wwPDB EM Validation Summary Report

Oct 27, 2024 – 07:44 PM JST

PDB ID	:	7XQP
EMDB ID	:	EMD-33401
Title	:	PSI-LHCI-LHCII-Lhcb9 supercomplex of Physcomitrella patens
Authors	:	Zhang, S.; Tang, K.L.; Li, X.Y.; Wang, W.D.; Yan, Q.J.; Shen, L.L.; Kuang, T.Y.; Han, G.Y.; Shen, J.R.; Zhang, X.
Deposited on	:	2022-05-08
Resolution	:	2.68 Å(reported)

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

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

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

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

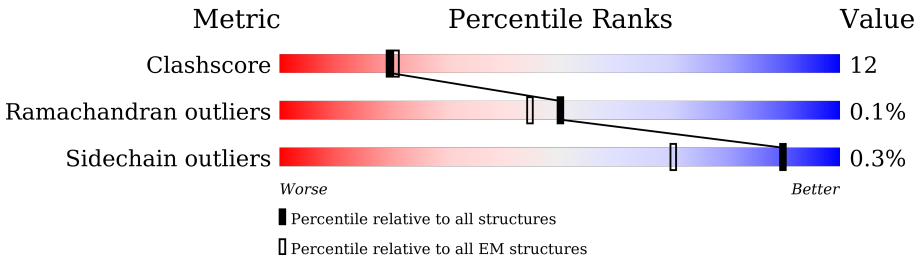
EMDB validation analysis	:	0.0.1.dev113
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.68 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	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	742	87% 13%
2	B	733	85% 15%
3	C	80	81% 19%
4	D	141	87% 13%
5	E	62	85% 15%
6	F	159	90% 10%
7	G	98	5% 84% 16%
8	H	95	93% 7%

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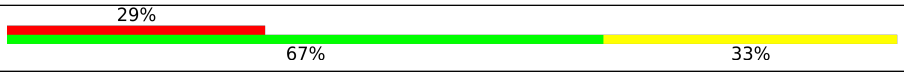
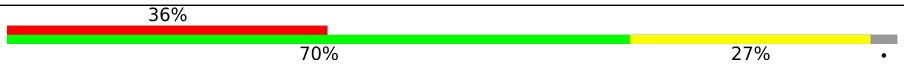
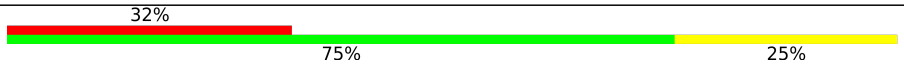
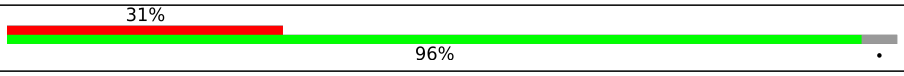
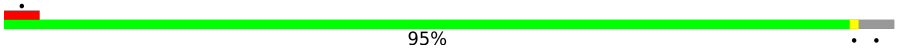
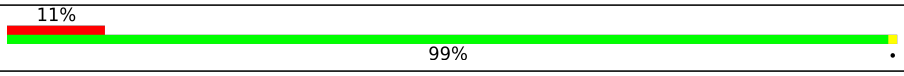
Mol	Chain	Length	Quality of chain
9	I	34	
10	J	41	
11	K	81	
12	L	163	
13	M	32	
14	O	89	
15	1	192	
15	5	192	
16	2	211	
16	6	211	
17	3	216	
17	7	216	
18	4	205	
18	8	205	
19	9	225	
20	a	227	
20	b	227	
20	c	227	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
21	CLA	1	303	X	-	-	-
21	CLA	1	304	X	-	-	-
21	CLA	1	305	X	-	-	-
21	CLA	1	306	X	-	-	-
21	CLA	1	308	X	-	-	-
21	CLA	1	309	X	-	-	-
21	CLA	1	310	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
21	CLA	1	311	X	-	-	-
21	CLA	1	312	X	-	-	-
21	CLA	1	313	X	-	-	-
21	CLA	1	314	X	-	-	-
21	CLA	1	315	X	-	-	-
21	CLA	1	316	X	-	-	-
21	CLA	2	603	X	-	-	-
21	CLA	2	604	X	-	-	-
21	CLA	2	608	X	-	-	-
21	CLA	2	609	X	-	X	-
21	CLA	2	610	X	-	-	-
21	CLA	2	611	X	-	-	-
21	CLA	2	612	X	-	-	-
21	CLA	2	613	X	-	-	-
21	CLA	3	401	X	-	-	-
21	CLA	3	402	X	-	-	-
21	CLA	3	403	X	-	-	-
21	CLA	3	404	X	-	-	-
21	CLA	3	405	X	-	-	-
21	CLA	3	406	X	-	-	-
21	CLA	3	408	X	-	-	-
21	CLA	3	409	X	-	X	-
21	CLA	3	410	X	-	-	-
21	CLA	3	411	X	-	-	-
21	CLA	3	412	X	-	-	-
21	CLA	3	413	X	-	-	-
21	CLA	3	414	X	-	-	-
21	CLA	3	415	X	-	-	-
21	CLA	4	601	X	-	-	-
21	CLA	4	602	X	-	-	-
21	CLA	4	603	X	-	-	-
21	CLA	4	604	X	-	-	-
21	CLA	4	608	X	-	-	-
21	CLA	4	610	X	-	-	-
21	CLA	4	611	X	-	-	-
21	CLA	4	612	X	-	-	-
21	CLA	4	613	X	-	-	-
21	CLA	5	602	X	-	-	-
21	CLA	5	603	X	-	-	-
21	CLA	5	604	X	-	-	-
21	CLA	5	605	X	-	-	-
21	CLA	5	607	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
21	CLA	5	608	X	-	-	-
21	CLA	5	609	X	-	-	-
21	CLA	5	610	X	-	-	-
21	CLA	5	611	X	-	-	-
21	CLA	5	612	X	-	-	-
21	CLA	5	613	X	-	-	-
21	CLA	5	614	X	-	-	-
21	CLA	6	603	X	-	-	-
21	CLA	6	604	X	-	-	-
21	CLA	6	608	X	-	-	-
21	CLA	6	609	X	-	-	-
21	CLA	6	610	X	-	-	-
21	CLA	6	611	X	-	-	-
21	CLA	6	612	X	-	-	-
21	CLA	6	613	X	-	-	-
21	CLA	7	401	X	-	-	-
21	CLA	7	402	X	-	-	-
21	CLA	7	403	X	-	-	-
21	CLA	7	404	X	-	-	-
21	CLA	7	405	X	-	-	-
21	CLA	7	408	X	-	-	-
21	CLA	7	409	X	-	-	-
21	CLA	7	410	X	-	-	-
21	CLA	7	411	X	-	-	-
21	CLA	7	412	X	-	-	-
21	CLA	7	413	X	-	-	-
21	CLA	7	414	X	-	-	-
21	CLA	8	601	X	-	-	-
21	CLA	8	602	X	-	-	-
21	CLA	8	603	X	-	-	-
21	CLA	8	604	X	-	-	-
21	CLA	8	608	X	-	-	-
21	CLA	8	609	X	-	X	-
21	CLA	8	610	X	-	-	-
21	CLA	8	611	X	-	-	-
21	CLA	8	612	X	-	-	-
21	CLA	8	618	X	-	-	-
21	CLA	9	602	X	-	-	-
21	CLA	9	603	X	-	-	-
21	CLA	9	604	X	-	-	-
21	CLA	9	610	X	-	-	-
21	CLA	9	611	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
21	CLA	9	612	X	-	-	-
21	CLA	9	613	X	-	-	-
21	CLA	A	802	X	-	-	-
21	CLA	A	803	X	-	-	-
21	CLA	A	804	X	-	-	-
21	CLA	A	805	X	-	-	-
21	CLA	A	806	X	-	-	-
21	CLA	A	807	X	-	-	-
21	CLA	A	808	X	-	-	-
21	CLA	A	809	X	-	-	-
21	CLA	A	810	X	-	-	-
21	CLA	A	811	X	-	-	-
21	CLA	A	812	X	-	-	-
21	CLA	A	813	X	-	-	-
21	CLA	A	814	X	-	-	-
21	CLA	A	815	X	-	-	-
21	CLA	A	816	X	-	-	-
21	CLA	A	817	X	-	-	-
21	CLA	A	818	X	-	-	-
21	CLA	A	819	X	-	-	-
21	CLA	A	820	X	-	-	-
21	CLA	A	821	X	-	-	-
21	CLA	A	822	X	-	-	-
21	CLA	A	823	X	-	-	-
21	CLA	A	824	X	-	-	-
21	CLA	A	825	X	-	-	-
21	CLA	A	826	X	-	-	-
21	CLA	A	827	X	-	-	-
21	CLA	A	828	X	-	-	-
21	CLA	A	829	X	-	-	-
21	CLA	A	830	X	-	-	-
21	CLA	A	831	X	-	-	-
21	CLA	A	832	X	-	-	-
21	CLA	A	833	X	-	-	-
21	CLA	A	834	X	-	-	-
21	CLA	A	835	X	-	-	-
21	CLA	A	836	X	-	-	-
21	CLA	A	837	X	-	-	-
21	CLA	A	838	X	-	-	-
21	CLA	A	839	X	-	-	-
21	CLA	A	840	X	-	-	-
21	CLA	A	841	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
21	CLA	A	842	X	-	-	-
21	CLA	A	852	X	-	-	-
21	CLA	B	801	X	-	-	-
21	CLA	B	802	X	-	-	-
21	CLA	B	803	X	-	-	-
21	CLA	B	804	X	-	-	-
21	CLA	B	805	X	-	-	-
21	CLA	B	806	X	-	-	-
21	CLA	B	807	X	-	-	-
21	CLA	B	808	X	-	-	-
21	CLA	B	809	X	-	-	-
21	CLA	B	810	X	-	-	-
21	CLA	B	811	X	-	-	-
21	CLA	B	812	X	-	-	-
21	CLA	B	813	X	-	-	-
21	CLA	B	814	X	-	-	-
21	CLA	B	815	X	-	-	-
21	CLA	B	816	X	-	-	-
21	CLA	B	817	X	-	-	-
21	CLA	B	818	X	-	-	-
21	CLA	B	819	X	-	-	-
21	CLA	B	820	X	-	-	-
21	CLA	B	821	X	-	-	-
21	CLA	B	822	X	-	-	-
21	CLA	B	823	X	-	-	-
21	CLA	B	824	X	-	-	-
21	CLA	B	825	X	-	-	-
21	CLA	B	826	X	-	-	-
21	CLA	B	827	X	-	-	-
21	CLA	B	828	X	-	-	-
21	CLA	B	829	X	-	-	-
21	CLA	B	830	X	-	-	-
21	CLA	B	831	X	-	-	-
21	CLA	B	832	X	-	-	-
21	CLA	B	833	X	-	-	-
21	CLA	B	834	X	-	-	-
21	CLA	B	835	X	-	-	-
21	CLA	B	836	X	-	-	-
21	CLA	B	837	X	-	-	-
21	CLA	B	838	X	-	-	-
21	CLA	B	839	X	-	-	-
21	CLA	B	840	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
21	CLA	F	302	X	-	-	-
21	CLA	F	304	X	-	-	-
21	CLA	F	305	X	-	-	-
21	CLA	G	202	X	-	-	-
21	CLA	G	203	X	-	-	-
21	CLA	G	204	X	-	-	-
21	CLA	H	201	X	-	-	-
21	CLA	J	102	X	-	-	-
21	CLA	K	201	X	-	-	-
21	CLA	K	202	X	-	-	-
21	CLA	K	203	X	-	-	-
21	CLA	K	204	X	-	-	-
21	CLA	L	302	X	-	-	-
21	CLA	L	303	X	-	-	-
21	CLA	L	304	X	-	-	-
21	CLA	O	201	X	-	-	-
21	CLA	O	202	X	-	-	-
21	CLA	O	203	X	-	-	-
21	CLA	O	204	X	-	-	-
21	CLA	a	602	X	-	-	-
21	CLA	a	603	X	-	-	-
21	CLA	a	604	X	-	-	-
21	CLA	a	610	X	-	-	-
21	CLA	a	611	X	-	-	-
21	CLA	a	612	X	-	-	-
21	CLA	a	613	X	-	-	-
21	CLA	a	614	X	-	-	-
21	CLA	b	303	X	-	-	-
21	CLA	b	304	X	-	-	-
21	CLA	b	305	X	-	-	-
21	CLA	b	311	X	-	-	-
21	CLA	b	312	X	-	-	-
21	CLA	b	313	X	-	-	-
21	CLA	b	314	X	-	-	-
21	CLA	b	315	X	-	-	-
21	CLA	c	602	X	-	-	-
21	CLA	c	603	X	-	-	-
21	CLA	c	604	X	-	-	-
21	CLA	c	610	X	-	-	-
21	CLA	c	611	X	-	-	-
21	CLA	c	612	X	-	-	-
21	CLA	c	613	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
21	CLA	c	614	X	-	-	-
24	BCR	K	205	-	-	X	-
29	CHL	1	302	X	-	-	-
29	CHL	1	307	X	-	-	-
29	CHL	2	601	X	-	-	-
29	CHL	2	602	X	-	-	-
29	CHL	2	605	X	-	-	-
29	CHL	2	606	X	-	-	-
29	CHL	2	607	X	-	-	-
29	CHL	2	614	X	-	-	-
29	CHL	3	407	X	-	-	-
29	CHL	4	605	X	-	-	-
29	CHL	4	606	X	-	-	-
29	CHL	4	607	X	-	-	-
29	CHL	4	614	X	-	-	-
29	CHL	5	601	X	-	-	-
29	CHL	5	606	X	-	-	-
29	CHL	6	601	X	-	-	-
29	CHL	6	602	X	-	-	-
29	CHL	6	605	X	-	-	-
29	CHL	6	606	X	-	-	-
29	CHL	6	607	X	-	-	-
29	CHL	6	614	X	-	-	-
29	CHL	7	406	X	-	-	-
29	CHL	8	605	X	-	-	-
29	CHL	8	606	X	-	-	-
29	CHL	8	607	X	-	-	-
29	CHL	8	613	X	-	-	-
29	CHL	9	601	X	-	-	-
29	CHL	9	605	X	-	-	-
29	CHL	9	606	X	-	-	-
29	CHL	9	607	X	-	-	-
29	CHL	9	608	X	-	-	-
29	CHL	9	609	X	-	-	-
29	CHL	a	601	X	-	-	-
29	CHL	a	605	X	-	-	-
29	CHL	a	606	X	-	-	-
29	CHL	a	607	X	-	-	-
29	CHL	a	608	X	-	-	-
29	CHL	a	609	X	-	-	-
29	CHL	b	302	X	-	-	-
29	CHL	b	306	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
29	CHL	b	307	X	-	-	-
29	CHL	b	308	X	-	-	-
29	CHL	b	309	X	-	-	-
29	CHL	b	310	X	-	-	-
29	CHL	c	601	X	-	-	-
29	CHL	c	605	X	-	-	-
29	CHL	c	606	X	-	-	-
29	CHL	c	607	X	-	-	-
29	CHL	c	608	X	-	-	-
29	CHL	c	609	X	-	-	-

2 Entry composition (i)

There are 32 unique types of molecules in this entry. The entry contains 56417 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	742	5836	3827	993	997	19	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	733	5849	3839	996	998	16	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	80	595	365	103	116	11	0	0

- Molecule 4 is a protein called Predicted protein PsaD.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	D	141	1104	707	196	198	3	0	0

- Molecule 5 is a protein called PsaE.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
5	E	62	487	309	87	91	0	0

- Molecule 6 is a protein called PSI-F.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	F	159	1230	796	210	221	3	0	0

- Molecule 7 is a protein called PSI-G.

Mol	Chain	Residues	Atoms				AltConf	Trace
7	G	98	Total	C	N	O	0	0
			749	483	128	138		

- Molecule 8 is a protein called PsaH photosystem I reaction center subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	95	Total	C	N	O	S	0	0
			740	476	125	138	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	34	Total	C	N	O	S	0	0
			266	181	35	48	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	41	Total	C	N	O	S	0	0
			325	222	48	54	1		

- Molecule 11 is a protein called PsaK.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	81	Total	C	N	O	S	0	0
			566	356	98	109	3		

- Molecule 12 is a protein called PSI subunit V.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	163	Total	C	N	O	S	0	0
			1229	808	197	222	2		

- Molecule 13 is a protein called Photosystem I reaction center subunit XII.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	32	Total	C	N	O	S	0	0
			238	155	38	44	1		

- Molecule 14 is a protein called PsaO.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	O	89	Total	C	N	O	S	0	0
			702	472	115	114	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
15	1	192	Total	C	N	O	S	0	0
			1478	965	247	265	1		
15	5	192	Total	C	N	O	S	0	0
			1475	962	247	265	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
16	2	211	Total	C	N	O	S	0	0
			1632	1062	274	292	4		
16	6	205	Total	C	N	O	S	0	0
			1587	1035	265	283	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
17	3	216	Total	C	N	O	S	0	0
			1670	1094	269	300	7		
17	7	213	Total	C	N	O	S	0	0
			1644	1076	265	296	7		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
18	4	205	Total	C	N	O	S	0	0
			1592	1033	266	288	5		
18	8	204	Total	C	N	O	S	0	0
			1585	1029	265	286	5		

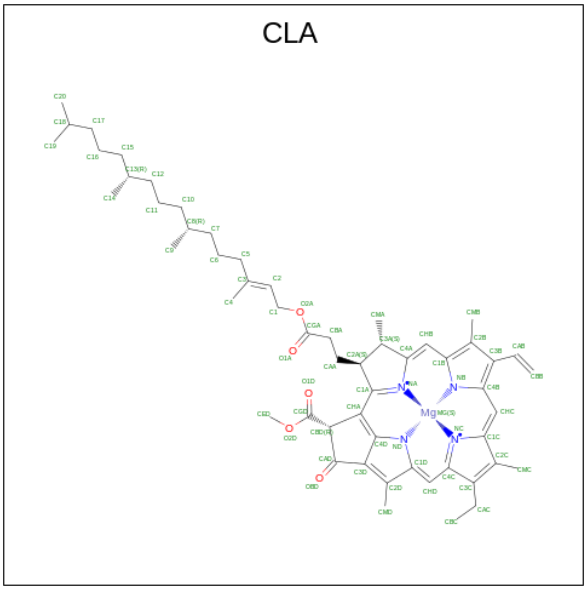
- Molecule 19 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	9	225	Total	C	N	O	S	0	0
			1747	1139	287	312	9		

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

Mol	Chain	Residues	Atoms	AltConf	Trace
20	a	218	Total C N O S 1651 1069 268 309 5	0	0
20	b	218	Total C N O S 1651 1069 268 309 5	0	0
20	c	227	Total C N O P S 1727 1110 284 327 1 5	0	0

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



Mol	Chain	Residues	Atoms	AltConf
21	A	1	Total C Mg N O 52 42 1 4 5	0
21	A	1	Total C Mg N O 52 42 1 4 5	0
21	A	1	Total C Mg N O 52 42 1 4 5	0
21	A	1	Total C Mg N O 65 55 1 4 5	0
21	A	1	Total C Mg N O 55 45 1 4 5	0
21	A	1	Total C Mg N O 65 55 1 4 5	0
21	A	1	Total C Mg N O 65 55 1 4 5	0
21	A	1	Total C Mg N O 45 35 1 4 5	0
21	A	1	Total C Mg N O 59 49 1 4 5	0

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Mol	Chain	Residues	Atoms					AltConf
21	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
21	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
21	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
21	A	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
21	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
21	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
21	A	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
21	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
21	A	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
21	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
21	A	1	Total	C	Mg	N	O	0
			44	34	1	4	5	
21	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
21	A	1	Total	C	Mg	N	O	0
			44	34	1	4	5	
21	A	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
21	A	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
21	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
21	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
21	A	1	Total	C	Mg	N	O	0
			64	54	1	4	5	
21	A	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
21	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
21	A	1	Total	C	Mg	N	O	0
			52	42	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
21	A	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
21	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
21	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
21	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
21	A	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
21	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
21	A	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
21	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
21	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
21	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
21	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
21	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
21	A	1	Total	C	Mg	N	O	0
			53	43	1	4	5	
21	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
21	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
21	B	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
21	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
21	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
21	B	1	Total	C	Mg	N	O	0
			63	53	1	4	5	
21	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
21	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
21	B	1	Total	C	Mg	N	O	0
			62	52	1	4	5	
21	B	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
21	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
21	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
21	B	1	Total	C	Mg	N	O	0
			44	34	1	4	5	
21	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
21	B	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
21	B	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
21	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
21	B	1	Total	C	Mg	N	O	0
			58	48	1	4	5	
21	B	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
21	B	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
21	B	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
21	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
21	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
21	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
21	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
21	B	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
21	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
21	B	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
21	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
21	B	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
21	B	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
21	B	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
21	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
21	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
21	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
21	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
21	B	1	Total	C	Mg	N	O	0
			64	54	1	4	5	
21	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
21	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
21	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
21	F	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
21	F	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
21	F	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
21	G	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
21	G	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
21	G	1	Total	C	Mg	N	O	0
			44	34	1	4	5	
21	H	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
21	J	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
21	K	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
21	K	1	Total	C	Mg	N	O	0
			50	40	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
21	K	1	Total	C	Mg	N	O	0
			44	34	1	4	5	
21	K	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
21	L	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
21	L	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
21	L	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
21	O	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
21	O	1	Total	C	Mg	N	O	0
			38	30	1	4	3	
21	O	1	Total	C	Mg	N	O	0
			50	42	1	4	3	
21	O	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
21	1	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
21	1	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
21	1	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
21	1	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
21	1	1	Total	C	Mg	N	O	0
			44	34	1	4	5	
21	1	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
21	1	1	Total	C	Mg	N	O	0
			43	33	1	4	5	
21	1	1	Total	C	Mg	N	O	0
			38	30	1	4	3	
21	1	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
21	1	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
21	1	1	Total	C	Mg	N	O	0
			38	30	1	4	3	
21	1	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
21	1	1	Total	C	Mg	N	O	0
			43	33	1	4	5	
21	2	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
21	2	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
21	2	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
21	2	1	Total	C	Mg	N	O	0
			51	42	1	4	4	
21	2	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
21	2	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
21	2	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
21	2	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
21	3	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
21	3	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
21	3	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
21	3	1	Total	C	Mg	N	O	0
			42	32	1	4	5	
21	3	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
21	3	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
21	3	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
21	3	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
21	3	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
21	3	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
21	3	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
21	3	1	Total	C	Mg	N	O	0
			40	32	1	4	3	

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Mol	Chain	Residues	Atoms					AltConf
21	3	1	Total	C	Mg	N	O	0
			36	30	1	4	1	
21	3	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
21	4	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
21	4	1	Total	C	Mg	N	O	0
			58	48	1	4	5	
21	4	1	Total	C	Mg	N	O	0
			44	34	1	4	5	
21	4	1	Total	C	Mg	N	O	0
			43	34	1	4	4	
21	4	1	Total	C	Mg	N	O	0
			43	34	1	4	4	
21	4	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
21	4	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
21	4	1	Total	C	Mg	N	O	0
			44	34	1	4	5	
21	4	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
21	4	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
21	5	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
21	5	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
21	5	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
21	5	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
21	5	1	Total	C	Mg	N	O	0
			44	34	1	4	5	
21	5	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
21	5	1	Total	C	Mg	N	O	0
			43	33	1	4	5	
21	5	1	Total	C	Mg	N	O	0
			38	30	1	4	3	
21	5	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
21	5	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
21	5	1	Total	C	Mg	N	O	0
			38	30	1	4	3	
21	5	1	Total	C	Mg	N	O	0
			43	33	1	4	5	
21	6	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
21	6	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
21	6	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
21	6	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
21	6	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
21	6	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
21	6	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
21	6	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
21	7	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
21	7	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
21	7	1	Total	C	Mg	N	O	0
			42	32	1	4	5	
21	7	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
21	7	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
21	7	1	Total	C	Mg	N	O	0
			44	34	1	4	5	
21	7	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
21	7	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
21	7	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
21	7	1	Total	C	Mg	N	O	0
			54	44	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
21	7	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
21	7	1	Total	C	Mg	N	O	0
			36	30	1	4	1	
21	7	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
21	8	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
21	8	1	Total	C	Mg	N	O	0
			58	48	1	4	5	
21	8	1	Total	C	Mg	N	O	0
			44	34	1	4	5	
21	8	1	Total	C	Mg	N	O	0
			43	34	1	4	4	
21	8	1	Total	C	Mg	N	O	0
			43	34	1	4	4	
21	8	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
21	8	1	Total	C	Mg	N	O	0
			44	34	1	4	5	
21	8	1	Total	C	Mg	N	O	0
			54	45	1	4	4	
21	8	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
21	8	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
21	9	1	Total	C	Mg	N	O	0
			53	43	1	4	5	
21	9	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
21	9	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
21	9	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
21	9	1	Total	C	Mg	N	O	0
			57	47	1	4	5	
21	9	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
21	9	1	Total	C	Mg	N	O	0
			53	43	1	4	5	
21	a	1	Total	C	Mg	N	O	0
			60	50	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
21	a	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
21	a	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
21	a	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
21	a	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
21	a	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
21	a	1	Total	C	Mg	N	O	0
			57	47	1	4	5	
21	a	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
21	b	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
21	b	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
21	b	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
21	b	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
21	b	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
21	b	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
21	b	1	Total	C	Mg	N	O	0
			53	43	1	4	5	
21	b	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
21	c	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
21	c	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
21	c	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
21	c	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
21	c	1	Total	C	Mg	N	O	0
			58	48	1	4	5	
21	c	1	Total	C	Mg	N	O	0
			44	35	1	4	4	

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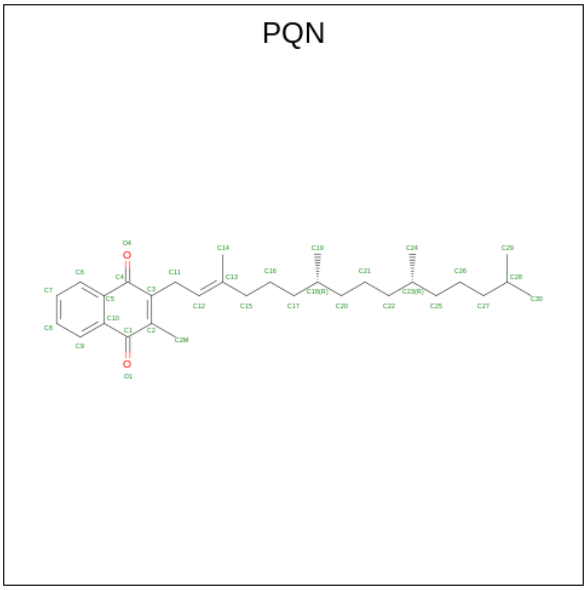
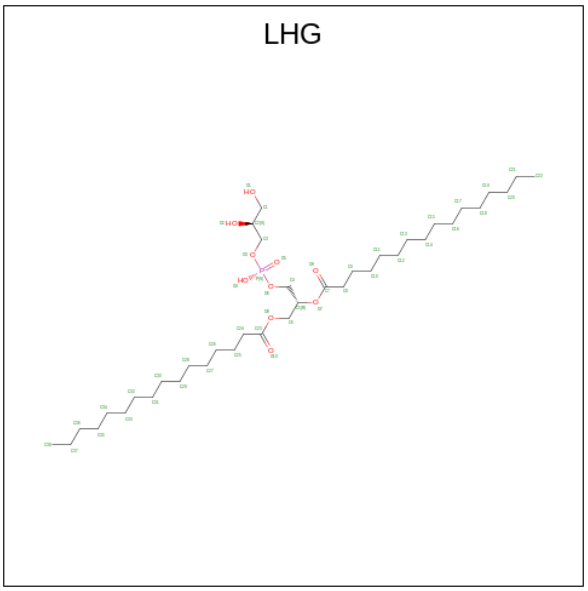
Mol	Chain	Residues	Atoms					AltConf
21	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
21	c	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

- Molecule 22 is PHYLLOQUINONE (three-letter code: PQN) (formula: $C_{31}H_{46}O_2$).



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

- Molecule 23 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula: $C_{38}H_{75}O_{10}P$).



Mol	Chain	Residues	Atoms				AltConf
23	A	1	Total	C	O	P	0
			49	38	10	1	
23	A	1	Total	C	O	P	0
			27	16	10	1	
23	A	1	Total	C	O	P	0
			49	38	10	1	
23	1	1	Total	C	O	P	0
			23	12	10	1	
23	1	1	Total	C	O	P	0
			28	17	10	1	
23	2	1	Total	C	O	P	0
			35	24	10	1	
23	4	1	Total	C	O	P	0
			37	26	10	1	
23	4	1	Total	C	O	P	0
			49	38	10	1	
23	5	1	Total	C	O	P	0
			28	17	10	1	
23	6	1	Total	C	O	P	0
			35	24	10	1	
23	8	1	Total	C	O	P	0
			37	26	10	1	
23	9	1	Total	C	O	P	0
			49	38	10	1	
23	a	1	Total	C	O	P	0
			49	38	10	1	
23	b	1	Total	C	O	P	0
			49	38	10	1	

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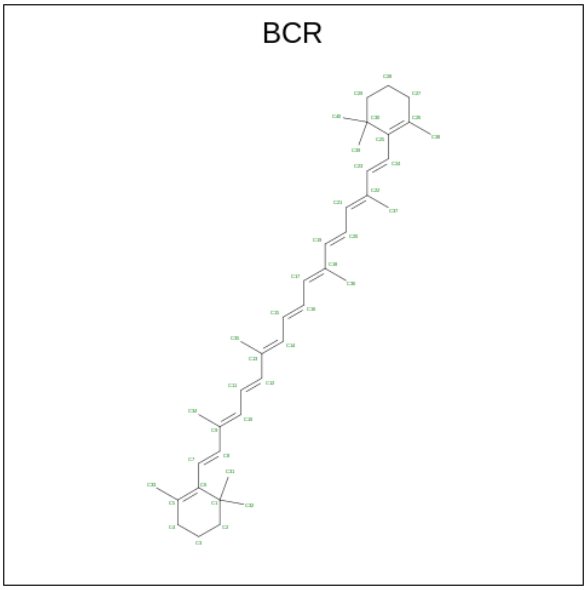
Mol	Chain	Residues	Atoms				AltConf
23	c	1	Total	C	O	P	0
			49	38	10	1	

- Molecule 24 is BETA-CAROTENE (three-letter code: BCR) (formula: $C_{40}H_{56}$).



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

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Mol	Chain	Residues	Atoms	AltConf
24	B	1	Total C 40 40	0
24	F	1	Total C 40 40	0
24	F	1	Total C 40 40	0
24	G	1	Total C 40 40	0
24	G	1	Total C 40 40	0
24	I	1	Total C 40 40	0
24	J	1	Total C 40 40	0
24	J	1	Total C 40 40	0
24	J	1	Total C 40 40	0
24	K	1	Total C 40 40	0
24	L	1	Total C 40 40	0
24	L	1	Total C 40 40	0
24	L	1	Total C 40 40	0
24	M	1	Total C 40 40	0
24	O	1	Total C 40 40	0
24	2	1	Total C 40 40	0
24	3	1	Total C 40 40	0
24	3	1	Total C 40 40	0
24	4	1	Total C 40 40	0
24	6	1	Total C 40 40	0
24	7	1	Total C 40 40	0

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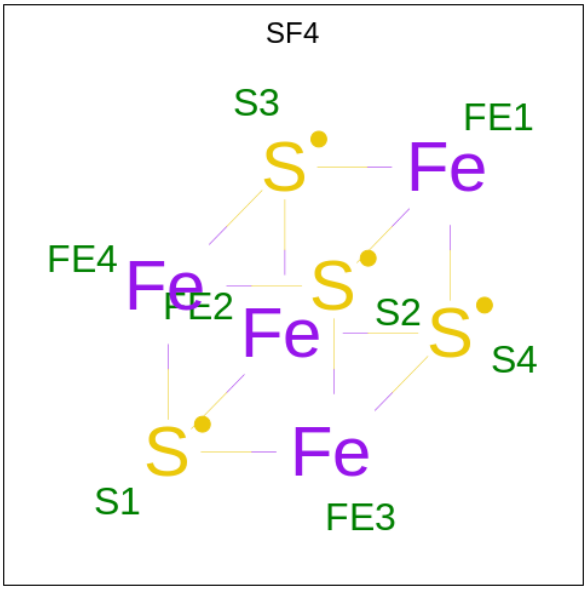
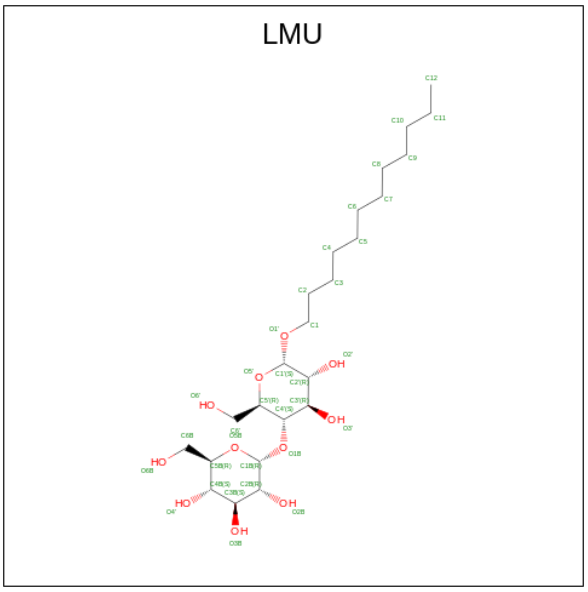
Mol	Chain	Residues	Atoms	AltConf
24	7	1	Total C 40 40	0
24	8	1	Total C 40 40	0

- Molecule 25 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).



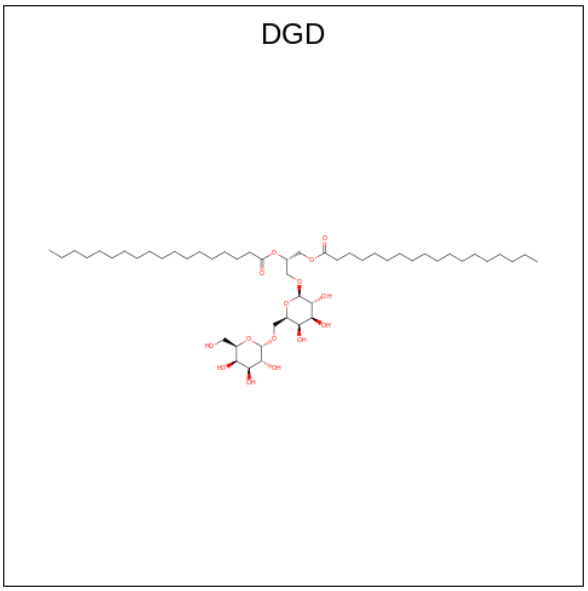
Mol	Chain	Residues	Atoms	AltConf
25	A	1	Total Fe S 8 4 4	0
25	C	1	Total Fe S 8 4 4	0
25	C	1	Total Fe S 8 4 4	0

- Molecule 26 is DODECYL-ALPHA-D-MALTOSIDE (three-letter code: LMU) (formula: $C_{24}H_{46}O_{11}$) (labeled as "Ligand of Interest" by depositor).



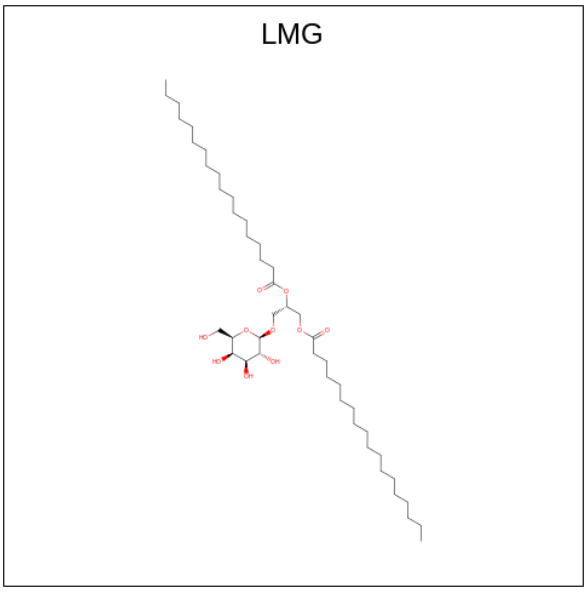
Mol	Chain	Residues	Atoms	AltConf
26	A	1	Total C O 35 24 11	0
26	A	1	Total C O 35 24 11	0
26	O	1	Total C O 35 24 11	0
26	3	1	Total C O 35 24 11	0
26	b	1	Total C O 35 24 11	0

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



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

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



Mol	Chain	Residues	Atoms			AltConf
28	G	1	Total	C	O	0
			55	45	10	
28	J	1	Total	C	O	0
			30	20	10	

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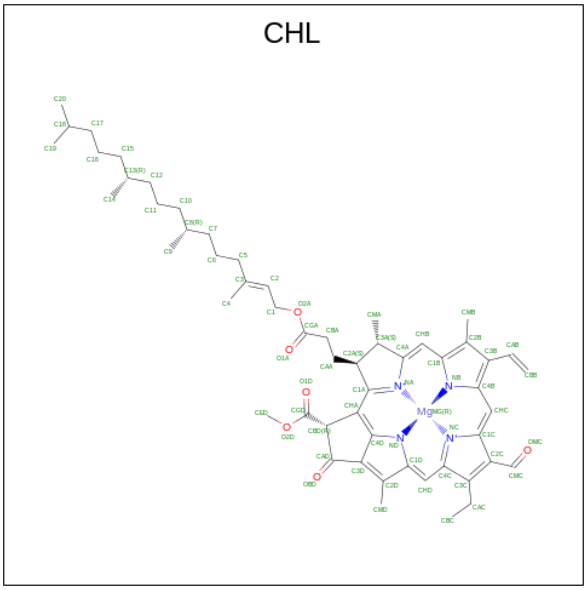
Mol	Chain	Residues	Atoms	AltConf
28	2	1	Total C O 13 7 6	0
28	6	1	Total C O 13 7 6	0

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



Mol	Chain	Residues	Atoms	AltConf
29	1	1	Total C Mg N O 51 40 1 4 6	0
29	1	1	Total C Mg N O 51 40 1 4 6	0
29	2	1	Total C Mg N O 53 42 1 4 6	0
29	2	1	Total C Mg N O 53 42 1 4 6	0
29	2	1	Total C Mg N O 46 35 1 4 6	0
29	2	1	Total C Mg N O 46 35 1 4 6	0
29	2	1	Total C Mg N O 51 40 1 4 6	0
29	2	1	Total C Mg N O 46 35 1 4 6	0
29	3	1	Total C Mg N O 40 32 1 4 3	0

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Mol	Chain	Residues	Atoms					AltConf
29	4	1	Total	C	Mg	N	O	0
			41	32	1	4	4	
29	4	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
29	4	1	Total	C	Mg	N	O	0
			51	40	1	4	6	
29	4	1	Total	C	Mg	N	O	0
			42	33	1	4	4	
29	5	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
29	5	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
29	6	1	Total	C	Mg	N	O	0
			44	34	1	4	5	
29	6	1	Total	C	Mg	N	O	0
			53	42	1	4	6	
29	6	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
29	6	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
29	6	1	Total	C	Mg	N	O	0
			51	40	1	4	6	
29	6	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
29	7	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
29	8	1	Total	C	Mg	N	O	0
			41	32	1	4	4	
29	8	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
29	8	1	Total	C	Mg	N	O	0
			51	40	1	4	6	
29	8	1	Total	C	Mg	N	O	0
			42	33	1	4	4	
29	9	1	Total	C	Mg	N	O	0
			43	34	1	4	4	
29	9	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
29	9	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
29	9	1	Total	C	Mg	N	O	0
			46	35	1	4	6	

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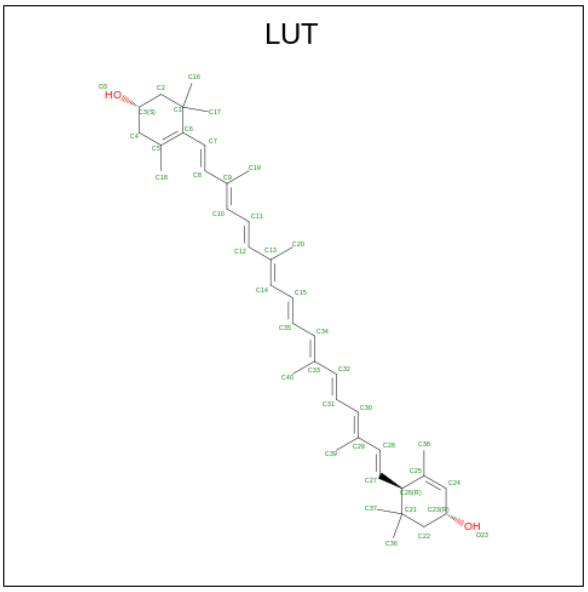
Mol	Chain	Residues	Atoms					AltConf
29	9	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
29	9	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
29	a	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
29	a	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
29	a	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
29	a	1	Total	C	Mg	N	O	0
			43	34	1	4	4	
29	a	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
29	a	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
29	b	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
29	b	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
29	b	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
29	b	1	Total	C	Mg	N	O	0
			53	42	1	4	6	
29	b	1	Total	C	Mg	N	O	0
			49	38	1	4	6	
29	b	1	Total	C	Mg	N	O	0
			52	41	1	4	6	
29	c	1	Total	C	Mg	N	O	0
			49	38	1	4	6	
29	c	1	Total	C	Mg	N	O	0
			43	34	1	4	4	
29	c	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
29	c	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
29	c	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
29	c	1	Total	C	Mg	N	O	0
			44	33	1	4	6	

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



Mol	Chain	Residues	Atoms	AltConf
30	1	1	Total C O 42 40 2	0
30	2	1	Total C O 42 40 2	0
30	3	1	Total C O 42 40 2	0
30	4	1	Total C O 42 40 2	0
30	5	1	Total C O 42 40 2	0
30	6	1	Total C O 42 40 2	0
30	7	1	Total C O 42 40 2	0
30	8	1	Total C O 42 40 2	0
30	9	1	Total C O 42 40 2	0
30	9	1	Total C O 42 40 2	0
30	a	1	Total C O 42 40 2	0
30	a	1	Total C O 42 40 2	0
30	b	1	Total C O 42 40 2	0
30	b	1	Total C O 42 40 2	0

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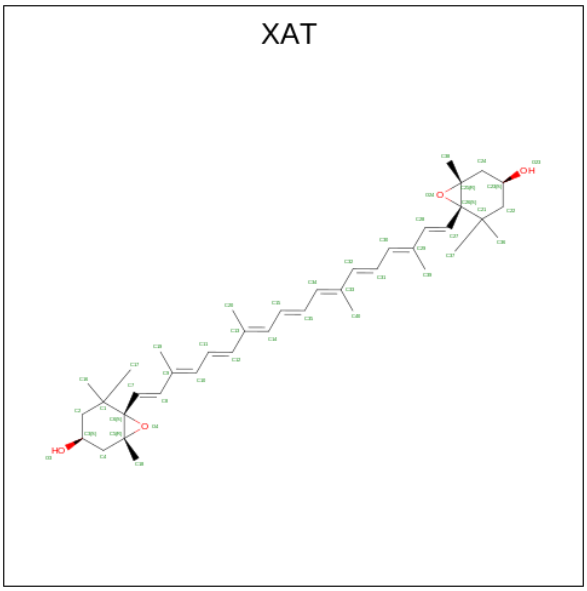
Mol	Chain	Residues	Atoms	AltConf
30	c	1	Total C O 42 40 2	0
30	c	1	Total C O 42 40 2	0

- Molecule 31 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
31	1	1	Total C O 44 40 4	0
31	2	1	Total C O 44 40 4	0
31	3	1	Total C O 44 40 4	0
31	4	1	Total C O 44 40 4	0
31	5	1	Total C O 44 40 4	0
31	6	1	Total C O 44 40 4	0
31	7	1	Total C O 44 40 4	0
31	8	1	Total C O 44 40 4	0
31	9	1	Total C O 44 40 4	0

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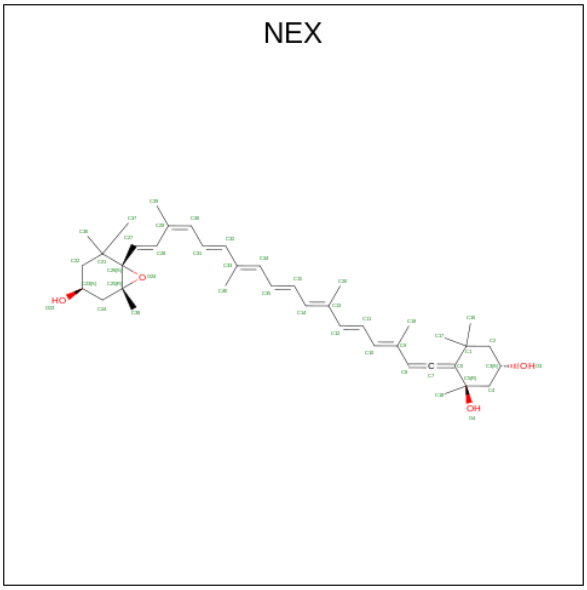
Mol	Chain	Residues	Atoms			AltConf
31	a	1	Total 44	C 40	O 4	0
31	c	1	Total 44	C 40	O 4	0

- Molecule 32 is (1R,3R)-6-{(3E,5E,7E,9E,11E,13E,15E,17E)-18-[(1S,4R,6R)-4-HYDROXY-2,2,6-TRIMETHYL-7-OXABICYCLO[4.1.0]HEPT-1-YL]-3,7,12,16-TETRAMETHYLOCTADECA-1,3,5,7,9,11,13,15,17-NONAENYLIDENE}-1,5,5-TRIMETHYLCYCLOHEXANE-1,3-DIOL (three-letter code: NEX) (formula: $C_{40}H_{56}O_4$).



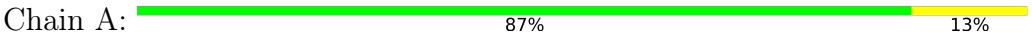
Mol	Chain	Residues	Atoms			AltConf
32	9	1	Total 44	C 40	O 4	0
32	b	1	Total 44	C 40	O 4	0
32	c	1	Total 44	C 40	O 4	0

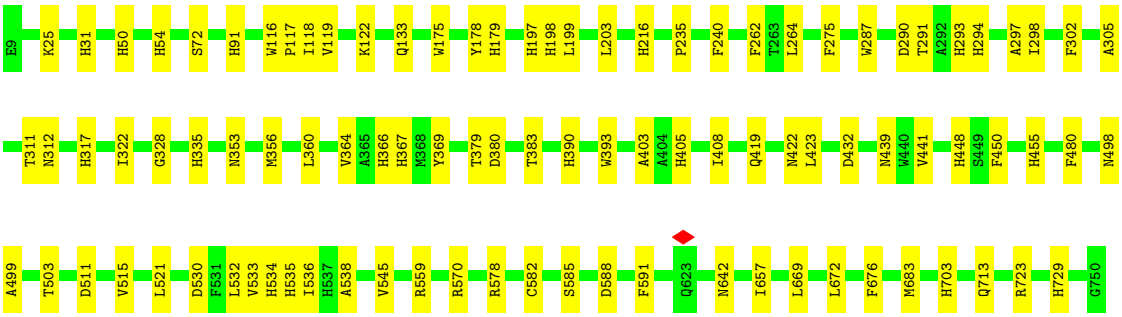
3 Residue-property plots (i)

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

• Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1

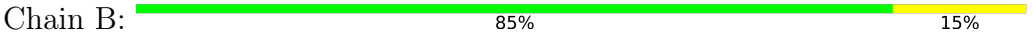
Chain A:

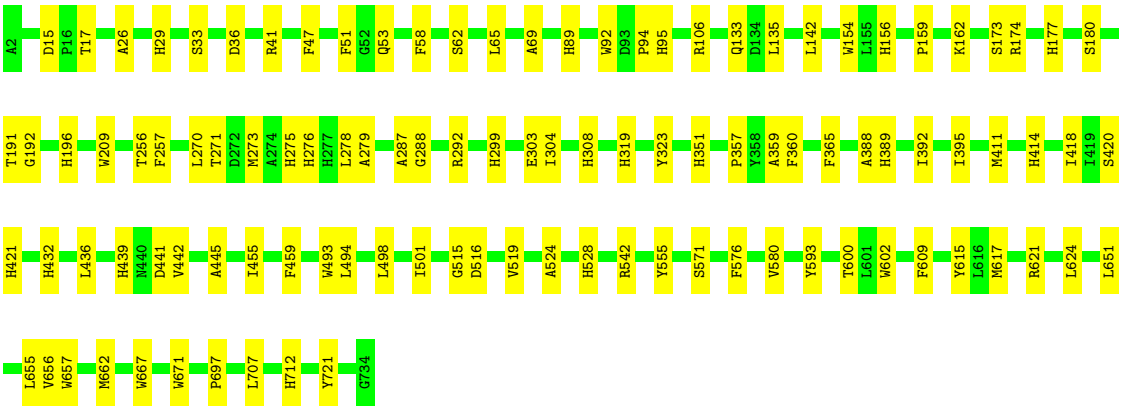




• Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

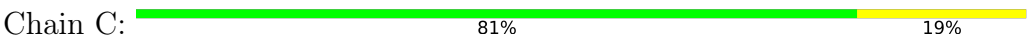
Chain B:

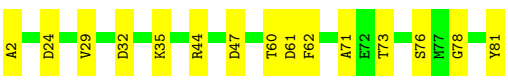




• Molecule 3: Photosystem I iron-sulfur center

Chain C:



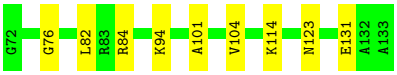


• Molecule 4: Predicted protein PsaD

Chain D:

• Molecule 5: PsaE

Chain E:

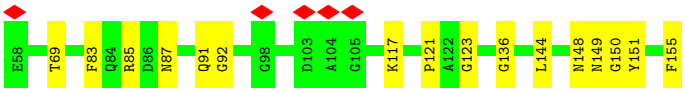


• Molecule 6: PSI-F

Chain F:

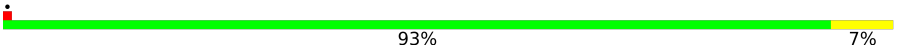
• Molecule 7: PSI-G

Chain G:



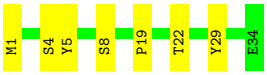
• Molecule 8: PsaH photosystem I reaction center subunit

Chain H:



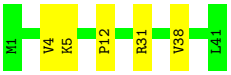
• Molecule 9: Photosystem I reaction center subunit VIII

Chain I:



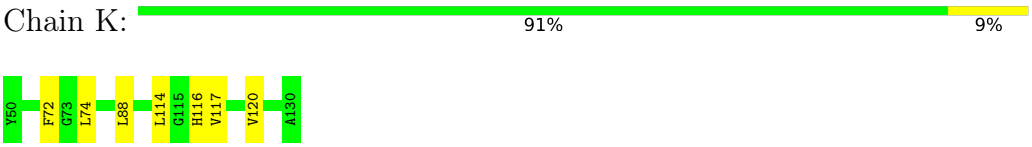
• Molecule 10: Photosystem I reaction center subunit IX

Chain J:



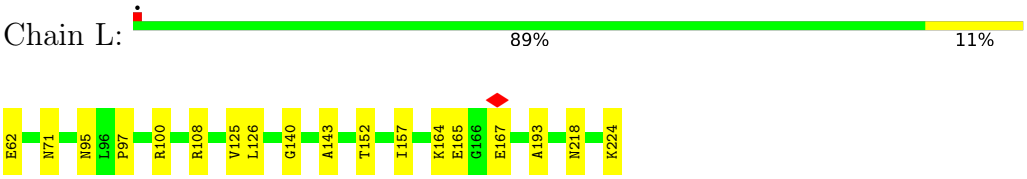
• Molecule 11: PsaK

Chain K:



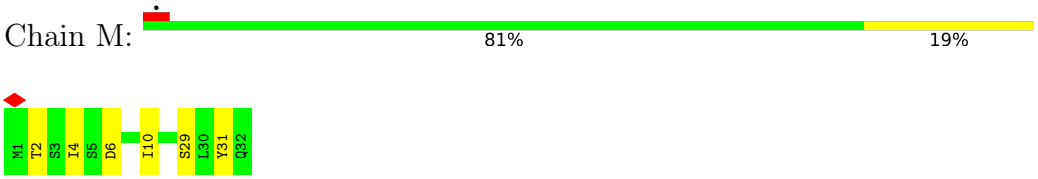
• Molecule 12: PSI subunit V

Chain L:



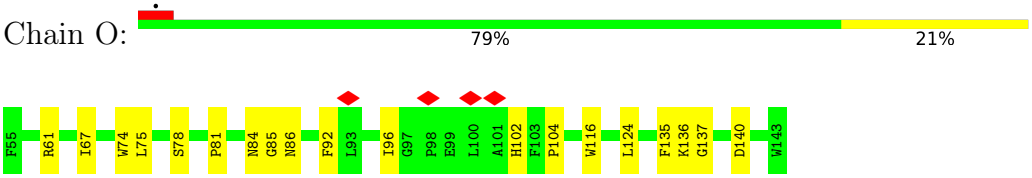
• Molecule 13: Photosystem I reaction center subunit XII

Chain M:



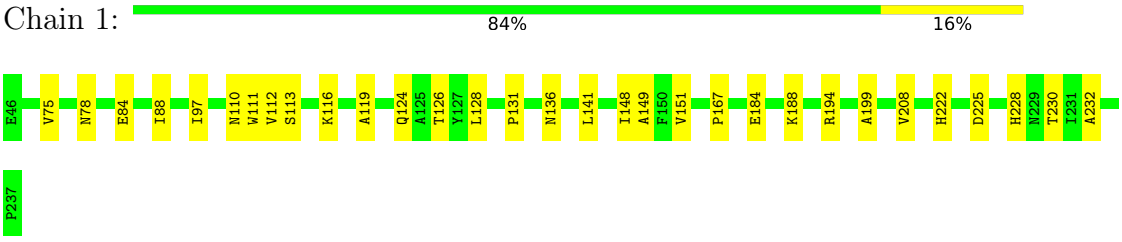
• Molecule 14: PsaO

Chain O:



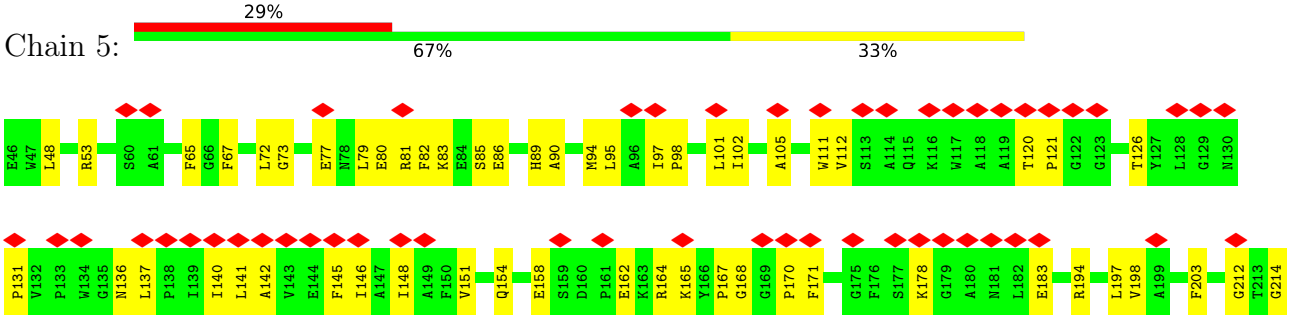
• Molecule 15: Chlorophyll a-b binding protein, chloroplastic

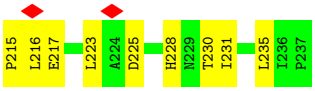
Chain 1:



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

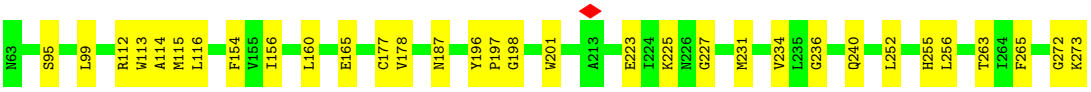
Chain 5:





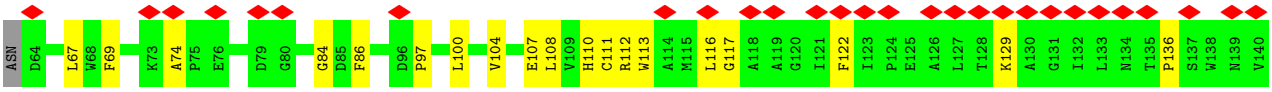
• Molecule 16: Chlorophyll a-b binding protein, chloroplastic

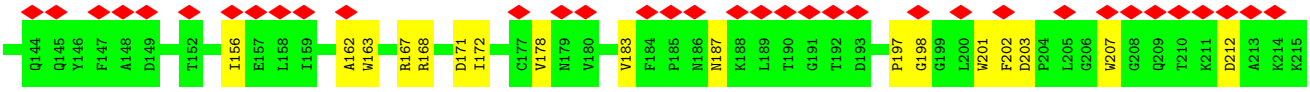
Chain 2:

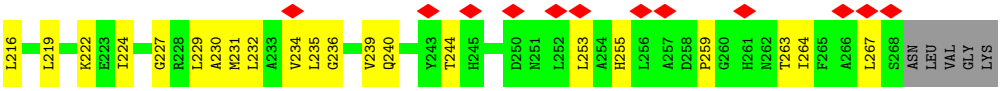


• Molecule 16: Chlorophyll a-b binding protein, chloroplastic

Chain 6:





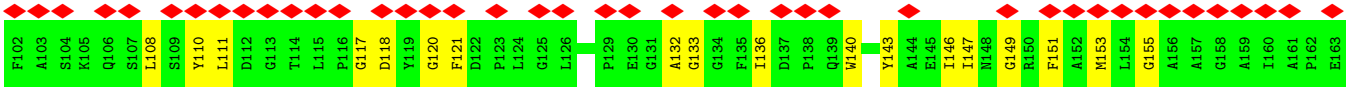


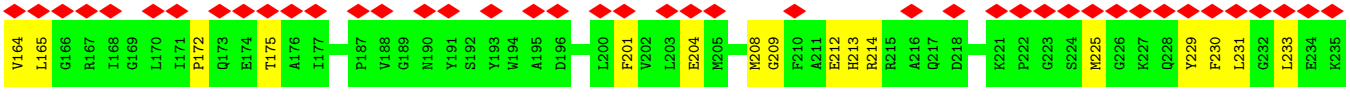
• Molecule 17: Chlorophyll a-b binding protein, chloroplastic

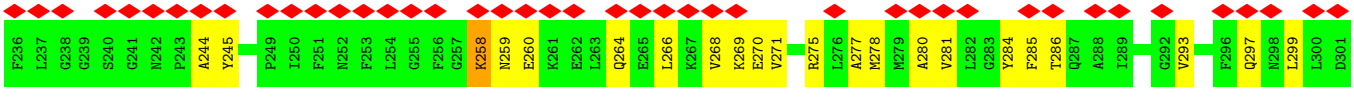
Chain 3:

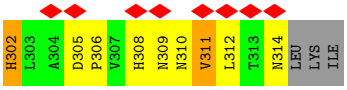
• Molecule 17: Chlorophyll a-b binding protein, chloroplastic

Chain 7:



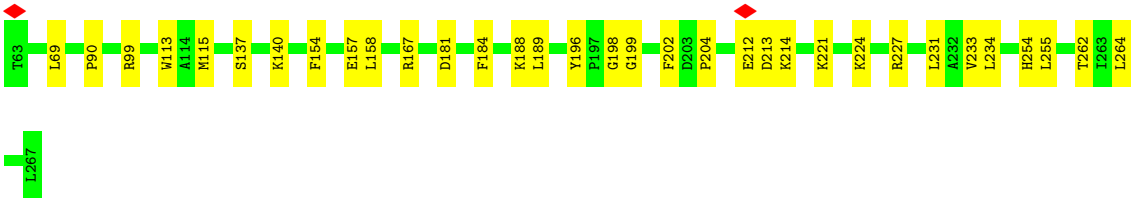






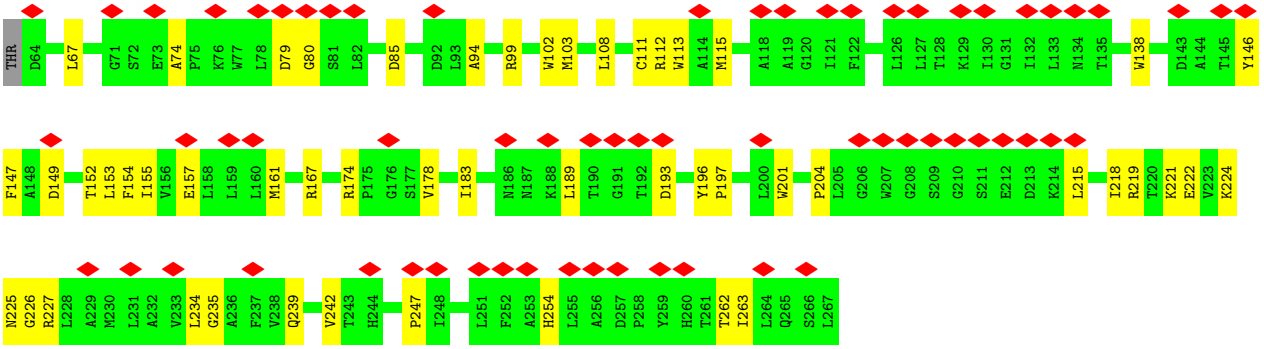
• Molecule 18: Chlorophyll a-b binding protein, chloroplastic

Chain 4:



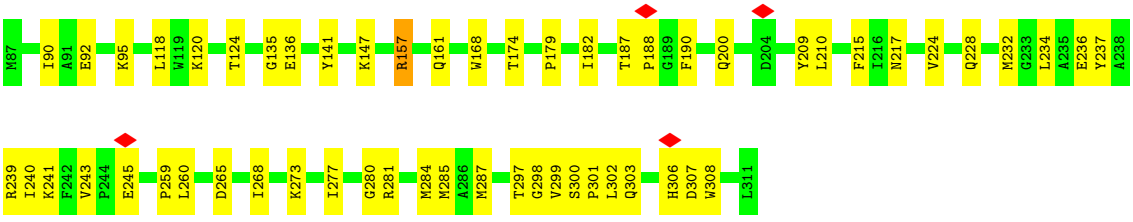
• Molecule 18: Chlorophyll a-b binding protein, chloroplastic

Chain 8:



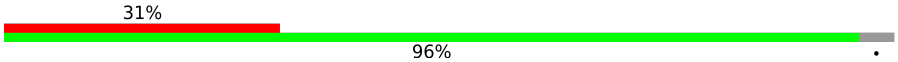
• Molecule 19: Chlorophyll a-b binding protein, chloroplastic

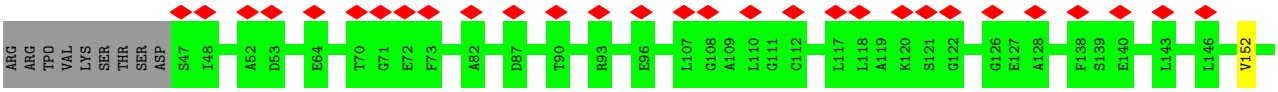
Chain 9:

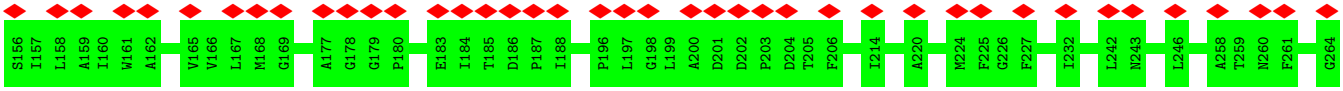


• Molecule 20: Chlorophyll a-b binding protein, chloroplastic

Chain a:

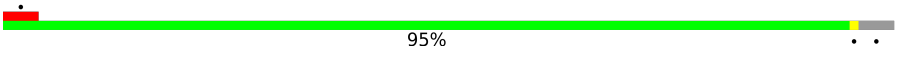


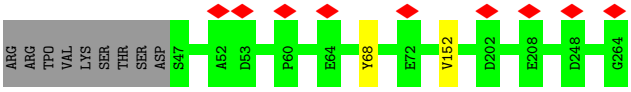




• Molecule 20: Chlorophyll a-b binding protein, chloroplastic

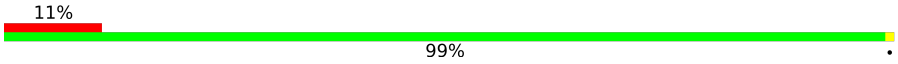
Chain b:

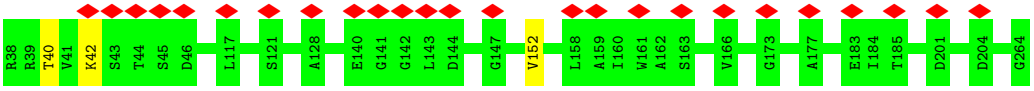




• Molecule 20: Chlorophyll a-b binding protein, chloroplastic

Chain c:





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	83777	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	78	Depositor
Minimum defocus (nm)	1600	Depositor
Maximum defocus (nm)	1900	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	4.400	Depositor
Minimum map value	-1.758	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.105	Depositor
Recommended contour level	0.45	Depositor
Map size (Å)	486.72003, 486.72003, 486.72003	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.014, 1.014, 1.014	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, LMU, LMG, TPO, PQN, CHL, XAT, LUT, DGD, SF4, CLA, BCR, NEX

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	0.28	0/6031	0.46	0/8227
2	B	0.30	0/6063	0.48	0/8274
3	C	0.28	0/605	0.55	0/821
4	D	0.28	0/1132	0.54	0/1532
5	E	0.28	0/498	0.51	0/677
6	F	0.27	0/1255	0.48	0/1696
7	G	0.28	0/767	0.50	0/1046
8	H	0.26	0/758	0.48	0/1022
9	I	0.28	0/273	0.41	0/373
10	J	0.26	0/334	0.43	0/457
11	K	0.25	0/572	0.46	0/773
12	L	0.27	0/1264	0.45	0/1727
13	M	0.28	0/239	0.42	0/322
14	O	0.26	0/729	0.47	0/997
15	1	0.28	0/1527	0.47	0/2088
15	5	0.27	0/1524	0.50	0/2084
16	2	0.29	0/1683	0.49	0/2300
16	6	0.25	0/1638	0.45	0/2241
17	3	0.30	0/1721	0.49	0/2335
17	7	0.28	0/1695	0.50	0/2302
18	4	0.26	0/1641	0.45	0/2244
18	8	0.25	0/1634	0.46	0/2234
19	9	0.29	0/1801	0.50	0/2451
20	a	0.27	0/1700	0.47	0/2316
20	b	0.27	0/1700	0.45	0/2316
20	c	0.26	0/1764	0.49	0/2399
All	All	0.28	0/40548	0.48	0/55254

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5836	0	5725	107	0
2	B	5849	0	5623	116	0
3	C	595	0	573	12	0
4	D	1104	0	1112	16	0
5	E	487	0	480	9	0
6	F	1230	0	1282	13	0
7	G	749	0	729	12	0
8	H	740	0	727	7	0
9	I	266	0	274	4	0
10	J	325	0	341	5	0
11	K	566	0	587	7	0
12	L	1229	0	1242	14	0
13	M	238	0	263	4	0
14	O	702	0	697	11	0
15	1	1478	0	1455	26	0
15	5	1475	0	1447	51	0
16	2	1632	0	1603	32	0
16	6	1587	0	1556	57	0
17	3	1670	0	1633	22	0
17	7	1644	0	1599	64	0
18	4	1592	0	1561	32	0
18	8	1585	0	1555	60	0
19	9	1747	0	1721	42	0
20	a	1651	0	1586	0	0
20	b	1651	0	1585	0	0
20	c	1727	0	1661	0	0
21	1	587	0	420	28	0
21	2	366	0	281	37	0
21	3	642	0	487	43	0
21	4	472	0	362	30	0
21	5	531	0	369	29	0
21	6	347	0	253	25	0
21	7	551	0	377	42	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
21	8	460	0	348	46	0
21	9	352	0	290	15	0
21	A	2422	0	2311	131	0
21	B	2312	0	2267	120	0
21	F	147	0	123	5	0
21	G	139	0	102	3	0
21	H	45	0	33	2	0
21	J	42	0	31	1	0
21	K	185	0	135	15	0
21	L	132	0	97	5	0
21	O	170	0	116	3	0
21	a	383	0	304	0	0
21	b	391	0	316	0	0
21	c	417	0	367	0	0
22	A	33	0	46	0	0
22	B	33	0	46	3	0
23	1	51	0	42	0	0
23	2	35	0	40	1	0
23	4	86	0	118	6	0
23	5	28	0	26	1	0
23	6	35	0	40	3	0
23	8	37	0	44	3	0
23	9	49	0	74	4	0
23	A	125	0	172	7	0
23	a	49	0	74	0	0
23	b	49	0	74	0	0
23	c	49	0	74	0	0
24	2	40	0	56	6	0
24	3	80	0	112	8	0
24	4	40	0	56	0	0
24	6	40	0	56	14	0
24	7	80	0	112	11	0
24	8	40	0	56	9	0
24	A	240	0	336	21	0
24	B	200	0	280	38	0
24	F	80	0	112	3	0
24	G	80	0	112	6	0
24	I	40	0	56	1	0
24	J	120	0	168	16	0
24	K	40	0	56	23	0
24	L	120	0	168	8	0
24	M	40	0	56	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
24	O	40	0	56	1	0
25	A	8	0	0	0	0
25	C	16	0	0	0	0
26	3	35	0	46	4	0
26	A	70	0	92	2	0
26	O	35	0	46	0	0
26	b	35	0	46	0	0
27	B	66	0	96	7	0
28	2	13	0	11	0	0
28	6	13	0	11	1	0
28	G	55	0	86	3	0
28	J	30	0	30	0	0
29	1	102	0	74	8	0
29	2	295	0	212	16	0
29	3	40	0	23	2	0
29	4	180	0	116	6	0
29	5	92	0	62	6	0
29	6	286	0	196	17	0
29	7	40	0	23	2	0
29	8	180	0	116	17	0
29	9	273	0	184	14	0
29	a	272	0	181	0	0
29	b	292	0	206	0	0
29	c	274	0	178	0	0
30	1	42	0	56	3	0
30	2	42	0	56	8	0
30	3	42	0	56	12	0
30	4	42	0	56	7	0
30	5	42	0	56	2	0
30	6	42	0	56	6	0
30	7	42	0	56	14	0
30	8	42	0	56	5	0
30	9	84	0	112	9	0
30	a	84	0	112	0	0
30	b	84	0	112	0	0
30	c	84	0	112	0	0
31	1	44	0	56	3	0
31	2	44	0	56	2	0
31	3	44	0	56	4	0
31	4	44	0	56	4	0
31	5	44	0	56	7	0
31	6	44	0	56	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
31	7	44	0	56	5	0
31	8	44	0	56	5	0
31	9	44	0	56	2	0
31	a	44	0	56	0	0
31	c	44	0	56	0	0
32	9	44	0	56	3	0
32	b	44	0	56	0	0
32	c	44	0	56	0	0
All	All	56417	0	54439	1134	0

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

The worst 5 of 1134 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)
21:3:409:CLA:C4	30:3:416:LUT:H28	1.47	1.43
21:A:852:CLA:O1D	21:B:801:CLA:H61	1.31	1.22
21:K:203:CLA:HMC1	24:K:205:BCR:H312	1.28	1.15
21:2:609:CLA:H43	30:2:616:LUT:H7	1.25	1.13
21:2:609:CLA:HBC2	21:2:609:CLA:HHD	1.30	1.10

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	740/742 (100%)	715 (97%)	25 (3%)	0	100	100
2	B	731/733 (100%)	701 (96%)	30 (4%)	0	100	100
3	C	78/80 (98%)	72 (92%)	6 (8%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	D	139/141 (99%)	132 (95%)	7 (5%)	0	100	100
5	E	60/62 (97%)	60 (100%)	0	0	100	100
6	F	157/159 (99%)	154 (98%)	3 (2%)	0	100	100
7	G	96/98 (98%)	94 (98%)	2 (2%)	0	100	100
8	H	93/95 (98%)	90 (97%)	3 (3%)	0	100	100
9	I	32/34 (94%)	29 (91%)	3 (9%)	0	100	100
10	J	39/41 (95%)	39 (100%)	0	0	100	100
11	K	79/81 (98%)	76 (96%)	3 (4%)	0	100	100
12	L	161/163 (99%)	153 (95%)	8 (5%)	0	100	100
13	M	30/32 (94%)	29 (97%)	0	1 (3%)	3	6
14	O	87/89 (98%)	79 (91%)	8 (9%)	0	100	100
15	1	190/192 (99%)	183 (96%)	7 (4%)	0	100	100
15	5	190/192 (99%)	176 (93%)	12 (6%)	2 (1%)	12	27
16	2	209/211 (99%)	201 (96%)	8 (4%)	0	100	100
16	6	203/211 (96%)	199 (98%)	4 (2%)	0	100	100
17	3	214/216 (99%)	203 (95%)	11 (5%)	0	100	100
17	7	211/216 (98%)	198 (94%)	12 (6%)	1 (0%)	25	46
18	4	203/205 (99%)	193 (95%)	10 (5%)	0	100	100
18	8	202/205 (98%)	192 (95%)	10 (5%)	0	100	100
19	9	223/225 (99%)	201 (90%)	22 (10%)	0	100	100
20	a	216/227 (95%)	208 (96%)	7 (3%)	1 (0%)	25	46
20	b	216/227 (95%)	208 (96%)	7 (3%)	1 (0%)	25	46
20	c	224/227 (99%)	215 (96%)	8 (4%)	1 (0%)	30	52
All	All	5023/5104 (98%)	4800 (96%)	216 (4%)	7 (0%)	50	71

5 of 7 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
15	5	170	PRO
20	b	152	VAL
20	c	152	VAL
20	a	152	VAL
13	M	4	ILE

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	603/603 (100%)	601 (100%)	2 (0%)	91 97
2	B	595/595 (100%)	593 (100%)	2 (0%)	91 97
3	C	67/67 (100%)	67 (100%)	0	100 100
4	D	115/115 (100%)	115 (100%)	0	100 100
5	E	52/52 (100%)	52 (100%)	0	100 100
6	F	129/129 (100%)	129 (100%)	0	100 100
7	G	78/78 (100%)	77 (99%)	1 (1%)	65 84
8	H	77/77 (100%)	77 (100%)	0	100 100
9	I	30/30 (100%)	30 (100%)	0	100 100
10	J	35/35 (100%)	35 (100%)	0	100 100
11	K	58/58 (100%)	58 (100%)	0	100 100
12	L	126/126 (100%)	126 (100%)	0	100 100
13	M	27/27 (100%)	27 (100%)	0	100 100
14	O	73/73 (100%)	73 (100%)	0	100 100
15	1	151/151 (100%)	151 (100%)	0	100 100
15	5	150/151 (99%)	149 (99%)	1 (1%)	81 92
16	2	168/168 (100%)	167 (99%)	1 (1%)	84 93
16	6	163/168 (97%)	163 (100%)	0	100 100
17	3	169/169 (100%)	169 (100%)	0	100 100
17	7	166/169 (98%)	164 (99%)	2 (1%)	67 85
18	4	164/164 (100%)	164 (100%)	0	100 100
18	8	163/164 (99%)	162 (99%)	1 (1%)	84 93
19	9	179/179 (100%)	178 (99%)	1 (1%)	84 93
20	a	165/173 (95%)	165 (100%)	0	100 100
20	b	165/173 (95%)	164 (99%)	1 (1%)	84 93
20	c	173/173 (100%)	172 (99%)	1 (1%)	84 93

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	4041/4067 (99%)	4028 (100%)	13 (0%)	90 97

5 of 13 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
17	7	258	LYS
17	7	302	HIS
20	c	42	LYS
19	9	157	ARG
20	b	68	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 6 such sidechains are listed below:

Mol	Chain	Res	Type
15	5	154	GLN
15	5	206	GLN
16	6	240	GLN
1	A	294	HIS
1	A	121	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)

1 non-standard protein/DNA/RNA residue is 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	$\#\|Z\| > 2$
20	TPO	c	40	20	8,10,11	1.58	1 (12%)	10,14,16	1.77	1 (10%)

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
20	TPO	c	40	20	-	2/9/11/13	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	c	40	TPO	P-O1P	3.35	1.61	1.50

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	c	40	TPO	P-OG1-CB	-4.89	108.44	123.21

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
20	c	40	TPO	CB-OG1-P-O2P
20	c	40	TPO	O-C-CA-CB

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

364 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	606	-	46,54,74	2.39	16 (34%)	49,90,114	3.48	24 (48%)
31	XAT	4	616	-	39,47,47	1.65	8 (20%)	54,74,74	1.62	11 (20%)
21	CLA	A	824	-	55,63,73	1.60	6 (10%)	64,101,113	1.44	8 (12%)
21	CLA	B	817	-	65,73,73	1.47	7 (10%)	76,113,113	1.39	8 (10%)
24	BCR	A	854	-	41,41,41	1.69	8 (19%)	56,56,56	1.44	8 (14%)
24	BCR	A	847	-	41,41,41	1.69	8 (19%)	56,56,56	1.39	9 (16%)
24	BCR	F	301	-	41,41,41	1.67	8 (19%)	56,56,56	1.56	9 (16%)
21	CLA	L	303	-	45,53,73	1.74	6 (13%)	52,89,113	1.62	9 (17%)
30	LUT	c	616	-	42,43,43	1.63	8 (19%)	51,60,60	1.57	11 (21%)
26	LMU	A	853	-	36,36,36	0.39	0	47,47,47	0.80	1 (2%)
21	CLA	8	608	18	43,51,73	1.93	7 (16%)	47,86,113	1.55	5 (10%)
29	CHL	5	601	15	46,54,74	2.30	14 (30%)	49,90,114	3.51	24 (48%)
29	CHL	2	614	-	46,54,74	2.31	16 (34%)	49,90,114	3.49	25 (51%)
30	LUT	9	615	-	42,43,43	1.63	8 (19%)	51,60,60	1.59	11 (21%)
29	CHL	b	306	20	46,54,74	2.36	16 (34%)	49,90,114	3.48	24 (48%)
21	CLA	A	839	-	45,53,73	1.81	6 (13%)	52,89,113	1.62	6 (11%)
21	CLA	1	304	-	55,63,73	1.61	6 (10%)	64,101,113	1.50	7 (10%)
21	CLA	G	204	7	43,52,73	1.83	5 (11%)	49,88,113	1.58	6 (12%)
21	CLA	4	602	18	57,66,73	1.56	6 (10%)	65,104,113	1.47	9 (13%)
21	CLA	8	602	18	57,66,73	1.58	5 (8%)	65,104,113	1.44	9 (13%)
21	CLA	G	203	-	50,58,73	1.70	6 (12%)	58,95,113	1.50	8 (13%)
23	LHG	A	855	-	48,48,48	0.27	0	51,54,54	0.37	0
29	CHL	2	605	-	46,54,74	2.31	14 (30%)	49,90,114	3.56	24 (48%)
29	CHL	a	605	20	44,53,74	2.42	16 (36%)	46,89,114	3.56	23 (50%)
29	CHL	6	605	-	46,54,74	2.34	16 (34%)	49,90,114	3.54	24 (48%)
21	CLA	7	401	17	45,53,73	1.79	6 (13%)	52,89,113	1.58	7 (13%)
21	CLA	7	414	-	39,48,73	1.89	6 (15%)	44,83,113	1.70	7 (15%)
29	CHL	1	302	15	51,59,74	2.20	14 (27%)	55,96,114	3.41	27 (49%)
21	CLA	F	304	-	45,53,73	1.80	6 (13%)	52,89,113	1.56	9 (17%)
29	CHL	4	614	18	42,50,74	2.41	14 (33%)	44,85,114	3.72	23 (52%)
24	BCR	3	419	-	41,41,41	1.73	8 (19%)	56,56,56	1.90	12 (21%)
24	BCR	J	103	-	41,41,41	1.76	8 (19%)	56,56,56	1.58	11 (19%)
21	CLA	5	604	-	49,57,73	1.72	5 (10%)	55,93,113	1.53	7 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
21	CLA	7	411	-	53,62,73	1.67	5 (9%)	61,100,113	1.42	9 (14%)
29	CHL	6	602	-	53,61,74	2.15	14 (26%)	57,98,114	3.36	29 (50%)
21	CLA	4	601	18	45,53,73	1.78	6 (13%)	52,89,113	1.59	6 (11%)
29	CHL	b	302	20	46,54,74	2.36	16 (34%)	49,90,114	3.50	23 (46%)
21	CLA	A	808	-	45,53,73	1.75	6 (13%)	52,89,113	1.65	7 (13%)
21	CLA	6	604	-	45,53,73	1.82	5 (11%)	52,89,113	1.56	6 (11%)
21	CLA	5	613	-	37,46,73	2.00	6 (16%)	46,81,113	1.71	9 (19%)
21	CLA	B	805	-	65,73,73	1.45	6 (9%)	76,113,113	1.40	7 (9%)
21	CLA	4	608	18	43,51,73	1.88	7 (16%)	47,86,113	1.59	5 (10%)
21	CLA	a	610	20	45,53,73	1.78	5 (11%)	52,89,113	1.58	6 (11%)
21	CLA	5	608	15	40,48,73	1.91	6 (15%)	50,83,113	1.71	9 (18%)
21	CLA	B	836	-	65,73,73	1.45	7 (10%)	76,113,113	1.48	7 (9%)
21	CLA	3	409	17	52,60,73	1.52	7 (13%)	60,97,113	2.27	20 (33%)
29	CHL	9	606	19	46,54,74	2.31	16 (34%)	49,90,114	3.55	23 (46%)
29	CHL	b	308	-	53,61,74	2.16	14 (26%)	57,98,114	3.40	28 (49%)
29	CHL	7	406	-	39,48,74	2.57	16 (41%)	44,83,114	3.86	25 (56%)
21	CLA	B	834	-	45,53,73	1.74	6 (13%)	52,89,113	1.68	8 (15%)
21	CLA	A	829	-	65,73,73	1.47	6 (9%)	76,113,113	1.32	7 (9%)
21	CLA	B	833	-	45,53,73	1.76	6 (13%)	52,89,113	1.58	7 (13%)
21	CLA	B	812	-	65,73,73	1.47	7 (10%)	76,113,113	1.38	8 (10%)
21	CLA	9	602	19	53,61,73	1.65	7 (13%)	61,98,113	1.51	9 (14%)
21	CLA	c	613	-	65,73,73	1.47	6 (9%)	76,113,113	1.40	6 (7%)
21	CLA	7	405	17	39,48,73	1.95	6 (15%)	48,83,113	1.69	8 (16%)
21	CLA	3	413	-	39,48,73	1.90	6 (15%)	44,83,113	1.62	7 (15%)
21	CLA	6	608	16	45,53,73	1.81	5 (11%)	52,89,113	1.52	6 (11%)
31	XAT	6	617	-	39,47,47	1.73	8 (20%)	54,74,74	1.79	12 (22%)
21	CLA	3	401	-	39,48,73	1.83	6 (15%)	44,83,113	1.80	8 (18%)
21	CLA	B	830	-	56,64,73	1.57	6 (10%)	65,102,113	1.43	7 (10%)
21	CLA	B	832	-	56,64,73	1.57	7 (12%)	65,102,113	1.56	8 (12%)
29	CHL	c	601	20	49,57,74	2.22	13 (26%)	52,93,114	3.44	24 (46%)
21	CLA	8	609	23	45,53,73	1.93	7 (15%)	52,89,113	2.06	11 (21%)
29	CHL	9	609	-	46,54,74	2.32	15 (32%)	49,90,114	3.56	25 (51%)
21	CLA	L	304	-	42,50,73	1.76	6 (14%)	48,85,113	1.64	6 (12%)
21	CLA	B	838	-	65,73,73	1.47	6 (9%)	76,113,113	1.34	7 (9%)
21	CLA	1	309	15	41,49,73	1.90	8 (19%)	47,84,113	2.29	17 (36%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
21	CLA	B	826	-	52,60,73	1.62	6 (11%)	60,97,113	1.54	8 (13%)
24	BCR	A	849	-	41,41,41	1.70	8 (19%)	56,56,56	1.71	12 (21%)
21	CLA	4	609	18	52,60,73	1.60	8 (15%)	60,97,113	2.33	19 (31%)
24	BCR	B	843	-	41,41,41	0.76	0	56,56,56	2.53	24 (42%)
21	CLA	8	618	-	41,49,73	1.83	7 (17%)	47,84,113	1.63	9 (19%)
31	XAT	2	617	-	39,47,47	1.65	8 (20%)	54,74,74	1.60	11 (20%)
21	CLA	c	612	20	44,52,73	1.81	6 (13%)	49,87,113	1.55	6 (12%)
21	CLA	1	312	15	45,53,73	1.81	6 (13%)	52,89,113	1.53	6 (11%)
21	CLA	4	604	-	43,51,73	1.78	6 (13%)	48,86,113	1.59	7 (14%)
21	CLA	b	313	20	45,53,73	1.80	6 (13%)	52,89,113	1.53	7 (13%)
31	XAT	a	618	-	39,47,47	1.68	8 (20%)	54,74,74	1.77	11 (20%)
24	BCR	J	101	-	41,41,41	1.75	8 (19%)	56,56,56	1.87	10 (17%)
21	CLA	3	408	17	59,67,73	1.58	7 (11%)	68,105,113	1.42	9 (13%)
30	LUT	8	614	-	42,43,43	1.67	8 (19%)	51,60,60	1.68	9 (17%)
21	CLA	A	828	-	60,68,73	1.52	6 (10%)	70,107,113	1.38	9 (12%)
21	CLA	1	303	15	61,69,73	1.51	6 (9%)	71,108,113	1.44	8 (11%)
29	CHL	5	606	-	46,54,74	2.37	16 (34%)	49,90,114	3.48	24 (48%)
21	CLA	1	311	23	37,46,73	1.97	7 (18%)	46,81,113	1.73	10 (21%)
21	CLA	A	831	-	55,63,73	1.60	6 (10%)	64,101,113	1.53	8 (12%)
21	CLA	B	801	-	65,73,73	2.06	16 (24%)	76,113,113	2.75	29 (38%)
21	CLA	A	825	-	65,73,73	1.45	6 (9%)	76,113,113	1.41	7 (9%)
23	LHG	A	844	-	48,48,48	0.27	0	51,54,54	0.35	0
30	LUT	7	415	-	42,43,43	1.68	8 (19%)	51,60,60	1.77	13 (25%)
21	CLA	A	836	1	45,53,73	1.79	6 (13%)	52,89,113	1.54	7 (13%)
23	LHG	1	319	21	27,27,48	0.35	0	30,33,54	0.47	0
21	CLA	B	803	-	55,63,73	1.60	6 (10%)	64,101,113	1.47	7 (10%)
29	CHL	2	606	-	46,54,74	2.28	14 (30%)	49,90,114	3.53	24 (48%)
29	CHL	a	606	-	46,54,74	2.35	15 (32%)	49,90,114	3.55	25 (51%)
29	CHL	6	606	-	46,54,74	2.33	15 (32%)	49,90,114	3.52	24 (48%)
21	CLA	B	835	-	65,73,73	1.44	6 (9%)	76,113,113	1.41	8 (10%)
29	CHL	4	605	-	41,49,74	2.20	13 (31%)	48,84,114	3.79	27 (56%)
21	CLA	A	834	-	65,73,73	1.47	6 (9%)	76,113,113	1.37	8 (10%)
29	CHL	9	601	19	43,51,74	2.34	15 (34%)	45,86,114	3.67	24 (53%)
21	CLA	1	305	-	49,57,73	1.69	6 (12%)	55,93,113	1.54	8 (14%)
21	CLA	2	603	-	45,53,73	1.83	7 (15%)	52,89,113	1.51	6 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
21	CLA	7	409	-	39,48,73	1.90	5 (12%)	44,83,113	1.67	7 (15%)
21	CLA	6	603	-	45,53,73	1.84	6 (13%)	52,89,113	1.59	7 (13%)
21	CLA	B	806	-	63,71,73	1.48	6 (9%)	73,110,113	1.44	8 (10%)
29	CHL	9	608	-	46,54,74	2.30	15 (32%)	49,90,114	3.52	23 (46%)
21	CLA	K	204	11	45,53,73	1.78	6 (13%)	52,89,113	1.57	6 (11%)
21	CLA	K	201	11	46,54,73	1.73	6 (13%)	53,90,113	1.56	6 (11%)
21	CLA	1	314	-	37,46,73	2.00	7 (18%)	46,81,113	1.69	11 (23%)
26	LMU	3	420	-	36,36,36	0.40	0	47,47,47	0.72	1 (2%)
24	BCR	L	301	-	41,41,41	1.69	8 (19%)	56,56,56	1.43	9 (16%)
29	CHL	c	606	20	46,54,74	2.35	16 (34%)	49,90,114	3.49	24 (48%)
21	CLA	A	809	1	59,67,73	1.53	6 (10%)	68,105,113	1.48	9 (13%)
21	CLA	3	411	17	43,51,73	1.82	6 (13%)	49,86,113	1.57	6 (12%)
21	CLA	A	841	-	65,73,73	1.48	6 (9%)	76,113,113	1.42	7 (9%)
21	CLA	B	810	-	54,62,73	1.67	7 (12%)	67,100,113	1.50	10 (14%)
21	CLA	c	602	20	60,68,73	1.54	7 (11%)	70,107,113	1.39	8 (11%)
21	CLA	A	804	-	65,73,73	1.47	6 (9%)	76,113,113	1.44	8 (10%)
24	BCR	7	417	-	41,41,41	1.73	8 (19%)	56,56,56	1.52	9 (16%)
30	LUT	9	614	-	42,43,43	1.63	8 (19%)	51,60,60	1.56	12 (23%)
21	CLA	3	405	-	40,49,73	1.85	7 (17%)	45,84,113	1.65	6 (13%)
24	BCR	B	845	-	41,41,41	1.71	8 (19%)	56,56,56	1.48	8 (14%)
21	CLA	O	204	-	39,48,73	1.91	6 (15%)	44,83,113	1.59	7 (15%)
21	CLA	B	837	-	63,72,73	1.49	6 (9%)	73,112,113	1.41	7 (9%)
21	CLA	8	603	-	43,52,73	1.84	5 (11%)	49,88,113	1.55	7 (14%)
23	LHG	c	619	21	48,48,48	0.26	0	51,54,54	0.31	0
21	CLA	A	801	-	52,60,73	1.97	6 (11%)	60,97,113	2.24	17 (28%)
21	CLA	B	815	-	53,62,73	1.65	7 (13%)	61,100,113	1.43	8 (13%)
21	CLA	B	821	-	55,63,73	1.63	6 (10%)	64,101,113	1.51	8 (12%)
21	CLA	B	816	-	52,60,73	1.65	7 (13%)	60,97,113	1.56	8 (13%)
21	CLA	5	611	15	45,53,73	1.79	6 (13%)	52,89,113	1.61	6 (11%)
21	CLA	1	316	15	43,51,73	1.89	8 (18%)	54,87,113	1.65	8 (14%)
21	CLA	A	832	-	45,53,73	1.74	6 (13%)	52,89,113	1.60	7 (13%)
29	CHL	b	309	-	49,57,74	2.22	13 (26%)	52,93,114	3.45	25 (48%)
29	CHL	a	607	-	43,51,74	2.31	14 (32%)	45,86,114	3.67	24 (53%)
21	CLA	3	410	-	39,48,73	1.91	5 (12%)	44,83,113	1.63	7 (15%)
21	CLA	B	813	-	43,52,73	1.77	6 (13%)	49,88,113	1.62	7 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
21	CLA	F	305	6	41,49,73	1.80	6 (14%)	47,84,113	1.64	7 (14%)
24	BCR	A	850	-	41,41,41	1.70	8 (19%)	56,56,56	1.78	9 (16%)
21	CLA	b	305	-	45,53,73	1.78	6 (13%)	52,89,113	1.60	6 (11%)
22	PQN	B	841	-	34,34,34	0.40	0	42,45,45	0.37	0
30	LUT	1	317	-	42,43,43	1.69	8 (19%)	51,60,60	1.70	9 (17%)
21	CLA	A	817	-	65,73,73	1.44	6 (9%)	76,113,113	1.40	7 (9%)
21	CLA	9	613	-	53,61,73	1.62	5 (9%)	61,98,113	1.52	8 (13%)
29	CHL	2	602	16	53,61,74	2.16	15 (28%)	57,98,114	3.38	28 (49%)
24	BCR	M	101	-	41,41,41	1.77	8 (19%)	56,56,56	1.83	12 (21%)
21	CLA	9	603	19	45,53,73	1.80	6 (13%)	52,89,113	1.61	6 (11%)
29	CHL	3	407	-	39,48,74	2.41	13 (33%)	44,83,114	3.58	24 (54%)
24	BCR	L	306	-	41,41,41	1.72	8 (19%)	56,56,56	1.78	11 (19%)
21	CLA	4	613	-	43,51,73	1.80	6 (13%)	49,86,113	1.56	7 (14%)
21	CLA	b	304	-	45,53,73	1.76	6 (13%)	52,89,113	1.63	7 (13%)
30	LUT	5	615	-	42,43,43	1.67	8 (19%)	51,60,60	1.69	10 (19%)
21	CLA	B	807	-	65,73,73	1.47	7 (10%)	76,113,113	1.39	8 (10%)
21	CLA	A	833	-	65,73,73	1.50	6 (9%)	76,113,113	1.36	7 (9%)
29	CHL	b	310	-	51,60,74	2.19	16 (31%)	54,97,114	3.34	27 (50%)
31	XAT	1	318	-	39,47,47	1.67	8 (20%)	54,74,74	1.62	12 (22%)
21	CLA	a	602	-	60,68,73	1.54	6 (10%)	70,107,113	1.43	7 (10%)
21	CLA	2	609	16	51,59,73	1.70	6 (11%)	58,95,113	2.08	15 (25%)
24	BCR	2	618	-	41,41,41	1.71	8 (19%)	56,56,56	1.55	10 (17%)
24	BCR	6	618	-	41,41,41	1.73	8 (19%)	56,56,56	1.65	10 (17%)
21	CLA	A	806	-	65,73,73	1.46	7 (10%)	76,113,113	1.40	6 (7%)
21	CLA	8	604	-	43,51,73	1.81	6 (13%)	48,86,113	1.64	6 (12%)
22	PQN	A	843	-	34,34,34	0.39	0	42,45,45	0.43	0
26	LMU	b	301	-	36,36,36	0.37	0	47,47,47	0.76	0
23	LHG	2	619	21	34,34,48	0.33	0	37,40,54	0.41	0
21	CLA	c	614	-	45,53,73	1.81	6 (13%)	52,89,113	1.50	6 (11%)
24	BCR	7	418	-	41,41,41	1.73	8 (19%)	56,56,56	1.98	12 (21%)
23	LHG	6	619	-	34,34,48	0.31	0	37,40,54	0.37	0
29	CHL	1	307	-	51,59,74	2.19	14 (27%)	55,96,114	3.43	27 (49%)
21	CLA	A	805	-	55,63,73	1.60	6 (10%)	64,101,113	1.45	7 (10%)
21	CLA	3	402	17	60,68,73	1.52	6 (10%)	70,107,113	1.43	8 (11%)
24	BCR	A	848	-	41,41,41	1.68	8 (19%)	56,56,56	1.36	8 (14%)
21	CLA	2	612	16	45,53,73	1.78	6 (13%)	52,89,113	1.59	7 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
21	CLA	A	802	-	52,60,73	1.66	7 (13%)	60,97,113	1.52	9 (15%)
21	CLA	5	607	-	43,52,73	1.83	5 (11%)	49,88,113	1.57	7 (14%)
21	CLA	4	611	18	44,52,73	1.79	6 (13%)	51,88,113	1.64	6 (11%)
24	BCR	B	846	-	41,41,41	0.75	0	56,56,56	1.94	18 (32%)
29	CHL	4	606	-	46,54,74	2.31	14 (30%)	49,90,114	3.55	23 (46%)
21	CLA	6	610	-	41,50,73	1.86	6 (14%)	49,85,113	1.59	6 (12%)
29	CHL	a	608	-	46,54,74	2.30	16 (34%)	49,90,114	3.51	24 (48%)
30	LUT	b	316	-	42,43,43	1.64	8 (19%)	51,60,60	1.59	9 (17%)
21	CLA	B	829	-	45,53,73	1.84	6 (13%)	52,89,113	1.70	7 (13%)
23	LHG	a	617	-	48,48,48	0.26	0	51,54,54	0.35	0
30	LUT	3	416	-	42,43,43	1.64	7 (16%)	51,60,60	1.68	11 (21%)
21	CLA	B	814	-	60,68,73	1.54	6 (10%)	70,107,113	1.47	8 (11%)
24	BCR	G	205	-	41,41,41	1.70	8 (19%)	56,56,56	1.56	10 (17%)
21	CLA	7	412	-	39,48,73	2.01	5 (12%)	44,83,113	1.61	7 (15%)
21	CLA	H	201	8	45,53,73	1.79	6 (13%)	52,89,113	1.55	6 (11%)
23	LHG	5	617	-	27,27,48	0.35	0	30,33,54	0.44	0
23	LHG	4	619	-	48,48,48	0.28	0	51,54,54	0.62	1 (1%)
21	CLA	a	613	-	57,65,73	1.60	5 (8%)	66,103,113	1.44	9 (13%)
21	CLA	5	610	-	37,46,73	1.99	7 (18%)	46,81,113	1.75	9 (19%)
21	CLA	c	610	20	45,53,73	1.76	5 (11%)	52,89,113	1.61	8 (15%)
29	CHL	c	607	-	46,54,74	2.39	16 (34%)	49,90,114	3.50	25 (51%)
21	CLA	A	813	-	54,62,73	1.59	6 (11%)	62,99,113	1.59	7 (11%)
21	CLA	A	840	-	65,73,73	1.45	6 (9%)	76,113,113	1.38	8 (10%)
21	CLA	9	611	23	57,65,73	1.58	6 (10%)	66,103,113	1.44	7 (10%)
21	CLA	7	403	-	41,50,73	1.94	7 (17%)	51,86,113	1.66	8 (15%)
30	LUT	c	615	-	42,43,43	1.64	8 (19%)	51,60,60	1.50	10 (19%)
29	CHL	c	608	-	46,54,74	2.34	15 (32%)	49,90,114	3.53	23 (46%)
21	CLA	A	810	-	45,53,73	1.75	6 (13%)	52,89,113	1.61	7 (13%)
21	CLA	a	603	-	41,49,73	1.85	6 (14%)	47,84,113	1.64	7 (14%)
21	CLA	7	404	-	40,49,73	1.86	6 (15%)	45,84,113	1.63	6 (13%)
21	CLA	A	811	-	45,53,73	1.74	6 (13%)	52,89,113	1.62	8 (15%)
21	CLA	A	823	-	56,64,73	1.62	7 (12%)	65,102,113	1.42	8 (12%)
30	LUT	4	615	-	42,43,43	1.66	8 (19%)	51,60,60	1.75	10 (19%)
21	CLA	3	403	-	55,63,73	1.65	7 (12%)	64,101,113	1.44	6 (9%)
21	CLA	A	826	-	65,73,73	1.46	6 (9%)	76,113,113	1.42	8 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
24	BCR	B	844	-	41,41,41	0.71	0	56,56,56	2.10	22 (39%)
21	CLA	9	604	-	45,53,73	1.75	7 (15%)	52,89,113	1.66	6 (11%)
21	CLA	B	811	-	45,53,73	1.84	7 (15%)	52,89,113	1.69	6 (11%)
21	CLA	7	410	-	43,51,73	1.82	5 (11%)	49,86,113	1.56	6 (12%)
21	CLA	b	311	20	54,62,73	1.61	6 (11%)	62,99,113	1.51	9 (14%)
21	CLA	a	604	-	46,55,73	1.75	6 (13%)	52,91,113	1.54	7 (13%)
23	LHG	1	301	21	22,22,48	0.34	0	25,28,54	0.67	1 (4%)
21	CLA	7	413	-	37,44,73	1.95	6 (16%)	42,77,113	1.68	7 (16%)
21	CLA	7	408	-	41,49,73	1.88	5 (12%)	47,84,113	1.62	7 (14%)
21	CLA	8	601	18	45,53,73	1.80	5 (11%)	52,89,113	1.55	6 (11%)
29	CHL	a	609	-	46,54,74	2.43	16 (34%)	49,90,114	3.56	24 (48%)
21	CLA	8	611	-	54,62,73	1.65	5 (9%)	62,99,113	1.44	8 (12%)
21	CLA	7	402	-	45,53,73	1.82	6 (13%)	52,89,113	1.58	7 (13%)
21	CLA	A	814	-	65,73,73	1.45	6 (9%)	76,113,113	1.44	8 (10%)
21	CLA	5	612	-	45,53,73	1.81	5 (11%)	52,89,113	1.57	6 (11%)
29	CHL	8	605	18	41,49,74	2.21	14 (34%)	48,84,114	3.76	28 (58%)
23	LHG	b	319	21	48,48,48	0.27	0	51,54,54	0.32	0
24	BCR	4	617	-	41,41,41	1.72	8 (19%)	56,56,56	1.46	9 (16%)
21	CLA	B	822	-	45,53,73	1.76	7 (15%)	52,89,113	1.61	6 (11%)
21	CLA	B	831	-	56,64,73	1.63	7 (12%)	65,102,113	1.42	10 (15%)
21	CLA	O	202	-	36,46,73	1.95	6 (16%)	41,80,113	1.69	8 (19%)
28	LMG	2	615	-	13,13,55	0.19	0	18,18,63	0.34	0
29	CHL	8	613	-	42,50,74	2.46	15 (35%)	44,85,114	3.62	23 (52%)
21	CLA	B	825	-	65,73,73	1.45	7 (10%)	76,113,113	1.42	8 (10%)
24	BCR	O	205	-	41,41,41	1.73	8 (19%)	56,56,56	1.67	11 (19%)
21	CLA	A	827	-	63,72,73	1.48	5 (7%)	73,112,113	1.43	7 (9%)
21	CLA	b	312	23	45,53,73	1.81	5 (11%)	52,89,113	1.54	6 (11%)
25	SF4	A	851	2,1	0,12,12	-	-	-		
30	LUT	2	616	-	42,43,43	1.65	8 (19%)	51,60,60	1.74	12 (23%)
21	CLA	A	837	-	51,59,73	1.70	7 (13%)	59,96,113	1.41	8 (13%)
29	CHL	6	607	-	51,59,74	2.26	16 (31%)	55,96,114	3.35	28 (50%)
32	NEX	9	617	-	38,46,46	1.61	7 (18%)	50,70,70	1.60	8 (16%)
21	CLA	3	415	-	39,48,73	1.88	6 (15%)	44,83,113	1.61	7 (15%)
21	CLA	A	835	-	50,58,73	1.64	5 (10%)	58,95,113	1.55	7 (12%)
21	CLA	b	303	20	59,67,73	1.56	6 (10%)	68,105,113	1.40	7 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
21	CLA	B	819	-	43,51,73	1.77	7 (16%)	49,86,113	1.61	7 (14%)
21	CLA	B	802	-	65,73,73	1.46	7 (10%)	76,113,113	1.41	7 (9%)
21	CLA	1	306	-	39,48,73	1.87	6 (15%)	45,82,113	1.70	7 (15%)
21	CLA	3	406	17	39,48,73	1.93	7 (17%)	48,83,113	1.68	8 (16%)
21	CLA	B	839	-	65,73,73	1.50	7 (10%)	76,113,113	1.38	8 (10%)
21	CLA	1	313	15	45,53,73	1.78	6 (13%)	52,89,113	1.57	8 (15%)
21	CLA	b	314	-	53,61,73	1.65	7 (13%)	61,98,113	1.51	7 (11%)
21	CLA	B	828	-	52,60,73	1.64	7 (13%)	60,97,113	1.51	7 (11%)
21	CLA	2	604	-	45,53,73	1.76	6 (13%)	52,89,113	1.60	7 (13%)
23	LHG	A	845	21	26,26,48	0.33	0	29,32,54	0.44	0
21	CLA	B	809	-	61,70,73	1.54	6 (9%)	70,109,113	1.35	7 (10%)
21	CLA	5	603	-	45,53,73	1.82	7 (15%)	52,89,113	1.53	7 (13%)
21	CLA	J	102	10	42,50,73	1.80	6 (14%)	48,85,113	1.58	6 (12%)
29	CHL	9	607	-	46,54,74	2.32	15 (32%)	49,90,114	3.52	23 (46%)
28	LMG	J	105	-	30,30,55	0.26	0	38,38,63	0.35	0
26	LMU	A	856	-	36,36,36	0.38	0	47,47,47	0.74	1 (2%)
21	CLA	B	804	-	65,73,73	1.50	7 (10%)	76,113,113	1.40	8 (10%)
21	CLA	3	412	-	53,62,73	1.64	6 (11%)	61,100,113	1.41	7 (11%)
23	LHG	9	618	21	48,48,48	0.27	0	51,54,54	0.33	0
31	XAT	7	416	-	39,47,47	1.70	8 (20%)	54,74,74	1.70	12 (22%)
21	CLA	c	603	-	55,63,73	1.60	6 (10%)	64,101,113	1.42	7 (10%)
29	CHL	9	605	19	46,54,74	2.36	16 (34%)	49,90,114	3.52	23 (46%)
21	CLA	O	201	23	42,50,73	1.77	6 (14%)	48,85,113	1.66	6 (12%)
21	CLA	5	614	15	43,51,73	1.90	6 (13%)	54,87,113	1.62	8 (14%)
28	LMG	G	206	-	55,55,55	0.21	0	63,63,63	0.26	0
21	CLA	G	202	-	45,53,73	1.77	6 (13%)	52,89,113	1.67	7 (13%)
21	CLA	3	404	-	41,50,73	1.90	7 (17%)	51,86,113	1.67	9 (17%)
21	CLA	2	611	-	41,49,73	1.82	6 (14%)	47,84,113	1.69	8 (17%)
21	CLA	A	820	-	44,52,73	1.82	6 (13%)	51,88,113	1.59	6 (11%)
21	CLA	6	611	-	41,49,73	1.86	5 (12%)	47,84,113	1.66	7 (14%)
24	BCR	F	303	-	41,41,41	1.72	8 (19%)	56,56,56	1.50	11 (19%)
21	CLA	B	827	-	65,73,73	1.46	6 (9%)	76,113,113	1.35	7 (9%)
31	XAT	5	616	-	39,47,47	1.65	8 (20%)	54,74,74	1.56	8 (14%)
21	CLA	1	308	-	43,52,73	1.82	6 (13%)	49,88,113	1.59	7 (14%)
29	CHL	c	609	20	43,52,74	2.46	16 (37%)	46,88,114	3.46	22 (47%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
21	CLA	b	315	-	45,53,73	1.80	6 (13%)	52,89,113	1.51	7 (13%)
21	CLA	c	604	-	45,53,73	1.78	7 (15%)	52,89,113	1.63	6 (11%)
21	CLA	9	610	19	54,62,73	1.59	6 (11%)	62,99,113	1.51	7 (11%)
30	LUT	a	615	-	42,43,43	1.64	7 (16%)	51,60,60	1.63	10 (19%)
21	CLA	4	603	-	43,52,73	1.84	6 (13%)	49,88,113	1.56	7 (14%)
29	CHL	4	607	-	51,59,74	2.15	14 (27%)	55,96,114	3.39	27 (49%)
32	NEX	c	618	-	38,46,46	1.60	7 (18%)	50,70,70	1.61	9 (18%)
24	BCR	3	418	-	41,41,41	1.69	8 (19%)	56,56,56	1.47	9 (16%)
21	CLA	c	611	23	58,66,73	1.56	6 (10%)	67,104,113	1.43	8 (11%)
24	BCR	K	205	-	41,41,41	0.74	0	56,56,56	2.13	19 (33%)
21	CLA	4	610	23	45,53,73	1.75	6 (13%)	52,89,113	1.60	6 (11%)
21	CLA	5	602	15	61,69,73	1.53	6 (9%)	71,108,113	1.39	8 (11%)
21	CLA	B	820	-	46,54,73	1.77	6 (13%)	53,90,113	1.54	7 (13%)
23	LHG	4	618	21	36,36,48	0.32	0	39,42,54	0.40	0
21	CLA	6	612	-	45,53,73	1.85	5 (11%)	52,89,113	1.60	7 (13%)
21	CLA	2	613	-	42,50,73	1.82	6 (14%)	48,85,113	1.60	7 (14%)
21	CLA	1	310	15	42,51,73	1.81	6 (14%)	48,87,113	1.62	7 (14%)
21	CLA	A	807	1	65,73,73	1.45	6 (9%)	76,113,113	1.41	6 (7%)
21	CLA	6	613	-	42,50,73	1.84	6 (14%)	48,85,113	1.58	7 (14%)
24	BCR	B	842	-	41,41,41	1.71	8 (19%)	56,56,56	1.44	8 (14%)
24	BCR	A	846	-	41,41,41	1.71	8 (19%)	56,56,56	1.63	9 (16%)
21	CLA	2	608	16	55,63,73	1.60	6 (10%)	64,101,113	1.43	8 (12%)
21	CLA	A	838	-	65,73,73	1.44	6 (9%)	76,113,113	1.44	7 (9%)
24	BCR	G	201	-	41,41,41	1.70	8 (19%)	56,56,56	1.53	9 (16%)
26	LMU	O	206	-	36,36,36	0.40	0	47,47,47	0.69	0
21	CLA	A	812	-	65,73,73	1.45	6 (9%)	76,113,113	1.33	8 (10%)
27	DGD	B	847	-	67,67,67	0.83	2 (2%)	81,81,81	0.98	3 (3%)
24	BCR	J	104	-	41,41,41	0.92	1 (2%)	56,56,56	2.29	20 (35%)
32	NEX	b	318	-	38,46,46	1.61	7 (18%)	50,70,70	1.59	8 (16%)
21	CLA	9	612	19	45,53,73	1.80	6 (13%)	52,89,113	1.54	6 (11%)
29	CHL	8	607	-	51,59,74	2.20	16 (31%)	55,96,114	3.35	28 (50%)
21	CLA	K	202	-	50,58,73	1.66	6 (12%)	58,95,113	1.66	11 (18%)
21	CLA	B	824	-	65,73,73	1.45	6 (9%)	76,113,113	1.43	8 (10%)
29	CHL	6	614	-	46,54,74	2.39	16 (34%)	49,90,114	3.46	25 (51%)
29	CHL	2	607	-	51,59,74	2.17	14 (27%)	55,96,114	3.41	27 (49%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
30	LUT	a	616	-	42,43,43	1.66	8 (19%)	51,60,60	1.57	10 (19%)
24	BCR	8	616	-	41,41,41	1.75	8 (19%)	56,56,56	1.49	9 (16%)
24	BCR	I	101	-	41,41,41	1.73	8 (19%)	56,56,56	1.49	10 (17%)
21	CLA	A	821	-	65,73,73	1.45	6 (9%)	76,113,113	1.42	9 (11%)
21	CLA	8	612	-	43,51,73	1.83	5 (11%)	49,86,113	1.56	7 (14%)
24	BCR	L	305	-	41,41,41	1.71	8 (19%)	56,56,56	1.46	8 (14%)
21	CLA	A	830	-	52,60,73	1.78	7 (13%)	60,97,113	2.10	16 (26%)
25	SF4	C	102	3	0,12,12	-	-	-		
21	CLA	4	612	-	55,63,73	1.62	6 (10%)	64,101,113	1.45	8 (12%)
21	CLA	3	414	-	37,44,73	1.93	7 (18%)	42,77,113	1.64	6 (14%)
21	CLA	7	407	17	43,52,73	2.35	11 (25%)	49,88,113	4.02	23 (46%)
29	CHL	c	605	-	42,51,74	2.39	15 (35%)	46,86,114	3.75	23 (50%)
21	CLA	A	842	-	65,73,73	1.47	7 (10%)	76,113,113	1.37	7 (9%)
29	CHL	b	307	-	46,54,74	2.30	14 (30%)	49,90,114	3.57	23 (46%)
21	CLA	A	852	-	52,60,73	1.65	7 (13%)	60,97,113	1.52	9 (15%)
21	CLA	a	614	-	41,49,73	1.85	6 (14%)	47,84,113	1.60	8 (17%)
28	LMG	6	615	-	13,13,55	0.20	0	18,18,63	0.49	0
21	CLA	A	818	-	52,60,73	1.73	7 (13%)	60,97,113	1.50	8 (13%)
31	XAT	c	617	-	39,47,47	1.67	8 (20%)	54,74,74	1.66	10 (18%)
21	CLA	L	302	12	45,53,73	1.77	6 (13%)	52,89,113	1.63	8 (15%)
21	CLA	A	816	-	42,50,73	1.77	6 (14%)	48,85,113	1.66	7 (14%)
21	CLA	8	610	-	44,52,73	1.82	6 (13%)	51,88,113	1.57	6 (11%)
21	CLA	6	609	-	42,50,73	1.82	6 (14%)	48,85,113	1.72	7 (14%)
21	CLA	2	610	23	41,50,73	1.81	6 (14%)	49,85,113	1.61	6 (12%)
21	CLA	5	605	-	39,48,73	1.90	6 (15%)	45,82,113	1.65	8 (17%)
21	CLA	a	611	-	47,55,73	1.75	5 (10%)	54,91,113	1.53	7 (12%)
21	CLA	B	823	-	65,73,73	1.46	6 (9%)	76,113,113	1.50	9 (11%)
30	LUT	b	317	-	42,43,43	1.62	8 (19%)	51,60,60	1.55	10 (19%)
21	CLA	O	203	-	49,58,73	1.66	6 (12%)	58,94,113	1.52	8 (13%)
25	SF4	C	101	3	0,12,12	-	-	-		
21	CLA	B	808	2	65,73,73	1.46	6 (9%)	76,113,113	1.40	6 (7%)
21	CLA	B	818	-	58,66,73	1.56	7 (12%)	67,104,113	1.42	7 (10%)
29	CHL	a	601	20	46,54,74	2.39	16 (34%)	49,90,114	3.54	24 (48%)
21	CLA	A	803	-	52,60,73	1.62	6 (11%)	60,97,113	1.53	9 (15%)
29	CHL	2	601	16	53,61,74	2.14	15 (28%)	57,98,114	3.36	28 (49%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
29	CHL	6	601	16	44,52,74	2.43	16 (36%)	51,88,114	3.79	26 (50%)
21	CLA	B	840	23	65,73,73	1.43	6 (9%)	76,113,113	1.43	7 (9%)
21	CLA	A	819	-	65,73,73	1.48	6 (9%)	76,113,113	1.38	8 (10%)
23	LHG	8	617	21	36,36,48	0.31	0	39,42,54	0.36	0
31	XAT	3	417	-	39,47,47	1.67	8 (20%)	54,74,74	1.60	9 (16%)
21	CLA	A	815	-	45,53,73	1.74	6 (13%)	52,89,113	1.62	7 (13%)
31	XAT	9	616	-	39,47,47	1.73	8 (20%)	54,74,74	2.33	15 (27%)
21	CLA	a	612	-	45,53,73	1.81	5 (11%)	52,89,113	1.56	6 (11%)
31	XAT	8	615	-	39,47,47	1.71	8 (20%)	54,74,74	1.67	9 (16%)
21	CLA	A	822	-	44,52,73	1.80	6 (13%)	51,88,113	1.65	7 (13%)
21	CLA	F	302	-	61,69,73	1.52	6 (9%)	71,108,113	1.43	9 (12%)
30	LUT	6	616	-	42,43,43	1.65	8 (19%)	51,60,60	1.66	12 (23%)
21	CLA	5	609	-	42,51,73	1.84	6 (14%)	48,87,113	1.60	7 (14%)
21	CLA	1	315	-	45,53,73	1.80	6 (13%)	52,89,113	1.57	7 (13%)
21	CLA	K	203	-	44,52,73	1.82	8 (18%)	55,88,113	1.66	8 (14%)

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	606	-	3/3/16/26	5/15/113/137	-
31	XAT	4	616	-	-	0/31/93/93	0/4/4/4
21	CLA	A	824	-	1/1/13/20	11/25/103/115	-
21	CLA	B	817	-	1/1/15/20	20/37/115/115	-
24	BCR	A	854	-	-	0/29/63/63	0/2/2/2
24	BCR	A	847	-	-	0/29/63/63	0/2/2/2
24	BCR	F	301	-	-	0/29/63/63	0/2/2/2
21	CLA	L	303	-	1/1/11/20	3/13/91/115	-
30	LUT	c	616	-	-	0/29/67/67	0/2/2/2
26	LMU	A	853	-	-	0/21/61/61	0/2/2/2
21	CLA	8	608	18	1/1/10/20	4/7/87/115	-
29	CHL	5	601	15	3/3/16/26	7/15/113/137	-
29	CHL	2	614	-	3/3/16/26	4/15/113/137	-
30	LUT	9	615	-	-	2/29/67/67	0/2/2/2
29	CHL	b	306	20	3/3/16/26	6/15/113/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	CLA	A	839	-	1/1/11/20	2/13/91/115	-
21	CLA	1	304	-	1/1/13/20	5/25/103/115	-
21	CLA	G	204	7	1/1/11/20	4/11/89/115	-
21	CLA	4	602	18	1/1/13/20	10/28/106/115	-
21	CLA	8	602	18	1/1/13/20	8/28/106/115	-
21	CLA	G	203	-	1/1/12/20	7/19/97/115	-
23	LHG	A	855	-	-	7/53/53/53	-
29	CHL	2	605	-	3/3/16/26	3/15/113/137	-
29	CHL	a	605	20	3/3/16/26	4/13/111/137	-
29	CHL	6	605	-	3/3/16/26	3/15/113/137	-
21	CLA	7	401	17	1/1/11/20	6/13/91/115	-
21	CLA	7	414	-	1/1/10/20	2/6/84/115	-
29	CHL	1	302	15	3/3/17/26	8/21/119/137	-
21	CLA	F	304	-	1/1/11/20	1/13/91/115	-
29	CHL	4	614	18	3/3/15/26	2/10/108/137	-
24	BCR	3	419	-	-	8/29/63/63	0/2/2/2
24	BCR	J	103	-	-	3/29/63/63	0/2/2/2
21	CLA	5	604	-	1/1/11/20	6/18/96/115	-
21	CLA	7	411	-	1/1/13/20	7/23/101/115	-
29	CHL	6	602	-	3/3/17/26	9/24/122/137	-
21	CLA	4	601	18	1/1/11/20	3/13/91/115	-
29	CHL	b	302	20	3/3/16/26	8/15/113/137	-
21	CLA	A	808	-	1/1/11/20	3/13/91/115	-
21	CLA	6	604	-	1/1/11/20	6/13/91/115	-
21	CLA	5	613	-	1/1/10/20	2/4/80/115	-
21	CLA	B	805	-	1/1/15/20	19/37/115/115	-
21	CLA	4	608	18	1/1/10/20	0/7/87/115	-
21	CLA	a	610	20	1/1/11/20	4/13/91/115	-
21	CLA	5	608	15	1/1/10/20	4/8/84/115	-
21	CLA	B	836	-	1/1/15/20	16/37/115/115	-
21	CLA	3	409	17	1/1/12/20	10/22/100/115	-
29	CHL	9	606	19	3/3/16/26	6/15/113/137	-
29	CHL	b	308	-	3/3/17/26	7/24/122/137	-
29	CHL	7	406	-	3/3/15/26	0/6/104/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	CLA	B	834	-	1/1/11/20	5/13/91/115	-
21	CLA	A	829	-	1/1/15/20	9/37/115/115	-
21	CLA	B	833	-	1/1/11/20	1/13/91/115	-
21	CLA	B	812	-	1/1/15/20	19/37/115/115	-
21	CLA	9	602	19	1/1/12/20	5/23/101/115	-
21	CLA	c	613	-	1/1/15/20	13/37/115/115	-
21	CLA	7	405	17	1/1/10/20	3/8/84/115	-
21	CLA	3	413	-	1/1/10/20	0/6/84/115	-
21	CLA	6	608	16	1/1/11/20	5/13/91/115	-
31	XAT	6	617	-	-	6/31/93/93	0/4/4/4
21	CLA	3	401	-	1/1/10/20	0/6/84/115	-
21	CLA	B	830	-	1/1/13/20	12/27/105/115	-
21	CLA	B	832	-	1/1/13/20	7/27/105/115	-
29	CHL	c	601	20	3/3/16/26	5/19/117/137	-
21	CLA	8	609	23	1/1/11/20	6/13/91/115	-
29	CHL	9	609	-	3/3/16/26	5/15/113/137	-
21	CLA	L	304	-	1/1/10/20	4/10/88/115	-
21	CLA	B	838	-	1/1/15/20	8/37/115/115	-
21	CLA	1	309	15	1/1/10/20	3/8/86/115	-
21	CLA	B	826	-	1/1/12/20	9/22/100/115	-
24	BCR	A	849	-	-	3/29/63/63	0/2/2/2
21	CLA	4	609	18	-	10/22/100/115	-
24	BCR	B	843	-	-	12/29/63/63	0/2/2/2
21	CLA	8	618	-	1/1/10/20	3/8/86/115	-
31	XAT	2	617	-	-	0/31/93/93	0/4/4/4
21	CLA	c	612	20	1/1/10/20	3/11/90/115	-
21	CLA	1	312	15	1/1/11/20	5/13/91/115	-
21	CLA	4	604	-	1/1/10/20	3/9/88/115	-
21	CLA	b	313	20	1/1/11/20	6/13/91/115	-
31	XAT	a	618	-	-	1/31/93/93	0/4/4/4
24	BCR	J	101	-	-	7/29/63/63	0/2/2/2
21	CLA	3	408	17	1/1/13/20	7/30/108/115	-
30	LUT	8	614	-	-	4/29/67/67	0/2/2/2
21	CLA	A	828	-	1/1/14/20	14/31/109/115	-
21	CLA	1	303	15	1/1/14/20	17/33/111/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	CHL	5	606	-	3/3/16/26	5/15/113/137	-
21	CLA	1	311	23	1/1/10/20	0/4/80/115	-
21	CLA	A	831	-	1/1/13/20	8/25/103/115	-
21	CLA	B	801	-	1/1/15/20	13/37/115/115	-
21	CLA	A	825	-	1/1/15/20	11/37/115/115	-
23	LHG	A	844	-	-	10/53/53/53	-
30	LUT	7	415	-	-	6/29/67/67	0/2/2/2
21	CLA	A	836	1	1/1/11/20	4/13/91/115	-
23	LHG	1	319	21	-	7/32/32/53	-
21	CLA	B	803	-	1/1/13/20	7/25/103/115	-
29	CHL	2	606	-	3/3/16/26	2/15/113/137	-
29	CHL	a	606	-	3/3/16/26	5/15/113/137	-
29	CHL	6	606	-	3/3/16/26	5/15/113/137	-
21	CLA	B	835	-	1/1/15/20	8/37/115/115	-
29	CHL	4	605	-	3/3/15/26	2/10/106/137	-
21	CLA	A	834	-	1/1/15/20	10/37/115/115	-
29	CHL	9	601	19	3/3/15/26	2/12/110/137	-
21	CLA	1	305	-	1/1/11/20	7/18/96/115	-
21	CLA	2	603	-	1/1/11/20	6/13/91/115	-
21	CLA	7	409	-	1/1/10/20	1/6/84/115	-
21	CLA	6	603	-	1/1/11/20	6/13/91/115	-
21	CLA	B	806	-	1/1/14/20	13/35/113/115	-
29	CHL	9	608	-	3/3/16/26	5/15/113/137	-
21	CLA	K	204	11	1/1/11/20	5/13/91/115	-
21	CLA	K	201	11	1/1/11/20	4/15/93/115	-
21	CLA	1	314	-	1/1/10/20	2/4/80/115	-
26	LMU	3	420	-	-	3/21/61/61	0/2/2/2
24	BCR	L	301	-	-	4/29/63/63	0/2/2/2
29	CHL	c	606	20	3/3/16/26	4/15/113/137	-
21	CLA	A	809	1	1/1/13/20	5/30/108/115	-
21	CLA	3	411	17	1/1/10/20	3/11/89/115	-
21	CLA	A	841	-	1/1/15/20	18/37/115/115	-
21	CLA	B	810	-	1/1/13/20	3/25/101/115	-
21	CLA	c	602	20	1/1/14/20	5/31/109/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	CLA	A	804	-	1/1/15/20	9/37/115/115	-
24	BCR	7	417	-	-	2/29/63/63	0/2/2/2
30	LUT	9	614	-	-	2/29/67/67	0/2/2/2
21	CLA	3	405	-	1/1/10/20	3/8/86/115	-
24	BCR	B	845	-	-	2/29/63/63	0/2/2/2
21	CLA	O	204	-	1/1/10/20	3/6/84/115	-
21	CLA	B	837	-	1/1/15/20	12/35/113/115	-
21	CLA	8	603	-	1/1/11/20	4/11/89/115	-
23	LHG	c	619	21	-	6/53/53/53	-
21	CLA	A	801	-	-	6/22/100/115	-
21	CLA	B	815	-	1/1/13/20	5/23/101/115	-
21	CLA	B	821	-	1/1/13/20	4/25/103/115	-
21	CLA	B	816	-	1/1/12/20	4/22/100/115	-
21	CLA	5	611	15	1/1/11/20	5/13/91/115	-
21	CLA	1	316	15	1/1/11/20	4/11/87/115	-
21	CLA	A	832	-	1/1/11/20	5/13/91/115	-
29	CHL	b	309	-	3/3/16/26	5/19/117/137	-
29	CHL	a	607	-	3/3/15/26	1/12/110/137	-
21	CLA	3	410	-	1/1/10/20	1/6/84/115	-
21	CLA	B	813	-	1/1/11/20	2/11/89/115	-
21	CLA	F	305	6	1/1/10/20	3/8/86/115	-
24	BCR	A	850	-	-	4/29/63/63	0/2/2/2
21	CLA	b	305	-	1/1/11/20	6/13/91/115	-
22	PQN	B	841	-	-	1/23/43/43	0/2/2/2
30	LUT	1	317	-	-	4/29/67/67	0/2/2/2
21	CLA	A	817	-	1/1/15/20	19/37/115/115	-
21	CLA	9	613	-	1/1/12/20	8/23/101/115	-
29	CHL	2	602	16	3/3/17/26	9/24/122/137	-
24	BCR	M	101	-	-	8/29/63/63	0/2/2/2
21	CLA	9	603	19	1/1/11/20	3/13/91/115	-
29	CHL	3	407	-	3/3/15/26	0/6/104/137	-
24	BCR	L	306	-	-	4/29/63/63	0/2/2/2
21	CLA	4	613	-	1/1/10/20	0/11/89/115	-
21	CLA	b	304	-	1/1/11/20	4/13/91/115	-
30	LUT	5	615	-	-	7/29/67/67	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	CLA	B	807	-	1/1/15/20	16/37/115/115	-
21	CLA	A	833	-	1/1/15/20	7/37/115/115	-
29	CHL	b	310	-	3/3/17/26	2/22/120/137	-
31	XAT	1	318	-	-	0/31/93/93	0/4/4/4
21	CLA	a	602	-	1/1/14/20	11/31/109/115	-
21	CLA	2	609	16	1/1/11/20	9/20/98/115	-
24	BCR	2	618	-	-	3/29/63/63	0/2/2/2
24	BCR	6	618	-	-	4/29/63/63	0/2/2/2
21	CLA	A	806	-	1/1/15/20	20/37/115/115	-
21	CLA	8	604	-	1/1/10/20	8/9/88/115	-
22	PQN	A	843	-	-	1/23/43/43	0/2/2/2
26	LMU	b	301	-	-	6/21/61/61	0/2/2/2
23	LHG	2	619	21	-	7/39/39/53	-
21	CLA	c	614	-	1/1/11/20	7/13/91/115	-
24	BCR	7	418	-	-	6/29/63/63	0/2/2/2
23	LHG	6	619	-	-	5/39/39/53	-
29	CHL	1	307	-	3/3/17/26	2/21/119/137	-
21	CLA	A	805	-	1/1/13/20	6/25/103/115	-
21	CLA	3	402	17	1/1/14/20	5/31/109/115	-
24	BCR	A	848	-	-	2/29/63/63	0/2/2/2
21	CLA	2	612	16	1/1/11/20	6/13/91/115	-
21	CLA	A	802	-	1/1/12/20	1/22/100/115	-
21	CLA	5	607	-	1/1/11/20	2/11/89/115	-
21	CLA	4	611	18	1/1/11/20	4/11/89/115	-
24	BCR	B	846	-	-	3/29/63/63	0/2/2/2
29	CHL	4	606	-	3/3/16/26	4/15/113/137	-
21	CLA	6	610	-	1/1/10/20	0/7/85/115	-
29	CHL	a	608	-	3/3/16/26	5/15/113/137	-
30	LUT	b	316	-	-	2/29/67/67	0/2/2/2
21	CLA	B	829	-	1/1/11/20	2/13/91/115	-
23	LHG	a	617	-	-	10/53/53/53	-
30	LUT	3	416	-	-	5/29/67/67	0/2/2/2
21	CLA	B	814	-	1/1/14/20	8/31/109/115	-
24	BCR	G	205	-	-	2/29/63/63	0/2/2/2
21	CLA	7	412	-	1/1/10/20	0/6/84/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	CLA	H	201	8	1/1/11/20	4/13/91/115	-
23	LHG	5	617	-	-	7/32/32/53	-
23	LHG	4	619	-	-	11/53/53/53	-
21	CLA	a	613	-	1/1/13/20	5/28/106/115	-
21	CLA	5	610	-	1/1/10/20	0/4/80/115	-
21	CLA	c	610	20	1/1/11/20	7/13/91/115	-
29	CHL	c	607	-	3/3/16/26	3/15/113/137	-
21	CLA	A	813	-	1/1/12/20	4/24/102/115	-
21	CLA	A	840	-	1/1/15/20	14/37/115/115	-
21	CLA	9	611	23	1/1/13/20	7/28/106/115	-
21	CLA	7	403	-	1/1/11/20	2/9/85/115	-
30	LUT	c	615	-	-	1/29/67/67	0/2/2/2
29	CHL	c	608	-	3/3/16/26	7/15/113/137	-
21	CLA	A	810	-	1/1/11/20	4/13/91/115	-
21	CLA	a	603	-	1/1/10/20	0/8/86/115	-
21	CLA	7	404	-	1/1/10/20	3/8/86/115	-
21	CLA	A	811	-	1/1/11/20	3/13/91/115	-
21	CLA	A	823	-	1/1/13/20	7/27/105/115	-
30	LUT	4	615	-	-	4/29/67/67	0/2/2/2
21	CLA	3	403	-	1/1/13/20	6/25/103/115	-
21	CLA	A	826	-	1/1/15/20	9/37/115/115	-
24	BCR	B	844	-	-	11/29/63/63	0/2/2/2
21	CLA	9	604	-	1/1/11/20	7/13/91/115	-
21	CLA	B	811	-	1/1/11/20	3/13/91/115	-
21	CLA	7	410	-	1/1/10/20	3/11/89/115	-
21	CLA	b	311	20	1/1/12/20	9/24/102/115	-
21	CLA	a	604	-	1/1/11/20	8/15/93/115	-
23	LHG	1	301	21	-	7/26/26/53	-
21	CLA	7	413	-	1/1/8/20	0/0/74/115	-
21	CLA	7	408	-	1/1/10/20	2/8/86/115	-
21	CLA	8	601	18	1/1/11/20	9/13/91/115	-
29	CHL	a	609	-	3/3/16/26	5/15/113/137	-
21	CLA	8	611	-	1/1/12/20	13/23/101/115	-
21	CLA	7	402	-	1/1/11/20	9/13/91/115	-
21	CLA	A	814	-	1/1/15/20	10/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	CLA	5	612	-	1/1/11/20	5/13/91/115	-
29	CHL	8	605	18	3/3/15/26	4/10/106/137	-
23	LHG	b	319	21	-	8/53/53/53	-
24	BCR	4	617	-	-	4/29/63/63	0/2/2/2
21	CLA	B	822	-	1/1/11/20	6/13/91/115	-
21	CLA	B	831	-	1/1/13/20	9/27/105/115	-
21	CLA	O	202	-	1/1/9/20	2/4/78/115	-
28	LMG	2	615	-	-	1/4/24/70	0/1/1/1
29	CHL	8	613	-	3/3/15/26	4/10/108/137	-
21	CLA	B	825	-	1/1/15/20	12/37/115/115	-
24	BCR	O	205	-	-	8/29/63/63	0/2/2/2
21	CLA	A	827	-	1/1/15/20	17/35/113/115	-
21	CLA	b	312	23	1/1/11/20	2/13/91/115	-
25	SF4	A	851	2,1	-	-	0/6/5/5
30	LUT	2	616	-	-	4/29/67/67	0/2/2/2
21	CLA	A	837	-	1/1/12/20	7/21/99/115	-
29	CHL	6	607	-	3/3/17/26	5/21/119/137	-
32	NEX	9	617	-	-	2/27/83/83	0/3/3/3
21	CLA	3	415	-	1/1/10/20	1/6/84/115	-
21	CLA	A	835	-	1/1/12/20	2/19/97/115	-
21	CLA	b	303	20	1/1/13/20	12/30/108/115	-
21	CLA	B	819	-	1/1/10/20	4/11/89/115	-
21	CLA	B	802	-	1/1/15/20	19/37/115/115	-
21	CLA	1	306	-	1/1/9/20	4/8/82/115	-
21	CLA	3	406	17	1/1/10/20	0/8/84/115	-
21	CLA	B	839	-	1/1/15/20	10/37/115/115	-
21	CLA	1	313	15	1/1/11/20	4/13/91/115	-
21	CLA	b	314	-	1/1/12/20	9/23/101/115	-
21	CLA	B	828	-	1/1/12/20	6/22/100/115	-
21	CLA	2	604	-	1/1/11/20	4/13/91/115	-
23	LHG	A	845	21	-	6/31/31/53	-
21	CLA	B	809	-	1/1/14/20	11/33/111/115	-
21	CLA	5	603	-	1/1/11/20	3/13/91/115	-
21	CLA	J	102	10	1/1/10/20	8/10/88/115	-
29	CHL	9	607	-	3/3/16/26	7/15/113/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	LMG	J	105	-	-	5/25/45/70	0/1/1/1
26	LMU	A	856	-	-	3/21/61/61	0/2/2/2
21	CLA	B	804	-	1/1/15/20	12/37/115/115	-
21	CLA	3	412	-	1/1/13/20	9/23/101/115	-
23	LHG	9	618	21	-	10/53/53/53	-
31	XAT	7	416	-	-	0/31/93/93	0/4/4/4
21	CLA	c	603	-	1/1/13/20	6/25/103/115	-
29	CHL	9	605	19	3/3/16/26	2/15/113/137	-
21	CLA	O	201	23	1/1/10/20	4/10/88/115	-
21	CLA	5	614	15	1/1/11/20	5/11/87/115	-
28	LMG	G	206	-	-	10/50/70/70	0/1/1/1
21	CLA	G	202	-	1/1/11/20	6/13/91/115	-
21	CLA	3	404	-	1/1/11/20	0/9/85/115	-
21	CLA	2	611	-	1/1/10/20	0/8/86/115	-
21	CLA	A	820	-	1/1/11/20	1/11/89/115	-
21	CLA	6	611	-	1/1/10/20	3/8/86/115	-
24	BCR	F	303	-	-	0/29/63/63	0/2/2/2
21	CLA	B	827	-	1/1/15/20	12/37/115/115	-
31	XAT	5	616	-	-	4/31/93/93	0/4/4/4
21	CLA	1	308	-	1/1/11/20	3/11/89/115	-
29	CHL	c	609	20	3/3/16/26	7/11/109/137	-
21	CLA	b	315	-	1/1/11/20	10/13/91/115	-
21	CLA	c	604	-	1/1/11/20	7/13/91/115	-
21	CLA	9	610	19	1/1/12/20	3/24/102/115	-
30	LUT	a	615	-	-	5/29/67/67	0/2/2/2
21	CLA	4	603	-	1/1/11/20	5/11/89/115	-
29	CHL	4	607	-	3/3/17/26	4/21/119/137	-
32	NEX	c	618	-	-	2/27/83/83	0/3/3/3
24	BCR	3	418	-	-	4/29/63/63	0/2/2/2
21	CLA	c	611	23	1/1/13/20	9/29/107/115	-
24	BCR	K	205	-	-	3/29/63/63	0/2/2/2
21	CLA	4	610	23	1/1/11/20	2/13/91/115	-
21	CLA	5	602	15	1/1/14/20	17/33/111/115	-
21	CLA	B	820	-	1/1/11/20	3/15/93/115	-
23	LHG	4	618	21	-	9/41/41/53	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	CLA	6	612	-	1/1/11/20	5/13/91/115	-
21	CLA	2	613	-	1/1/10/20	1/10/88/115	-
21	CLA	1	310	15	1/1/11/20	3/9/87/115	-
21	CLA	A	807	1	1/1/15/20	11/37/115/115	-
21	CLA	6	613	-	1/1/10/20	4/10/88/115	-
24	BCR	B	842	-	-	0/29/63/63	0/2/2/2
24	BCR	A	846	-	-	4/29/63/63	0/2/2/2
21	CLA	2	608	16	1/1/13/20	8/25/103/115	-
21	CLA	A	838	-	1/1/15/20	13/37/115/115	-
24	BCR	G	201	-	-	0/29/63/63	0/2/2/2
26	LMU	O	206	-	-	5/21/61/61	0/2/2/2
21	CLA	A	812	-	1/1/15/20	5/37/115/115	-
27	DGD	B	847	-	-	16/55/95/95	0/2/2/2
24	BCR	J	104	-	-	9/29/63/63	0/2/2/2
32	NEX	b	318	-	-	2/27/83/83	0/3/3/3
21	CLA	9	612	19	1/1/11/20	4/13/91/115	-
29	CHL	8	607	-	3/3/17/26	5/21/119/137	-
21	CLA	K	202	-	1/1/12/20	2/19/97/115	-
21	CLA	B	824	-	1/1/15/20	10/37/115/115	-
29	CHL	6	614	-	3/3/16/26	5/15/113/137	-
29	CHL	2	607	-	3/3/17/26	4/21/119/137	-
30	LUT	a	616	-	-	4/29/67/67	0/2/2/2
24	BCR	8	616	-	-	6/29/63/63	0/2/2/2
24	BCR	I	101	-	-	4/29/63/63	0/2/2/2
21	CLA	A	821	-	1/1/15/20	11/37/115/115	-
21	CLA	8	612	-	1/1/10/20	3/11/89/115	-
24	BCR	L	305	-	-	2/29/63/63	0/2/2/2
21	CLA	A	830	-	1/1/12/20	4/22/100/115	-
25	SF4	C	102	3	-	-	0/6/5/5
21	CLA	4	612	-	1/1/13/20	5/25/103/115	-
21	CLA	3	414	-	1/1/8/20	0/0/74/115	-
21	CLA	7	407	17	-	5/11/89/115	-
29	CHL	c	605	-	3/3/15/26	3/9/107/137	-
21	CLA	A	842	-	1/1/15/20	14/37/115/115	-
29	CHL	b	307	-	3/3/16/26	3/15/113/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	CLA	A	852	-	1/1/12/20	6/22/100/115	-
21	CLA	a	614	-	1/1/10/20	2/8/86/115	-
28	LMG	6	615	-	-	3/4/24/70	0/1/1/1
21	CLA	A	818	-	1/1/12/20	8/22/100/115	-
31	XAT	c	617	-	-	1/31/93/93	0/4/4/4
21	CLA	L	302	12	1/1/11/20	7/13/91/115	-
21	CLA	A	816	-	1/1/10/20	3/10/88/115	-
21	CLA	8	610	-	1/1/11/20	6/11/89/115	-
21	CLA	6	609	-	1/1/10/20	5/10/88/115	-
21	CLA	2	610	23	1/1/10/20	1/7/85/115	-
21	CLA	5	605	-	1/1/9/20	4/8/82/115	-
21	CLA	a	611	-	1/1/11/20	6/16/94/115	-
21	CLA	B	823	-	1/1/15/20	12/37/115/115	-
30	LUT	b	317	-	-	2/29/67/67	0/2/2/2
21	CLA	O	203	-	1/1/11/20	4/17/95/115	-
25	SF4	C	101	3	-	-	0/6/5/5
21	CLA	B	808	2	1/1/15/20	7/37/115/115	-
21	CLA	B	818	-	1/1/13/20	9/29/107/115	-
29	CHL	a	601	20	3/3/16/26	4/15/113/137	-
21	CLA	A	803	-	1/1/12/20	7/22/100/115	-
29	CHL	2	601	16	3/3/17/26	10/24/122/137	-
29	CHL	6	601	16	3/3/16/26	6/11/109/137	-
21	CLA	B	840	23	1/1/15/20	6/37/115/115	-
21	CLA	A	819	-	1/1/15/20	16/37/115/115	-
23	LHG	8	617	21	-	9/41/41/53	-
31	XAT	3	417	-	-	0/31/93/93	0/4/4/4
21	CLA	A	815	-	1/1/11/20	5/13/91/115	-
31	XAT	9	616	-	-	8/31/93/93	0/4/4/4
21	CLA	a	612	-	1/1/11/20	5/13/91/115	-
31	XAT	8	615	-	-	0/31/93/93	0/4/4/4
21	CLA	A	822	-	1/1/11/20	1/11/89/115	-
21	CLA	F	302	-	1/1/14/20	8/33/111/115	-
30	LUT	6	616	-	-	2/29/67/67	0/2/2/2
21	CLA	5	609	-	1/1/11/20	3/9/87/115	-
21	CLA	1	315	-	1/1/11/20	4/13/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	CLA	K	203	-	1/1/11/20	2/13/89/115	-

The worst 5 of 2580 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	7	412	CLA	C4B-NB	8.30	1.42	1.35
21	A	818	CLA	C4B-NB	8.22	1.42	1.35
21	7	407	CLA	C1D-ND	8.02	1.47	1.37
21	6	603	CLA	C4B-NB	7.91	1.42	1.35
21	B	811	CLA	C4B-NB	7.88	1.42	1.35

The worst 5 of 3657 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	7	407	CLA	CAC-C3C-C4C	16.81	146.62	124.81
21	7	407	CLA	C1D-ND-C4D	-10.68	98.75	106.33
29	a	601	CHL	C1D-ND-C4D	10.07	113.49	106.33
29	9	601	CHL	C1D-ND-C4D	10.04	113.47	106.33
29	c	609	CHL	C1D-ND-C4D	10.00	113.44	106.33

5 of 368 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
21	A	802	CLA	ND
21	A	803	CLA	ND
21	A	804	CLA	ND
21	A	805	CLA	ND
21	A	806	CLA	ND

5 of 1981 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
21	A	801	CLA	CBD-CGD-O2D-CED
21	A	804	CLA	C1A-C2A-CAA-CBA
21	A	805	CLA	C3A-C2A-CAA-CBA
21	A	806	CLA	CHA-CBD-CGD-O1D
21	A	806	CLA	CHA-CBD-CGD-O2D

There are no ring outliers.

277 monomers are involved in 815 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
29	8	606	CHL	2	0
31	4	616	XAT	4	0
21	A	824	CLA	3	0
21	B	817	CLA	7	0
24	A	854	BCR	13	0
24	A	847	BCR	3	0
24	F	301	BCR	2	0
21	L	303	CLA	1	0
21	8	608	CLA	2	0
29	5	601	CHL	3	0
29	2	614	CHL	5	0
30	9	615	LUT	6	0
21	A	839	CLA	2	0
21	1	304	CLA	4	0
21	G	204	CLA	1	0
21	4	602	CLA	5	0
21	8	602	CLA	4	0
23	A	855	LHG	4	0
29	6	605	CHL	1	0
21	7	401	CLA	7	0
21	7	414	CLA	1	0
29	1	302	CHL	2	0
21	F	304	CLA	2	0
29	4	614	CHL	1	0
24	3	419	BCR	1	0
24	J	103	BCR	3	0
21	5	604	CLA	2	0
21	7	411	CLA	2	0
29	6	602	CHL	3	0
21	4	601	CLA	2	0
21	A	808	CLA	3	0
21	6	604	CLA	9	0
21	5	613	CLA	1	0
21	B	805	CLA	5	0
21	4	608	CLA	1	0
21	5	608	CLA	2	0
21	B	836	CLA	5	0
21	3	409	CLA	22	0
29	9	606	CHL	1	0
29	7	406	CHL	2	0
21	B	834	CLA	2	0
21	A	829	CLA	2	0
21	B	812	CLA	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
21	9	602	CLA	2	0
21	3	413	CLA	2	0
21	6	608	CLA	3	0
31	6	617	XAT	9	0
21	3	401	CLA	2	0
21	B	830	CLA	3	0
21	B	832	CLA	5	0
21	8	609	CLA	25	0
29	9	609	CHL	5	0
21	L	304	CLA	2	0
21	B	838	CLA	2	0
21	1	309	CLA	11	0
21	B	826	CLA	2	0
24	A	849	BCR	4	0
21	4	609	CLA	16	0
24	B	843	BCR	20	0
21	8	618	CLA	2	0
31	2	617	XAT	2	0
21	1	312	CLA	2	0
24	J	101	BCR	5	0
21	3	408	CLA	8	0
30	8	614	LUT	5	0
21	A	828	CLA	5	0
21	1	303	CLA	2	0
29	5	606	CHL	3	0
21	A	831	CLA	1	0
21	B	801	CLA	8	0
21	A	825	CLA	4	0
23	A	844	LHG	2	0
30	7	415	LUT	14	0
21	A	836	CLA	1	0
21	B	803	CLA	2	0
29	2	606	CHL	2	0
29	6	606	CHL	1	0
21	B	835	CLA	2	0
21	A	834	CLA	5	0
29	9	601	CHL	3	0
21	2	603	CLA	2	0
21	6	603	CLA	4	0
21	B	806	CLA	2	0
29	9	608	CHL	1	0
21	K	204	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
21	K	201	CLA	5	0
21	1	314	CLA	1	0
26	3	420	LMU	4	0
24	L	301	BCR	3	0
21	A	809	CLA	1	0
21	3	411	CLA	1	0
21	A	841	CLA	4	0
21	B	810	CLA	1	0
21	A	804	CLA	3	0
24	7	417	BCR	8	0
30	9	614	LUT	3	0
21	3	405	CLA	1	0
24	B	845	BCR	3	0
21	B	837	CLA	6	0
21	8	603	CLA	2	0
21	A	801	CLA	2	0
21	B	815	CLA	3	0
21	B	821	CLA	1	0
21	B	816	CLA	3	0
21	5	611	CLA	1	0
21	A	832	CLA	2	0
21	B	813	CLA	3	0
21	F	305	CLA	2	0
24	A	850	BCR	1	0
22	B	841	PQN	3	0
30	1	317	LUT	3	0
21	A	817	CLA	4	0
21	9	613	CLA	2	0
29	2	602	CHL	3	0
24	M	101	BCR	3	0
21	9	603	CLA	1	0
29	3	407	CHL	2	0
24	L	306	BCR	3	0
21	4	613	CLA	3	0
30	5	615	LUT	2	0
21	B	807	CLA	6	0
21	A	833	CLA	6	0
31	1	318	XAT	3	0
21	2	609	CLA	24	0
24	2	618	BCR	6	0
24	6	618	BCR	14	0
21	A	806	CLA	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
21	8	604	CLA	4	0
23	2	619	LHG	1	0
24	7	418	BCR	4	0
23	6	619	LHG	3	0
29	1	307	CHL	6	0
21	A	805	CLA	5	0
21	3	402	CLA	1	0
21	A	802	CLA	4	0
21	5	607	CLA	3	0
21	4	611	CLA	2	0
24	B	846	BCR	5	0
29	4	606	CHL	1	0
21	6	610	CLA	3	0
21	B	829	CLA	2	0
30	3	416	LUT	12	0
21	B	814	CLA	4	0
24	G	205	BCR	2	0
21	7	412	CLA	1	0
21	H	201	CLA	2	0
23	5	617	LHG	1	0
23	4	619	LHG	1	0
21	5	610	CLA	1	0
21	A	813	CLA	2	0
21	A	840	CLA	8	0
21	9	611	CLA	5	0
21	A	810	CLA	4	0
21	7	404	CLA	4	0
21	A	823	CLA	1	0
30	4	615	LUT	7	0
21	3	403	CLA	1	0
21	A	826	CLA	2	0
24	B	844	BCR	8	0
21	9	604	CLA	2	0
21	B	811	CLA	1	0
21	7	410	CLA	2	0
21	7	413	CLA	1	0
21	7	408	CLA	5	0
21	8	611	CLA	5	0
21	7	402	CLA	9	0
21	A	814	CLA	2	0
21	5	612	CLA	1	0
29	8	605	CHL	5	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
21	B	822	CLA	3	0
21	B	831	CLA	6	0
21	O	202	CLA	1	0
29	8	613	CHL	4	0
21	B	825	CLA	3	0
24	O	205	BCR	1	0
21	A	827	CLA	7	0
30	2	616	LUT	8	0
21	A	837	CLA	3	0
29	6	607	CHL	5	0
32	9	617	NEX	3	0
21	3	415	CLA	3	0
21	A	835	CLA	3	0
21	B	819	CLA	1	0
21	B	802	CLA	3	0
21	1	306	CLA	3	0
21	3	406	CLA	1	0
21	B	839	CLA	5	0
21	1	313	CLA	1	0
21	B	828	CLA	3	0
21	2	604	CLA	3	0
23	A	845	LHG	1	0
21	B	809	CLA	4	0
21	5	603	CLA	4	0
21	J	102	CLA	1	0
29	9	607	CHL	2	0
26	A	856	LMU	2	0
21	B	804	CLA	2	0
21	3	412	CLA	1	0
23	9	618	LHG	4	0
31	7	416	XAT	5	0
29	9	605	CHL	2	0
21	O	201	CLA	1	0
21	5	614	CLA	1	0
28	G	206	LMG	3	0
21	G	202	CLA	2	0
21	3	404	CLA	4	0
21	2	611	CLA	1	0
21	A	820	CLA	1	0
21	6	611	CLA	1	0
24	F	303	BCR	1	0
21	B	827	CLA	12	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
31	5	616	XAT	7	0
21	1	308	CLA	2	0
21	9	610	CLA	2	0
21	4	603	CLA	1	0
29	4	607	CHL	4	0
24	3	418	BCR	7	0
24	K	205	BCR	23	0
21	5	602	CLA	12	0
21	B	820	CLA	1	0
23	4	618	LHG	5	0
21	6	612	CLA	3	0
21	2	613	CLA	2	0
21	1	310	CLA	1	0
21	A	807	CLA	2	0
21	6	613	CLA	2	0
24	B	842	BCR	3	0
24	A	846	BCR	1	0
21	2	608	CLA	4	0
21	A	838	CLA	4	0
24	G	201	BCR	5	0
21	A	812	CLA	6	0
27	B	847	DGD	7	0
24	J	104	BCR	8	0
21	9	612	CLA	1	0
29	8	607	CHL	6	0
21	K	202	CLA	1	0
21	B	824	CLA	3	0
29	6	614	CHL	4	0
29	2	607	CHL	3	0
24	8	616	BCR	9	0
24	I	101	BCR	1	0
21	A	821	CLA	6	0
21	8	612	CLA	2	0
24	L	305	BCR	2	0
21	A	830	CLA	3	0
21	4	612	CLA	1	0
21	7	407	CLA	18	0
21	A	842	CLA	6	0
21	A	852	CLA	8	0
28	6	615	LMG	1	0
21	A	818	CLA	6	0
21	L	302	CLA	2	0

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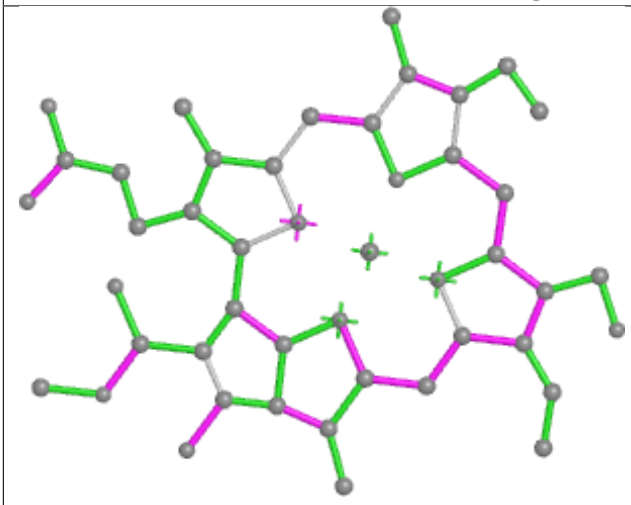
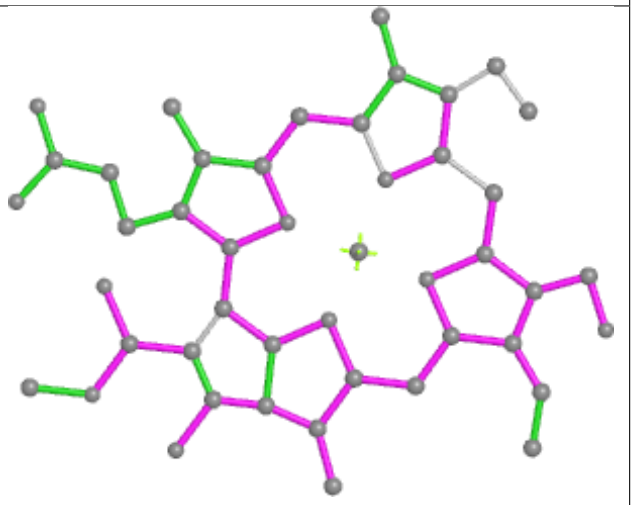
Mol	Chain	Res	Type	Clashes	Symm-Clashes
21	A	816	CLA	2	0
21	8	610	CLA	1	0
21	6	609	CLA	3	0
21	2	610	CLA	3	0
21	5	605	CLA	2	0
21	B	823	CLA	4	0
21	O	203	CLA	1	0
21	B	808	CLA	3	0
21	B	818	CLA	2	0
21	A	803	CLA	3	0
29	2	601	CHL	3	0
29	6	601	CHL	3	0
21	B	840	CLA	1	0
21	A	819	CLA	6	0
23	8	617	LHG	3	0
31	3	417	XAT	4	0
31	9	616	XAT	2	0
31	8	615	XAT	5	0
21	A	822	CLA	3	0
21	F	302	CLA	1	0
30	6	616	LUT	6	0
21	5	609	CLA	1	0
21	1	315	CLA	2	0
21	K	203	CLA	8	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.

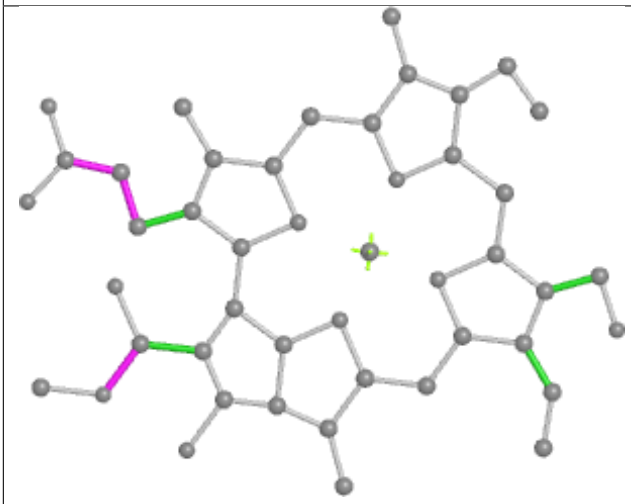
Ligand CHL 8 606



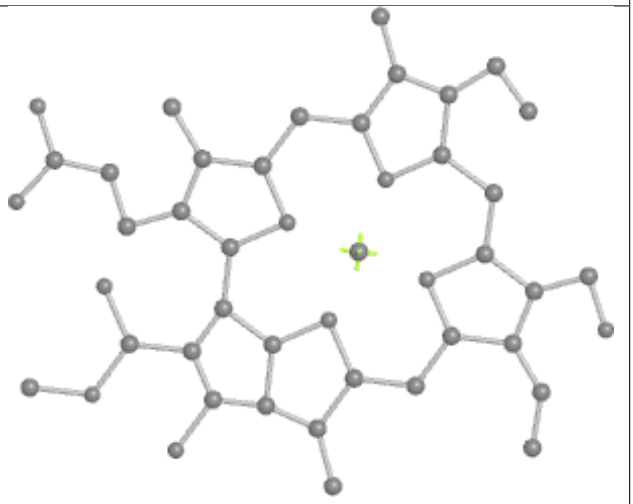
Bond lengths



Bond angles

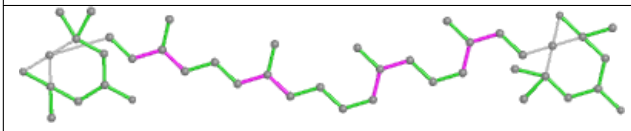


Torsions

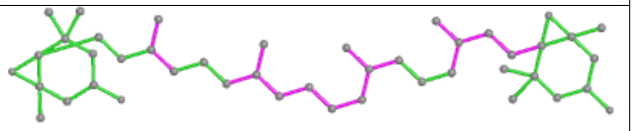


Rings

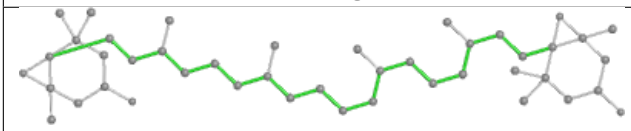
Ligand XAT 4 616



Bond lengths



Bond angles



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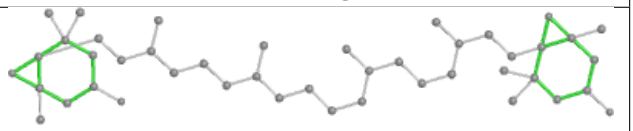
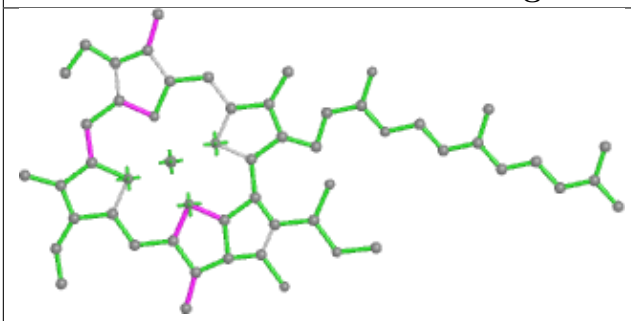


Rings

Ligand CLA A 824



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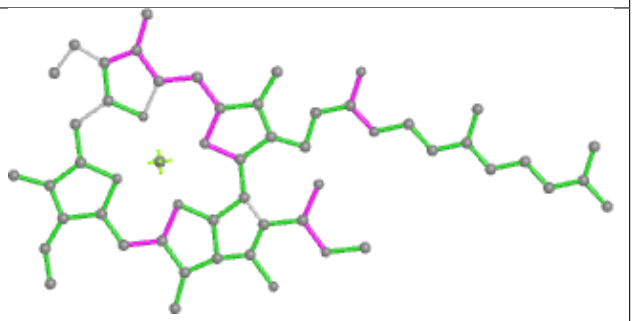
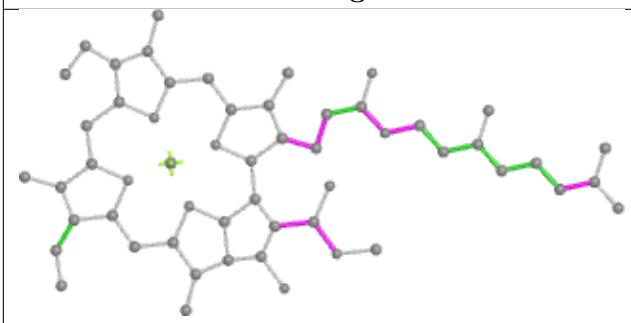


Bond angles



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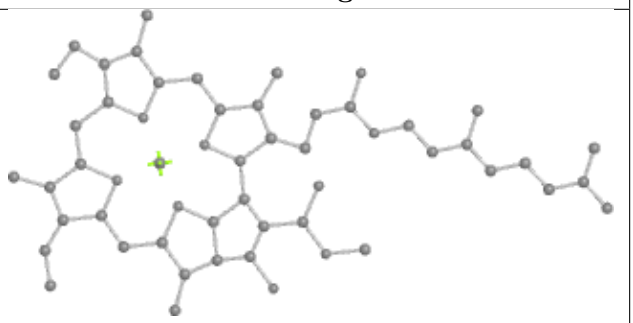
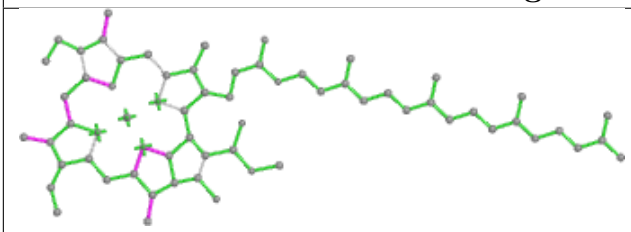


Rings

Ligand CLA B 817



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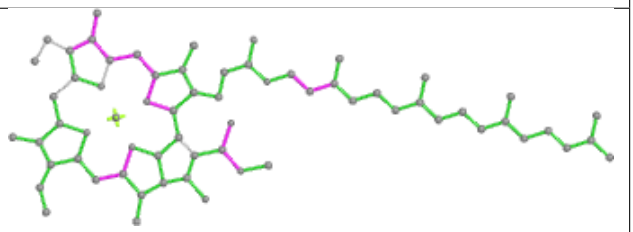
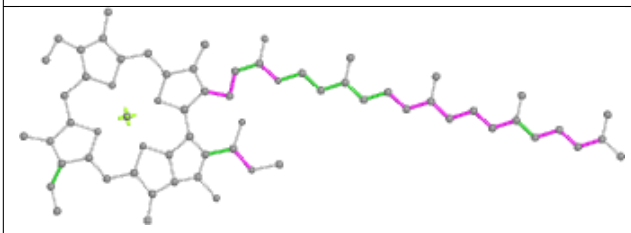


Bond angles



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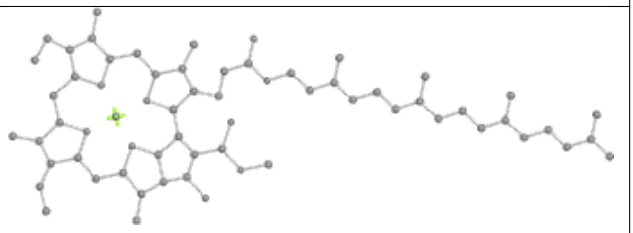
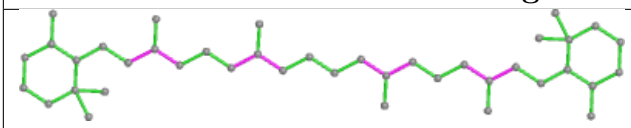


Rings

Ligand BCR A 854



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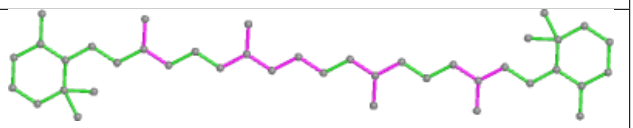

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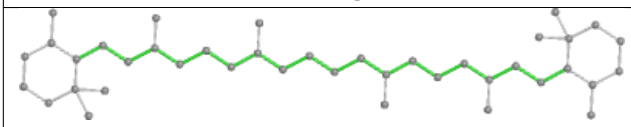

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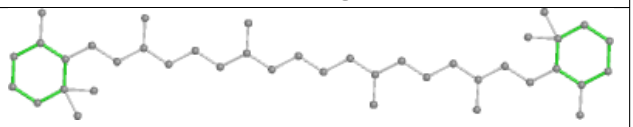

Rings

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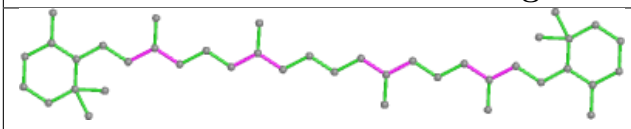
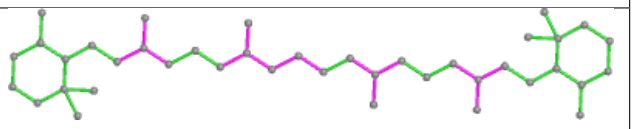
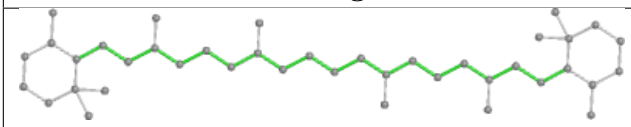
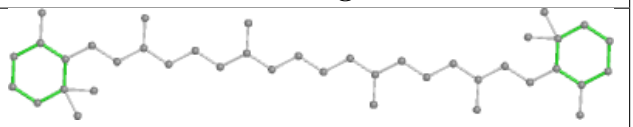
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

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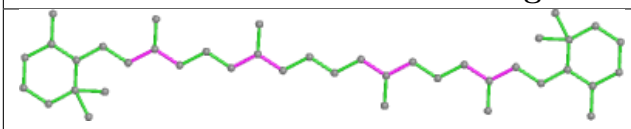
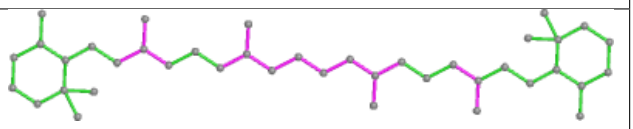
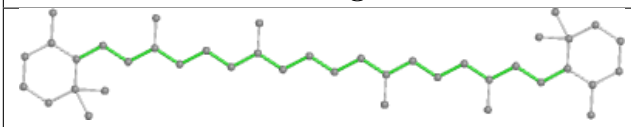
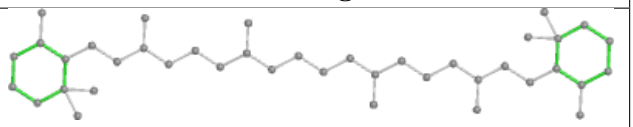
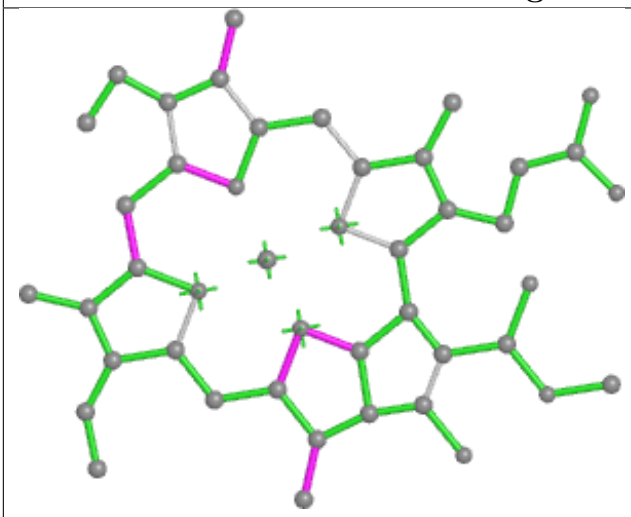
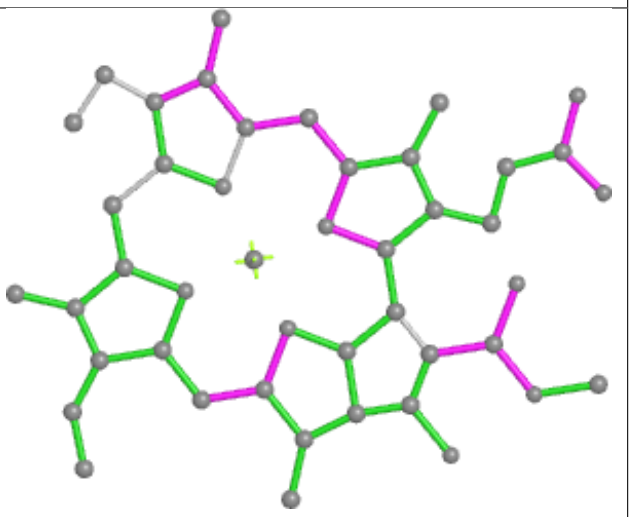
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

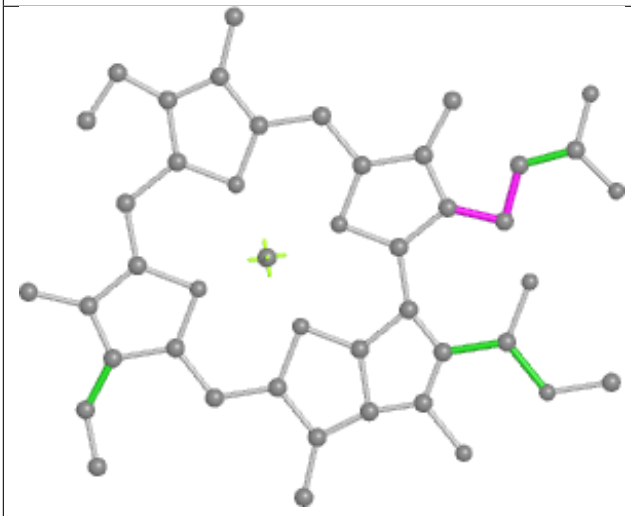
Ligand CLA L 303



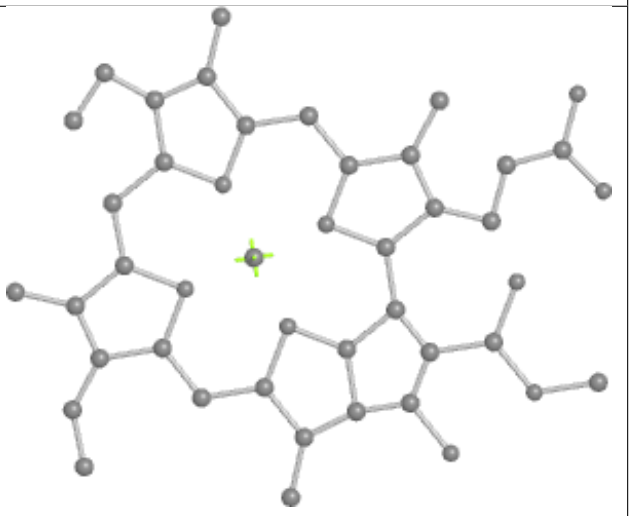
Bond lengths



Bond angles

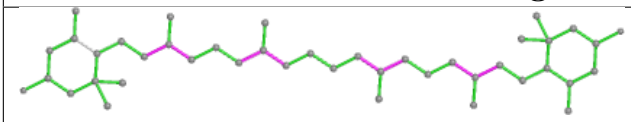


Torsions



Rings

Ligand LUT c 616



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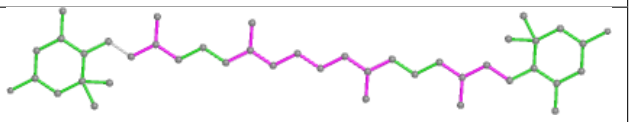
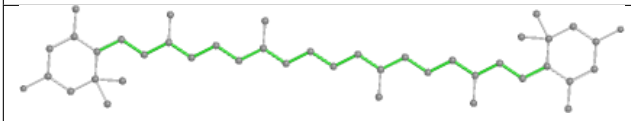


Bond angles



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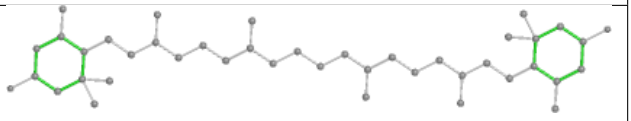
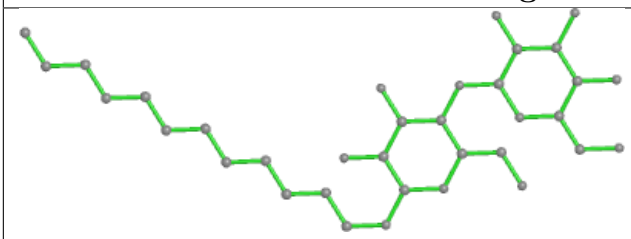


Rings

Ligand LMU A 853



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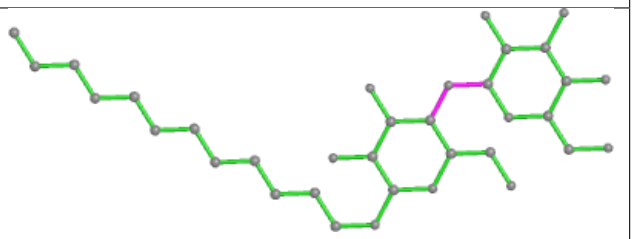
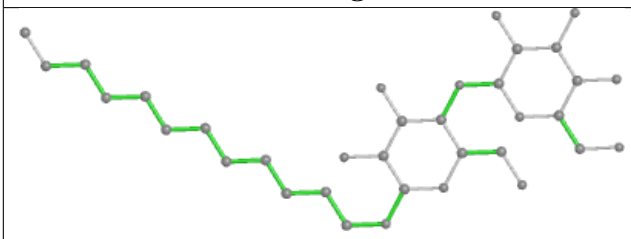


Bond angles



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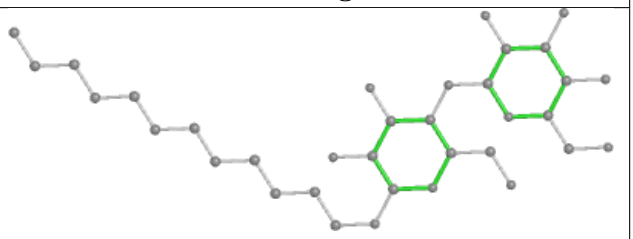
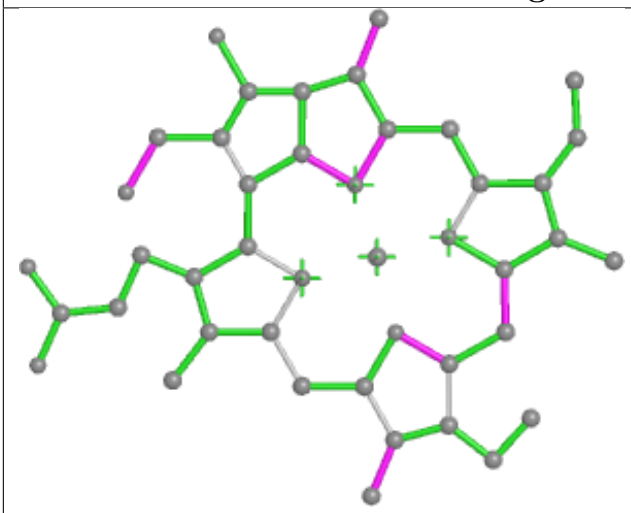
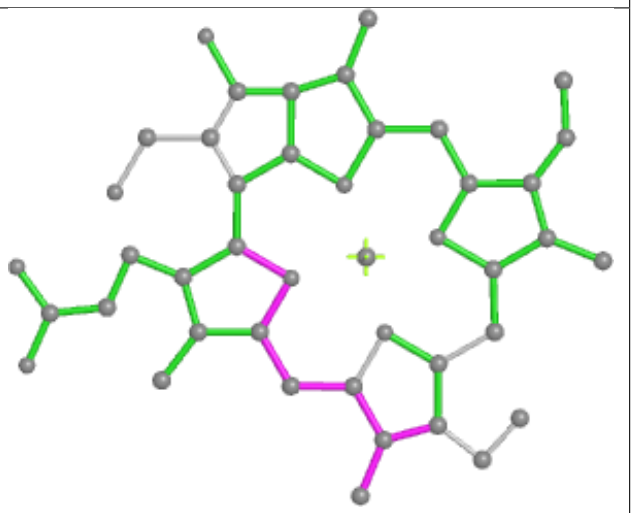


Rings

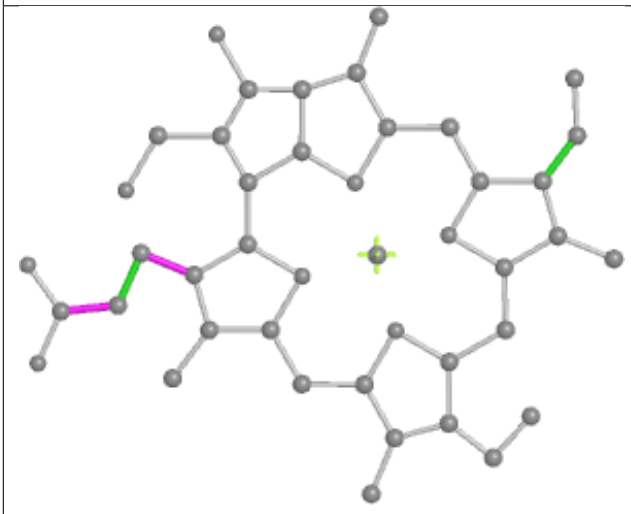
Ligand CLA 8 608



Bond lengths



Bond angles



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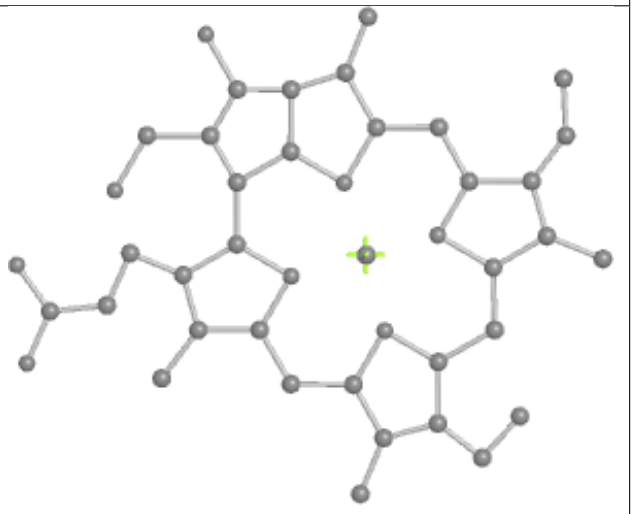
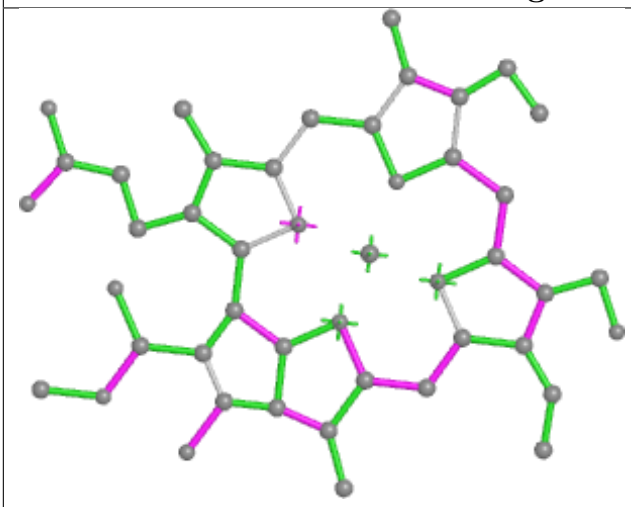


Rings

Ligand CHL 5 601



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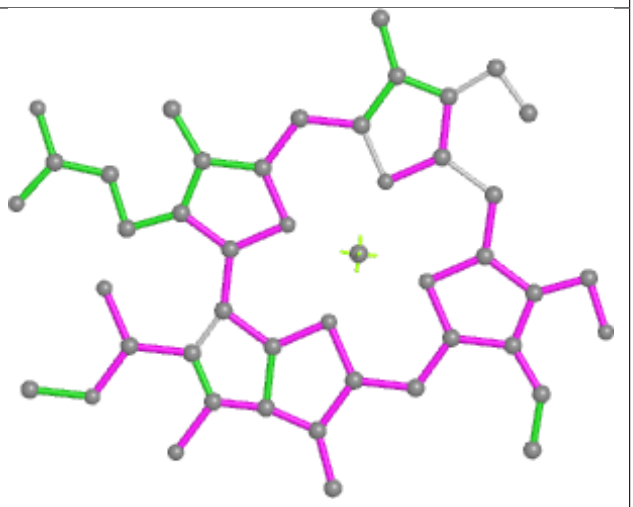

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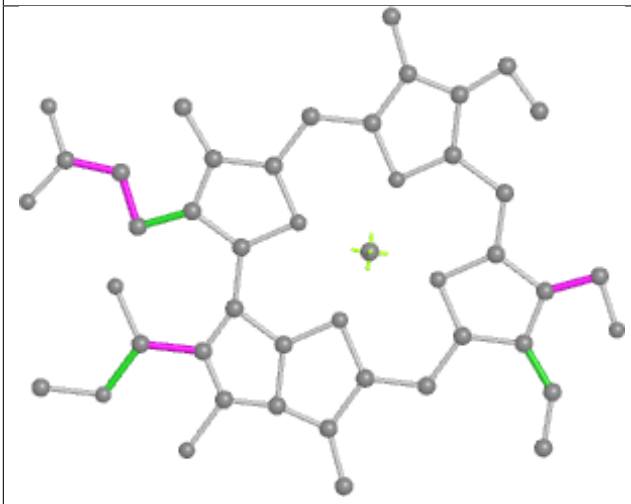

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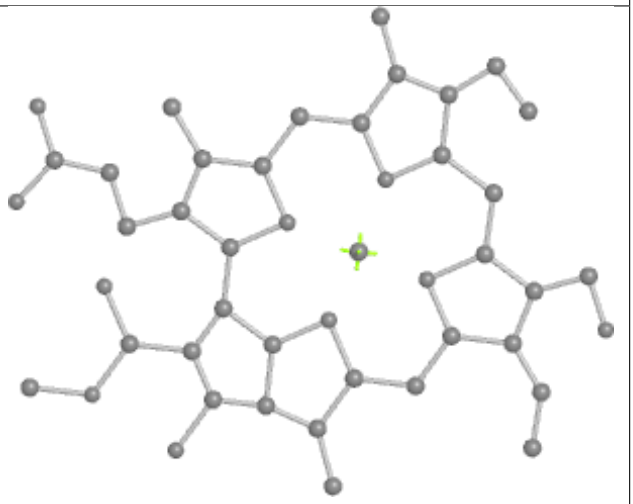
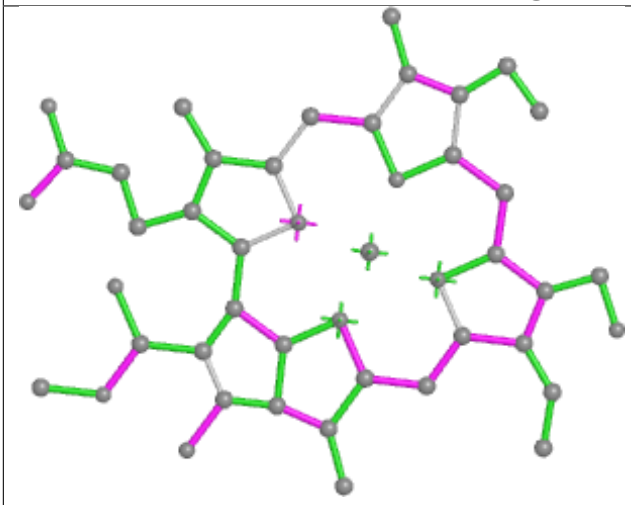


Rings

Ligand CHL 2 614



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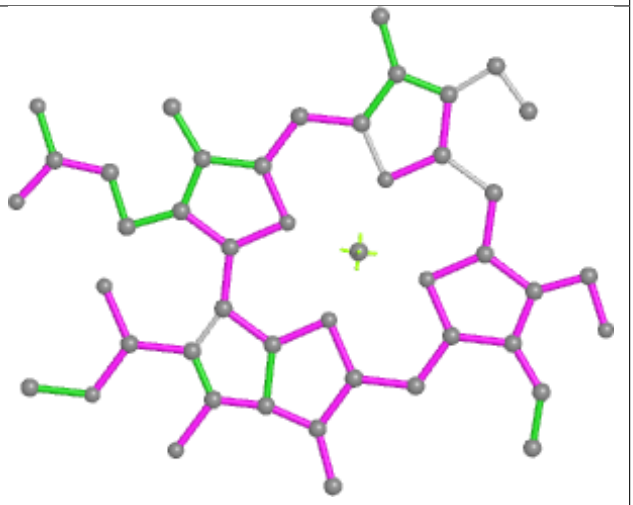

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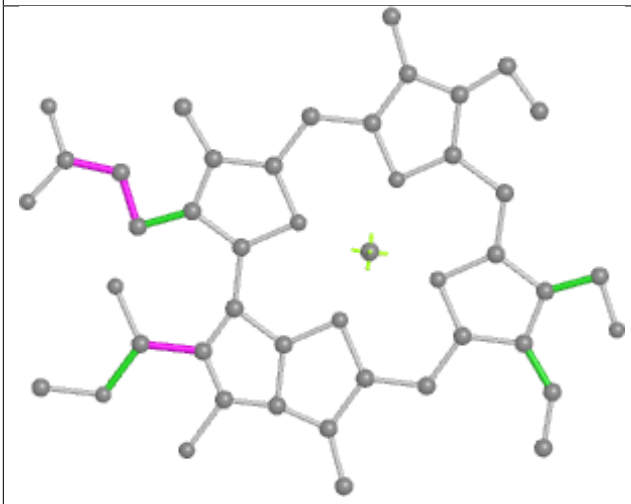

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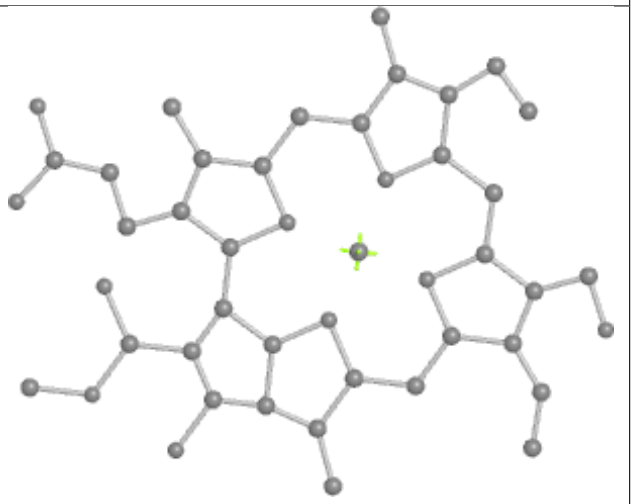
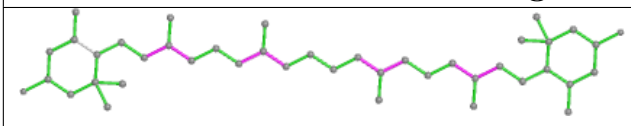


Rings

Ligand LUT 9 615



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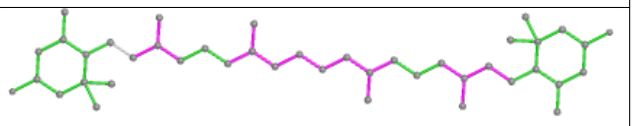

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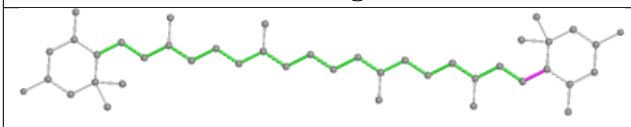

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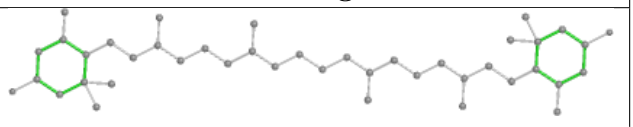
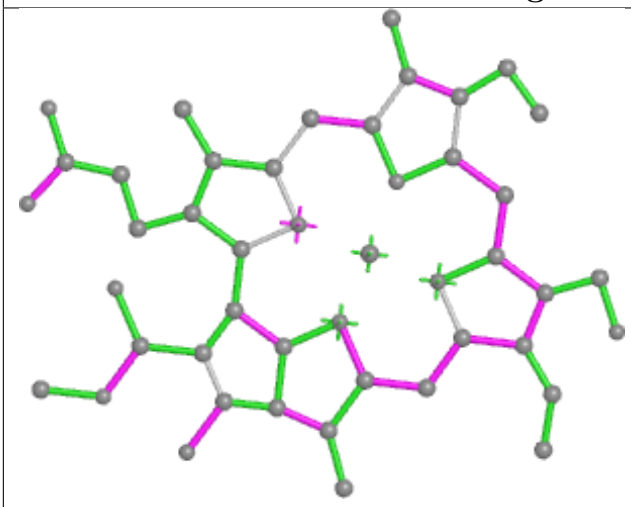


Rings

Ligand CHL b 306



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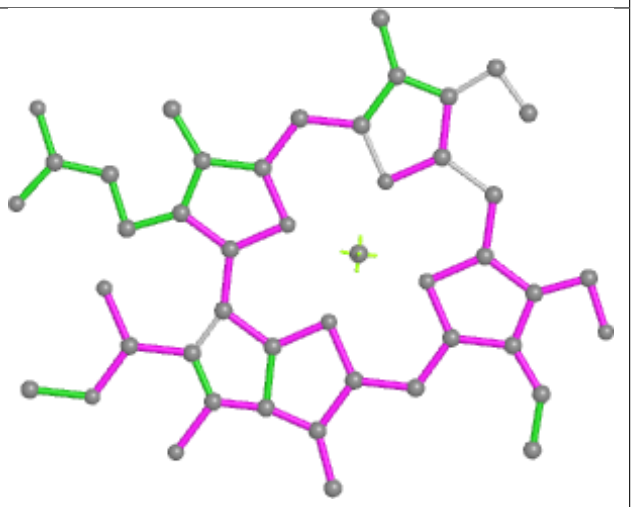

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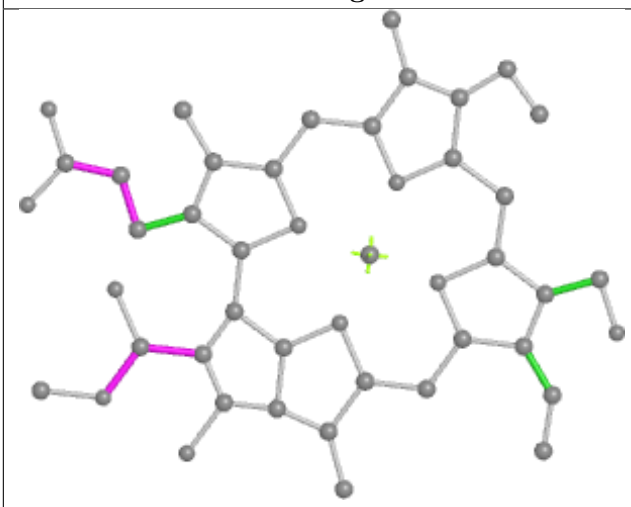

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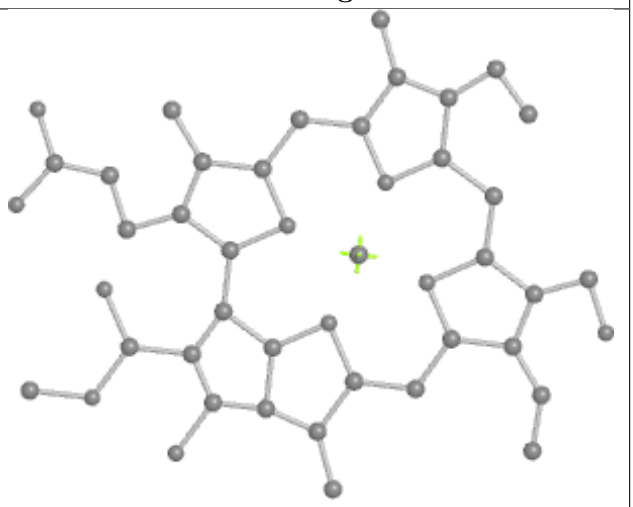
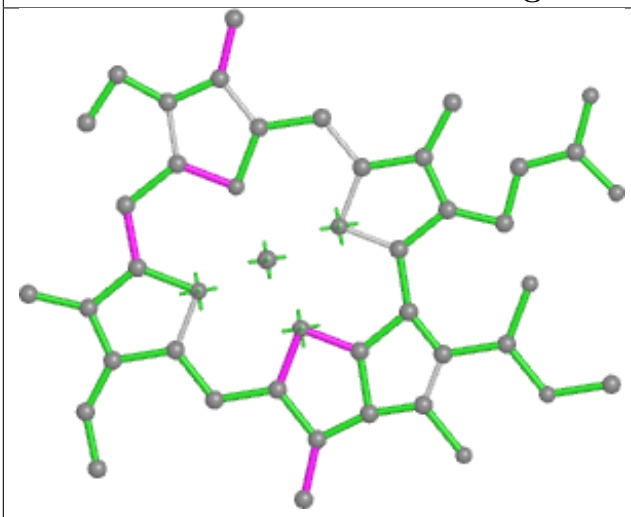


Rings

Ligand CLA A 839



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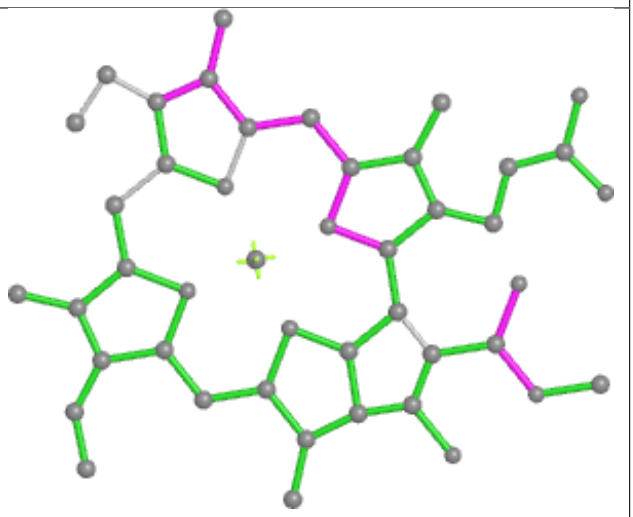

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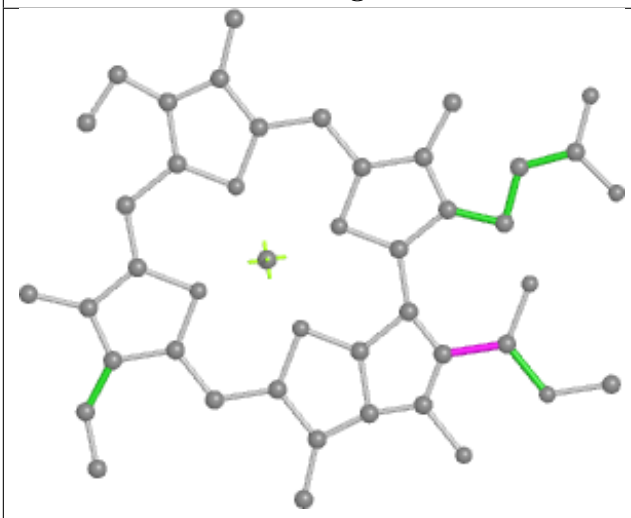

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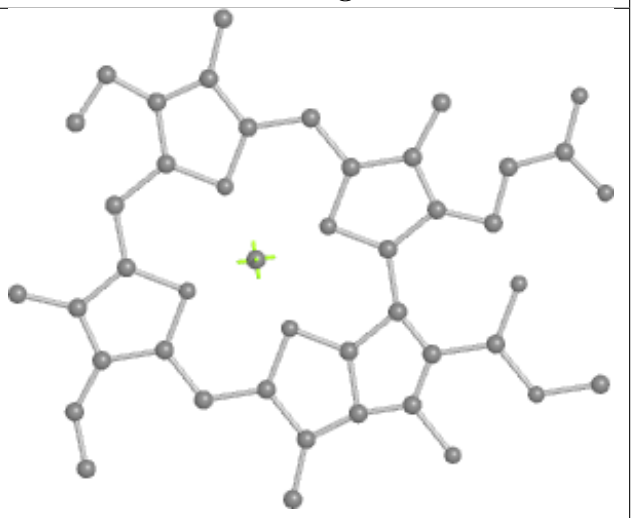
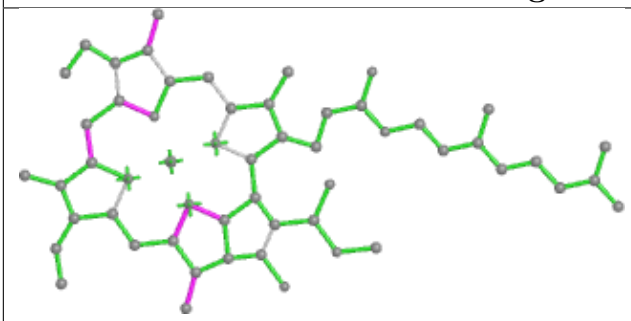


Rings

Ligand CLA 1 304



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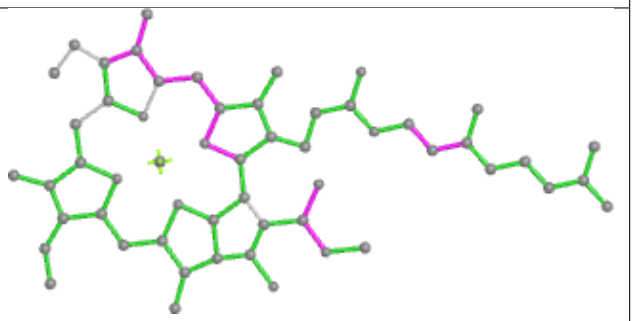

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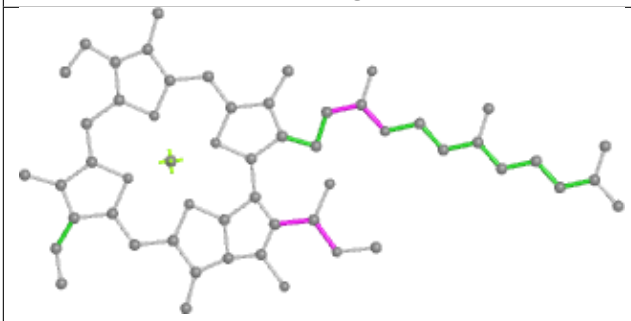

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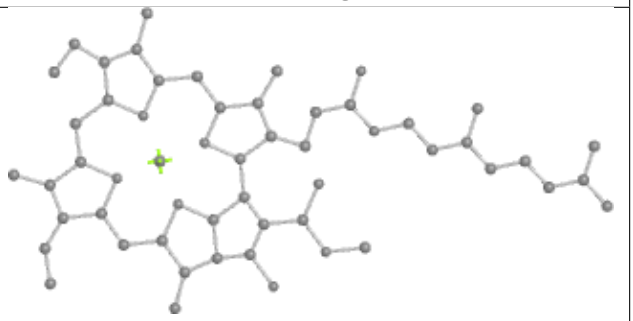
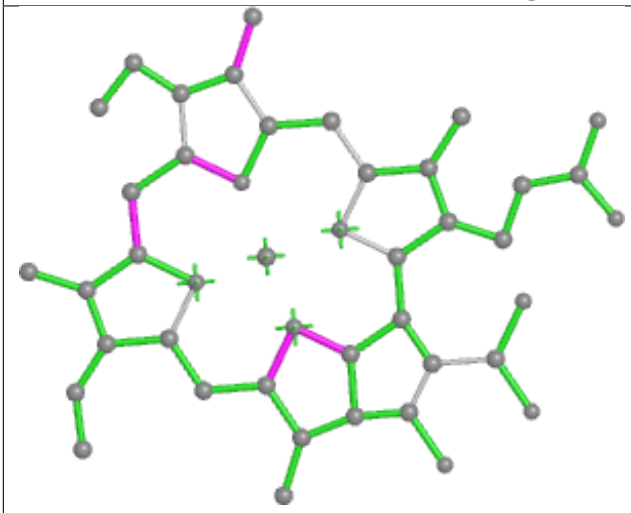


Rings

Ligand CLA G 204



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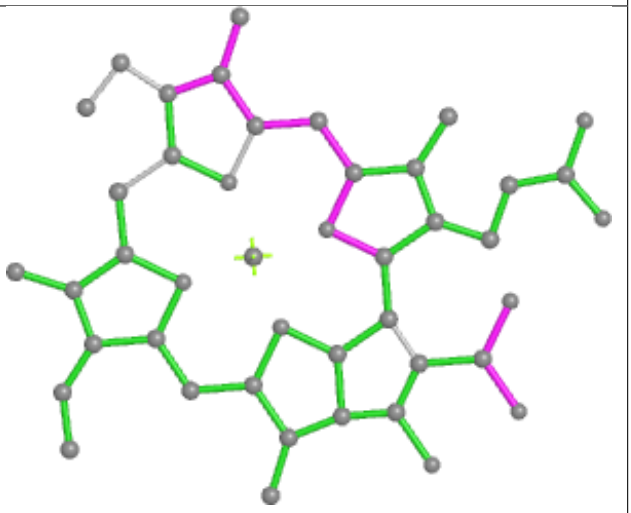
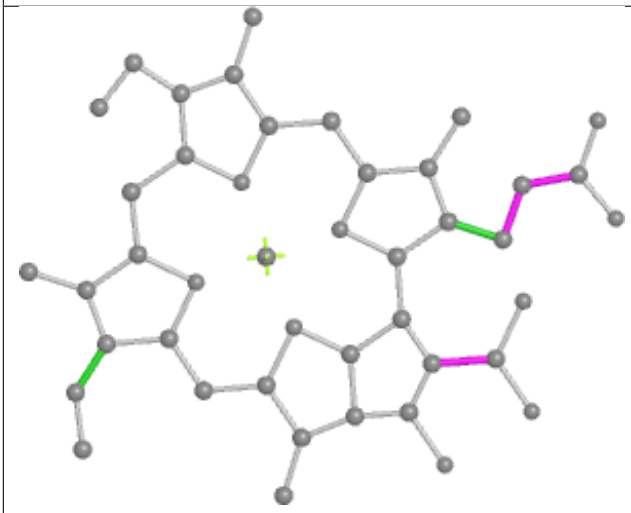


Bond angles



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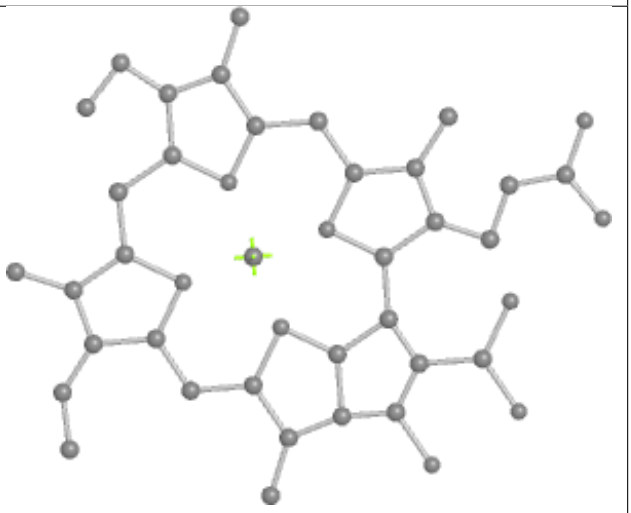
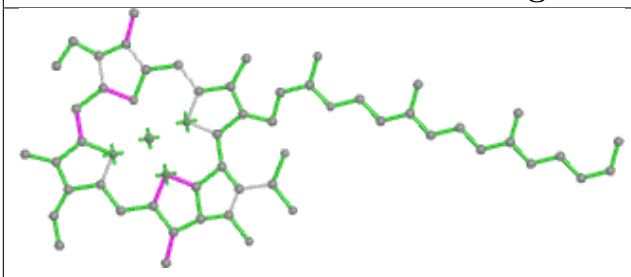
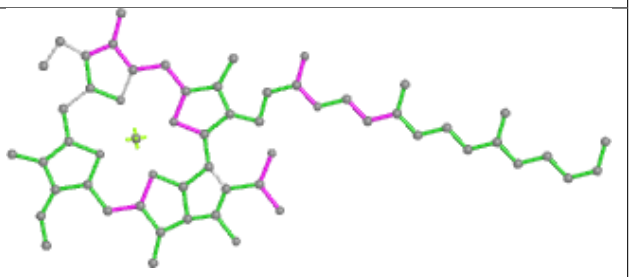
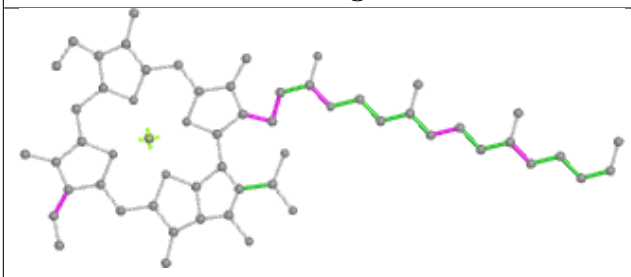
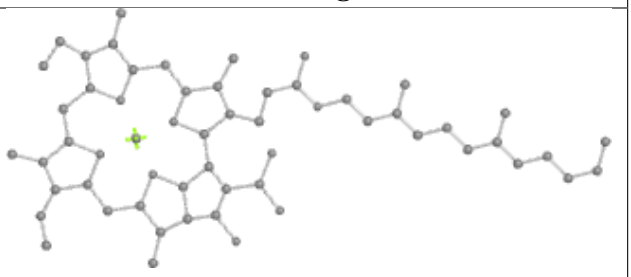


Rings

Ligand CLA 4 602	
 Bond lengths	 Bond angles
 Torsions	 Rings

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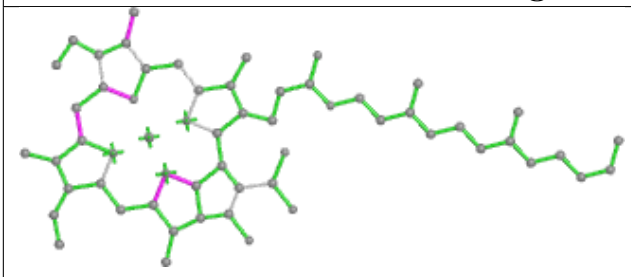
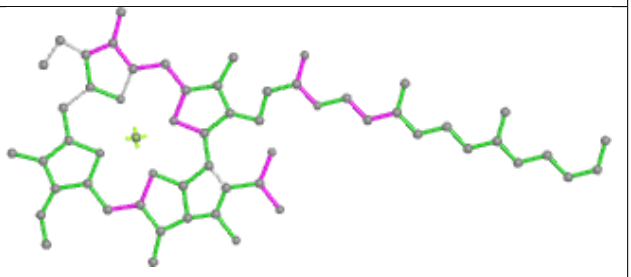
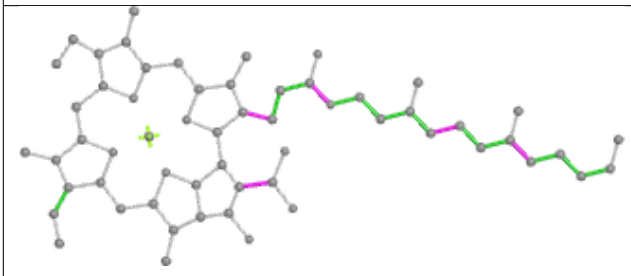
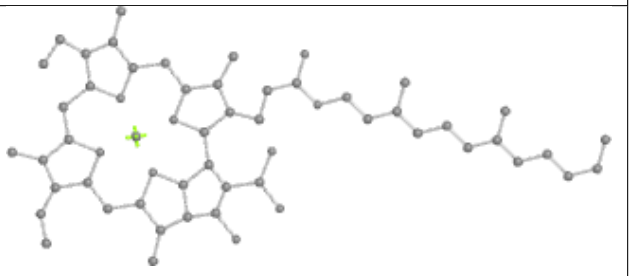
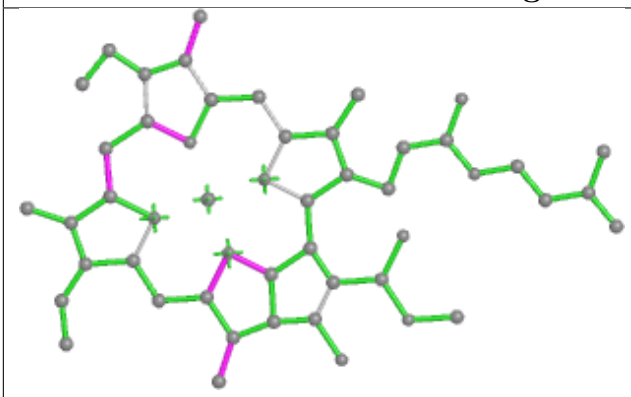
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA G 203



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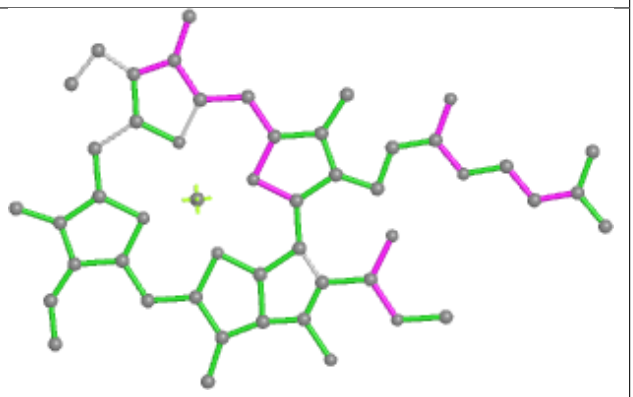
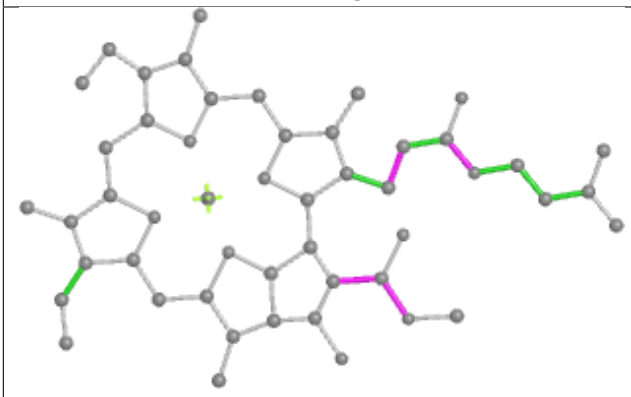


Bond angles



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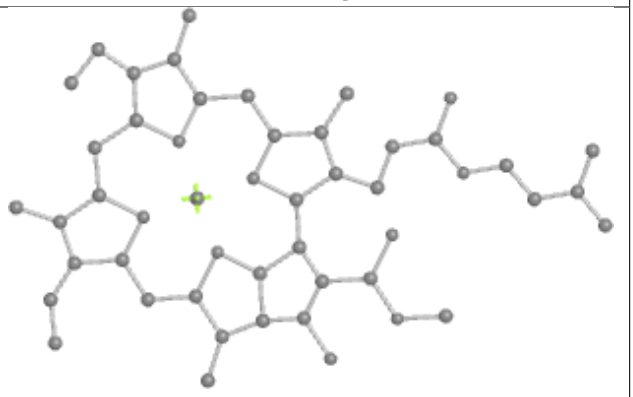
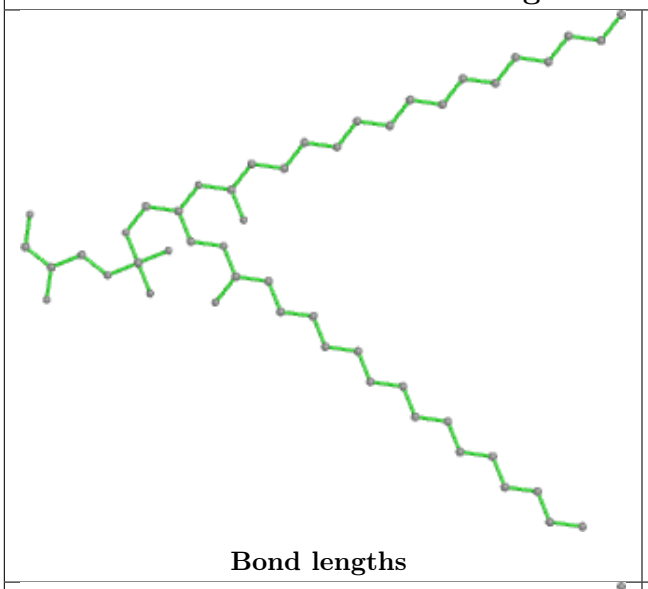


Rings

Ligand LHG A 855



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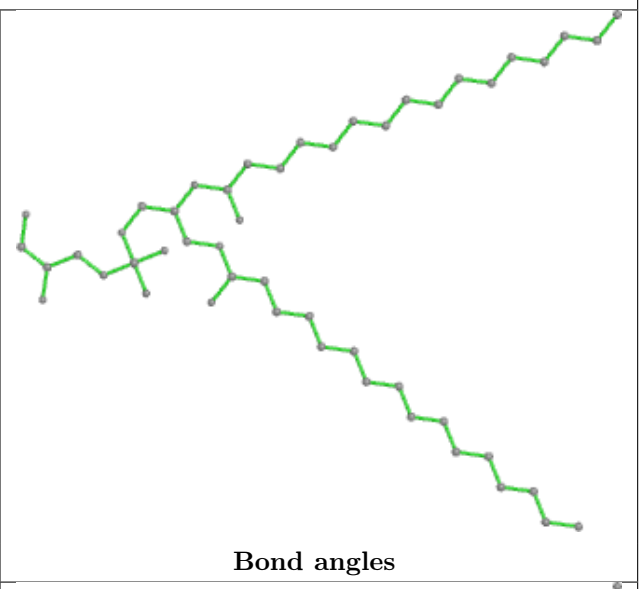
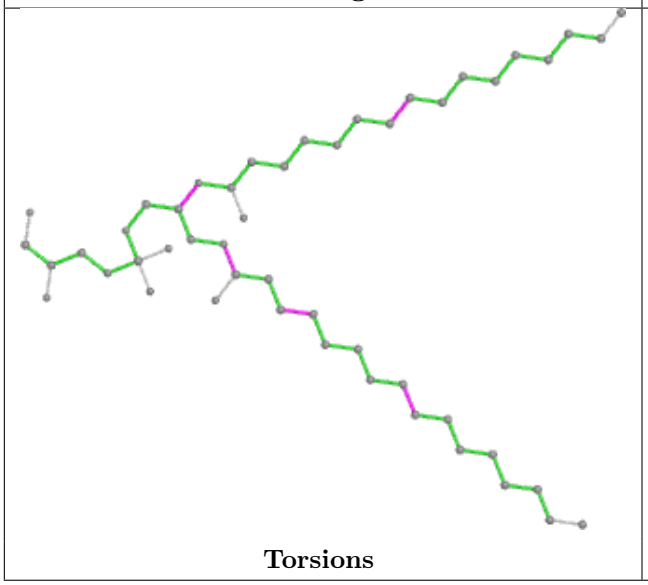


Bond angles



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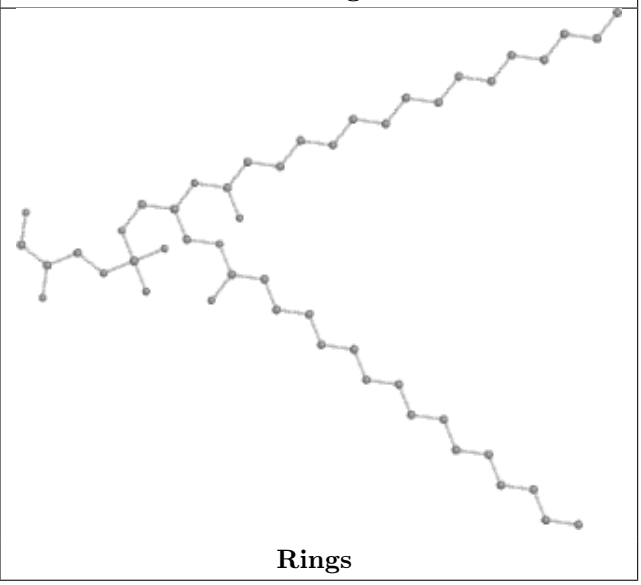
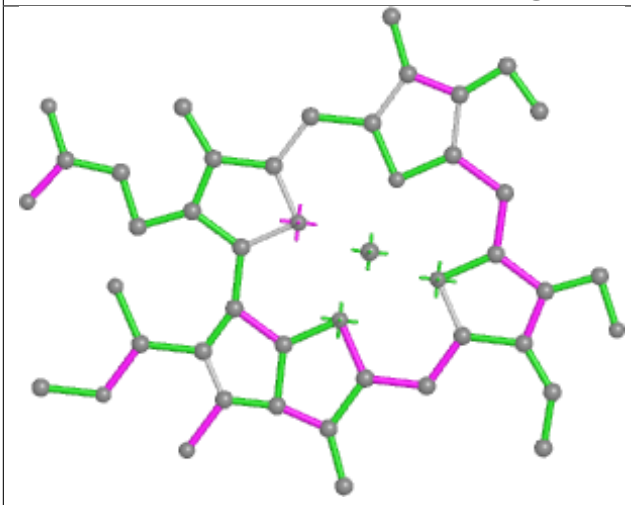


Rings

Ligand CHL 2 605



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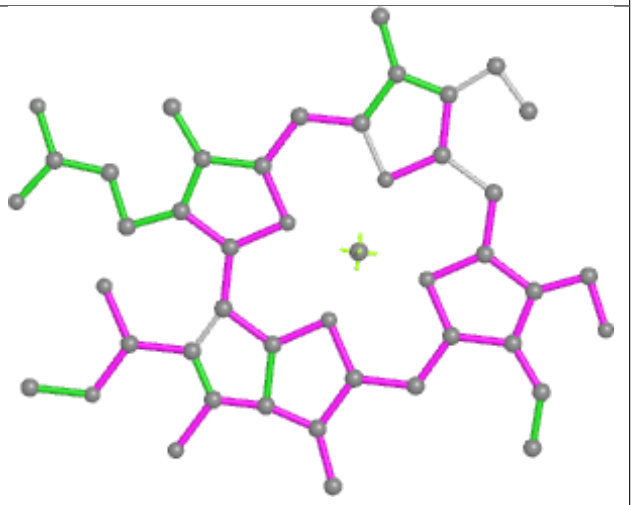
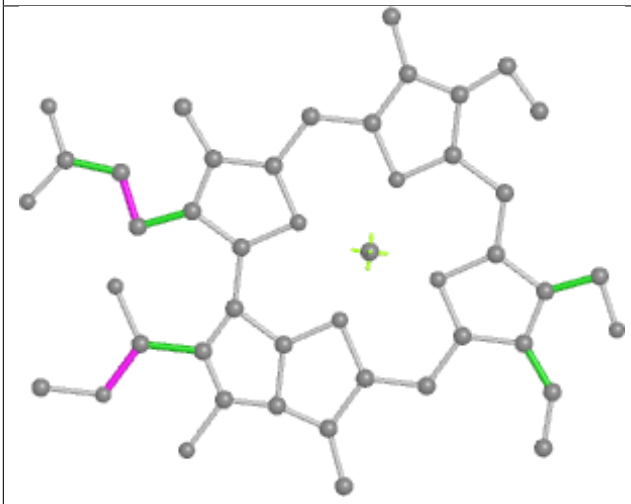


Bond angles



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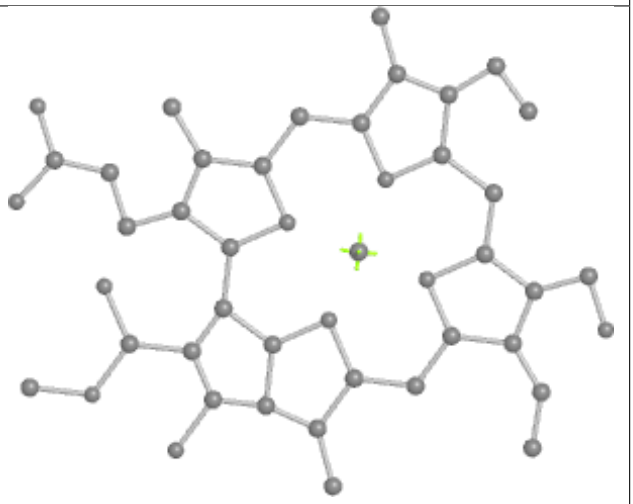
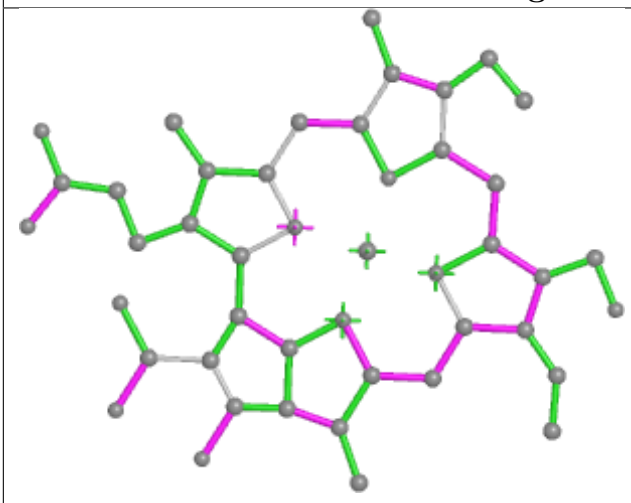


Rings

Ligand CHL a 605



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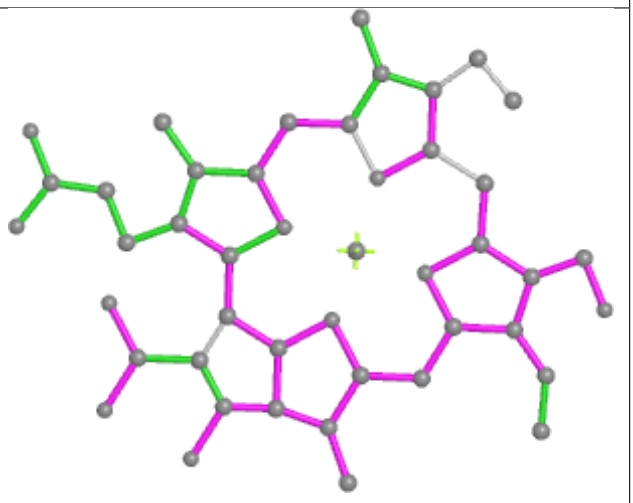
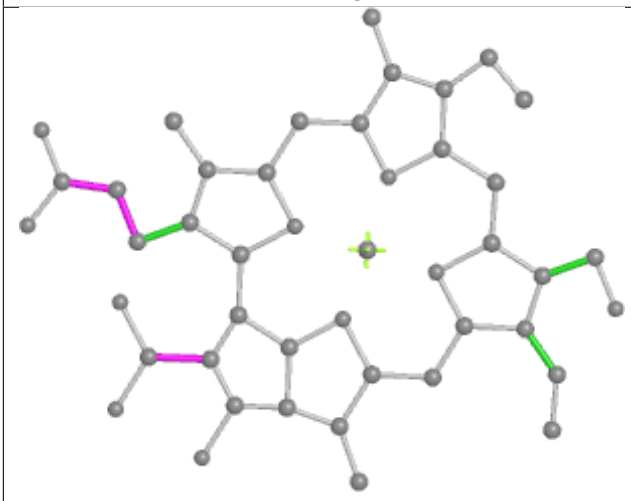
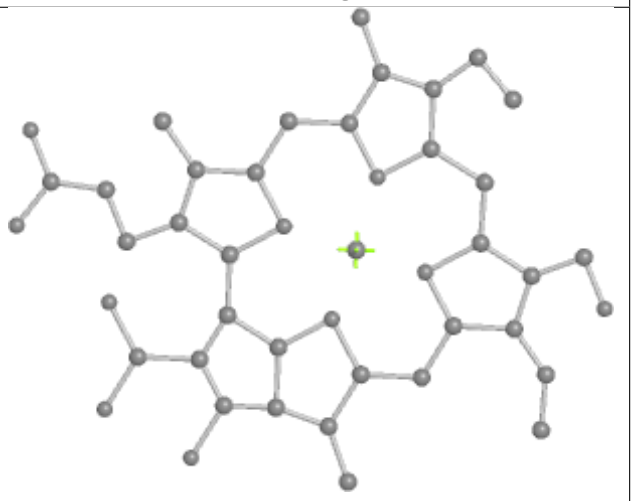


Bond angles



Torsions



Rings

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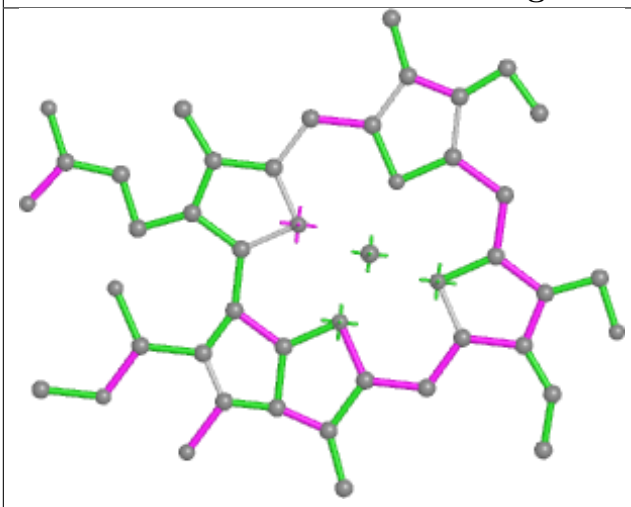

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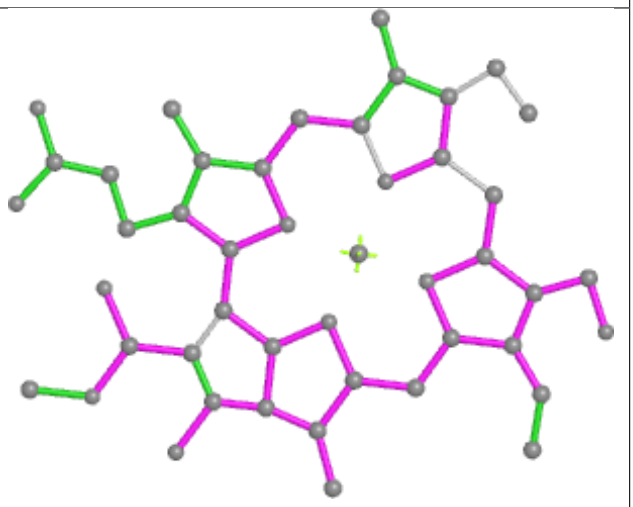

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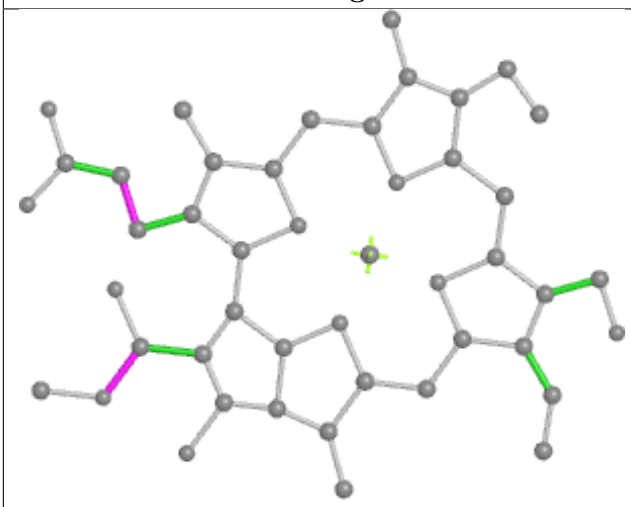

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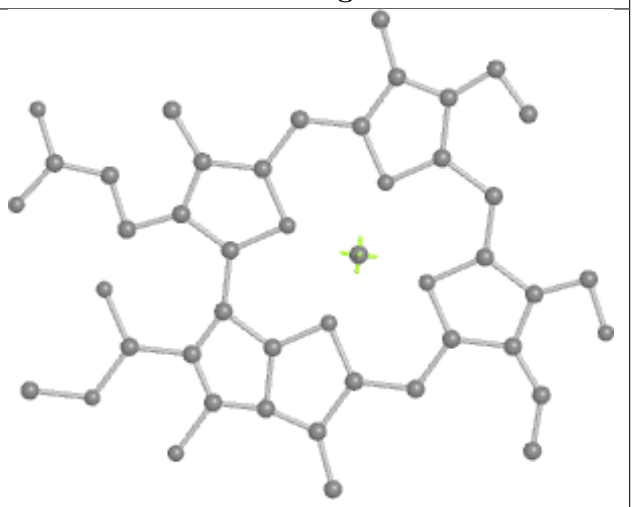

Rings

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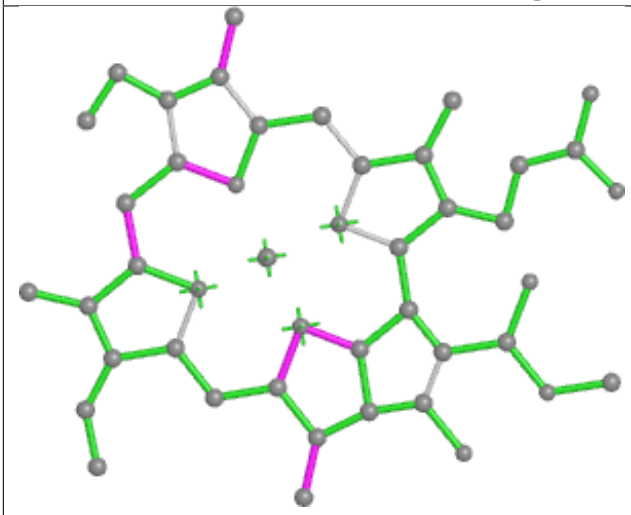

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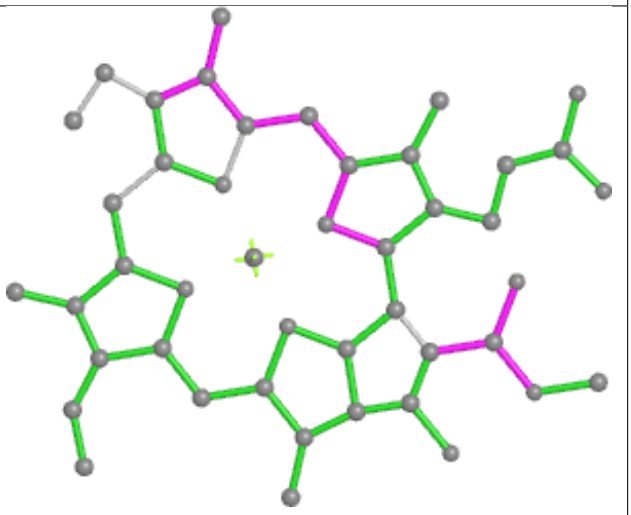

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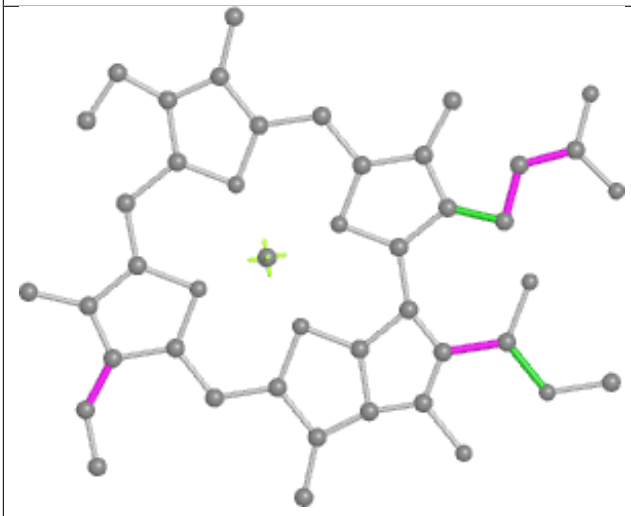

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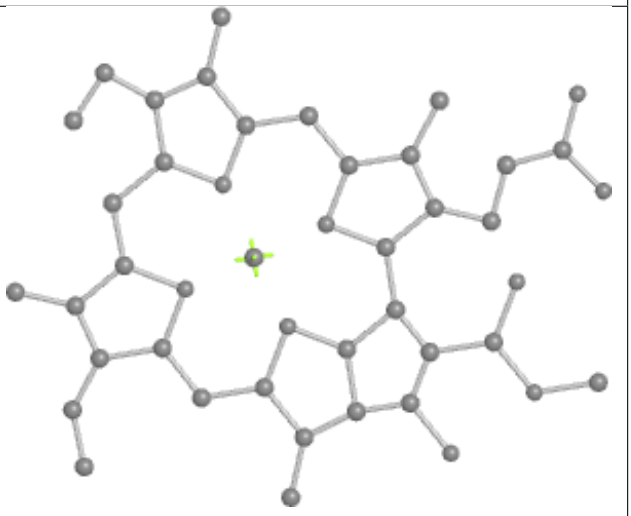

Rings

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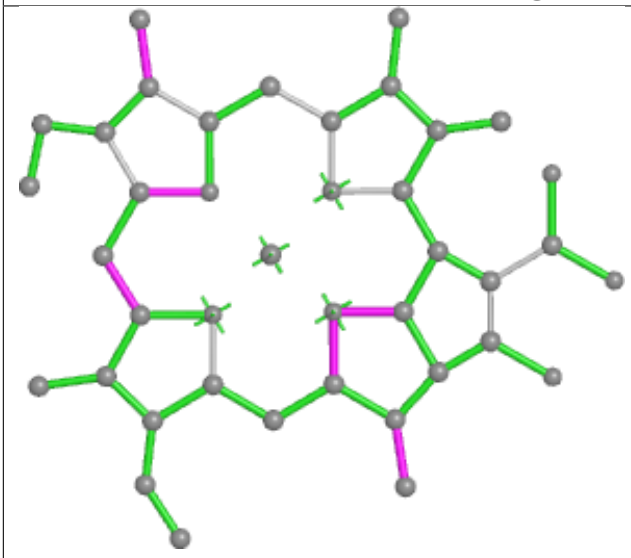

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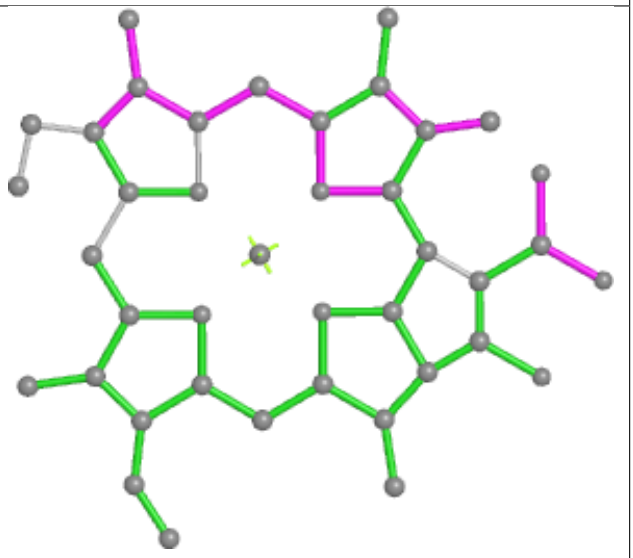
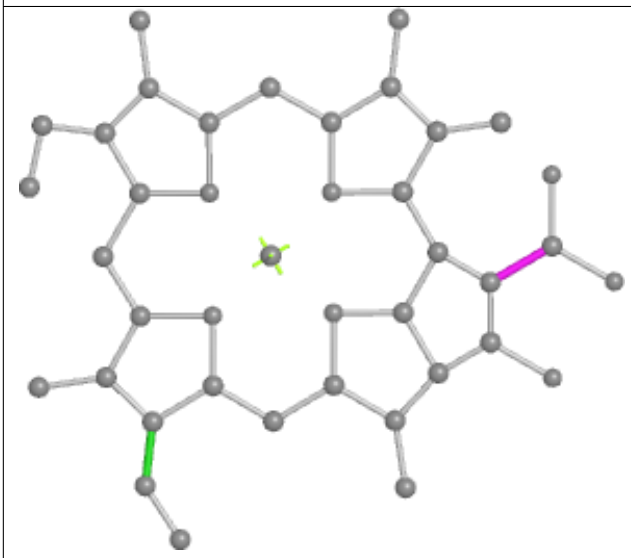


Bond angles



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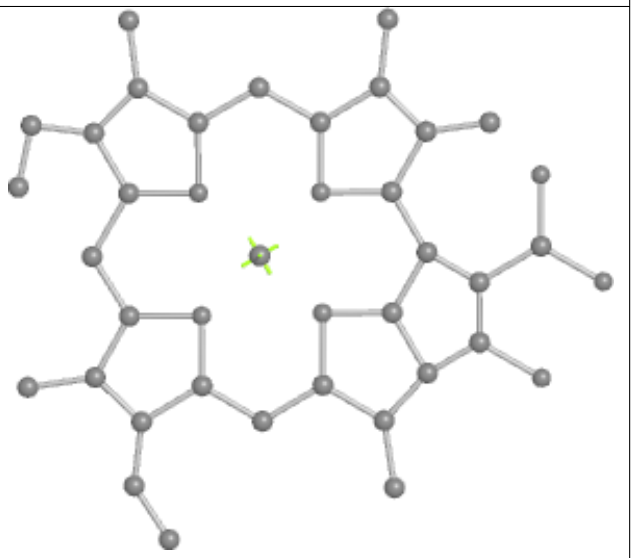
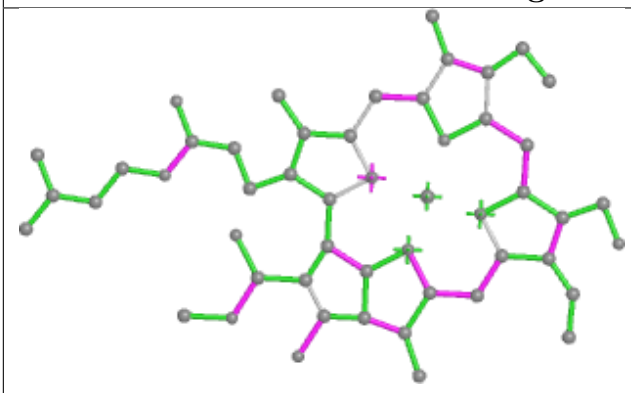


Rings

Ligand CHL 1 302



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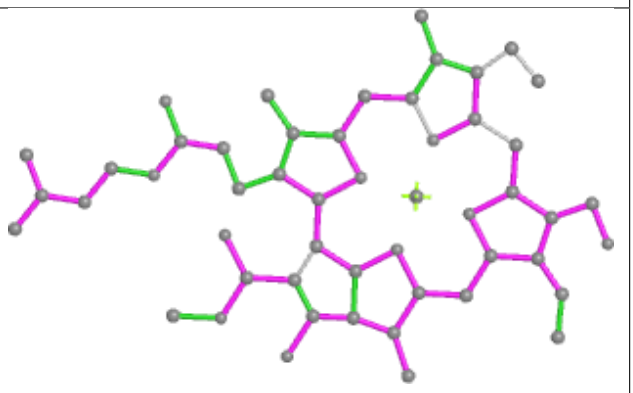

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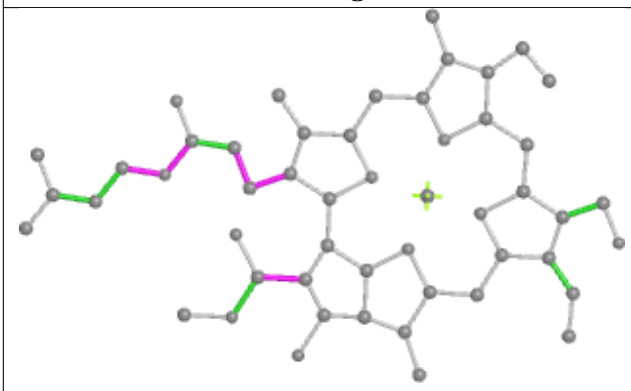

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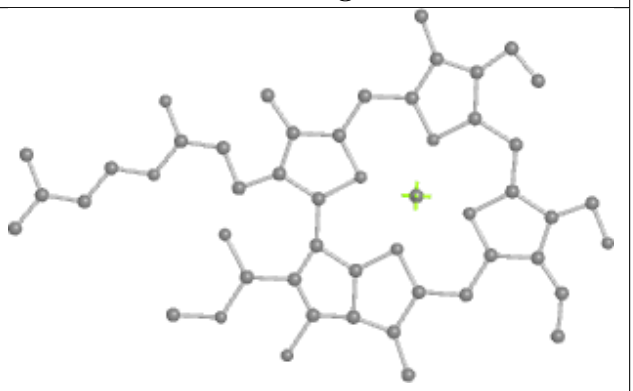

Rings

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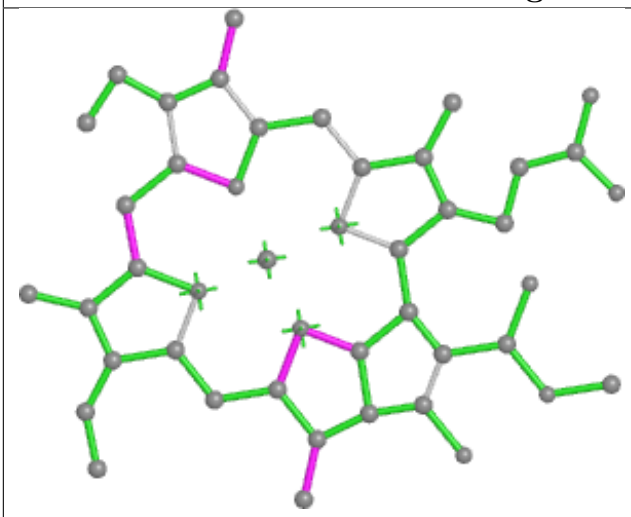

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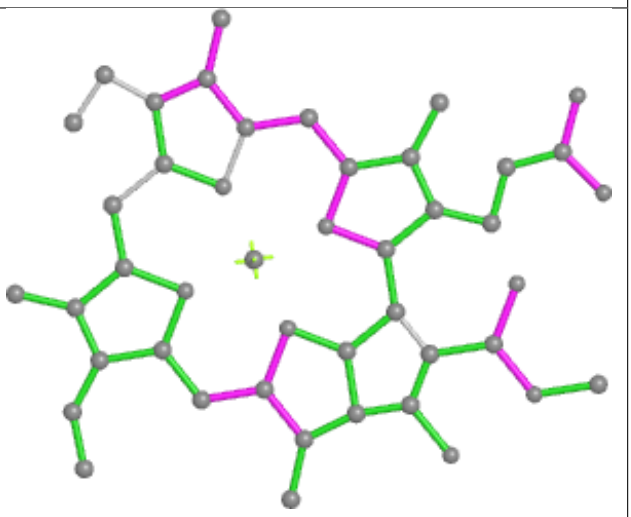

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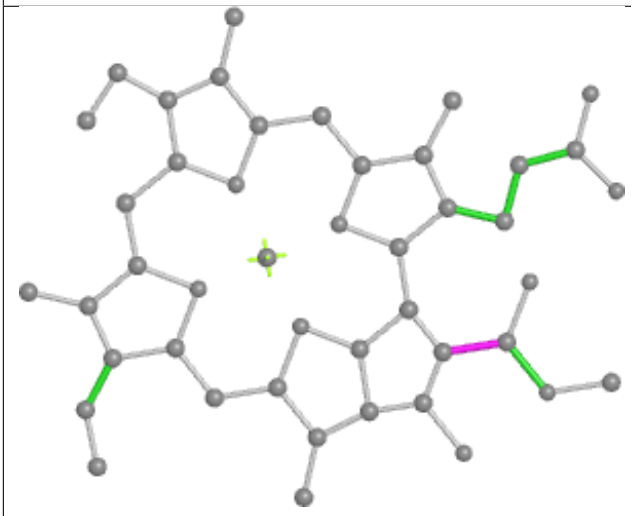

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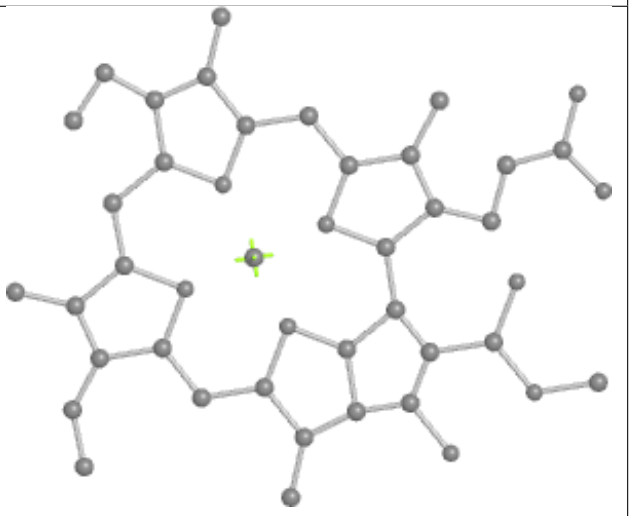

Rings

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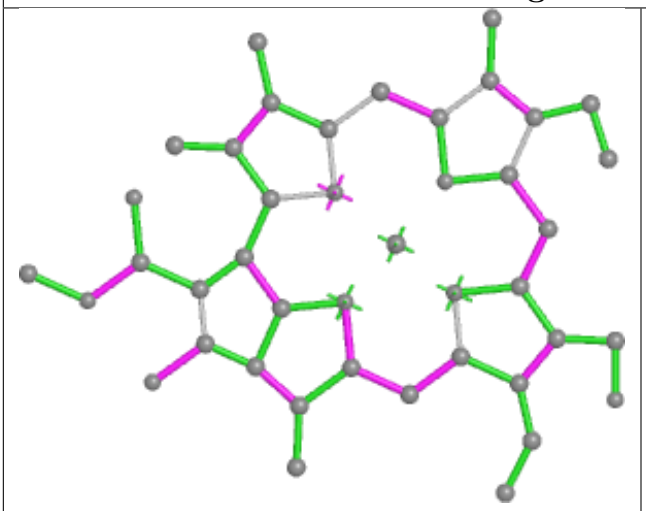

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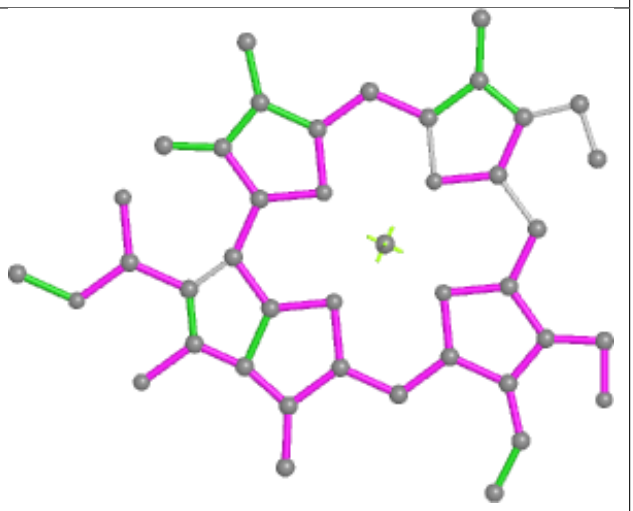

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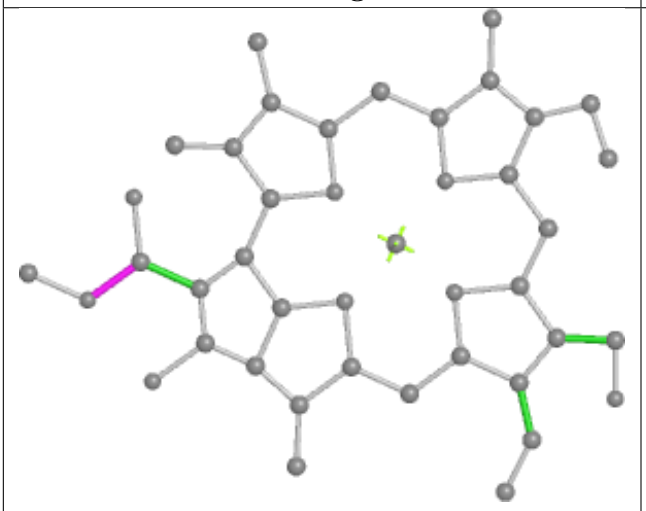

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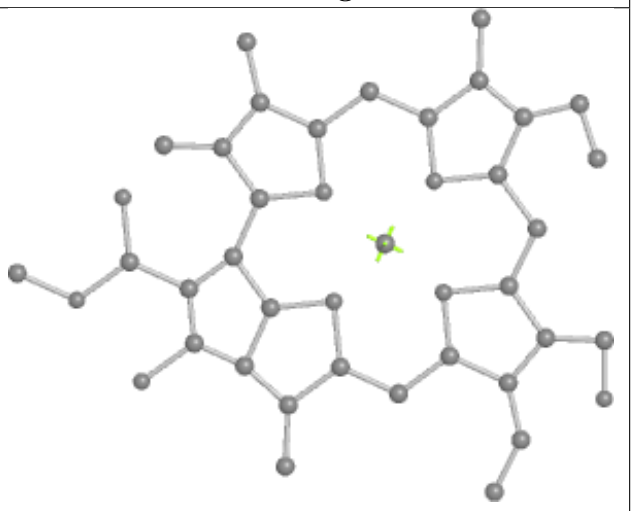
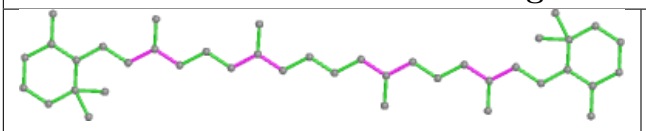


Rings

Ligand BCR 3 419



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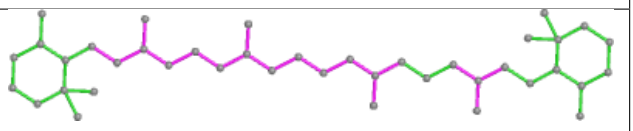

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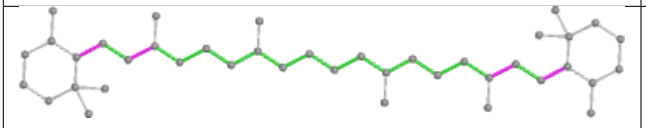
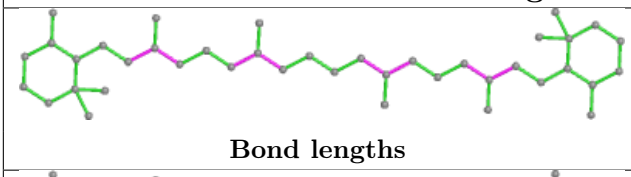


Torsions

Rings

Ligand BCR J 103



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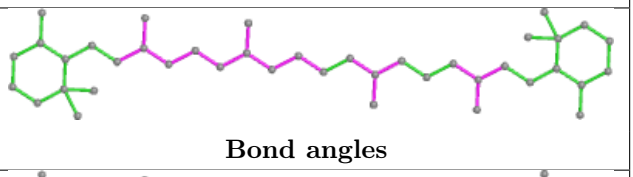
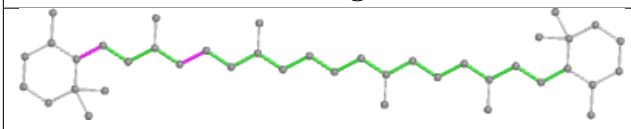


Bond angles



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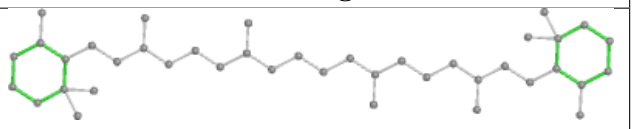
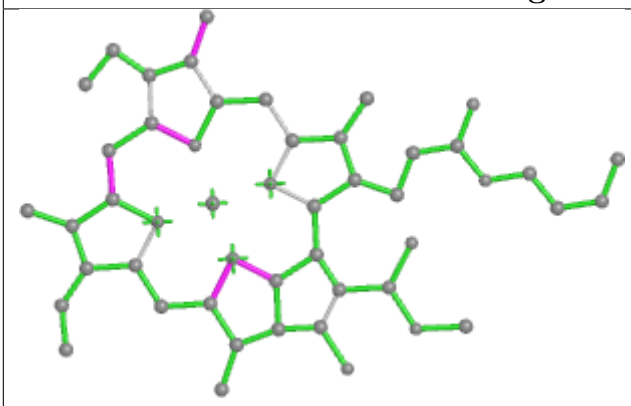


Rings

Ligand CLA 5 604



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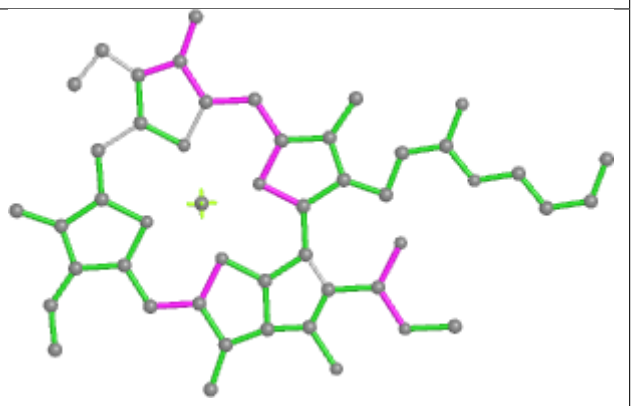

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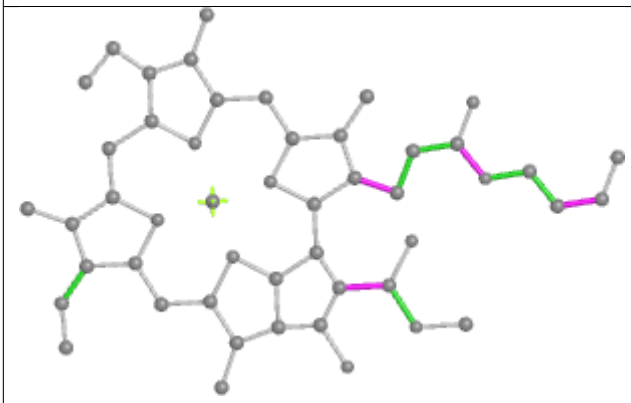

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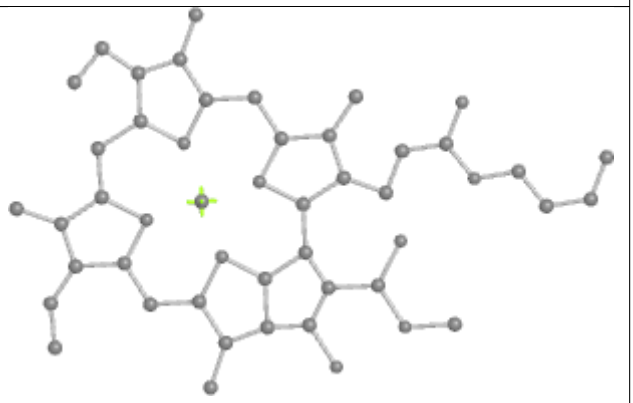
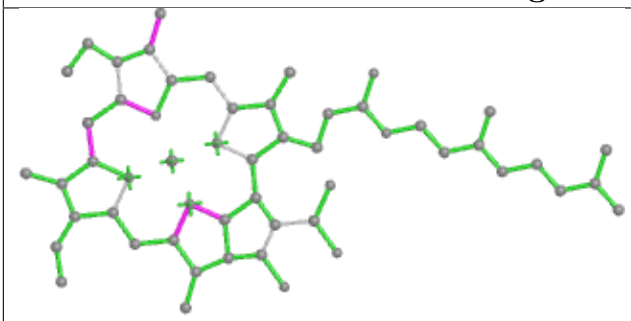


Rings

Ligand CLA 7 411



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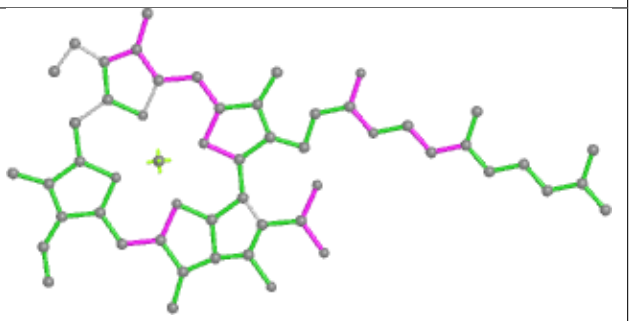

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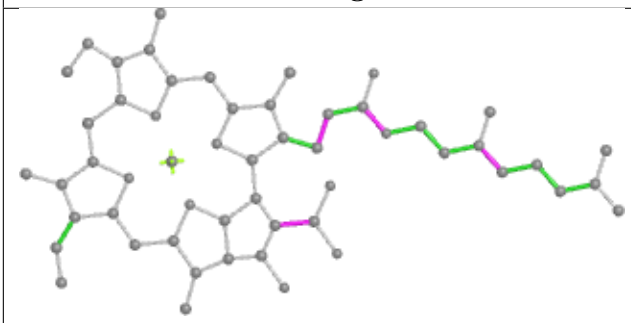

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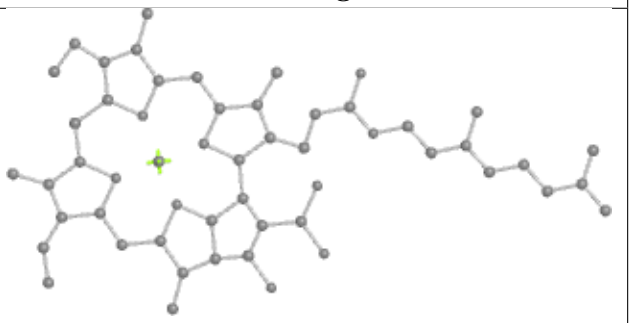
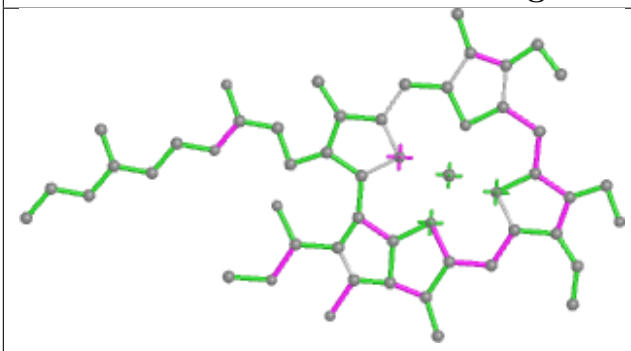


Rings

Ligand CHL 6 602



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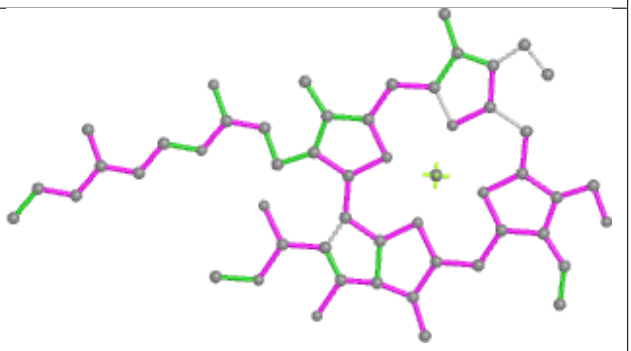
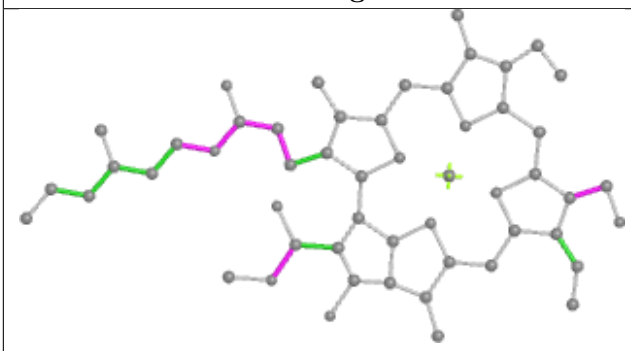


Bond angles



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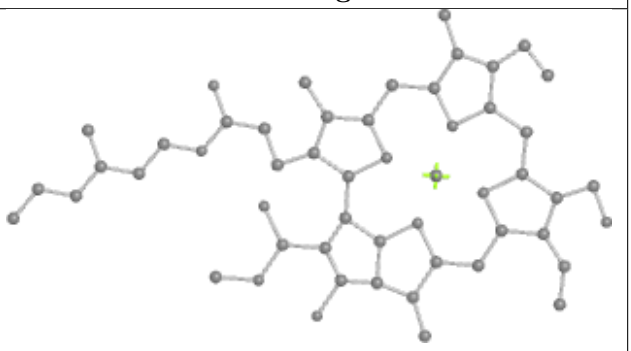

Rings

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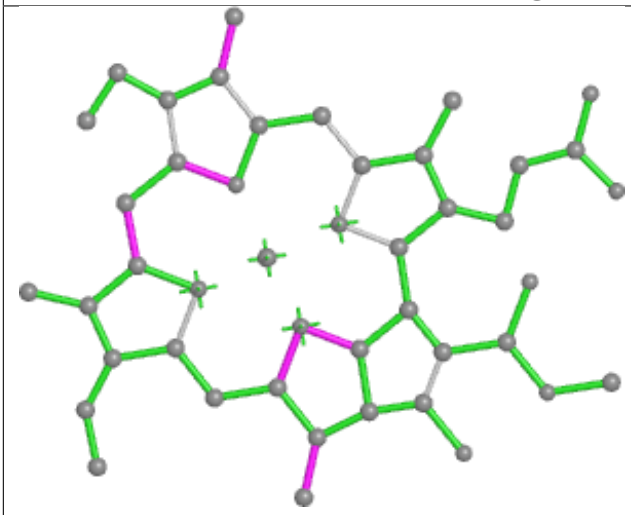

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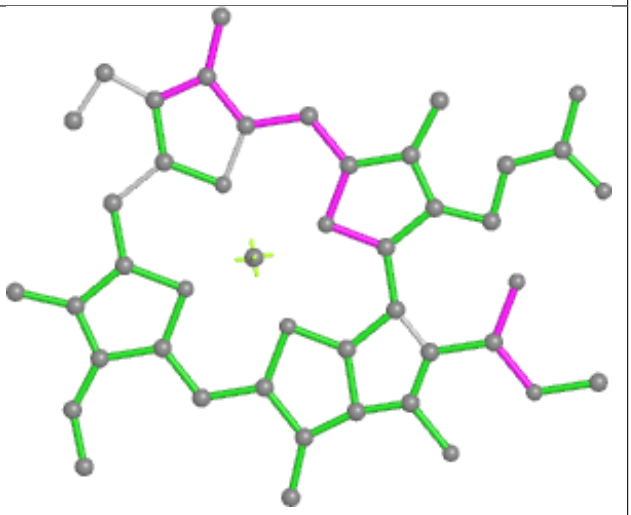

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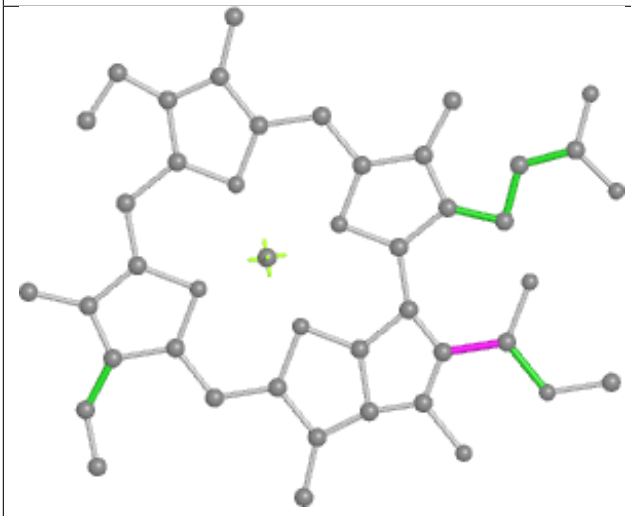
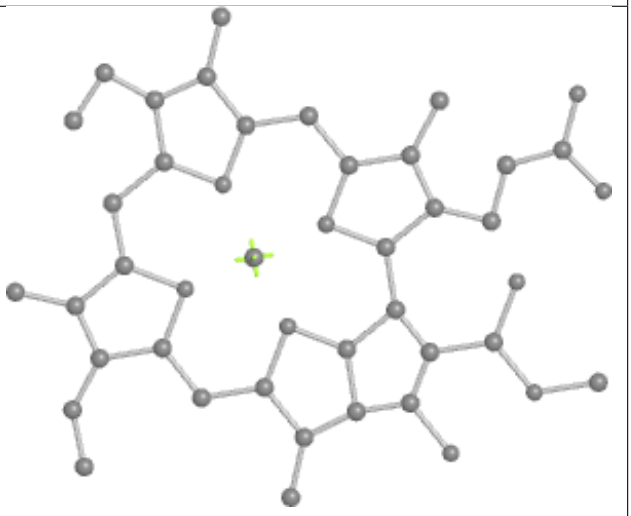
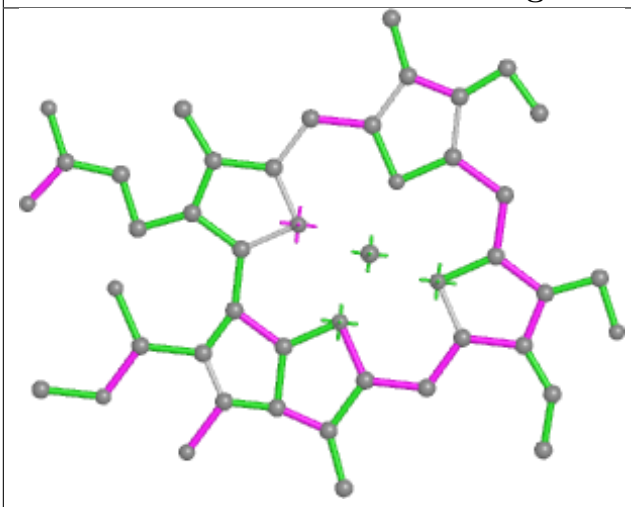


Torsions

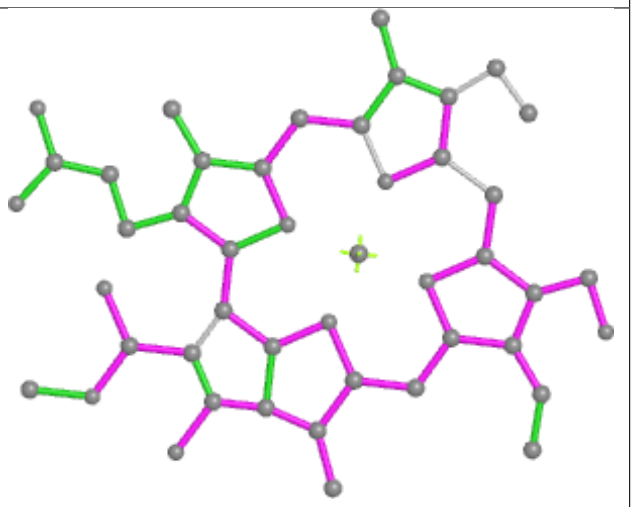


Rings

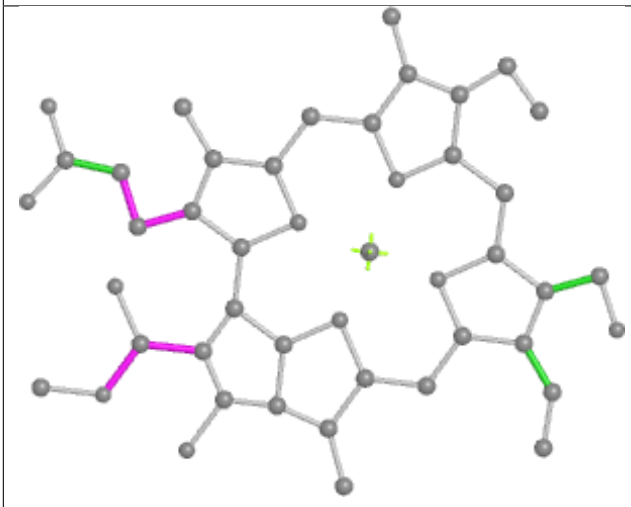
Ligand CHL b 302



Bond lengths



Bond angles



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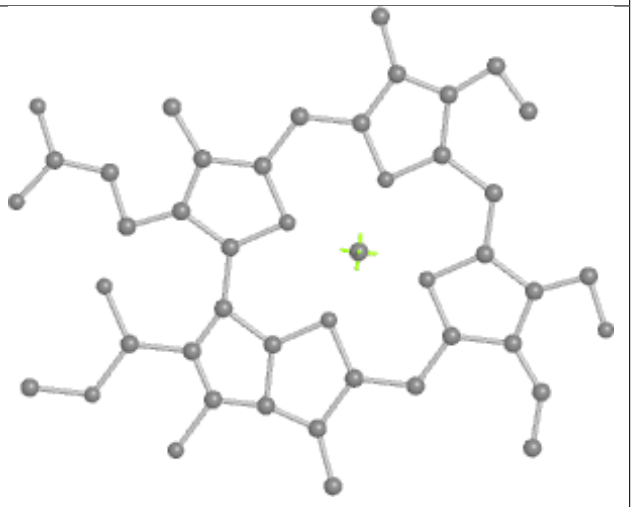
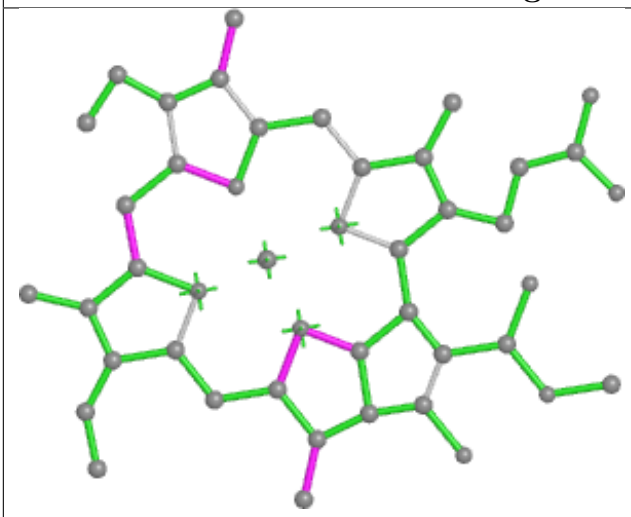


Rings

Ligand CLA A 808



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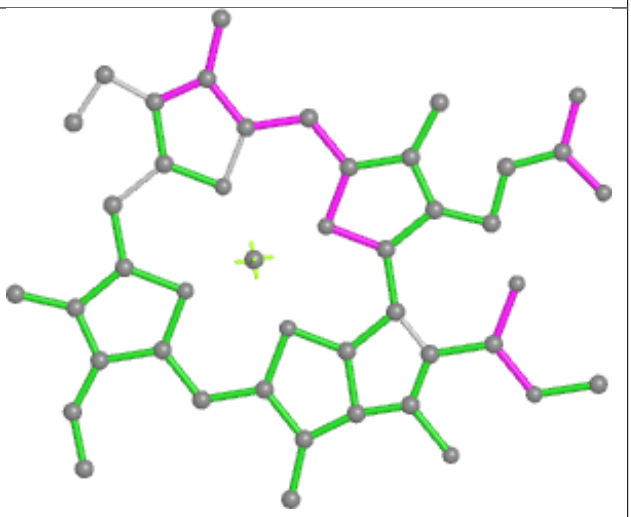

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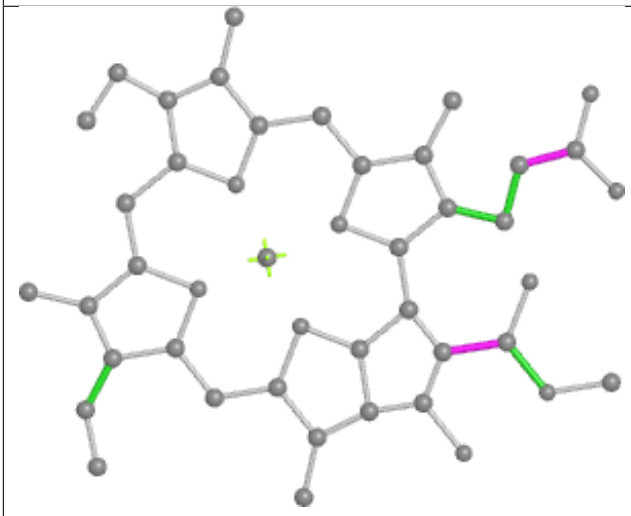

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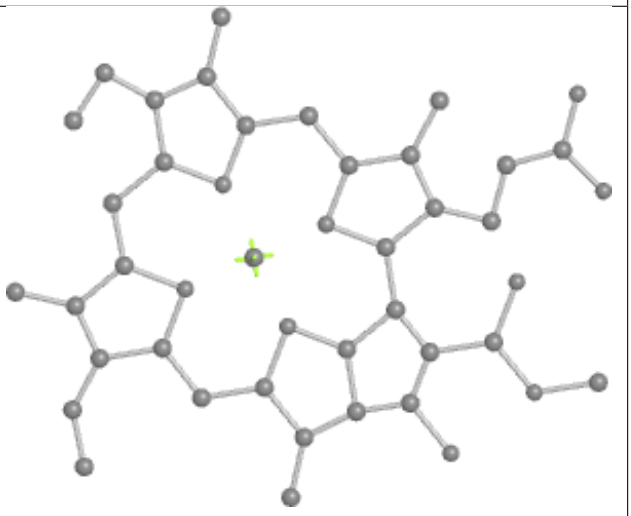
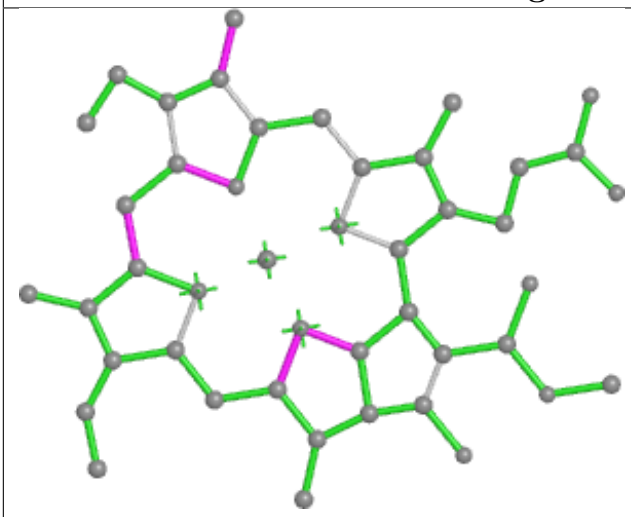


Rings

Ligand CLA 6 604



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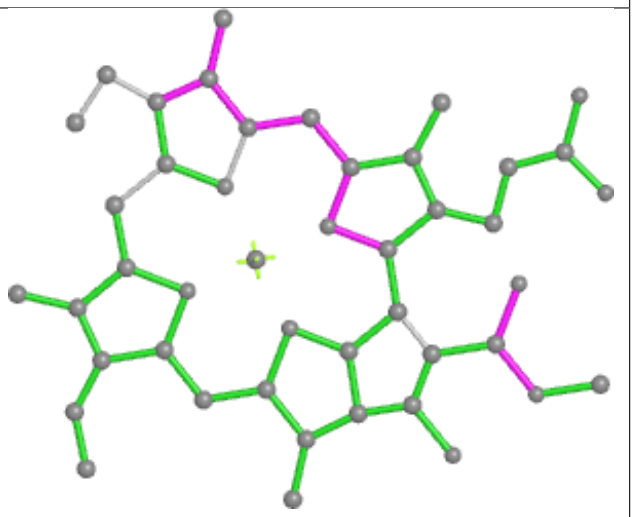
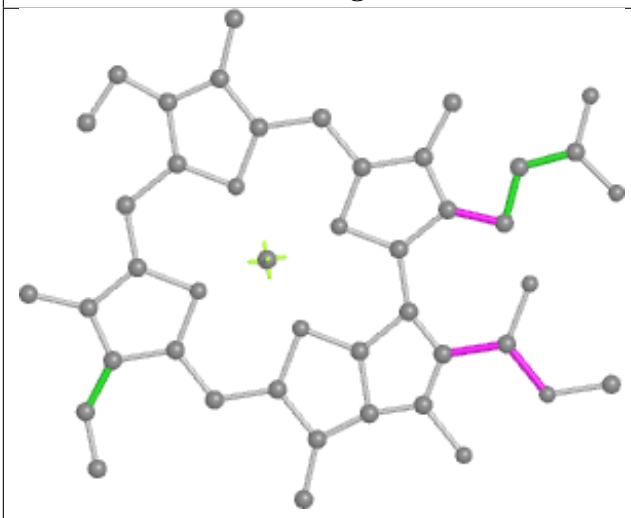


Bond angles



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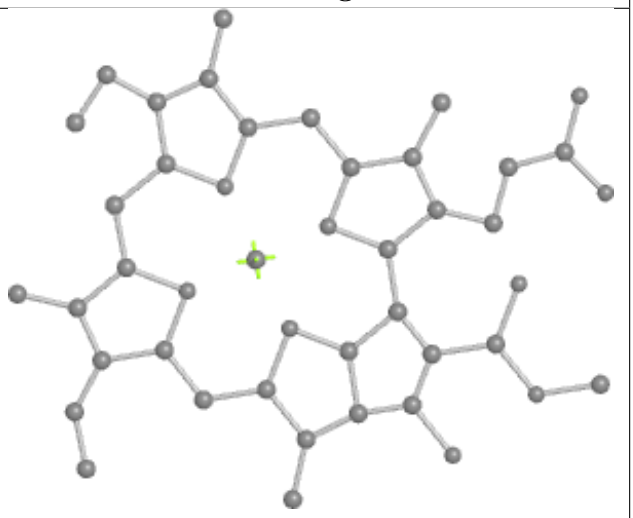
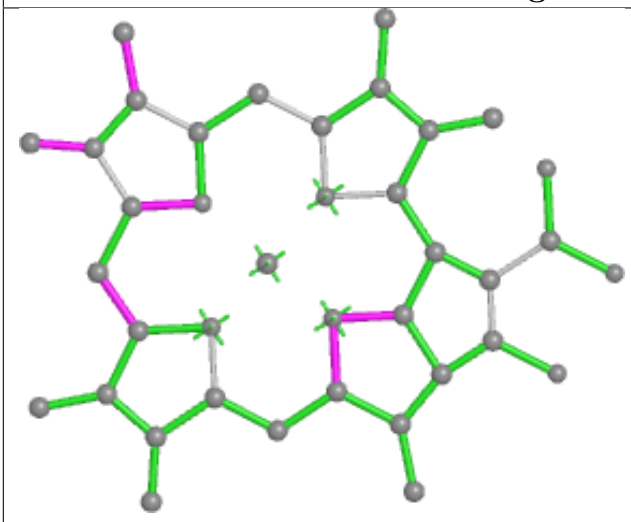


Rings

Ligand CLA 5 613



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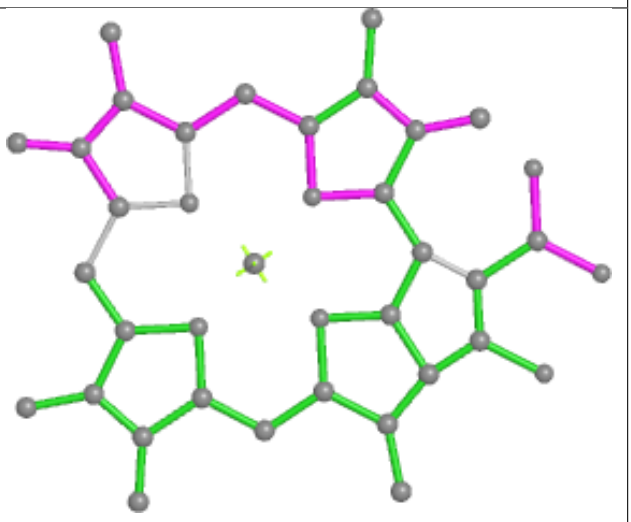
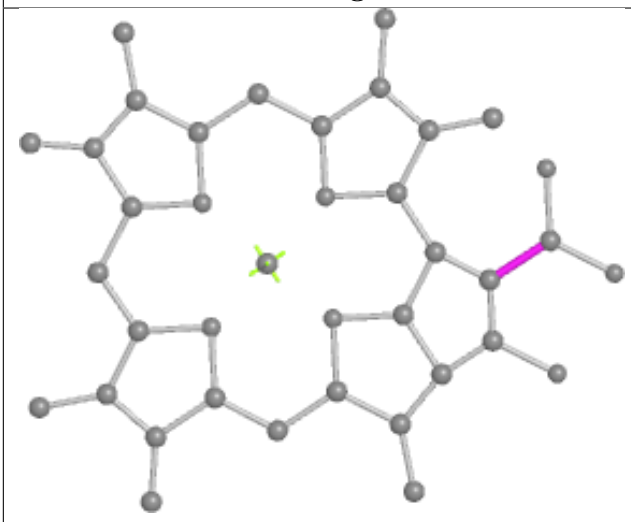


Bond angles



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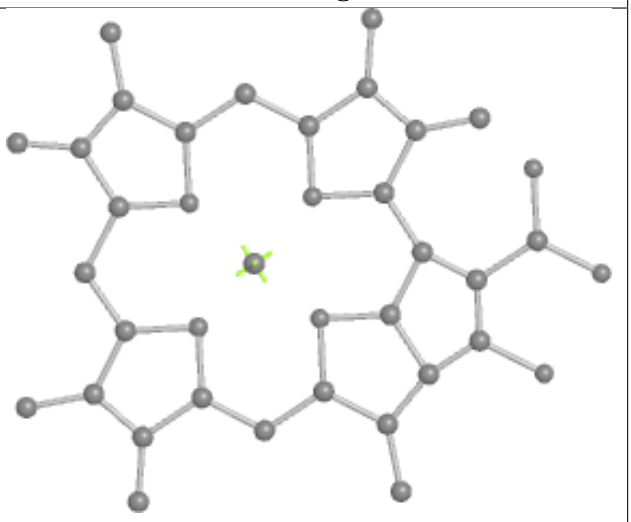
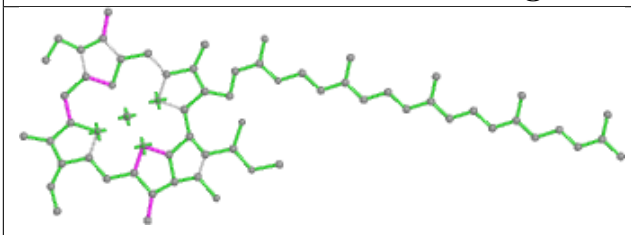


Rings

Ligand CLA B 805



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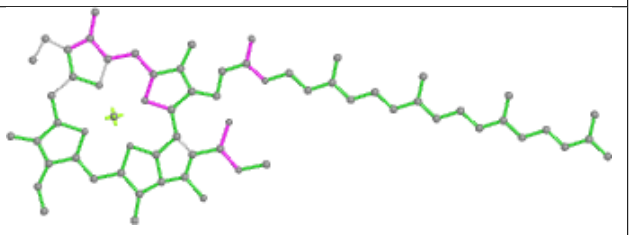
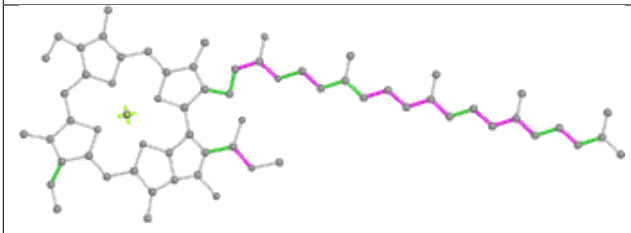


Bond angles



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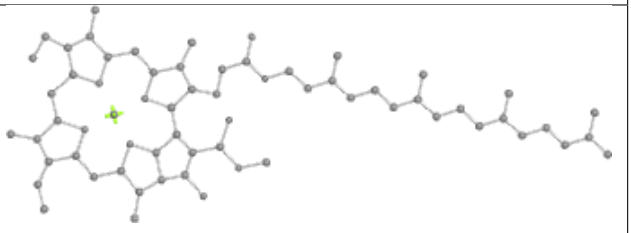
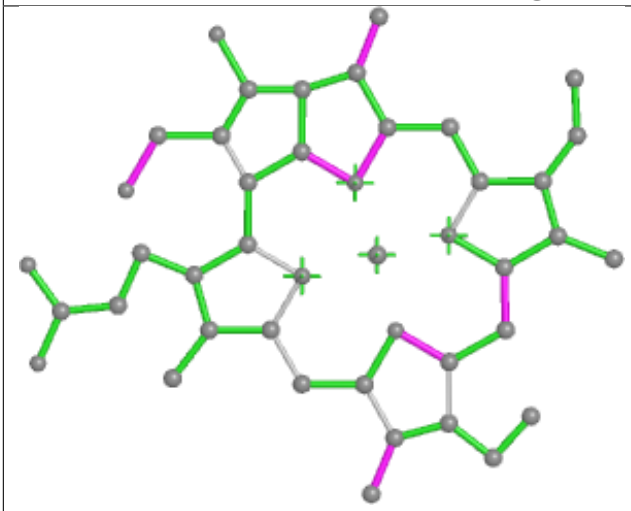


Rings

Ligand CLA 4 608



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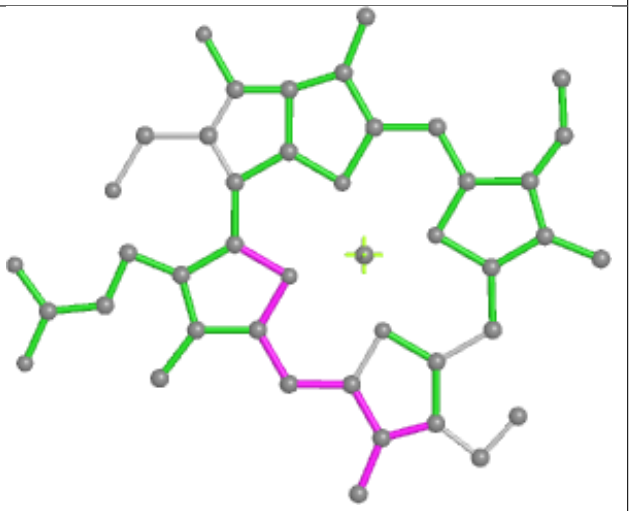
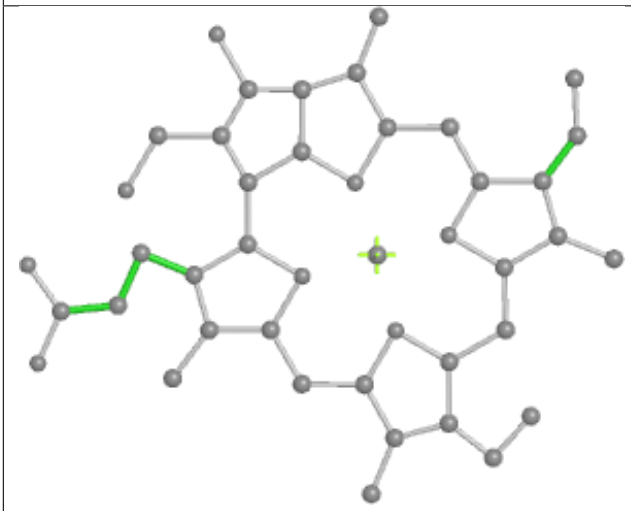


Bond angles



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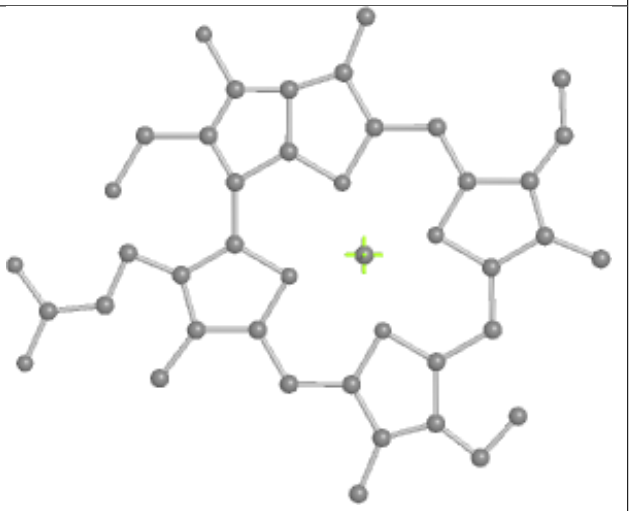
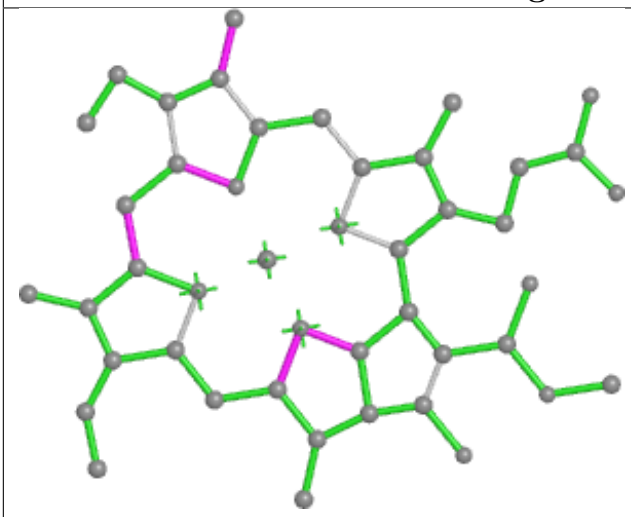


Rings

Ligand CLA a 610



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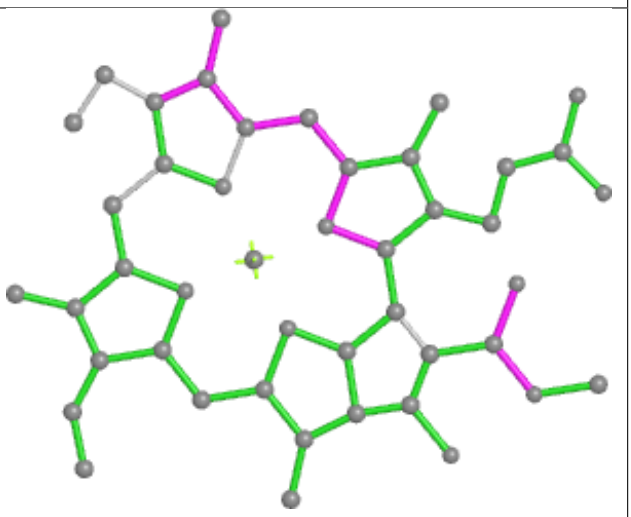

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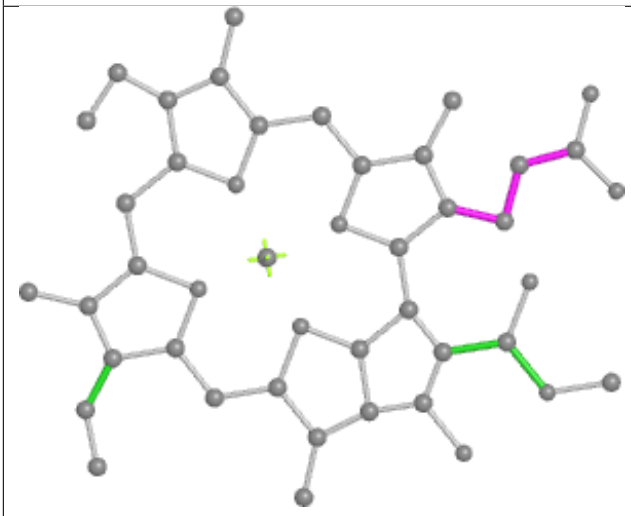

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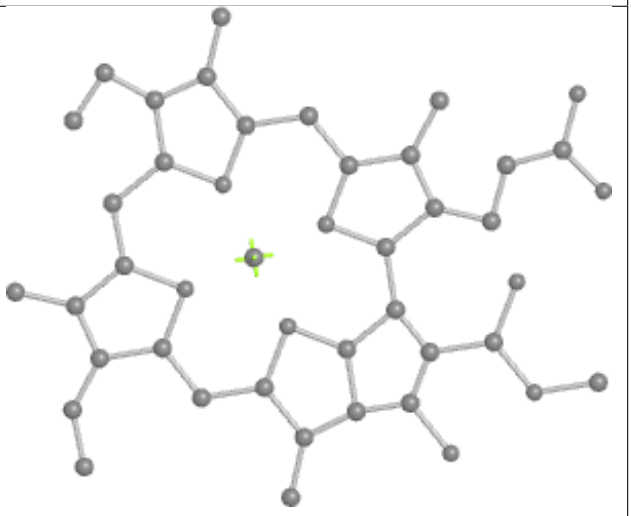
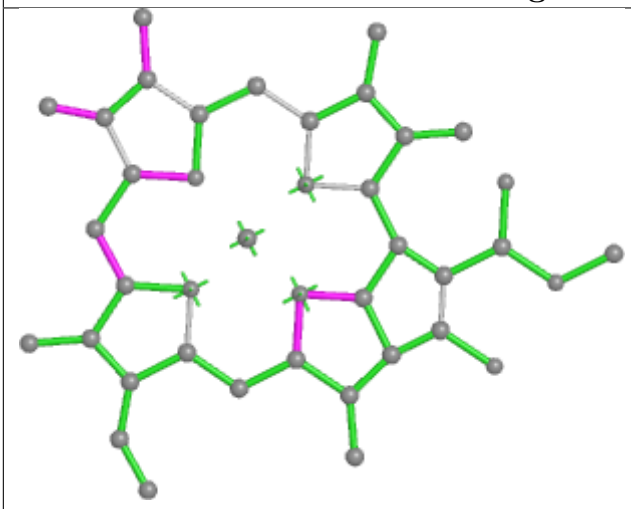


Rings

Ligand CLA 5 608



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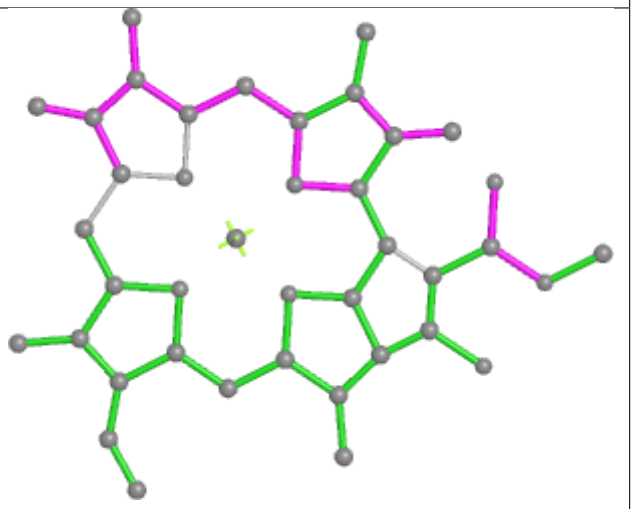

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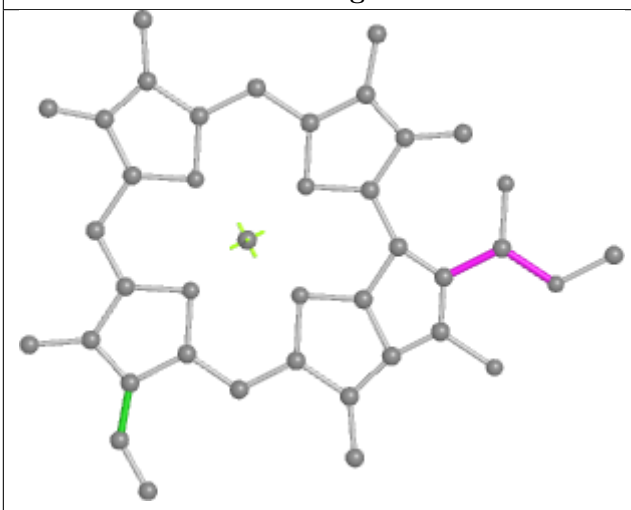

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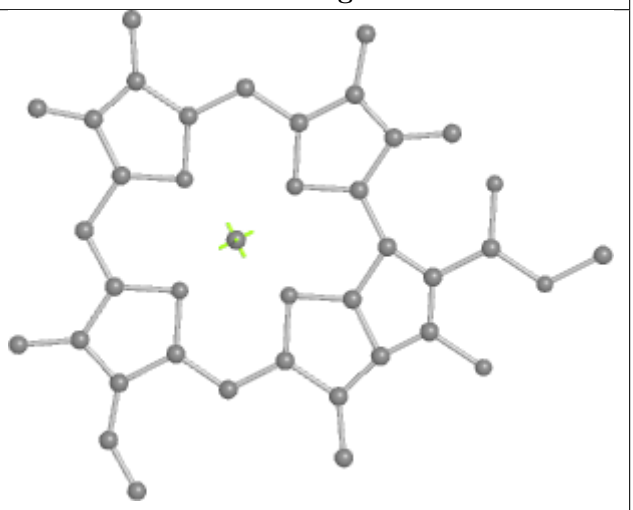
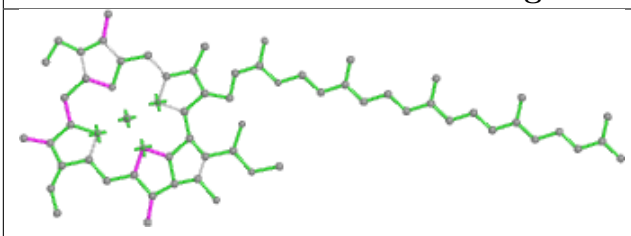


Rings

Ligand CLA B 836



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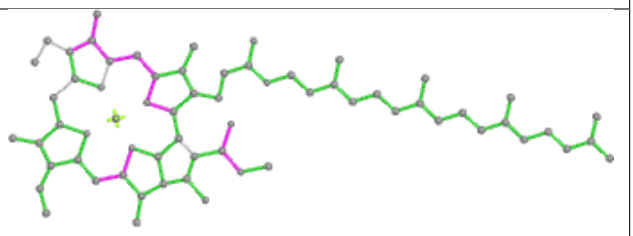
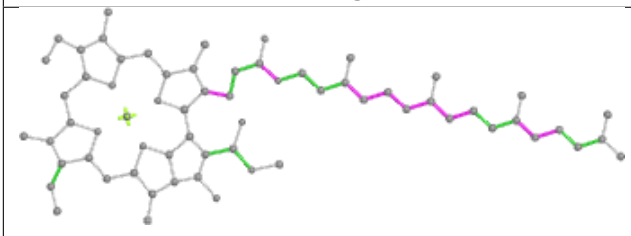


Bond angles



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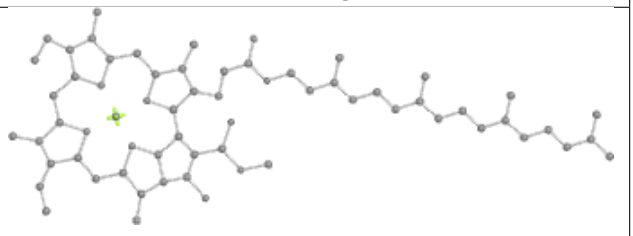
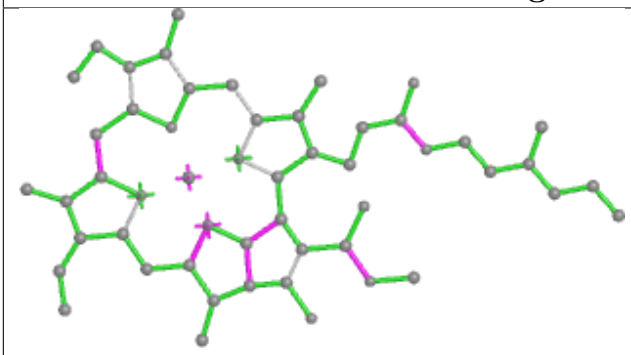


Rings

Ligand CLA 3 409



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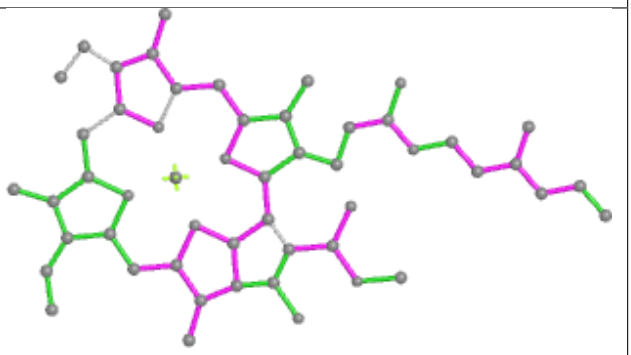
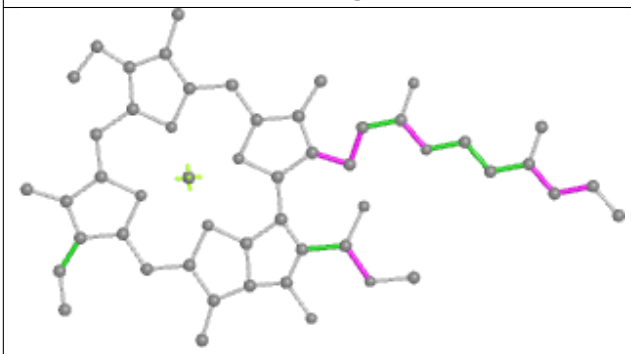


Bond angles



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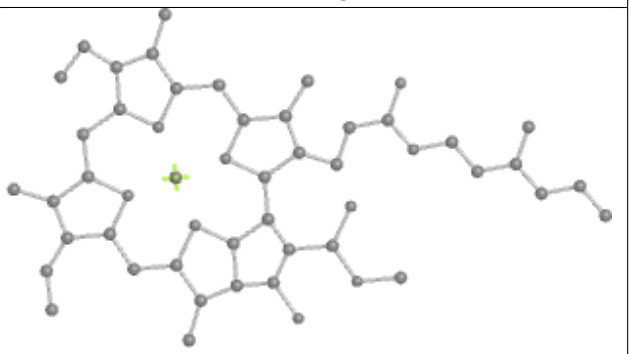
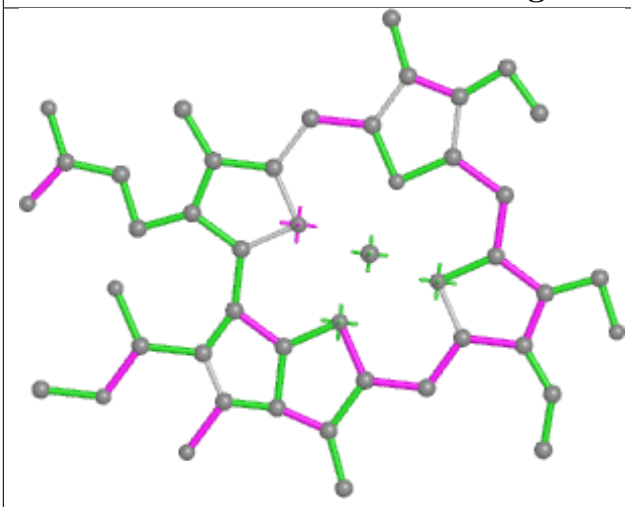


Rings

Ligand CHL 9 606



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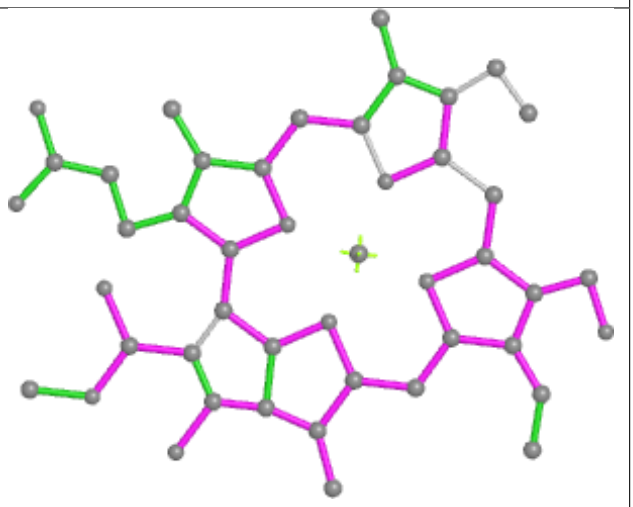
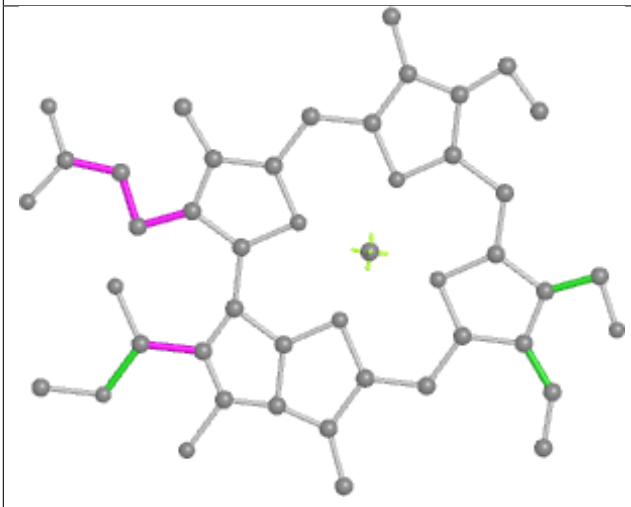


Bond angles



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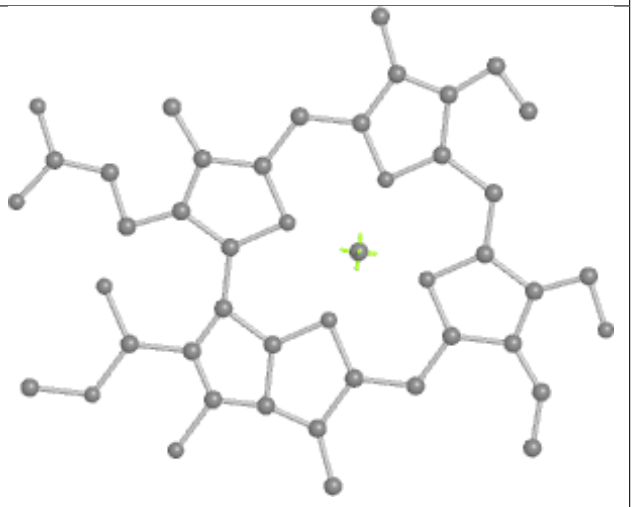
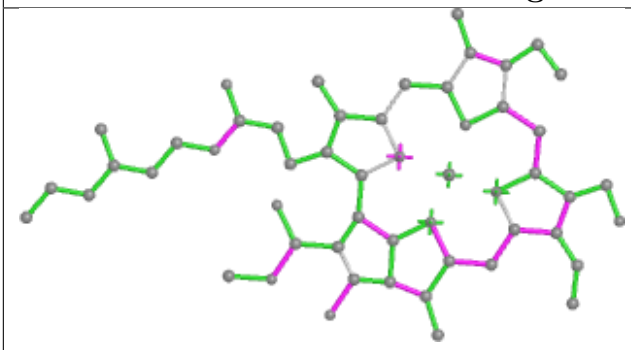


Rings

Ligand CHL b 308



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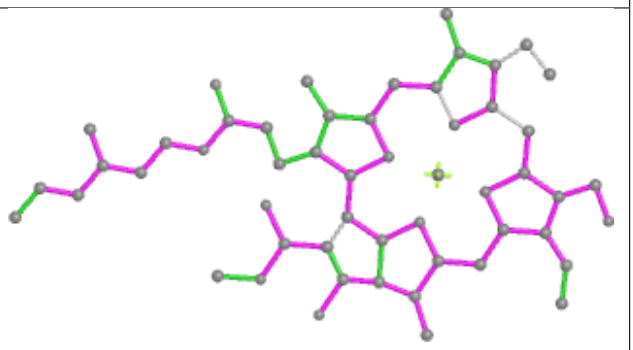
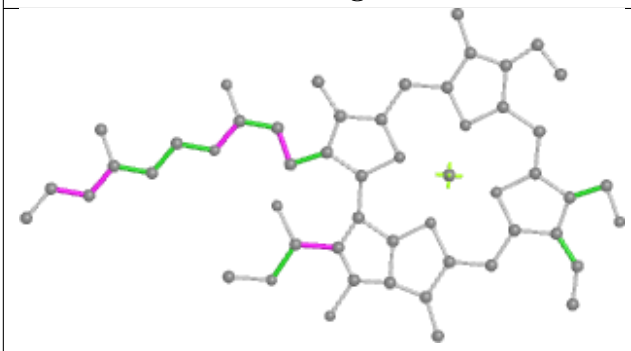


Bond angles



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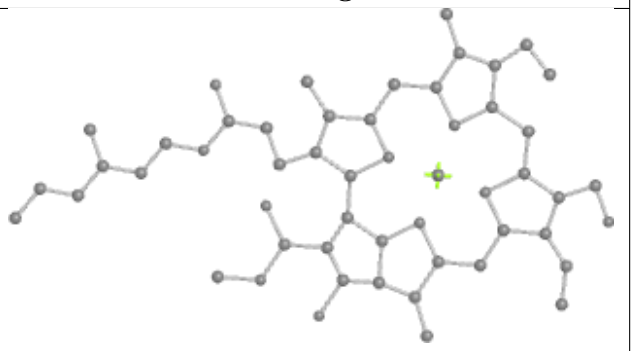
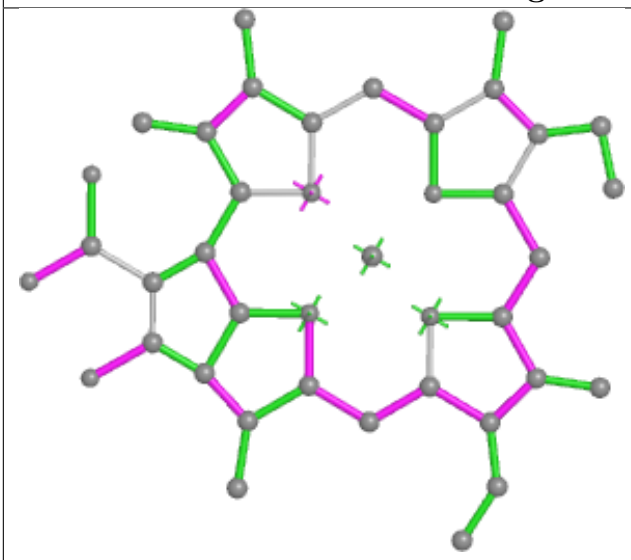


Rings

Ligand CHL 7 406



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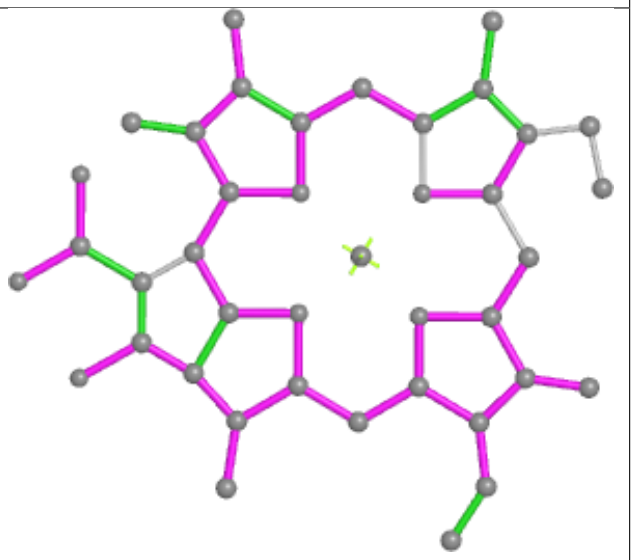
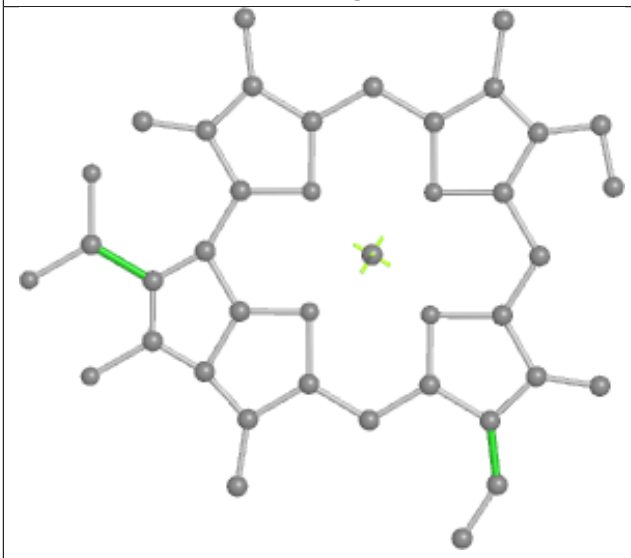
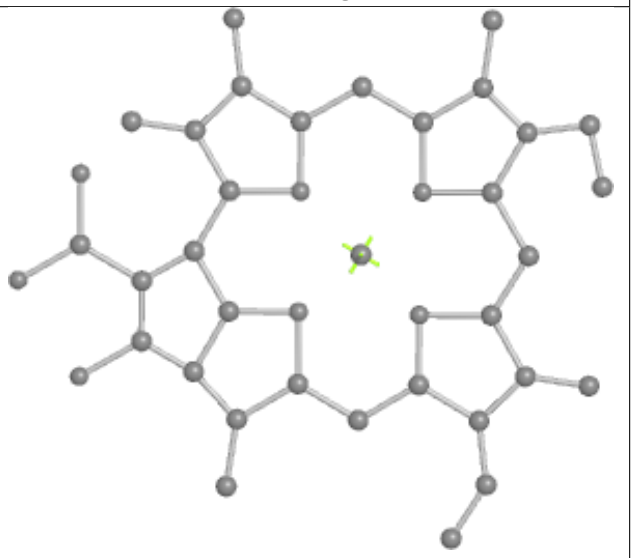


Bond angles

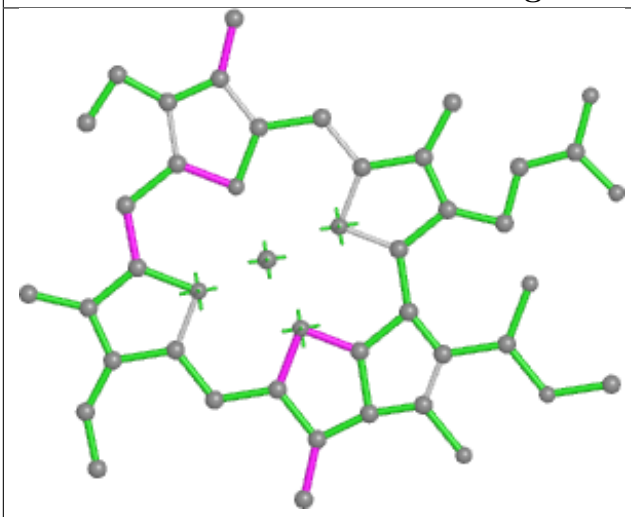


Torsions

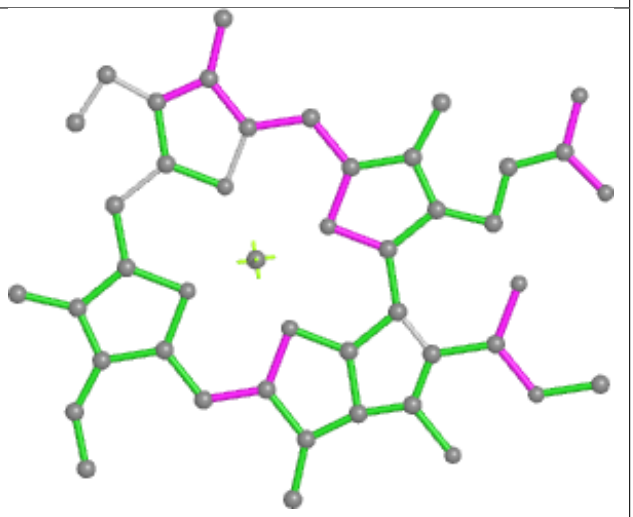


Rings

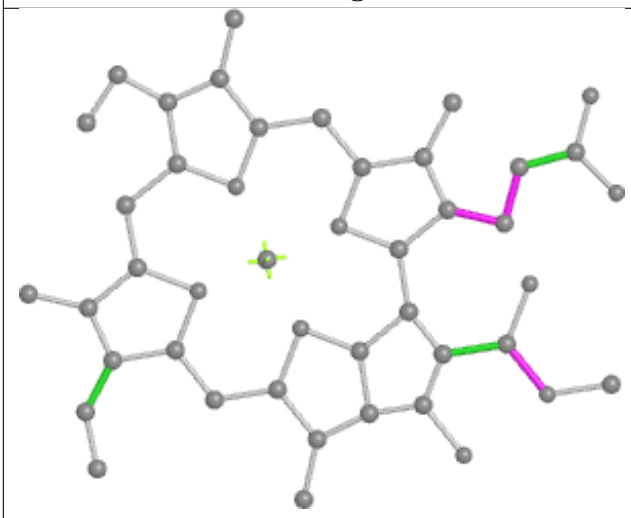
Ligand CLA B 834



Bond lengths



Bond angles



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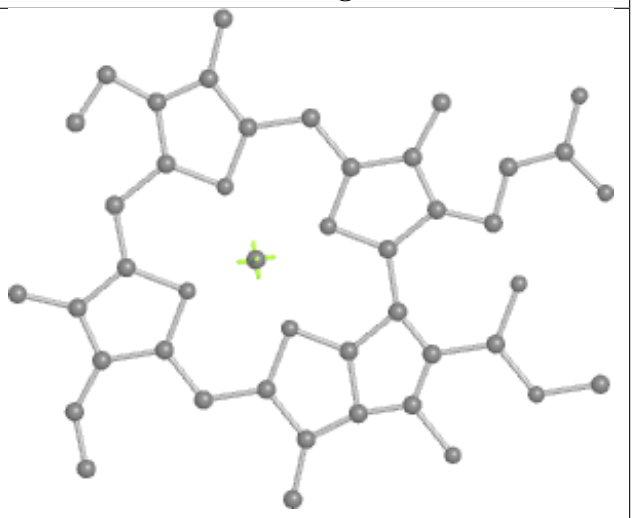
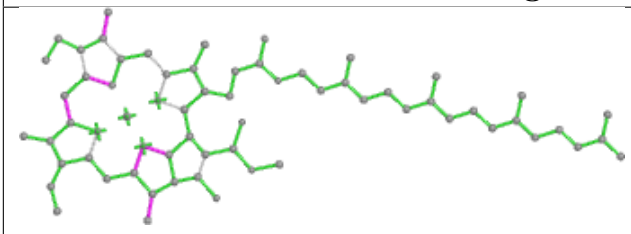


Rings

Ligand CLA A 829



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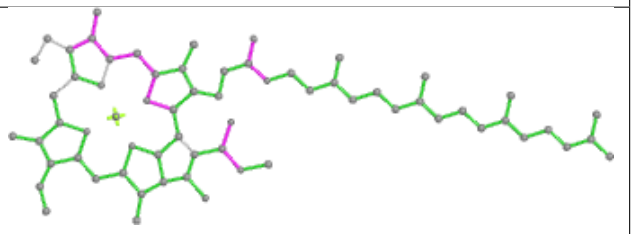

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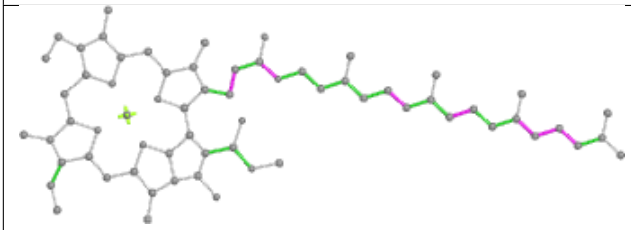

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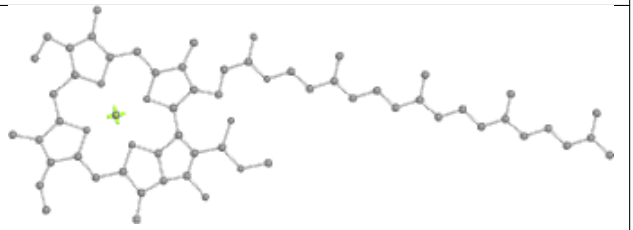

Rings

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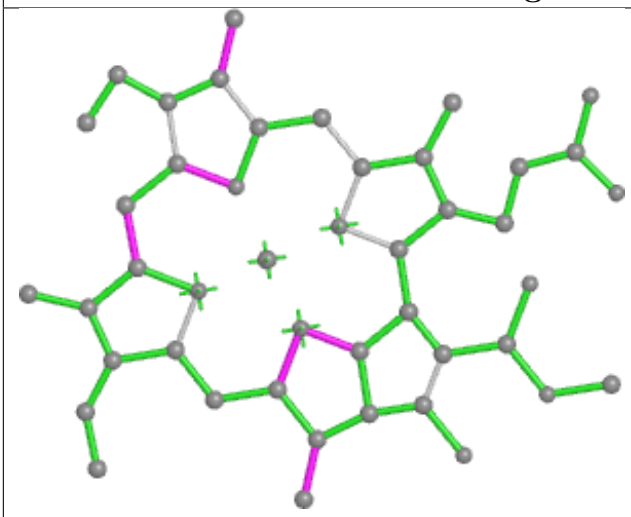

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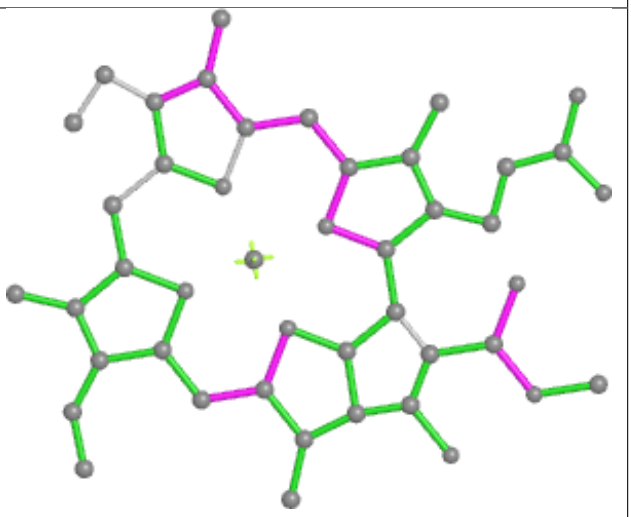
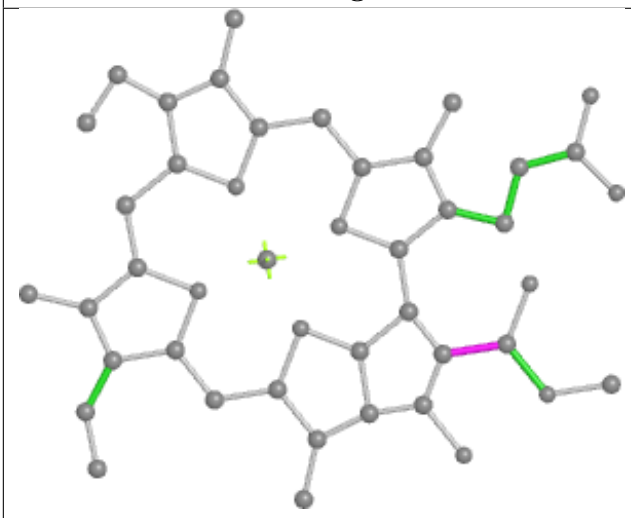


Bond angles



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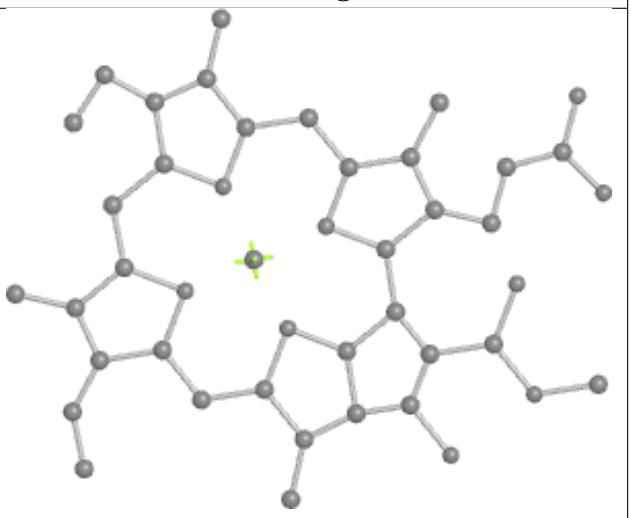

Rings

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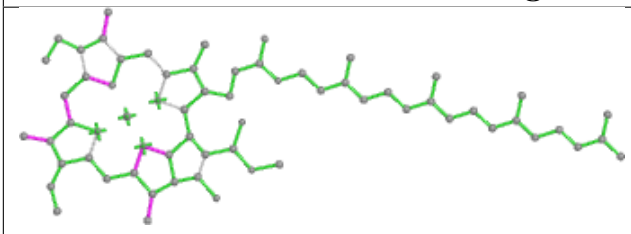
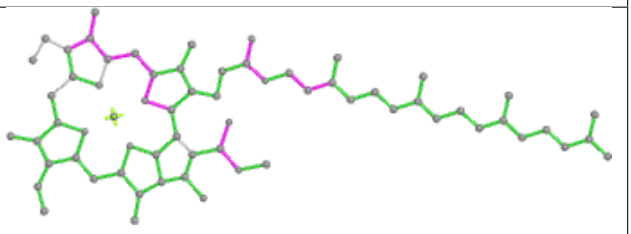
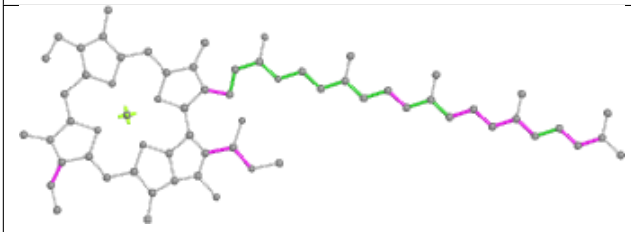


Bond lengths



Bond angles



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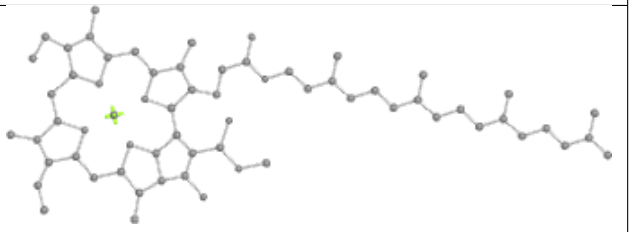

Rings

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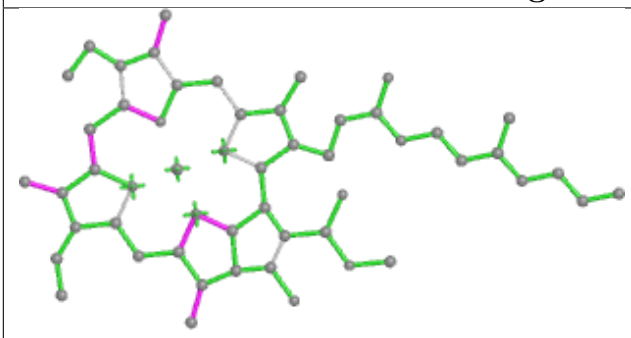
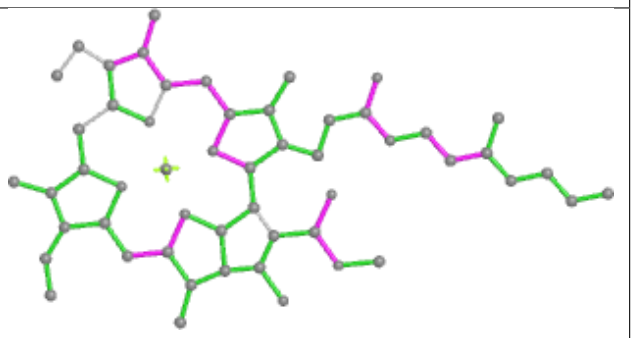
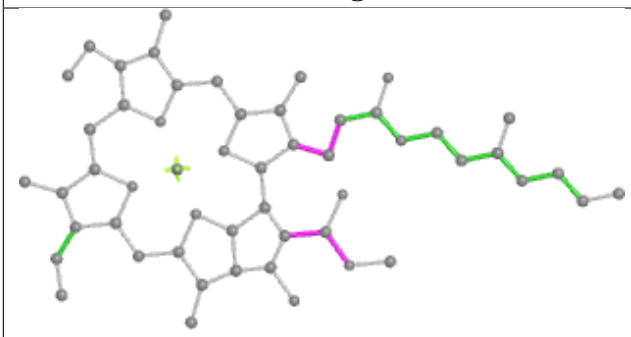
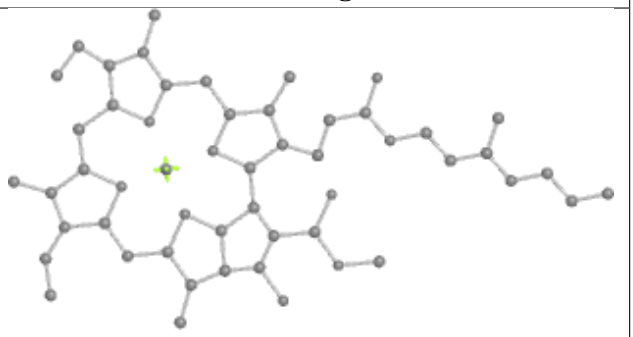
	
Bond lengths	Bond angles
	
Torsions	Rings

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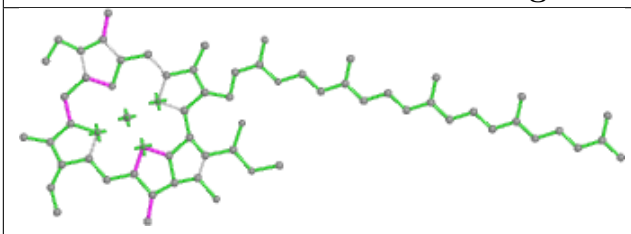
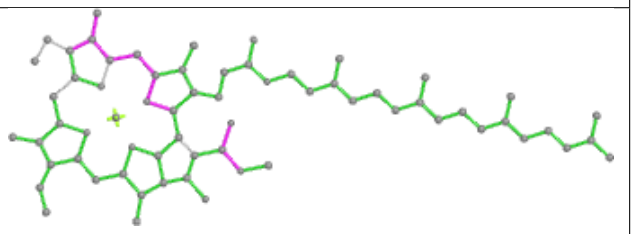
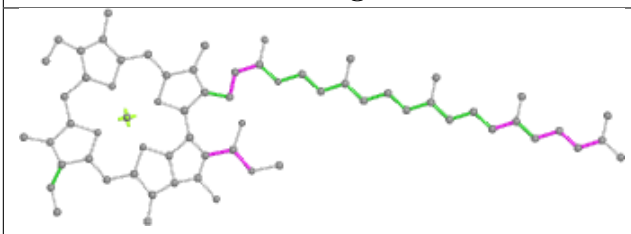
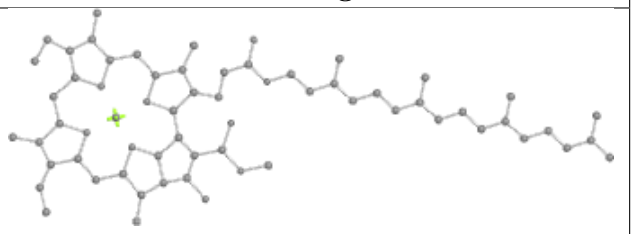
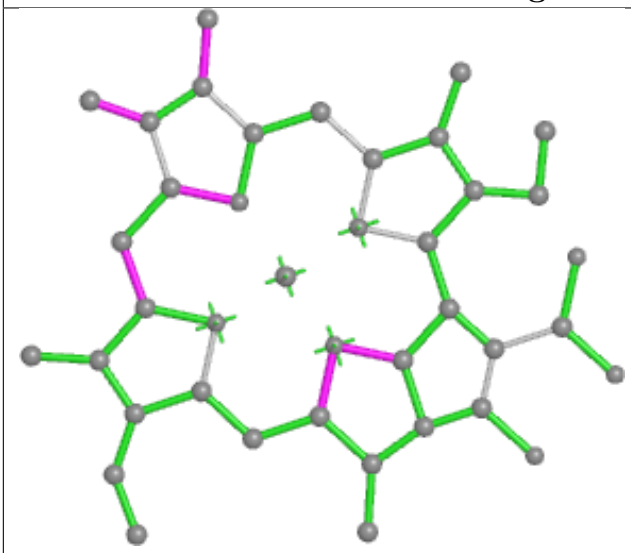
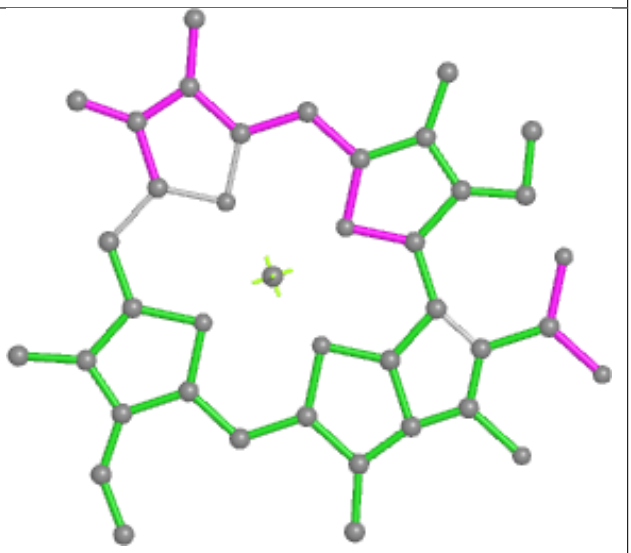
	
Bond lengths	Bond angles
	
Torsions	Rings

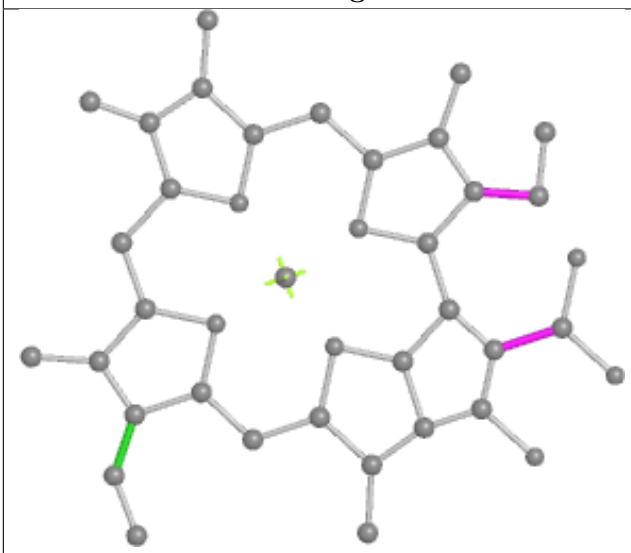
Ligand CLA 7 405



Bond lengths



Bond angles



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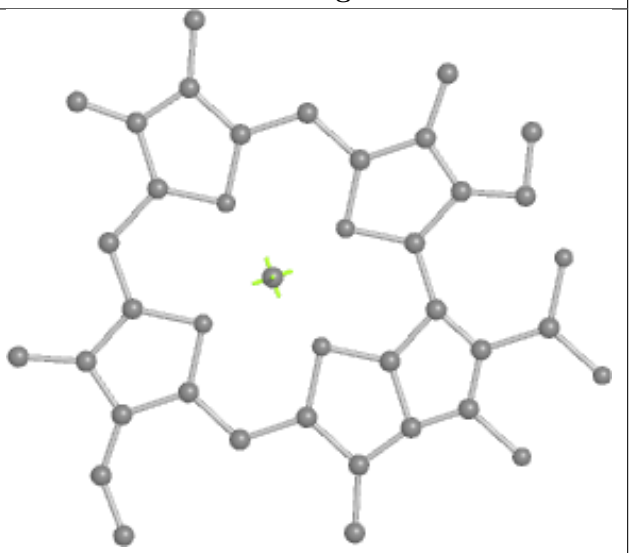
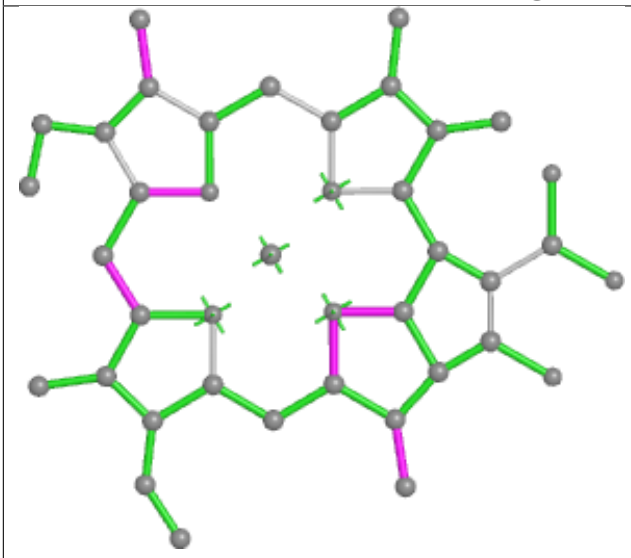


Rings

Ligand CLA 3 413



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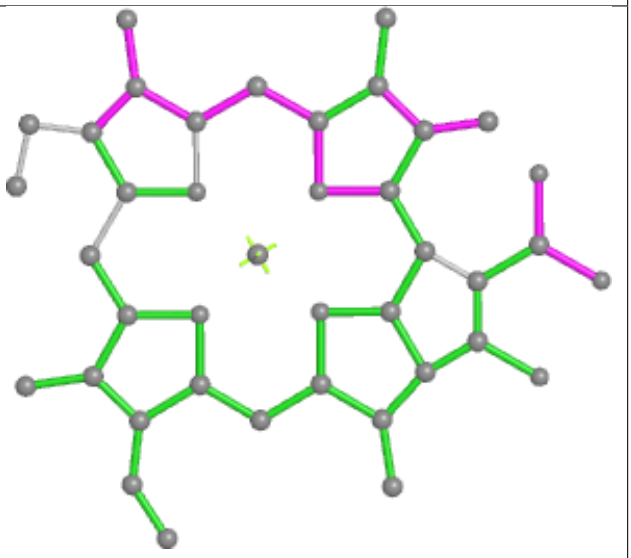
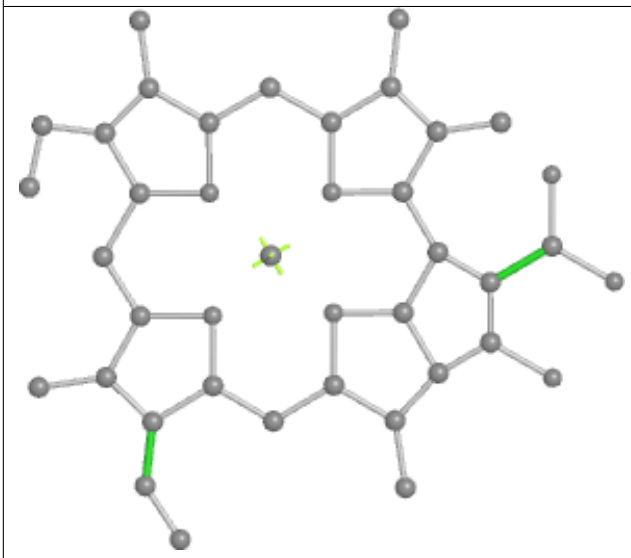


Bond angles



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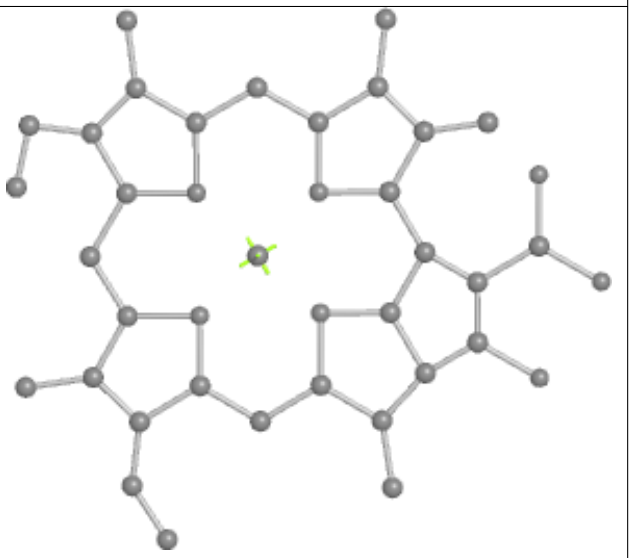
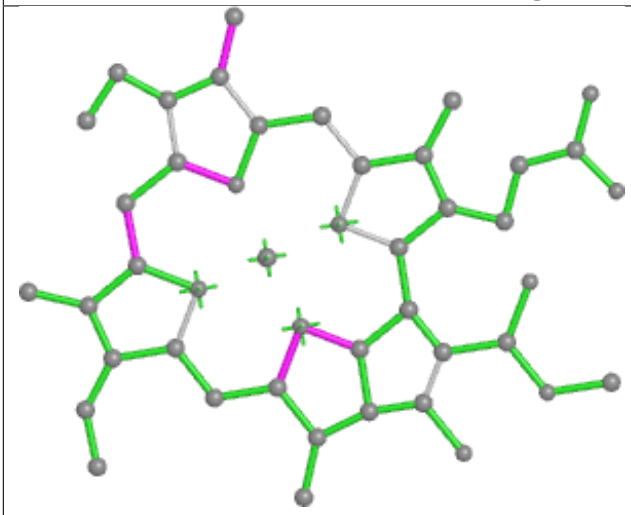


Rings

Ligand CLA 6 608



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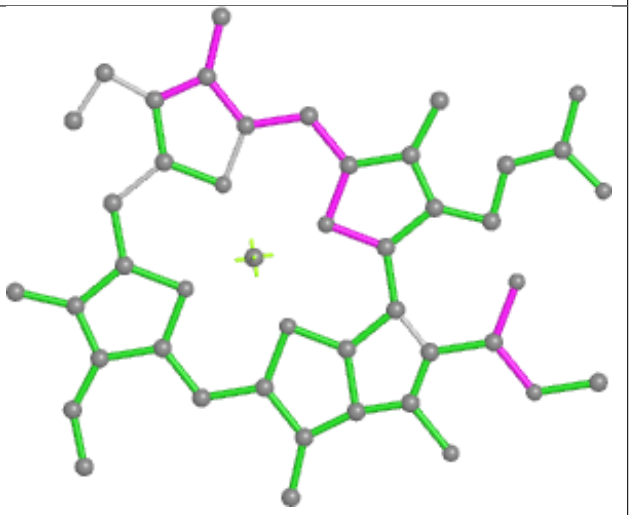
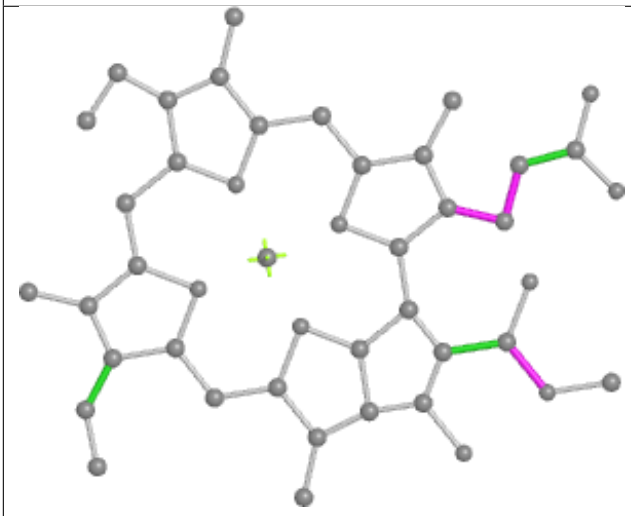


Bond angles



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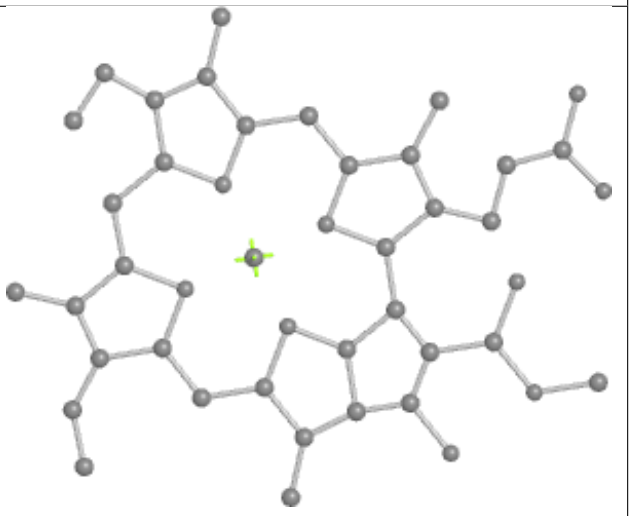
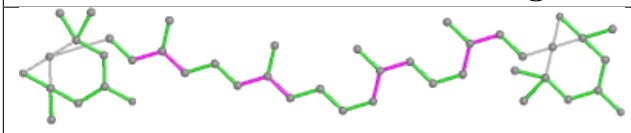


Rings

Ligand XAT 6 617



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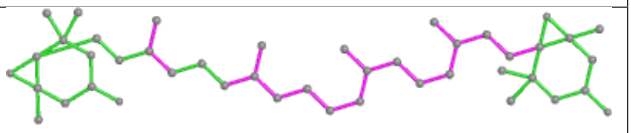
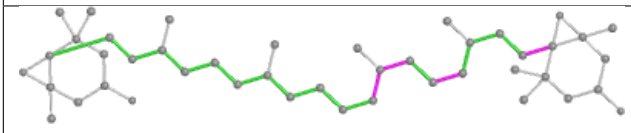


Bond angles



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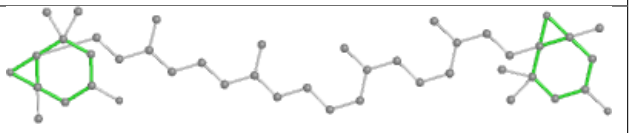
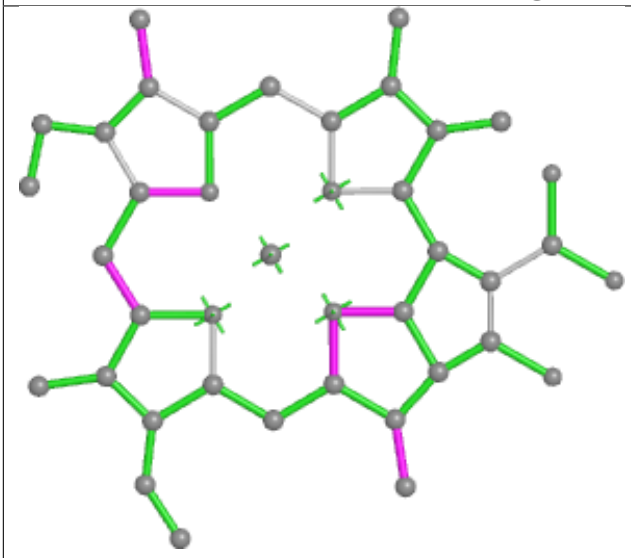


Rings

Ligand CLA 3 401



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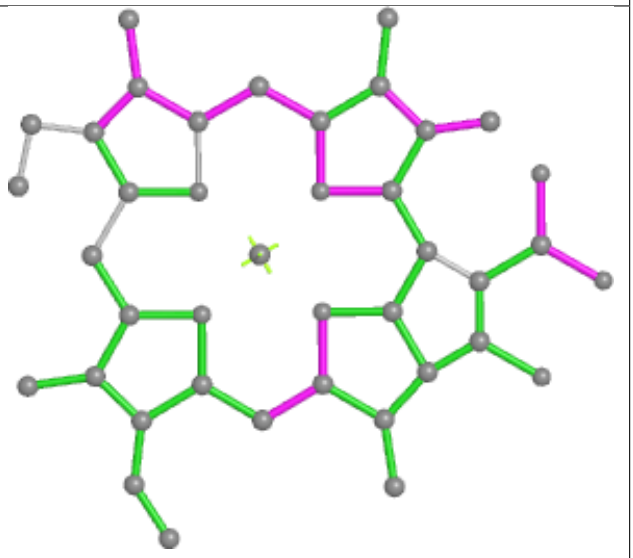
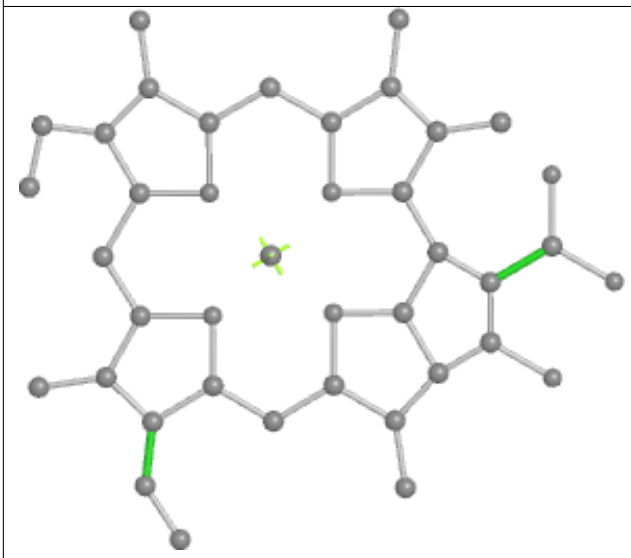


Bond angles



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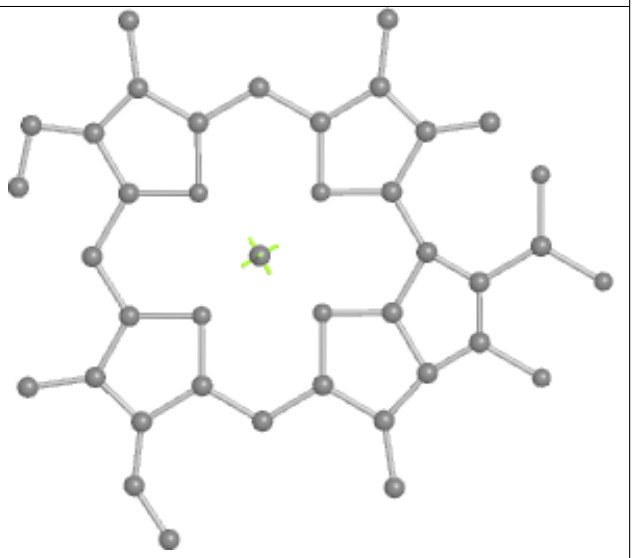
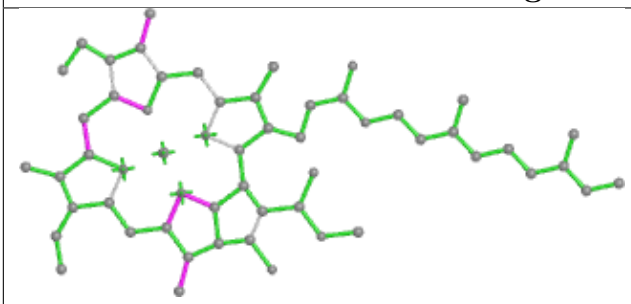


Rings

Ligand CLA B 830



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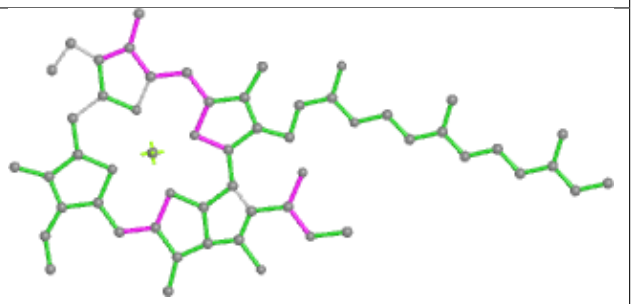
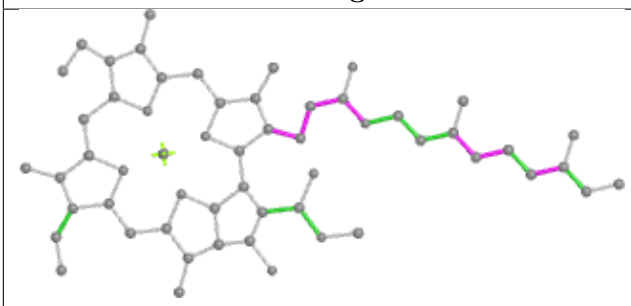
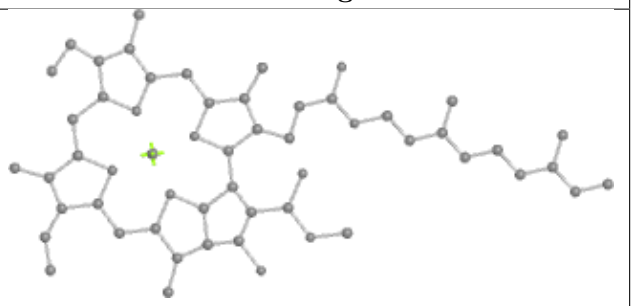


Bond angles

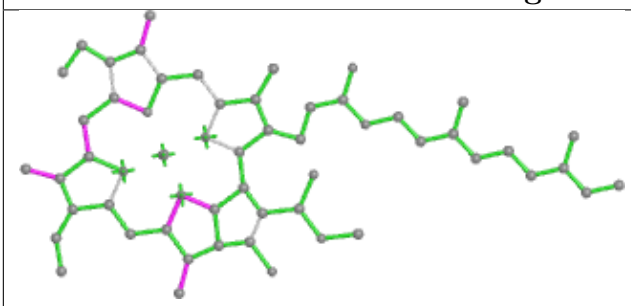


Torsions

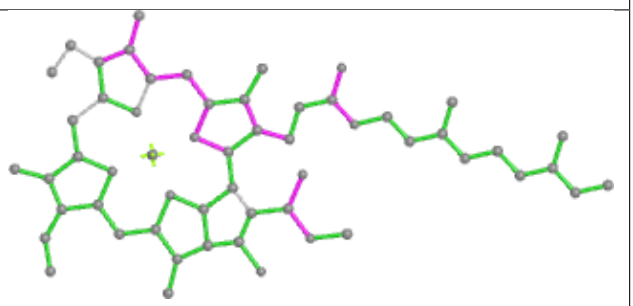


Rings

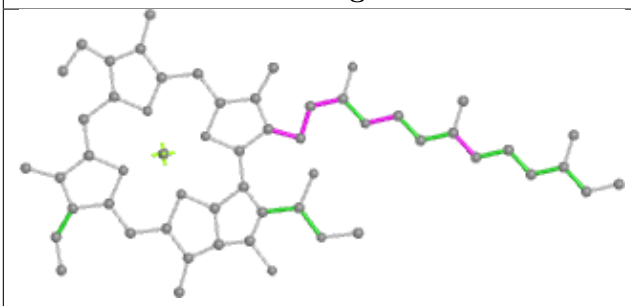
Ligand CLA B 832



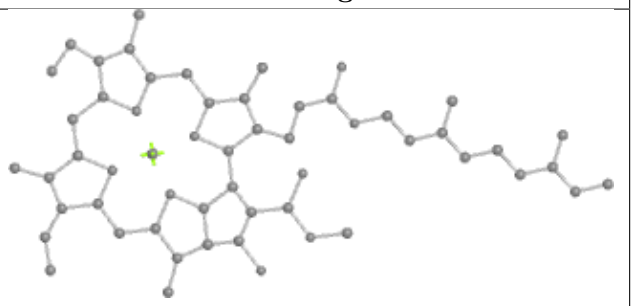
Bond lengths



Bond angles

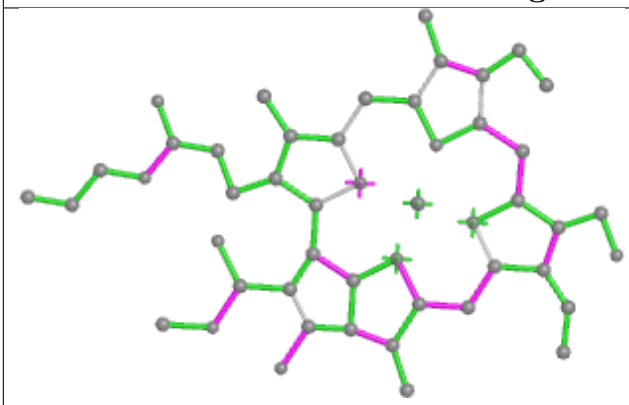


Torsions



Rings

Ligand CHL c 601



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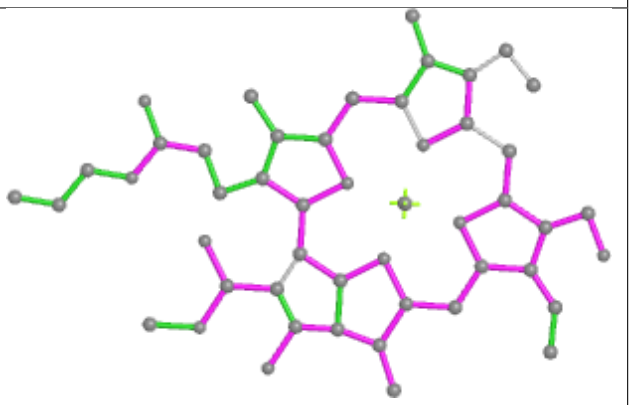

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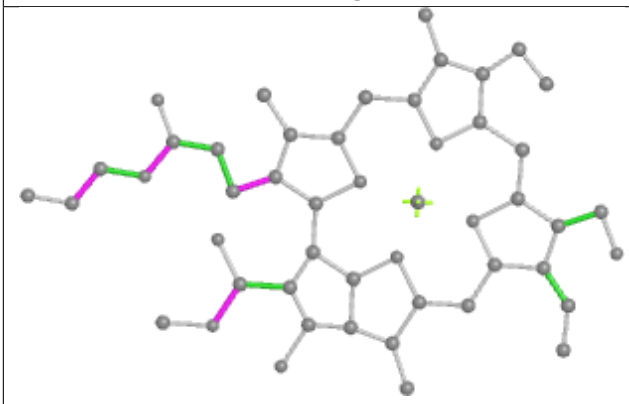

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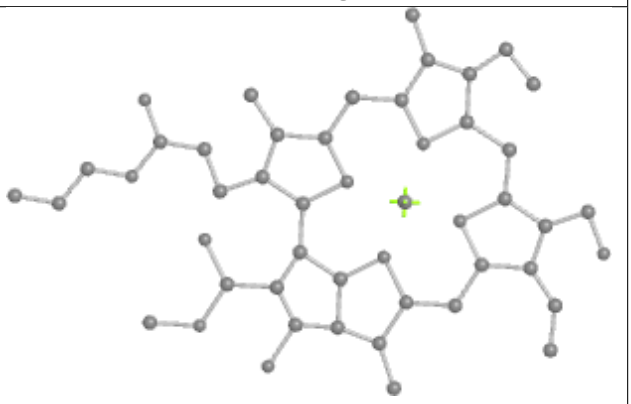
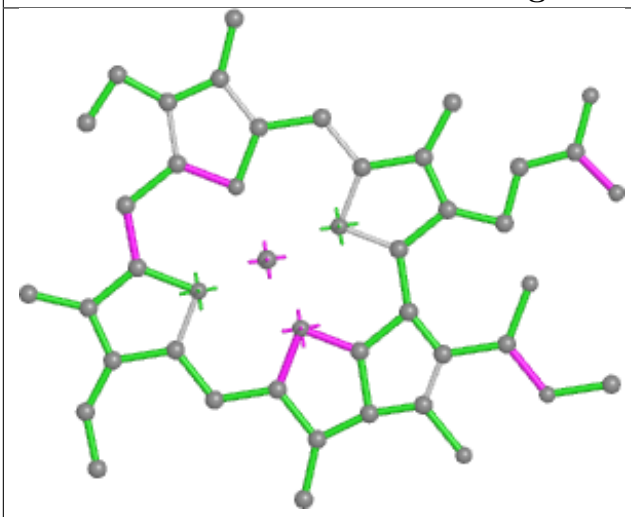


Rings

Ligand CLA 8 609



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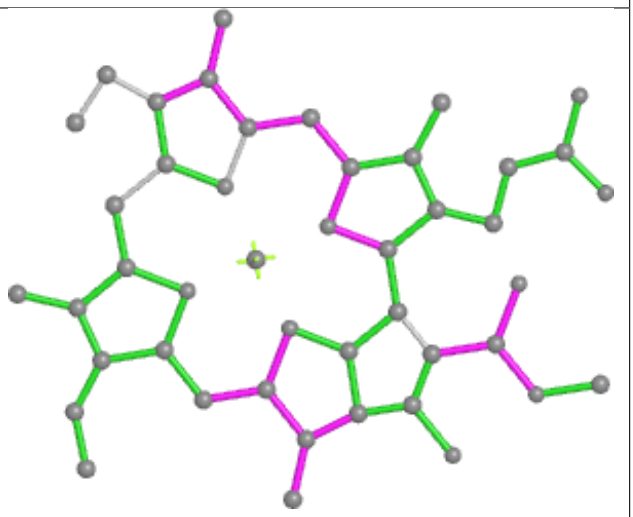

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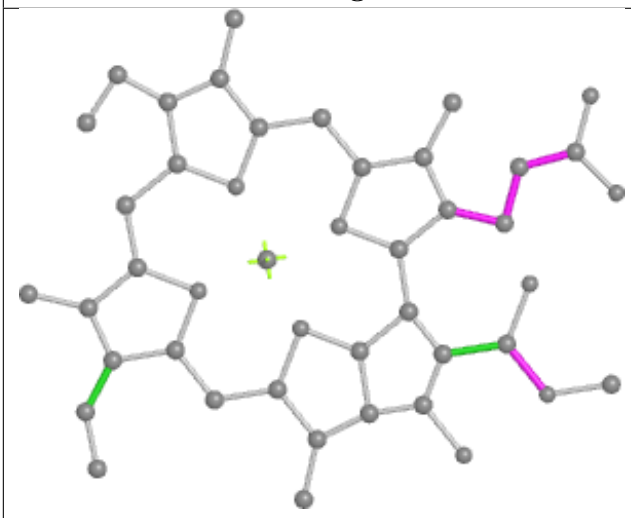

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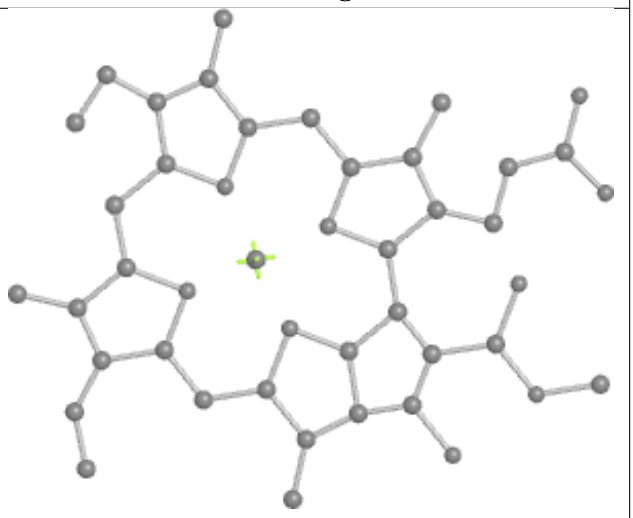

Rings

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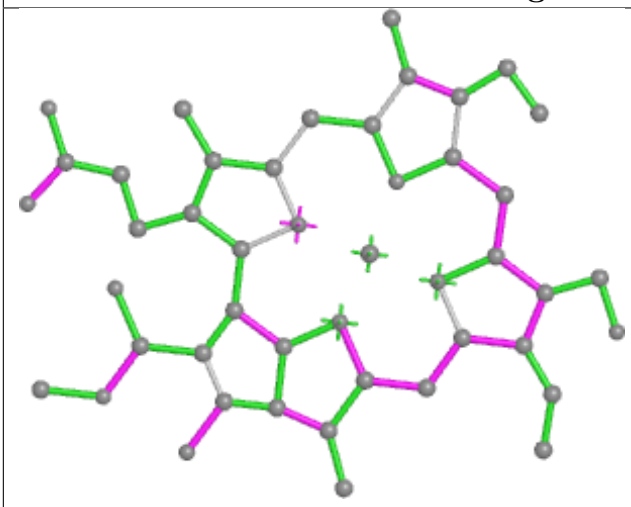

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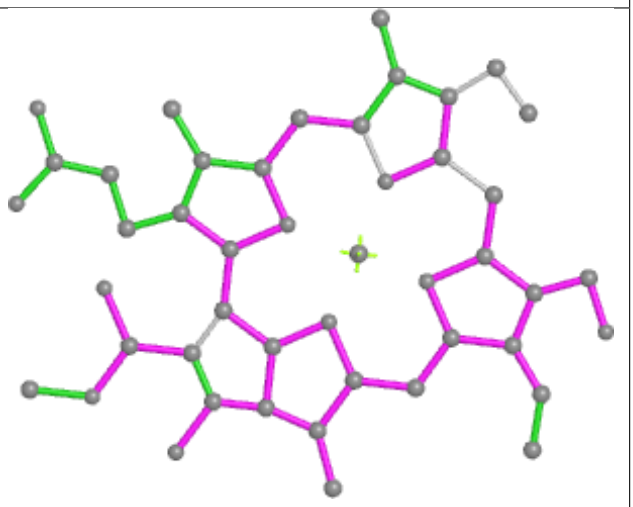
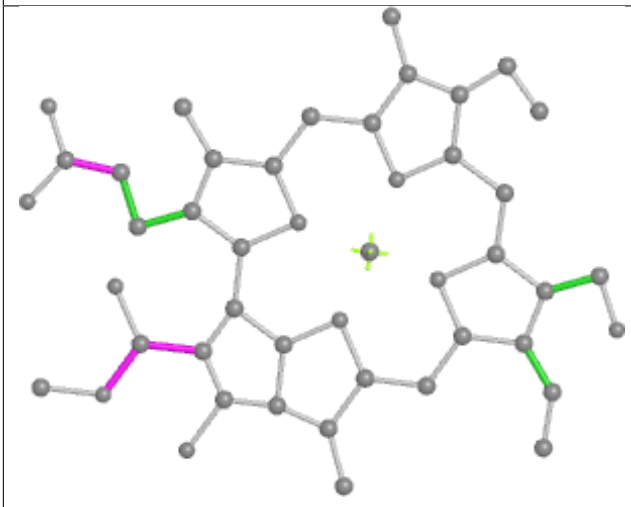


Bond angles



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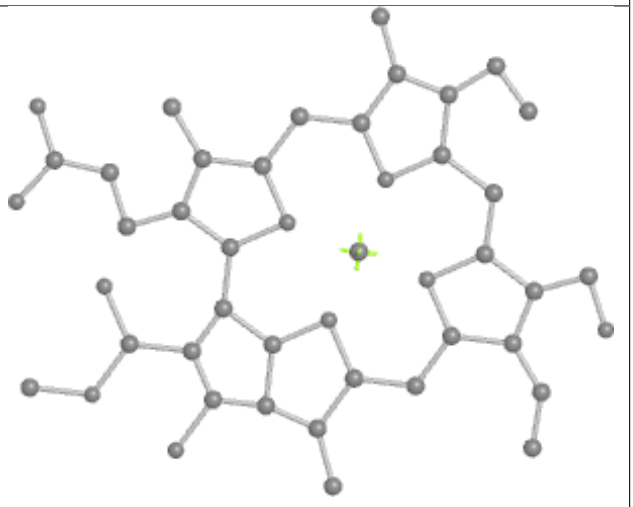
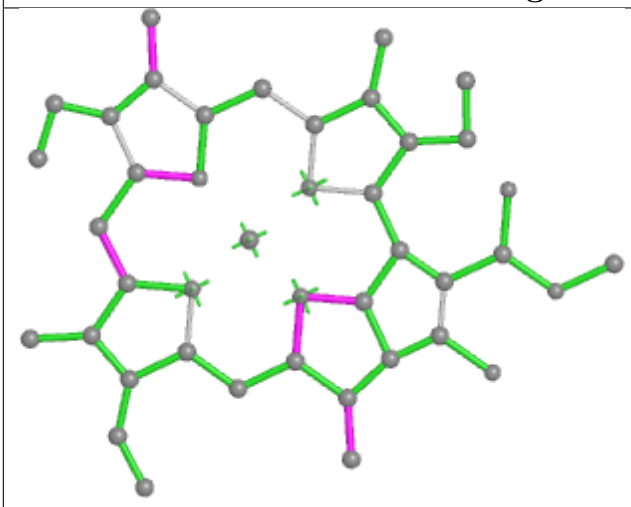


Rings

Ligand CLA L 304



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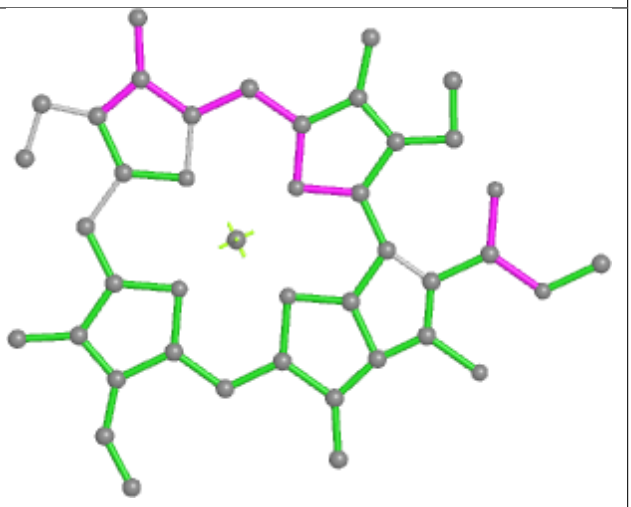

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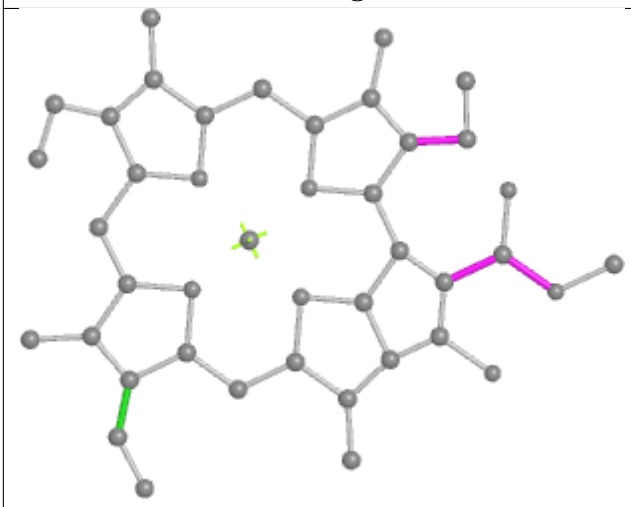

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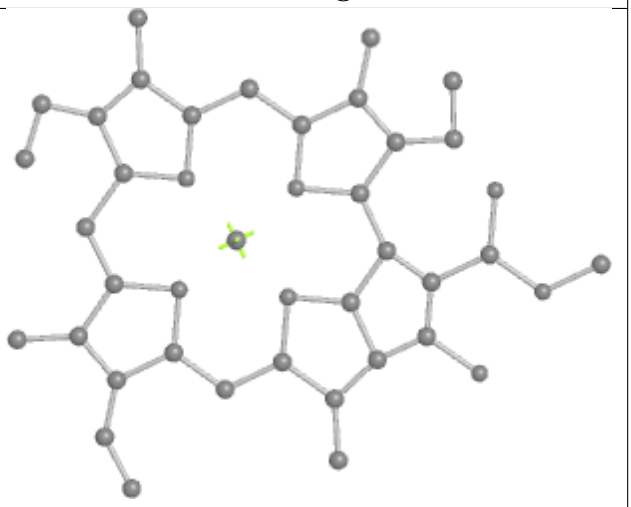
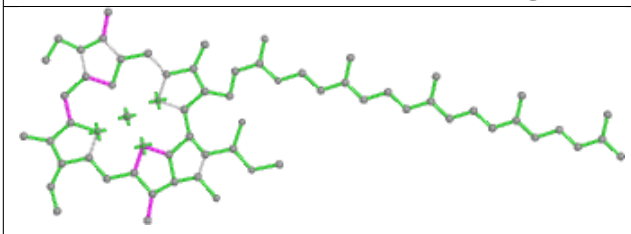


Rings

Ligand CLA B 838



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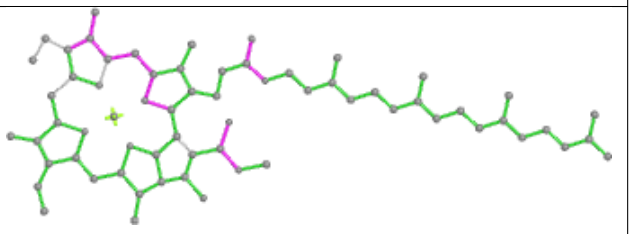

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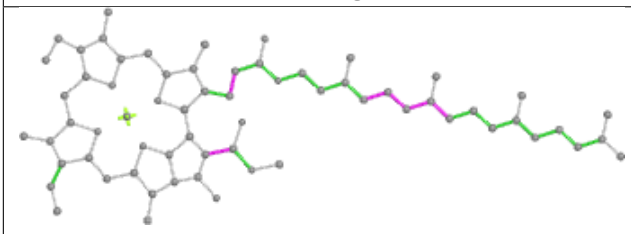

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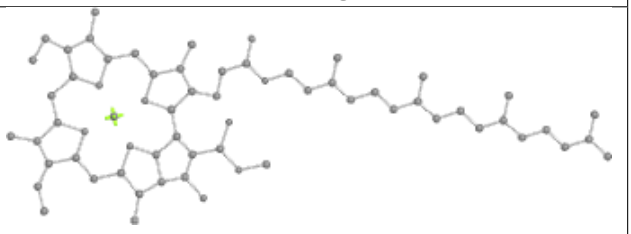
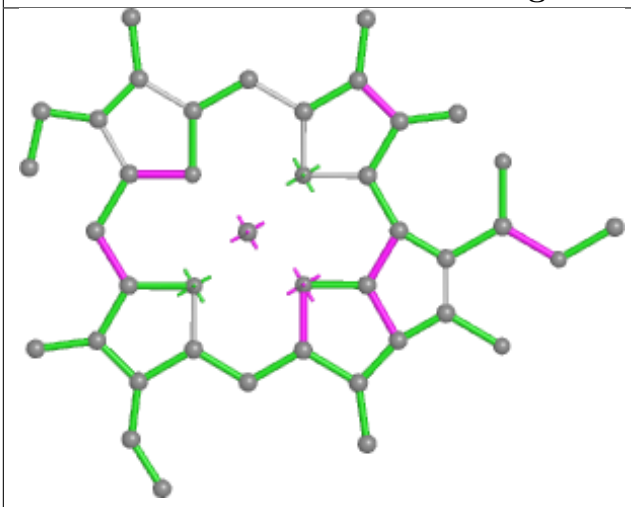


Rings

Ligand CLA 1 309



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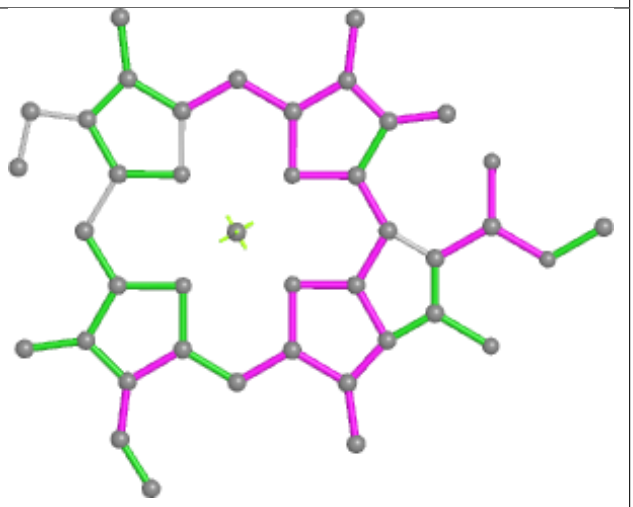
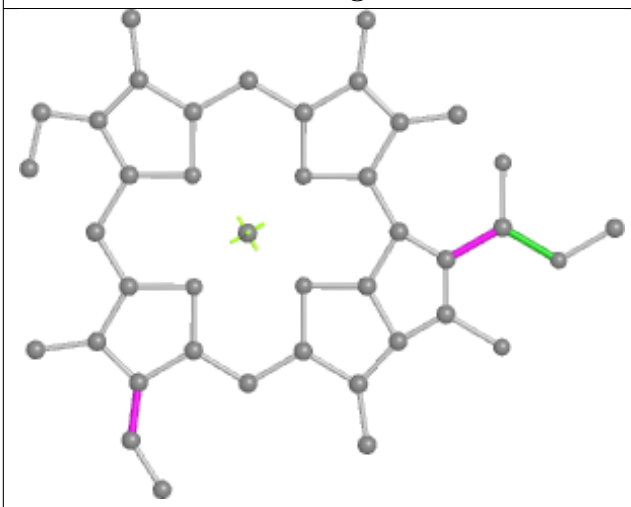


Bond angles



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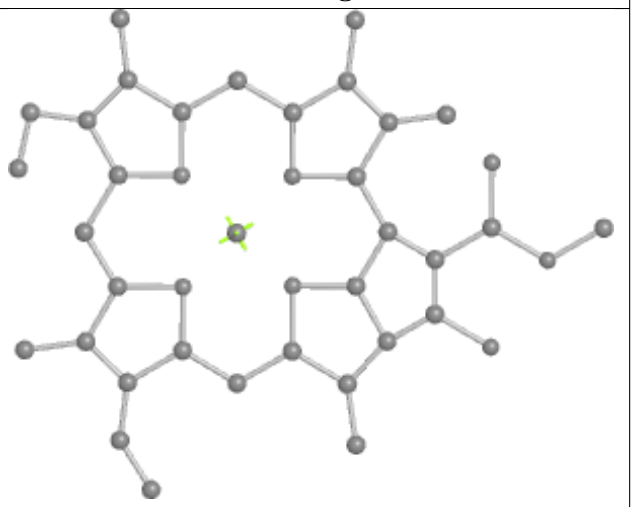
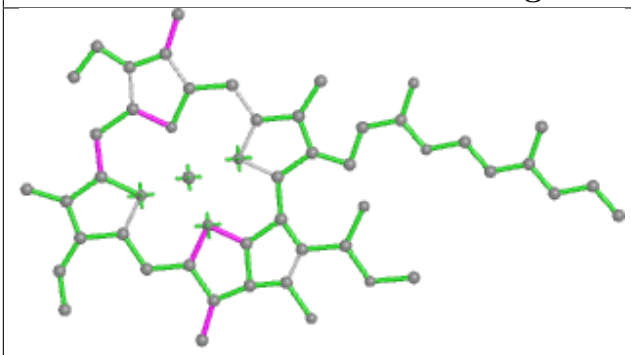


Rings

Ligand CLA B 826



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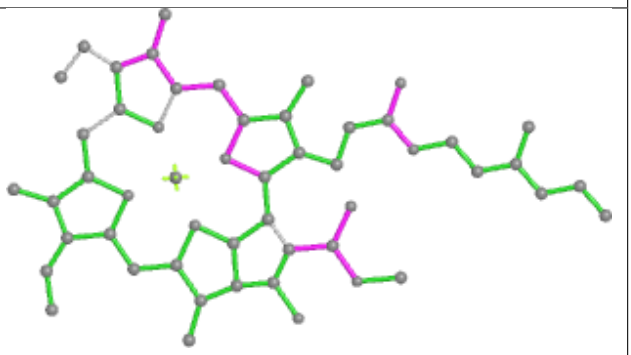
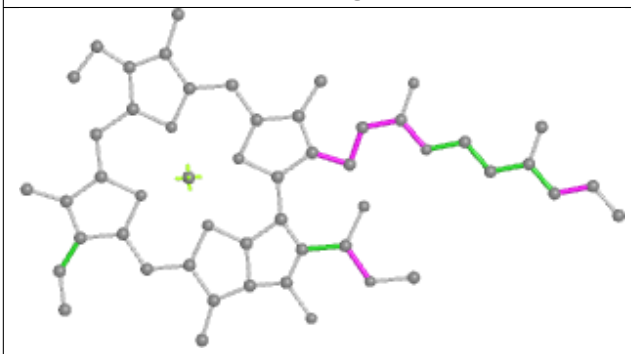


Bond angles



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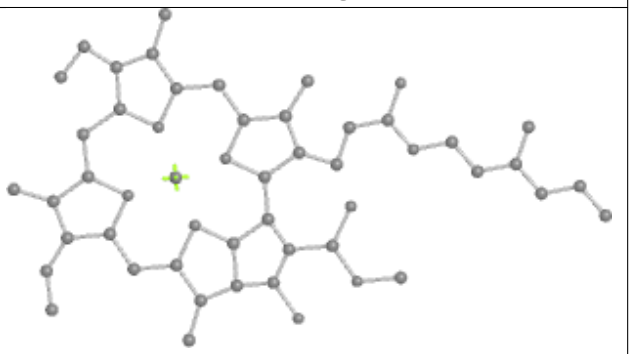
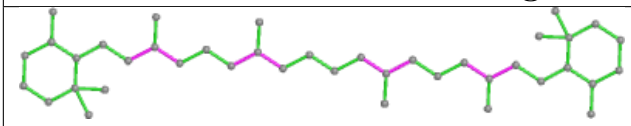


Rings

Ligand BCR A 849



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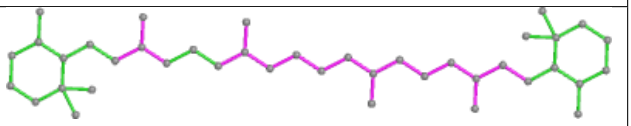
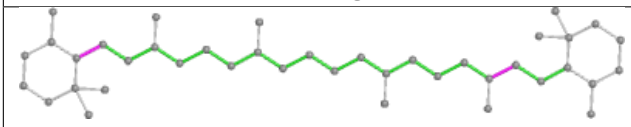


Bond angles



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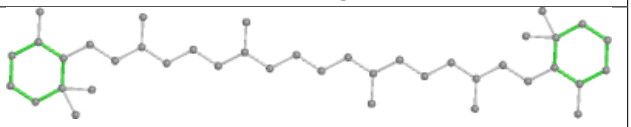
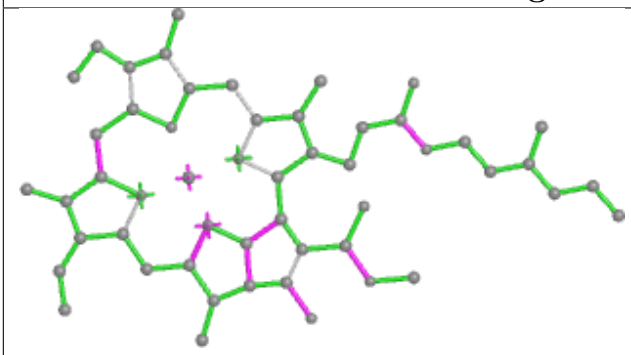


Rings

Ligand CLA 4 609



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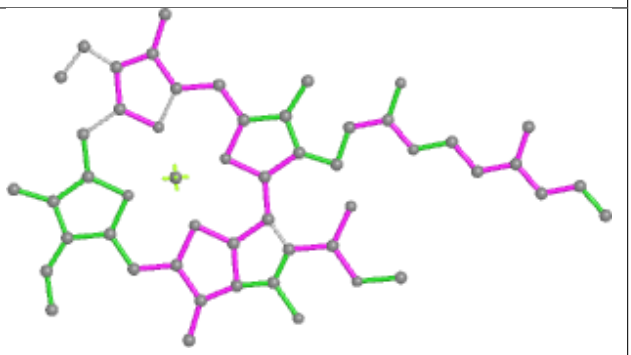
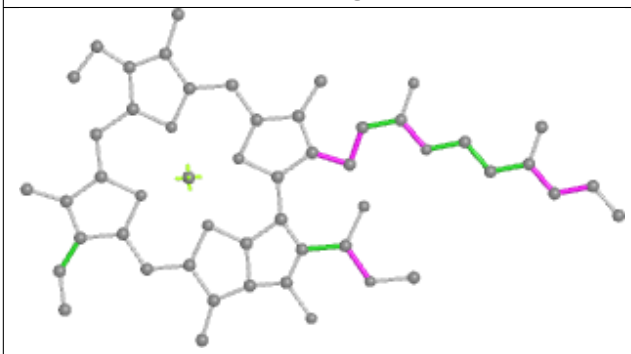


Bond angles



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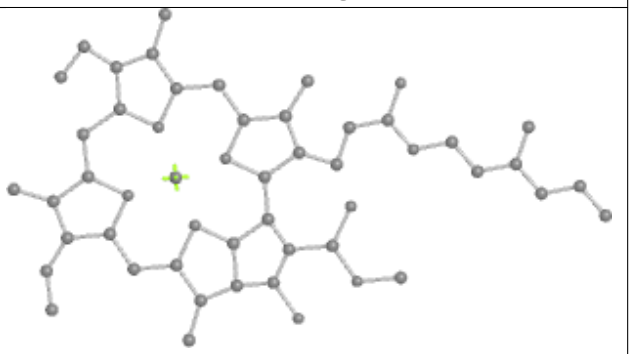
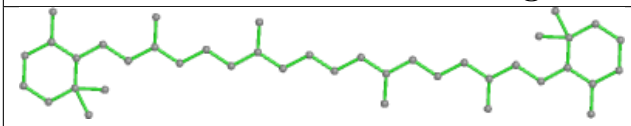


Rings

Ligand BCR B 843



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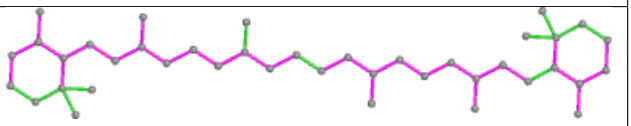
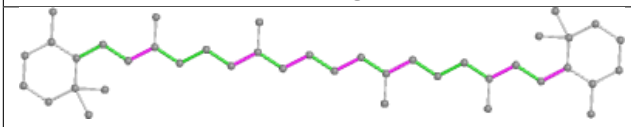


Bond angles



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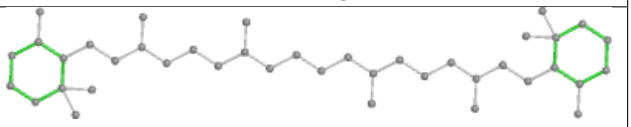
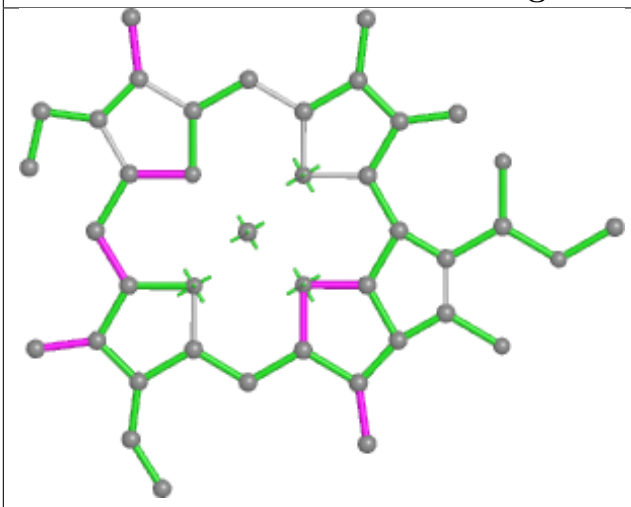


Rings

Ligand CLA 8 618



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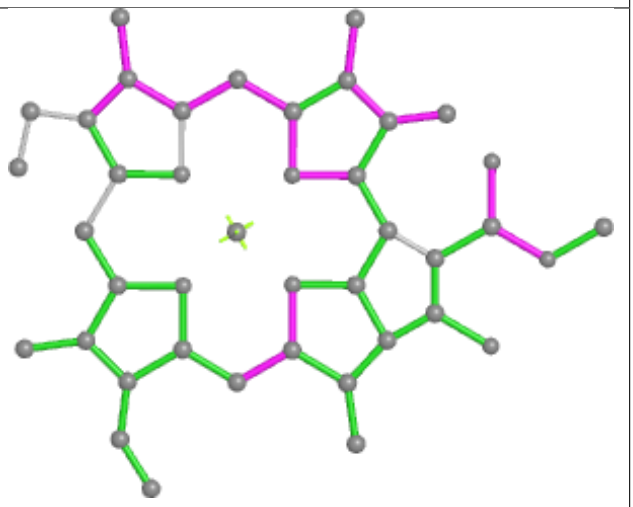
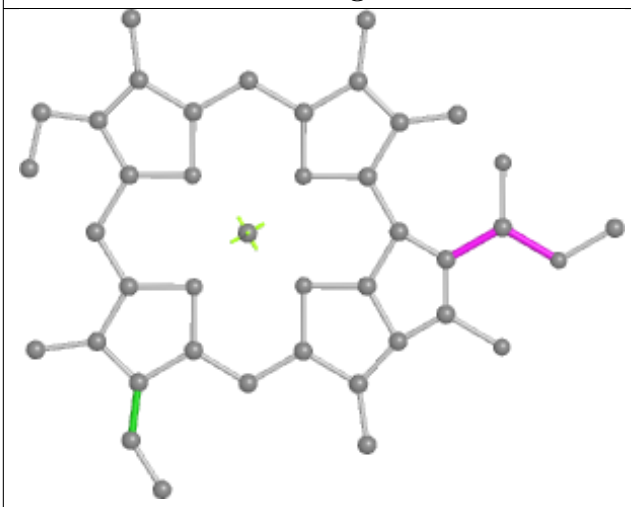


Bond angles



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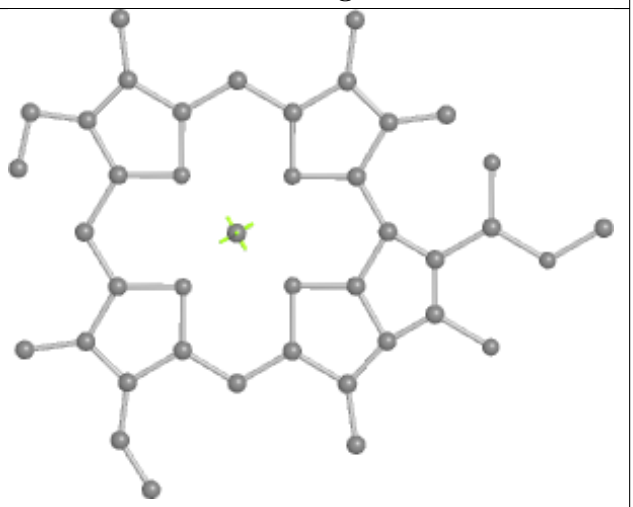
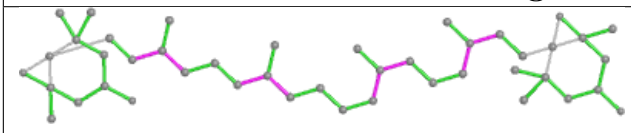


Rings

Ligand XAT 2 617



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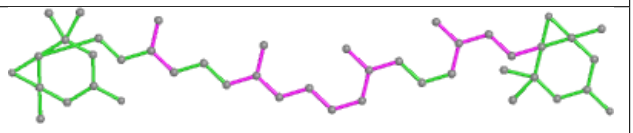
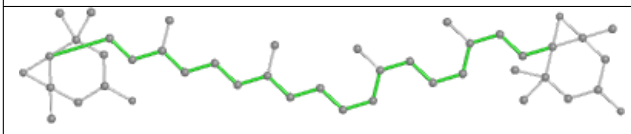
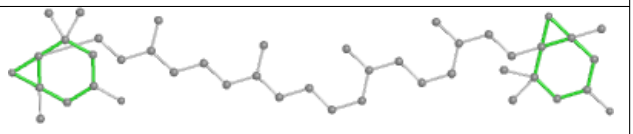


Bond angles

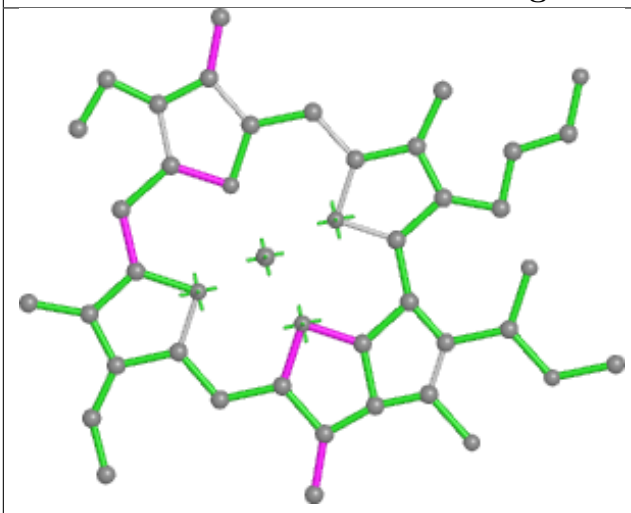


Torsions



Rings

Ligand CLA c 612



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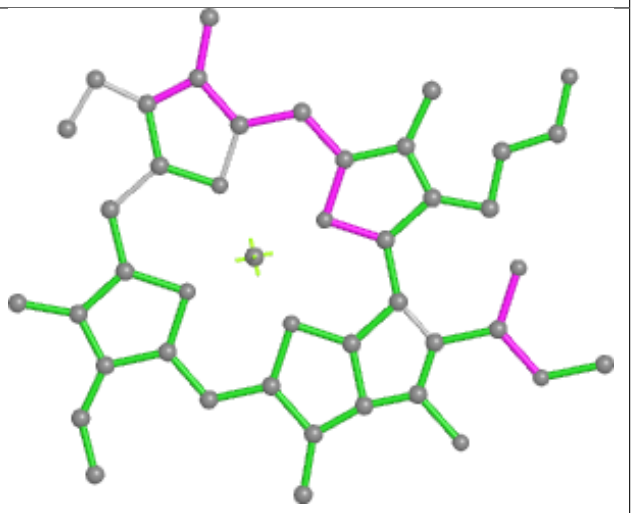
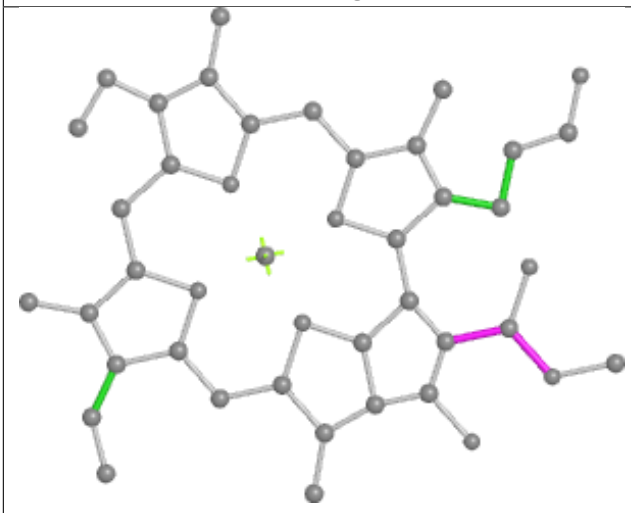


Bond angles



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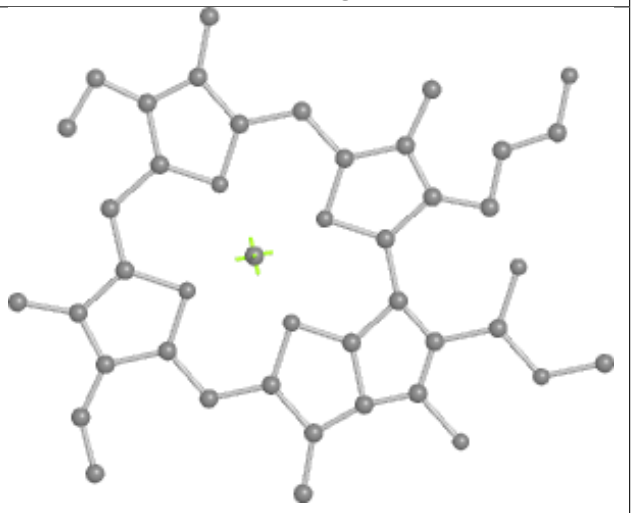
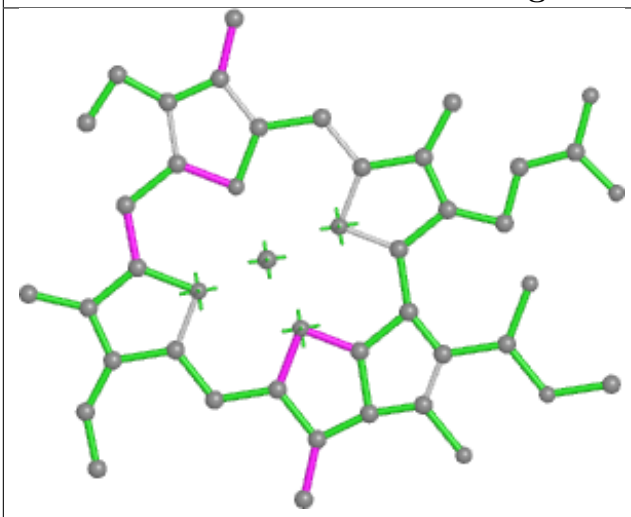


Rings

Ligand CLA 1 312



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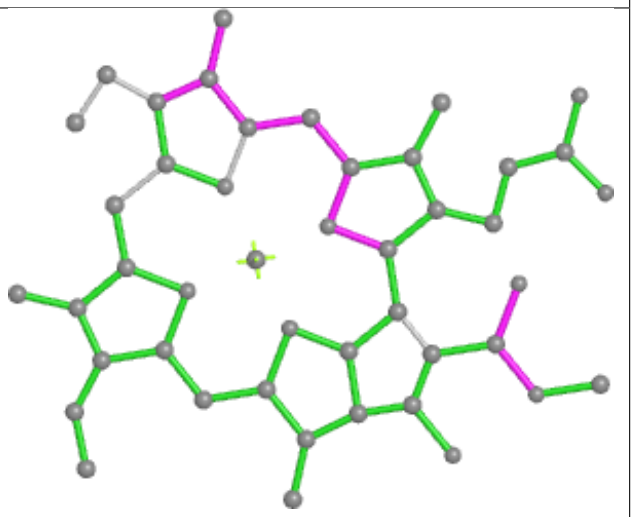

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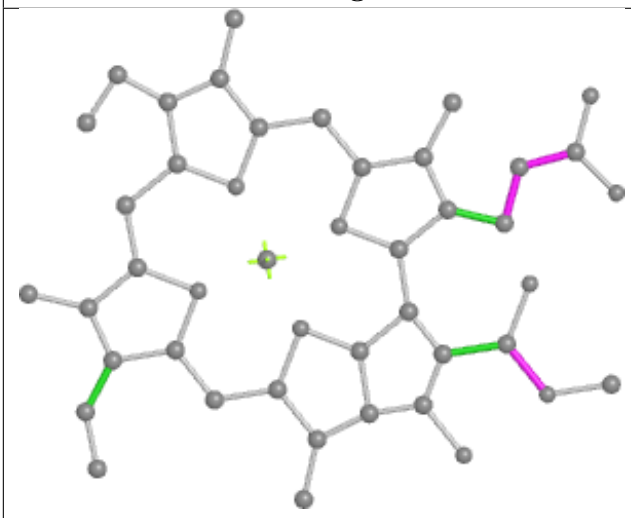

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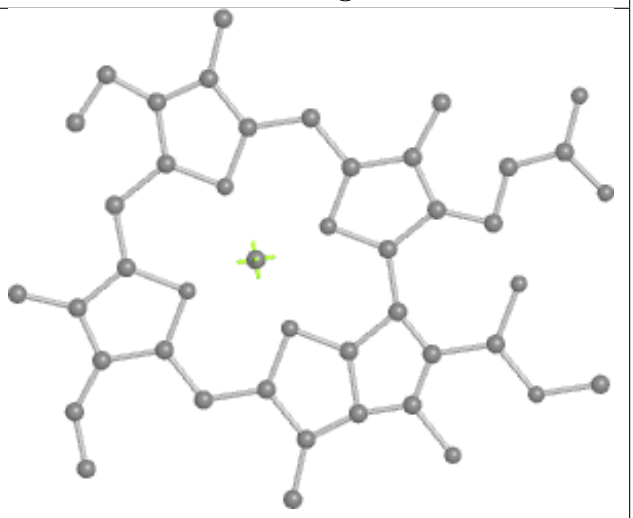
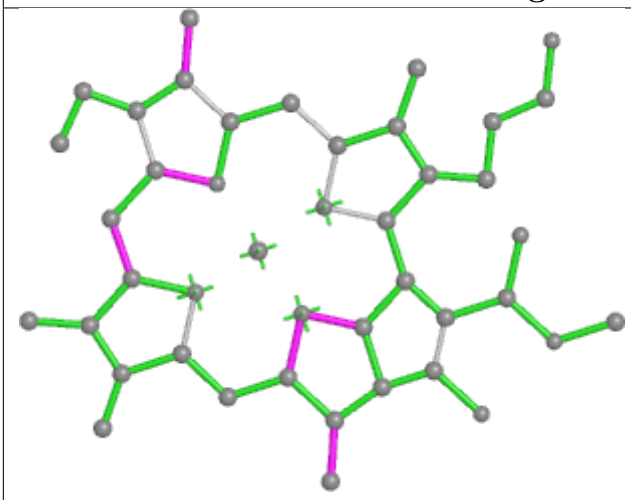


Rings

Ligand CLA 4 604



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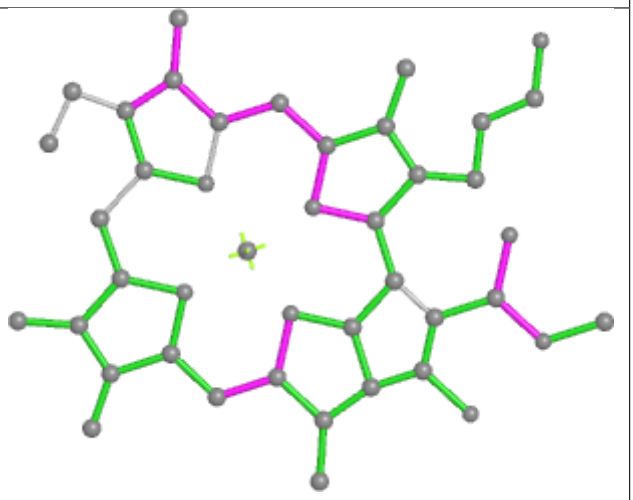

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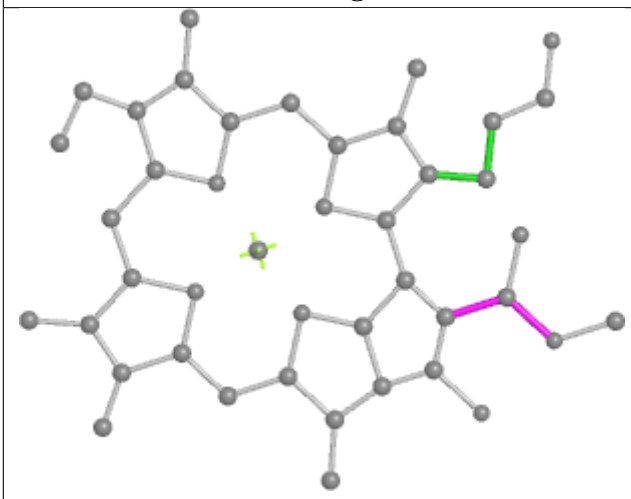

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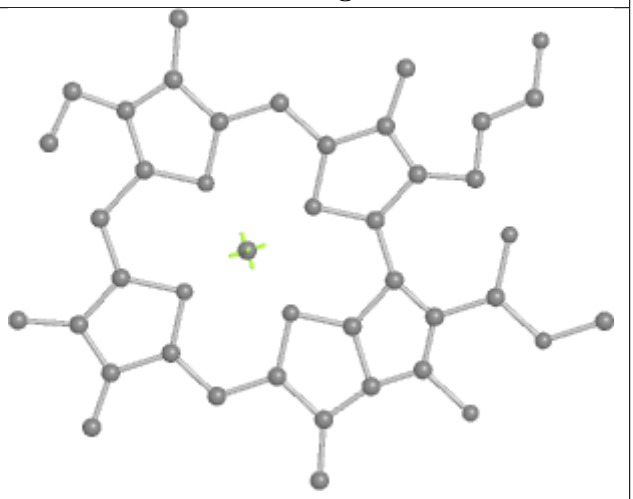
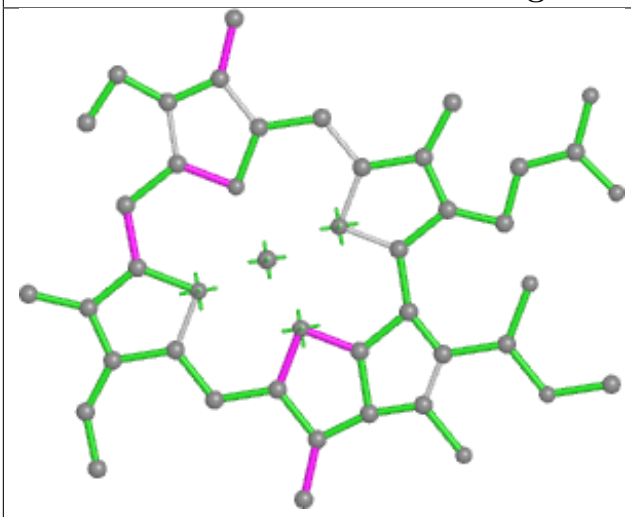


Rings

Ligand CLA b 313



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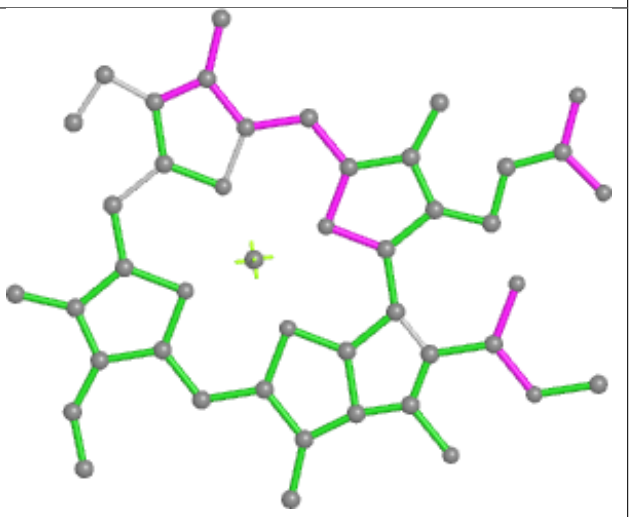

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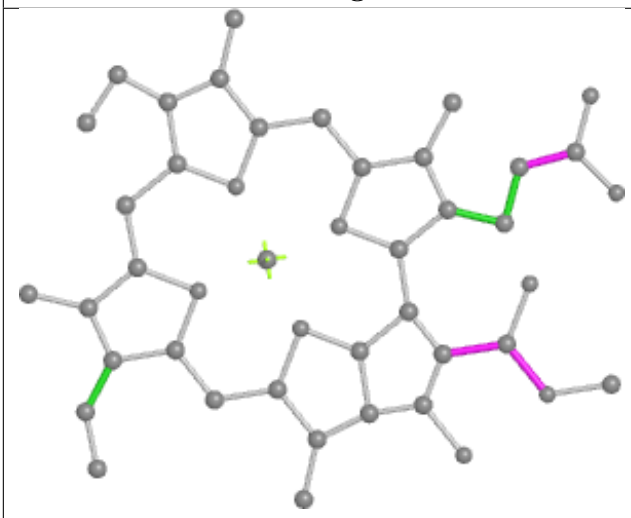

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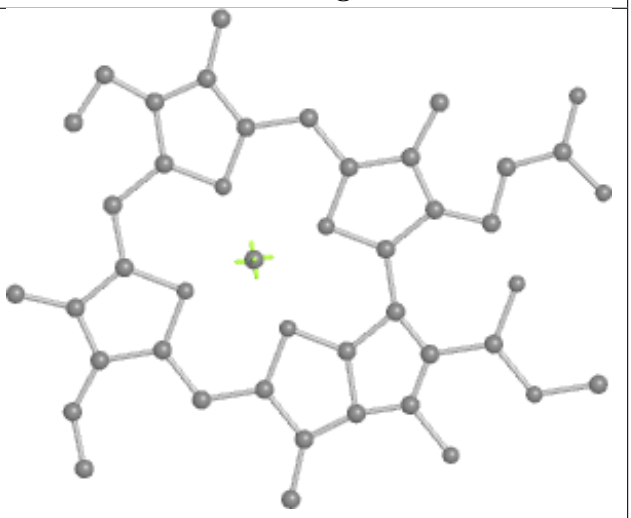

Rings

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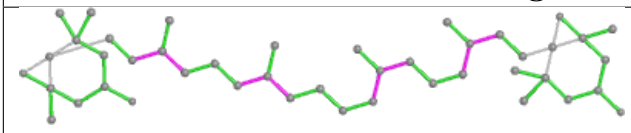

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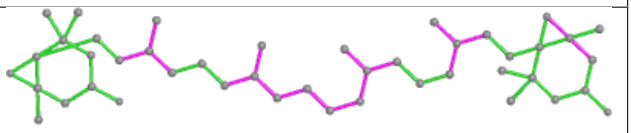
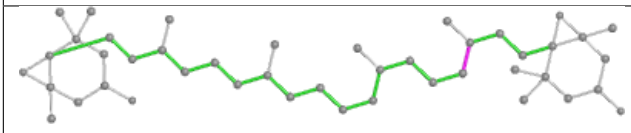


Bond angles



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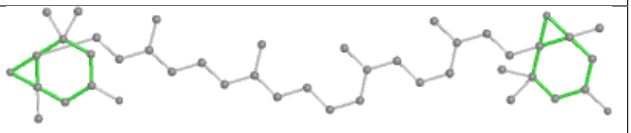
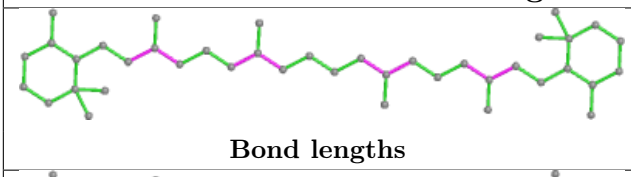


Rings

Ligand BCR J 101



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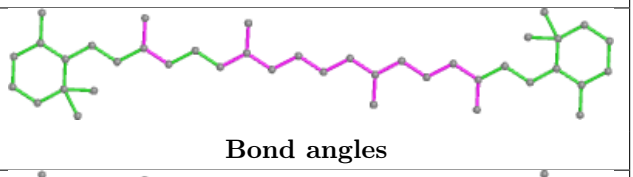

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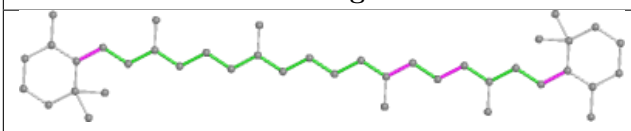

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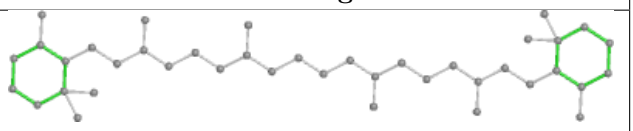
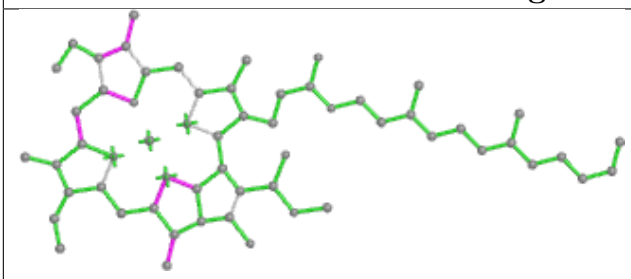


Rings

Ligand CLA 3 408



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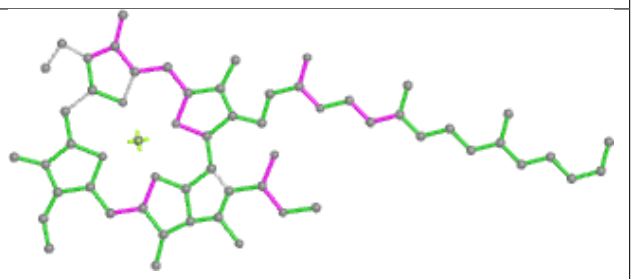

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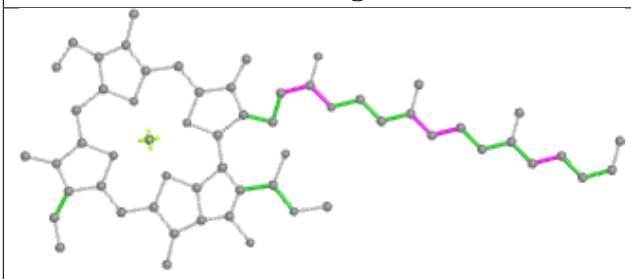

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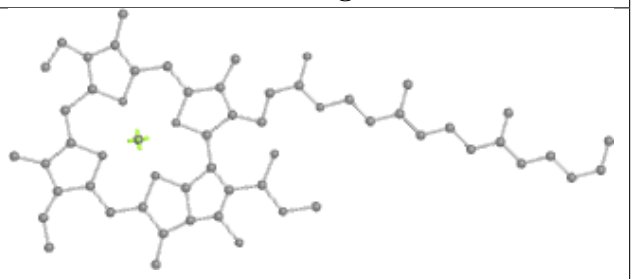
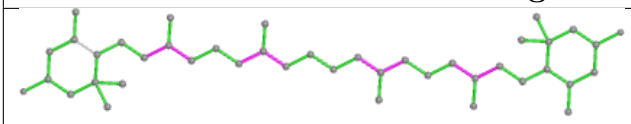


Rings

Ligand LUT 8 614



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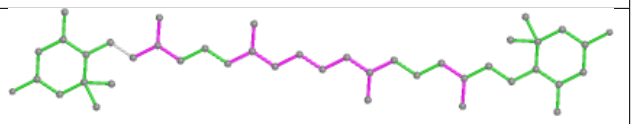

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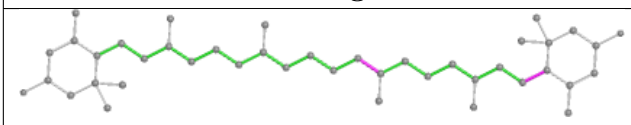

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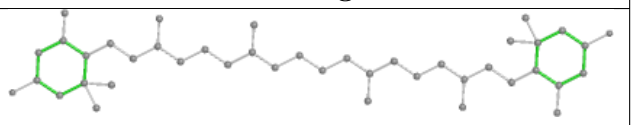
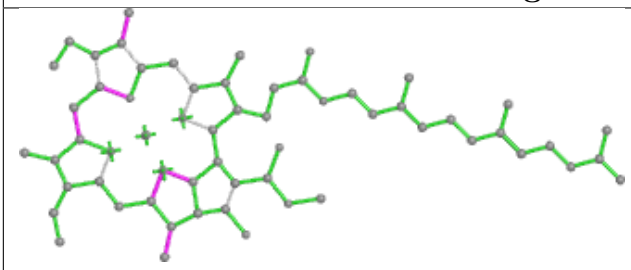
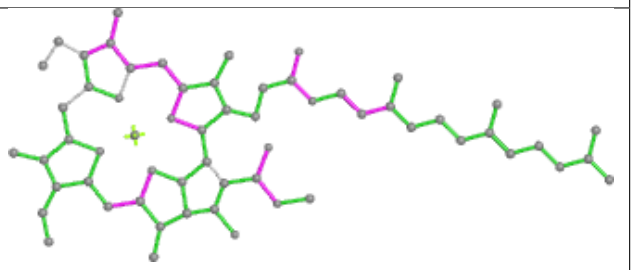
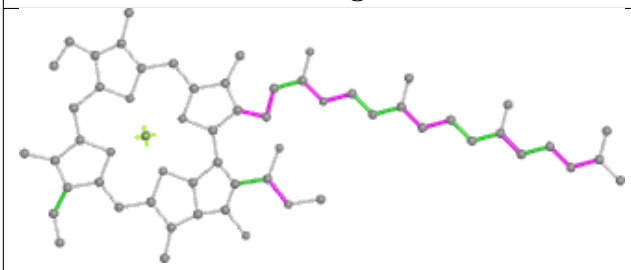
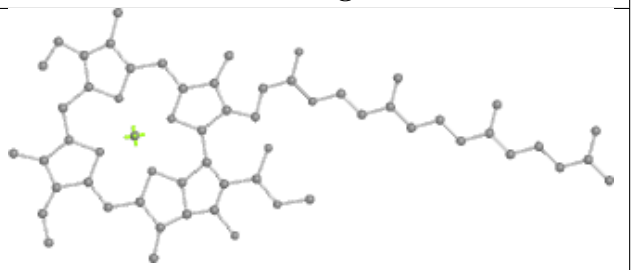


Rings

Ligand CLA A 828	
 Bond lengths	 Bond angles
 Torsions	 Rings

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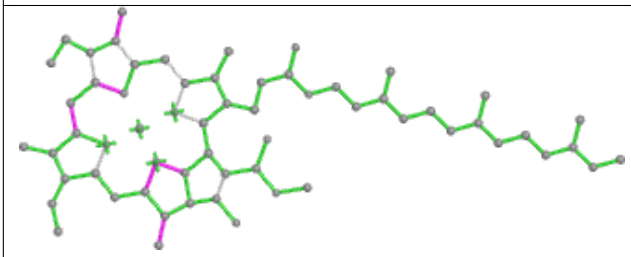
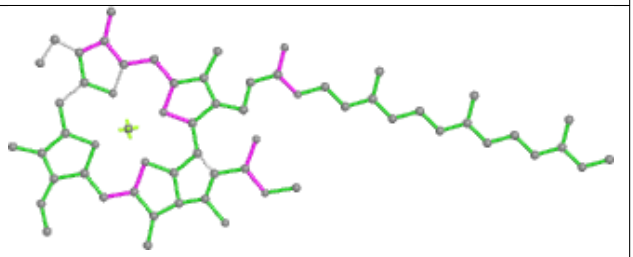
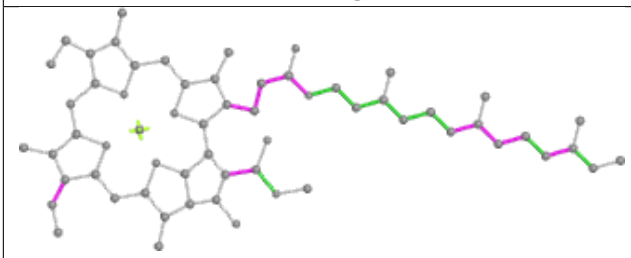
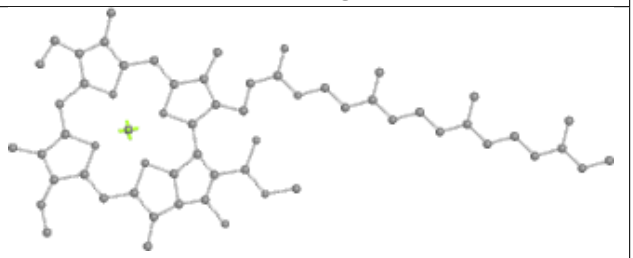
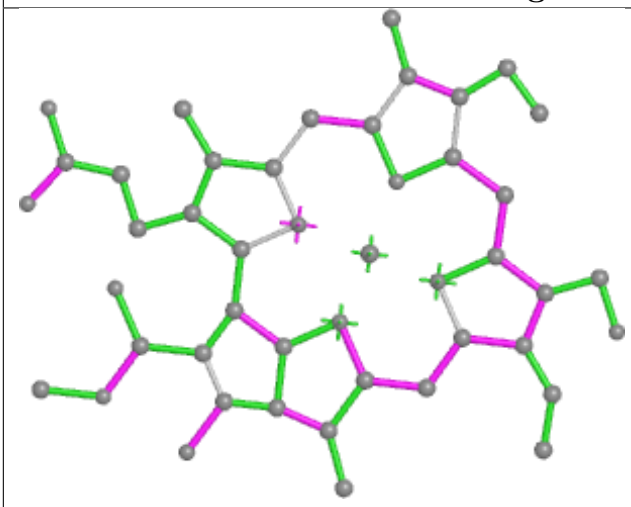
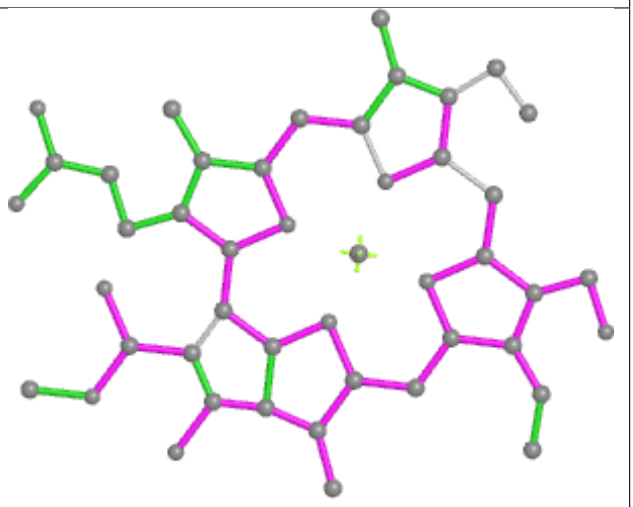
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CHL 5 606



Bond lengths



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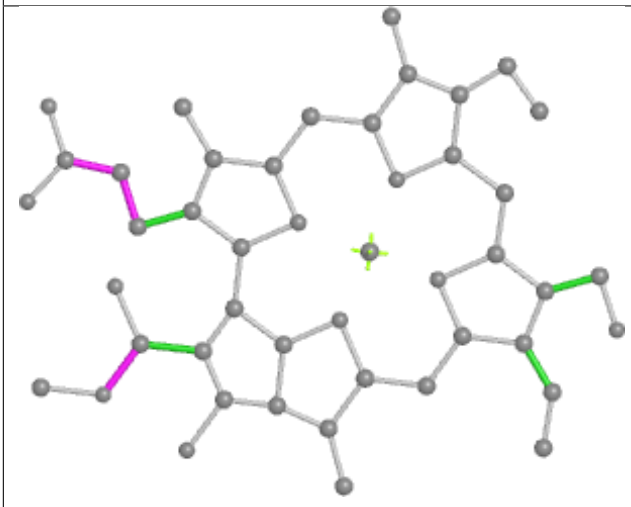

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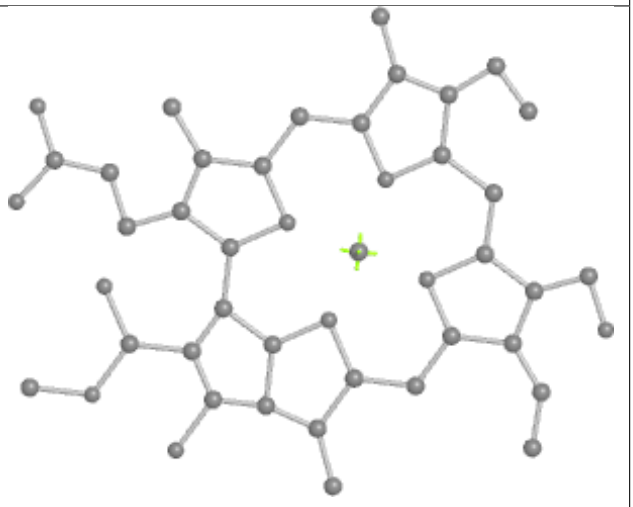
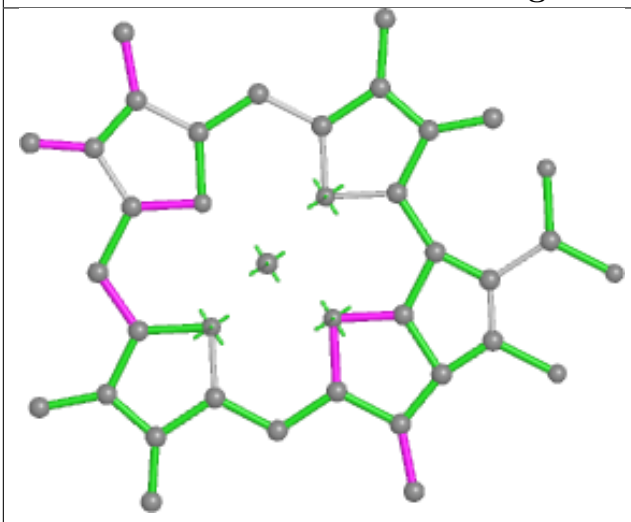


Rings

Ligand CLA 1 311



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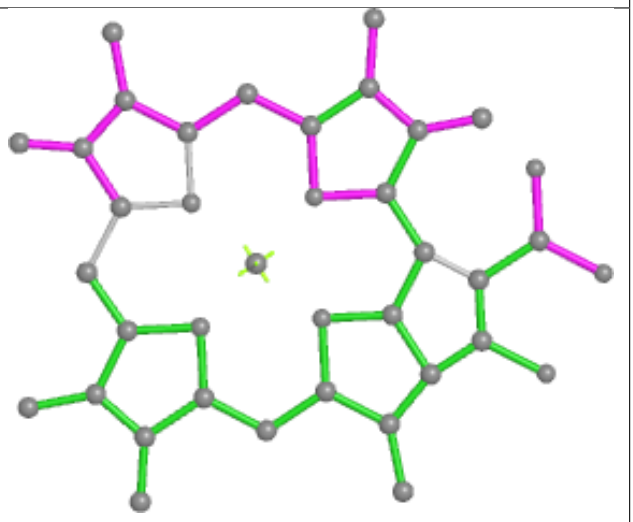
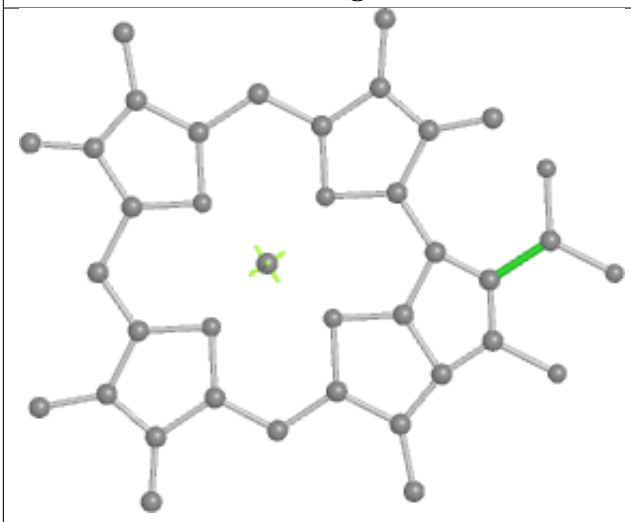


Bond angles



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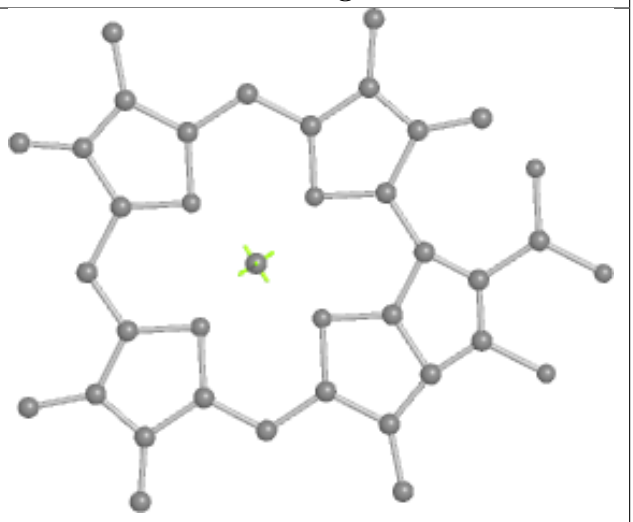
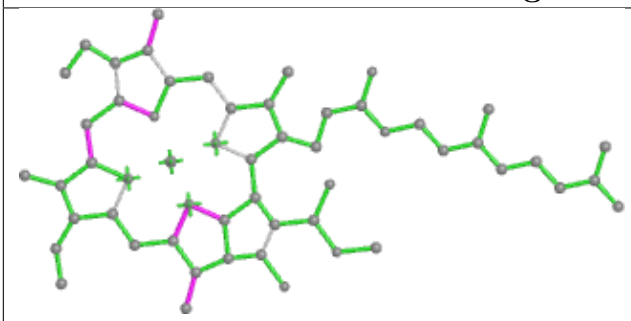


Rings

Ligand CLA A 831



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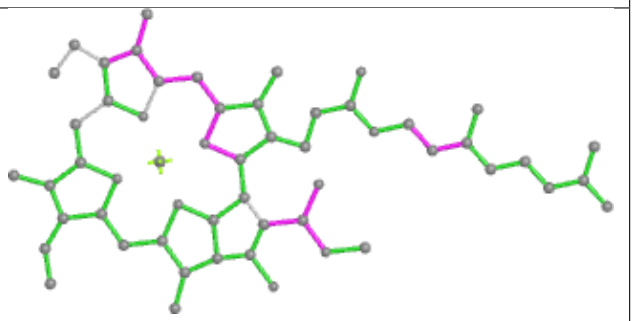
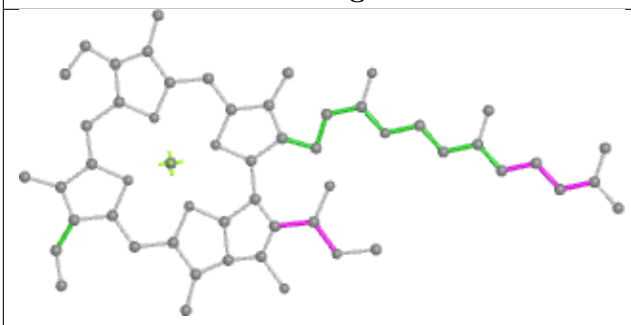
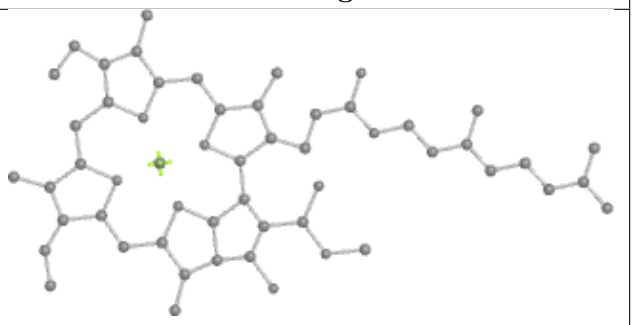


Bond angles

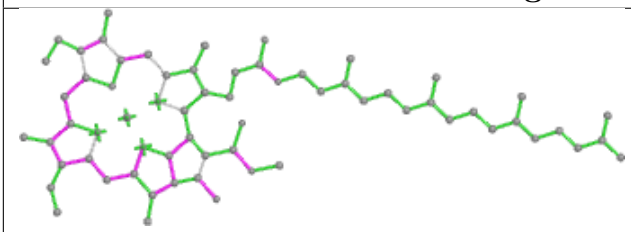


Torsions

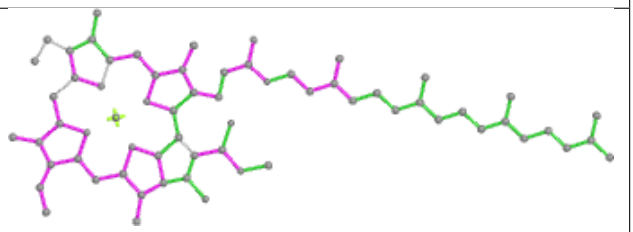


Rings

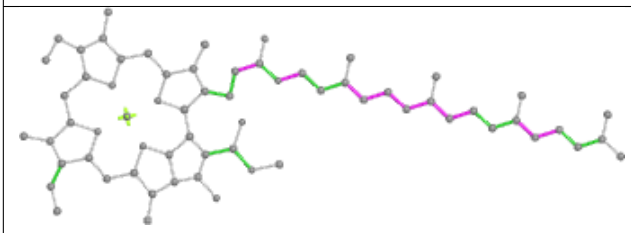
Ligand CLA B 801



Bond lengths



Bond angles



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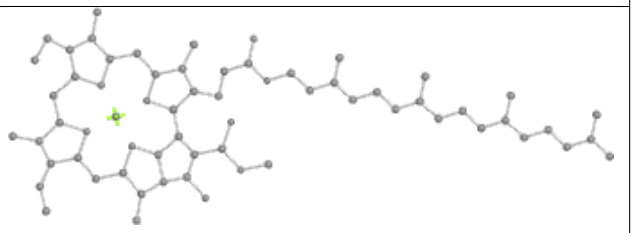
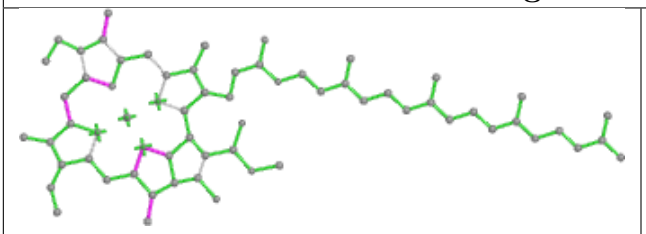


Rings

Ligand CLA A 825



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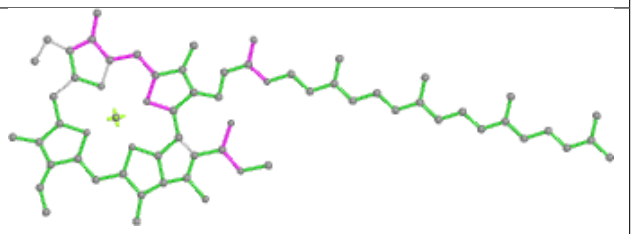
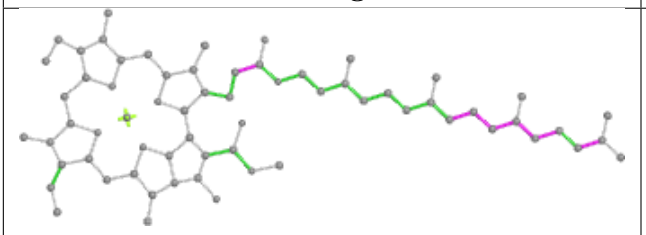


Bond angles



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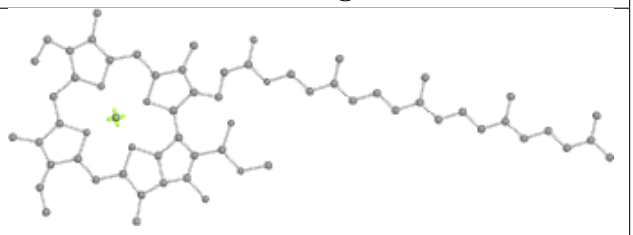
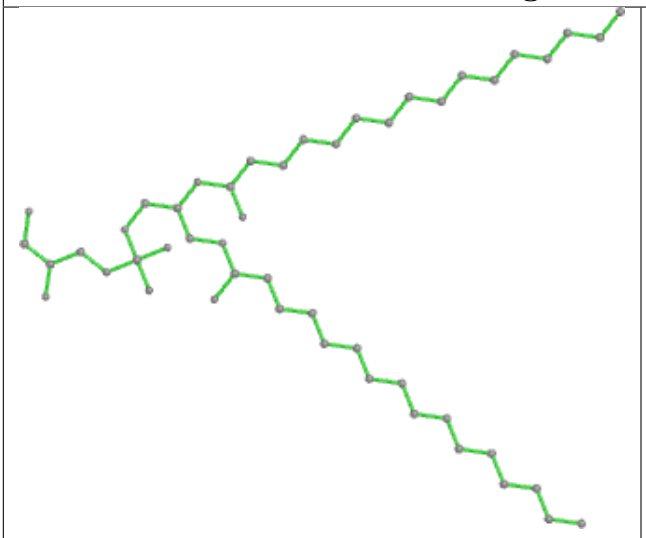


Rings

Ligand LHG A 844



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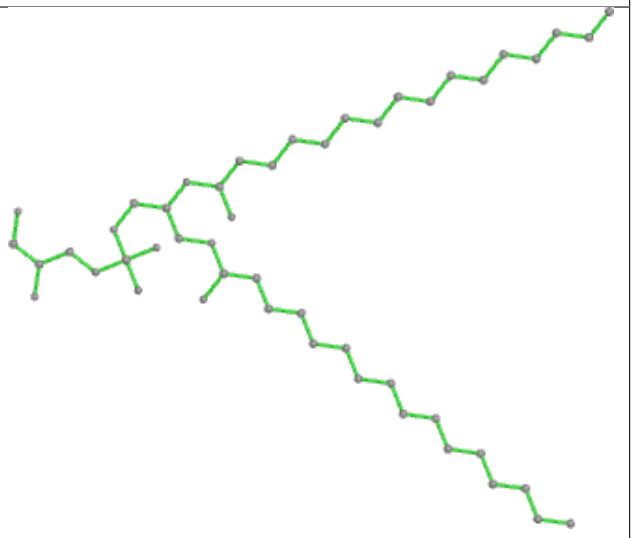

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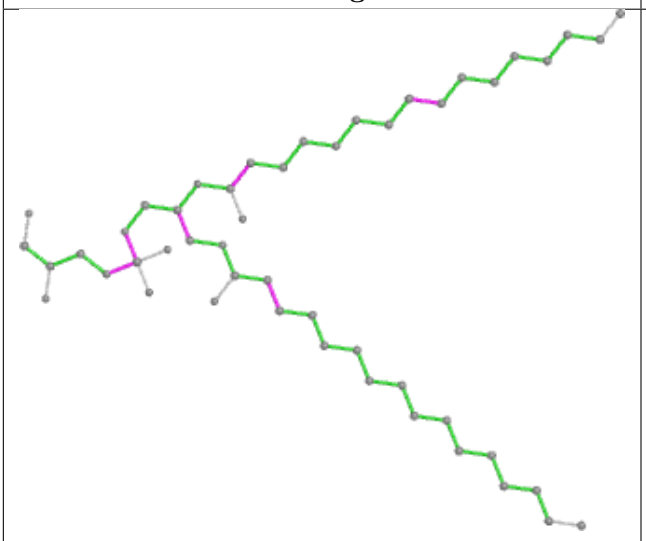

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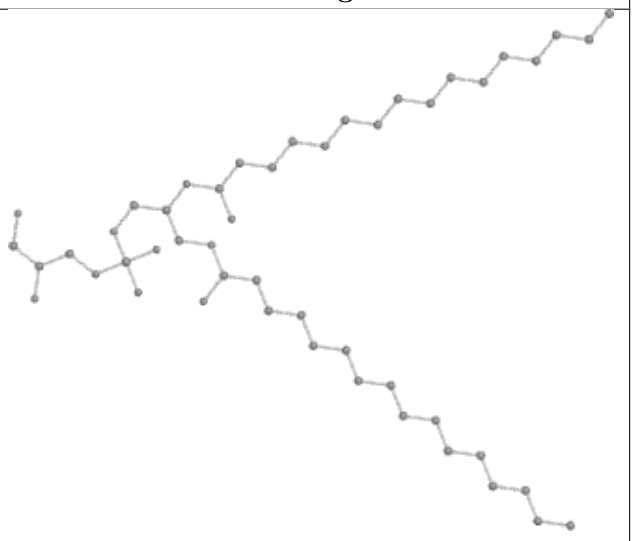
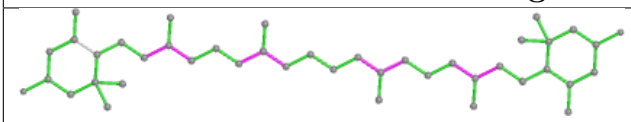


Rings

Ligand LUT 7 415



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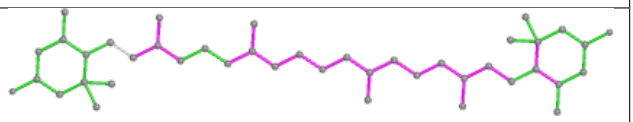

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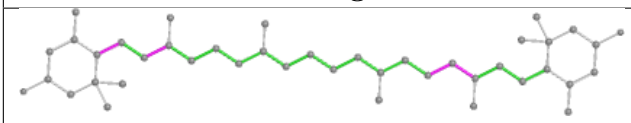

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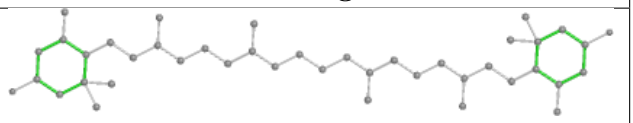
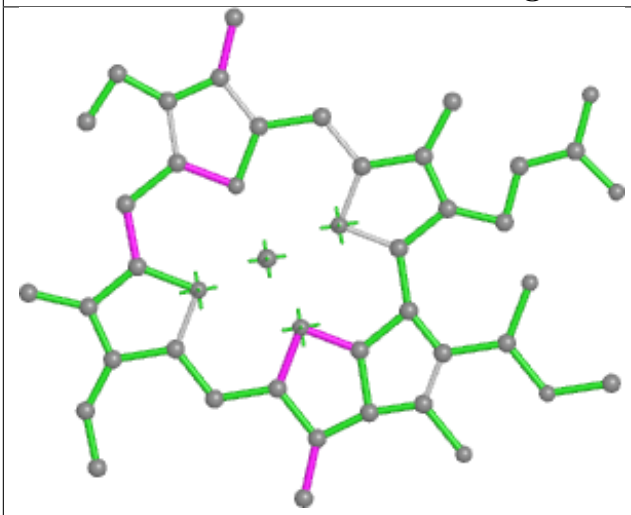


Rings

Ligand CLA A 836



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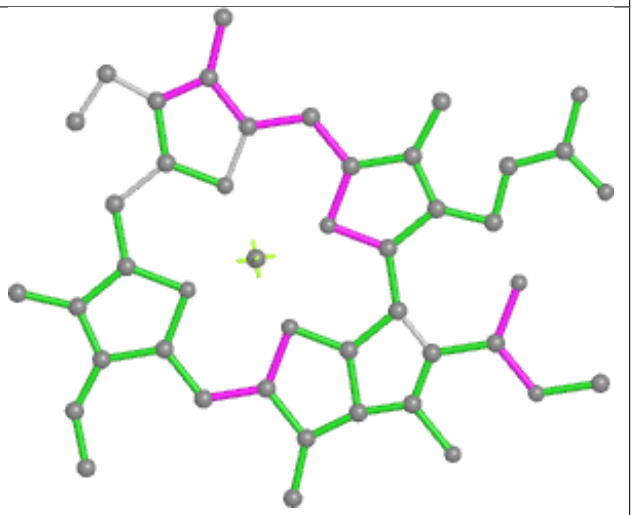

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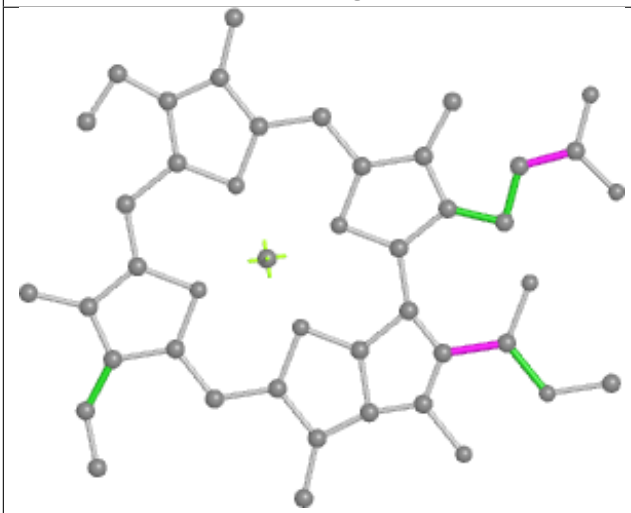

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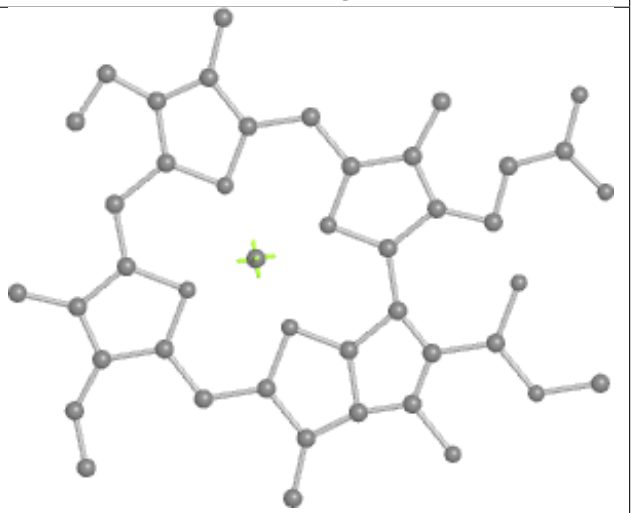
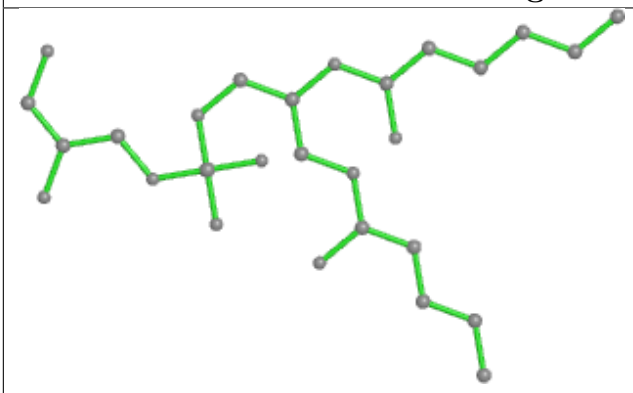


Rings

Ligand LHG 1 319



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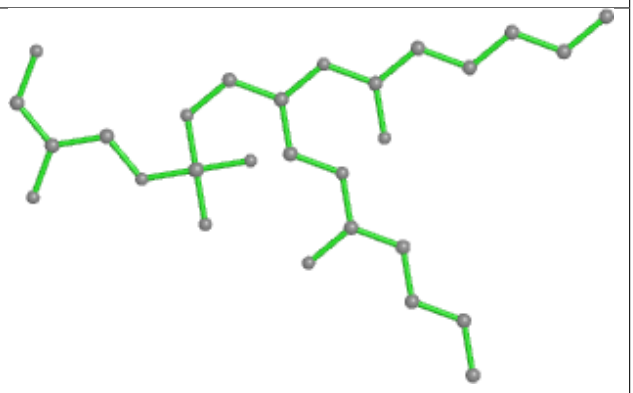
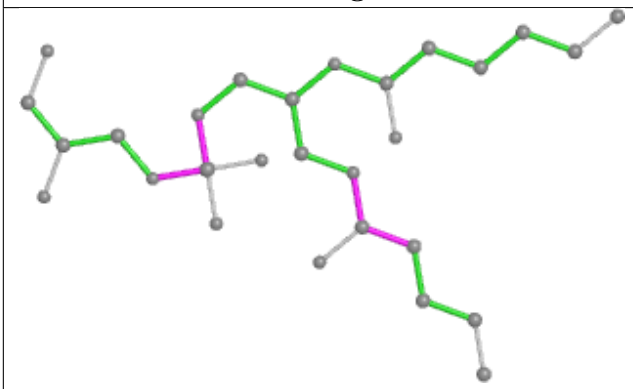


Bond angles



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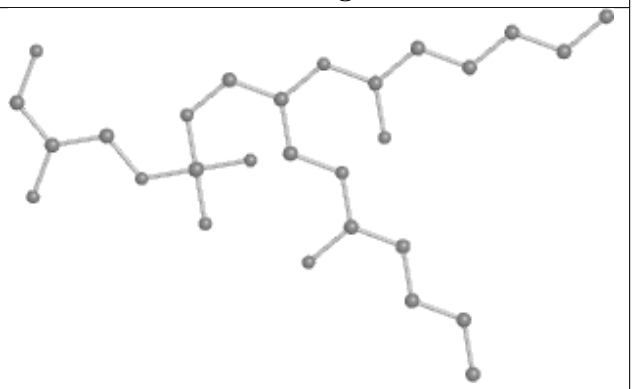
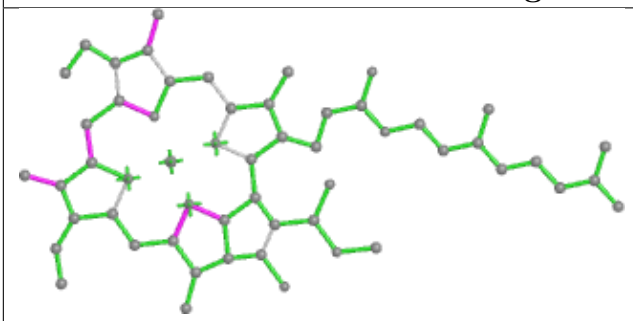


Rings

Ligand CLA B 803



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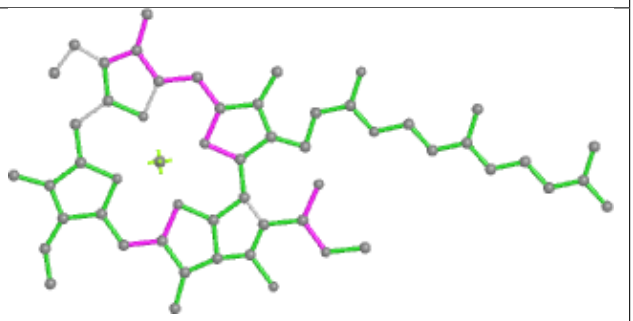

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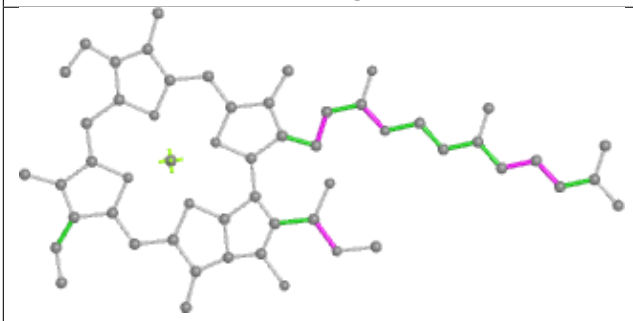

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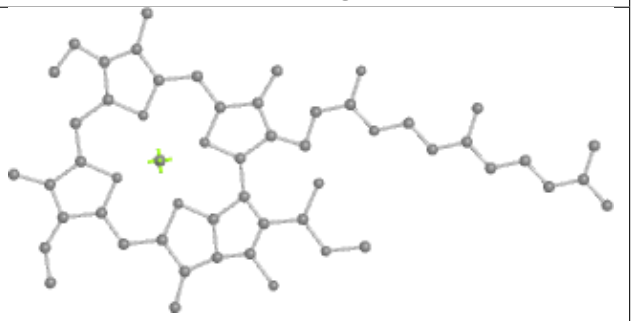
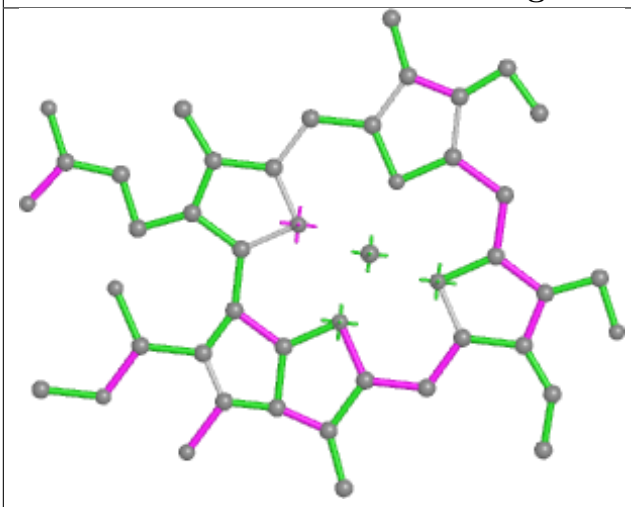


Rings

Ligand CHL 2 606



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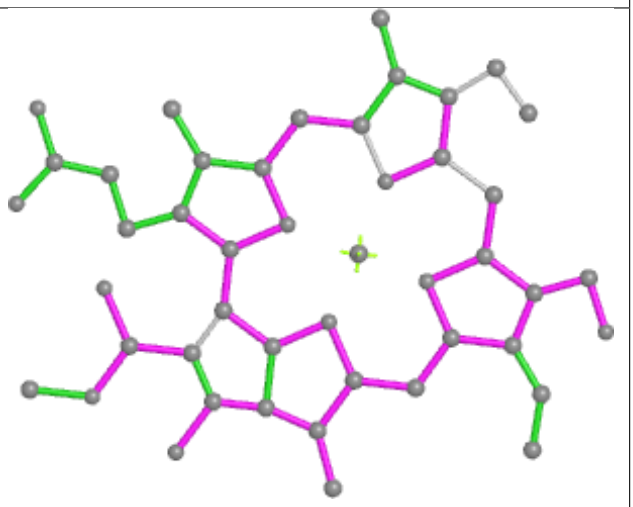
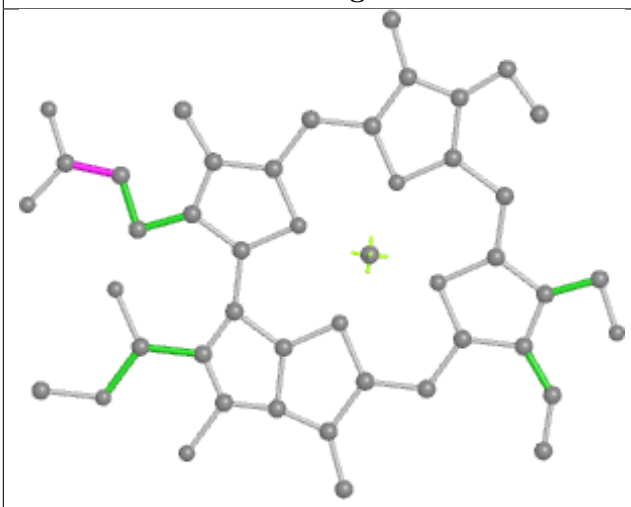


Bond angles



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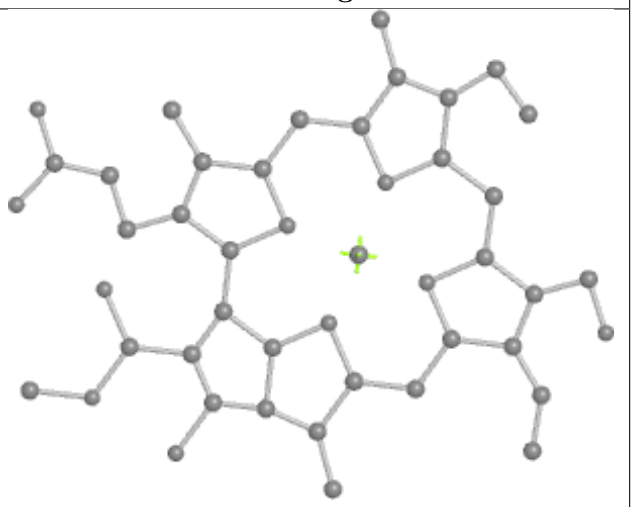
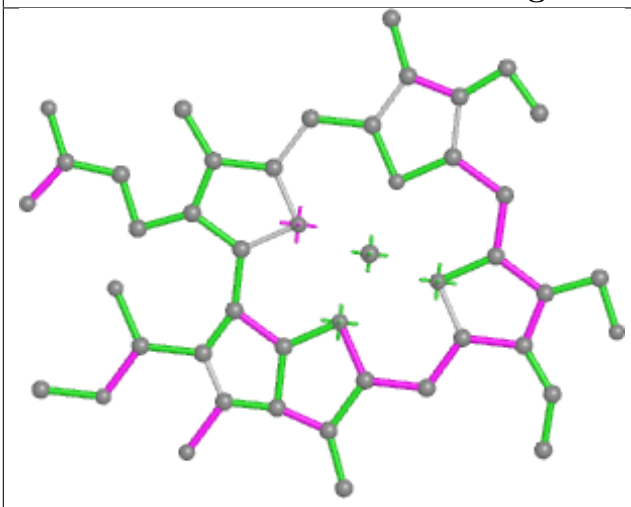


Rings

Ligand CHL a 606



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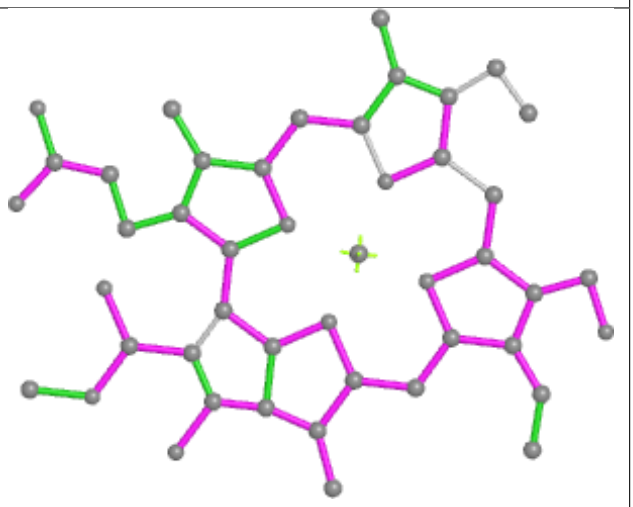

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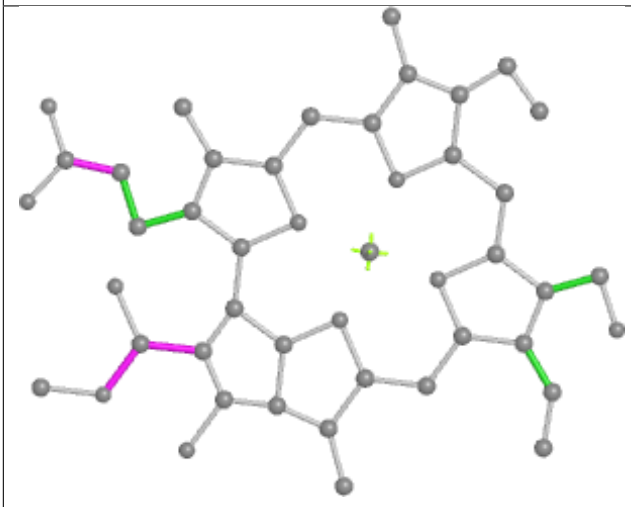

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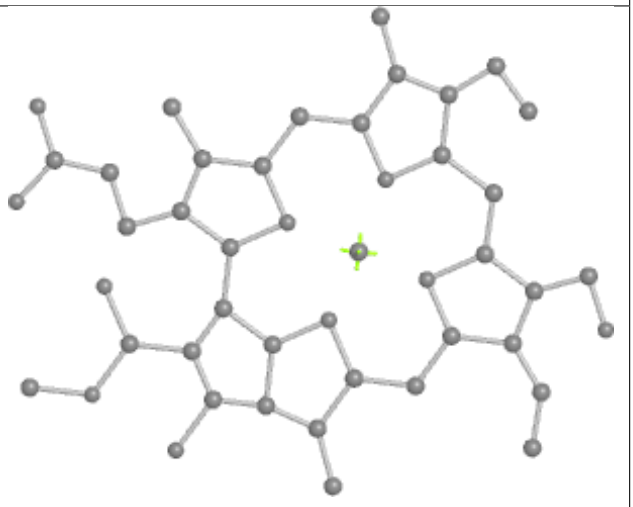
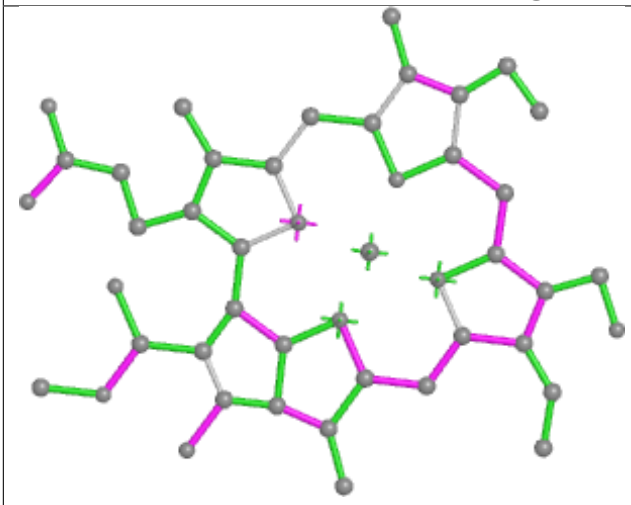


Rings

Ligand CHL 6 606



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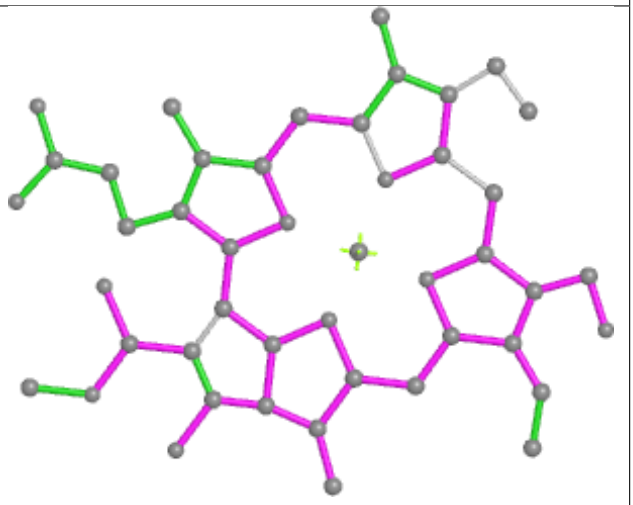
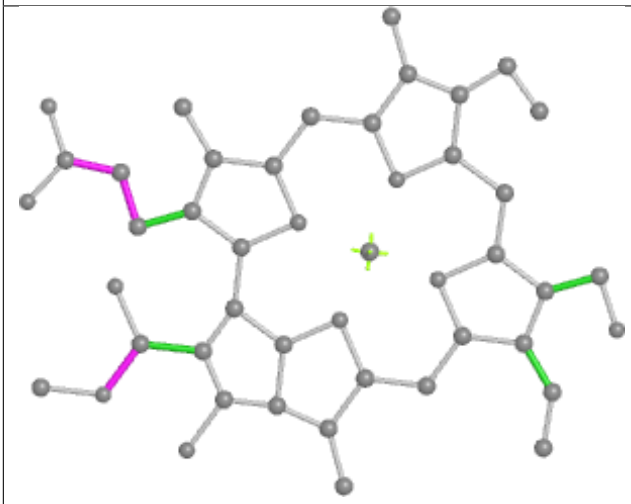


Bond angles



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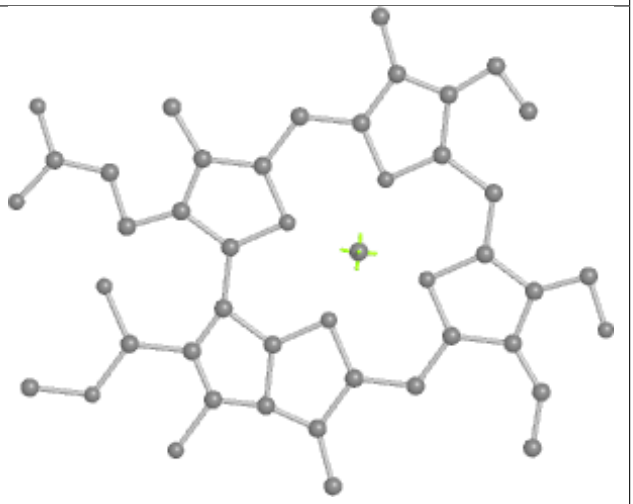
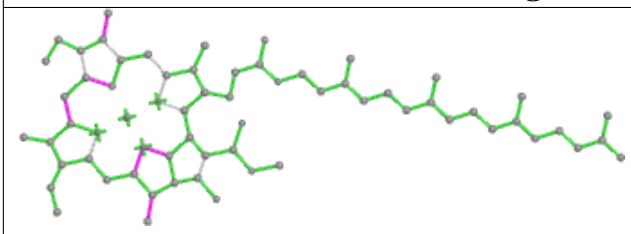


Rings

Ligand CLA B 835



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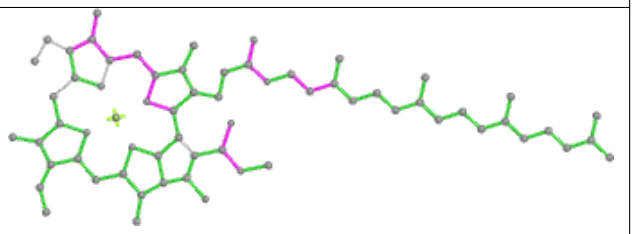
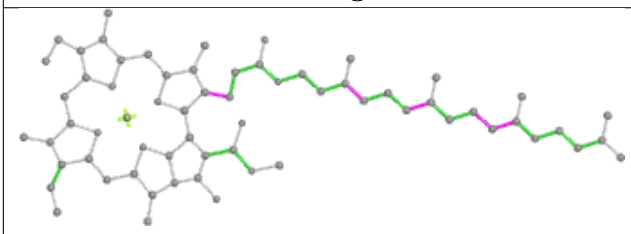


Bond angles



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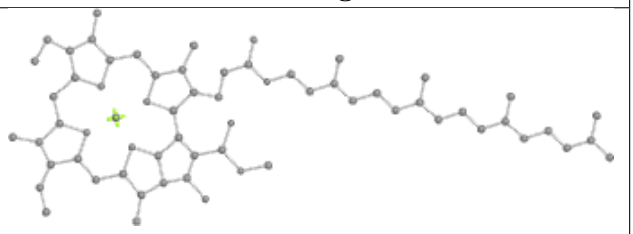
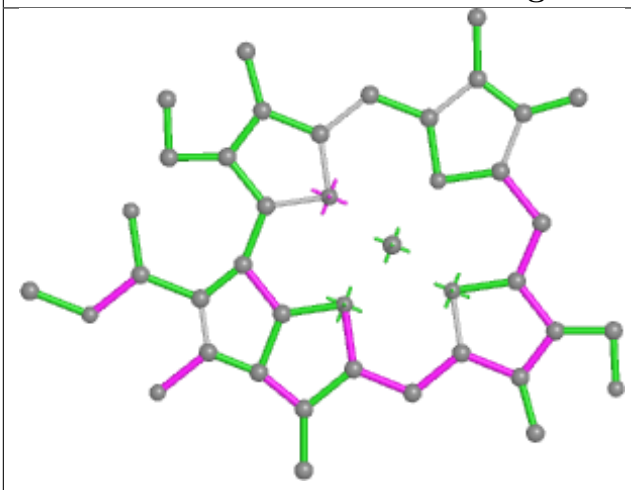


Rings

Ligand CHL 4 605



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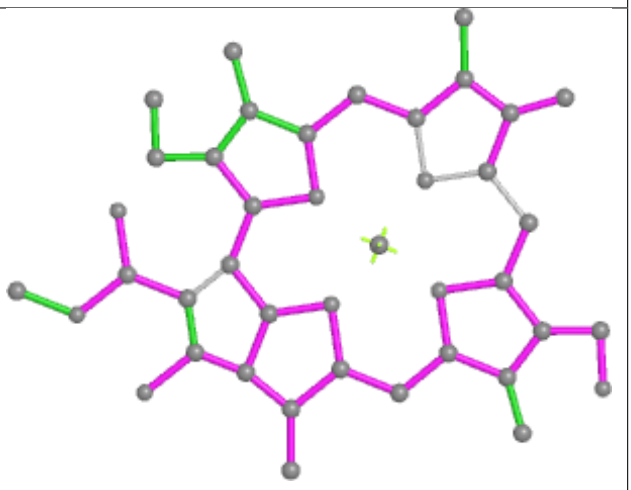
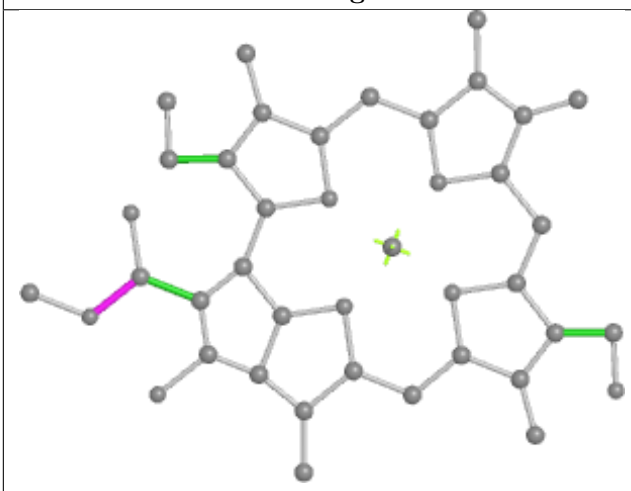


Bond angles



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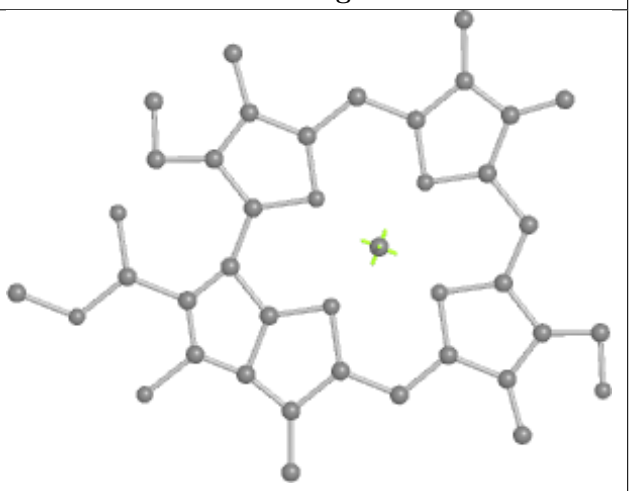
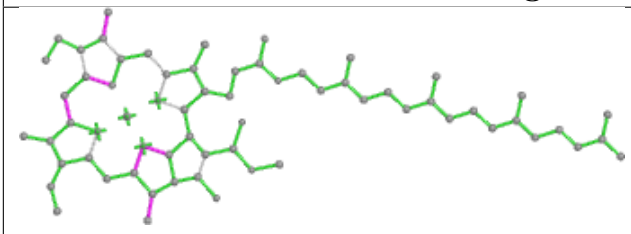


Rings

Ligand CLA A 834



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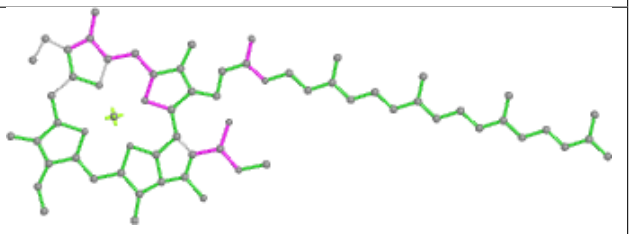

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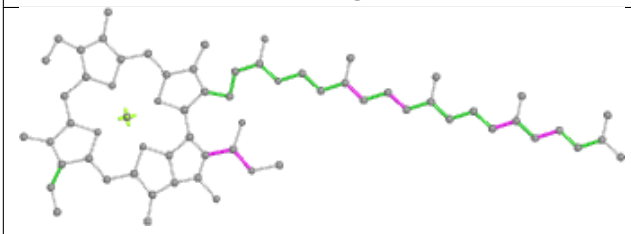

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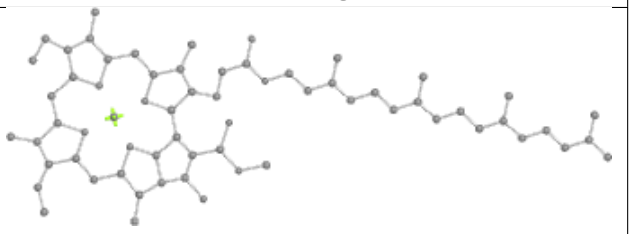
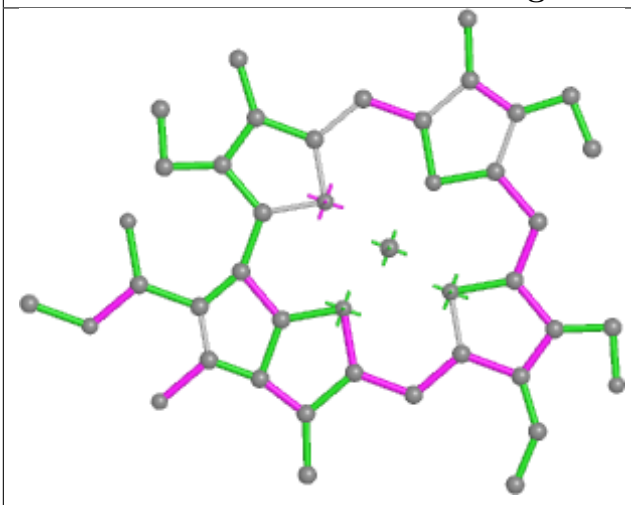


Rings

Ligand CHL 9 601



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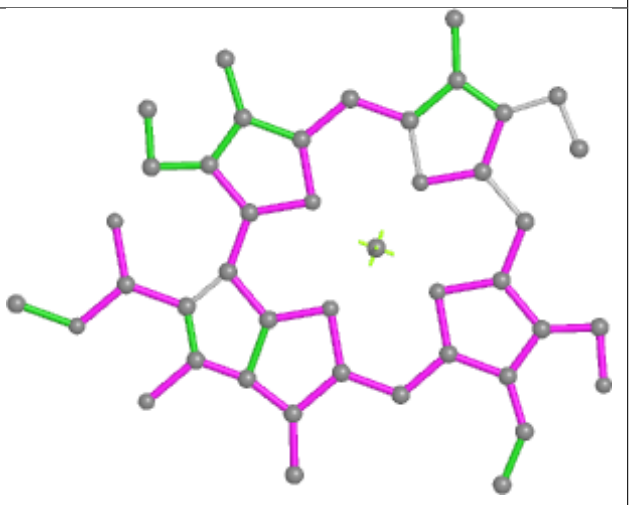

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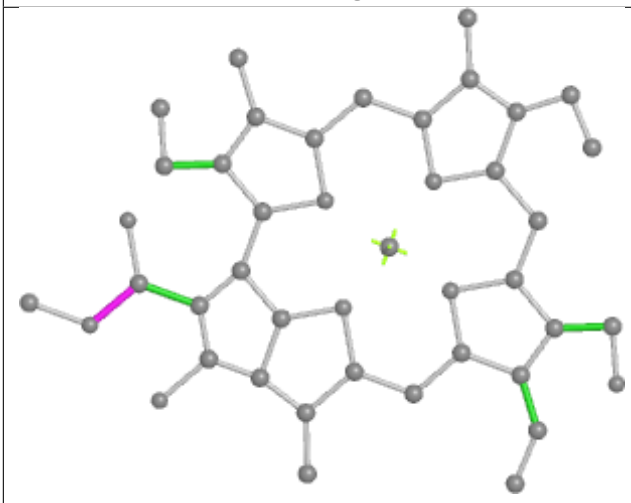

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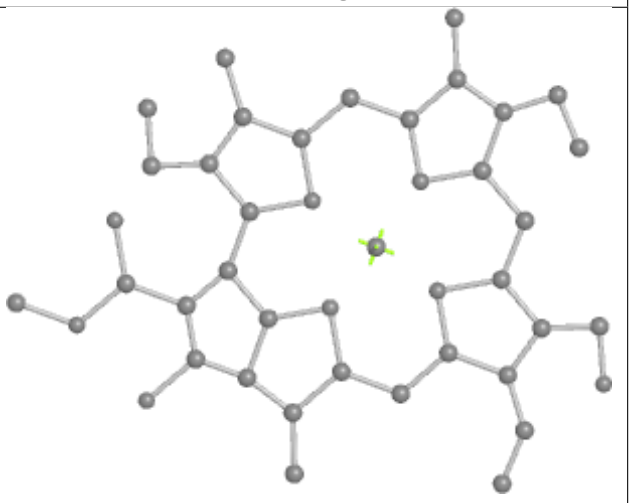
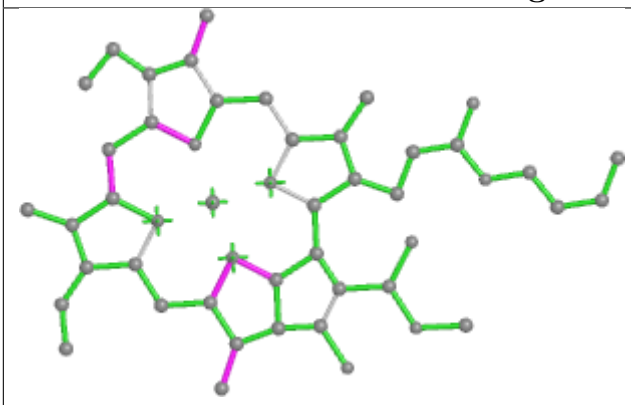


Rings

Ligand CLA 1 305



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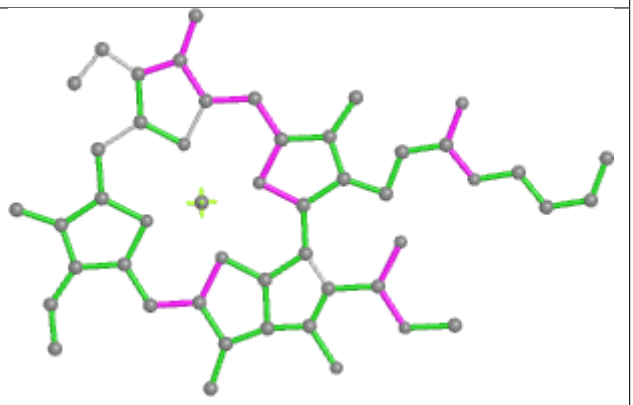

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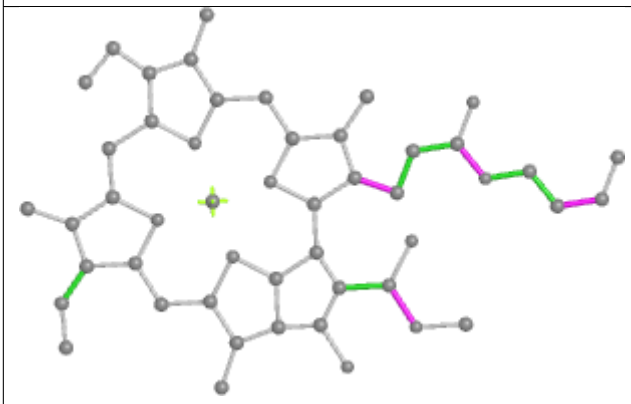

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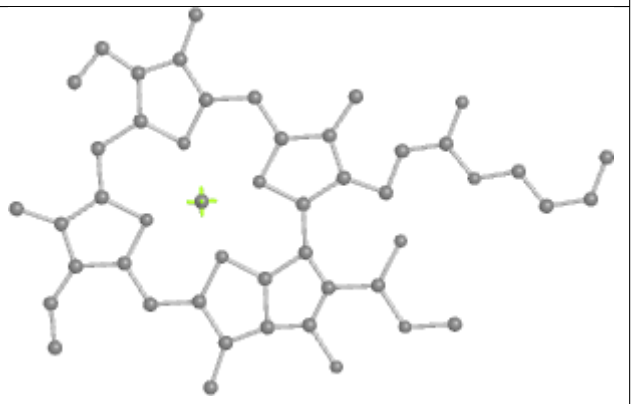
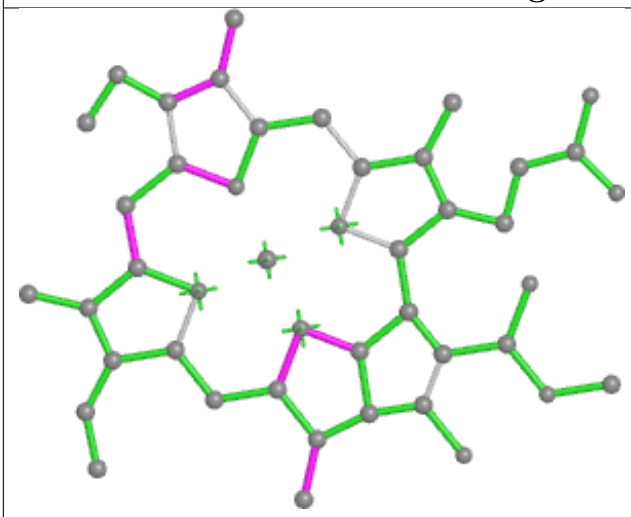


Rings

Ligand CLA 2 603



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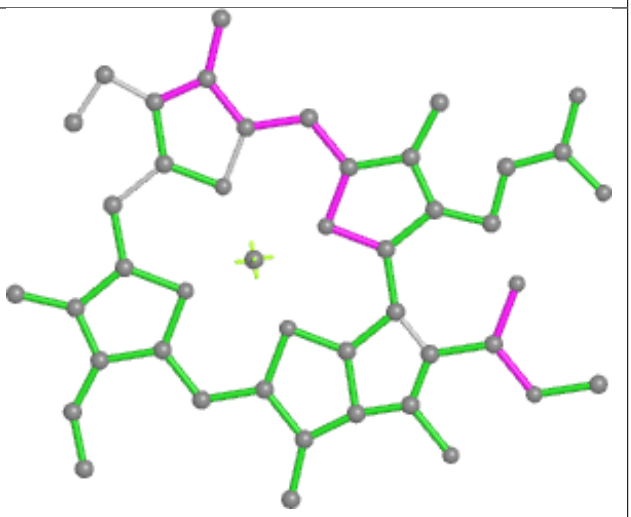

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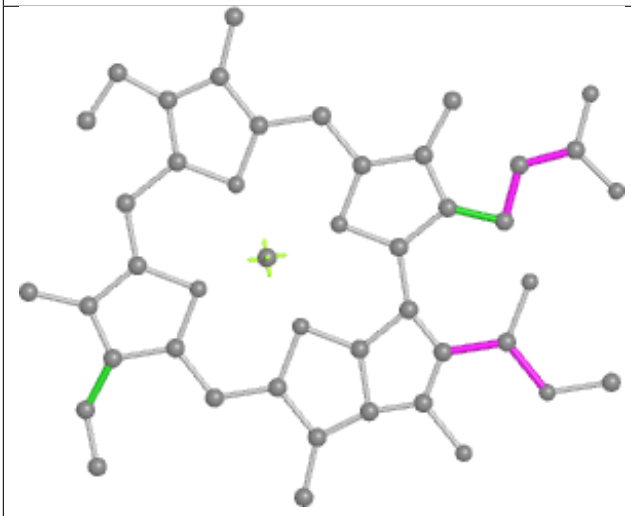

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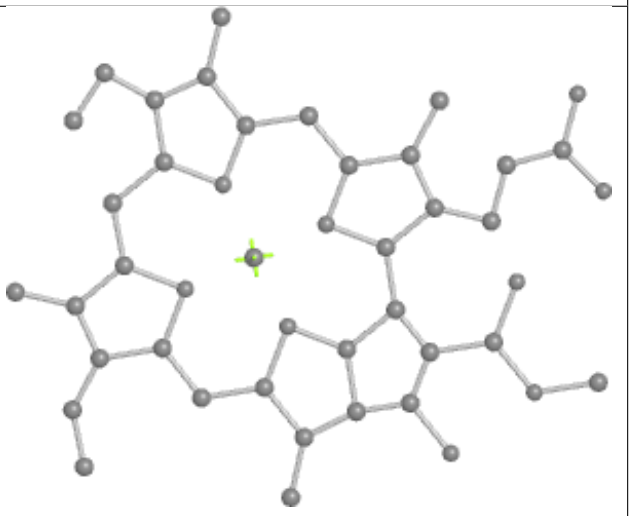
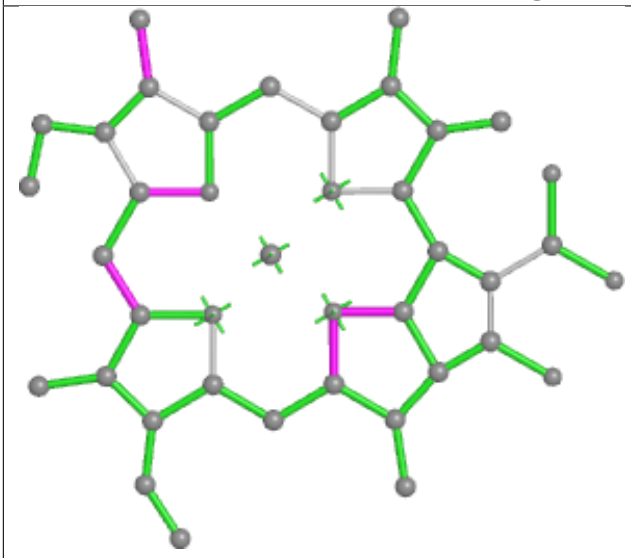


Rings

Ligand CLA 7 409



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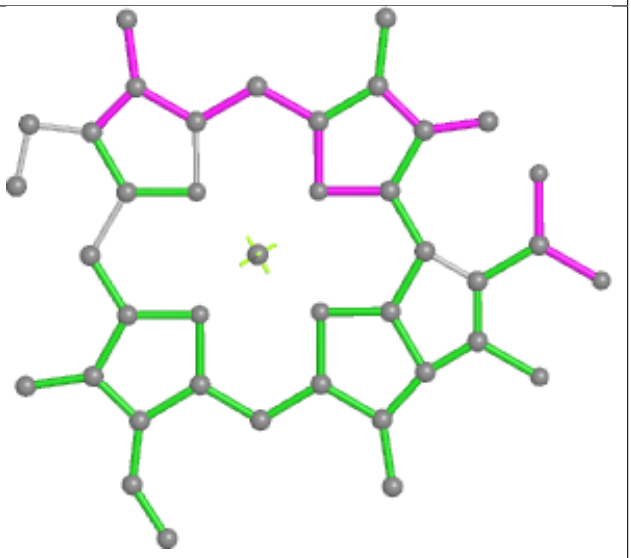

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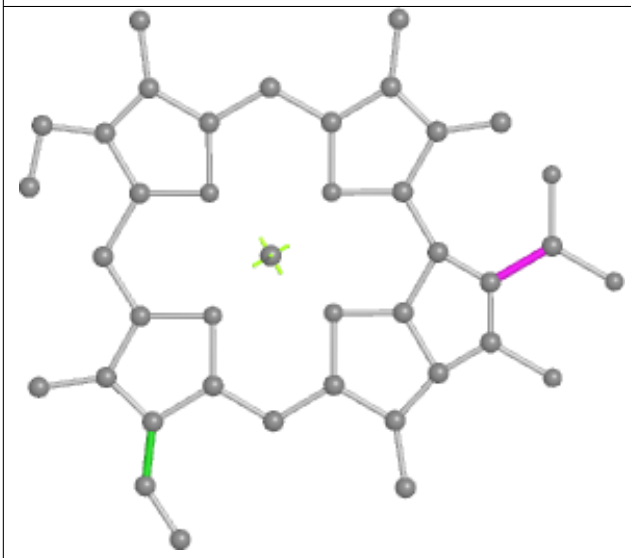

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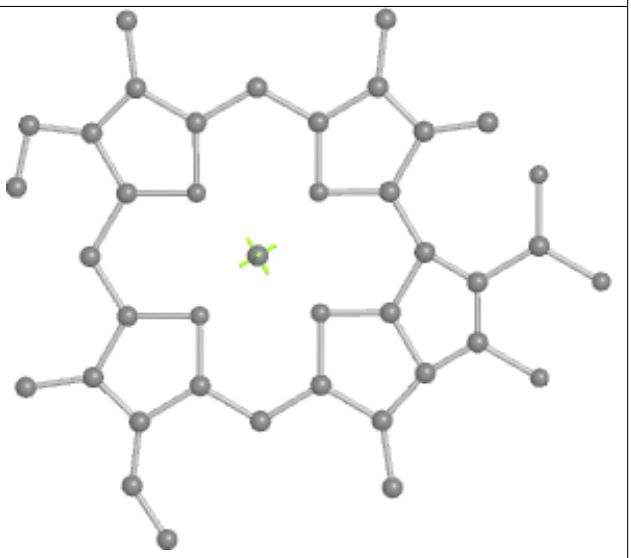
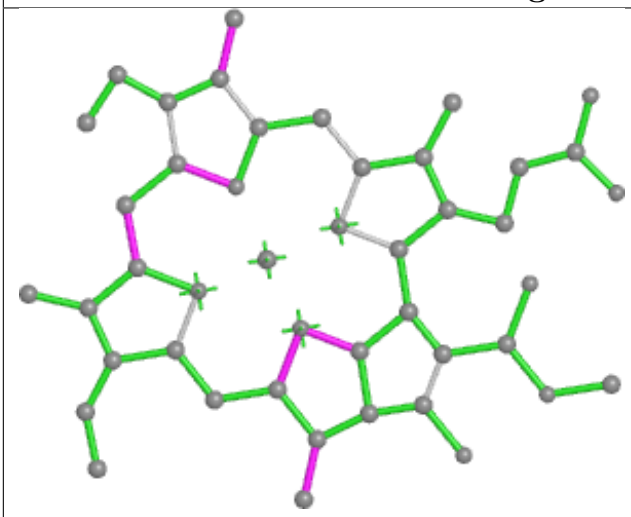


Rings

Ligand CLA 6 603



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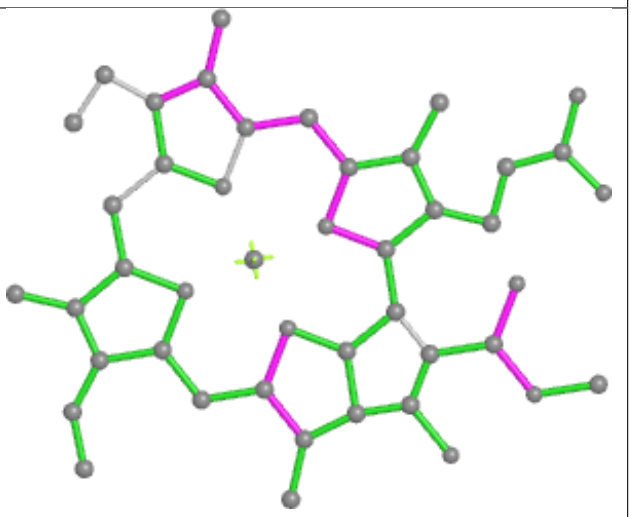

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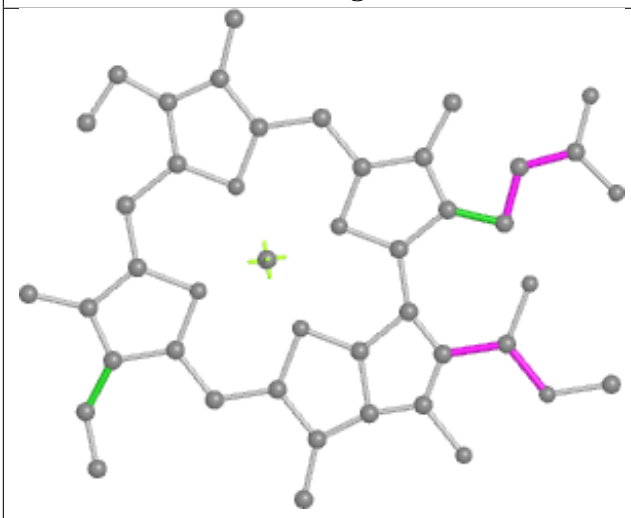

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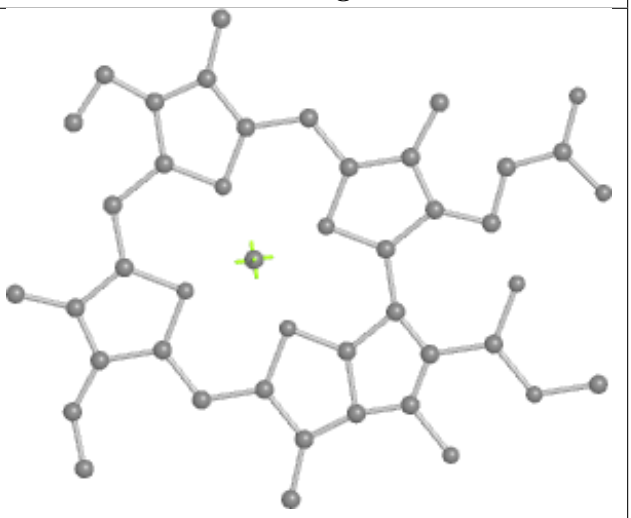
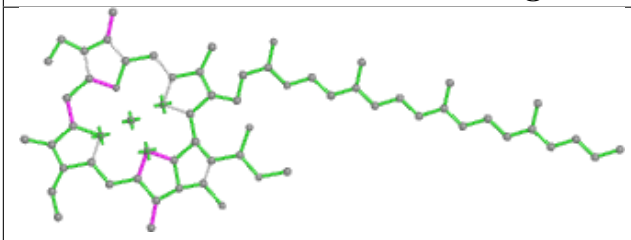


Rings

Ligand CLA B 806



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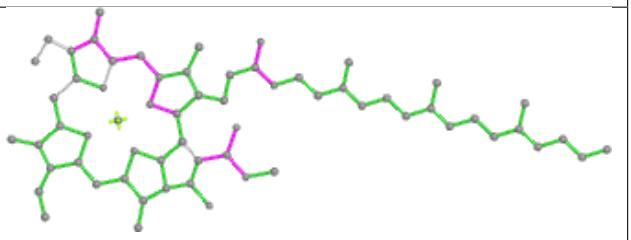
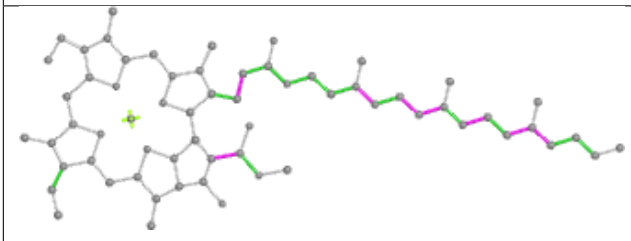


Bond angles



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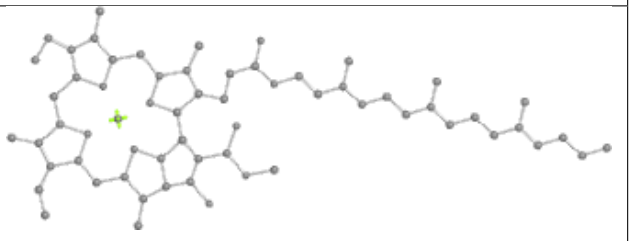
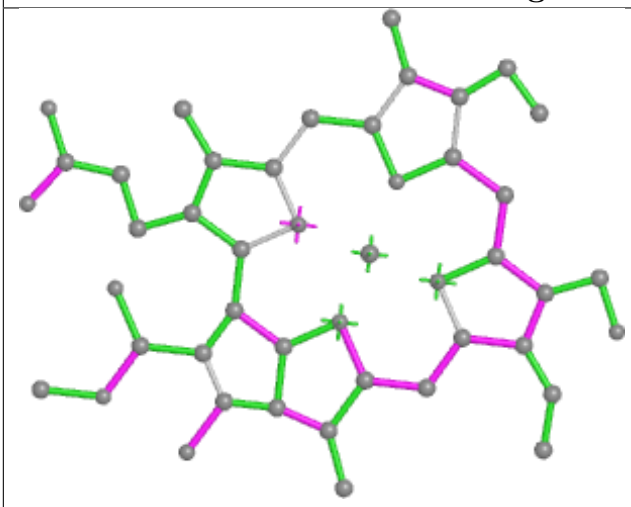


Rings

Ligand CHL 9 608



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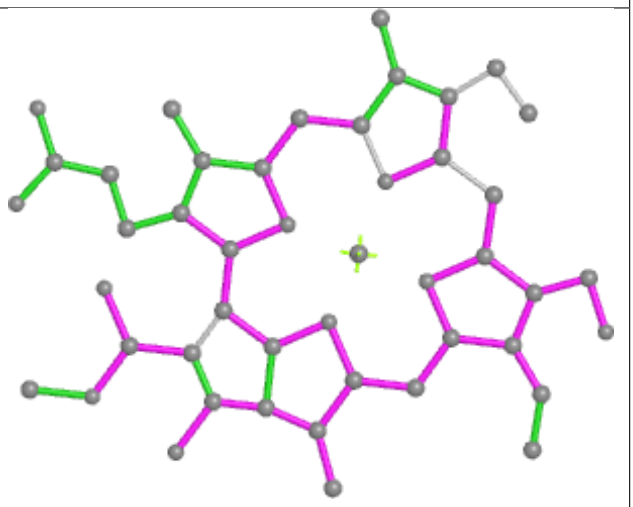
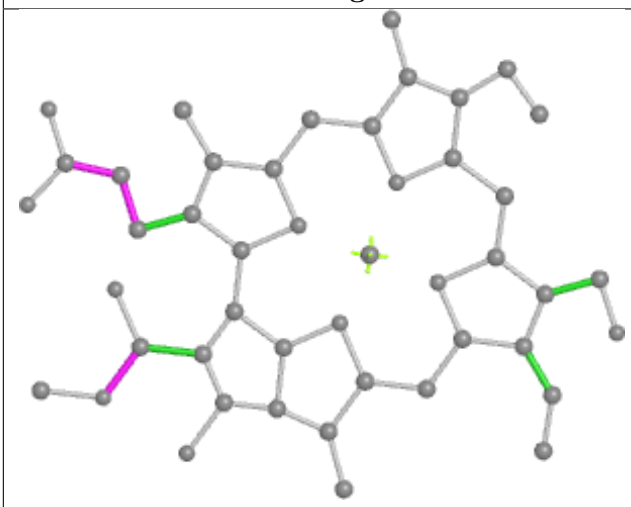


Bond angles



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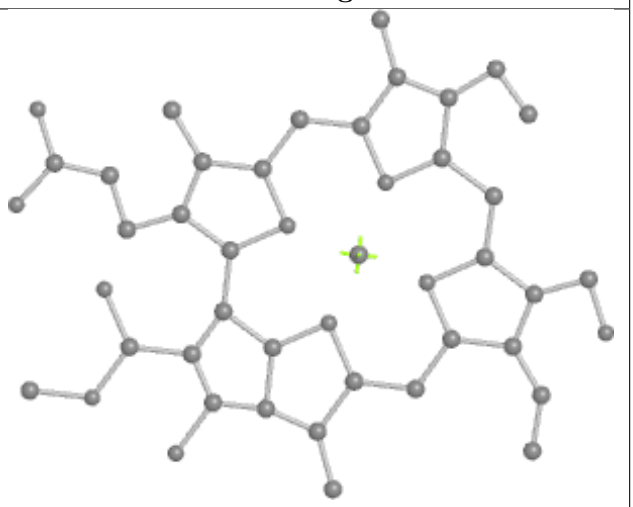
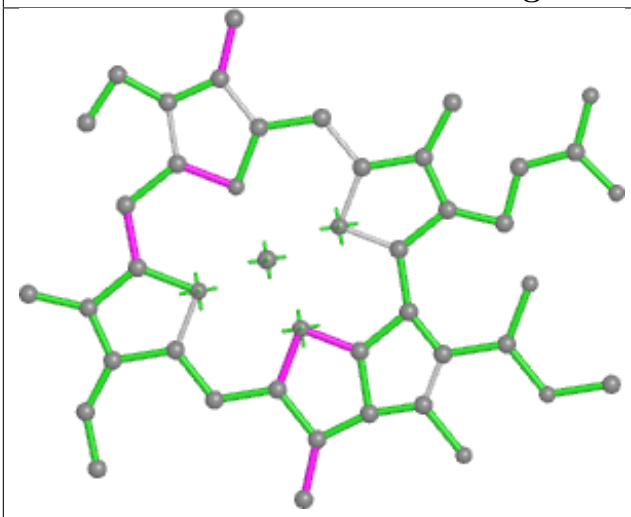


Rings

Ligand CLA K 204



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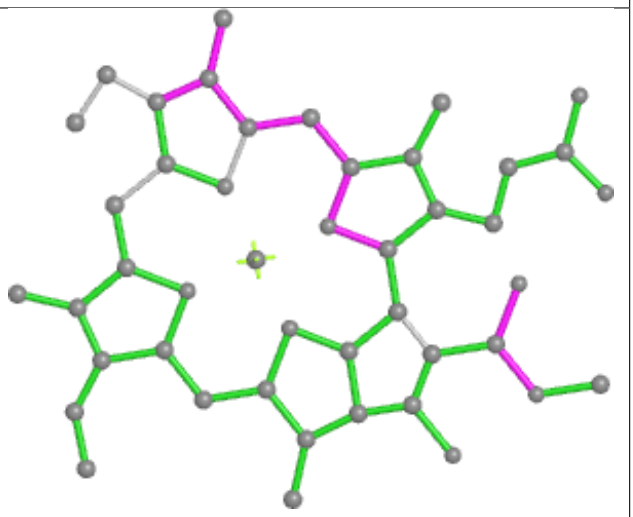

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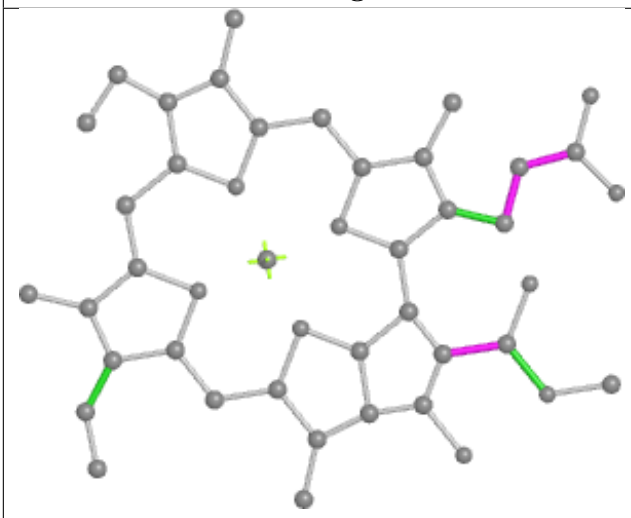

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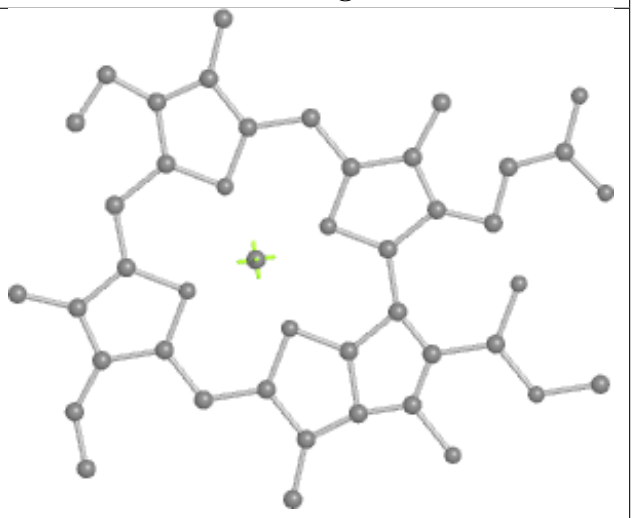

Rings

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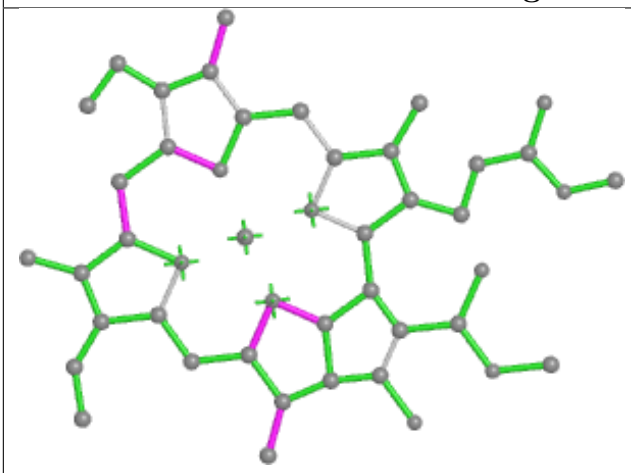

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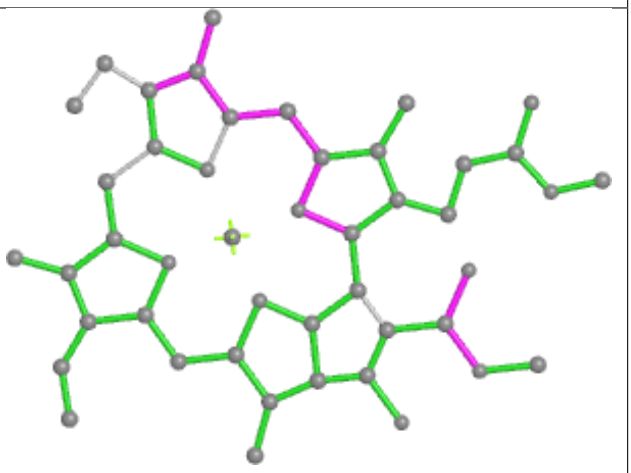

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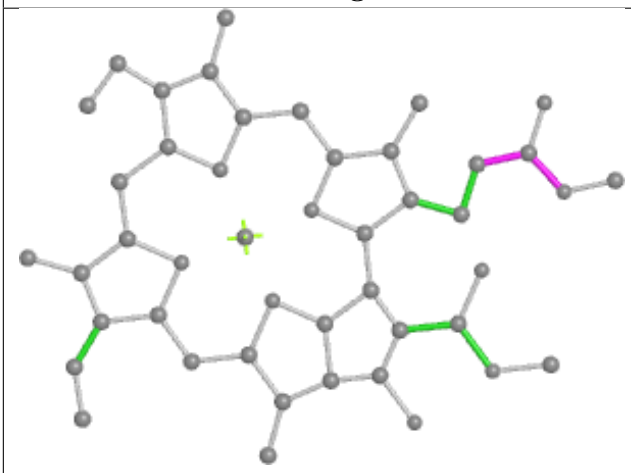

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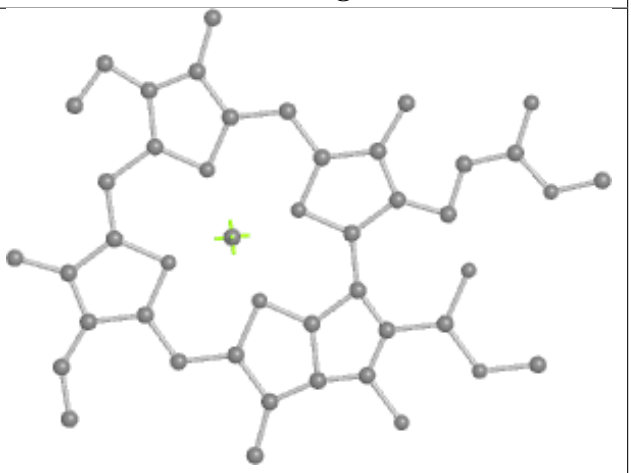
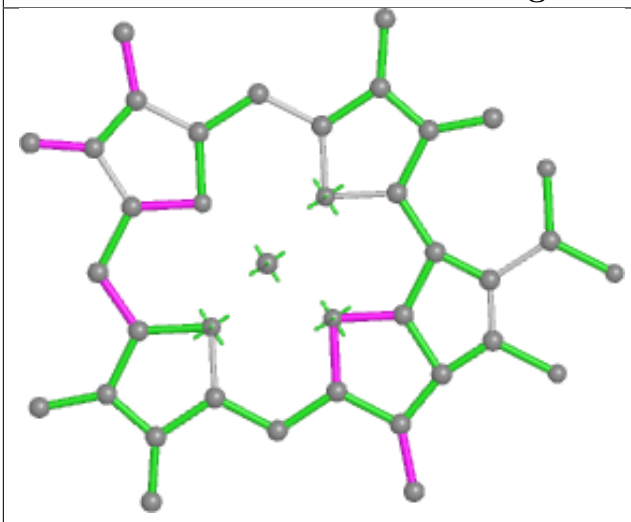


Rings

Ligand CLA 1 314



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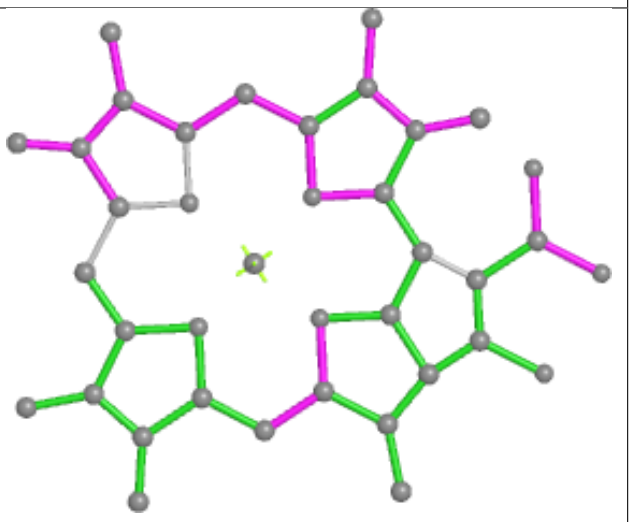
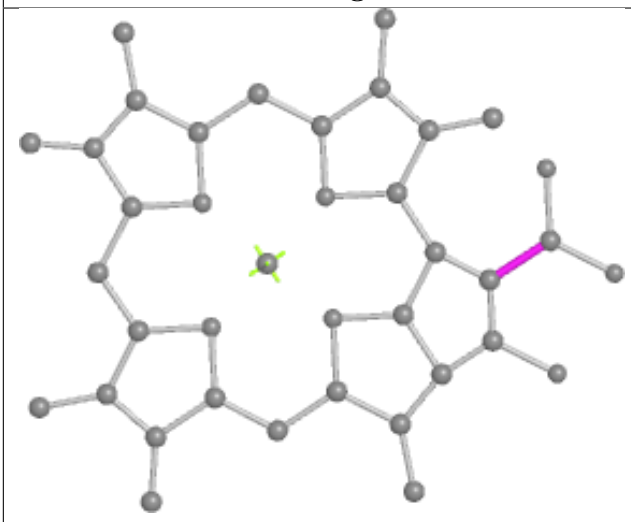


Bond angles



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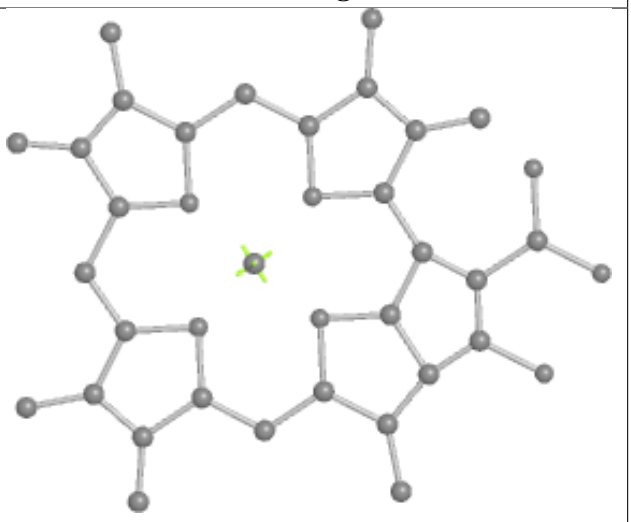
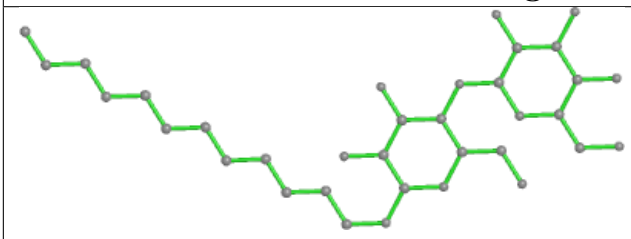


Rings

Ligand LMU 3 420



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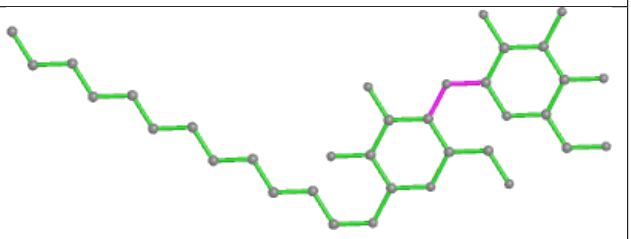
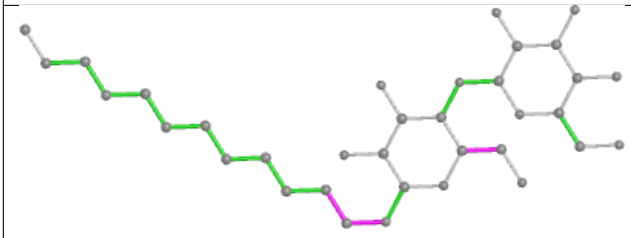
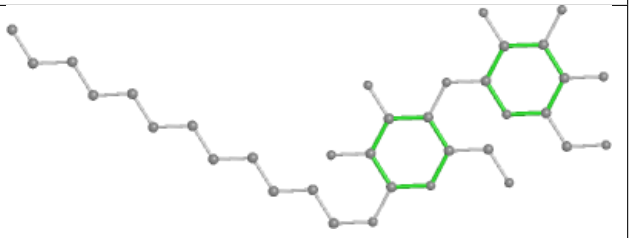


Bond angles

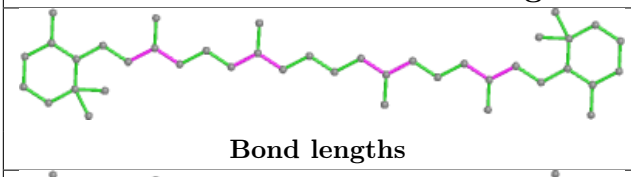


Torsions



Rings

Ligand BCR L 301



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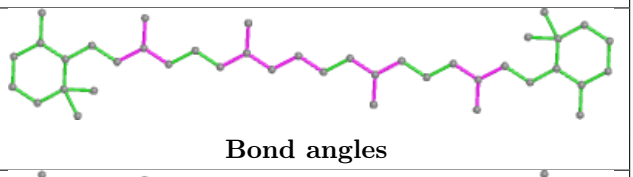
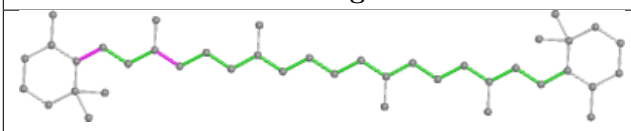
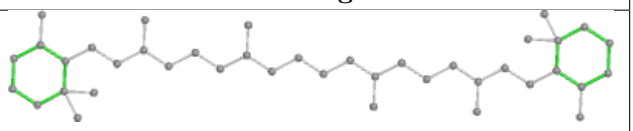


Bond angles

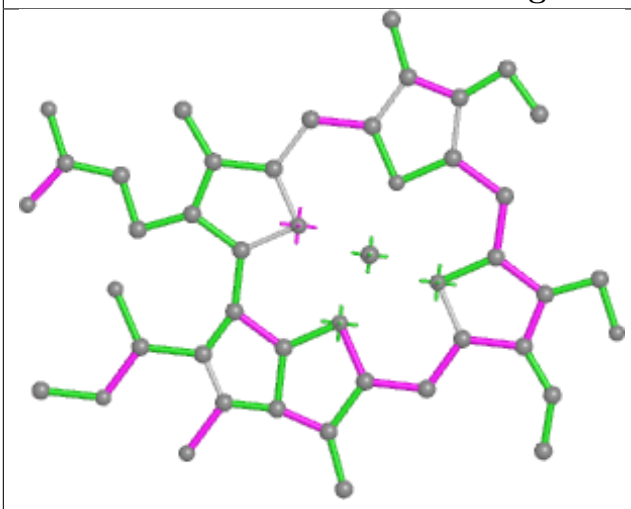


Torsions

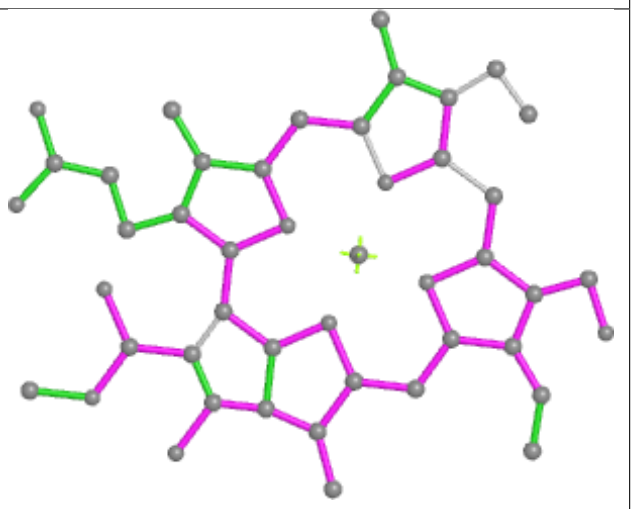


Rings

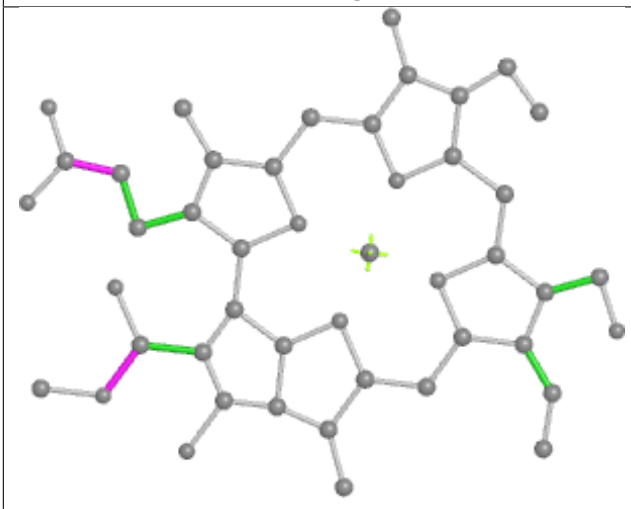
Ligand CHL c 606



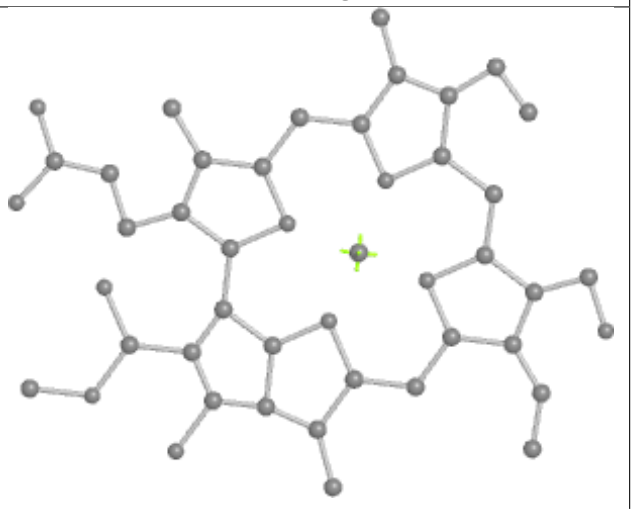
Bond lengths



Bond angles

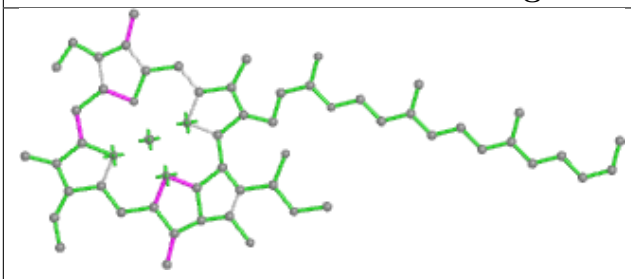


Torsions



Rings

Ligand CLA A 809



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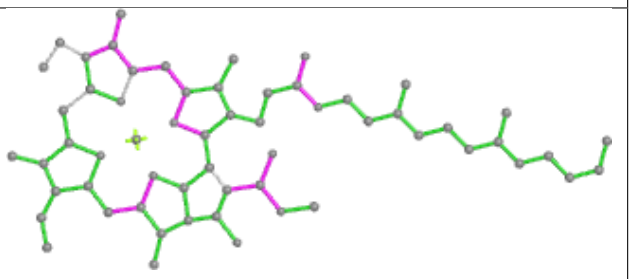
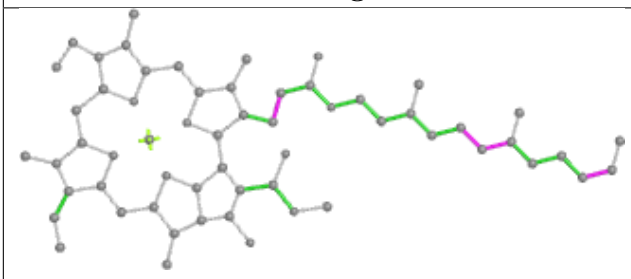


Bond angles



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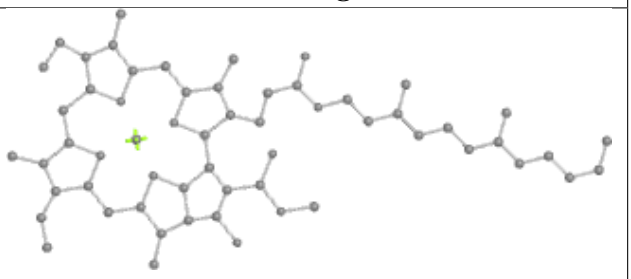
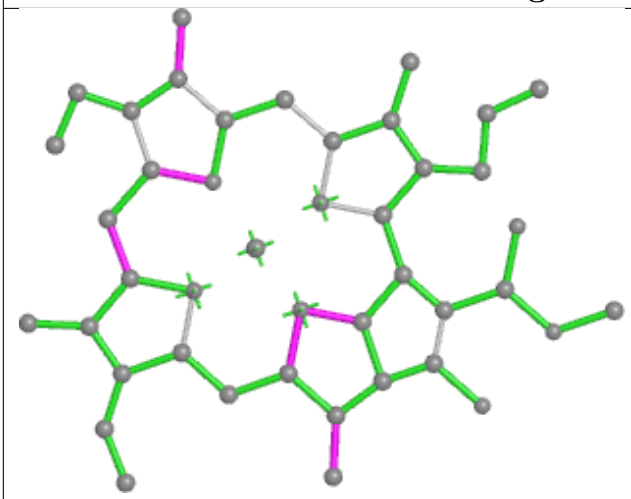


Rings

Ligand CLA 3 411



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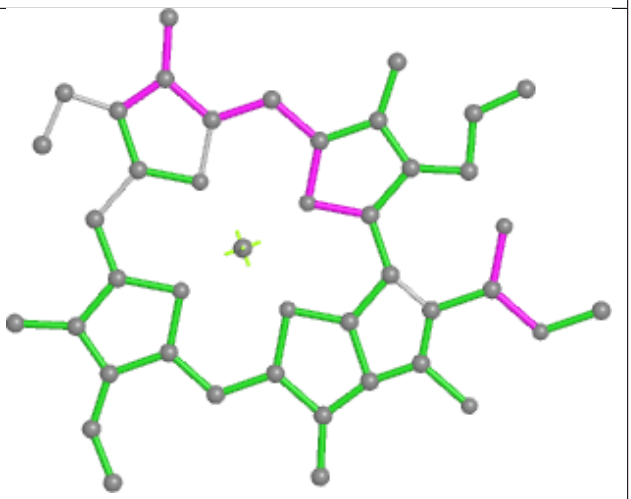
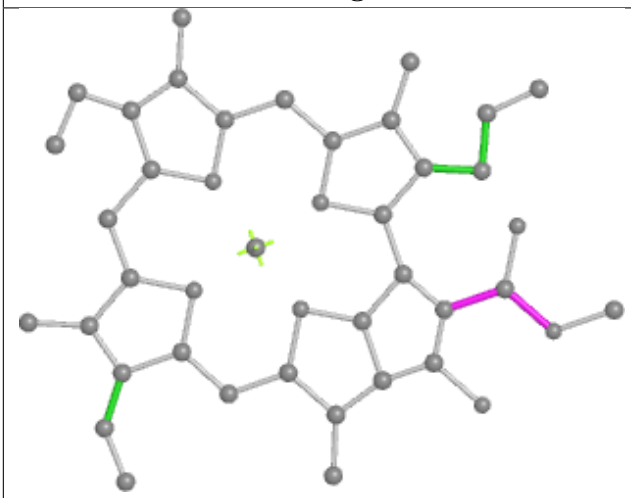


Bond angles



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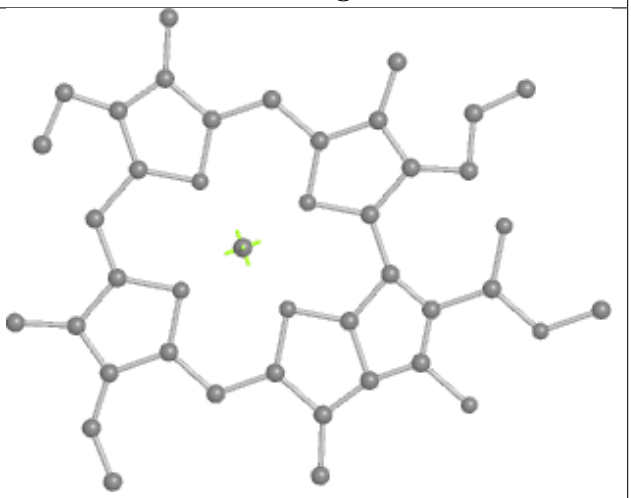
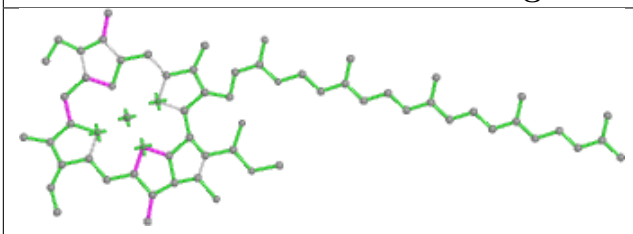
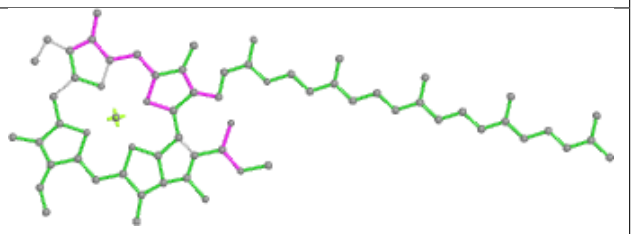


Rings

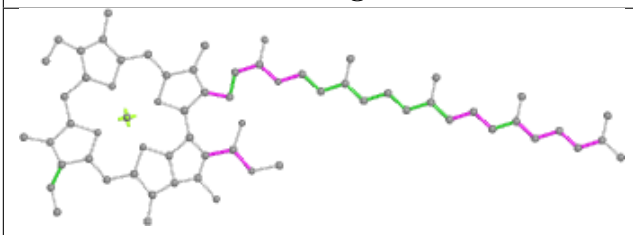
Ligand CLA A 841



Bond lengths



Bond angles



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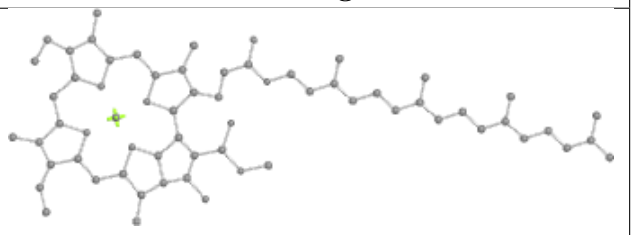
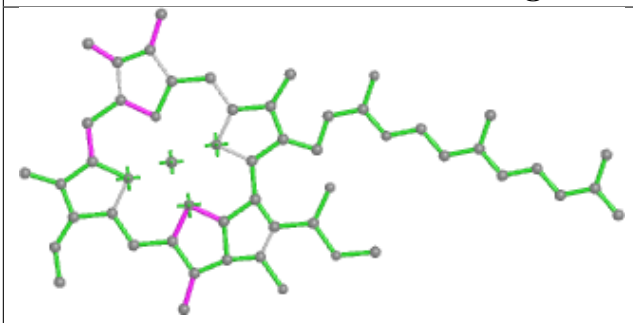
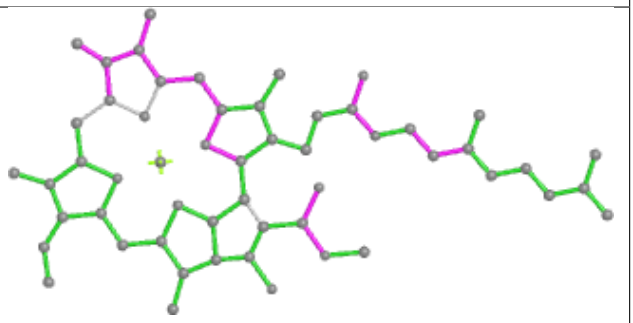


Rings

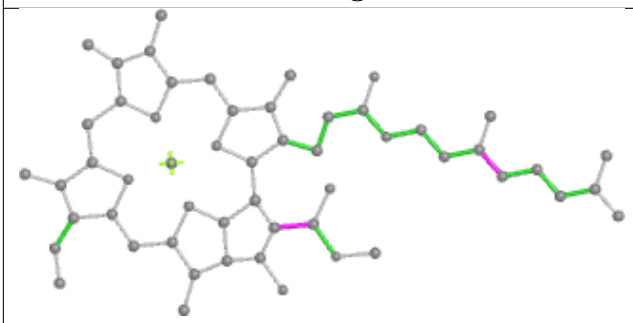
Ligand CLA B 810



Bond lengths



Bond angles



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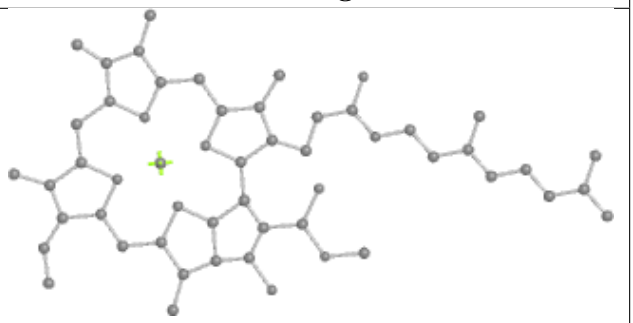
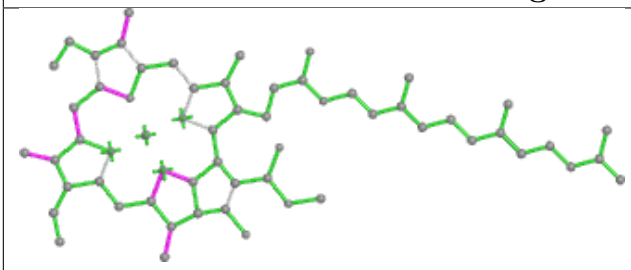


Rings

Ligand CLA c 602



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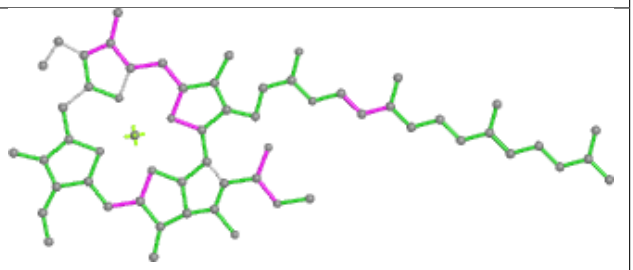
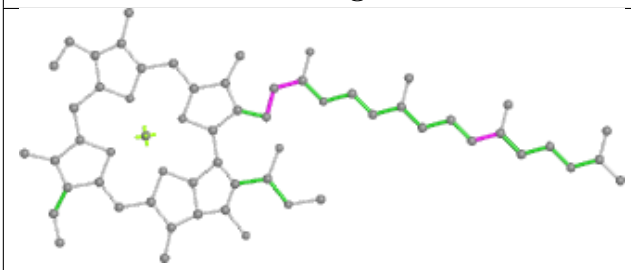


Bond angles



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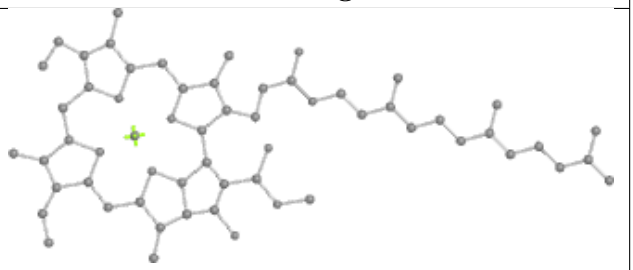
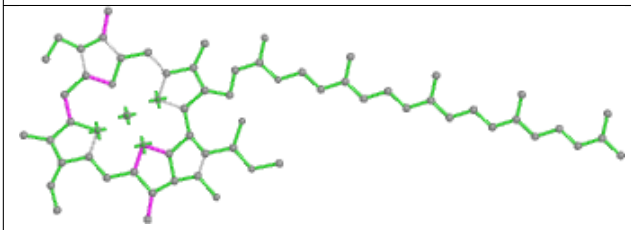


Rings

Ligand CLA A 804



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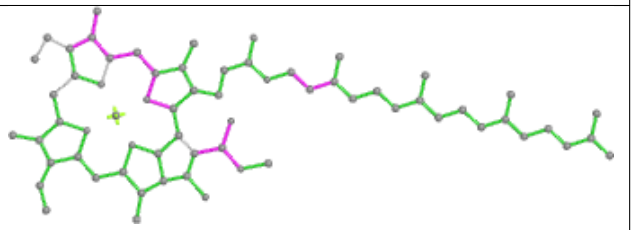
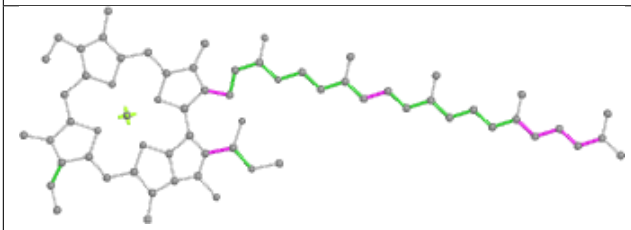


Bond angles



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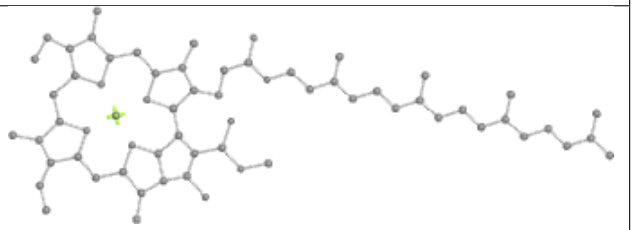
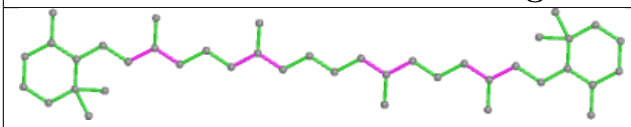
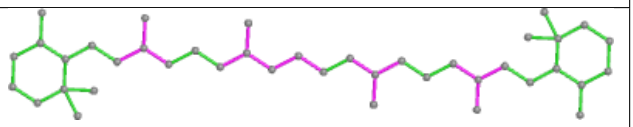


Rings

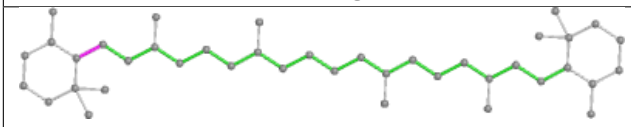
Ligand BCR 7 417



Bond lengths



Bond angles



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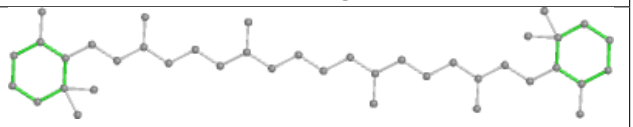
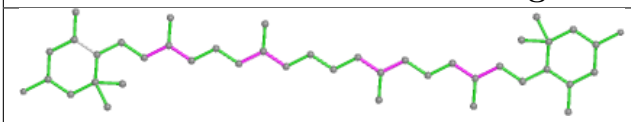
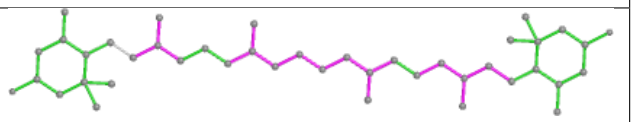


Rings

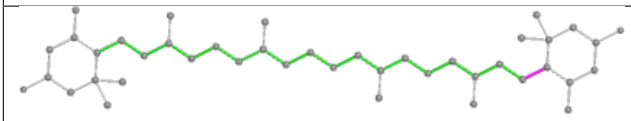
Ligand LUT 9 614



Bond lengths



Bond angles



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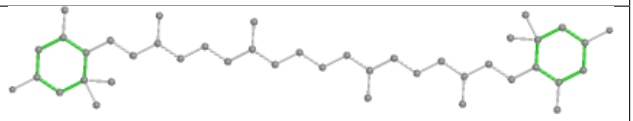
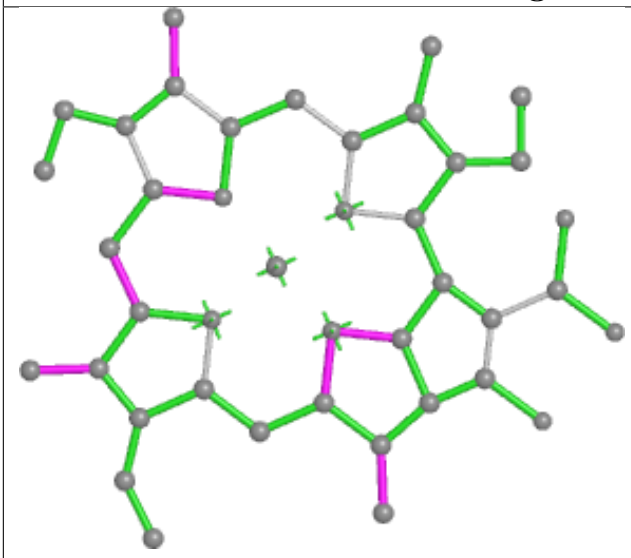


Rings

Ligand CLA 3 405



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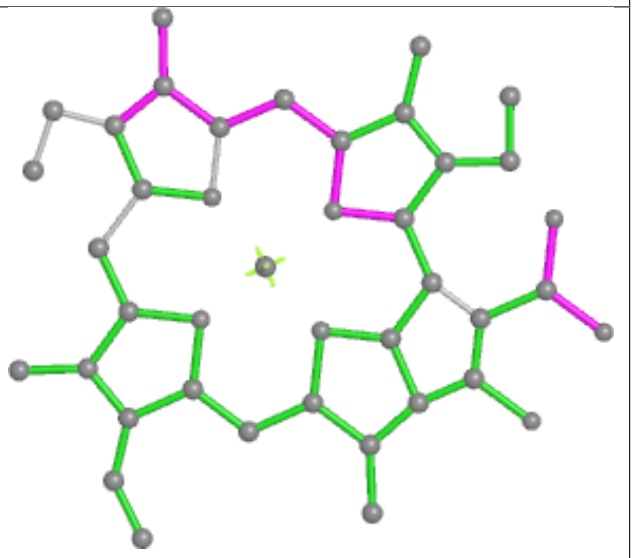
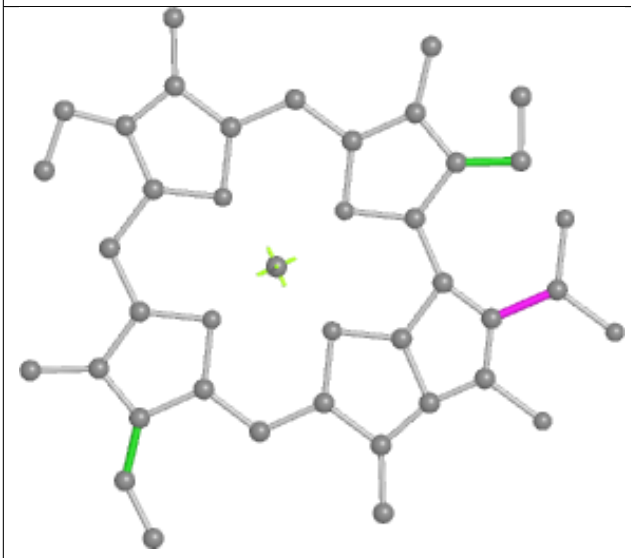


Bond angles



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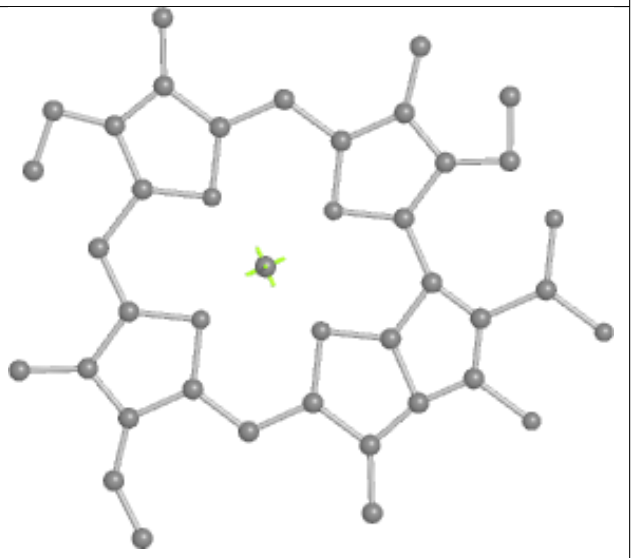
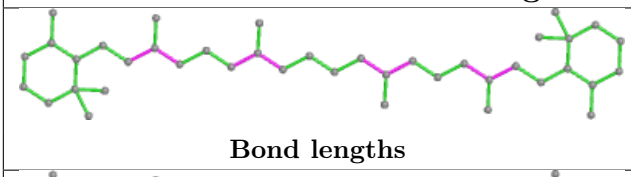
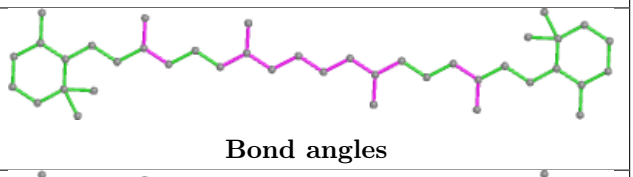


Rings

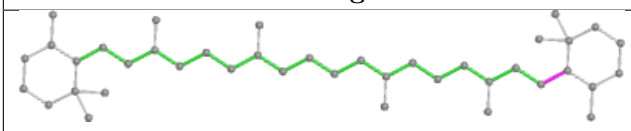
Ligand BCR B 845



Bond lengths



Bond angles



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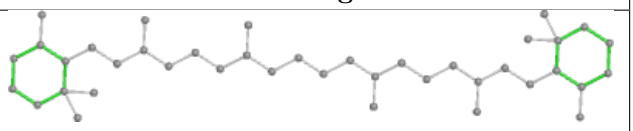
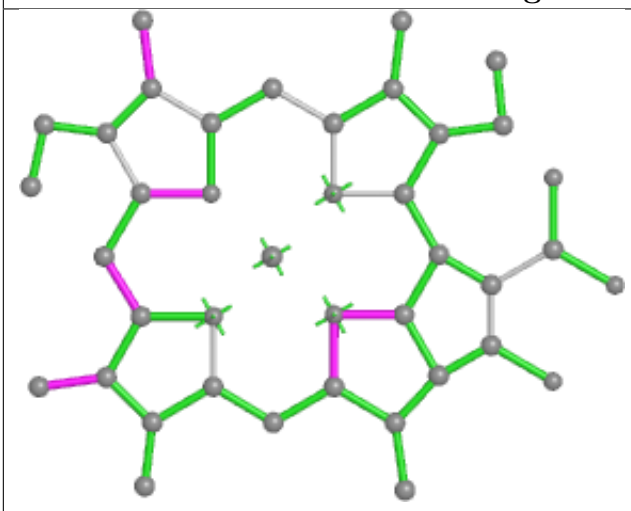


Rings

Ligand CLA O 204



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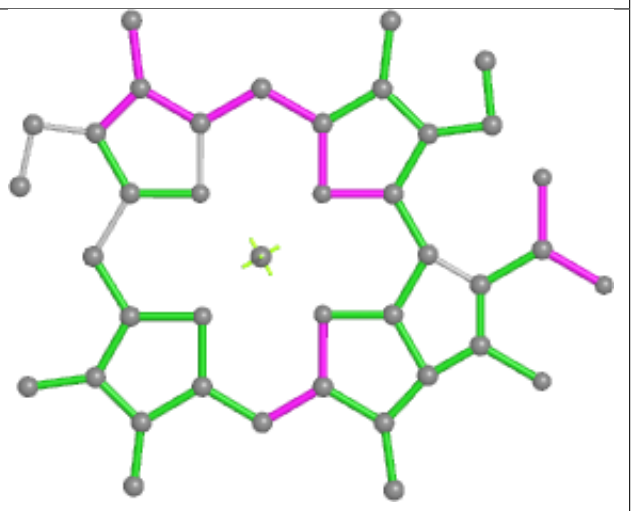
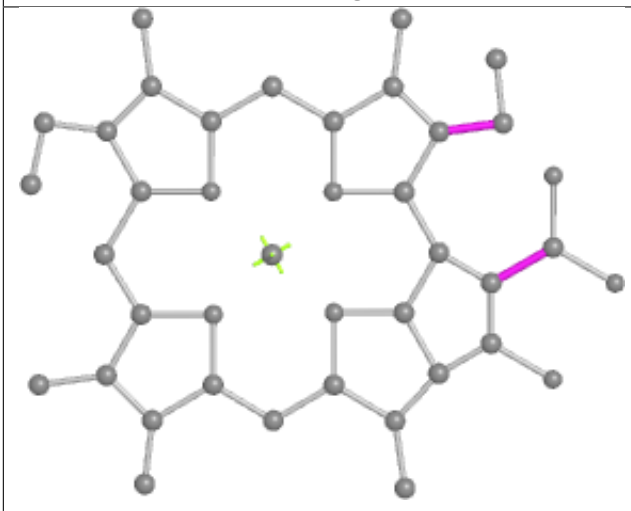


Bond angles



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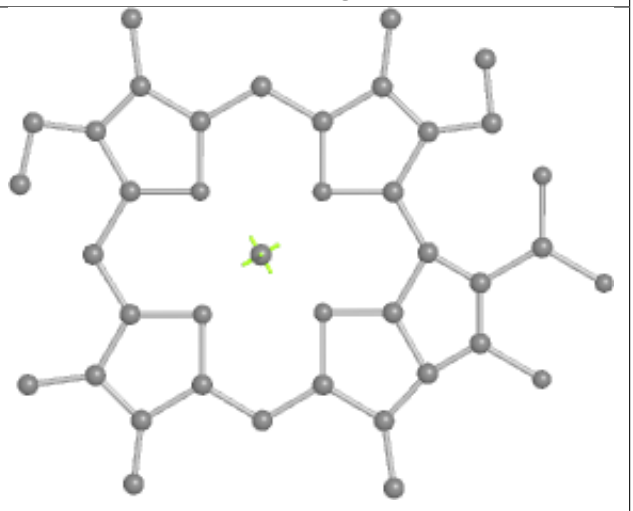
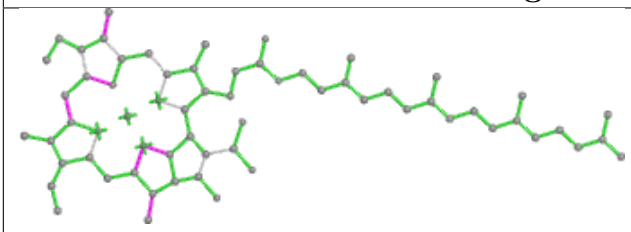
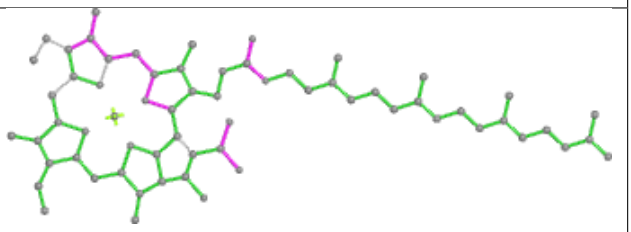


Rings

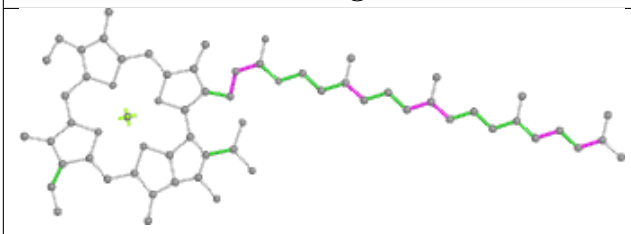
Ligand CLA B 837



Bond lengths



Bond angles



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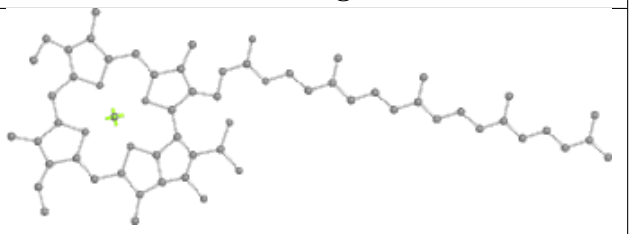
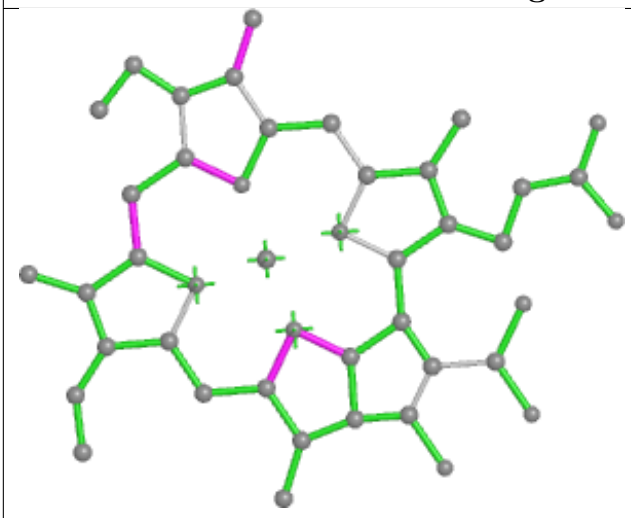


Rings

Ligand CLA 8 603



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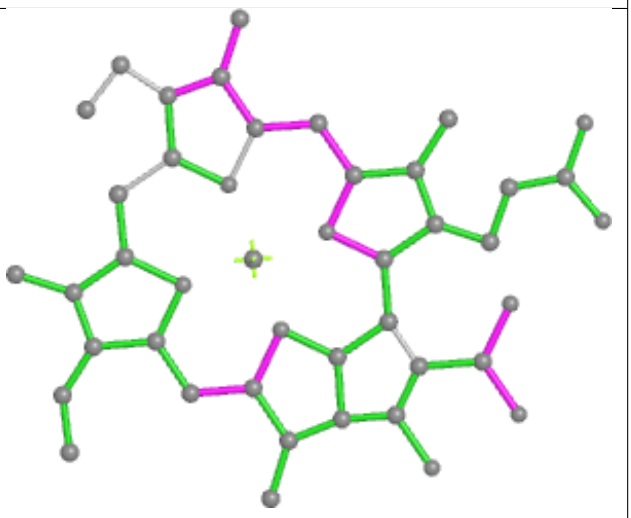

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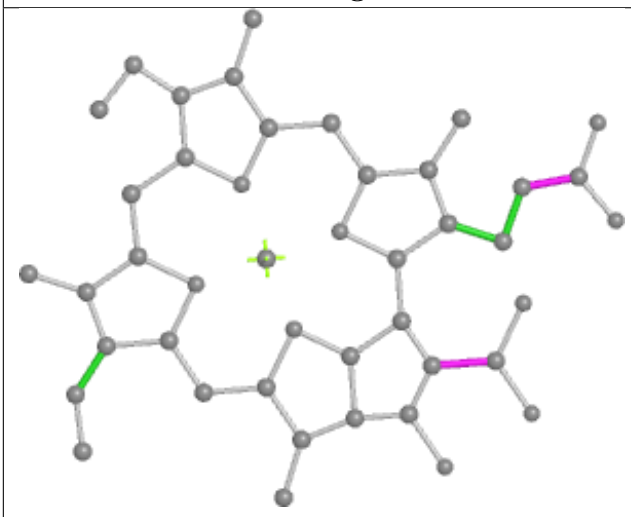

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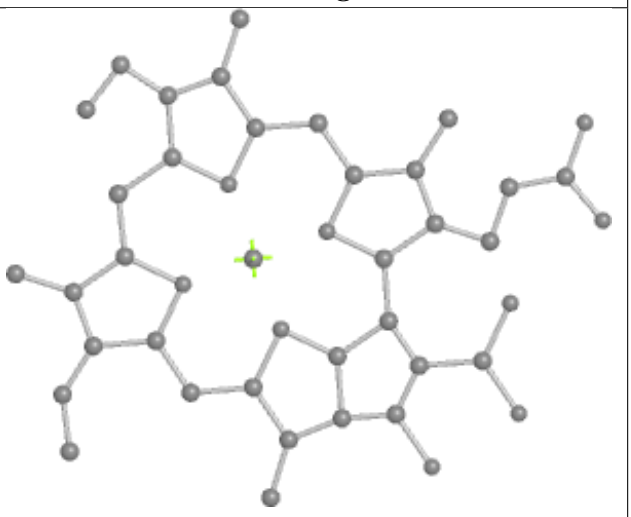
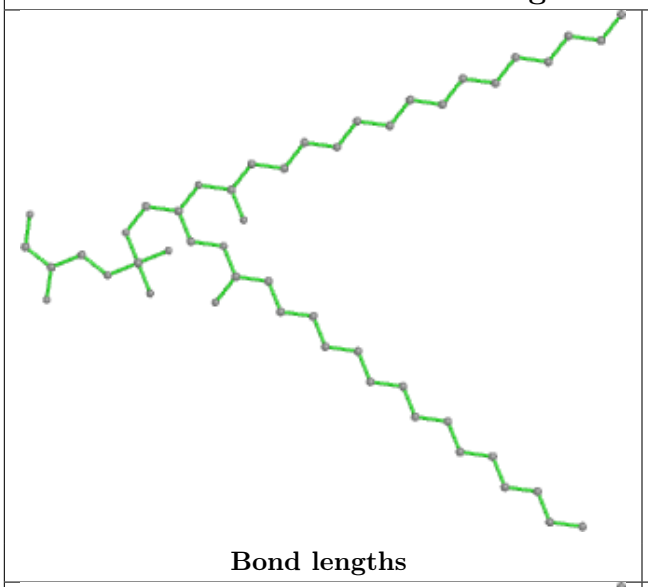


Rings

Ligand LHG c 619



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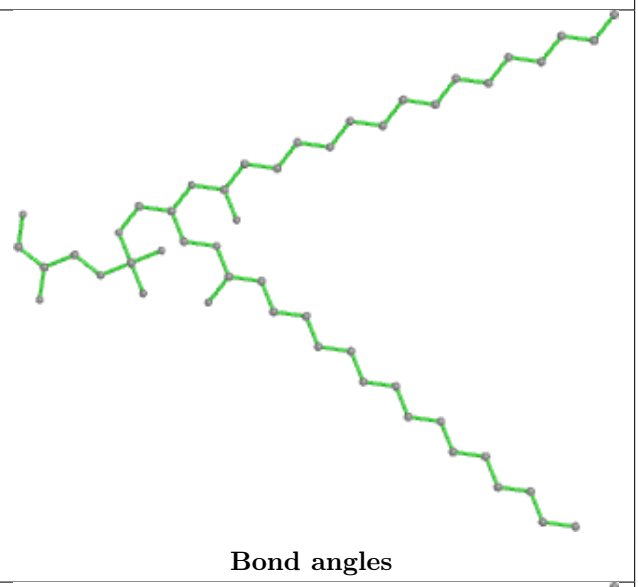

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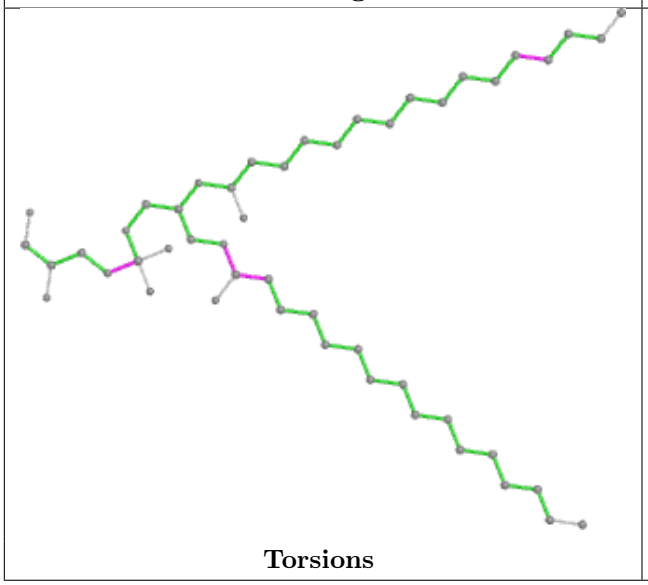

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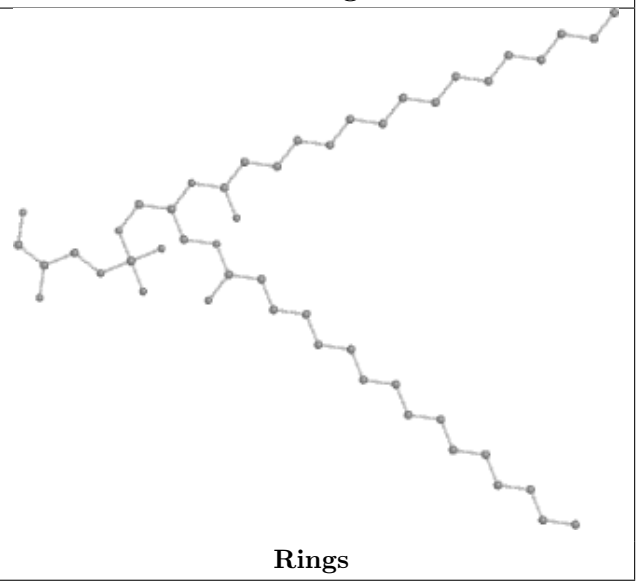
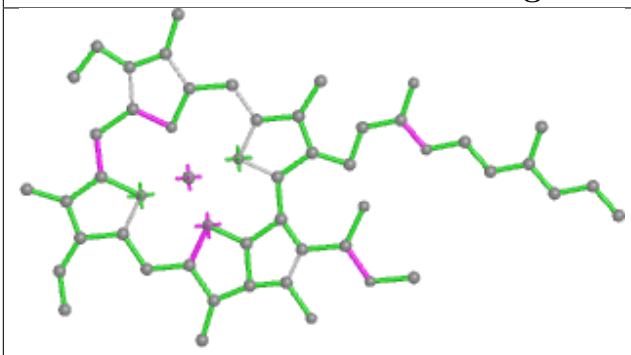


Rings

Ligand CLA A 801



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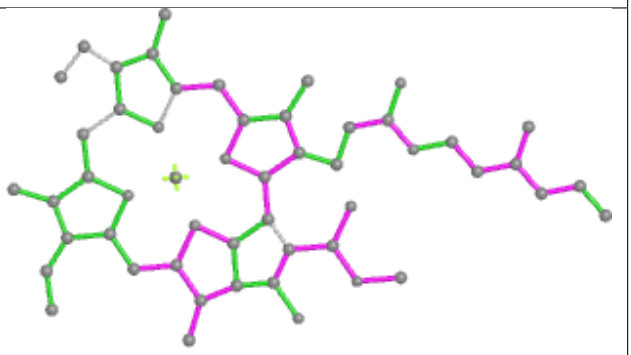

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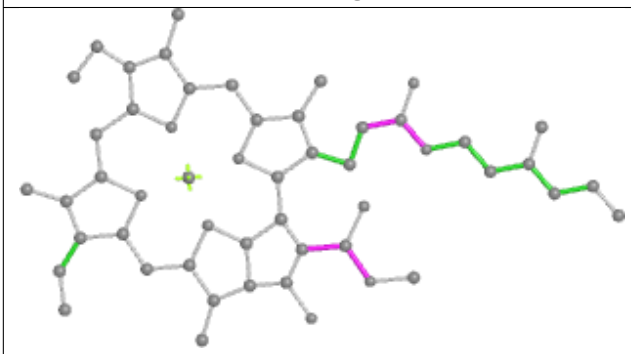

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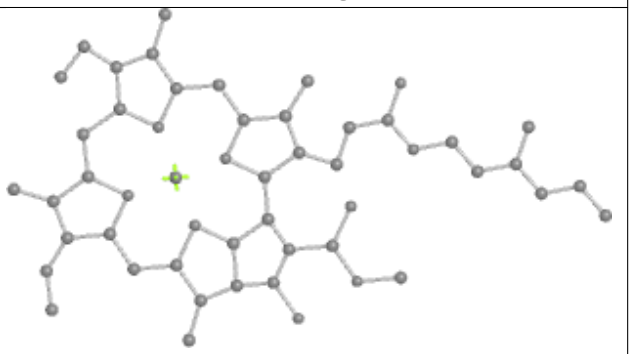
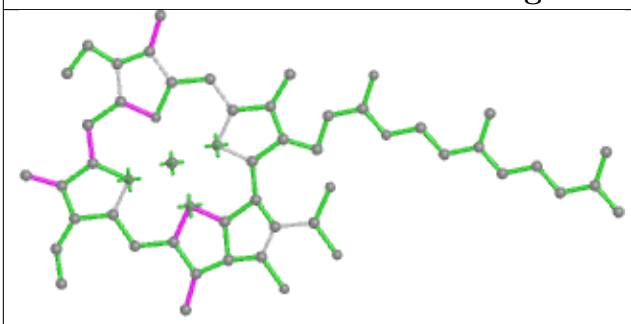


Rings

Ligand CLA B 815



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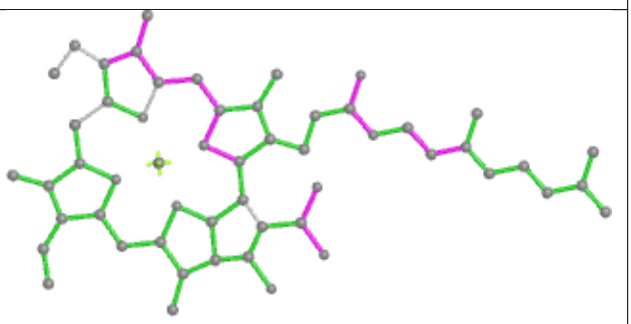
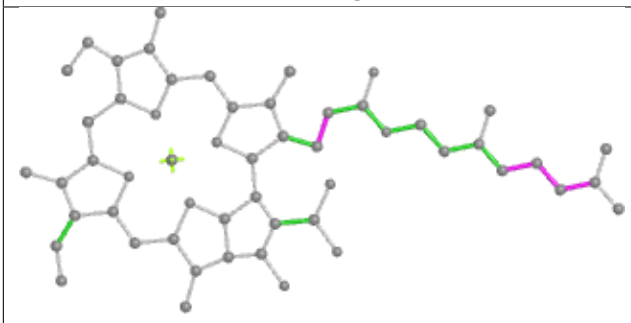


Bond angles



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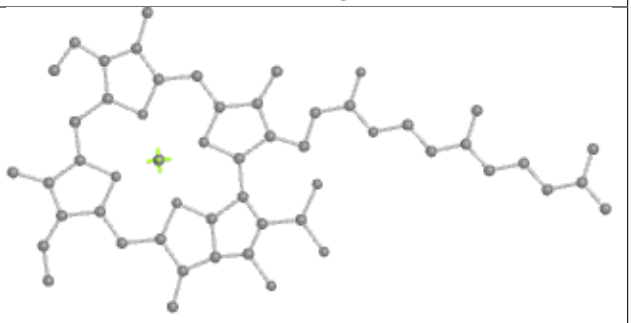

Rings

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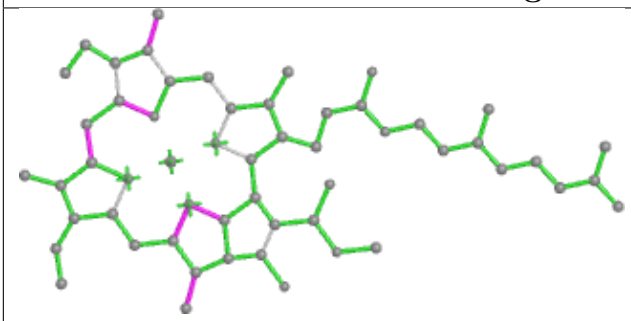

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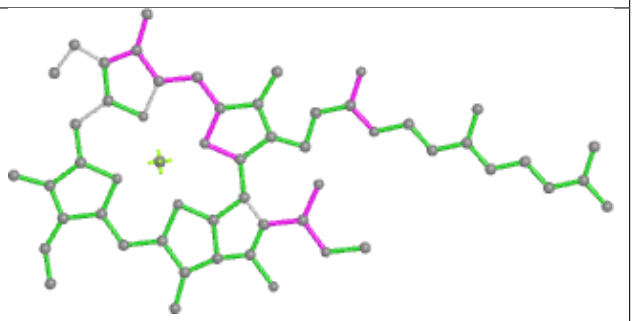
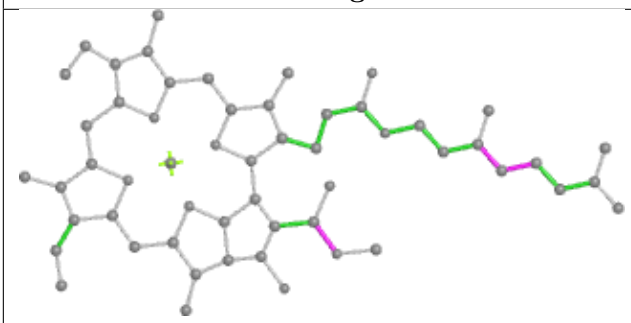


Bond angles



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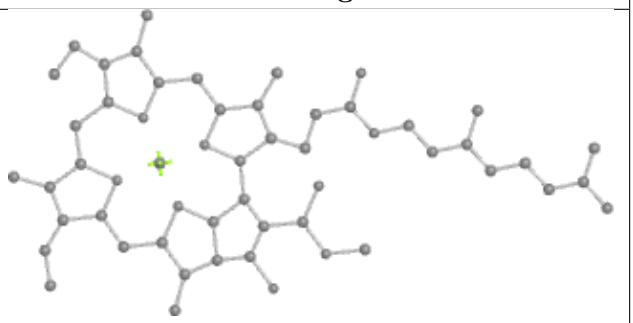

Rings

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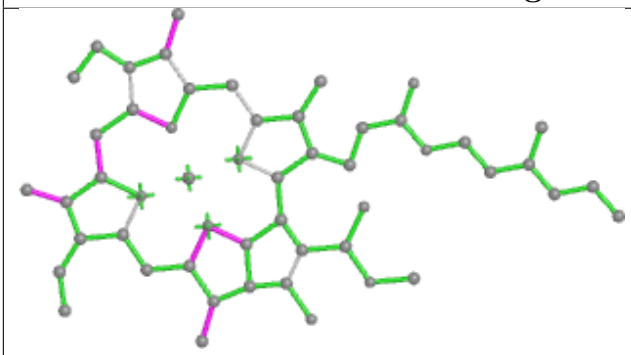

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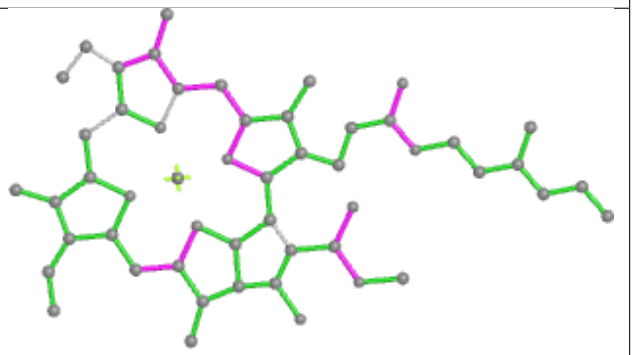

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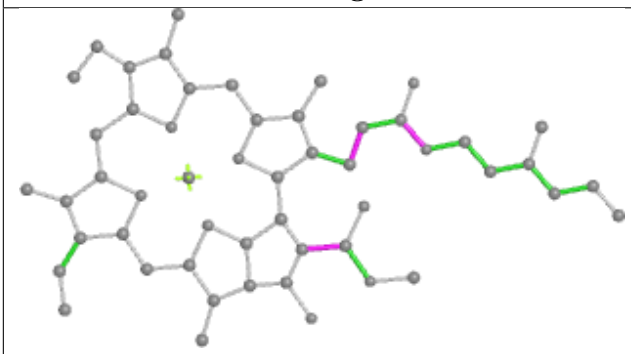

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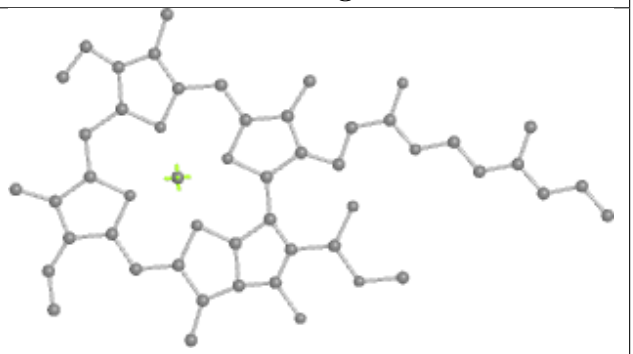
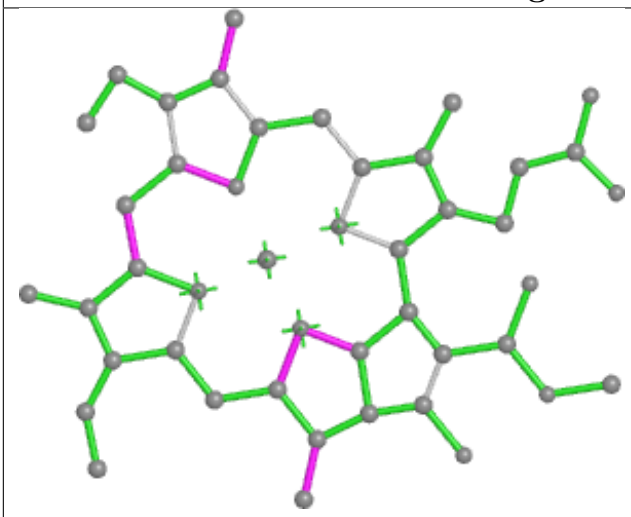


Rings

Ligand CLA 5 611



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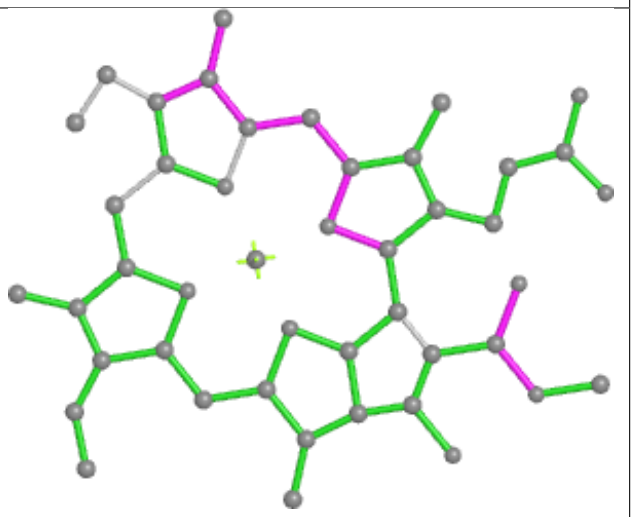

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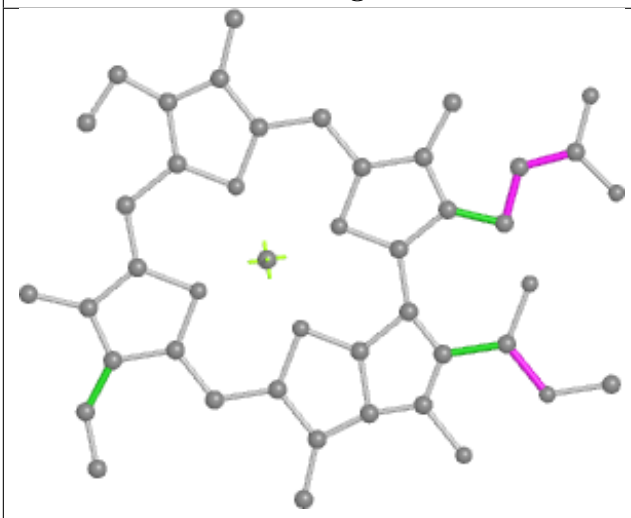

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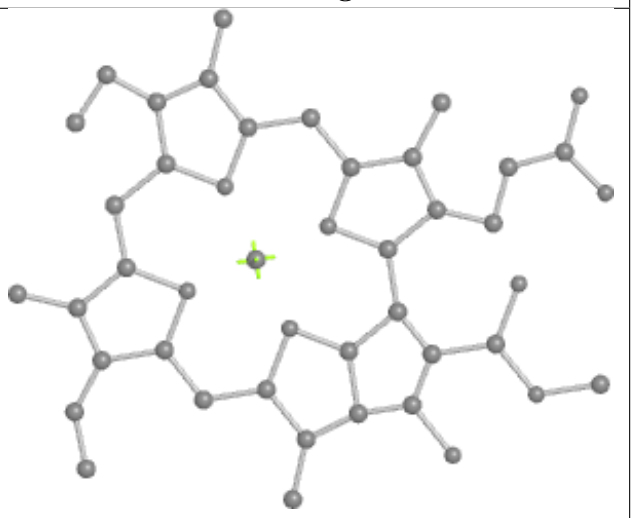
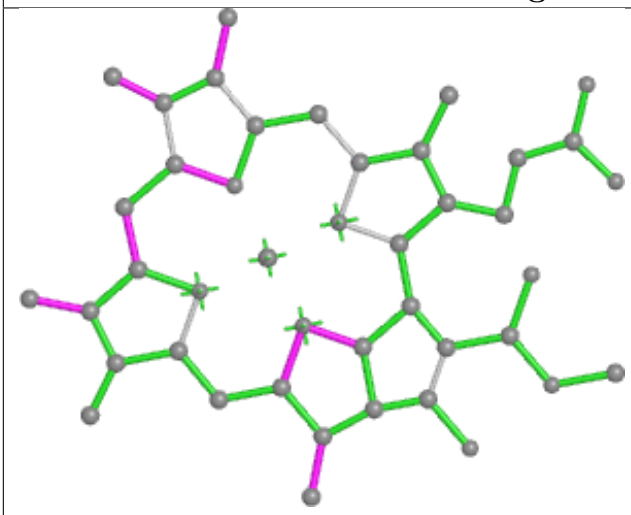


Rings

Ligand CLA 1 316



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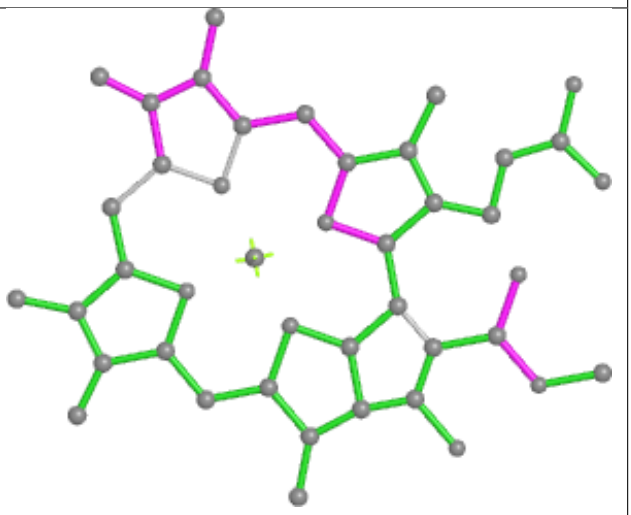

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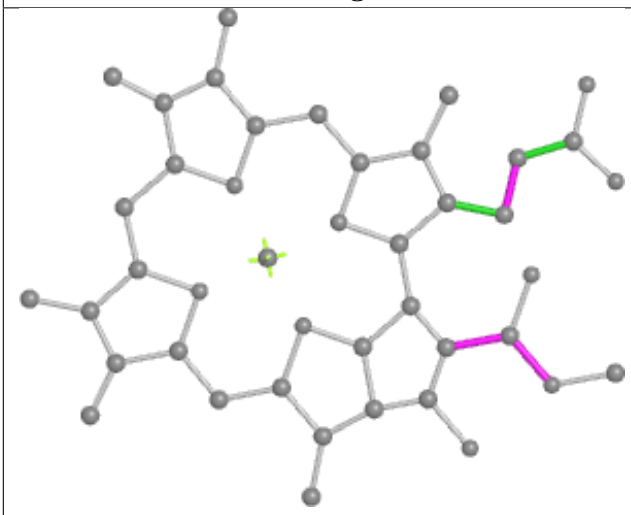

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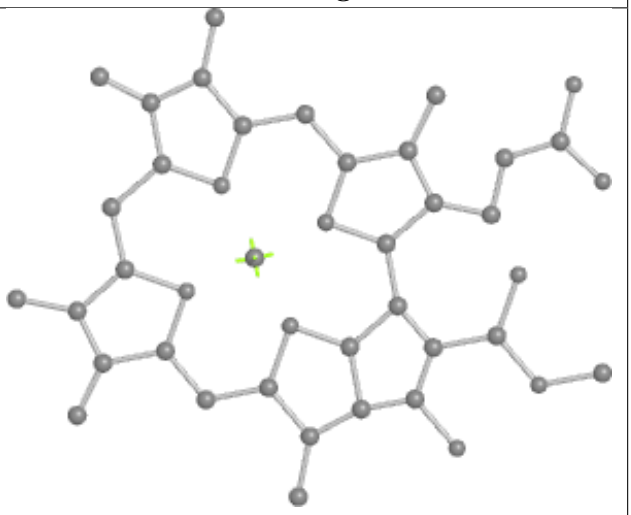
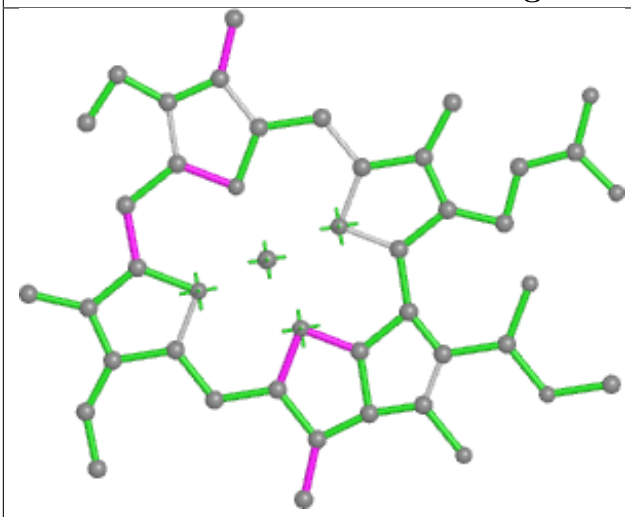


Rings

Ligand CLA A 832



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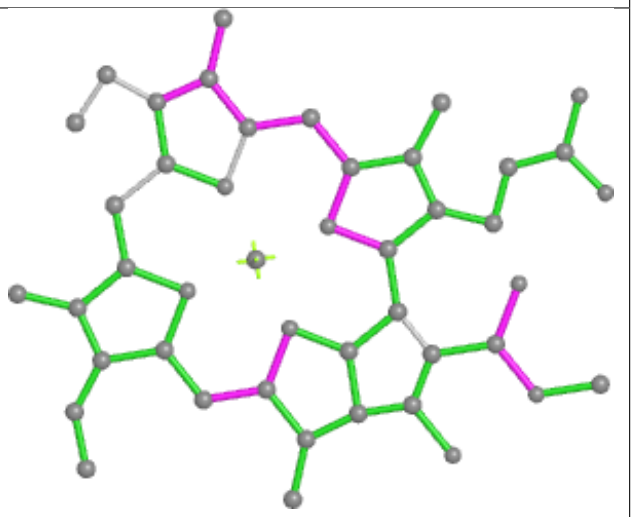

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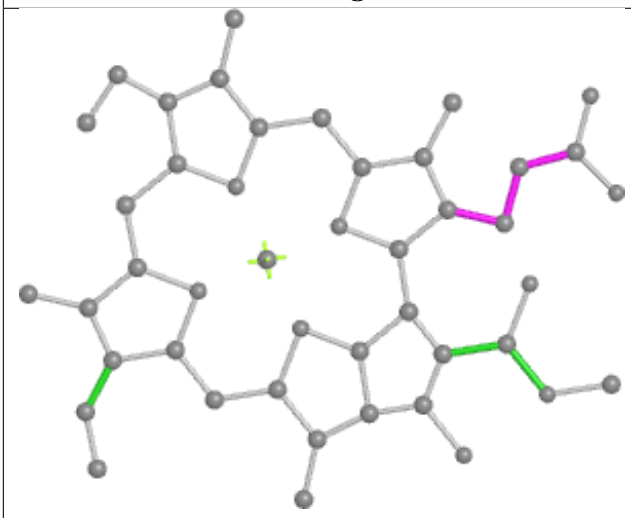

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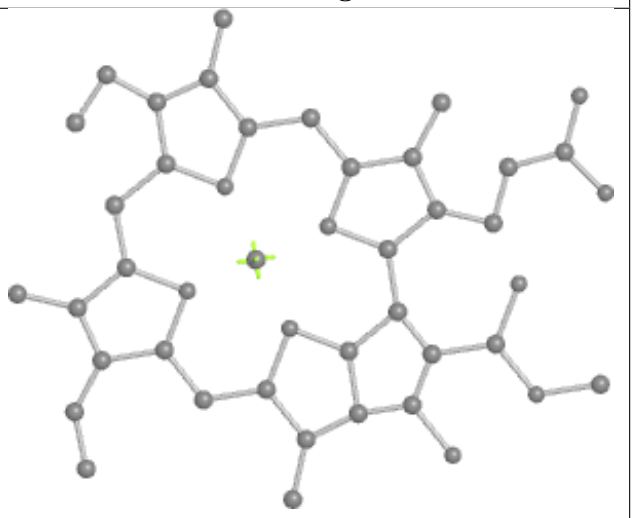
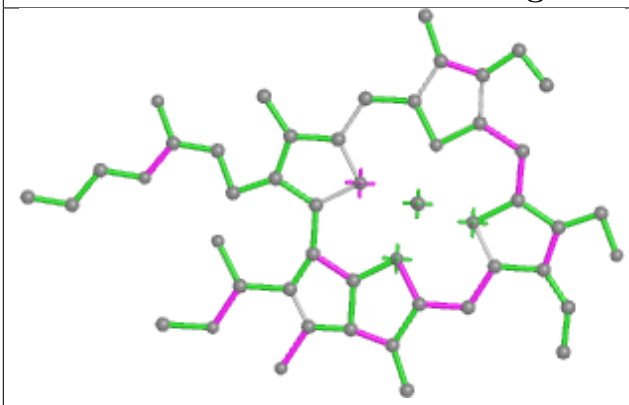


Rings

Ligand CHL b 309



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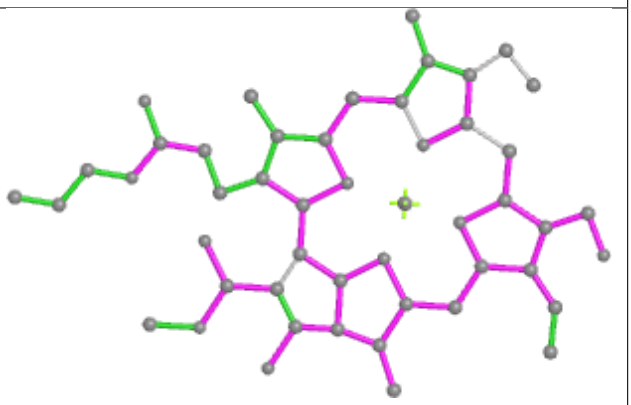
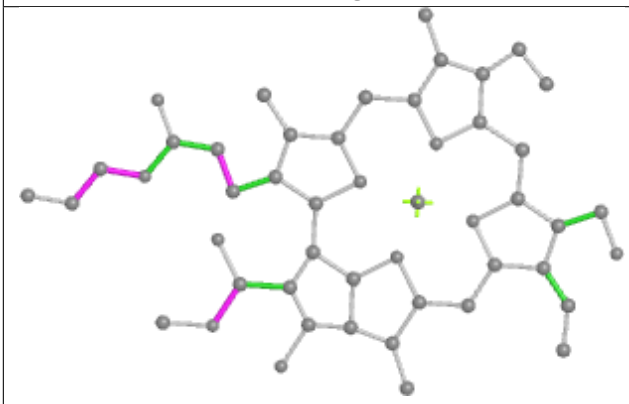


Bond angles



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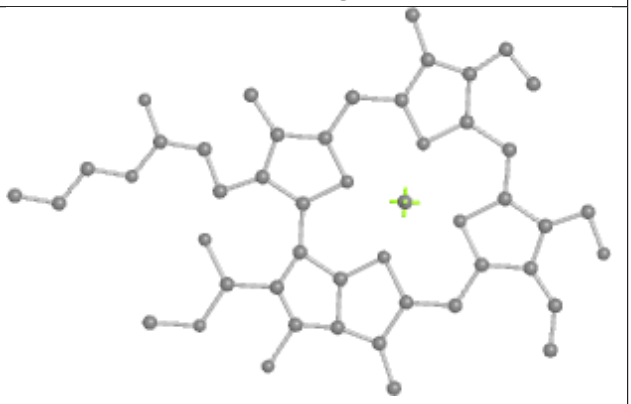
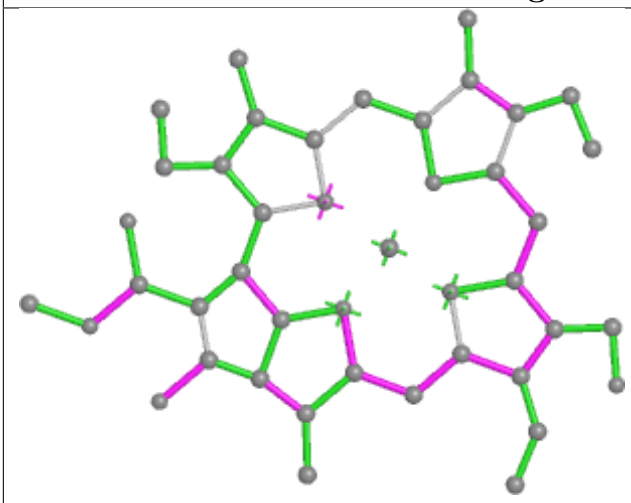


Rings

Ligand CHL a 607



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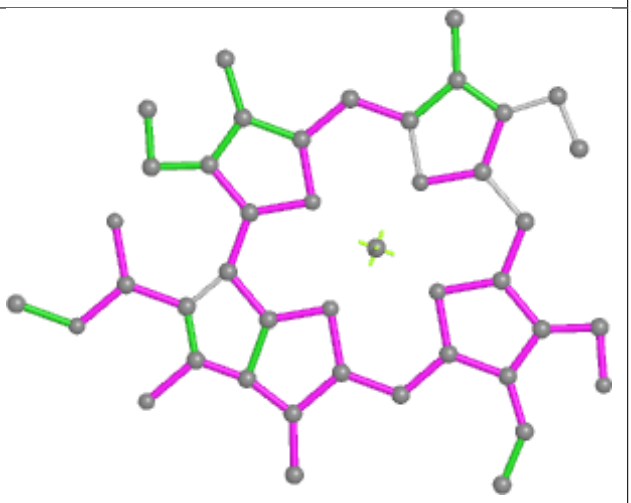
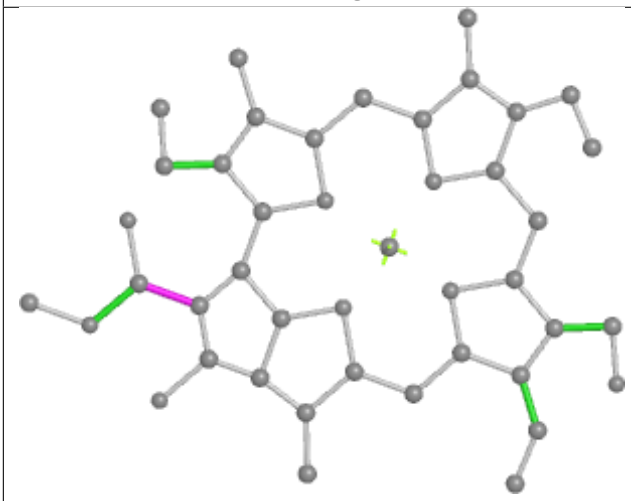


Bond angles



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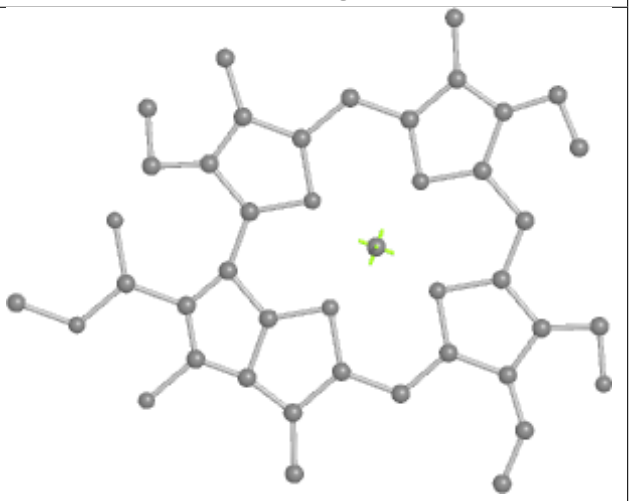
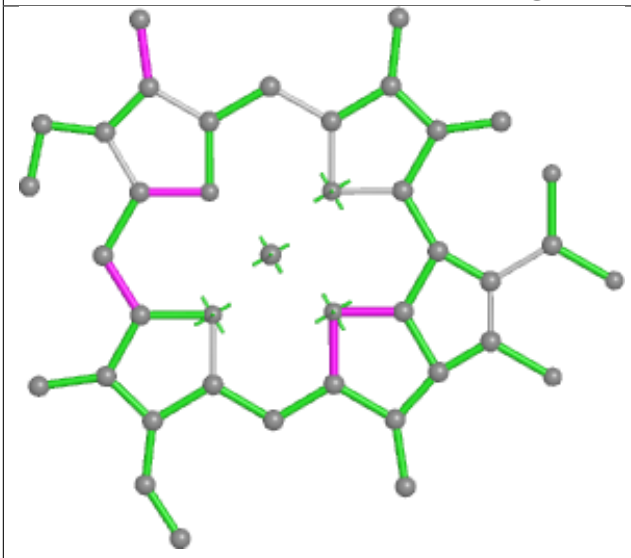


Rings

Ligand CLA 3 410



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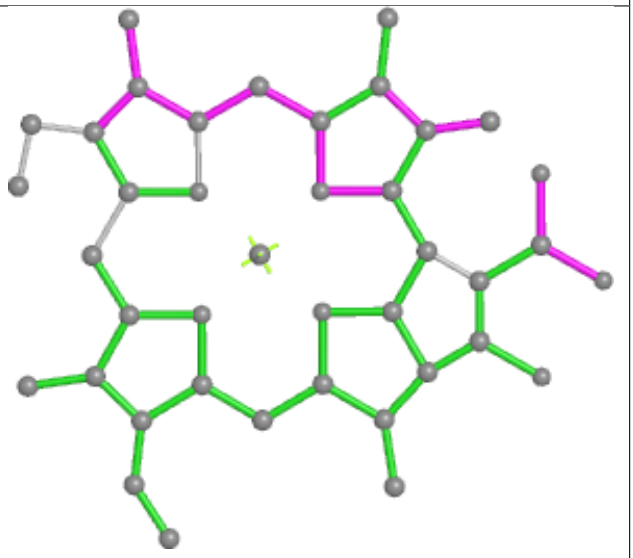
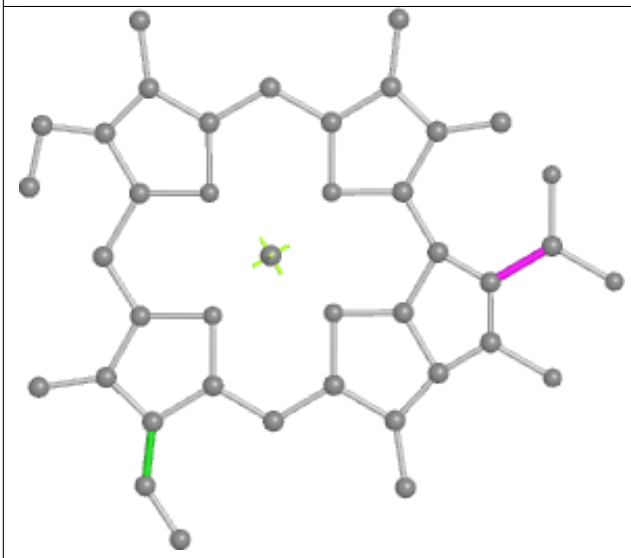


Bond angles



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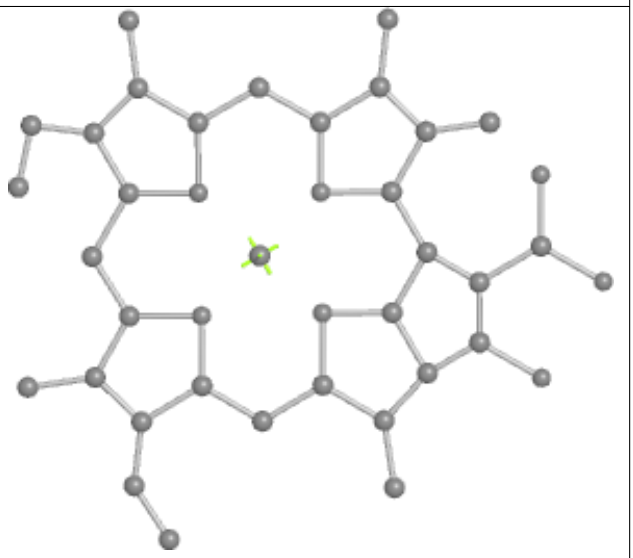
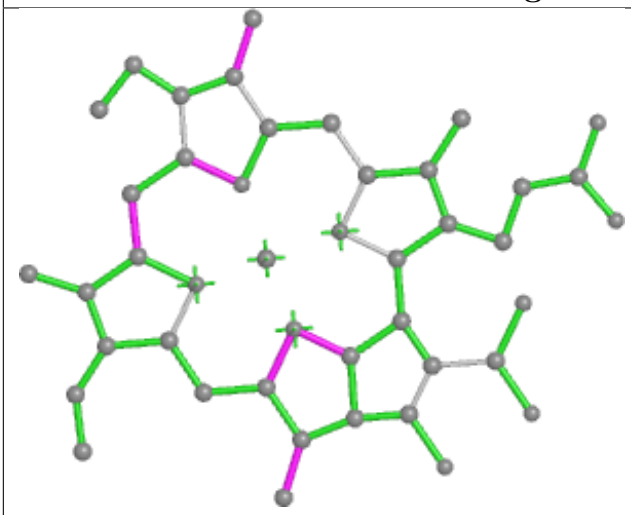
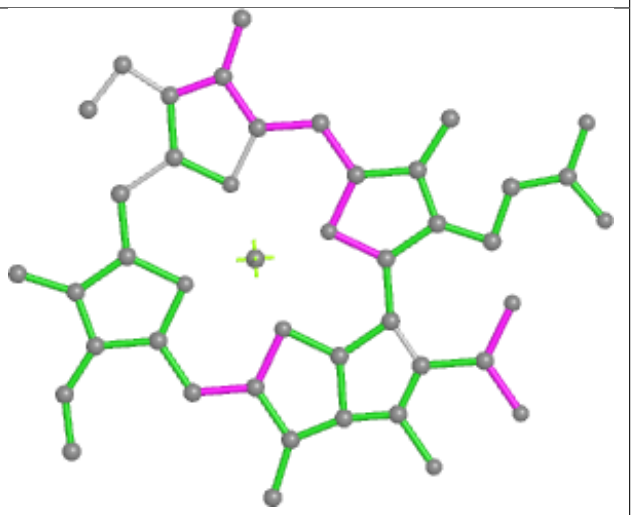


Rings

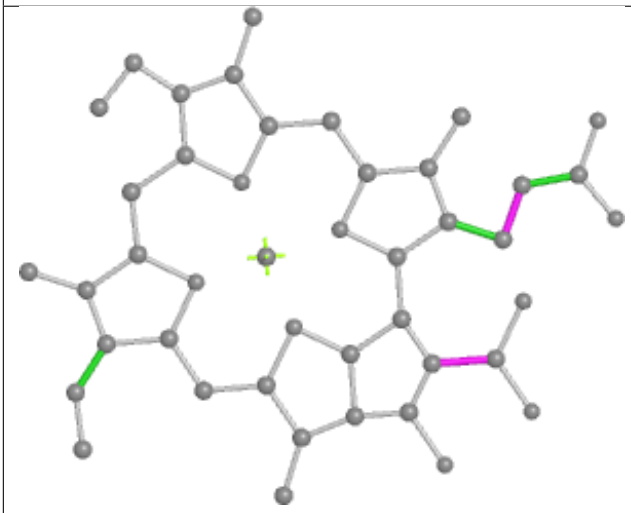
Ligand CLA B 813



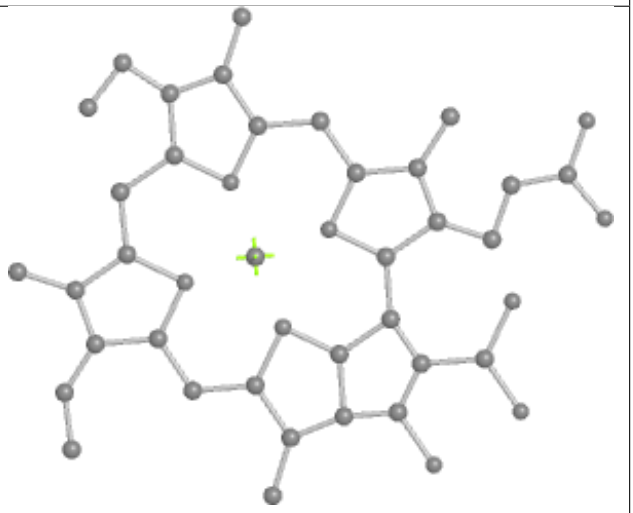
Bond lengths



Bond angles

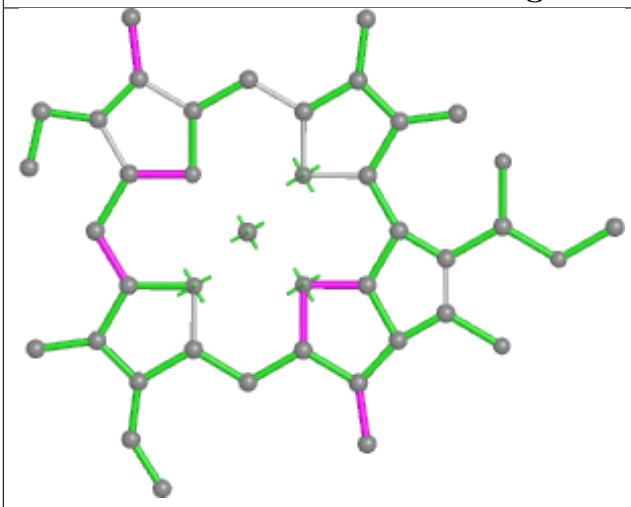


Torsions



Rings

Ligand CLA F 305



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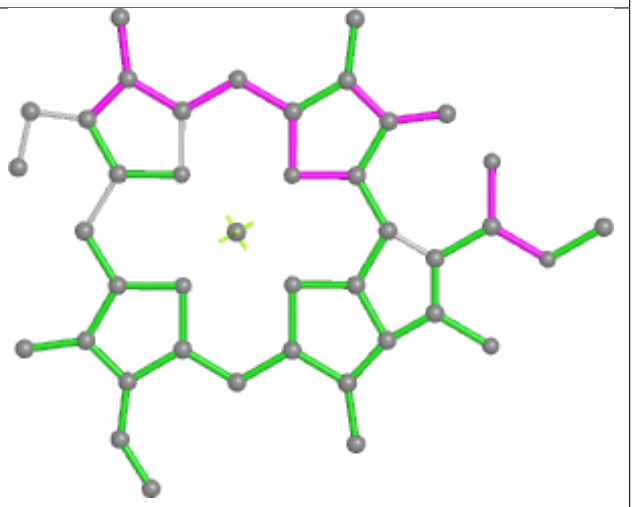

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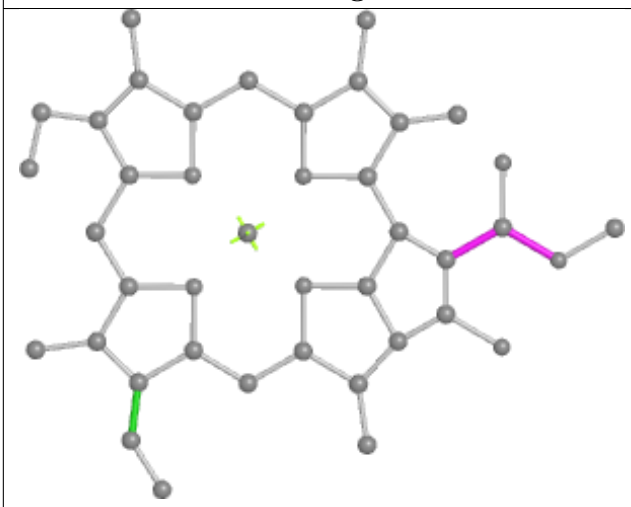

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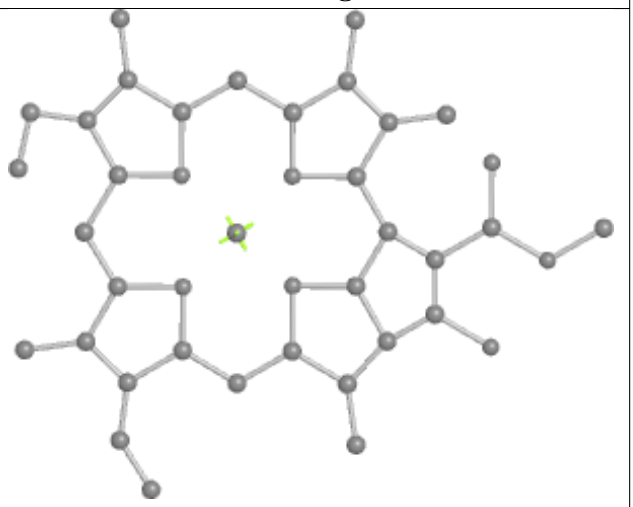
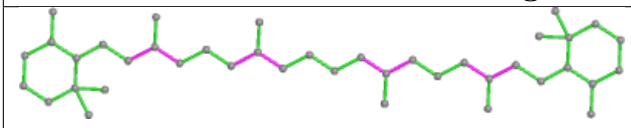


Rings

Ligand BCR A 850



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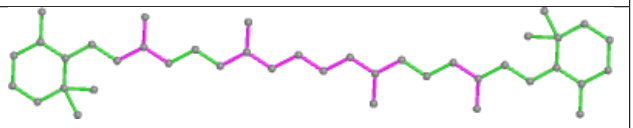
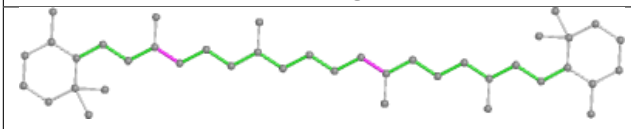


Bond angles



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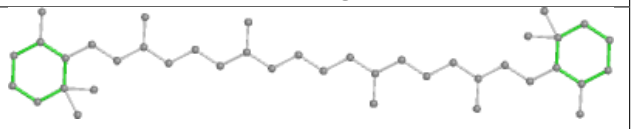
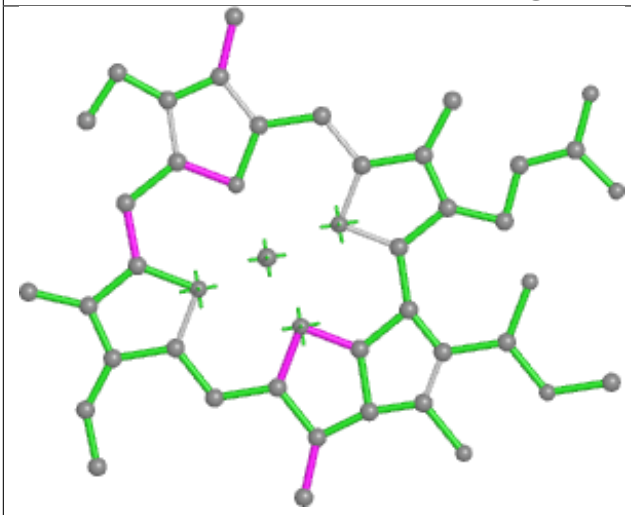


Rings

Ligand CLA b 305



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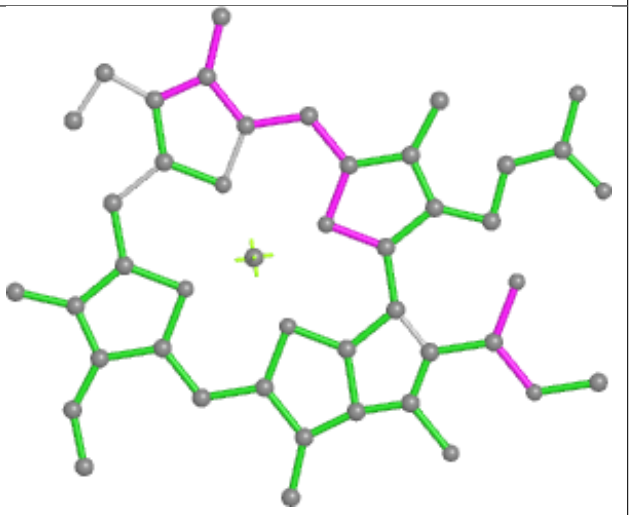
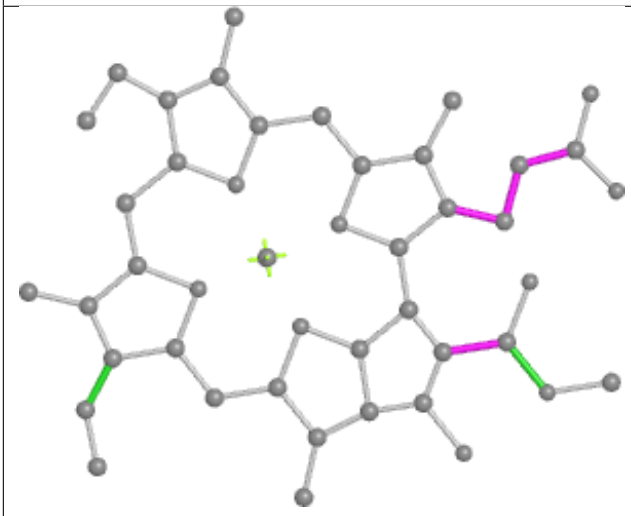


Bond angles



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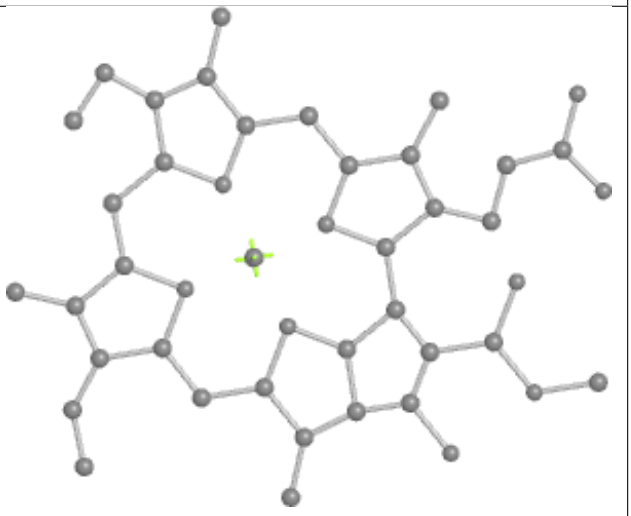
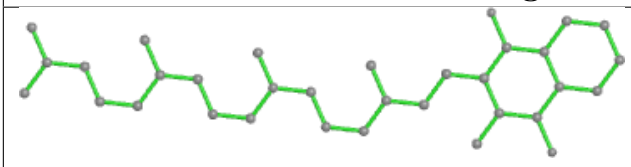


Rings

Ligand PQN B 841



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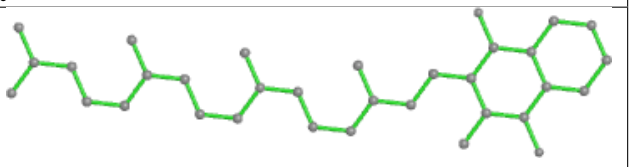

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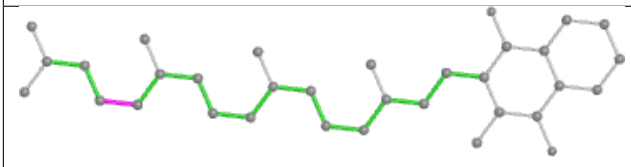

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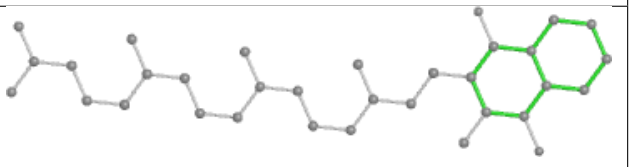
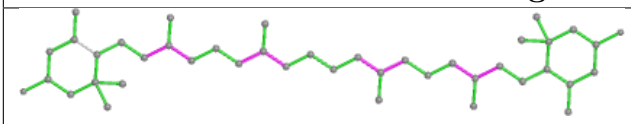


Rings

Ligand LUT 1 317



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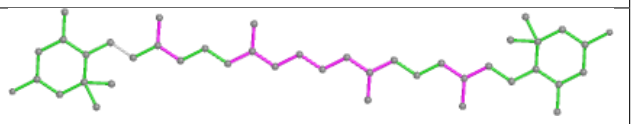
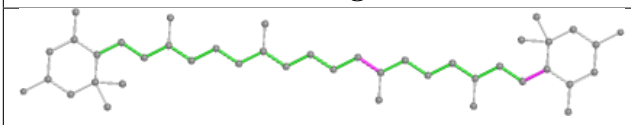


Bond angles



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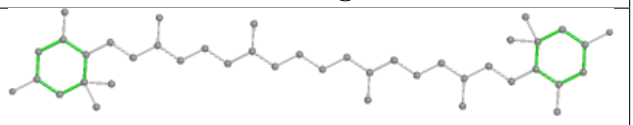
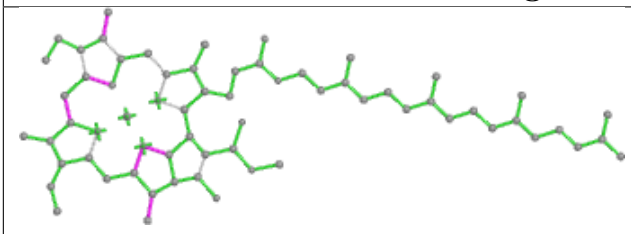


Rings

Ligand CLA A 817



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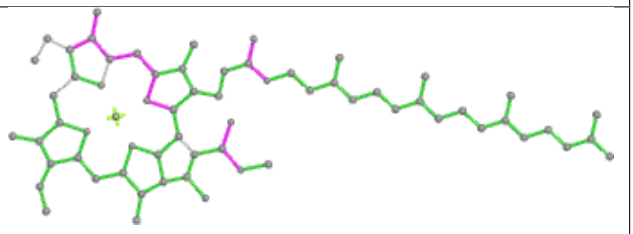

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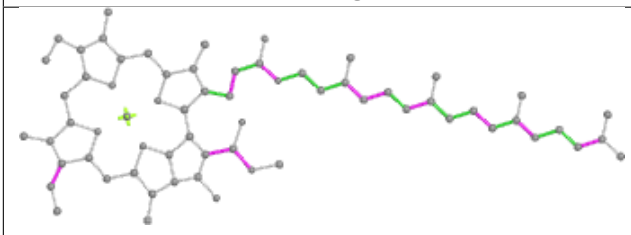

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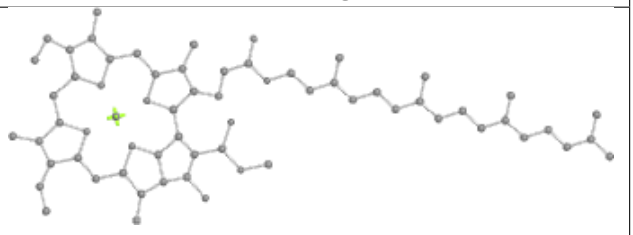
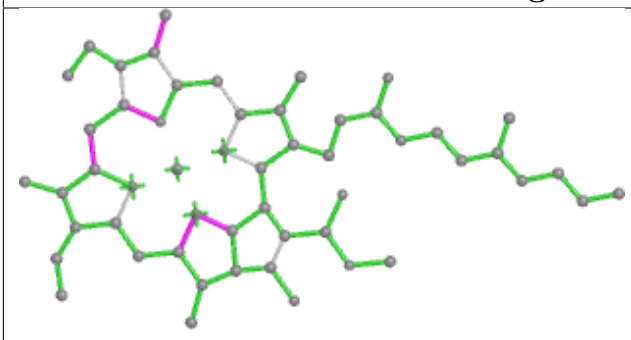


Rings

Ligand CLA 9 613



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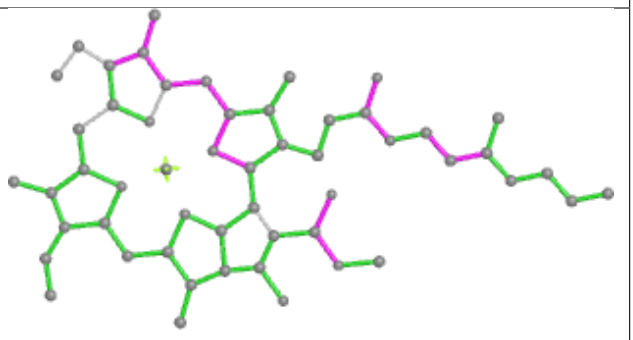
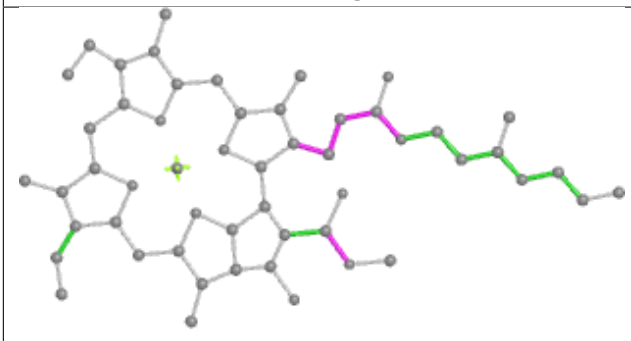


Bond angles



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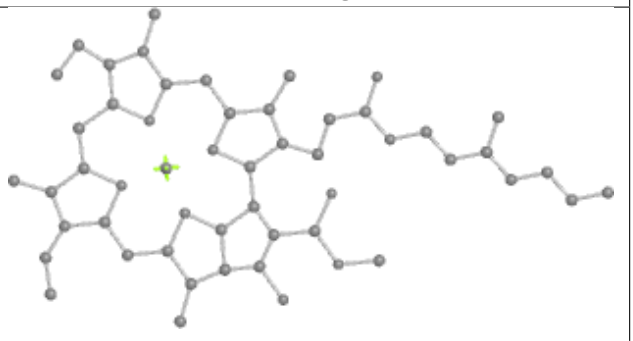
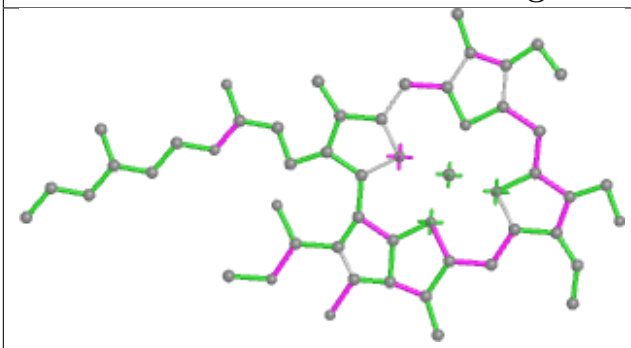


Rings

Ligand CHL 2 602



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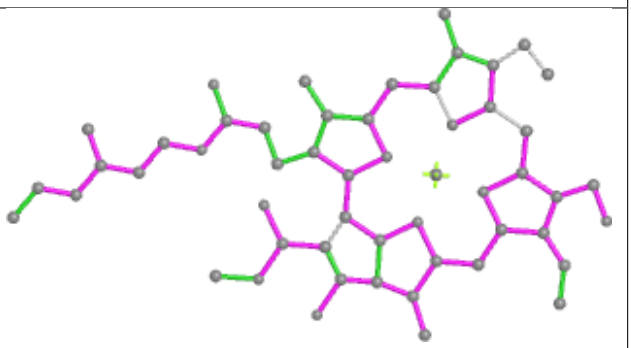
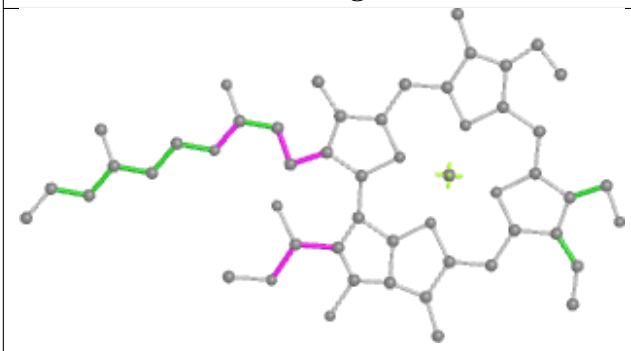


Bond angles



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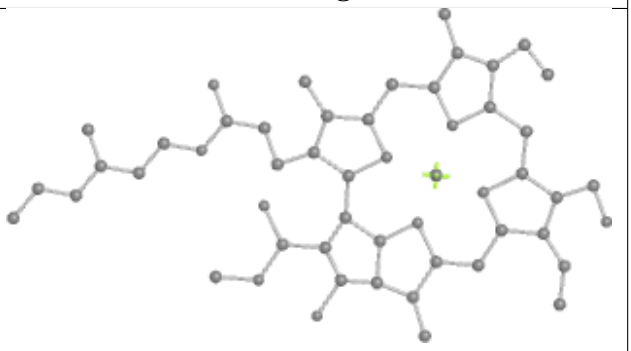
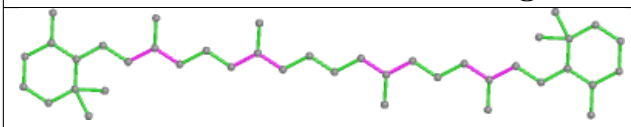


Rings

Ligand BCR M 101



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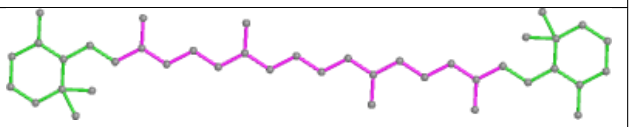
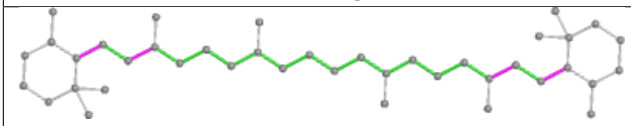


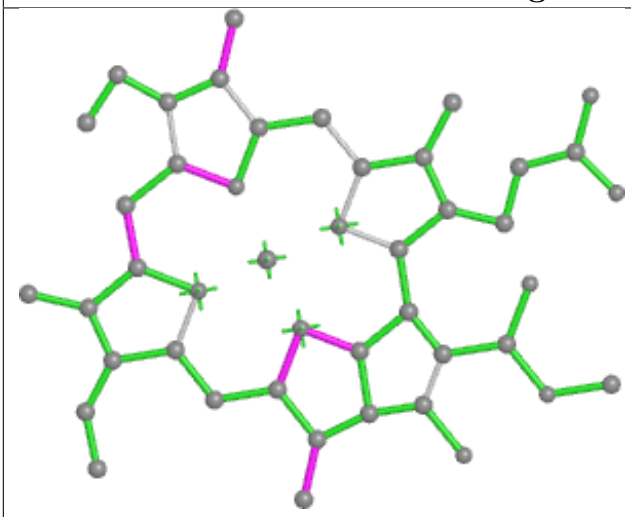
Bond angles



Torsions

Rings

Ligand CLA 9 603



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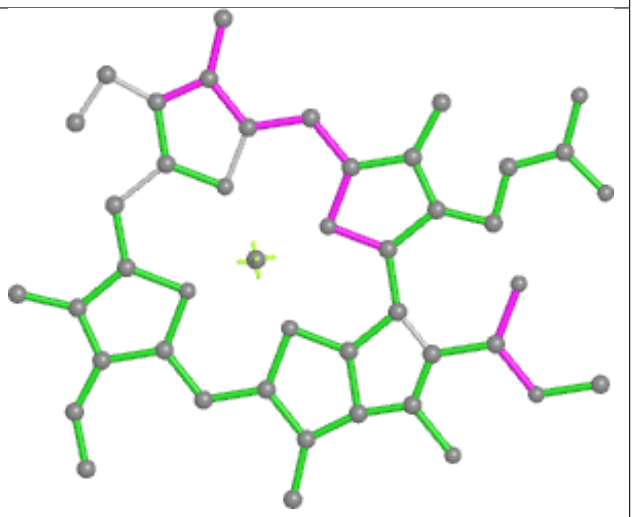

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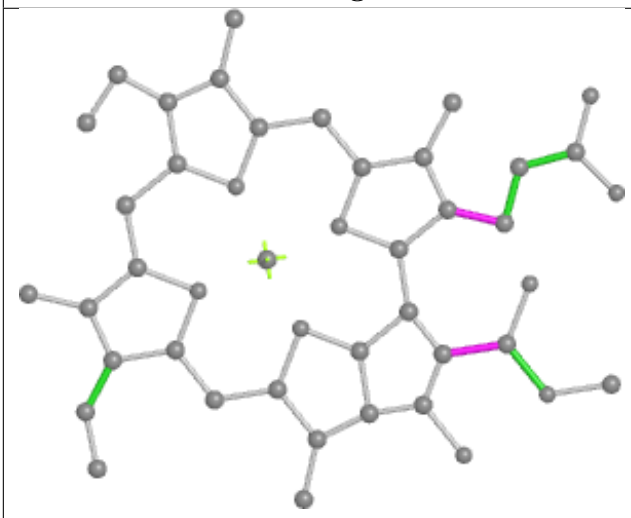

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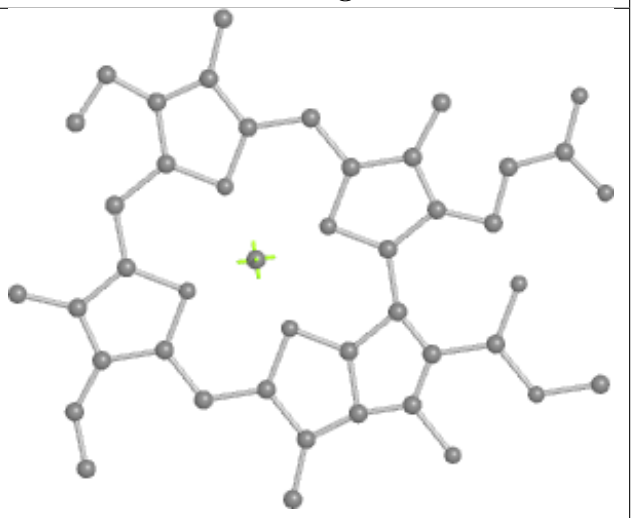
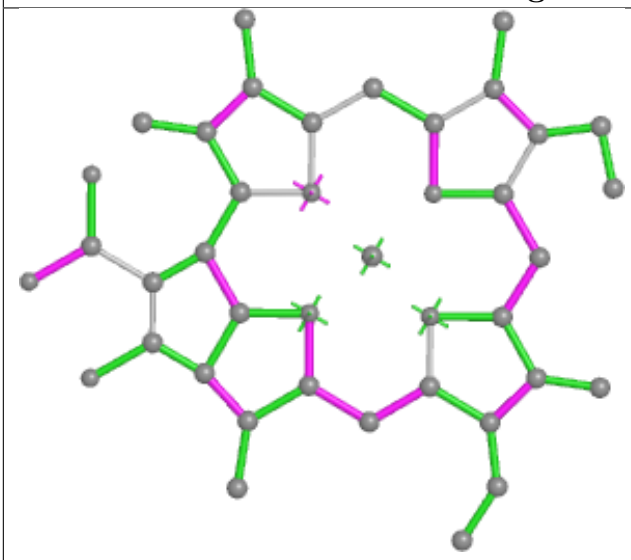


Rings

Ligand CHL 3 407



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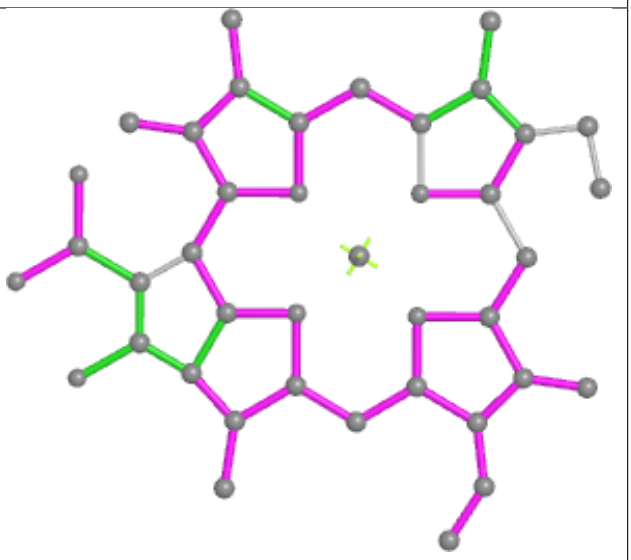
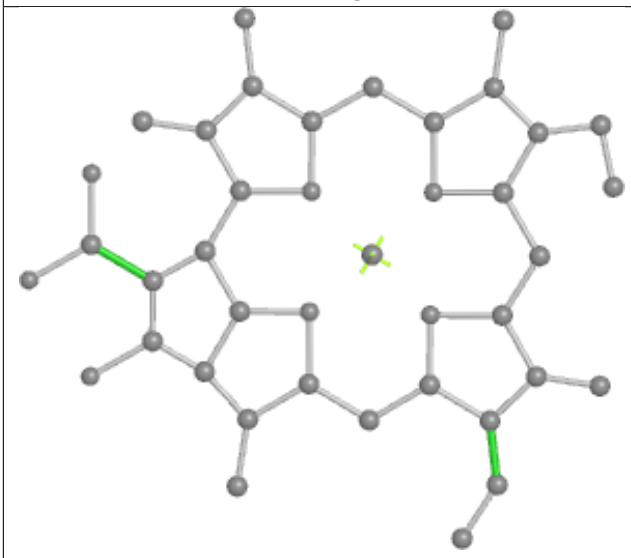


Bond angles



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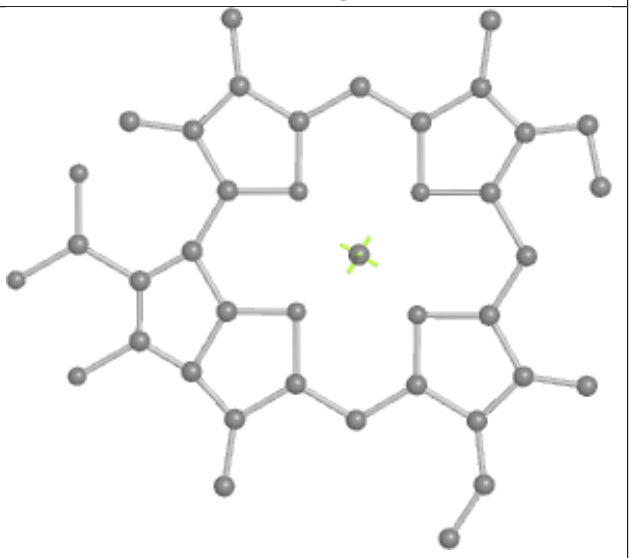
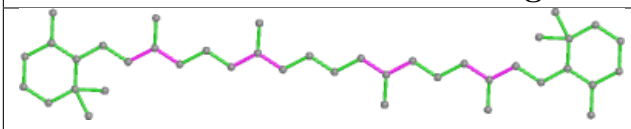


Rings

Ligand BCR L 306



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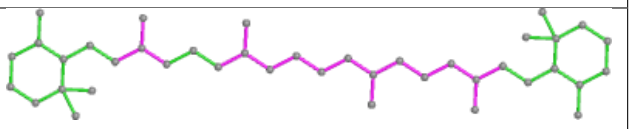
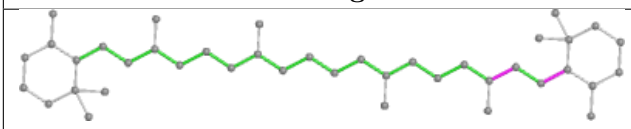
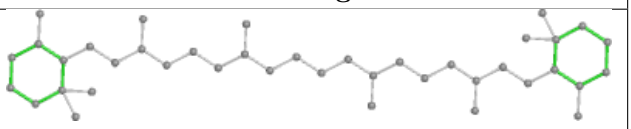


Bond angles

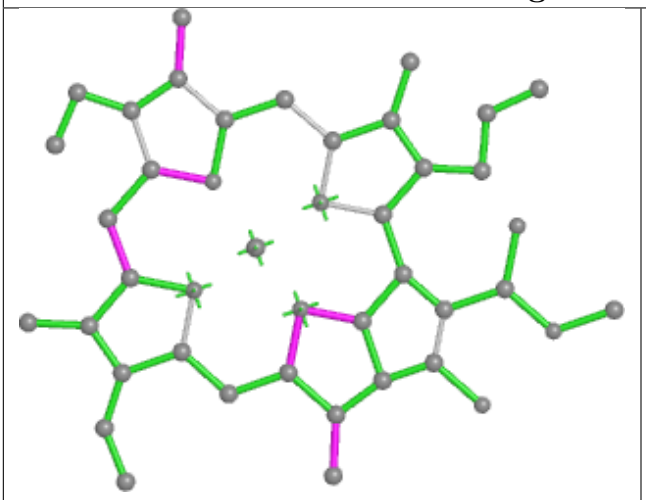


Torsions

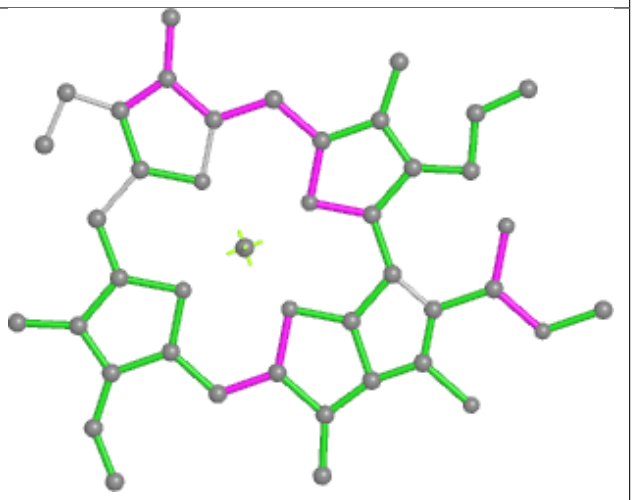


Rings

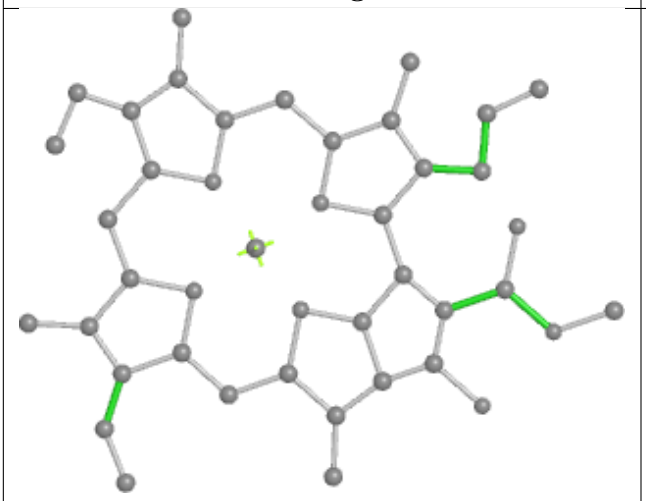
Ligand CLA 4 613



Bond lengths



Bond angles



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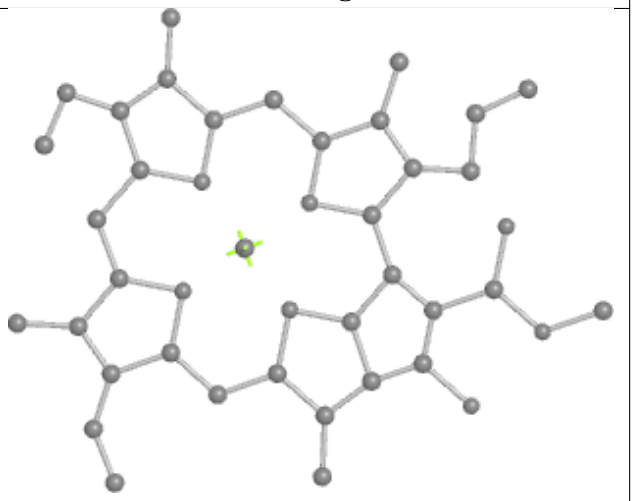
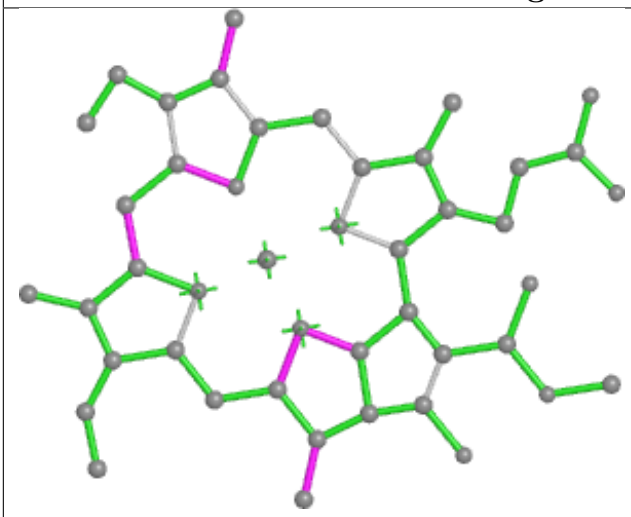


Rings

Ligand CLA b 304



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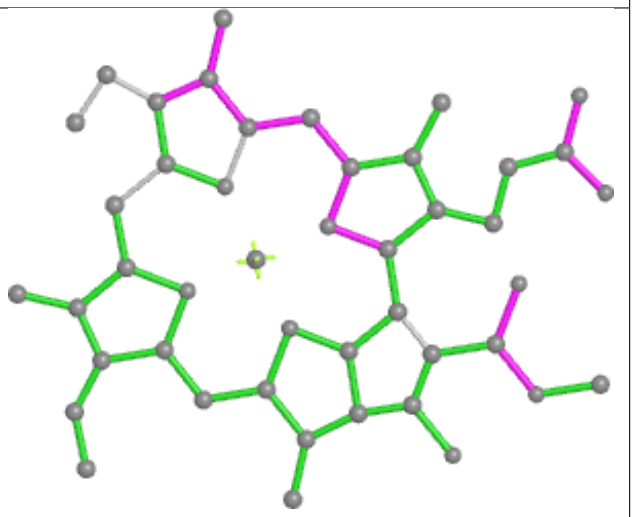
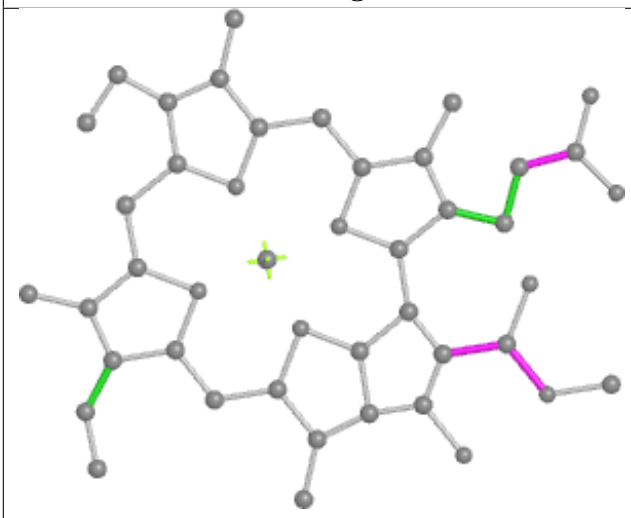


Bond angles



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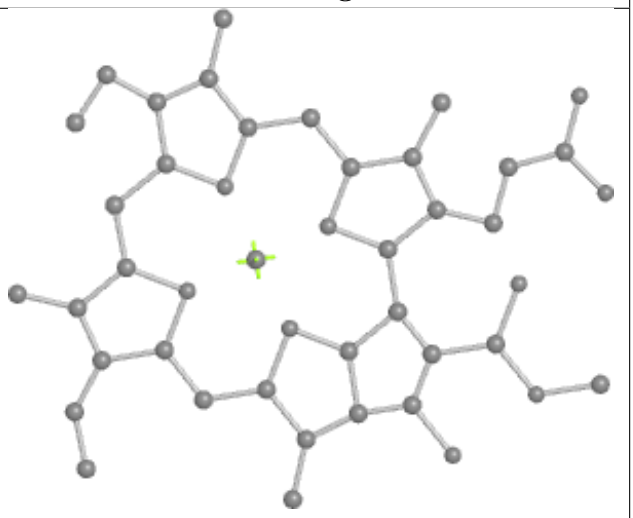
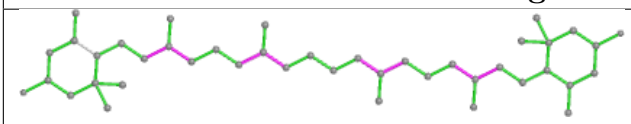


Rings

Ligand LUT 5 615



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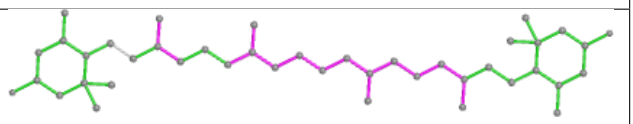
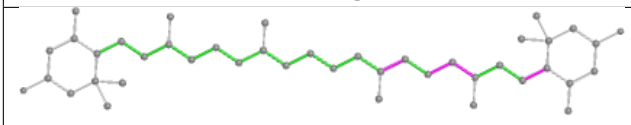


Bond angles



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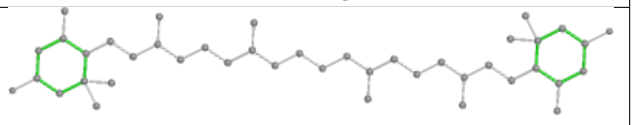
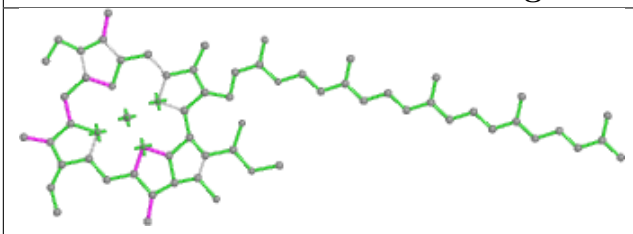


Rings

Ligand CLA B 807



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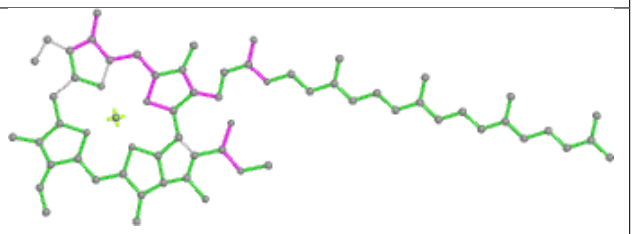
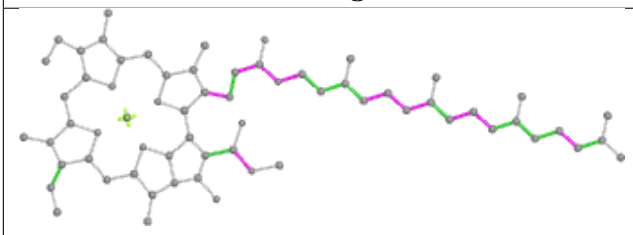


Bond angles



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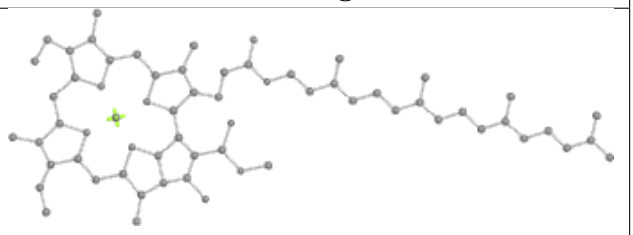
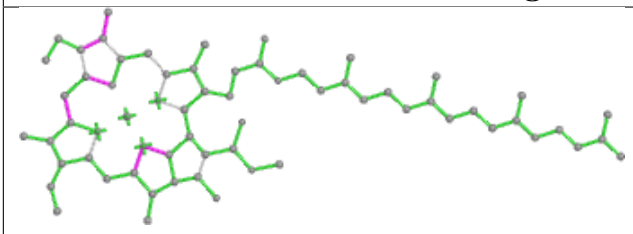


Rings

Ligand CLA A 833



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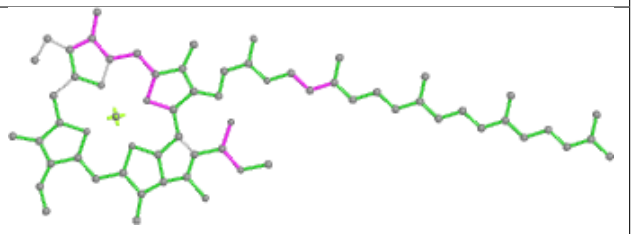
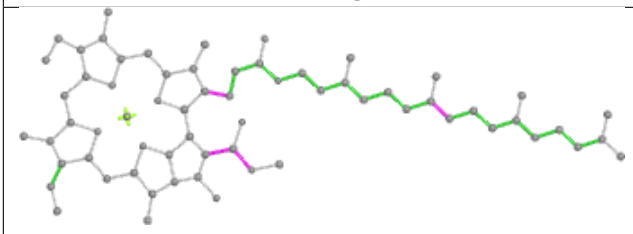


Bond angles



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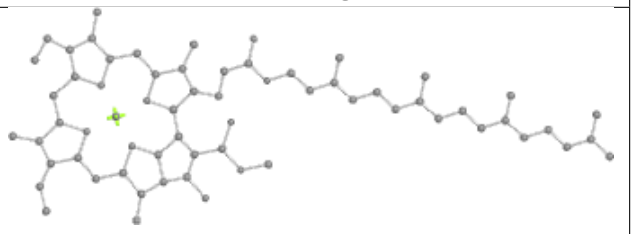
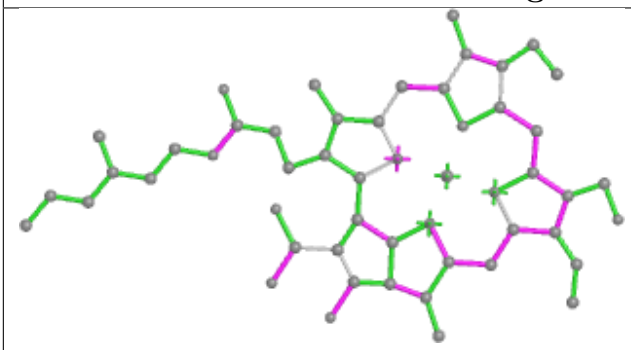
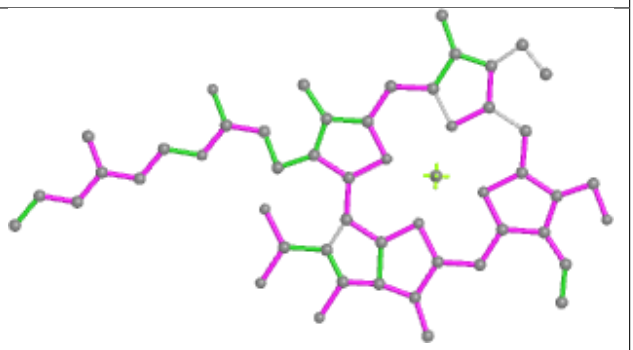
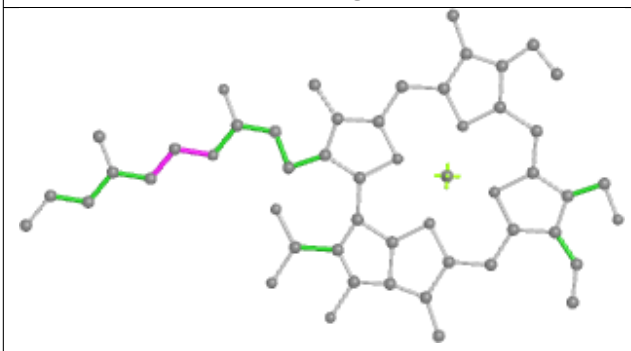
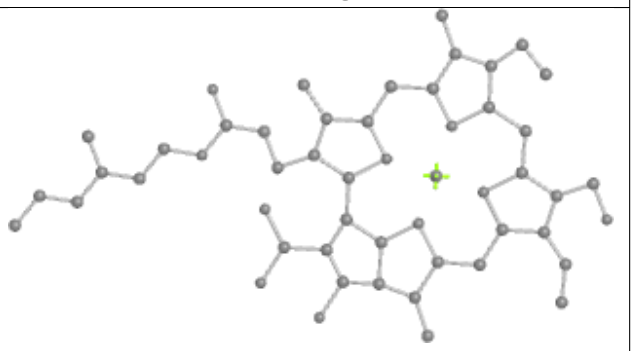
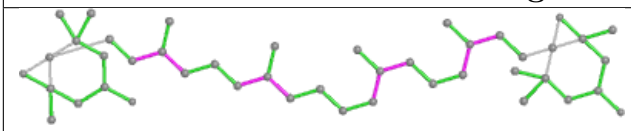
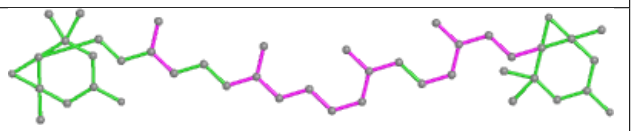
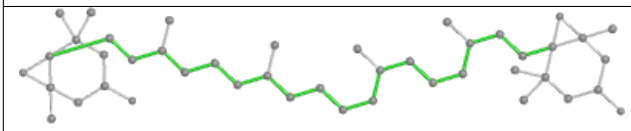
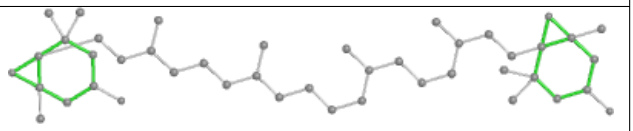
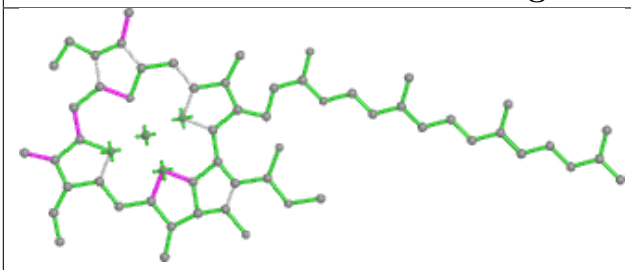


Rings

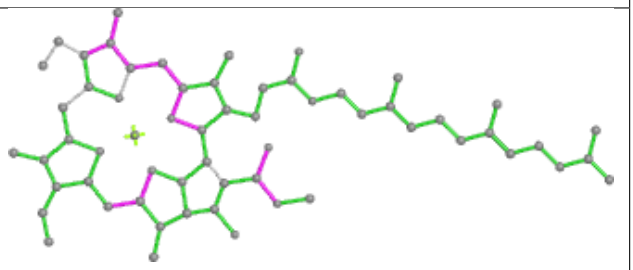
Ligand CHL b 310	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand XAT 1 318	
 Bond lengths	 Bond angles
 Torsions	 Rings

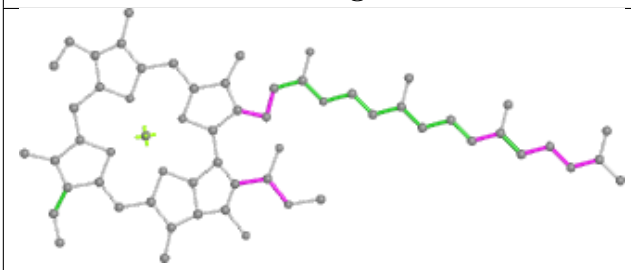
Ligand CLA a 602



Bond lengths



Bond angles



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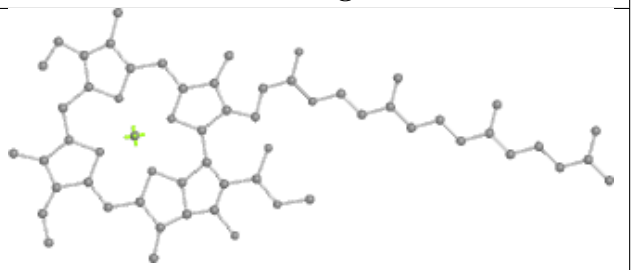
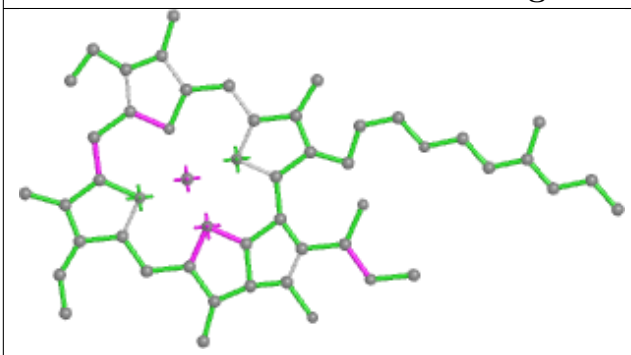


Rings

Ligand CLA 2 609



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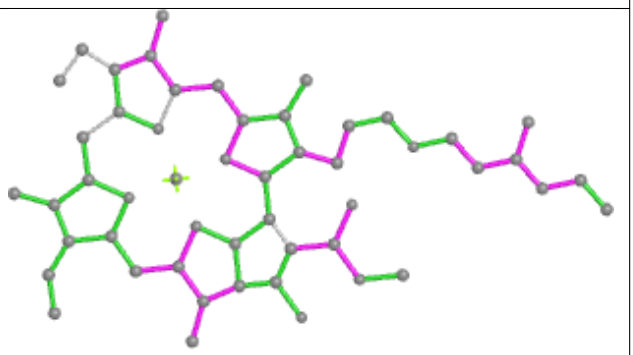
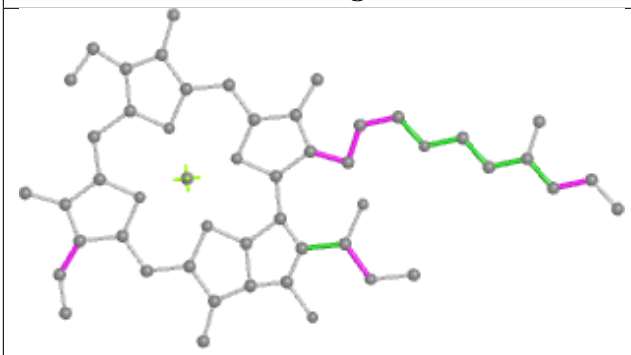


Bond angles



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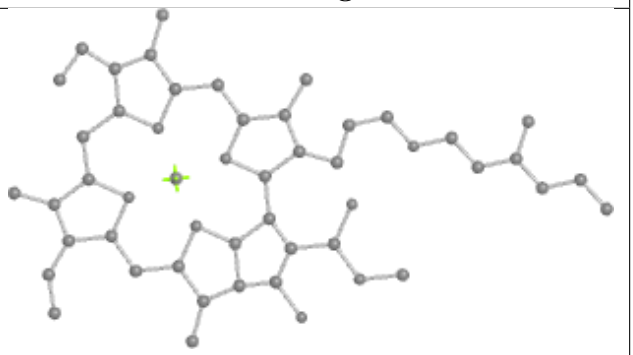
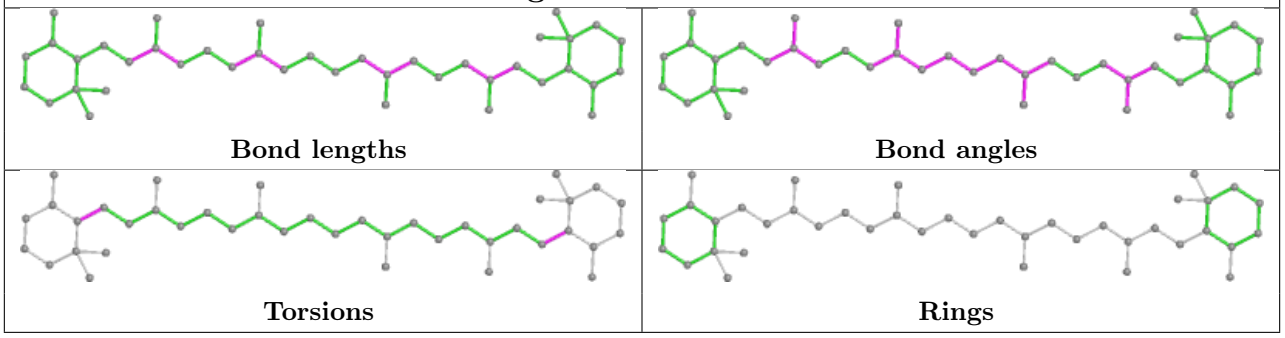


Rings

Ligand BCR 2 618



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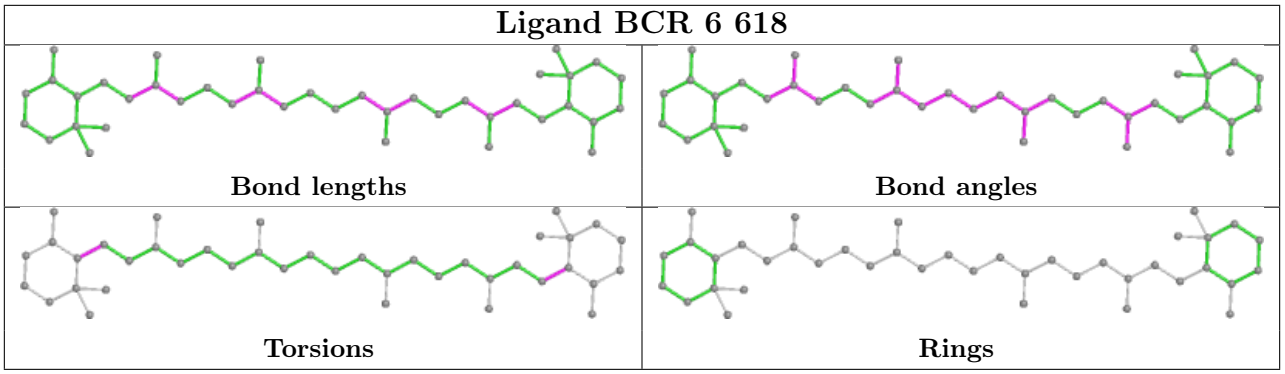
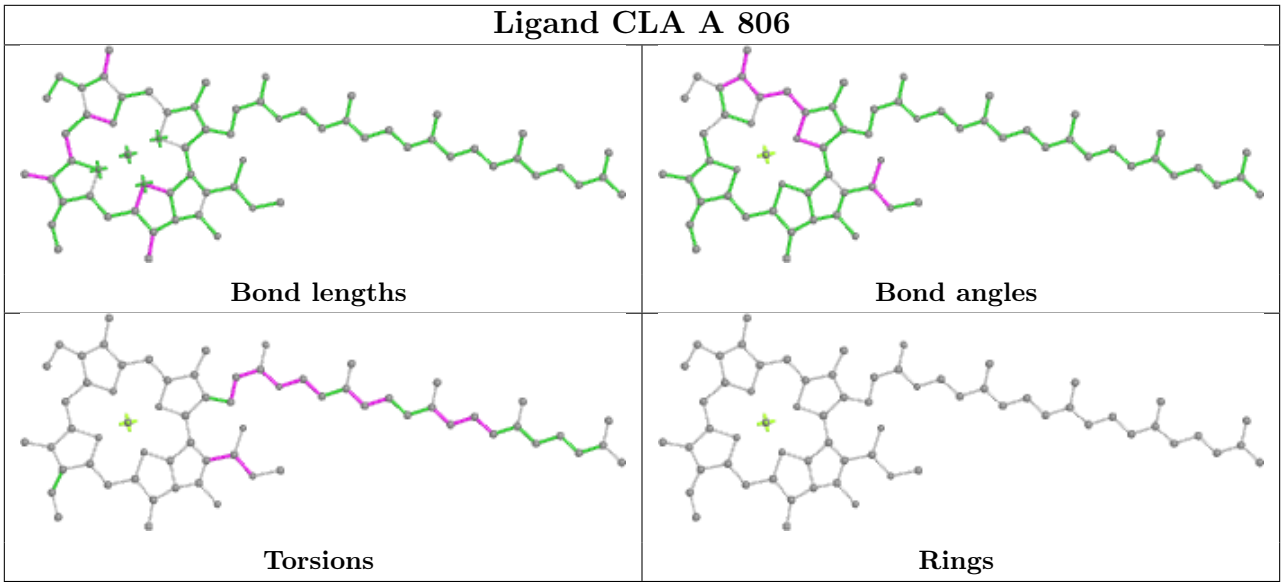
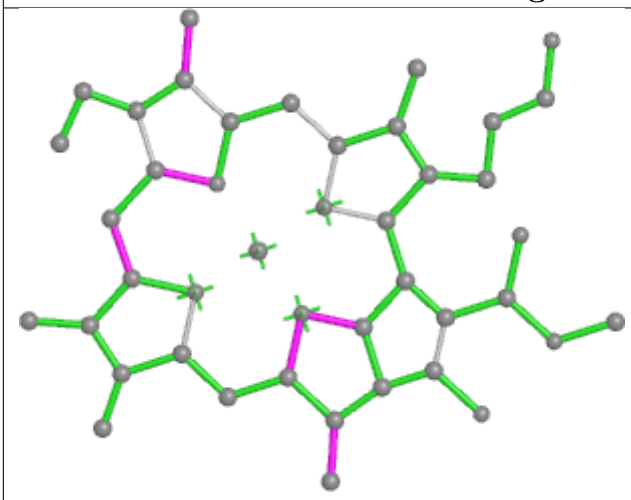


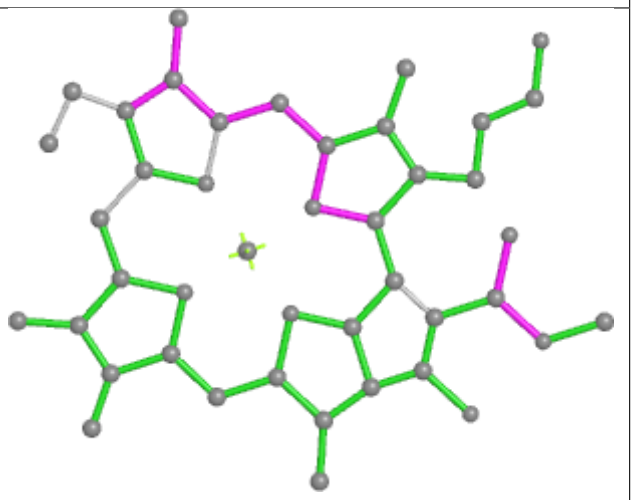
Ligand CLA A 806



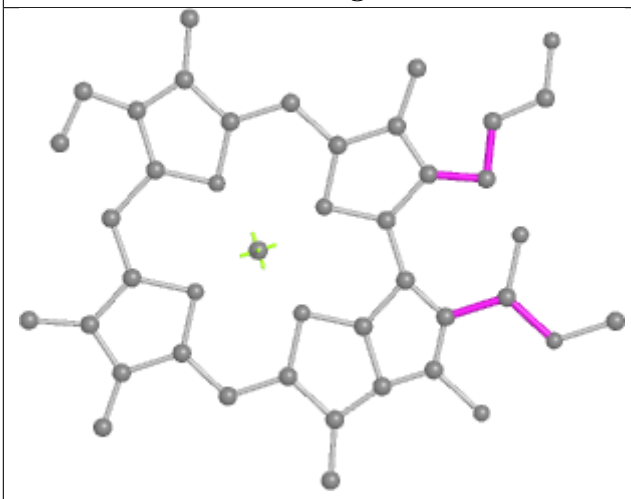
Ligand CLA 8 604



Bond lengths



Bond angles



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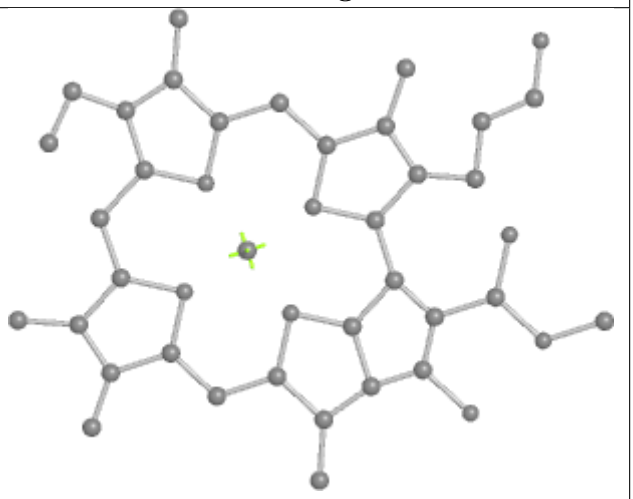
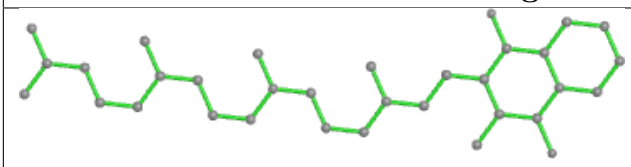
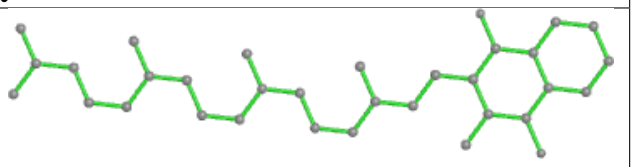


Rings

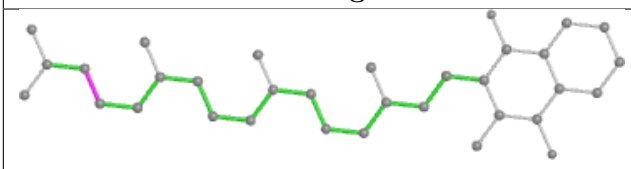
Ligand PQN A 843



Bond lengths



Bond angles



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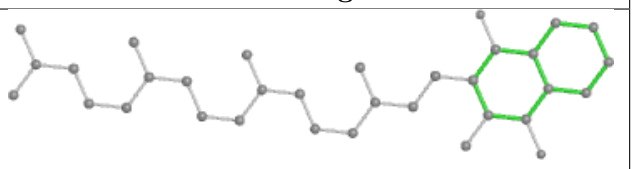
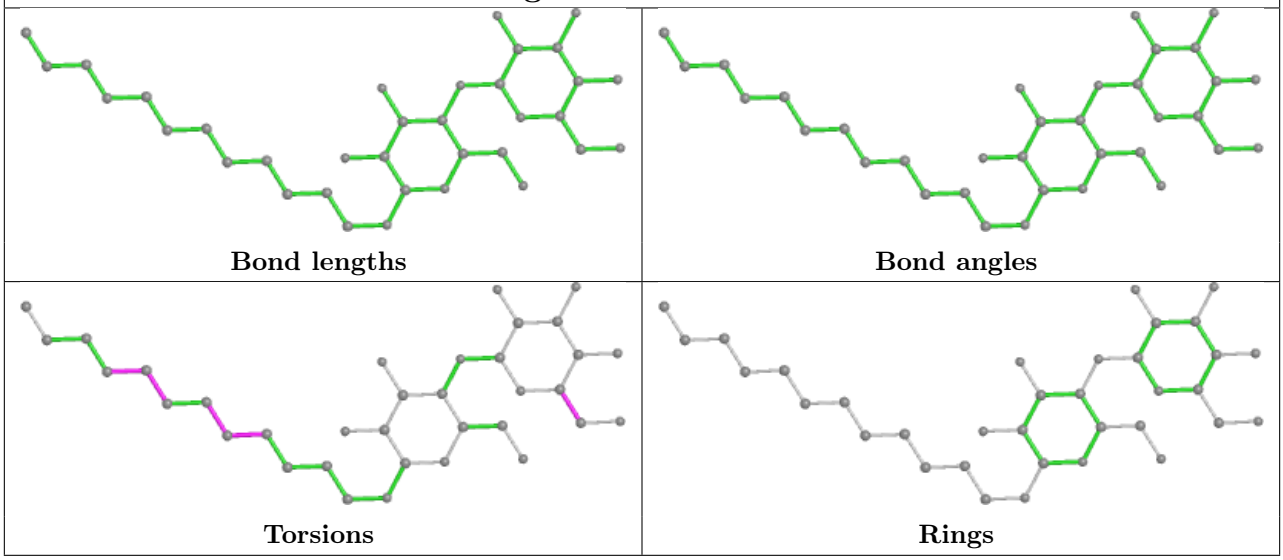
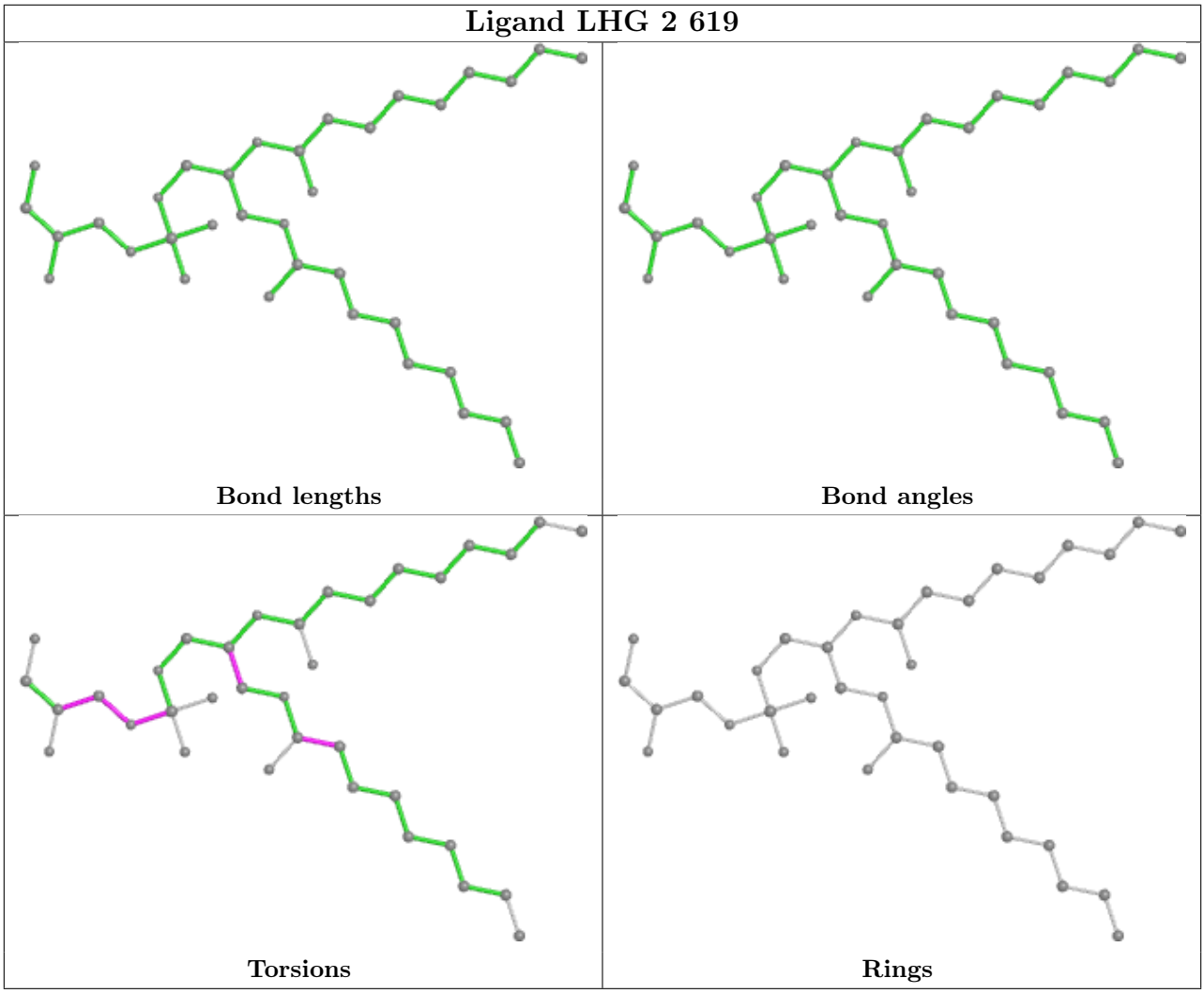


Rings

Ligand LMU b 301



Ligand LHG 2 619



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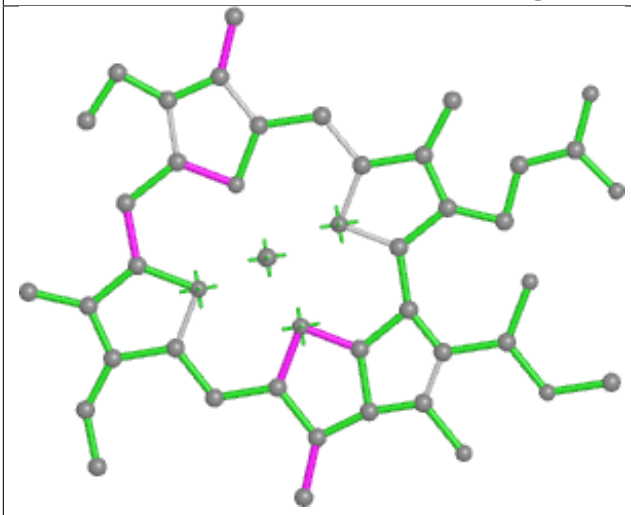
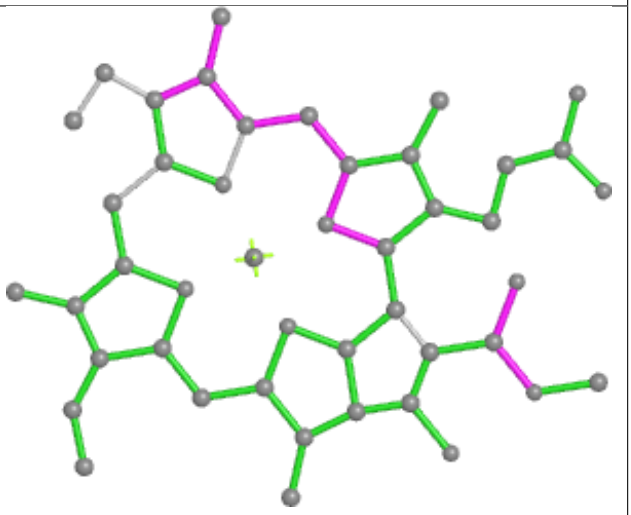
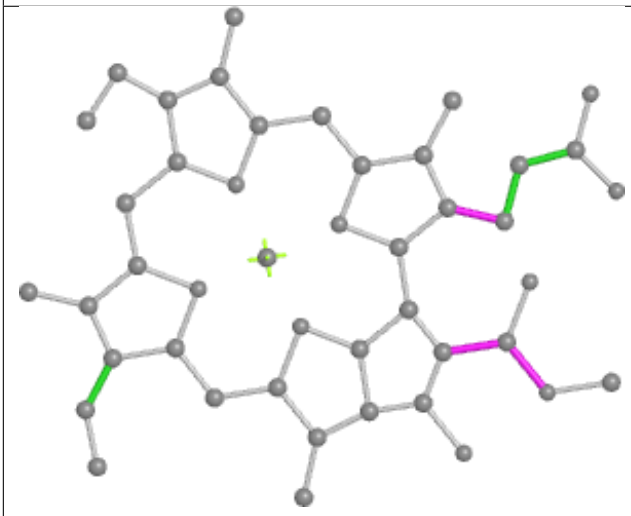


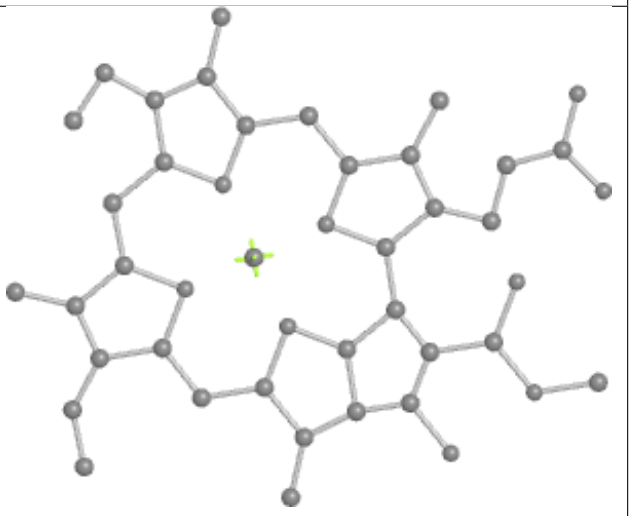
Bond lengths



Bond angles

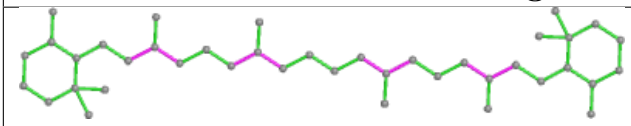


Torsions



Rings

Ligand BCR 7 418



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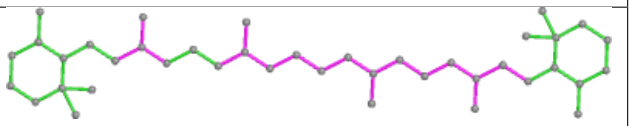

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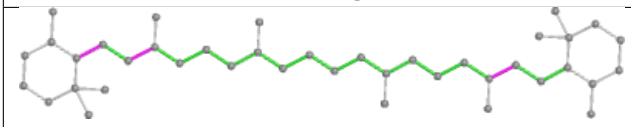
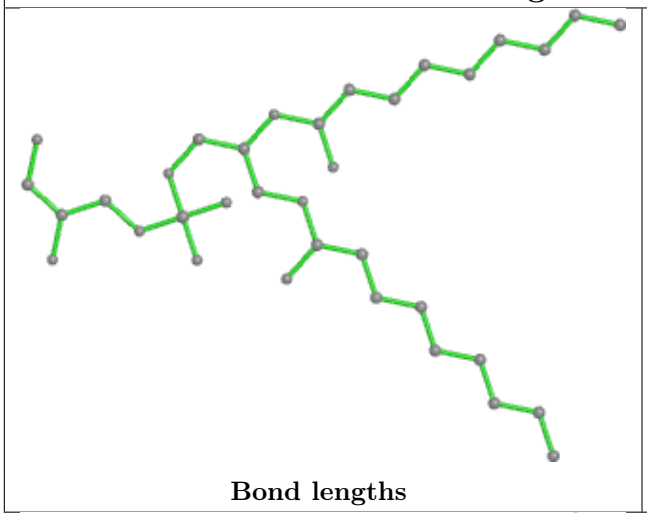


Torsions

Rings

Ligand LHG 6 619



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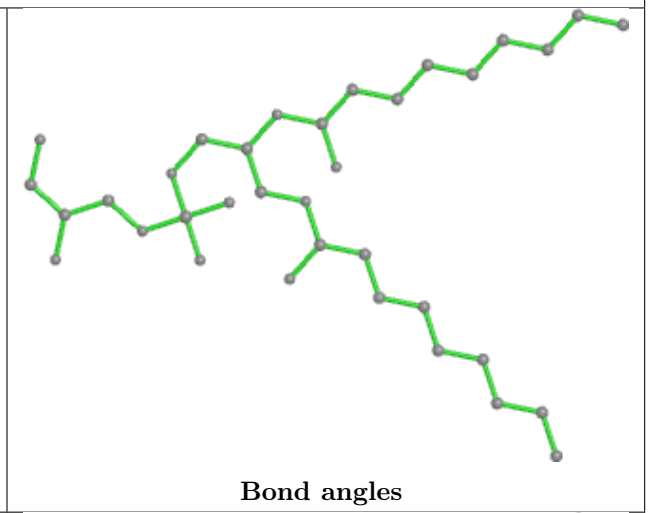
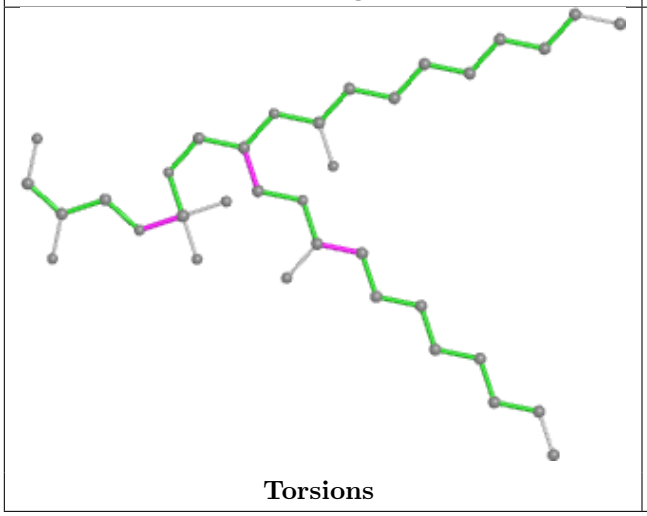


Bond angles



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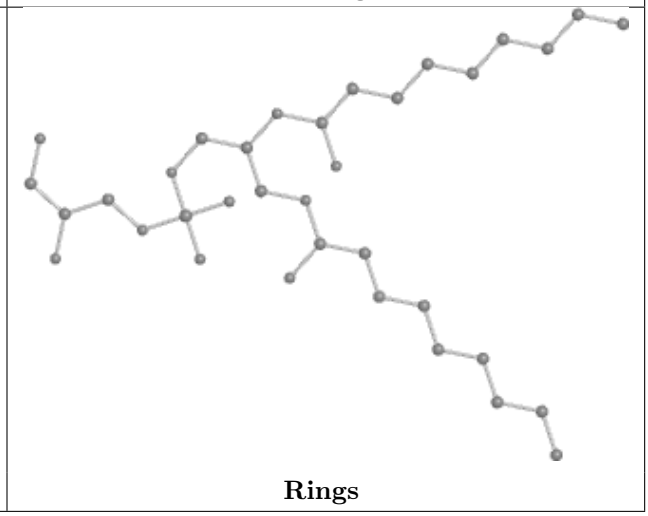
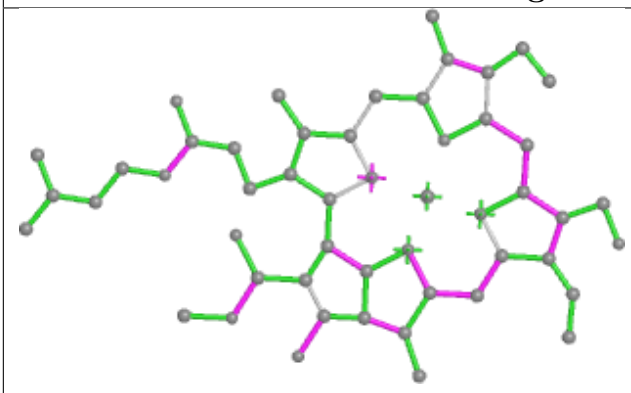


Rings

Ligand CHL 1 307



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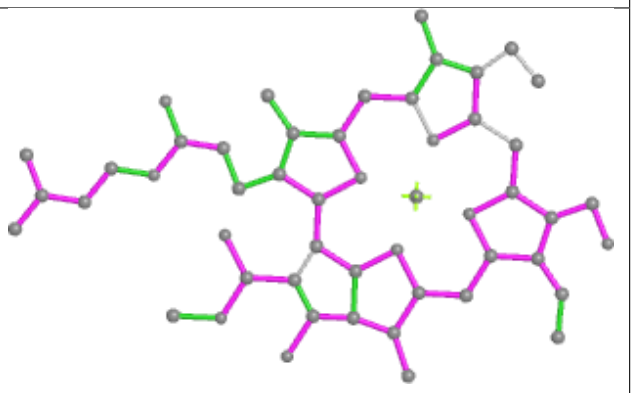
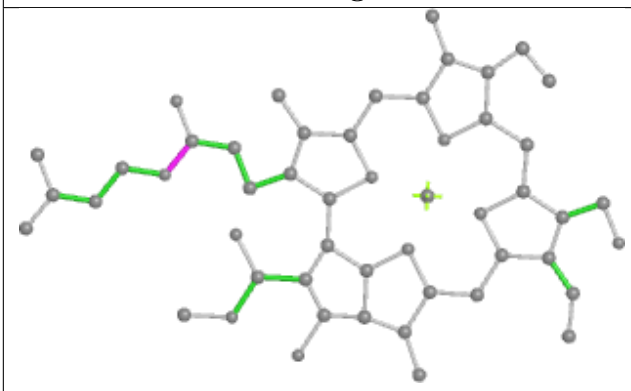


Bond angles



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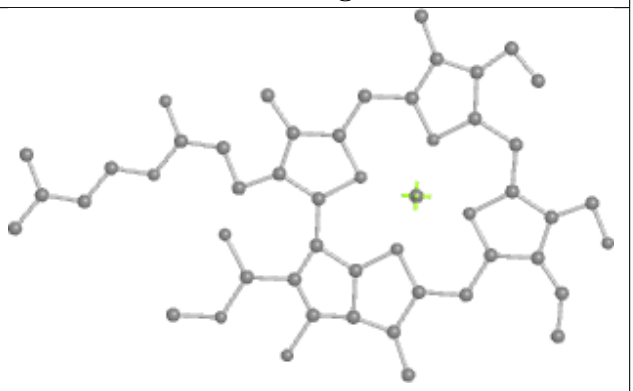
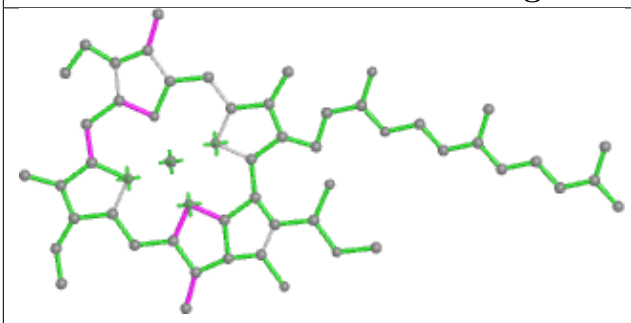


Rings

Ligand CLA A 805



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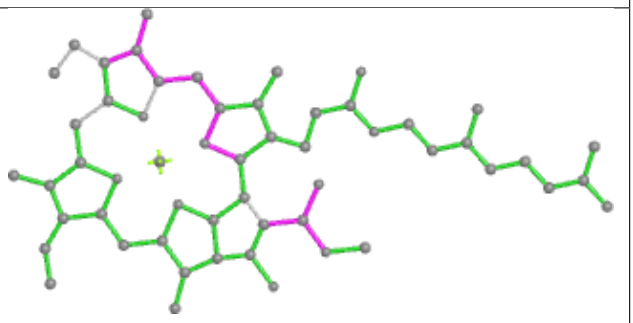
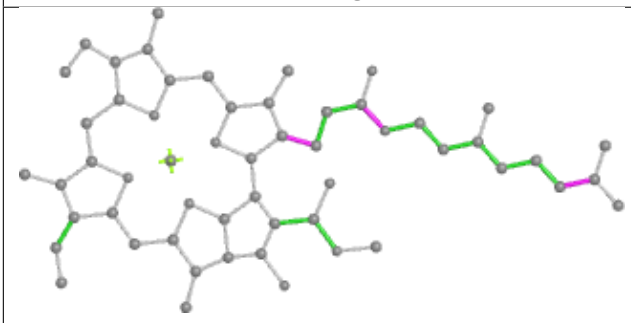


Bond angles



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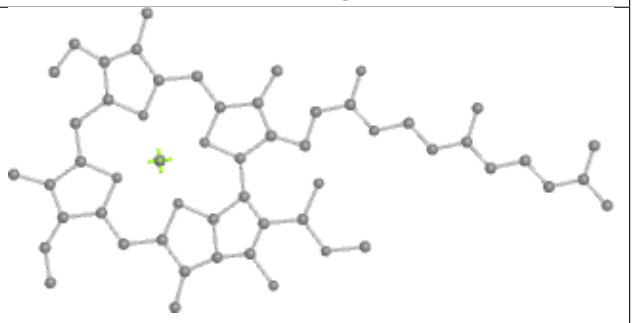
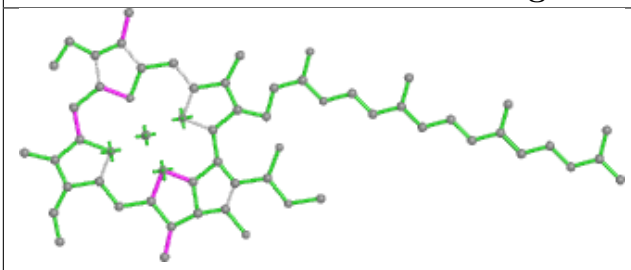


Rings

Ligand CLA 3 402



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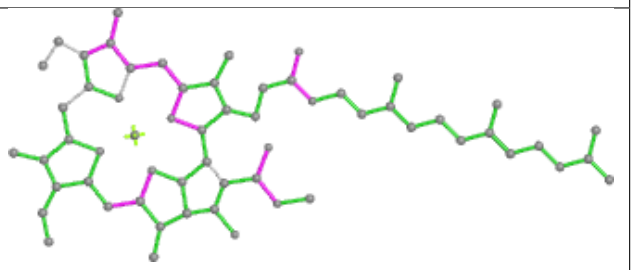

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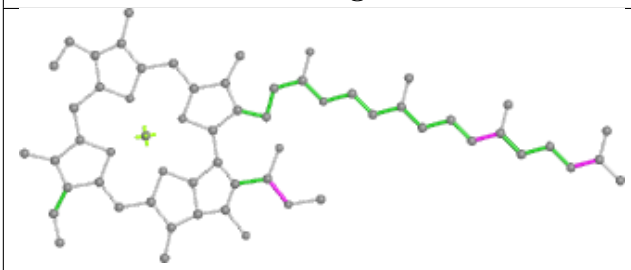

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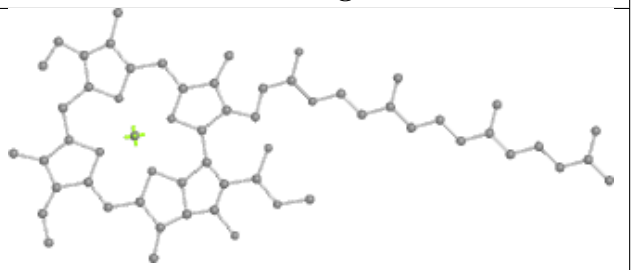
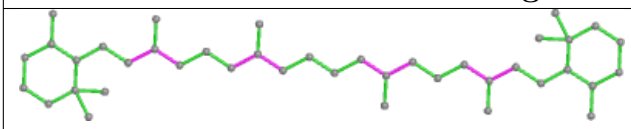


Rings

Ligand BCR A 848



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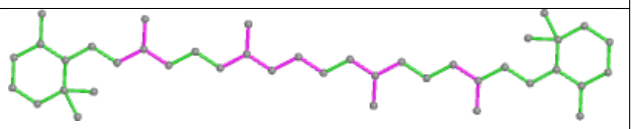
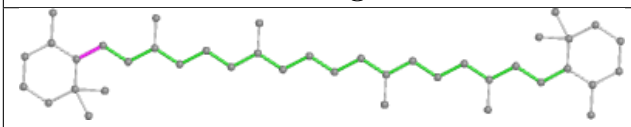


Bond angles



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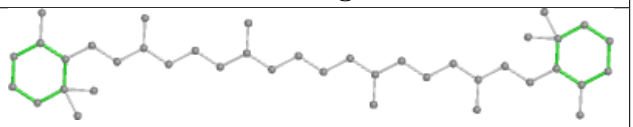
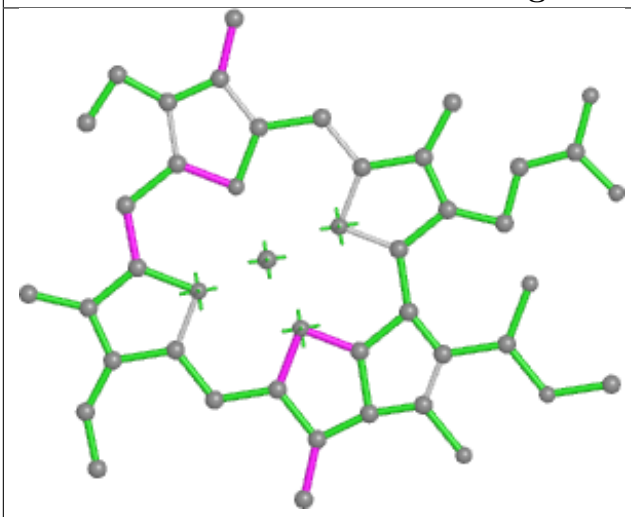


Rings

Ligand CLA 2 612



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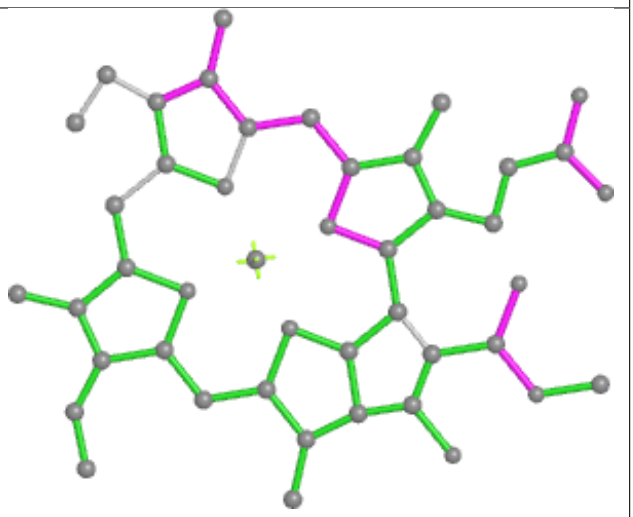

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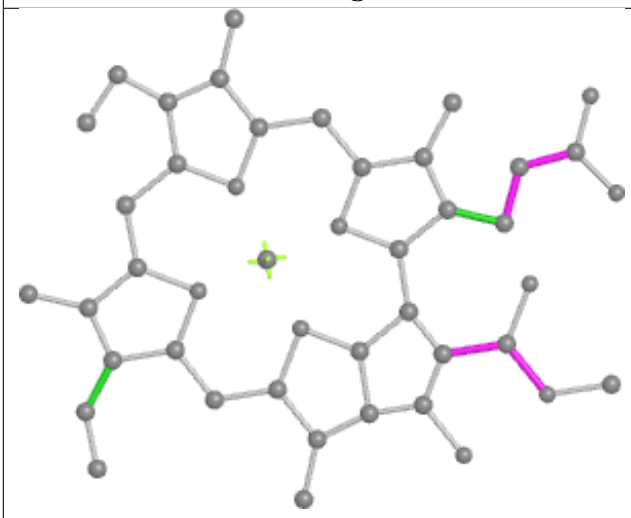

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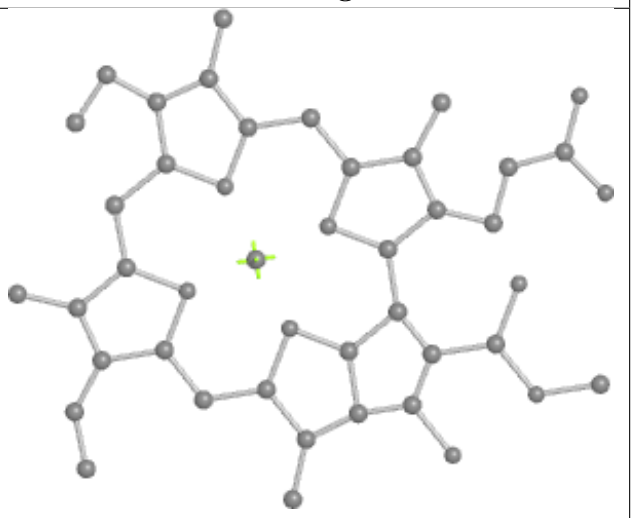
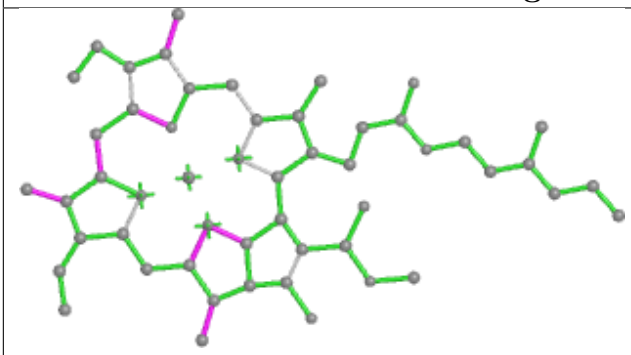
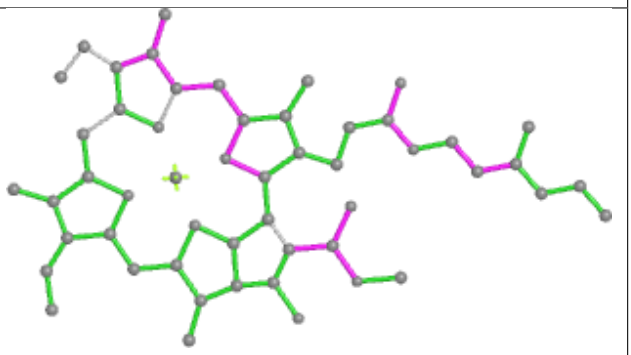
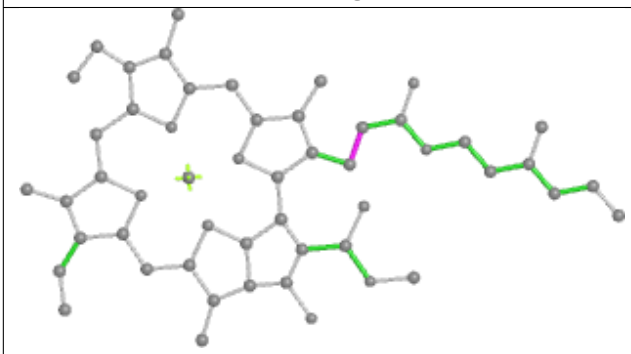
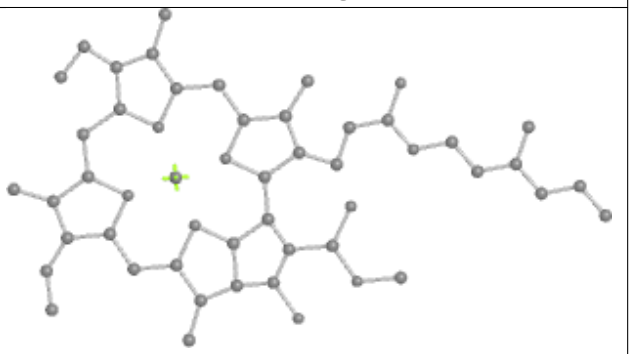
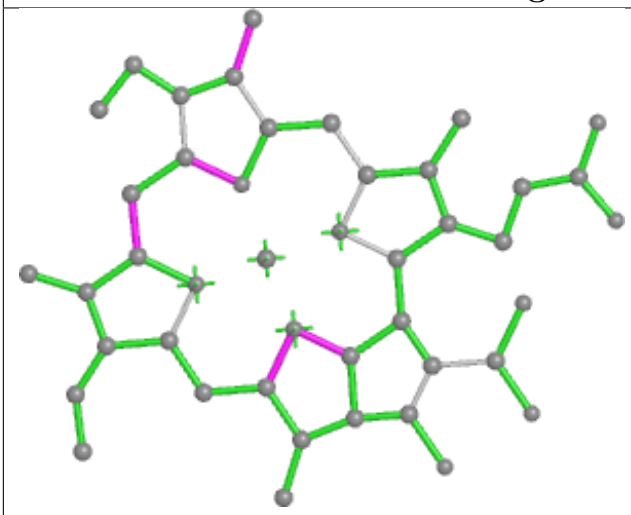


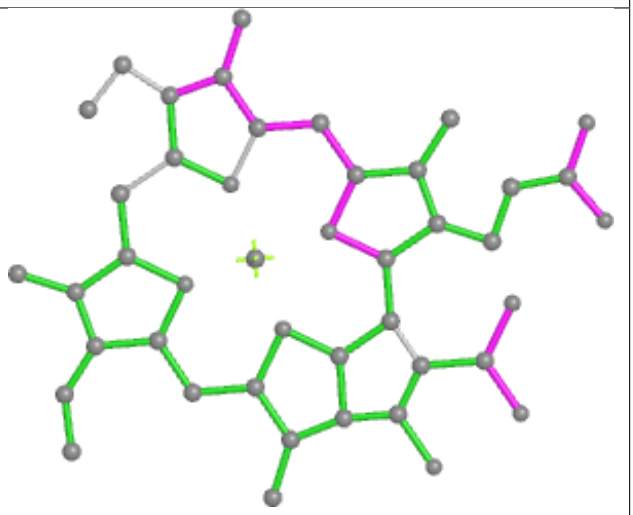
Rings

Ligand CLA A 802	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

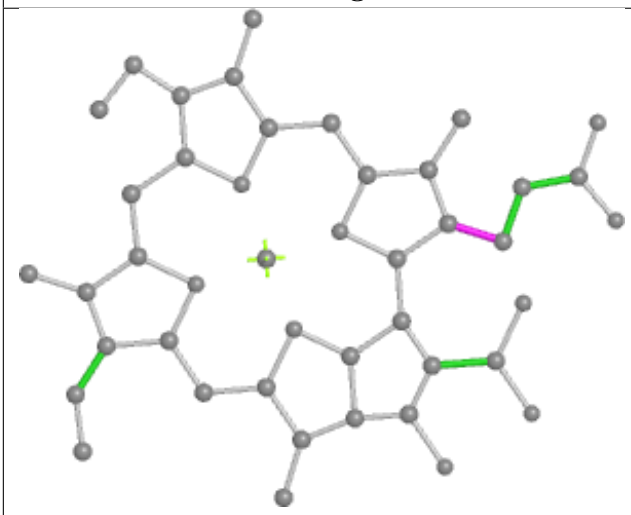
Ligand CLA 5 607



Bond lengths



Bond angles



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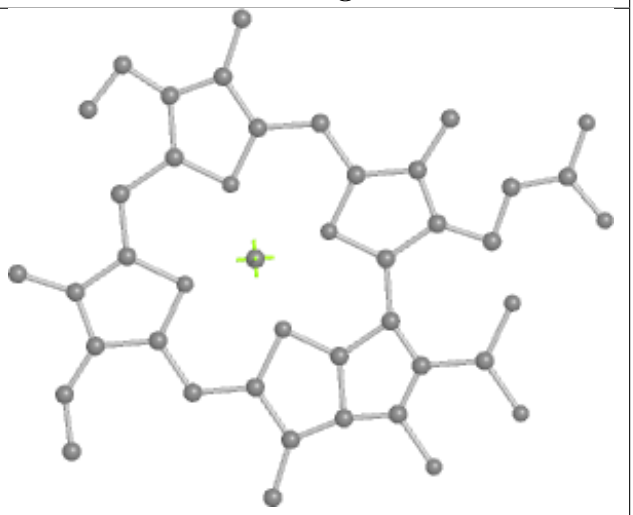
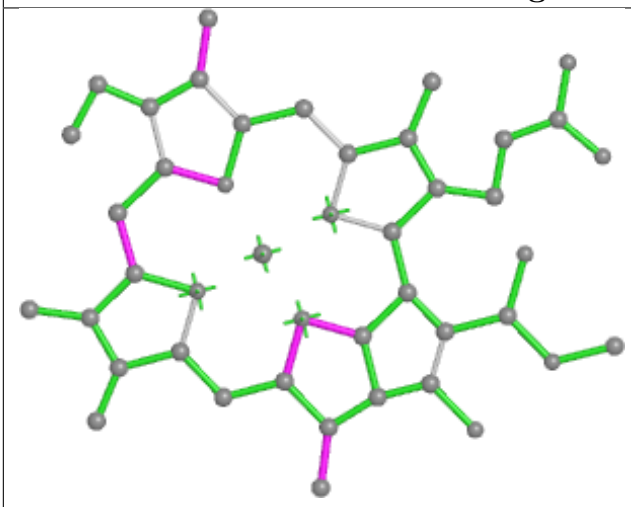


Rings

Ligand CLA 4 611



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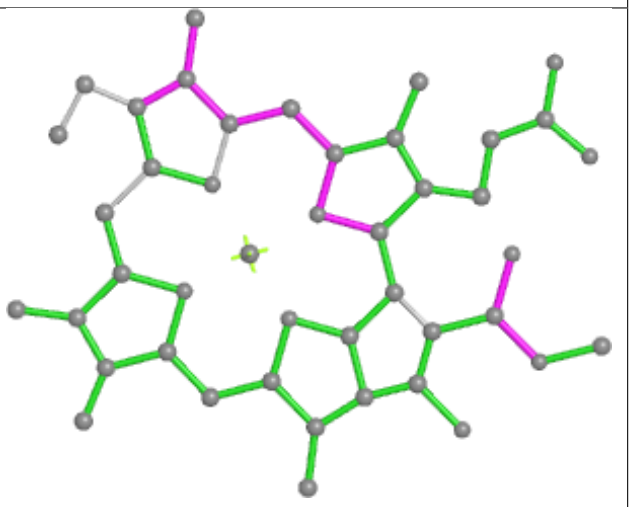
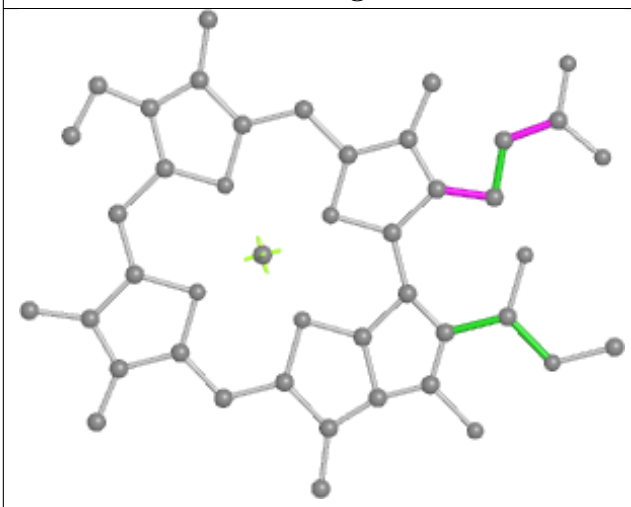


Bond angles



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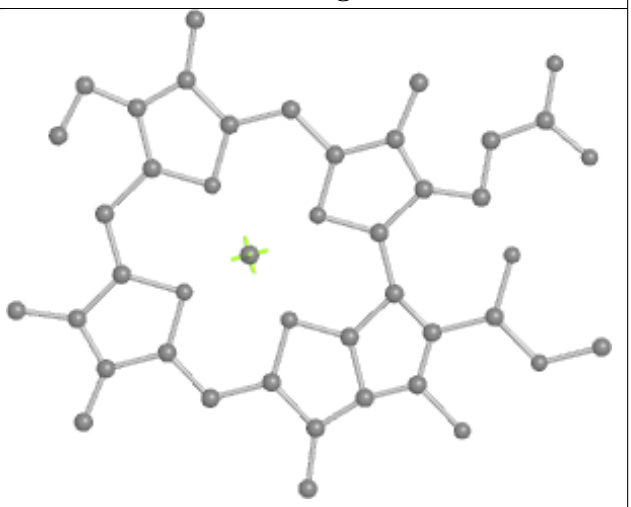
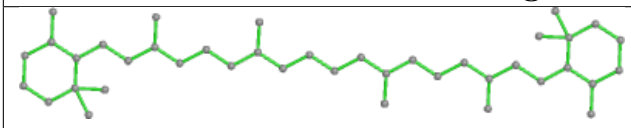


Rings

Ligand BCR B 846



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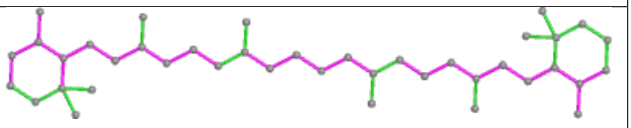
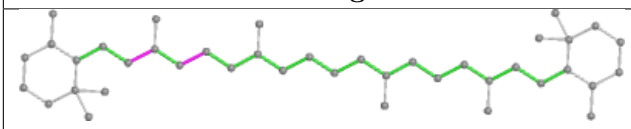


Bond angles



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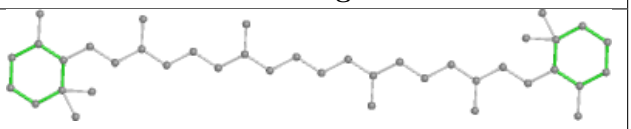
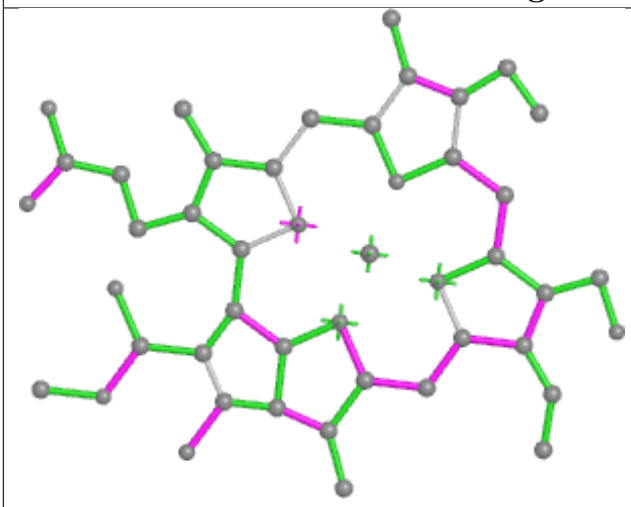


Rings

Ligand CHL 4 606



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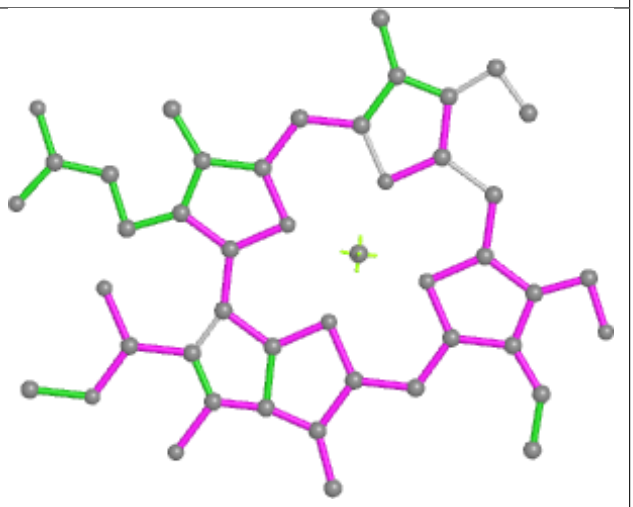
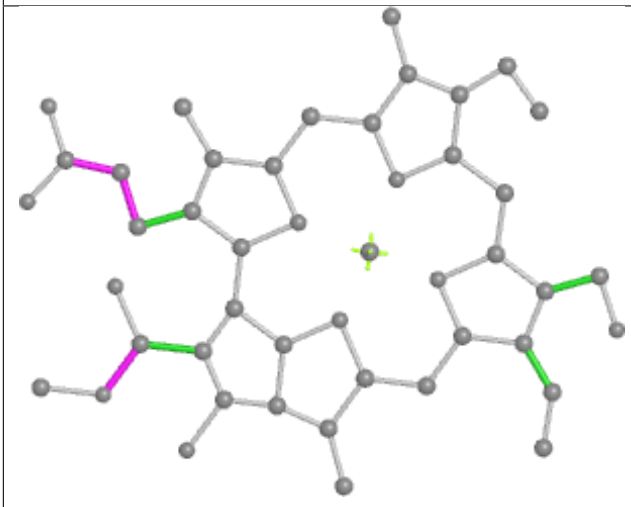


Bond angles



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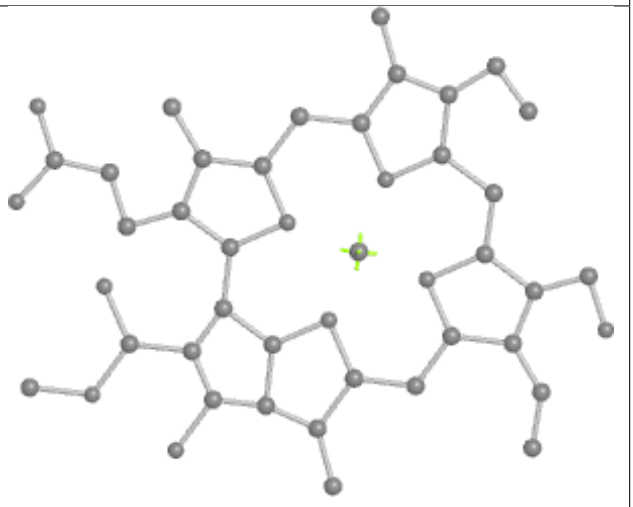
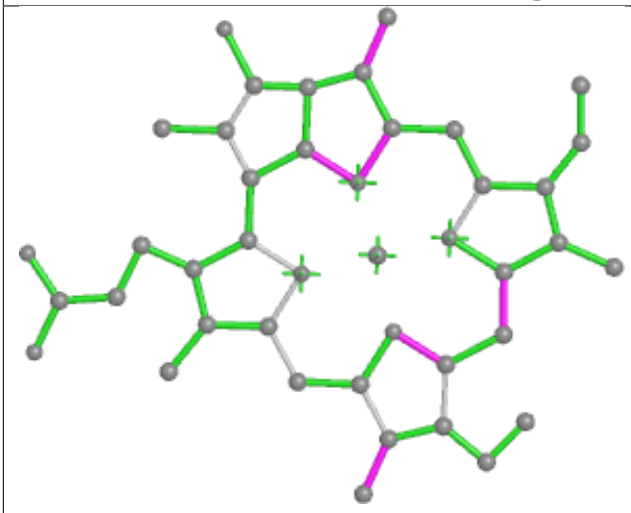
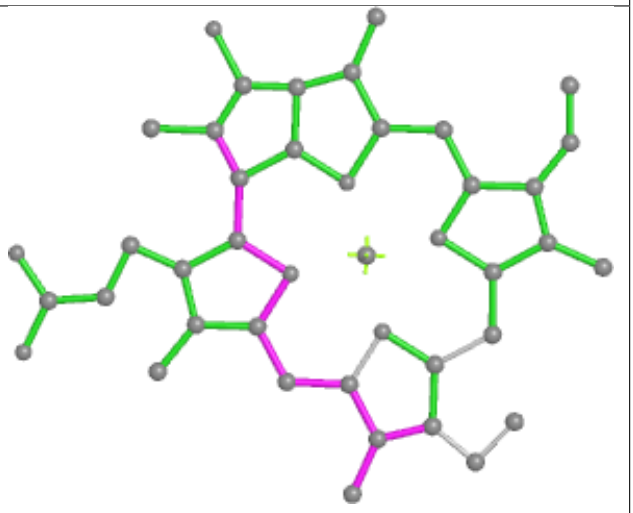


Rings

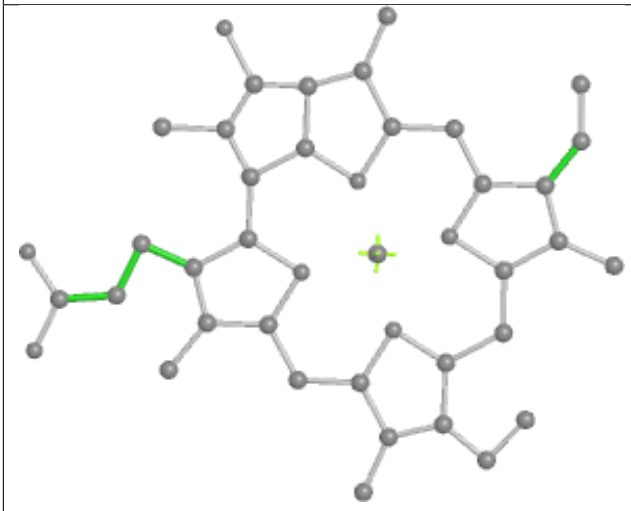
Ligand CLA 6 610



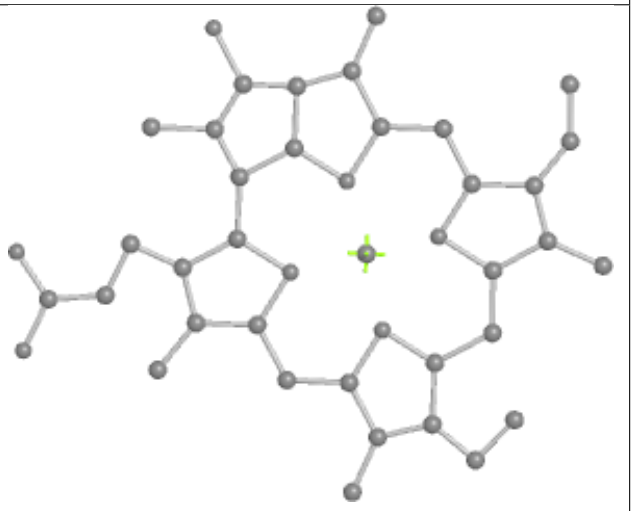
Bond lengths



Bond angles

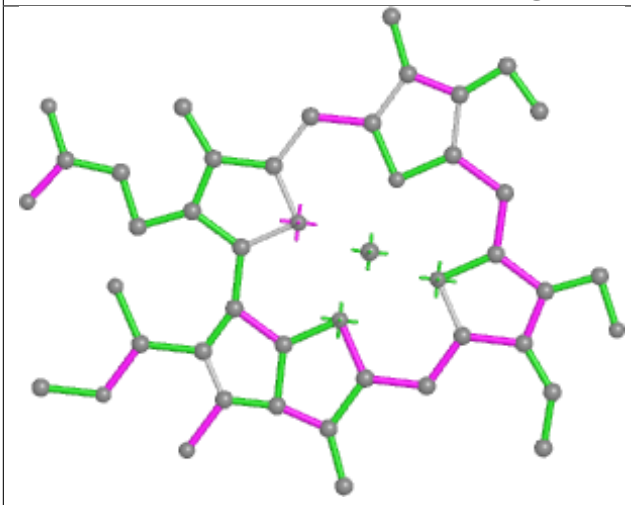


Torsions



Rings

Ligand CHL a 608



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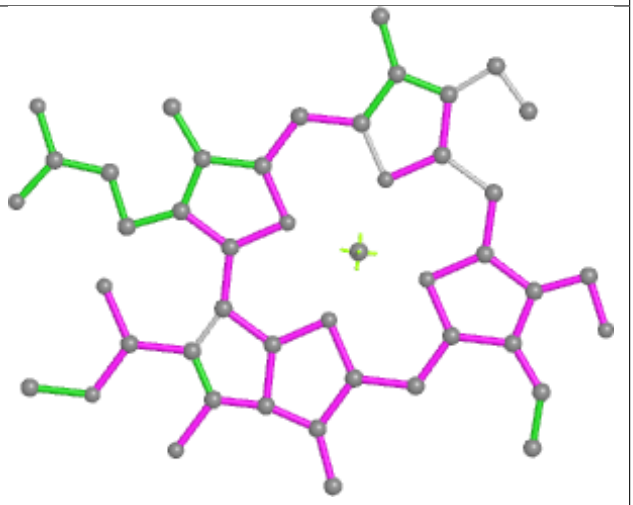
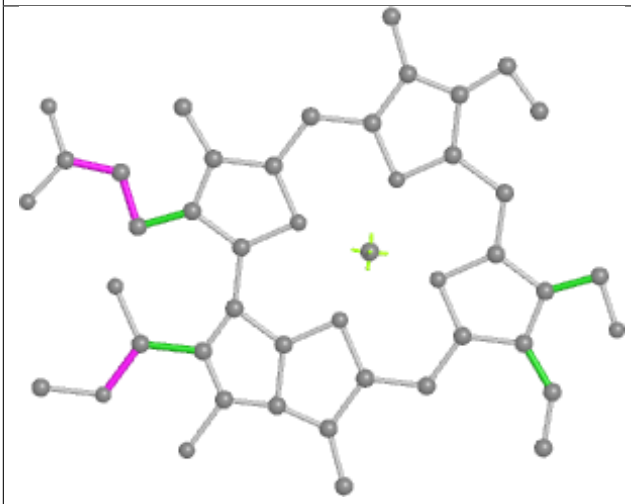


Bond angles



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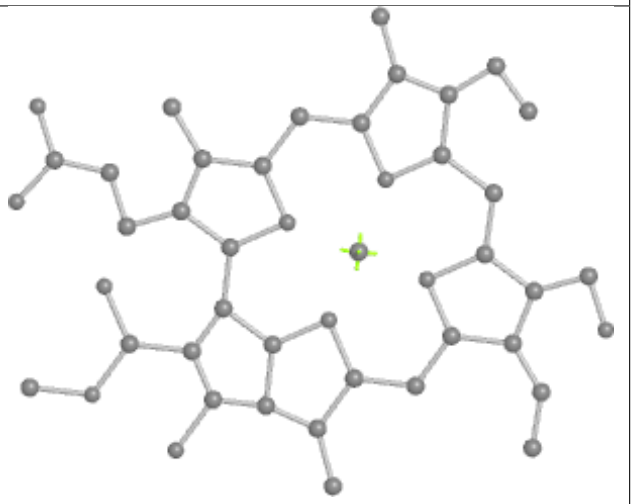
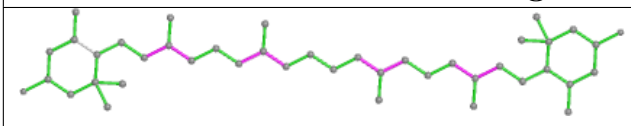


Rings

Ligand LUT b 316



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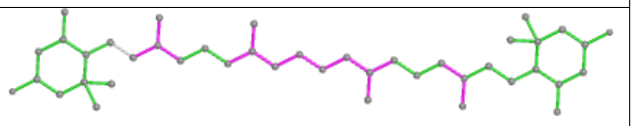
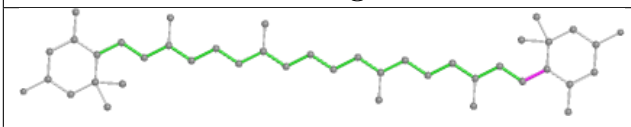


Bond angles



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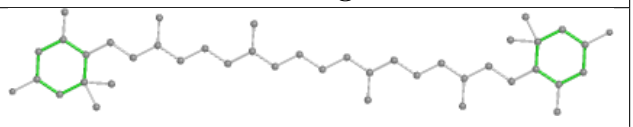
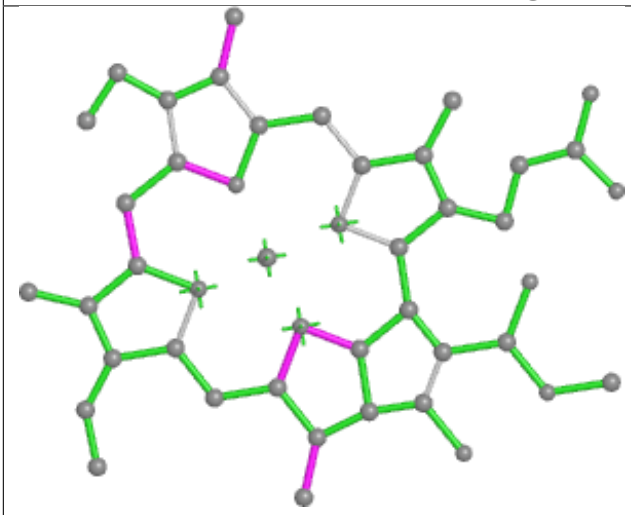


Rings

Ligand CLA B 829



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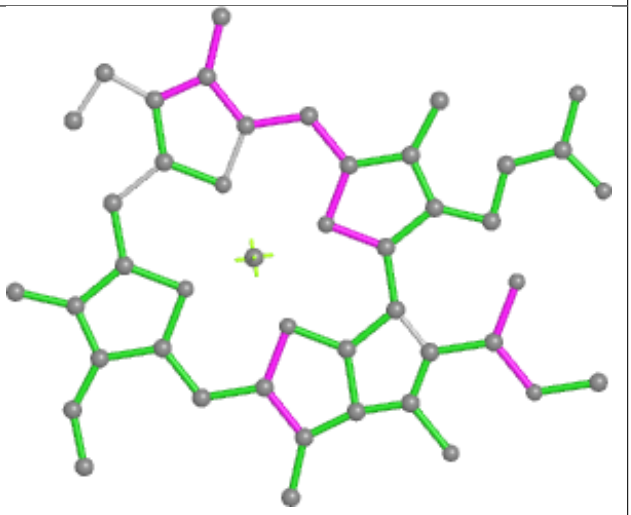

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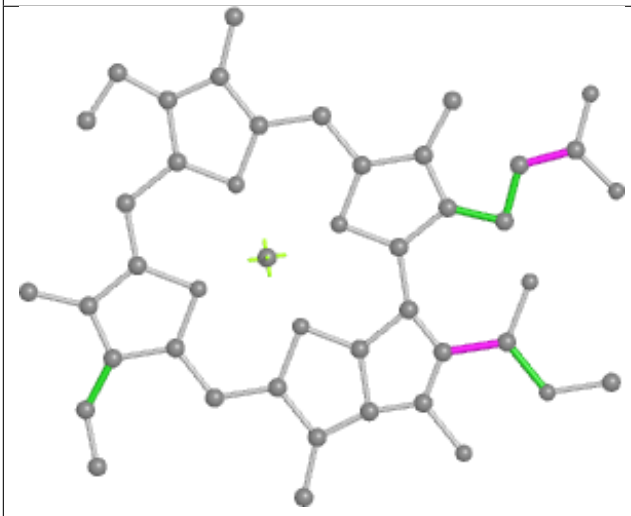

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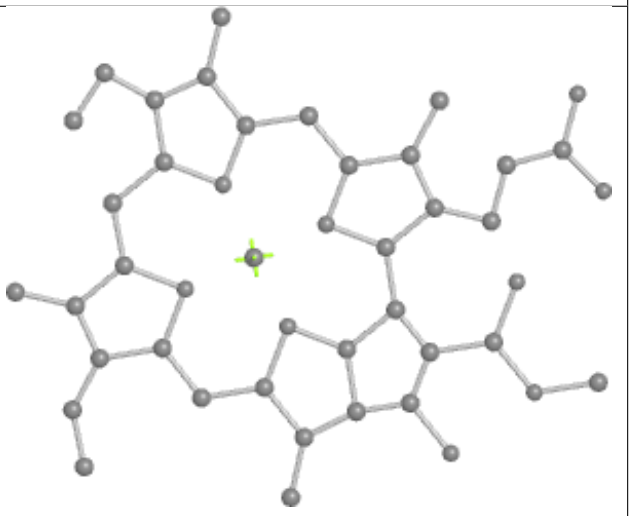
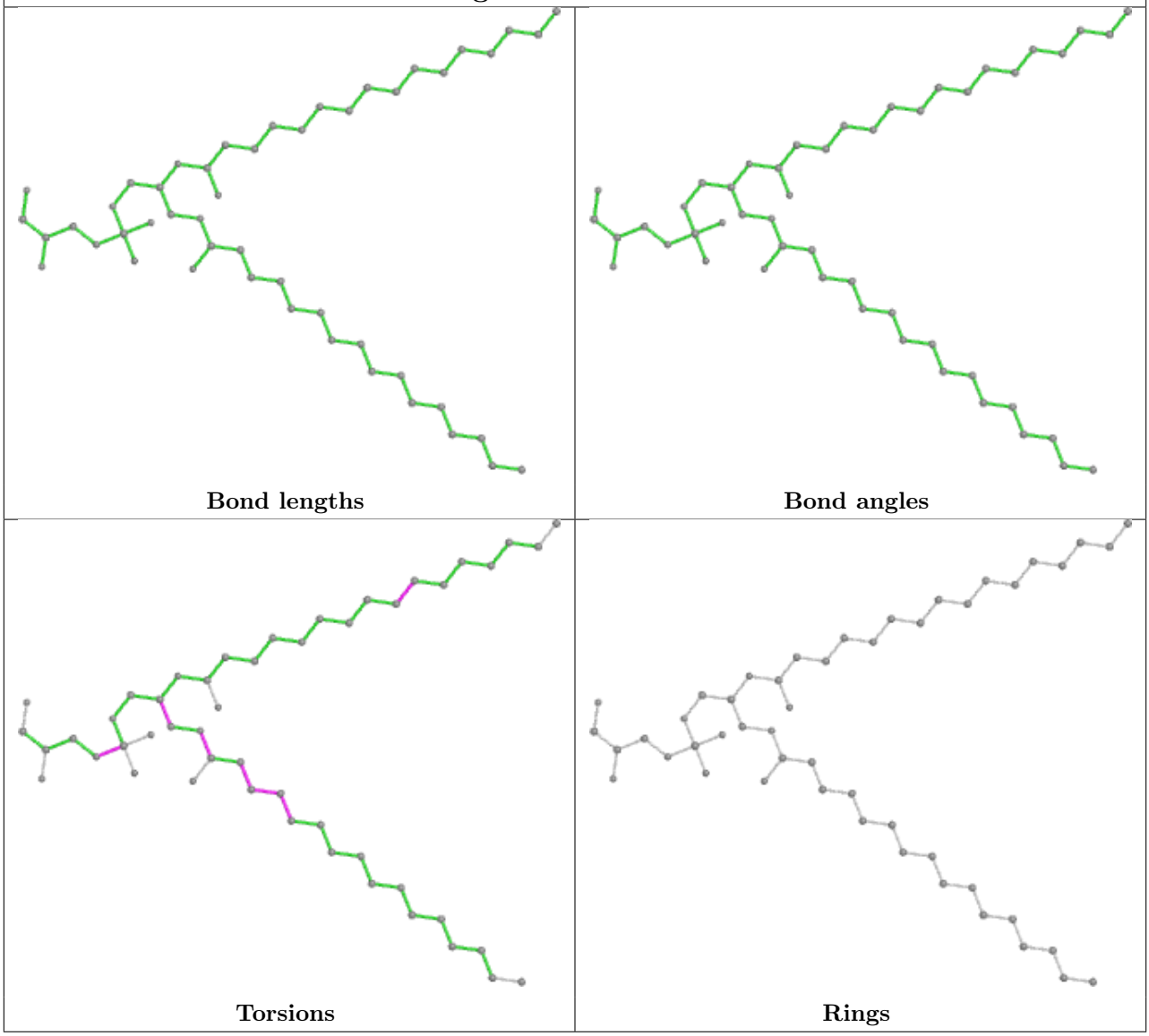
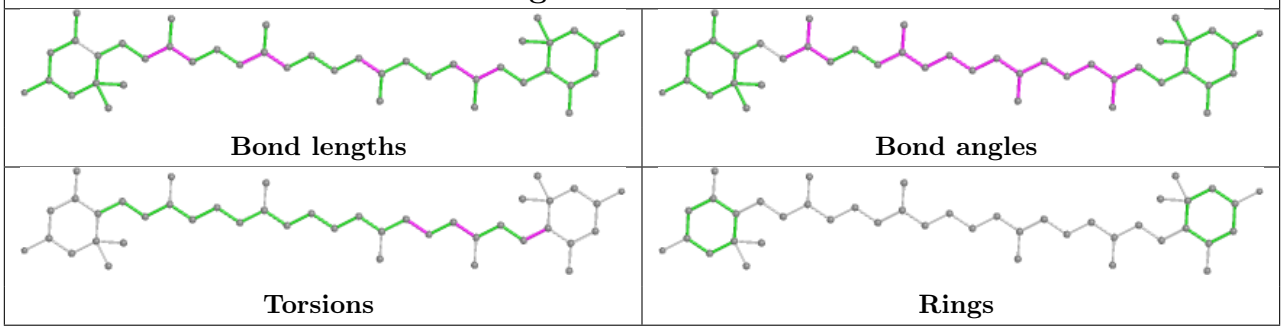


Rings

Ligand LHG a 617



Ligand LUT 3 416



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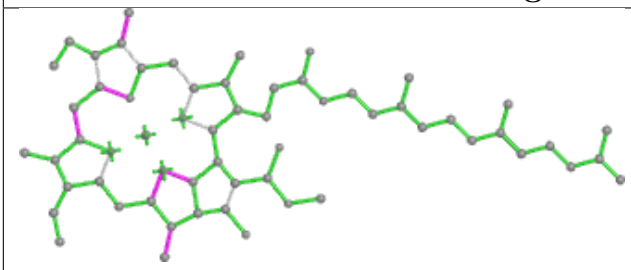

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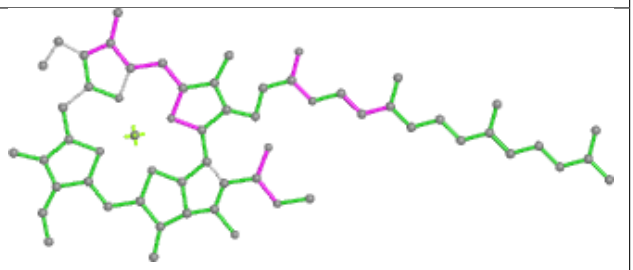
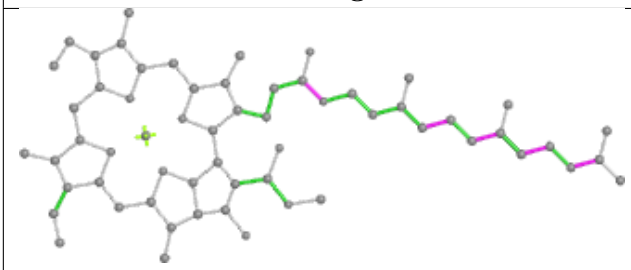


Bond angles



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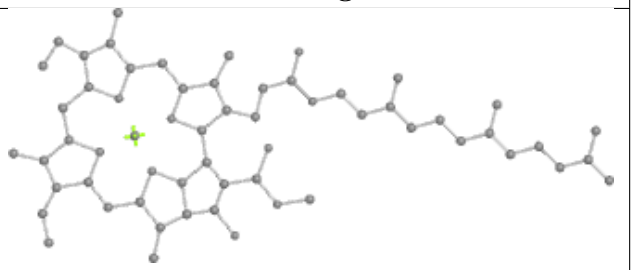
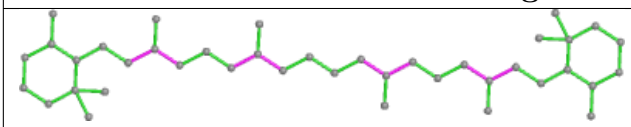


Rings

Ligand BCR G 205



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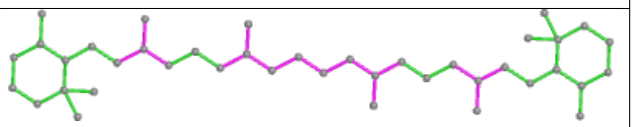
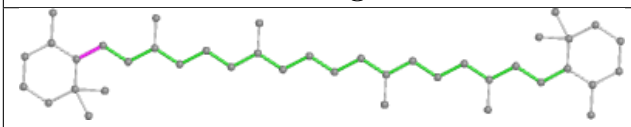


Bond angles



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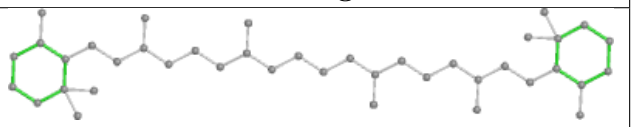
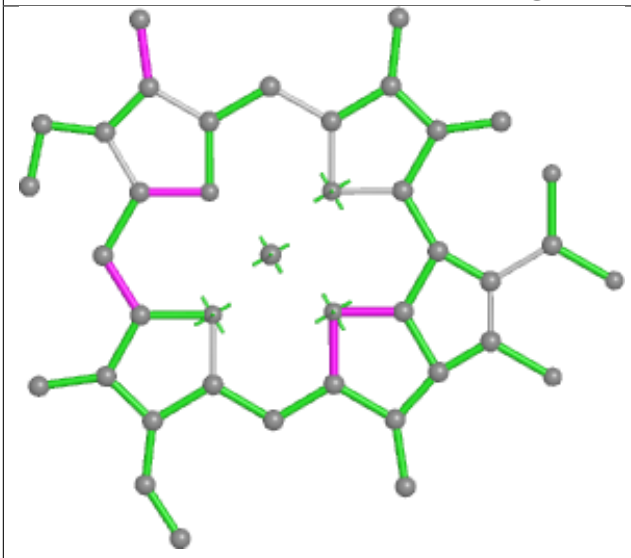


Rings

Ligand CLA 7 412



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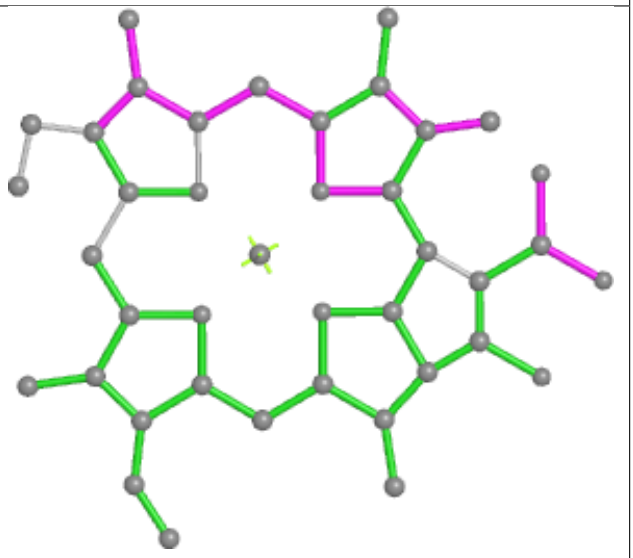
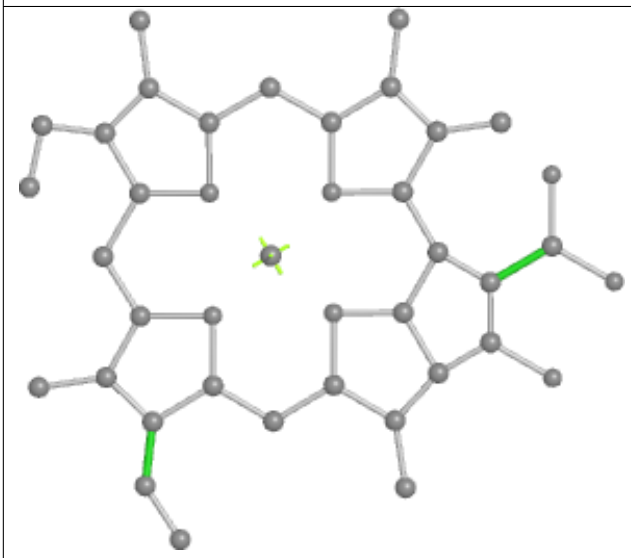


Bond angles



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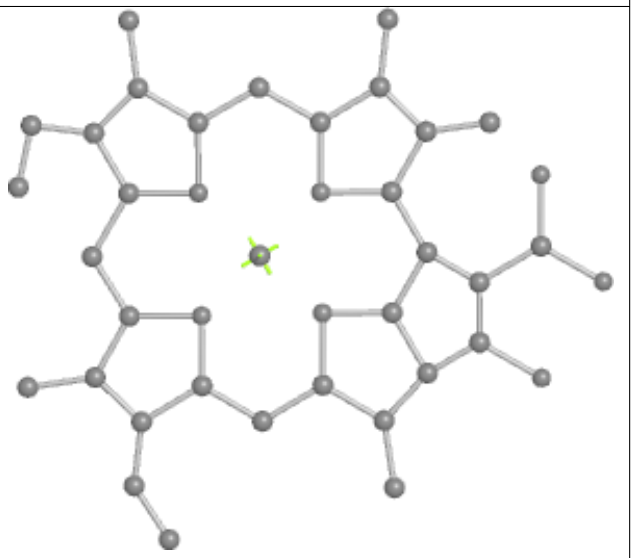
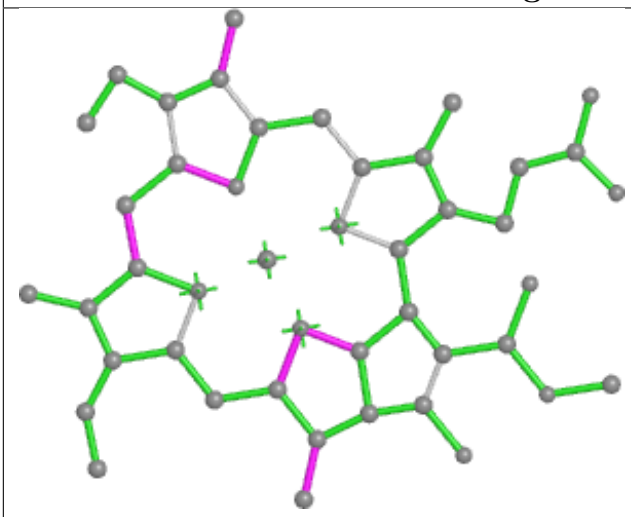


Rings

Ligand CLA H 201



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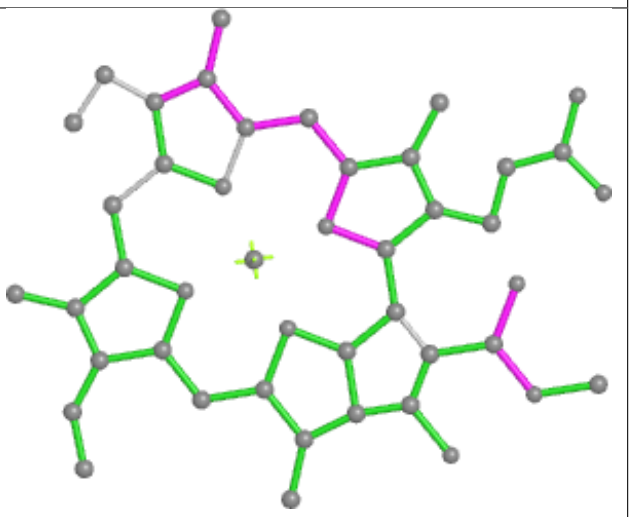

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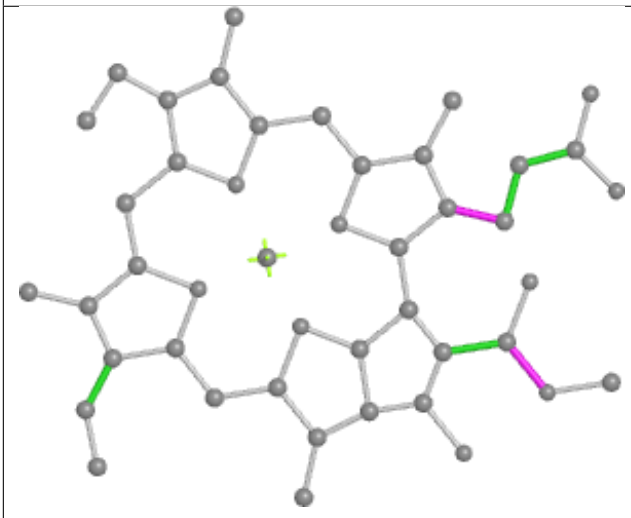

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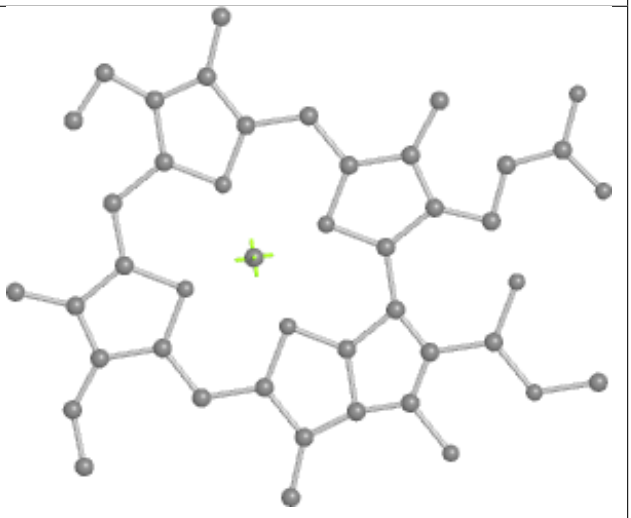
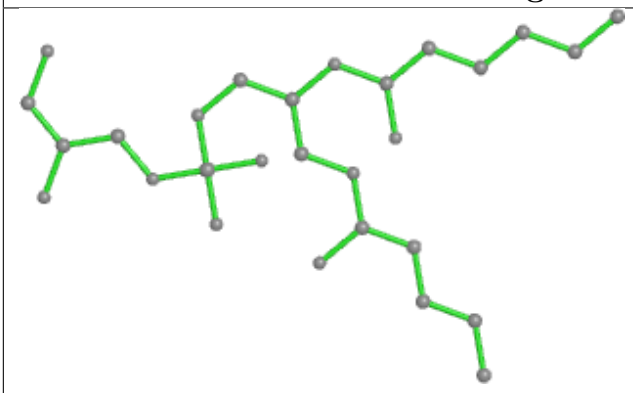


Rings

Ligand LHG 5 617



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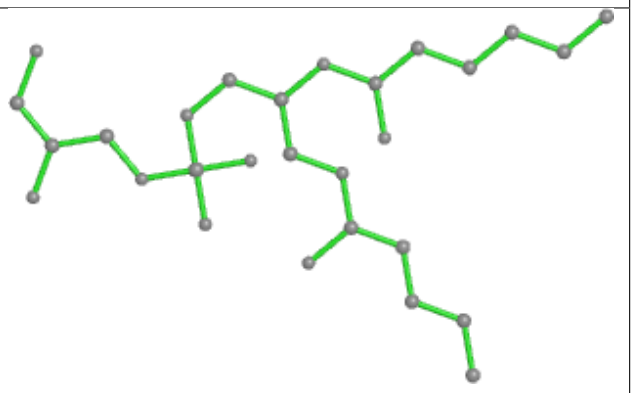
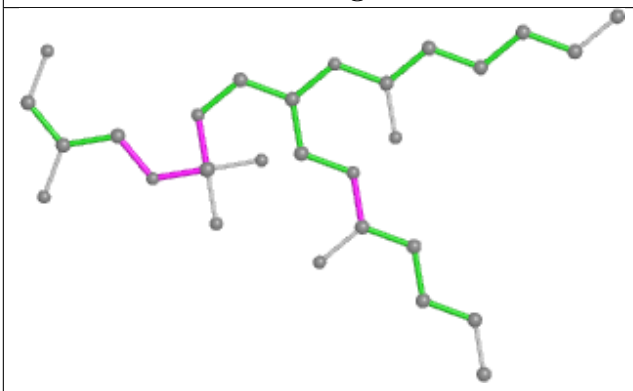


Bond angles



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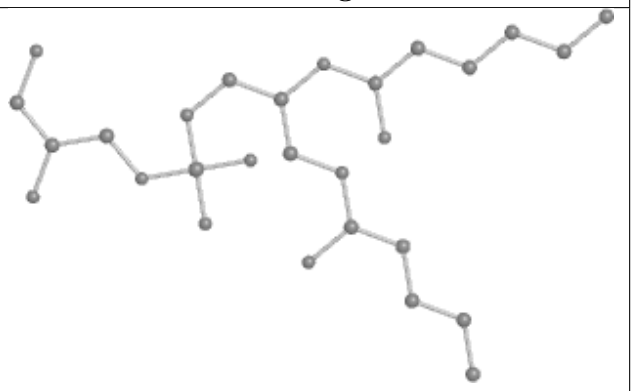
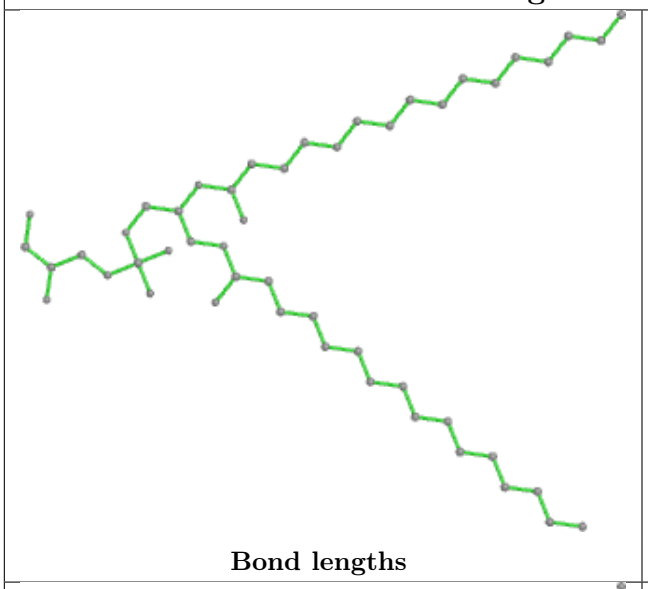


Rings

Ligand LHG 4 619



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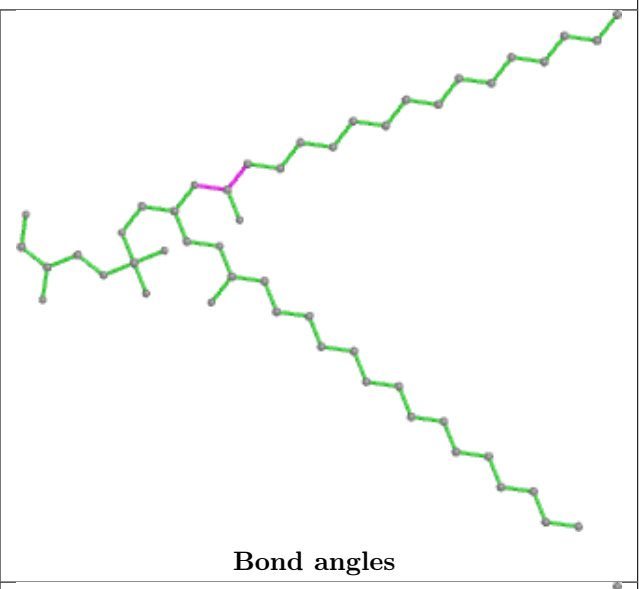
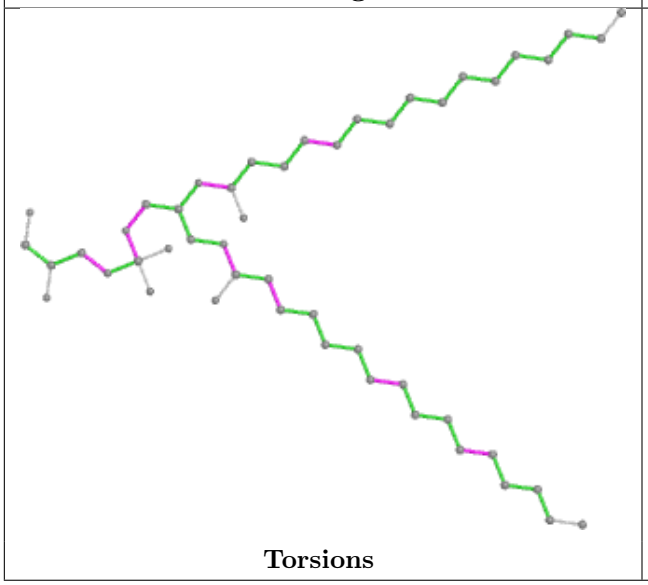


Bond angles



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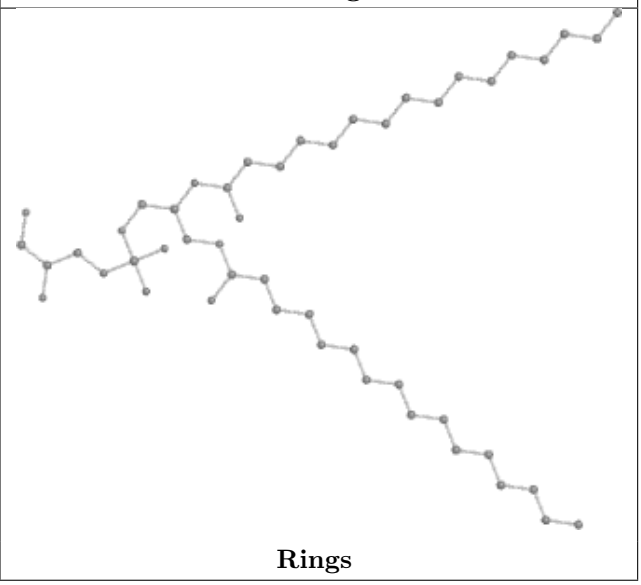
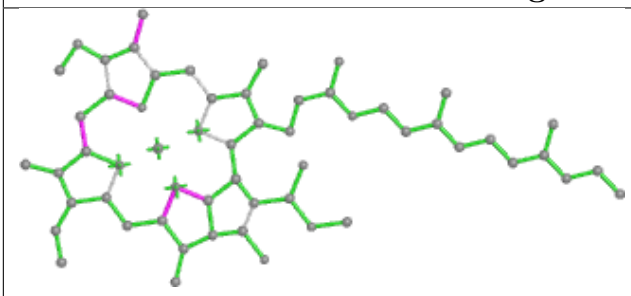


Rings

Ligand CLA a 613



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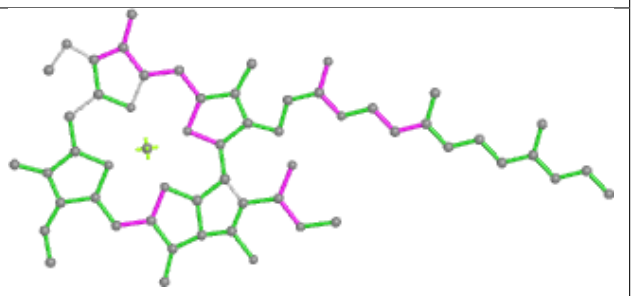
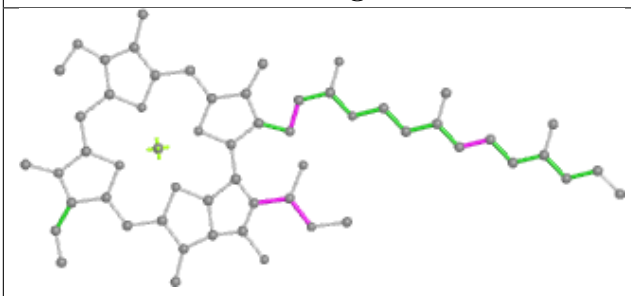


Bond angles



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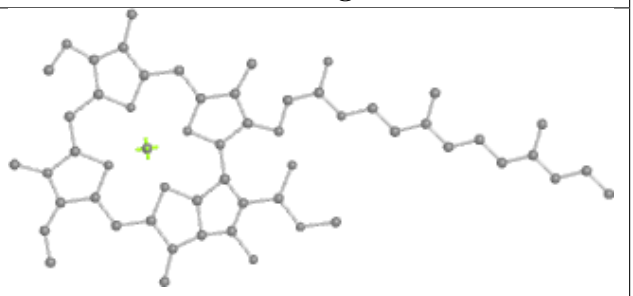
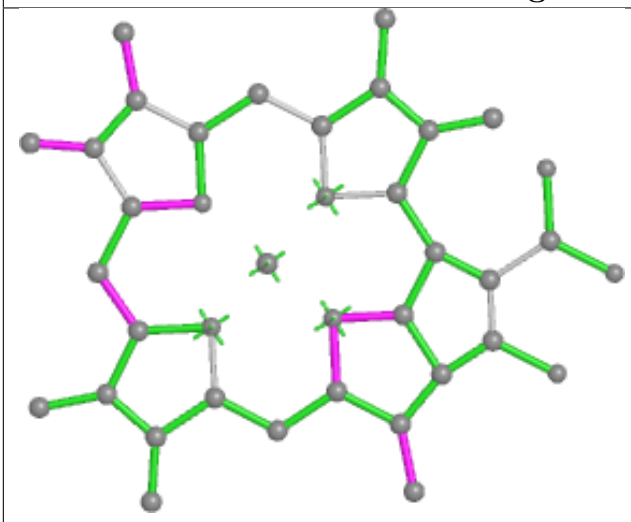


Rings

Ligand CLA 5 610



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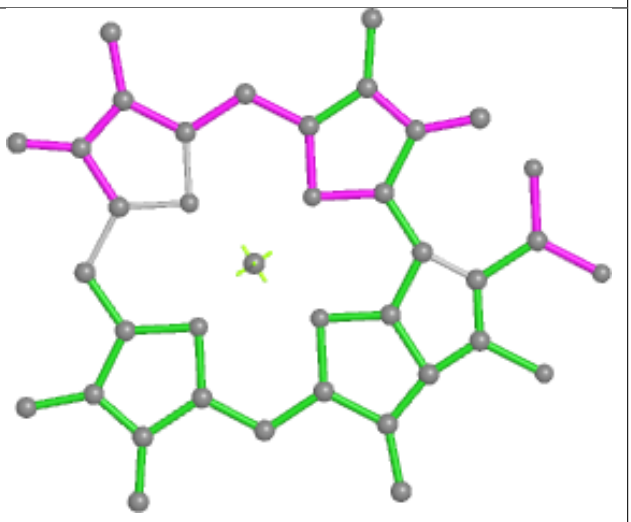
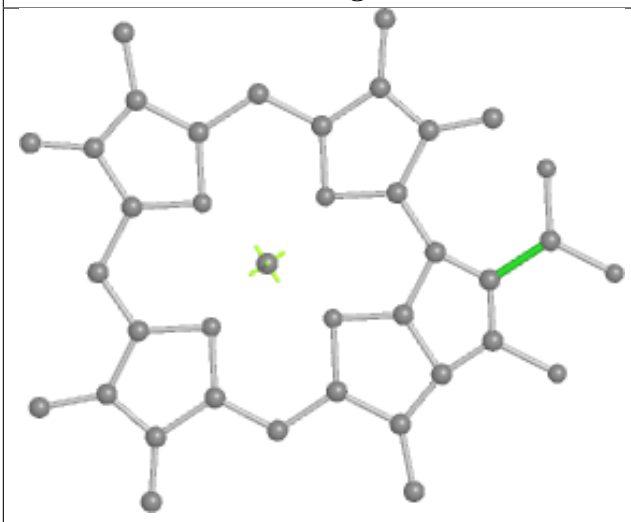


Bond angles



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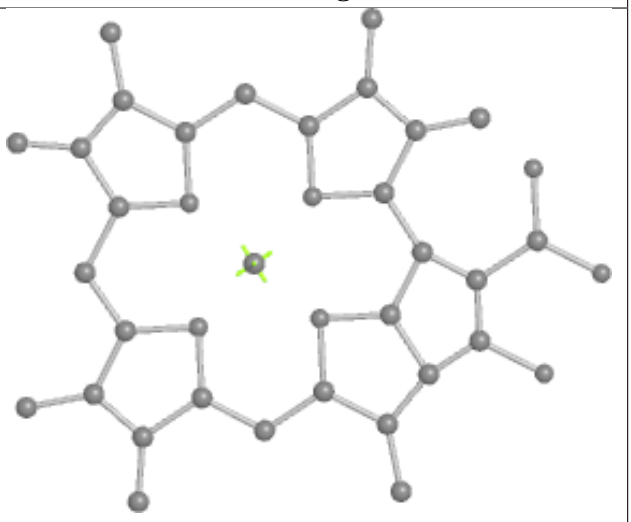
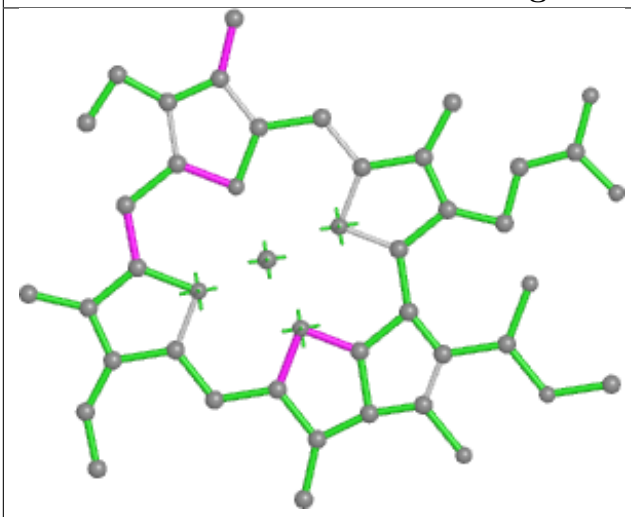
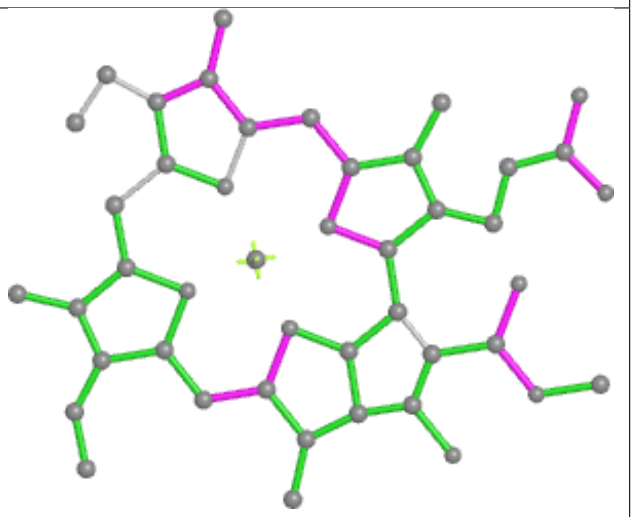


Rings

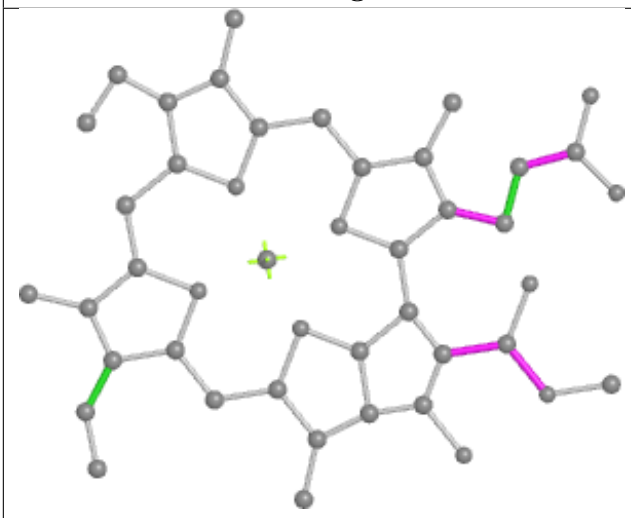
Ligand CLA c 610



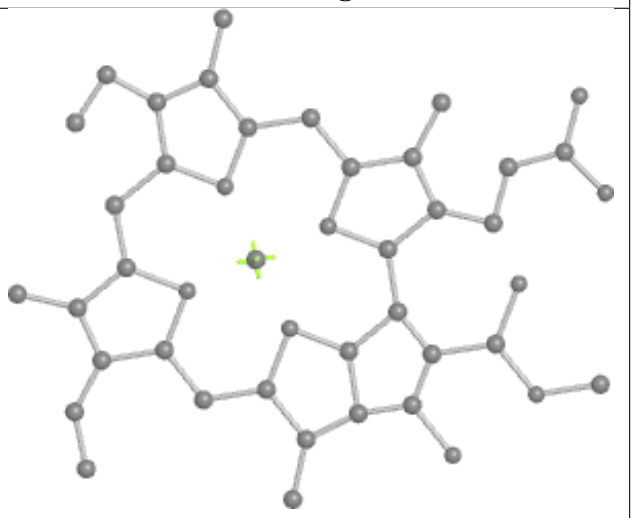
Bond lengths



Bond angles

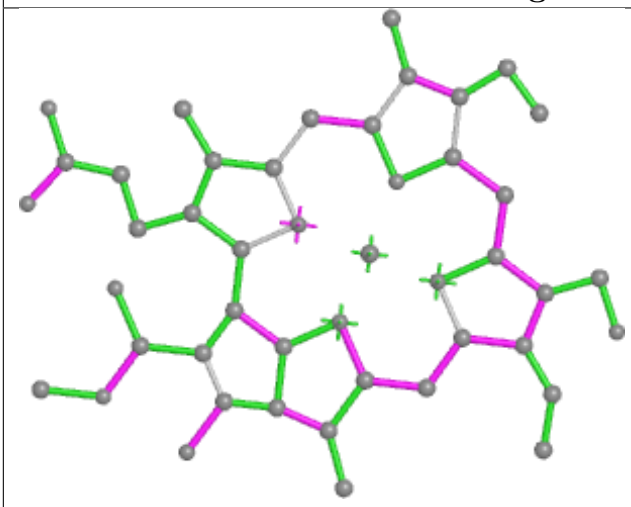


Torsions



Rings

Ligand CHL c 607



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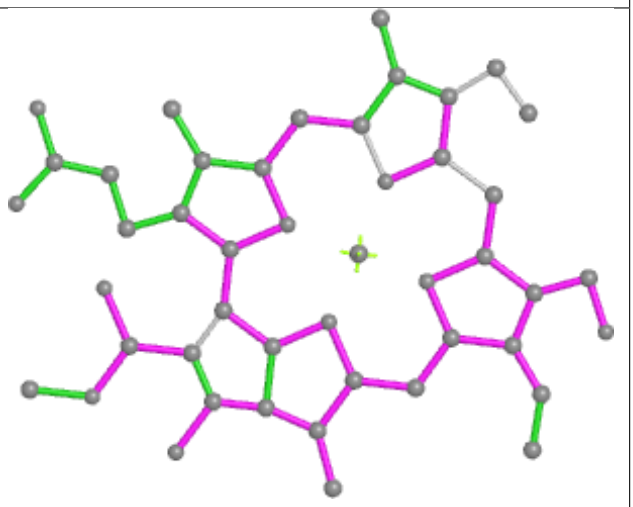

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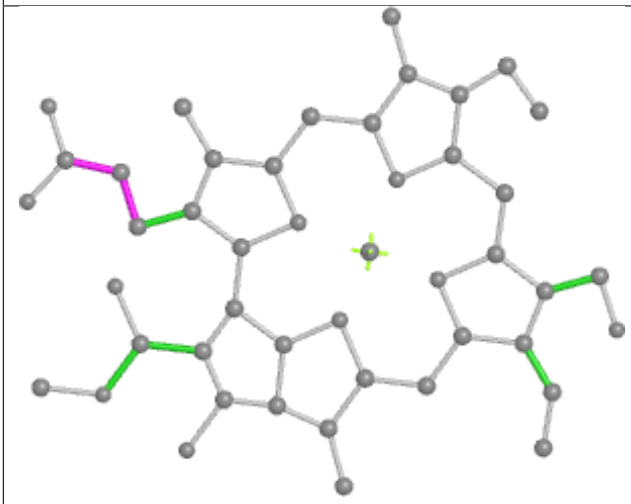

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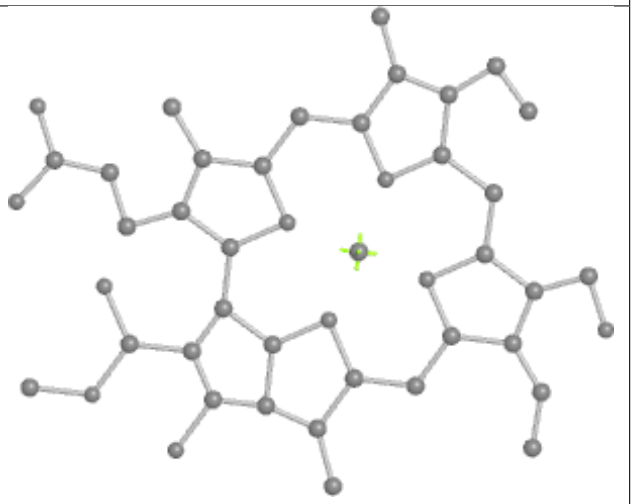
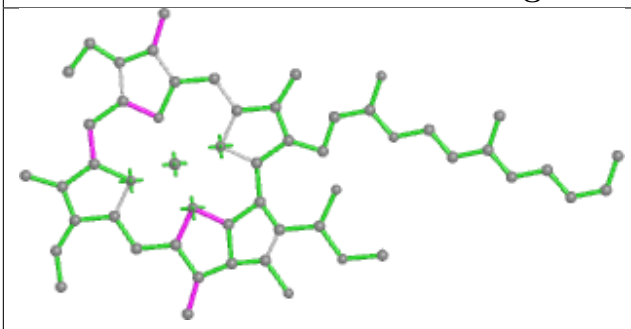


Rings

Ligand CLA A 813



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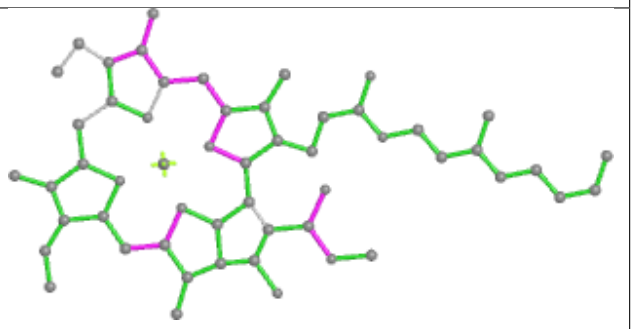
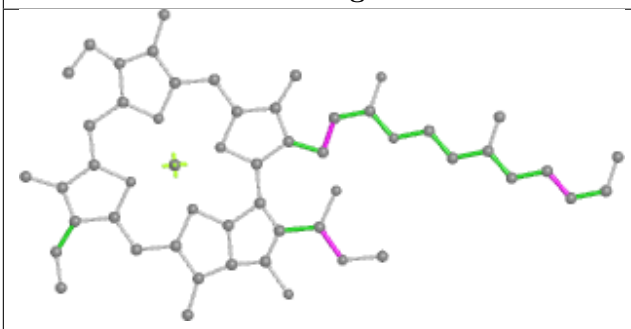


Bond angles



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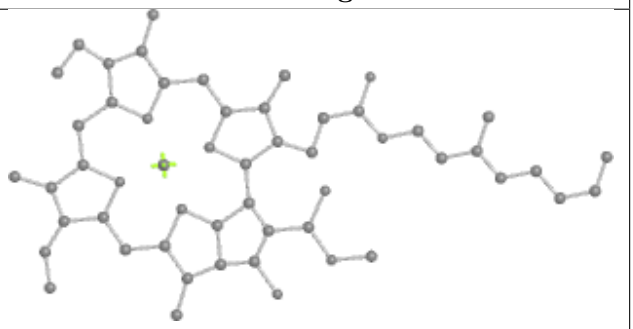
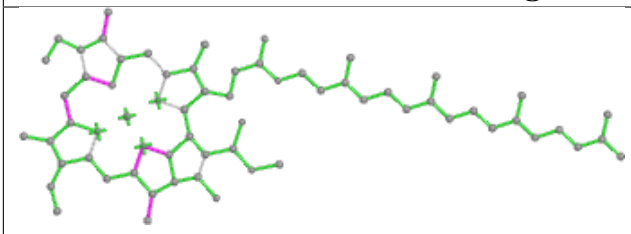


Rings

Ligand CLA A 840



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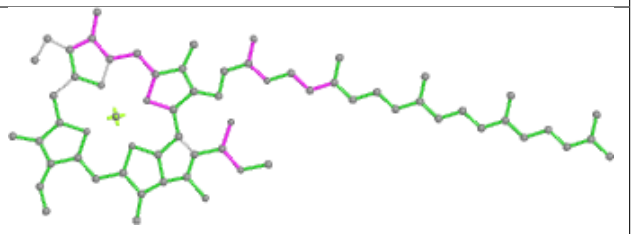
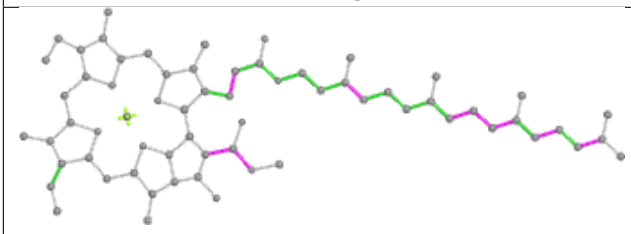


Bond angles



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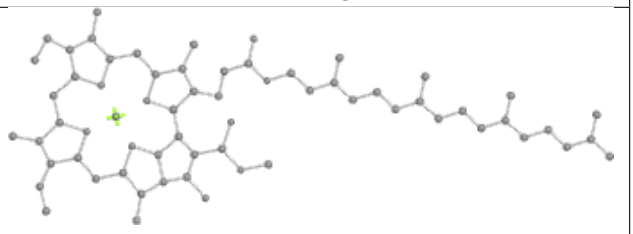
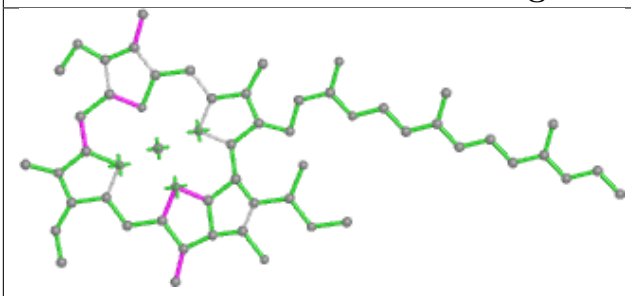


Rings

Ligand CLA 9 611



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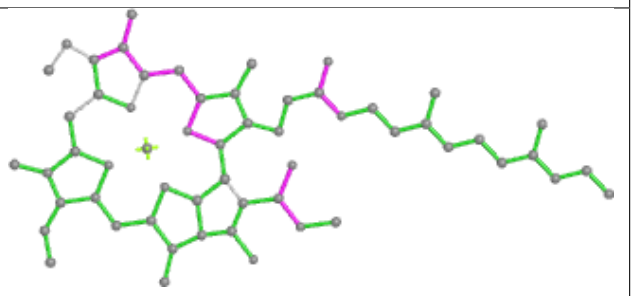

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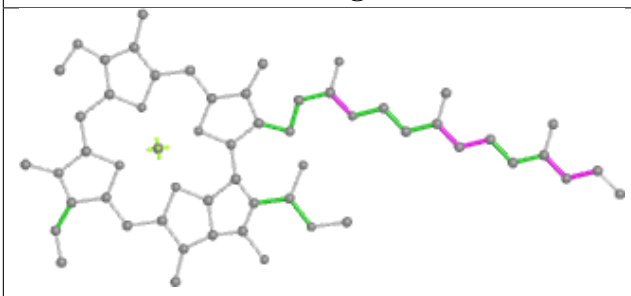

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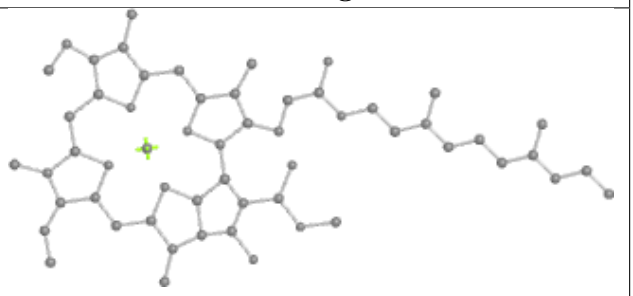
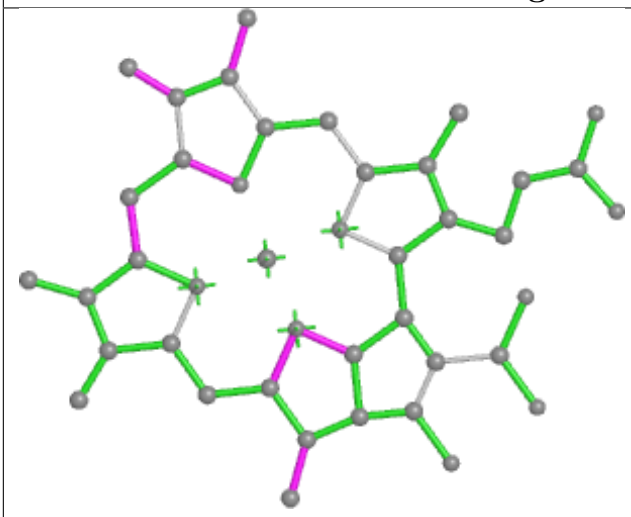


Rings

Ligand CLA 7 403



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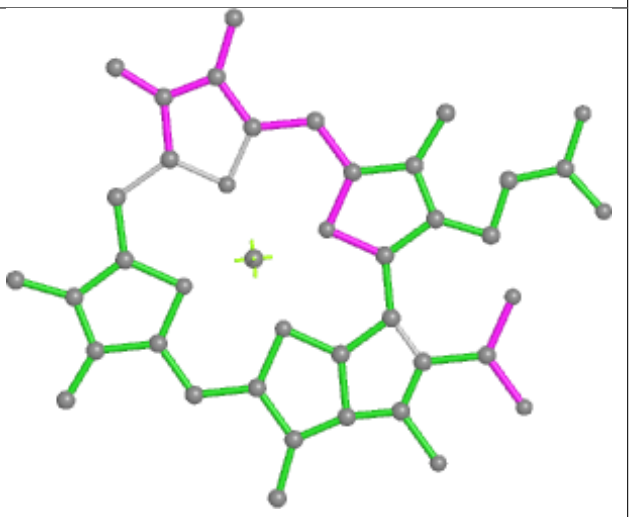
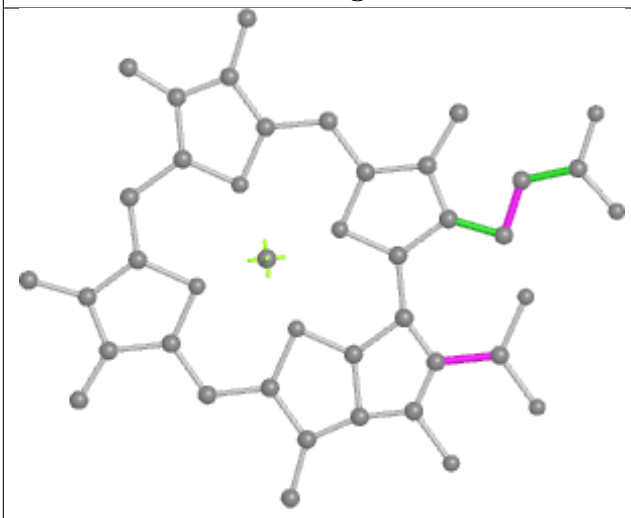


Bond angles



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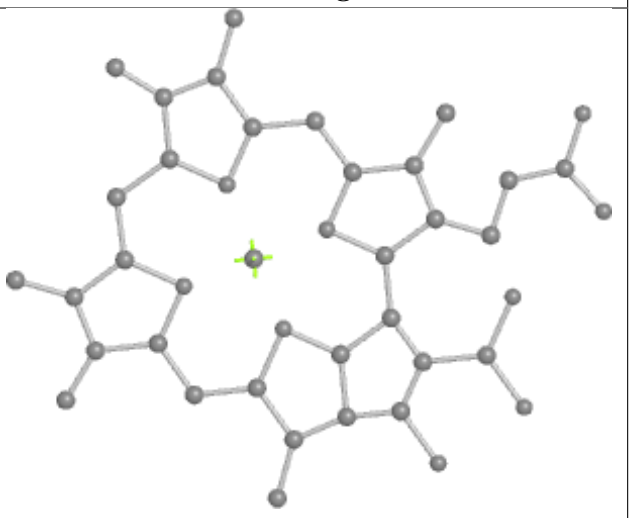
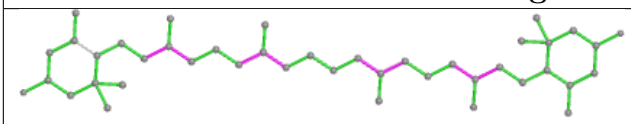


Rings

Ligand LUT c 615



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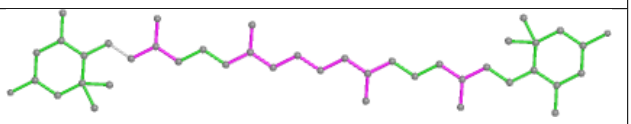
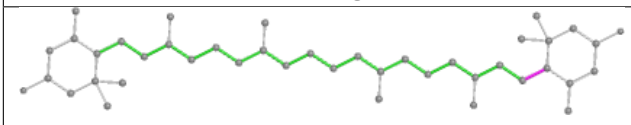


Bond angles



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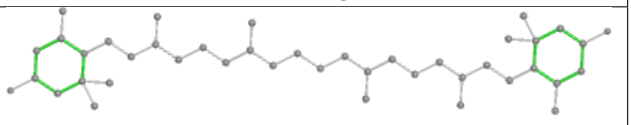
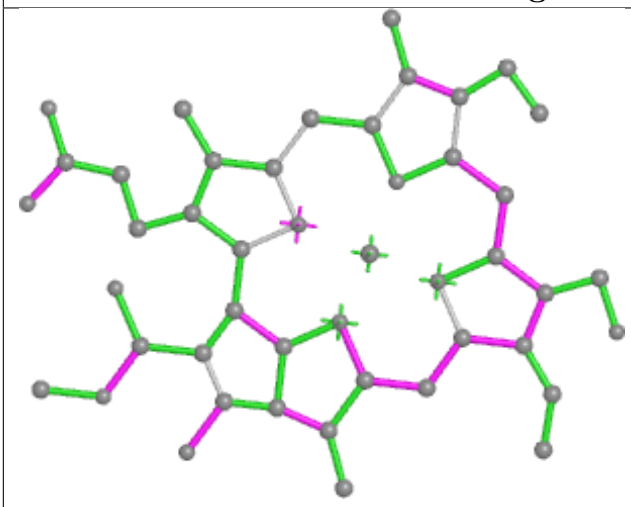


Rings

Ligand CHL c 608



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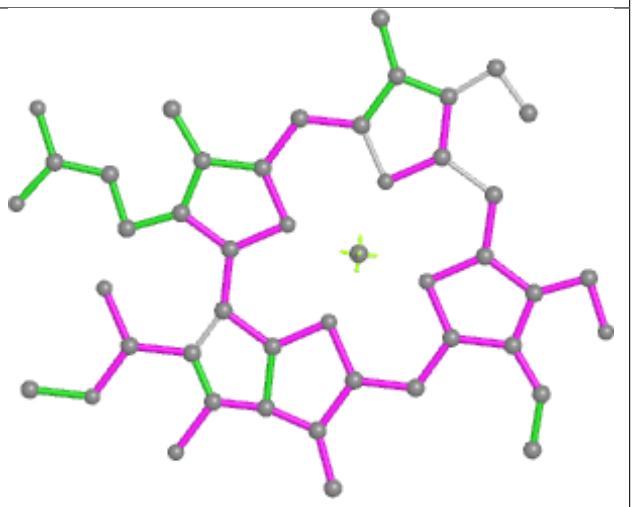
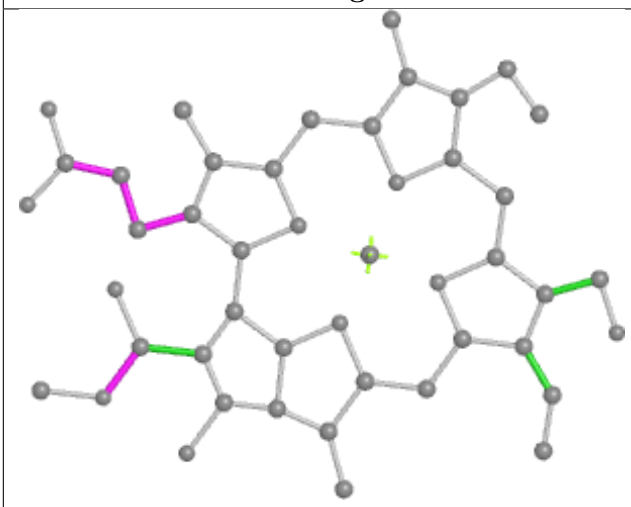


Bond angles



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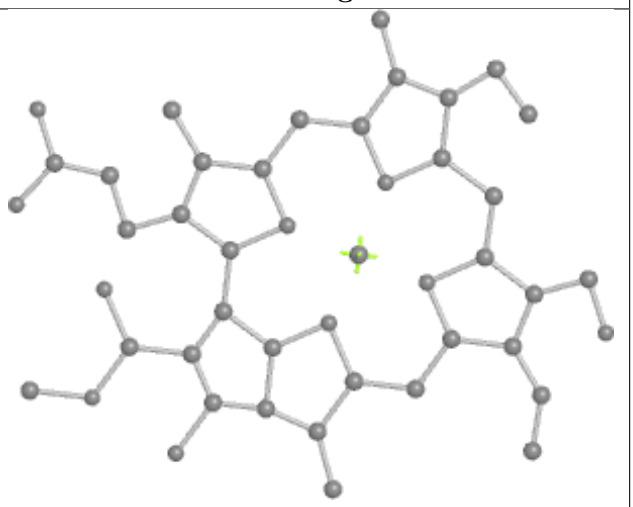
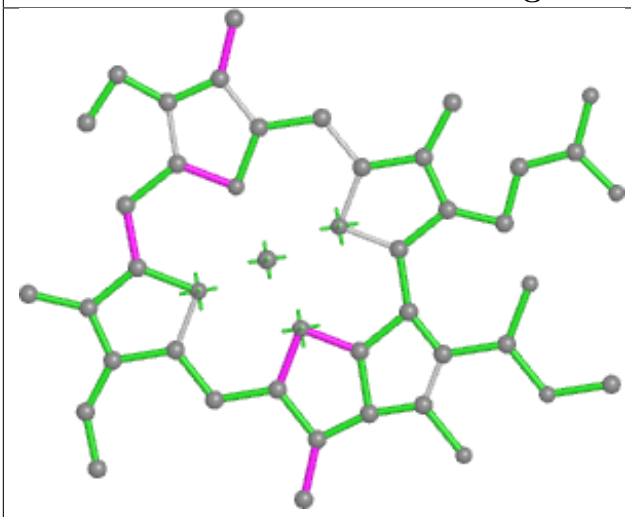
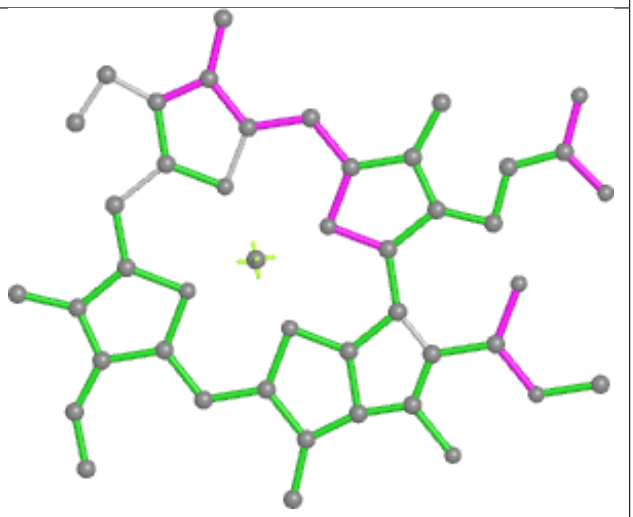


Rings

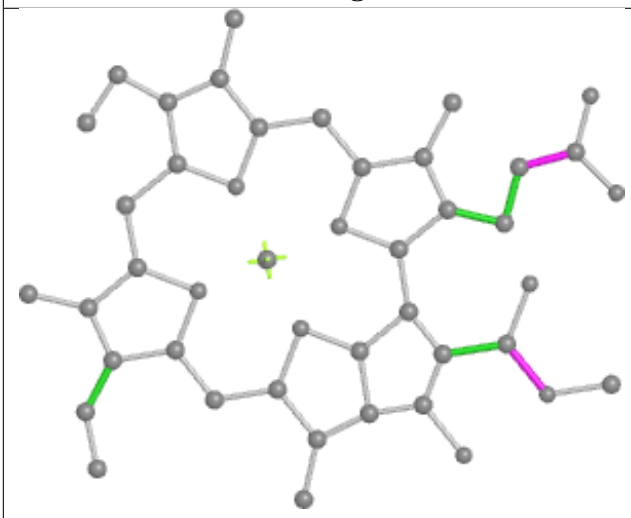
Ligand CLA A 810



Bond lengths



Bond angles



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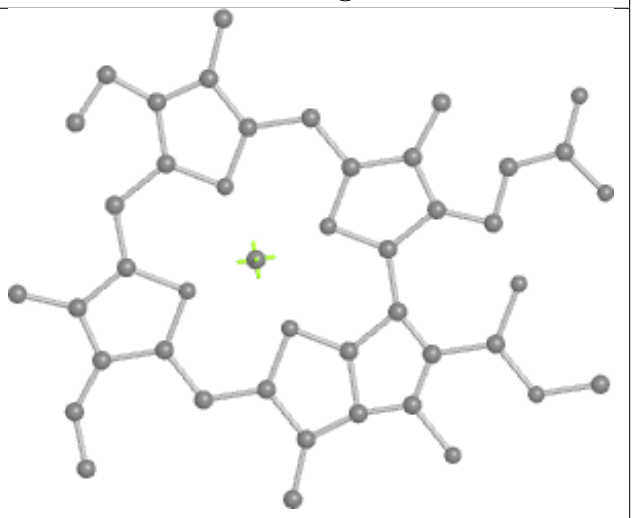
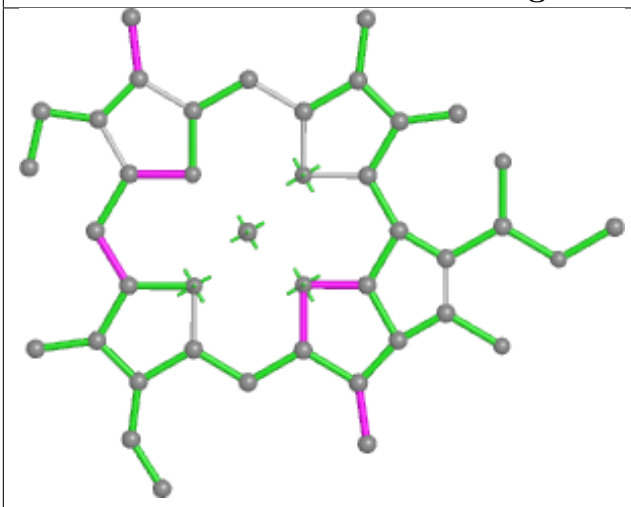


Rings

Ligand CLA a 603



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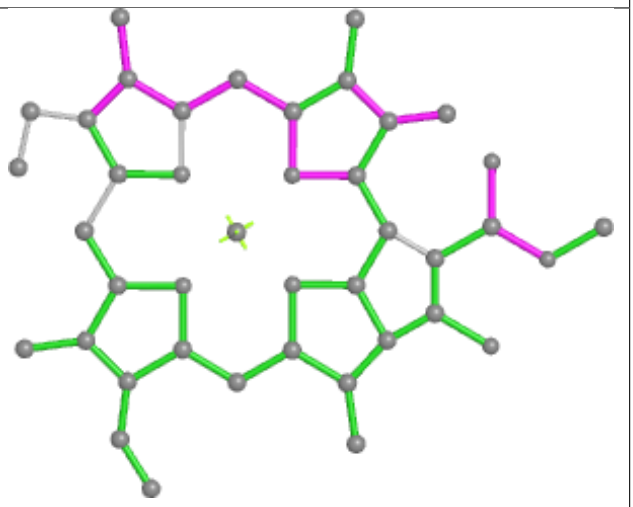
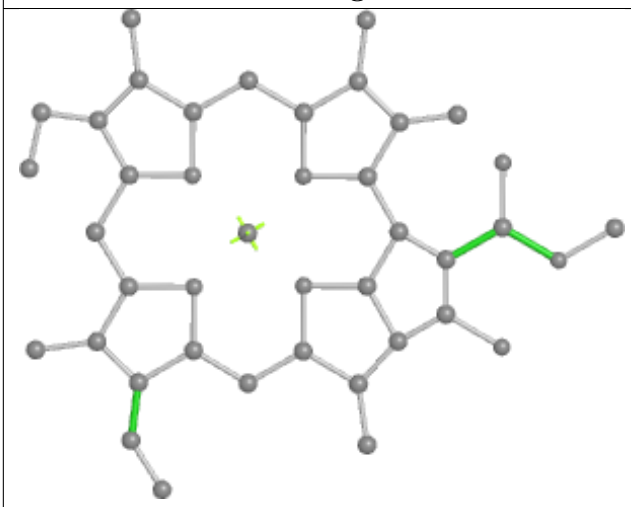


Bond angles



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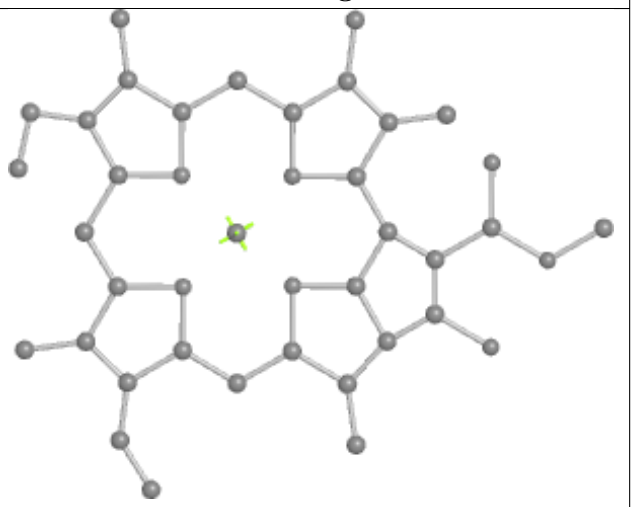
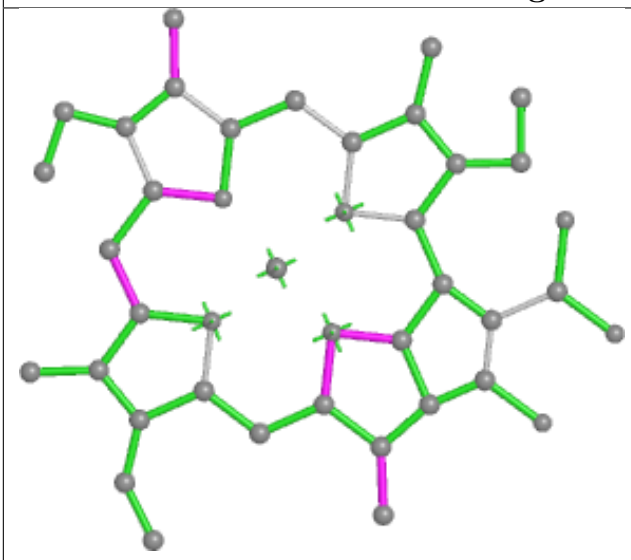
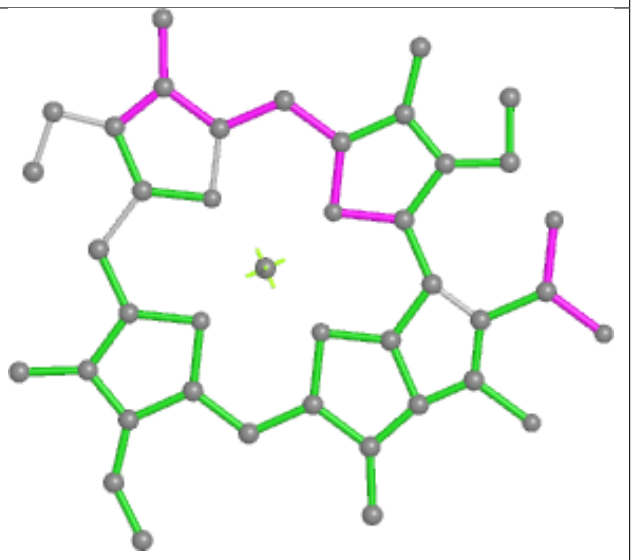


Rings

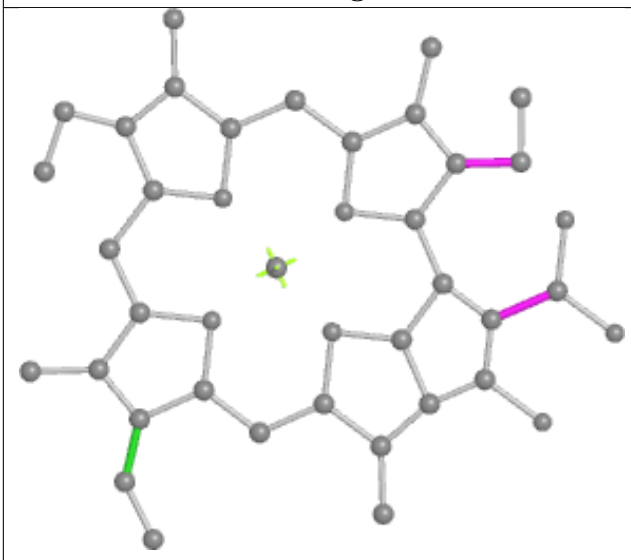
Ligand CLA 7 404



Bond lengths



Bond angles



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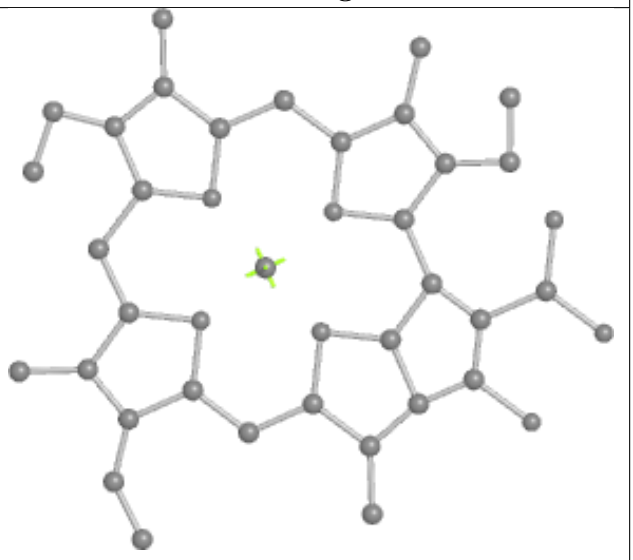
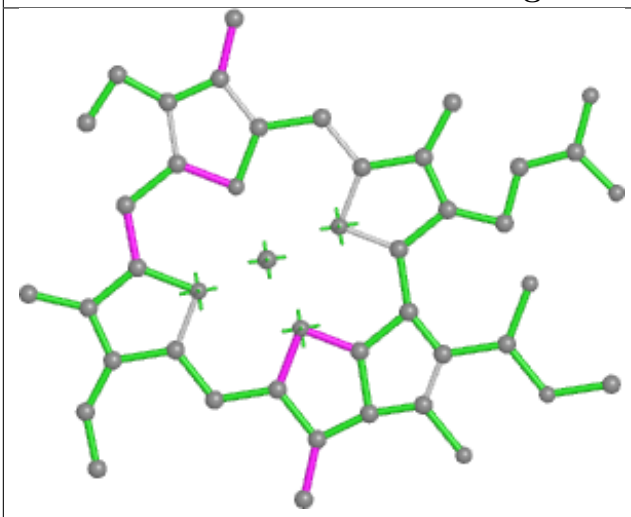


Rings

Ligand CLA A 811



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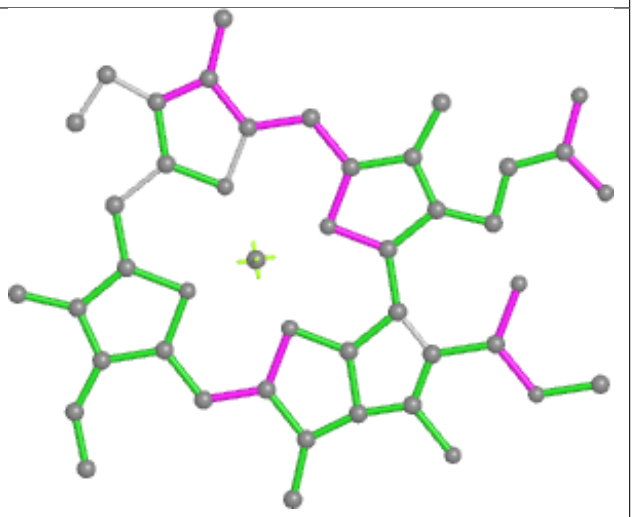
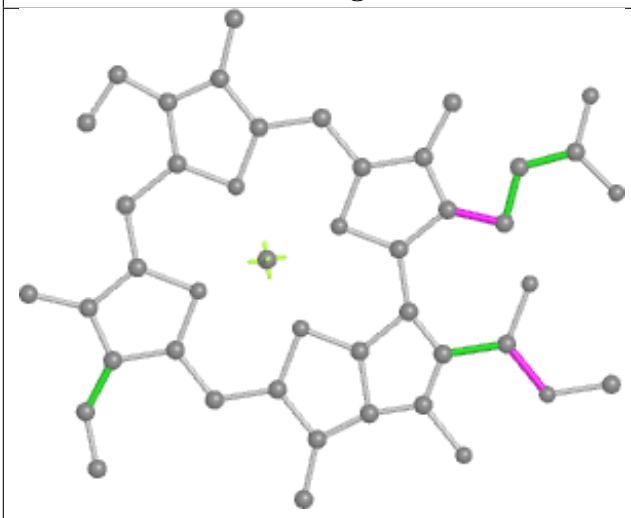


Bond angles



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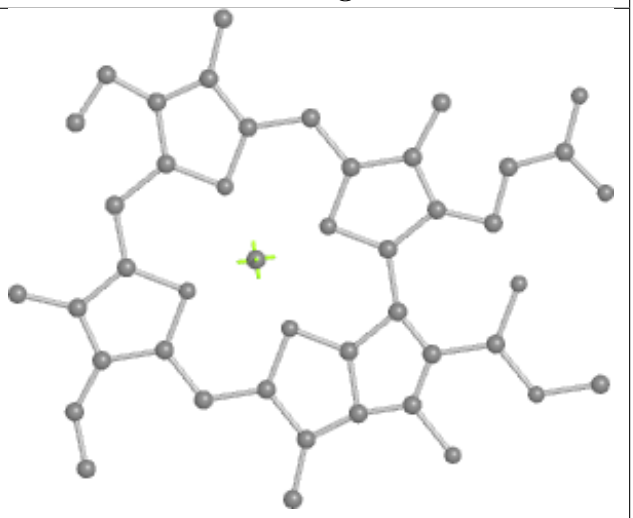
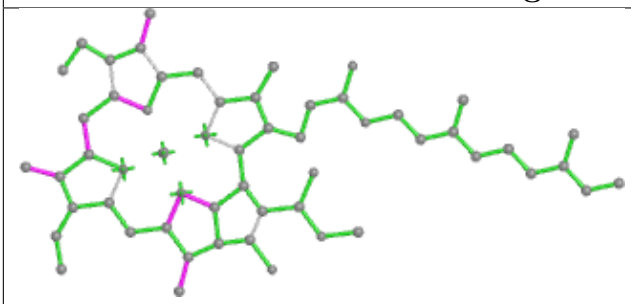


Rings

Ligand CLA A 823



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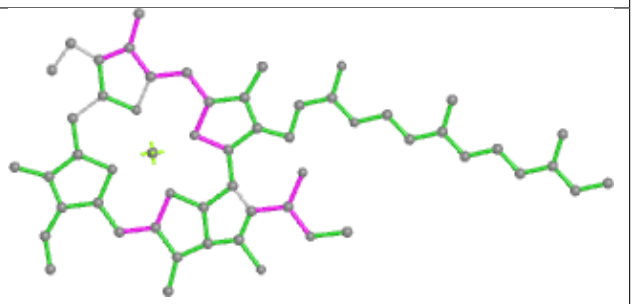
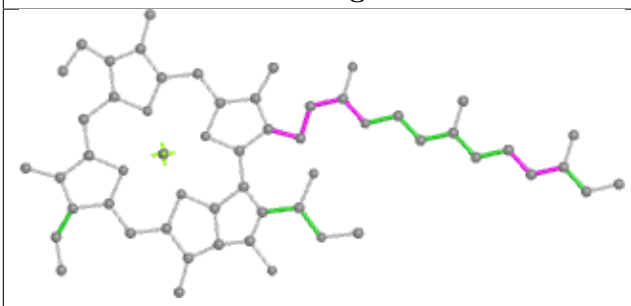
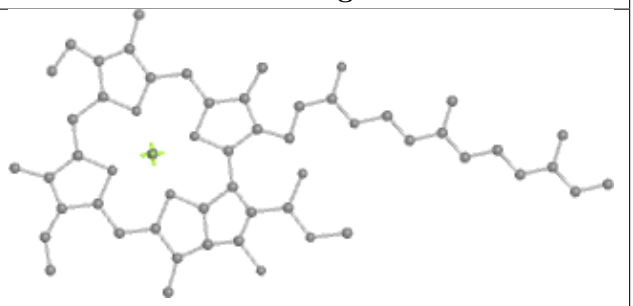


Bond angles

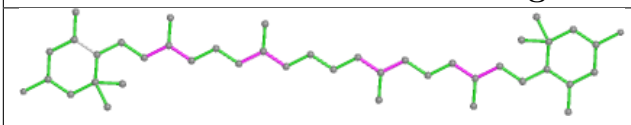


Torsions

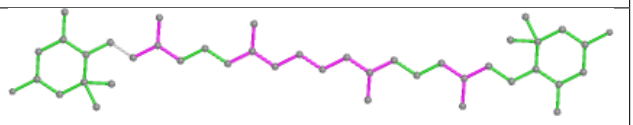


Rings

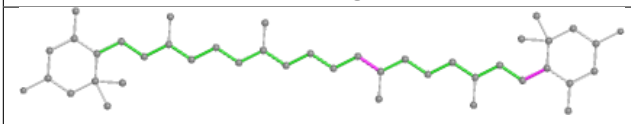
Ligand LUT 4 615



Bond lengths



Bond angles



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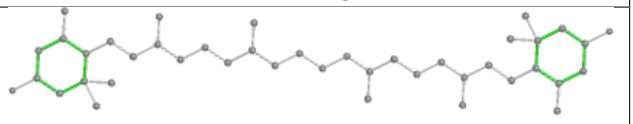
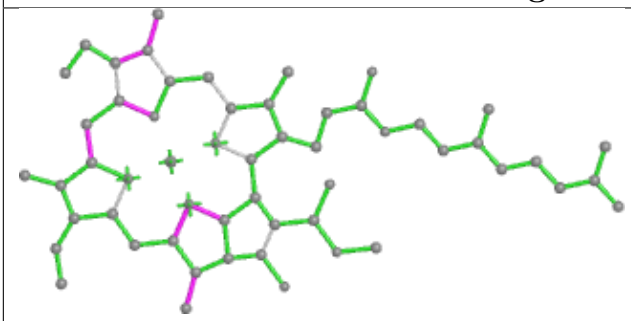


Rings

Ligand CLA 3 403



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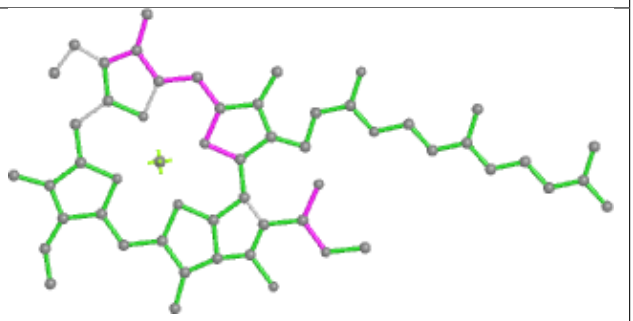

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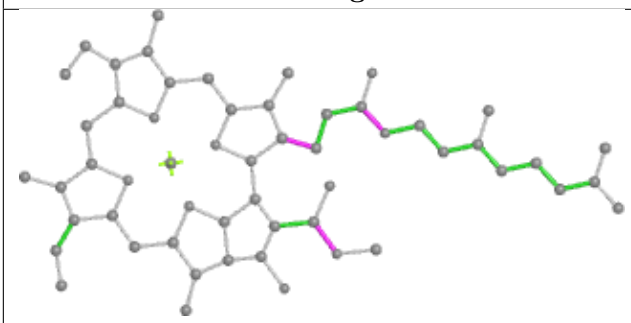

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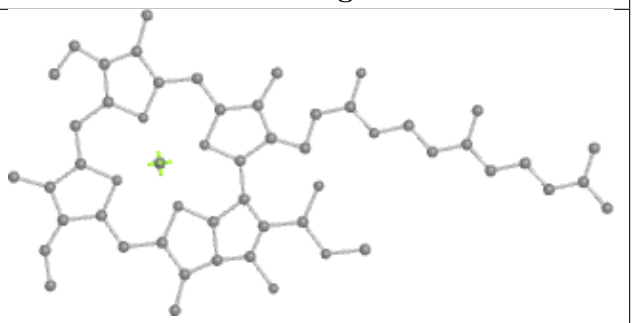
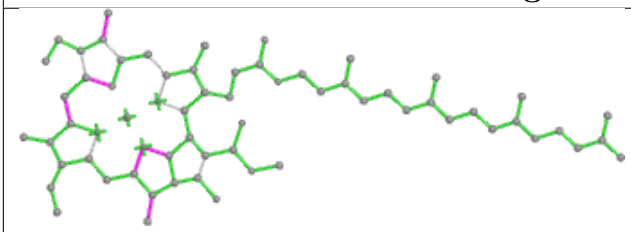


Rings

Ligand CLA A 826



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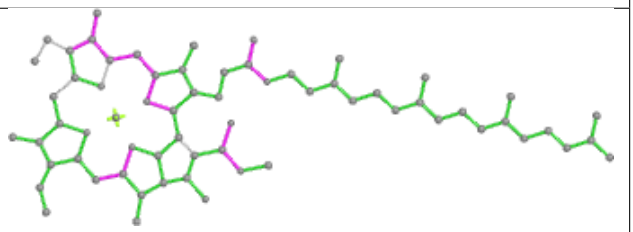
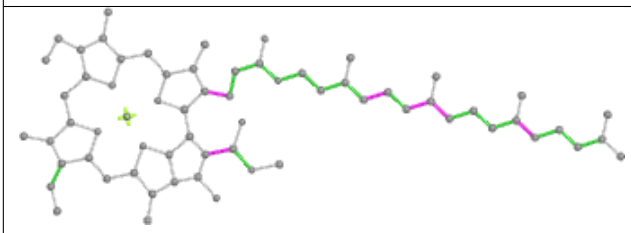


Bond angles



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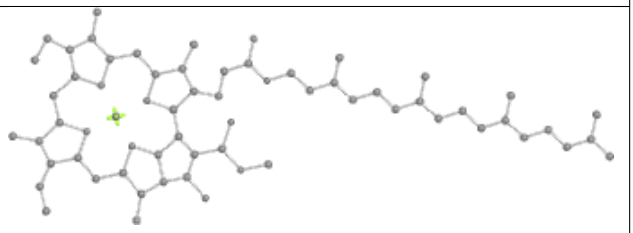
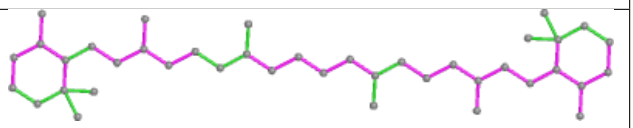


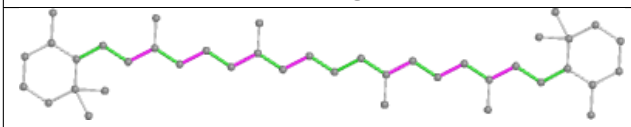
Rings

Ligand BCR B 844

Bond lengths



Bond angles



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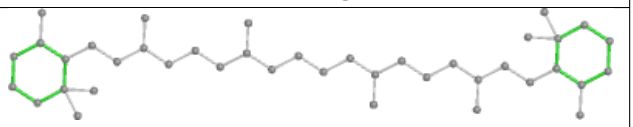
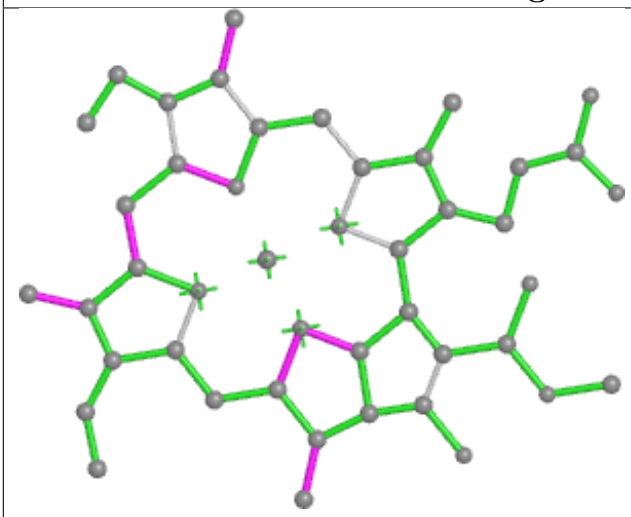


Rings

Ligand CLA 9 604



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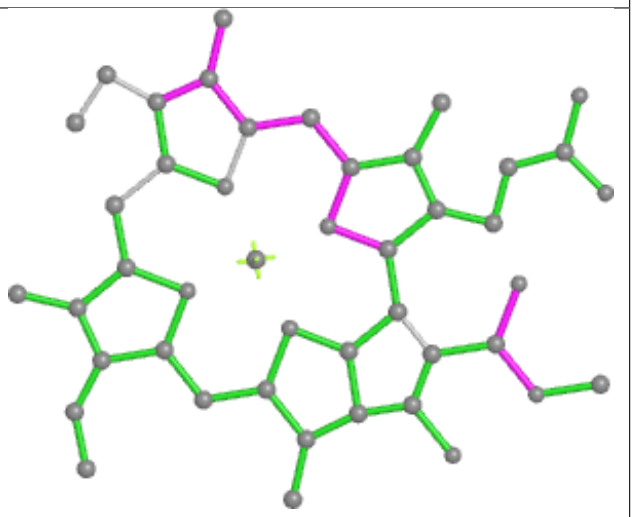

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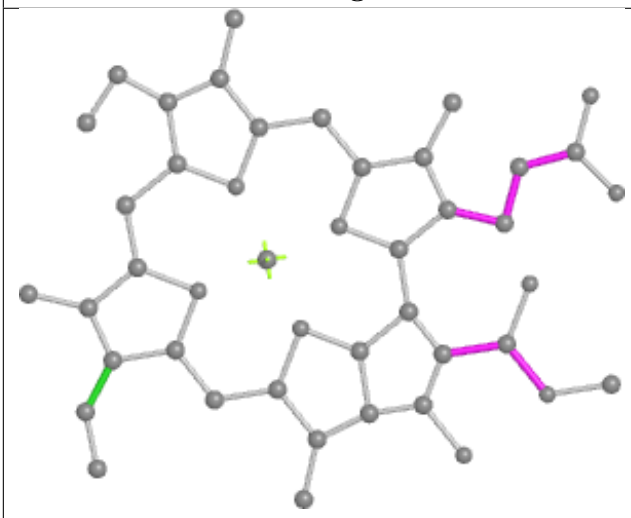

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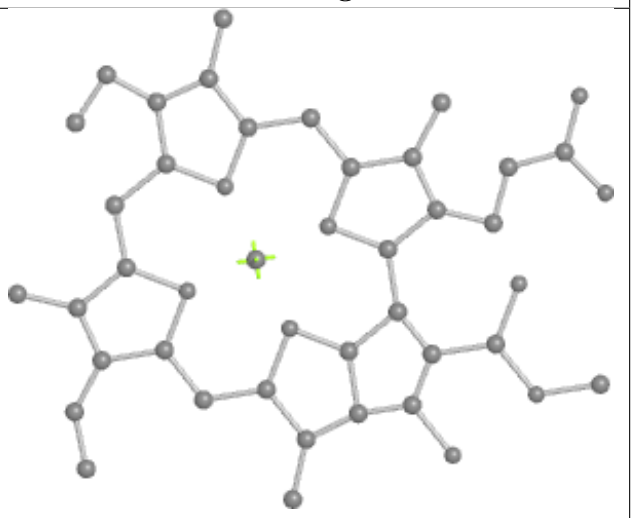
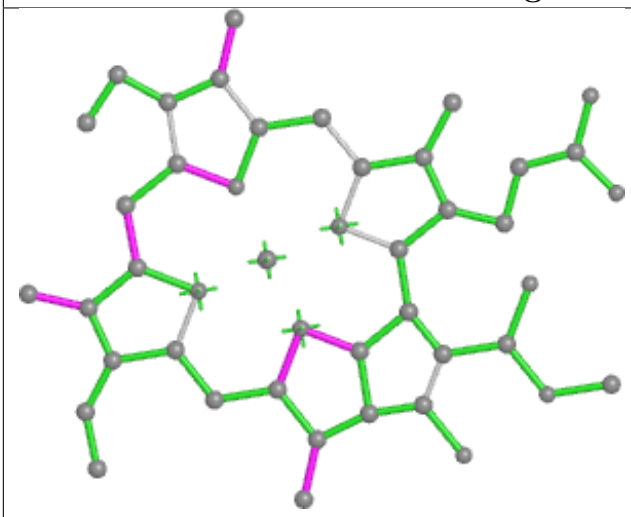


Rings

Ligand CLA B 811



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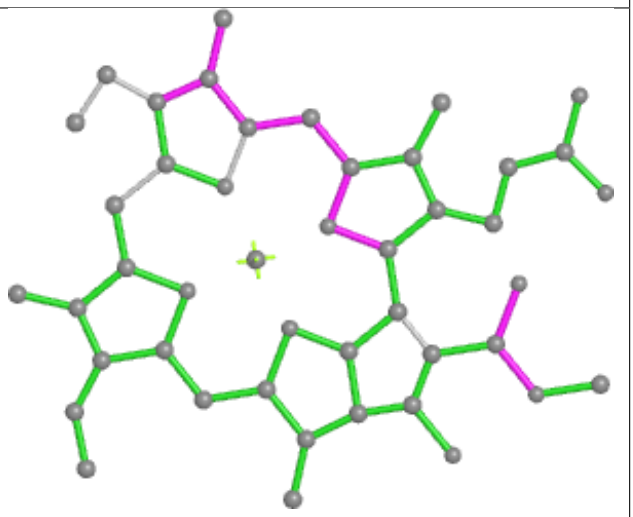

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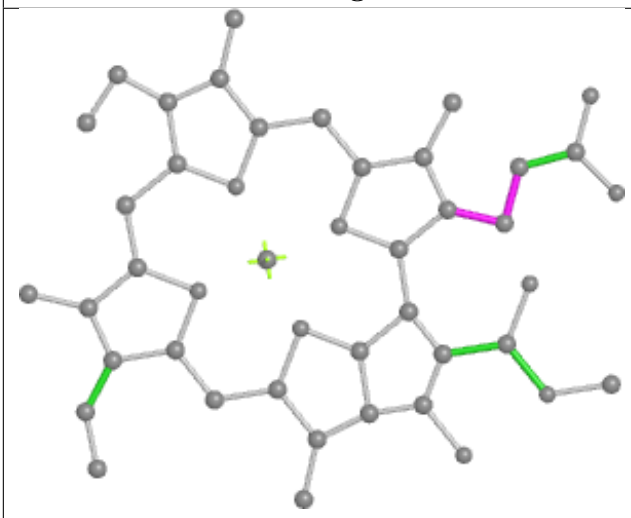

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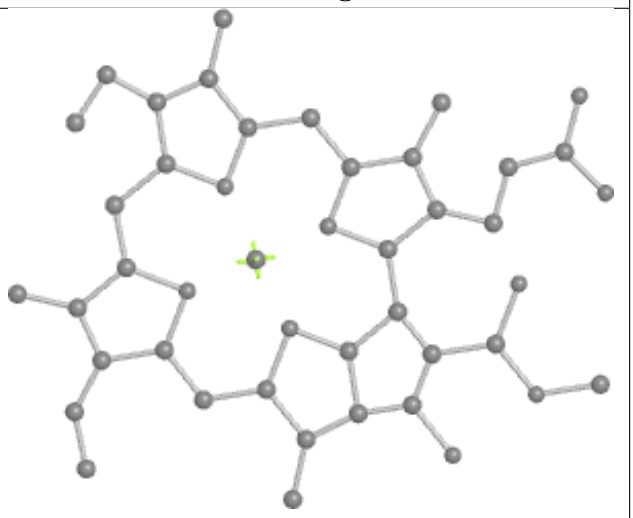
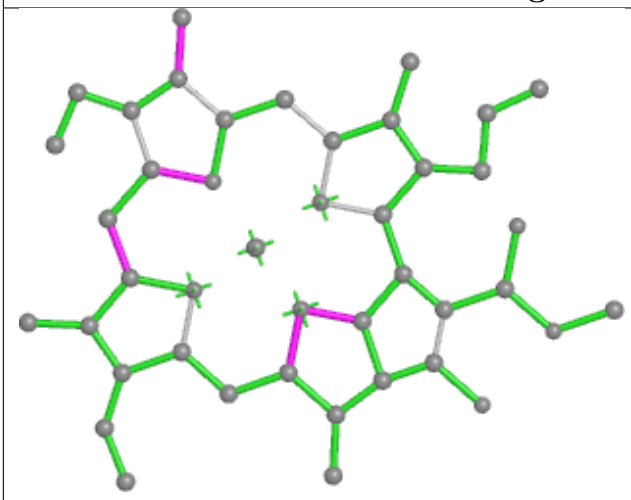


Rings

Ligand CLA 7 410



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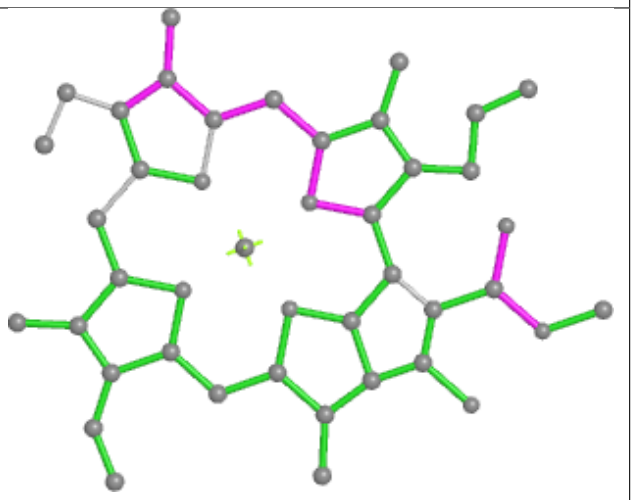
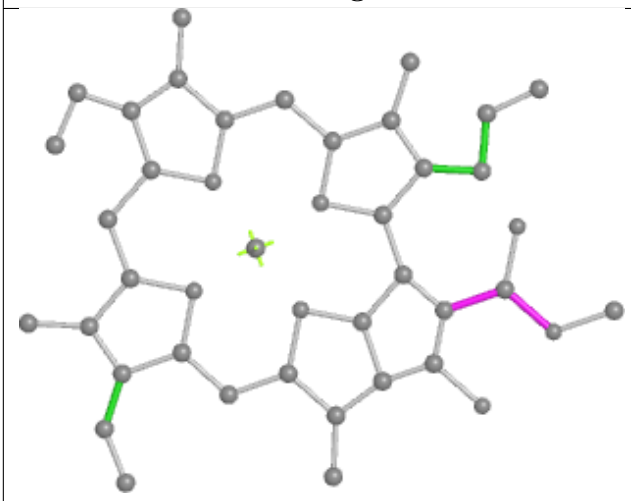


Bond angles



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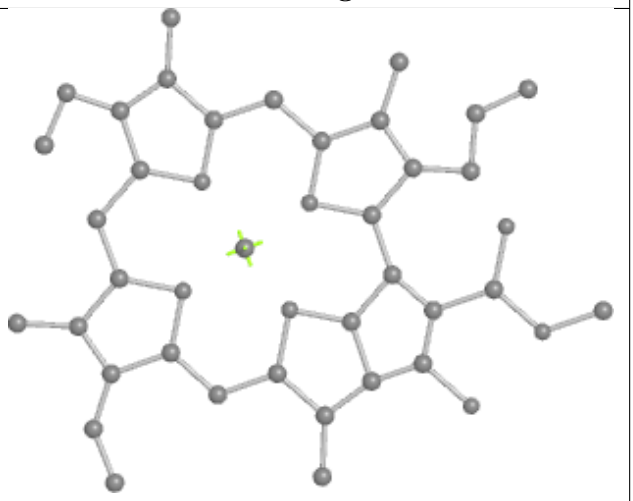
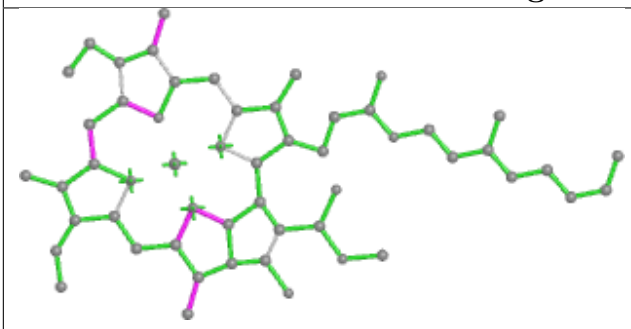


Rings

Ligand CLA b 311



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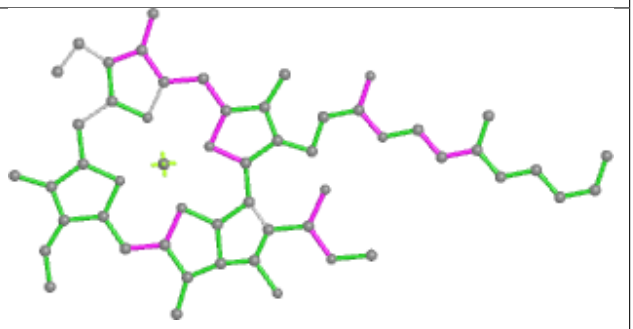
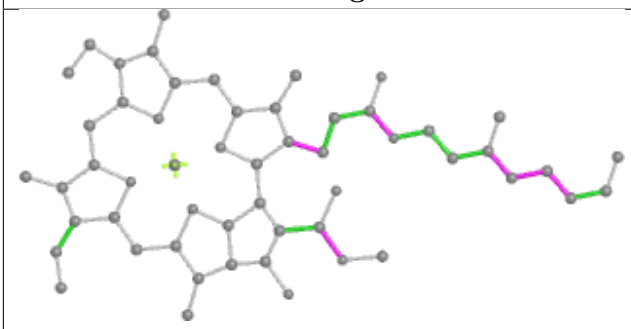


Bond angles



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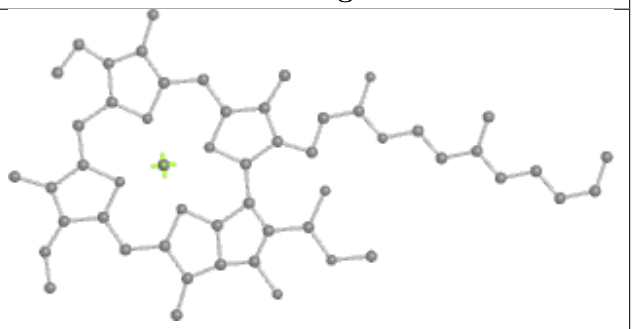
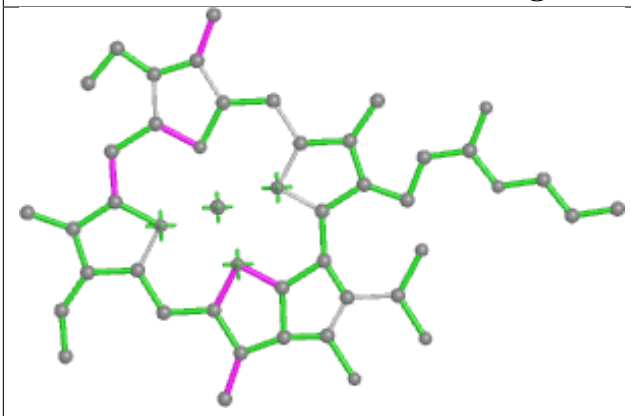


Rings

Ligand CLA a 604



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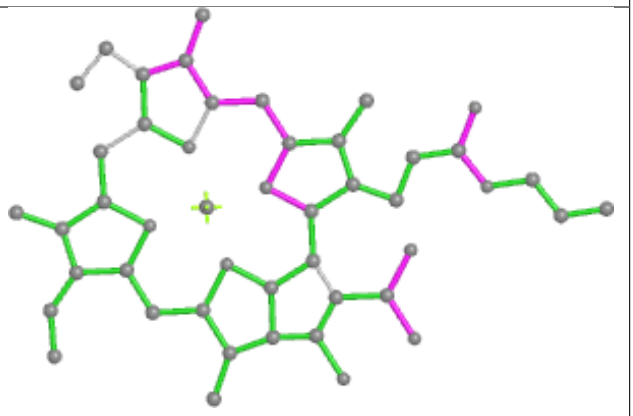
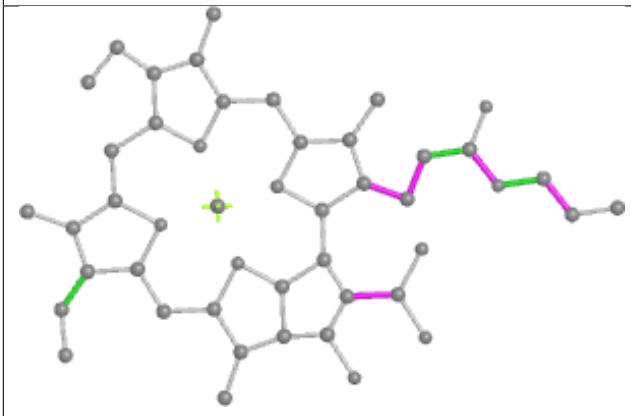


Bond angles



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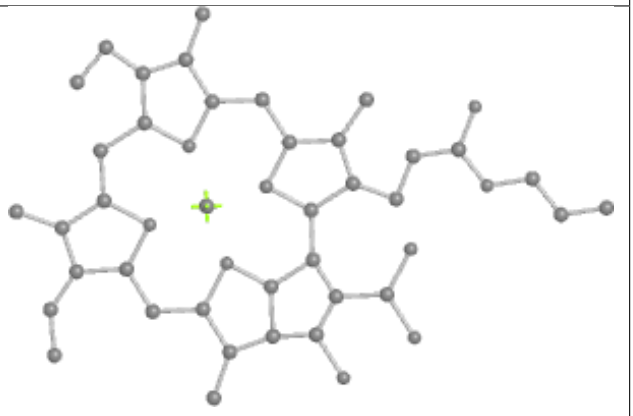
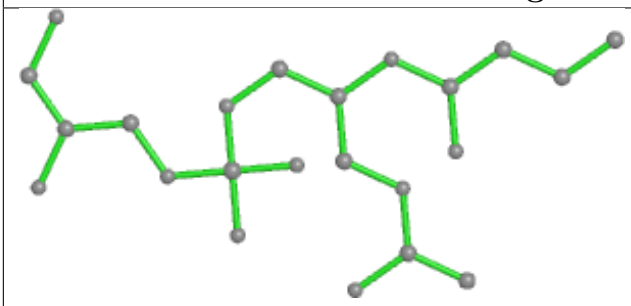


Rings

Ligand LHG 1 301



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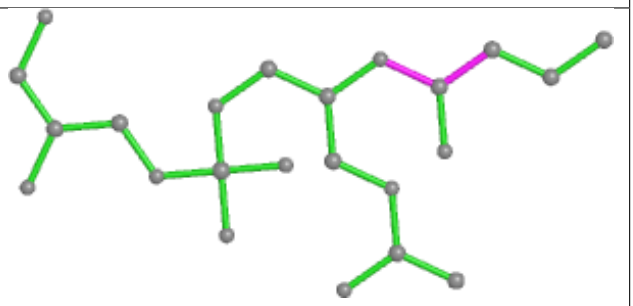

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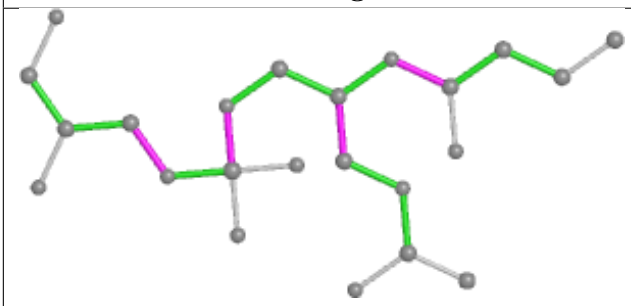

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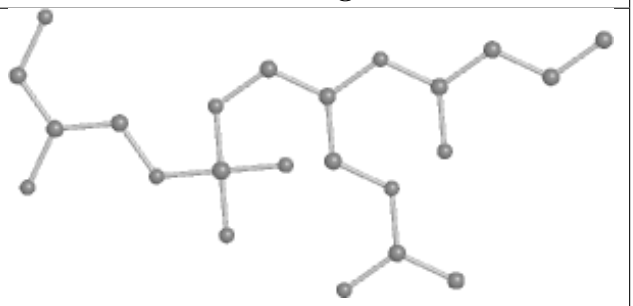
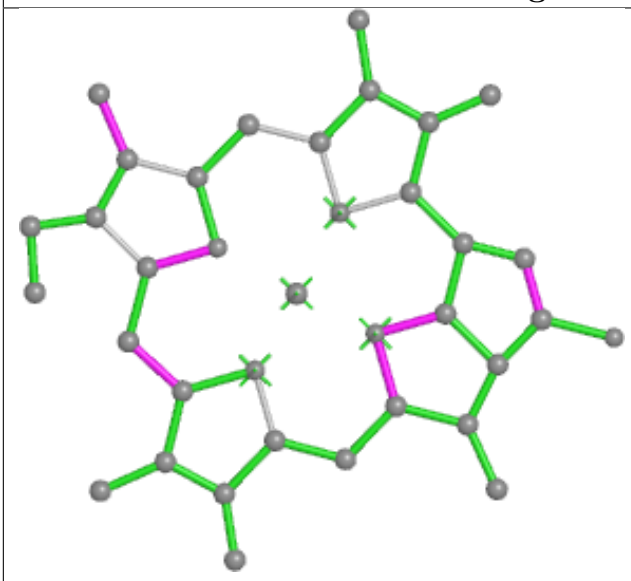


Rings

Ligand CLA 7 413



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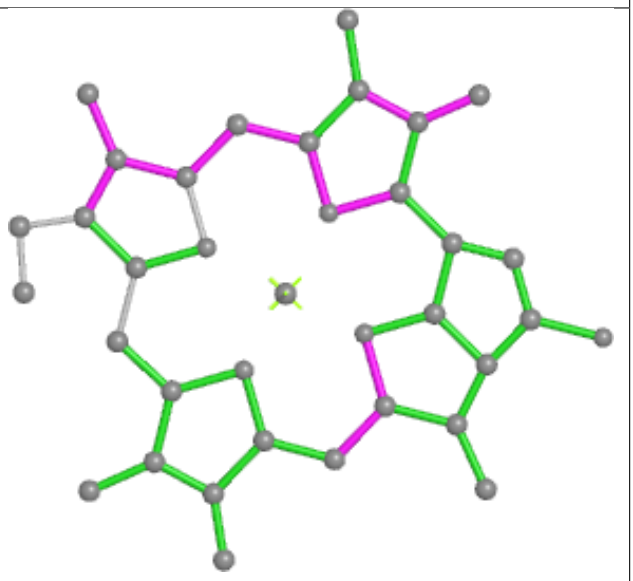

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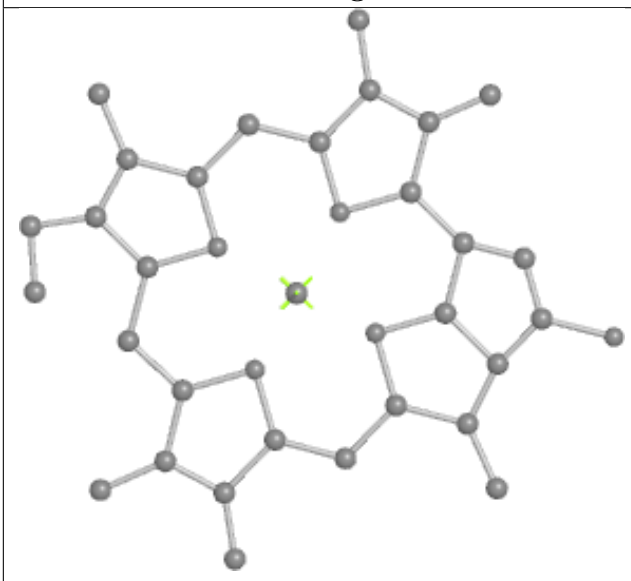

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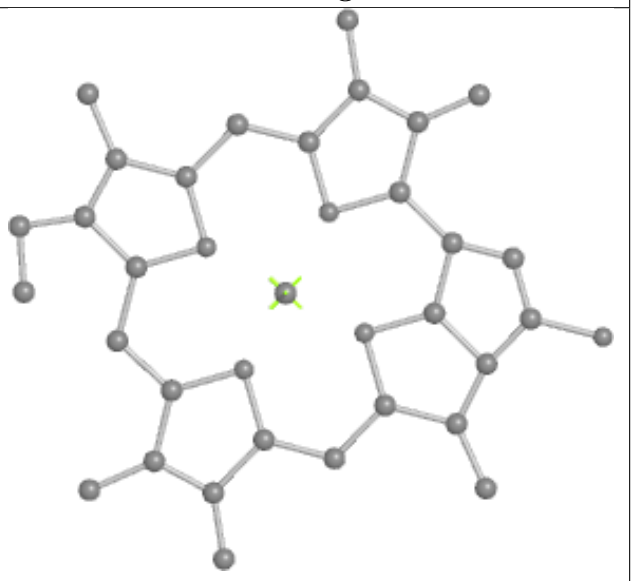
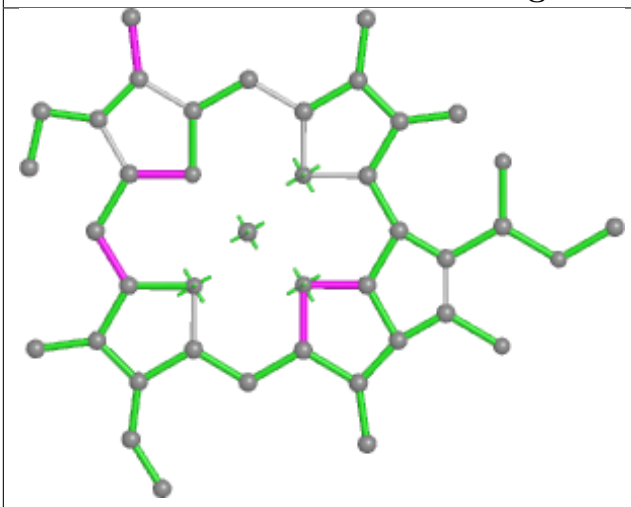


Rings

Ligand CLA 7 408



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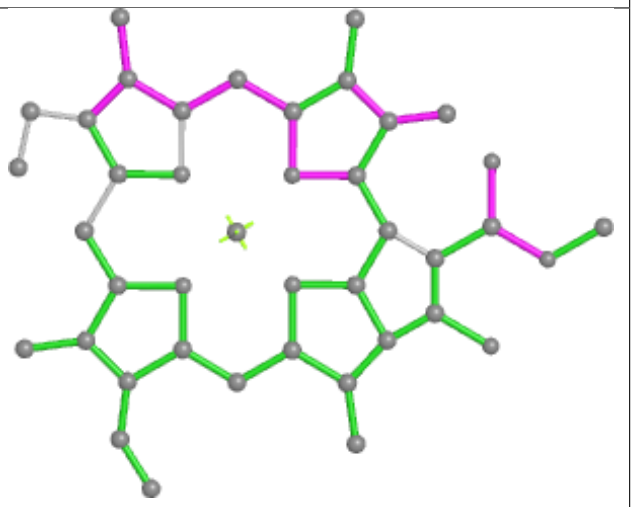
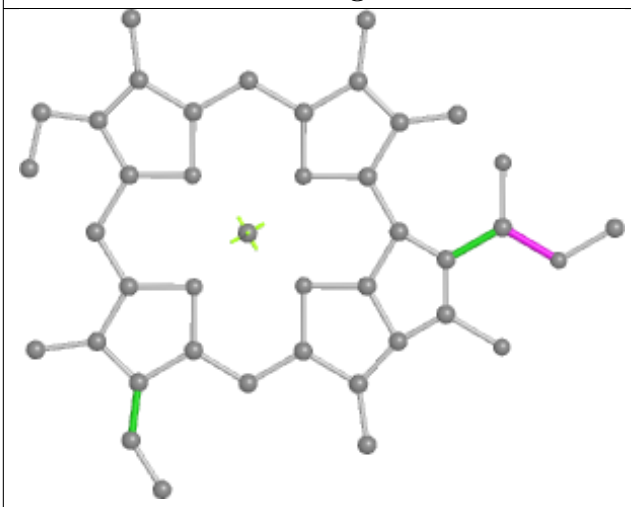


Bond angles



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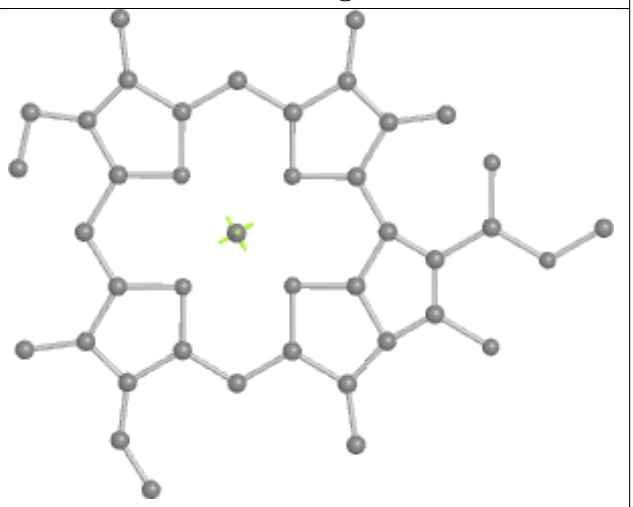
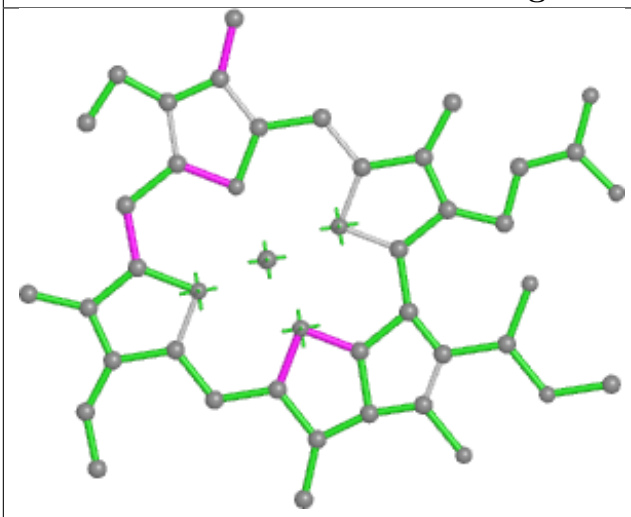


Rings

Ligand CLA 8 601



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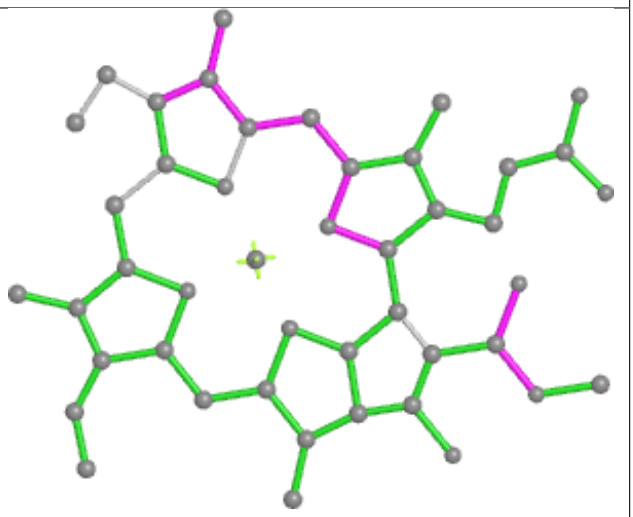
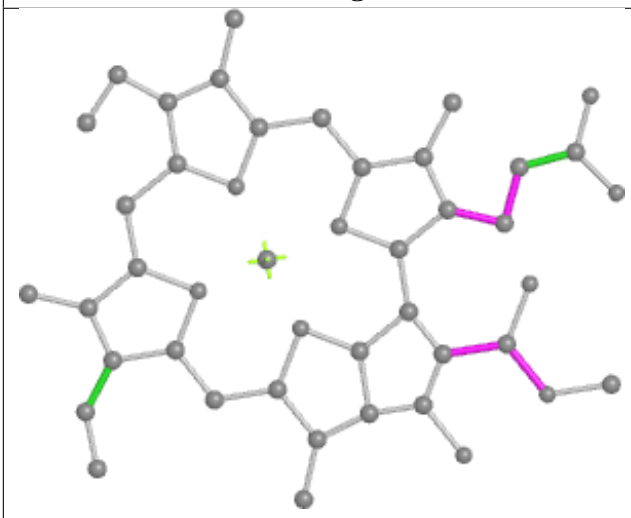


Bond angles



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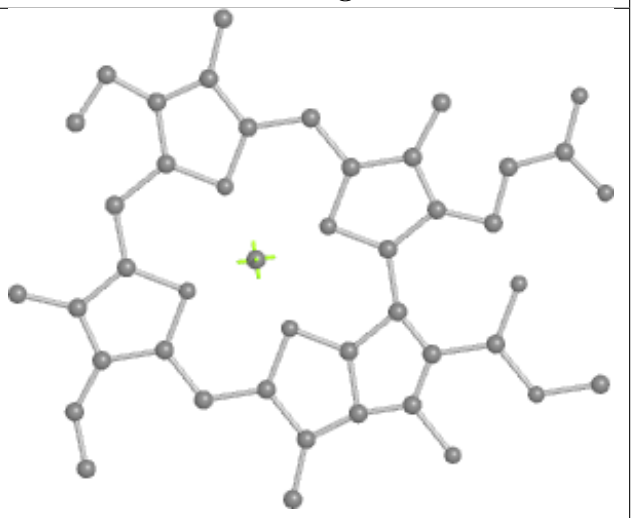
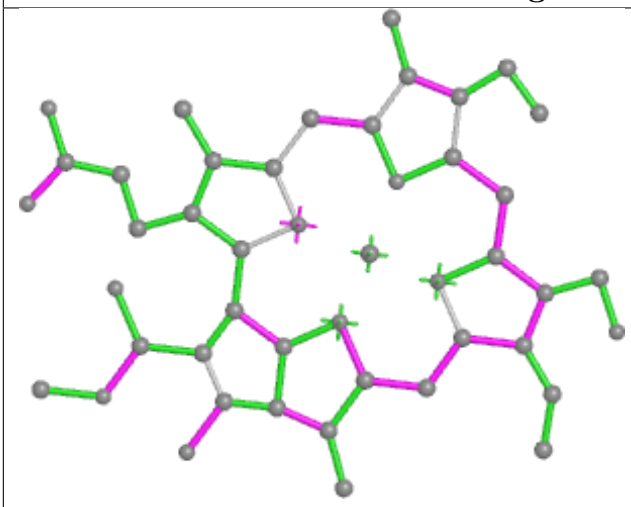


Rings

Ligand CHL a 609



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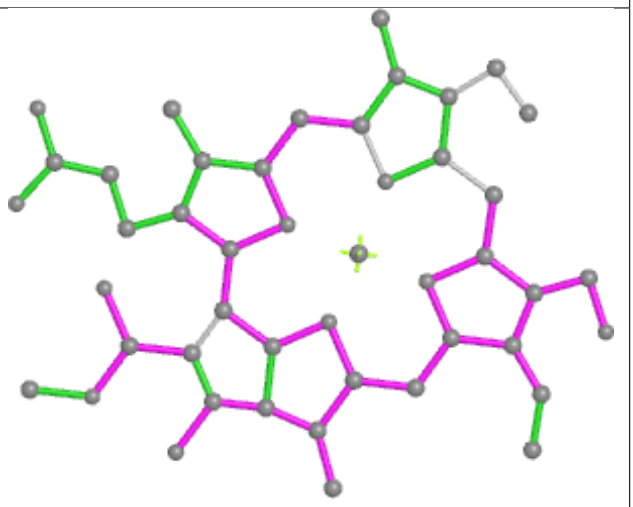

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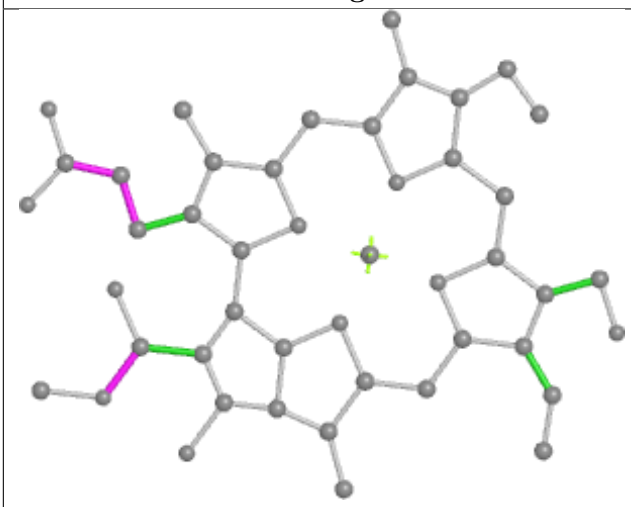

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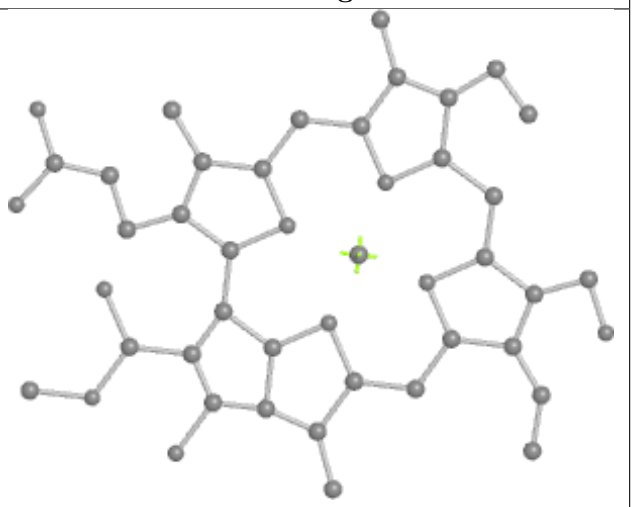
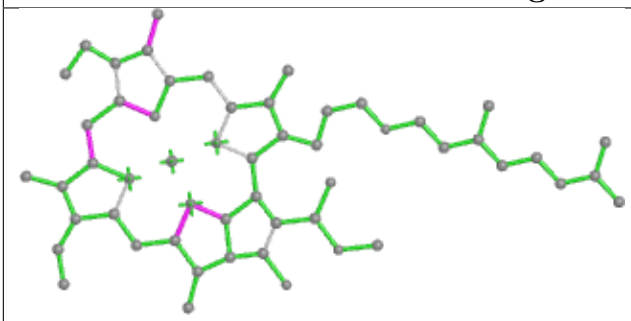


Rings

Ligand CLA 8 611



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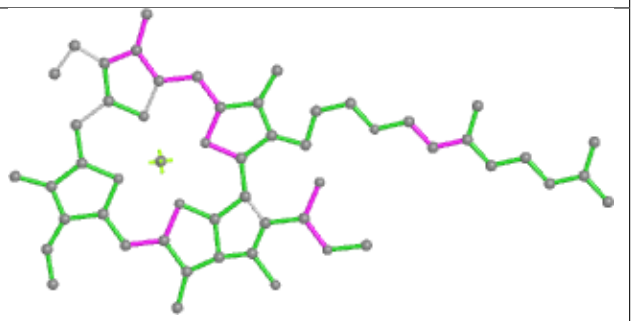

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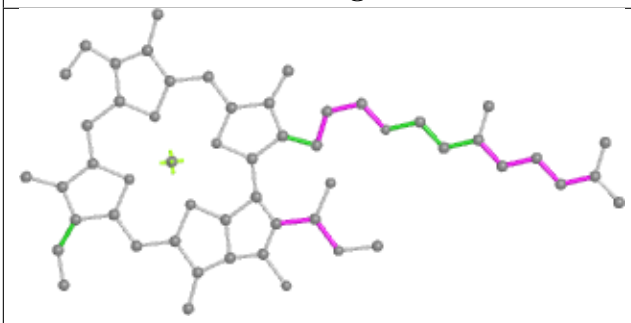

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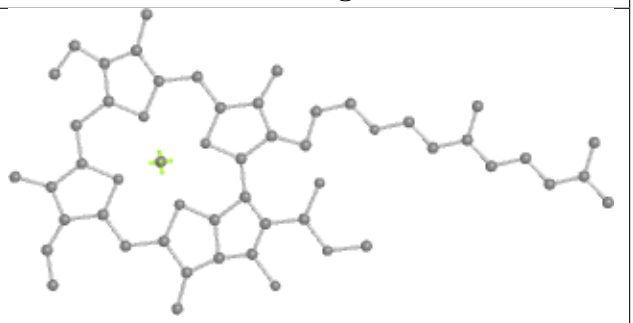
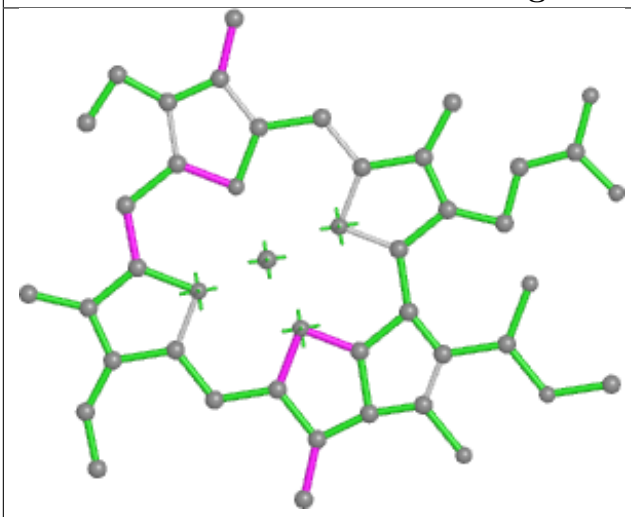


Rings

Ligand CLA 7 402



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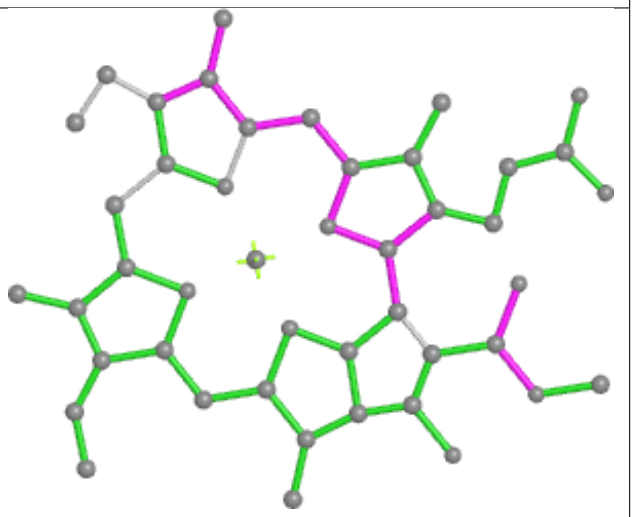

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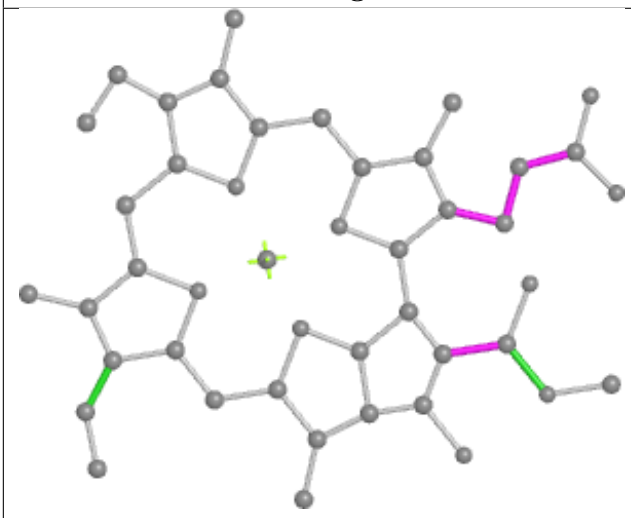

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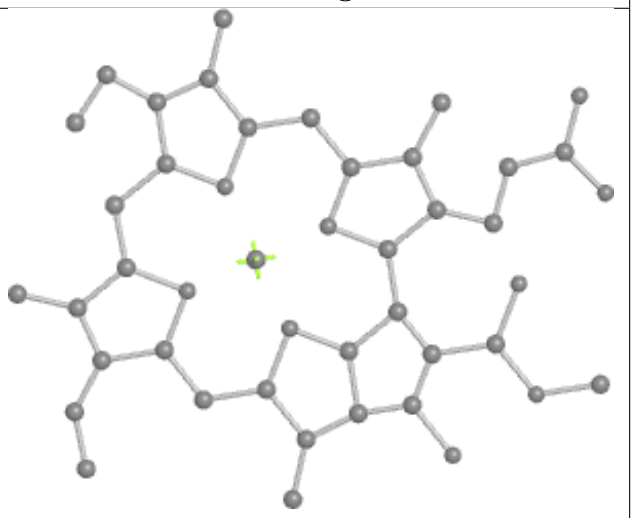
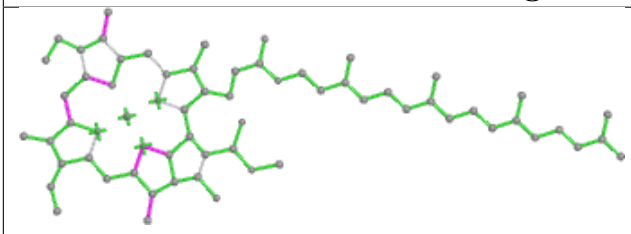


Rings

Ligand CLA A 814



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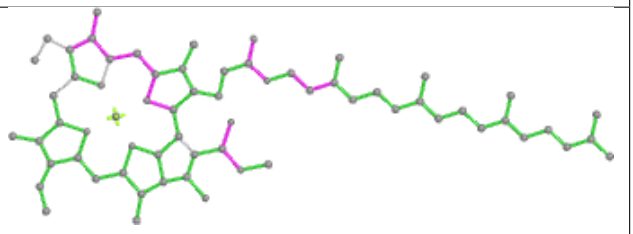
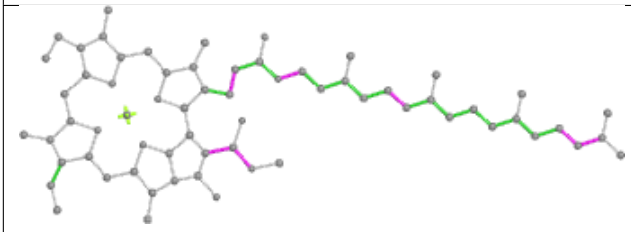


Bond angles



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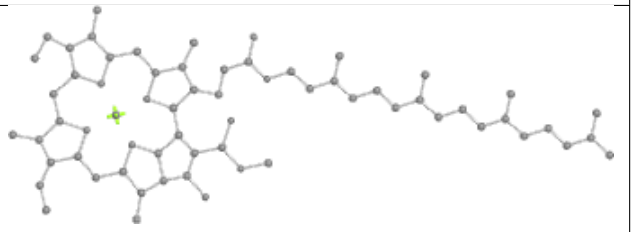
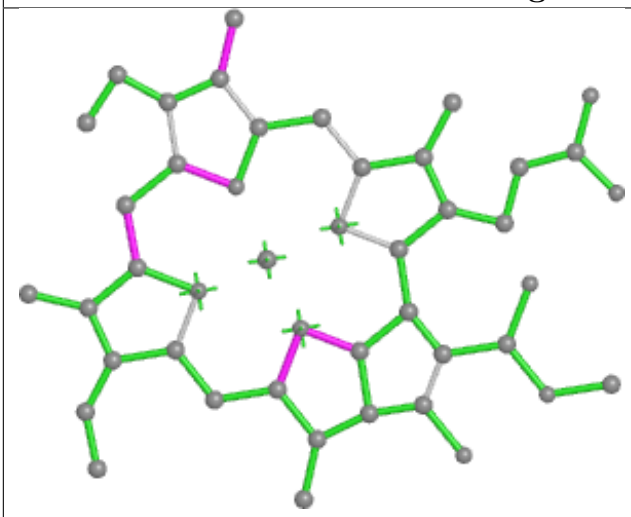


Rings

Ligand CLA 5 612



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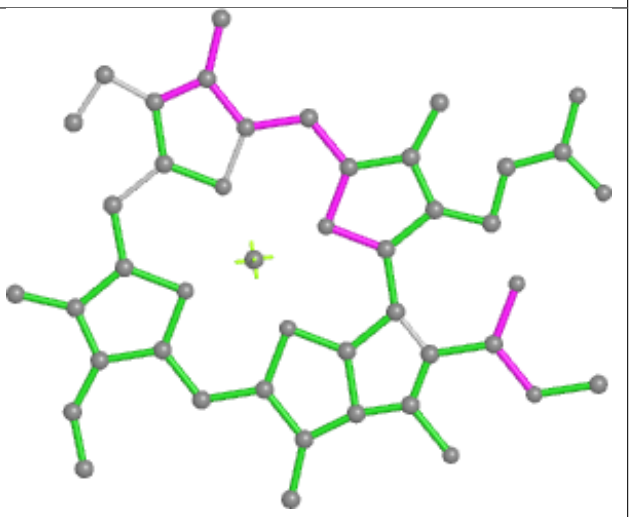

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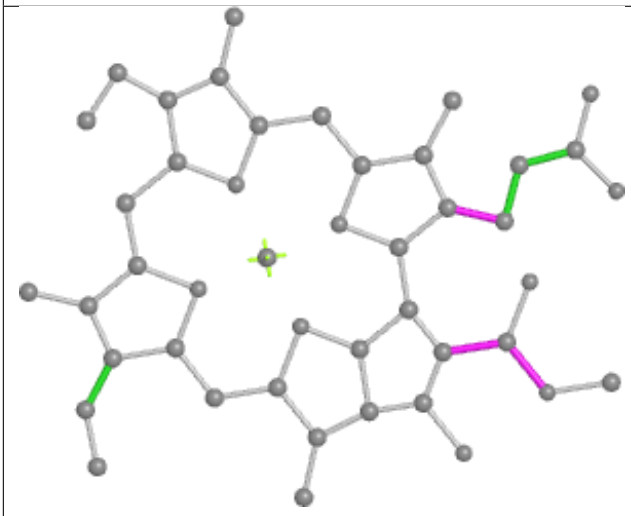

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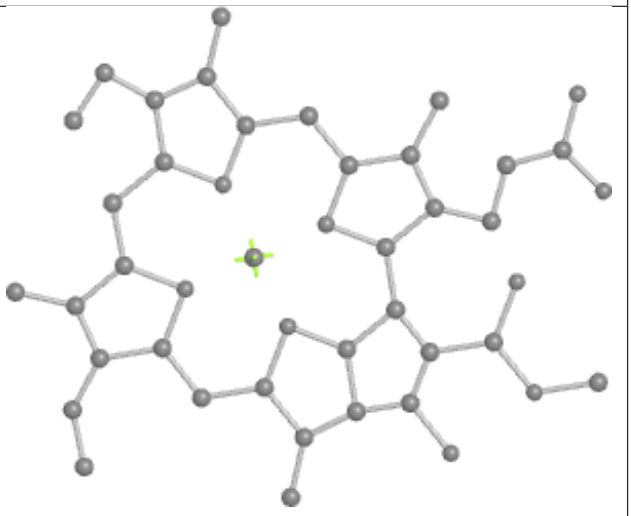
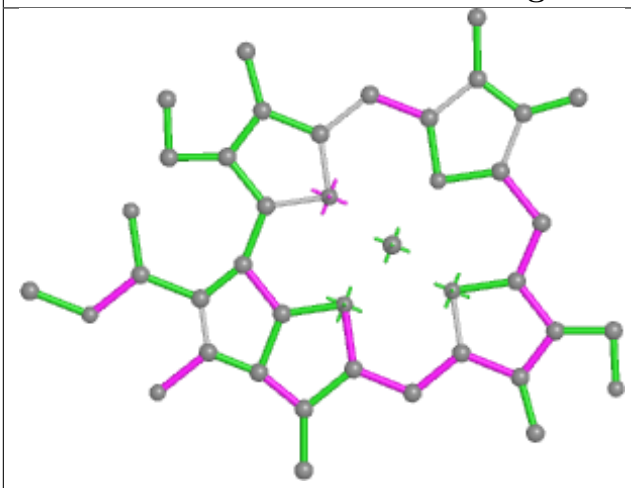


Rings

Ligand CHL 8 605



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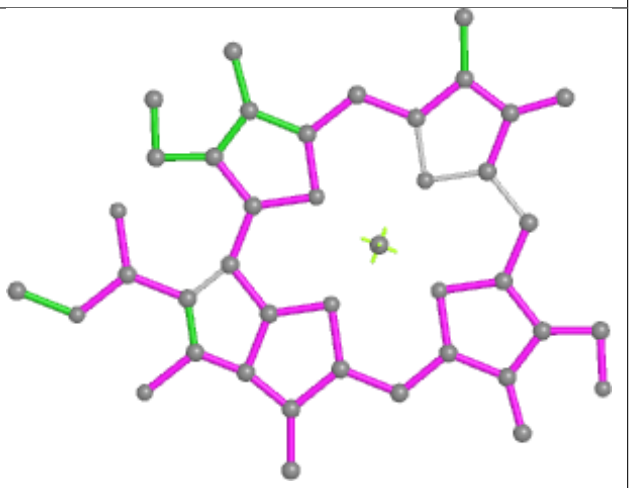

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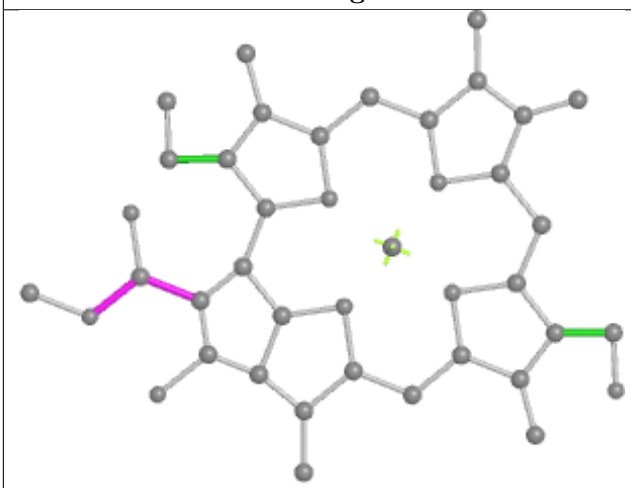

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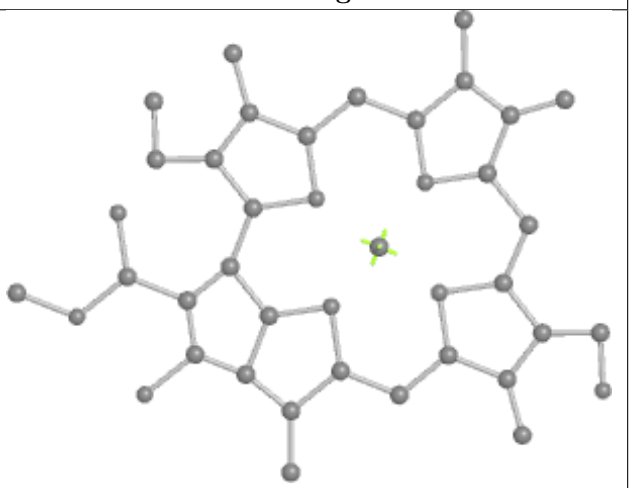
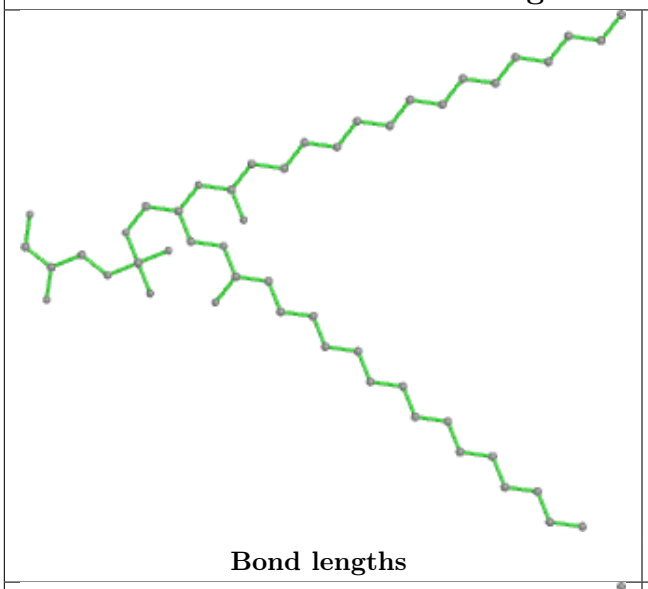


Rings

Ligand LHG b 319



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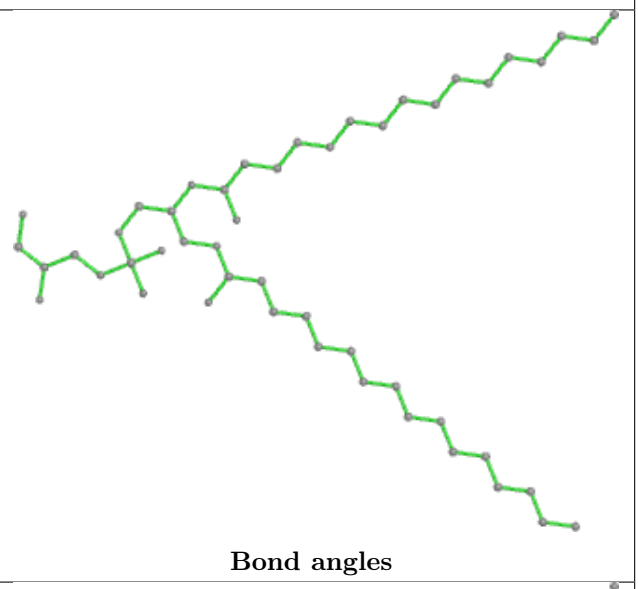

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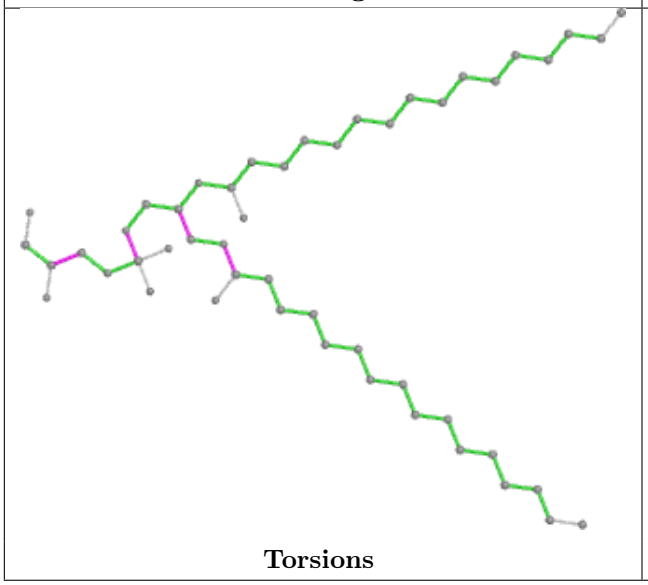

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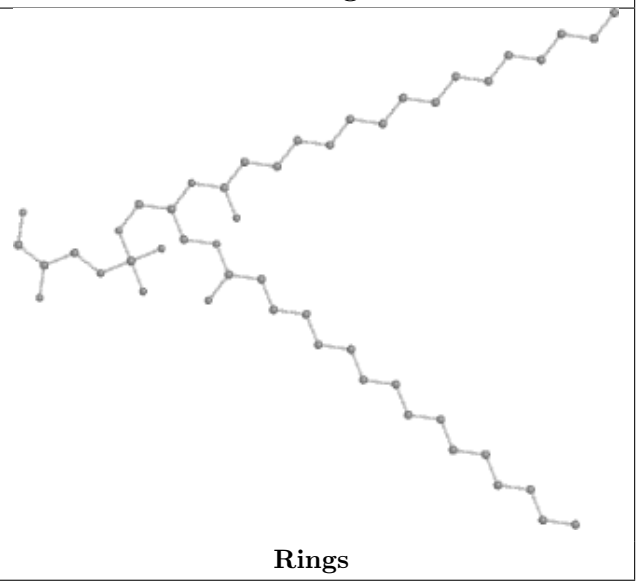
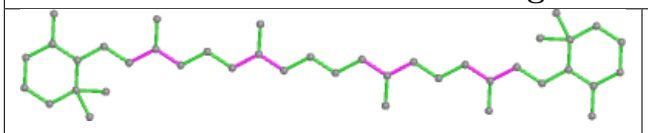


Rings

Ligand BCR 4 617



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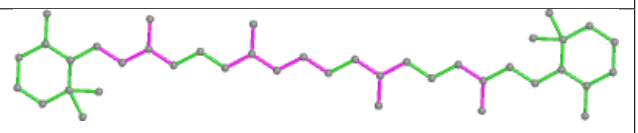

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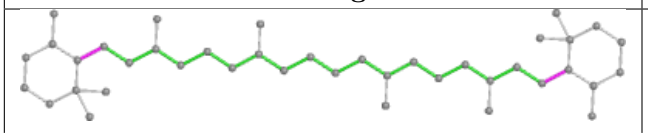

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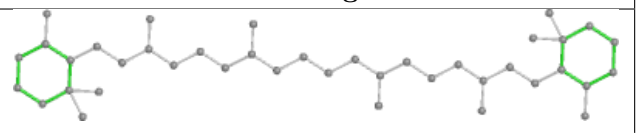
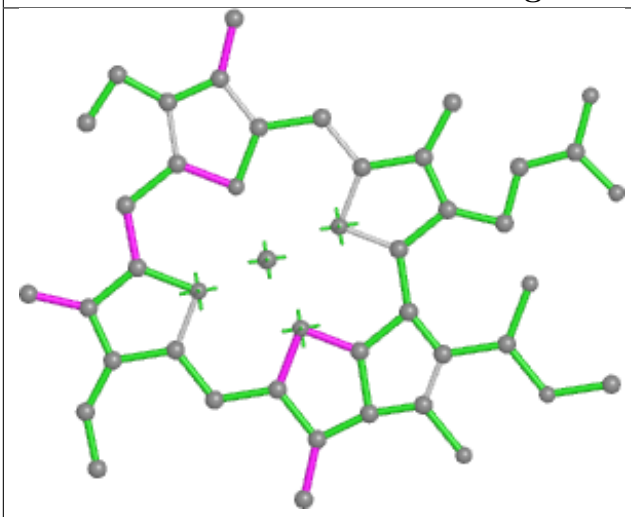


Rings

Ligand CLA B 822



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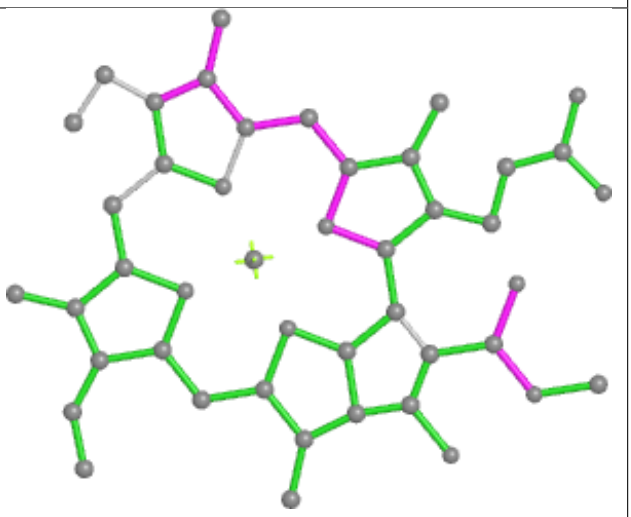
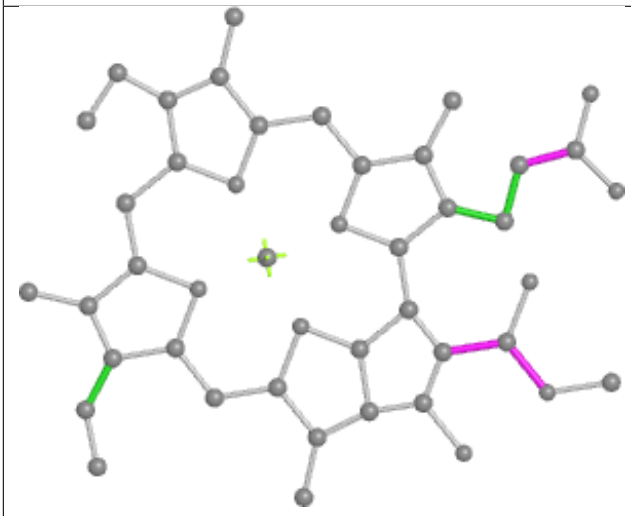


Bond angles



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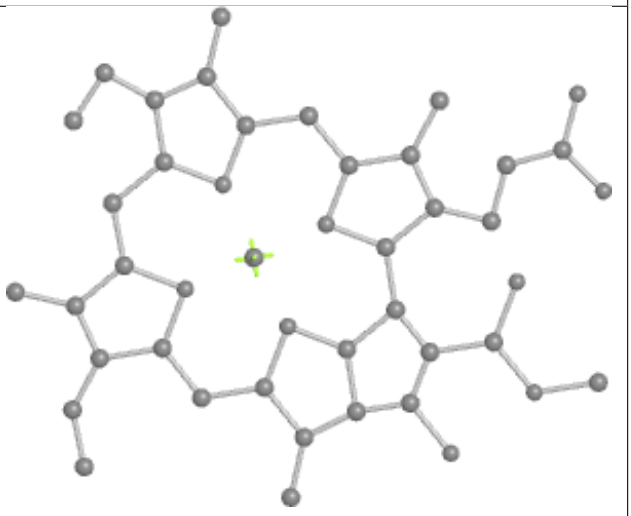

Rings

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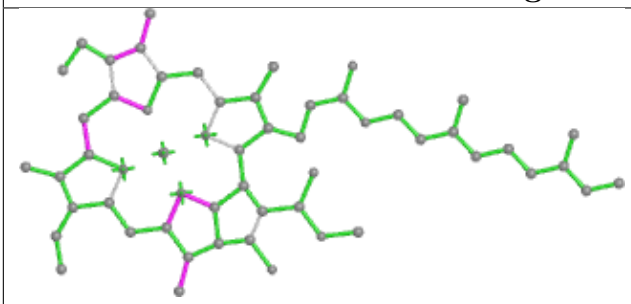

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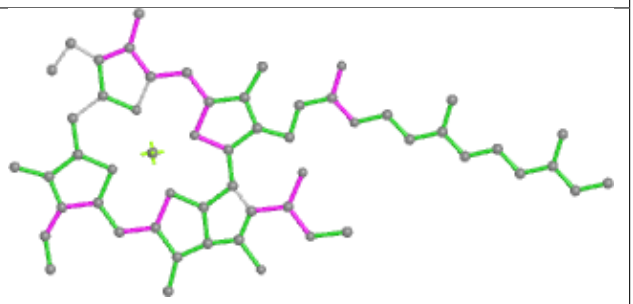
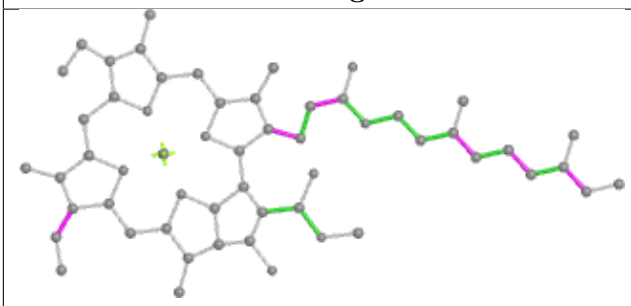


Bond angles



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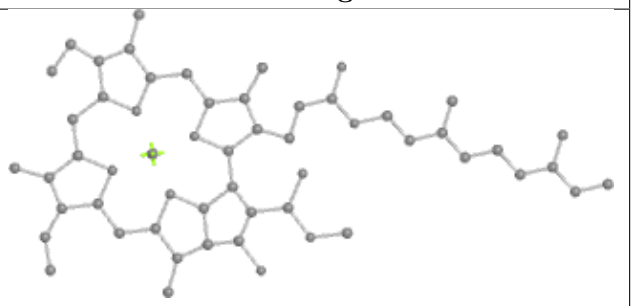
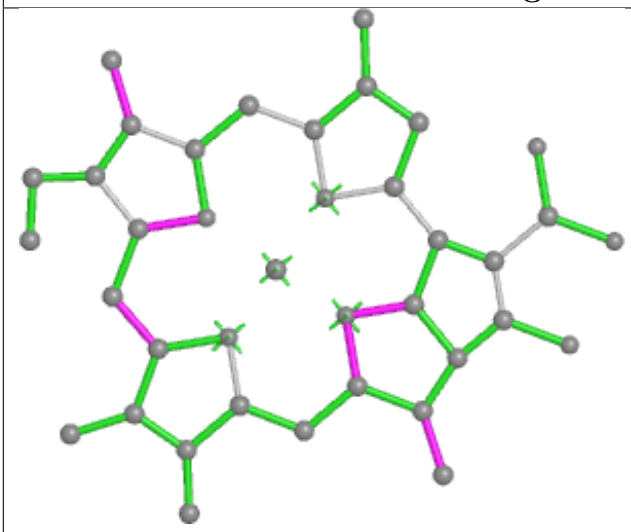


Rings

Ligand CLA O 202



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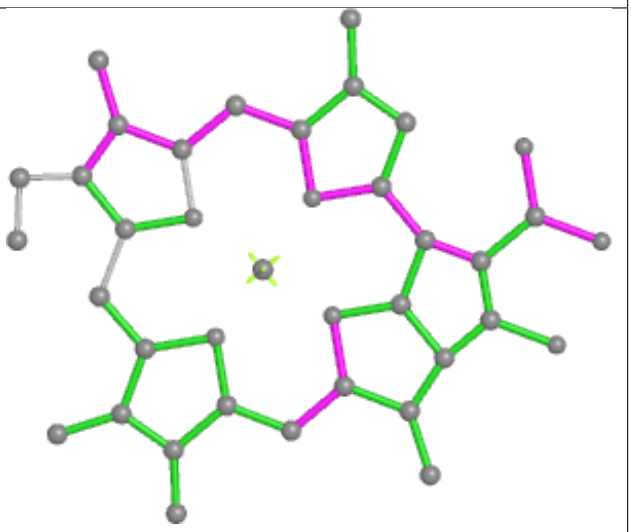
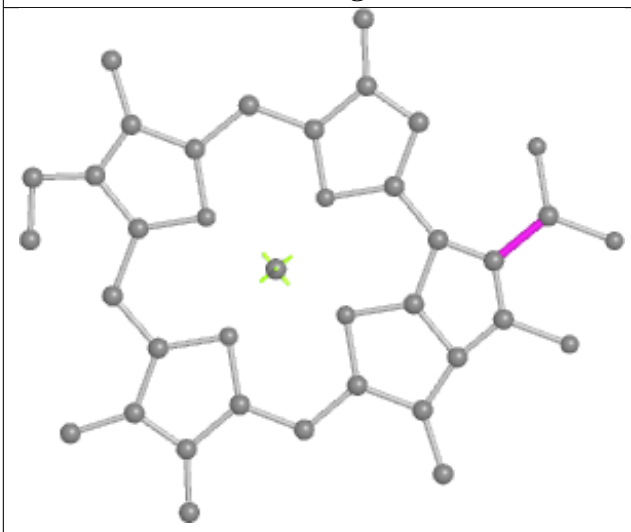


Bond angles



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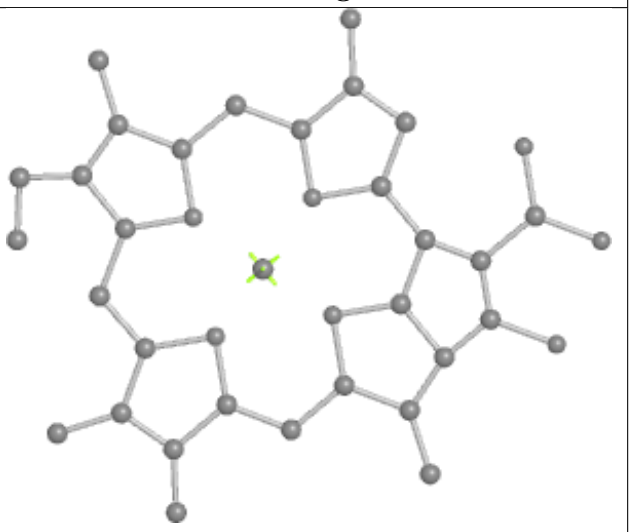
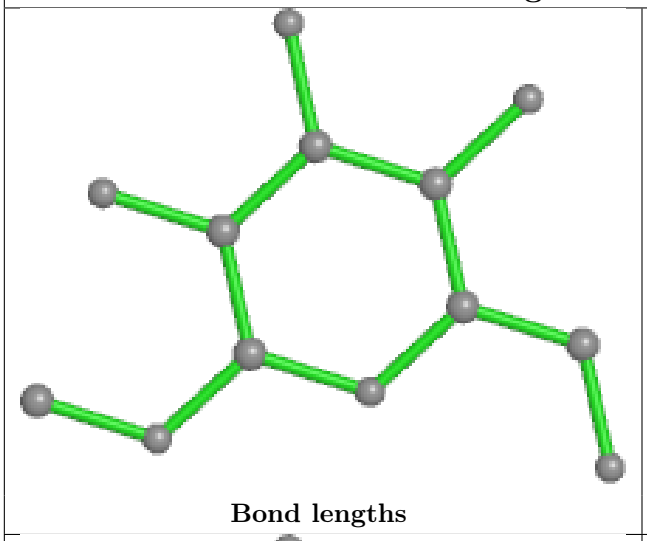


Rings

Ligand LMG 2 615



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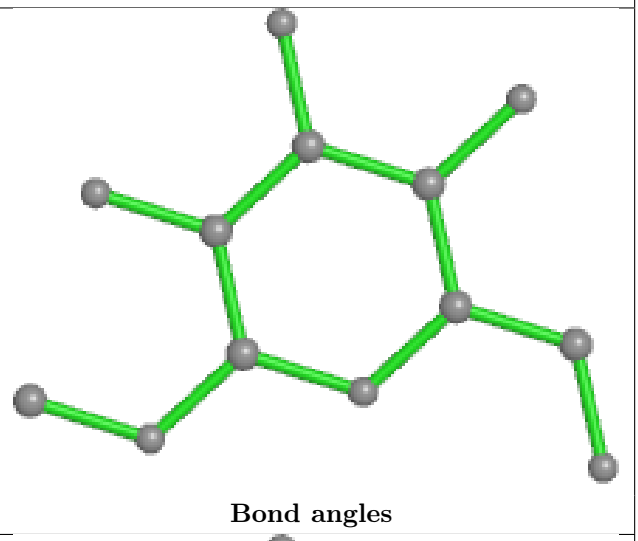
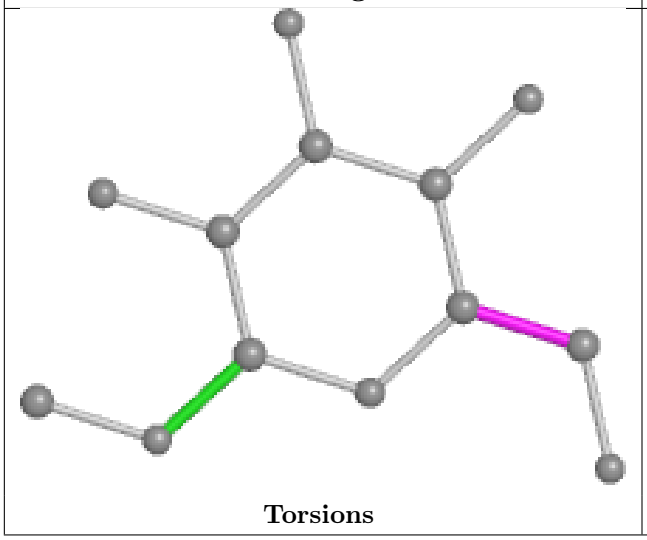


Bond angles



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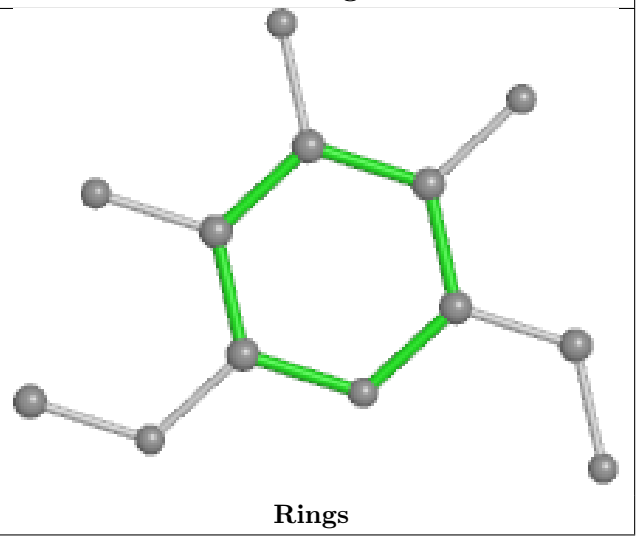
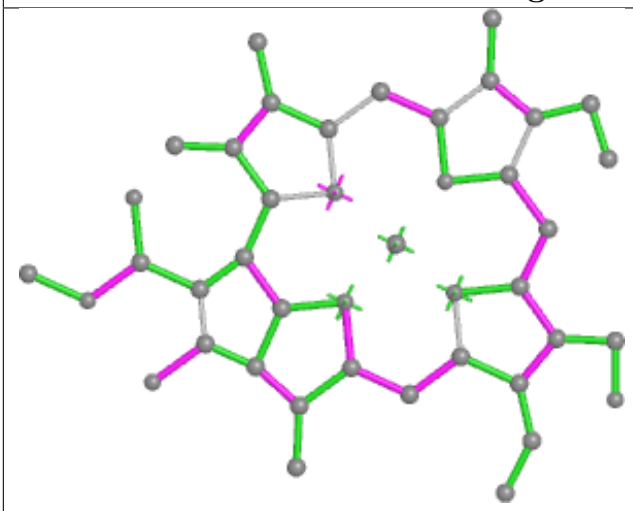


Rings

Ligand CHL 8 613



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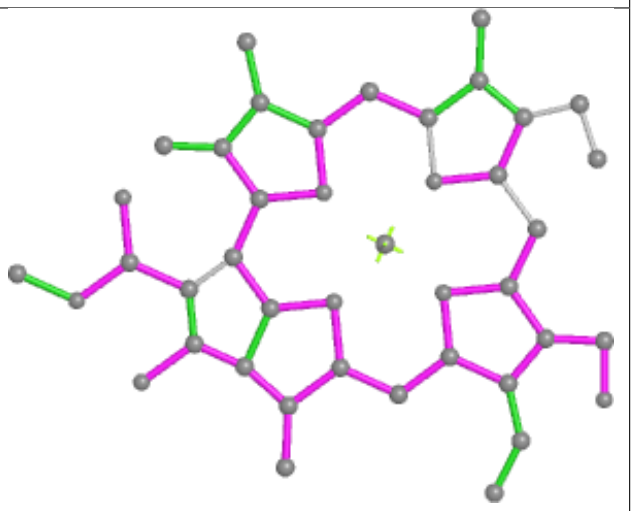
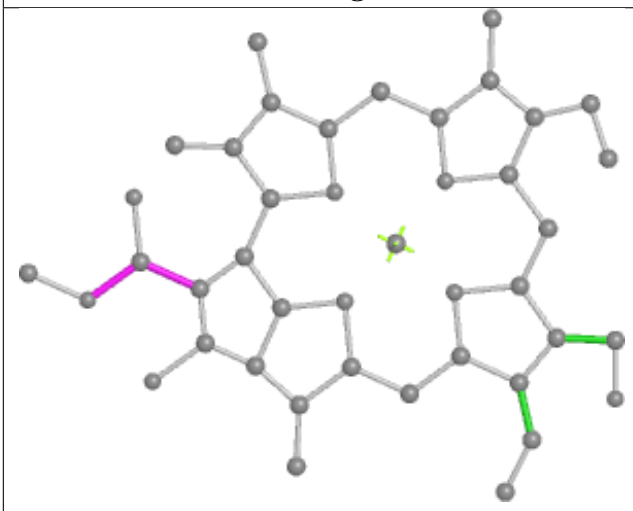
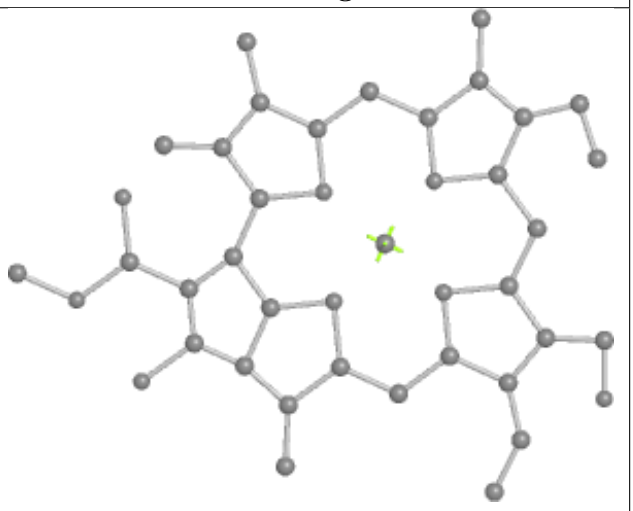


Bond angles

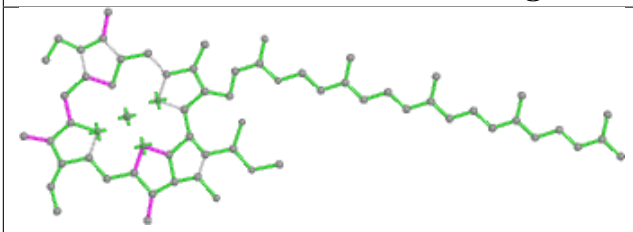


Torsions



Rings

Ligand CLA B 825



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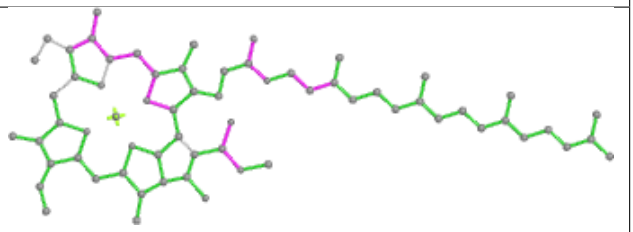

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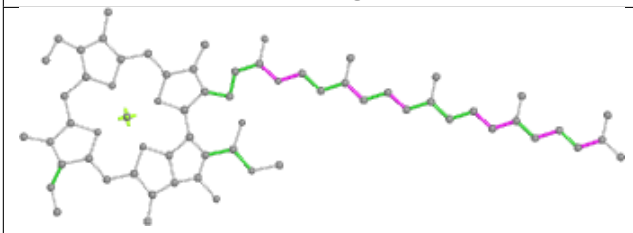

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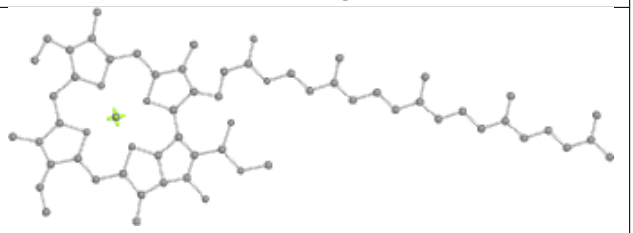
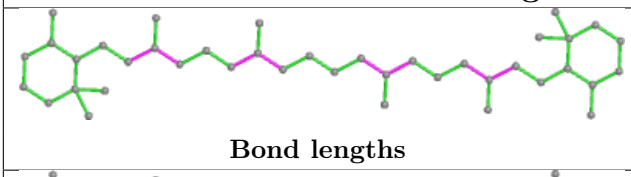


Rings

Ligand BCR O 205



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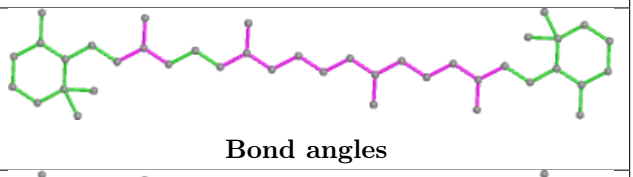

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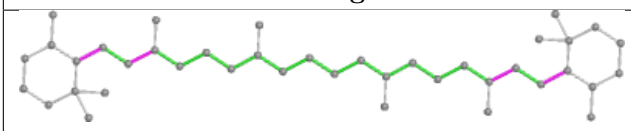

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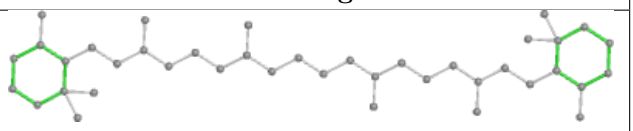
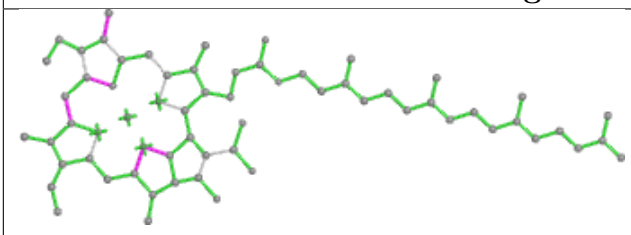


Rings

Ligand CLA A 827



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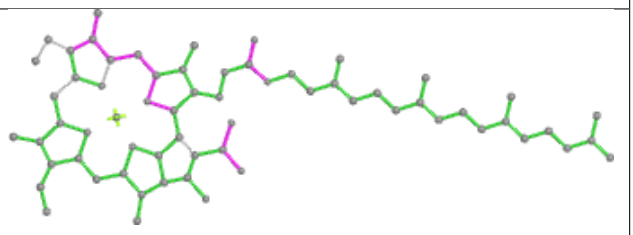

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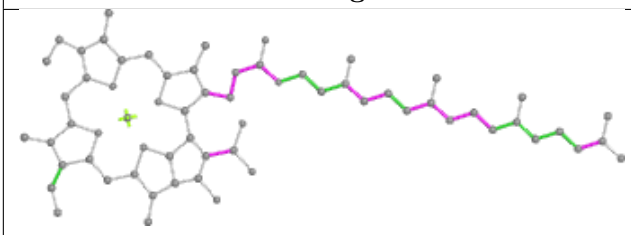

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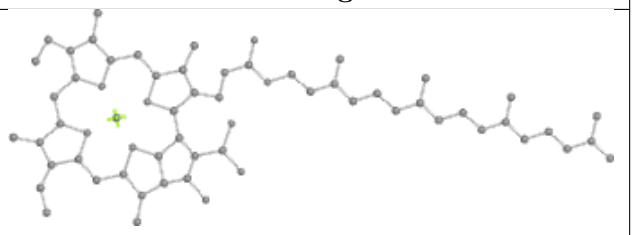
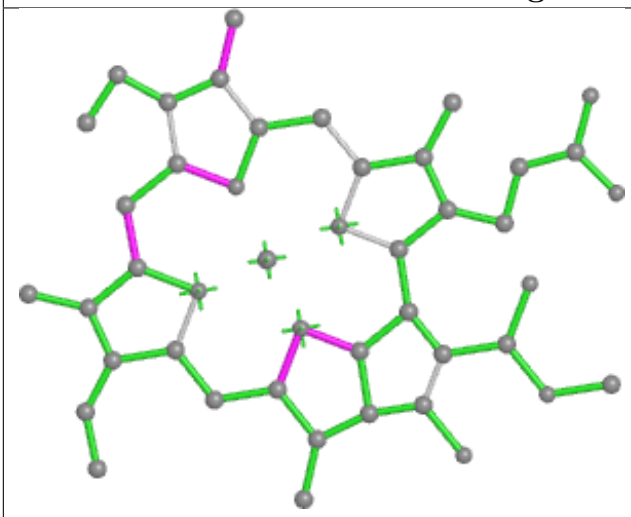


Rings

Ligand CLA b 312



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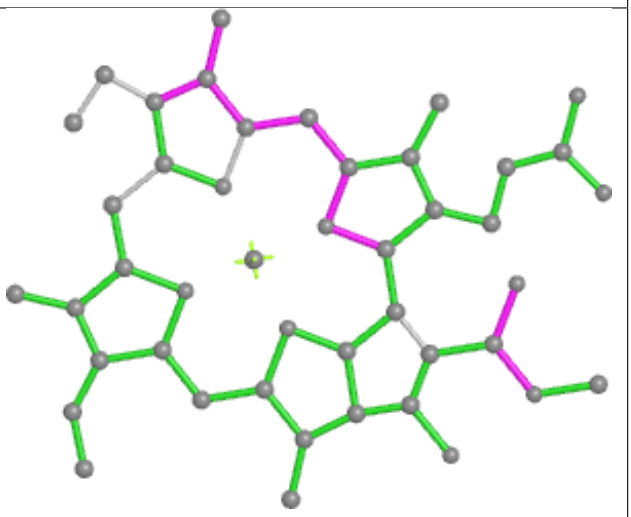

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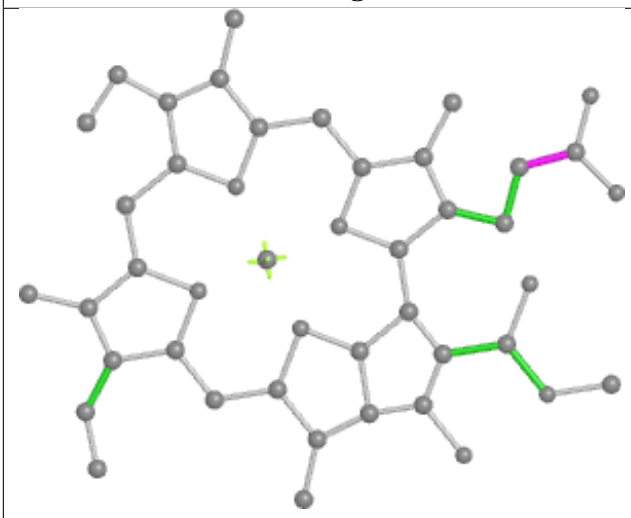

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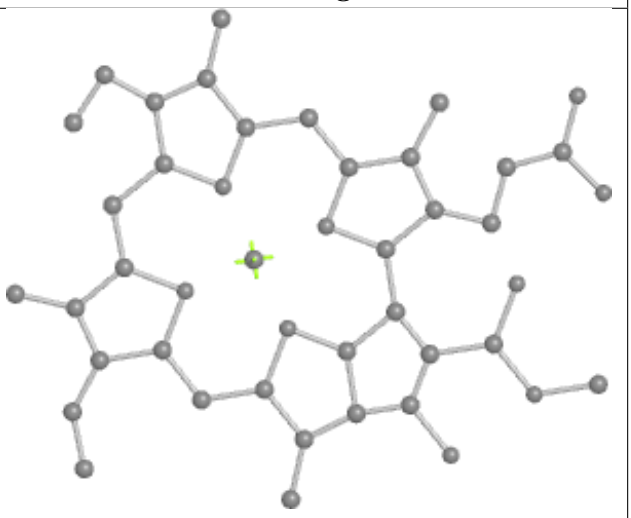
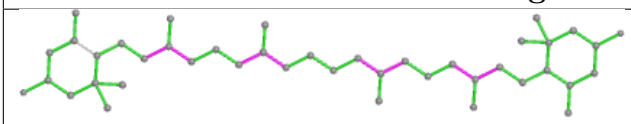


Rings

Ligand LUT 2 616



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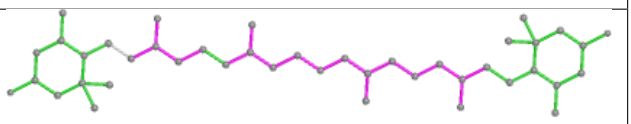

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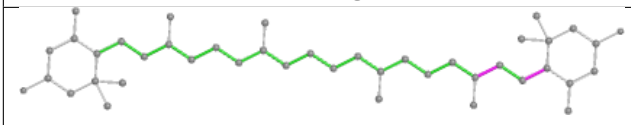
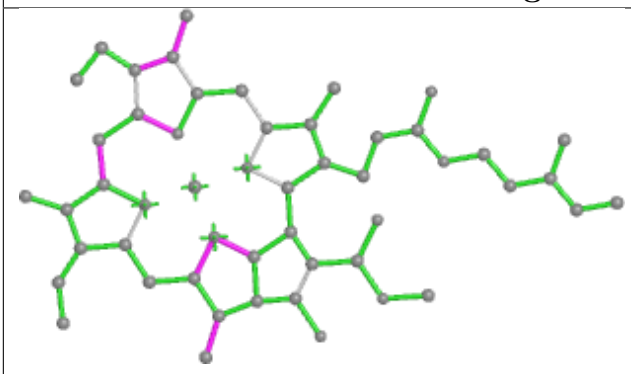


Torsions

Rings

Ligand CLA A 837



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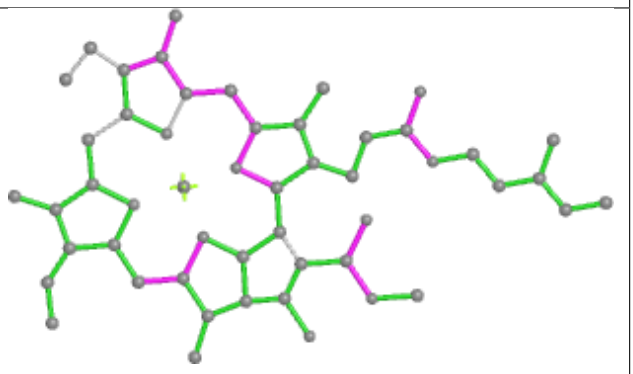

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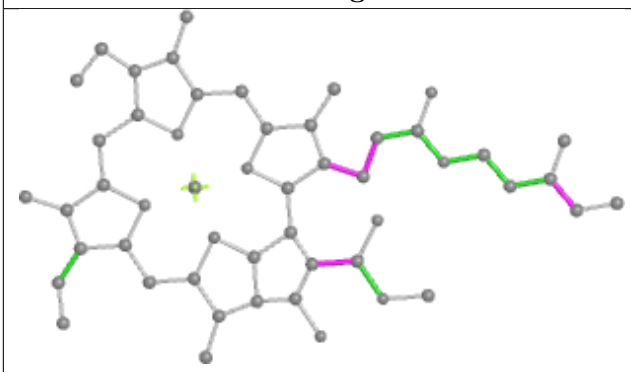

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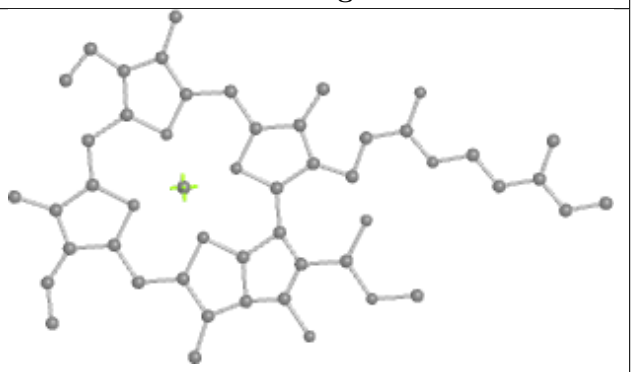
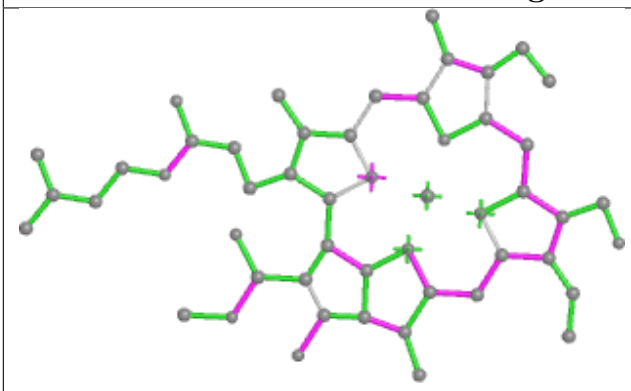


Rings

Ligand CHL 6 607



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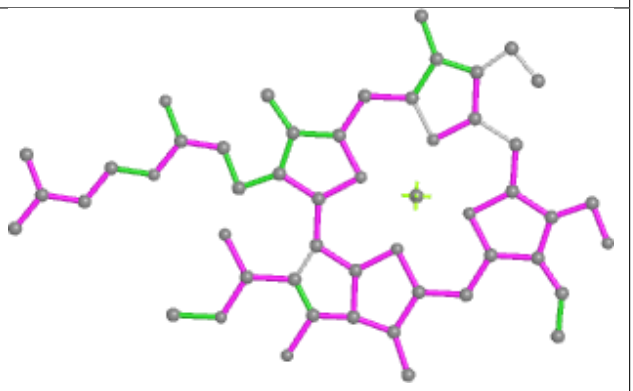

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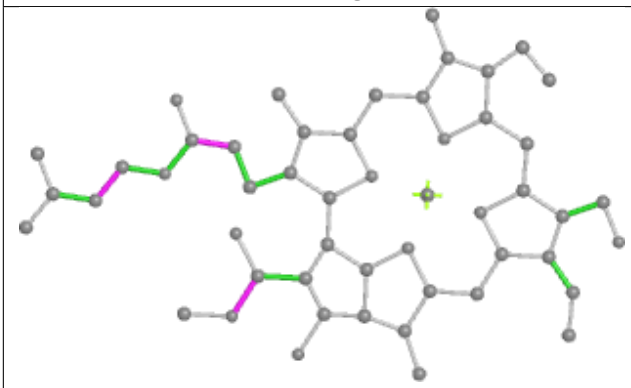

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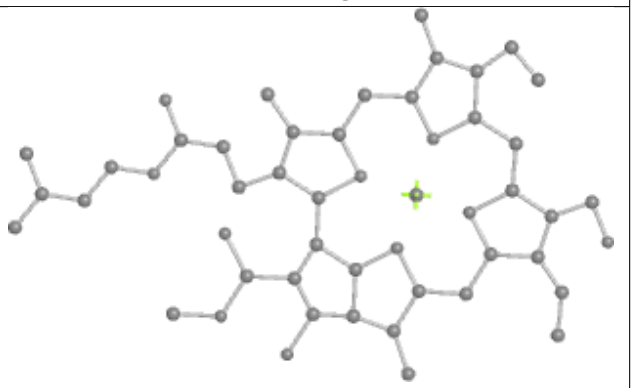
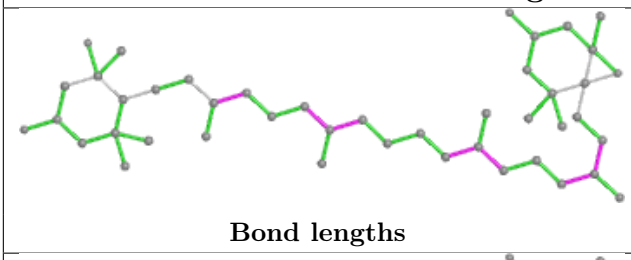


Rings

Ligand NEX 9 617



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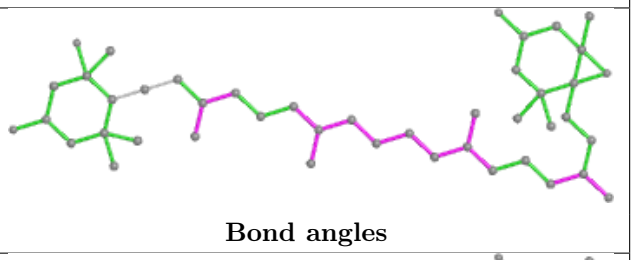

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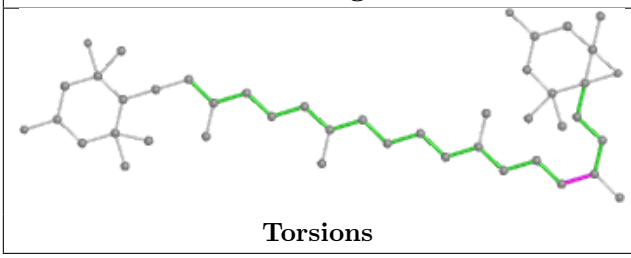

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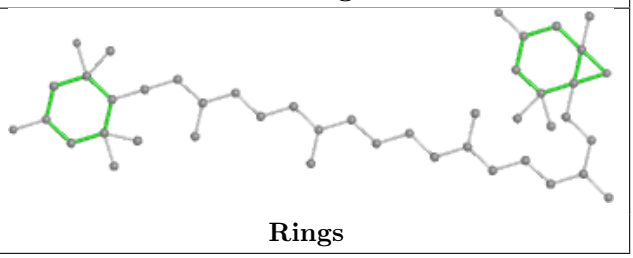
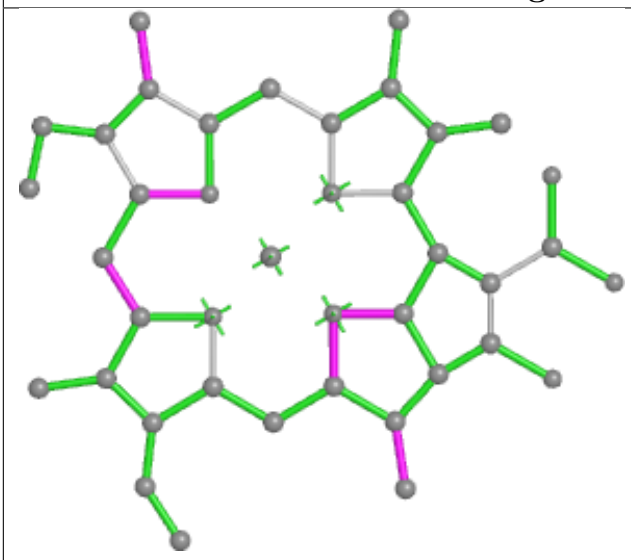


Rings

Ligand CLA 3 415



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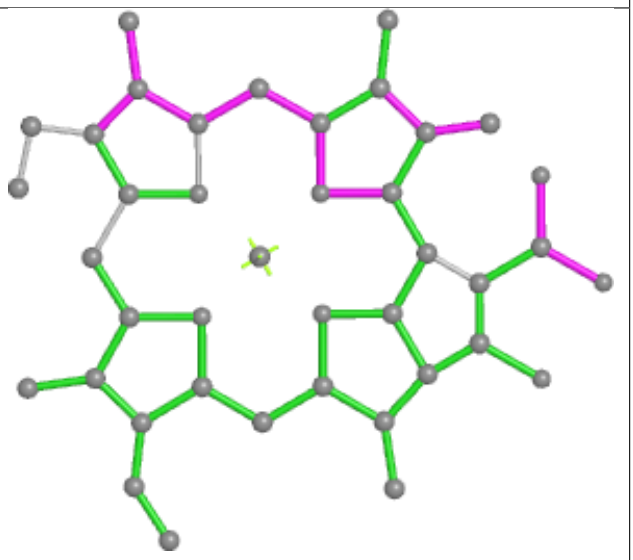
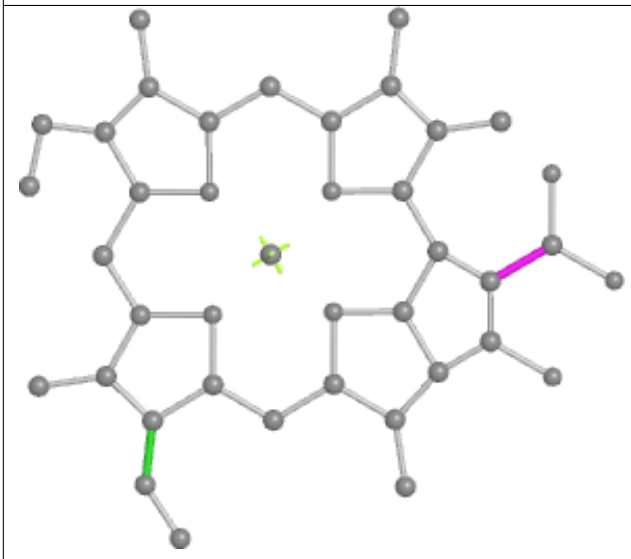


Bond angles



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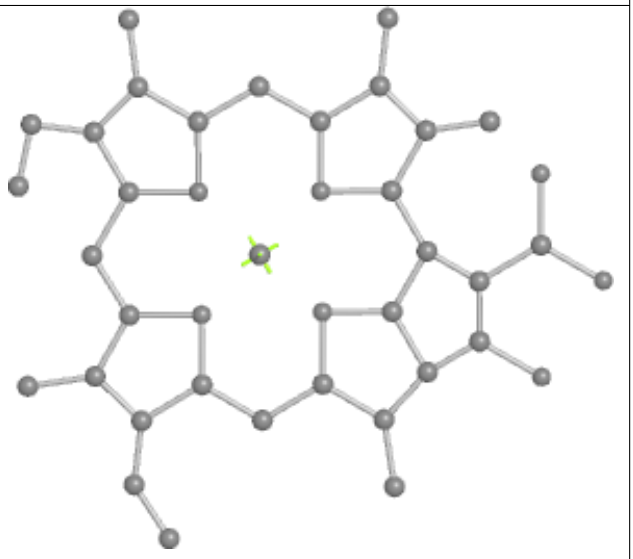
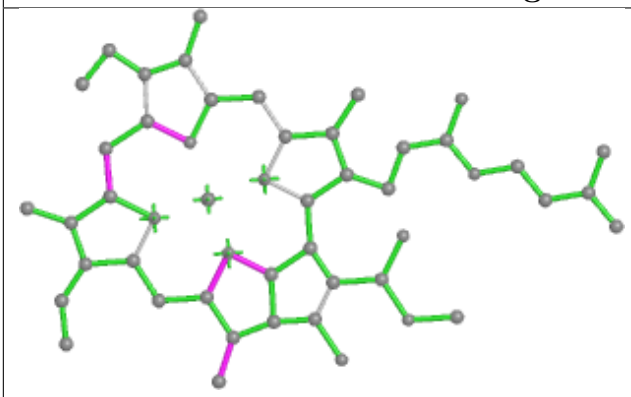
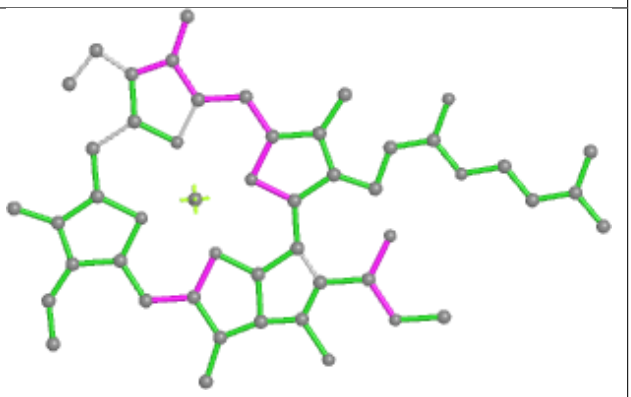
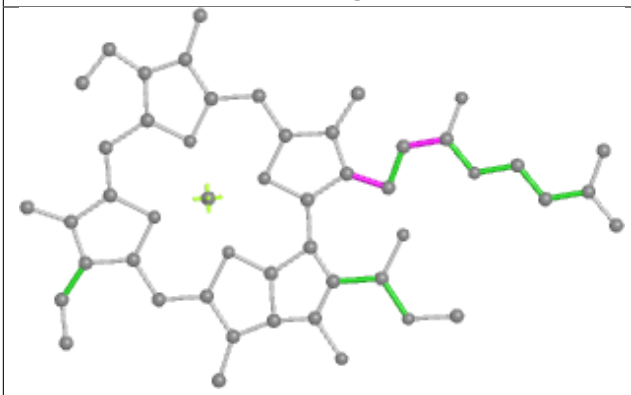
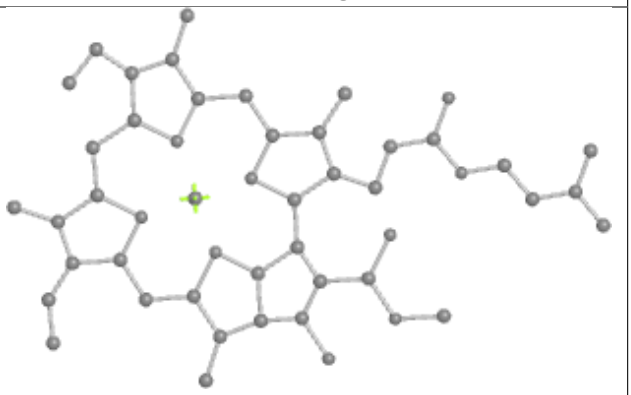
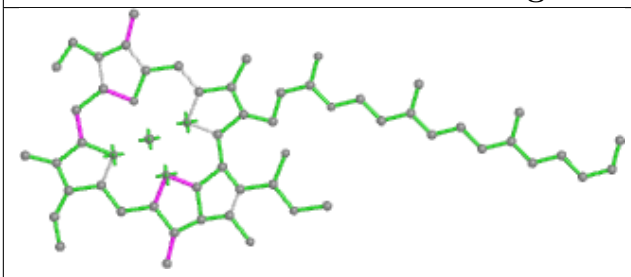
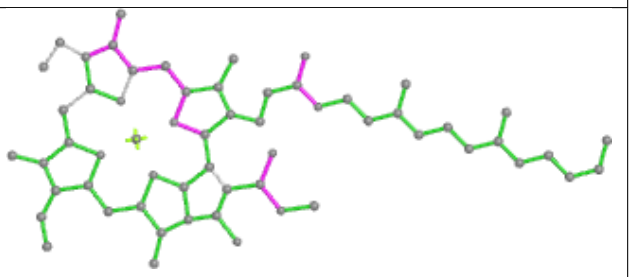
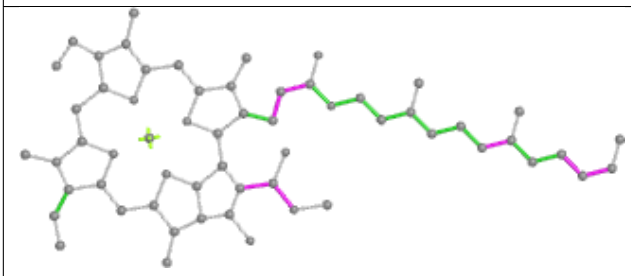
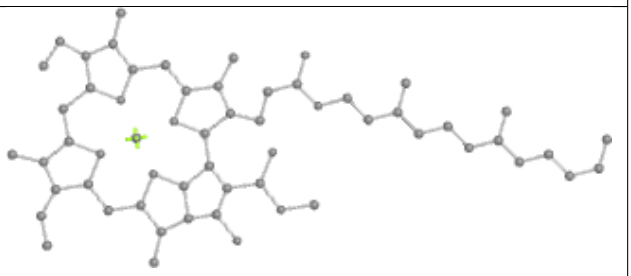
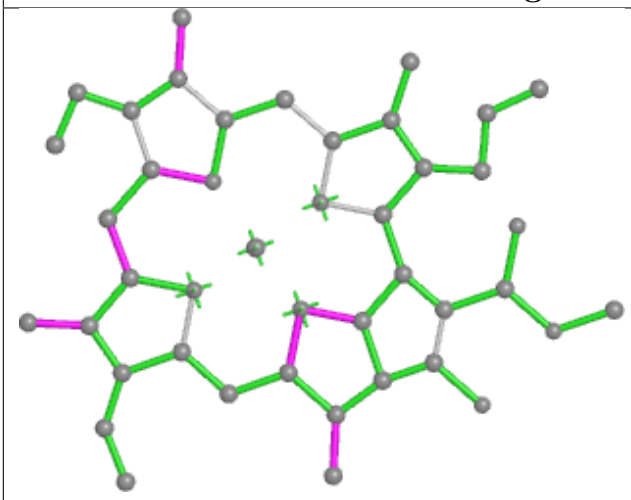


Rings

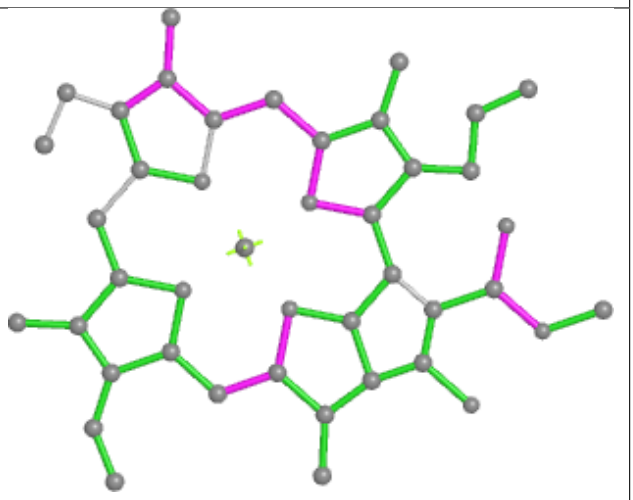
Ligand CLA A 835	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA b 303	
	
Bond lengths	Bond angles
	
Torsions	Rings

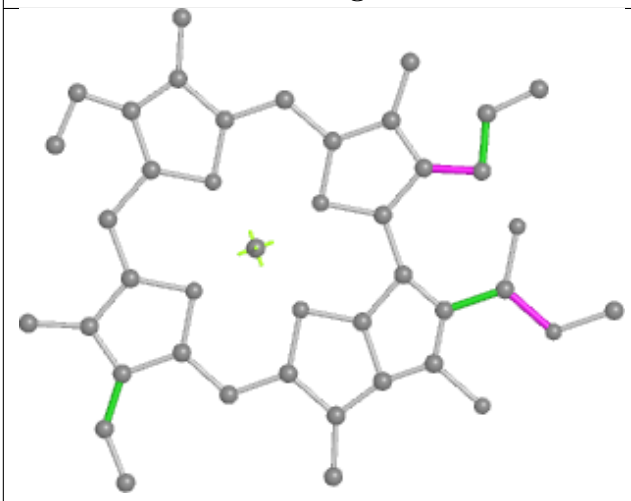
Ligand CLA B 819



Bond lengths



Bond angles



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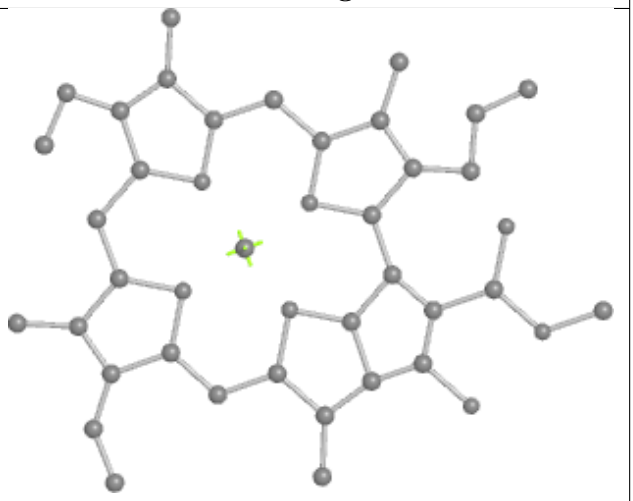
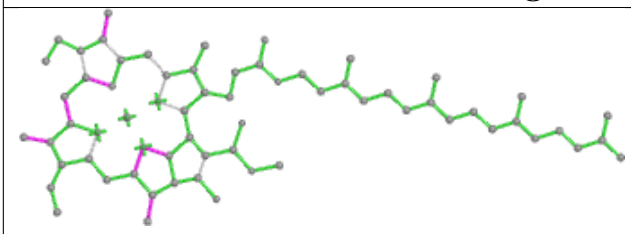
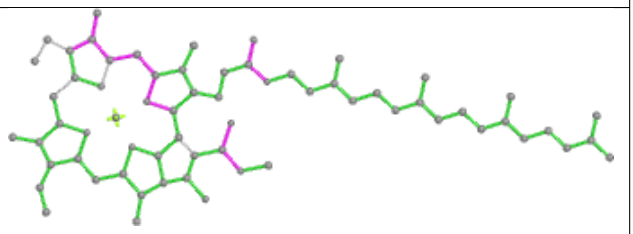


Rings

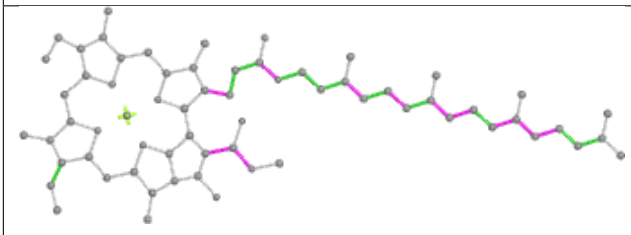
Ligand CLA B 802



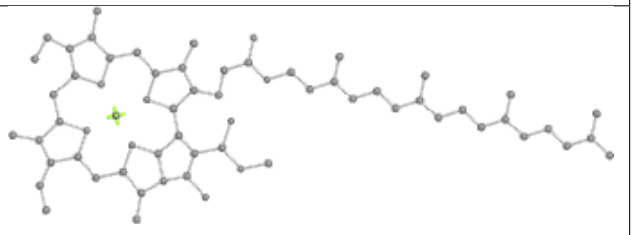
Bond lengths



Bond angles

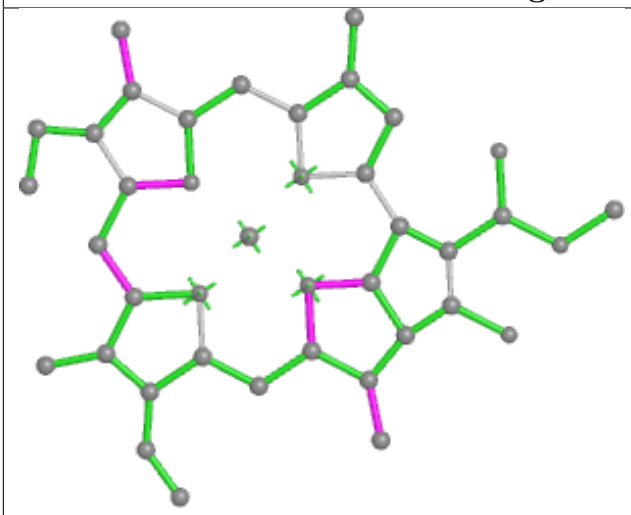


Torsions



Rings

Ligand CLA 1 306



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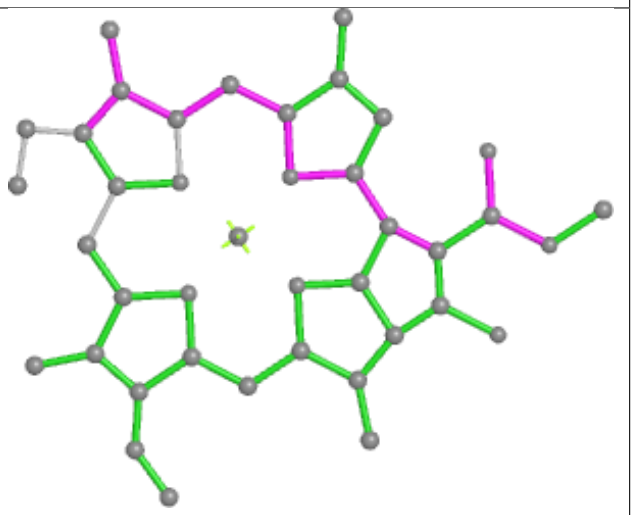

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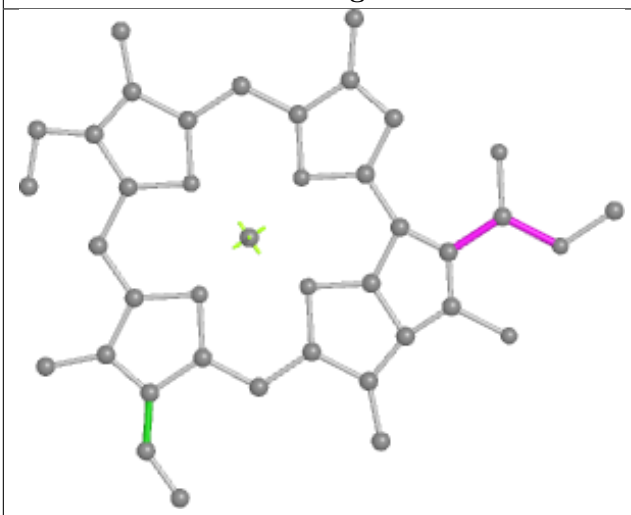

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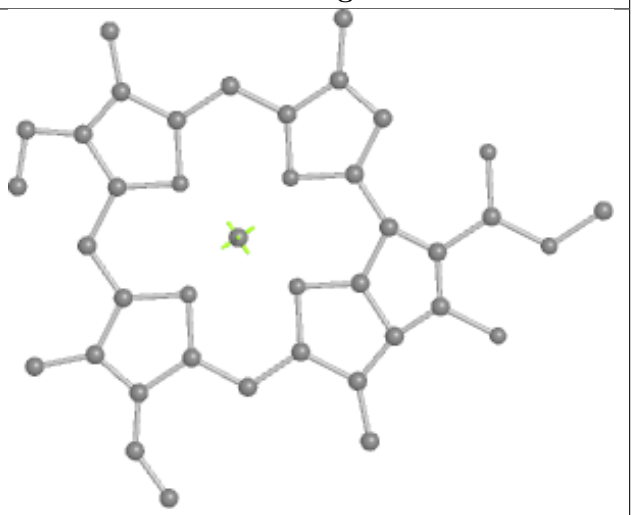
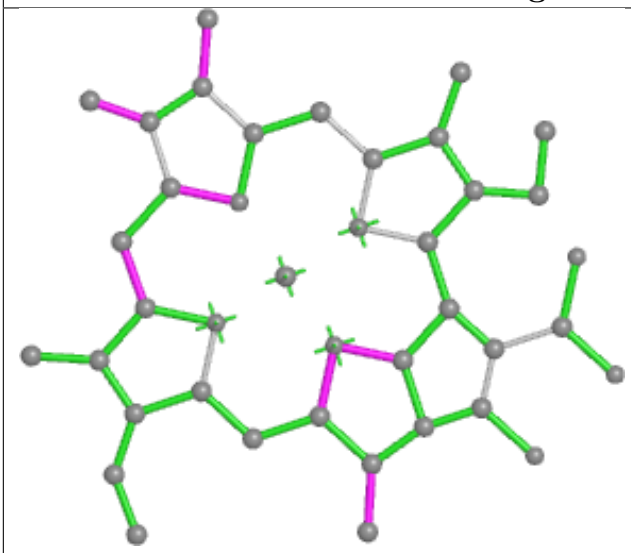


Rings

Ligand CLA 3 406



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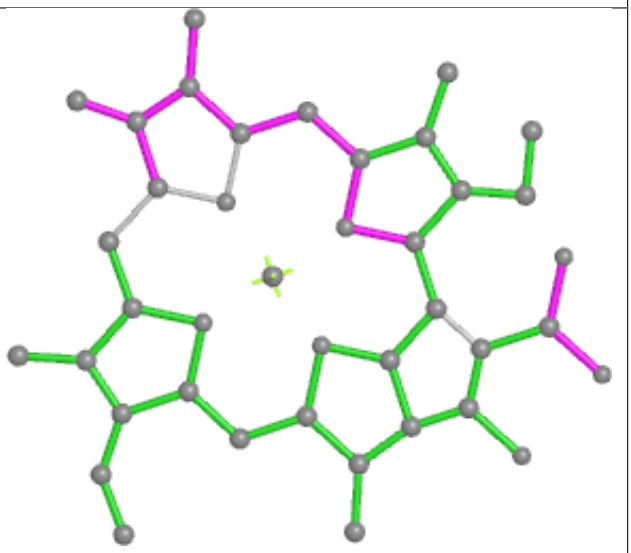

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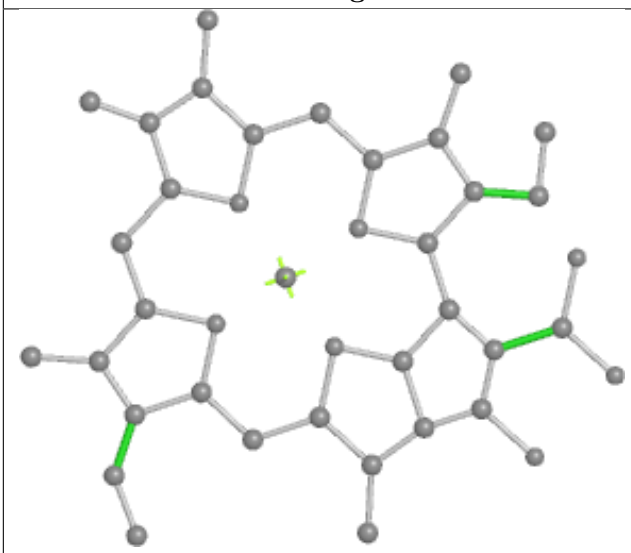

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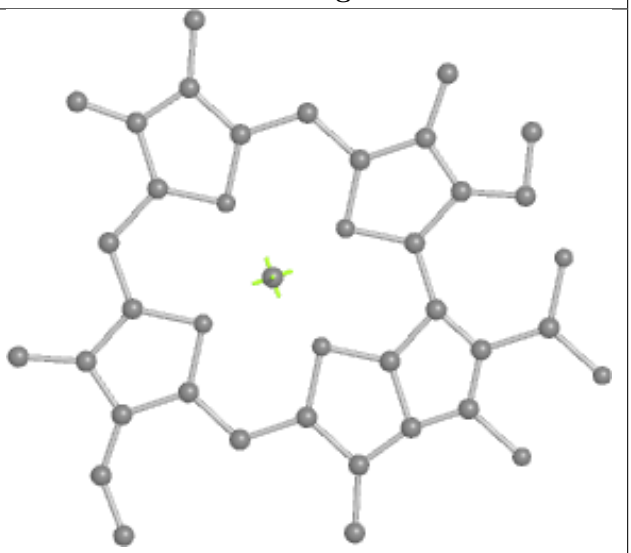
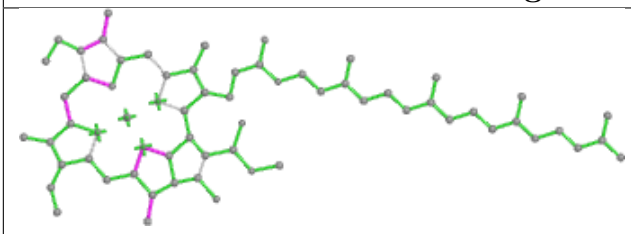


Rings

Ligand CLA B 839



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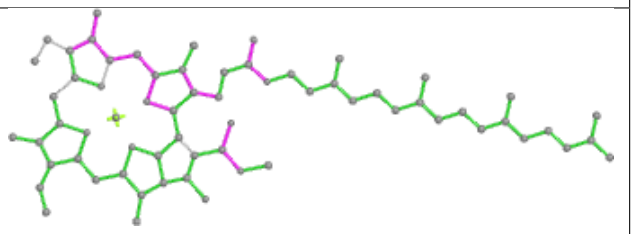

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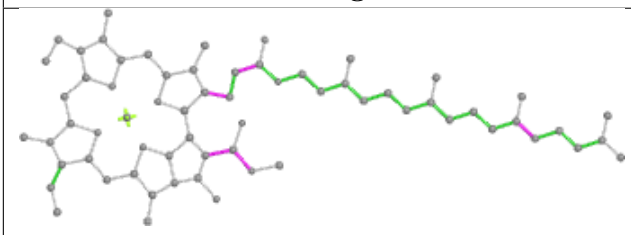

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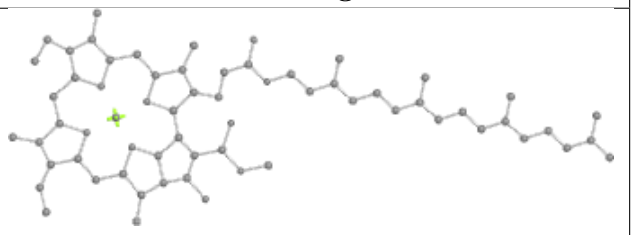
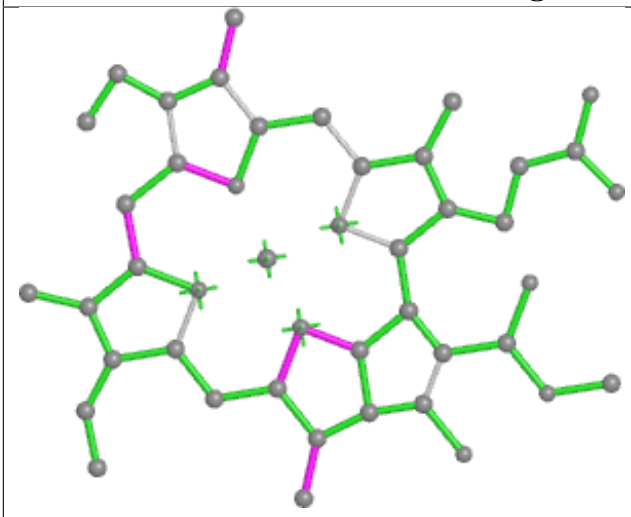


Rings

Ligand CLA 1 313



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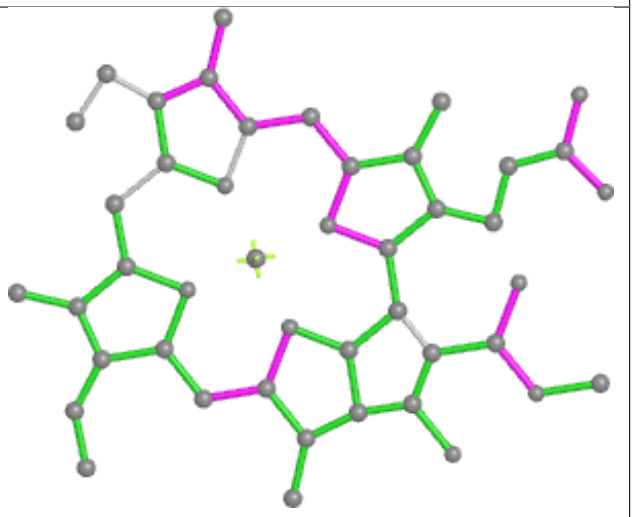

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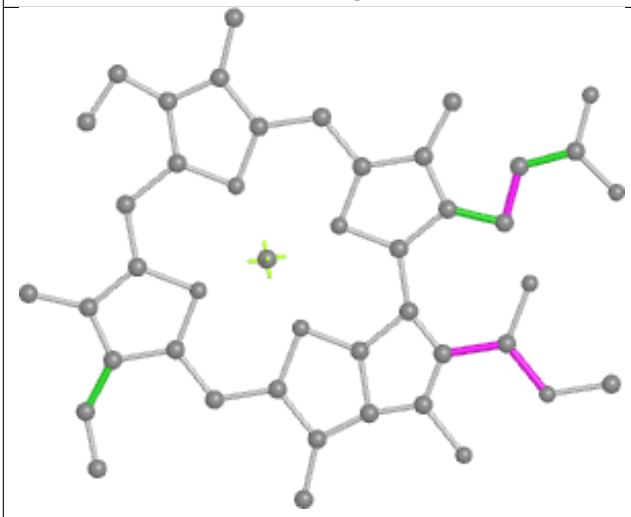

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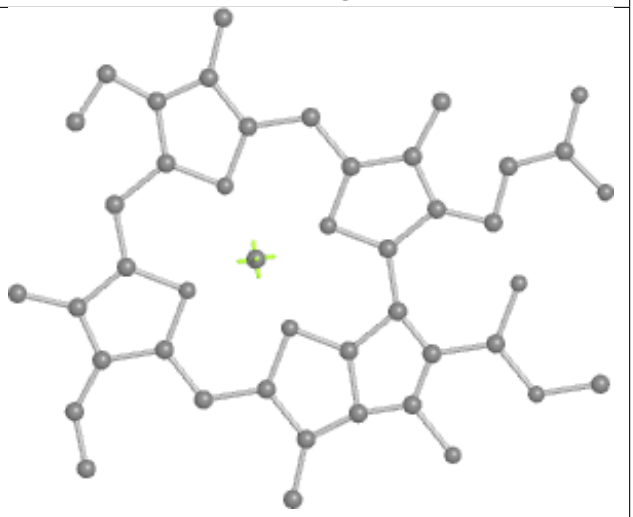
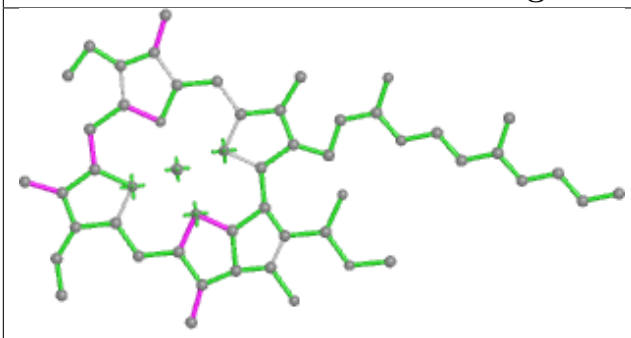


Rings

Ligand CLA b 314



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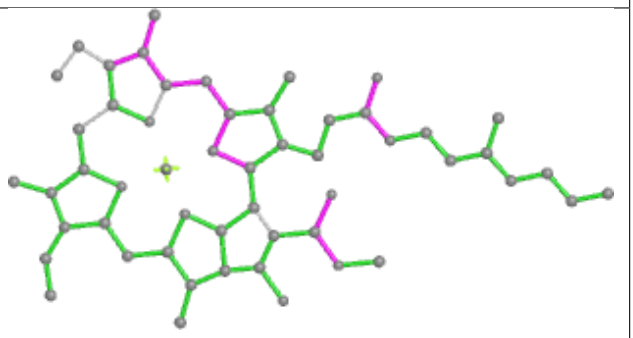

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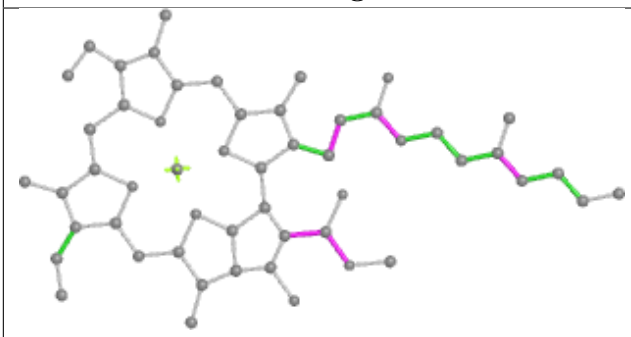

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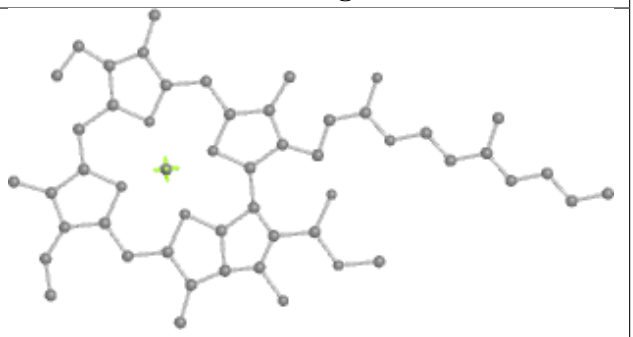
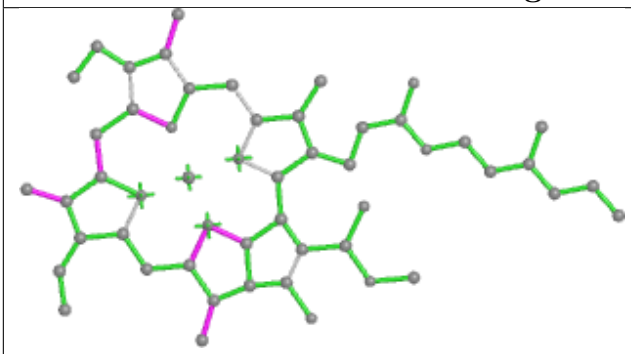


Rings

Ligand CLA B 828



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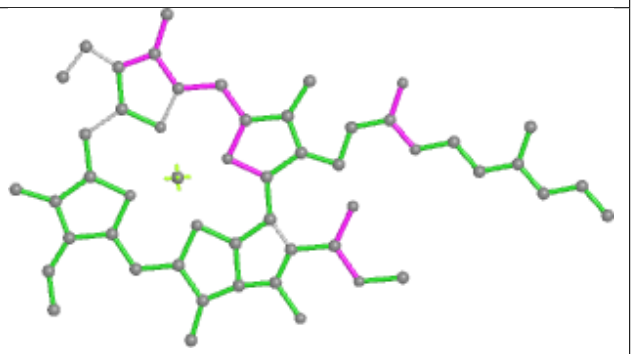
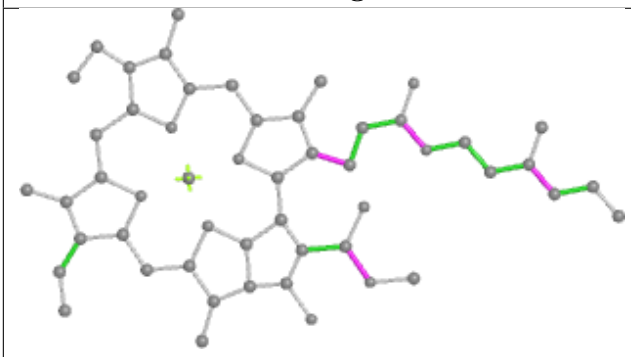


Bond angles



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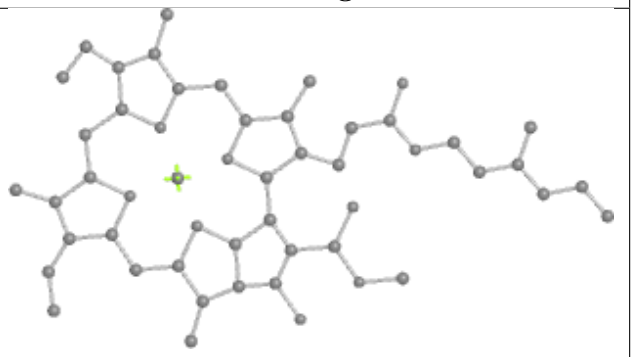
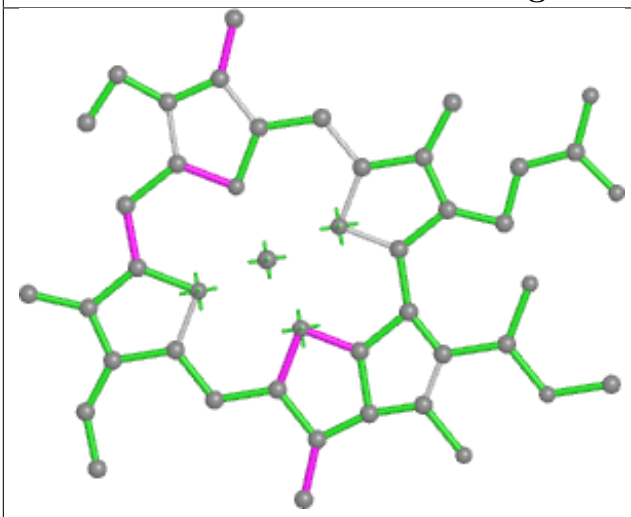


Rings

Ligand CLA 2 604



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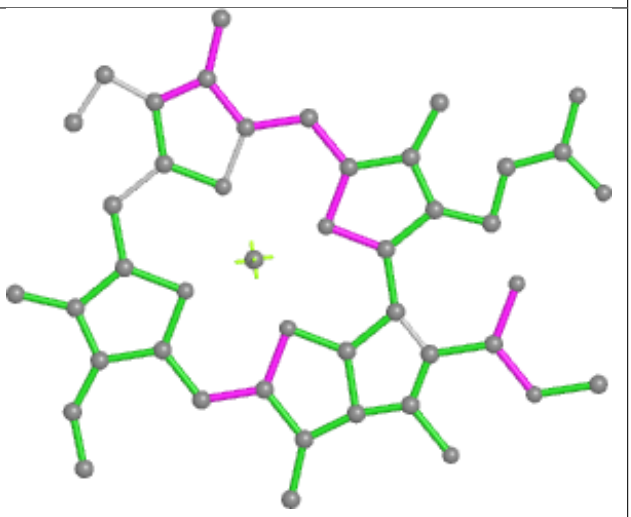
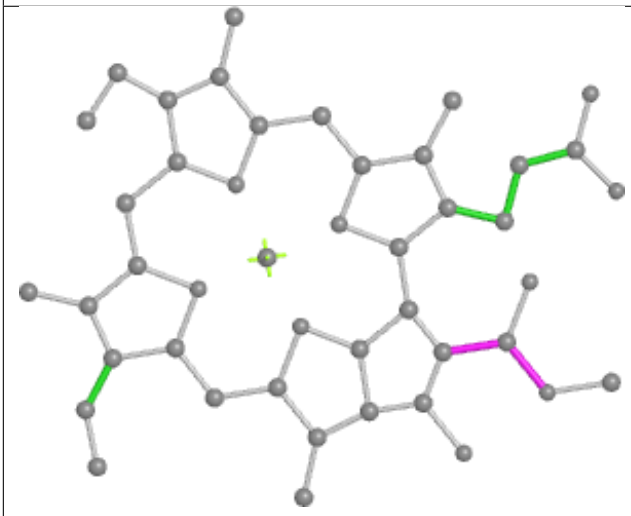


Bond angles



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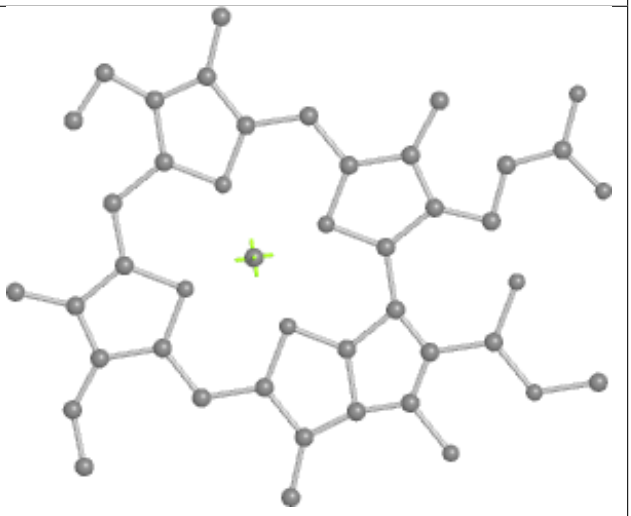
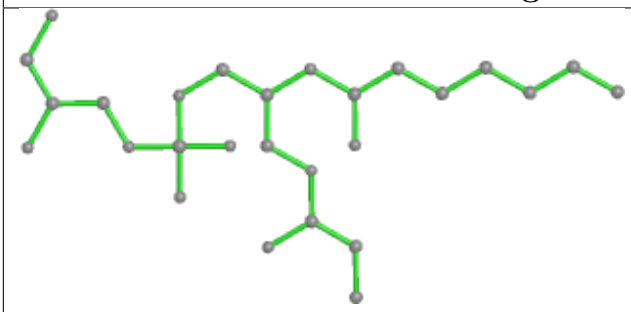


Rings

Ligand LHG A 845



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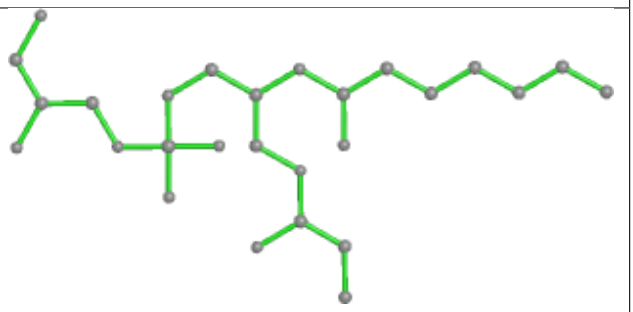
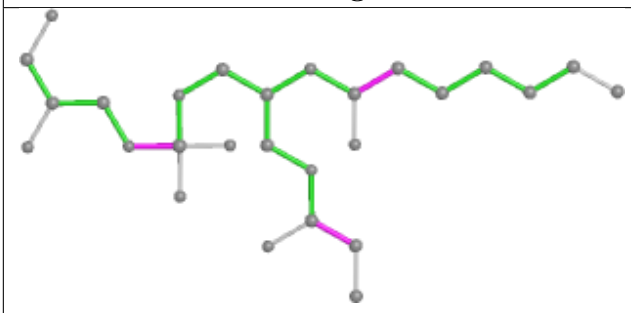


Bond angles



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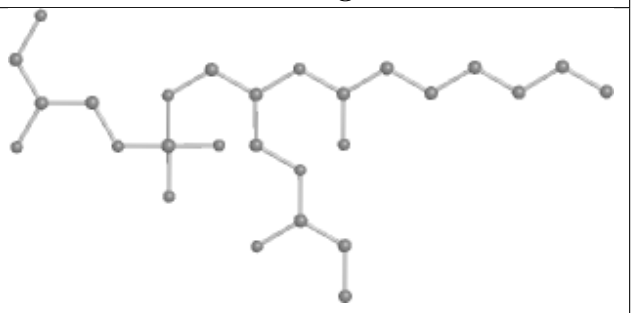
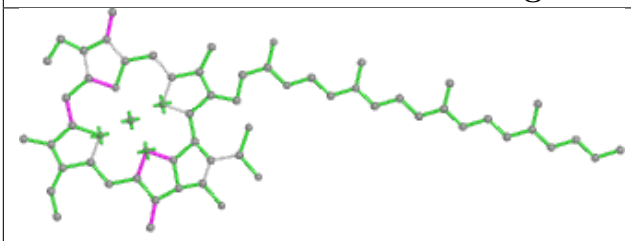


Rings

Ligand CLA B 809



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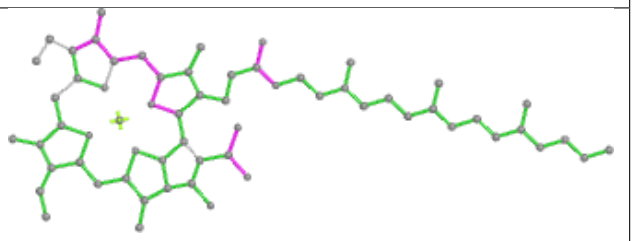
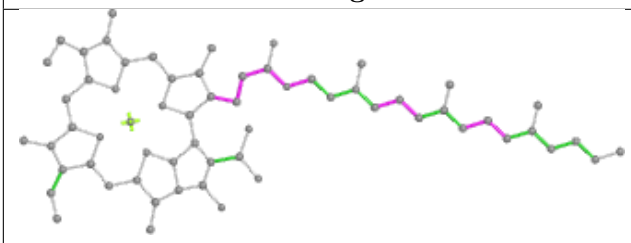


Bond angles



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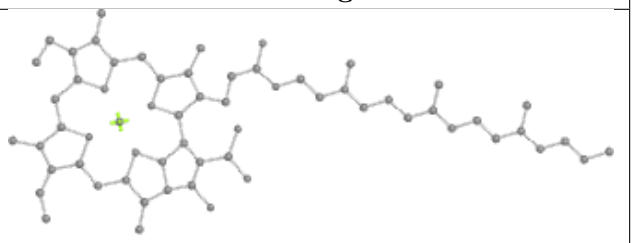
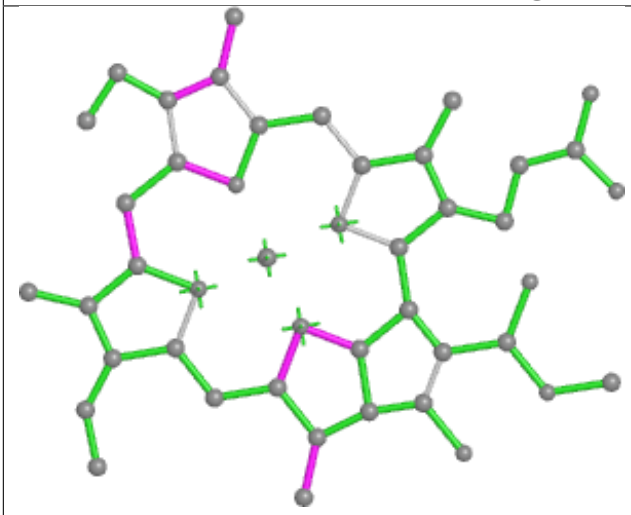


Rings

Ligand CLA 5 603



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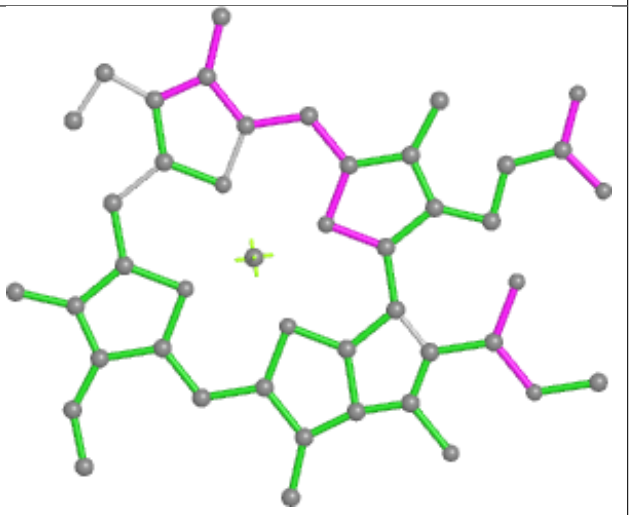

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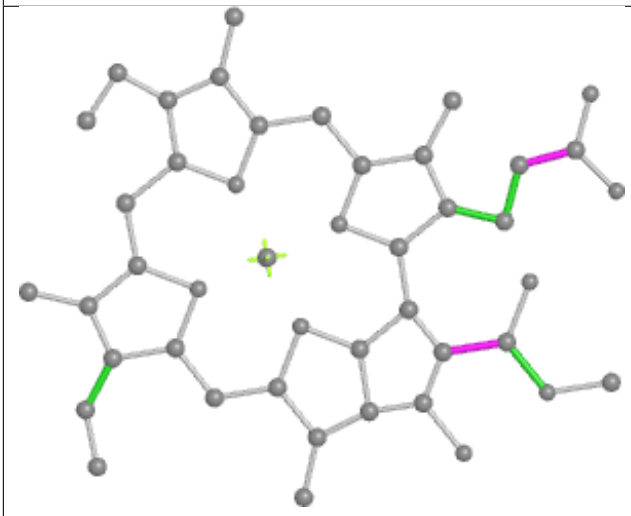

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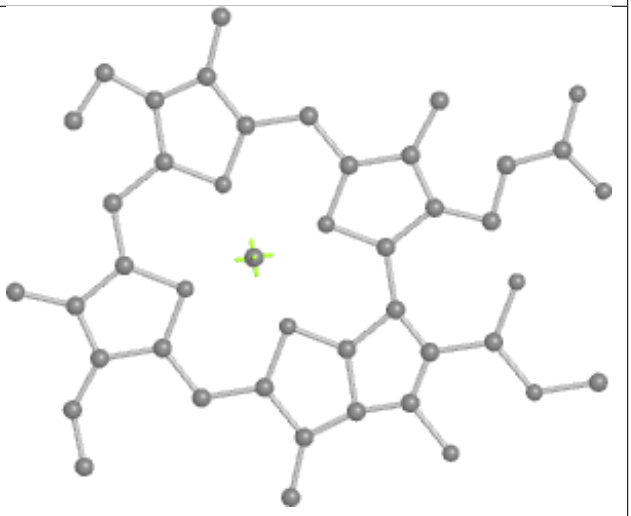
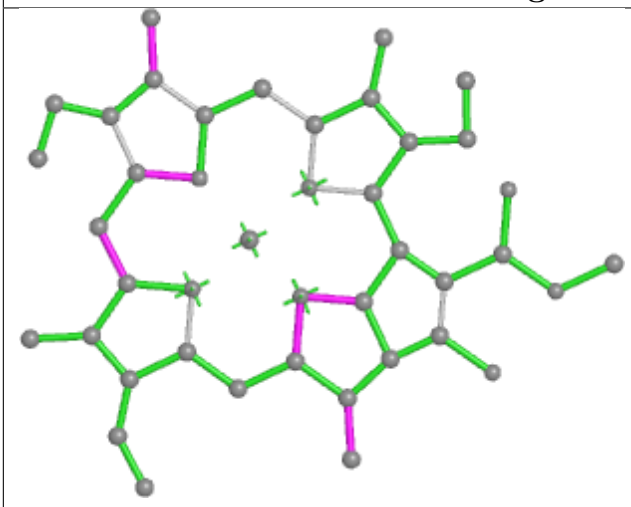


Rings

Ligand CLA J 102



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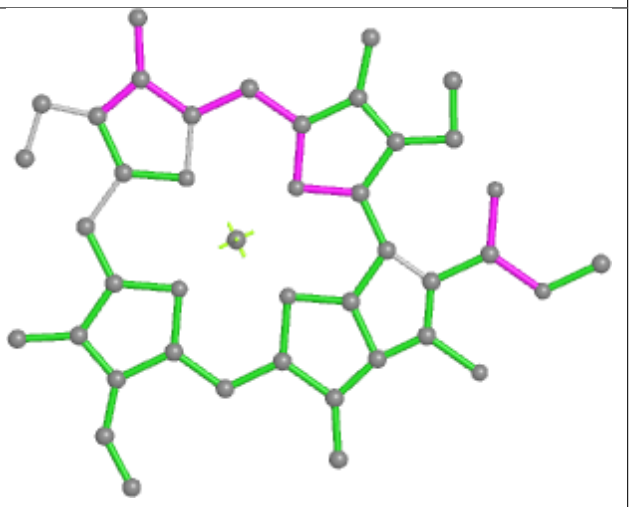
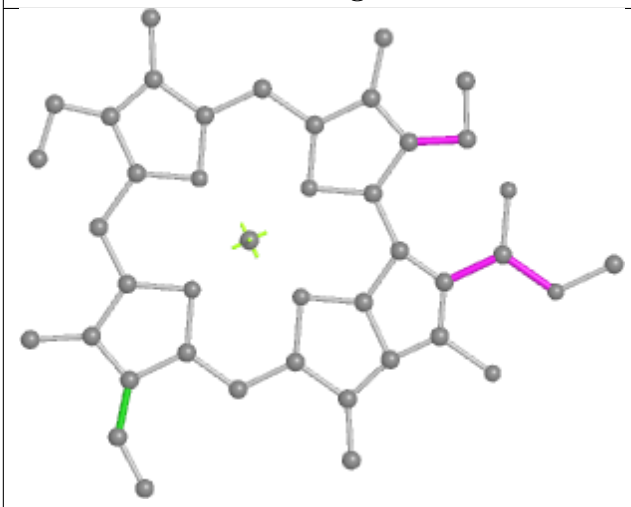


Bond angles



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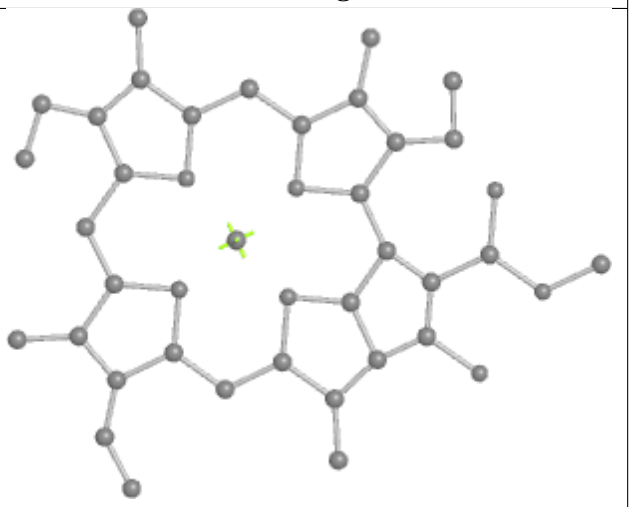
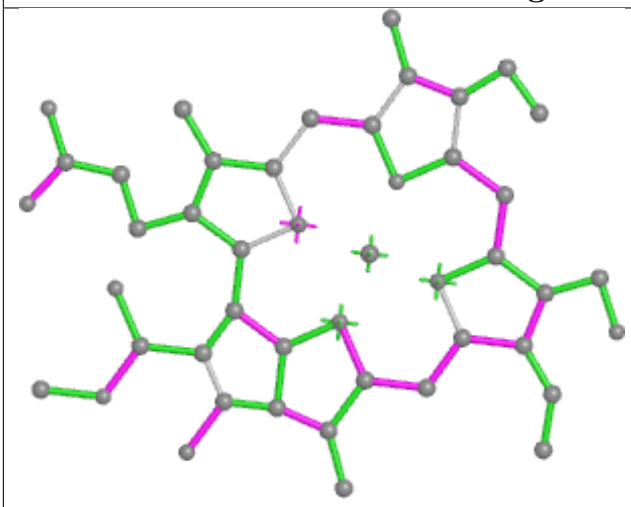


Rings

Ligand CHL 9 607



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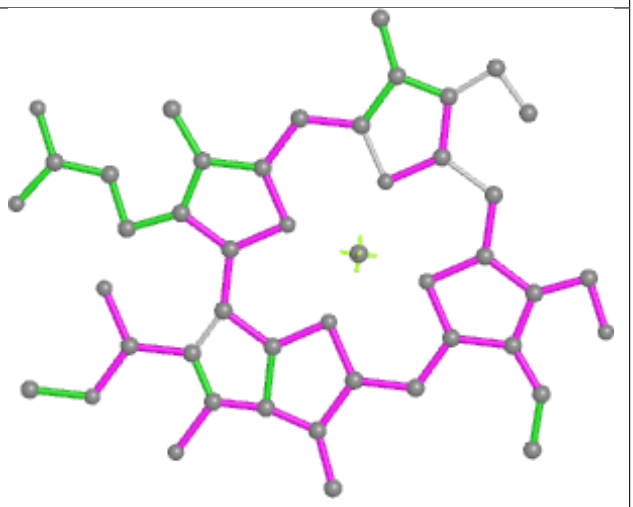

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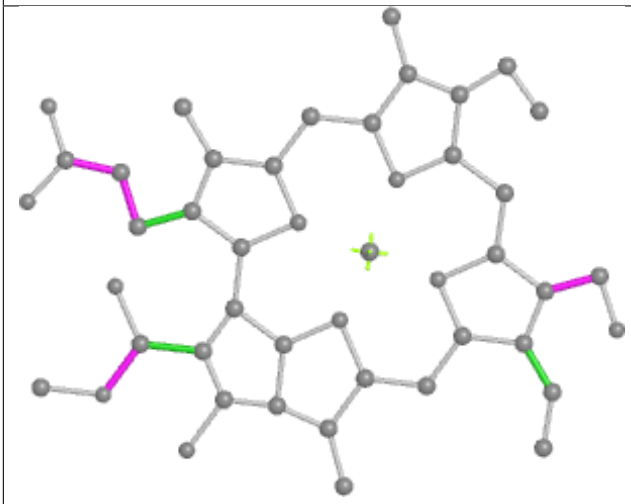
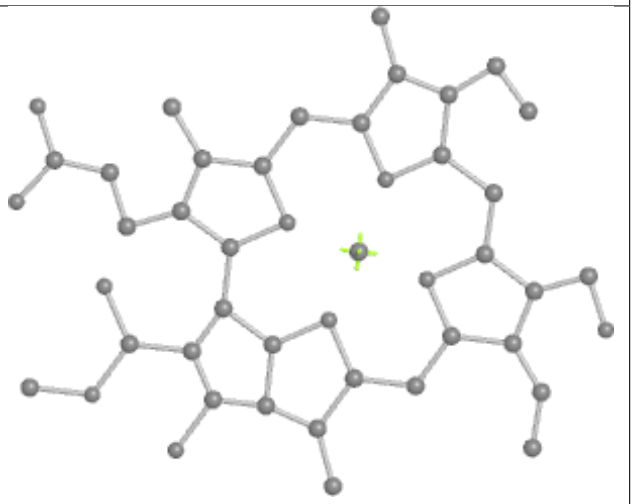
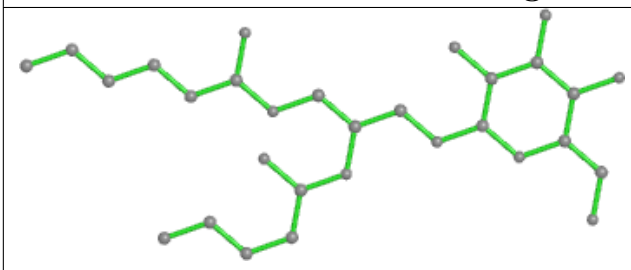


Torsions



Rings

Ligand LMG J 105



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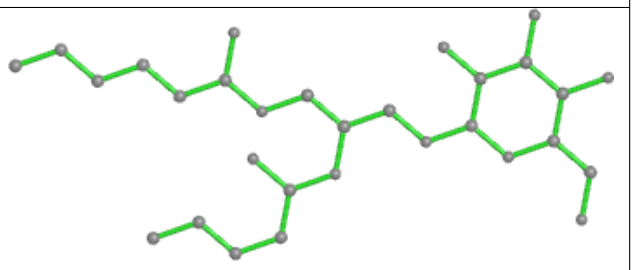
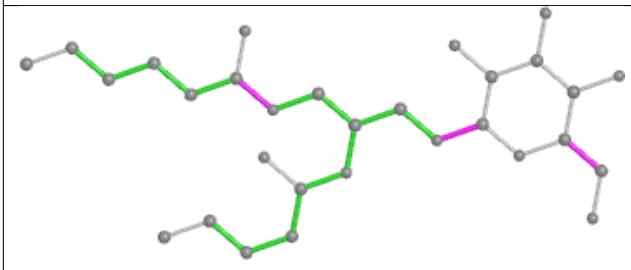


Bond angles



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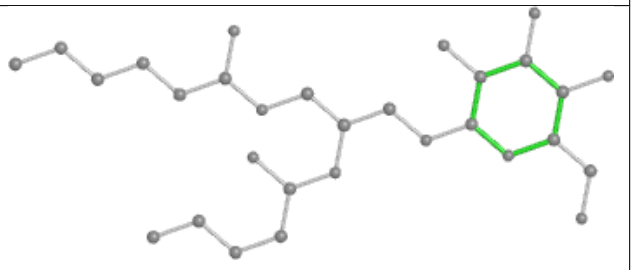
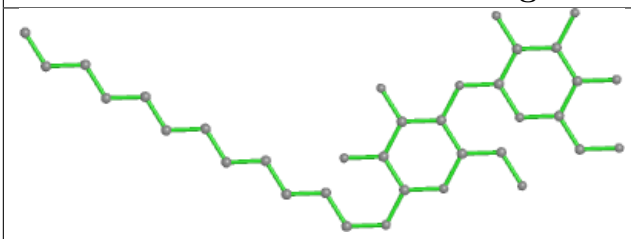


Rings

Ligand LMU A 856



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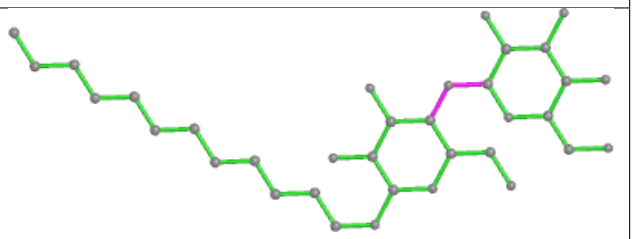
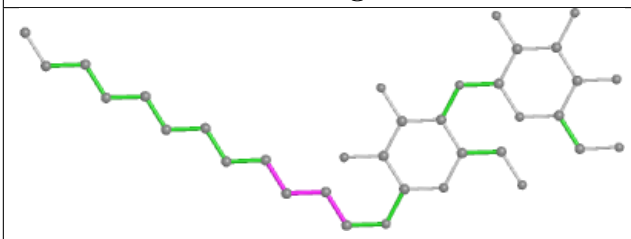


Bond angles



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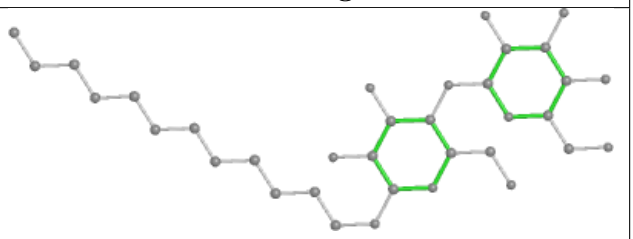
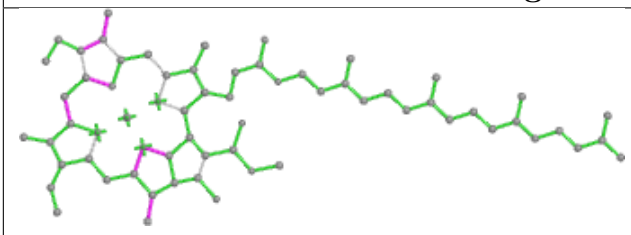


Rings

Ligand CLA B 804



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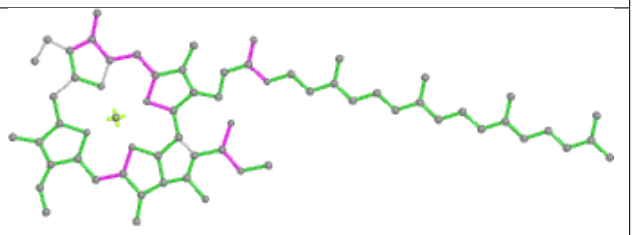

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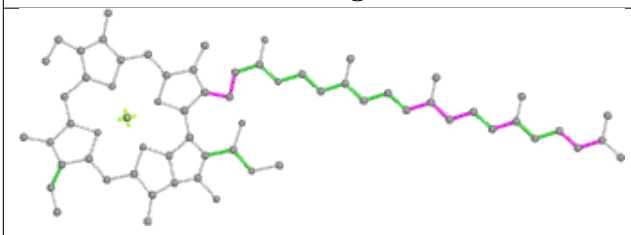

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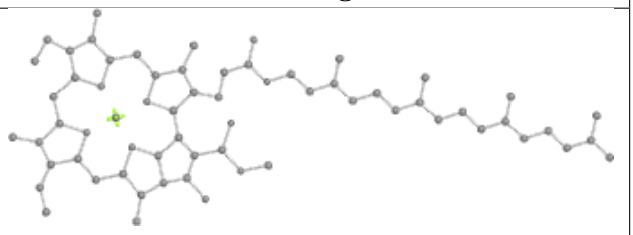
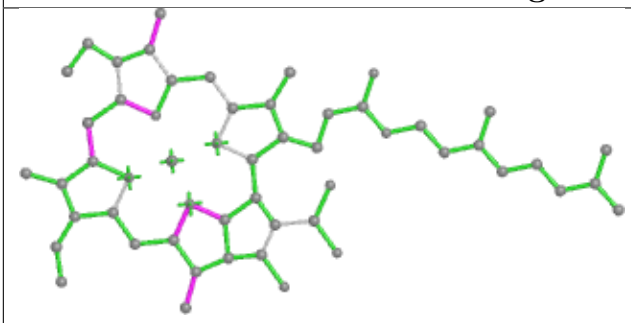


Rings

Ligand CLA 3 412



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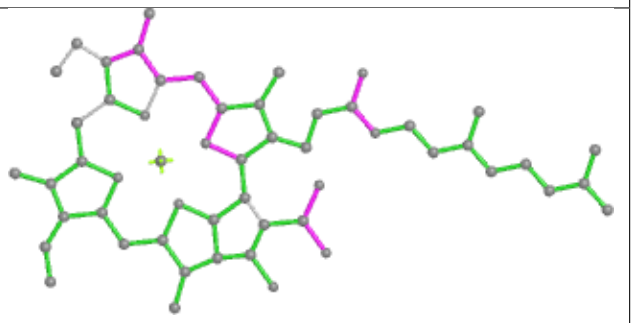
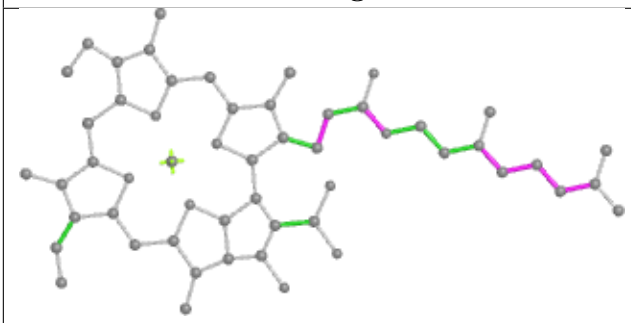


Bond angles



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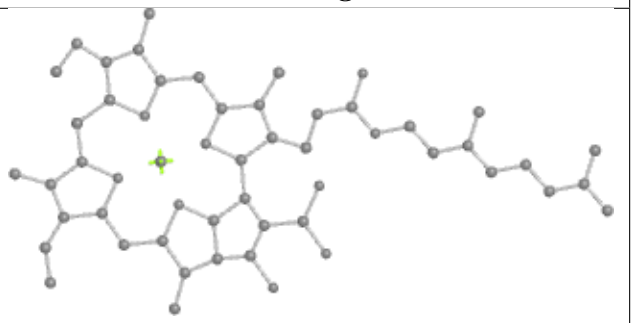
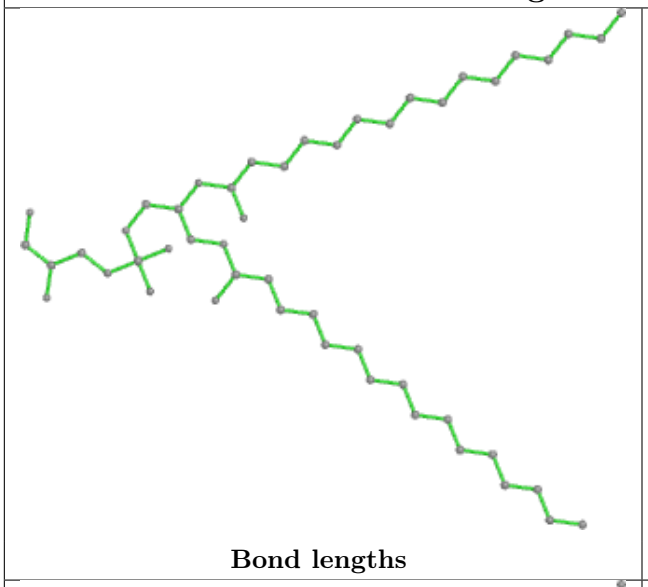


Rings

Ligand LHG 9 618



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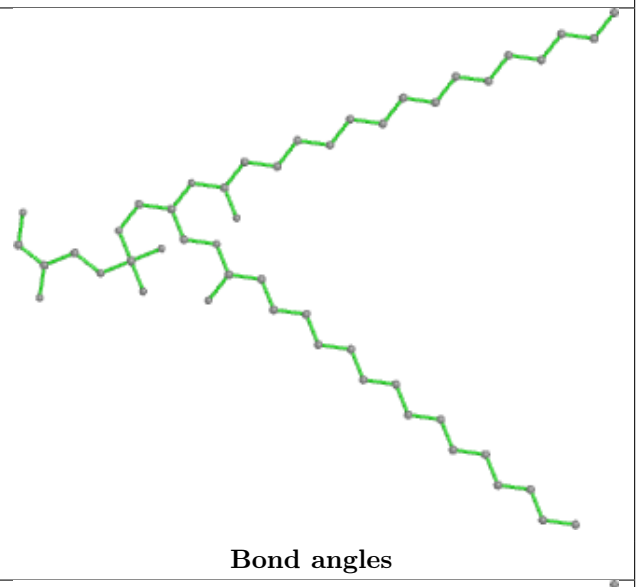

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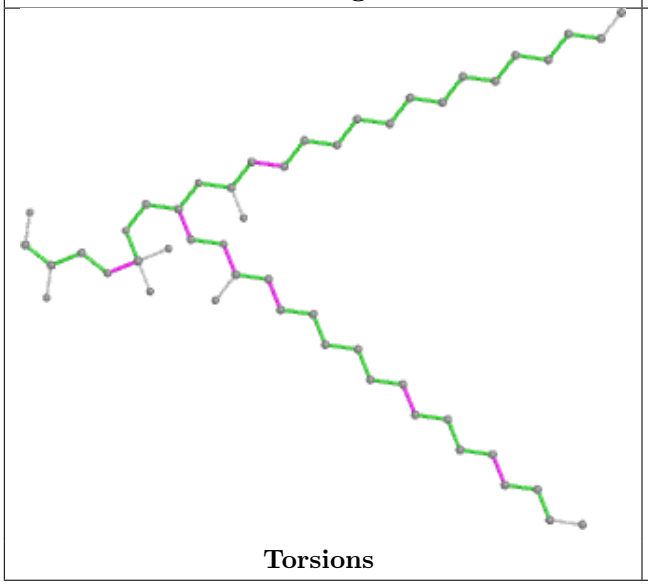

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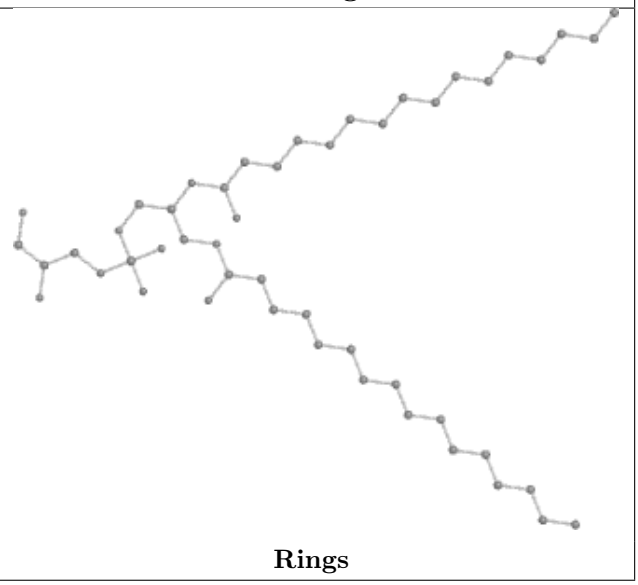
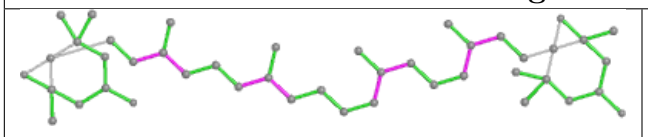


Rings

Ligand XAT 7 416



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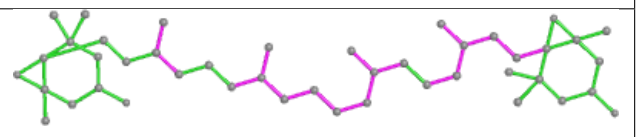

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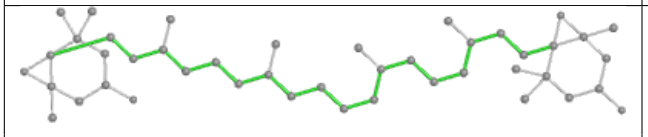

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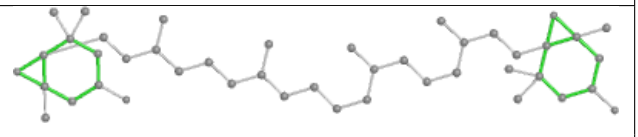
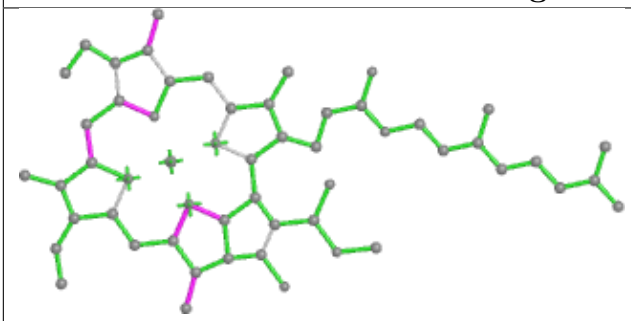


Rings

Ligand CLA c 603



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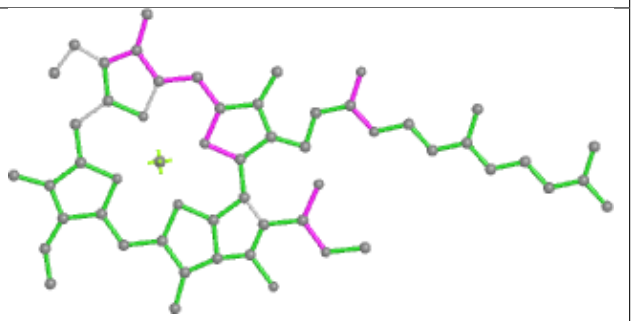
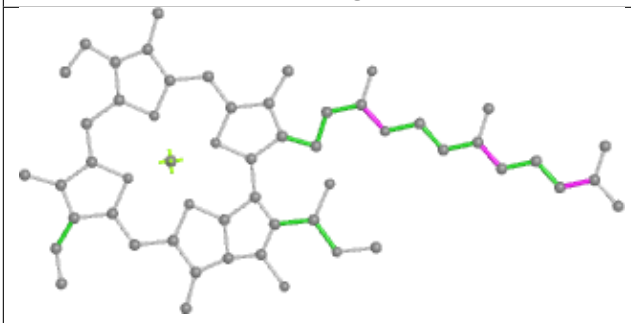


Bond angles



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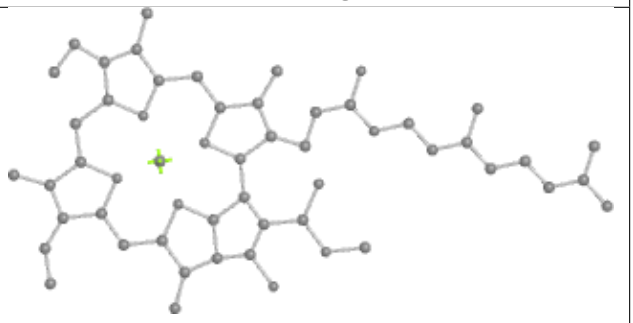
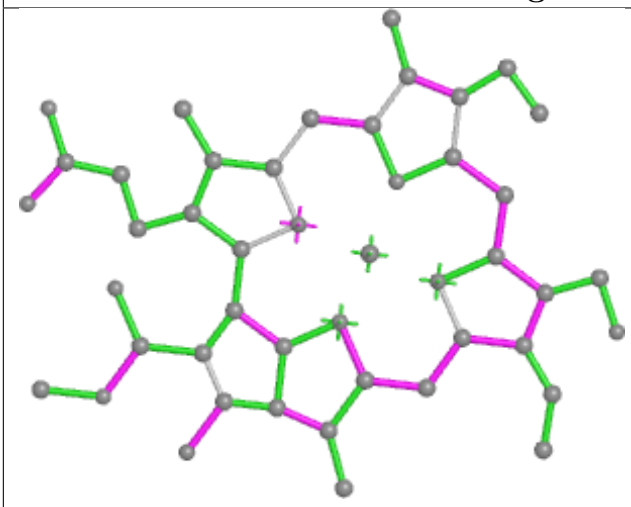


Rings

Ligand CHL 9 605



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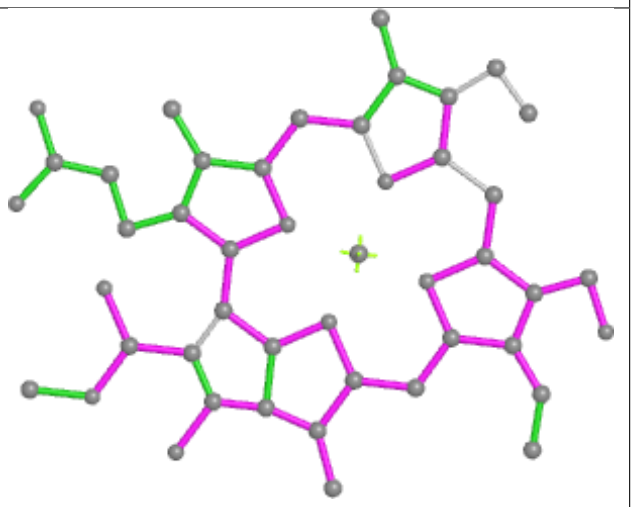

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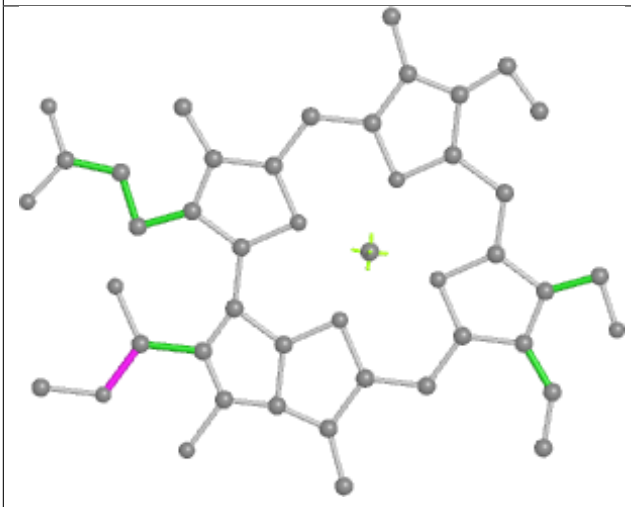

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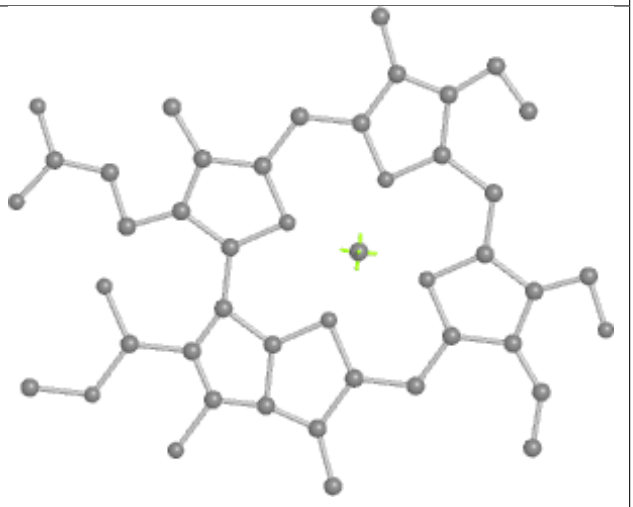
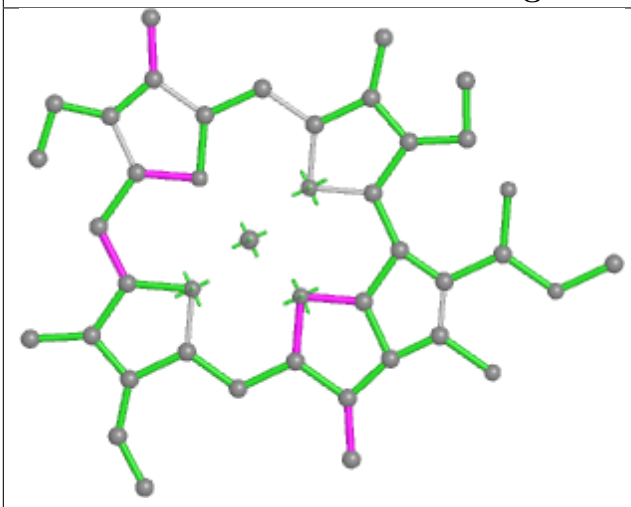


Rings

Ligand CLA O 201



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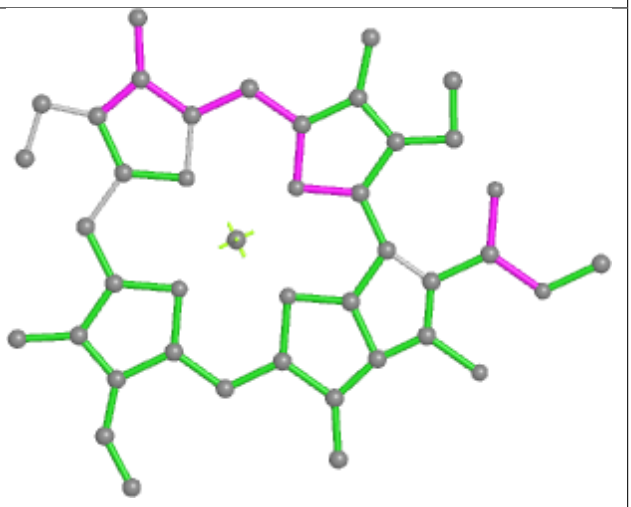
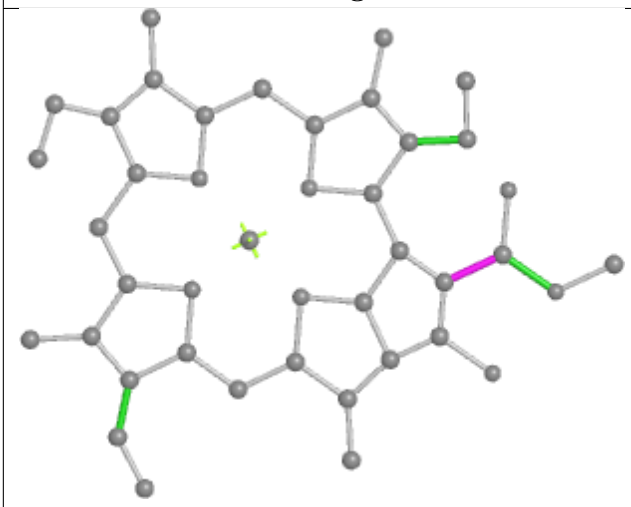


Bond angles



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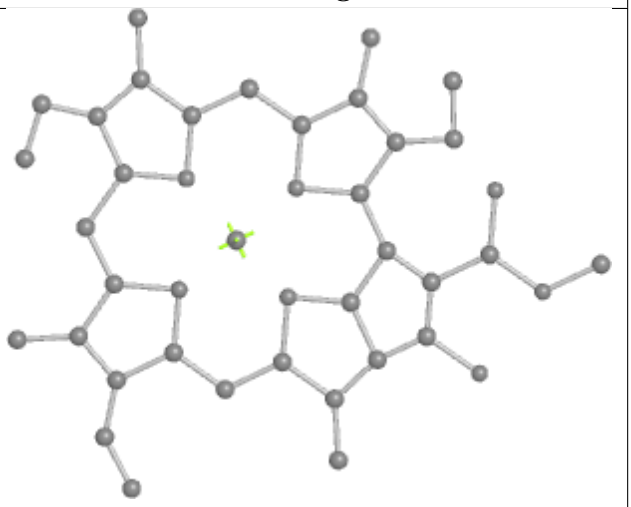
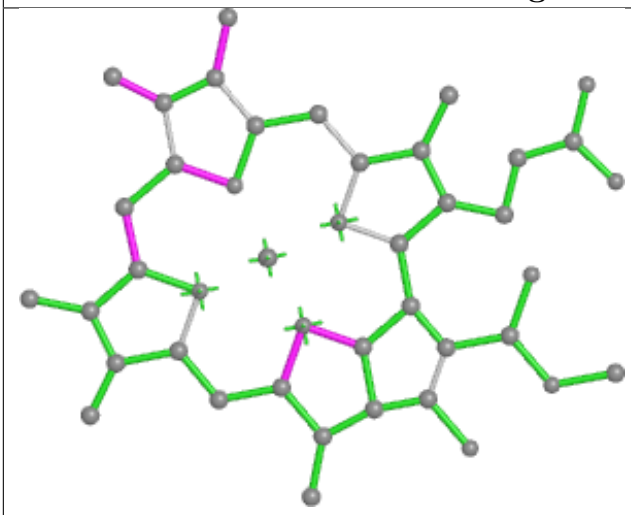


Rings

Ligand CLA 5 614



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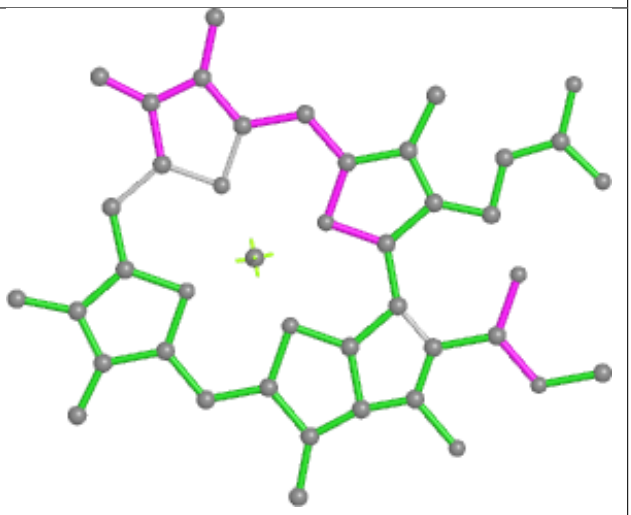
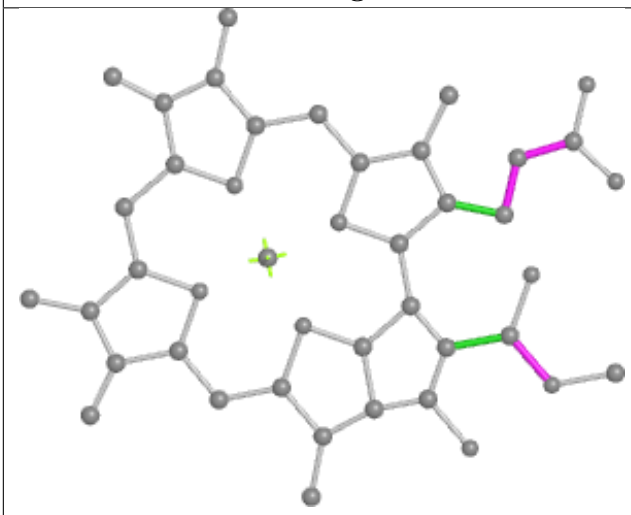


Bond angles



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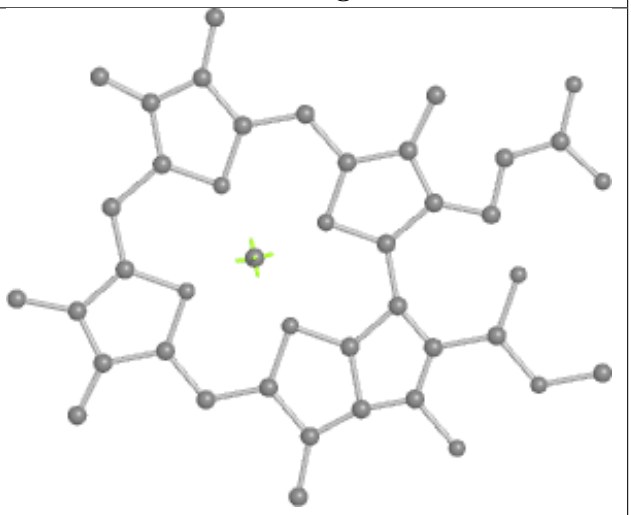
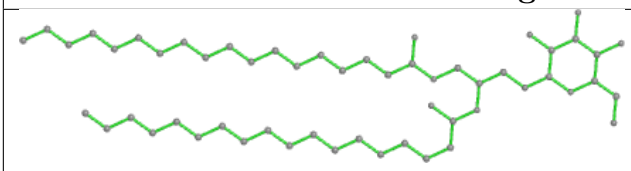


Rings

Ligand LMG G 206



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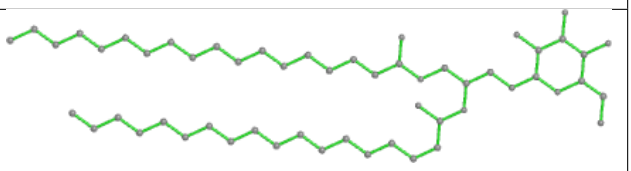
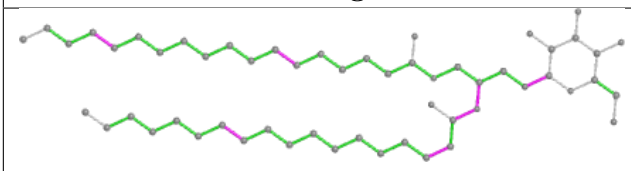


Bond angles



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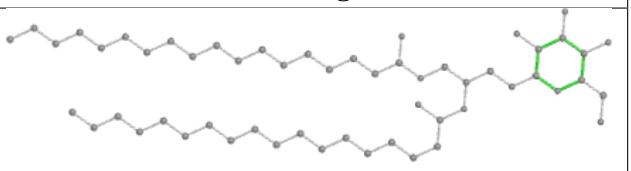
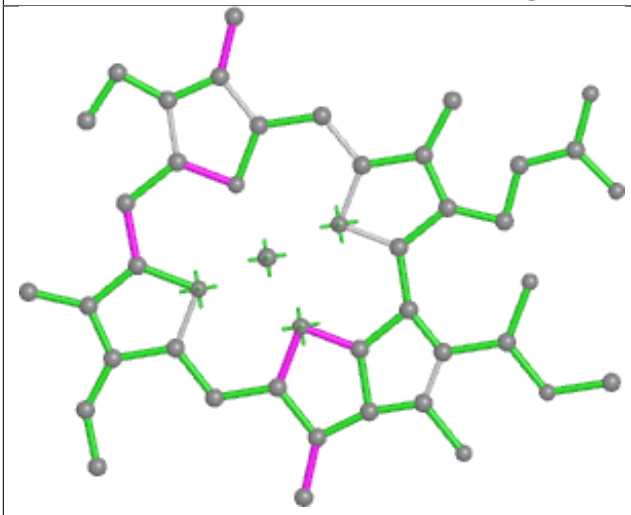


Rings

Ligand CLA G 202



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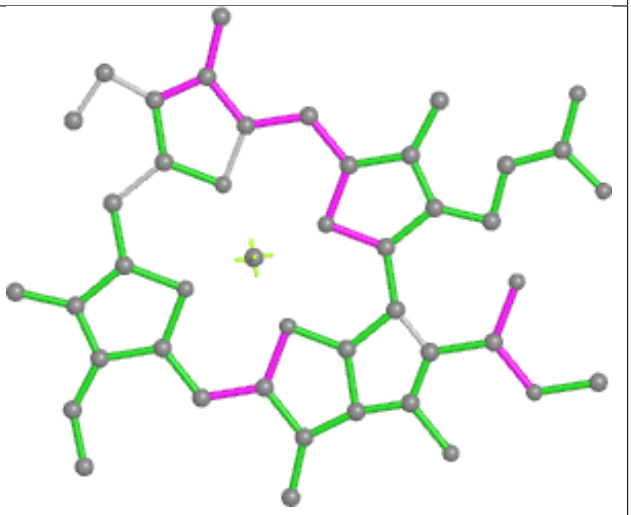
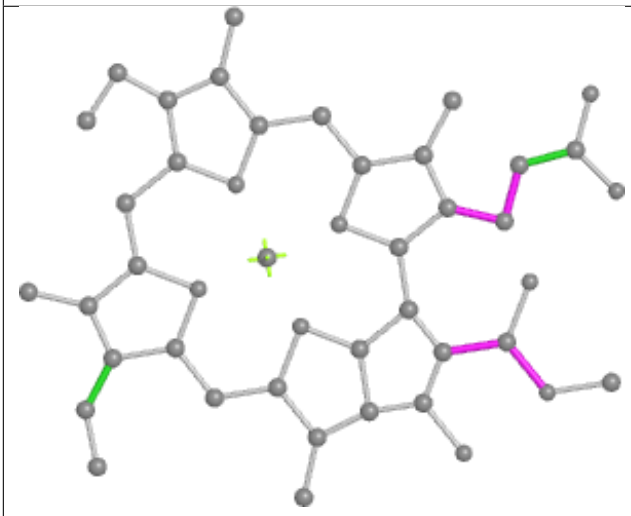


Bond angles



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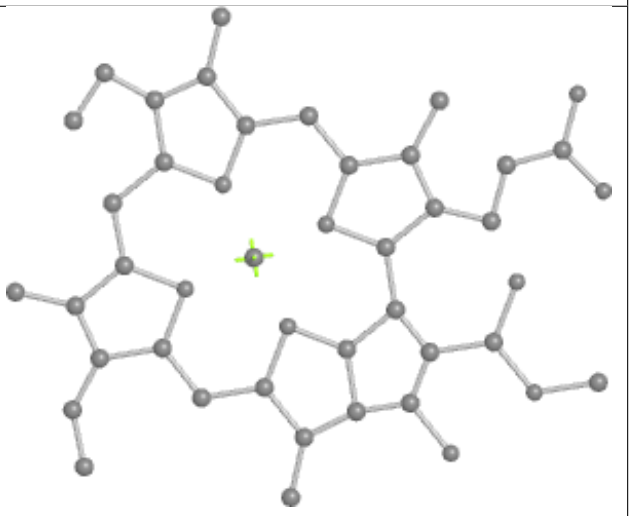
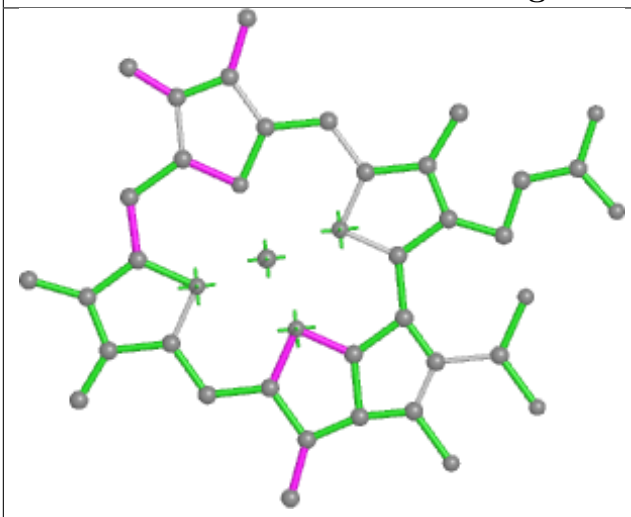


Rings

Ligand CLA 3 404



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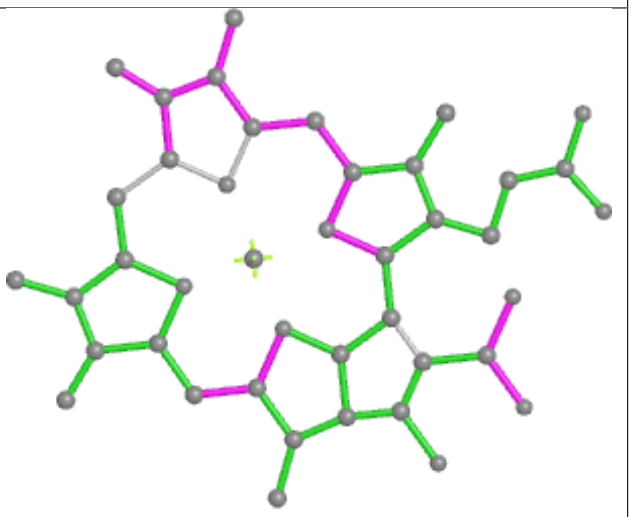
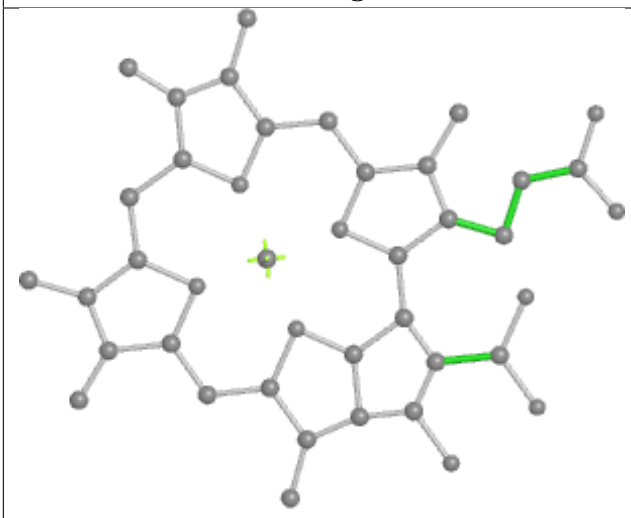


Bond angles



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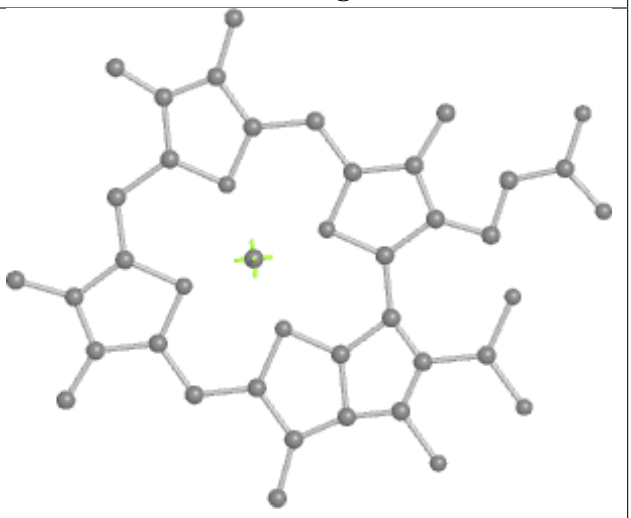
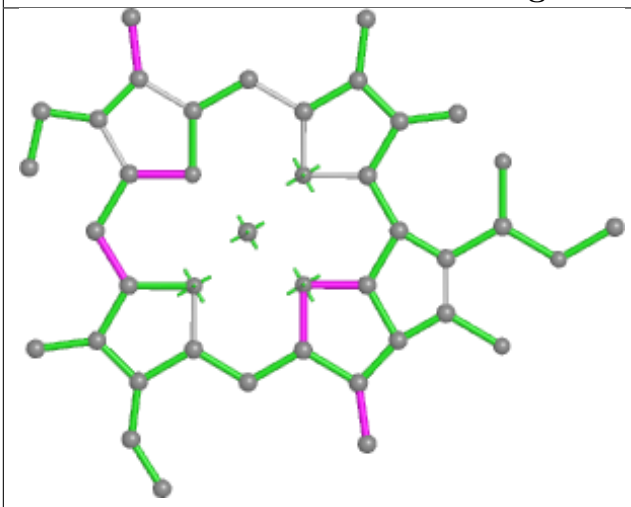


Rings

Ligand CLA 2 611



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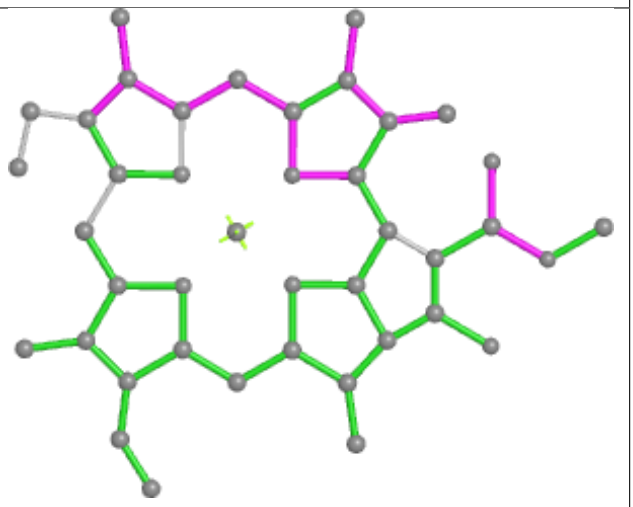
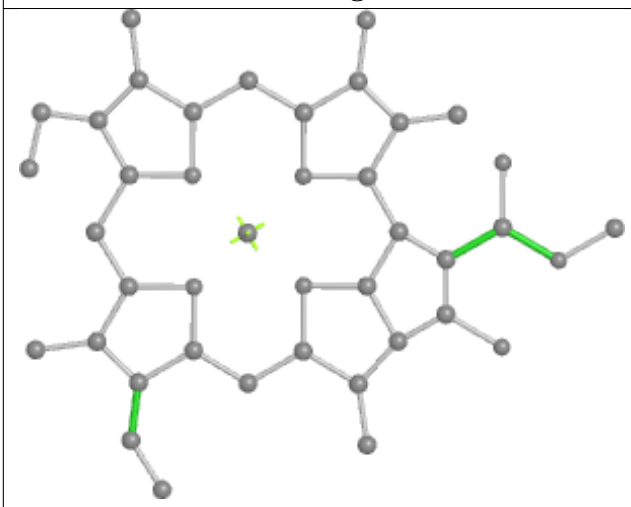


Bond angles



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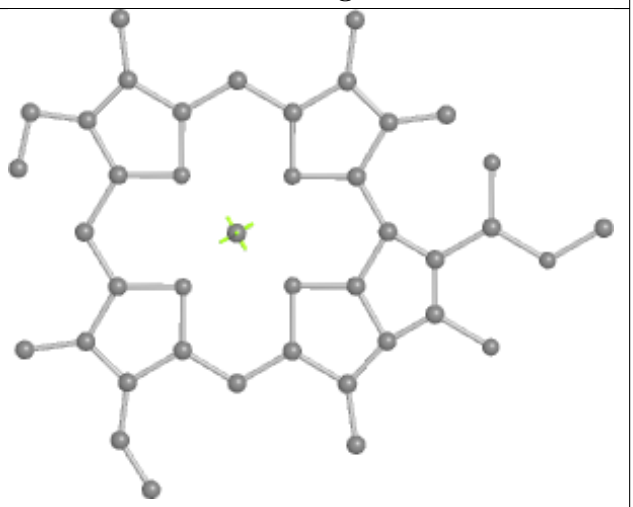
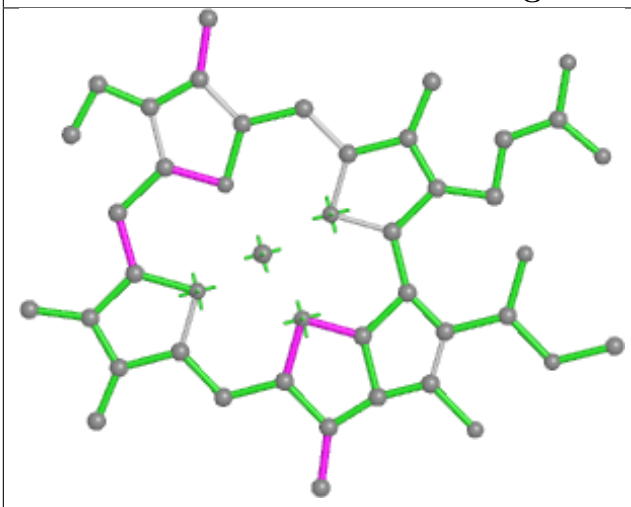


Rings

Ligand CLA A 820



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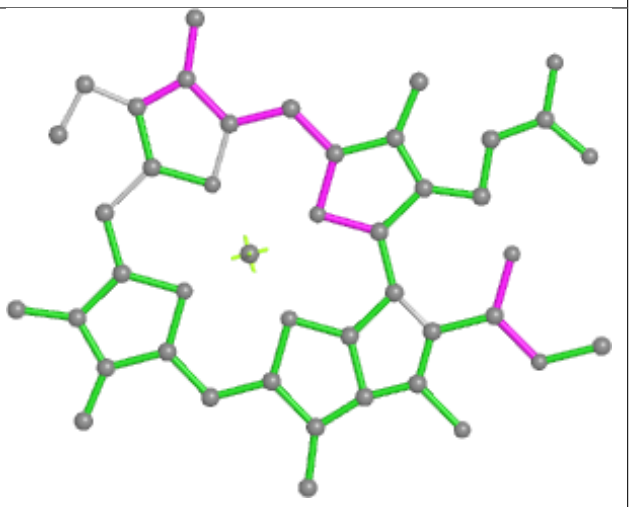
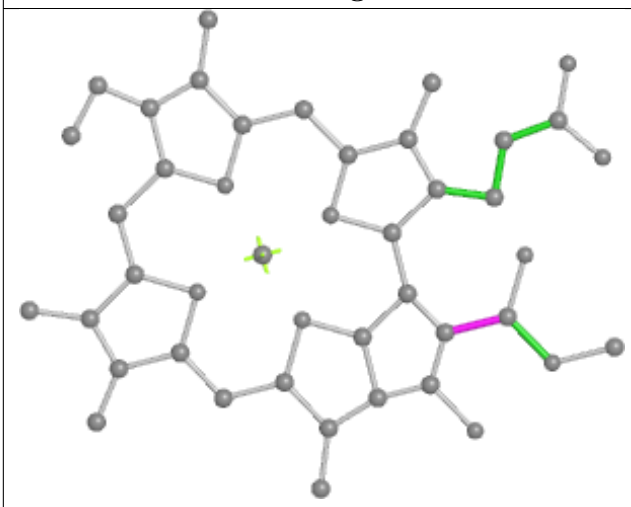


Bond angles



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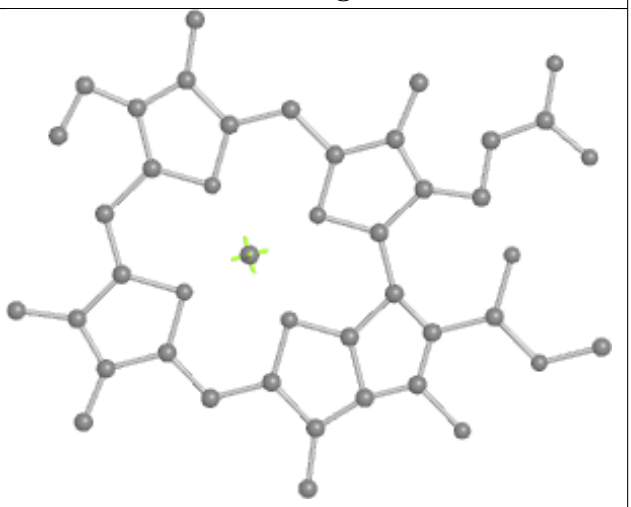
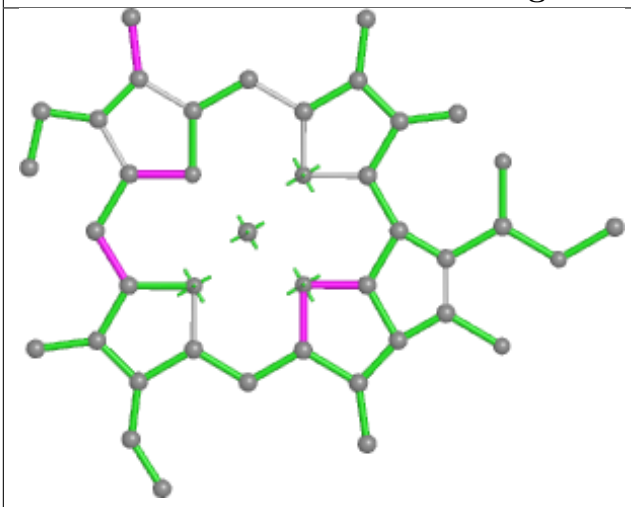


Rings

Ligand CLA 6 611



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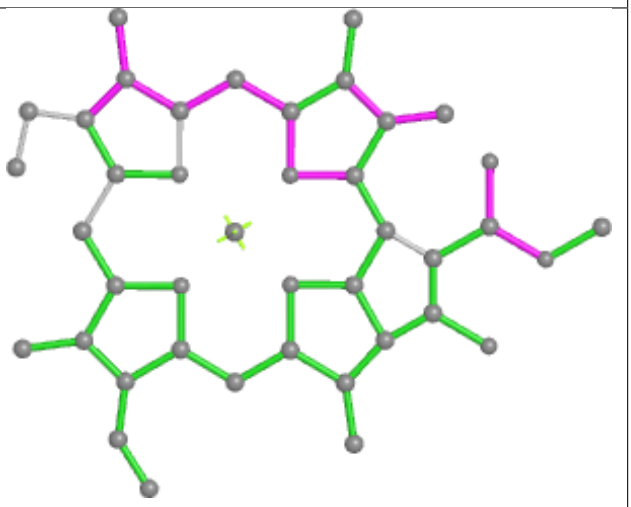

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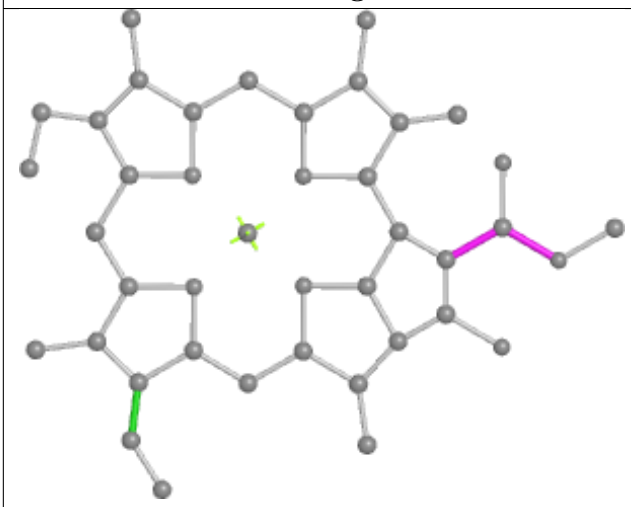

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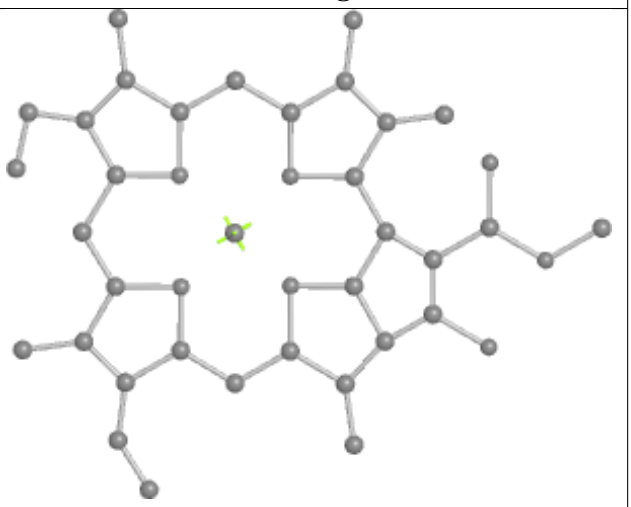
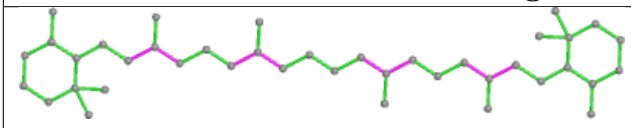


Rings

Ligand BCR F 303



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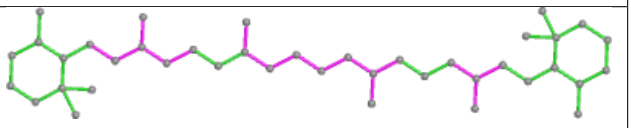

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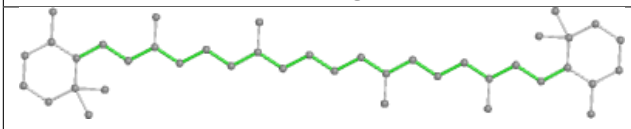

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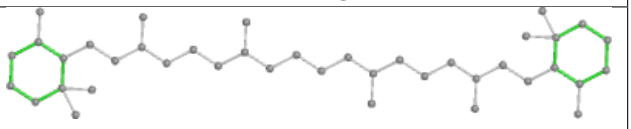

Rings

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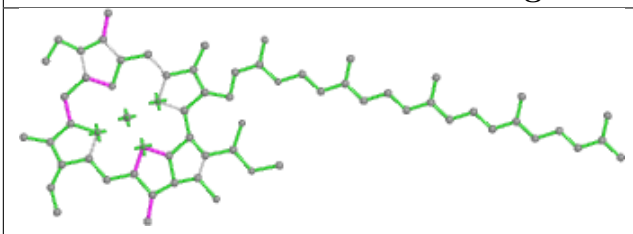

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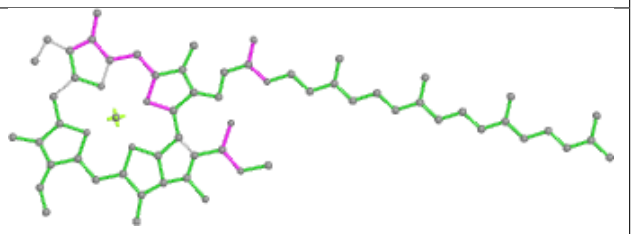

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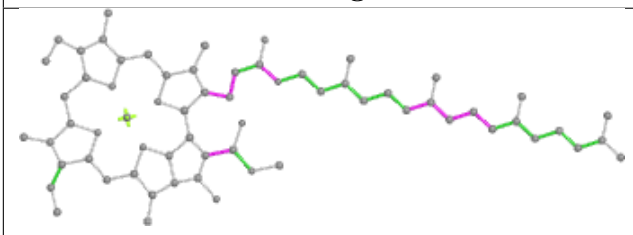

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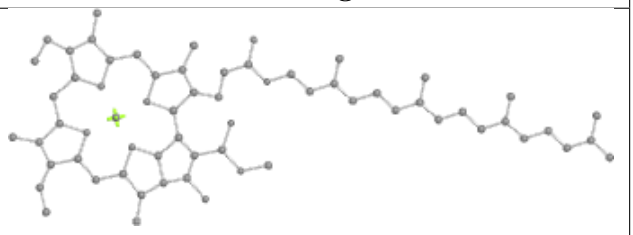
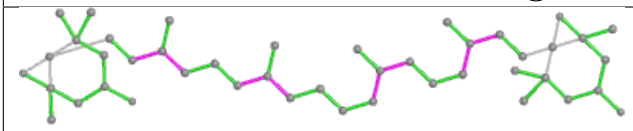


Rings

Ligand XAT 5 616



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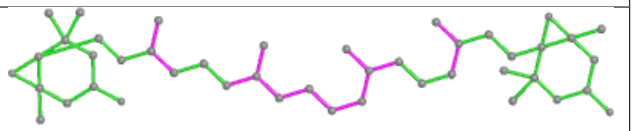

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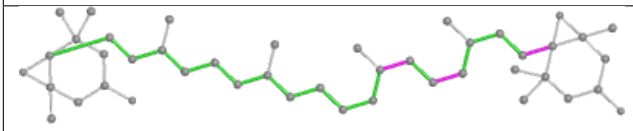

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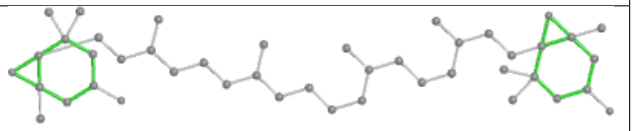
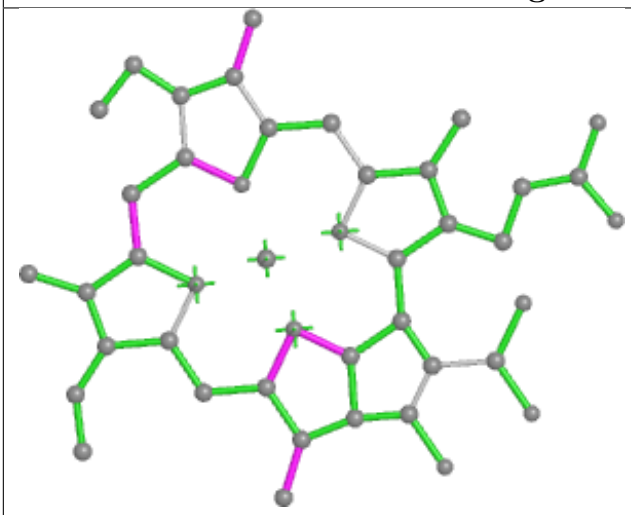


Rings

Ligand CLA 1 308



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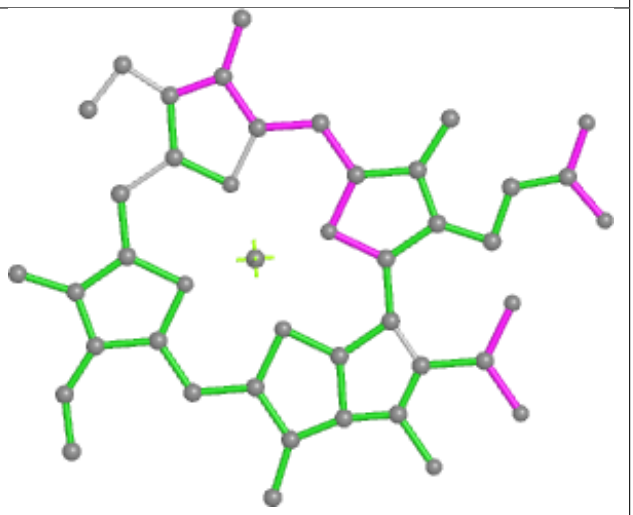

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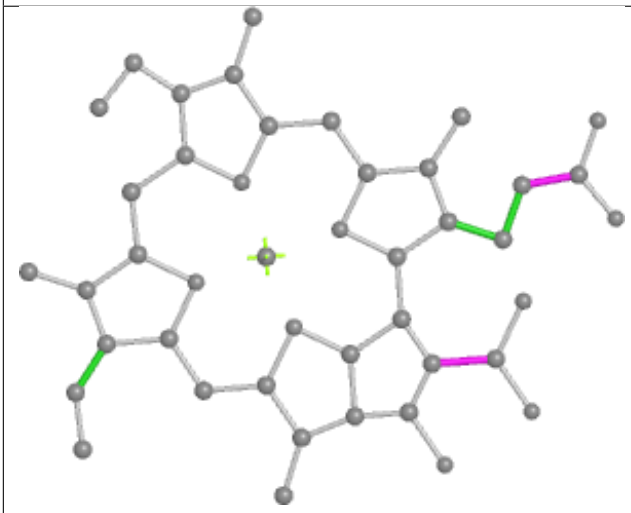

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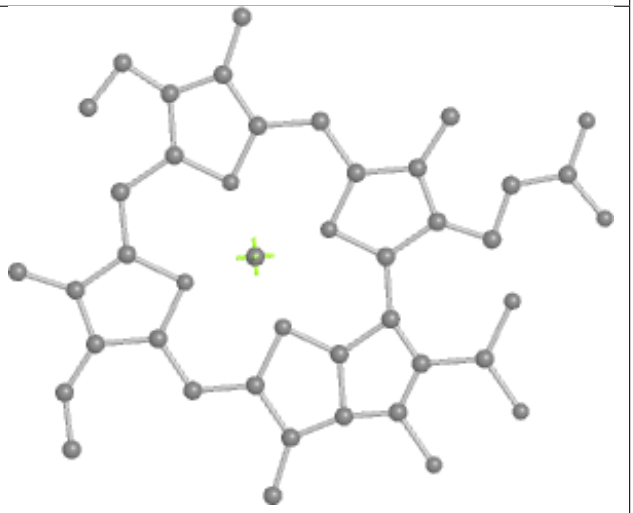
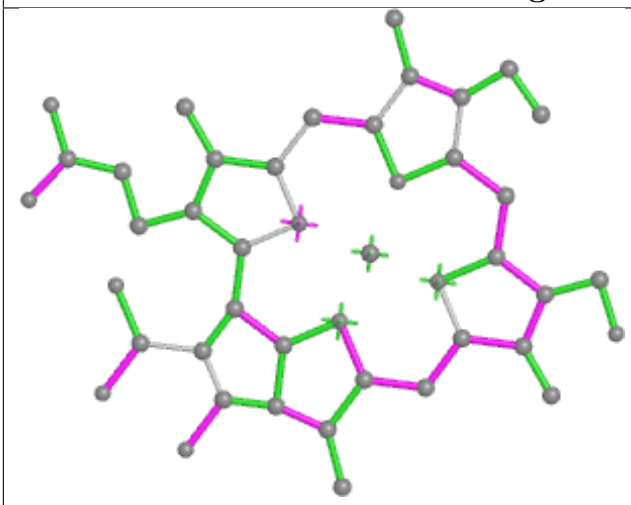


Rings

Ligand CHL c 609



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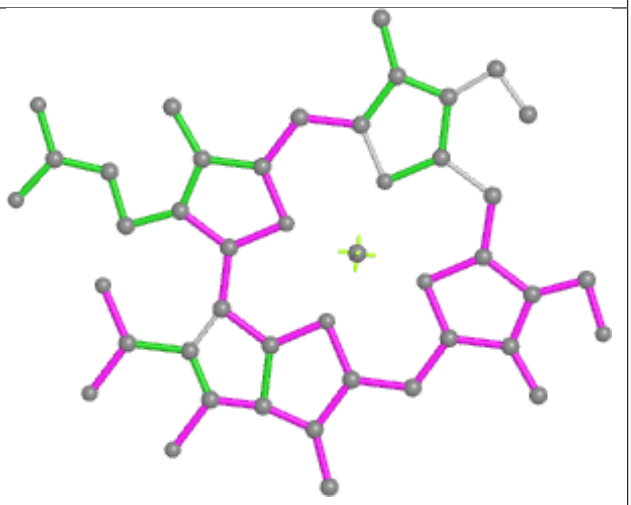

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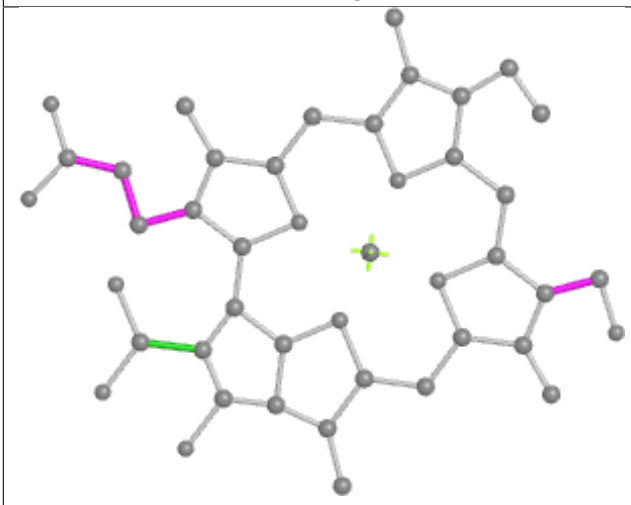

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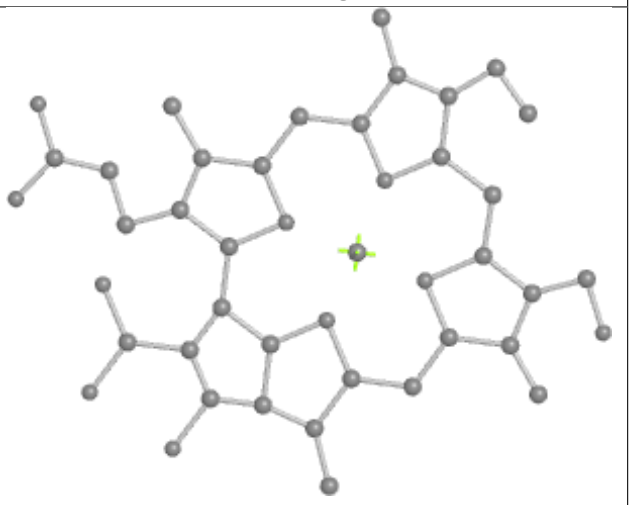
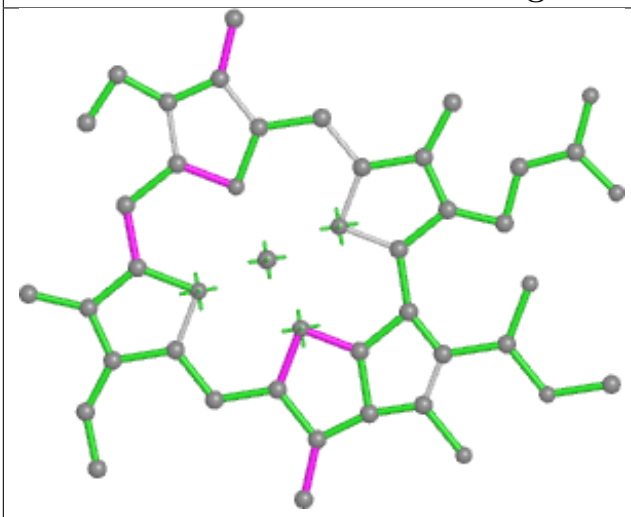


Rings

Ligand CLA b 315



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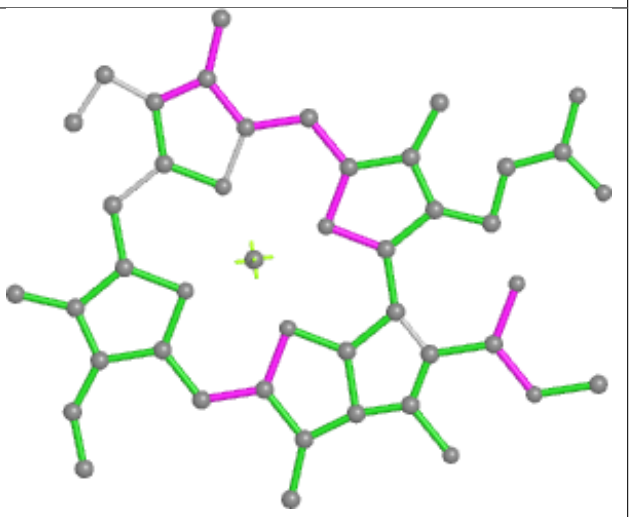
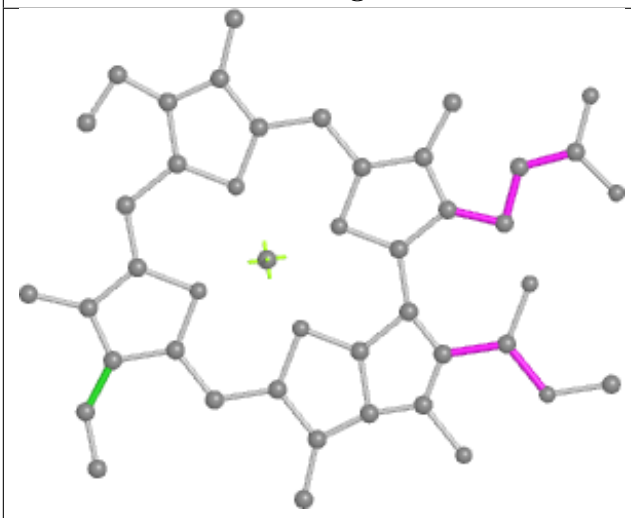


Bond angles



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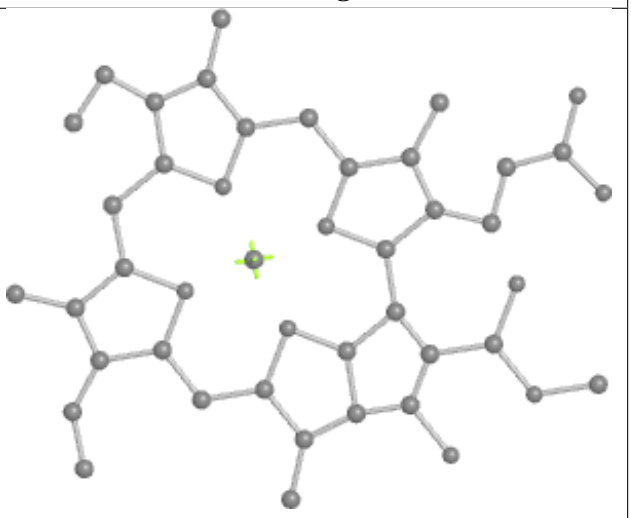
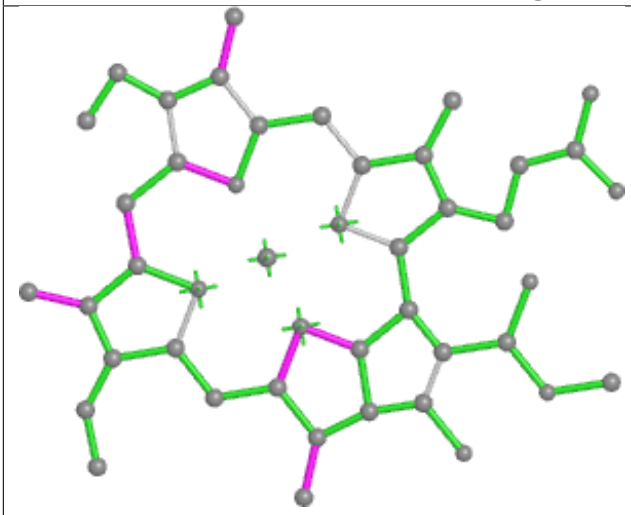


Rings

Ligand CLA c 604



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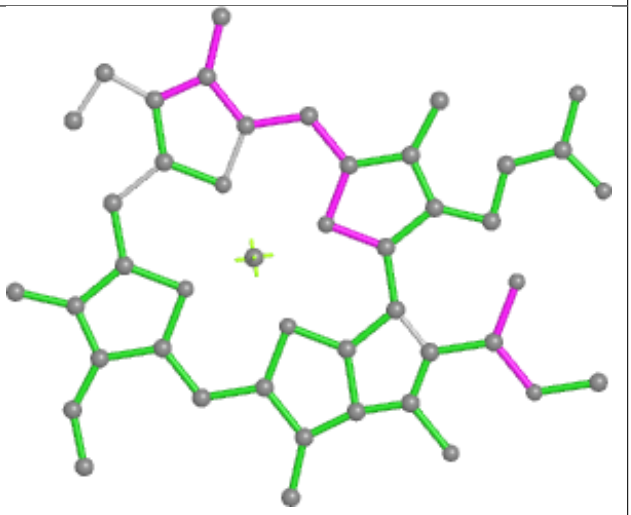
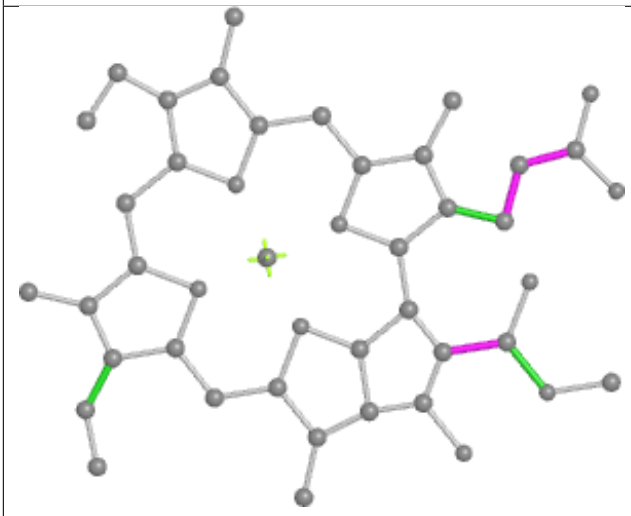


Bond angles



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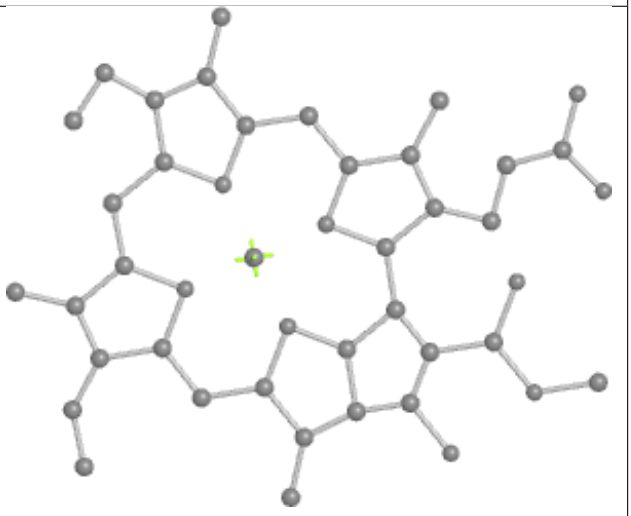
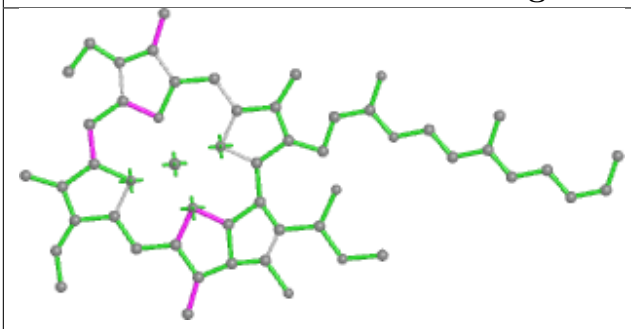


Rings

Ligand CLA 9 610



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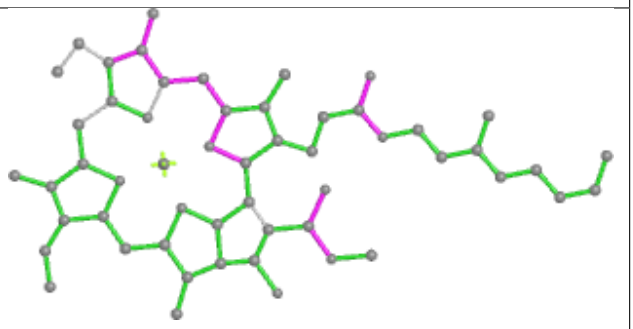
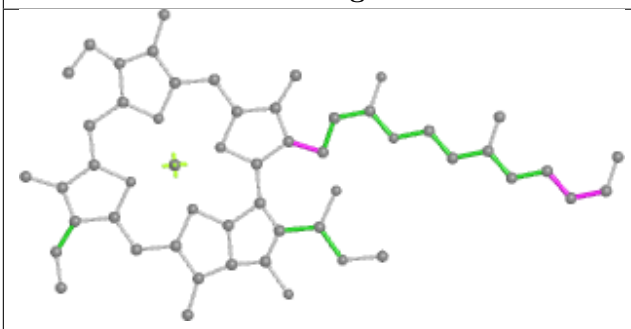


Bond angles



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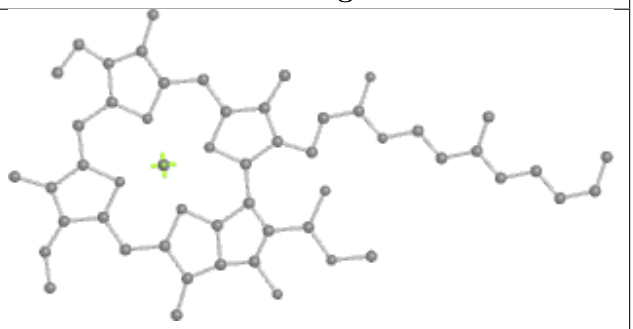
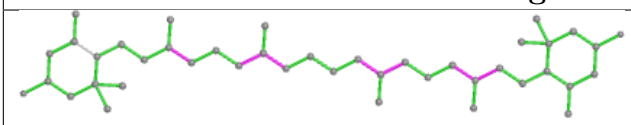


Rings

Ligand LUT a 615



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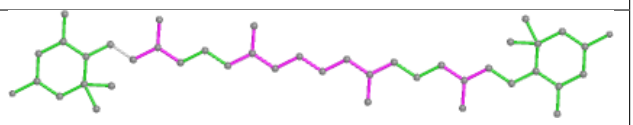
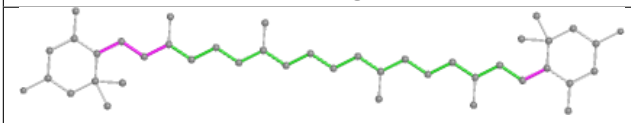


Bond angles



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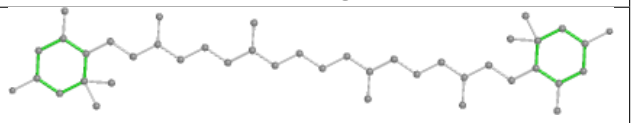
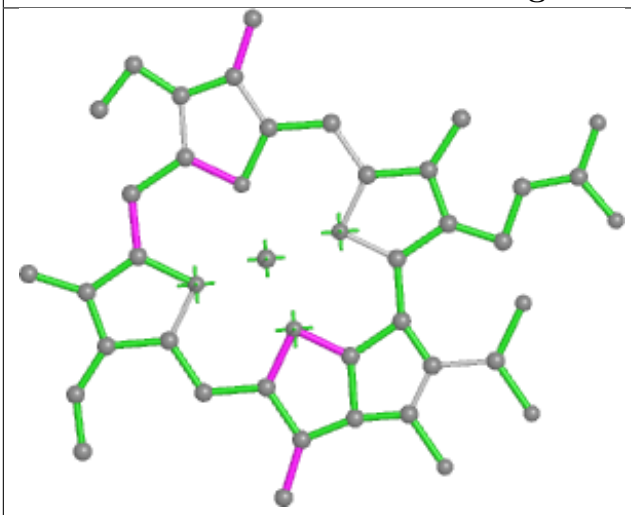
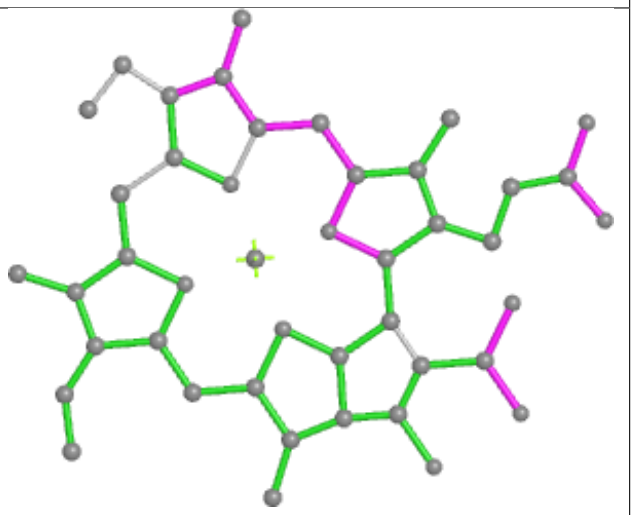


Rings

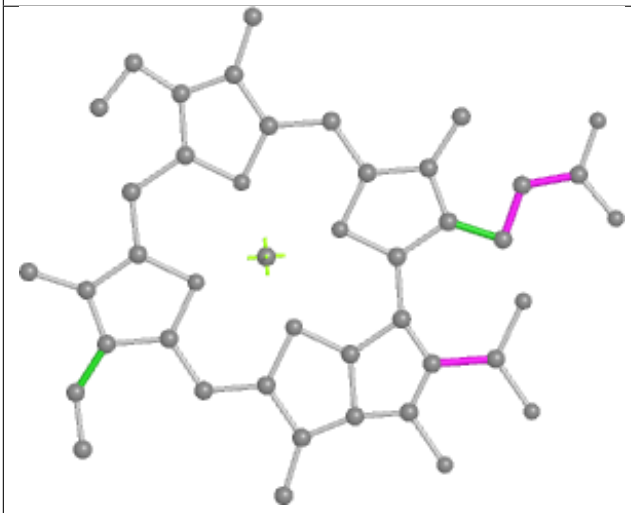
Ligand CLA 4 603



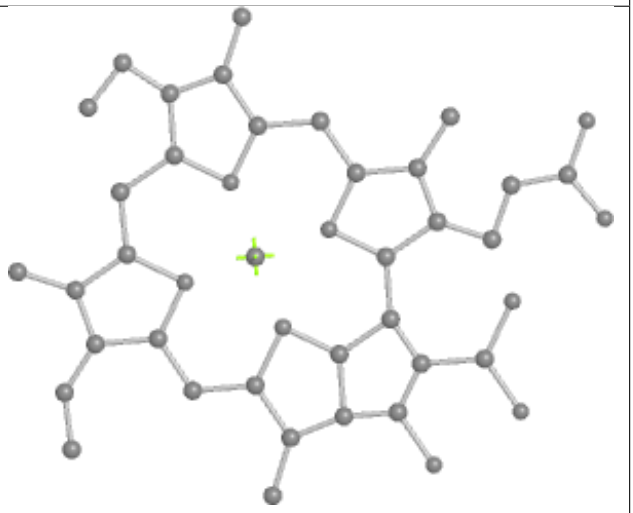
Bond lengths



Bond angles

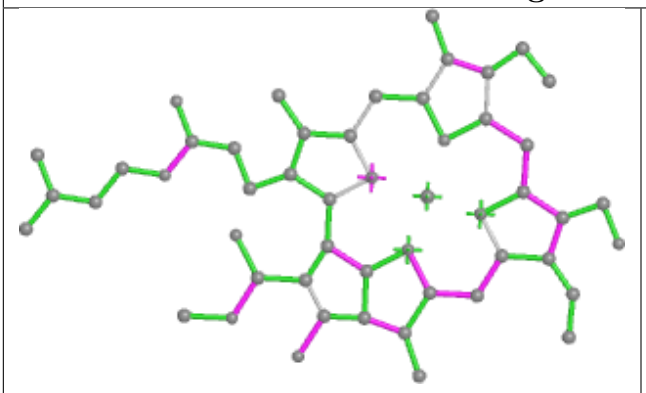


Torsions



Rings

Ligand CHL 4 607



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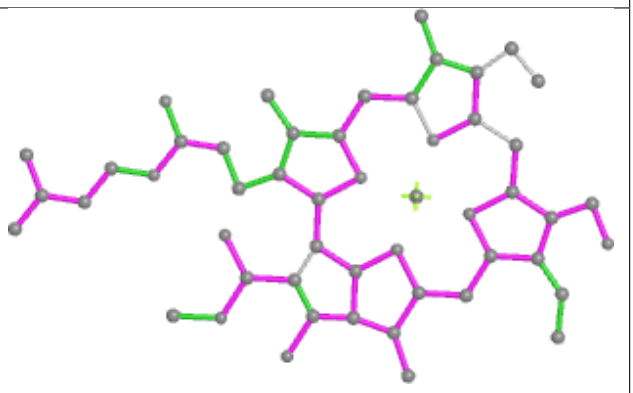
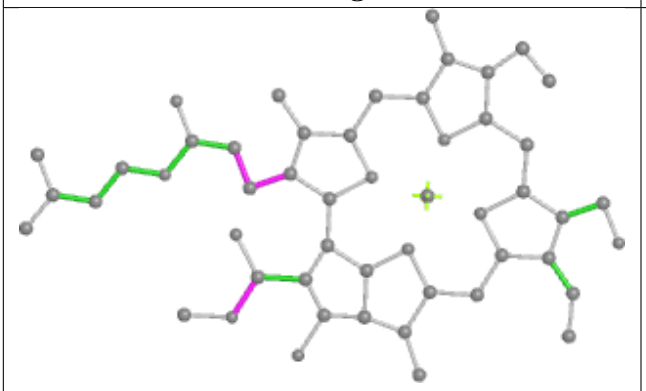


Bond angles



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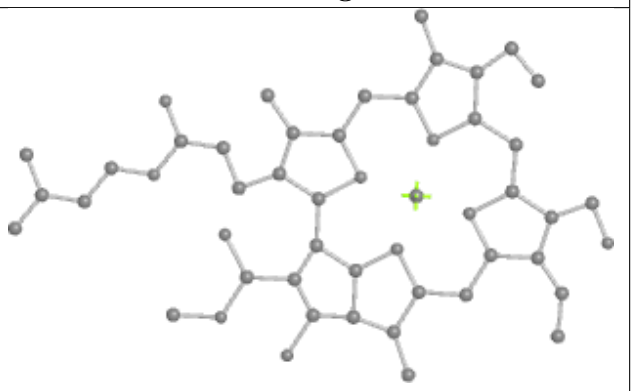
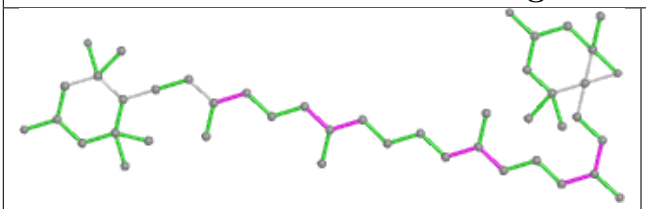


Rings

Ligand NEX c 618



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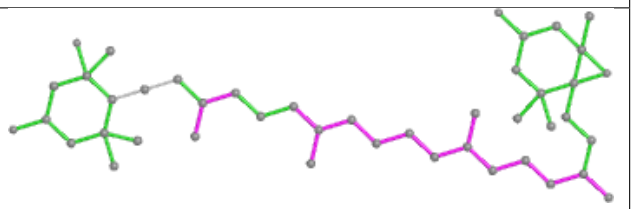
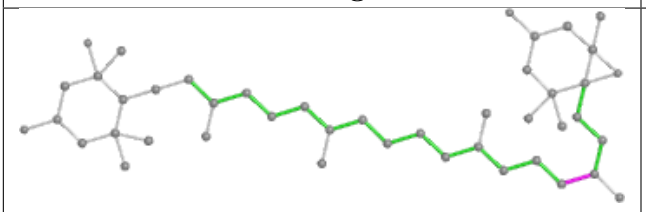


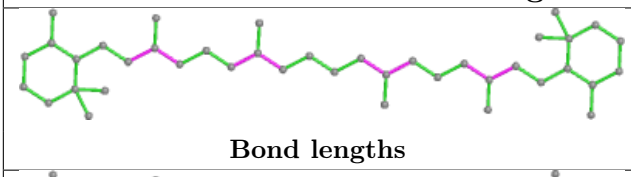
Bond angles



Torsions

Rings

Ligand BCR 3 418



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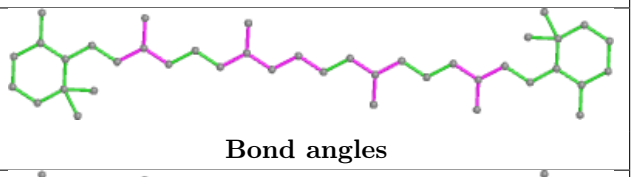
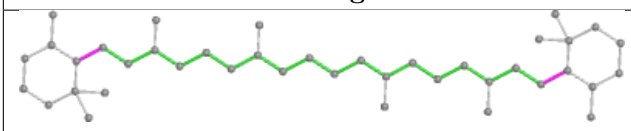


Bond angles



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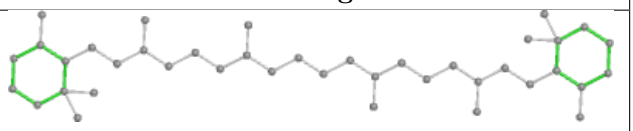
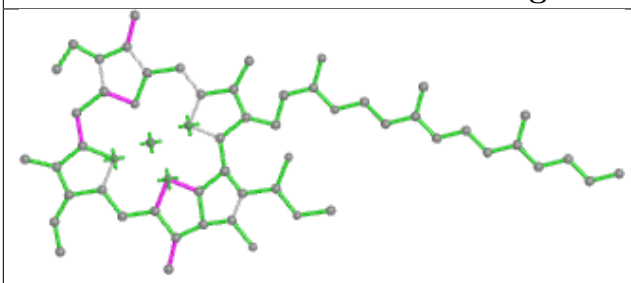


Rings

Ligand CLA c 611



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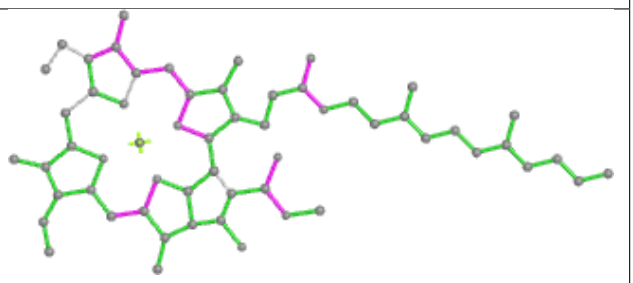
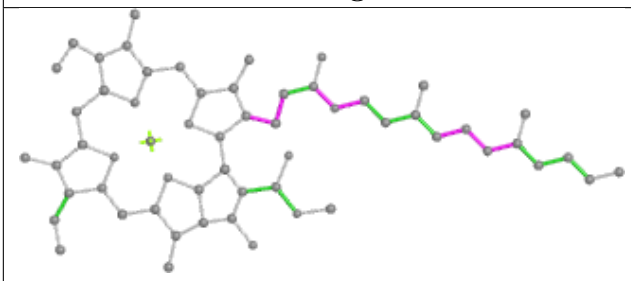


Bond angles



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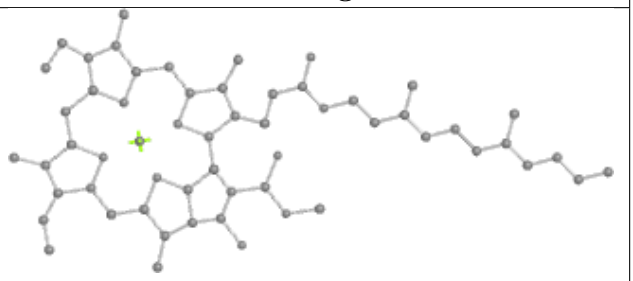
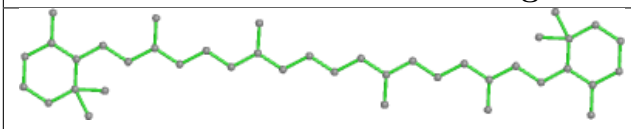


Rings

Ligand BCR K 205



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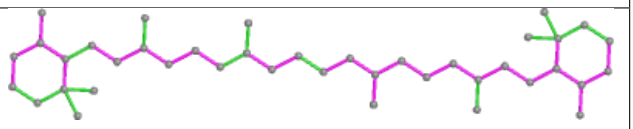
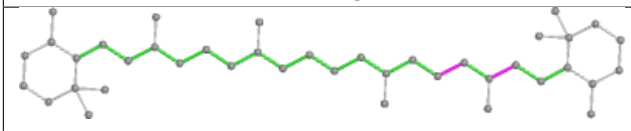


Bond angles



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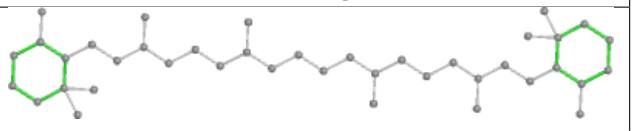
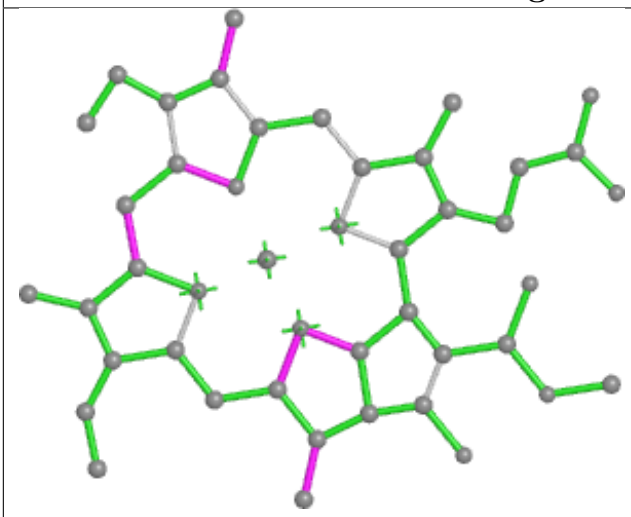


Rings

Ligand CLA 4 610



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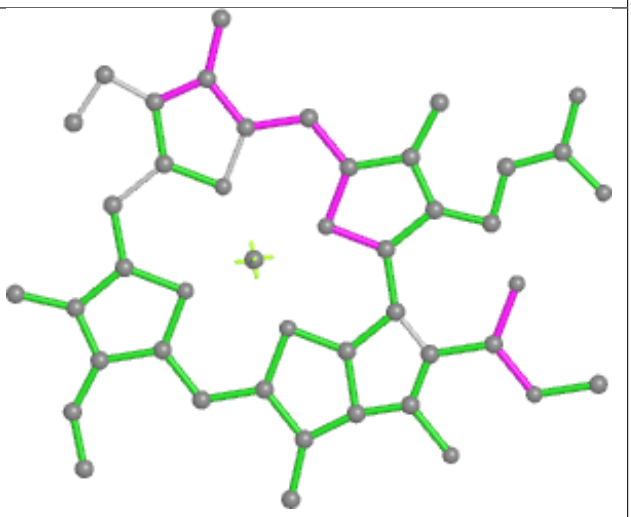

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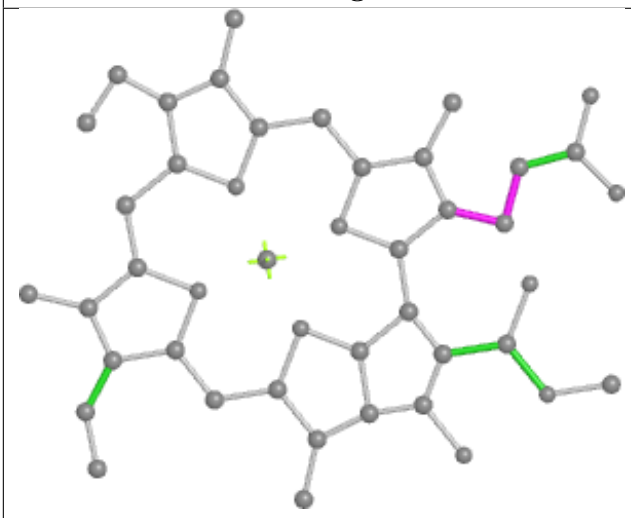

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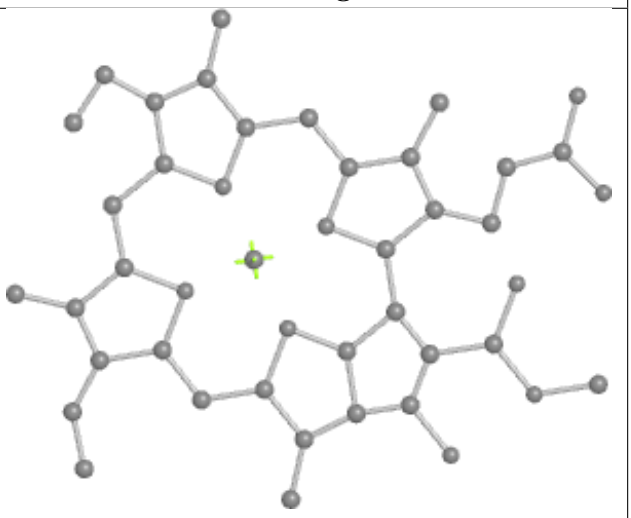
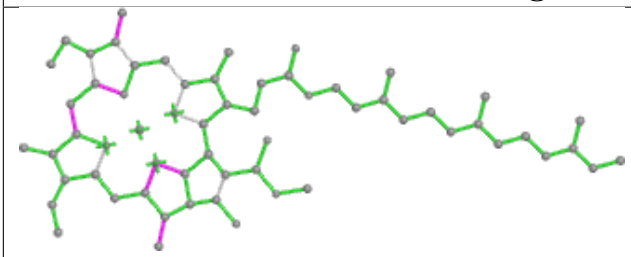


Rings

Ligand CLA 5 602



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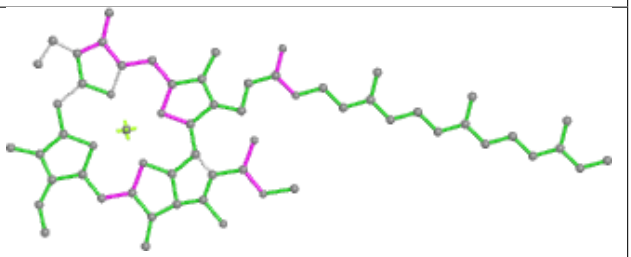

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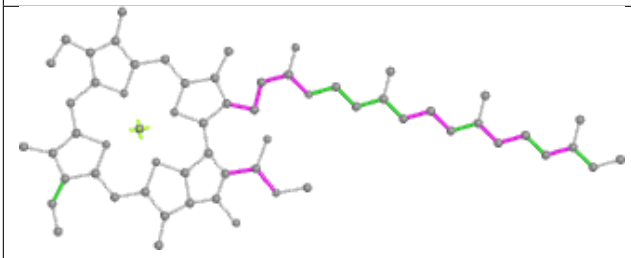

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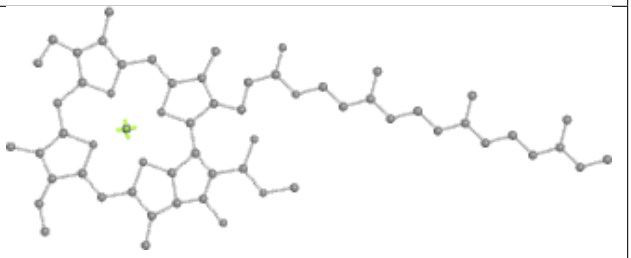
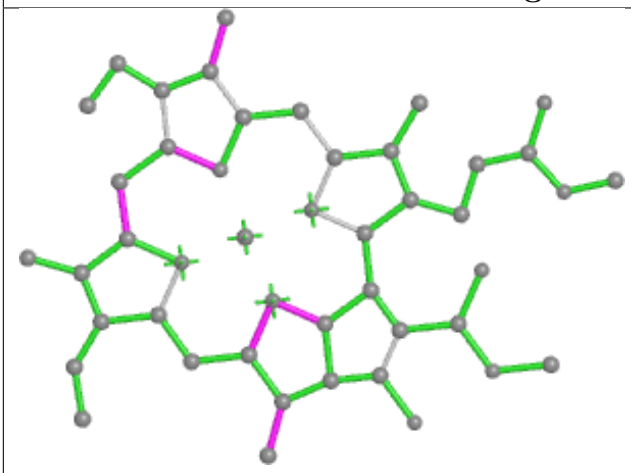
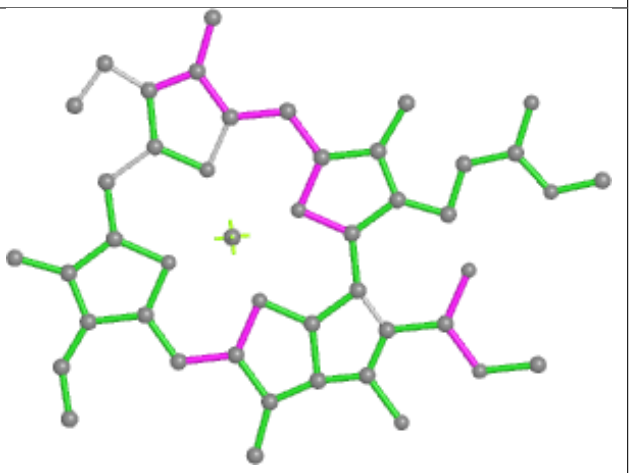


Rings

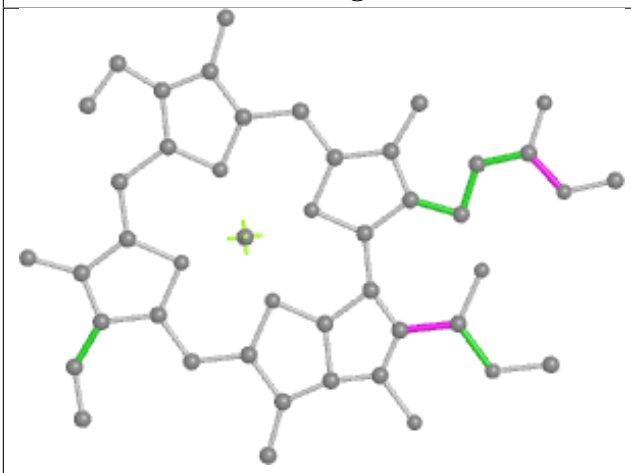
Ligand CLA B 820



Bond lengths



Bond angles



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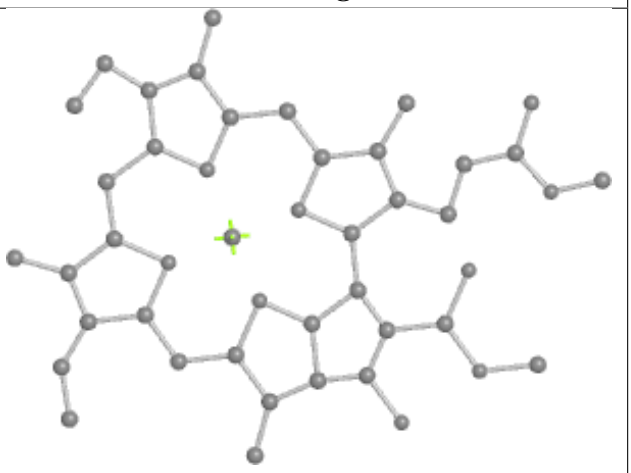
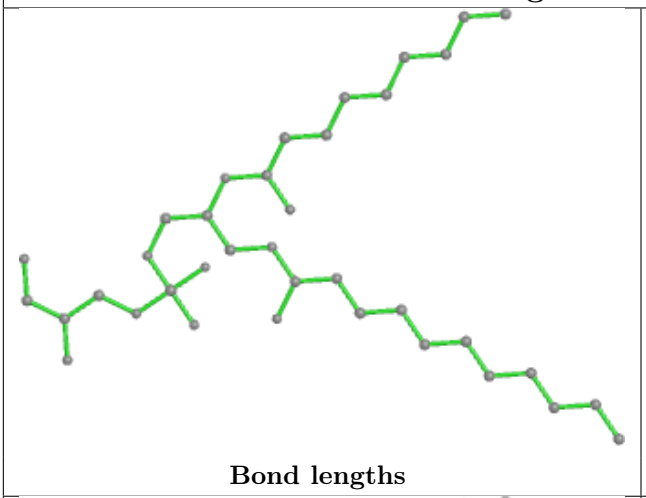


Rings

Ligand LHG 4 618



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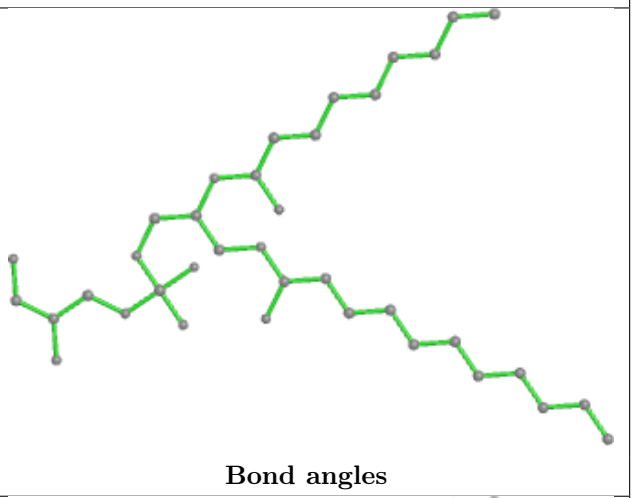
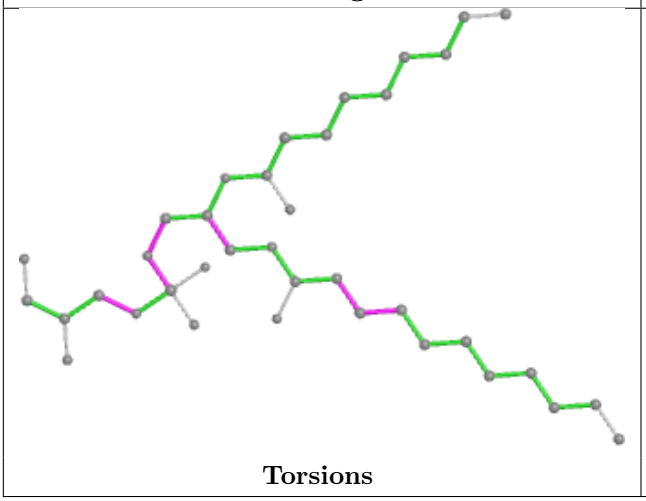


Bond angles



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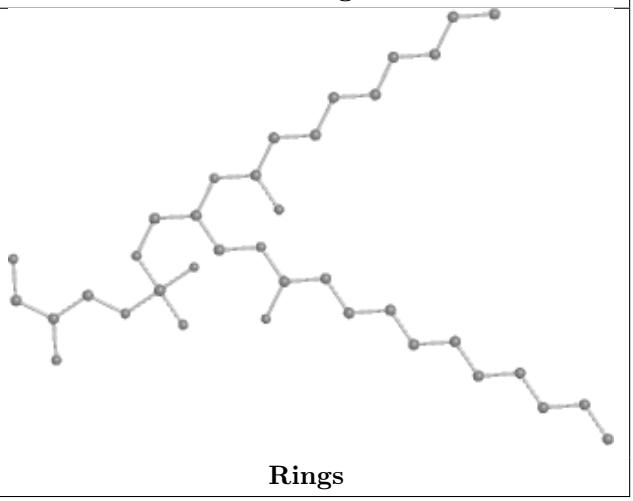
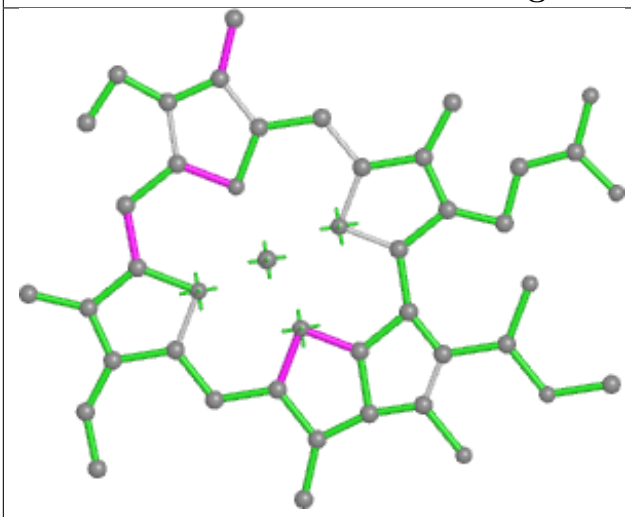


Rings

Ligand CLA 6 612



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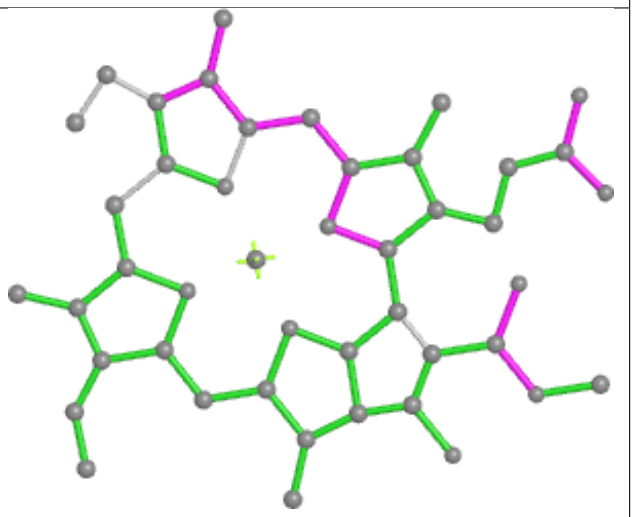

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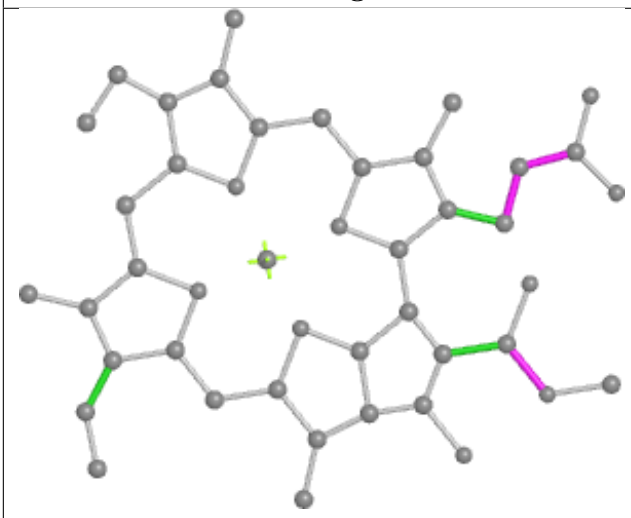

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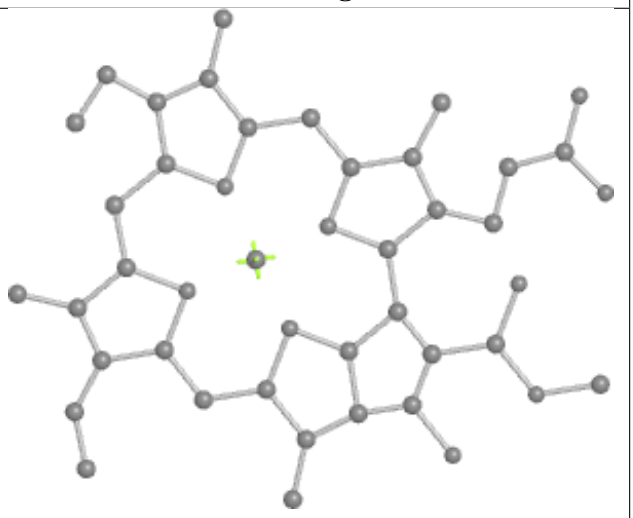
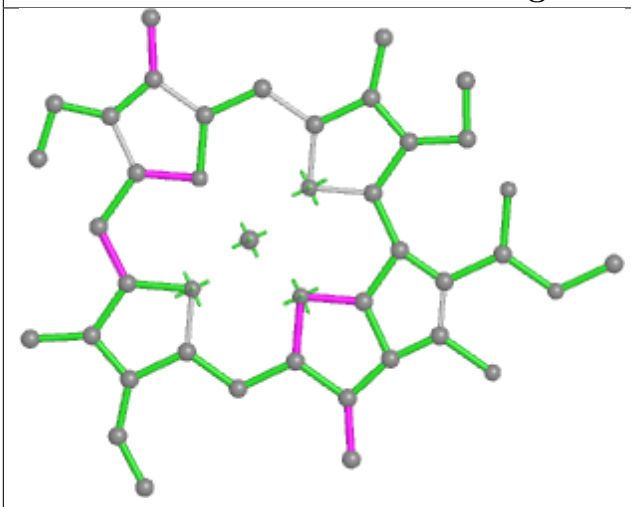


Rings

Ligand CLA 2 613



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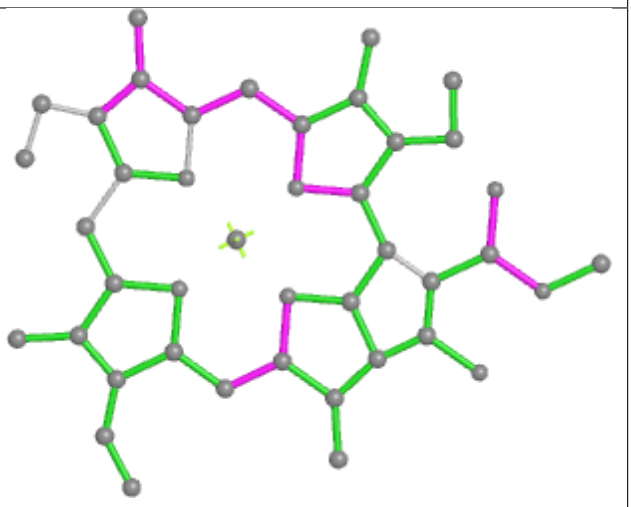
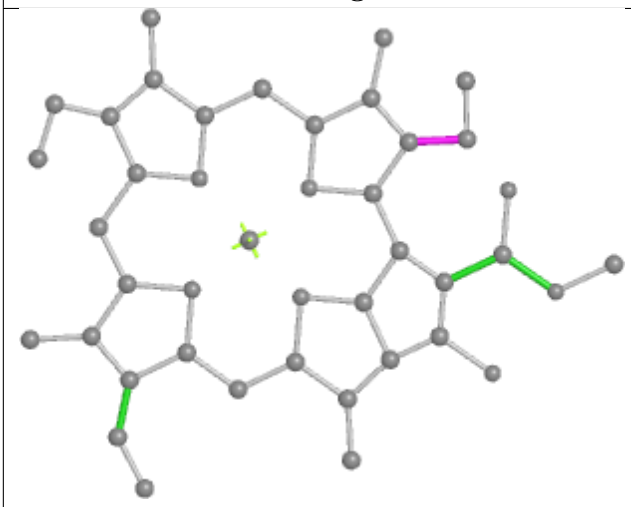


Bond angles



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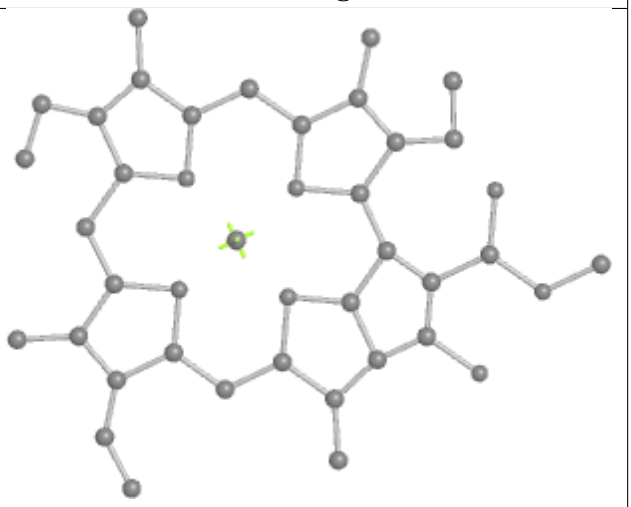
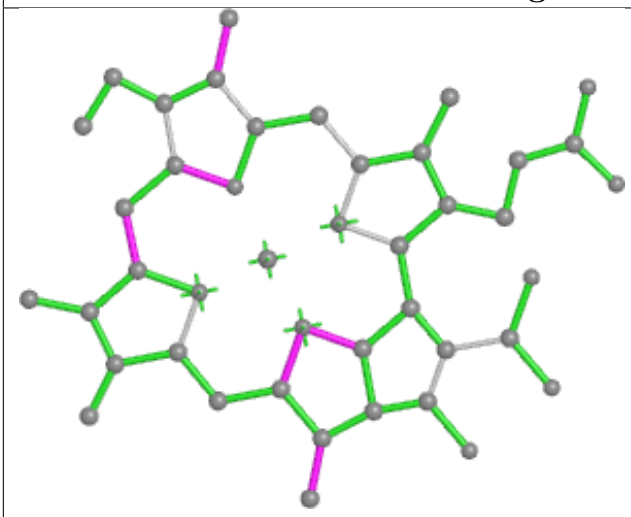


Rings

Ligand CLA 1 310



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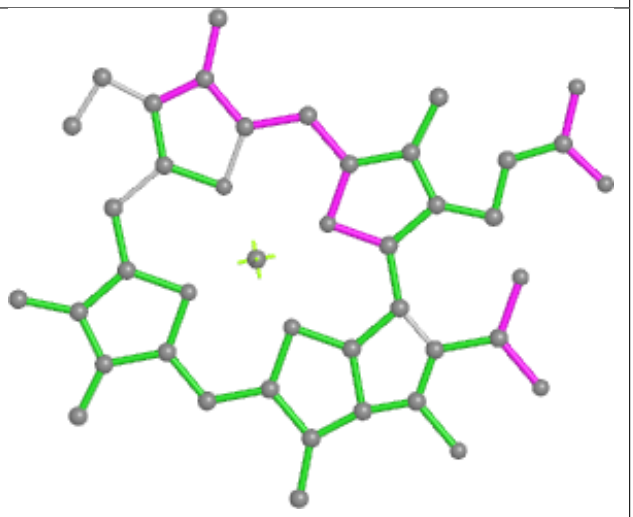
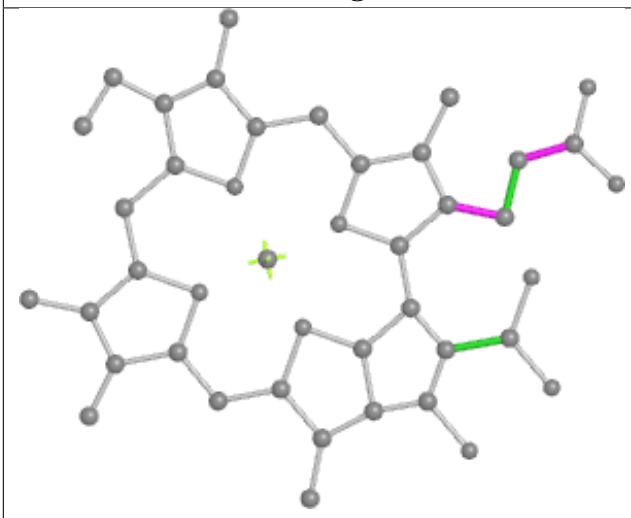


Bond angles



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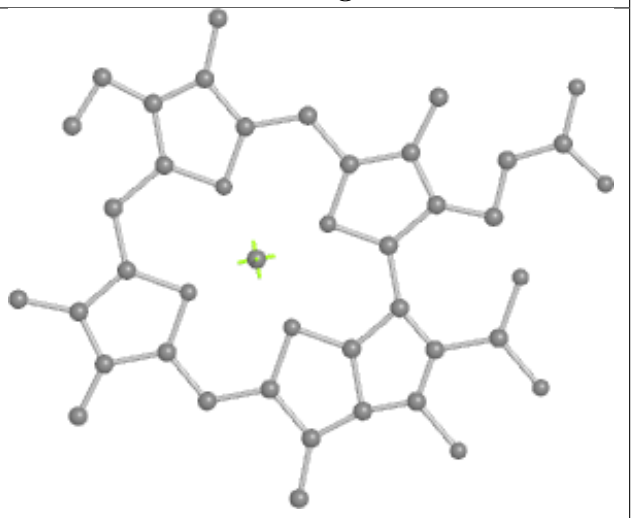
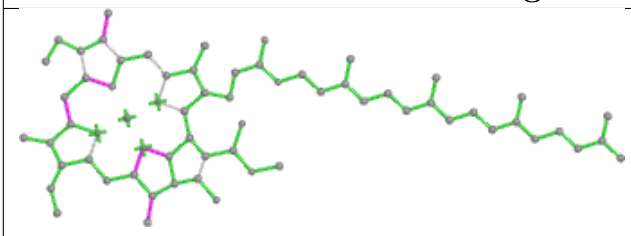
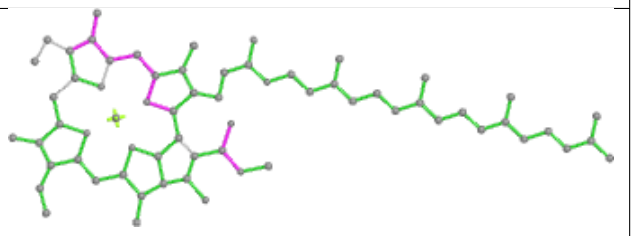


Rings

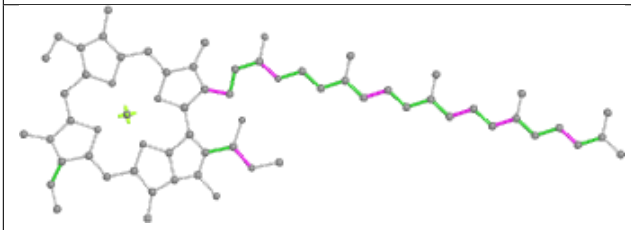
Ligand CLA A 807



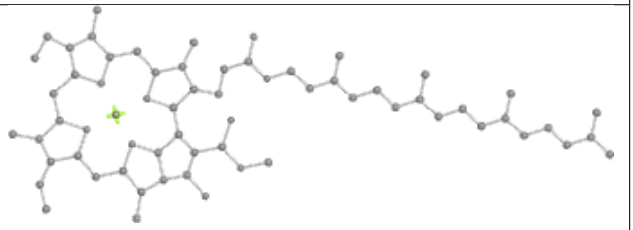
Bond lengths



Bond angles

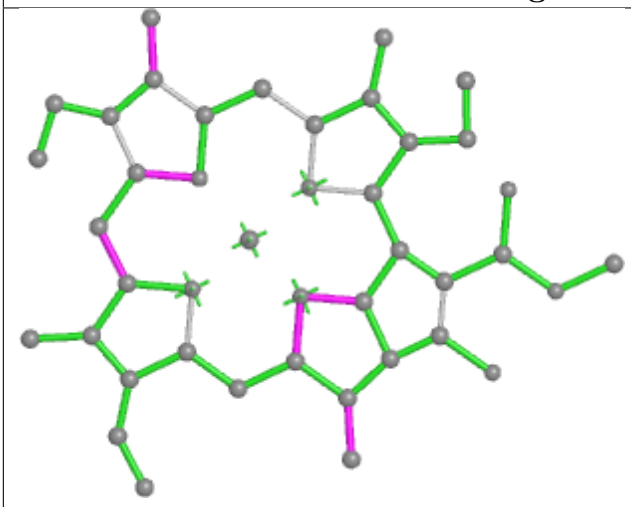


Torsions



Rings

Ligand CLA 6 613



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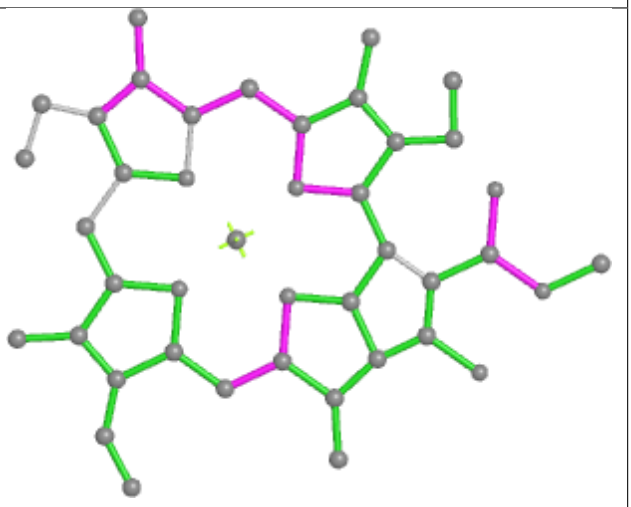

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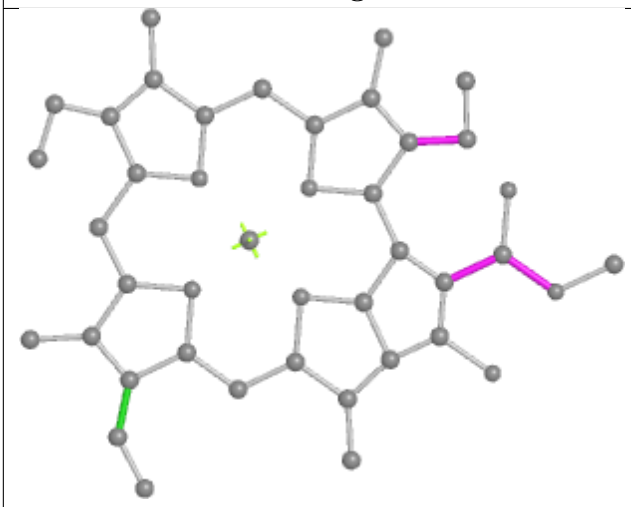

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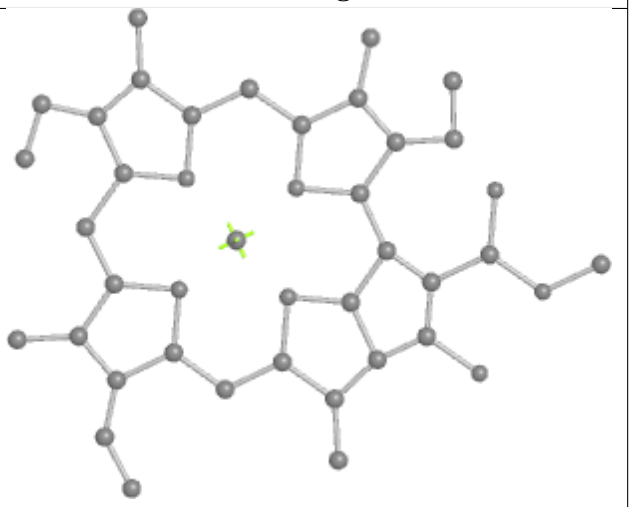
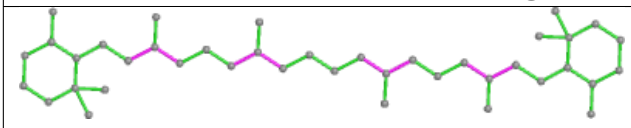


Rings

Ligand BCR B 842



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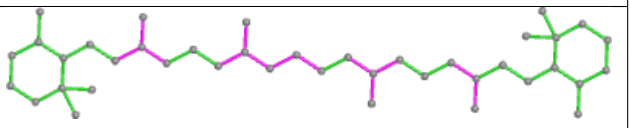
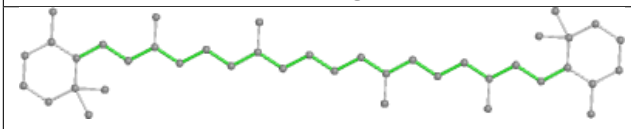


Bond angles



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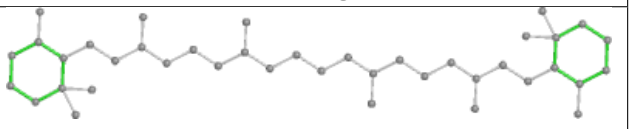
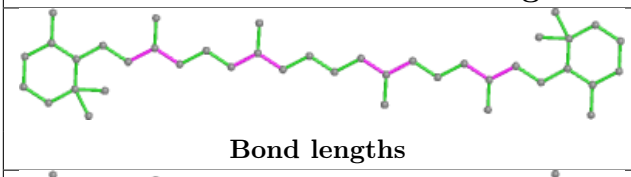


Rings

Ligand BCR A 846



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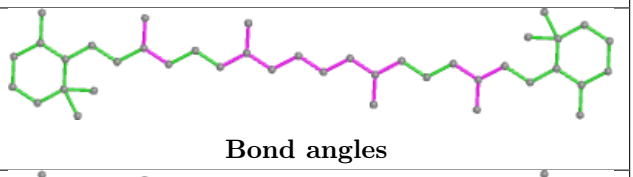
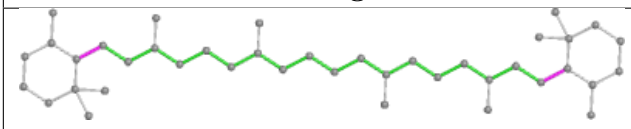


Bond angles



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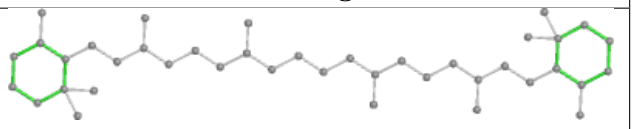
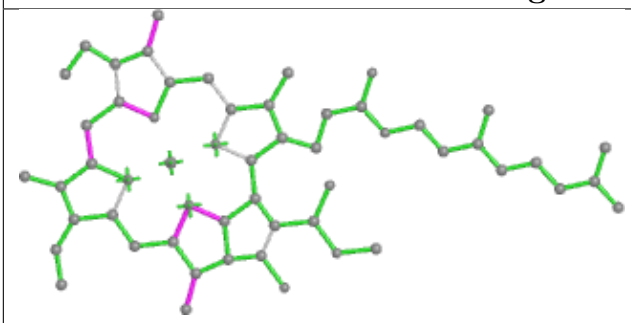


Rings

Ligand CLA 2 608



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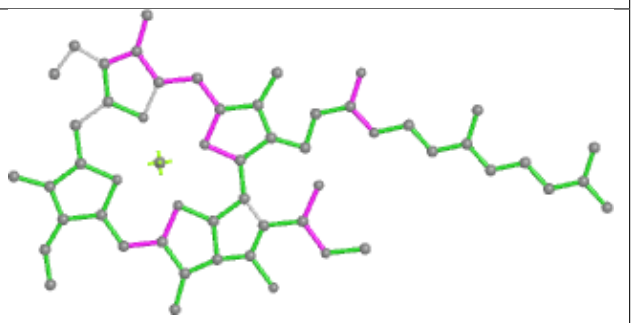

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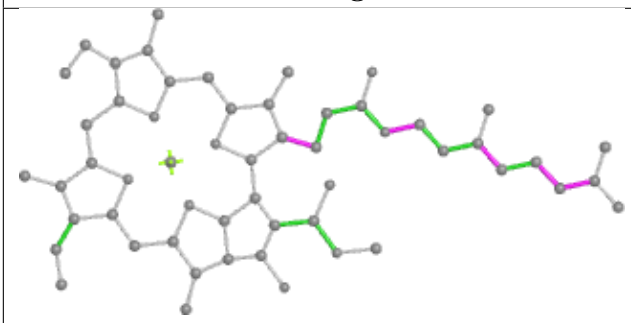

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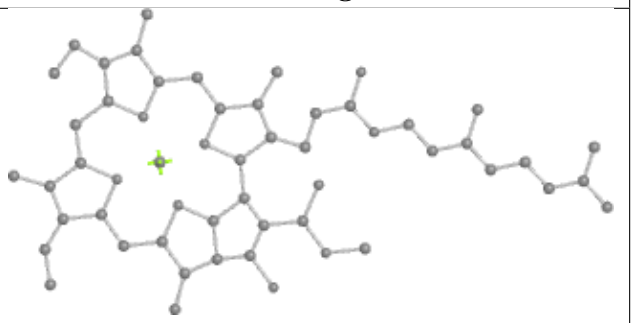
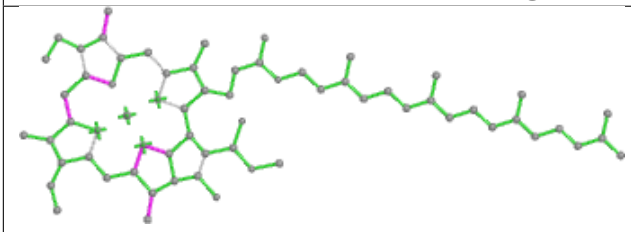


Rings

Ligand CLA A 838



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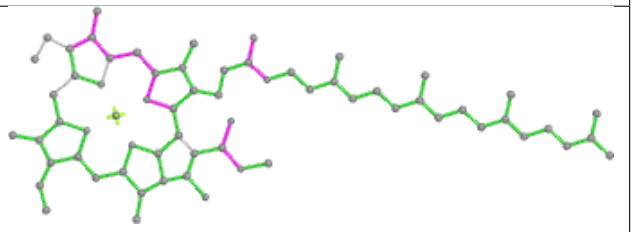

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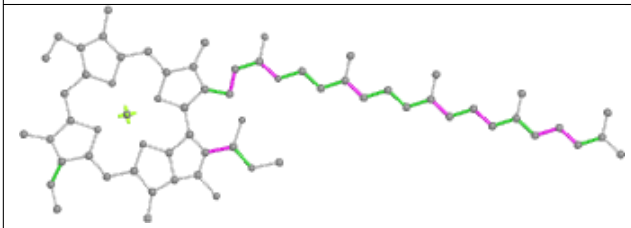

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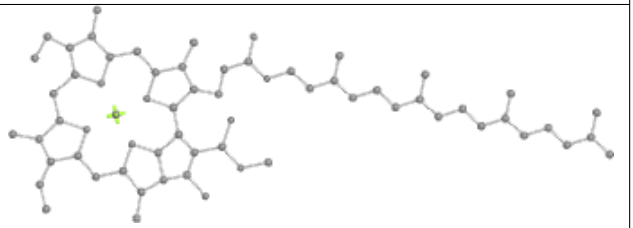
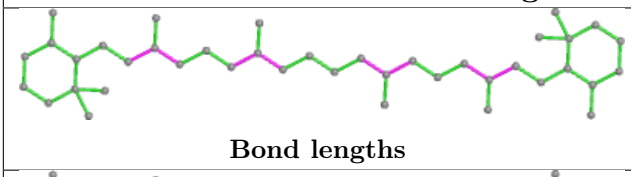


Rings

Ligand BCR G 201



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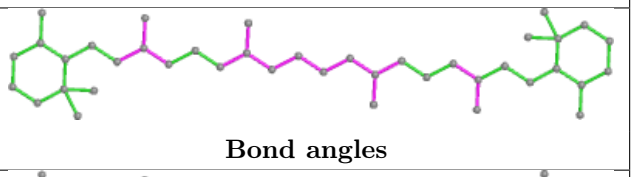
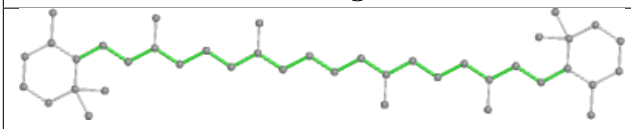


Bond angles



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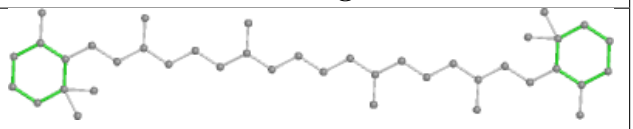
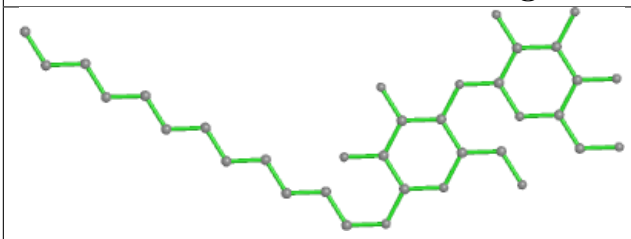
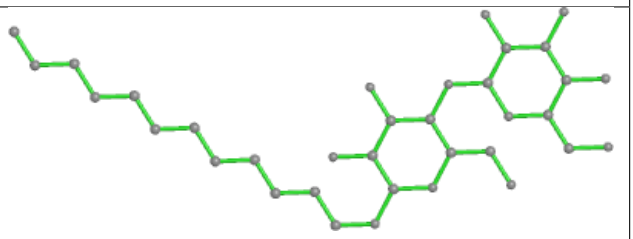


Rings

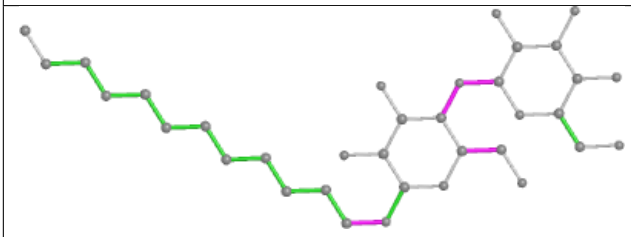
Ligand LMU O 206



Bond lengths



Bond angles



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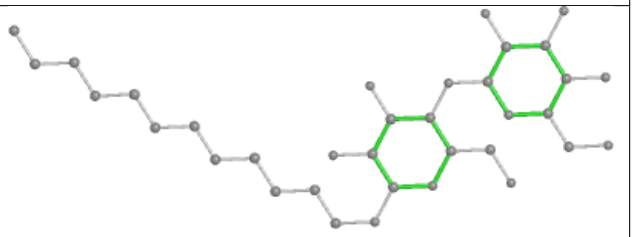
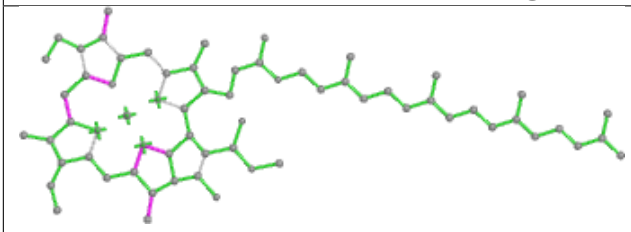


Rings

Ligand CLA A 812



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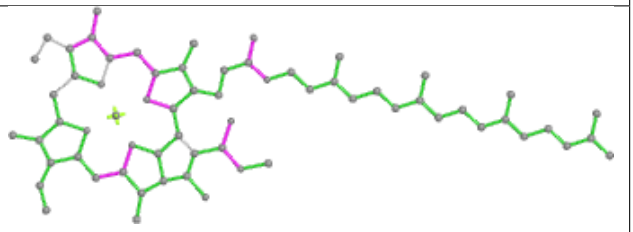
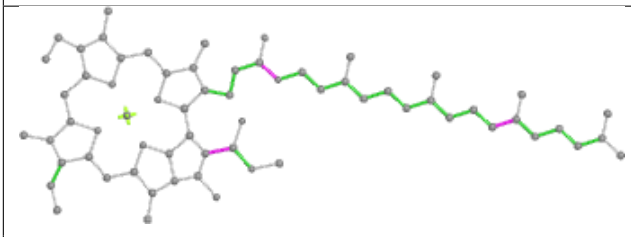


Bond angles



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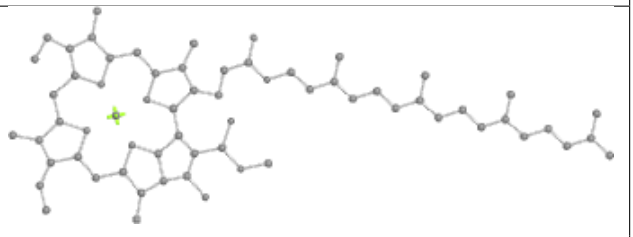
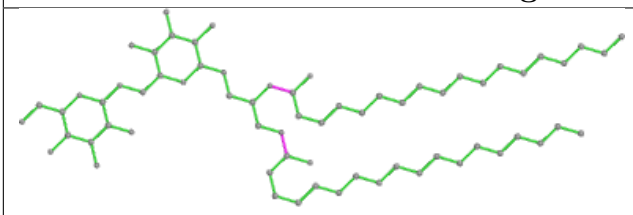


Rings

Ligand DGD B 847



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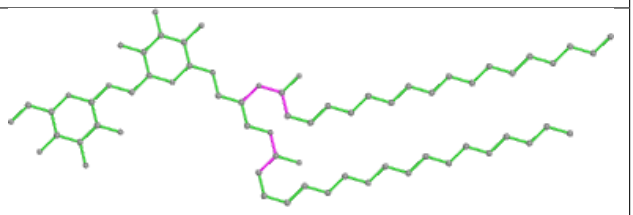
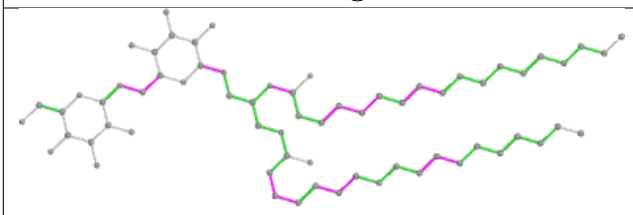


Bond angles



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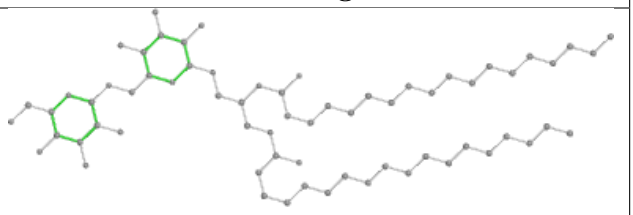
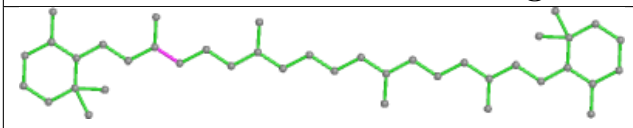


Rings

Ligand BCR J 104



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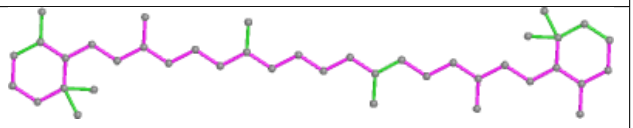
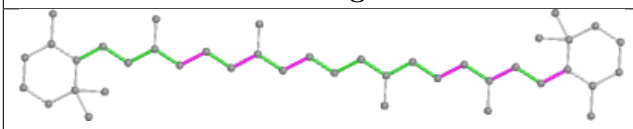


Bond angles



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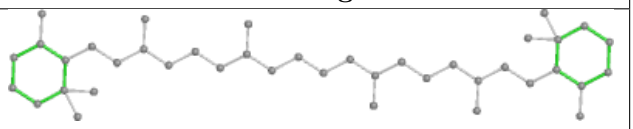
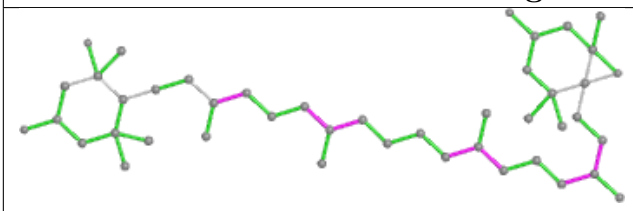


Rings

Ligand NEX b 318



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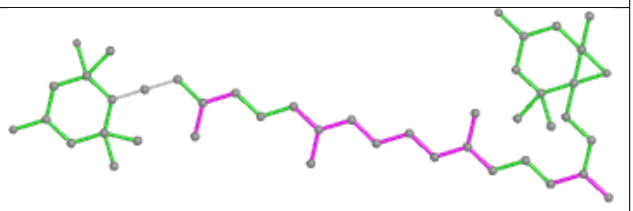
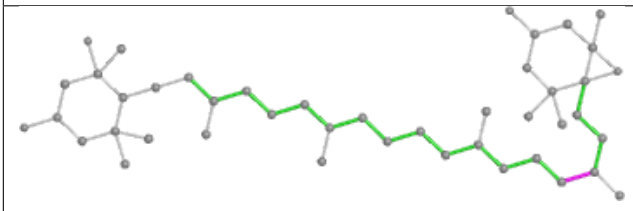


Bond angles



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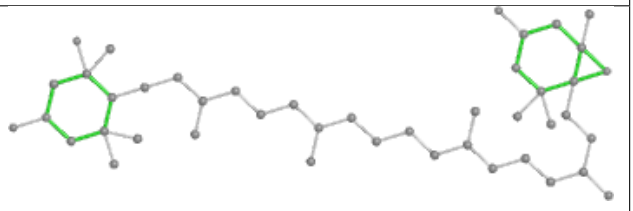
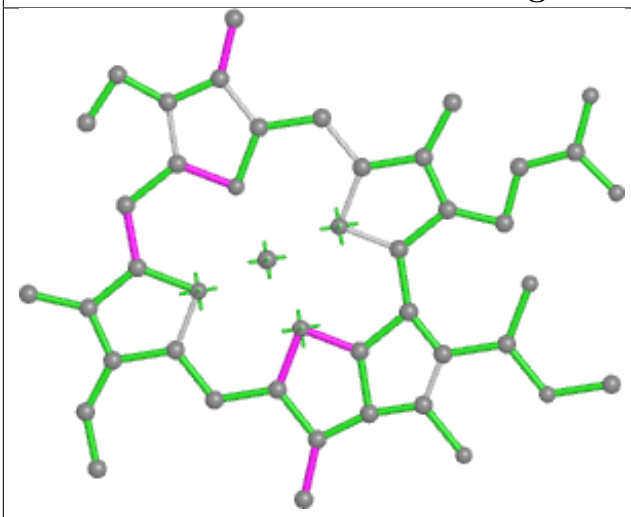


Rings

Ligand CLA 9 612



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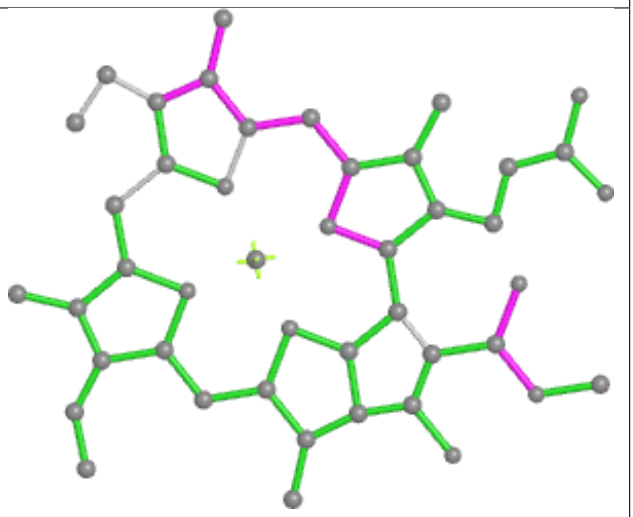
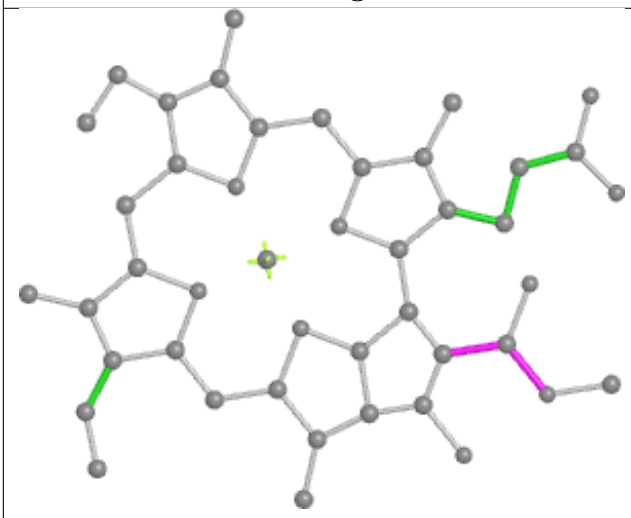
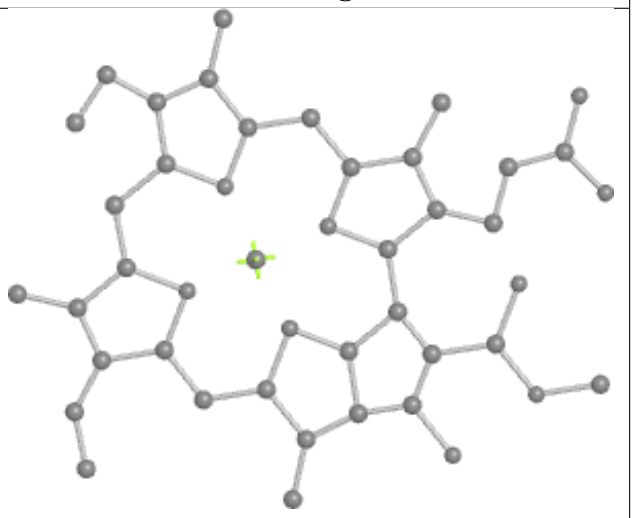


Bond angles

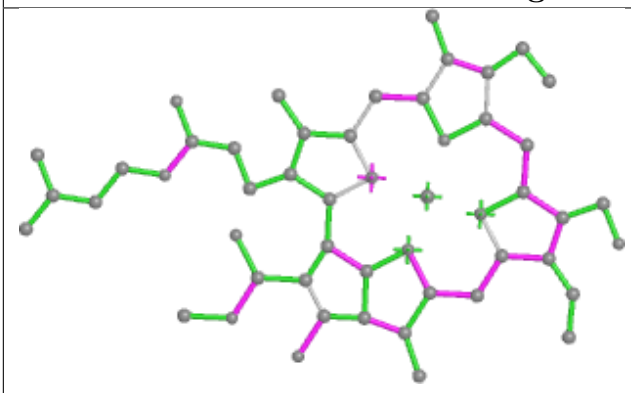


Torsions

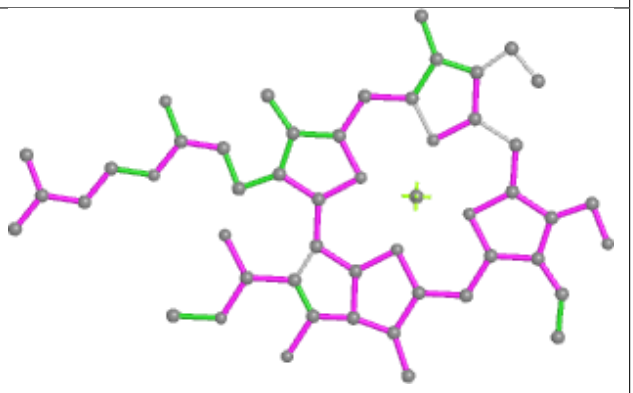


Rings

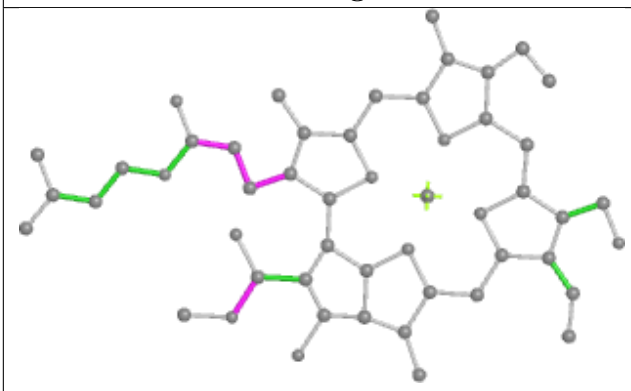
Ligand CHL 8 607



Bond lengths



Bond angles



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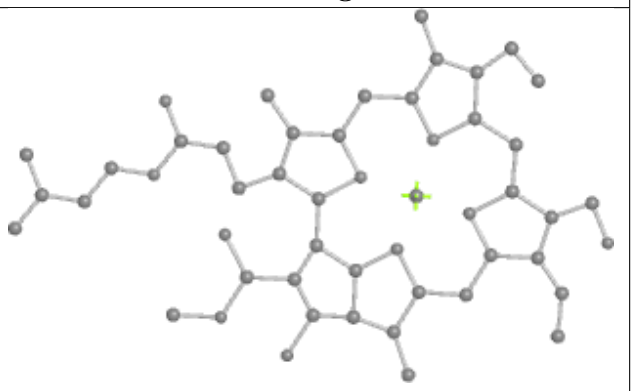

Rings

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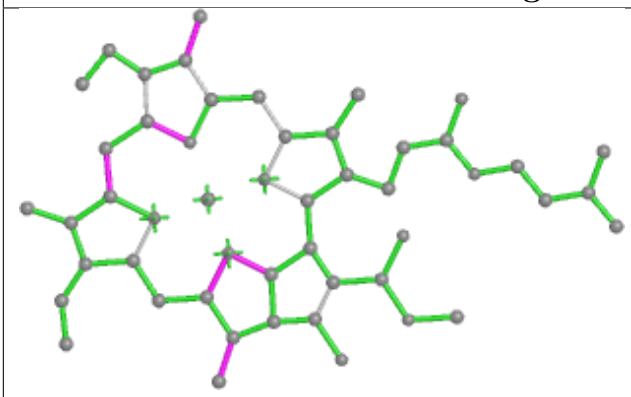
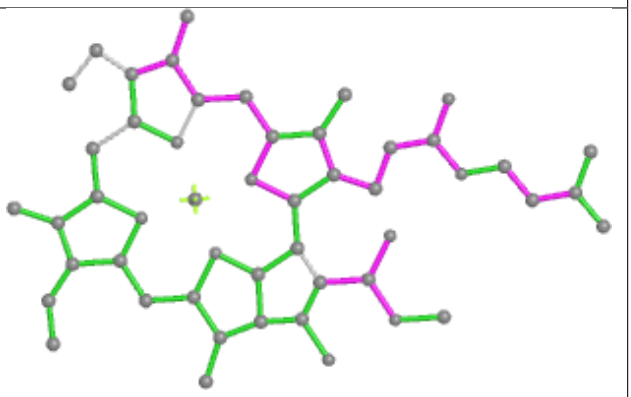
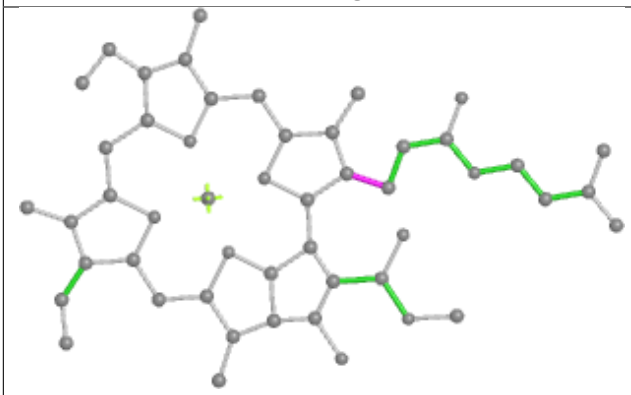
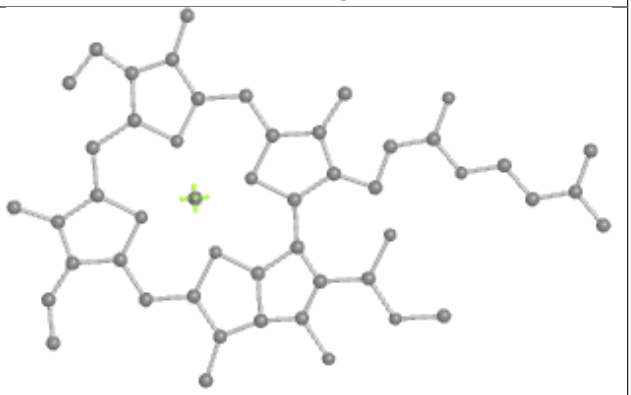
 Bond lengths	 Bond angles
 Torsions	 Rings

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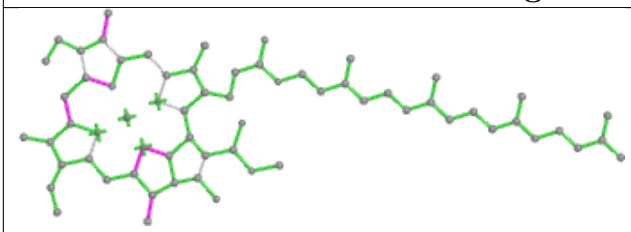
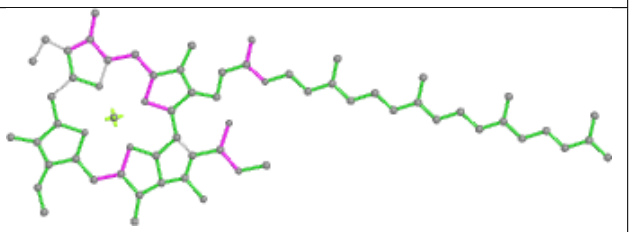
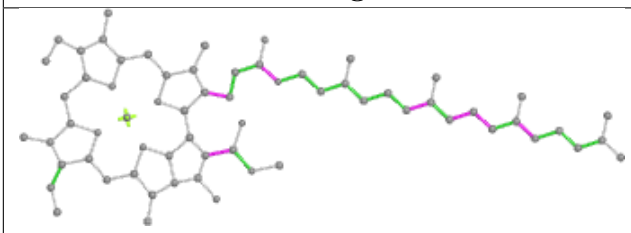
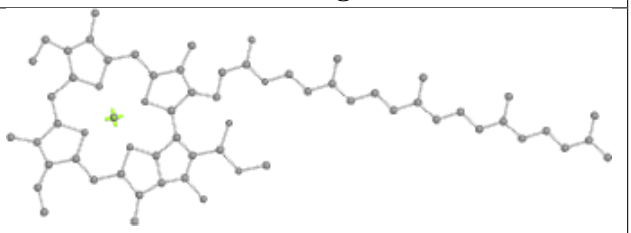
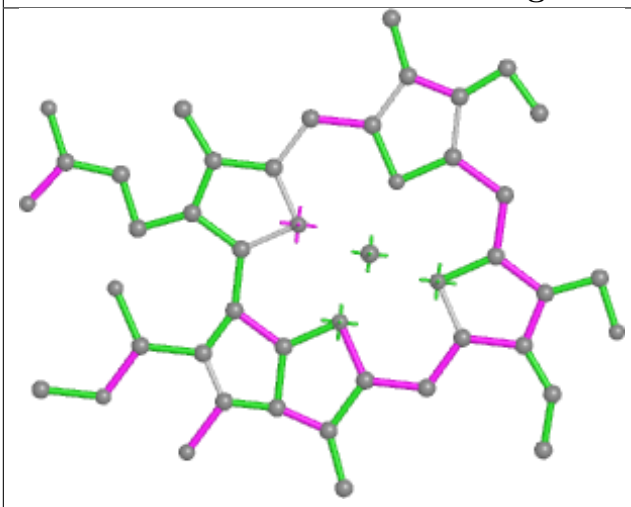
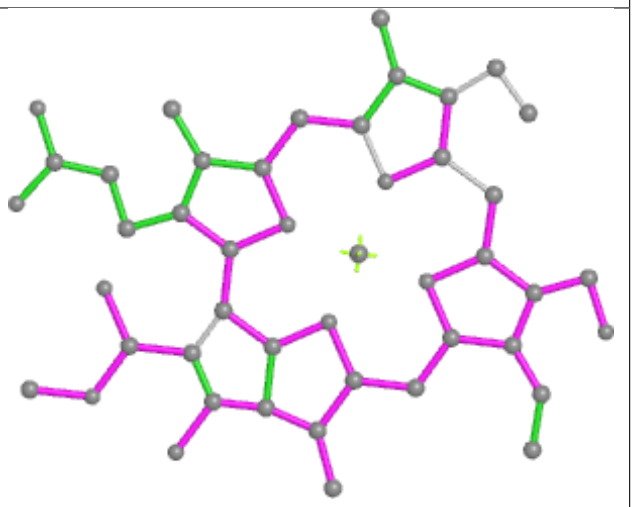
 Bond lengths	 Bond angles
 Torsions	 Rings

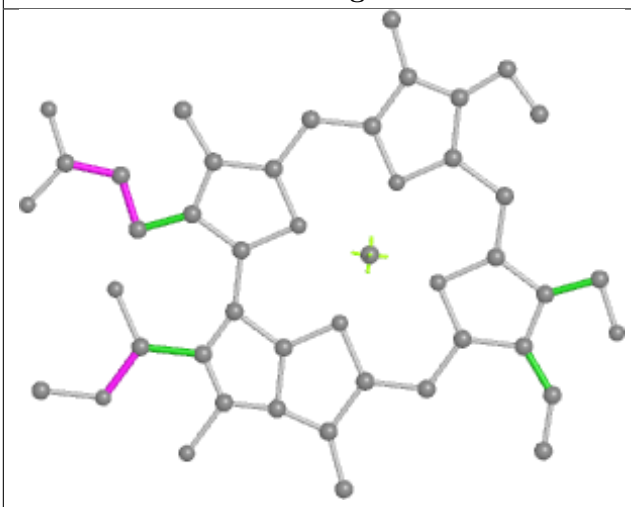
Ligand CHL 6 614



Bond lengths



Bond angles



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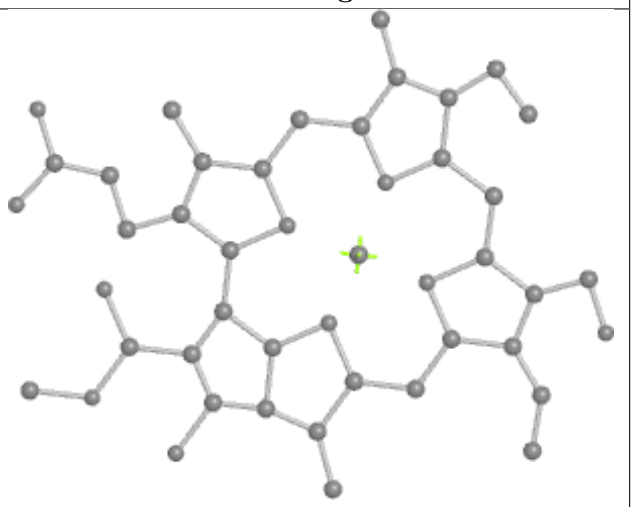
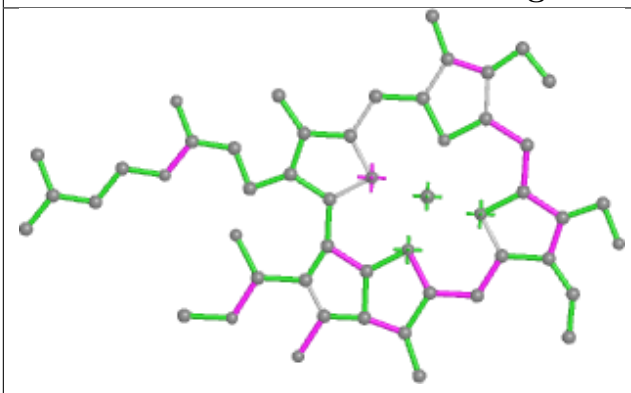


Rings

Ligand CHL 2 607



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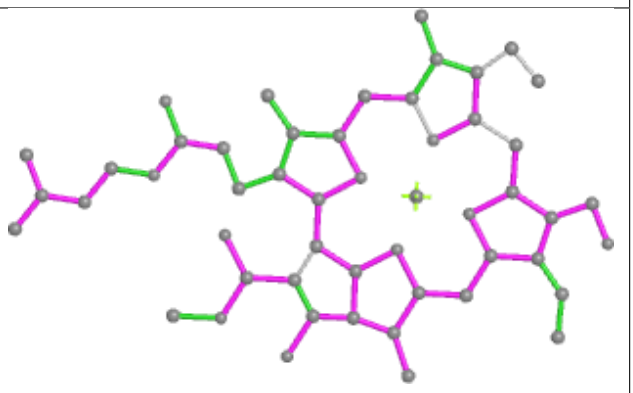
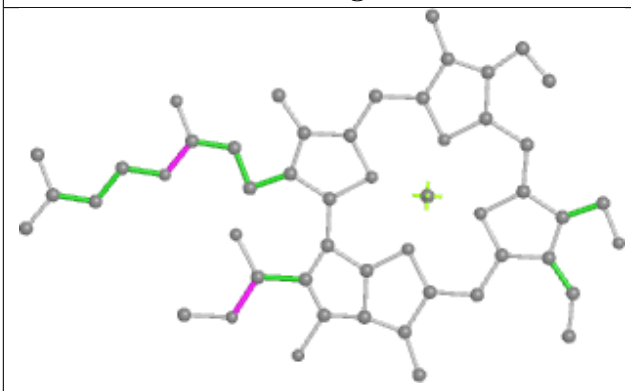


Bond angles



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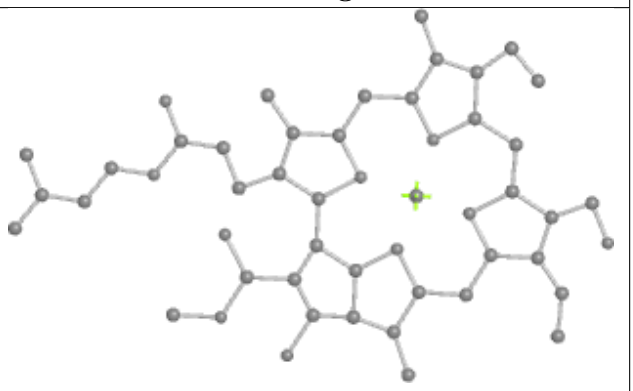
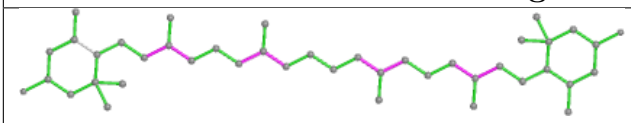


Rings

Ligand LUT a 616



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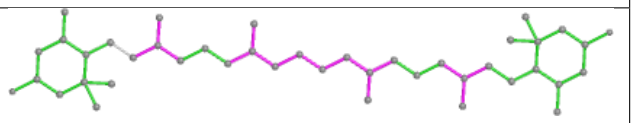
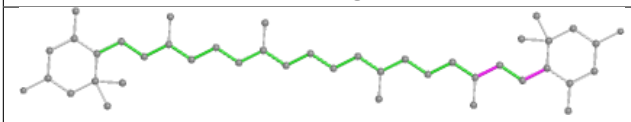


Bond angles



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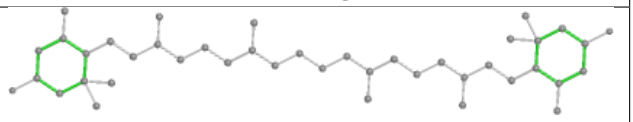
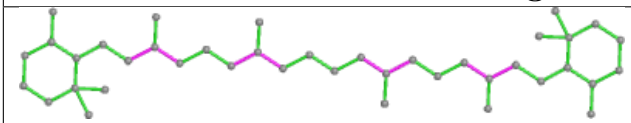


Rings

Ligand BCR 8 616



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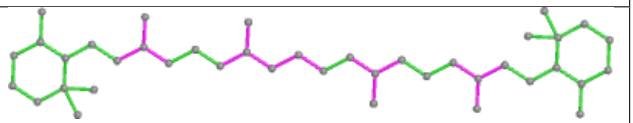

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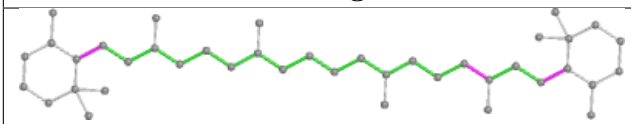

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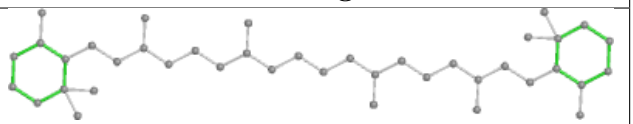
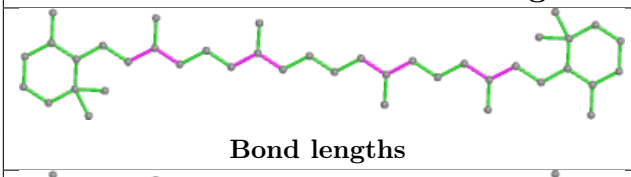


Rings

Ligand BCR I 101



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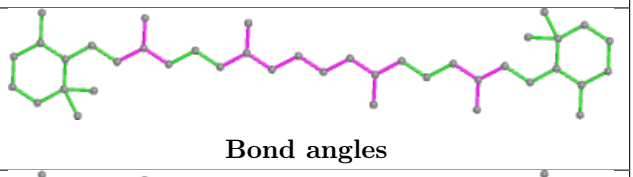

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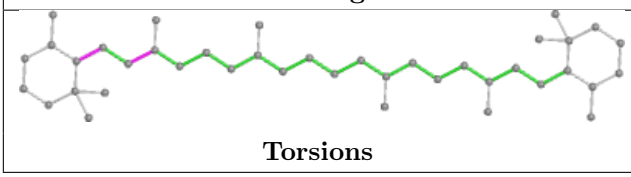

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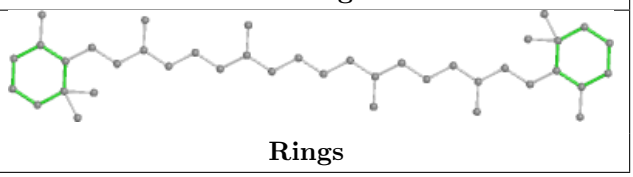
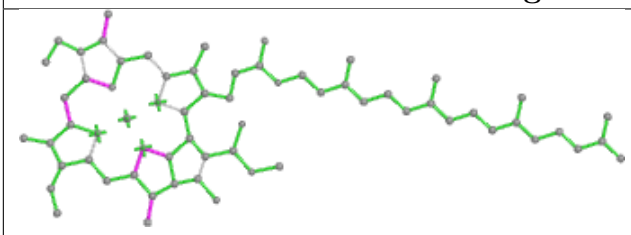


Rings

Ligand CLA A 821



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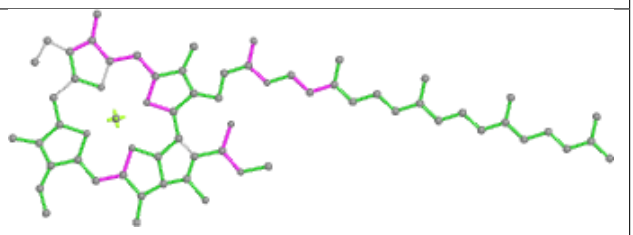
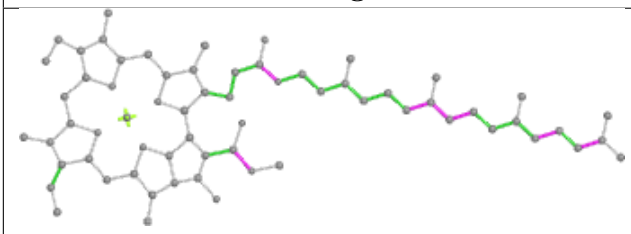


Bond angles



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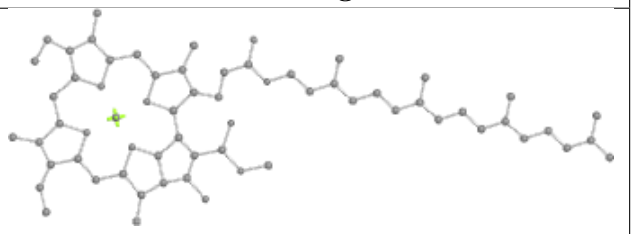
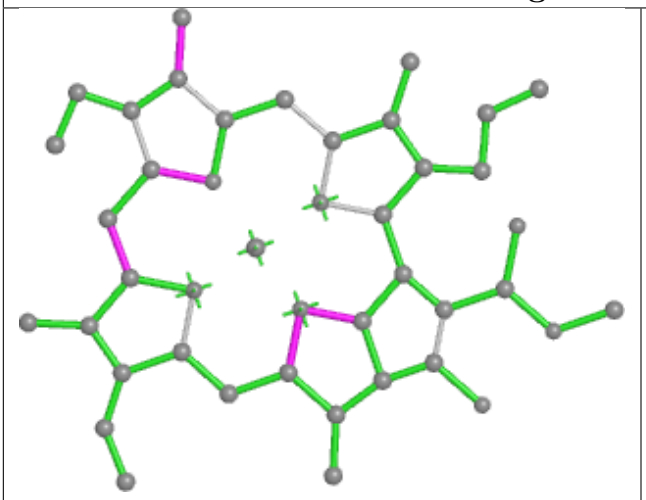


Rings

Ligand CLA 8 612



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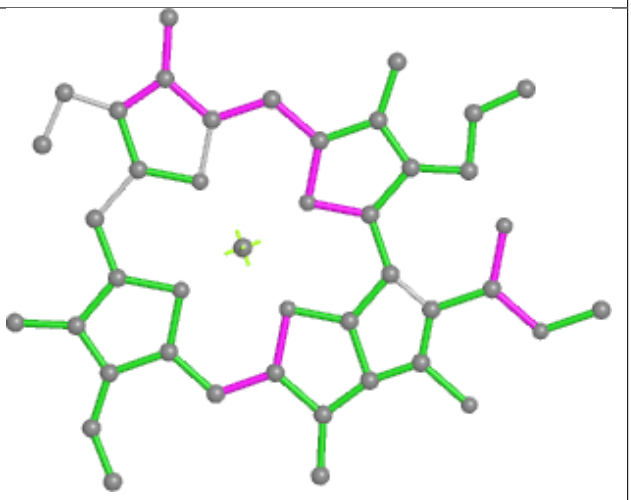
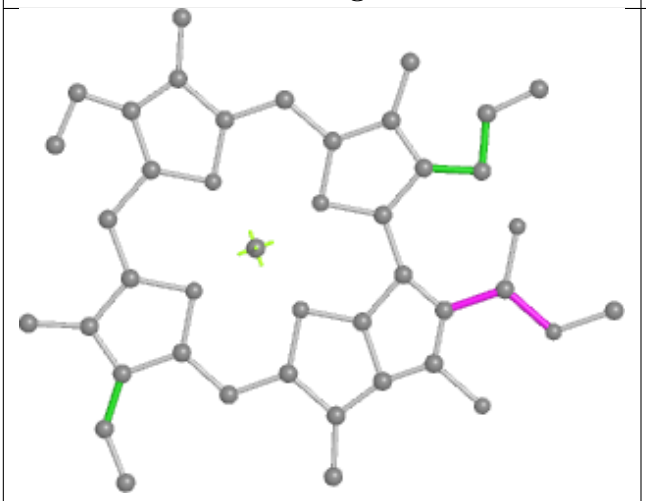


Bond angles



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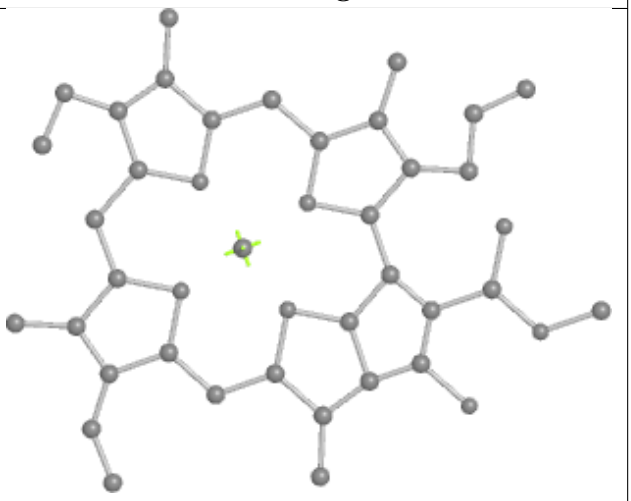
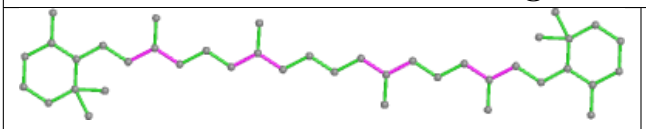


Rings

Ligand BCR L 305



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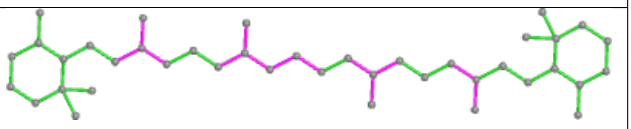
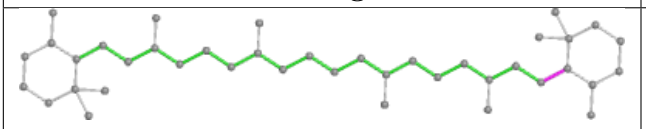


Bond angles



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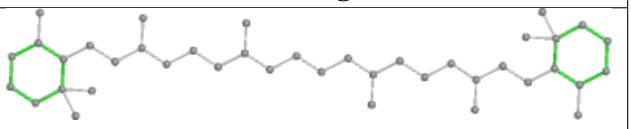
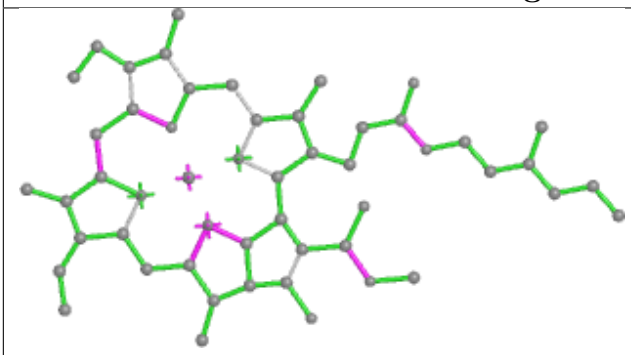
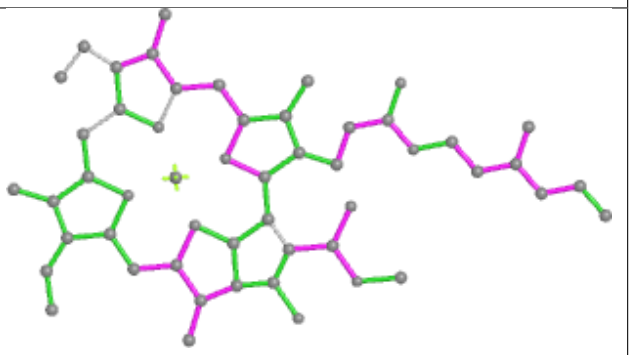
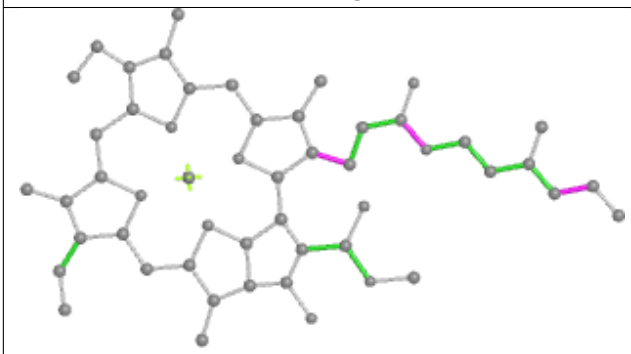
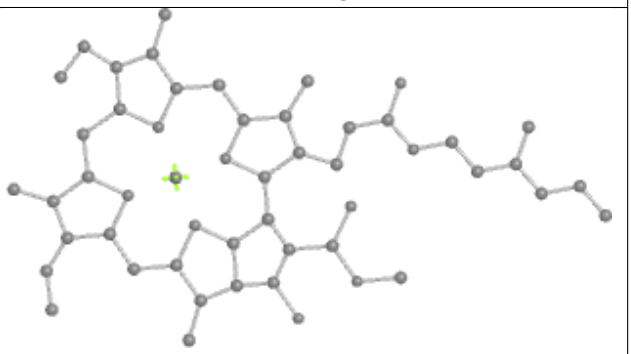
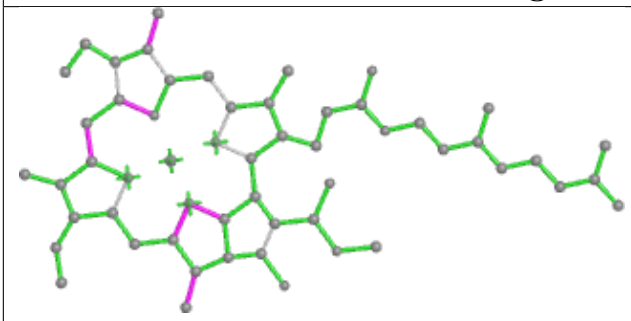
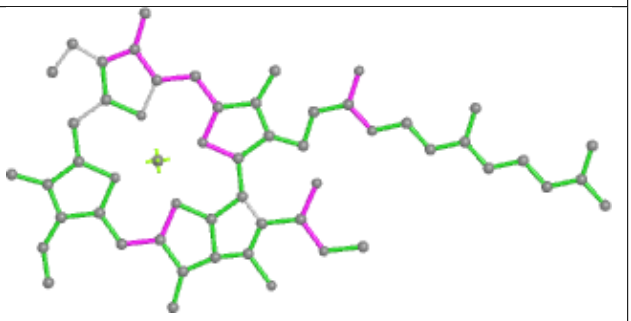
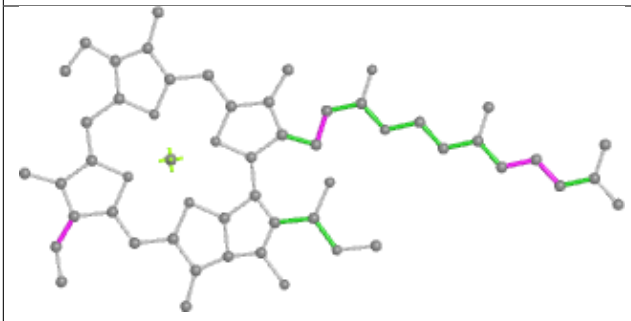
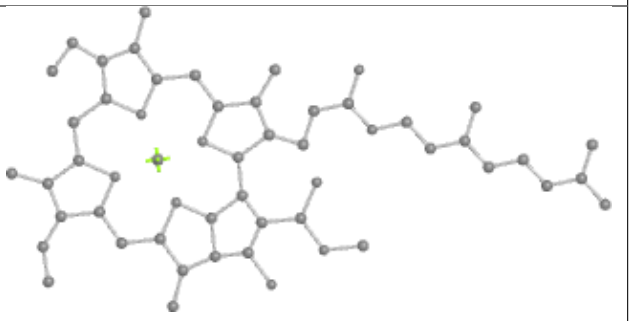


Rings

Ligand CLA A 830	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA 4 612	
	
Bond lengths	Bond angles
	
Torsions	Rings

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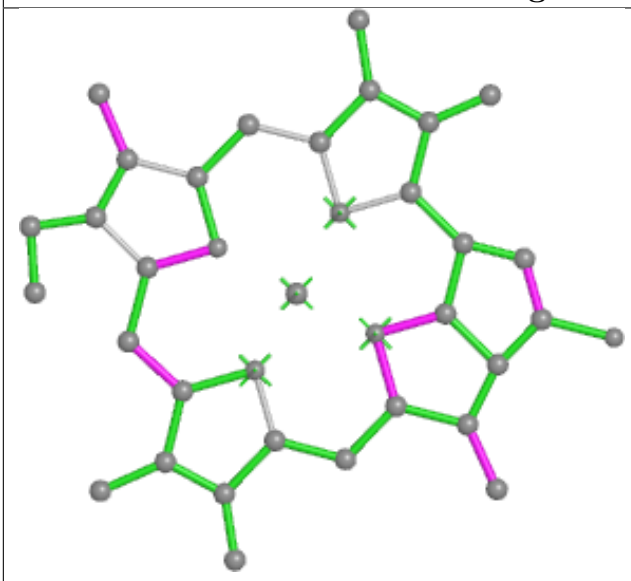

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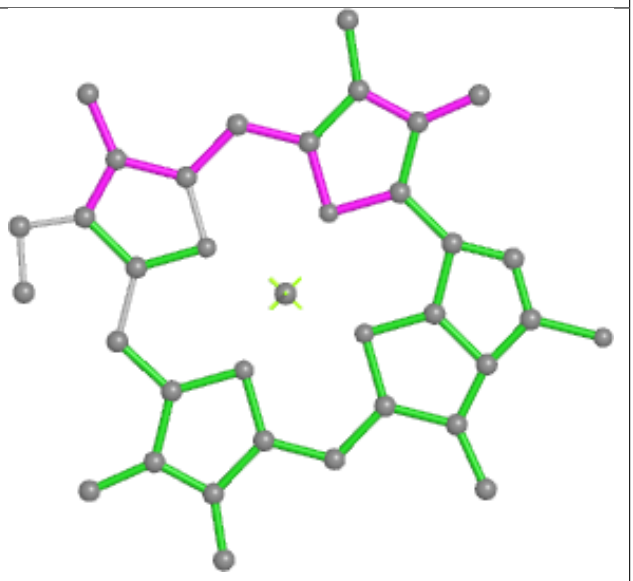
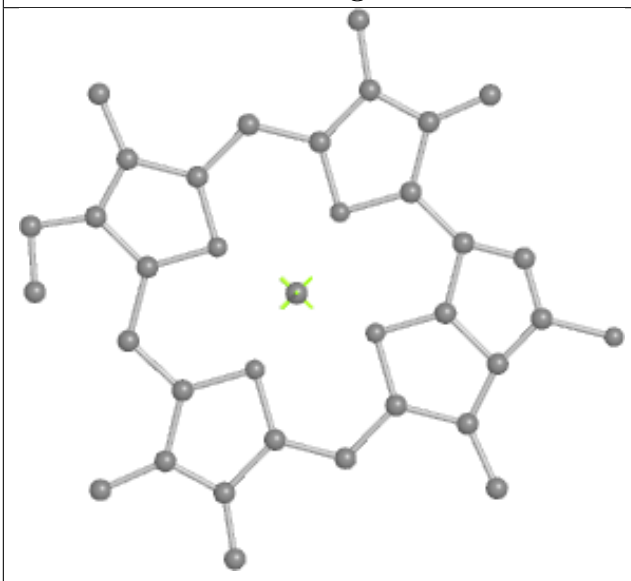


Bond angles



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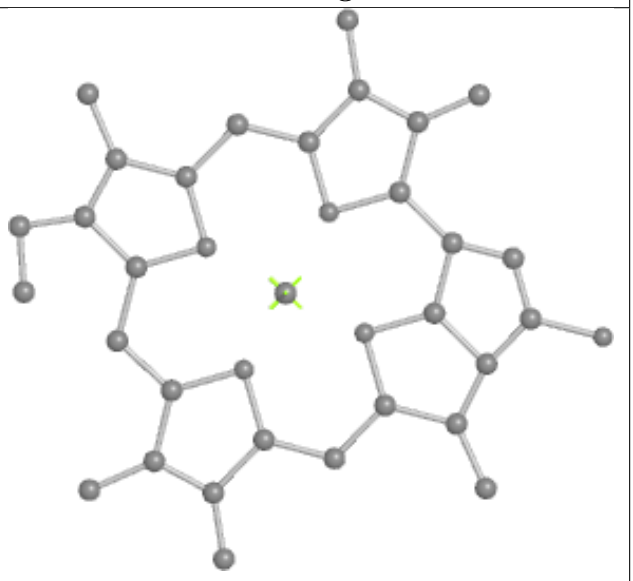
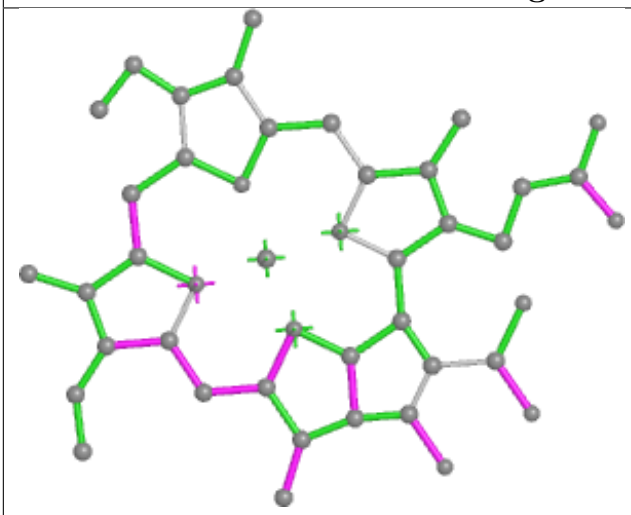


Rings

Ligand CLA 7 407



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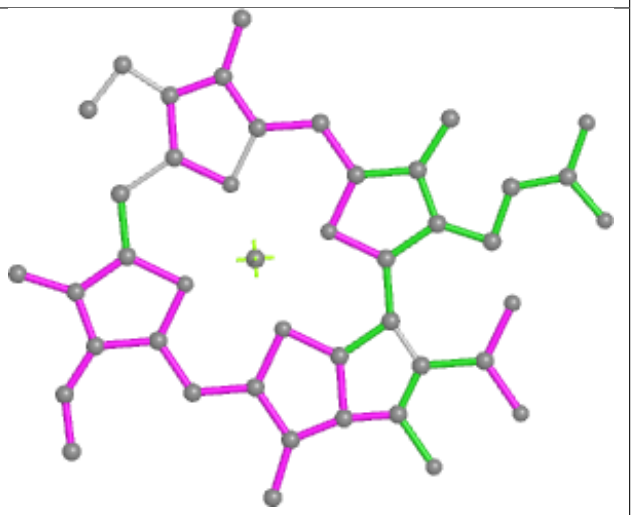
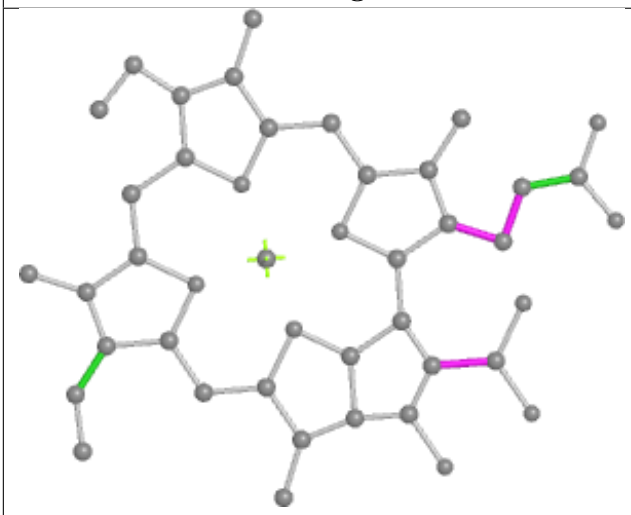


Bond angles



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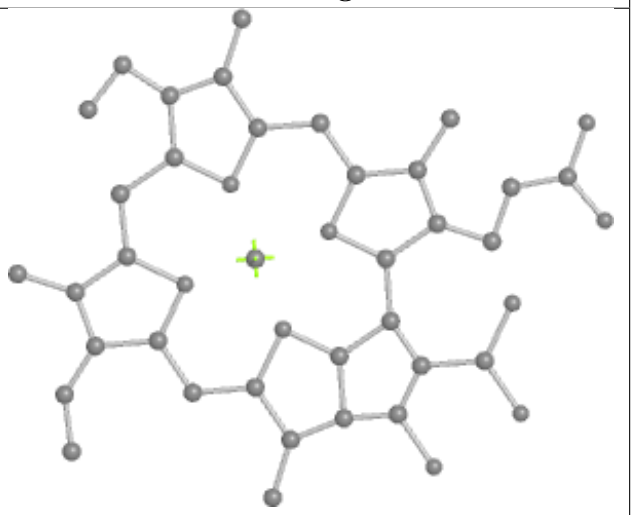
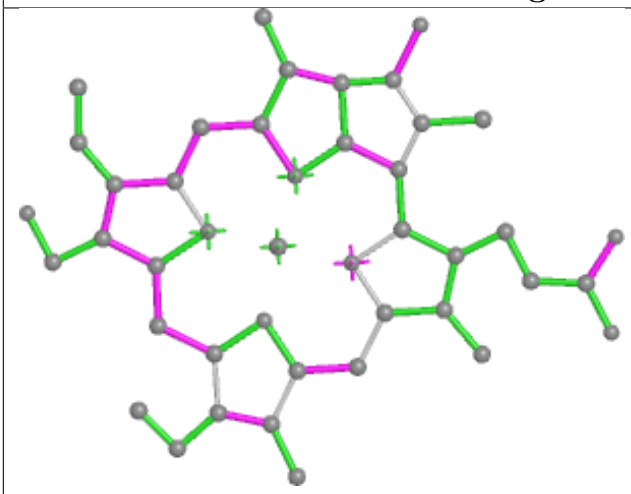


Rings

Ligand CHL c 605



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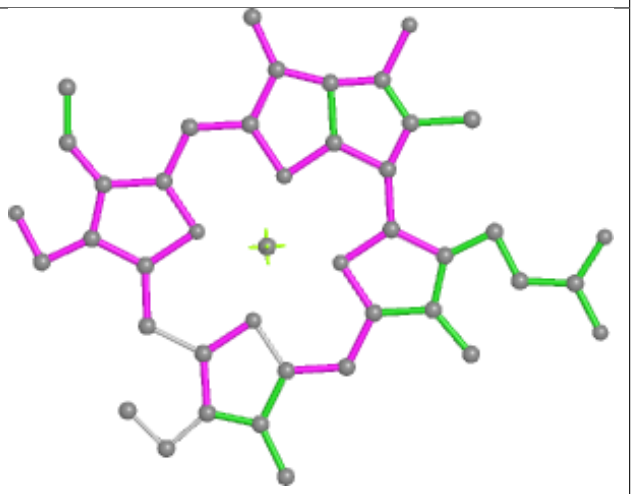
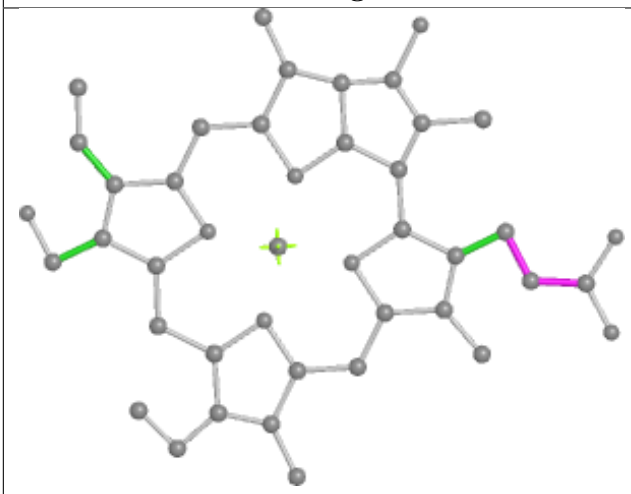


Bond angles



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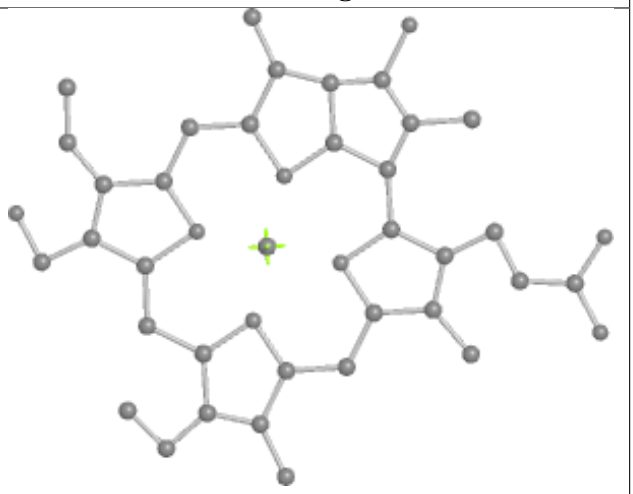
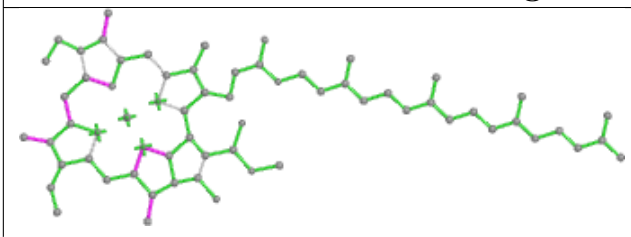


Rings

Ligand CLA A 842



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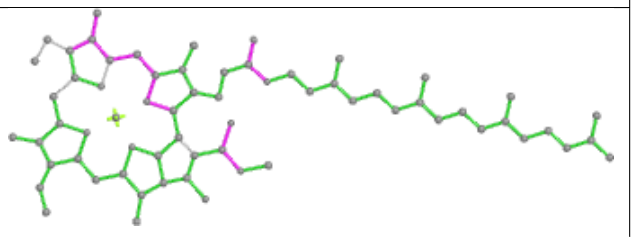

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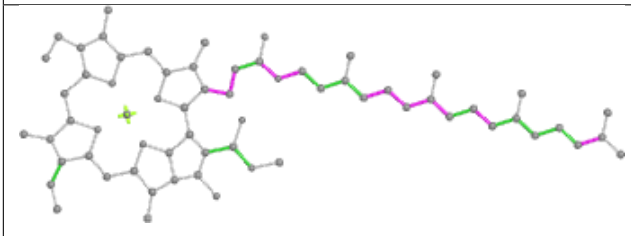

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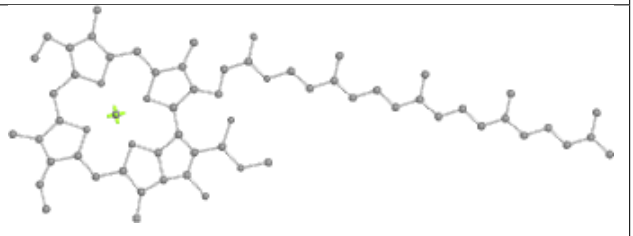
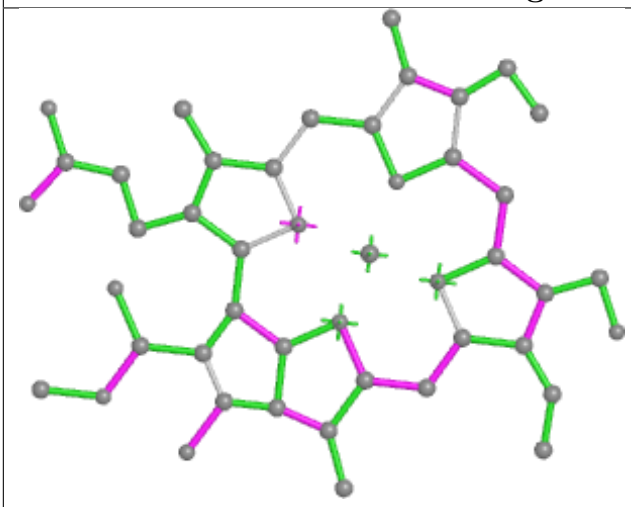


Rings

Ligand CHL b 307



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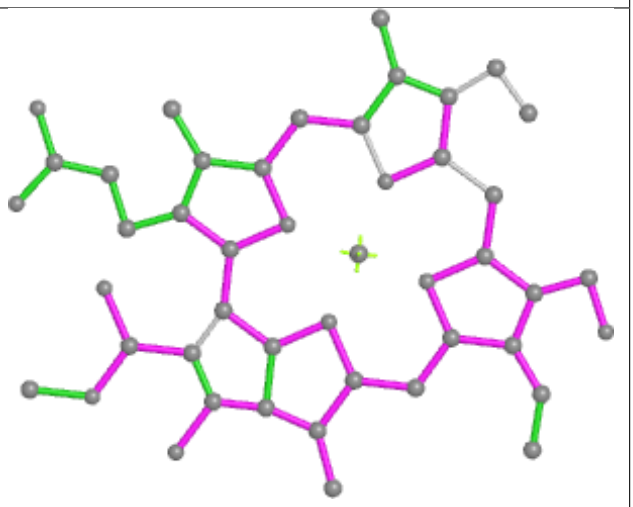

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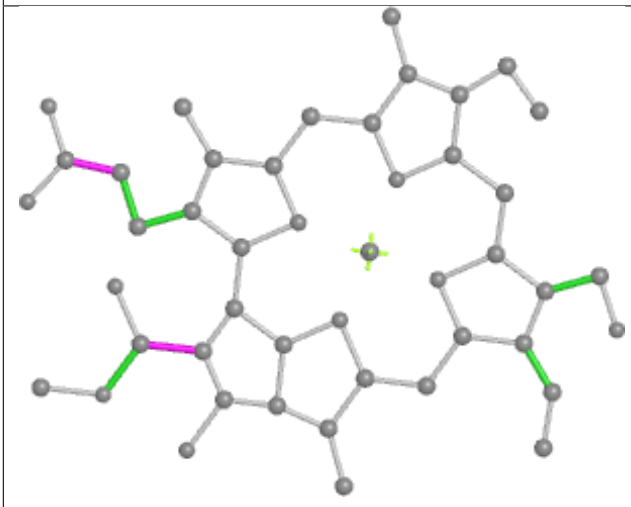

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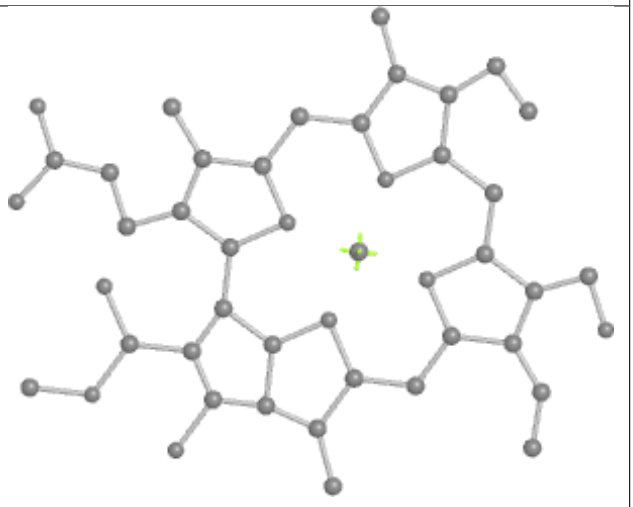

Rings

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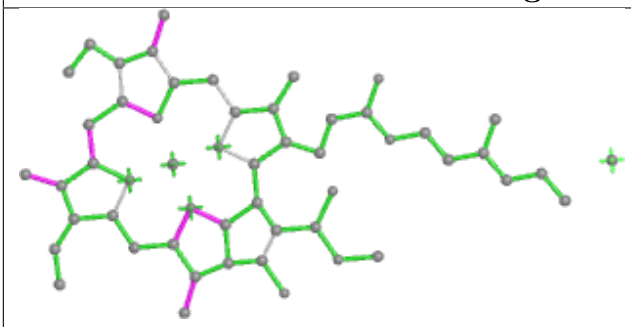

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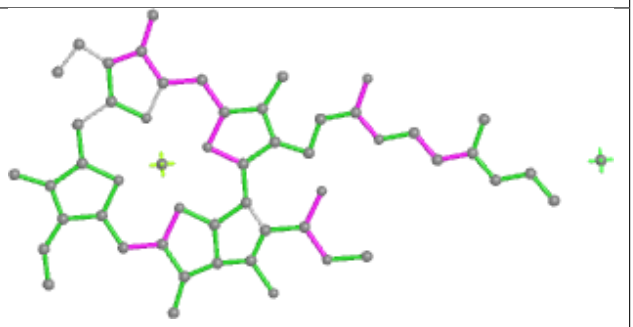
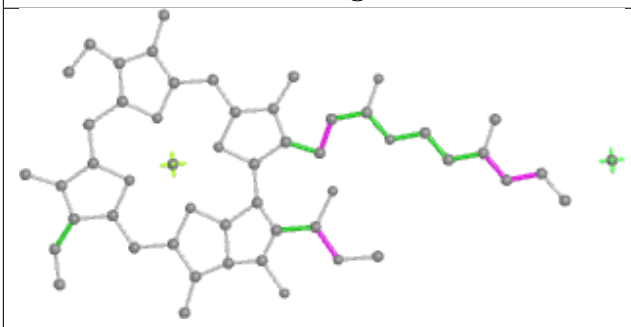


Bond angles



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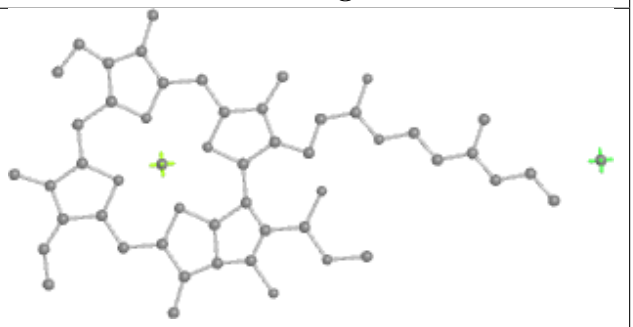
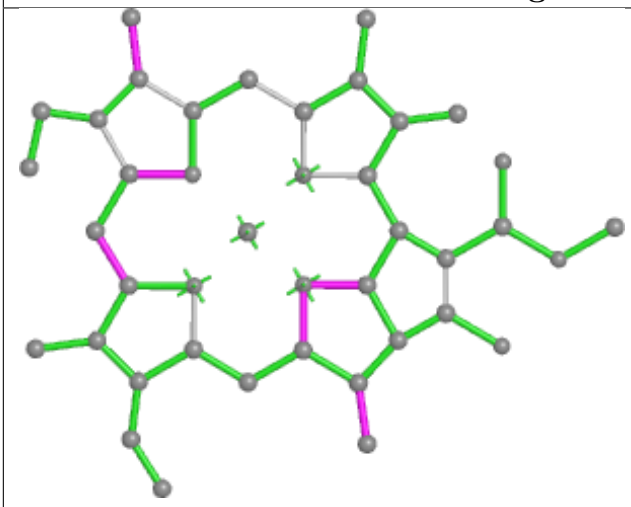


Rings

Ligand CLA a 614



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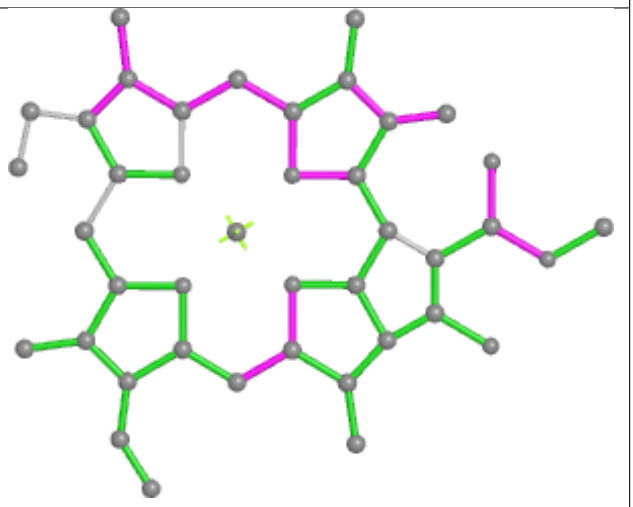

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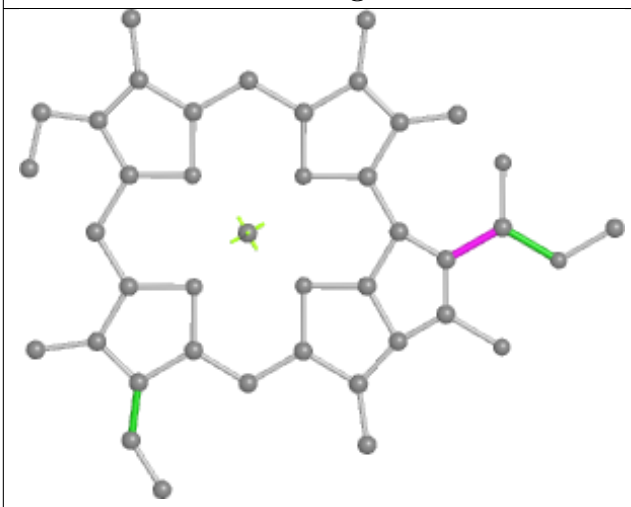

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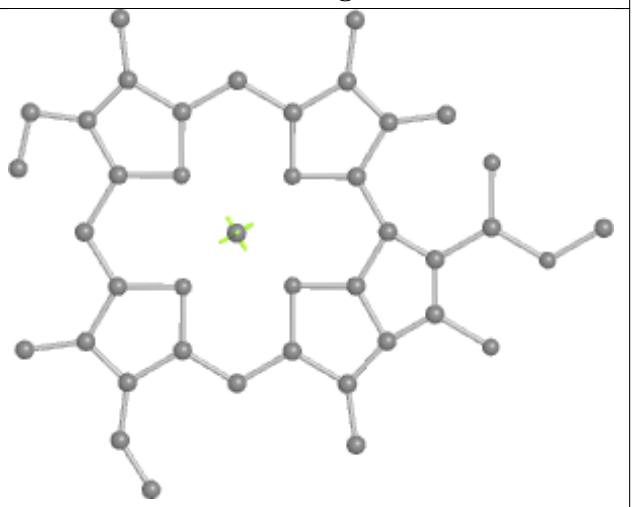

Rings

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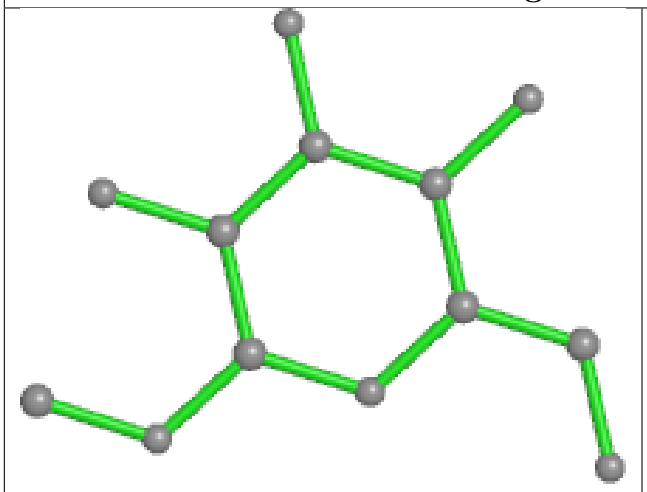

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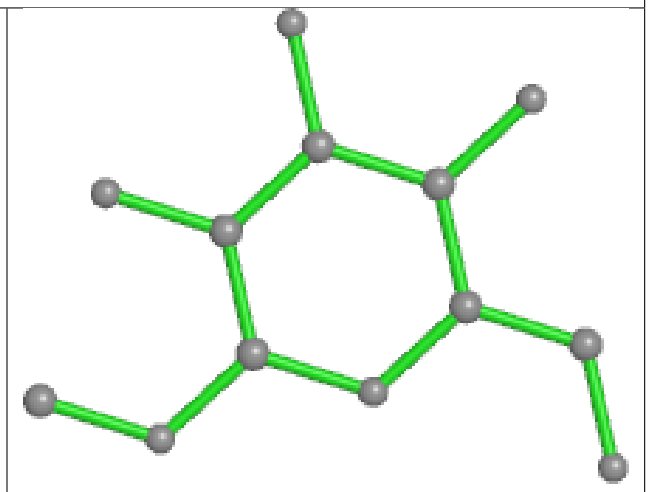
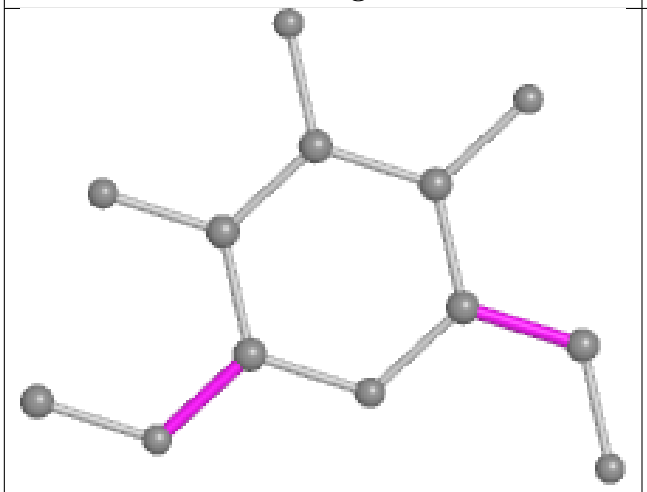


Bond angles



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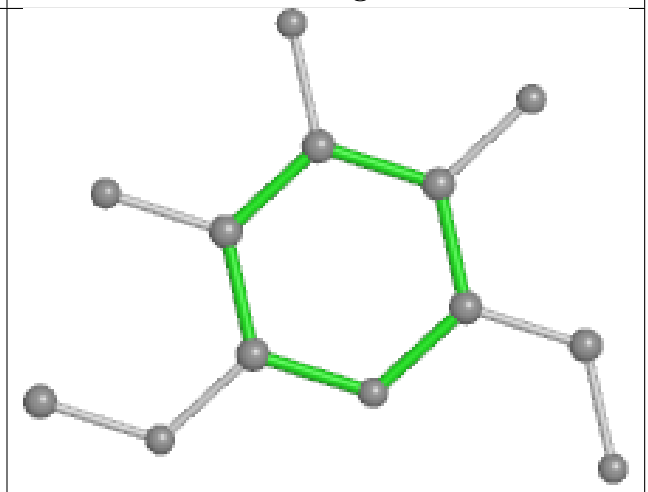
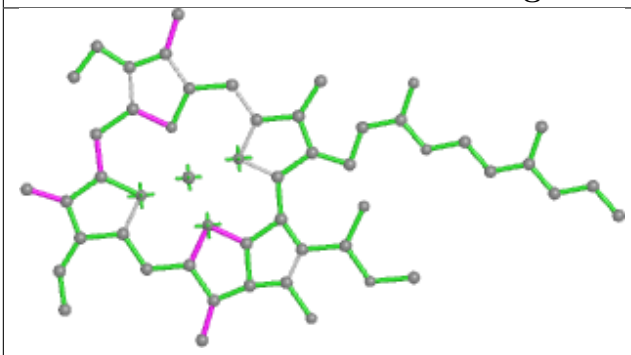


Rings

Ligand CLA A 818



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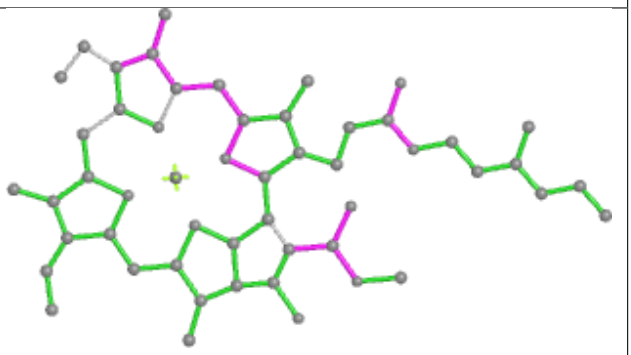
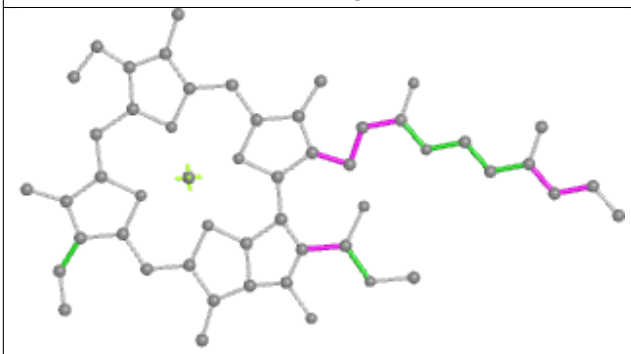


Bond angles



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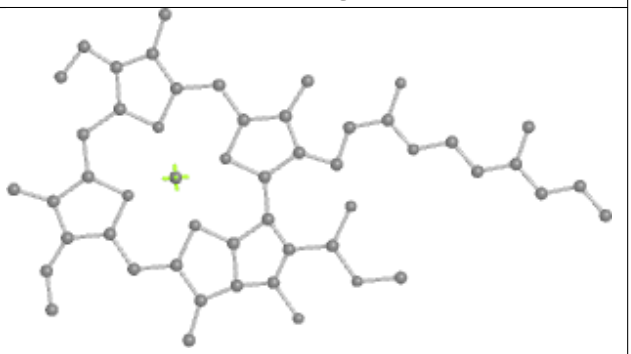
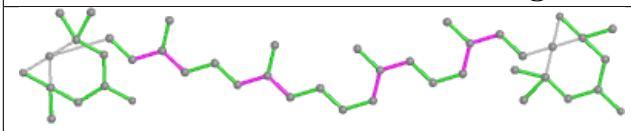


Rings

Ligand XAT c 617



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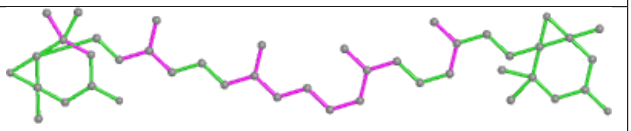
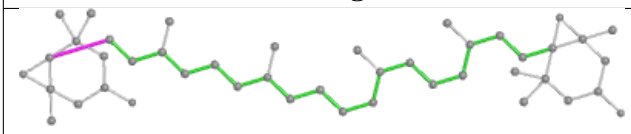


Bond angles



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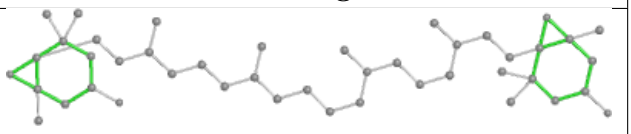
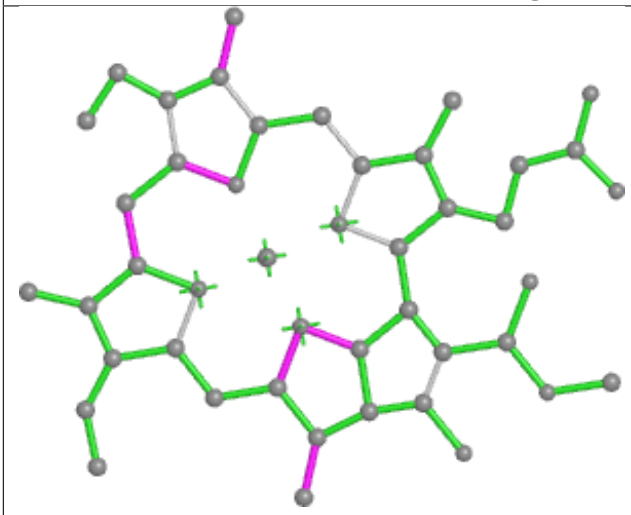


Rings

Ligand CLA L 302



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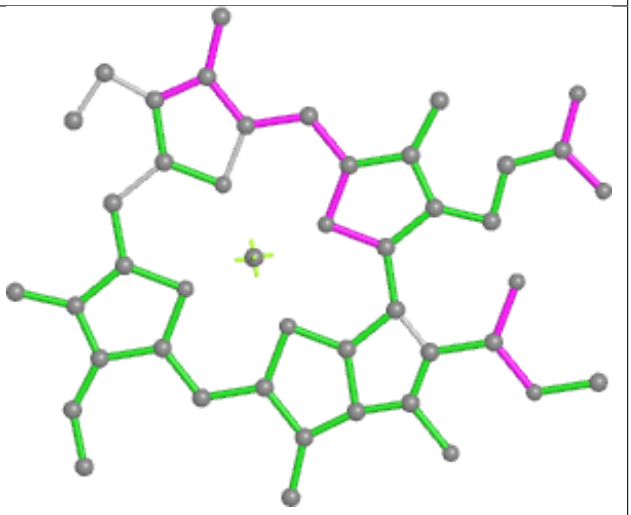
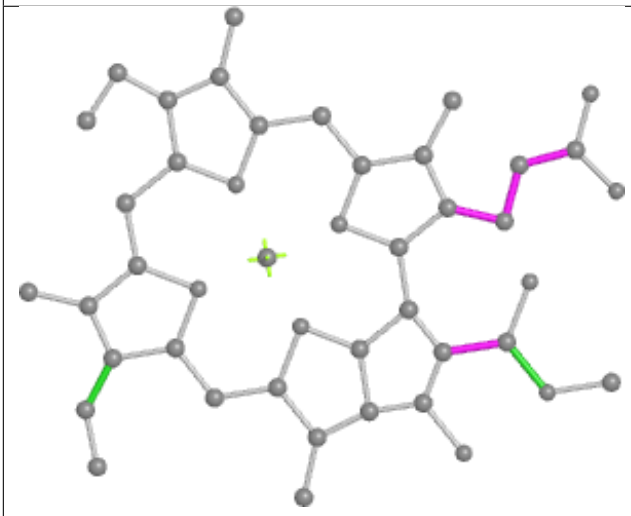


Bond angles



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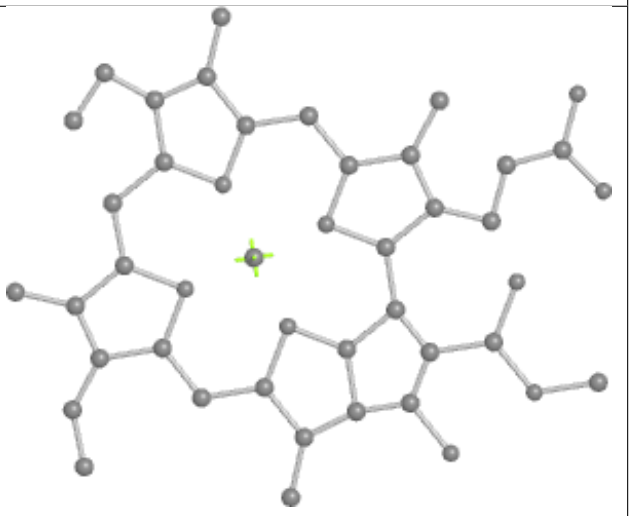
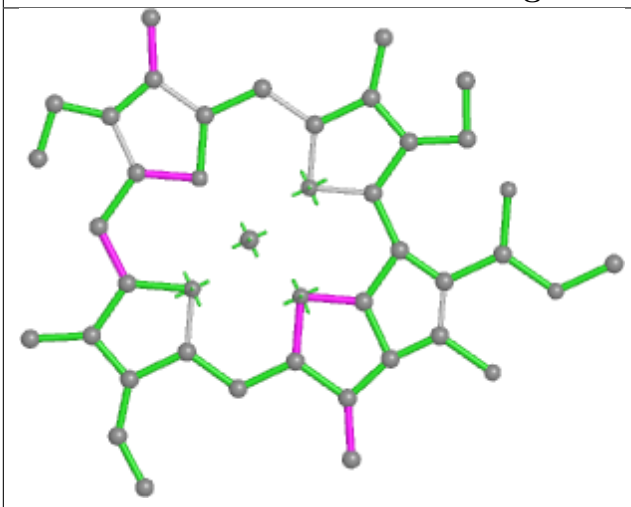


Rings

Ligand CLA A 816



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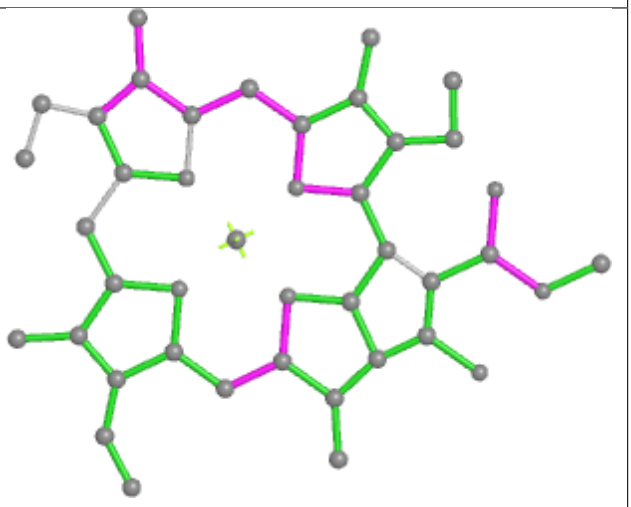
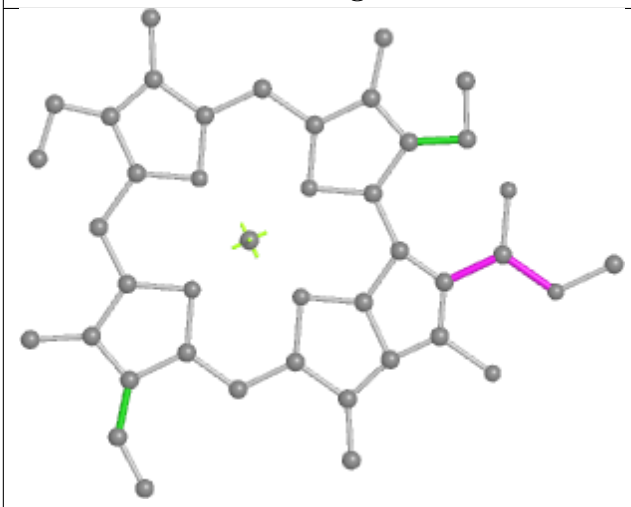
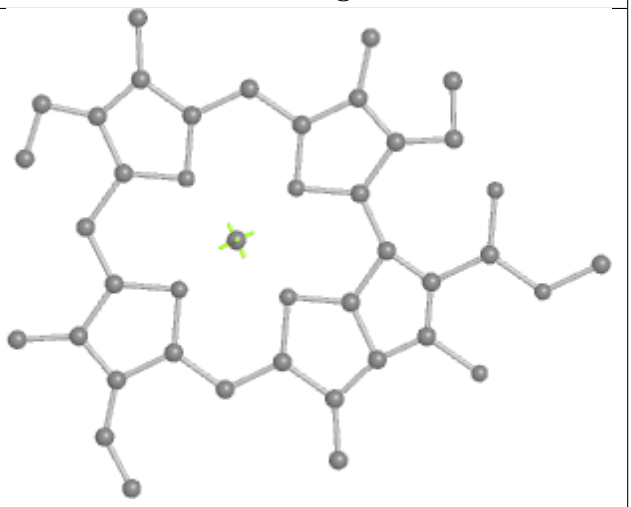


Bond angles

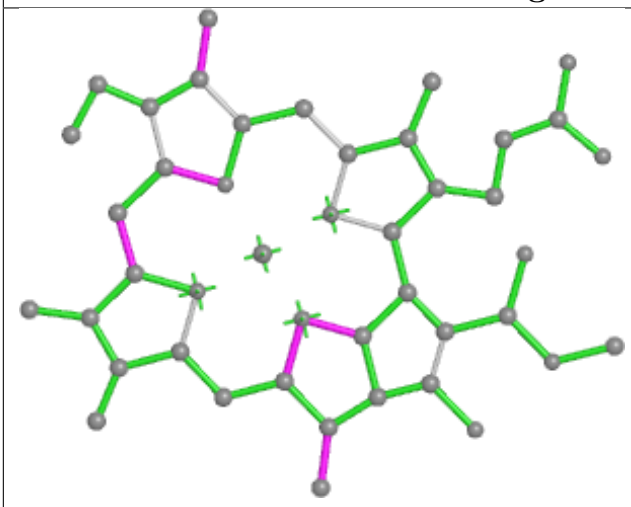


Torsions



Rings

Ligand CLA 8 610



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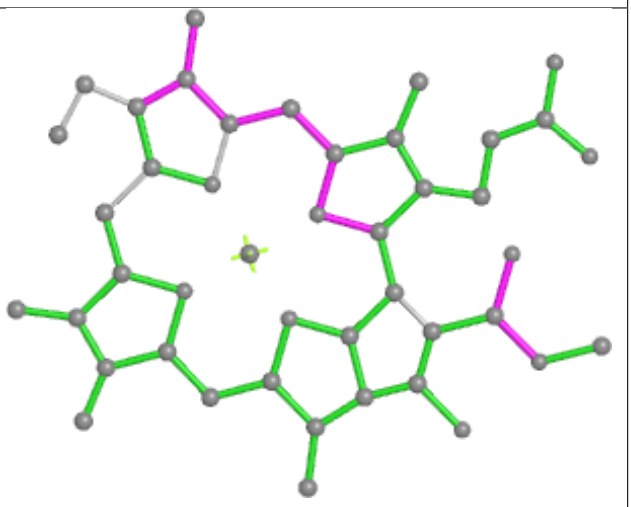
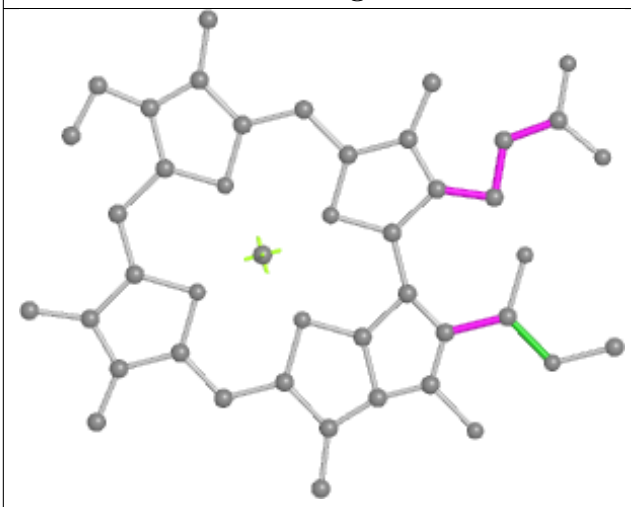


Bond angles



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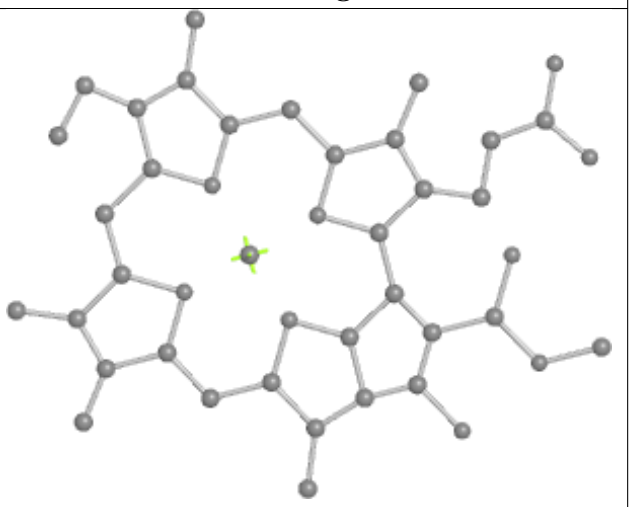
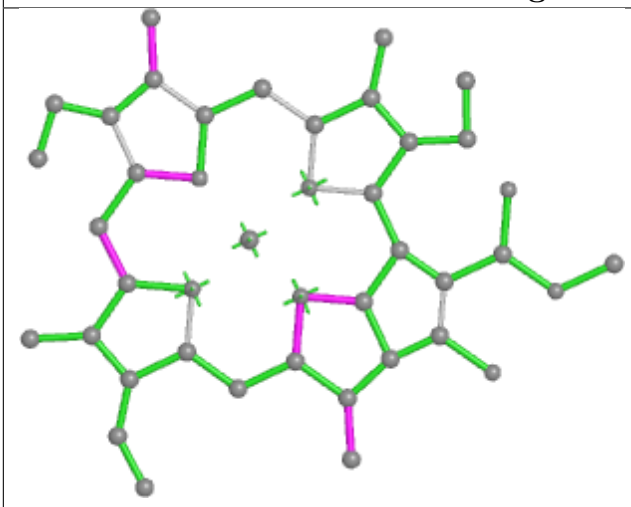


Rings

Ligand CLA 6 609



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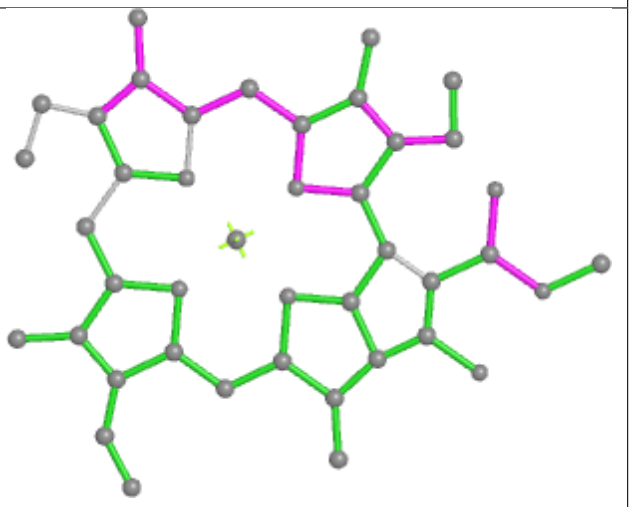

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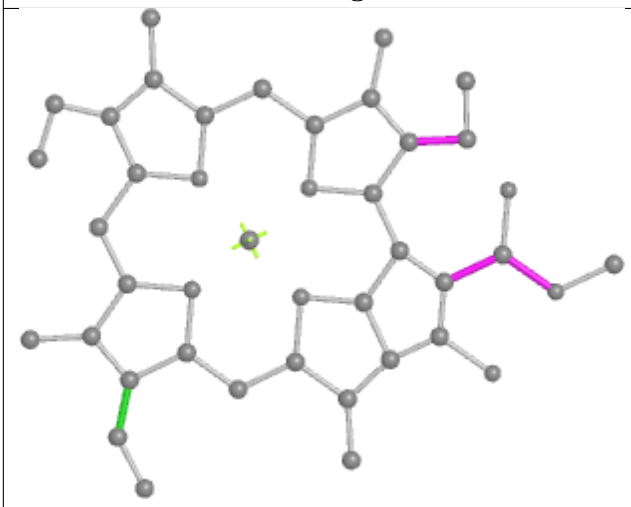

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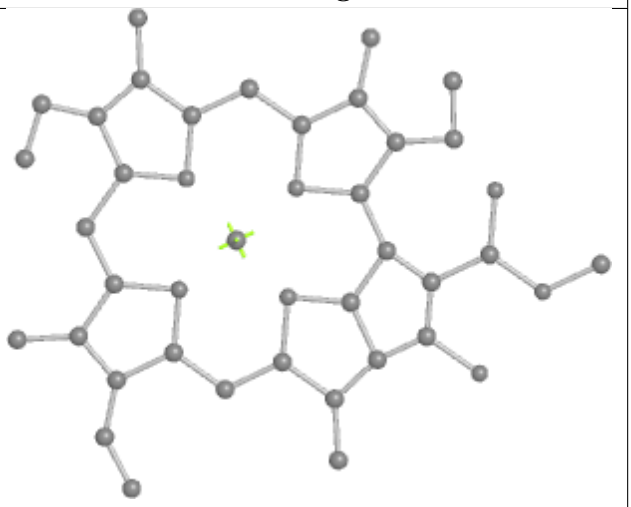
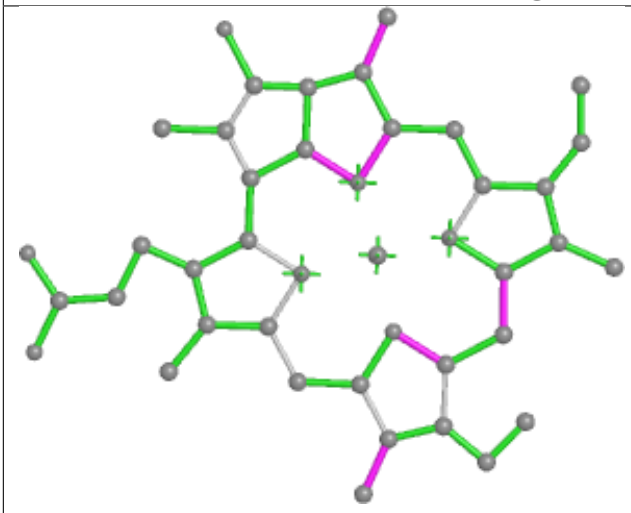


Rings

Ligand CLA 2 610



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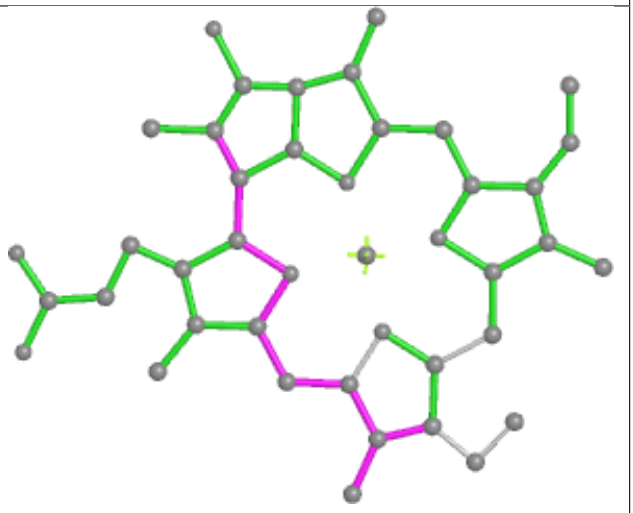

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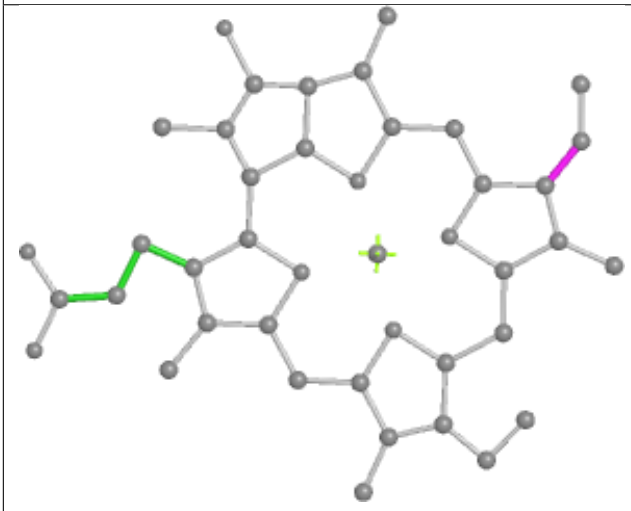

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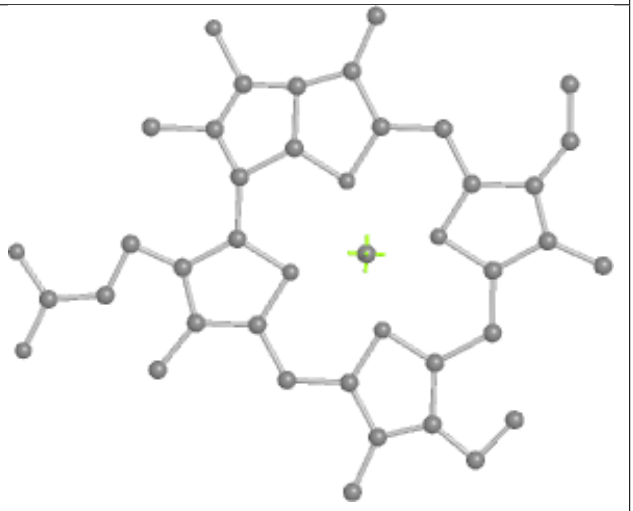

Rings

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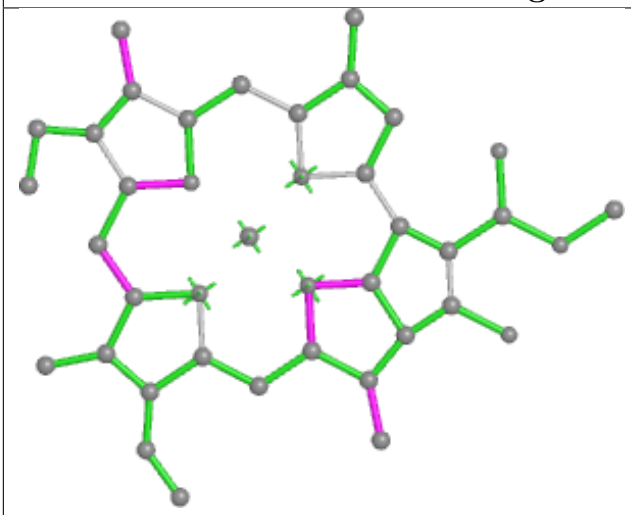

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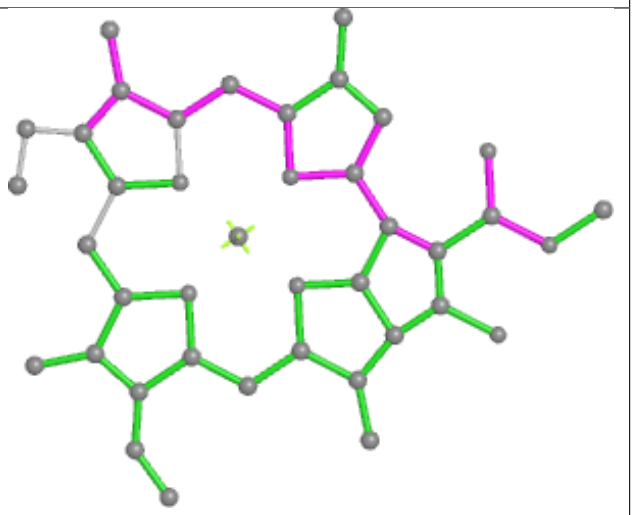

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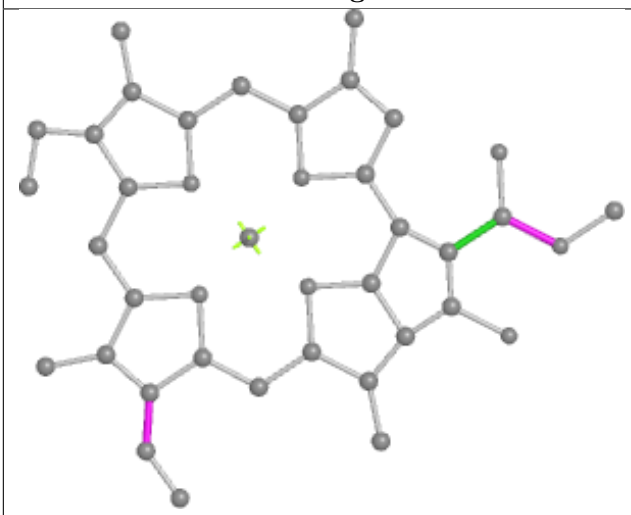

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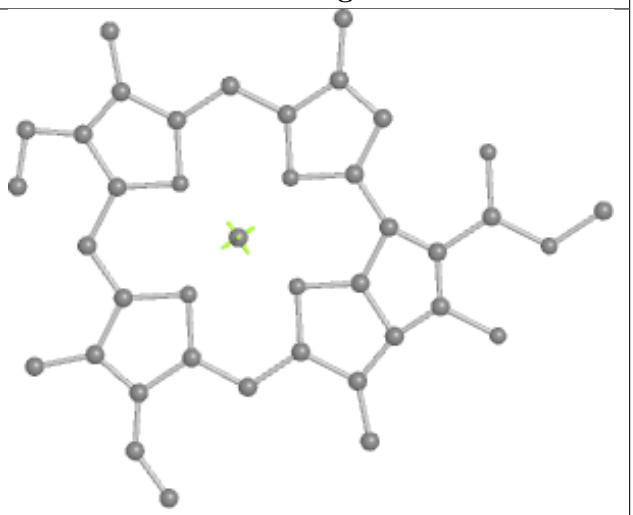

Rings

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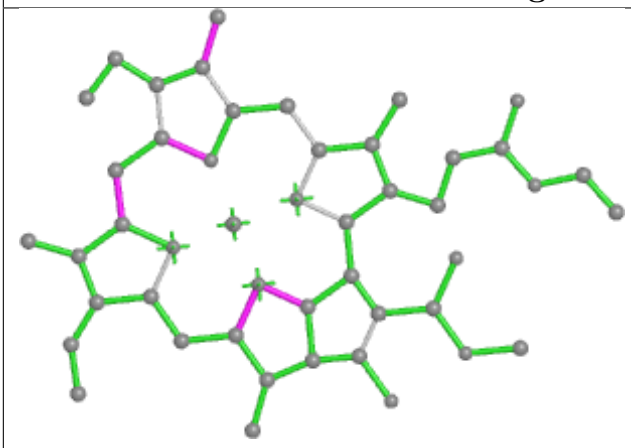

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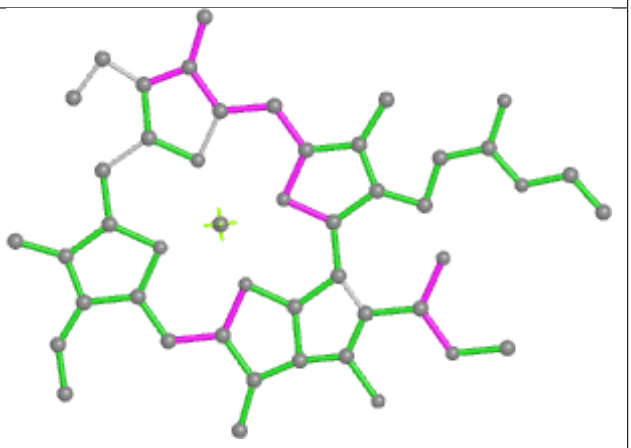

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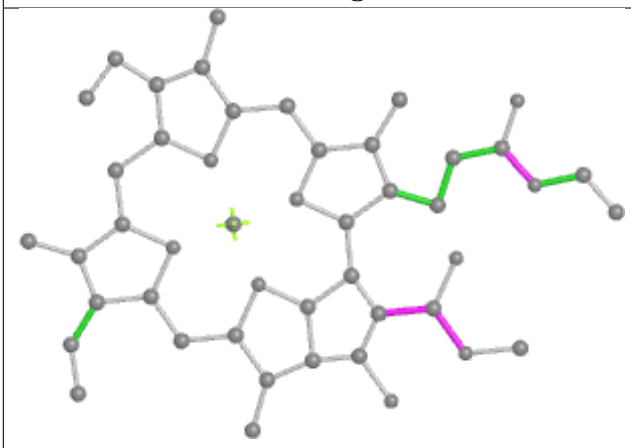

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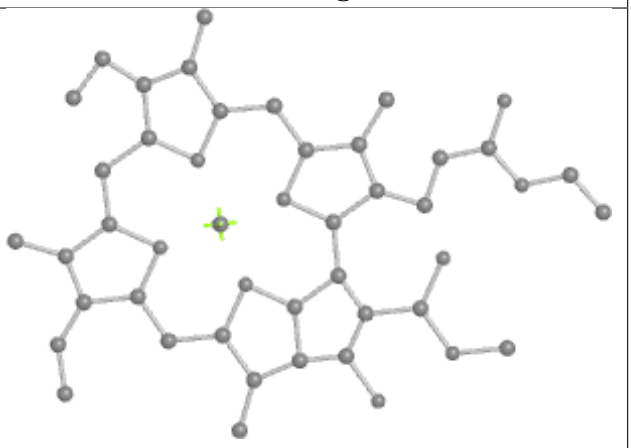
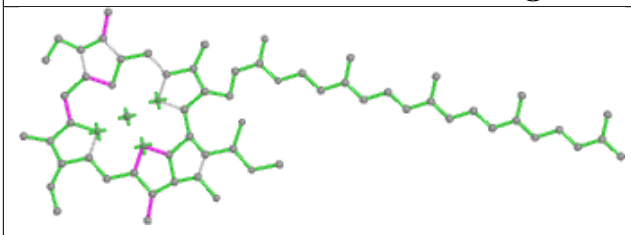


Rings

Ligand CLA B 823



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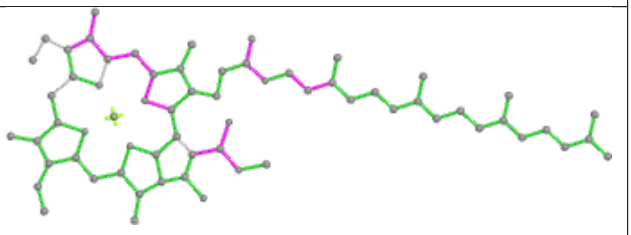

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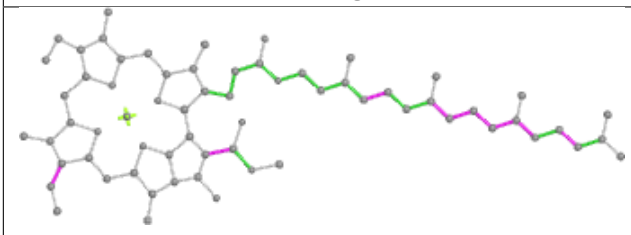

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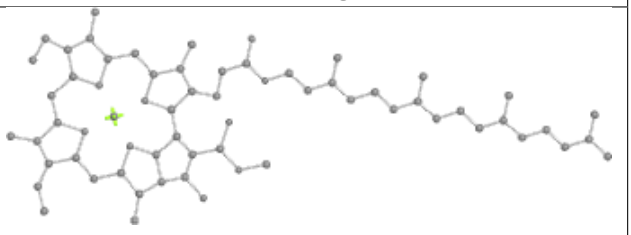
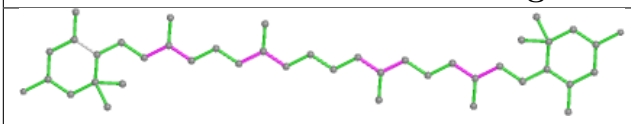


Rings

Ligand LUT b 317



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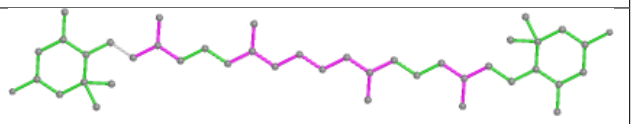

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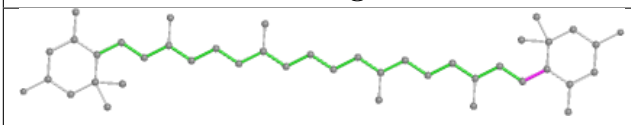

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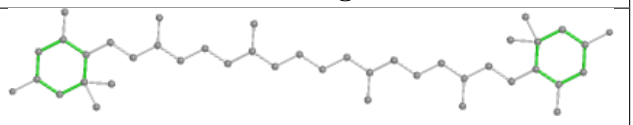
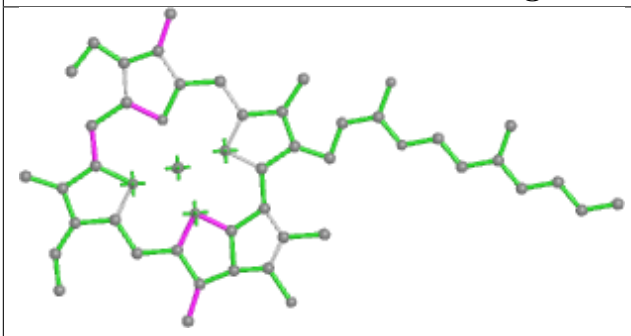


Rings

Ligand CLA O 203



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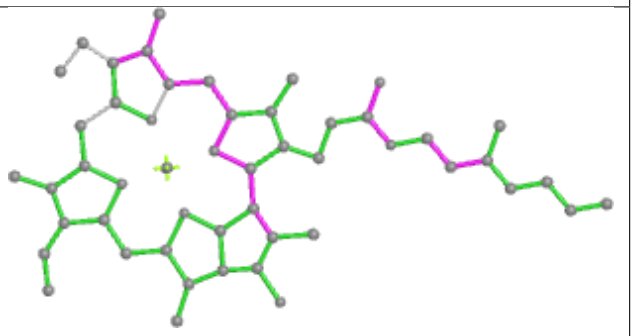

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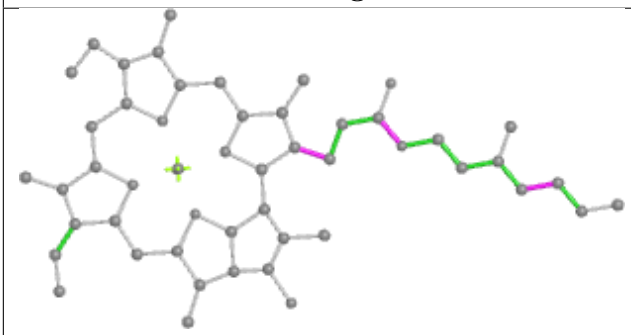

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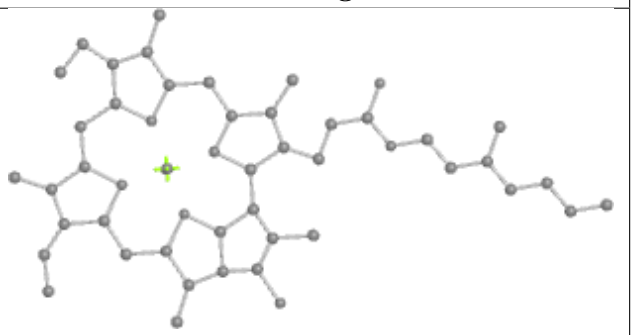

Rings

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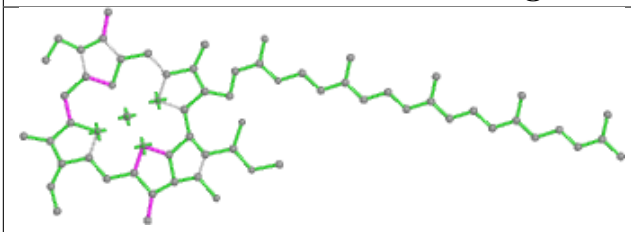

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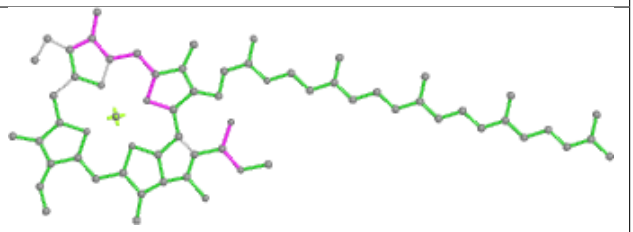
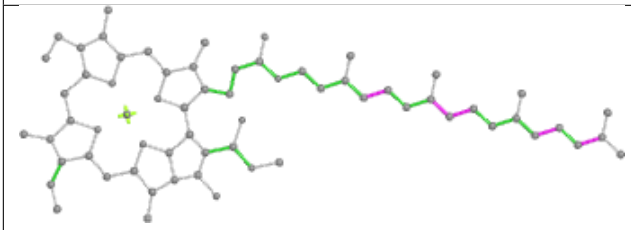


Bond angles



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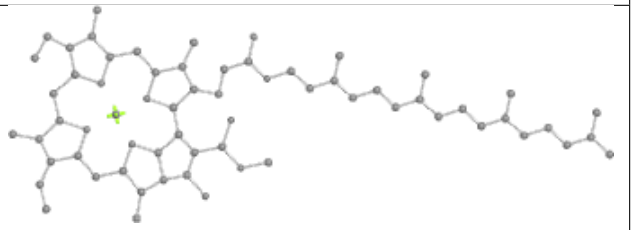

Rings

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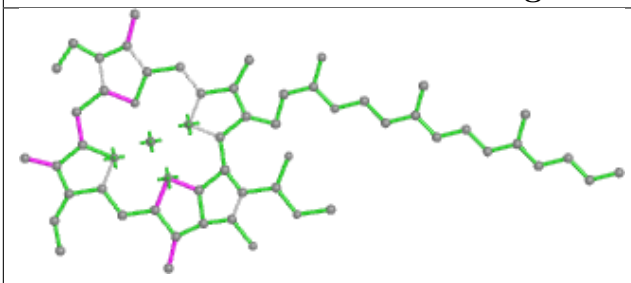
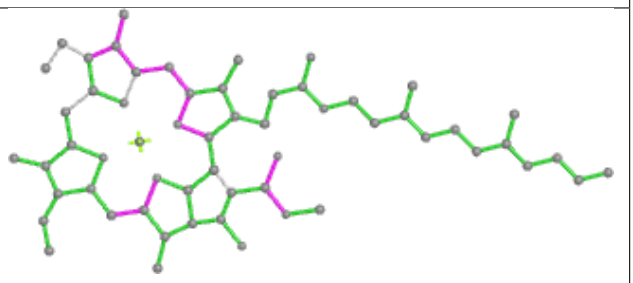
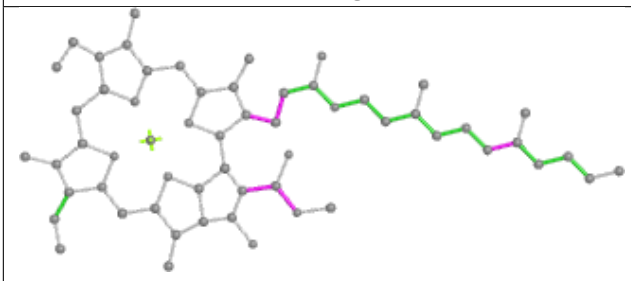
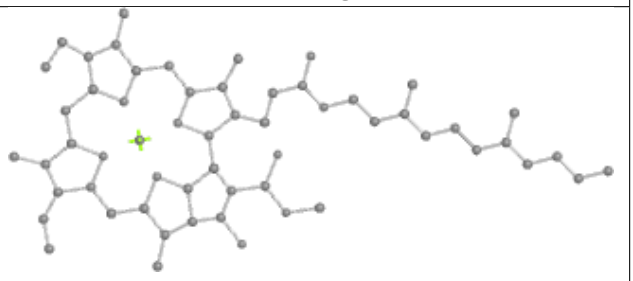
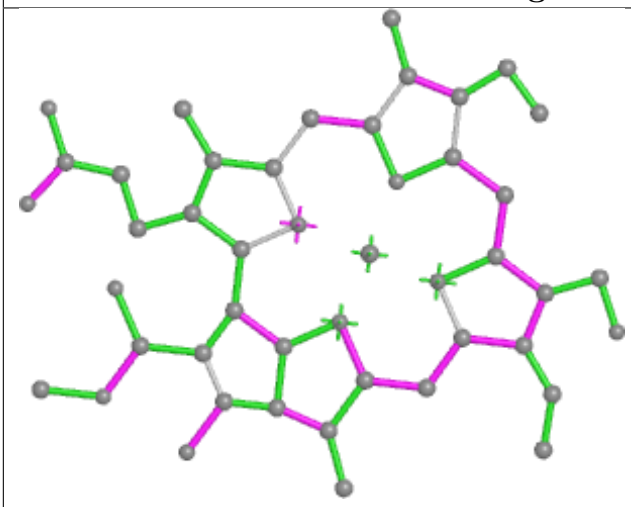
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

Ligand CHL a 601



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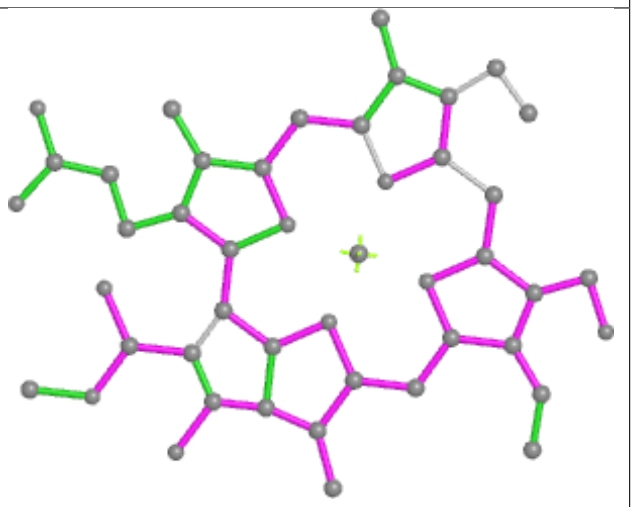
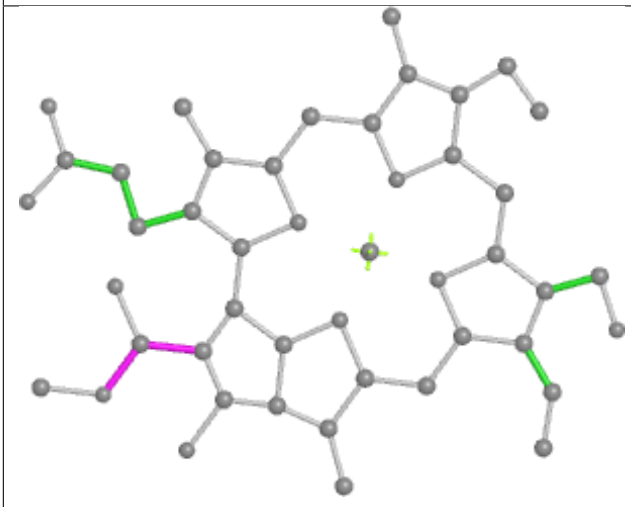


Bond angles



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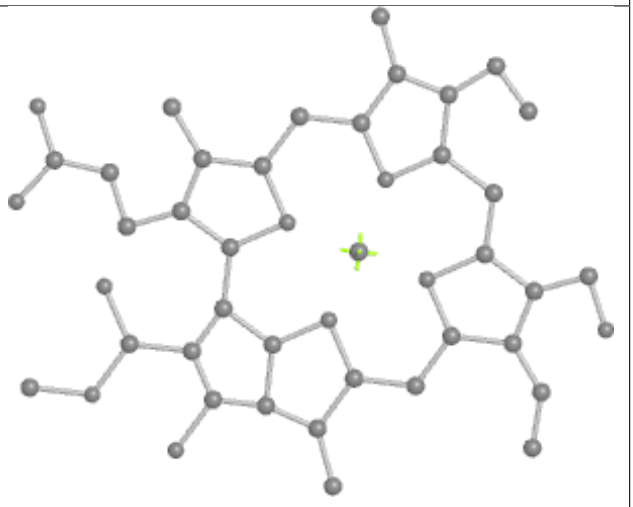
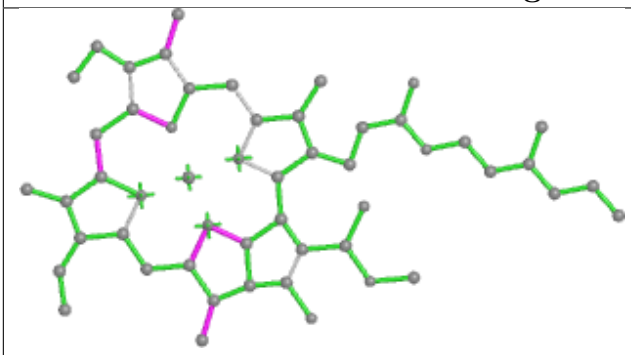


Rings

Ligand CLA A 803



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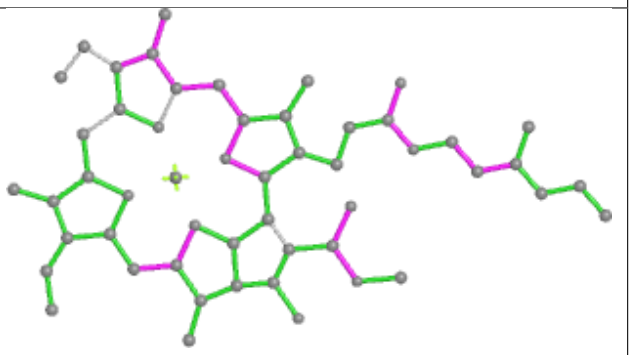

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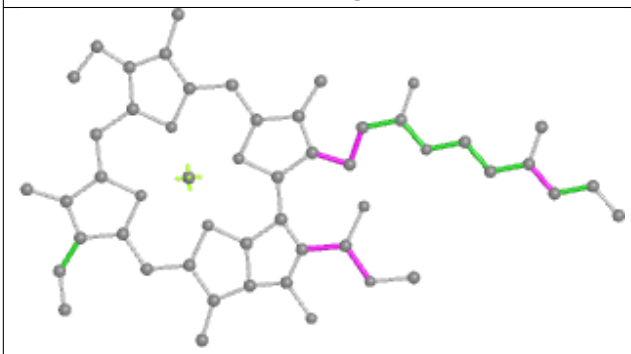

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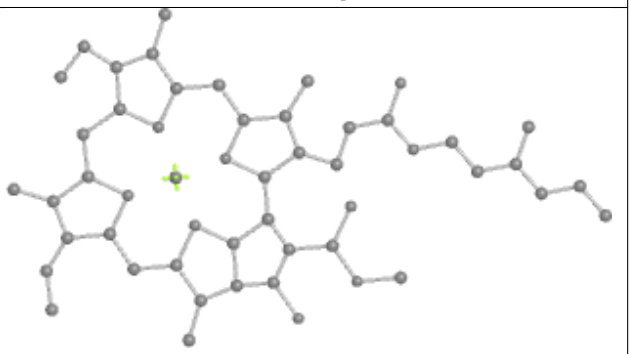
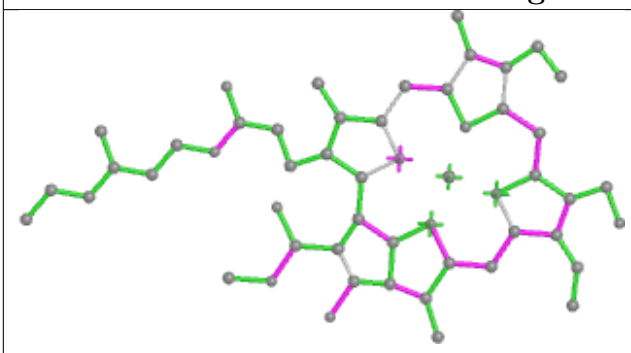
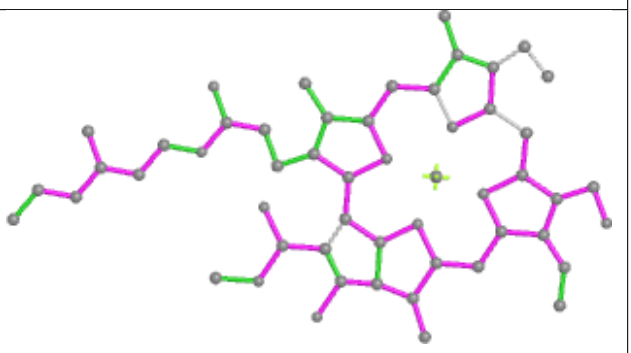


Rings

Ligand CHL 2 601



Bond lengths



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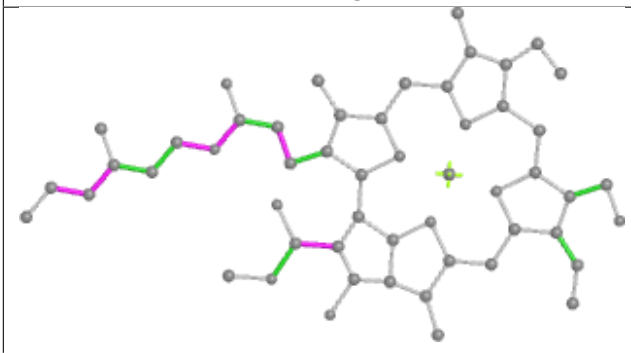

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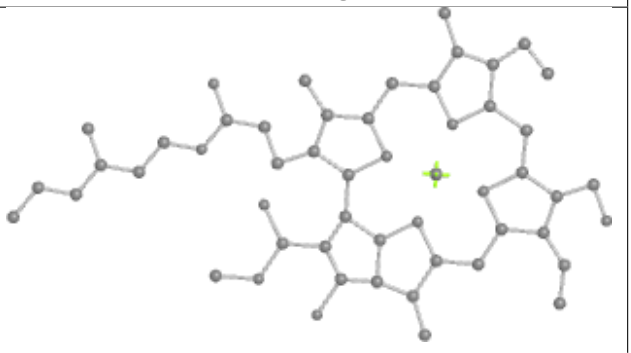
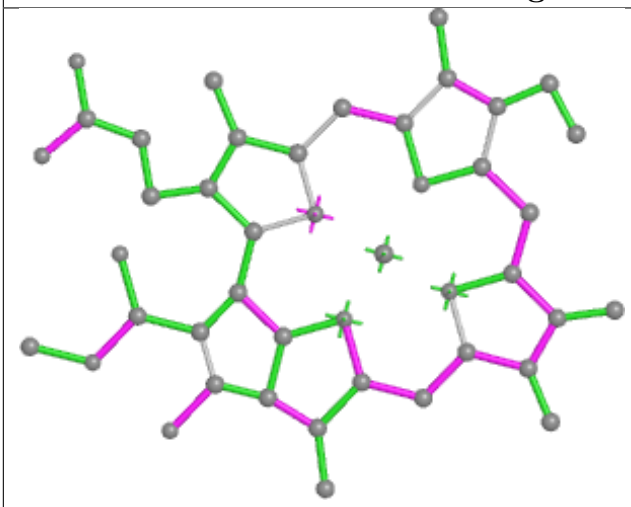


Rings

Ligand CHL 6 601



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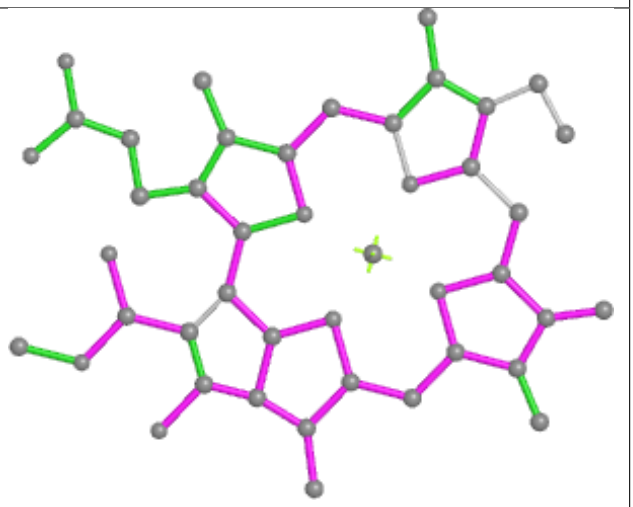

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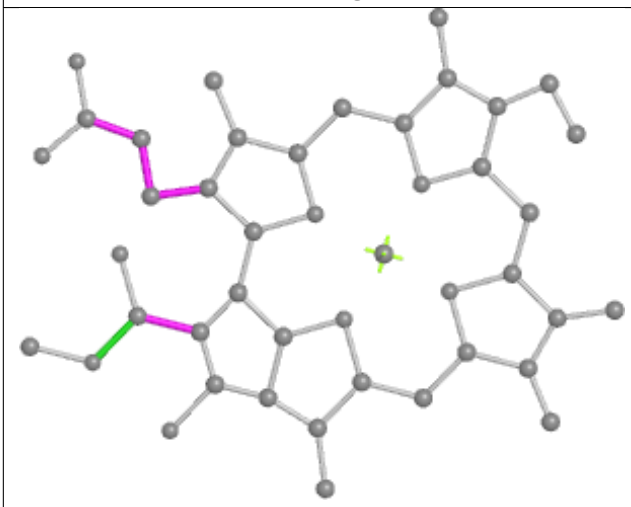

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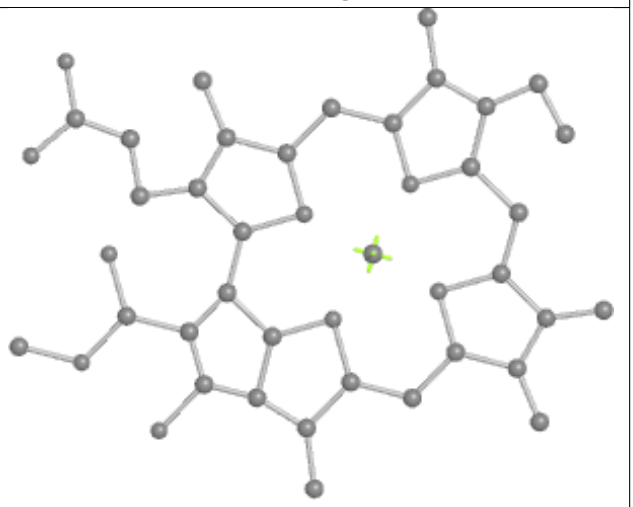
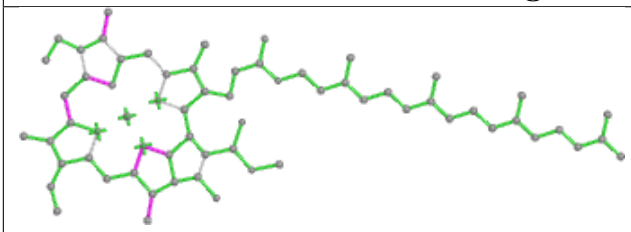


Rings

Ligand CLA B 840



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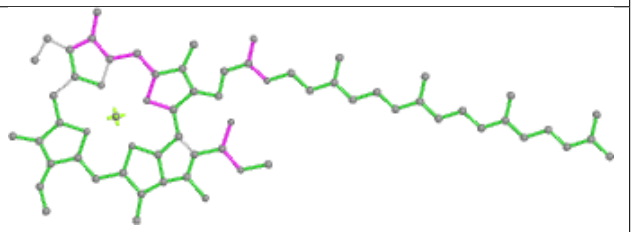

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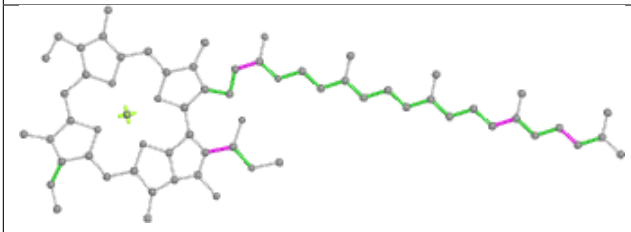

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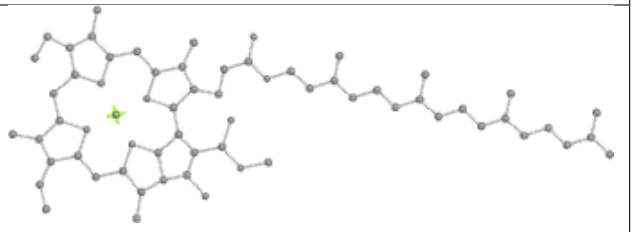
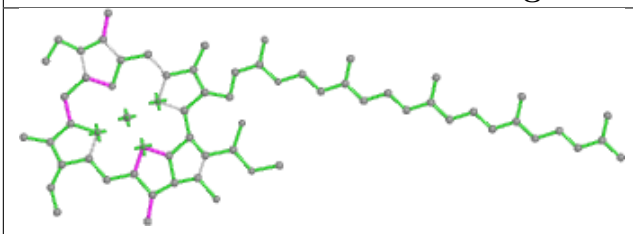


Rings

Ligand CLA A 819



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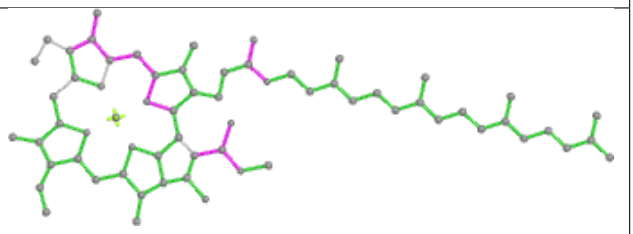

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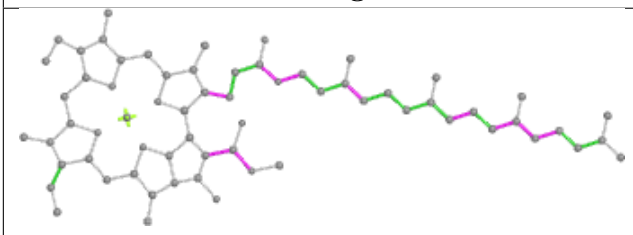

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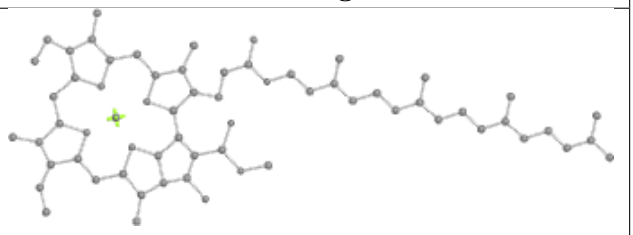
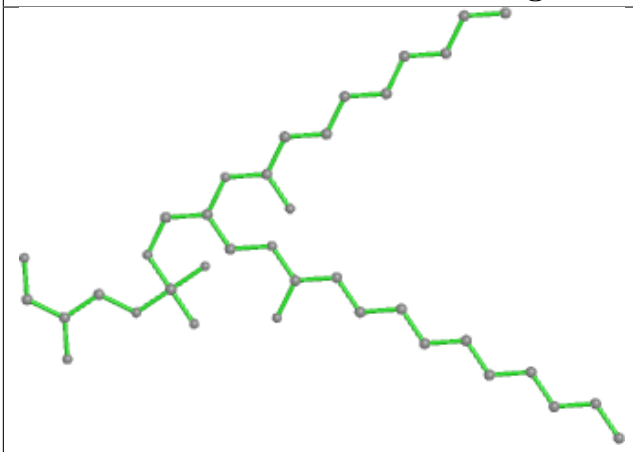


Rings

Ligand LHG 8 617



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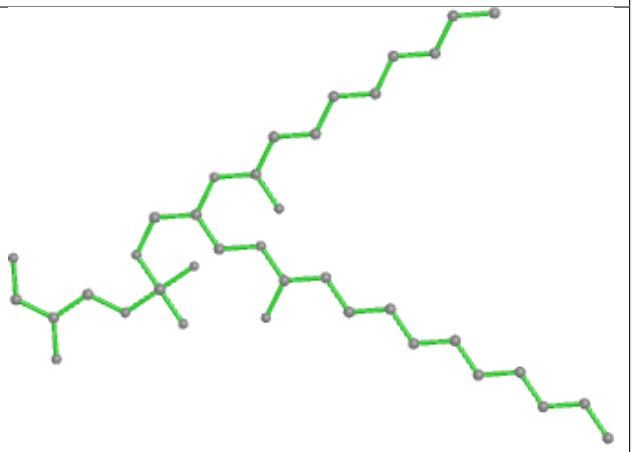

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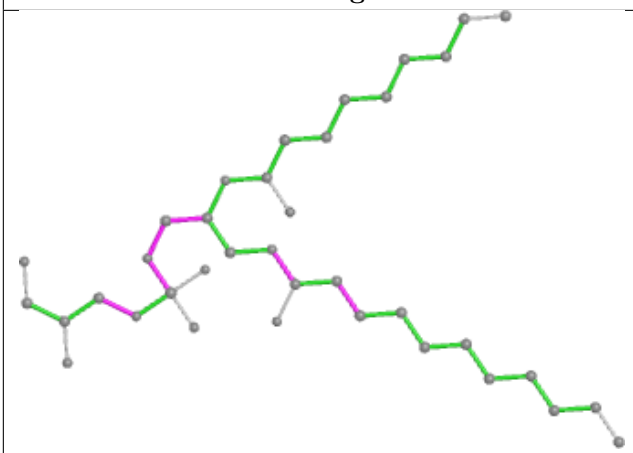

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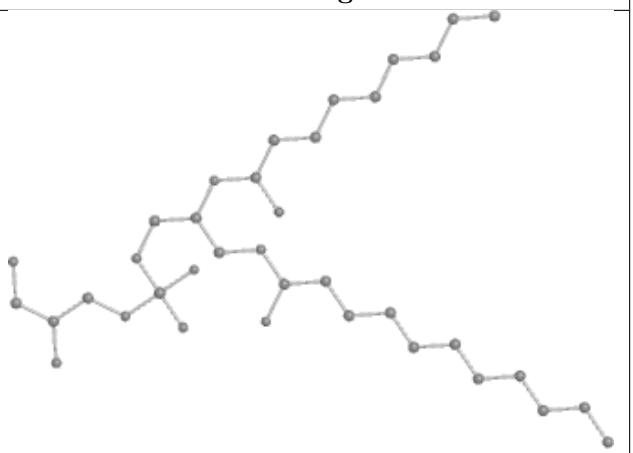
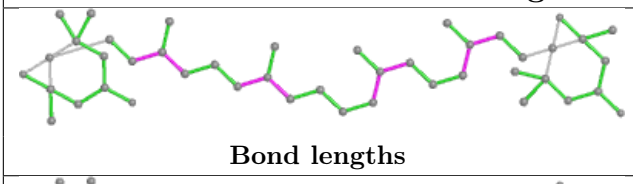


Rings

Ligand XAT 3 417



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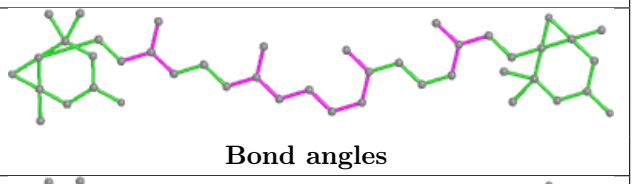
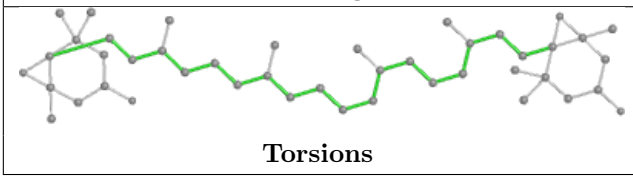


Bond angles



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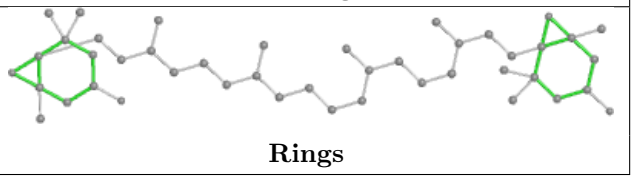
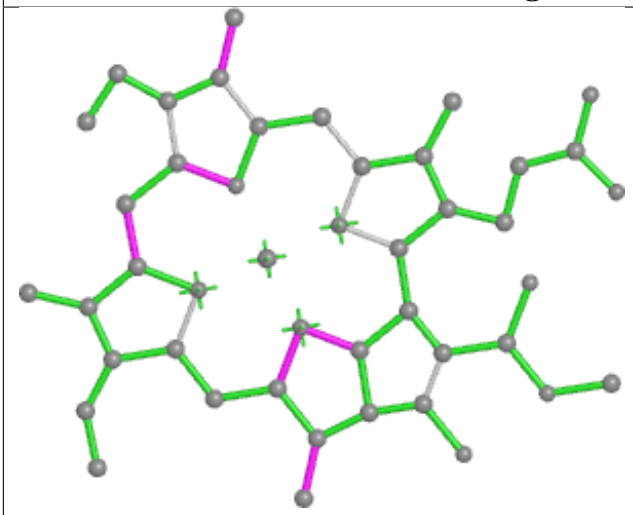


Rings

Ligand CLA A 815



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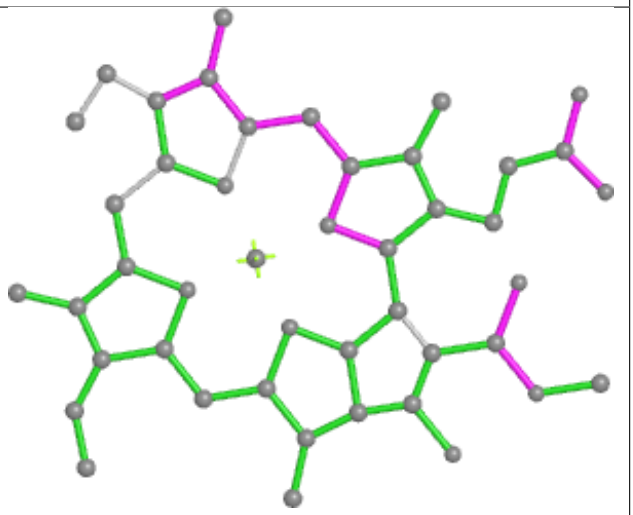

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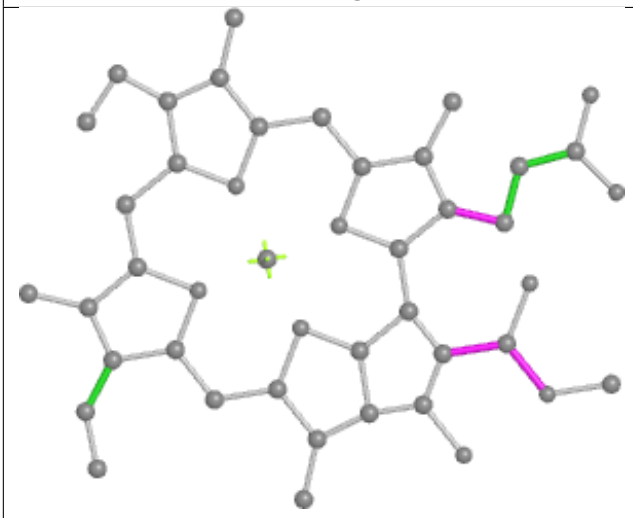

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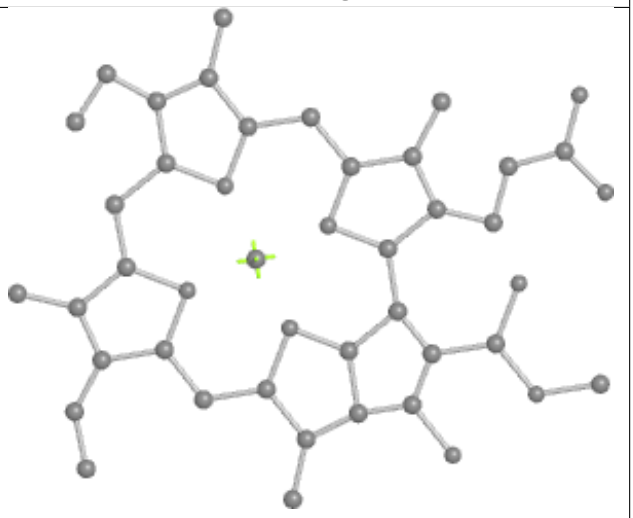
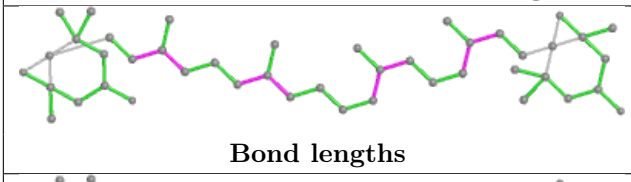


Rings

Ligand XAT 9 616



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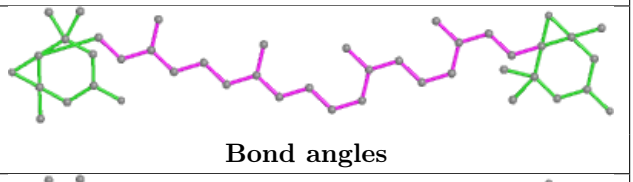

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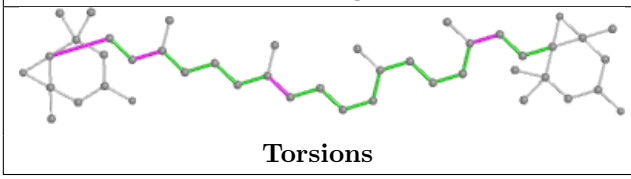

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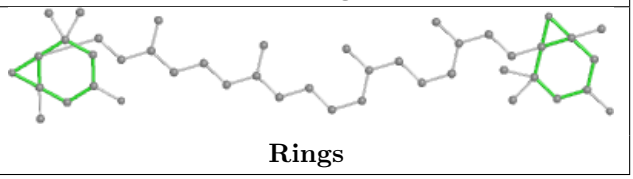
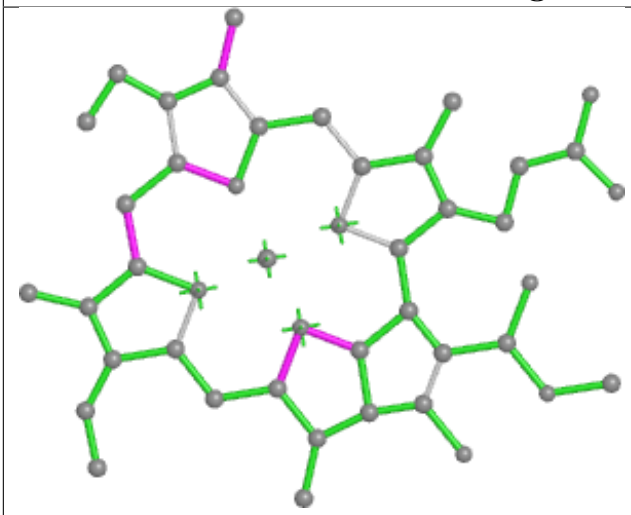


Rings

Ligand CLA a 612



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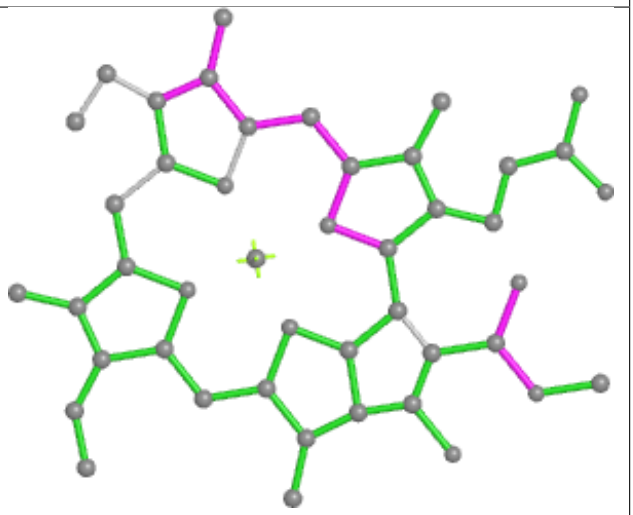

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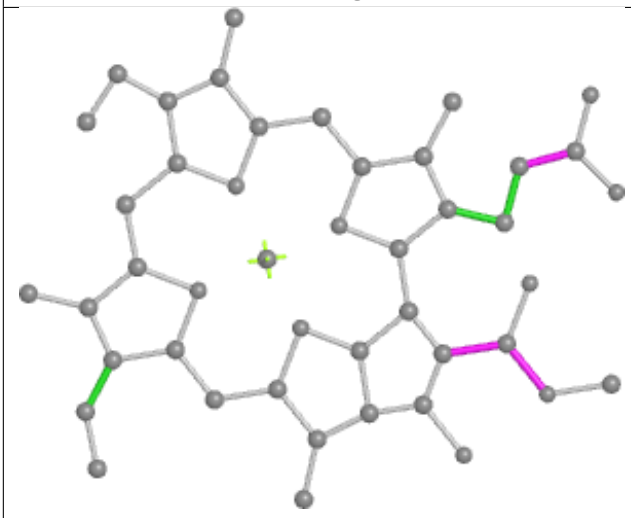

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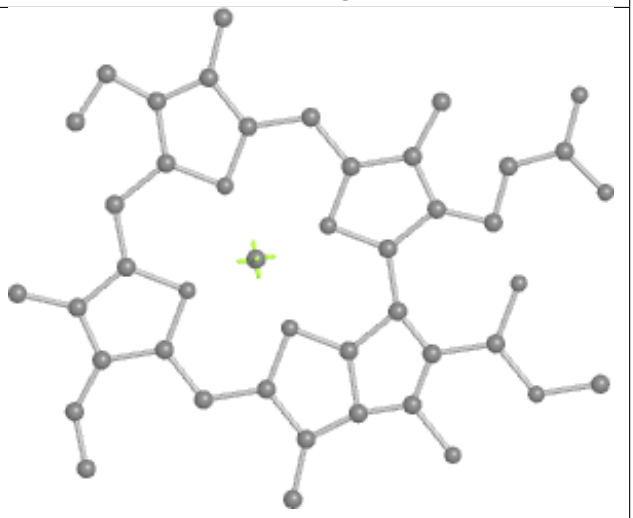
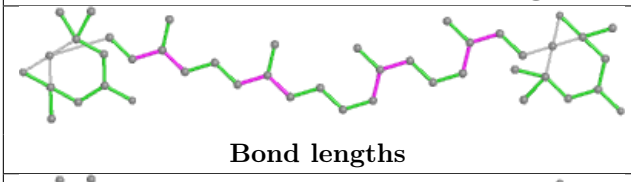


Rings

Ligand XAT 8 615



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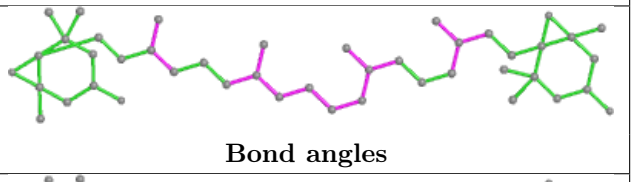

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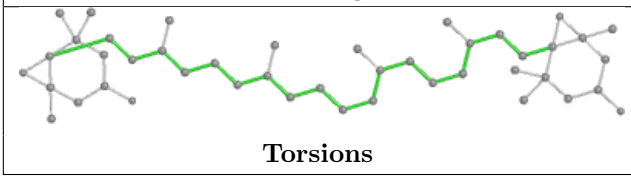

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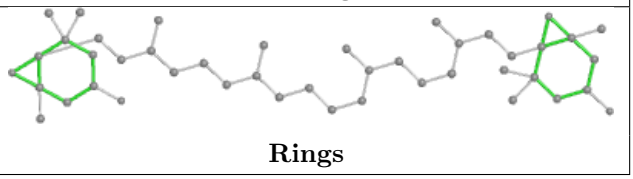
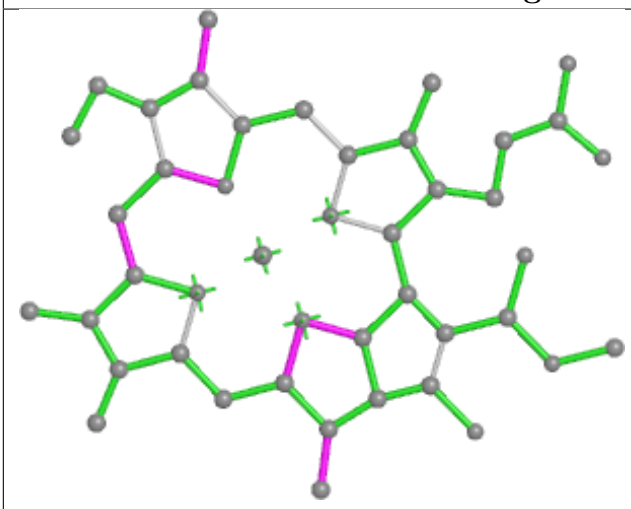


Rings

Ligand CLA A 822



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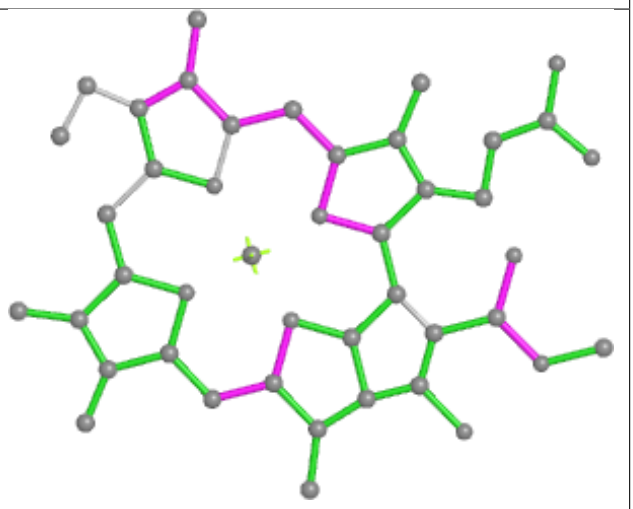
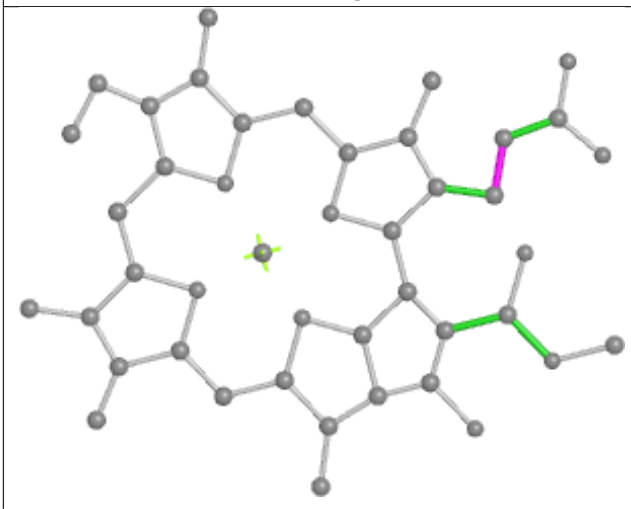


Bond angles



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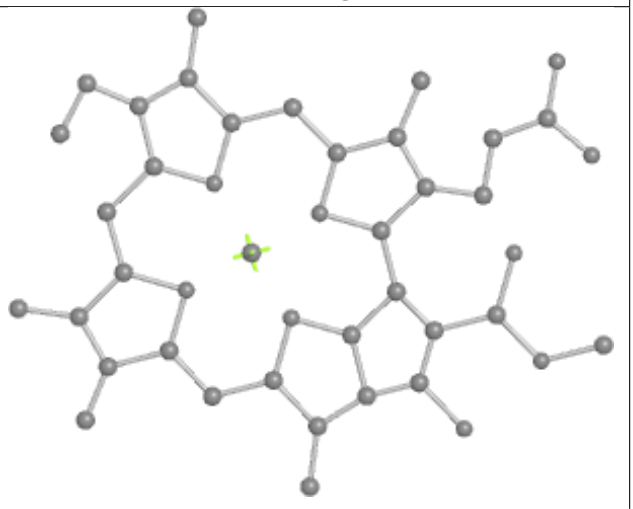
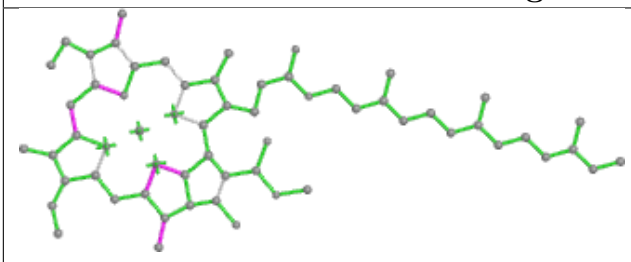
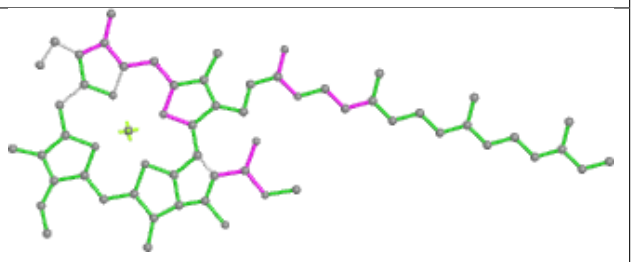
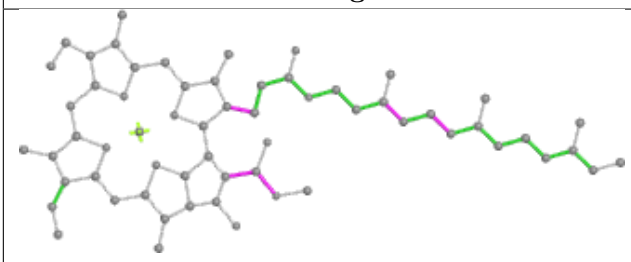
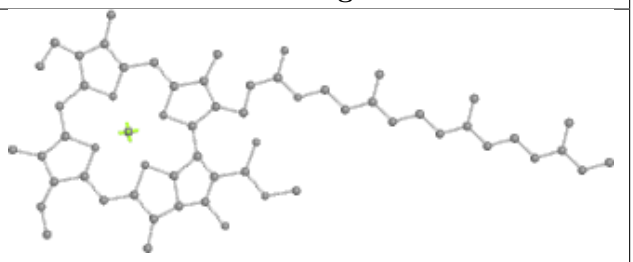


Rings

Ligand CLA F 302	
	
Bond lengths	Bond angles
	
Torsions	Rings

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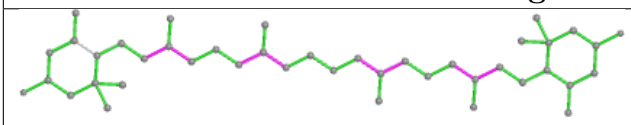
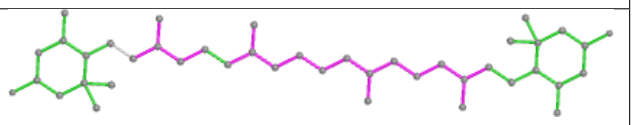
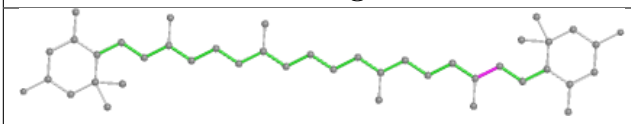
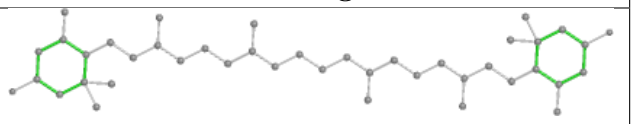
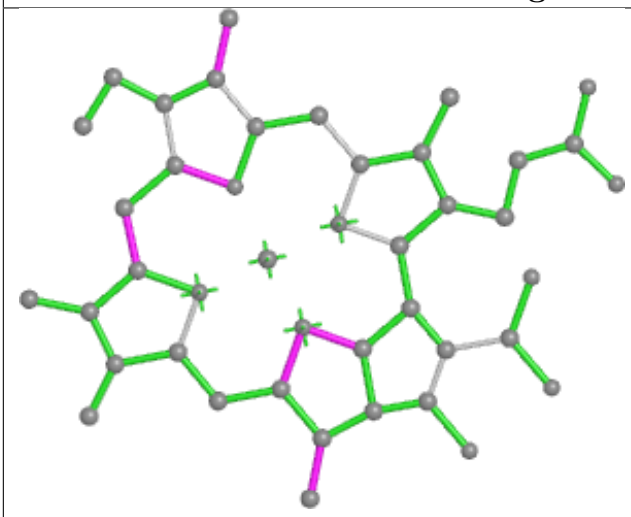
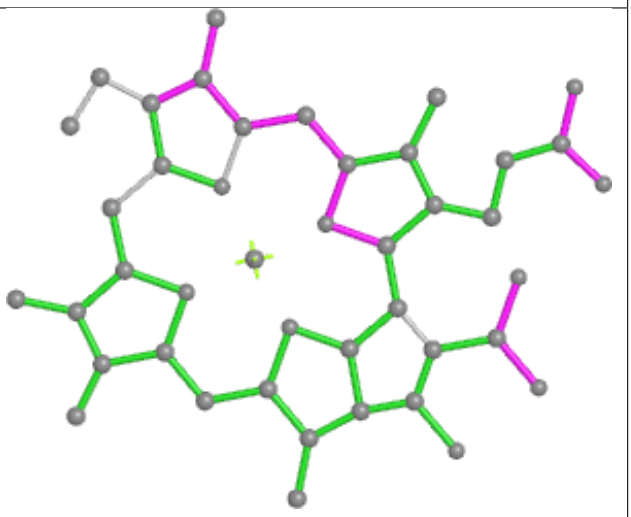
	
Bond lengths	Bond angles
	
Torsions	Rings

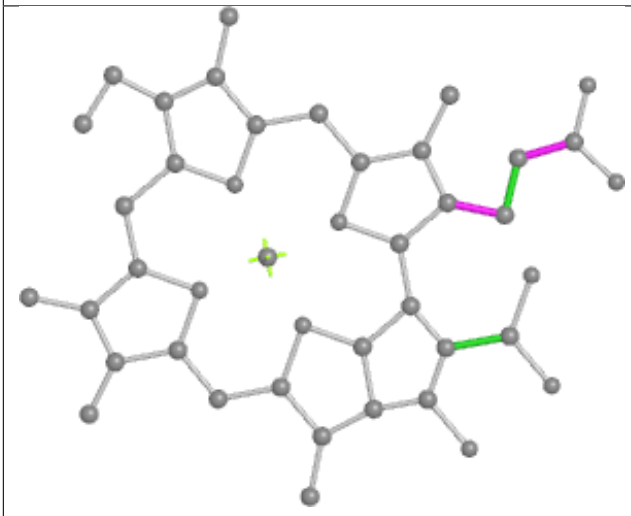
Ligand CLA 5 609



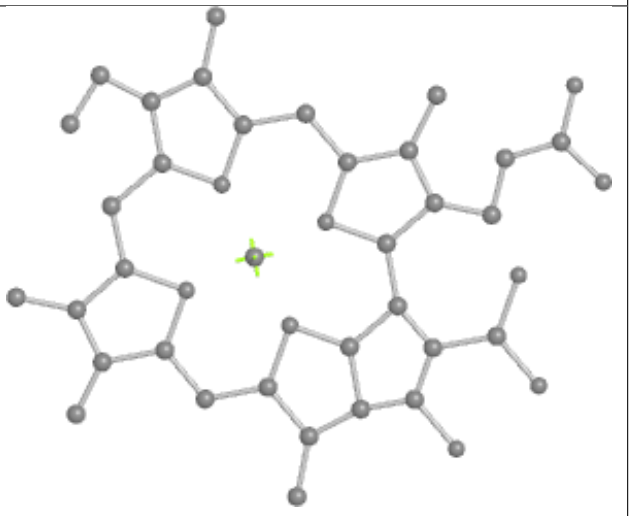
Bond lengths



Bond angles

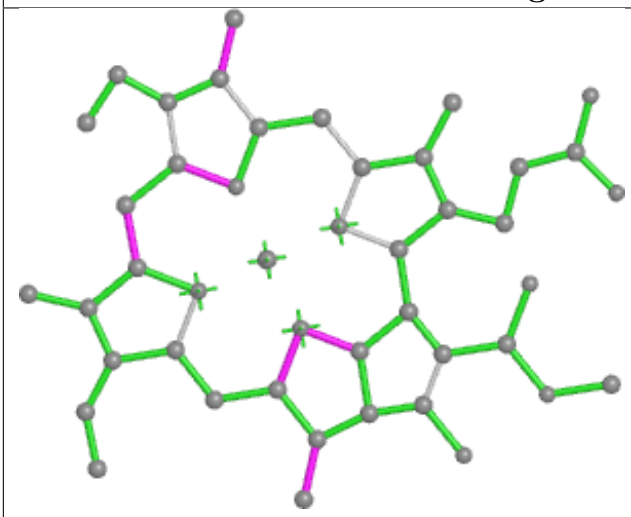


Torsions

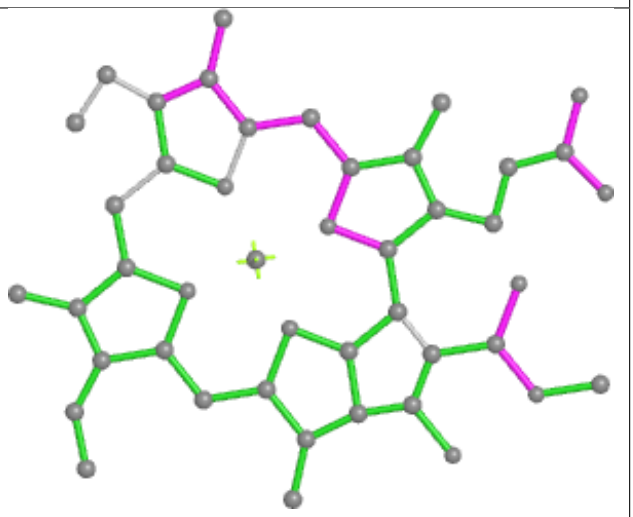


Rings

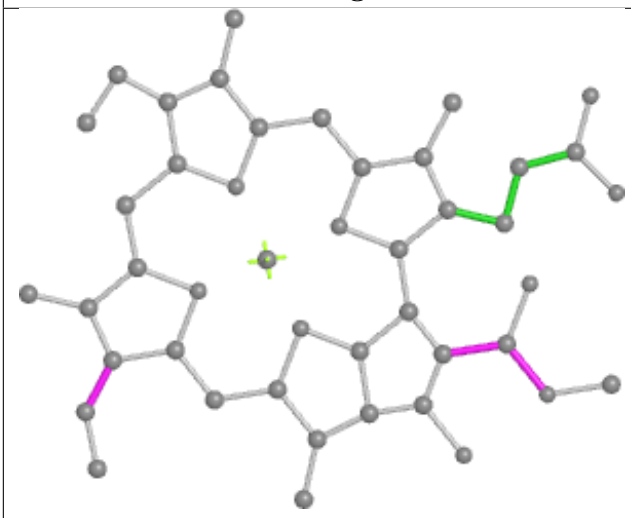
Ligand CLA 1 315



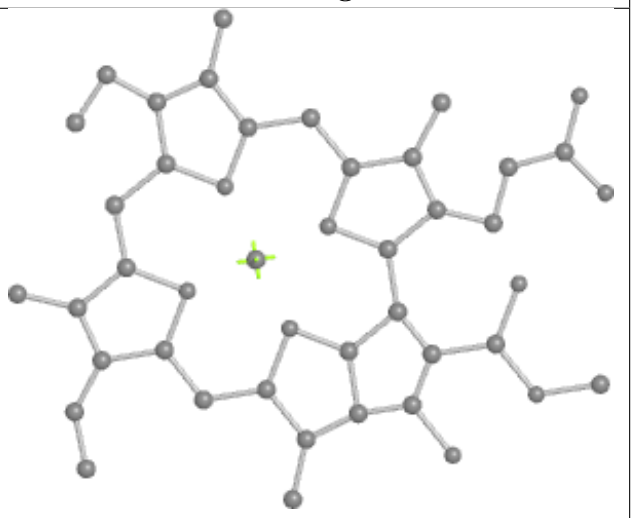
Bond lengths



Bond angles

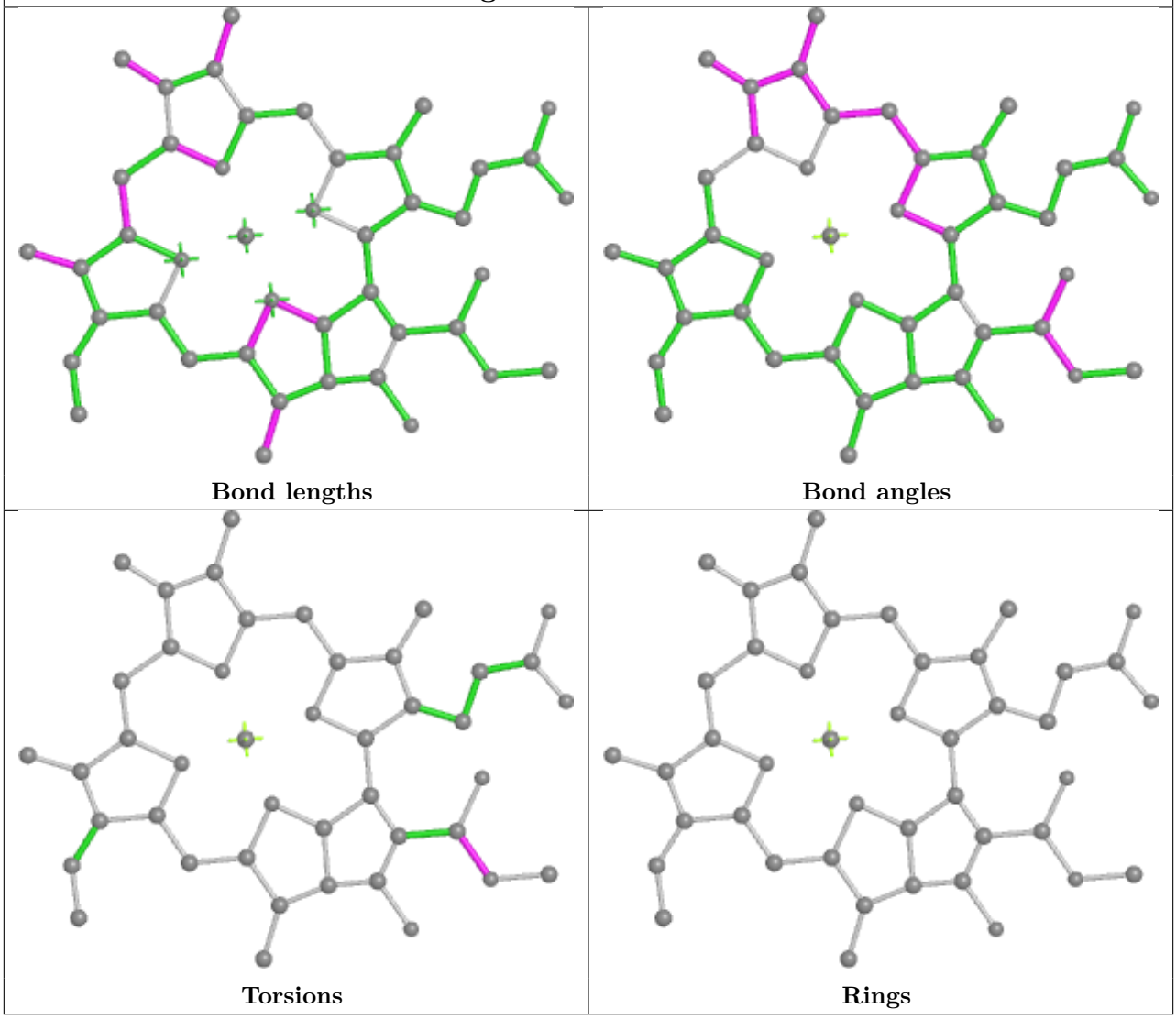


Torsions



Rings

Ligand CLA K 203



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.

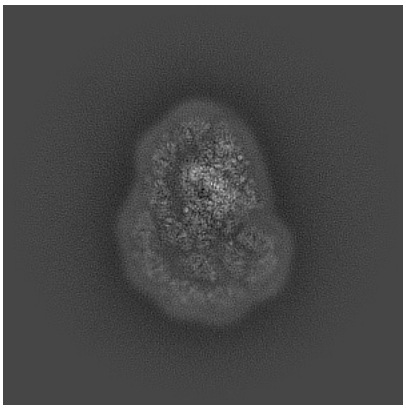
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-33401. These allow visual inspection of the internal detail of the map and identification of artifacts.

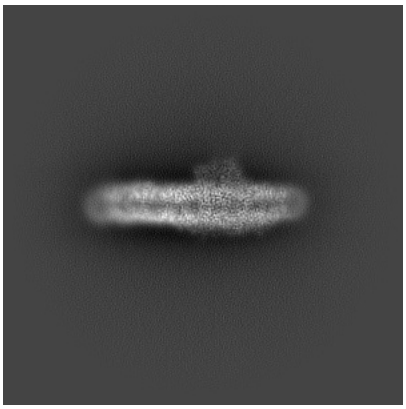
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

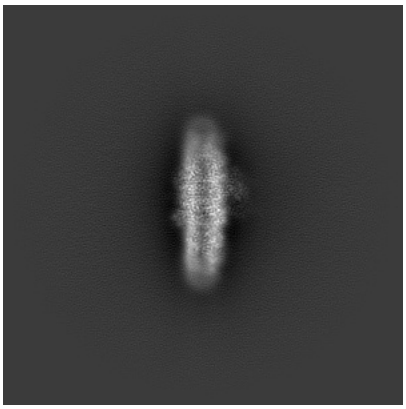
6.1.1 Primary map



X

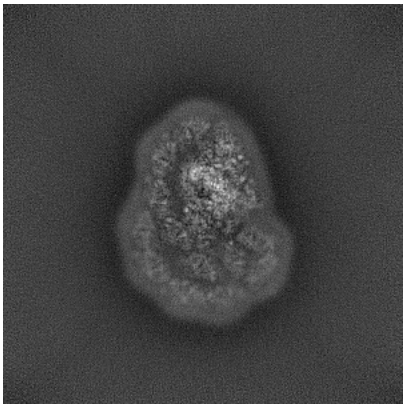


Y

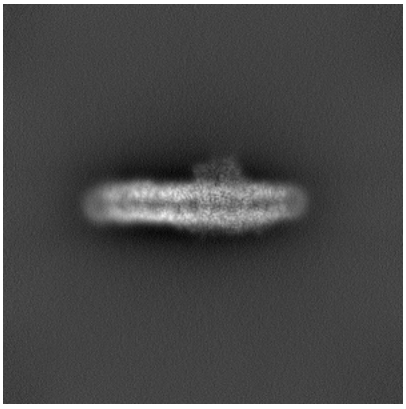


Z

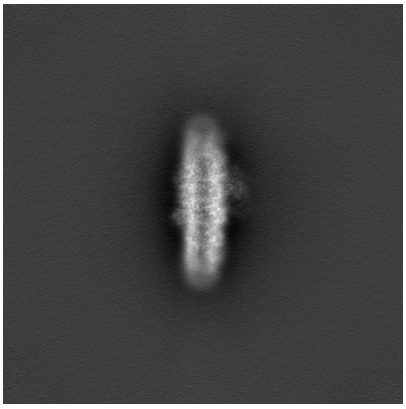
6.1.2 Raw map



X



Y

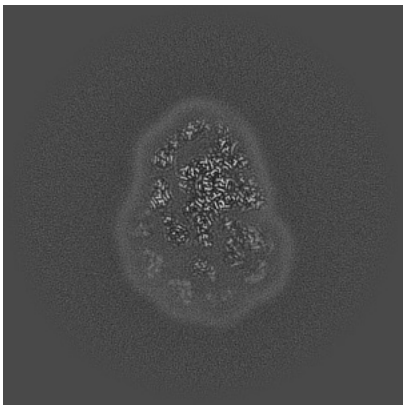


Z

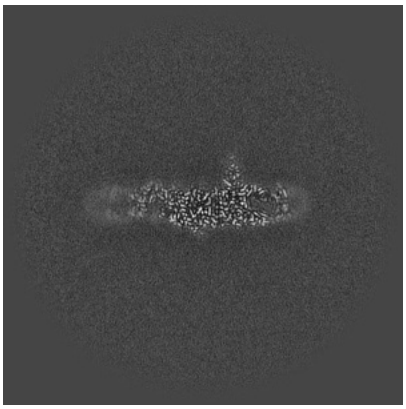
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

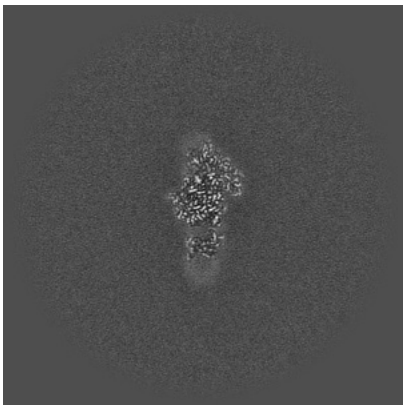
6.2.1 Primary map



X Index: 240

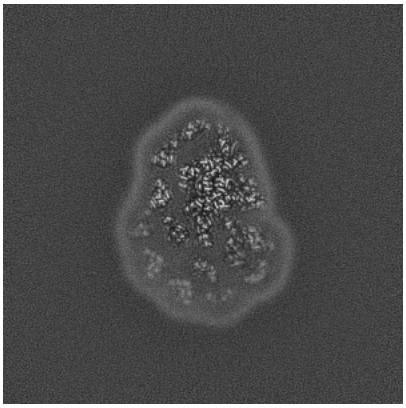


Y Index: 240

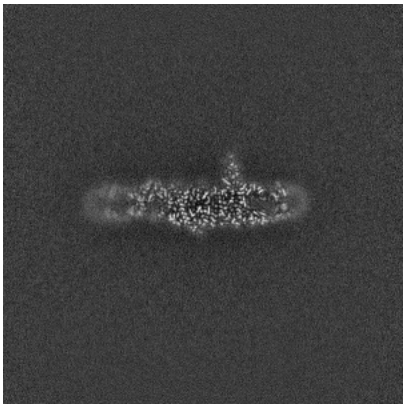


Z Index: 240

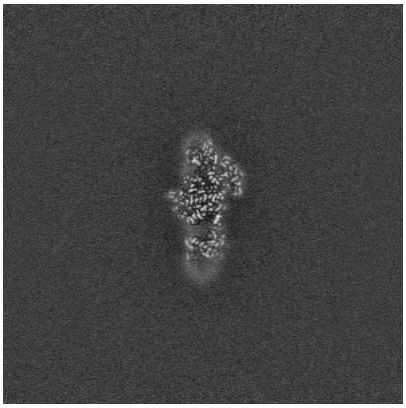
6.2.2 Raw map



X Index: 240



Y Index: 240

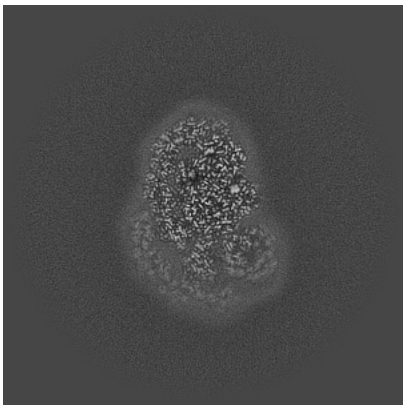


Z Index: 240

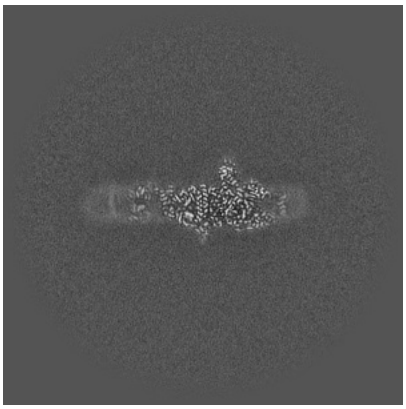
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

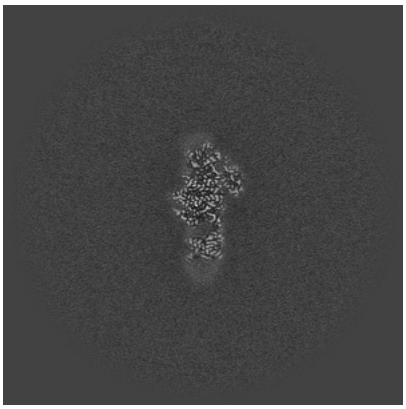
6.3.1 Primary map



X Index: 252

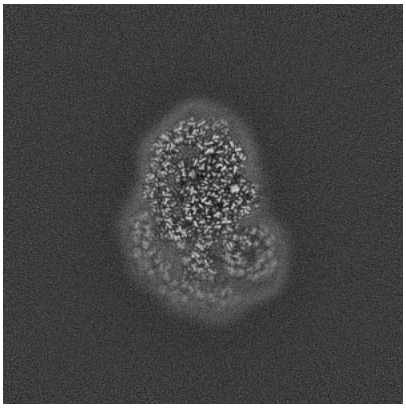


Y Index: 247

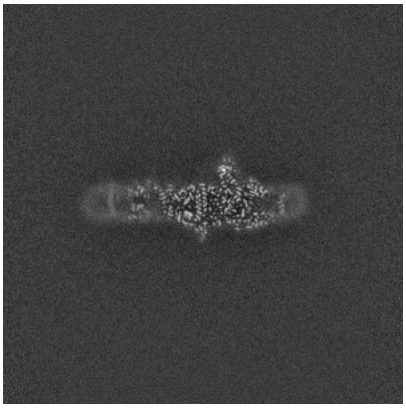


Z Index: 243

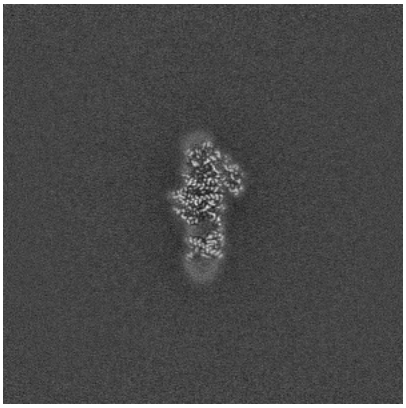
6.3.2 Raw map



X Index: 252



Y Index: 247

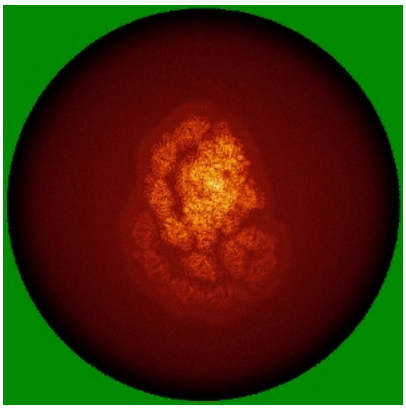


Z Index: 242

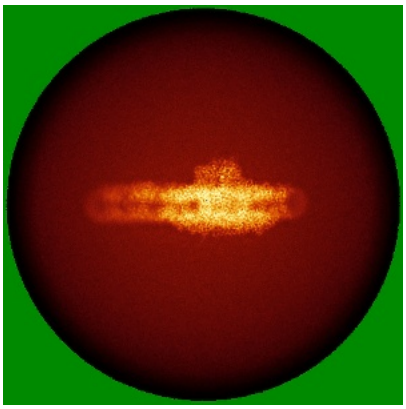
The images above show the largest variance slices of the map in three orthogonal directions.

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

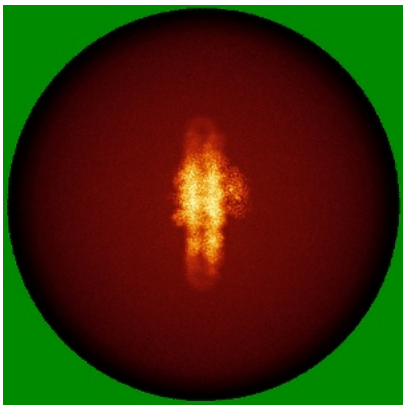
6.4.1 Primary map



X

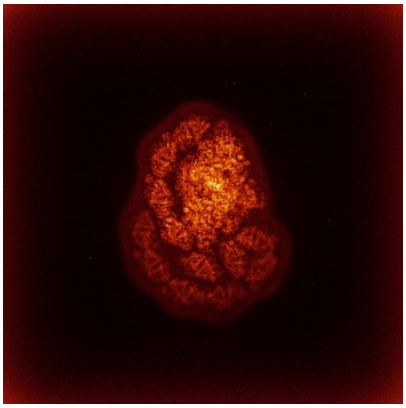


Y

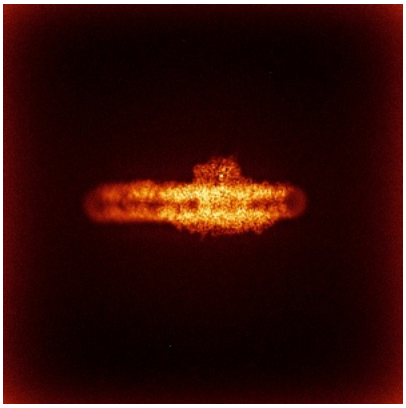


Z

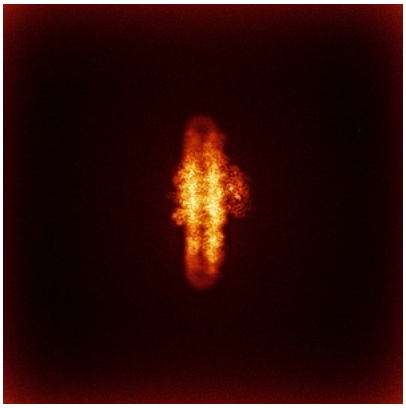
6.4.2 Raw map



X



Y

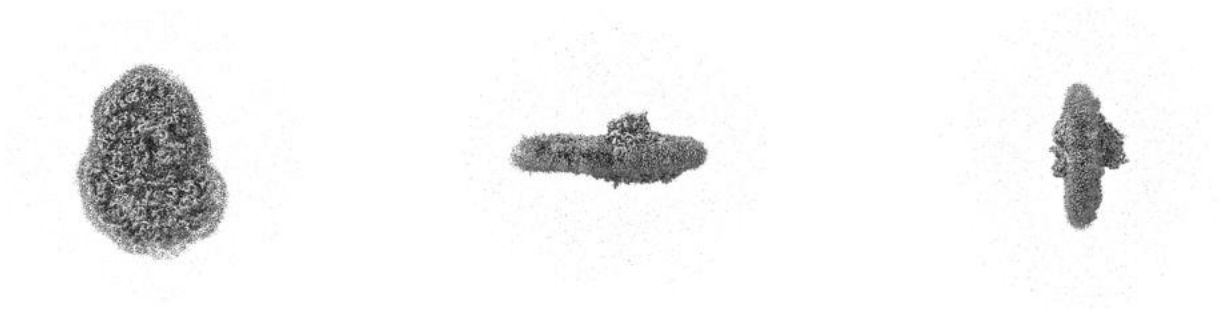


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views (i)

6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.45. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map

X Y Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

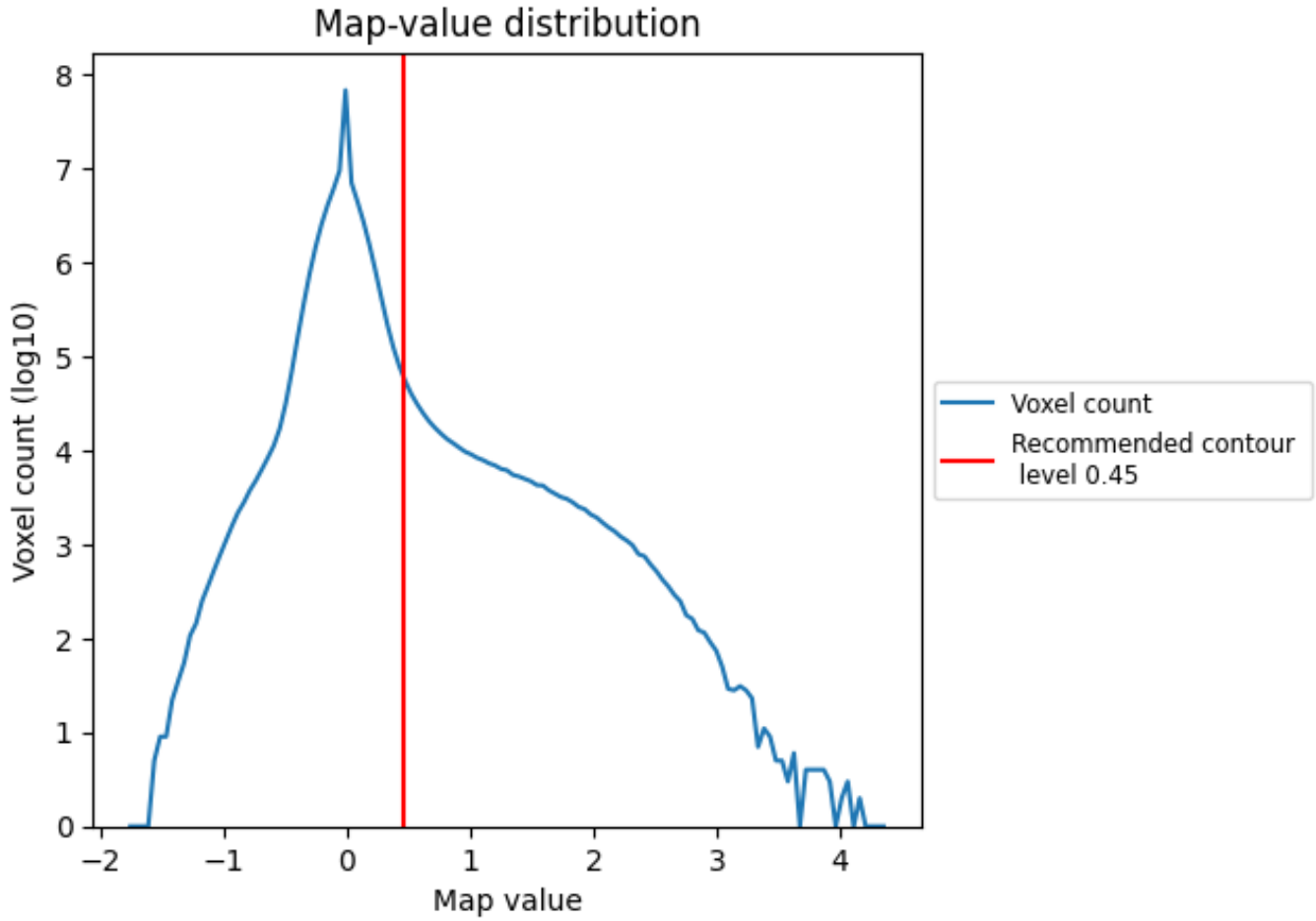
6.6 Mask visualisation (i)

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

7 Map analysis

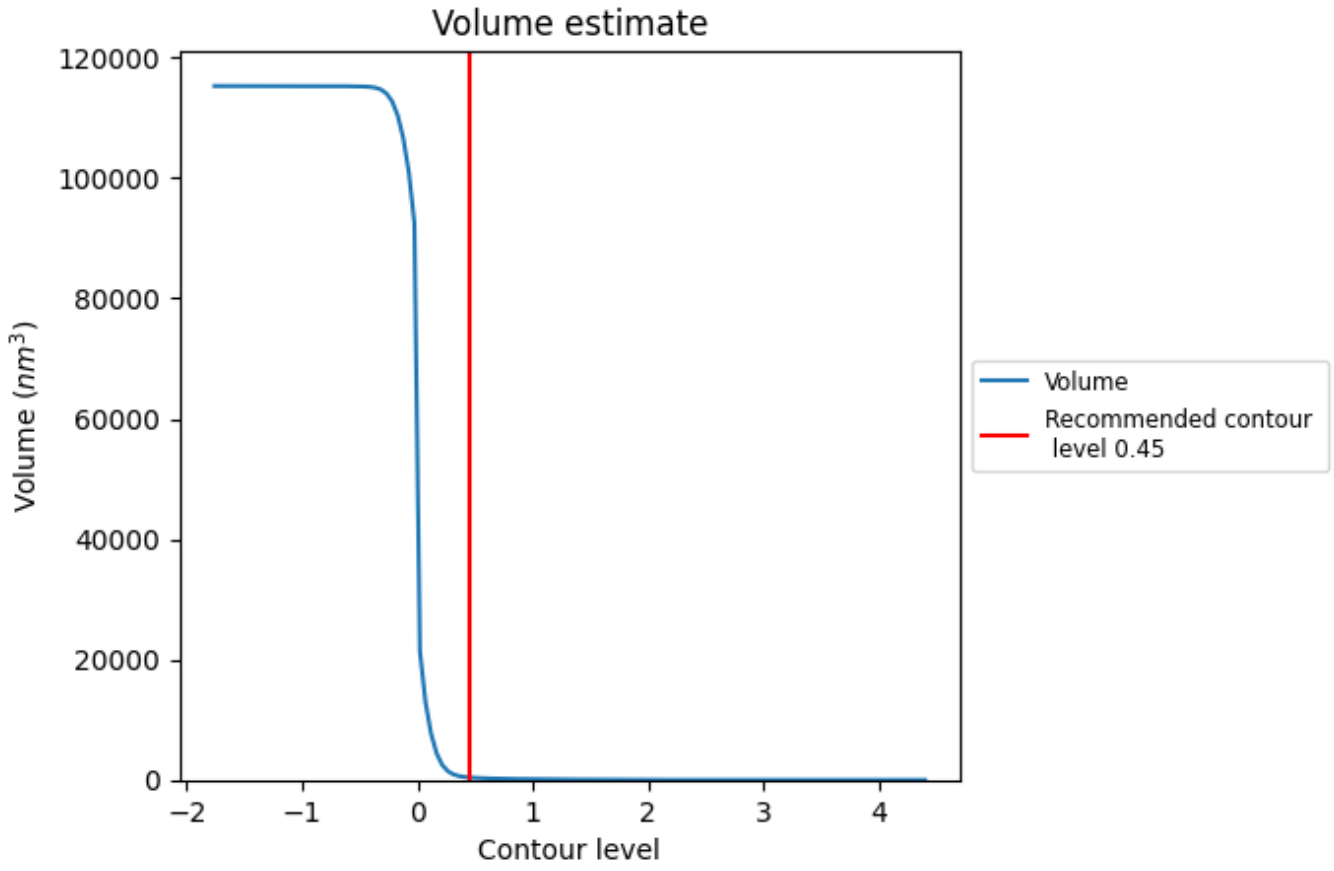
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

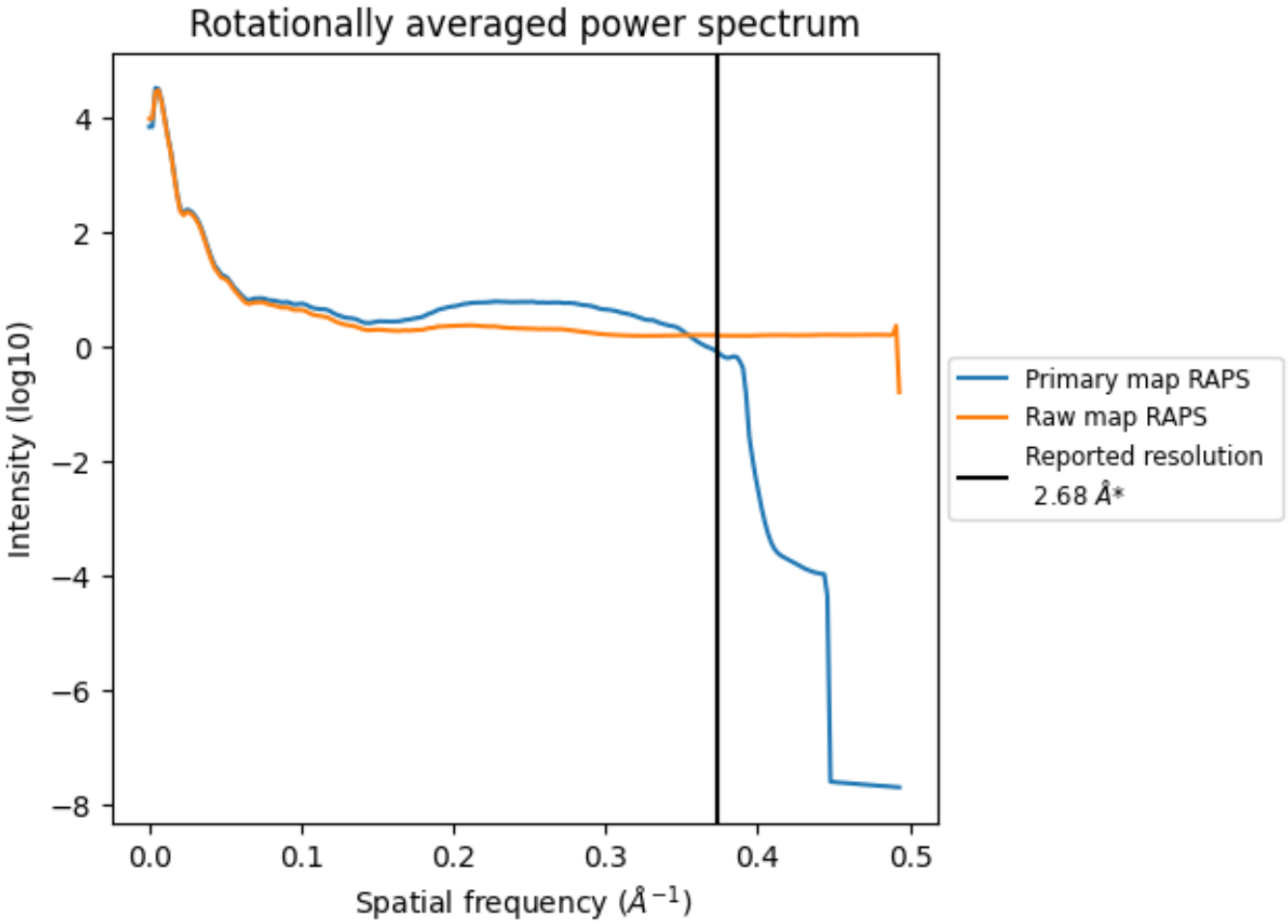
7.2 Volume estimate



The volume at the recommended contour level is 418 nm^3; this corresponds to an approximate mass of 378 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)

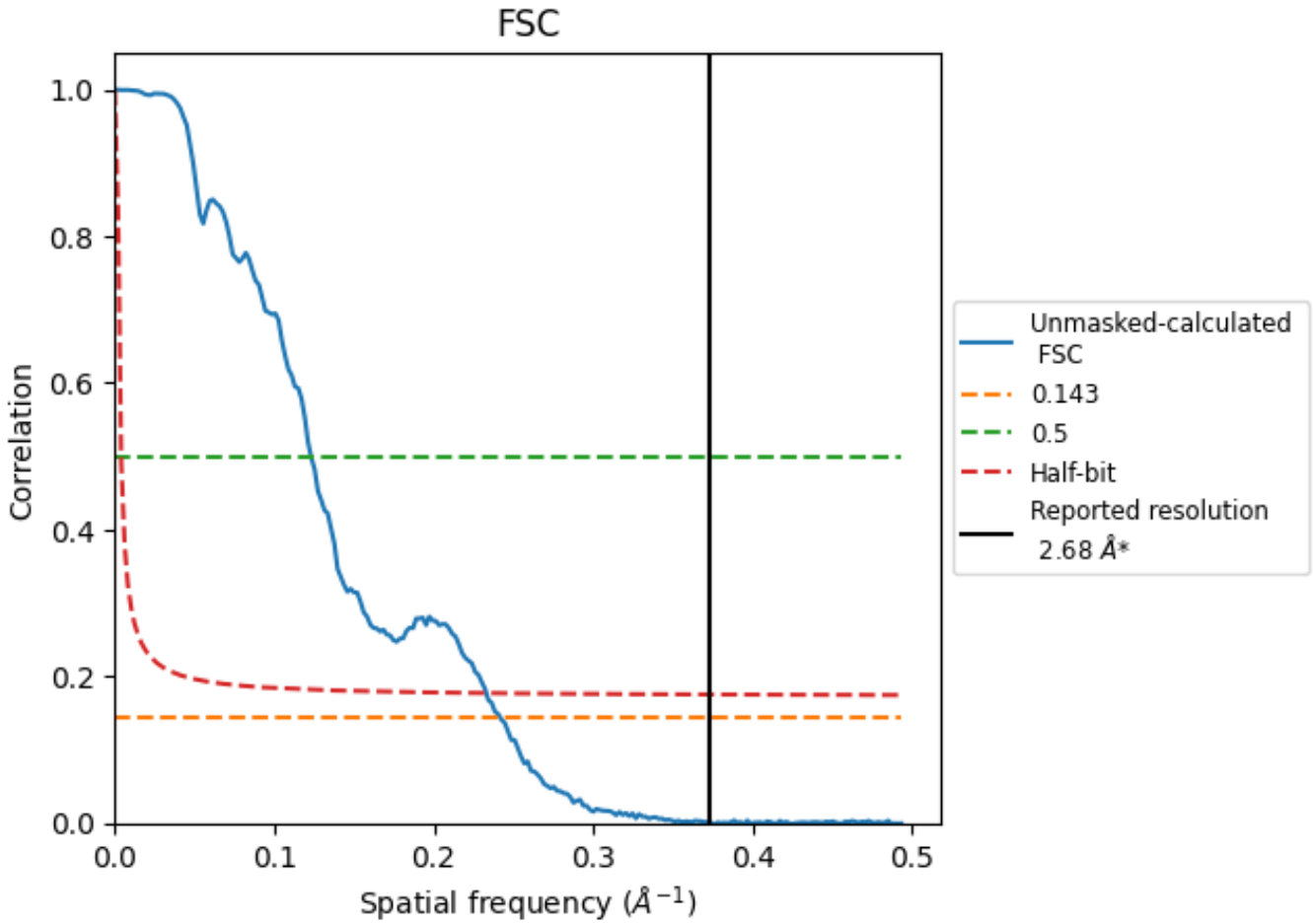


*Reported resolution corresponds to spatial frequency of 0.373 Å^{-1}

8 Fourier-Shell correlation

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.373 Å^{-1}

8.2 Resolution estimates (i)

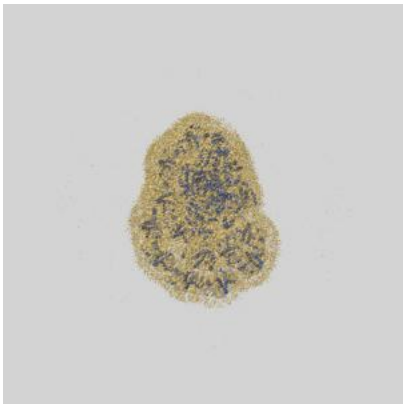
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.68	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.14	8.13	4.29

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.14 differs from the reported value 2.68 by more than 10 %

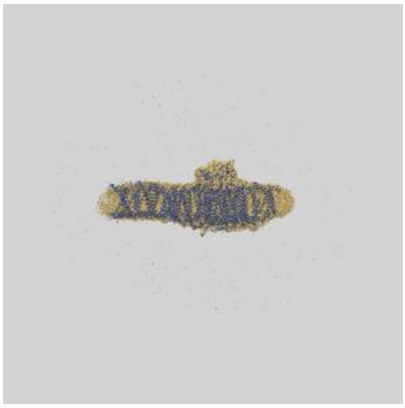
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-33401 and PDB model 7XQP. Per-residue inclusion information can be found in section 3 on page 38.

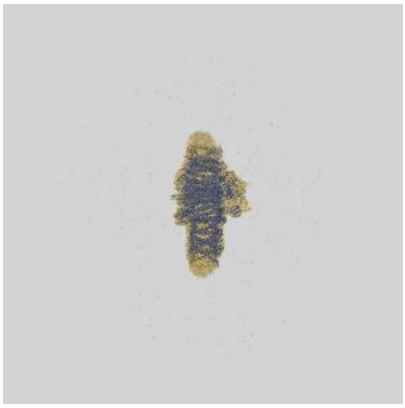
9.1 Map-model overlay



X



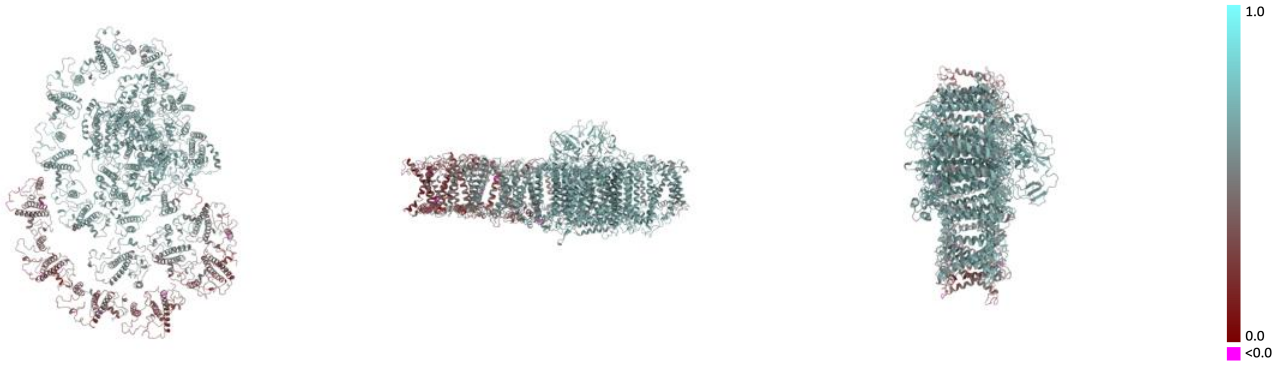
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.45 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.

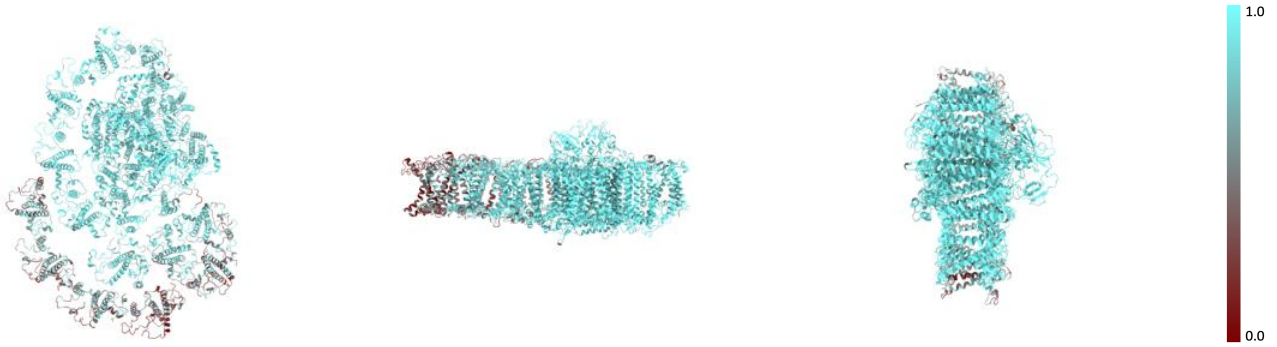
9.2 Q-score mapped to coordinate model (i)



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.

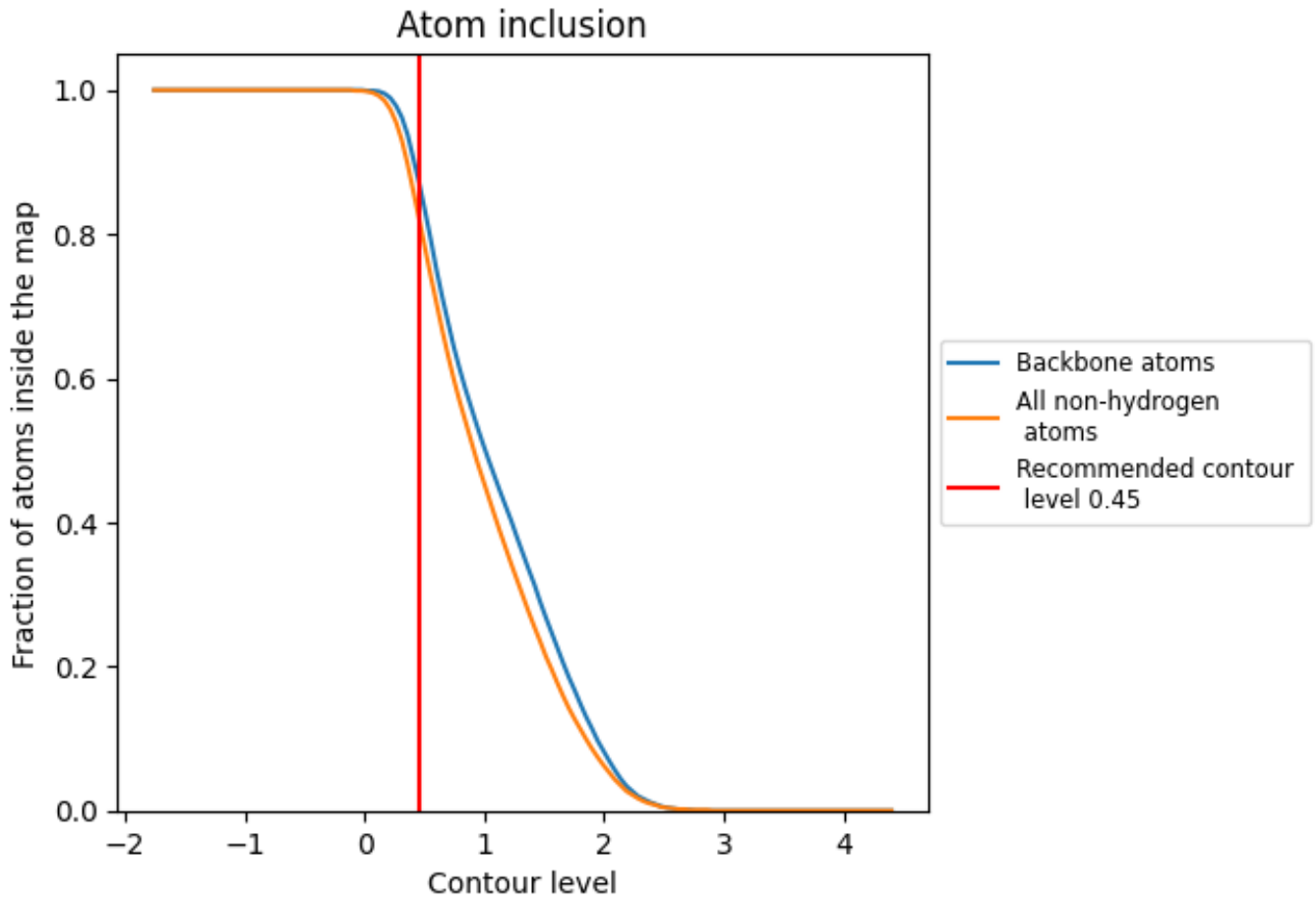
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.45).

9.4 Atom inclusion (i)



At the recommended contour level, 88% of all backbone atoms, 83% 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 (0.45) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8260	0.5360
1	0.9160	0.5760
2	0.9220	0.5910
3	0.9350	0.6030
4	0.9200	0.5810
5	0.5830	0.3590
6	0.5300	0.3330
7	0.3390	0.2870
8	0.5420	0.3320
9	0.8250	0.5250
A	0.9620	0.6340
B	0.9610	0.6300
C	0.9730	0.6210
D	0.9470	0.6150
E	0.9410	0.6070
F	0.9220	0.6030
G	0.7980	0.5530
H	0.8880	0.5780
I	0.9470	0.6180
J	0.9350	0.6110
K	0.9400	0.6090
L	0.9430	0.6120
M	0.8980	0.5880
O	0.8320	0.5260
a	0.5470	0.3560
b	0.7680	0.4910
c	0.7450	0.4660