wwPDB EM Validation Summary Report

Nov 4, 2024 – 12:03 PM JST

PDB ID	:	7Y8A
EMDB ID	:	EMD-33683
Title	:	Cryo-EM structure of cryptophyte photosystem I
Authors	:	Zhao, L.S.; Zhang, Y.Z.; Liu, L.N.; Li, K.
Deposited on	:	2022-06-23
Resolution	:	2.71 Å(reported)

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

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

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

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

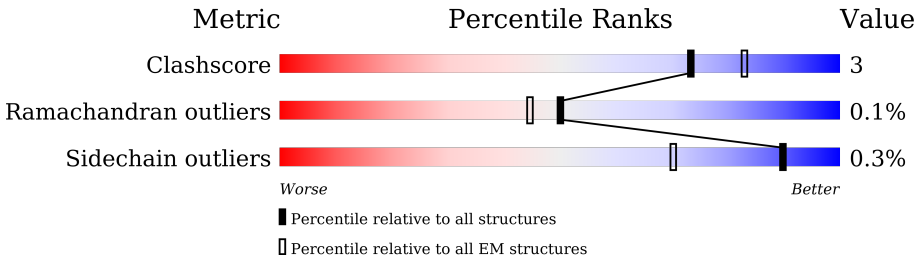
EMDB validation analysis	:	0.0.1.dev113
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (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 2.71 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	1	222	72% 9% 19%
2	2	216	70% 7% 22%
3	3	236	73% 24%
4	4	217	78% 19%
5	5	229	69% 13% 18%
6	6	215	73% 7% 20%
7	7	230	70% 7% 23%
8	8	227	68% 8% 24%

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Mol	Chain	Length	Quality of chain
9	9	220	5% 73% 8% 18%
10	A	752	91% 7%
11	B	734	91% 9%
12	C	81	86% 11%
13	D	141	90% 6%
14	E	64	89% 6% 5%
15	F	183	80% 8% 13%
16	I	36	86% 6% 8%
17	J	42	93% 7%
18	K	87	82% 8% 10%
19	L	153	7% 90% 5%
20	M	30	93% 7%
21	O	154	14% 56% 40%
22	R	133	61% 8% 31%
23	X	164	30% 79% 10% 12%
24	Z	242	60% 37%
25	a	215	80% 20%
26	b	218	80% 19%

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
27	CLA	1	601	X	-	-	-
27	CLA	1	602	X	-	-	-
27	CLA	1	603	X	-	-	-
27	CLA	1	604	X	-	-	-
27	CLA	1	605	X	-	-	-
27	CLA	1	606	X	-	-	-
27	CLA	1	607	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
27	CLA	1	608	X	-	-	-
27	CLA	1	609	X	-	-	-
27	CLA	1	611	X	-	-	-
27	CLA	1	612	X	-	-	-
27	CLA	1	613	X	-	-	-
27	CLA	2	601	X	-	-	-
27	CLA	2	602	X	-	-	-
27	CLA	2	603	X	-	-	-
27	CLA	2	604	X	-	-	-
27	CLA	2	605	X	-	-	-
27	CLA	2	606	X	-	-	-
27	CLA	2	607	X	-	-	-
27	CLA	2	608	X	-	-	-
27	CLA	2	609	X	-	-	-
27	CLA	2	611	X	-	-	-
27	CLA	2	612	X	-	-	-
27	CLA	3	601	X	-	-	-
27	CLA	3	602	X	-	-	-
27	CLA	3	603	X	-	-	-
27	CLA	3	604	X	-	-	-
27	CLA	3	605	X	-	-	-
27	CLA	3	607	X	-	-	-
27	CLA	3	608	X	-	-	-
27	CLA	3	609	X	-	-	-
27	CLA	3	610	X	-	-	-
27	CLA	3	611	X	-	-	-
27	CLA	3	612	X	-	-	-
27	CLA	4	601	X	-	-	-
27	CLA	4	602	X	-	-	-
27	CLA	4	603	X	-	-	-
27	CLA	4	604	X	-	-	-
27	CLA	4	606	X	-	-	-
27	CLA	4	607	X	-	-	-
27	CLA	4	608	X	-	-	-
27	CLA	4	609	X	-	-	-
27	CLA	4	610	X	-	-	-
27	CLA	4	611	X	-	-	-
27	CLA	5	601	X	-	-	-
27	CLA	5	602	X	-	-	-
27	CLA	5	603	X	-	-	-
27	CLA	5	604	X	-	-	-
27	CLA	5	605	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
27	CLA	5	606	X	-	-	-
27	CLA	5	607	X	-	-	-
27	CLA	5	608	X	-	-	-
27	CLA	5	609	X	-	-	-
27	CLA	5	611	X	-	-	-
27	CLA	5	612	X	-	-	-
27	CLA	5	613	X	-	-	-
27	CLA	6	601	X	-	-	-
27	CLA	6	602	X	-	-	-
27	CLA	6	603	X	-	-	-
27	CLA	6	604	X	-	-	-
27	CLA	6	605	X	-	-	-
27	CLA	6	606	X	-	-	-
27	CLA	6	607	X	-	-	-
27	CLA	6	608	X	-	-	-
27	CLA	6	609	X	-	-	-
27	CLA	6	611	X	-	-	-
27	CLA	6	612	X	-	-	-
27	CLA	7	302	X	-	-	-
27	CLA	7	303	X	-	-	-
27	CLA	7	304	X	-	-	-
27	CLA	7	305	X	-	-	-
27	CLA	7	306	X	-	-	-
27	CLA	7	308	X	-	-	-
27	CLA	7	309	X	-	-	-
27	CLA	7	310	X	-	-	-
27	CLA	7	312	X	-	-	-
27	CLA	7	313	X	-	-	-
27	CLA	8	601	X	-	-	-
27	CLA	8	602	X	-	-	-
27	CLA	8	603	X	-	-	-
27	CLA	8	604	X	-	-	-
27	CLA	8	605	X	-	-	-
27	CLA	8	606	X	-	-	-
27	CLA	8	607	X	-	-	-
27	CLA	8	608	X	-	-	-
27	CLA	8	615	X	-	-	-
27	CLA	9	601	X	-	-	-
27	CLA	9	602	X	-	-	-
27	CLA	9	603	X	-	-	-
27	CLA	9	604	X	-	-	-
27	CLA	9	605	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
27	CLA	9	606	X	-	-	-
27	CLA	9	607	X	-	-	-
27	CLA	9	608	X	-	-	-
27	CLA	9	609	X	-	-	-
27	CLA	9	611	X	-	-	-
27	CLA	9	612	X	-	-	-
27	CLA	9	613	X	-	-	-
27	CLA	9	614	X	-	-	-
27	CLA	A	801	X	-	-	-
27	CLA	A	802	X	-	-	-
27	CLA	A	803	X	-	-	-
27	CLA	A	804	X	-	-	-
27	CLA	A	805	X	-	-	-
27	CLA	A	806	X	-	-	-
27	CLA	A	807	X	-	-	-
27	CLA	A	808	X	-	-	-
27	CLA	A	809	X	-	-	-
27	CLA	A	810	X	-	-	-
27	CLA	A	811	X	-	-	-
27	CLA	A	812	X	-	-	-
27	CLA	A	813	X	-	-	-
27	CLA	A	814	X	-	-	-
27	CLA	A	815	X	-	-	-
27	CLA	A	816	X	-	-	-
27	CLA	A	817	X	-	-	-
27	CLA	A	818	X	-	-	-
27	CLA	A	819	X	-	-	-
27	CLA	A	820	X	-	-	-
27	CLA	A	821	X	-	-	-
27	CLA	A	822	X	-	-	-
27	CLA	A	823	X	-	-	-
27	CLA	A	824	X	-	-	-
27	CLA	A	825	X	-	-	-
27	CLA	A	826	X	-	-	-
27	CLA	A	827	X	-	-	-
27	CLA	A	828	X	-	-	-
27	CLA	A	829	X	-	-	-
27	CLA	A	830	X	-	-	-
27	CLA	A	831	X	-	-	-
27	CLA	A	832	X	-	-	-
27	CLA	A	833	X	-	-	-
27	CLA	A	834	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
27	CLA	A	835	X	-	-	-
27	CLA	A	836	X	-	-	-
27	CLA	A	837	X	-	-	-
27	CLA	A	838	X	-	-	-
27	CLA	A	839	X	-	-	-
27	CLA	A	840	X	-	-	-
27	CLA	A	841	X	-	-	-
27	CLA	A	842	X	-	-	-
27	CLA	A	843	X	-	-	-
27	CLA	A	844	X	-	-	-
27	CLA	B	801	X	-	-	-
27	CLA	B	802	X	-	-	-
27	CLA	B	803	X	-	-	-
27	CLA	B	804	X	-	-	-
27	CLA	B	805	X	-	-	-
27	CLA	B	806	X	-	-	-
27	CLA	B	807	X	-	-	-
27	CLA	B	808	X	-	-	-
27	CLA	B	809	X	-	-	-
27	CLA	B	810	X	-	-	-
27	CLA	B	811	X	-	-	-
27	CLA	B	812	X	-	-	-
27	CLA	B	813	X	-	-	-
27	CLA	B	814	X	-	-	-
27	CLA	B	815	X	-	-	-
27	CLA	B	816	X	-	-	-
27	CLA	B	817	X	-	-	-
27	CLA	B	818	X	-	-	-
27	CLA	B	819	X	-	-	-
27	CLA	B	820	X	-	-	-
27	CLA	B	821	X	-	-	-
27	CLA	B	822	X	-	-	-
27	CLA	B	823	X	-	-	-
27	CLA	B	824	X	-	-	-
27	CLA	B	825	X	-	-	-
27	CLA	B	826	X	-	-	-
27	CLA	B	827	X	-	-	-
27	CLA	B	828	X	-	-	-
27	CLA	B	829	X	-	-	-
27	CLA	B	830	X	-	-	-
27	CLA	B	831	X	-	-	-
27	CLA	B	832	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
27	CLA	B	833	X	-	-	-
27	CLA	B	834	X	-	-	-
27	CLA	B	835	X	-	-	-
27	CLA	B	836	X	-	-	-
27	CLA	B	837	X	-	-	-
27	CLA	B	838	X	-	-	-
27	CLA	B	839	X	-	-	-
27	CLA	B	840	X	-	-	-
27	CLA	B	841	X	-	-	-
27	CLA	F	202	X	-	-	-
27	CLA	F	203	X	-	-	-
27	CLA	F	204	X	-	-	-
27	CLA	J	102	X	-	-	-
27	CLA	K	101	X	-	-	-
27	CLA	K	102	X	-	-	-
27	CLA	L	201	X	-	-	-
27	CLA	L	202	X	-	-	-
27	CLA	L	203	X	-	-	-
27	CLA	O	201	X	-	-	-
27	CLA	O	202	X	-	-	-
27	CLA	O	203	X	-	-	-
27	CLA	O	204	X	-	-	-
27	CLA	R	202	X	-	-	-
27	CLA	Z	301	X	-	-	-
27	CLA	Z	304	X	-	-	-
27	CLA	Z	305	X	-	-	-
27	CLA	Z	306	X	-	-	-
27	CLA	Z	310	X	-	-	-
27	CLA	a	601	X	-	-	-
27	CLA	a	602	X	-	-	-
27	CLA	a	603	X	-	-	-
27	CLA	a	604	X	-	-	-
27	CLA	a	605	X	-	-	-
27	CLA	a	606	X	-	-	-
27	CLA	a	607	X	-	-	-
27	CLA	a	608	X	-	-	-
27	CLA	a	610	X	-	-	-
27	CLA	a	611	X	-	-	-
27	CLA	b	601	X	-	-	-
27	CLA	b	602	X	-	-	-
27	CLA	b	603	X	-	-	-
27	CLA	b	604	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
27	CLA	b	606	X	-	-	-
27	CLA	b	607	X	-	-	-
27	CLA	b	608	X	-	-	-
27	CLA	b	610	X	-	-	-
27	CLA	b	611	X	-	-	-

2 Entry composition (i)

There are 39 unique types of molecules in this entry. The entry contains 53404 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 ACPI-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	1	179	1338	861	227	242	8	0	0

- Molecule 2 is a protein called ACPI-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	2	168	1320	872	215	230	3	0	0

- Molecule 3 is a protein called ACPI-3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	3	180	1362	875	231	246	10	0	0

- Molecule 4 is a protein called ACPI-4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	4	176	1366	891	224	245	6	0	0

- Molecule 5 is a protein called ACPI-5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	5	188	1403	908	234	253	8	0	0

- Molecule 6 is a protein called ACPI-6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	6	173	1305	846	217	232	10	0	0

- Molecule 7 is a protein called ACPI-7.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	7	177	Total	C	N	O	S	0	0
			1337	861	230	238	8		

- Molecule 8 is a protein called ACPI-8.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	8	173	Total	C	N	O	S	0	0
			1298	842	217	235	4		

- Molecule 9 is a protein called ACPI-12.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	9	180	Total	C	N	O	S	0	0
			1349	864	230	243	12		

- Molecule 10 is a protein called Photosystem I P700 chlorophyll a apoprotein A1.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	A	741	Total	C	N	O	S	0	0
			5824	3804	992	1000	28		

- Molecule 11 is a protein called Photosystem I P700 chlorophyll a apoprotein A2.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	B	731	Total	C	N	O	S	0	0
			5828	3847	982	984	15		

- Molecule 12 is a protein called Photosystem I iron-sulfur center.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	C	80	Total	C	N	O	S	0	0
			591	361	103	115	12		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
13	D	137	Total	C	N	O	S	0	0
			1070	685	184	198	3		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
14	E	61	Total	C	N	O	0	0
			491	312	85	94		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
15	F	160	Total	C	N	O	S	0	0
			1258	814	214	228	2		

- Molecule 16 is a protein called Photosystem I reaction center subunit VIII.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	I	33	Total	C	N	O	S	0	0
			258	180	34	42	2		

- Molecule 17 is a protein called Photosystem I reaction center subunit IX.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	J	42	Total	C	N	O	S	0	0
			342	232	49	58	3		

- Molecule 18 is a protein called Photosystem I reaction center subunit PsaK.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	K	78	Total	C	N	O	S	0	0
			553	358	90	102	3		

- Molecule 19 is a protein called Photosystem I reaction center subunit XI.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	L	147	Total	C	N	O	S	0	0
			1119	730	180	207	2		

- Molecule 20 is a protein called Photosystem I reaction center subunit XII.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	M	30	Total	C	N	O	S	0	0
			227	152	35	39	1		

- Molecule 21 is a protein called PsaO.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	O	92	Total	C	N	O	S	0	0
			709	481	104	123	1		

- Molecule 22 is a protein called PsaR.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	R	92	Total	C	N	O	S	0	0
			680	439	112	127	2		

- Molecule 23 is a protein called Unk1.

Mol	Chain	Residues	Atoms				AltConf	Trace
23	X	145	Total	C	N	O	0	0
			725	435	145	145		

- Molecule 24 is a protein called ACPI-S.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	Z	153	Total	C	N	O	S	0	0
			1130	721	188	211	10		

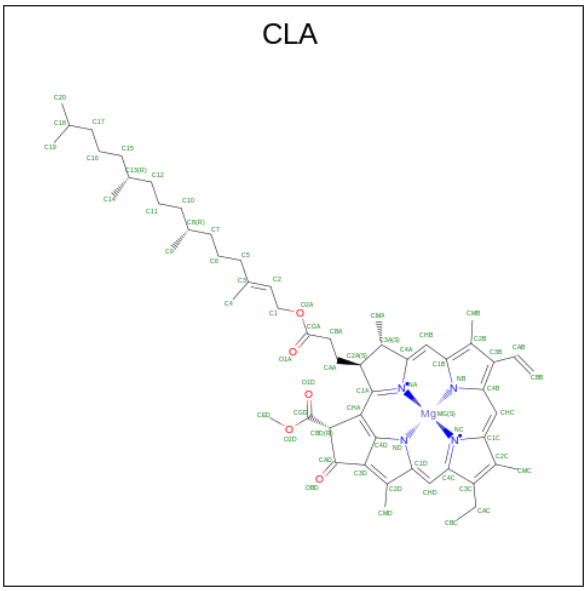
- Molecule 25 is a protein called ACPI-13.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	a	171	Total	C	N	O	S	0	0
			1271	823	207	231	10		

- Molecule 26 is a protein called ACPI-14.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	b	176	Total	C	N	O	S	0	0
			1368	891	224	244	9		

- Molecule 27 is CHLOROPHYLL A (three-letter code: CLA) (formula: $C_{55}H_{72}MgN_4O_5$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
27	1	1	Total 45	C 35	Mg 1	N 4	O 5	0
27	1	1	Total 59	C 49	Mg 1	N 4	O 5	0
27	1	1	Total 52	C 42	Mg 1	N 4	O 5	0
27	1	1	Total 45	C 35	Mg 1	N 4	O 5	0
27	1	1	Total 42	C 34	Mg 1	N 4	O 3	0
27	1	1	Total 45	C 35	Mg 1	N 4	O 5	0
27	1	1	Total 45	C 35	Mg 1	N 4	O 5	0
27	1	1	Total 60	C 50	Mg 1	N 4	O 5	0
27	1	1	Total 41	C 33	Mg 1	N 4	O 3	0
27	1	1	Total 45	C 35	Mg 1	N 4	O 5	0
27	1	1	Total 60	C 50	Mg 1	N 4	O 5	0
27	1	1	Total 45	C 35	Mg 1	N 4	O 5	0
27	2	1	Total 42	C 34	Mg 1	N 4	O 3	0
27	2	1	Total 59	C 49	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
27	2	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
27	2	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
27	2	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
27	2	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
27	2	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
27	2	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
27	2	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
27	2	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
27	2	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
27	3	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
27	3	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
27	3	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
27	3	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	3	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
27	3	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
27	3	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
27	3	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	3	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	3	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
27	3	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
27	4	1	Total	C	Mg	N	O	0
			55	45	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
27	4	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
27	4	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
27	4	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
27	4	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
27	4	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
27	4	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	4	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
27	4	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	4	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	5	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
27	5	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
27	5	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
27	5	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
27	5	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
27	5	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
27	5	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
27	5	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
27	5	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
27	5	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
27	5	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
27	5	1	Total	C	Mg	N	O	0
			41	33	1	4	3	

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Mol	Chain	Residues	Atoms					AltConf
27	6	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
27	6	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	6	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
27	6	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
27	6	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
27	6	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
27	6	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
27	6	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
27	6	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
27	6	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
27	6	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
27	7	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
27	7	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	7	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
27	7	1	Total	C	Mg	N	O	0
			53	43	1	4	5	
27	7	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
27	7	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
27	7	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
27	7	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
27	7	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
27	7	1	Total	C	Mg	N	O	0
			50	40	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
27	8	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
27	8	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
27	8	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	8	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	8	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
27	8	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
27	8	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
27	8	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	8	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	9	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
27	9	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
27	9	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
27	9	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
27	9	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
27	9	1	Total	C	Mg	N	O	0
			64	54	1	4	5	
27	9	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	9	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
27	9	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
27	9	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
27	9	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
27	9	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
27	9	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
27	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	A	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
27	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	A	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
27	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	A	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
27	A	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
27	A	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
27	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	A	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
27	A	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
27	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
27	A	1	Total	C	Mg	N	O	0
			62	52	1	4	5	
27	A	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
27	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms	AltConf
27	A	1	Total C Mg N O 55 45 1 4 5	0
27	A	1	Total C Mg N O 65 55 1 4 5	0
27	A	1	Total C Mg N O 65 55 1 4 5	0
27	A	1	Total C Mg N O 65 55 1 4 5	0
27	A	1	Total C Mg N O 65 55 1 4 5	0
27	A	1	Total C Mg N O 65 55 1 4 5	0
27	A	1	Total C Mg N O 65 55 1 4 5	0
27	A	1	Total C Mg N O 65 55 1 4 5	0
27	A	1	Total C Mg N O 50 40 1 4 5	0
27	A	1	Total C Mg N O 60 50 1 4 5	0
27	A	1	Total C Mg N O 65 55 1 4 5	0
27	A	1	Total C Mg N O 65 55 1 4 5	0
27	A	1	Total C Mg N O 65 55 1 4 5	0
27	A	1	Total C Mg N O 55 45 1 4 5	0
27	A	1	Total C Mg N O 60 50 1 4 5	0
27	A	1	Total C Mg N O 55 45 1 4 5	0
27	A	1	Total C Mg N O 65 55 1 4 5	0
27	A	1	Total C Mg N O 65 55 1 4 5	0
27	A	1	Total C Mg N O 65 55 1 4 5	0
27	A	1	Total C Mg N O 55 45 1 4 5	0
27	A	1	Total C Mg N O 65 55 1 4 5	0

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Mol	Chain	Residues	Atoms	AltConf
27	A	1	Total C Mg N O 65 55 1 4 5	0
27	A	1	Total C Mg N O 65 55 1 4 5	0
27	A	1	Total C Mg N O 65 55 1 4 5	0
27	B	1	Total C Mg N O 65 55 1 4 5	0
27	B	1	Total C Mg N O 65 55 1 4 5	0
27	B	1	Total C Mg N O 45 35 1 4 5	0
27	B	1	Total C Mg N O 65 55 1 4 5	0
27	B	1	Total C Mg N O 65 55 1 4 5	0
27	B	1	Total C Mg N O 65 55 1 4 5	0
27	B	1	Total C Mg N O 65 55 1 4 5	0
27	B	1	Total C Mg N O 65 55 1 4 5	0
27	B	1	Total C Mg N O 65 55 1 4 5	0
27	B	1	Total C Mg N O 60 50 1 4 5	0
27	B	1	Total C Mg N O 55 45 1 4 5	0
27	B	1	Total C Mg N O 65 55 1 4 5	0
27	B	1	Total C Mg N O 61 51 1 4 5	0
27	B	1	Total C Mg N O 42 34 1 4 3	0
27	B	1	Total C Mg N O 65 55 1 4 5	0
27	B	1	Total C Mg N O 59 49 1 4 5	0
27	B	1	Total C Mg N O 60 50 1 4 5	0
27	B	1	Total C Mg N O 60 50 1 4 5	0

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Mol	Chain	Residues	Atoms					AltConf
27	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
27	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
27	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
27	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
27	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
27	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
27	B	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
27	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
27	B	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
27	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	B	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
27	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
27	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	B	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
27	F	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
27	F	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
27	F	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
27	J	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
27	K	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	K	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
27	L	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
27	L	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
27	L	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
27	O	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
27	O	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
27	O	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
27	O	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
27	R	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
27	Z	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
27	Z	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
27	Z	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
27	Z	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
27	Z	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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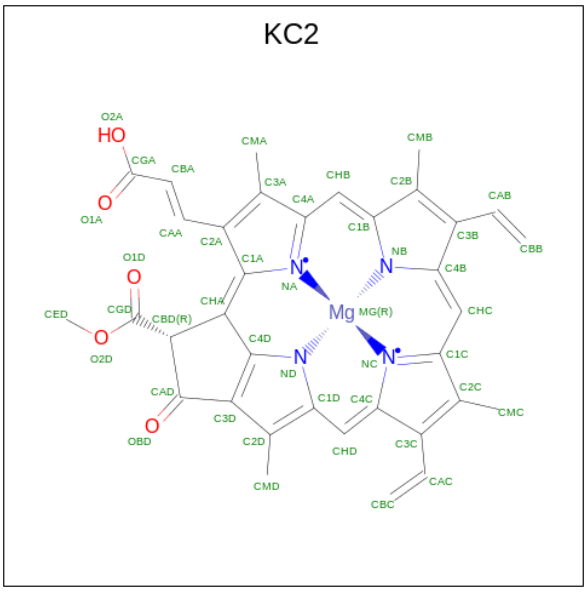
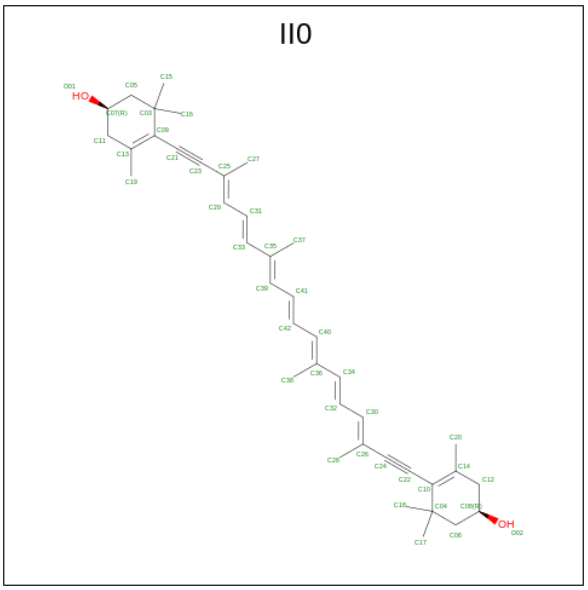
Mol	Chain	Residues	Atoms					AltConf
27	a	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
27	a	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
27	a	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
27	a	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
27	a	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
27	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	a	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
27	a	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
27	a	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
27	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	b	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
27	b	1	Total	C	Mg	N	O	0
			64	54	1	4	5	
27	b	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
27	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	b	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
27	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
27	b	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
27	b	1	Total	C	Mg	N	O	0
			55	45	1	4	5	

- Molecule 28 is Chlorophyll c2 (three-letter code: KC2) (formula: $C_{35}H_{28}MgN_4O_5$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
28	1	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
28	2	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
28	3	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
28	4	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
28	5	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
28	6	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
28	6	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
28	7	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
28	7	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
28	9	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
28	Z	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
28	a	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
28	b	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
28	b	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

- Molecule 29 is (1 {R})-3,5,5-trimethyl-4-[(3 {E},5 {E},7 {E},9 {E},11 {E},13 {E},15 {E})-3,7,12,16-tetramethyl-18-[(4 {R})-2,6,6-trimethyl-4-oxidanyl-cyclohexen-1-yl]octadeca-3,5,7,9,11,13,15-heptaen-1,17-diynyl]cyclohex-3-en-1-ol (three-letter code: II0) (formula: $C_{40}H_{52}O_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	AltConf
29	1	1	Total C O 42 40 2	0
29	1	1	Total C O 42 40 2	0
29	1	1	Total C O 42 40 2	0
29	1	1	Total C O 42 40 2	0
29	2	1	Total C O 42 40 2	0
29	2	1	Total C O 42 40 2	0
29	2	1	Total C O 42 40 2	0
29	3	1	Total C O 42 40 2	0
29	3	1	Total C O 42 40 2	0
29	3	1	Total C O 42 40 2	0
29	3	1	Total C O 42 40 2	0

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Mol	Chain	Residues	Atoms			AltConf
29	3	1	Total	C	O	0
			42	40	2	
29	4	1	Total	C	O	0
			42	40	2	
29	4	1	Total	C	O	0
			42	40	2	
29	4	1	Total	C	O	0
			42	40	2	
29	4	1	Total	C	O	0
			42	40	2	
29	5	1	Total	C	O	0
			42	40	2	
29	5	1	Total	C	O	0
			42	40	2	
29	5	1	Total	C	O	0
			42	40	2	
29	5	1	Total	C	O	0
			42	40	2	
29	5	1	Total	C	O	0
			42	40	2	
29	6	1	Total	C	O	0
			42	40	2	
29	6	1	Total	C	O	0
			42	40	2	
29	7	1	Total	C	O	0
			42	40	2	
29	7	1	Total	C	O	0
			42	40	2	
29	7	1	Total	C	O	0
			42	40	2	
29	7	1	Total	C	O	0
			42	40	2	
29	7	1	Total	C	O	0
			42	40	2	
29	8	1	Total	C	O	0
			42	40	2	
29	8	1	Total	C	O	0
			42	40	2	
29	8	1	Total	C	O	0
			42	40	2	
29	9	1	Total	C	O	0
			42	40	2	

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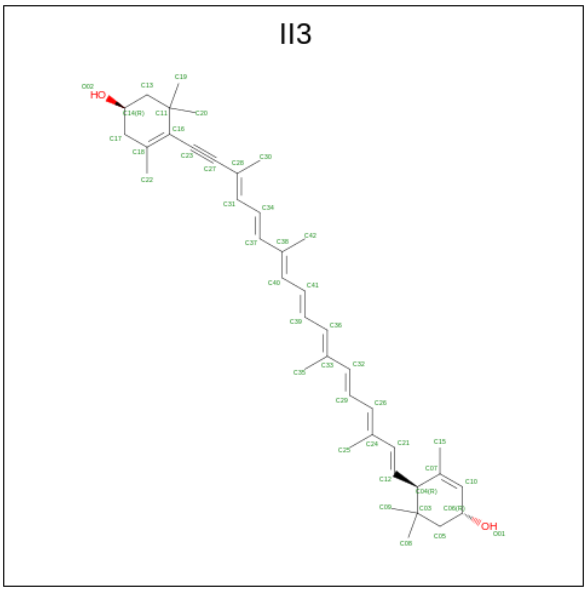
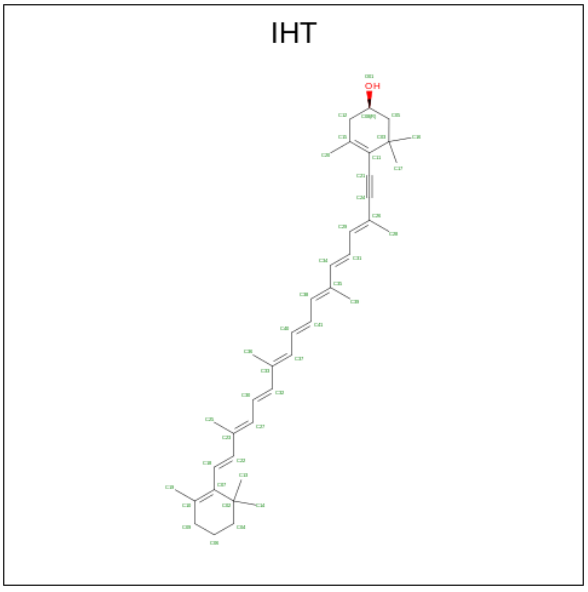
Mol	Chain	Residues	Atoms			AltConf
29	9	1	Total	C	O	0
			42	40	2	
29	9	1	Total	C	O	0
			42	40	2	
29	9	1	Total	C	O	0
			42	40	2	
29	B	1	Total	C	O	0
			42	40	2	
29	J	1	Total	C	O	0
			42	40	2	
29	O	1	Total	C	O	0
			42	40	2	
29	O	1	Total	C	O	0
			42	40	2	
29	R	1	Total	C	O	0
			42	40	2	
29	Z	1	Total	C	O	0
			42	40	2	
29	a	1	Total	C	O	0
			42	40	2	
29	a	1	Total	C	O	0
			42	40	2	
29	a	1	Total	C	O	0
			42	40	2	
29	a	1	Total	C	O	0
			42	40	2	
29	b	1	Total	C	O	0
			42	40	2	
29	b	1	Total	C	O	0
			42	40	2	

- Molecule 30 is (1 {R})-3,5,5-trimethyl-4-[(3 {E},5 {E},7 {E},9 {E},11 {E},13 {E},15 {E},17 {E})-3,7,12,16-tetramethyl-18-[(1 {R},4 {R})-2,6,6-trimethyl-4-oxidanyl-cyclohex-2-en-1-yl]octadeca-3,5,7,9,11,13,15,17-octaen-1-ynyl]cyclohex-3-en-1-ol (three-letter code: II3) (formula: $C_{40}H_{54}O_2$) (labeled as "Ligand of Interest" by depositor).



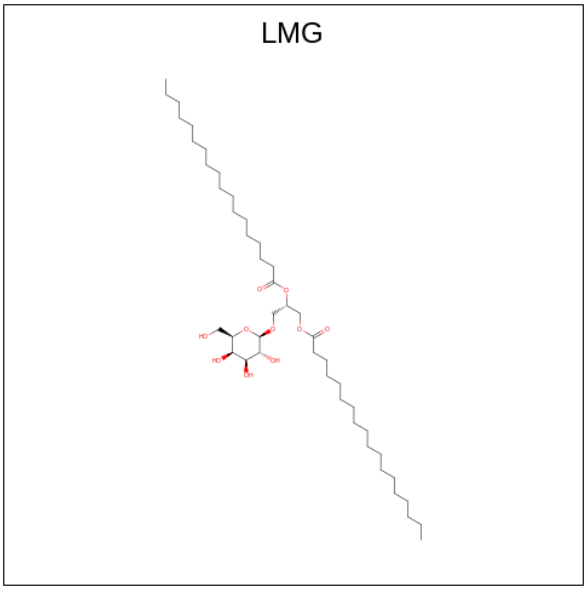
Mol	Chain	Residues	Atoms			AltConf
30	1	1	Total	C	O	0
			42	40	2	
30	b	1	Total	C	O	0
			42	40	2	

- Molecule 31 is (1 {R})-3,5,5-trimethyl-4-[(3 {E},5 {E},7 {E},9 {E},11 {E},13 {E},15 {E},17 {E})-3,7,12,16-tetramethyl-18-(2,6,6-trimethylcyclohexen-1-yl)octadeca-3,5,7,9,11,13,15,17-octaen-1-ynyl]cyclohex-3-en-1-ol (three-letter code: IHT) (formula: $C_{40}H_{54}O$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
31	1	1	Total	C	O	0
			41	40	1	
31	2	1	Total	C	O	0
			41	40	1	
31	5	1	Total	C	O	0
			41	40	1	
31	6	1	Total	C	O	0
			41	40	1	
31	8	1	Total	C	O	0
			41	40	1	
31	9	1	Total	C	O	0
			41	40	1	
31	A	1	Total	C	O	0
			41	40	1	
31	L	1	Total	C	O	0
			41	40	1	
31	Z	1	Total	C	O	0
			41	40	1	
31	a	1	Total	C	O	0
			41	40	1	

- Molecule 32 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: LMG) (formula: $C_{45}H_{86}O_{10}$).



Mol	Chain	Residues	Atoms			AltConf
32	2	1	Total	C	O	0
			36	26	10	

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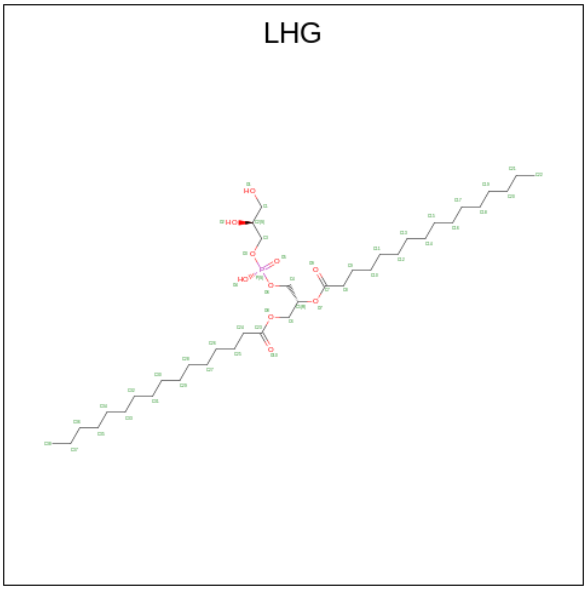
Mol	Chain	Residues	Atoms	AltConf
32	3	1	Total C O 30 20 10	0
32	3	1	Total C O 32 22 10	0
32	6	1	Total C O 32 22 10	0
32	8	1	Total C O 52 42 10	0
32	8	1	Total C O 51 41 10	0
32	F	1	Total C O 32 22 10	0

- Molecule 33 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula: $C_{38}H_{75}O_{10}P$).



Mol	Chain	Residues	Atoms	AltConf
33	2	1	Total C O P 22 12 9 1	0
33	2	1	Total C O P 39 28 10 1	0
33	2	1	Total C O P 42 31 10 1	0
33	3	1	Total C O P 49 38 10 1	0
33	3	1	Total C O P 34 23 10 1	0

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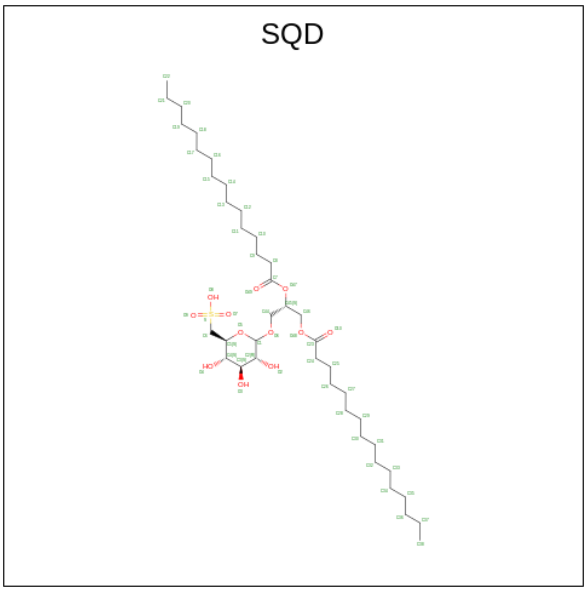
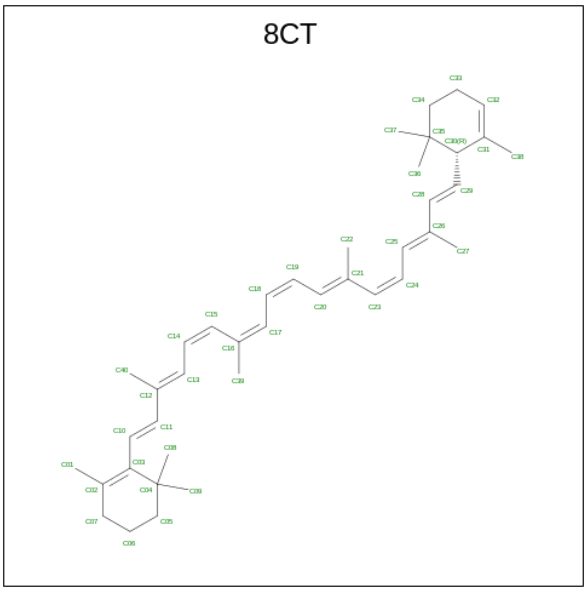
Mol	Chain	Residues	Atoms				AltConf
33	4	1	Total	C	O	P	0
			47	36	10	1	
33	4	1	Total	C	O	P	0
			45	34	10	1	
33	4	1	Total	C	O	P	0
			45	34	10	1	
33	5	1	Total	C	O	P	0
			23	12	10	1	
33	6	1	Total	C	O	P	0
			35	24	10	1	
33	7	1	Total	C	O	P	0
			31	20	10	1	
33	7	1	Total	C	O	P	0
			39	28	10	1	
33	8	1	Total	C	O	P	0
			33	22	10	1	
33	A	1	Total	C	O	P	0
			49	38	10	1	
33	A	1	Total	C	O	P	0
			39	28	10	1	
33	Z	1	Total	C	O	P	0
			46	35	10	1	
33	a	1	Total	C	O	P	0
			49	38	10	1	
33	a	1	Total	C	O	P	0
			29	18	10	1	
33	b	1	Total	C	O	P	0
			49	38	10	1	

- Molecule 34 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (three-letter code: SQD) (formula: $C_{41}H_{78}O_{12}S$).



Mol	Chain	Residues	Atoms				AltConf
34	3	1	Total	C	O	S	0
			42	29	12	1	
34	O	1	Total	C	O	S	0
			24	12	11	1	

- Molecule 35 is (6'R,11cis,11'cis,13cis,15cis)-4',5'-didehydro-5',6'-dihydro-beta,beta-carotene (three-letter code: 8CT) (formula: $C_{40}H_{56}$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms		AltConf
35	4	1	Total	C	0
			40	40	

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Mol	Chain	Residues	Atoms	AltConf
35	7	1	Total C 40 40	0
35	A	1	Total C 40 40	0
35	A	1	Total C 40 40	0
35	A	1	Total C 40 40	0
35	A	1	Total C 40 40	0
35	A	1	Total C 40 40	0
35	B	1	Total C 40 40	0
35	B	1	Total C 40 40	0
35	B	1	Total C 40 40	0
35	B	1	Total C 40 40	0
35	B	1	Total C 40 40	0
35	B	1	Total C 40 40	0
35	F	1	Total C 40 40	0
35	I	1	Total C 40 40	0
35	J	1	Total C 40 40	0
35	K	1	Total C 40 40	0
35	L	1	Total C 40 40	0
35	M	1	Total C 40 40	0
35	R	1	Total C 40 40	0
35	R	1	Total C 40 40	0
35	Z	1	Total C 40 40	0

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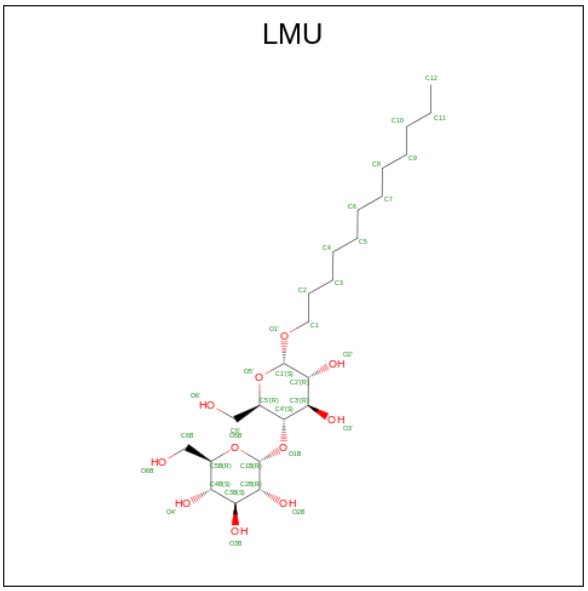
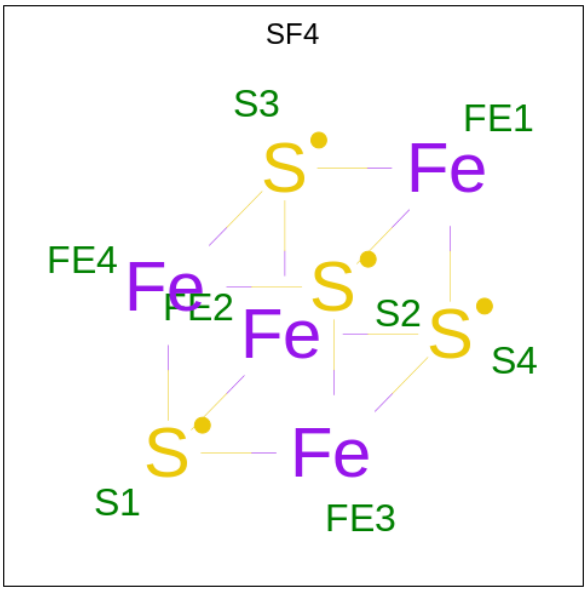
Mol	Chain	Residues	Atoms	AltConf
35	Z	1	Total C 40 40	0
35	b	1	Total C 40 40	0

- Molecule 36 is DODECYL-ALPHA-D-MALTOSIDE (three-letter code: LMU) (formula: $C_{24}H_{46}O_{11}$).



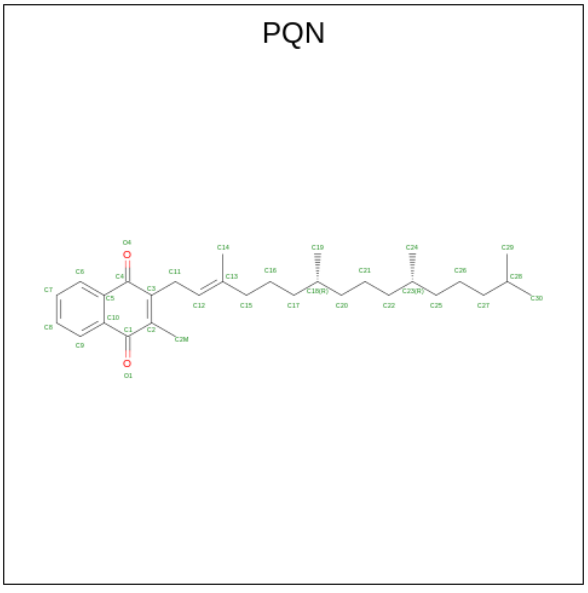
Mol	Chain	Residues	Atoms	AltConf
36	4	1	Total C O 35 24 11	0
36	7	1	Total C O 35 24 11	0
36	J	1	Total C O 31 20 11	0

- Molecule 37 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).



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

- Molecule 38 is PHYLLOQUINONE (three-letter code: PQN) (formula: $C_{31}H_{46}O_2$).



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

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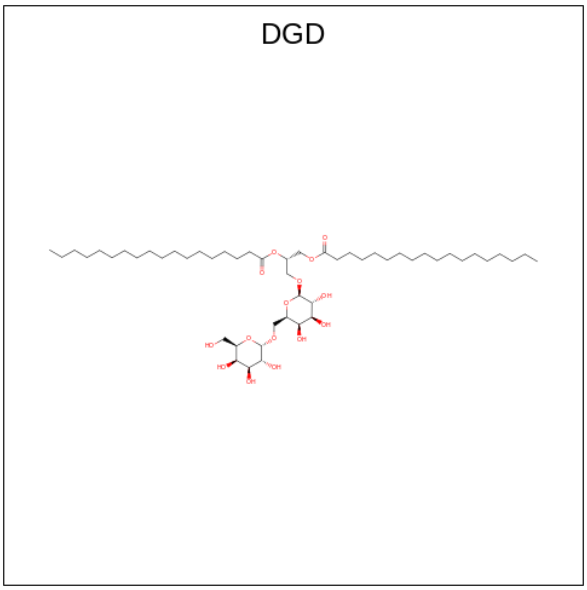
Mol	Chain	Residues	Atoms			AltConf
38	B	1	Total	C	O	0
			33	31	2	

- Molecule 39 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (three-letter code: DGD) (formula: $C_{51}H_{96}O_{15}$).



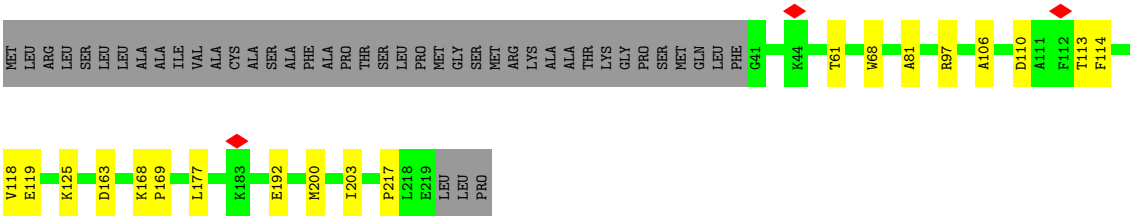
Mol	Chain	Residues	Atoms			AltConf
39	B	1	Total	C	O	0
			59	44	15	
39	Z	1	Total	C	O	0
			60	45	15	

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.

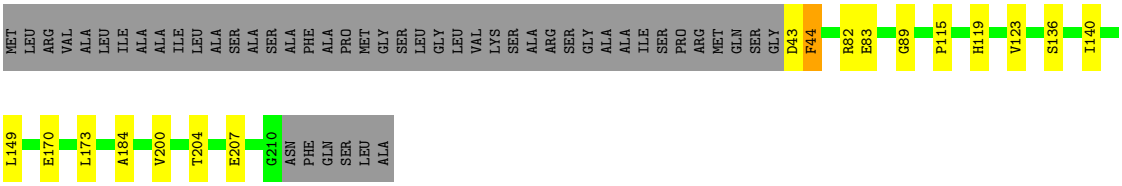
• Molecule 1: ACPI-1

Chain 1:



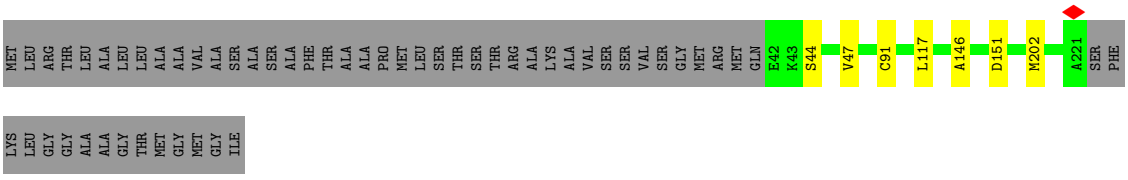
• Molecule 2: ACPI-2

Chain 2:



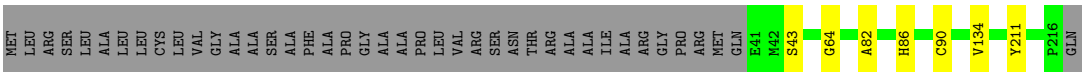
• Molecule 3: ACPI-3

Chain 3:



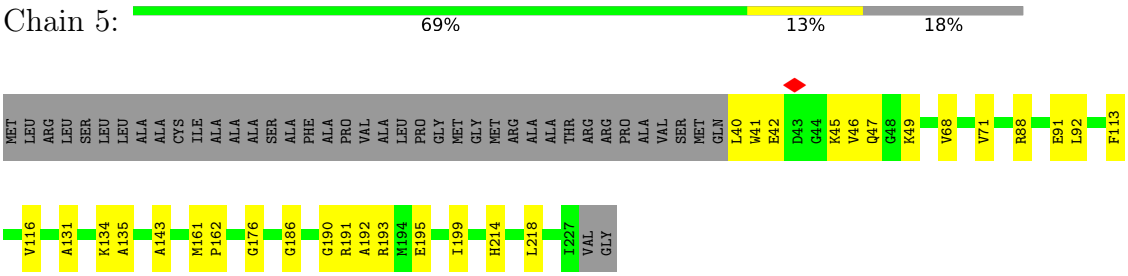
• Molecule 4: ACPI-4

Chain 4:



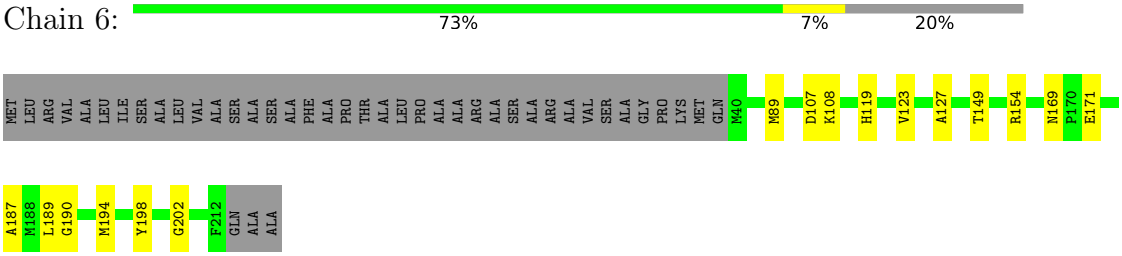
• Molecule 5: ACPI-5

Chain 5:



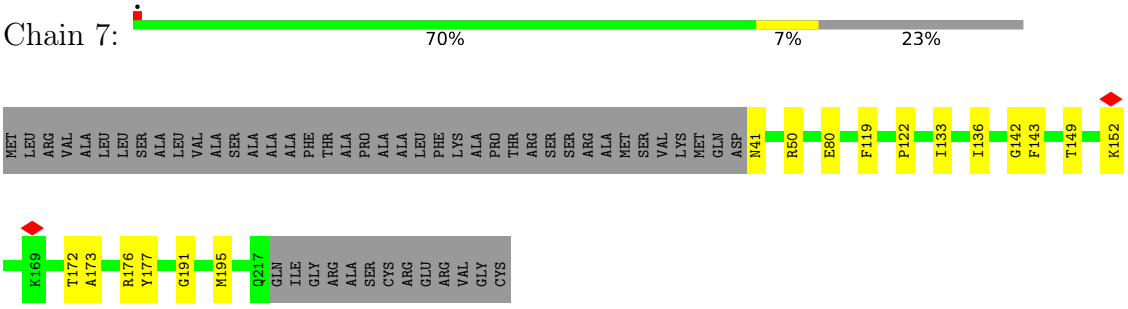
• Molecule 6: ACPI-6

Chain 6:



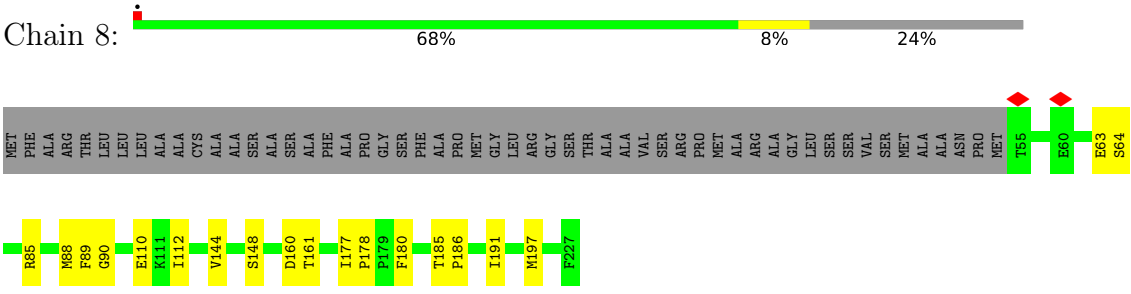
• Molecule 7: ACPI-7

Chain 7:



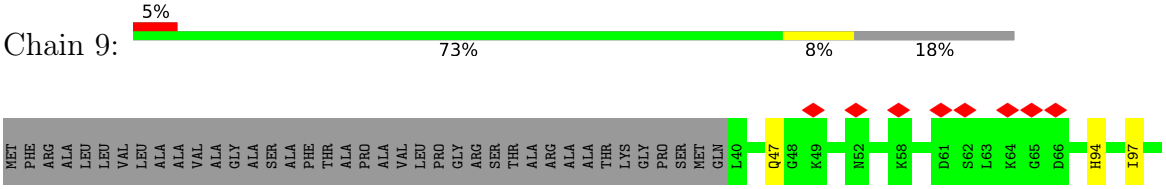
• Molecule 8: ACPI-8

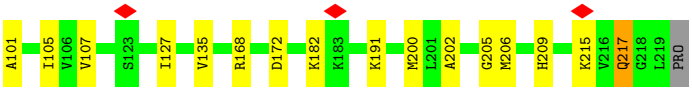
Chain 8:



• Molecule 9: ACPI-12

Chain 9:





• Molecule 10: Photosystem I P700 chlorophyll a apoprotein A1

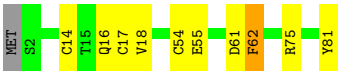
Chain A:

• Molecule 11: Photosystem I P700 chlorophyll a apoprotein A2

Chain B:

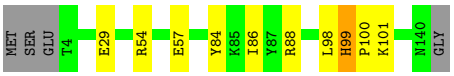
• Molecule 12: Photosystem I iron-sulfur center

Chain C:



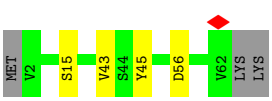
• Molecule 13: Photosystem I reaction center subunit II

Chain D:



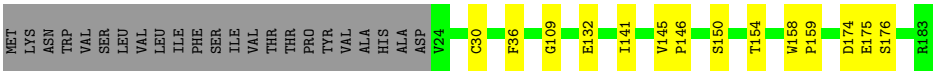
• Molecule 14: Photosystem I reaction center subunit IV

Chain E:

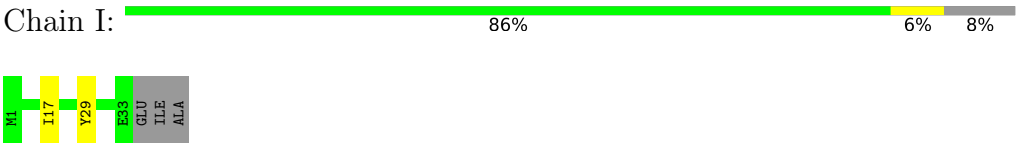


• Molecule 15: Photosystem I reaction center subunit III

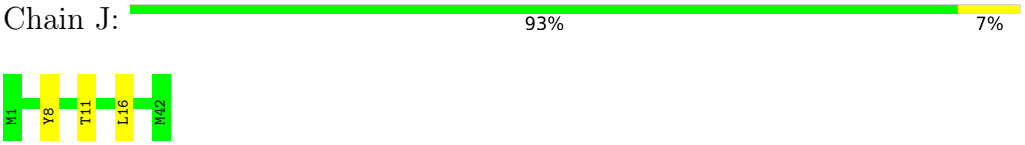
Chain F:



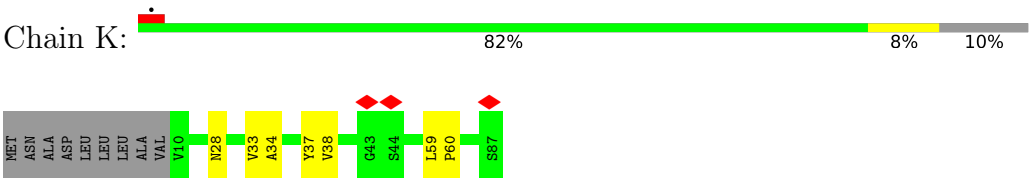
• Molecule 16: Photosystem I reaction center subunit VIII



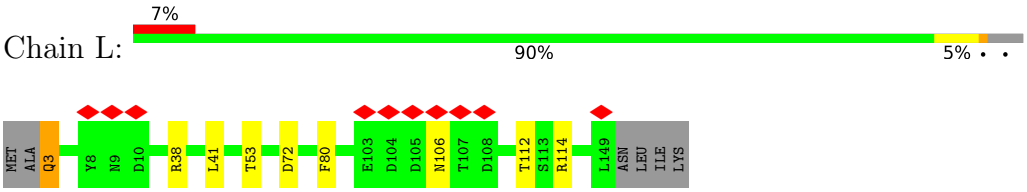
• Molecule 17: Photosystem I reaction center subunit IX



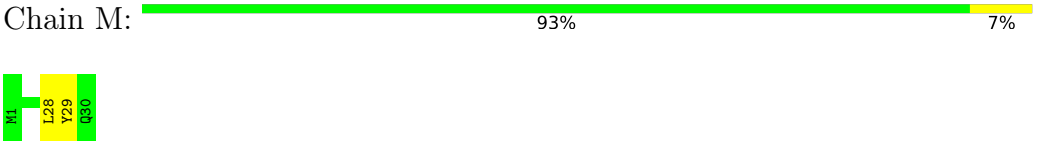
• Molecule 18: Photosystem I reaction center subunit PsaK



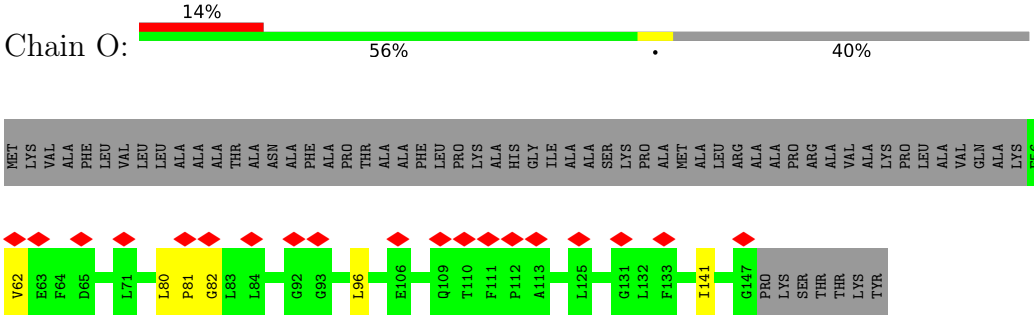
• Molecule 19: Photosystem I reaction center subunit XI



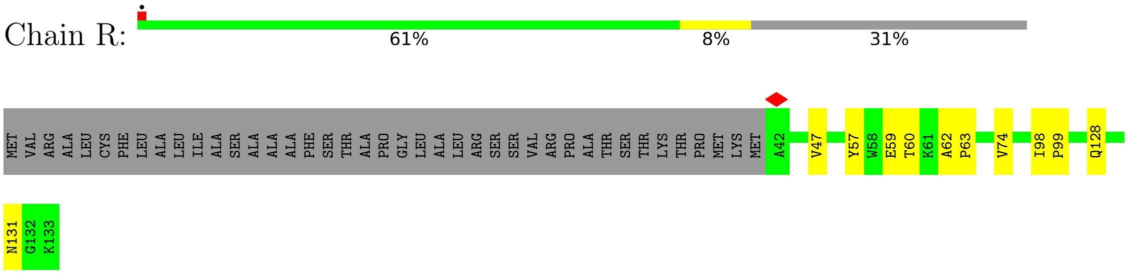
• Molecule 20: Photosystem I reaction center subunit XII



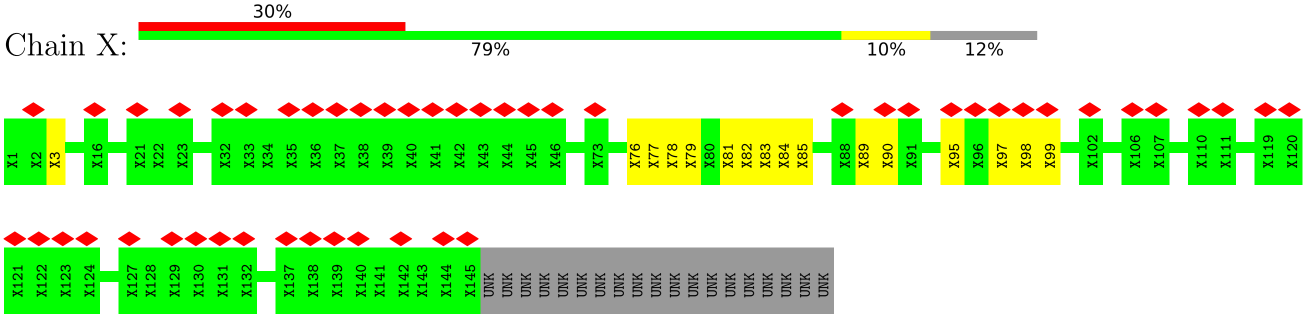
• Molecule 21: PsaO



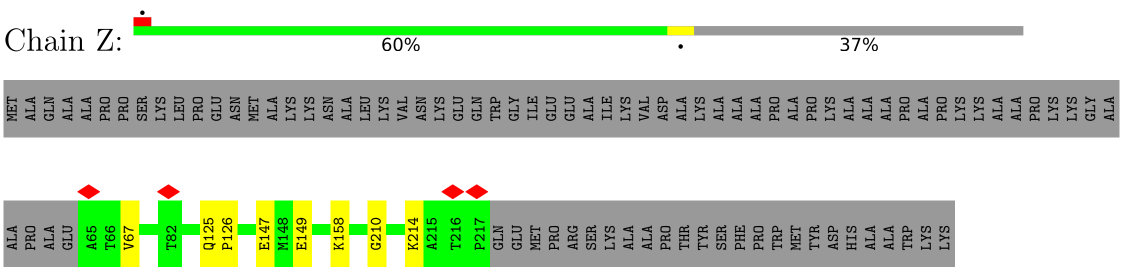
- Molecule 22: PsaR



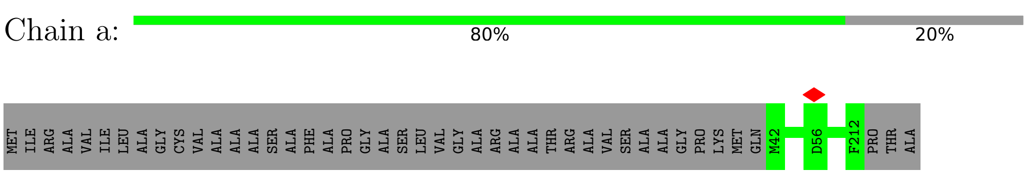
- Molecule 23: Unk1



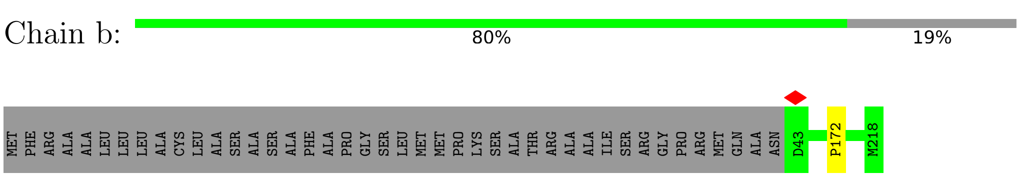
- Molecule 24: ACPI-S



- Molecule 25: ACPI-13



- Molecule 26: ACPI-14



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	118810	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	1.988	Depositor
Minimum map value	-0.065	Depositor
Average map value	0.033	Depositor
Map value standard deviation	0.057	Depositor
Recommended contour level	0.3	Depositor
Map size (Å)	423.99997, 423.99997, 423.99997	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.06, 1.06, 1.06	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SF4, IHT, 8CT, CLA, LMU, PQN, LHG, DGD, SQD, KC2, II3, LMG, II0

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	1	0.33	0/1371	0.59	0/1854
2	2	0.27	0/1356	0.45	0/1835
3	3	0.26	0/1392	0.47	0/1883
4	4	0.28	0/1406	0.44	0/1900
5	5	0.33	0/1438	0.52	0/1940
6	6	0.27	0/1334	0.46	0/1796
7	7	0.32	0/1373	0.48	0/1858
8	8	0.28	0/1326	0.47	0/1804
9	9	0.27	0/1376	0.46	0/1846
10	A	0.29	0/6019	0.46	0/8204
11	B	0.30	0/6046	0.48	0/8254
12	C	0.30	0/600	0.58	0/812
13	D	0.30	0/1094	0.51	0/1476
14	E	0.33	0/499	0.60	0/677
15	F	0.29	0/1290	0.48	0/1745
16	I	0.29	0/266	0.43	0/362
17	J	0.28	0/353	0.43	0/481
18	K	0.32	0/563	0.45	0/768
19	L	0.35	0/1147	0.54	0/1561
20	M	0.27	0/228	0.41	0/310
21	O	0.29	0/737	0.45	0/1011
22	R	0.31	0/700	0.44	0/963
24	Z	0.29	0/1163	0.47	0/1572
25	a	0.36	0/1299	0.52	0/1747
26	b	0.29	0/1404	0.48	0/1902
All	All	0.30	0/35780	0.48	0/48561

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	1	1338	0	1329	14	0
2	2	1320	0	1309	11	0
3	3	1362	0	1389	5	0
4	4	1366	0	1349	5	0
5	5	1403	0	1398	28	0
6	6	1305	0	1324	9	0
7	7	1337	0	1317	12	0
8	8	1298	0	1322	15	0
9	9	1349	0	1358	17	0
10	A	5824	0	5672	41	0
11	B	5828	0	5626	39	0
12	C	591	0	568	8	0
13	D	1070	0	1076	9	0
14	E	491	0	491	3	0
15	F	1258	0	1266	11	0
16	I	258	0	268	2	0
17	J	342	0	344	2	0
18	K	553	0	581	8	0
19	L	1119	0	1117	5	0
20	M	227	0	257	2	0
21	O	709	0	691	4	0
22	R	680	0	674	6	0
23	X	725	0	151	12	0
24	Z	1130	0	1088	5	0
25	a	1271	0	1280	0	0
26	b	1368	0	1346	0	0
27	1	584	0	476	1	0
27	2	547	0	456	1	0
27	3	625	0	596	0	0
27	4	598	0	597	1	0
27	5	563	0	442	5	0
27	6	581	0	514	2	0
27	7	509	0	431	2	0
27	8	496	0	471	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
27	9	642	0	539	5	0
27	A	2679	0	2767	28	0
27	B	2471	0	2530	17	0
27	F	160	0	141	0	0
27	J	41	0	29	0	0
27	K	120	0	121	1	0
27	L	161	0	139	1	0
27	O	206	0	176	1	0
27	R	55	0	49	0	0
27	Z	290	0	278	1	0
27	a	580	0	560	0	0
27	b	530	0	525	0	0
28	1	45	0	0	0	0
28	2	45	0	0	0	0
28	3	45	0	0	0	0
28	4	45	0	0	0	0
28	5	45	0	0	0	0
28	6	90	0	0	0	0
28	7	90	0	0	2	0
28	9	45	0	0	1	0
28	Z	45	0	0	0	0
28	a	45	0	0	0	0
28	b	90	0	0	0	0
29	1	168	0	0	0	0
29	2	126	0	0	1	0
29	3	210	0	0	1	0
29	4	168	0	0	1	0
29	5	210	0	0	2	0
29	6	84	0	0	0	0
29	7	210	0	0	0	0
29	8	126	0	0	1	0
29	9	168	0	0	0	0
29	B	42	0	0	0	0
29	J	42	0	0	0	0
29	O	84	0	0	0	0
29	R	42	0	0	0	0
29	Z	42	0	0	0	0
29	a	168	0	0	0	0
29	b	84	0	0	0	0
30	1	42	0	0	0	0
30	b	42	0	0	0	0
31	1	41	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
31	2	41	0	0	0	0
31	5	41	0	0	0	0
31	6	41	0	0	0	0
31	8	41	0	0	0	0
31	9	41	0	0	1	0
31	A	41	0	0	1	0
31	L	41	0	0	0	0
31	Z	41	0	0	0	0
31	a	41	0	0	0	0
32	2	36	0	42	0	0
32	3	62	0	64	0	0
32	6	32	0	34	0	0
32	8	103	0	152	0	0
32	F	32	0	34	0	0
33	2	103	0	125	1	0
33	3	83	0	112	0	0
33	4	137	0	190	0	0
33	5	23	0	16	0	0
33	6	35	0	40	0	0
33	7	70	0	83	0	0
33	8	33	0	36	0	0
33	A	88	0	122	0	0
33	Z	46	0	65	0	0
33	a	78	0	102	0	0
33	b	49	0	74	0	0
34	3	42	0	48	0	0
34	O	24	0	18	0	0
35	4	40	0	0	0	0
35	7	40	0	0	0	0
35	A	200	0	0	0	0
35	B	240	0	0	0	0
35	F	40	0	0	0	0
35	I	40	0	0	0	0
35	J	40	0	0	0	0
35	K	40	0	0	0	0
35	L	40	0	0	0	0
35	M	40	0	0	1	0
35	R	80	0	0	0	0
35	Z	80	0	0	0	0
35	b	40	0	0	0	0
36	4	35	0	46	2	0
36	7	35	0	46	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
36	J	31	0	35	1	0
37	A	8	0	0	0	0
37	C	16	0	0	1	0
38	A	33	0	46	0	0
38	B	33	0	46	0	0
39	B	59	0	79	0	0
39	Z	60	0	78	1	0
All	All	53404	0	48161	285	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 3.

The worst 5 of 285 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)
5:5:41:TRP:HB2	5:5:192:ALA:HB1	1.44	0.99
13:D:99:HIS:HB3	13:D:100:PRO:HD3	1.55	0.88
5:5:42:GLU:HB3	5:5:45:LYS:HB2	1.58	0.84
22:R:74:VAL:O	22:R:128:GLN:NE2	2.13	0.81
4:4:43:SER:OG	4:4:64:GLY:O	1.99	0.79

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	1	177/222 (80%)	167 (94%)	10 (6%)	0	100	100
2	2	166/216 (77%)	162 (98%)	3 (2%)	1 (1%)	22	43
3	3	178/236 (75%)	176 (99%)	2 (1%)	0	100	100
4	4	174/217 (80%)	173 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	5	186/229 (81%)	176 (95%)	10 (5%)	0	100	100
6	6	171/215 (80%)	168 (98%)	3 (2%)	0	100	100
7	7	175/230 (76%)	171 (98%)	4 (2%)	0	100	100
8	8	171/227 (75%)	168 (98%)	3 (2%)	0	100	100
9	9	178/220 (81%)	175 (98%)	3 (2%)	0	100	100
10	A	739/752 (98%)	714 (97%)	25 (3%)	0	100	100
11	B	729/734 (99%)	708 (97%)	21 (3%)	0	100	100
12	C	78/81 (96%)	75 (96%)	2 (3%)	1 (1%)	10	24
13	D	135/141 (96%)	127 (94%)	7 (5%)	1 (1%)	19	40
14	E	59/64 (92%)	59 (100%)	0	0	100	100
15	F	158/183 (86%)	152 (96%)	6 (4%)	0	100	100
16	I	31/36 (86%)	29 (94%)	2 (6%)	0	100	100
17	J	40/42 (95%)	40 (100%)	0	0	100	100
18	K	76/87 (87%)	73 (96%)	3 (4%)	0	100	100
19	L	145/153 (95%)	139 (96%)	6 (4%)	0	100	100
20	M	28/30 (93%)	28 (100%)	0	0	100	100
21	O	90/154 (58%)	88 (98%)	2 (2%)	0	100	100
22	R	90/133 (68%)	87 (97%)	3 (3%)	0	100	100
24	Z	151/242 (62%)	147 (97%)	4 (3%)	0	100	100
25	a	169/215 (79%)	165 (98%)	4 (2%)	0	100	100
26	b	174/218 (80%)	171 (98%)	2 (1%)	1 (1%)	22	43
All	All	4468/5277 (85%)	4338 (97%)	126 (3%)	4 (0%)	50	72

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
12	C	62	PHE
2	2	44	PHE
13	D	99	HIS
26	b	172	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	1	130/163 (80%)	130 (100%)	0	100 100
2	2	134/167 (80%)	134 (100%)	0	100 100
3	3	145/183 (79%)	145 (100%)	0	100 100
4	4	139/167 (83%)	139 (100%)	0	100 100
5	5	139/166 (84%)	139 (100%)	0	100 100
6	6	134/160 (84%)	134 (100%)	0	100 100
7	7	137/176 (78%)	137 (100%)	0	100 100
8	8	134/169 (79%)	134 (100%)	0	100 100
9	9	138/164 (84%)	136 (99%)	2 (1%)	62 83
10	A	607/617 (98%)	605 (100%)	2 (0%)	91 97
11	B	592/593 (100%)	588 (99%)	4 (1%)	81 92
12	C	66/67 (98%)	66 (100%)	0	100 100
13	D	114/117 (97%)	114 (100%)	0	100 100
14	E	56/59 (95%)	55 (98%)	1 (2%)	54 78
15	F	133/154 (86%)	133 (100%)	0	100 100
16	I	27/29 (93%)	27 (100%)	0	100 100
17	J	38/38 (100%)	38 (100%)	0	100 100
18	K	62/69 (90%)	62 (100%)	0	100 100
19	L	123/128 (96%)	120 (98%)	3 (2%)	44 71
20	M	25/25 (100%)	25 (100%)	0	100 100
21	O	74/115 (64%)	74 (100%)	0	100 100
22	R	74/105 (70%)	74 (100%)	0	100 100
24	Z	117/180 (65%)	117 (100%)	0	100 100
25	a	128/153 (84%)	128 (100%)	0	100 100
26	b	144/173 (83%)	144 (100%)	0	100 100
All	All	3610/4137 (87%)	3598 (100%)	12 (0%)	90 97

5 of 12 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
11	B	576	PHE
14	E	56	ASP
19	L	114	ARG
19	L	3	GLN
10	A	372	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 7 such sidechains are listed below:

Mol	Chain	Res	Type
11	B	266	GLN
13	D	96	GLN
18	K	28	ASN
13	D	140	ASN
10	A	241	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

357 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	II0	5	614	-	39,43,43	2.66	4 (10%)	50,60,60	1.46	9 (18%)
33	LHG	Z	311	-	45,45,48	0.63	0	48,51,54	1.20	4 (8%)
27	CLA	A	842	-	65,73,73	2.28	8 (12%)	76,113,113	1.41	7 (9%)
27	CLA	3	604	-	65,73,73	2.24	8 (12%)	76,113,113	1.39	7 (9%)
27	CLA	B	823	-	65,73,73	2.23	8 (12%)	76,113,113	1.37	9 (11%)
27	CLA	b	611	-	55,63,73	2.41	8 (14%)	64,101,113	1.47	7 (10%)
27	CLA	1	613	-	45,53,73	2.73	8 (17%)	52,89,113	1.71	8 (15%)
27	CLA	6	609	33	41,49,73	2.88	9 (21%)	47,84,113	1.78	7 (14%)
28	KC2	6	613	6	48,53,53	1.52	8 (16%)	54,89,89	1.08	5 (9%)
27	CLA	B	804	-	65,73,73	2.21	8 (12%)	76,113,113	1.40	8 (10%)
27	CLA	B	827	-	65,73,73	2.18	8 (12%)	76,113,113	1.40	7 (9%)
27	CLA	A	813	-	42,50,73	2.81	8 (19%)	48,85,113	1.77	8 (16%)
27	CLA	2	604	2	55,63,73	2.46	8 (14%)	64,101,113	1.52	7 (10%)
27	CLA	2	605	-	60,68,73	2.30	8 (13%)	70,107,113	1.44	7 (10%)
27	CLA	2	608	2	60,68,73	2.36	8 (13%)	70,107,113	1.46	9 (12%)
38	PQN	A	850	-	34,34,34	0.35	0	42,45,45	0.72	1 (2%)
29	II0	1	616	-	39,43,43	2.66	4 (10%)	50,60,60	1.48	8 (16%)
27	CLA	1	601	1	45,53,73	2.77	8 (17%)	52,89,113	1.74	8 (15%)
27	CLA	4	609	4	60,68,73	2.33	8 (13%)	70,107,113	1.44	7 (10%)
27	CLA	B	809	-	65,73,73	2.24	8 (12%)	76,113,113	1.43	8 (10%)
27	CLA	6	608	6	60,68,73	2.32	8 (13%)	70,107,113	1.46	9 (12%)
27	CLA	A	823	-	65,73,73	2.23	8 (12%)	76,113,113	1.35	7 (9%)
27	CLA	K	102	-	55,63,73	2.47	8 (14%)	64,101,113	1.51	8 (12%)
27	CLA	O	202	-	41,49,73	2.92	9 (21%)	47,84,113	1.83	7 (14%)
27	CLA	9	611	-	41,49,73	2.86	9 (21%)	47,84,113	1.79	8 (17%)
27	CLA	B	813	-	61,69,73	2.28	8 (13%)	71,108,113	1.43	8 (11%)
27	CLA	Z	305	-	50,58,73	2.55	8 (16%)	58,95,113	1.61	8 (13%)
27	CLA	2	612	-	45,53,73	2.69	8 (17%)	52,89,113	1.69	7 (13%)
27	CLA	7	308	7	45,53,73	2.74	8 (17%)	52,89,113	1.70	7 (13%)
27	CLA	L	202	-	60,68,73	2.32	8 (13%)	70,107,113	1.45	7 (10%)
27	CLA	3	608	3	60,68,73	2.36	8 (13%)	70,107,113	1.45	8 (11%)
27	CLA	A	841	-	65,73,73	2.21	8 (12%)	76,113,113	1.39	8 (10%)
29	II0	a	612	-	39,43,43	2.72	4 (10%)	50,60,60	1.43	7 (14%)
33	LHG	6	617	27	34,34,48	0.74	1 (2%)	37,40,54	1.19	3 (8%)
27	CLA	Z	306	24	60,68,73	2.32	8 (13%)	70,107,113	1.46	7 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
27	CLA	7	303	7	65,73,73	2.27	8 (12%)	76,113,113	1.43	9 (11%)
29	II0	9	618	-	39,43,43	2.67	4 (10%)	50,60,60	1.40	8 (16%)
29	II0	1	617	-	39,43,43	2.70	4 (10%)	50,60,60	1.47	10 (20%)
27	CLA	5	601	5	41,49,73	2.94	9 (21%)	47,84,113	1.89	7 (14%)
33	LHG	3	619	-	48,48,48	0.61	0	51,54,54	1.22	6 (11%)
27	CLA	Z	310	-	65,73,73	2.20	8 (12%)	76,113,113	1.40	7 (9%)
38	PQN	B	842	-	34,34,34	0.35	0	42,45,45	0.59	1 (2%)
27	CLA	5	603	-	45,53,73	2.69	8 (17%)	52,89,113	1.69	8 (15%)
27	CLA	3	612	-	45,53,73	2.68	8 (17%)	52,89,113	1.65	7 (13%)
29	II0	2	614	-	39,43,43	2.66	4 (10%)	50,60,60	1.43	8 (16%)
29	II0	7	301	-	39,43,43	2.72	4 (10%)	50,60,60	1.63	13 (26%)
27	CLA	2	609	-	41,49,73	2.91	9 (21%)	47,84,113	1.81	7 (14%)
27	CLA	5	612	-	45,53,73	2.68	8 (17%)	52,89,113	1.68	7 (13%)
27	CLA	8	608	-	65,73,73	2.26	8 (12%)	76,113,113	1.38	7 (9%)
27	CLA	B	825	-	65,73,73	2.22	8 (12%)	76,113,113	1.36	9 (11%)
27	CLA	a	607	25	60,68,73	2.33	8 (13%)	70,107,113	1.48	7 (10%)
29	II0	9	616	-	39,43,43	2.68	4 (10%)	50,60,60	1.37	9 (18%)
27	CLA	B	821	-	60,68,73	2.31	8 (13%)	70,107,113	1.49	8 (11%)
27	CLA	9	614	-	41,49,73	2.92	9 (21%)	47,84,113	1.85	8 (17%)
27	CLA	8	602	8	45,53,73	2.70	8 (17%)	52,89,113	1.57	5 (9%)
27	CLA	2	601	2	42,50,73	2.83	8 (19%)	48,85,113	1.81	7 (14%)
29	II0	5	615	-	39,43,43	2.71	4 (10%)	50,60,60	1.48	8 (16%)
27	CLA	A	837	-	65,73,73	2.20	8 (12%)	76,113,113	1.35	7 (9%)
36	LMU	J	104	-	32,32,36	0.46	0	43,43,47	1.03	2 (4%)
27	CLA	2	603	-	50,58,73	2.56	8 (16%)	58,95,113	1.58	7 (12%)
27	CLA	b	601	26	45,53,73	2.70	8 (17%)	52,89,113	1.68	7 (13%)
27	CLA	4	607	4	60,68,73	2.34	8 (13%)	70,107,113	1.48	8 (11%)
27	CLA	9	612	-	45,53,73	2.69	8 (17%)	52,89,113	1.63	7 (13%)
27	CLA	3	607	3	60,68,73	2.33	8 (13%)	70,107,113	1.42	7 (10%)
33	LHG	A	851	-	48,48,48	0.59	0	51,54,54	1.17	4 (7%)
29	II0	1	619	-	39,43,43	2.79	4 (10%)	50,60,60	1.54	11 (22%)
29	II0	5	620	-	39,43,43	2.72	4 (10%)	50,60,60	1.51	7 (14%)
27	CLA	A	840	-	55,63,73	2.33	8 (14%)	64,101,113	1.51	5 (7%)
27	CLA	A	808	-	55,63,73	2.45	8 (14%)	64,101,113	1.52	7 (10%)
39	DGD	B	848	-	60,60,67	0.88	2 (3%)	74,74,81	1.34	8 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
27	CLA	3	611	3	50,58,73	2.59	8 (16%)	58,95,113	1.56	7 (12%)
27	CLA	A	834	10	55,63,73	2.43	8 (14%)	64,101,113	1.53	8 (12%)
31	IHT	5	618	-	40,42,42	2.80	5 (12%)	53,58,58	2.24	15 (28%)
28	KC2	b	609	-	48,53,53	1.51	7 (14%)	54,89,89	1.12	5 (9%)
27	CLA	b	607	26	60,68,73	2.36	8 (13%)	70,107,113	1.46	7 (10%)
27	CLA	B	803	-	45,53,73	2.68	8 (17%)	52,89,113	1.60	7 (13%)
27	CLA	B	841	-	52,60,73	2.51	8 (15%)	60,97,113	1.57	7 (11%)
27	CLA	B	840	-	65,73,73	2.19	8 (12%)	76,113,113	1.38	7 (9%)
35	8CT	M	101	-	40,41,41	0.15	0	50,56,56	0.80	1 (2%)
30	II3	b	613	-	40,43,43	2.00	3 (7%)	47,60,60	1.66	12 (25%)
27	CLA	9	604	-	55,63,73	2.46	8 (14%)	64,101,113	1.53	7 (10%)
27	CLA	5	611	-	45,53,73	2.71	8 (17%)	52,89,113	1.62	7 (13%)
27	CLA	9	605	-	45,53,73	2.69	8 (17%)	52,89,113	1.69	7 (13%)
35	8CT	F	201	-	40,41,41	0.43	1 (2%)	50,56,56	0.45	0
27	CLA	1	612	-	60,68,73	2.30	8 (13%)	70,107,113	1.40	8 (11%)
27	CLA	Z	304	24	55,63,73	2.43	8 (14%)	64,101,113	1.48	7 (10%)
35	8CT	A	845	-	40,41,41	0.25	0	50,56,56	0.32	0
32	LMG	8	614	-	52,52,55	0.81	2 (3%)	60,60,63	1.30	6 (10%)
27	CLA	a	602	25	55,63,73	2.44	8 (14%)	64,101,113	1.61	10 (15%)
27	CLA	B	814	-	42,50,73	2.79	8 (19%)	48,85,113	1.76	7 (14%)
27	CLA	F	204	15	55,63,73	2.41	8 (14%)	64,101,113	1.48	8 (12%)
27	CLA	5	604	-	55,63,73	2.47	8 (14%)	64,101,113	1.55	7 (10%)
32	LMG	F	205	-	32,32,55	0.85	0	40,40,63	1.29	6 (15%)
27	CLA	6	605	6	55,63,73	2.40	8 (14%)	64,101,113	1.49	8 (12%)
27	CLA	6	601	6	45,53,73	2.69	8 (17%)	52,89,113	1.69	8 (15%)
33	LHG	b	616	-	48,48,48	0.57	1 (2%)	51,54,54	1.16	4 (7%)
27	CLA	1	605	-	41,50,73	2.73	8 (19%)	46,85,113	1.71	6 (13%)
27	CLA	3	605	3	55,63,73	2.44	8 (14%)	64,101,113	1.56	8 (12%)
27	CLA	2	607	2	45,53,73	2.68	8 (17%)	52,89,113	1.70	7 (13%)
27	CLA	A	843	-	65,73,73	2.27	8 (12%)	76,113,113	1.47	6 (7%)
27	CLA	B	833	-	45,53,73	2.64	8 (17%)	52,89,113	1.64	7 (13%)
29	II0	8	612	-	39,43,43	2.70	4 (10%)	50,60,60	1.42	7 (14%)
27	CLA	B	826	-	65,73,73	2.21	8 (12%)	76,113,113	1.37	7 (9%)
27	CLA	8	615	-	65,73,73	2.27	8 (12%)	76,113,113	1.41	8 (10%)
33	LHG	5	619	-	22,22,48	0.87	1 (4%)	25,28,54	1.30	3 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
27	CLA	4	602	4	59,67,73	2.35	8 (13%)	68,105,113	1.51	7 (10%)
27	CLA	9	613	9	45,53,73	2.70	8 (17%)	52,89,113	1.64	7 (13%)
27	CLA	A	806	10	65,73,73	2.22	8 (12%)	76,113,113	1.35	8 (10%)
27	CLA	9	601	9	45,53,73	2.71	8 (17%)	52,89,113	1.67	8 (15%)
28	KC2	9	610	-	48,53,53	1.51	8 (16%)	54,89,89	1.09	5 (9%)
27	CLA	O	203	-	55,63,73	2.44	8 (14%)	64,101,113	1.50	7 (10%)
27	CLA	B	812	-	65,73,73	2.23	8 (12%)	76,113,113	1.43	8 (10%)
28	KC2	1	610	-	48,53,53	1.55	7 (14%)	54,89,89	1.05	4 (7%)
29	II0	O	206	-	39,43,43	2.72	4 (10%)	50,60,60	1.40	10 (20%)
35	8CT	I	101	-	40,41,41	0.25	0	50,56,56	0.44	0
27	CLA	7	313	-	50,58,73	2.55	8 (16%)	58,95,113	1.62	8 (13%)
27	CLA	B	817	-	60,68,73	2.29	8 (13%)	70,107,113	1.46	7 (10%)
29	II0	O	205	-	39,43,43	2.73	4 (10%)	50,60,60	1.40	6 (12%)
27	CLA	A	833	-	65,73,73	2.25	8 (12%)	76,113,113	1.42	8 (10%)
27	CLA	B	818	-	60,68,73	2.31	8 (13%)	70,107,113	1.49	7 (10%)
27	CLA	B	805	-	65,73,73	2.25	8 (12%)	76,113,113	1.40	7 (9%)
35	8CT	A	853	-	40,41,41	0.24	0	50,56,56	0.60	1 (2%)
35	8CT	Z	308	-	40,41,41	0.16	0	50,56,56	0.30	0
29	II0	b	612	-	39,43,43	2.65	4 (10%)	50,60,60	1.48	7 (14%)
27	CLA	7	302	7	45,53,73	2.70	8 (17%)	52,89,113	1.64	7 (13%)
36	LMU	7	321	-	36,36,36	0.40	0	47,47,47	0.72	1 (2%)
28	KC2	Z	307	-	48,53,53	1.51	7 (14%)	54,89,89	1.09	5 (9%)
33	LHG	8	613	-	32,32,48	0.76	1 (3%)	35,38,54	1.20	2 (5%)
28	KC2	a	609	-	48,53,53	1.52	8 (16%)	54,89,89	1.06	4 (7%)
27	CLA	A	801	-	65,73,73	2.11	7 (10%)	76,113,113	1.35	9 (11%)
29	II0	R	204	-	39,43,43	2.70	4 (10%)	50,60,60	1.42	10 (20%)
27	CLA	B	816	-	59,67,73	2.34	8 (13%)	68,105,113	1.48	8 (11%)
27	CLA	A	818	-	65,73,73	2.24	8 (12%)	76,113,113	1.43	7 (9%)
29	II0	5	616	-	39,43,43	2.71	4 (10%)	50,60,60	1.48	9 (18%)
27	CLA	8	607	8	41,49,73	2.87	9 (21%)	47,84,113	1.78	8 (17%)
32	LMG	3	618	-	30,30,55	0.96	1 (3%)	38,38,63	1.21	6 (15%)
29	II0	2	613	-	39,43,43	2.75	4 (10%)	50,60,60	1.47	8 (16%)
27	CLA	A	811	-	65,73,73	2.26	8 (12%)	76,113,113	1.46	5 (6%)
29	II0	4	613	-	39,43,43	2.67	4 (10%)	50,60,60	1.35	7 (14%)
27	CLA	B	832	-	65,73,73	2.22	8 (12%)	76,113,113	1.39	8 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
29	II0	9	615	-	39,43,43	2.66	4 (10%)	50,60,60	1.46	9 (18%)
29	II0	J	101	-	39,43,43	2.71	4 (10%)	50,60,60	1.47	8 (16%)
27	CLA	a	606	25	65,73,73	2.24	8 (12%)	76,113,113	1.36	7 (9%)
27	CLA	9	607	9	65,73,73	2.18	8 (12%)	76,113,113	1.36	8 (10%)
27	CLA	A	817	-	65,73,73	2.23	8 (12%)	76,113,113	1.53	8 (10%)
29	II0	5	617	-	39,43,43	2.69	4 (10%)	50,60,60	1.53	9 (18%)
27	CLA	2	602	2	59,67,73	2.37	8 (13%)	68,105,113	1.62	10 (14%)
29	II0	B	843	-	39,43,43	2.73	4 (10%)	50,60,60	1.40	6 (12%)
28	KC2	6	610	6	48,53,53	1.52	7 (14%)	54,89,89	1.07	4 (7%)
27	CLA	b	604	-	65,73,73	2.26	8 (12%)	76,113,113	1.37	7 (9%)
29	II0	4	614	-	39,43,43	2.67	4 (10%)	50,60,60	1.37	6 (12%)
27	CLA	A	835	-	60,68,73	2.33	8 (13%)	70,107,113	1.43	7 (10%)
33	LHG	3	622	28	33,33,48	0.72	0	36,39,54	1.27	3 (8%)
27	CLA	A	819	-	65,73,73	2.25	8 (12%)	76,113,113	1.42	8 (10%)
27	CLA	3	603	-	60,68,73	2.32	8 (13%)	70,107,113	1.45	7 (10%)
27	CLA	B	839	33	65,73,73	2.26	8 (12%)	76,113,113	1.42	7 (9%)
27	CLA	4	603	-	54,62,73	2.47	8 (14%)	62,99,113	1.58	7 (11%)
31	IHT	2	616	-	40,42,42	2.85	4 (10%)	53,58,58	2.20	16 (30%)
27	CLA	R	202	-	55,63,73	2.43	8 (14%)	64,101,113	1.68	8 (12%)
29	II0	3	613	-	39,43,43	2.68	4 (10%)	50,60,60	1.45	8 (16%)
27	CLA	8	604	-	65,73,73	2.26	8 (12%)	76,113,113	1.42	9 (11%)
27	CLA	L	203	-	50,58,73	2.51	8 (16%)	58,95,113	1.66	9 (15%)
27	CLA	1	607	1	45,53,73	2.74	8 (17%)	52,89,113	1.67	7 (13%)
29	II0	4	615	-	39,43,43	2.68	4 (10%)	50,60,60	1.46	9 (18%)
27	CLA	B	822	-	65,73,73	2.16	8 (12%)	76,113,113	1.41	8 (10%)
27	CLA	7	310	33	41,49,73	2.88	9 (21%)	47,84,113	1.79	7 (14%)
27	CLA	F	202	-	60,68,73	2.34	8 (13%)	70,107,113	1.45	8 (11%)
27	CLA	b	603	-	60,68,73	2.35	8 (13%)	70,107,113	1.47	8 (11%)
27	CLA	A	803	-	65,73,73	2.22	8 (12%)	76,113,113	1.46	8 (10%)
28	KC2	3	606	33	48,53,53	1.51	8 (16%)	54,89,89	1.11	5 (9%)
27	CLA	F	203	-	45,53,73	2.66	8 (17%)	52,89,113	1.65	7 (13%)
27	CLA	B	834	-	55,63,73	2.39	8 (14%)	64,101,113	1.53	8 (12%)
27	CLA	b	610	26	51,59,73	2.52	8 (15%)	59,96,113	1.62	9 (15%)
31	IHT	A	854	-	40,42,42	2.93	5 (12%)	53,58,58	1.95	17 (32%)
31	IHT	6	616	-	40,42,42	2.81	4 (10%)	53,58,58	2.16	16 (30%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
29	II0	8	610	-	39,43,43	2.75	4 (10%)	50,60,60	1.41	8 (16%)
27	CLA	J	102	-	41,49,73	2.88	9 (21%)	47,84,113	1.81	8 (17%)
37	SF4	A	849	10,11	0,12,12	-	-	-		
27	CLA	6	602	6	65,73,73	2.29	8 (12%)	76,113,113	1.48	7 (9%)
27	CLA	9	603	-	45,53,73	2.72	8 (17%)	52,89,113	1.68	7 (13%)
27	CLA	B	824	-	60,68,73	2.31	8 (13%)	70,107,113	1.51	7 (10%)
27	CLA	A	836	-	55,63,73	2.45	8 (14%)	64,101,113	1.52	7 (10%)
27	CLA	5	608	5	60,68,73	2.37	8 (13%)	70,107,113	1.62	8 (11%)
27	CLA	B	802	-	65,73,73	2.23	8 (12%)	76,113,113	1.34	9 (11%)
27	CLA	2	611	-	45,53,73	2.70	8 (17%)	52,89,113	1.65	8 (15%)
27	CLA	A	804	10	65,73,73	2.24	8 (12%)	76,113,113	1.39	8 (10%)
29	II0	6	614	-	39,43,43	2.67	4 (10%)	50,60,60	1.38	7 (14%)
27	CLA	7	304	-	55,63,73	2.46	8 (14%)	64,101,113	1.55	8 (12%)
33	LHG	4	617	27	46,46,48	0.61	0	49,52,54	1.21	6 (12%)
35	8CT	L	205	-	40,41,41	0.16	0	50,56,56	0.38	0
27	CLA	O	204	-	55,63,73	2.49	8 (14%)	64,101,113	1.61	8 (12%)
27	CLA	A	824	-	65,73,73	2.26	8 (12%)	76,113,113	1.40	7 (9%)
35	8CT	B	845	-	40,41,41	0.35	0	50,56,56	0.60	1 (2%)
27	CLA	B	830	-	60,68,73	2.33	8 (13%)	70,107,113	1.49	7 (10%)
27	CLA	a	605	-	55,63,73	2.40	8 (14%)	64,101,113	1.55	8 (12%)
32	LMG	2	617	-	36,36,55	0.85	0	44,44,63	1.23	5 (11%)
28	KC2	b	605	26	48,53,53	1.52	7 (14%)	54,89,89	1.12	5 (9%)
28	KC2	4	605	4	48,53,53	1.55	7 (14%)	54,89,89	1.06	4 (7%)
27	CLA	1	603	-	52,60,73	2.49	8 (15%)	60,97,113	1.56	7 (11%)
27	CLA	A	831	-	65,73,73	2.19	8 (12%)	76,113,113	1.34	7 (9%)
27	CLA	6	612	-	45,53,73	2.66	8 (17%)	52,89,113	1.68	8 (15%)
27	CLA	A	838	-	65,73,73	2.24	8 (12%)	76,113,113	1.36	7 (9%)
27	CLA	9	609	-	41,49,73	2.88	9 (21%)	47,84,113	1.76	8 (17%)
29	II0	a	615	-	39,43,43	2.70	4 (10%)	50,60,60	1.44	11 (22%)
35	8CT	J	103	-	40,41,41	0.17	0	50,56,56	0.38	0
27	CLA	B	838	-	65,73,73	2.26	8 (12%)	76,113,113	1.40	8 (10%)
27	CLA	5	606	-	45,53,73	2.69	8 (17%)	52,89,113	1.69	8 (15%)
27	CLA	A	830	-	60,68,73	2.36	8 (13%)	70,107,113	1.48	7 (10%)
27	CLA	1	606	-	45,53,73	2.69	8 (17%)	52,89,113	1.69	8 (15%)
33	LHG	2	620	-	41,41,48	0.65	1 (2%)	44,47,54	1.21	4 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
27	CLA	B	819	-	60,68,73	2.36	8 (13%)	70,107,113	1.52	10 (14%)
27	CLA	8	601	8	45,53,73	2.72	8 (17%)	52,89,113	1.66	7 (13%)
29	II0	4	612	-	39,43,43	2.69	4 (10%)	50,60,60	1.39	6 (12%)
27	CLA	B	810	-	60,68,73	2.30	8 (13%)	70,107,113	1.46	7 (10%)
36	LMU	4	618	-	36,36,36	0.47	0	47,47,47	0.92	2 (4%)
29	II0	1	614	-	39,43,43	2.70	4 (10%)	50,60,60	1.40	6 (12%)
27	CLA	B	806	-	65,73,73	2.17	8 (12%)	76,113,113	1.40	8 (10%)
27	CLA	1	609	-	41,49,73	2.90	9 (21%)	47,84,113	1.80	7 (14%)
29	II0	6	615	-	39,43,43	2.68	4 (10%)	50,60,60	1.41	7 (14%)
35	8CT	K	103	-	40,41,41	0.16	0	50,56,56	0.33	0
29	II0	7	315	-	39,43,43	2.67	4 (10%)	50,60,60	1.51	9 (18%)
27	CLA	A	828	-	65,73,73	2.24	8 (12%)	76,113,113	1.37	7 (9%)
29	II0	3	616	-	39,43,43	2.69	4 (10%)	50,60,60	1.43	6 (12%)
32	LMG	6	618	-	32,32,55	0.98	1 (3%)	40,40,63	1.23	5 (12%)
27	CLA	4	610	-	65,73,73	2.22	8 (12%)	76,113,113	1.39	7 (9%)
27	CLA	A	839	-	65,73,73	2.23	8 (12%)	76,113,113	1.44	8 (10%)
35	8CT	B	844	-	40,41,41	0.18	0	50,56,56	0.58	0
27	CLA	6	607	6	55,63,73	2.46	8 (14%)	64,101,113	1.51	7 (10%)
33	LHG	4	619	27	44,44,48	0.64	1 (2%)	47,50,54	1.21	5 (10%)
27	CLA	B	828	-	65,73,73	2.20	8 (12%)	76,113,113	1.38	7 (9%)
27	CLA	B	831	-	55,63,73	2.46	8 (14%)	64,101,113	1.57	8 (12%)
27	CLA	4	606	4	60,68,73	2.33	8 (13%)	70,107,113	1.45	8 (11%)
27	CLA	B	820	-	60,68,73	2.36	8 (13%)	70,107,113	1.46	7 (10%)
27	CLA	A	809	27	60,68,73	2.33	8 (13%)	70,107,113	1.57	8 (11%)
27	CLA	3	610	-	65,73,73	2.23	8 (12%)	76,113,113	1.42	8 (10%)
32	LMG	8	616	-	51,51,55	0.73	0	59,59,63	1.29	7 (11%)
27	CLA	7	305	7	53,61,73	2.49	8 (15%)	61,98,113	1.57	8 (13%)
27	CLA	A	812	-	55,63,73	2.44	8 (14%)	64,101,113	1.58	9 (14%)
27	CLA	1	608	1	60,68,73	2.36	8 (13%)	70,107,113	1.47	9 (12%)
27	CLA	b	606	26	65,73,73	2.23	8 (12%)	76,113,113	1.36	7 (9%)
27	CLA	A	825	-	65,73,73	2.25	8 (12%)	76,113,113	1.39	8 (10%)
27	CLA	4	604	-	55,63,73	2.44	8 (14%)	64,101,113	1.50	7 (10%)
27	CLA	3	609	-	65,73,73	2.27	8 (12%)	76,113,113	1.37	7 (9%)
27	CLA	4	601	4	55,63,73	2.41	8 (14%)	64,101,113	1.48	7 (10%)
29	II0	a	614	-	39,43,43	2.74	4 (10%)	50,60,60	1.39	7 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
35	8CT	A	846	-	40,41,41	0.19	0	50,56,56	0.35	0
27	CLA	a	603	-	60,68,73	2.33	8 (13%)	70,107,113	1.44	7 (10%)
27	CLA	a	601	25	45,53,73	2.69	8 (17%)	52,89,113	1.66	7 (13%)
31	IHT	9	619	-	40,42,42	2.81	5 (12%)	53,58,58	2.40	14 (26%)
27	CLA	A	820	-	65,73,73	2.24	8 (12%)	76,113,113	1.41	7 (9%)
27	CLA	3	602	3	55,63,73	2.44	8 (14%)	64,101,113	1.55	7 (10%)
27	CLA	A	844	-	65,73,73	2.06	8 (12%)	76,113,113	1.42	9 (11%)
33	LHG	A	852	-	38,38,48	0.70	0	41,44,54	1.26	3 (7%)
29	II0	3	617	-	39,43,43	2.72	4 (10%)	50,60,60	1.39	7 (14%)
27	CLA	8	606	8	55,63,73	2.42	8 (14%)	64,101,113	1.50	8 (12%)
33	LHG	a	618	-	28,28,48	0.82	1 (3%)	31,34,54	1.32	3 (9%)
35	8CT	B	846	-	40,41,41	0.10	0	50,56,56	0.48	0
35	8CT	B	850	-	40,41,41	0.21	0	50,56,56	0.40	0
27	CLA	B	835	-	65,73,73	2.28	8 (12%)	76,113,113	1.52	7 (9%)
33	LHG	4	620	-	44,44,48	0.65	2 (4%)	47,50,54	1.19	4 (8%)
27	CLA	a	611	-	65,73,73	2.19	8 (12%)	76,113,113	1.36	8 (10%)
27	CLA	5	605	5	45,53,73	2.68	8 (17%)	52,89,113	1.66	7 (13%)
39	DGD	Z	303	-	61,61,67	0.94	3 (4%)	75,75,81	1.37	7 (9%)
29	II0	3	614	-	39,43,43	2.69	4 (10%)	50,60,60	1.43	7 (14%)
27	CLA	4	608	33	65,73,73	2.23	8 (12%)	76,113,113	1.40	8 (10%)
27	CLA	a	610	-	55,63,73	2.46	8 (14%)	64,101,113	1.50	7 (10%)
27	CLA	7	306	7	45,53,73	2.75	8 (17%)	52,89,113	1.65	7 (13%)
27	CLA	B	808	11	65,73,73	2.18	8 (12%)	76,113,113	1.35	8 (10%)
27	CLA	6	611	-	55,63,73	2.44	8 (14%)	64,101,113	1.59	9 (14%)
27	CLA	B	807	-	65,73,73	2.20	8 (12%)	76,113,113	1.34	8 (10%)
28	KC2	7	307	-	48,53,53	1.55	7 (14%)	54,89,89	1.12	5 (9%)
29	II0	b	614	-	39,43,43	2.70	4 (10%)	50,60,60	1.45	8 (16%)
27	CLA	A	810	-	65,73,73	2.24	8 (12%)	76,113,113	1.38	9 (11%)
29	II0	2	615	-	39,43,43	2.72	4 (10%)	50,60,60	1.50	10 (20%)
27	CLA	B	837	-	65,73,73	2.24	8 (12%)	76,113,113	1.39	7 (9%)
27	CLA	1	611	-	45,53,73	2.75	8 (17%)	52,89,113	1.68	7 (13%)
31	IHT	1	618	-	40,42,42	2.83	5 (12%)	53,58,58	2.05	14 (26%)
29	II0	8	611	-	39,43,43	2.73	4 (10%)	50,60,60	1.32	6 (12%)
35	8CT	B	849	-	40,41,41	0.33	0	50,56,56	0.72	1 (2%)
27	CLA	5	607	5	45,53,73	2.68	8 (17%)	52,89,113	1.65	7 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
27	CLA	8	605	8	50,58,73	2.53	8 (16%)	58,95,113	1.62	9 (15%)
27	CLA	a	608	-	60,68,73	2.34	8 (13%)	70,107,113	1.49	9 (12%)
27	CLA	4	611	-	65,73,73	2.21	8 (12%)	76,113,113	1.38	8 (10%)
27	CLA	6	604	-	60,68,73	2.35	8 (13%)	70,107,113	1.46	7 (10%)
27	CLA	O	201	-	55,63,73	2.43	8 (14%)	64,101,113	1.54	10 (15%)
29	II0	7	317	-	39,43,43	2.71	4 (10%)	50,60,60	1.53	9 (18%)
37	SF4	C	102	12	0,12,12	-	-	-		
35	8CT	R	201	-	40,41,41	0.20	0	50,56,56	0.41	0
35	8CT	Z	309	-	40,41,41	0.23	0	50,56,56	0.63	1 (2%)
27	CLA	L	201	19	51,59,73	2.53	8 (15%)	59,96,113	1.58	7 (11%)
27	CLA	B	829	-	45,53,73	2.70	8 (17%)	52,89,113	1.76	8 (15%)
35	8CT	R	203	-	40,41,41	0.16	0	50,56,56	0.46	1 (2%)
27	CLA	3	601	3	45,53,73	2.71	8 (17%)	52,89,113	1.62	7 (13%)
28	KC2	5	610	5	48,53,53	1.52	7 (14%)	54,89,89	1.06	5 (9%)
27	CLA	A	821	-	55,63,73	2.42	8 (14%)	64,101,113	1.58	7 (10%)
35	8CT	4	616	-	40,41,41	0.18	0	50,56,56	0.31	0
35	8CT	b	615	-	40,41,41	0.22	0	50,56,56	0.30	0
27	CLA	7	312	-	55,63,73	2.44	8 (14%)	64,101,113	1.52	7 (10%)
27	CLA	B	811	-	55,63,73	2.44	8 (14%)	64,101,113	1.55	7 (10%)
35	8CT	7	318	-	40,41,41	0.41	1 (2%)	50,56,56	0.59	0
27	CLA	7	309	7	55,63,73	2.43	8 (14%)	64,101,113	1.57	9 (14%)
29	II0	Z	312	-	39,43,43	2.67	4 (10%)	50,60,60	1.39	8 (16%)
35	8CT	A	848	-	40,41,41	0.37	0	50,56,56	0.56	0
30	II3	1	615	-	40,43,43	2.03	3 (7%)	47,60,60	1.57	9 (19%)
27	CLA	B	836	-	47,55,73	2.58	8 (17%)	54,91,113	1.62	7 (12%)
28	KC2	7	311	7	48,53,53	1.51	8 (16%)	54,89,89	1.10	4 (7%)
34	SQD	O	207	-	23,24,54	1.57	4 (17%)	31,34,65	1.39	4 (12%)
27	CLA	A	822	-	65,73,73	2.26	8 (12%)	76,113,113	1.39	7 (9%)
27	CLA	2	606	-	45,53,73	2.69	8 (17%)	52,89,113	1.64	7 (13%)
31	IHT	8	609	-	40,42,42	2.80	4 (10%)	53,58,58	2.33	16 (30%)
33	LHG	2	618	-	21,21,48	0.75	0	23,26,54	1.25	2 (8%)
37	SF4	C	101	12	0,12,12	-	-	-		
33	LHG	a	617	-	48,48,48	0.60	1 (2%)	51,54,54	1.20	5 (9%)
31	IHT	a	616	-	40,42,42	2.81	4 (10%)	53,58,58	2.33	17 (32%)
35	8CT	A	847	-	40,41,41	0.23	0	50,56,56	0.77	1 (2%)
27	CLA	9	606	-	64,72,73	2.21	8 (12%)	74,111,113	1.41	9 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
27	CLA	5	613	5	41,49,73	2.90	9 (21%)	47,84,113	1.76	8 (17%)
29	II0	3	615	-	39,43,43	2.70	4 (10%)	50,60,60	1.37	8 (16%)
27	CLA	6	603	-	45,53,73	2.69	8 (17%)	52,89,113	1.70	7 (13%)
27	CLA	b	608	-	65,73,73	2.25	8 (12%)	76,113,113	1.38	8 (10%)
31	IHT	L	204	-	40,42,42	2.83	4 (10%)	53,58,58	2.23	16 (30%)
27	CLA	5	609	-	41,49,73	2.90	9 (21%)	47,84,113	1.77	7 (14%)
29	II0	7	314	-	39,43,43	2.68	4 (10%)	50,60,60	1.43	8 (16%)
33	LHG	2	619	-	38,38,48	0.69	1 (2%)	41,44,54	1.25	4 (9%)
28	KC2	2	610	-	48,53,53	1.53	7 (14%)	54,89,89	1.07	5 (9%)
27	CLA	1	602	1	59,67,73	2.37	8 (13%)	68,105,113	1.49	8 (11%)
35	8CT	B	847	-	40,41,41	0.16	0	50,56,56	0.46	0
27	CLA	9	602	9	55,63,73	2.45	8 (14%)	64,101,113	1.57	8 (12%)
27	CLA	1	604	1	45,53,73	2.72	8 (17%)	52,89,113	1.64	7 (13%)
27	CLA	K	101	-	65,73,73	2.24	8 (12%)	76,113,113	1.34	7 (9%)
27	CLA	8	603	-	65,73,73	2.27	8 (12%)	76,113,113	1.40	7 (9%)
27	CLA	Z	301	-	60,68,73	2.39	8 (13%)	70,107,113	1.46	7 (10%)
29	II0	9	617	-	39,43,43	2.71	4 (10%)	50,60,60	1.46	8 (16%)
31	IHT	Z	302	-	40,42,42	2.84	4 (10%)	53,58,58	2.12	14 (26%)
33	LHG	7	320	27	38,38,48	0.65	0	41,44,54	1.17	3 (7%)
27	CLA	A	814	-	45,53,73	2.71	8 (17%)	52,89,113	1.68	7 (13%)
27	CLA	9	608	9	55,63,73	2.43	8 (14%)	64,101,113	1.54	8 (12%)
27	CLA	B	801	-	65,73,73	2.12	8 (12%)	76,113,113	1.33	8 (10%)
27	CLA	B	815	-	65,73,73	2.28	8 (12%)	76,113,113	1.43	8 (10%)
27	CLA	a	604	-	60,68,73	2.37	8 (13%)	70,107,113	1.48	6 (8%)
27	CLA	A	832	-	65,73,73	2.23	8 (12%)	76,113,113	1.36	7 (9%)
29	II0	7	316	-	39,43,43	2.73	4 (10%)	50,60,60	1.45	8 (16%)
27	CLA	5	602	5	55,63,73	2.46	8 (14%)	64,101,113	1.53	7 (10%)
27	CLA	A	807	10	50,58,73	2.56	8 (16%)	58,95,113	1.62	8 (13%)
32	LMG	3	620	-	32,32,55	0.91	0	40,40,63	1.28	6 (15%)
29	II0	a	613	-	39,43,43	2.68	4 (10%)	50,60,60	1.43	8 (16%)
27	CLA	A	829	-	50,58,73	2.55	8 (16%)	58,95,113	1.66	7 (12%)
27	CLA	A	805	-	50,58,73	2.57	8 (16%)	58,95,113	1.62	7 (12%)
33	LHG	7	319	-	30,30,48	0.75	1 (3%)	33,36,54	1.20	3 (9%)
27	CLA	b	602	26	64,72,73	2.29	8 (12%)	74,111,113	1.48	9 (12%)
27	CLA	A	827	-	65,73,73	2.14	8 (12%)	76,113,113	1.38	8 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
27	CLA	A	815	-	62,70,73	2.31	8 (12%)	72,109,113	1.42	7 (9%)
27	CLA	A	826	-	65,73,73	2.13	8 (12%)	76,113,113	1.35	8 (10%)
27	CLA	A	816	-	60,68,73	2.30	8 (13%)	70,107,113	1.47	7 (10%)
34	SQD	3	621	-	41,42,54	1.33	4 (9%)	50,53,65	1.09	3 (6%)
27	CLA	6	606	-	55,63,73	2.45	8 (14%)	64,101,113	1.59	9 (14%)
27	CLA	A	802	27	55,63,73	2.41	8 (14%)	64,101,113	1.50	7 (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
29	II0	5	614	-	-	2/21/67/67	0/2/2/2
33	LHG	Z	311	-	-	23/50/50/53	-
27	CLA	A	842	-	1/1/15/20	6/37/115/115	-
27	CLA	3	604	-	1/1/15/20	3/37/115/115	-
27	CLA	B	823	-	1/1/15/20	10/37/115/115	-
27	CLA	b	611	-	1/1/13/20	4/25/103/115	-
27	CLA	1	613	-	1/1/11/20	3/13/91/115	-
27	CLA	6	609	33	1/1/10/20	0/8/86/115	-
28	KC2	6	613	6	-	9/15/71/71	-
27	CLA	B	804	-	1/1/15/20	10/37/115/115	-
27	CLA	B	827	-	1/1/15/20	6/37/115/115	-
27	CLA	A	813	-	1/1/10/20	1/10/88/115	-
27	CLA	2	604	2	1/1/13/20	1/25/103/115	-
27	CLA	2	605	-	1/1/14/20	4/31/109/115	-
27	CLA	2	608	2	1/1/14/20	6/31/109/115	-
38	PQN	A	850	-	-	10/23/43/43	0/2/2/2
29	II0	1	616	-	-	2/21/67/67	0/2/2/2
27	CLA	1	601	1	1/1/11/20	3/13/91/115	-
27	CLA	4	609	4	1/1/14/20	4/31/109/115	-
27	CLA	B	809	-	1/1/15/20	8/37/115/115	-
27	CLA	6	608	6	1/1/14/20	5/31/109/115	-
27	CLA	A	823	-	1/1/15/20	10/37/115/115	-
27	CLA	K	102	-	1/1/13/20	3/25/103/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	CLA	O	202	-	1/1/10/20	2/8/86/115	-
27	CLA	9	611	-	1/1/10/20	3/8/86/115	-
27	CLA	B	813	-	1/1/14/20	11/33/111/115	-
27	CLA	Z	305	-	1/1/12/20	1/19/97/115	-
27	CLA	2	612	-	1/1/11/20	3/13/91/115	-
27	CLA	7	308	7	1/1/11/20	1/13/91/115	-
27	CLA	L	202	-	1/1/14/20	9/31/109/115	-
27	CLA	3	608	3	1/1/14/20	2/31/109/115	-
27	CLA	A	841	-	1/1/15/20	5/37/115/115	-
29	II0	a	612	-	-	2/21/67/67	0/2/2/2
33	LHG	6	617	27	-	16/39/39/53	-
27	CLA	Z	306	24	1/1/14/20	11/31/109/115	-
27	CLA	7	303	7	1/1/15/20	7/37/115/115	-
29	II0	9	618	-	-	2/21/67/67	0/2/2/2
29	II0	1	617	-	-	2/21/67/67	0/2/2/2
27	CLA	5	601	5	1/1/10/20	0/8/86/115	-
33	LHG	3	619	-	-	23/53/53/53	-
27	CLA	Z	310	-	1/1/15/20	5/37/115/115	-
38	PQN	B	842	-	-	5/23/43/43	0/2/2/2
27	CLA	5	603	-	1/1/11/20	3/13/91/115	-
27	CLA	3	612	-	1/1/11/20	2/13/91/115	-
29	II0	2	614	-	-	0/21/67/67	0/2/2/2
29	II0	7	301	-	-	2/21/67/67	0/2/2/2
27	CLA	2	609	-	1/1/10/20	0/8/86/115	-
27	CLA	5	612	-	1/1/11/20	3/13/91/115	-
27	CLA	8	608	-	1/1/15/20	4/37/115/115	-
27	CLA	B	825	-	1/1/15/20	2/37/115/115	-
27	CLA	a	607	25	1/1/14/20	3/31/109/115	-
29	II0	9	616	-	-	2/21/67/67	0/2/2/2
27	CLA	B	821	-	1/1/14/20	9/31/109/115	-
27	CLA	9	614	-	1/1/10/20	1/8/86/115	-
27	CLA	8	602	8	1/1/11/20	3/13/91/115	-
27	CLA	2	601	2	1/1/10/20	3/10/88/115	-
29	II0	5	615	-	-	1/21/67/67	0/2/2/2
27	CLA	A	837	-	1/1/15/20	7/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
36	LMU	J	104	-	-	9/17/57/61	0/2/2/2
27	CLA	2	603	-	1/1/12/20	4/19/97/115	-
27	CLA	b	601	26	1/1/11/20	3/13/91/115	-
27	CLA	4	607	4	1/1/14/20	5/31/109/115	-
27	CLA	9	612	-	1/1/11/20	2/13/91/115	-
27	CLA	3	607	3	1/1/14/20	4/31/109/115	-
33	LHG	A	851	-	-	22/53/53/53	-
29	II0	1	619	-	-	1/21/67/67	0/2/2/2
29	II0	5	620	-	-	1/21/67/67	0/2/2/2
27	CLA	A	840	-	1/1/13/20	3/25/103/115	-
27	CLA	A	808	-	1/1/13/20	2/25/103/115	-
39	DGD	B	848	-	-	15/48/88/95	0/2/2/2
27	CLA	3	611	3	1/1/12/20	2/19/97/115	-
27	CLA	A	834	10	1/1/13/20	7/25/103/115	-
31	IHT	5	618	-	-	1/25/65/65	0/2/2/2
28	KC2	b	609	-	-	2/15/71/71	-
27	CLA	b	607	26	1/1/14/20	5/31/109/115	-
27	CLA	B	803	-	1/1/11/20	3/13/91/115	-
27	CLA	B	841	-	1/1/12/20	5/22/100/115	-
27	CLA	B	840	-	1/1/15/20	1/37/115/115	-
35	8CT	M	101	-	-	5/29/63/63	0/2/2/2
30	II3	b	613	-	-	1/25/67/67	0/2/2/2
27	CLA	9	604	-	1/1/13/20	1/25/103/115	-
27	CLA	5	611	-	1/1/11/20	6/13/91/115	-
27	CLA	9	605	-	1/1/11/20	2/13/91/115	-
35	8CT	F	201	-	-	4/29/63/63	0/2/2/2
27	CLA	1	612	-	1/1/14/20	6/31/109/115	-
27	CLA	Z	304	24	1/1/13/20	2/25/103/115	-
35	8CT	A	845	-	-	1/29/63/63	0/2/2/2
32	LMG	8	614	-	-	23/47/67/70	0/1/1/1
27	CLA	a	602	25	1/1/13/20	9/25/103/115	-
27	CLA	B	814	-	1/1/10/20	4/10/88/115	-
27	CLA	F	204	15	1/1/13/20	4/25/103/115	-
27	CLA	5	604	-	1/1/13/20	9/25/103/115	-
32	LMG	F	205	-	-	11/27/47/70	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	CLA	6	605	6	1/1/13/20	5/25/103/115	-
27	CLA	6	601	6	1/1/11/20	2/13/91/115	-
33	LHG	b	616	-	-	25/53/53/53	-
27	CLA	1	605	-	1/1/10/20	1/9/87/115	-
27	CLA	3	605	3	1/1/13/20	2/25/103/115	-
27	CLA	2	607	2	1/1/11/20	0/13/91/115	-
27	CLA	A	843	-	1/1/15/20	10/37/115/115	-
27	CLA	B	833	-	1/1/11/20	1/13/91/115	-
29	II0	8	612	-	-	1/21/67/67	0/2/2/2
27	CLA	B	826	-	1/1/15/20	11/37/115/115	-
27	CLA	8	615	-	1/1/15/20	5/37/115/115	-
33	LHG	5	619	-	-	14/26/26/53	-
27	CLA	4	602	4	1/1/13/20	2/30/108/115	-
27	CLA	9	613	9	1/1/11/20	1/13/91/115	-
27	CLA	A	806	10	1/1/15/20	7/37/115/115	-
27	CLA	9	601	9	1/1/11/20	5/13/91/115	-
28	KC2	9	610	-	-	6/15/71/71	-
27	CLA	O	203	-	1/1/13/20	4/25/103/115	-
27	CLA	B	812	-	1/1/15/20	13/37/115/115	-
28	KC2	1	610	-	-	7/15/71/71	-
29	II0	O	206	-	-	1/21/67/67	0/2/2/2
35	8CT	I	101	-	-	3/29/63/63	0/2/2/2
27	CLA	7	313	-	1/1/12/20	6/19/97/115	-
27	CLA	B	817	-	1/1/14/20	1/31/109/115	-
29	II0	O	205	-	-	2/21/67/67	0/2/2/2
27	CLA	A	833	-	1/1/15/20	4/37/115/115	-
27	CLA	B	818	-	1/1/14/20	1/31/109/115	-
27	CLA	B	805	-	1/1/15/20	10/37/115/115	-
35	8CT	A	853	-	-	6/29/63/63	0/2/2/2
35	8CT	Z	308	-	-	6/29/63/63	0/2/2/2
29	II0	b	612	-	-	1/21/67/67	0/2/2/2
27	CLA	7	302	7	1/1/11/20	0/13/91/115	-
36	LMU	7	321	-	-	8/21/61/61	0/2/2/2
28	KC2	Z	307	-	-	7/15/71/71	-
33	LHG	8	613	-	-	21/37/37/53	-
28	KC2	a	609	-	-	3/15/71/71	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	CLA	A	801	-	1/1/15/20	8/37/115/115	-
29	II0	R	204	-	-	2/21/67/67	0/2/2/2
27	CLA	B	816	-	1/1/13/20	12/30/108/115	-
27	CLA	A	818	-	1/1/15/20	7/37/115/115	-
29	II0	5	616	-	-	1/21/67/67	0/2/2/2
27	CLA	8	607	8	1/1/10/20	1/8/86/115	-
32	LMG	3	618	-	-	9/25/45/70	0/1/1/1
29	II0	2	613	-	-	1/21/67/67	0/2/2/2
27	CLA	A	811	-	1/1/15/20	12/37/115/115	-
29	II0	4	613	-	-	1/21/67/67	0/2/2/2
27	CLA	B	832	-	1/1/15/20	15/37/115/115	-
29	II0	9	615	-	-	1/21/67/67	0/2/2/2
29	II0	J	101	-	-	1/21/67/67	0/2/2/2
27	CLA	a	606	25	1/1/15/20	4/37/115/115	-
27	CLA	9	607	9	1/1/15/20	10/37/115/115	-
27	CLA	A	817	-	1/1/15/20	13/37/115/115	-
29	II0	5	617	-	-	2/21/67/67	0/2/2/2
27	CLA	2	602	2	1/1/13/20	12/30/108/115	-
29	II0	B	843	-	-	2/21/67/67	0/2/2/2
28	KC2	6	610	6	-	6/15/71/71	-
27	CLA	b	604	-	1/1/15/20	16/37/115/115	-
29	II0	4	614	-	-	2/21/67/67	0/2/2/2
27	CLA	A	835	-	1/1/14/20	6/31/109/115	-
33	LHG	3	622	28	-	13/38/38/53	-
27	CLA	A	819	-	1/1/15/20	5/37/115/115	-
27	CLA	3	603	-	1/1/14/20	3/31/109/115	-
27	CLA	B	839	33	1/1/15/20	5/37/115/115	-
27	CLA	4	603	-	1/1/12/20	5/24/102/115	-
31	IHT	2	616	-	-	2/25/65/65	0/2/2/2
27	CLA	R	202	-	1/1/13/20	10/25/103/115	-
29	II0	3	613	-	-	2/21/67/67	0/2/2/2
27	CLA	8	604	-	1/1/15/20	4/37/115/115	-
27	CLA	L	203	-	1/1/12/20	5/19/97/115	-
27	CLA	1	607	1	1/1/11/20	0/13/91/115	-
29	II0	4	615	-	-	0/21/67/67	0/2/2/2
27	CLA	B	822	-	1/1/15/20	7/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	CLA	7	310	33	1/1/10/20	0/8/86/115	-
27	CLA	F	202	-	1/1/14/20	10/31/109/115	-
27	CLA	b	603	-	1/1/14/20	7/31/109/115	-
27	CLA	A	803	-	1/1/15/20	8/37/115/115	-
28	KC2	3	606	33	-	8/15/71/71	-
27	CLA	F	203	-	1/1/11/20	3/13/91/115	-
27	CLA	B	834	-	1/1/13/20	2/25/103/115	-
27	CLA	b	610	26	1/1/12/20	9/21/99/115	-
31	IHT	A	854	-	-	2/25/65/65	0/2/2/2
31	IHT	6	616	-	-	3/25/65/65	0/2/2/2
29	II0	8	610	-	-	2/21/67/67	0/2/2/2
27	CLA	J	102	-	1/1/10/20	1/8/86/115	-
37	SF4	A	849	10,11	-	-	0/6/5/5
27	CLA	6	602	6	1/1/15/20	7/37/115/115	-
27	CLA	9	603	-	1/1/11/20	5/13/91/115	-
27	CLA	B	824	-	1/1/14/20	5/31/109/115	-
27	CLA	A	836	-	1/1/13/20	1/25/103/115	-
27	CLA	5	608	5	1/1/14/20	10/31/109/115	-
27	CLA	B	802	-	1/1/15/20	8/37/115/115	-
27	CLA	2	611	-	1/1/11/20	2/13/91/115	-
27	CLA	A	804	10	1/1/15/20	16/37/115/115	-
29	II0	6	614	-	-	1/21/67/67	0/2/2/2
27	CLA	7	304	-	1/1/13/20	1/25/103/115	-
33	LHG	4	617	27	-	18/51/51/53	-
35	8CT	L	205	-	-	2/29/63/63	0/2/2/2
27	CLA	O	204	-	1/1/13/20	8/25/103/115	-
27	CLA	A	824	-	1/1/15/20	3/37/115/115	-
35	8CT	B	845	-	-	8/29/63/63	0/2/2/2
27	CLA	B	830	-	1/1/14/20	0/31/109/115	-
27	CLA	a	605	-	1/1/13/20	10/25/103/115	-
32	LMG	2	617	-	-	8/31/51/70	0/1/1/1
28	KC2	b	605	26	-	7/15/71/71	-
28	KC2	4	605	4	-	7/15/71/71	-
27	CLA	1	603	-	1/1/12/20	4/22/100/115	-
27	CLA	A	831	-	1/1/15/20	11/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	CLA	6	612	-	1/1/11/20	2/13/91/115	-
27	CLA	A	838	-	1/1/15/20	3/37/115/115	-
27	CLA	9	609	-	1/1/10/20	3/8/86/115	-
29	II0	a	615	-	-	1/21/67/67	0/2/2/2
35	8CT	J	103	-	-	7/29/63/63	0/2/2/2
27	CLA	B	838	-	1/1/15/20	5/37/115/115	-
27	CLA	5	606	-	1/1/11/20	5/13/91/115	-
27	CLA	A	830	-	1/1/14/20	4/31/109/115	-
27	CLA	1	606	-	1/1/11/20	0/13/91/115	-
33	LHG	2	620	-	-	17/46/46/53	-
27	CLA	B	819	-	1/1/14/20	8/31/109/115	-
27	CLA	8	601	8	1/1/11/20	3/13/91/115	-
29	II0	4	612	-	-	2/21/67/67	0/2/2/2
27	CLA	B	810	-	1/1/14/20	4/31/109/115	-
36	LMU	4	618	-	-	11/21/61/61	0/2/2/2
29	II0	1	614	-	-	2/21/67/67	0/2/2/2
27	CLA	B	806	-	1/1/15/20	4/37/115/115	-
27	CLA	1	609	-	1/1/10/20	1/8/86/115	-
29	II0	6	615	-	-	1/21/67/67	0/2/2/2
35	8CT	K	103	-	-	3/29/63/63	0/2/2/2
29	II0	7	315	-	-	1/21/67/67	0/2/2/2
27	CLA	A	828	-	1/1/15/20	7/37/115/115	-
29	II0	3	616	-	-	2/21/67/67	0/2/2/2
32	LMG	6	618	-	-	5/27/47/70	0/1/1/1
27	CLA	4	610	-	1/1/15/20	7/37/115/115	-
27	CLA	A	839	-	1/1/15/20	13/37/115/115	-
35	8CT	B	844	-	-	3/29/63/63	0/2/2/2
27	CLA	6	607	6	1/1/13/20	2/25/103/115	-
33	LHG	4	619	27	-	20/49/49/53	-
27	CLA	B	828	-	1/1/15/20	9/37/115/115	-
27	CLA	B	831	-	1/1/13/20	8/25/103/115	-
27	CLA	4	606	4	1/1/14/20	4/31/109/115	-
27	CLA	B	820	-	1/1/14/20	8/31/109/115	-
27	CLA	A	809	27	1/1/14/20	3/31/109/115	-
27	CLA	3	610	-	1/1/15/20	8/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	LMG	8	616	-	-	24/46/66/70	0/1/1/1
27	CLA	7	305	7	1/1/12/20	6/23/101/115	-
27	CLA	A	812	-	1/1/13/20	3/25/103/115	-
27	CLA	1	608	1	1/1/14/20	3/31/109/115	-
27	CLA	b	606	26	1/1/15/20	4/37/115/115	-
27	CLA	A	825	-	1/1/15/20	7/37/115/115	-
27	CLA	4	604	-	1/1/13/20	9/25/103/115	-
27	CLA	3	609	-	1/1/15/20	0/37/115/115	-
27	CLA	4	601	4	1/1/13/20	5/25/103/115	-
29	II0	a	614	-	-	2/21/67/67	0/2/2/2
35	8CT	A	846	-	-	3/29/63/63	0/2/2/2
27	CLA	a	603	-	1/1/14/20	5/31/109/115	-
27	CLA	a	601	25	1/1/11/20	6/13/91/115	-
31	IHT	9	619	-	-	3/25/65/65	0/2/2/2
27	CLA	A	820	-	1/1/15/20	8/37/115/115	-
27	CLA	3	602	3	1/1/13/20	2/25/103/115	-
27	CLA	A	844	-	1/1/15/20	6/37/115/115	-
33	LHG	A	852	-	-	20/43/43/53	-
29	II0	3	617	-	-	2/21/67/67	0/2/2/2
27	CLA	8	606	8	1/1/13/20	3/25/103/115	-
33	LHG	a	618	-	-	16/33/33/53	-
35	8CT	B	846	-	-	8/29/63/63	0/2/2/2
35	8CT	B	850	-	-	9/29/63/63	0/2/2/2
27	CLA	B	835	-	1/1/15/20	9/37/115/115	-
33	LHG	4	620	-	-	17/49/49/53	-
27	CLA	a	611	-	1/1/15/20	5/37/115/115	-
27	CLA	5	605	5	1/1/11/20	2/13/91/115	-
39	DGD	Z	303	-	-	27/49/89/95	0/2/2/2
29	II0	3	614	-	-	0/21/67/67	0/2/2/2
27	CLA	4	608	33	1/1/15/20	2/37/115/115	-
27	CLA	a	610	-	1/1/13/20	6/25/103/115	-
27	CLA	7	306	7	1/1/11/20	4/13/91/115	-
27	CLA	B	808	11	1/1/15/20	8/37/115/115	-
27	CLA	6	611	-	1/1/13/20	4/25/103/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	CLA	B	807	-	1/1/15/20	9/37/115/115	-
28	KC2	7	307	-	-	6/15/71/71	-
29	II0	b	614	-	-	0/21/67/67	0/2/2/2
27	CLA	A	810	-	1/1/15/20	16/37/115/115	-
29	II0	2	615	-	-	2/21/67/67	0/2/2/2
27	CLA	B	837	-	1/1/15/20	3/37/115/115	-
27	CLA	1	611	-	1/1/11/20	3/13/91/115	-
31	IHT	1	618	-	-	2/25/65/65	0/2/2/2
29	II0	8	611	-	-	2/21/67/67	0/2/2/2
35	8CT	B	849	-	-	4/29/63/63	0/2/2/2
27	CLA	5	607	5	1/1/11/20	0/13/91/115	-
27	CLA	8	605	8	1/1/12/20	3/19/97/115	-
27	CLA	a	608	-	1/1/14/20	7/31/109/115	-
27	CLA	4	611	-	1/1/15/20	9/37/115/115	-
27	CLA	6	604	-	1/1/14/20	6/31/109/115	-
27	CLA	O	201	-	1/1/13/20	3/25/103/115	-
29	II0	7	317	-	-	1/21/67/67	0/2/2/2
37	SF4	C	102	12	-	-	0/6/5/5
35	8CT	R	201	-	-	7/29/63/63	0/2/2/2
35	8CT	Z	309	-	-	6/29/63/63	0/2/2/2
27	CLA	L	201	19	1/1/12/20	1/21/99/115	-
27	CLA	B	829	-	1/1/11/20	0/13/91/115	-
35	8CT	R	203	-	-	4/29/63/63	0/2/2/2
27	CLA	3	601	3	1/1/11/20	4/13/91/115	-
28	KC2	5	610	5	-	4/15/71/71	-
27	CLA	A	821	-	1/1/13/20	2/25/103/115	-
35	8CT	4	616	-	-	5/29/63/63	0/2/2/2
35	8CT	b	615	-	-	6/29/63/63	0/2/2/2
27	CLA	7	312	-	1/1/13/20	5/25/103/115	-
27	CLA	B	811	-	1/1/13/20	6/25/103/115	-
35	8CT	7	318	-	-	9/29/63/63	0/2/2/2
27	CLA	7	309	7	1/1/13/20	7/25/103/115	-
29	II0	Z	312	-	-	1/21/67/67	0/2/2/2
35	8CT	A	848	-	-	1/29/63/63	0/2/2/2
30	II3	1	615	-	-	1/25/67/67	0/2/2/2
27	CLA	B	836	-	1/1/11/20	1/16/94/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	KC2	7	311	7	-	7/15/71/71	-
34	SQD	O	207	-	-	7/18/38/69	0/1/1/1
27	CLA	A	822	-	1/1/15/20	8/37/115/115	-
27	CLA	2	606	-	1/1/11/20	2/13/91/115	-
31	IHT	8	609	-	-	1/25/65/65	0/2/2/2
33	LHG	2	618	-	-	9/24/24/53	-
37	SF4	C	101	12	-	-	0/6/5/5
33	LHG	a	617	-	-	25/53/53/53	-
31	IHT	a	616	-	-	6/25/65/65	0/2/2/2
35	8CT	A	847	-	-	9/29/63/63	0/2/2/2
27	CLA	9	606	-	1/1/14/20	10/36/114/115	-
27	CLA	5	613	5	1/1/10/20	1/8/86/115	-
29	II0	3	615	-	-	1/21/67/67	0/2/2/2
27	CLA	6	603	-	1/1/11/20	5/13/91/115	-
27	CLA	b	608	-	1/1/15/20	7/37/115/115	-
31	IHT	L	204	-	-	2/25/65/65	0/2/2/2
27	CLA	5	609	-	1/1/10/20	0/8/86/115	-
29	II0	7	314	-	-	0/21/67/67	0/2/2/2
33	LHG	2	619	-	-	17/43/43/53	-
28	KC2	2	610	-	-	6/15/71/71	-
27	CLA	1	602	1	1/1/13/20	6/30/108/115	-
35	8CT	B	847	-	-	4/29/63/63	0/2/2/2
27	CLA	9	602	9	1/1/13/20	7/25/103/115	-
27	CLA	1	604	1	1/1/11/20	1/13/91/115	-
27	CLA	K	101	-	1/1/15/20	6/37/115/115	-
27	CLA	8	603	-	1/1/15/20	8/37/115/115	-
27	CLA	Z	301	-	1/1/14/20	11/31/109/115	-
29	II0	9	617	-	-	2/21/67/67	0/2/2/2
31	IHT	Z	302	-	-	2/25/65/65	0/2/2/2
33	LHG	7	320	27	-	20/43/43/53	-
27	CLA	A	814	-	1/1/11/20	5/13/91/115	-
27	CLA	9	608	9	1/1/13/20	9/25/103/115	-
27	CLA	B	801	-	1/1/15/20	5/37/115/115	-
27	CLA	B	815	-	1/1/15/20	9/37/115/115	-
27	CLA	a	604	-	1/1/14/20	9/31/109/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	CLA	A	832	-	1/1/15/20	6/37/115/115	-
29	II0	7	316	-	-	2/21/67/67	0/2/2/2
27	CLA	5	602	5	1/1/13/20	4/25/103/115	-
27	CLA	A	807	10	1/1/12/20	2/19/97/115	-
32	LMG	3	620	-	-	11/27/47/70	0/1/1/1
29	II0	a	613	-	-	2/21/67/67	0/2/2/2
27	CLA	A	829	-	1/1/12/20	4/19/97/115	-
27	CLA	A	805	-	1/1/12/20	1/19/97/115	-
33	LHG	7	319	-	-	9/35/35/53	-
27	CLA	b	602	26	1/1/14/20	14/36/114/115	-
27	CLA	A	827	-	1/1/15/20	5/37/115/115	-
27	CLA	A	815	-	1/1/14/20	1/34/112/115	-
27	CLA	A	826	-	1/1/15/20	5/37/115/115	-
27	CLA	A	816	-	1/1/14/20	7/31/109/115	-
34	SQD	3	621	-	-	14/37/57/69	0/1/1/1
27	CLA	6	606	-	1/1/13/20	8/25/103/115	-
27	CLA	A	802	27	1/1/13/20	3/25/103/115	-

The worst 5 of 2160 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	1	601	CLA	C1B-NB	10.96	1.45	1.35
27	5	608	CLA	C1B-NB	10.93	1.45	1.35
27	5	601	CLA	C1B-NB	10.92	1.45	1.35
27	A	811	CLA	C1B-NB	10.91	1.44	1.35
27	O	204	CLA	C1B-NB	10.88	1.44	1.35

The worst 5 of 2443 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	8	609	IHT	C02-C07-C10	-10.15	108.32	122.61
31	9	619	IHT	C02-C07-C10	-10.12	108.35	122.61
31	L	204	IHT	C02-C07-C10	-9.21	109.64	122.61
31	5	618	IHT	C02-C07-C10	-8.96	110.00	122.61
31	6	616	IHT	C02-C07-C10	-8.07	111.24	122.61

5 of 222 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
27	1	601	CLA	ND
27	1	602	CLA	ND
27	1	603	CLA	ND
27	1	604	CLA	ND
27	1	605	CLA	ND

5 of 1972 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
27	1	603	CLA	C1A-C2A-CAA-CBA
27	2	601	CLA	C3A-C2A-CAA-CBA
27	2	601	CLA	CHA-CBD-CGD-O1D
27	2	601	CLA	CHA-CBD-CGD-O2D
27	2	602	CLA	C3A-C2A-CAA-CBA

There are no ring outliers.

73 monomers are involved in 87 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
27	A	842	CLA	1	0
27	B	809	CLA	1	0
27	A	823	CLA	2	0
27	K	102	CLA	1	0
27	7	308	CLA	1	0
29	2	614	II0	1	0
27	5	612	CLA	1	0
27	8	608	CLA	1	0
27	B	825	CLA	1	0
27	8	602	CLA	2	0
27	A	837	CLA	1	0
36	J	104	LMU	1	0
29	5	620	II0	2	0
27	A	840	CLA	1	0
27	A	808	CLA	1	0
27	A	834	CLA	1	0
27	B	840	CLA	1	0
35	M	101	8CT	1	0
27	9	604	CLA	2	0
27	Z	304	CLA	1	0
27	5	604	CLA	1	0
27	6	605	CLA	1	0
27	A	843	CLA	1	0
28	9	610	KC2	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
27	B	812	CLA	1	0
27	7	313	CLA	1	0
36	7	321	LMU	1	0
27	A	801	CLA	1	0
27	B	816	CLA	1	0
27	A	818	CLA	3	0
27	A	811	CLA	1	0
29	4	613	II0	1	0
27	B	832	CLA	2	0
27	9	607	CLA	1	0
27	A	819	CLA	1	0
27	B	839	CLA	1	0
27	B	822	CLA	1	0
27	B	834	CLA	4	0
31	A	854	IHT	1	0
29	8	610	II0	1	0
27	A	836	CLA	3	0
27	5	608	CLA	2	0
27	B	802	CLA	1	0
27	2	611	CLA	1	0
27	A	824	CLA	2	0
27	B	830	CLA	1	0
27	A	838	CLA	1	0
36	4	618	LMU	2	0
27	4	606	CLA	1	0
27	A	809	CLA	1	0
27	A	812	CLA	1	0
31	9	619	IHT	1	0
27	A	844	CLA	3	0
39	Z	303	DGD	1	0
29	3	614	II0	1	0
27	6	611	CLA	1	0
27	B	807	CLA	1	0
27	A	810	CLA	3	0
27	8	605	CLA	2	0
27	O	201	CLA	1	0
37	C	102	SF4	1	0
27	L	201	CLA	1	0
27	A	821	CLA	1	0
28	7	311	KC2	2	0
27	9	606	CLA	1	0
27	5	609	CLA	1	0

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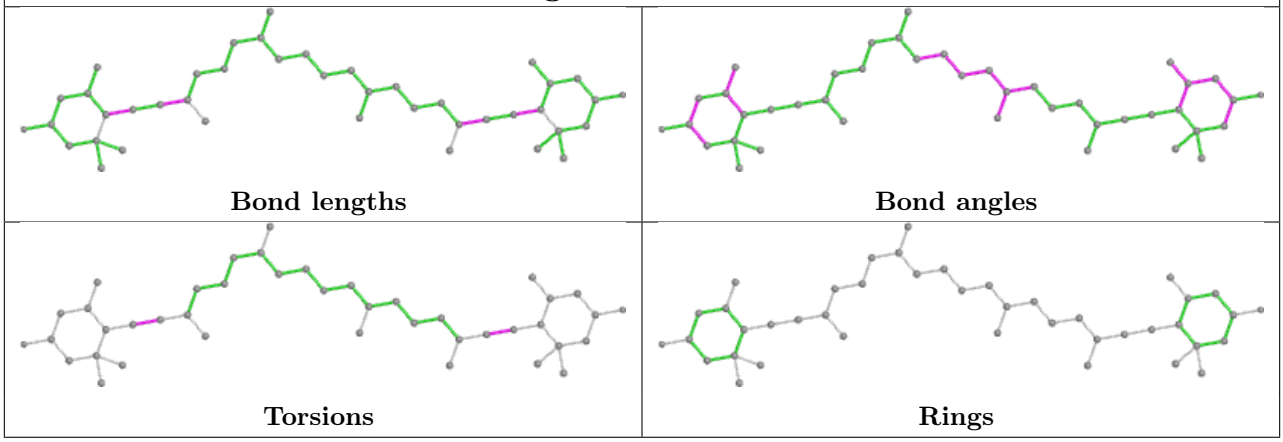
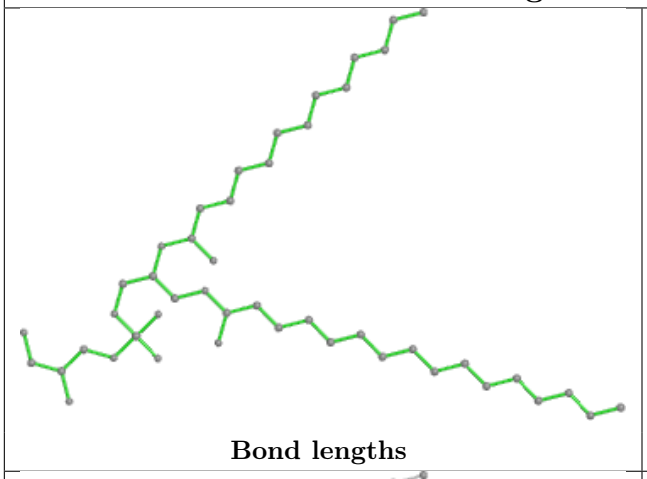
Mol	Chain	Res	Type	Clashes	Symm-Clashes
33	2	619	LHG	1	0
27	9	602	CLA	1	0
27	1	604	CLA	1	0
27	8	603	CLA	1	0
27	B	801	CLA	2	0
27	B	815	CLA	1	0
27	A	826	CLA	1	0

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

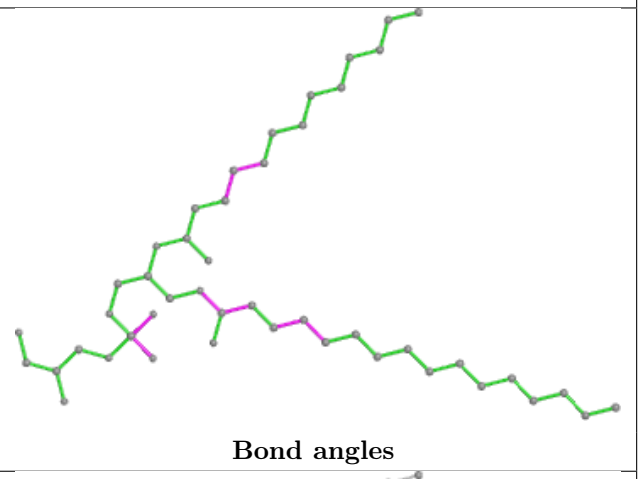
Ligand II0 5 614



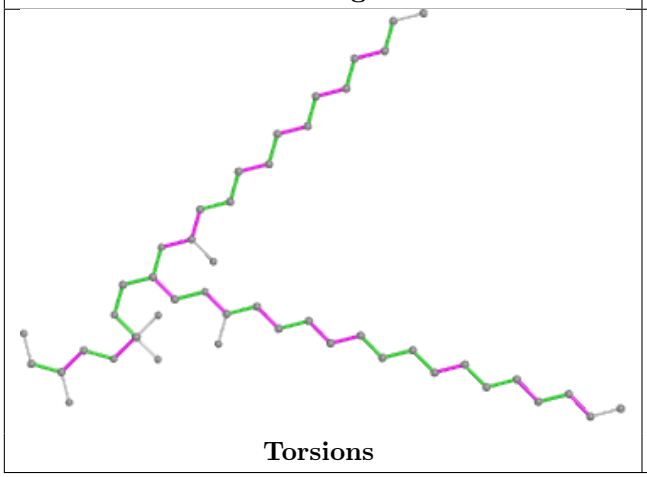
Ligand LHG Z 311



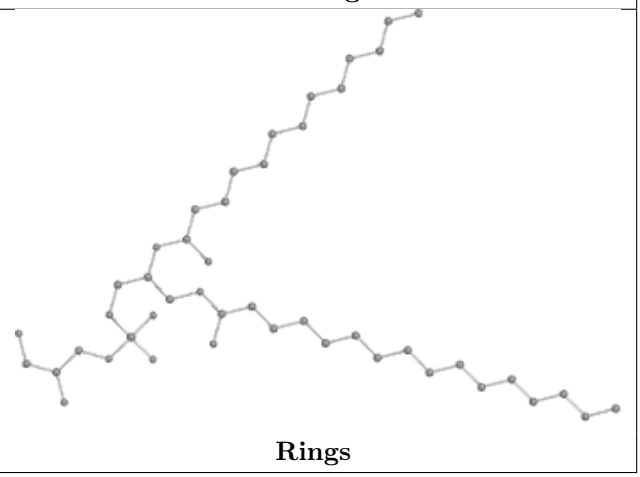
Bond lengths



Bond angles

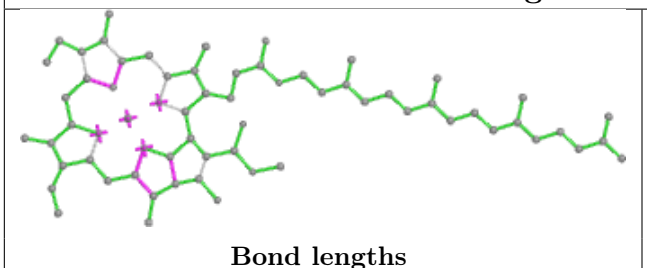


Torsions

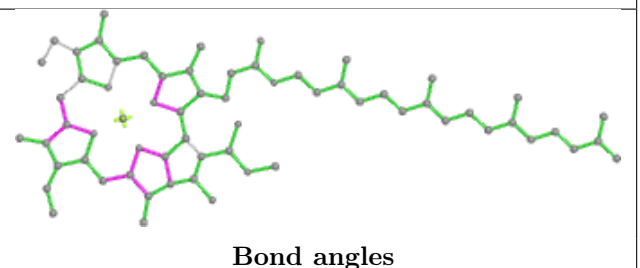


Rings

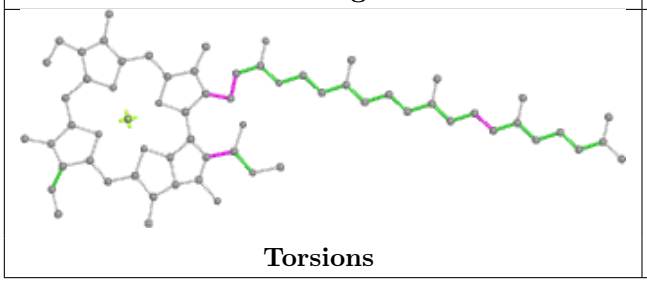
Ligand CLA A 842



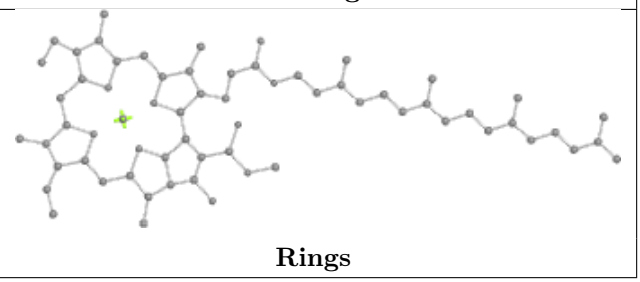
Bond lengths



Bond angles

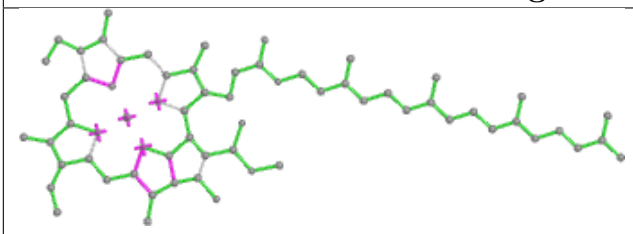


Torsions

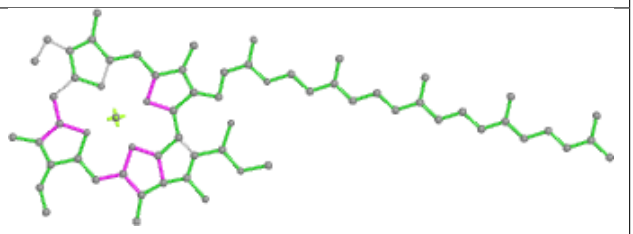


Rings

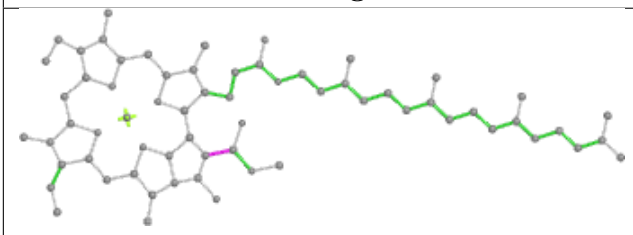
Ligand CLA 3 604



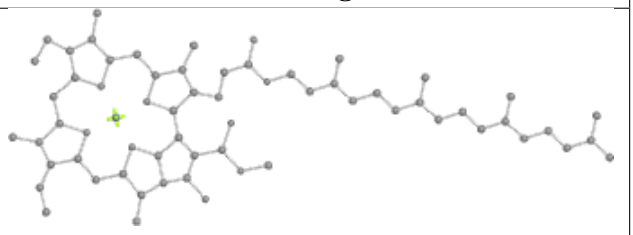
Bond lengths



Bond angles

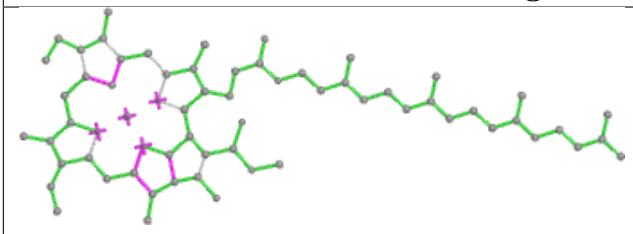


Torsions

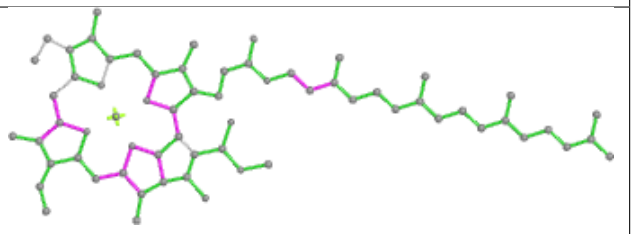


Rings

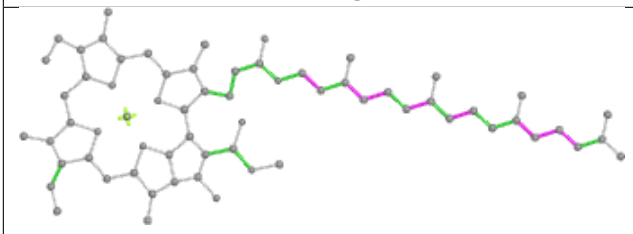
Ligand CLA B 823



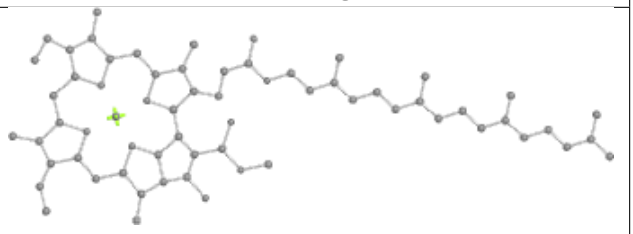
Bond lengths



Bond angles

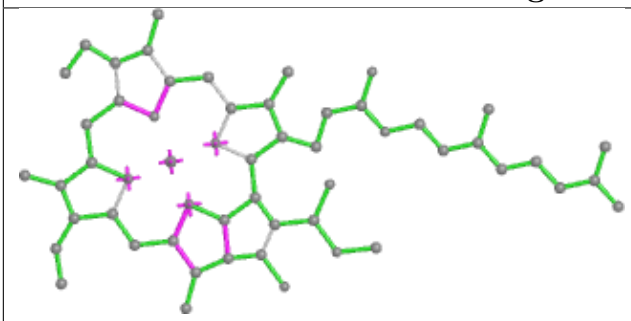


Torsions

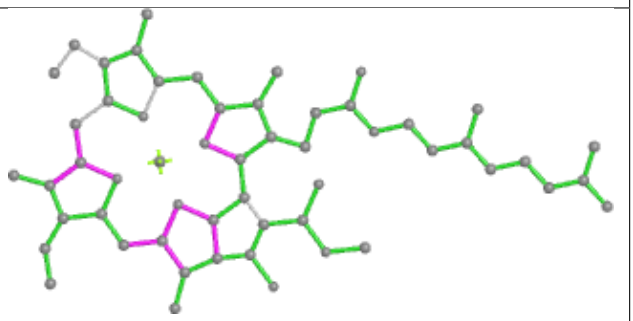


Rings

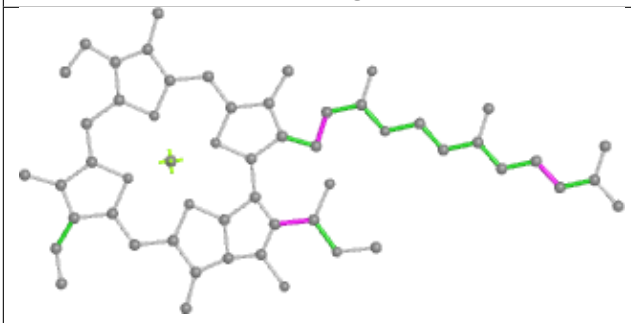
Ligand CLA b 611



Bond lengths



Bond angles



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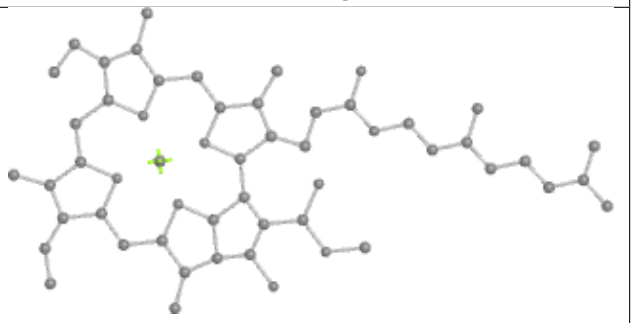
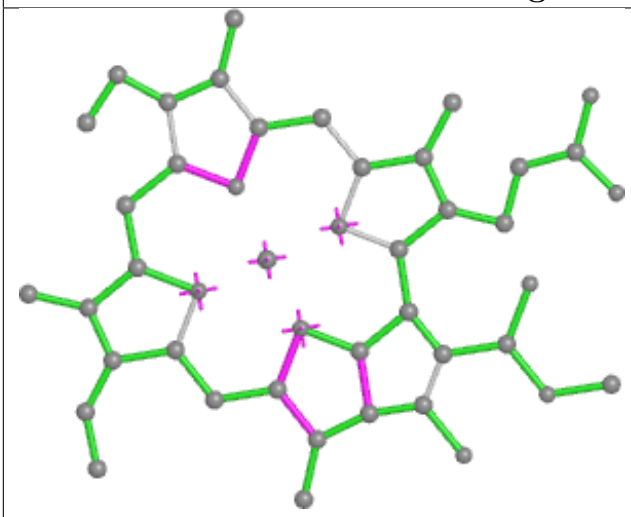


Rings

Ligand CLA 1 613



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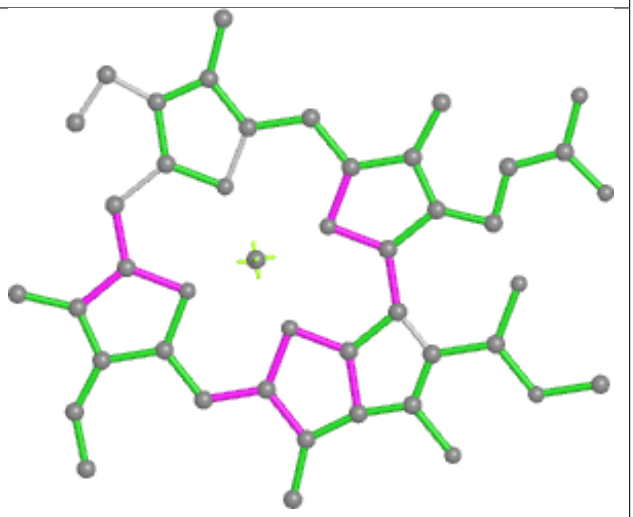
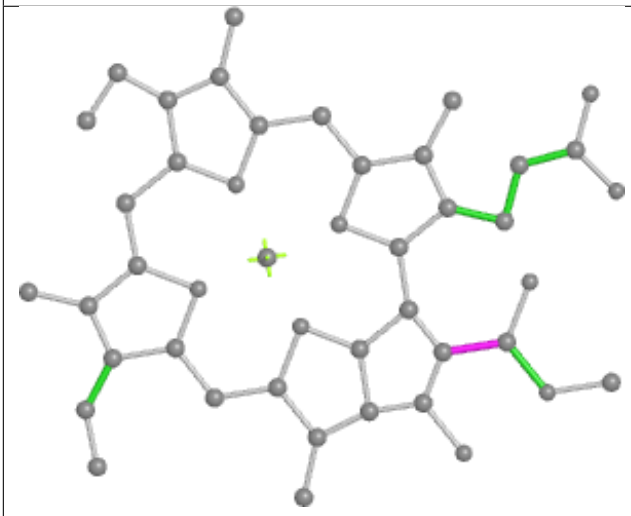


Bond angles



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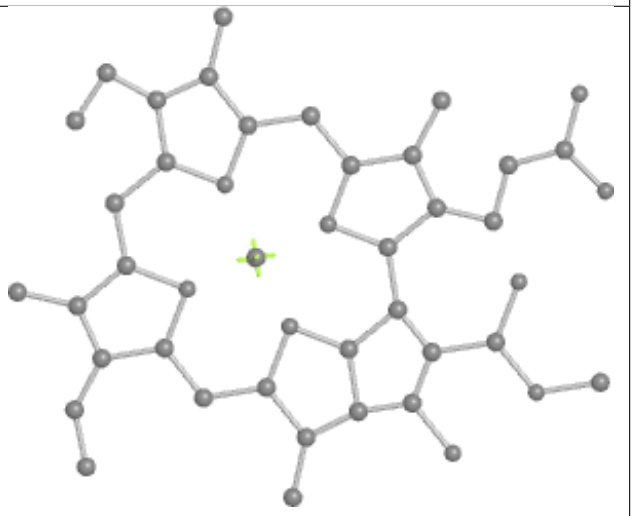
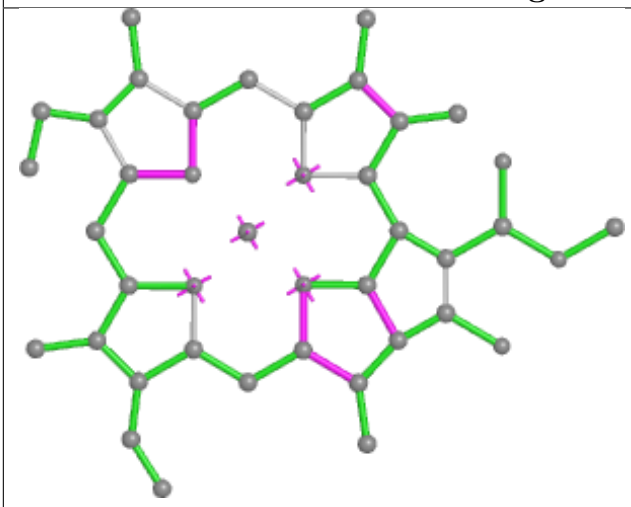


Rings

Ligand CLA 6 609



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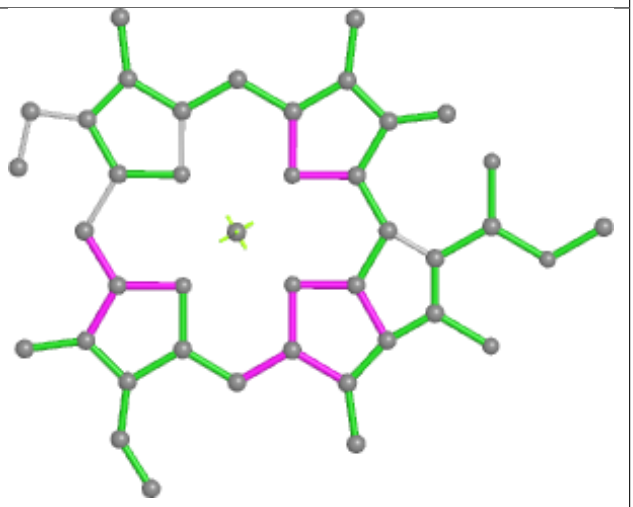
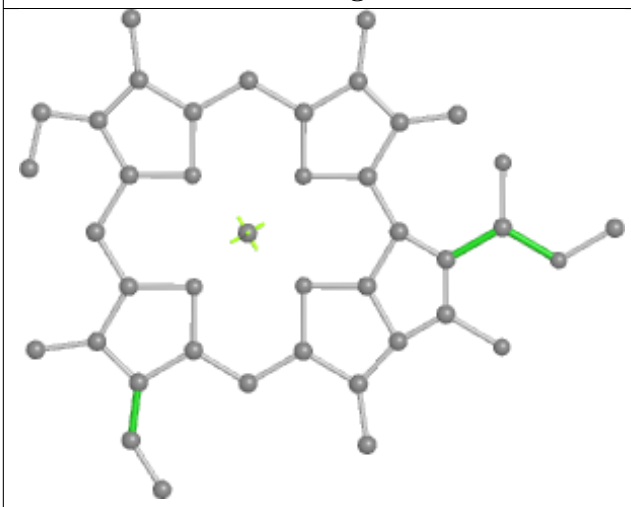
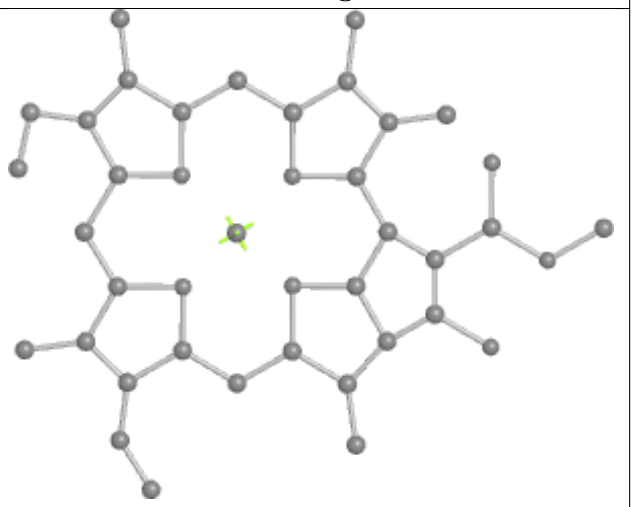


Bond angles

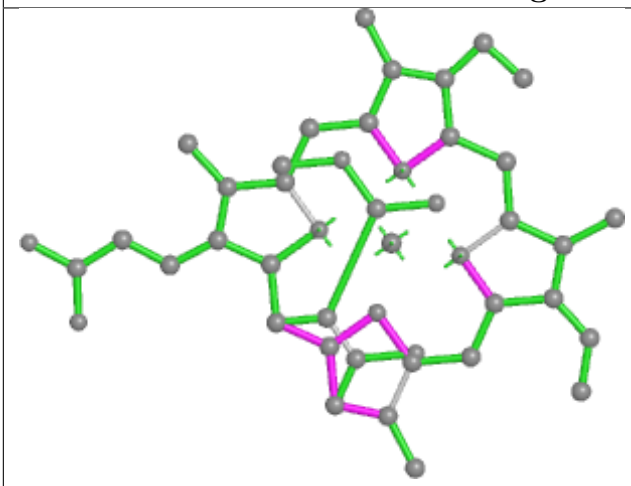


Torsions

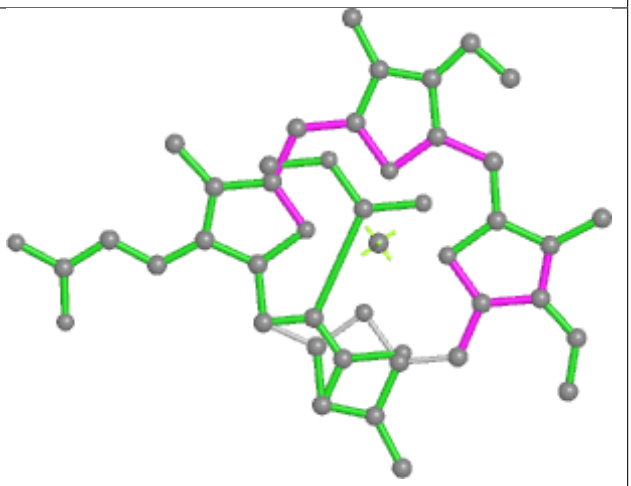


Rings

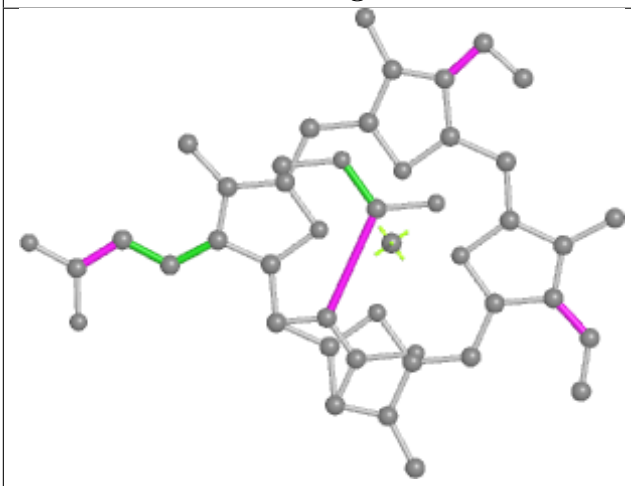
Ligand KC2 6 613



Bond lengths



Bond angles



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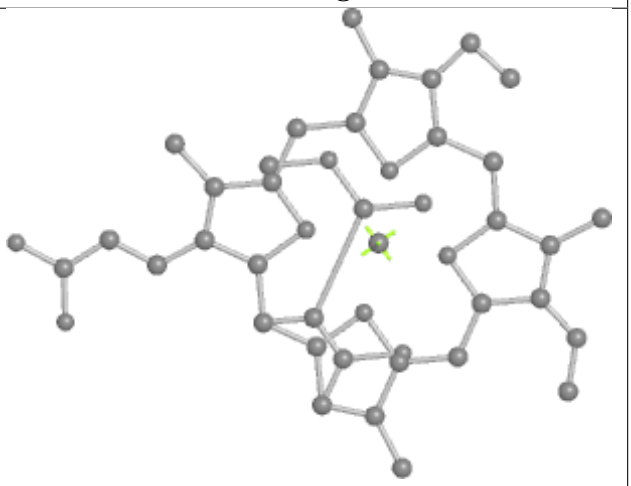
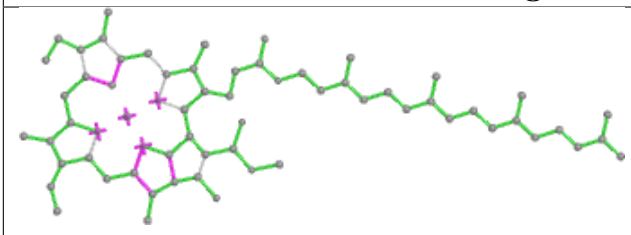


Rings

Ligand CLA B 804



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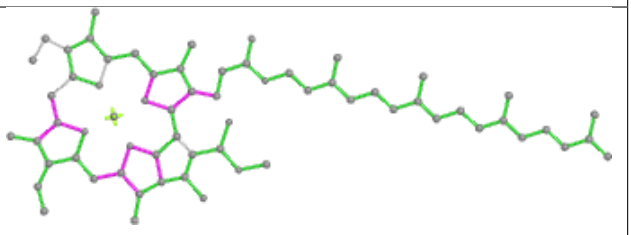
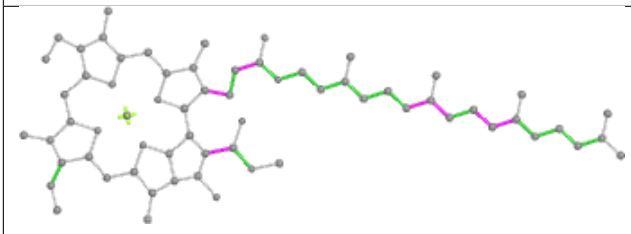
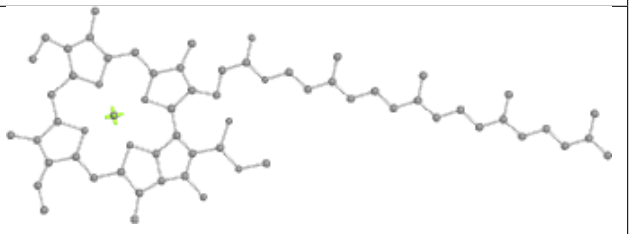


Bond angles

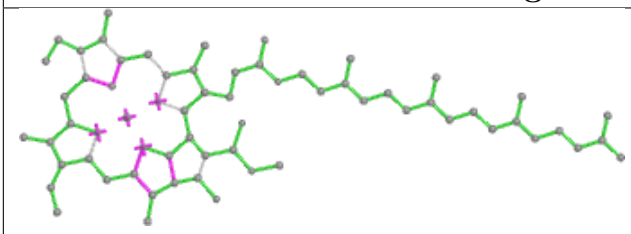


Torsions

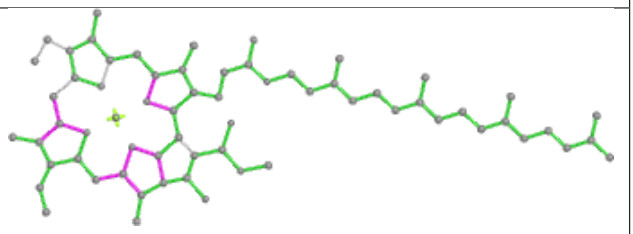


Rings

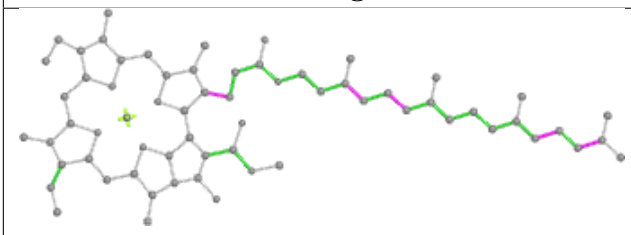
Ligand CLA B 827



Bond lengths



Bond angles



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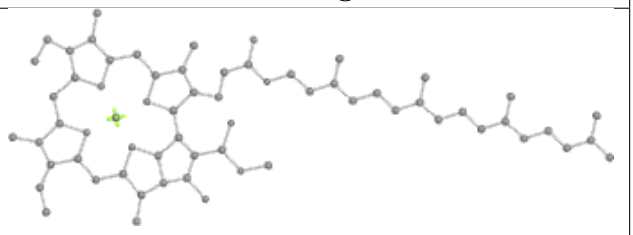
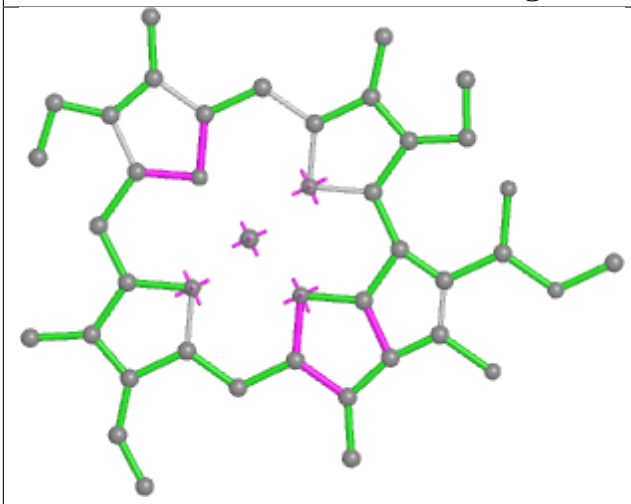


Rings

Ligand CLA A 813



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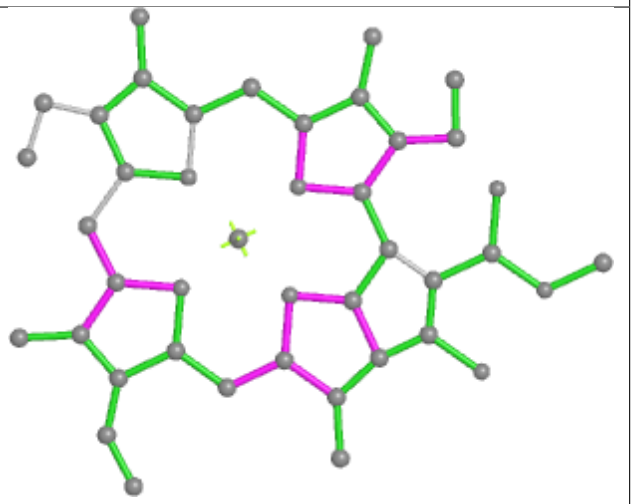
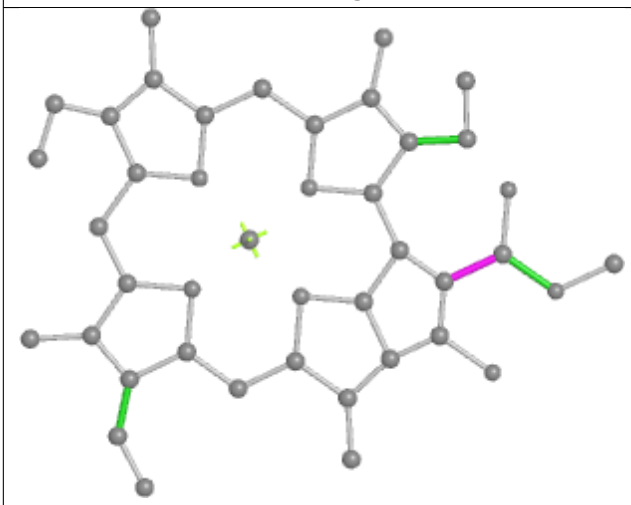


Bond angles



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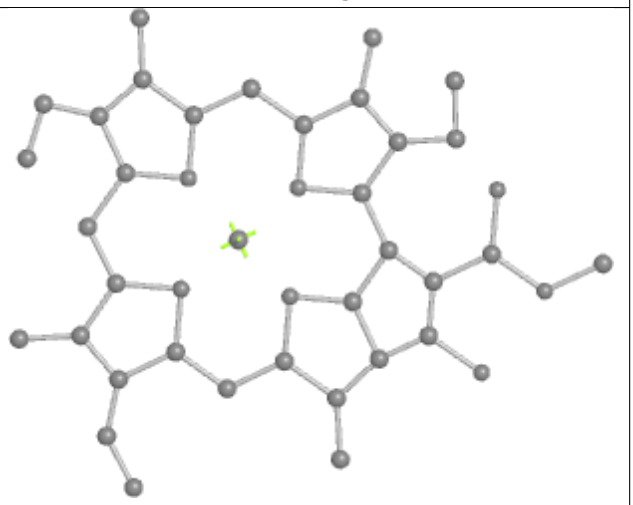
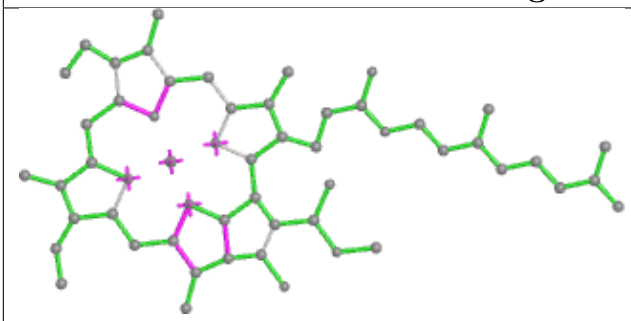


Rings

Ligand CLA 2 604



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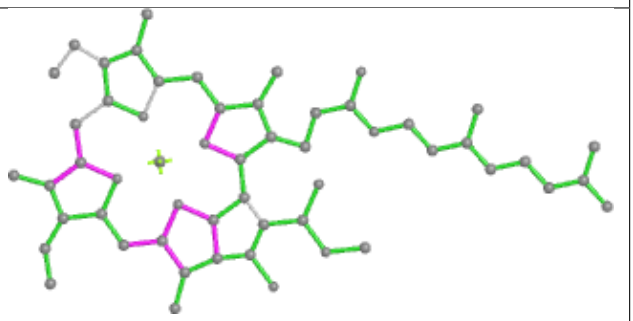
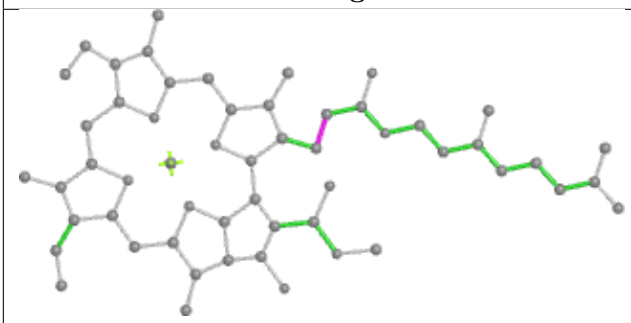
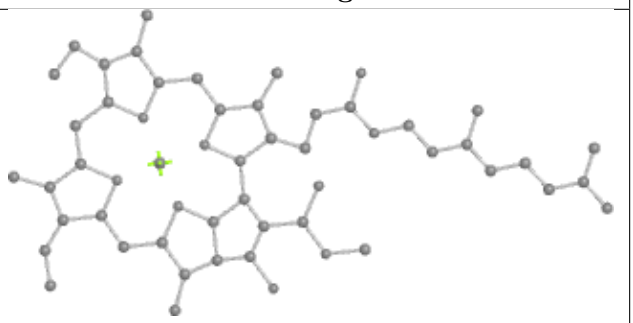


Bond angles

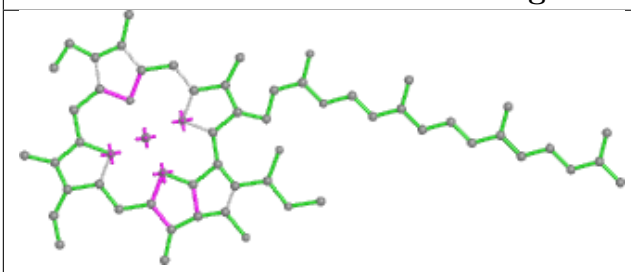


Torsions

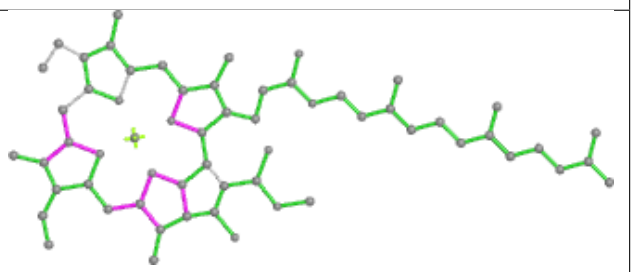


Rings

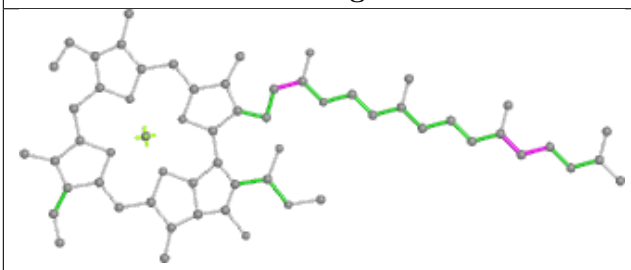
Ligand CLA 2 605



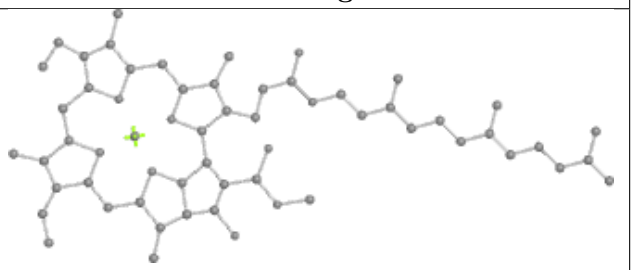
Bond lengths



Bond angles

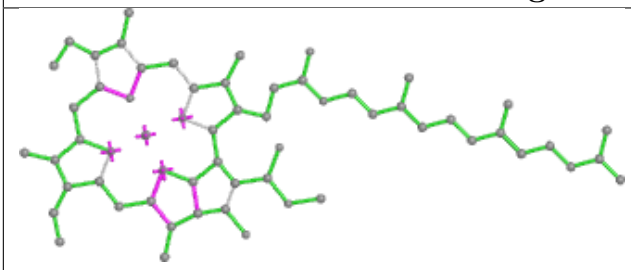


Torsions

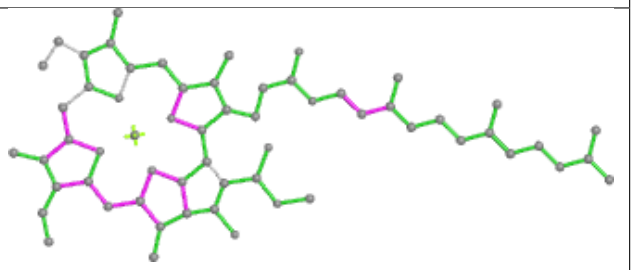


Rings

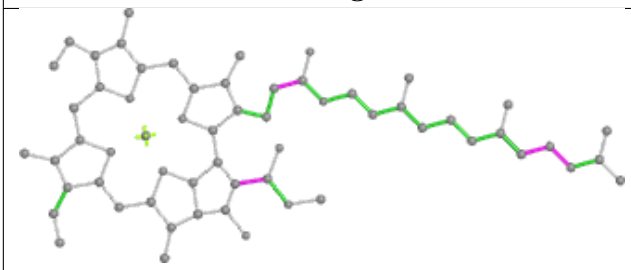
Ligand CLA 2 608



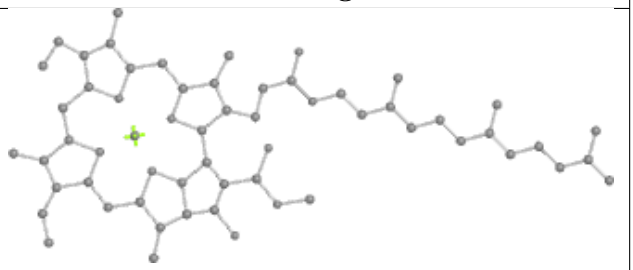
Bond lengths



Bond angles

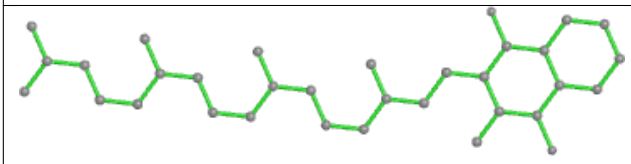


Torsions



Rings

Ligand PQN A 850



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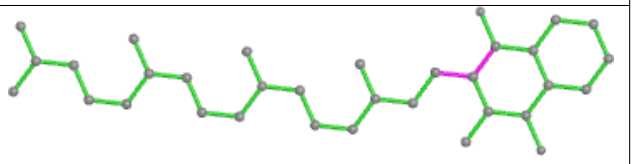
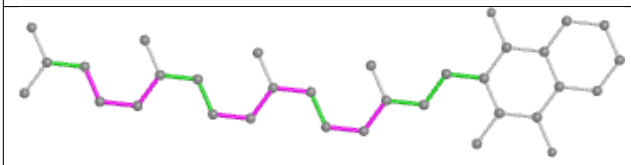
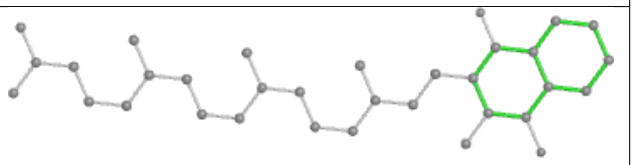


Bond angles

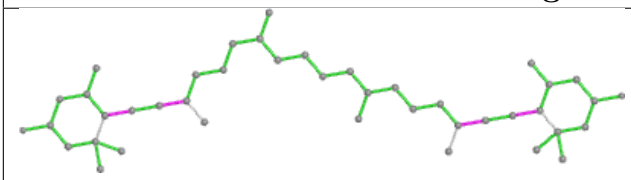


Torsions



Rings

Ligand II0 1 616



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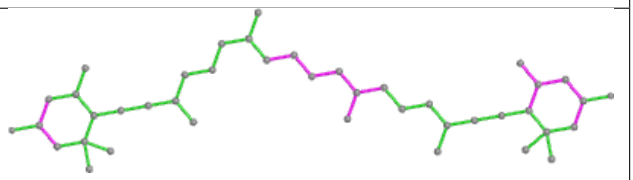
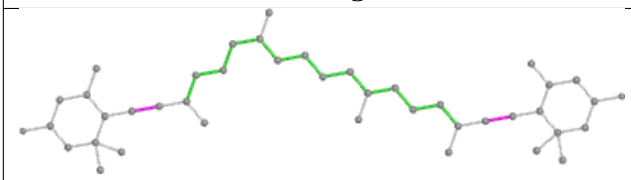


Bond angles



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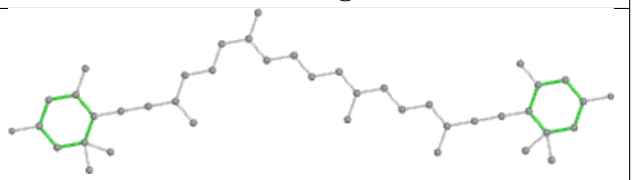
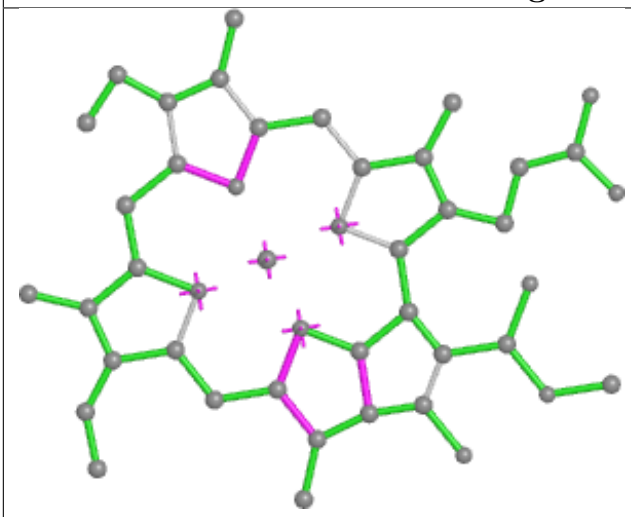


Rings

Ligand CLA 1 601



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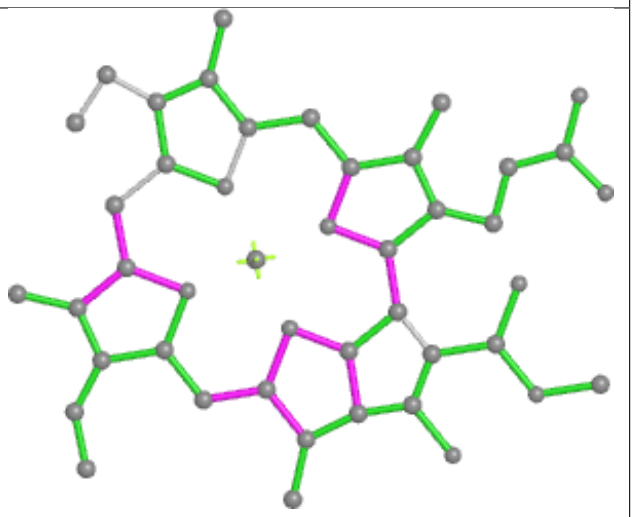
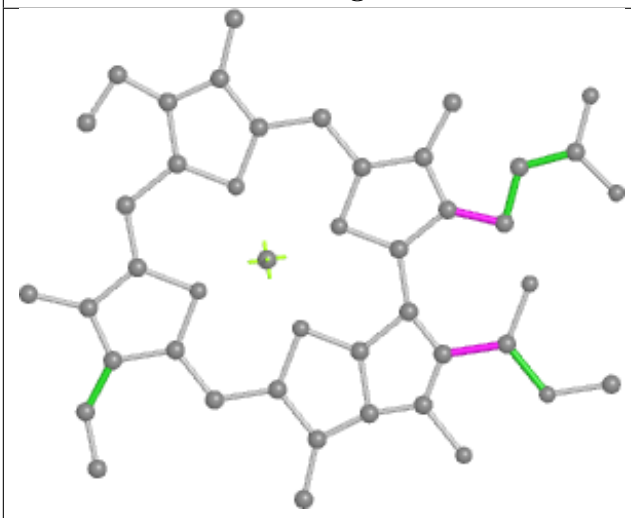


Bond angles



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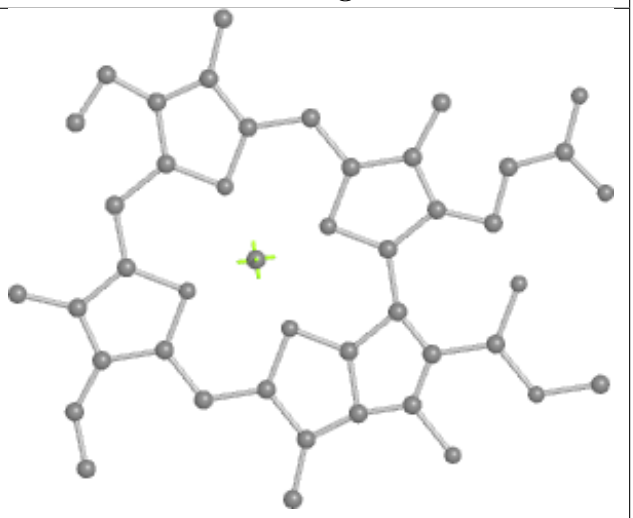
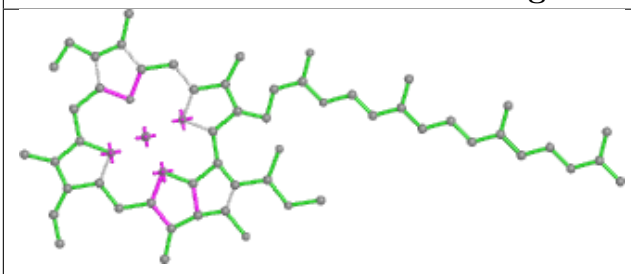


Rings

Ligand CLA 4 609



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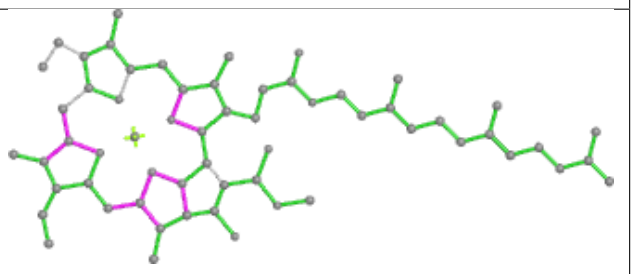

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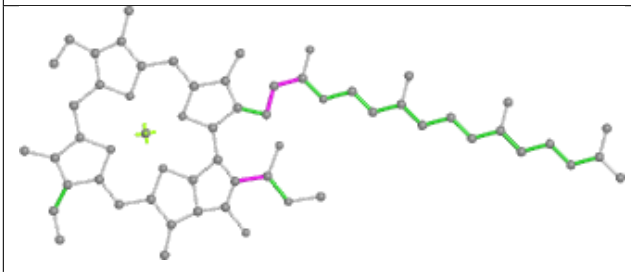

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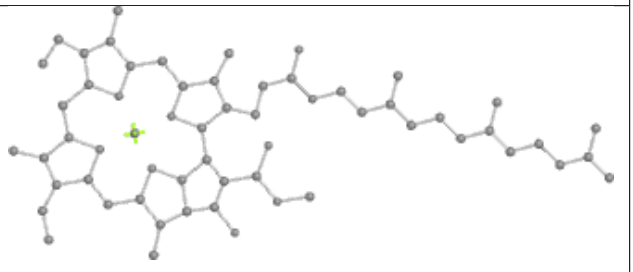
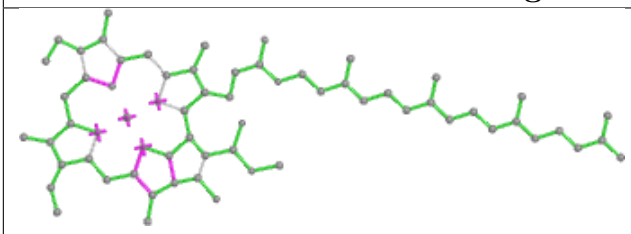
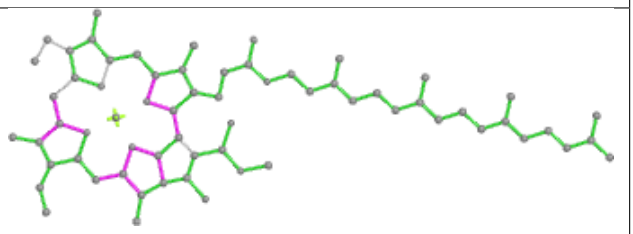
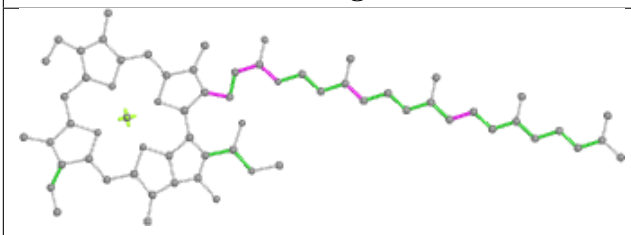
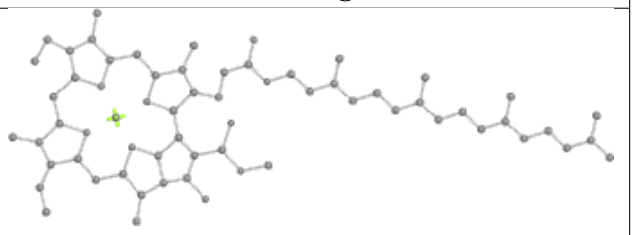
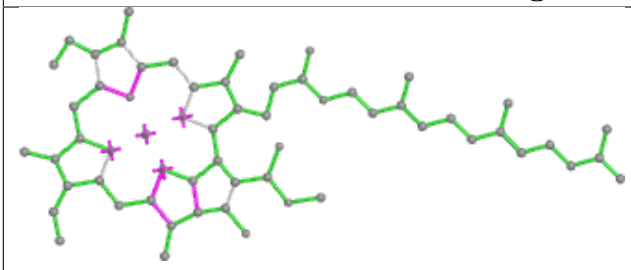
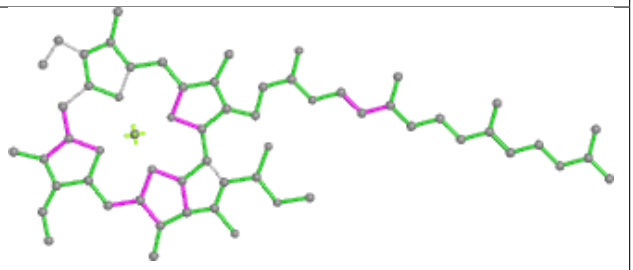
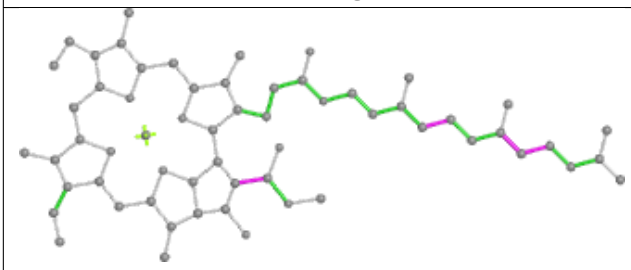
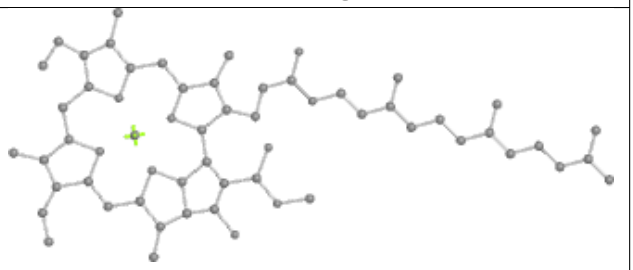
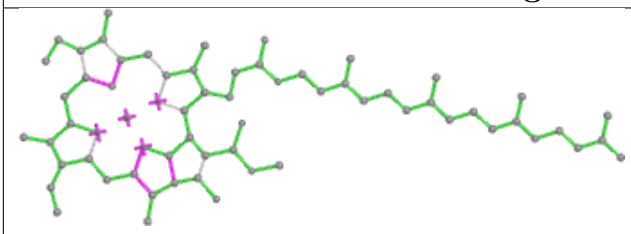


Rings

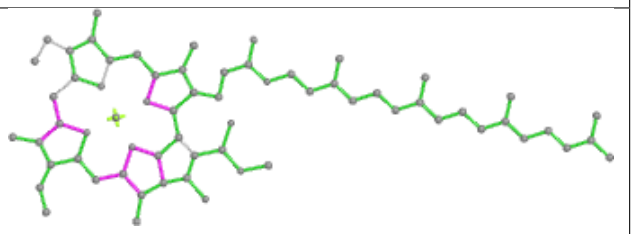
Ligand CLA B 809	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA 6 608	
 Bond lengths	 Bond angles
 Torsions	 Rings

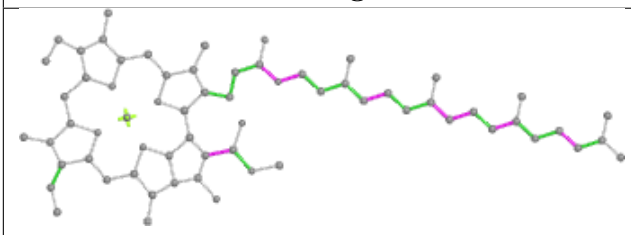
Ligand CLA A 823



Bond lengths



Bond angles



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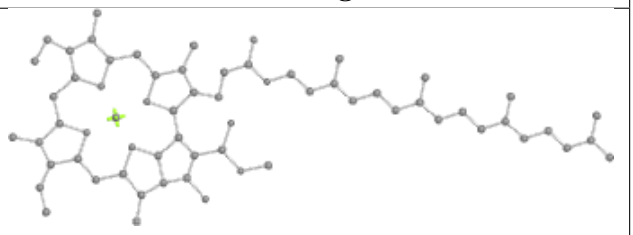
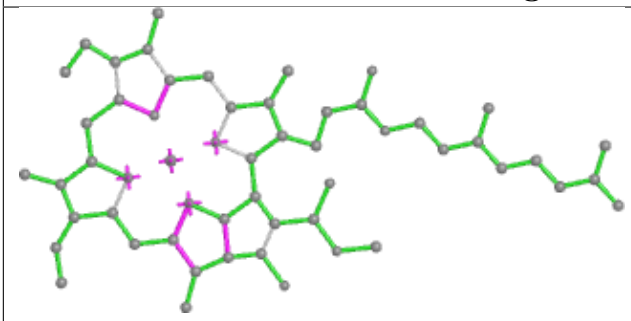
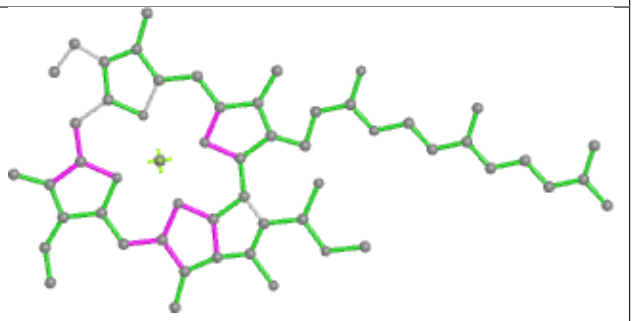


Rings

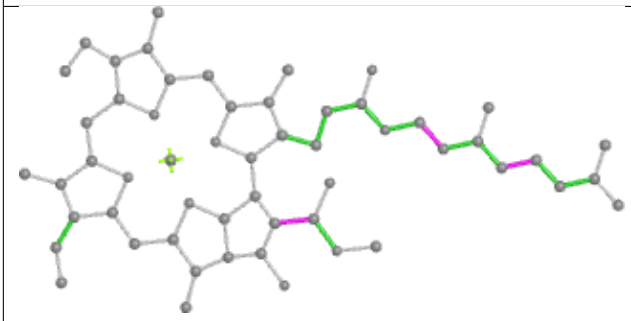
Ligand CLA K 102



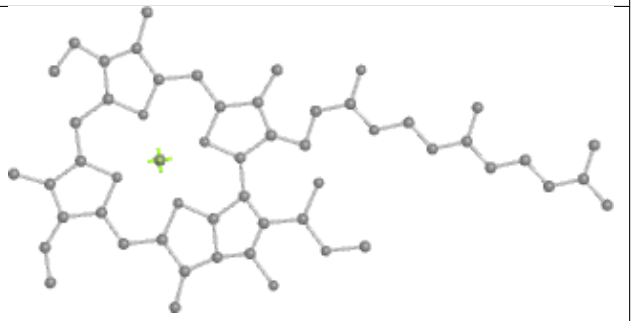
Bond lengths



Bond angles

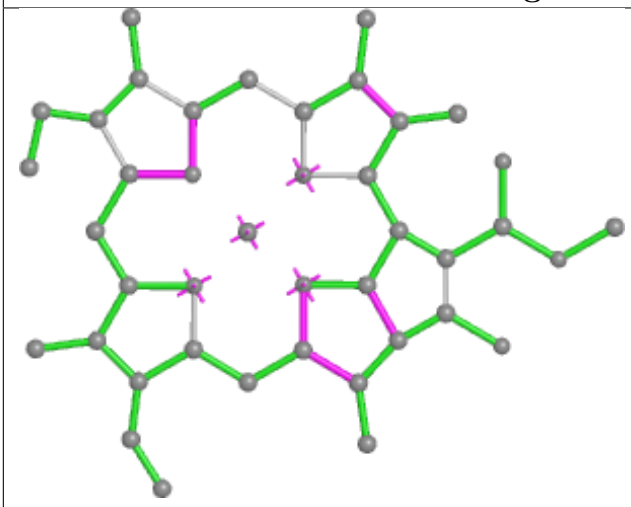


Torsions

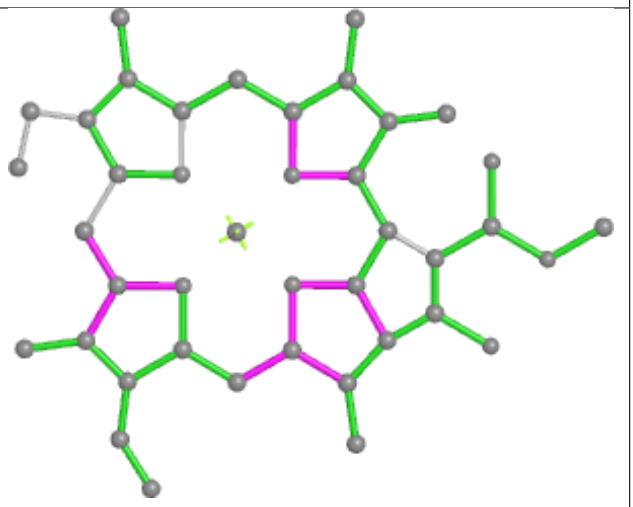


Rings

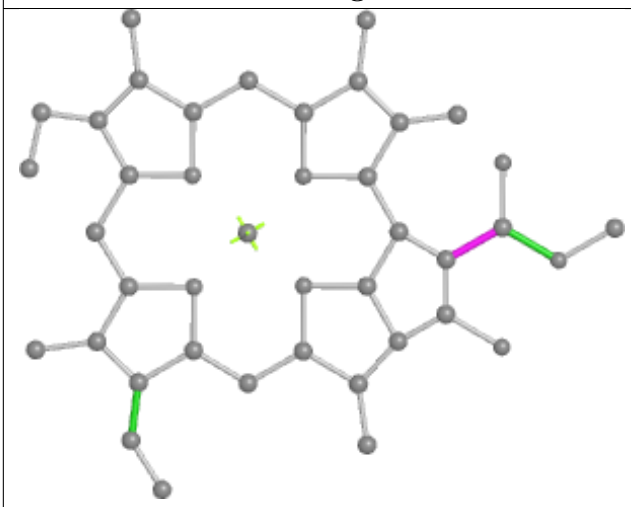
Ligand CLA O 202



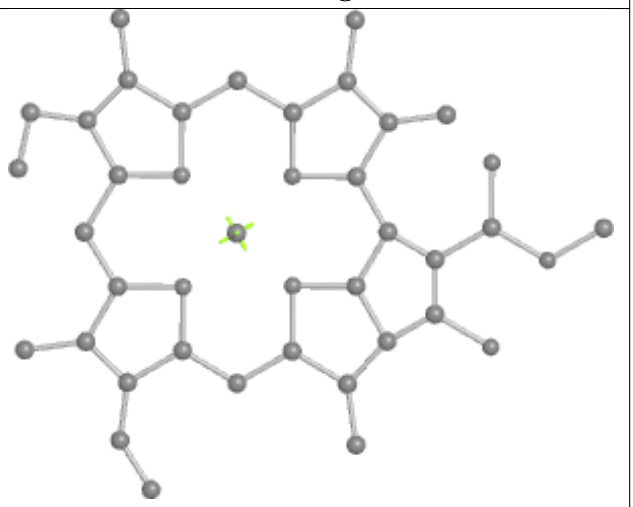
Bond lengths



Bond angles

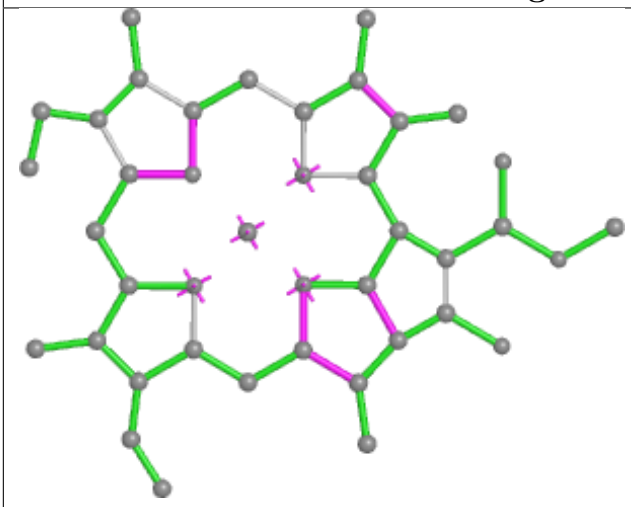


Torsions



Rings

Ligand CLA 9 611



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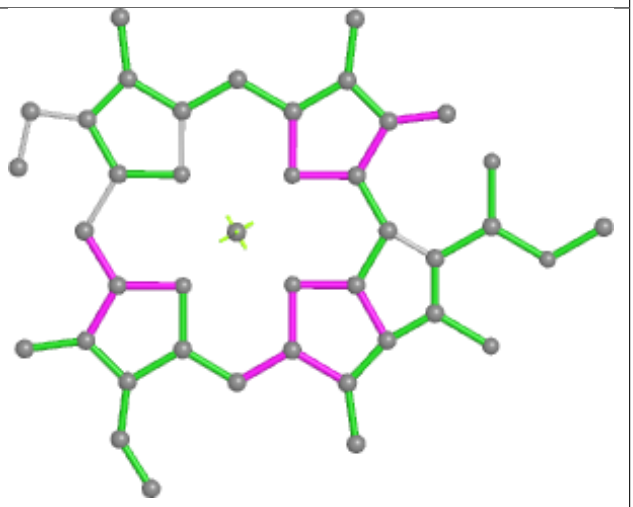
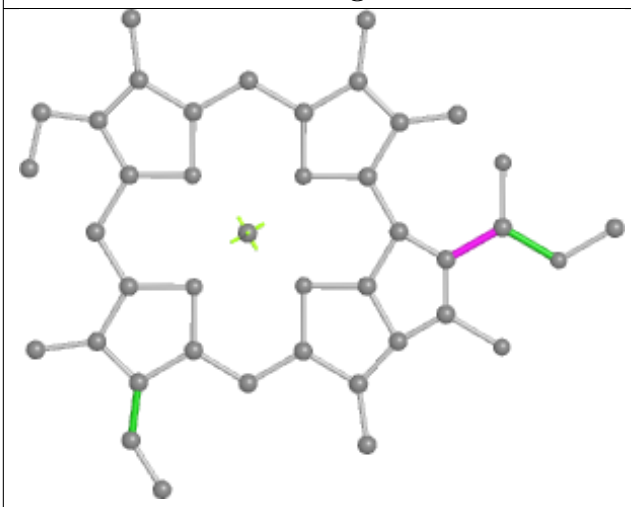
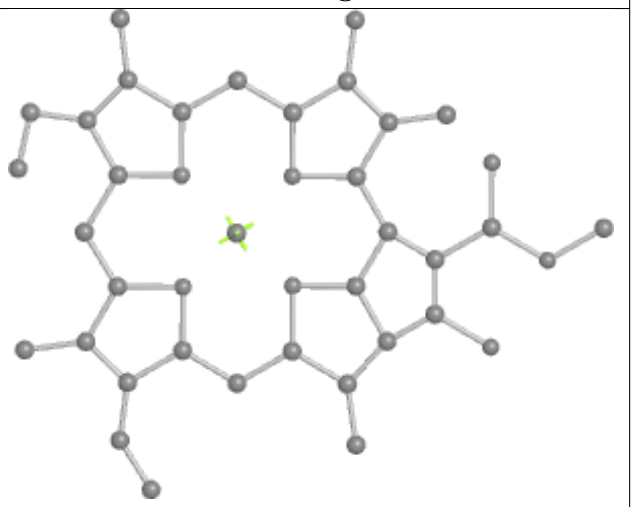


Bond angles

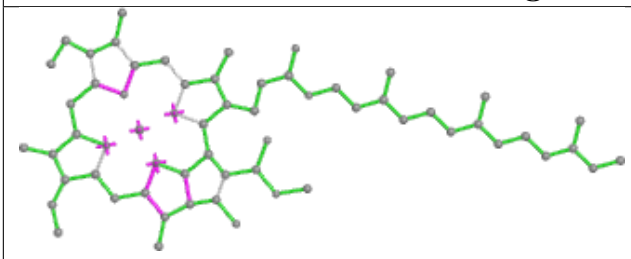


Torsions

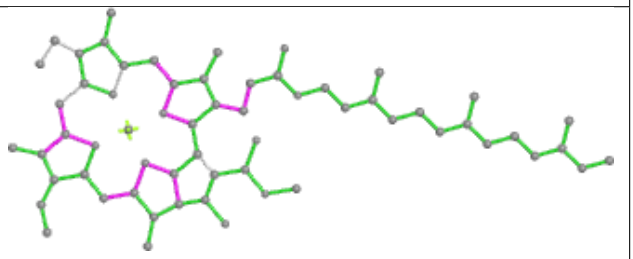


Rings

Ligand CLA B 813



Bond lengths



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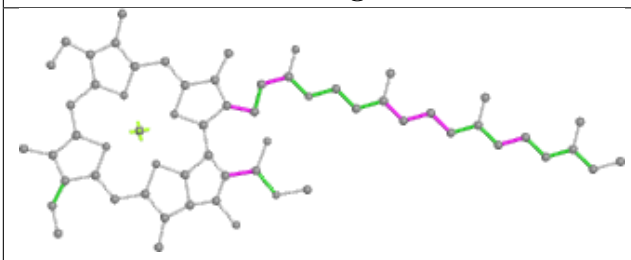

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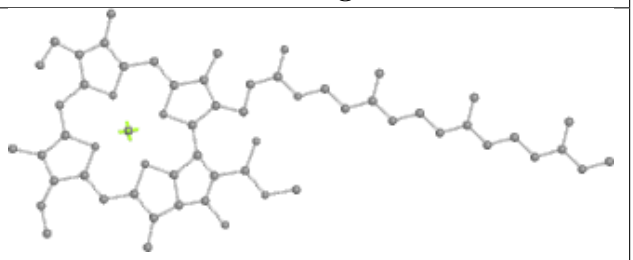
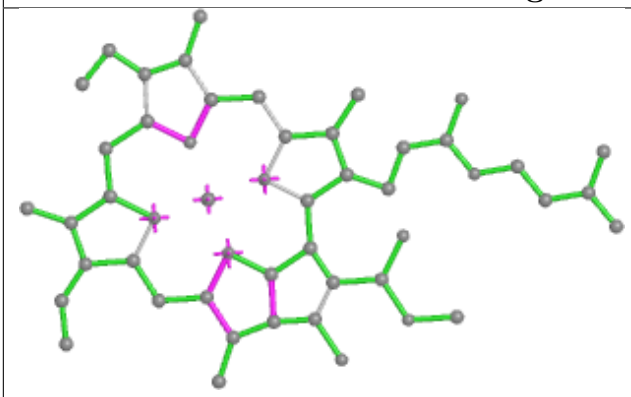
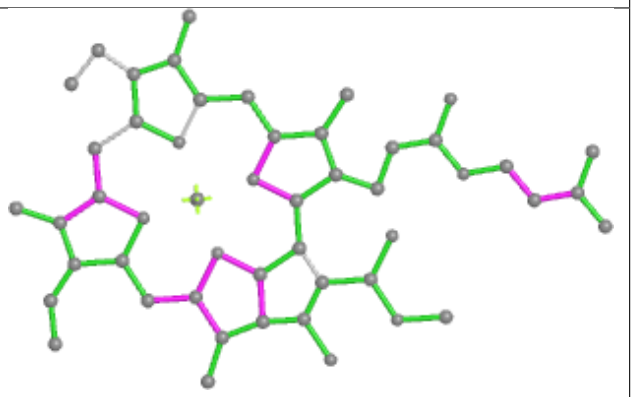


Rings

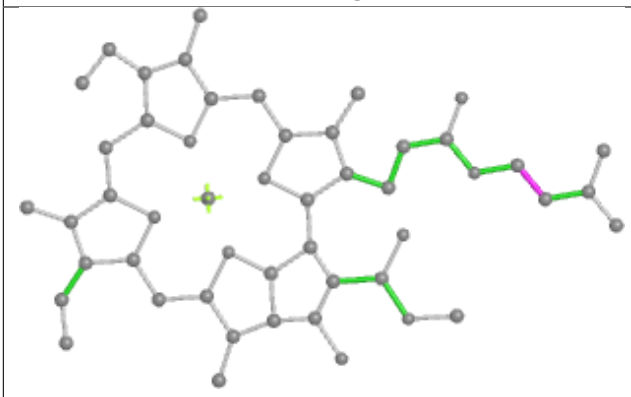
Ligand CLA Z 305



Bond lengths



Bond angles



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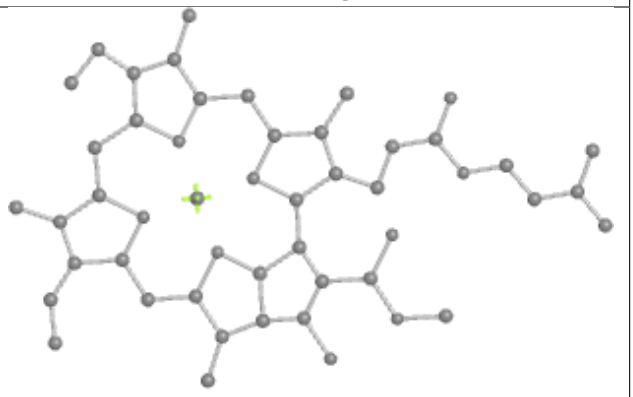
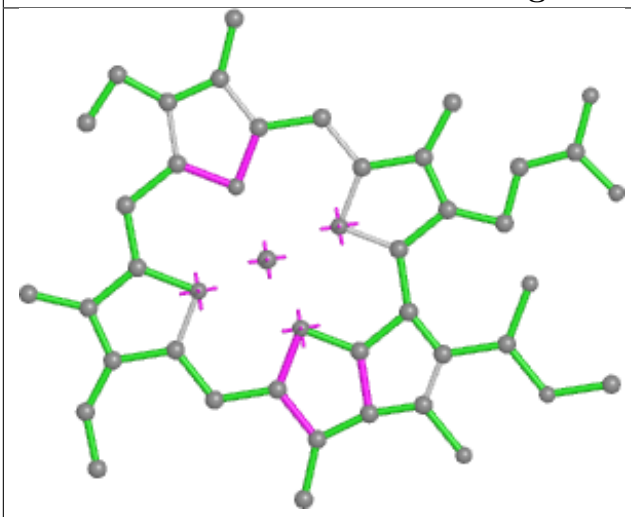
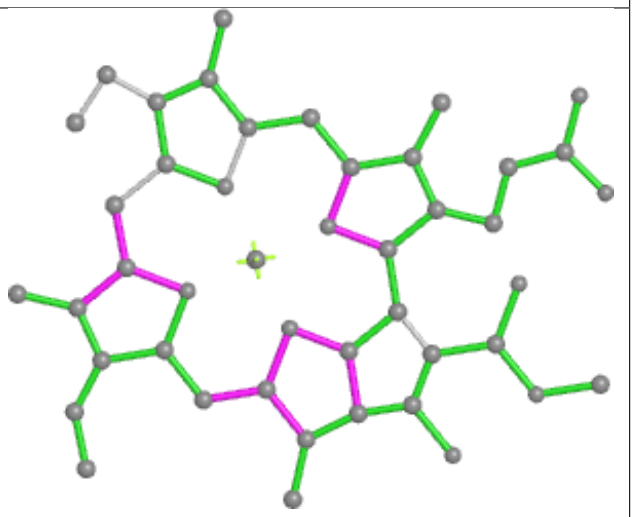


Rings

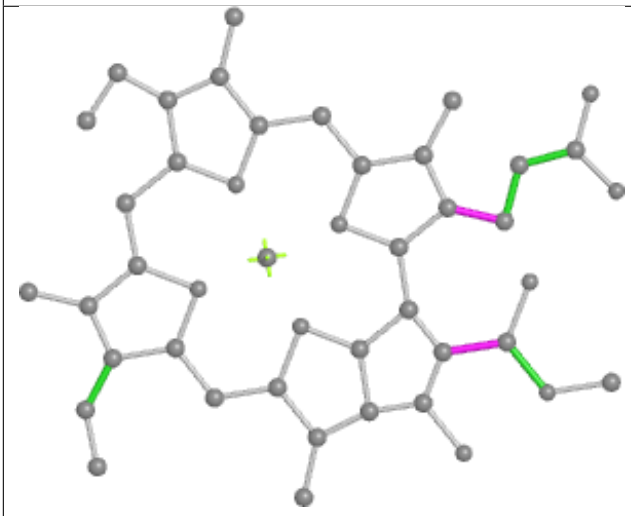
Ligand CLA 2 612



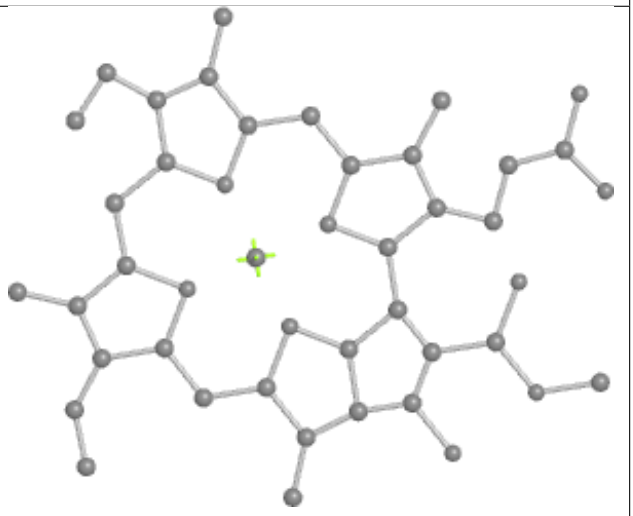
Bond lengths



Bond angles

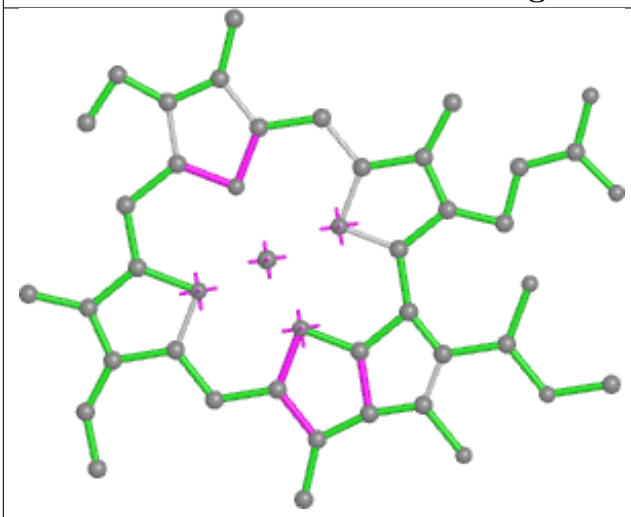


Torsions

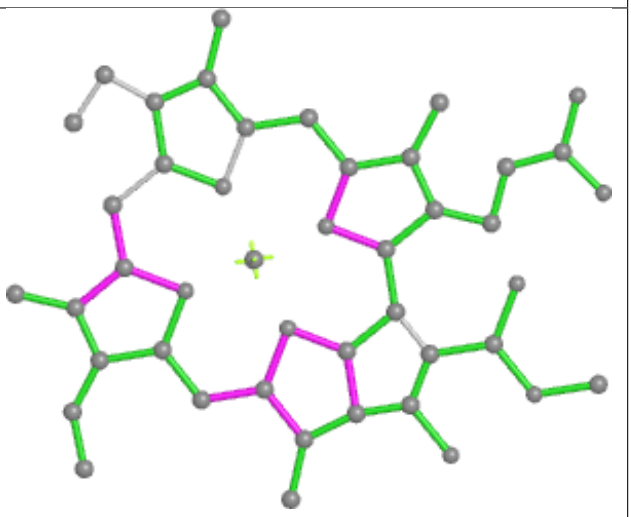


Rings

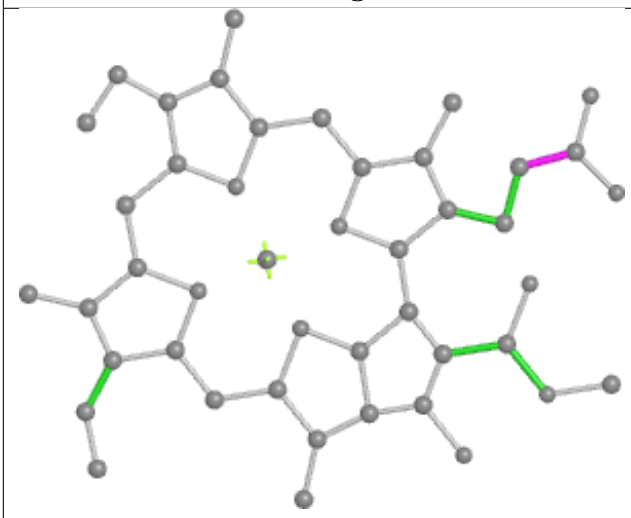
Ligand CLA 7 308



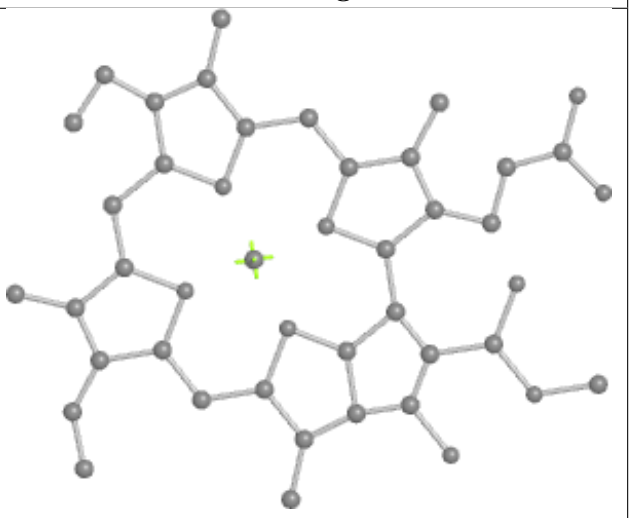
Bond lengths



Bond angles

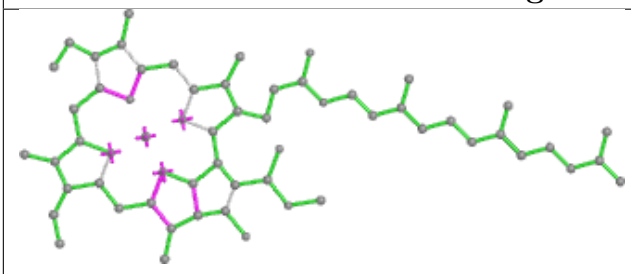


Torsions

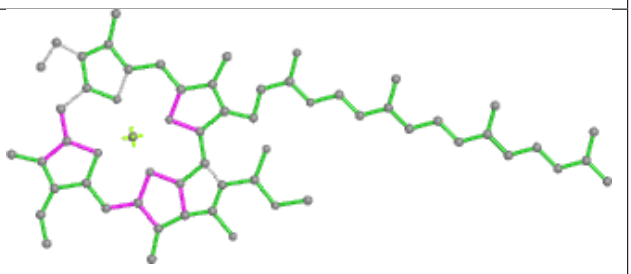


Rings

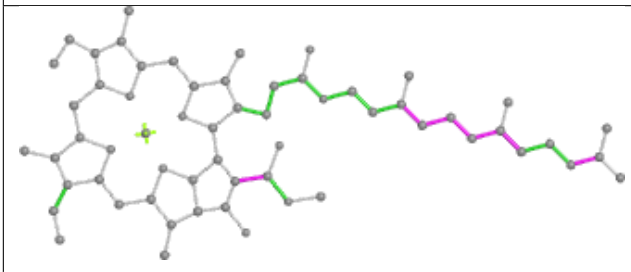
Ligand CLA L 202



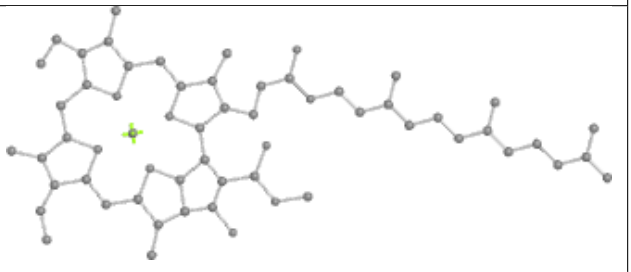
Bond lengths



Bond angles

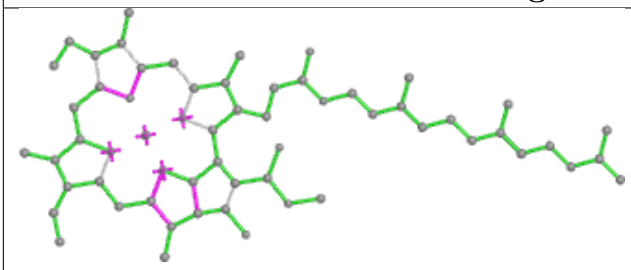


Torsions



Rings

Ligand CLA 3 608



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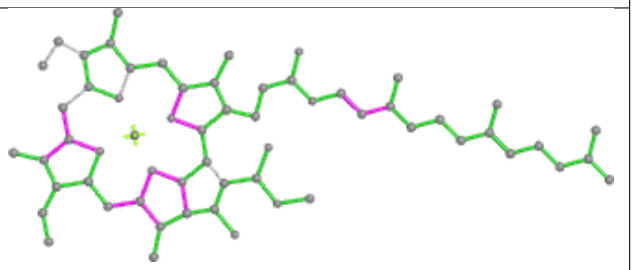

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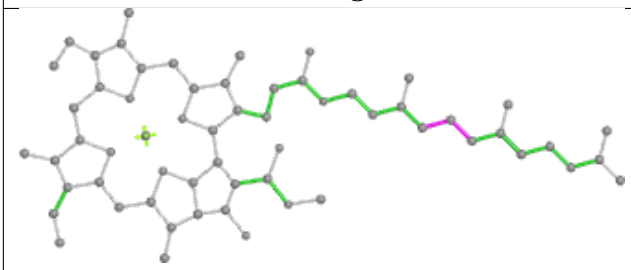

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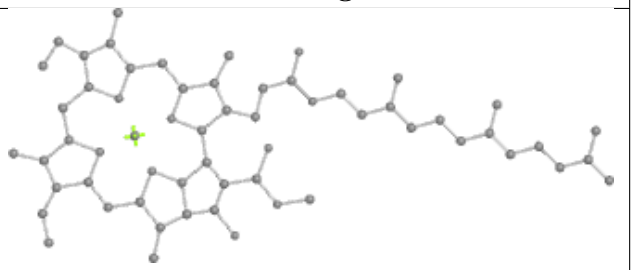
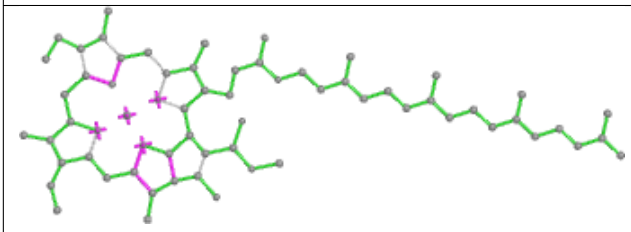


Rings

Ligand CLA A 841



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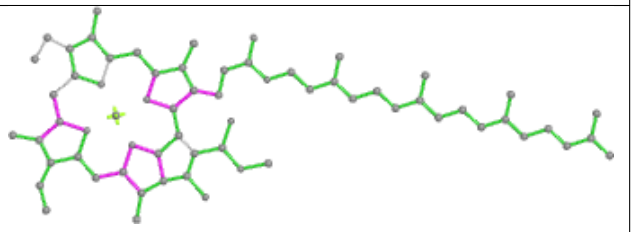

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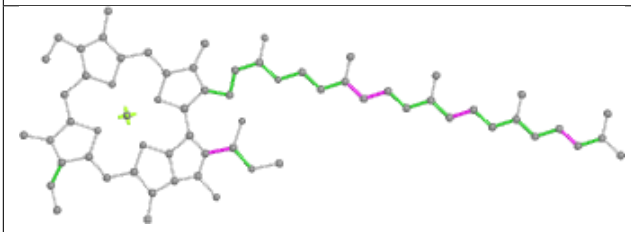

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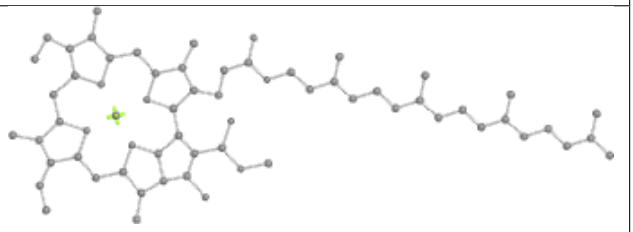
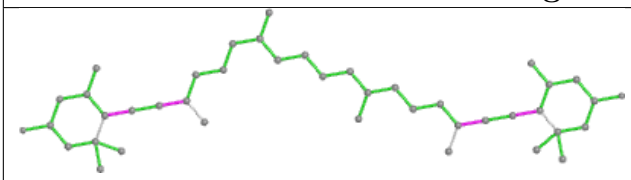


Rings

Ligand II0 a 612



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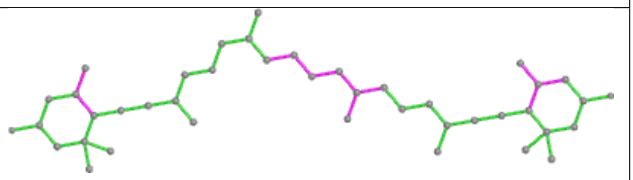
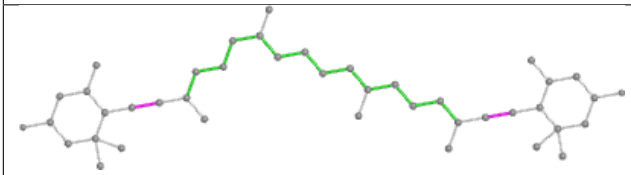


Bond angles



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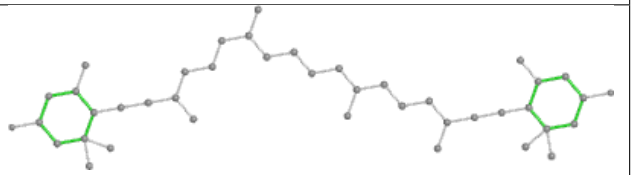
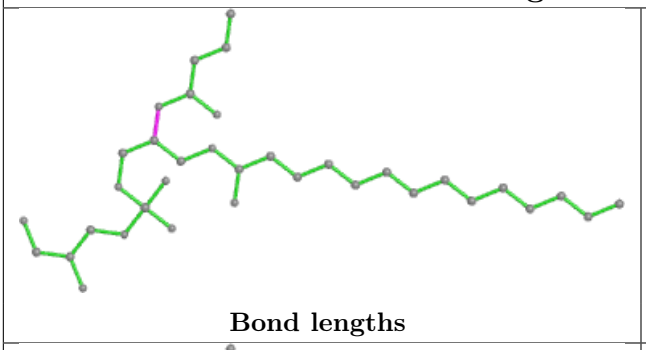


Rings

Ligand LHG 6 617



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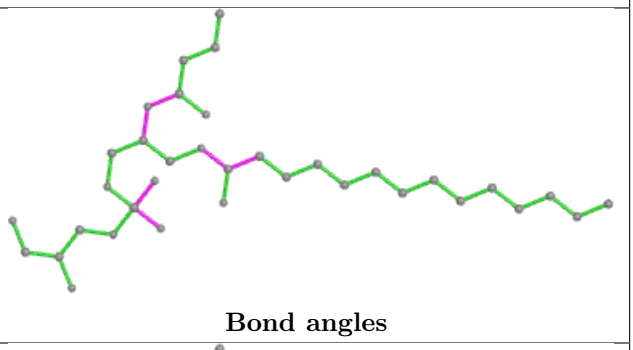

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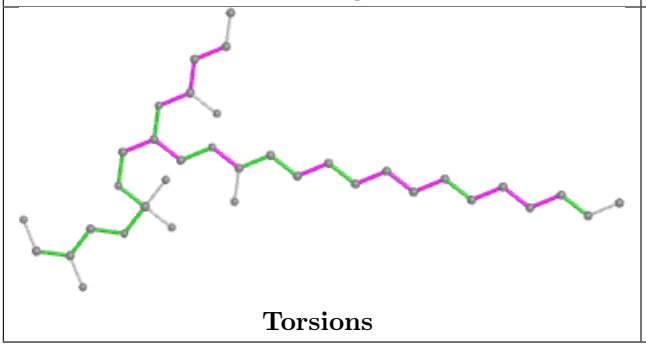

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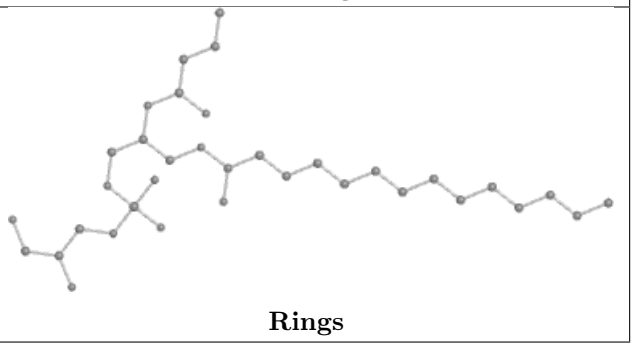
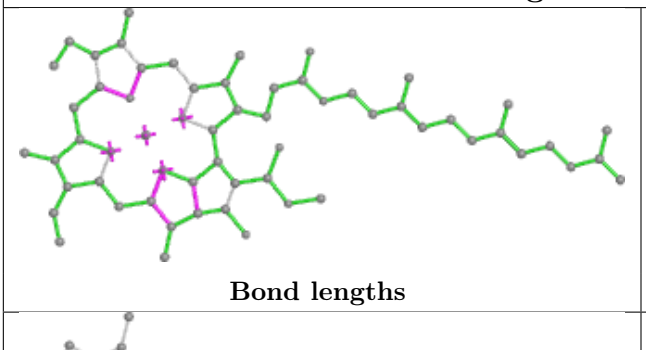


Rings

Ligand CLA Z 306



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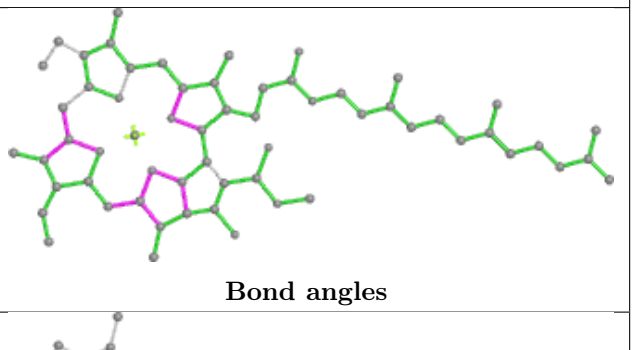

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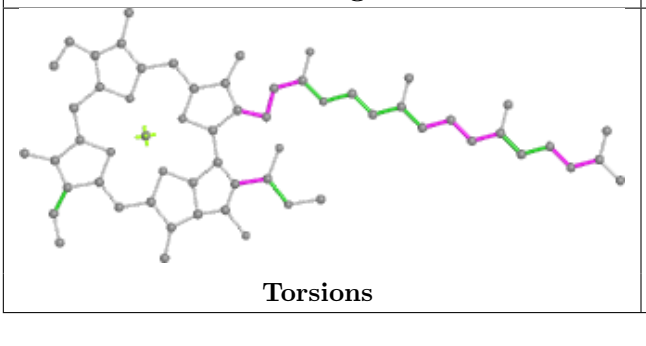

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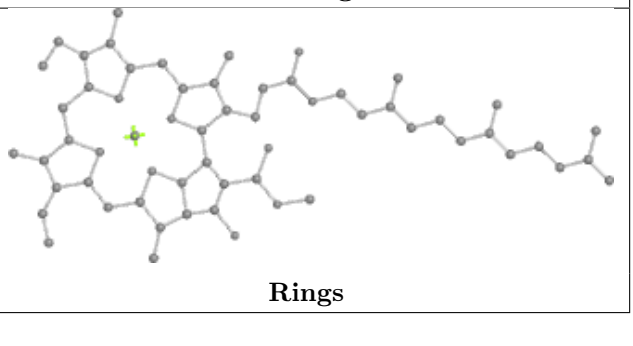
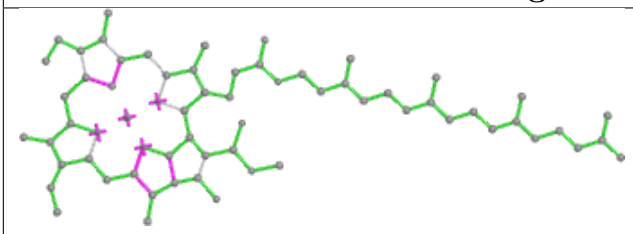


Rings

Ligand CLA 7 303



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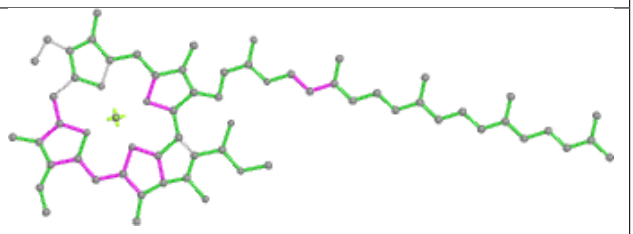

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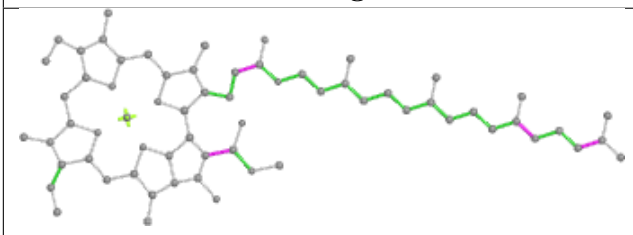

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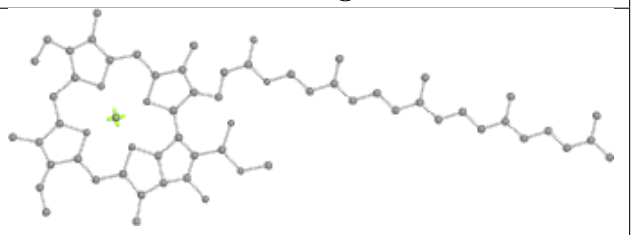
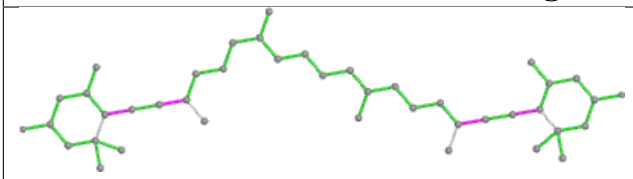


Rings

Ligand II0 9 618



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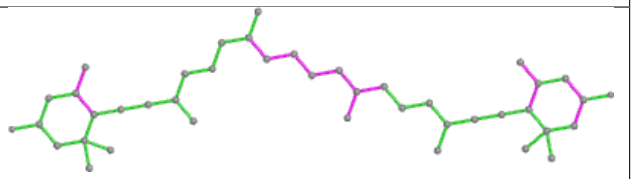

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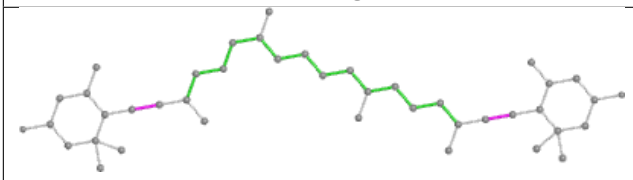

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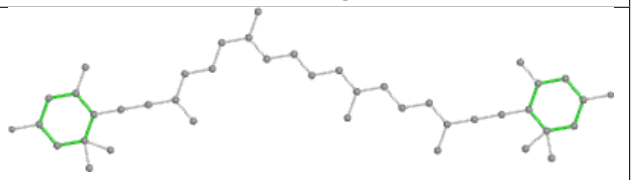
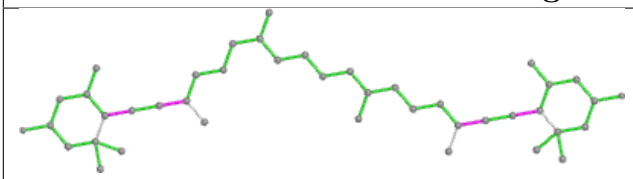


Rings

Ligand II0 1 617



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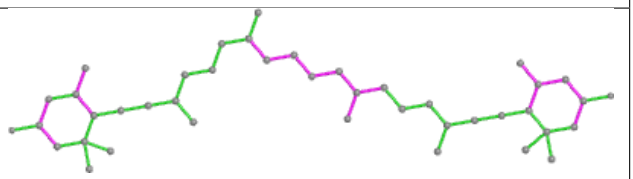

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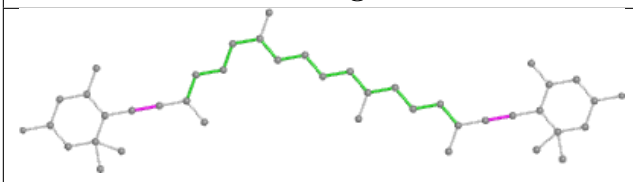

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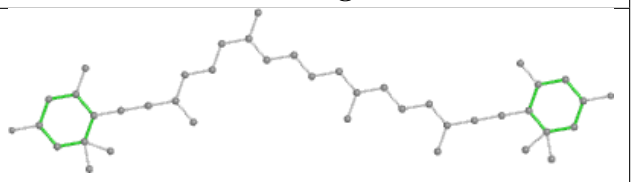
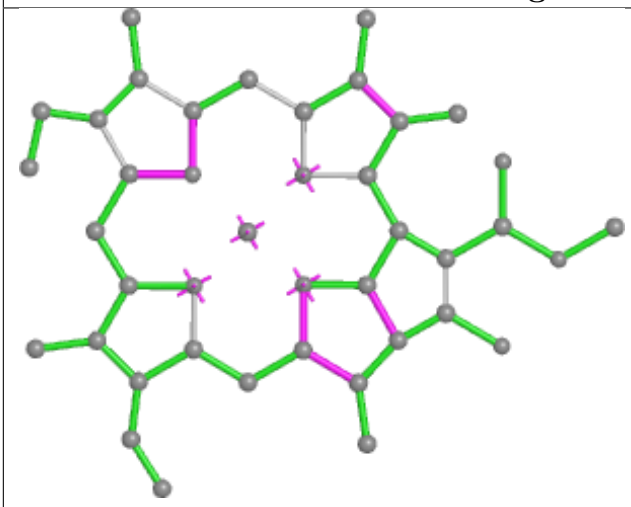


Rings

Ligand CLA 5 601



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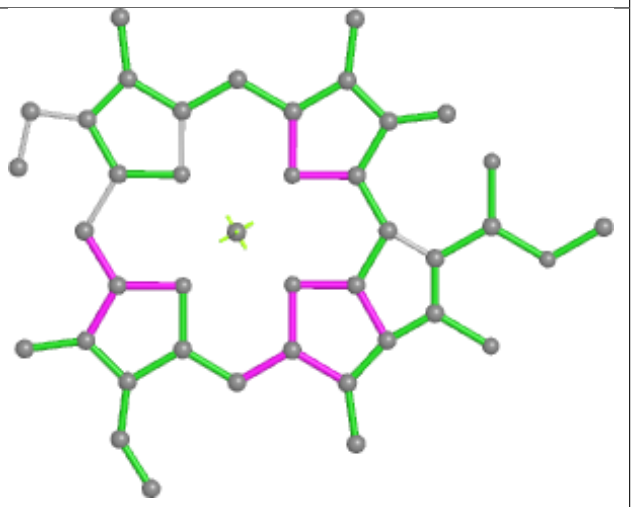
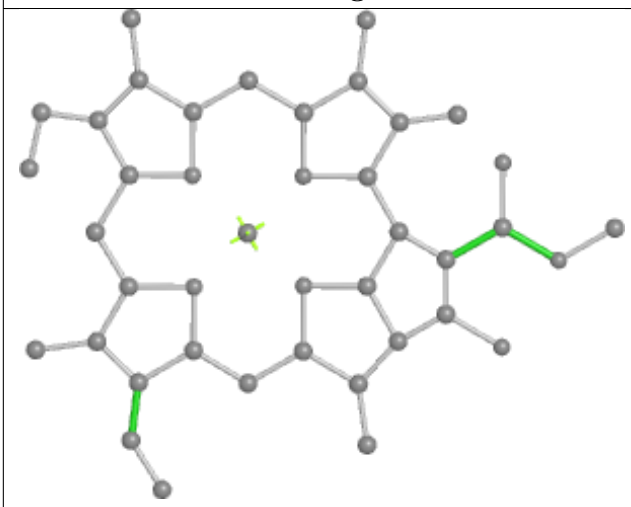


Bond angles



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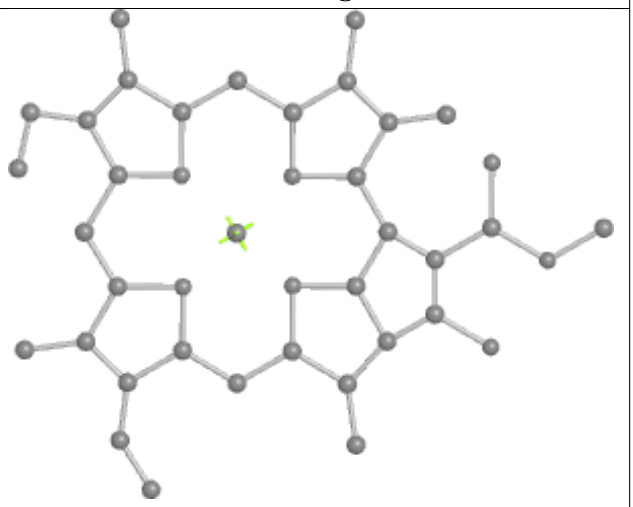
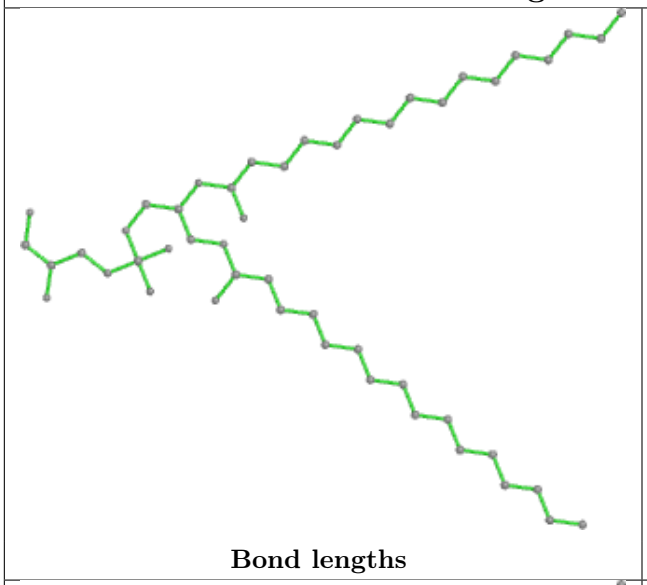


Rings

Ligand LHG 3 619



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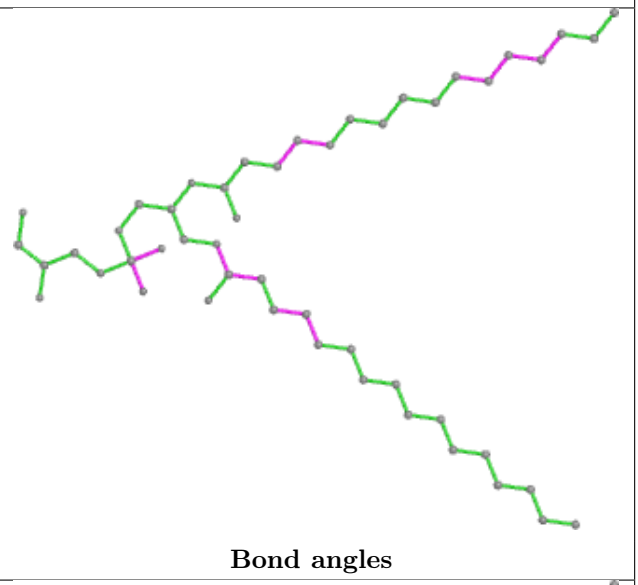
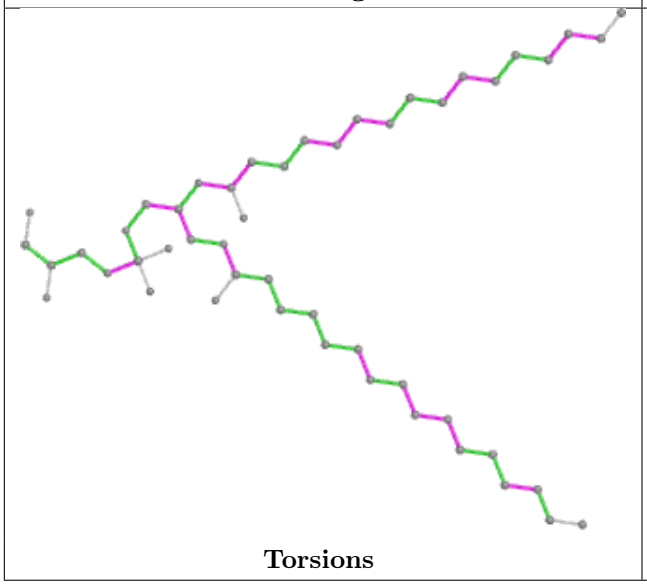


Bond angles



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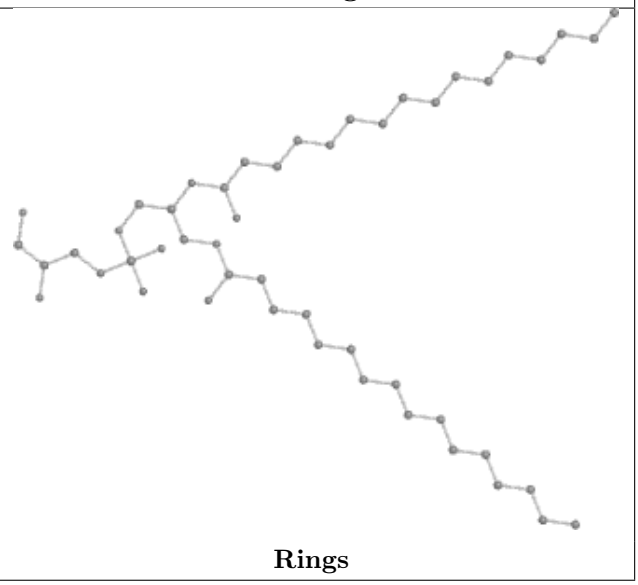
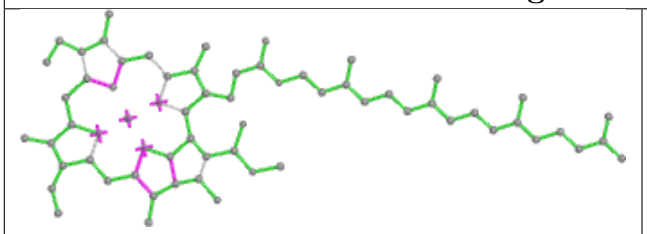


Rings

Ligand CLA Z 310



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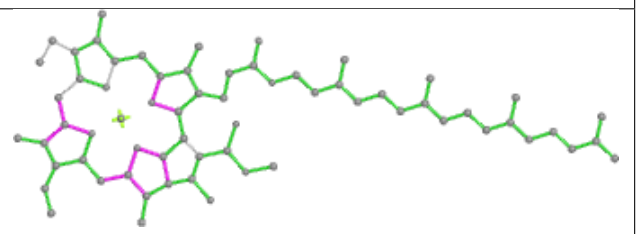
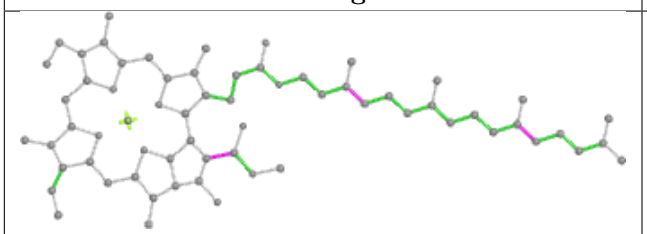


Bond angles



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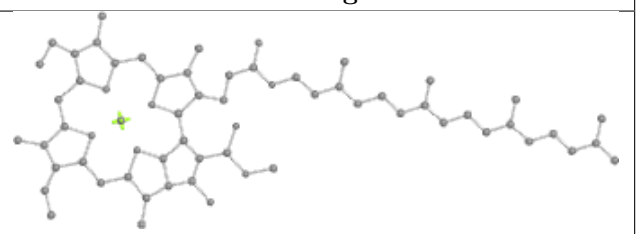
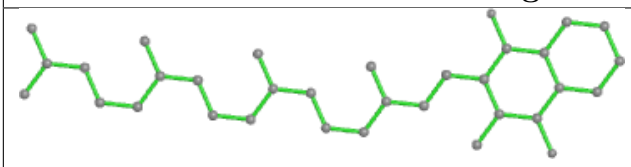
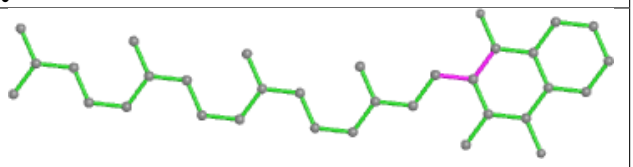


Rings

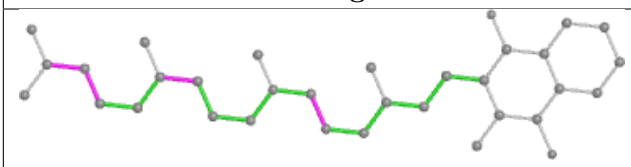
Ligand PQN B 842



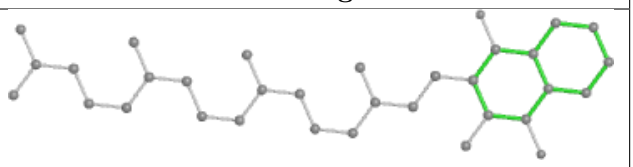
Bond lengths



Bond angles

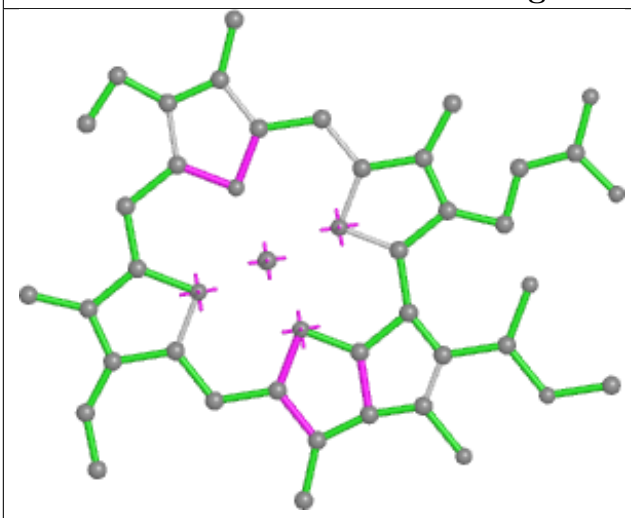


Torsions

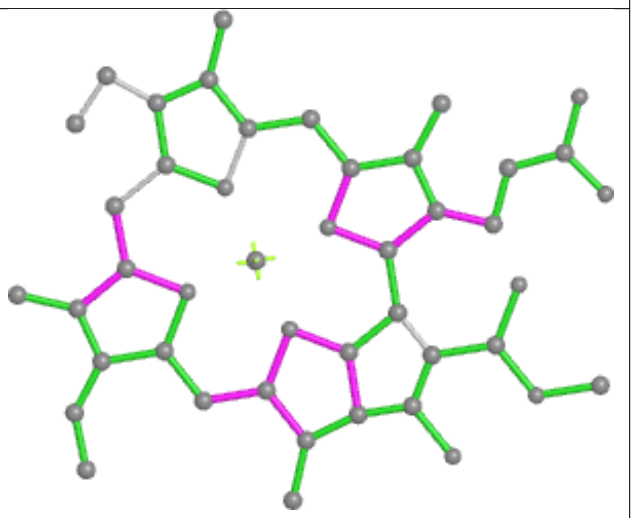


Rings

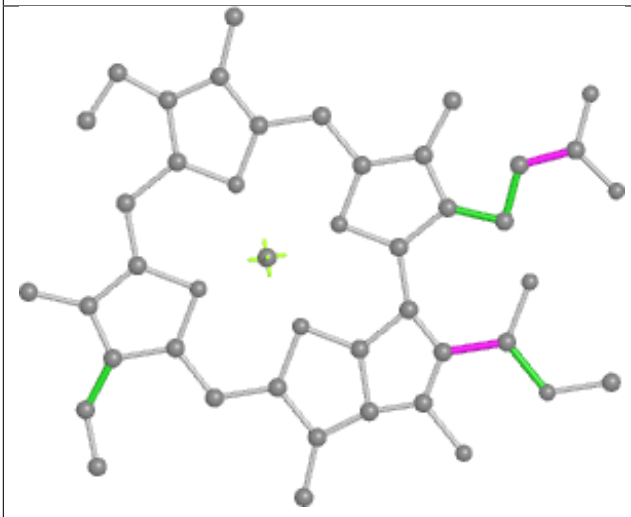
Ligand CLA 5 603



Bond lengths



Bond angles



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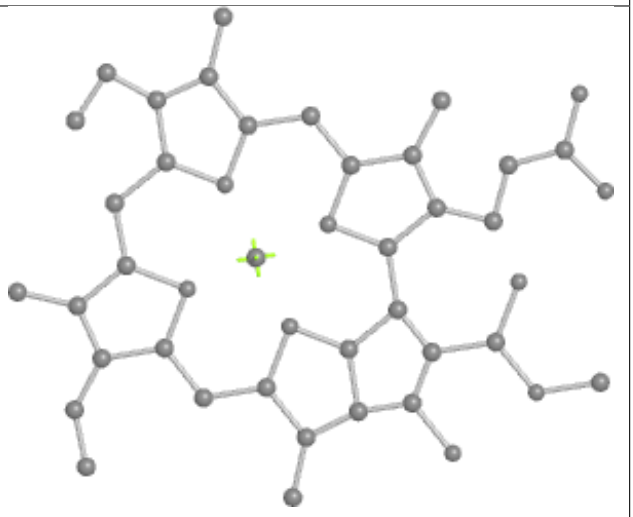
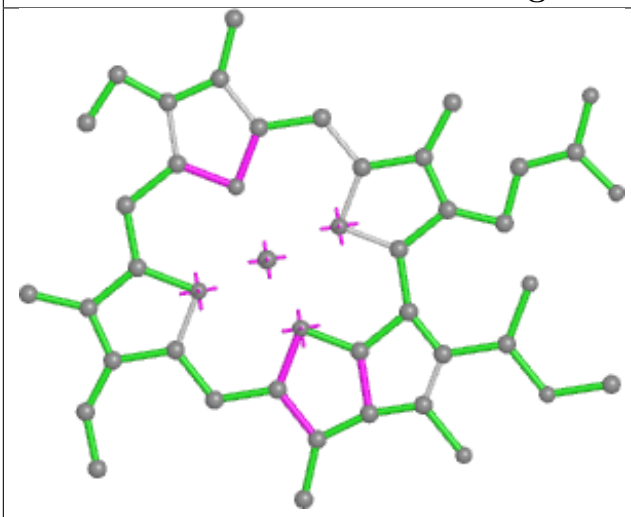
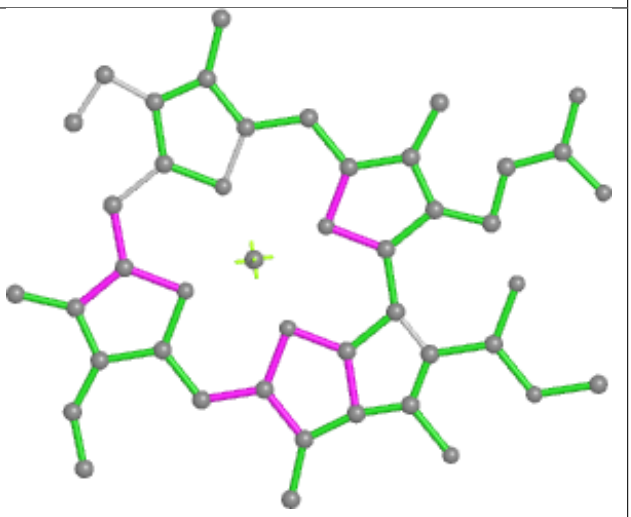


Rings

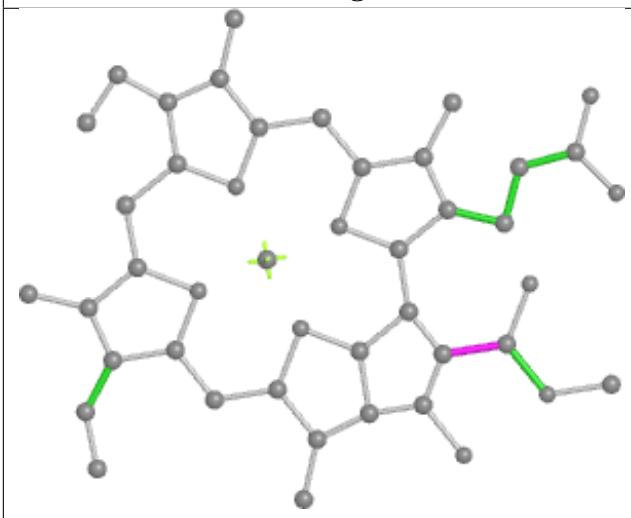
Ligand CLA 3 612



Bond lengths



Bond angles



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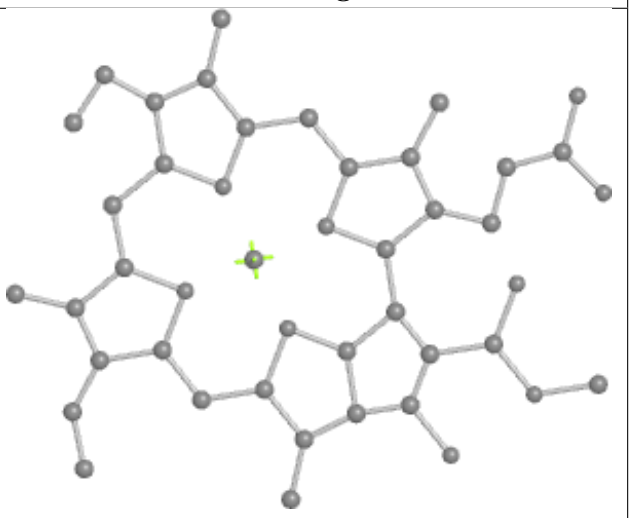
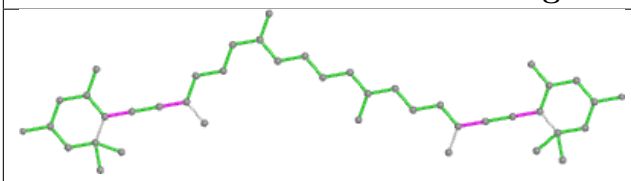
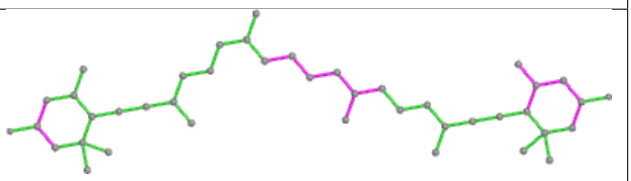


Rings

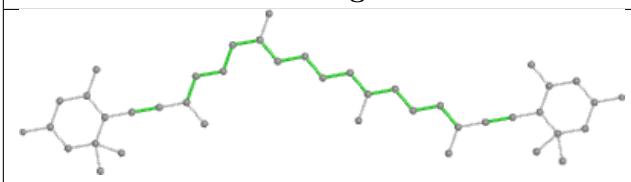
Ligand II0 2 614



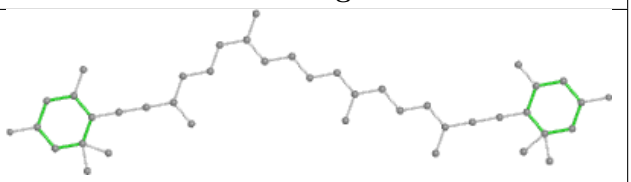
Bond lengths



Bond angles

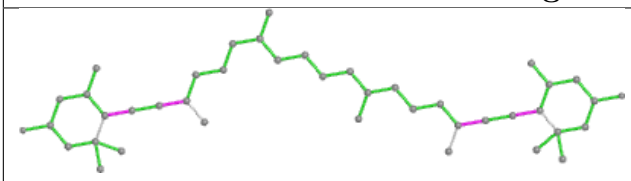


Torsions



Rings

Ligand II0 7 301



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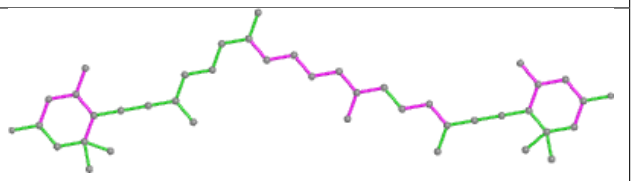

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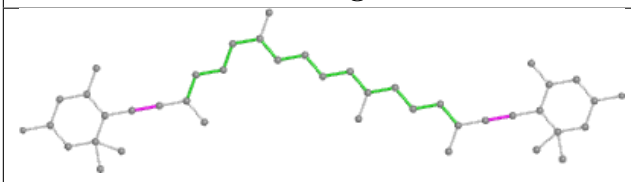

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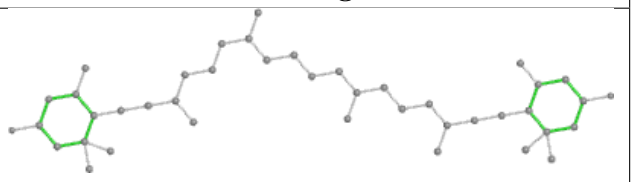
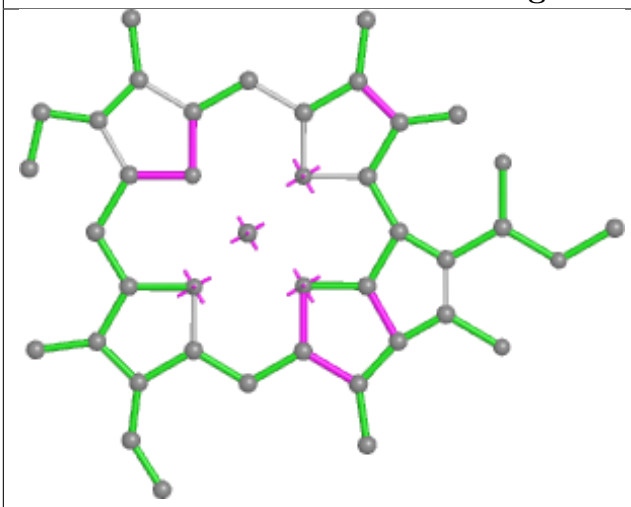


Rings

Ligand CLA 2 609



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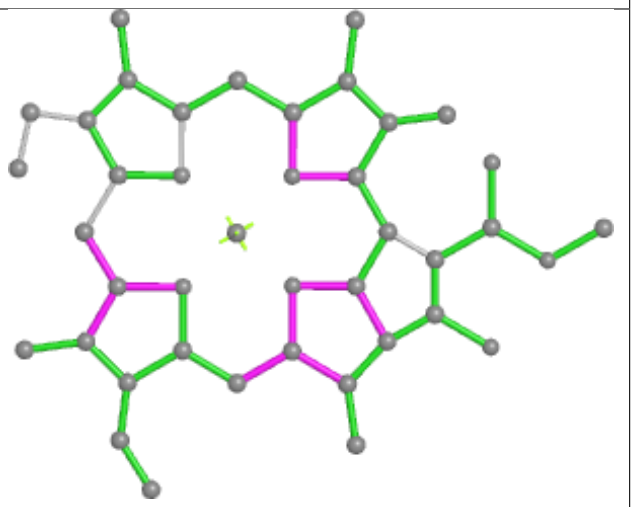

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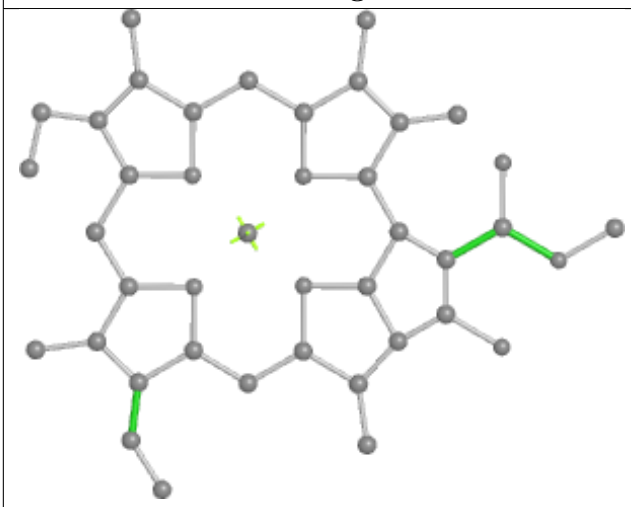

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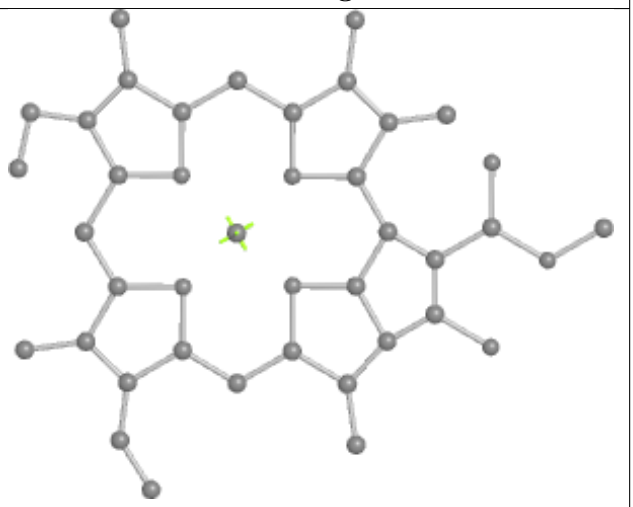
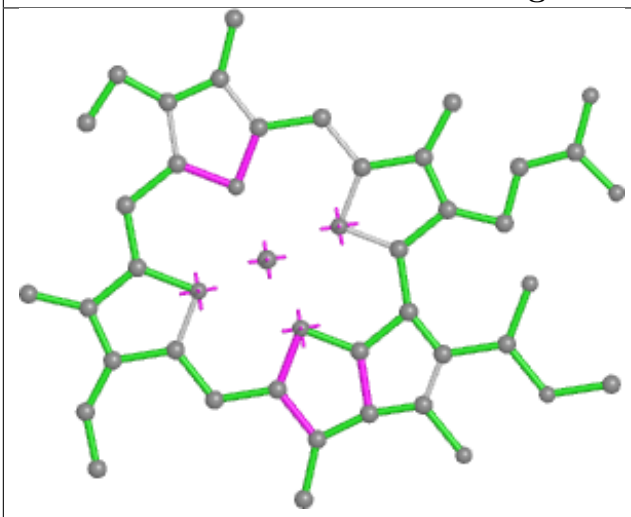


Rings

Ligand CLA 5 612



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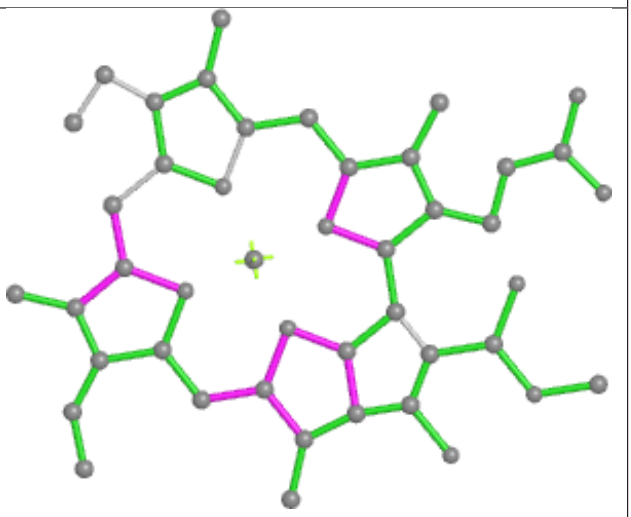

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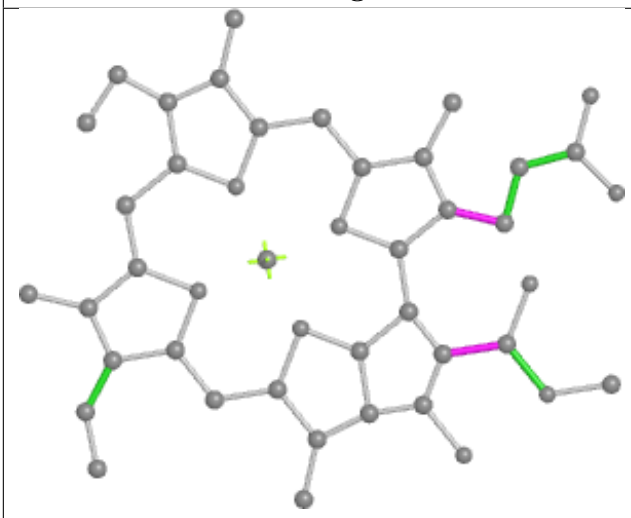

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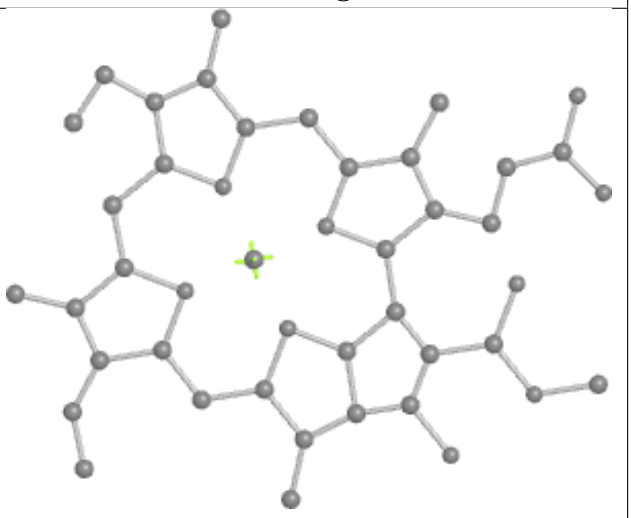
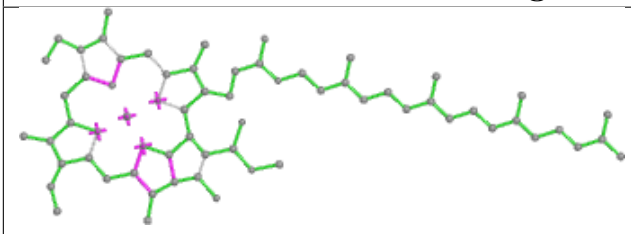


Rings

Ligand CLA 8 608



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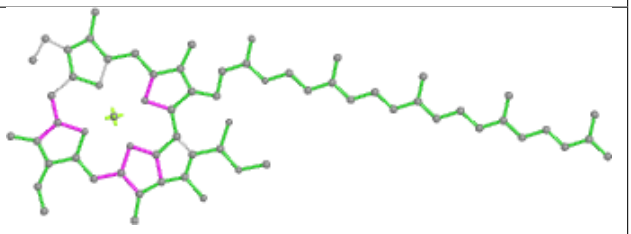
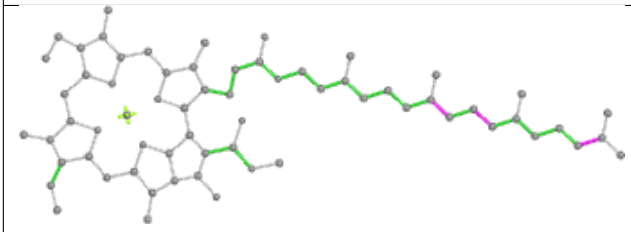


Bond angles



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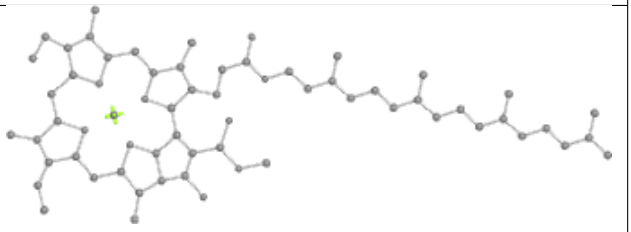
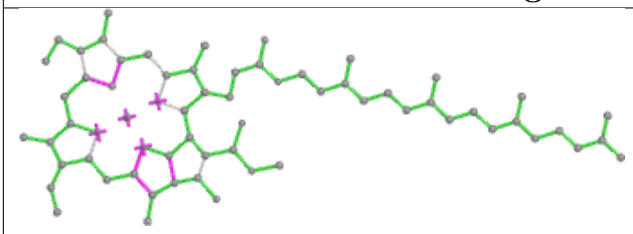
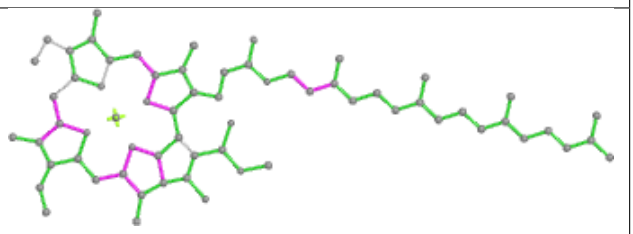


Rings

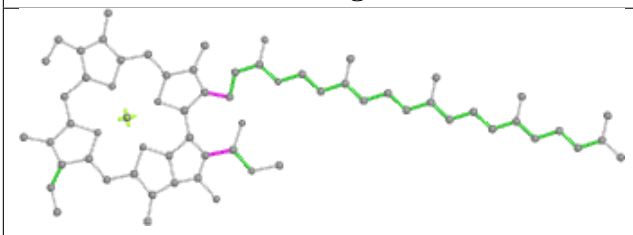
Ligand CLA B 825



Bond lengths



Bond angles



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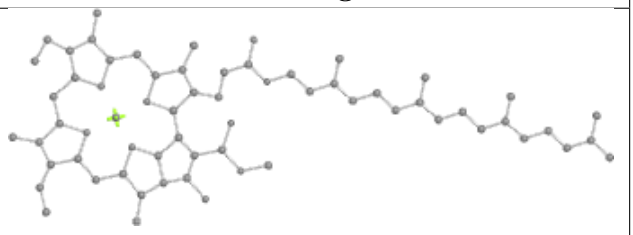
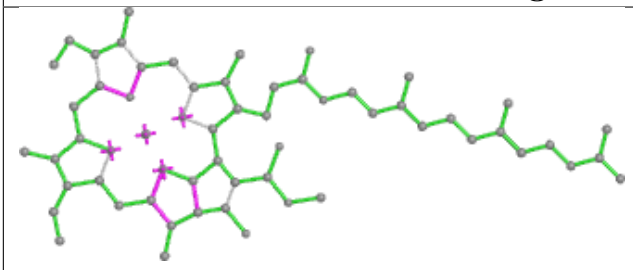


Rings

Ligand CLA a 607



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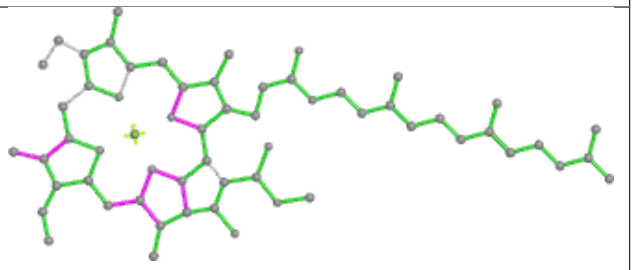
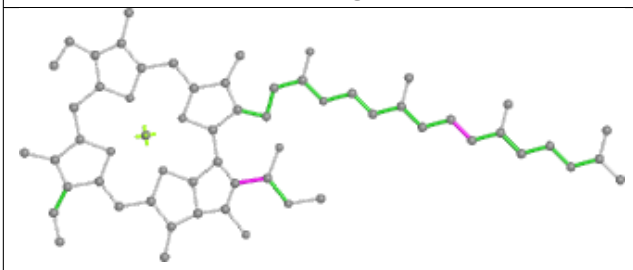


Bond angles



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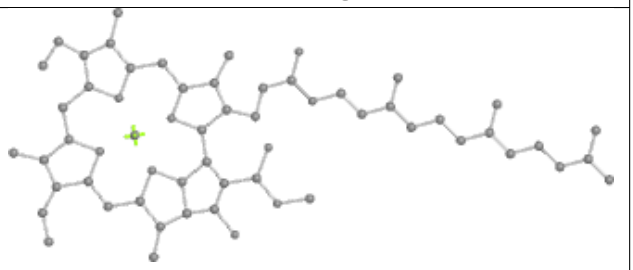
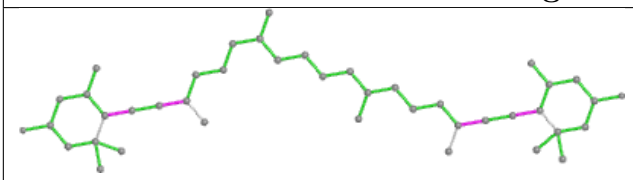


Rings

Ligand II0 9 616



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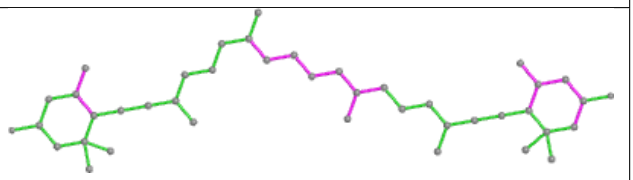
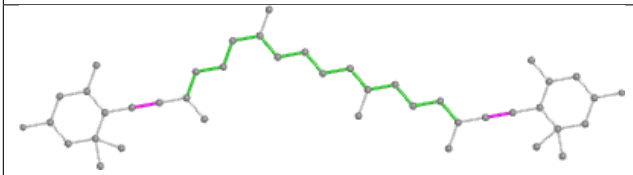
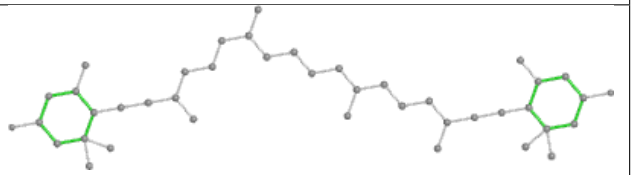


Bond angles

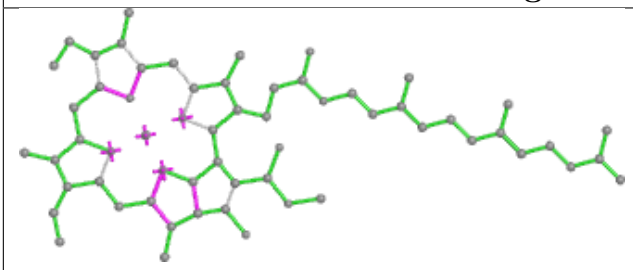


Torsions

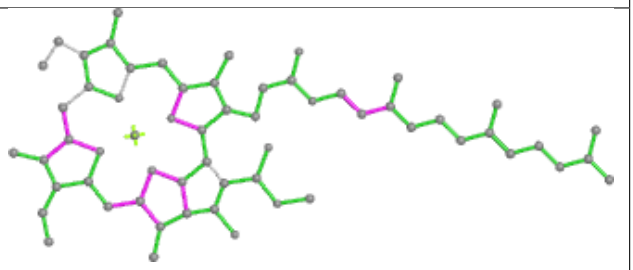


Rings

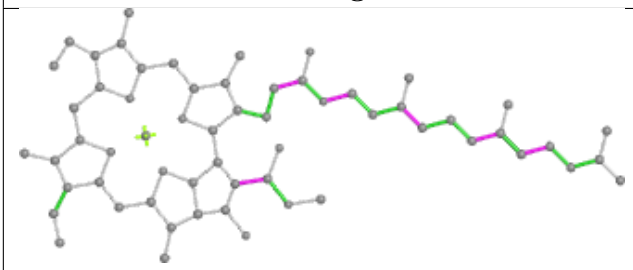
Ligand CLA B 821



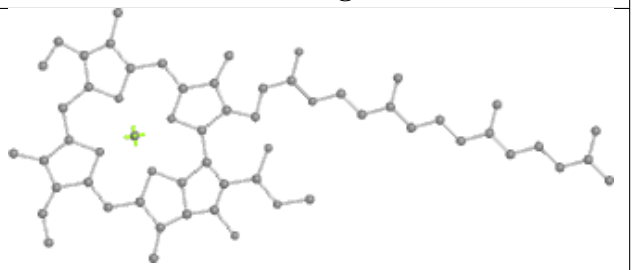
Bond lengths



Bond angles

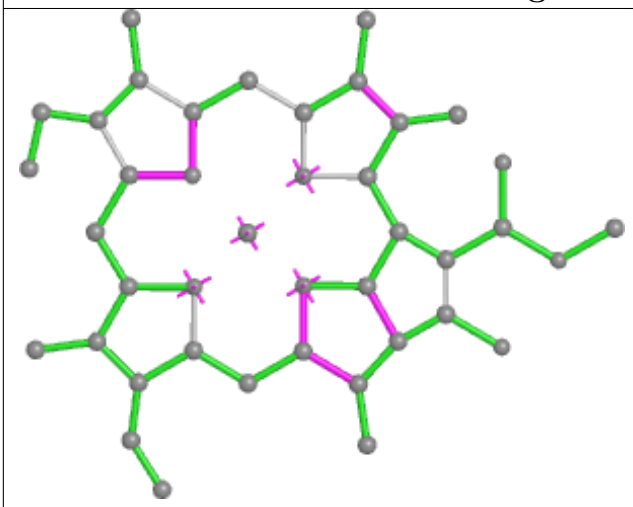


Torsions

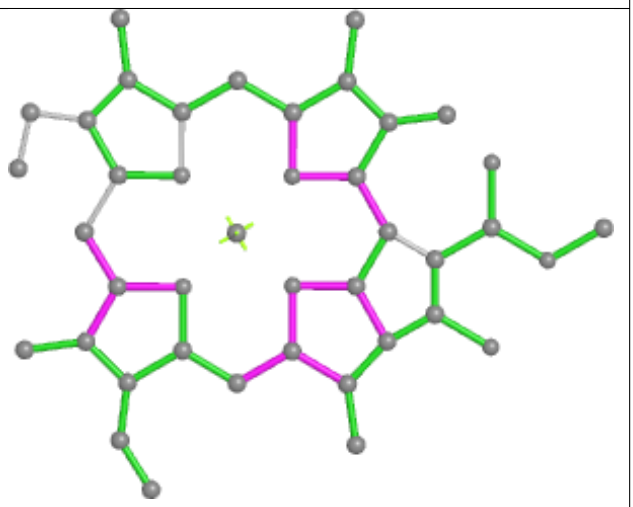


Rings

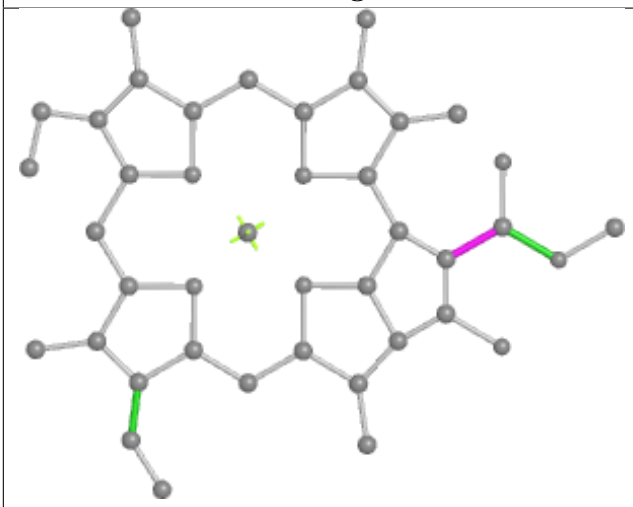
Ligand CLA 9 614



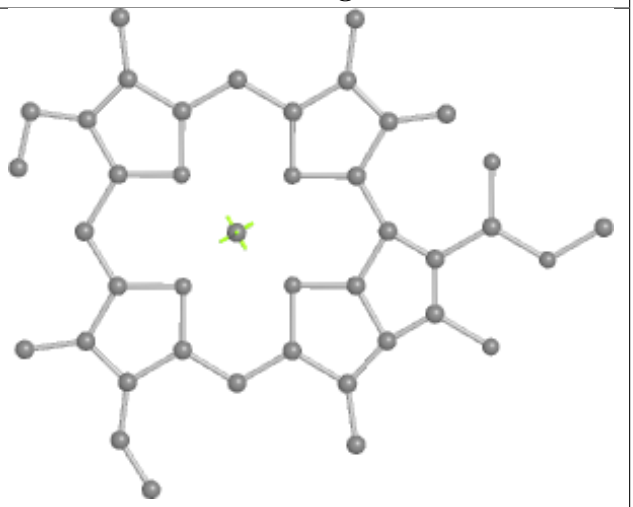
Bond lengths



Bond angles

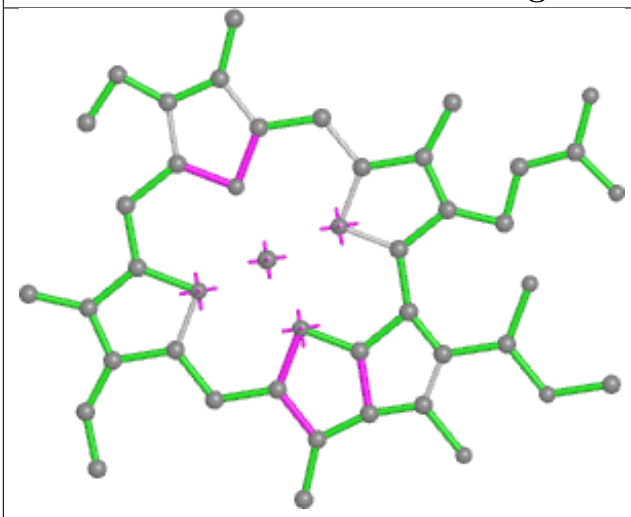


Torsions

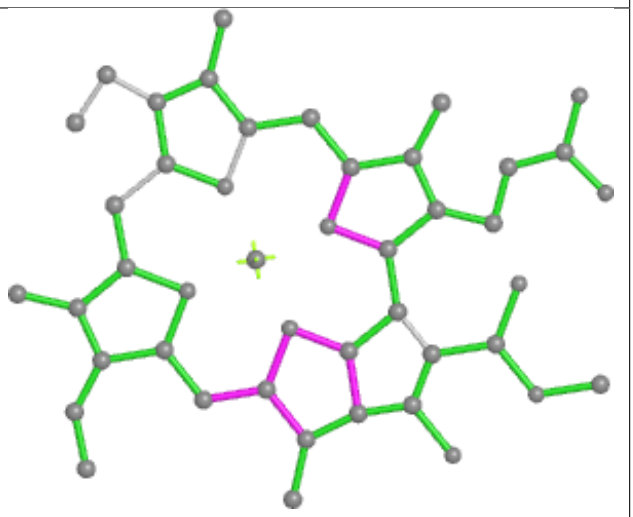


Rings

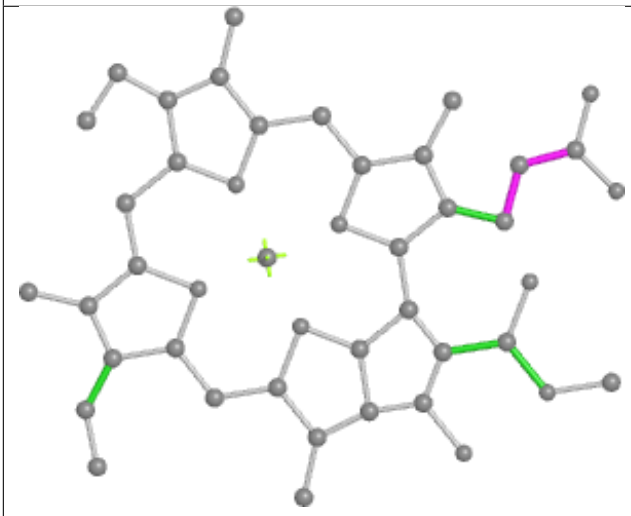
Ligand CLA 8 602



Bond lengths



Bond angles



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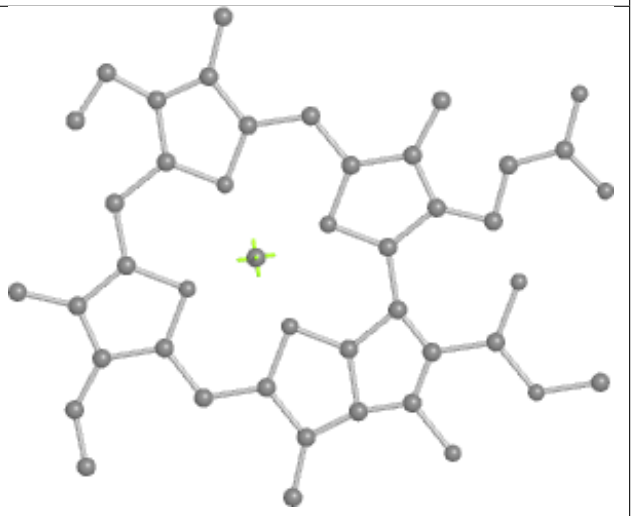
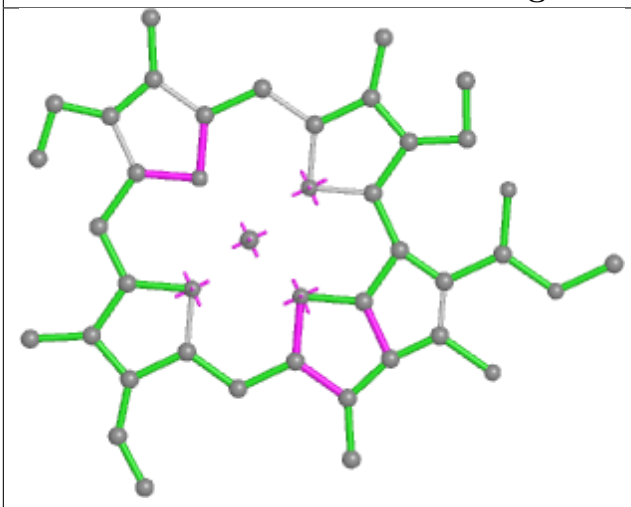


Rings

Ligand CLA 2 601



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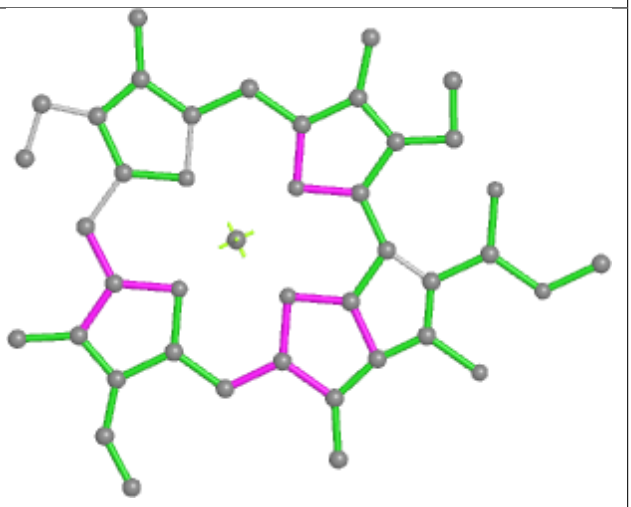
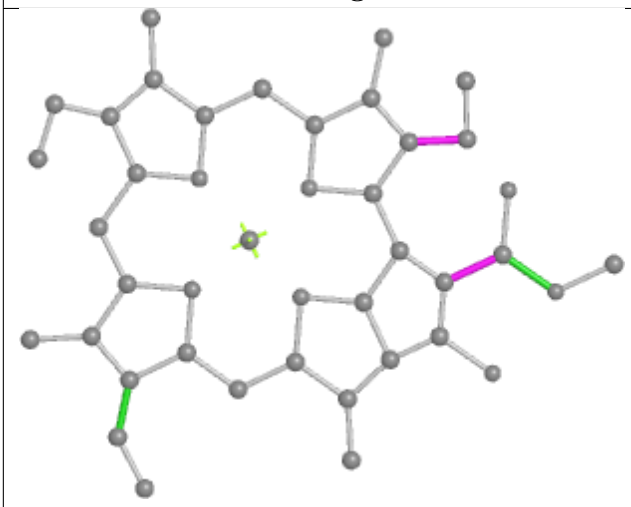


Bond angles



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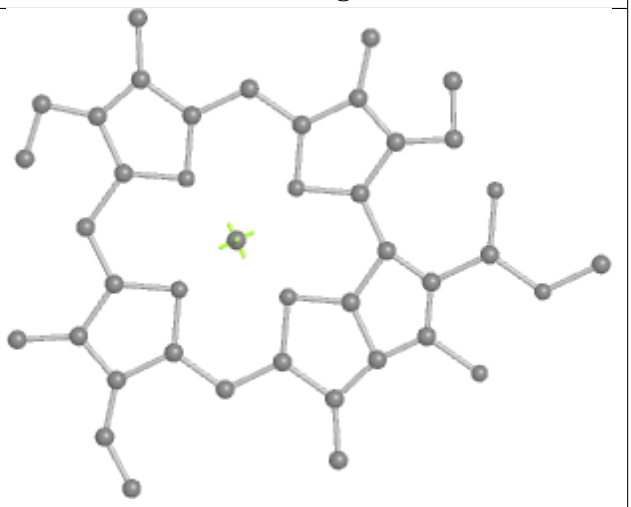
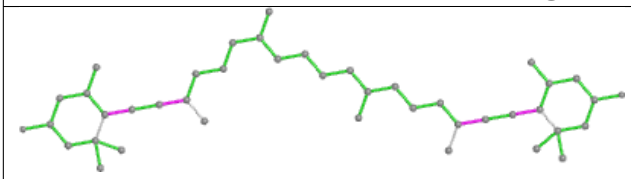


Rings

Ligand II0 5 615



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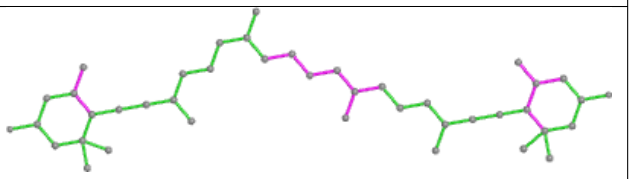
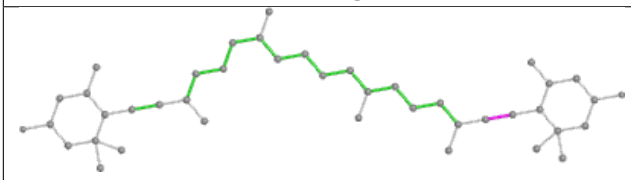
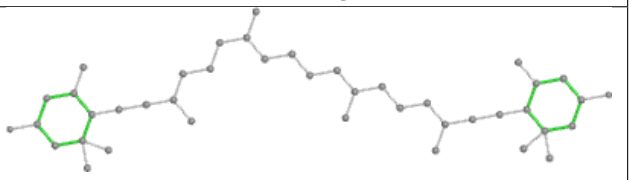


Bond angles

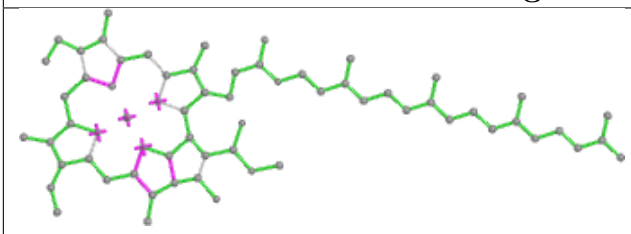


Torsions

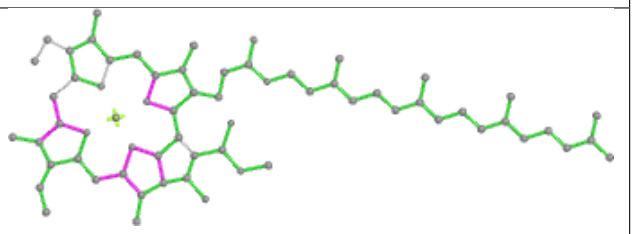


Rings

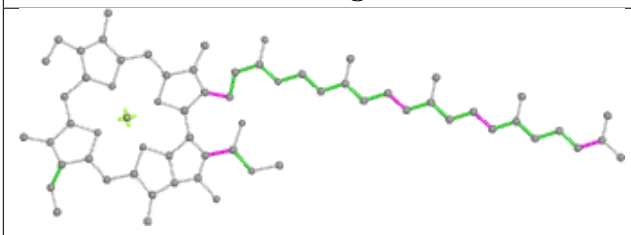
Ligand CLA A 837



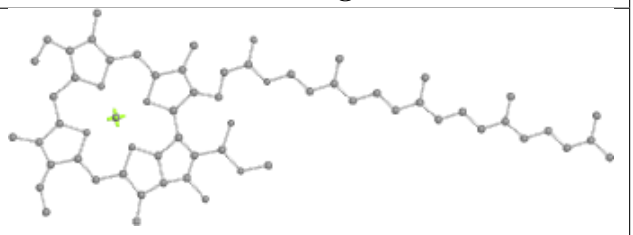
Bond lengths



Bond angles

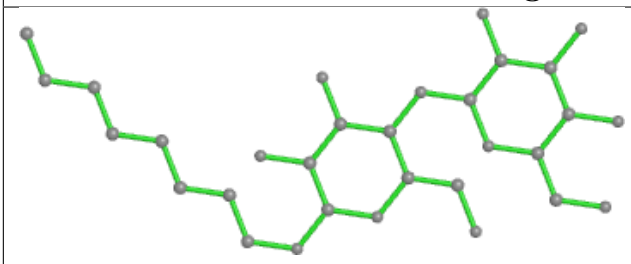


Torsions

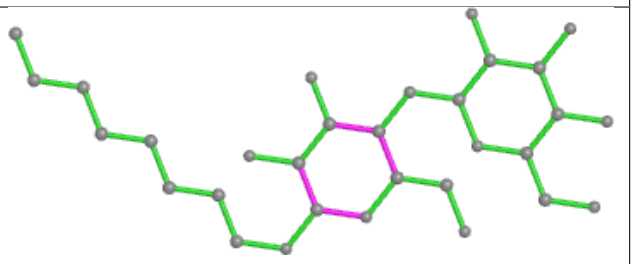


Rings

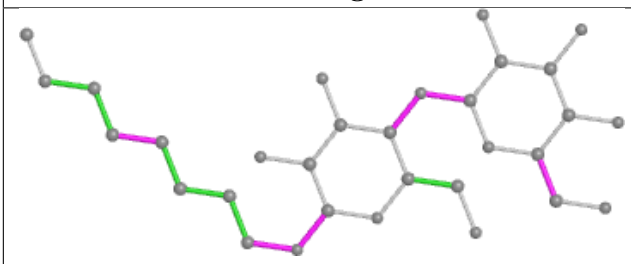
Ligand LMU J 104



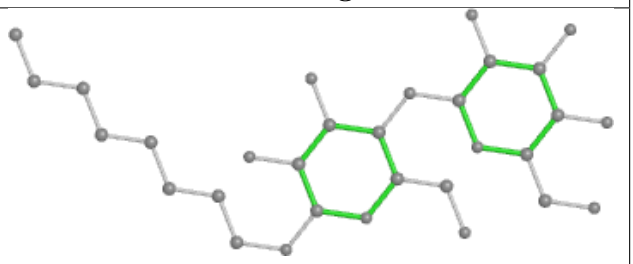
Bond lengths



Bond angles

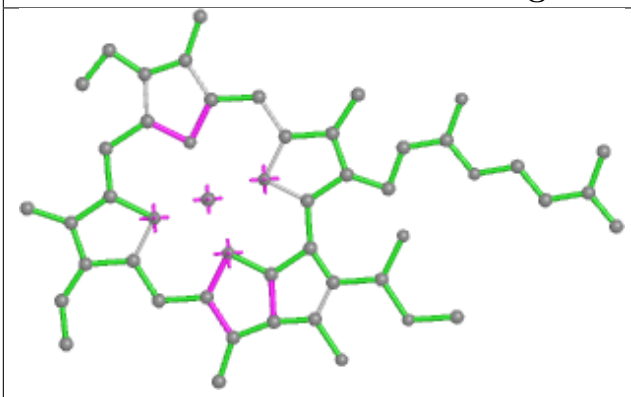


Torsions

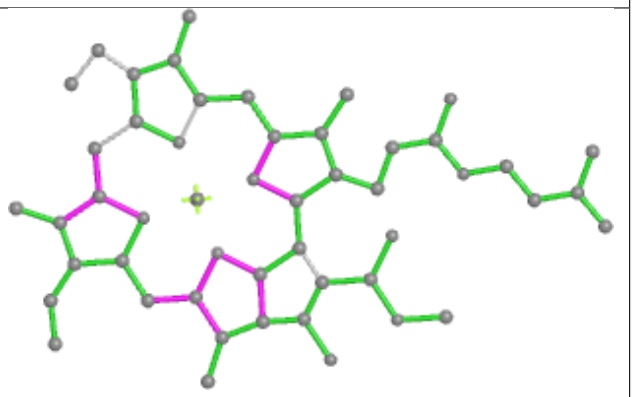


Rings

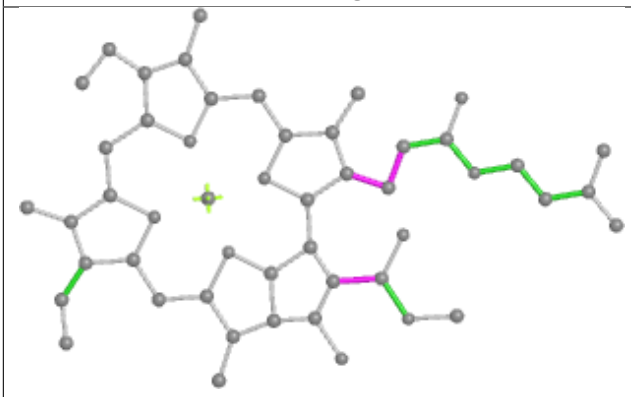
Ligand CLA 2 603



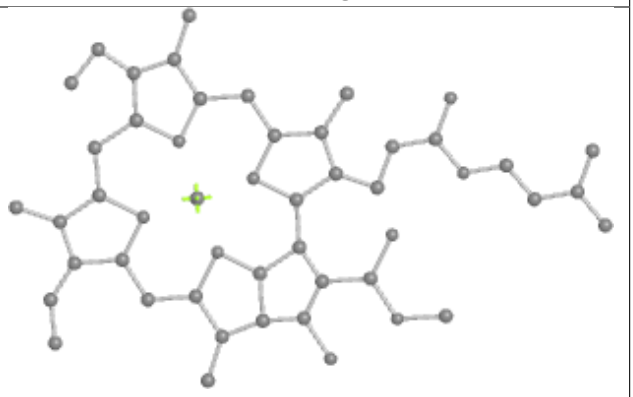
Bond lengths



Bond angles

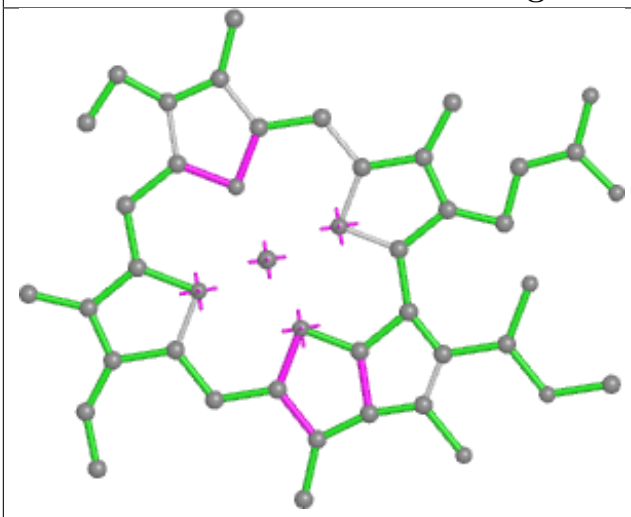


Torsions



Rings

Ligand CLA b 601



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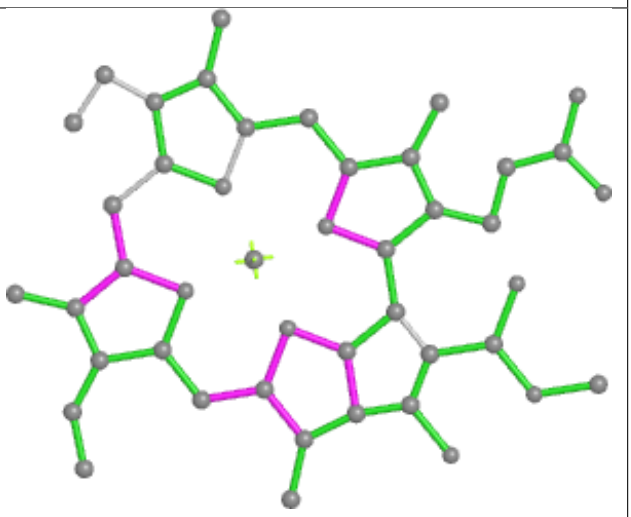

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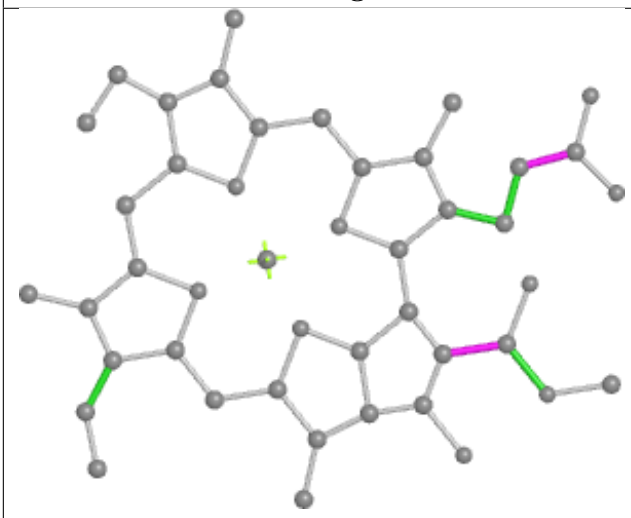

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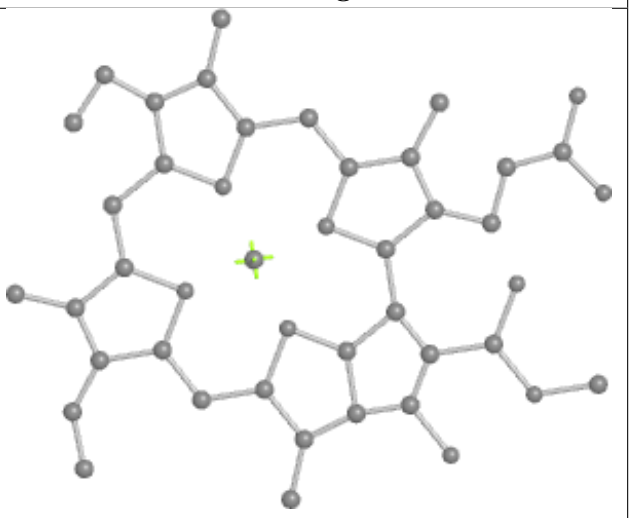
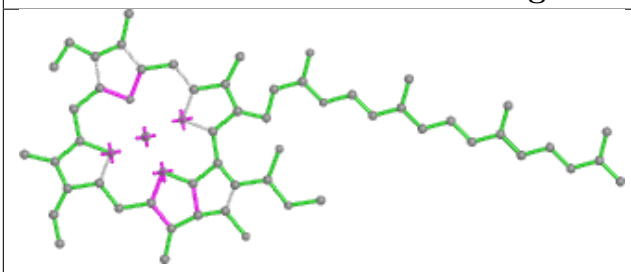


Rings

Ligand CLA 4 607



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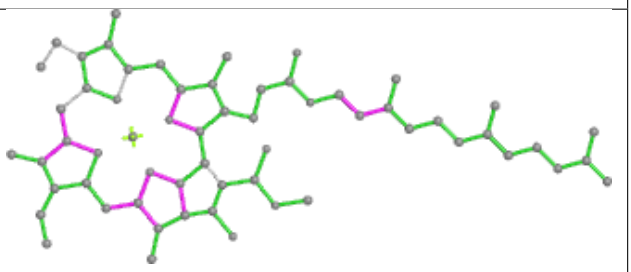
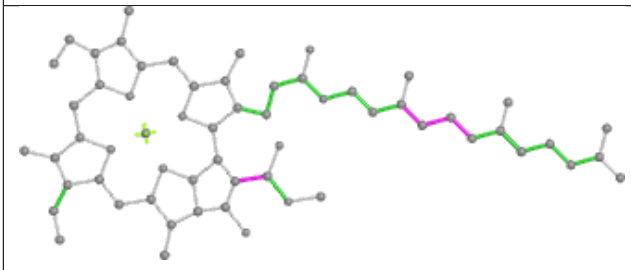


Bond angles



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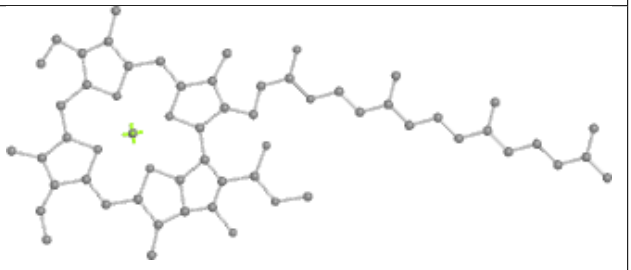
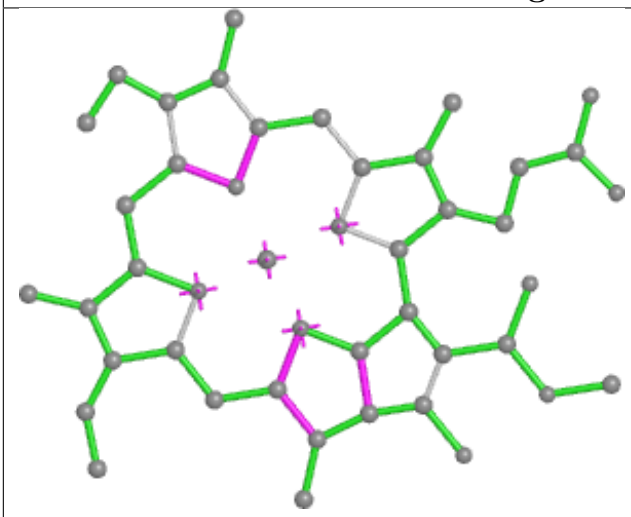


Rings

Ligand CLA 9 612



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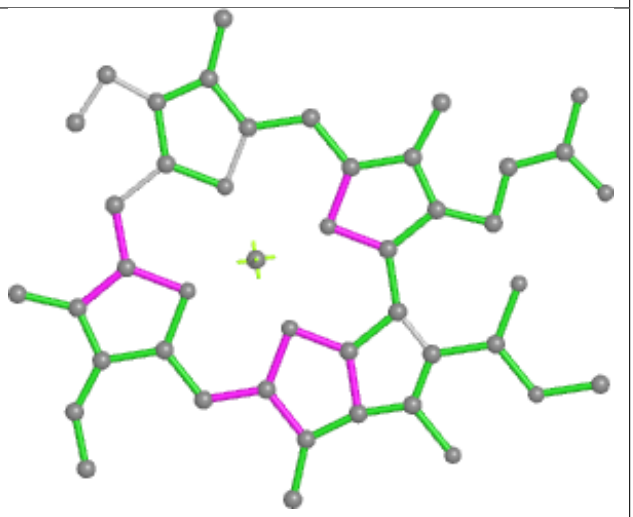
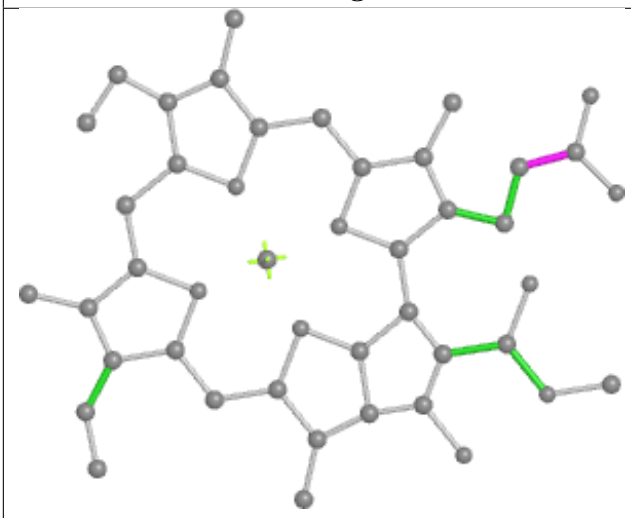


Bond angles



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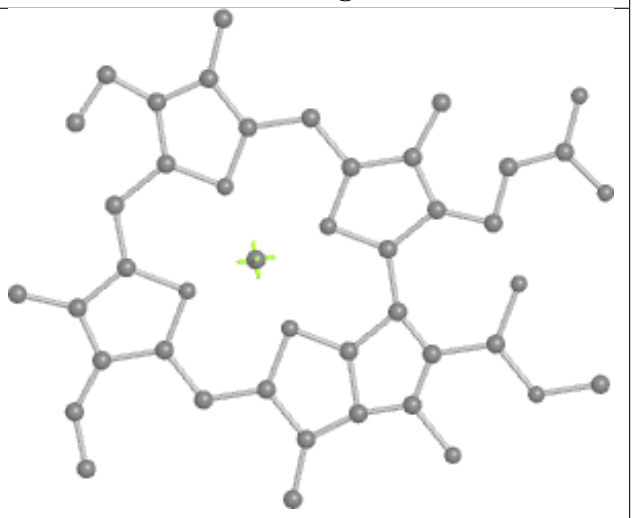
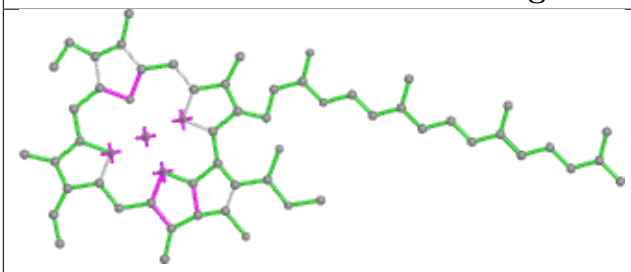


Rings

Ligand CLA 3 607



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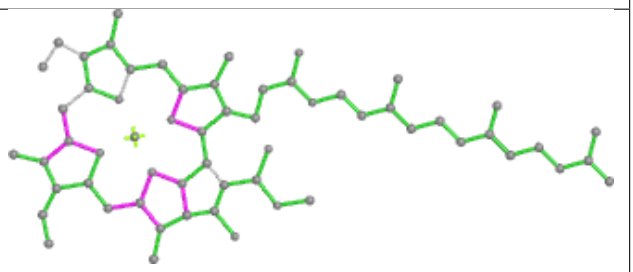
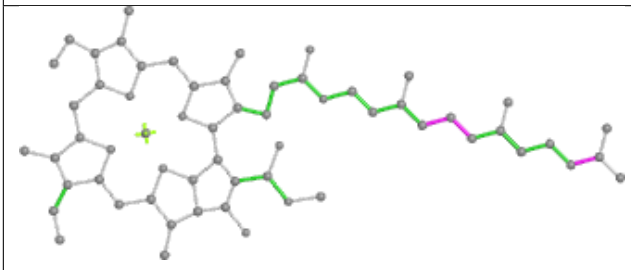


Bond angles



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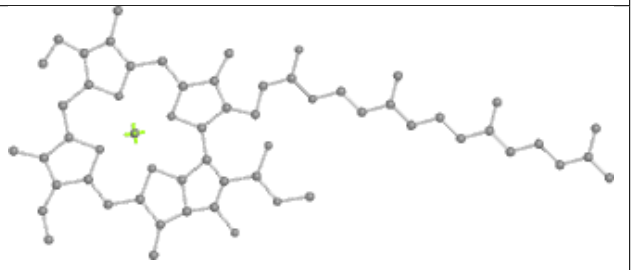
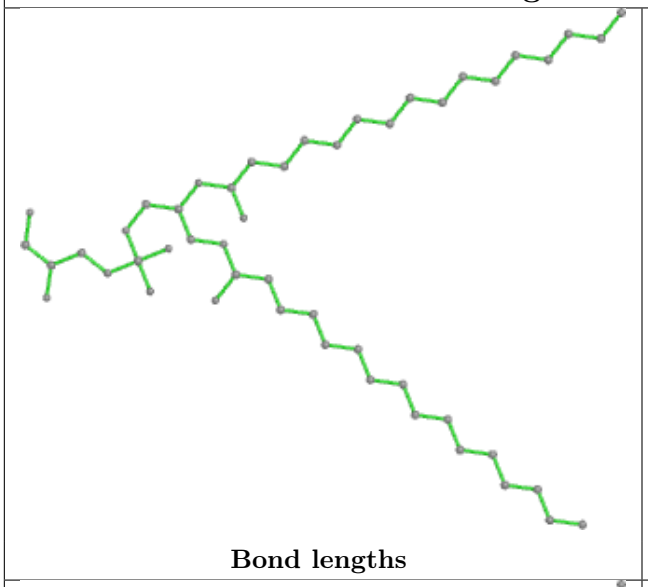


Rings

Ligand LHG A 851



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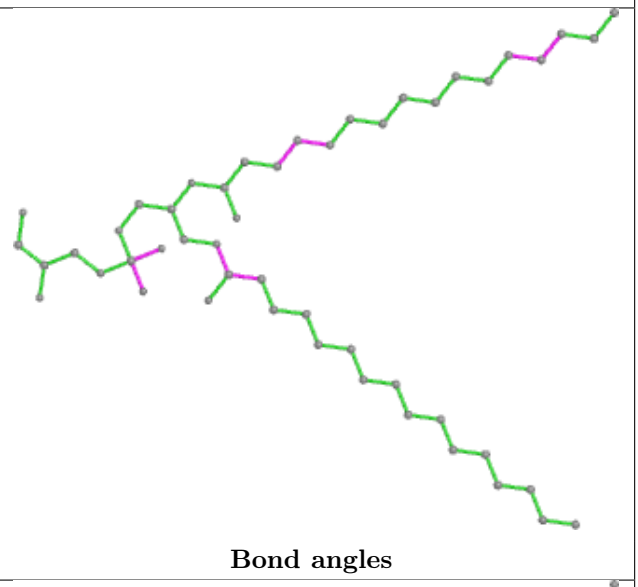
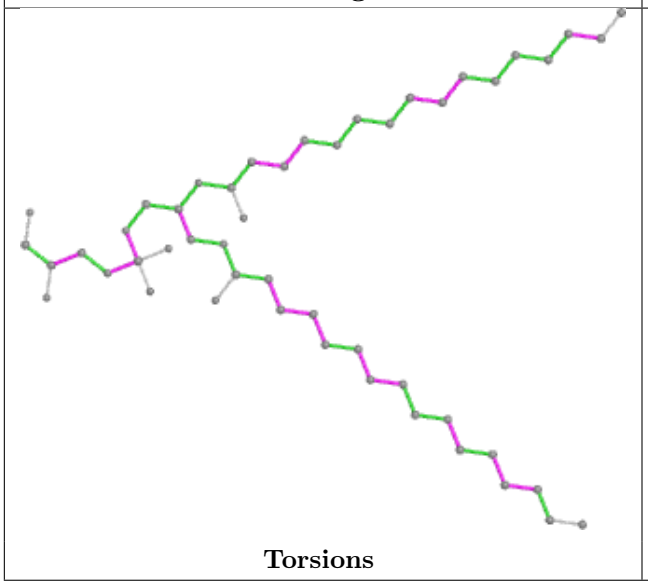


Bond angles



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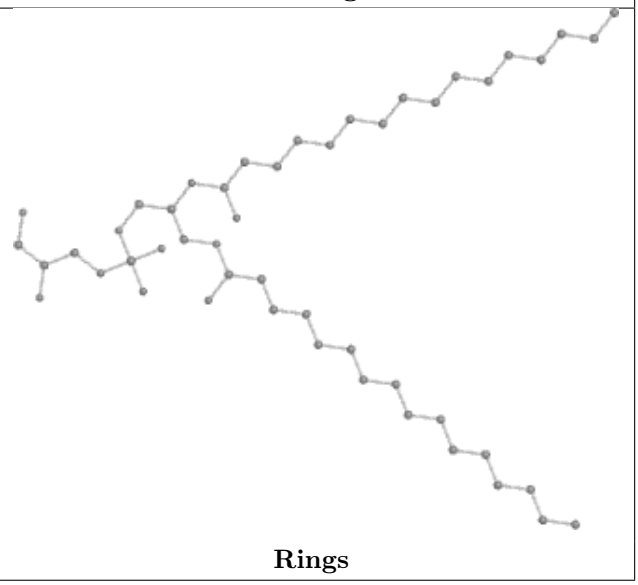
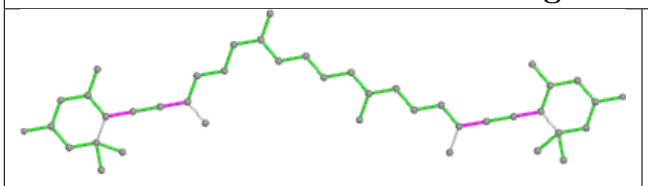


Rings

Ligand II0 1 619



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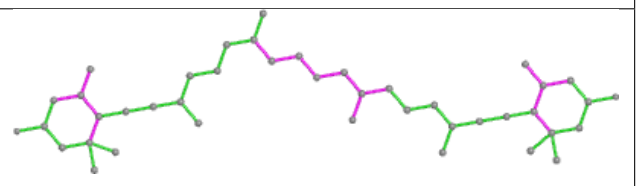
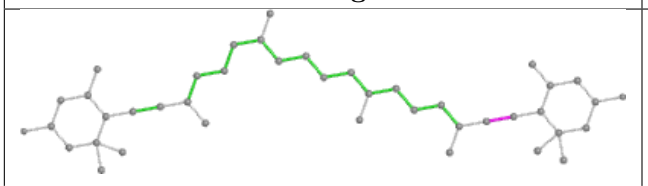


Bond angles



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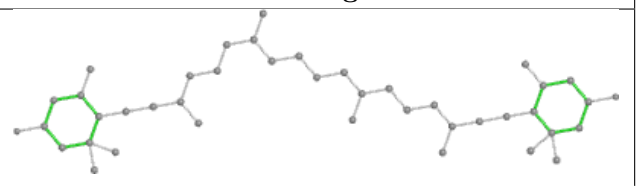
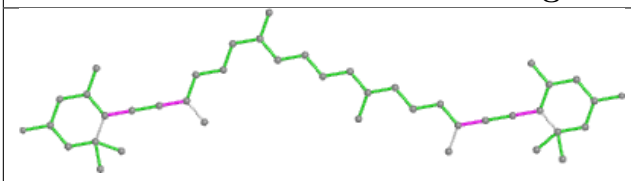


Rings

Ligand II0 5 620



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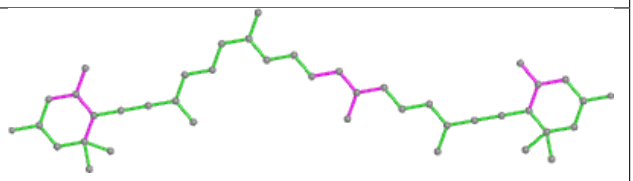
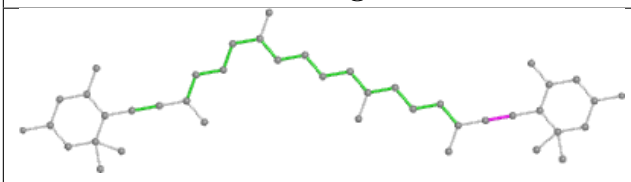


Bond angles



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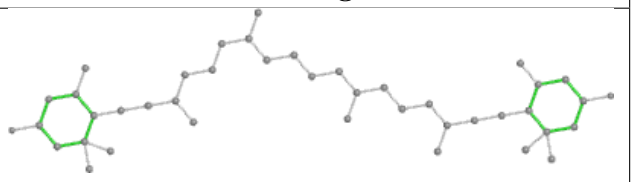
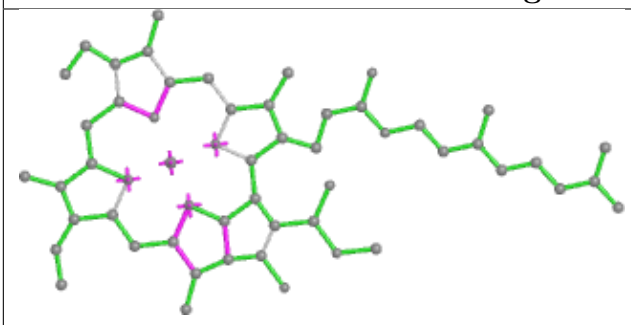
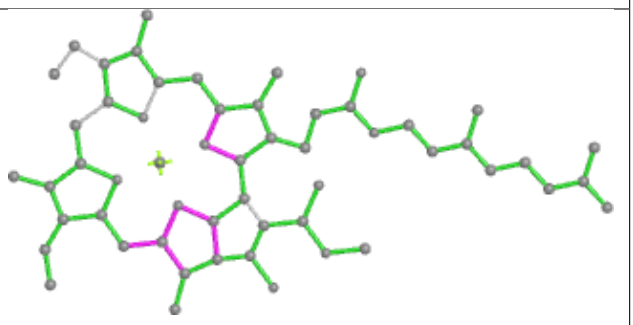


Rings

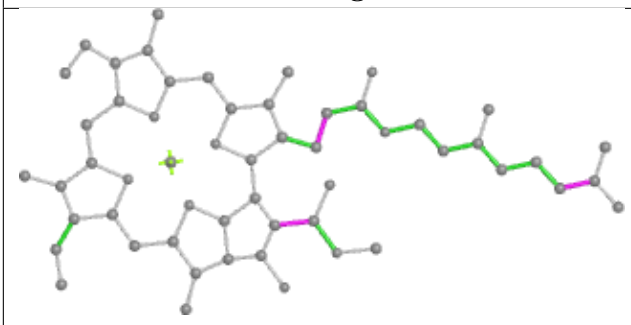
Ligand CLA A 840



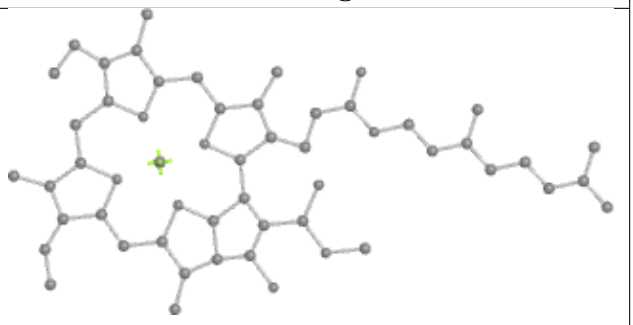
Bond lengths



Bond angles

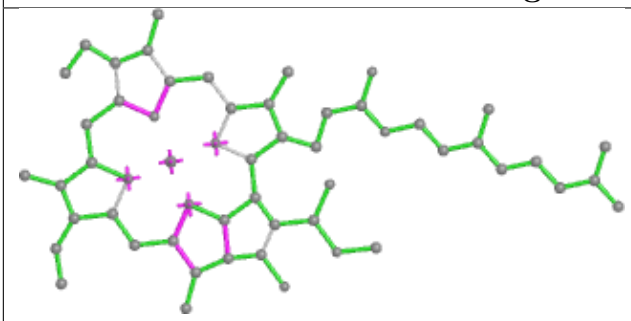


Torsions

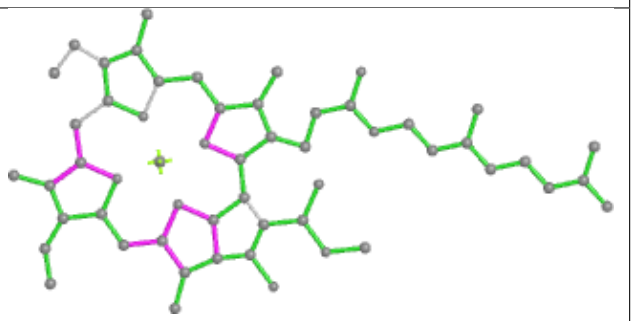


Rings

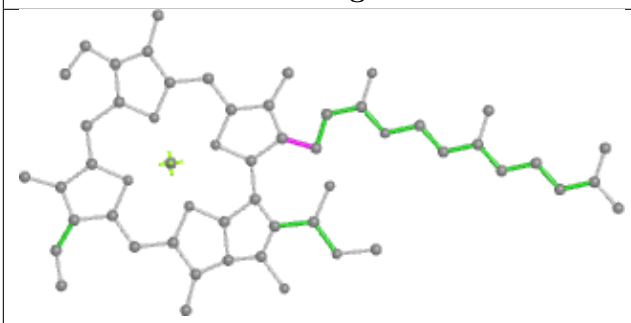
Ligand CLA A 808



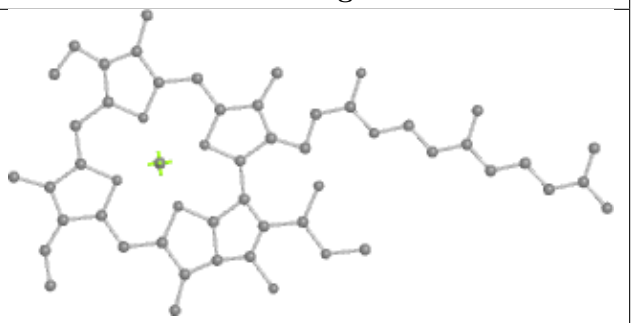
Bond lengths



Bond angles

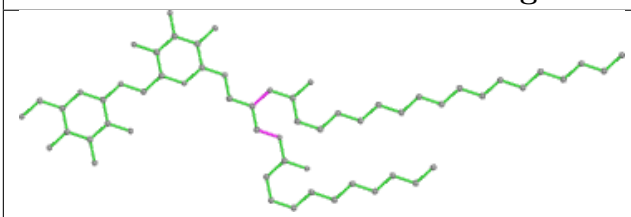


Torsions

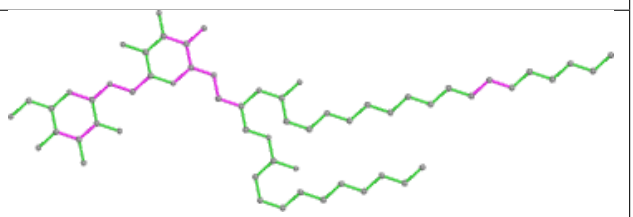


Rings

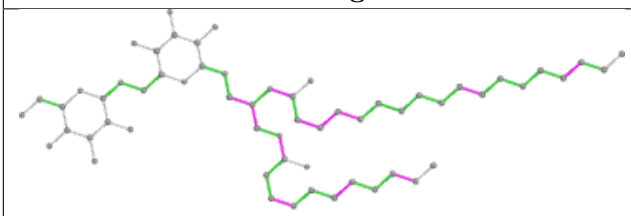
Ligand DGD B 848



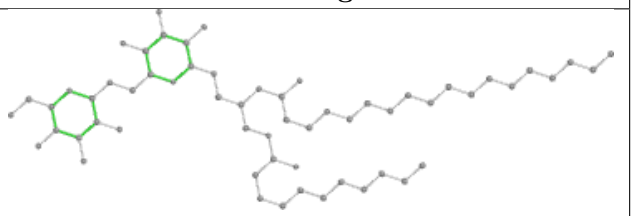
Bond lengths



Bond angles

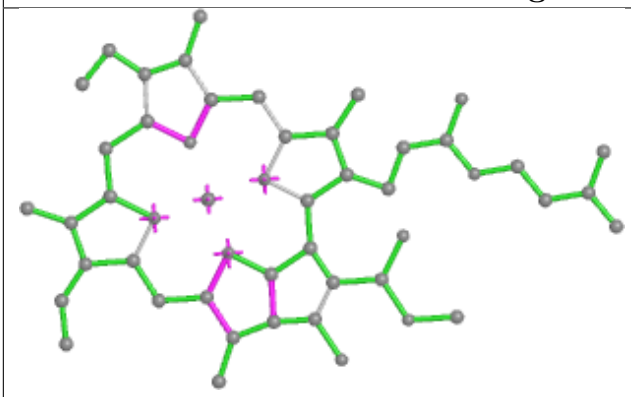


Torsions



Rings

Ligand CLA 3 611



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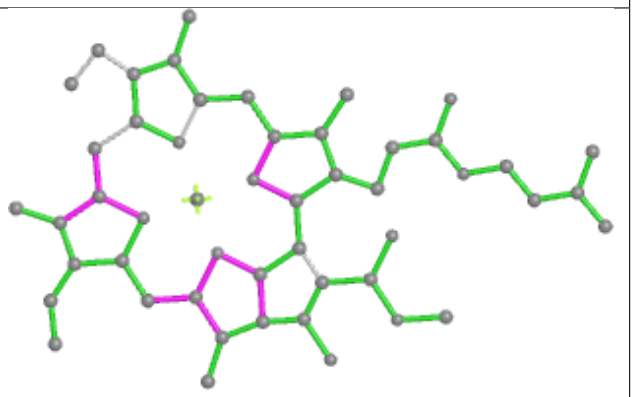
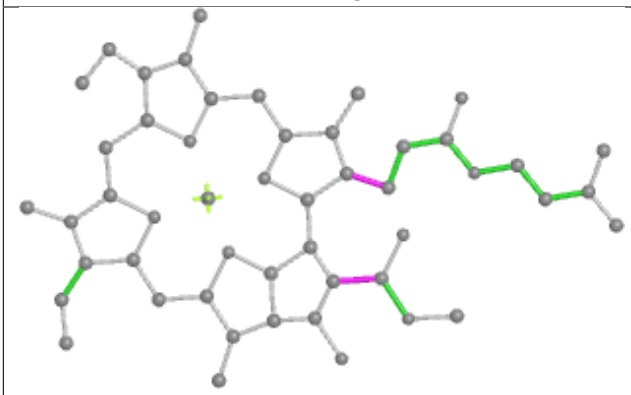
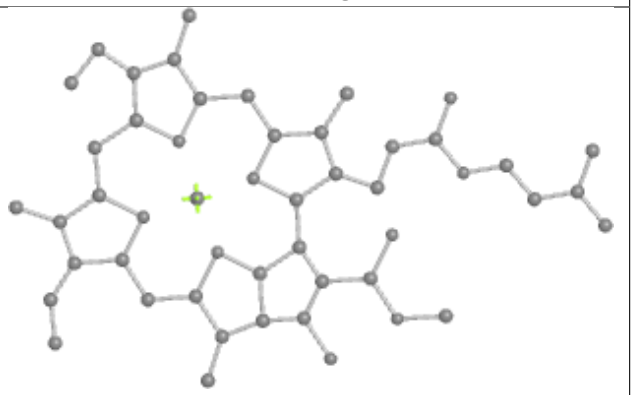


Bond angles

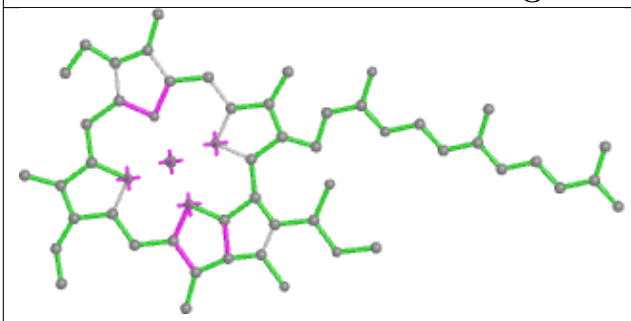


Torsions

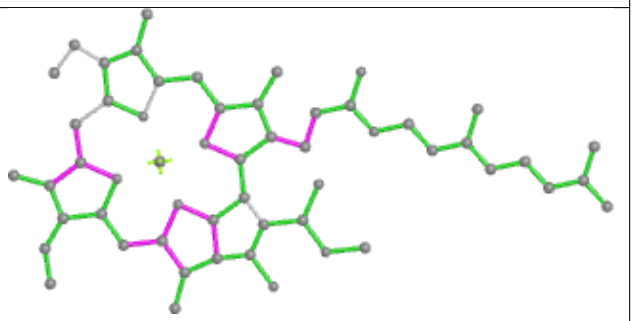


Rings

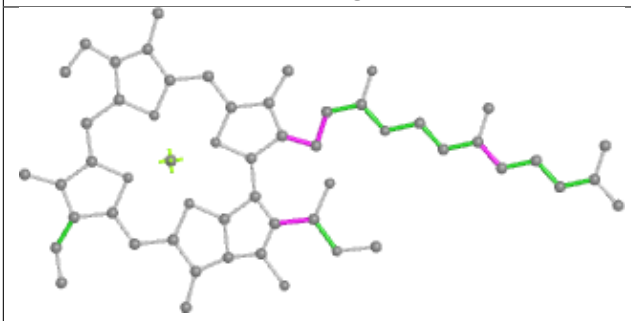
Ligand CLA A 834



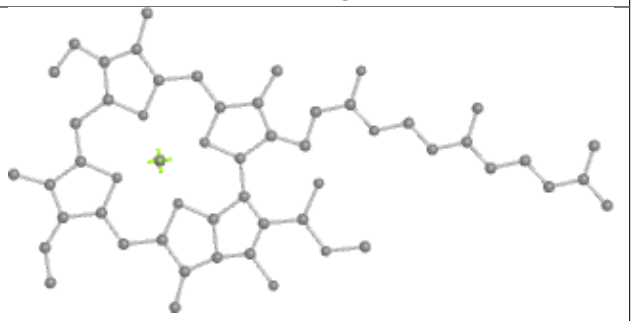
Bond lengths



Bond angles

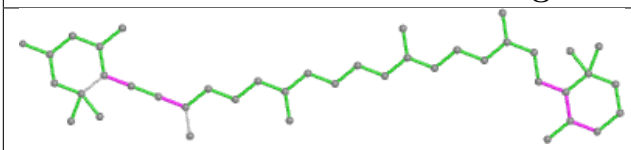


Torsions

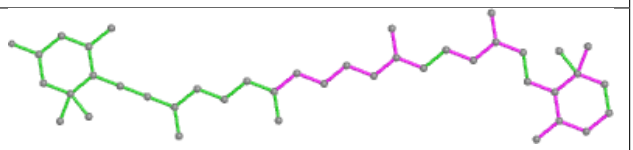


Rings

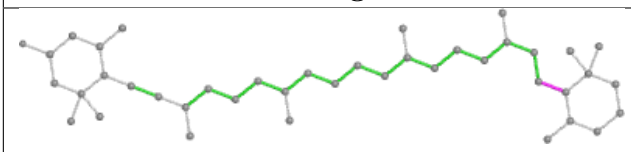
Ligand IHT 5 618



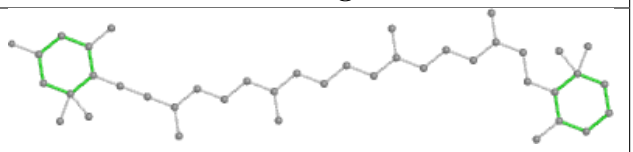
Bond lengths



Bond angles

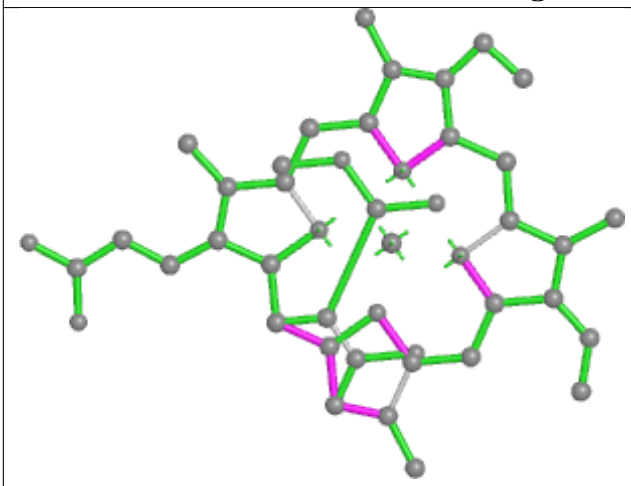


Torsions

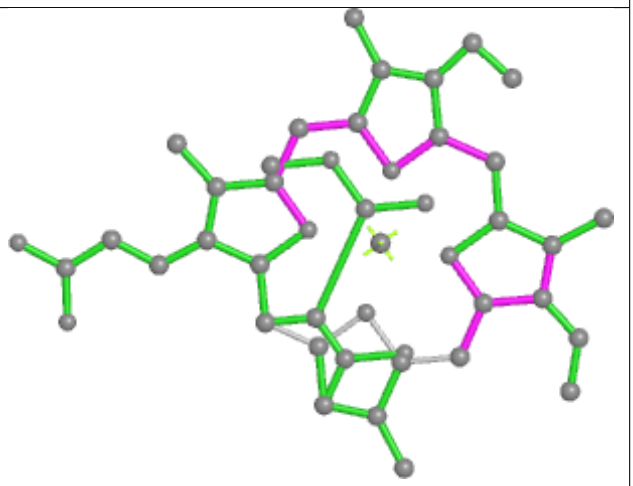


Rings

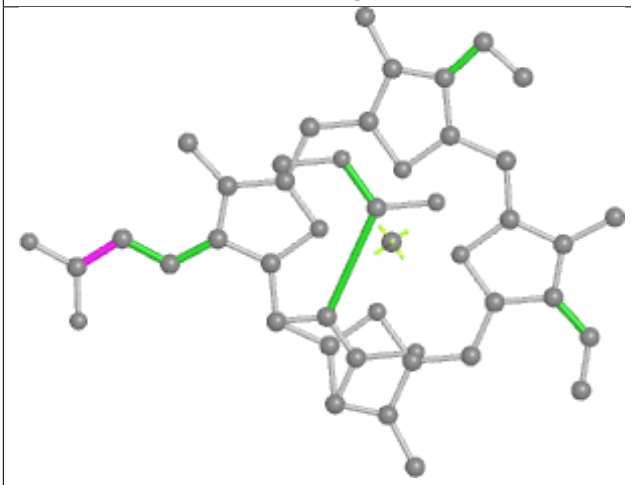
Ligand KC2 b 609



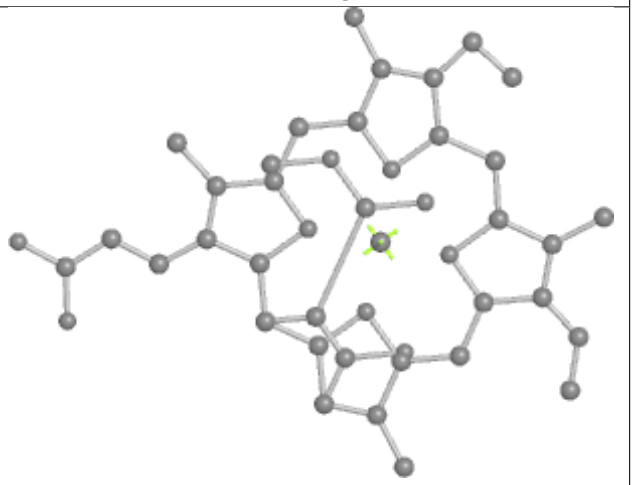
Bond lengths



Bond angles

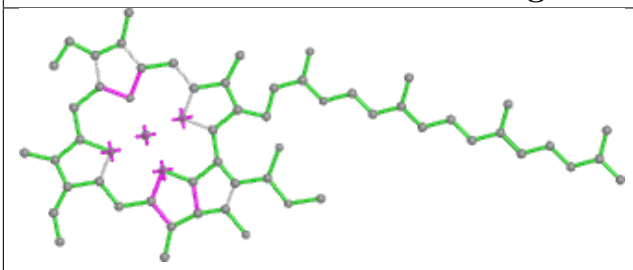


Torsions

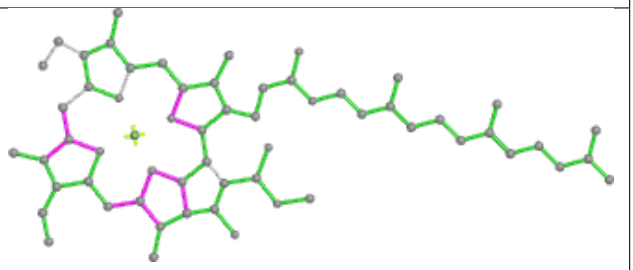


Rings

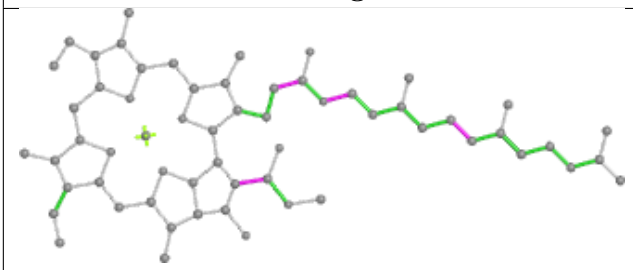
Ligand CLA b 607



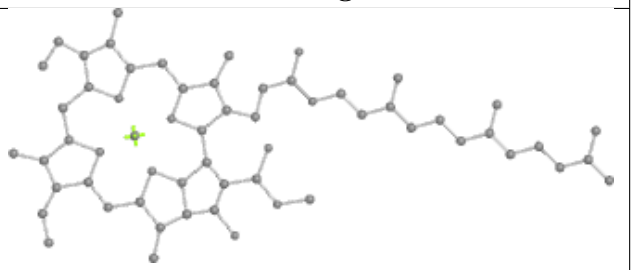
Bond lengths



Bond angles

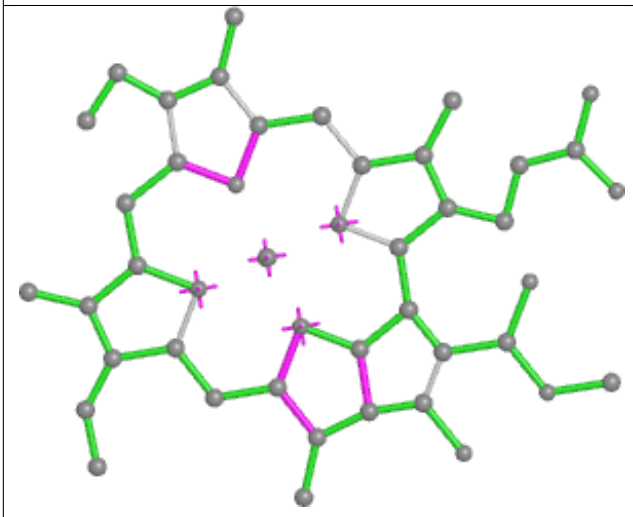


Torsions



Rings

Ligand CLA B 803



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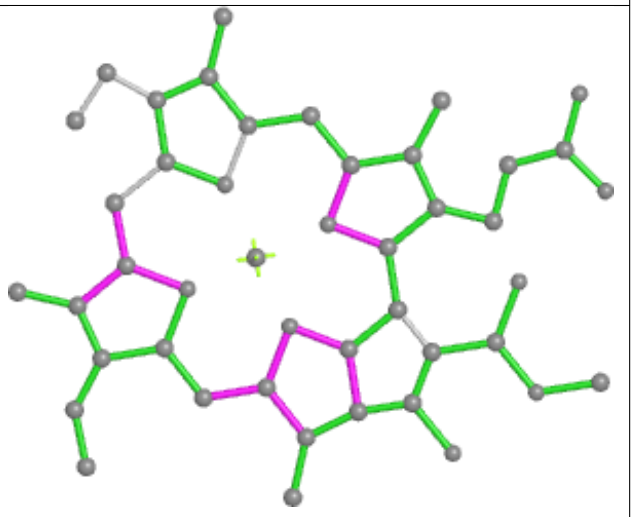
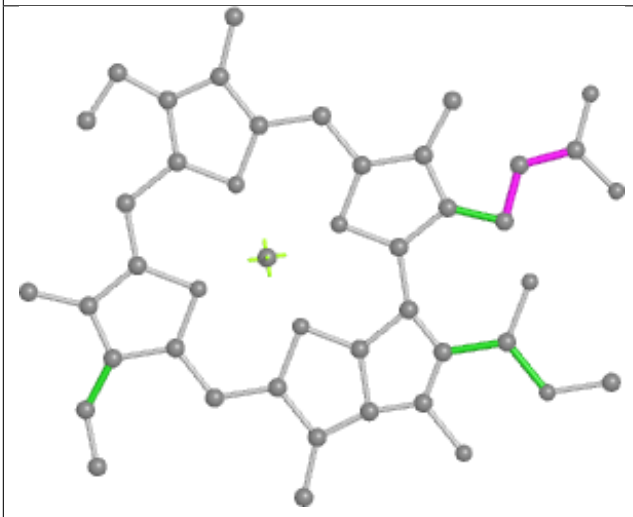
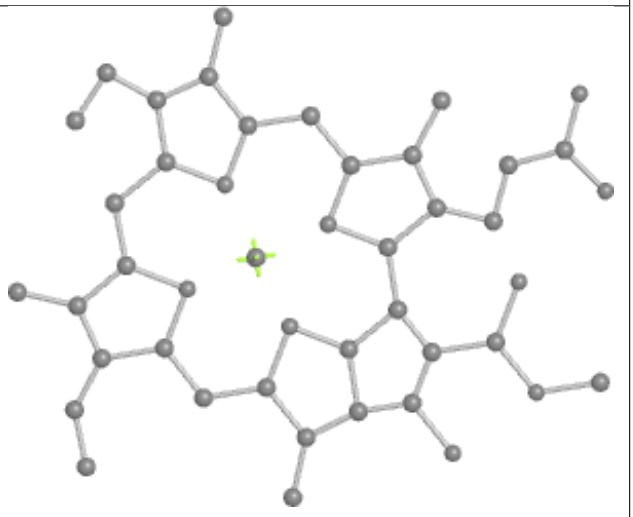


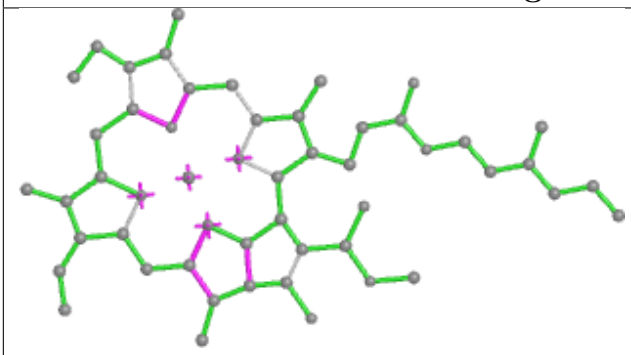
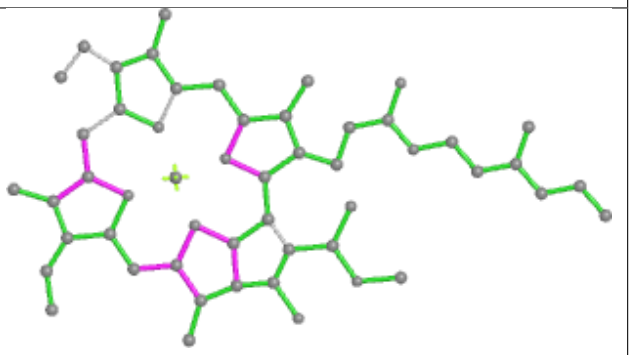
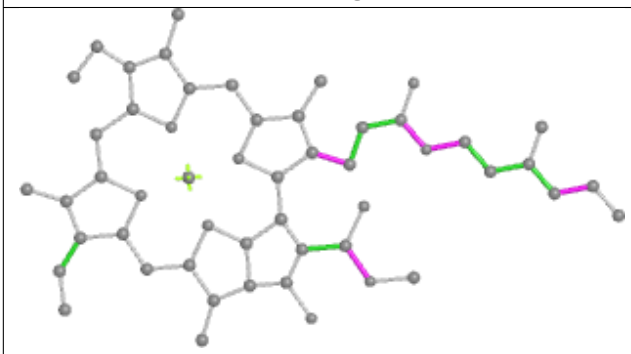
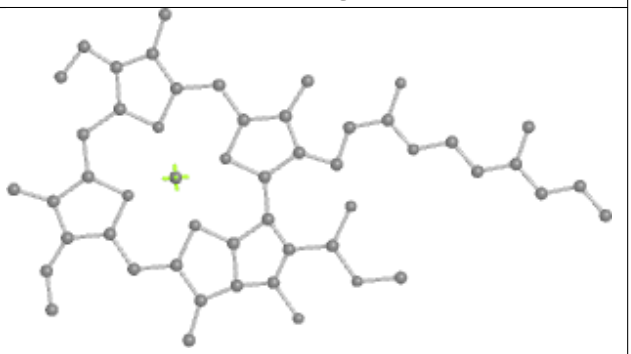
Bond angles

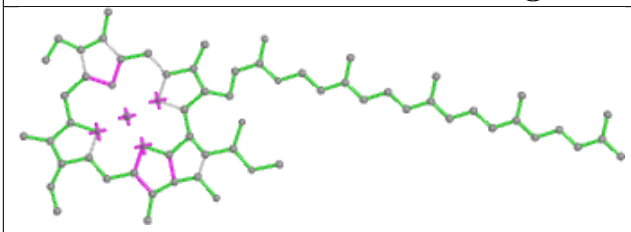
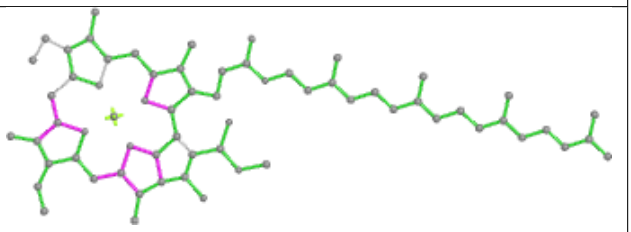
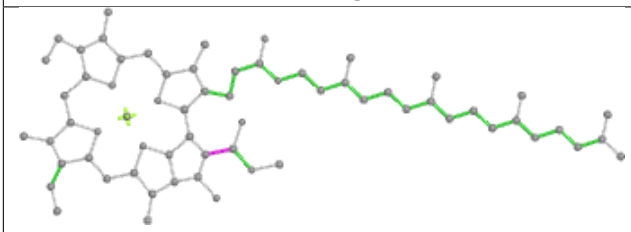
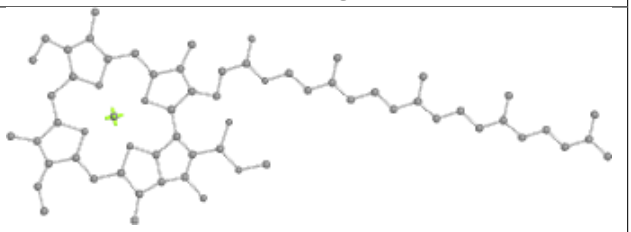


Torsions

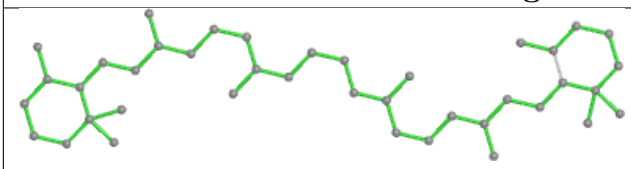


Rings

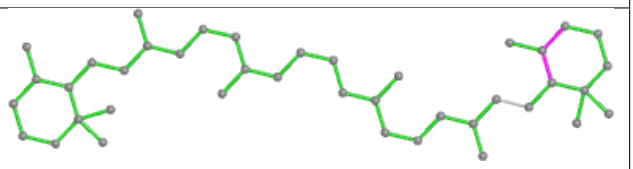
Ligand CLA B 841	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA B 840	
	
Bond lengths	Bond angles
	
Torsions	Rings

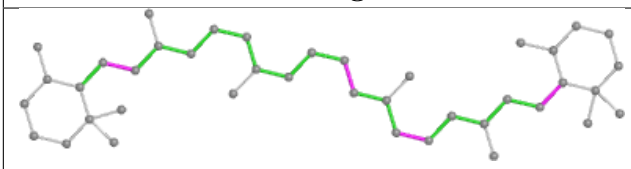
Ligand 8CT M 101



Bond lengths



Bond angles



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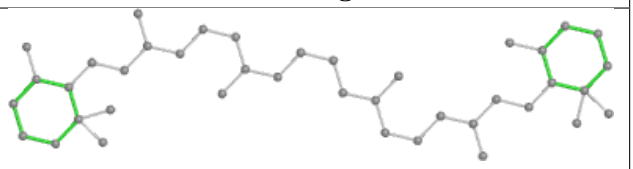
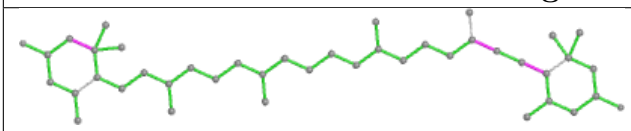


Rings

Ligand II3 b 613



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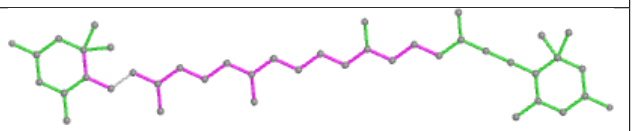

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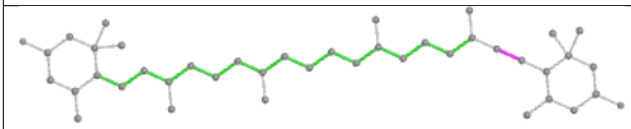

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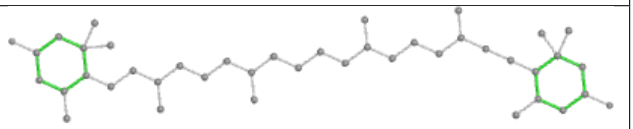
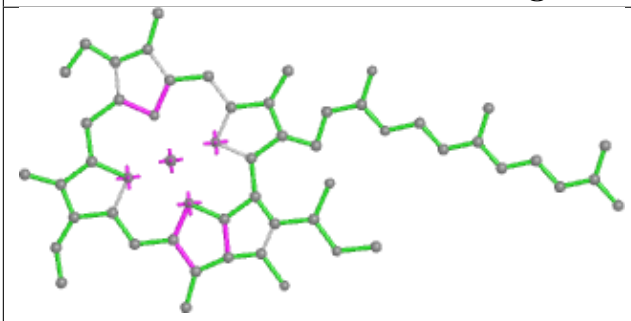
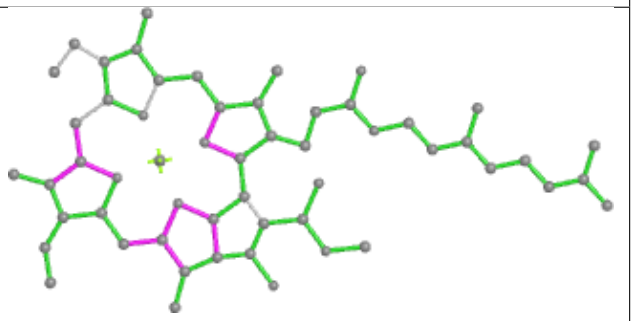


Rings

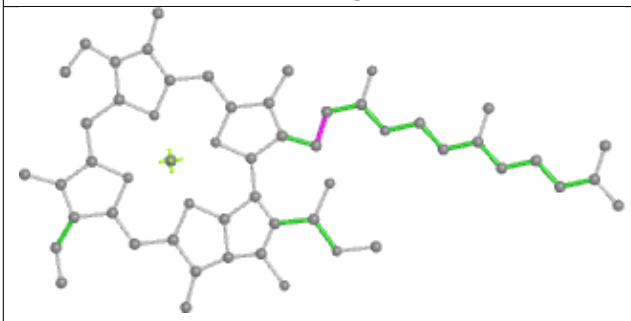
Ligand CLA 9 604



Bond lengths



Bond angles



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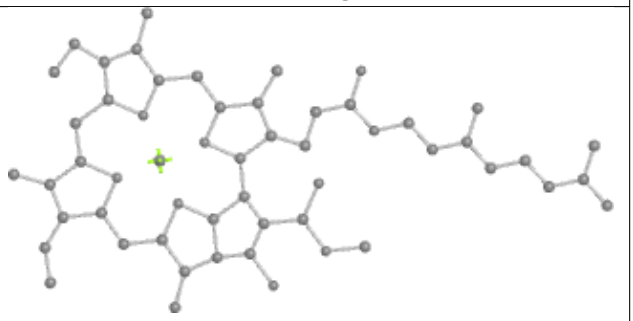
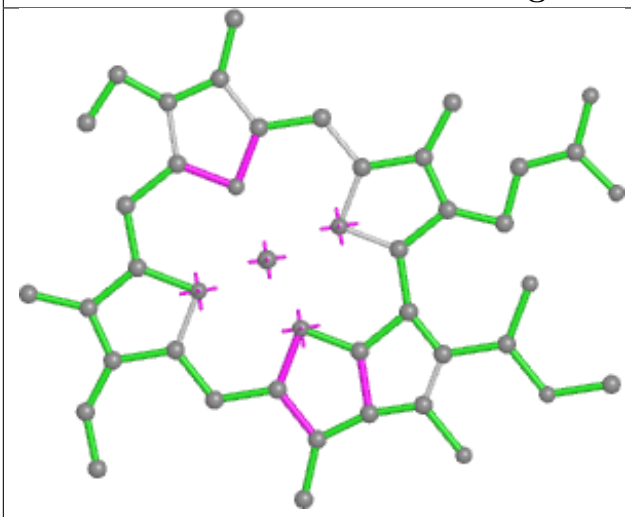


Rings

Ligand CLA 5 611



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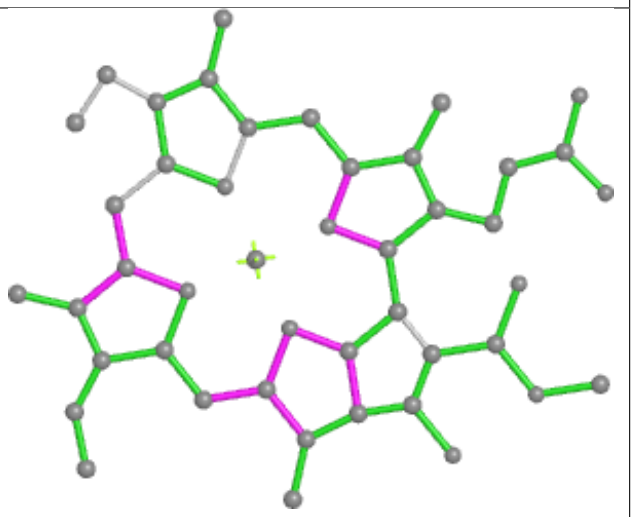

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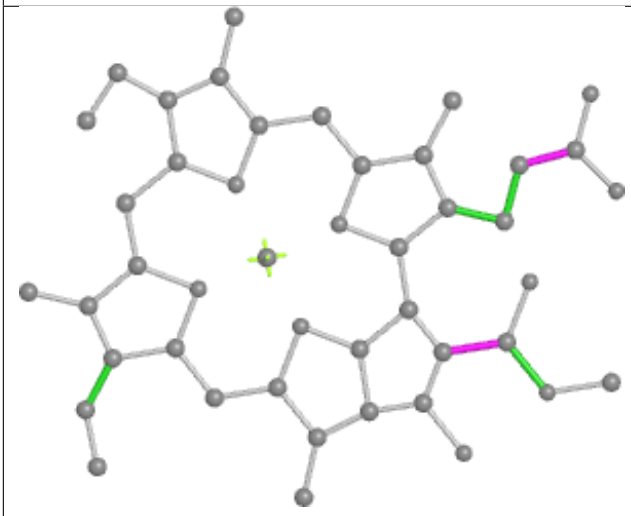

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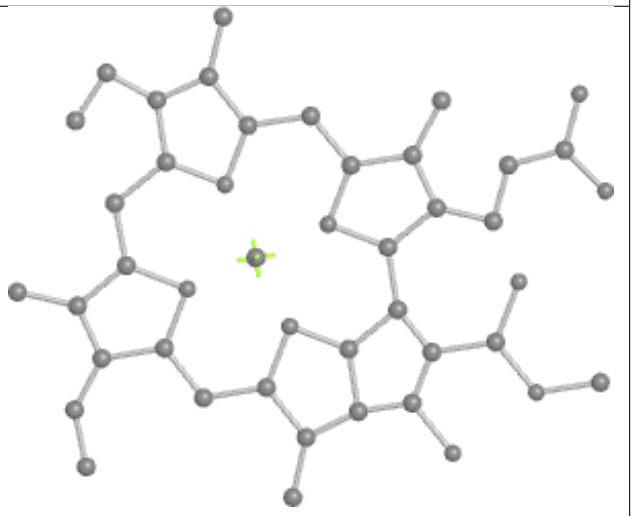
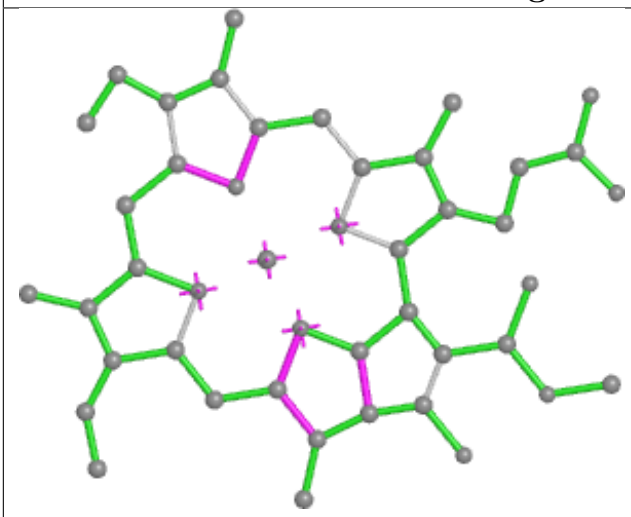


Rings

Ligand CLA 9 605



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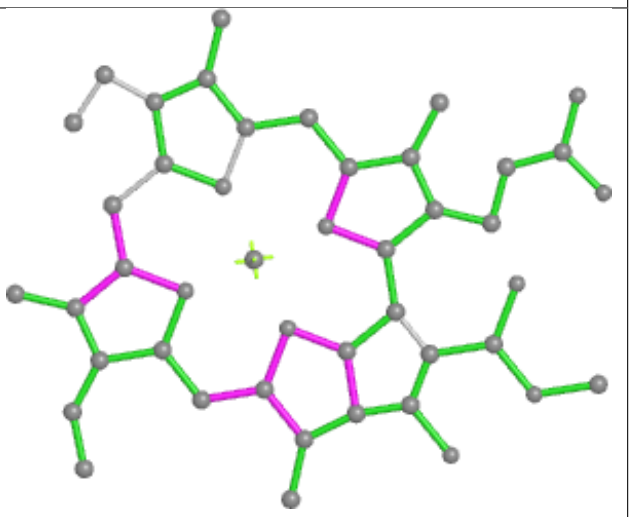
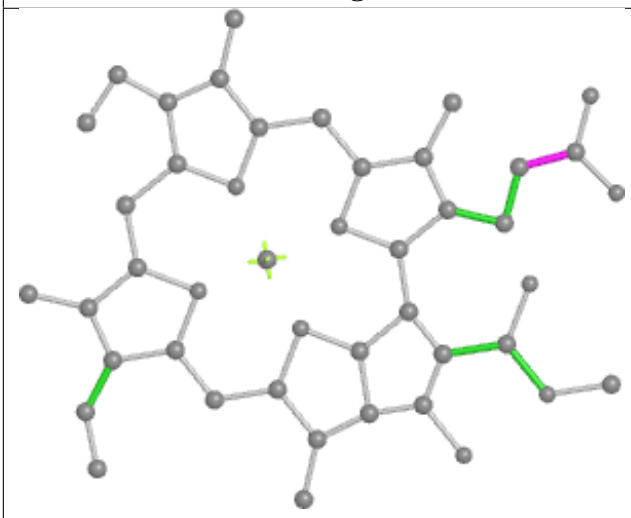
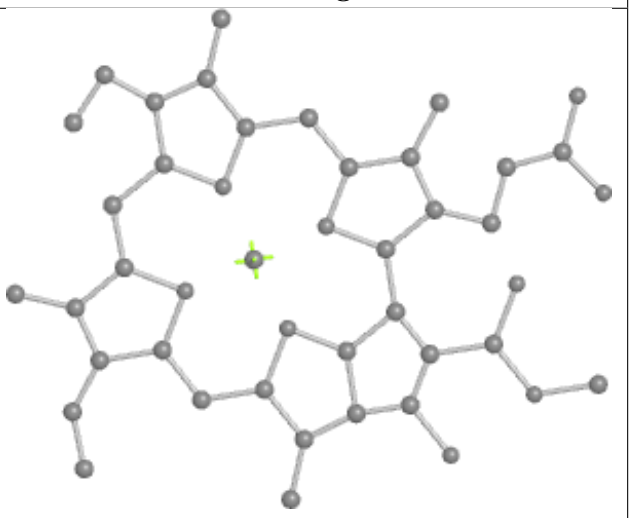


Bond angles

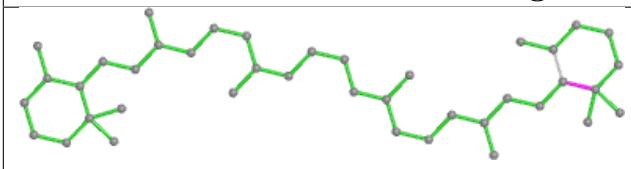


Torsions

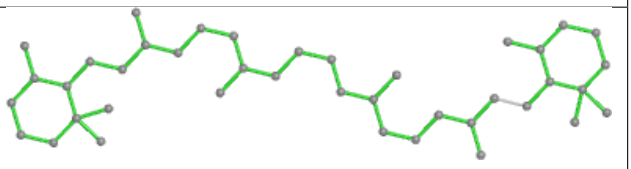


Rings

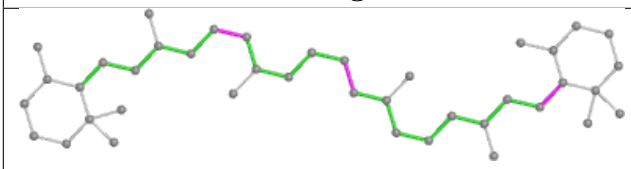
Ligand 8CT F 201



Bond lengths



Bond angles



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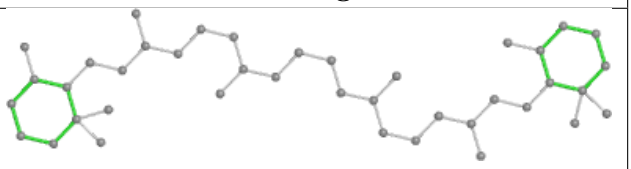
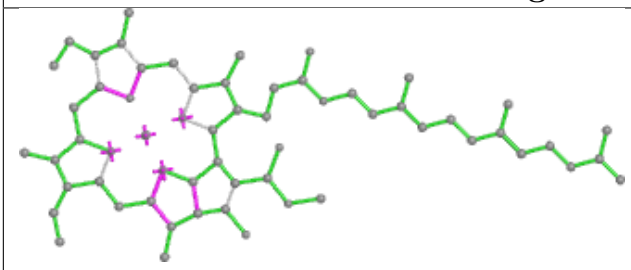
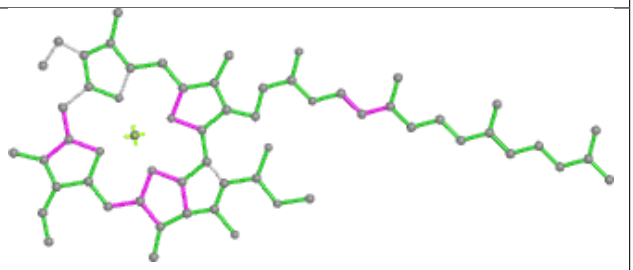


Rings

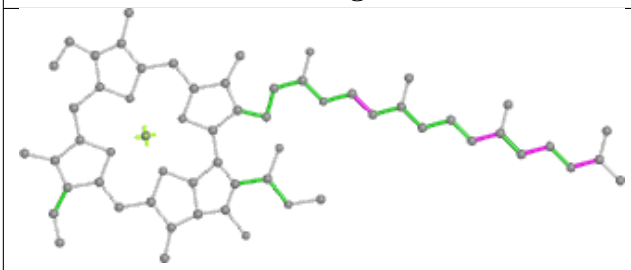
Ligand CLA 1 612



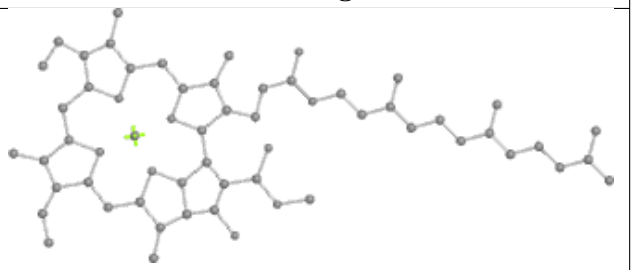
Bond lengths



Bond angles

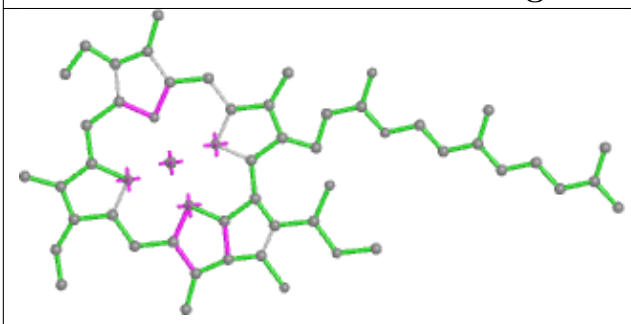


Torsions



Rings

Ligand CLA Z 304



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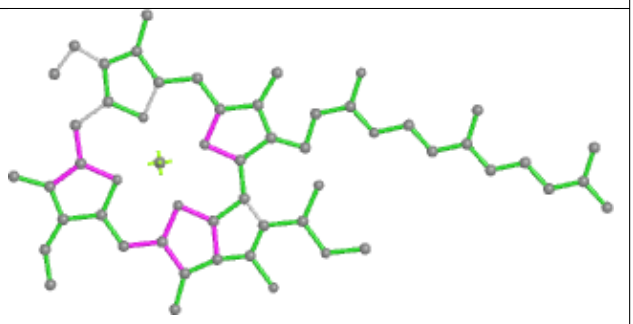
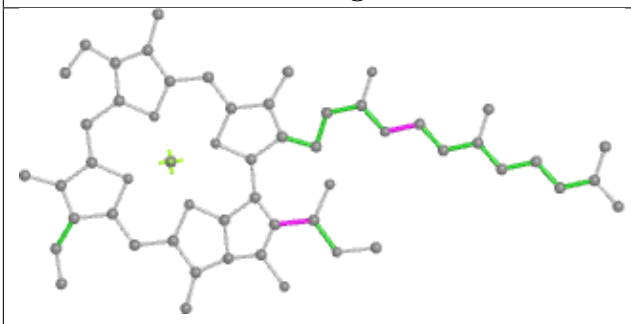


Bond angles



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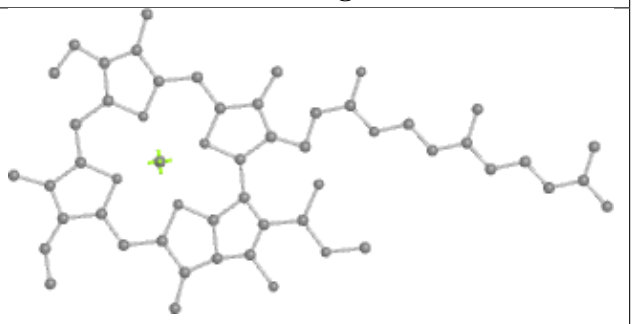
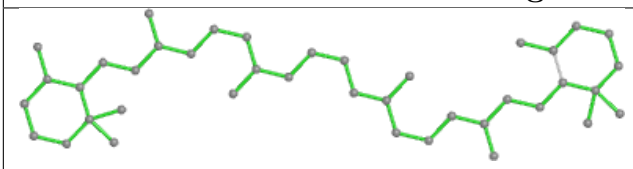
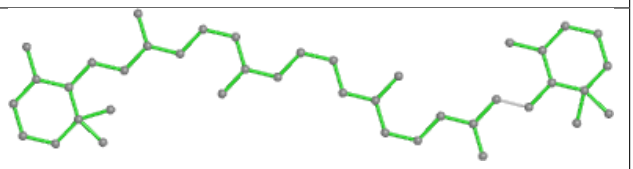


Rings

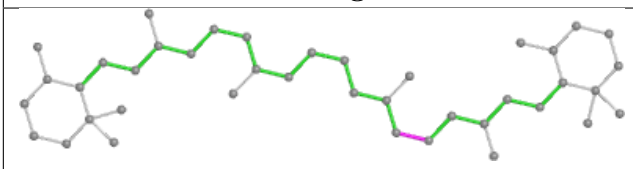
Ligand 8CT A 845



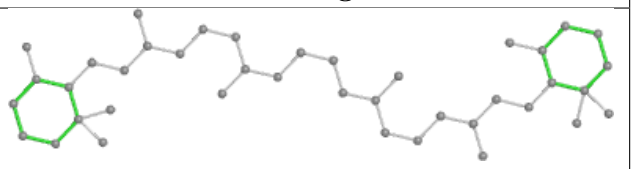
Bond lengths



Bond angles

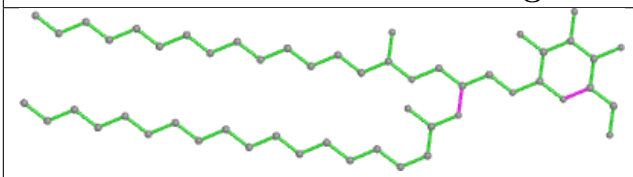


Torsions



Rings

Ligand LMG 8 614



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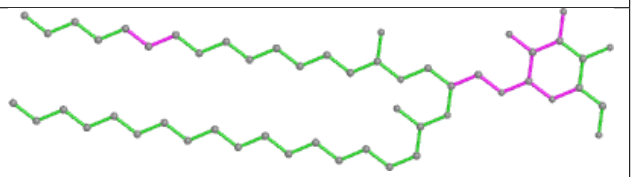
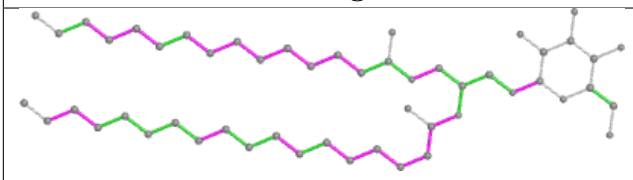
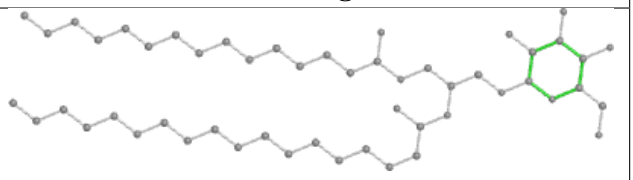


Bond angles

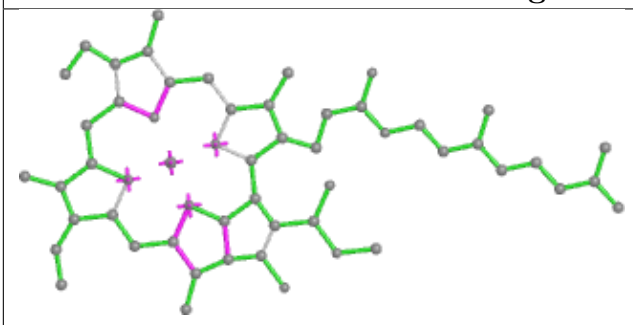


Torsions

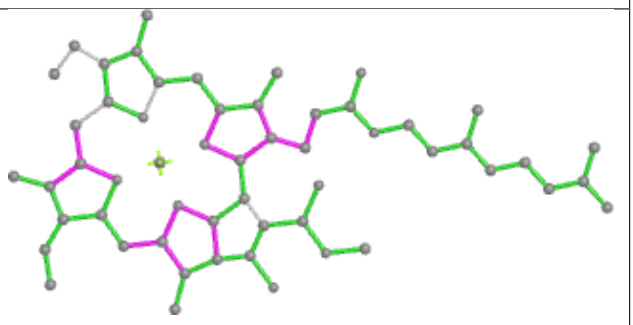


Rings

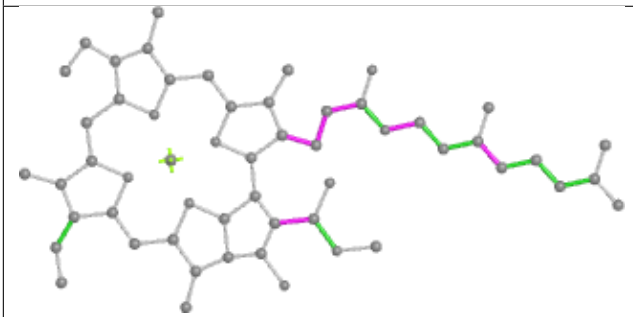
Ligand CLA a 602



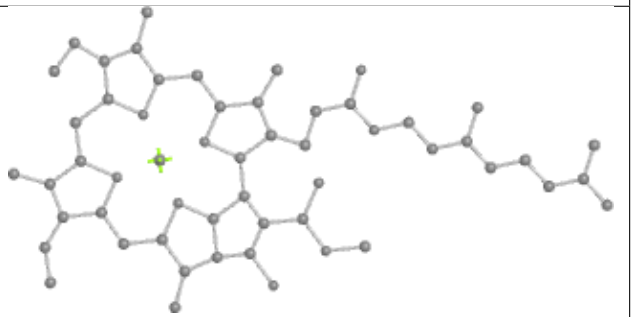
Bond lengths



Bond angles

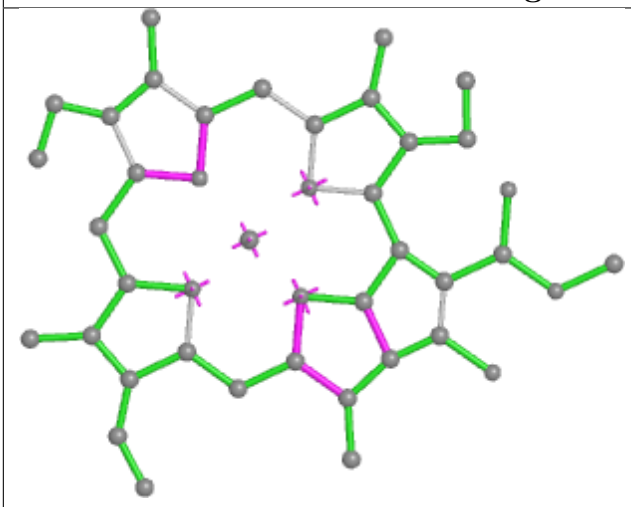


Torsions

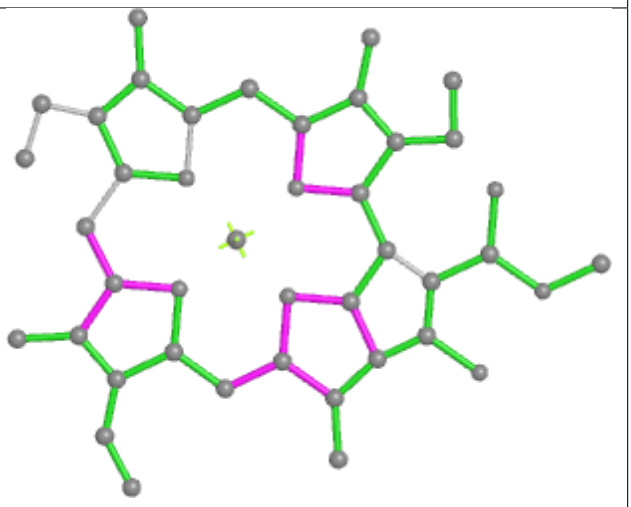


Rings

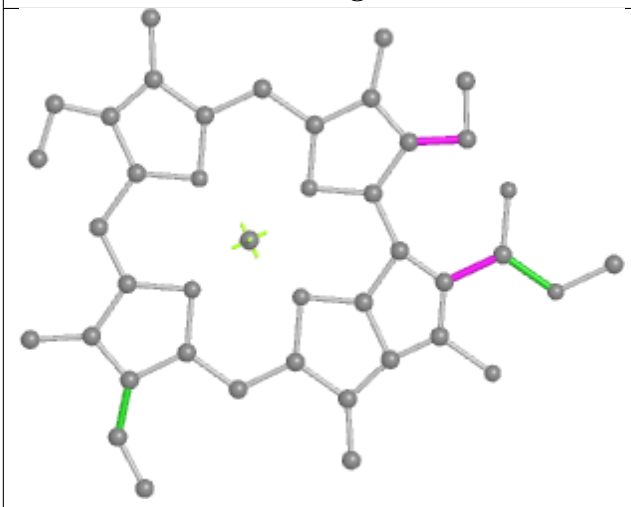
Ligand CLA B 814



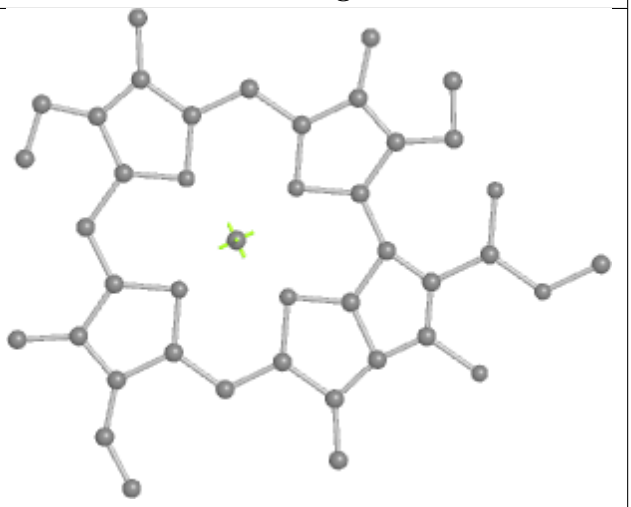
Bond lengths



Bond angles

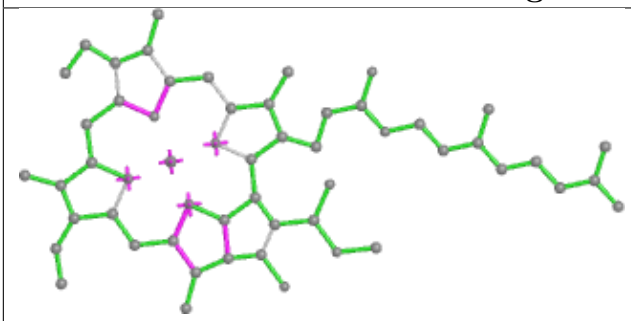


Torsions



Rings

Ligand CLA F 204



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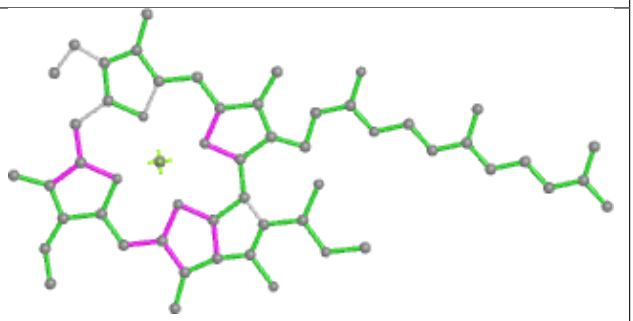
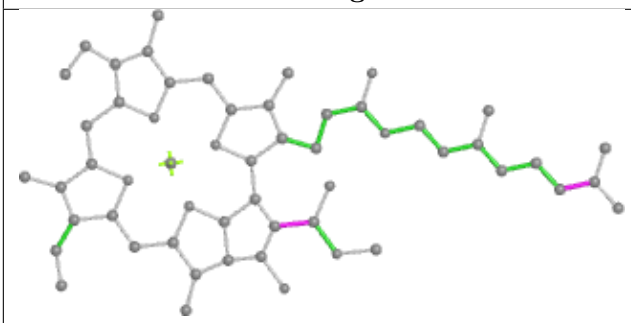


Bond angles



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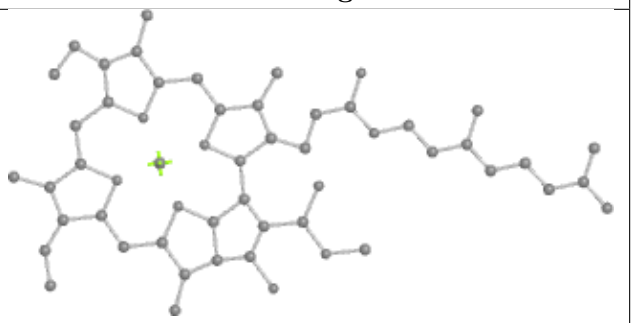
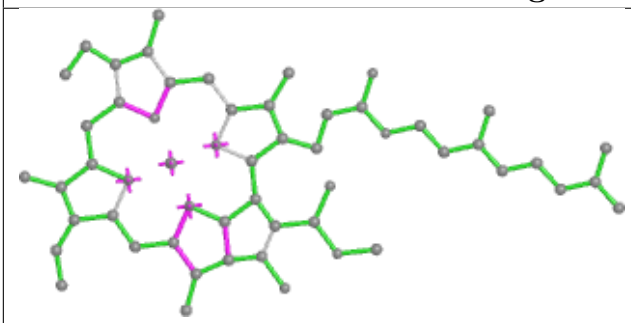


Rings

Ligand CLA 5 604



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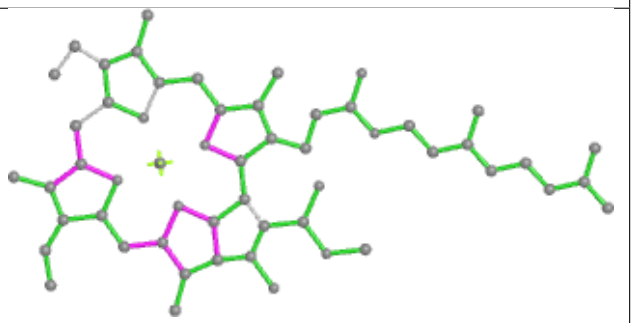
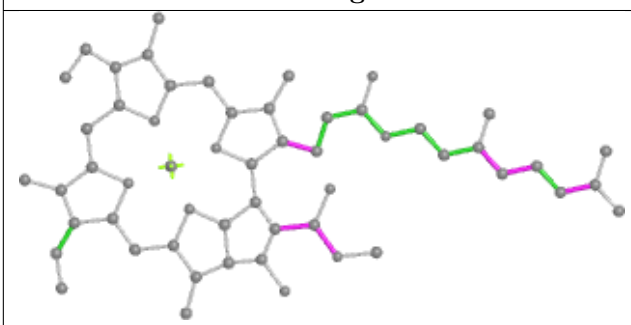


Bond angles



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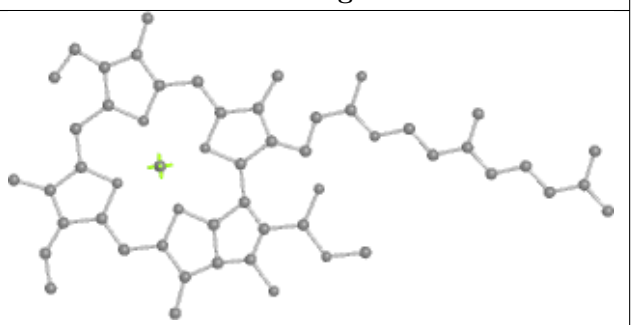
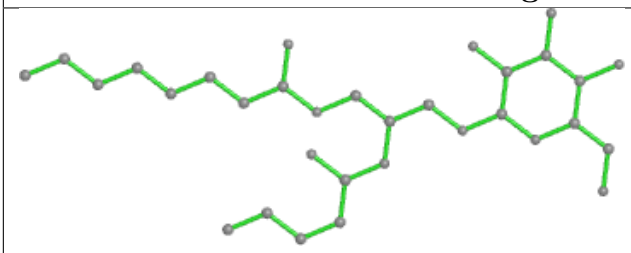


Rings

Ligand LMG F 205



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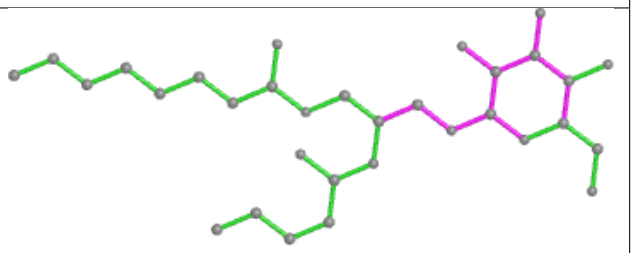
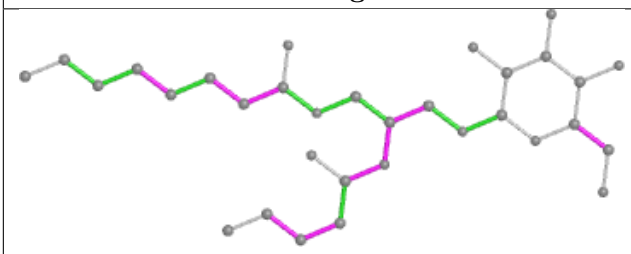


Bond angles



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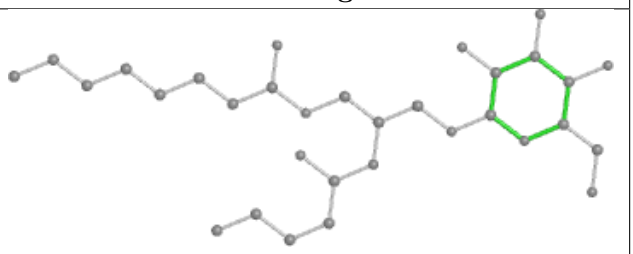
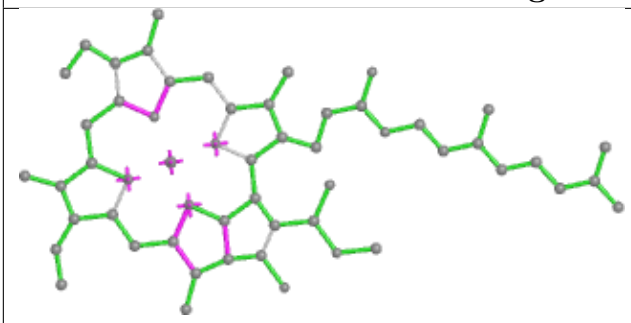


Rings

Ligand CLA 6 605



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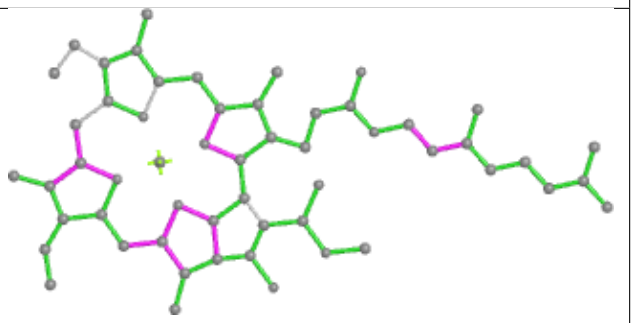
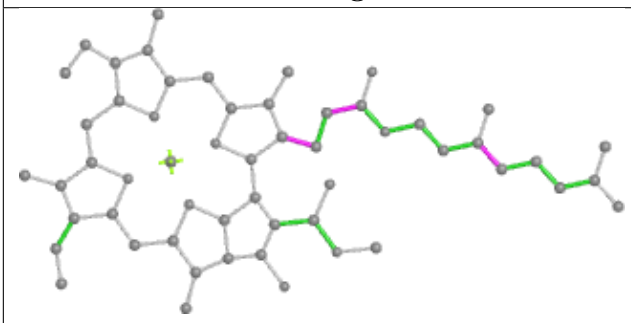


Bond angles



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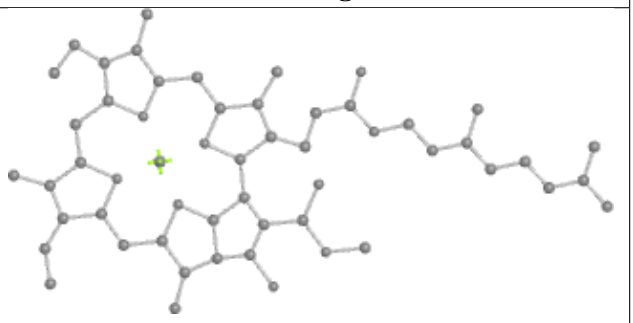
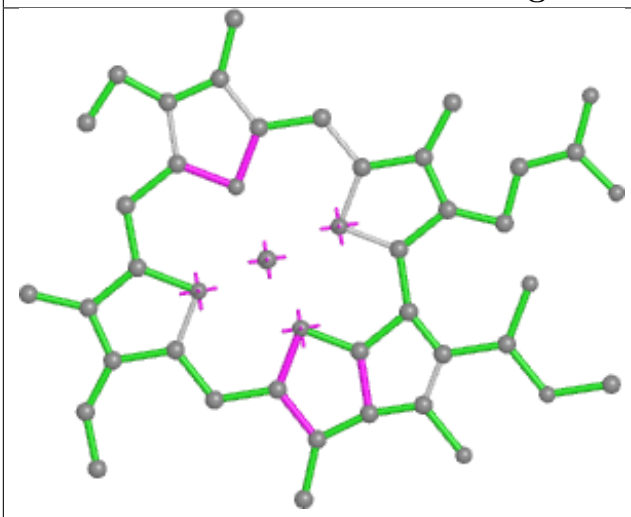


Rings

Ligand CLA 6 601



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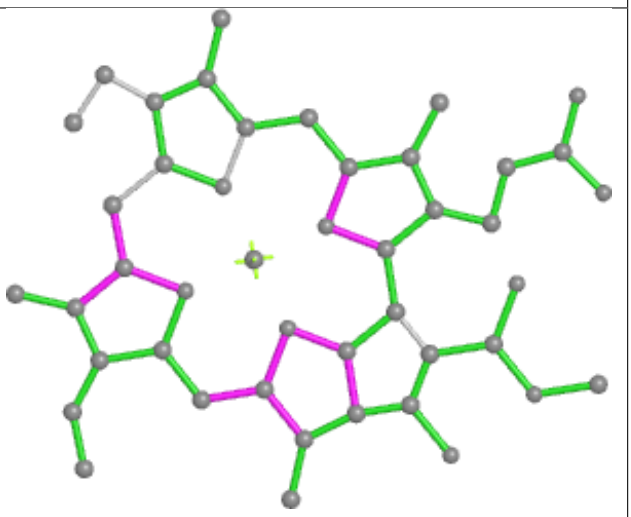
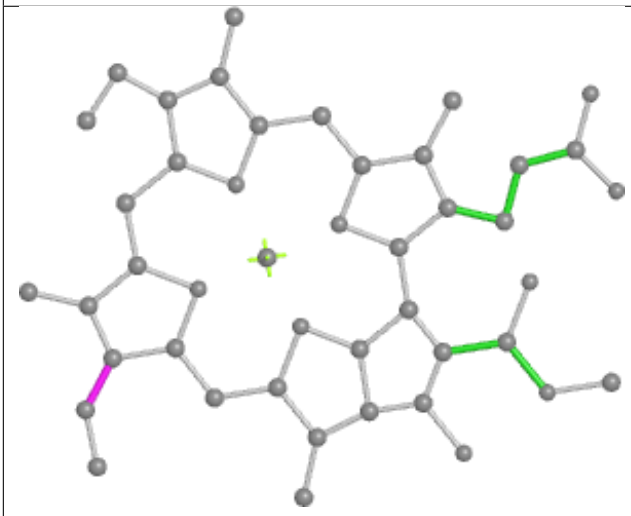


Bond angles



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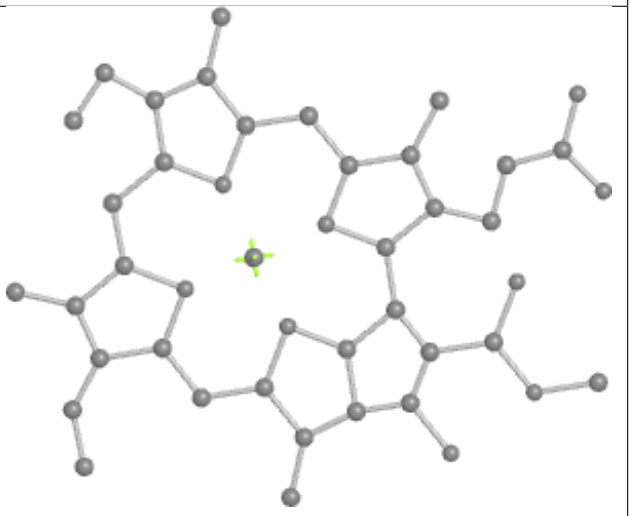
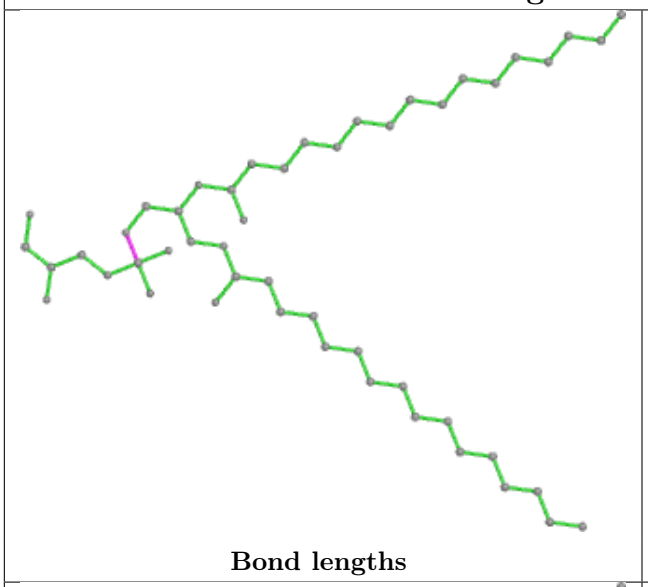
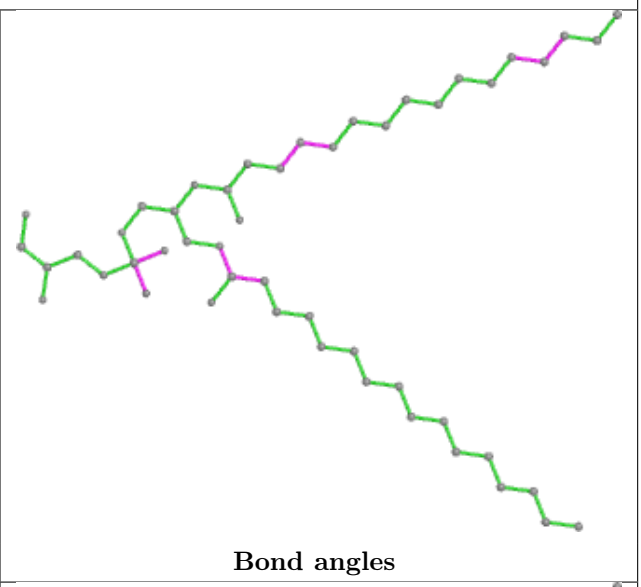


Rings

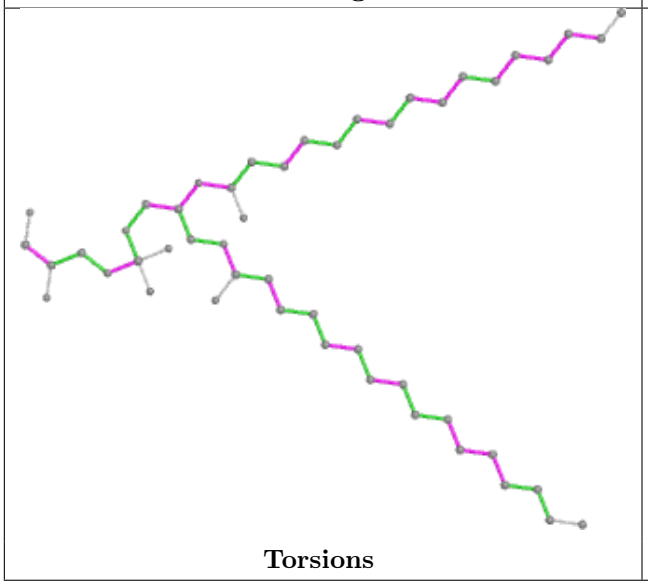
Ligand LHG b 616



Bond lengths



Bond angles



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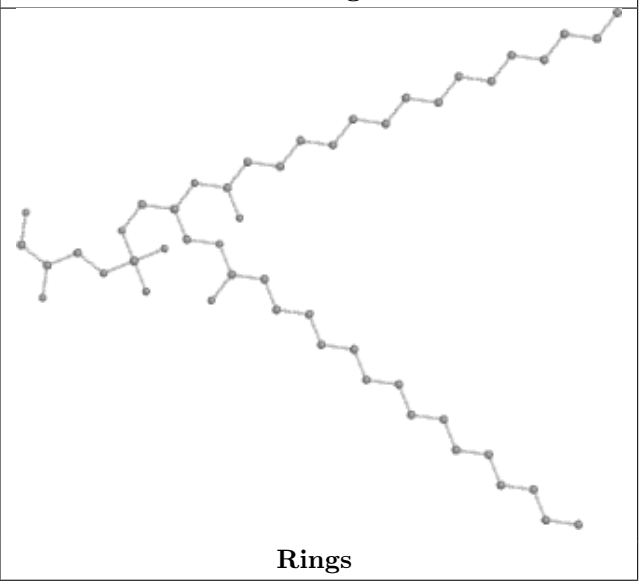
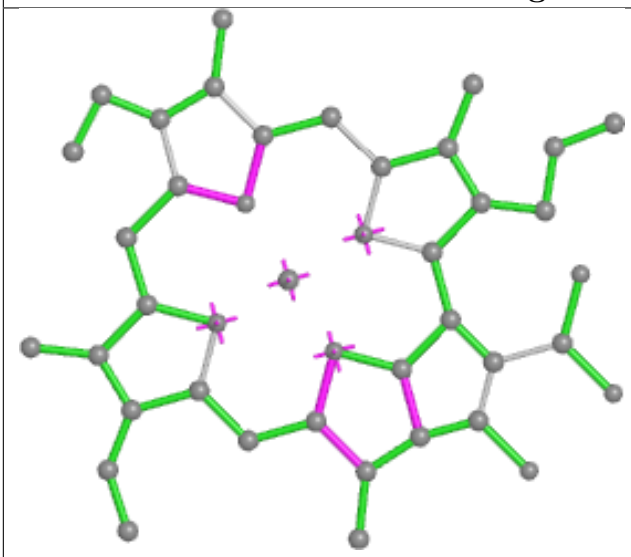


Rings

Ligand CLA 1 605



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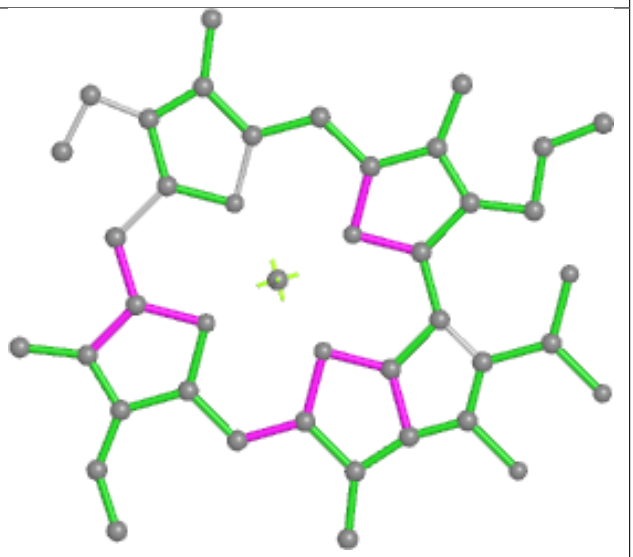
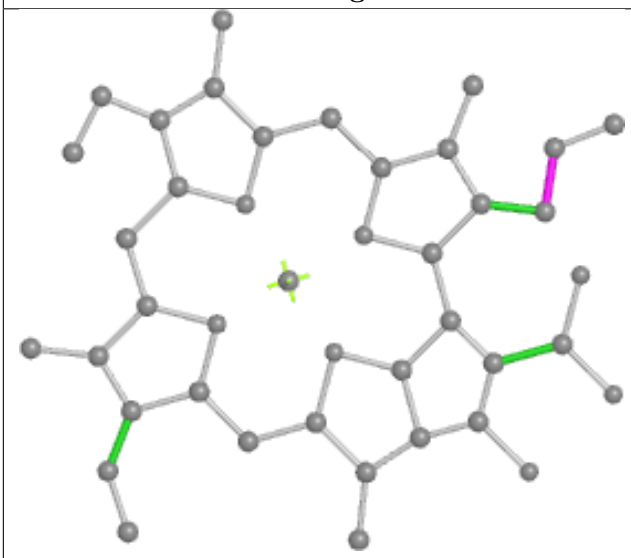
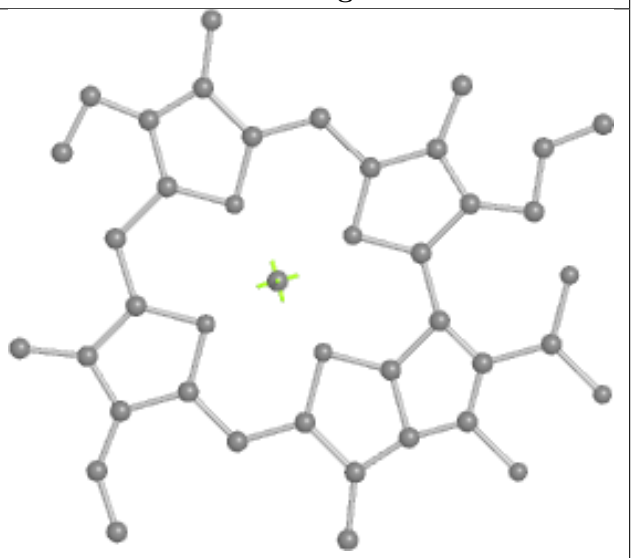


Bond angles

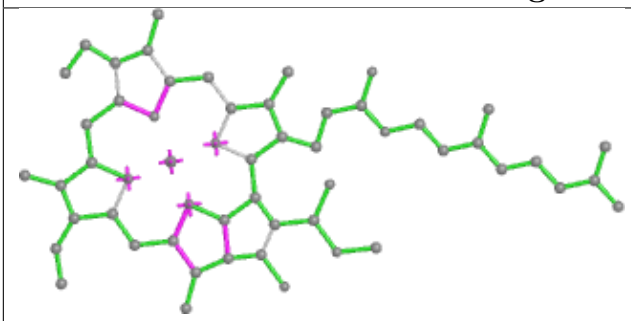


Torsions

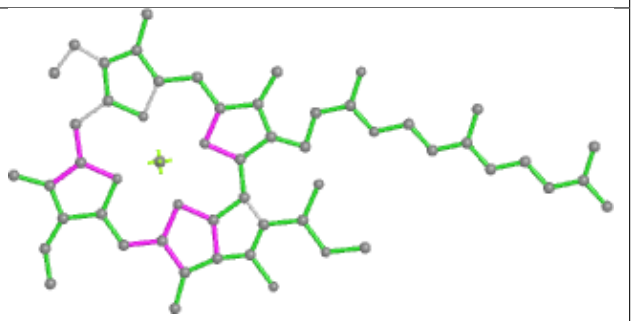


Rings

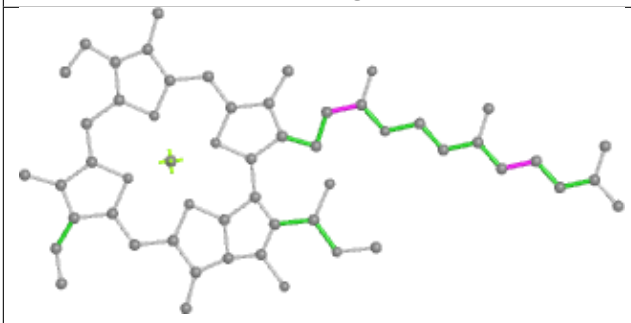
Ligand CLA 3 605



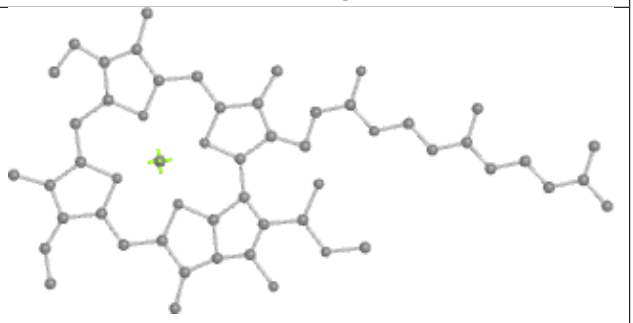
Bond lengths



Bond angles

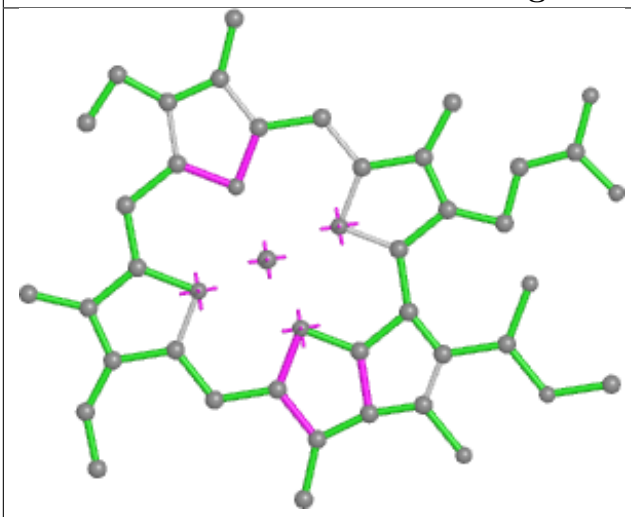


Torsions

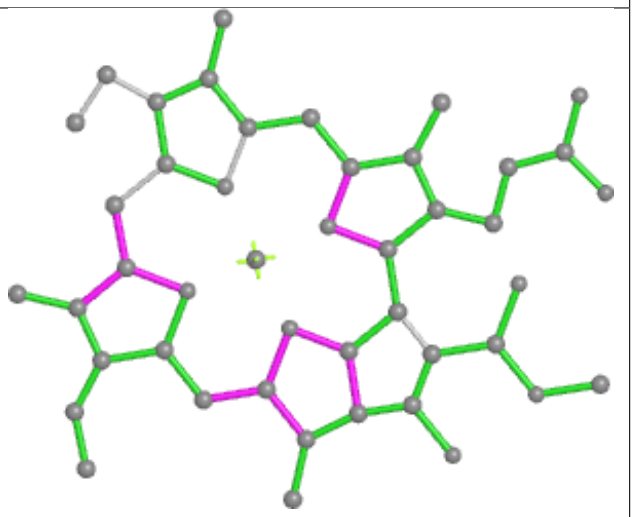


Rings

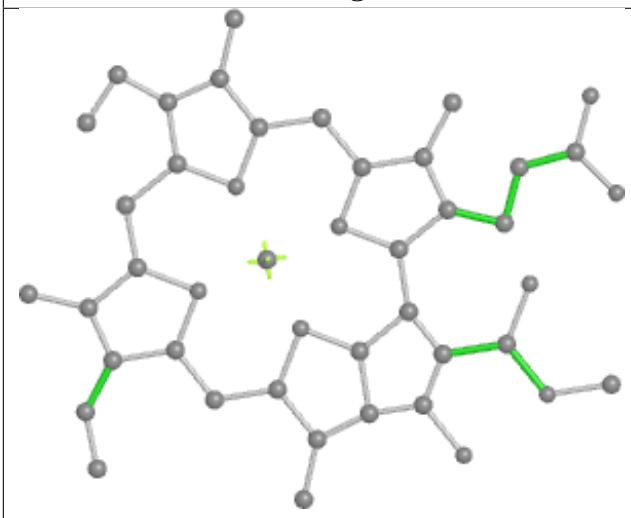
Ligand CLA 2 607



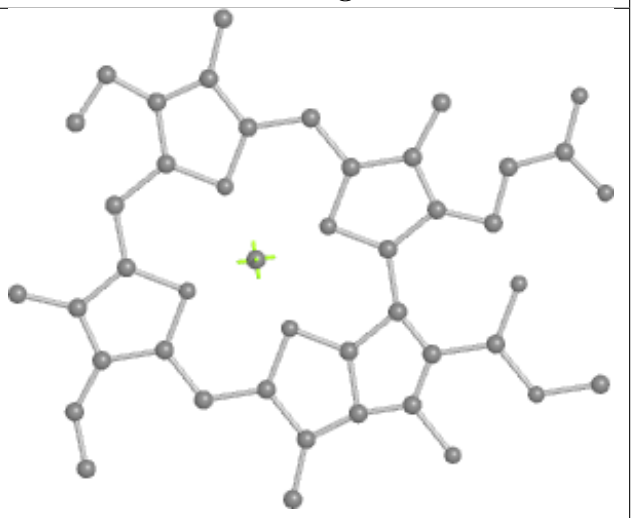
Bond lengths



Bond angles

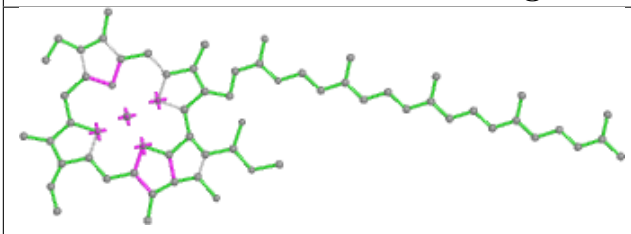


Torsions



Rings

Ligand CLA A 843



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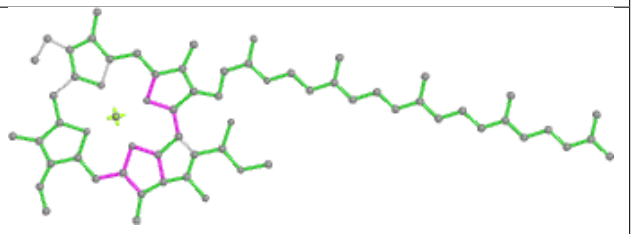
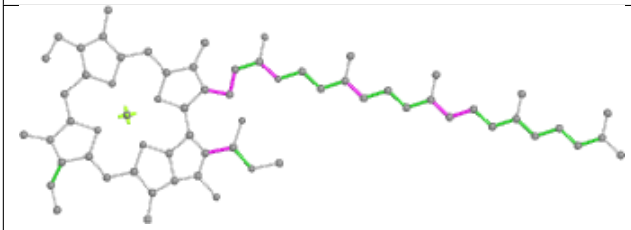
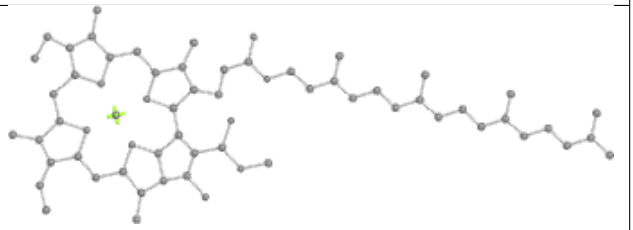


Bond angles

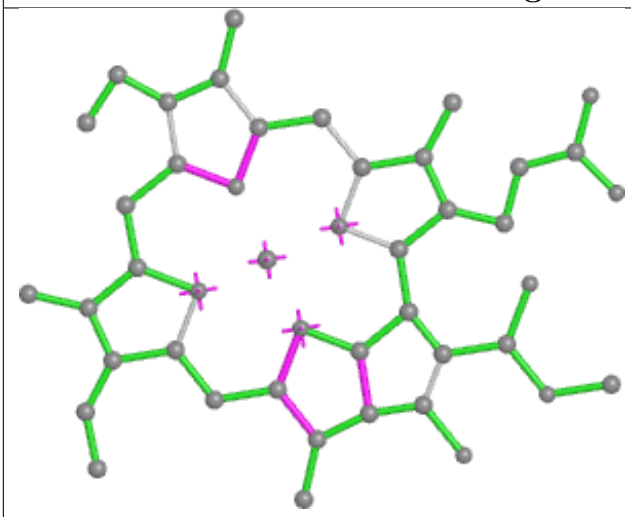


Torsions

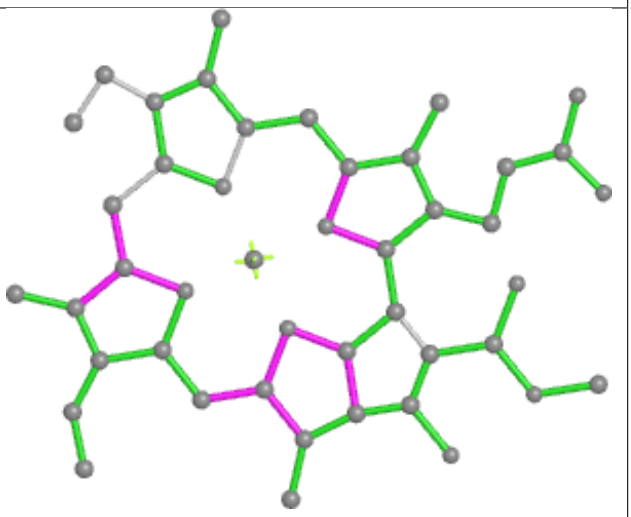


Rings

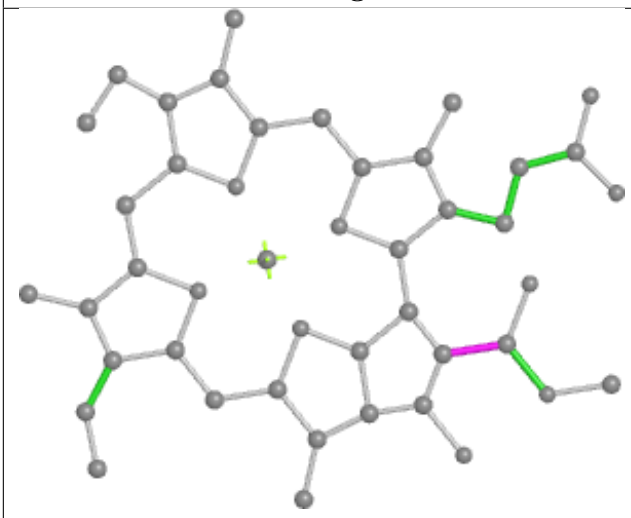
Ligand CLA B 833



Bond lengths



Bond angles



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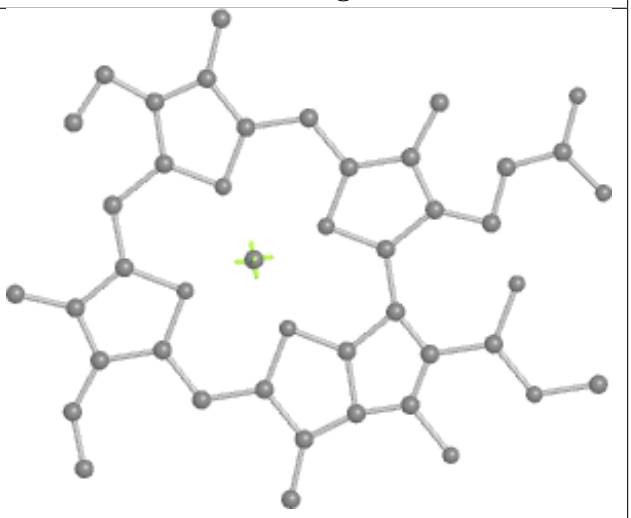
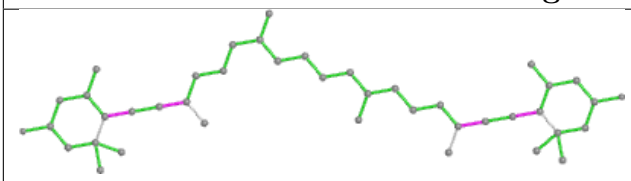
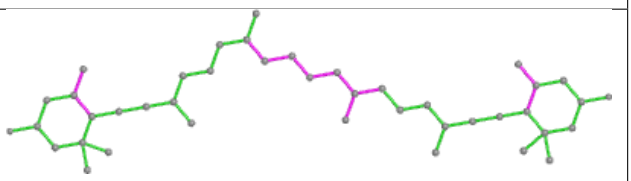


Rings

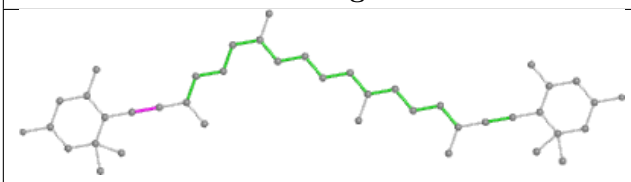
Ligand II0 8 612



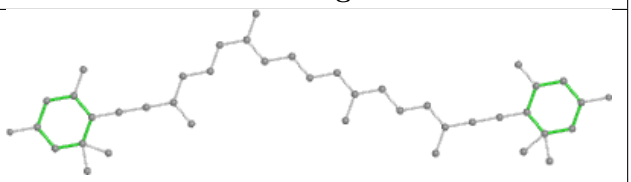
Bond lengths



Bond angles

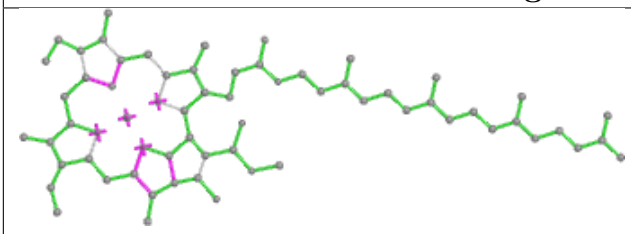


Torsions

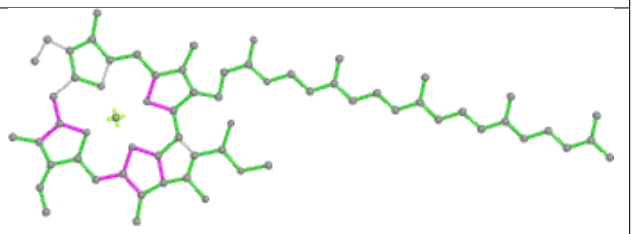


Rings

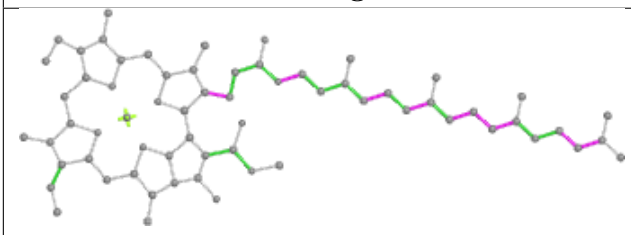
Ligand CLA B 826



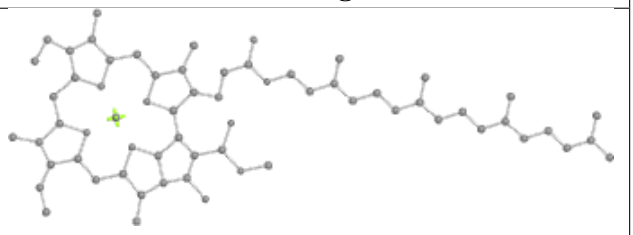
Bond lengths



Bond angles

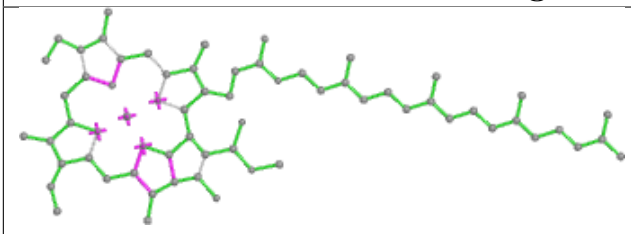


Torsions

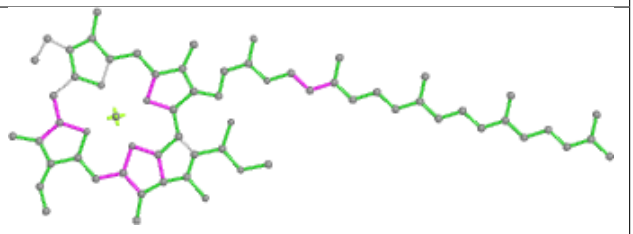


Rings

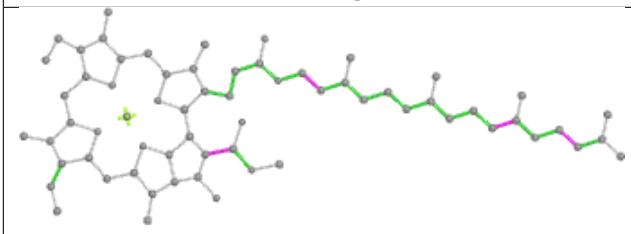
Ligand CLA 8 615



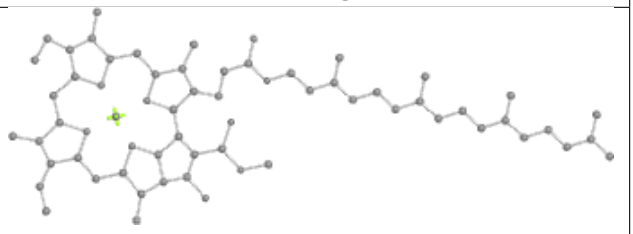
Bond lengths



Bond angles

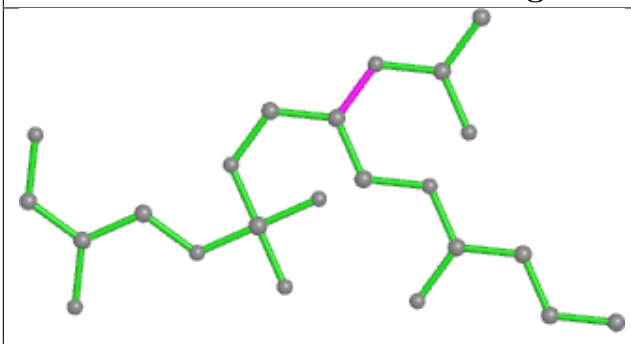


Torsions

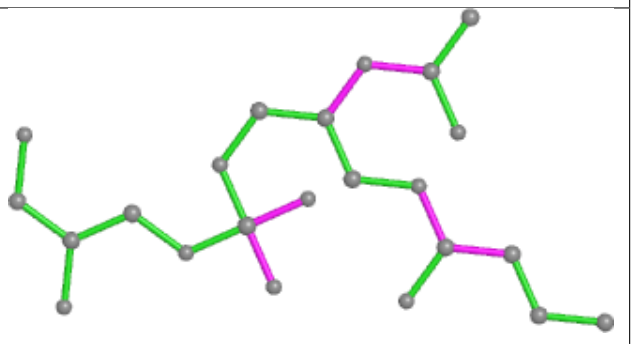


Rings

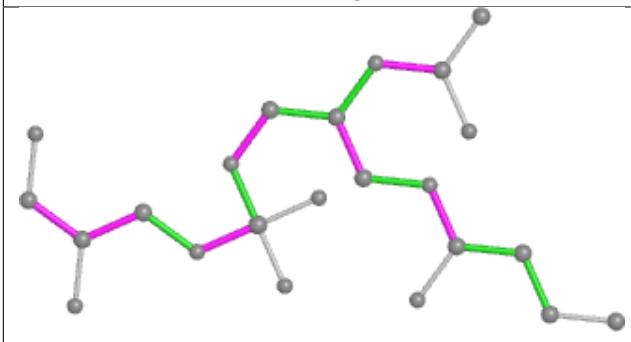
Ligand LHG 5 619



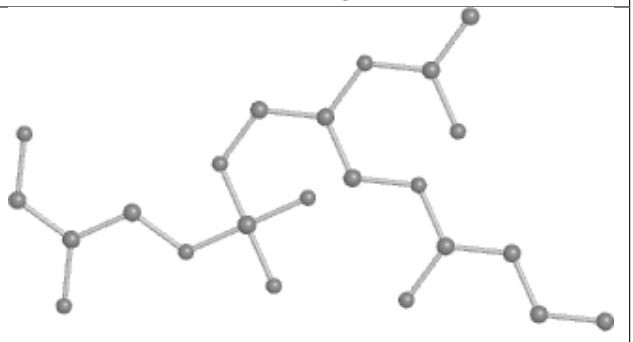
Bond lengths



Bond angles

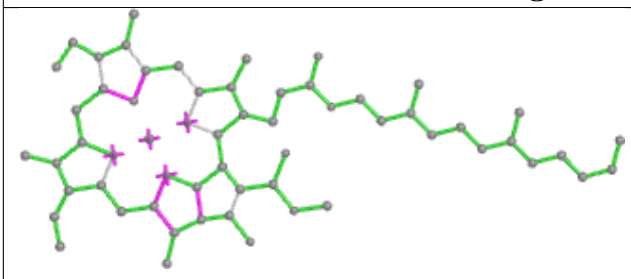


Torsions



Rings

Ligand CLA 4 602



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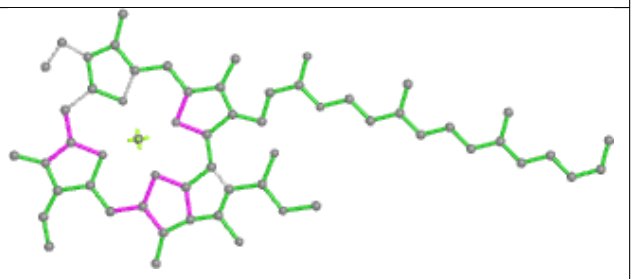
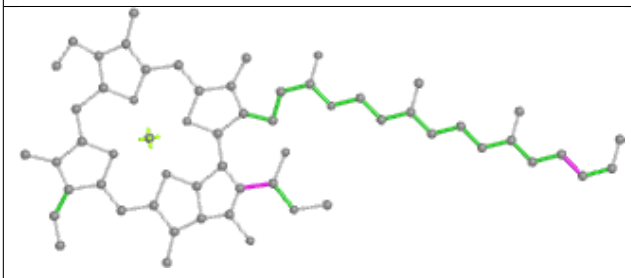


Bond angles



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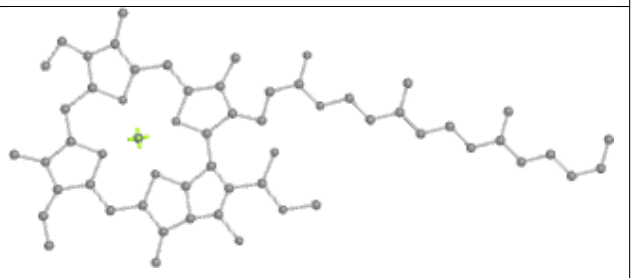
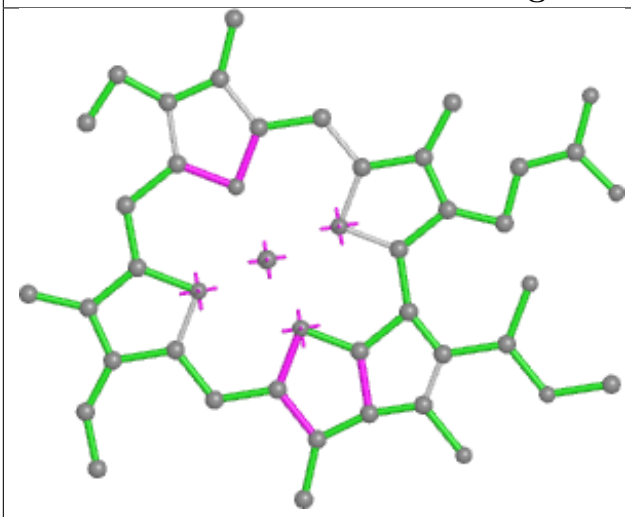


Rings

Ligand CLA 9 613



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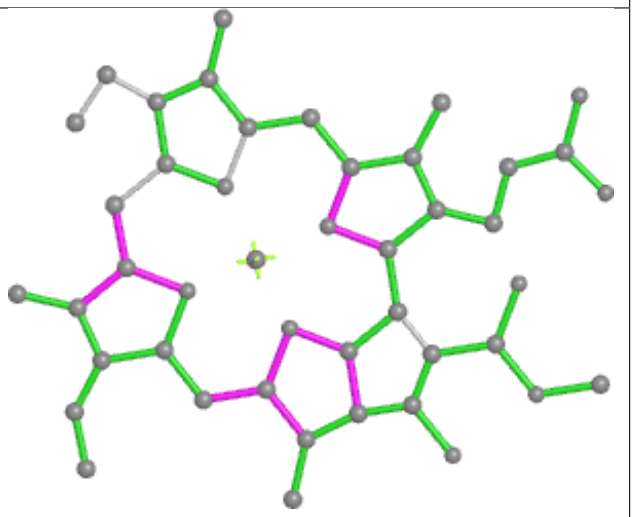
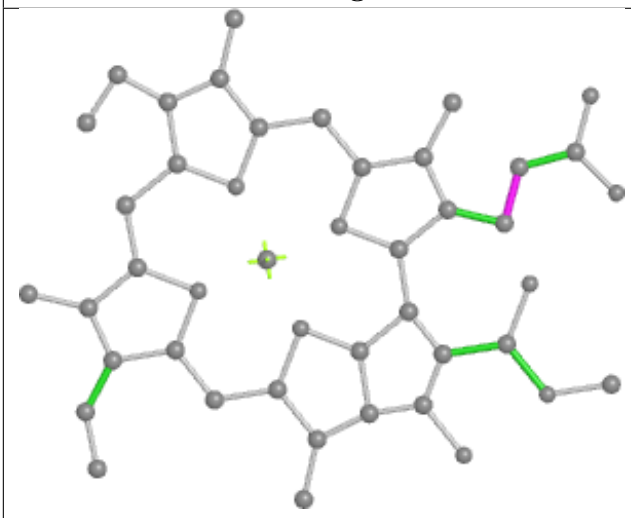


Bond angles



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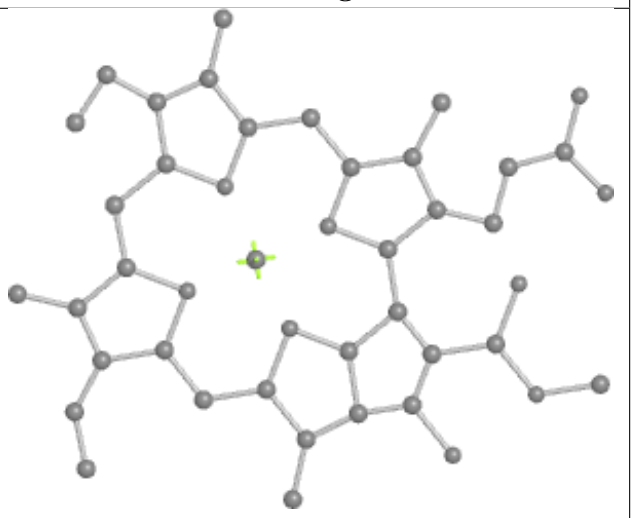
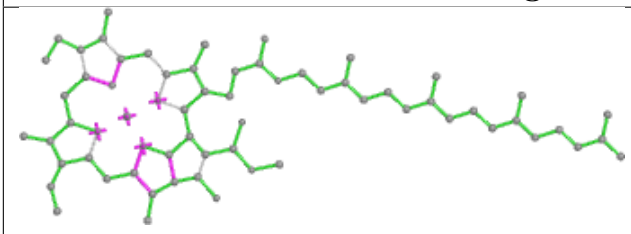


Rings

Ligand CLA A 806



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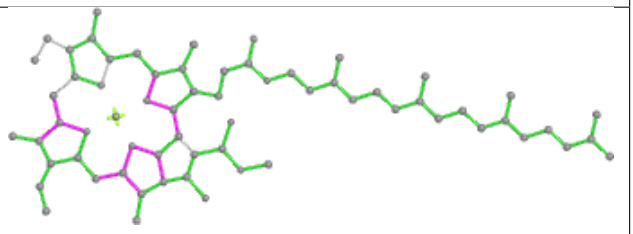
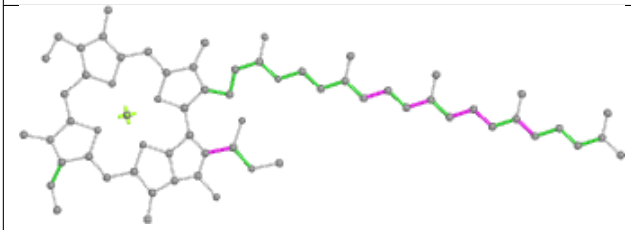


Bond angles



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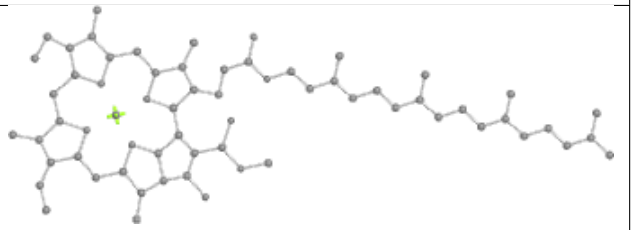
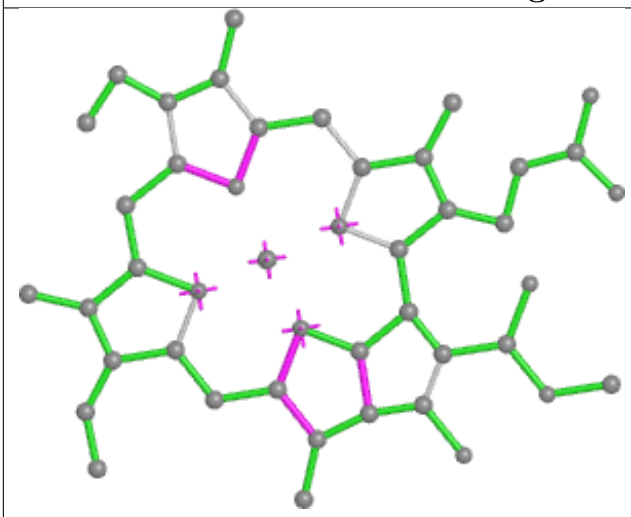


Rings

Ligand CLA 9 601



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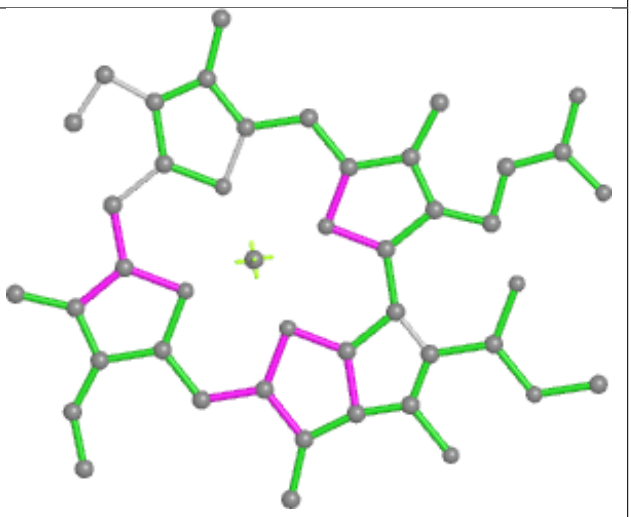
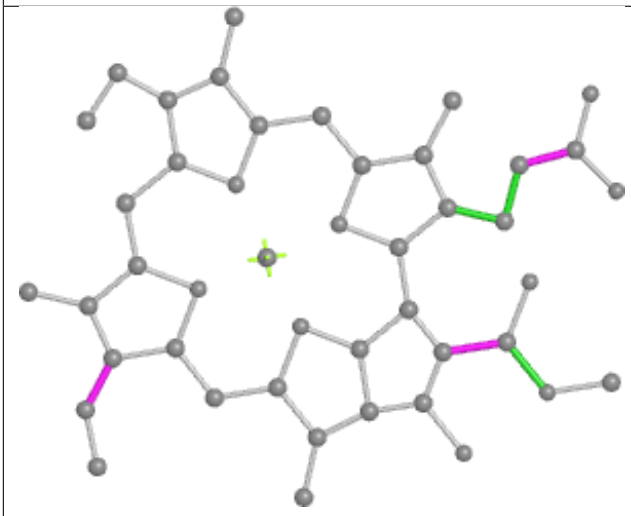


Bond angles



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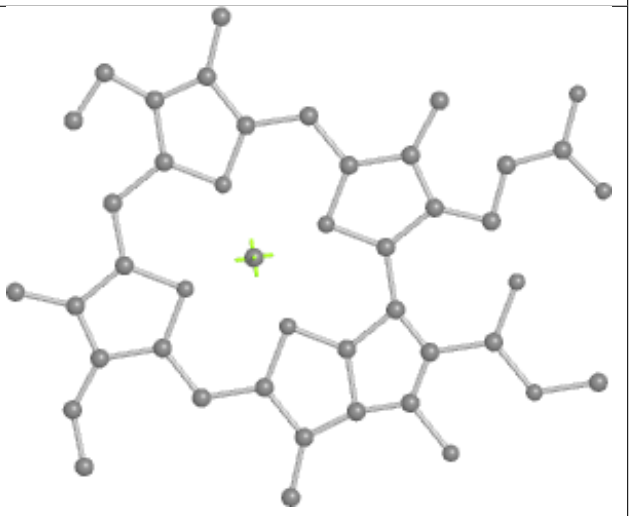
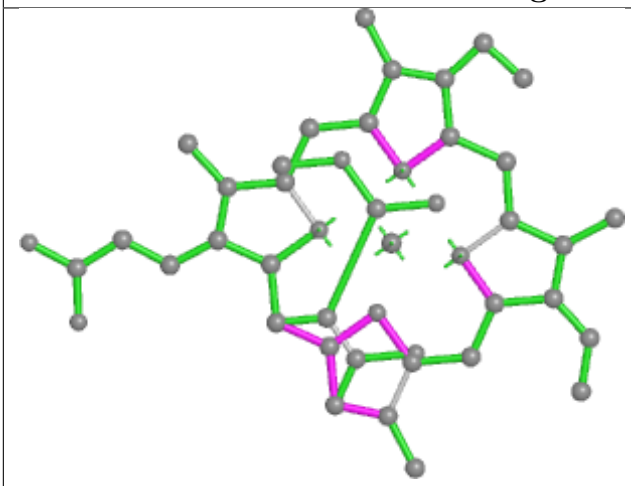


Rings

Ligand KC2 9 610



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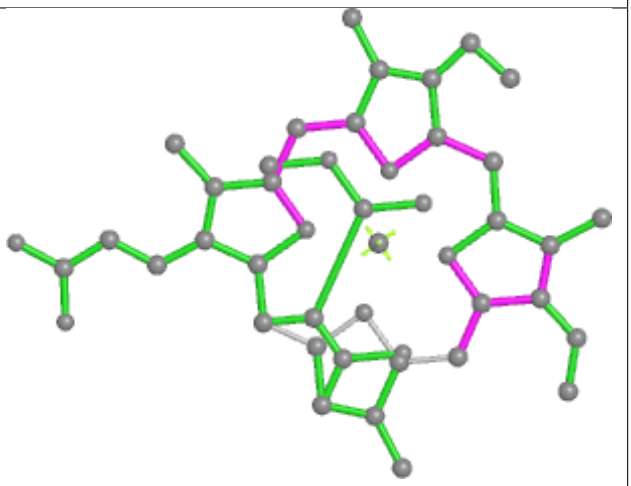
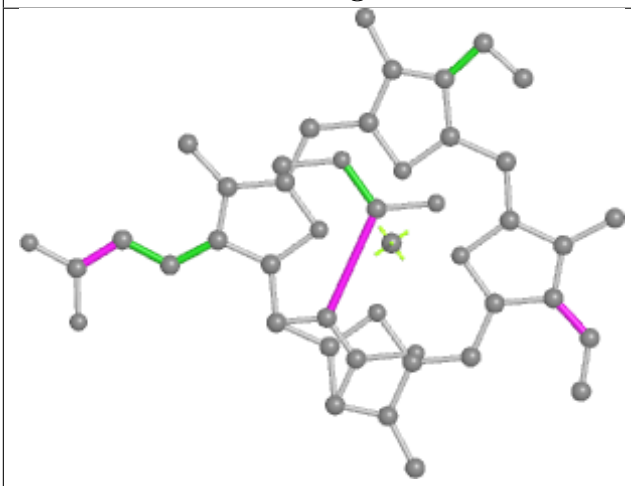


Bond angles



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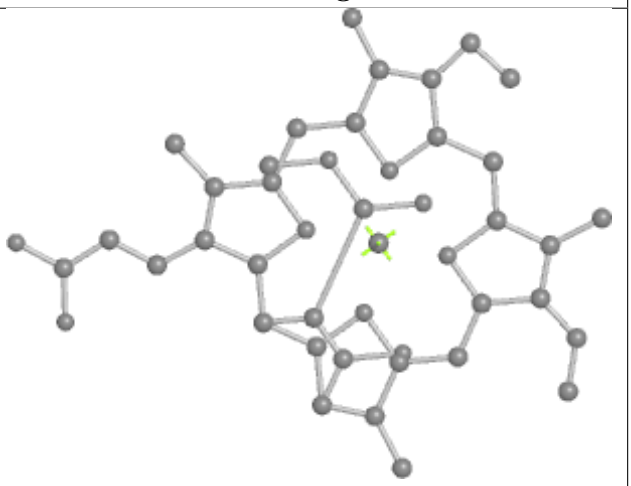
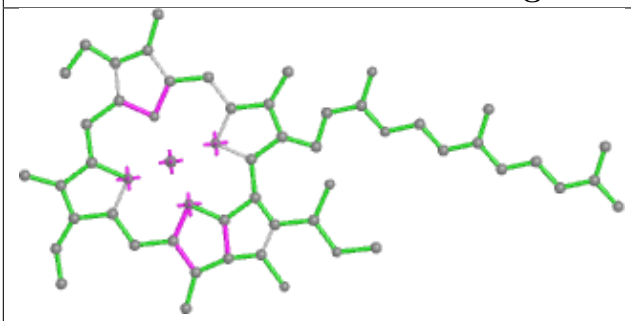


Rings

Ligand CLA O 203



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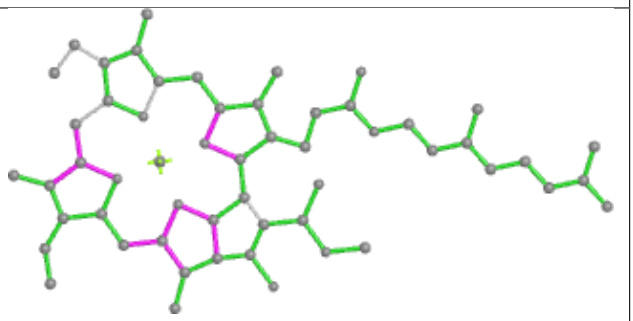
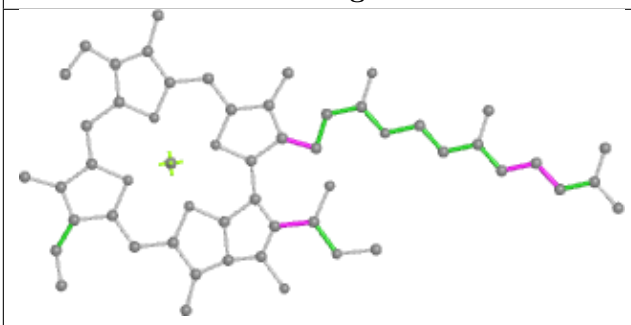


Bond angles



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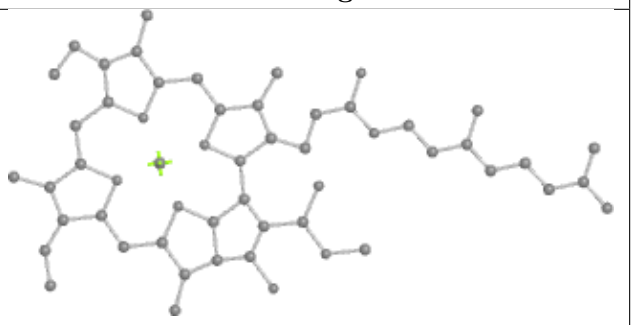
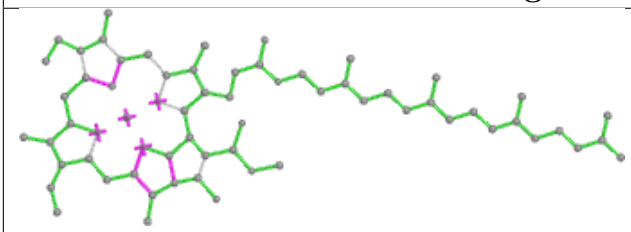


Rings

Ligand CLA B 812



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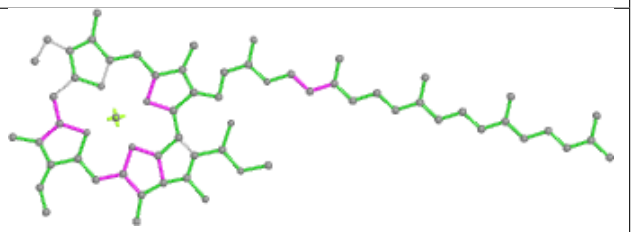
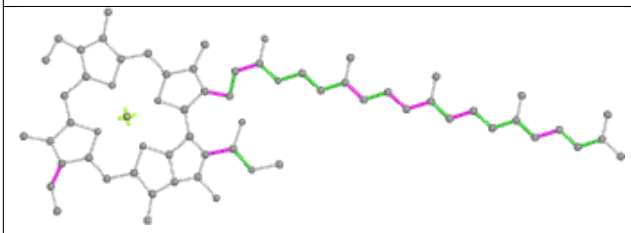


Bond angles



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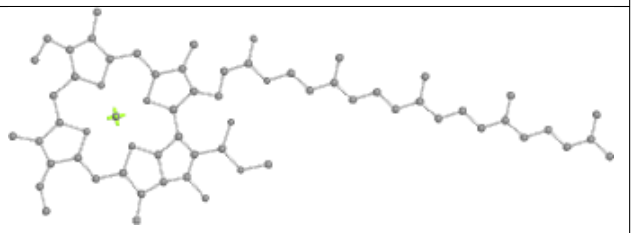
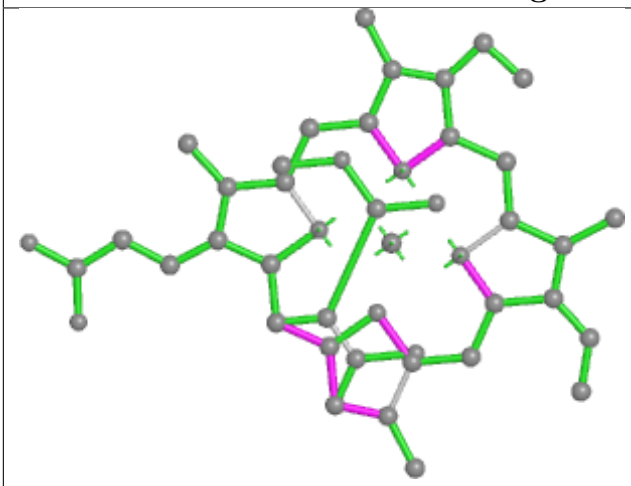
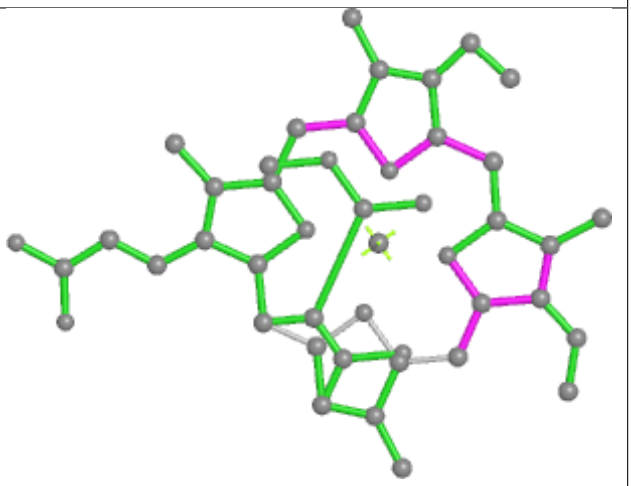


Rings

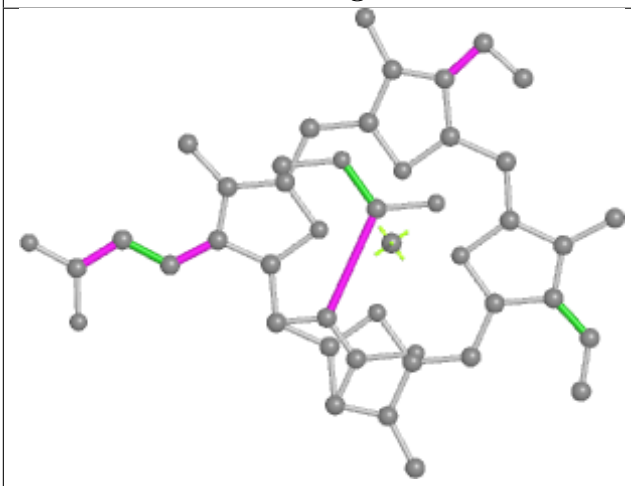
Ligand KC2 1 610



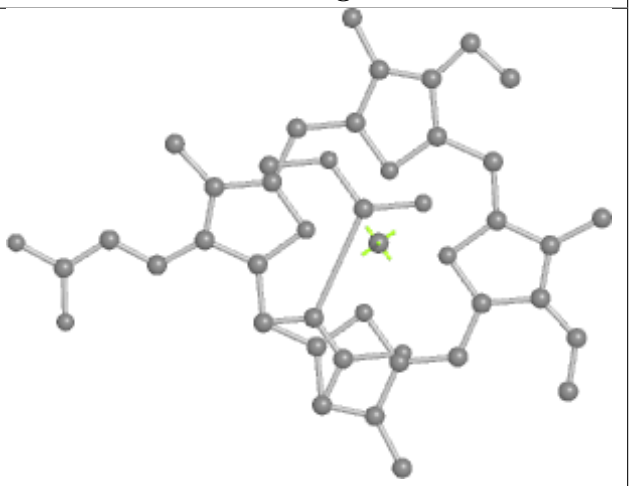
Bond lengths



Bond angles

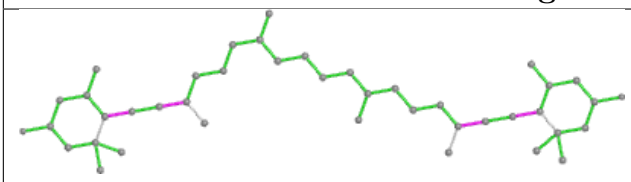


Torsions



Rings

Ligand II0 O 206



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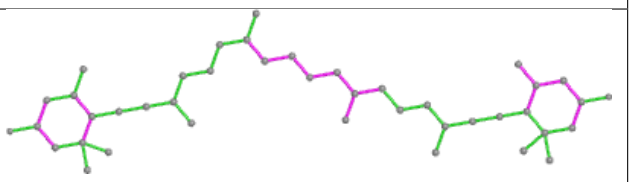
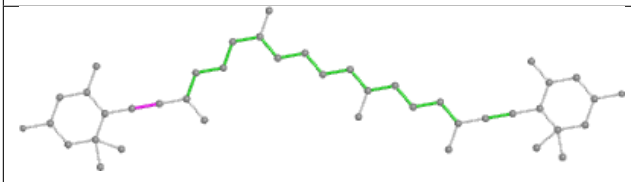
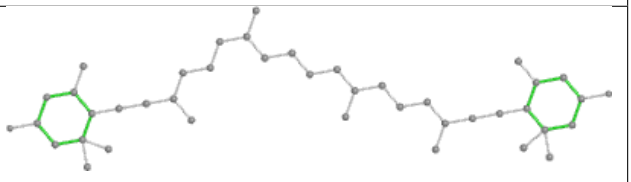


Bond angles

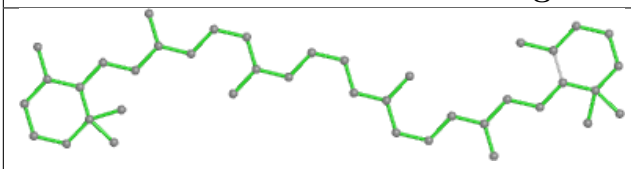


Torsions



Rings

Ligand 8CT I 101



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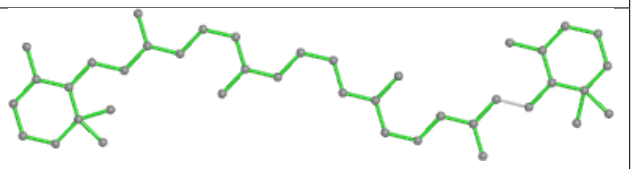
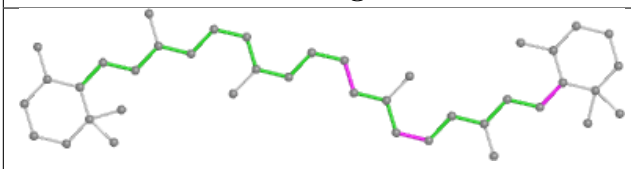
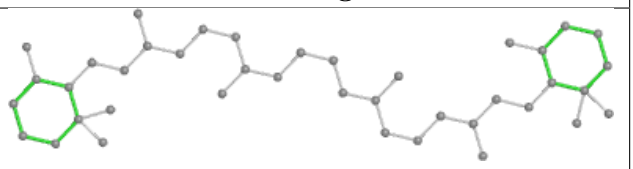


Bond angles

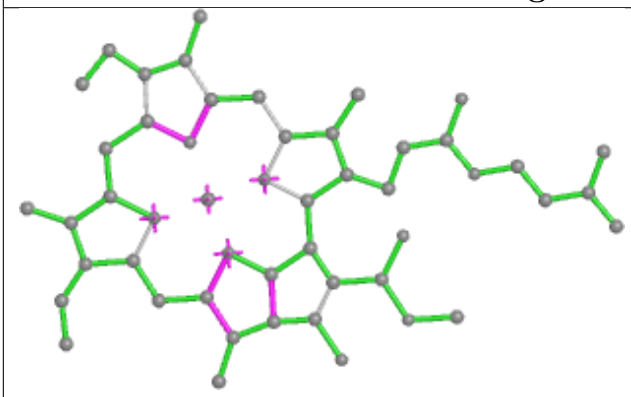


Torsions



Rings

Ligand CLA 7 313



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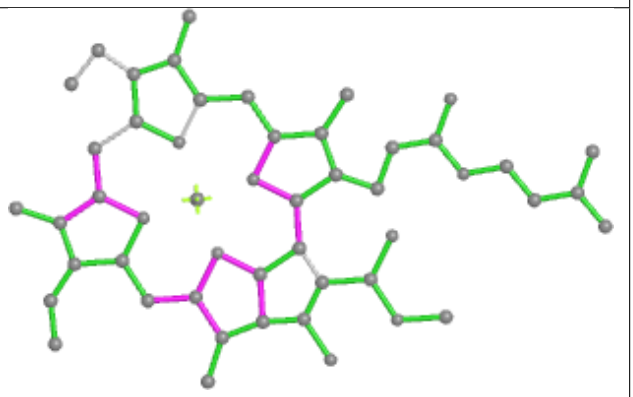
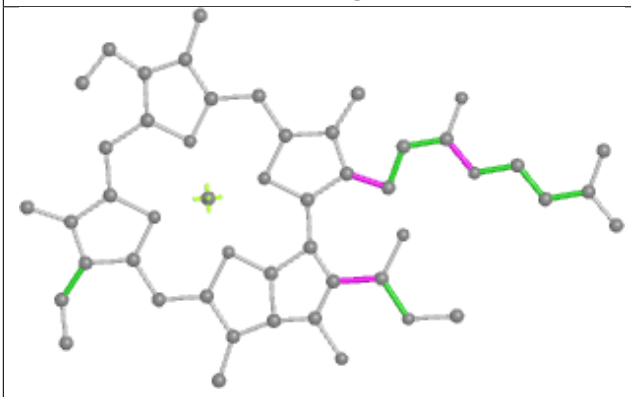
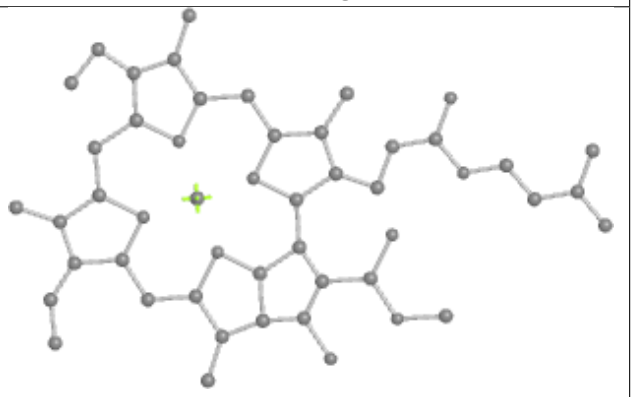


Bond angles

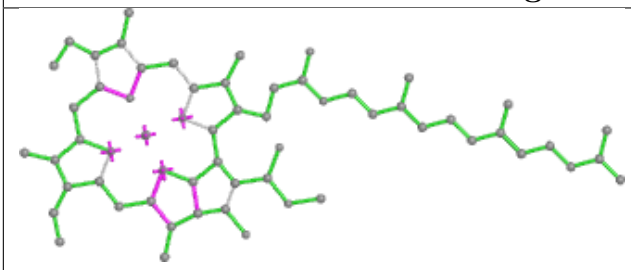


Torsions

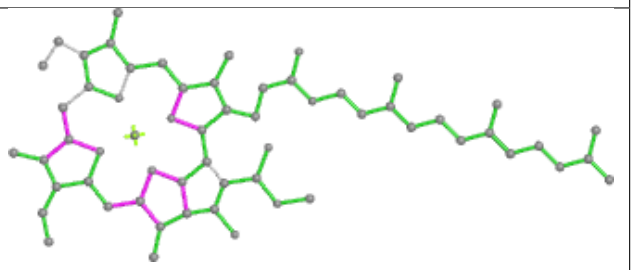


Rings

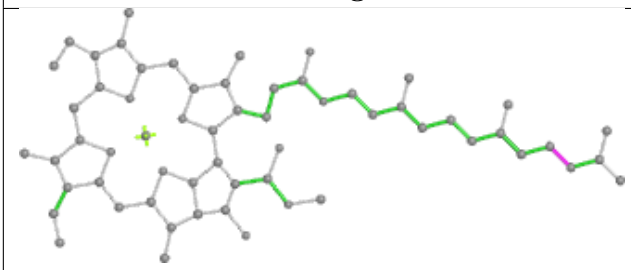
Ligand CLA B 817



Bond lengths



Bond angles



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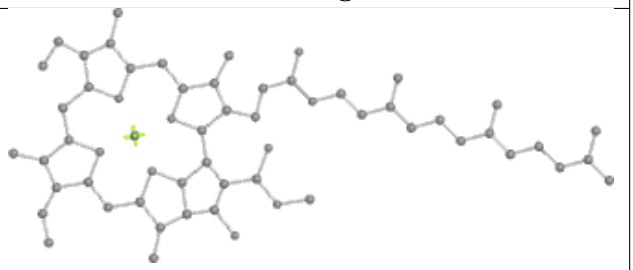
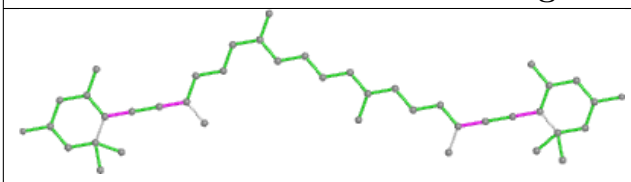


Rings

Ligand II0 O 205



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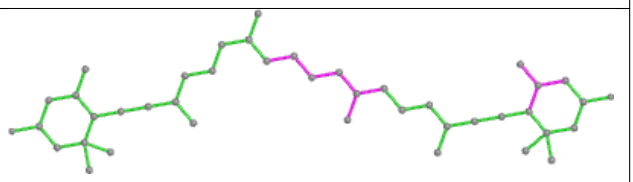
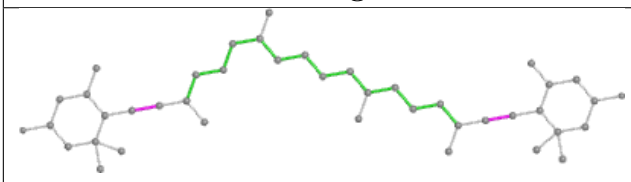
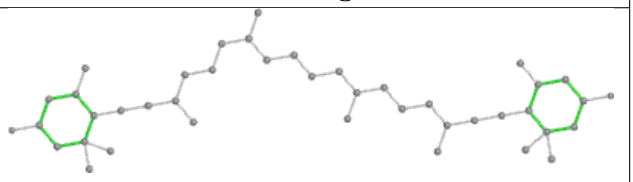


Bond angles

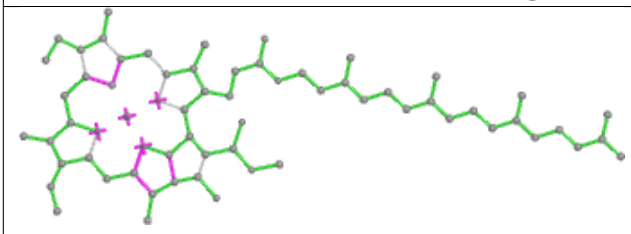


Torsions

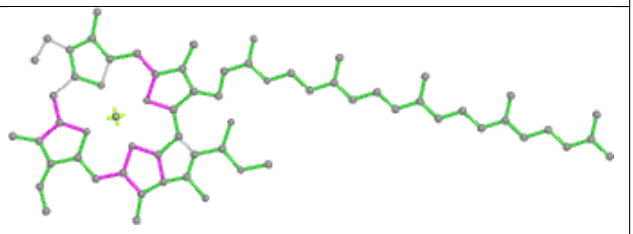


Rings

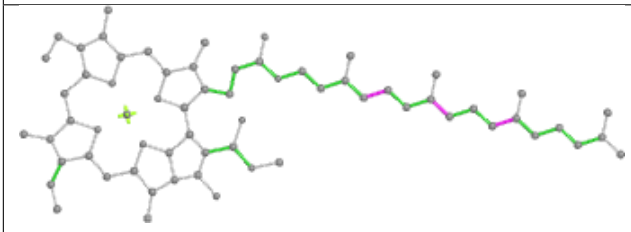
Ligand CLA A 833



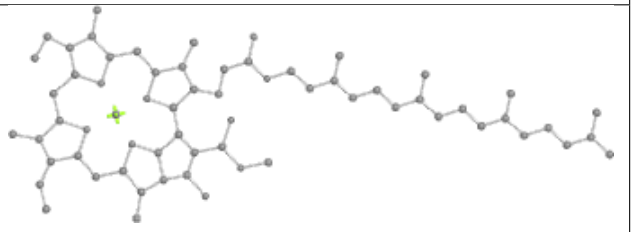
Bond lengths



Bond angles

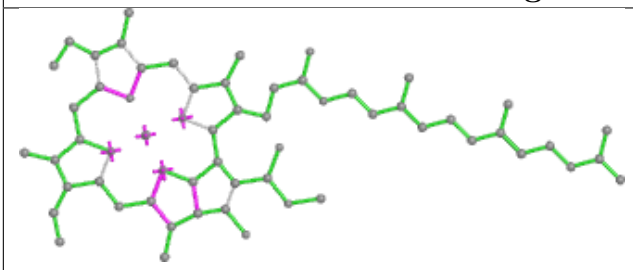


Torsions

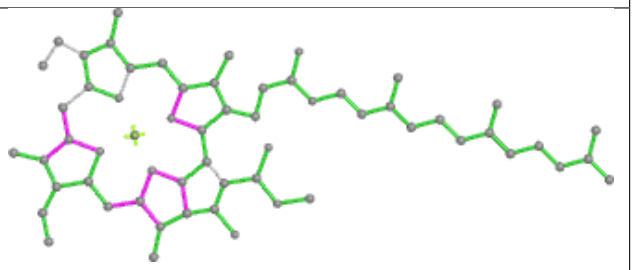


Rings

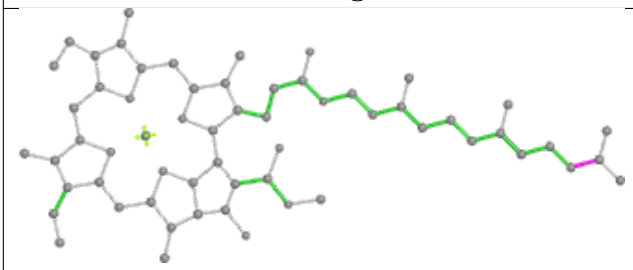
Ligand CLA B 818



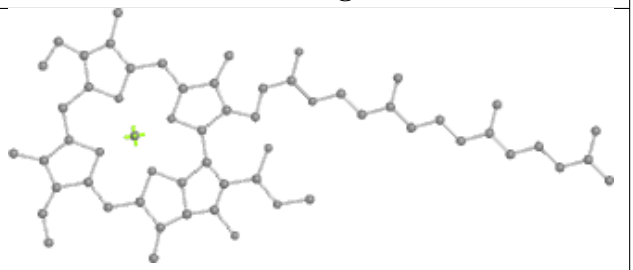
Bond lengths



Bond angles

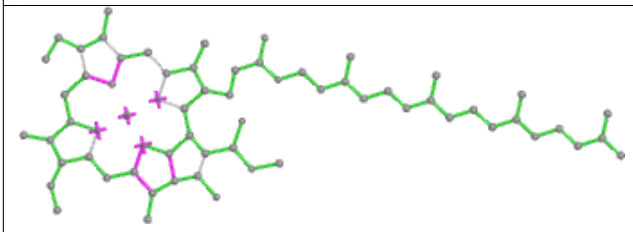


Torsions

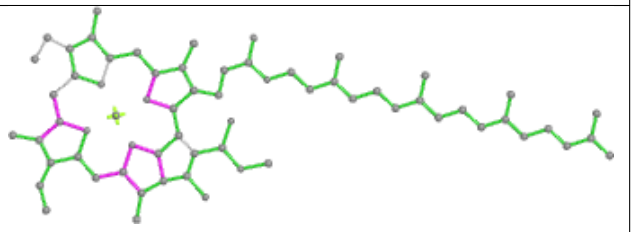


Rings

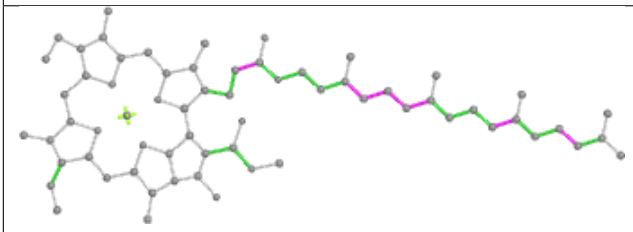
Ligand CLA B 805



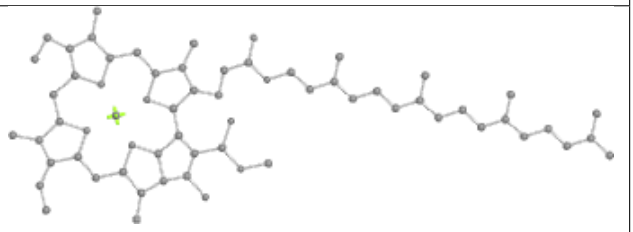
Bond lengths



Bond angles

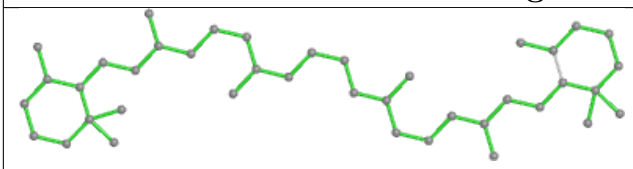


Torsions

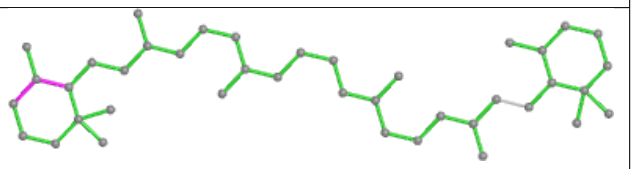


Rings

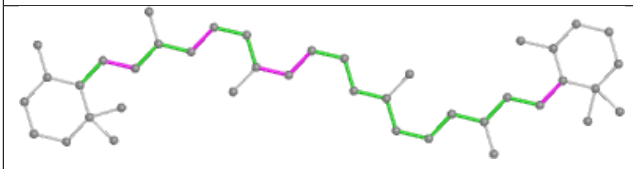
Ligand 8CT A 853



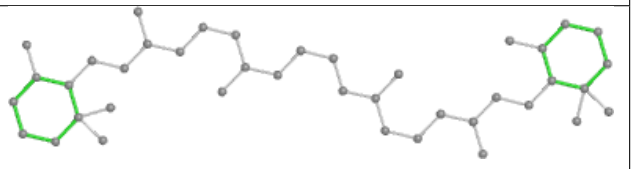
Bond lengths



Bond angles

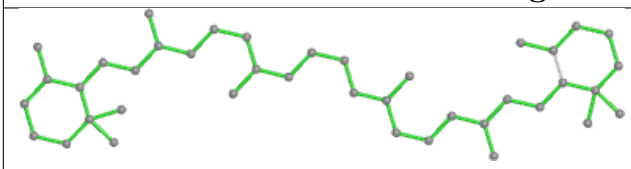


Torsions



Rings

Ligand 8CT Z 308



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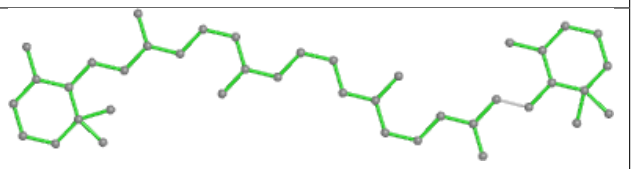
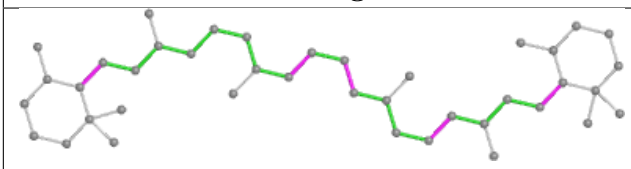
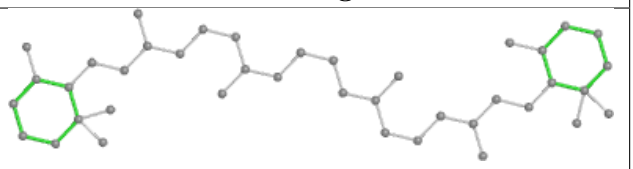


Bond angles

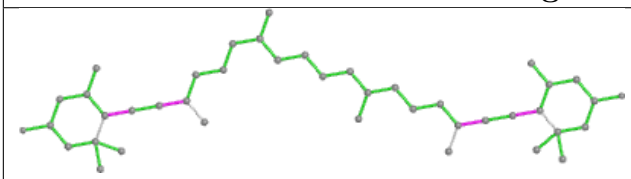


Torsions



Rings

Ligand II0 b 612



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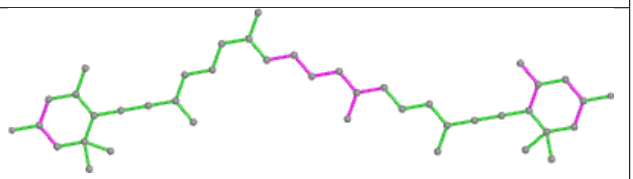
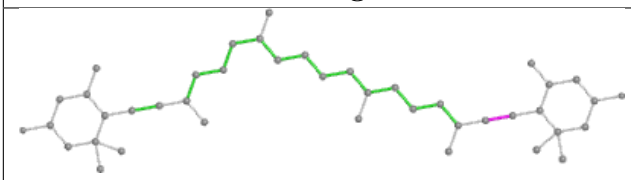


Bond angles



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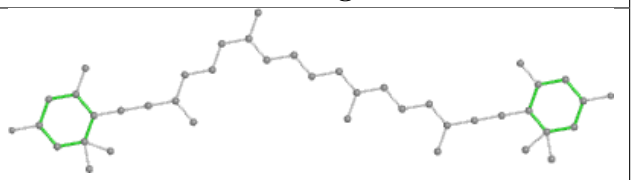
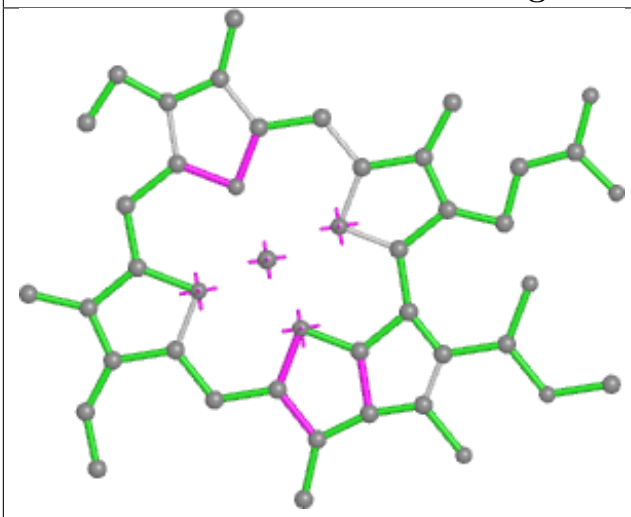


Rings

Ligand CLA 7 302



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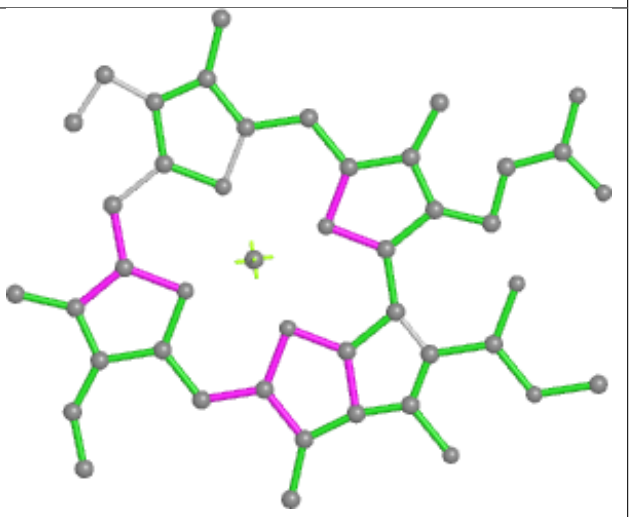
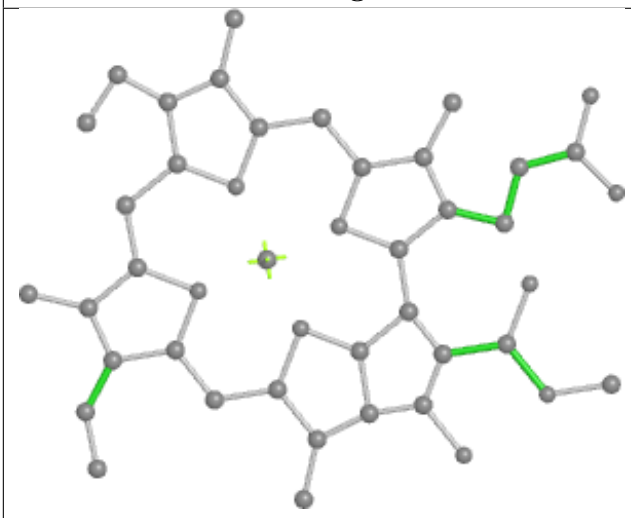


Bond angles



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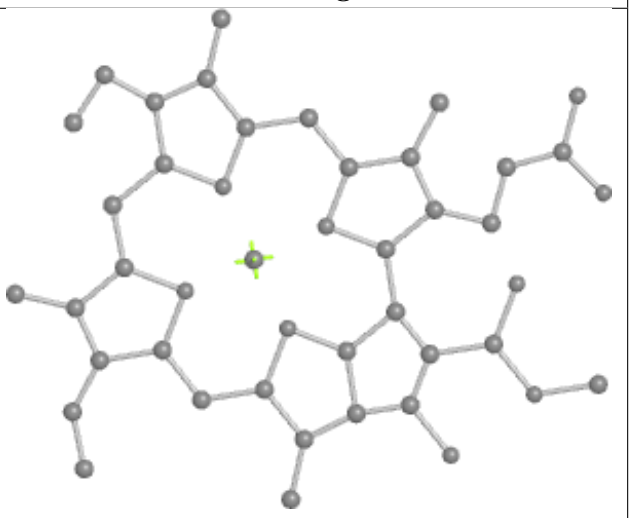
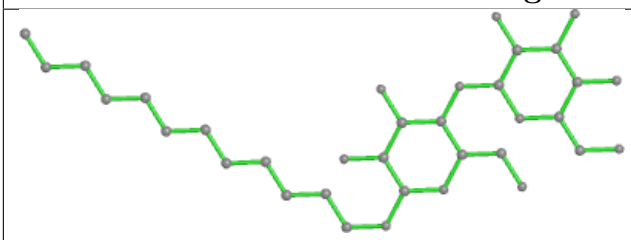


Rings

Ligand LMU 7 321



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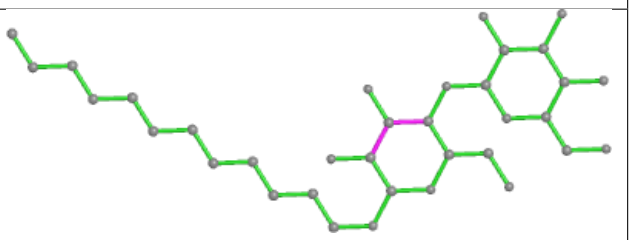
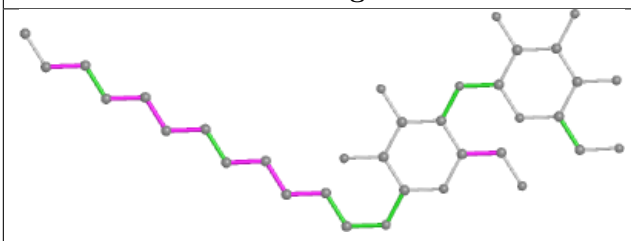


Bond angles



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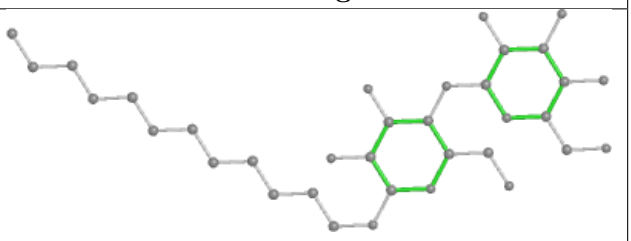
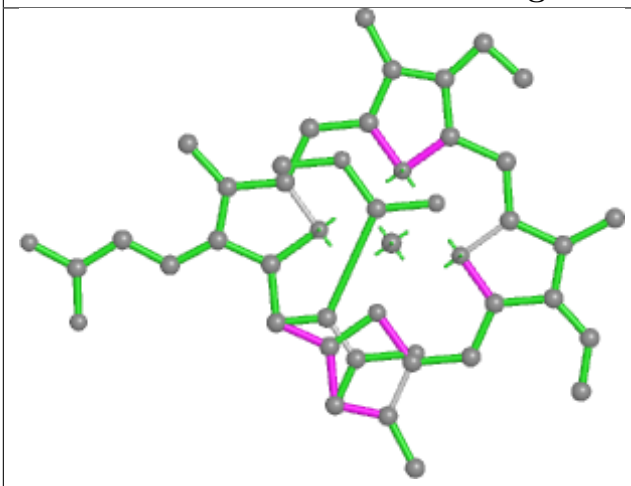
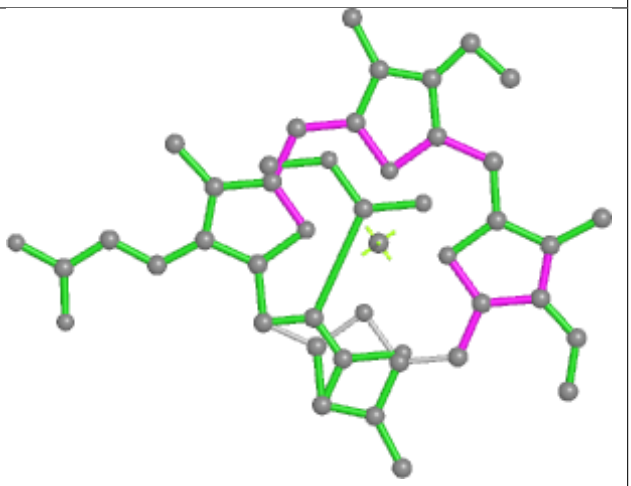


Rings

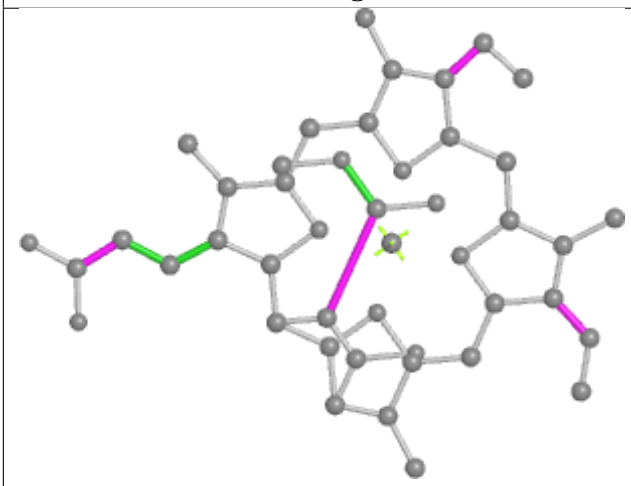
Ligand KC2 Z 307



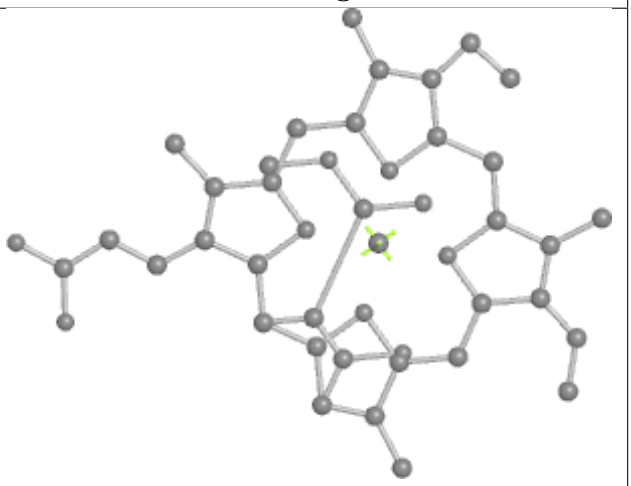
Bond lengths



Bond angles

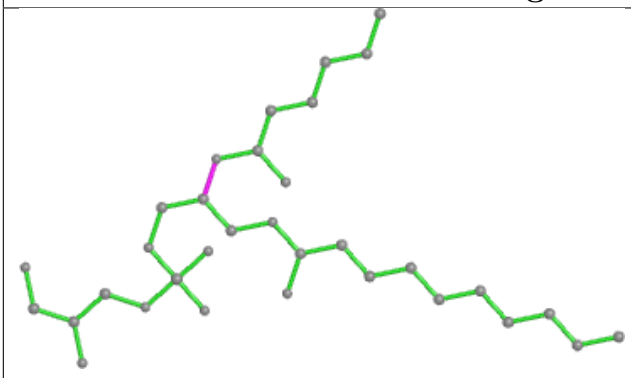


Torsions

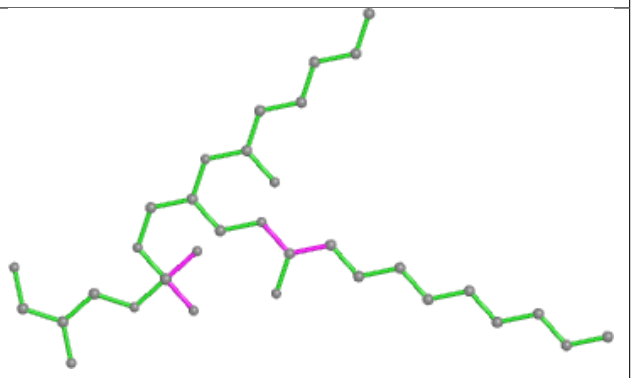


Rings

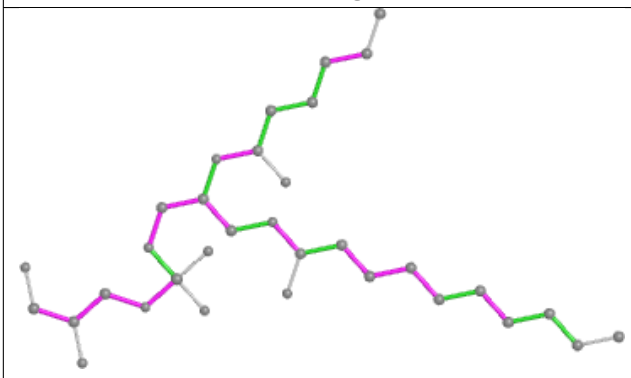
Ligand LHG 8 613



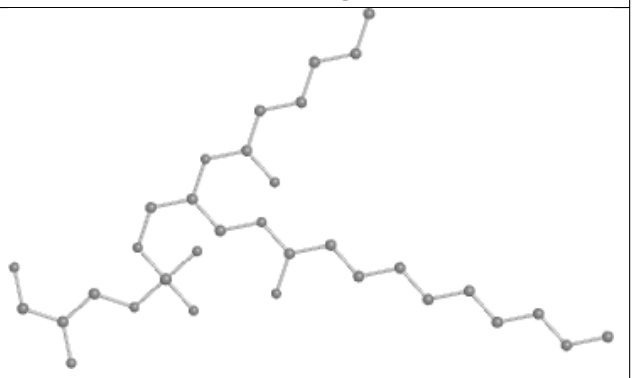
Bond lengths



Bond angles

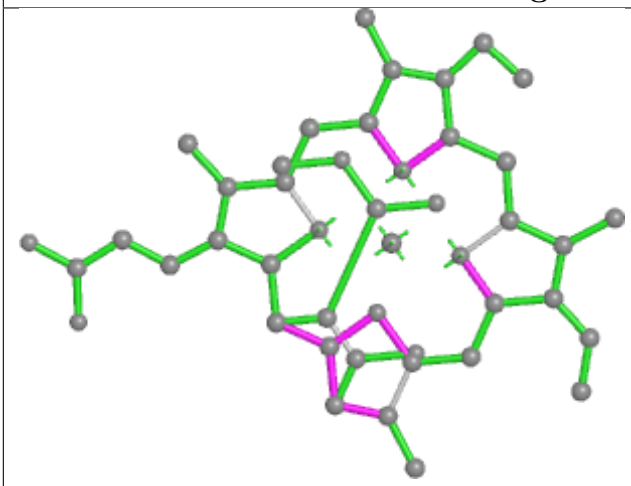


Torsions

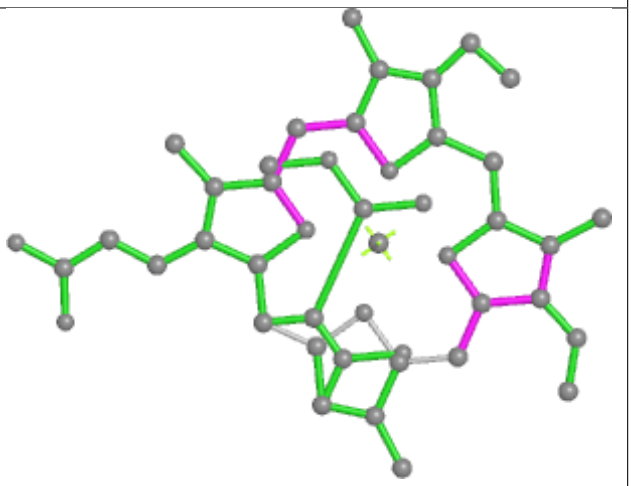


Rings

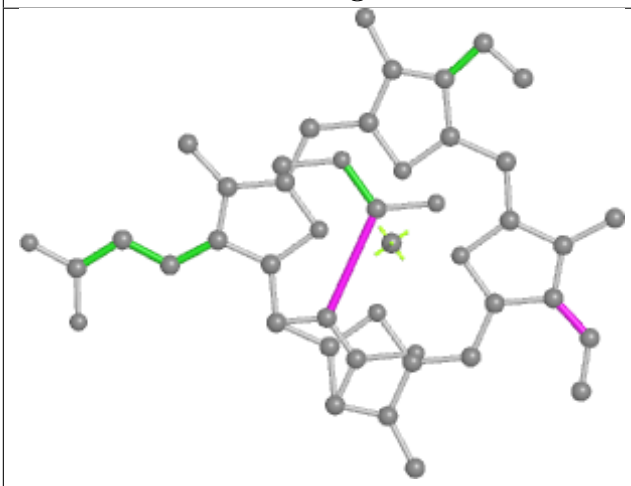
Ligand KC2 a 609



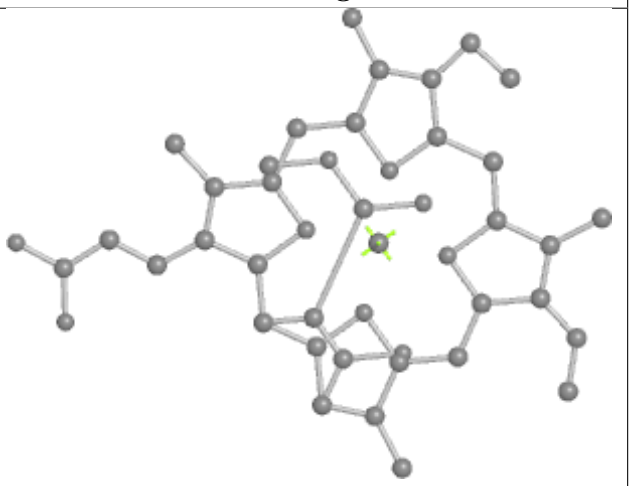
Bond lengths



Bond angles

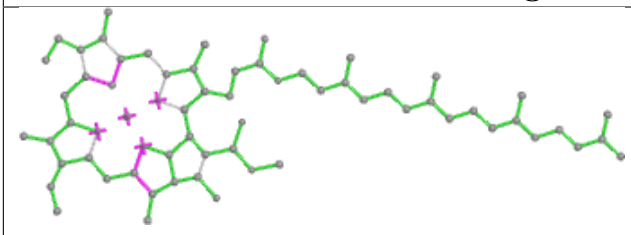


Torsions



Rings

Ligand CLA A 801



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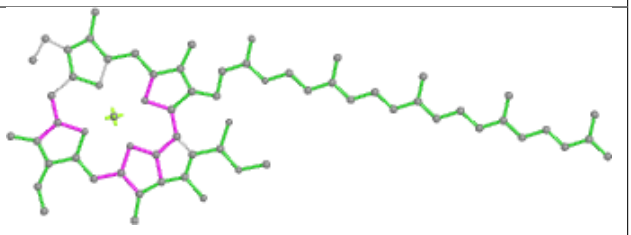
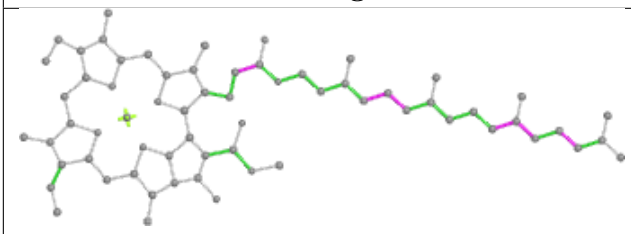
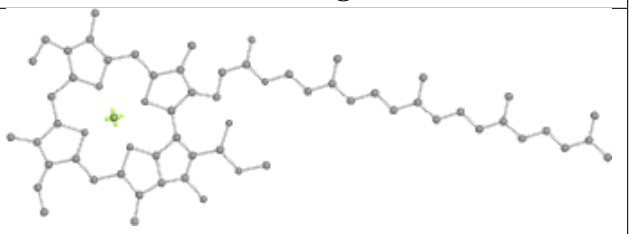


Bond angles

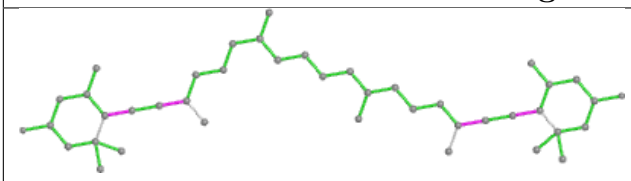


Torsions



Rings

Ligand II0 R 204



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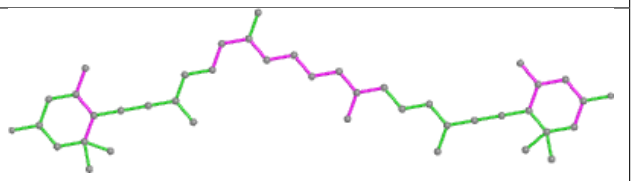
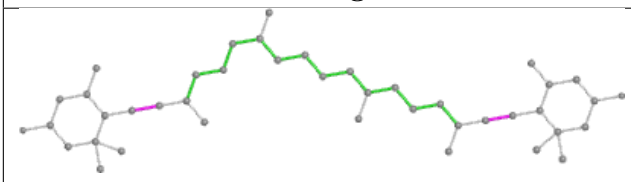


Bond angles



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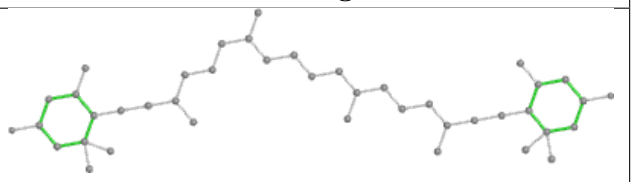
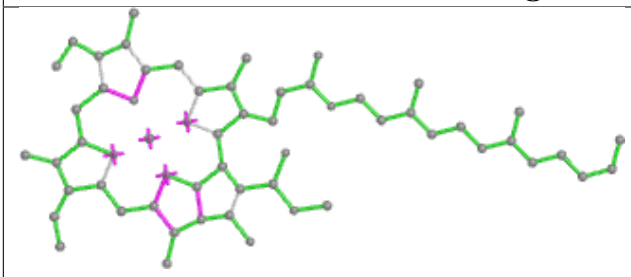
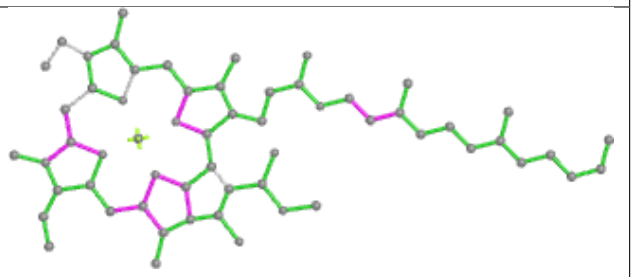


Rings

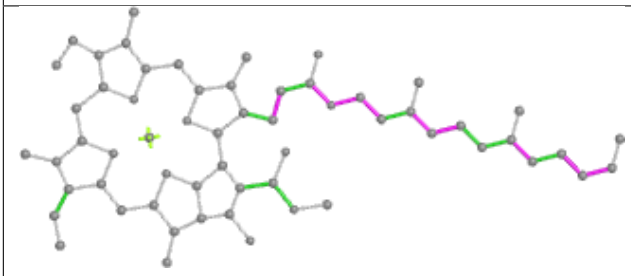
Ligand CLA B 816



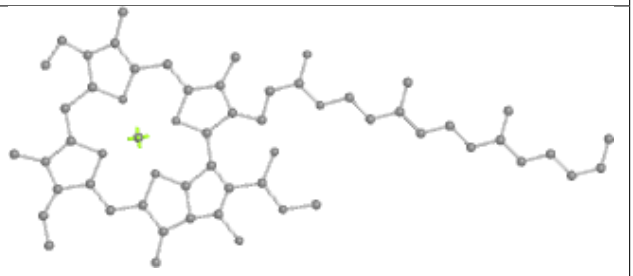
Bond lengths



Bond angles

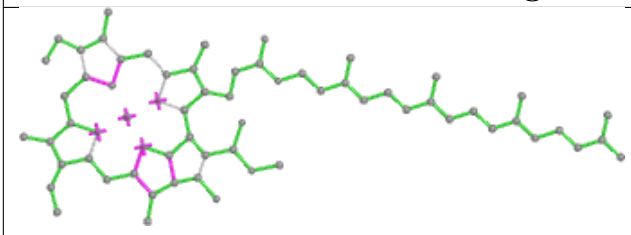


Torsions



Rings

Ligand CLA A 818



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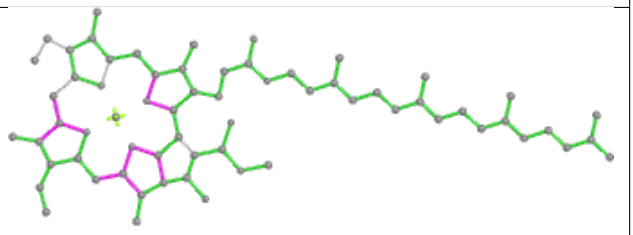
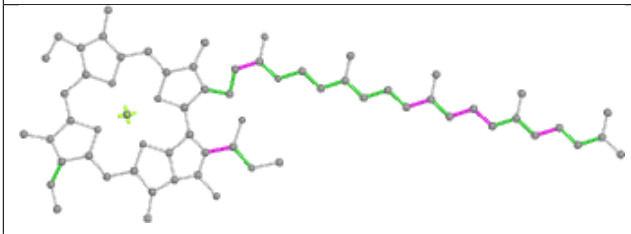
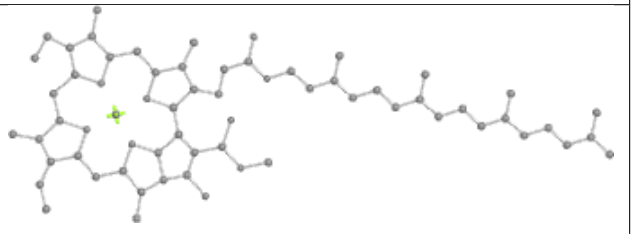


Bond angles

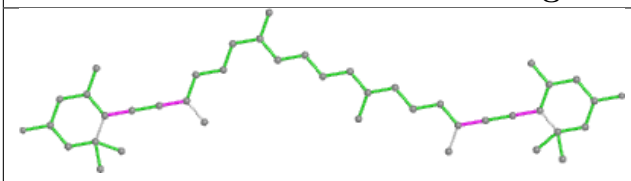


Torsions

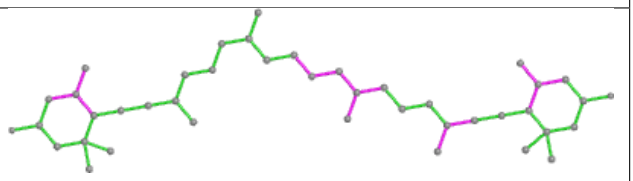


Rings

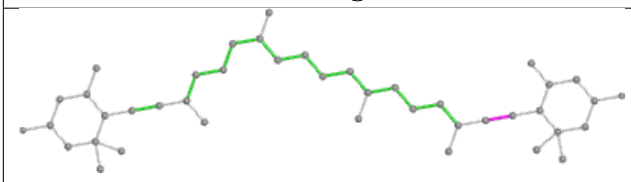
Ligand II0 5 616



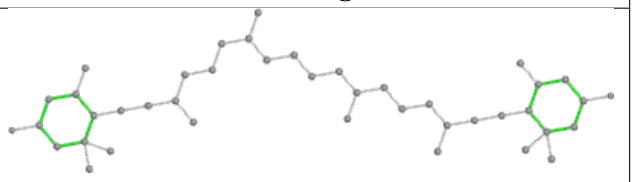
Bond lengths



Bond angles

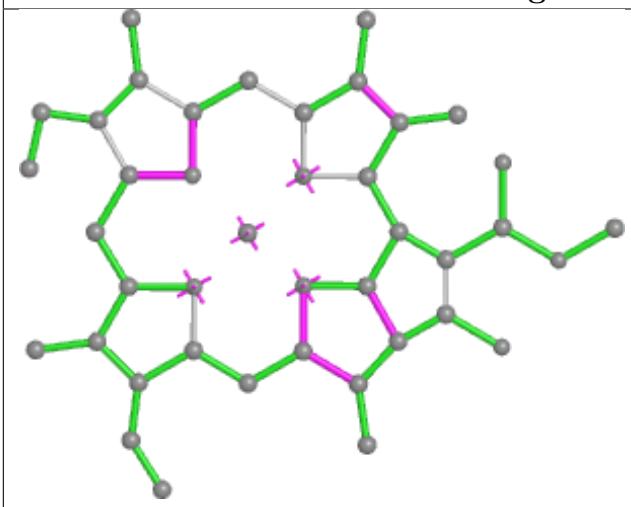


Torsions

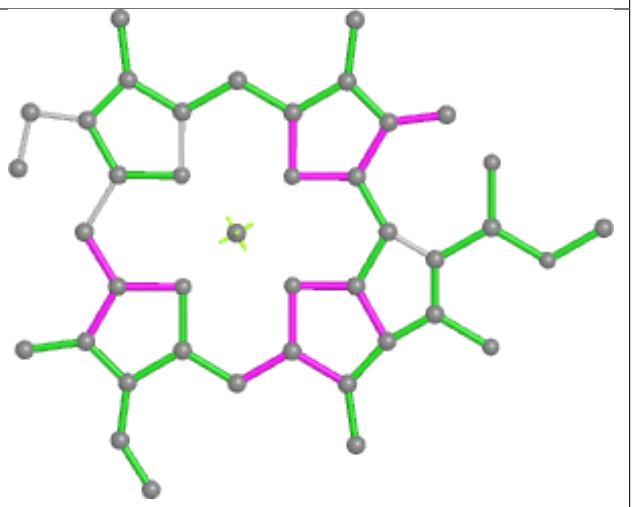


Rings

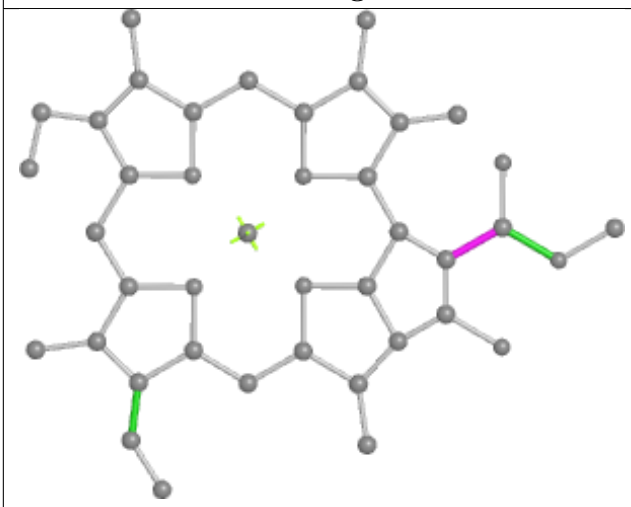
Ligand CLA 8 607



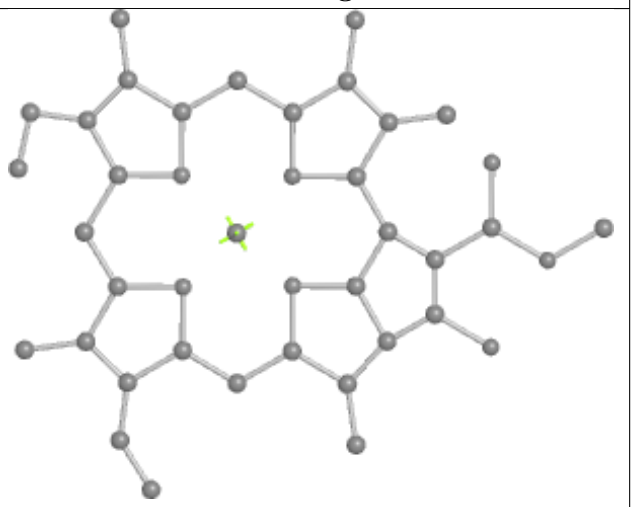
Bond lengths



Bond angles

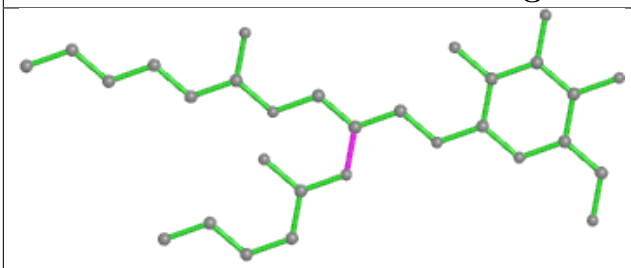


Torsions



Rings

Ligand LMG 3 618



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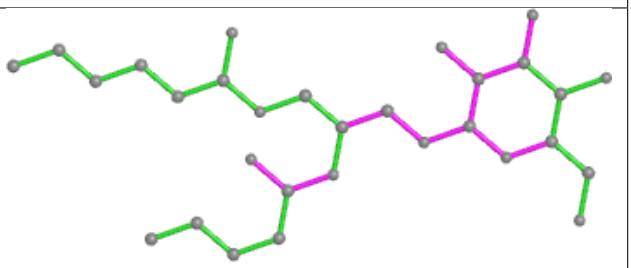

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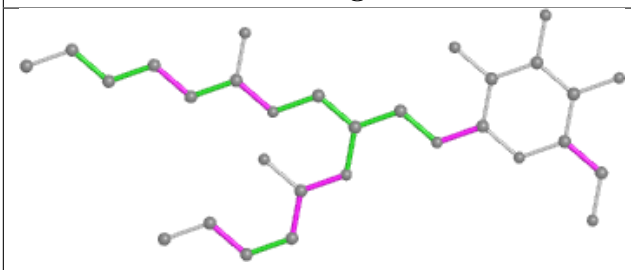

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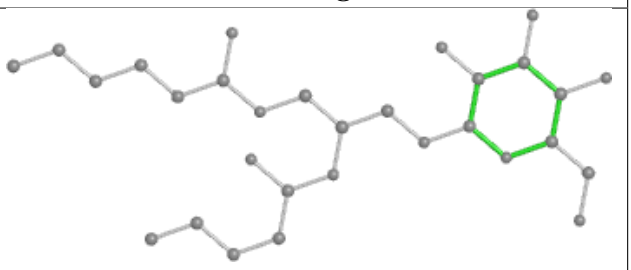
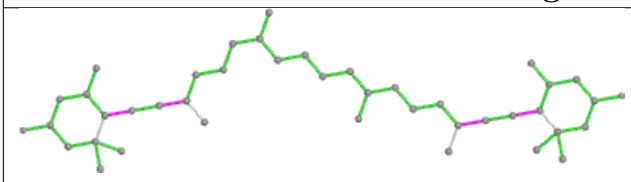


Rings

Ligand II0 2 613



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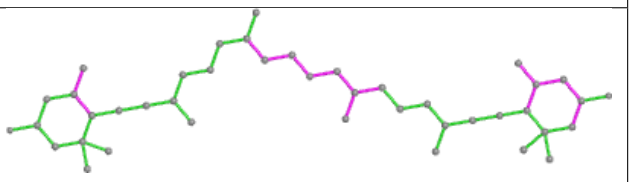

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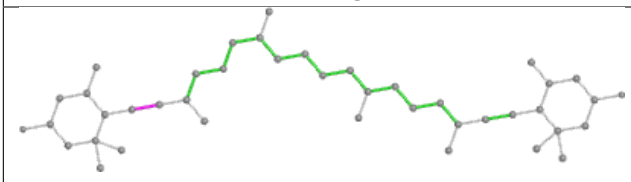

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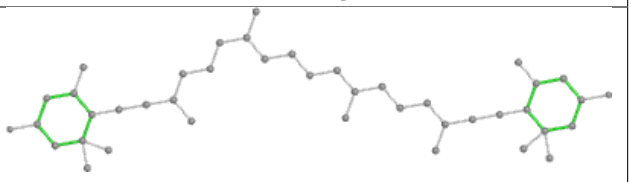
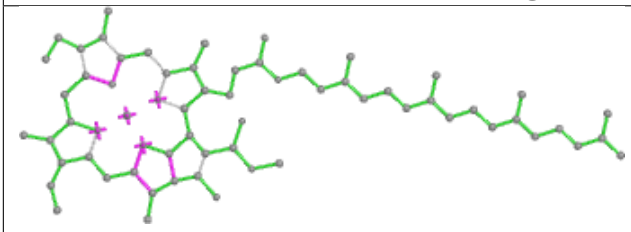


Rings

Ligand CLA A 811



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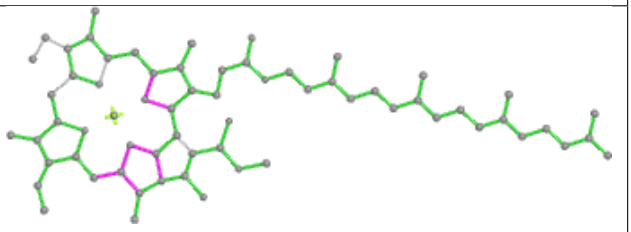
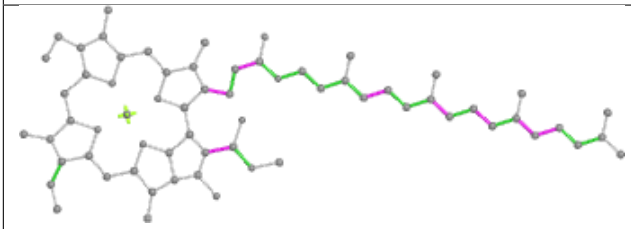


Bond angles



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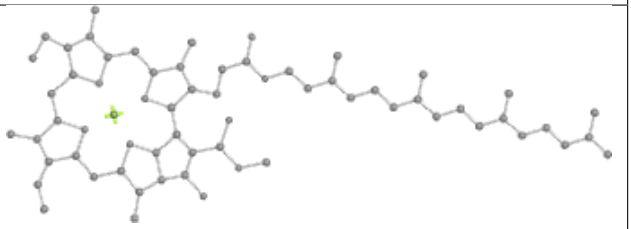
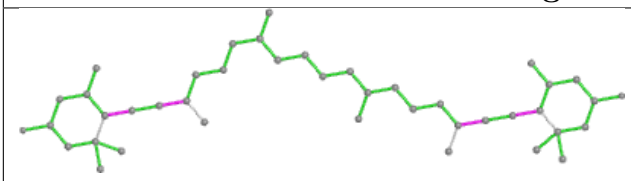


Rings

Ligand II0 4 613



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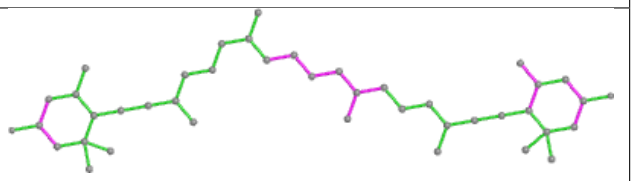

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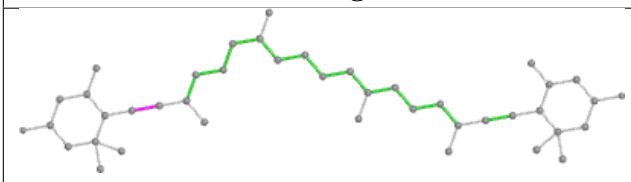

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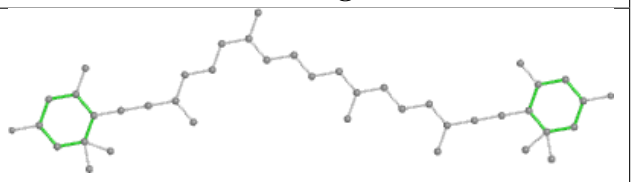
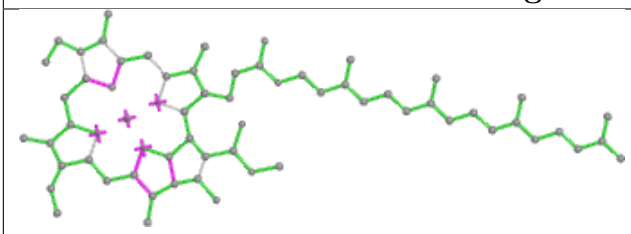


Rings

Ligand CLA B 832



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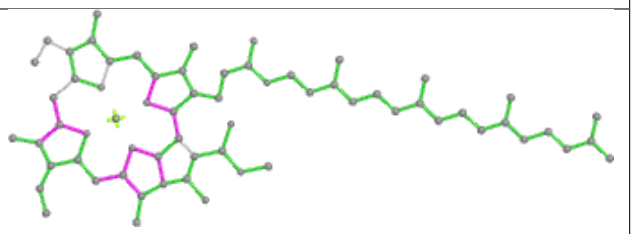

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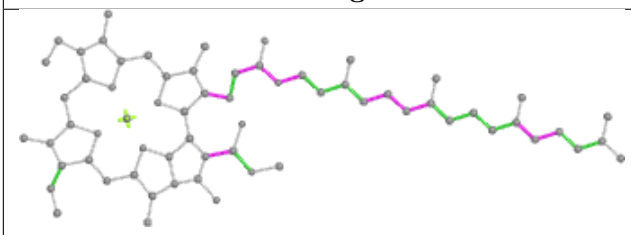

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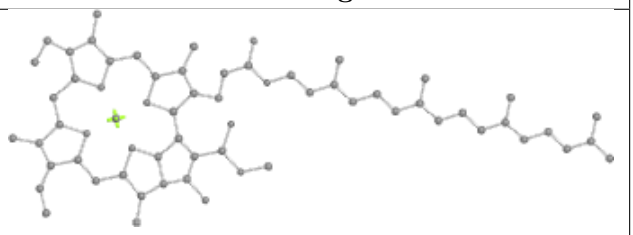
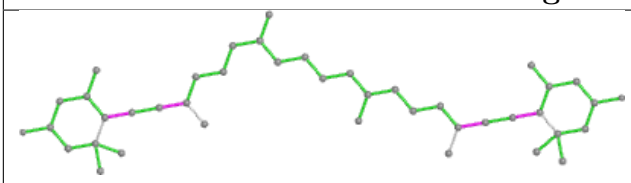


Rings

Ligand II0 9 615



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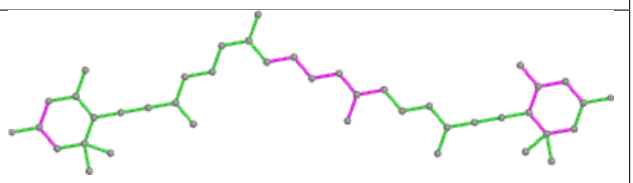

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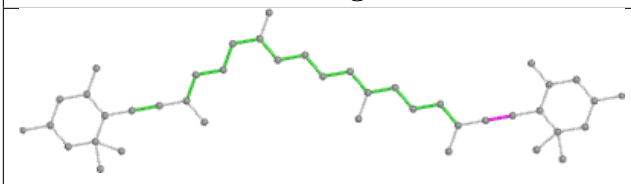

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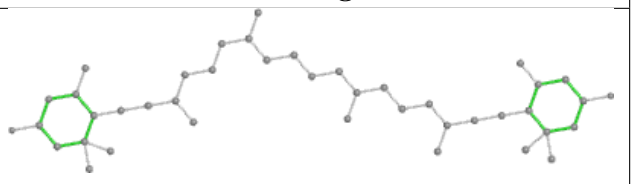
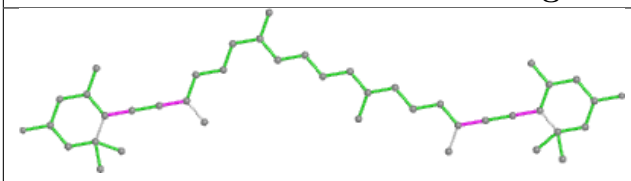


Rings

Ligand II0 J 101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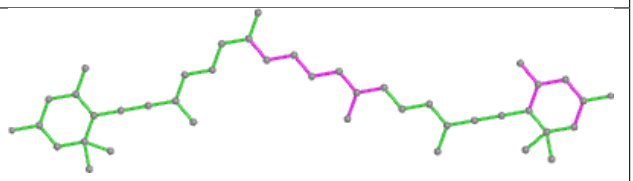
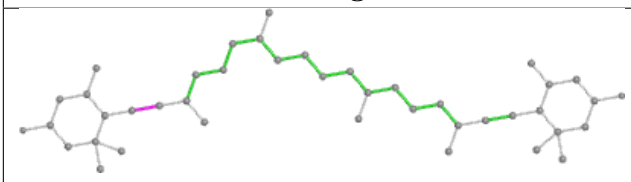

Bond angles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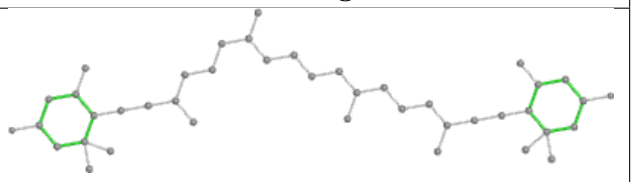
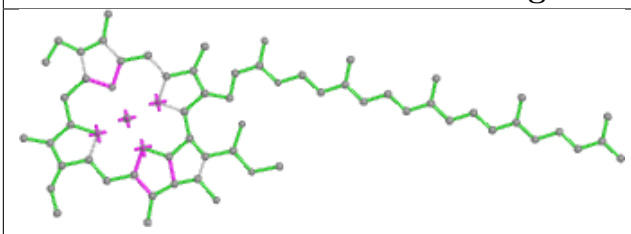
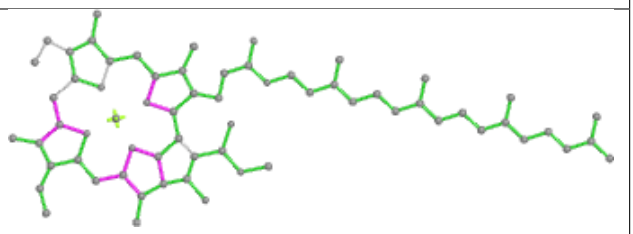
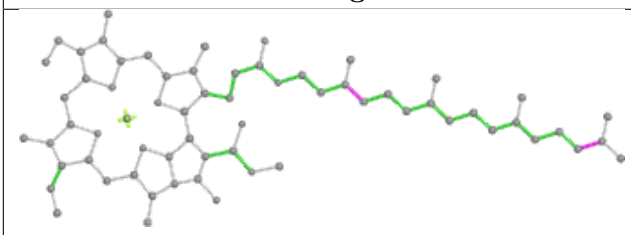

Rings

Ligand CLA a 606


Bond lengths


Bond angles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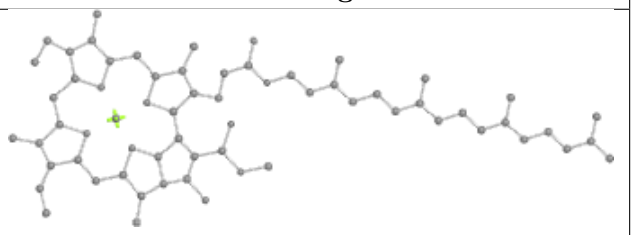
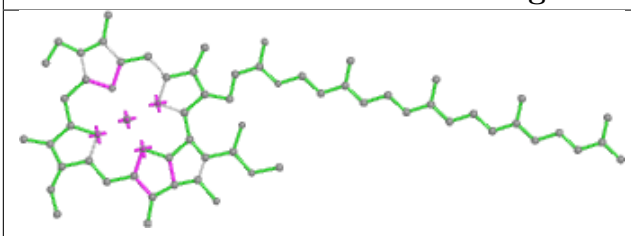

Rings

Ligand CLA 9 607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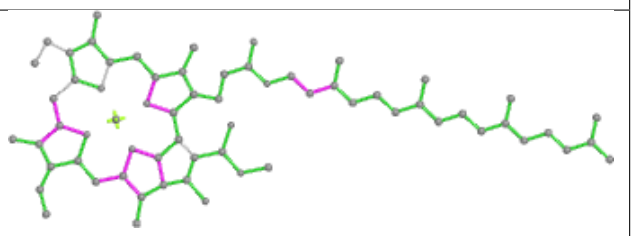
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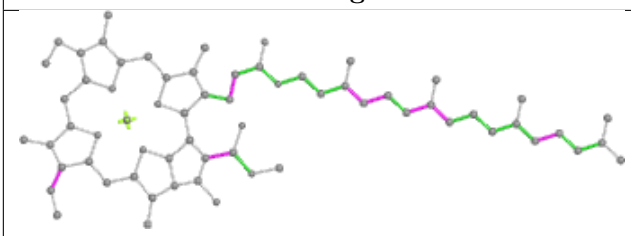
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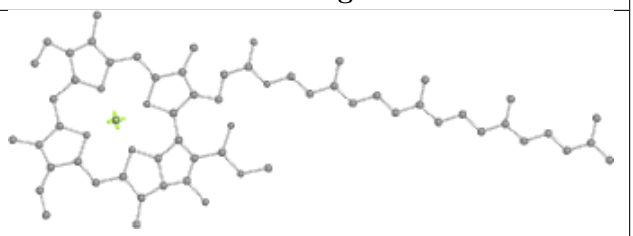
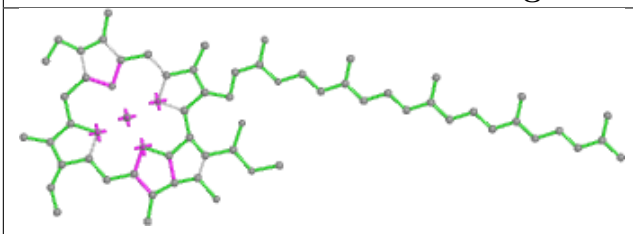
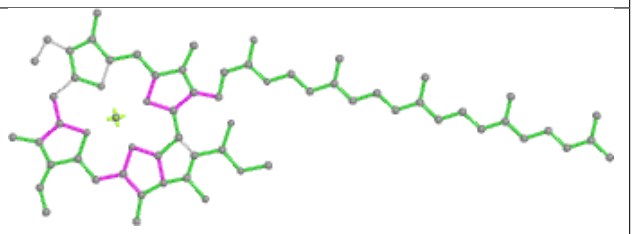

Rings

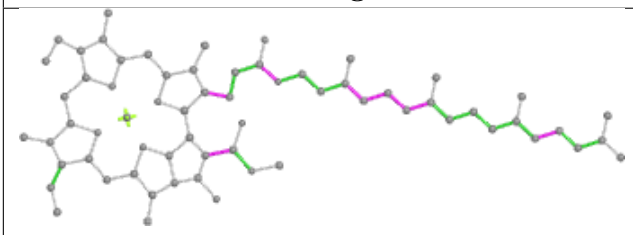
Ligand CLA A 817



Bond lengths



Bond angles



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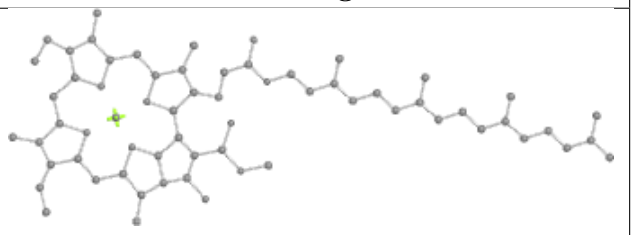
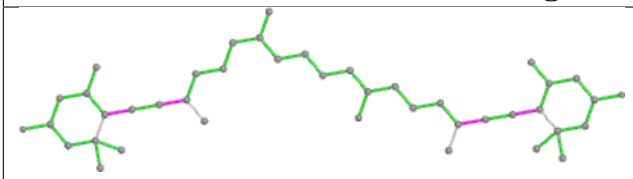


Rings

Ligand II0 5 617



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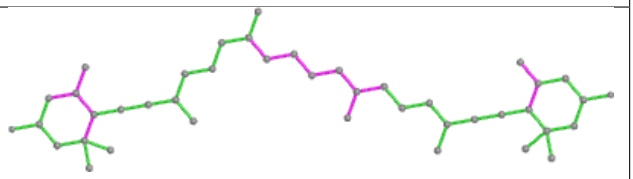
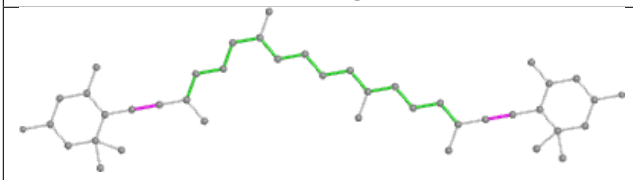


Bond angles



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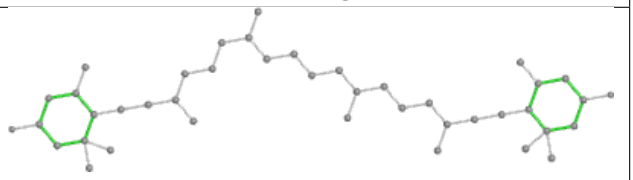
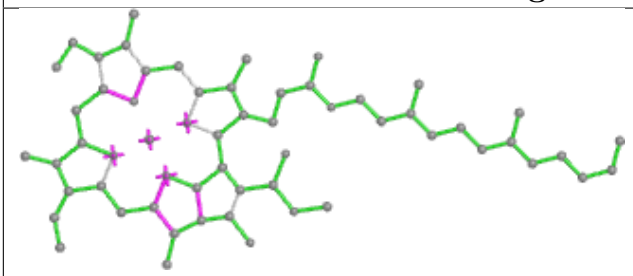


Rings

Ligand CLA 2 602



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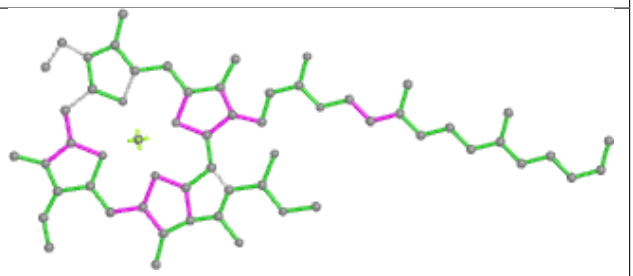
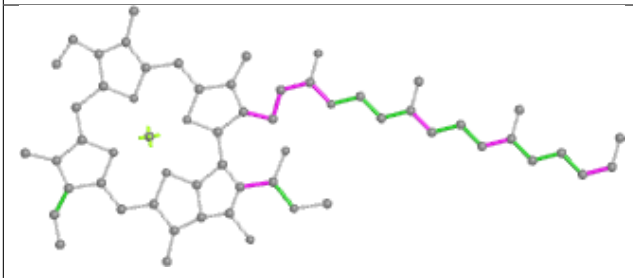
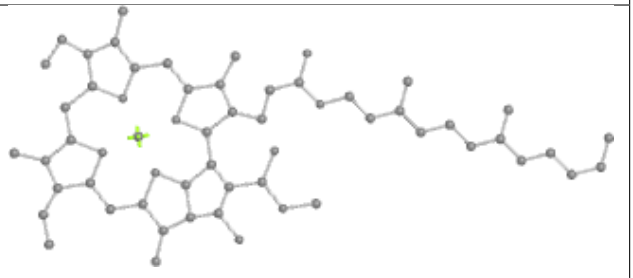


Bond angles

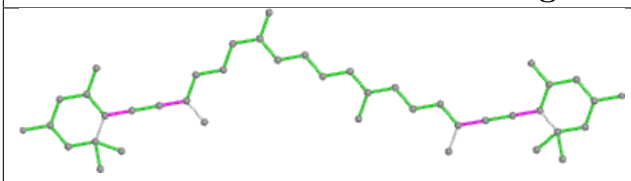


Torsions



Rings

Ligand II0 B 843



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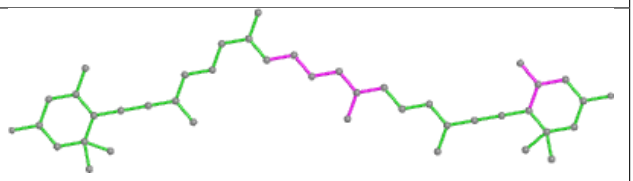
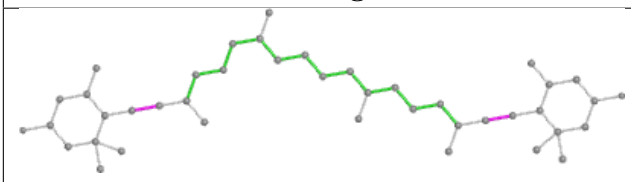
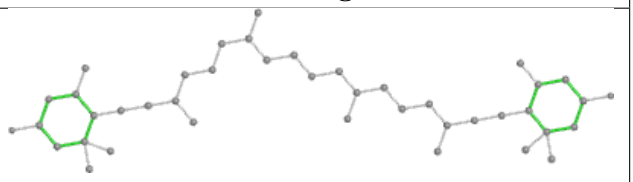


Bond angles

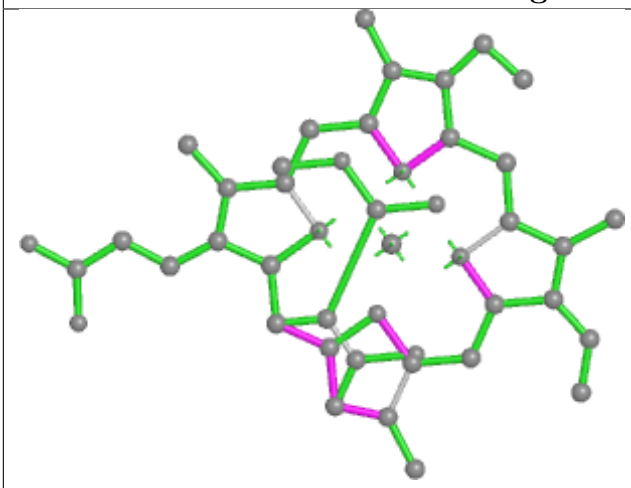


Torsions

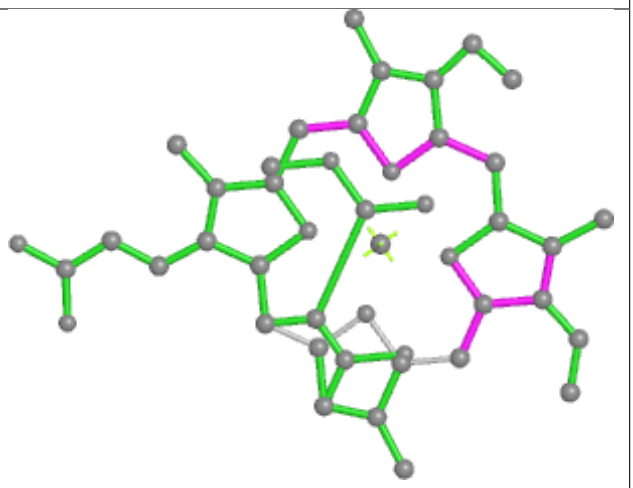


Rings

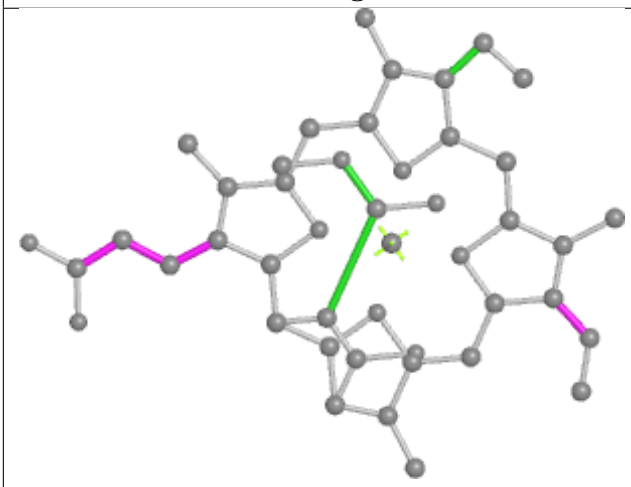
Ligand KC2 6 610



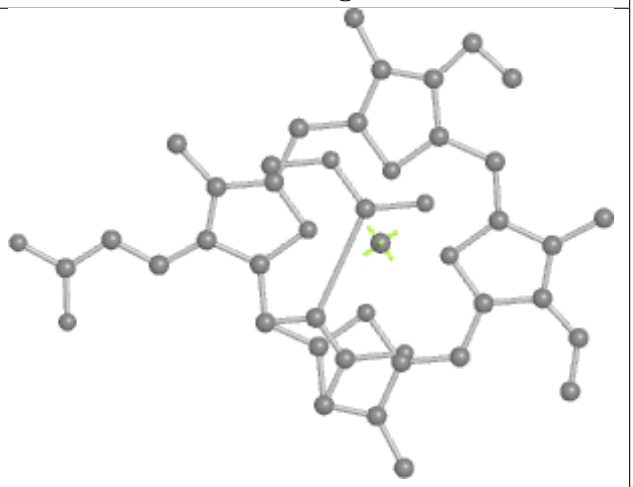
Bond lengths



Bond angles

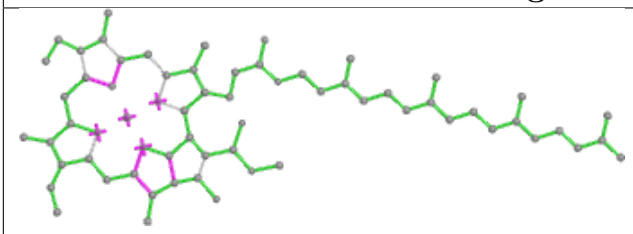


Torsions

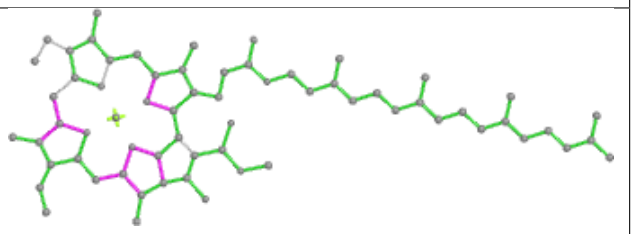


Rings

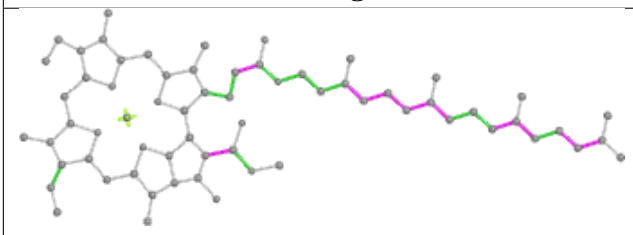
Ligand CLA b 604



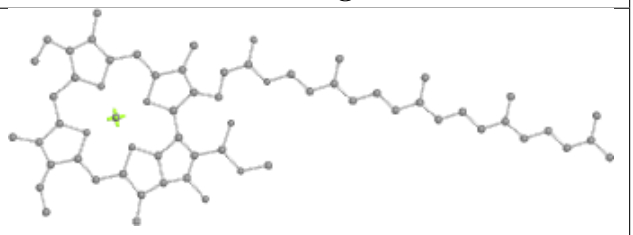
Bond lengths



Bond angles

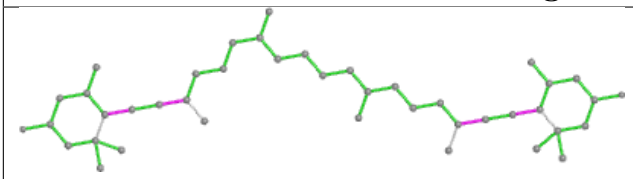


Torsions



Rings

Ligand II0 4 614



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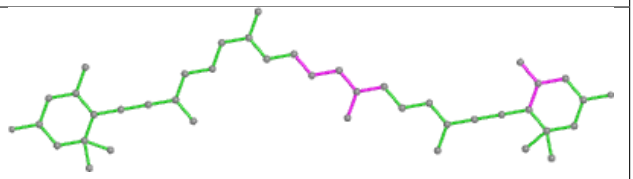

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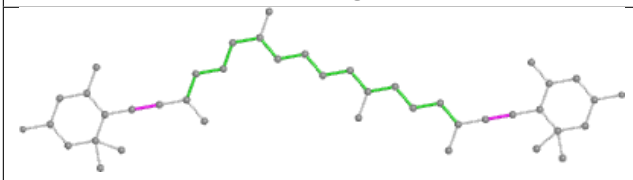

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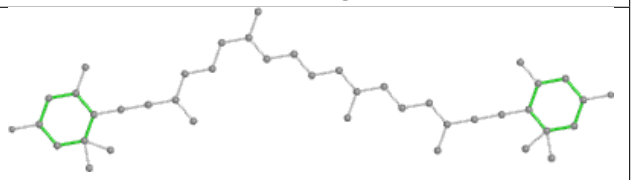
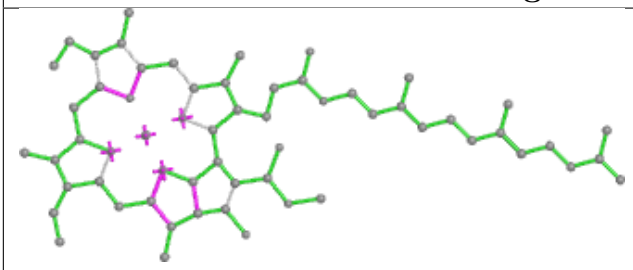


Rings

Ligand CLA A 835



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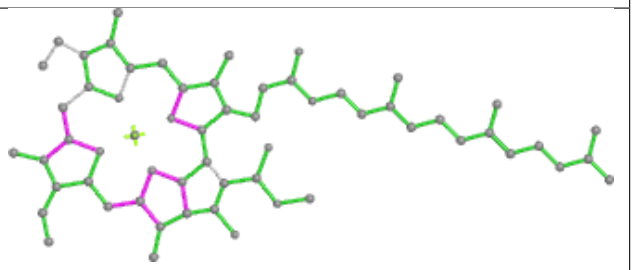
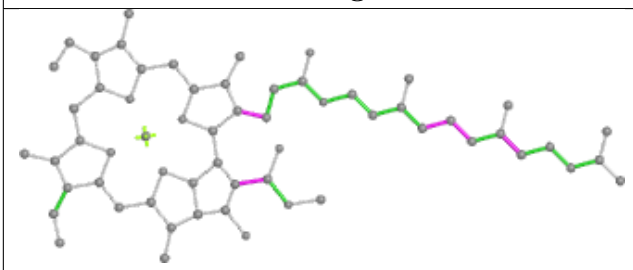
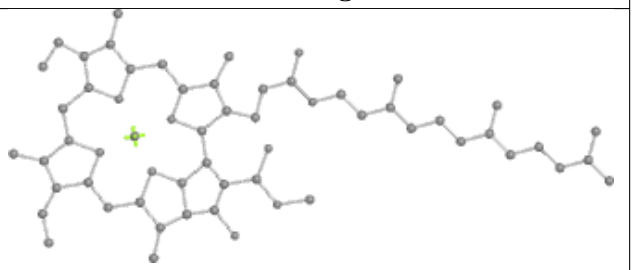


Bond angles

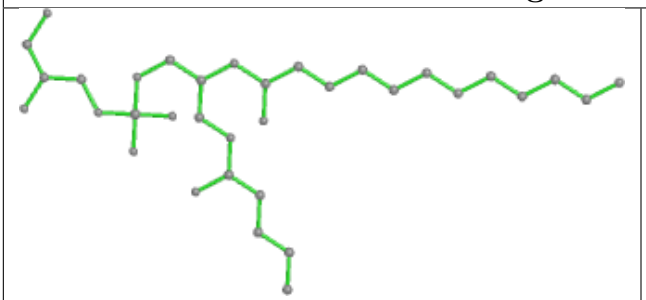


Torsions

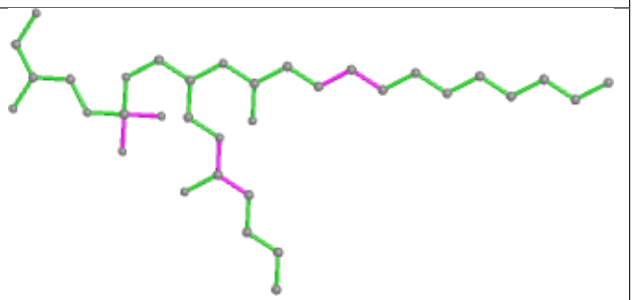


Rings

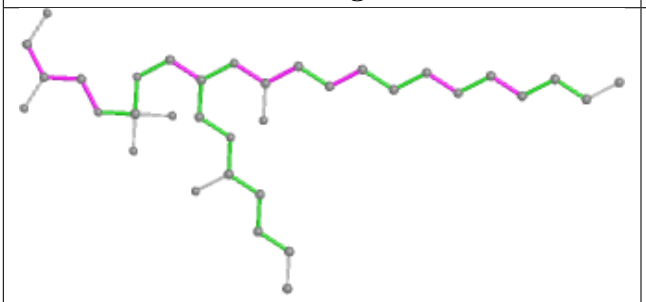
Ligand LHG 3 622



Bond lengths



Bond angles



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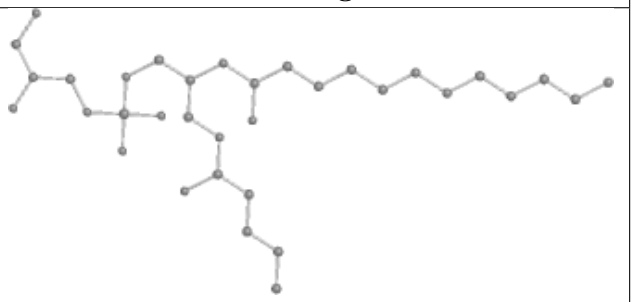
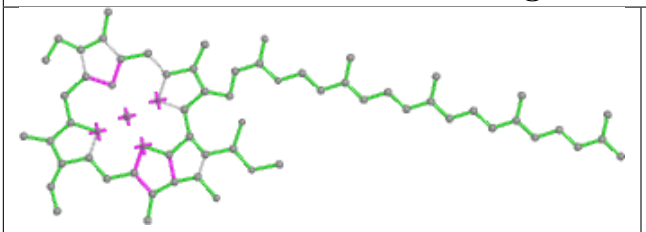
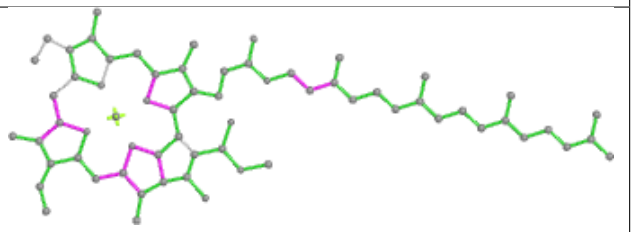


Rings

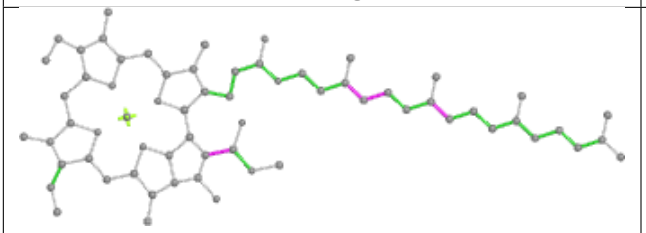
Ligand CLA A 819



Bond lengths



Bond angles



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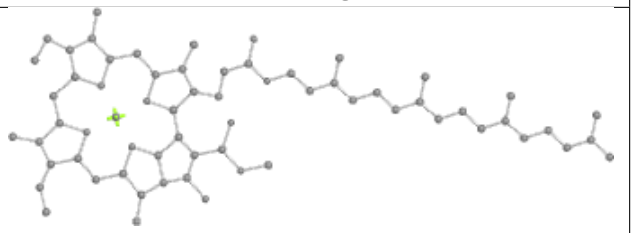
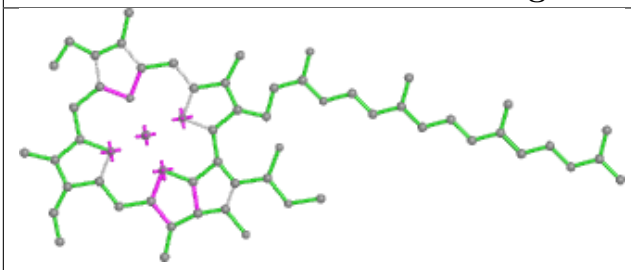
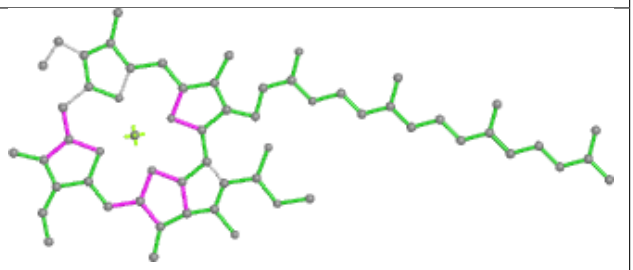
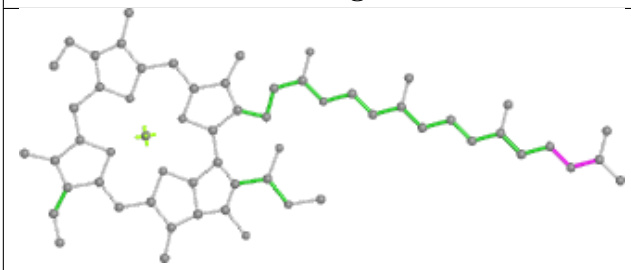
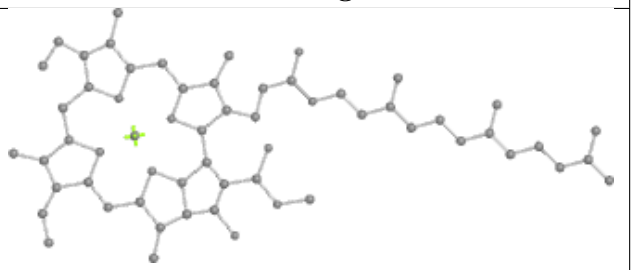
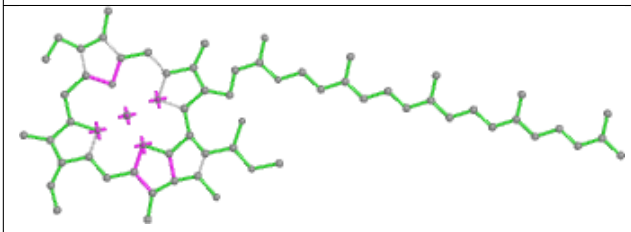
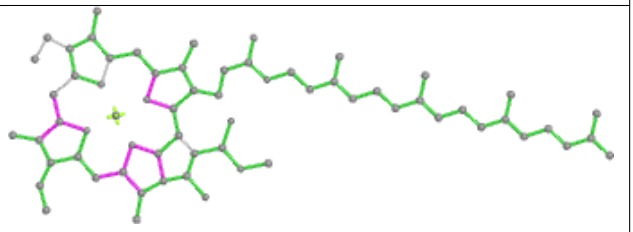
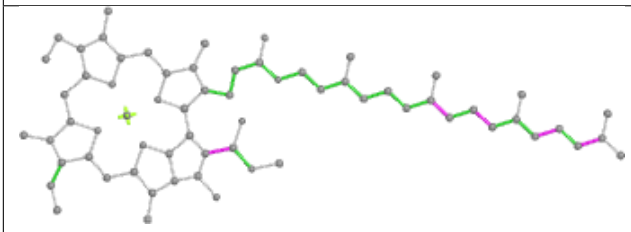
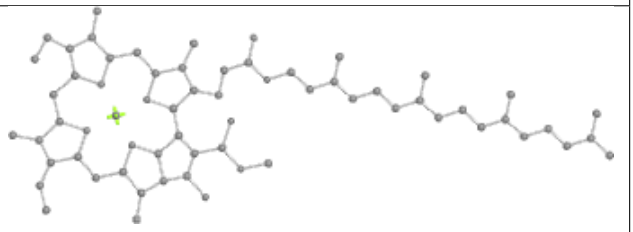
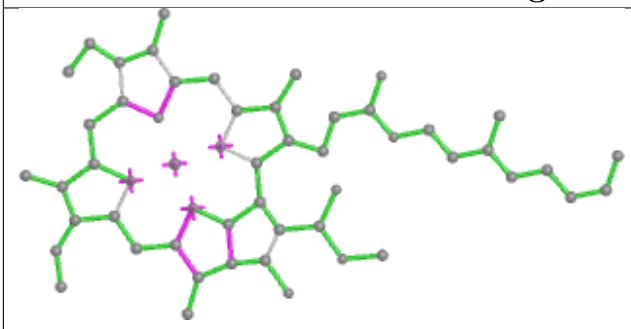


Rings

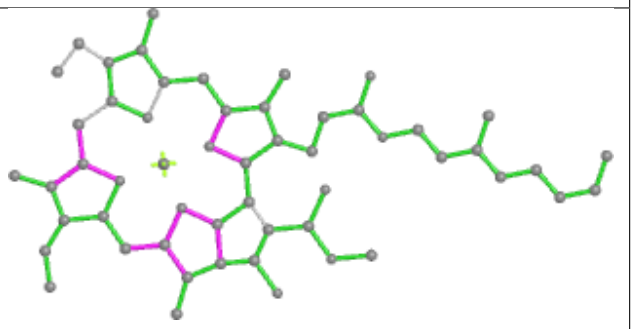
Ligand CLA 3 603	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA B 839	
 Bond lengths	 Bond angles
 Torsions	 Rings

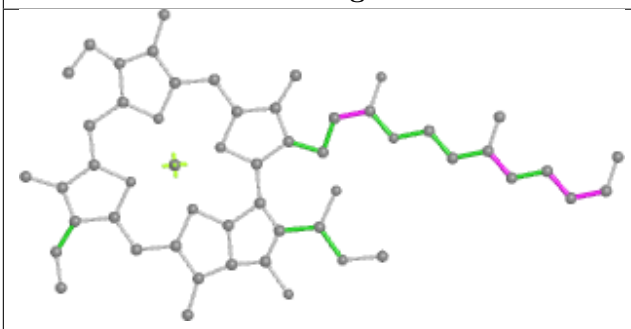
Ligand CLA 4 603



Bond lengths



Bond angles



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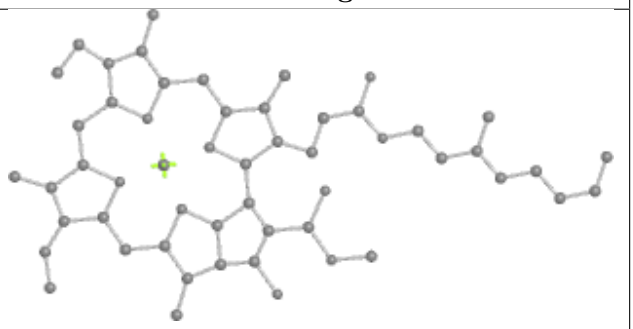
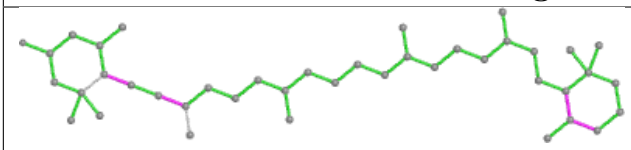
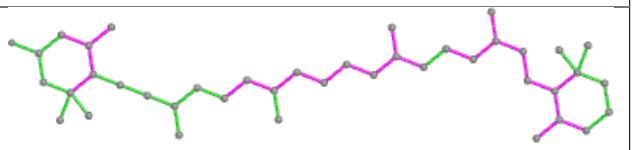


Rings

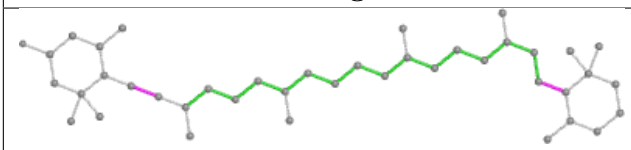
Ligand IHT 2 616



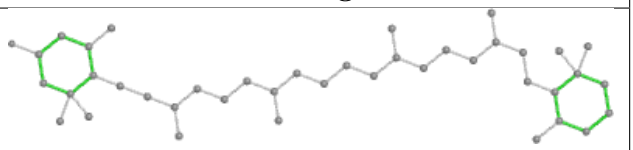
Bond lengths



Bond angles

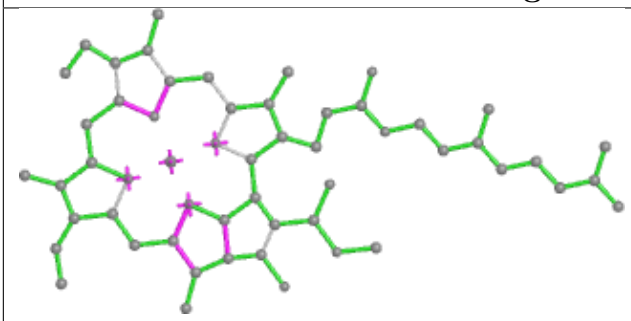


Torsions



Rings

Ligand CLA R 202



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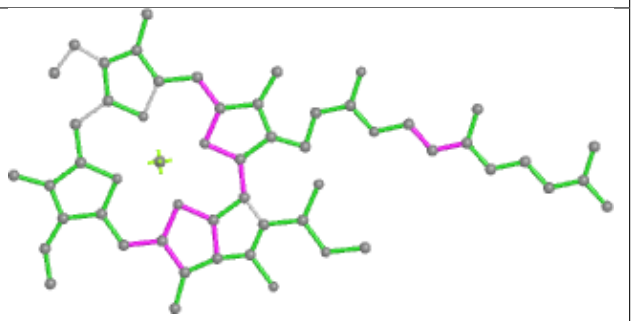
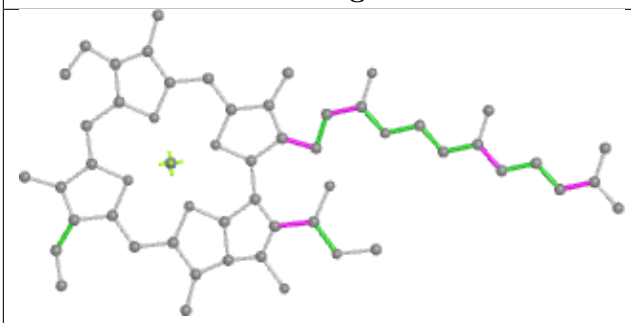
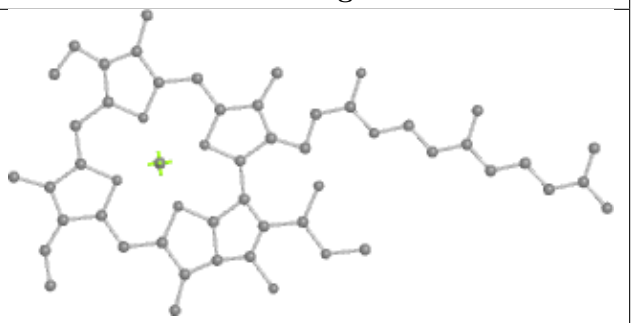


Bond angles

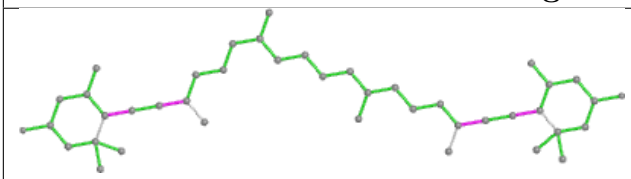


Torsions



Rings

Ligand II0 3 613



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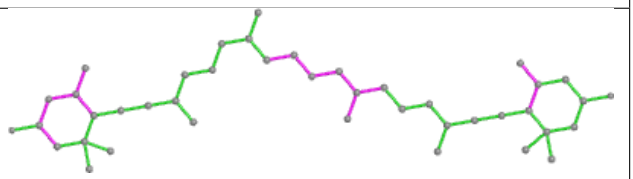
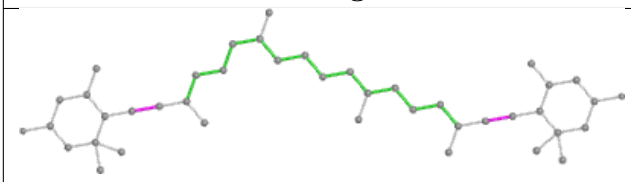
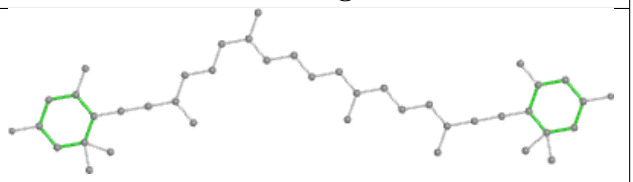


Bond angles

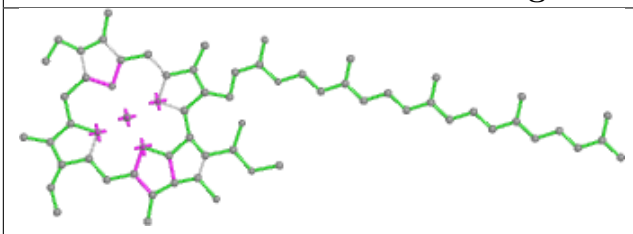


Torsions



Rings

Ligand CLA 8 604



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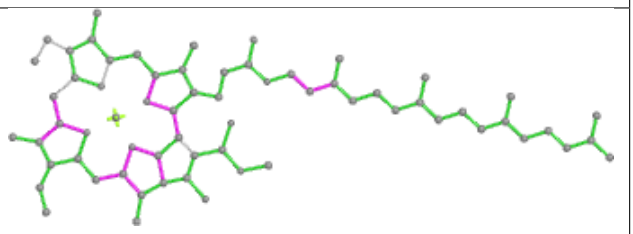
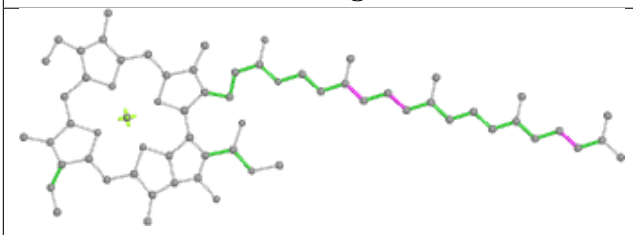
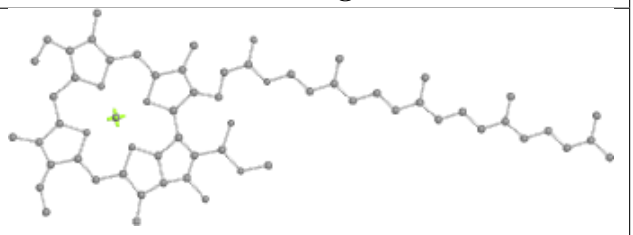


Bond angles

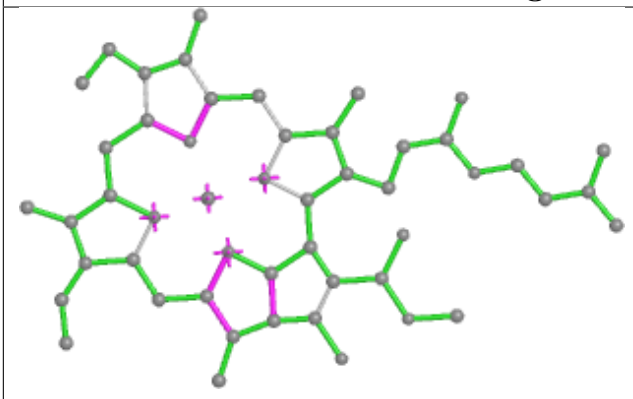


Torsions

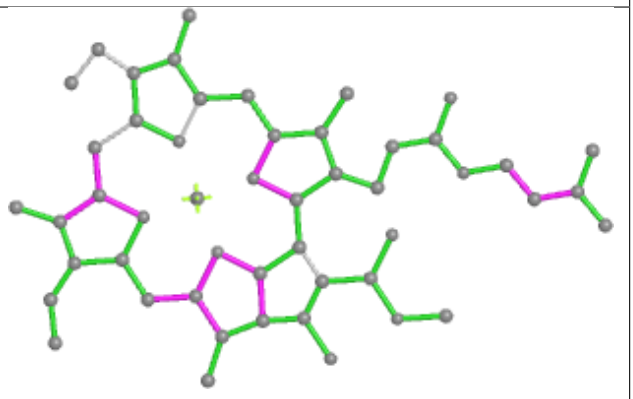


Rings

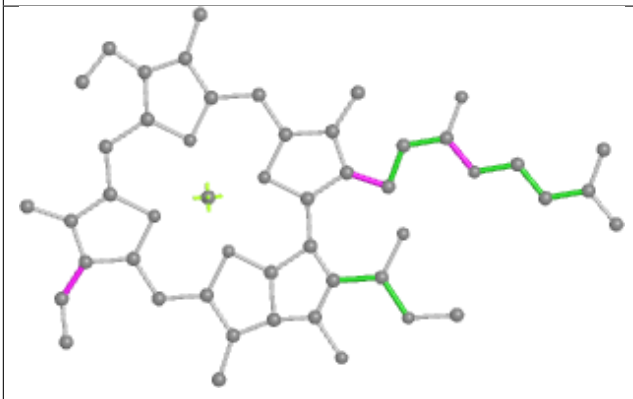
Ligand CLA L 203



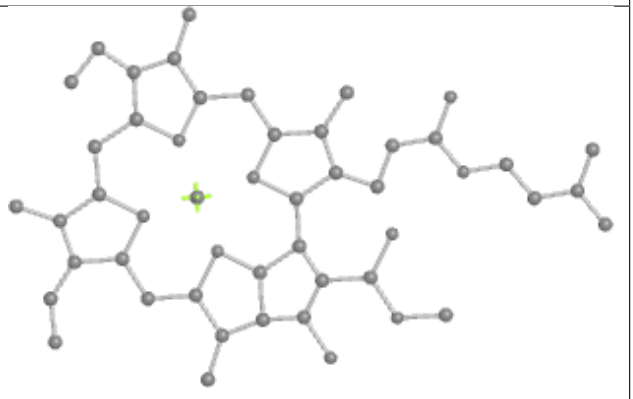
Bond lengths



Bond angles

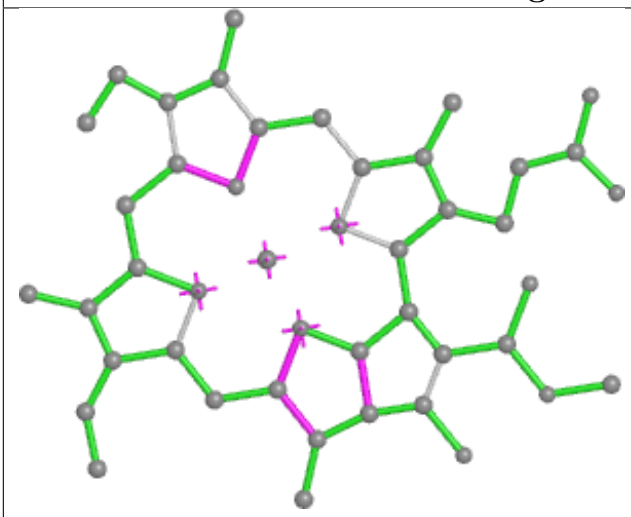


Torsions

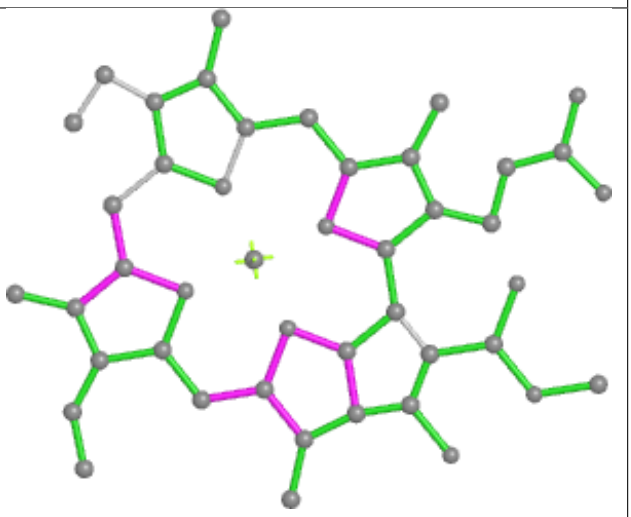


Rings

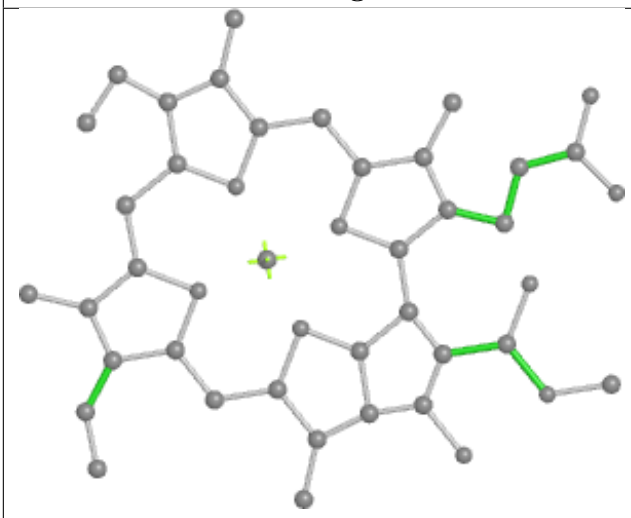
Ligand CLA 1 607



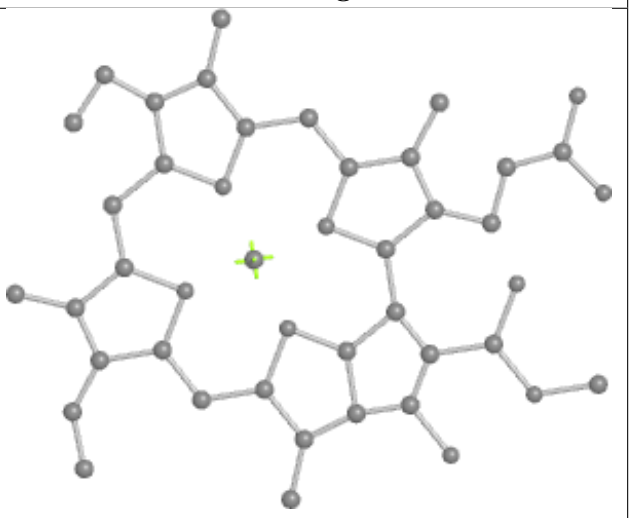
Bond lengths



Bond angles

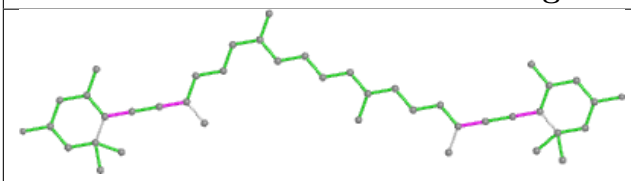


Torsions

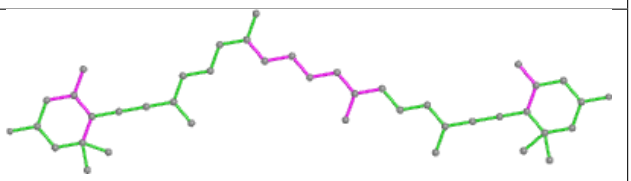


Rings

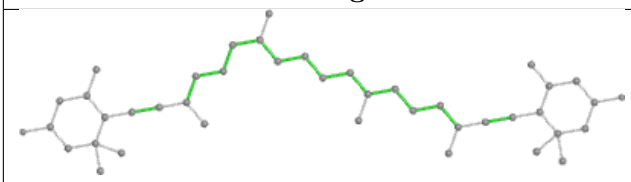
Ligand II0 4 615



Bond lengths



Bond angles



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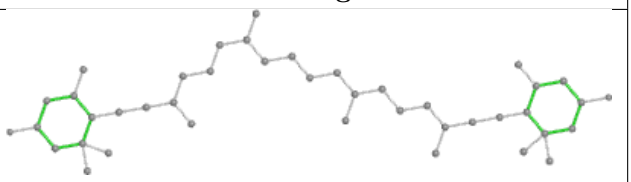
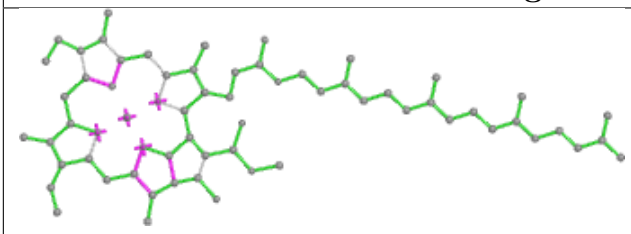
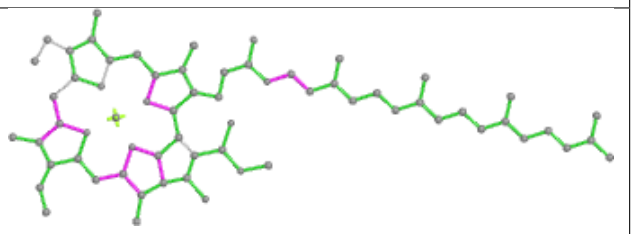


Rings

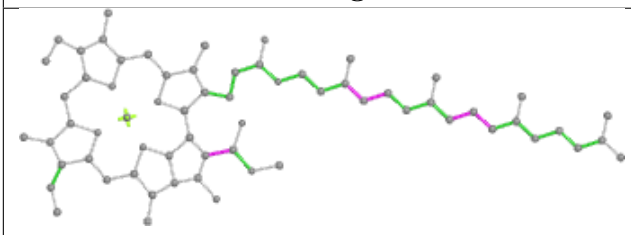
Ligand CLA B 822



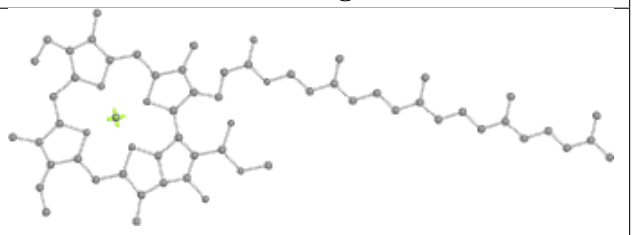
Bond lengths



Bond angles

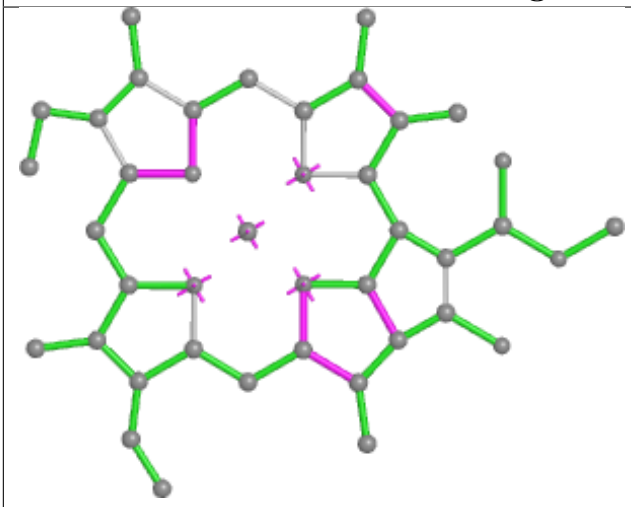


Torsions

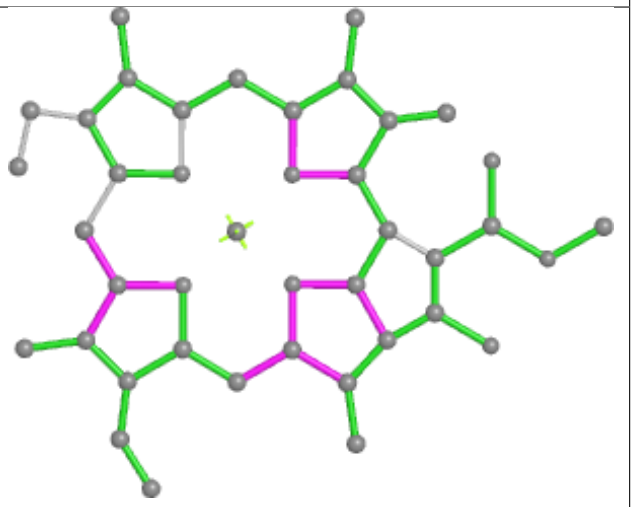


Rings

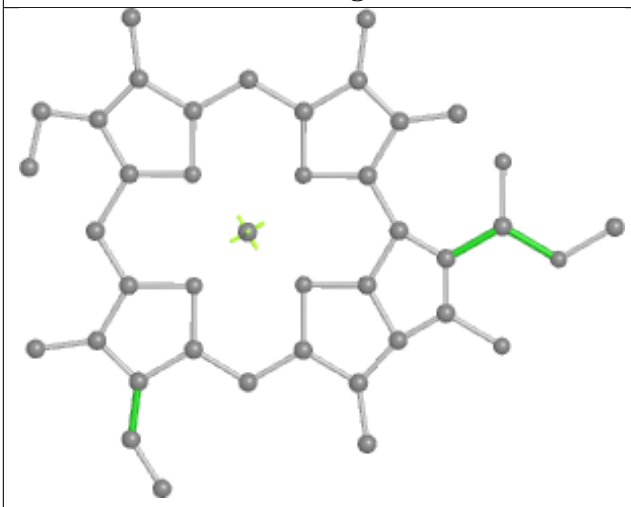
Ligand CLA 7 310



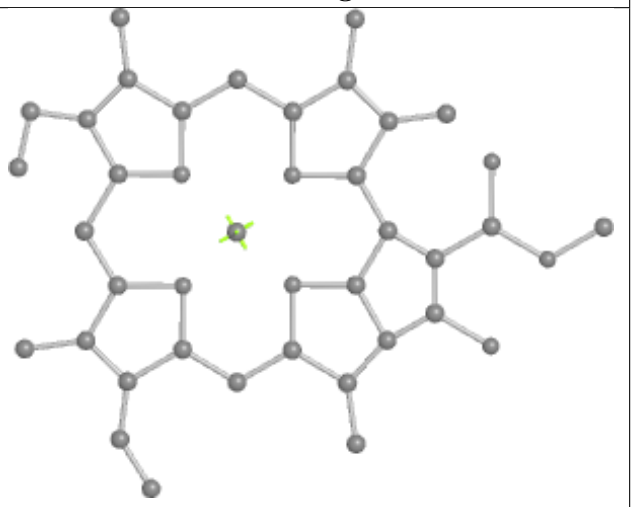
Bond lengths



Bond angles

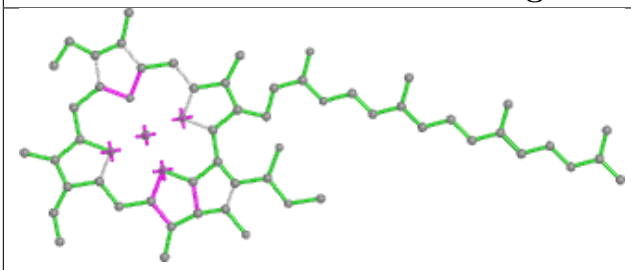


Torsions



Rings

Ligand CLA F 202



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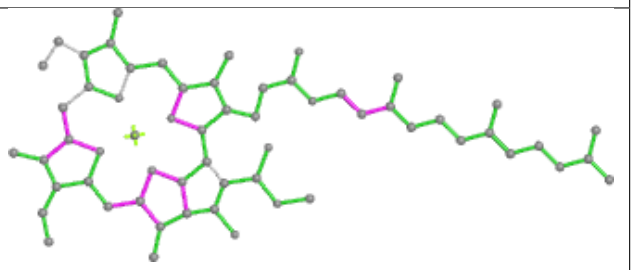
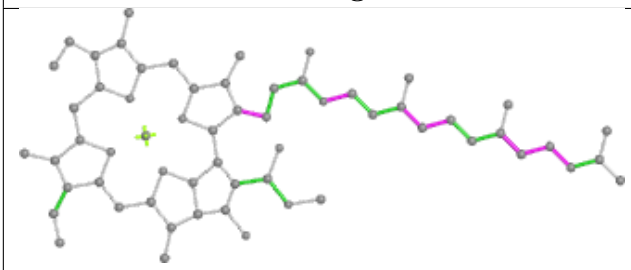


Bond angles



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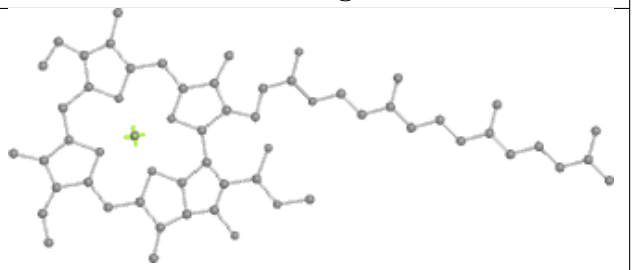
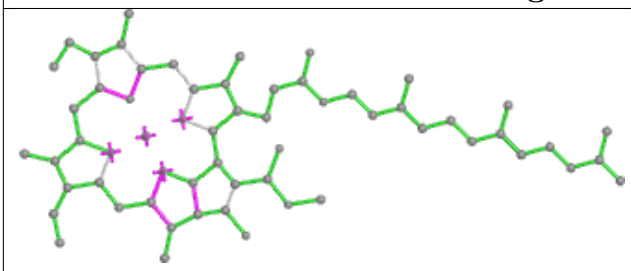


Rings

Ligand CLA b 603



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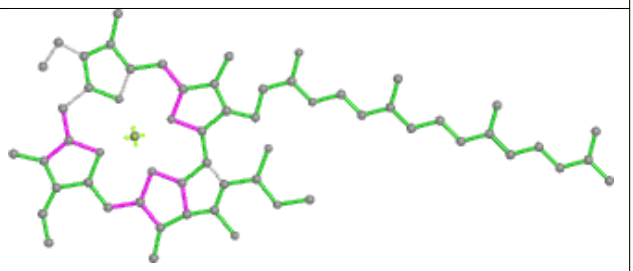
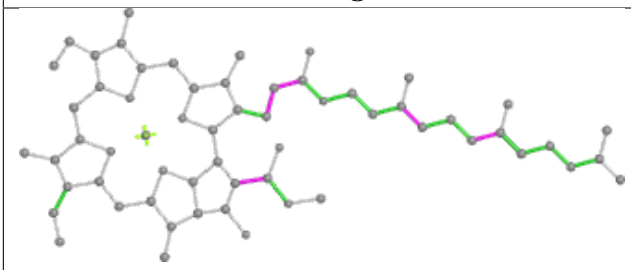


Bond angles



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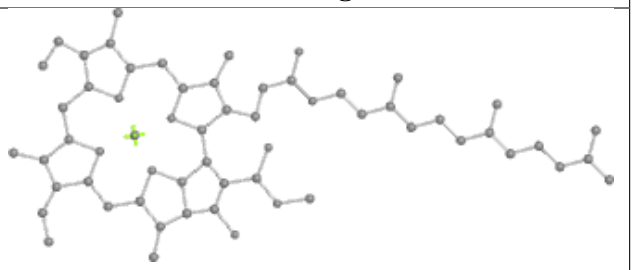
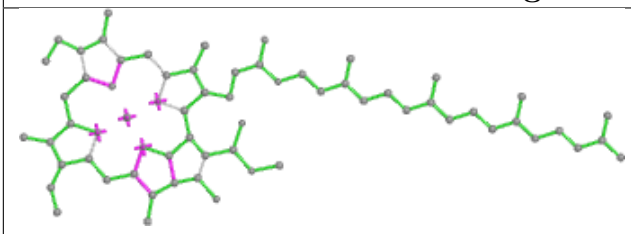


Rings

Ligand CLA A 803



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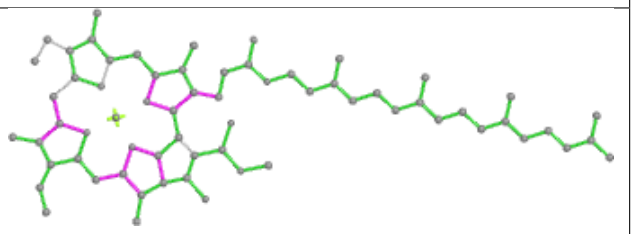
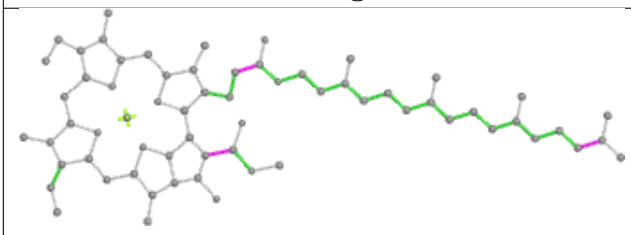


Bond angles



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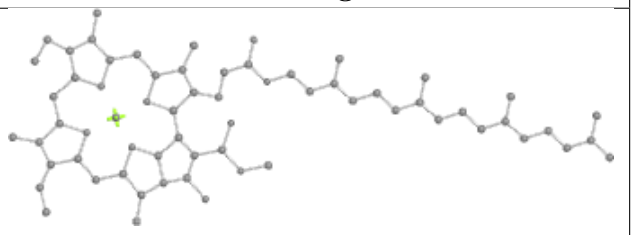
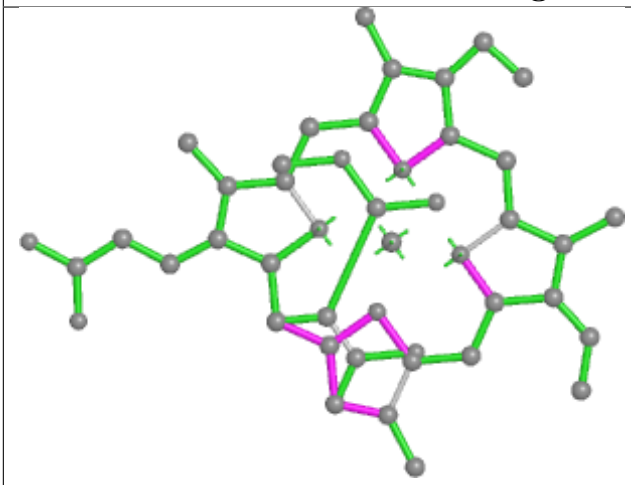


Rings

Ligand KC2 3 606



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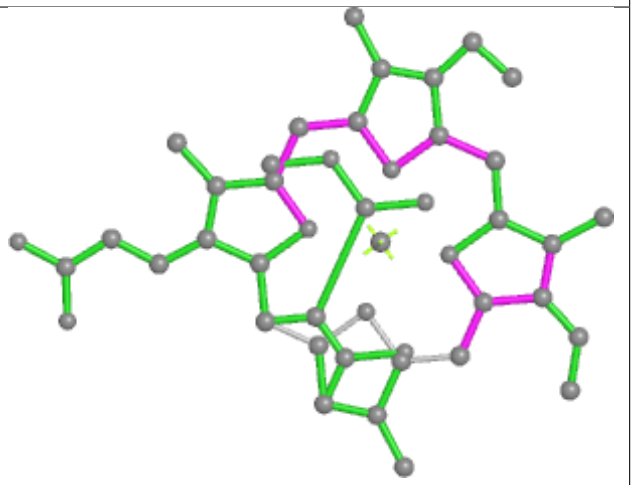
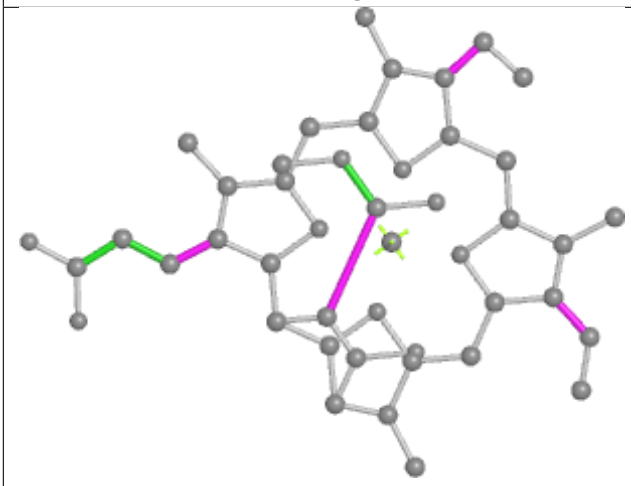


Bond angles



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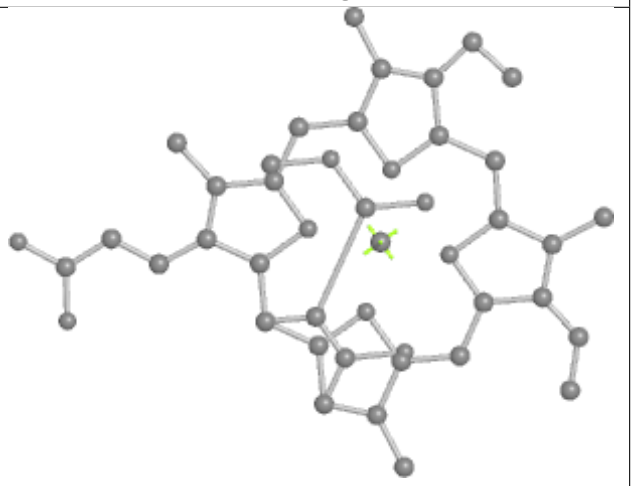
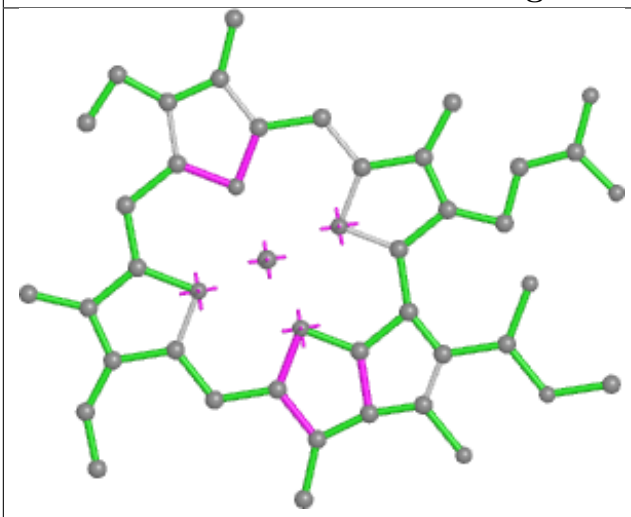


Rings

Ligand CLA F 203



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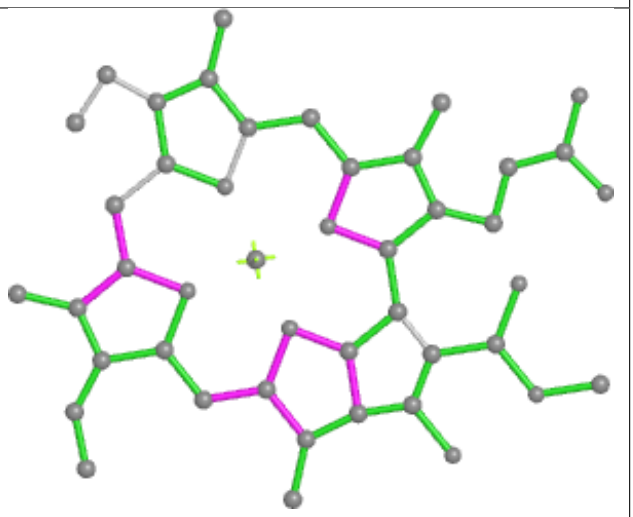
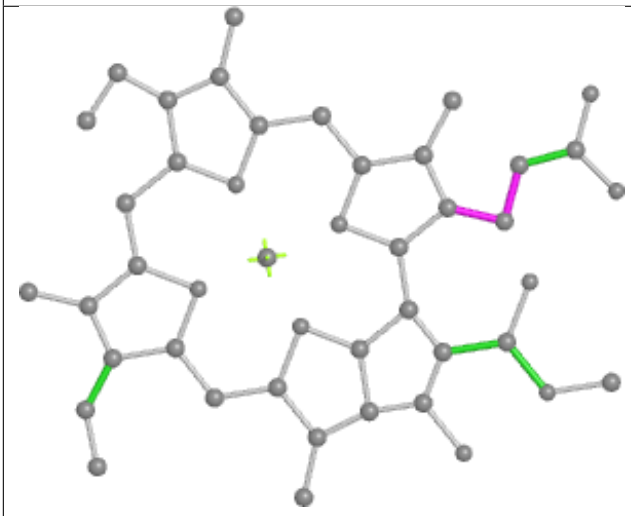


Bond angles



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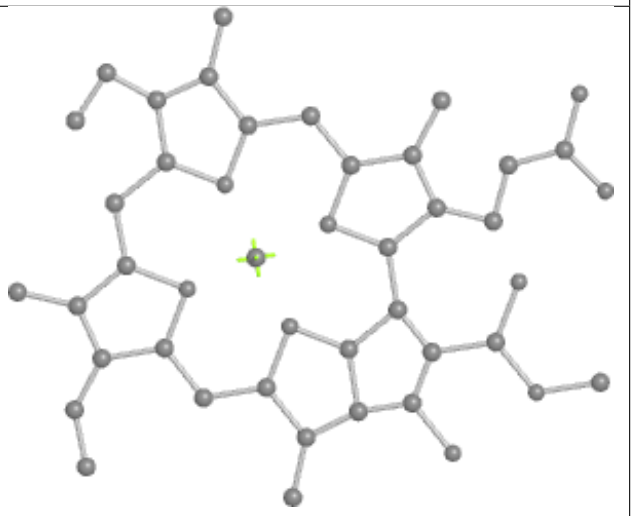
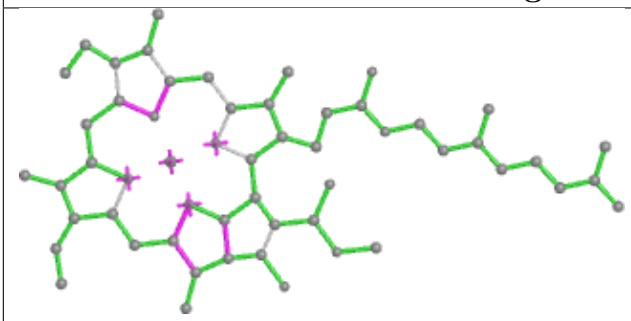


Rings

Ligand CLA B 834



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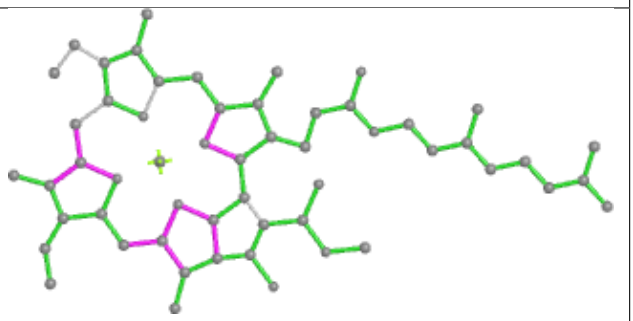
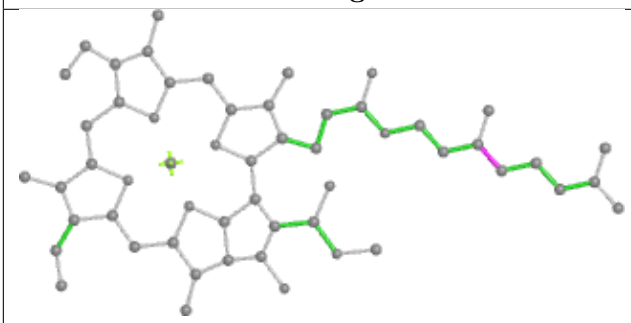


Bond angles



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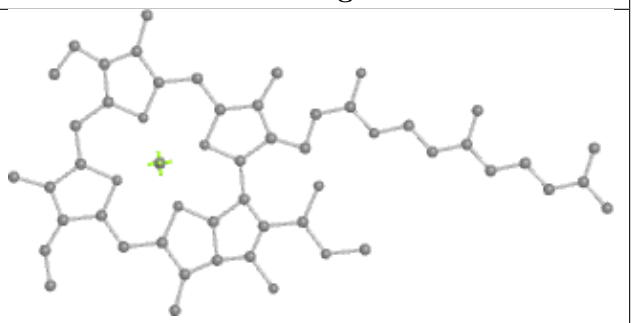
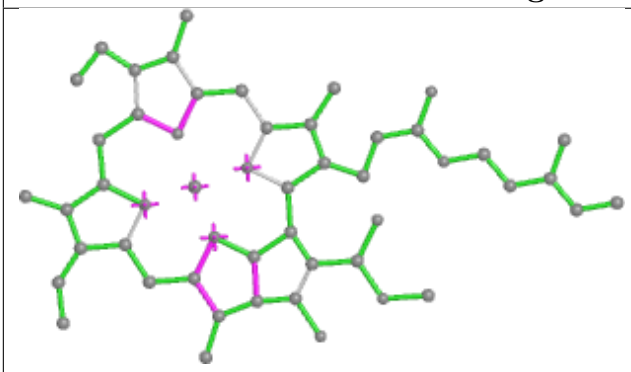
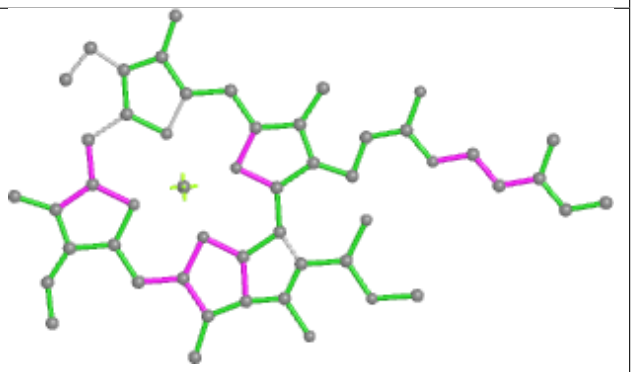


Rings

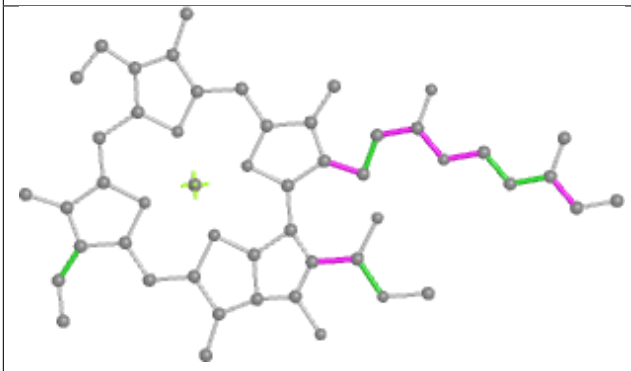
Ligand CLA b 610



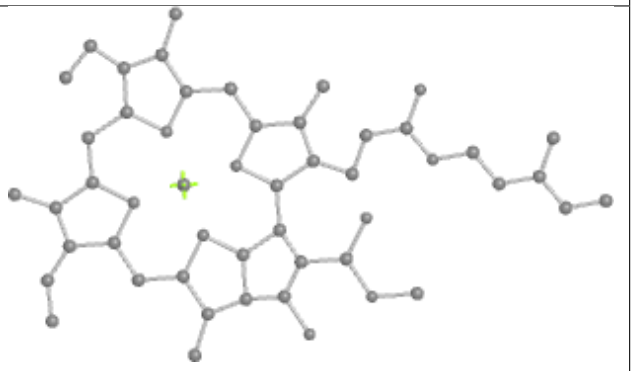
Bond lengths



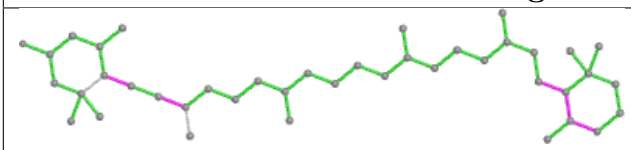
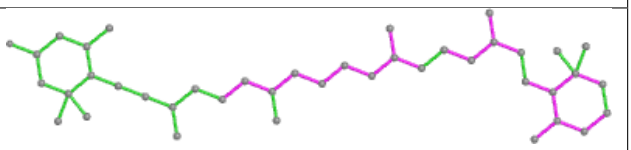
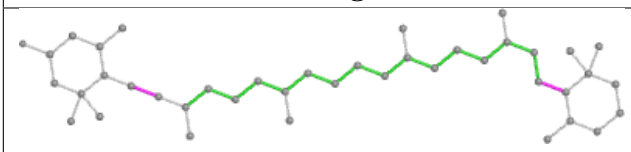
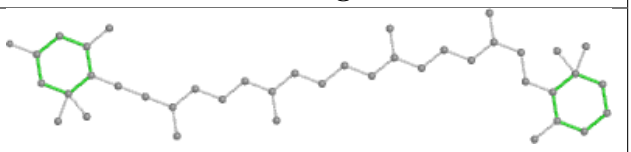
Bond angles

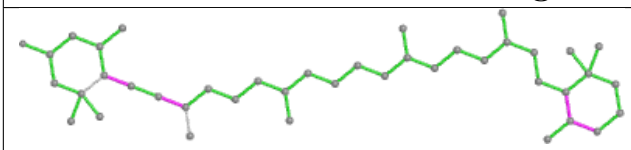
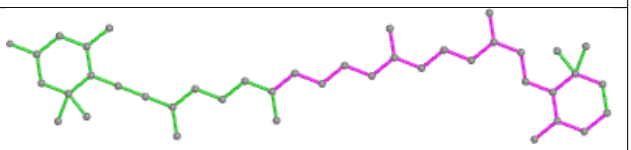
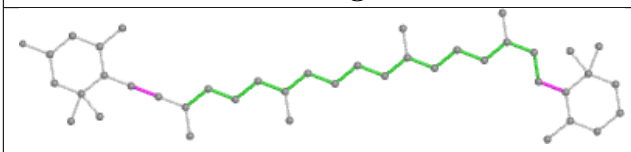
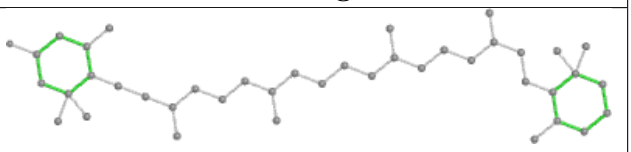


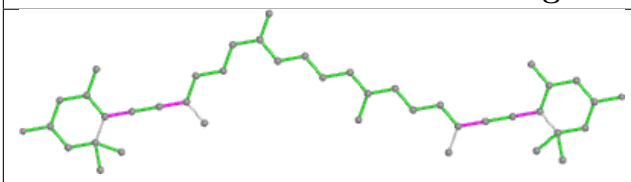
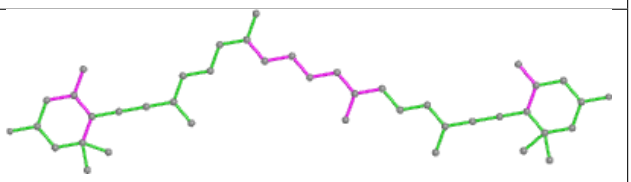
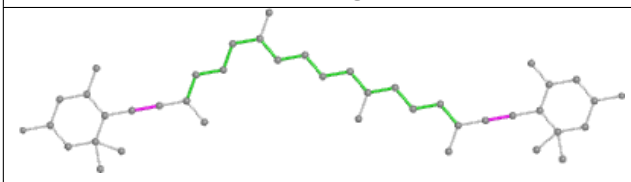
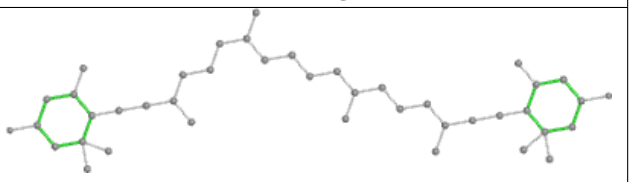
Torsions



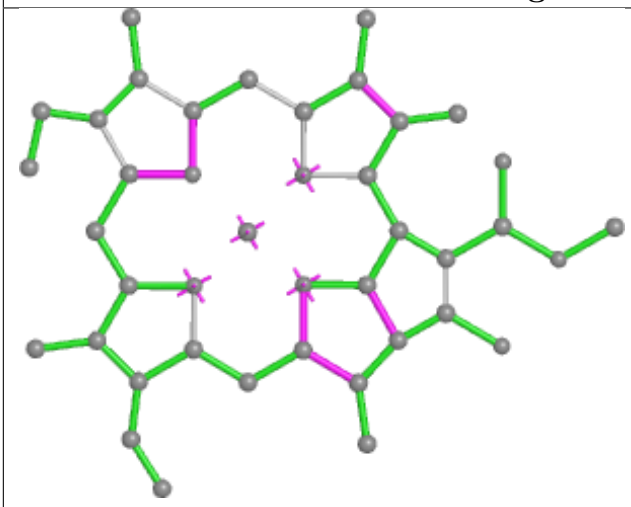
Rings

Ligand IHT A 854	
 Bond lengths	 Bond angles
 Torsions	 Rings

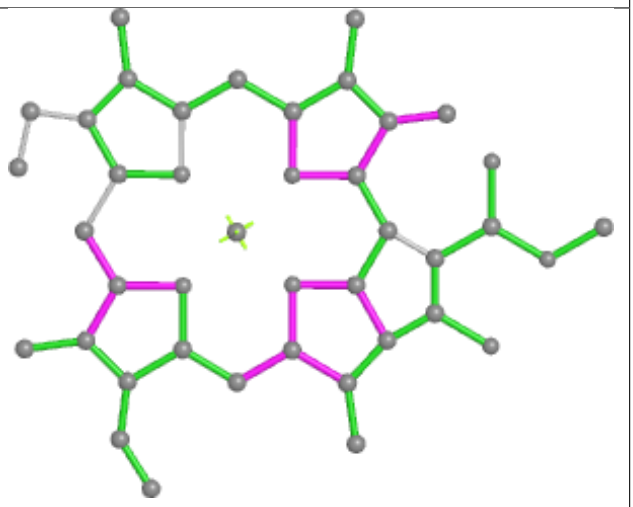
Ligand IHT 6 616	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand II0 8 610	
 Bond lengths	 Bond angles
 Torsions	 Rings

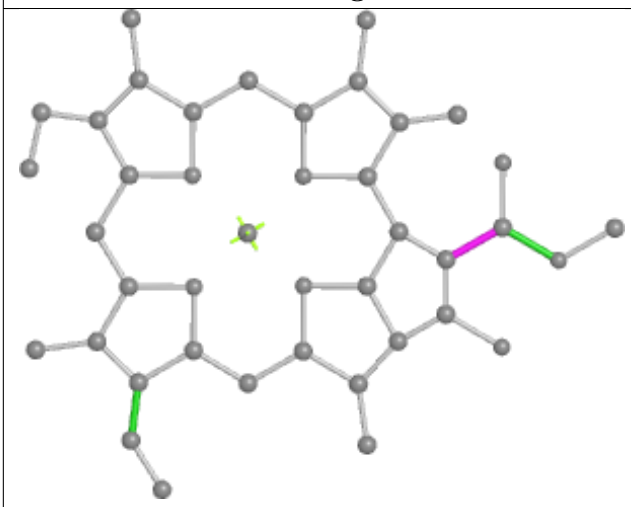
Ligand CLA J 102



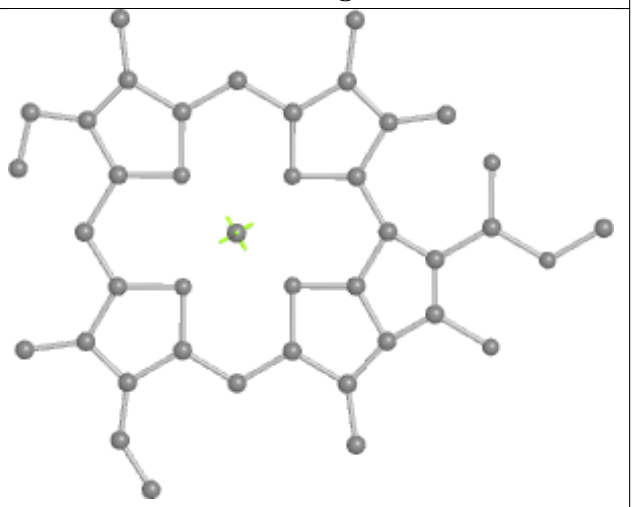
Bond lengths



Bond angles

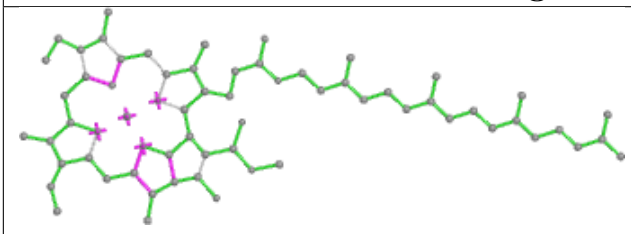


Torsions

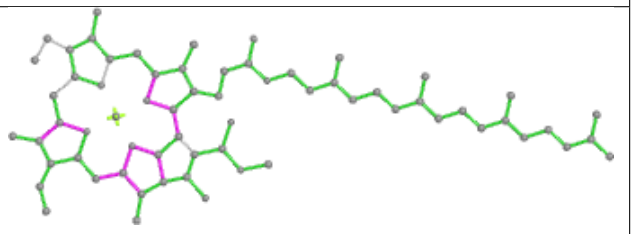


Rings

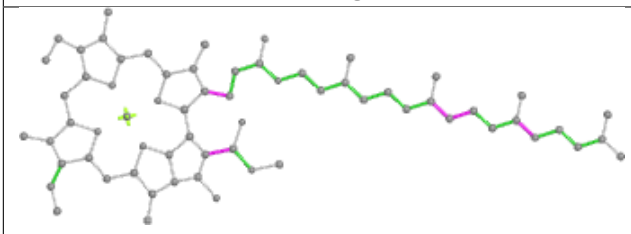
Ligand CLA 6 602



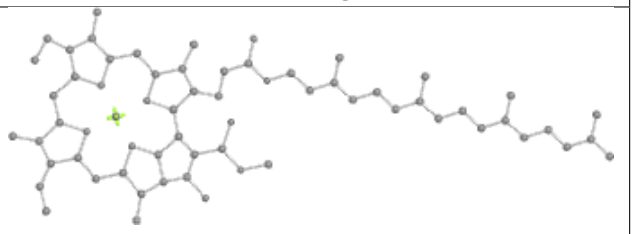
Bond lengths



Bond angles

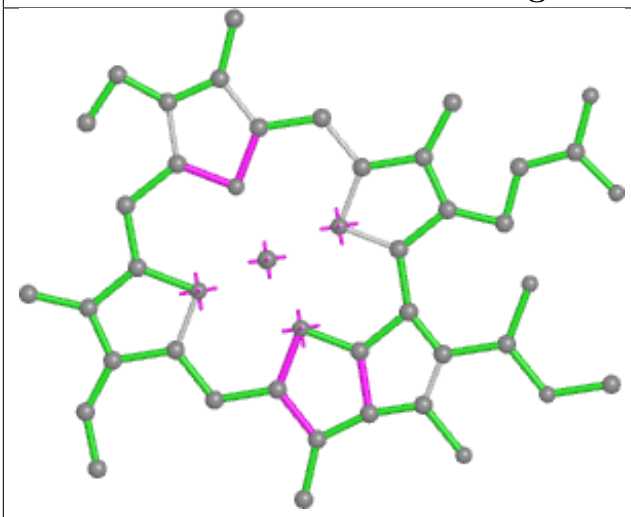


Torsions

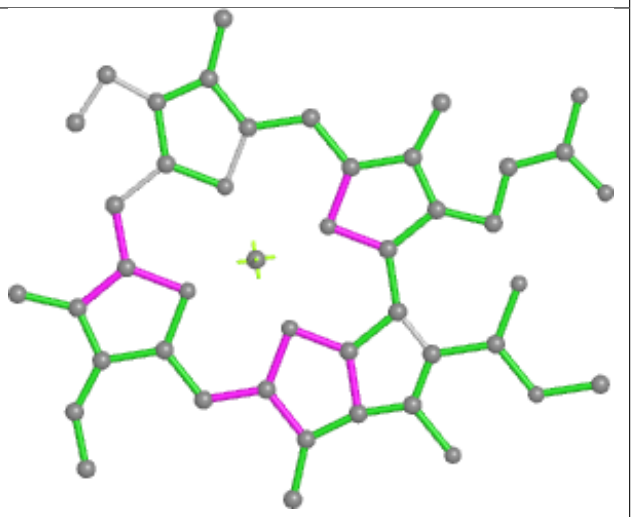


Rings

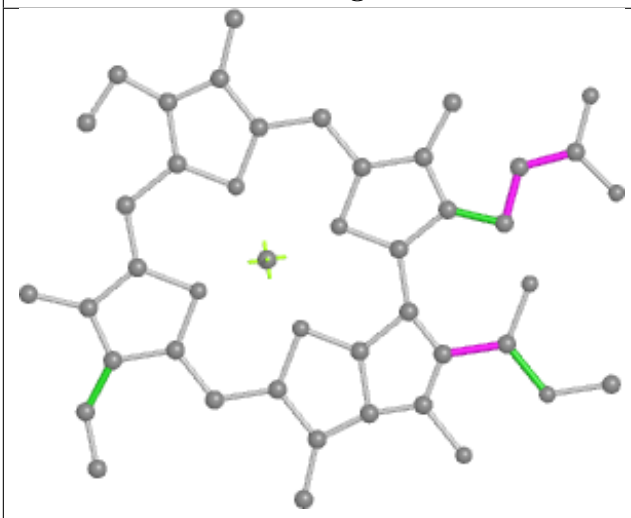
Ligand CLA 9 603



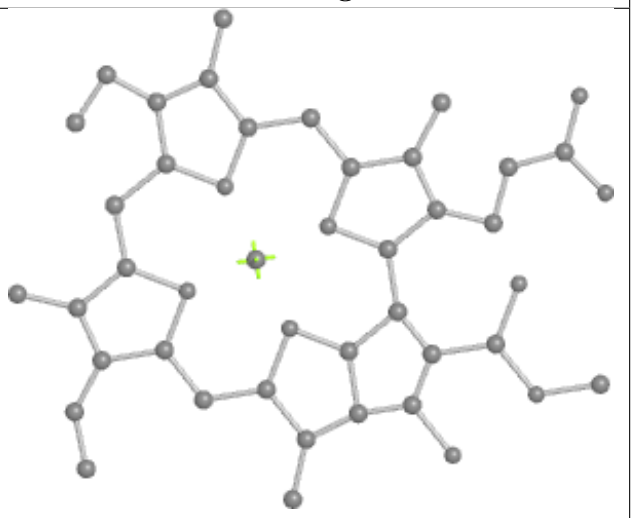
Bond lengths



Bond angles

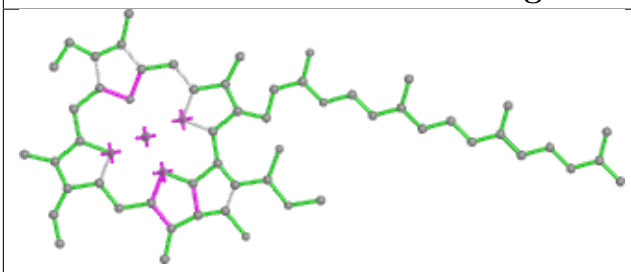


Torsions

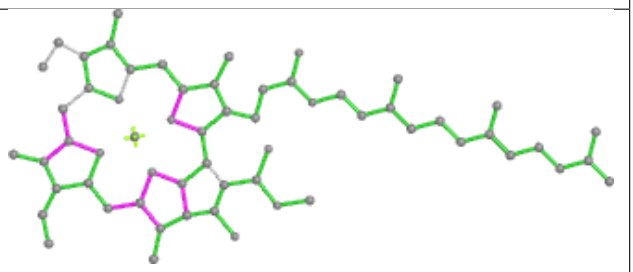


Rings

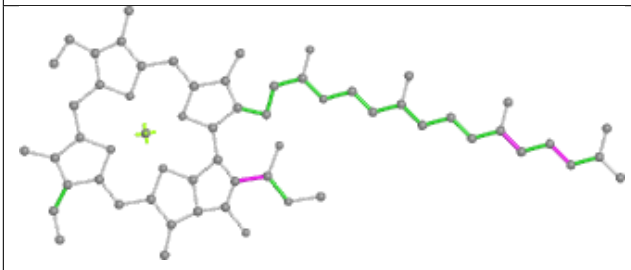
Ligand CLA B 824



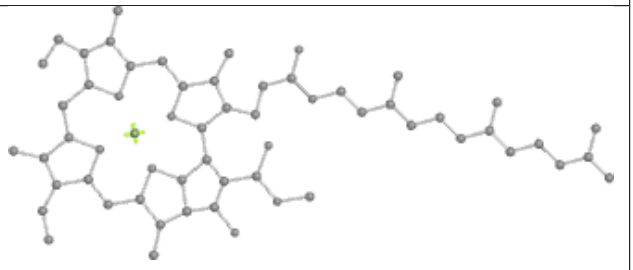
Bond lengths



Bond angles

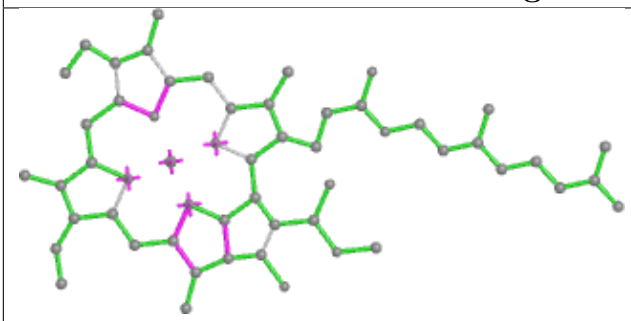


Torsions



Rings

Ligand CLA A 836



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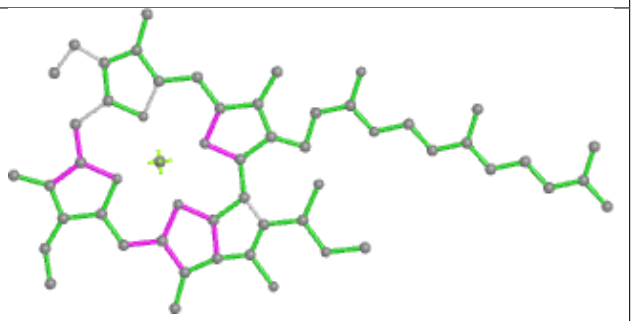

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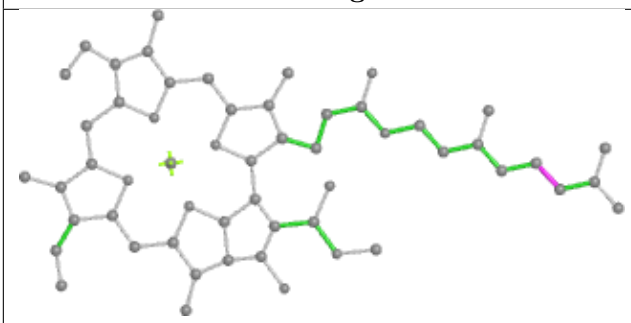

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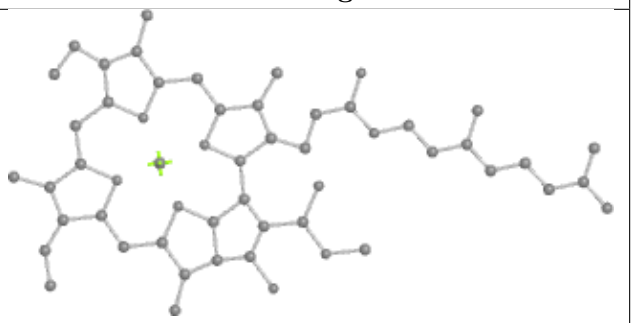
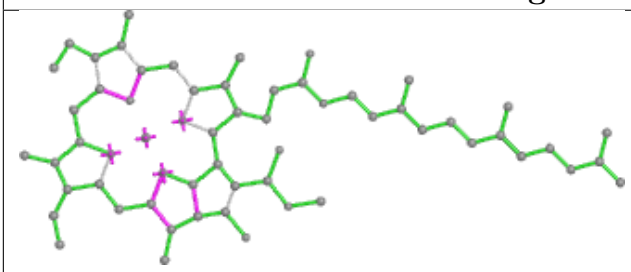


Rings

Ligand CLA 5 608



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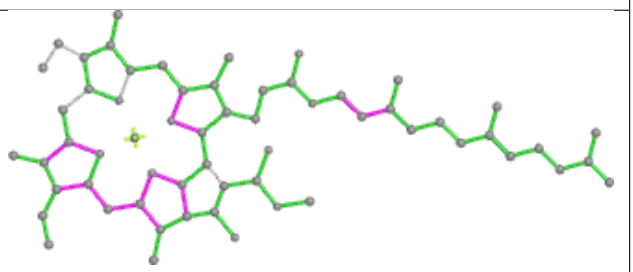
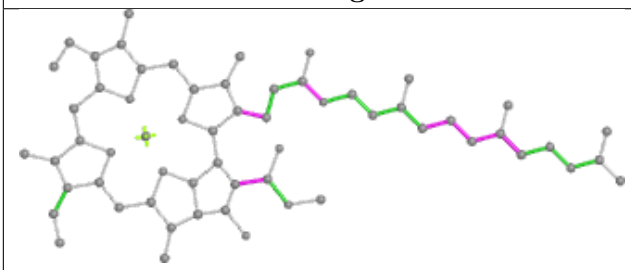


Bond angles



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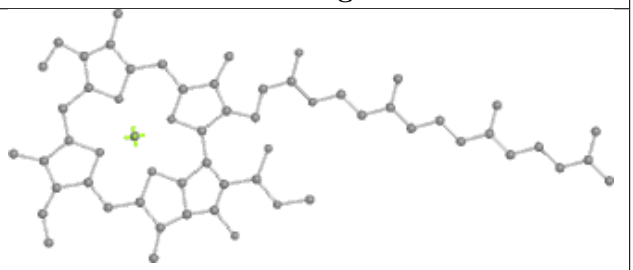
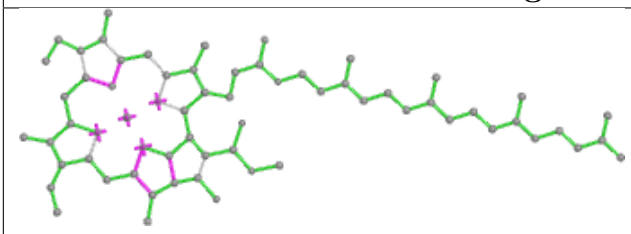


Rings

Ligand CLA B 802



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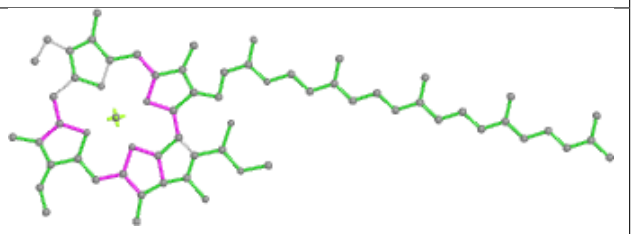
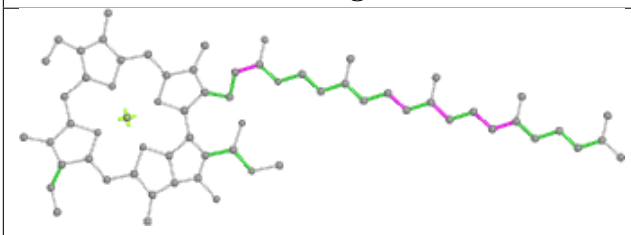


Bond angles



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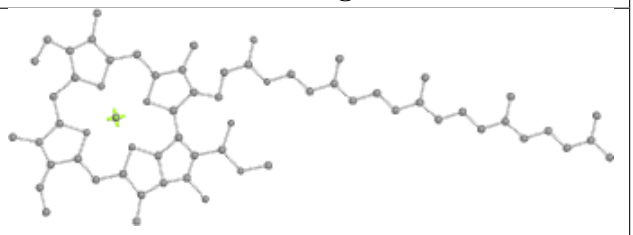
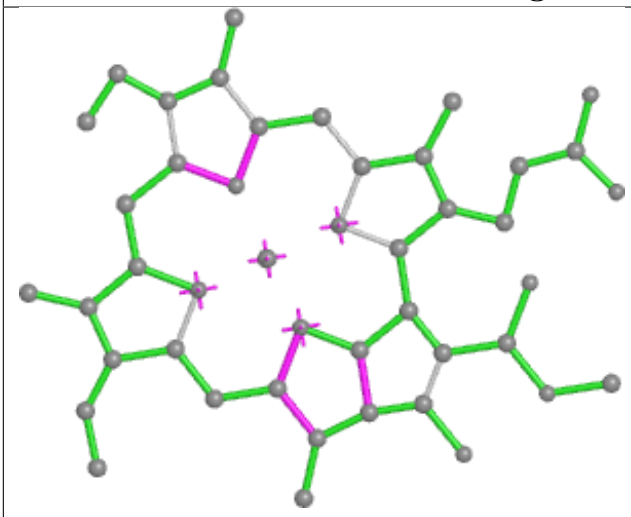


Rings

Ligand CLA 2 611



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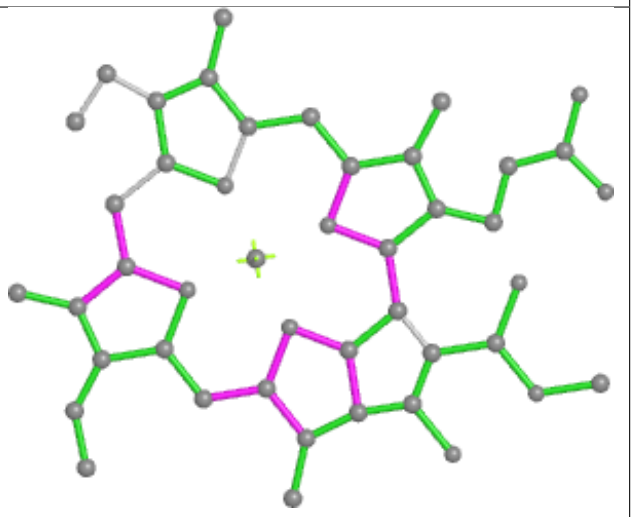
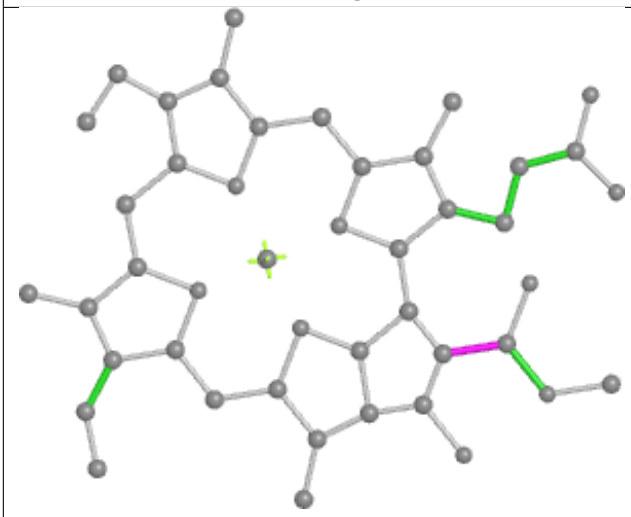


Bond angles



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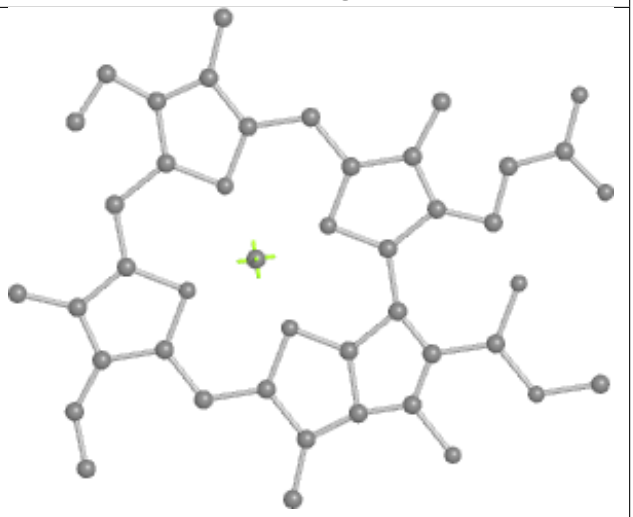
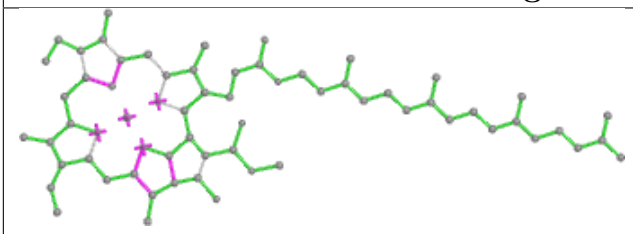


Rings

Ligand CLA A 804



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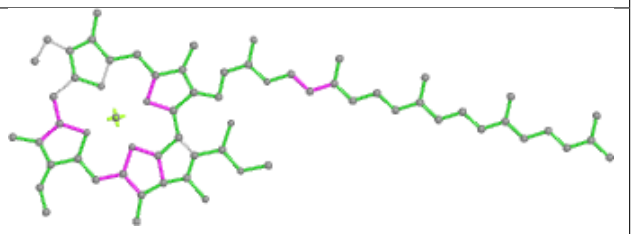

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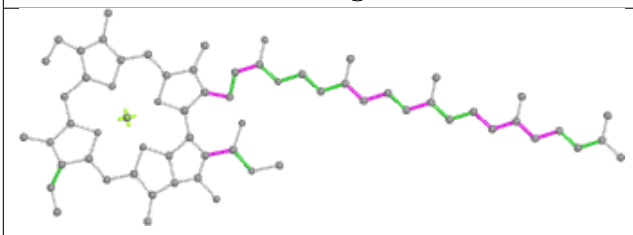

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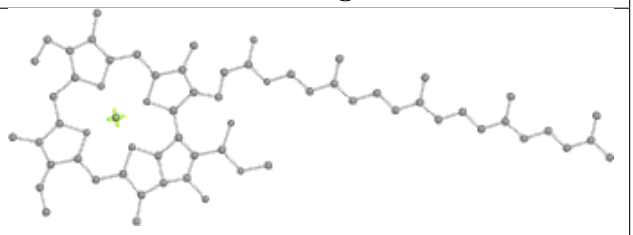
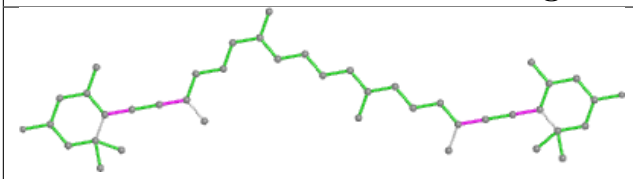


Rings

Ligand II0 6 614



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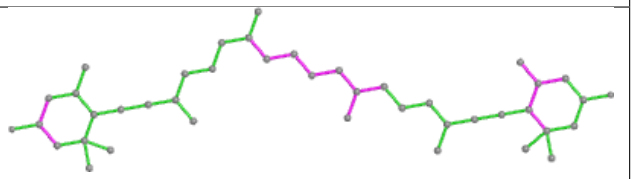
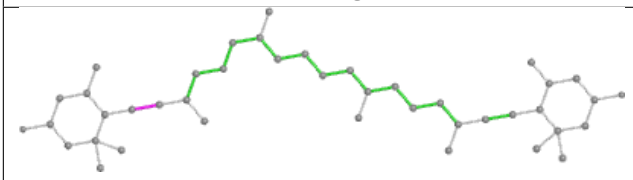


Bond angles



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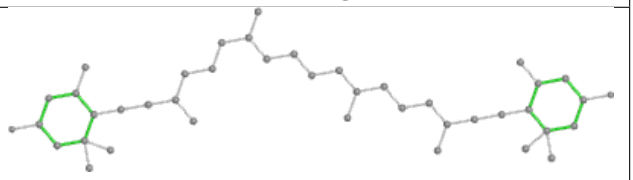
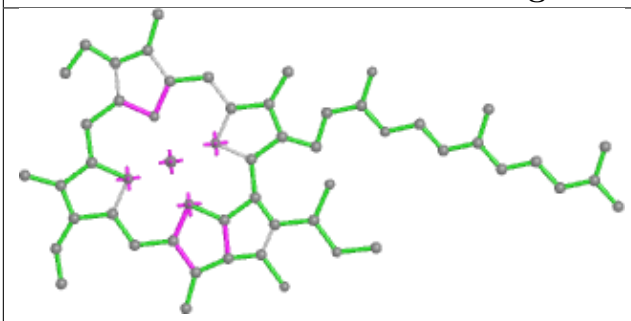


Rings

Ligand CLA 7 304



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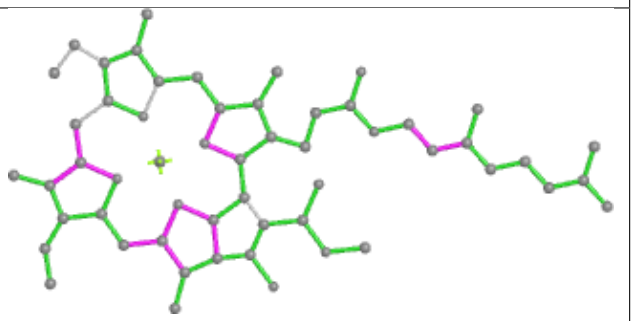
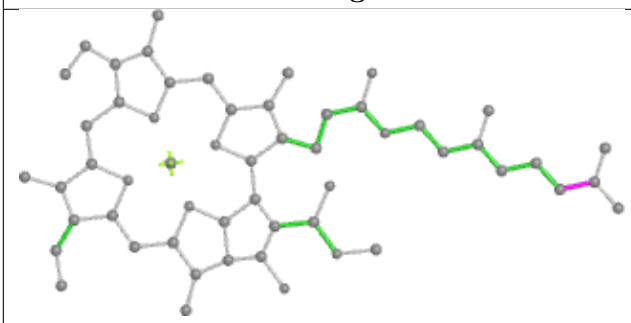


Bond angles



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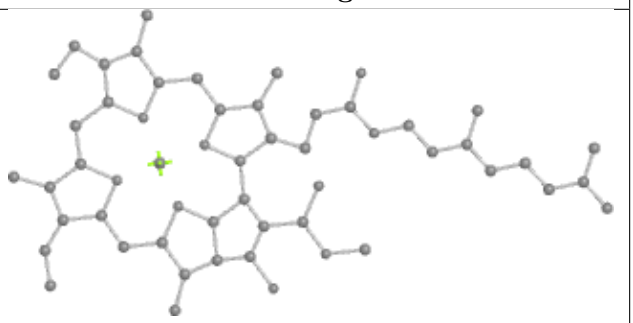
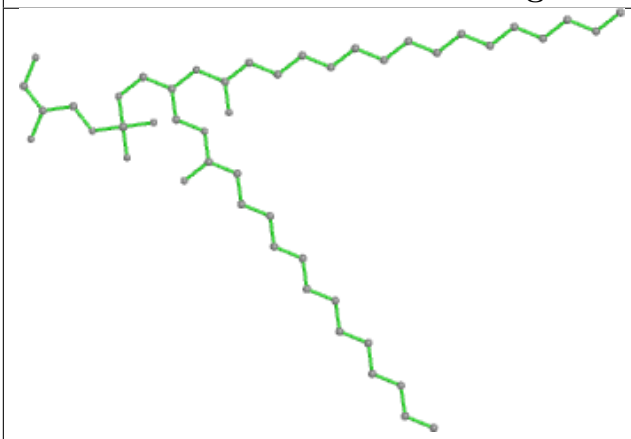


Rings

Ligand LHG 4 617



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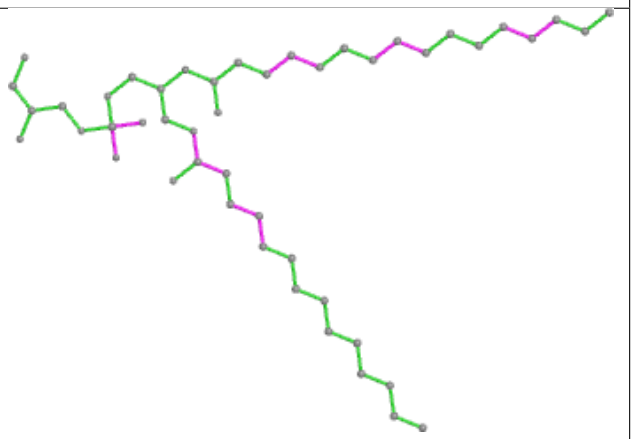
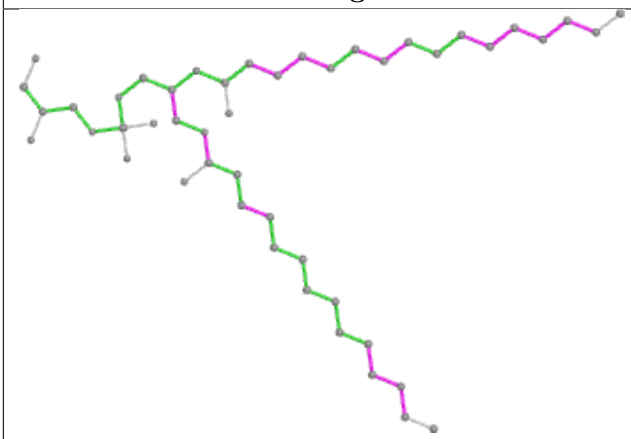
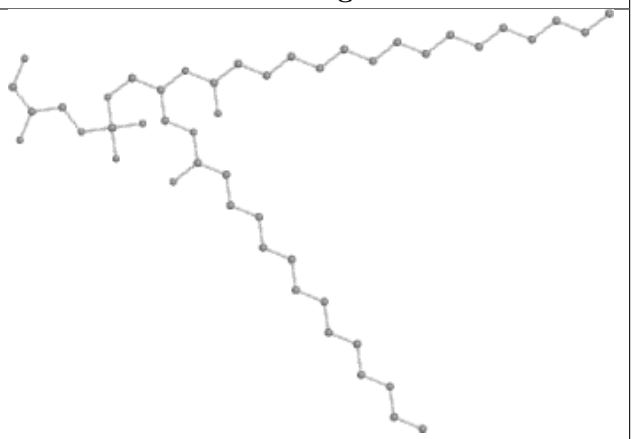


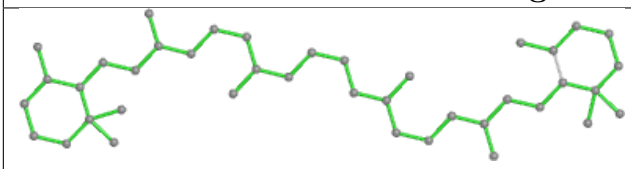
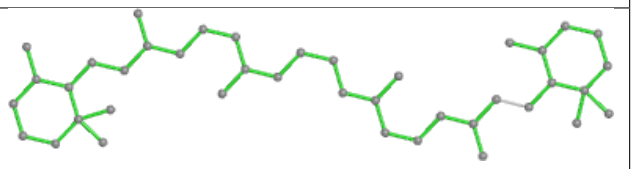
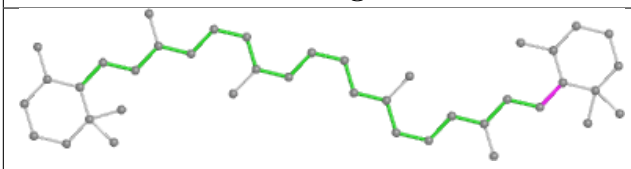
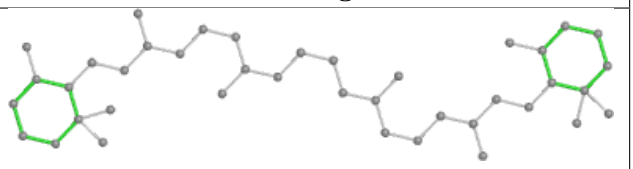
Bond angles

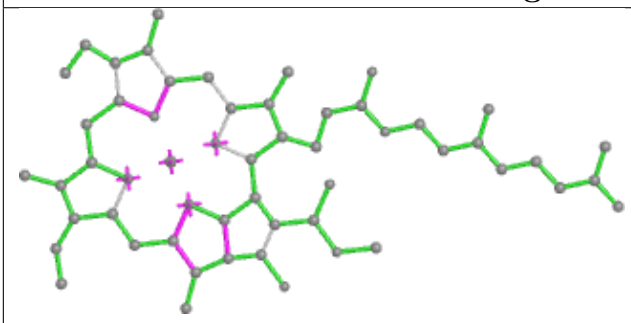
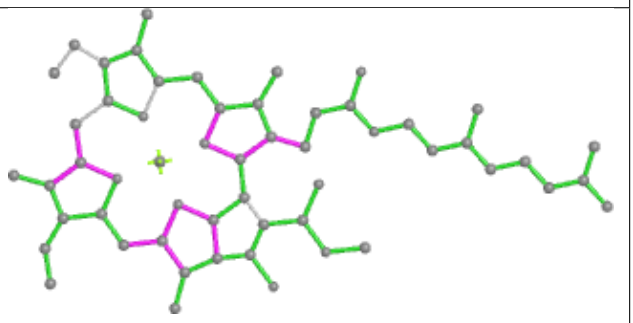
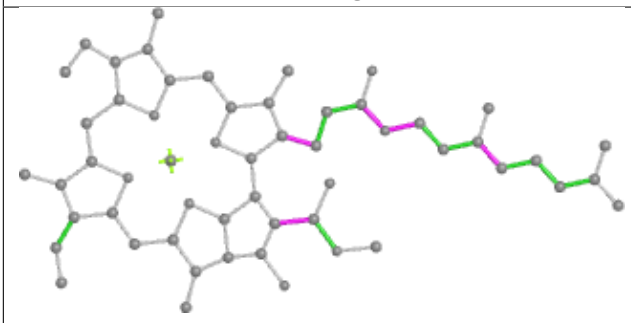
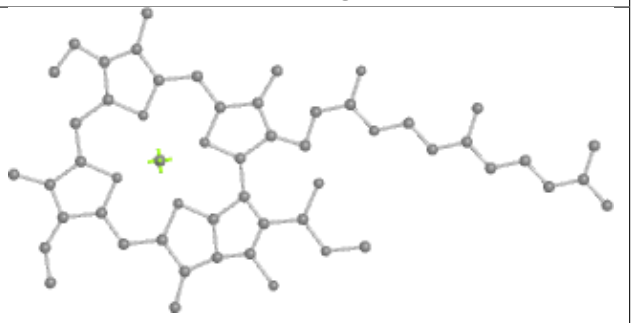


Torsions

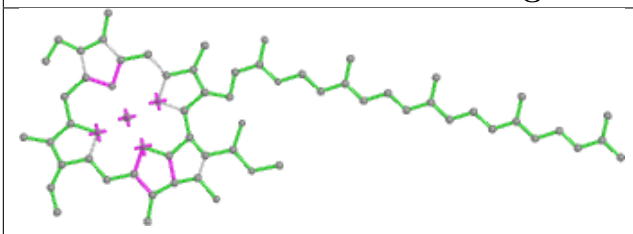


Rings

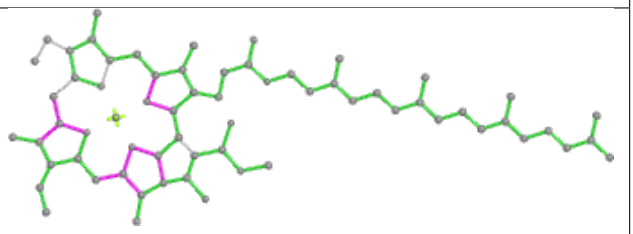
Ligand 8CT L 205	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA O 204	
 Bond lengths	 Bond angles
 Torsions	 Rings

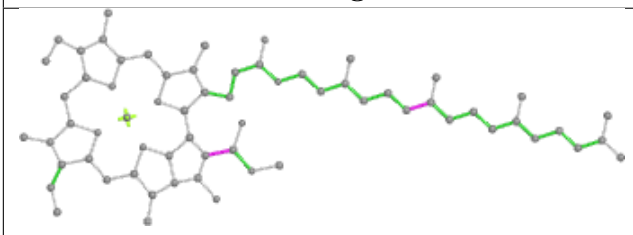
Ligand CLA A 824



Bond lengths



Bond angles



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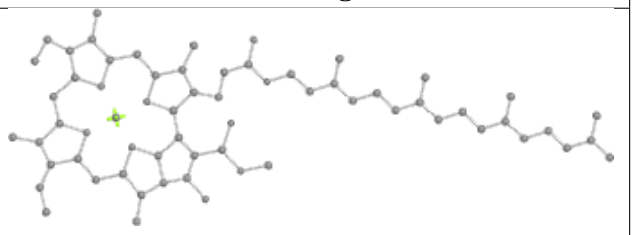
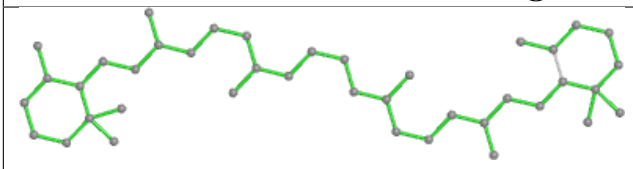
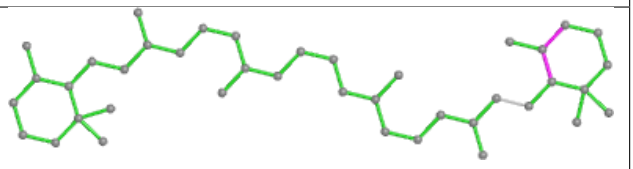


Rings

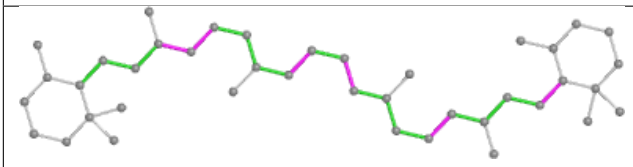
Ligand 8CT B 845



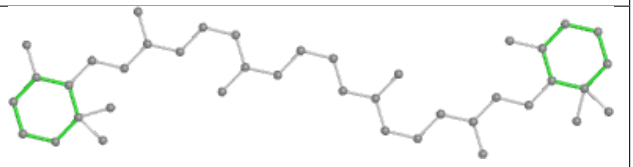
Bond lengths



Bond angles

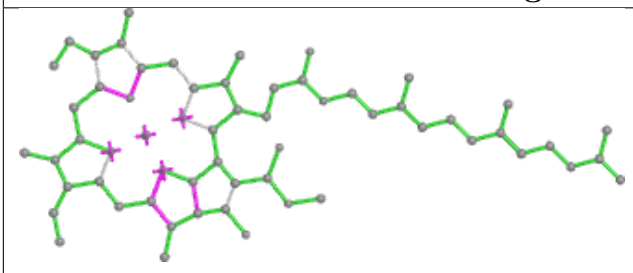


Torsions

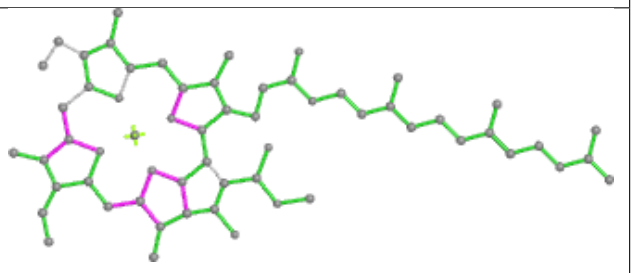


Rings

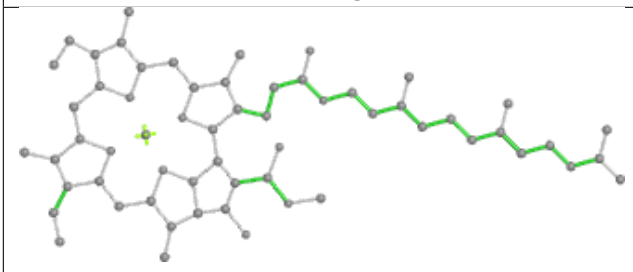
Ligand CLA B 830



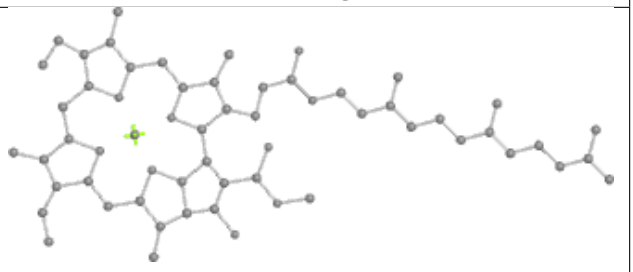
Bond lengths



Bond angles

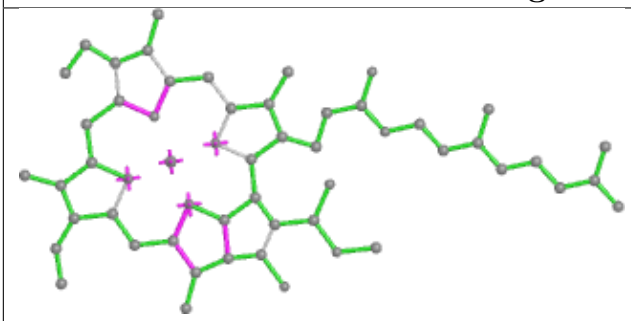


Torsions

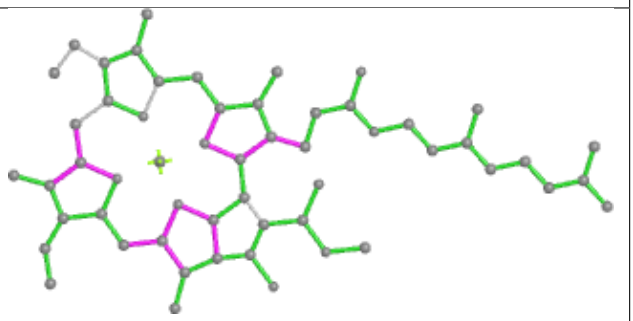


Rings

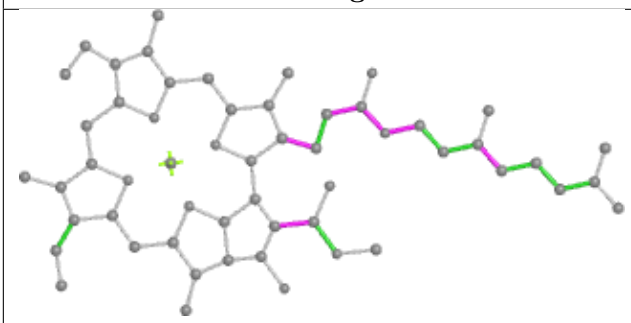
Ligand CLA a 605



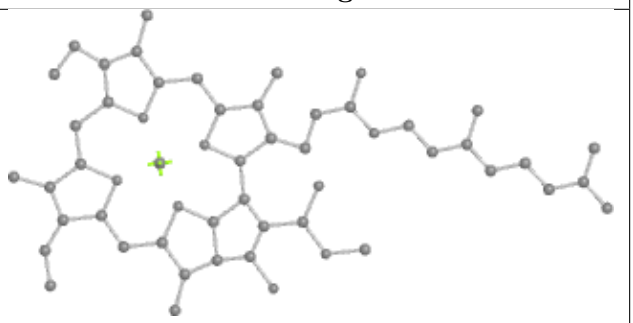
Bond lengths



Bond angles

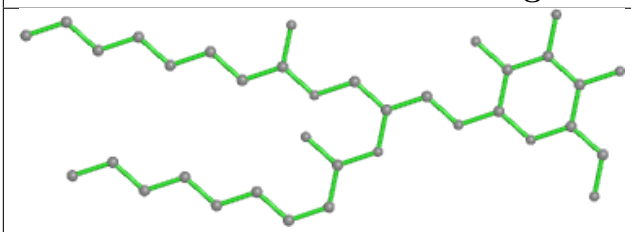


Torsions

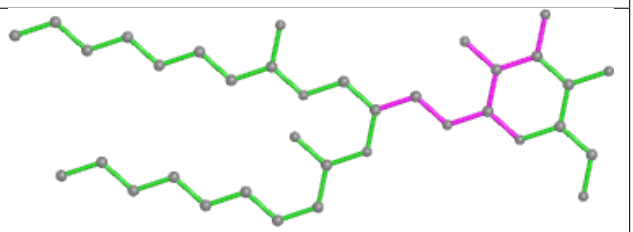


Rings

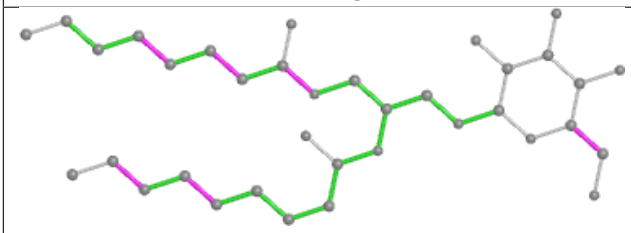
Ligand LMG 2 617



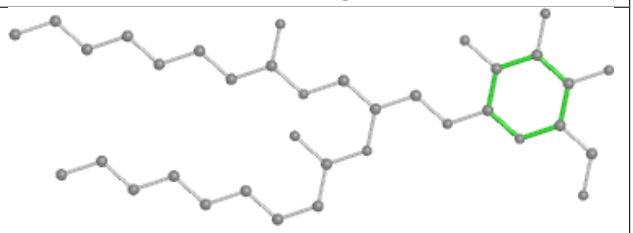
Bond lengths



Bond angles

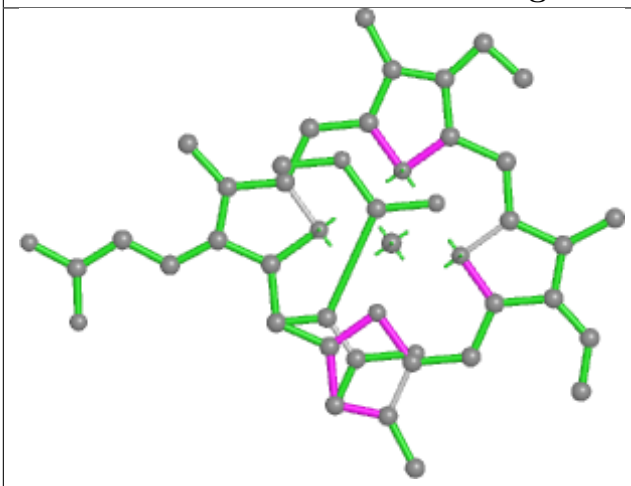


Torsions



Rings

Ligand KC2 b 605



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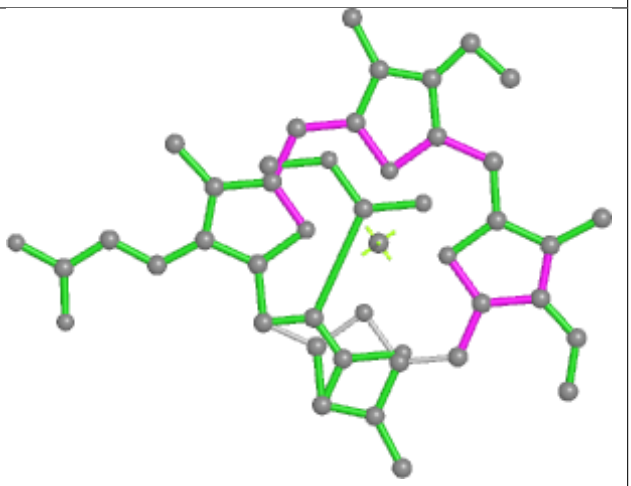
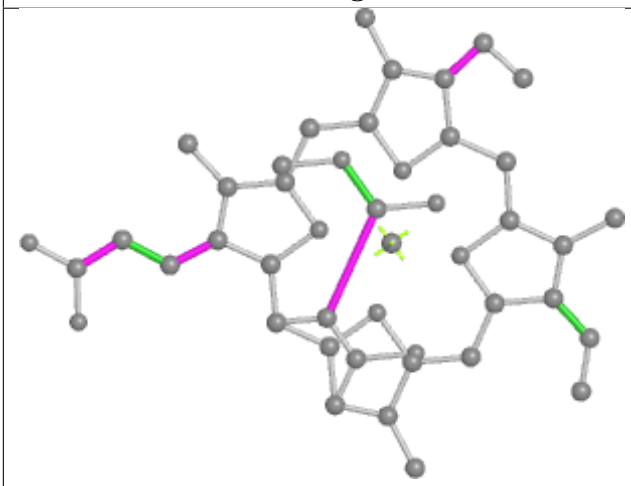


Bond angles



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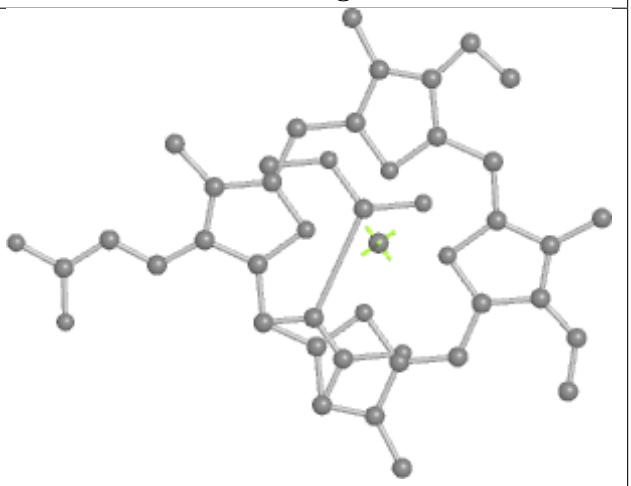
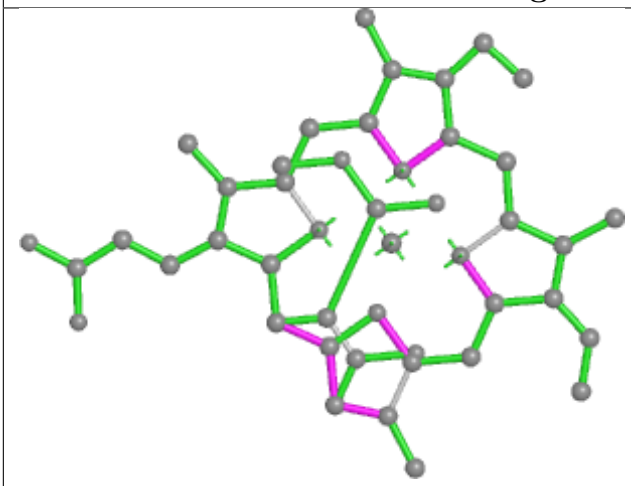


Rings

Ligand KC2 4 605



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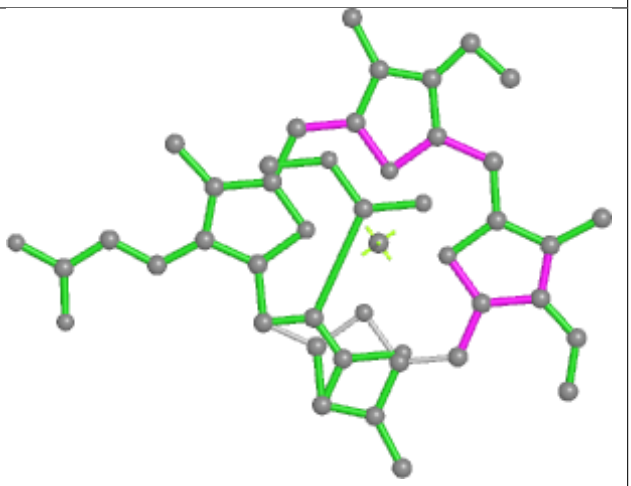

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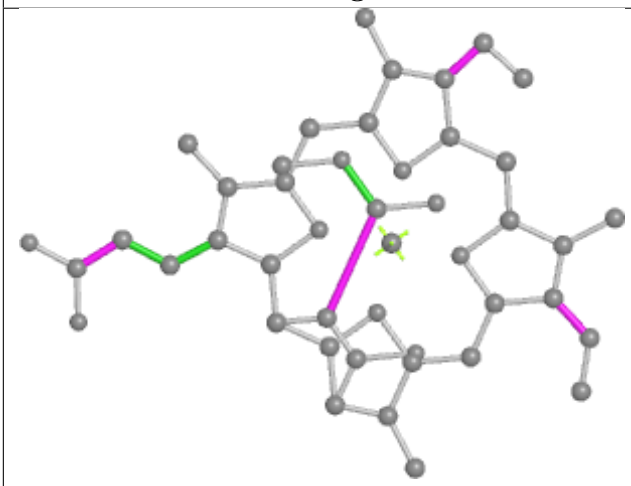

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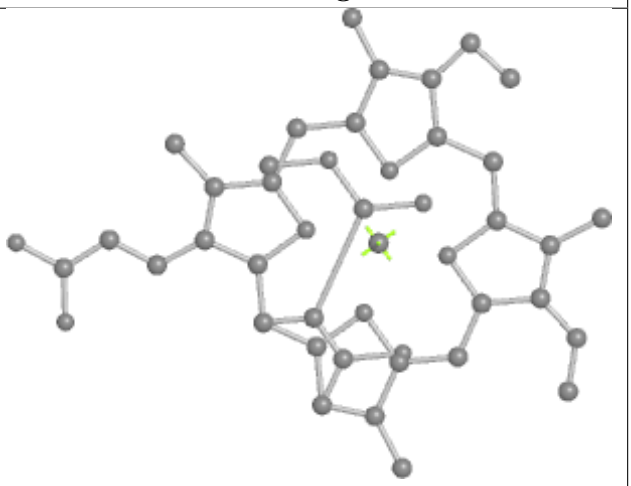
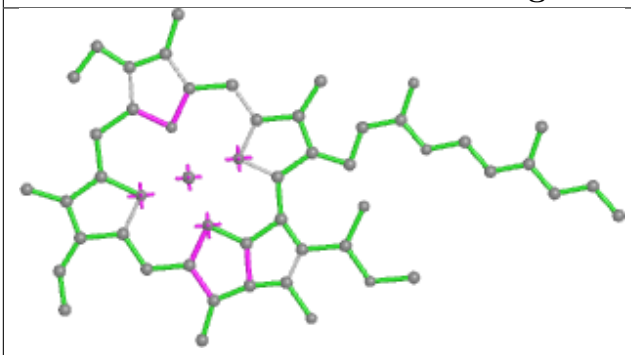
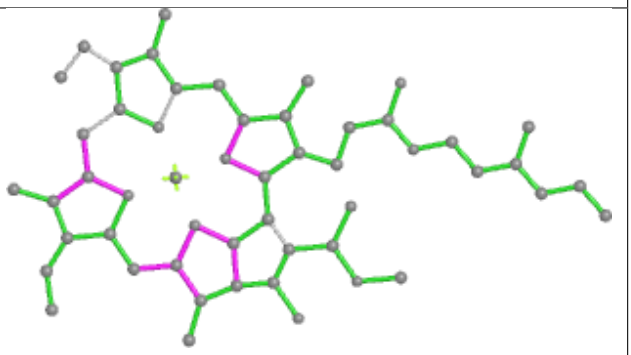
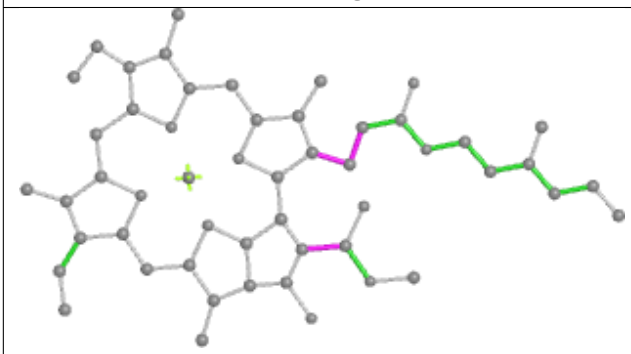
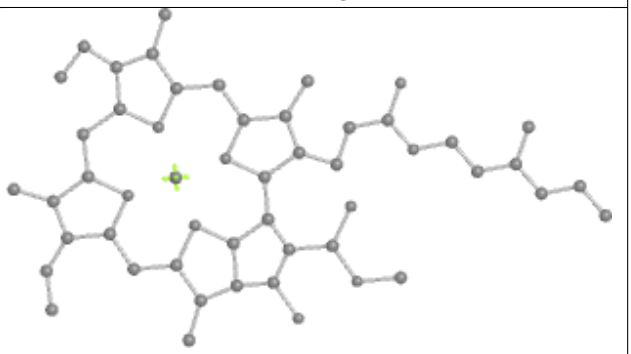
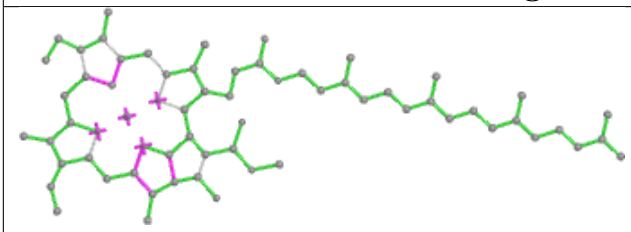
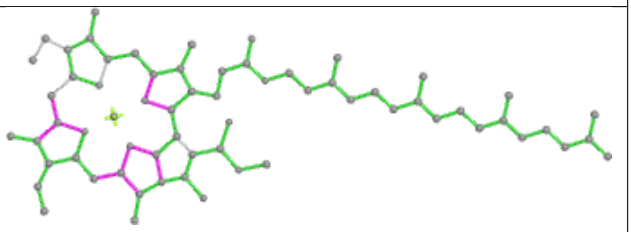
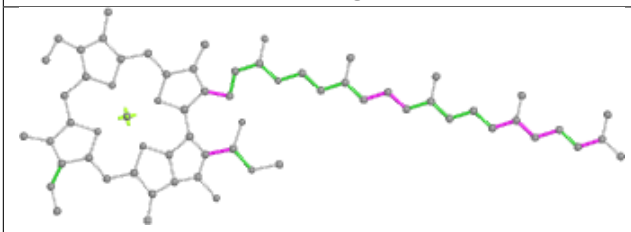
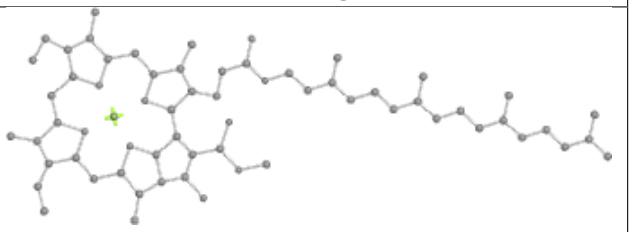
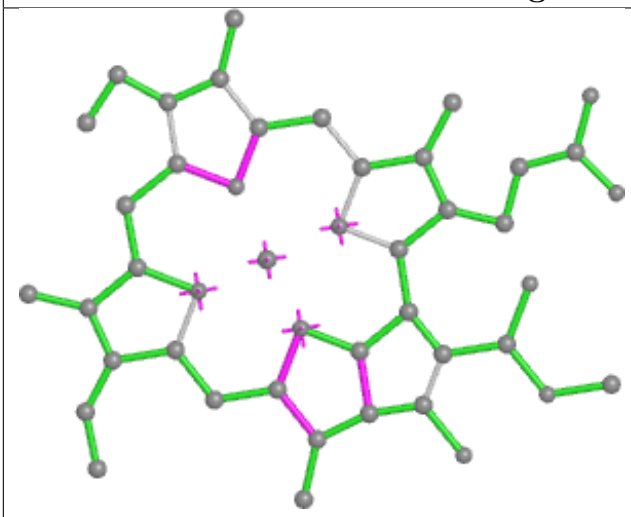


Rings

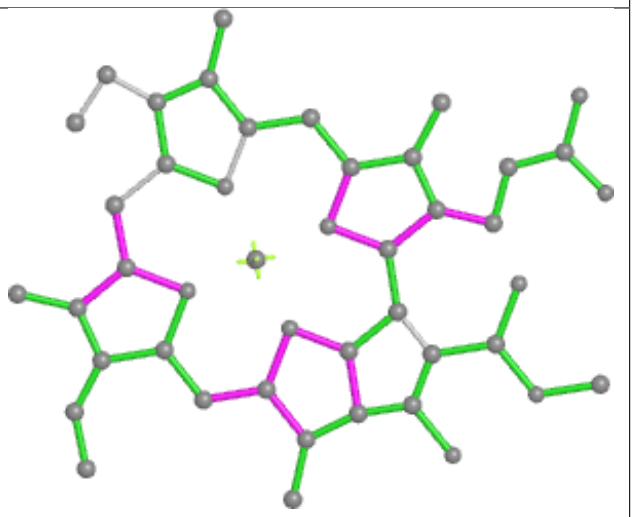
Ligand CLA 1 603	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA A 831	
	
Bond lengths	Bond angles
	
Torsions	Rings

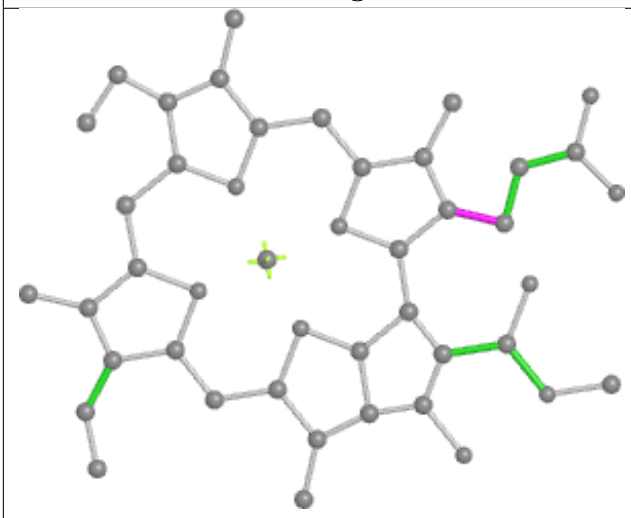
Ligand CLA 6 612



Bond lengths



Bond angles



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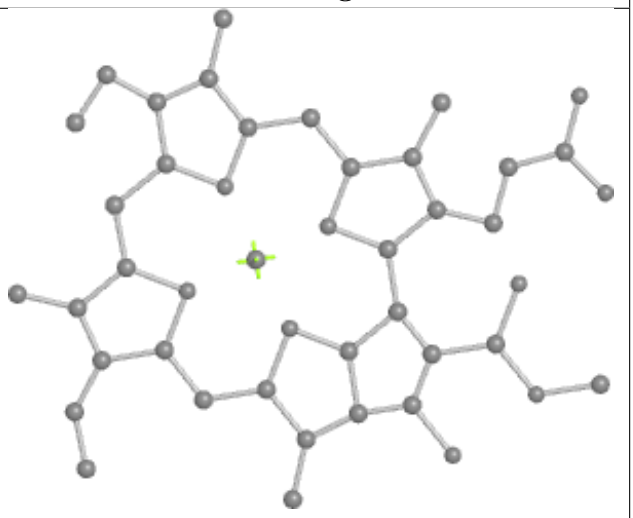
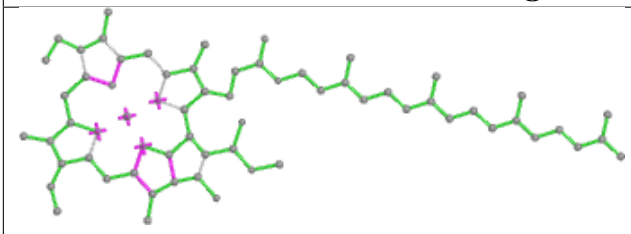


Rings

Ligand CLA A 838



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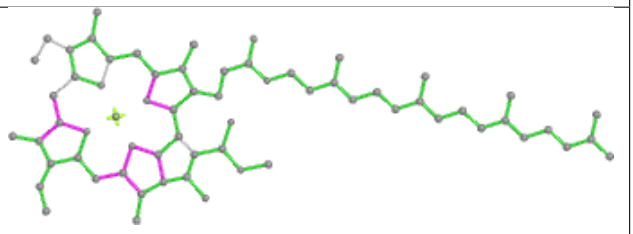
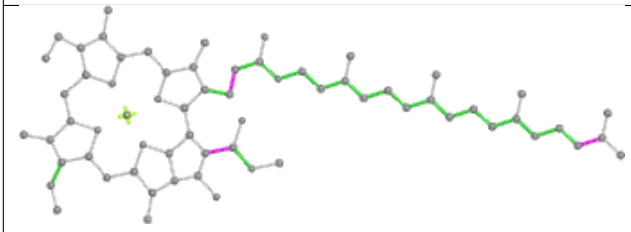


Bond angles



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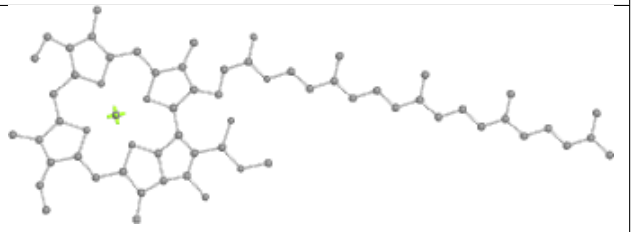
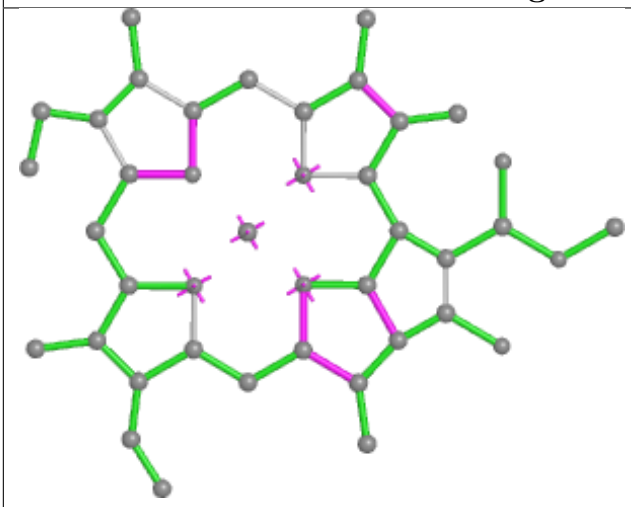


Rings

Ligand CLA 9 609



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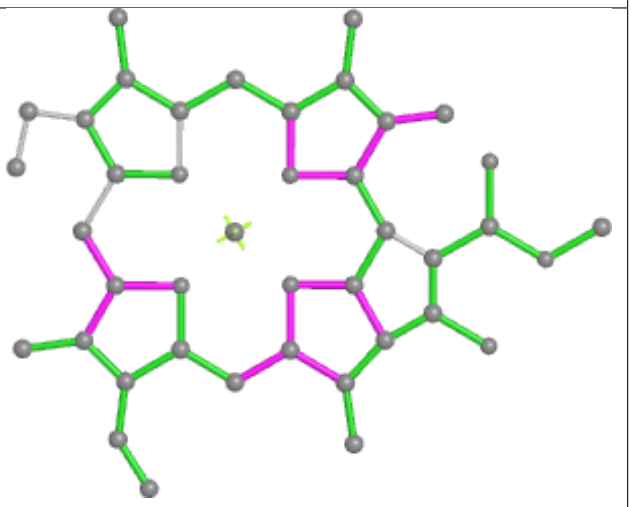

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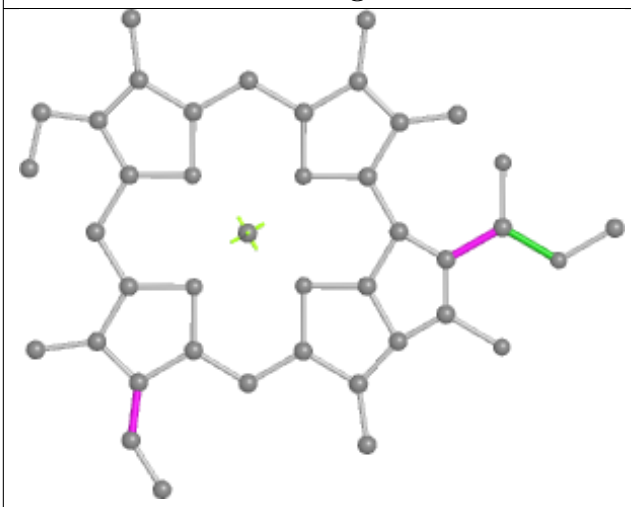

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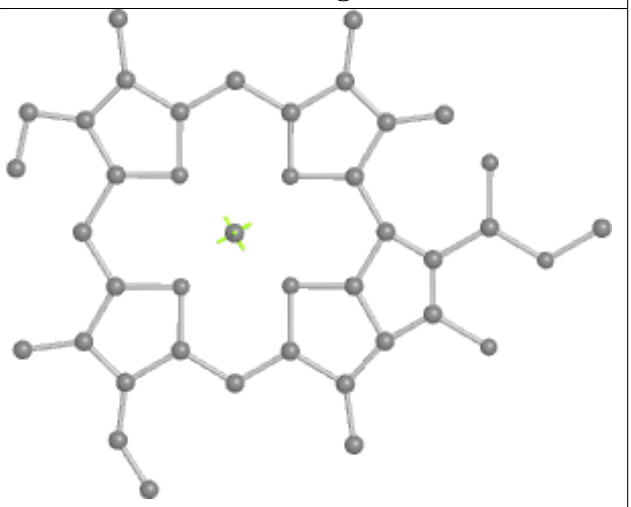
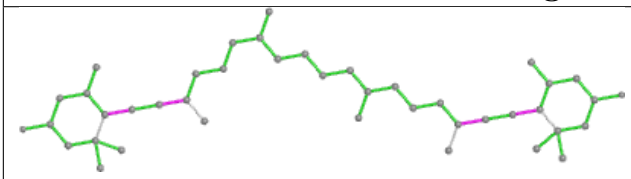


Rings

Ligand II0 a 615



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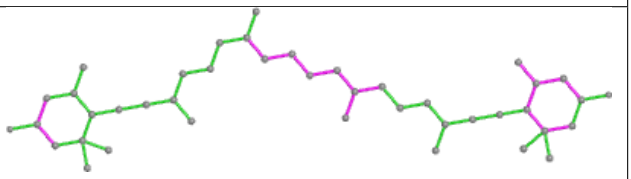
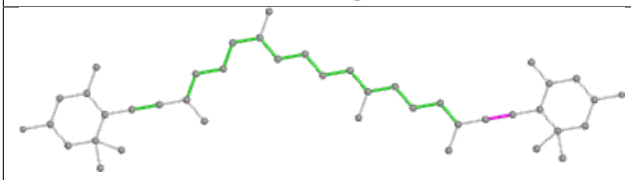


Bond angles



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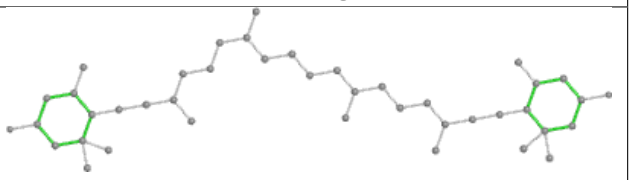
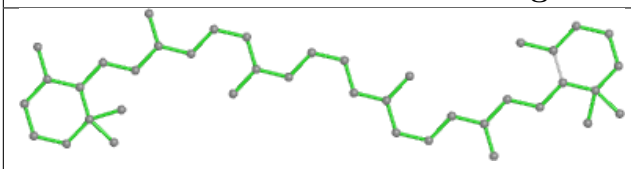
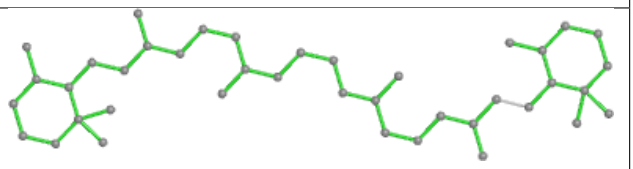


Rings

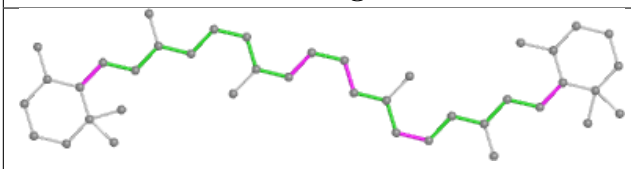
Ligand 8CT J 103



Bond lengths



Bond angles



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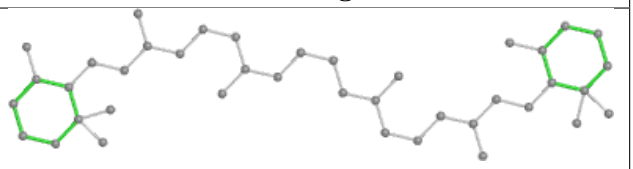
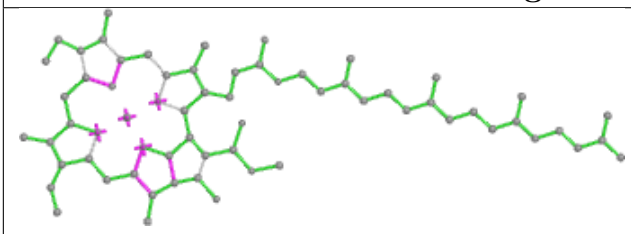


Rings

Ligand CLA B 838



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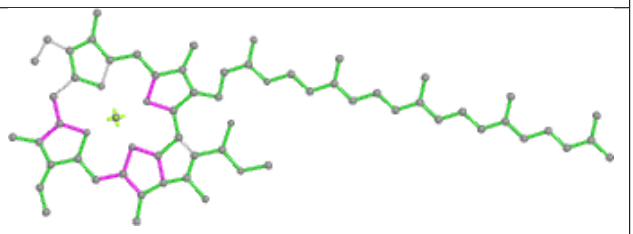
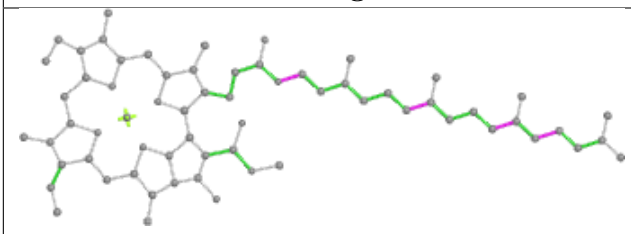
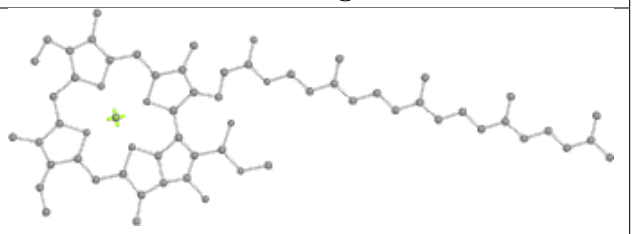


Bond angles

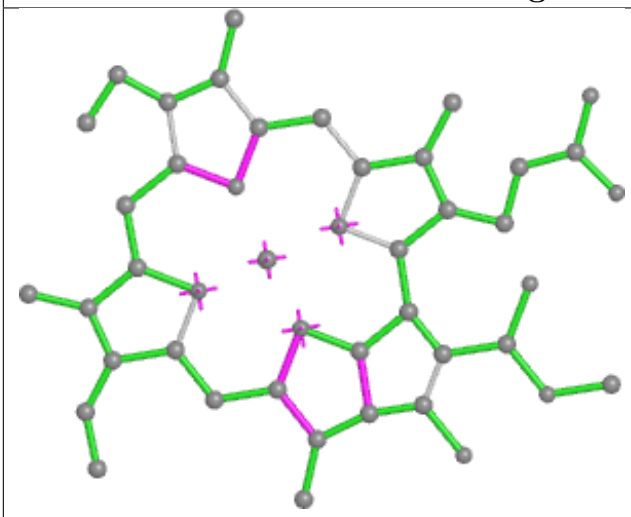


Torsions

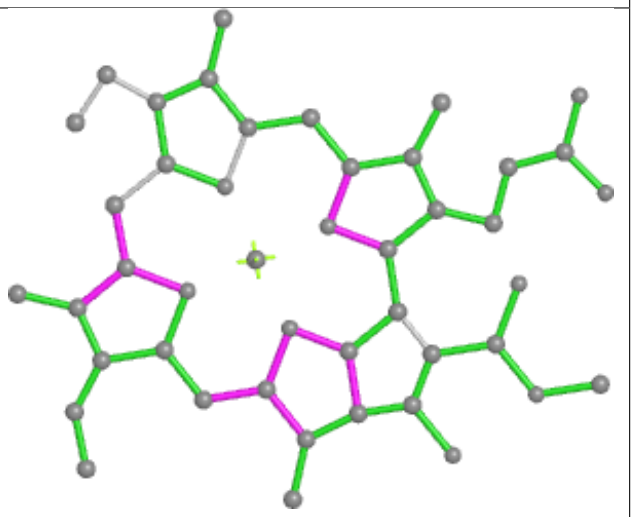


Rings

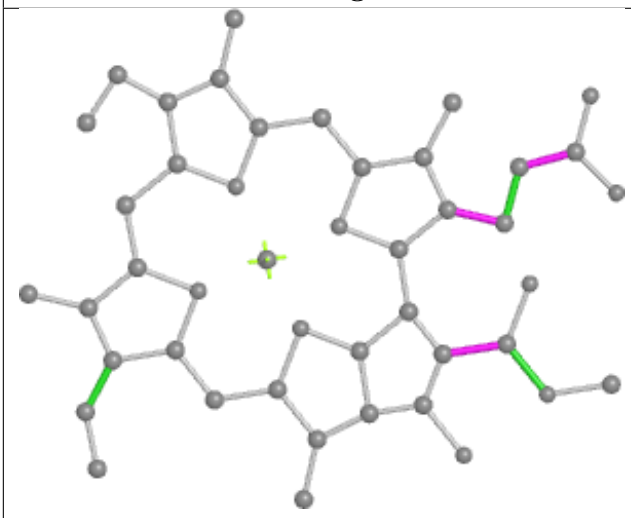
Ligand CLA 5 606



Bond lengths



Bond angles



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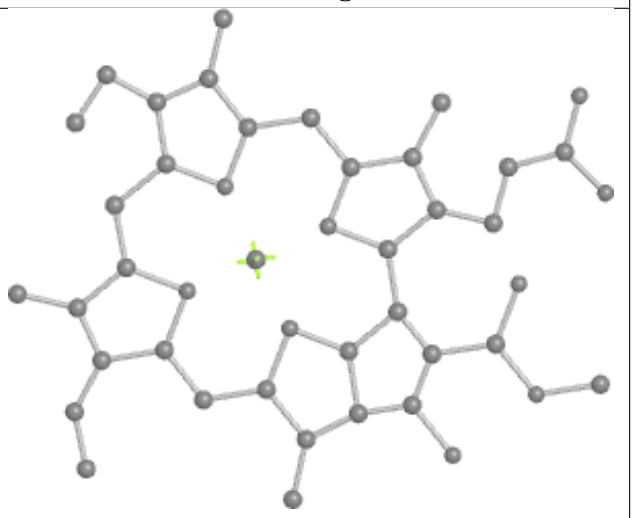
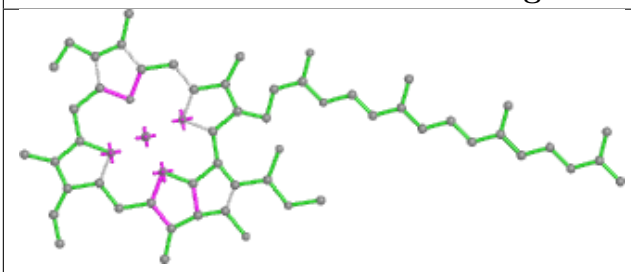


Rings

Ligand CLA A 830



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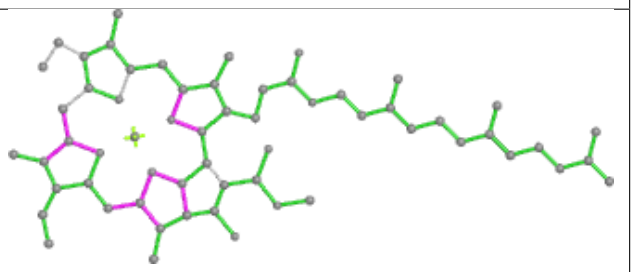
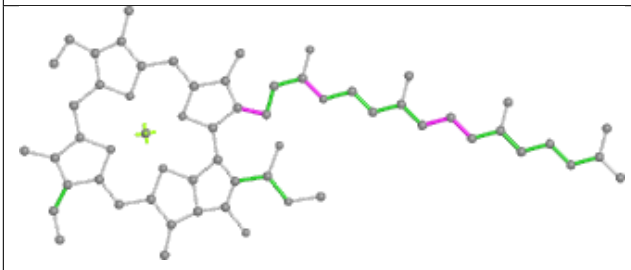
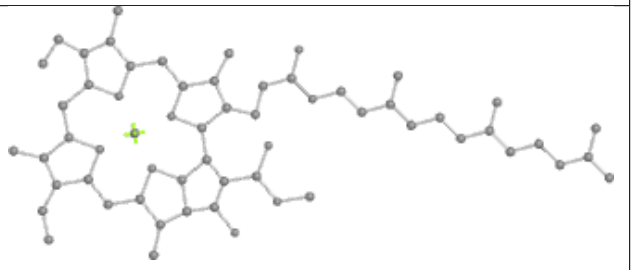


Bond angles

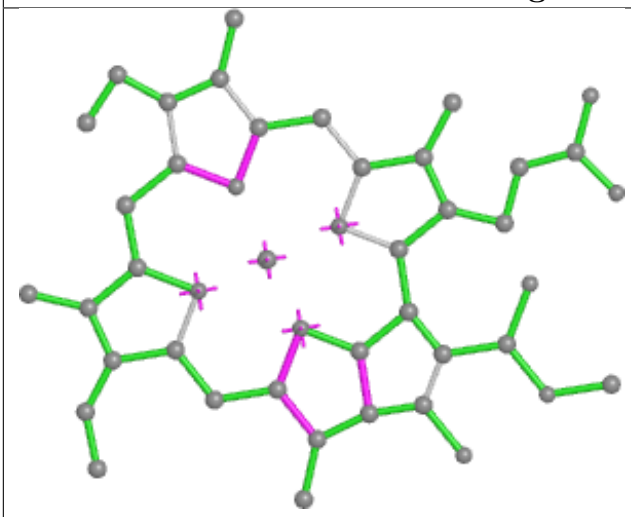


Torsions

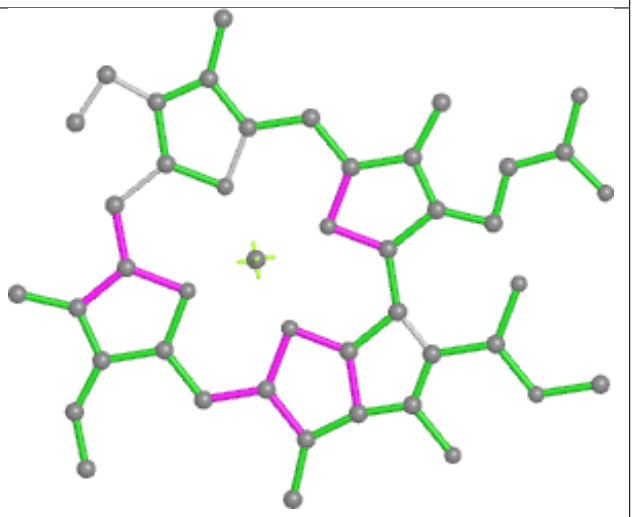


Rings

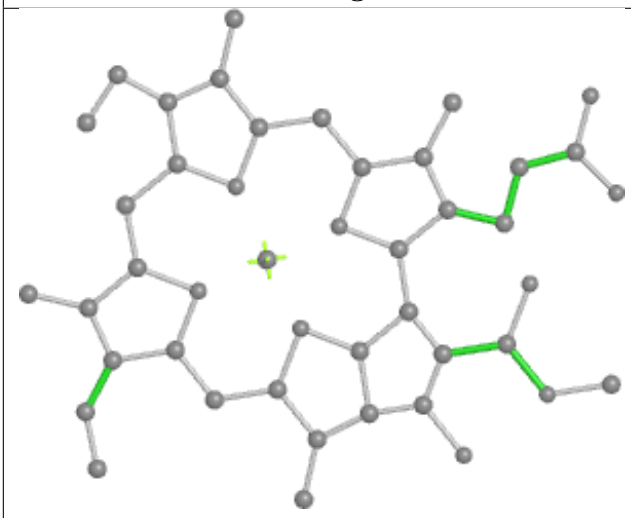
Ligand CLA 1 606



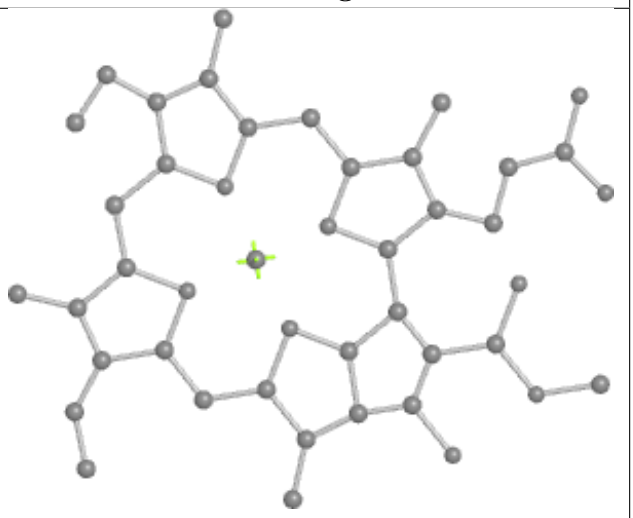
Bond lengths



Bond angles

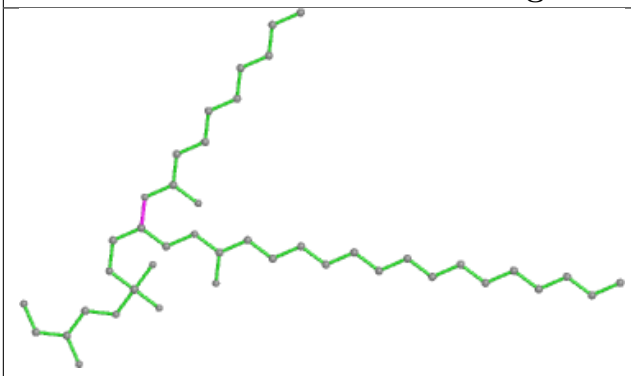


Torsions



Rings

Ligand LHG 2 620



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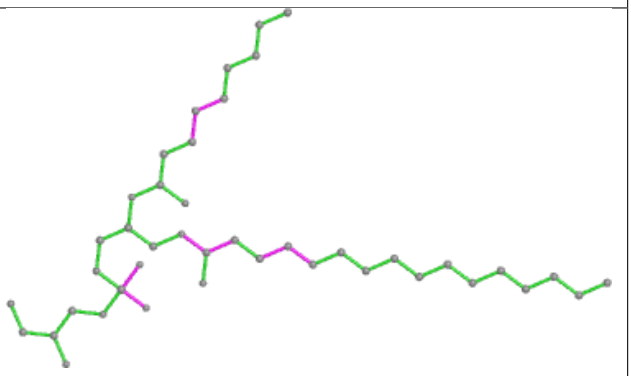
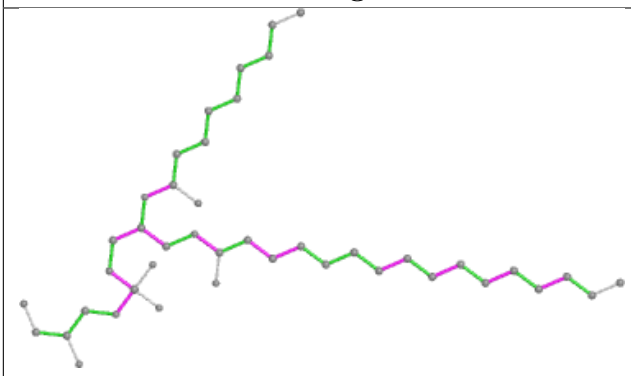
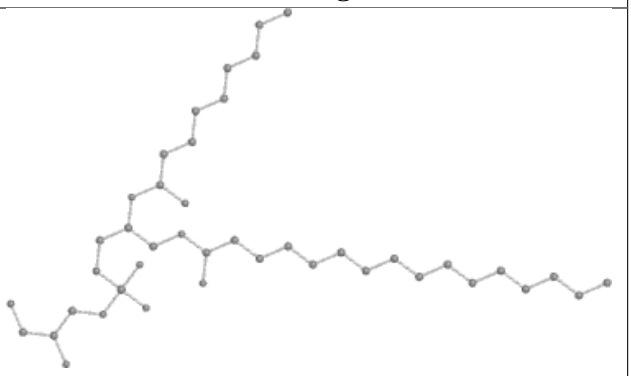


Bond angles

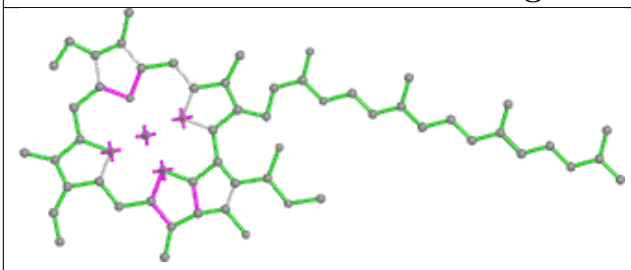


Torsions

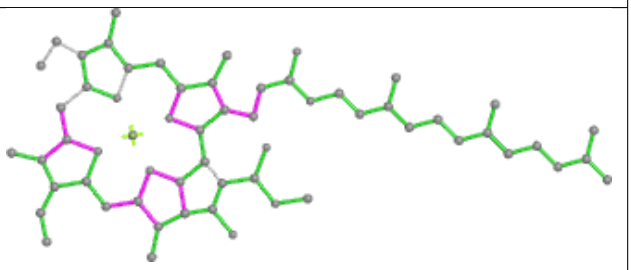


Rings

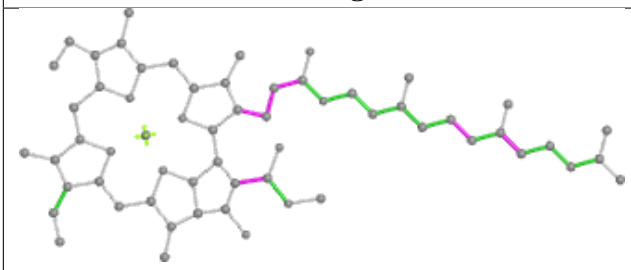
Ligand CLA B 819



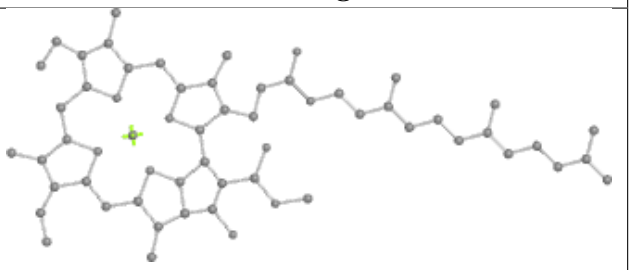
Bond lengths



Bond angles

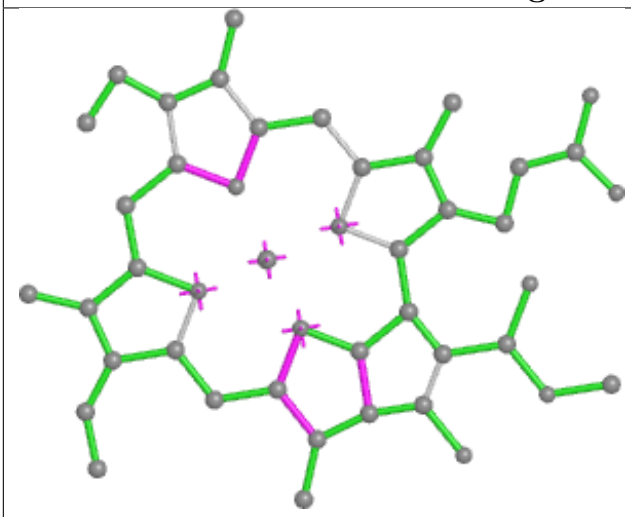


Torsions



Rings

Ligand CLA 8 601



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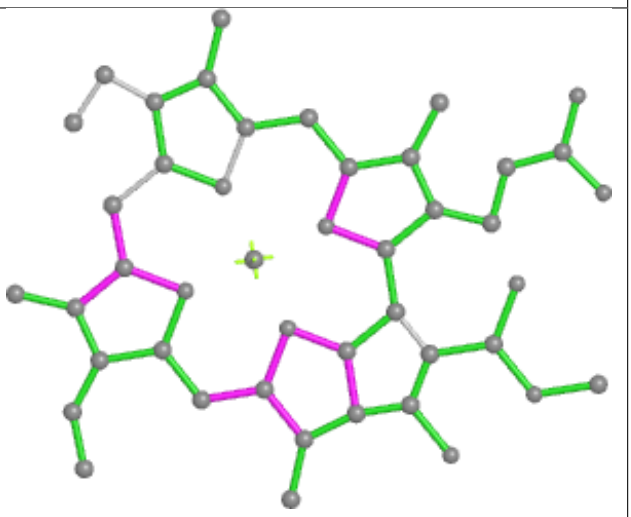
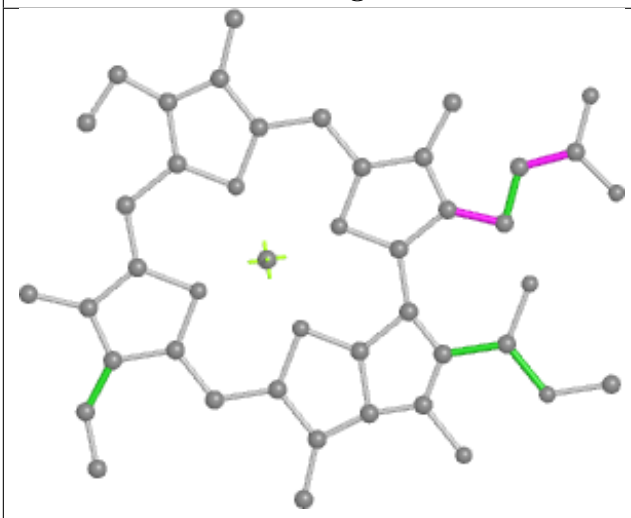


Bond angles



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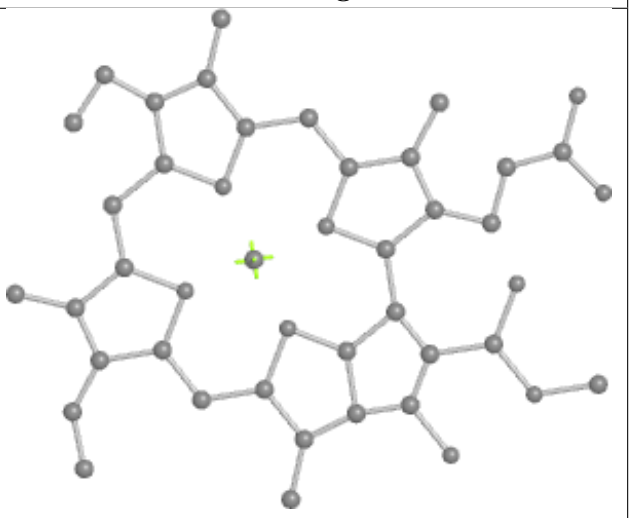
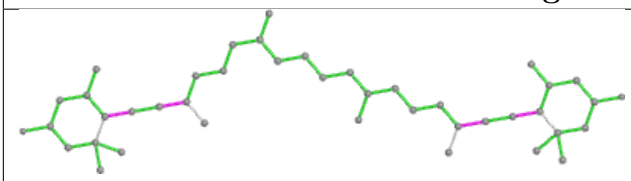


Rings

Ligand II0 4 612



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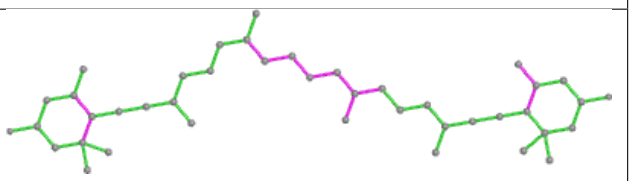

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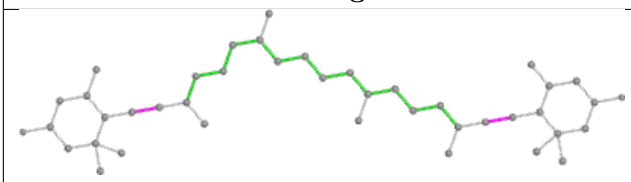

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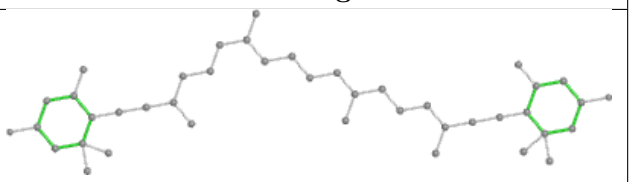
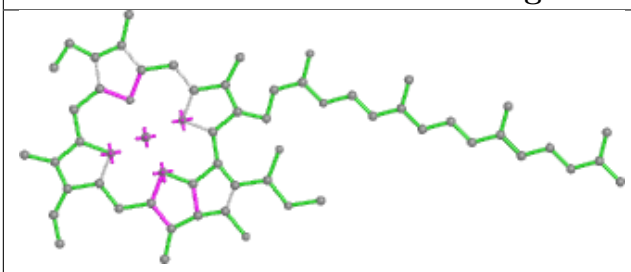


Rings

Ligand CLA B 810



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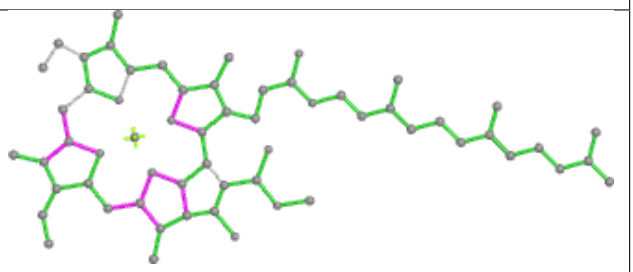
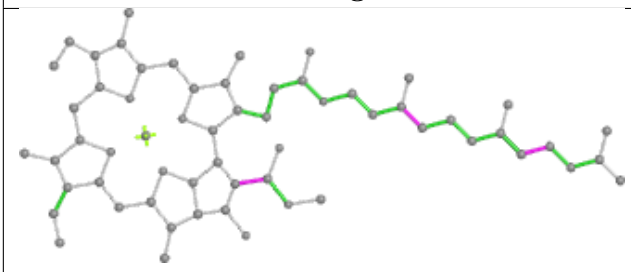


Bond angles



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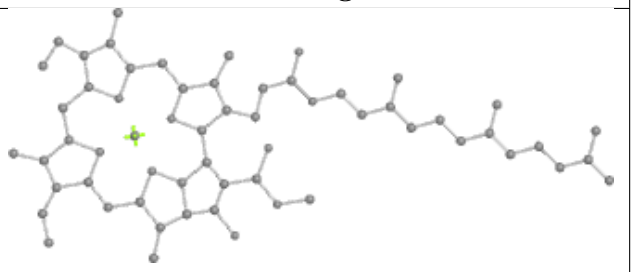
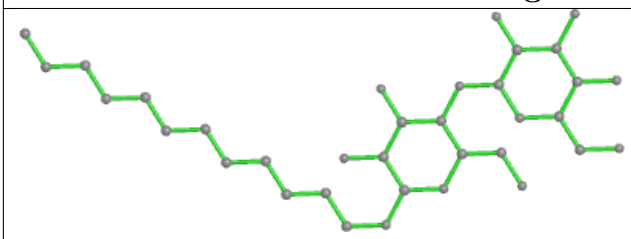


Rings

Ligand LMU 4 618



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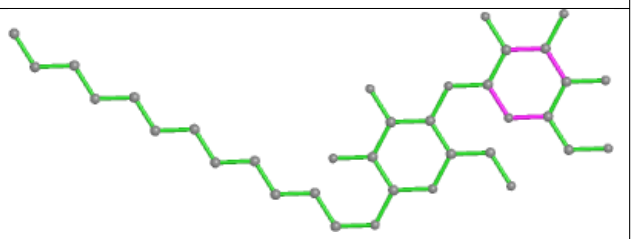
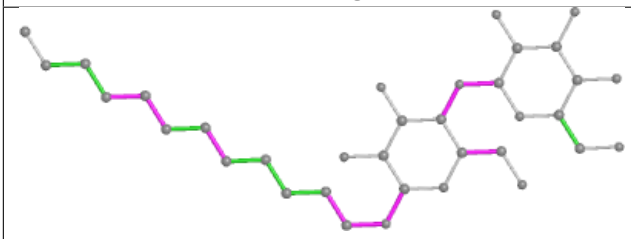


Bond angles



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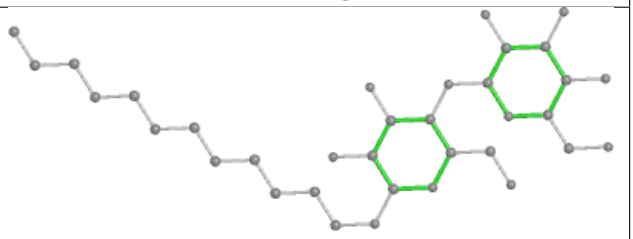
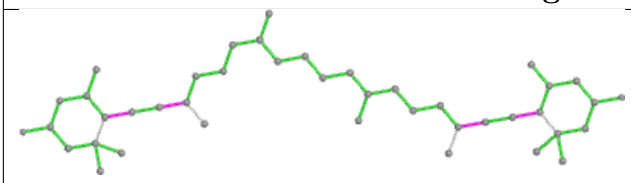


Rings

Ligand II0 1 614



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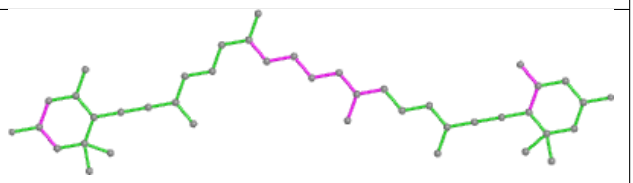

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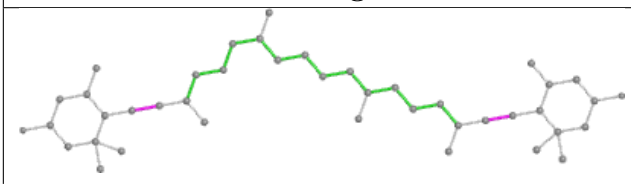

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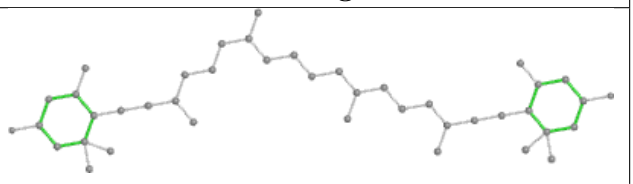
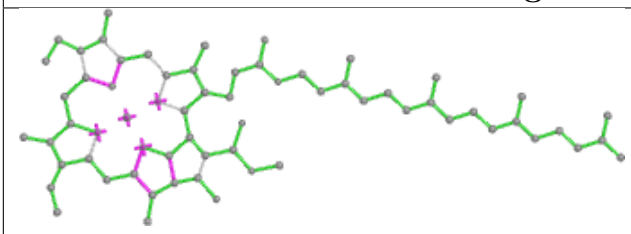


Rings

Ligand CLA B 806



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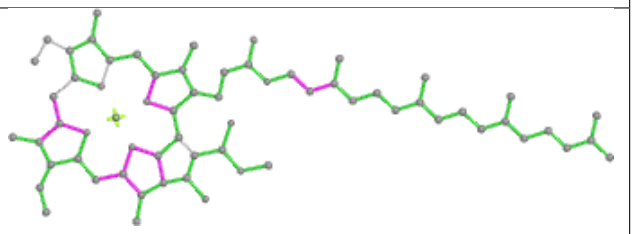
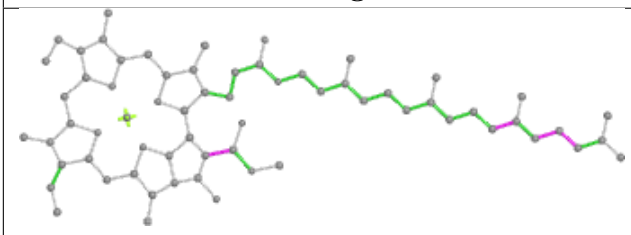


Bond angles



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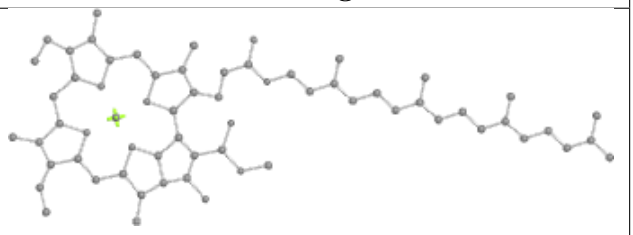
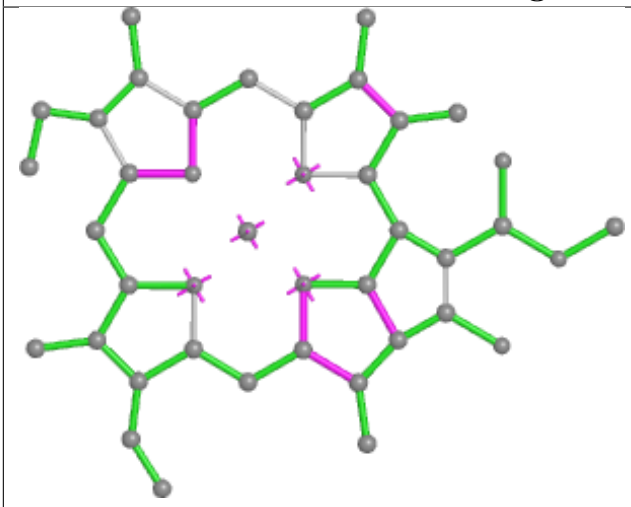


Rings

Ligand CLA 1 609



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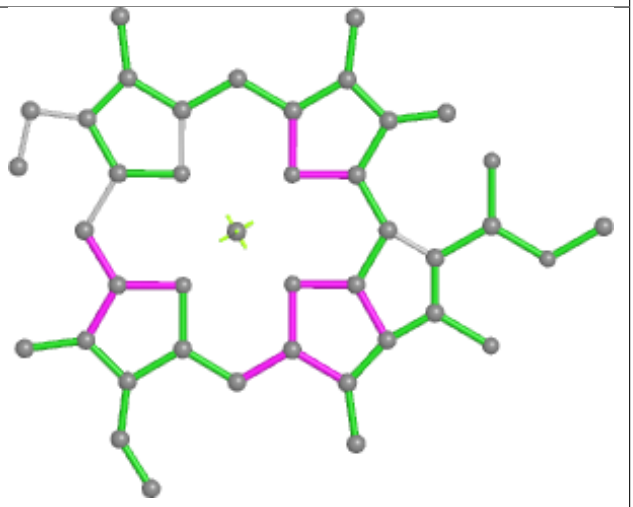

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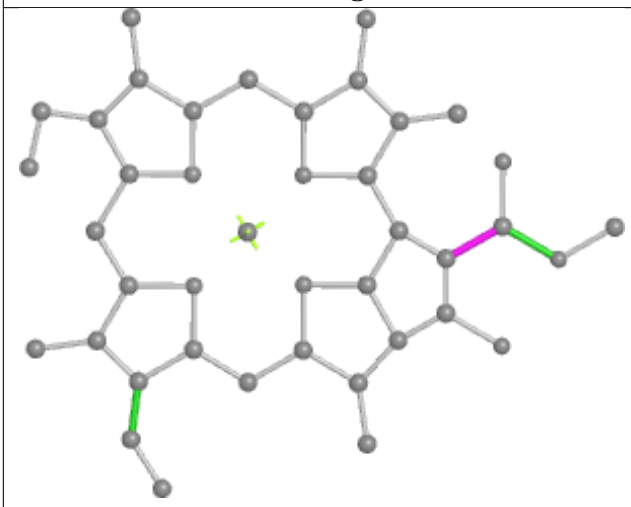

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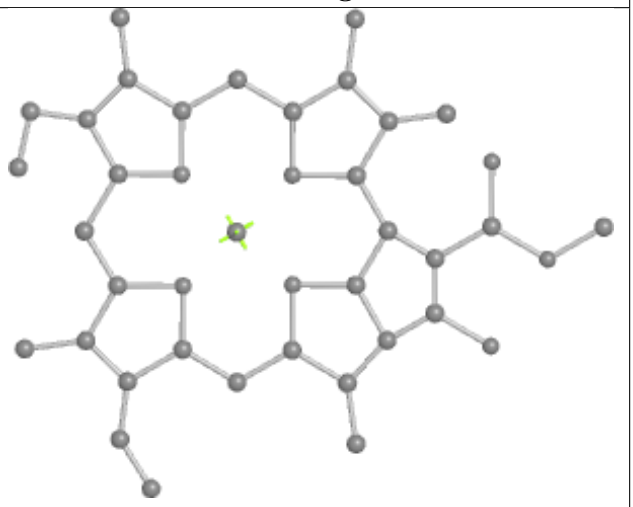
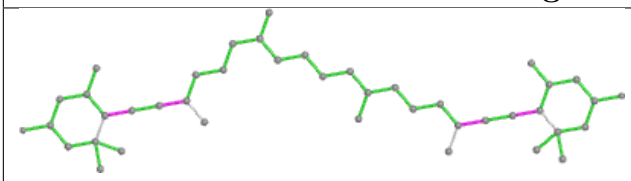


Rings

Ligand II0 6 615



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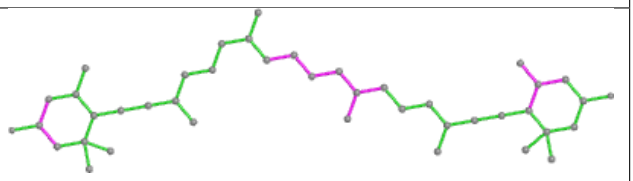
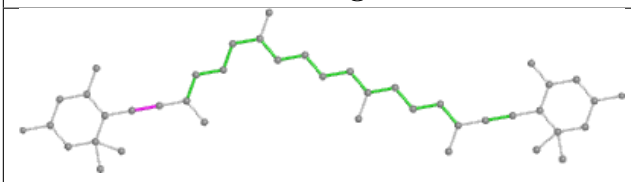


Bond angles



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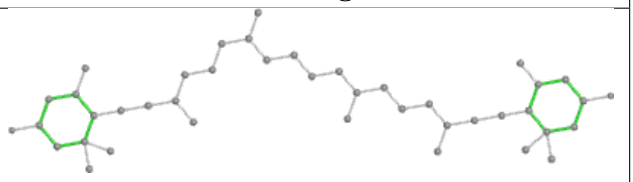
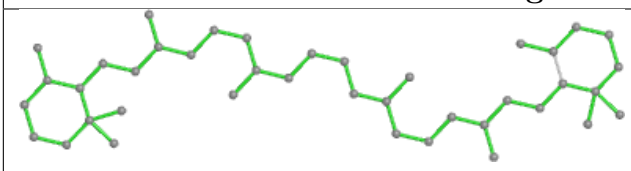


Rings

Ligand 8CT K 103



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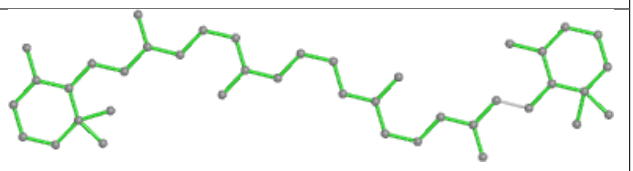
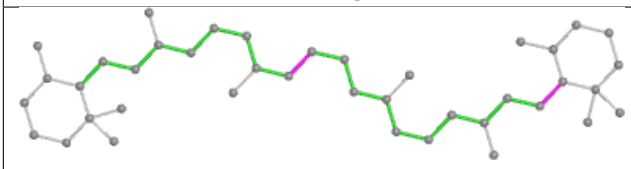
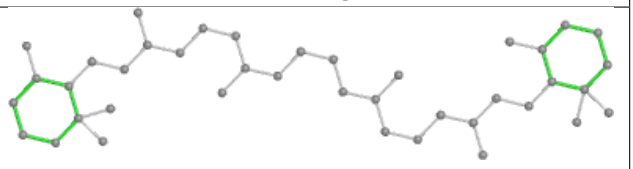


Bond angles

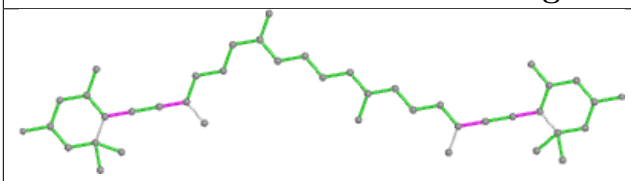


Torsions



Rings

Ligand II0 7 315



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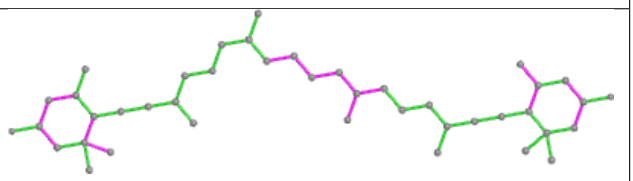
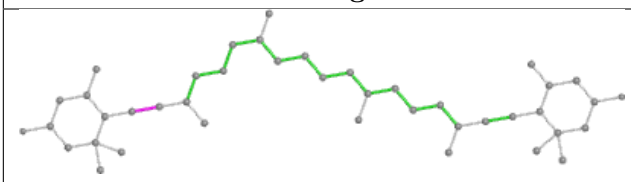
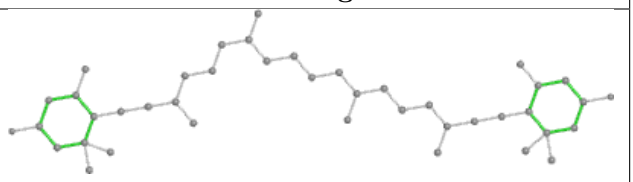


Bond angles

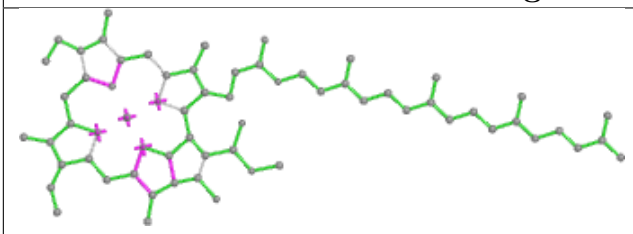


Torsions



Rings

Ligand CLA A 828



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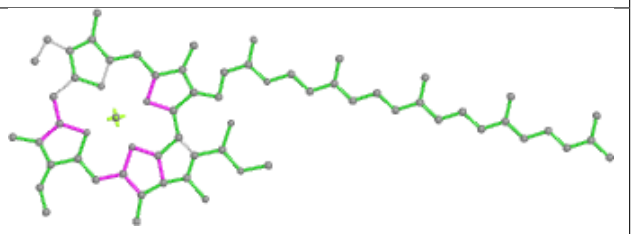
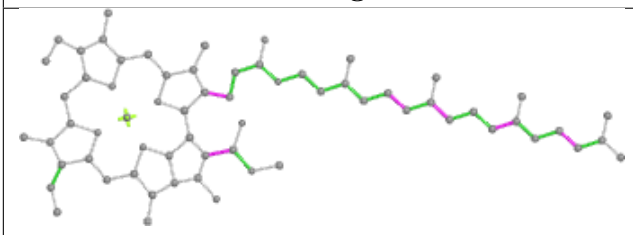


Bond angles



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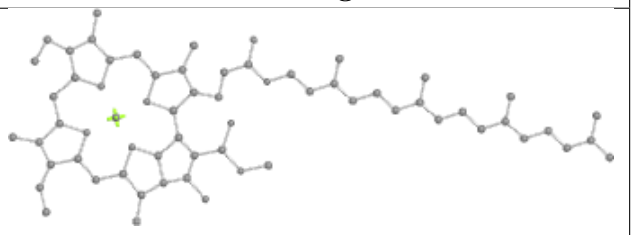
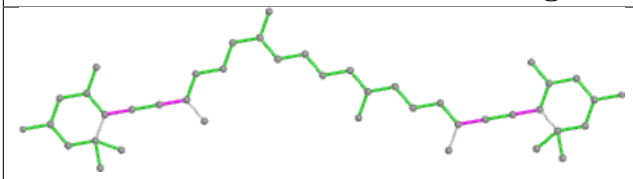


Rings

Ligand II0 3 616



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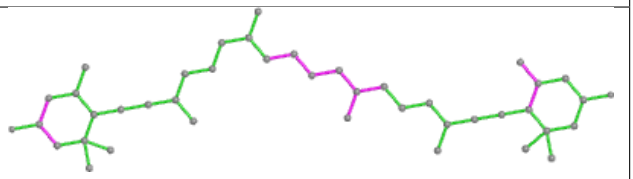
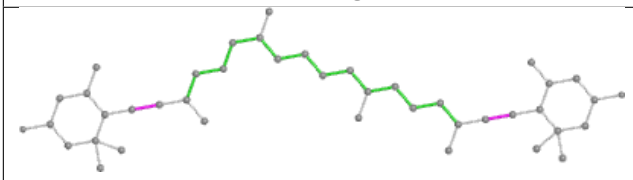
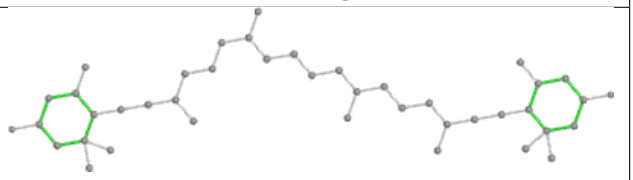


Bond angles

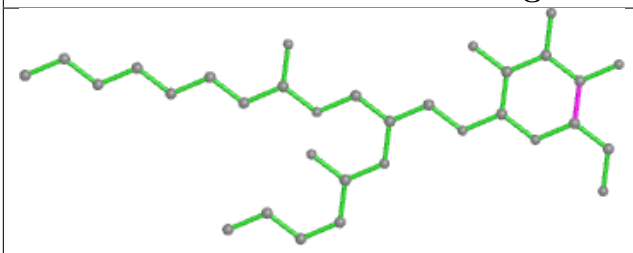


Torsions



Rings

Ligand LMG 6 618



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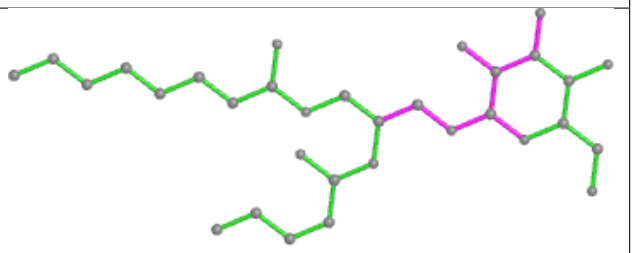
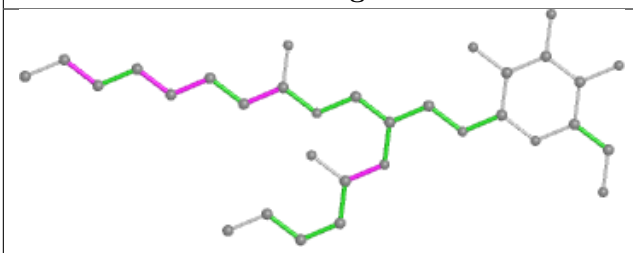
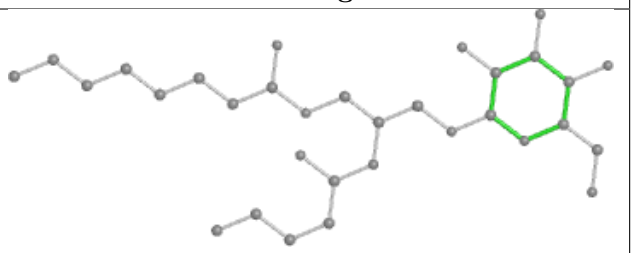


Bond angles

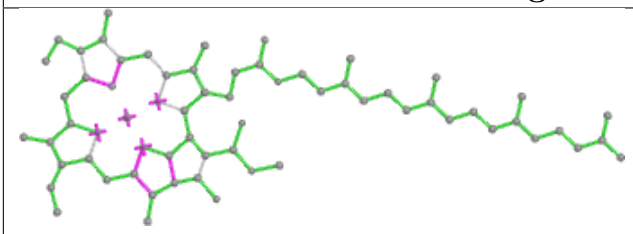


Torsions

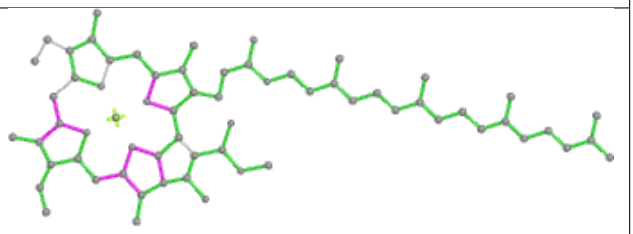


Rings

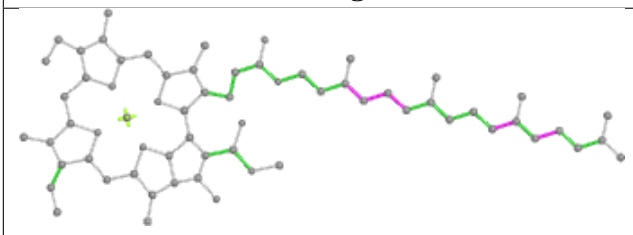
Ligand CLA 4 610



Bond lengths



Bond angles



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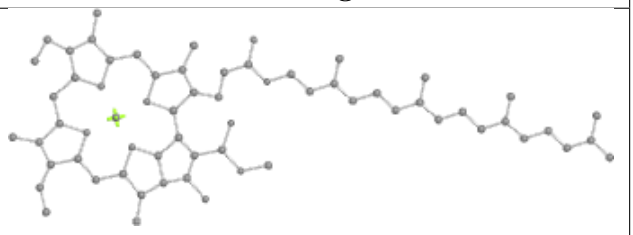
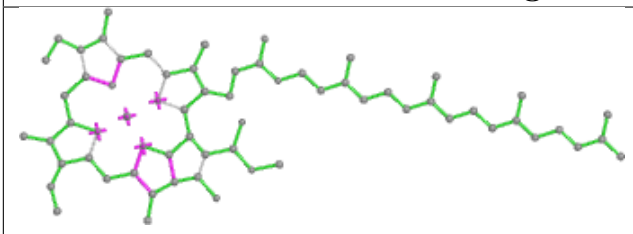
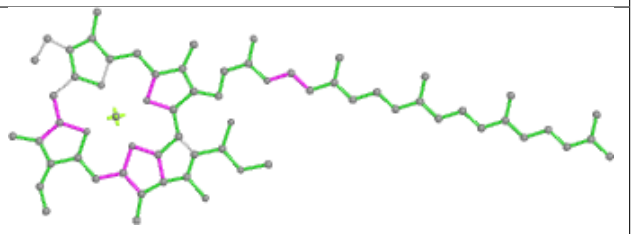


Rings

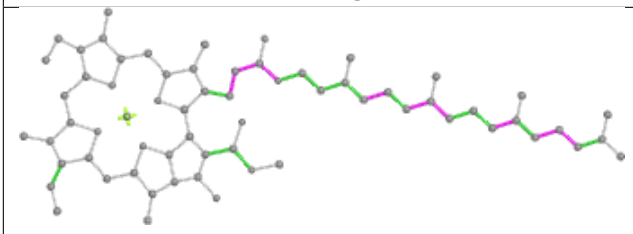
Ligand CLA A 839



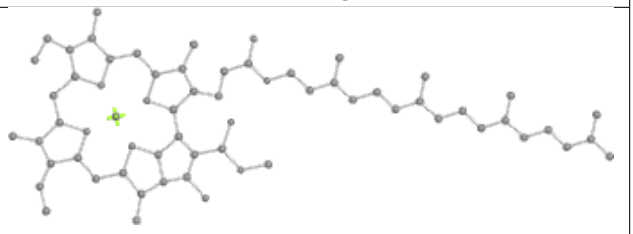
Bond lengths



Bond angles

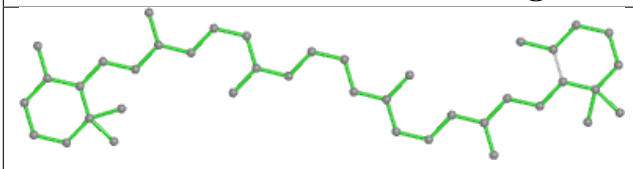


Torsions



Rings

Ligand 8CT B 844



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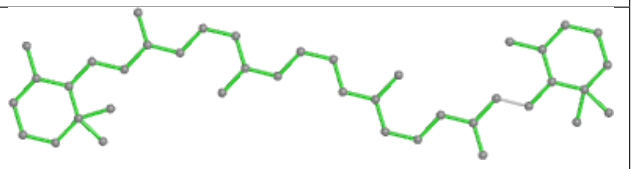
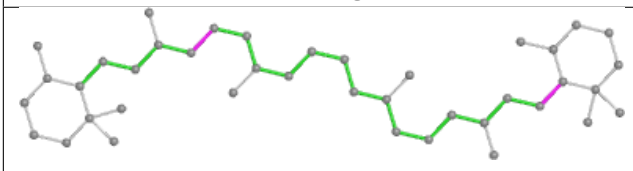


Bond angles



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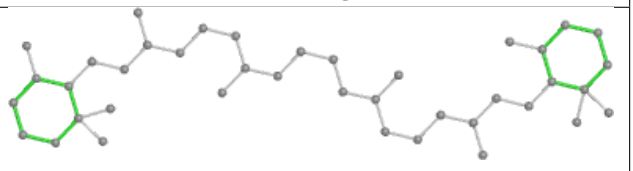
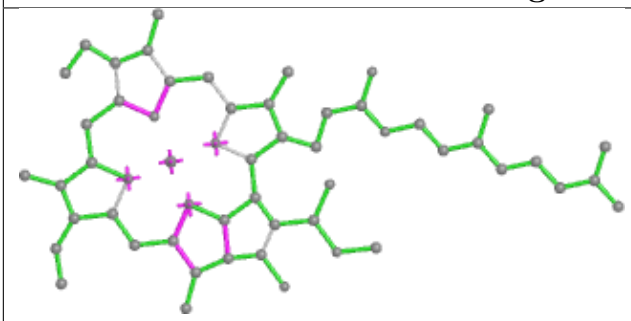
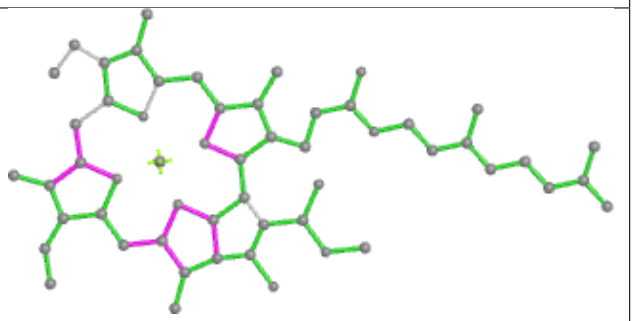


Rings

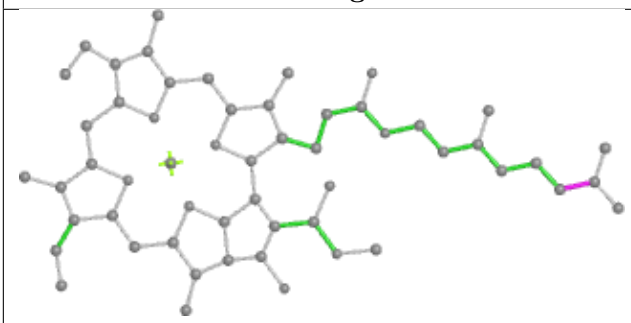
Ligand CLA 6 607



Bond lengths



Bond angles



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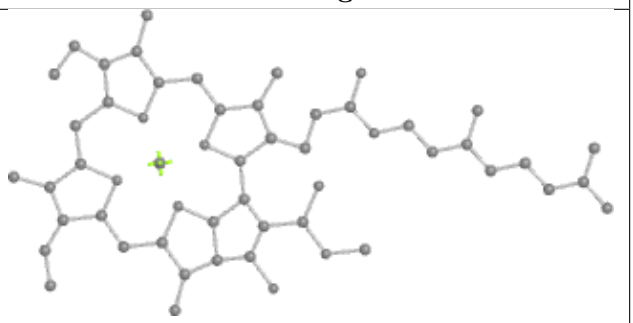
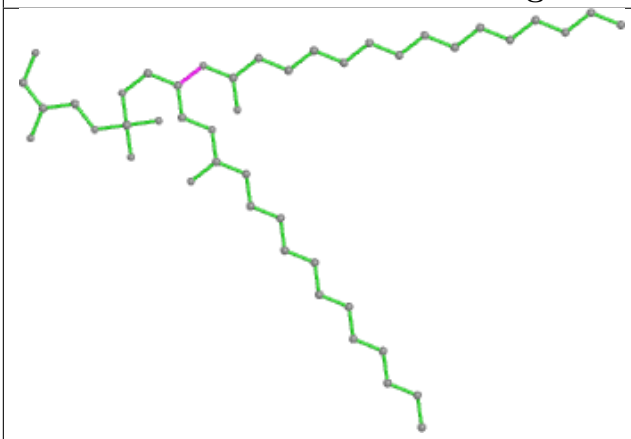


Rings

Ligand LHG 4 619



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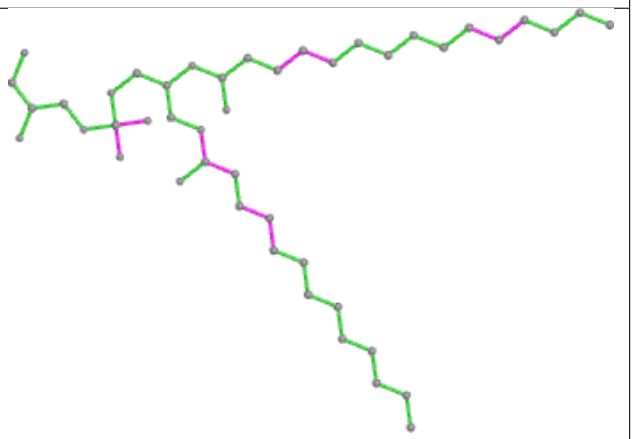
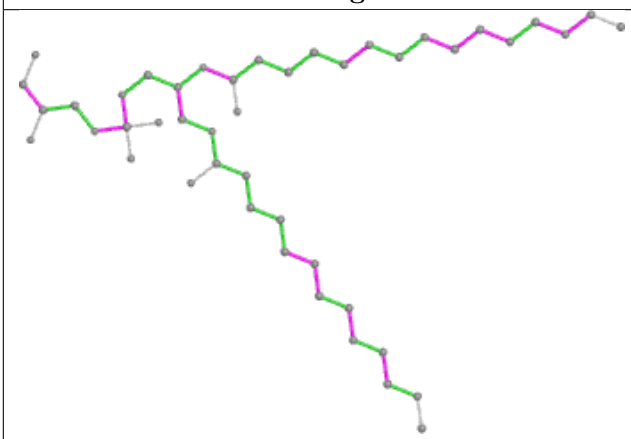


Bond angles



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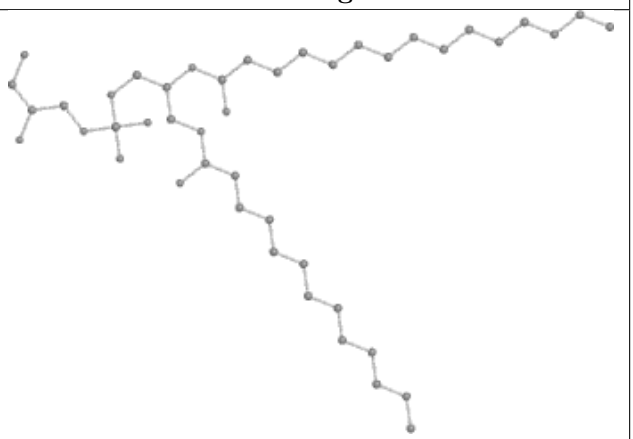
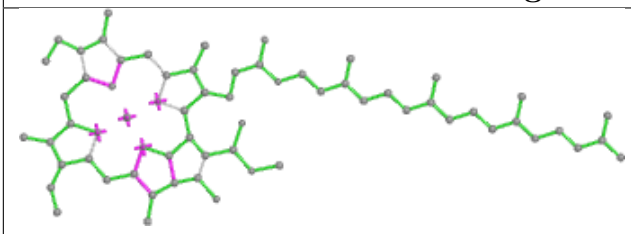


Rings

Ligand CLA B 828



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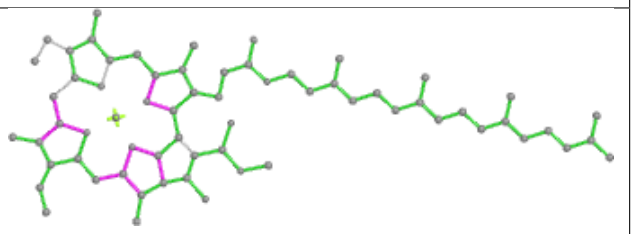

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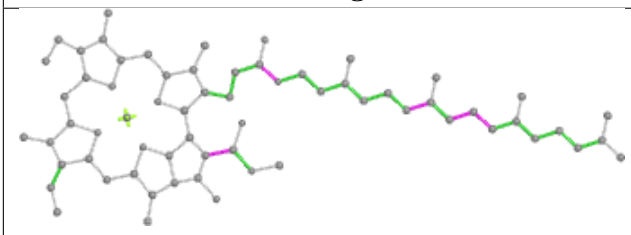

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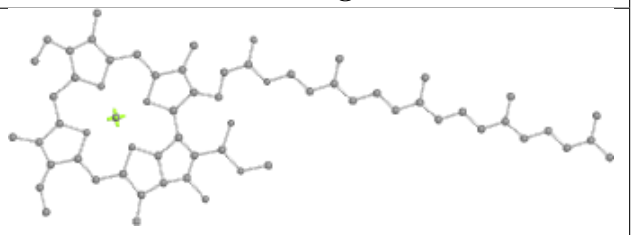
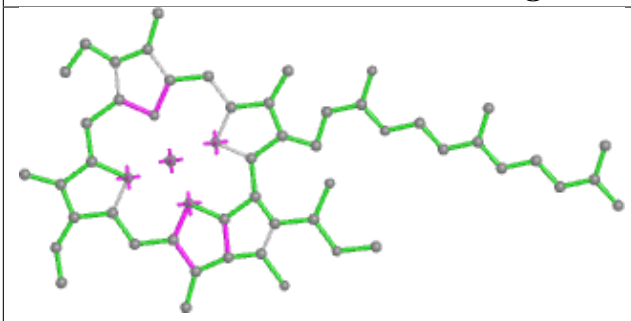
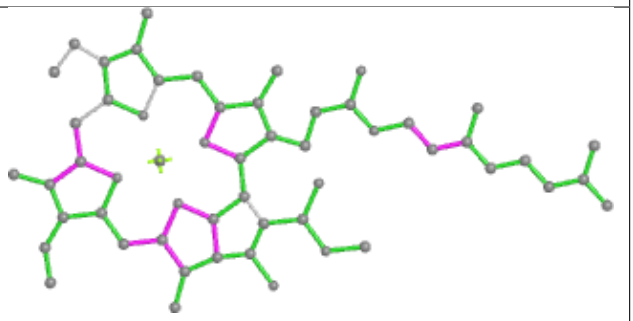


Rings

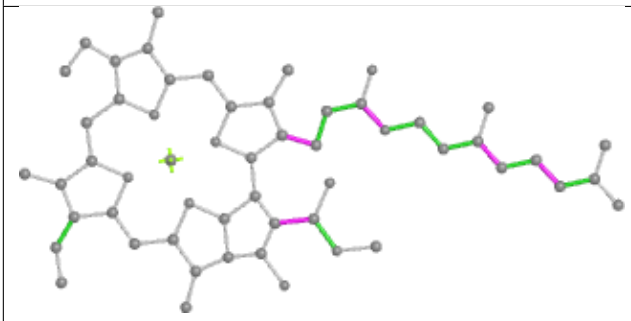
Ligand CLA B 831



Bond lengths



Bond angles



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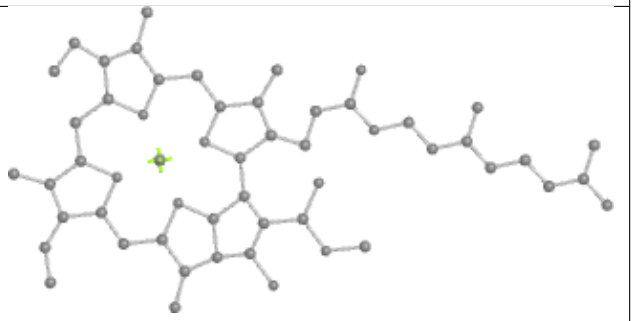
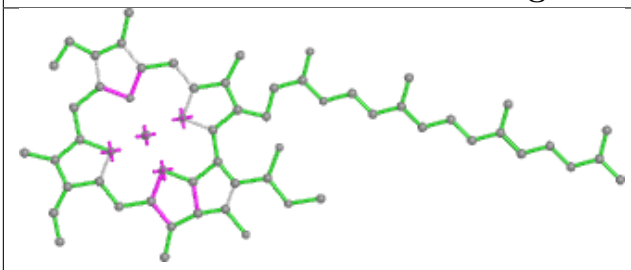
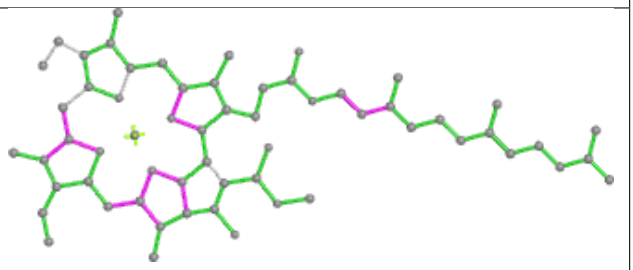


Rings

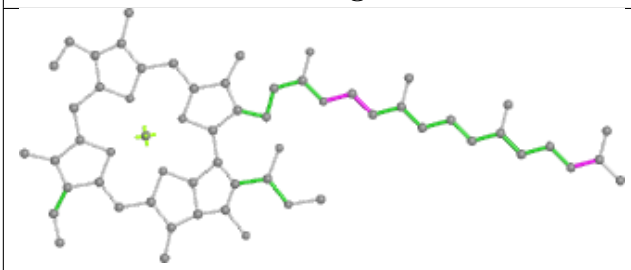
Ligand CLA 4 606



Bond lengths



Bond angles



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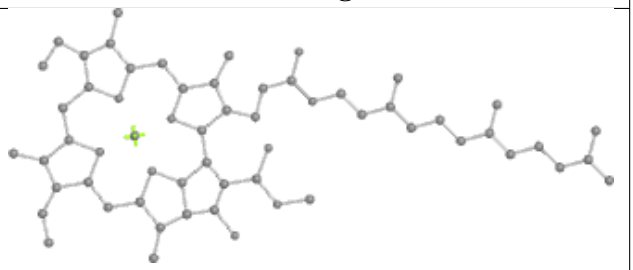
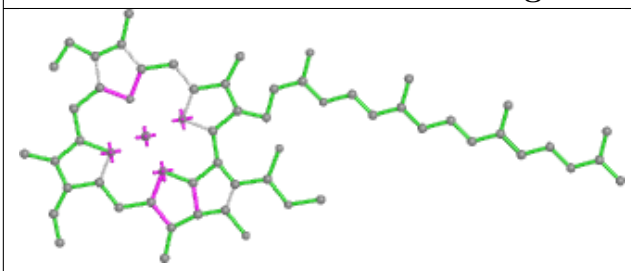
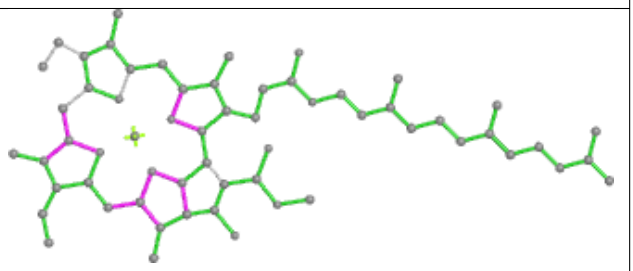


Rings

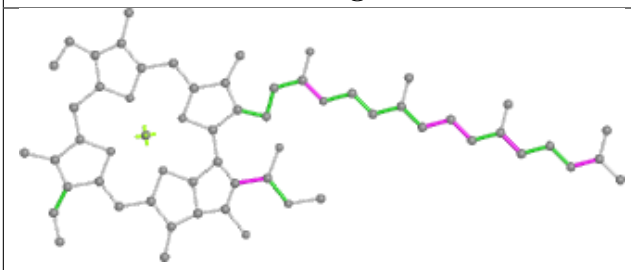
Ligand CLA B 820



Bond lengths



Bond angles



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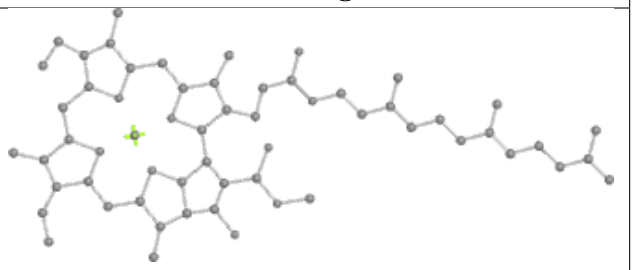
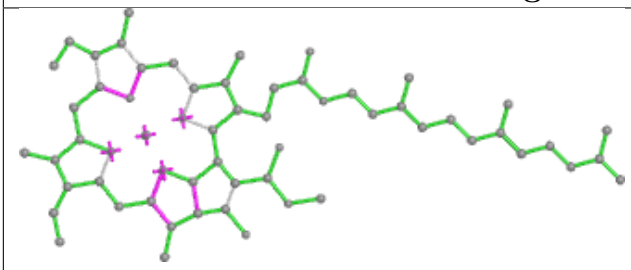
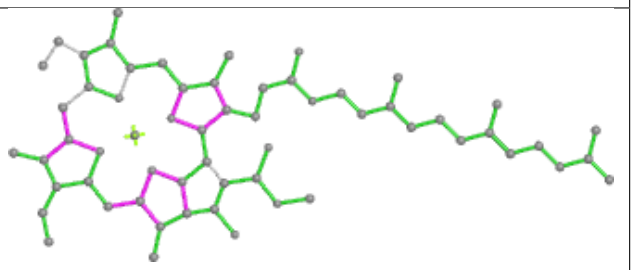


Rings

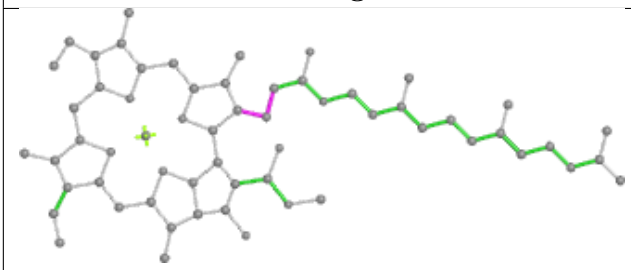
Ligand CLA A 809



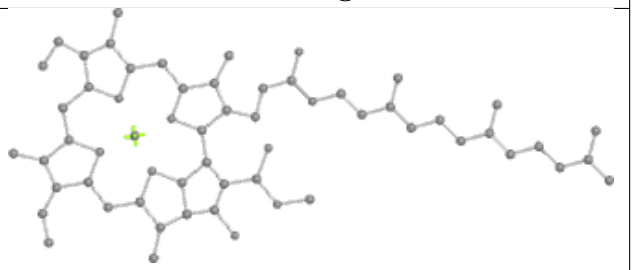
Bond lengths



Bond angles

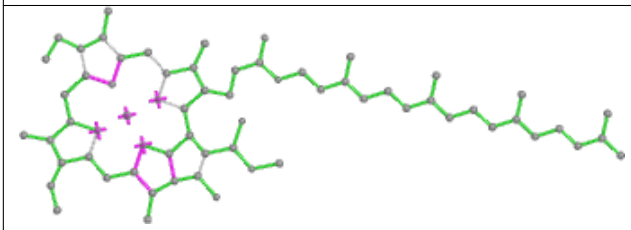


Torsions

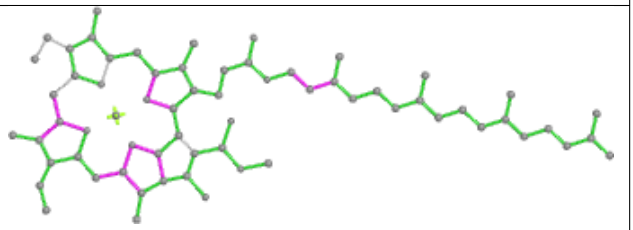


Rings

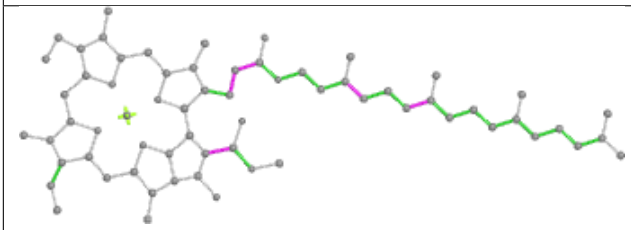
Ligand CLA 3 610



Bond lengths



Bond angles



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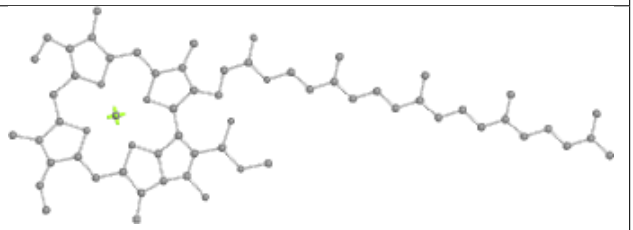
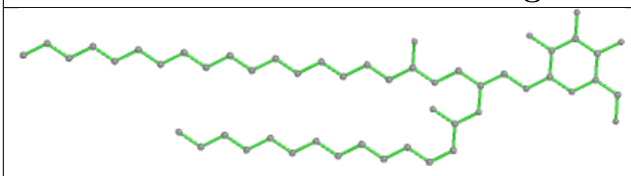


Rings

Ligand LMG 8 616



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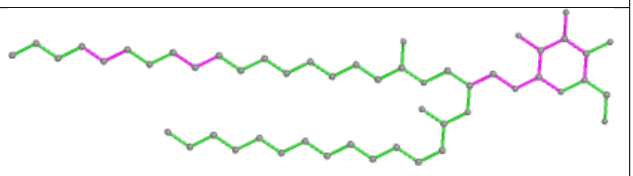
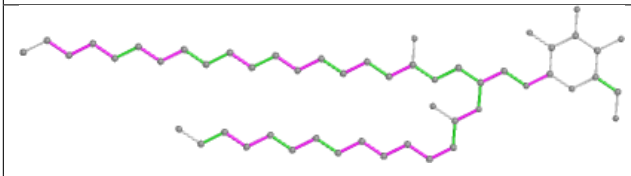
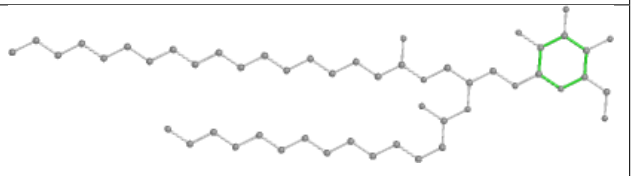


Bond angles

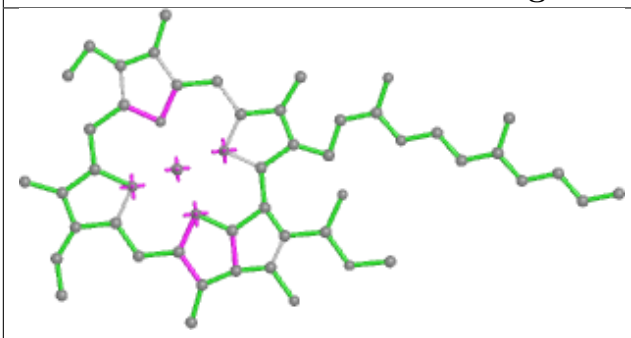


Torsions



Rings

Ligand CLA 7 305



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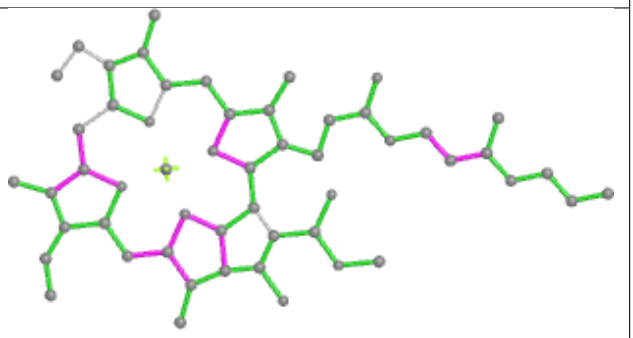
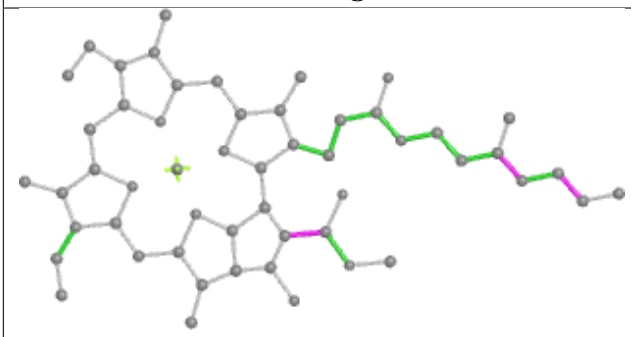


Bond angles



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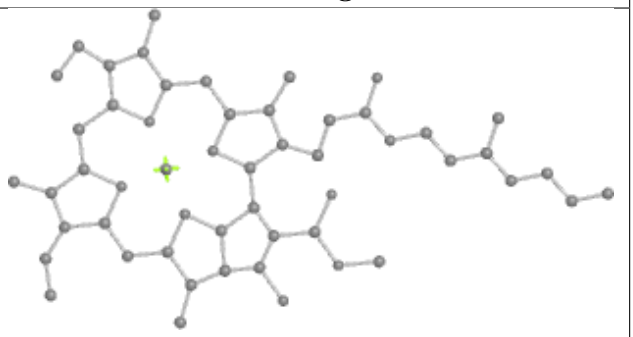
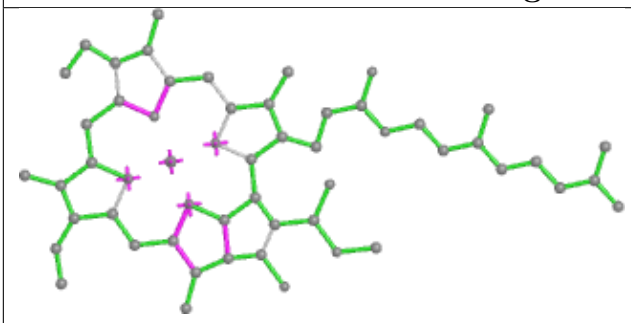
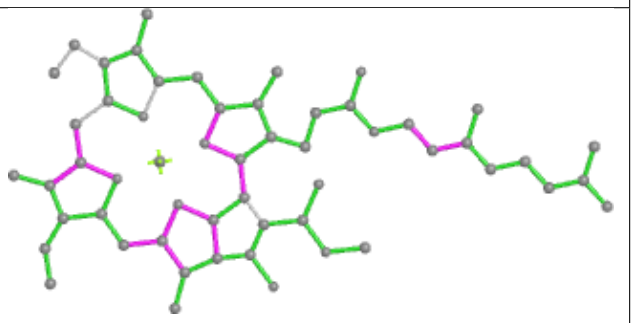


Rings

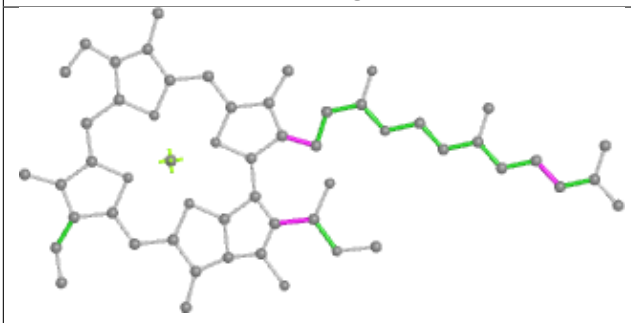
Ligand CLA A 812



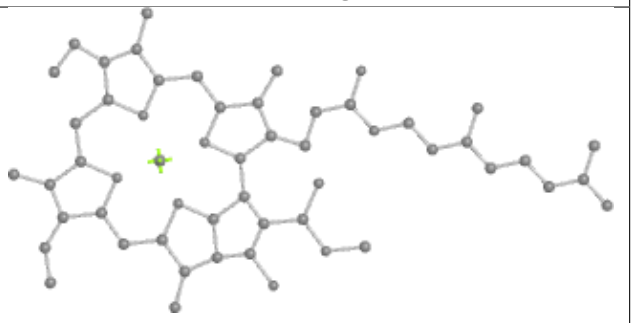
Bond lengths



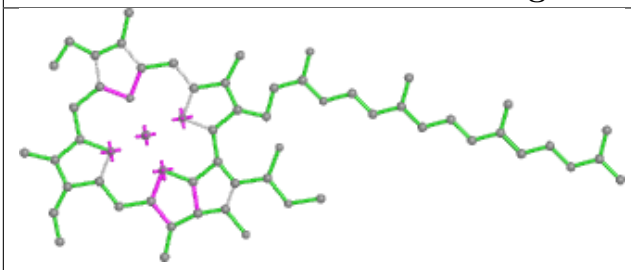
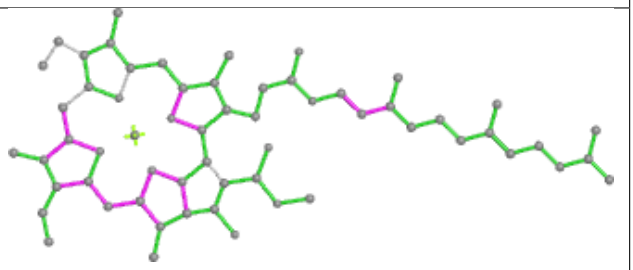
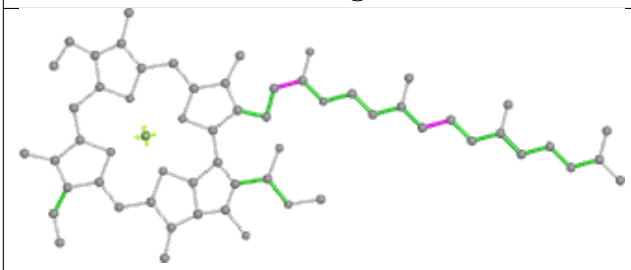
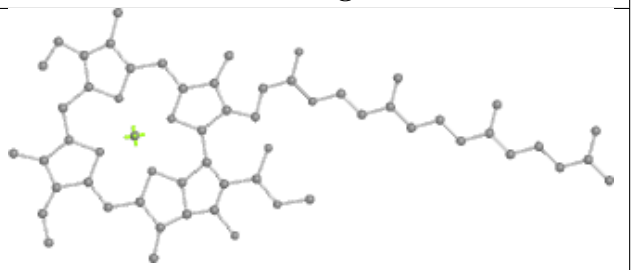
Bond angles

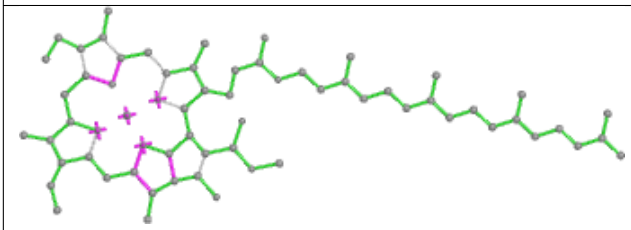
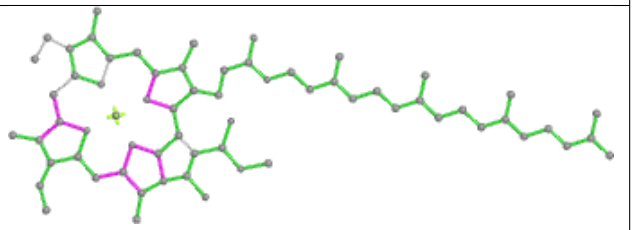
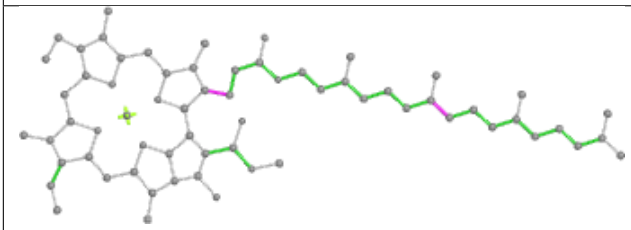
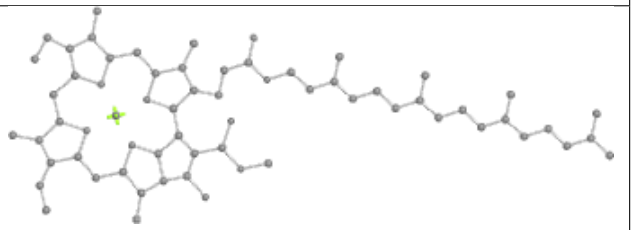


Torsions

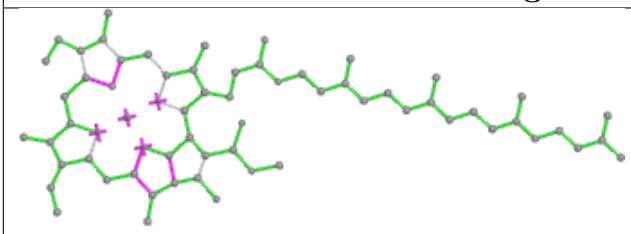


Rings

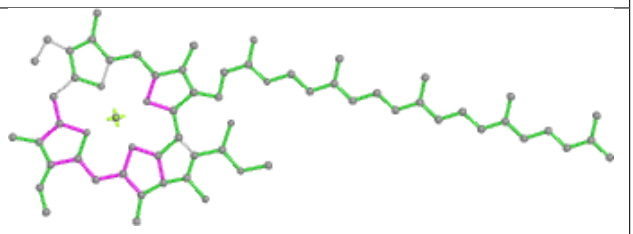
Ligand CLA 1 608	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

Ligand CLA b 606	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

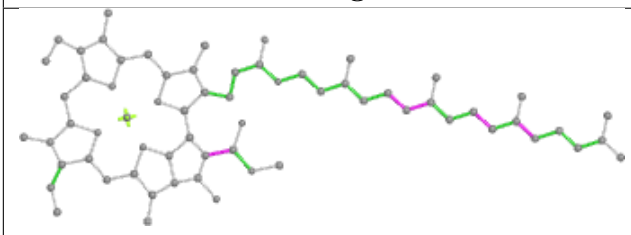
Ligand CLA A 825



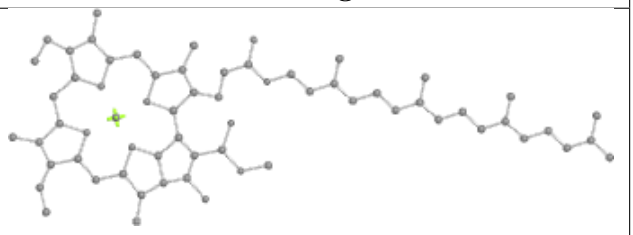
Bond lengths



Bond angles

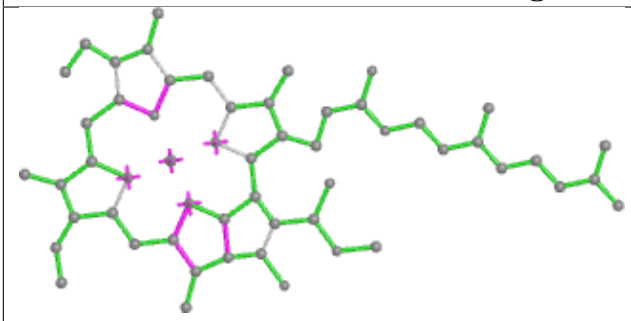


Torsions



Rings

Ligand CLA 4 604



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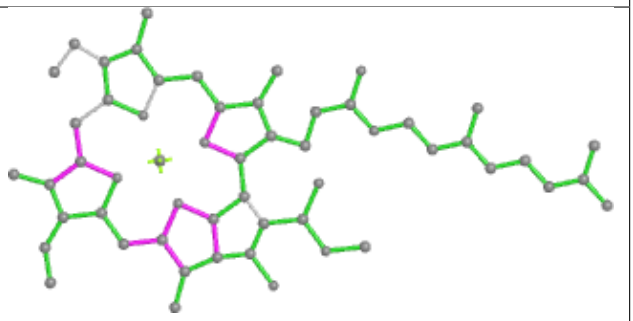
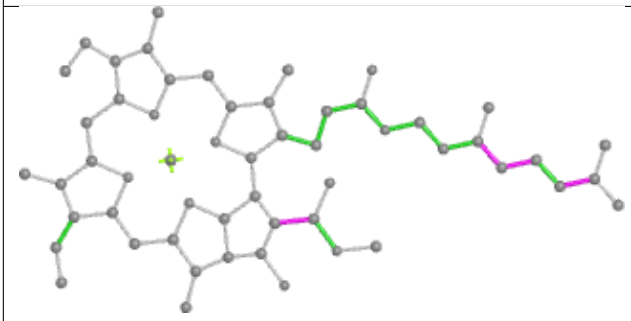


Bond angles



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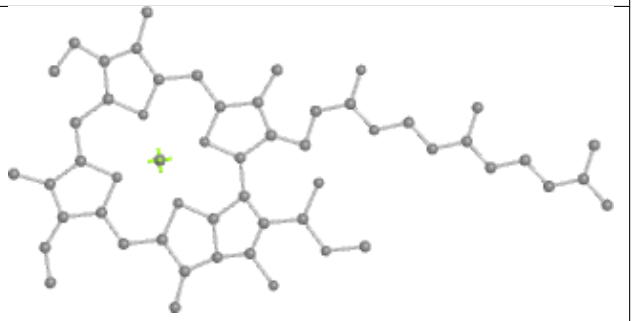
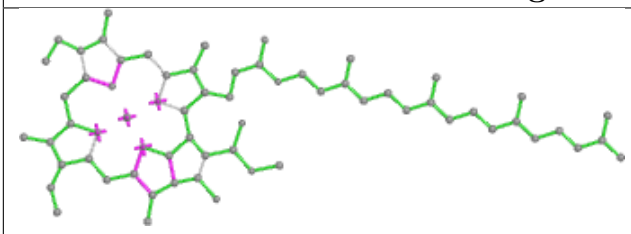


Rings

Ligand CLA 3 609



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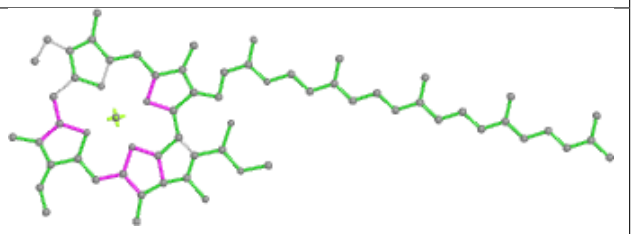
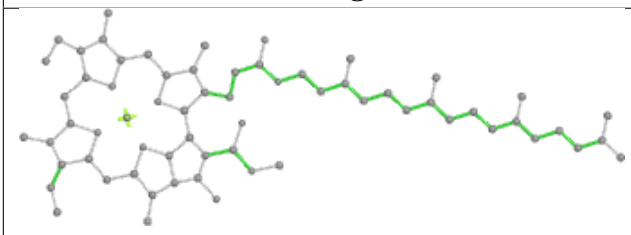


Bond angles



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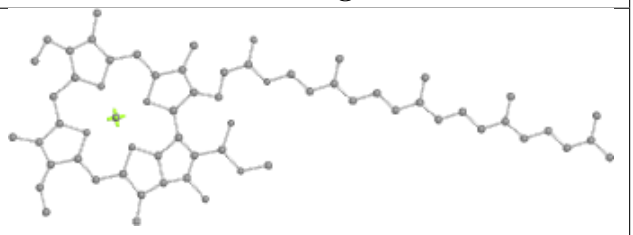
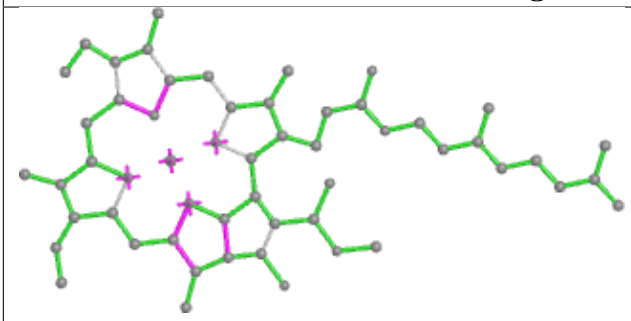


Rings

Ligand CLA 4 601



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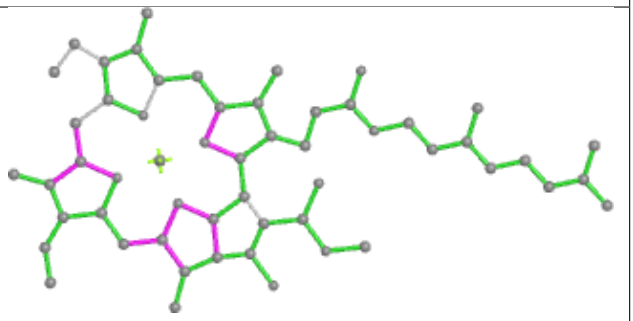
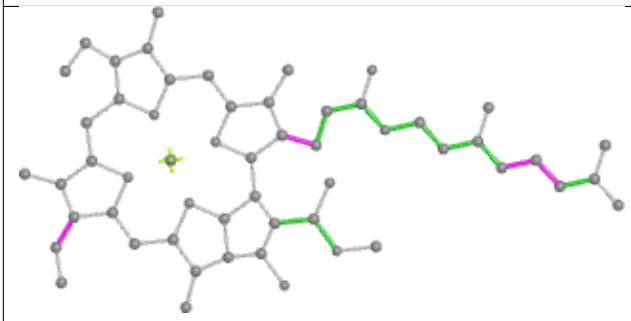


Bond angles



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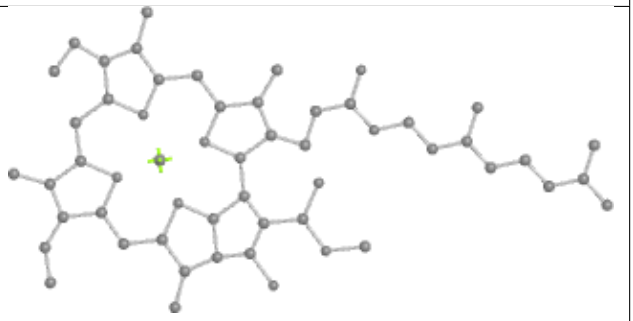
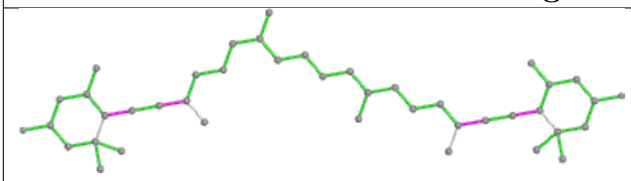


Rings

Ligand II0 a 614



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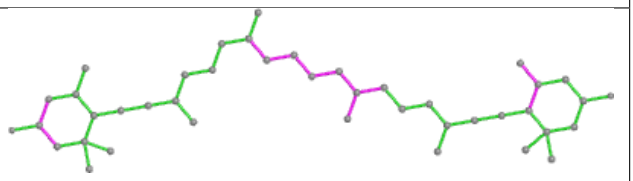
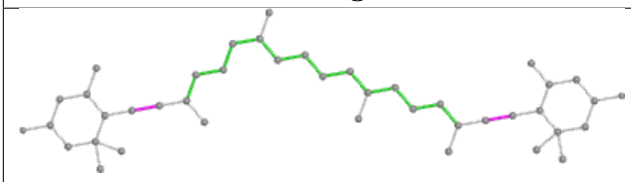


Bond angles



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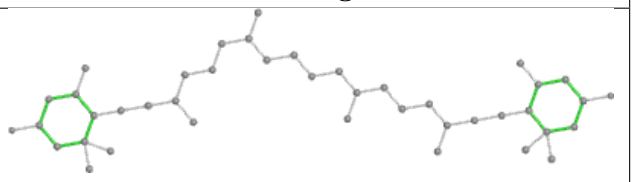
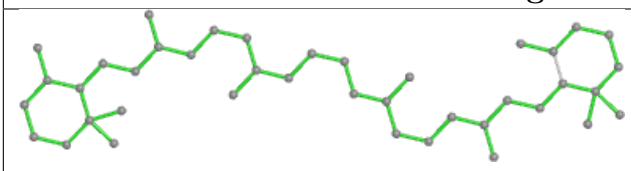


Rings

Ligand 8CT A 846



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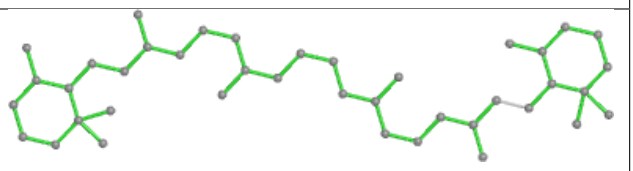

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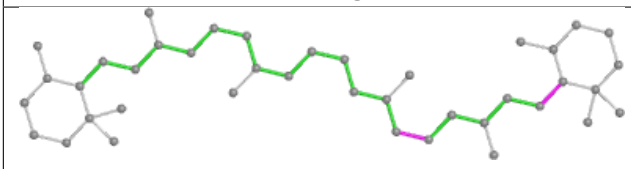

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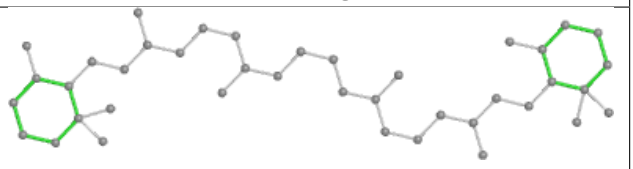
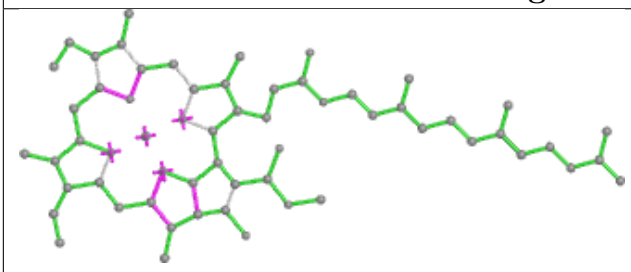


Rings

Ligand CLA a 603



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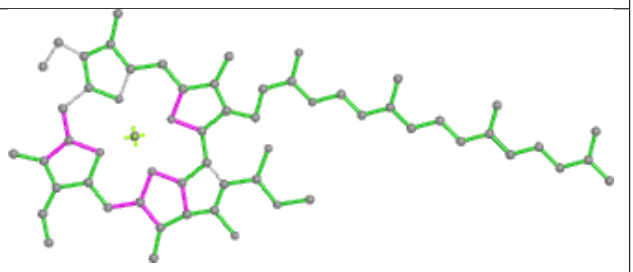
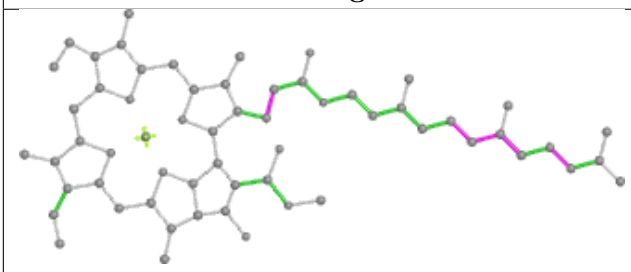


Bond angles



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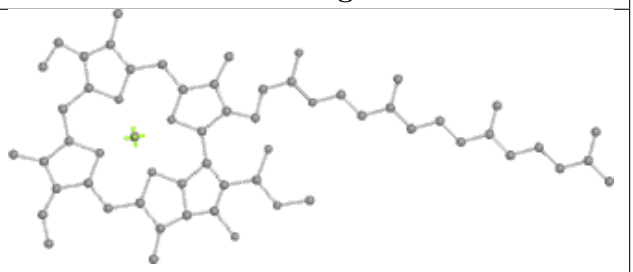
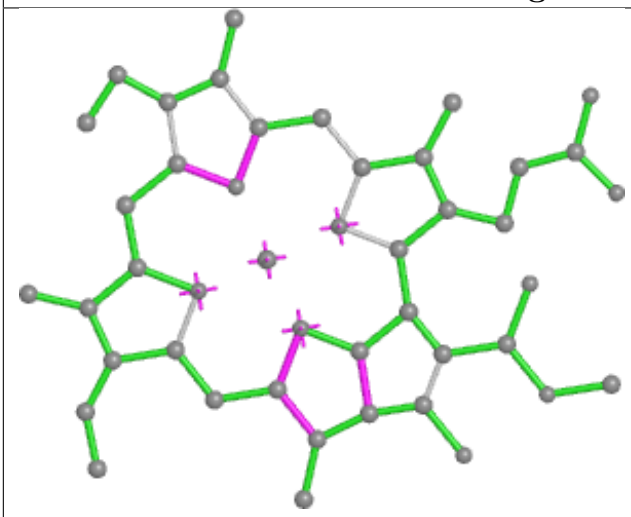


Rings

Ligand CLA a 601



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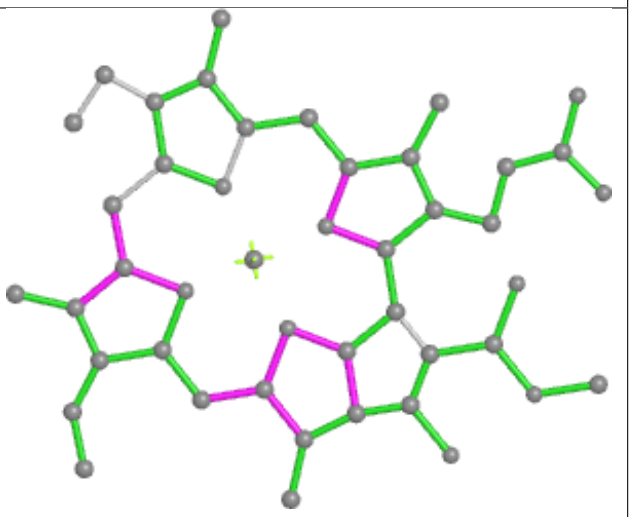
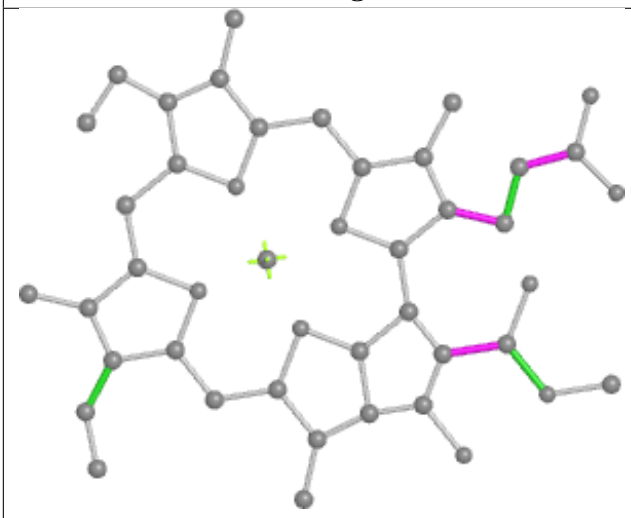


Bond angles



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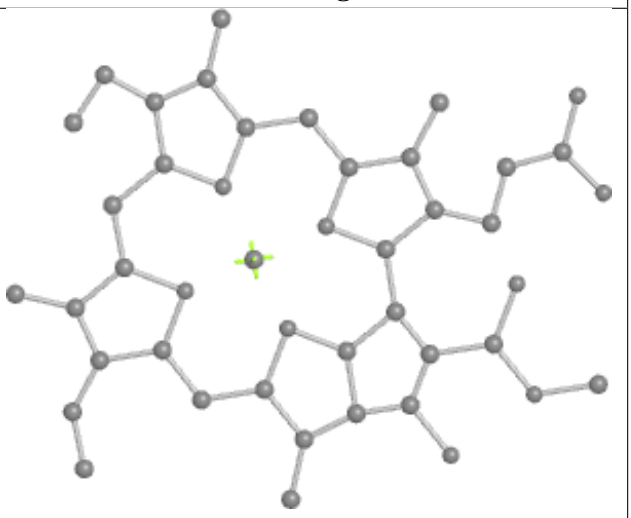
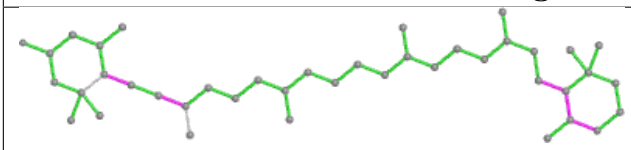
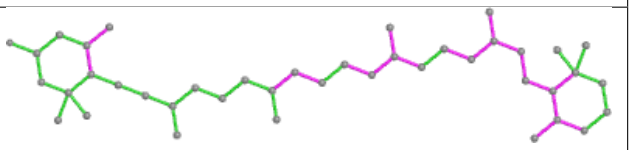


Rings

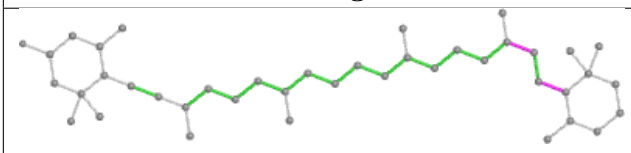
Ligand IHT 9 619



Bond lengths



Bond angles



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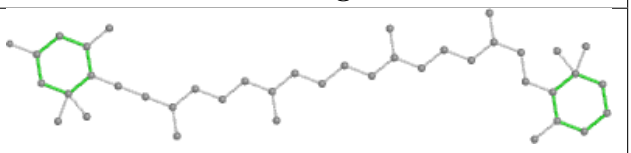
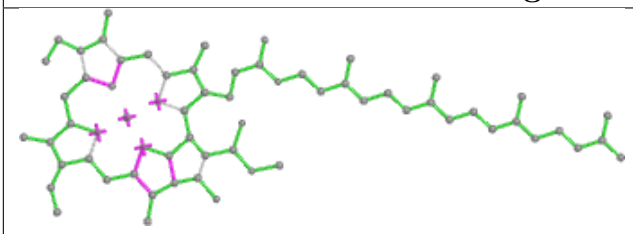


Rings

Ligand CLA A 820



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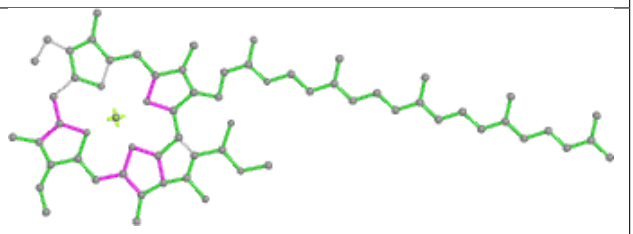
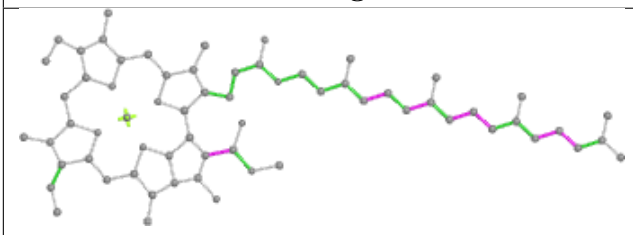


Bond angles



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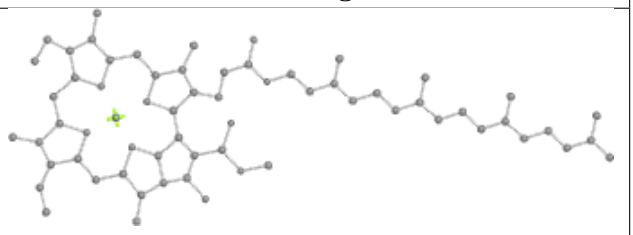
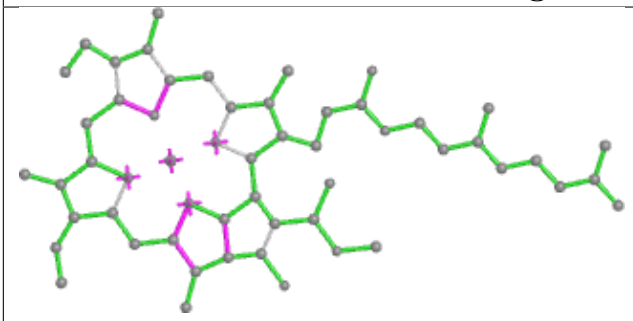


Rings

Ligand CLA 3 602



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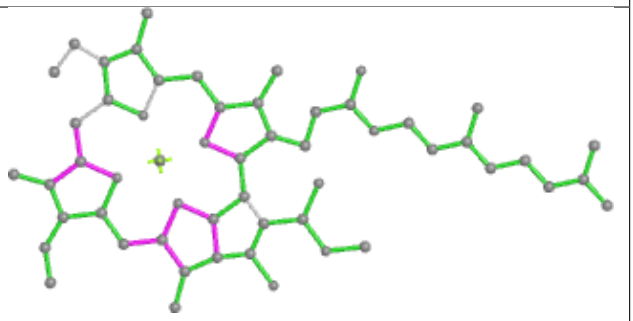
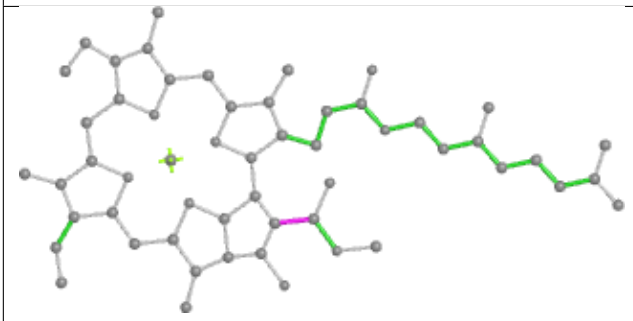


Bond angles



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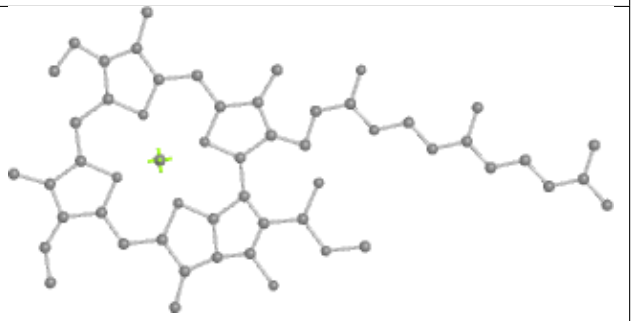
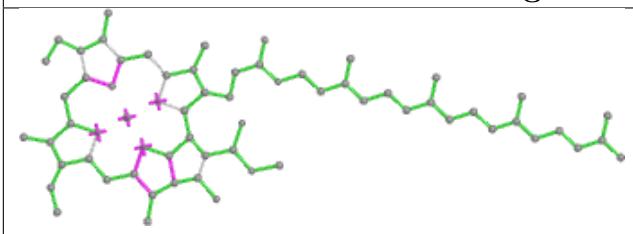


Rings

Ligand CLA A 844



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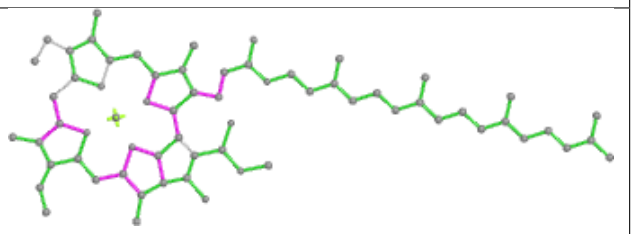
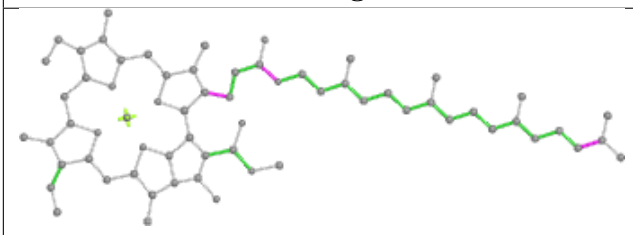


Bond angles



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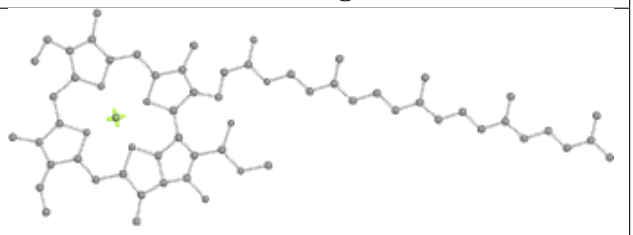
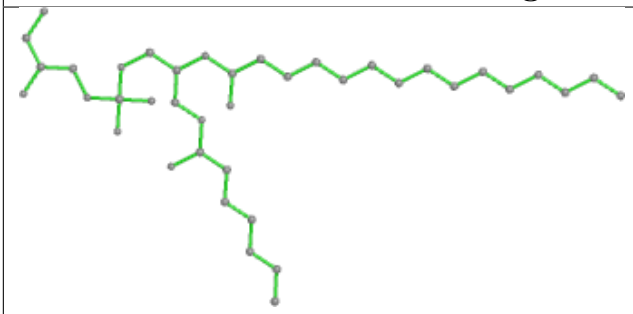
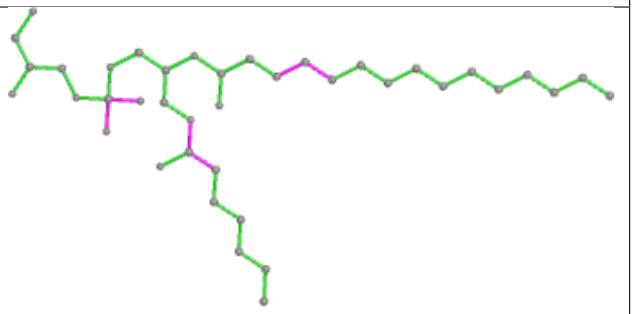


Rings

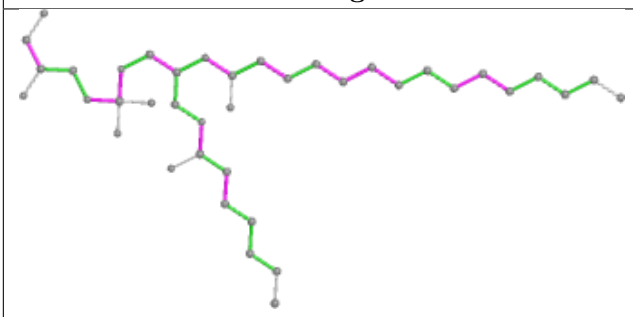
Ligand LHG A 852



Bond lengths



Bond angles



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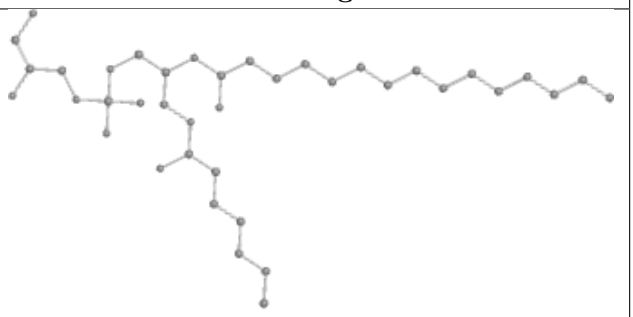
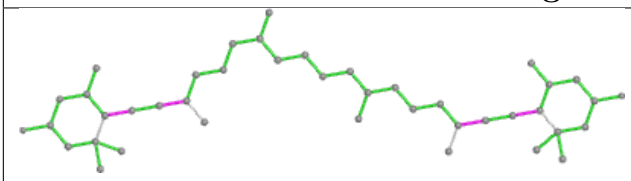
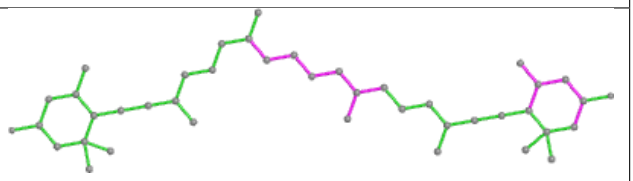


Rings

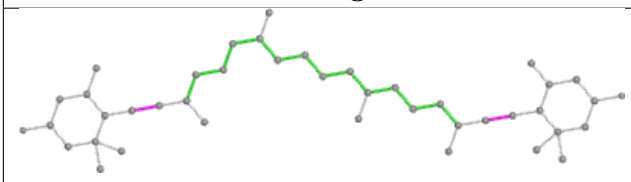
Ligand II0 3 617



Bond lengths



Bond angles



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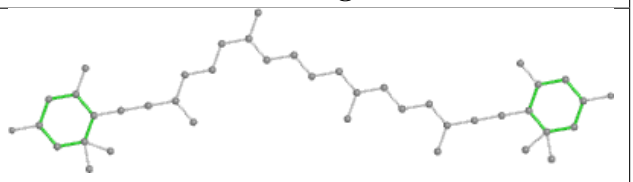
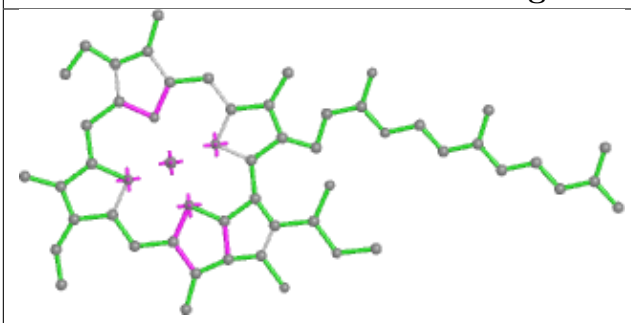
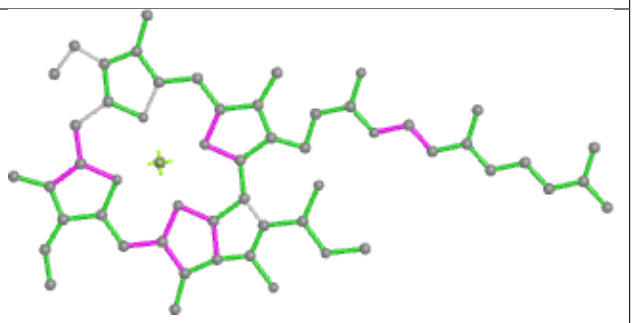


Rings

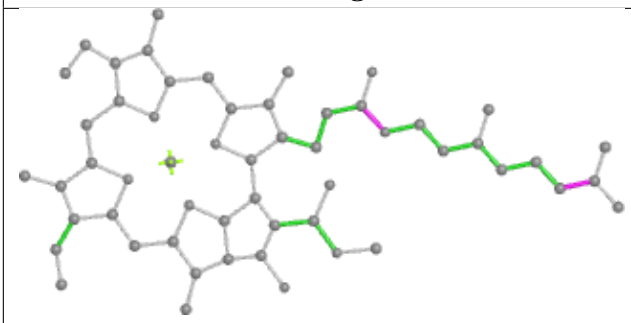
Ligand CLA 8 606



Bond lengths



Bond angles



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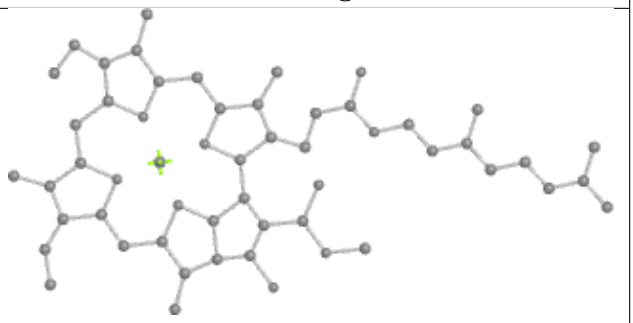
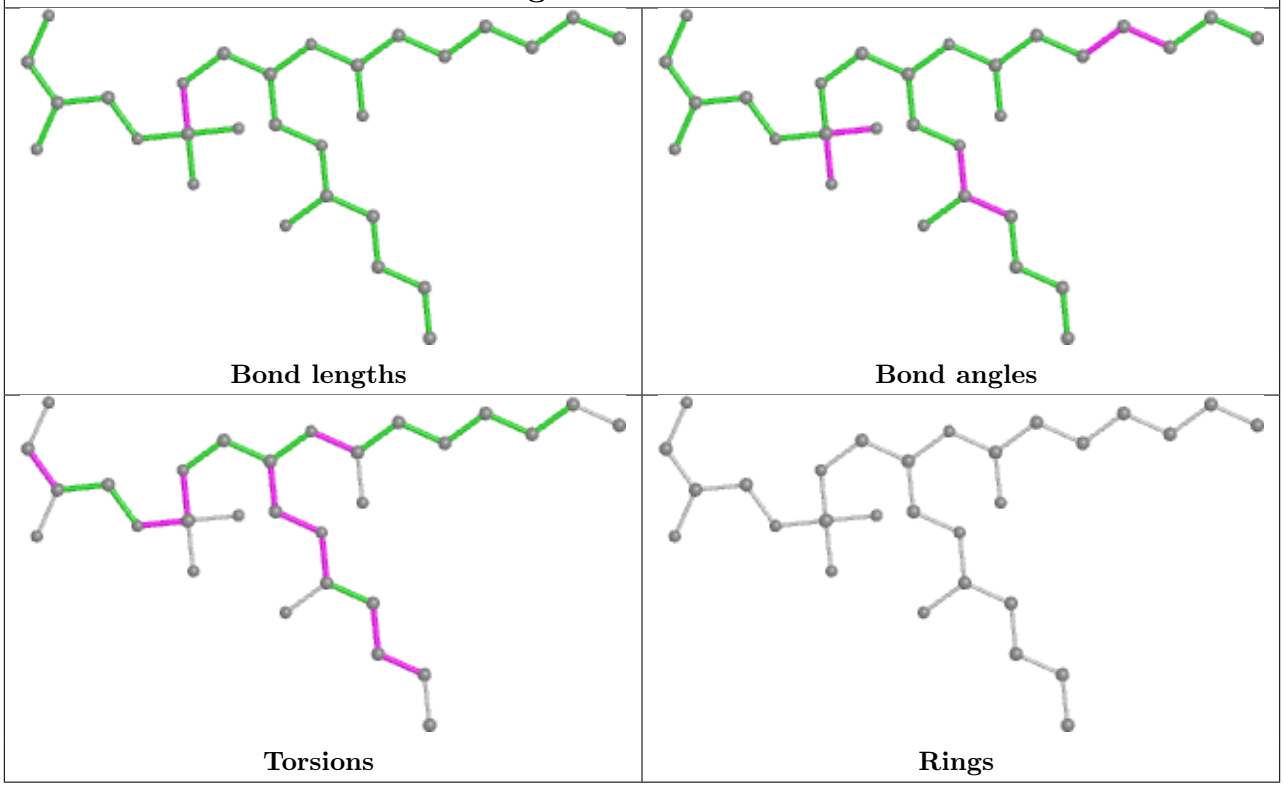
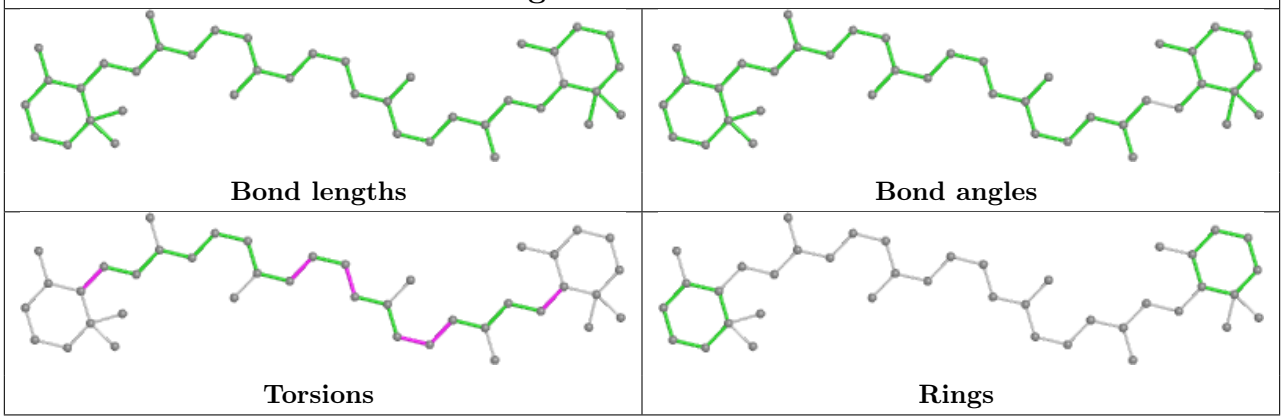


Rings

Ligand LHG a 618



Ligand 8CT B 846



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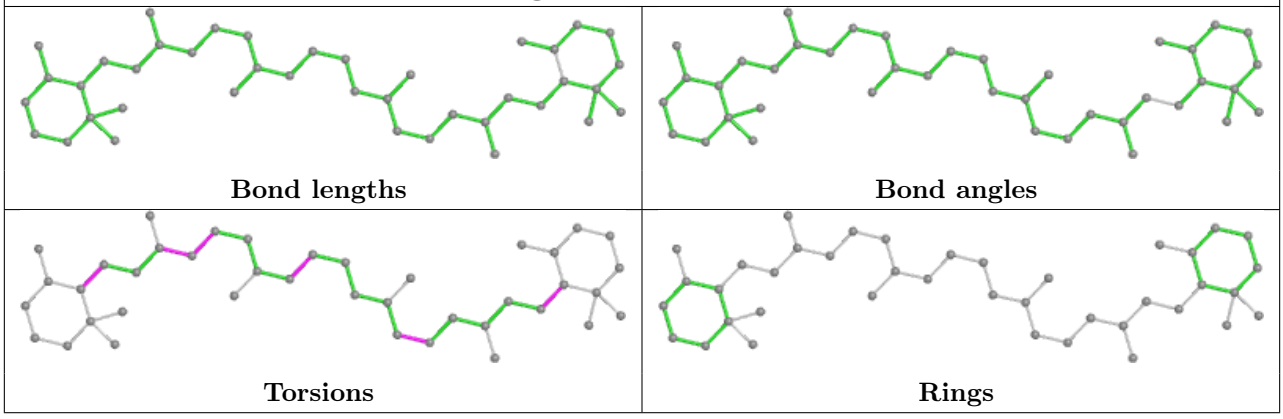
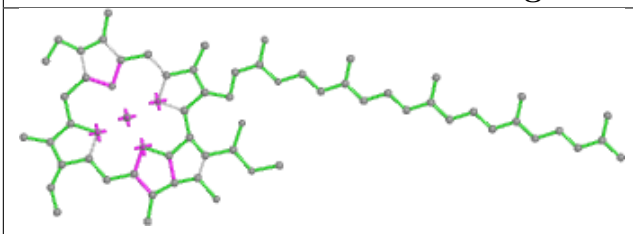
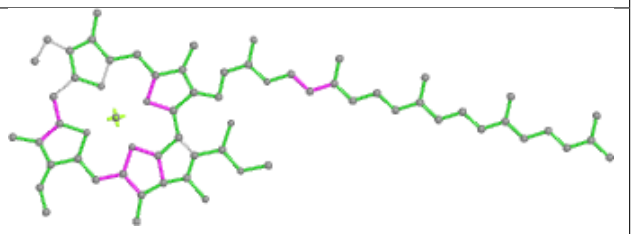


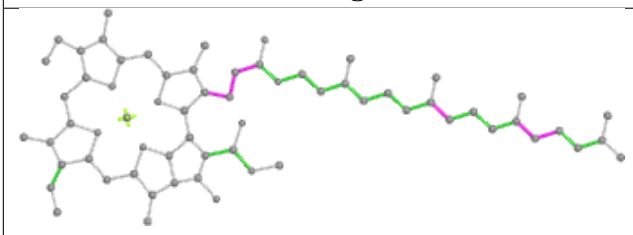
Ligand CLA B 835



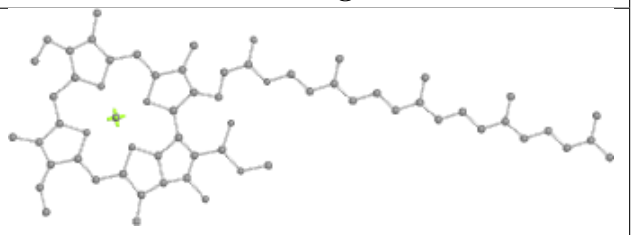
Bond lengths



Bond angles

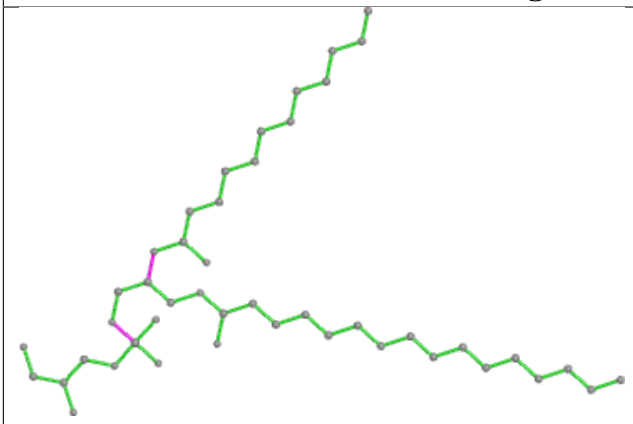


Torsions



Rings

Ligand LHG 4 620



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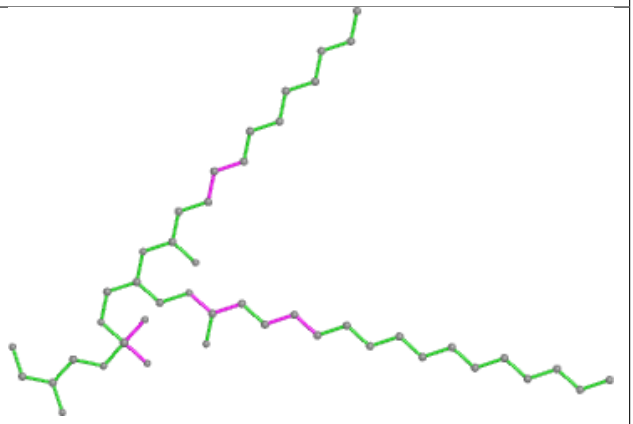
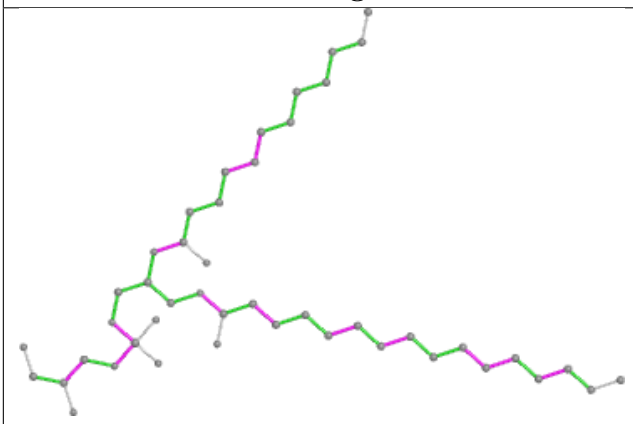


Bond angles



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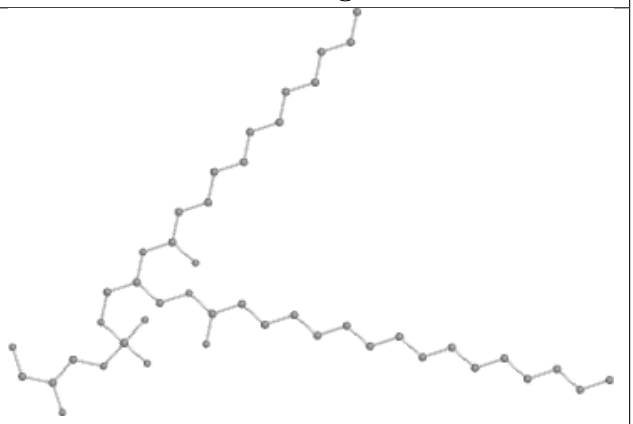
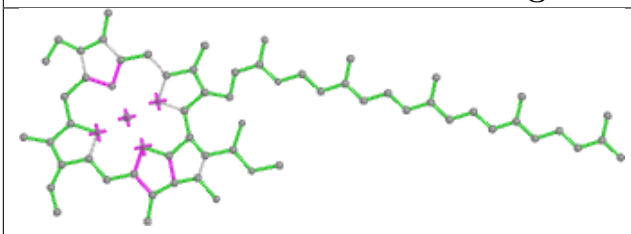
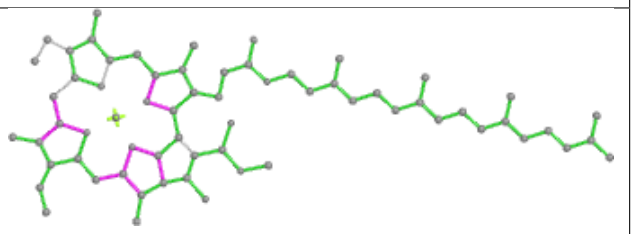


Rings

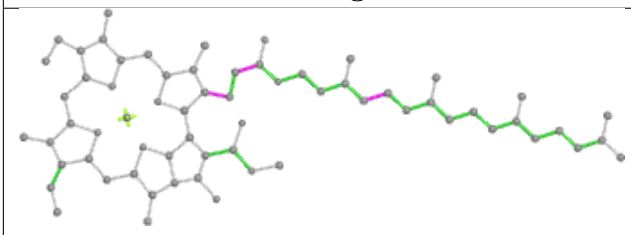
Ligand CLA a 611



Bond lengths



Bond angles



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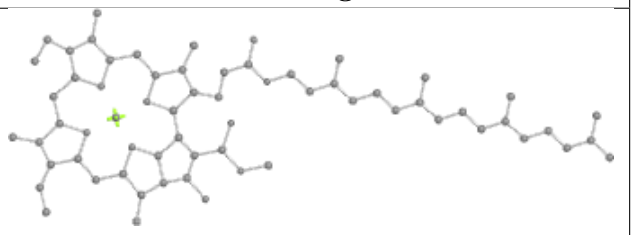
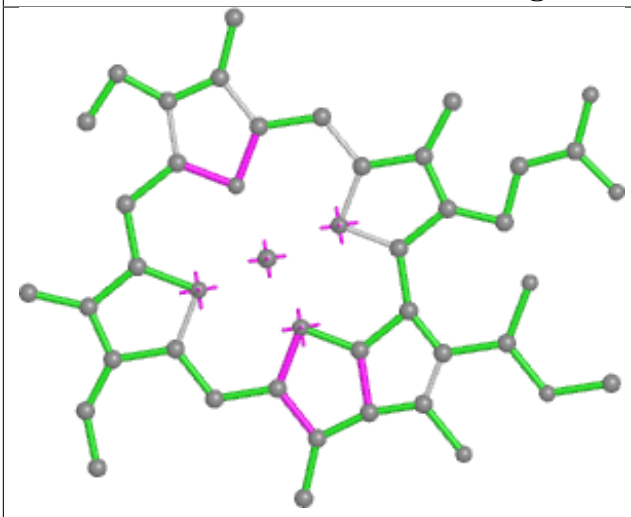
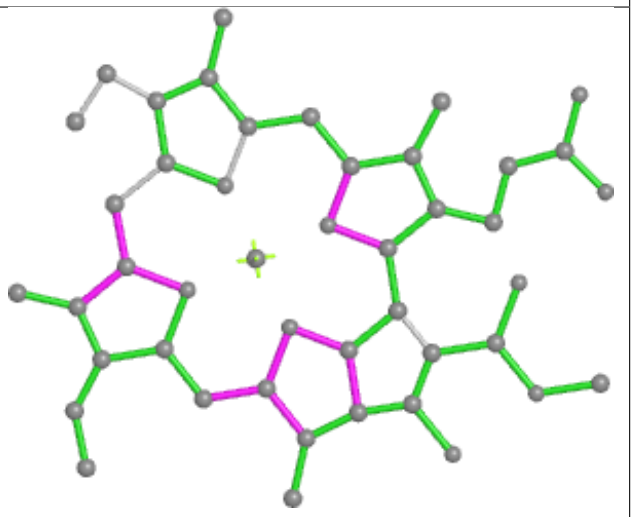


Rings

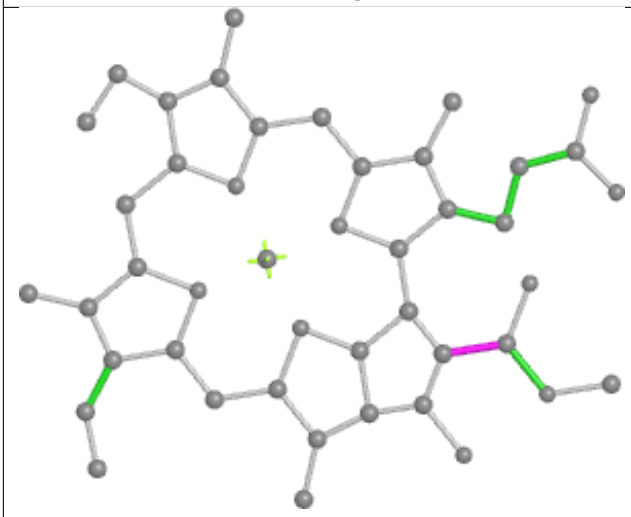
Ligand CLA 5 605



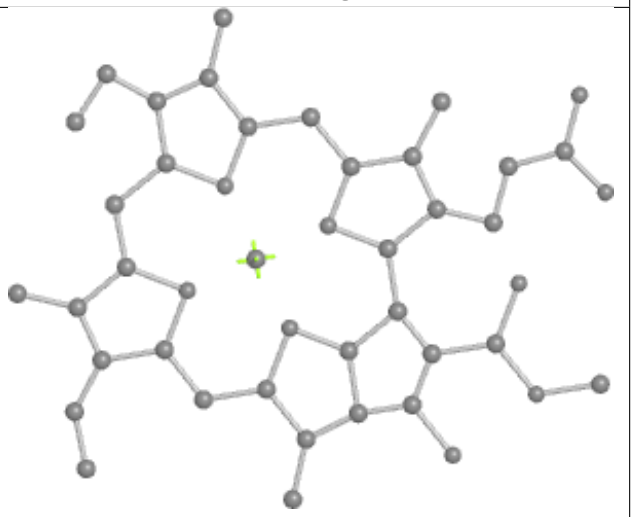
Bond lengths



Bond angles

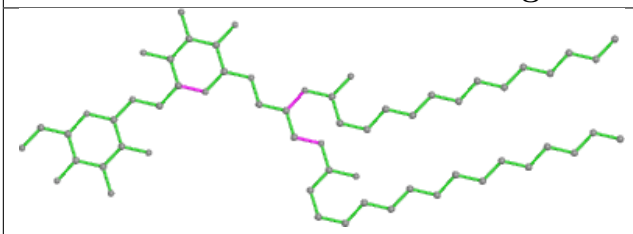


Torsions

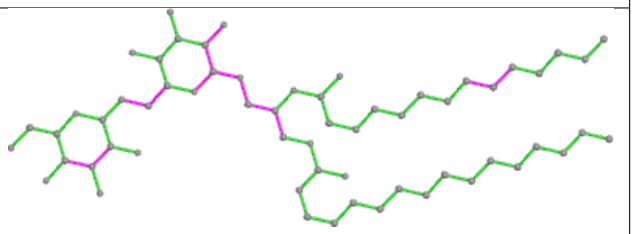


Rings

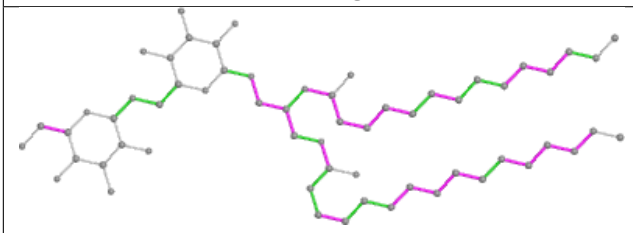
Ligand DGD Z 303



Bond lengths



Bond angles



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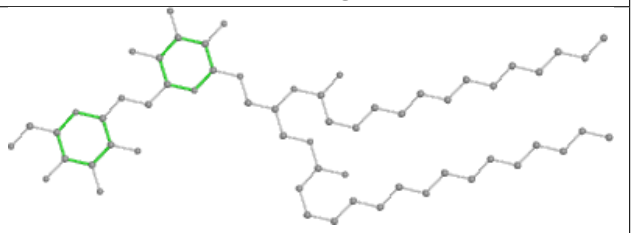
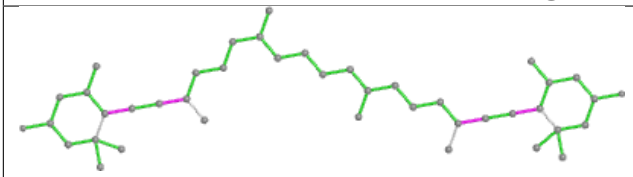
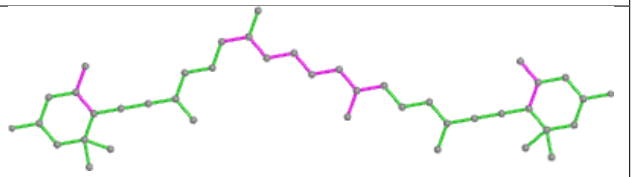


Rings

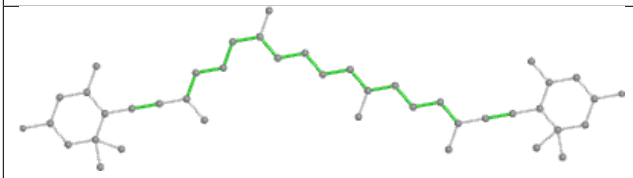
Ligand II0 3 614



Bond lengths



Bond angles



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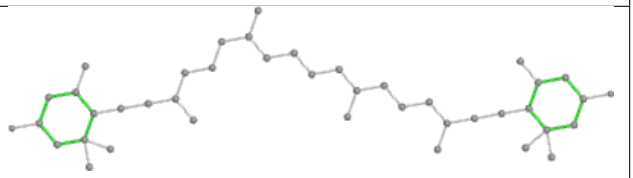
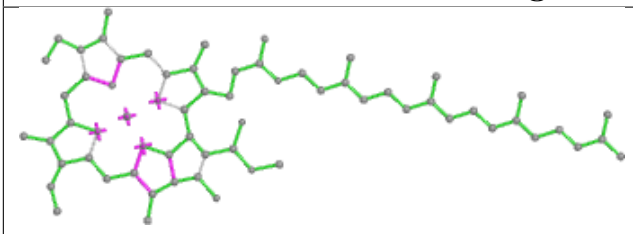


Rings

Ligand CLA 4 608



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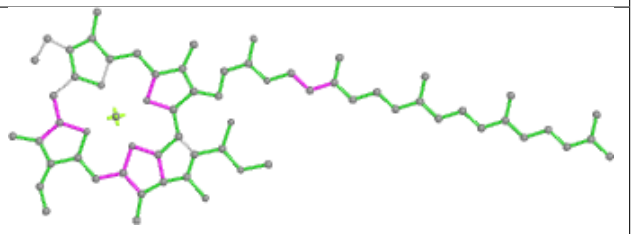
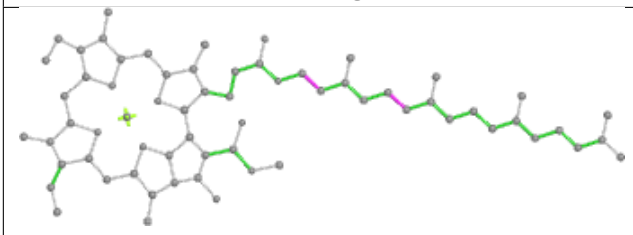


Bond angles



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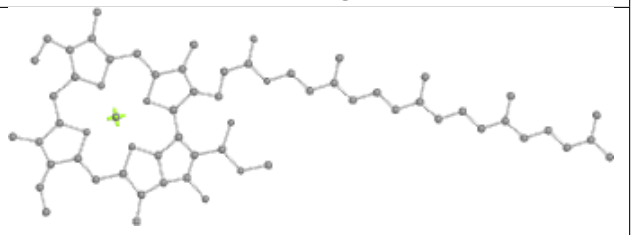
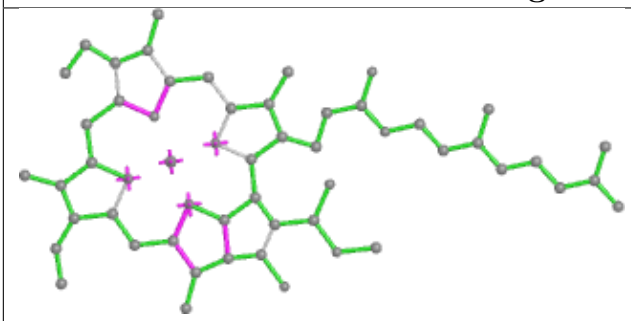
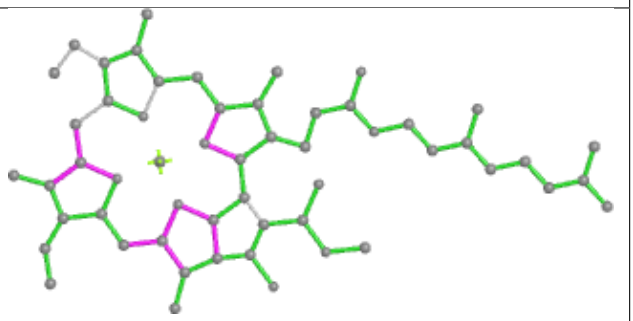


Rings

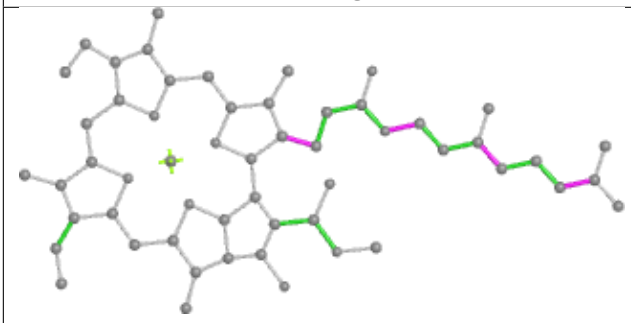
Ligand CLA a 610



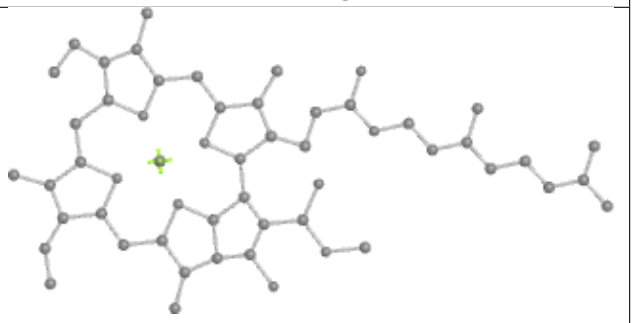
Bond lengths



Bond angles

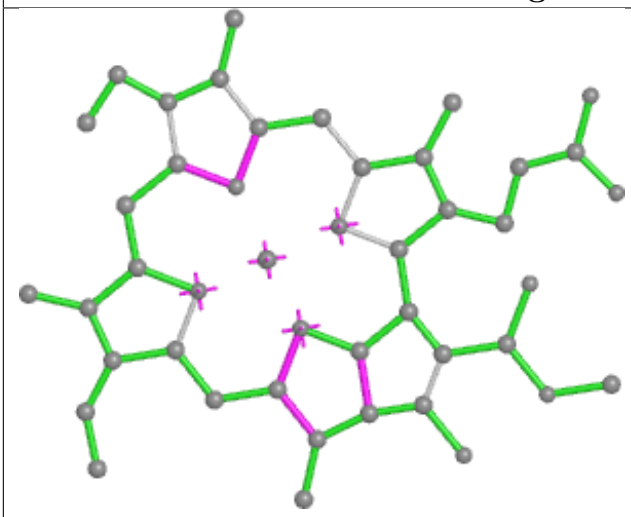


Torsions

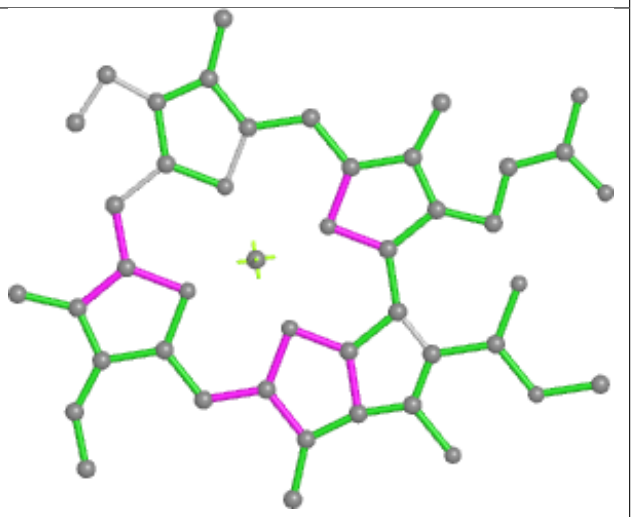


Rings

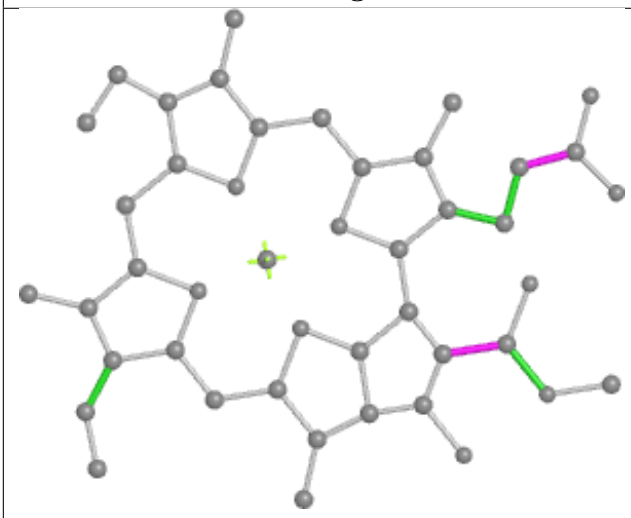
Ligand CLA 7 306



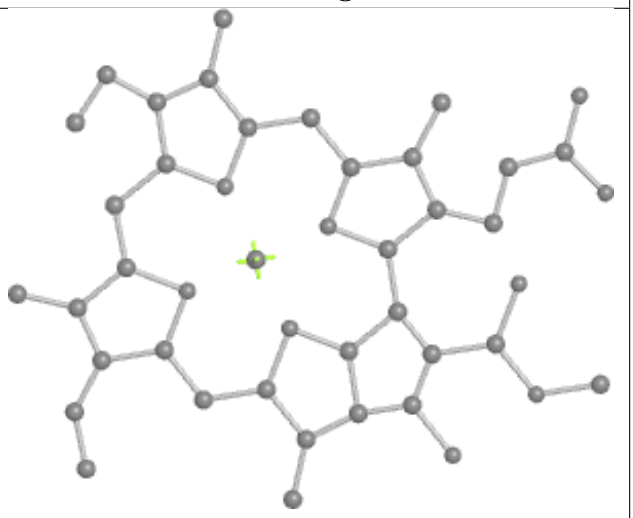
Bond lengths



Bond angles

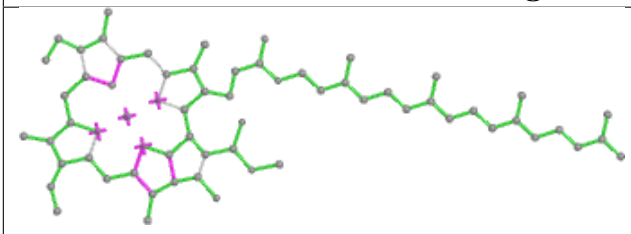


Torsions

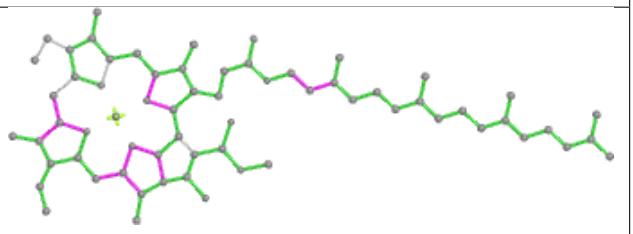


Rings

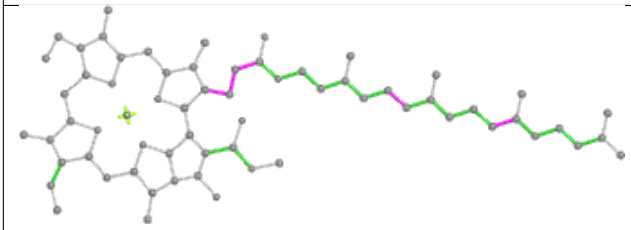
Ligand CLA B 808



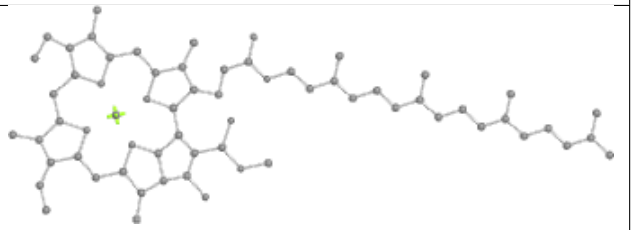
Bond lengths



Bond angles

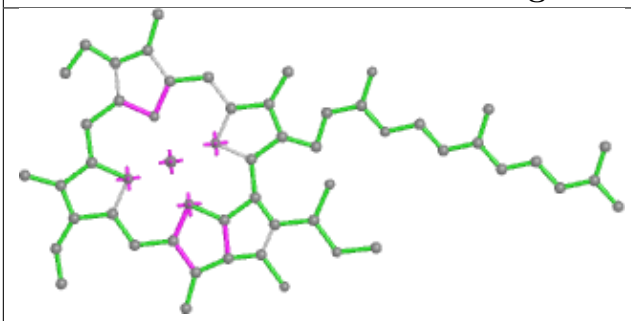


Torsions



Rings

Ligand CLA 6 611



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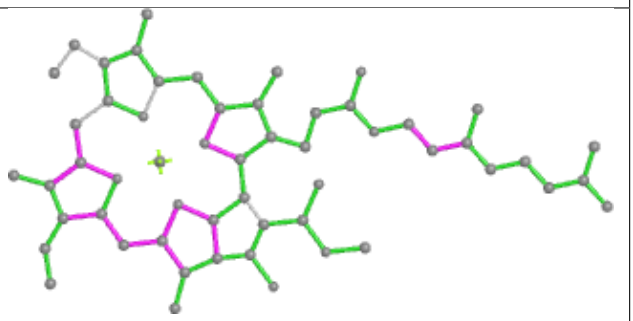
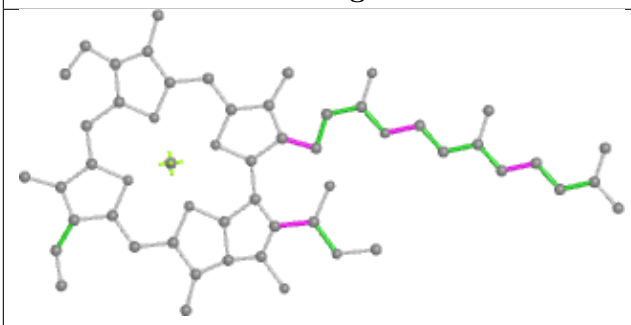
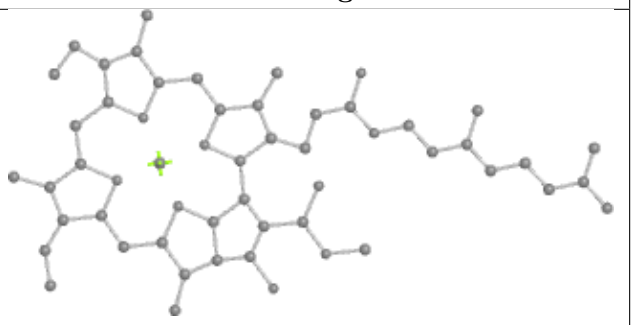


Bond angles

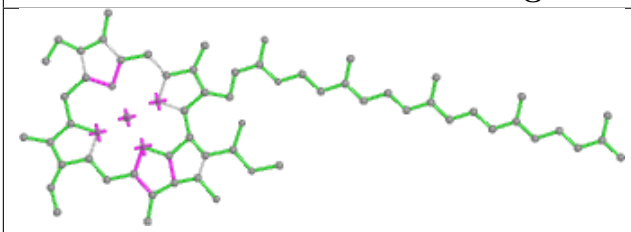


Torsions

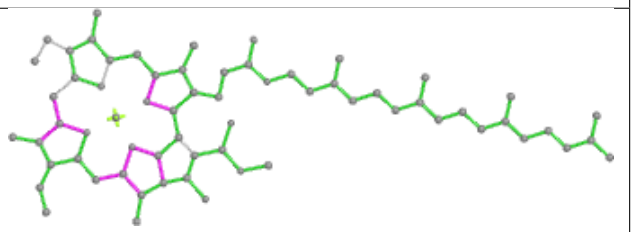


Rings

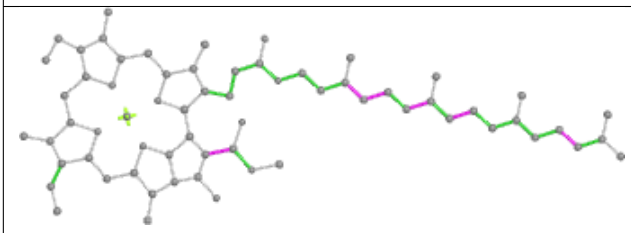
Ligand CLA B 807



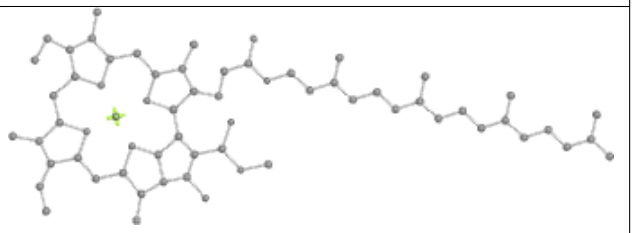
Bond lengths



Bond angles

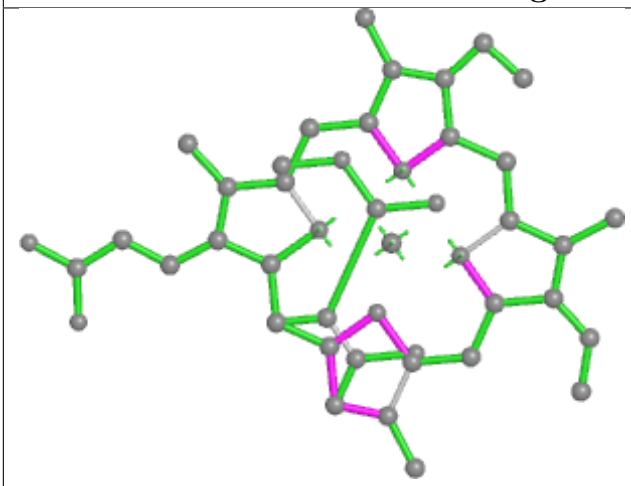


Torsions

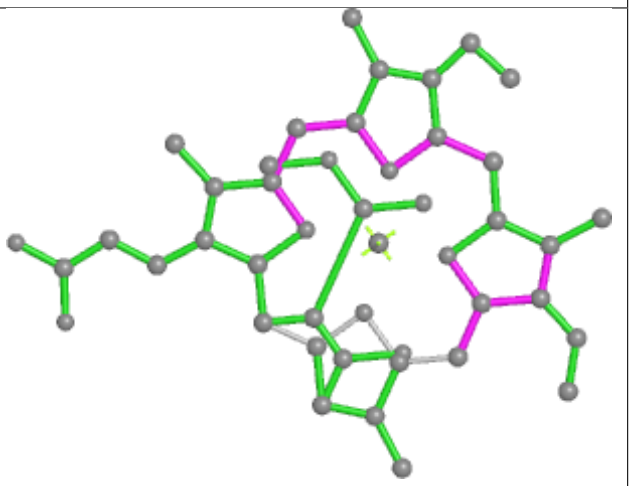


Rings

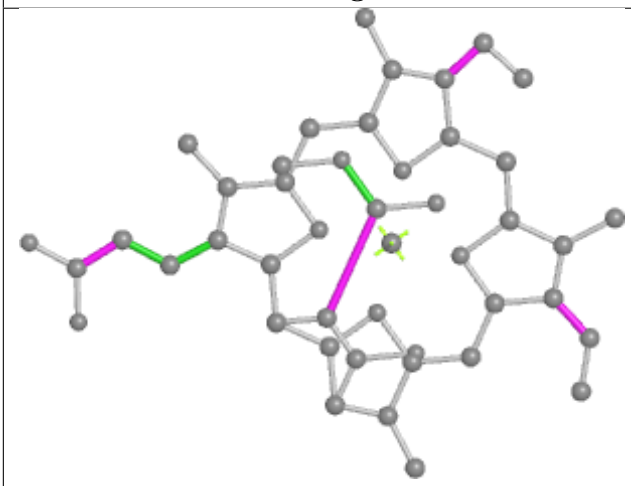
Ligand KC2 7 307



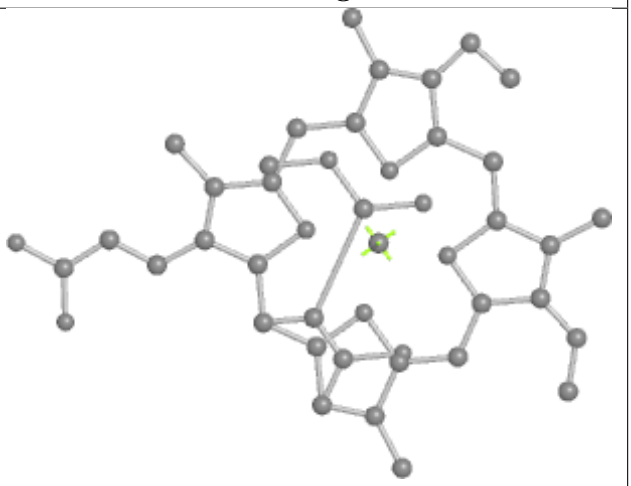
Bond lengths



Bond angles

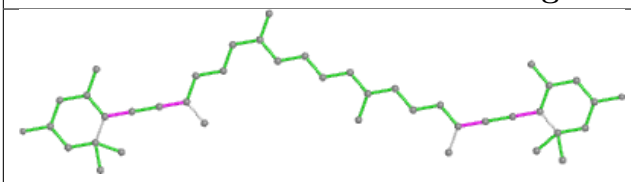


Torsions

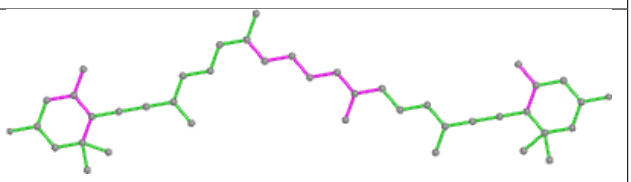


Rings

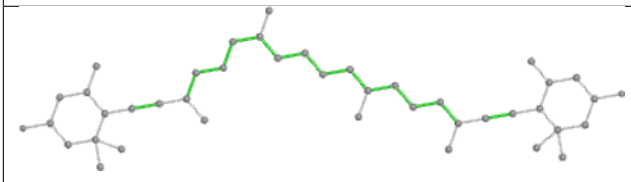
Ligand II0 b 614



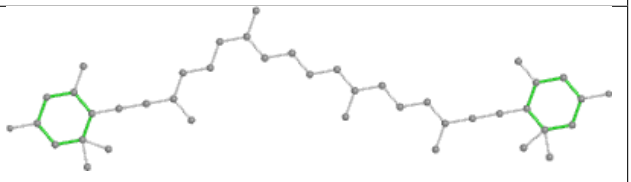
Bond lengths



Bond angles

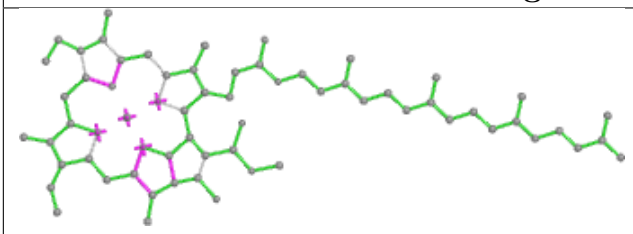


Torsions

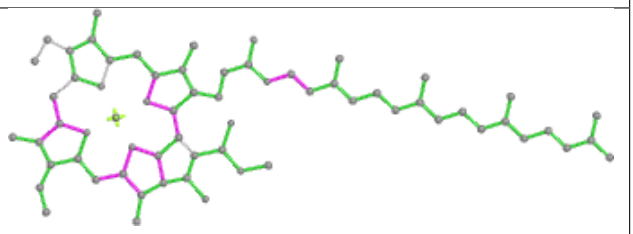


Rings

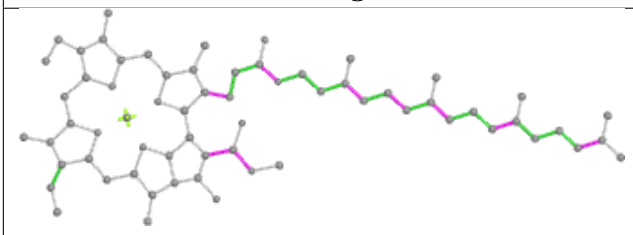
Ligand CLA A 810



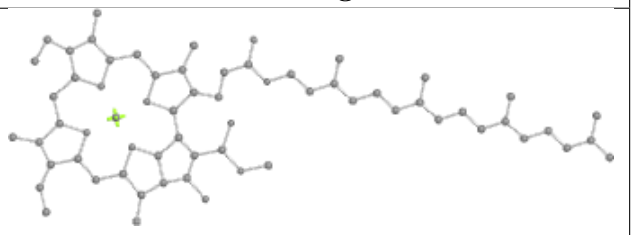
Bond lengths



Bond angles

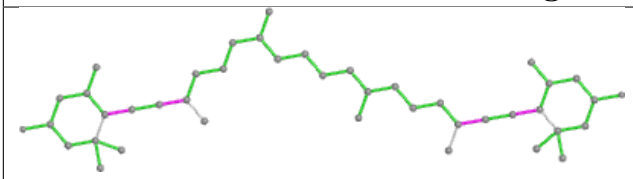


Torsions



Rings

Ligand II0 2 615



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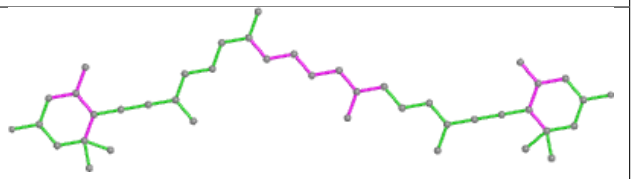

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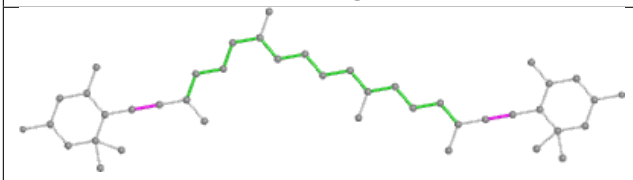

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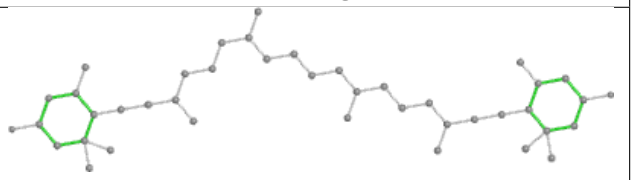

Rings

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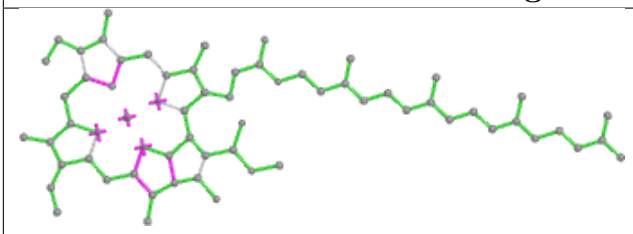

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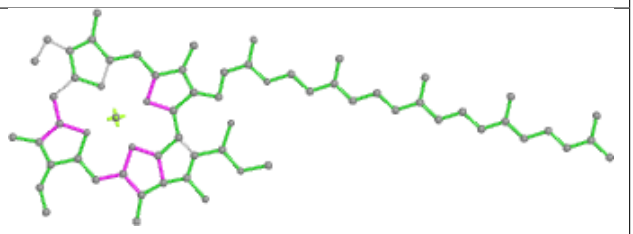

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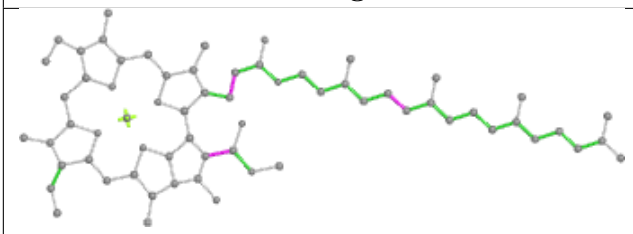

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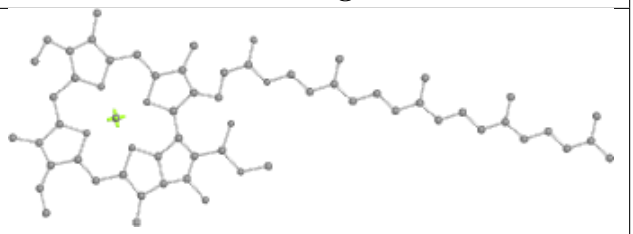

Rings

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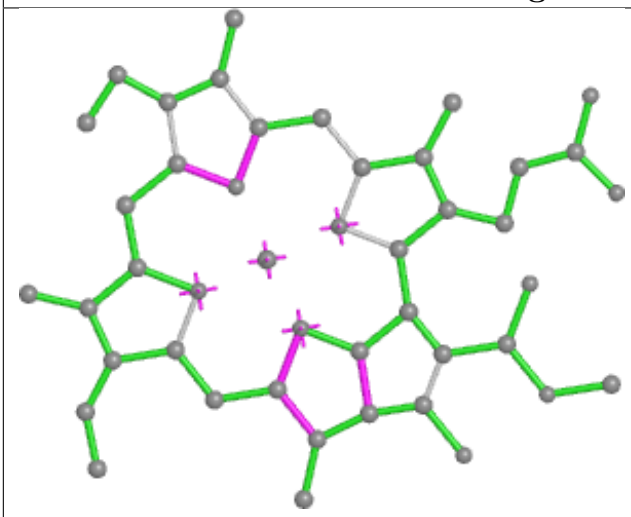

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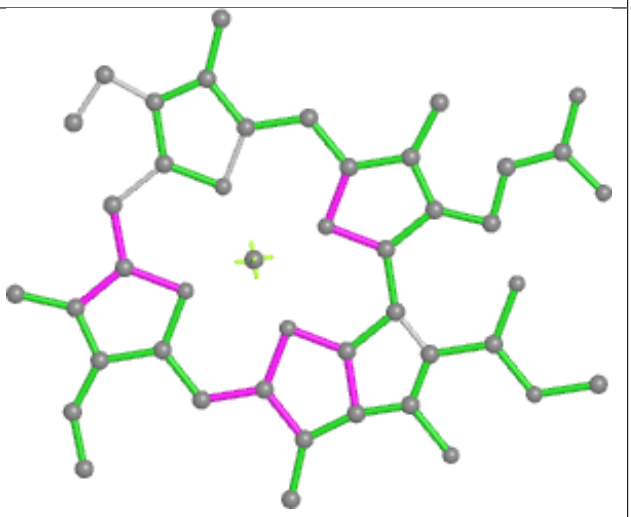

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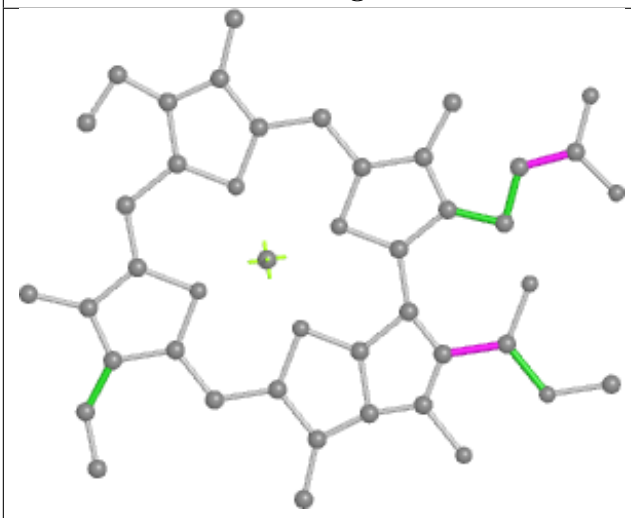

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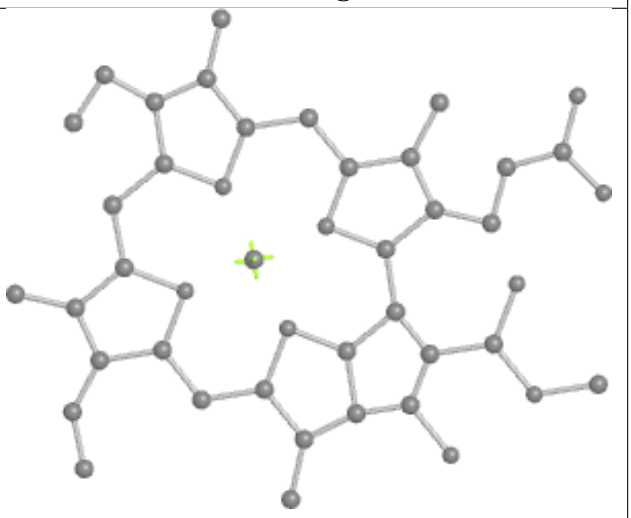

Rings

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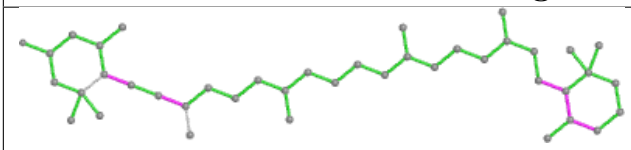

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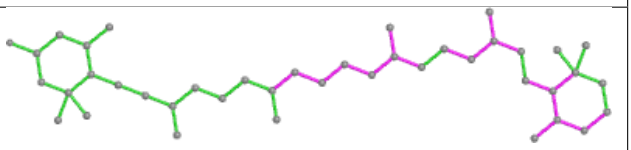

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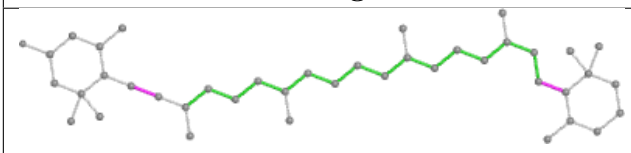

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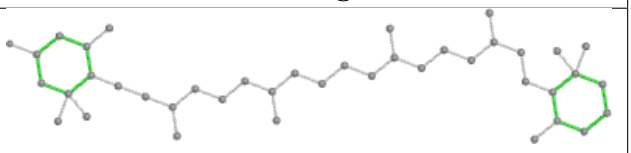

Rings

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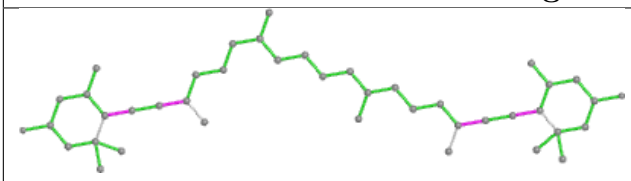

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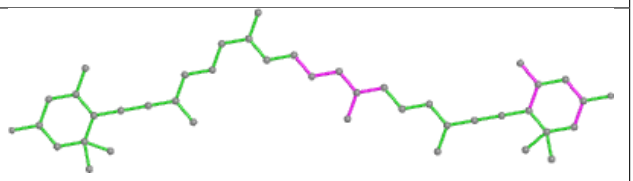

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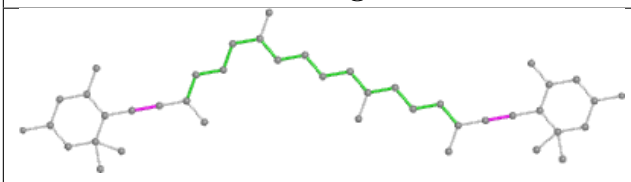

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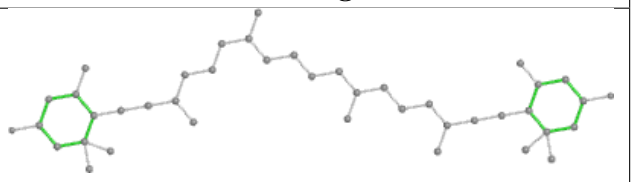

Rings

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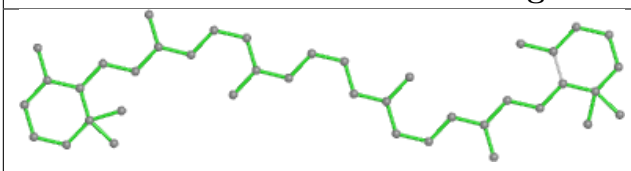

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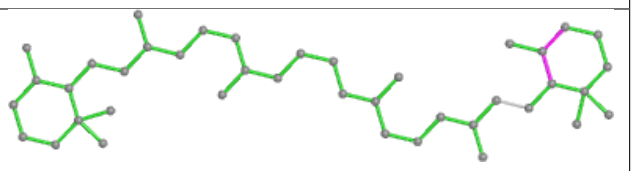

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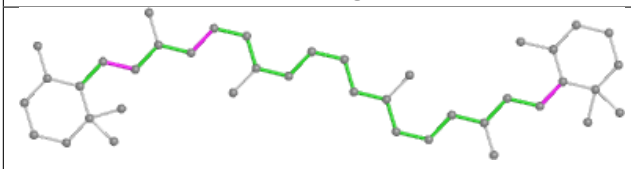

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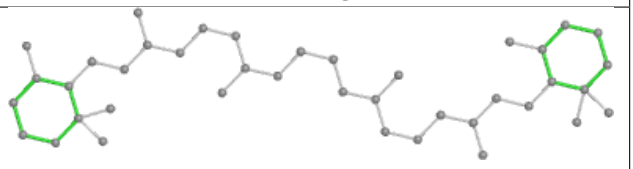
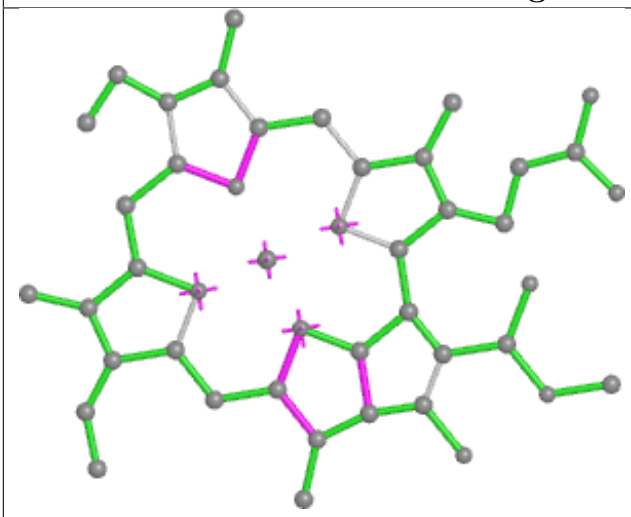


Rings

Ligand CLA 5 607



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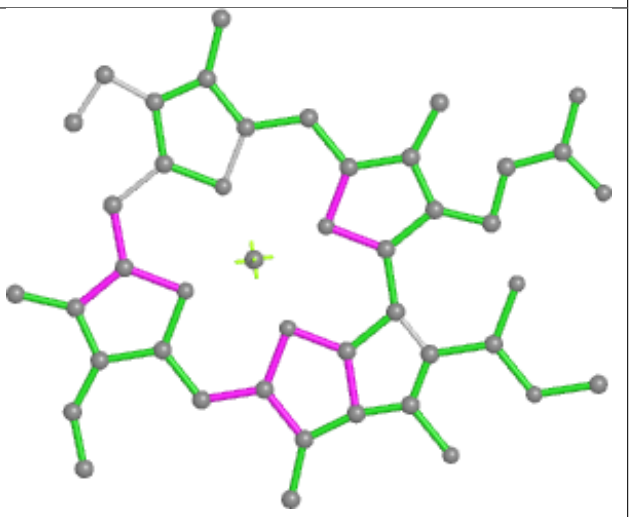

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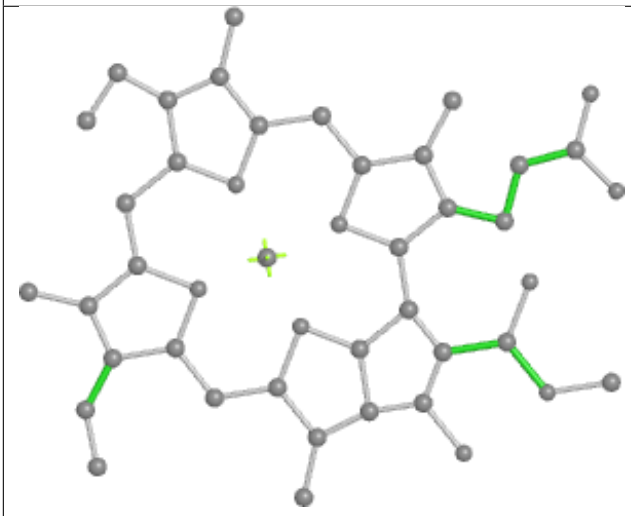

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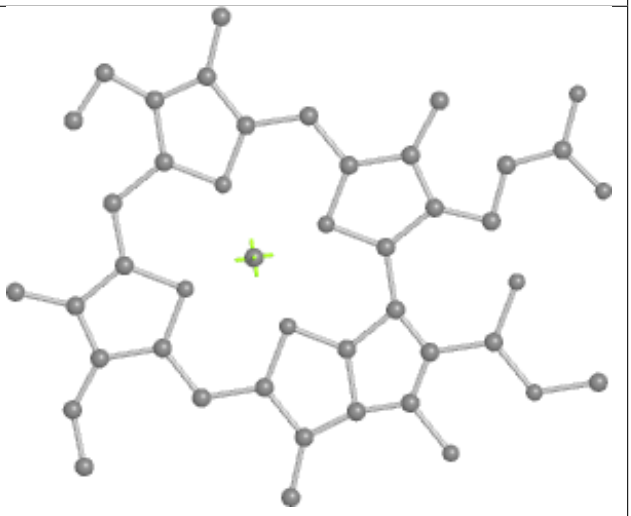

Rings

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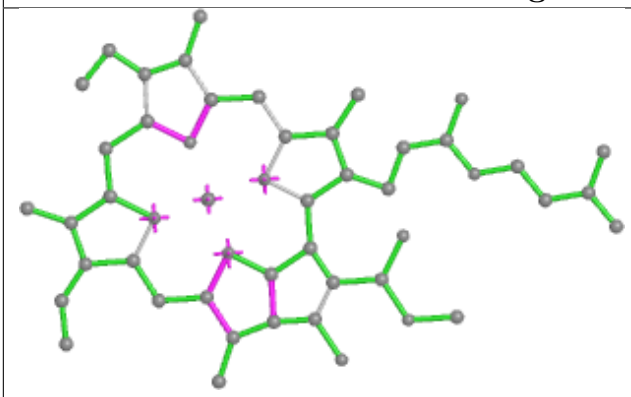

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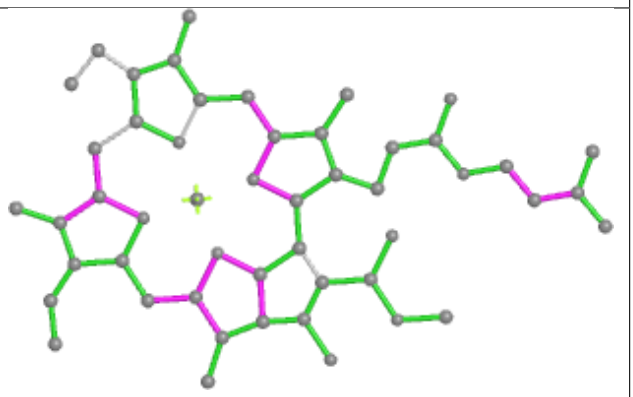

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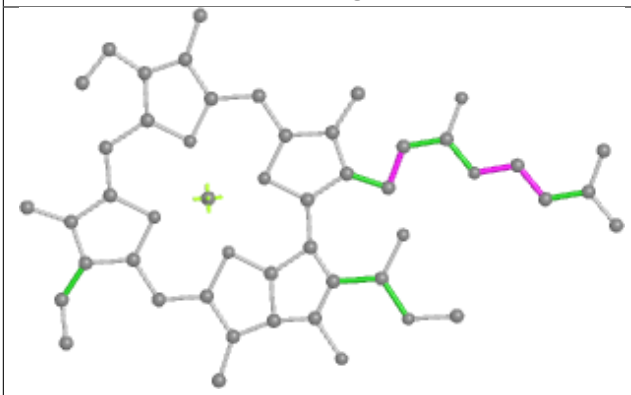

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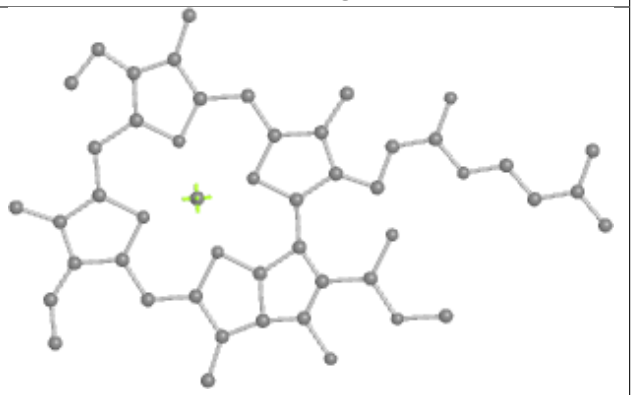

Rings

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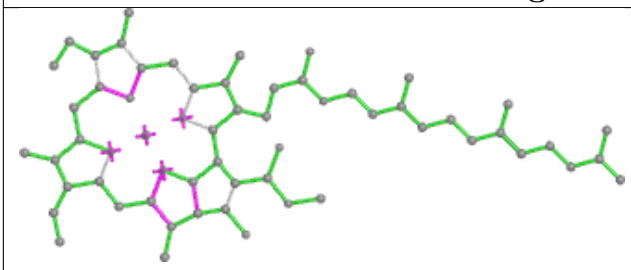

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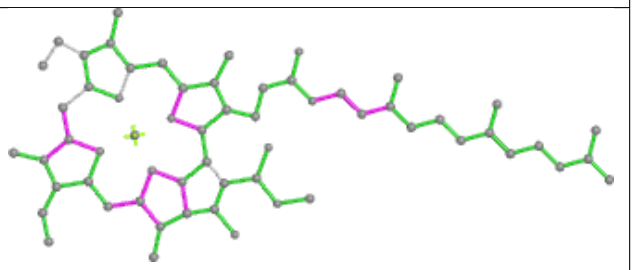

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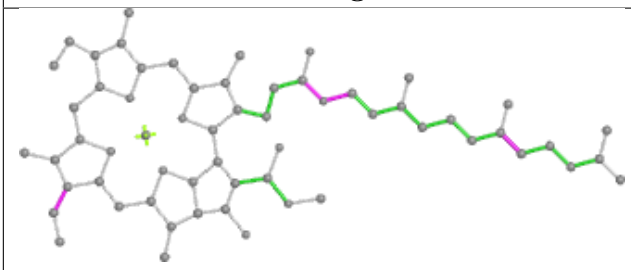

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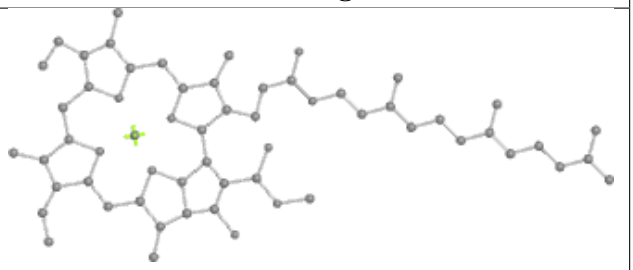

Rings

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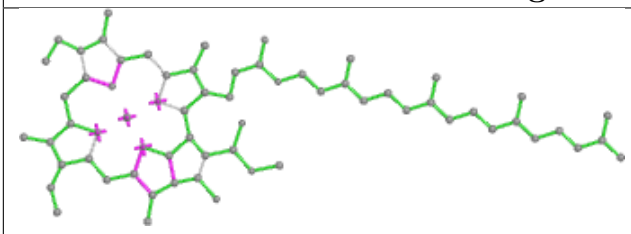
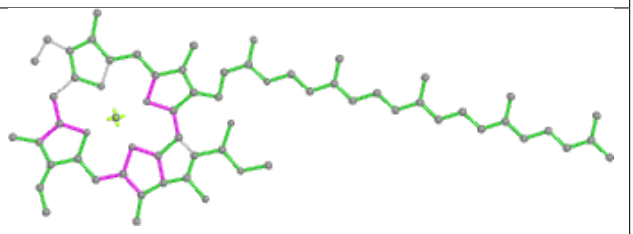
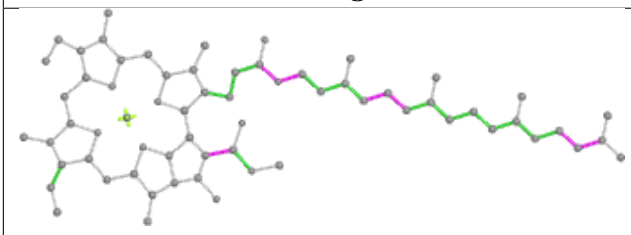
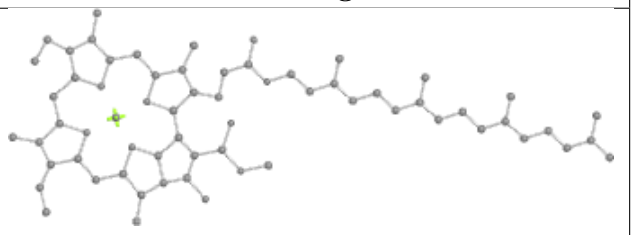
	
Bond lengths	Bond angles
	
Torsions	Rings

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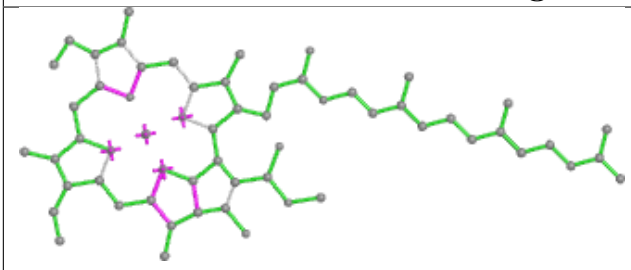
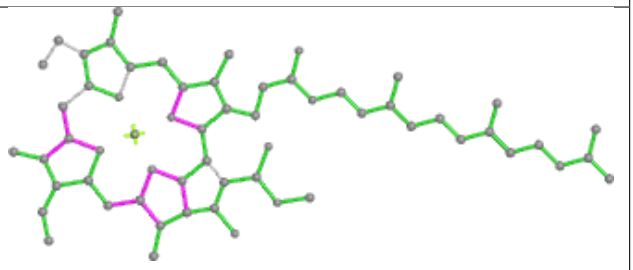
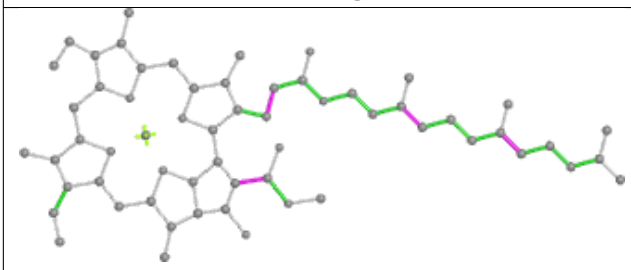
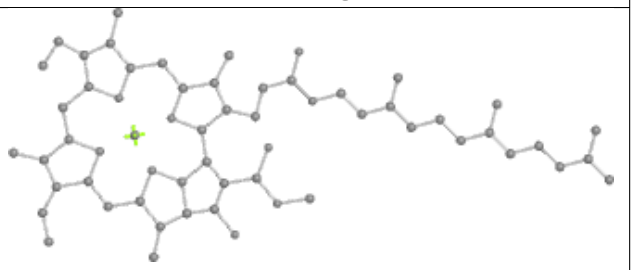
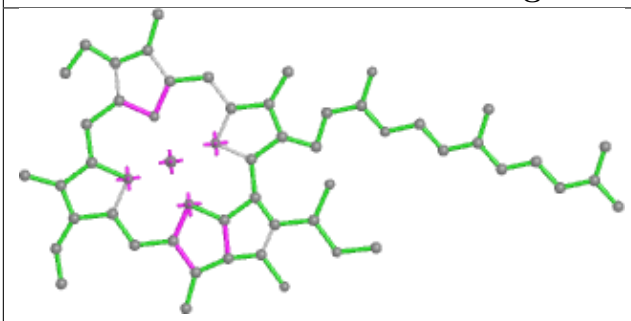
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA O 201



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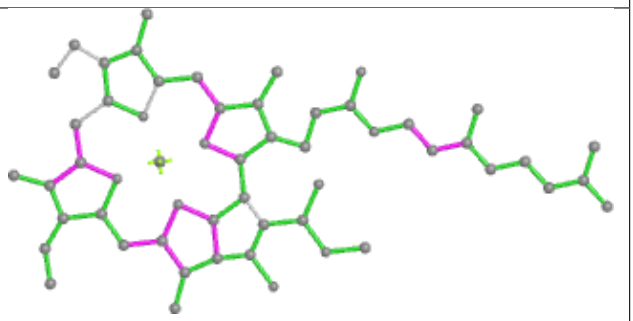

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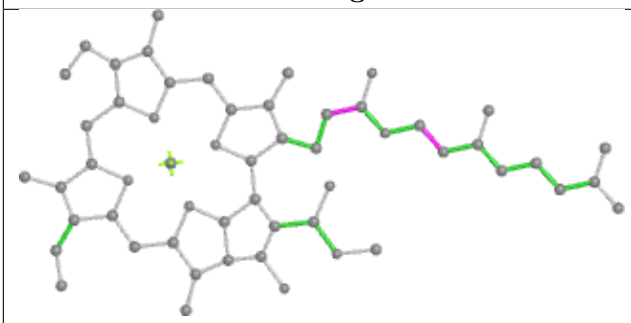

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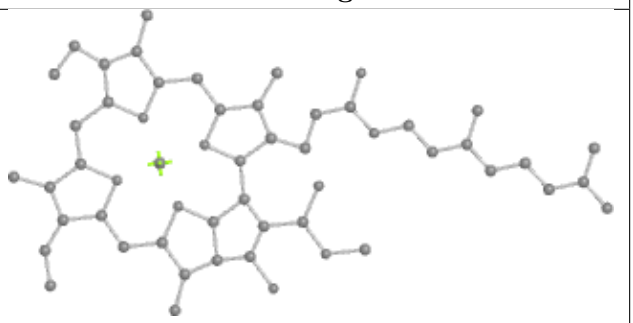
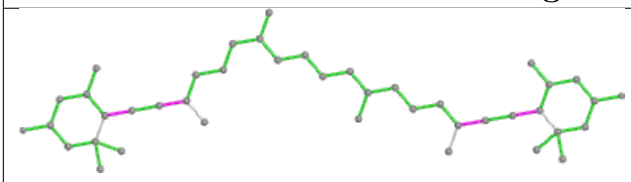


Rings

Ligand II0 7 317



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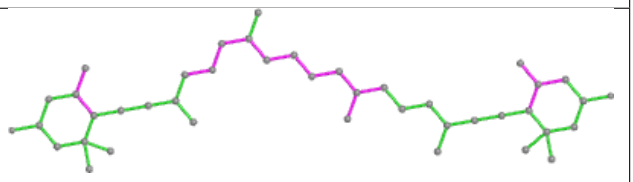
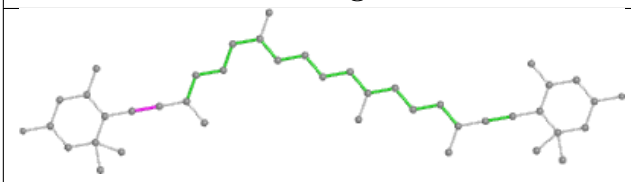


Bond angles



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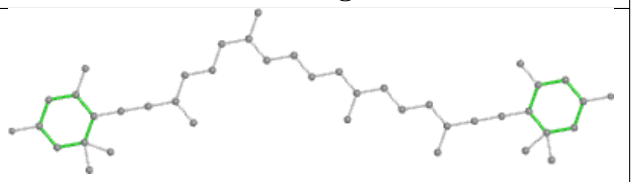
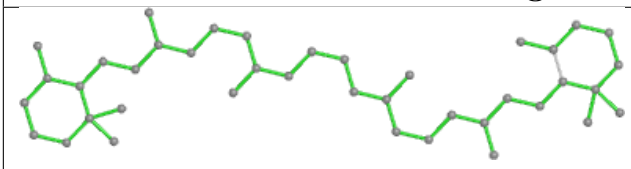
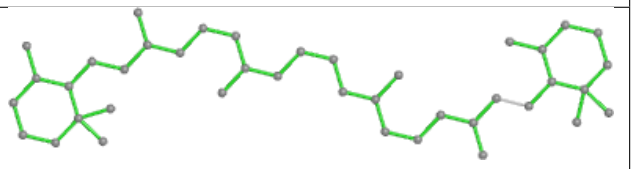


Rings

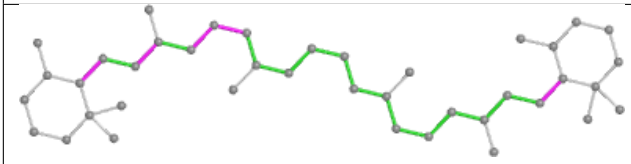
Ligand 8CT R 201



Bond lengths



Bond angles



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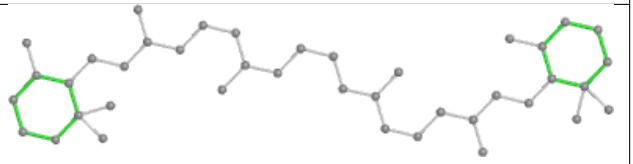
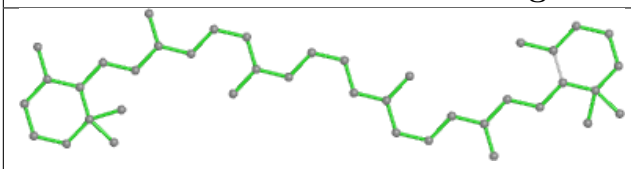
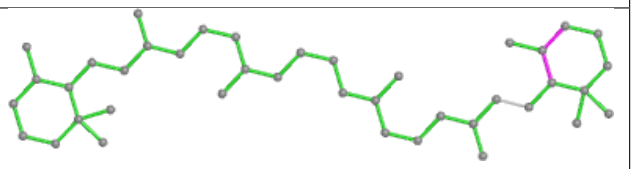


Rings

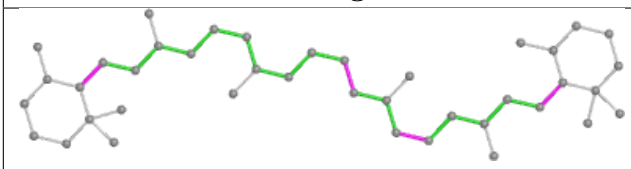
Ligand 8CT Z 309



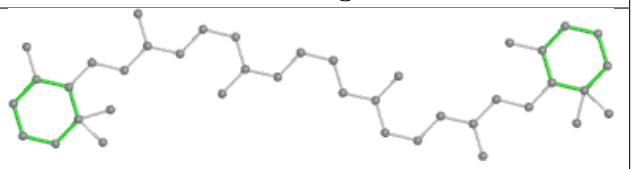
Bond lengths



Bond angles

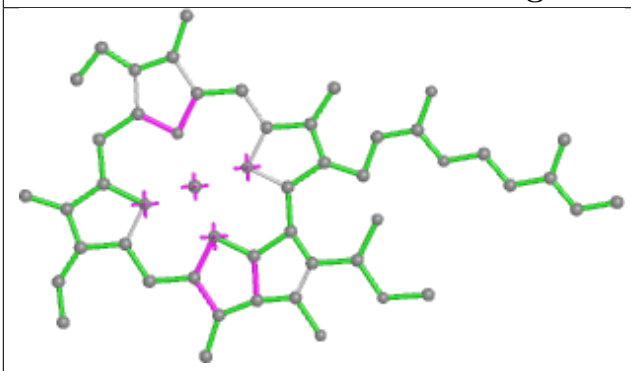


Torsions

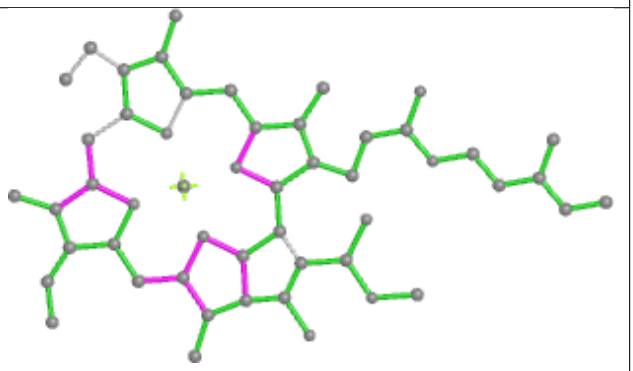


Rings

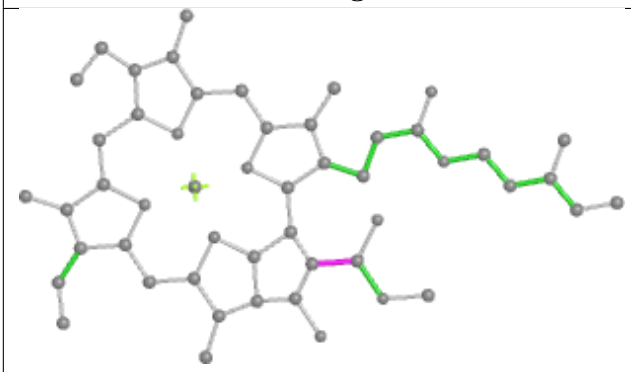
Ligand CLA L 201



Bond lengths



Bond angles



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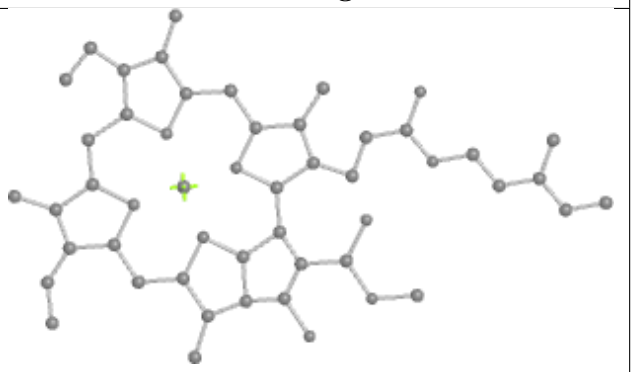
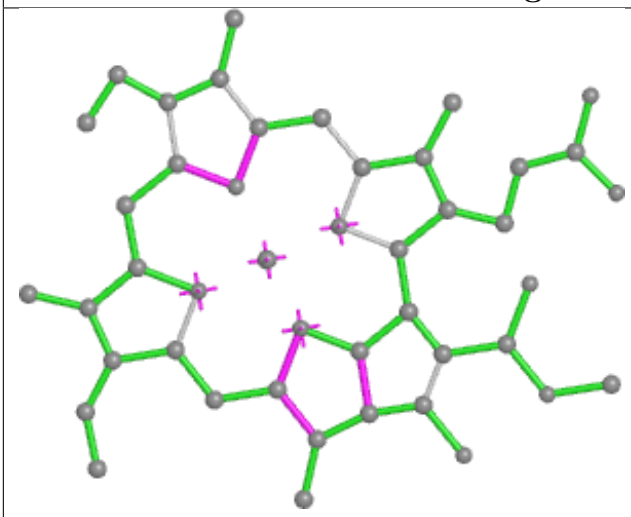


Rings

Ligand CLA B 829



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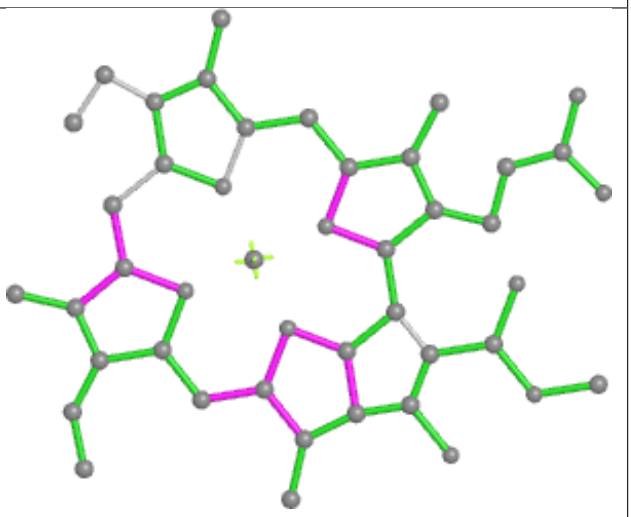

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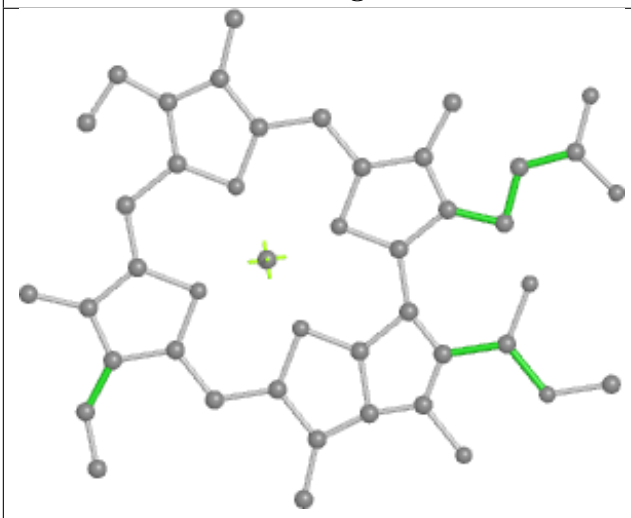
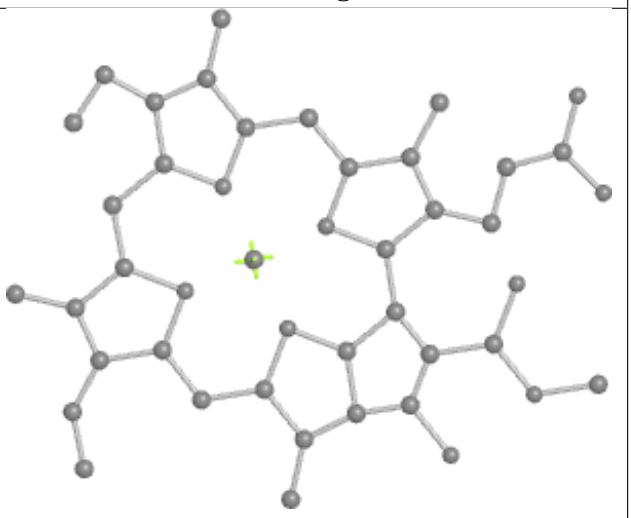
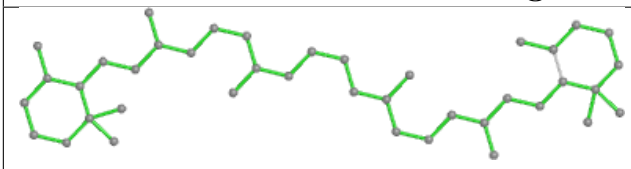


Torsions



Rings

Ligand 8CT R 203



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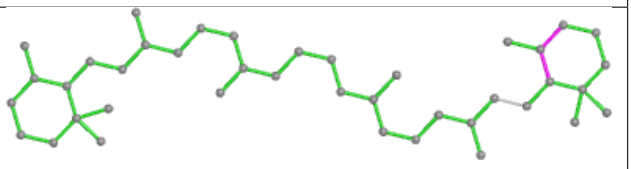
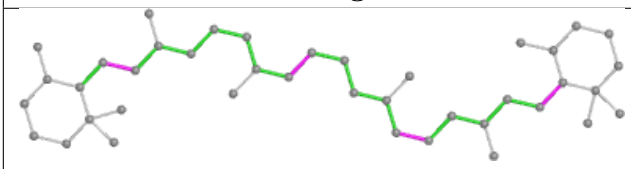


Bond angles



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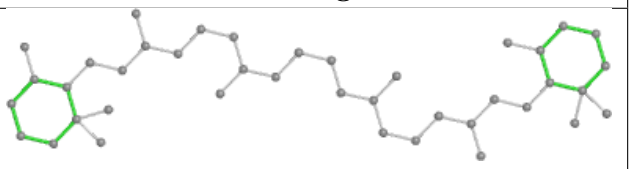
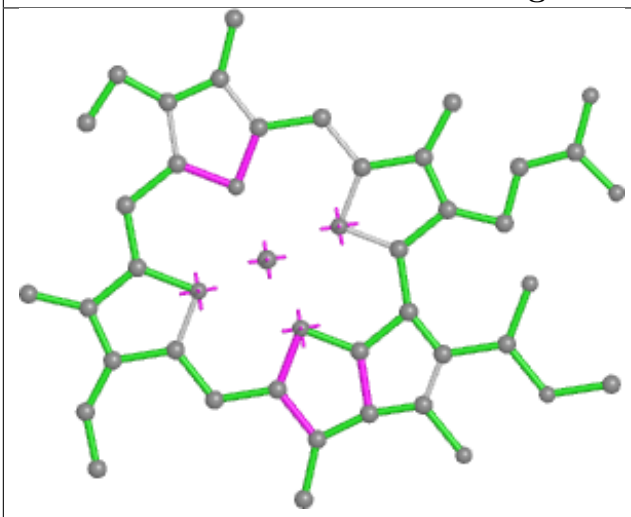


Rings

Ligand CLA 3 601



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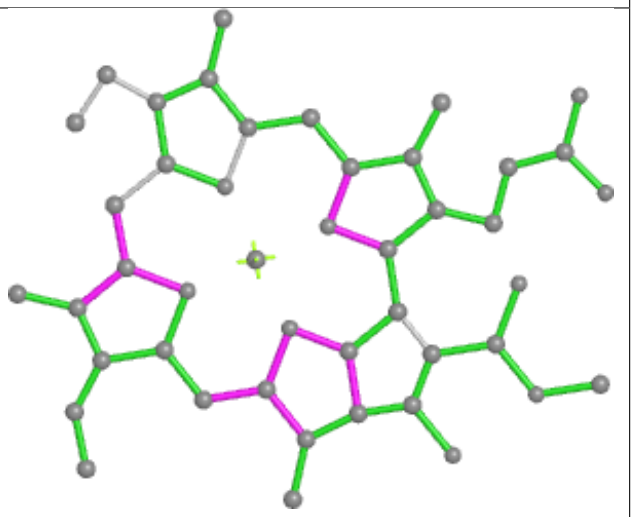
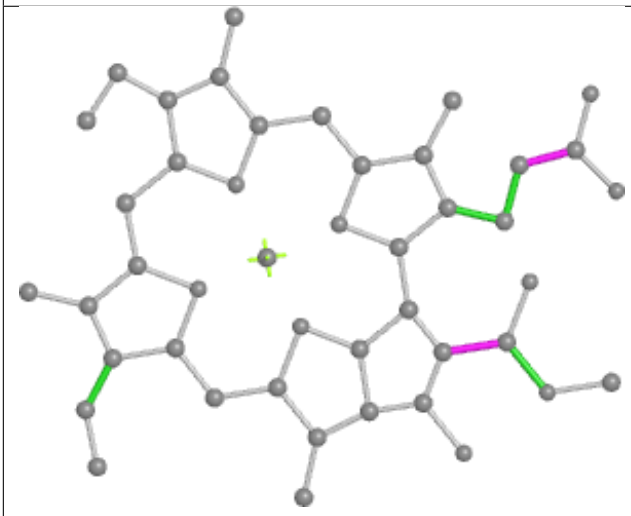


Bond angles



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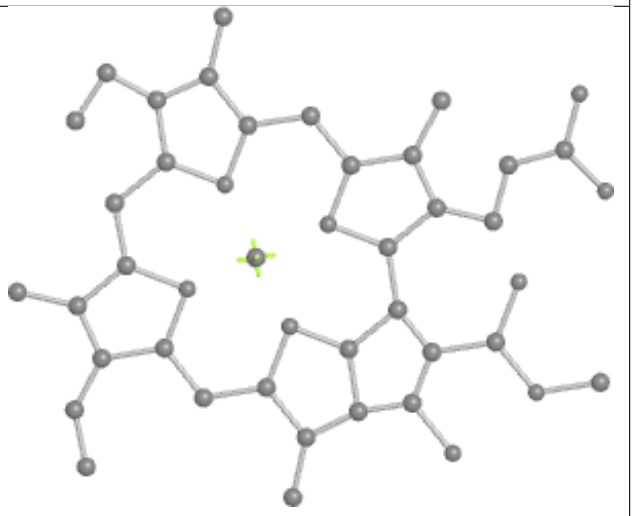
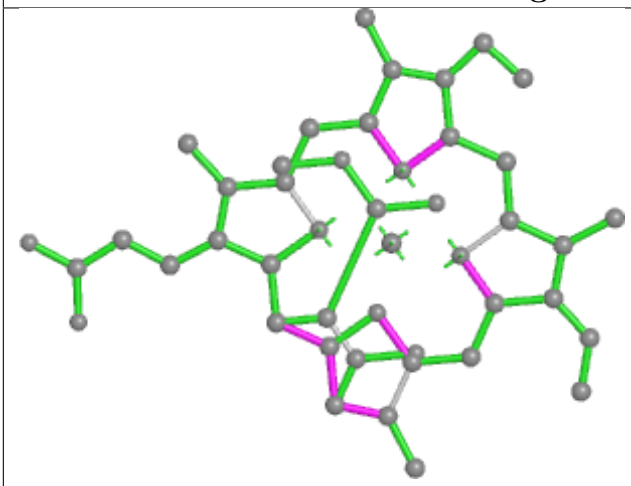
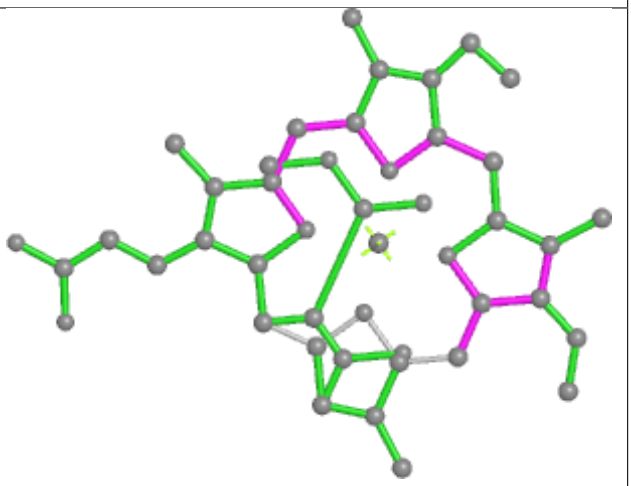


Rings

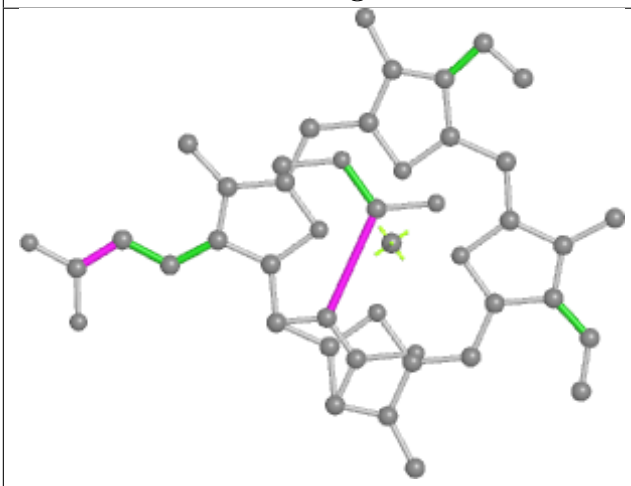
Ligand KC2 5 610



Bond lengths



Bond angles



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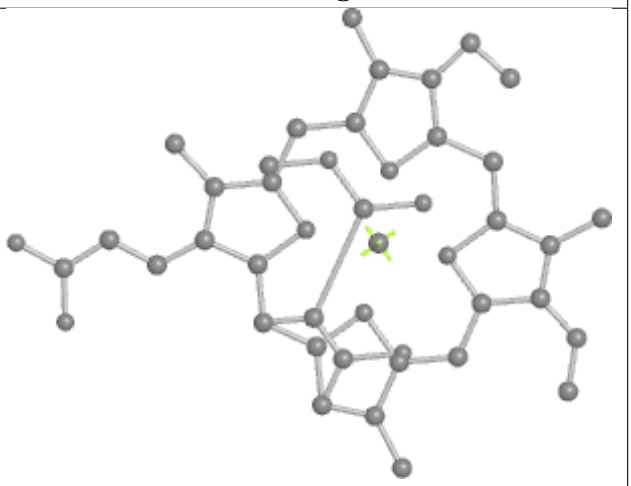
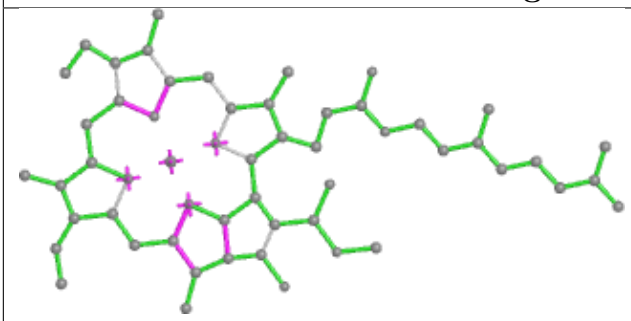
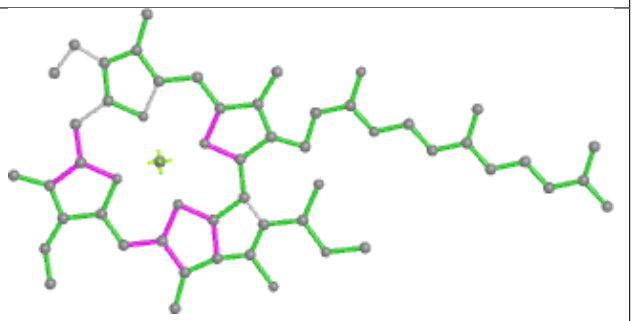


Rings

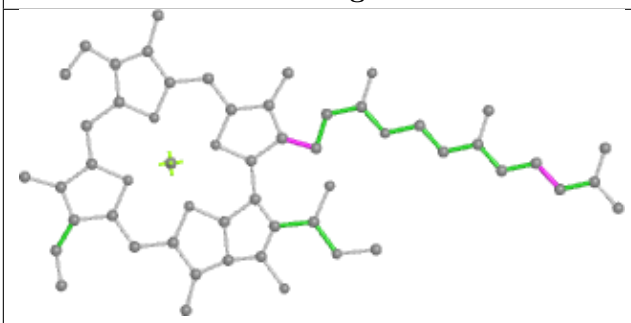
Ligand CLA A 821



Bond lengths



Bond angles



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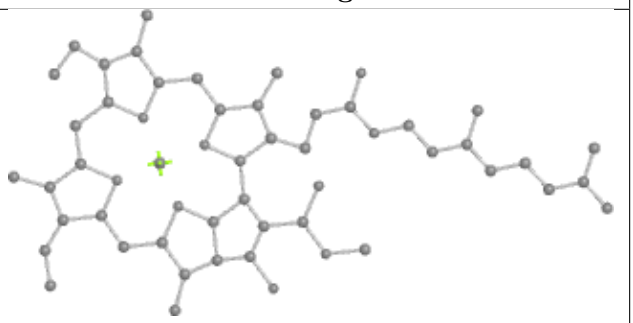
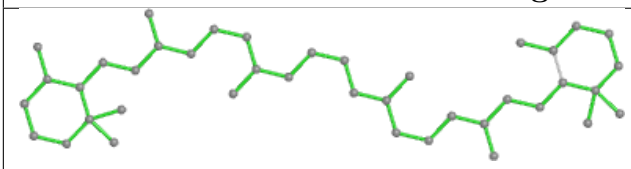


Rings

Ligand 8CT 4 616



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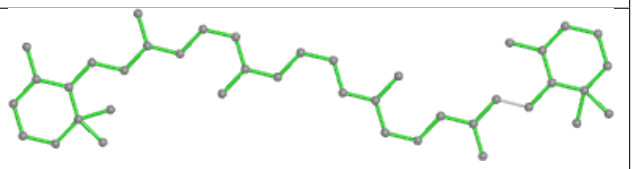

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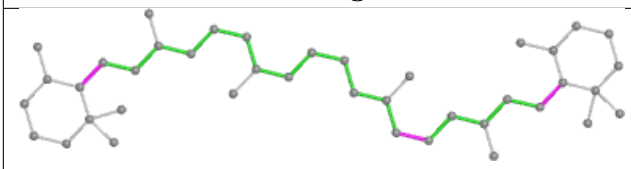
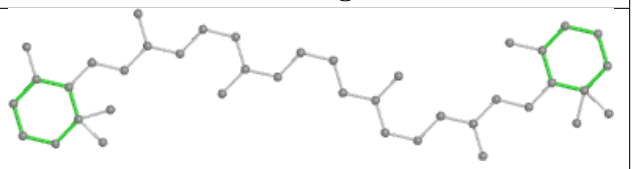
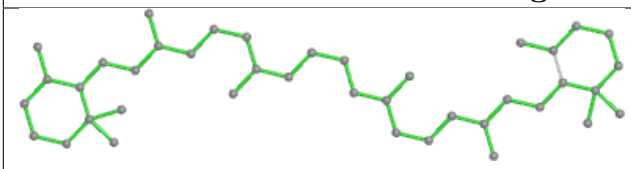


Torsions

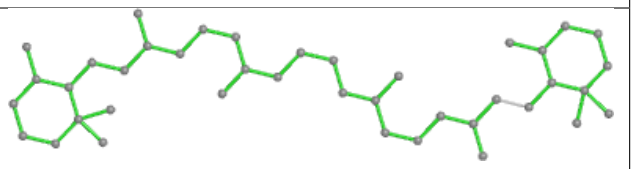


Rings

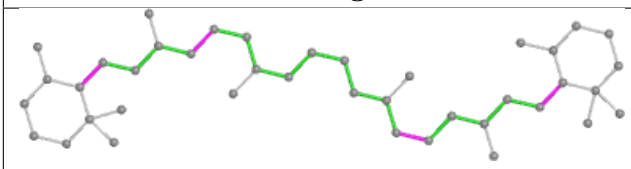
Ligand 8CT b 615



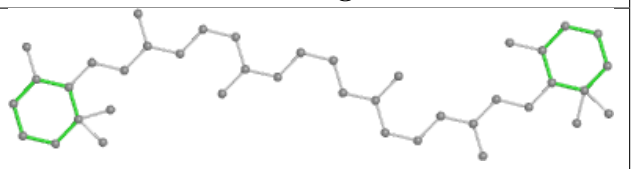
Bond lengths



Bond angles

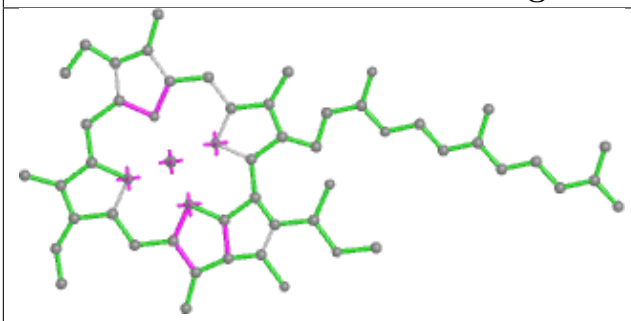


Torsions



Rings

Ligand CLA 7 312



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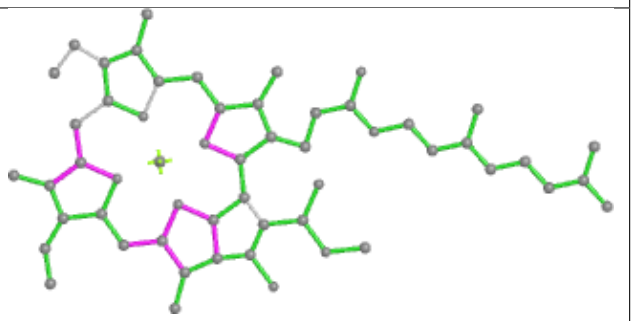
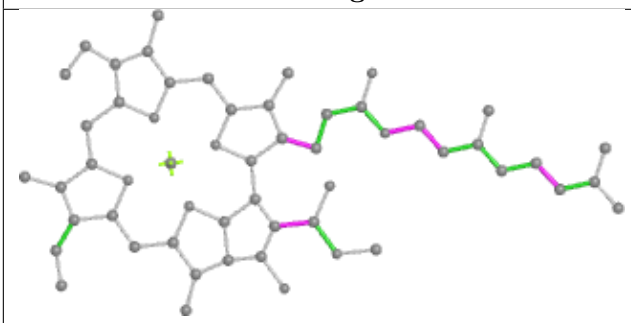
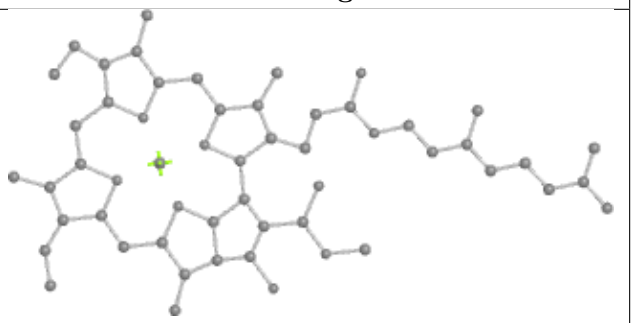


Bond angles

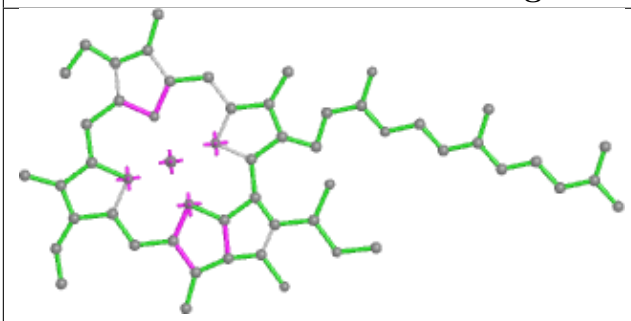


Torsions



Rings

Ligand CLA B 811



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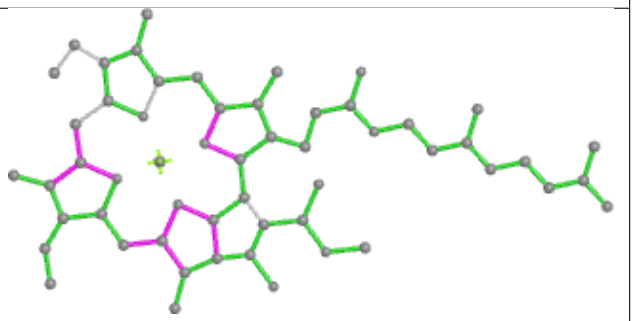
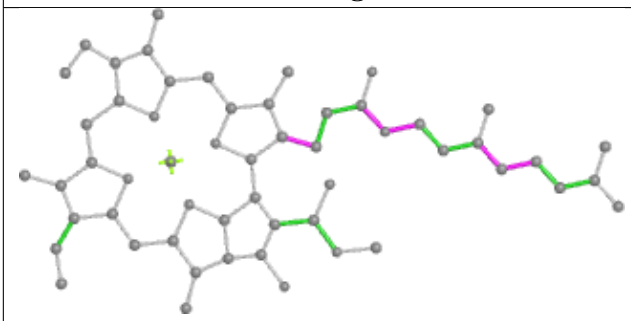


Bond angles



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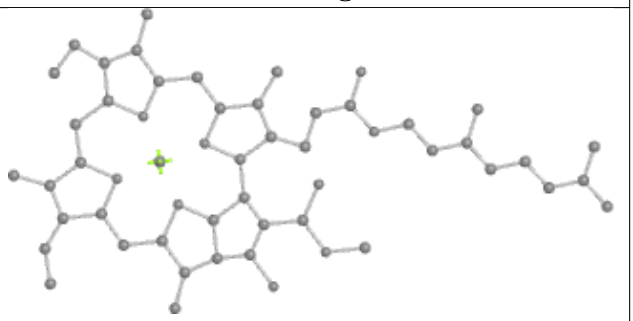
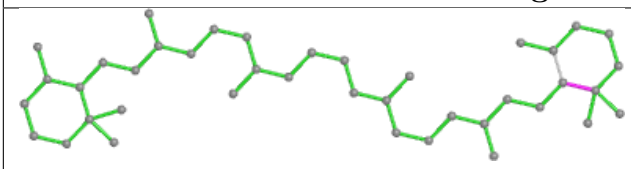
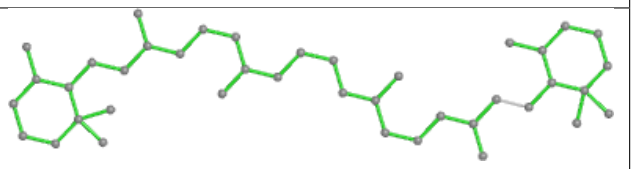


Rings

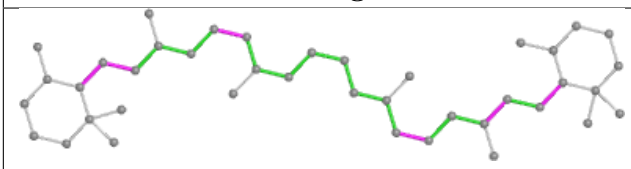
Ligand 8CT 7 318



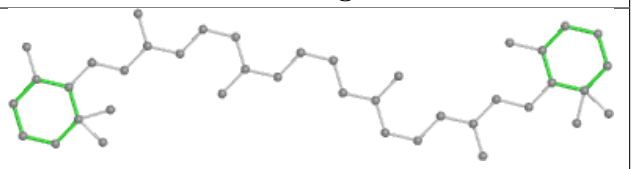
Bond lengths



Bond angles

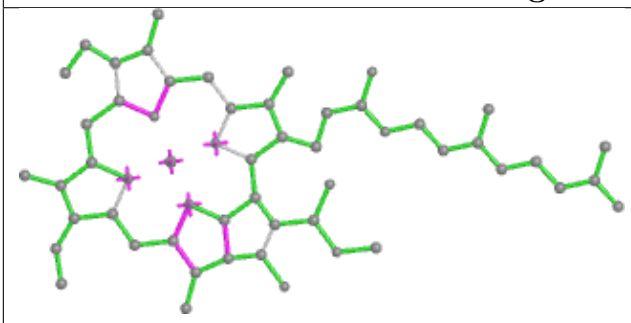


Torsions



Rings

Ligand CLA 7 309



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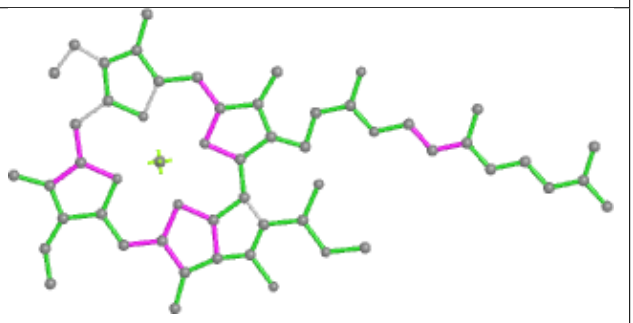
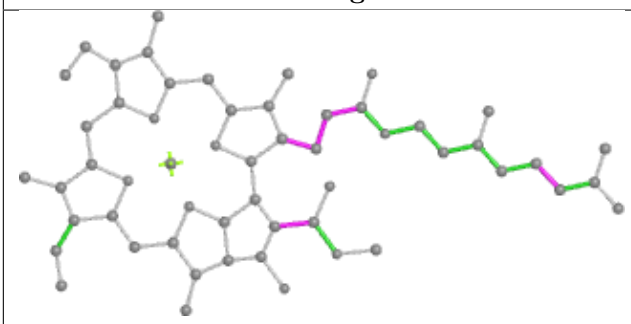
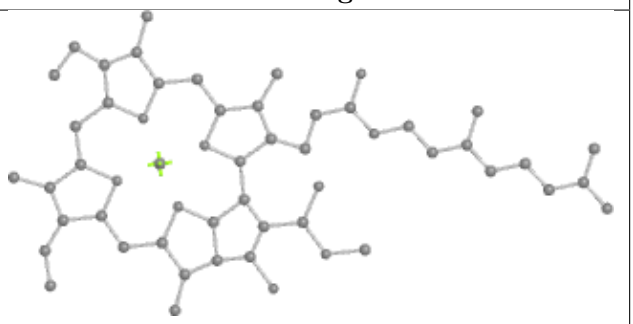


Bond angles

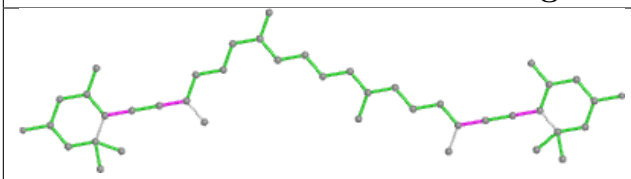


Torsions



Rings

Ligand II0 Z 312



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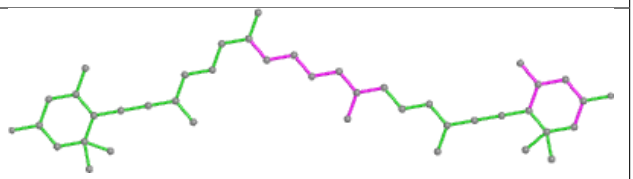
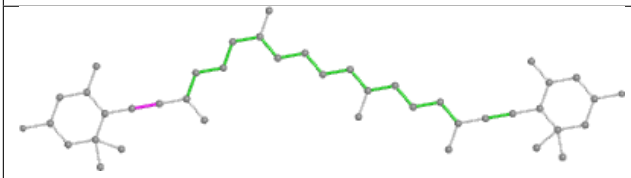
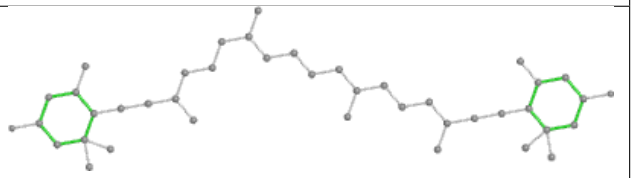


Bond angles

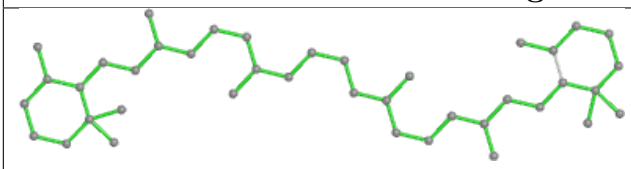


Torsions

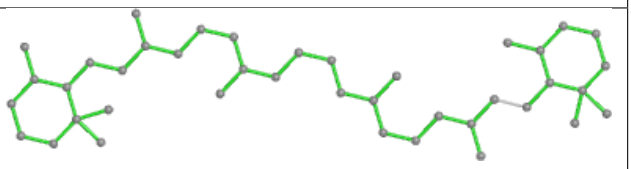


Rings

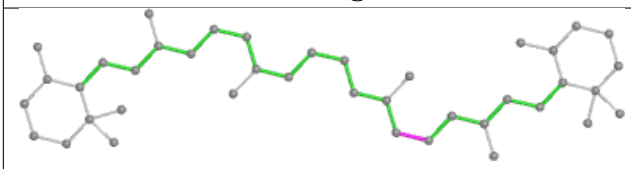
Ligand 8CT A 848



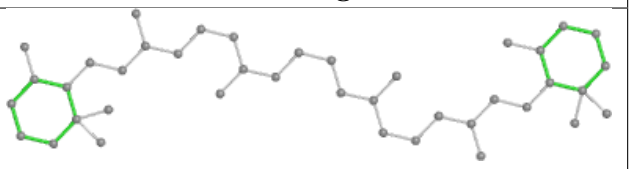
Bond lengths



Bond angles

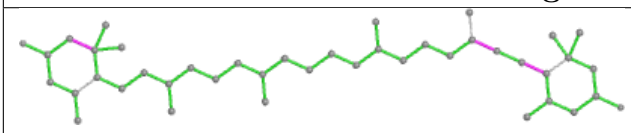


Torsions

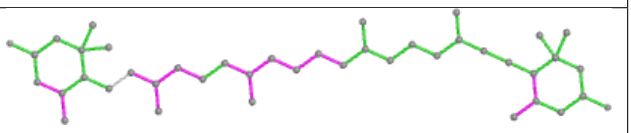


Rings

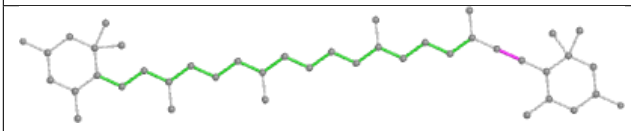
Ligand II3 1 615



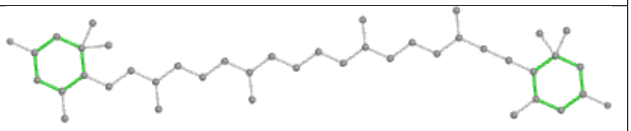
Bond lengths



Bond angles

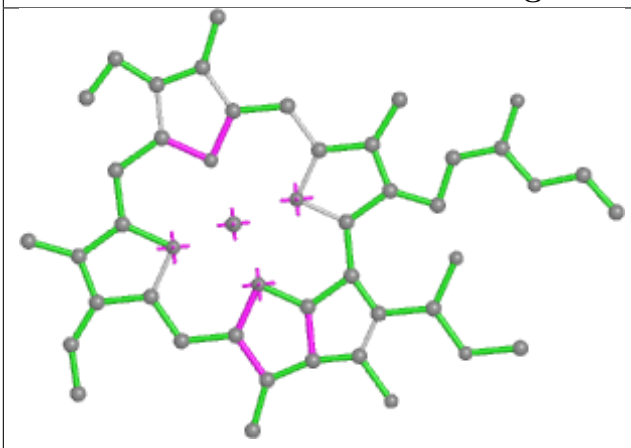


Torsions



Rings

Ligand CLA B 836



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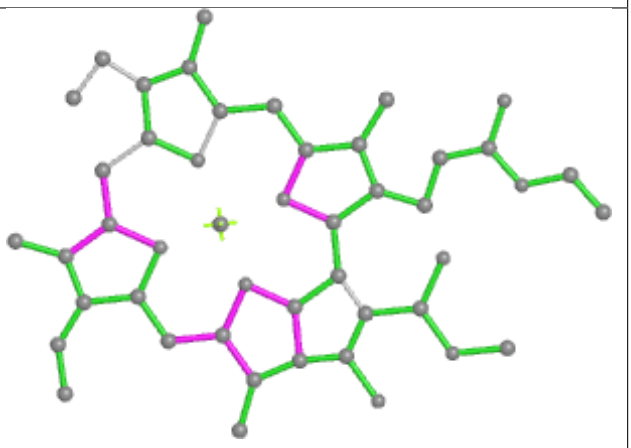
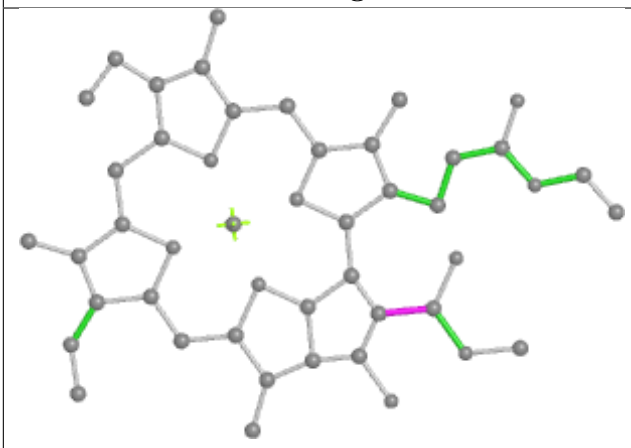


Bond angles



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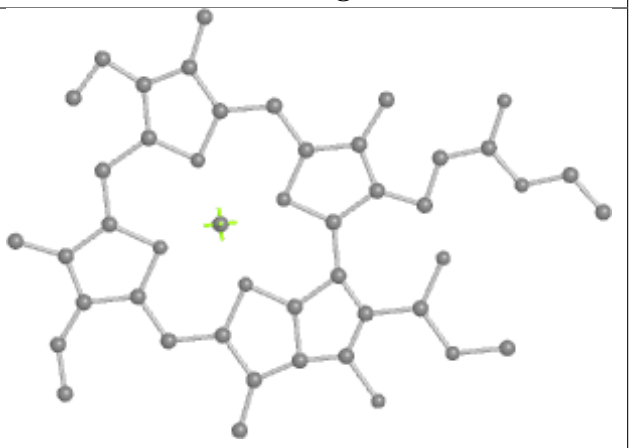
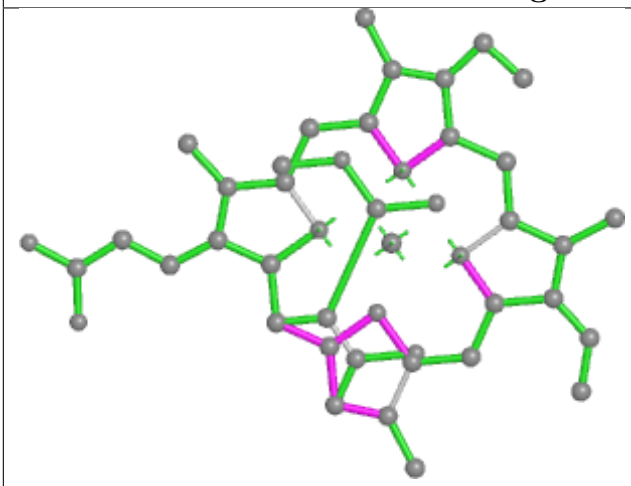


Rings

Ligand KC2 7 311



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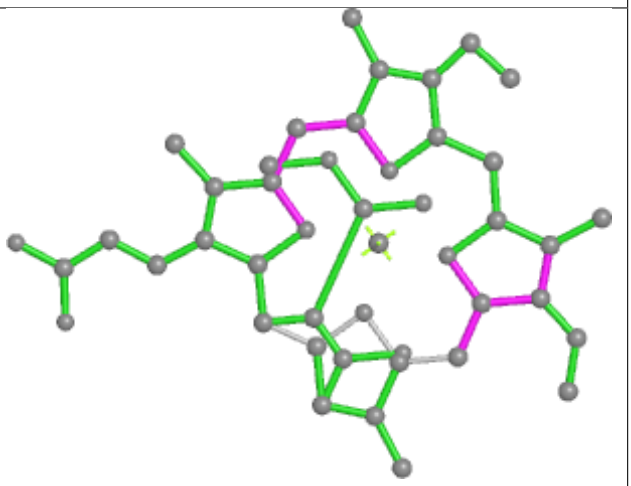

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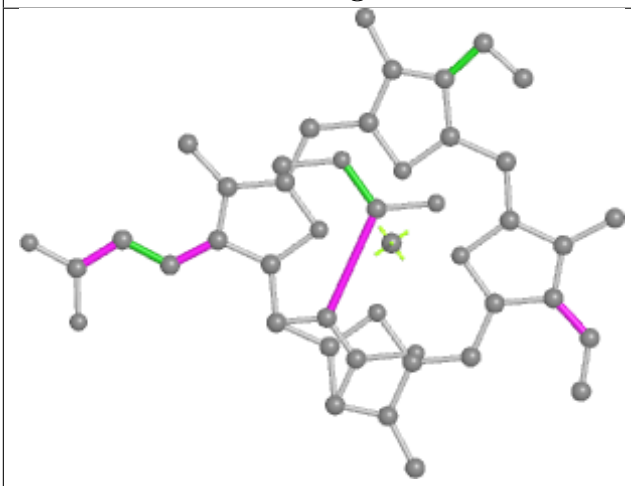

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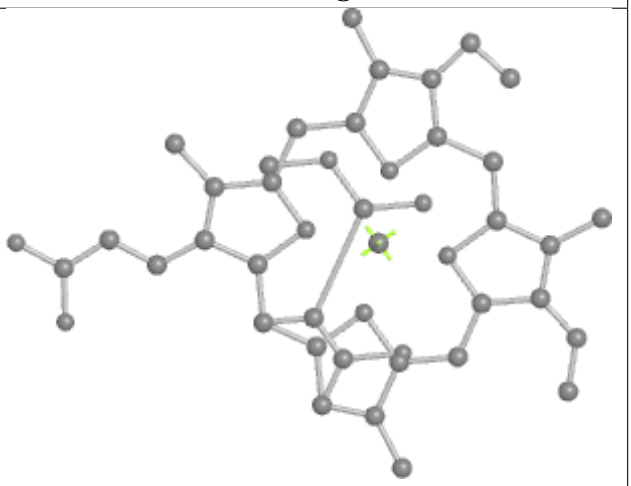
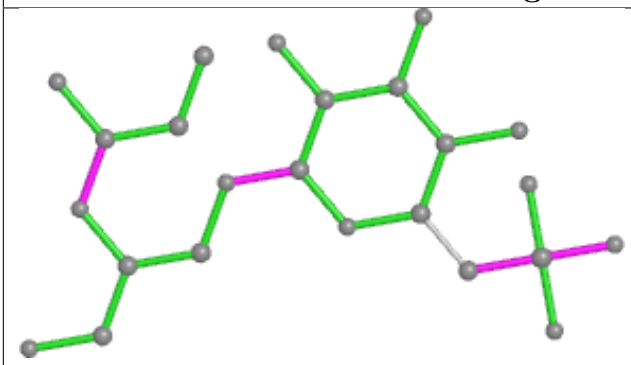


Rings

Ligand SQD O 207



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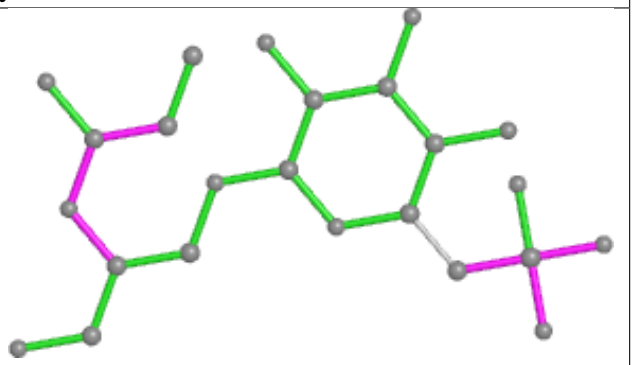

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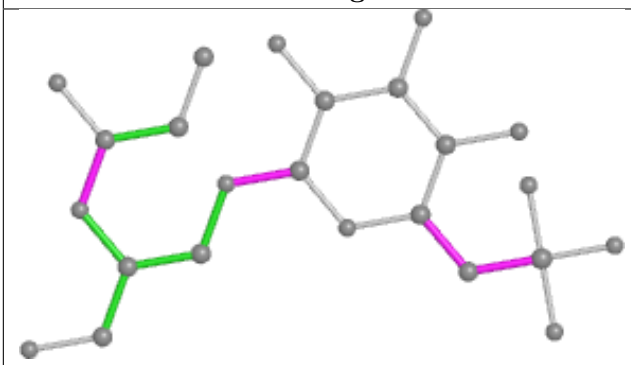

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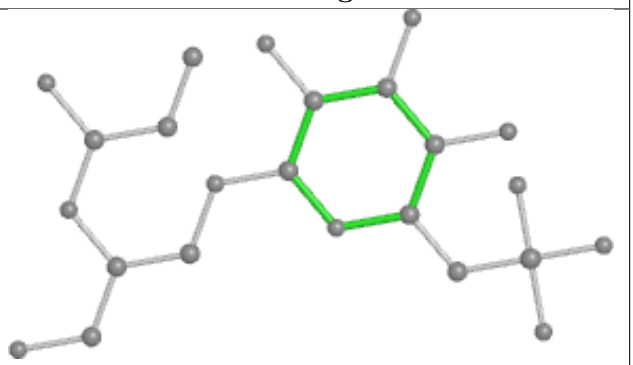
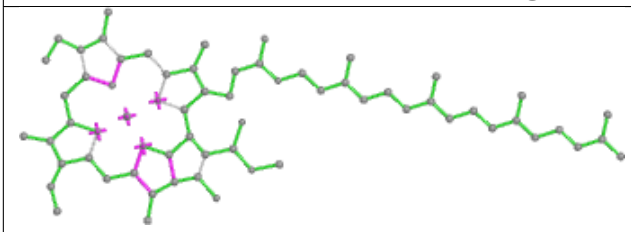


Rings

Ligand CLA A 822



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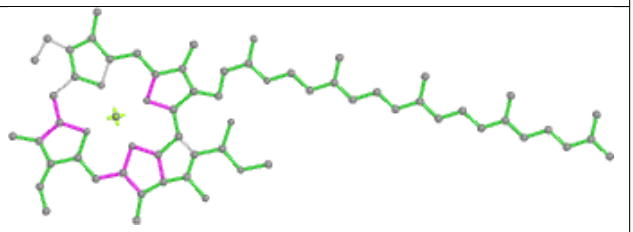

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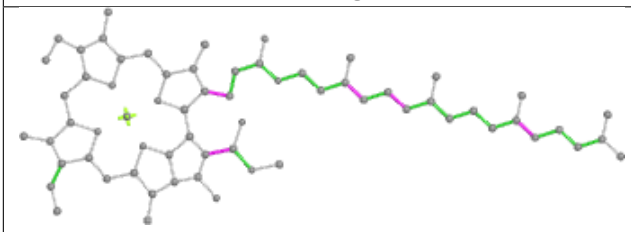

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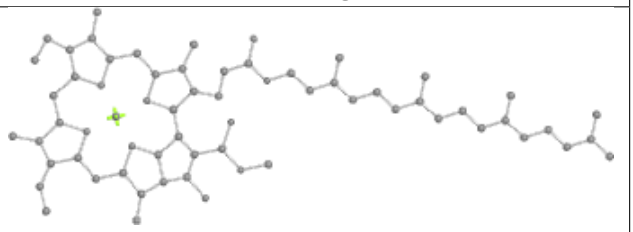
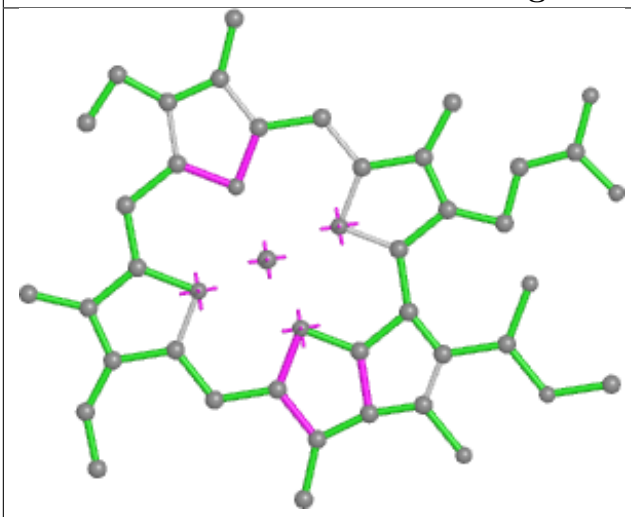


Rings

Ligand CLA 2 606



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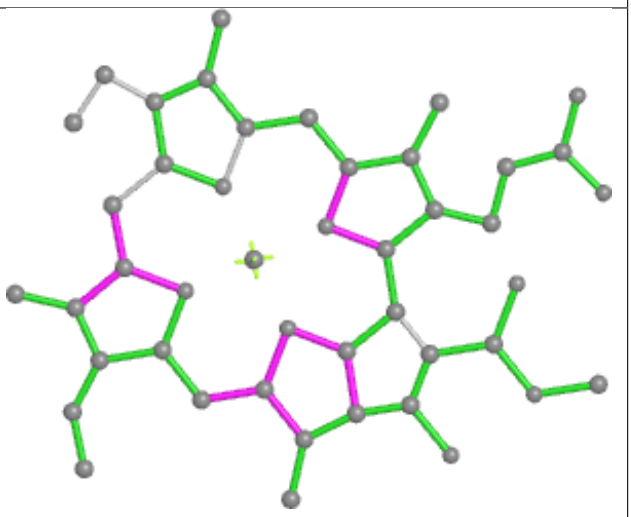

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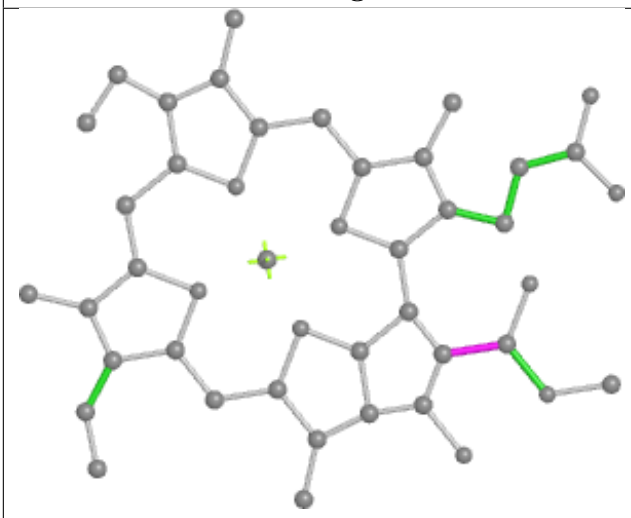

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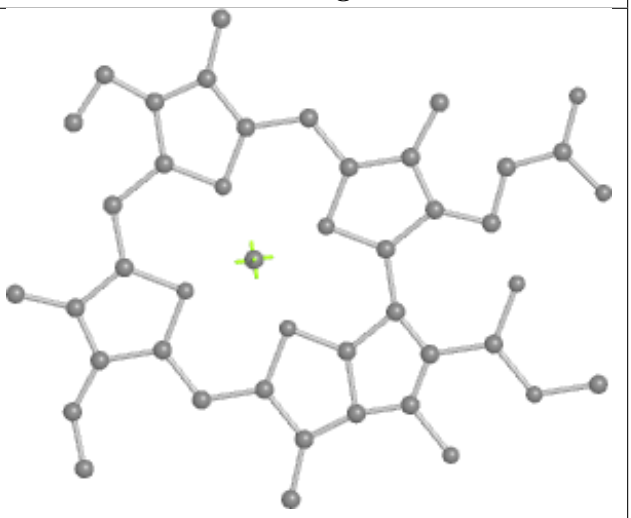
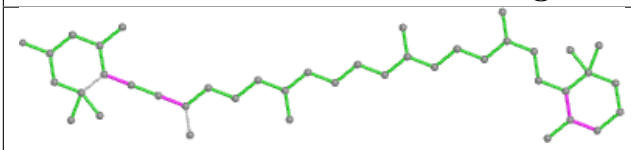


Rings

Ligand IHT 8 609



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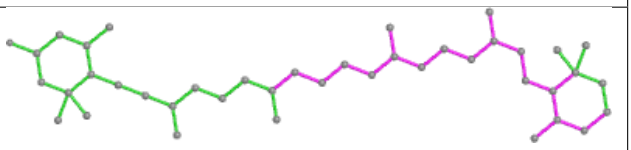

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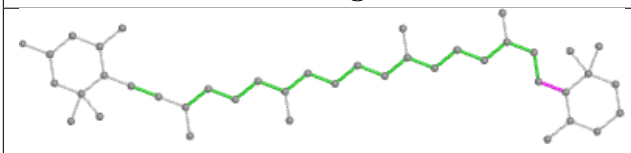

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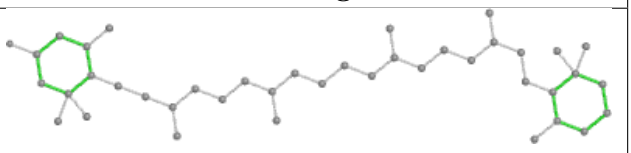
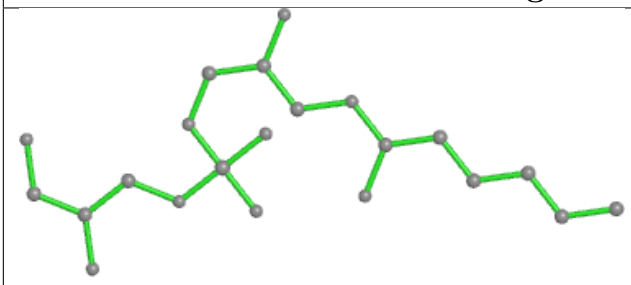


Rings

Ligand LHG 2 618



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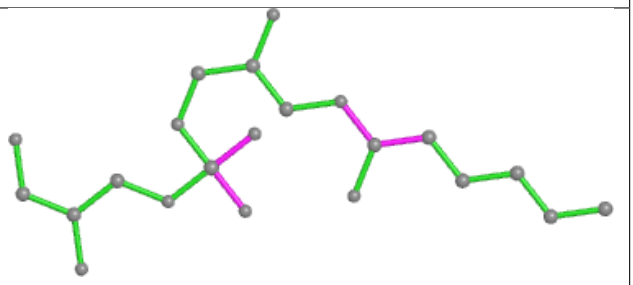

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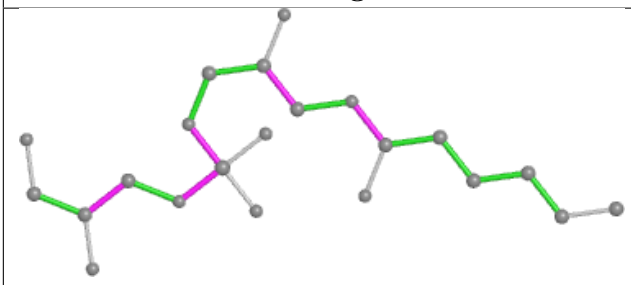

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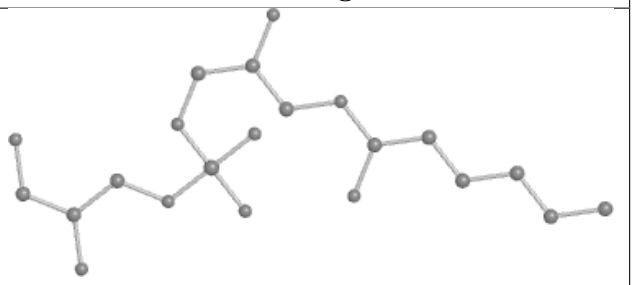

Rings

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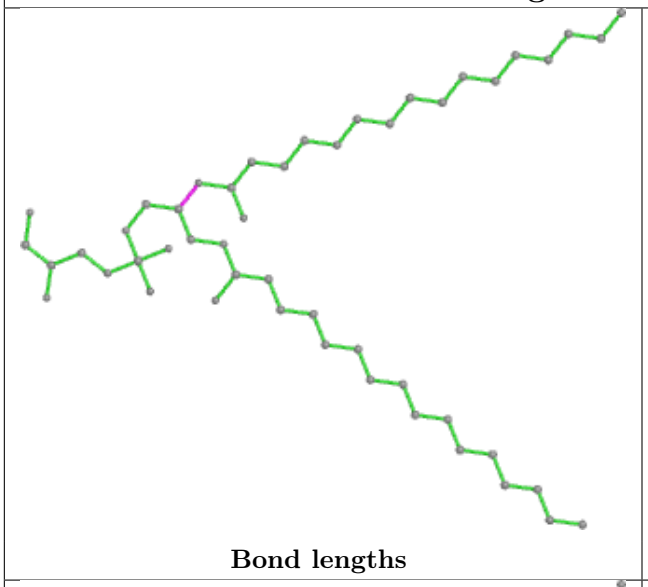

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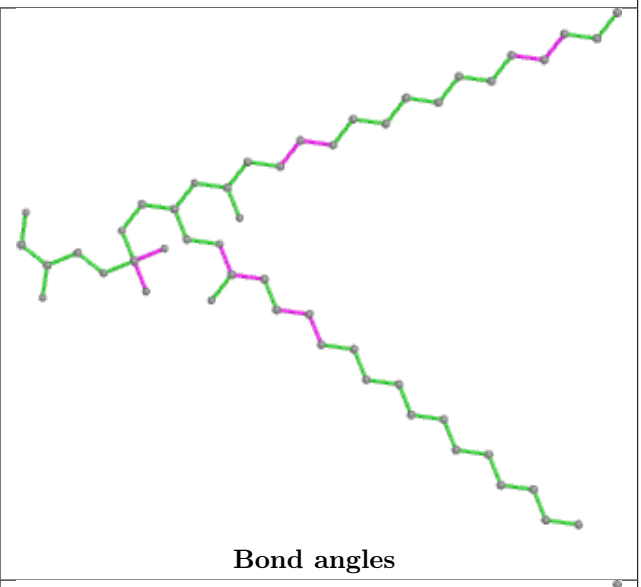
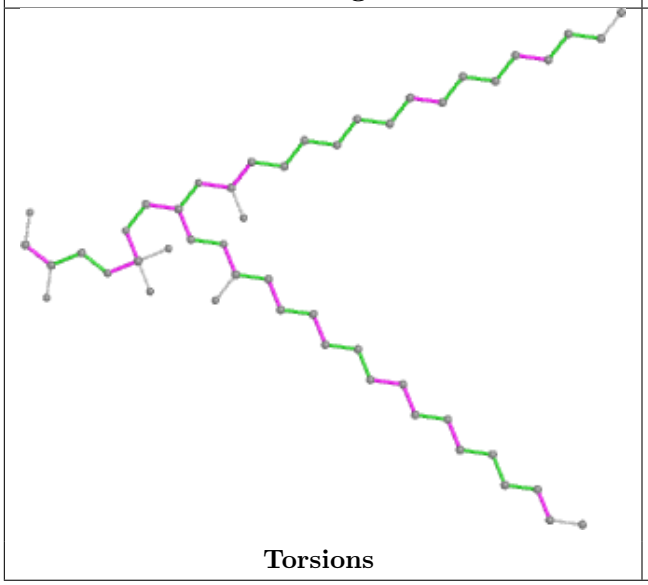


Bond angles



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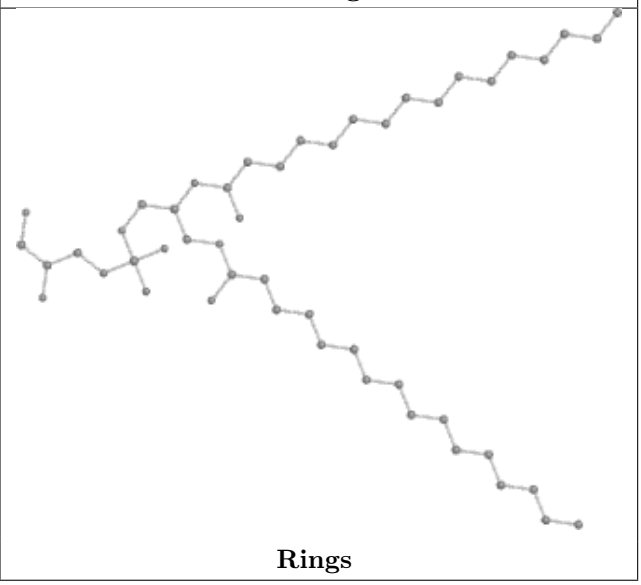

Rings

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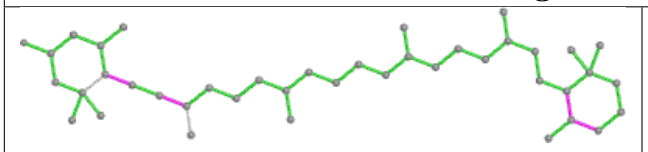

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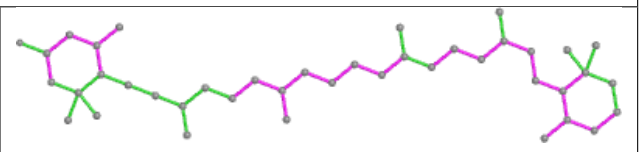
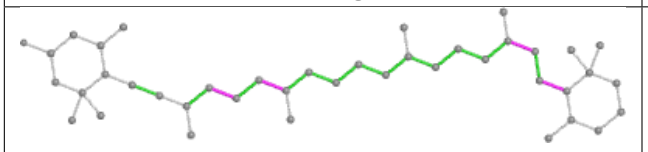


Bond angles



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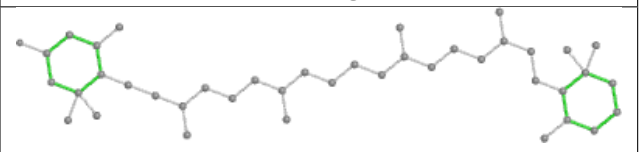
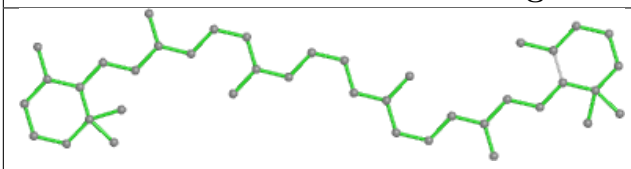
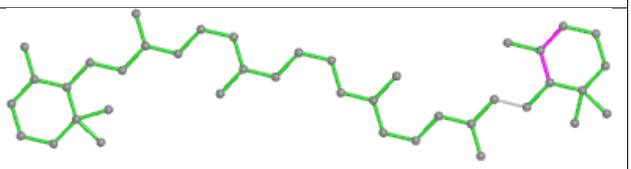
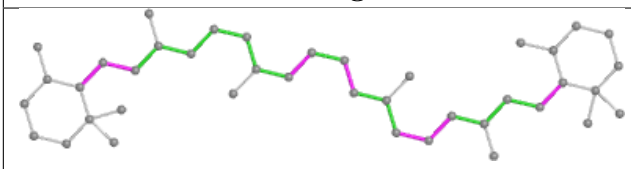
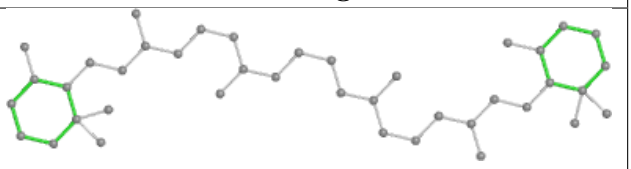
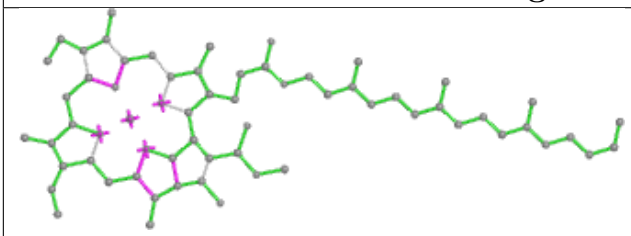
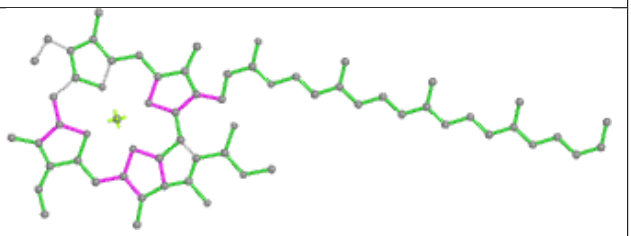
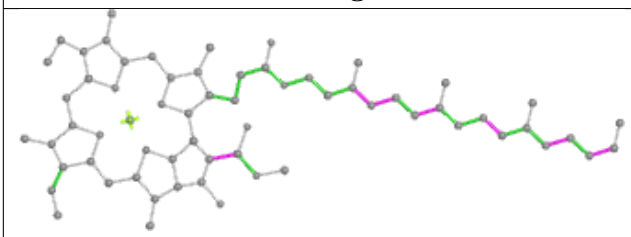
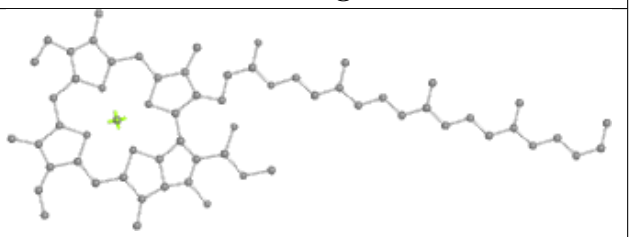
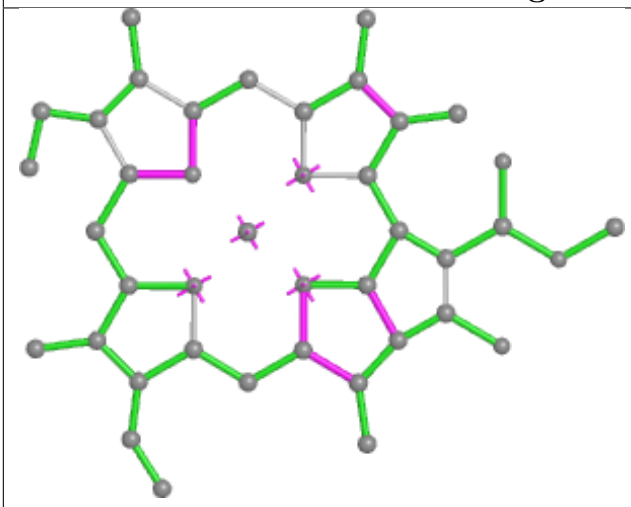


Rings

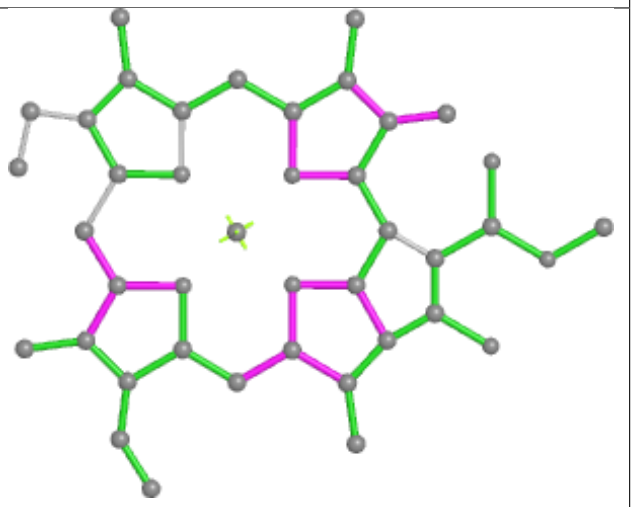
Ligand 8CT A 847	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA 9 606	
 Bond lengths	 Bond angles
 Torsions	 Rings

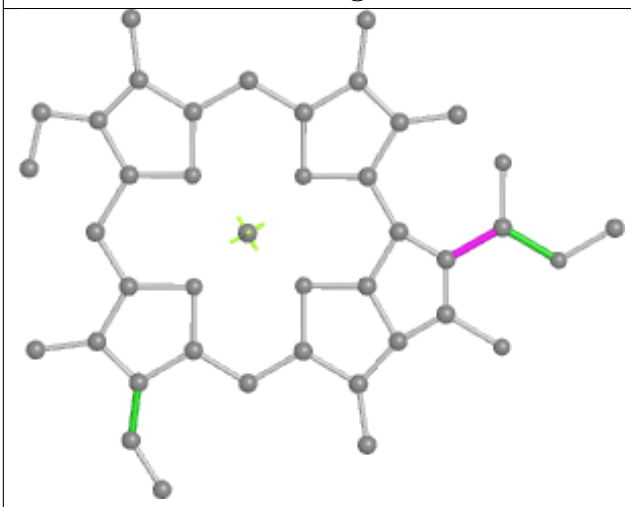
Ligand CLA 5 613



Bond lengths



Bond angles



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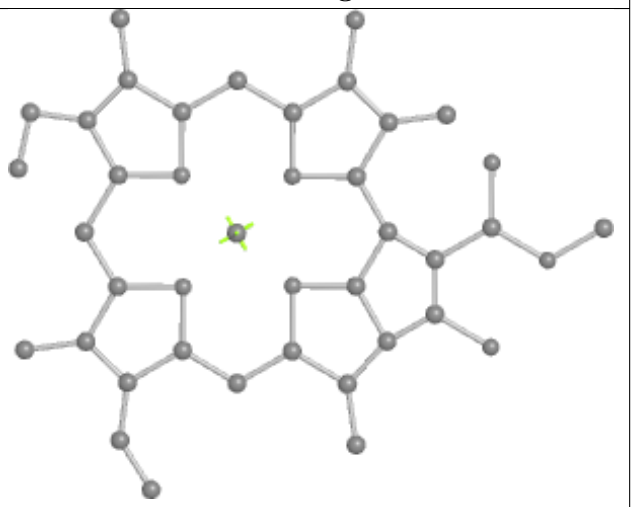
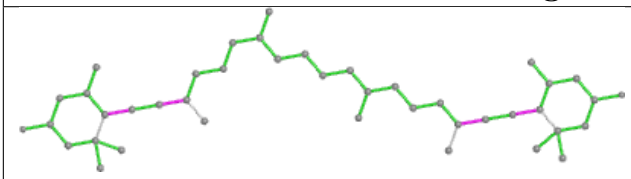


Rings

Ligand II0 3 615



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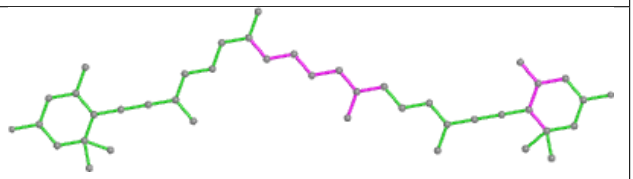
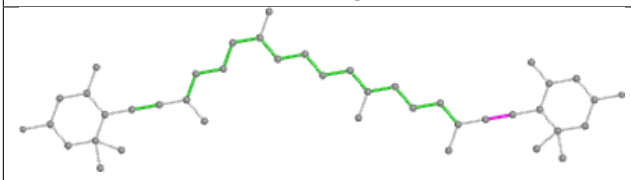


Bond angles



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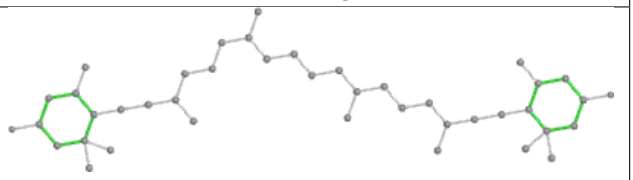
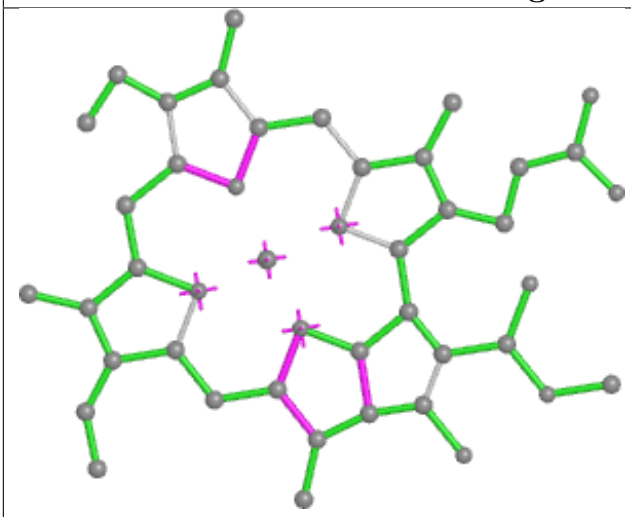
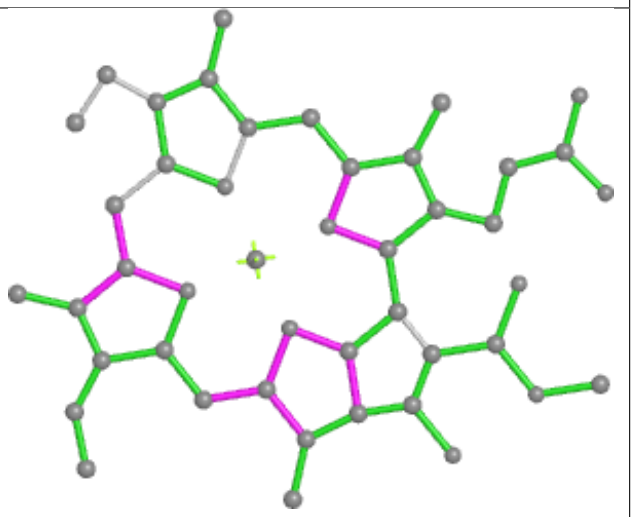


Rings

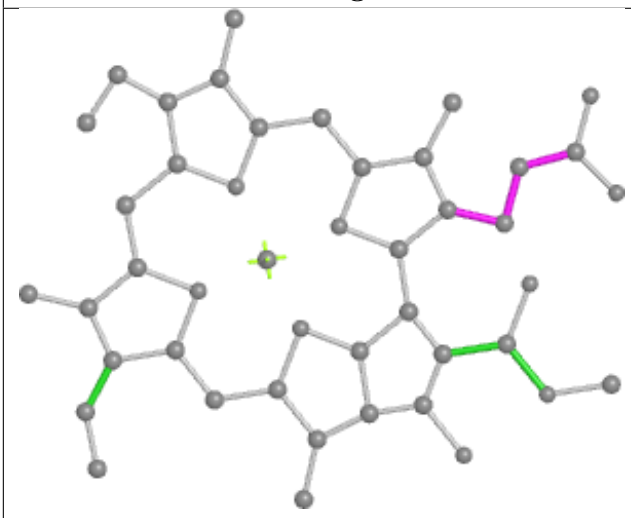
Ligand CLA 6 603



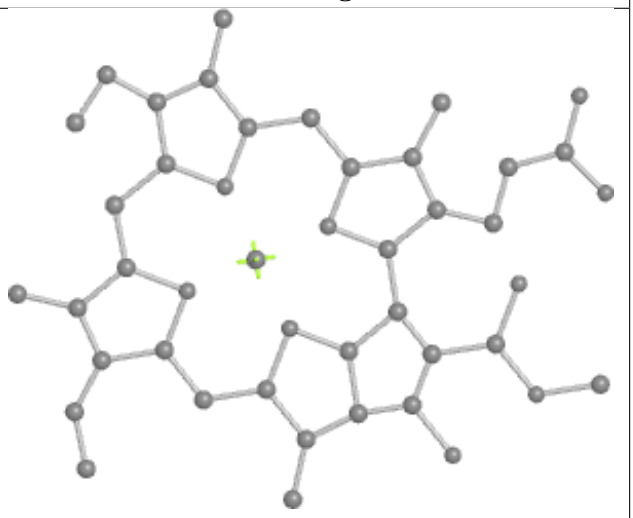
Bond lengths



Bond angles

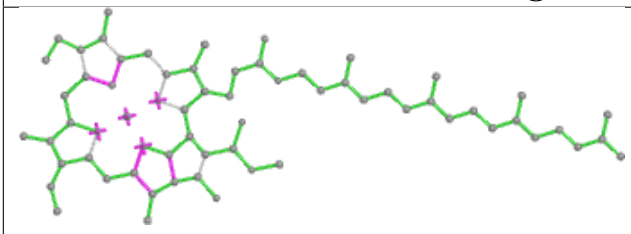


Torsions

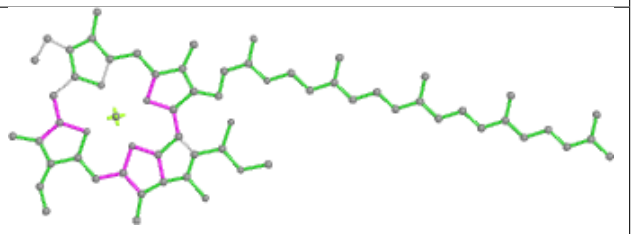


Rings

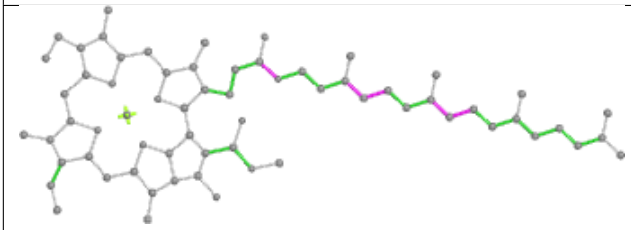
Ligand CLA b 608



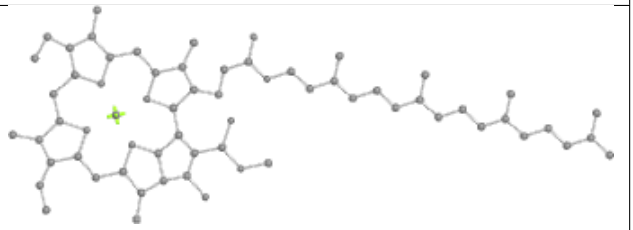
Bond lengths



Bond angles

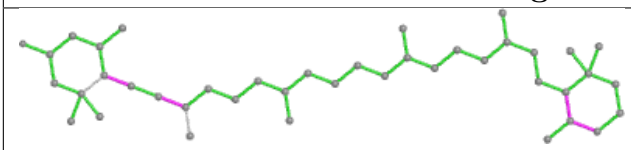


Torsions



Rings

Ligand IHT L 204



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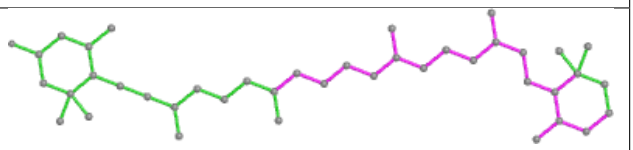

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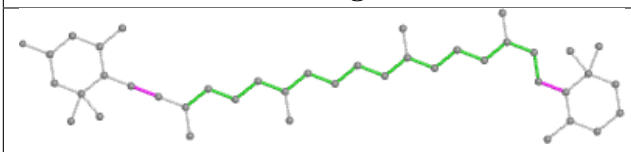

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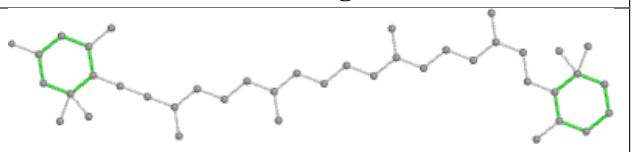
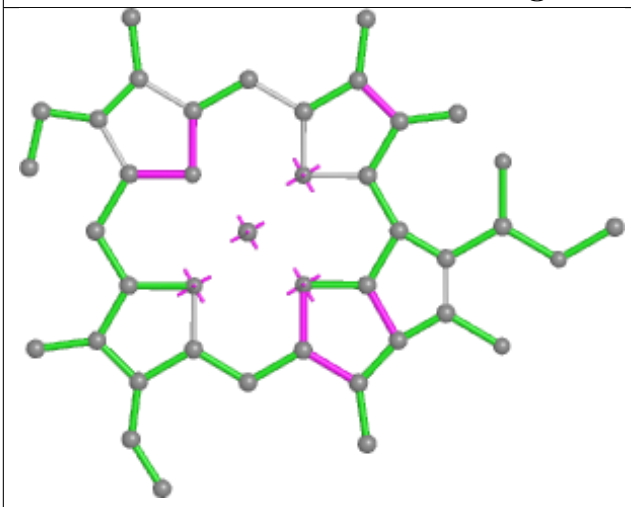


Rings

Ligand CLA 5 609



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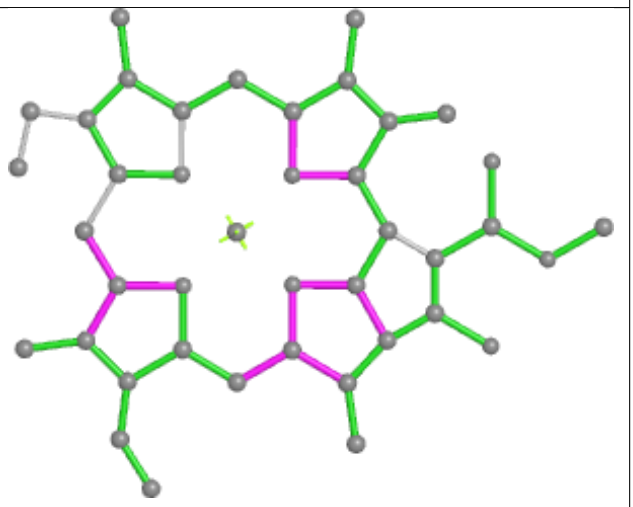

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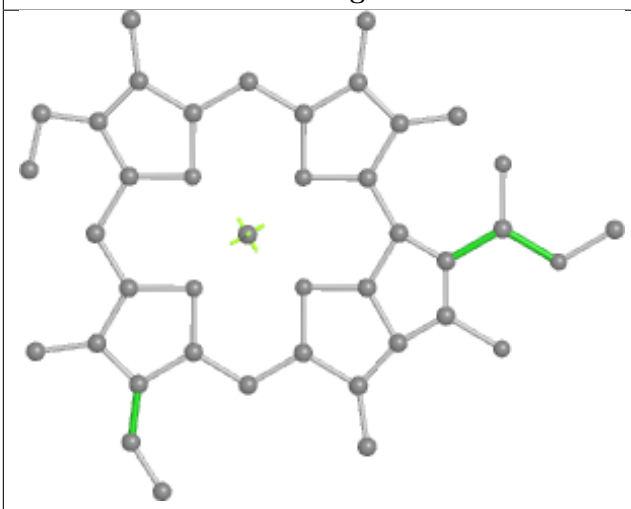

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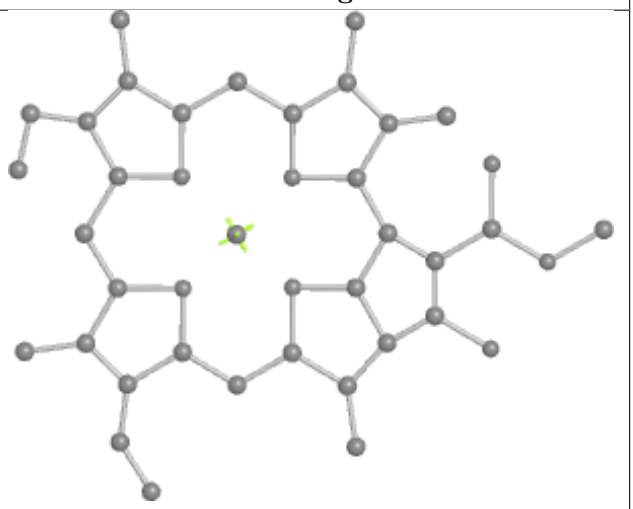
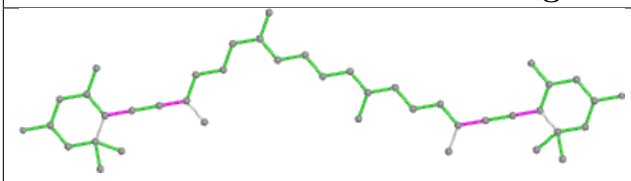


Rings

Ligand II0 7 314



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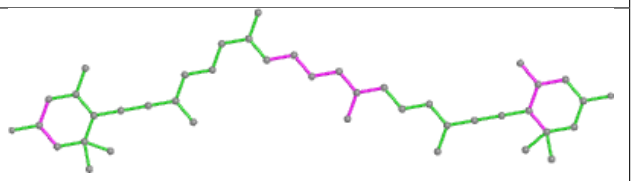

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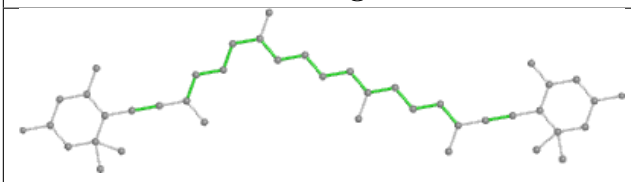

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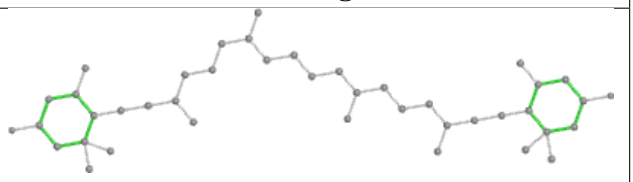
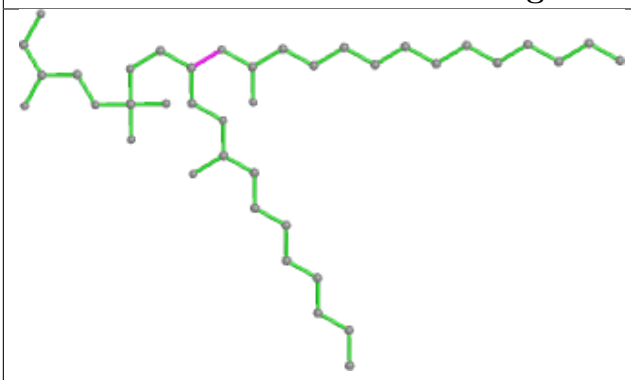


Rings

Ligand LHG 2 619



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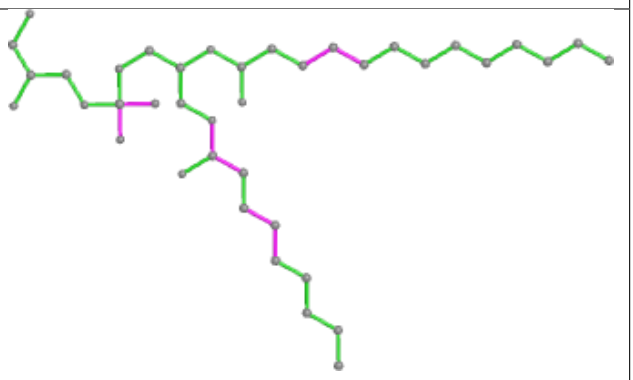

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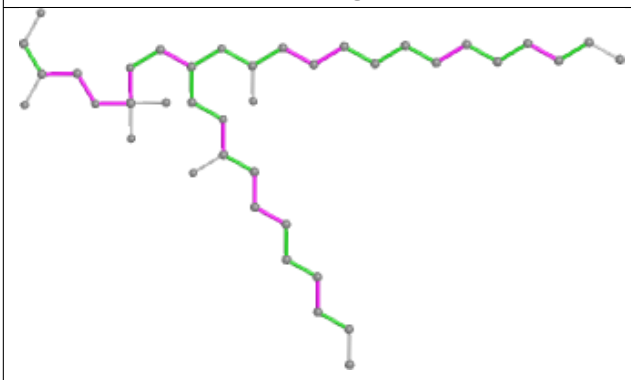

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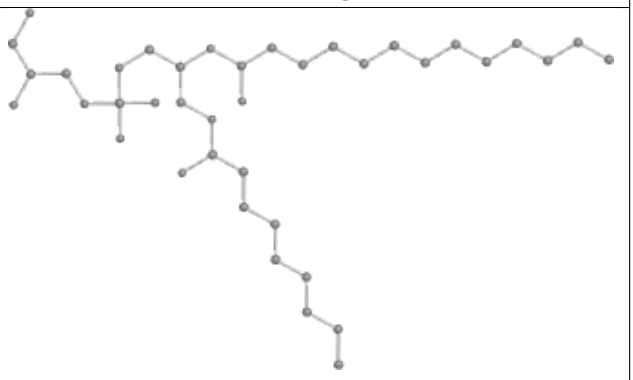
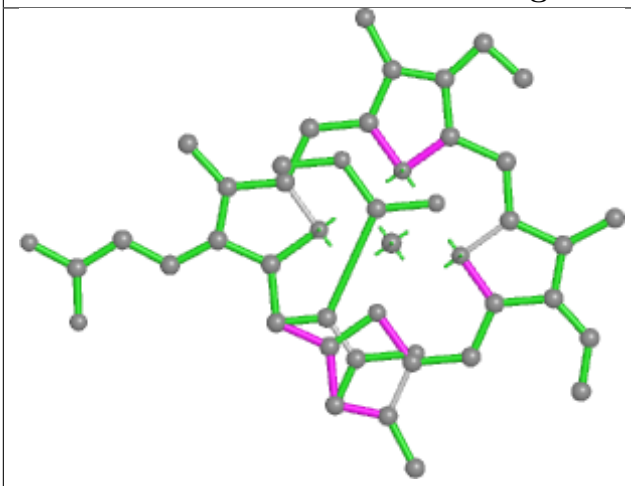


Rings

Ligand KC2 2 610



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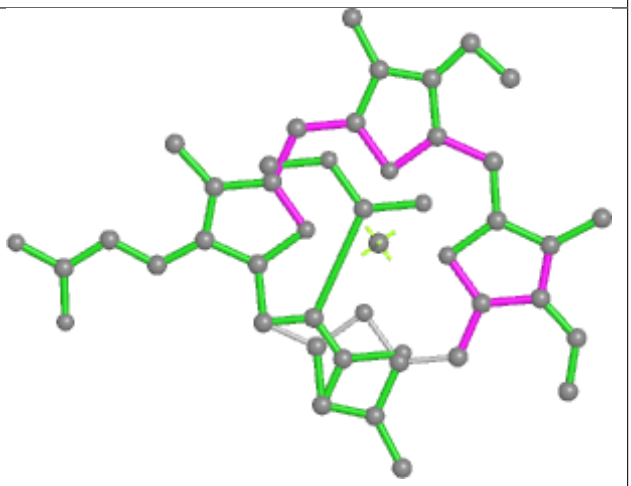

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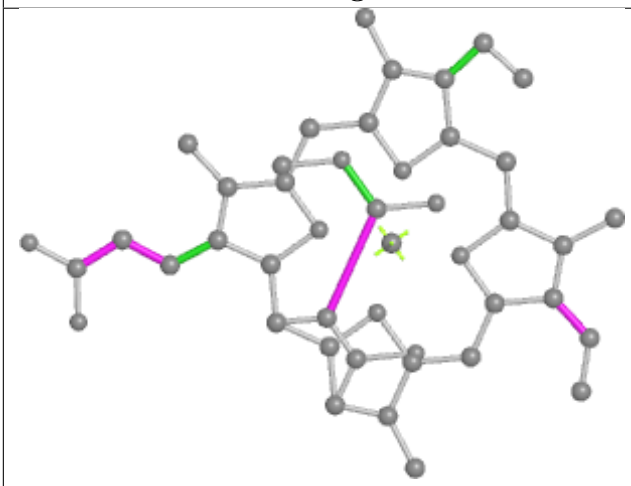

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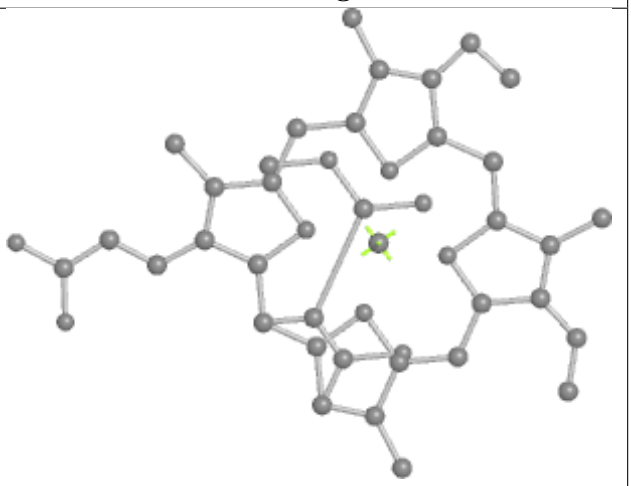
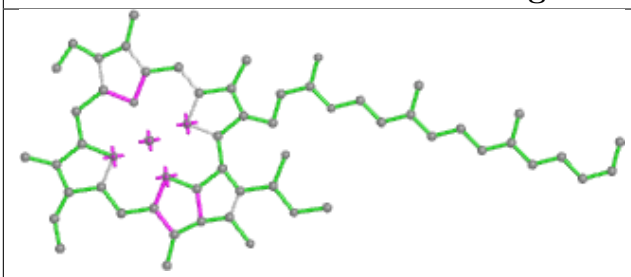


Rings

Ligand CLA 1 602



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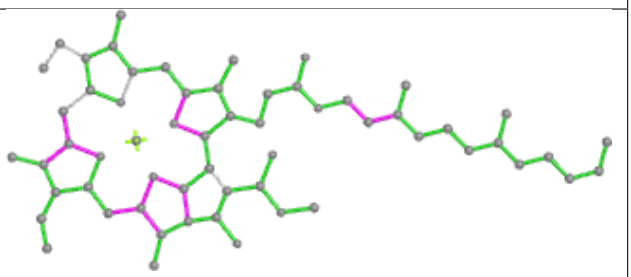
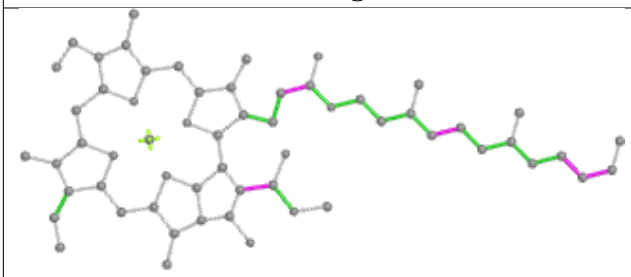


Bond angles



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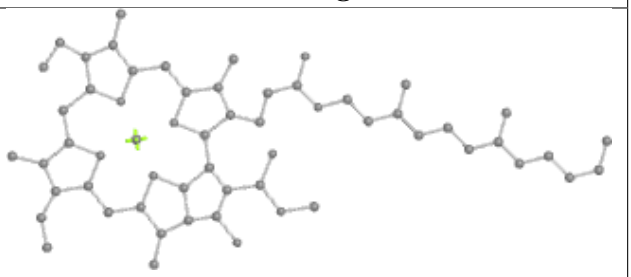
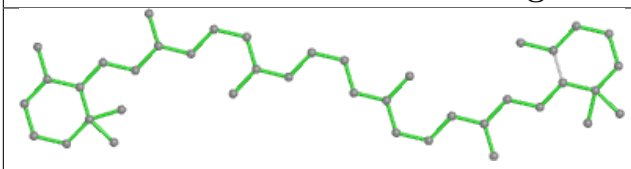
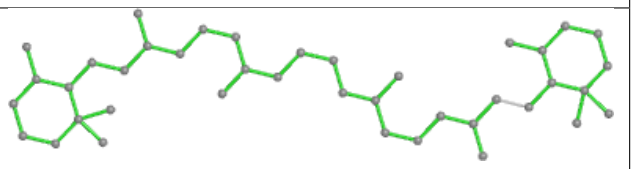
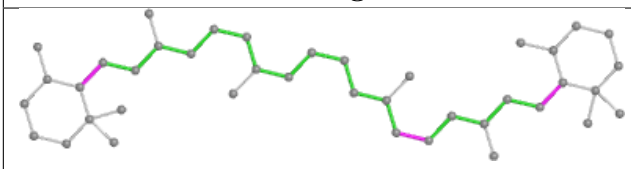
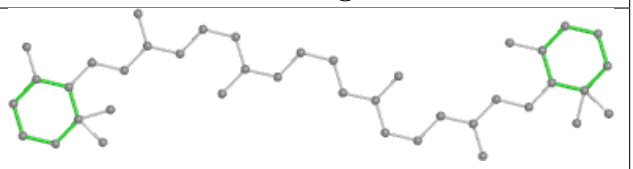
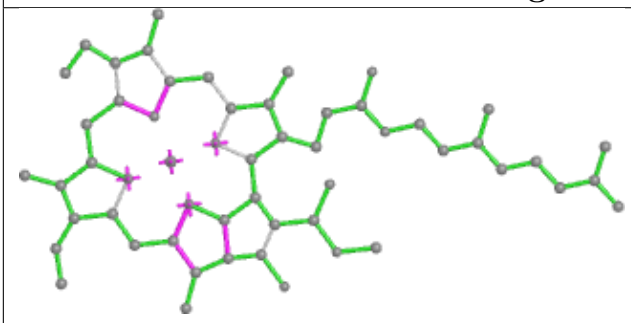
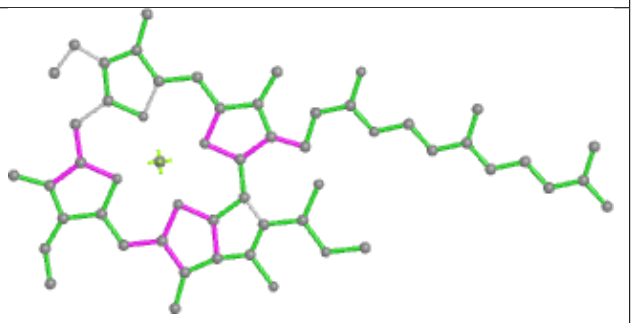
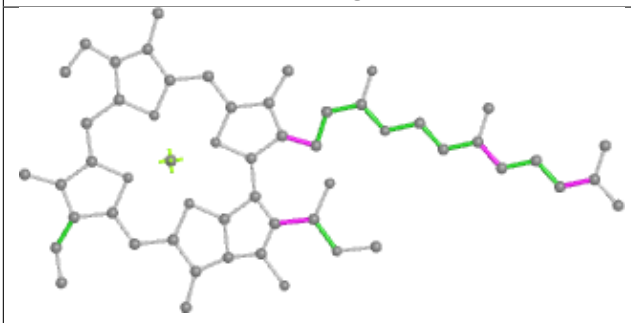
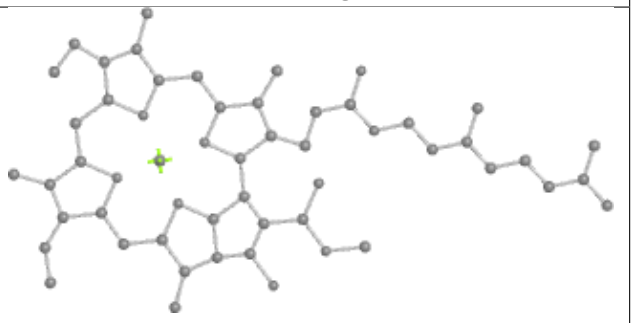
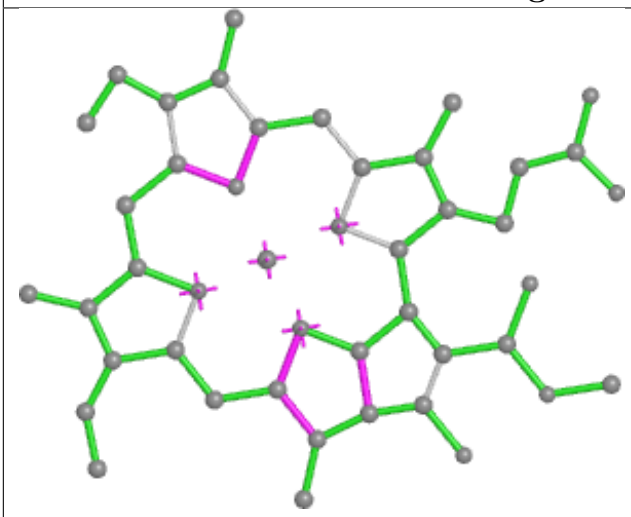


Rings

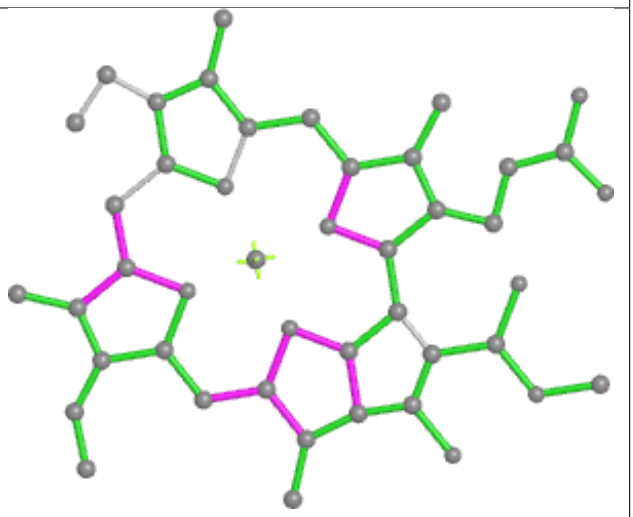
Ligand 8CT B 847	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA 9 602	
 Bond lengths	 Bond angles
 Torsions	 Rings

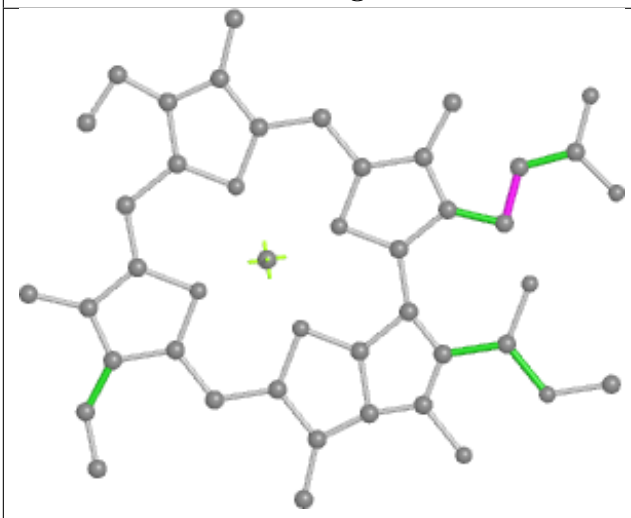
Ligand CLA 1 604



Bond lengths



Bond angles



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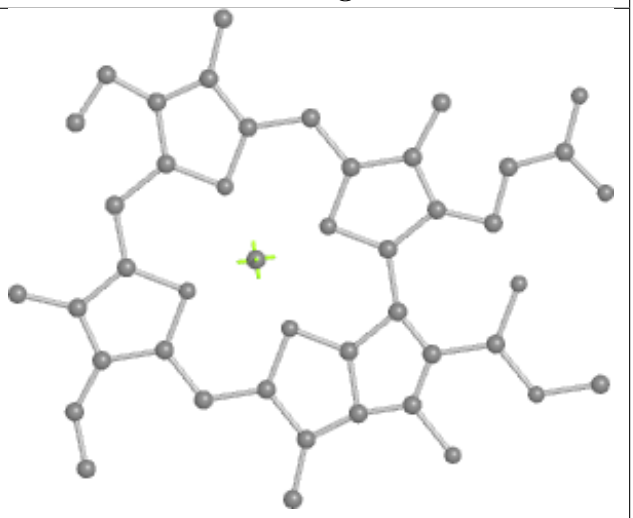
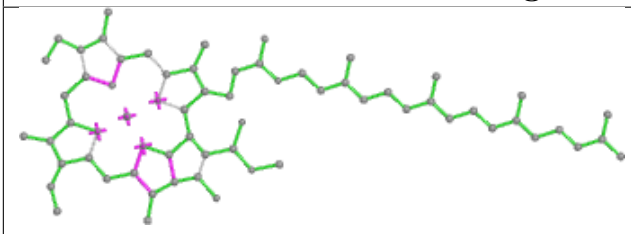


Rings

Ligand CLA K 101



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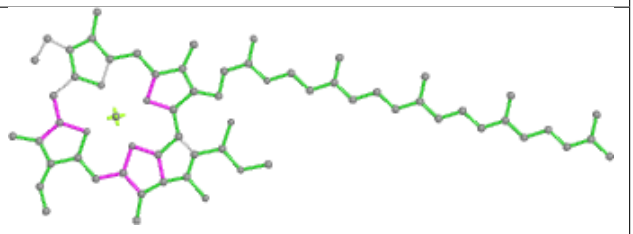
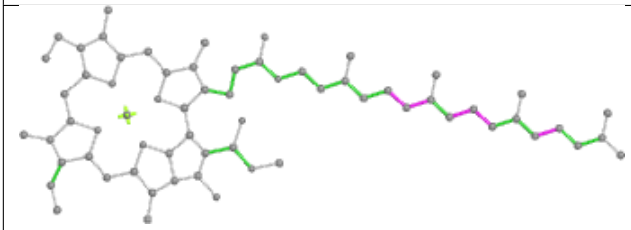


Bond angles



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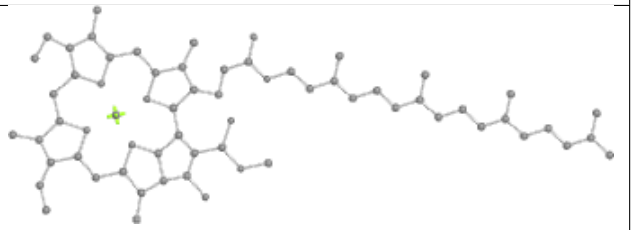
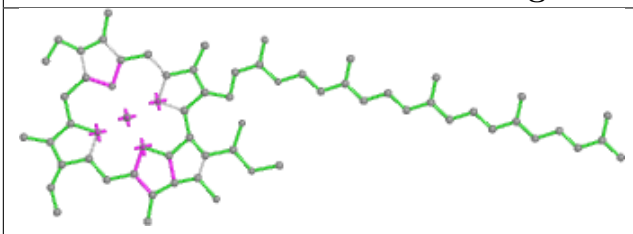


Rings

Ligand CLA 8 603



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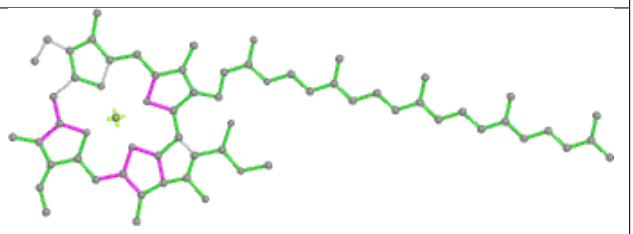
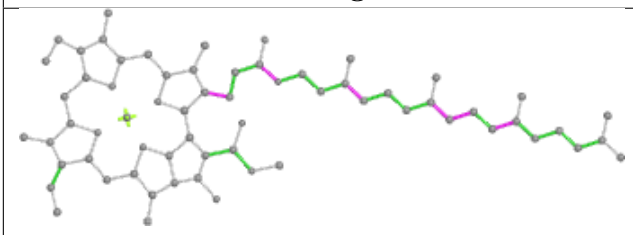


Bond angles



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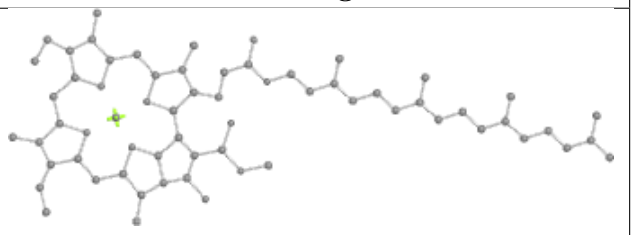
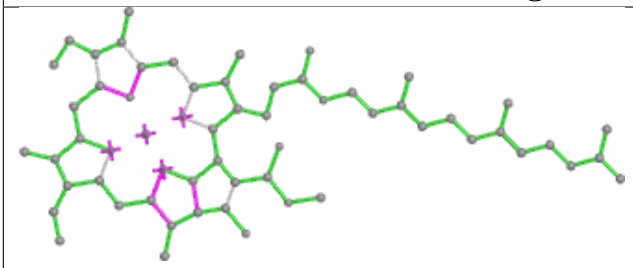
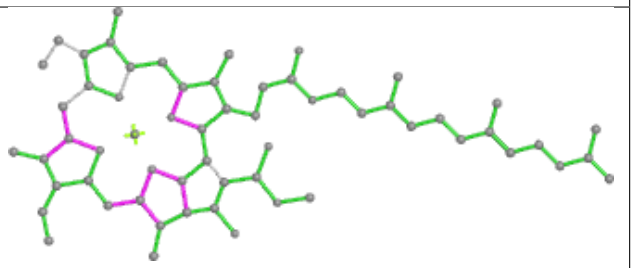


Rings

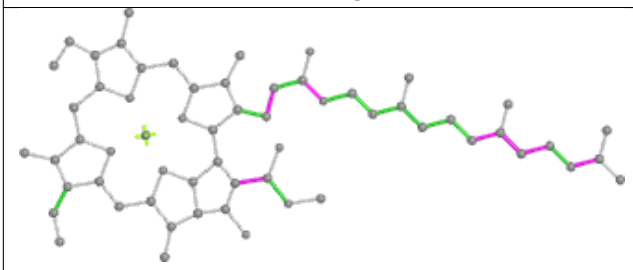
Ligand CLA Z 301



Bond lengths



Bond angles



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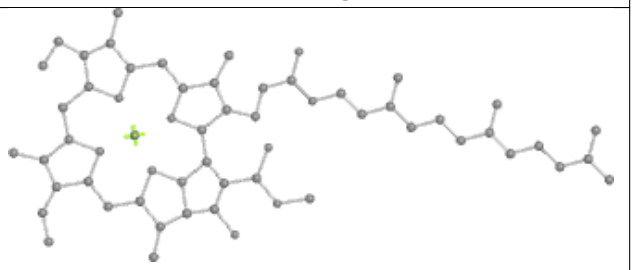
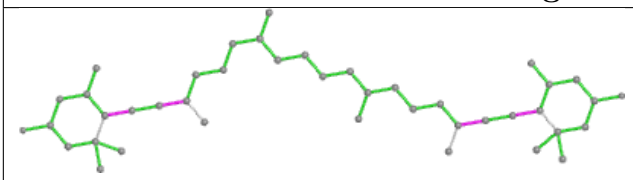
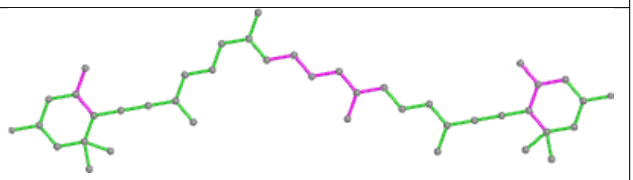


Rings

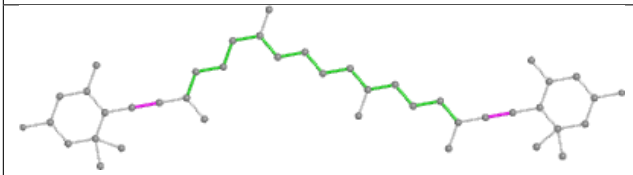
Ligand II0 9 617



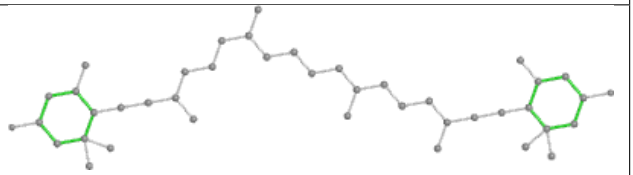
Bond lengths



Bond angles

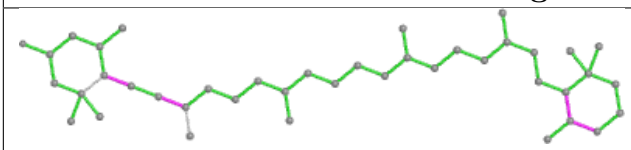


Torsions

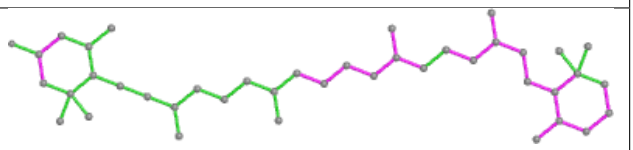


Rings

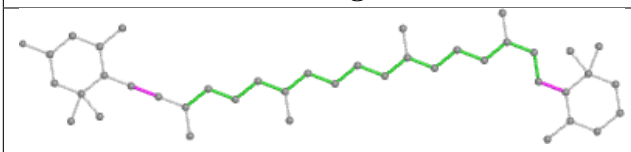
Ligand IHT Z 302



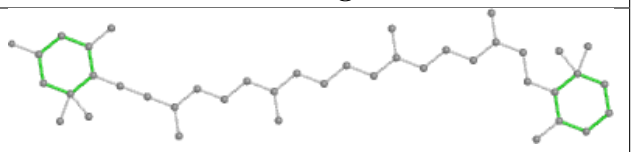
Bond lengths



Bond angles

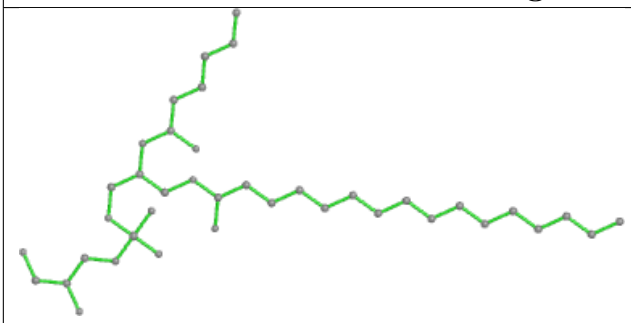


Torsions

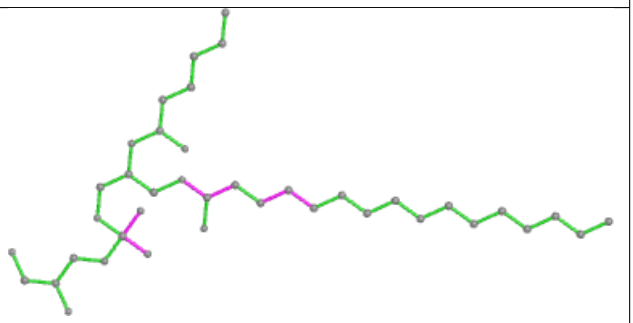


Rings

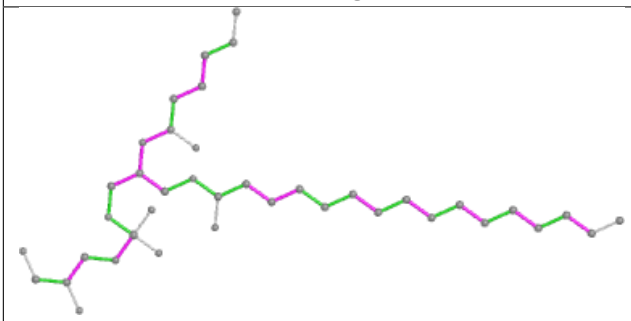
Ligand LHG 7 320



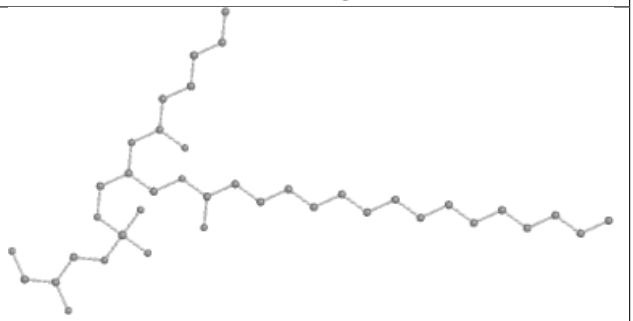
Bond lengths



Bond angles

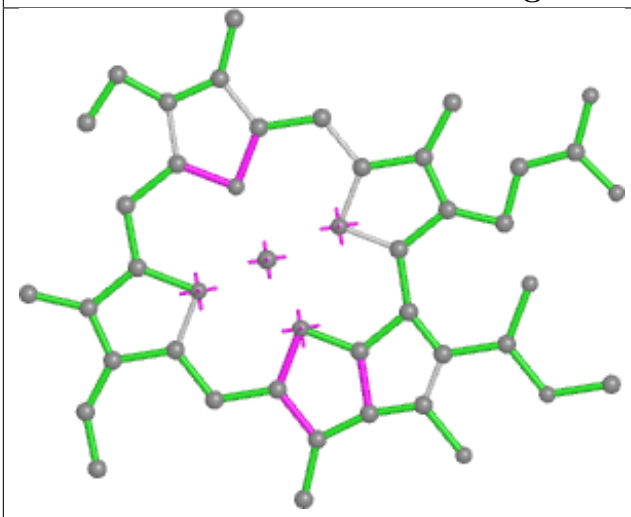


Torsions

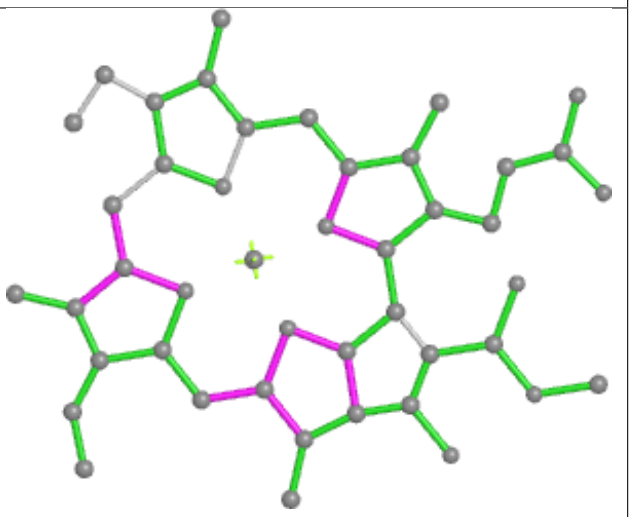


Rings

Ligand CLA A 814



Bond lengths



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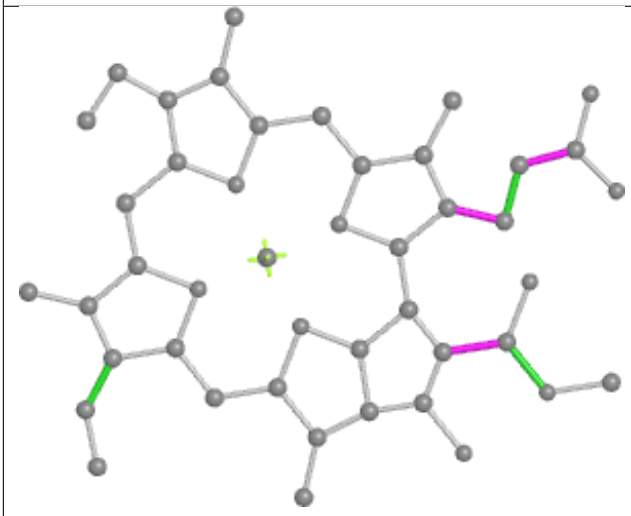

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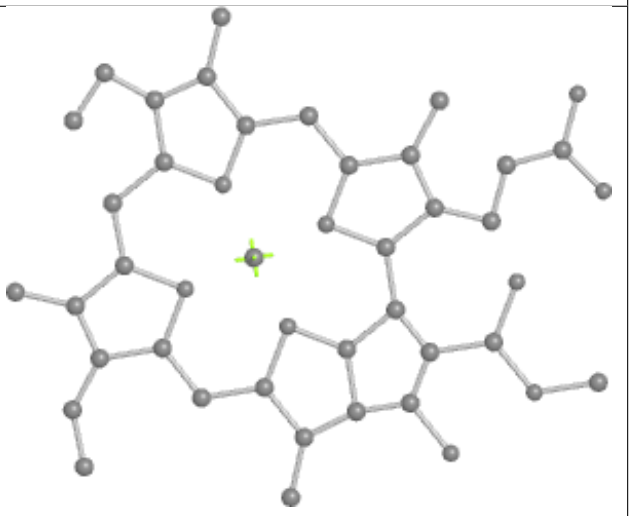
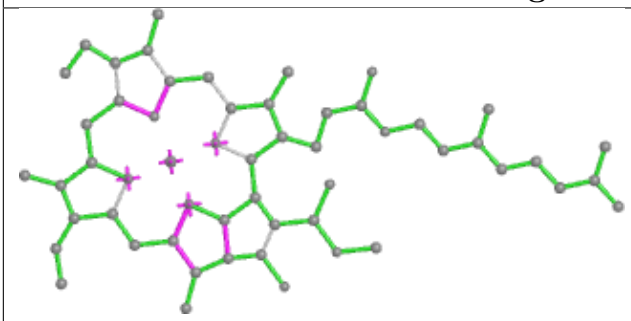
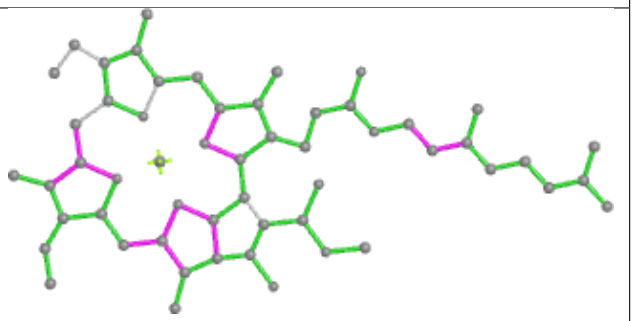


Rings

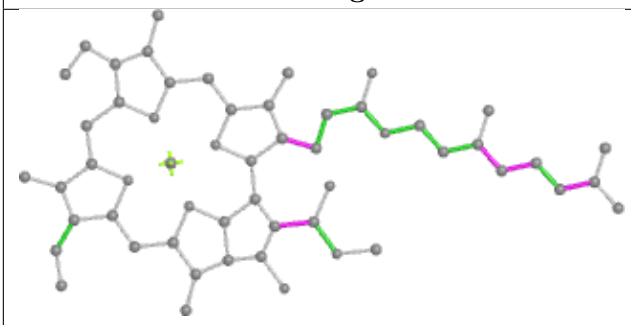
Ligand CLA 9 608



Bond lengths



Bond angles



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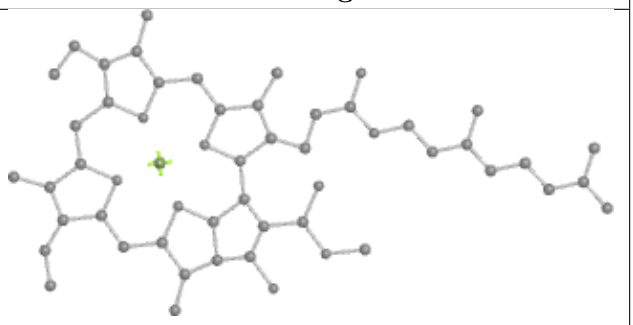
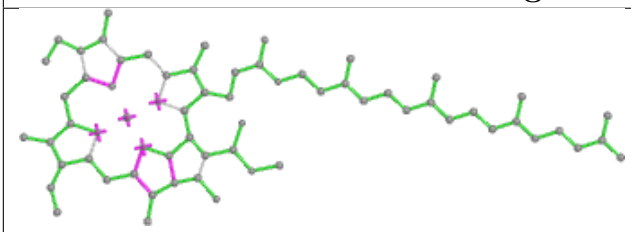


Rings

Ligand CLA B 801



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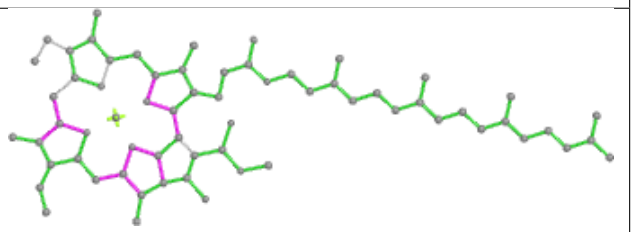
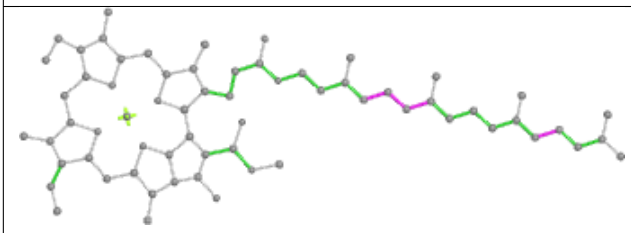
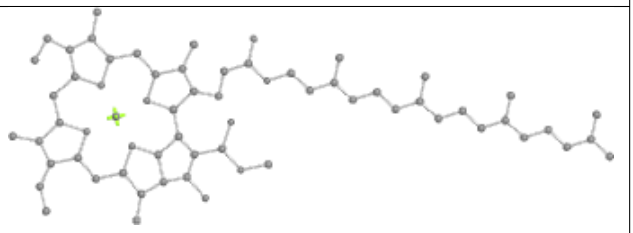


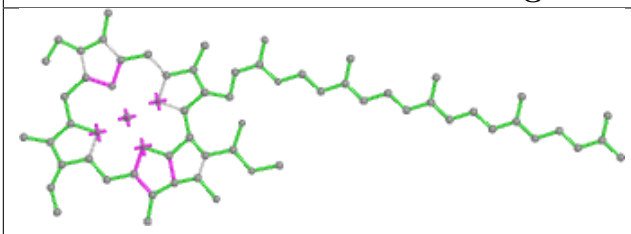
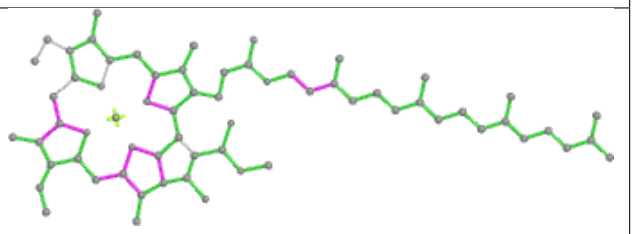
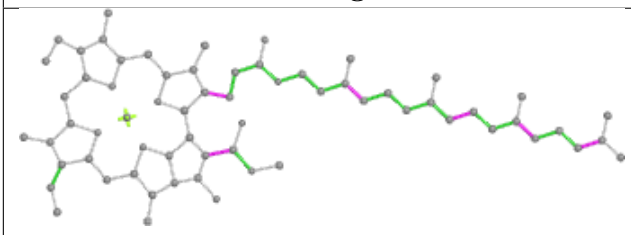
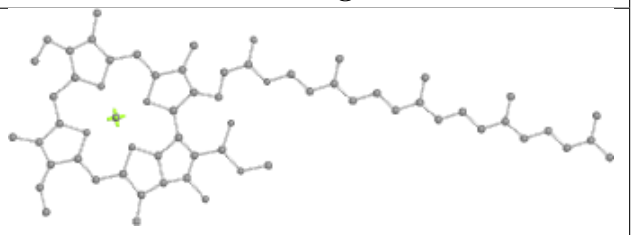
Bond angles

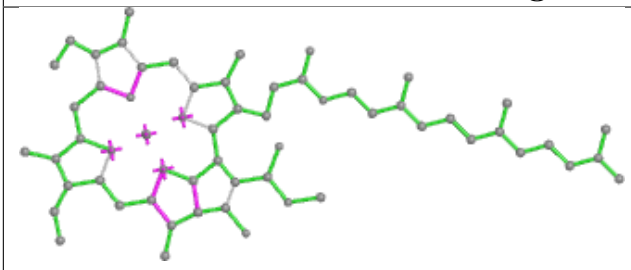
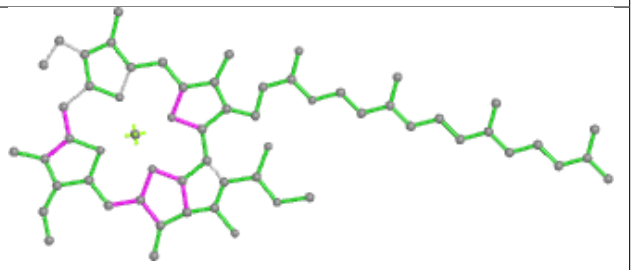
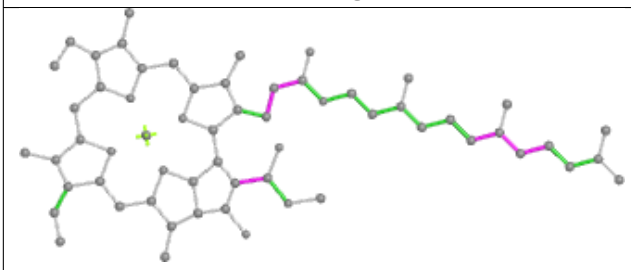
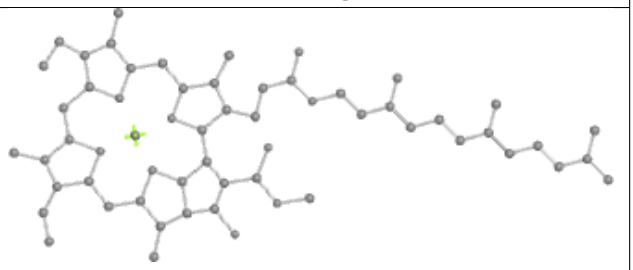


Torsions

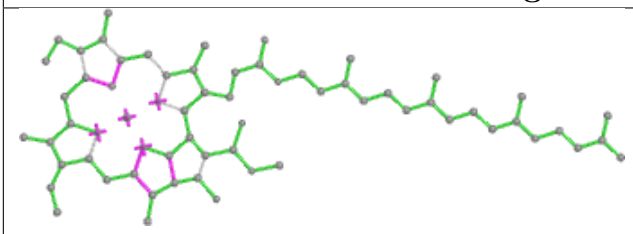


Rings

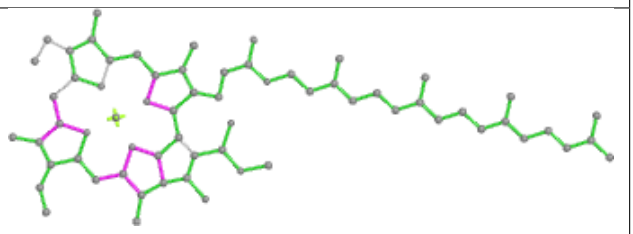
Ligand CLA B 815	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA a 604	
 Bond lengths	 Bond angles
 Torsions	 Rings

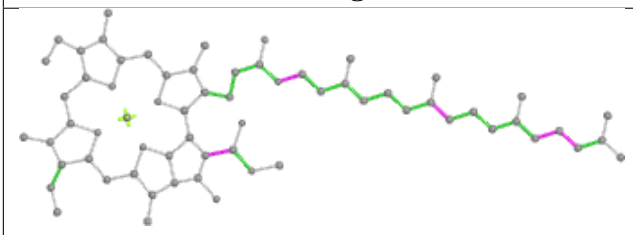
Ligand CLA A 832



Bond lengths



Bond angles



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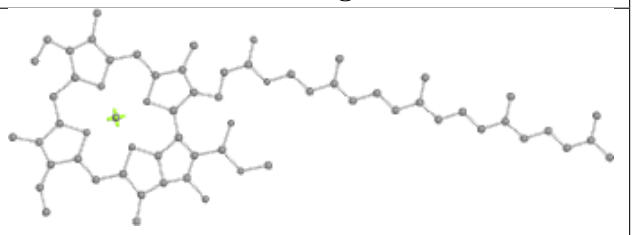
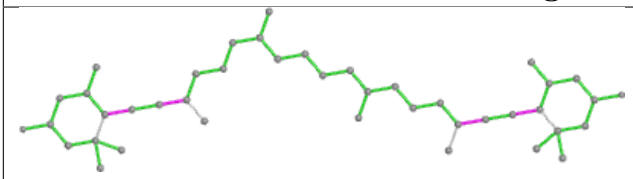


Rings

Ligand II0 7 316



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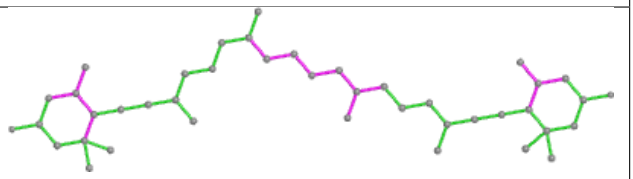
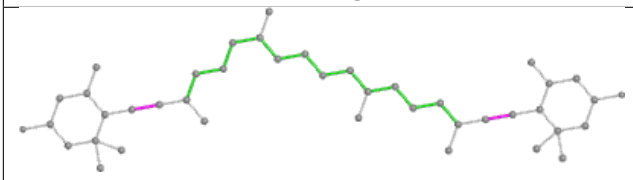


Bond angles



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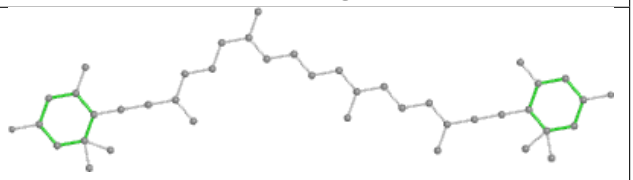
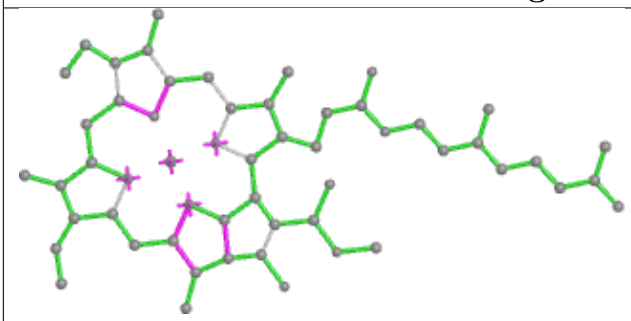
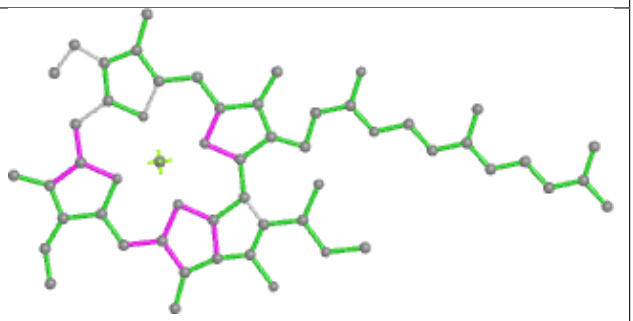


Rings

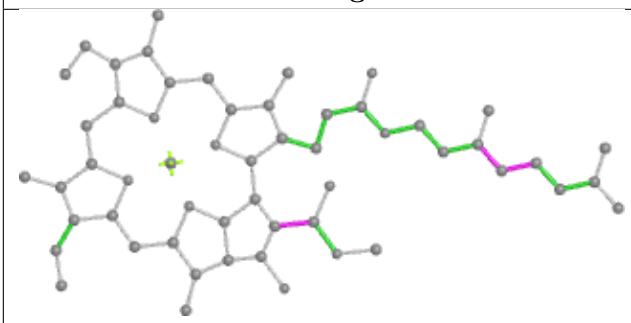
Ligand CLA 5 602



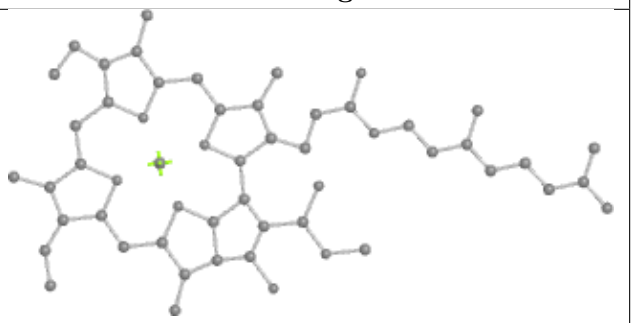
Bond lengths



Bond angles

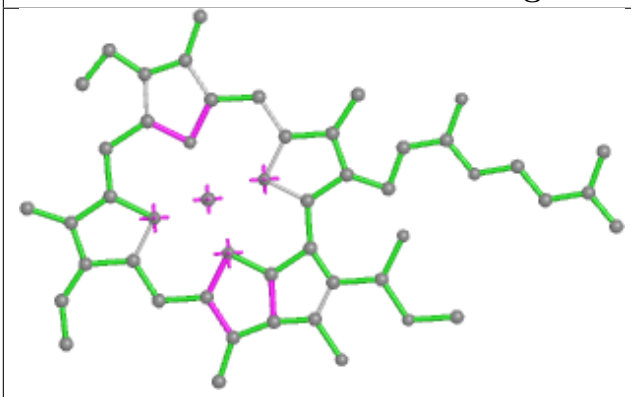


Torsions

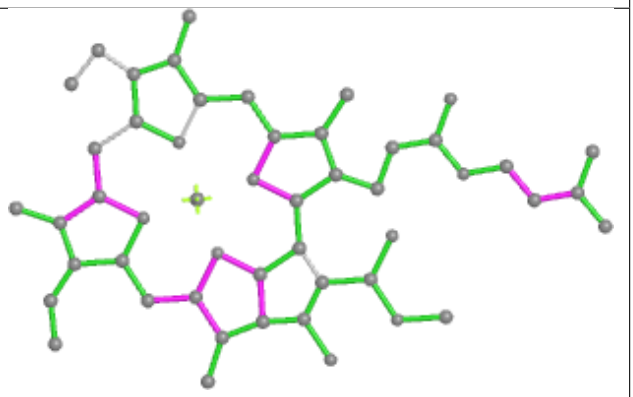


Rings

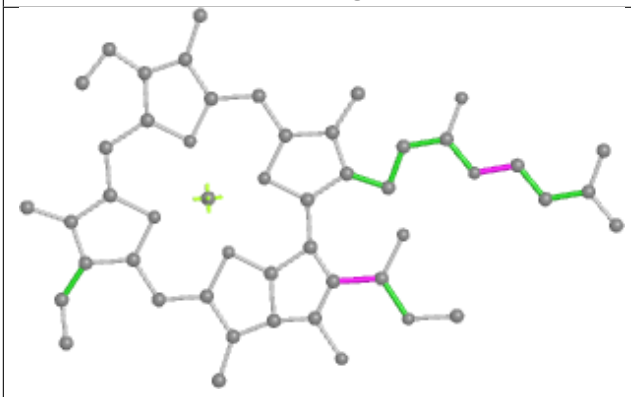
Ligand CLA A 807



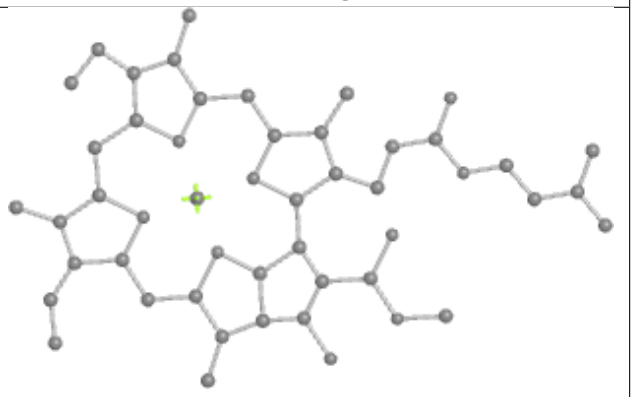
Bond lengths



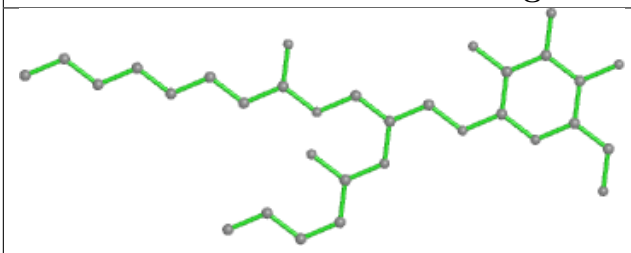
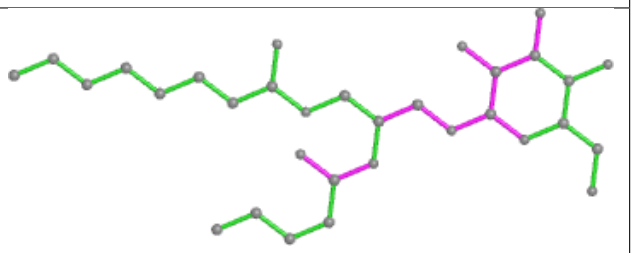
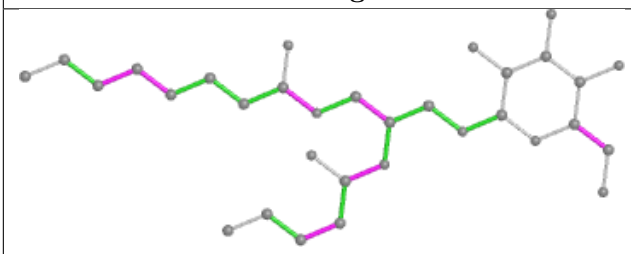
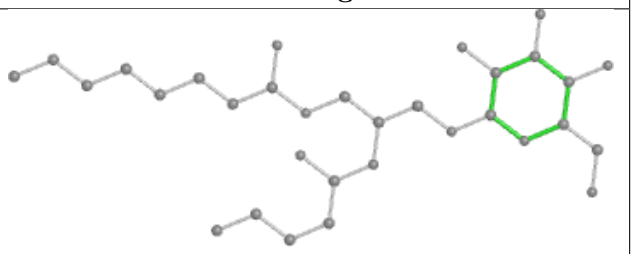
Bond angles

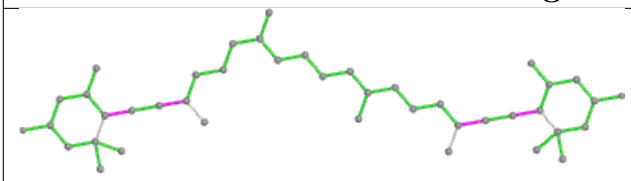
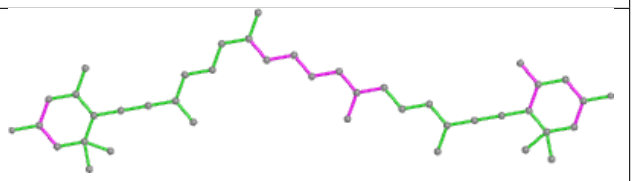
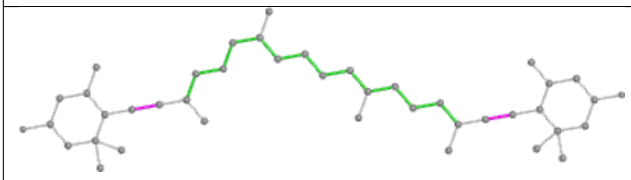
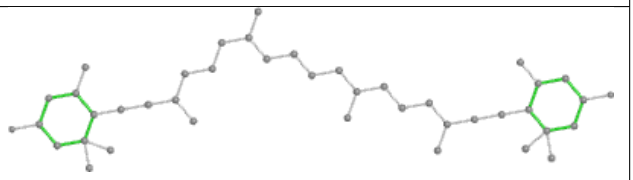


Torsions

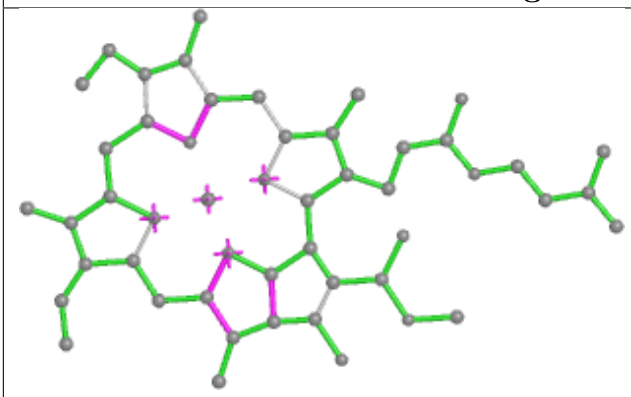


Rings

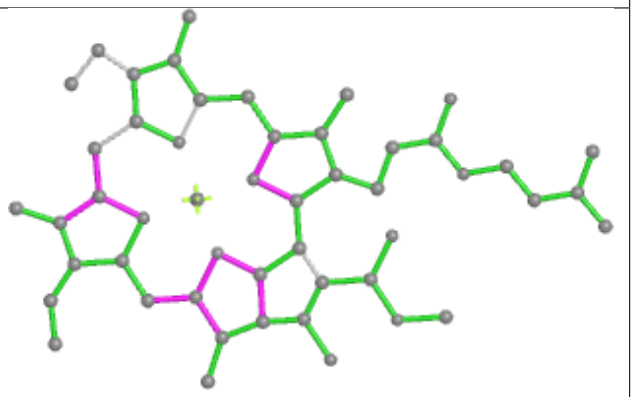
Ligand LMG 3 620	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand II0 a 613	
 Bond lengths	 Bond angles
 Torsions	 Rings

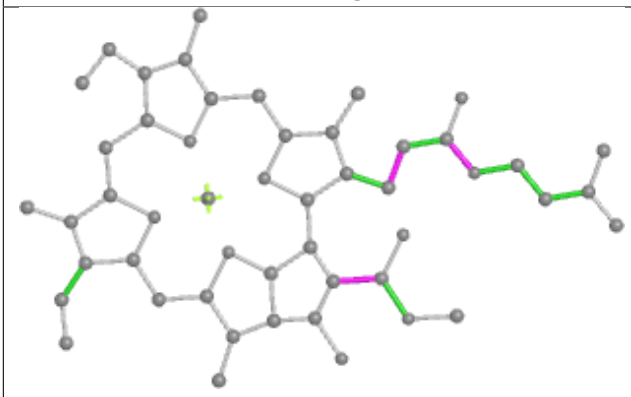
Ligand CLA A 829



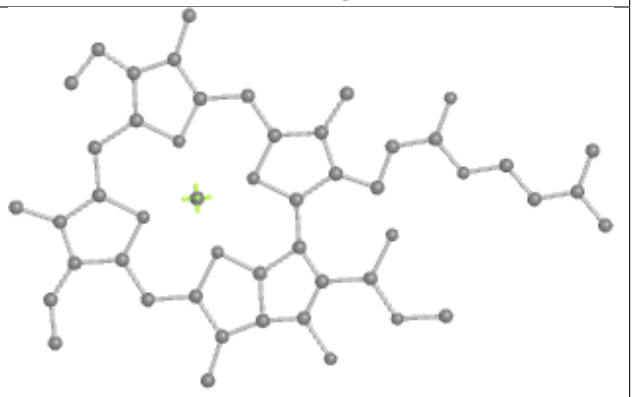
Bond lengths



Bond angles

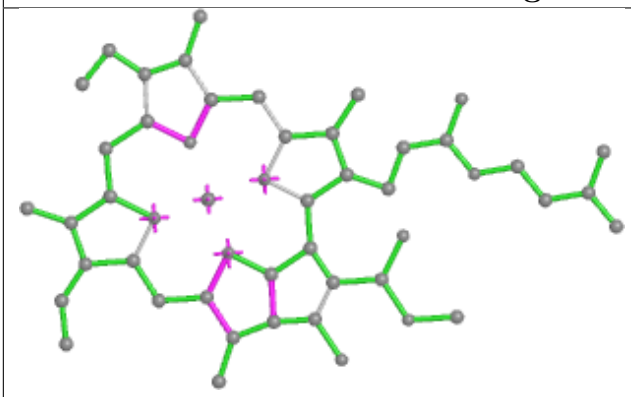


Torsions

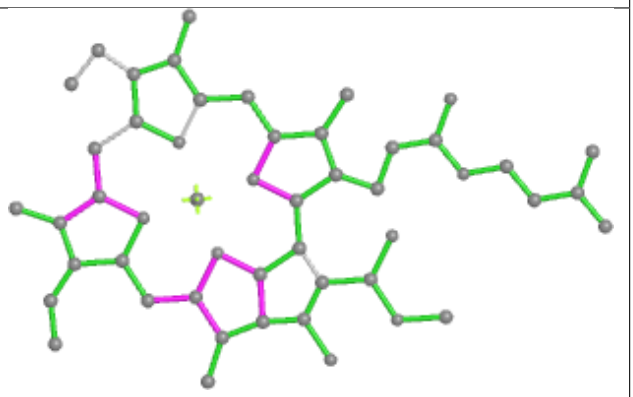


Rings

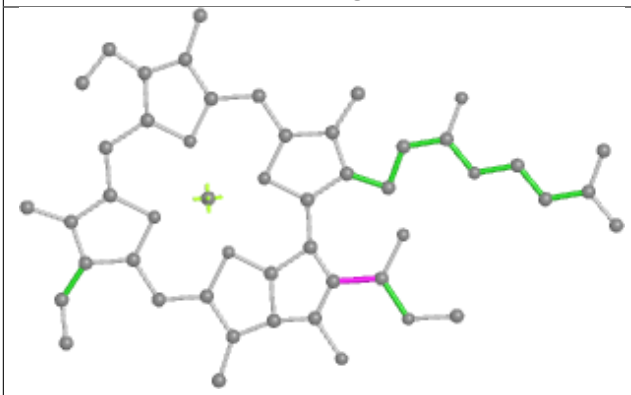
Ligand CLA A 805



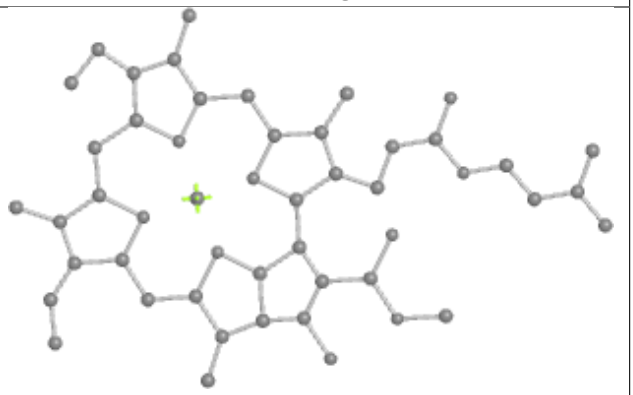
Bond lengths



Bond angles

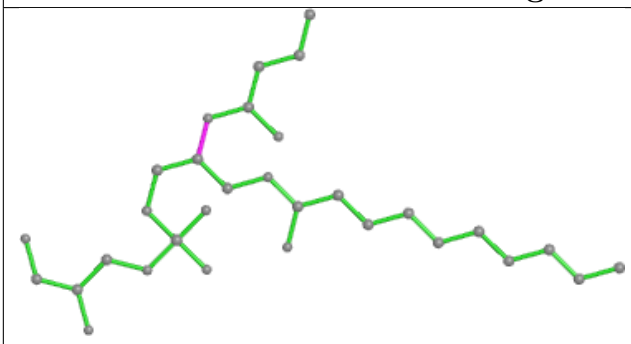


Torsions

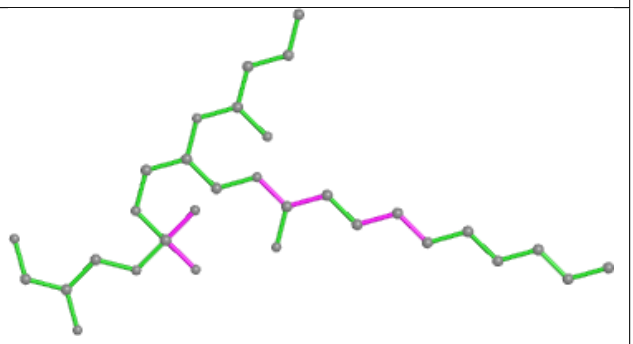


Rings

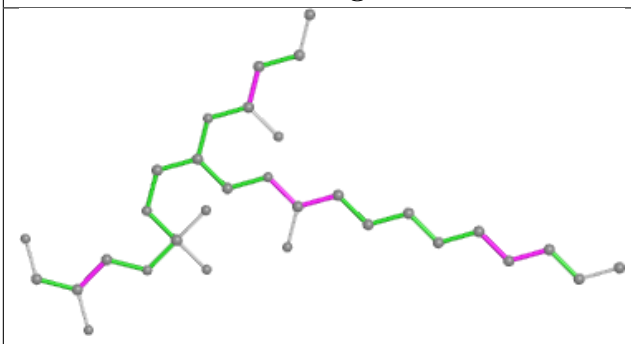
Ligand LHG 7 319



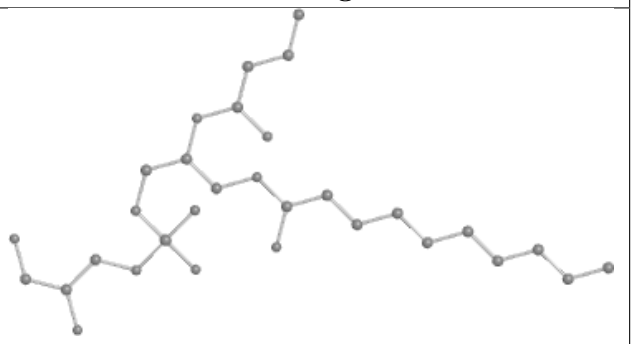
Bond lengths



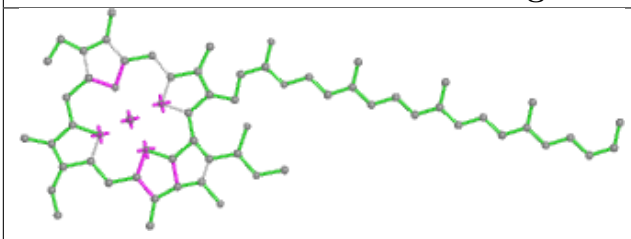
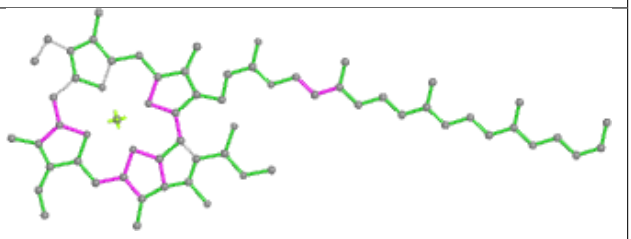
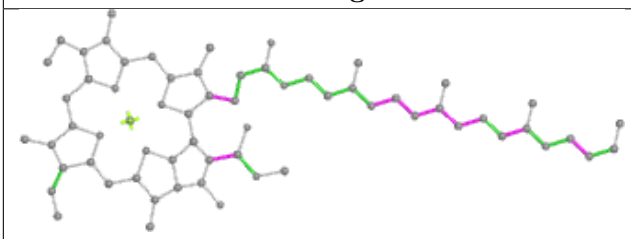
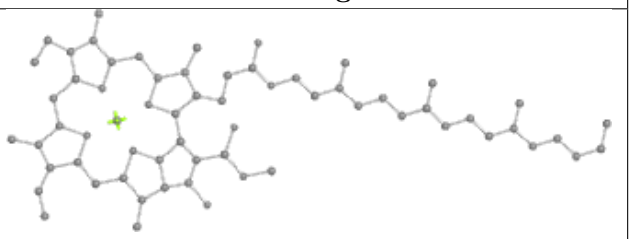
Bond angles

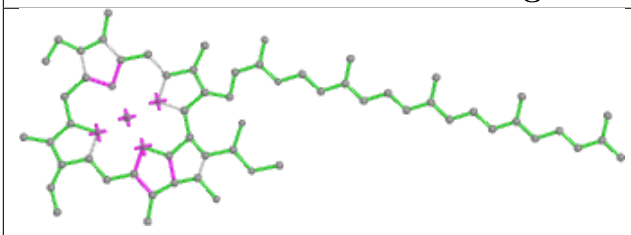
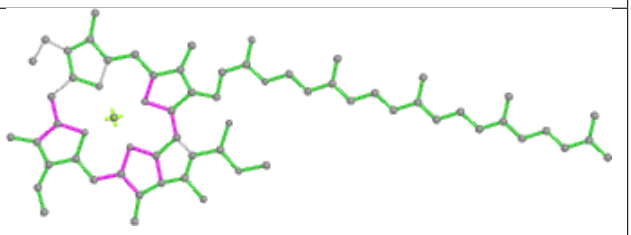
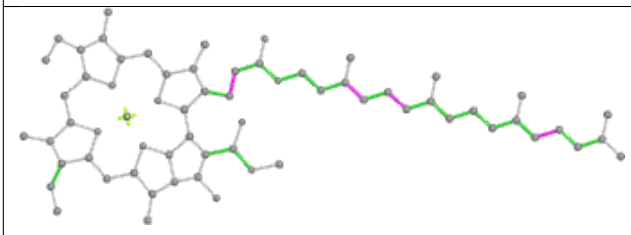
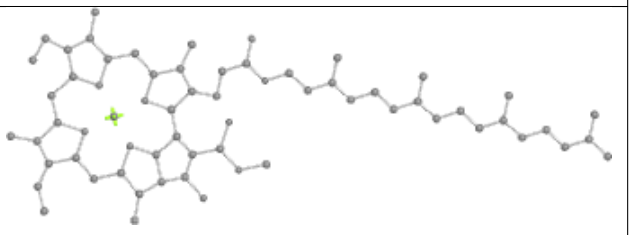


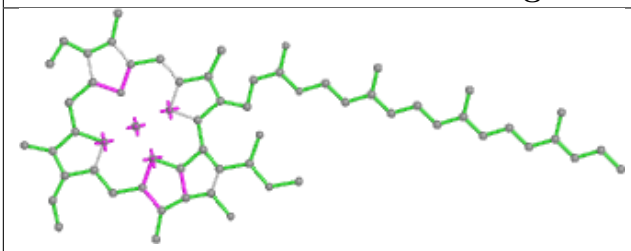
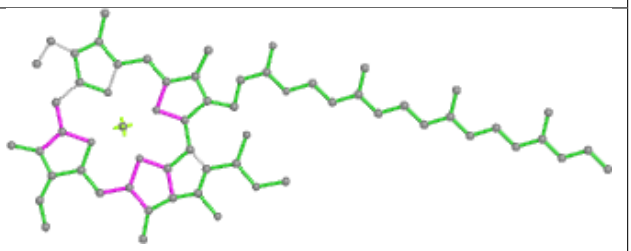
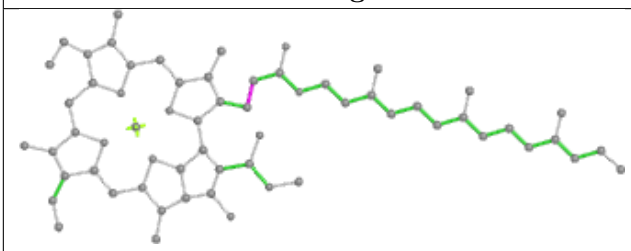
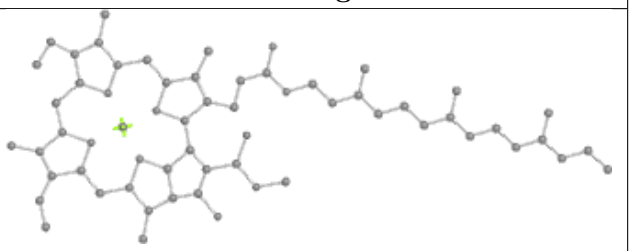
Torsions

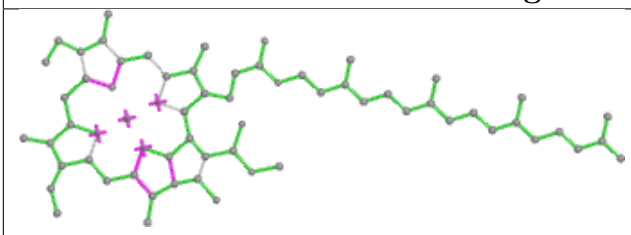
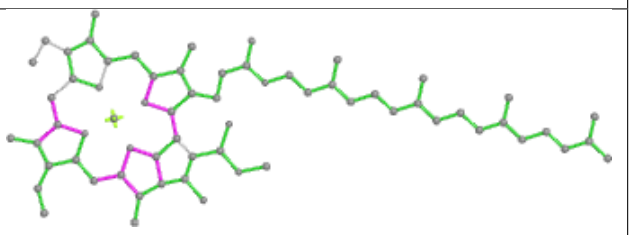
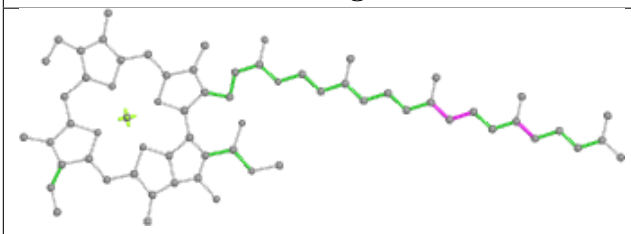
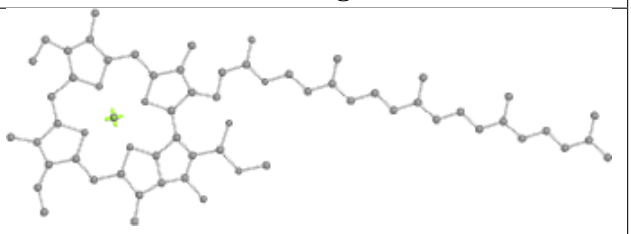


Rings

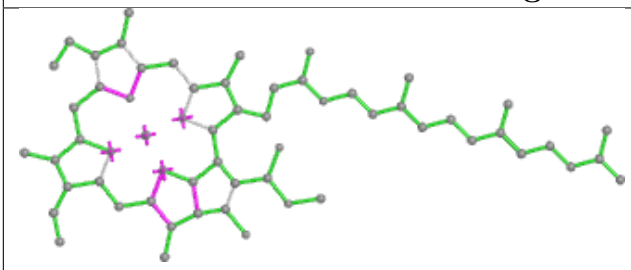
Ligand CLA b 602	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA A 827	
 Bond lengths	 Bond angles
 Torsions	 Rings

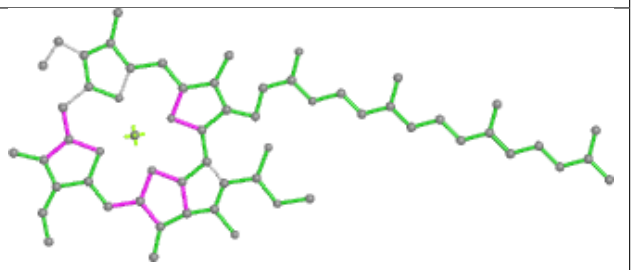
Ligand CLA A 815	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA A 826	
 Bond lengths	 Bond angles
 Torsions	 Rings

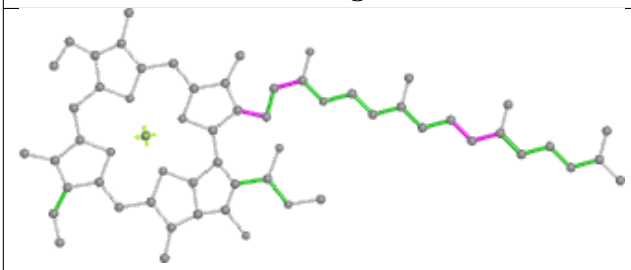
Ligand CLA A 816



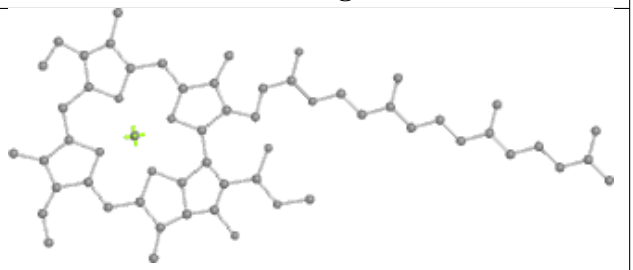
Bond lengths



Bond angles

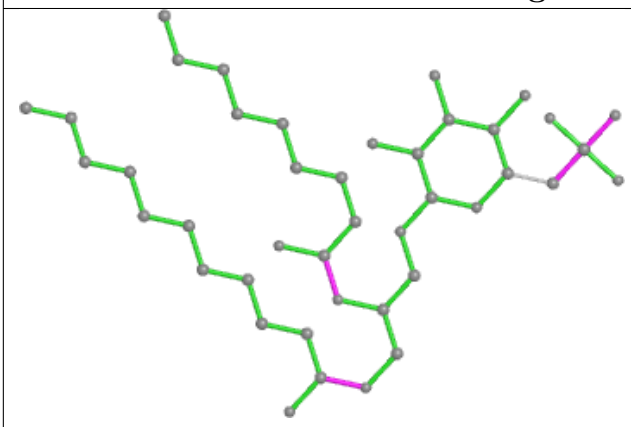


Torsions

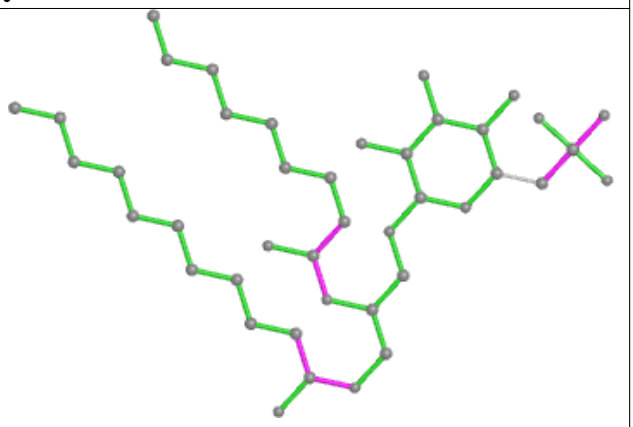


Rings

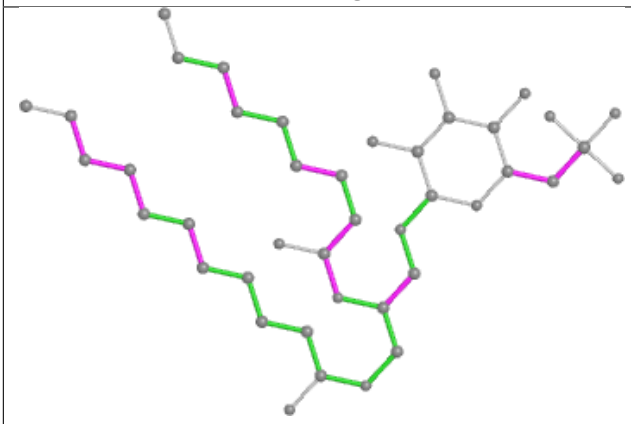
Ligand SQD 3 621



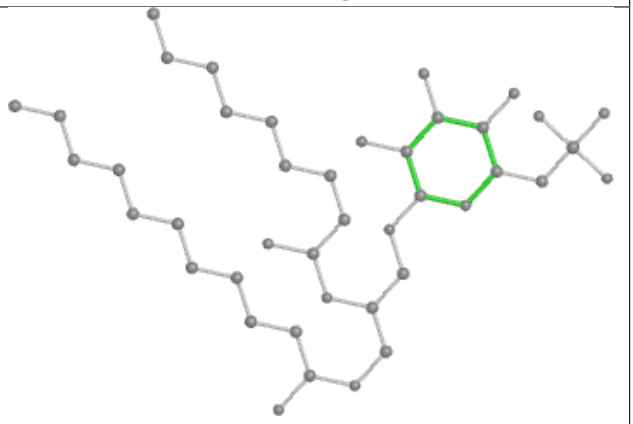
Bond lengths



Bond angles

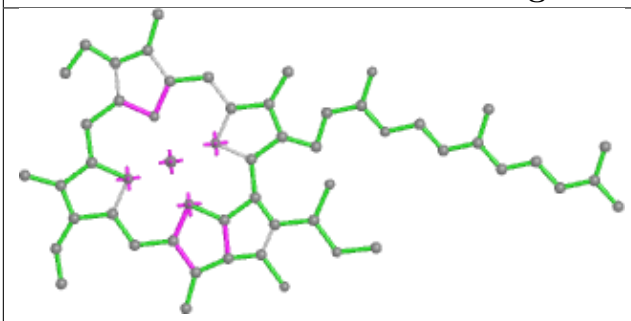


Torsions

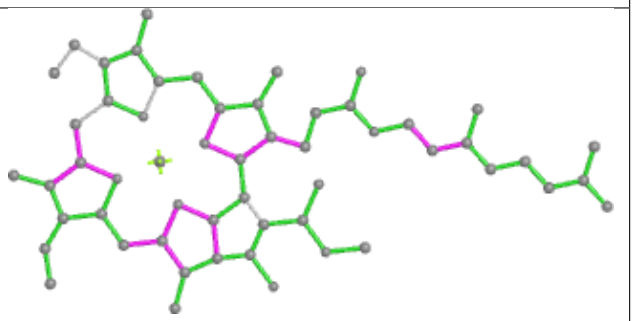


Rings

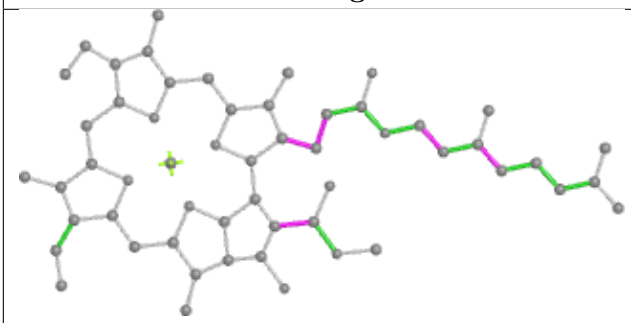
Ligand CLA 6 606



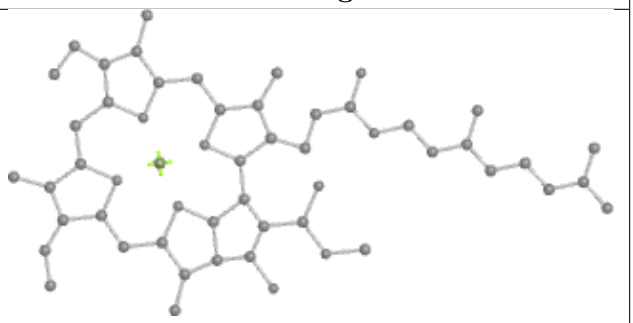
Bond lengths



Bond angles

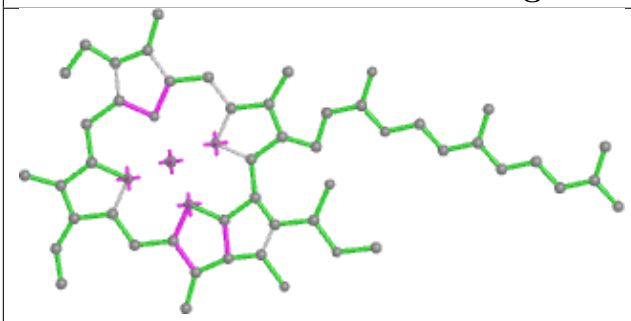


Torsions

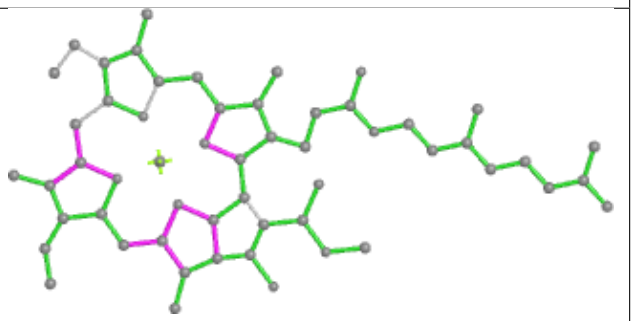


Rings

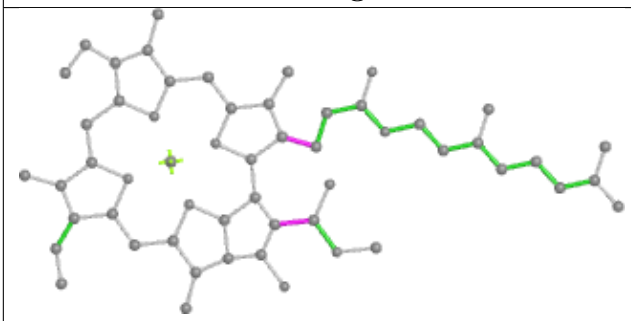
Ligand CLA A 802



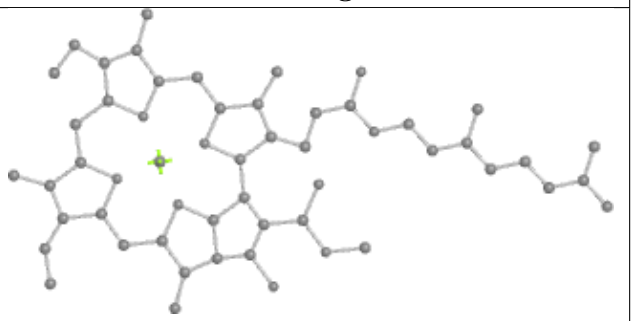
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

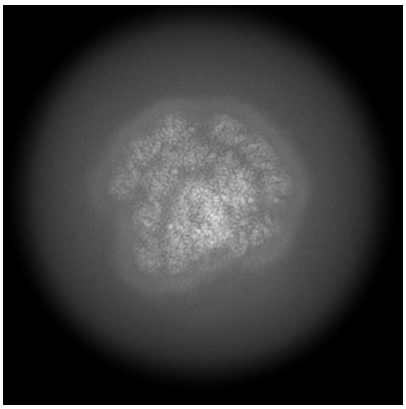
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-33683. These allow visual inspection of the internal detail of the map and identification of artifacts.

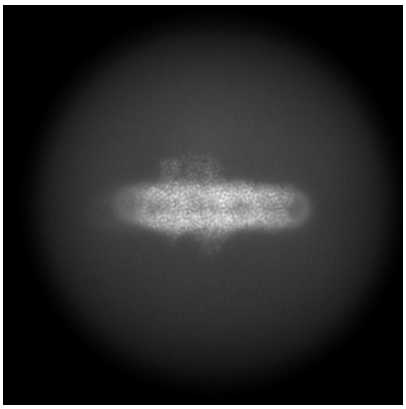
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

6.1.1 Primary map



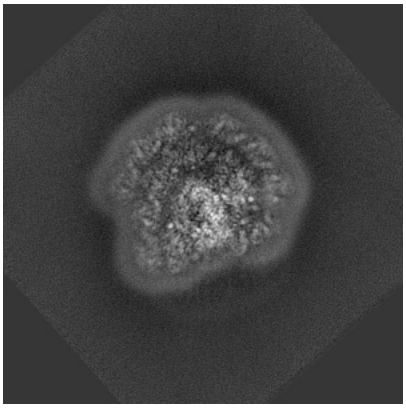
X



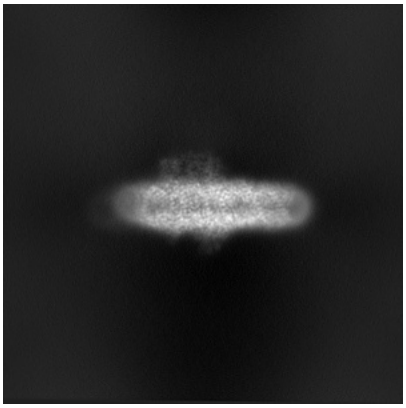
Y

Z

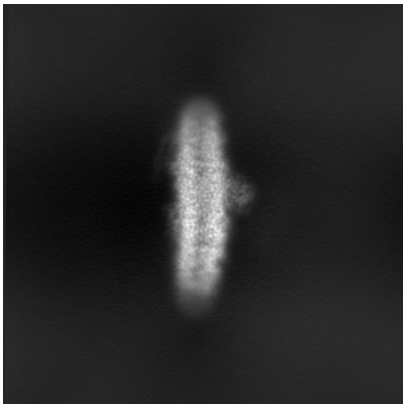
6.1.2 Raw map



X



Y

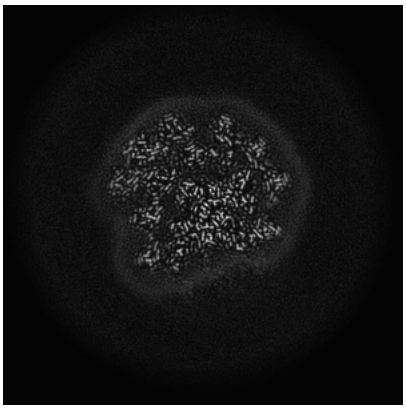


Z

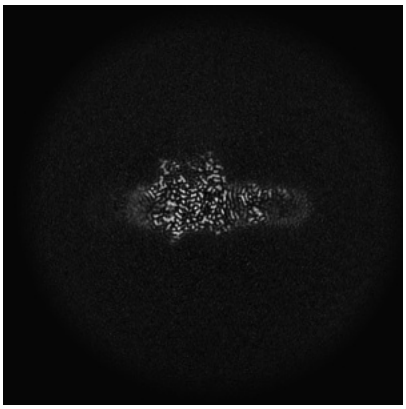
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

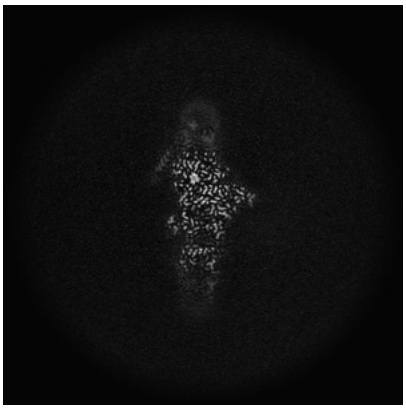
6.2.1 Primary map



X Index: 200

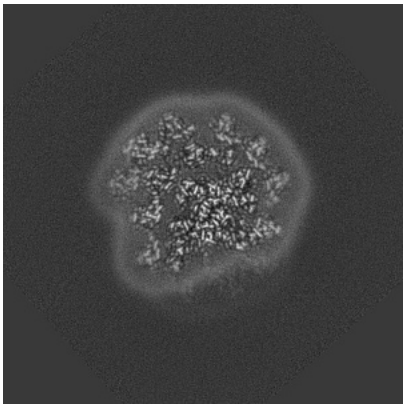


Y Index: 200

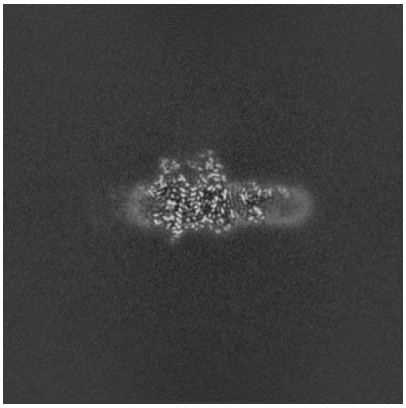


Z Index: 200

6.2.2 Raw map



X Index: 200



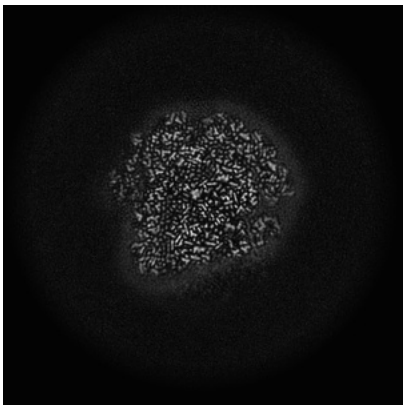
Y Index: 200

Z Index: 200

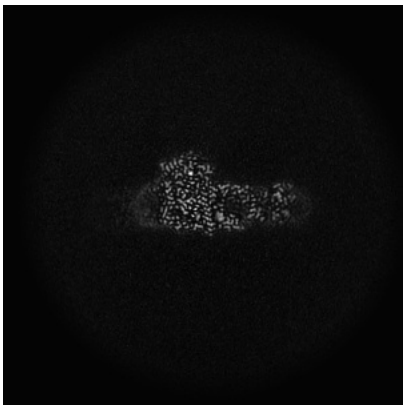
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

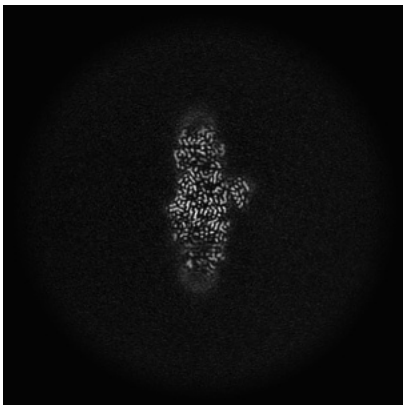
6.3.1 Primary map



X Index: 210

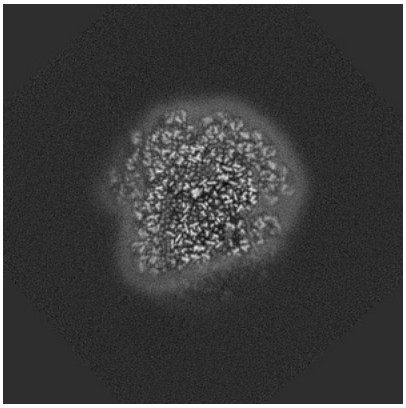


Y Index: 212

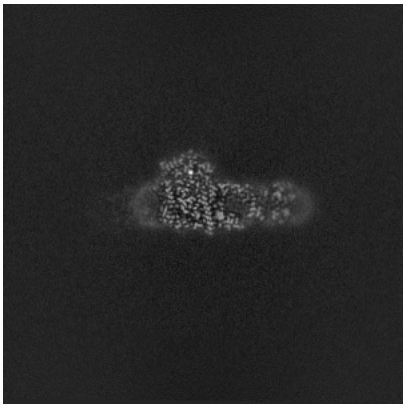


Z Index: 174

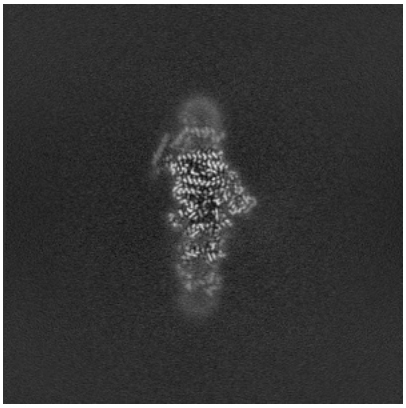
6.3.2 Raw map



X Index: 210



Y Index: 212

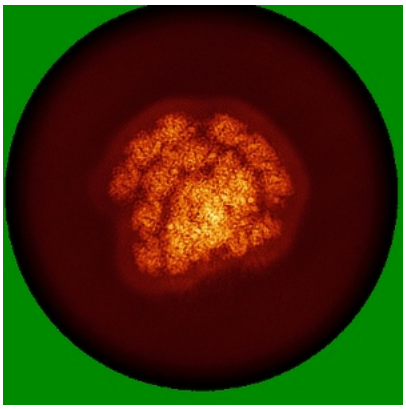


Z Index: 206

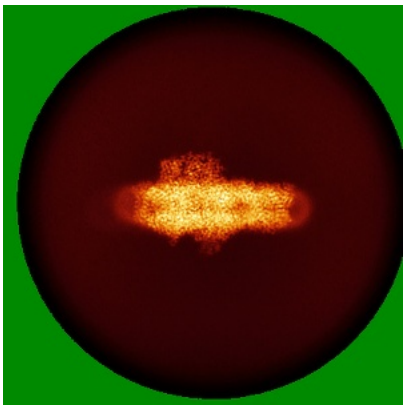
The images above show the largest variance slices of the map in three orthogonal directions.

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

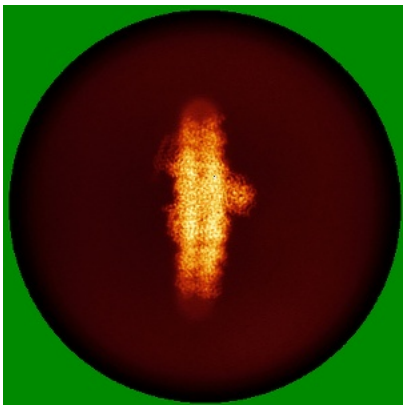
6.4.1 Primary map



X

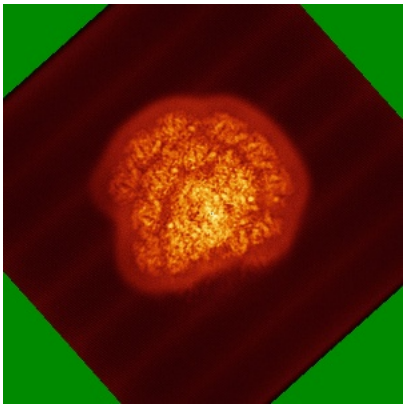


Y

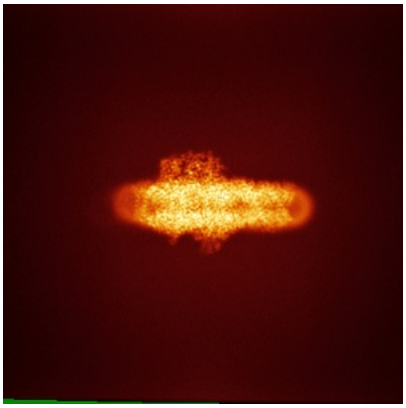


Z

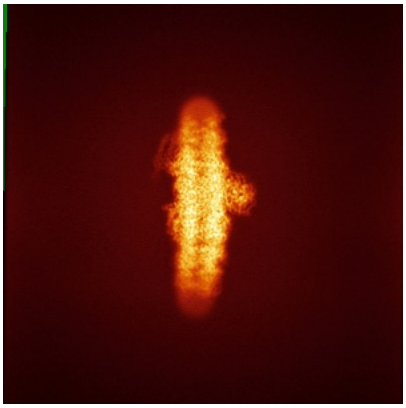
6.4.2 Raw map



X



Y

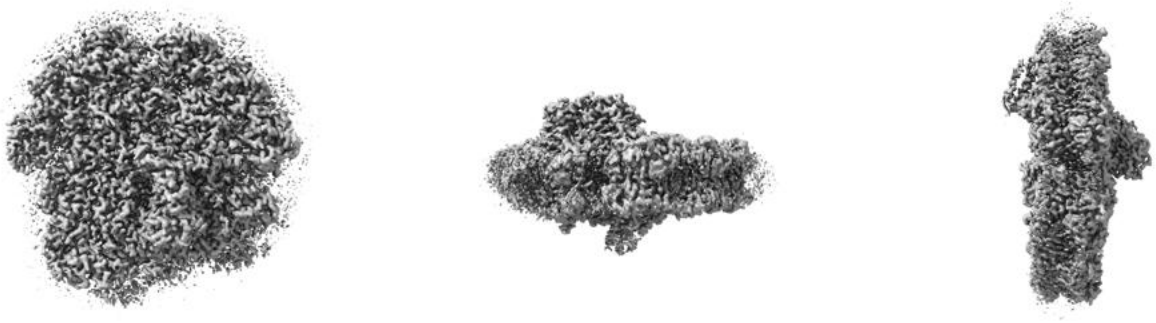


Z

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 0.3. 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.

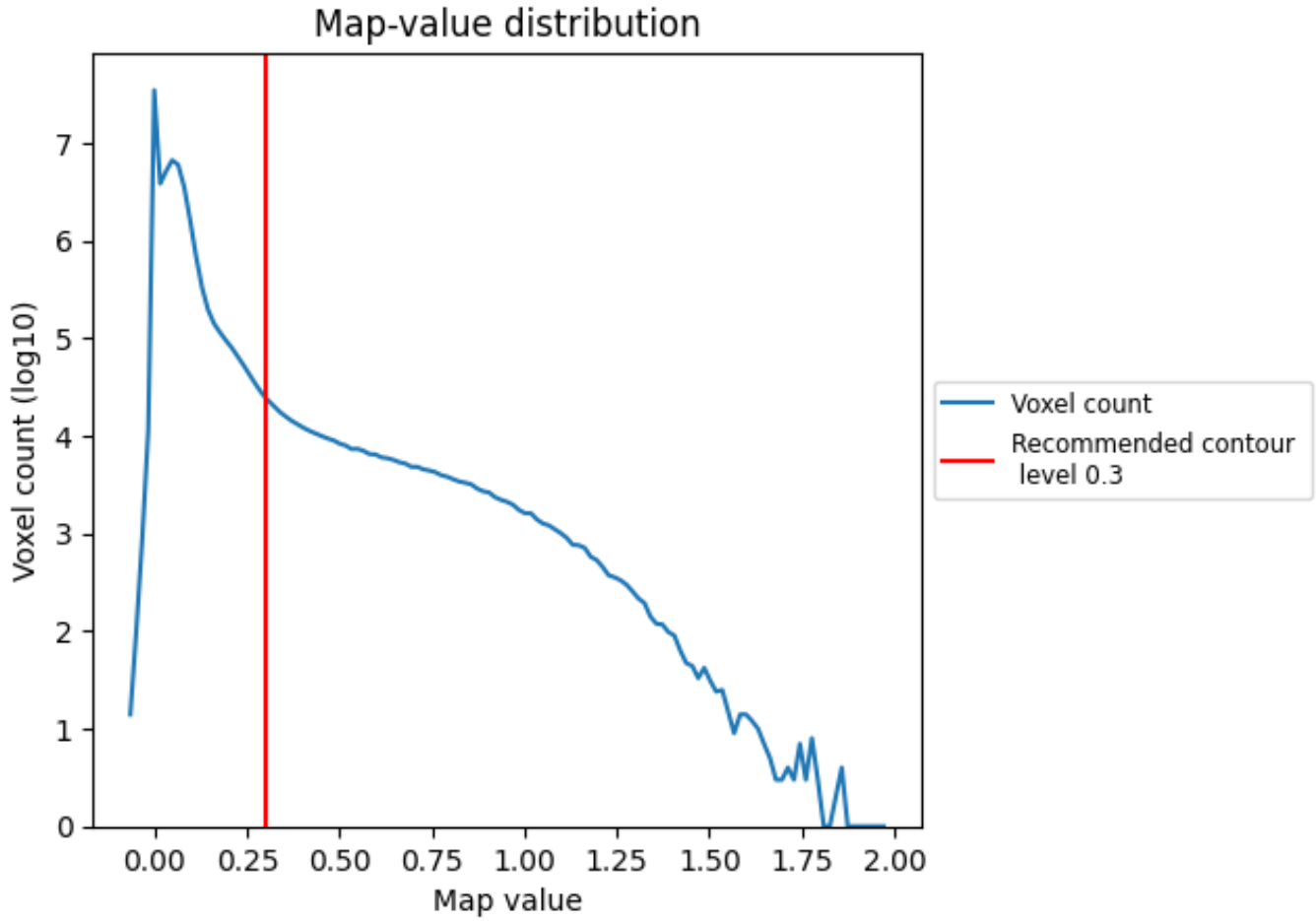
6.6 Mask visualisation (i)

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

7 Map analysis

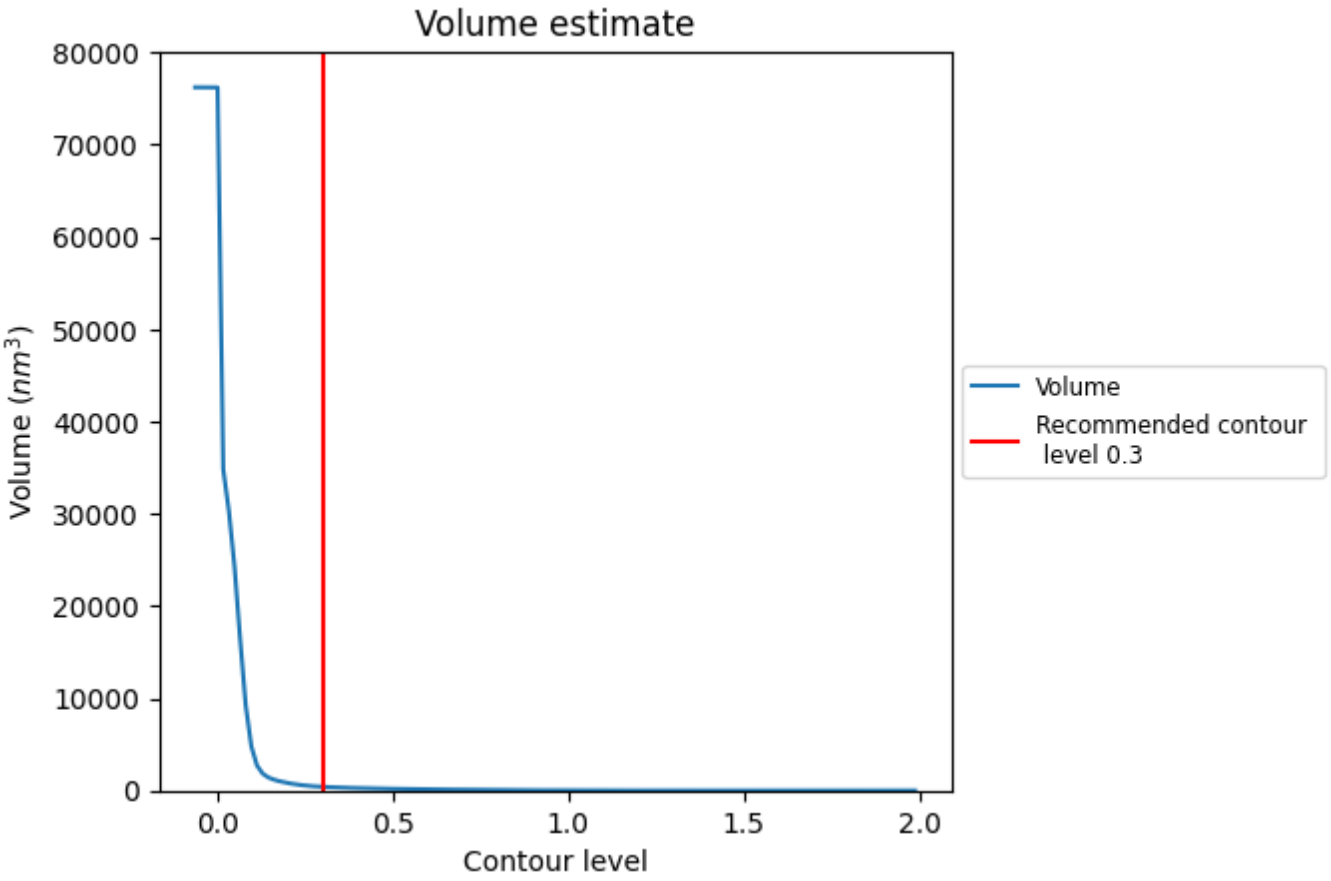
This section contains the results of statistical analysis of the map.

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.

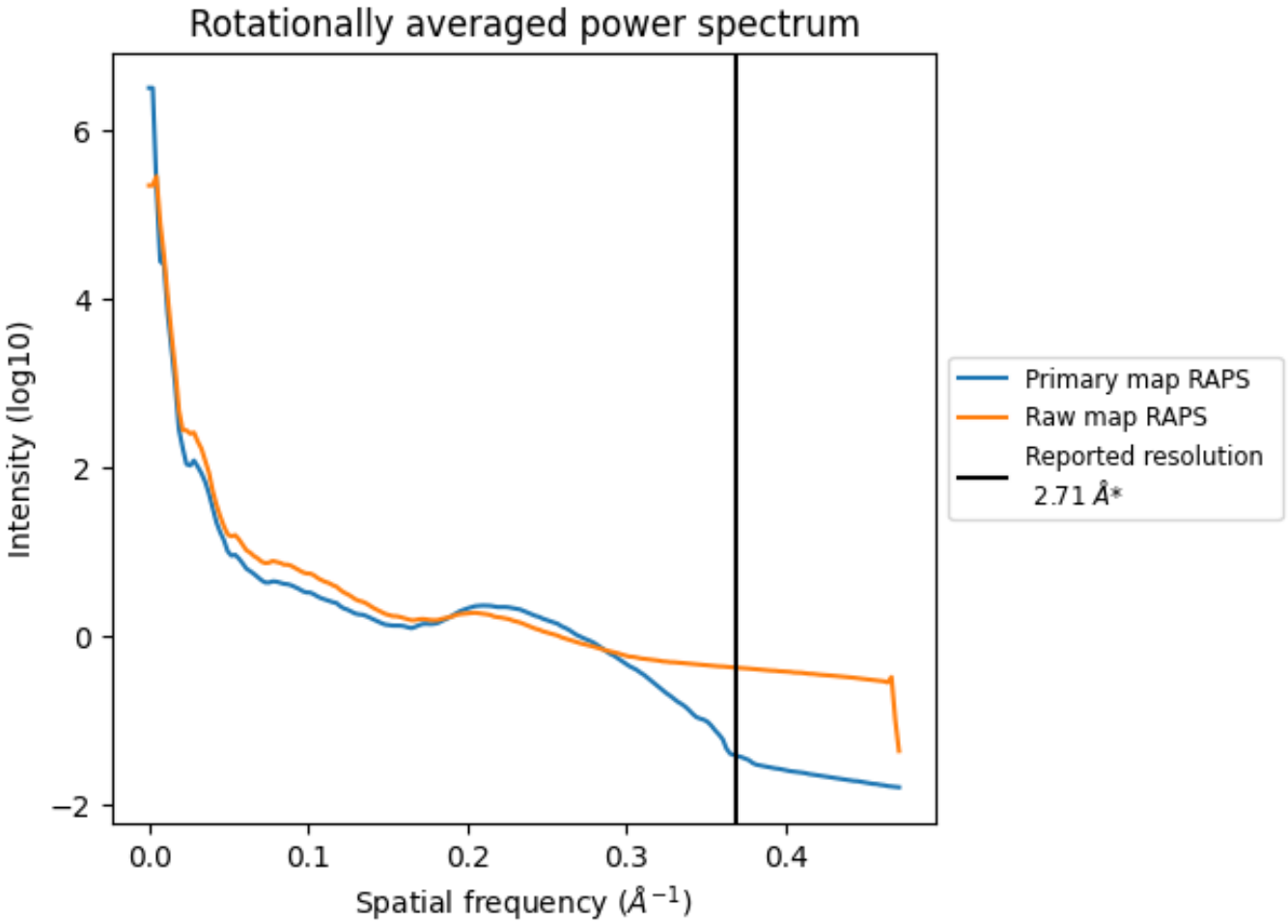
7.2 Volume estimate



The volume at the recommended contour level is 402 nm^3; this corresponds to an approximate mass of 363 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)

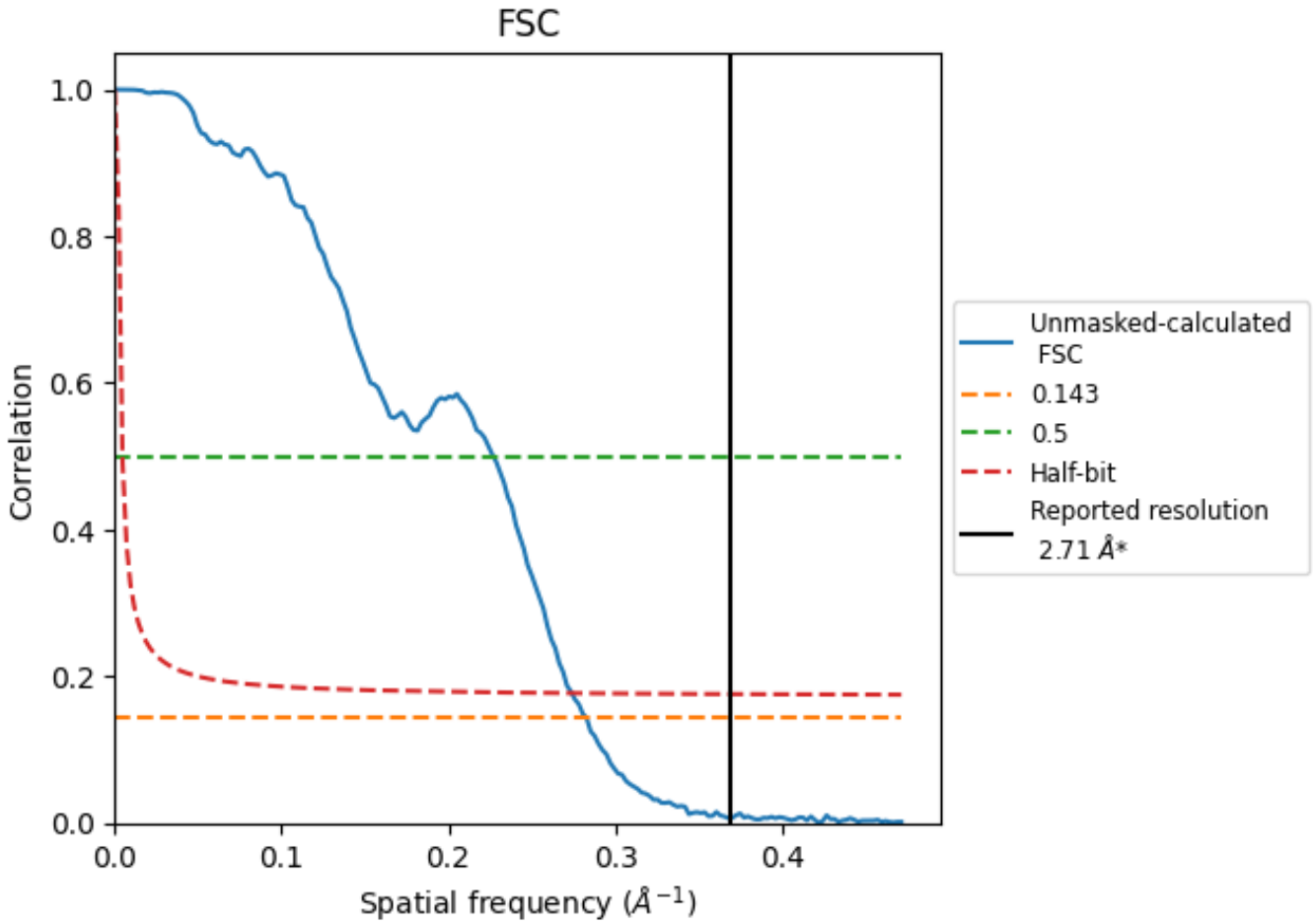


*Reported resolution corresponds to spatial frequency of 0.369 $Å^{-1}$

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 0.369 Å^{-1}

8.2 Resolution estimates (i)

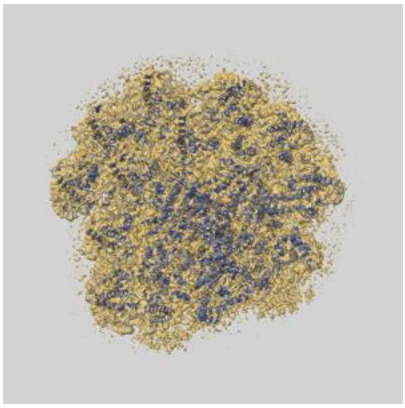
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.71	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.54	4.41	3.65

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.54 differs from the reported value 2.71 by more than 10 %

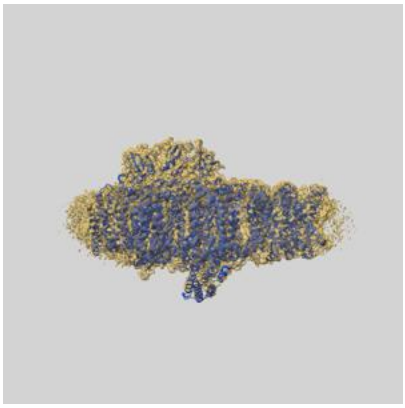
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-33683 and PDB model 7Y8A. Per-residue inclusion information can be found in section 3 on page 38.

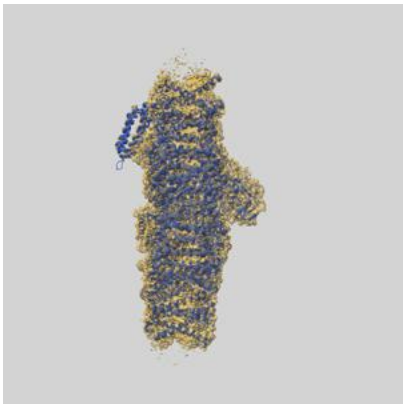
9.1 Map-model overlay



X



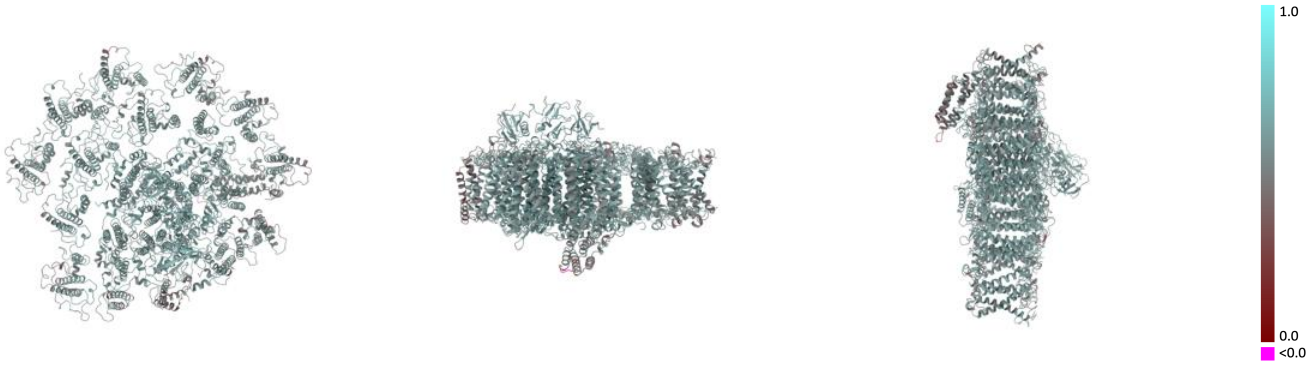
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.3 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.

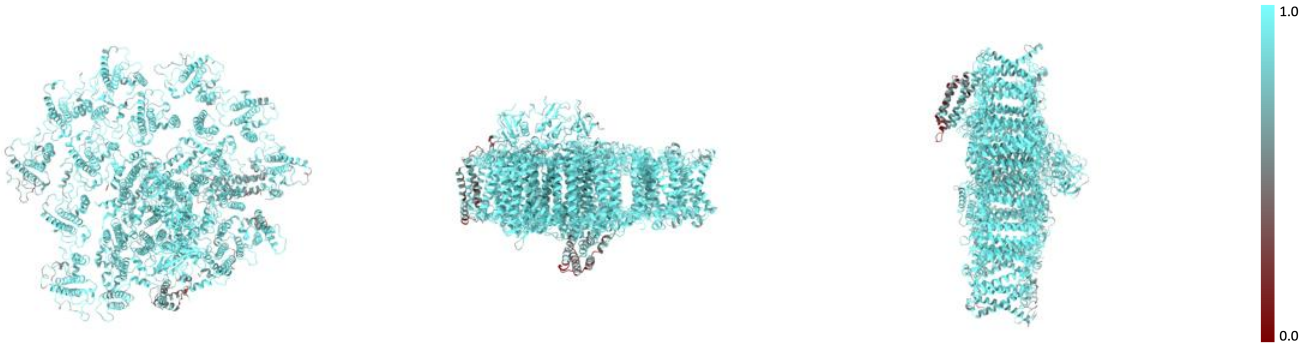
9.2 Q-score mapped to coordinate model (i)



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.

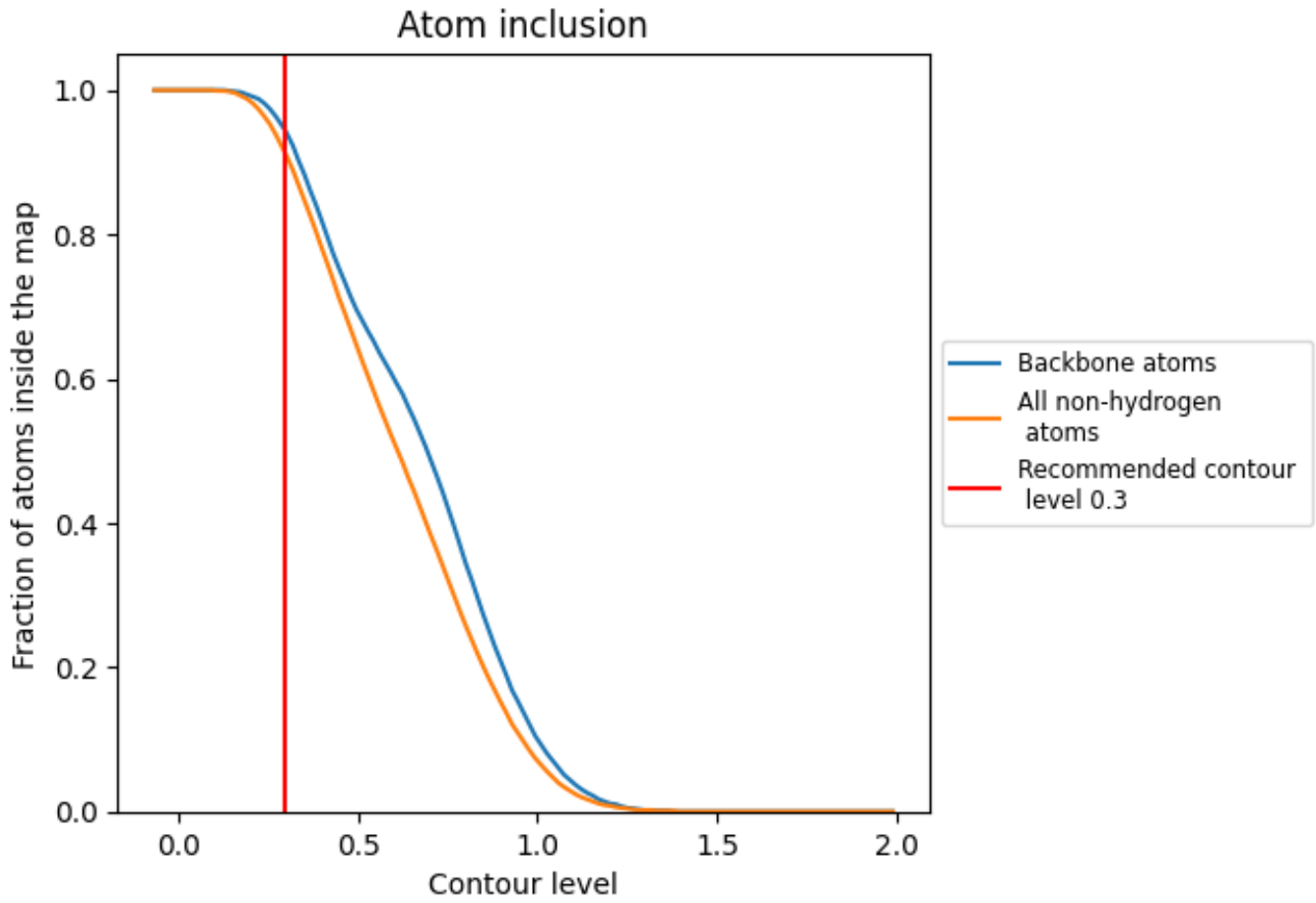
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.3).

9.4 Atom inclusion (i)



At the recommended contour level, 94% of all backbone atoms, 91% 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 (0.3) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9110	0.5810
1	0.8440	0.5270
2	0.9210	0.5810
3	0.9450	0.6080
4	0.9400	0.5980
5	0.8730	0.5370
6	0.9080	0.5580
7	0.8780	0.5340
8	0.8870	0.5560
9	0.7800	0.5420
A	0.9690	0.6140
B	0.9730	0.6220
C	0.9680	0.6020
D	0.9470	0.5840
E	0.8740	0.5850
F	0.9230	0.5960
I	0.9760	0.6120
J	0.9610	0.6110
K	0.8740	0.5370
L	0.8760	0.5640
M	0.9430	0.5940
O	0.5870	0.4700
R	0.9360	0.5890
X	0.5590	0.4670
Z	0.8960	0.5790
a	0.9040	0.5640
b	0.9200	0.5640