wwPDB EM Validation Summary Report

Oct 1, 2024 – 10:22 AM JST

PDB ID	:	6IJJ
EMDB ID	:	EMD-9678
Title	:	Photosystem I of Chlamydomonas reinhardtii
Authors	:	Pan, X.; Ma, J.; Su, X.; Liu, Z.; Zhang, X.; Li, M.
Deposited on	:	2018-10-10
Resolution	:	2.89 Å(reported)

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

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

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

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

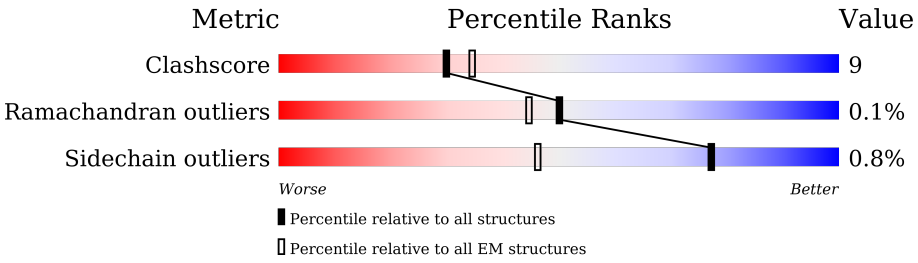
EMDB validation analysis	:	0.0.1.dev113
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.89 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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

Mol	Chain	Length	Quality of chain
1	A	751	82% 17%
2	B	735	11% 85% 14%
3	C	81	75% 23%
4	D	196	57% 15% 27%
5	E	143	6% 41% 55%
6	F	227	15% 65% 7% 28%
7	I	106	25% 18% 12% 70%
8	J	41	27% 83% 17%

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Mol	Chain	Length	Quality of chain
9	K	160	29% 47% 6% 47%
10	L	258	41% 33% 7% 59%
11	1	248	62% 66% 12% 22%
11	a	248	50% 78% 22%
12	3	298	9% 60% 13% 26%
13	4	290	17% 64% 8% 28%
14	5	274	10% 66% 17% 18%
15	6	318	10% 61% 11% 28%
16	7	241	9% 71% 16% 12%
17	8	272	12% 68% 10% 21%

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
18	CLA	1	601	X	-	-	-
18	CLA	1	602	X	-	-	-
18	CLA	1	603	X	-	-	-
18	CLA	1	604	X	-	-	-
18	CLA	1	606	X	-	-	-
18	CLA	1	607	X	-	-	-
18	CLA	1	608	X	-	-	-
18	CLA	1	609	X	-	-	-
18	CLA	1	610	X	-	-	-
18	CLA	1	611	X	-	-	-
18	CLA	1	612	X	-	-	-
18	CLA	1	613	X	-	-	-
18	CLA	1	614	X	-	-	-
18	CLA	1	616	X	-	-	-
18	CLA	3	602	X	-	-	-
18	CLA	3	603	X	-	-	-
18	CLA	3	604	X	-	-	-
18	CLA	3	606	X	-	-	-
18	CLA	3	607	X	-	-	-
18	CLA	3	608	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
18	CLA	3	609	X	-	-	-
18	CLA	3	610	X	-	-	-
18	CLA	3	611	X	-	-	-
18	CLA	3	612	X	-	-	-
18	CLA	3	613	X	-	-	-
18	CLA	3	614	X	-	-	-
18	CLA	3	615	X	-	-	-
18	CLA	3	617	X	-	-	-
18	CLA	4	602	X	-	-	-
18	CLA	4	603	X	-	-	-
18	CLA	4	604	X	-	-	-
18	CLA	4	606	X	-	-	-
18	CLA	4	607	X	-	-	-
18	CLA	4	608	X	-	-	-
18	CLA	4	609	X	-	-	-
18	CLA	4	610	X	-	-	-
18	CLA	4	611	X	-	-	-
18	CLA	4	613	X	-	-	-
18	CLA	4	614	X	-	-	-
18	CLA	4	616	X	-	-	-
18	CLA	4	618	X	-	-	-
18	CLA	5	601	X	-	-	-
18	CLA	5	602	X	-	-	-
18	CLA	5	603	X	-	-	-
18	CLA	5	604	X	-	-	-
18	CLA	5	606	X	-	-	-
18	CLA	5	607	X	-	-	-
18	CLA	5	608	X	-	-	-
18	CLA	5	609	X	-	-	-
18	CLA	5	610	X	-	-	-
18	CLA	5	611	X	-	-	-
18	CLA	5	612	X	-	-	-
18	CLA	5	613	X	-	-	-
18	CLA	5	614	X	-	-	-
18	CLA	5	616	X	-	-	-
18	CLA	5	617	X	-	-	-
18	CLA	5	618	X	-	-	-
18	CLA	6	601	X	-	-	-
18	CLA	6	602	X	-	-	-
18	CLA	6	603	X	-	-	-
18	CLA	6	604	X	-	-	-
18	CLA	6	606	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
18	CLA	6	607	X	-	-	-
18	CLA	6	608	X	-	-	-
18	CLA	6	609	X	-	-	-
18	CLA	6	610	X	-	-	-
18	CLA	6	611	X	-	-	-
18	CLA	6	612	X	-	-	-
18	CLA	6	613	X	-	-	-
18	CLA	6	614	X	-	-	-
18	CLA	6	616	X	-	-	-
18	CLA	6	617	X	-	-	-
18	CLA	6	618	X	-	-	-
18	CLA	6	620	X	-	-	-
18	CLA	7	602	X	-	-	-
18	CLA	7	603	X	-	-	-
18	CLA	7	604	X	-	-	-
18	CLA	7	606	X	-	-	-
18	CLA	7	607	X	-	-	-
18	CLA	7	608	X	-	-	-
18	CLA	7	609	X	-	-	-
18	CLA	7	610	X	-	-	-
18	CLA	7	611	X	-	-	-
18	CLA	7	613	X	-	-	-
18	CLA	7	614	X	-	-	-
18	CLA	7	615	X	-	-	-
18	CLA	7	616	X	-	-	-
18	CLA	8	601	X	-	-	-
18	CLA	8	602	X	-	-	-
18	CLA	8	603	X	-	-	-
18	CLA	8	604	X	-	-	-
18	CLA	8	606	X	-	-	-
18	CLA	8	607	X	-	-	-
18	CLA	8	608	X	-	-	-
18	CLA	8	609	X	-	-	-
18	CLA	8	610	X	-	-	-
18	CLA	8	611	X	-	-	-
18	CLA	8	613	X	-	-	-
18	CLA	8	614	X	-	-	-
18	CLA	A	801	X	-	-	-
18	CLA	A	802	X	-	-	-
18	CLA	A	803	X	-	-	-
18	CLA	A	804	X	-	-	-
18	CLA	A	805	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
18	CLA	A	806	X	-	-	-
18	CLA	A	807	X	-	-	-
18	CLA	A	808	X	-	-	-
18	CLA	A	809	X	-	-	-
18	CLA	A	810	X	-	-	-
18	CLA	A	811	X	-	-	-
18	CLA	A	812	X	-	-	-
18	CLA	A	813	X	-	-	-
18	CLA	A	814	X	-	-	-
18	CLA	A	815	X	-	-	-
18	CLA	A	816	X	-	-	-
18	CLA	A	817	X	-	-	-
18	CLA	A	818	X	-	-	-
18	CLA	A	819	X	-	-	-
18	CLA	A	820	X	-	-	-
18	CLA	A	821	X	-	-	-
18	CLA	A	822	X	-	-	-
18	CLA	A	823	X	-	-	-
18	CLA	A	824	X	-	-	-
18	CLA	A	825	X	-	-	-
18	CLA	A	826	X	-	-	-
18	CLA	A	827	X	-	-	-
18	CLA	A	828	X	-	-	-
18	CLA	A	829	X	-	-	-
18	CLA	A	830	X	-	-	-
18	CLA	A	831	X	-	-	-
18	CLA	A	832	X	-	-	-
18	CLA	A	833	X	-	-	-
18	CLA	A	834	X	-	-	-
18	CLA	A	835	X	-	-	-
18	CLA	A	836	X	-	-	-
18	CLA	A	837	X	-	-	-
18	CLA	A	838	X	-	-	-
18	CLA	A	839	X	-	-	-
18	CLA	A	840	X	-	-	-
18	CLA	A	841	X	-	-	-
18	CLA	A	842	X	-	-	-
18	CLA	A	843	X	-	-	-
18	CLA	A	845	X	-	-	-
18	CLA	A	854	X	-	-	-
18	CLA	B	802	X	-	-	-
18	CLA	B	803	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
18	CLA	B	804	X	-	-	-
18	CLA	B	805	X	-	-	-
18	CLA	B	806	X	-	-	-
18	CLA	B	807	X	-	-	-
18	CLA	B	808	X	-	-	-
18	CLA	B	809	X	-	-	-
18	CLA	B	810	X	-	-	-
18	CLA	B	811	X	-	-	-
18	CLA	B	812	X	-	-	-
18	CLA	B	813	X	-	-	-
18	CLA	B	814	X	-	-	-
18	CLA	B	815	X	-	-	-
18	CLA	B	816	X	-	-	-
18	CLA	B	817	X	-	-	-
18	CLA	B	818	X	-	-	-
18	CLA	B	819	X	-	-	-
18	CLA	B	820	X	-	-	-
18	CLA	B	821	X	-	-	-
18	CLA	B	822	X	-	-	-
18	CLA	B	823	X	-	-	-
18	CLA	B	824	X	-	-	-
18	CLA	B	825	X	-	-	-
18	CLA	B	826	X	-	-	-
18	CLA	B	827	X	-	-	-
18	CLA	B	828	X	-	-	-
18	CLA	B	829	X	-	-	-
18	CLA	B	830	X	-	-	-
18	CLA	B	831	X	-	-	-
18	CLA	B	832	X	-	-	-
18	CLA	B	833	X	-	-	-
18	CLA	B	834	X	-	-	-
18	CLA	B	835	X	-	-	-
18	CLA	B	836	X	-	-	-
18	CLA	B	837	X	-	-	-
18	CLA	B	838	X	-	-	-
18	CLA	B	839	X	-	-	-
18	CLA	B	840	X	-	-	-
18	CLA	B	841	X	-	-	-
18	CLA	F	301	X	-	-	-
18	CLA	F	304	X	-	-	-
18	CLA	J	101	X	-	-	-
18	CLA	K	201	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
18	CLA	K	203	X	-	-	-
18	CLA	K	204	X	-	-	-
18	CLA	K	206	X	-	-	-
18	CLA	L	302	X	-	-	-
18	CLA	L	303	X	-	-	-
18	CLA	L	304	X	-	-	-
18	CLA	a	601	X	-	-	-
18	CLA	a	602	X	-	-	-
18	CLA	a	603	X	-	-	-
18	CLA	a	604	X	-	-	-
18	CLA	a	606	X	-	-	-
18	CLA	a	607	X	-	-	-
18	CLA	a	608	X	-	-	-
18	CLA	a	609	X	-	-	-
18	CLA	a	610	X	-	-	-
18	CLA	a	611	X	-	-	-
18	CLA	a	612	X	-	-	-
18	CLA	a	613	X	-	-	-
18	CLA	a	614	X	-	-	-
18	CLA	a	616	X	-	-	-

2 Entry composition (i)

There are 28 unique types of molecules in this entry. The entry contains 44968 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called PsaA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	741	Total	C	N	O	S	0	0
			5819	3805	993	999	22		

- Molecule 2 is a protein called PsaB.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	731	Total	C	N	O	S	0	0
			5812	3818	975	1001	18		

- Molecule 3 is a protein called PsaC.

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

- Molecule 4 is a protein called PsaD.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	144	Total	C	N	O	S	0	0
			1129	722	200	200	7		

- Molecule 5 is a protein called PsaE.

Mol	Chain	Residues	Atoms				AltConf	Trace
5	E	64	Total	C	N	O	0	0
			505	322	89	94		

- Molecule 6 is a protein called PsaF.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	164	Total	C	N	O	S	0	0
			1254	811	209	231	3		

- Molecule 7 is a protein called PsaI.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	I	32	Total	C	N	O	S	0	0
			242	166	34	41	1		

- Molecule 8 is a protein called PsaJ.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	J	41	Total	C	N	O	S	0	0
			337	231	47	58	1		

- Molecule 9 is a protein called PsaK.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	K	85	Total	C	N	O	S	0	0
			578	368	99	109	2		

- Molecule 10 is a protein called PsaL.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	L	105	Total	C	N	O	S	0	0
			761	502	122	135	2		

- Molecule 11 is a protein called Lhca1.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	1	193	Total	C	N	O	S	0	0
			1433	932	239	259	3		
11	a	194	Total	C	N	O	S	0	0
			1444	941	240	260	3		

- Molecule 12 is a protein called Lhca3.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	3	221	Total	C	N	O	S	0	0
			1683	1099	271	305	8		

- Molecule 13 is a protein called Lhca4.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	4	210	Total	C	N	O	S	0	0
			1631	1071	263	292	5		

- Molecule 14 is a protein called Lhca5.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	5	226	Total	C	N	O	S	0	0
			1765	1149	295	313	8		

- Molecule 15 is a protein called Lhca6.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	6	230	Total	C	N	O	S	0	0
			1771	1167	293	305	6		

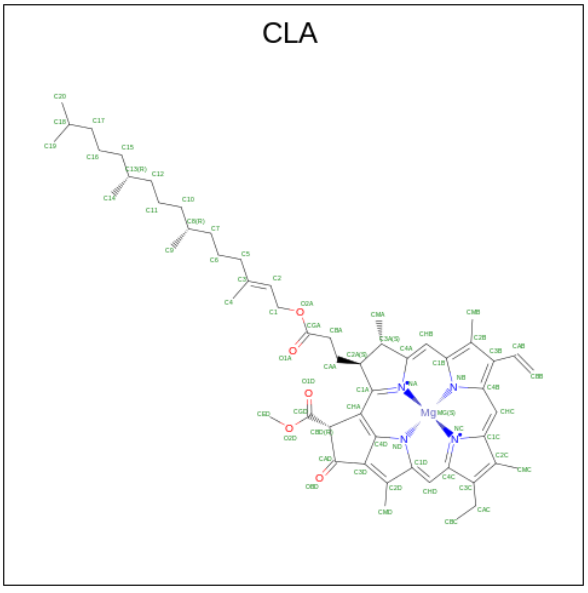
- Molecule 16 is a protein called Lhca7.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	7	213	Total	C	N	O	S	0	0
			1649	1072	274	297	6		

- Molecule 17 is a protein called Lhca8.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	8	215	Total	C	N	O	S	0	0
			1630	1058	278	290	4		

- Molecule 18 is CHLOROPHYLL A (three-letter code: CLA) (formula: $C_{55}H_{72}MgN_4O_5$).



Mol	Chain	Residues	Atoms					AltConf
18	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	A	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
18	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	A	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
18	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	A	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
18	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	A	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
18	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	A	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
18	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
18	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
18	A	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
18	A	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
18	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	A	1	Total	C	Mg	N	O	0
			53	43	1	4	5	
18	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
18	A	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
18	A	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
18	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	A	1	Total	C	Mg	N	O	0
			64	55	1	4	4	
18	A	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
18	A	1	Total	C	Mg	N	O	0
			64	55	1	4	4	
18	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	A	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
18	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
18	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	A	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
18	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
18	A	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
18	A	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
18	A	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
18	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	A	1	Total	C	Mg	N	O	0
			64	54	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
18	A	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
18	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	B	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
18	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	B	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
18	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	B	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
18	B	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
18	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	B	1	Total	C	Mg	N	O	0
			64	54	1	4	5	
18	B	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
18	B	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
18	B	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
18	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
18	B	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
18	B	1	Total	C	Mg	N	O	0
			50	40	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
18	B	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
18	B	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
18	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
18	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	B	1	Total	C	Mg	N	O	0
			62	52	1	4	5	
18	B	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
18	B	1	Total	C	Mg	N	O	0
			62	52	1	4	5	
18	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	B	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
18	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
18	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
18	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
18	B	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
18	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	B	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
18	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	B	1	Total	C	Mg	N	O	0
			44	35	1	4	4	

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Mol	Chain	Residues	Atoms					AltConf
18	F	1	Total	C	Mg	N	O	0
			57	47	1	4	5	
18	F	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
18	F	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
18	J	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
18	K	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
18	K	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	K	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
18	K	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
18	L	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
18	L	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
18	L	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
18	1	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
18	1	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
18	1	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
18	1	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
18	1	1	Total	C	Mg	N	O	0
			39	32	1	4	2	
18	1	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
18	1	1	Total	C	Mg	N	O	0
			44	34	1	4	5	
18	1	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
18	1	1	Total	C	Mg	N	O	0
			39	31	1	4	3	
18	1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
18	1	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
18	1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	1	1	Total	C	Mg	N	O	0
			37	29	1	4	3	
18	1	1	Total	C	Mg	N	O	0
			43	33	1	4	5	
18	a	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
18	a	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
18	a	1	Total	C	Mg	N	O	0
			54	45	1	4	4	
18	a	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
18	a	1	Total	C	Mg	N	O	0
			44	35	1	4	4	
18	a	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
18	a	1	Total	C	Mg	N	O	0
			44	34	1	4	5	
18	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	a	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
18	a	1	Total	C	Mg	N	O	0
			38	30	1	4	3	
18	a	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
18	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	a	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
18	a	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
18	3	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
18	3	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
18	3	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
18	3	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
18	3	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
18	3	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
18	3	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
18	3	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	3	1	Total	C	Mg	N	O	0
			38	30	1	4	3	
18	3	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
18	3	1	Total	C	Mg	N	O	0
			53	44	1	4	4	
18	3	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
18	3	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
18	3	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
18	4	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	4	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
18	4	1	Total	C	Mg	N	O	0
			44	34	1	4	5	
18	4	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
18	4	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
18	4	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
18	4	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	4	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
18	4	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
18	4	1	Total	C	Mg	N	O	0
			42	34	1	4	3	

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Mol	Chain	Residues	Atoms					AltConf
18	4	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
18	4	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	4	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
18	4	1	Total	C	Mg	N	O	0
			43	33	1	4	5	
18	4	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
18	5	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
18	5	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	5	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
18	5	1	Total	C	Mg	N	O	0
			63	53	1	4	5	
18	5	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
18	5	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	5	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
18	5	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	5	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
18	5	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
18	5	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
18	5	1	Total	C	Mg	N	O	0
			64	55	1	4	4	
18	5	1	Total	C	Mg	N	O	0
			44	34	1	4	5	
18	5	1	Total	C	Mg	N	O	0
			42	33	1	4	4	
18	5	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
18	5	1	Total	C	Mg	N	O	0
			40	32	1	4	3	

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Mol	Chain	Residues	Atoms					AltConf
18	5	1	Total	C	Mg	N	O	0
			43	33	1	4	5	
18	6	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	6	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	6	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
18	6	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	6	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
18	6	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
18	6	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
18	6	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
18	6	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	6	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
18	6	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
18	6	1	Total	C	Mg	N	O	0
			64	54	1	4	5	
18	6	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
18	6	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	6	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
18	6	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
18	6	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
18	7	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
18	7	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	7	1	Total	C	Mg	N	O	0
			44	34	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
18	7	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
18	7	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
18	7	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
18	7	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
18	7	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
18	7	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	7	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
18	7	1	Total	C	Mg	N	O	0
			44	34	1	4	5	
18	7	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	7	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
18	7	1	Total	C	Mg	N	O	0
			39	32	1	4	2	
18	7	1	Total	C	Mg	N	O	0
			43	33	1	4	5	
18	8	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	8	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
18	8	1	Total	C	Mg	N	O	0
			44	34	1	4	5	
18	8	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
18	8	1	Total	C	Mg	N	O	0
			64	54	1	4	5	
18	8	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
18	8	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
18	8	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
18	8	1	Total	C	Mg	N	O	0
			60	50	1	4	5	

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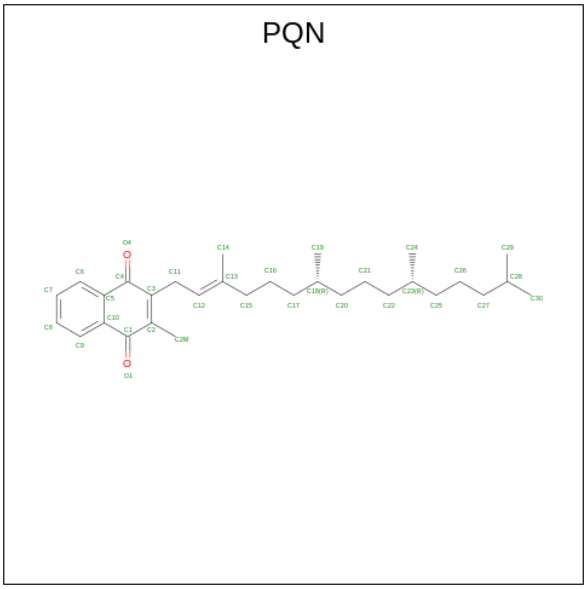
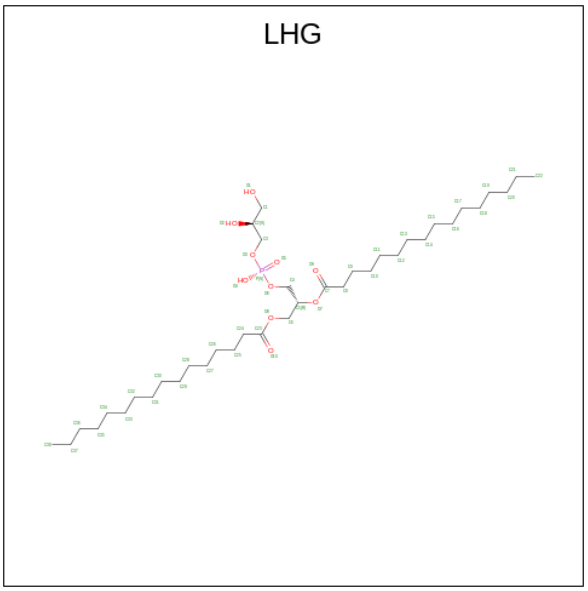
Mol	Chain	Residues	Atoms					AltConf
18	8	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
18	8	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
18	8	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	8	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
18	8	1	Total	C	Mg	N	O	0
			43	33	1	4	5	

- Molecule 19 is PHYLLOQUINONE (three-letter code: PQN) (formula: $C_{31}H_{46}O_2$).



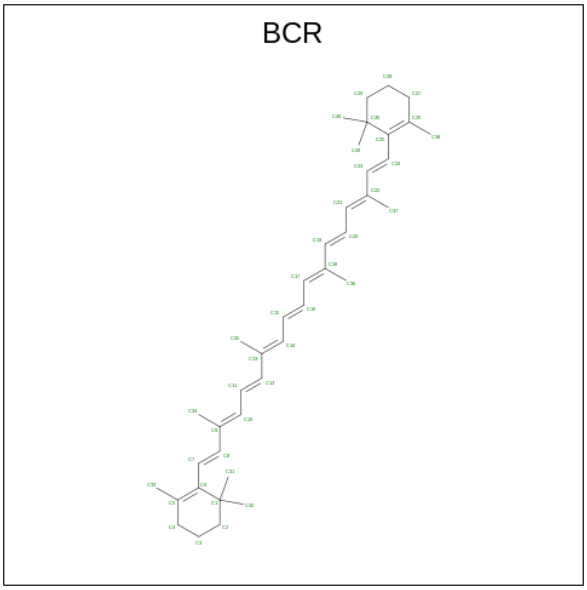
Mol	Chain	Residues	Atoms			AltConf
19	A	1	Total	C	O	0
			33	31	2	
19	B	1	Total	C	O	0
			33	31	2	

- Molecule 20 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula: $C_{38}H_{75}O_{10}P$).



Mol	Chain	Residues	Atoms				AltConf
20	A	1	Total	C	O	P	0
			49	38	10	1	
20	A	1	Total	C	O	P	0
			30	19	10	1	
20	B	1	Total	C	O	P	0
			36	26	9	1	
20	1	1	Total	C	O	P	0
			49	38	10	1	
20	a	1	Total	C	O	P	0
			49	38	10	1	
20	3	1	Total	C	O	P	0
			45	34	10	1	
20	3	1	Total	C	O	P	0
			49	38	10	1	
20	4	1	Total	C	O	P	0
			49	38	10	1	
20	5	1	Total	C	O	P	0
			49	38	10	1	
20	5	1	Total	C	O	P	0
			49	38	10	1	
20	6	1	Total	C	O	P	0
			48	37	10	1	
20	7	1	Total	C	O	P	0
			37	26	10	1	
20	8	1	Total	C	O	P	0
			49	38	10	1	
20	8	1	Total	C	O	P	0
			49	38	10	1	

- Molecule 21 is BETA-CAROTENE (three-letter code: BCR) (formula: $C_{40}H_{56}$).



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

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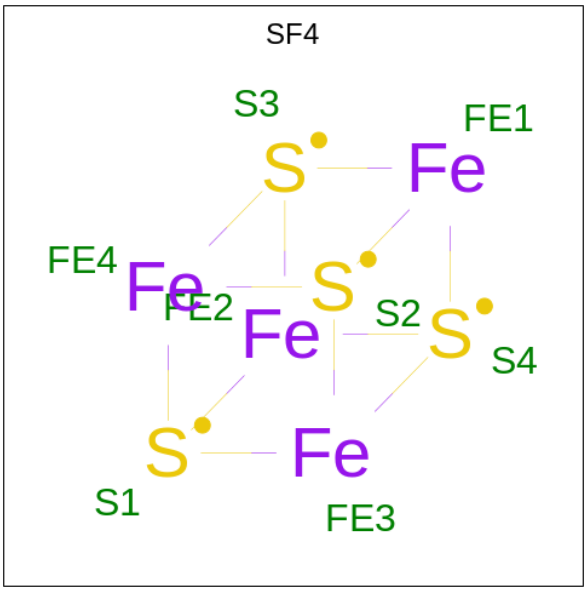
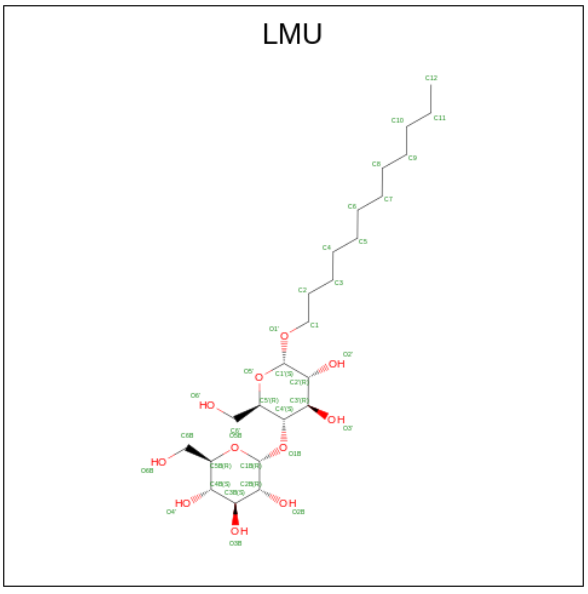
Mol	Chain	Residues	Atoms	AltConf
21	F	1	Total C 40 40	0
21	J	1	Total C 40 40	0
21	K	1	Total C 40 40	0
21	K	1	Total C 40 40	0
21	L	1	Total C 40 40	0
21	L	1	Total C 40 40	0
21	1	1	Total C 40 40	0
21	a	1	Total C 40 40	0
21	3	1	Total C 40 40	0
21	3	1	Total C 40 40	0
21	3	1	Total C 40 40	0
21	4	1	Total C 40 40	0
21	5	1	Total C 40 40	0
21	6	1	Total C 40 40	0
21	7	1	Total C 40 40	0
21	7	1	Total C 40 40	0
21	8	1	Total C 40 40	0

- Molecule 22 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).



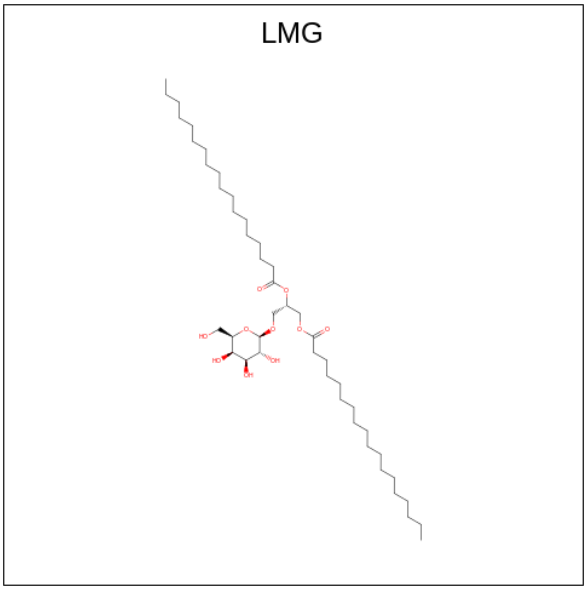
Mol	Chain	Residues	Atoms	AltConf
22	A	1	Total Fe S 8 4 4	0
22	C	1	Total Fe S 8 4 4	0
22	C	1	Total Fe S 8 4 4	0

- Molecule 23 is DODECYL-ALPHA-D-MALTOSIDE (three-letter code: LMU) (formula: $C_{24}H_{46}O_{11}$).



Mol	Chain	Residues	Atoms	AltConf
23	A	1	Total C O 33 23 10	0
23	A	1	Total C O 34 24 10	0
23	A	1	Total C O 34 24 10	0
23	K	1	Total C O 35 24 11	0
23	5	1	Total C O 33 22 11	0
23	8	1	Total C O 35 24 11	0
23	8	1	Total C O 35 24 11	0

- Molecule 24 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: LMG) (formula: $C_{45}H_{86}O_{10}$).



Mol	Chain	Residues	Atoms	AltConf
24	A	1	Total C O 40 30 10	0
24	J	1	Total C O 40 30 10	0
24	4	1	Total C O 40 30 10	0
24	4	1	Total C O 40 30 10	0

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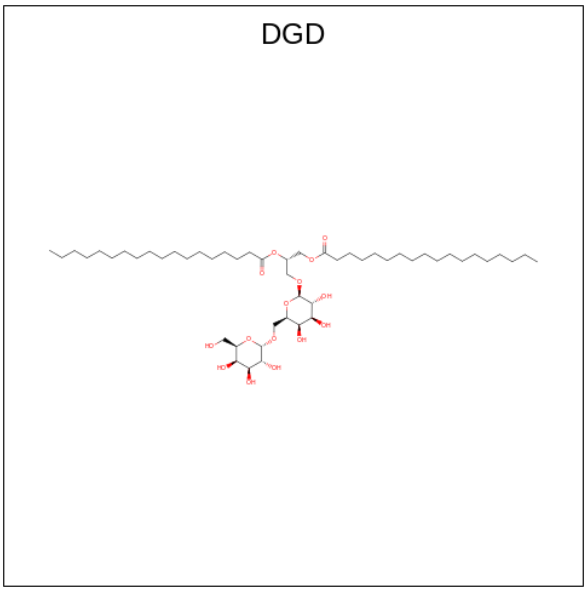
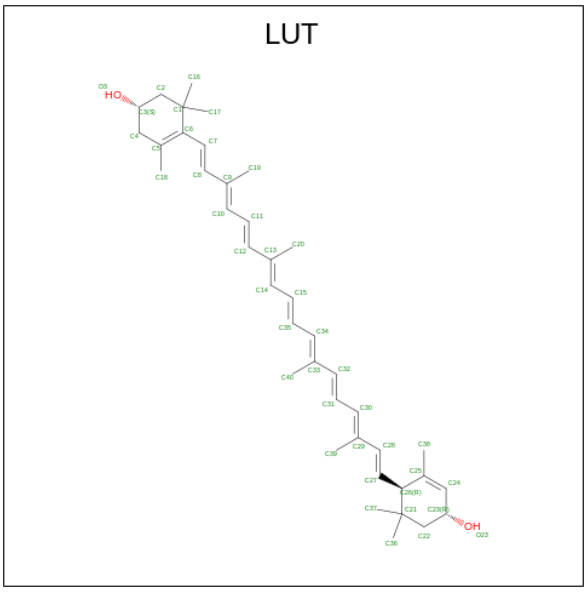
Mol	Chain	Residues	Atoms			AltConf
24	5	1	Total 40	C 30	O 10	0
24	5	1	Total 40	C 30	O 10	0
24	7	1	Total 44	C 34	O 10	0

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



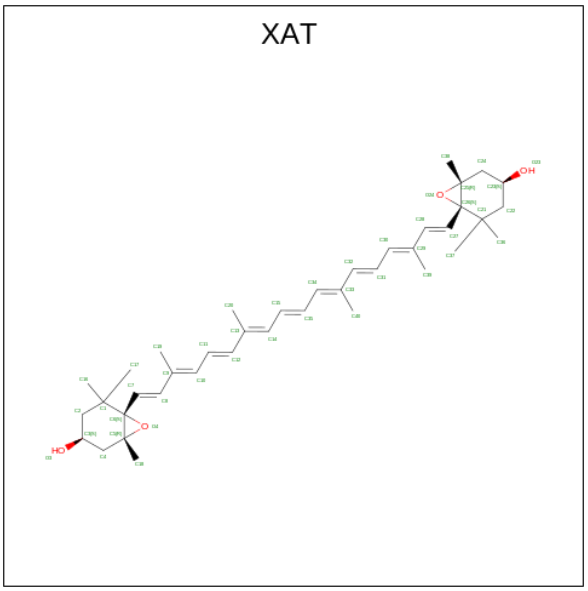
Mol	Chain	Residues	Atoms			AltConf
25	B	1	Total 62	C 47	O 15	0
25	J	1	Total 58	C 43	O 15	0

- Molecule 26 is (3R,3'R,6S)-4,5-DIDEHYDRO-5,6-DIHYDRO-BETA,BETA-CAROTENE-3 ,3'-DIOL (three-letter code: LUT) (formula: $C_{40}H_{56}O_2$).



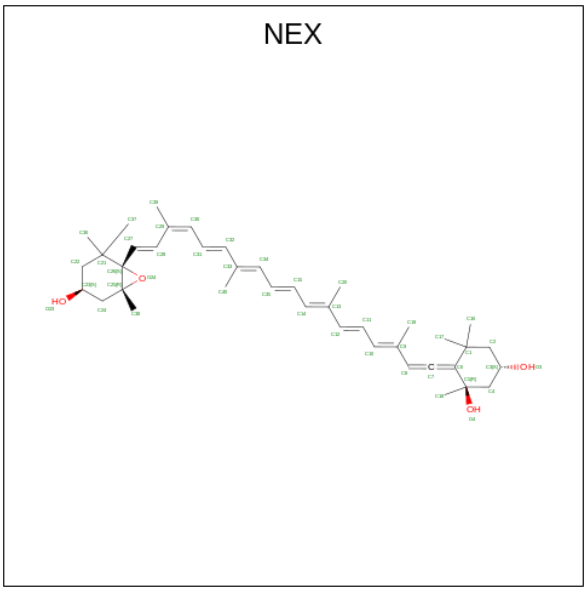
Mol	Chain	Residues	Atoms	AltConf
26	1	1	Total C O 42 40 2	0
26	a	1	Total C O 42 40 2	0
26	3	1	Total C O 42 40 2	0
26	4	1	Total C O 42 40 2	0
26	5	1	Total C O 42 40 2	0
26	6	1	Total C O 42 40 2	0
26	7	1	Total C O 42 40 2	0
26	8	1	Total C O 42 40 2	0

- Molecule 27 is (3S,5R,6S,3'S,5'R,6'S)-5,6,5',6'-DIEPOXY-5,6,5',6'- TETRAHYDRO-BETA ,BETA-CAROTENE-3,3'-DIOL (three-letter code: XAT) (formula: $C_{40}H_{56}O_4$).



Mol	Chain	Residues	Atoms			AltConf
27	1	1	Total	C	O	0
			44	40	4	
27	a	1	Total	C	O	0
			44	40	4	
27	3	1	Total	C	O	0
			44	40	4	
27	4	1	Total	C	O	0
			44	40	4	
27	5	1	Total	C	O	0
			44	40	4	
27	6	1	Total	C	O	0
			44	40	4	
27	7	1	Total	C	O	0
			44	40	4	
27	8	1	Total	C	O	0
			44	40	4	

- Molecule 28 is (1R,3R)-6-{(3E,5E,7E,9E,11E,13E,15E,17E)-18-[(1S,4R,6R)-4-HYDROXY-2,2,6-TRIMETHYL-7-OXABICYCLO[4.1.0]HEPT-1-YL]-3,7,12,16-TETRAMETHYLOCTADECA-1,3,5,7,9,11,13,15,17-NONAENYLIDENE}-1,5,5-TRIMETHYLCYCLOHEXANE-1,3-DIOL (three-letter code: NEX) (formula: $C_{40}H_{56}O_4$).



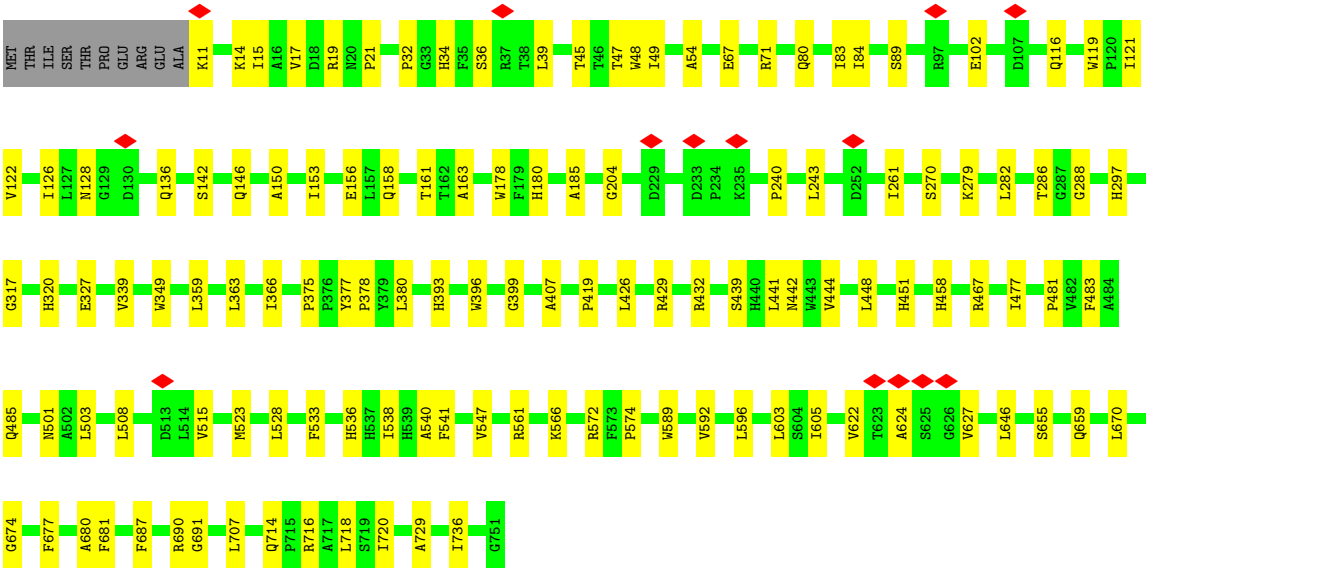
Mol	Chain	Residues	Atoms			AltConf
28	5	1	Total	C	O	0
			44	40	4	
28	6	1	Total	C	O	0
			44	40	4	

3 Residue-property plots (i)

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

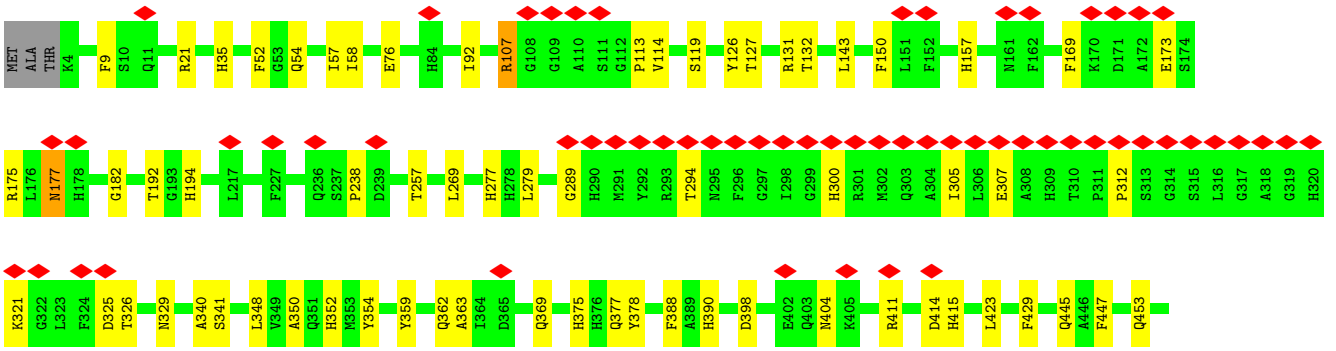
• Molecule 1: PsaA

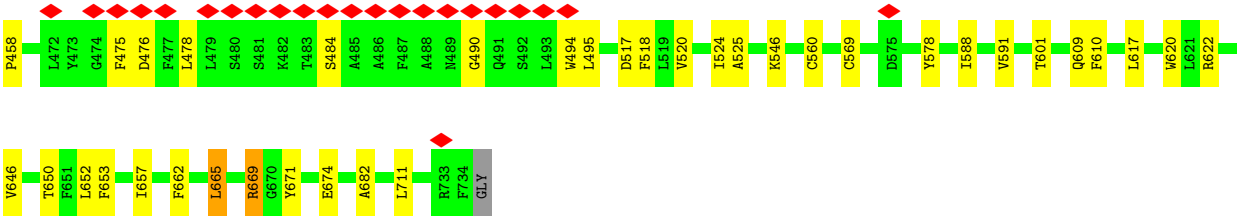
Chain A:



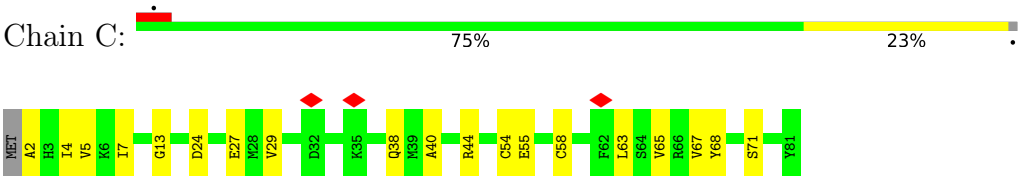
• Molecule 2: PsaB

Chain B:

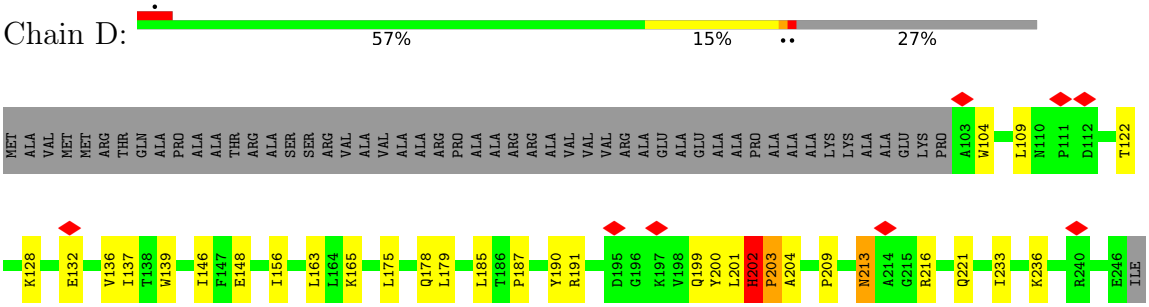




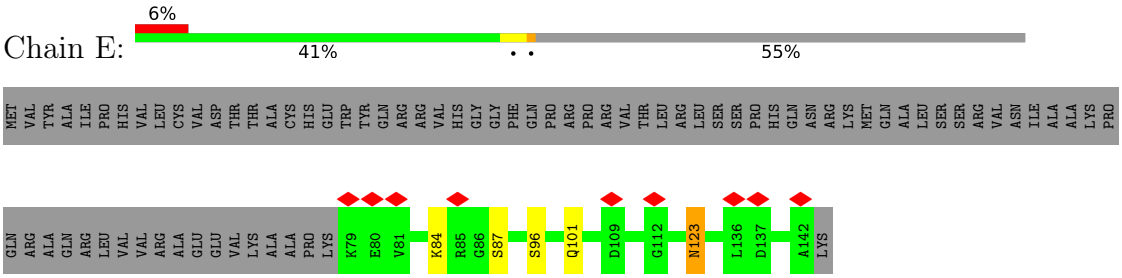
• Molecule 3: PsaC



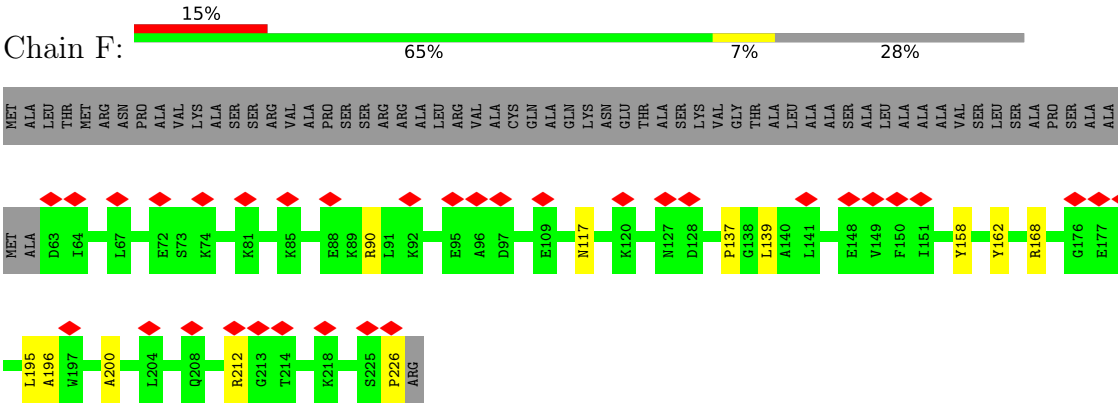
• Molecule 4: PsaD



• Molecule 5: PsaE

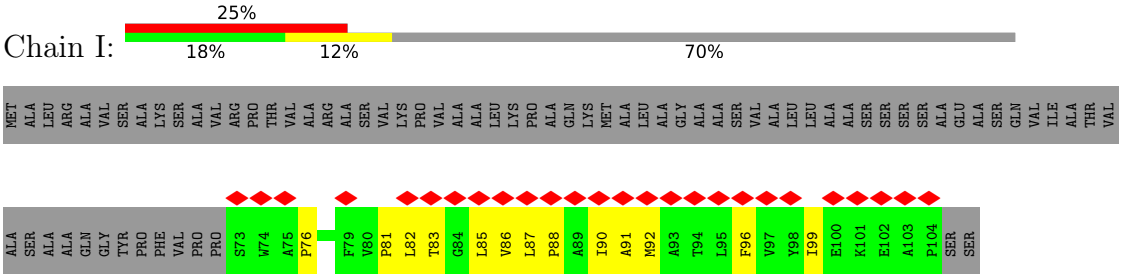


• Molecule 6: PsaF



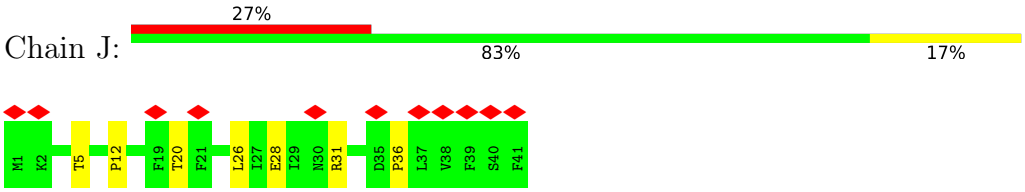
• Molecule 7: PsaI

Chain I:



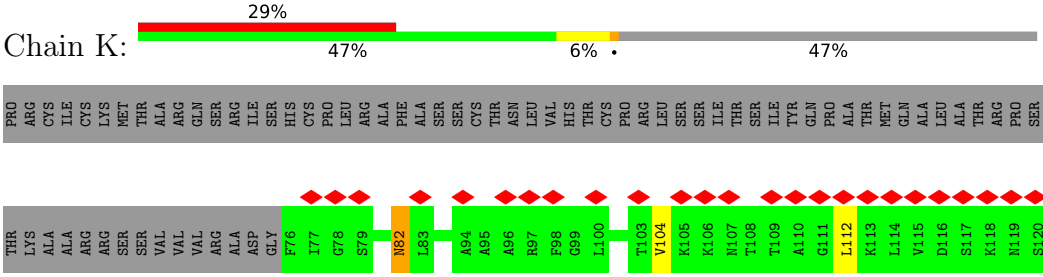
• Molecule 8: PsaJ

Chain J:



• Molecule 9: PsaK

Chain K:

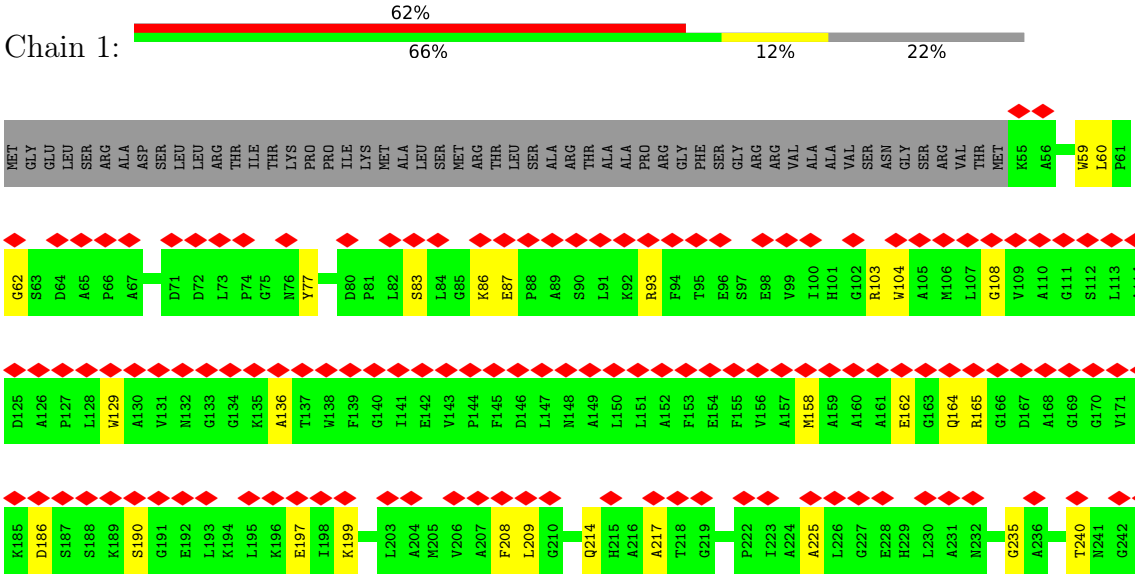


• Molecule 10: PsaL

Chain L:

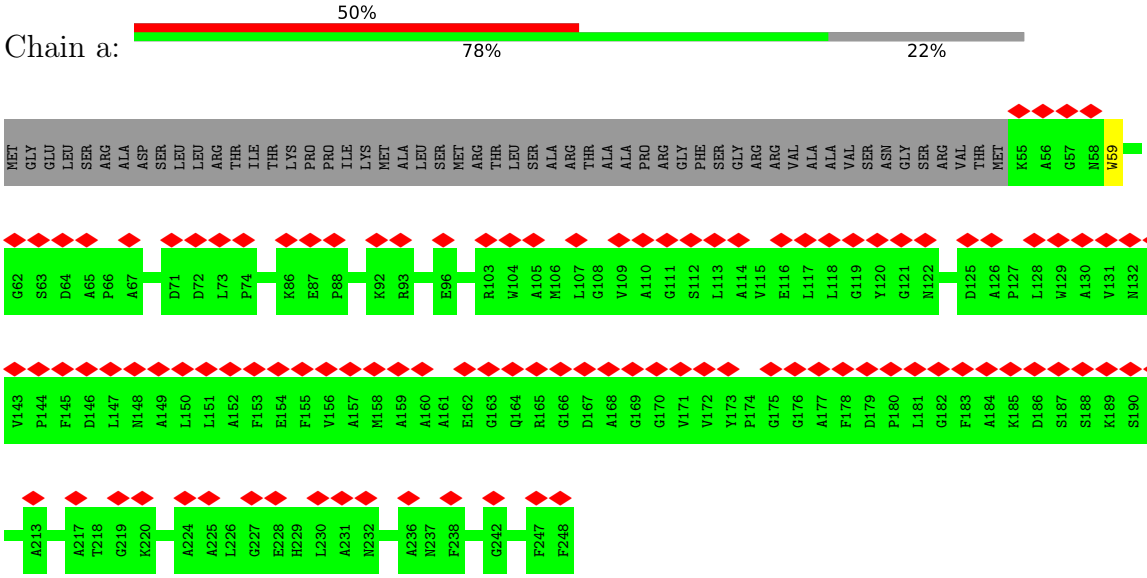
• Molecule 11: Lhca1

Chain 1:



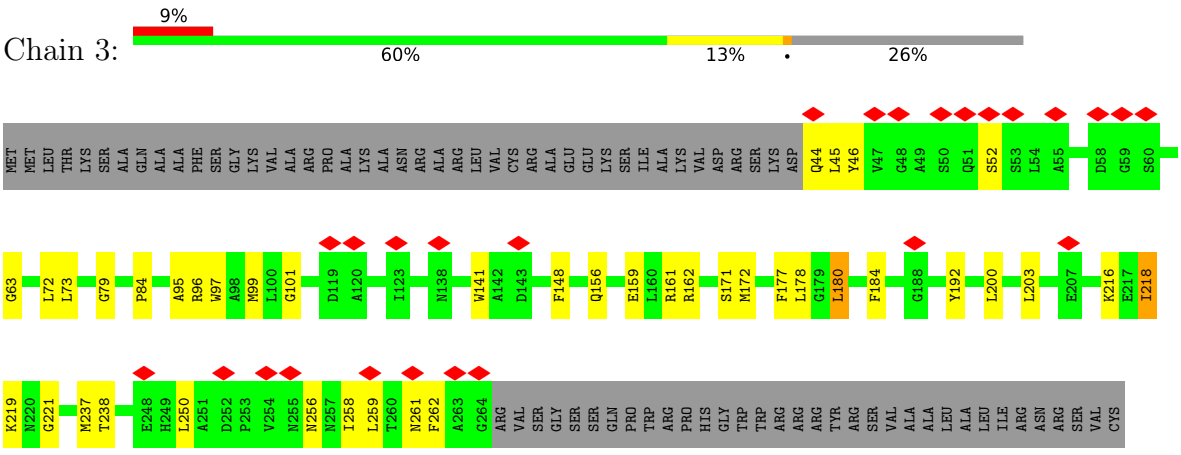
• Molecule 11: Lhca1

Chain a:



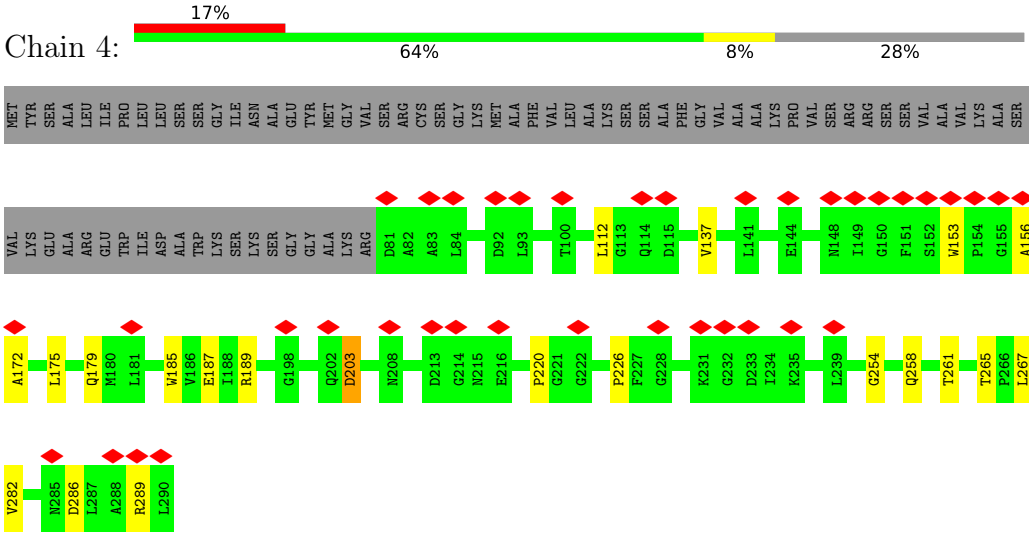
• Molecule 12: Lhca3

Chain 3:



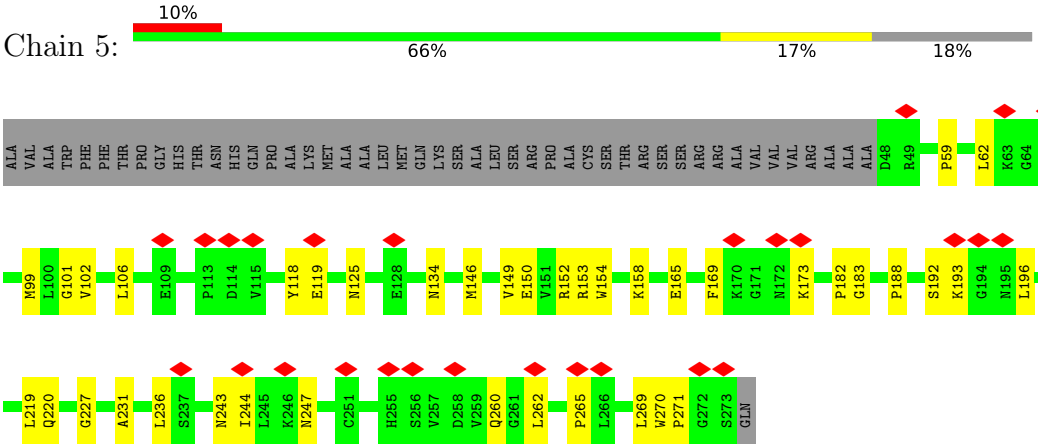
• Molecule 13: Lhca4

Chain 4:



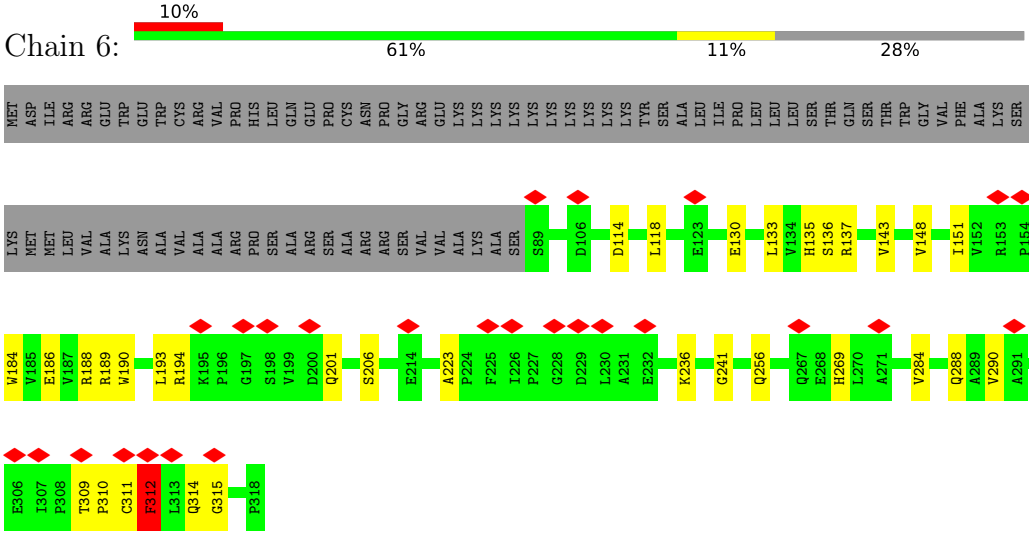
• Molecule 14: Lhca5

Chain 5:



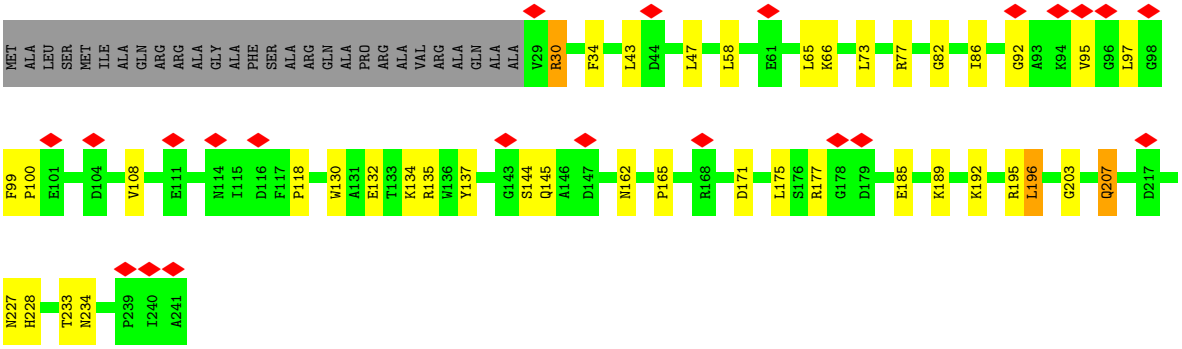
• Molecule 15: Lhca6

Chain 6:

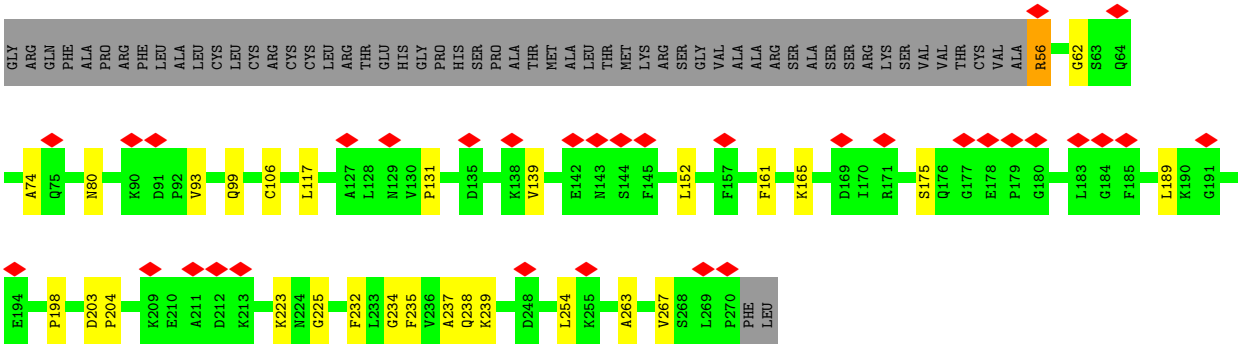


• Molecule 16: Lhca7

Chain 7:



• Molecule 17: Lhca8



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	58955	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 ($e^-/Å^2$)	60.0	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.391	Depositor
Minimum map value	-0.159	Depositor
Average map value	0.004	Depositor
Map value standard deviation	0.022	Depositor
Recommended contour level	0.07	Depositor
Map size (Å)	208.0, 208.0, 208.0	wwPDB
Map dimensions	200, 200, 200	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.04, 1.04, 1.04	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	0.42	0/6015	0.57	1/8201 (0.0%)
2	B	0.41	0/6024	0.58	3/8225 (0.0%)
3	C	0.42	0/610	0.65	0/826
4	D	0.38	0/1157	0.60	0/1563
5	E	0.38	0/515	0.53	0/700
6	F	0.35	0/1280	0.55	0/1733
7	I	0.32	0/250	0.58	0/345
8	J	0.36	0/349	0.56	0/478
9	K	0.30	0/583	0.65	0/790
10	L	0.30	0/779	0.61	1/1063 (0.1%)
11	1	0.32	0/1478	0.55	0/2012
11	a	0.32	0/1490	0.54	0/2028
12	3	0.39	0/1731	0.65	2/2349 (0.1%)
13	4	0.33	0/1686	0.53	0/2300
14	5	0.36	0/1820	0.58	1/2480 (0.0%)
15	6	0.35	0/1833	0.57	0/2505
16	7	0.38	0/1701	0.60	1/2310 (0.0%)
17	8	0.36	0/1680	0.63	0/2288
All	All	0.38	0/30981	0.58	9/42196 (0.0%)

There are no bond length outliers.

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	3	180	LEU	CA-CB-CG	6.97	131.34	115.30
2	B	665	LEU	CB-CG-CD2	-6.66	99.68	111.00
12	3	200	LEU	CA-CB-CG	6.59	130.46	115.30
16	7	196	LEU	CA-CB-CG	6.08	129.29	115.30
14	5	106	LEU	CA-CB-CG	5.88	128.82	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5819	0	5672	100	0
2	B	5812	0	5569	83	0
3	C	600	0	589	12	0
4	D	1129	0	1144	33	0
5	E	505	0	504	4	0
6	F	1254	0	1288	14	0
7	I	242	0	252	9	0
8	J	337	0	336	7	0
9	K	578	0	617	9	0
10	L	761	0	768	18	0
11	1	1433	0	1387	25	0
11	a	1444	0	1396	0	0
12	3	1683	0	1641	33	0
13	4	1631	0	1587	21	0
14	5	1765	0	1738	39	0
15	6	1771	0	1772	27	0
16	7	1649	0	1589	35	0
17	8	1630	0	1609	25	0
18	1	675	0	541	23	0
18	3	724	0	628	22	0
18	4	782	0	686	23	0
18	5	878	0	758	36	0
18	6	893	0	809	25	0
18	7	758	0	641	20	0
18	8	727	0	635	17	0
18	A	2625	0	2614	122	0
18	B	2277	0	2218	91	0
18	F	140	0	113	5	0
18	J	42	0	31	0	0
18	K	201	0	171	5	0
18	L	135	0	99	8	0
18	a	722	0	618	0	0
19	A	33	0	46	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	B	33	0	46	2	0
20	1	49	0	74	2	0
20	3	94	0	137	6	0
20	4	49	0	74	4	0
20	5	98	0	148	5	0
20	6	48	0	69	1	0
20	7	37	0	44	5	0
20	8	98	0	148	9	0
20	A	79	0	104	3	0
20	B	36	0	41	1	0
20	a	49	0	74	0	0
21	1	40	0	56	2	0
21	3	120	0	168	13	0
21	4	40	0	56	3	0
21	5	40	0	56	3	0
21	6	40	0	56	4	0
21	7	80	0	112	5	0
21	8	40	0	56	2	0
21	A	240	0	336	24	0
21	B	280	0	392	20	0
21	F	40	0	56	6	0
21	J	40	0	56	2	0
21	K	80	0	112	6	0
21	L	80	0	112	8	0
21	a	40	0	56	0	0
22	A	8	0	0	0	0
22	C	16	0	0	0	0
23	5	33	0	39	0	0
23	8	70	0	92	1	0
23	A	101	0	130	6	0
23	K	35	0	46	0	0
24	4	80	0	100	1	0
24	5	80	0	100	3	0
24	7	44	0	61	0	0
24	A	40	0	50	0	0
24	J	40	0	50	4	0
25	B	62	0	85	3	0
25	J	58	0	77	3	0
26	1	42	0	56	3	0
26	3	42	0	56	2	0
26	4	42	0	56	6	0
26	5	42	0	56	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
26	6	42	0	56	2	0
26	7	42	0	56	3	0
26	8	42	0	56	5	0
26	a	42	0	56	0	0
27	1	44	0	56	3	0
27	3	44	0	56	2	0
27	4	44	0	56	2	0
27	5	44	0	56	6	0
27	6	44	0	56	2	0
27	7	44	0	56	4	0
27	8	44	0	56	2	0
27	a	44	0	56	0	0
28	5	44	0	56	4	0
28	6	44	0	56	4	0
All	All	44968	0	44543	755	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 9.

The worst 5 of 755 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)
4:D:202:HIS:HB3	4:D:203:PRO:CD	1.63	1.28
4:D:202:HIS:CB	4:D:203:PRO:HD3	1.75	1.16
4:D:202:HIS:HB3	4:D:203:PRO:HD3	1.17	1.12
4:D:202:HIS:CG	4:D:203:PRO:HD3	1.95	1.01
12:3:46:TYR:OH	20:3:624:LHG:HC42	1.80	0.82

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	739/751 (98%)	708 (96%)	31 (4%)	0	100	100
2	B	729/735 (99%)	699 (96%)	30 (4%)	0	100	100
3	C	78/81 (96%)	74 (95%)	4 (5%)	0	100	100
4	D	142/196 (72%)	131 (92%)	9 (6%)	2 (1%)	9	31
5	E	62/143 (43%)	58 (94%)	4 (6%)	0	100	100
6	F	162/227 (71%)	149 (92%)	13 (8%)	0	100	100
7	I	30/106 (28%)	28 (93%)	2 (7%)	0	100	100
8	J	39/41 (95%)	37 (95%)	2 (5%)	0	100	100
9	K	83/160 (52%)	73 (88%)	10 (12%)	0	100	100
10	L	101/258 (39%)	98 (97%)	3 (3%)	0	100	100
11	1	191/248 (77%)	171 (90%)	19 (10%)	1 (0%)	25	56
11	a	192/248 (77%)	175 (91%)	16 (8%)	1 (0%)	25	56
12	3	219/298 (74%)	202 (92%)	17 (8%)	0	100	100
13	4	208/290 (72%)	196 (94%)	12 (6%)	0	100	100
14	5	224/274 (82%)	198 (88%)	26 (12%)	0	100	100
15	6	228/318 (72%)	206 (90%)	21 (9%)	1 (0%)	30	60
16	7	211/241 (88%)	193 (92%)	18 (8%)	0	100	100
17	8	213/272 (78%)	198 (93%)	15 (7%)	0	100	100
All	All	3851/4887 (79%)	3594 (93%)	252 (6%)	5 (0%)	50	77

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	D	202	HIS
4	D	203	PRO
15	6	312	PHE
11	1	59	TRP
11	a	59	TRP

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	601/610 (98%)	600 (100%)	1 (0%)	92 98
2	B	595/597 (100%)	590 (99%)	5 (1%)	79 93
3	C	69/70 (99%)	69 (100%)	0	100 100
4	D	120/152 (79%)	118 (98%)	2 (2%)	56 83
5	E	55/123 (45%)	54 (98%)	1 (2%)	54 82
6	F	126/169 (75%)	125 (99%)	1 (1%)	79 93
7	I	26/76 (34%)	26 (100%)	0	100 100
8	J	37/37 (100%)	37 (100%)	0	100 100
9	K	59/123 (48%)	58 (98%)	1 (2%)	56 83
10	L	74/198 (37%)	73 (99%)	1 (1%)	62 86
11	1	136/180 (76%)	136 (100%)	0	100 100
11	a	137/180 (76%)	137 (100%)	0	100 100
12	3	167/230 (73%)	165 (99%)	2 (1%)	67 89
13	4	165/226 (73%)	164 (99%)	1 (1%)	84 95
14	5	183/219 (84%)	182 (100%)	1 (0%)	86 96
15	6	184/260 (71%)	182 (99%)	2 (1%)	70 90
16	7	164/181 (91%)	159 (97%)	5 (3%)	36 71
17	8	161/207 (78%)	158 (98%)	3 (2%)	52 81
All	All	3059/3838 (80%)	3033 (99%)	26 (1%)	77 93

5 of 26 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
13	4	203	ASP
15	6	312	PHE
17	8	99	GLN
15	6	311	CYS
16	7	30	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 14 such sidechains are listed below:

Mol	Chain	Res	Type
5	E	123	ASN
13	4	114	GLN
16	7	234	ASN
15	6	314	GLN

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Mol	Chain	Res	Type
16	7	227	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

299 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	$\#\|Z\| > 2$
26	LUT	6	619	-	42,43,43	0.76	0	51,60,60	1.57	12 (23%)
18	CLA	a	601	11	53,62,73	1.62	8 (15%)	61,100,113	1.47	7 (11%)
18	CLA	3	614	-	39,48,73	1.87	7 (17%)	44,83,113	1.66	7 (15%)
18	CLA	A	811	-	65,73,73	1.43	7 (10%)	76,113,113	1.44	7 (9%)
24	LMG	4	624	-	40,40,55	0.91	1 (2%)	48,48,63	1.22	4 (8%)
18	CLA	B	840	-	65,73,73	1.46	8 (12%)	76,113,113	1.52	6 (7%)
18	CLA	A	837	1	45,53,73	1.78	8 (17%)	52,89,113	1.74	10 (19%)
18	CLA	6	608	-	51,59,73	1.64	7 (13%)	59,96,113	1.60	6 (10%)
18	CLA	7	613	16	65,73,73	1.46	8 (12%)	76,113,113	1.43	9 (11%)
18	CLA	8	616	17	43,51,73	1.87	6 (13%)	54,87,113	1.82	12 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
21	BCR	K	202	-	41,41,41	0.72	0	56,56,56	2.06	15 (26%)
18	CLA	5	608	-	50,58,73	1.63	8 (16%)	58,95,113	1.69	8 (13%)
21	BCR	1	619	-	41,41,41	0.66	0	56,56,56	1.93	16 (28%)
27	XAT	1	618	-	39,47,47	0.86	1 (2%)	54,74,74	2.59	20 (37%)
18	CLA	B	822	-	42,50,73	1.85	5 (11%)	48,85,113	1.67	7 (14%)
18	CLA	5	603	-	54,62,73	1.68	9 (16%)	67,100,113	1.42	8 (11%)
18	CLA	6	616	15	65,73,73	1.45	6 (9%)	76,113,113	1.59	11 (14%)
27	XAT	8	620	-	39,47,47	0.92	1 (2%)	54,74,74	2.67	19 (35%)
24	LMG	J	104	-	40,40,55	0.90	2 (5%)	48,48,63	1.22	4 (8%)
28	NEX	5	624	-	38,46,46	1.00	1 (2%)	50,70,70	2.18	16 (32%)
18	CLA	6	606	-	39,48,73	1.83	6 (15%)	44,83,113	1.75	8 (18%)
21	BCR	B	847	-	41,41,41	0.73	0	56,56,56	2.00	18 (32%)
18	CLA	8	613	17	65,73,73	1.45	8 (12%)	76,113,113	1.56	8 (10%)
18	CLA	4	603	13	44,52,73	1.83	8 (18%)	55,88,113	1.76	10 (18%)
18	CLA	4	611	20	42,50,73	1.78	7 (16%)	48,85,113	1.60	8 (16%)
18	CLA	A	817	-	45,53,73	1.71	7 (15%)	52,89,113	1.97	11 (21%)
21	BCR	A	848	-	41,41,41	0.77	0	56,56,56	1.86	15 (26%)
18	CLA	1	612	11	45,53,73	1.77	6 (13%)	52,89,113	1.63	7 (13%)
18	CLA	4	610	13	61,69,73	1.48	7 (11%)	71,108,113	1.55	8 (11%)
18	CLA	3	608	-	55,63,73	1.64	11 (20%)	64,101,113	1.49	7 (10%)
26	LUT	5	620	-	42,43,43	0.77	0	51,60,60	1.64	13 (25%)
21	BCR	L	301	-	41,41,41	0.75	0	56,56,56	1.84	15 (26%)
21	BCR	B	846	-	41,41,41	0.73	0	56,56,56	2.05	16 (28%)
19	PQN	A	844	-	34,34,34	2.87	11 (32%)	42,45,45	2.23	7 (16%)
18	CLA	A	820	-	65,73,73	1.47	10 (15%)	76,113,113	1.65	11 (14%)
18	CLA	A	824	-	41,49,73	1.82	6 (14%)	47,84,113	1.76	11 (23%)
18	CLA	7	612	16	44,52,73	1.86	8 (18%)	51,88,113	1.53	9 (17%)
18	CLA	L	304	-	45,53,73	1.79	5 (11%)	52,89,113	1.62	6 (11%)
18	CLA	A	819	-	59,67,73	1.58	10 (16%)	68,105,113	1.39	5 (7%)
18	CLA	A	835	-	61,69,73	1.47	9 (14%)	71,108,113	1.68	12 (16%)
18	CLA	4	602	13	60,68,73	1.46	8 (13%)	70,107,113	1.62	8 (11%)
18	CLA	5	609	14	65,73,73	1.46	8 (12%)	76,113,113	1.46	9 (11%)
18	CLA	6	611	20	42,50,73	1.75	7 (16%)	48,85,113	1.61	7 (14%)
18	CLA	6	612	15	40,49,73	1.83	7 (17%)	45,84,113	1.77	7 (15%)
18	CLA	6	618	15	39,48,73	1.87	8 (20%)	48,83,113	1.84	9 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
21	BCR	A	850	-	41,41,41	0.75	0	56,56,56	1.95	15 (26%)
18	CLA	3	615	-	39,48,73	1.90	8 (20%)	44,83,113	1.78	7 (15%)
18	CLA	B	805	-	65,73,73	1.39	8 (12%)	76,113,113	1.53	8 (10%)
23	LMU	A	859	-	35,35,36	1.27	3 (8%)	43,45,47	1.23	4 (9%)
18	CLA	A	826	-	64,72,73	1.42	8 (12%)	74,111,113	1.55	8 (10%)
21	BCR	7	623	-	41,41,41	0.71	0	56,56,56	1.81	13 (23%)
27	XAT	6	621	-	39,47,47	0.92	2 (5%)	54,74,74	2.72	20 (37%)
18	CLA	A	845	20	50,58,73	1.66	7 (14%)	58,95,113	1.59	6 (10%)
18	CLA	5	616	14	41,50,73	1.89	9 (21%)	50,85,113	1.62	8 (16%)
18	CLA	5	618	14	39,48,73	1.92	8 (20%)	48,83,113	1.79	9 (18%)
20	LHG	A	846	-	48,48,48	0.71	1 (2%)	51,54,54	1.27	6 (11%)
18	CLA	B	814	-	64,72,73	1.43	8 (12%)	74,111,113	1.53	7 (9%)
18	CLA	5	617	-	50,58,73	1.66	8 (16%)	58,95,113	1.62	8 (13%)
18	CLA	A	823	-	42,50,73	1.77	9 (21%)	48,85,113	1.71	7 (14%)
18	CLA	B	813	-	65,73,73	1.46	7 (10%)	76,113,113	1.46	9 (11%)
18	CLA	a	607	-	45,53,73	1.75	6 (13%)	52,89,113	1.65	8 (15%)
18	CLA	6	604	-	65,73,73	1.45	9 (13%)	76,113,113	1.38	7 (9%)
18	CLA	A	836	-	65,73,73	1.46	9 (13%)	76,113,113	1.44	7 (9%)
18	CLA	4	618	13	39,48,73	1.91	8 (20%)	48,83,113	1.79	10 (20%)
18	CLA	4	612	13	40,49,73	1.84	7 (17%)	45,84,113	1.69	8 (17%)
18	CLA	a	612	11	45,53,73	1.77	7 (15%)	52,89,113	1.62	7 (13%)
18	CLA	a	604	-	49,57,73	1.68	7 (14%)	55,93,113	1.74	9 (16%)
18	CLA	A	821	-	53,61,73	1.59	8 (15%)	61,98,113	1.59	7 (11%)
18	CLA	5	606	-	39,48,73	1.91	7 (17%)	44,83,113	1.56	7 (15%)
18	CLA	8	612	17	40,49,73	1.80	7 (17%)	45,84,113	1.75	9 (20%)
18	CLA	B	827	-	62,70,73	1.46	8 (12%)	72,109,113	1.53	7 (9%)
18	CLA	4	604	-	54,62,73	1.67	8 (14%)	67,100,113	1.46	9 (13%)
20	LHG	6	623	18	47,47,48	0.65	1 (2%)	50,53,54	1.27	6 (12%)
21	BCR	8	621	-	41,41,41	0.71	0	56,56,56	1.94	18 (32%)
21	BCR	7	621	-	41,41,41	0.73	0	56,56,56	2.02	22 (39%)
27	XAT	a	618	-	39,47,47	0.87	1 (2%)	54,74,74	2.61	20 (37%)
18	CLA	6	610	15	65,73,73	1.44	7 (10%)	76,113,113	1.40	7 (9%)
18	CLA	5	614	-	45,52,73	1.91	7 (15%)	48,87,113	1.65	8 (16%)
24	LMG	A	860	-	40,40,55	0.93	2 (5%)	48,48,63	1.27	5 (10%)
18	CLA	7	604	-	54,62,73	1.59	7 (12%)	63,100,113	1.62	8 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
18	CLA	B	820	-	50,58,73	1.70	6 (12%)	58,95,113	1.62	7 (12%)
18	CLA	B	828	-	65,73,73	1.43	9 (13%)	76,113,113	1.46	8 (10%)
18	CLA	B	836	-	50,58,73	1.62	7 (14%)	58,95,113	1.65	6 (10%)
18	CLA	6	613	-	63,72,73	1.47	8 (12%)	73,112,113	1.49	9 (12%)
18	CLA	8	603	-	44,52,73	1.80	8 (18%)	55,88,113	1.79	9 (16%)
18	CLA	A	809	1	65,73,73	1.40	7 (10%)	76,113,113	1.49	7 (9%)
20	LHG	3	623	-	44,44,48	0.60	0	47,50,54	1.26	6 (12%)
20	LHG	1	620	18	48,48,48	0.60	0	51,54,54	1.24	6 (11%)
18	CLA	B	811	-	54,62,73	1.63	7 (12%)	67,100,113	1.52	9 (13%)
27	XAT	4	620	-	39,47,47	0.89	1 (2%)	54,74,74	2.61	18 (33%)
18	CLA	5	607	-	65,73,73	1.45	8 (12%)	76,113,113	1.70	13 (17%)
18	CLA	8	601	17	65,73,73	1.46	10 (15%)	76,113,113	1.44	10 (13%)
18	CLA	a	616	11	45,53,73	1.74	6 (13%)	52,89,113	1.55	7 (13%)
18	CLA	7	602	16	65,73,73	1.44	9 (13%)	76,113,113	1.40	8 (10%)
23	LMU	8	625	-	36,36,36	1.19	2 (5%)	47,47,47	1.27	6 (12%)
21	BCR	L	305	-	41,41,41	0.68	0	56,56,56	1.77	12 (21%)
18	CLA	K	206	9	45,53,73	1.77	7 (15%)	52,89,113	1.68	7 (13%)
18	CLA	7	615	-	38,47,73	1.91	7 (18%)	46,81,113	1.74	8 (17%)
18	CLA	1	609	11	40,48,73	1.96	6 (15%)	50,83,113	1.78	10 (20%)
18	CLA	B	834	-	60,68,73	1.55	8 (13%)	70,107,113	1.47	9 (12%)
18	CLA	1	610	11	38,47,73	1.93	7 (18%)	44,81,113	1.73	8 (18%)
18	CLA	3	602	12	60,68,73	1.45	9 (15%)	70,107,113	1.51	7 (10%)
18	CLA	B	810	-	65,73,73	1.46	6 (9%)	76,113,113	1.40	7 (9%)
18	CLA	K	203	-	65,73,73	1.48	6 (9%)	76,113,113	1.41	10 (13%)
18	CLA	4	613	13	65,73,73	1.47	7 (10%)	76,113,113	1.45	7 (9%)
23	LMU	5	628	-	34,34,36	1.26	2 (5%)	45,45,47	1.31	7 (15%)
18	CLA	5	619	-	43,51,73	1.85	8 (18%)	54,87,113	1.95	11 (20%)
22	SF4	A	853	-	0,12,12	-	-	-		
18	CLA	1	601	11	53,62,73	1.62	8 (15%)	61,100,113	1.45	9 (14%)
18	CLA	A	802	-	65,73,73	1.39	8 (12%)	76,113,113	1.71	10 (13%)
21	BCR	5	622	-	41,41,41	0.69	0	56,56,56	2.11	20 (35%)
18	CLA	1	606	11	37,47,73	1.92	6 (16%)	41,80,113	1.70	7 (17%)
18	CLA	3	607	12	56,64,73	1.61	7 (12%)	69,102,113	1.54	11 (15%)
23	LMU	K	208	-	36,36,36	1.21	2 (5%)	47,47,47	1.33	5 (10%)
21	BCR	a	619	-	41,41,41	0.69	0	56,56,56	1.93	16 (28%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
18	CLA	B	807	-	52,60,73	1.64	9 (17%)	60,97,113	1.53	9 (15%)
18	CLA	A	833	-	45,53,73	1.72	6 (13%)	52,89,113	1.77	6 (11%)
18	CLA	1	603	-	53,62,73	1.65	6 (11%)	61,100,113	1.61	8 (13%)
21	BCR	A	852	-	41,41,41	0.78	1 (2%)	56,56,56	2.10	16 (28%)
18	CLA	A	810	1	50,58,73	1.66	10 (20%)	58,95,113	1.52	10 (17%)
18	CLA	a	614	-	55,62,73	1.70	7 (12%)	60,99,113	1.50	7 (11%)
18	CLA	A	832	-	50,58,73	1.64	8 (16%)	58,95,113	1.60	8 (13%)
18	CLA	3	606	-	53,62,73	1.63	7 (13%)	61,100,113	1.51	7 (11%)
18	CLA	B	829	-	65,73,73	1.51	9 (13%)	76,113,113	1.68	9 (11%)
18	CLA	B	821	-	46,54,73	1.80	6 (13%)	53,90,113	1.60	8 (15%)
18	CLA	F	301	-	57,65,73	1.59	9 (15%)	66,103,113	1.41	9 (13%)
18	CLA	7	614	-	42,50,73	1.78	7 (16%)	48,85,113	1.67	8 (16%)
18	CLA	8	614	-	56,64,73	1.54	7 (12%)	65,102,113	1.58	9 (13%)
21	BCR	A	856	-	41,41,41	0.72	0	56,56,56	1.96	17 (30%)
25	DGD	B	850	-	63,63,67	0.98	1 (1%)	77,77,81	1.42	11 (14%)
27	XAT	7	620	-	39,47,47	0.91	2 (5%)	54,74,74	2.67	20 (37%)
18	CLA	B	841	20	44,52,73	1.82	5 (11%)	50,87,113	1.60	9 (18%)
18	CLA	8	609	17	45,53,73	1.73	7 (15%)	52,89,113	1.71	6 (11%)
18	CLA	B	802	-	65,73,73	1.46	9 (13%)	76,113,113	1.35	8 (10%)
18	CLA	8	610	17	60,68,73	1.44	7 (11%)	70,107,113	1.50	7 (10%)
18	CLA	4	607	-	45,53,73	1.75	7 (15%)	52,89,113	1.73	7 (13%)
18	CLA	B	817	-	59,67,73	1.54	9 (15%)	68,105,113	1.58	8 (11%)
20	LHG	5	625	-	48,48,48	0.61	0	51,54,54	1.25	6 (11%)
18	CLA	F	304	-	41,49,73	1.82	6 (14%)	47,84,113	1.70	9 (19%)
21	BCR	3	621	-	41,41,41	0.70	0	56,56,56	2.46	20 (35%)
18	CLA	A	830	-	65,73,73	1.43	8 (12%)	76,113,113	1.53	10 (13%)
18	CLA	A	840	-	52,60,73	1.62	7 (13%)	60,97,113	1.68	11 (18%)
18	CLA	B	803	-	65,73,73	1.39	9 (13%)	76,113,113	1.92	13 (17%)
18	CLA	B	812	-	43,51,73	1.80	6 (13%)	49,86,113	1.62	6 (12%)
18	CLA	8	604	-	50,58,73	1.65	6 (12%)	58,95,113	1.63	7 (12%)
20	LHG	8	622	18	48,48,48	0.94	2 (4%)	51,54,54	1.04	3 (5%)
18	CLA	3	604	-	65,73,73	1.47	7 (10%)	76,113,113	1.46	6 (7%)
18	CLA	A	806	-	65,73,73	1.47	9 (13%)	76,113,113	1.66	11 (14%)
21	BCR	K	207	-	41,41,41	0.75	0	56,56,56	1.78	14 (25%)
21	BCR	6	622	-	41,41,41	0.72	0	56,56,56	1.95	17 (30%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
18	CLA	6	614	-	60,68,73	1.52	7 (11%)	70,107,113	1.51	7 (10%)
18	CLA	B	819	-	55,63,73	1.63	7 (12%)	64,101,113	1.52	6 (9%)
25	DGD	J	103	-	59,59,67	0.99	3 (5%)	73,73,81	1.47	10 (13%)
22	SF4	C	101	-	0,12,12	-	-	-		
21	BCR	B	844	-	41,41,41	0.73	0	56,56,56	2.03	18 (32%)
18	CLA	K	204	-	46,54,73	1.70	7 (15%)	53,90,113	1.65	6 (11%)
18	CLA	8	606	-	64,72,73	1.50	7 (10%)	75,112,113	1.35	6 (8%)
18	CLA	A	822	-	65,73,73	1.47	8 (12%)	76,113,113	1.53	7 (9%)
18	CLA	B	823	-	45,53,73	1.79	6 (13%)	52,89,113	1.58	6 (11%)
26	LUT	8	619	-	42,43,43	0.77	0	51,60,60	1.58	10 (19%)
18	CLA	A	854	-	65,73,73	1.46	9 (13%)	76,113,113	1.57	11 (14%)
20	LHG	5	623	18	48,48,48	0.62	1 (2%)	51,54,54	1.25	6 (11%)
18	CLA	F	303	-	42,50,73	1.87	8 (19%)	48,85,113	1.65	7 (14%)
18	CLA	4	601	13	65,73,73	1.50	10 (15%)	76,113,113	1.32	7 (9%)
21	BCR	A	849	-	41,41,41	0.83	0	56,56,56	2.03	18 (32%)
18	CLA	6	602	15	65,73,73	1.46	9 (13%)	76,113,113	1.45	8 (10%)
24	LMG	5	626	-	40,40,55	0.88	0	48,48,63	1.20	5 (10%)
21	BCR	F	305	-	41,41,41	0.78	0	56,56,56	2.14	18 (32%)
23	LMU	8	624	-	36,36,36	1.20	2 (5%)	47,47,47	0.96	2 (4%)
27	XAT	5	621	-	39,47,47	0.93	0	54,74,74	2.78	21 (38%)
21	BCR	B	848	-	41,41,41	0.79	0	56,56,56	1.78	11 (19%)
21	BCR	B	801	-	41,41,41	0.71	0	56,56,56	2.01	13 (23%)
21	BCR	4	621	-	41,41,41	0.68	0	56,56,56	1.94	16 (28%)
18	CLA	8	608	-	51,59,73	1.69	8 (15%)	59,96,113	1.65	8 (13%)
18	CLA	A	818	-	60,68,73	1.48	7 (11%)	70,107,113	1.64	7 (10%)
18	CLA	5	602	14	65,73,73	1.44	7 (10%)	76,113,113	1.54	7 (9%)
18	CLA	5	604	-	63,71,73	1.53	8 (12%)	78,111,113	1.45	9 (11%)
18	CLA	7	609	16	45,53,73	1.67	6 (13%)	52,89,113	1.86	9 (17%)
26	LUT	a	617	-	42,43,43	0.74	0	51,60,60	1.58	12 (23%)
21	BCR	B	843	-	41,41,41	0.70	0	56,56,56	1.94	15 (26%)
23	LMU	A	857	-	34,34,36	1.38	3 (8%)	44,44,47	1.26	4 (9%)
18	CLA	A	812	-	65,73,73	1.41	7 (10%)	76,113,113	1.50	8 (10%)
18	CLA	4	616	13	43,51,73	1.85	8 (18%)	54,87,113	1.71	8 (14%)
27	XAT	3	619	-	39,47,47	0.93	2 (5%)	54,74,74	2.63	21 (38%)
18	CLA	5	601	14	56,64,73	1.58	7 (12%)	65,102,113	1.48	6 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
28	NEX	6	624	-	38,46,46	0.93	2 (5%)	50,70,70	2.28	16 (32%)
18	CLA	A	831	-	65,73,73	1.53	10 (15%)	76,113,113	1.70	14 (18%)
18	CLA	A	814	-	65,73,73	1.39	7 (10%)	76,113,113	1.58	10 (13%)
21	BCR	B	845	-	41,41,41	0.71	0	56,56,56	1.96	17 (30%)
18	CLA	A	838	-	50,58,73	1.56	7 (14%)	58,95,113	1.78	8 (13%)
18	CLA	3	617	12	39,48,73	1.84	9 (23%)	44,83,113	1.67	8 (18%)
18	CLA	5	610	14	54,62,73	1.60	7 (12%)	62,99,113	1.61	7 (11%)
18	CLA	3	612	12	43,51,73	1.79	7 (16%)	49,86,113	1.63	8 (16%)
18	CLA	7	606	-	41,49,73	1.84	8 (19%)	47,84,113	1.72	7 (14%)
18	CLA	1	608	-	43,52,73	1.85	5 (11%)	49,88,113	1.58	6 (12%)
18	CLA	7	603	-	43,52,73	1.79	8 (18%)	49,88,113	1.66	7 (14%)
21	BCR	3	620	-	41,41,41	0.72	0	56,56,56	2.06	19 (33%)
18	CLA	A	828	-	64,72,73	1.42	7 (10%)	74,111,113	1.53	7 (9%)
18	CLA	A	807	1	65,73,73	1.48	10 (15%)	76,113,113	1.43	7 (9%)
18	CLA	1	611	20	65,73,73	1.44	6 (9%)	76,113,113	1.48	8 (10%)
18	CLA	B	806	2	65,73,73	1.45	10 (15%)	76,113,113	1.45	9 (11%)
18	CLA	6	609	15	45,53,73	1.76	9 (20%)	52,89,113	1.67	8 (15%)
18	CLA	6	617	-	45,53,73	1.75	7 (15%)	52,89,113	1.57	6 (11%)
18	CLA	7	601	16	60,68,73	1.50	8 (13%)	70,107,113	1.55	9 (12%)
18	CLA	B	825	-	62,70,73	1.49	8 (12%)	72,109,113	1.39	8 (11%)
18	CLA	A	805	-	52,60,73	1.61	8 (15%)	60,97,113	1.64	8 (13%)
18	CLA	B	824	-	65,73,73	1.54	7 (10%)	76,113,113	1.45	9 (11%)
18	CLA	B	804	-	41,49,73	1.78	8 (19%)	47,84,113	1.78	8 (17%)
18	CLA	L	302	10	45,53,73	1.80	5 (11%)	52,89,113	1.73	8 (15%)
18	CLA	3	603	-	55,63,73	1.62	8 (14%)	64,101,113	1.70	12 (18%)
18	CLA	3	611	20	37,46,73	1.95	7 (18%)	46,81,113	1.81	10 (21%)
18	CLA	B	835	-	45,53,73	1.77	6 (13%)	52,89,113	1.82	9 (17%)
18	CLA	5	612	14	40,49,73	1.80	7 (17%)	45,84,113	1.75	8 (17%)
19	PQN	B	842	-	34,34,34	2.90	11 (32%)	42,45,45	2.04	5 (11%)
18	CLA	B	831	-	65,73,73	1.43	7 (10%)	76,113,113	1.50	6 (7%)
18	CLA	7	607	-	42,50,73	1.79	7 (16%)	48,85,113	1.72	9 (18%)
26	LUT	1	617	-	42,43,43	0.74	0	51,60,60	1.66	14 (27%)
18	CLA	7	608	-	50,58,73	1.68	10 (20%)	58,95,113	1.56	9 (15%)
18	CLA	B	830	-	43,51,73	1.82	9 (20%)	49,86,113	1.81	9 (18%)
18	CLA	A	839	-	55,63,73	1.57	9 (16%)	64,101,113	1.52	8 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
20	LHG	4	622	18	48,48,48	0.62	1 (2%)	51,54,54	1.25	7 (13%)
18	CLA	B	809	2	65,73,73	1.42	9 (13%)	76,113,113	1.49	6 (7%)
18	CLA	1	602	11	61,69,73	1.49	7 (11%)	71,108,113	1.43	7 (9%)
18	CLA	A	816	-	45,53,73	1.72	7 (15%)	52,89,113	1.83	7 (13%)
20	LHG	B	851	18	35,35,48	0.72	1 (2%)	38,40,54	1.33	5 (13%)
21	BCR	J	102	-	41,41,41	0.70	0	56,56,56	1.99	18 (32%)
18	CLA	a	609	11	65,73,73	1.49	6 (9%)	76,113,113	1.43	8 (10%)
18	CLA	A	827	-	59,67,73	1.50	8 (13%)	68,105,113	1.59	10 (14%)
18	CLA	a	610	11	59,67,73	1.55	9 (15%)	69,106,113	1.40	7 (10%)
18	CLA	4	606	-	39,48,73	1.83	7 (17%)	44,83,113	1.71	7 (15%)
18	CLA	6	620	-	45,53,73	1.74	10 (22%)	52,89,113	1.87	11 (21%)
24	LMG	4	623	-	40,40,55	0.89	1 (2%)	48,48,63	1.23	4 (8%)
18	CLA	6	607	-	41,49,73	1.83	8 (19%)	51,84,113	1.87	10 (19%)
18	CLA	4	609	13	61,69,73	1.51	7 (11%)	71,108,113	1.53	10 (14%)
26	LUT	4	619	-	42,43,43	0.79	0	51,60,60	1.62	11 (21%)
18	CLA	a	611	20	37,46,73	1.96	7 (18%)	46,81,113	1.78	9 (19%)
18	CLA	A	813	-	54,62,73	1.53	7 (12%)	62,99,113	1.70	6 (9%)
18	CLA	B	839	-	65,73,73	1.43	8 (12%)	76,113,113	1.47	8 (10%)
18	CLA	8	607	-	41,49,73	1.86	8 (19%)	51,84,113	1.74	9 (17%)
18	CLA	4	614	-	56,64,73	1.60	8 (14%)	65,102,113	1.49	7 (10%)
18	CLA	A	843	-	64,72,73	1.42	8 (12%)	74,111,113	1.44	7 (9%)
18	CLA	8	611	20	42,50,73	1.78	7 (16%)	48,85,113	1.63	8 (16%)
20	LHG	A	847	18	29,29,48	0.83	1 (3%)	32,35,54	1.29	3 (9%)
20	LHG	8	623	-	48,48,48	0.61	0	51,54,54	1.26	6 (11%)
18	CLA	B	816	-	55,63,73	1.56	7 (12%)	64,101,113	1.59	6 (9%)
18	CLA	3	613	12	52,61,73	1.61	8 (15%)	59,98,113	1.62	8 (13%)
18	CLA	a	606	11	43,52,73	1.79	6 (13%)	48,87,113	1.65	5 (10%)
18	CLA	A	815	-	50,58,73	1.67	9 (18%)	58,95,113	1.56	9 (15%)
18	CLA	B	837	-	65,73,73	1.46	7 (10%)	76,113,113	1.42	8 (10%)
18	CLA	A	801	-	65,73,73	1.48	9 (13%)	76,113,113	1.40	7 (9%)
18	CLA	1	604	-	49,57,73	1.69	6 (12%)	55,93,113	1.75	8 (14%)
18	CLA	1	616	11	43,51,73	1.91	8 (18%)	54,87,113	1.64	8 (14%)
18	CLA	a	613	-	65,73,73	1.49	7 (10%)	76,113,113	1.49	8 (10%)
18	CLA	4	608	-	65,73,73	1.44	7 (10%)	76,113,113	1.44	7 (9%)
18	CLA	7	616	16	43,51,73	1.85	7 (16%)	54,87,113	1.66	8 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
21	BCR	3	622	-	41,41,41	0.71	0	56,56,56	2.61	21 (37%)
18	CLA	B	833	-	65,73,73	1.47	7 (10%)	76,113,113	1.53	10 (13%)
18	CLA	A	803	-	65,73,73	1.46	10 (15%)	76,113,113	1.54	7 (9%)
18	CLA	7	610	16	65,73,73	1.43	9 (13%)	76,113,113	1.42	10 (13%)
18	CLA	a	602	11	61,69,73	1.51	7 (11%)	71,108,113	1.43	7 (9%)
18	CLA	B	832	-	60,68,73	1.49	7 (11%)	70,107,113	1.61	9 (12%)
18	CLA	J	101	8	42,50,73	1.82	6 (14%)	48,85,113	1.73	8 (16%)
21	BCR	A	851	-	41,41,41	0.79	0	56,56,56	2.14	14 (25%)
18	CLA	L	303	-	45,53,73	1.76	5 (11%)	52,89,113	1.60	7 (13%)
24	LMG	7	624	-	44,44,55	0.83	0	52,52,63	1.25	5 (9%)
18	CLA	A	829	-	65,73,73	1.41	8 (12%)	76,113,113	1.54	7 (9%)
18	CLA	8	602	17	60,68,73	1.51	7 (11%)	70,107,113	1.50	8 (11%)
22	SF4	C	102	-	0,12,12	-	-	-		
26	LUT	3	618	-	42,43,43	0.79	0	51,60,60	1.55	9 (17%)
18	CLA	K	201	9	45,53,73	1.77	7 (15%)	52,89,113	1.87	12 (23%)
20	LHG	7	622	18	36,36,48	0.74	1 (2%)	39,42,54	1.28	4 (10%)
18	CLA	A	808	-	50,58,73	1.61	7 (14%)	58,95,113	1.70	9 (15%)
18	CLA	A	842	-	65,73,73	1.44	8 (12%)	76,113,113	1.45	6 (7%)
18	CLA	B	808	-	65,73,73	1.43	8 (12%)	76,113,113	1.64	10 (13%)
18	CLA	5	611	20	42,50,73	1.78	6 (14%)	48,85,113	1.64	7 (14%)
18	CLA	B	815	-	43,51,73	1.73	7 (16%)	49,86,113	1.75	7 (14%)
18	CLA	a	608	-	43,52,73	1.81	6 (13%)	49,88,113	1.64	7 (14%)
20	LHG	a	620	18	48,48,48	0.64	1 (2%)	51,54,54	1.25	6 (11%)
18	CLA	B	838	-	47,55,73	1.66	7 (14%)	54,91,113	1.64	7 (12%)
18	CLA	B	826	-	55,63,73	1.57	7 (12%)	64,101,113	1.69	6 (9%)
18	CLA	a	603	-	54,62,73	1.63	7 (12%)	62,99,113	1.57	8 (12%)
24	LMG	5	627	-	40,40,55	0.86	0	48,48,63	1.20	3 (6%)
23	LMU	A	858	-	34,35,36	1.29	2 (5%)	42,45,47	1.22	5 (11%)
20	LHG	3	624	18	48,48,48	0.63	0	51,54,54	1.22	6 (11%)
18	CLA	5	613	14	64,72,73	1.45	7 (10%)	74,111,113	1.53	7 (9%)
18	CLA	A	834	-	65,73,73	1.43	8 (12%)	76,113,113	1.48	7 (9%)
18	CLA	1	613	-	65,73,73	1.48	6 (9%)	76,113,113	1.45	8 (10%)
26	LUT	7	619	-	42,43,43	0.89	2 (4%)	51,60,60	1.85	14 (27%)
18	CLA	6	603	-	54,62,73	1.64	8 (14%)	67,100,113	1.51	9 (13%)
18	CLA	B	818	-	60,68,73	1.49	8 (13%)	70,107,113	1.61	8 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
18	CLA	A	825	-	65,73,73	1.42	8 (12%)	76,113,113	1.46	9 (11%)
18	CLA	1	607	-	39,48,73	1.87	7 (17%)	44,83,113	1.70	7 (15%)
18	CLA	A	804	-	65,73,73	1.46	8 (12%)	76,113,113	1.46	8 (10%)
18	CLA	1	614	-	37,45,73	2.08	8 (21%)	44,79,113	1.82	10 (22%)
18	CLA	3	609	12	60,68,73	1.52	8 (13%)	70,107,113	1.64	11 (15%)
18	CLA	6	601	15	65,73,73	1.43	8 (12%)	76,113,113	1.56	8 (10%)
18	CLA	7	611	20	59,67,73	1.47	7 (11%)	68,105,113	1.58	7 (10%)
18	CLA	A	841	-	65,73,73	1.45	9 (13%)	76,113,113	1.42	7 (9%)
18	CLA	3	610	12	65,73,73	1.45	9 (13%)	76,113,113	1.44	7 (9%)

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
26	LUT	6	619	-	-	2/29/67/67	0/2/2/2
18	CLA	a	601	11	1/1/13/20	6/23/101/115	-
18	CLA	3	614	-	1/1/10/20	0/6/84/115	-
18	CLA	A	811	-	1/1/15/20	15/37/115/115	-
24	LMG	4	624	-	-	13/35/55/70	0/1/1/1
18	CLA	B	840	-	1/1/15/20	7/37/115/115	-
18	CLA	A	837	1	1/1/11/20	8/13/91/115	-
18	CLA	6	608	-	1/1/12/20	7/21/99/115	-
18	CLA	7	613	16	1/1/15/20	12/37/115/115	-
18	CLA	8	616	17	-	11/11/87/115	-
21	BCR	K	202	-	-	4/29/63/63	0/2/2/2
18	CLA	5	608	-	1/1/12/20	7/19/97/115	-
21	BCR	1	619	-	-	0/29/63/63	0/2/2/2
27	XAT	1	618	-	-	1/31/93/93	0/4/4/4
18	CLA	B	822	-	1/1/10/20	2/10/88/115	-
18	CLA	5	603	-	1/1/13/20	7/25/101/115	-
18	CLA	6	616	15	1/1/15/20	18/37/115/115	-
27	XAT	8	620	-	-	2/31/93/93	0/4/4/4
24	LMG	J	104	-	-	17/35/55/70	0/1/1/1
28	NEX	5	624	-	-	2/27/83/83	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	CLA	6	606	-	1/1/10/20	4/6/84/115	-
21	BCR	B	847	-	-	2/29/63/63	0/2/2/2
18	CLA	8	613	17	1/1/15/20	19/37/115/115	-
18	CLA	4	603	13	1/1/11/20	5/13/89/115	-
18	CLA	4	611	20	1/1/10/20	4/10/88/115	-
18	CLA	A	817	-	1/1/11/20	4/13/91/115	-
21	BCR	A	848	-	-	4/29/63/63	0/2/2/2
18	CLA	1	612	11	1/1/11/20	7/13/91/115	-
18	CLA	4	610	13	1/1/14/20	7/33/111/115	-
18	CLA	3	608	-	1/1/13/20	7/25/103/115	-
26	LUT	5	620	-	-	2/29/67/67	0/2/2/2
21	BCR	L	301	-	-	5/29/63/63	0/2/2/2
21	BCR	B	846	-	-	2/29/63/63	0/2/2/2
19	PQN	A	844	-	-	7/23/43/43	0/2/2/2
18	CLA	A	820	-	1/1/15/20	16/37/115/115	-
18	CLA	A	824	-	1/1/10/20	2/8/86/115	-
18	CLA	7	612	16	-	5/11/89/115	-
18	CLA	L	304	-	1/1/11/20	7/13/91/115	-
18	CLA	A	819	-	1/1/13/20	8/30/108/115	-
18	CLA	A	835	-	1/1/14/20	11/33/111/115	-
18	CLA	4	602	13	1/1/14/20	7/31/109/115	-
18	CLA	5	609	14	1/1/15/20	12/37/115/115	-
18	CLA	6	611	20	1/1/10/20	2/10/88/115	-
18	CLA	6	612	15	1/1/10/20	3/8/86/115	-
18	CLA	6	618	15	1/1/10/20	2/8/84/115	-
21	BCR	A	850	-	-	0/29/63/63	0/2/2/2
18	CLA	3	615	-	1/1/10/20	1/6/84/115	-
18	CLA	B	805	-	1/1/15/20	14/37/115/115	-
23	LMU	A	859	-	-	9/21/57/61	0/2/2/2
18	CLA	A	826	-	1/1/14/20	13/35/113/115	-
21	BCR	7	623	-	-	3/29/63/63	0/2/2/2
27	XAT	6	621	-	-	2/31/93/93	0/4/4/4
18	CLA	A	845	20	1/1/12/20	11/19/97/115	-
18	CLA	5	616	14	1/1/10/20	4/8/84/115	-
18	CLA	5	618	14	1/1/10/20	0/8/84/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	LHG	A	846	-	-	34/53/53/53	-
18	CLA	B	814	-	1/1/14/20	13/36/114/115	-
18	CLA	5	617	-	1/1/12/20	8/19/97/115	-
18	CLA	A	823	-	1/1/10/20	2/10/88/115	-
18	CLA	B	813	-	1/1/15/20	21/37/115/115	-
18	CLA	a	607	-	1/1/11/20	5/13/91/115	-
18	CLA	6	604	-	1/1/15/20	18/37/115/115	-
18	CLA	A	836	-	1/1/15/20	13/37/115/115	-
18	CLA	4	618	13	1/1/10/20	1/8/84/115	-
18	CLA	4	612	13	-	2/8/86/115	-
18	CLA	a	612	11	1/1/11/20	5/13/91/115	-
18	CLA	a	604	-	1/1/11/20	10/18/96/115	-
18	CLA	A	821	-	1/1/12/20	11/23/101/115	-
18	CLA	5	606	-	1/1/10/20	3/6/84/115	-
18	CLA	8	612	17	-	2/8/86/115	-
18	CLA	B	827	-	1/1/14/20	17/34/112/115	-
18	CLA	4	604	-	1/1/13/20	10/25/101/115	-
20	LHG	6	623	18	-	26/52/52/53	-
21	BCR	8	621	-	-	6/29/63/63	0/2/2/2
21	BCR	7	621	-	-	2/29/63/63	0/2/2/2
27	XAT	a	618	-	-	1/31/93/93	0/4/4/4
18	CLA	6	610	15	1/1/15/20	10/37/115/115	-
18	CLA	5	614	-	1/1/10/20	7/13/87/115	-
24	LMG	A	860	-	-	14/35/55/70	0/1/1/1
18	CLA	7	604	-	1/1/13/20	8/23/101/115	-
18	CLA	B	820	-	1/1/12/20	8/19/97/115	-
18	CLA	B	828	-	1/1/15/20	13/37/115/115	-
18	CLA	B	836	-	1/1/12/20	6/19/97/115	-
18	CLA	6	613	-	1/1/15/20	14/35/113/115	-
18	CLA	8	603	-	1/1/11/20	7/13/89/115	-
18	CLA	A	809	1	1/1/15/20	10/37/115/115	-
20	LHG	3	623	-	-	22/49/49/53	-
20	LHG	1	620	18	-	17/53/53/53	-
18	CLA	B	811	-	1/1/13/20	9/25/101/115	-
27	XAT	4	620	-	-	1/31/93/93	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	CLA	5	607	-	1/1/15/20	15/37/115/115	-
18	CLA	8	601	17	1/1/15/20	16/37/115/115	-
18	CLA	a	616	11	1/1/11/20	4/13/91/115	-
18	CLA	7	602	16	1/1/15/20	13/37/115/115	-
23	LMU	8	625	-	-	11/21/61/61	0/2/2/2
21	BCR	L	305	-	-	10/29/63/63	0/2/2/2
18	CLA	K	206	9	1/1/11/20	7/13/91/115	-
18	CLA	7	615	-	1/1/9/20	2/5/81/115	-
18	CLA	1	609	11	1/1/10/20	3/8/84/115	-
18	CLA	B	834	-	1/1/14/20	11/31/109/115	-
18	CLA	1	610	11	1/1/9/20	0/6/80/115	-
18	CLA	3	602	12	1/1/14/20	5/31/109/115	-
18	CLA	B	810	-	1/1/15/20	12/37/115/115	-
18	CLA	K	203	-	1/1/15/20	10/37/115/115	-
18	CLA	4	613	13	1/1/15/20	13/37/115/115	-
23	LMU	5	628	-	-	12/19/59/61	0/2/2/2
18	CLA	5	619	-	-	7/11/87/115	-
22	SF4	A	853	-	-	-	0/6/5/5
18	CLA	1	601	11	1/1/13/20	3/23/101/115	-
18	CLA	A	802	-	1/1/15/20	11/37/115/115	-
21	BCR	5	622	-	-	6/29/63/63	0/2/2/2
18	CLA	1	606	11	1/1/8/20	1/5/79/115	-
18	CLA	3	607	12	1/1/13/20	6/28/104/115	-
23	LMU	K	208	-	-	12/21/61/61	0/2/2/2
21	BCR	a	619	-	-	2/29/63/63	0/2/2/2
18	CLA	B	807	-	1/1/12/20	5/22/100/115	-
18	CLA	A	833	-	1/1/11/20	2/13/91/115	-
18	CLA	1	603	-	1/1/13/20	13/23/101/115	-
21	BCR	A	852	-	-	7/29/63/63	0/2/2/2
18	CLA	A	810	1	1/1/12/20	5/19/97/115	-
18	CLA	a	614	-	1/1/12/20	7/25/99/115	-
18	CLA	A	832	-	1/1/12/20	4/19/97/115	-
18	CLA	3	606	-	1/1/13/20	8/23/101/115	-
18	CLA	B	829	-	1/1/15/20	10/37/115/115	-
18	CLA	B	821	-	1/1/11/20	7/14/92/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	CLA	F	301	-	1/1/13/20	8/28/106/115	-
18	CLA	7	614	-	1/1/10/20	4/10/88/115	-
18	CLA	8	614	-	1/1/13/20	8/27/105/115	-
21	BCR	A	856	-	-	7/29/63/63	0/2/2/2
25	DGD	B	850	-	-	23/51/91/95	0/2/2/2
27	XAT	7	620	-	-	1/31/93/93	0/4/4/4
18	CLA	B	841	20	1/1/10/20	5/12/90/115	-
18	CLA	8	609	17	1/1/11/20	4/13/91/115	-
18	CLA	B	802	-	1/1/15/20	18/37/115/115	-
18	CLA	8	610	17	1/1/14/20	7/31/109/115	-
18	CLA	4	607	-	1/1/11/20	6/13/91/115	-
18	CLA	B	817	-	1/1/13/20	10/30/108/115	-
20	LHG	5	625	-	-	31/53/53/53	-
18	CLA	F	304	-	1/1/10/20	4/8/86/115	-
21	BCR	3	621	-	-	6/29/63/63	0/2/2/2
18	CLA	A	830	-	1/1/15/20	18/37/115/115	-
18	CLA	A	840	-	1/1/12/20	4/22/100/115	-
18	CLA	B	803	-	1/1/15/20	12/37/115/115	-
18	CLA	B	812	-	1/1/10/20	3/11/89/115	-
18	CLA	8	604	-	1/1/12/20	11/19/97/115	-
20	LHG	8	622	18	-	25/53/53/53	-
18	CLA	3	604	-	1/1/15/20	7/37/115/115	-
18	CLA	A	806	-	1/1/15/20	15/37/115/115	-
21	BCR	K	207	-	-	4/29/63/63	0/2/2/2
21	BCR	6	622	-	-	6/29/63/63	0/2/2/2
18	CLA	6	614	-	1/1/14/20	11/31/109/115	-
18	CLA	B	819	-	1/1/13/20	6/25/103/115	-
25	DGD	J	103	-	-	26/47/87/95	0/2/2/2
22	SF4	C	101	-	-	-	0/6/5/5
21	BCR	B	844	-	-	9/29/63/63	0/2/2/2
18	CLA	K	204	-	1/1/11/20	7/15/93/115	-
18	CLA	8	606	-	1/1/15/20	9/35/113/115	-
18	CLA	A	822	-	1/1/15/20	11/37/115/115	-
18	CLA	B	823	-	1/1/11/20	5/13/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	LUT	8	619	-	-	2/29/67/67	0/2/2/2
18	CLA	A	854	-	1/1/15/20	14/37/115/115	-
20	LHG	5	623	18	-	24/53/53/53	-
18	CLA	F	303	-	-	5/10/88/115	-
18	CLA	4	601	13	-	16/37/115/115	-
21	BCR	A	849	-	-	2/29/63/63	0/2/2/2
18	CLA	6	602	15	1/1/15/20	7/37/115/115	-
24	LMG	5	626	-	-	26/35/55/70	0/1/1/1
21	BCR	F	305	-	-	2/29/63/63	0/2/2/2
23	LMU	8	624	-	-	10/21/61/61	0/2/2/2
27	XAT	5	621	-	-	2/31/93/93	0/4/4/4
21	BCR	B	848	-	-	4/29/63/63	0/2/2/2
21	BCR	B	801	-	-	4/29/63/63	0/2/2/2
21	BCR	4	621	-	-	4/29/63/63	0/2/2/2
18	CLA	8	608	-	1/1/12/20	9/21/99/115	-
18	CLA	A	818	-	1/1/14/20	13/31/109/115	-
18	CLA	5	602	14	1/1/15/20	5/37/115/115	-
18	CLA	5	604	-	1/1/15/20	15/35/111/115	-
18	CLA	7	609	16	1/1/11/20	6/13/91/115	-
26	LUT	a	617	-	-	5/29/67/67	0/2/2/2
21	BCR	B	843	-	-	5/29/63/63	0/2/2/2
23	LMU	A	857	-	-	9/19/56/61	0/2/2/2
18	CLA	A	812	-	1/1/15/20	15/37/115/115	-
18	CLA	4	616	13	1/1/11/20	7/11/87/115	-
27	XAT	3	619	-	-	2/31/93/93	0/4/4/4
18	CLA	5	601	14	1/1/13/20	6/27/105/115	-
28	NEX	6	624	-	-	4/27/83/83	0/3/3/3
18	CLA	A	831	-	1/1/15/20	9/37/115/115	-
18	CLA	A	814	-	1/1/15/20	18/37/115/115	-
21	BCR	B	845	-	-	4/29/63/63	0/2/2/2
18	CLA	A	838	-	1/1/12/20	7/19/97/115	-
18	CLA	3	617	12	1/1/10/20	2/6/84/115	-
18	CLA	5	610	14	1/1/12/20	3/24/102/115	-
18	CLA	3	612	12	1/1/10/20	3/11/89/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	CLA	7	606	-	1/1/10/20	2/8/86/115	-
18	CLA	1	608	-	1/1/11/20	0/11/89/115	-
18	CLA	7	603	-	1/1/11/20	4/11/89/115	-
21	BCR	3	620	-	-	5/29/63/63	0/2/2/2
18	CLA	A	828	-	1/1/14/20	10/35/113/115	-
18	CLA	A	807	1	1/1/15/20	13/37/115/115	-
18	CLA	1	611	20	1/1/15/20	11/37/115/115	-
18	CLA	B	806	2	1/1/15/20	11/37/115/115	-
18	CLA	6	609	15	1/1/11/20	4/13/91/115	-
18	CLA	6	617	-	1/1/11/20	5/13/91/115	-
18	CLA	7	601	16	-	12/31/109/115	-
18	CLA	B	825	-	1/1/14/20	9/34/112/115	-
18	CLA	A	805	-	1/1/12/20	3/22/100/115	-
18	CLA	B	824	-	1/1/15/20	12/37/115/115	-
18	CLA	B	804	-	1/1/10/20	3/8/86/115	-
18	CLA	L	302	10	1/1/11/20	7/13/91/115	-
18	CLA	3	603	-	1/1/13/20	7/25/103/115	-
18	CLA	3	611	20	1/1/10/20	0/4/80/115	-
18	CLA	B	835	-	1/1/11/20	7/13/91/115	-
18	CLA	5	612	14	1/1/10/20	2/8/86/115	-
19	PQN	B	842	-	-	9/23/43/43	0/2/2/2
18	CLA	B	831	-	1/1/15/20	10/37/115/115	-
18	CLA	7	607	-	1/1/10/20	6/10/88/115	-
26	LUT	1	617	-	-	4/29/67/67	0/2/2/2
18	CLA	7	608	-	1/1/12/20	3/19/97/115	-
18	CLA	B	830	-	1/1/10/20	5/11/89/115	-
18	CLA	A	839	-	1/1/13/20	4/25/103/115	-
20	LHG	4	622	18	-	25/53/53/53	-
18	CLA	B	809	2	1/1/15/20	18/37/115/115	-
18	CLA	1	602	11	1/1/14/20	7/33/111/115	-
18	CLA	A	816	-	1/1/11/20	4/13/91/115	-
20	LHG	B	851	18	-	19/39/39/53	-
21	BCR	J	102	-	-	7/29/63/63	0/2/2/2
18	CLA	a	609	11	1/1/15/20	20/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	CLA	A	827	-	1/1/13/20	6/30/108/115	-
18	CLA	a	610	11	1/1/14/20	4/29/107/115	-
18	CLA	4	606	-	1/1/10/20	2/6/84/115	-
18	CLA	6	620	-	1/1/11/20	7/13/91/115	-
24	LMG	4	623	-	-	12/35/55/70	0/1/1/1
18	CLA	6	607	-	1/1/10/20	4/10/86/115	-
18	CLA	4	609	13	1/1/14/20	6/33/111/115	-
26	LUT	4	619	-	-	2/29/67/67	0/2/2/2
18	CLA	a	611	20	1/1/10/20	0/4/80/115	-
18	CLA	A	813	-	1/1/12/20	4/24/102/115	-
18	CLA	B	839	-	1/1/15/20	9/37/115/115	-
18	CLA	8	607	-	1/1/10/20	5/10/86/115	-
18	CLA	4	614	-	1/1/13/20	12/27/105/115	-
18	CLA	A	843	-	1/1/14/20	16/35/113/115	-
18	CLA	8	611	20	1/1/10/20	4/10/88/115	-
20	LHG	A	847	18	-	17/34/34/53	-
20	LHG	8	623	-	-	33/53/53/53	-
18	CLA	B	816	-	1/1/13/20	10/25/103/115	-
18	CLA	3	613	12	1/1/12/20	5/21/99/115	-
18	CLA	a	606	11	1/1/10/20	4/10/88/115	-
18	CLA	A	815	-	1/1/12/20	8/19/97/115	-
18	CLA	B	837	-	1/1/15/20	6/37/115/115	-
18	CLA	A	801	-	1/1/15/20	9/37/115/115	-
18	CLA	1	604	-	1/1/11/20	10/18/96/115	-
18	CLA	1	616	11	1/1/11/20	4/11/87/115	-
18	CLA	a	613	-	1/1/15/20	11/37/115/115	-
18	CLA	4	608	-	1/1/15/20	13/37/115/115	-
18	CLA	7	616	16	1/1/11/20	7/11/87/115	-
21	BCR	3	622	-	-	8/29/63/63	0/2/2/2
18	CLA	B	833	-	1/1/15/20	16/37/115/115	-
18	CLA	A	803	-	1/1/15/20	7/37/115/115	-
18	CLA	7	610	16	1/1/15/20	8/37/115/115	-
18	CLA	a	602	11	1/1/14/20	6/33/111/115	-
18	CLA	B	832	-	1/1/14/20	8/31/109/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	CLA	J	101	8	1/1/10/20	5/10/88/115	-
21	BCR	A	851	-	-	5/29/63/63	0/2/2/2
18	CLA	L	303	-	1/1/11/20	6/13/91/115	-
24	LMG	7	624	-	-	15/39/59/70	0/1/1/1
18	CLA	A	829	-	1/1/15/20	8/37/115/115	-
18	CLA	8	602	17	1/1/14/20	7/31/109/115	-
26	LUT	3	618	-	-	2/29/67/67	0/2/2/2
22	SF4	C	102	-	-	-	0/6/5/5
18	CLA	K	201	9	1/1/11/20	8/13/91/115	-
20	LHG	7	622	18	-	24/41/41/53	-
18	CLA	A	808	-	1/1/12/20	4/19/97/115	-
18	CLA	A	842	-	1/1/15/20	10/37/115/115	-
18	CLA	B	808	-	1/1/15/20	14/37/115/115	-
18	CLA	5	611	20	1/1/10/20	5/10/88/115	-
18	CLA	B	815	-	1/1/10/20	4/11/89/115	-
18	CLA	a	608	-	1/1/11/20	2/11/89/115	-
20	LHG	a	620	18	-	10/53/53/53	-
18	CLA	B	838	-	1/1/11/20	6/16/94/115	-
18	CLA	B	826	-	1/1/13/20	6/25/103/115	-
18	CLA	a	603	-	1/1/12/20	6/23/101/115	-
24	LMG	5	627	-	-	15/35/55/70	0/1/1/1
23	LMU	A	858	-	-	7/21/57/61	0/2/2/2
20	LHG	3	624	18	-	27/53/53/53	-
18	CLA	5	613	14	1/1/14/20	20/35/113/115	-
18	CLA	A	834	-	1/1/15/20	12/37/115/115	-
18	CLA	1	613	-	1/1/15/20	9/37/115/115	-
26	LUT	7	619	-	-	2/29/67/67	0/2/2/2
18	CLA	6	603	-	1/1/13/20	7/25/101/115	-
18	CLA	B	818	-	1/1/14/20	15/31/109/115	-
18	CLA	A	825	-	1/1/15/20	20/37/115/115	-
18	CLA	1	607	-	1/1/10/20	0/6/84/115	-
18	CLA	A	804	-	1/1/15/20	14/37/115/115	-
18	CLA	1	614	-	1/1/9/20	0/4/76/115	-
18	CLA	3	609	12	1/1/14/20	20/31/109/115	-
18	CLA	6	601	15	1/1/15/20	16/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	CLA	7	611	20	1/1/13/20	12/29/107/115	-
18	CLA	A	841	-	1/1/15/20	18/37/115/115	-
18	CLA	3	610	12	1/1/15/20	6/37/115/115	-

The worst 5 of 1701 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	B	842	PQN	C12-C13	8.68	1.53	1.33
19	A	844	PQN	C12-C13	8.32	1.52	1.33
18	7	612	CLA	C4B-NB	8.02	1.42	1.35
19	A	844	PQN	O1-C1	8.02	1.40	1.23
19	B	842	PQN	O1-C1	7.81	1.39	1.23

The worst 5 of 2702 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	5	621	XAT	O24-C25-C24	11.52	122.04	113.38
18	B	803	CLA	C4A-NA-C1A	9.21	110.84	106.71
18	8	613	CLA	C4A-NA-C1A	9.08	110.79	106.71
27	6	621	XAT	O24-C25-C24	8.96	120.11	113.38
27	8	620	XAT	O24-C25-C24	8.87	120.04	113.38

5 of 208 chirality outliers are listed below:

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

5 of 2486 torsion outliers are listed below:

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

There are no ring outliers.

235 monomers are involved in 528 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
26	6	619	LUT	2	0
18	3	614	CLA	1	0
18	A	811	CLA	6	0
24	4	624	LMG	1	0
18	B	840	CLA	3	0
18	A	837	CLA	1	0
18	6	608	CLA	1	0
18	7	613	CLA	1	0
18	8	616	CLA	1	0
21	K	202	BCR	2	0
18	5	608	CLA	3	0
21	1	619	BCR	2	0
27	1	618	XAT	3	0
18	6	616	CLA	5	0
27	8	620	XAT	2	0
24	J	104	LMG	4	0
28	5	624	NEX	4	0
21	B	847	BCR	4	0
18	8	613	CLA	5	0
18	4	603	CLA	1	0
18	A	817	CLA	1	0
21	A	848	BCR	3	0
18	1	612	CLA	1	0
18	4	610	CLA	3	0
18	3	608	CLA	4	0
26	5	620	LUT	4	0
21	L	301	BCR	4	0
21	B	846	BCR	3	0
19	A	844	PQN	3	0
18	A	820	CLA	5	0
18	A	824	CLA	1	0
18	7	612	CLA	3	0
18	L	304	CLA	2	0
18	A	819	CLA	3	0
18	A	835	CLA	4	0
18	4	602	CLA	3	0
18	5	609	CLA	5	0
18	6	611	CLA	1	0
18	6	612	CLA	2	0
21	A	850	BCR	4	0
18	3	615	CLA	1	0
18	B	805	CLA	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	A	859	LMU	3	0
18	A	826	CLA	1	0
21	7	623	BCR	1	0
27	6	621	XAT	2	0
18	A	845	CLA	1	0
18	5	616	CLA	1	0
18	5	618	CLA	2	0
20	A	846	LHG	3	0
18	B	814	CLA	1	0
18	5	617	CLA	1	0
18	A	823	CLA	1	0
18	B	813	CLA	6	0
18	6	604	CLA	4	0
18	A	836	CLA	5	0
18	4	612	CLA	1	0
18	A	821	CLA	1	0
18	5	606	CLA	2	0
18	8	612	CLA	1	0
18	B	827	CLA	5	0
20	6	623	LHG	1	0
21	8	621	BCR	2	0
21	7	621	BCR	4	0
18	6	610	CLA	2	0
18	5	614	CLA	1	0
18	7	604	CLA	2	0
18	B	828	CLA	3	0
18	6	613	CLA	2	0
18	A	809	CLA	3	0
20	3	623	LHG	1	0
20	1	620	LHG	2	0
18	B	811	CLA	3	0
27	4	620	XAT	2	0
18	5	607	CLA	5	0
18	8	601	CLA	1	0
18	7	602	CLA	2	0
21	L	305	BCR	4	0
18	K	206	CLA	1	0
18	1	609	CLA	5	0
18	B	834	CLA	3	0
18	1	610	CLA	1	0
18	B	810	CLA	3	0
18	K	203	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	4	613	CLA	3	0
18	5	619	CLA	3	0
18	1	601	CLA	2	0
18	A	802	CLA	5	0
21	5	622	BCR	3	0
18	1	606	CLA	1	0
18	3	607	CLA	2	0
18	B	807	CLA	4	0
18	A	833	CLA	1	0
18	1	603	CLA	6	0
21	A	852	BCR	3	0
18	A	810	CLA	2	0
18	3	606	CLA	2	0
18	B	829	CLA	7	0
18	B	821	CLA	1	0
18	F	301	CLA	3	0
18	7	614	CLA	1	0
18	8	614	CLA	2	0
21	A	856	BCR	6	0
25	B	850	DGD	3	0
27	7	620	XAT	4	0
18	B	841	CLA	3	0
18	B	802	CLA	2	0
18	8	610	CLA	4	0
18	4	607	CLA	1	0
18	B	817	CLA	5	0
20	5	625	LHG	3	0
18	F	304	CLA	1	0
21	3	621	BCR	3	0
18	A	830	CLA	5	0
18	A	840	CLA	4	0
18	B	803	CLA	3	0
18	B	812	CLA	1	0
18	8	604	CLA	1	0
20	8	622	LHG	7	0
18	3	604	CLA	2	0
18	A	806	CLA	7	0
21	K	207	BCR	4	0
21	6	622	BCR	4	0
18	B	819	CLA	2	0
25	J	103	DGD	3	0
21	B	844	BCR	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	K	204	CLA	1	0
18	8	606	CLA	1	0
18	A	822	CLA	3	0
26	8	619	LUT	5	0
18	A	854	CLA	5	0
20	5	623	LHG	2	0
18	F	303	CLA	1	0
18	4	601	CLA	4	0
21	A	849	BCR	5	0
18	6	602	CLA	1	0
21	F	305	BCR	6	0
23	8	624	LMU	1	0
27	5	621	XAT	6	0
21	B	848	BCR	2	0
21	B	801	BCR	4	0
21	4	621	BCR	3	0
18	8	608	CLA	2	0
18	A	818	CLA	5	0
18	5	602	CLA	5	0
18	5	604	CLA	3	0
21	B	843	BCR	3	0
23	A	857	LMU	1	0
18	A	812	CLA	5	0
18	4	616	CLA	1	0
27	3	619	XAT	2	0
28	6	624	NEX	4	0
18	A	831	CLA	3	0
18	A	814	CLA	7	0
21	B	845	BCR	2	0
18	A	838	CLA	1	0
18	3	617	CLA	5	0
18	5	610	CLA	5	0
18	3	612	CLA	2	0
18	1	608	CLA	3	0
21	3	620	BCR	6	0
18	A	828	CLA	8	0
18	A	807	CLA	3	0
18	1	611	CLA	1	0
18	B	806	CLA	5	0
18	6	609	CLA	1	0
18	6	617	CLA	2	0
18	7	601	CLA	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	B	825	CLA	3	0
18	B	824	CLA	5	0
18	L	302	CLA	5	0
18	B	835	CLA	1	0
18	5	612	CLA	2	0
19	B	842	PQN	2	0
18	B	831	CLA	5	0
26	1	617	LUT	3	0
18	7	608	CLA	6	0
18	B	830	CLA	1	0
18	A	839	CLA	4	0
20	4	622	LHG	4	0
18	B	809	CLA	3	0
18	1	602	CLA	2	0
18	A	816	CLA	1	0
20	B	851	LHG	1	0
21	J	102	BCR	2	0
18	A	827	CLA	2	0
18	4	606	CLA	1	0
18	6	620	CLA	3	0
18	6	607	CLA	1	0
18	4	609	CLA	3	0
26	4	619	LUT	6	0
18	A	813	CLA	2	0
18	B	839	CLA	1	0
18	8	607	CLA	1	0
18	4	614	CLA	1	0
18	A	843	CLA	2	0
18	8	611	CLA	2	0
20	8	623	LHG	2	0
18	A	815	CLA	1	0
18	B	837	CLA	6	0
18	A	801	CLA	5	0
18	1	616	CLA	1	0
18	4	608	CLA	3	0
21	3	622	BCR	4	0
18	B	833	CLA	3	0
18	A	803	CLA	1	0
18	7	610	CLA	3	0
18	B	832	CLA	4	0
21	A	851	BCR	4	0
18	L	303	CLA	1	0

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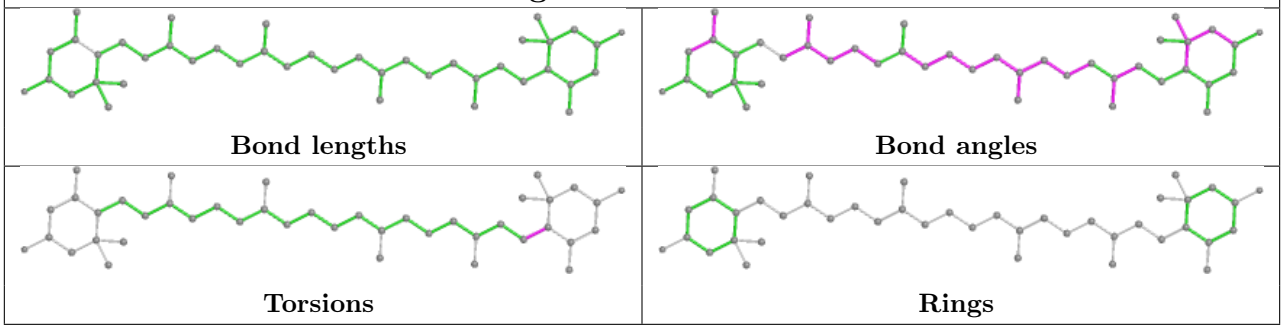
Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	A	829	CLA	9	0
26	3	618	LUT	2	0
18	K	201	CLA	2	0
20	7	622	LHG	5	0
18	A	808	CLA	2	0
18	A	842	CLA	6	0
18	B	808	CLA	5	0
18	B	838	CLA	3	0
18	B	826	CLA	1	0
24	5	627	LMG	3	0
23	A	858	LMU	2	0
20	3	624	LHG	5	0
18	5	613	CLA	4	0
18	A	834	CLA	3	0
18	1	613	CLA	2	0
26	7	619	LUT	3	0
18	6	603	CLA	1	0
18	B	818	CLA	4	0
18	A	825	CLA	3	0
18	A	804	CLA	3	0
18	3	609	CLA	3	0
18	6	601	CLA	3	0
18	7	611	CLA	2	0
18	A	841	CLA	4	0
18	3	610	CLA	4	0

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

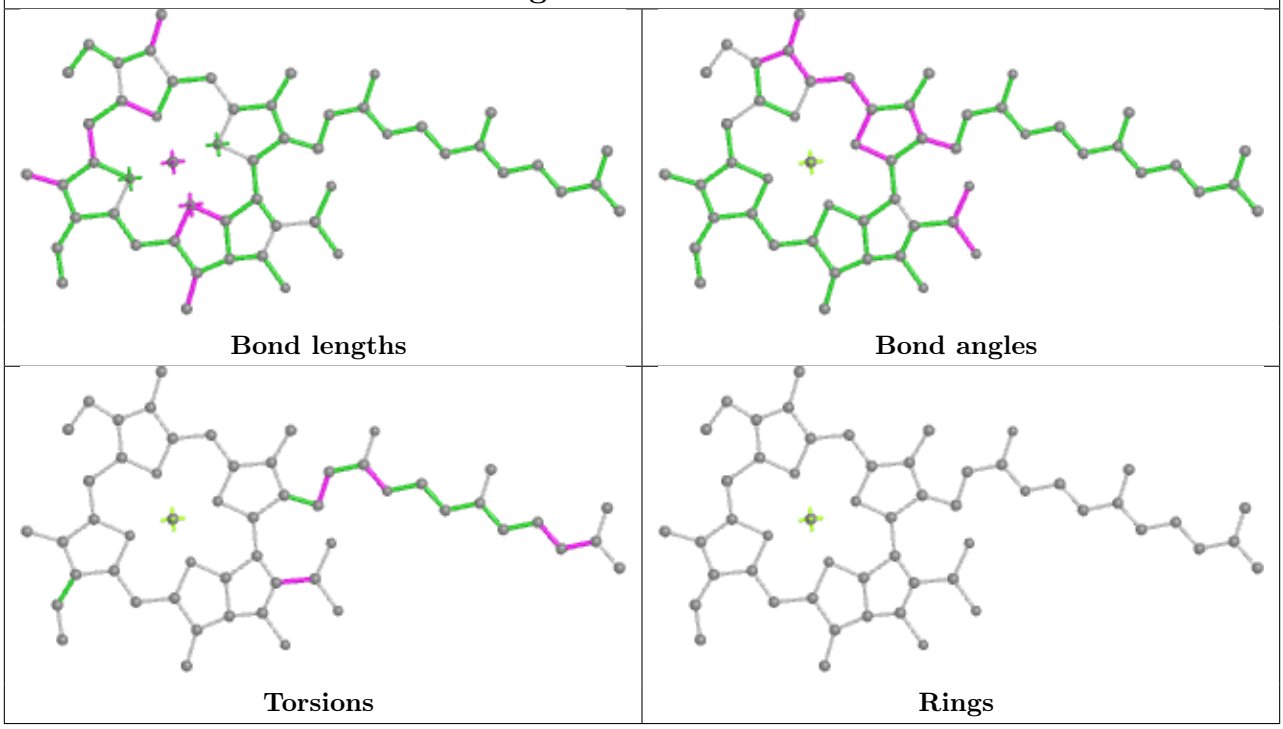
Ligand LUT 6 619



Bond lengths | Bond angles

Torsions | Rings

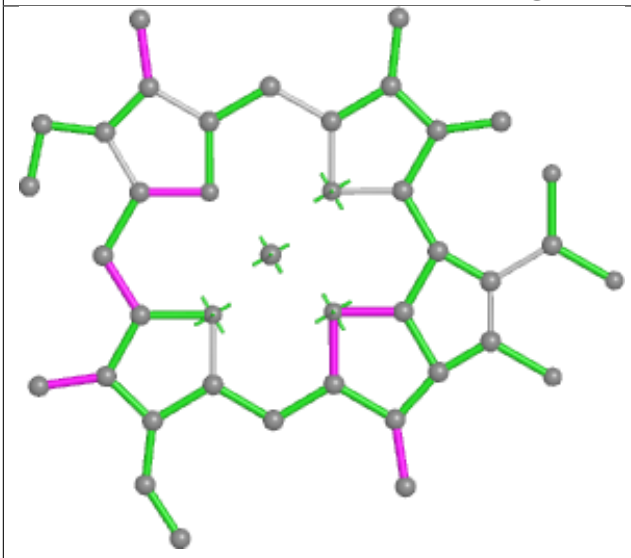
Ligand CLA a 601



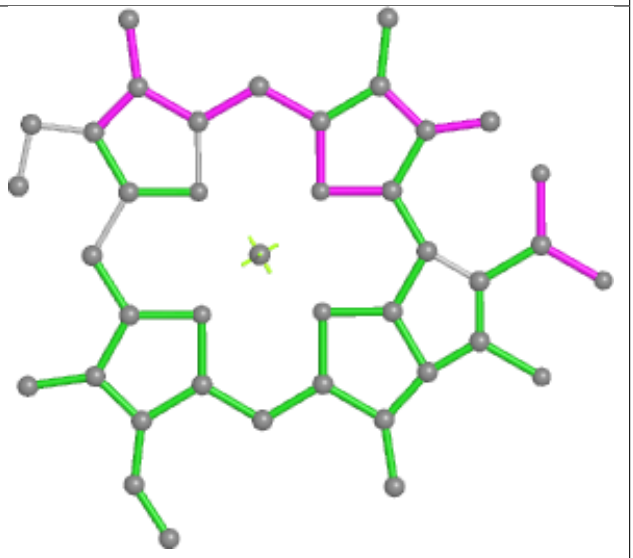
Bond lengths | Bond angles

Torsions | Rings

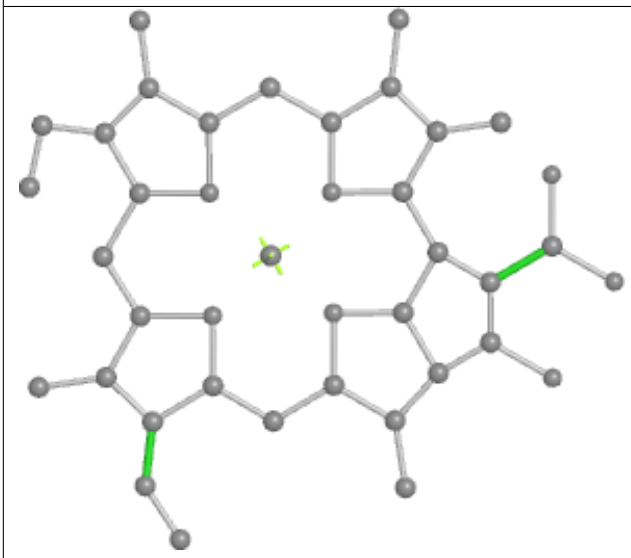
Ligand CLA 3 614



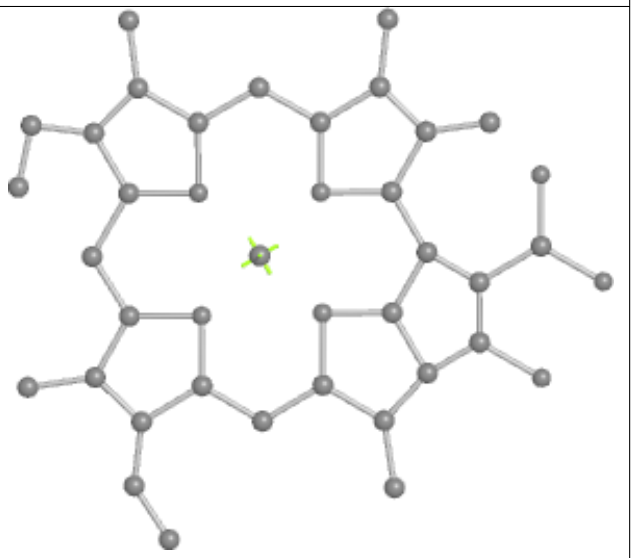
Bond lengths



Bond angles

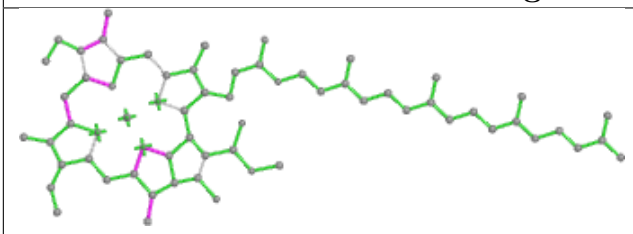


Torsions

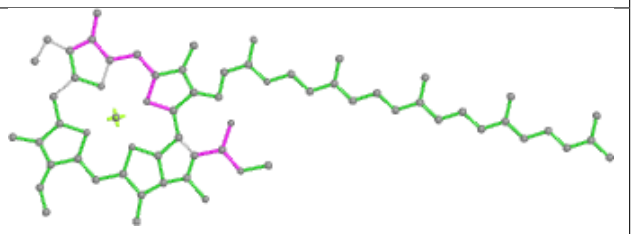


Rings

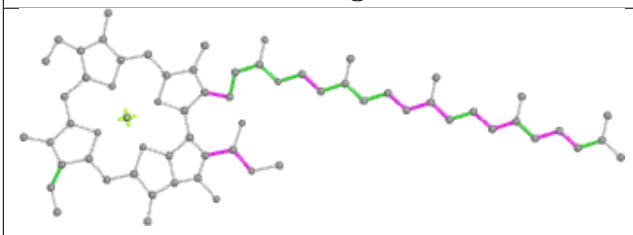
Ligand CLA A 811



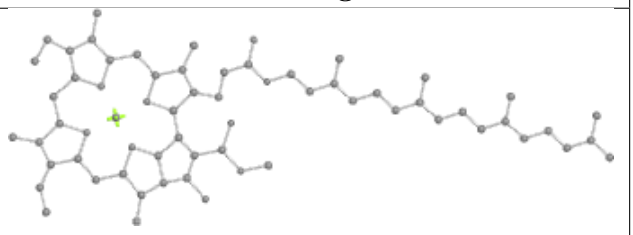
Bond lengths



Bond angles

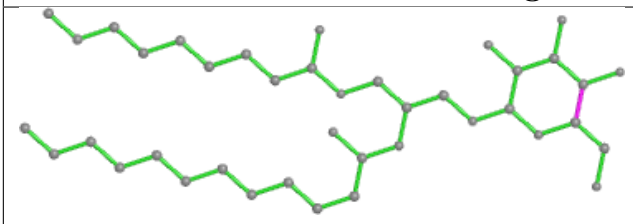


Torsions

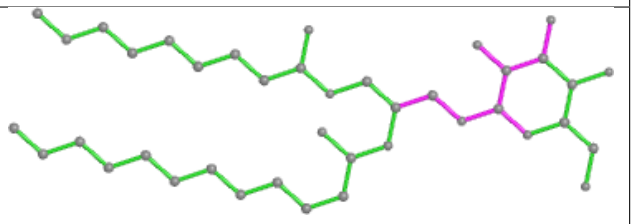


Rings

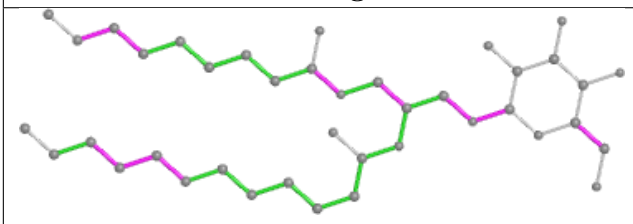
Ligand LMG 4 624



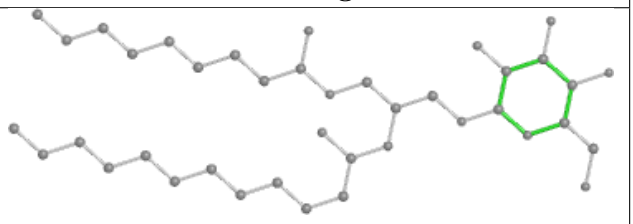
Bond lengths



Bond angles

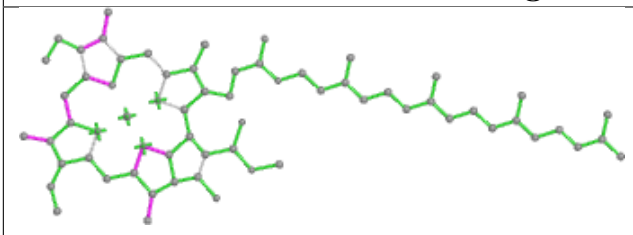


Torsions

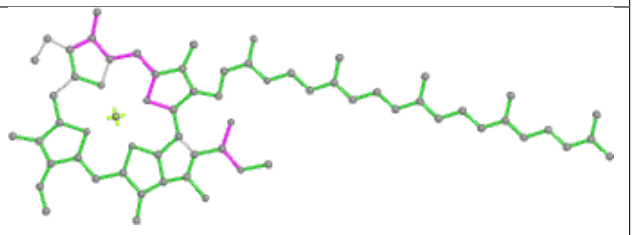


Rings

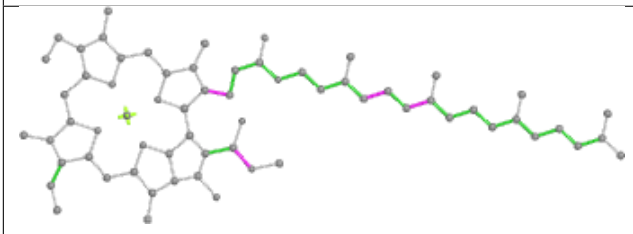
Ligand CLA B 840



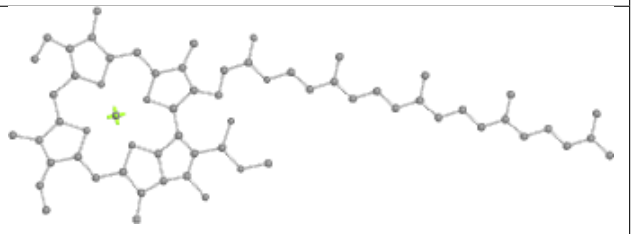
Bond lengths



Bond angles

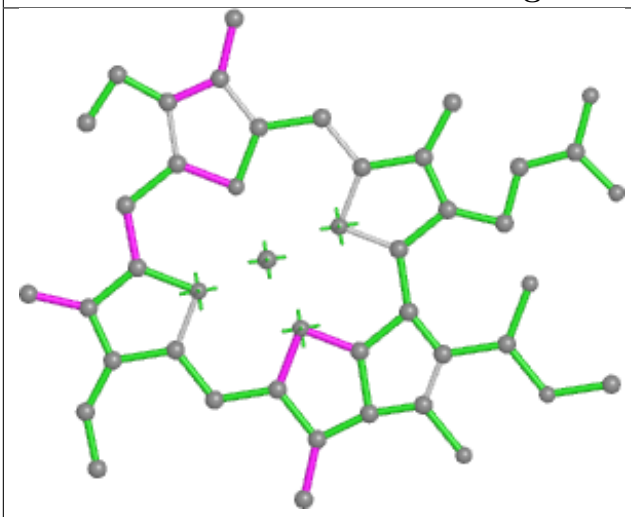


Torsions

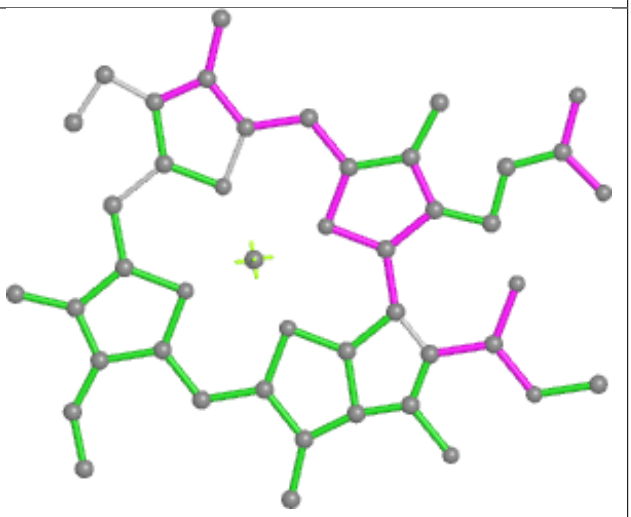


Rings

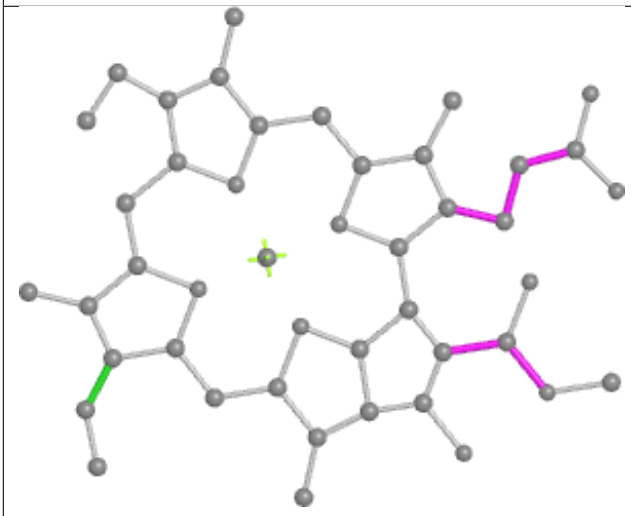
Ligand CLA A 837



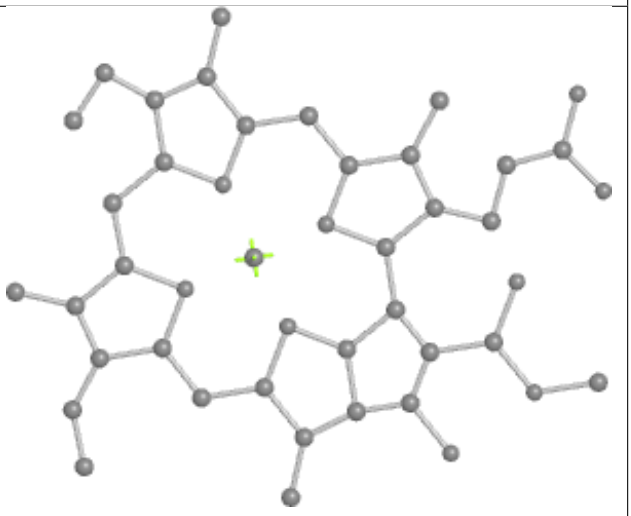
Bond lengths



Bond angles

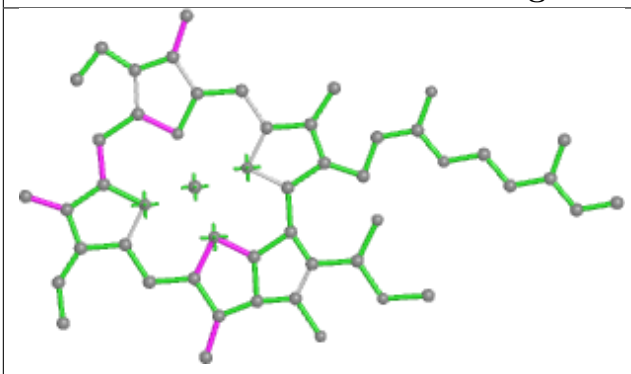


Torsions

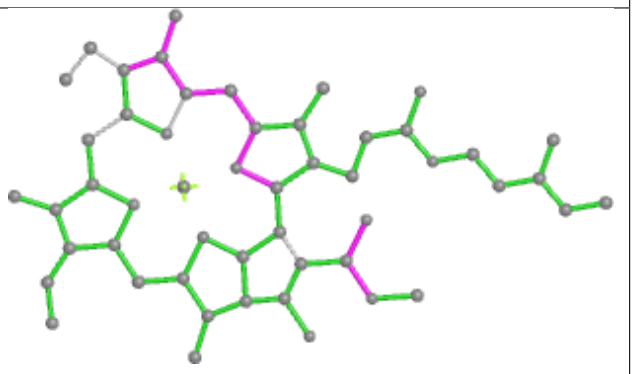


Rings

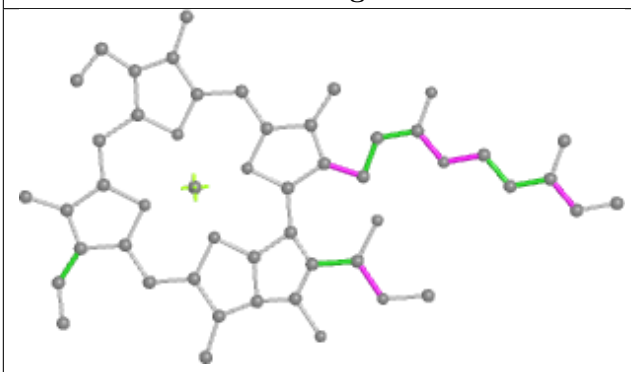
Ligand CLA 6 608



Bond lengths



Bond angles



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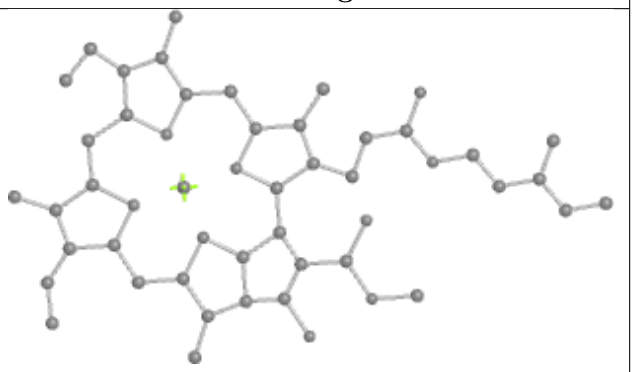

Rings

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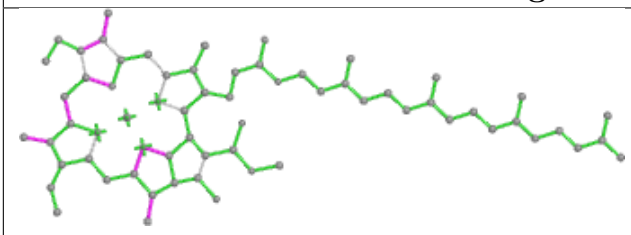

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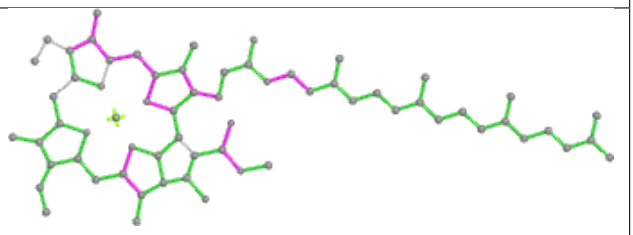
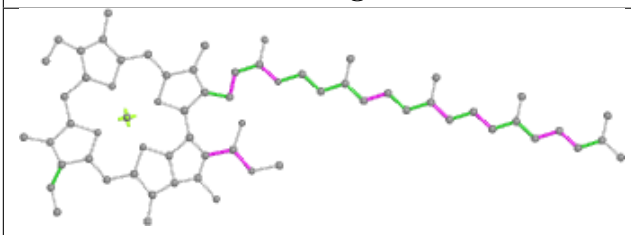


Bond angles



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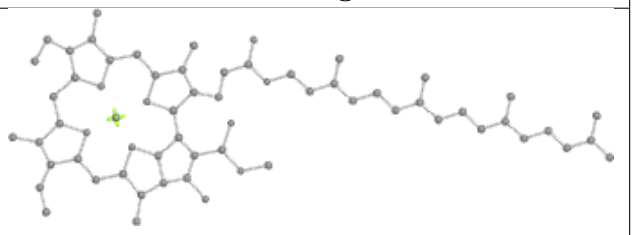

Rings

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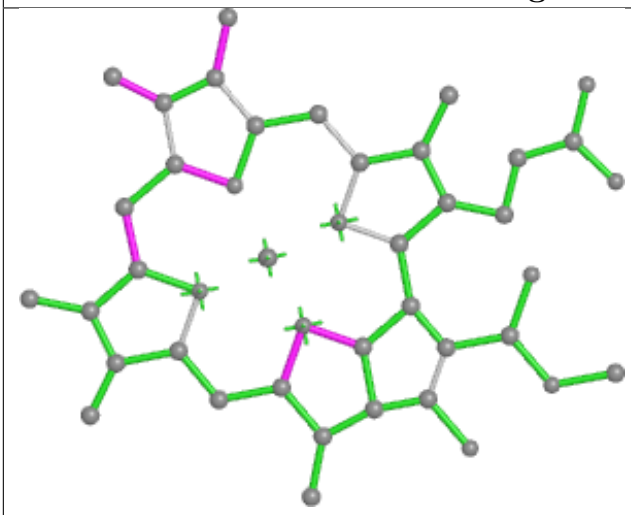
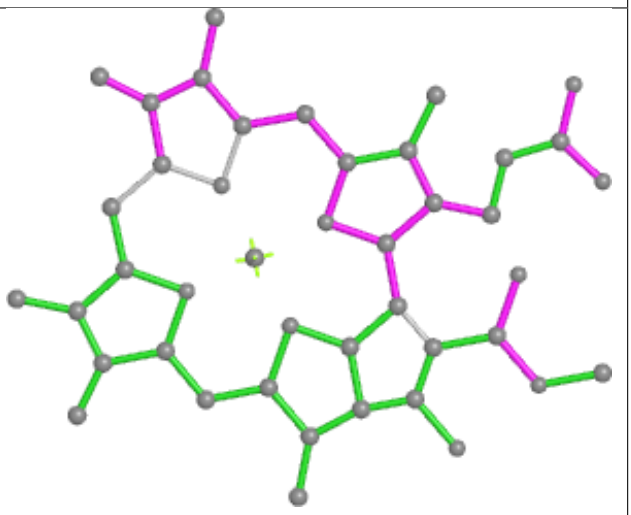
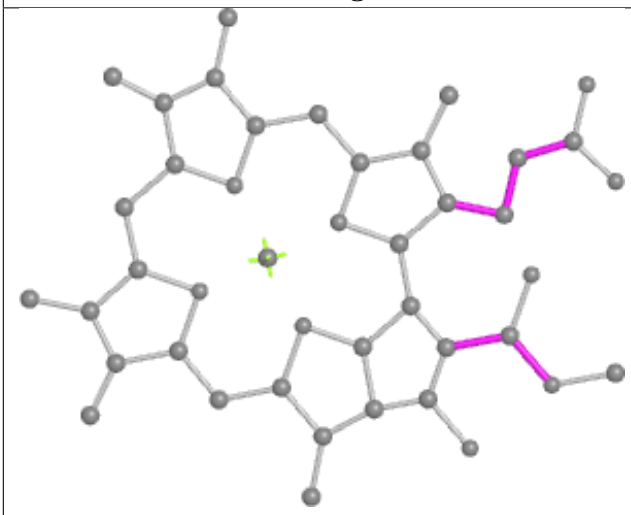


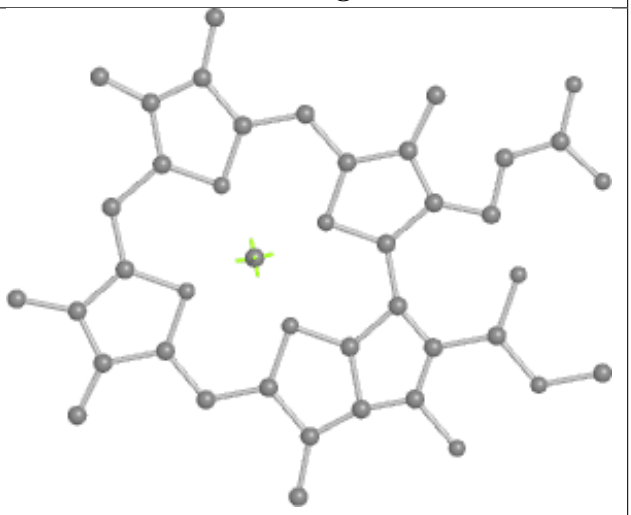
Bond lengths



Bond angles

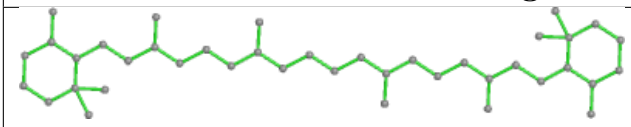


Torsions

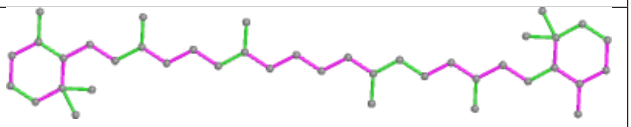


Rings

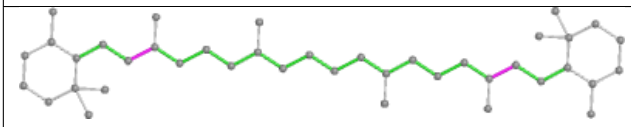
Ligand BCR K 202



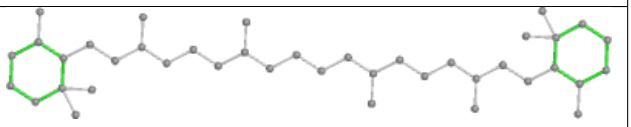
Bond lengths



Bond angles

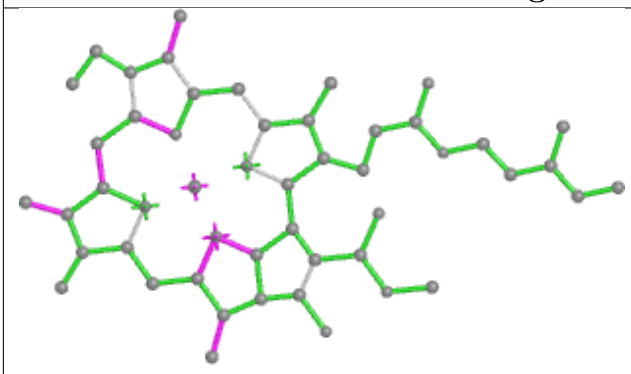


Torsions

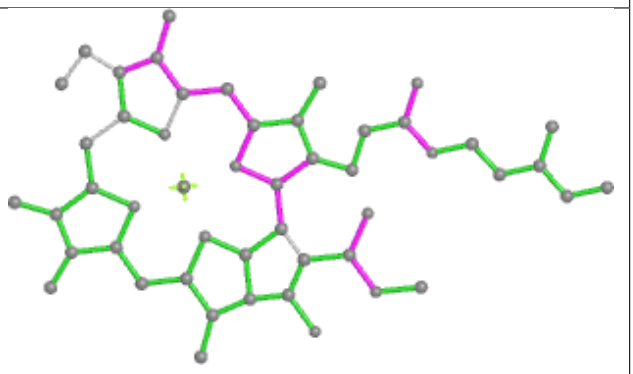


Rings

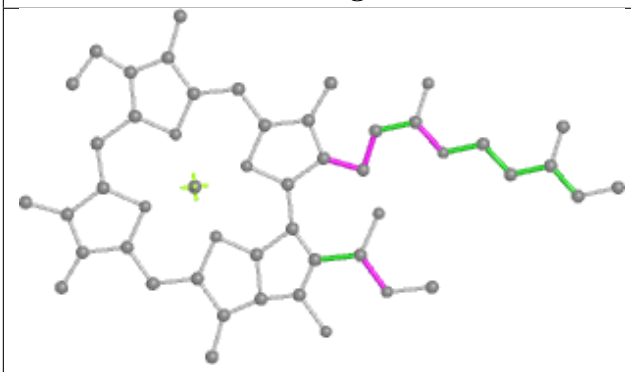
Ligand CLA 5 608



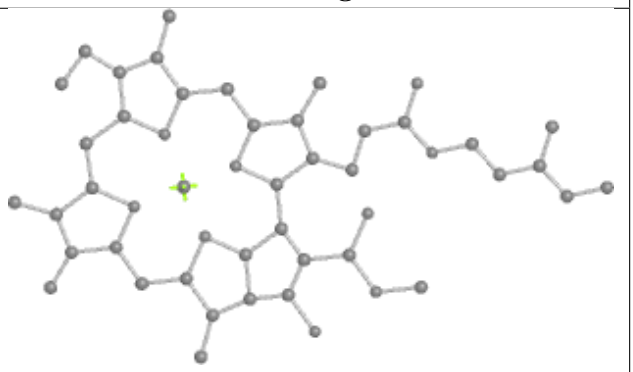
Bond lengths



Bond angles

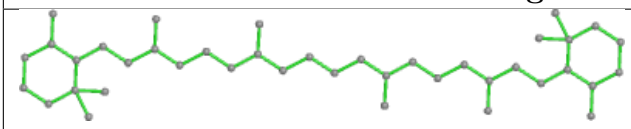


Torsions

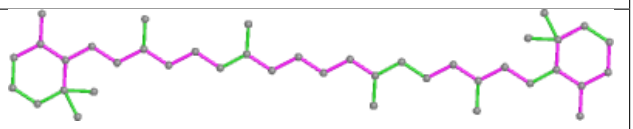


Rings

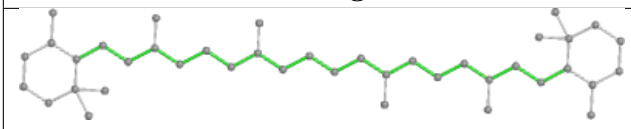
Ligand BCR 1 619



Bond lengths



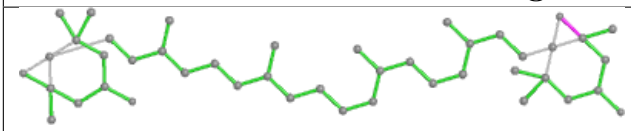
Bond angles



Torsions

Rings

Ligand XAT 1 618



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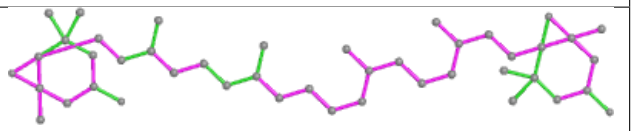
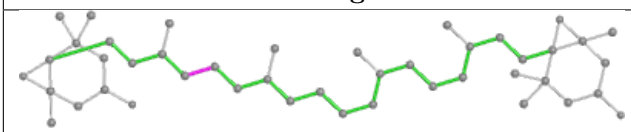


Bond angles



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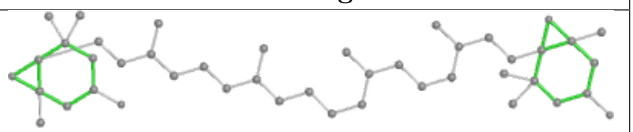
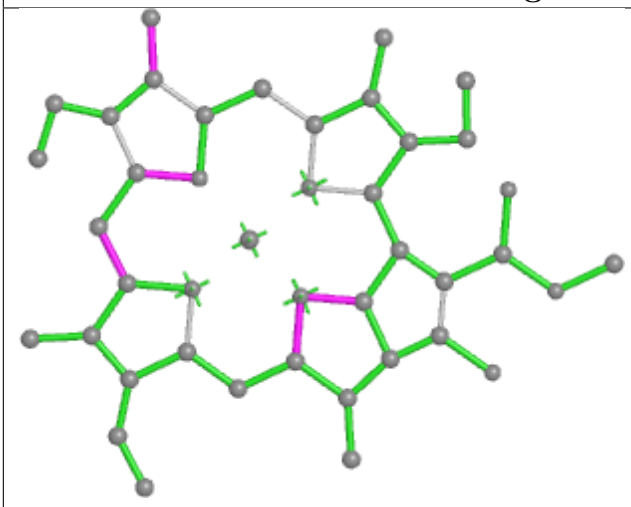
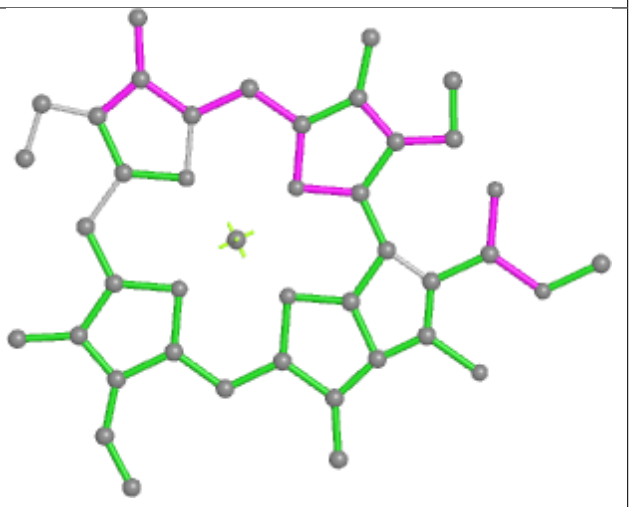


Rings

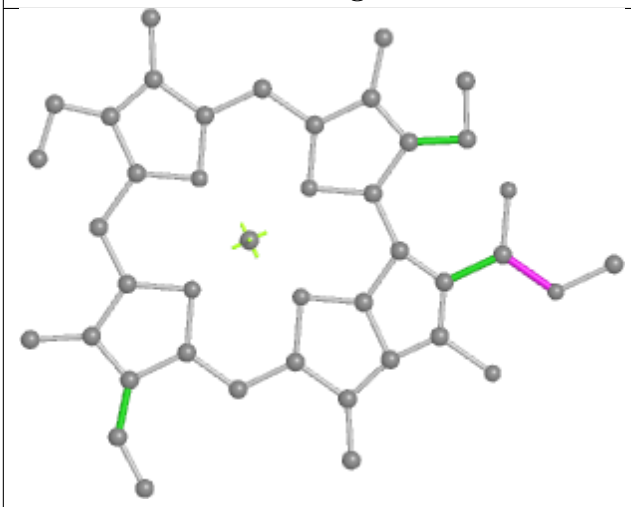
Ligand CLA B 822



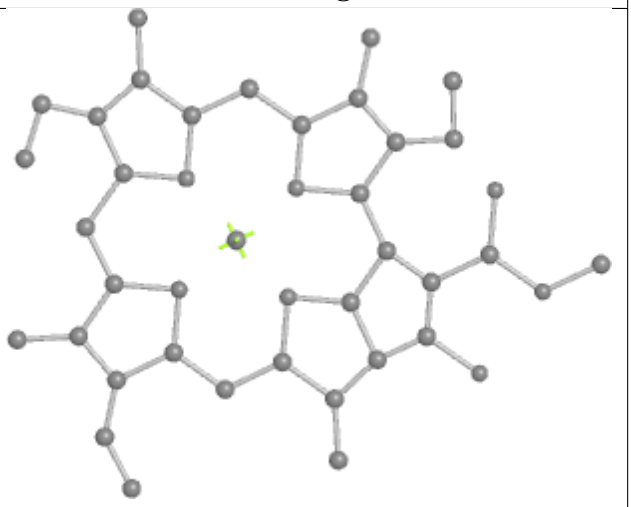
Bond lengths



Bond angles

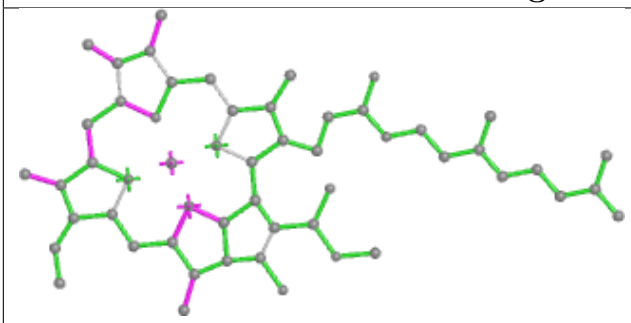


Torsions

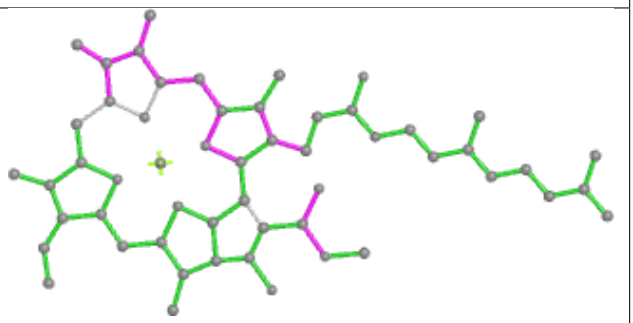


Rings

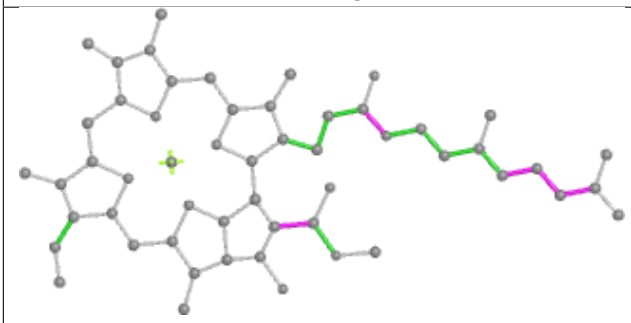
Ligand CLA 5 603



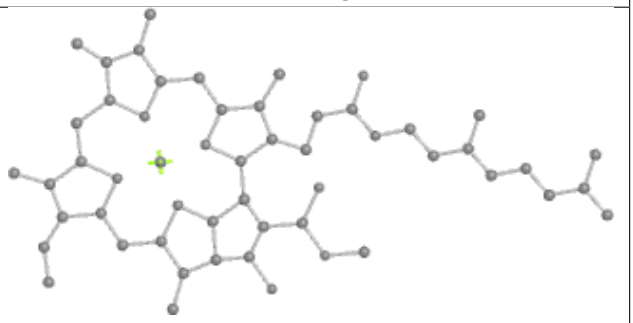
Bond lengths



Bond angles

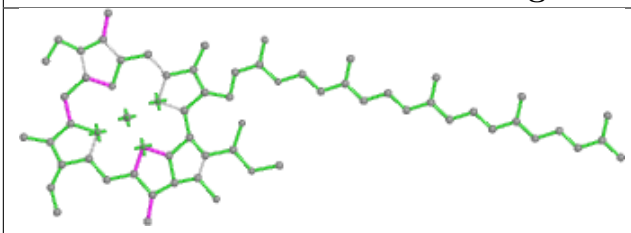


Torsions

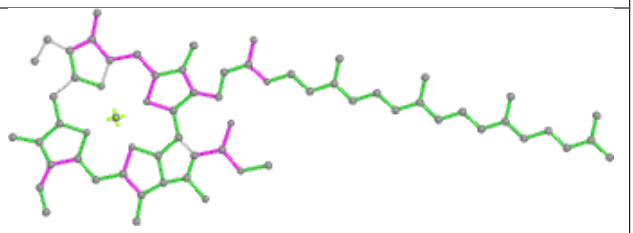


Rings

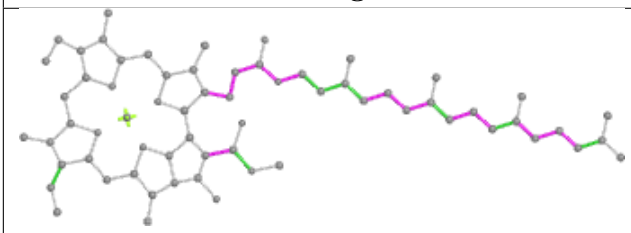
Ligand CLA 6 616



Bond lengths



Bond angles



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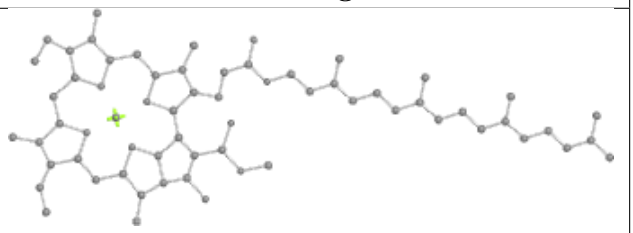
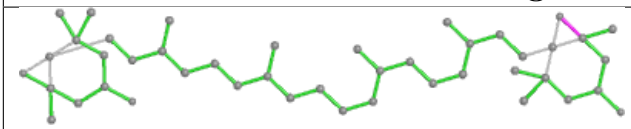


Rings

Ligand XAT 8 620



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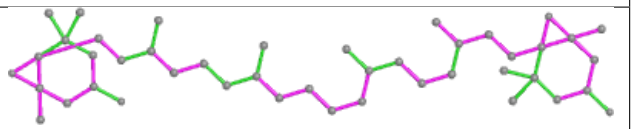
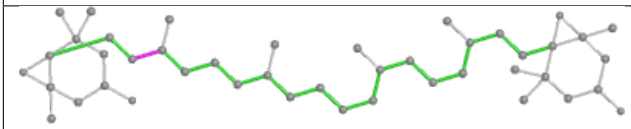


Bond angles



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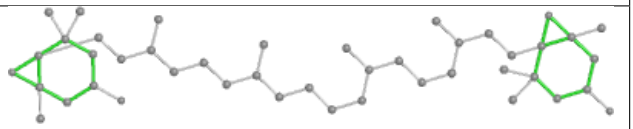
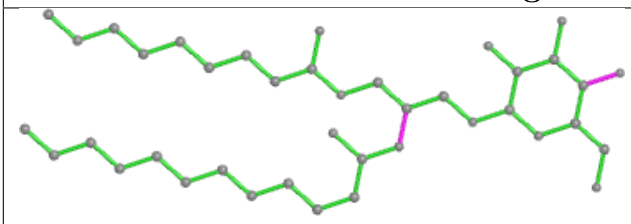


Rings

Ligand LMG J 104



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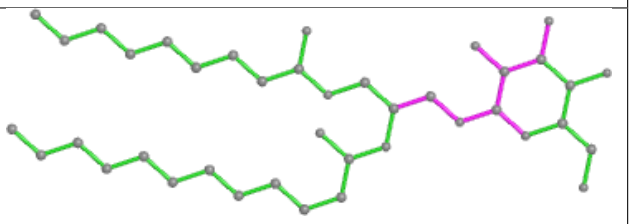
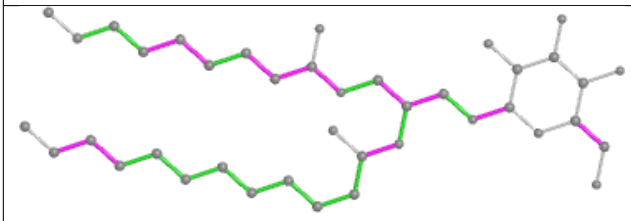


Bond angles



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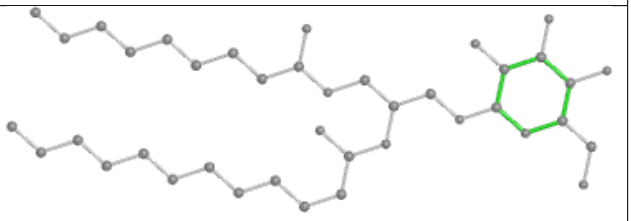
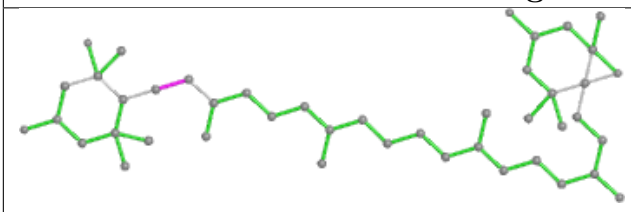
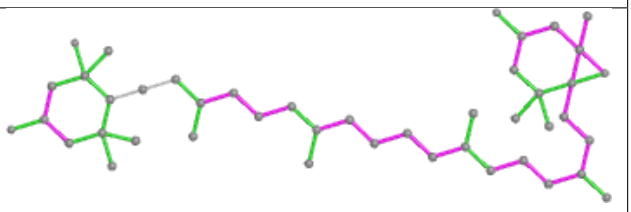


Rings

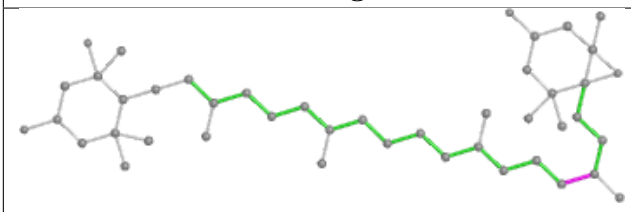
Ligand NEX 5 624



Bond lengths



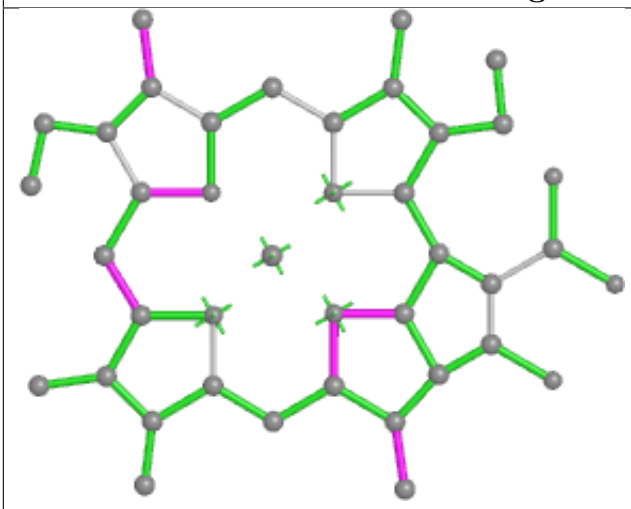
Bond angles



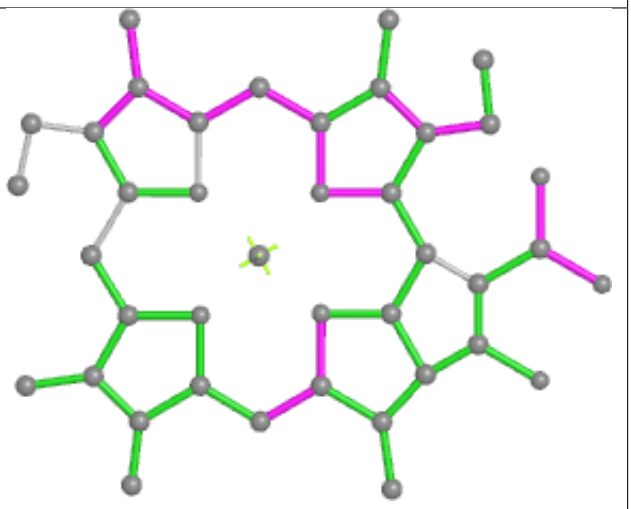
Torsions

Rings

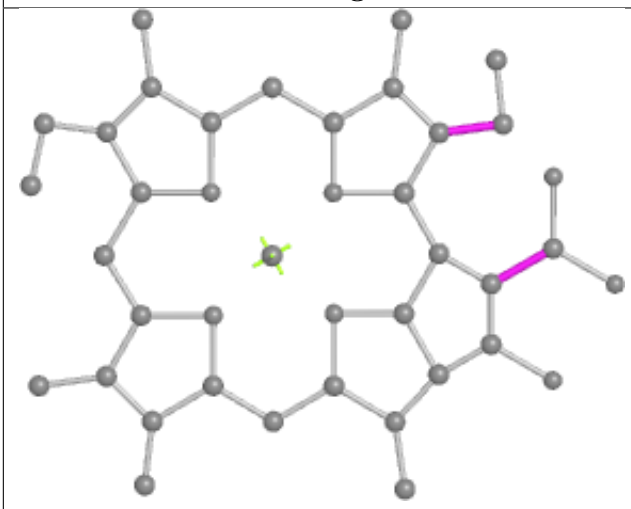
Ligand CLA 6 606



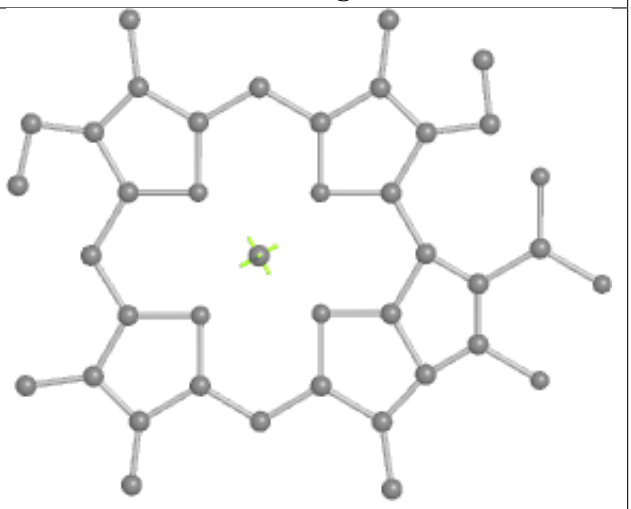
Bond lengths



Bond angles

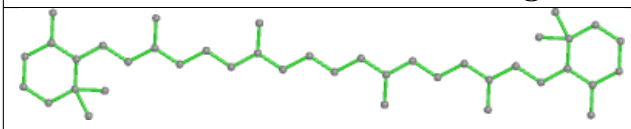


Torsions

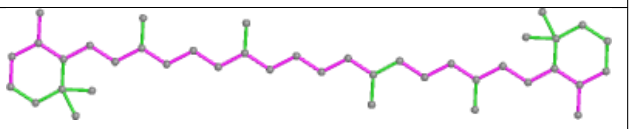


Rings

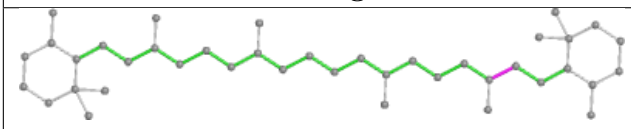
Ligand BCR B 847



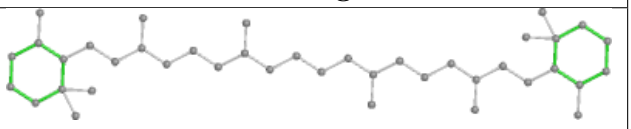
Bond lengths



Bond angles

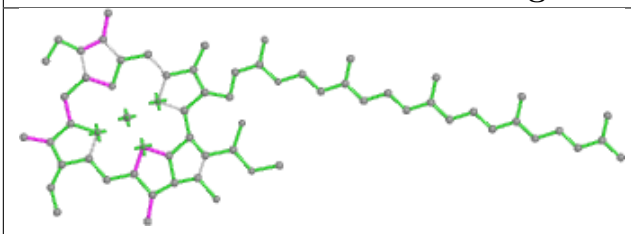


Torsions



Rings

Ligand CLA 8 613



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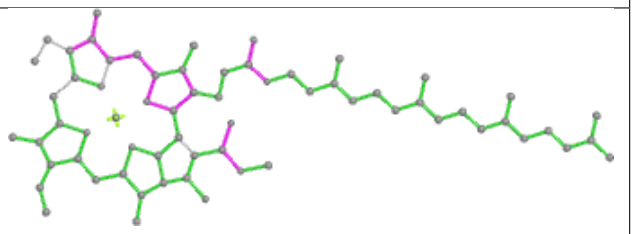
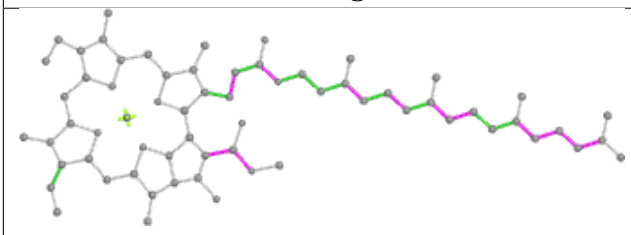
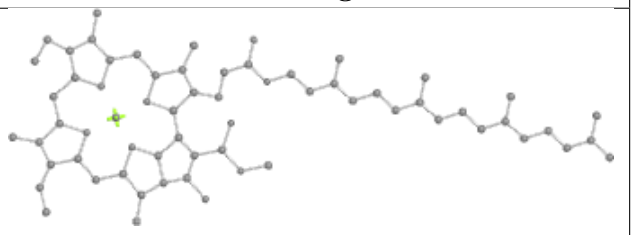


Bond angles

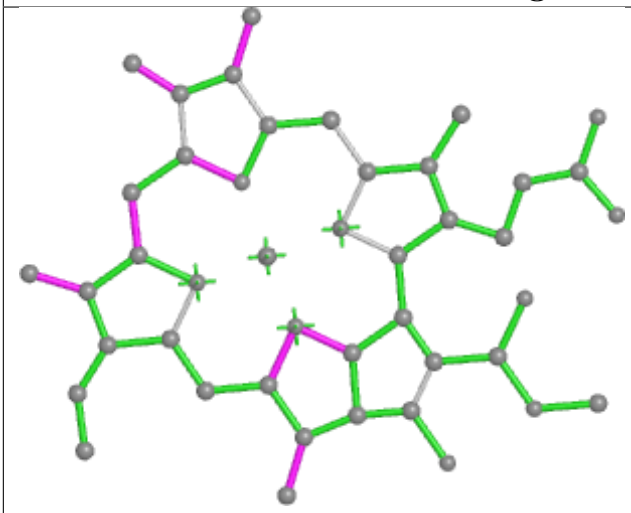


Torsions



Rings

Ligand CLA 4 603



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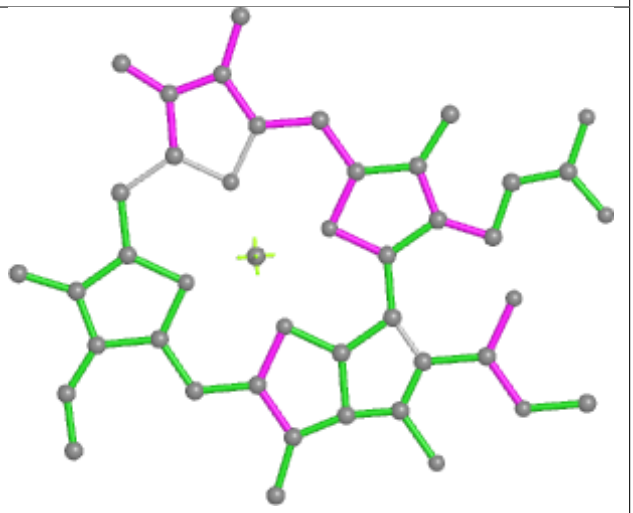
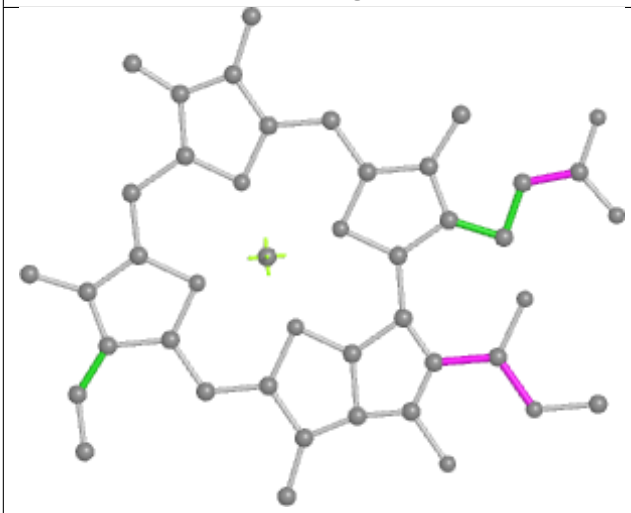
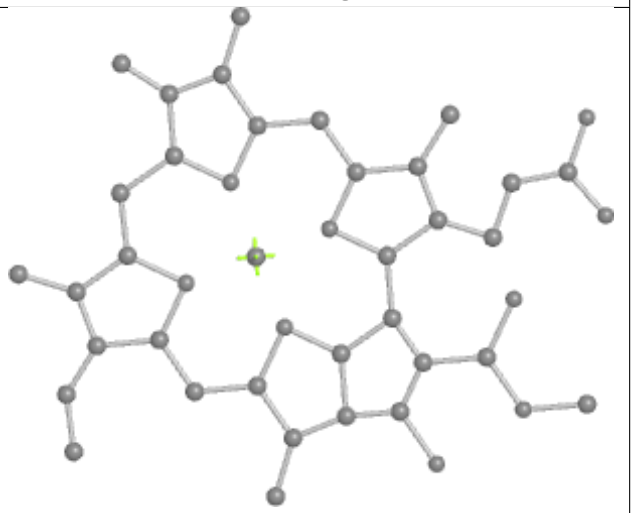


Bond angles

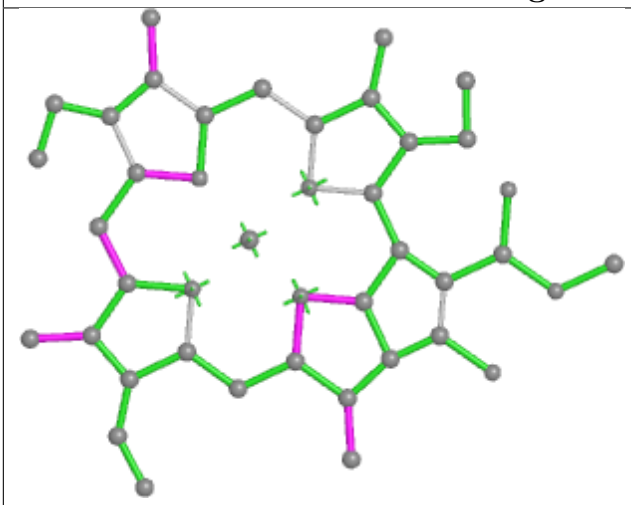


Torsions

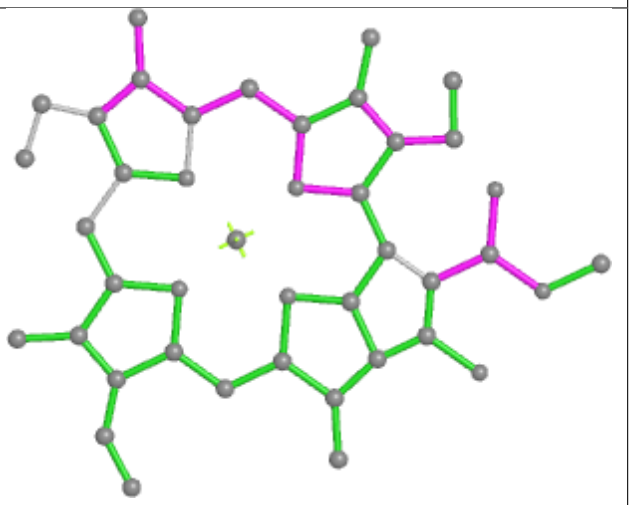


Rings

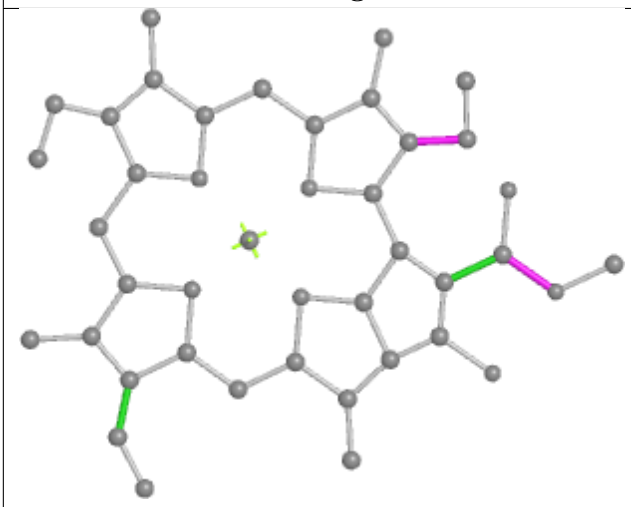
Ligand CLA 4 611



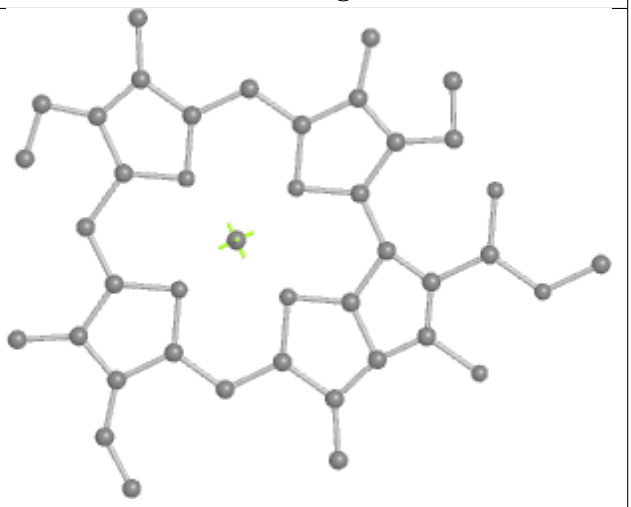
Bond lengths



Bond angles

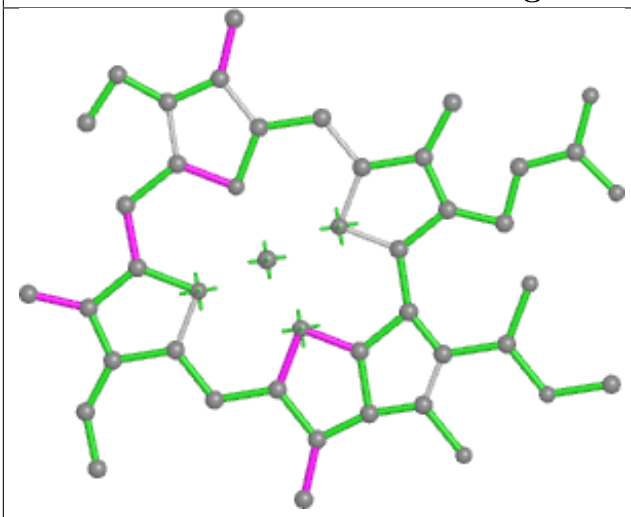


Torsions

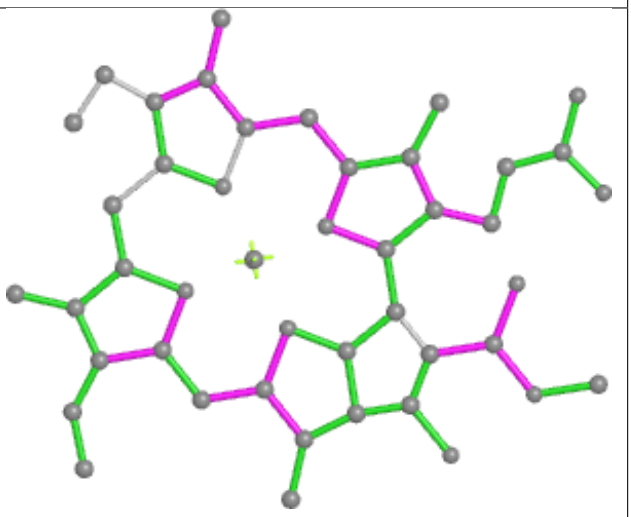


Rings

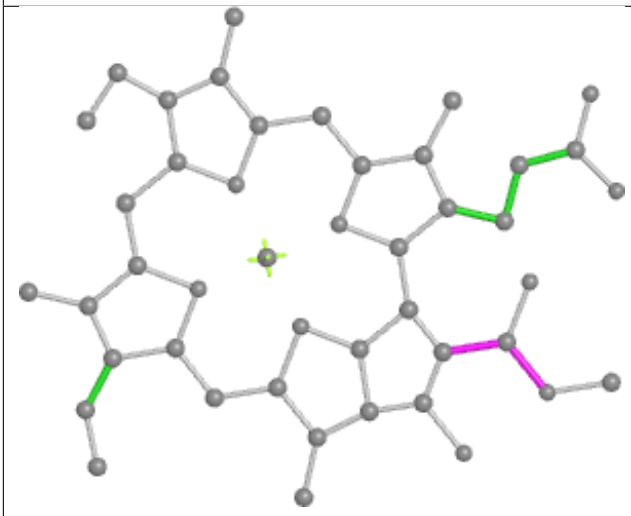
Ligand CLA A 817



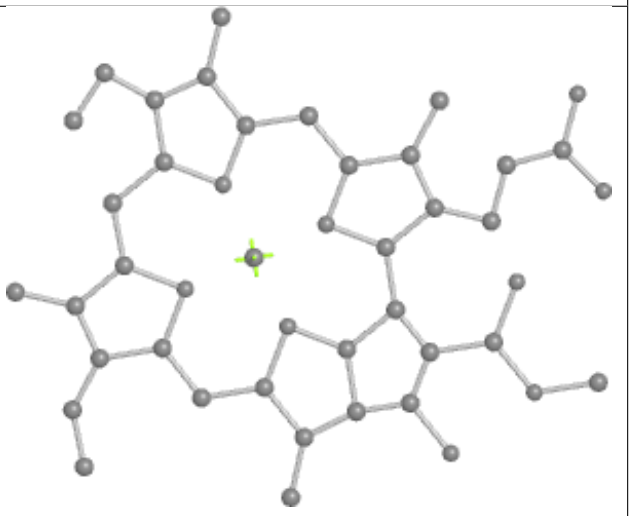
Bond lengths



Bond angles

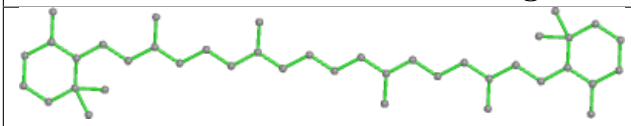


Torsions

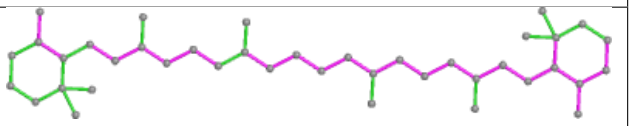


Rings

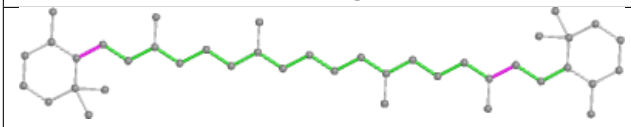
Ligand BCR A 848



Bond lengths



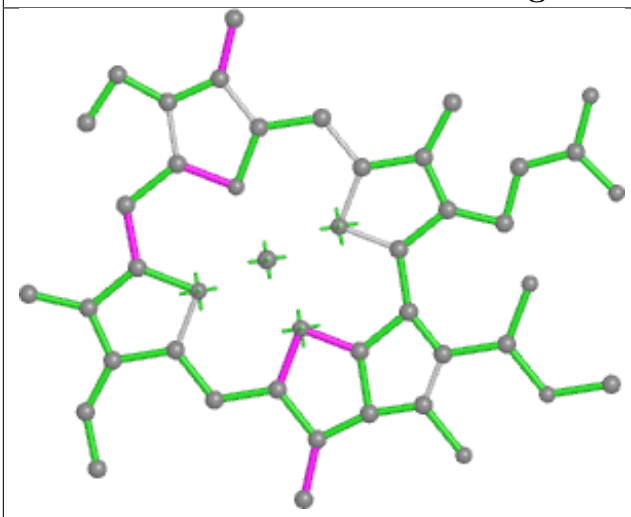
Bond angles



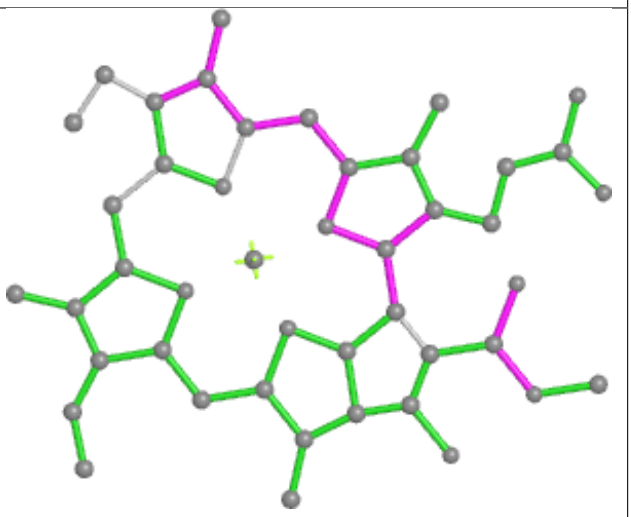
Torsions

Rings

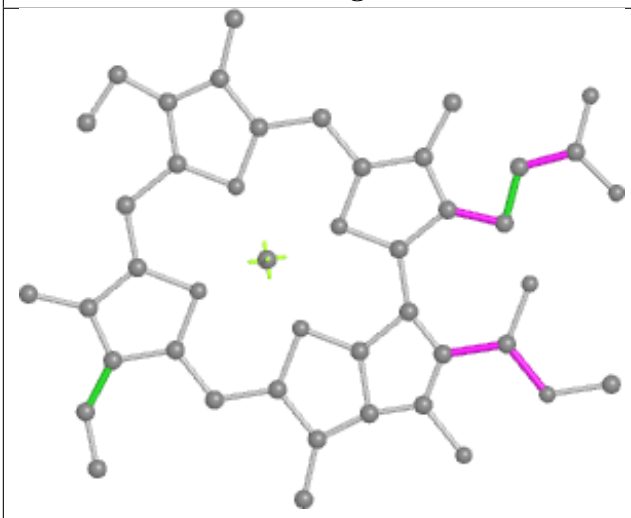
Ligand CLA 1 612



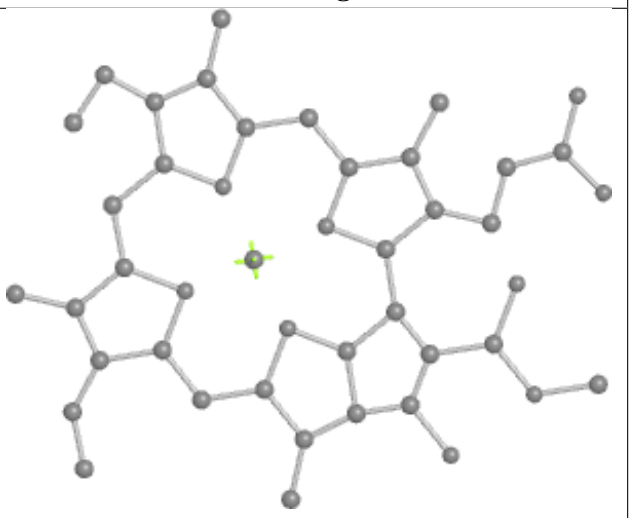
Bond lengths



Bond angles

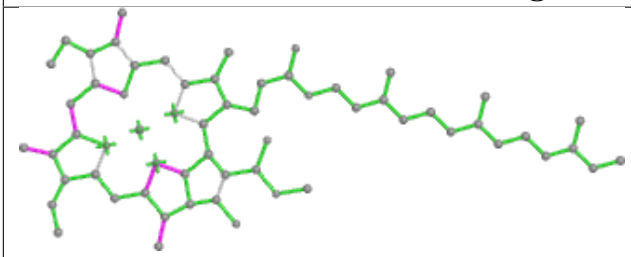


Torsions

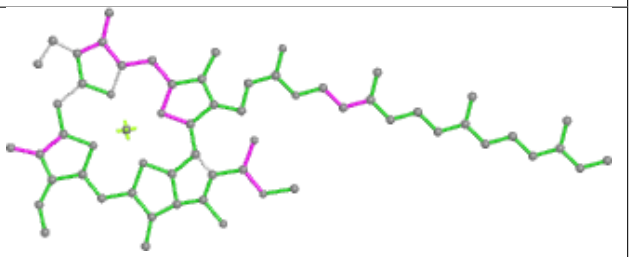


Rings

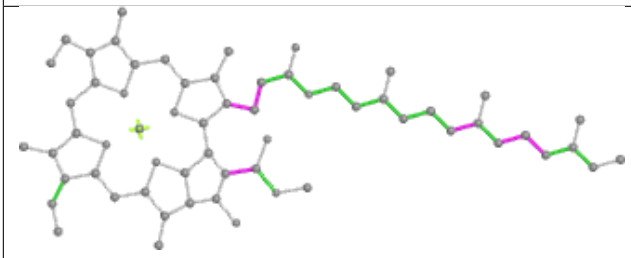
Ligand CLA 4 610



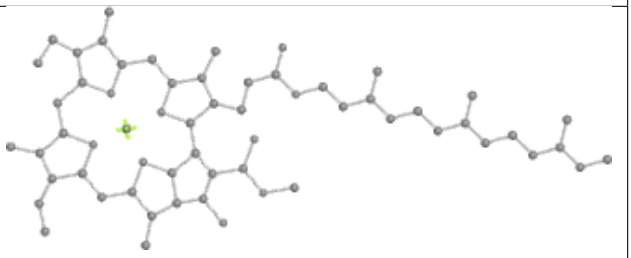
Bond lengths



Bond angles

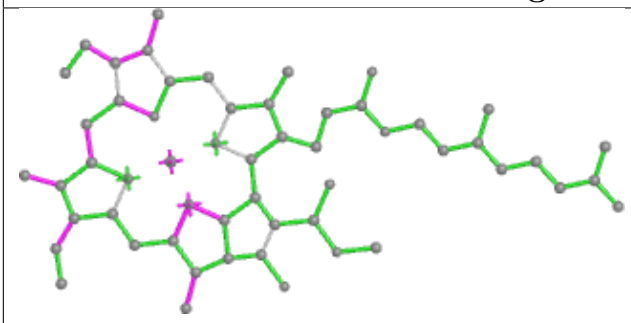


Torsions

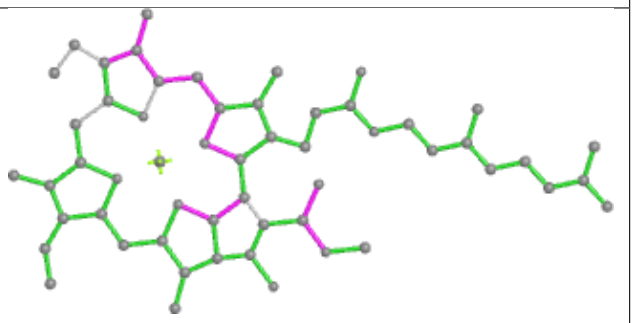


Rings

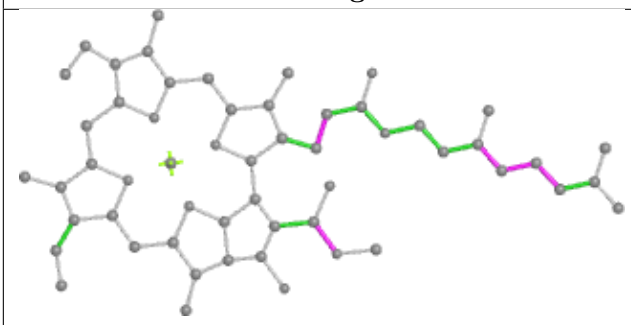
Ligand CLA 3 608



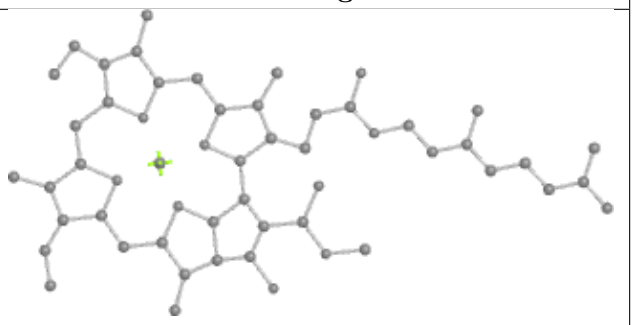
Bond lengths



Bond angles

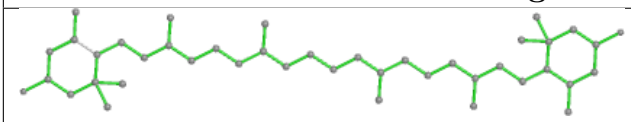


Torsions

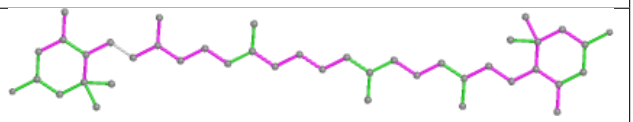


Rings

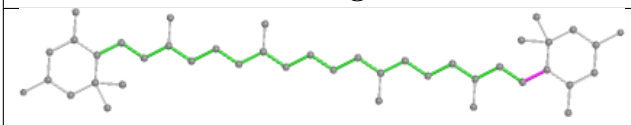
Ligand LUT 5 620



Bond lengths



Bond angles



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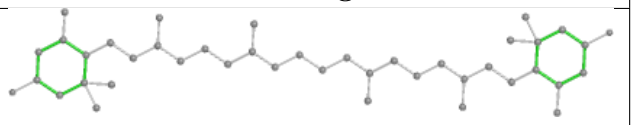
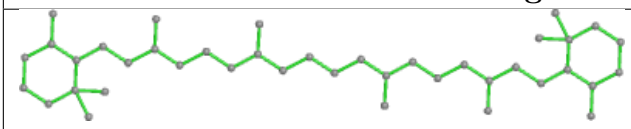
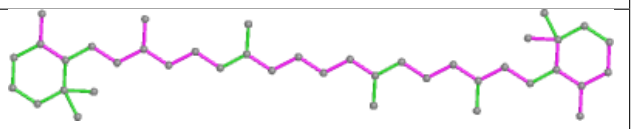


Rings

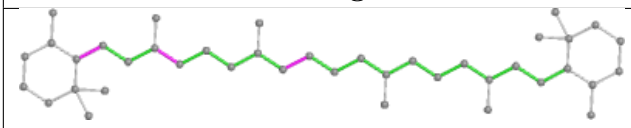
Ligand BCR L 301



Bond lengths



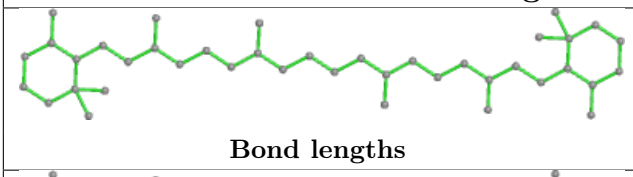
Bond angles



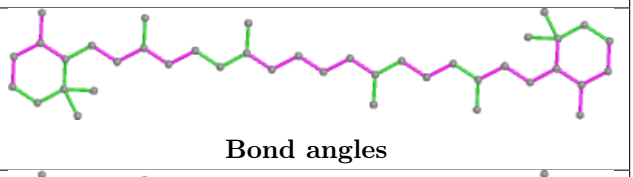
Torsions

Rings

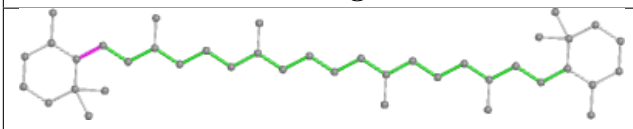
Ligand BCR B 846



Bond lengths



Bond angles



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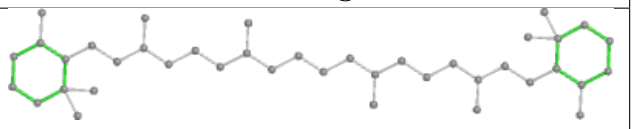
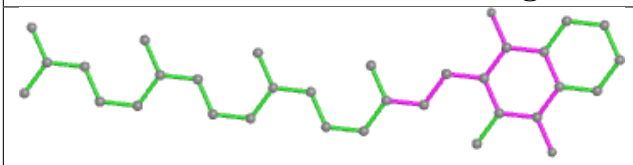


Rings

Ligand PQN A 844



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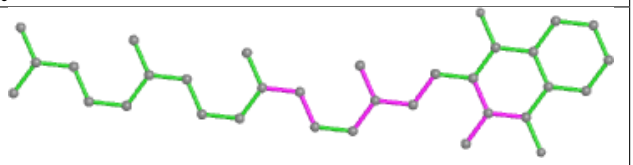
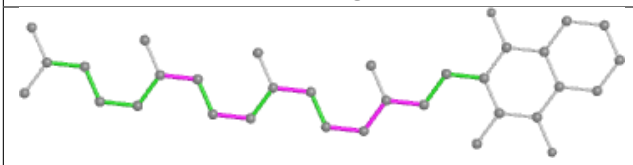
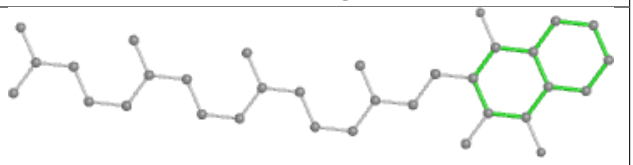


Bond angles

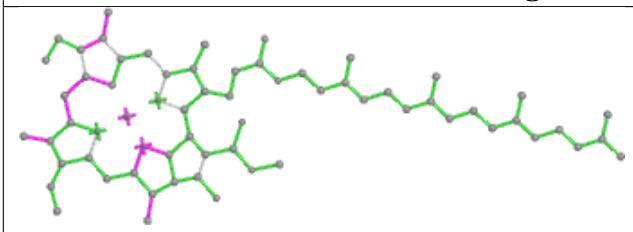


Torsions

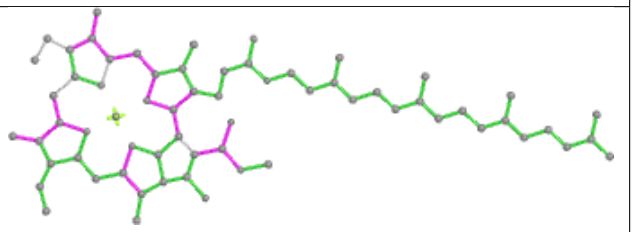


Rings

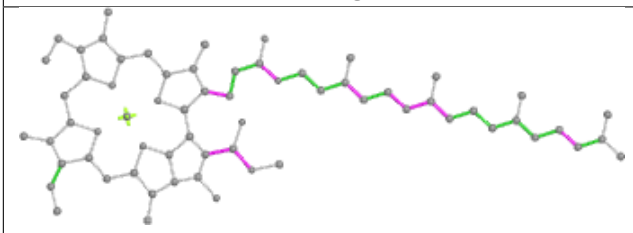
Ligand CLA A 820



Bond lengths



Bond angles



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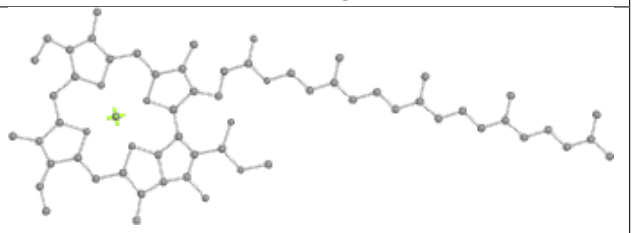
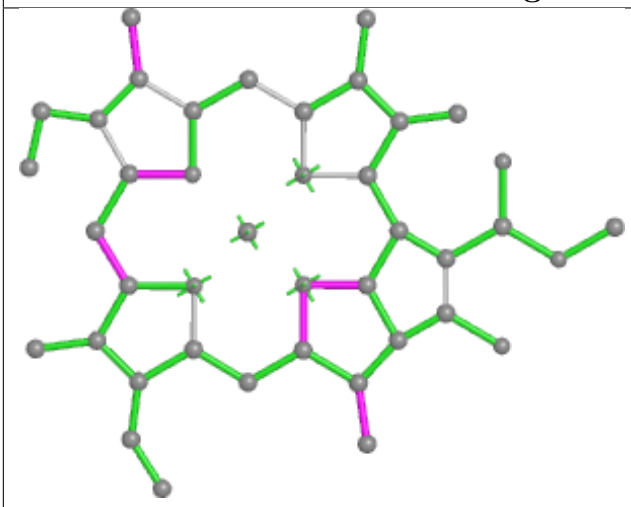
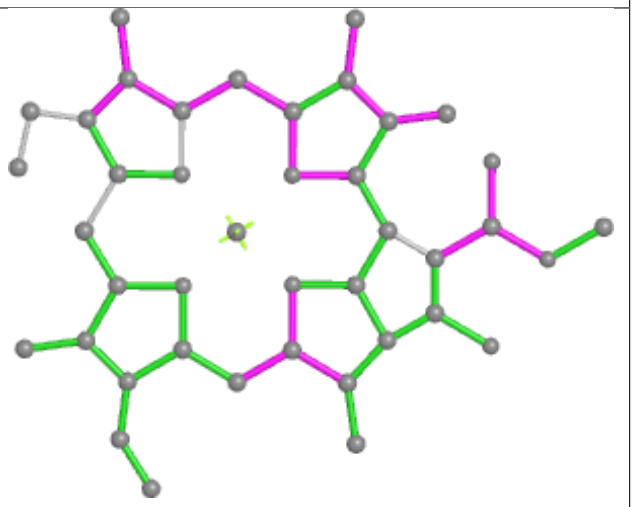


Rings

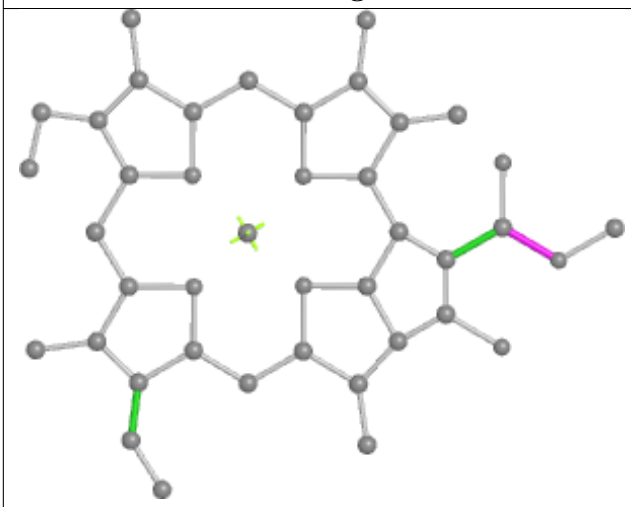
Ligand CLA A 824



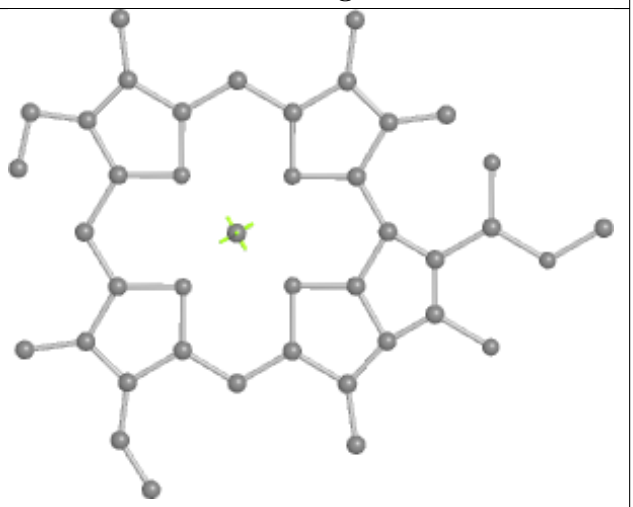
Bond lengths



Bond angles

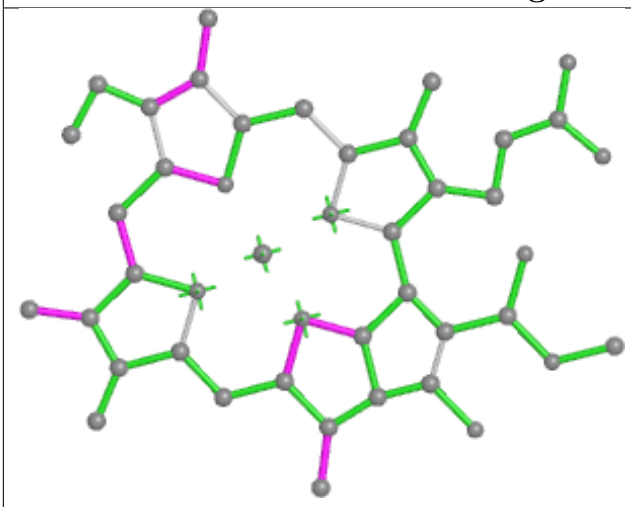


Torsions

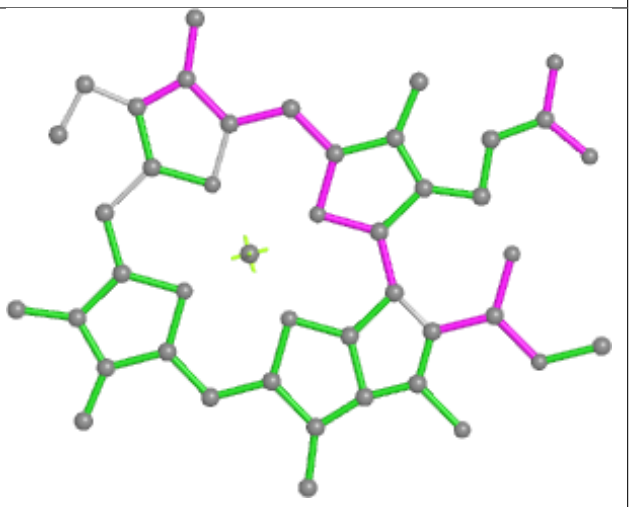


Rings

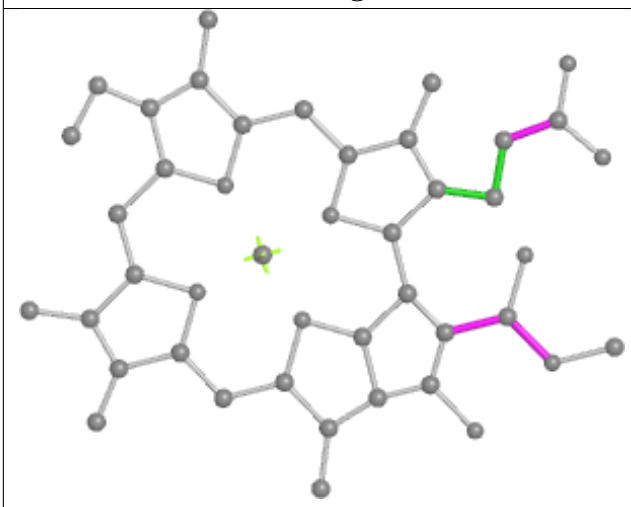
Ligand CLA 7 612



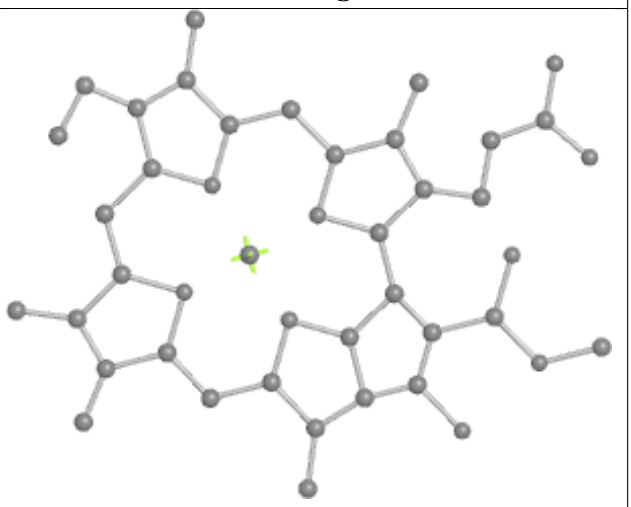
Bond lengths



Bond angles

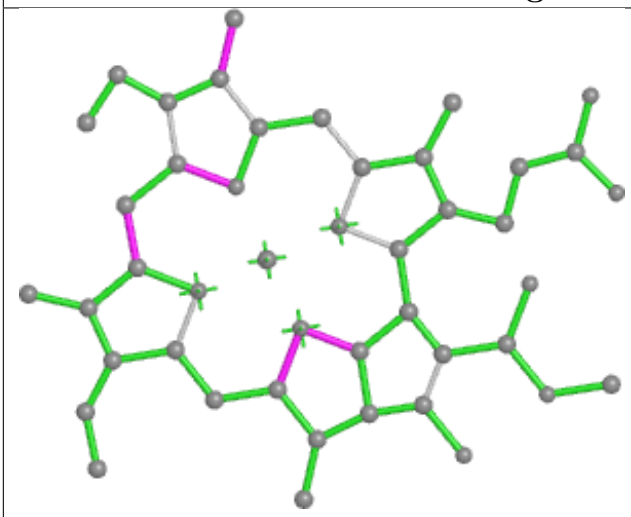


Torsions

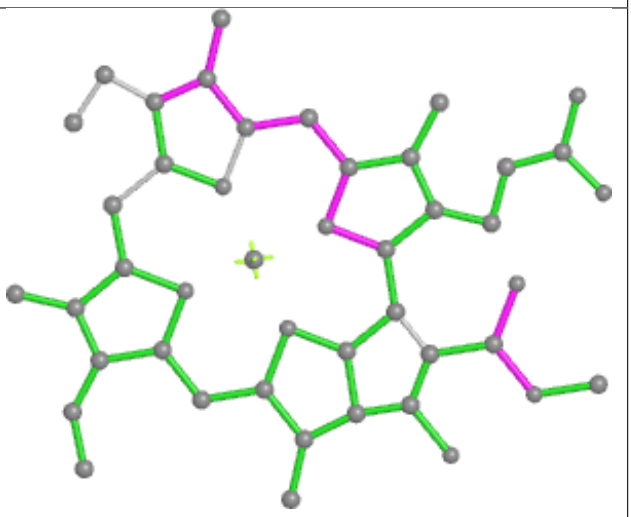


Rings

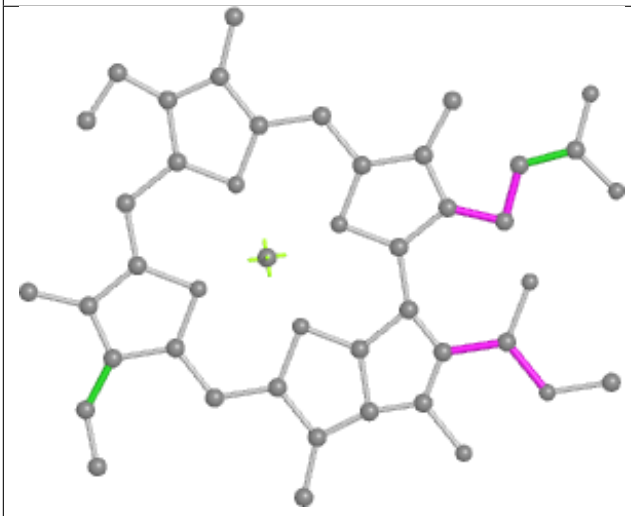
Ligand CLA L 304



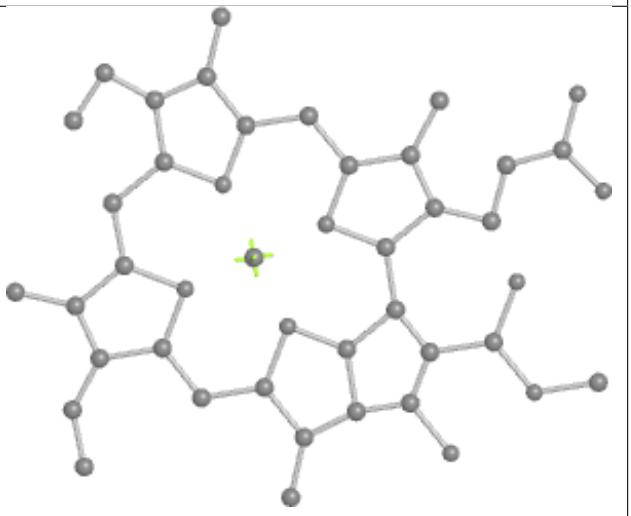
Bond lengths



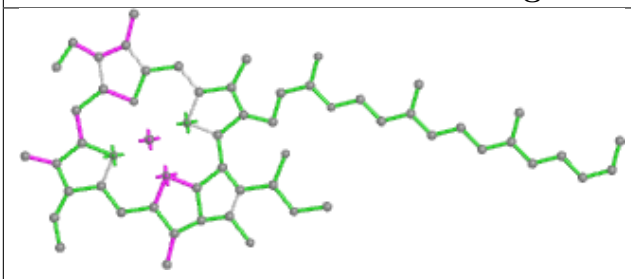
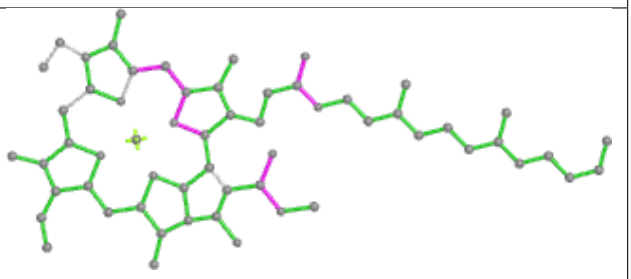
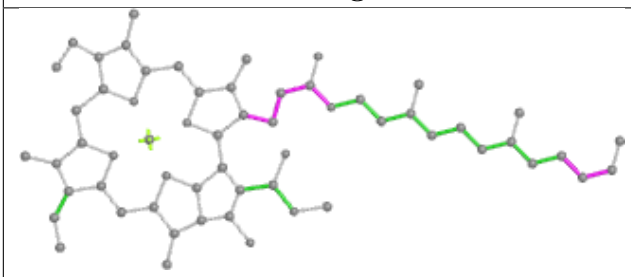
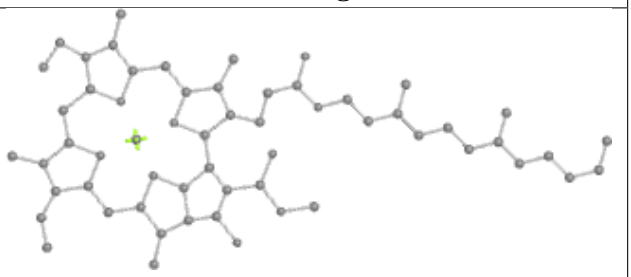
Bond angles

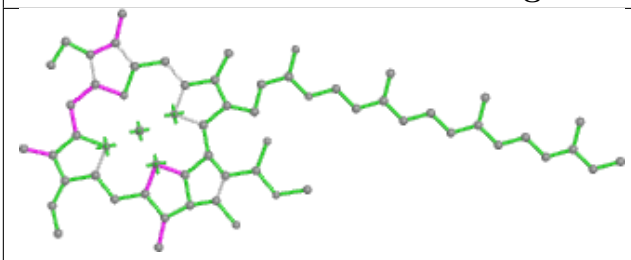
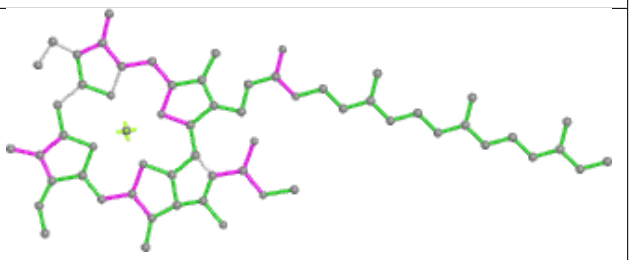
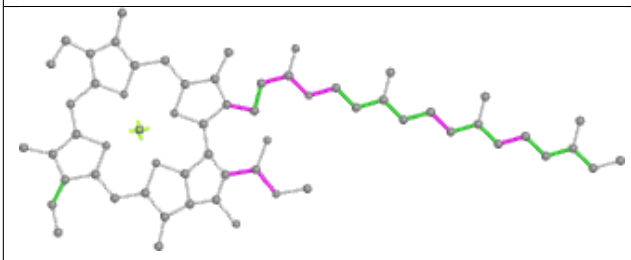
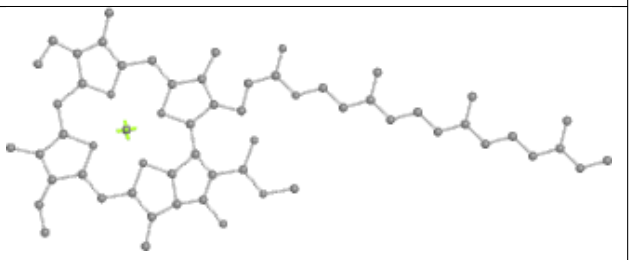


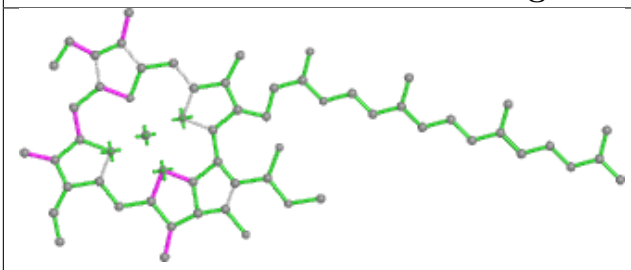
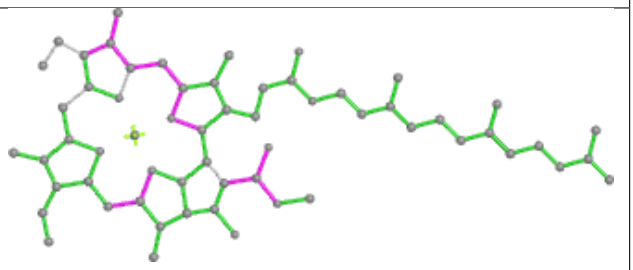
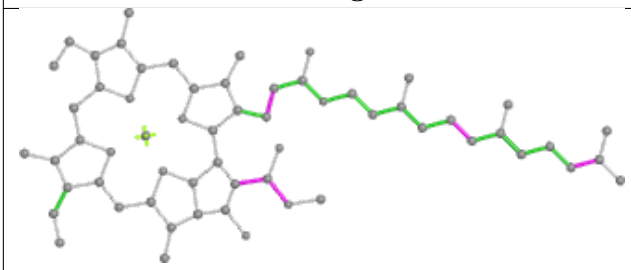
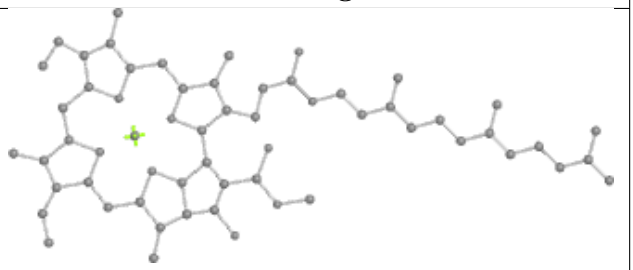
Torsions

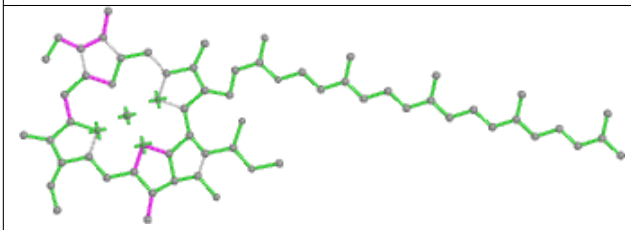
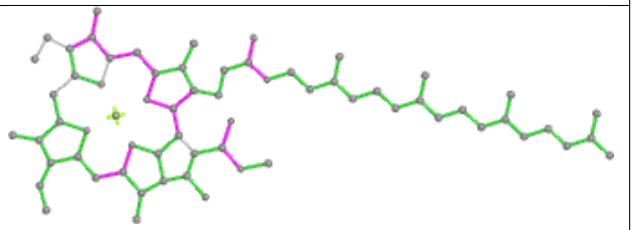
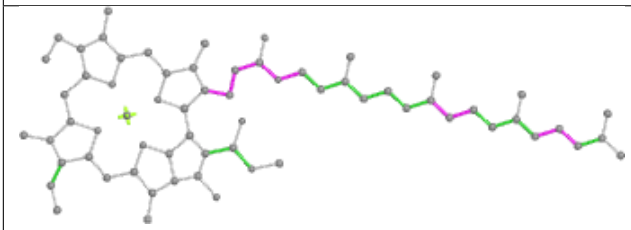
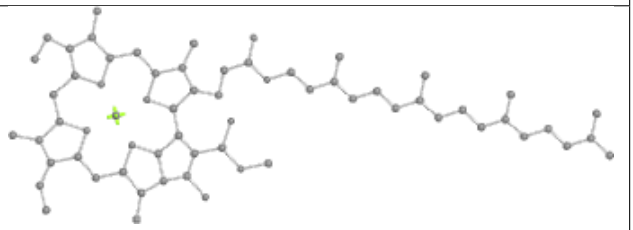


Rings

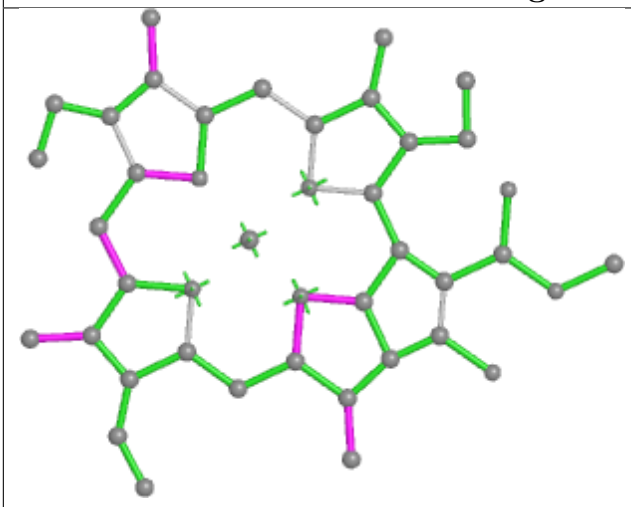
Ligand CLA A 819	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA A 835	
 Bond lengths	 Bond angles
 Torsions	 Rings

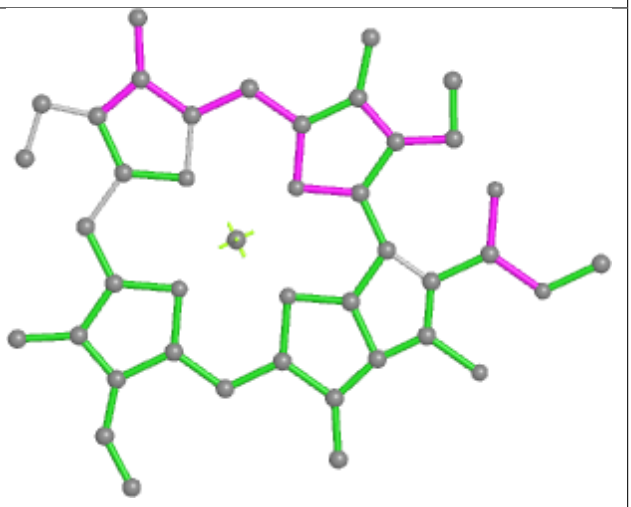
Ligand CLA 4 602	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA 5 609	
 Bond lengths	 Bond angles
 Torsions	 Rings

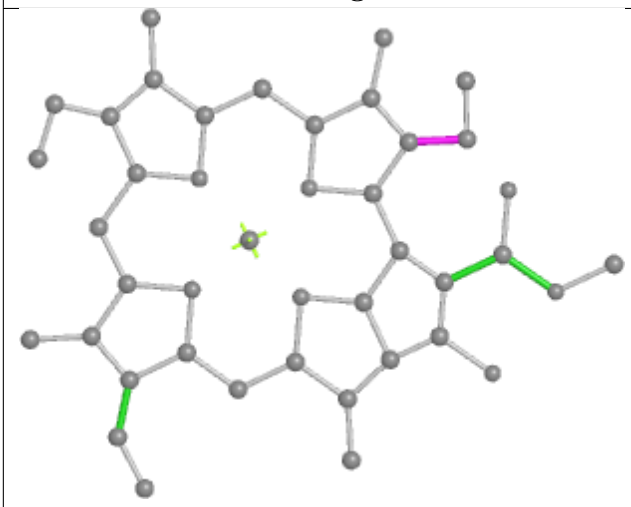
Ligand CLA 6 611



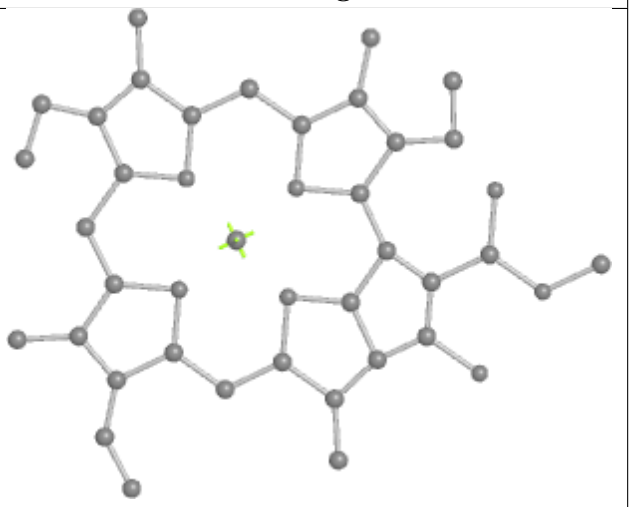
Bond lengths



Bond angles

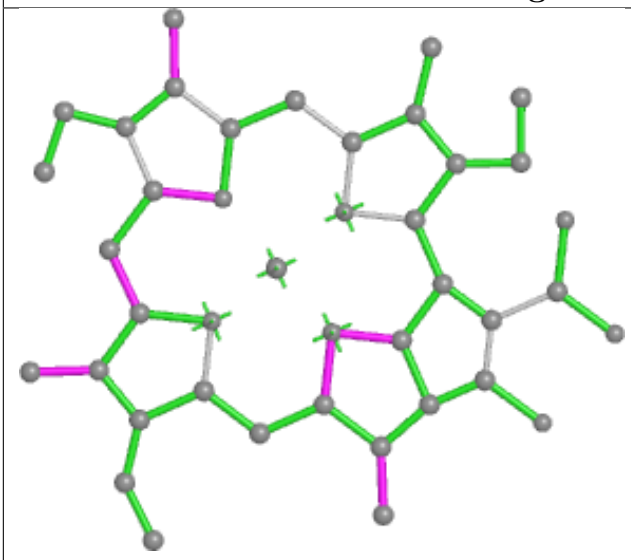


Torsions

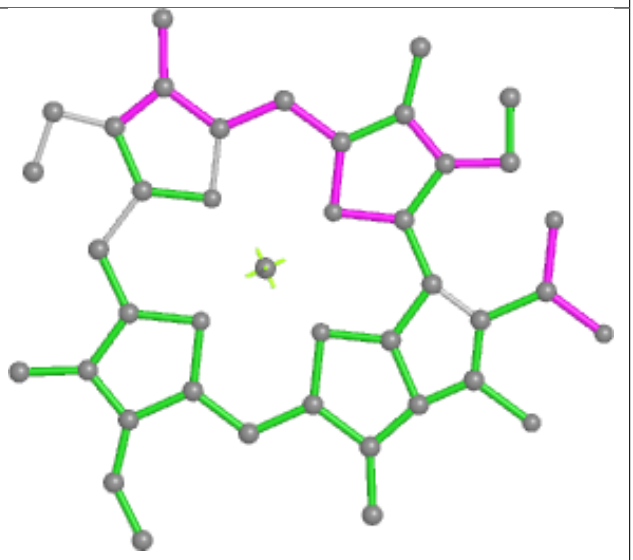


Rings

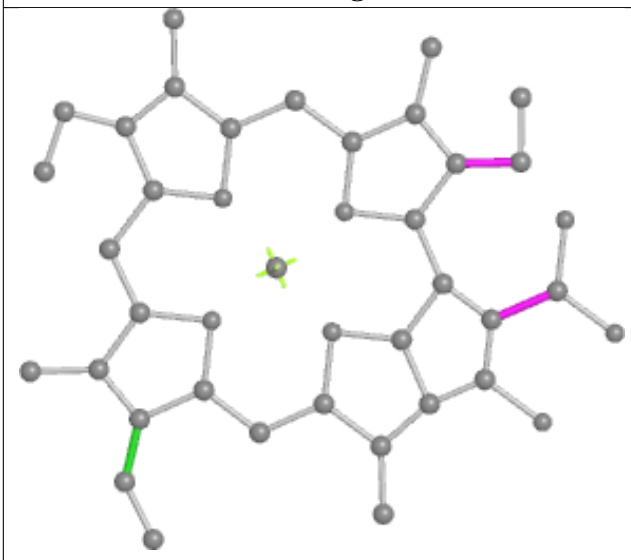
Ligand CLA 6 612



Bond lengths



Bond angles



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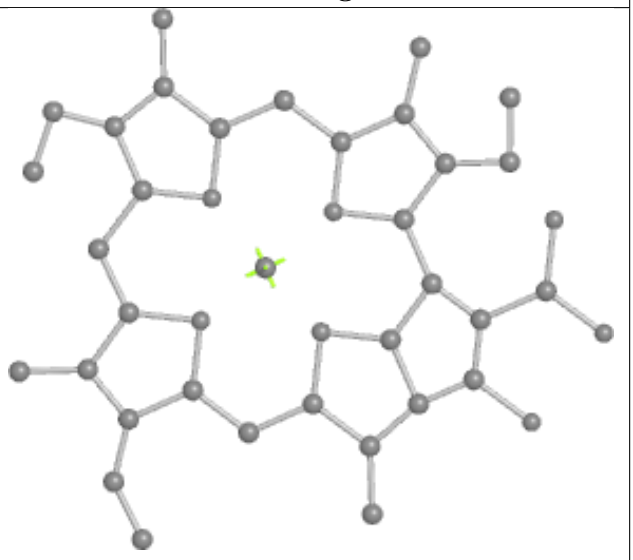
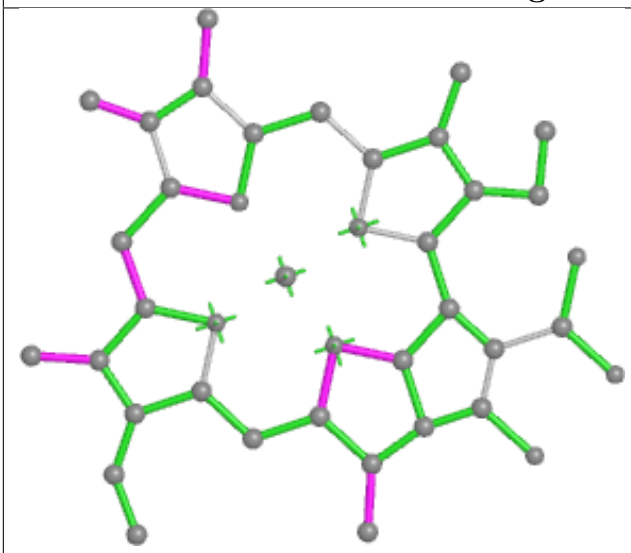
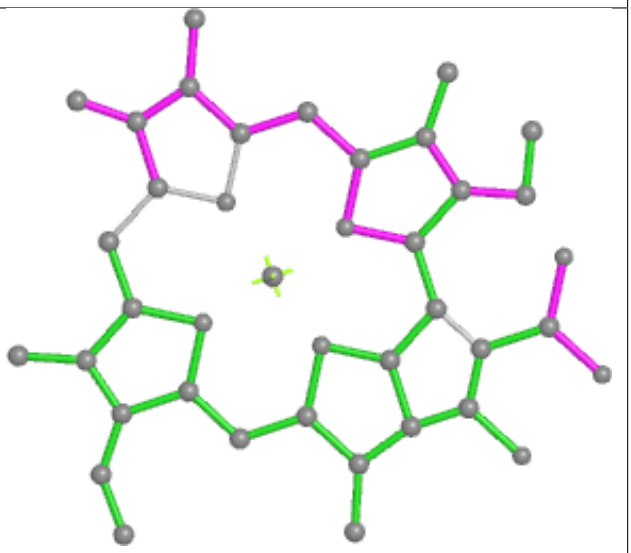


Rings

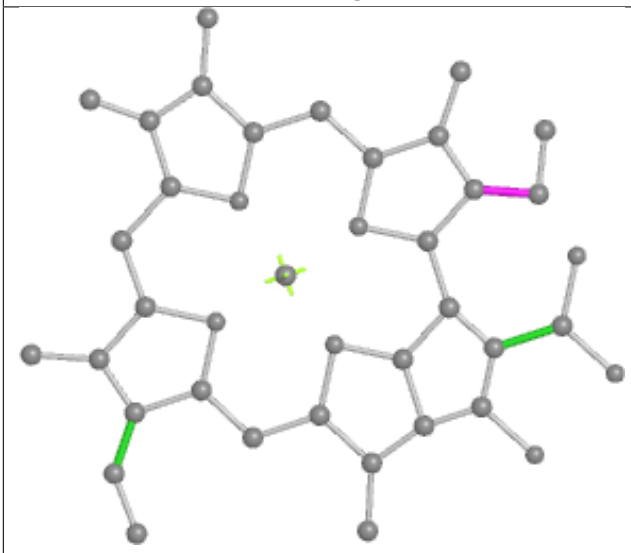
Ligand CLA 6 618



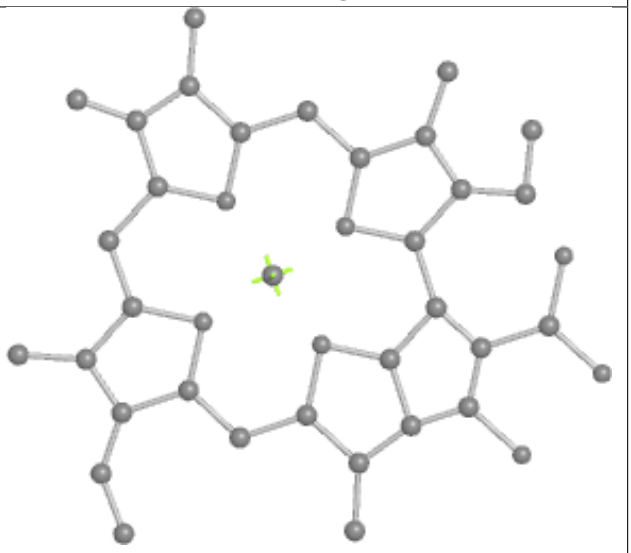
Bond lengths



Bond angles



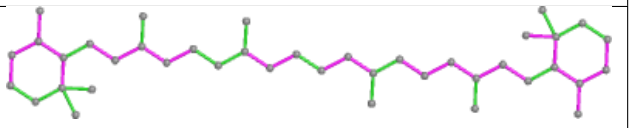
Torsions



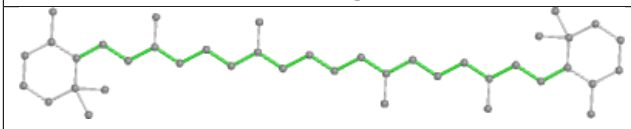
Rings

Ligand BCR A 850

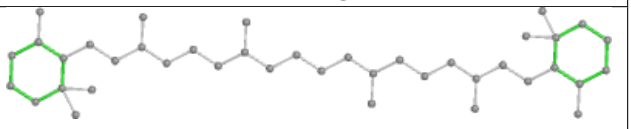
Bond lengths



Bond angles

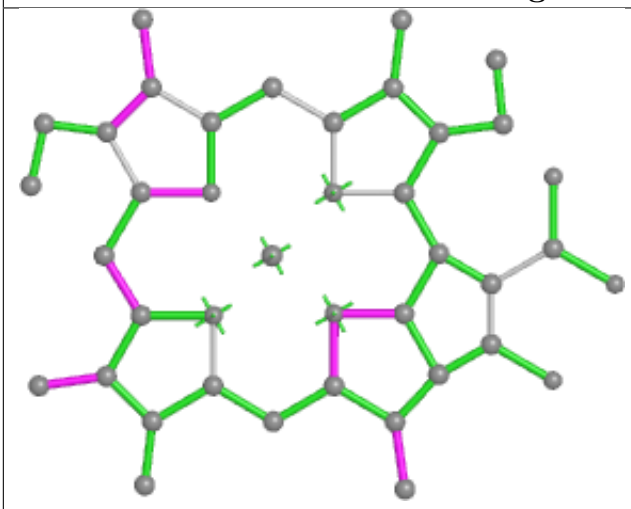


Torsions

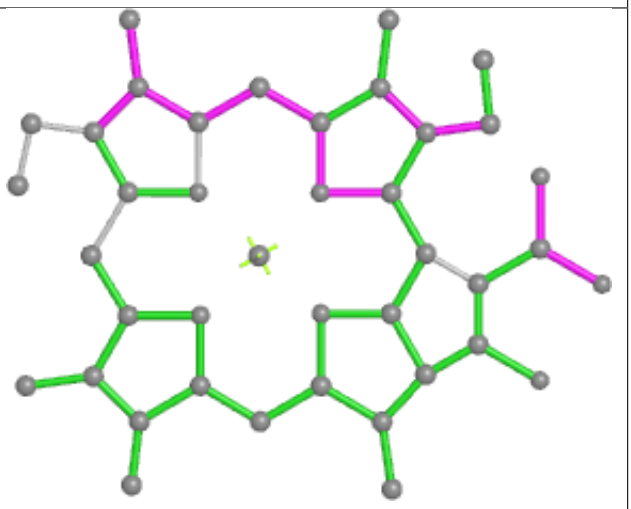


Rings

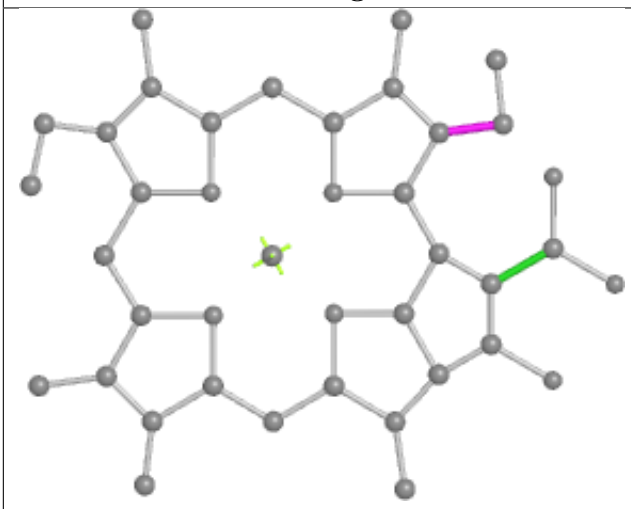
Ligand CLA 3 615



Bond lengths



Bond angles



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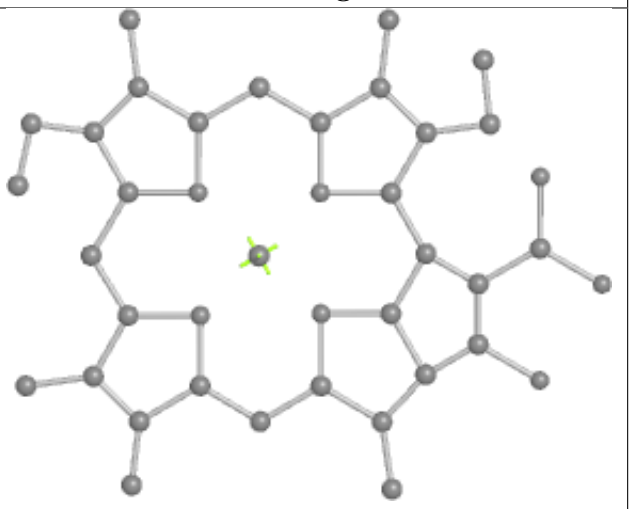
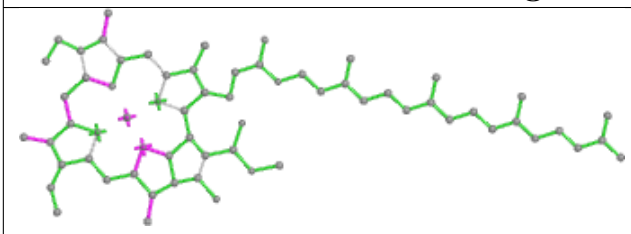
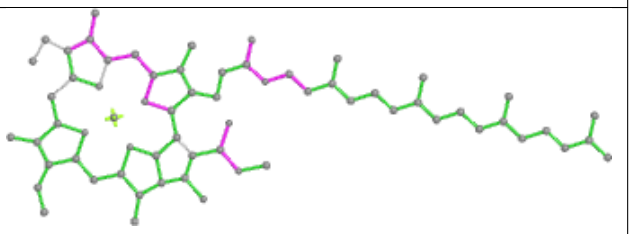


Rings

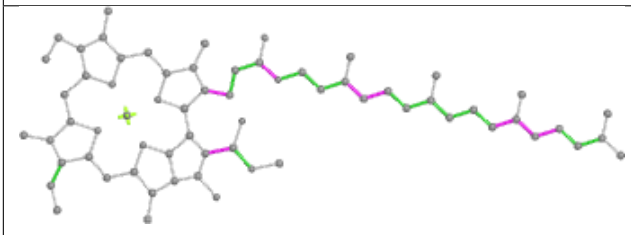
Ligand CLA B 805



Bond lengths



Bond angles



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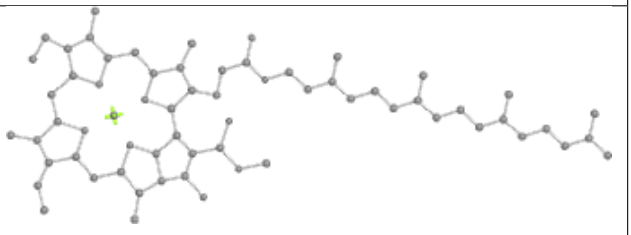
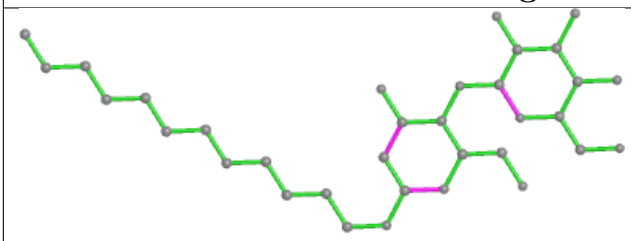
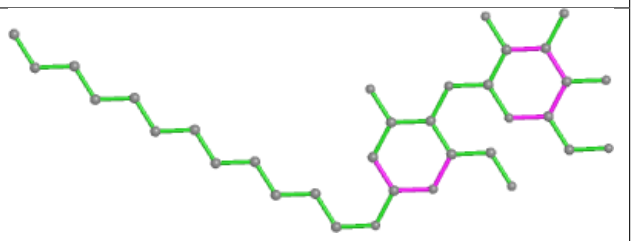


Rings

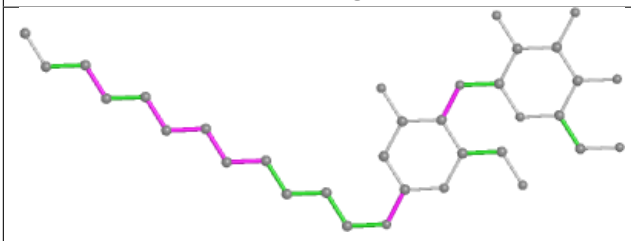
Ligand LMU A 859



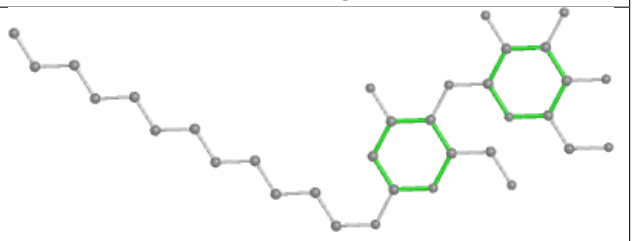
Bond lengths



Bond angles

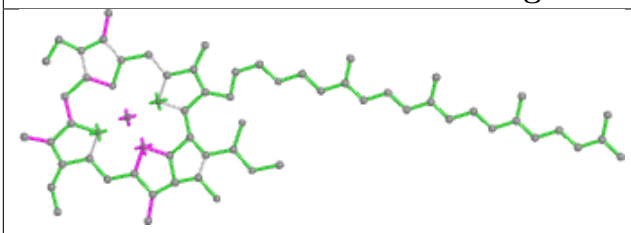


Torsions

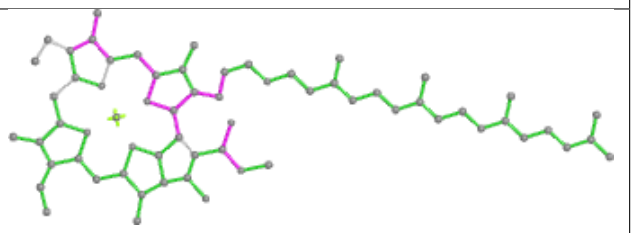


Rings

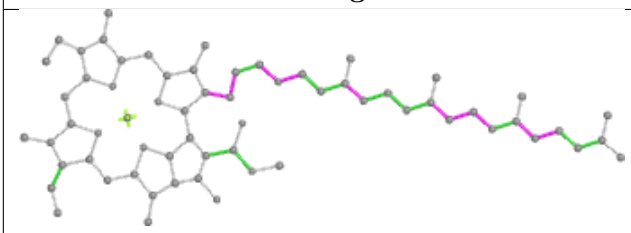
Ligand CLA A 826



Bond lengths



Bond angles



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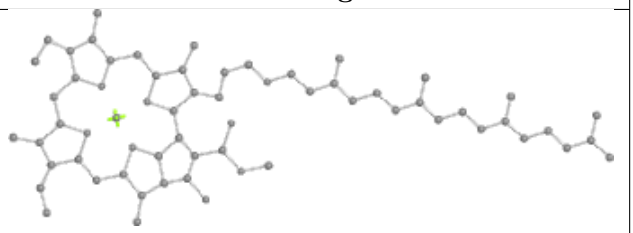
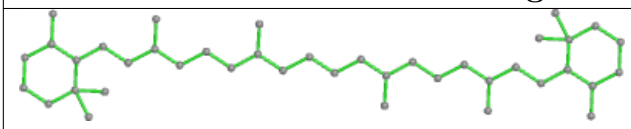
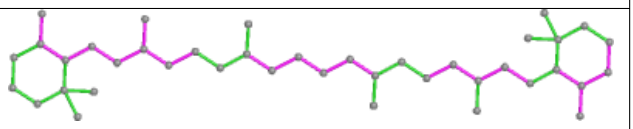


Rings

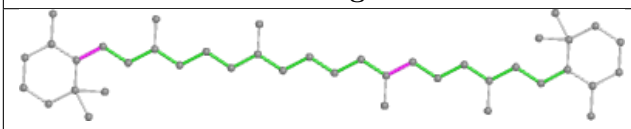
Ligand BCR 7 623



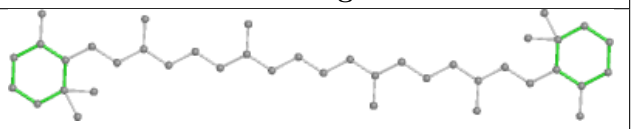
Bond lengths



Bond angles

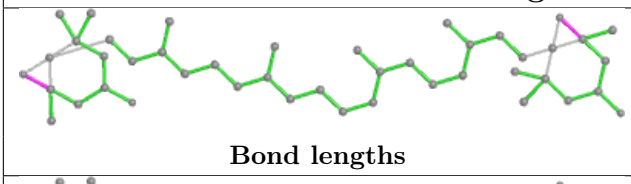


Torsions

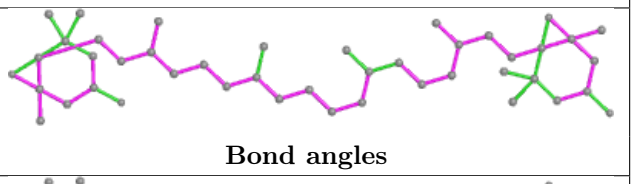


Rings

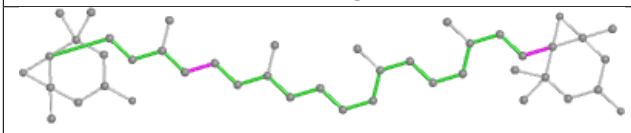
Ligand XAT 6 621



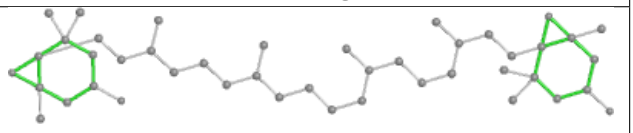
Bond lengths



Bond angles

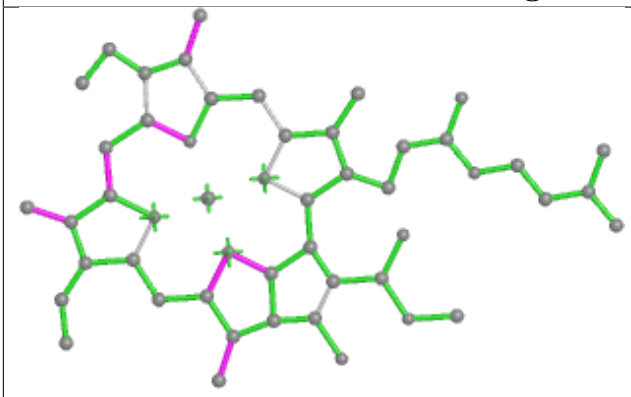


Torsions

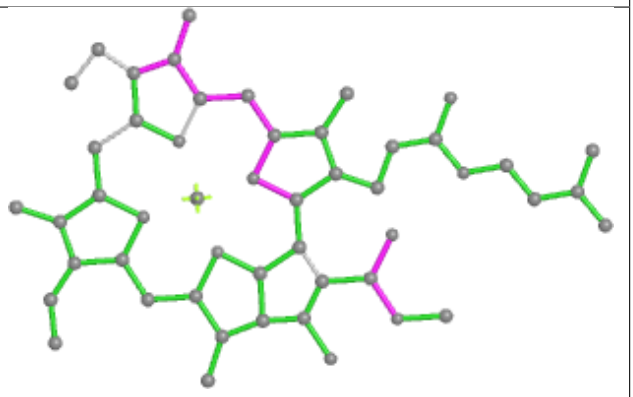


Rings

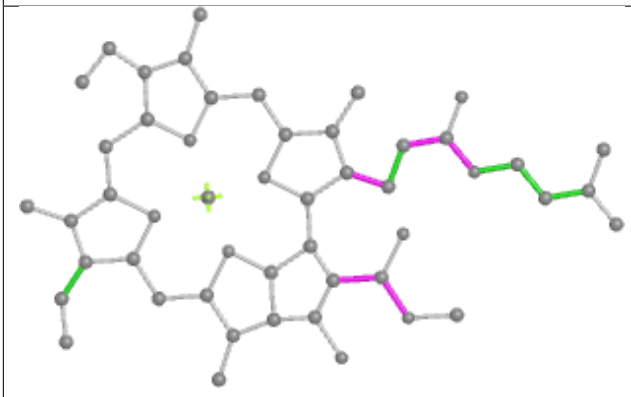
Ligand CLA A 845



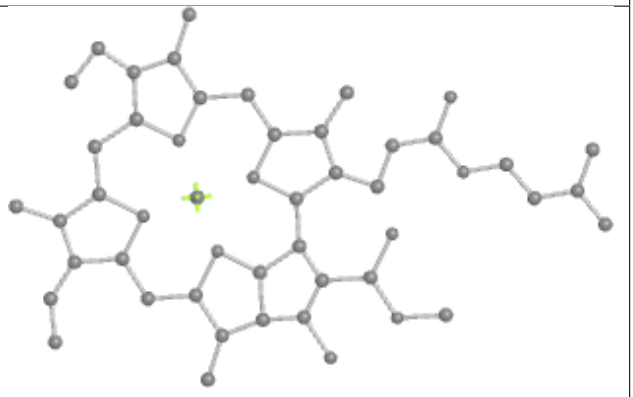
Bond lengths



Bond angles

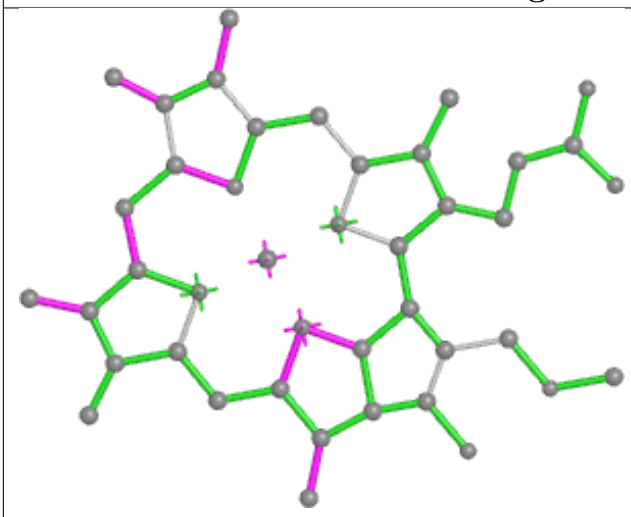


Torsions

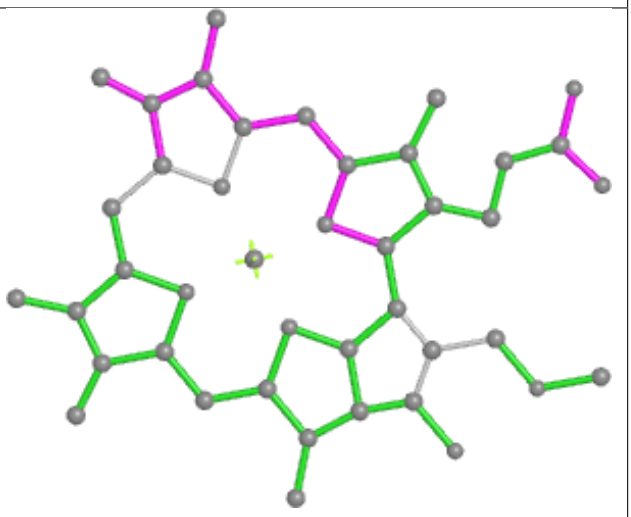


Rings

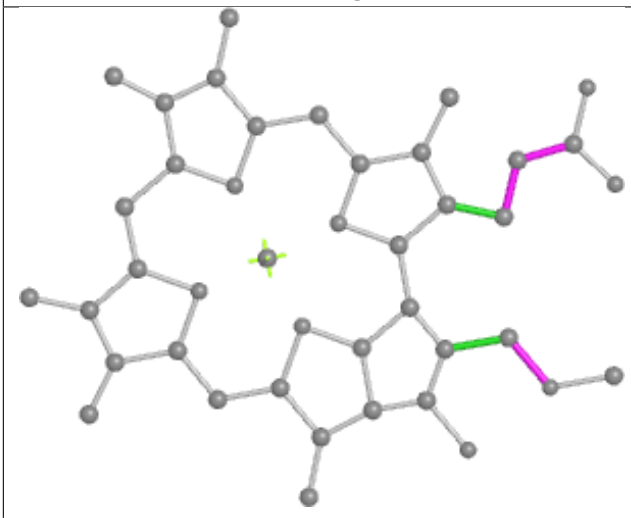
Ligand CLA 5 616



Bond lengths



Bond angles



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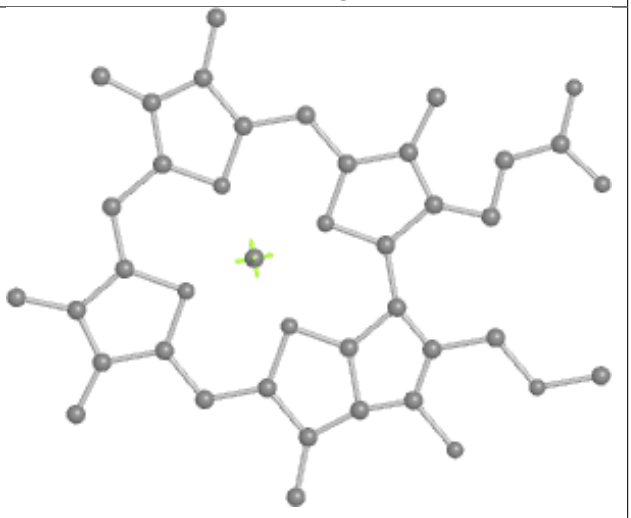
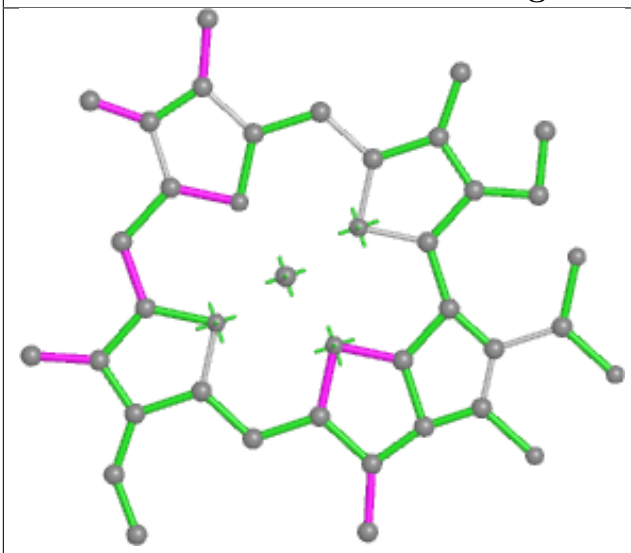
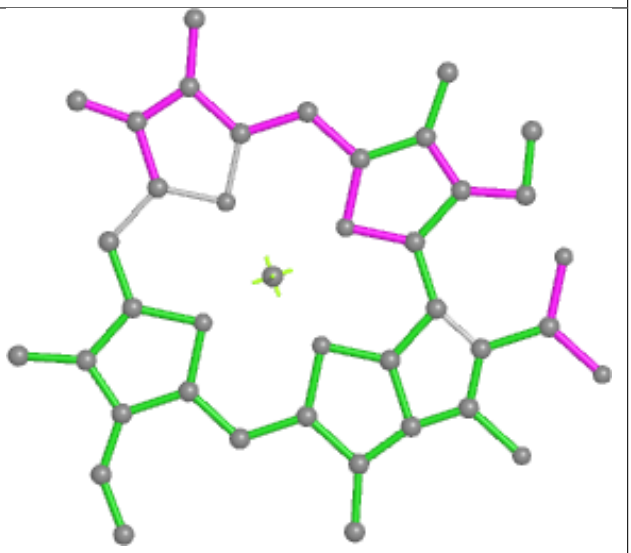


Rings

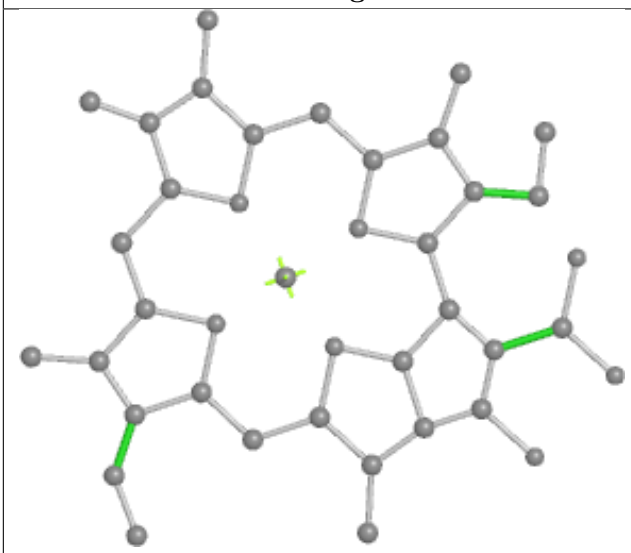
Ligand CLA 5 618



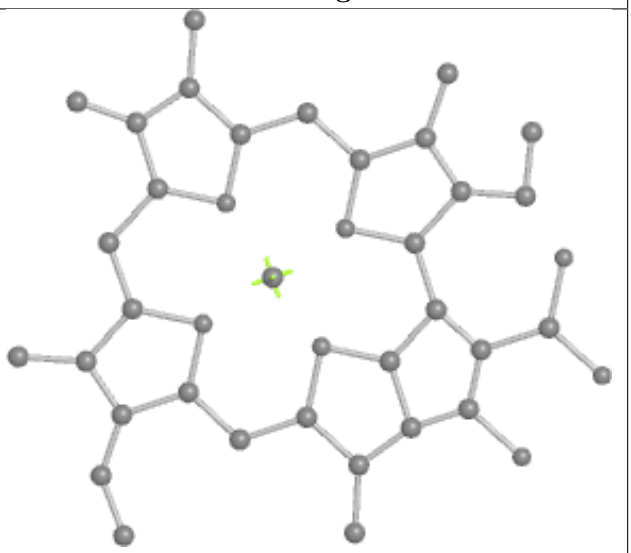
Bond lengths



Bond angles

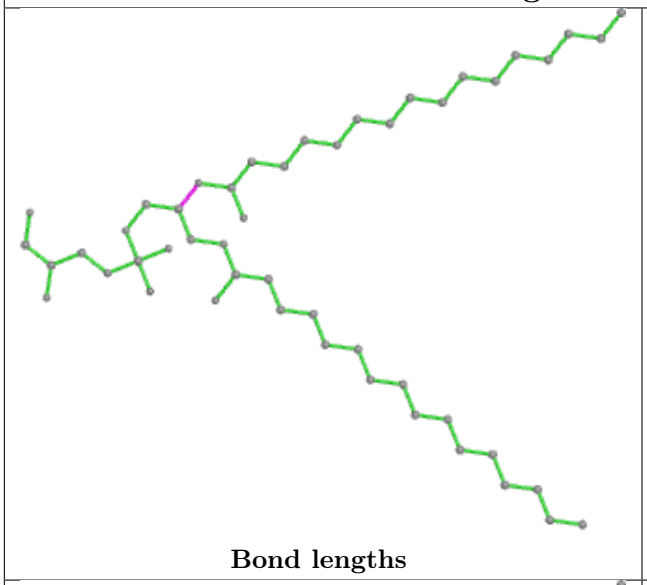


Torsions

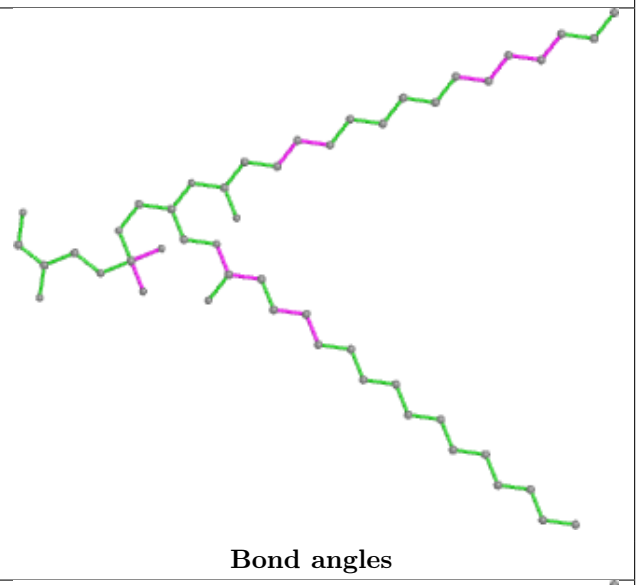


Rings

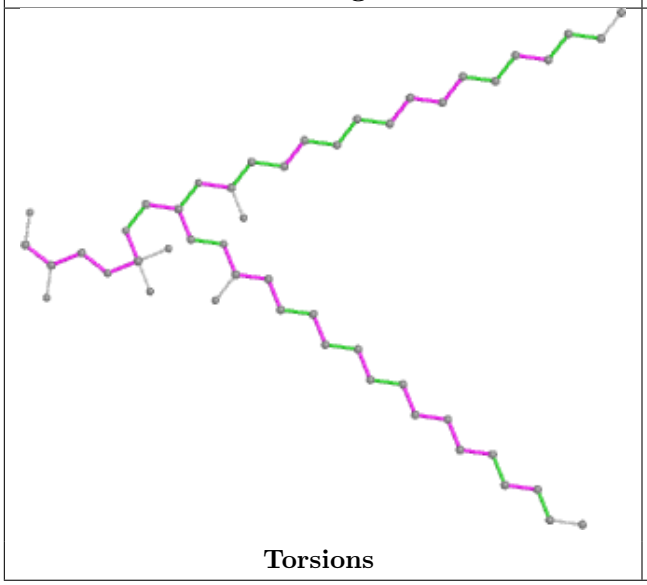
Ligand LHG A 846



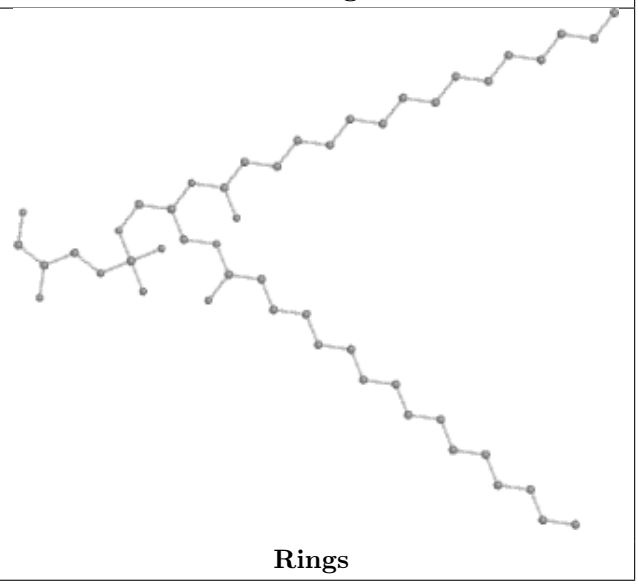
Bond lengths



Bond angles

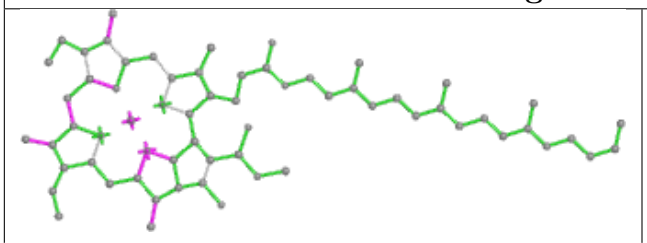


Torsions

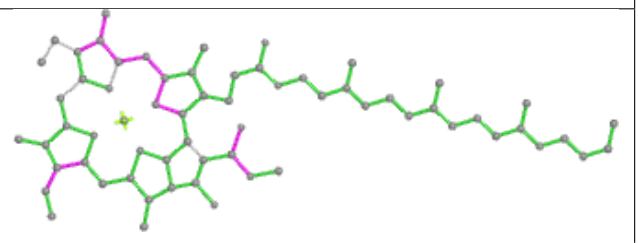


Rings

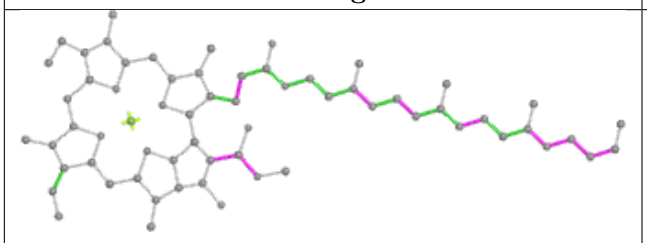
Ligand CLA B 814



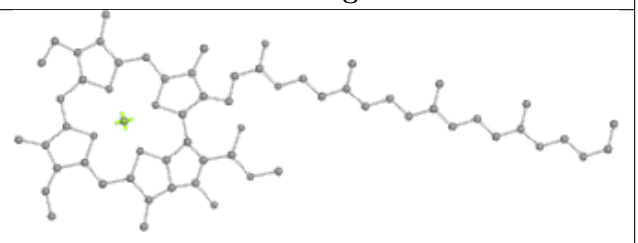
Bond lengths



Bond angles

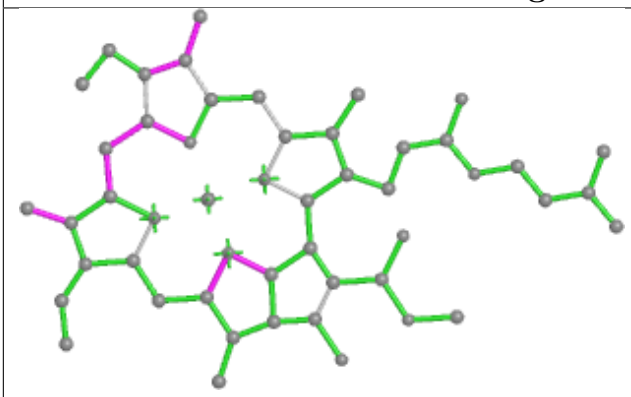


Torsions

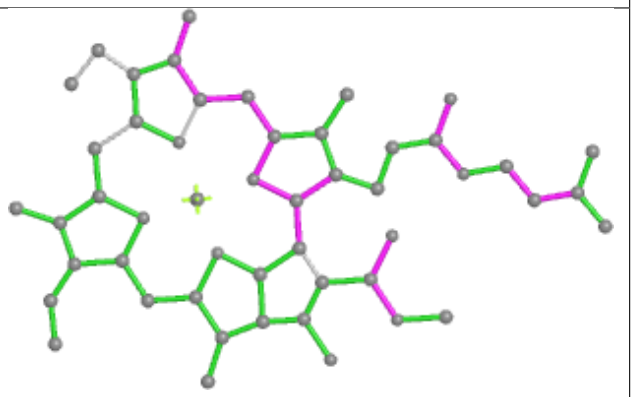


Rings

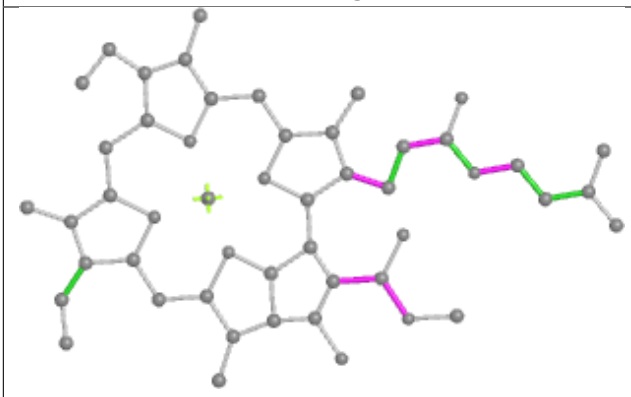
Ligand CLA 5 617



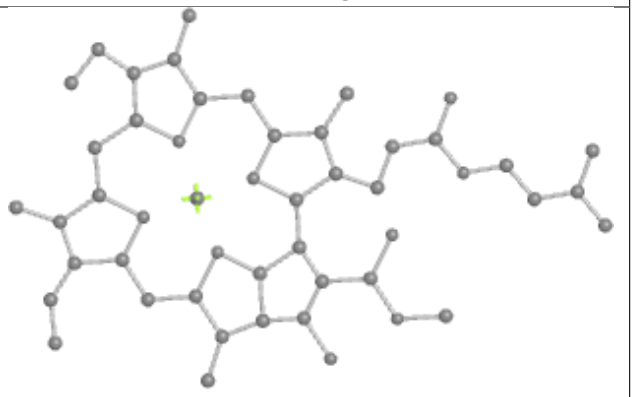
Bond lengths



Bond angles

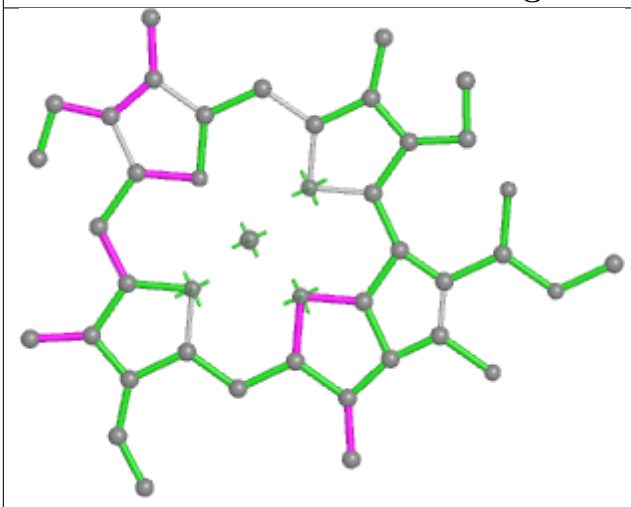


Torsions

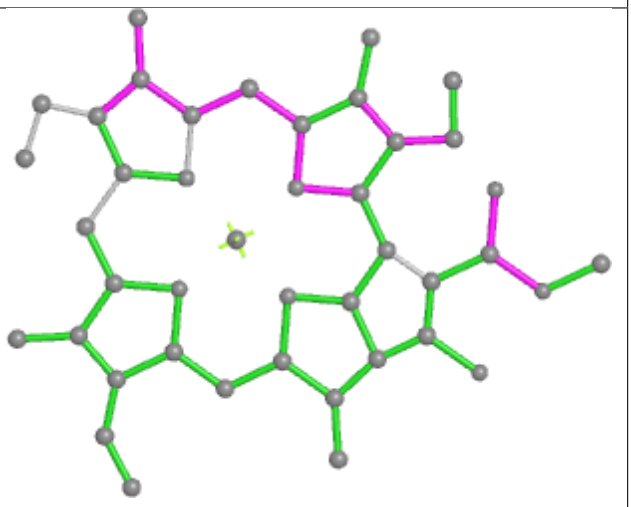


Rings

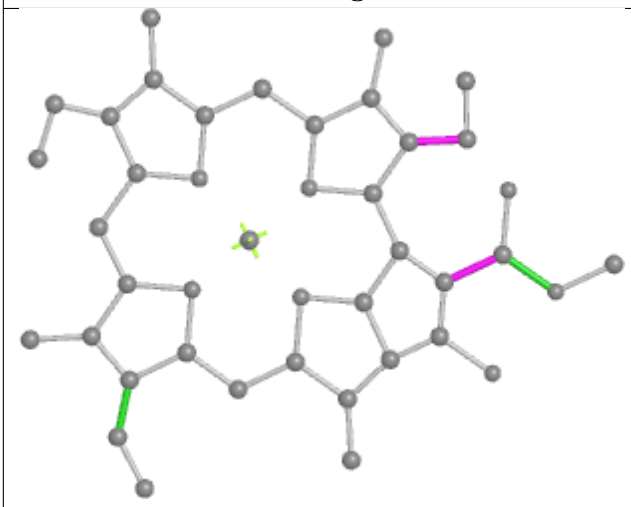
Ligand CLA A 823



Bond lengths



Bond angles



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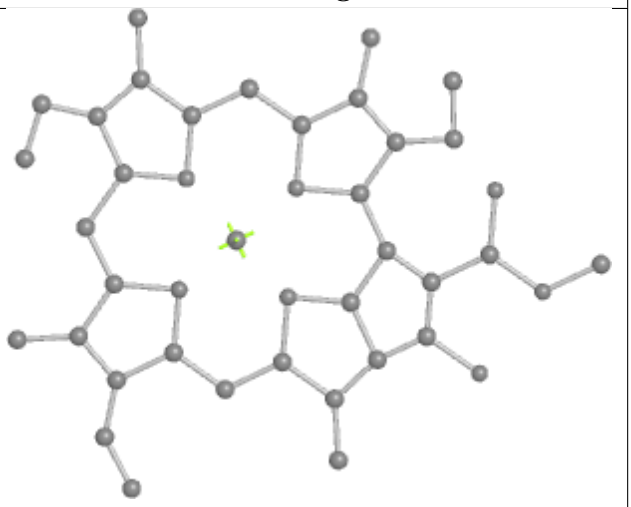
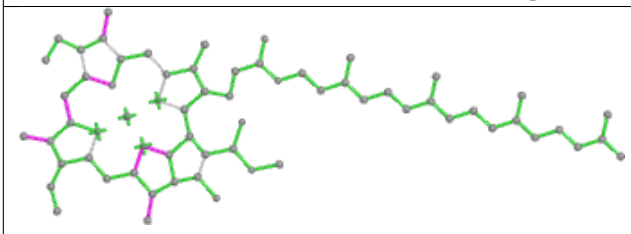
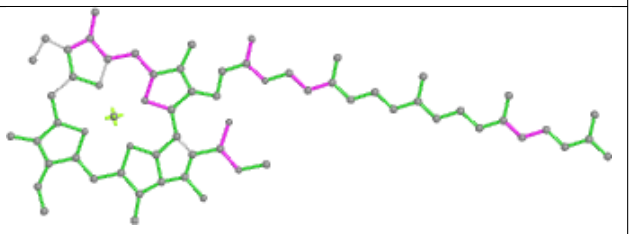


Rings

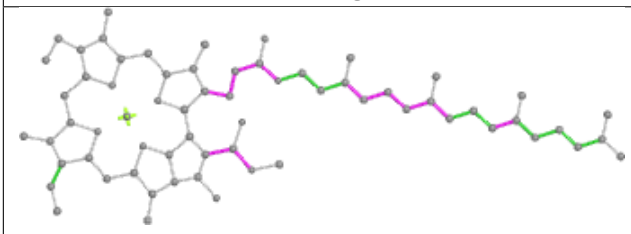
Ligand CLA B 813



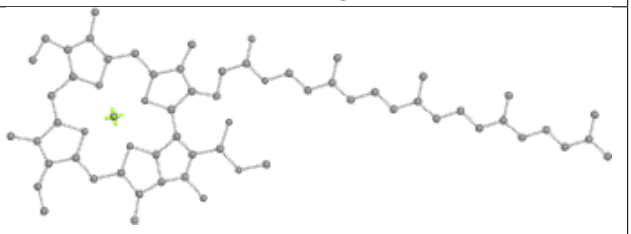
Bond lengths



Bond angles

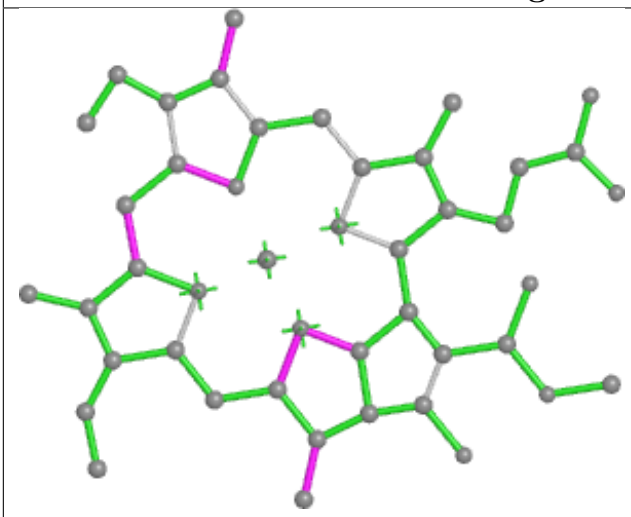


Torsions

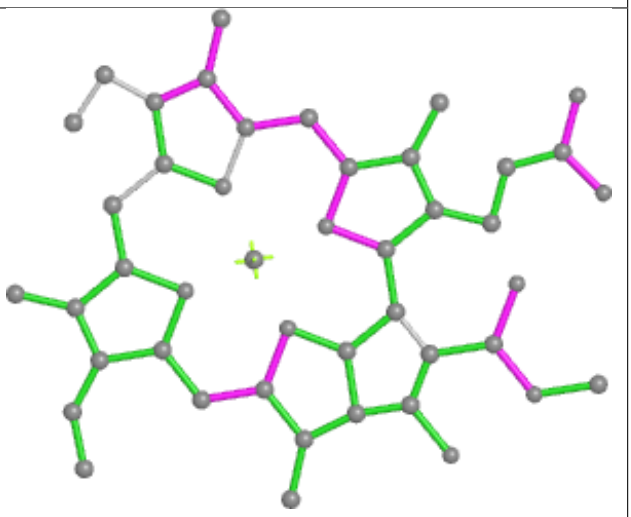


Rings

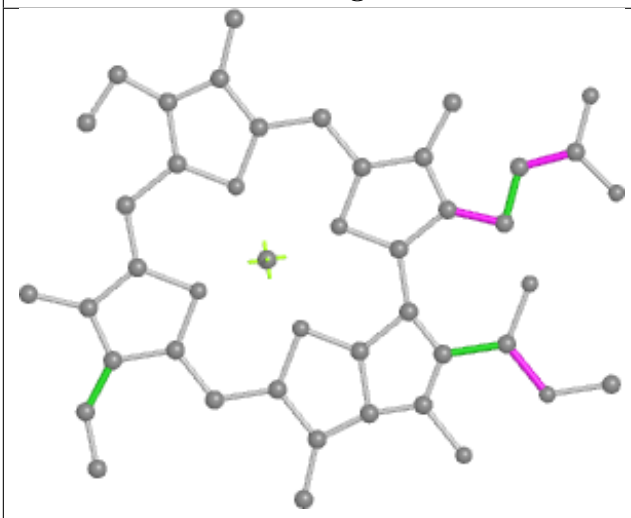
Ligand CLA a 607



Bond lengths



Bond angles



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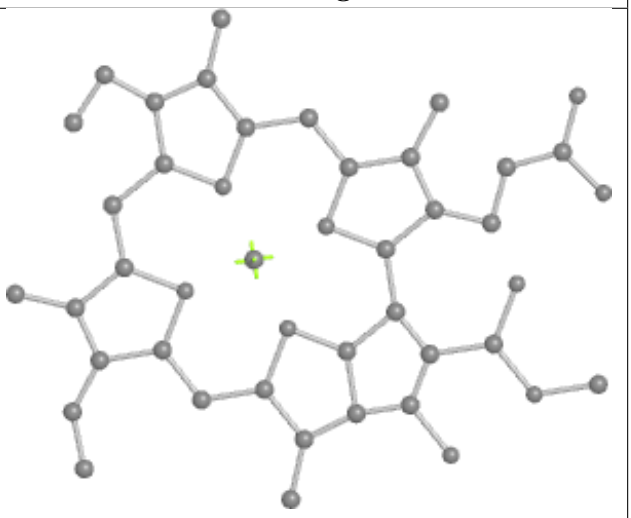
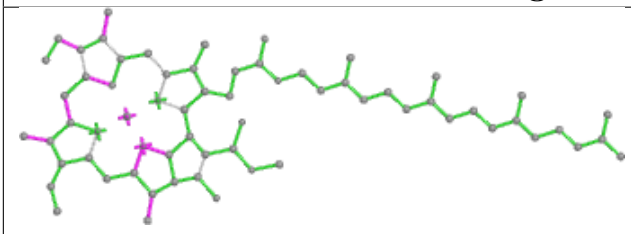
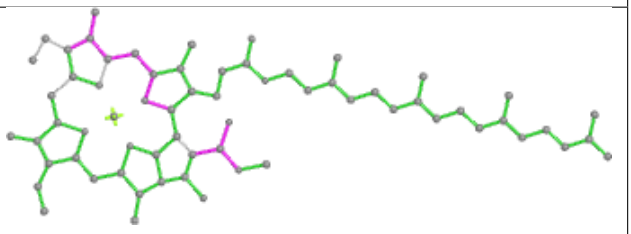


Rings

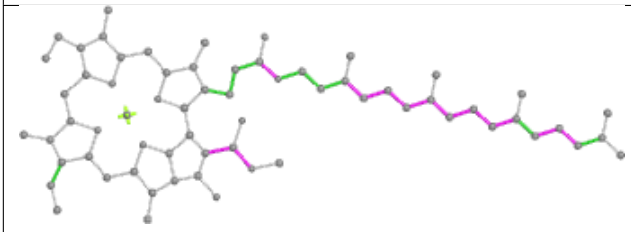
Ligand CLA 6 604



Bond lengths



Bond angles



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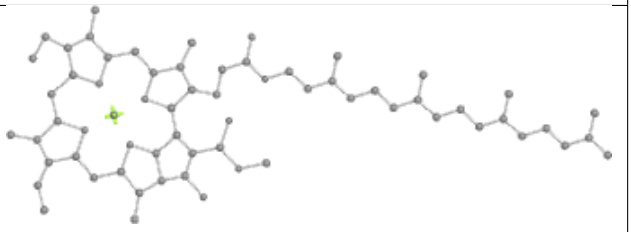
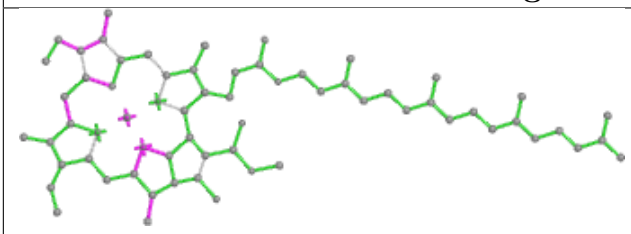


Rings

Ligand CLA A 836



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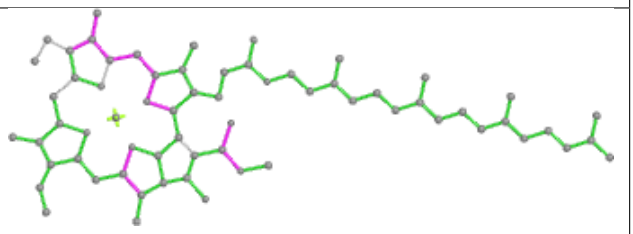
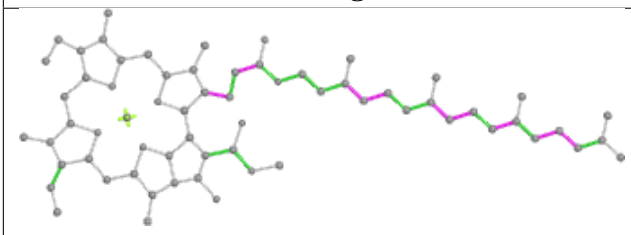


Bond angles



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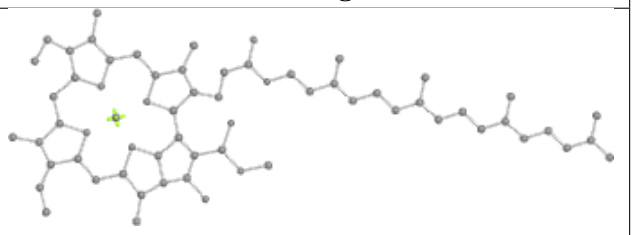
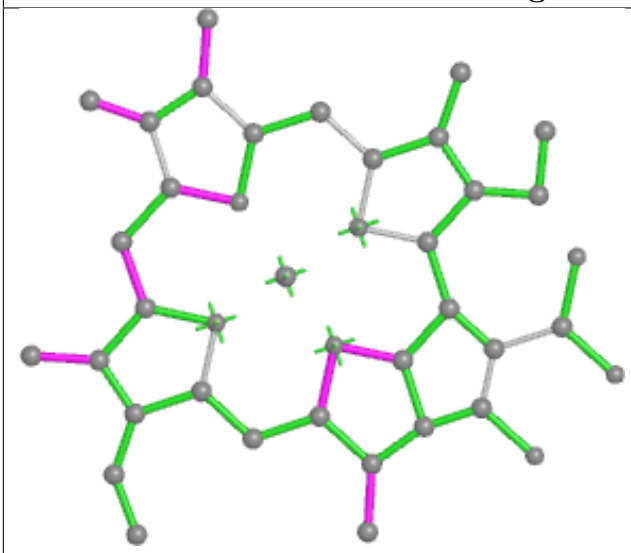


Rings

Ligand CLA 4 618



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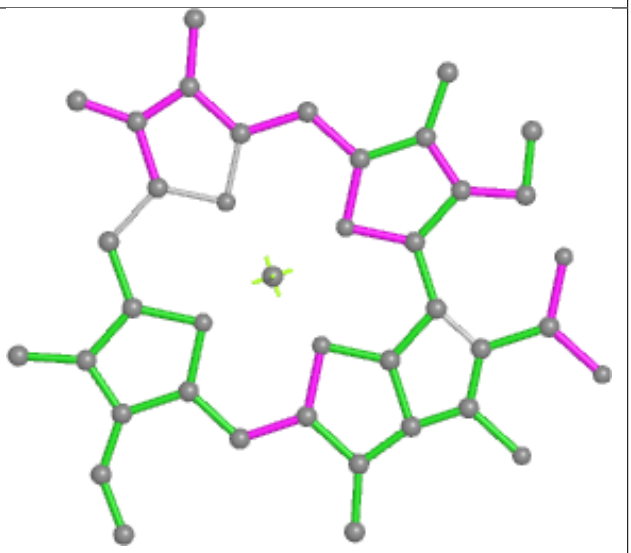
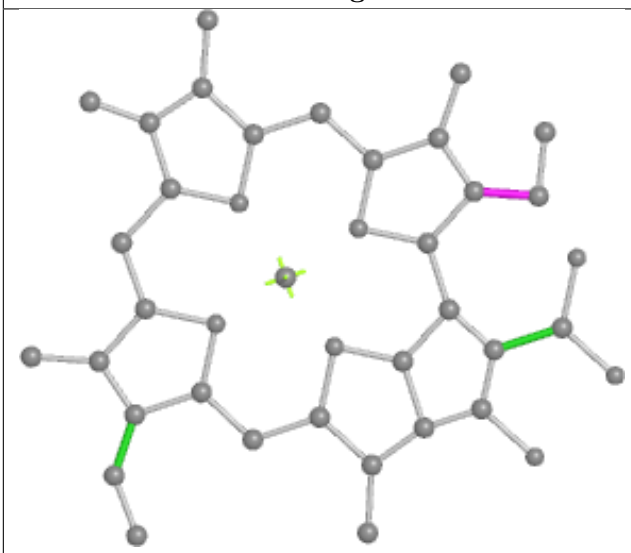


Bond angles



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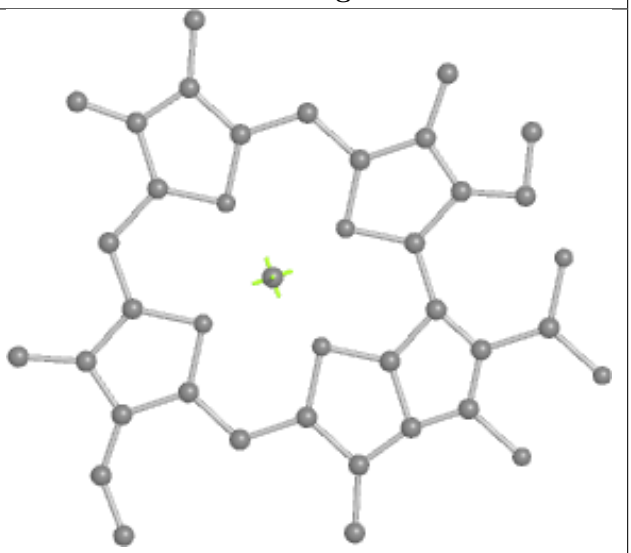
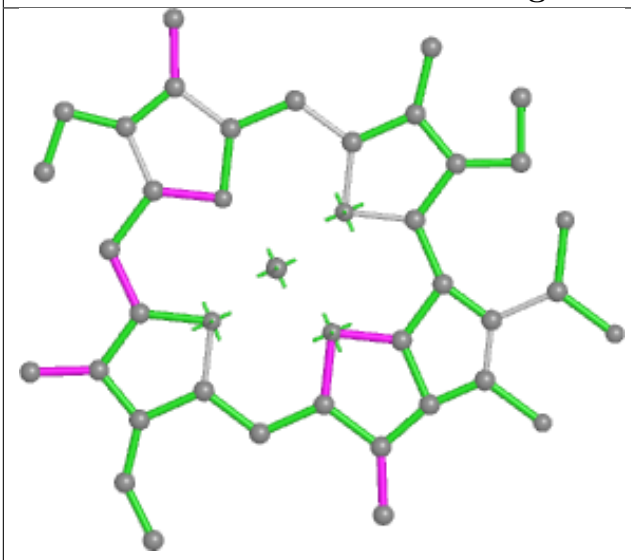
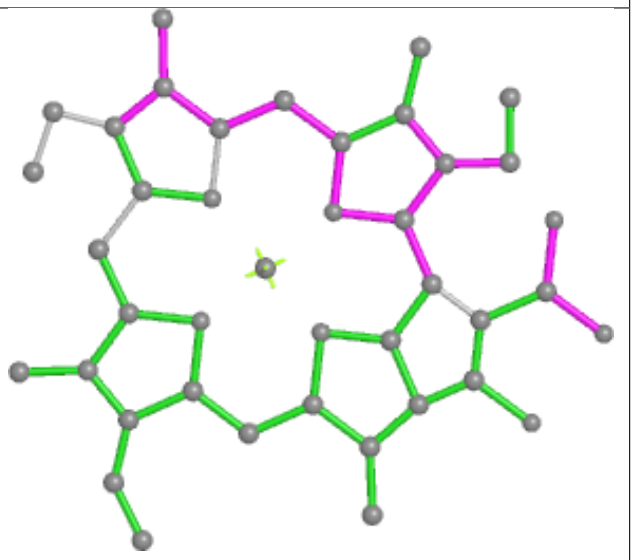


Rings

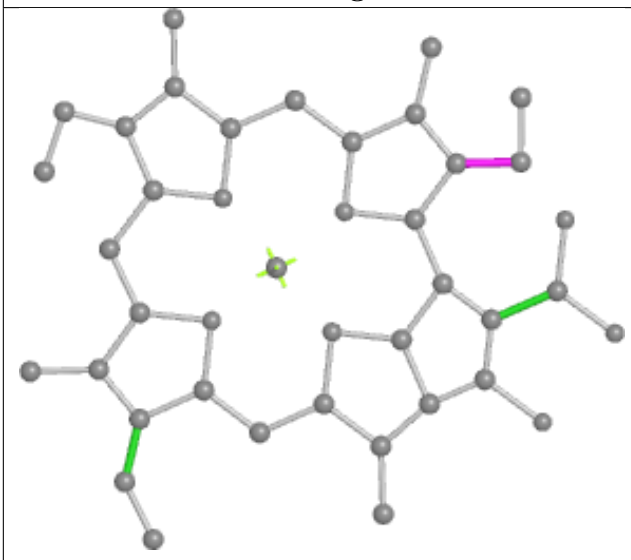
Ligand CLA 4 612



Bond lengths



Bond angles



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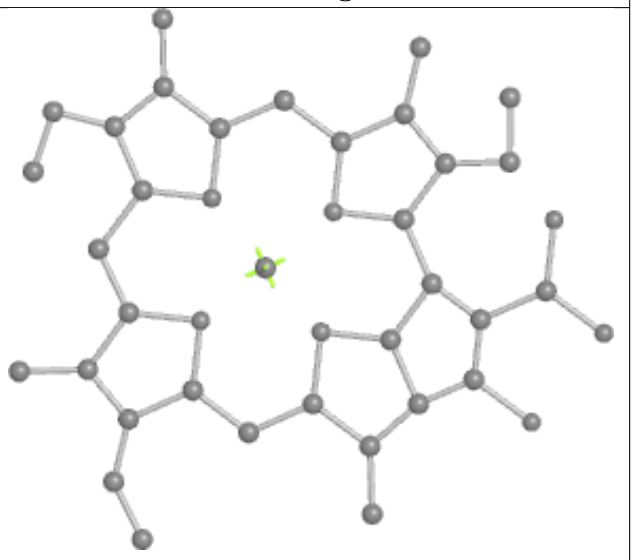
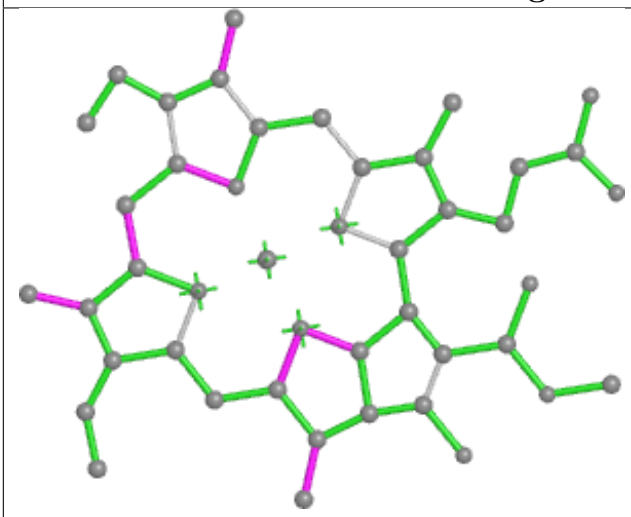


Rings

Ligand CLA a 612



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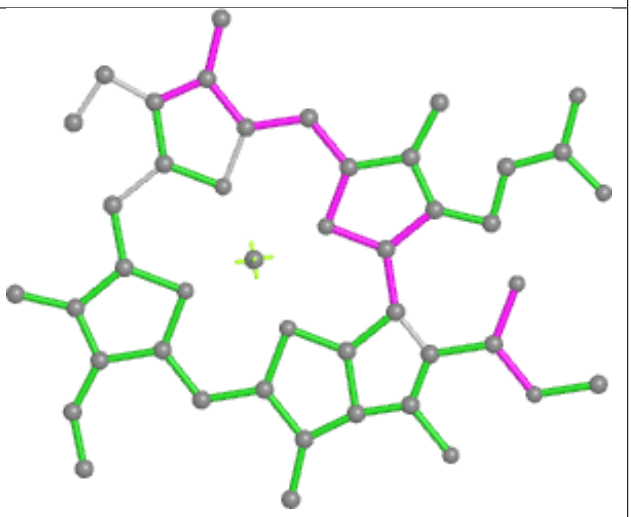
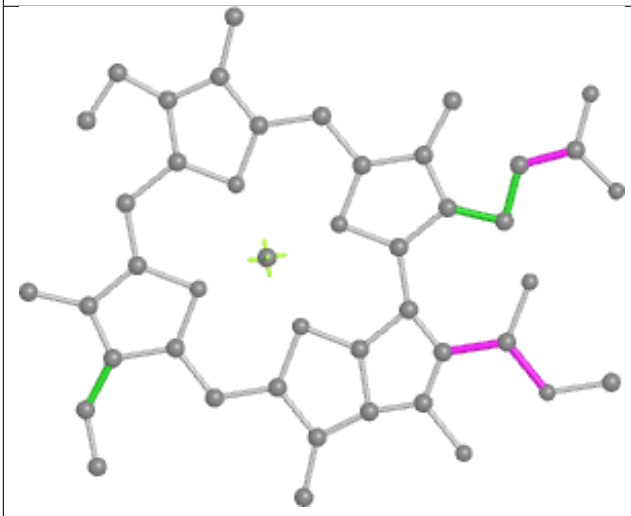
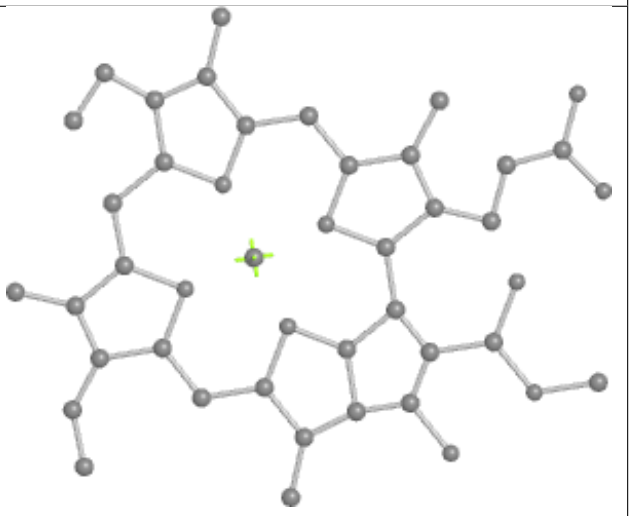


Bond angles

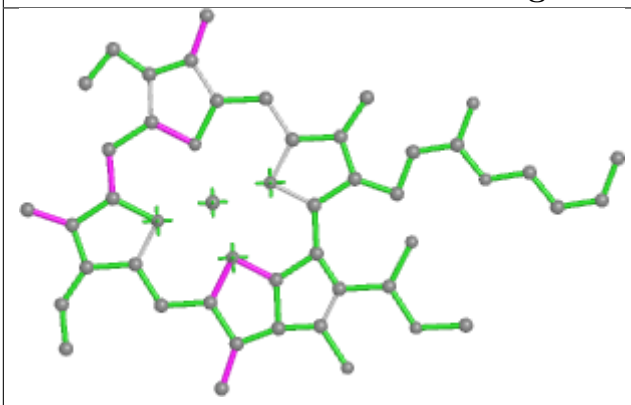


Torsions

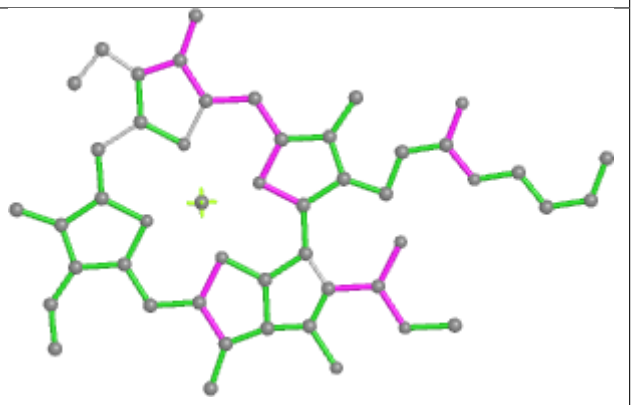


Rings

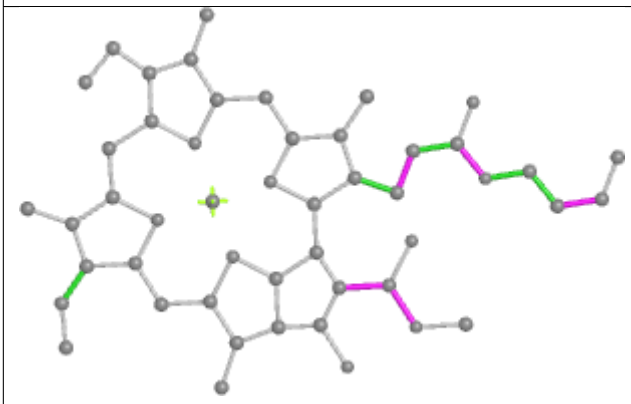
Ligand CLA a 604



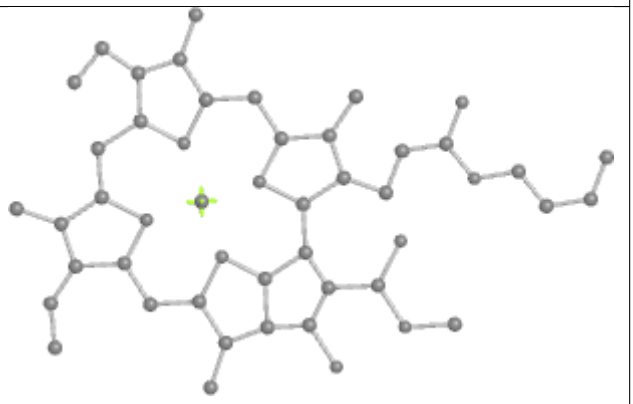
Bond lengths



Bond angles

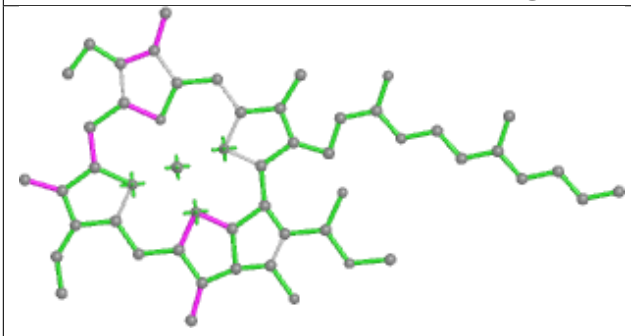


Torsions

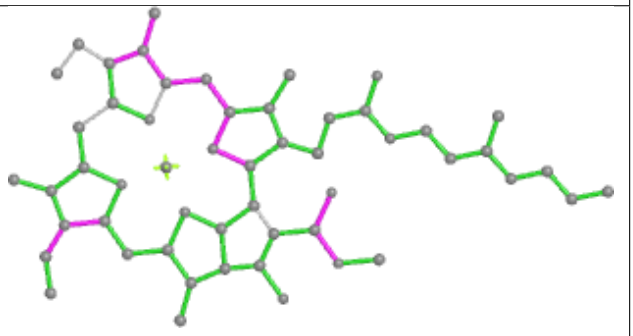


Rings

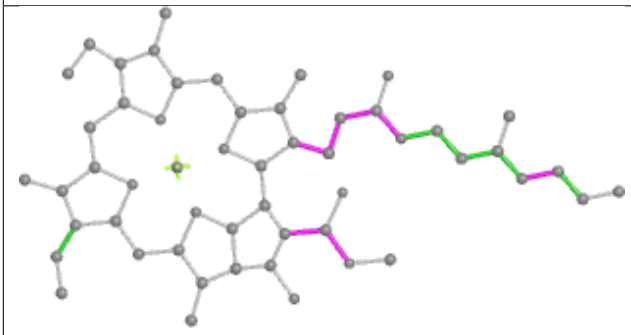
Ligand CLA A 821



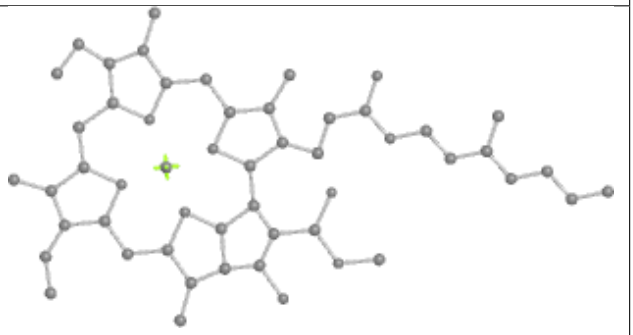
Bond lengths



Bond angles

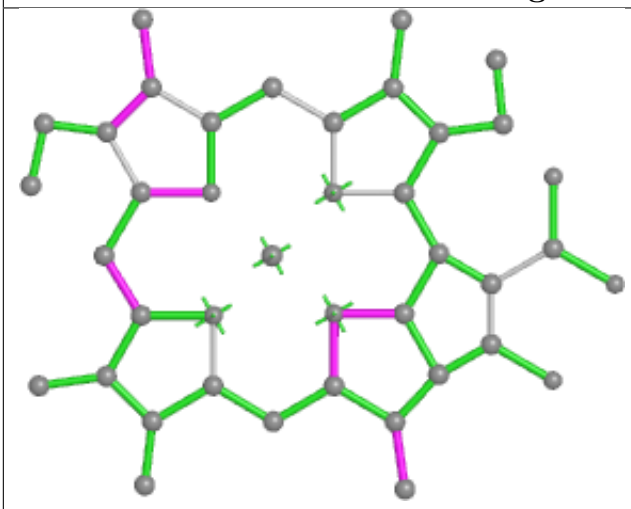


Torsions

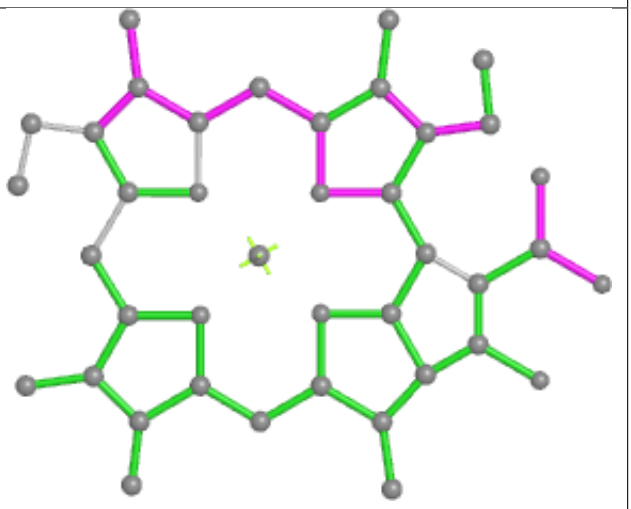


Rings

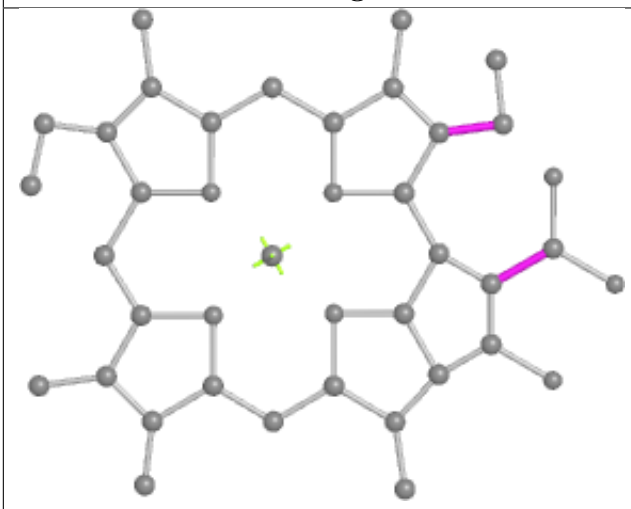
Ligand CLA 5 606



Bond lengths



Bond angles



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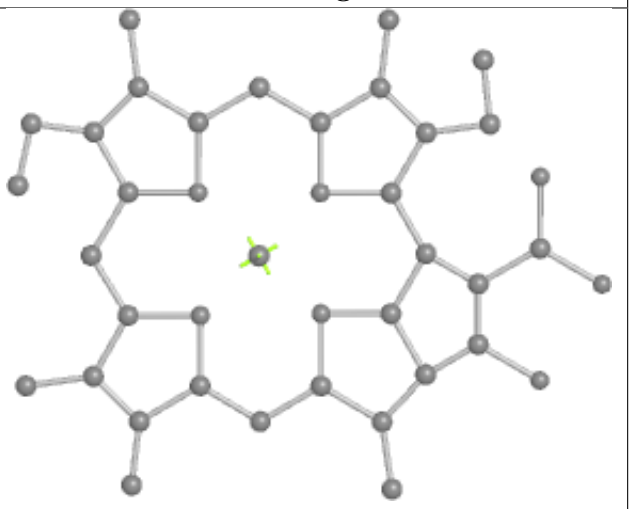
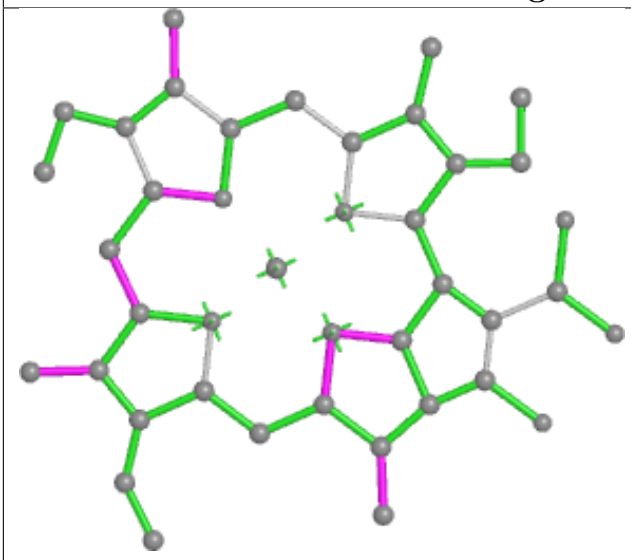
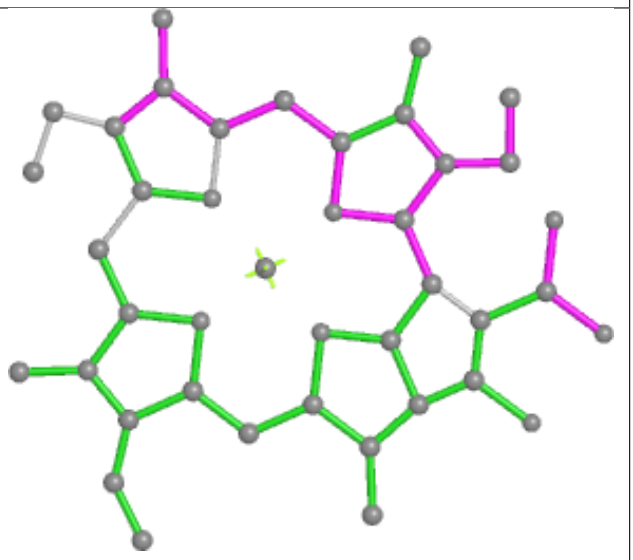


Rings

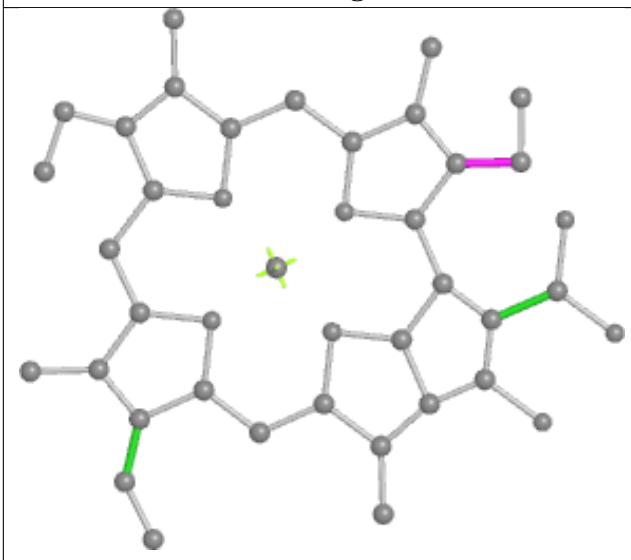
Ligand CLA 8 612



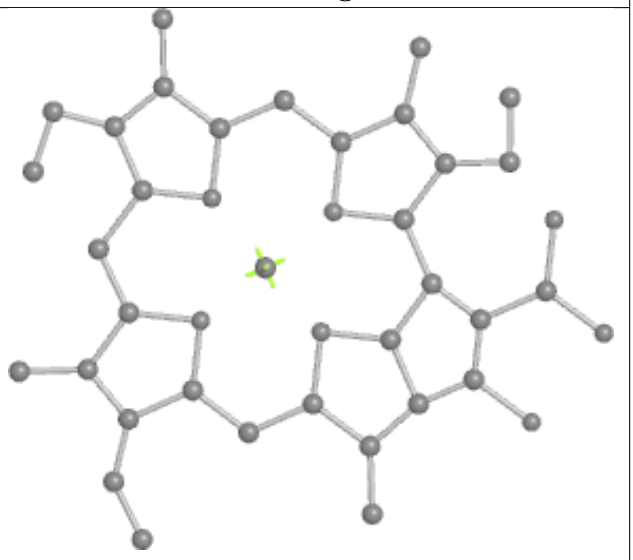
Bond lengths



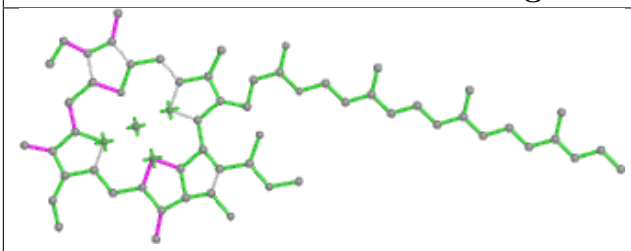
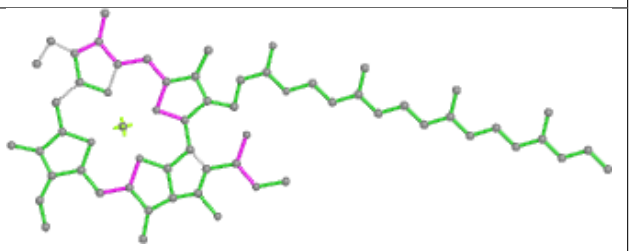
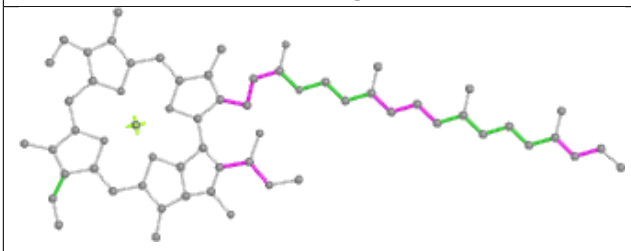
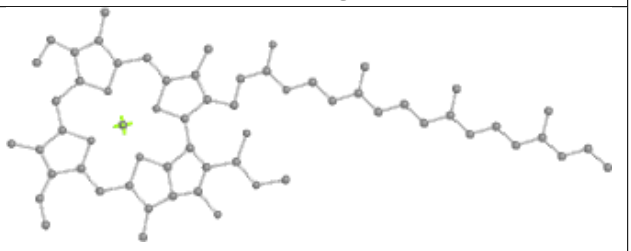
Bond angles

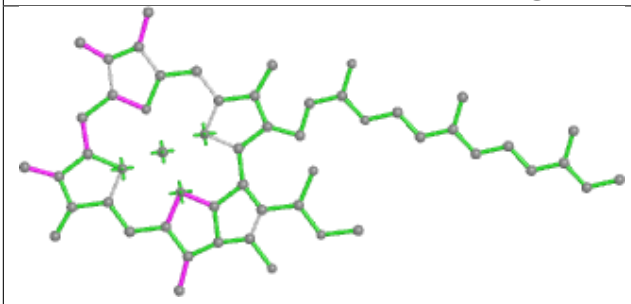
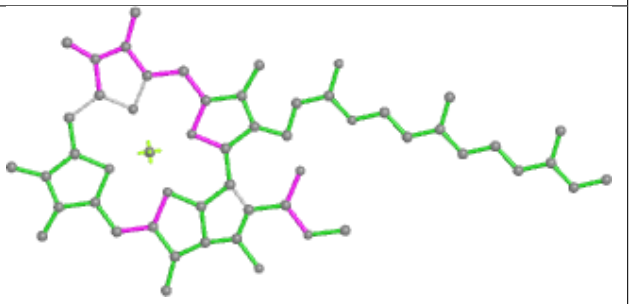
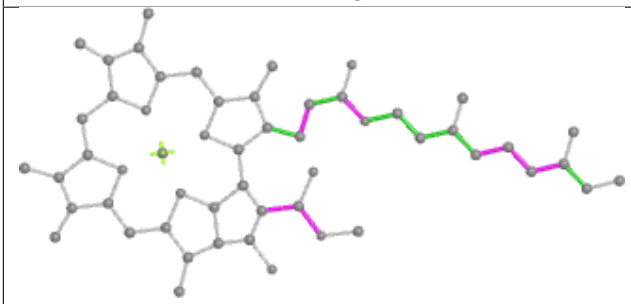
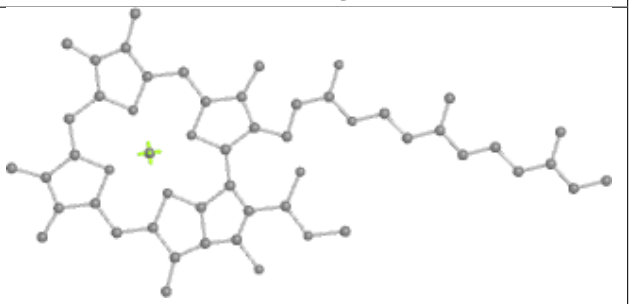


Torsions

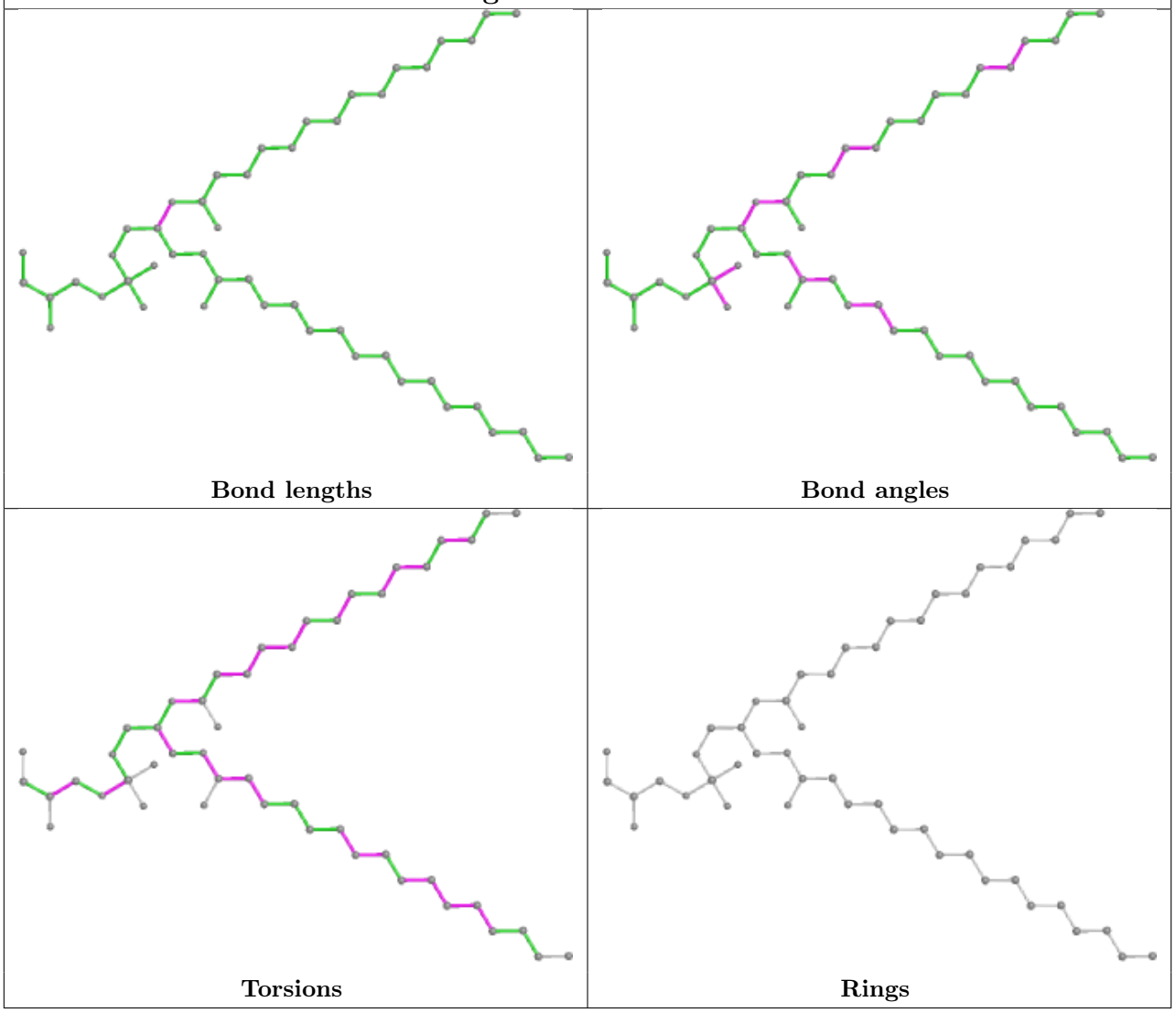


Rings

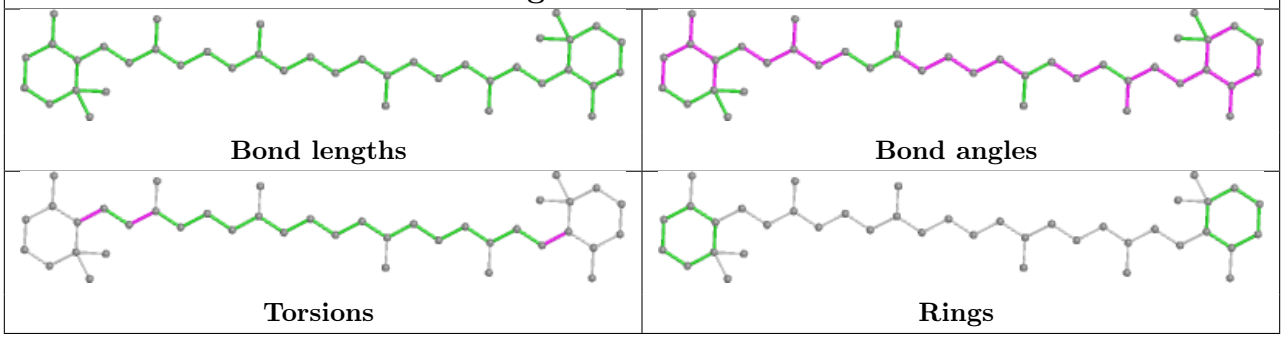
Ligand CLA B 827	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA 4 604	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand LHG 6 623



Ligand BCR 8 621



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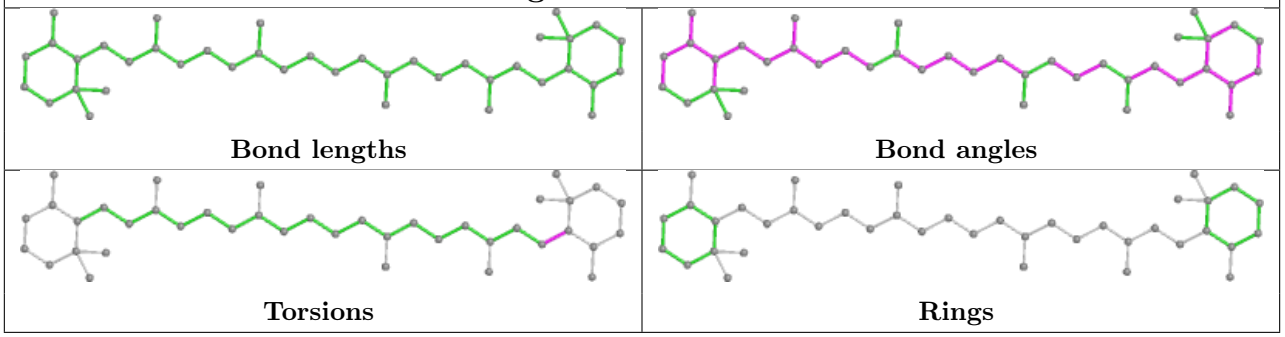
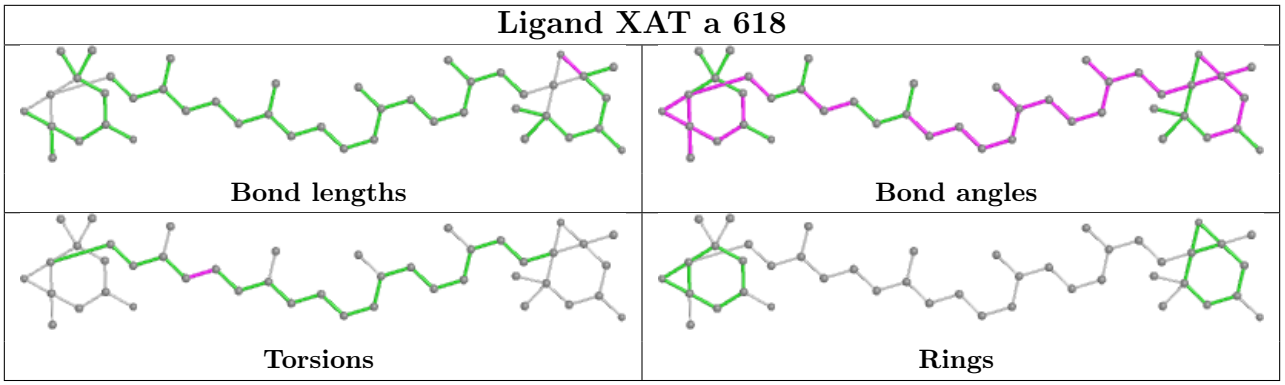


Ligand XAT a 618



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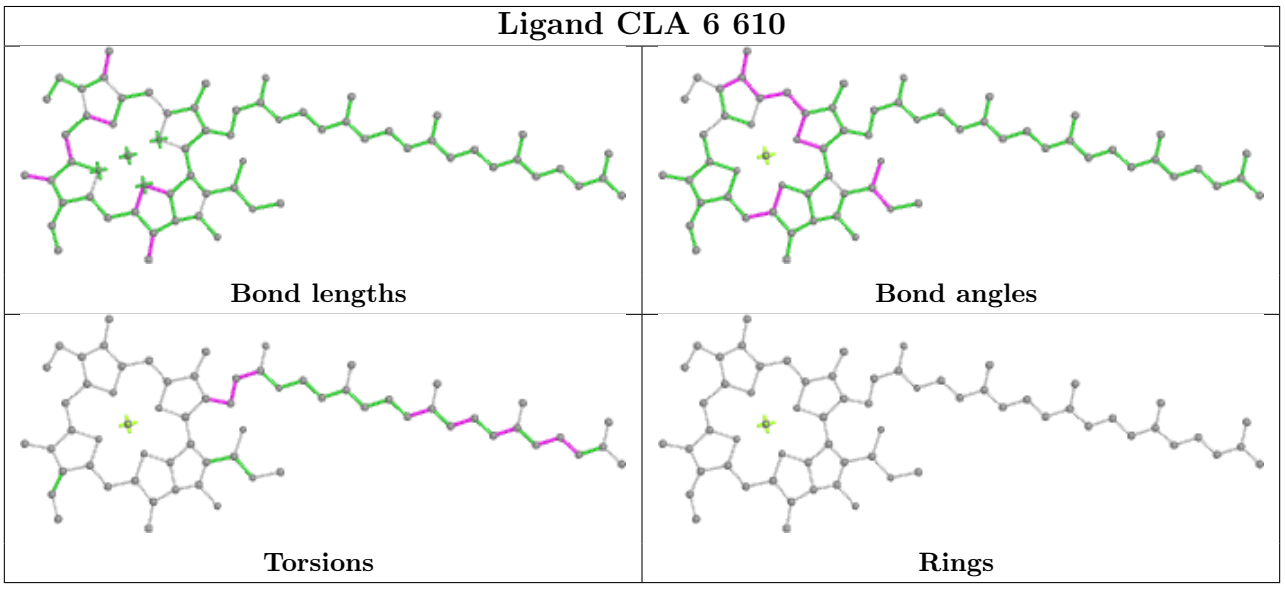
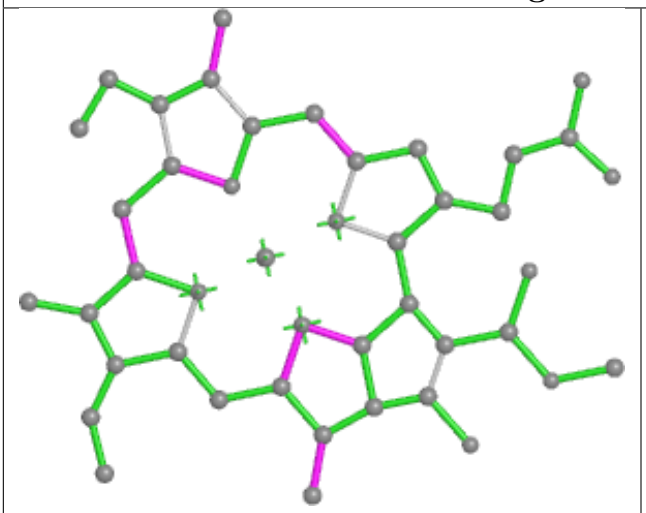
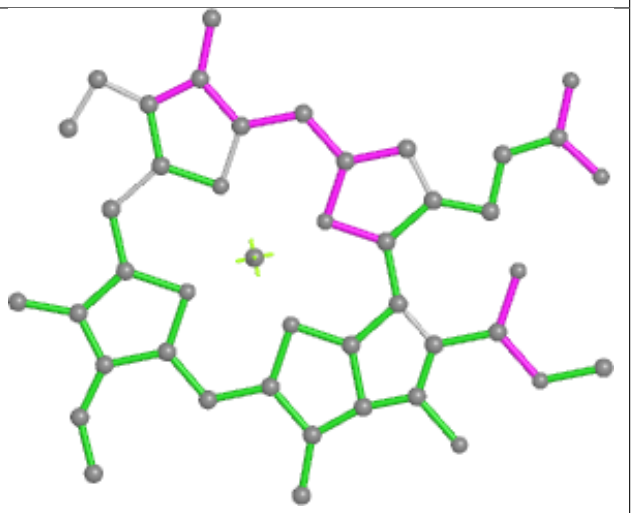


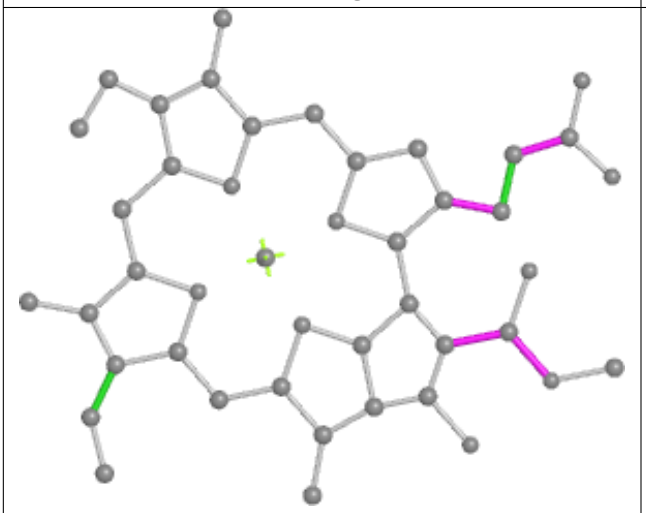
Ligand CLA 5 614



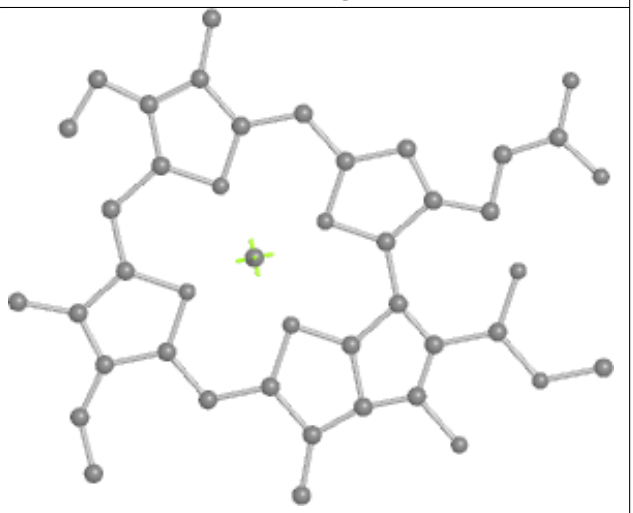
Bond lengths



Bond angles

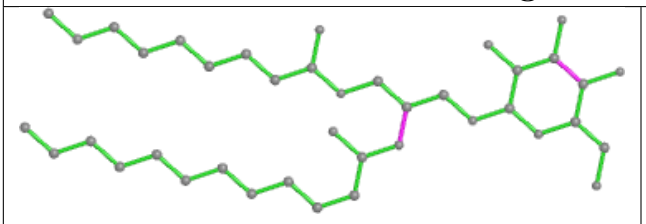


Torsions

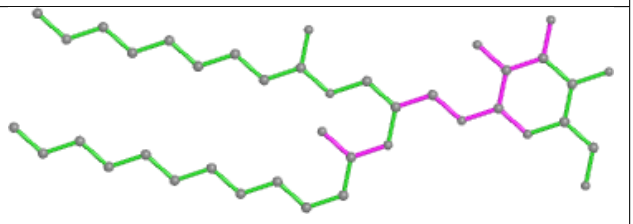


Rings

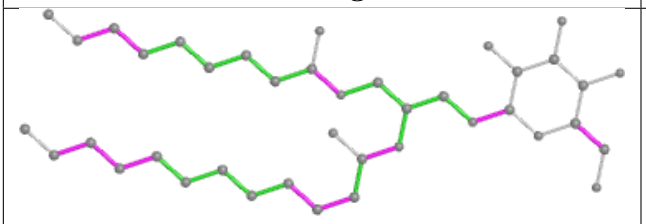
Ligand LMG A 860



Bond lengths



Bond angles



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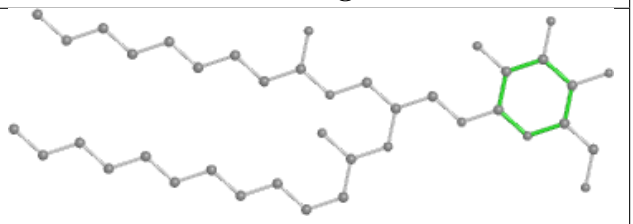
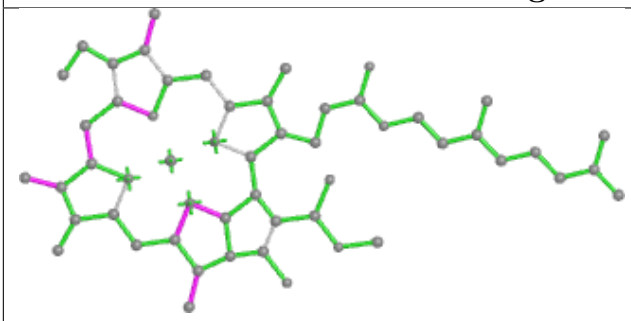


Rings

Ligand CLA 7 604



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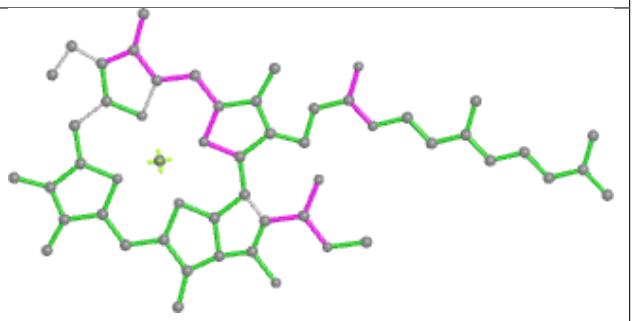
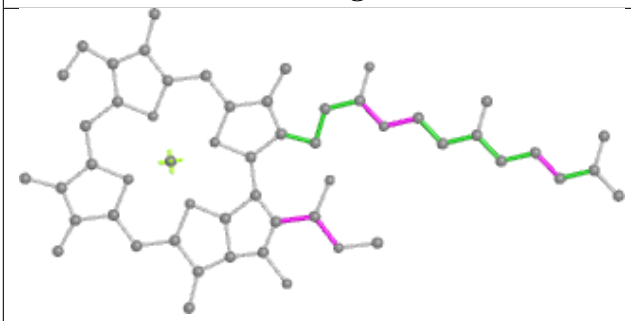


Bond angles



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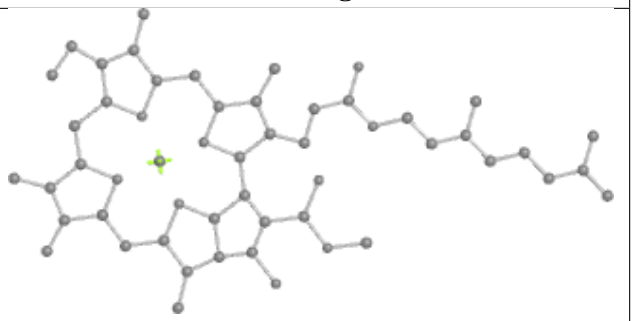
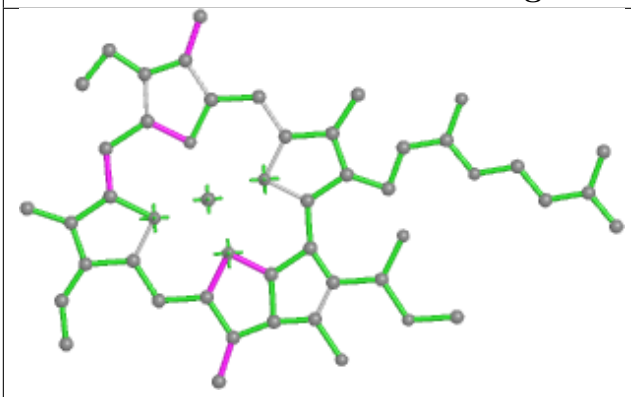
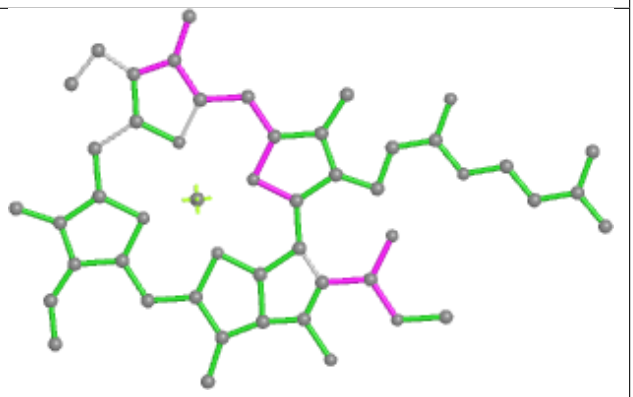


Rings

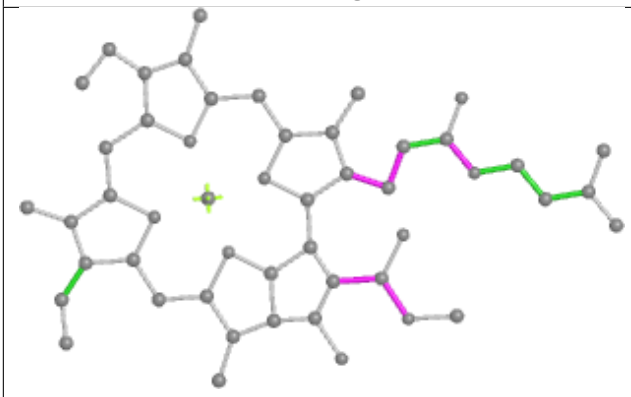
Ligand CLA B 820



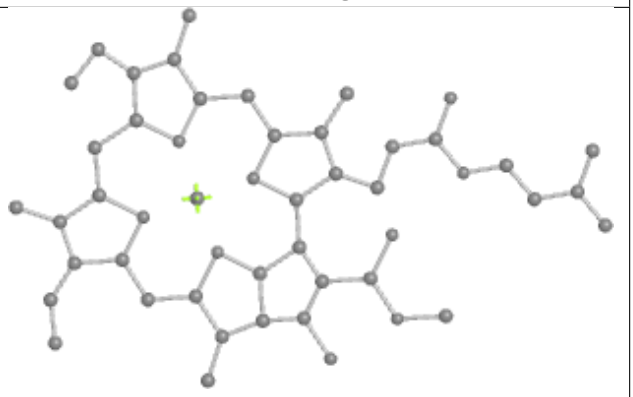
Bond lengths



Bond angles

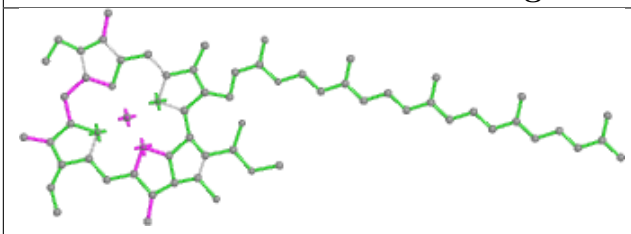


Torsions



Rings

Ligand CLA B 828



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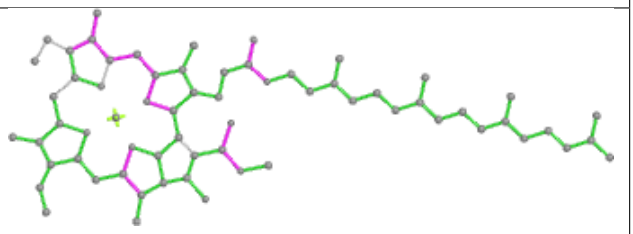
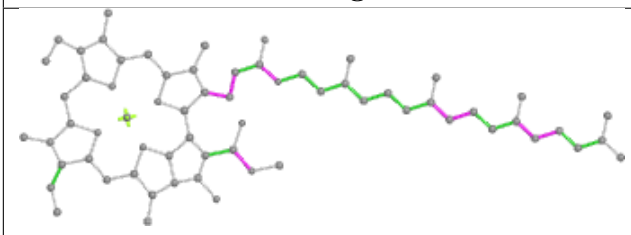
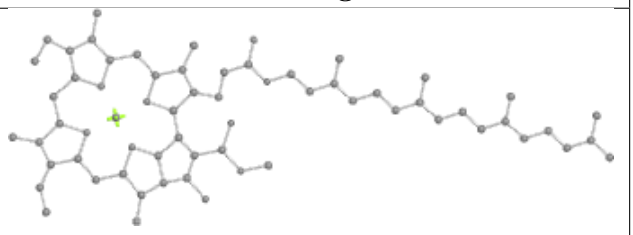


Bond angles

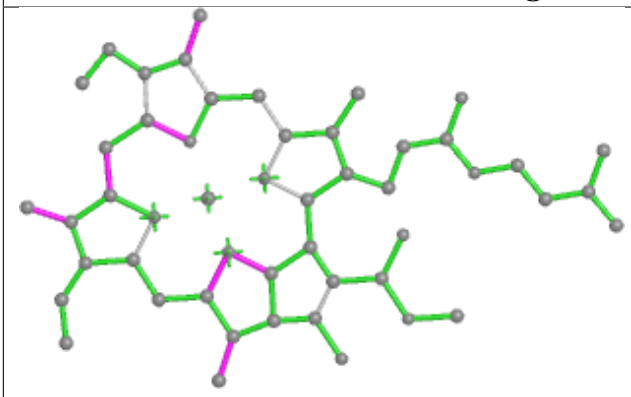


Torsions

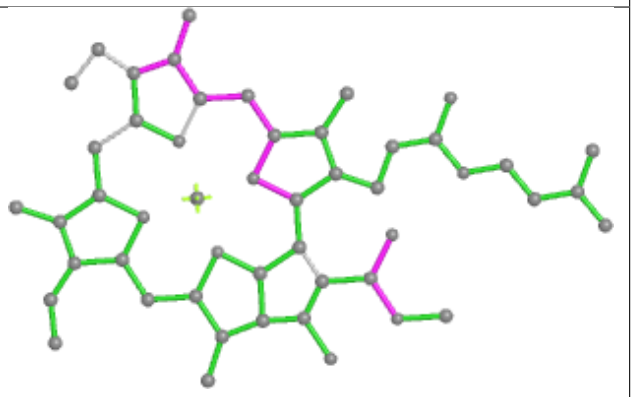


Rings

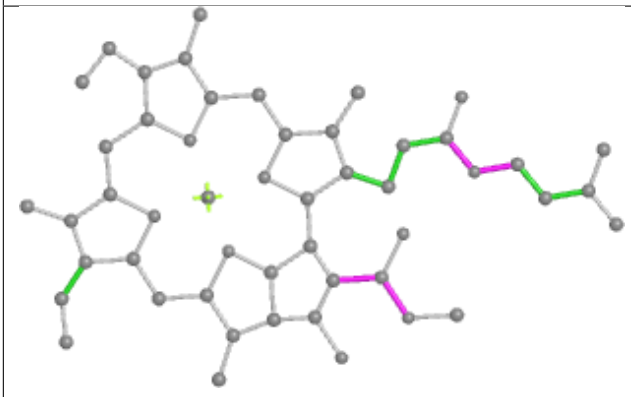
Ligand CLA B 836



Bond lengths



Bond angles



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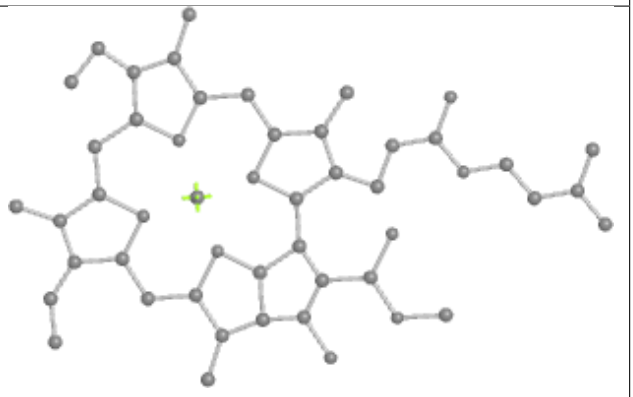
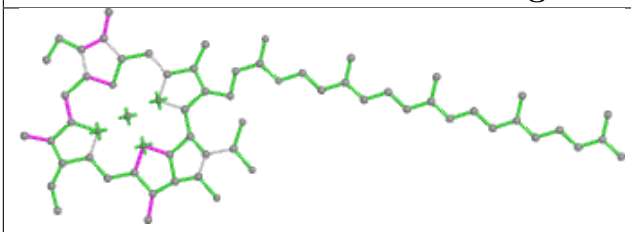
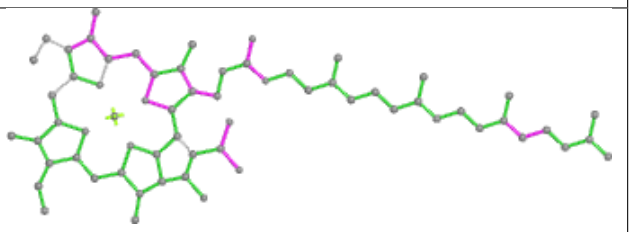


Rings

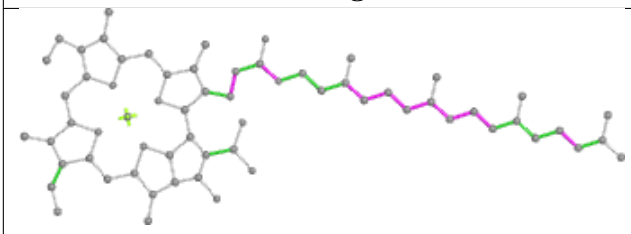
Ligand CLA 6 613



Bond lengths



Bond angles



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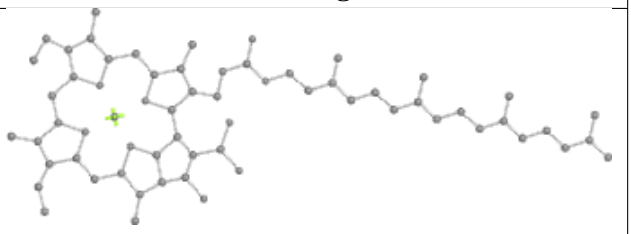
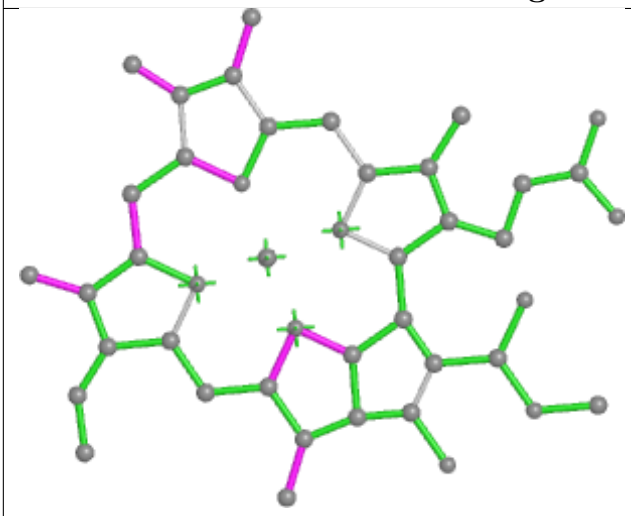
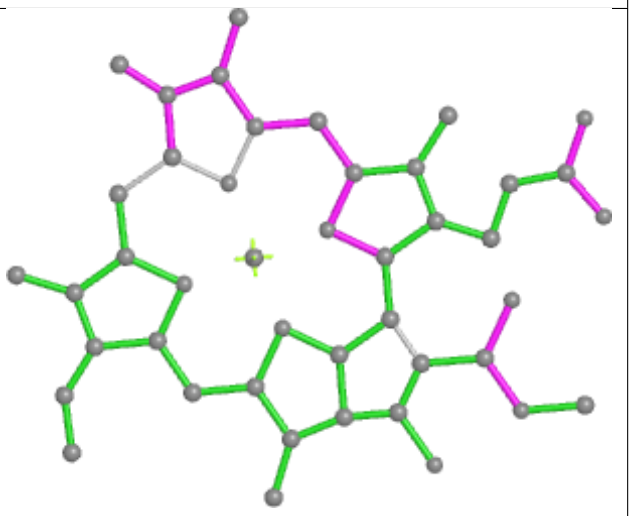


Rings

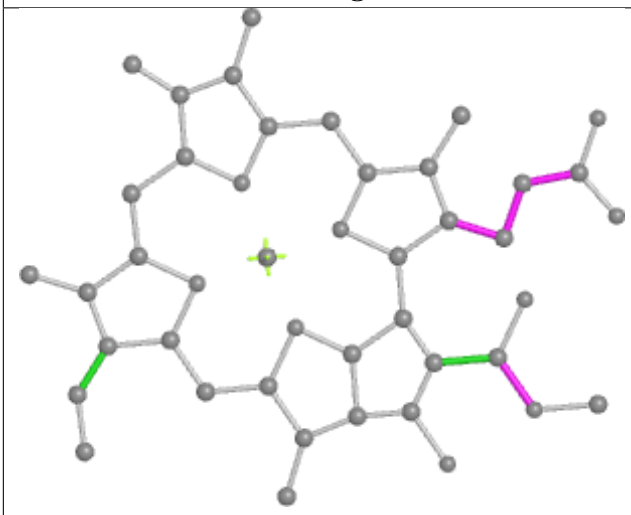
Ligand CLA 8 603



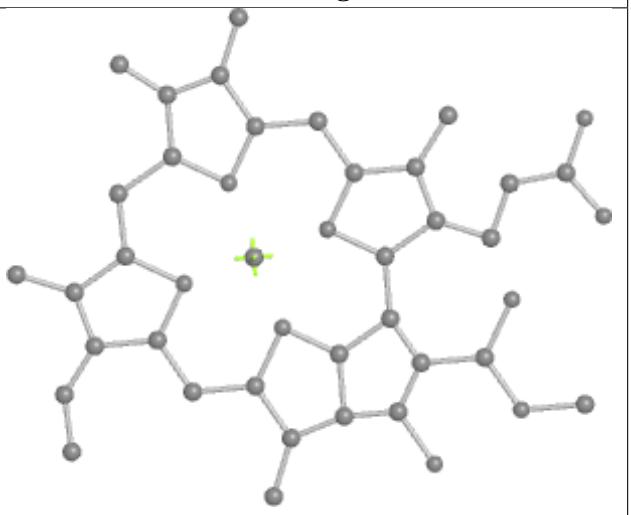
Bond lengths



Bond angles

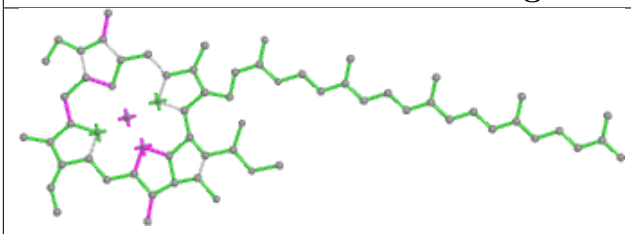


Torsions

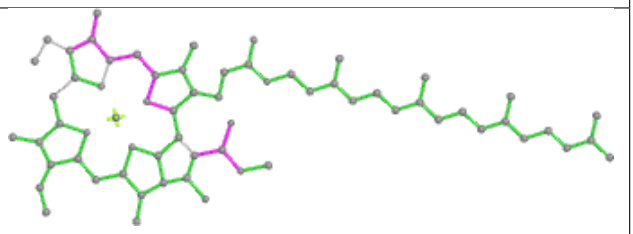


Rings

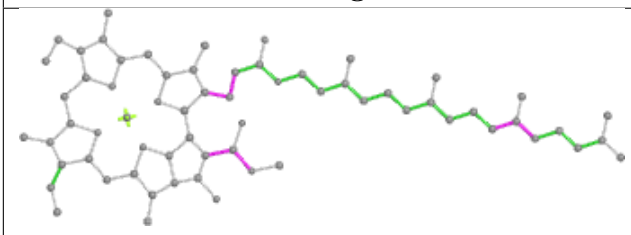
Ligand CLA A 809



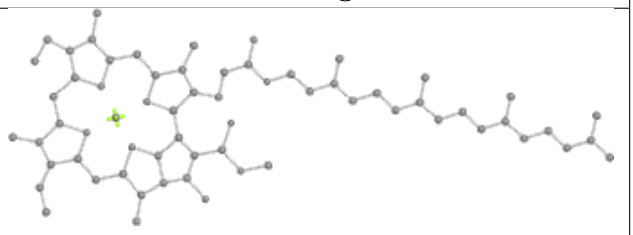
Bond lengths



Bond angles

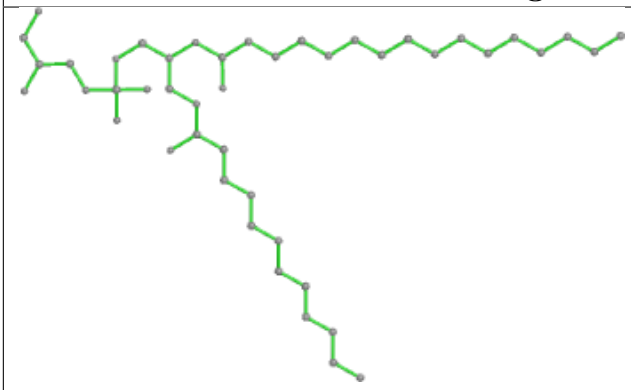


Torsions

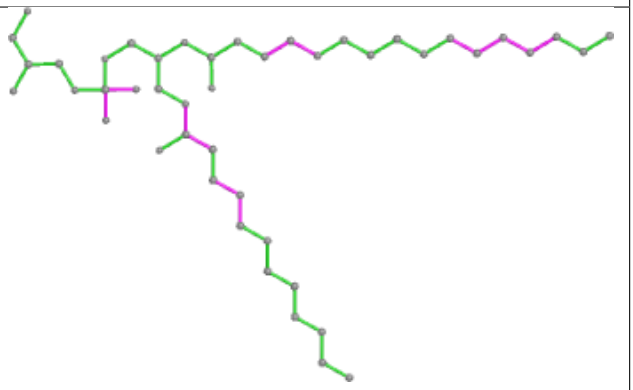


Rings

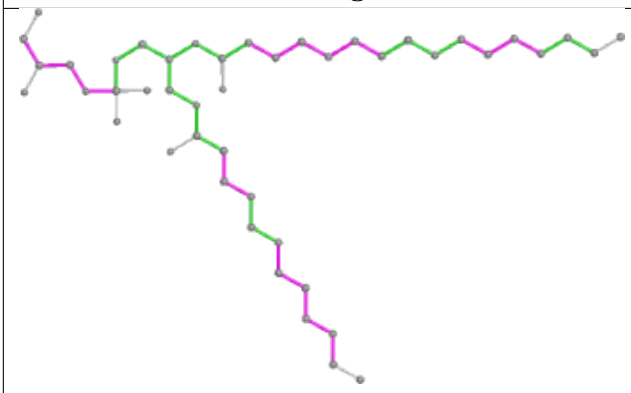
Ligand LHG 3 623



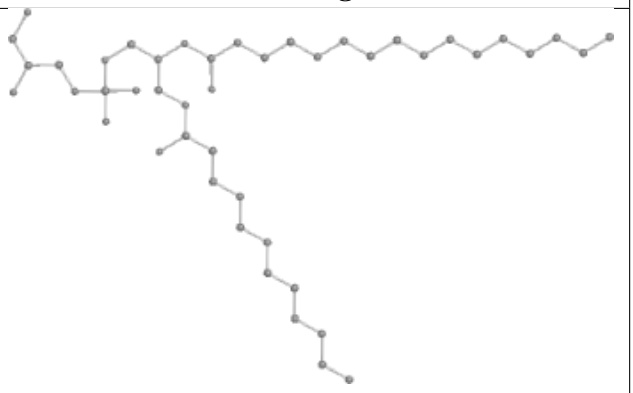
Bond lengths



Bond angles

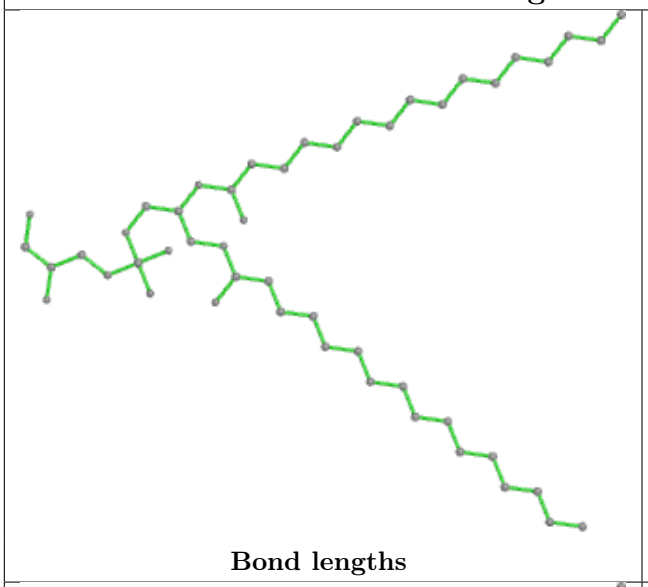


Torsions



Rings

Ligand LHG 1 620



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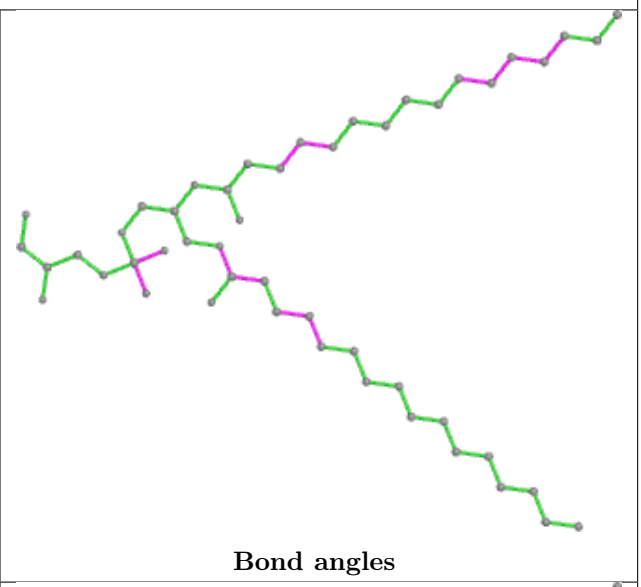
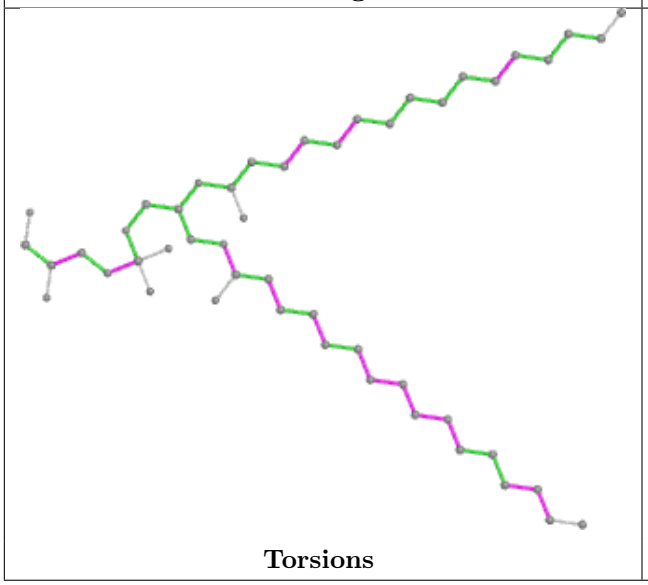


Bond angles



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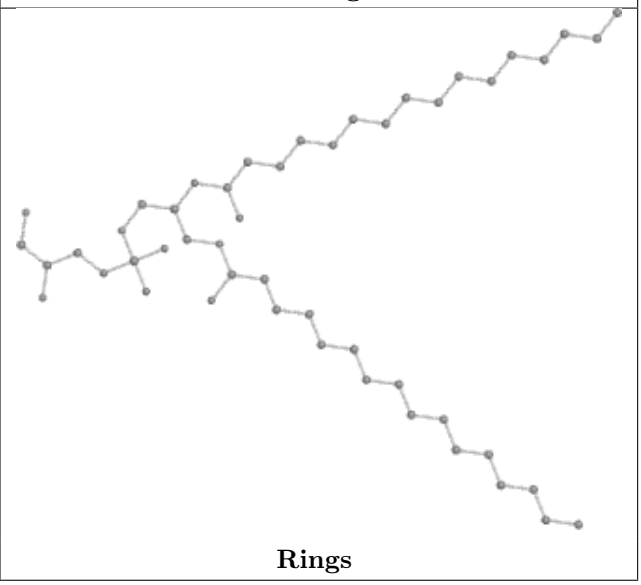
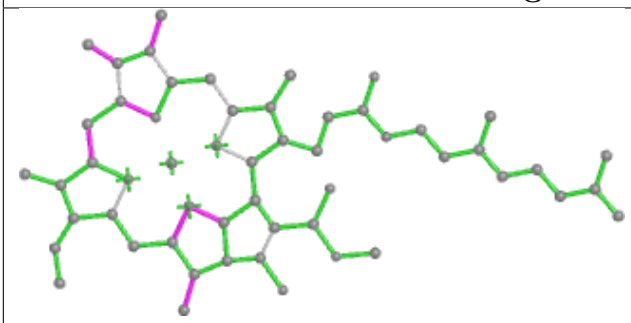
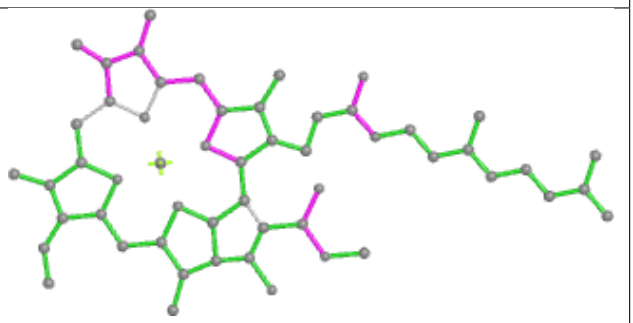


Rings

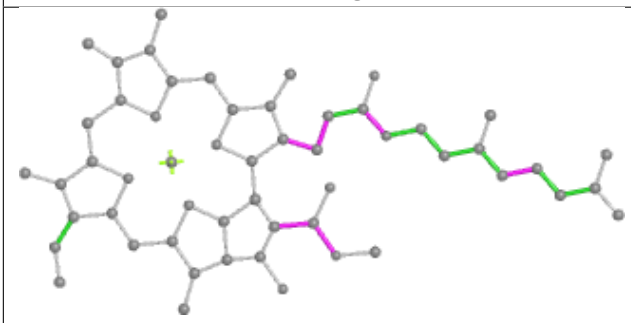
Ligand CLA B 811



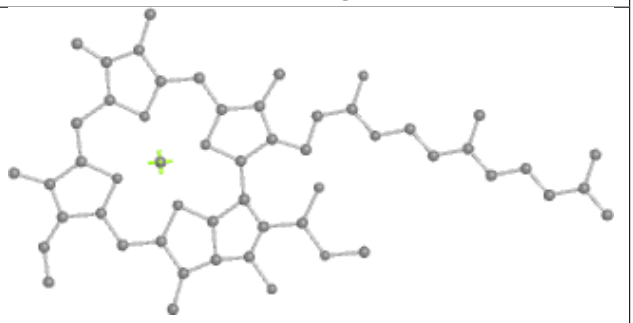
Bond lengths



Bond angles

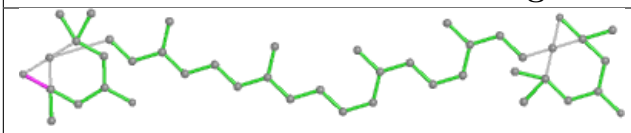


Torsions

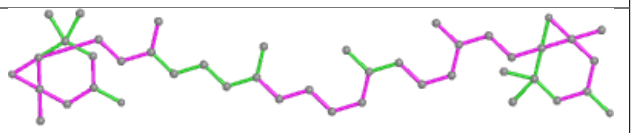


Rings

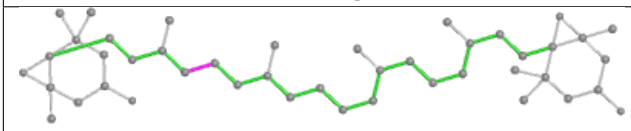
Ligand XAT 4 620



Bond lengths



Bond angles



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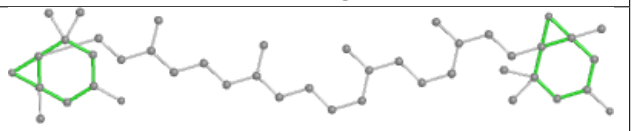
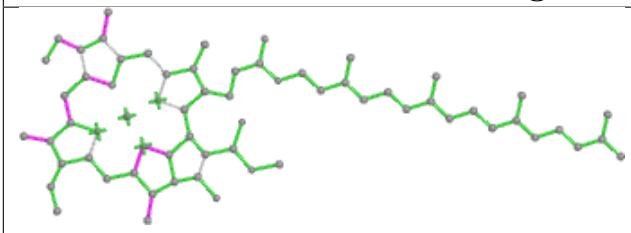
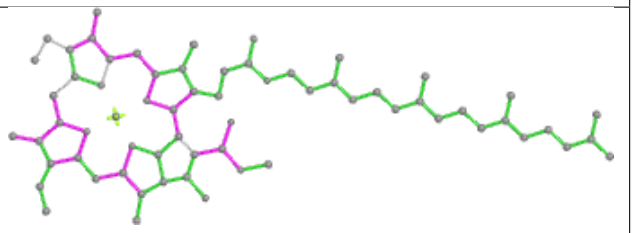


Rings

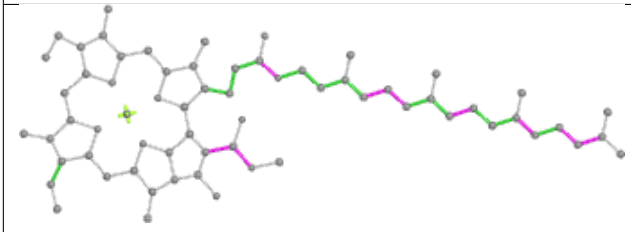
Ligand CLA 5 607



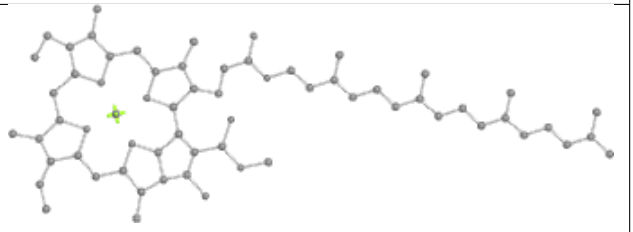
Bond lengths



Bond angles

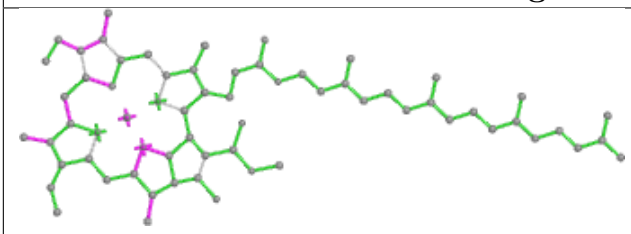


Torsions

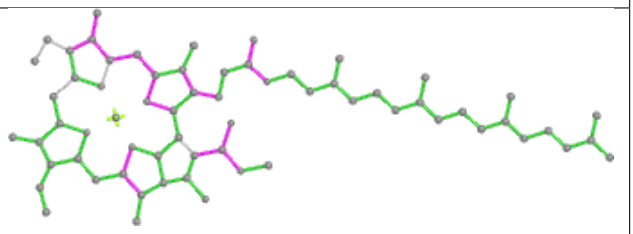


Rings

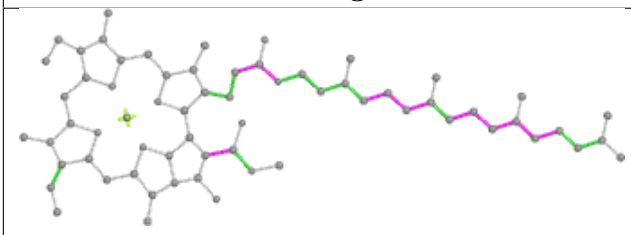
Ligand CLA 8 601



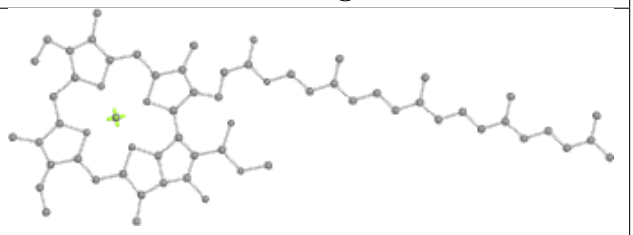
Bond lengths



Bond angles

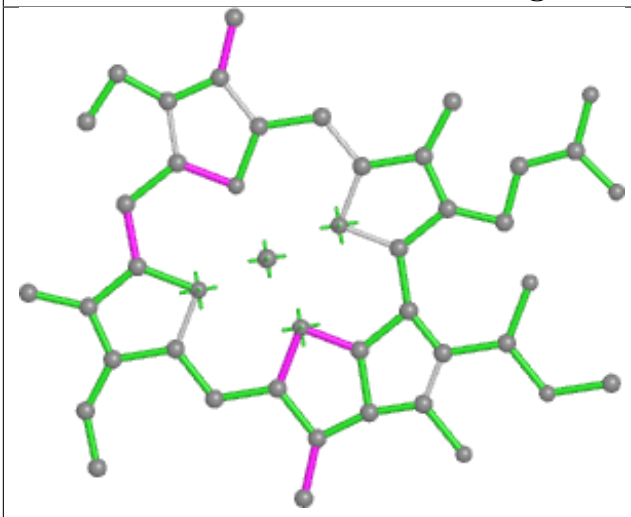


Torsions



Rings

Ligand CLA a 616



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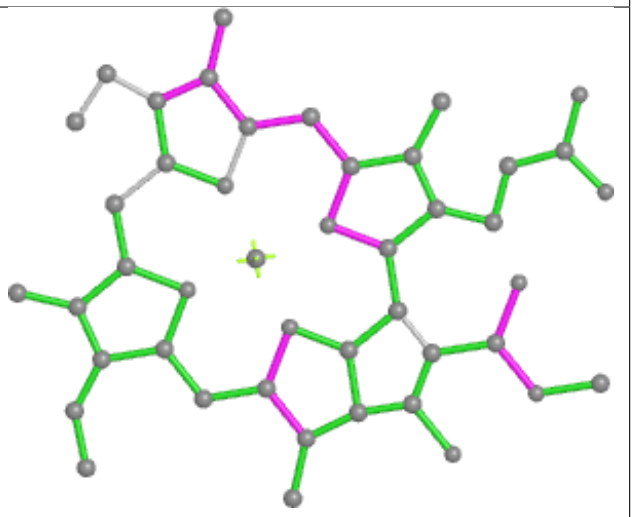
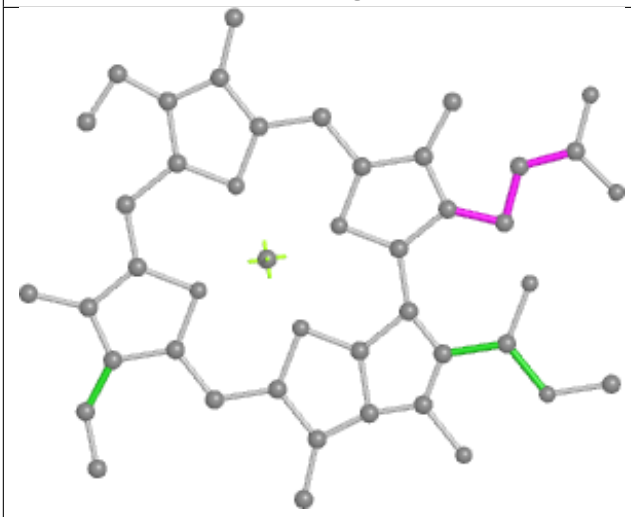
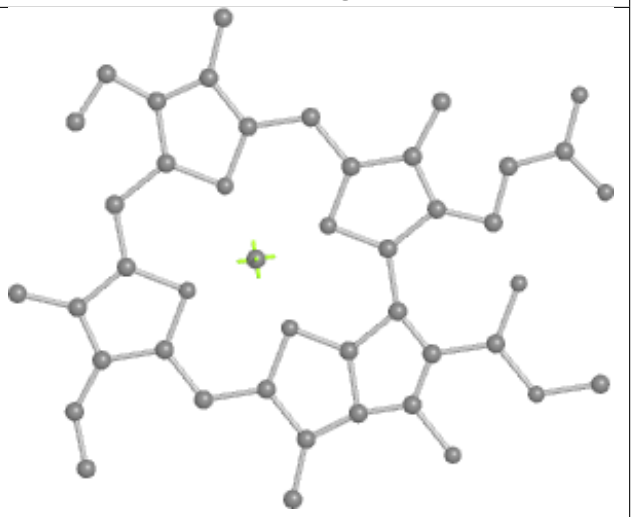


Bond angles

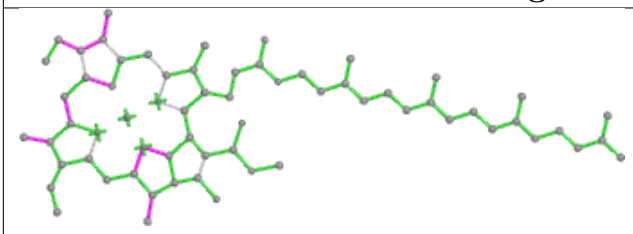


Torsions

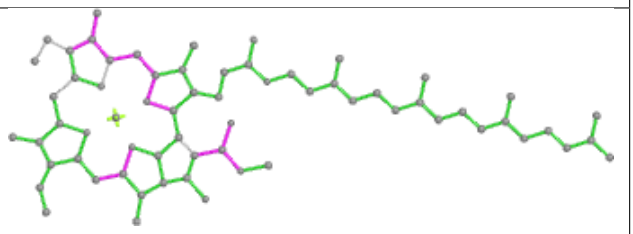


Rings

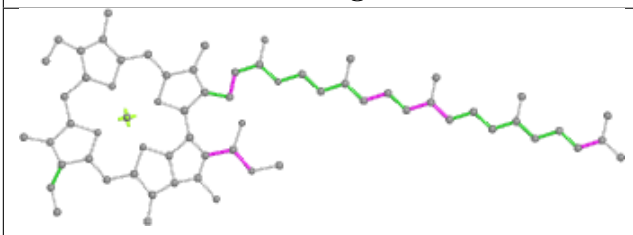
Ligand CLA 7 602



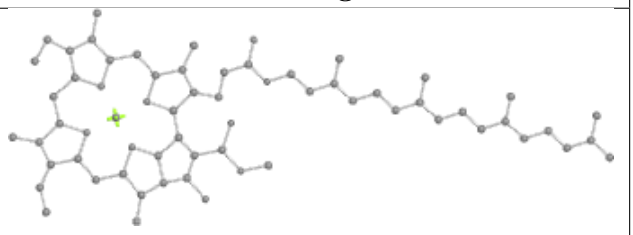
Bond lengths



Bond angles

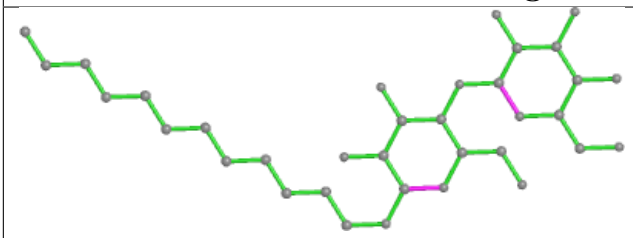


Torsions

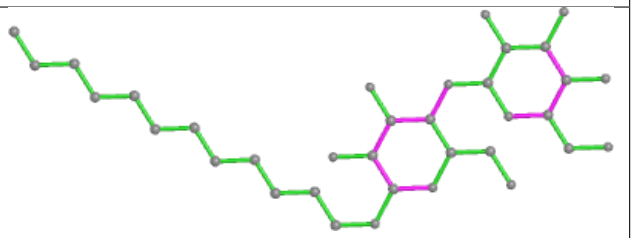


Rings

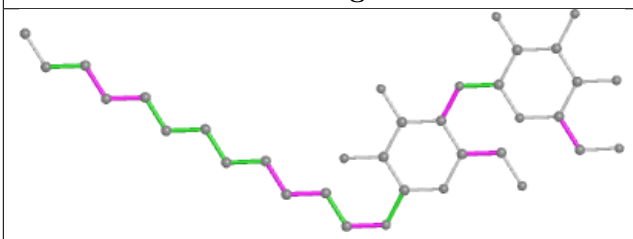
Ligand LMU 8 625



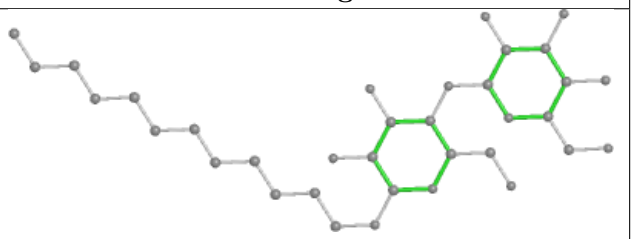
Bond lengths



Bond angles

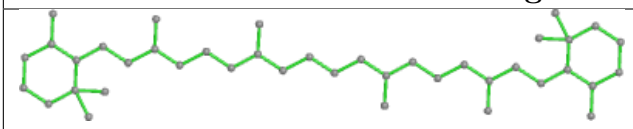


Torsions



Rings

Ligand BCR L 305



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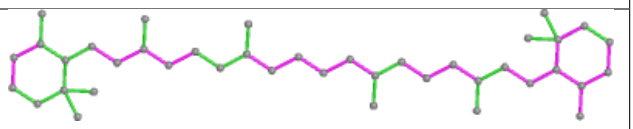
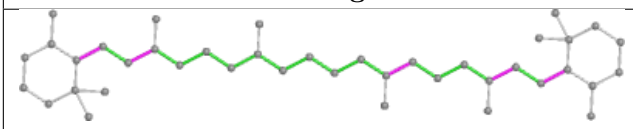
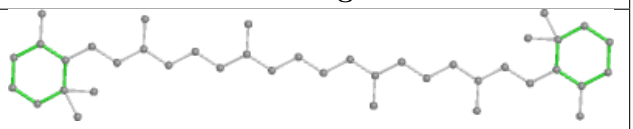


Bond angles

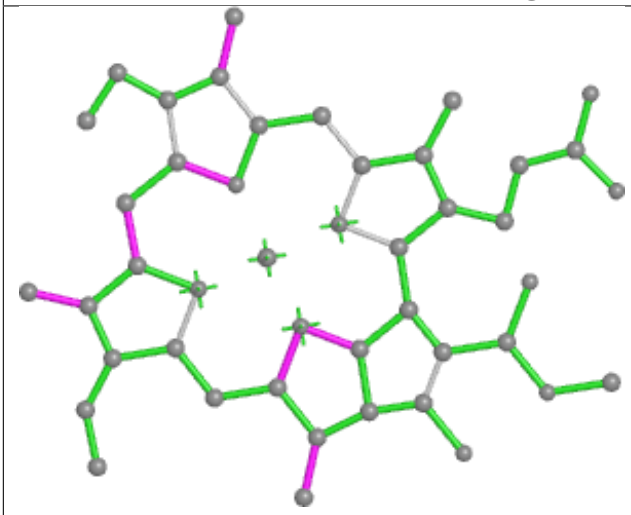


Torsions



Rings

Ligand CLA K 206



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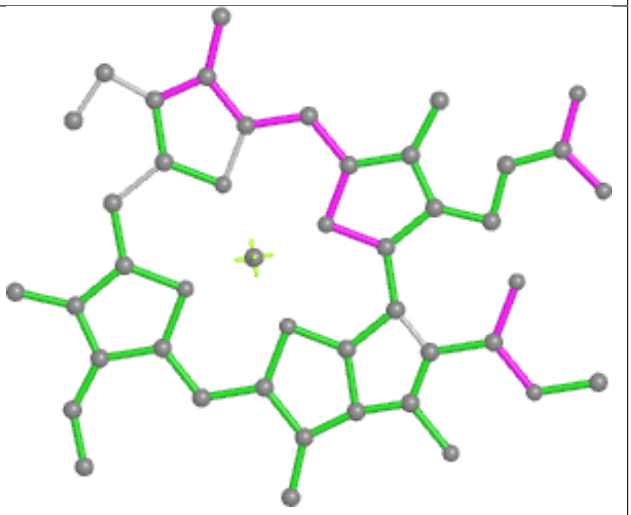
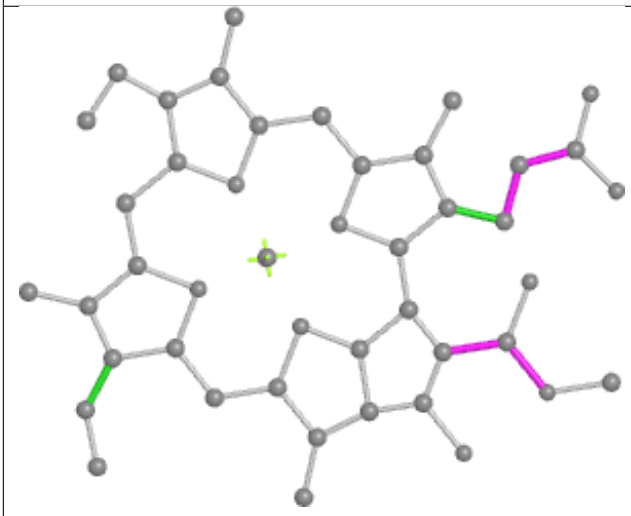


Bond angles



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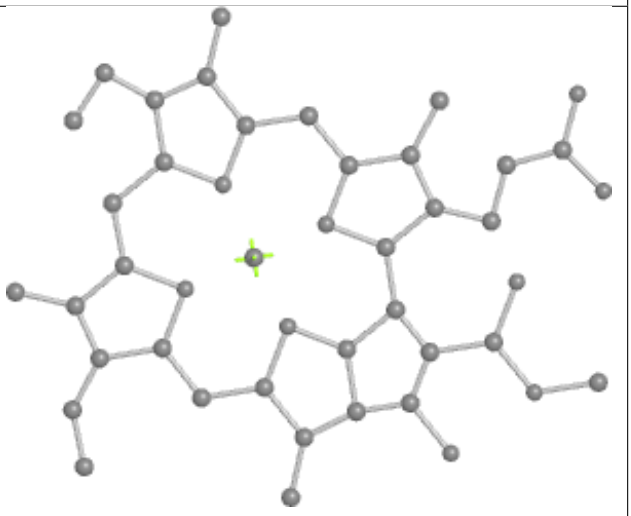
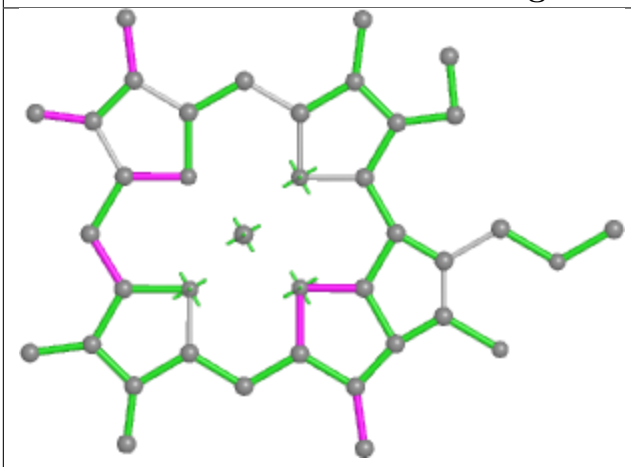
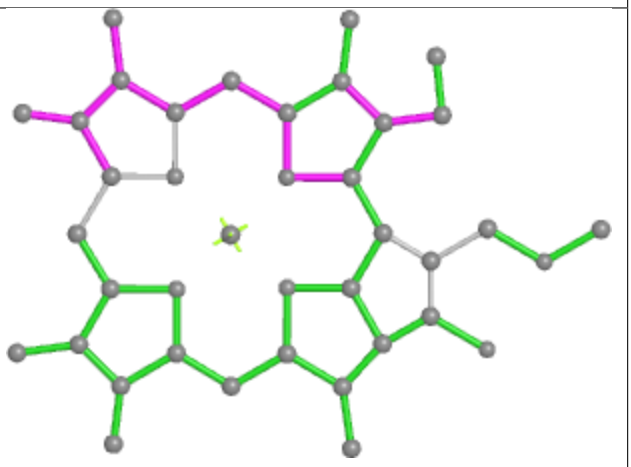


Rings

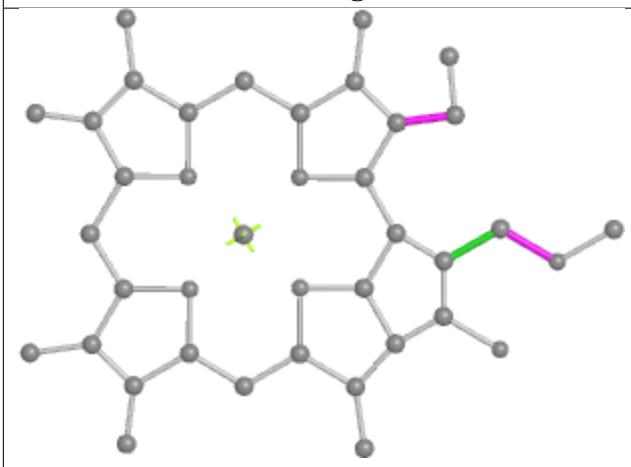
Ligand CLA 7 615



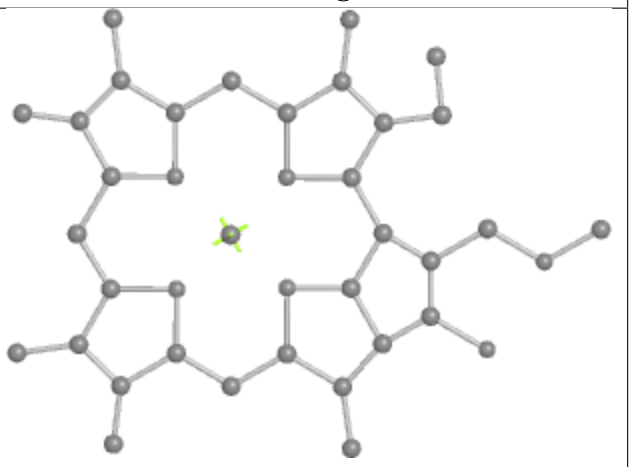
Bond lengths



Bond angles

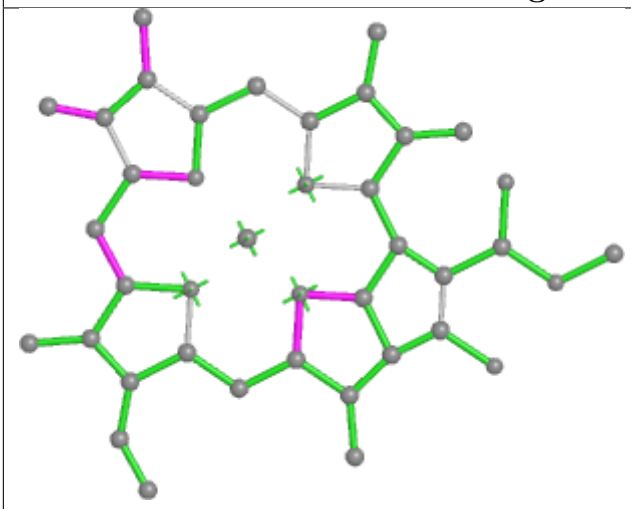


Torsions

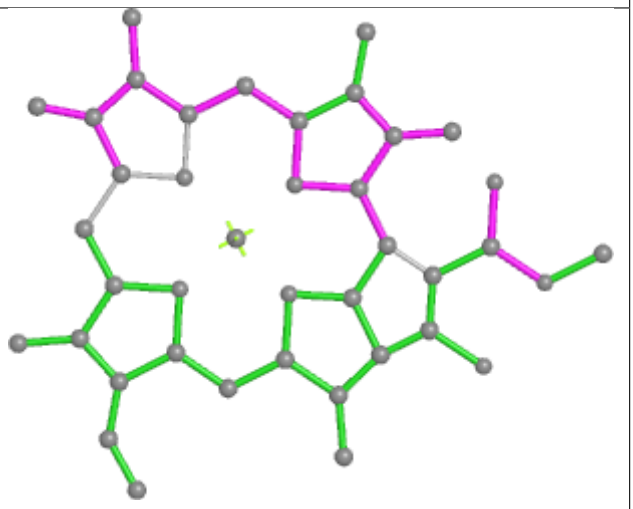


Rings

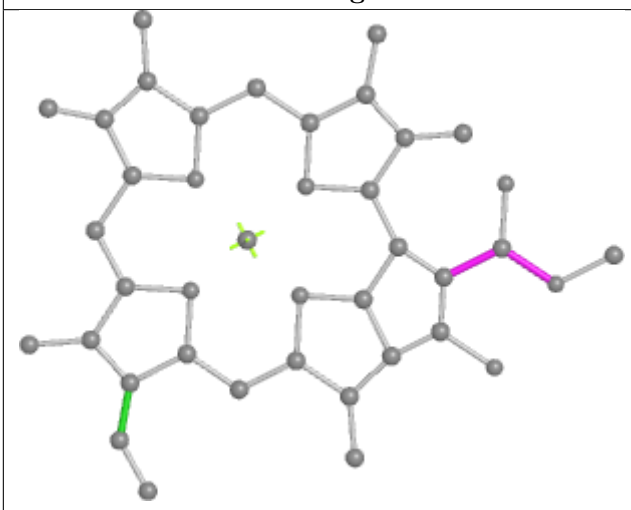
Ligand CLA 1 609



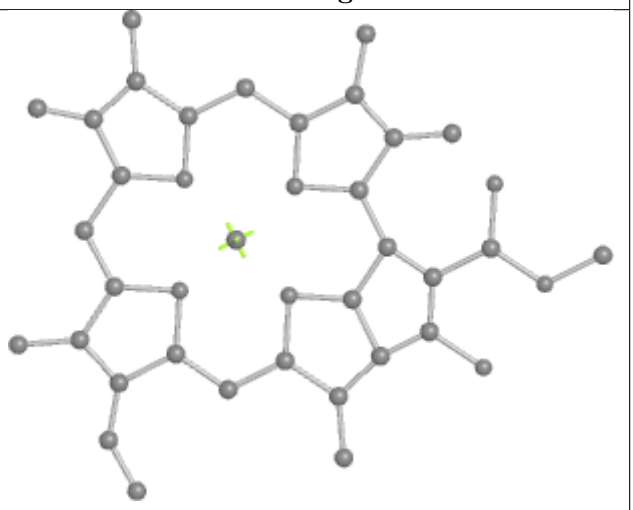
Bond lengths



Bond angles

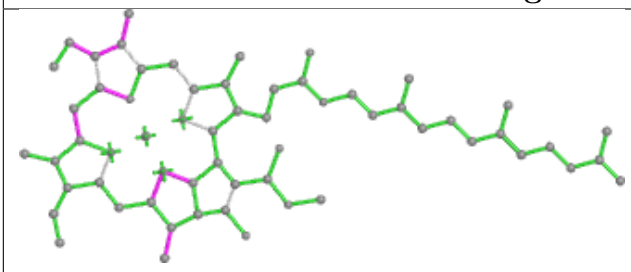


Torsions

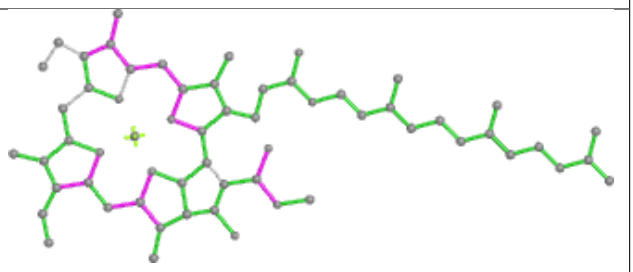


Rings

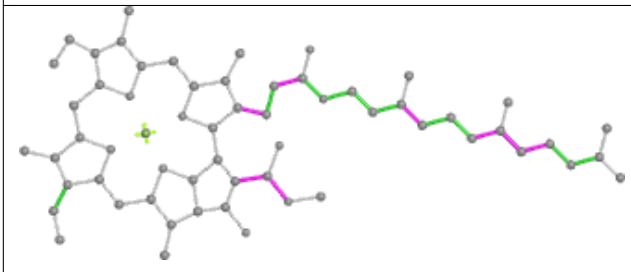
Ligand CLA B 834



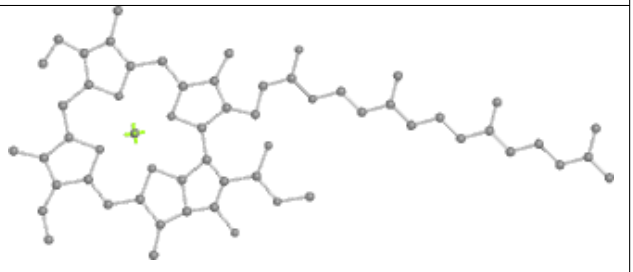
Bond lengths



Bond angles

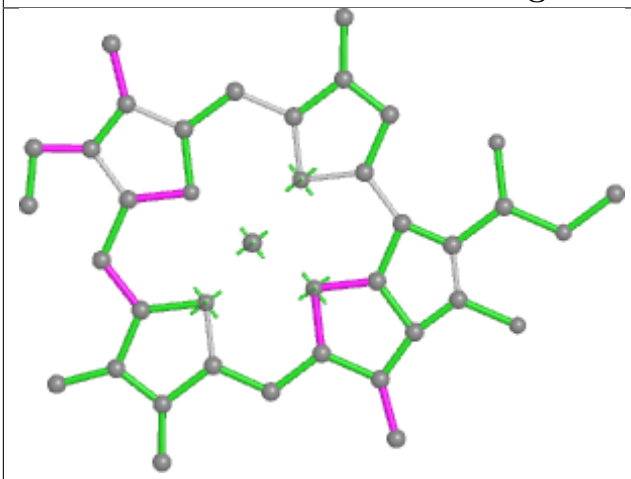


Torsions

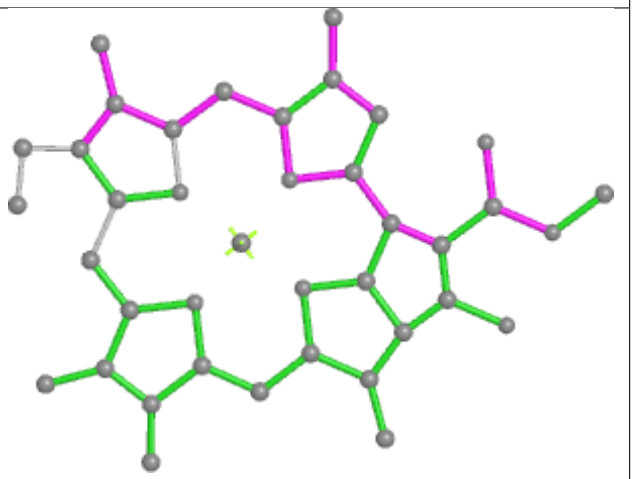


Rings

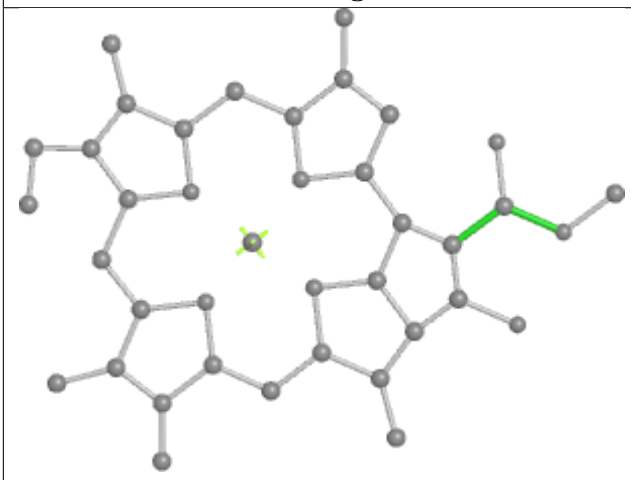
Ligand CLA 1 610



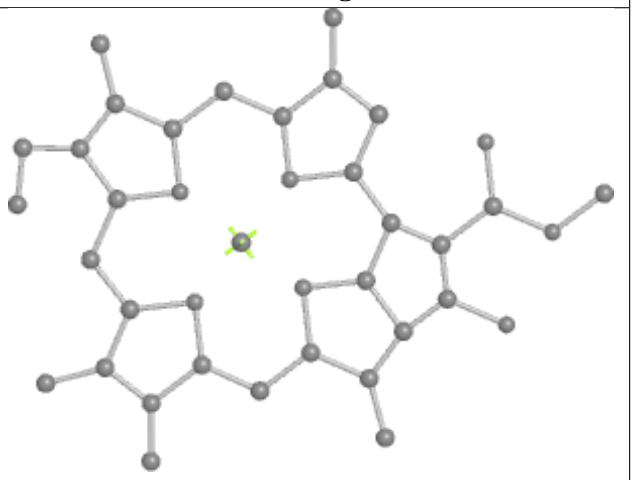
Bond lengths



Bond angles

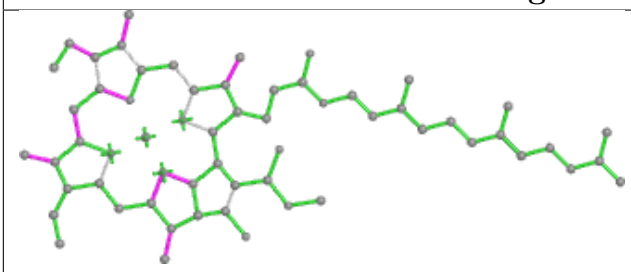


Torsions

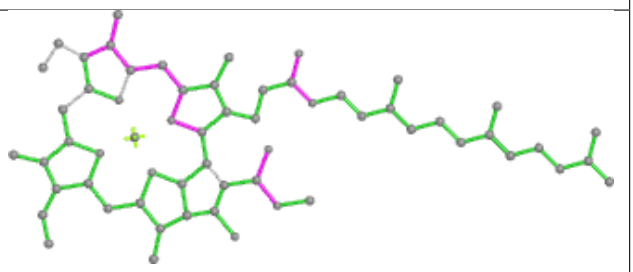


Rings

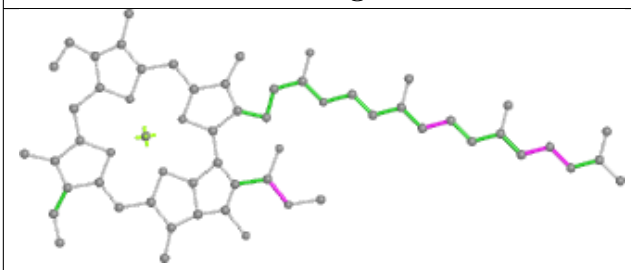
Ligand CLA 3 602



Bond lengths



Bond angles



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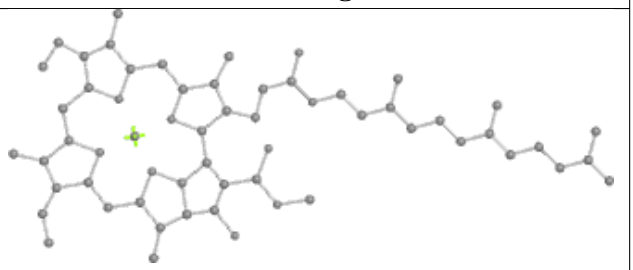
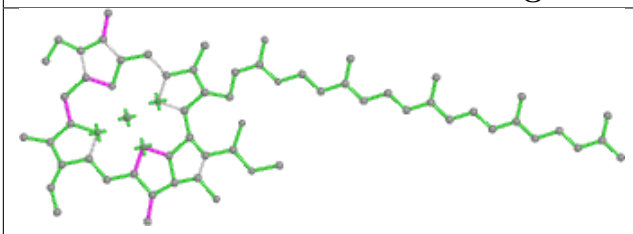
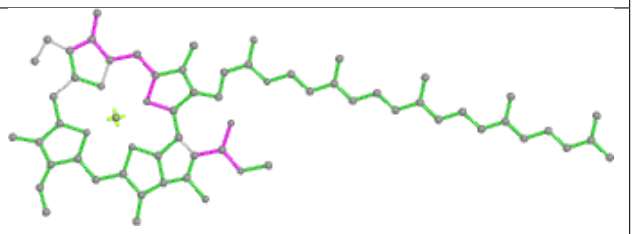


Rings

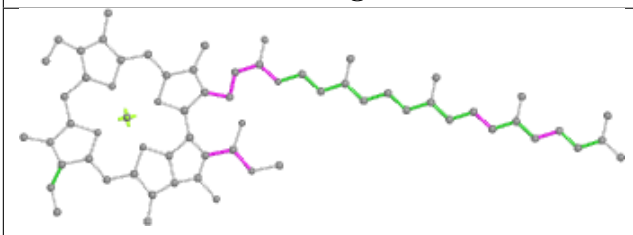
Ligand CLA B 810



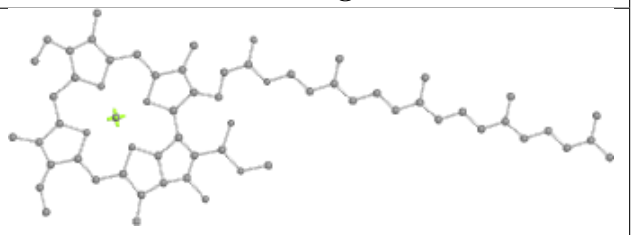
Bond lengths



Bond angles

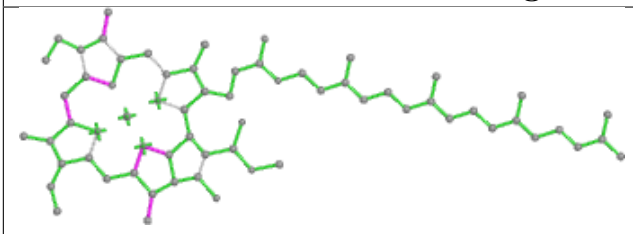


Torsions

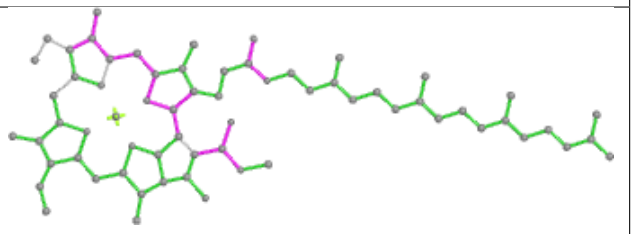


Rings

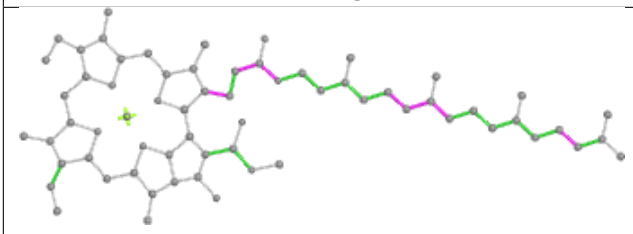
Ligand CLA K 203



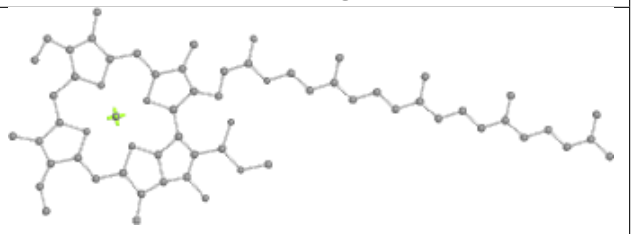
Bond lengths



Bond angles

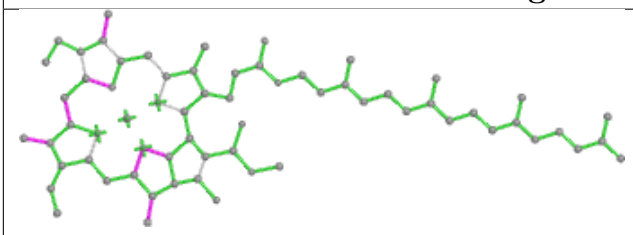


Torsions

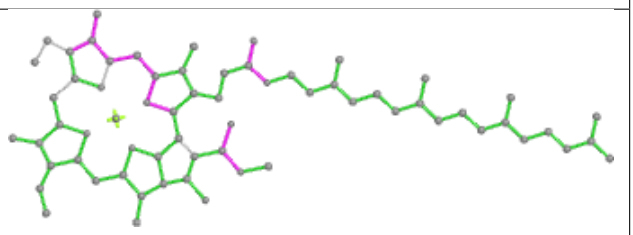


Rings

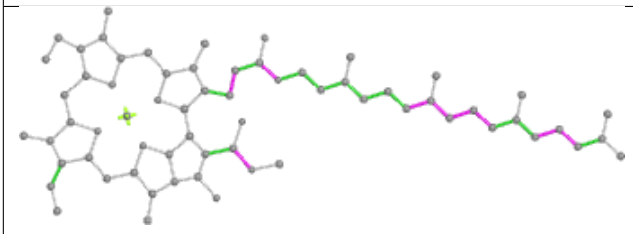
Ligand CLA 4 613



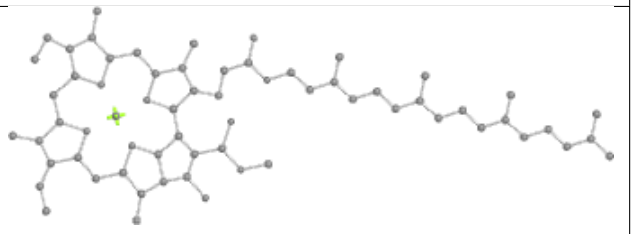
Bond lengths



Bond angles

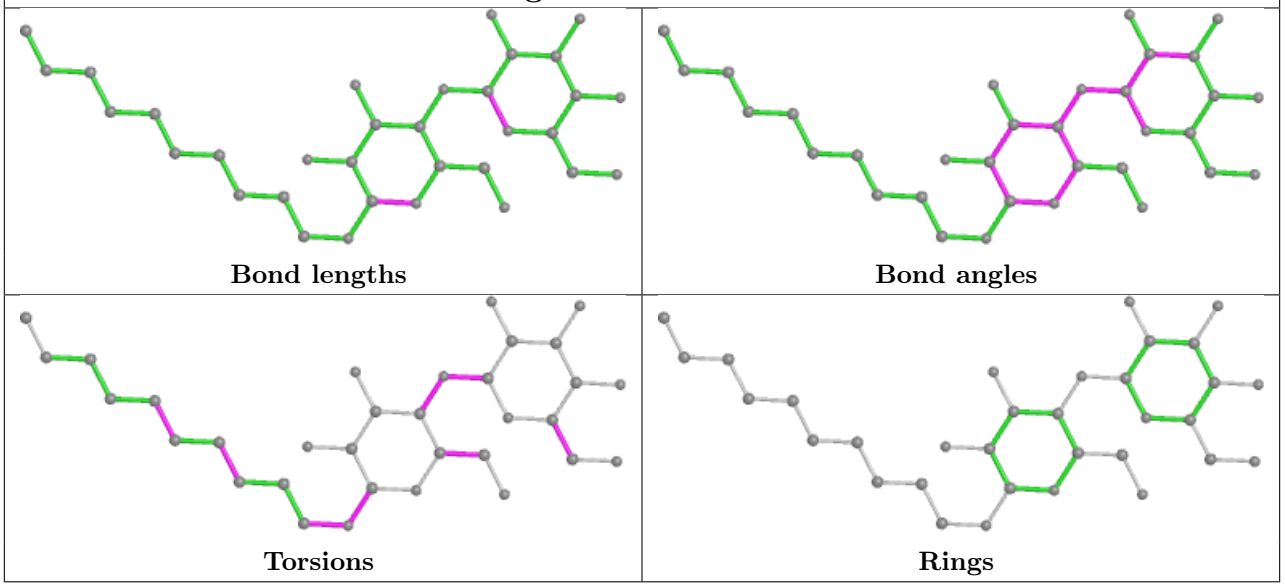


Torsions

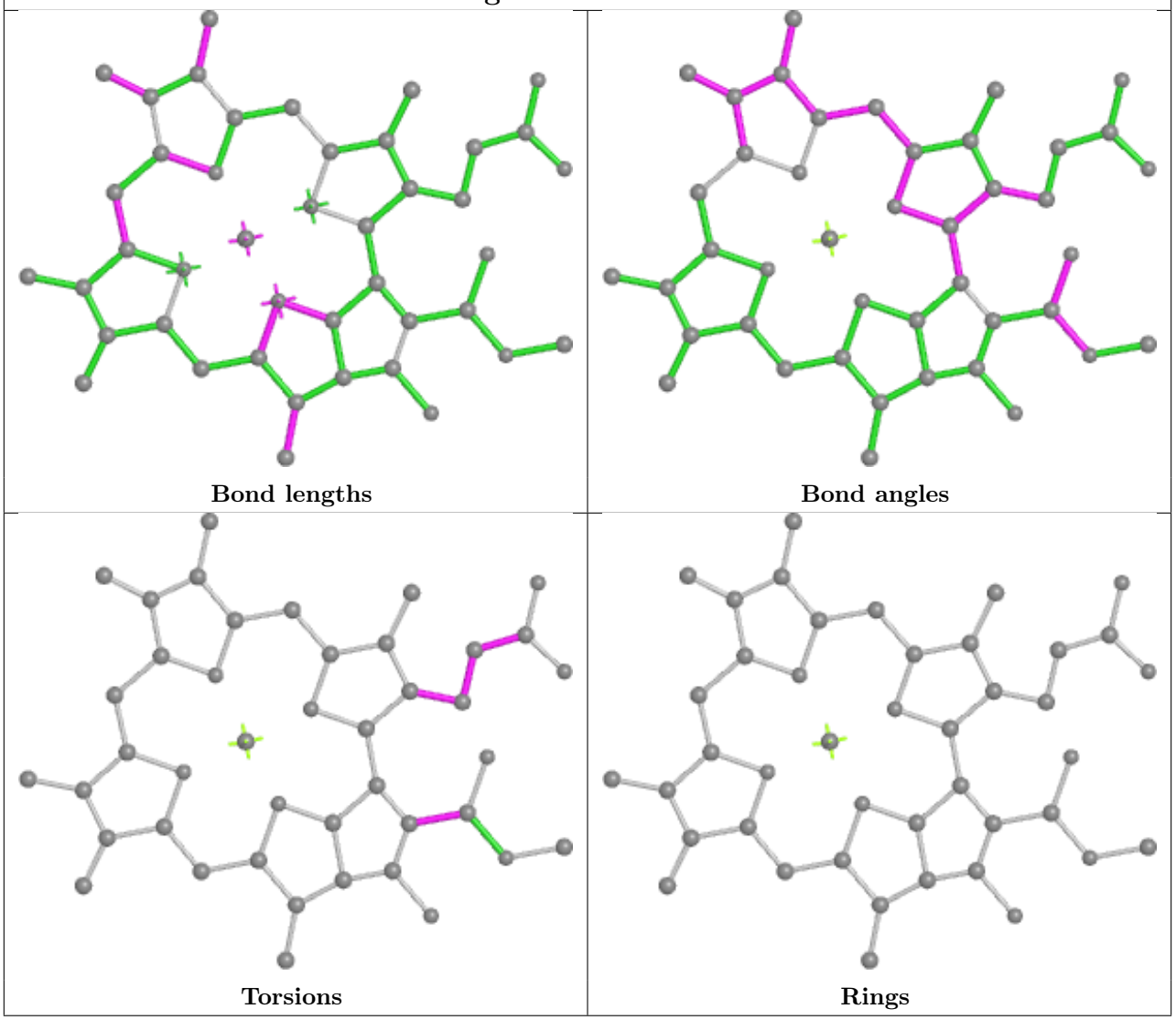


Rings

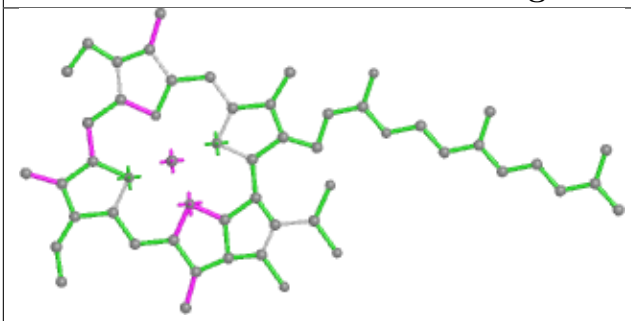
Ligand LMU 5 628



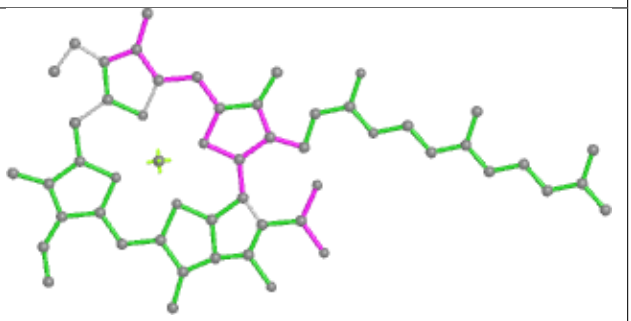
Ligand CLA 5 619



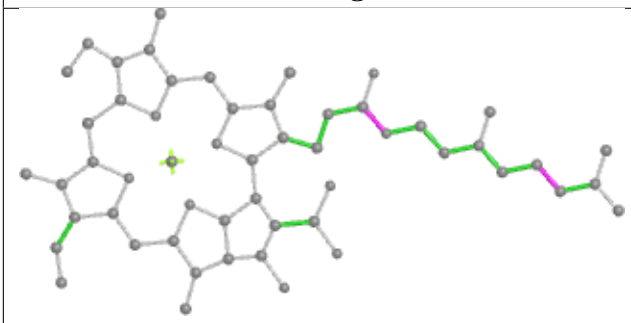
Ligand CLA 1 601



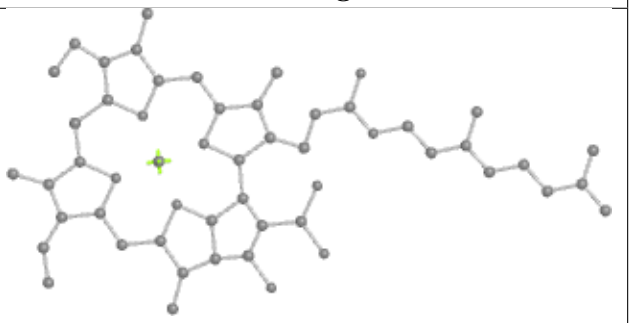
Bond lengths



Bond angles

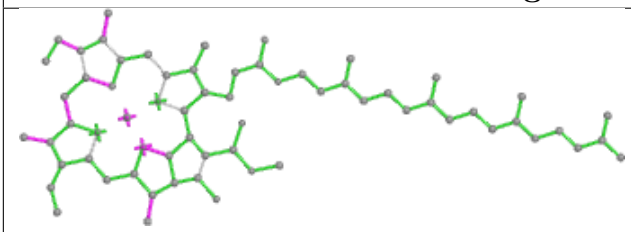


Torsions

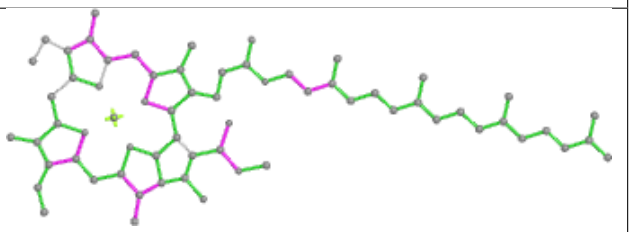


Rings

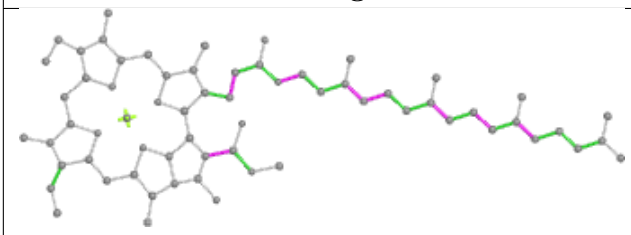
Ligand CLA A 802



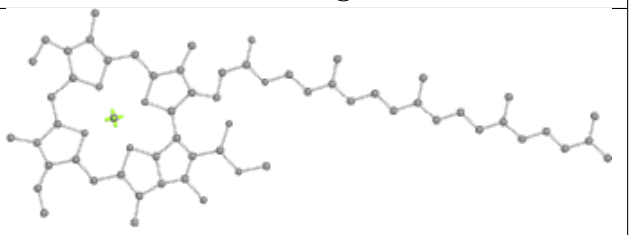
Bond lengths



Bond angles

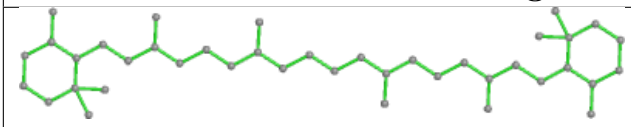


Torsions

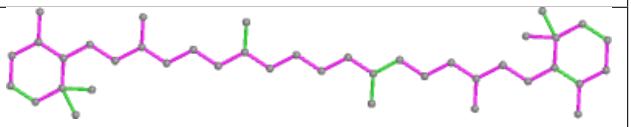


Rings

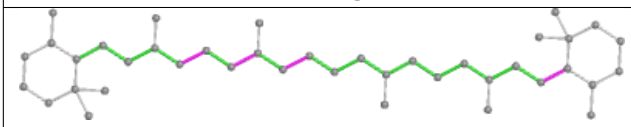
Ligand BCR 5 622



Bond lengths



Bond angles



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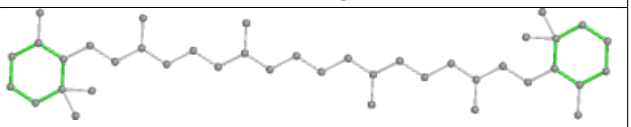
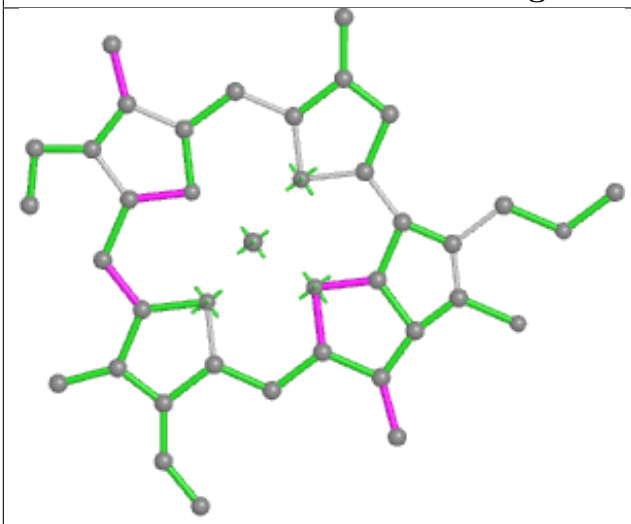
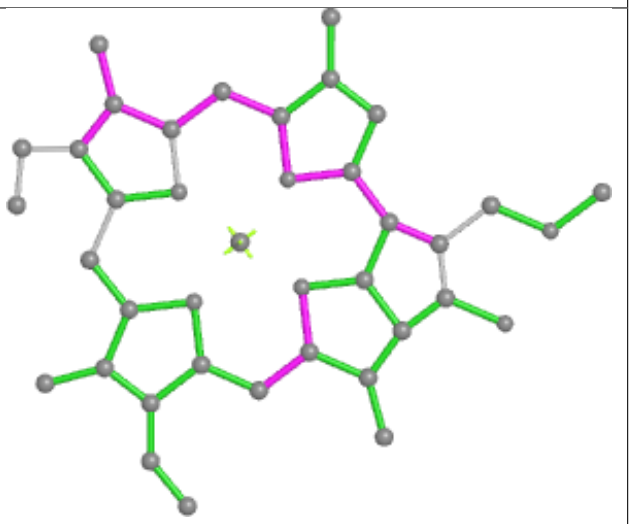


Rings

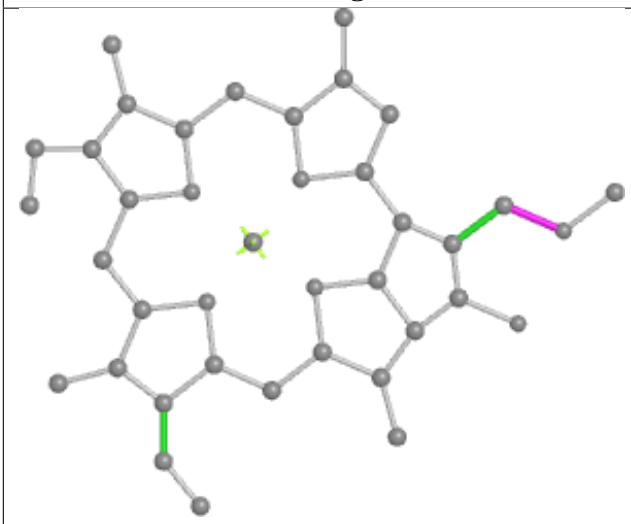
Ligand CLA 1 606



Bond lengths



Bond angles



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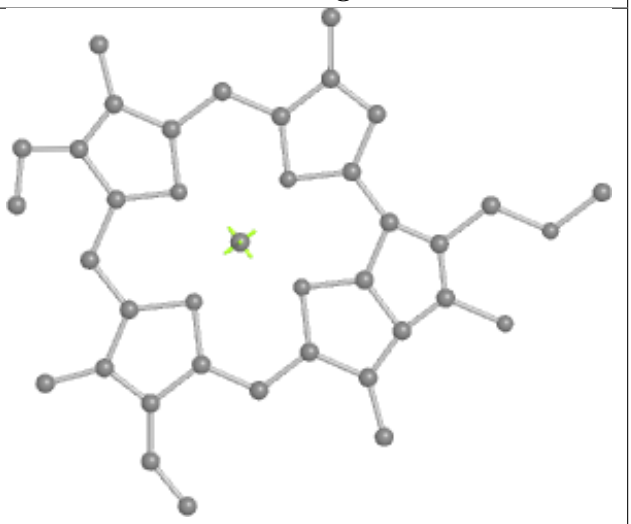
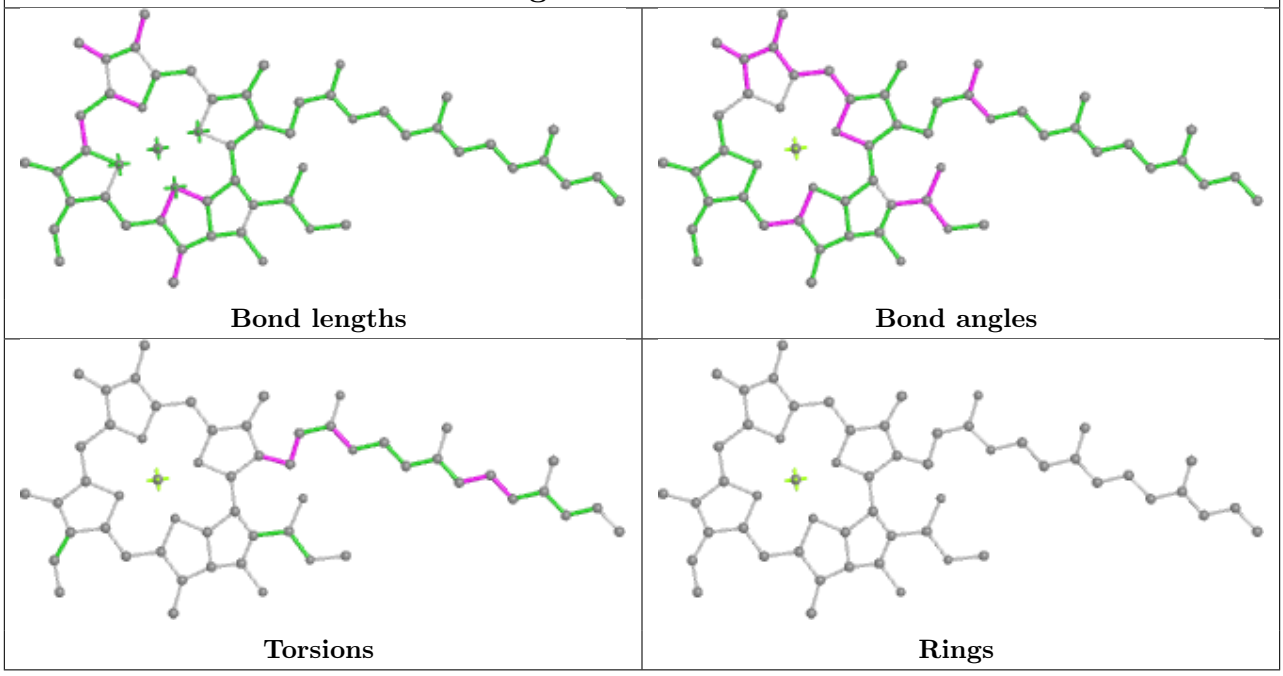
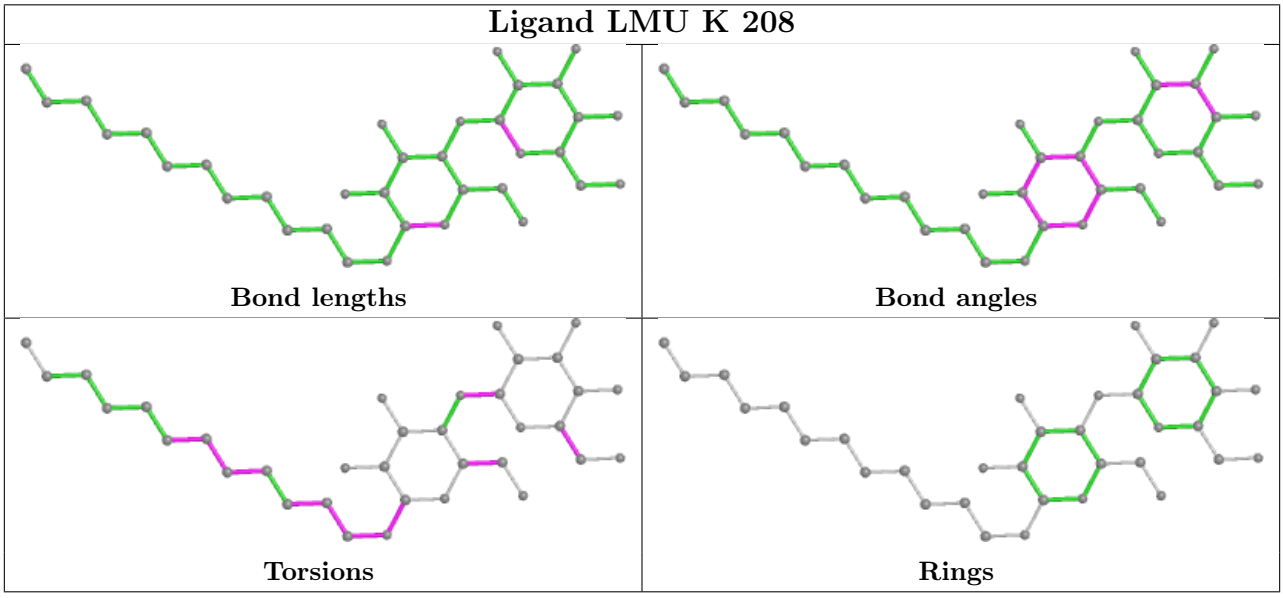


Rings

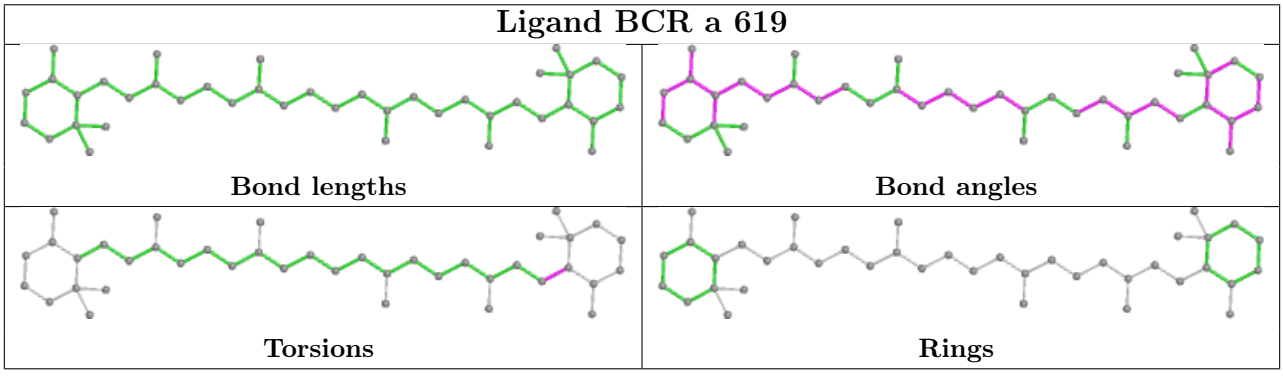
Ligand CLA 3 607

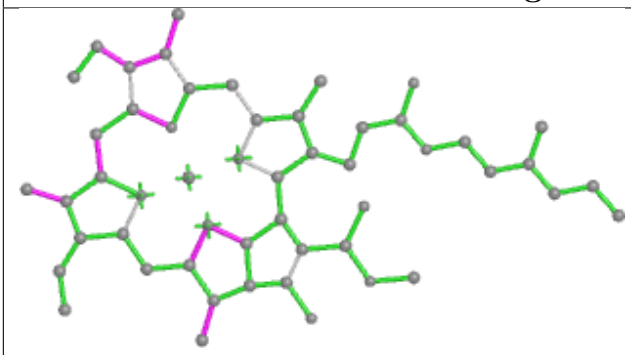
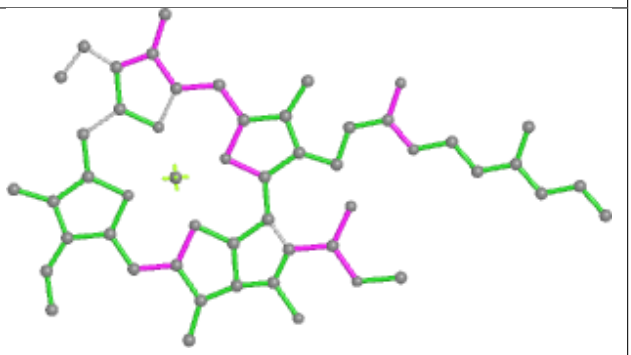
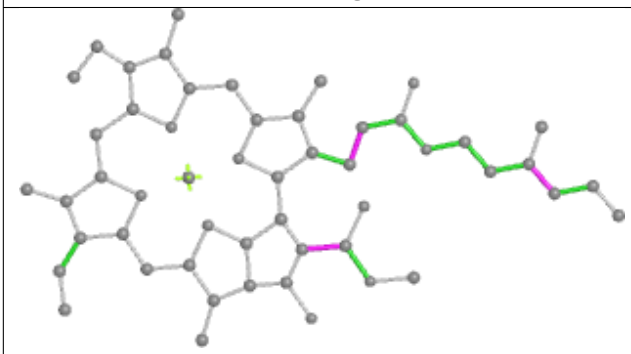
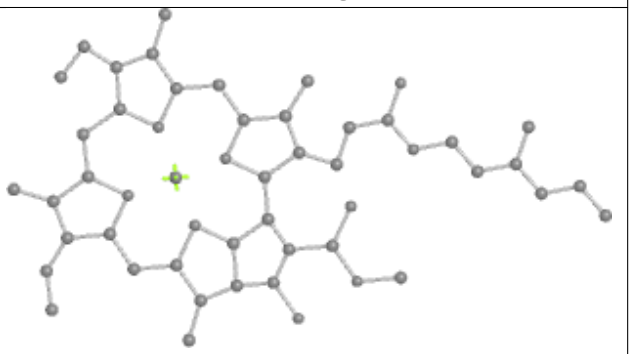


Ligand LMU K 208

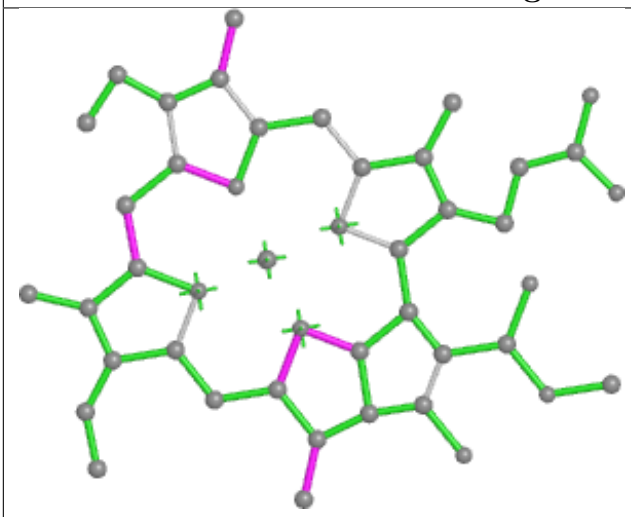


Ligand BCR a 619

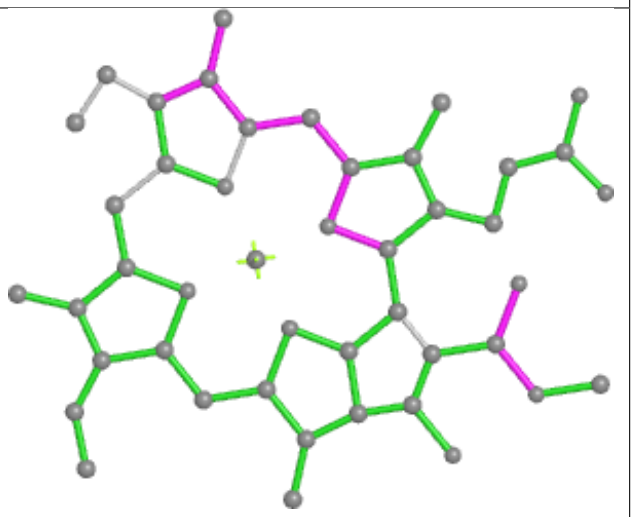


Ligand CLA B 807	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

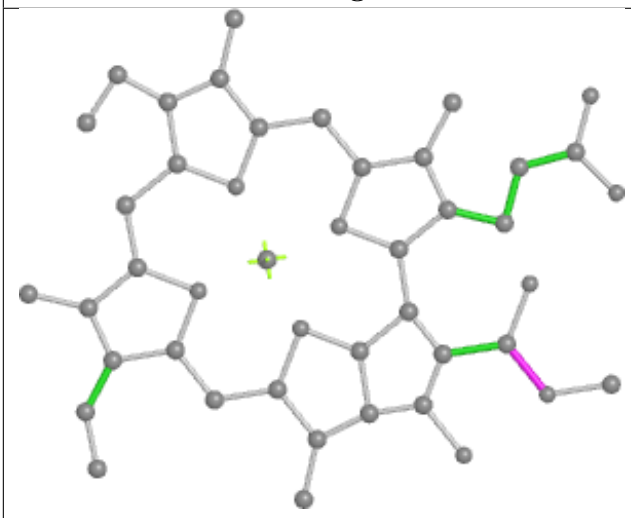
Ligand CLA A 833



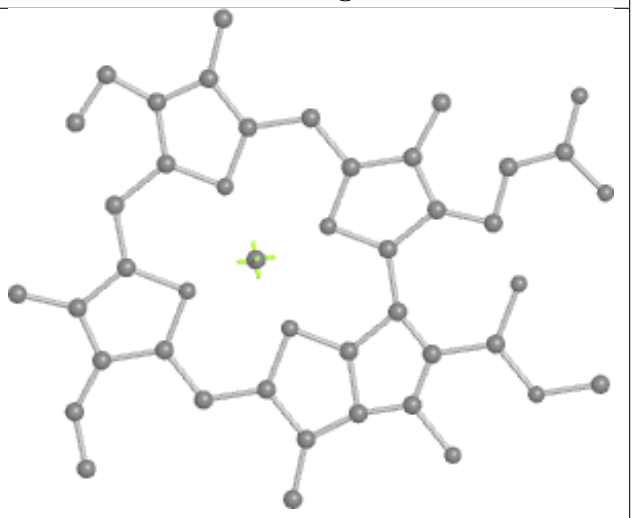
Bond lengths



Bond angles

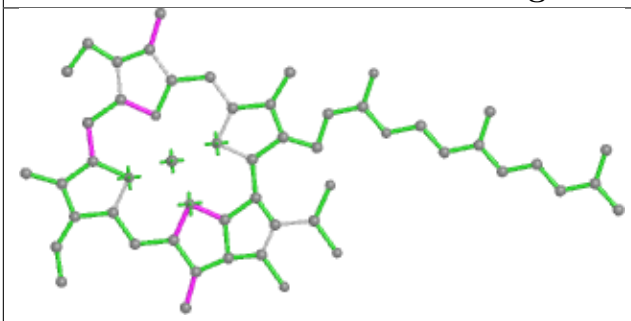


Torsions

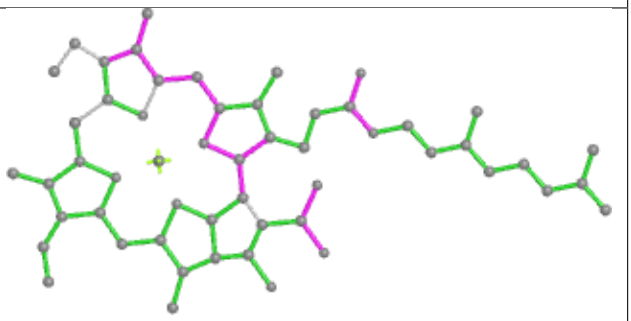


Rings

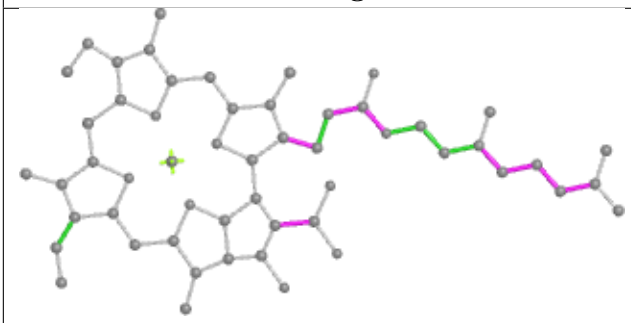
Ligand CLA 1 603



Bond lengths



Bond angles



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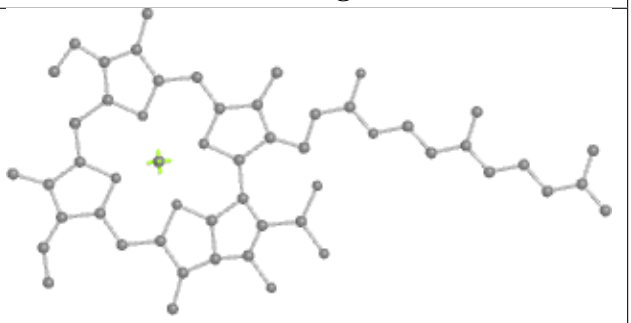
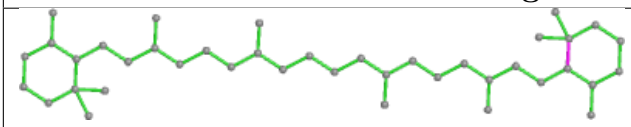
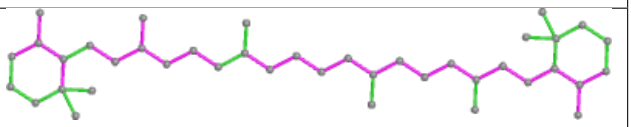


Rings

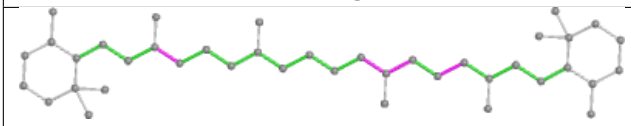
Ligand BCR A 852



Bond lengths

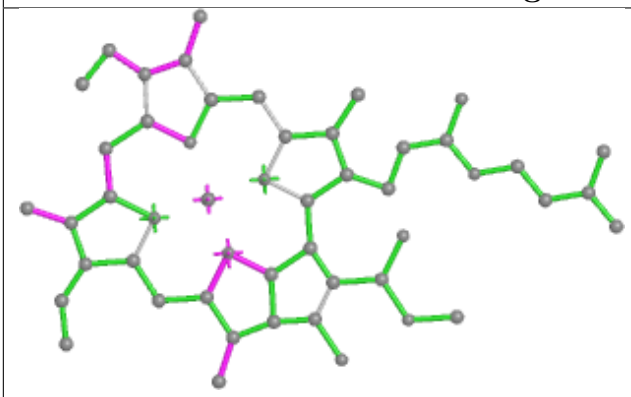
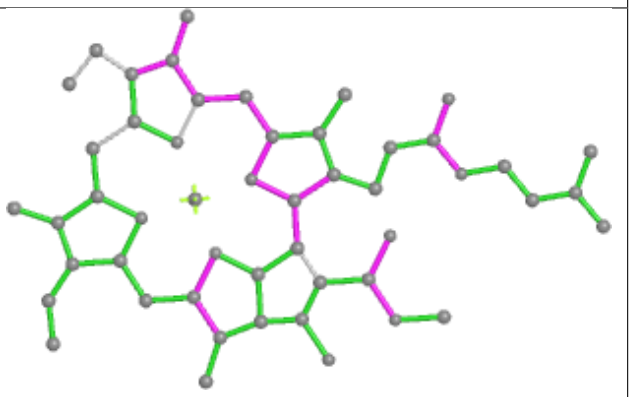
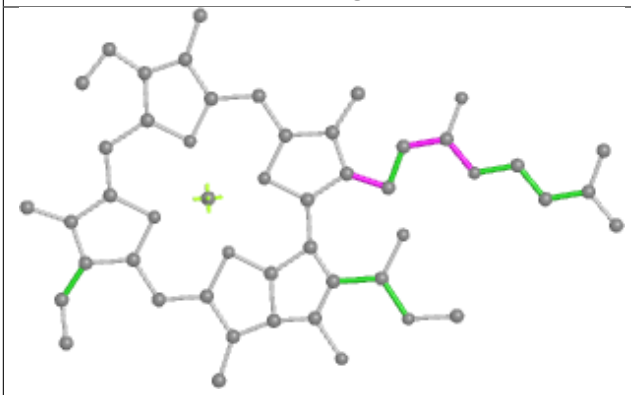
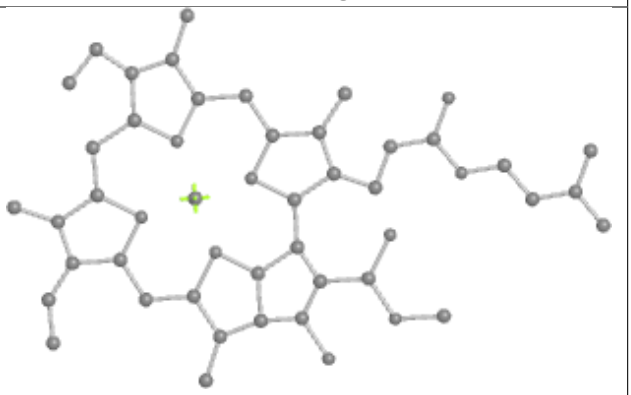


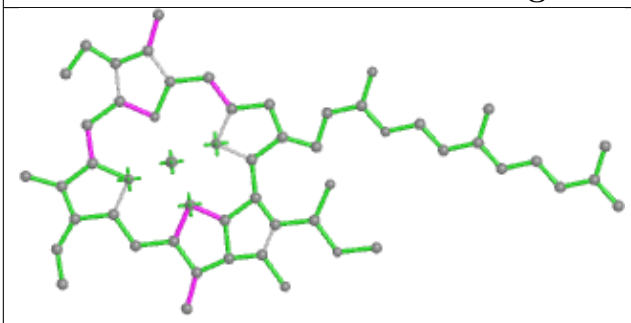
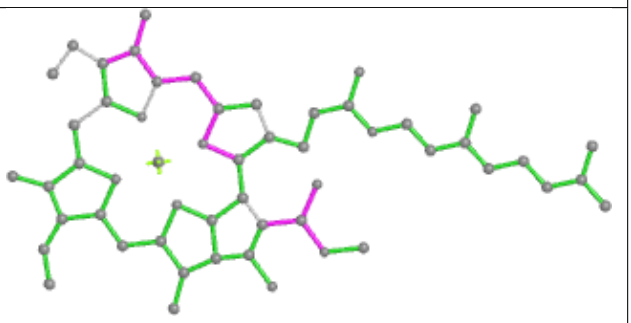
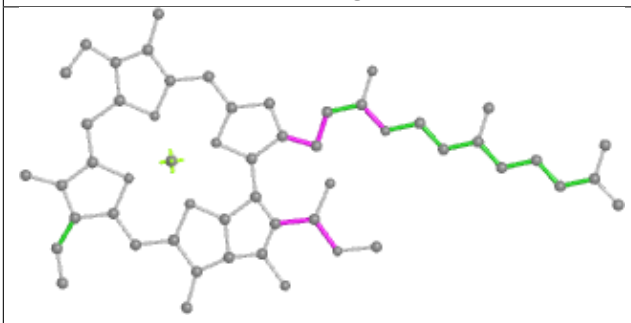
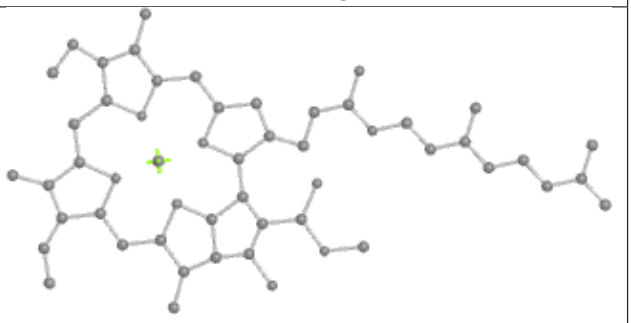
Bond angles



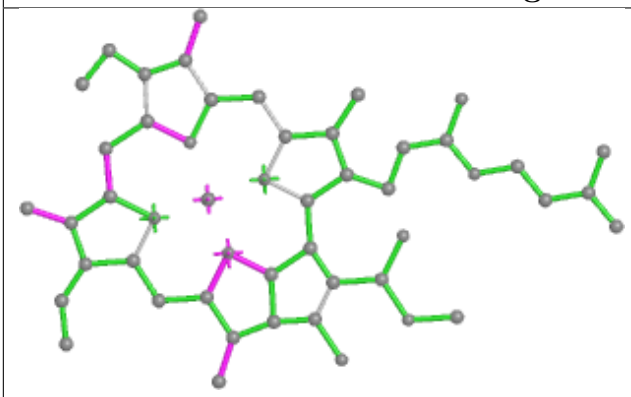
Torsions

Rings

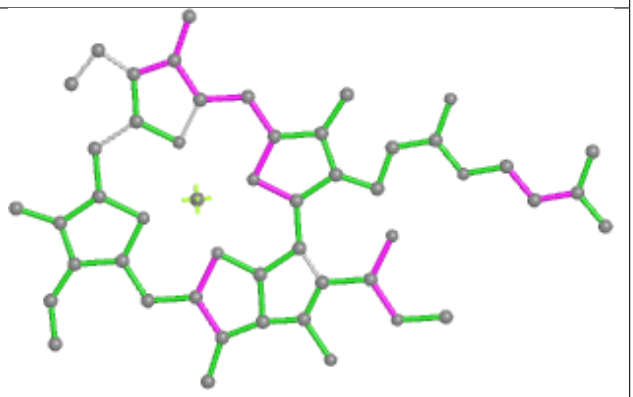
Ligand CLA A 810	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA a 614	
 Bond lengths	 Bond angles
 Torsions	 Rings

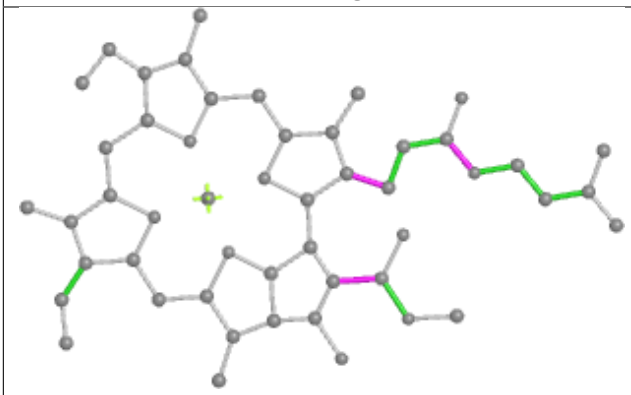
Ligand CLA A 832



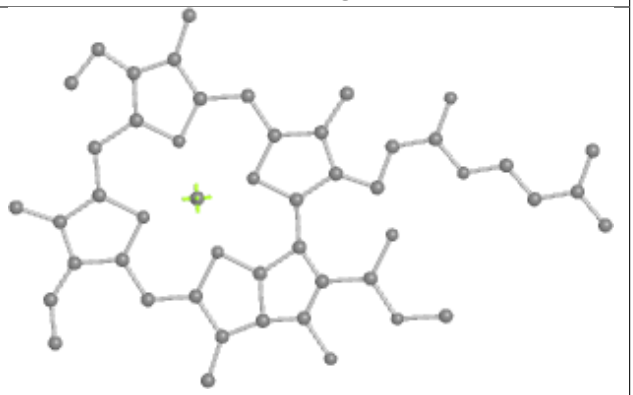
Bond lengths



Bond angles

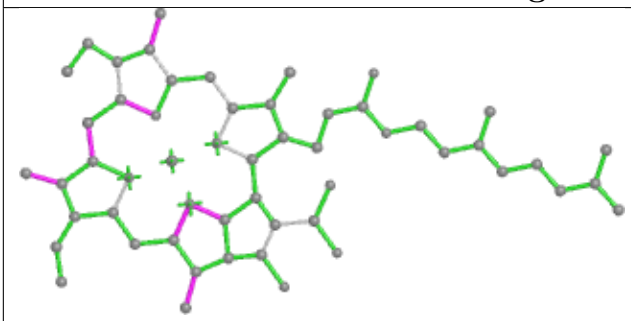


Torsions

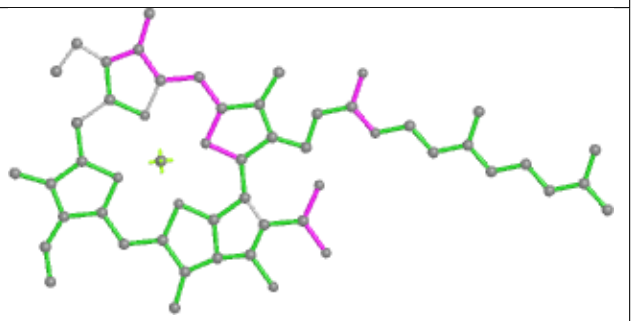


Rings

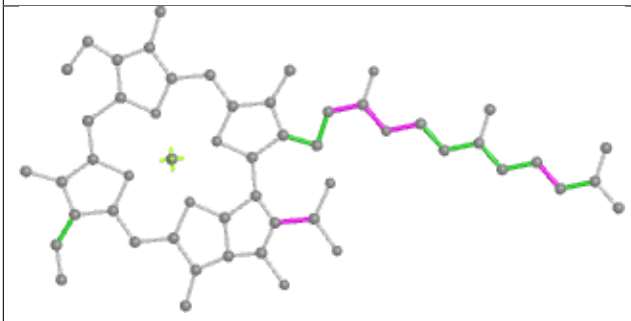
Ligand CLA 3 606



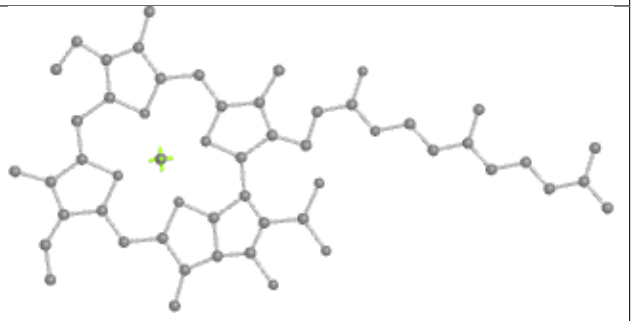
Bond lengths



Bond angles

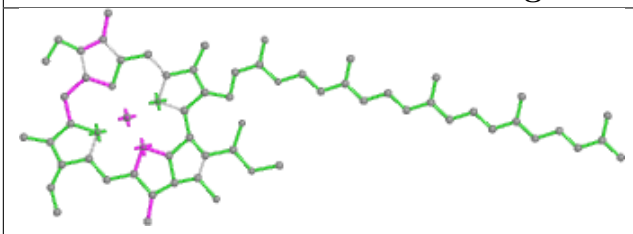


Torsions

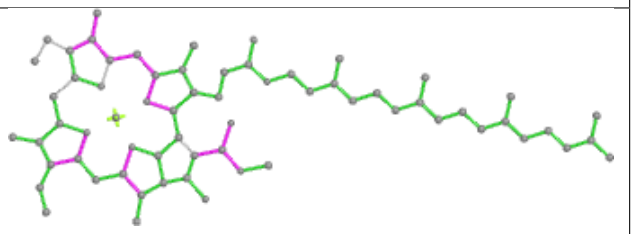


Rings

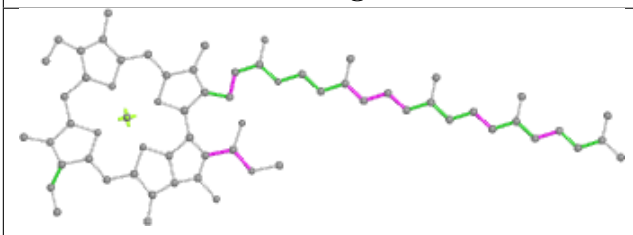
Ligand CLA B 829



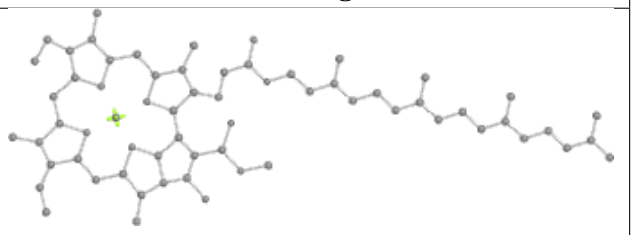
Bond lengths



Bond angles

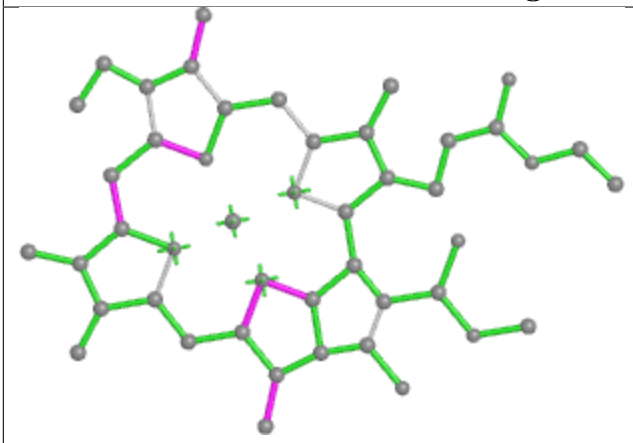


Torsions

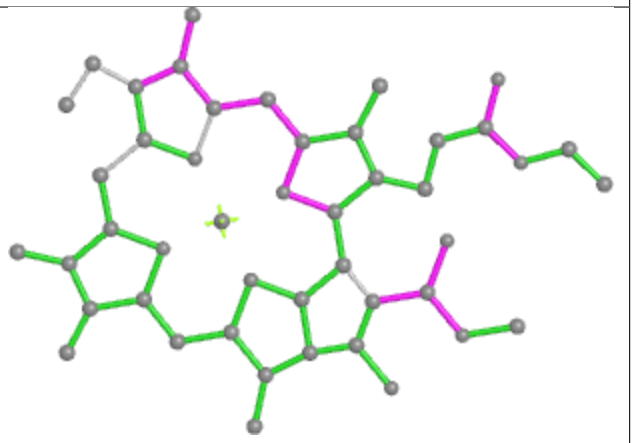


Rings

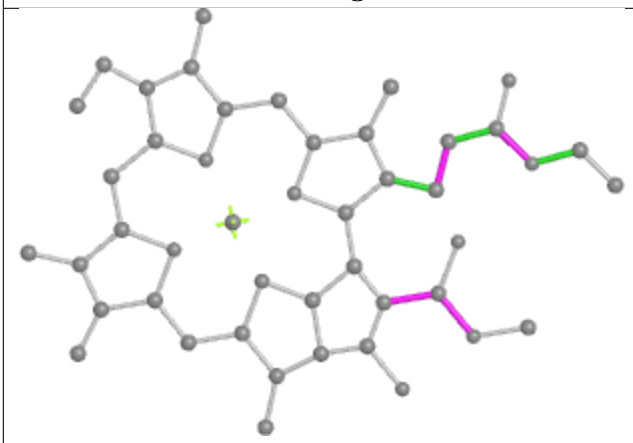
Ligand CLA B 821



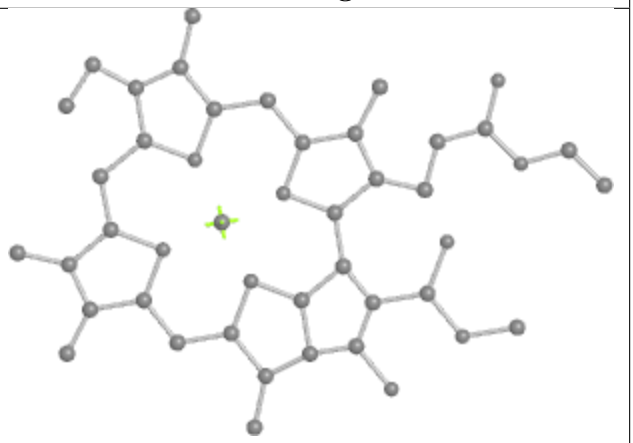
Bond lengths



Bond angles

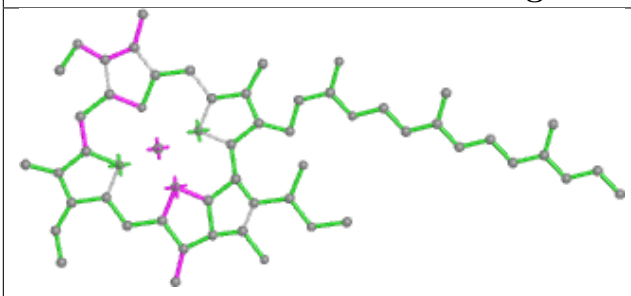


Torsions

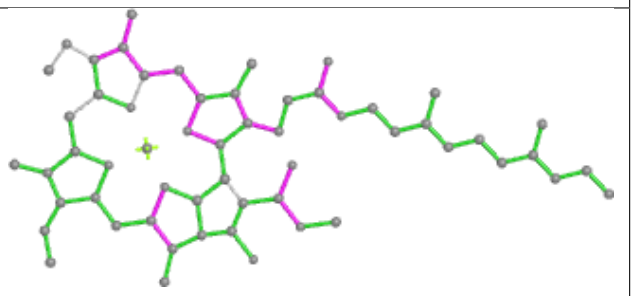


Rings

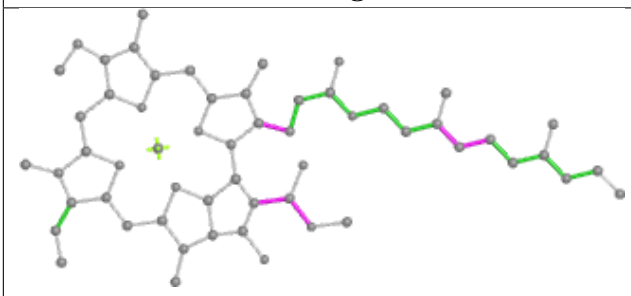
Ligand CLA F 301



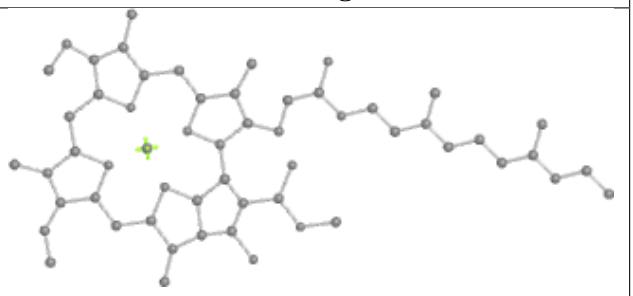
Bond lengths



Bond angles

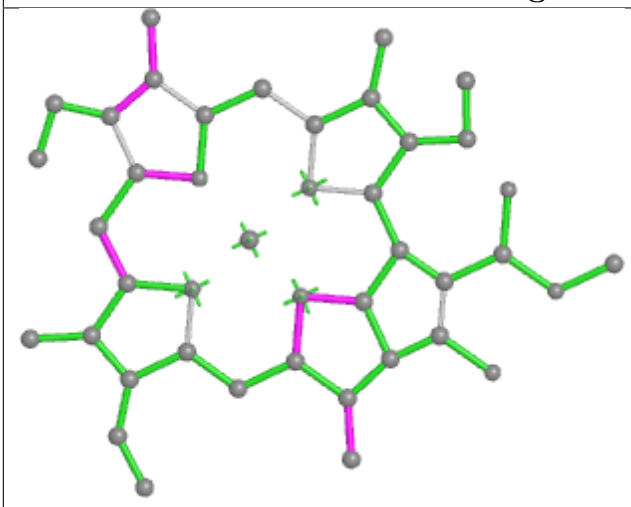


Torsions

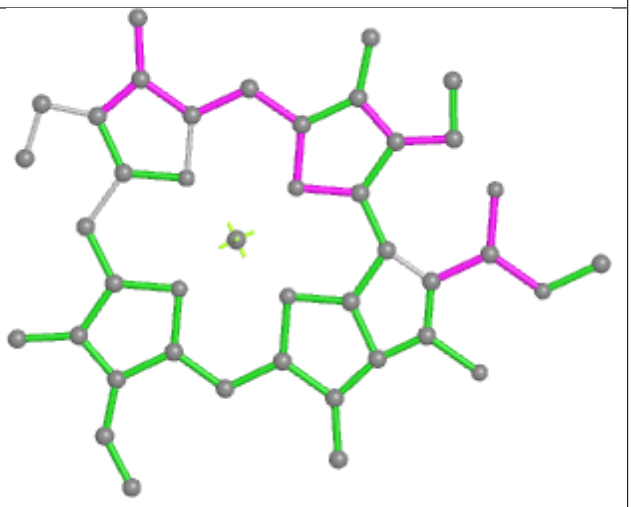


Rings

Ligand CLA 7 614



Bond lengths



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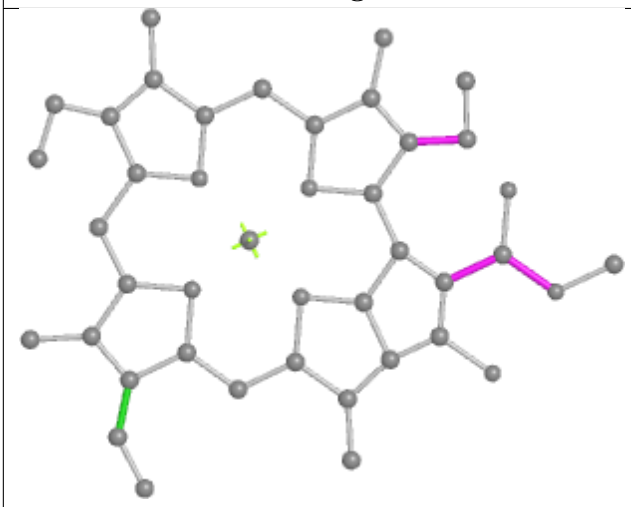
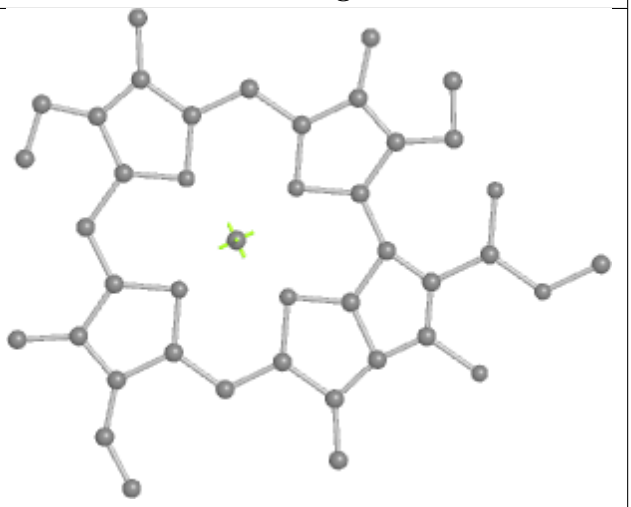
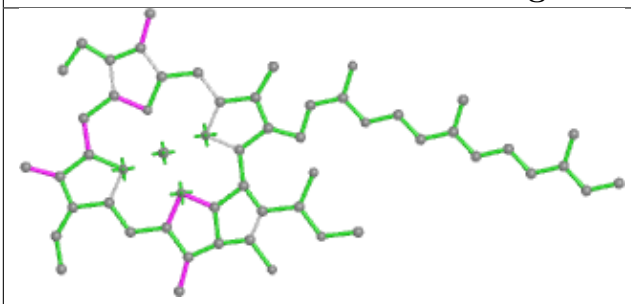


Torsions



Rings

Ligand CLA 8 614



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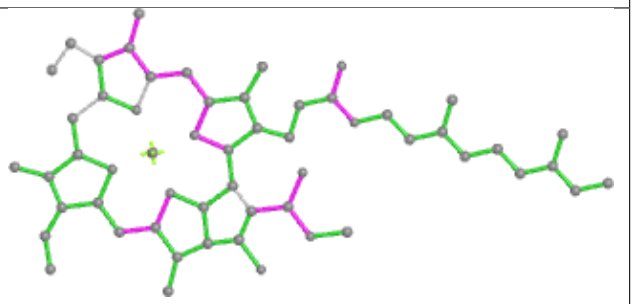
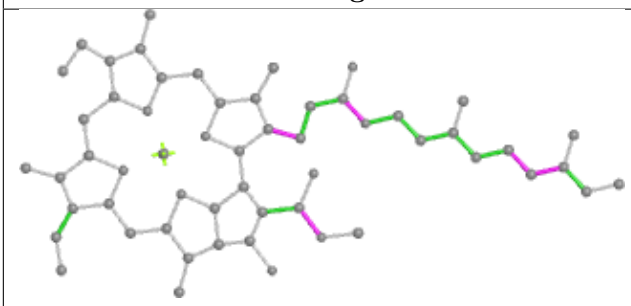
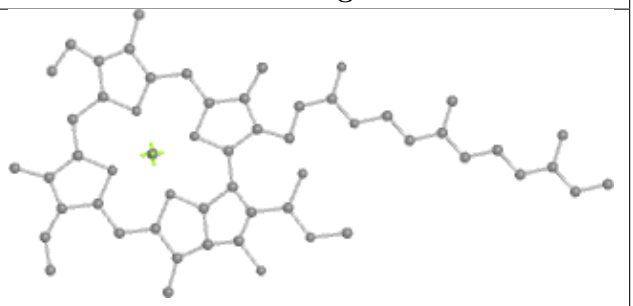


Bond angles

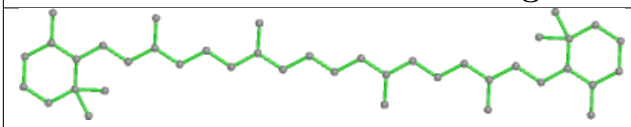


Torsions

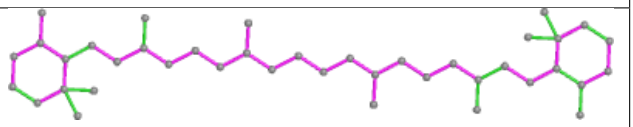


Rings

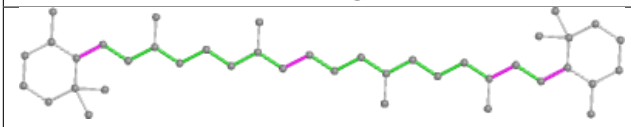
Ligand BCR A 856



Bond lengths



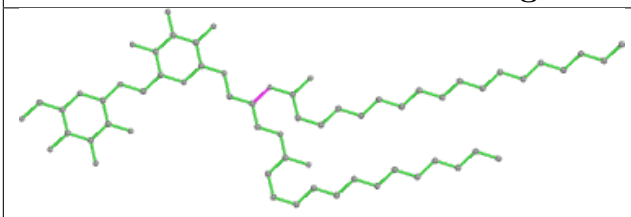
Bond angles



Torsions

Rings

Ligand DGD B 850



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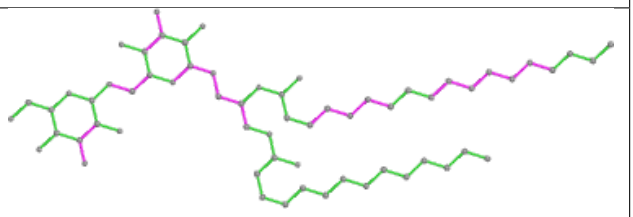

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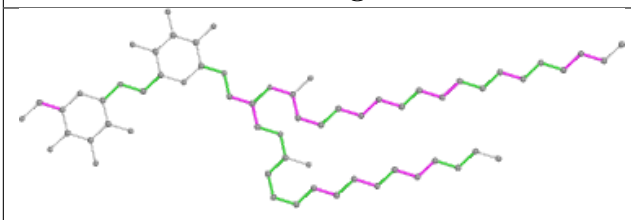

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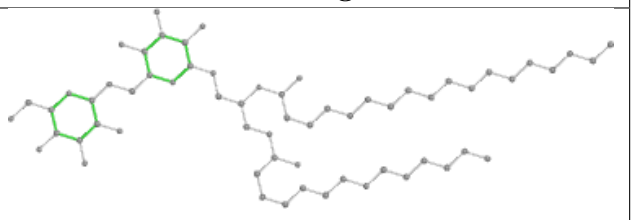
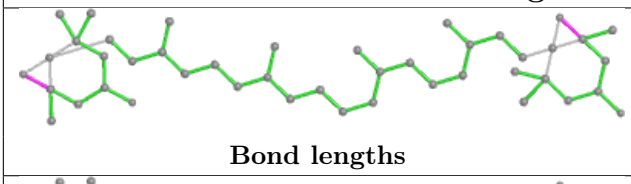


Rings

Ligand XAT 7 620



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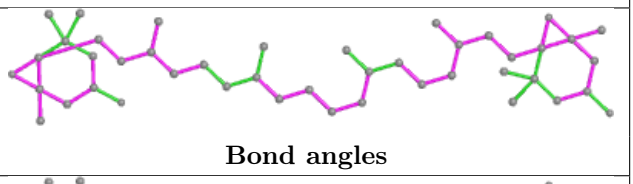
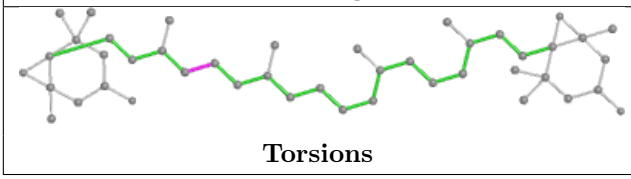


Bond angles



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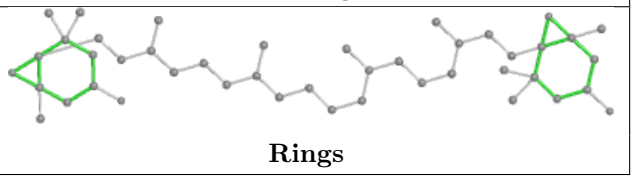
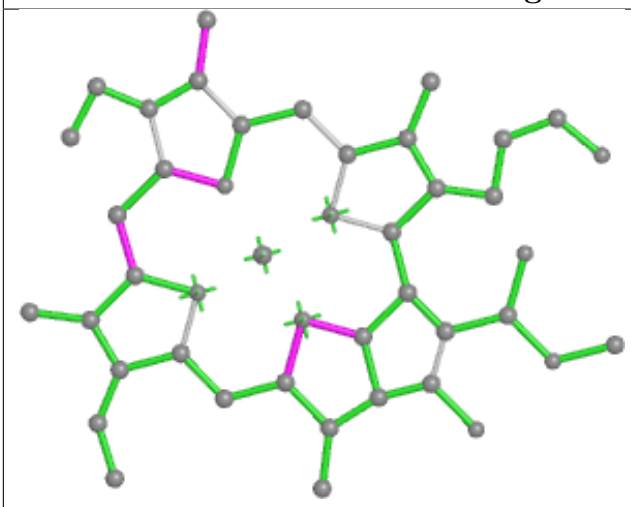


Rings

Ligand CLA B 841



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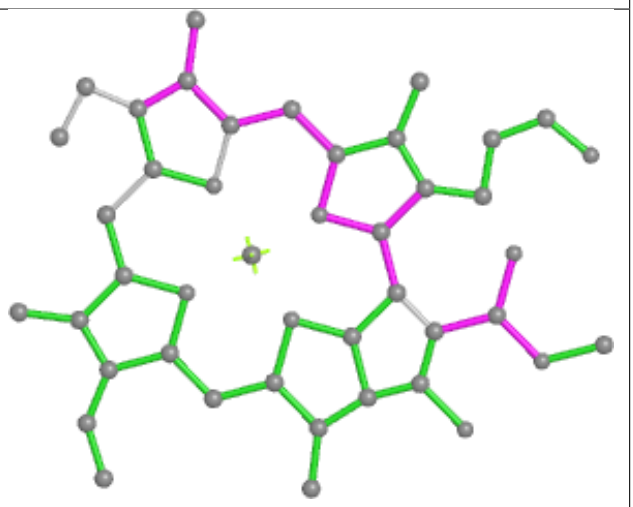
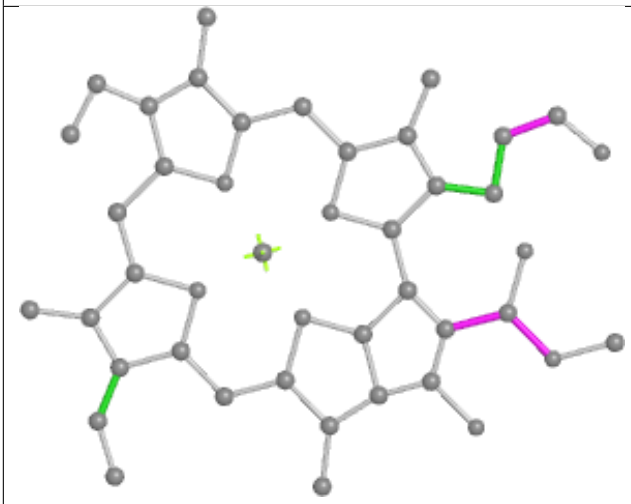


Bond angles



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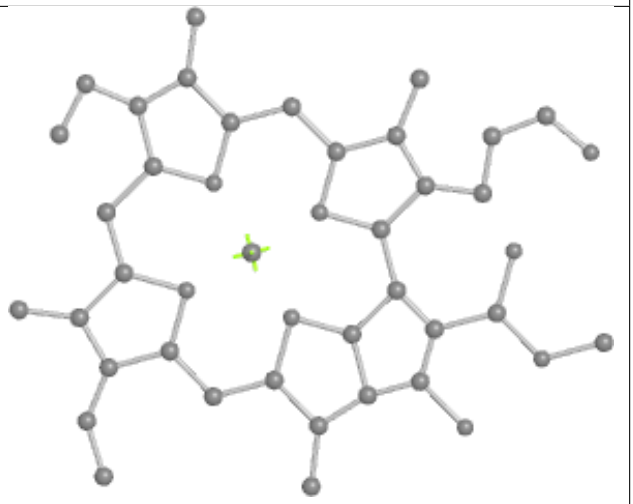
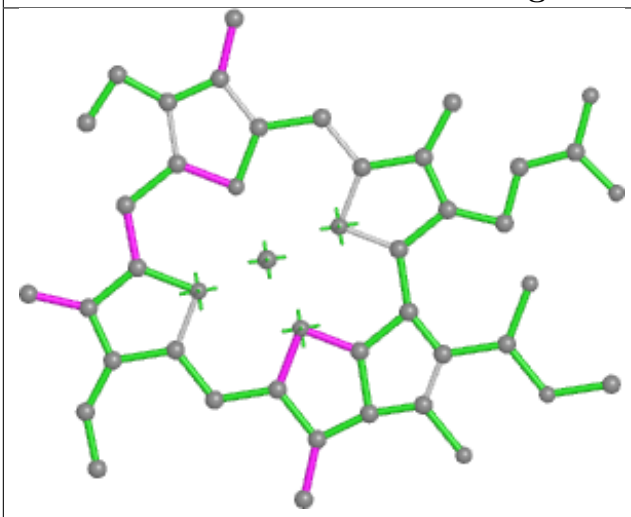


Rings

Ligand CLA 8 609



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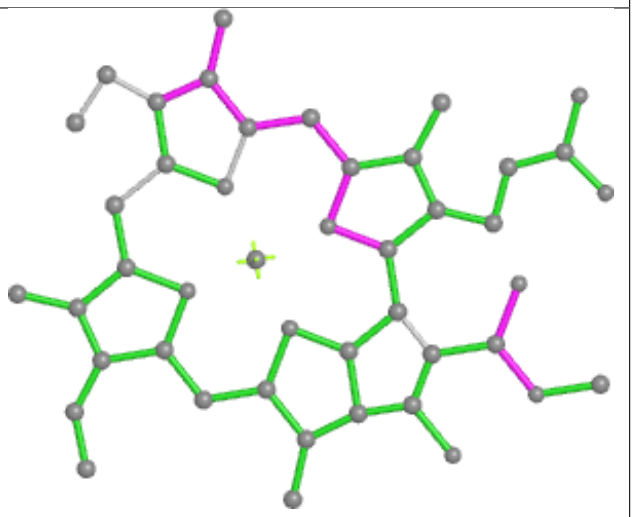
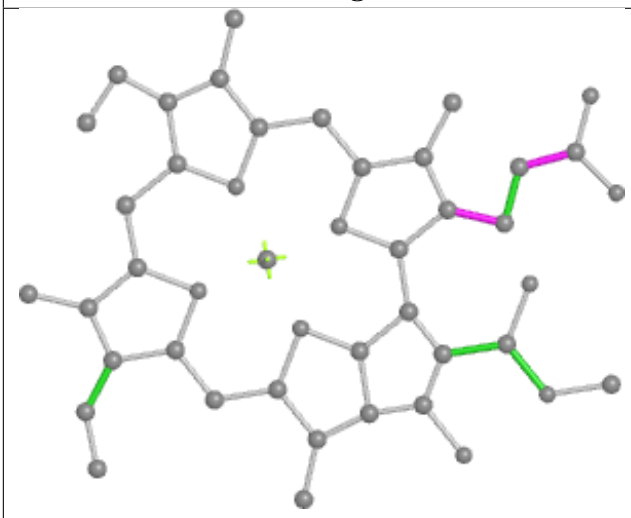


Bond angles



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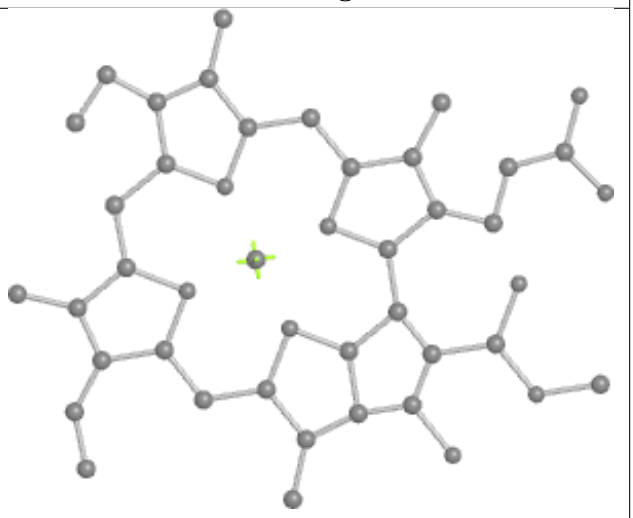
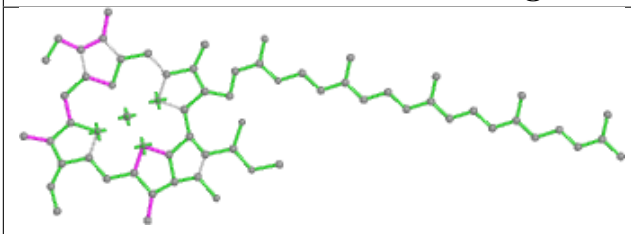


Rings

Ligand CLA B 802



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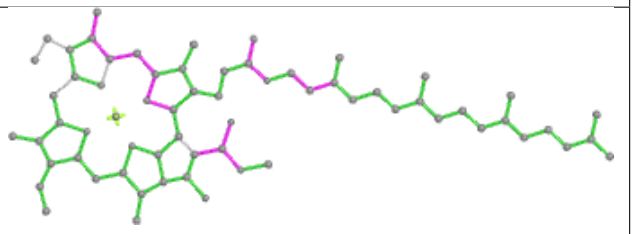
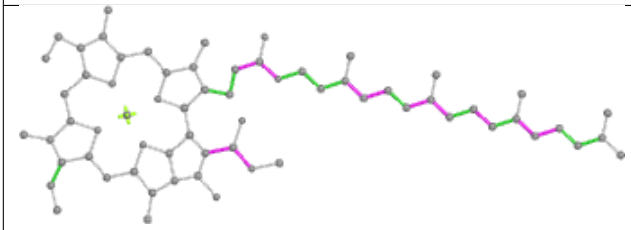


Bond angles



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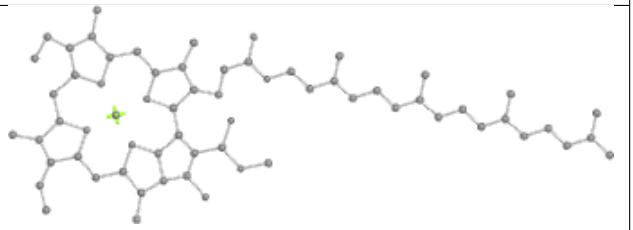
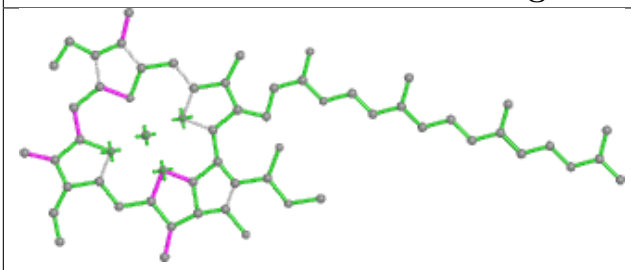
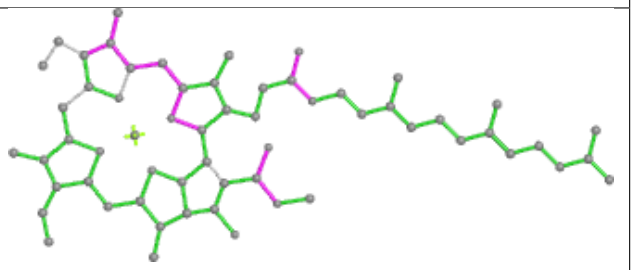


Rings

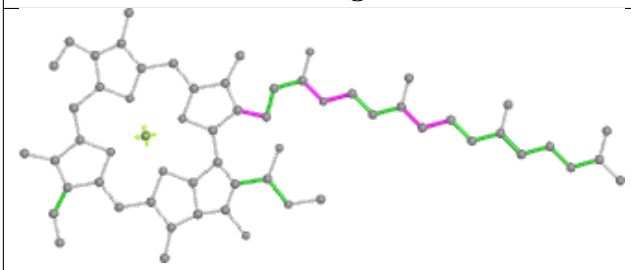
Ligand CLA 8 610



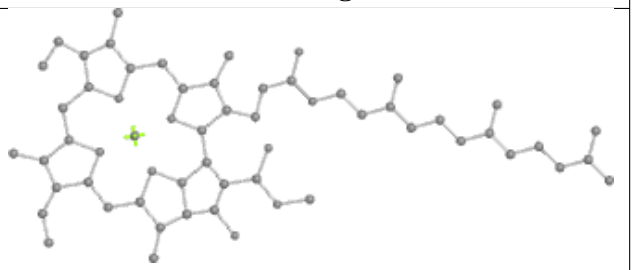
Bond lengths



Bond angles

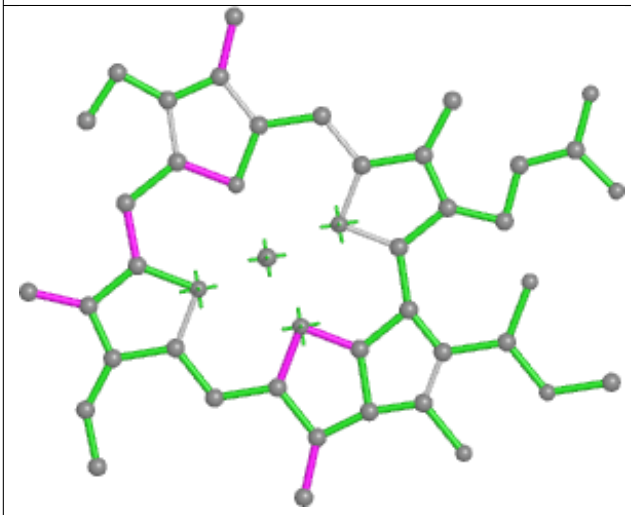


Torsions



Rings

Ligand CLA 4 607



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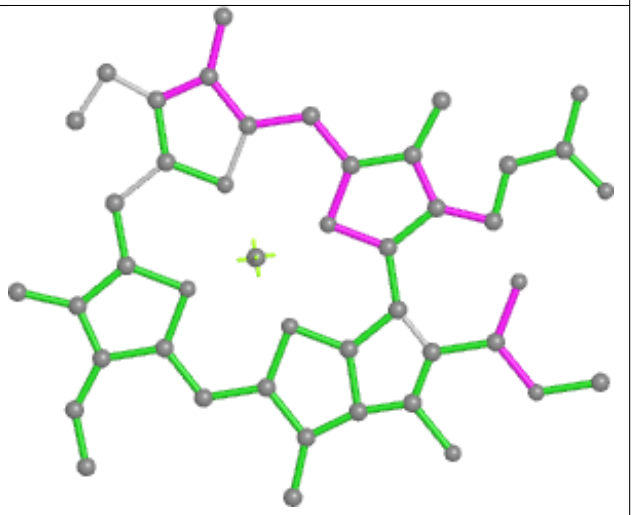

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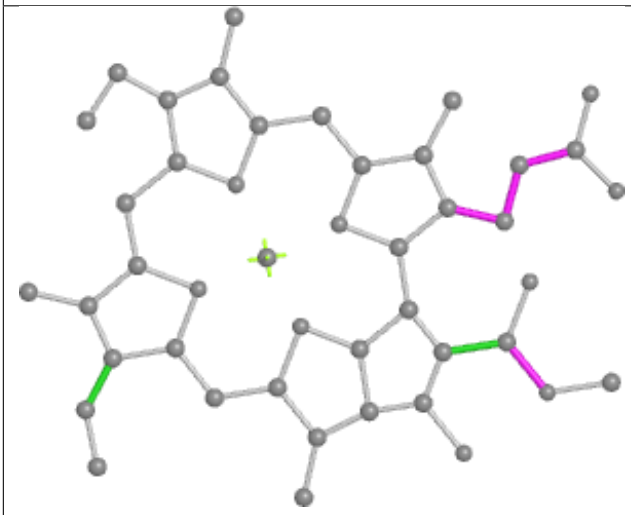

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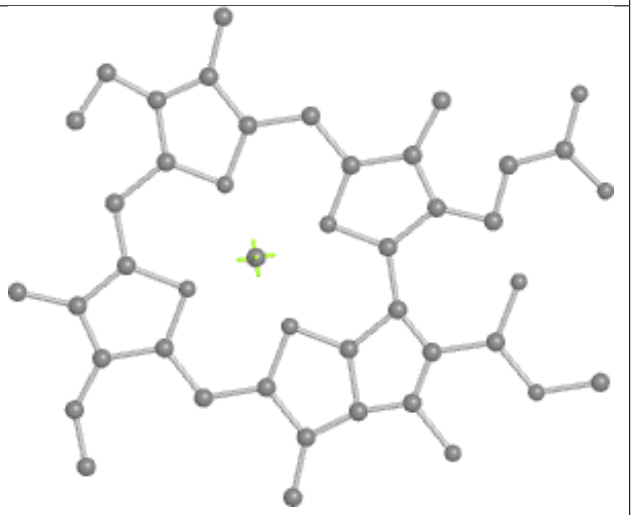
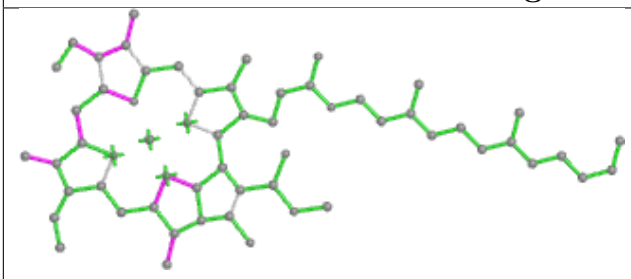
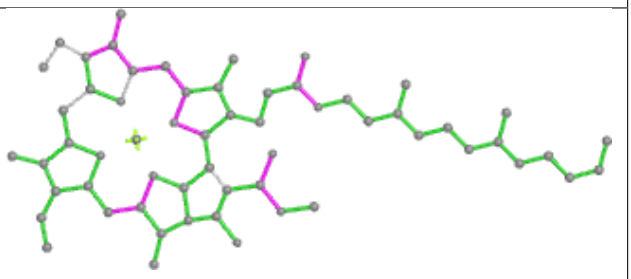
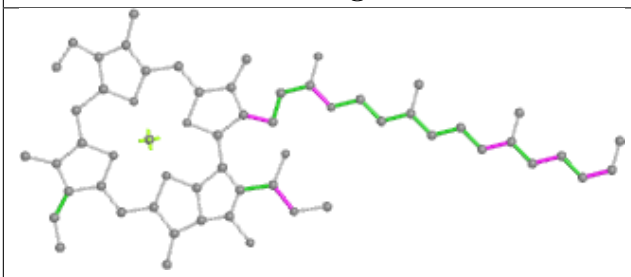
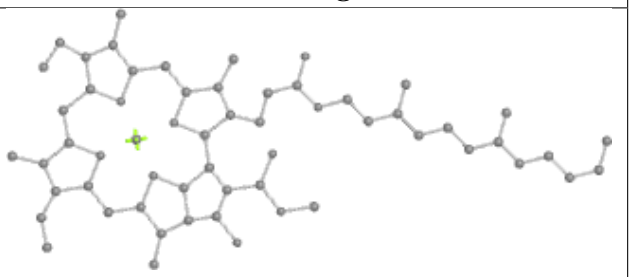
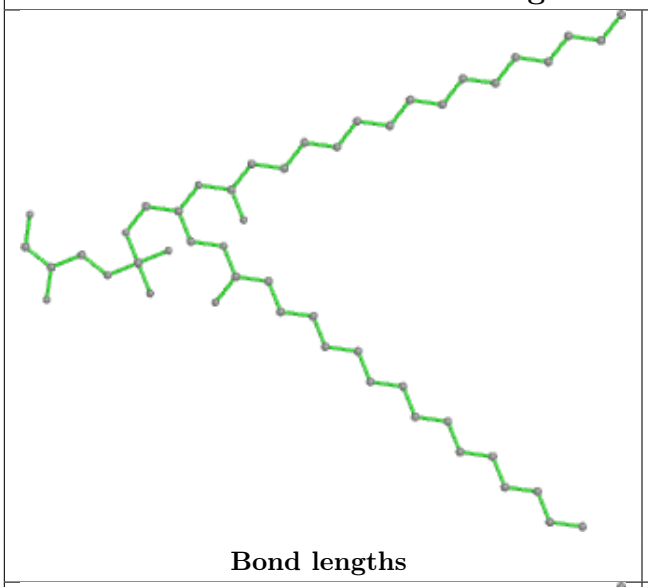


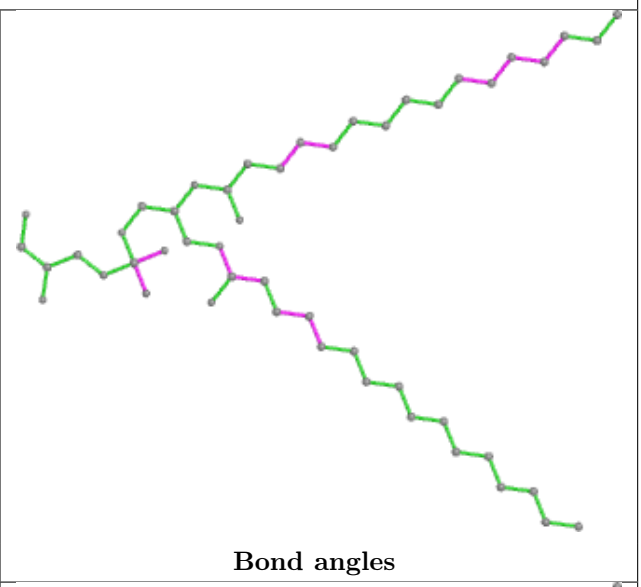
Rings

Ligand CLA B 817	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

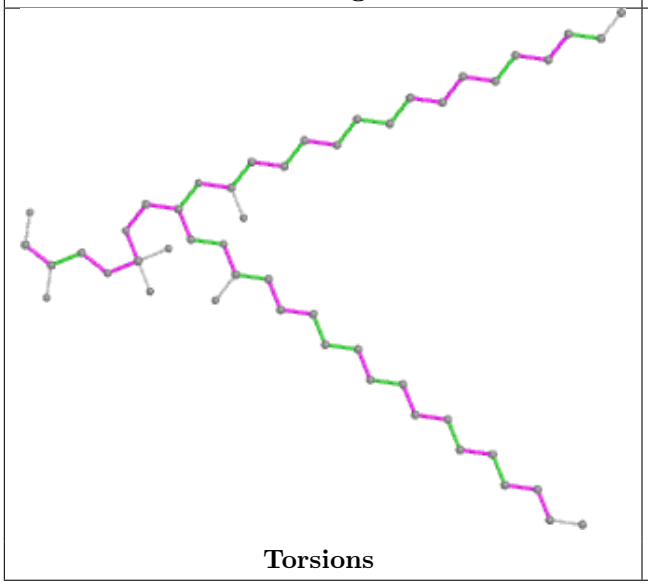
Ligand LHG 5 625



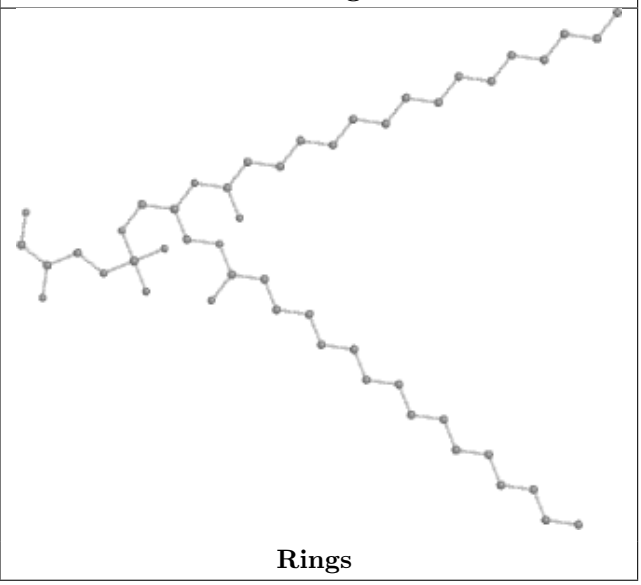
Bond lengths



Bond angles

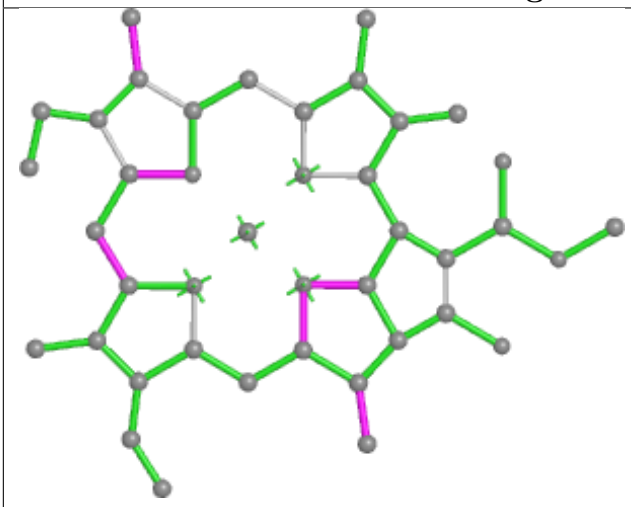


Torsions

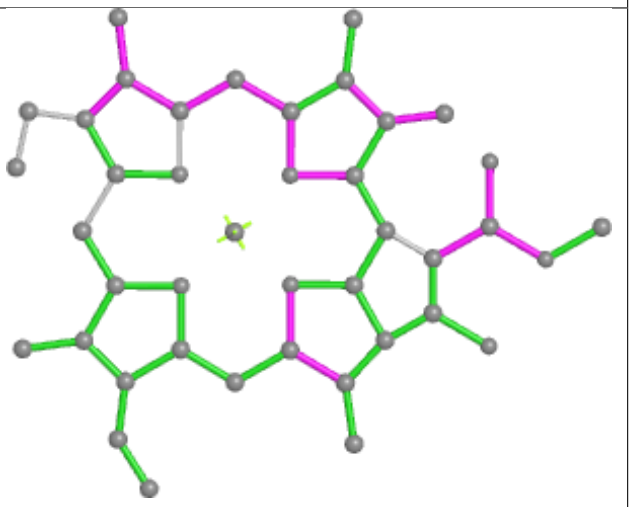


Rings

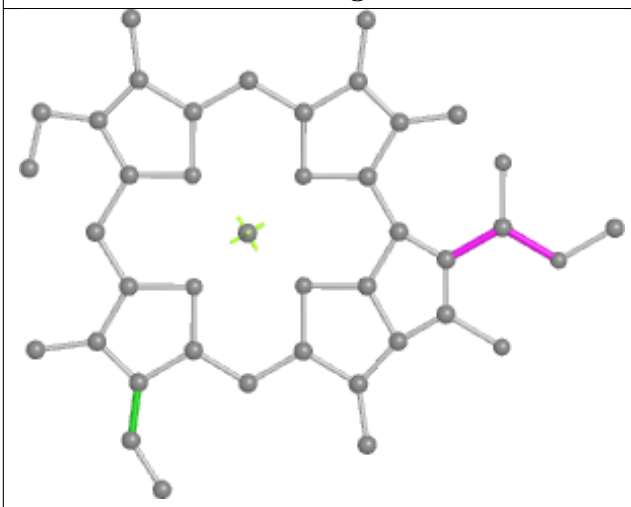
Ligand CLA F 304



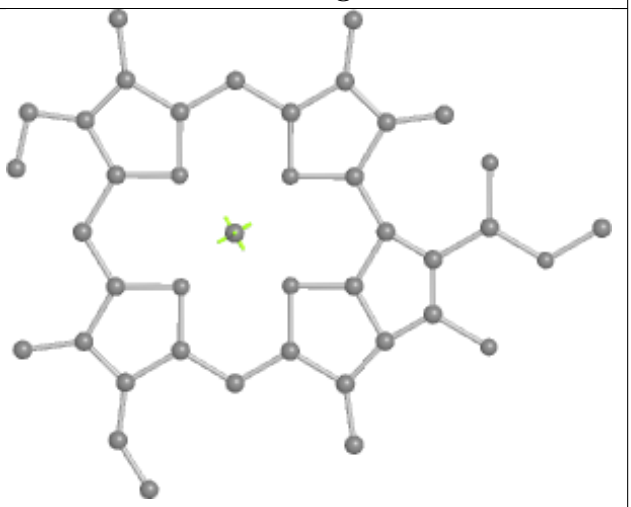
Bond lengths



Bond angles

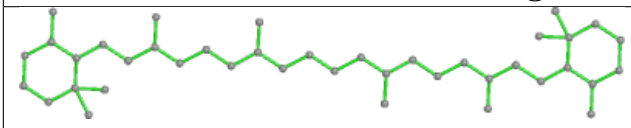


Torsions

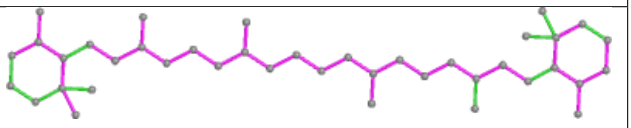


Rings

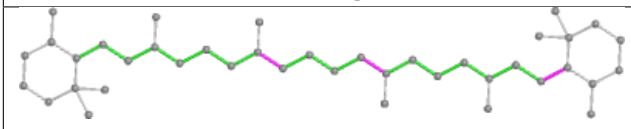
Ligand BCR 3 621



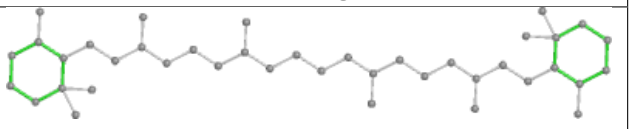
Bond lengths



Bond angles

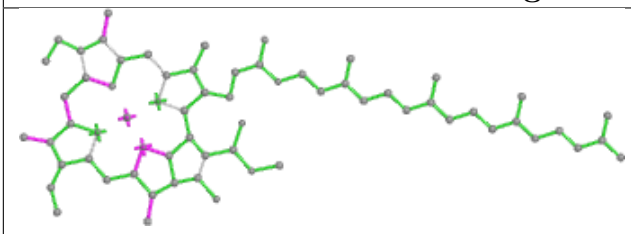


Torsions

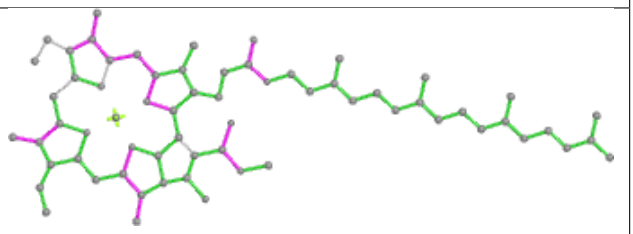


Rings

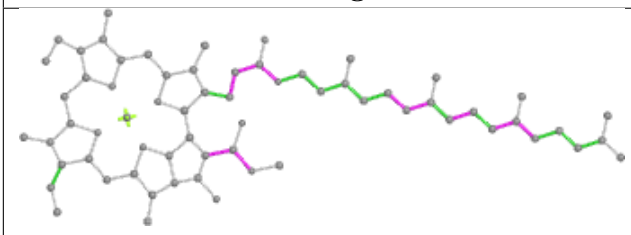
Ligand CLA A 830



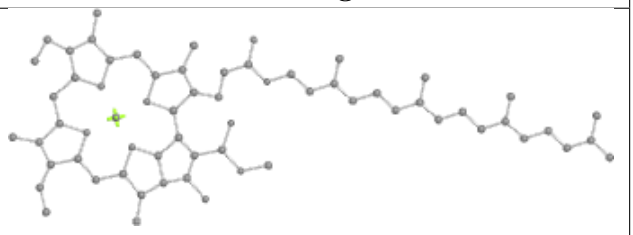
Bond lengths



Bond angles

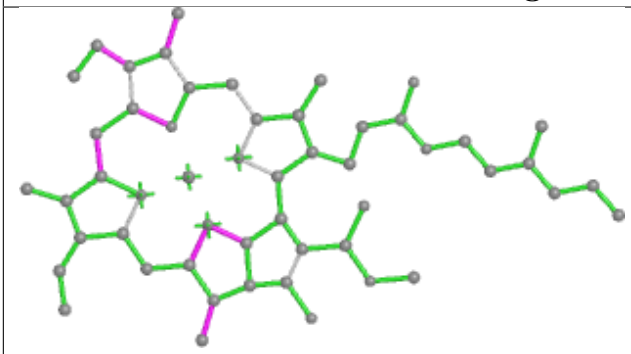


Torsions

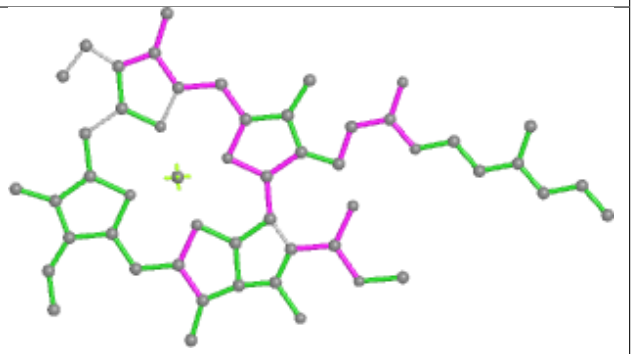


Rings

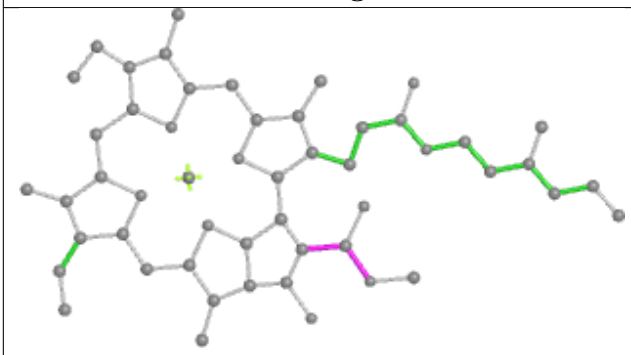
Ligand CLA A 840



Bond lengths



Bond angles



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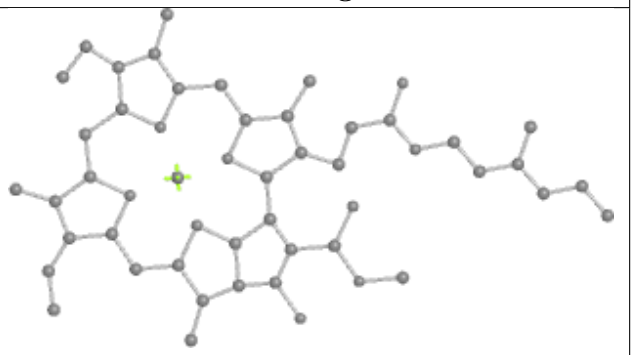
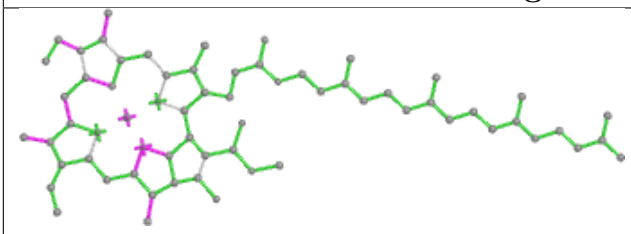
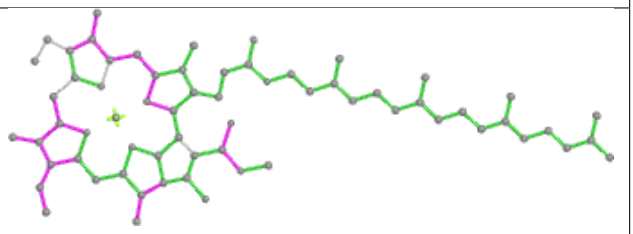


Rings

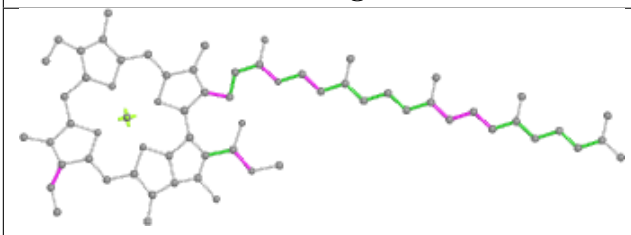
Ligand CLA B 803



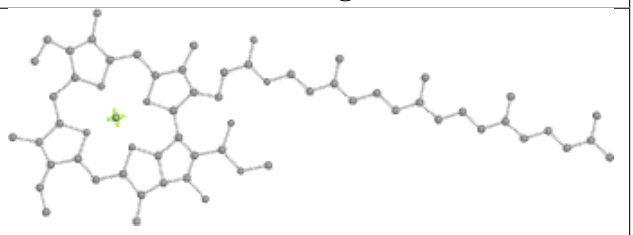
Bond lengths



Bond angles

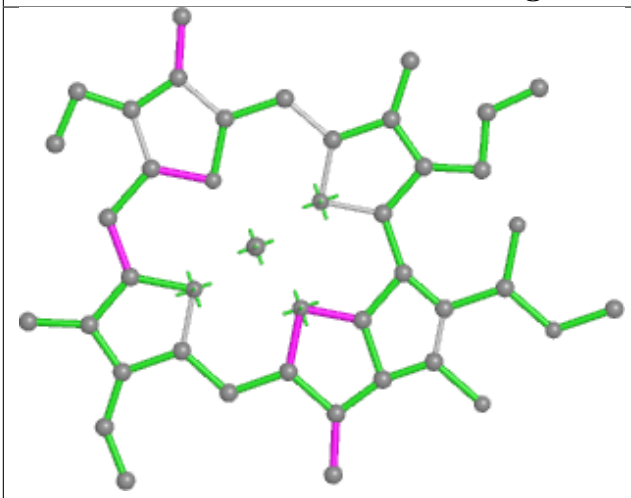


Torsions

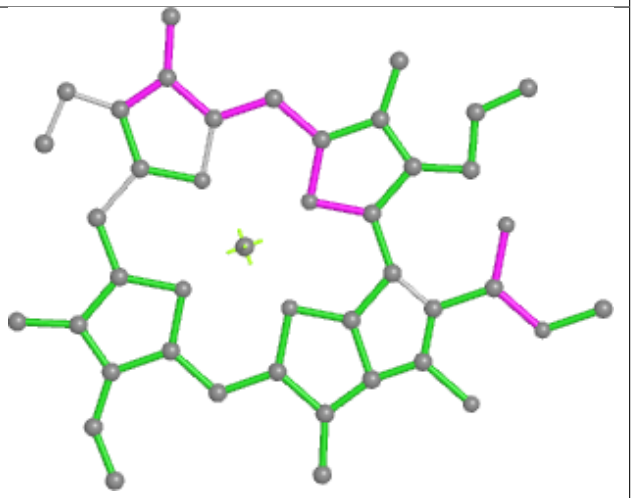


Rings

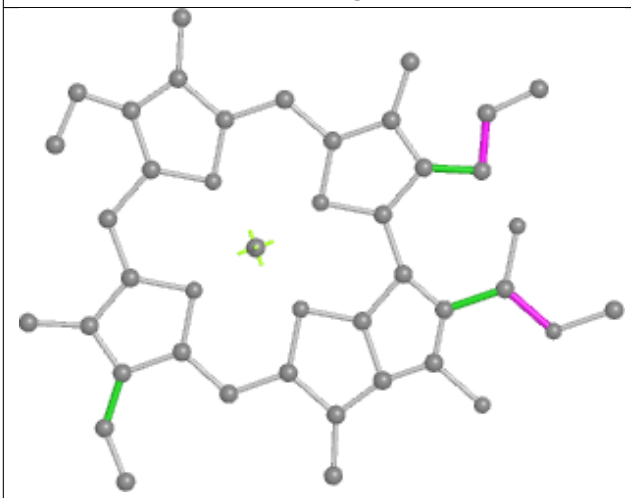
Ligand CLA B 812



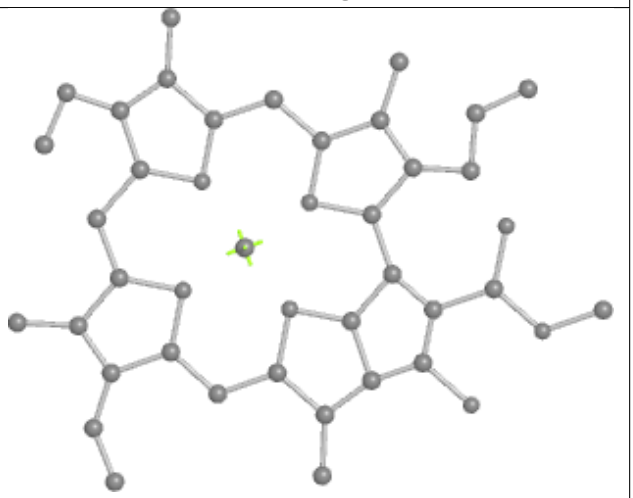
Bond lengths



Bond angles

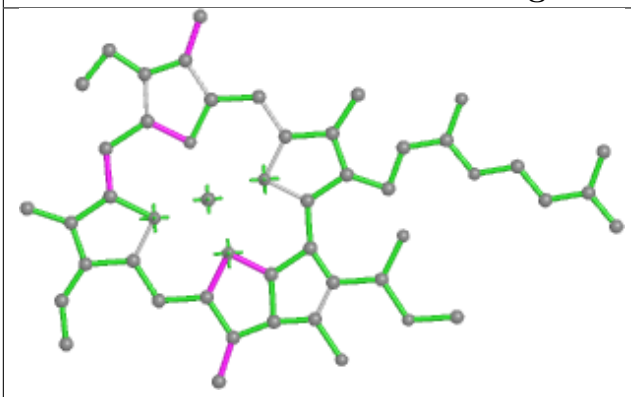


Torsions

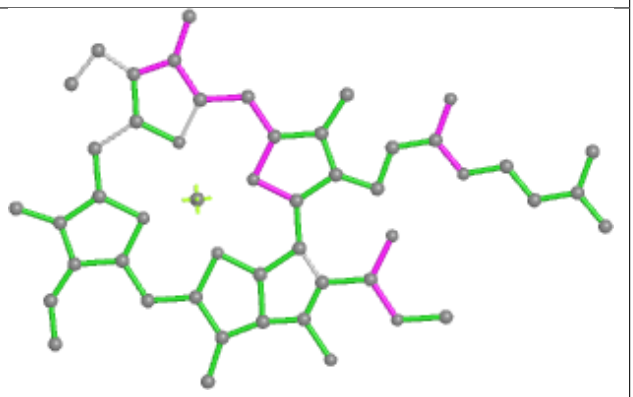


Rings

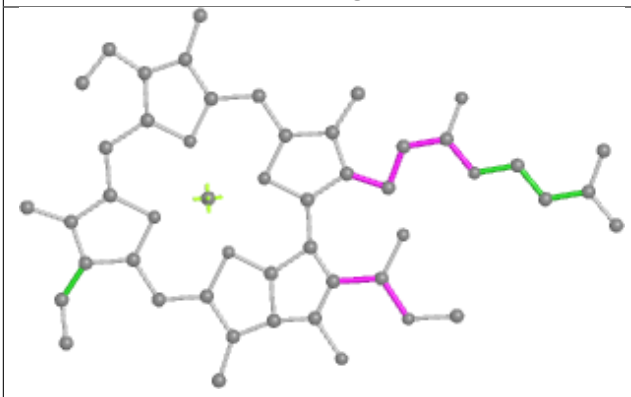
Ligand CLA 8 604



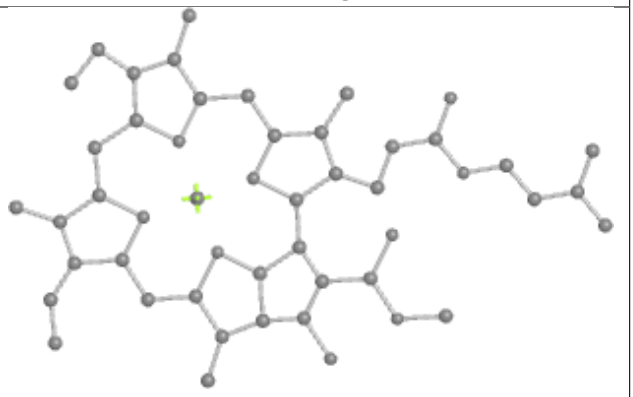
Bond lengths



Bond angles

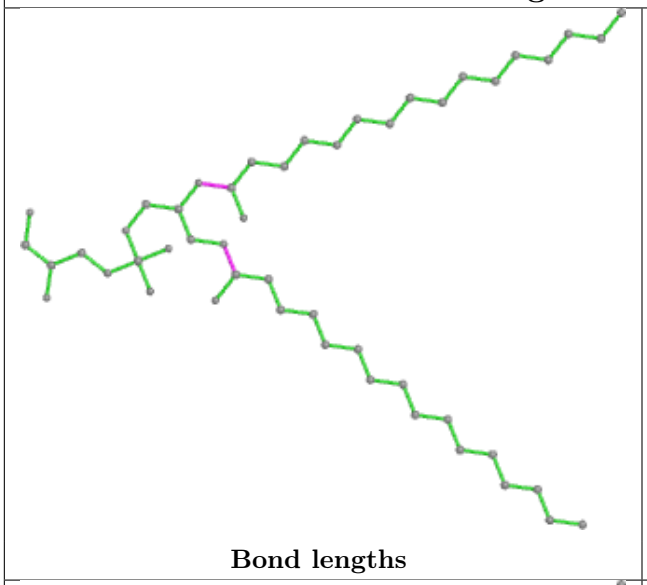


Torsions



Rings

Ligand LHG 8 622



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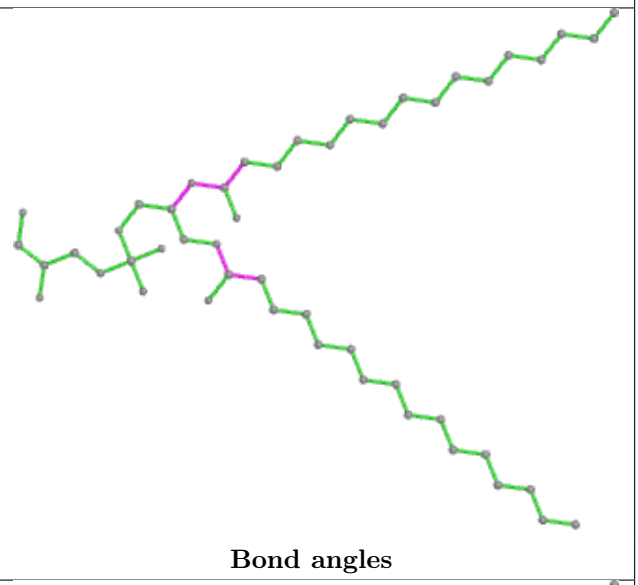
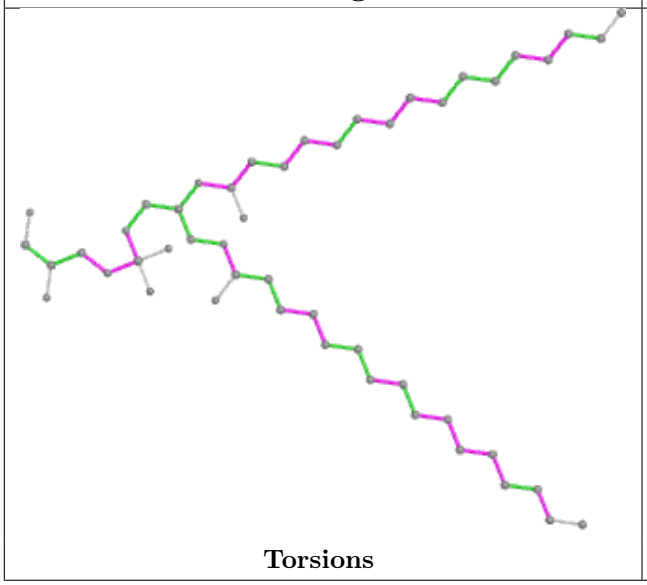


Bond angles



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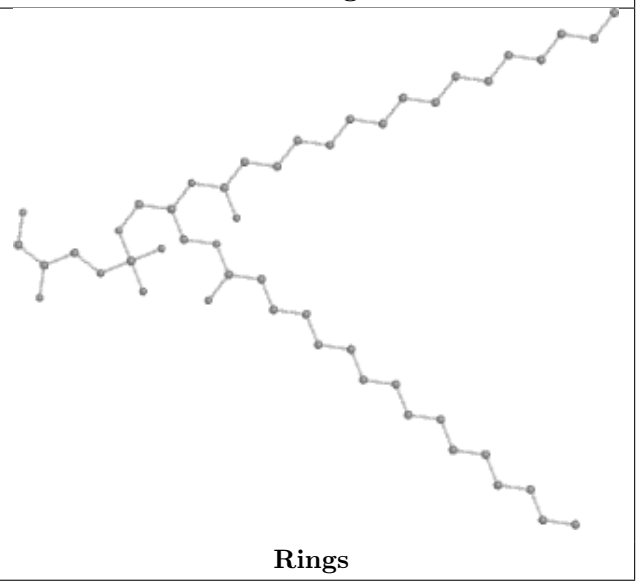
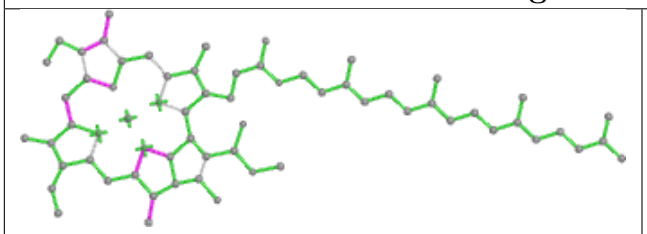
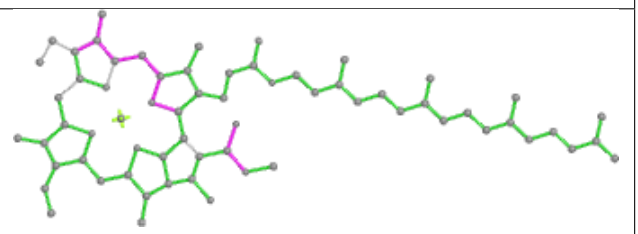


Rings

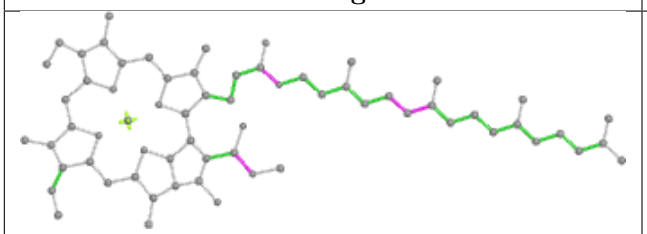
Ligand CLA 3 604



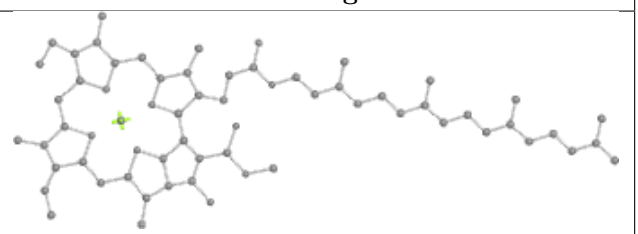
Bond lengths



Bond angles

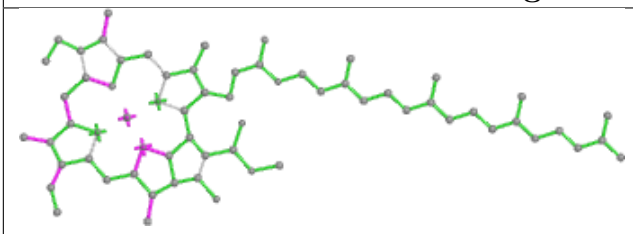


Torsions

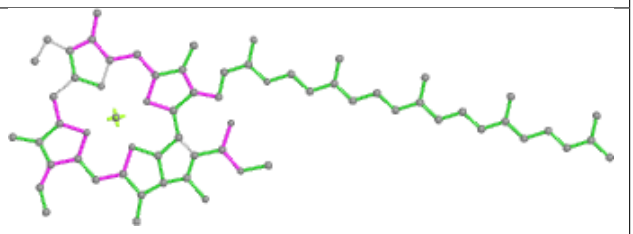


Rings

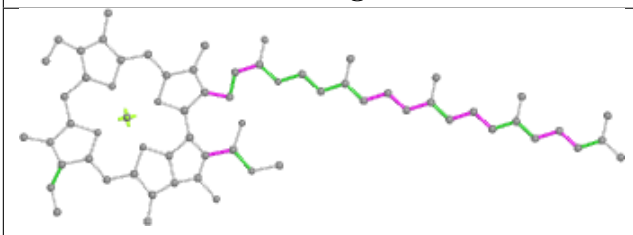
Ligand CLA A 806



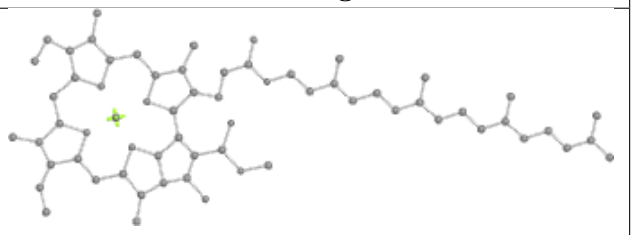
Bond lengths



Bond angles

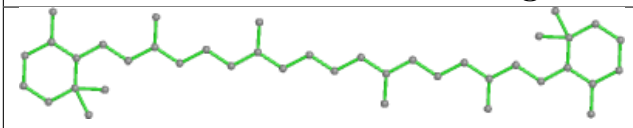


Torsions

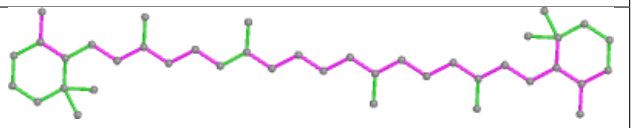


Rings

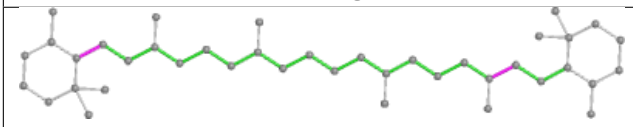
Ligand BCR K 207



Bond lengths



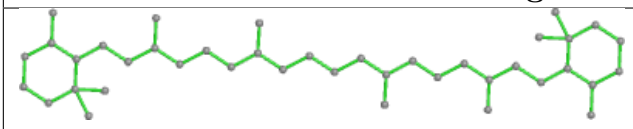
Bond angles



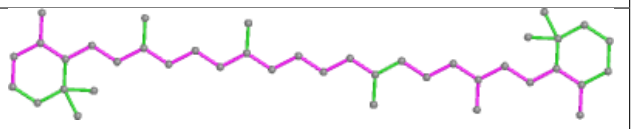
Torsions

Rings

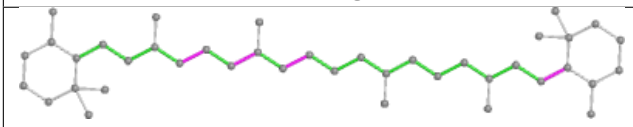
Ligand BCR 6 622



Bond lengths



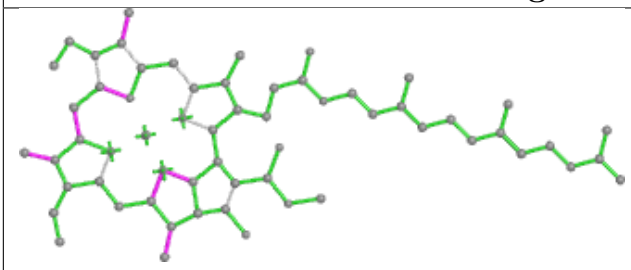
Bond angles



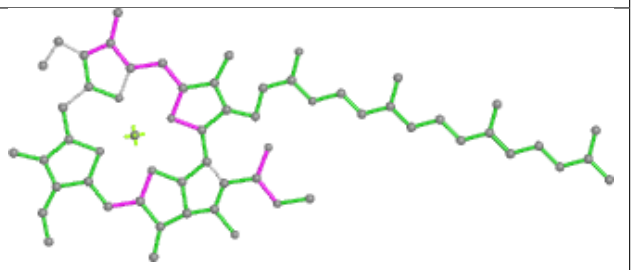
Torsions

Rings

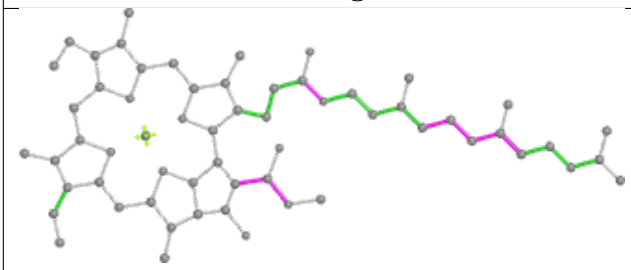
Ligand CLA 6 614



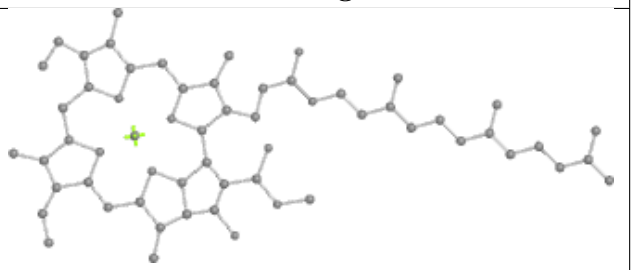
Bond lengths



Bond angles

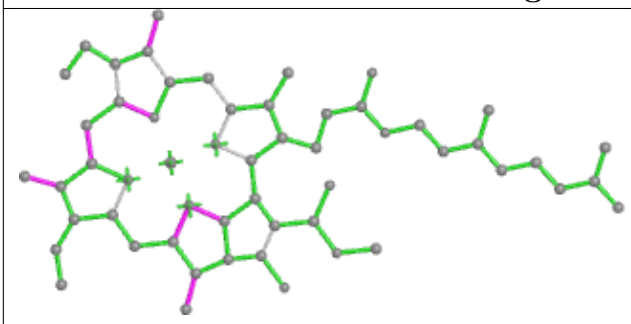


Torsions

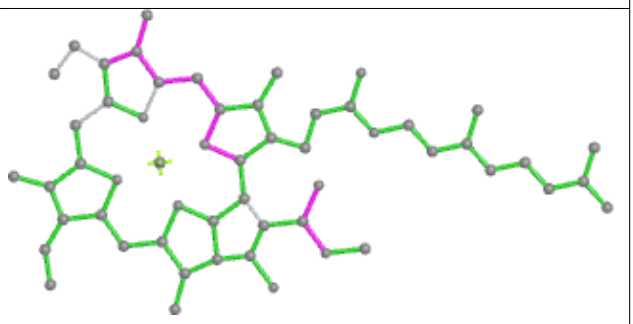


Rings

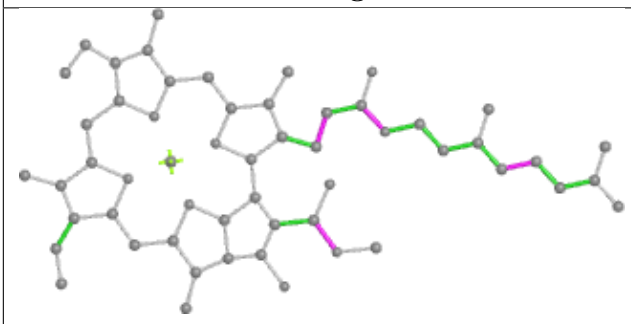
Ligand CLA B 819



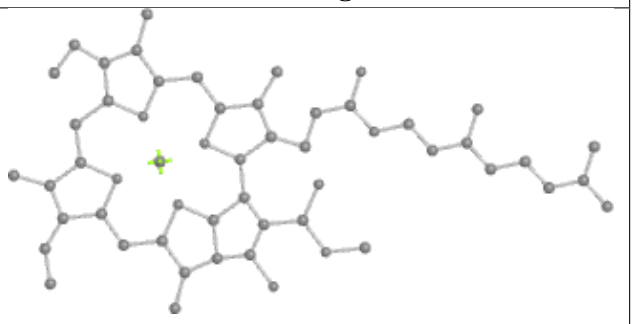
Bond lengths



Bond angles

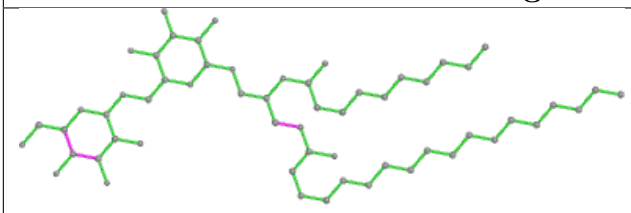


Torsions

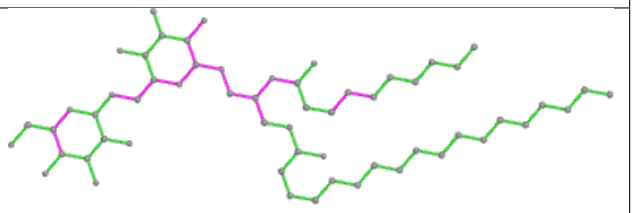


Rings

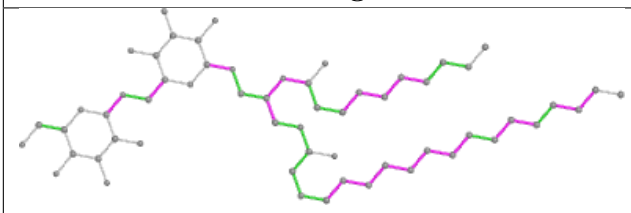
Ligand DGD J 103



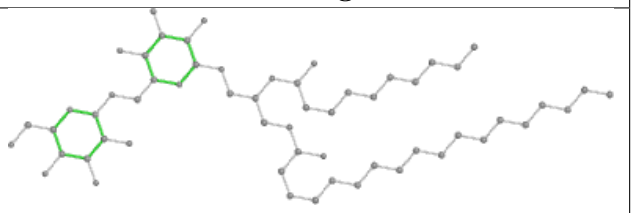
Bond lengths



Bond angles

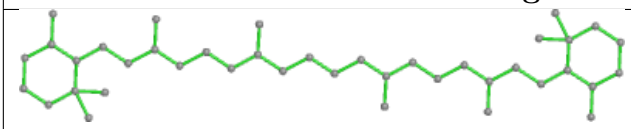


Torsions

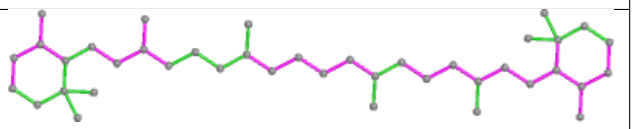


Rings

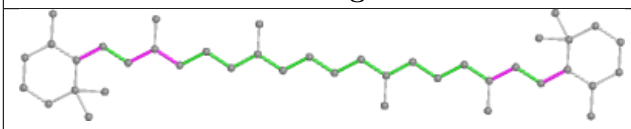
Ligand BCR B 844



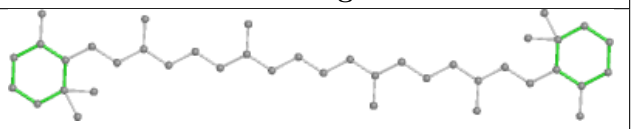
Bond lengths



Bond angles

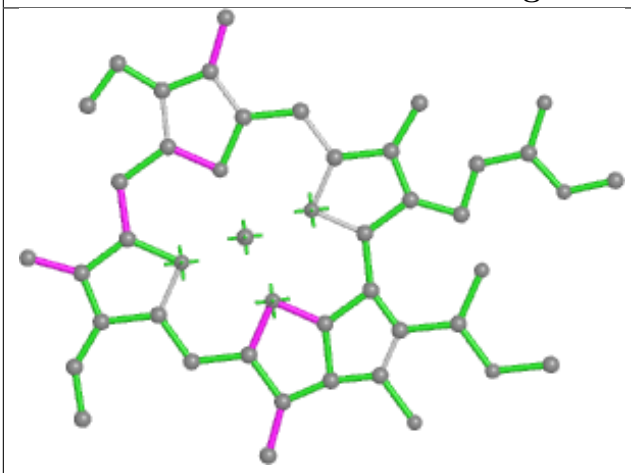


Torsions

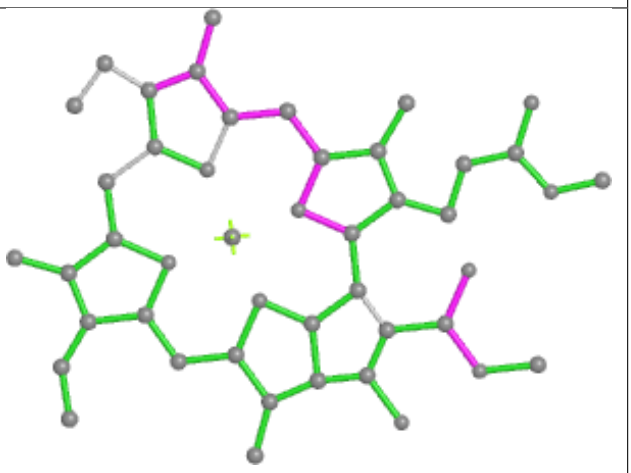


Rings

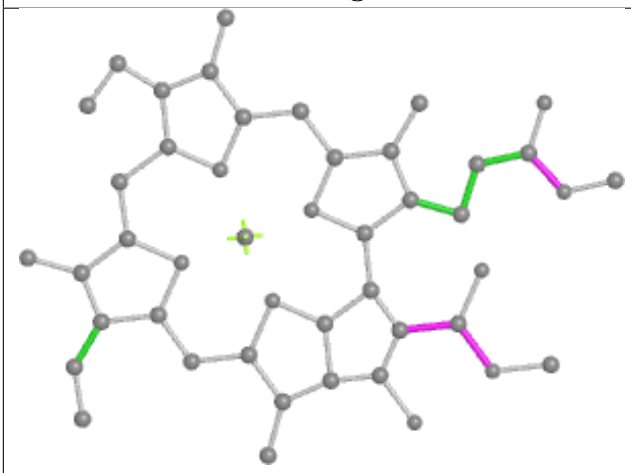
Ligand CLA K 204



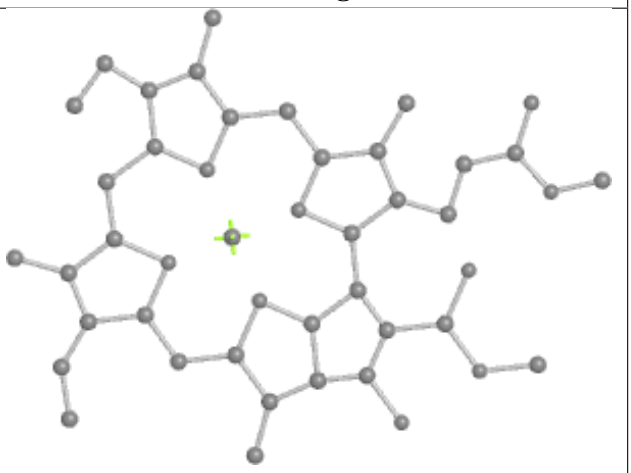
Bond lengths



Bond angles

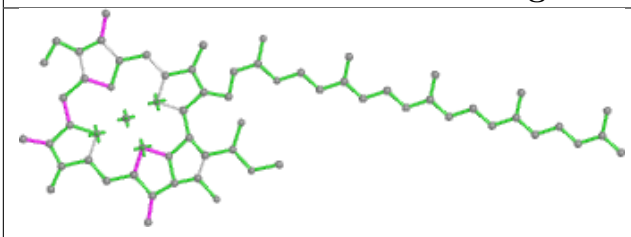


Torsions

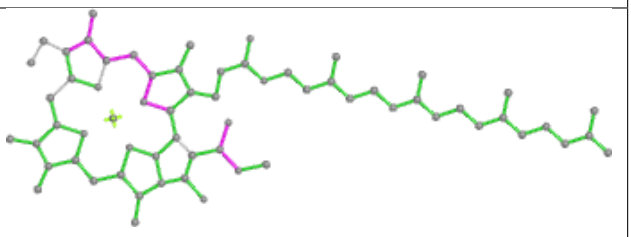


Rings

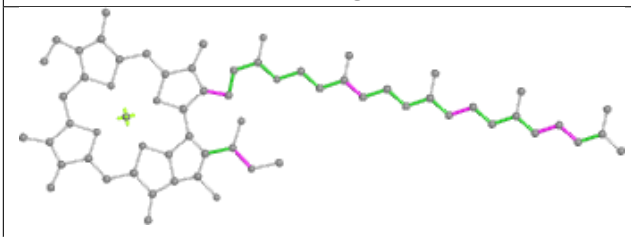
Ligand CLA 8 606



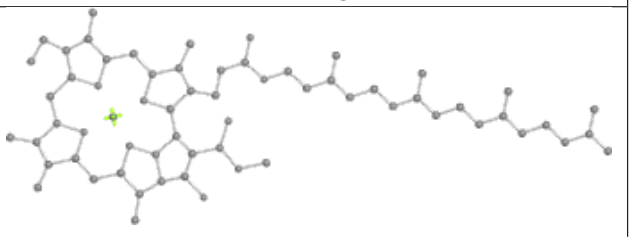
Bond lengths



Bond angles

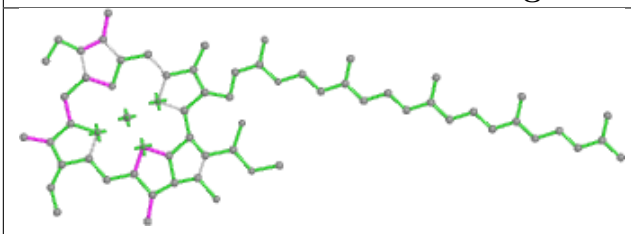


Torsions

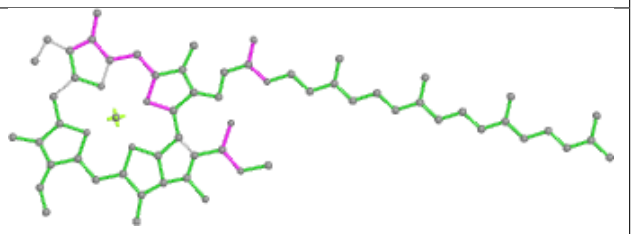


Rings

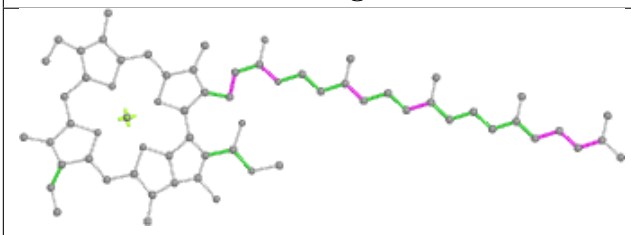
Ligand CLA A 822



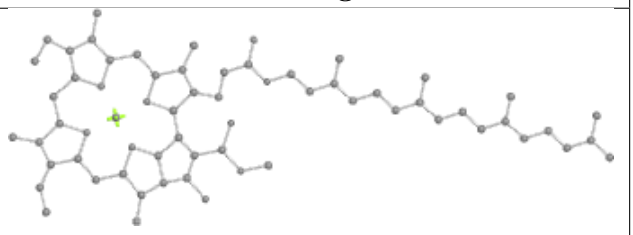
Bond lengths



Bond angles

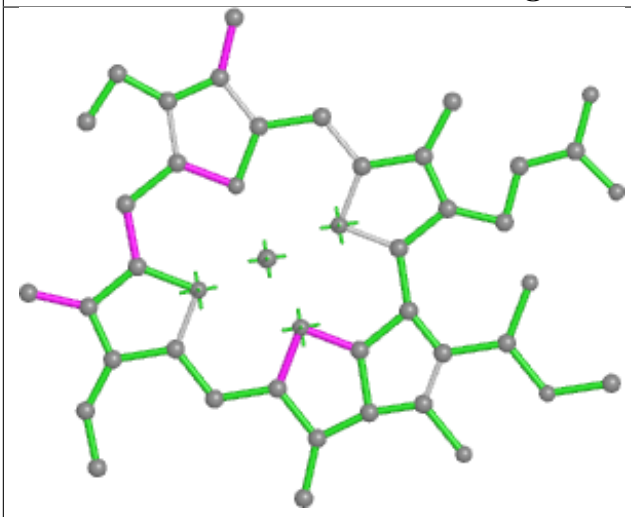


Torsions

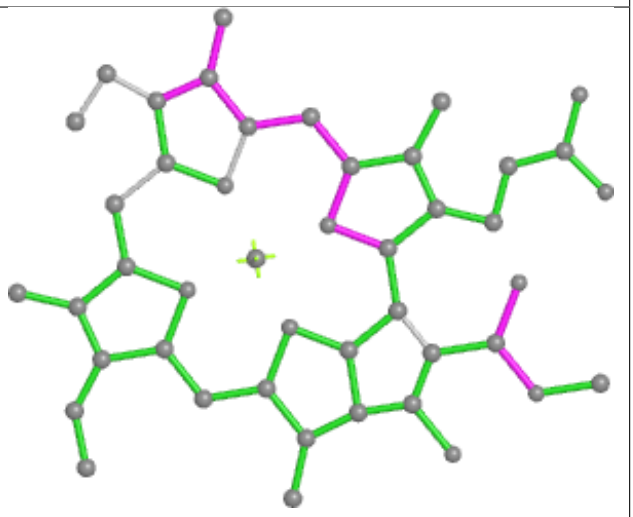


Rings

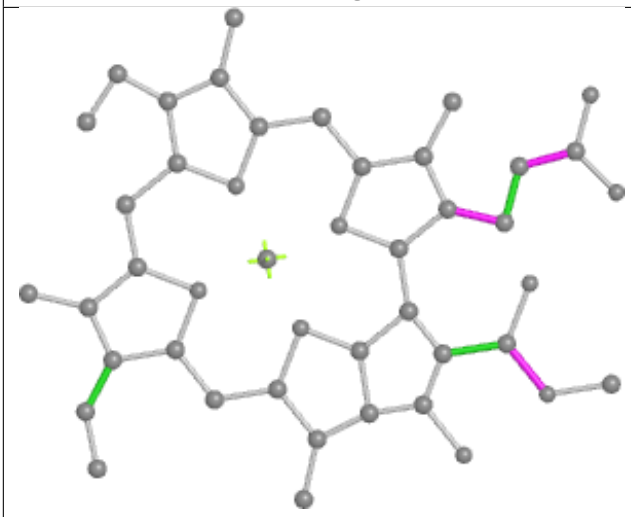
Ligand CLA B 823



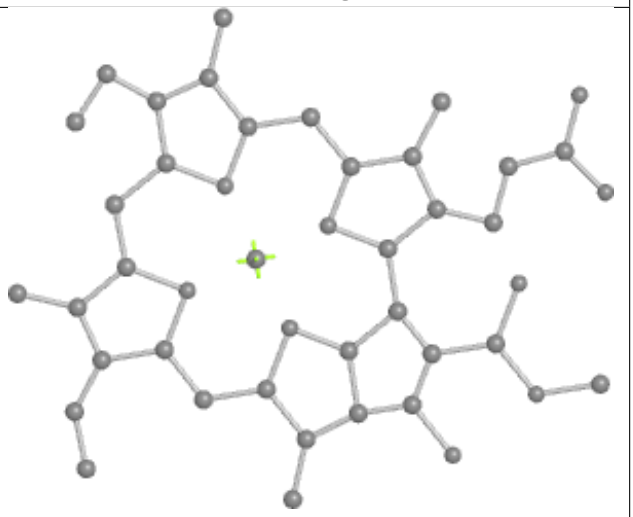
Bond lengths



Bond angles

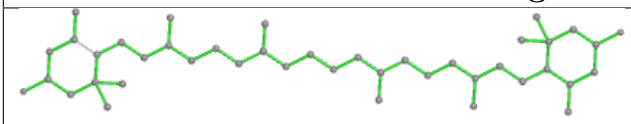


Torsions

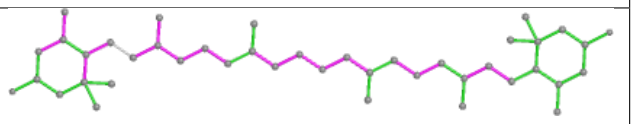


Rings

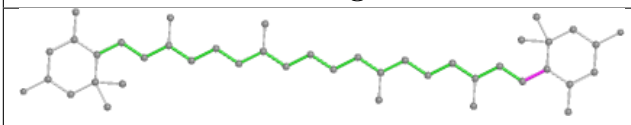
Ligand LUT 8 619



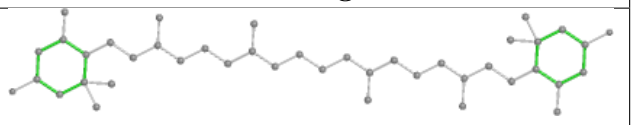
Bond lengths



Bond angles

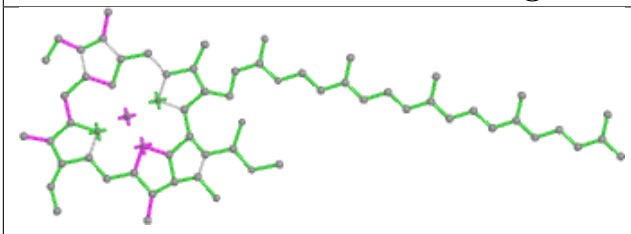


Torsions

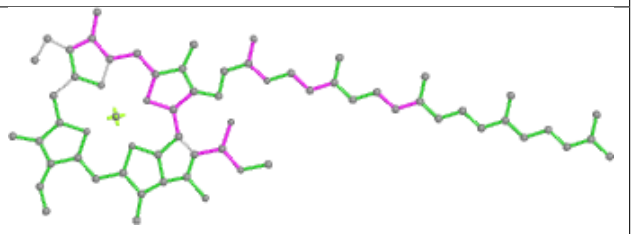


Rings

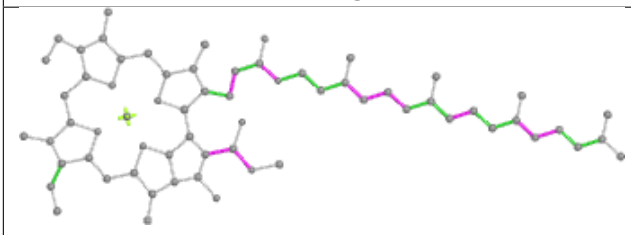
Ligand CLA A 854



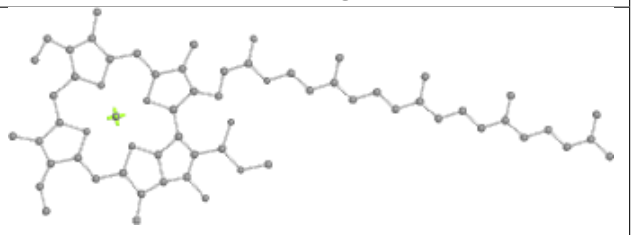
Bond lengths



Bond angles

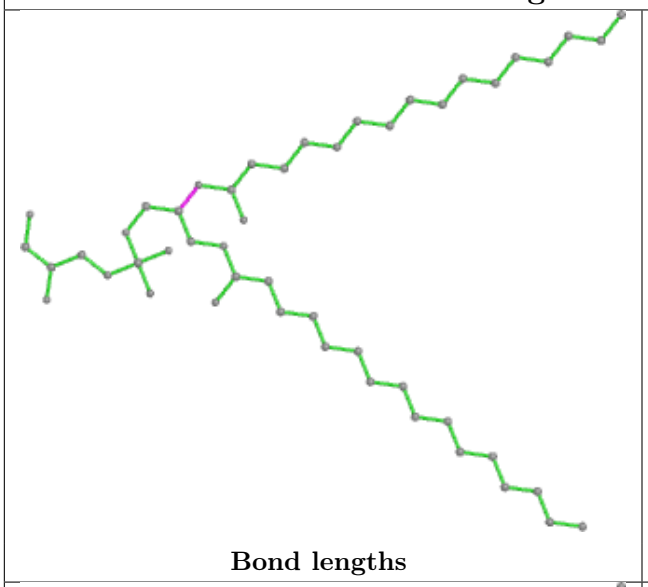


Torsions

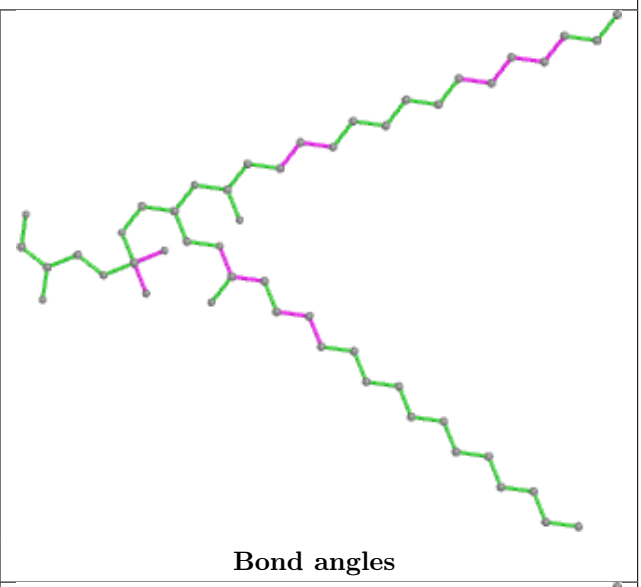


Rings

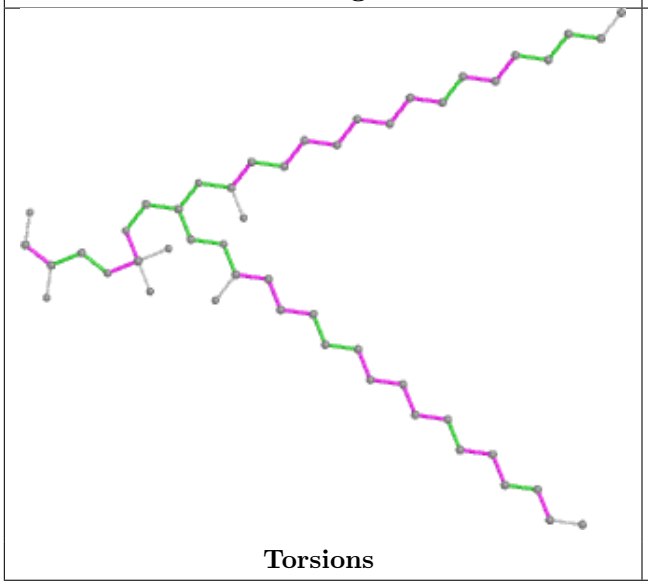
Ligand LHG 5 623



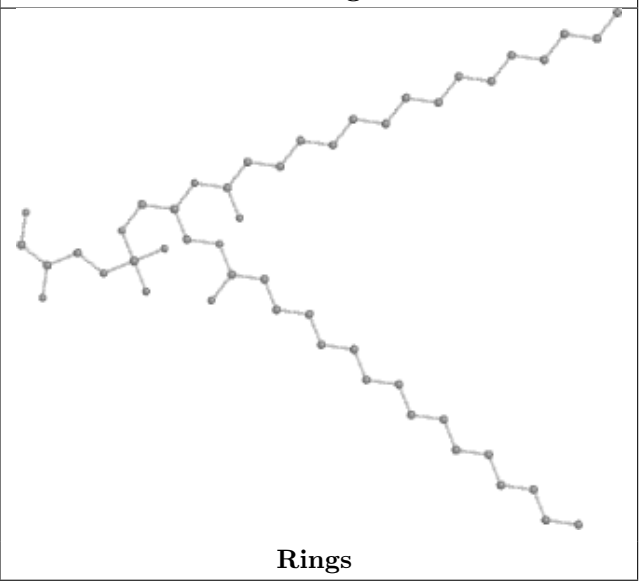
Bond lengths



Bond angles

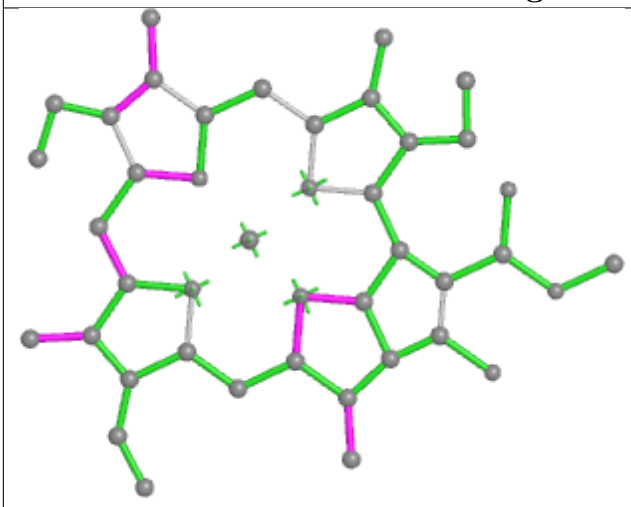


Torsions

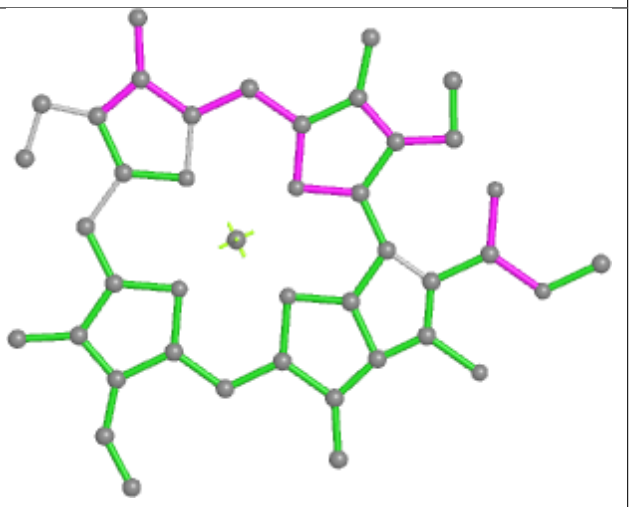


Rings

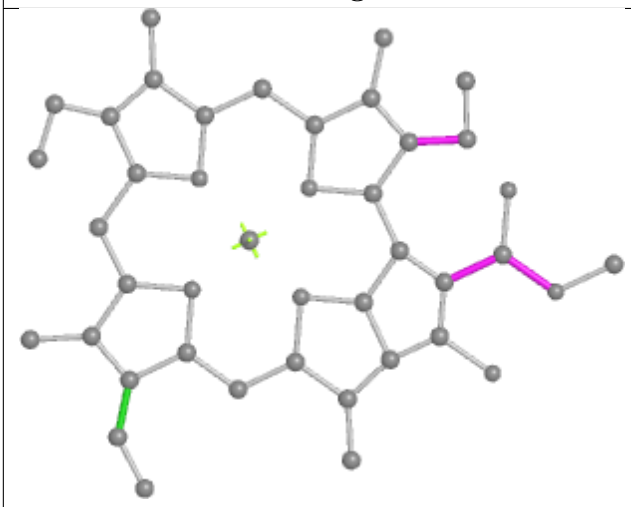
Ligand CLA F 303



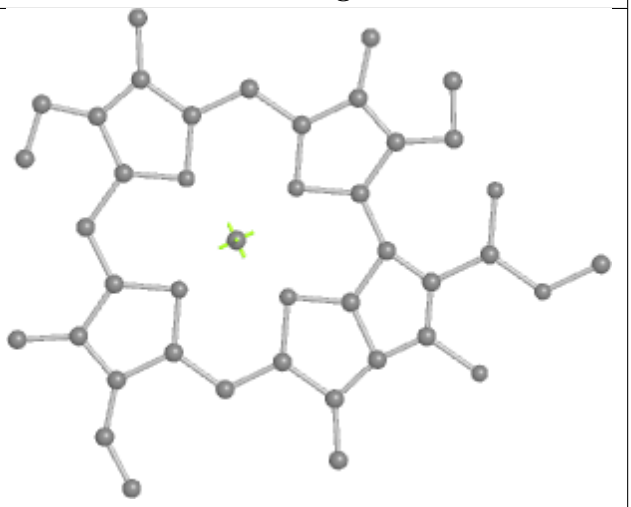
Bond lengths



Bond angles

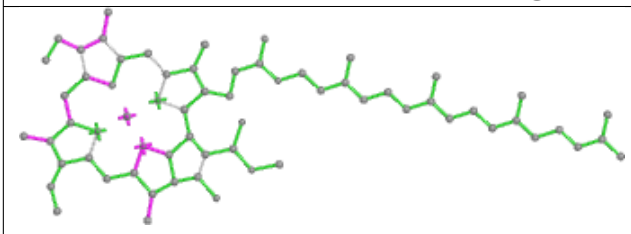


Torsions

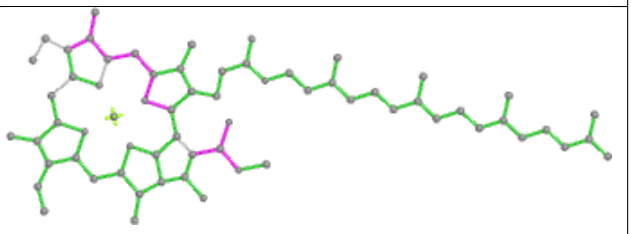


Rings

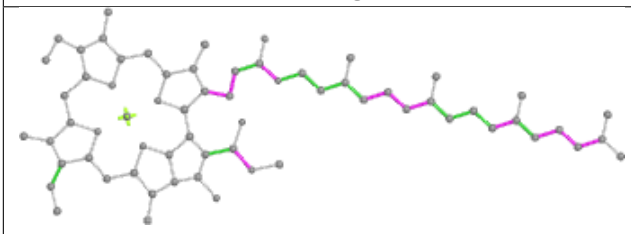
Ligand CLA 4 601



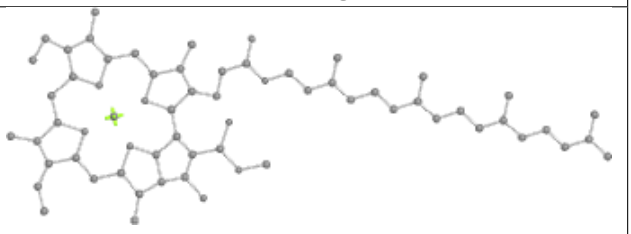
Bond lengths



Bond angles

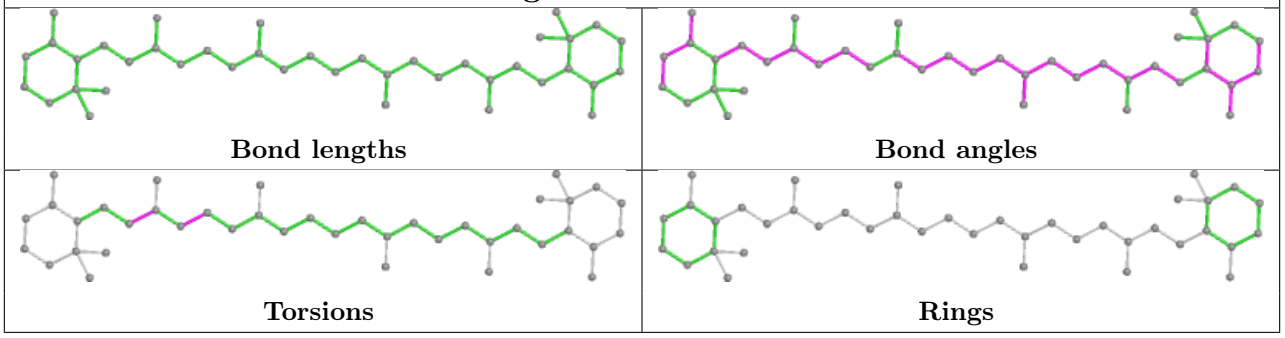


Torsions

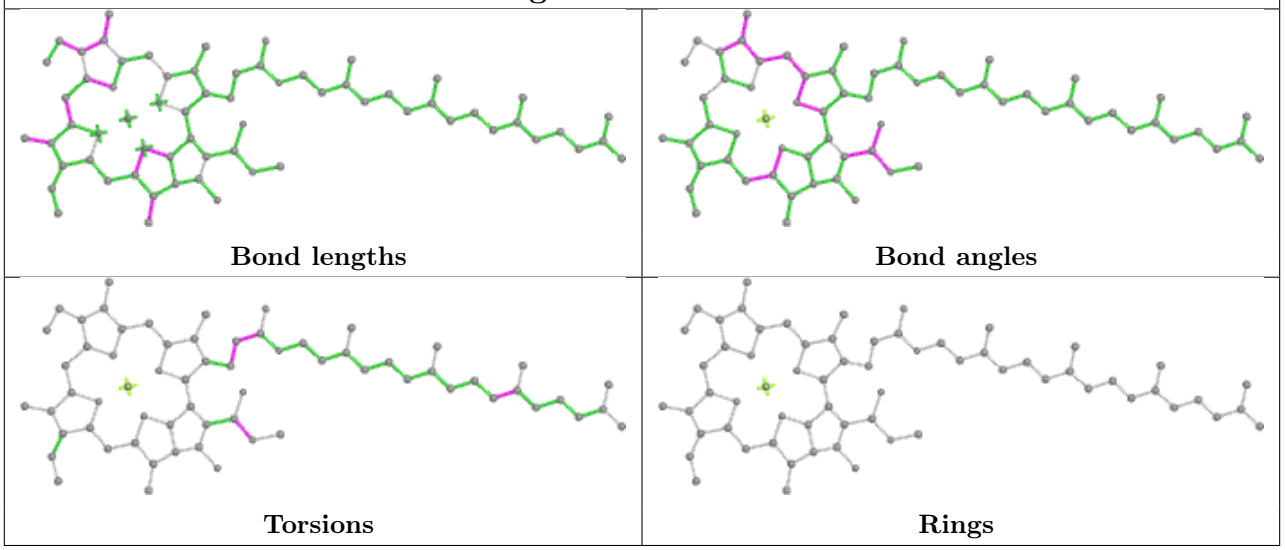


Rings

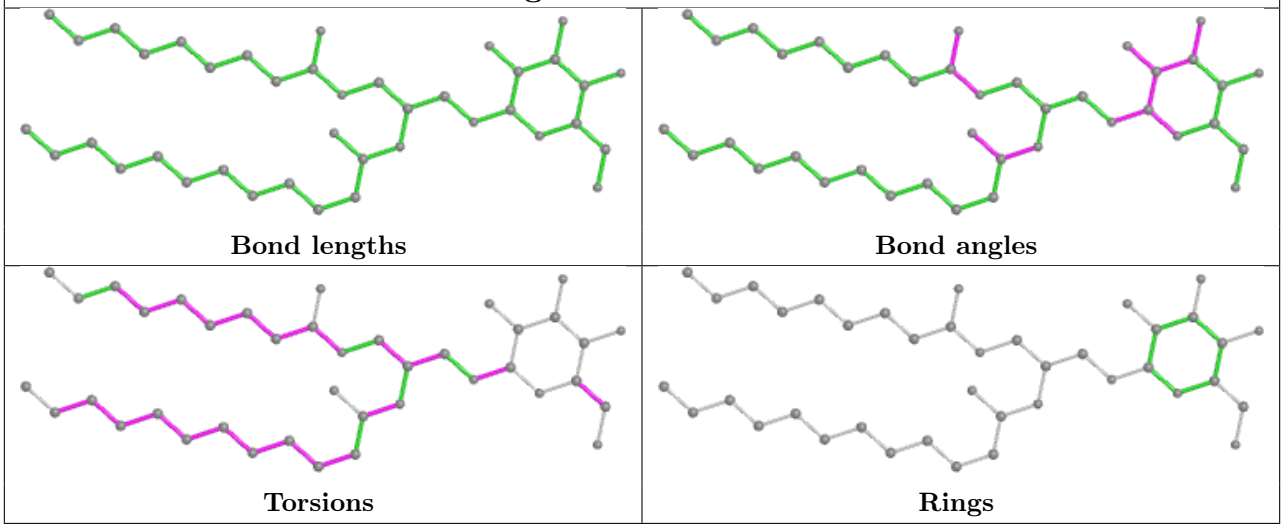
Ligand BCR A 849



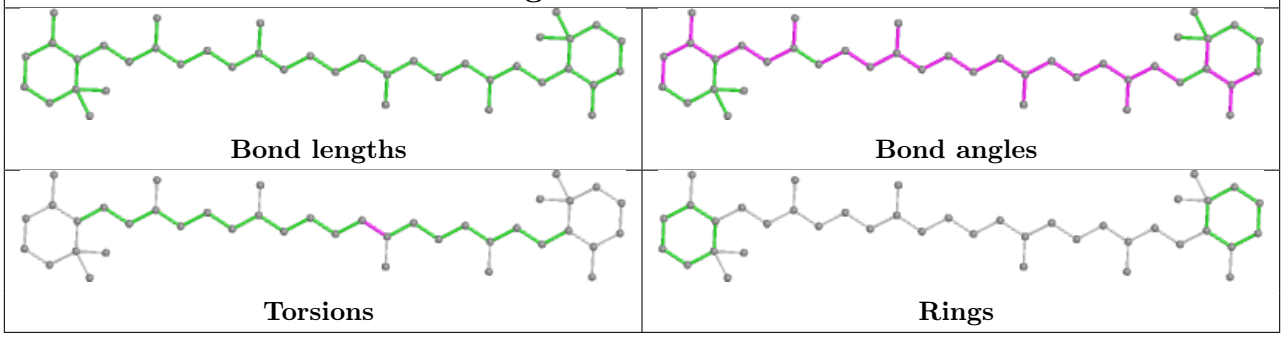
Ligand CLA 6 602



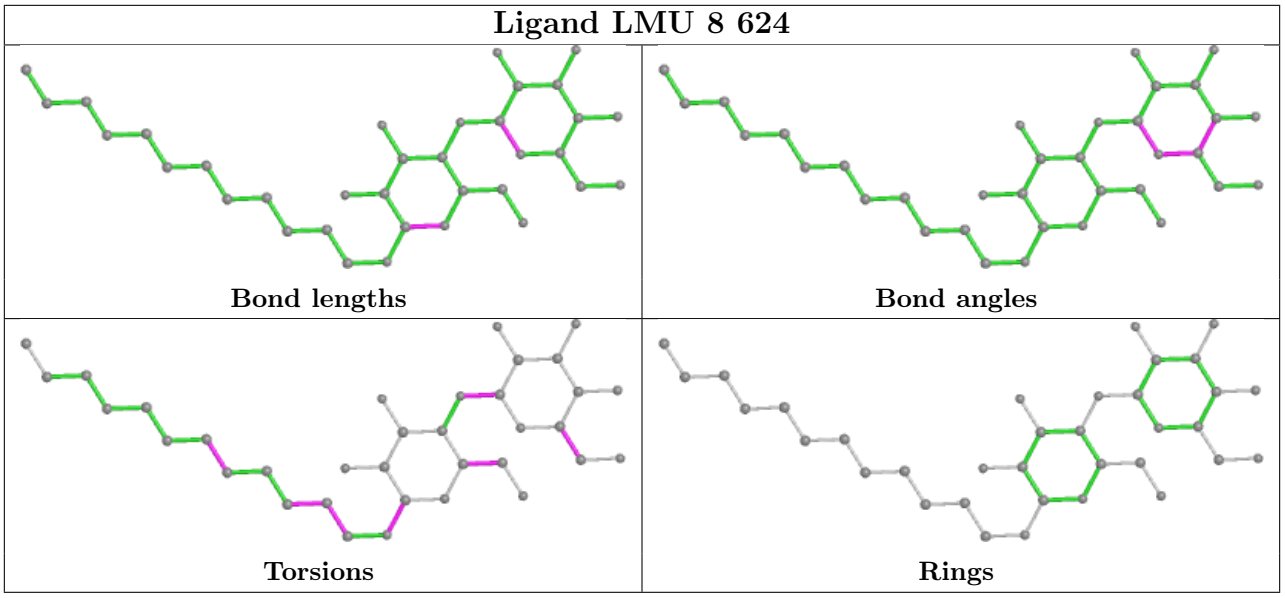
Ligand LMG 5 626



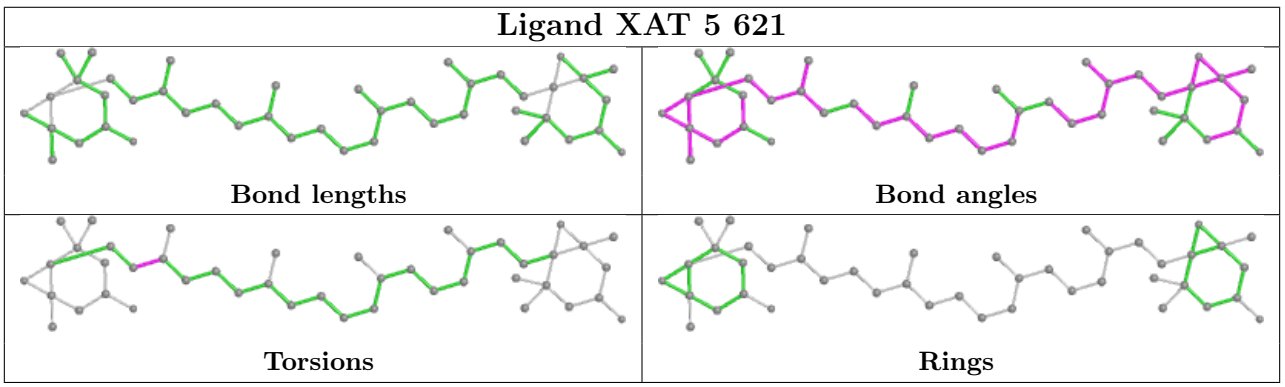
Ligand BCR F 305



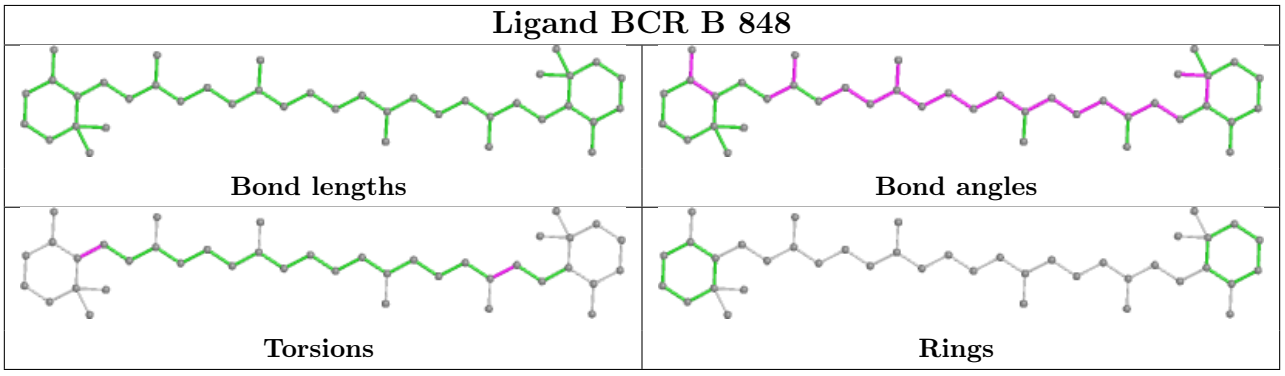
Ligand LMU 8 624



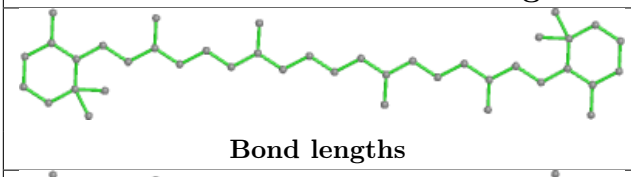
Ligand XAT 5 621



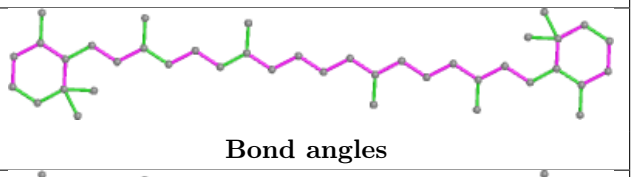
Ligand BCR B 848



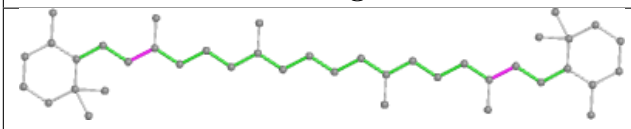
Ligand BCR B 801



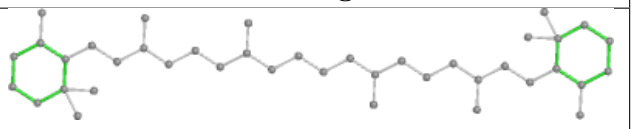
Bond lengths



Bond angles

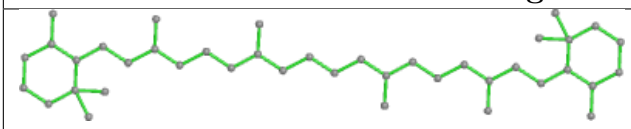


Torsions

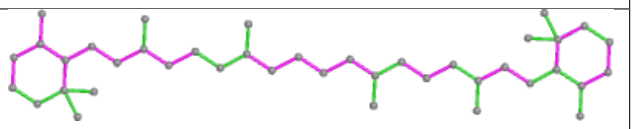


Rings

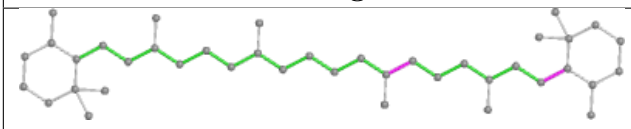
Ligand BCR 4 621



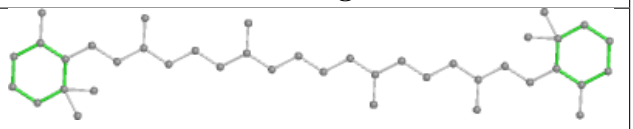
Bond lengths



Bond angles

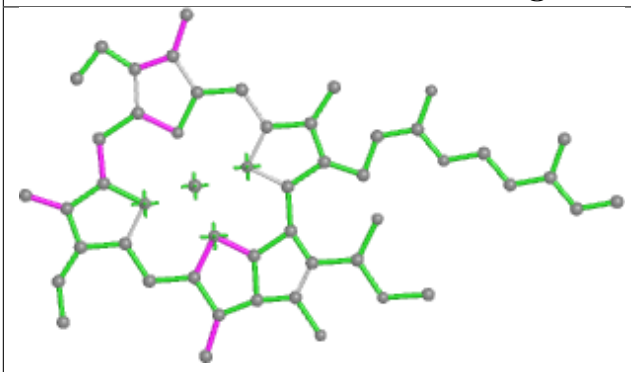


Torsions

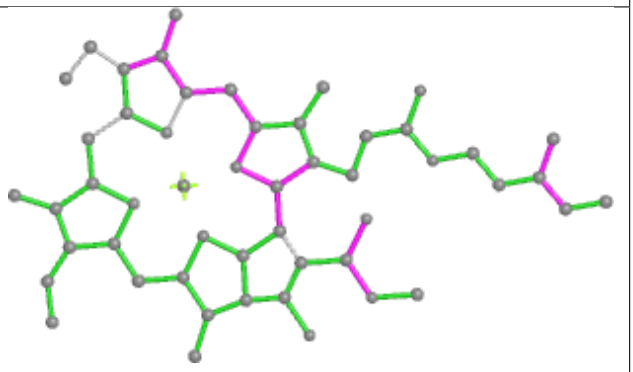


Rings

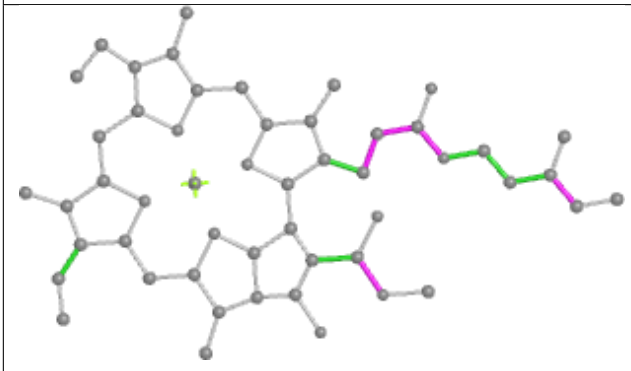
Ligand CLA 8 608



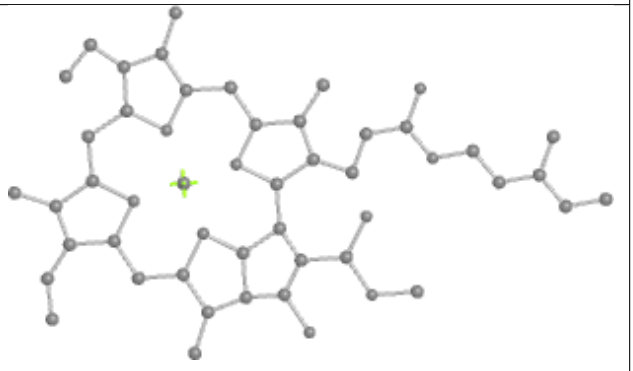
Bond lengths



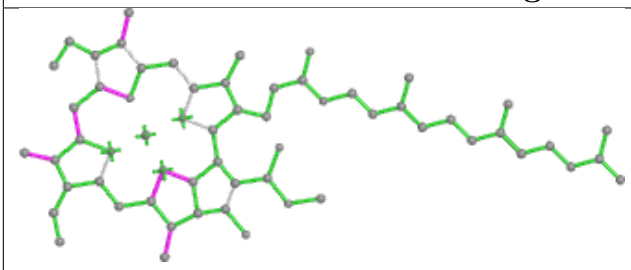
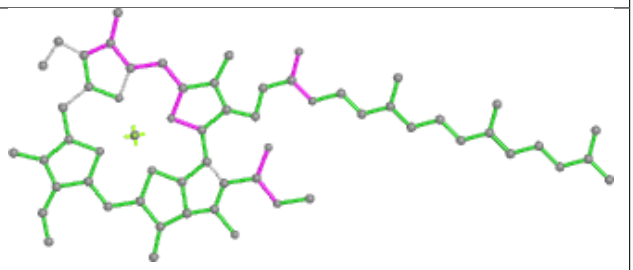
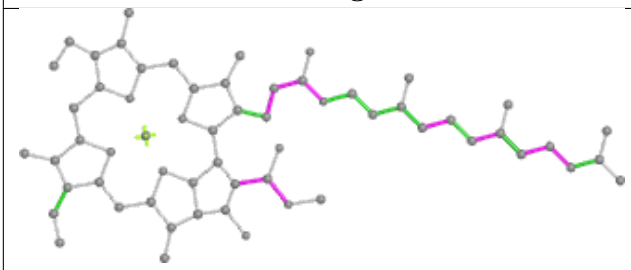
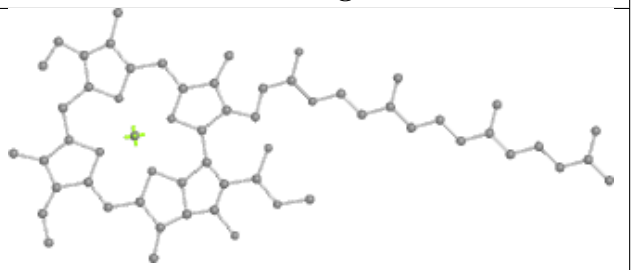
Bond angles

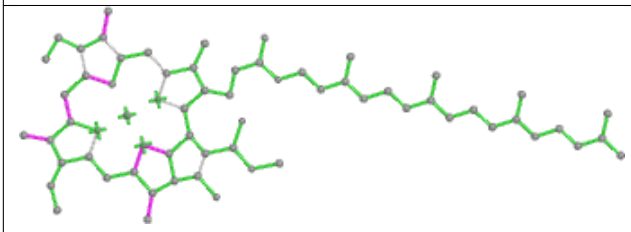
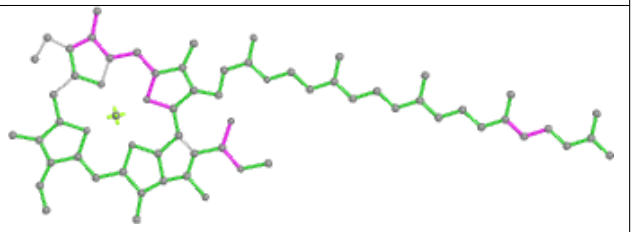
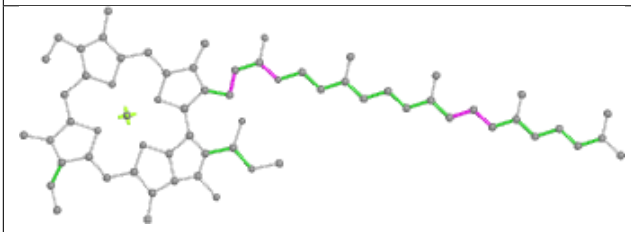
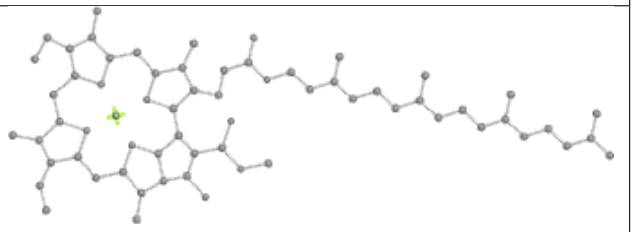


Torsions

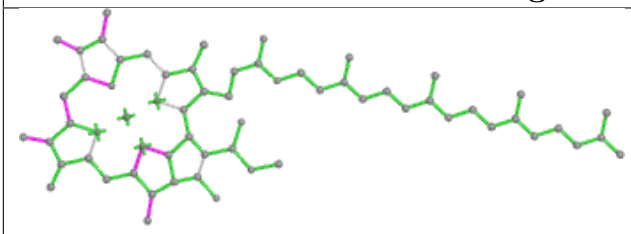


Rings

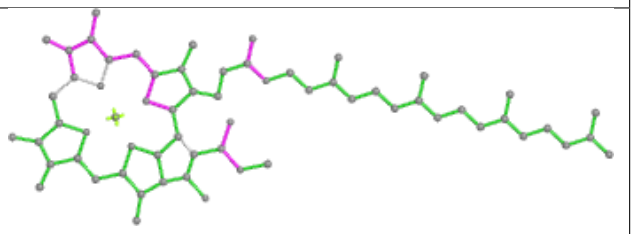
Ligand CLA A 818	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA 5 602	
 Bond lengths	 Bond angles
 Torsions	 Rings

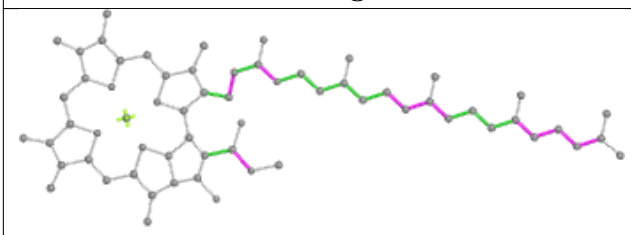
Ligand CLA 5 604



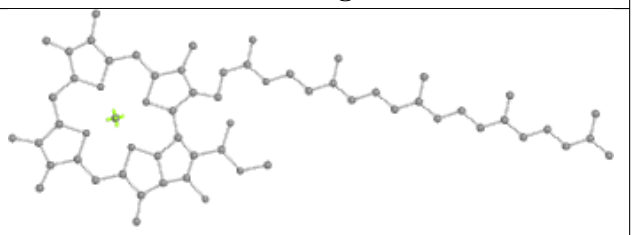
Bond lengths



Bond angles

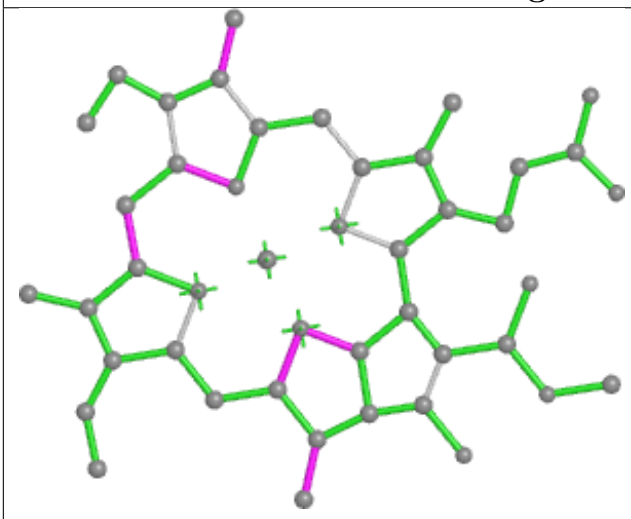


Torsions

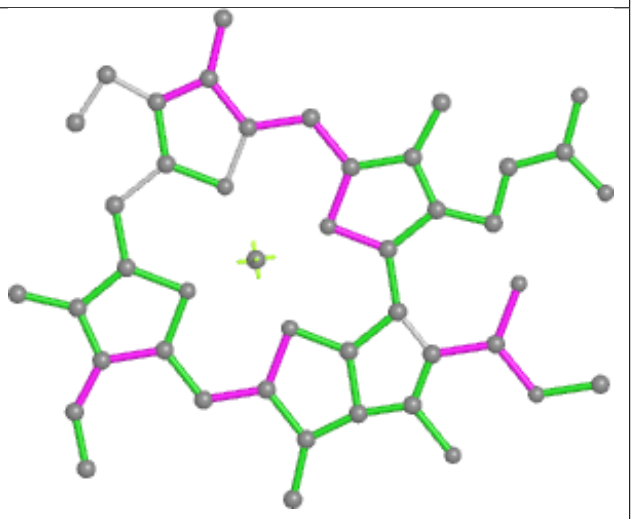


Rings

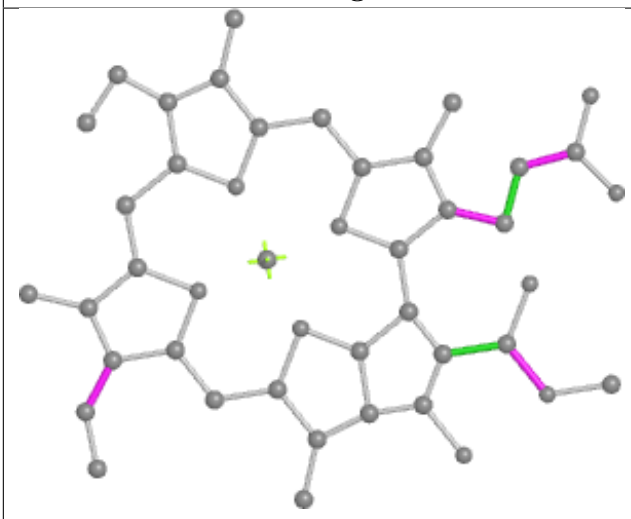
Ligand CLA 7 609



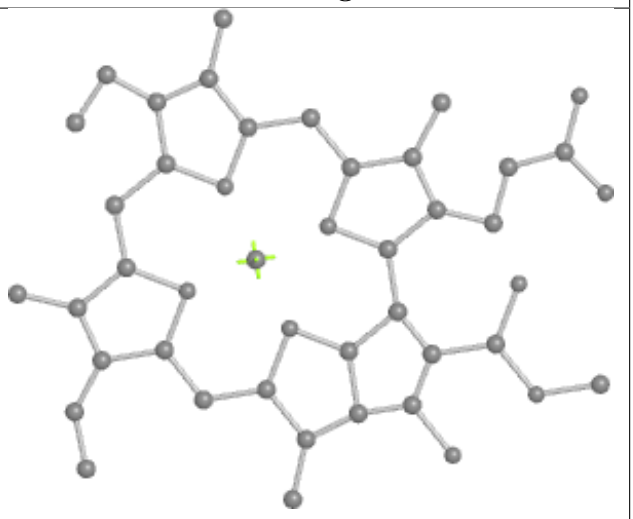
Bond lengths



Bond angles

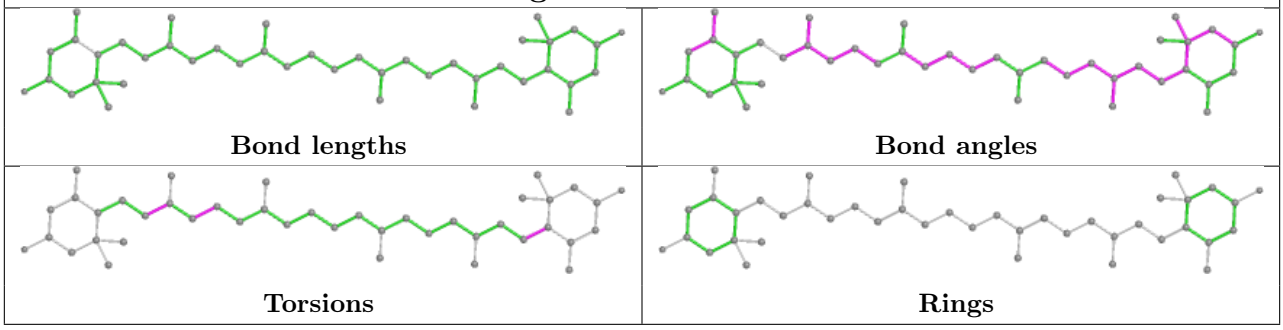


Torsions

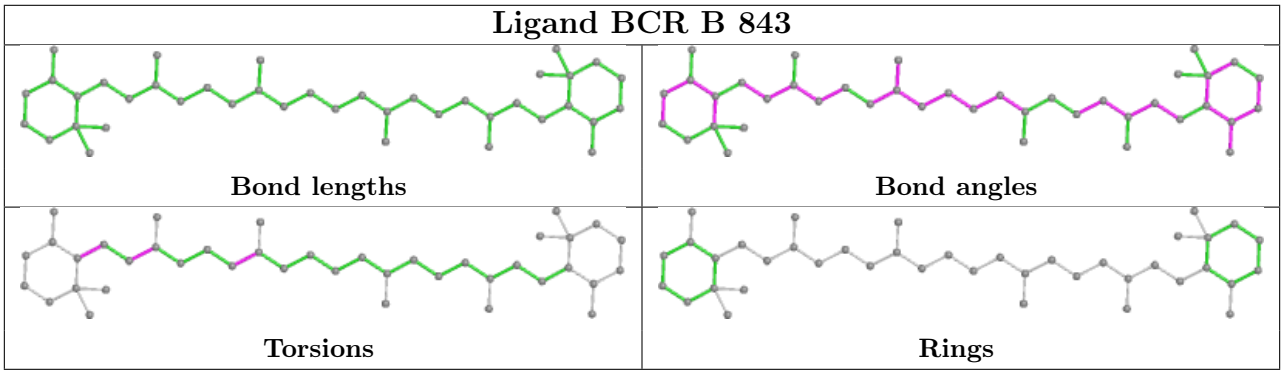


Rings

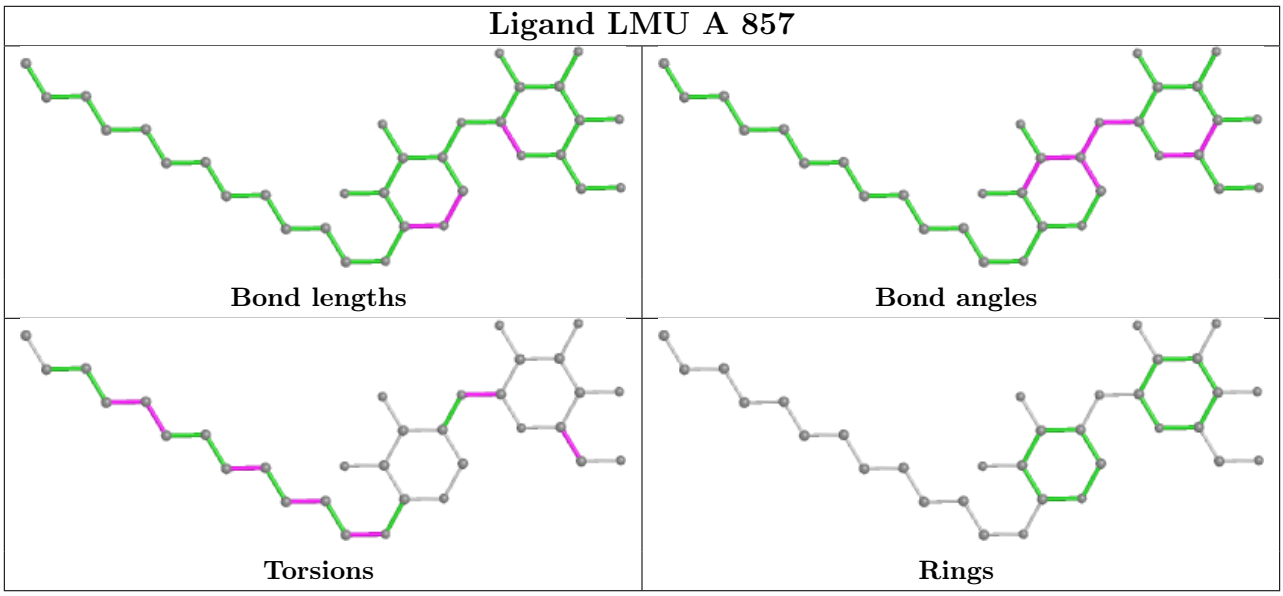
Ligand LUT a 617



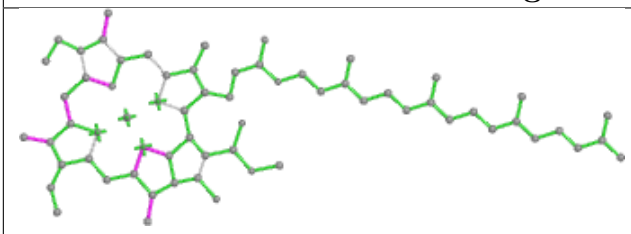
Ligand BCR B 843



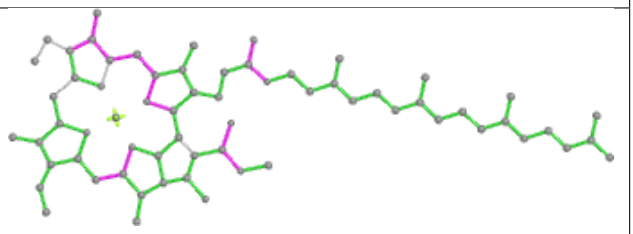
Ligand LMU A 857



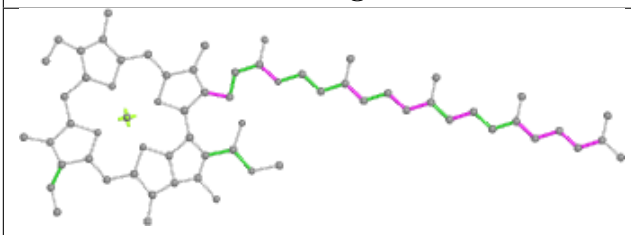
Ligand CLA A 812



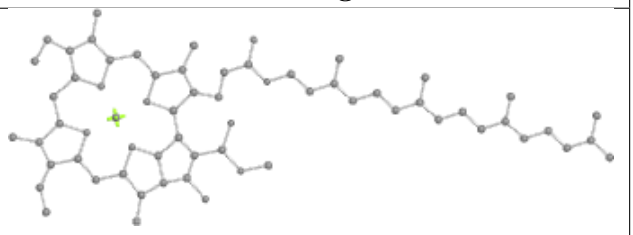
Bond lengths



Bond angles

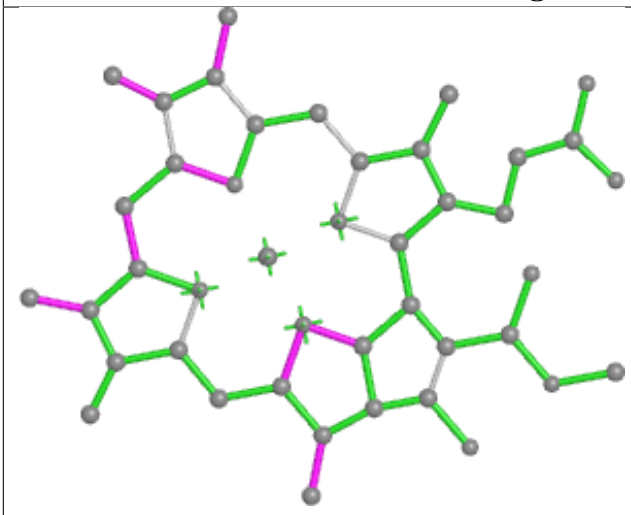


Torsions

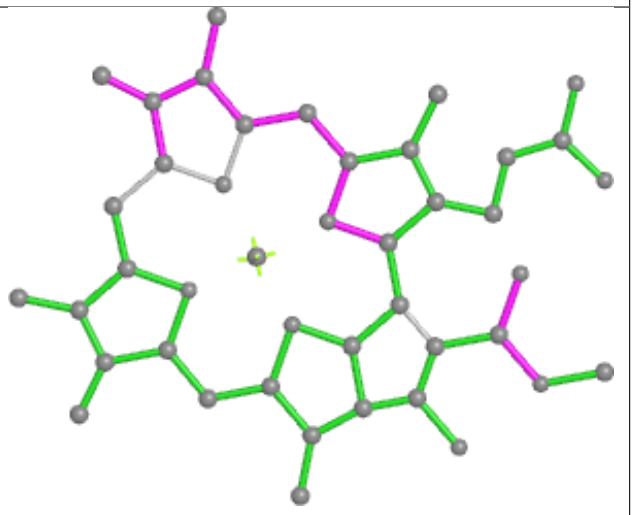


Rings

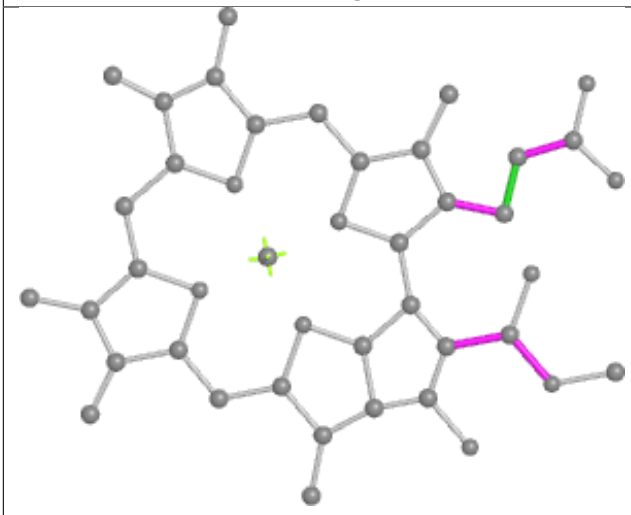
Ligand CLA 4 616



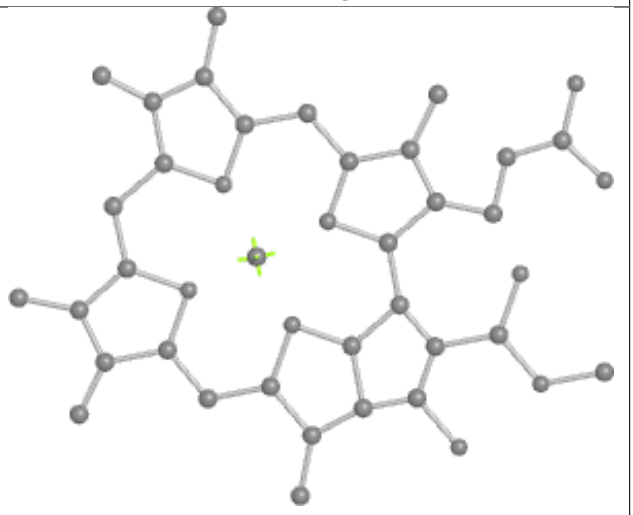
Bond lengths



Bond angles

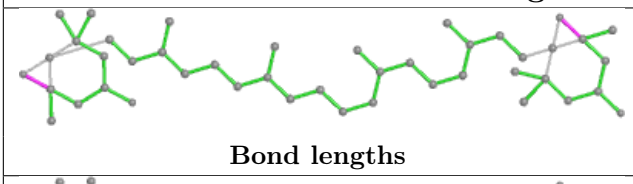


Torsions

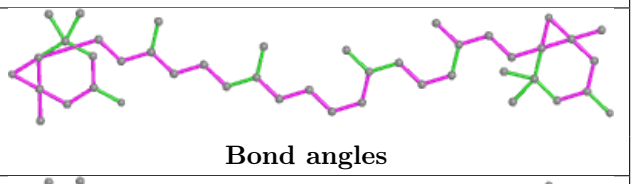


Rings

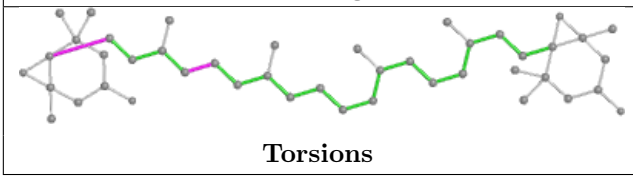
Ligand XAT 3 619



Bond lengths



Bond angles



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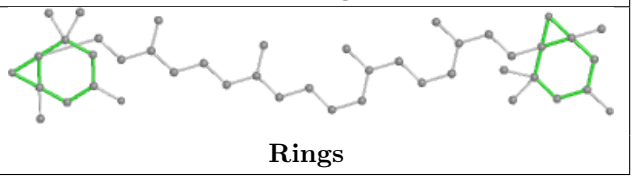
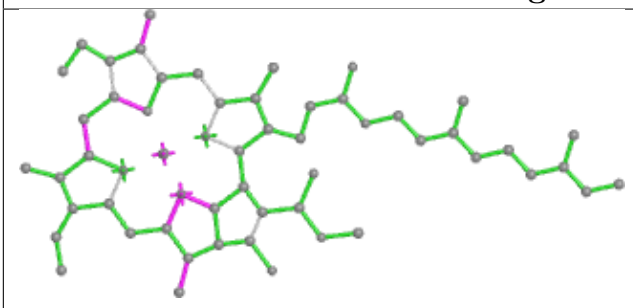


Rings

Ligand CLA 5 601



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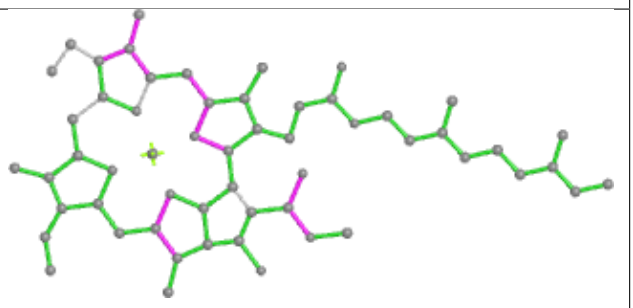
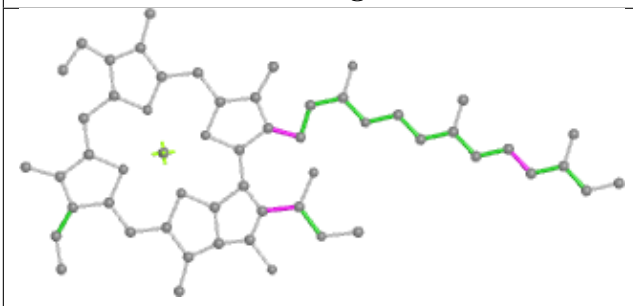


Bond angles



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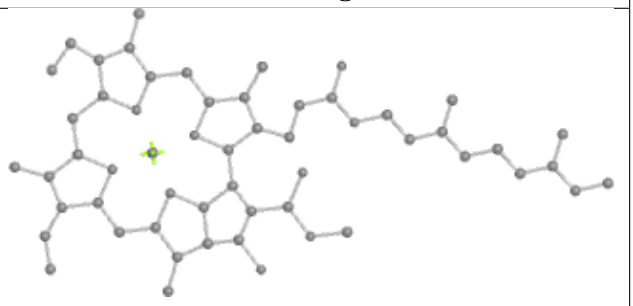
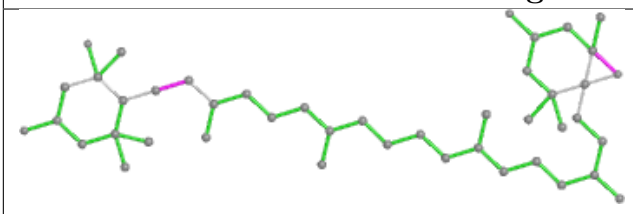
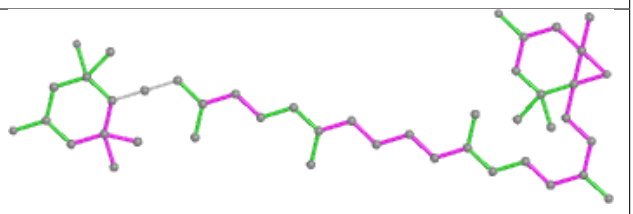


Rings

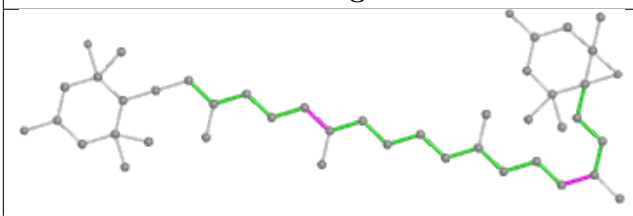
Ligand NEX 6 624



Bond lengths



Bond angles



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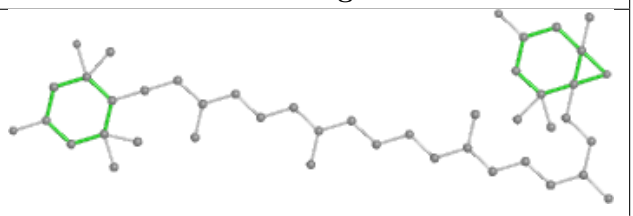
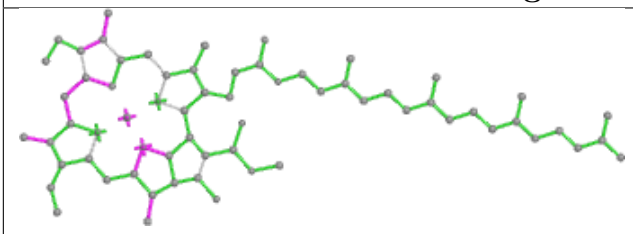
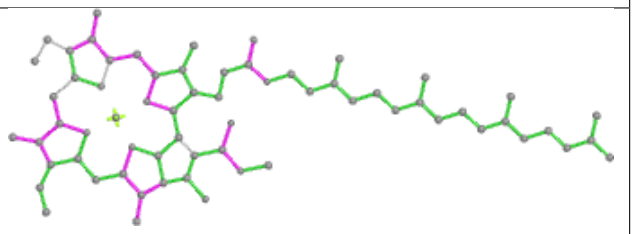


Rings

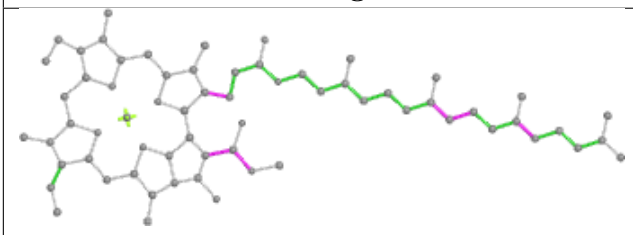
Ligand CLA A 831



Bond lengths



Bond angles



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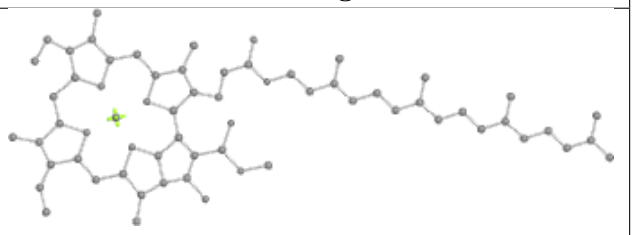
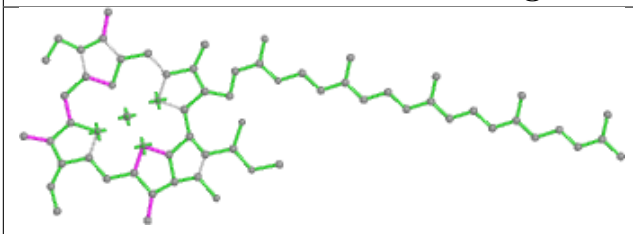
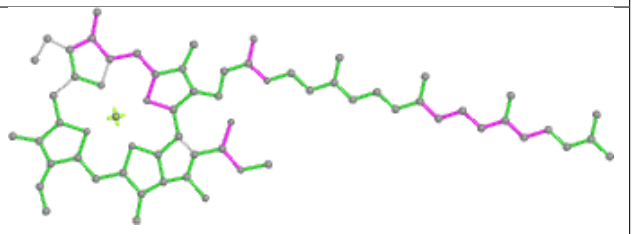


Rings

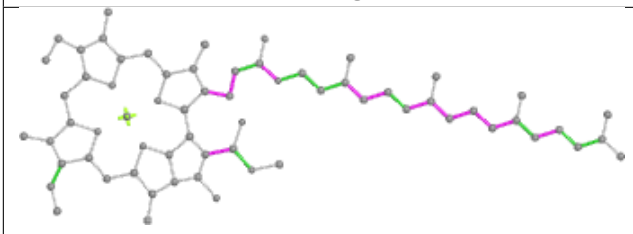
Ligand CLA A 814



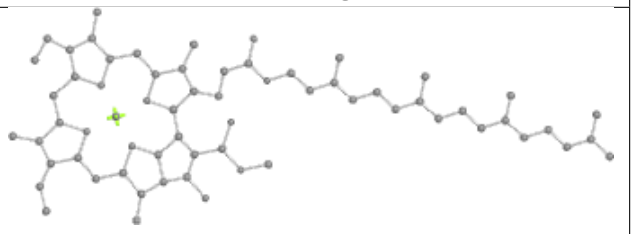
Bond lengths



Bond angles

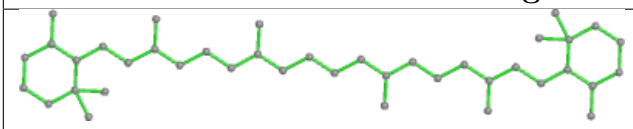


Torsions

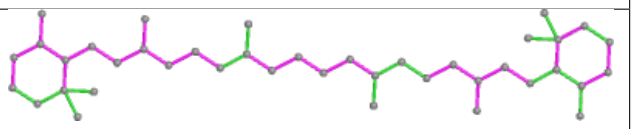


Rings

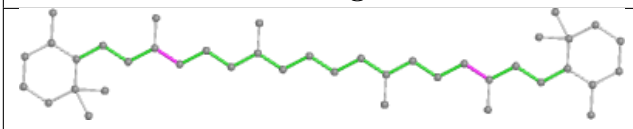
Ligand BCR B 845



Bond lengths



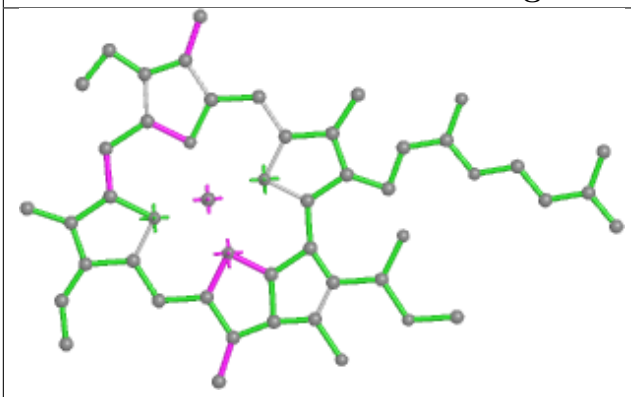
Bond angles



Torsions

Rings

Ligand CLA A 838



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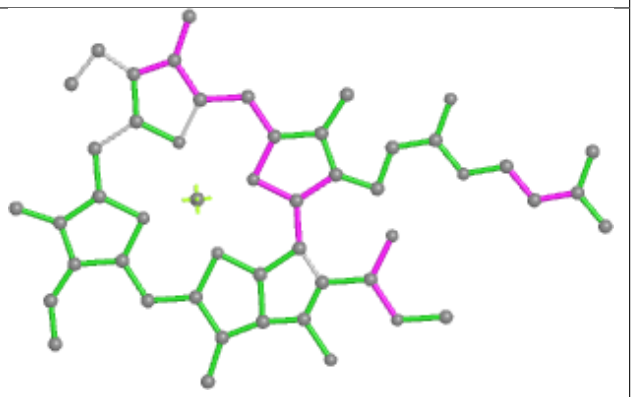
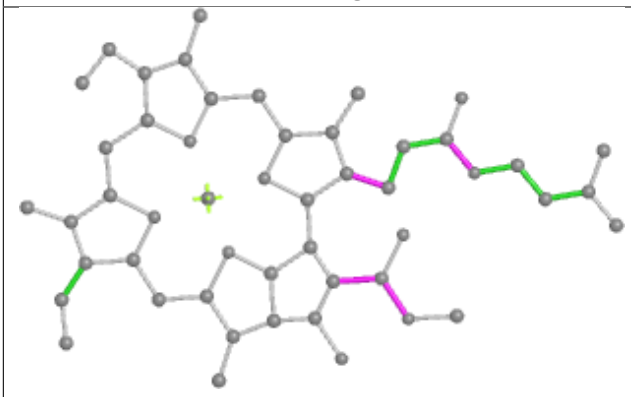
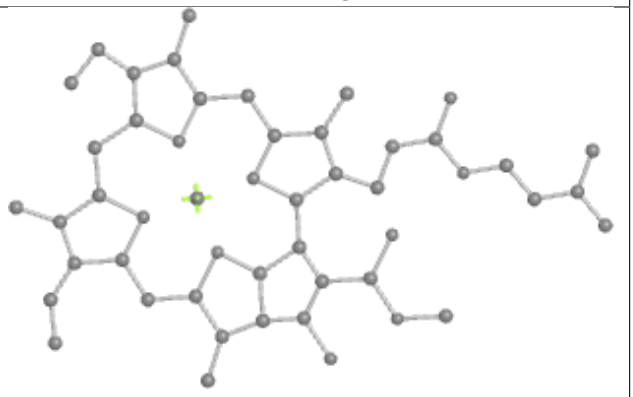


Bond angles

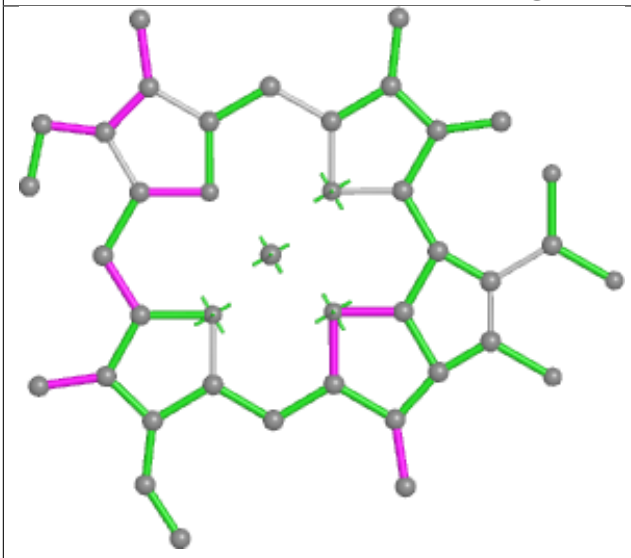


Torsions



Rings

Ligand CLA 3 617



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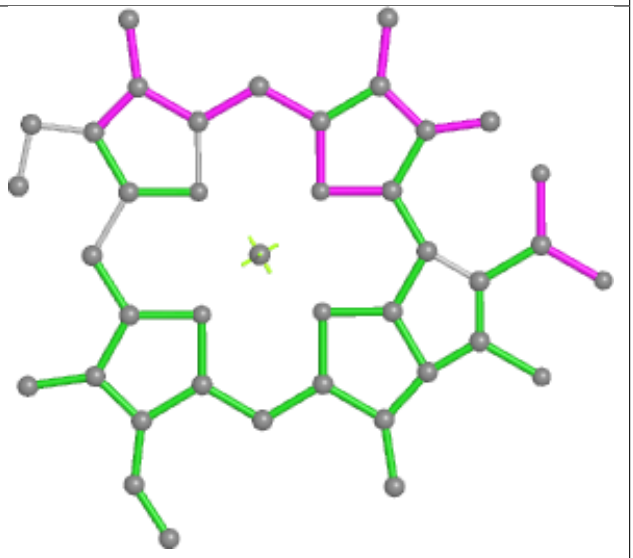
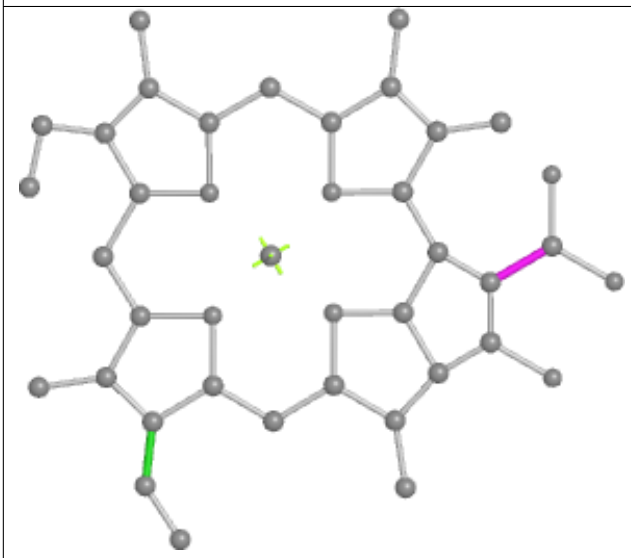
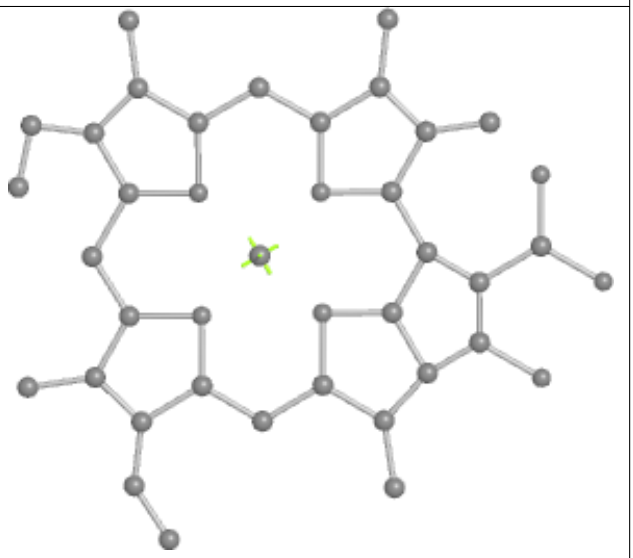


Bond angles

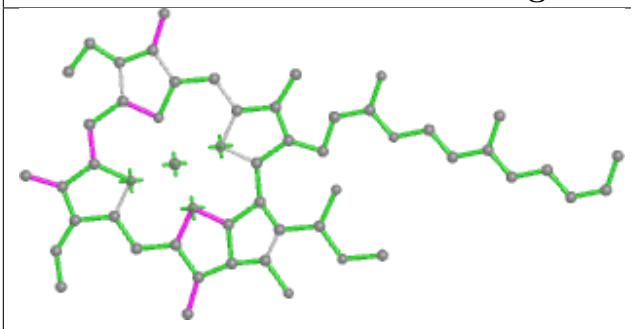


Torsions

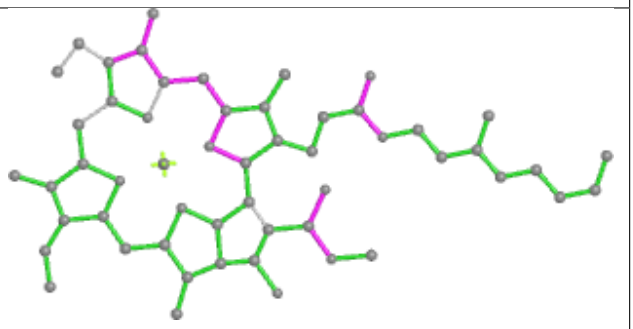


Rings

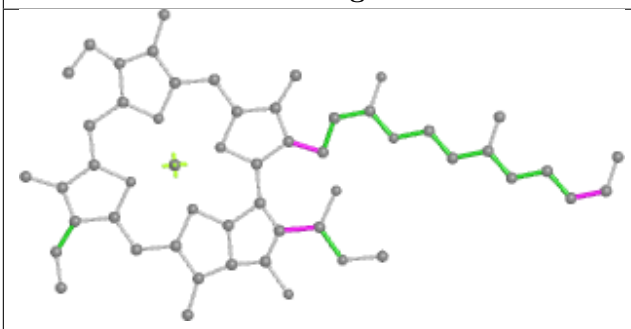
Ligand CLA 5 610



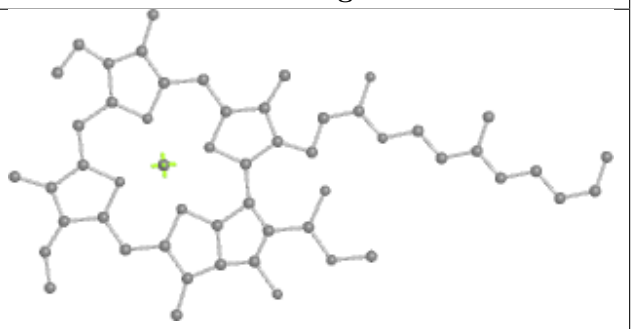
Bond lengths



Bond angles

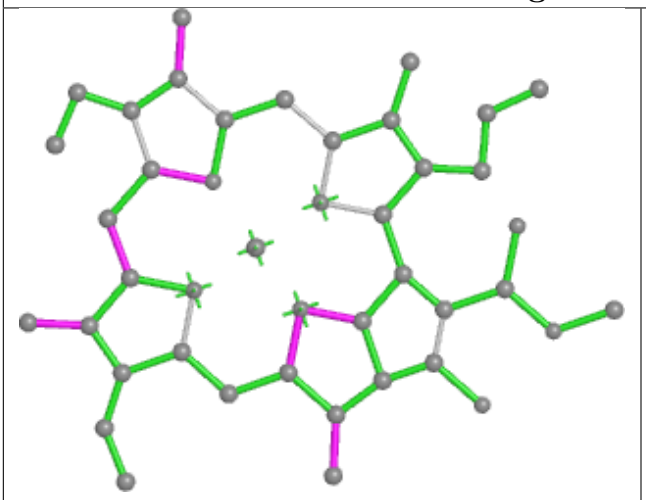


Torsions

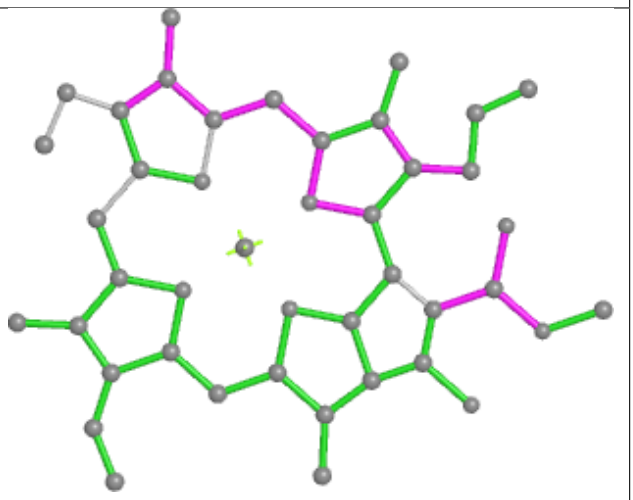


Rings

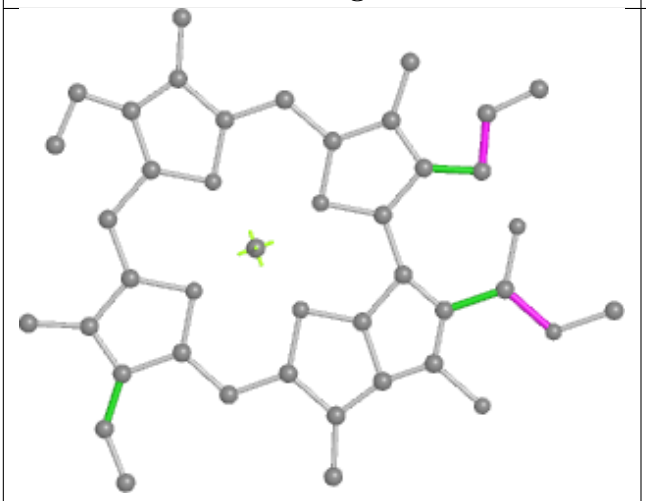
Ligand CLA 3 612



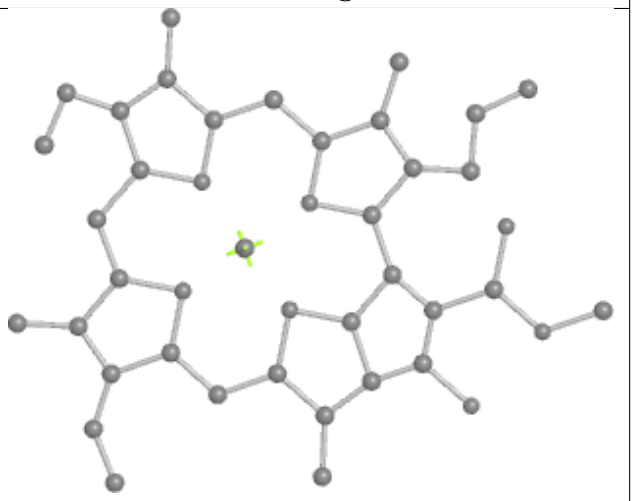
Bond lengths



Bond angles

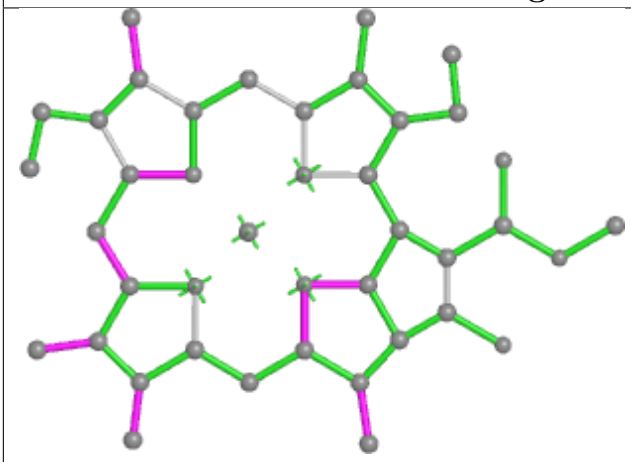


Torsions

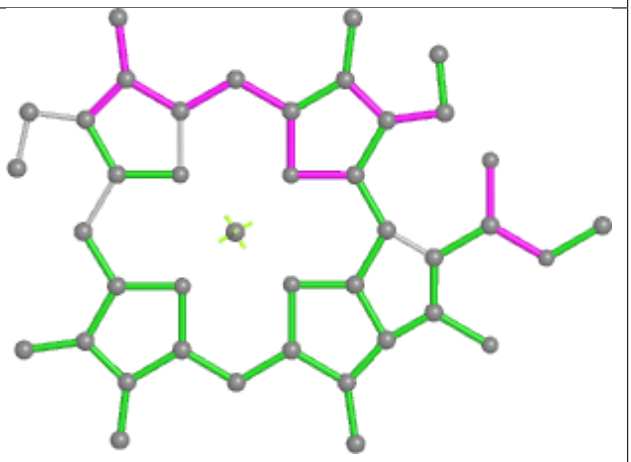


Rings

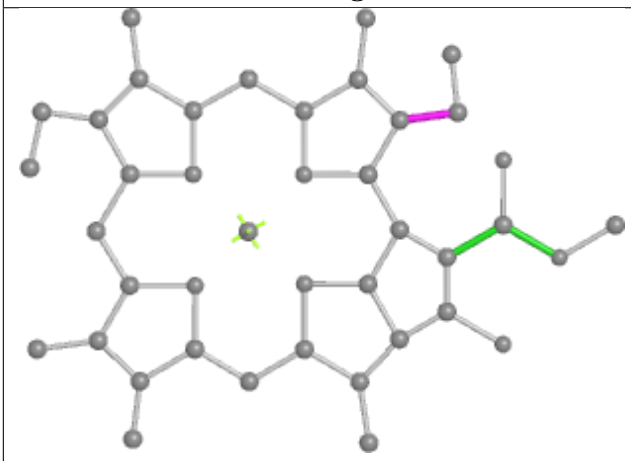
Ligand CLA 7 606



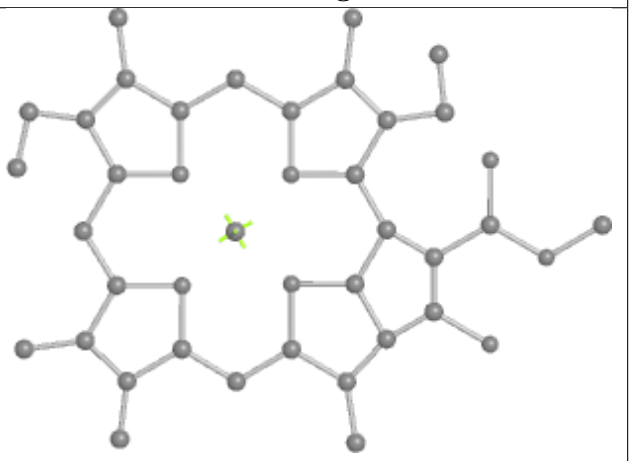
Bond lengths



Bond angles

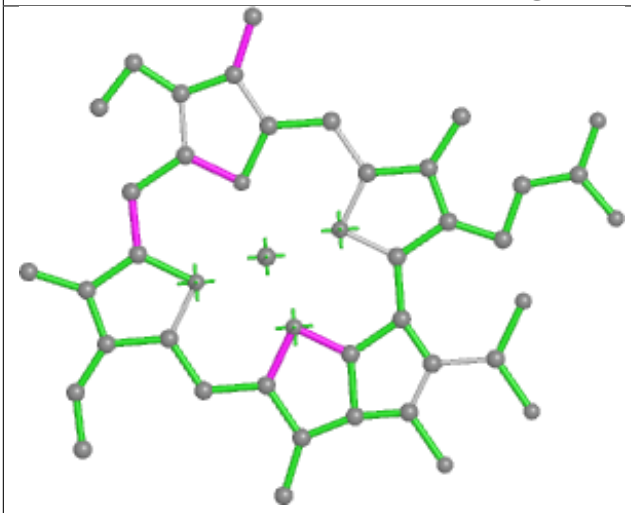


Torsions

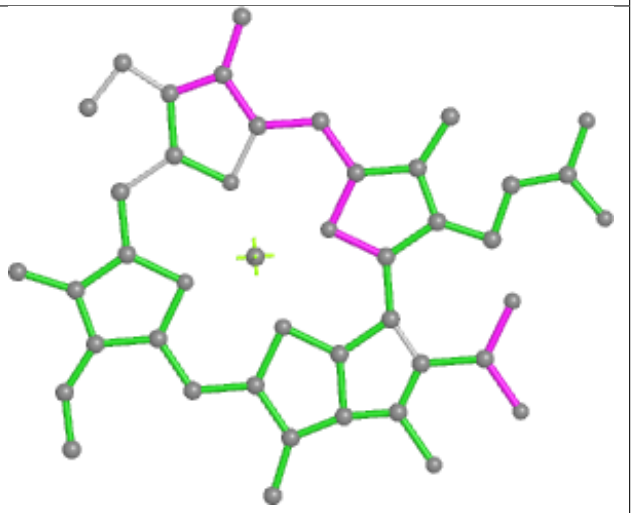


Rings

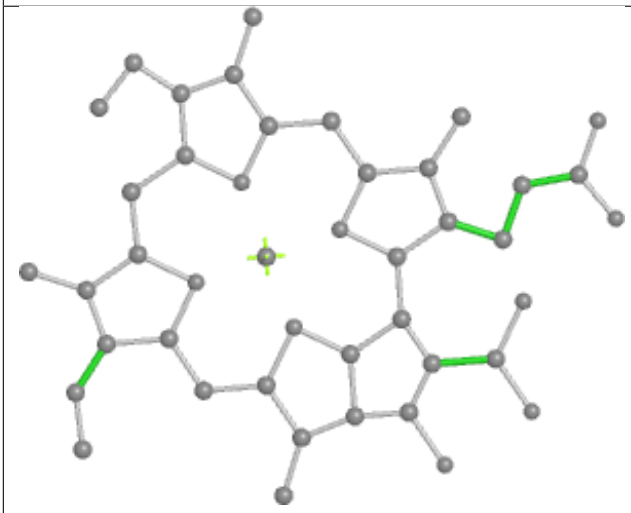
Ligand CLA 1 608



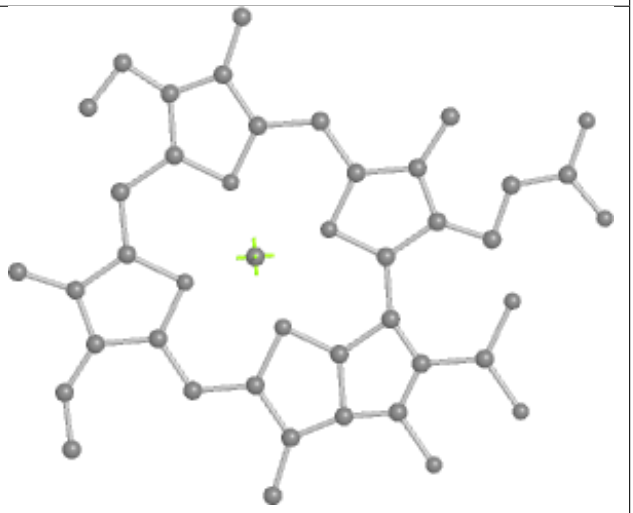
Bond lengths



Bond angles

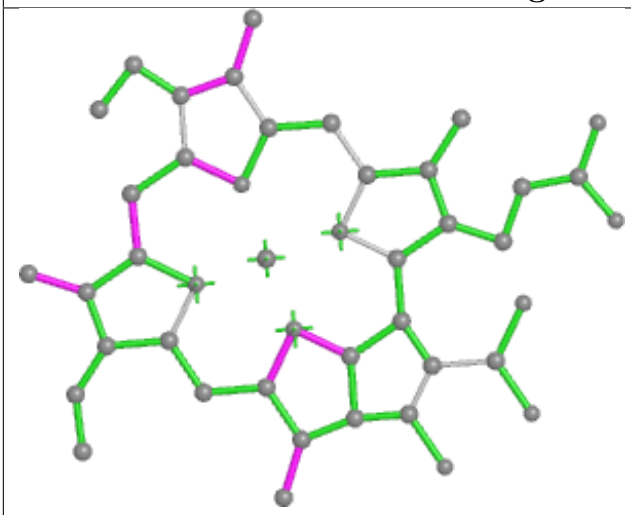


Torsions



Rings

Ligand CLA 7 603



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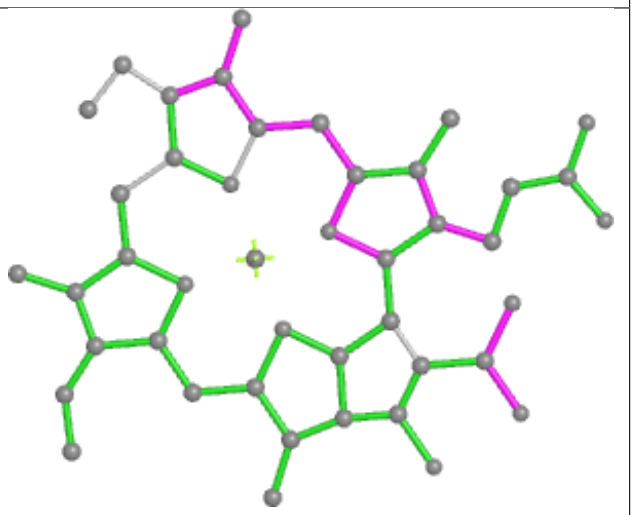
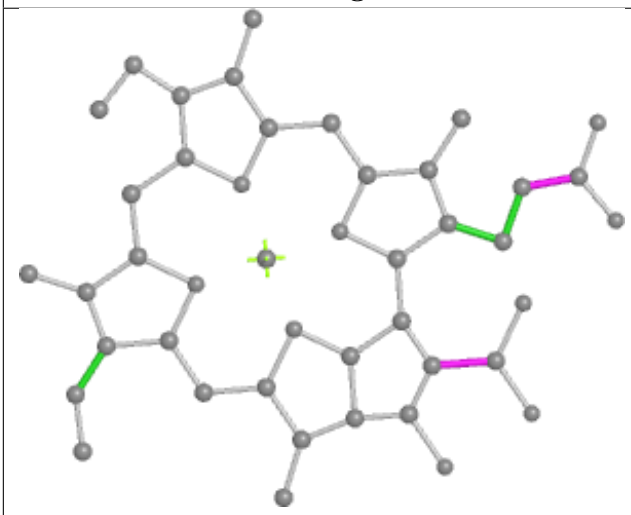
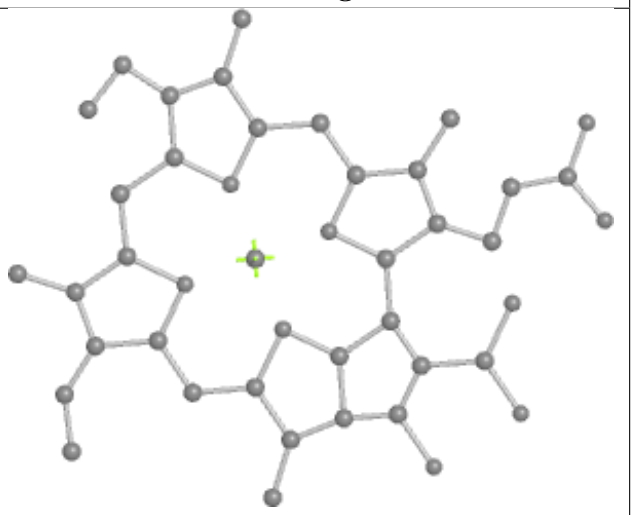


Bond angles

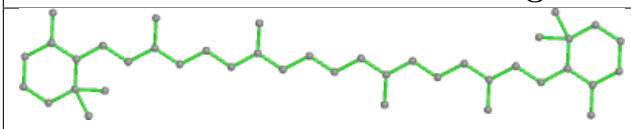


Torsions

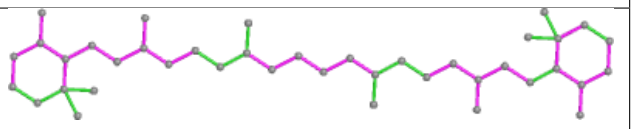


Rings

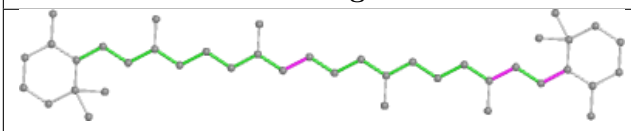
Ligand BCR 3 620



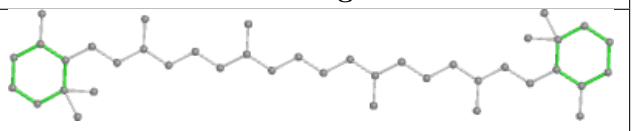
Bond lengths



Bond angles

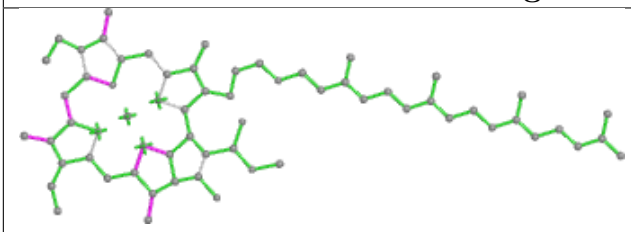


Torsions

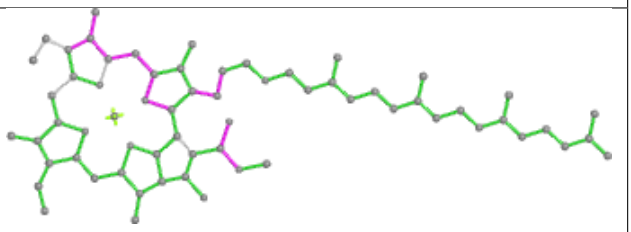


Rings

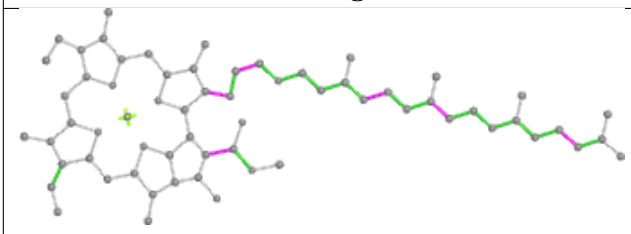
Ligand CLA A 828



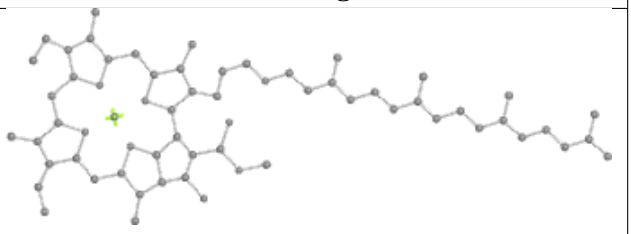
Bond lengths



Bond angles

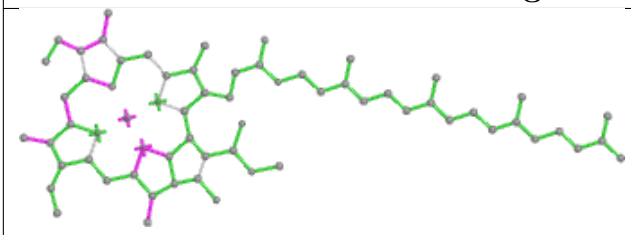


Torsions

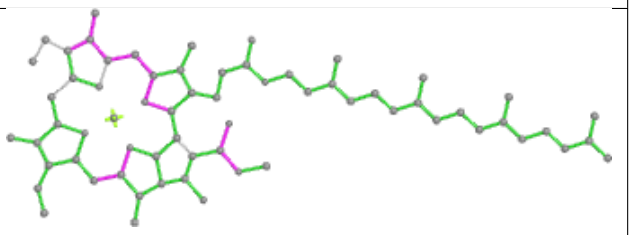


Rings

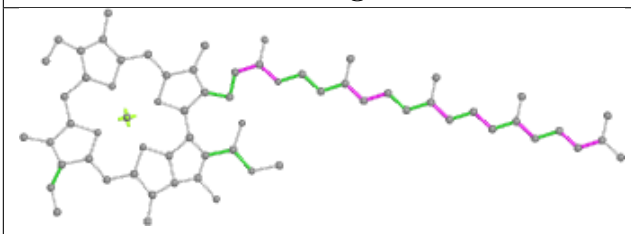
Ligand CLA A 807



Bond lengths



Bond angles



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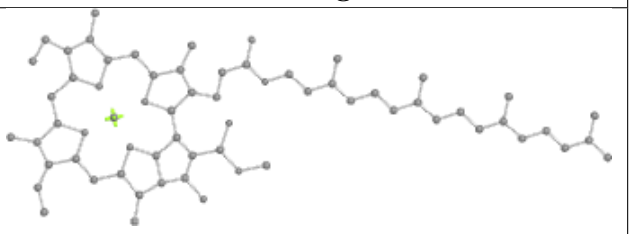
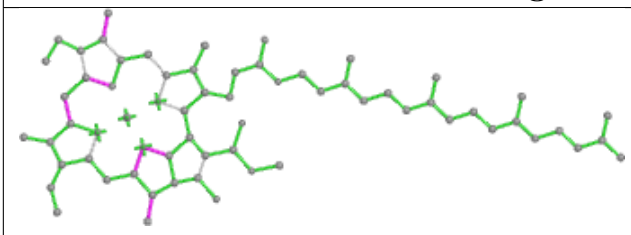
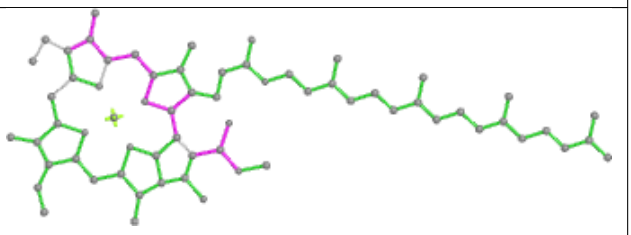


Rings

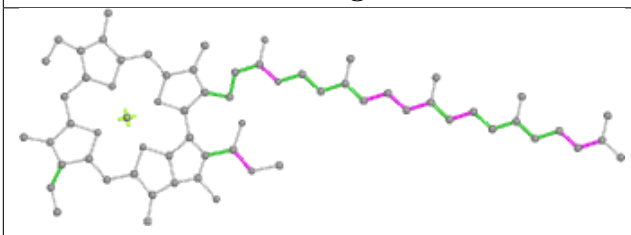
Ligand CLA 1 611



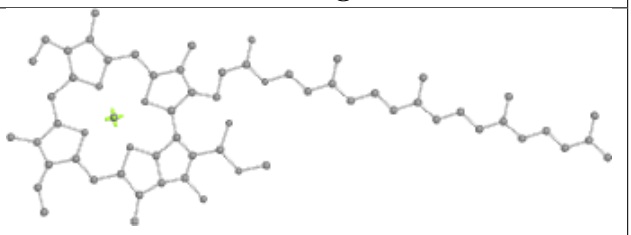
Bond lengths



Bond angles

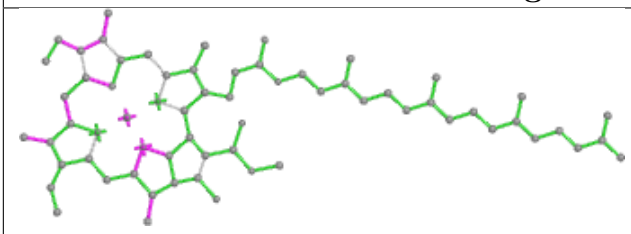


Torsions

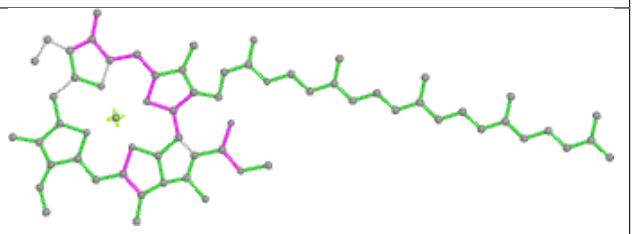


Rings

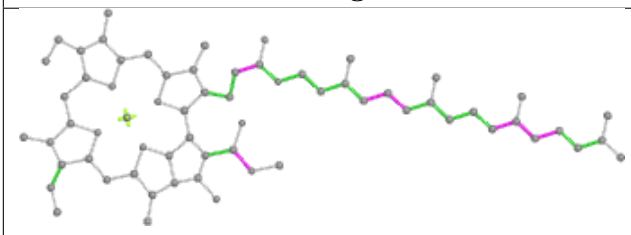
Ligand CLA B 806



Bond lengths



Bond angles



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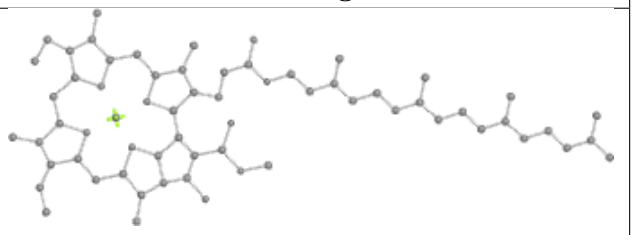
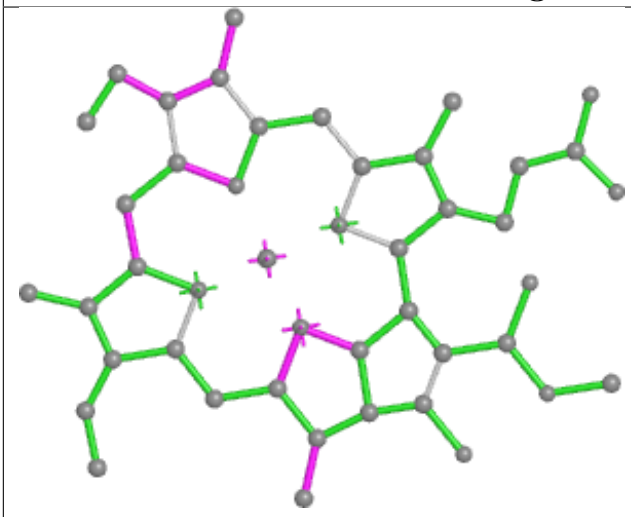
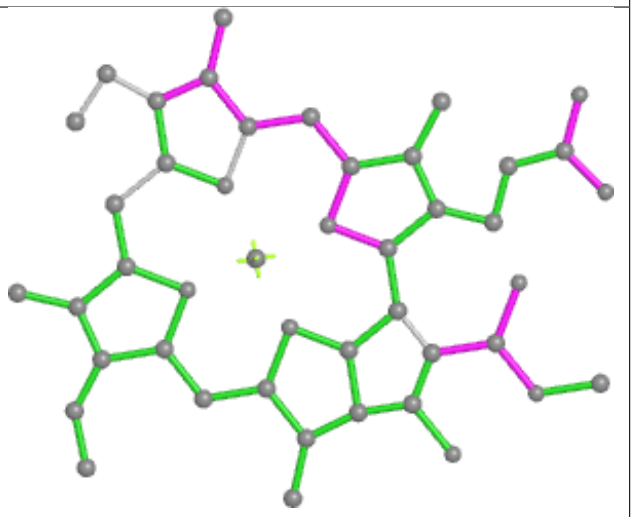


Rings

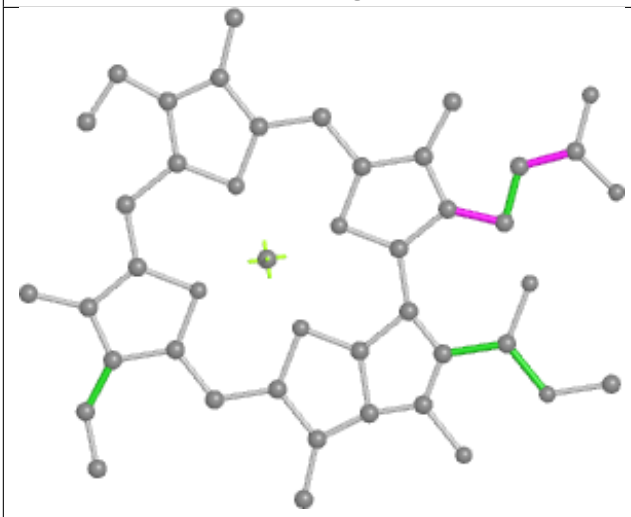
Ligand CLA 6 609



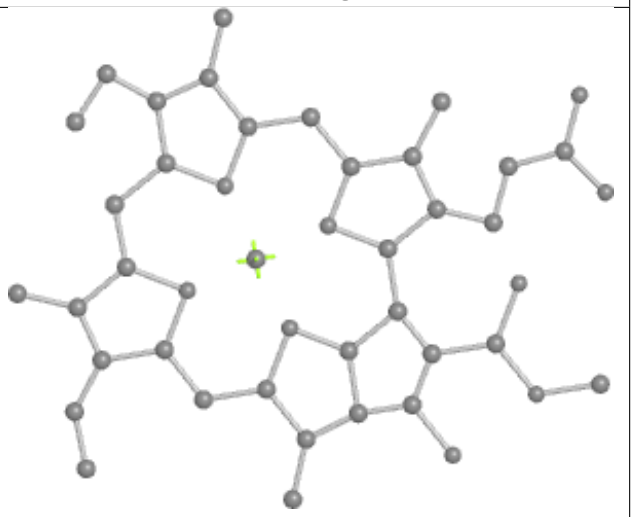
Bond lengths



Bond angles

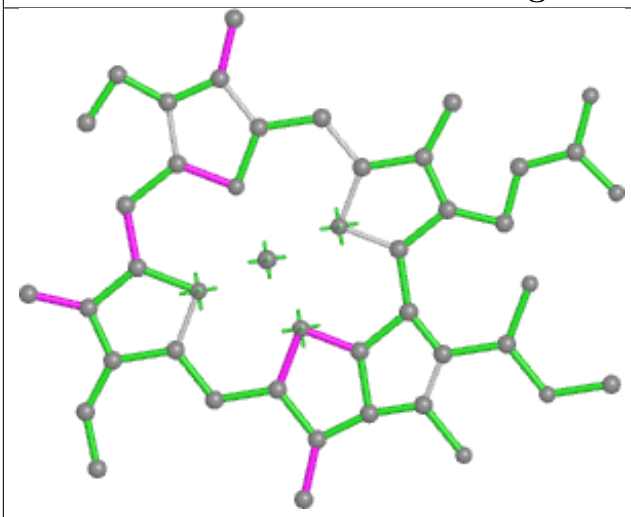


Torsions

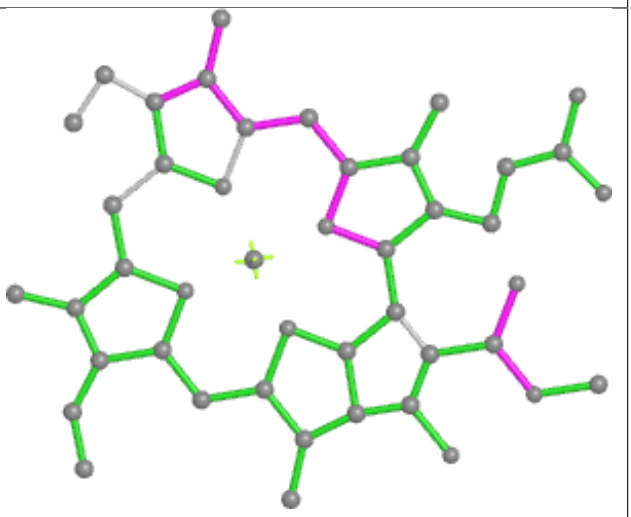


Rings

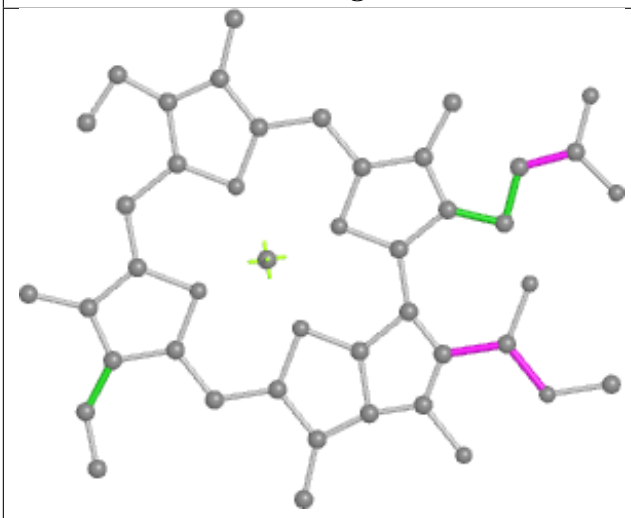
Ligand CLA 6 617



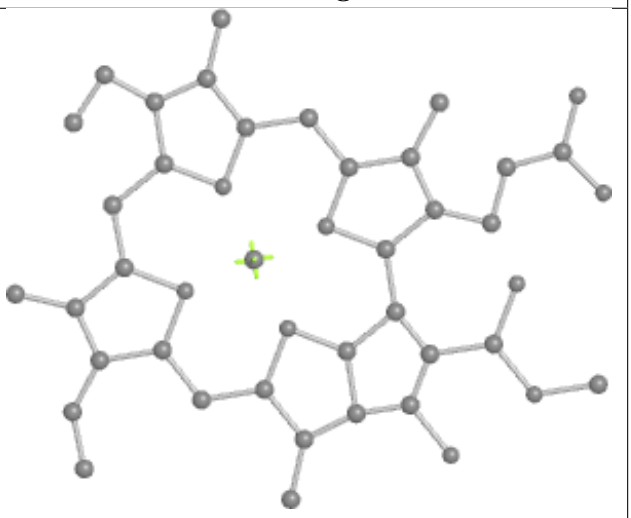
Bond lengths



Bond angles

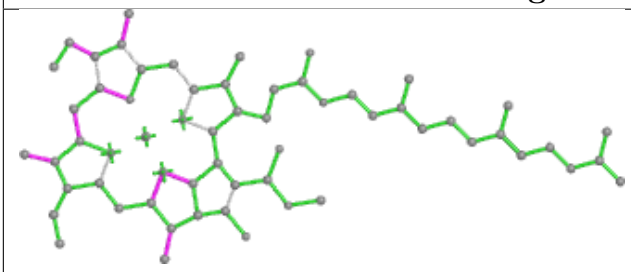


Torsions

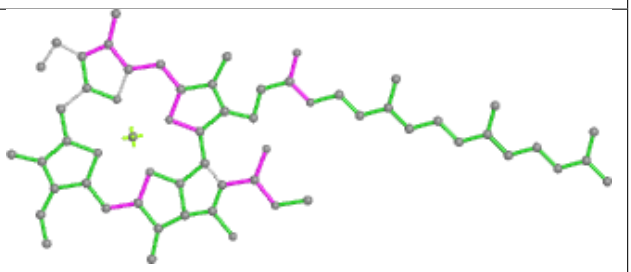


Rings

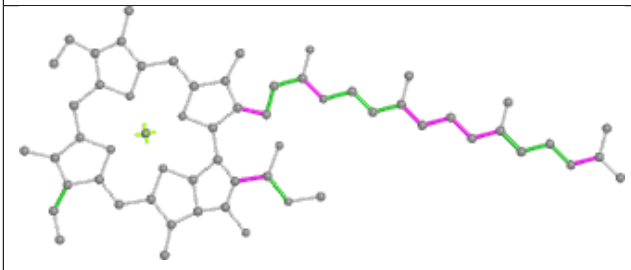
Ligand CLA 7 601



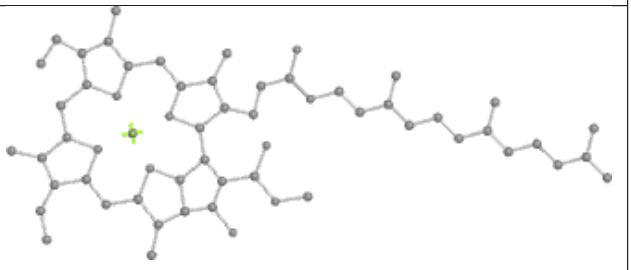
Bond lengths



Bond angles

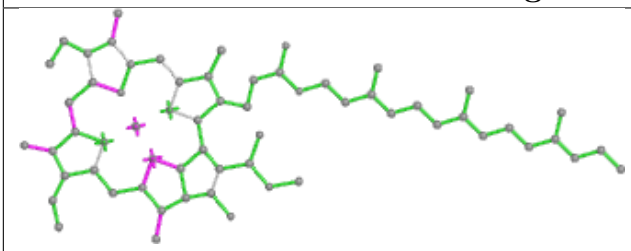


Torsions

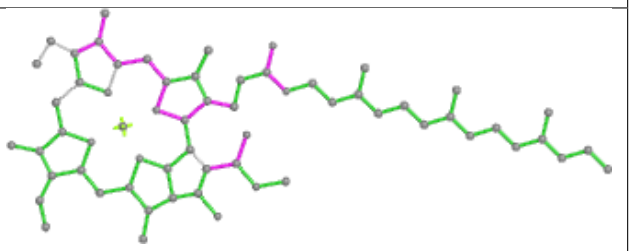


Rings

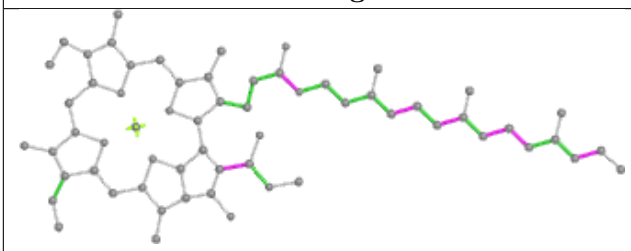
Ligand CLA B 825



Bond lengths



Bond angles



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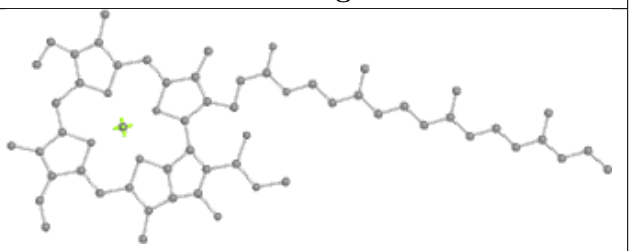
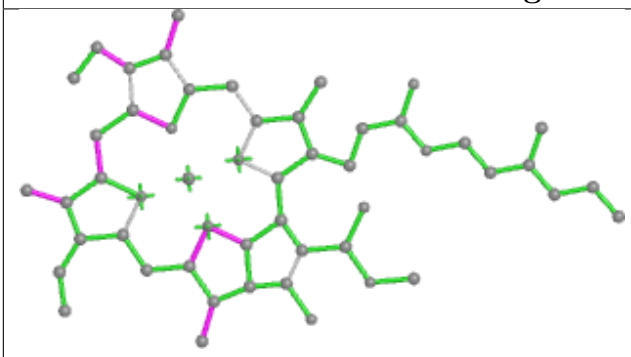
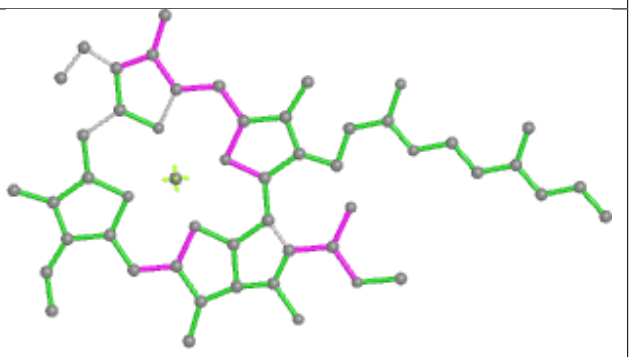


Rings

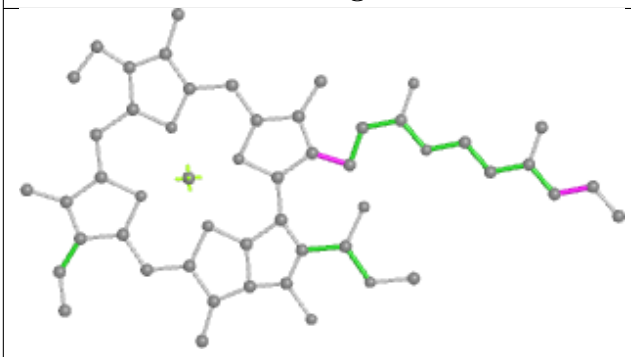
Ligand CLA A 805



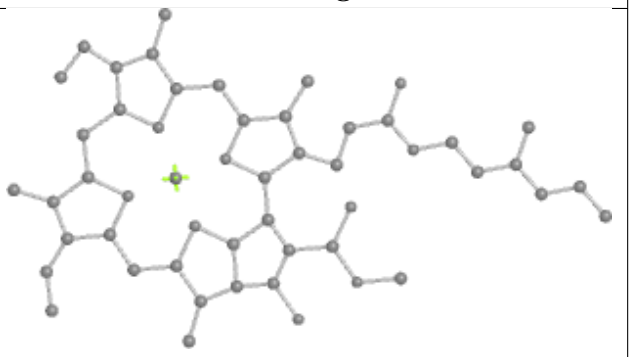
Bond lengths



Bond angles

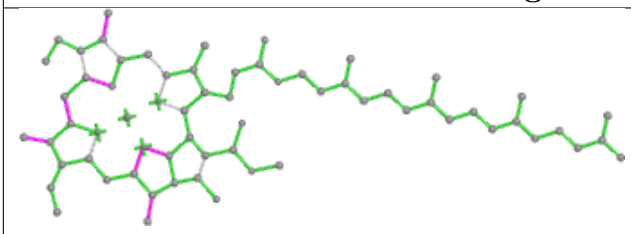


Torsions

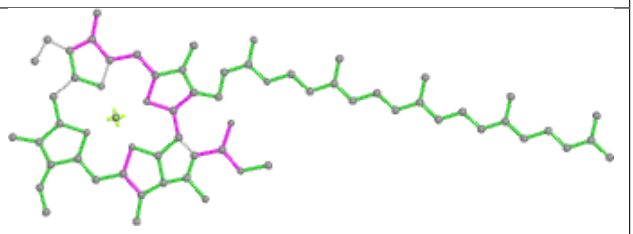


Rings

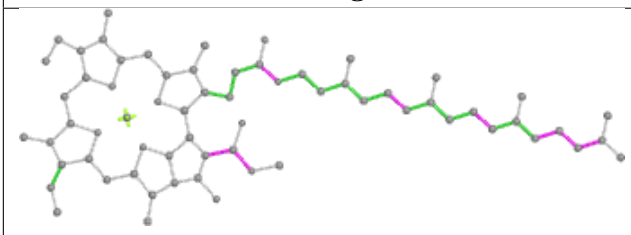
Ligand CLA B 824



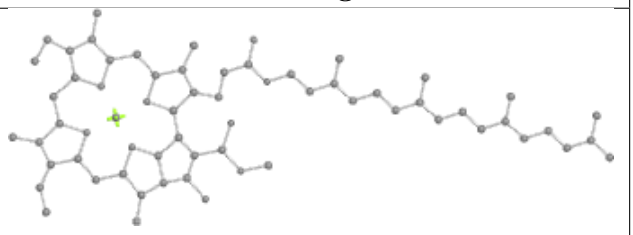
Bond lengths



Bond angles

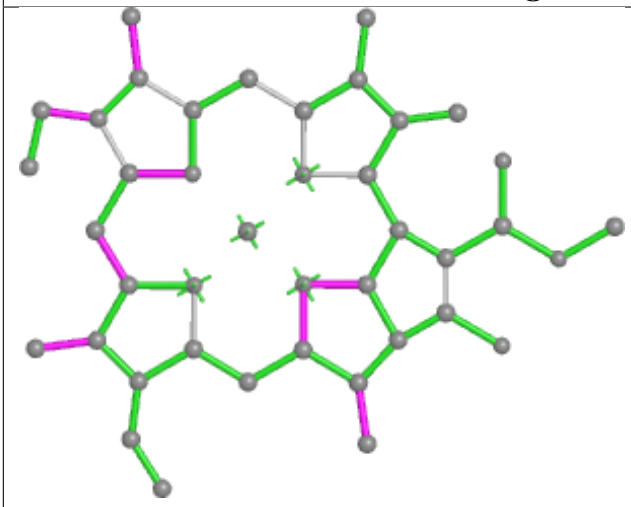


Torsions

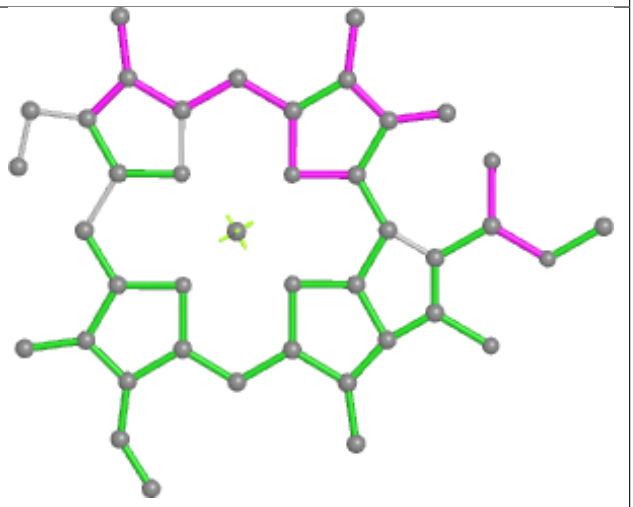


Rings

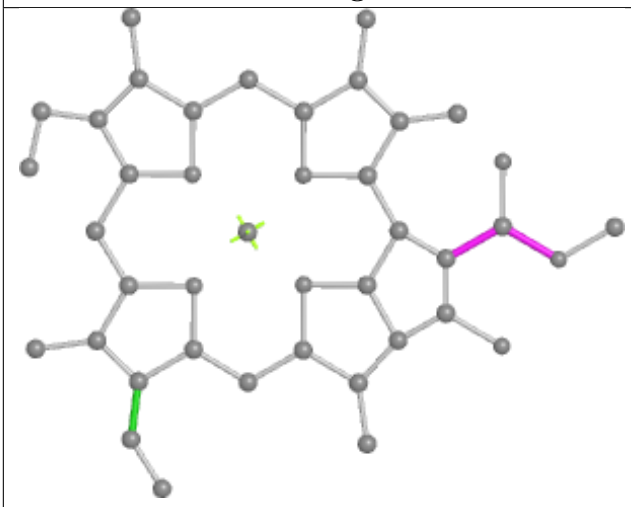
Ligand CLA B 804



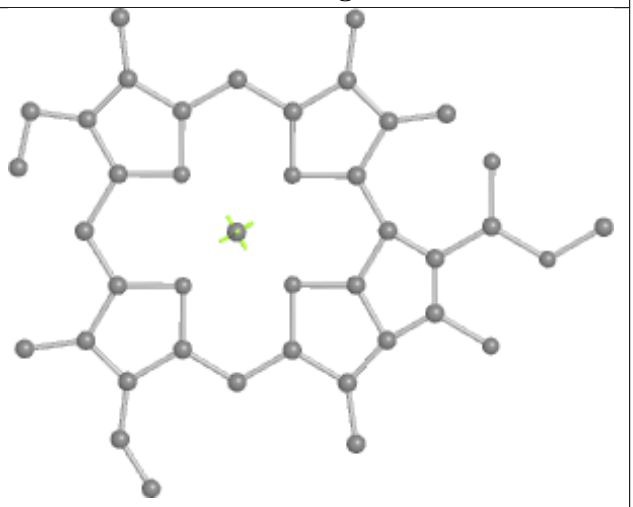
Bond lengths



Bond angles

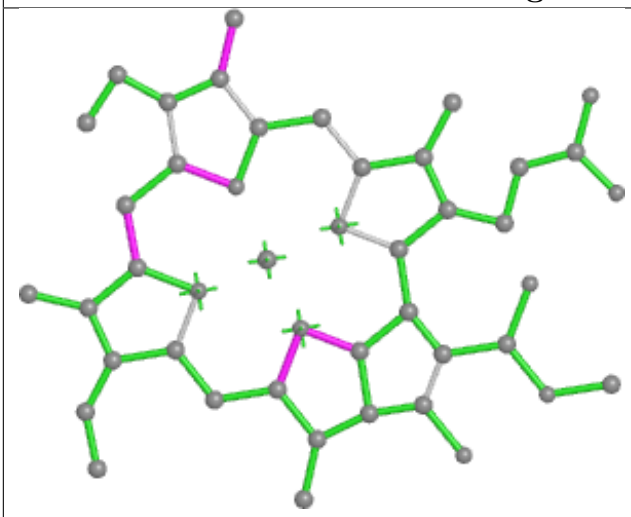


Torsions

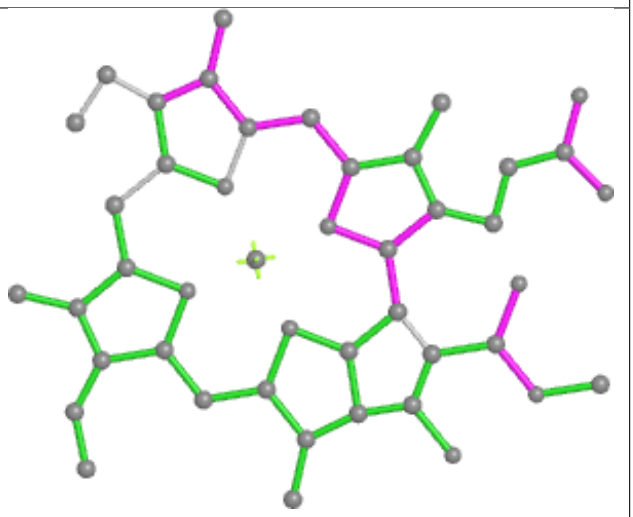


Rings

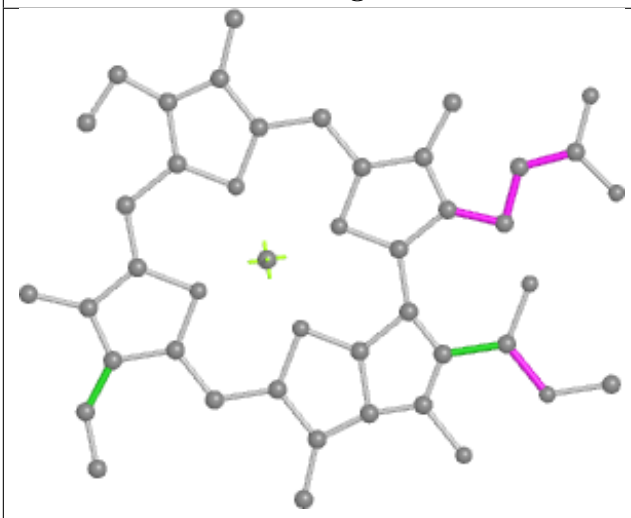
Ligand CLA L 302



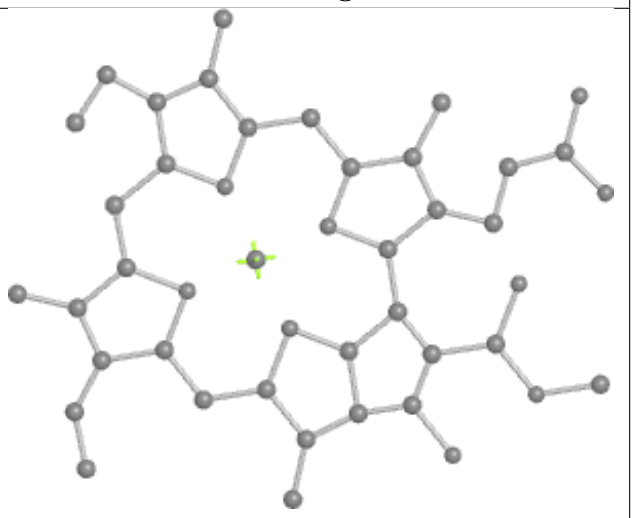
Bond lengths



Bond angles

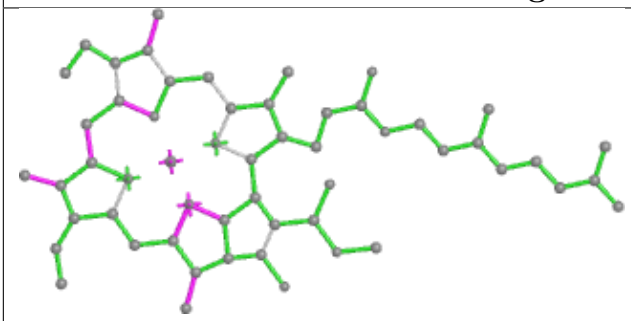


Torsions

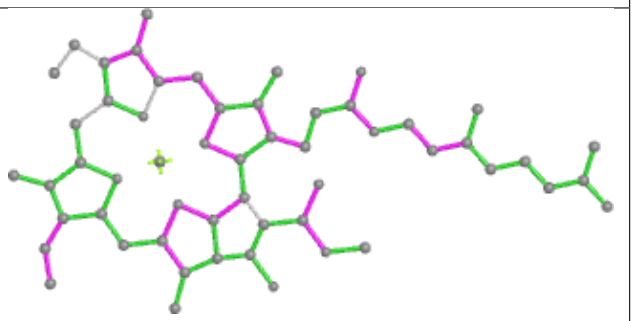


Rings

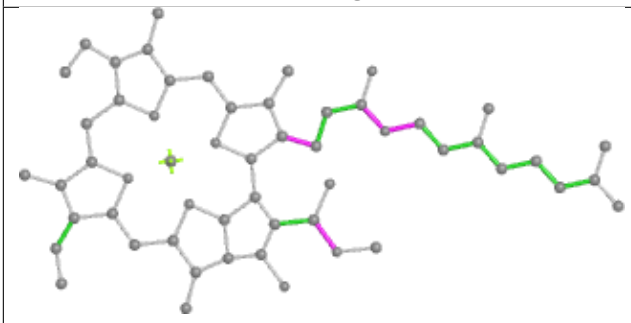
Ligand CLA 3 603



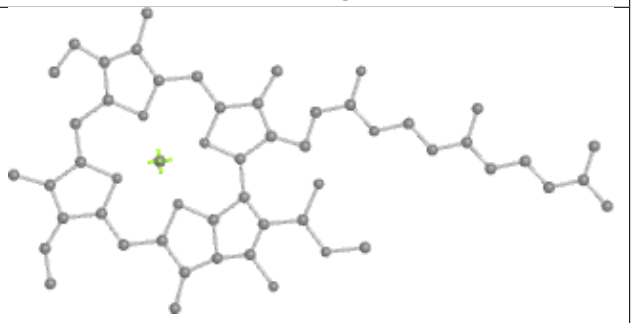
Bond lengths



Bond angles

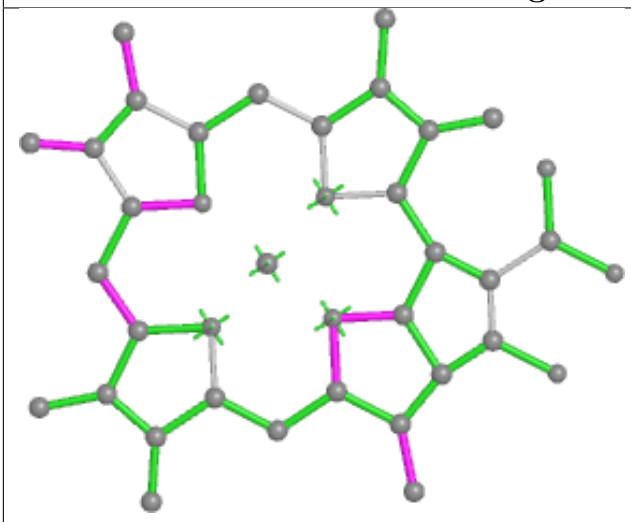


Torsions

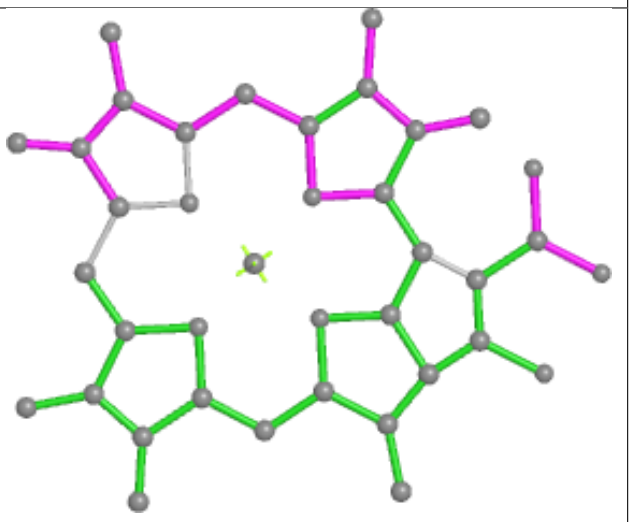


Rings

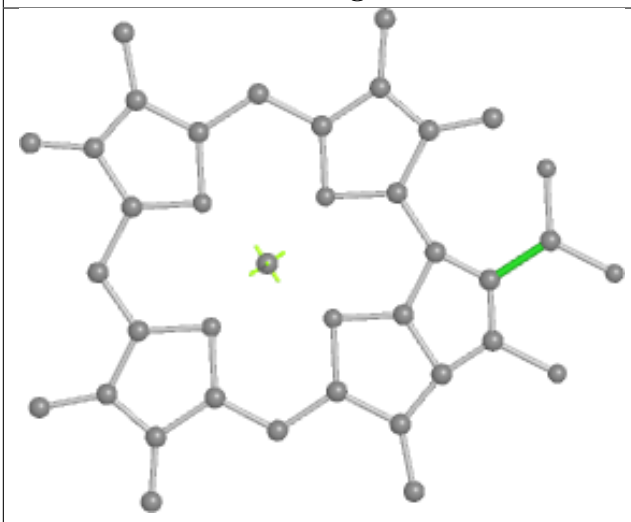
Ligand CLA 3 611



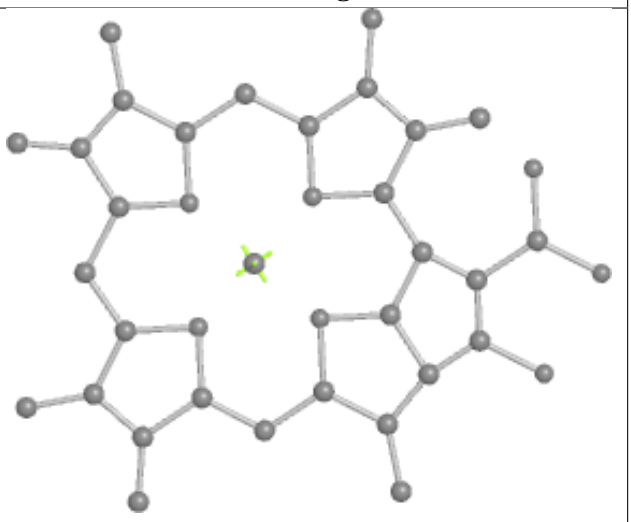
Bond lengths



Bond angles

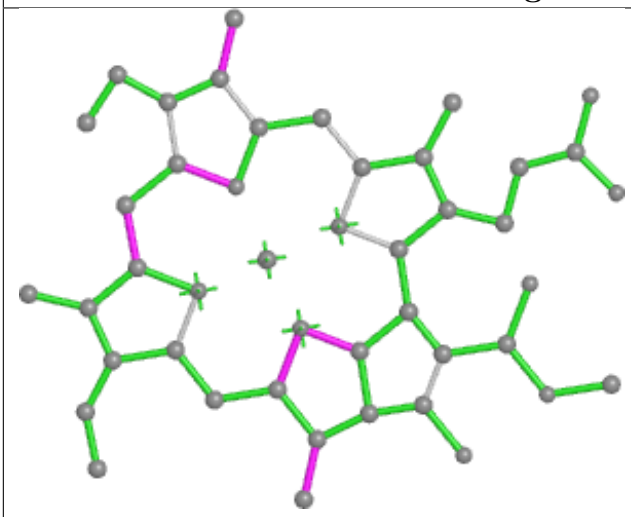


Torsions

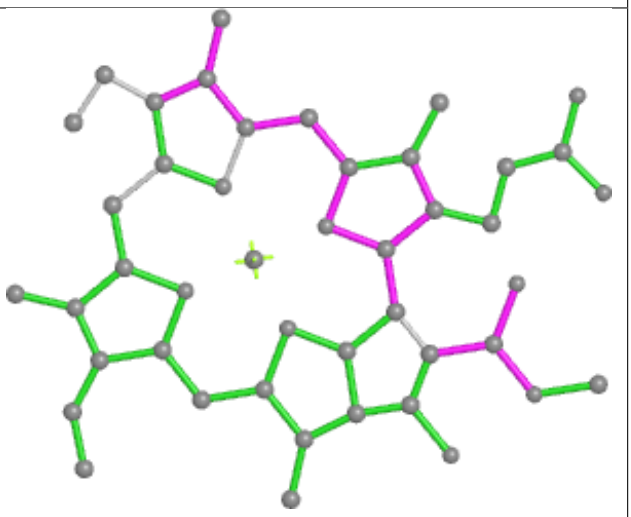


Rings

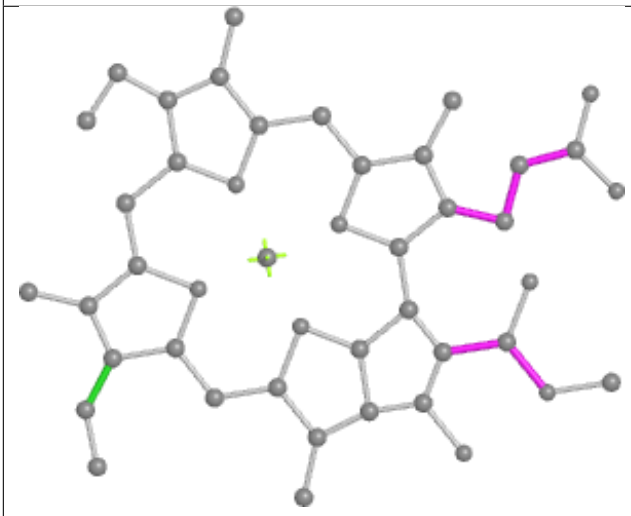
Ligand CLA B 835



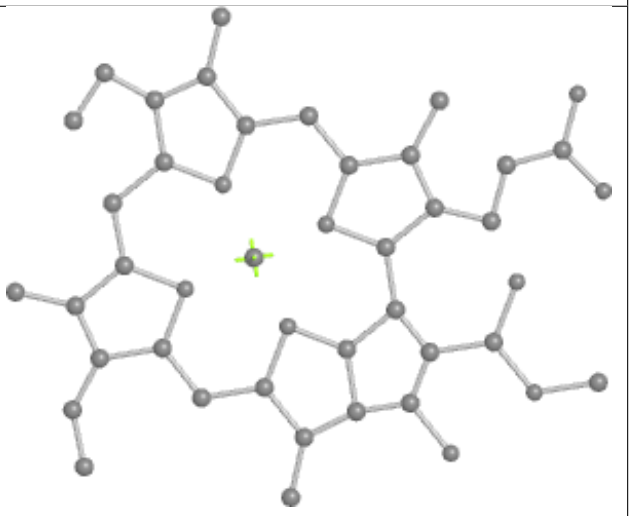
Bond lengths



Bond angles

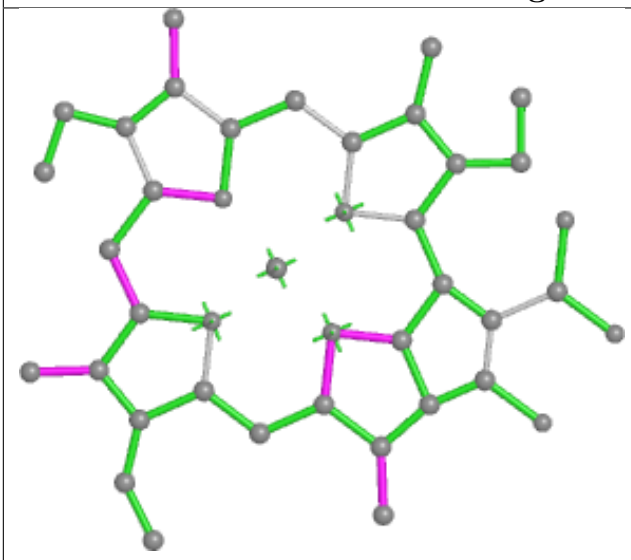


Torsions

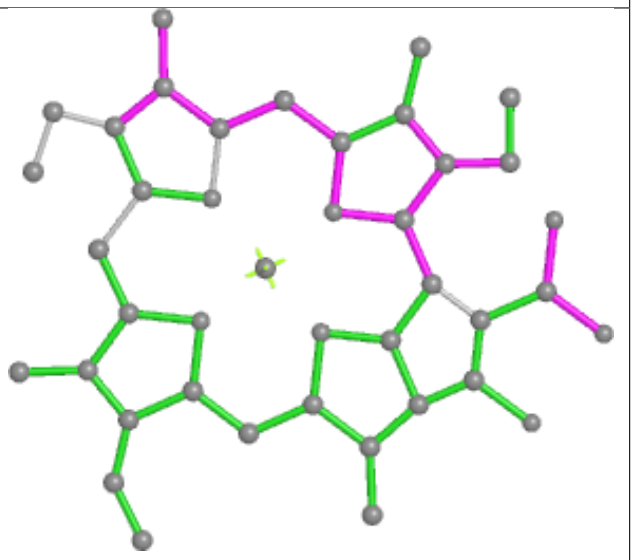


Rings

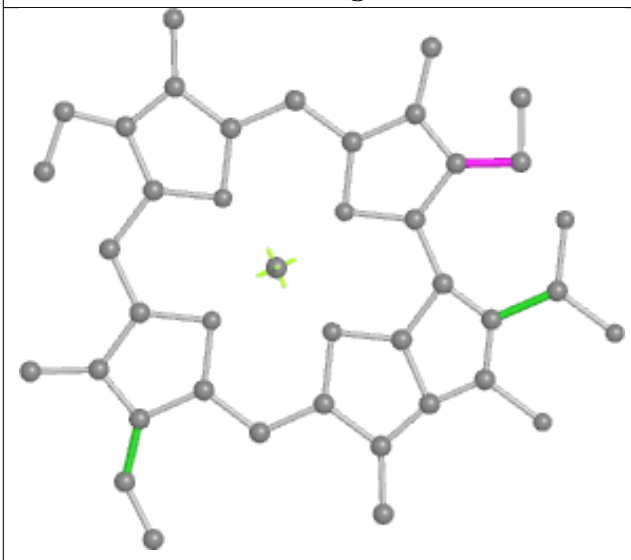
Ligand CLA 5 612



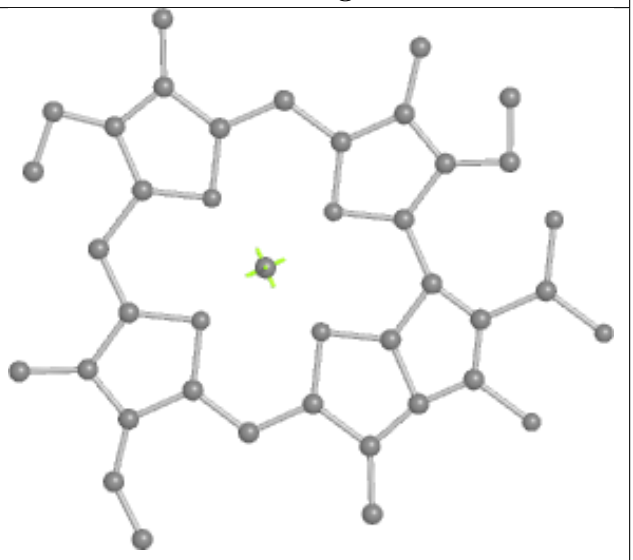
Bond lengths



Bond angles

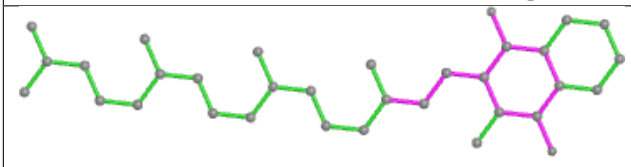


Torsions

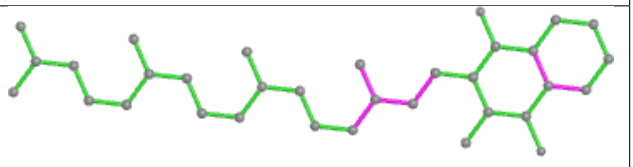


Rings

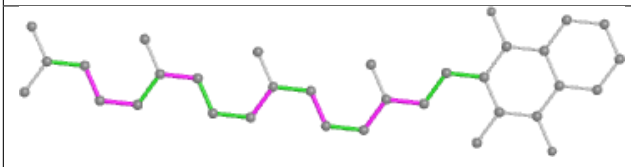
Ligand PQN B 842



Bond lengths



Bond angles



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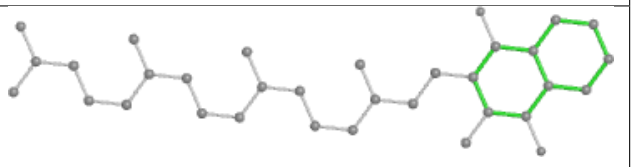
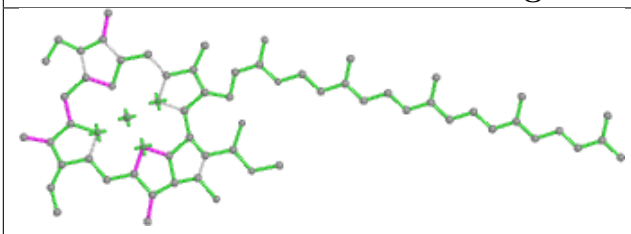
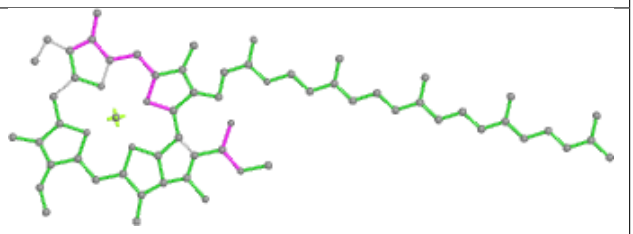


Rings

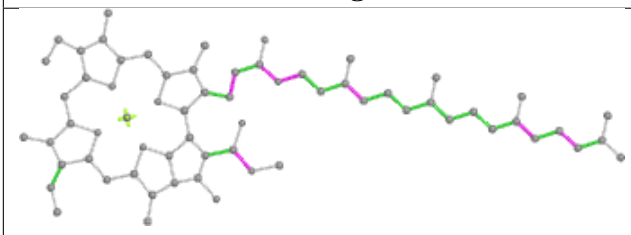
Ligand CLA B 831



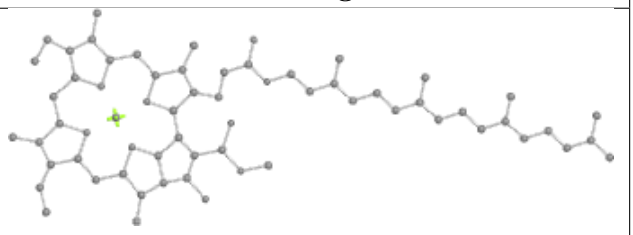
Bond lengths



Bond angles

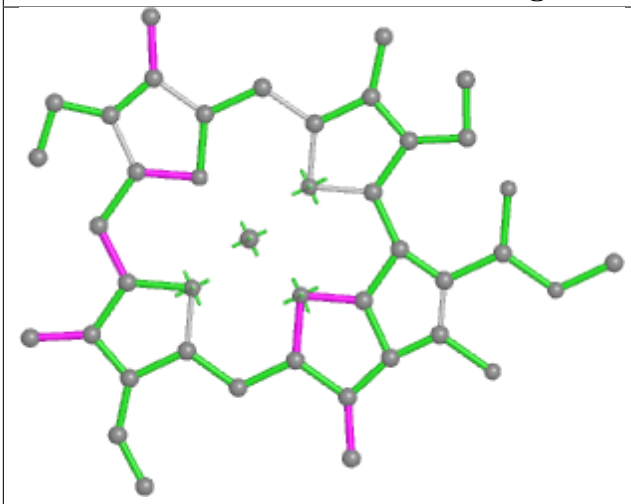


Torsions

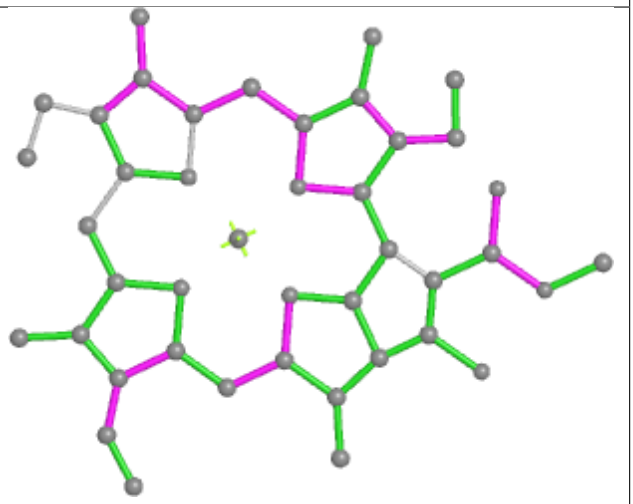


Rings

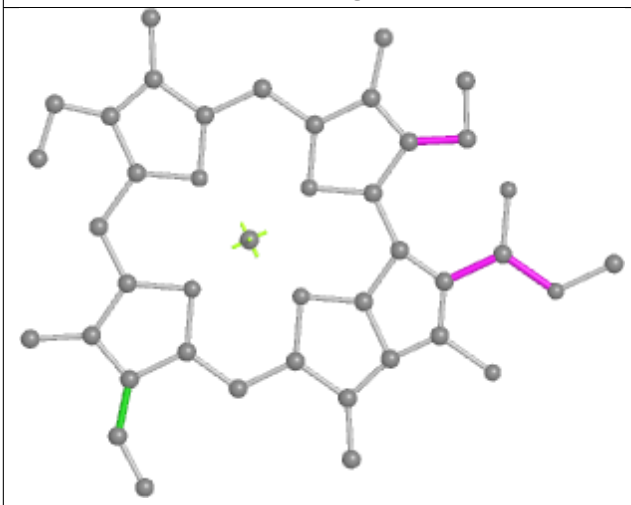
Ligand CLA 7 607



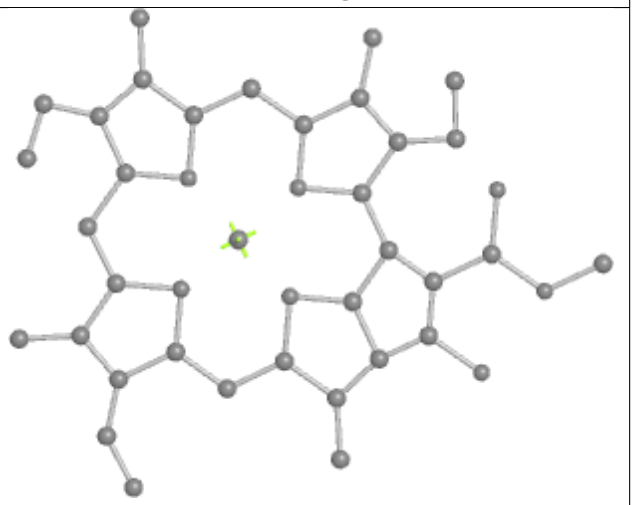
Bond lengths



Bond angles

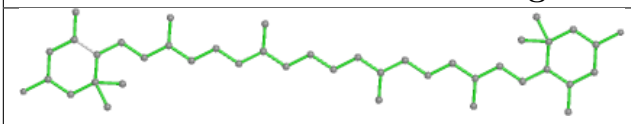


Torsions

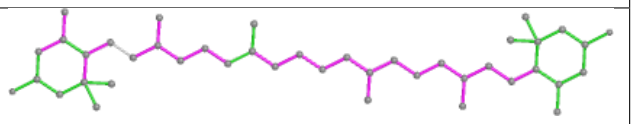


Rings

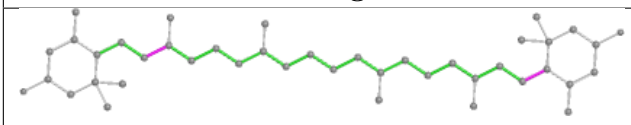
Ligand LUT 1 617



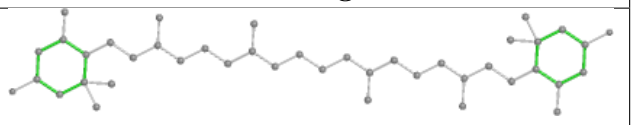
Bond lengths



Bond angles

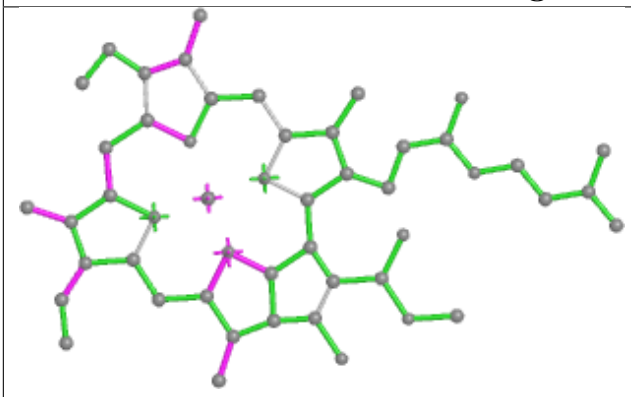


Torsions

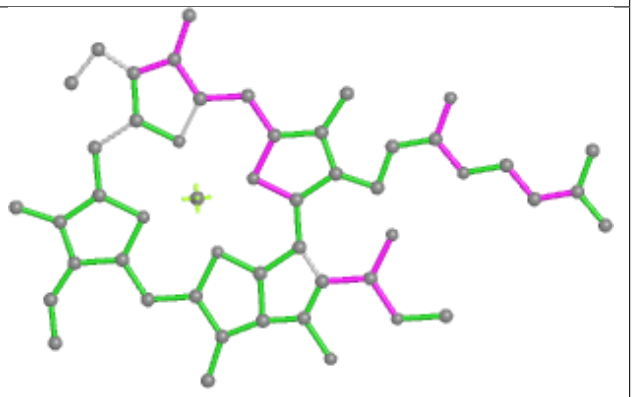


Rings

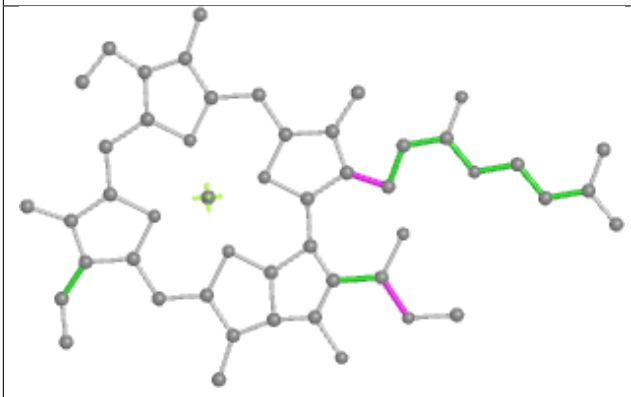
Ligand CLA 7 608



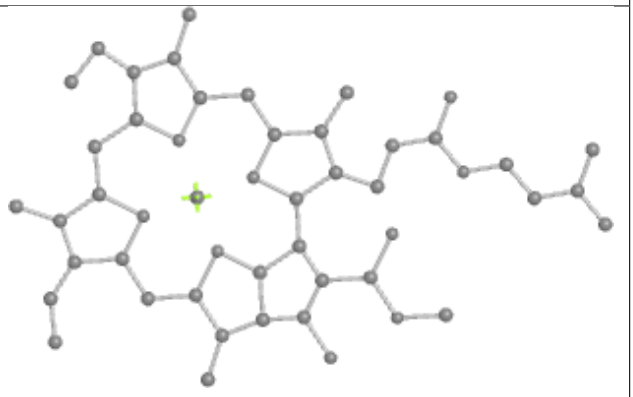
Bond lengths



Bond angles

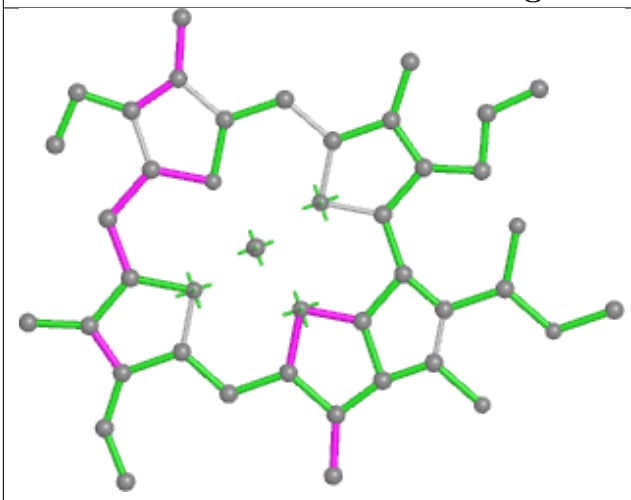


Torsions

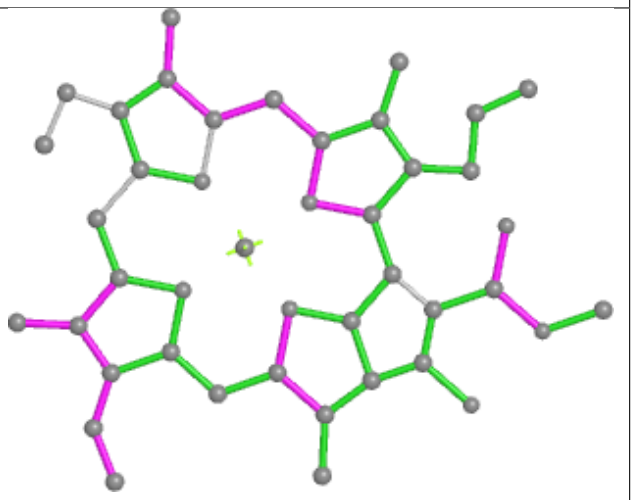


Rings

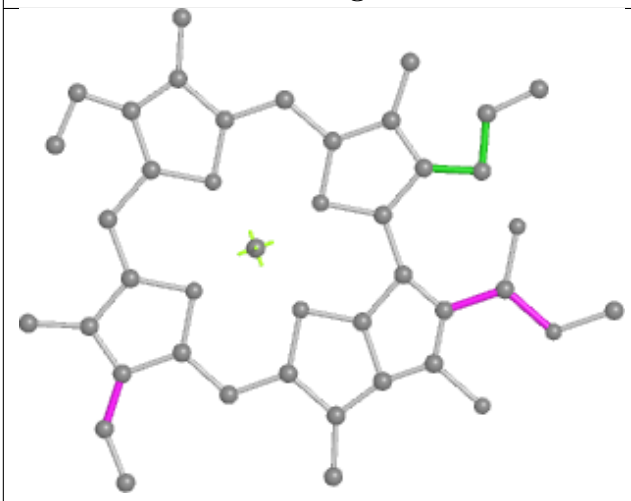
Ligand CLA B 830



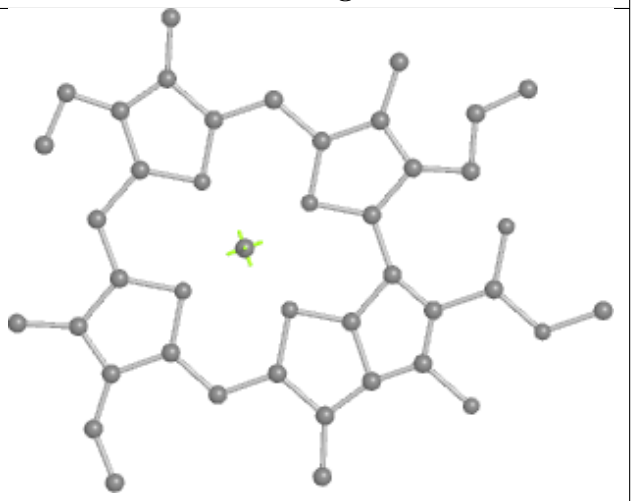
Bond lengths



Bond angles

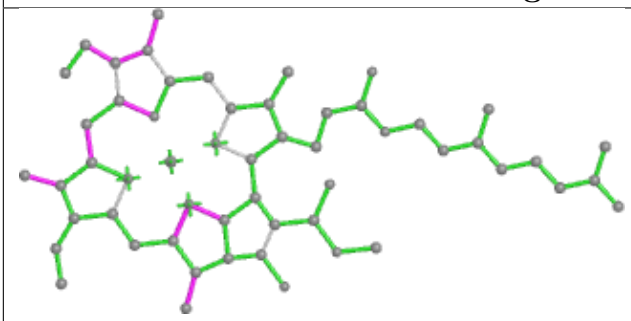


Torsions

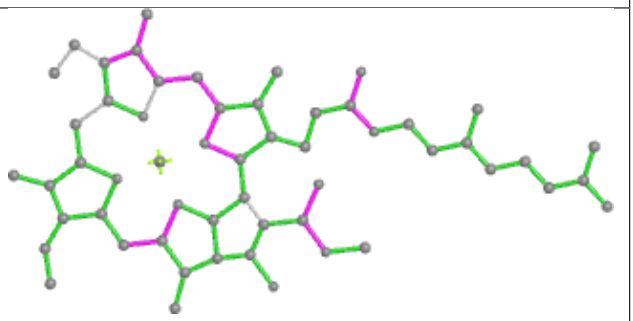


Rings

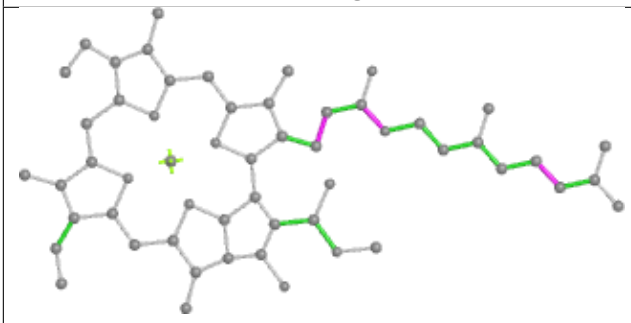
Ligand CLA A 839



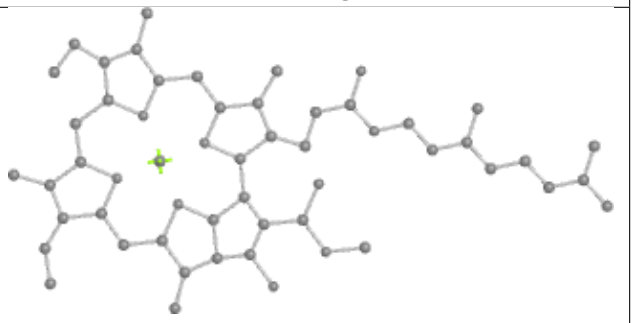
Bond lengths



Bond angles

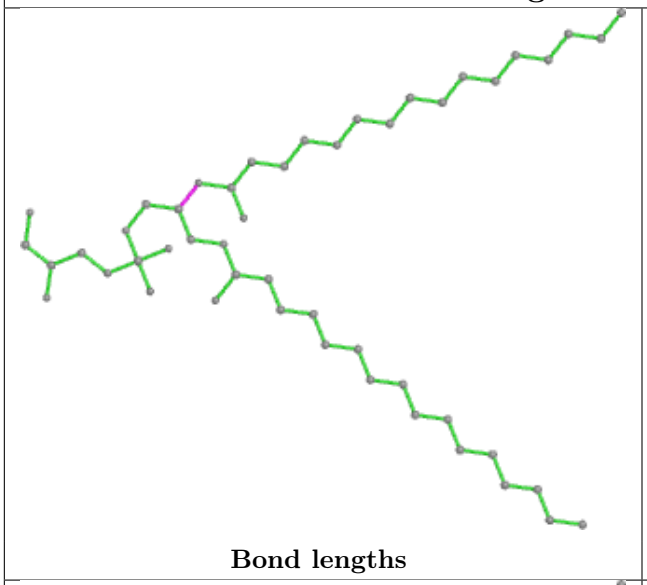


Torsions

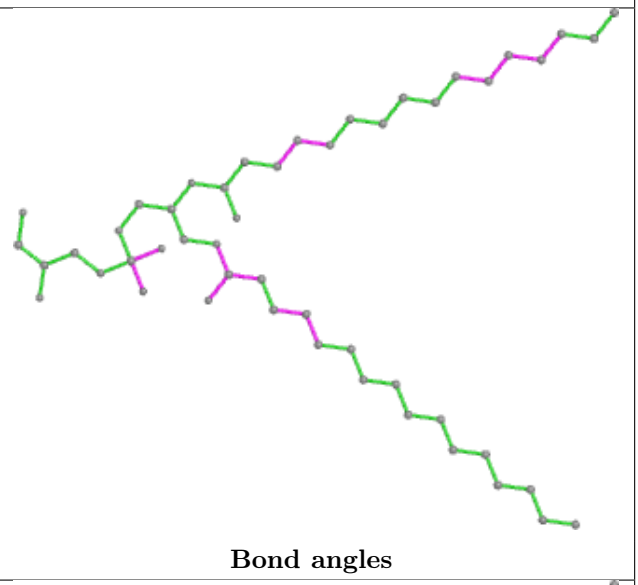


Rings

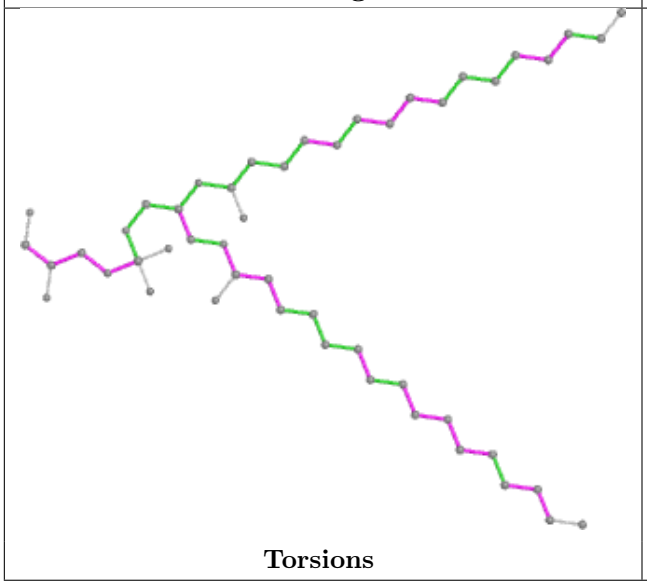
Ligand LHG 4 622



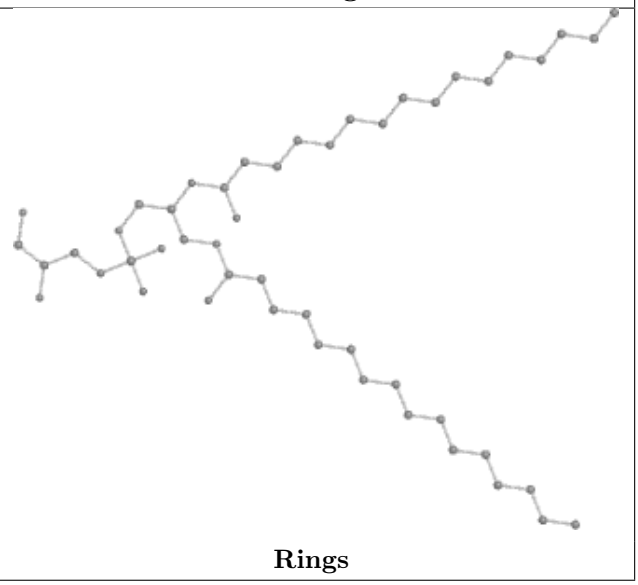
Bond lengths



Bond angles

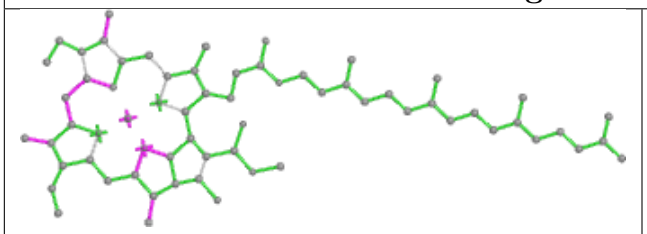


Torsions

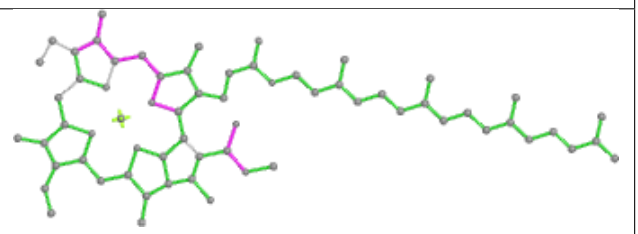


Rings

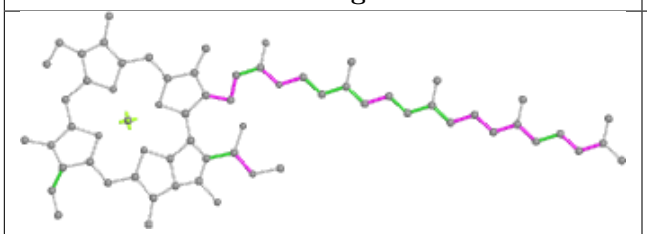
Ligand CLA B 809



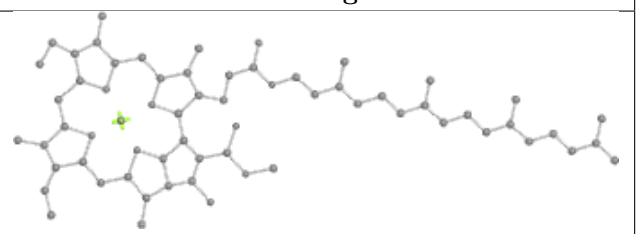
Bond lengths



Bond angles

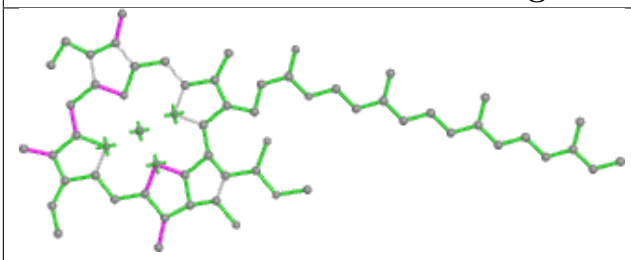


Torsions

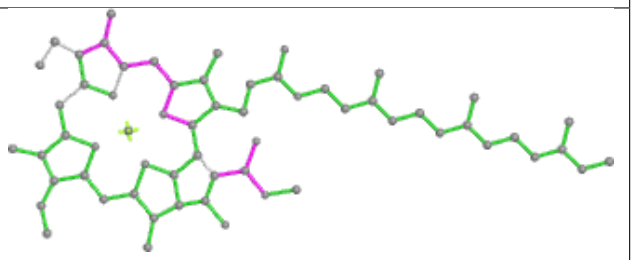


Rings

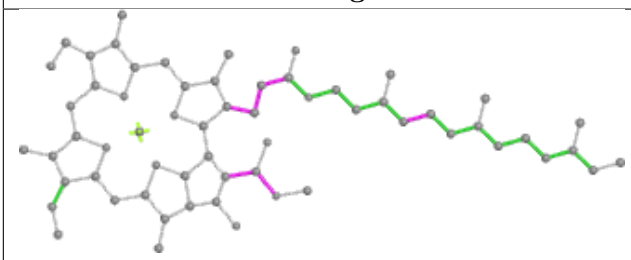
Ligand CLA 1 602



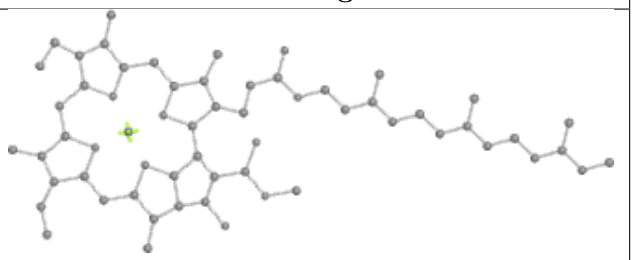
Bond lengths



Bond angles

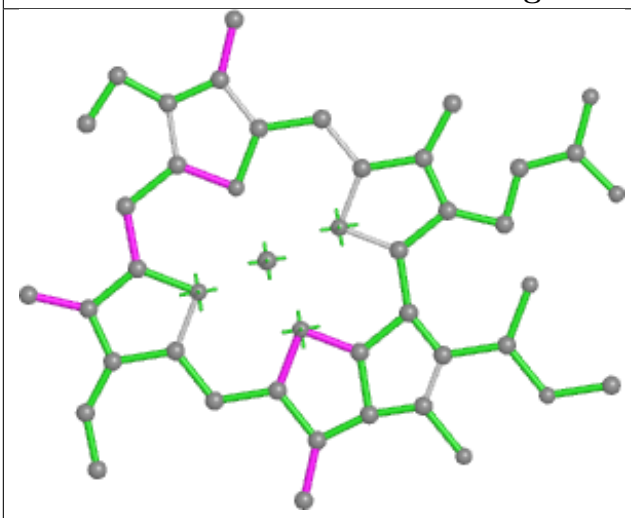


Torsions

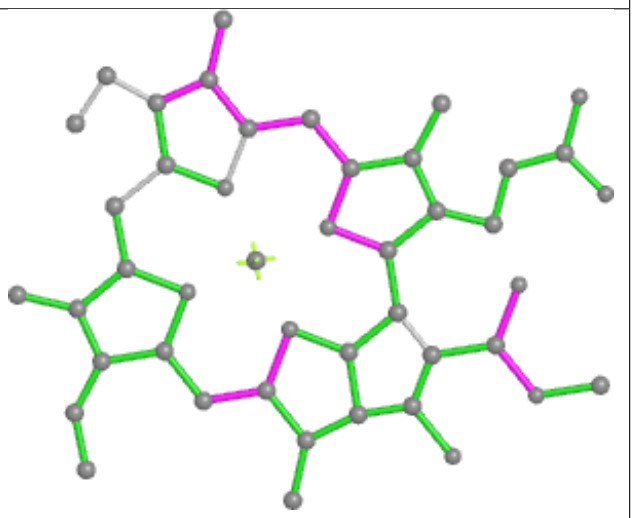


Rings

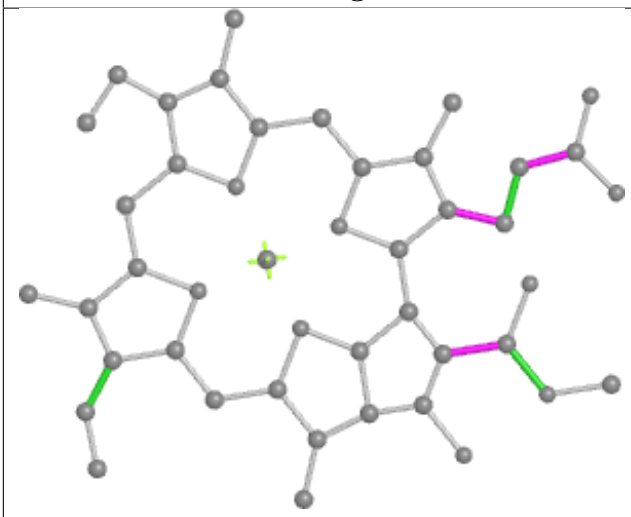
Ligand CLA A 816



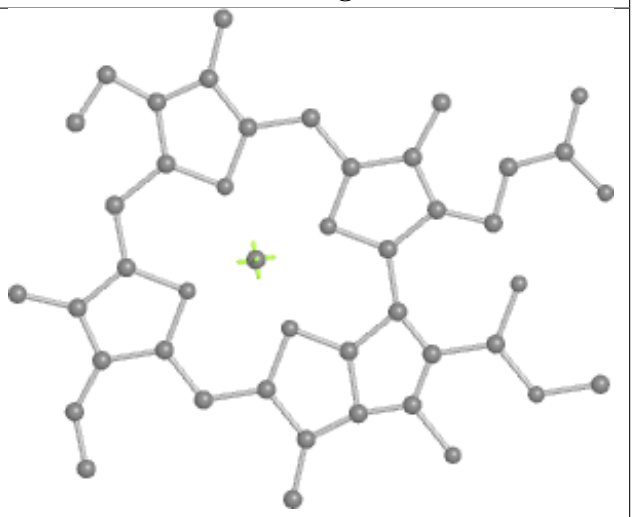
Bond lengths



Bond angles

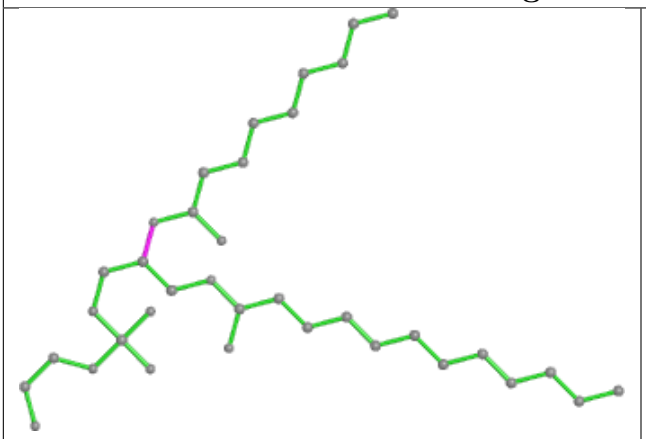


Torsions



Rings

Ligand LHG B 851



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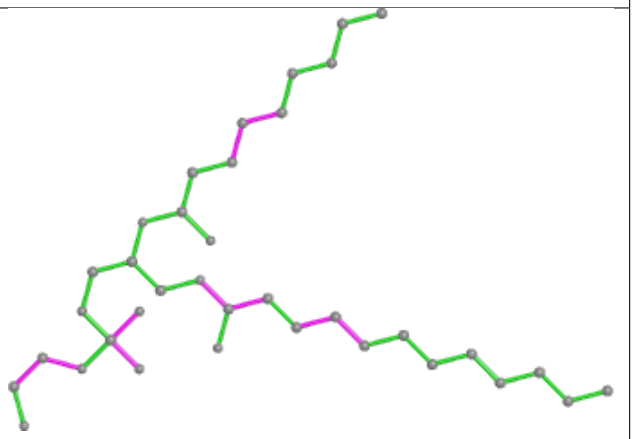
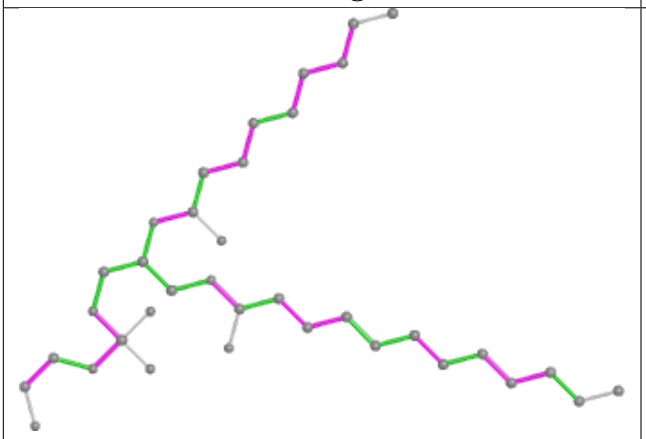


Bond angles



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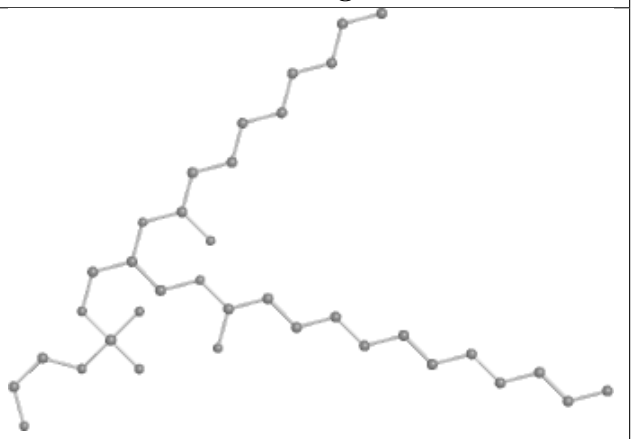
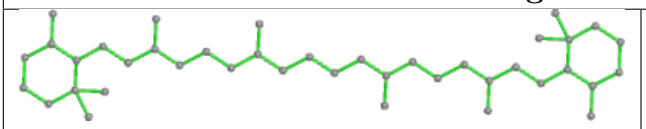
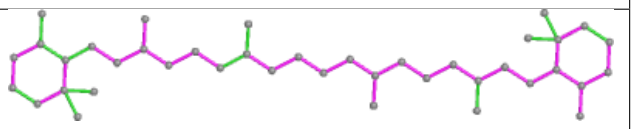


Rings

Ligand BCR J 102



Bond lengths

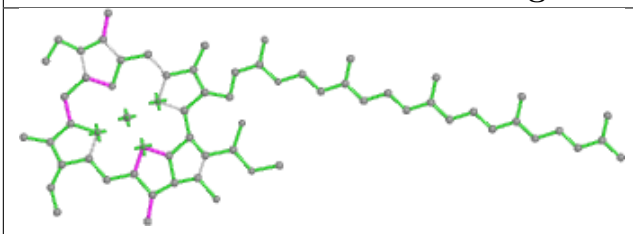


Bond angles

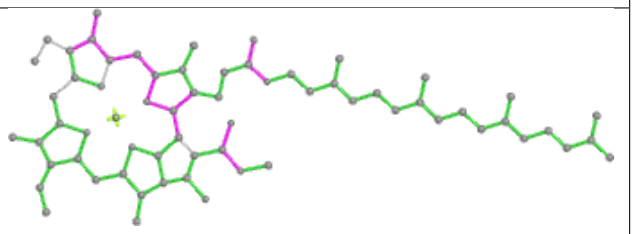
Torsions

Rings

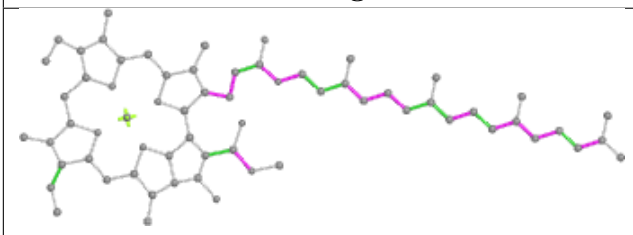
Ligand CLA a 609



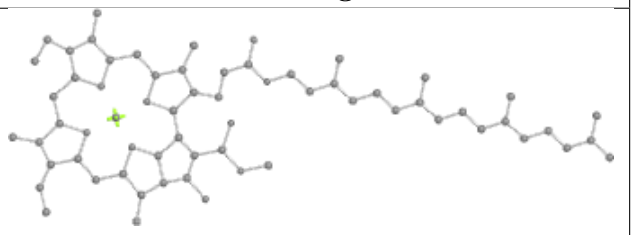
Bond lengths



Bond angles

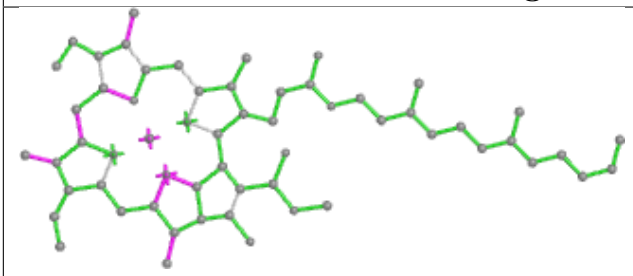


Torsions

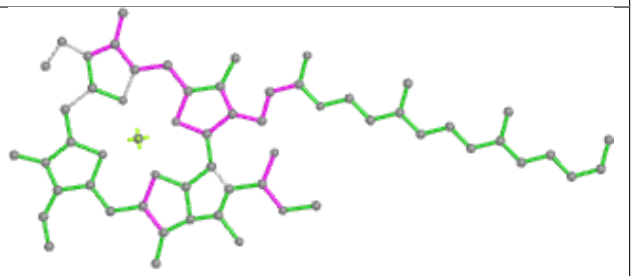


Rings

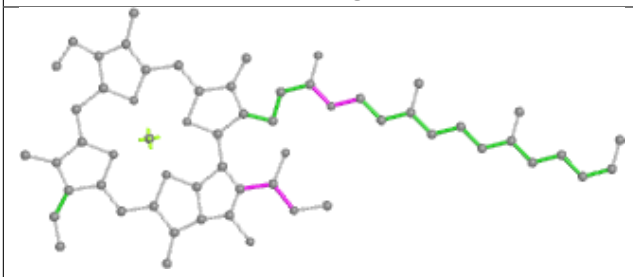
Ligand CLA A 827



Bond lengths



Bond angles



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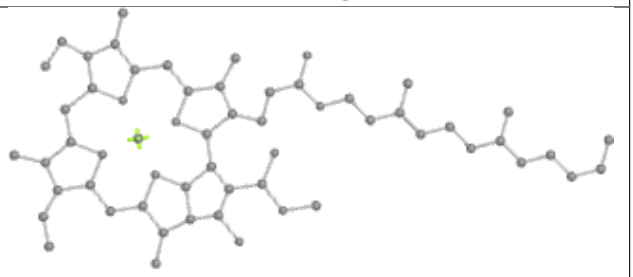
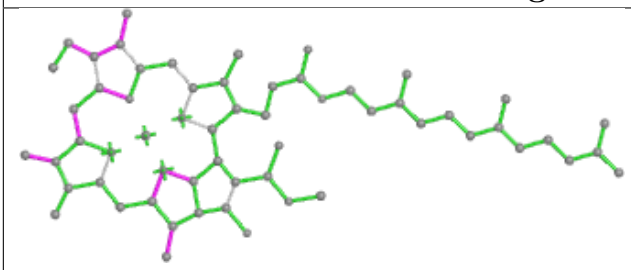


Rings

Ligand CLA a 610



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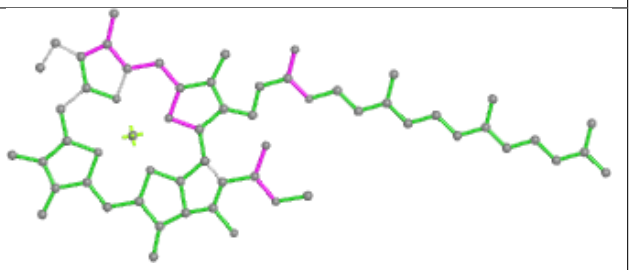
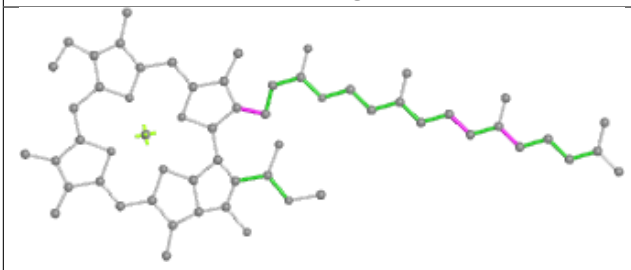


Bond angles



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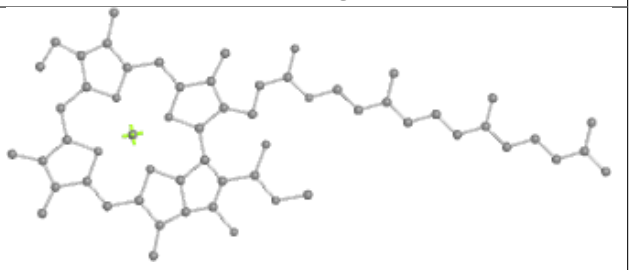
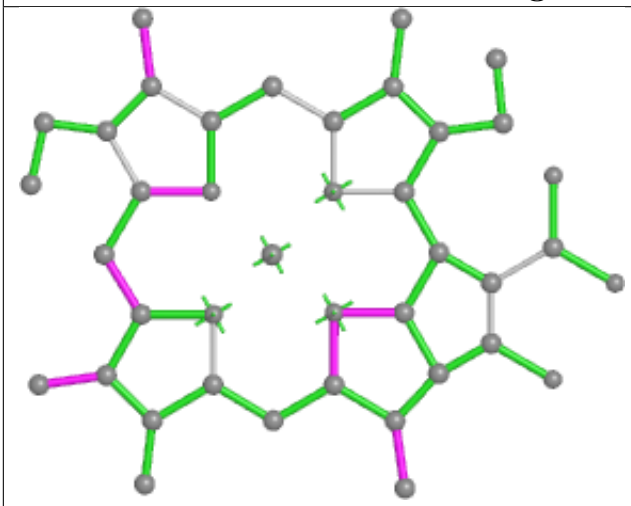
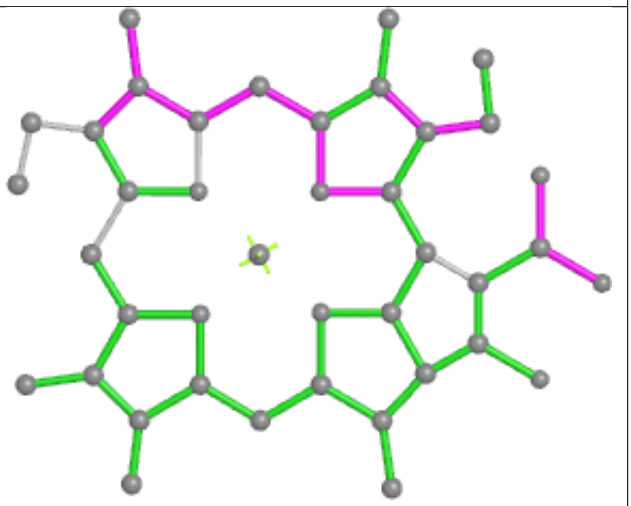


Rings

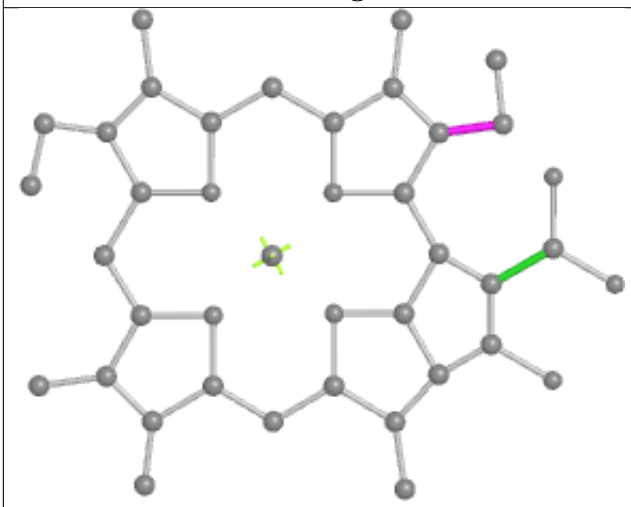
Ligand CLA 4 606



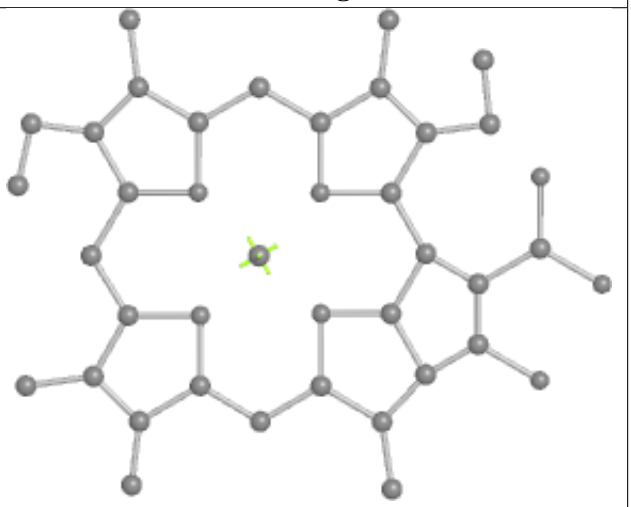
Bond lengths



Bond angles

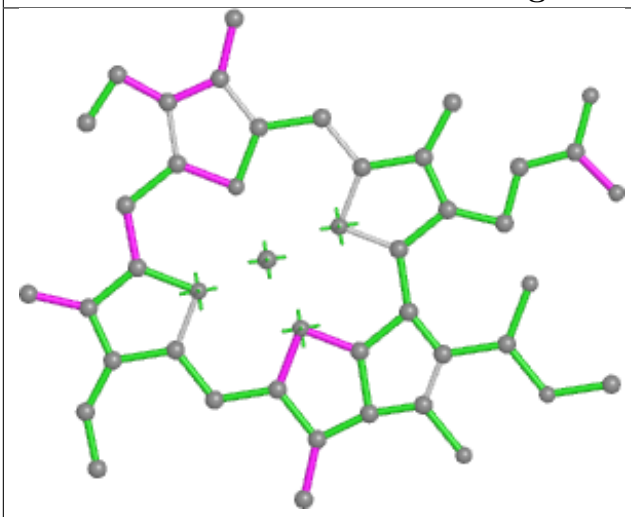


Torsions

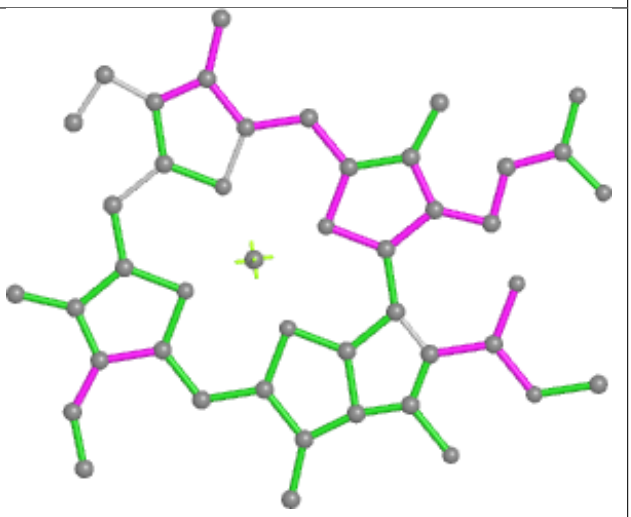


Rings

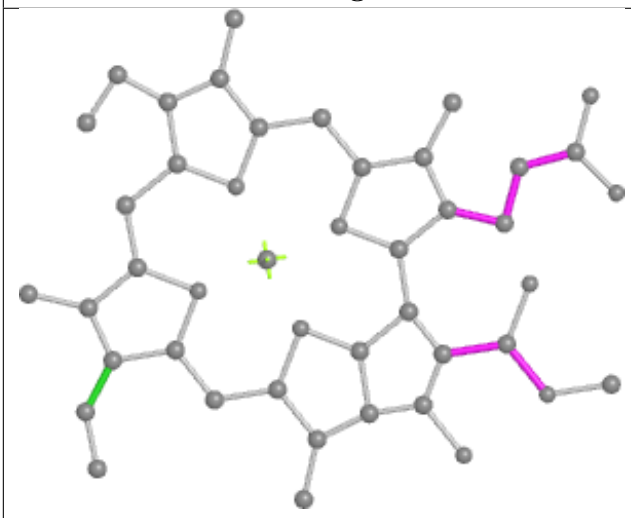
Ligand CLA 6 620



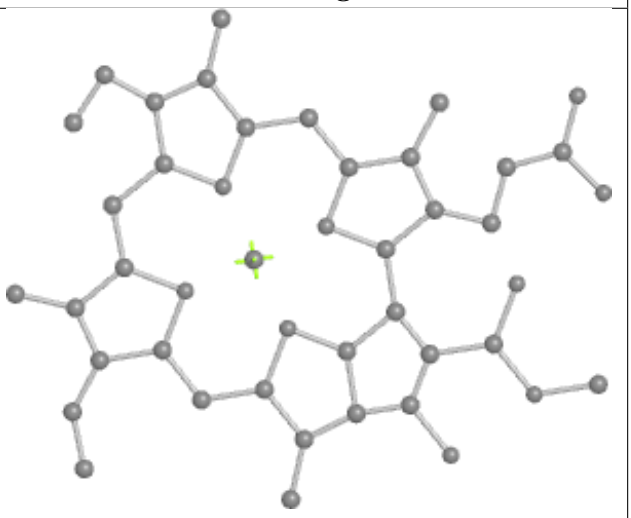
Bond lengths



Bond angles

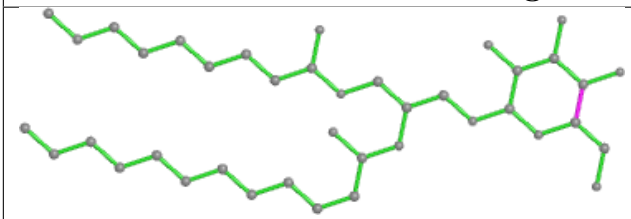


Torsions



Rings

Ligand LMG 4 623



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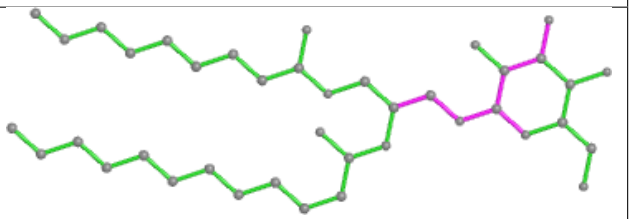
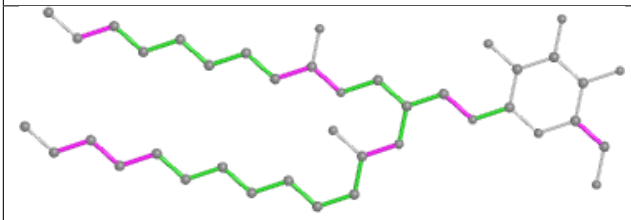


Bond angles



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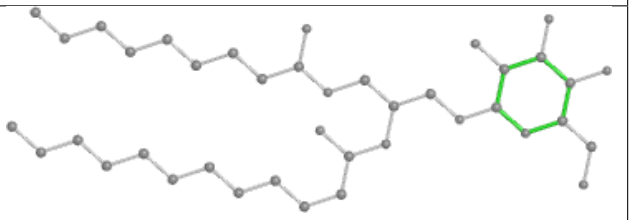
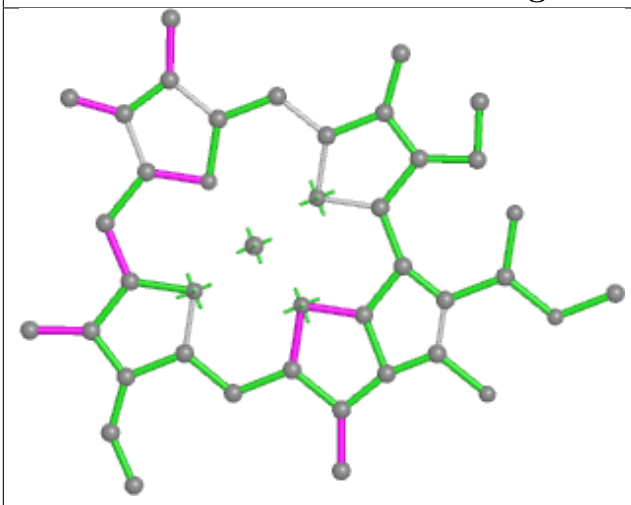
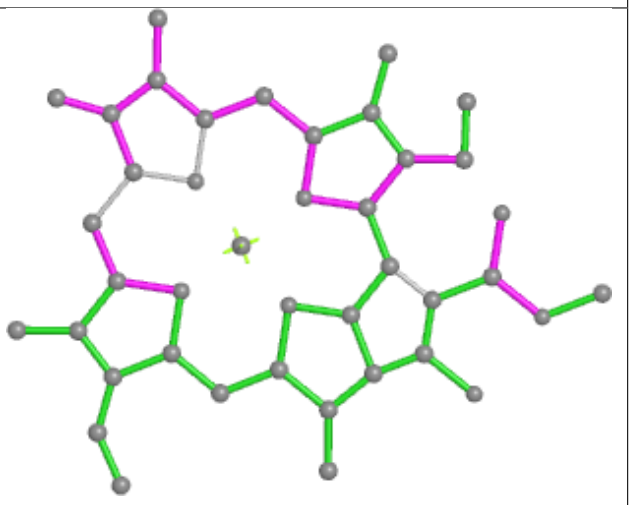


Rings

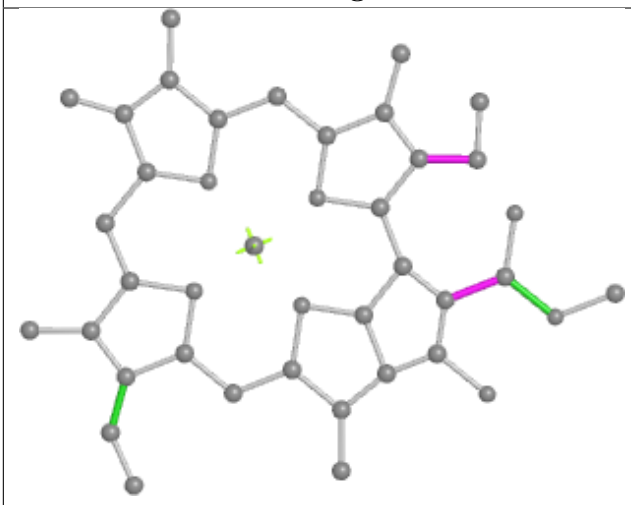
Ligand CLA 6 607



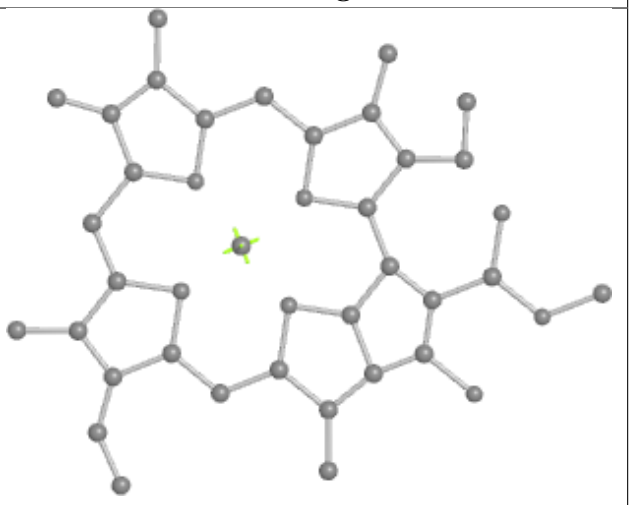
Bond lengths



Bond angles

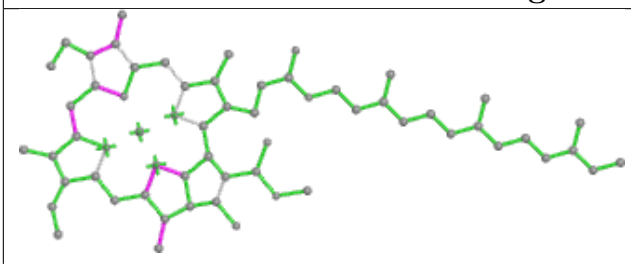


Torsions

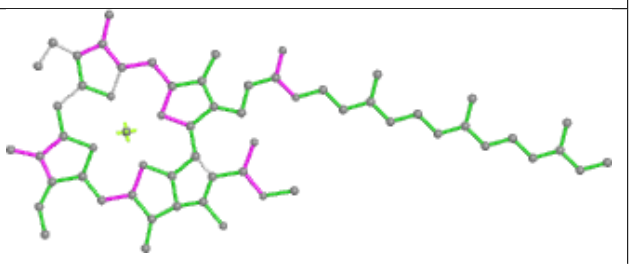


Rings

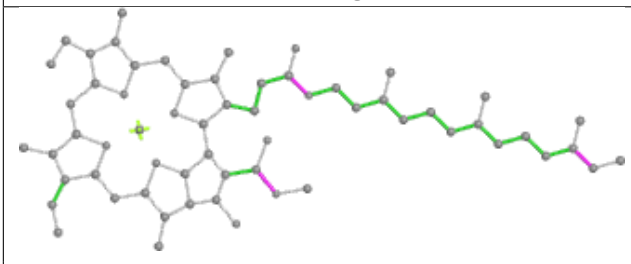
Ligand CLA 4 609



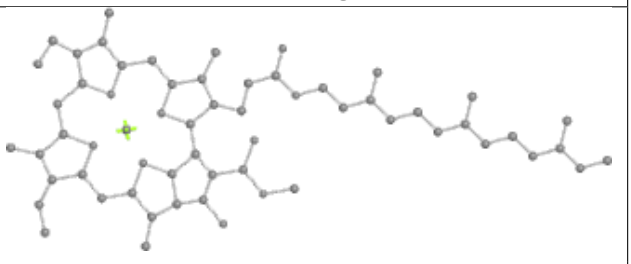
Bond lengths



Bond angles

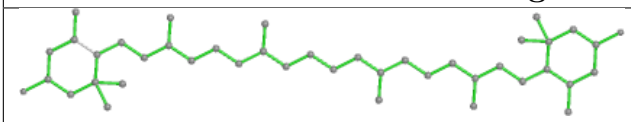


Torsions

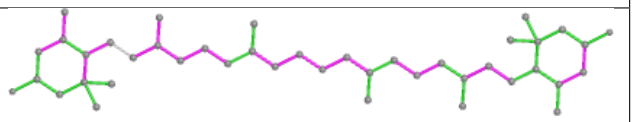


Rings

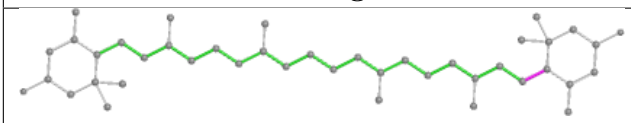
Ligand LUT 4 619



Bond lengths



Bond angles



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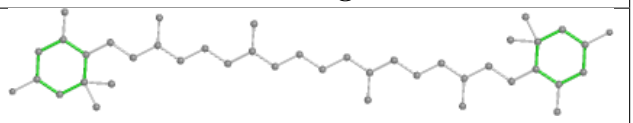
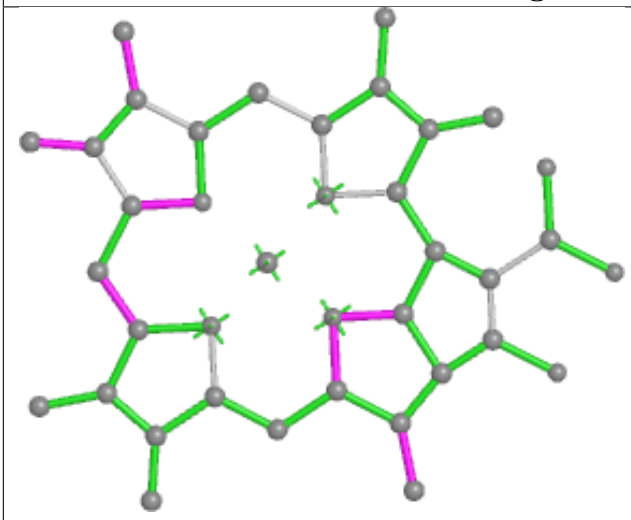


Rings

Ligand CLA a 611



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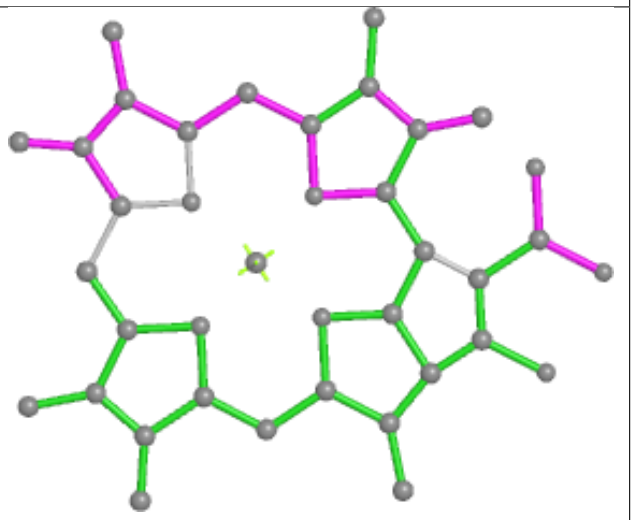
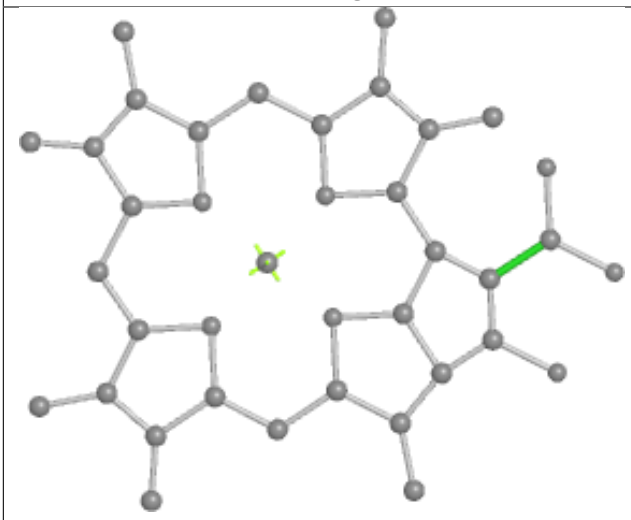


Bond angles



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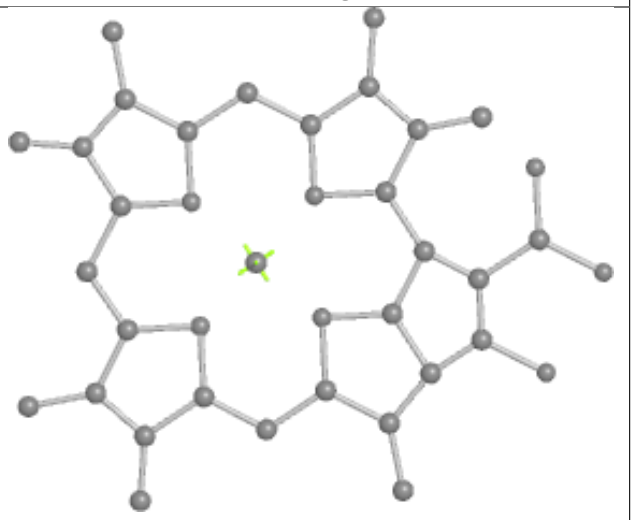
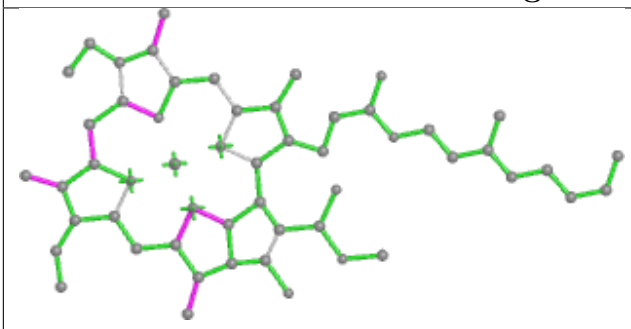
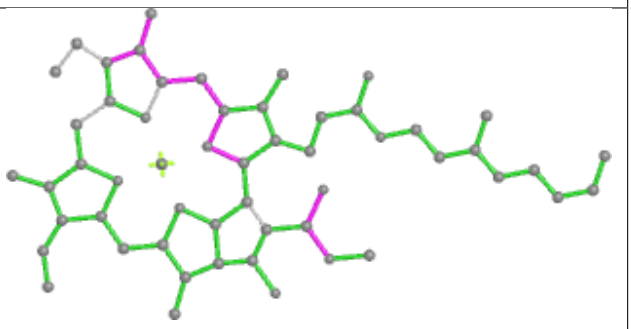
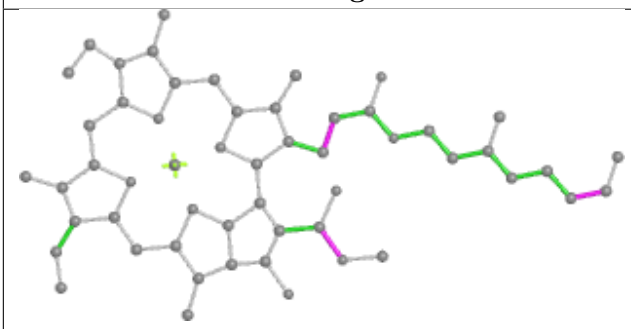
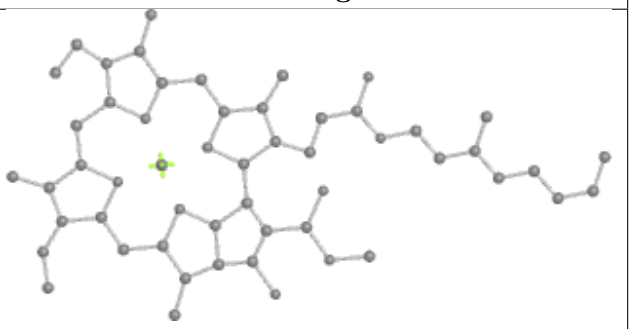
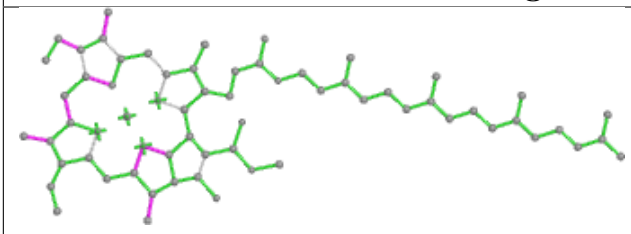
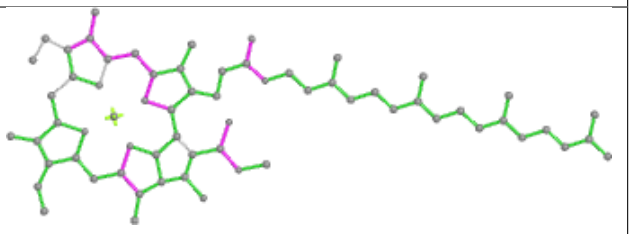
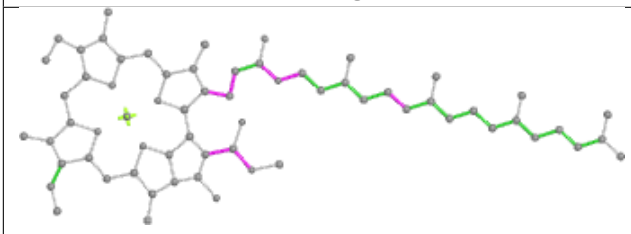
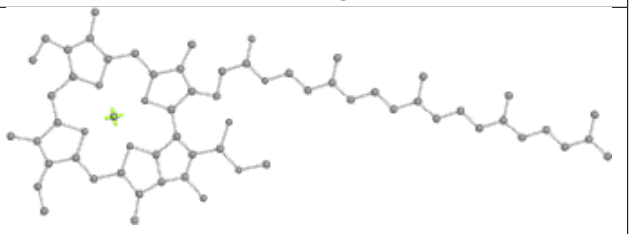
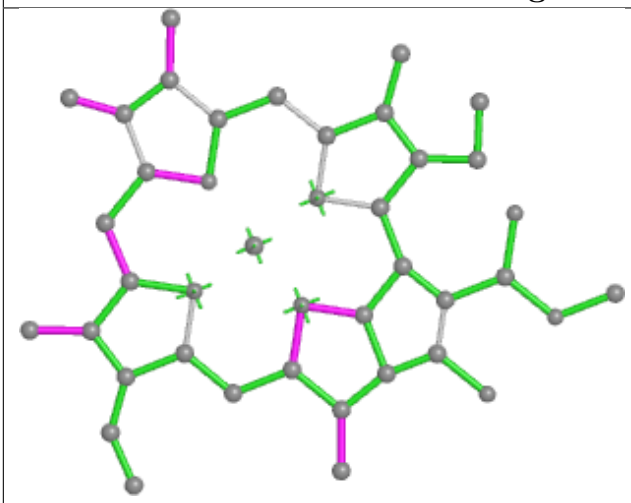


Rings

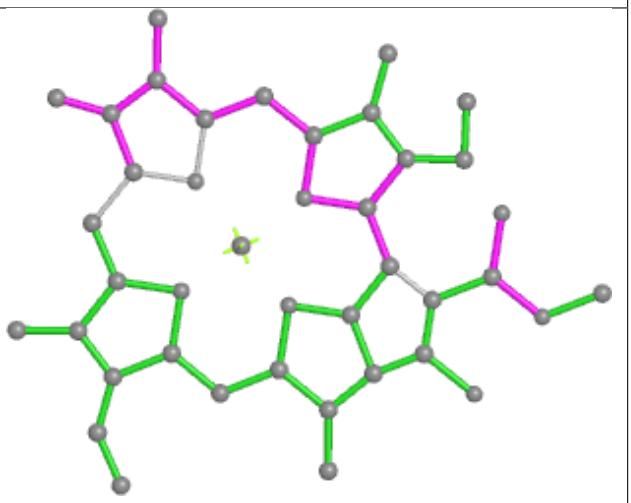
Ligand CLA A 813	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA B 839	
	
Bond lengths	Bond angles
	
Torsions	Rings

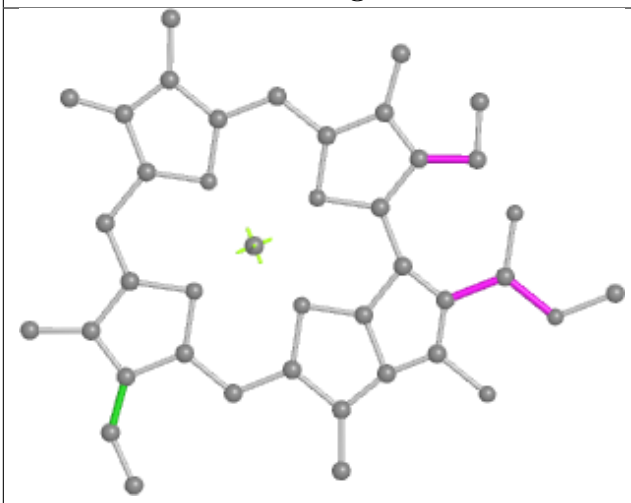
Ligand CLA 8 607



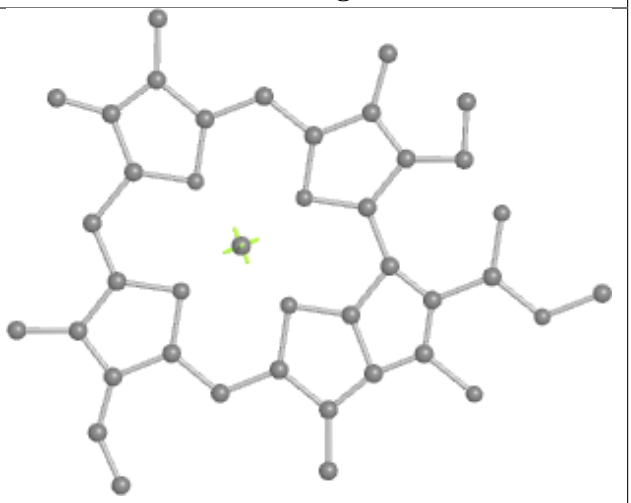
Bond lengths



Bond angles

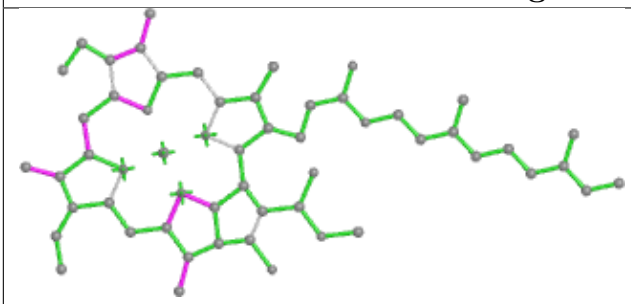


Torsions

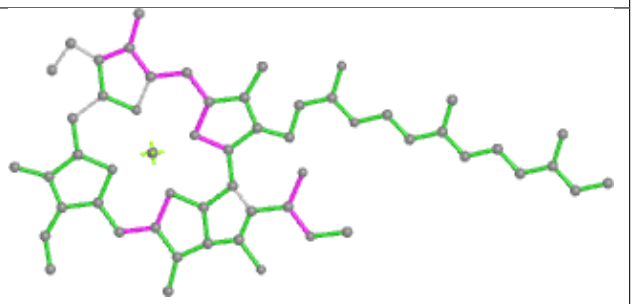


Rings

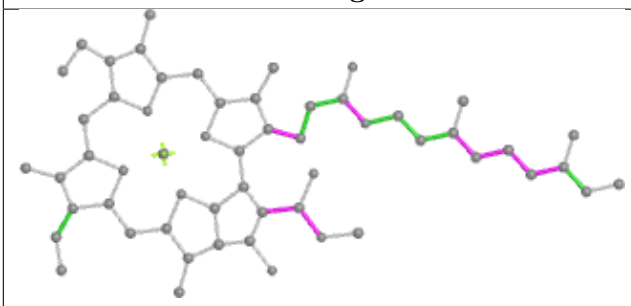
Ligand CLA 4 614



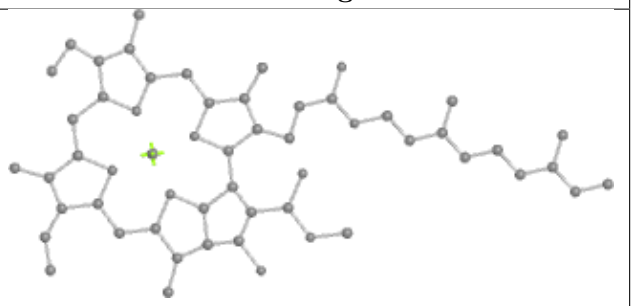
Bond lengths



Bond angles

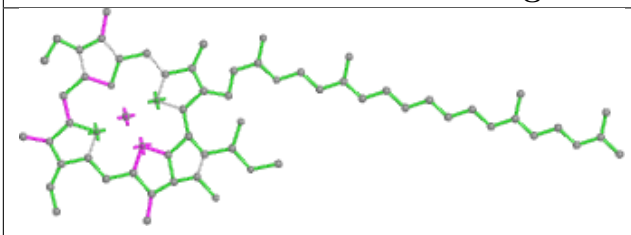


Torsions

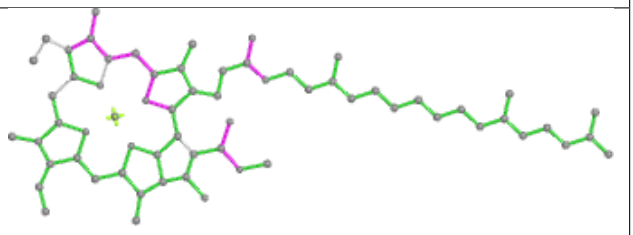


Rings

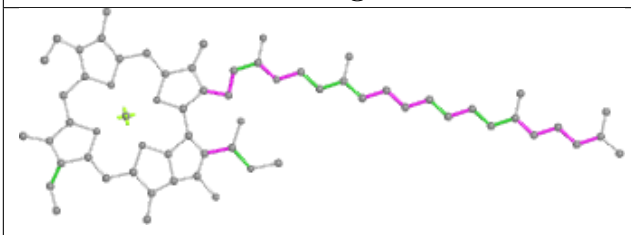
Ligand CLA A 843



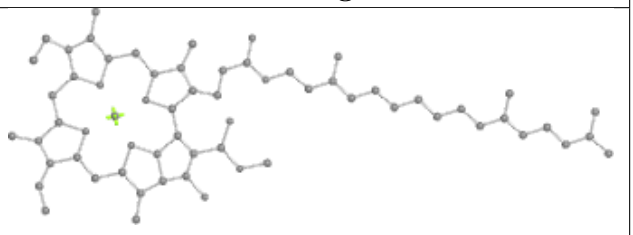
Bond lengths



Bond angles

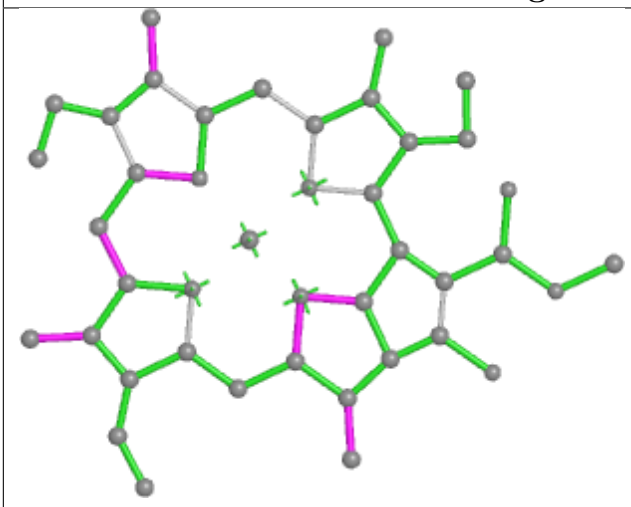


Torsions

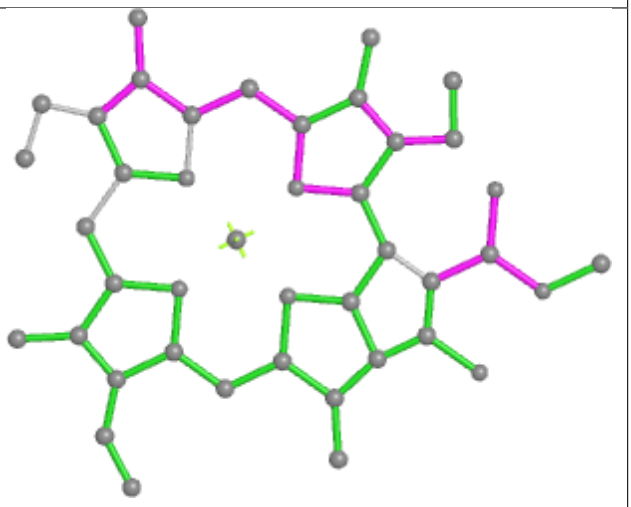


Rings

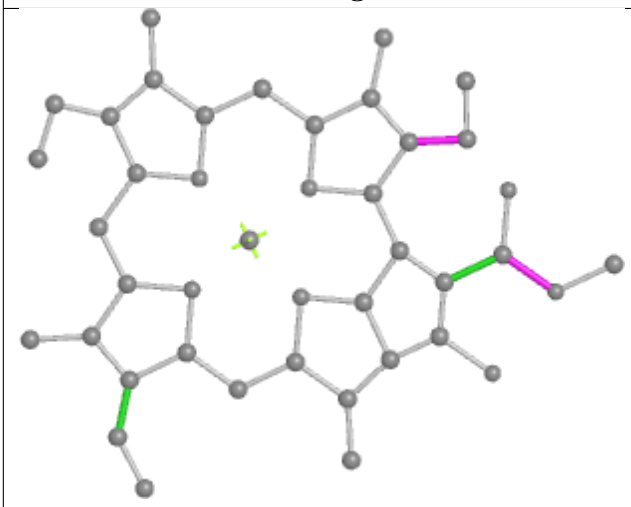
Ligand CLA 8 611



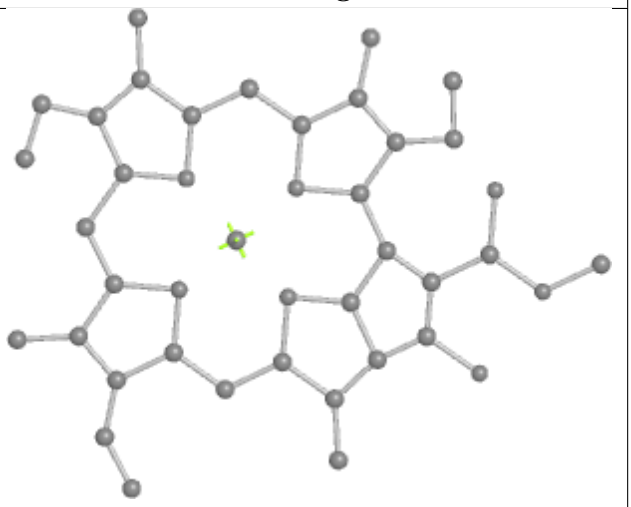
Bond lengths



Bond angles

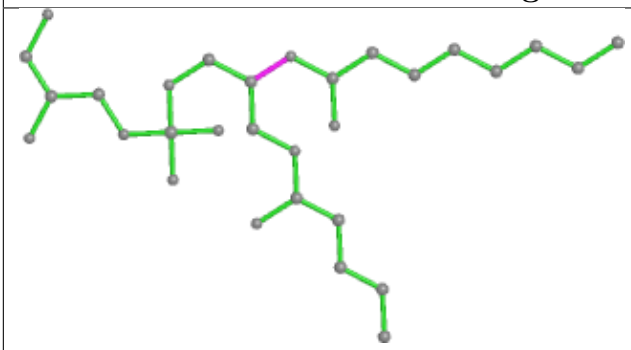


Torsions

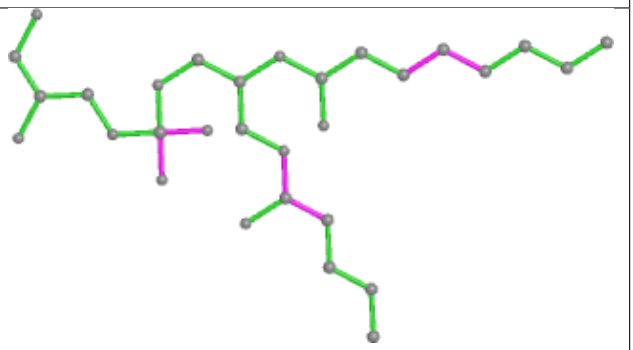


Rings

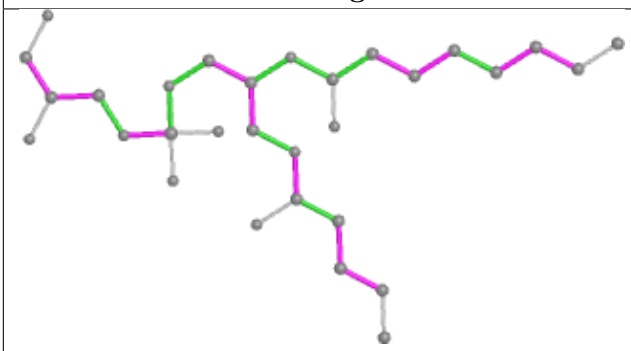
Ligand LHG A 847



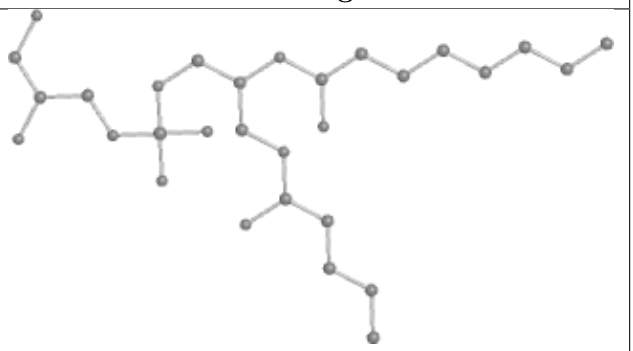
Bond lengths



Bond angles

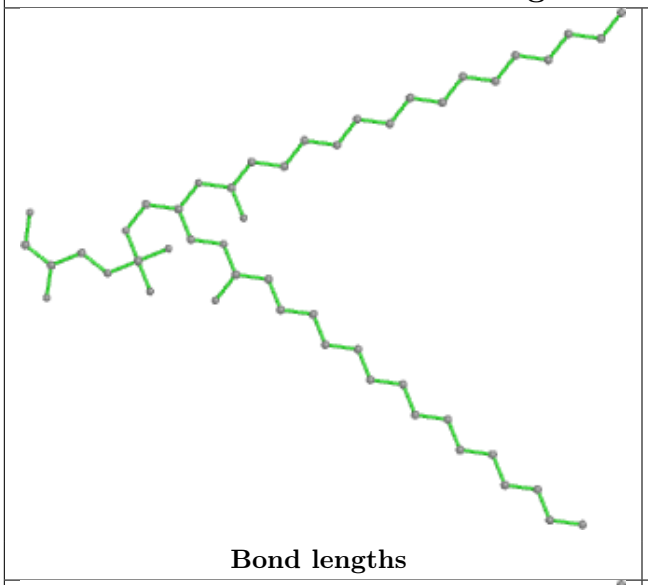


Torsions

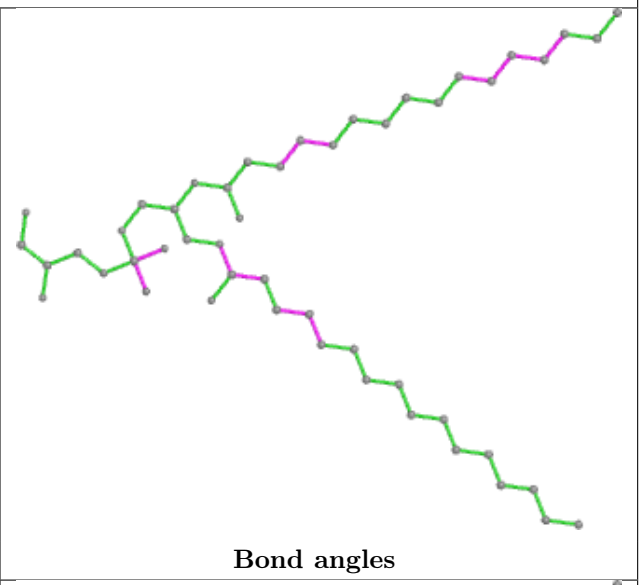


Rings

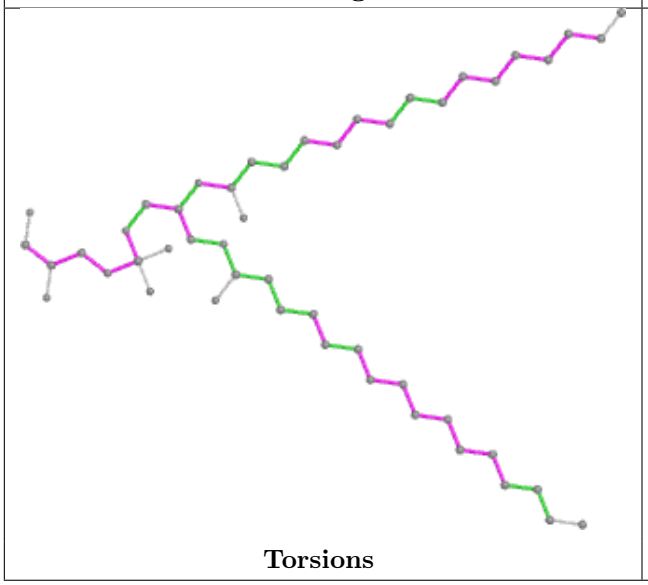
Ligand LHG 8 623



Bond lengths



Bond angles



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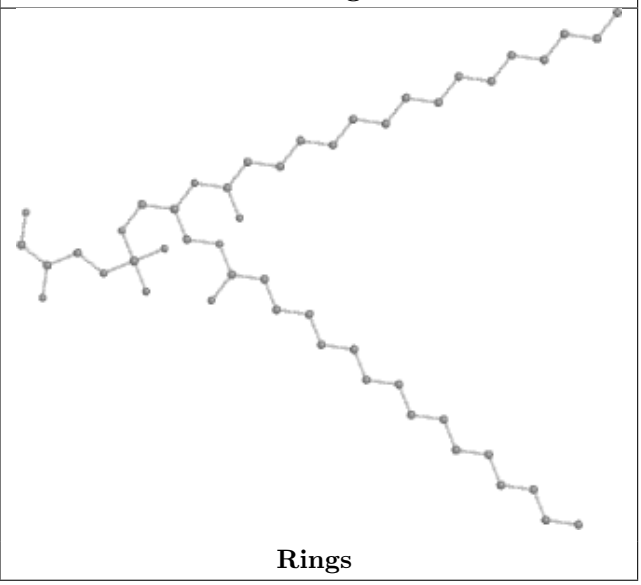
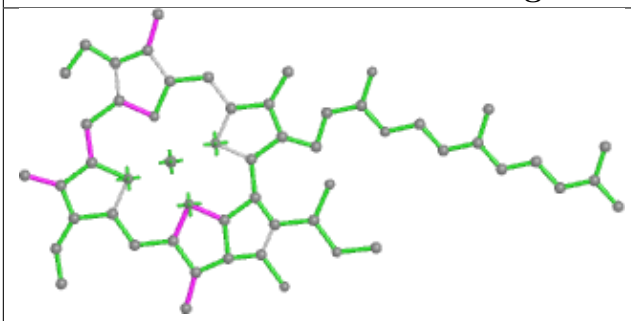
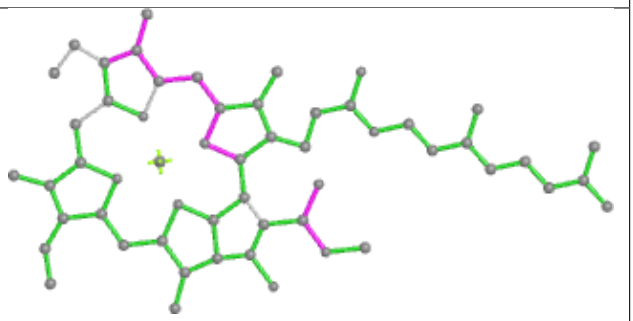


Rings

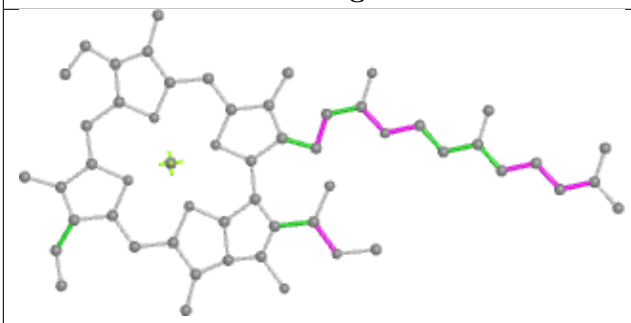
Ligand CLA B 816



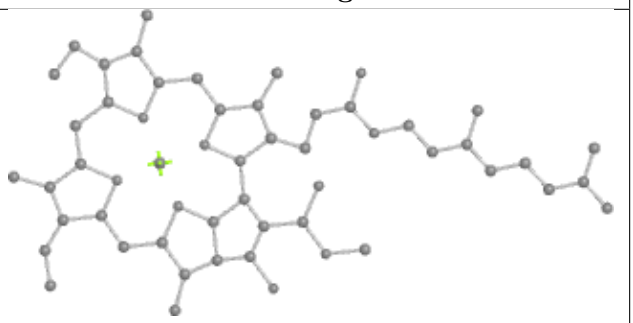
Bond lengths



Bond angles

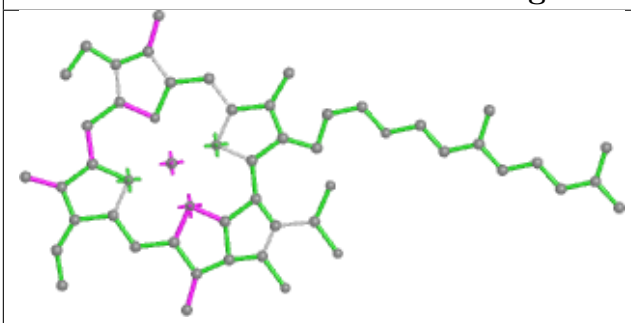


Torsions

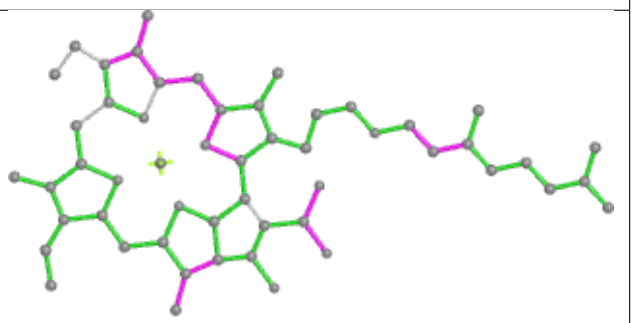


Rings

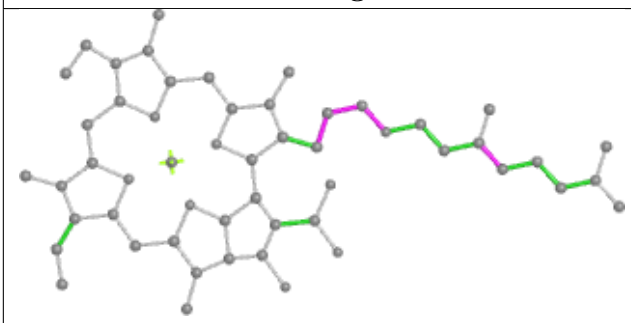
Ligand CLA 3 613



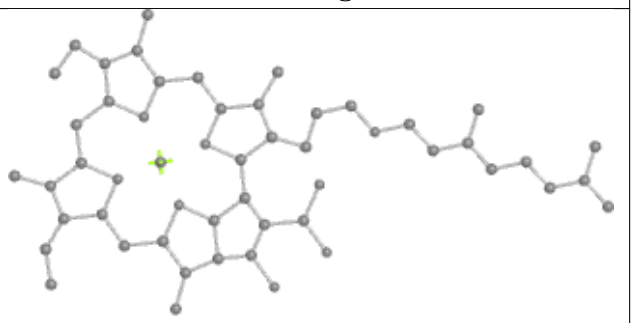
Bond lengths



Bond angles

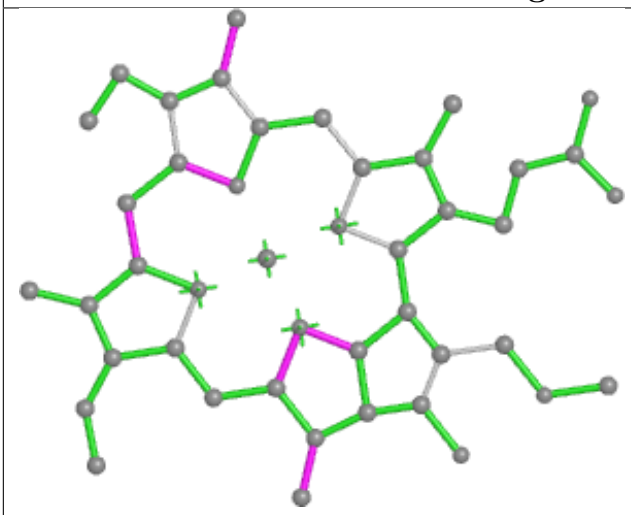


Torsions

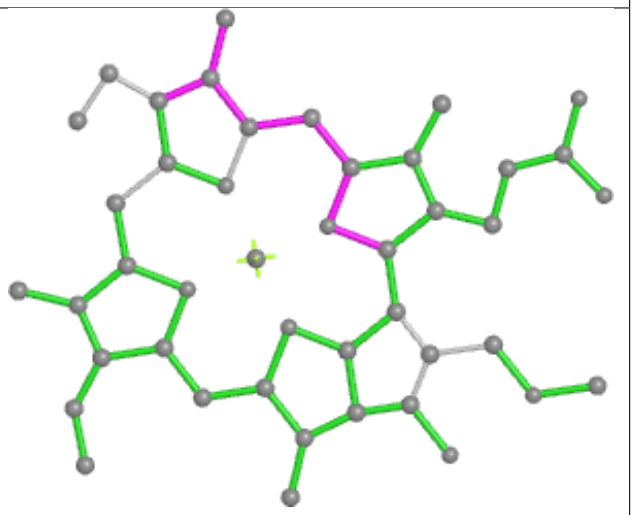


Rings

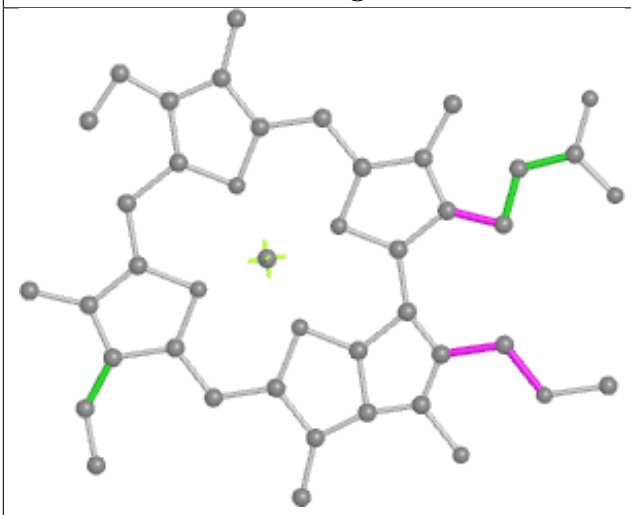
Ligand CLA a 606



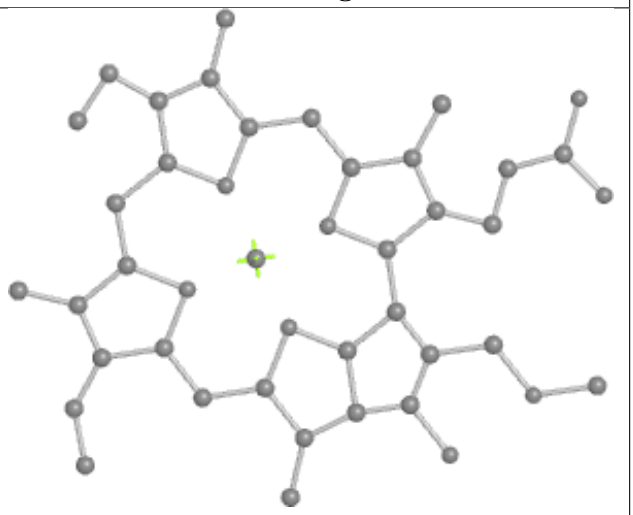
Bond lengths



Bond angles

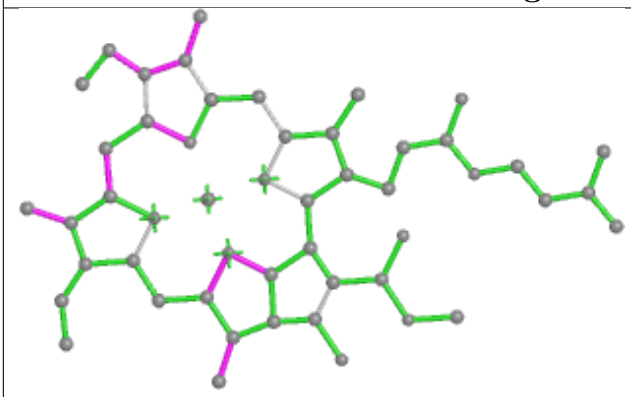


Torsions

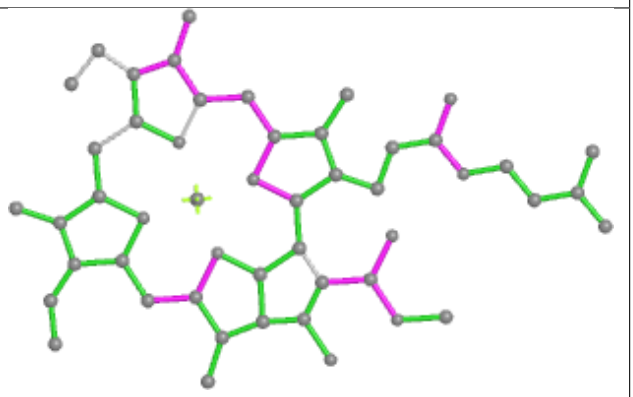


Rings

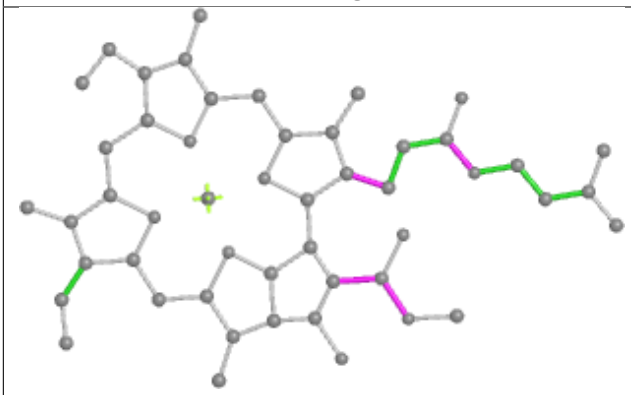
Ligand CLA A 815



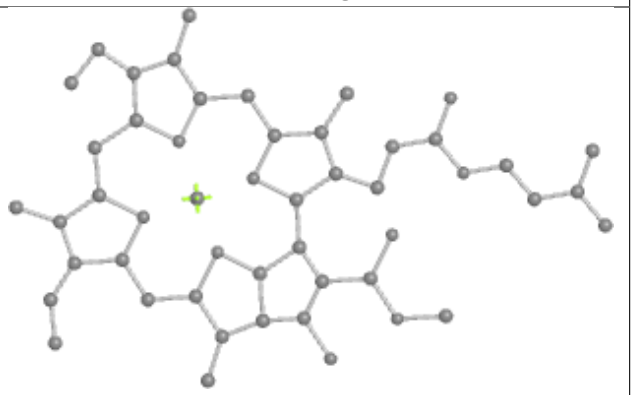
Bond lengths



Bond angles

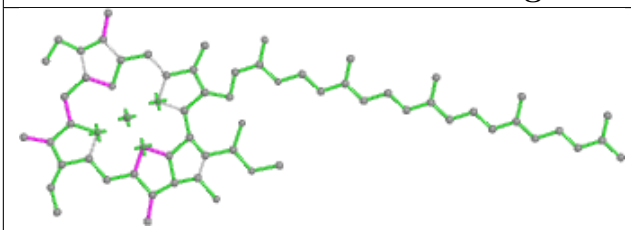


Torsions

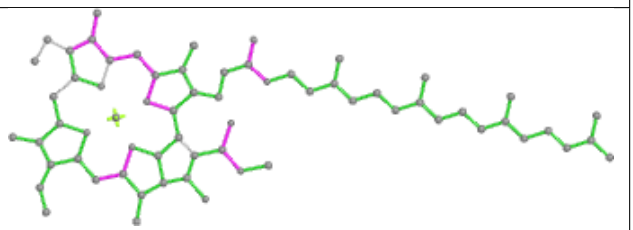


Rings

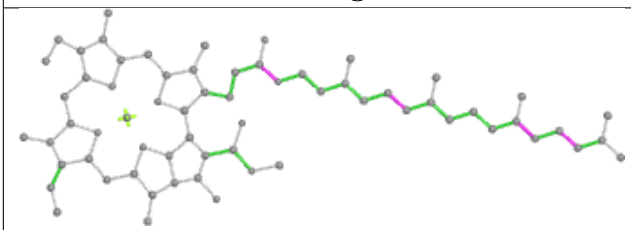
Ligand CLA B 837



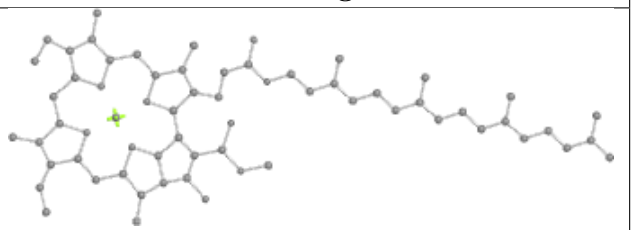
Bond lengths



Bond angles

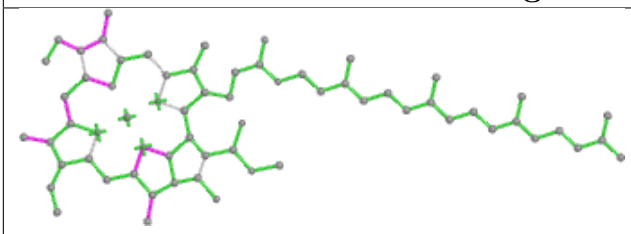


Torsions

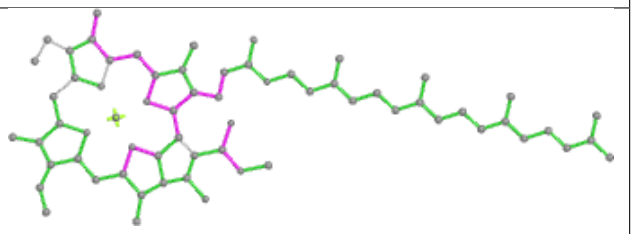


Rings

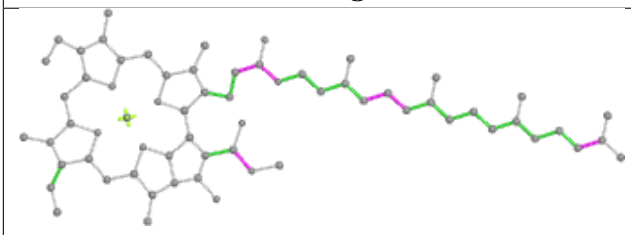
Ligand CLA A 801



Bond lengths



Bond angles



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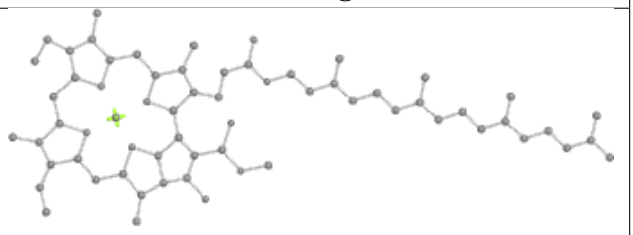
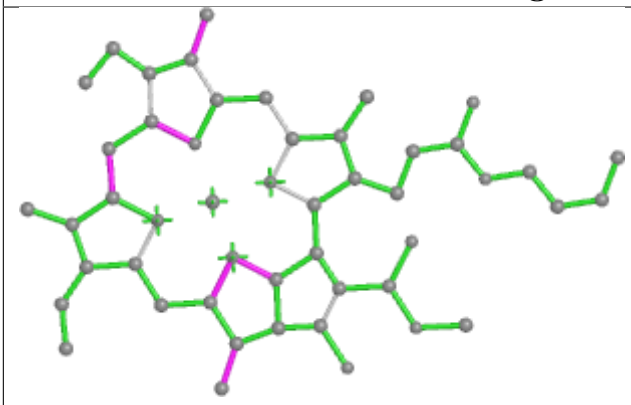
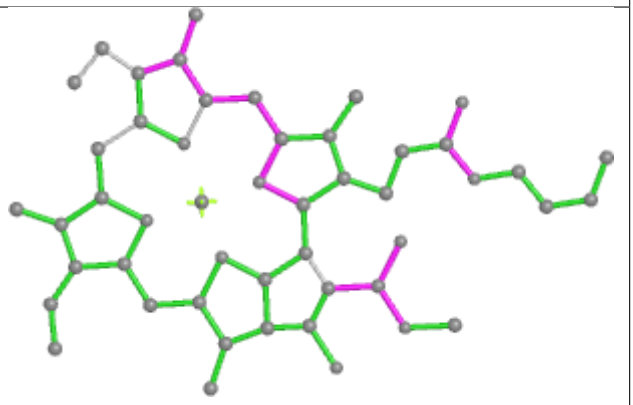


Rings

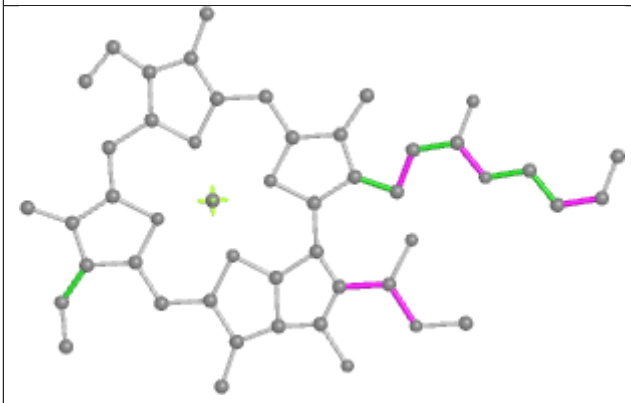
Ligand CLA 1 604



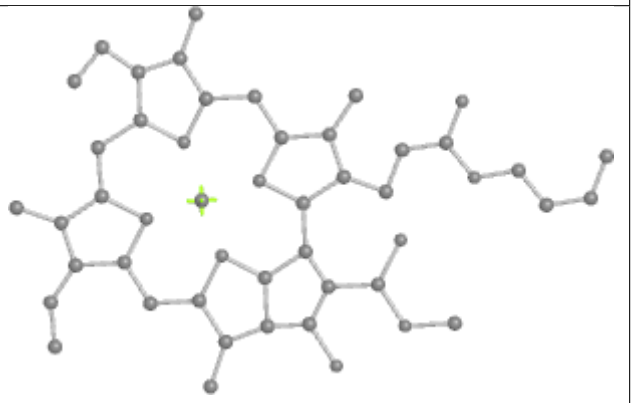
Bond lengths



Bond angles

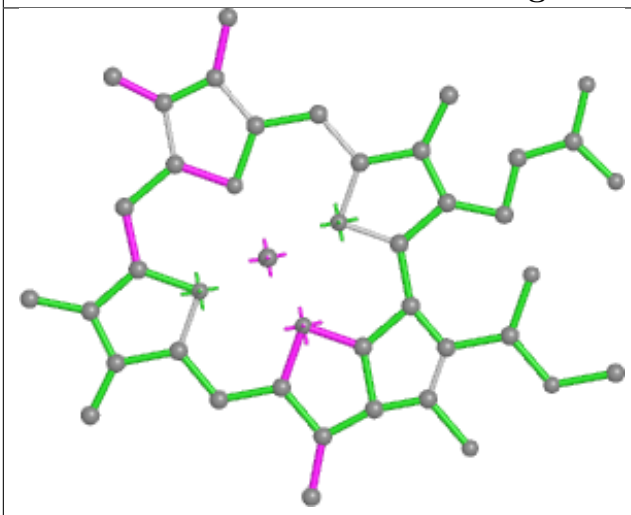


Torsions

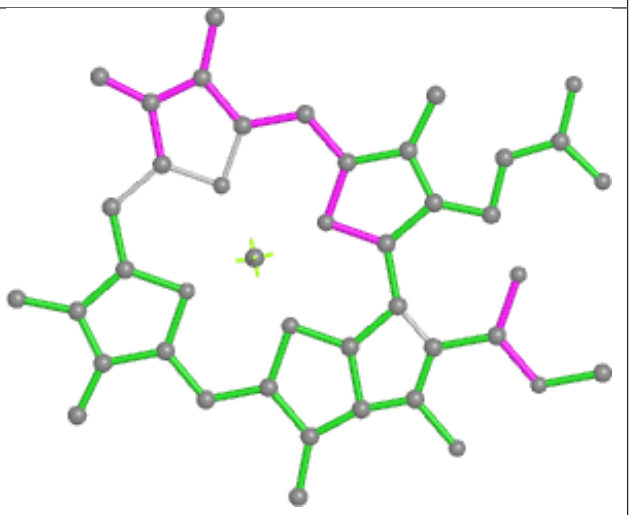


Rings

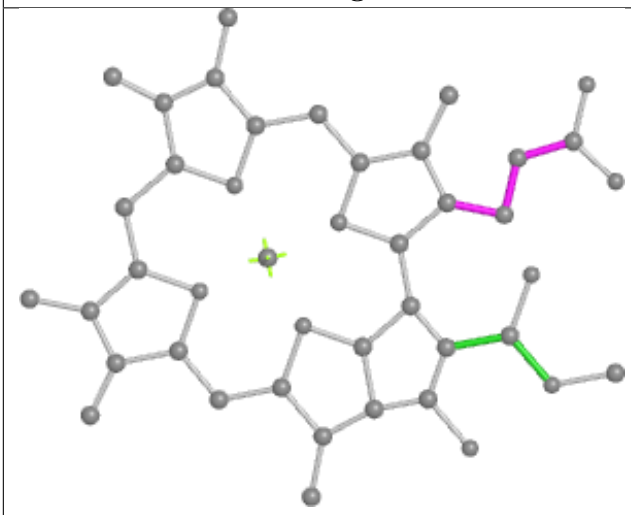
Ligand CLA 1 616



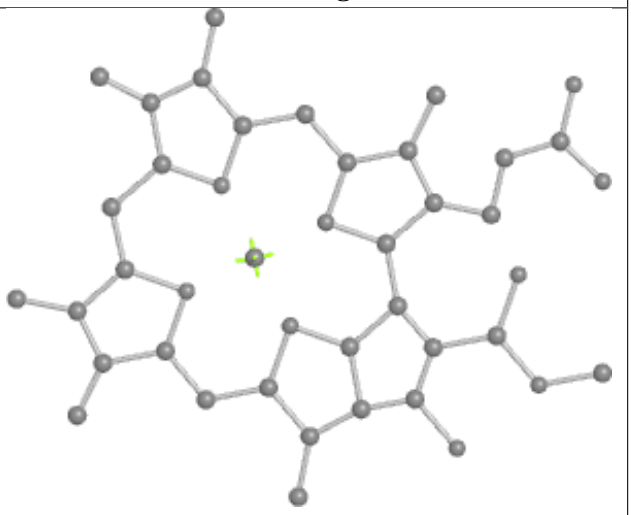
Bond lengths



Bond angles

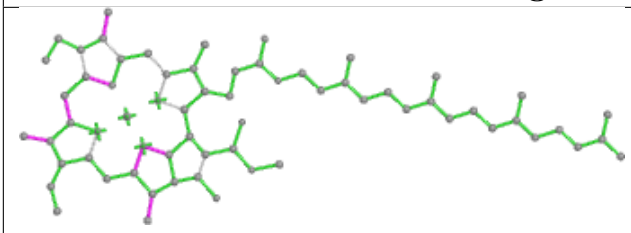


Torsions

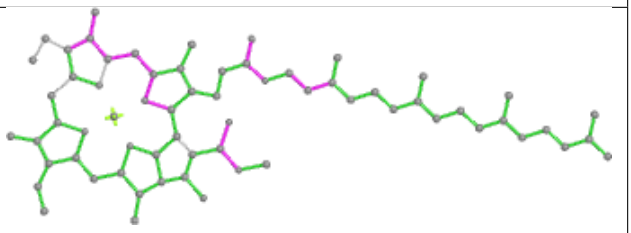


Rings

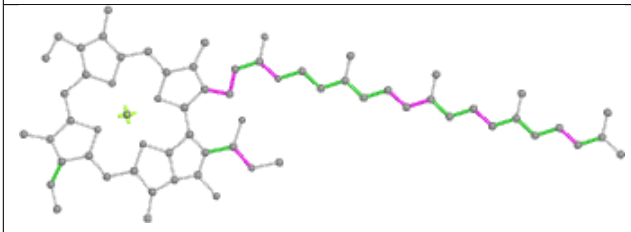
Ligand CLA a 613



Bond lengths



Bond angles



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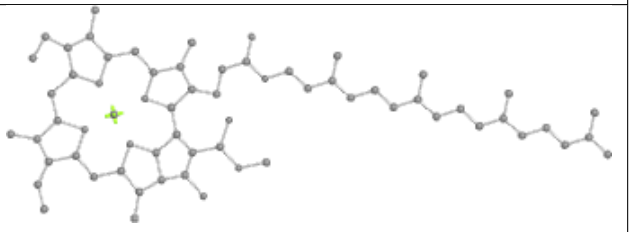
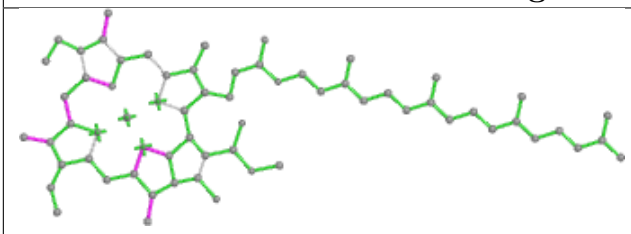
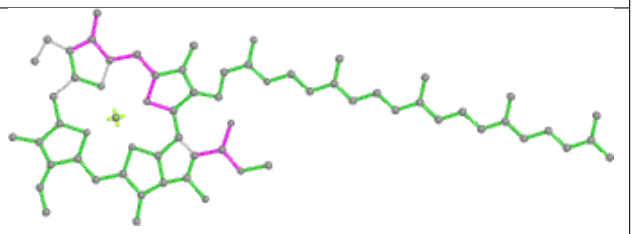


Rings

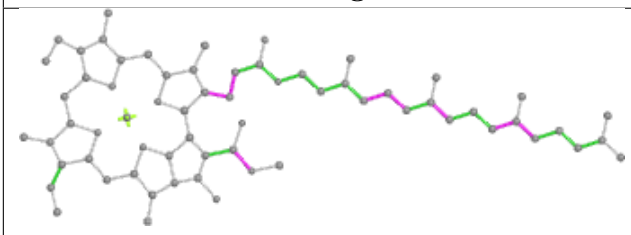
Ligand CLA 4 608



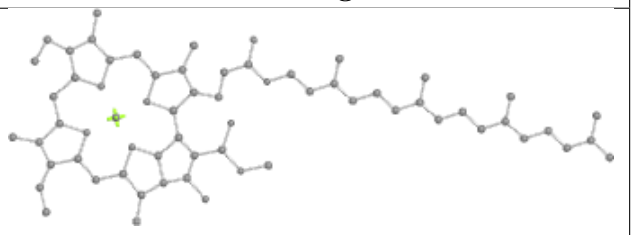
Bond lengths



Bond angles

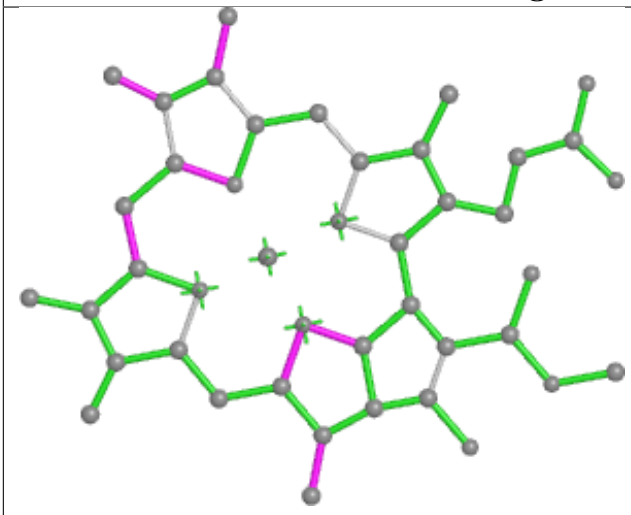


Torsions

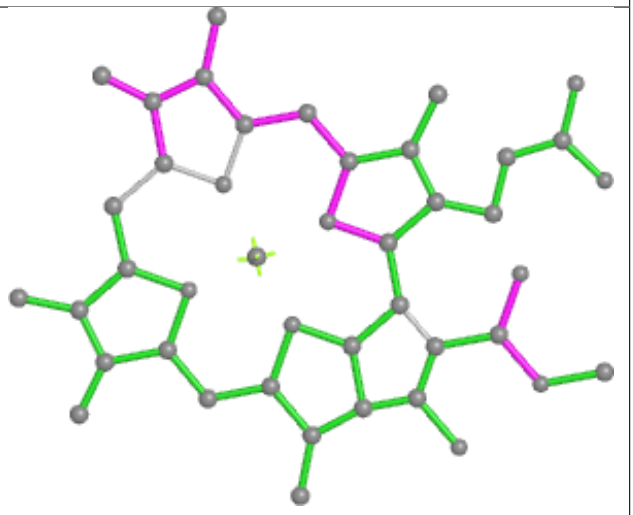


Rings

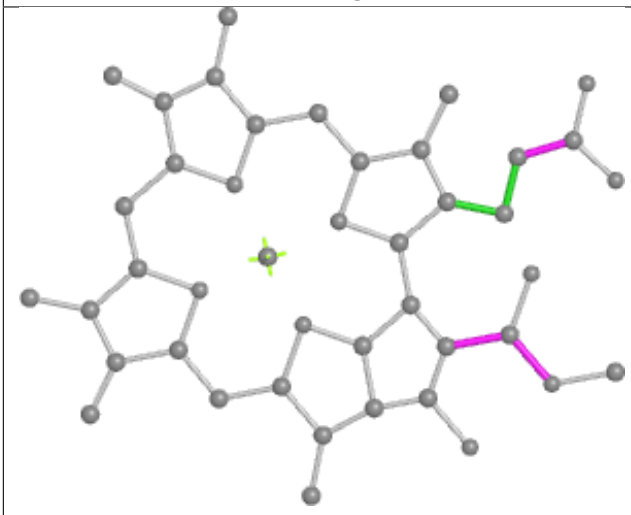
Ligand CLA 7 616



Bond lengths



Bond angles



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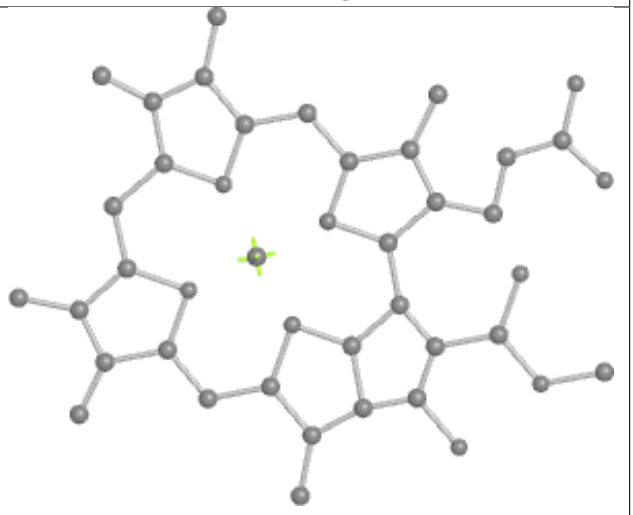
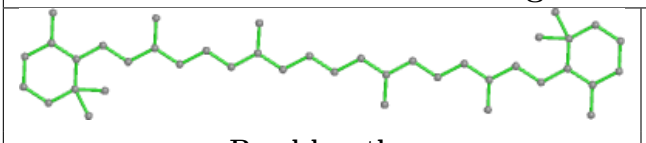


Rings

Ligand BCR 3 622



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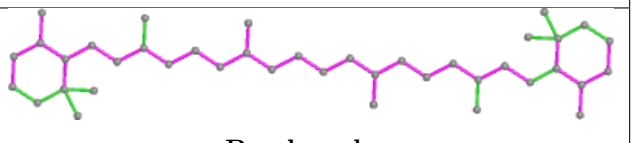
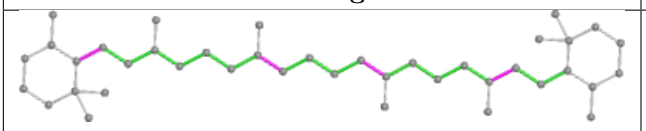
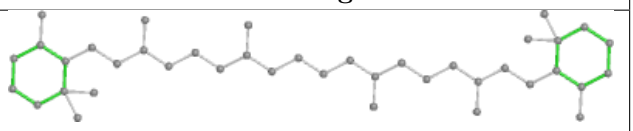


Bond angles

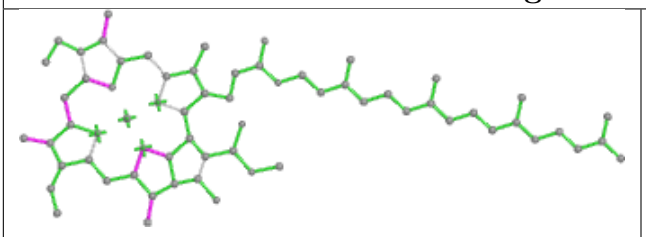


Torsions

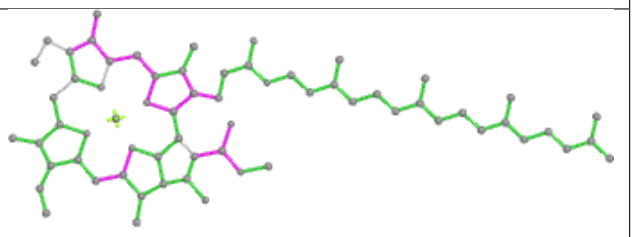


Rings

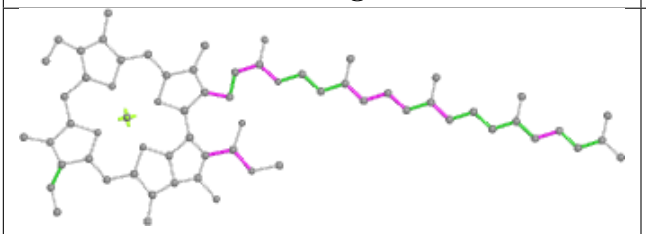
Ligand CLA B 833



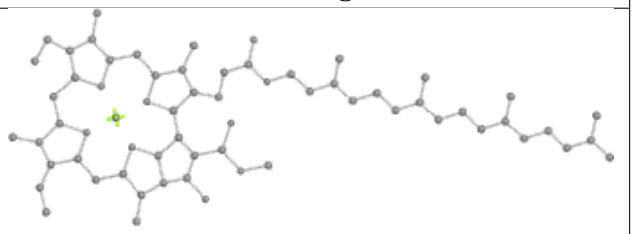
Bond lengths



Bond angles

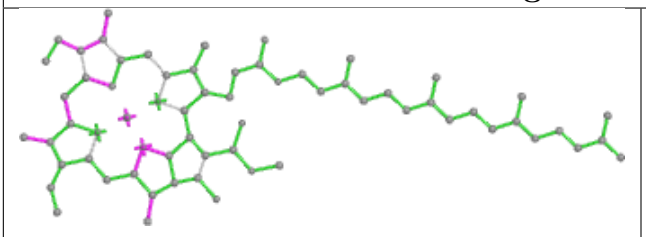


Torsions

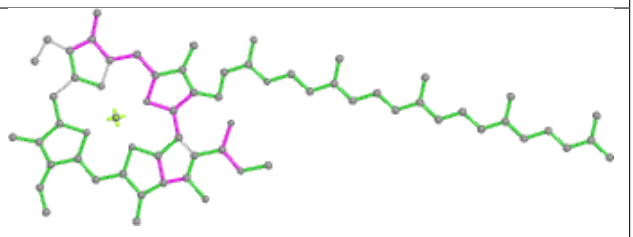


Rings

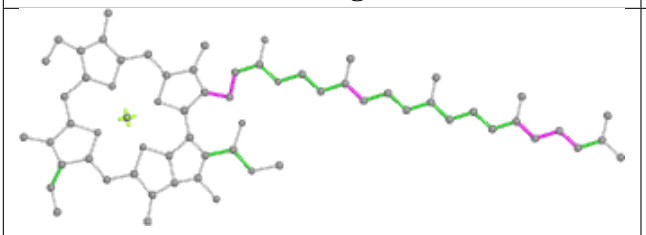
Ligand CLA A 803



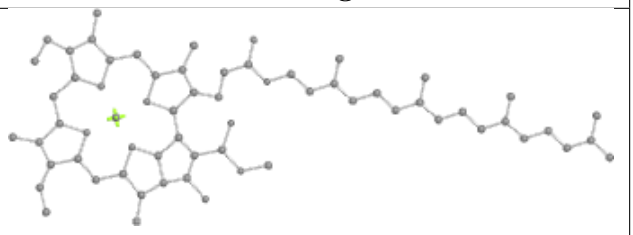
Bond lengths



Bond angles

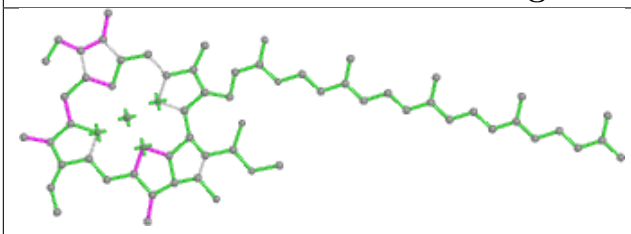


Torsions



Rings

Ligand CLA 7 610



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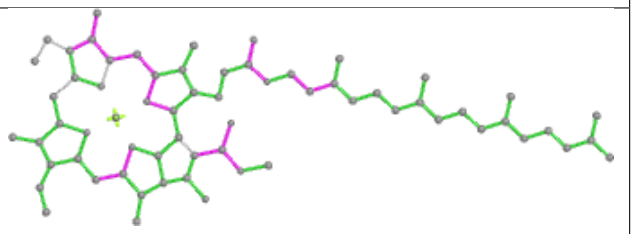
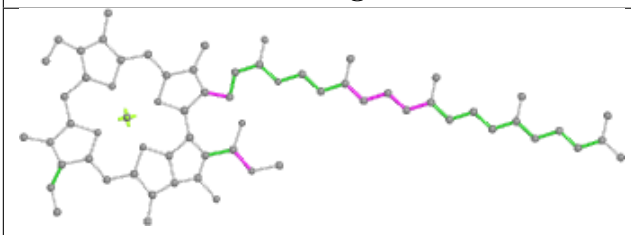
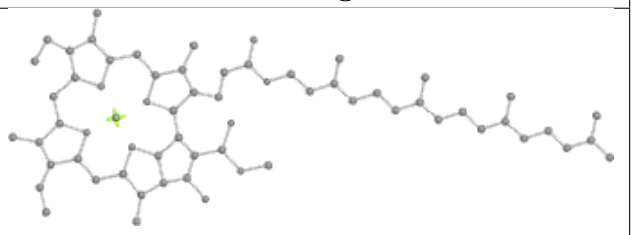


Bond angles

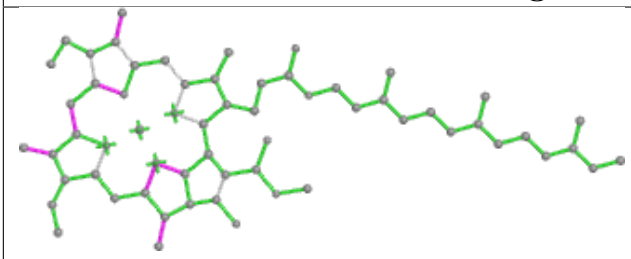


Torsions

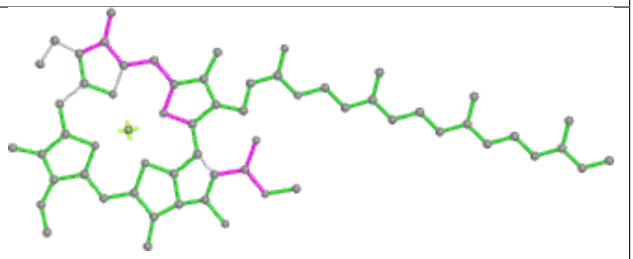


Rings

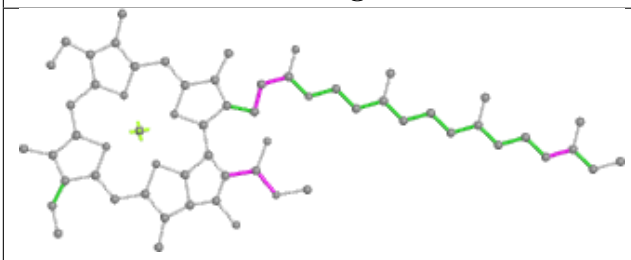
Ligand CLA a 602



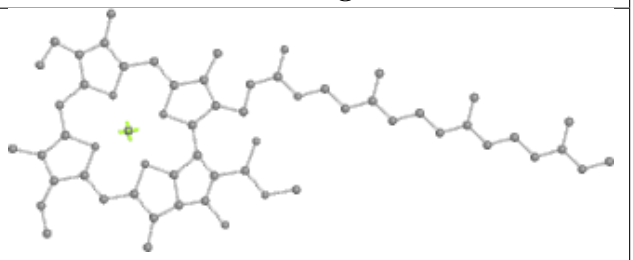
Bond lengths



Bond angles

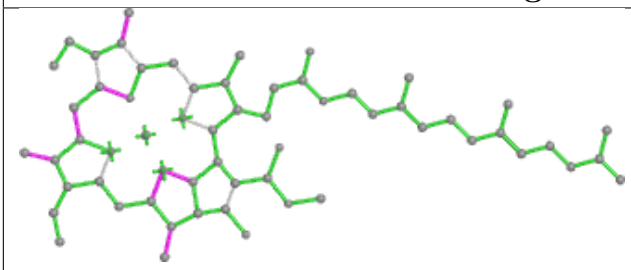


Torsions

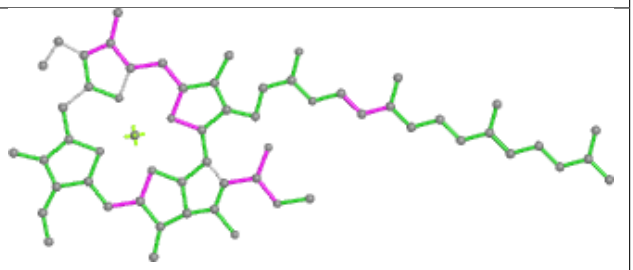


Rings

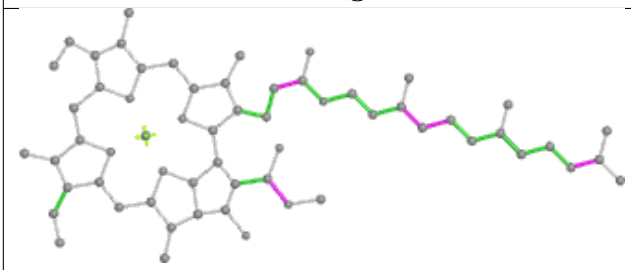
Ligand CLA B 832



Bond lengths



Bond angles



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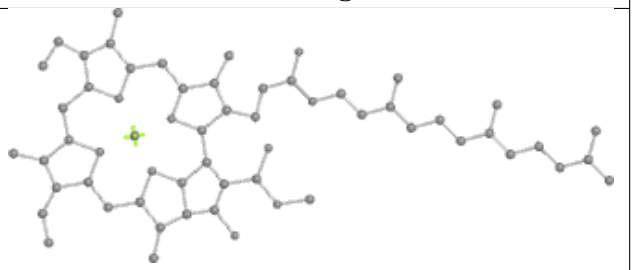
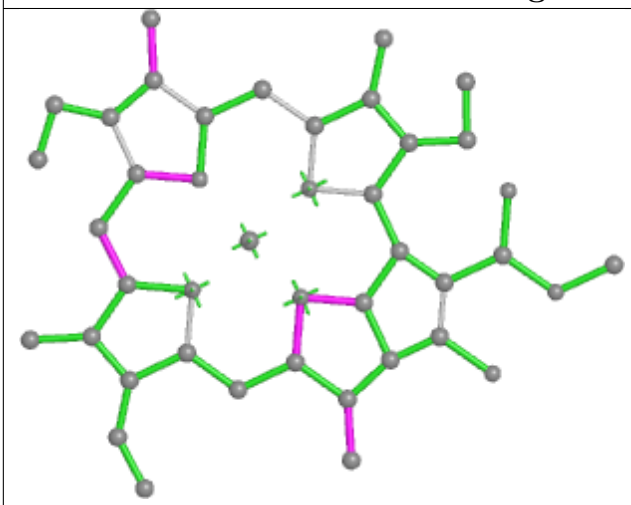
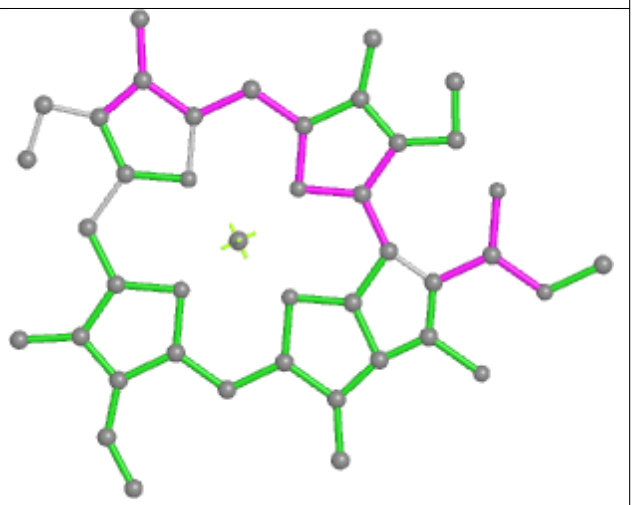


Rings

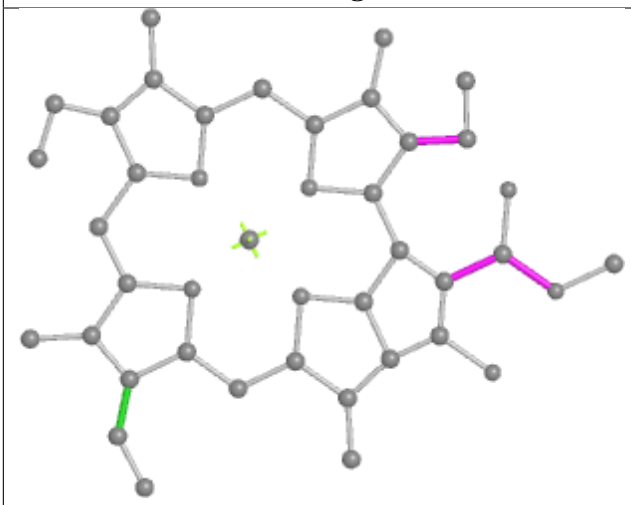
Ligand CLA J 101



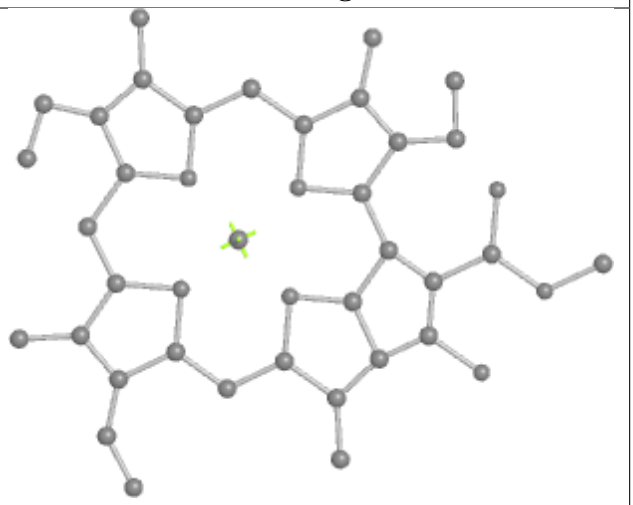
Bond lengths



Bond angles

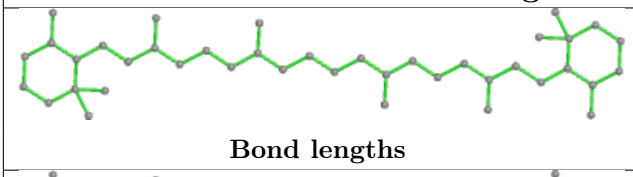


Torsions

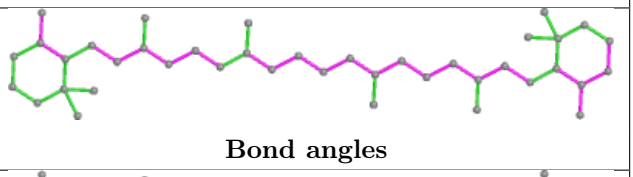


Rings

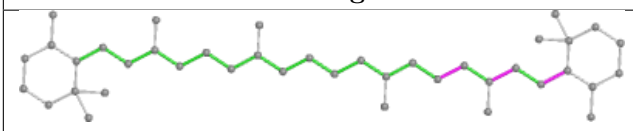
Ligand BCR A 851



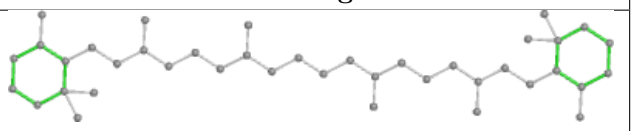
Bond lengths



Bond angles

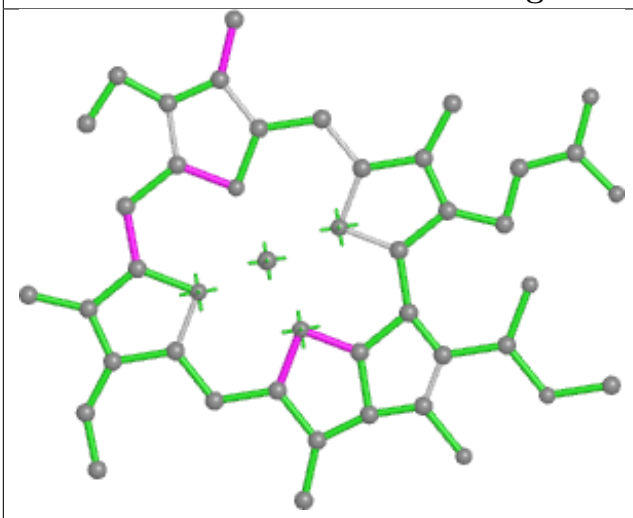


Torsions

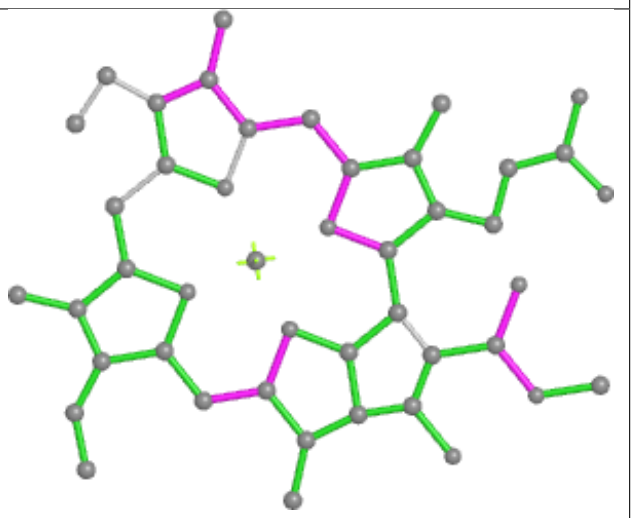


Rings

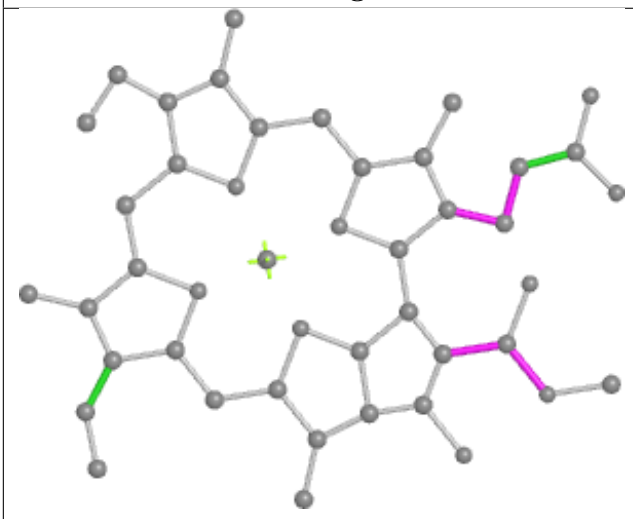
Ligand CLA L 303



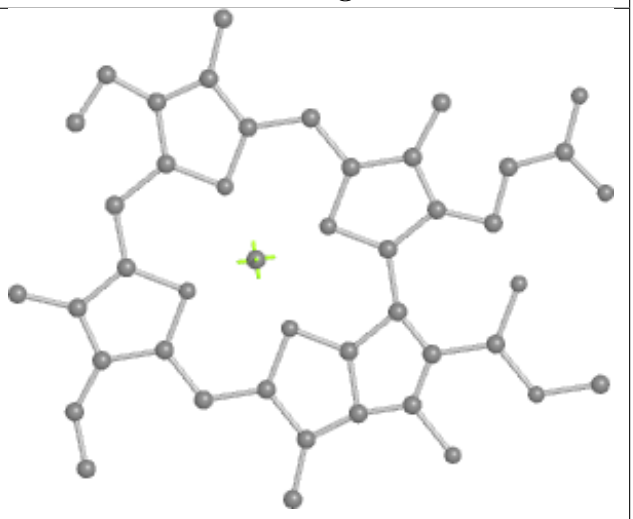
Bond lengths



Bond angles

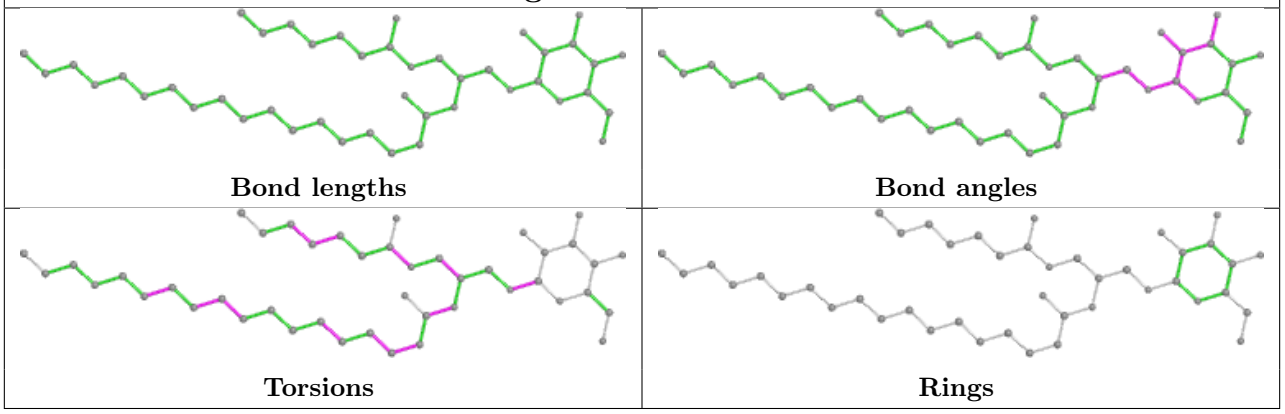


Torsions

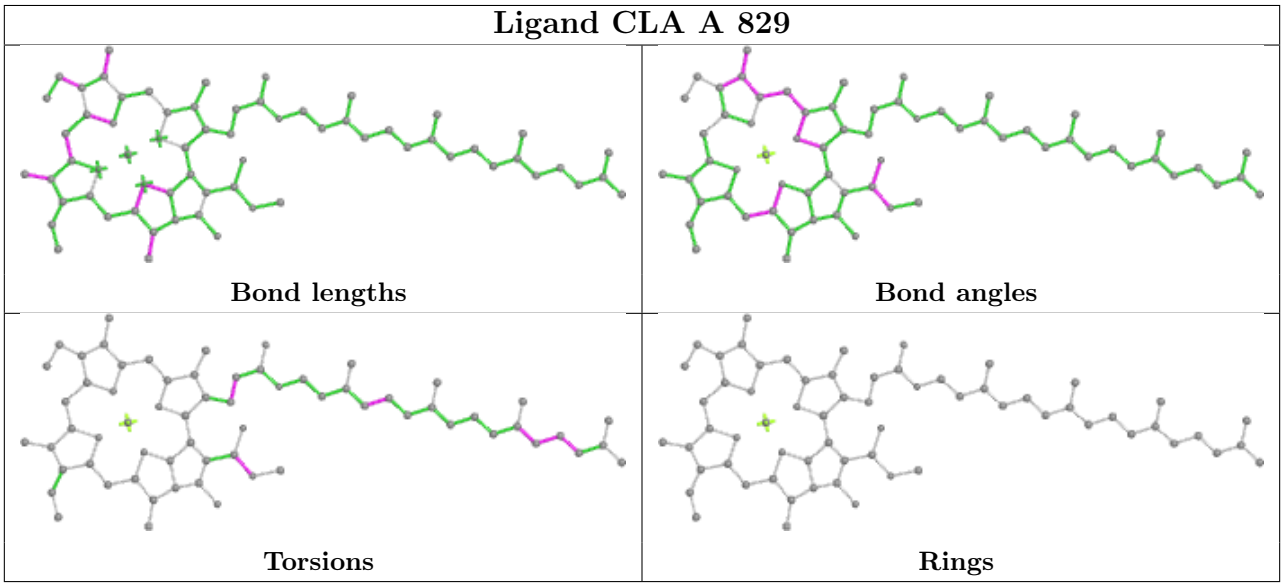


Rings

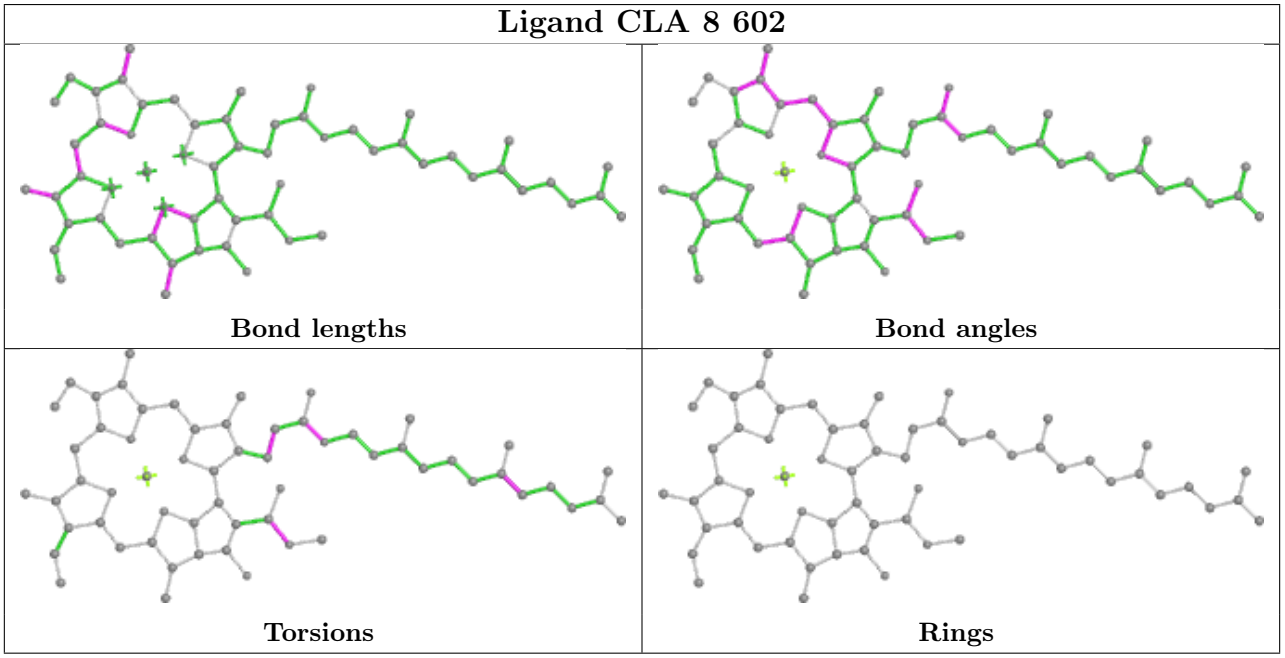
Ligand LMG 7 624



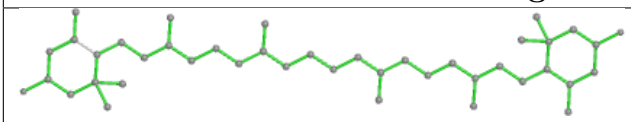
Ligand CLA A 829



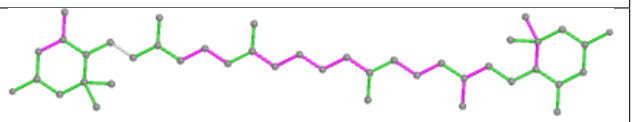
Ligand CLA 8 602



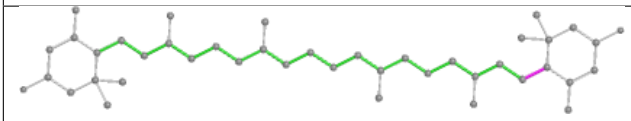
Ligand LUT 3 618



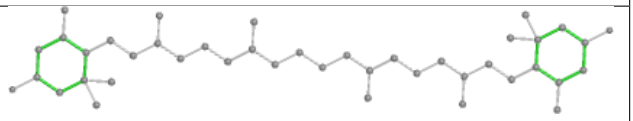
Bond lengths



Bond angles

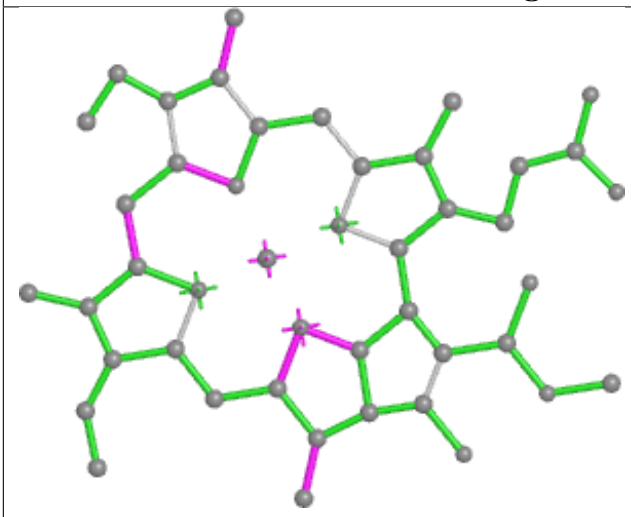


Torsions

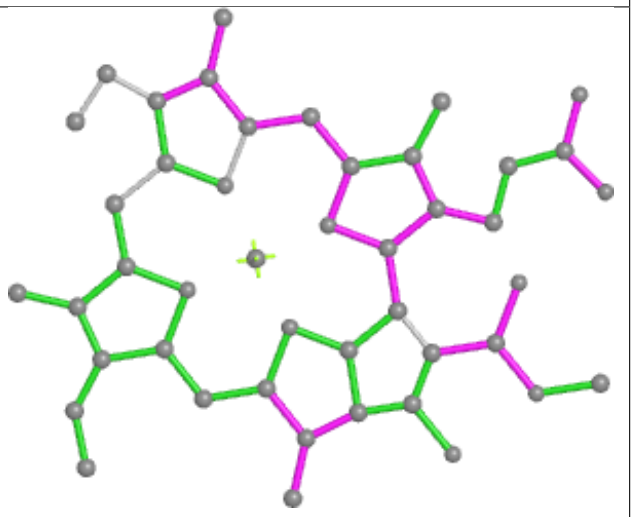


Rings

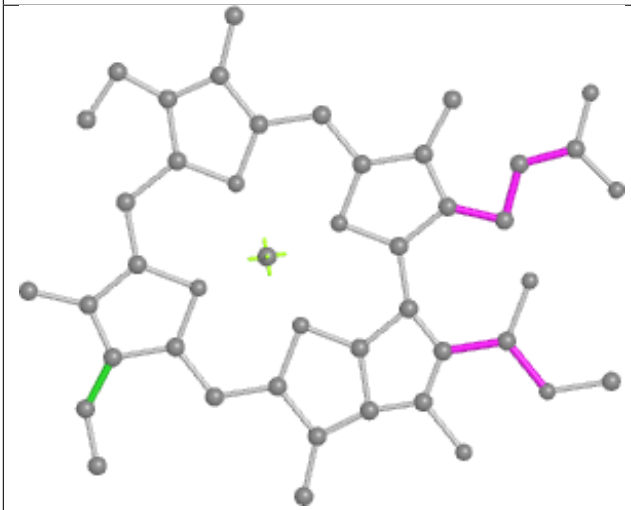
Ligand CLA K 201



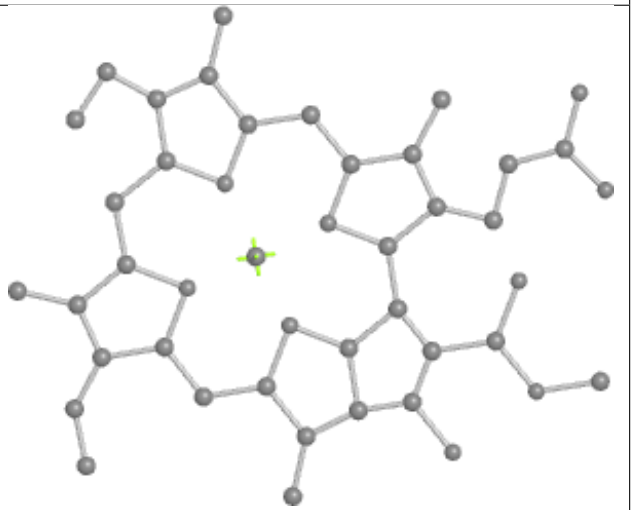
Bond lengths



Bond angles

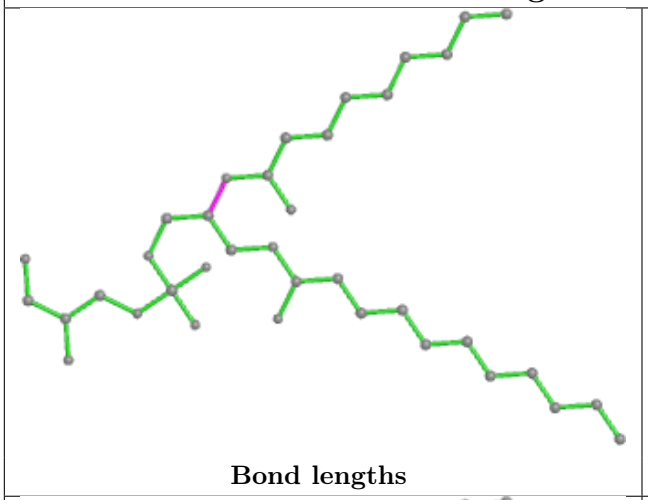


Torsions

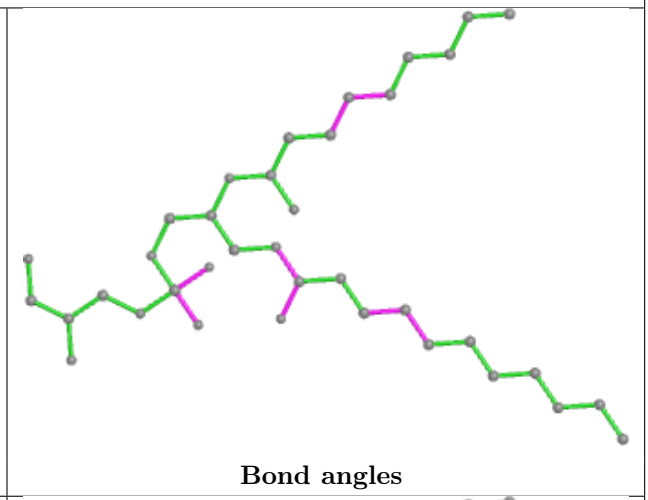


Rings

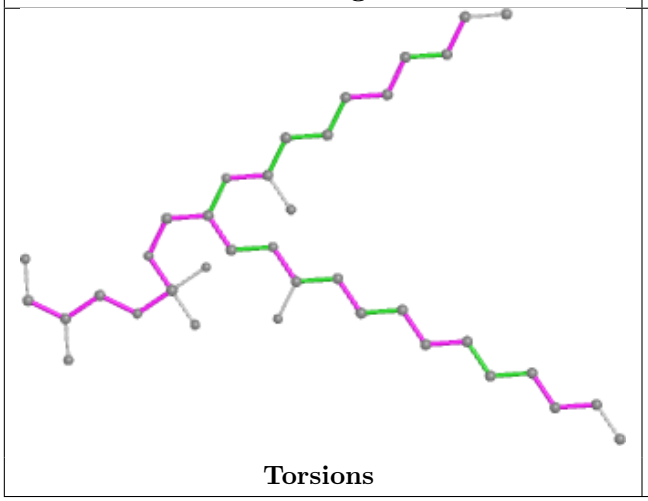
Ligand LHG 7 622



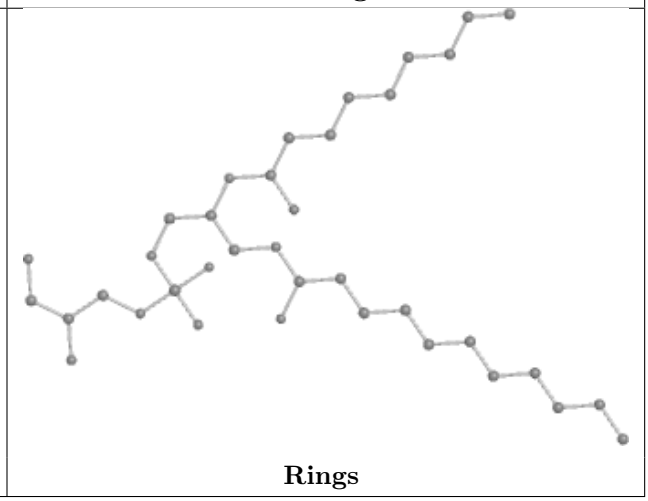
Bond lengths



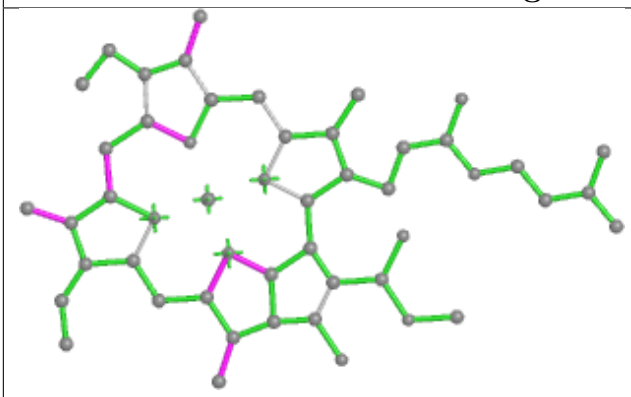
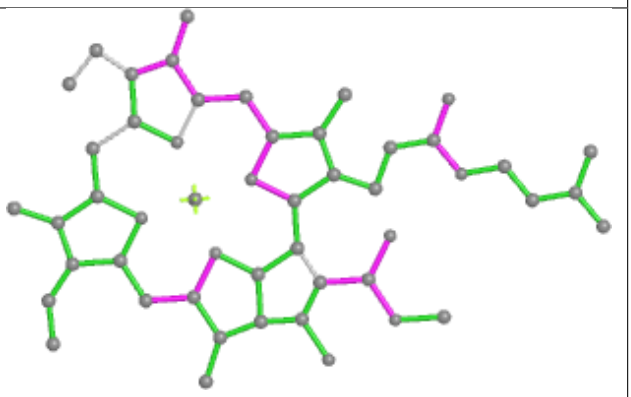
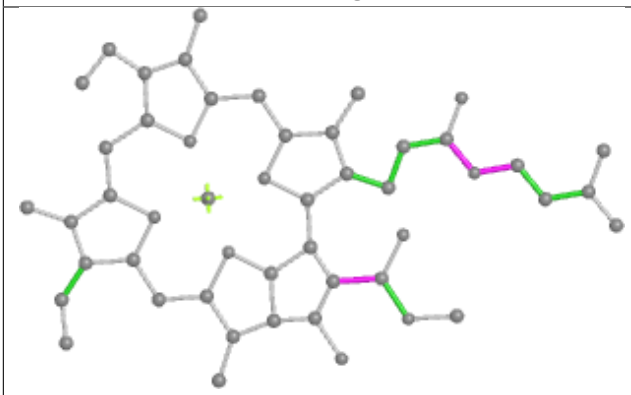
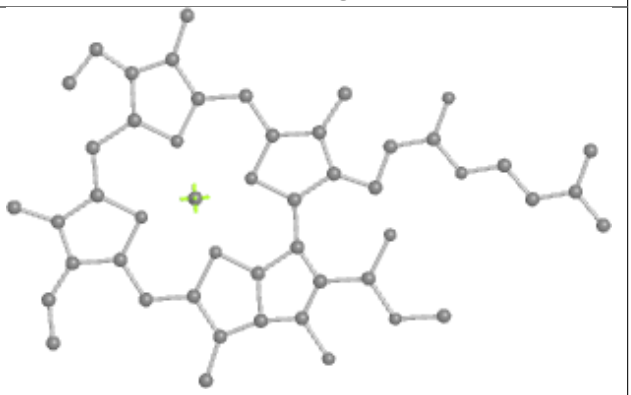
Bond angles

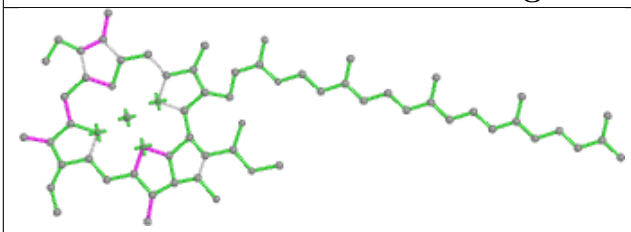
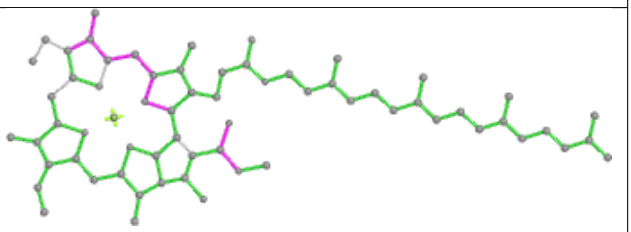
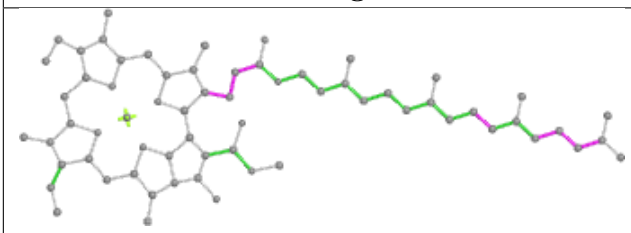
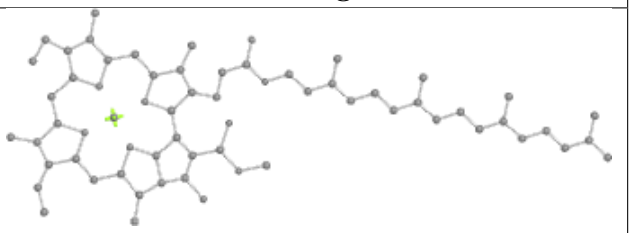


Torsions

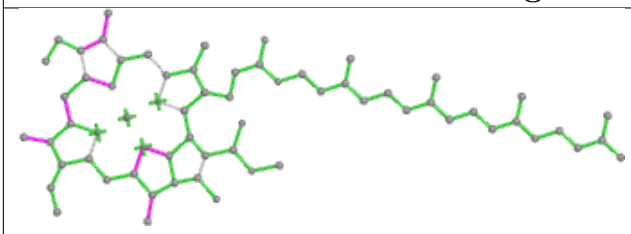


Rings

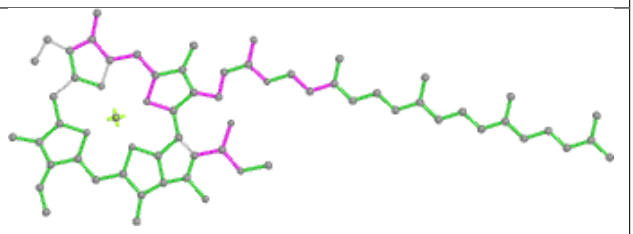
Ligand CLA A 808	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA A 842	
	
Bond lengths	Bond angles
	
Torsions	Rings

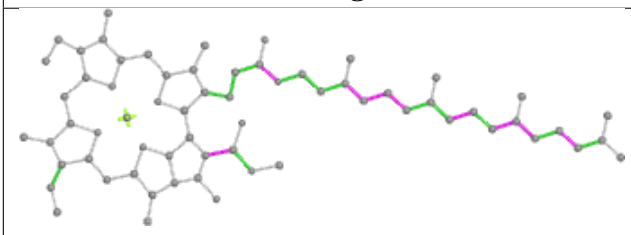
Ligand CLA B 808



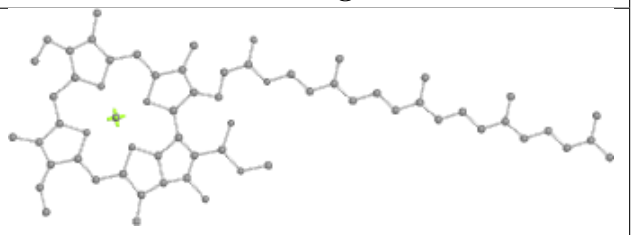
Bond lengths



Bond angles

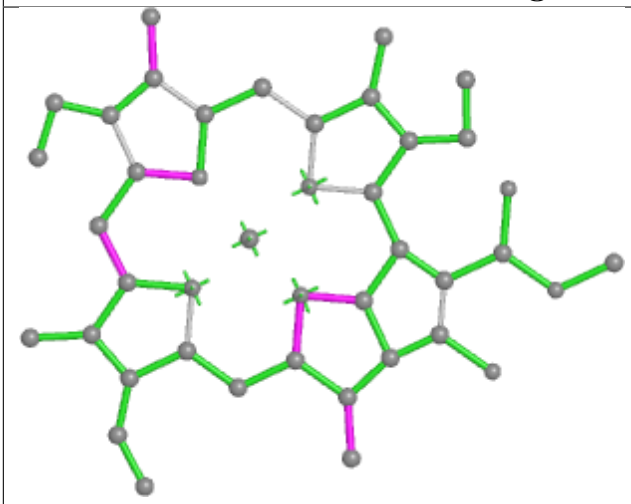


Torsions

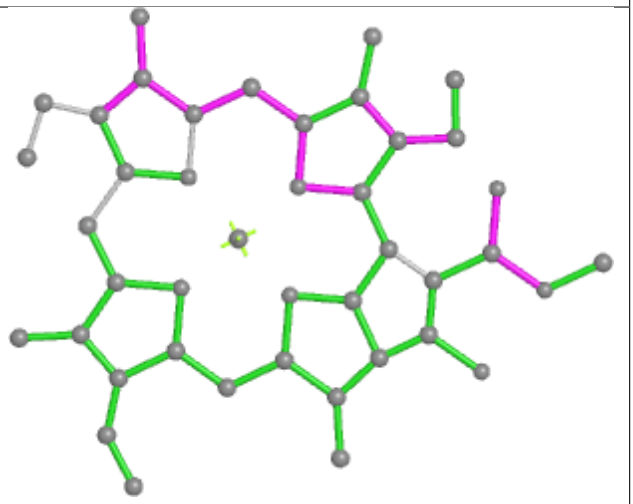


Rings

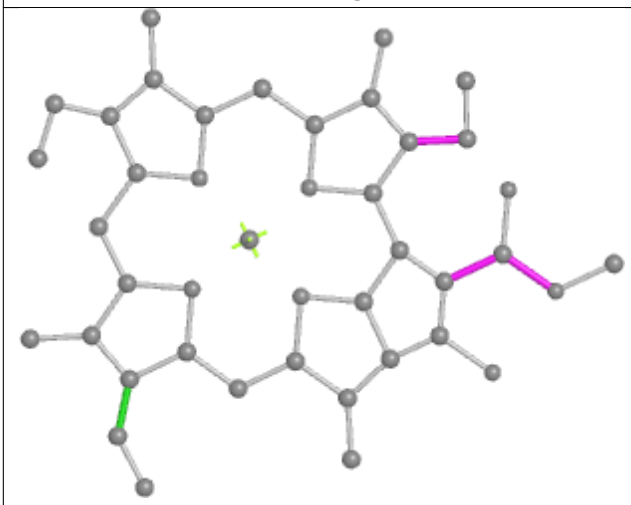
Ligand CLA 5 611



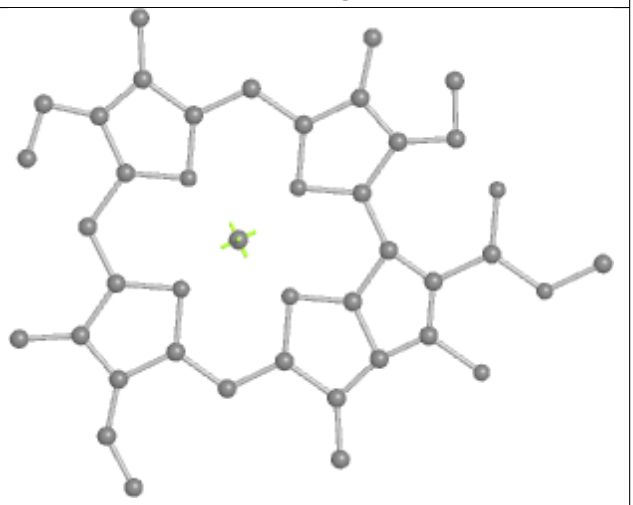
Bond lengths



Bond angles

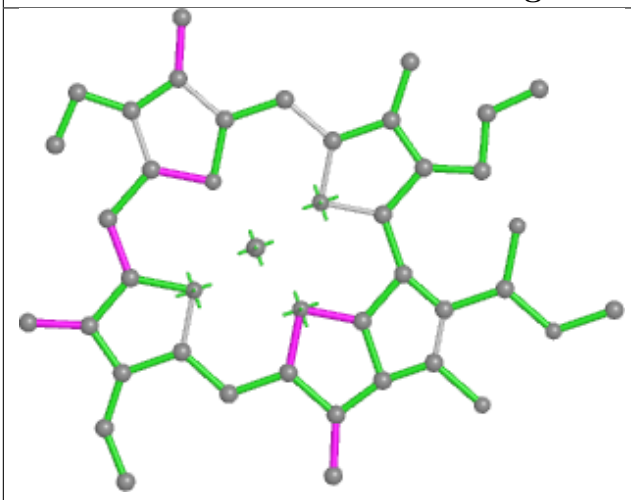


Torsions

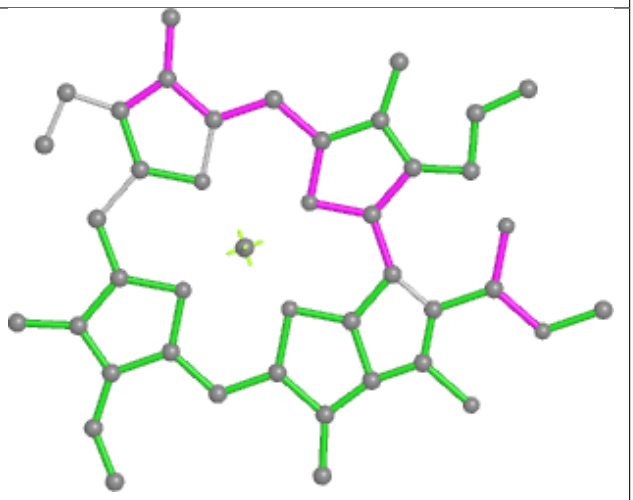


Rings

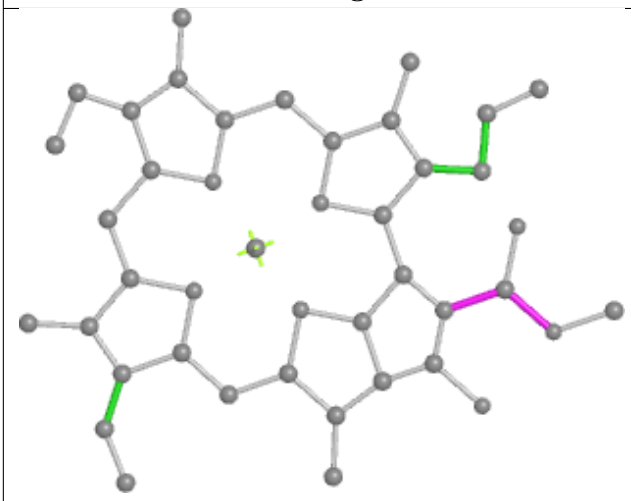
Ligand CLA B 815



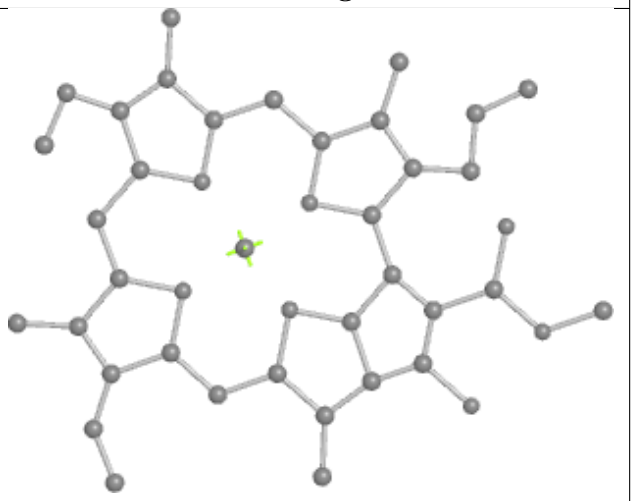
Bond lengths



Bond angles

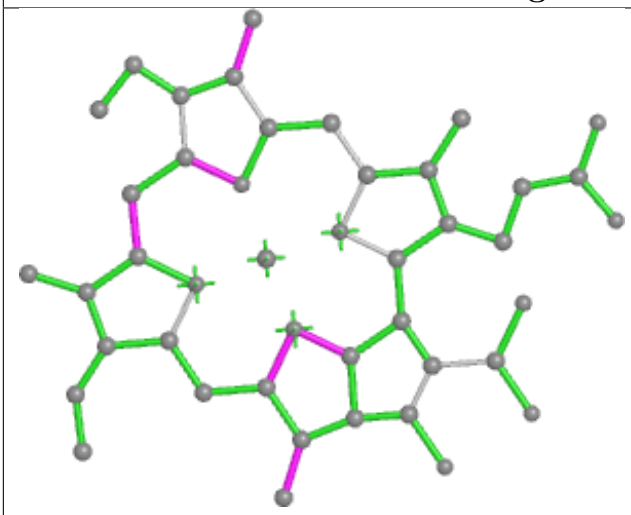


Torsions

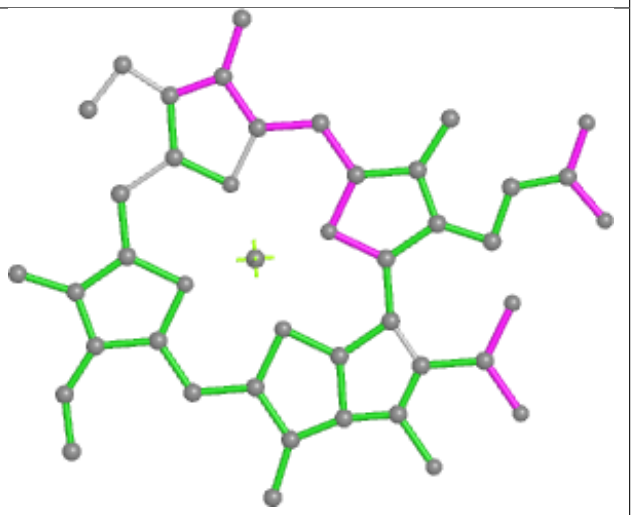


Rings

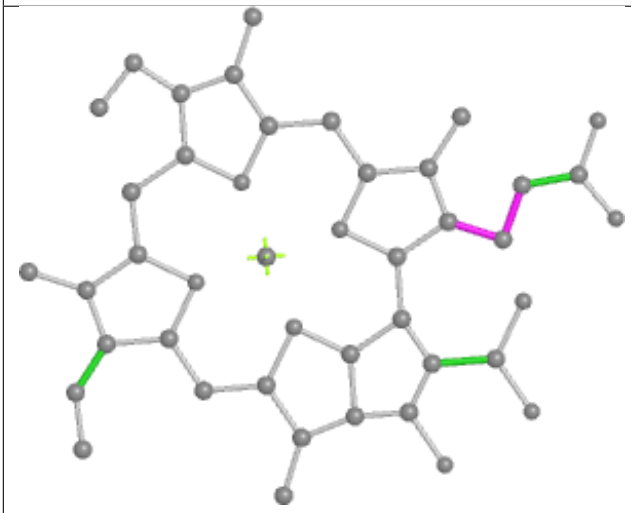
Ligand CLA a 608



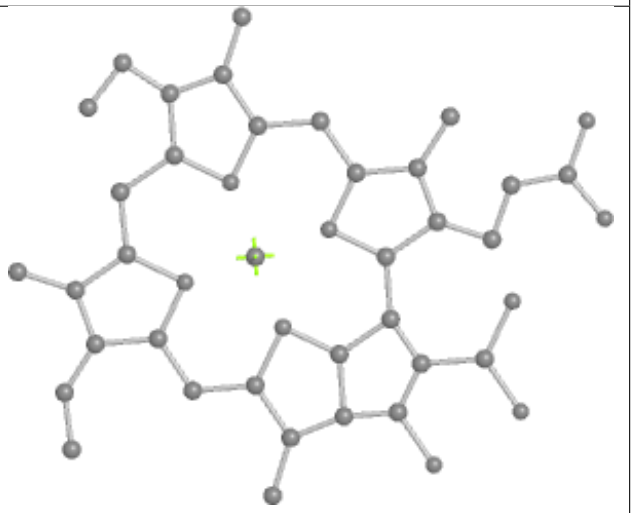
Bond lengths



Bond angles

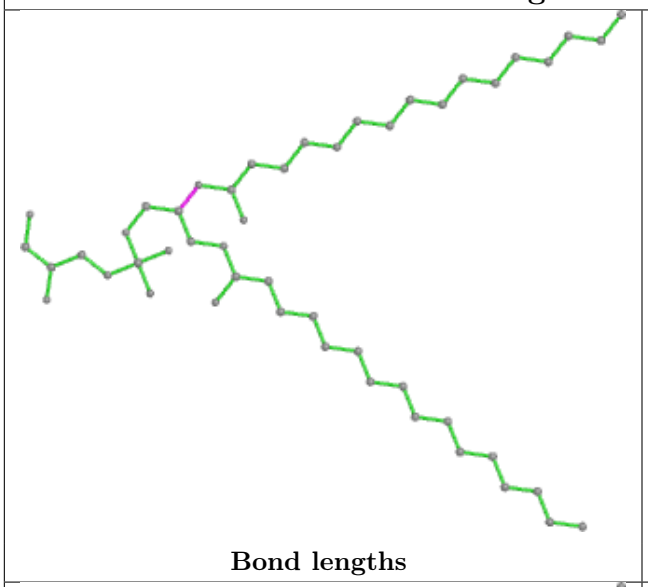


Torsions

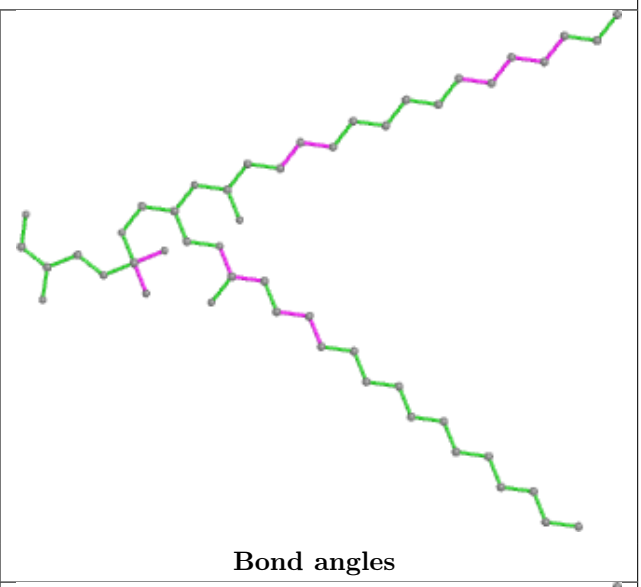


Rings

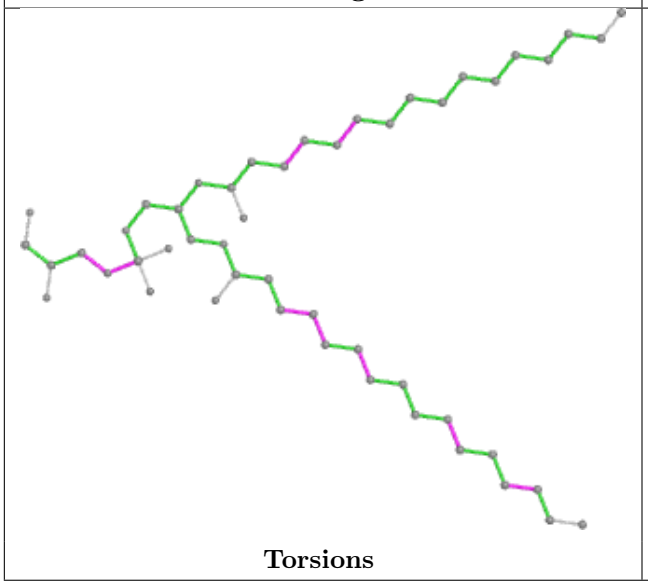
Ligand LHG a 620



Bond lengths



Bond angles



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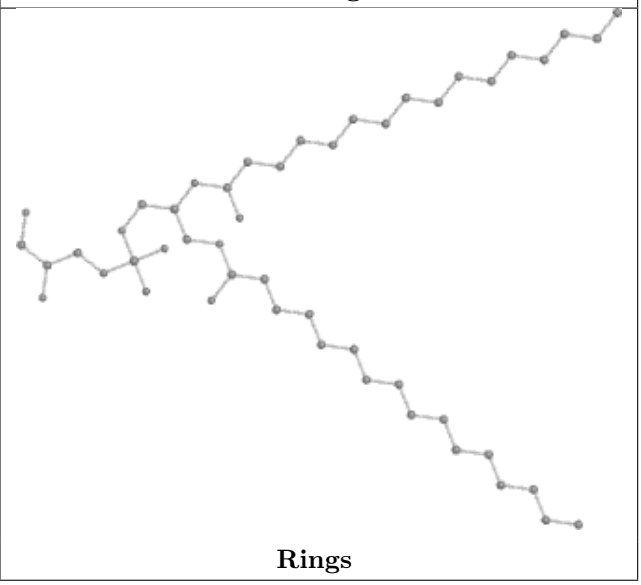
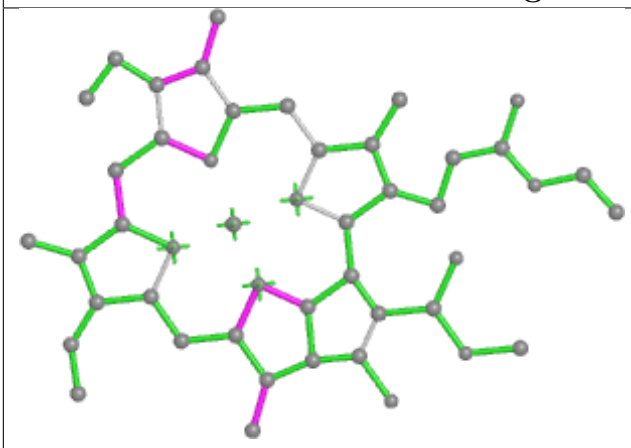
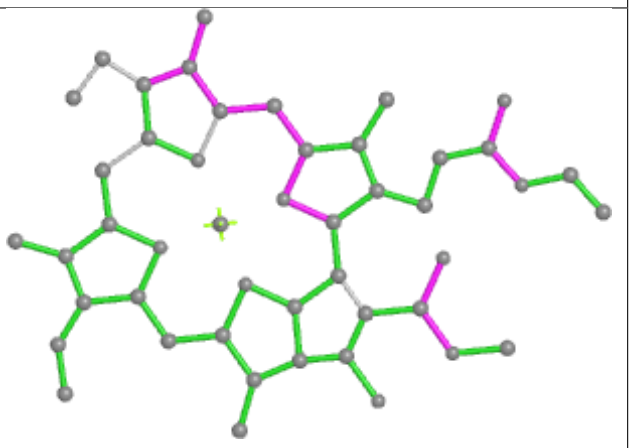


Rings

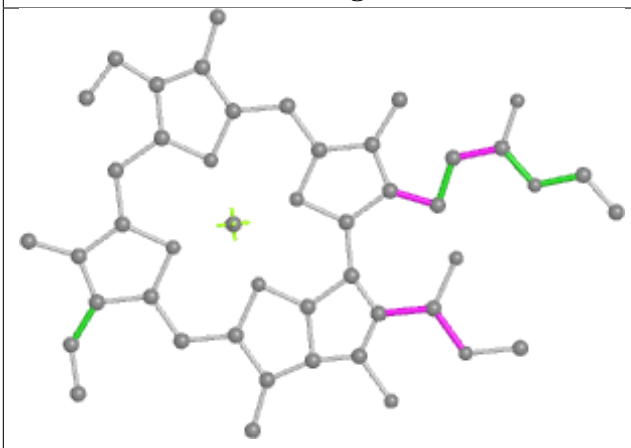
Ligand CLA B 838



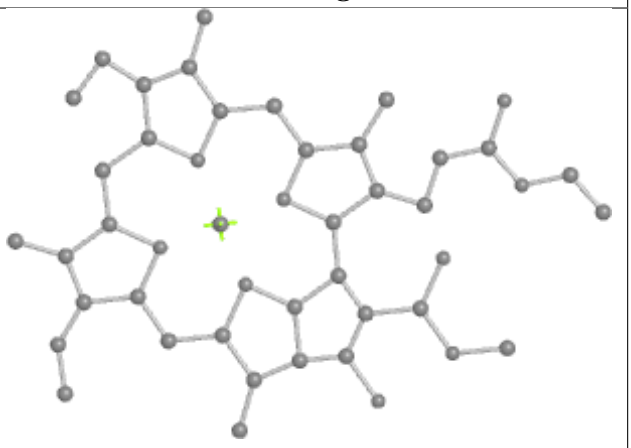
Bond lengths



Bond angles

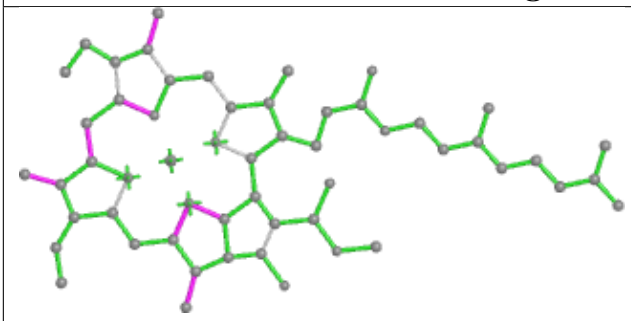


Torsions

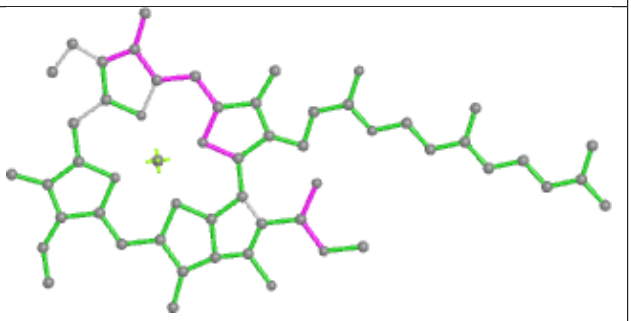


Rings

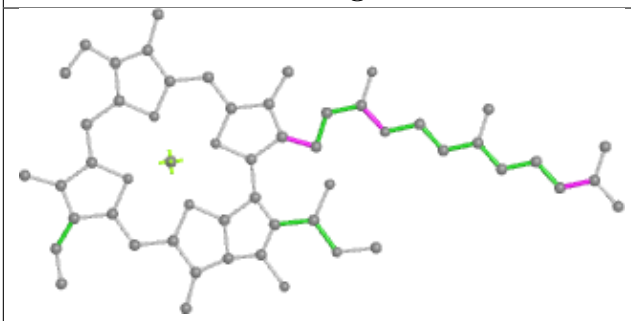
Ligand CLA B 826



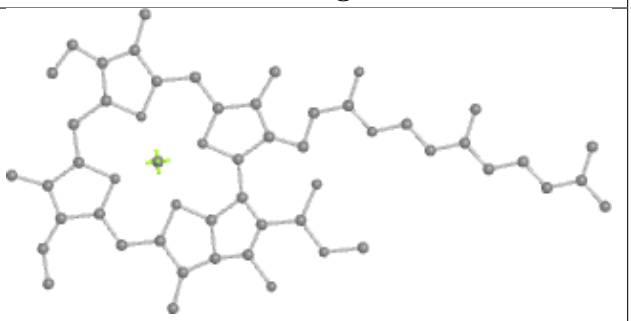
Bond lengths



Bond angles

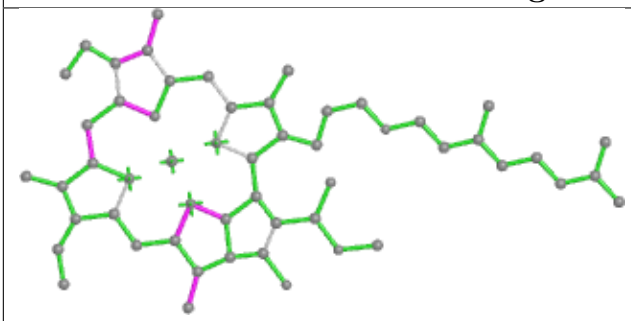


Torsions

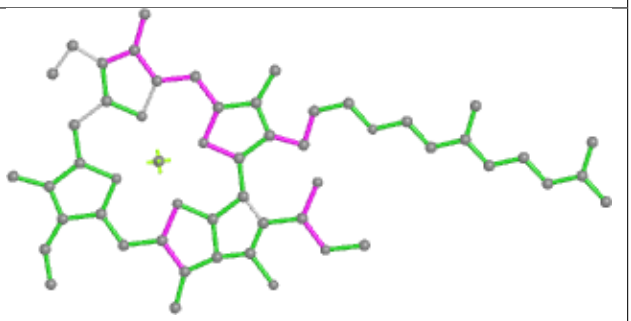


Rings

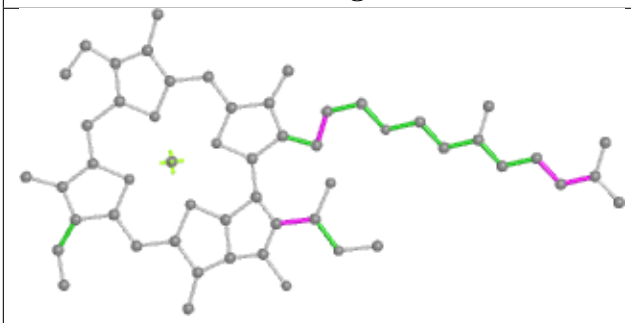
Ligand CLA a 603



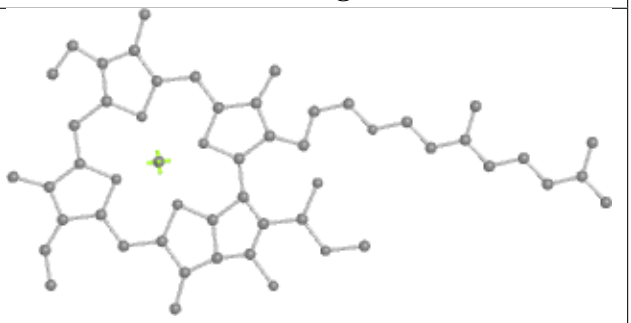
Bond lengths



Bond angles

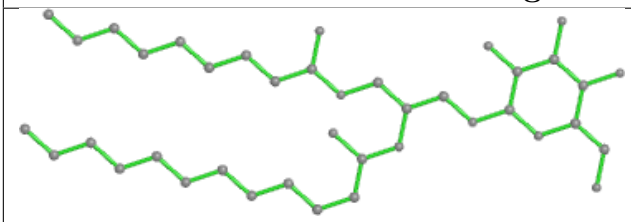


Torsions

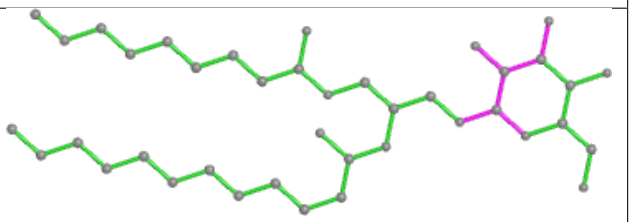


Rings

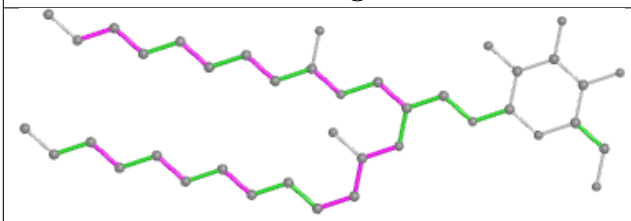
Ligand LMG 5 627



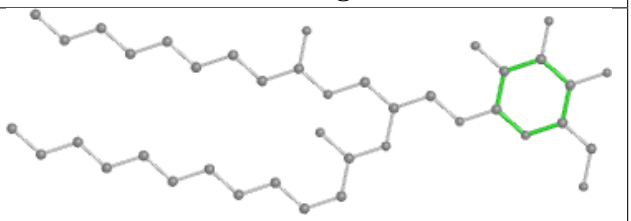
Bond lengths



Bond angles

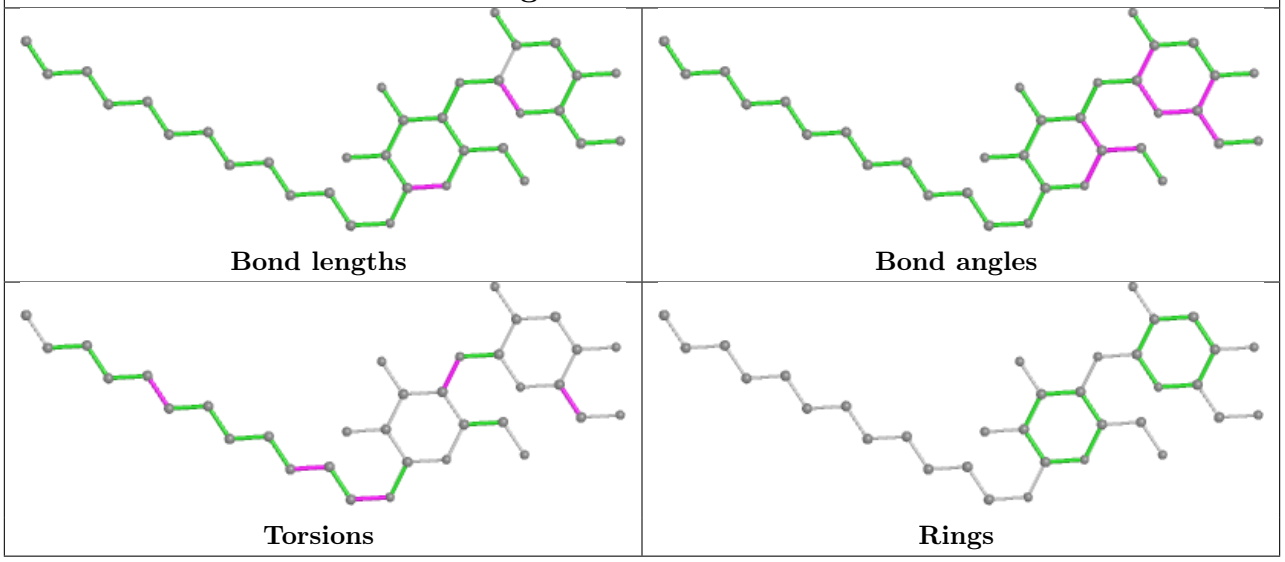


Torsions

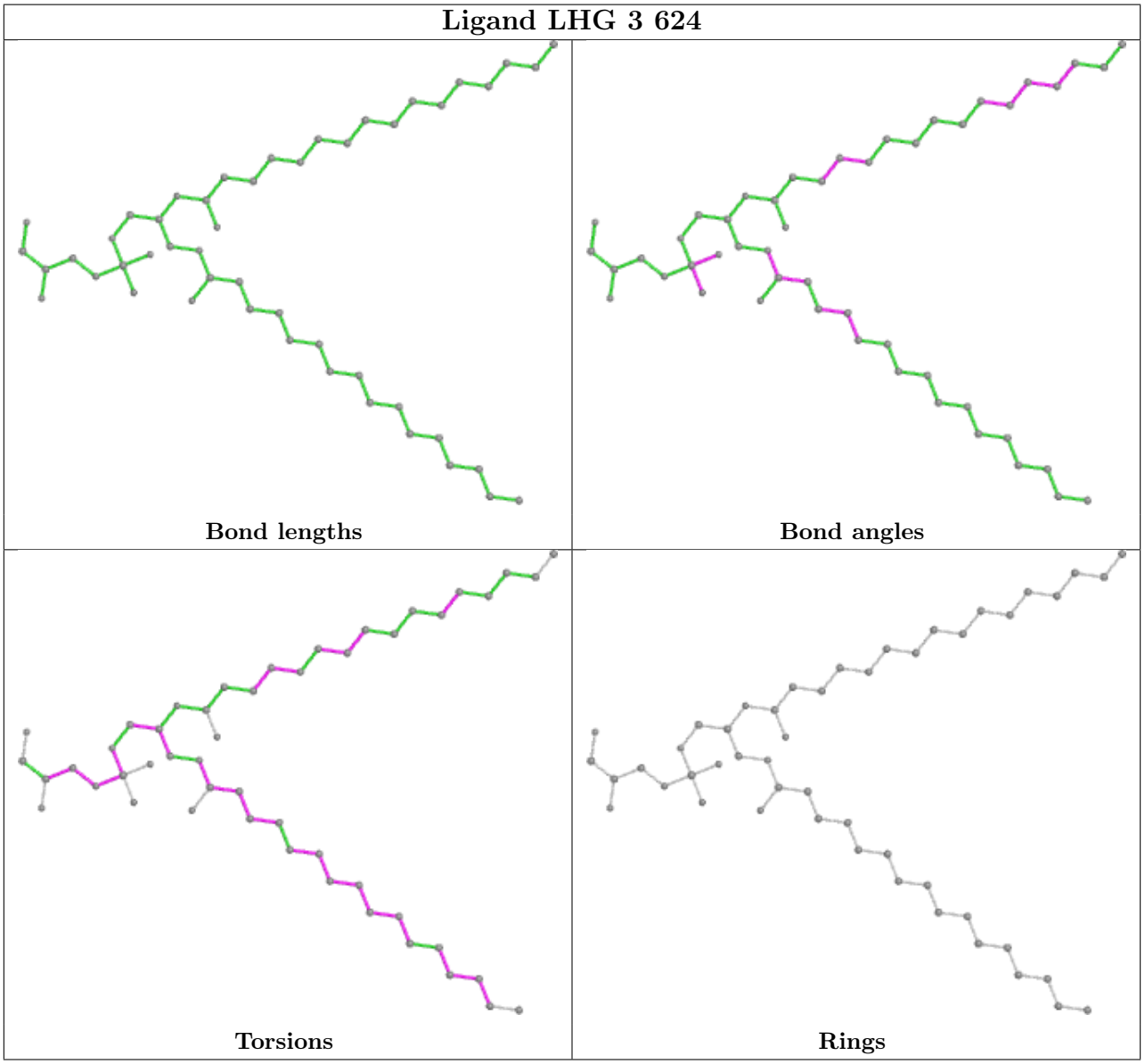


Rings

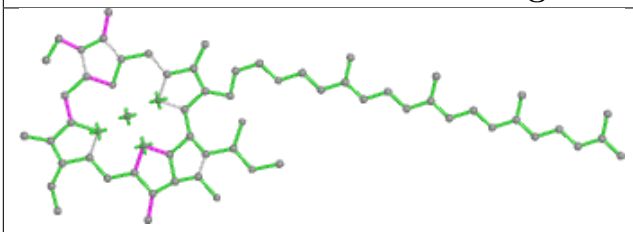
Ligand LMU A 858



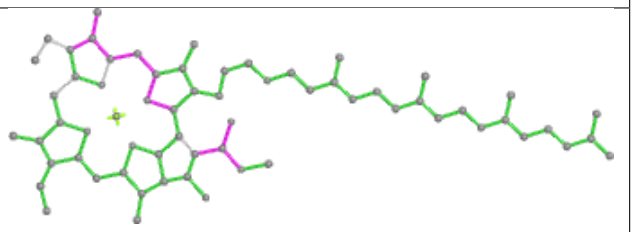
Ligand LHG 3 624



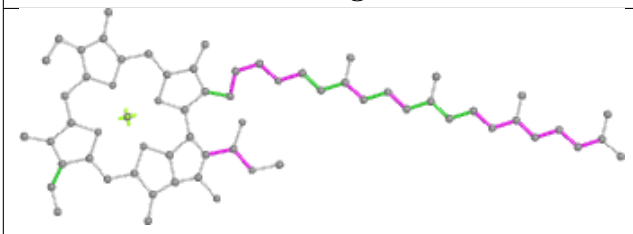
Ligand CLA 5 613



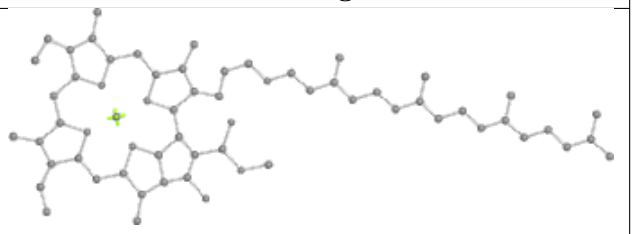
Bond lengths



Bond angles

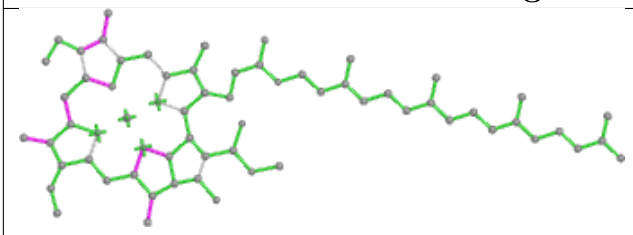


Torsions

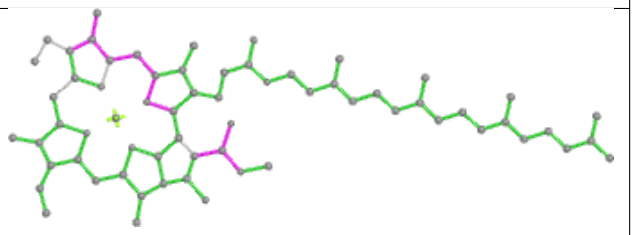


Rings

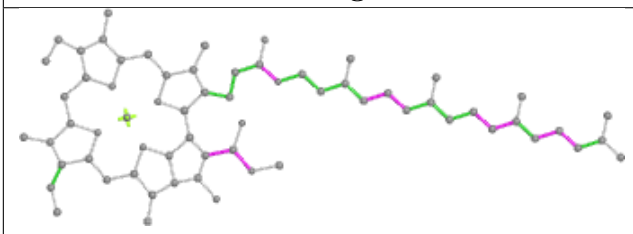
Ligand CLA A 834



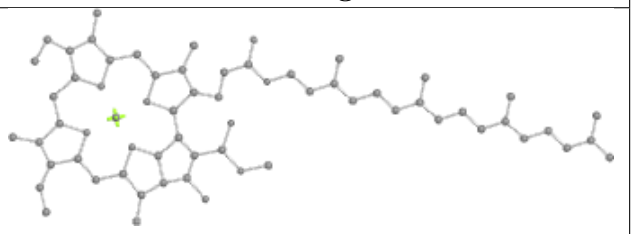
Bond lengths



Bond angles

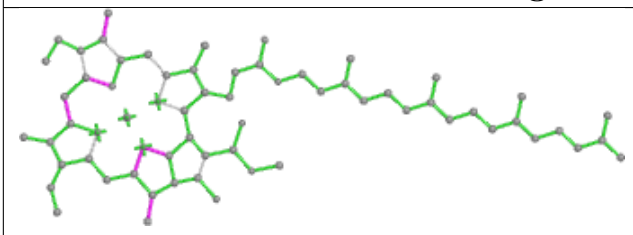


Torsions

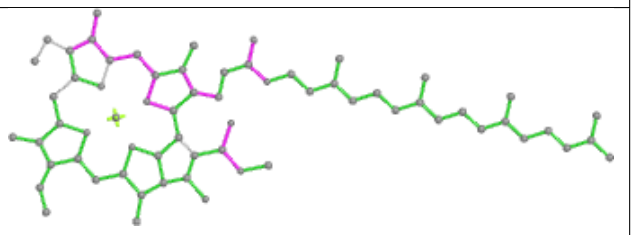


Rings

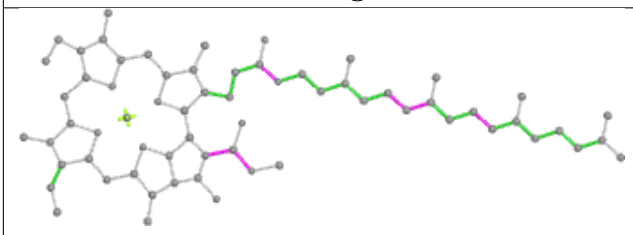
Ligand CLA 1 613



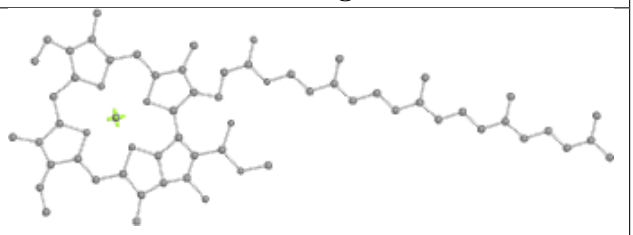
Bond lengths



Bond angles

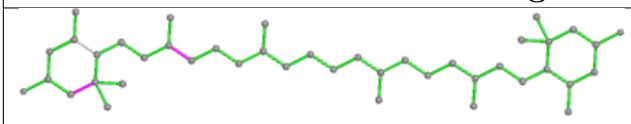


Torsions

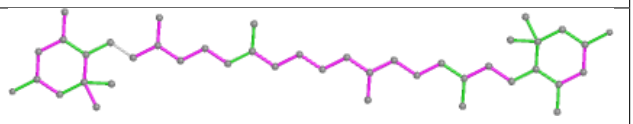


Rings

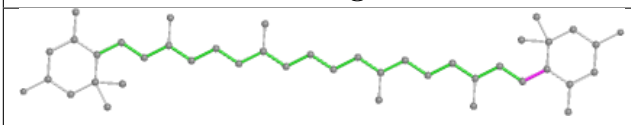
Ligand LUT 7 619



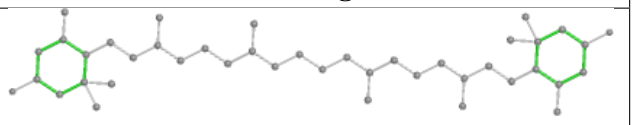
Bond lengths



Bond angles

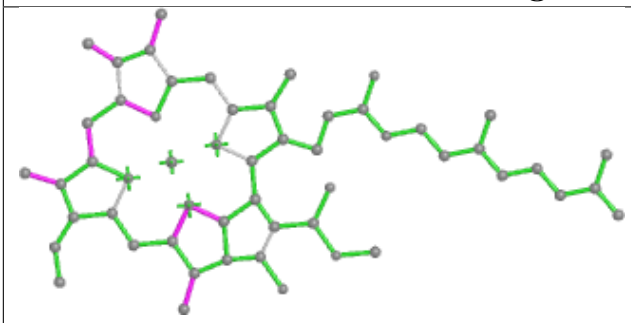


Torsions

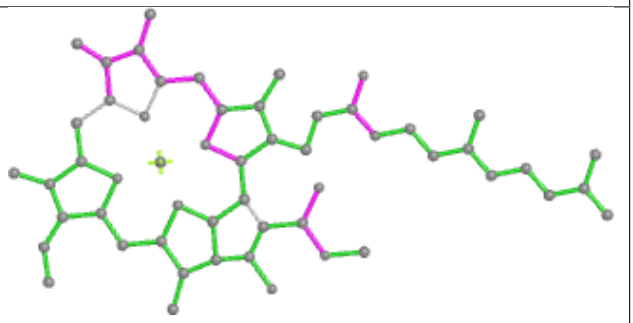


Rings

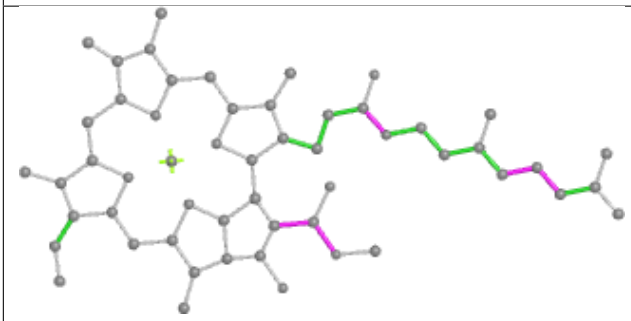
Ligand CLA 6 603



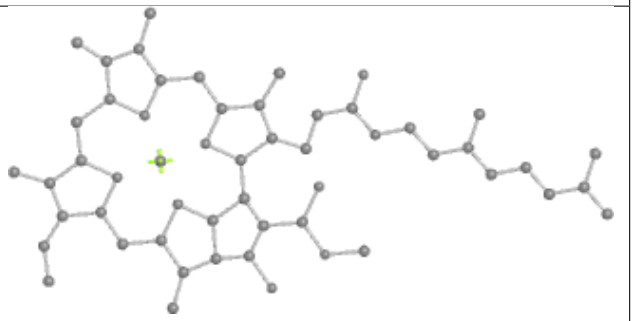
Bond lengths



Bond angles

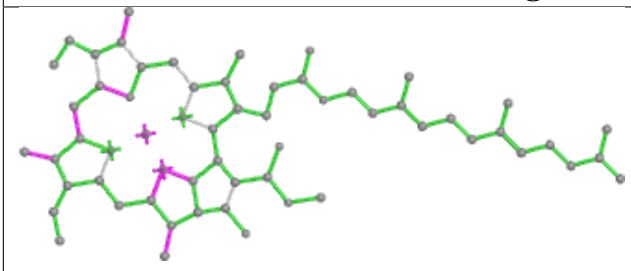


Torsions

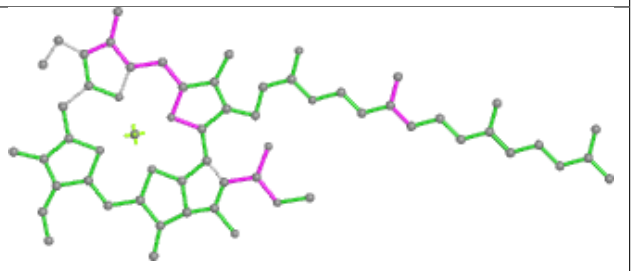


Rings

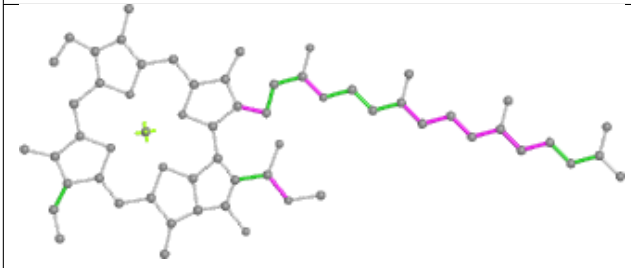
Ligand CLA B 818



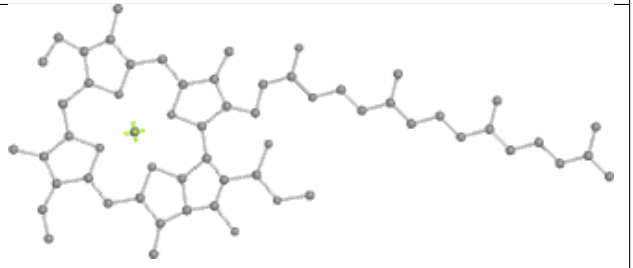
Bond lengths



Bond angles

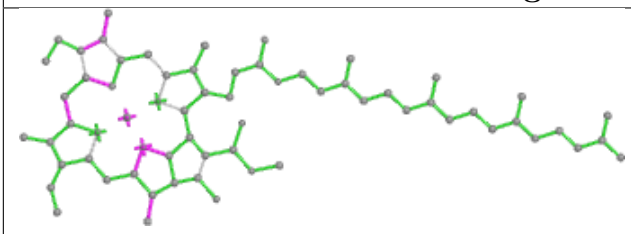


Torsions

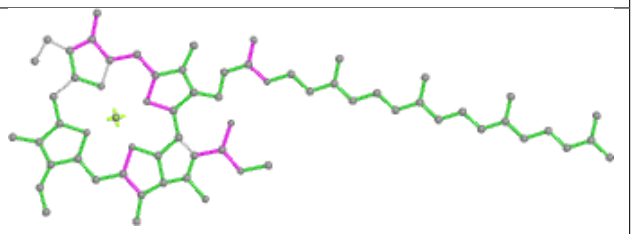


Rings

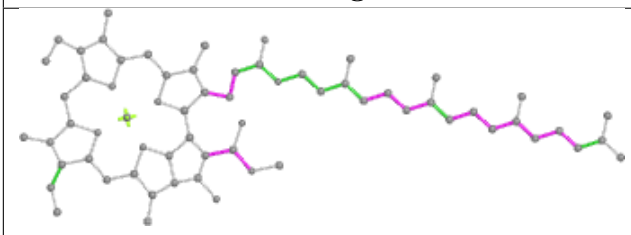
Ligand CLA A 825



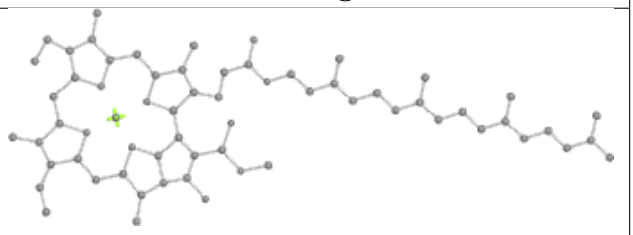
Bond lengths



Bond angles

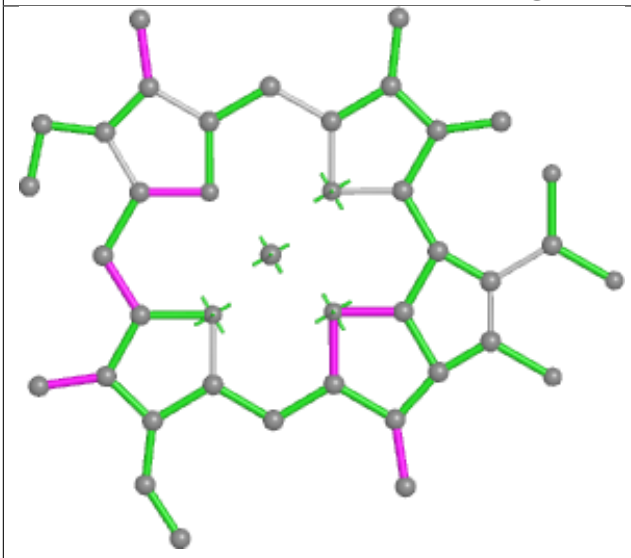


Torsions

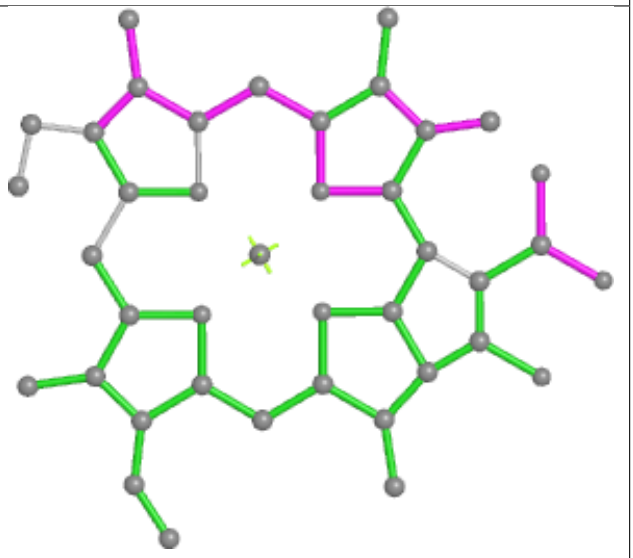


Rings

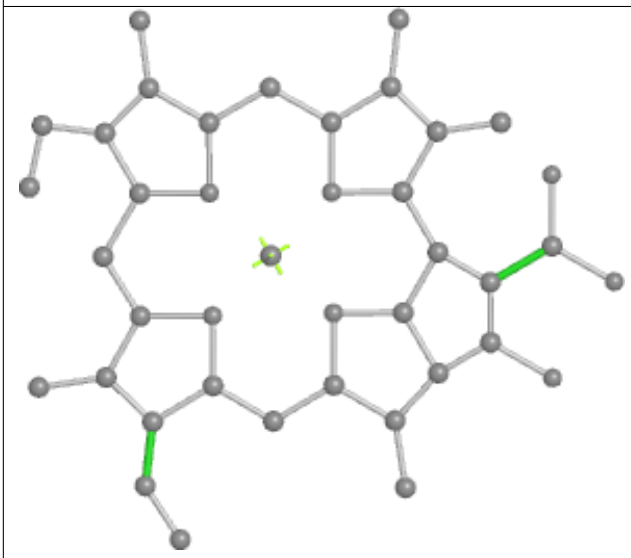
Ligand CLA 1 607



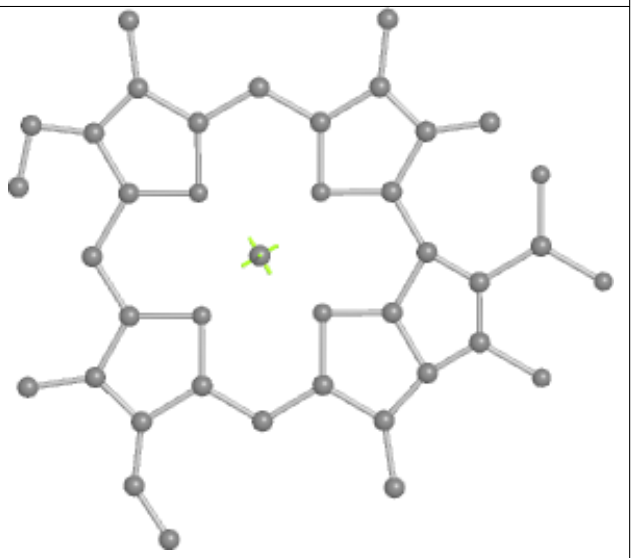
Bond lengths



Bond angles

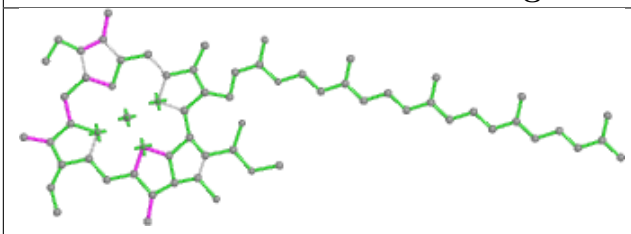


Torsions

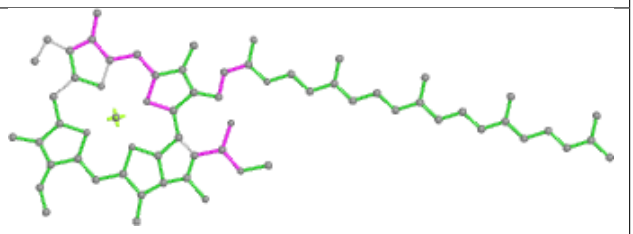


Rings

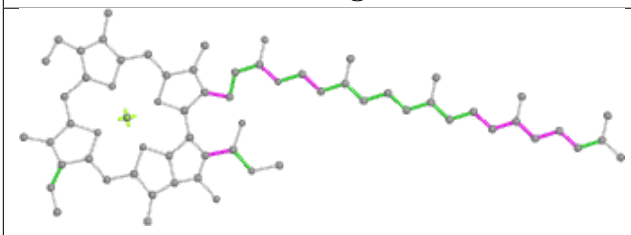
Ligand CLA A 804



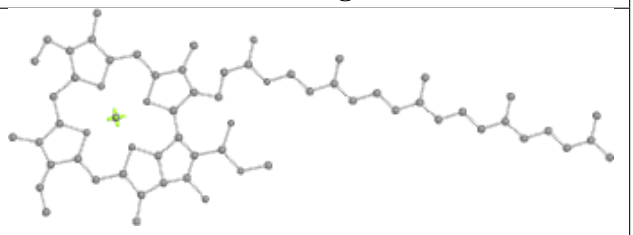
Bond lengths



Bond angles

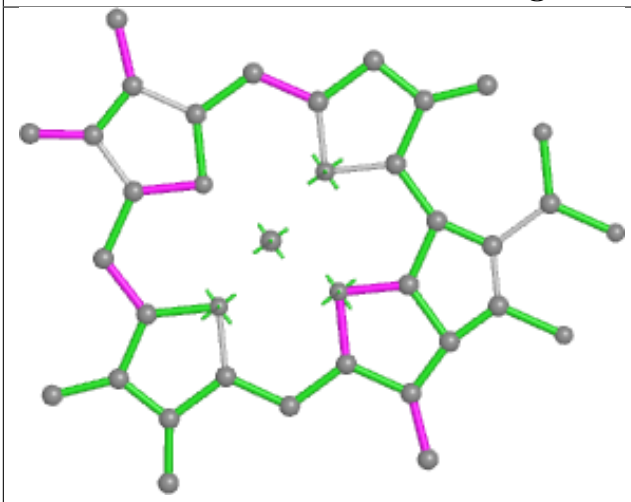


Torsions

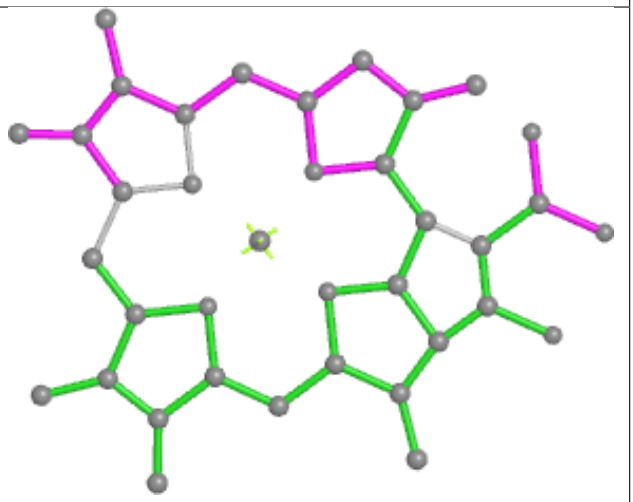


Rings

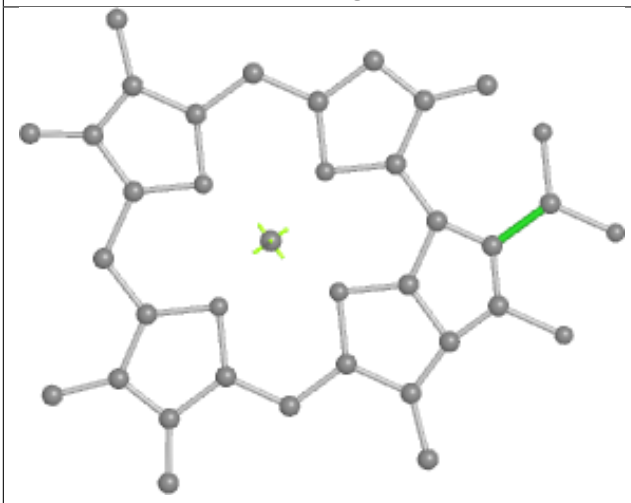
Ligand CLA 1 614



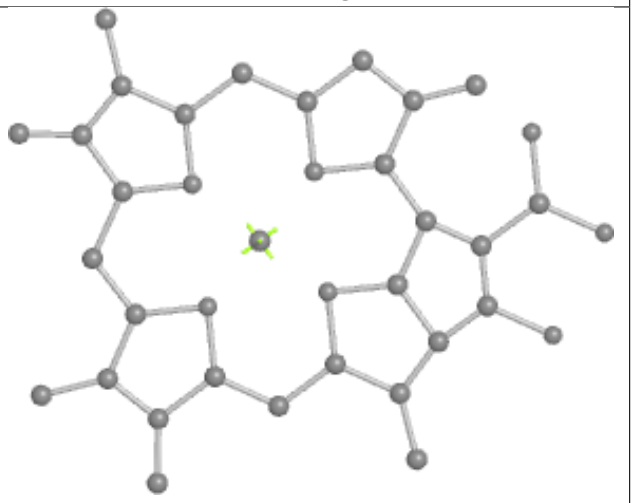
Bond lengths



Bond angles

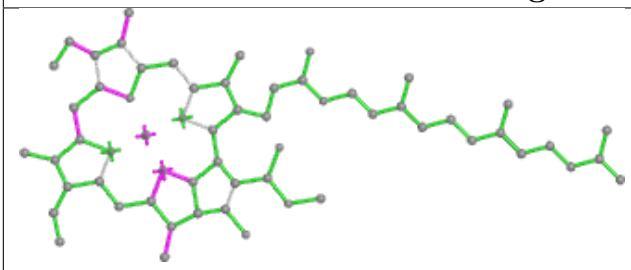


Torsions

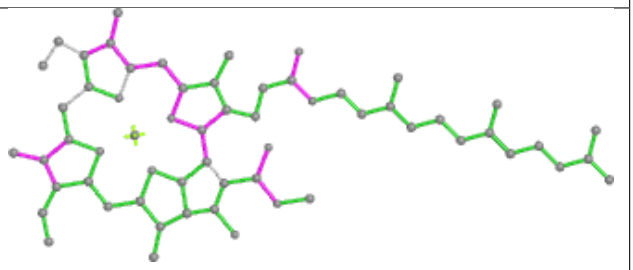


Rings

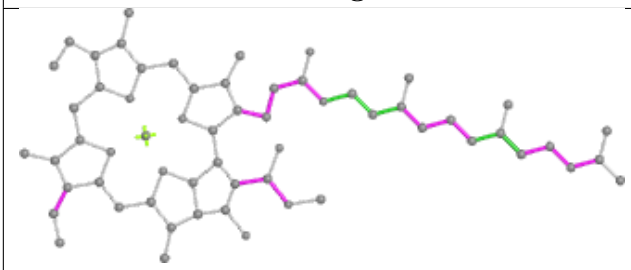
Ligand CLA 3 609



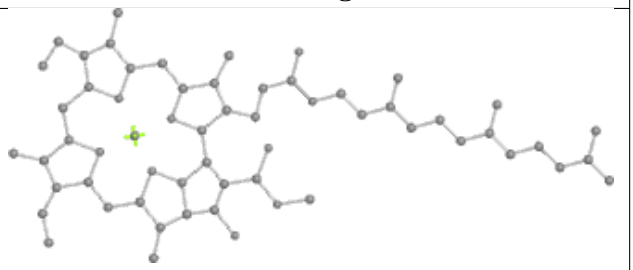
Bond lengths



Bond angles

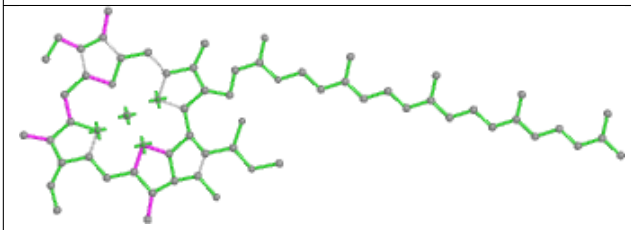


Torsions

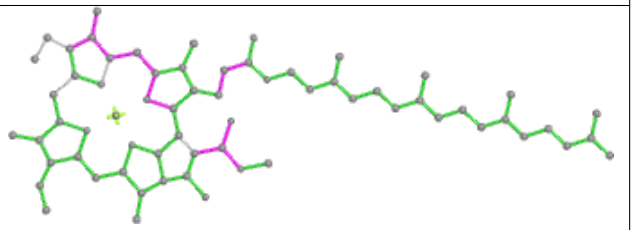


Rings

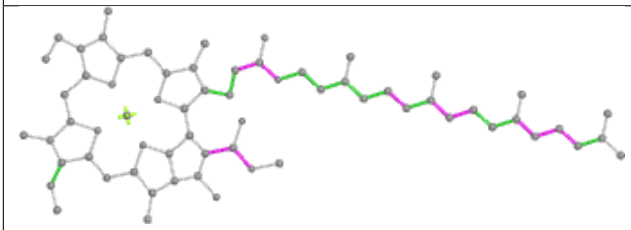
Ligand CLA 6 601



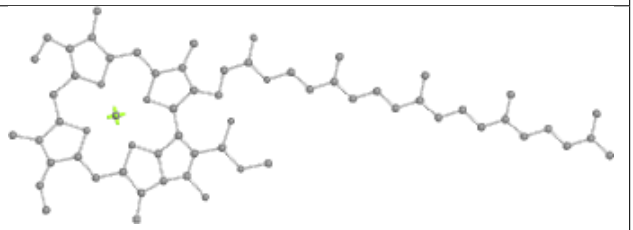
Bond lengths



Bond angles

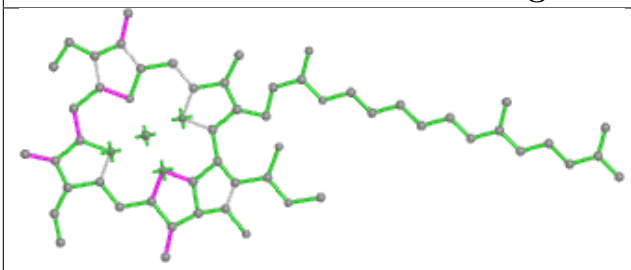


Torsions

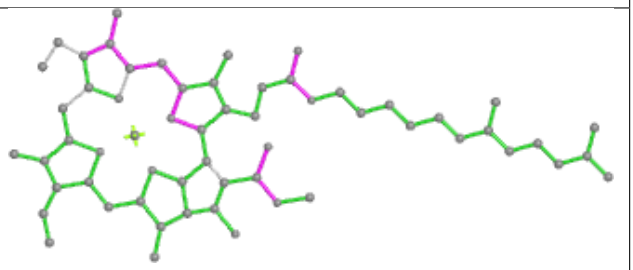


Rings

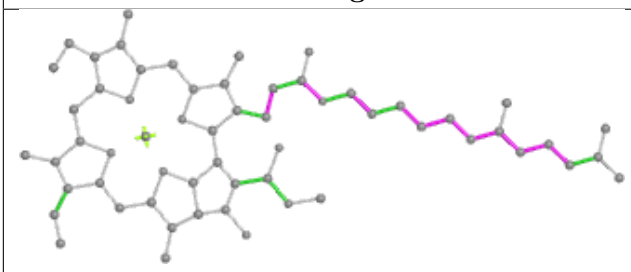
Ligand CLA 7 611



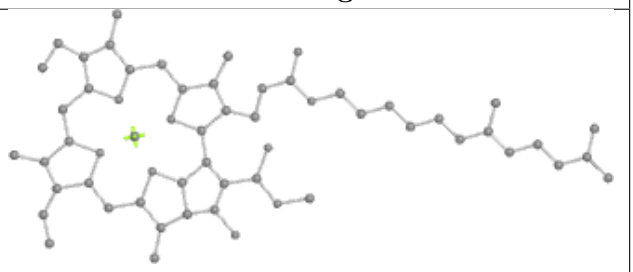
Bond lengths



Bond angles

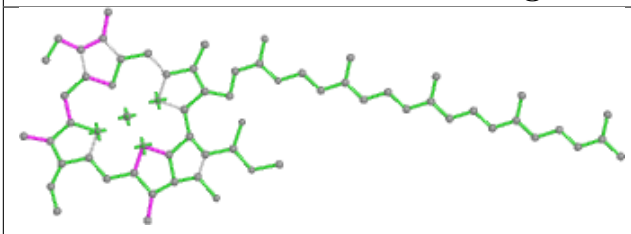


Torsions

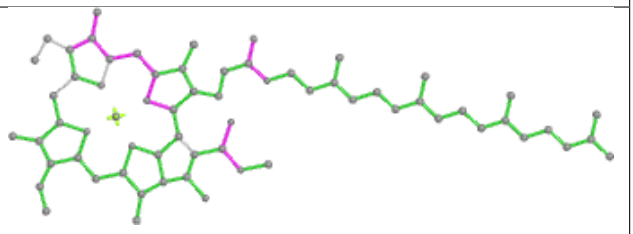


Rings

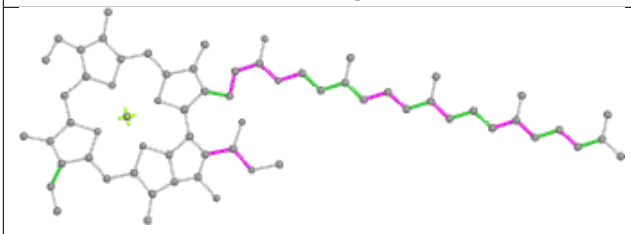
Ligand CLA A 841



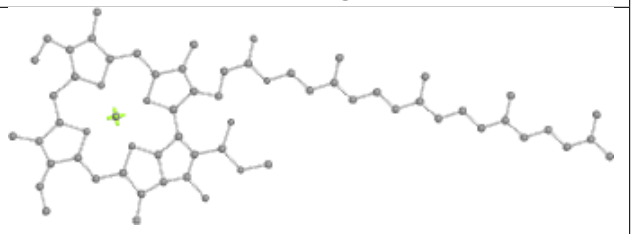
Bond lengths



Bond angles

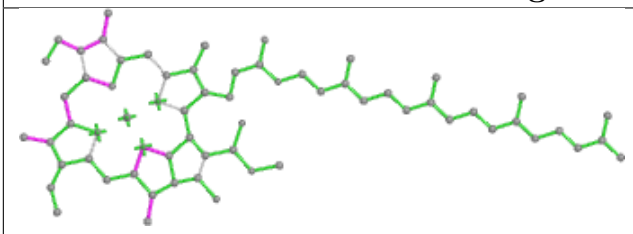


Torsions

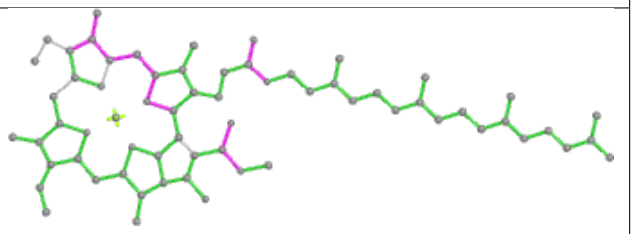


Rings

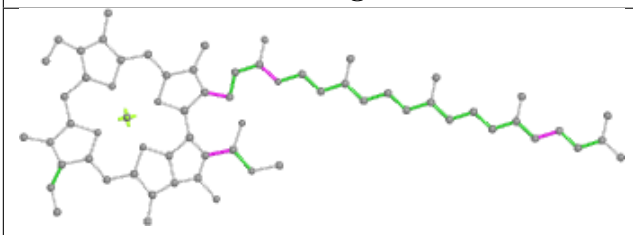
Ligand CLA 3 610



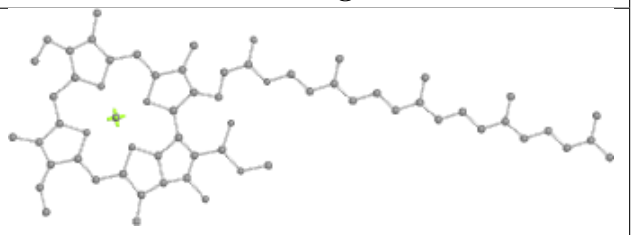
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

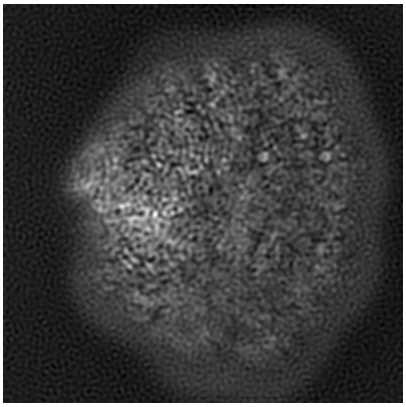
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-9678. These allow visual inspection of the internal detail of the map and identification of artifacts.

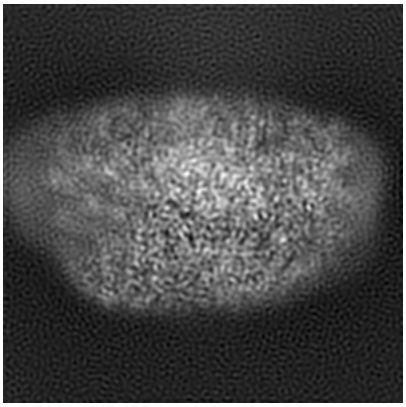
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

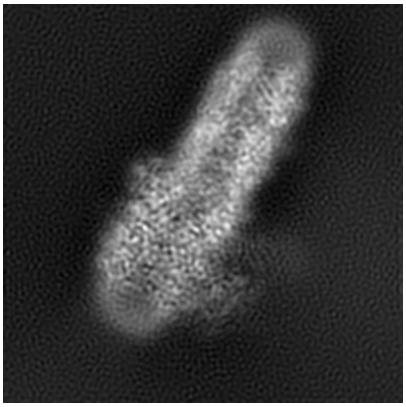
6.1.1 Primary map



X



Y

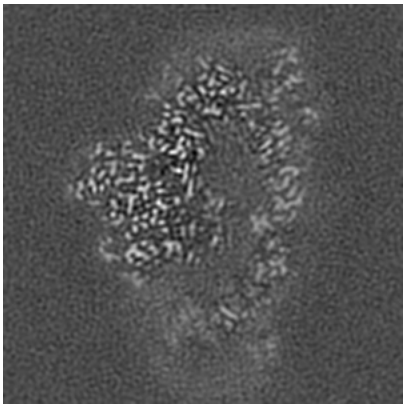


Z

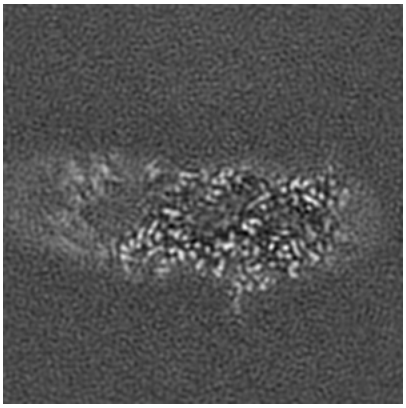
The images above show the map projected in three orthogonal directions.

6.2 Central slices

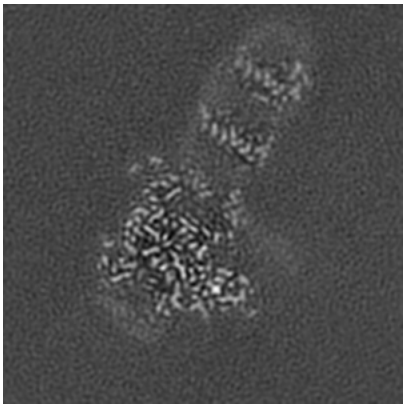
6.2.1 Primary map



X Index: 100



Y Index: 100

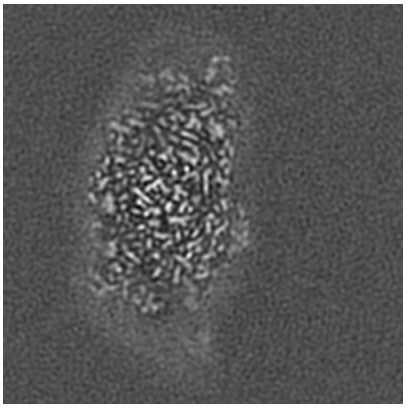


Z Index: 100

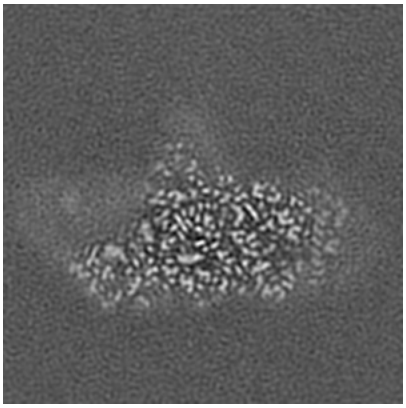
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

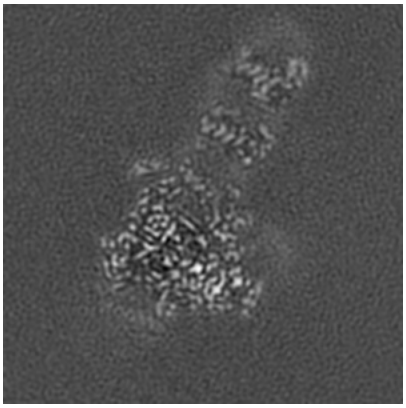
6.3.1 Primary map



X Index: 80



Y Index: 82

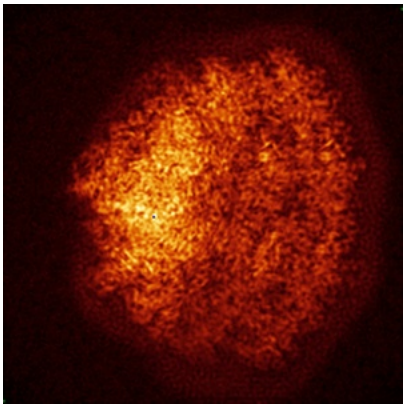


Z Index: 98

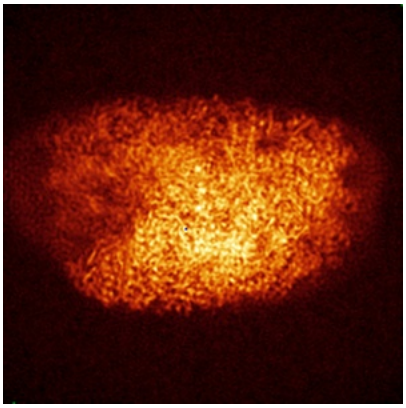
The images above show the largest variance slices of the map in three orthogonal directions.

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

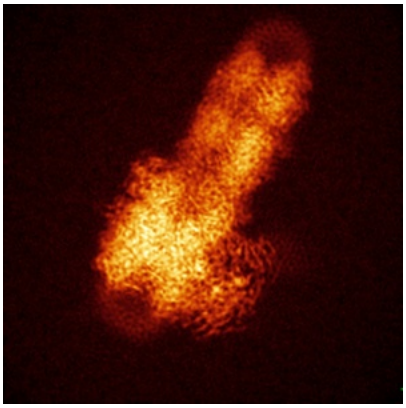
6.4.1 Primary map



X



Y

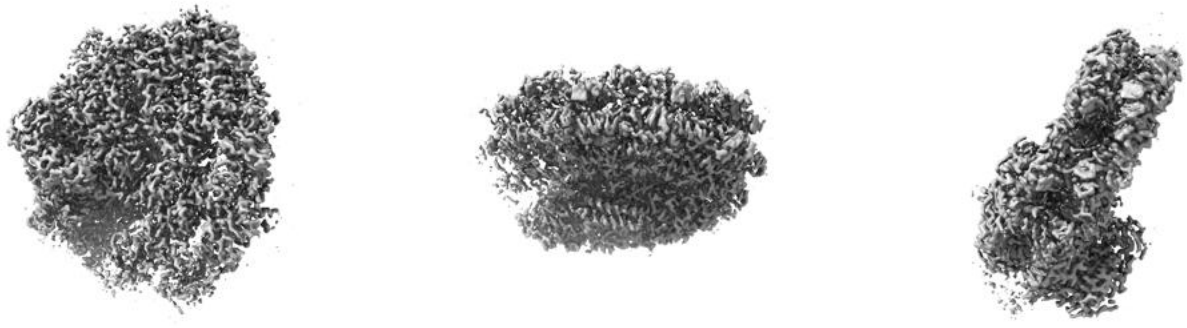


Z

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

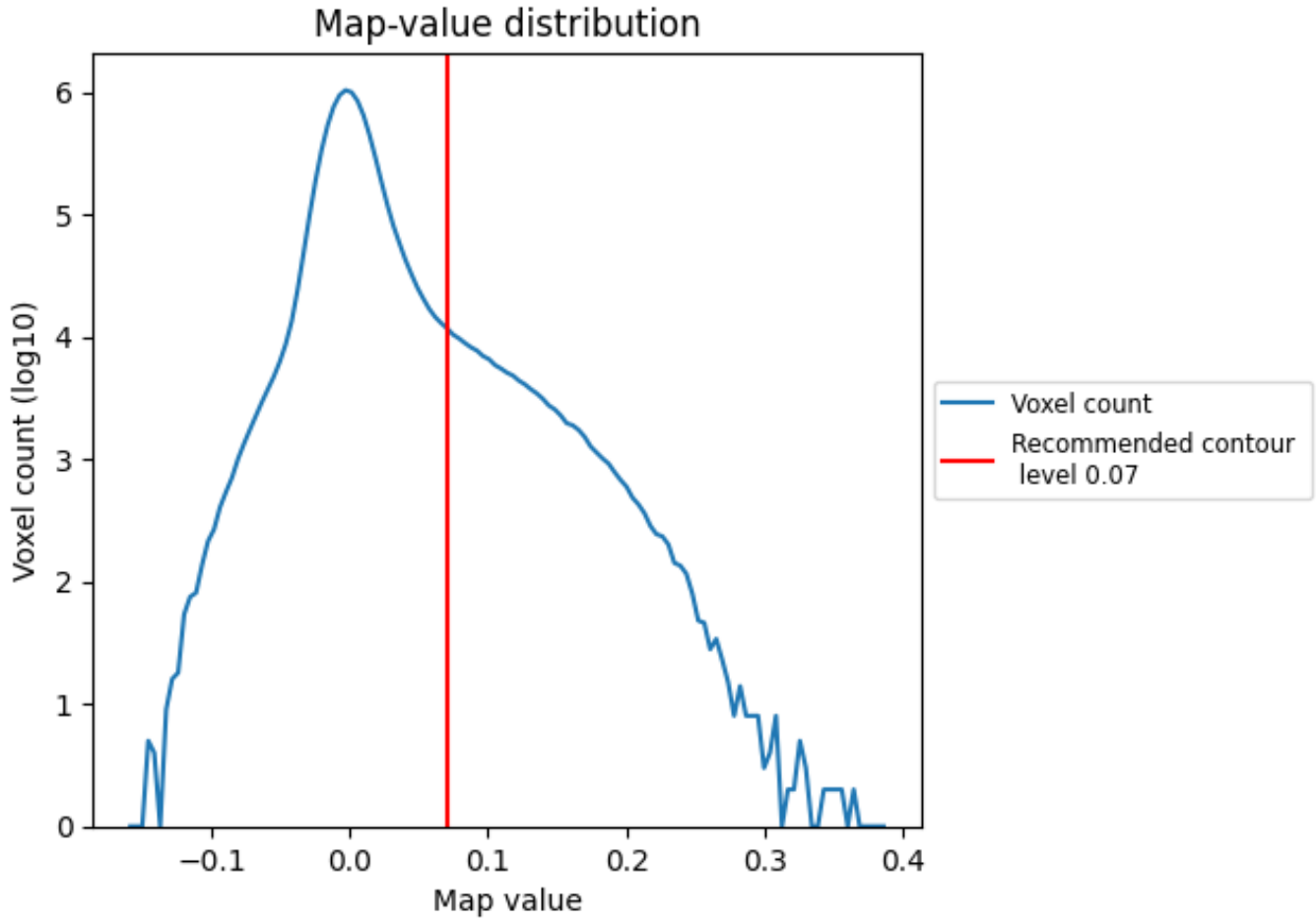
6.6 Mask visualisation (i)

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

7 Map analysis

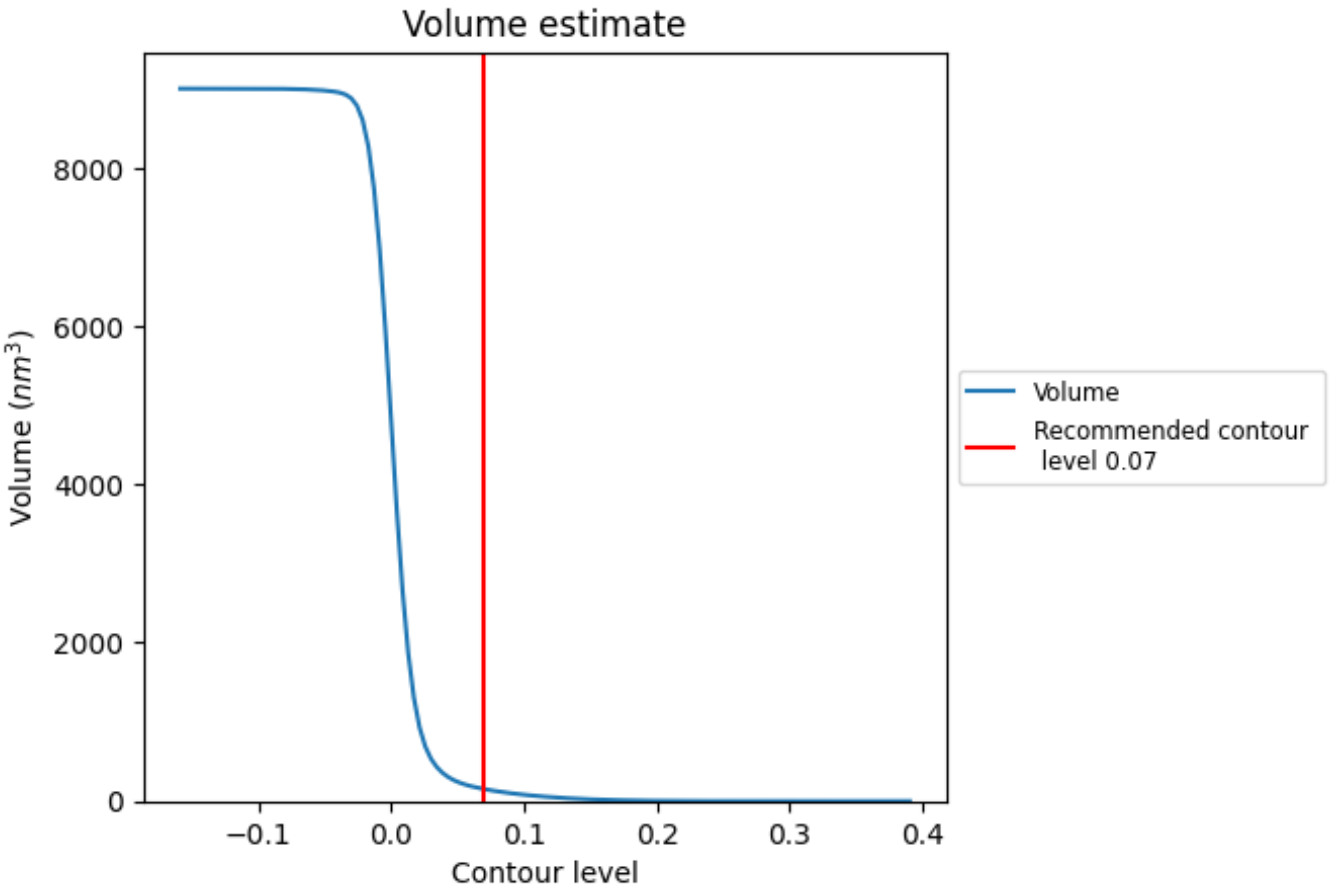
This section contains the results of statistical analysis of the map.

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.

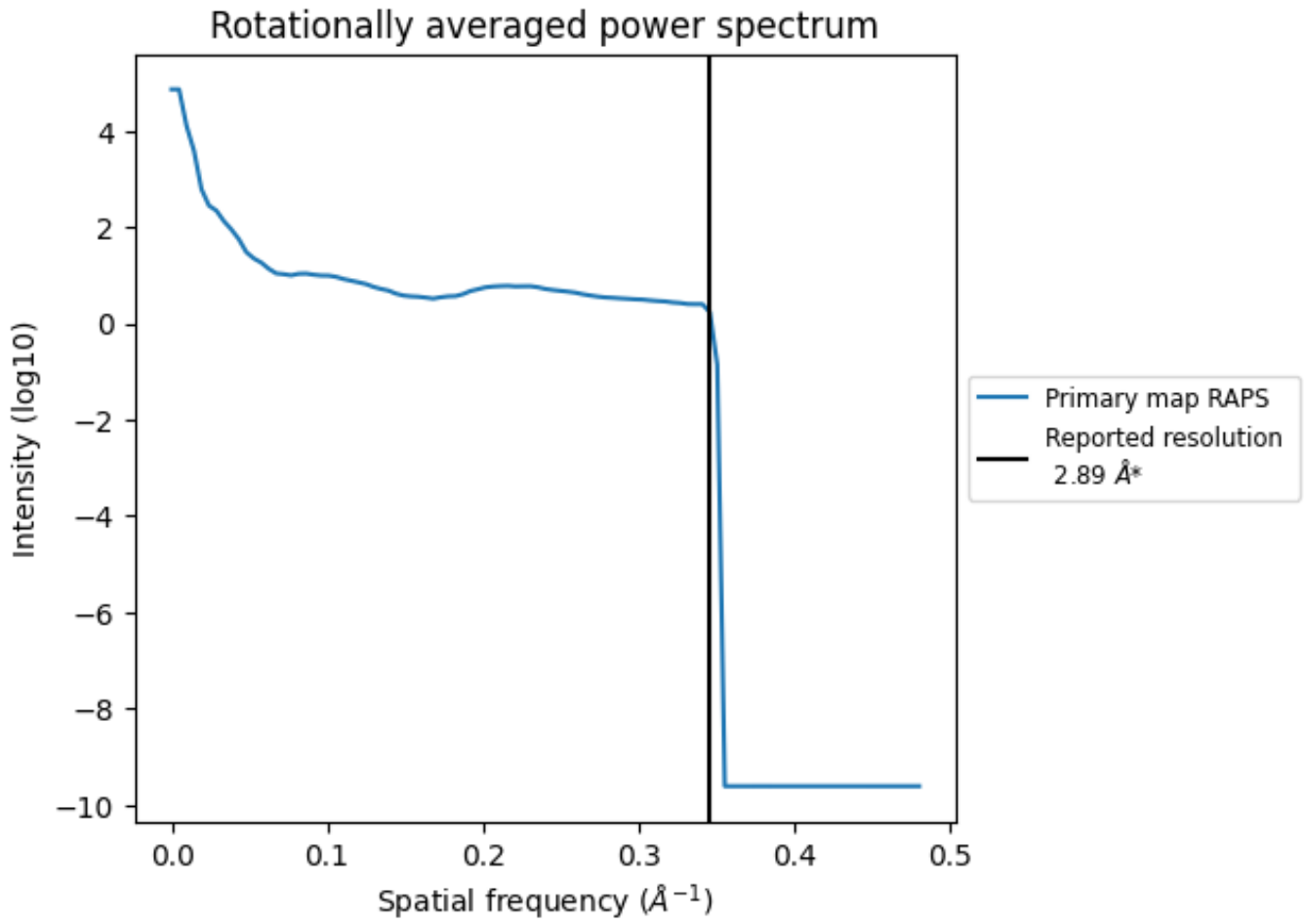
7.2 Volume estimate (i)



The volume at the recommended contour level is 153 nm^3; this corresponds to an approximate mass of 138 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 0.346 Å^{-1}

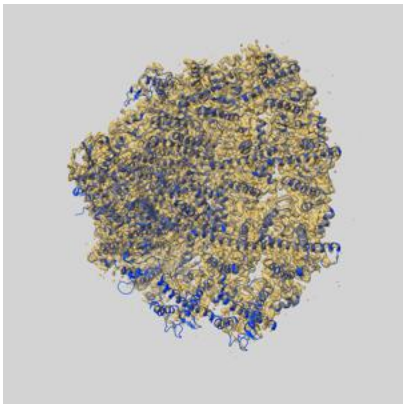
8 Fourier-Shell correlation

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

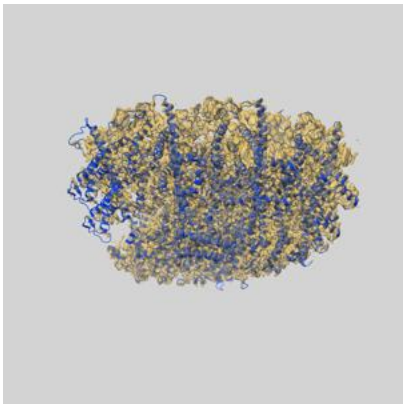
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-9678 and PDB model 6IJJ. Per-residue inclusion information can be found in section 3 on page 32.

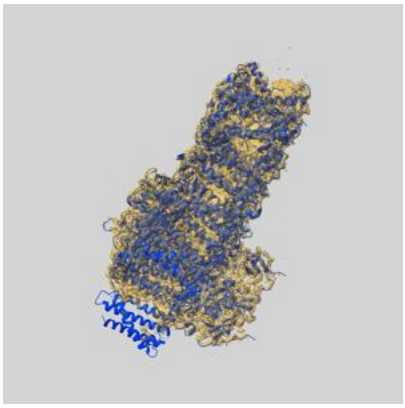
9.1 Map-model overlay



X



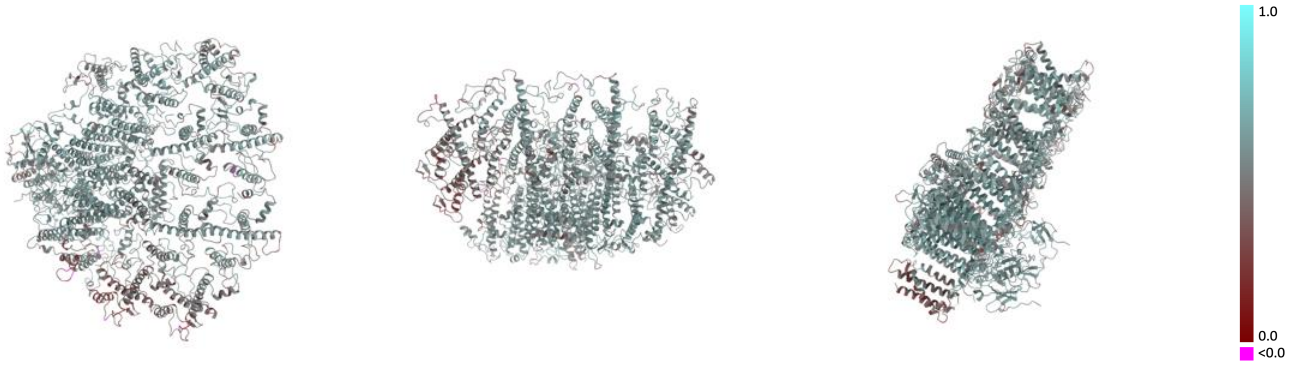
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.07 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.

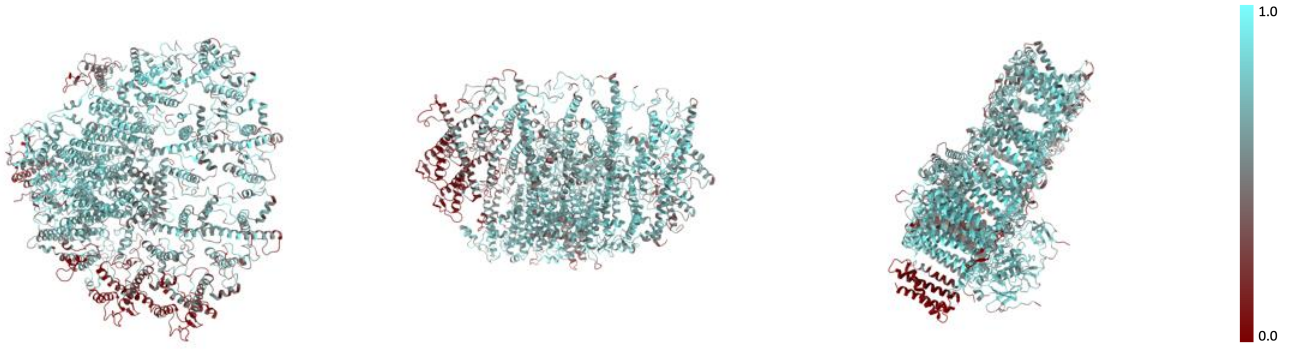
9.2 Q-score mapped to coordinate model (i)



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.

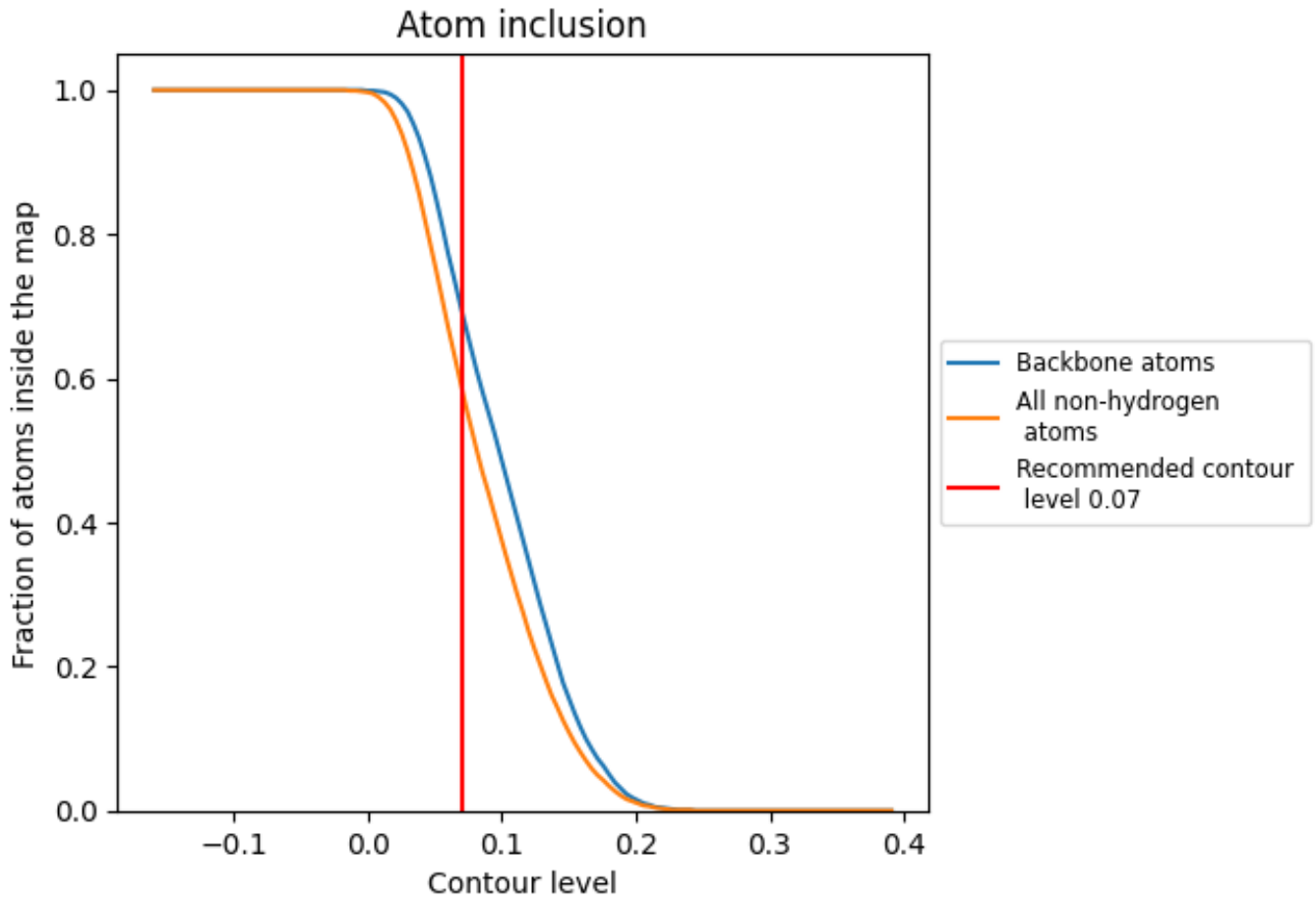
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.07).

9.4 Atom inclusion (i)



At the recommended contour level, 70% of all backbone atoms, 59% 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 (0.07) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5900	0.5370
1	0.2230	0.3740
3	0.6650	0.5730
4	0.5480	0.5270
5	0.5940	0.5430
6	0.6170	0.5440
7	0.6350	0.5530
8	0.5860	0.5300
A	0.7670	0.6020
B	0.6290	0.5440
C	0.7910	0.5640
D	0.6830	0.5550
E	0.6790	0.5520
F	0.5240	0.5090
I	0.2080	0.4660
J	0.3890	0.5120
K	0.3660	0.5030
L	0.0220	0.3540
a	0.3300	0.4660