wwPDB EM Validation Summary Report (i)

Apr 5, 2026 – 09:26 PM UTC

PDB ID	:	9K1E / pdb_00009k1e
EMDB ID	:	EMD-61973
Title	:	Structural insights into photosystem I complex of Bryopsis corticulans
Authors	:	Liu, X.Y.; Wang, W.D.
Deposited on	:	2024-10-16
Resolution	:	2.68 Å(reported)

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

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

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

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

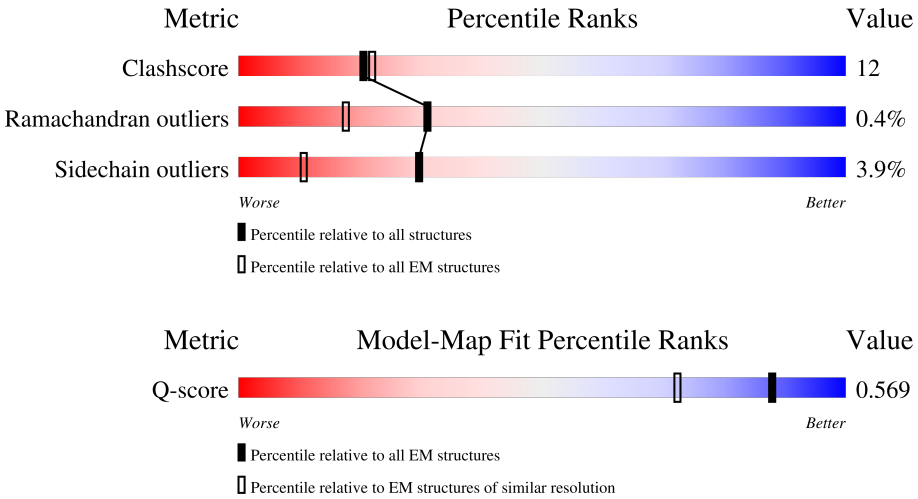
EMDB validation analysis	:	0.0.1.dev132
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.68 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	9255 (2.18 - 3.18)

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	0	245	9% 61% 24% • 13%
2	1	226	• 56% 28% • 14%
2	5	226	6% 62% 22% • 14%
3	2	256	70% 13% • 16%

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Mol	Chain	Length	Quality of chain
4	3	281	62% 18% 19%
5	6	267	69% 16% 14%
6	7	264	66% 19% 14%
7	4	248	48% 29% 6% 17%
7	8	248	59% 21% 17%
8	9	222	60% 18% 6% 15%
9	A	751	72% 26%
10	B	734	76% 23%
11	D	198	55% 17% 28%
12	E	91	62% 8% 30%
13	F	236	58% 11% 30%
14	G	167	36% 16% 44%
15	I	36	6% 67% 28%
16	J	41	63% 34%
17	L	204	9% 64% 15% 21%
18	C	81	77% 22%
19	K	123	55% 9% 35%
20	M	32	84% 12%
21	O	137	6% 57% 9% 33%
22	H	133	13% 59% 11% 29%

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
23	CHL	0	301	X	-	-	-
23	CHL	0	302	X	-	-	-
23	CHL	0	305	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
23	CHL	0	306	X	-	-	-
23	CHL	1	301	X	-	-	-
23	CHL	1	304	X	-	-	-
23	CHL	1	305	X	-	-	-
23	CHL	1	306	X	-	-	-
23	CHL	1	312	X	-	-	-
23	CHL	2	301	X	-	-	-
23	CHL	2	304	X	-	-	-
23	CHL	2	305	X	-	-	-
23	CHL	2	306	X	-	-	-
23	CHL	2	307	X	-	-	-
23	CHL	2	312	X	-	-	-
23	CHL	3	301	X	-	-	-
23	CHL	3	302	X	-	-	-
23	CHL	3	305	X	-	-	-
23	CHL	3	307	X	-	-	-
23	CHL	4	301	X	-	-	-
23	CHL	4	302	X	-	-	-
23	CHL	4	305	X	-	-	-
23	CHL	4	306	X	-	-	-
23	CHL	4	307	X	-	-	-
23	CHL	4	308	X	-	-	-
23	CHL	4	313	X	-	-	-
23	CHL	4	315	X	-	-	-
23	CHL	5	301	X	-	-	-
23	CHL	5	304	X	-	-	-
23	CHL	5	305	X	-	-	-
23	CHL	5	306	X	-	-	-
23	CHL	5	312	X	-	-	-
23	CHL	6	301	X	-	-	-
23	CHL	6	302	X	-	-	-
23	CHL	6	305	X	-	-	-
23	CHL	6	306	X	-	-	-
23	CHL	6	307	X	-	-	-
23	CHL	6	308	X	-	-	-
23	CHL	6	313	X	-	-	-
23	CHL	6	315	X	-	-	-
23	CHL	6	323	X	-	-	-
23	CHL	7	301	X	-	-	-
23	CHL	7	302	X	-	-	-
23	CHL	7	305	X	-	-	-
23	CHL	7	306	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
23	CHL	7	307	X	-	-	-
23	CHL	7	313	X	-	-	-
23	CHL	8	301	X	-	-	-
23	CHL	8	303	X	-	-	-
23	CHL	8	306	X	-	-	-
23	CHL	8	307	X	-	-	-
23	CHL	8	308	X	-	-	-
23	CHL	8	309	X	-	-	-
23	CHL	8	314	X	-	-	-
23	CHL	8	316	X	-	-	-
23	CHL	9	301	X	-	-	-
23	CHL	9	305	X	-	-	-
23	CHL	9	306	X	-	-	-
23	CHL	9	312	X	-	-	-
24	CLA	0	303	X	-	-	-
24	CLA	0	304	X	-	-	-
24	CLA	0	307	X	-	-	-
24	CLA	0	308	X	-	-	-
24	CLA	0	309	X	-	-	-
24	CLA	0	310	X	-	-	-
24	CLA	0	311	X	-	-	-
24	CLA	0	312	X	-	-	-
24	CLA	0	313	X	-	-	-
24	CLA	0	319	X	-	-	-
24	CLA	1	302	X	-	-	-
24	CLA	1	303	X	-	-	-
24	CLA	1	307	X	-	-	-
24	CLA	1	308	X	-	-	-
24	CLA	1	309	X	-	-	-
24	CLA	1	310	X	-	-	-
24	CLA	1	311	X	-	-	-
24	CLA	1	313	X	-	-	-
24	CLA	2	302	X	-	-	-
24	CLA	2	303	X	-	-	-
24	CLA	2	308	X	-	-	-
24	CLA	2	309	X	-	-	-
24	CLA	2	310	X	-	-	-
24	CLA	2	311	X	-	-	-
24	CLA	2	313	X	-	-	-
24	CLA	3	303	X	-	-	-
24	CLA	3	304	X	-	-	-
24	CLA	3	306	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
24	CLA	3	308	X	-	-	-
24	CLA	3	309	X	-	-	-
24	CLA	3	310	X	-	-	-
24	CLA	3	311	X	-	-	-
24	CLA	3	312	X	-	-	-
24	CLA	3	313	X	-	-	-
24	CLA	3	314	X	-	-	-
24	CLA	3	315	X	-	-	-
24	CLA	4	303	X	-	-	-
24	CLA	4	304	X	-	-	-
24	CLA	4	309	X	-	-	-
24	CLA	4	310	X	-	-	-
24	CLA	4	311	X	-	-	-
24	CLA	4	312	X	-	-	-
24	CLA	4	314	X	-	-	-
24	CLA	5	302	X	-	-	-
24	CLA	5	303	X	-	-	-
24	CLA	5	307	X	-	-	-
24	CLA	5	308	X	-	-	-
24	CLA	5	309	X	-	-	-
24	CLA	5	310	X	-	-	-
24	CLA	5	311	X	-	-	-
24	CLA	5	313	X	-	-	-
24	CLA	6	303	X	-	-	-
24	CLA	6	304	X	-	-	-
24	CLA	6	309	X	-	-	-
24	CLA	6	310	X	-	-	-
24	CLA	6	311	X	-	-	-
24	CLA	6	312	X	-	-	-
24	CLA	6	314	X	-	-	-
24	CLA	6	316	X	-	-	-
24	CLA	6	317	X	-	-	-
24	CLA	6	318	X	-	-	-
24	CLA	7	303	X	-	-	-
24	CLA	7	304	X	-	-	-
24	CLA	7	308	X	-	-	-
24	CLA	7	309	X	-	-	-
24	CLA	7	310	X	-	-	-
24	CLA	7	311	X	-	-	-
24	CLA	7	312	X	-	-	-
24	CLA	7	314	X	-	-	-
24	CLA	7	315	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
24	CLA	7	316	X	-	-	-
24	CLA	7	317	X	-	-	-
24	CLA	8	304	X	-	-	-
24	CLA	8	305	X	-	-	-
24	CLA	8	310	X	-	-	-
24	CLA	8	311	X	-	-	-
24	CLA	8	312	X	-	-	-
24	CLA	8	313	X	-	-	-
24	CLA	8	315	X	-	-	-
24	CLA	9	302	X	-	-	-
24	CLA	9	303	X	-	-	-
24	CLA	9	304	X	-	-	-
24	CLA	9	307	X	-	-	-
24	CLA	9	308	X	-	-	-
24	CLA	9	309	X	-	-	-
24	CLA	9	310	X	-	-	-
24	CLA	9	311	X	-	-	-
24	CLA	A	801	X	-	-	-
24	CLA	A	802	X	-	-	-
24	CLA	A	803	X	-	-	-
24	CLA	A	804	X	-	-	-
24	CLA	A	805	X	-	-	-
24	CLA	A	806	X	-	-	-
24	CLA	A	807	X	-	-	-
24	CLA	A	808	X	-	-	-
24	CLA	A	809	X	-	-	-
24	CLA	A	810	X	-	-	-
24	CLA	A	811	X	-	-	-
24	CLA	A	812	X	-	-	-
24	CLA	A	813	X	-	-	-
24	CLA	A	814	X	-	-	-
24	CLA	A	815	X	-	-	-
24	CLA	A	816	X	-	-	-
24	CLA	A	817	X	-	-	-
24	CLA	A	818	X	-	-	-
24	CLA	A	819	X	-	-	-
24	CLA	A	820	X	-	-	-
24	CLA	A	821	X	-	-	-
24	CLA	A	822	X	-	-	-
24	CLA	A	823	X	-	-	-
24	CLA	A	824	X	-	-	-
24	CLA	A	825	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
24	CLA	A	826	X	-	-	-
24	CLA	A	827	X	-	-	-
24	CLA	A	828	X	-	-	-
24	CLA	A	829	X	-	-	-
24	CLA	A	830	X	-	-	-
24	CLA	A	831	X	-	-	-
24	CLA	A	832	X	-	-	-
24	CLA	A	833	X	-	-	-
24	CLA	A	834	X	-	-	-
24	CLA	A	835	X	-	-	-
24	CLA	A	836	X	-	-	-
24	CLA	A	837	X	-	-	-
24	CLA	A	838	X	-	-	-
24	CLA	A	839	X	-	-	-
24	CLA	A	840	X	-	-	-
24	CLA	A	848	X	-	-	-
24	CLA	A	853	X	-	-	-
24	CLA	B	801	X	-	-	-
24	CLA	B	802	X	-	-	-
24	CLA	B	804	X	-	-	-
24	CLA	B	805	X	-	-	-
24	CLA	B	806	X	-	-	-
24	CLA	B	807	X	-	-	-
24	CLA	B	808	X	-	-	-
24	CLA	B	809	X	-	-	-
24	CLA	B	810	X	-	-	-
24	CLA	B	811	X	-	-	-
24	CLA	B	812	X	-	-	-
24	CLA	B	813	X	-	-	-
24	CLA	B	814	X	-	-	-
24	CLA	B	815	X	-	-	-
24	CLA	B	816	X	-	-	-
24	CLA	B	817	X	-	-	-
24	CLA	B	818	X	-	-	-
24	CLA	B	819	X	-	-	-
24	CLA	B	820	X	-	-	-
24	CLA	B	821	X	-	-	-
24	CLA	B	822	X	-	-	-
24	CLA	B	823	X	-	-	-
24	CLA	B	824	X	-	-	-
24	CLA	B	825	X	-	-	-
24	CLA	B	826	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
24	CLA	B	827	X	-	-	-
24	CLA	B	828	X	-	-	-
24	CLA	B	829	X	-	-	-
24	CLA	B	830	X	-	-	-
24	CLA	B	831	X	-	-	-
24	CLA	B	832	X	-	-	-
24	CLA	B	833	X	-	-	-
24	CLA	B	834	X	-	-	-
24	CLA	B	835	X	-	-	-
24	CLA	B	836	X	-	-	-
24	CLA	B	837	X	-	-	-
24	CLA	B	838	X	-	-	-
24	CLA	B	839	X	-	-	-
24	CLA	B	840	X	-	-	-
24	CLA	B	841	X	-	-	-
24	CLA	F	302	X	-	-	-
24	CLA	F	303	X	-	-	-
24	CLA	G	101	X	-	-	-
24	CLA	G	102	X	-	-	-
24	CLA	G	103	X	-	-	-
24	CLA	H	201	X	-	-	-
24	CLA	H	202	X	-	-	-
24	CLA	H	203	X	-	-	-
24	CLA	H	204	X	-	-	-
24	CLA	H	205	X	-	-	-
24	CLA	J	103	X	-	-	-
24	CLA	K	101	X	-	-	-
24	CLA	K	102	X	-	-	-
24	CLA	K	103	X	-	-	-
24	CLA	K	104	X	-	-	-
24	CLA	L	201	X	-	-	-
24	CLA	L	202	X	-	-	-
24	CLA	L	203	X	-	-	-
24	CLA	L	206	X	-	-	-
24	CLA	O	201	X	-	-	-
24	CLA	O	204	X	-	-	-
24	CLA	O	205	X	-	-	-
24	CLA	O	206	X	-	-	-
24	CLA	O	209	X	-	-	-
32	CL0	A	852	X	-	-	-

2 Entry composition (i)

There are 34 unique types of molecules in this entry. The entry contains 54077 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 Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	0	213	Total	C	N	O	S	0	0
			1640	1063	270	296	11		

- Molecule 2 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	1	195	Total	C	N	O	S	0	0
			1478	950	243	273	12		
2	5	195	Total	C	N	O	S	0	0
			1484	956	243	273	12		

- Molecule 3 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	2	216	Total	C	N	O	S	0	0
			1667	1082	269	304	12		

- Molecule 4 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	3	228	Total	C	N	O	S	0	0
			1768	1141	288	329	10		

- Molecule 5 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	6	229	Total	C	N	O	S	0	0
			1797	1182	292	313	10		

- Molecule 6 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	7	228	Total	C	N	O	S	0	0
			1758	1137	291	319	11		

- Molecule 7 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	8	205	Total	C	N	O	S	0	0
			1574	1035	256	274	9		
7	4	207	Total	C	N	O	S	0	0
			1569	1030	257	273	9		

- Molecule 8 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	9	189	Total	C	N	O	S	0	0
			1453	932	245	267	9		

- Molecule 9 is a protein called Photosystem I P700 chlorophyll a apoprotein A1.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	A	746	Total	C	N	O	S	0	0
			5872	3836	998	1016	22		

- Molecule 10 is a protein called photosystem I.

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

- Molecule 11 is a protein called Photosystem I reaction center subunit II, chloroplastic.

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

- Molecule 12 is a protein called PsaE.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	E	64	Total	C	N	O	S	0	0
			509	323	90	95	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
13	F	165	Total	C	N	O	S	0	0
			1273	810	224	235	4		

- Molecule 14 is a protein called PsaG.

Mol	Chain	Residues	Atoms				AltConf	Trace
14	G	93	Total	C	N	O	0	0
			726	471	119	136		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
15	I	35	Total	C	N	O	S	0	0
			262	180	37	43	2		

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

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

- Molecule 17 is a protein called PSI subunit V.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	L	162	Total	C	N	O	S	0	0
			1195	773	192	226	4		

- Molecule 18 is a protein called Photosystem I iron-sulfur center.

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

- Molecule 19 is a protein called PsaK.

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

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

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

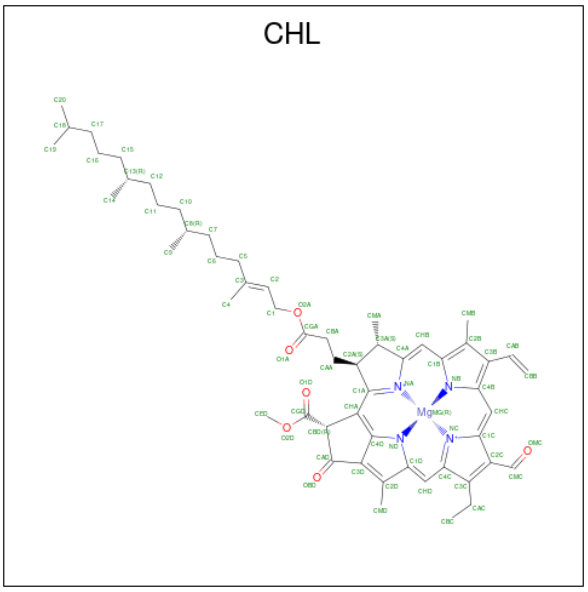
- Molecule 21 is a protein called PsaO.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	O	92	Total	C	N	O	S	0	0
			728	488	116	120	4		

- Molecule 22 is a protein called PsaH.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	H	94	Total	C	N	O	S	0	0
			717	451	126	139	1		

- Molecule 23 is CHLOROPHYLL B (CCD ID: CHL) (formula: $C_{55}H_{70}MgN_4O_6$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
23	0	1	Total	C	Mg	N	O	0
			52	41	1	4	6	
23	0	1	Total	C	Mg	N	O	0
			64	53	1	4	6	
23	0	1	Total	C	Mg	N	O	0
			51	40	1	4	6	
23	0	1	Total	C	Mg	N	O	0
			48	37	1	4	6	

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Mol	Chain	Residues	Atoms					AltConf
23	1	1	Total	C	Mg	N	O	0
			64	53	1	4	6	
23	1	1	Total	C	Mg	N	O	0
			51	40	1	4	6	
23	1	1	Total	C	Mg	N	O	0
			48	37	1	4	6	
23	1	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
23	1	1	Total	C	Mg	N	O	0
			62	51	1	4	6	
23	2	1	Total	C	Mg	N	O	0
			64	53	1	4	6	
23	2	1	Total	C	Mg	N	O	0
			43	34	1	4	4	
23	2	1	Total	C	Mg	N	O	0
			48	37	1	4	6	
23	2	1	Total	C	Mg	N	O	0
			51	40	1	4	6	
23	2	1	Total	C	Mg	N	O	0
			47	36	1	4	6	
23	2	1	Total	C	Mg	N	O	0
			51	40	1	4	6	
23	3	1	Total	C	Mg	N	O	0
			61	50	1	4	6	
23	3	1	Total	C	Mg	N	O	0
			62	51	1	4	6	
23	3	1	Total	C	Mg	N	O	0
			51	40	1	4	6	
23	3	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
23	5	1	Total	C	Mg	N	O	0
			64	53	1	4	6	
23	5	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
23	5	1	Total	C	Mg	N	O	0
			48	37	1	4	6	
23	5	1	Total	C	Mg	N	O	0
			47	36	1	4	6	
23	5	1	Total	C	Mg	N	O	0
			47	36	1	4	6	
23	6	1	Total	C	Mg	N	O	0
			61	50	1	4	6	

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Mol	Chain	Residues	Atoms					AltConf
23	6	1	Total	C	Mg	N	O	0
			64	53	1	4	6	
23	6	1	Total	C	Mg	N	O	0
			43	34	1	4	4	
23	6	1	Total	C	Mg	N	O	0
			51	40	1	4	6	
23	6	1	Total	C	Mg	N	O	0
			51	40	1	4	6	
23	6	1	Total	C	Mg	N	O	0
			60	49	1	4	6	
23	6	1	Total	C	Mg	N	O	0
			52	41	1	4	6	
23	6	1	Total	C	Mg	N	O	0
			43	34	1	4	4	
23	6	1	Total	C	Mg	N	O	0
			61	50	1	4	6	
23	7	1	Total	C	Mg	N	O	0
			63	52	1	4	6	
23	7	1	Total	C	Mg	N	O	0
			64	53	1	4	6	
23	7	1	Total	C	Mg	N	O	0
			48	37	1	4	6	
23	7	1	Total	C	Mg	N	O	0
			61	50	1	4	6	
23	7	1	Total	C	Mg	N	O	0
			51	40	1	4	6	
23	7	1	Total	C	Mg	N	O	0
			47	36	1	4	6	
23	8	1	Total	C	Mg	N	O	0
			52	41	1	4	6	
23	8	1	Total	C	Mg	N	O	0
			64	53	1	4	6	
23	8	1	Total	C	Mg	N	O	0
			47	36	1	4	6	
23	8	1	Total	C	Mg	N	O	0
			51	40	1	4	6	
23	8	1	Total	C	Mg	N	O	0
			51	40	1	4	6	
23	8	1	Total	C	Mg	N	O	0
			47	36	1	4	6	
23	8	1	Total	C	Mg	N	O	0
			56	45	1	4	6	

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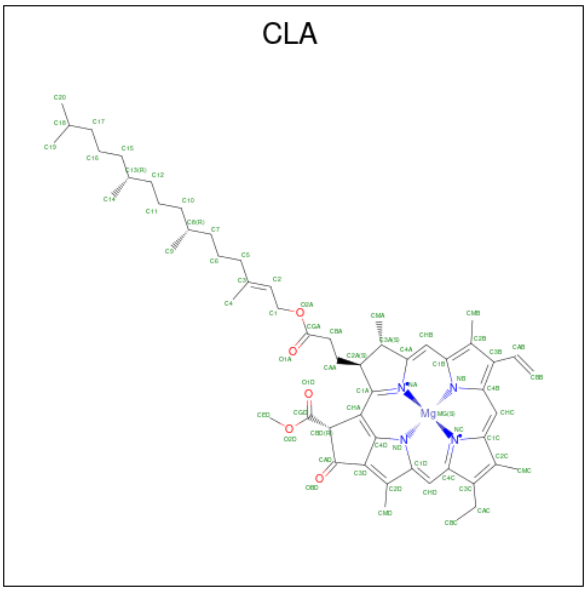
Mol	Chain	Residues	Atoms					AltConf
23	8	1	Total	C	Mg	N	O	0
			43	34	1	4	4	
23	9	1	Total	C	Mg	N	O	0
			47	36	1	4	6	
23	9	1	Total	C	Mg	N	O	0
			51	40	1	4	6	
23	9	1	Total	C	Mg	N	O	0
			48	37	1	4	6	
23	9	1	Total	C	Mg	N	O	0
			47	36	1	4	6	
23	4	1	Total	C	Mg	N	O	0
			61	50	1	4	6	
23	4	1	Total	C	Mg	N	O	0
			53	42	1	4	6	
23	4	1	Total	C	Mg	N	O	0
			43	34	1	4	4	
23	4	1	Total	C	Mg	N	O	0
			48	37	1	4	6	
23	4	1	Total	C	Mg	N	O	0
			51	40	1	4	6	
23	4	1	Total	C	Mg	N	O	0
			47	36	1	4	6	
23	4	1	Total	C	Mg	N	O	0
			51	40	1	4	6	
23	4	1	Total	C	Mg	N	O	0
			54	43	1	4	6	

- Molecule 24 is CHLOROPHYLL A (CCD ID: CLA) (formula: $C_{55}H_{72}MgN_4O_5$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
24	0	1	Total 62	C 52	Mg 1	N 4	O 5	0
24	0	1	Total 52	C 42	Mg 1	N 4	O 5	0
24	0	1	Total 60	C 50	Mg 1	N 4	O 5	0
24	0	1	Total 60	C 50	Mg 1	N 4	O 5	0
24	0	1	Total 41	C 33	Mg 1	N 4	O 3	0
24	0	1	Total 47	C 37	Mg 1	N 4	O 5	0
24	0	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	0	1	Total 46	C 36	Mg 1	N 4	O 5	0
24	0	1	Total 45	C 35	Mg 1	N 4	O 5	0
24	0	1	Total 46	C 36	Mg 1	N 4	O 5	0
24	1	1	Total 56	C 46	Mg 1	N 4	O 5	0
24	1	1	Total 52	C 42	Mg 1	N 4	O 5	0
24	1	1	Total 45	C 35	Mg 1	N 4	O 5	0
24	1	1	Total 55	C 45	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
24	1	1	Total	C	Mg	N	O	0
			63	53	1	4	5	
24	1	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
24	1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
24	1	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
24	2	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
24	2	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
24	2	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
24	2	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
24	2	1	Total	C	Mg	N	O	0
			48	38	1	4	5	
24	2	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
24	2	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
24	3	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
24	3	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
24	3	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
24	3	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
24	3	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
24	3	1	Total	C	Mg	N	O	0
			62	52	1	4	5	
24	3	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
24	3	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
24	3	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
24	3	1	Total	C	Mg	N	O	0
			46	36	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
24	3	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
24	5	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
24	5	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
24	5	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
24	5	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
24	5	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
24	5	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
24	5	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
24	5	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
24	6	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
24	6	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
24	6	1	Total	C	Mg	N	O	0
			58	48	1	4	5	
24	6	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
24	6	1	Total	C	Mg	N	O	0
			48	38	1	4	5	
24	6	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
24	6	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
24	6	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
24	6	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
24	6	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
24	7	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
24	7	1	Total	C	Mg	N	O	0
			55	45	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
24	7	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
24	7	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
24	7	1	Total	C	Mg	N	O	0
			37	31	1	4	1	
24	7	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
24	7	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
24	7	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
24	7	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
24	7	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
24	7	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
24	8	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
24	8	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
24	8	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
24	8	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
24	8	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
24	8	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
24	8	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
24	9	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
24	9	1	Total	C	Mg	N	O	0
			48	38	1	4	5	
24	9	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
24	9	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
24	9	1	Total	C	Mg	N	O	0
			60	50	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
24	9	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
24	9	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
24	9	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
24	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
24	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
24	A	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
24	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
24	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
24	A	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
24	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
24	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
24	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
24	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
24	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
24	A	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
24	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
24	A	1	Total	C	Mg	N	O	0
			57	47	1	4	5	
24	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
24	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
24	A	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
24	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
24	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
24	A	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
24	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
24	A	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
24	A	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
24	A	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
24	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
24	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
24	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
24	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
24	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
24	A	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
24	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
24	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
24	A	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
24	A	1	Total	C	Mg	N	O	0
			57	47	1	4	5	
24	A	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
24	A	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
24	A	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
24	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
24	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
24	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
24	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
24	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
24	B	1	Total	C	Mg	N	O	0
			58	48	1	4	5	
24	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
24	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
24	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
24	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
24	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
24	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
24	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
24	B	1	Total	C	Mg	N	O	0
			62	52	1	4	5	
24	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
24	B	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
24	B	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
24	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
24	B	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
24	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
24	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
24	B	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
24	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
24	B	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
24	B	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
24	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
24	B	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
24	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
24	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
24	B	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
24	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
24	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
24	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
24	B	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
24	B	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
24	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
24	B	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
24	B	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
24	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
24	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
24	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
24	B	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
24	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
24	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
24	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
24	F	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
24	F	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
24	G	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
24	G	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
24	G	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
24	J	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
24	L	1	Total	C	Mg	N	O	0
			58	48	1	4	5	
24	L	1	Total	C	Mg	N	O	0
			63	53	1	4	5	
24	L	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
24	L	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
24	K	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
24	K	1	Total	C	Mg	N	O	0
			53	43	1	4	5	
24	K	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
24	K	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
24	O	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
24	O	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
24	O	1	Total	C	Mg	N	O	0
			38	30	1	4	3	
24	O	1	Total	C	Mg	N	O	0
			38	30	1	4	3	
24	O	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
24	H	1	Total	C	Mg	N	O	0
			46	36	1	4	5	

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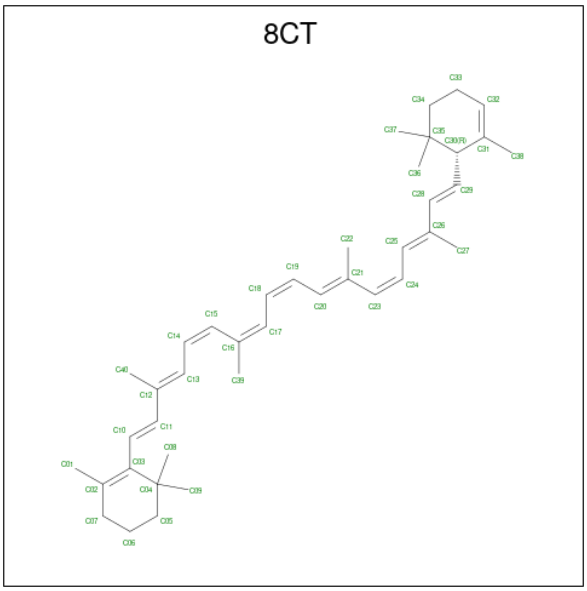
Mol	Chain	Residues	Atoms					AltConf
24	H	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
24	H	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
24	H	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
24	H	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
24	4	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
24	4	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
24	4	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
24	4	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
24	4	1	Total	C	Mg	N	O	0
			48	38	1	4	5	
24	4	1	Total	C	Mg	N	O	0
			53	43	1	4	5	
24	4	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

- Molecule 25 is (6'R,11cis,11'cis,13cis,15cis)-4',5'-didehydro-5',6'-dihydro-beta,beta-carotene (CCD ID: 8CT) (formula: $C_{40}H_{56}$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	AltConf
25	0	1	Total C 40 40	0
25	1	1	Total C 40 40	0
25	2	1	Total C 40 40	0
25	3	1	Total C 40 40	0
25	3	1	Total C 40 40	0
25	3	1	Total C 40 40	0
25	6	1	Total C 40 40	0
25	6	1	Total C 40 40	0
25	7	1	Total C 40 40	0
25	7	1	Total C 40 40	0
25	8	1	Total C 40 40	0
25	9	1	Total C 40 40	0
25	A	1	Total C 40 40	0
25	A	1	Total C 40 40	0
25	A	1	Total C 40 40	0
25	A	1	Total C 40 40	0
25	A	1	Total C 40 40	0
25	B	1	Total C 40 40	0
25	B	1	Total C 40 40	0
25	B	1	Total C 40 40	0
25	B	1	Total C 40 40	0
25	B	1	Total C 40 40	0

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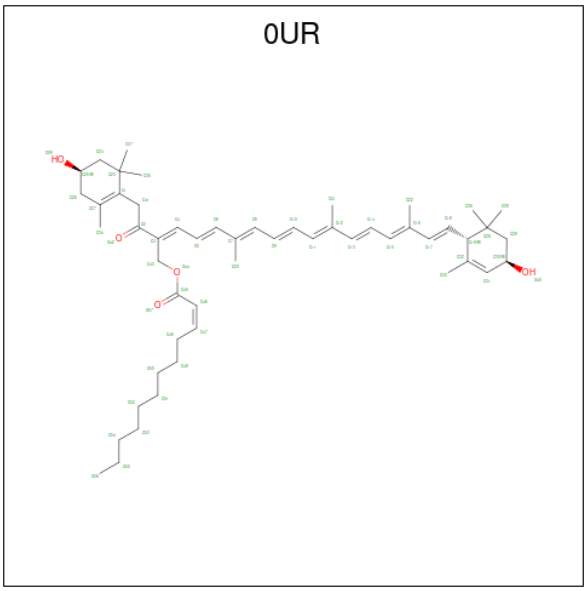
Mol	Chain	Residues	Atoms	AltConf
25	B	1	Total C 40 40	0
25	B	1	Total C 40 40	0
25	F	1	Total C 40 40	0
25	F	1	Total C 40 40	0
25	G	1	Total C 40 40	0
25	I	1	Total C 40 40	0
25	J	1	Total C 40 40	0
25	J	1	Total C 40 40	0
25	L	1	Total C 40 40	0
25	L	1	Total C 40 40	0
25	L	1	Total C 40 40	0
25	K	1	Total C 40 40	0
25	M	1	Total C 40 40	0
25	O	1	Total C 40 40	0
25	O	1	Total C 40 40	0
25	4	1	Total C 40 40	0

- Molecule 26 is Siphonein (CCD ID: 0UR) (formula: $C_{52}H_{76}O_5$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	AltConf
26	0	1	Total C O 52 47 5	0
26	0	1	Total C O 52 47 5	0
26	1	1	Total C O 52 47 5	0
26	1	1	Total C O 52 47 5	0
26	2	1	Total C O 51 46 5	0
26	2	1	Total C O 50 45 5	0
26	3	1	Total C O 51 46 5	0
26	5	1	Total C O 51 46 5	0
26	5	1	Total C O 52 47 5	0
26	6	1	Total C O 51 46 5	0
26	6	1	Total C O 52 47 5	0
26	7	1	Total C O 51 46 5	0
26	8	1	Total C O 51 46 5	0
26	8	1	Total C O 52 47 5	0

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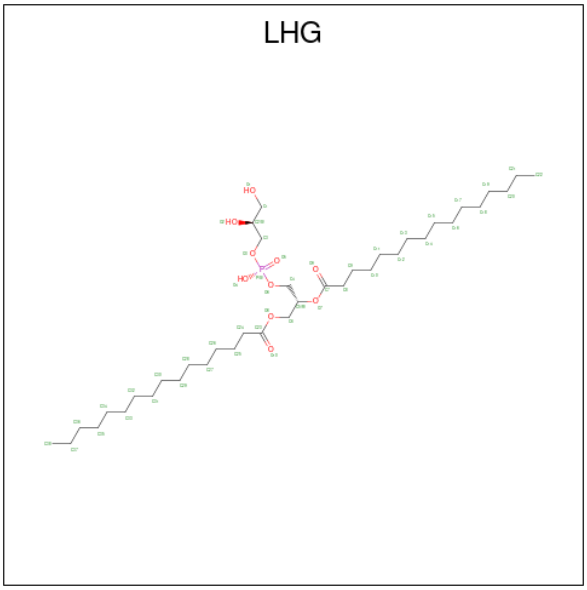
Mol	Chain	Residues	Atoms	AltConf
26	9	1	Total C O 52 47 5	0
26	9	1	Total C O 52 47 5	0
26	O	1	Total C O 52 47 5	0
26	4	1	Total C O 51 46 5	0
26	4	1	Total C O 50 45 5	0

- Molecule 27 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: $C_{38}H_{75}O_{10}P$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	AltConf
27	0	1	Total C O P 49 38 10 1	0
27	1	1	Total C O P 49 38 10 1	0
27	1	1	Total C O P 43 32 10 1	0
27	2	1	Total C O P 32 21 10 1	0
27	2	1	Total C O P 32 21 10 1	0
27	3	1	Total C O P 36 25 10 1	0

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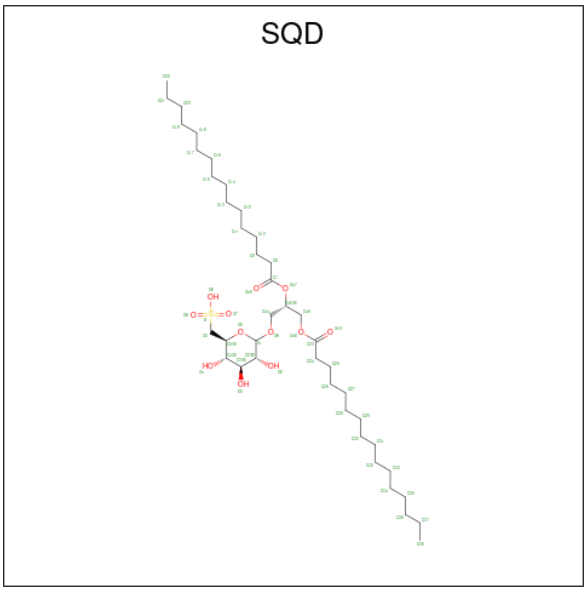
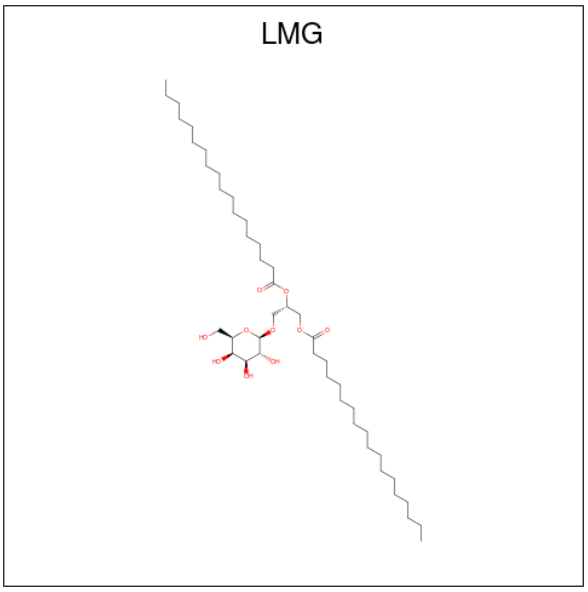
Mol	Chain	Residues	Atoms				AltConf
27	3	1	Total	C	O	P	0
			37	26	10	1	
27	3	1	Total	C	O	P	0
			43	34	8	1	
27	5	1	Total	C	O	P	0
			37	26	10	1	
27	6	1	Total	C	O	P	0
			37	26	10	1	
27	7	1	Total	C	O	P	0
			30	19	10	1	
27	7	1	Total	C	O	P	0
			38	27	10	1	
27	7	1	Total	C	O	P	0
			39	28	10	1	
27	8	1	Total	C	O	P	0
			31	20	10	1	
27	8	1	Total	C	O	P	0
			44	33	10	1	
27	9	1	Total	C	O	P	0
			47	36	10	1	
27	A	1	Total	C	O	P	0
			49	38	10	1	
27	A	1	Total	C	O	P	0
			27	16	10	1	
27	A	1	Total	C	O	P	0
			42	31	10	1	
27	B	1	Total	C	O	P	0
			23	12	10	1	
27	B	1	Total	C	O	P	0
			38	27	10	1	
27	I	1	Total	C	O	P	0
			46	35	10	1	
27	L	1	Total	C	O	P	0
			31	20	10	1	

- Molecule 28 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (CCD ID: SQD) (formula: $C_{41}H_{78}O_{12}S$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
28	0	1	Total	C	O	S	0
			36	26	9	1	

- Molecule 29 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
29	2	1	Total	C	O	0
			36	26	10	
29	3	1	Total	C	O	0
			36	26	10	

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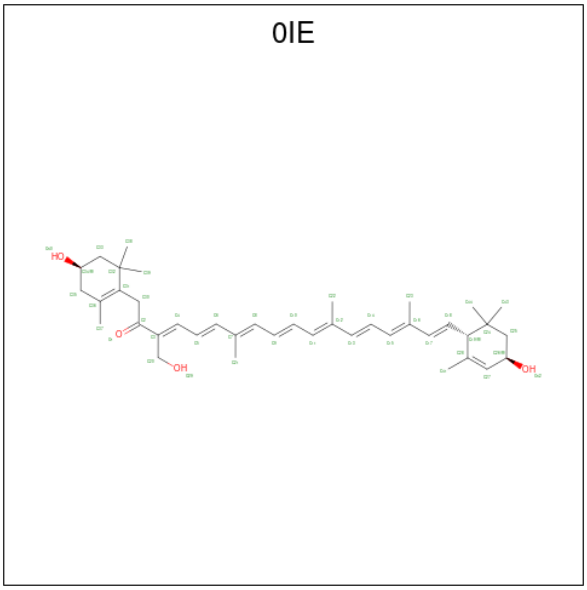
Mol	Chain	Residues	Atoms	AltConf
29	9	1	Total C O 55 45 10	0
29	A	1	Total C O 36 26 10	0
29	A	1	Total C O 37 27 10	0
29	J	1	Total C O 29 19 10	0
29	J	1	Total C O 46 36 10	0
29	M	1	Total C O 42 32 10	0
29	O	1	Total C O 31 21 10	0
29	O	1	Total C O 39 29 10	0

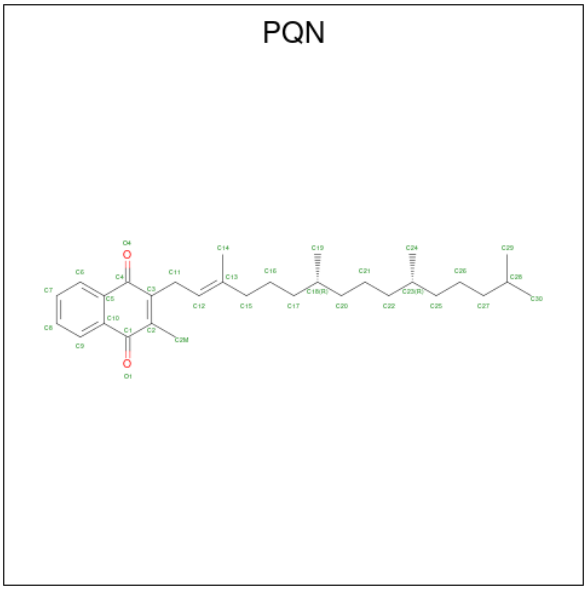
- Molecule 30 is Siphonaxanthin (CCD ID: 0IE) (formula: $C_{40}H_{56}O_4$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	AltConf
30	3	1	Total C O 44 40 4	0
30	7	1	Total C O 44 40 4	0

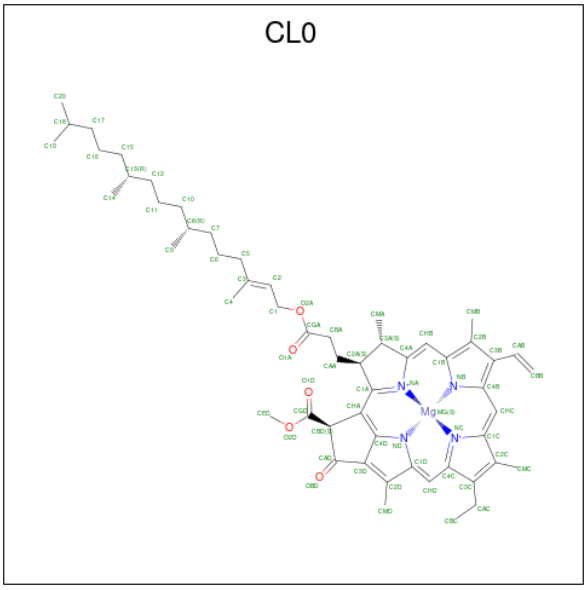
- Molecule 31 is PHYLLOQUINONE (CCD ID: PQN) (formula: $C_{31}H_{46}O_2$) (labeled as "Lig-

and of Interest" by depositor).



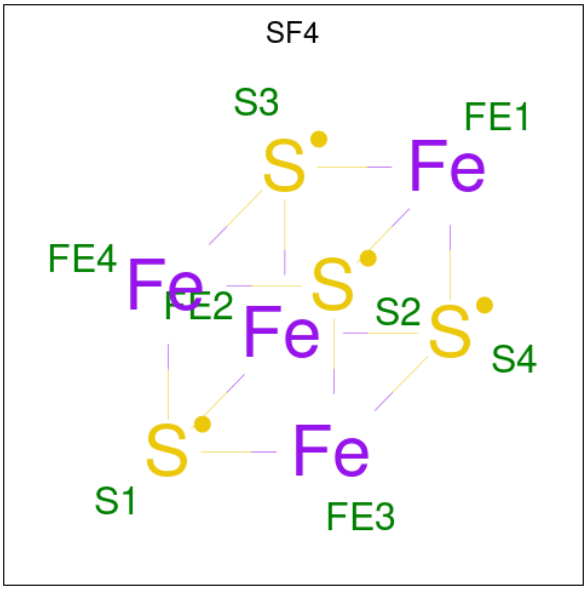
Mol	Chain	Residues	Atoms	AltConf
31	A	1	Total C O 33 31 2	0
31	B	1	Total C O 33 31 2	0

- Molecule 32 is CHLOROPHYLL A ISOMER (CCD ID: CL0) (formula: $C_{55}H_{72}MgN_4O_5$) (labeled as "Ligand of Interest" by depositor).



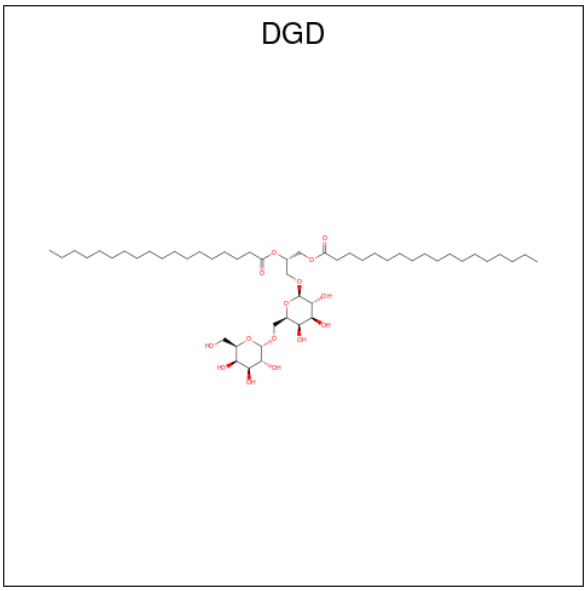
Mol	Chain	Residues	Atoms					AltConf
32	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

- Molecule 33 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 34 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: $C_{51}H_{96}O_{15}$) (labeled as "Ligand of Interest" by depositor).

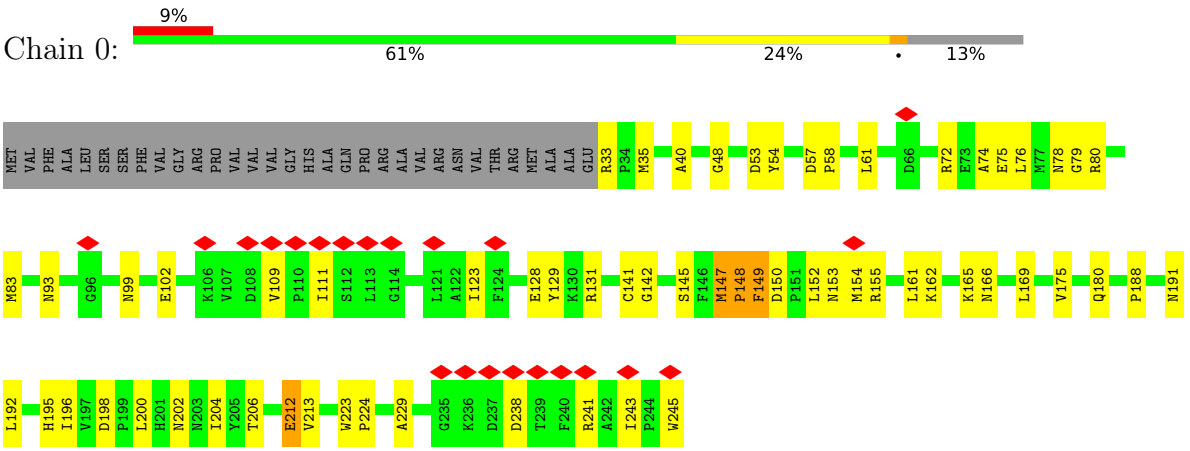


Mol	Chain	Residues	Atoms			AltConf
34	B	1	Total	C	O	0
			56	41	15	

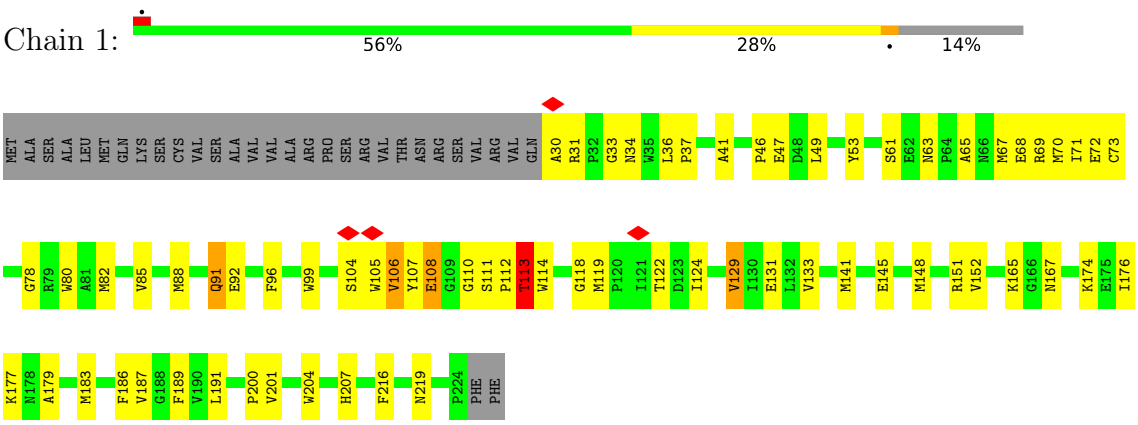
3 Residue-property plots (i)

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

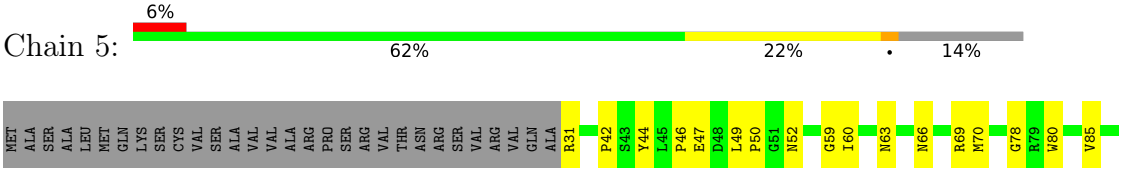
• Molecule 1: Chlorophyll a-b binding protein, chloroplastic

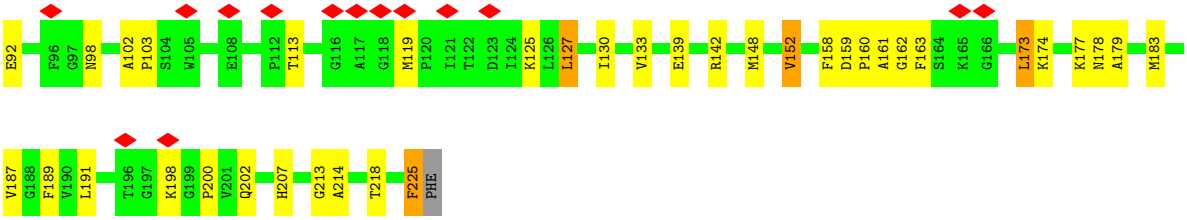


• Molecule 2: Chlorophyll a-b binding protein, chloroplastic



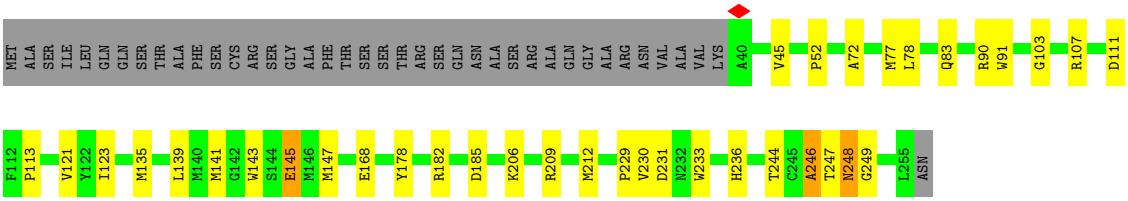
• Molecule 2: Chlorophyll a-b binding protein, chloroplastic





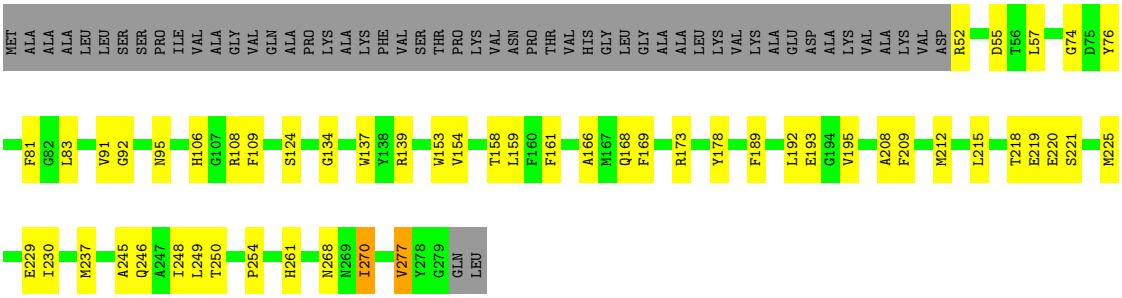
• Molecule 3: Chlorophyll a-b binding protein, chloroplastic

Chain 2:



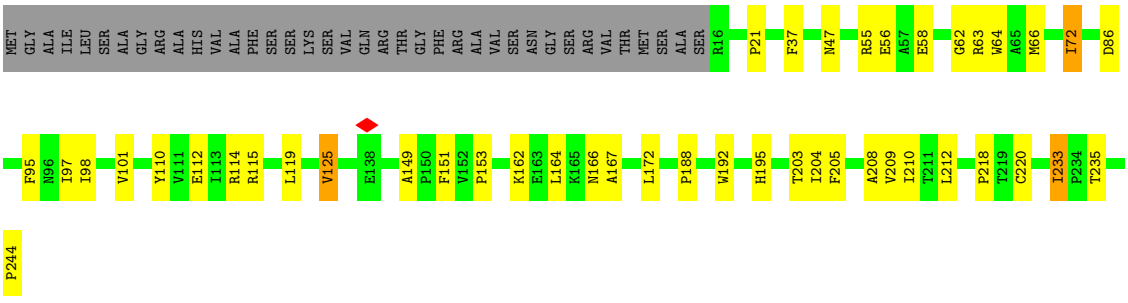
• Molecule 4: Chlorophyll a-b binding protein, chloroplastic

Chain 3:



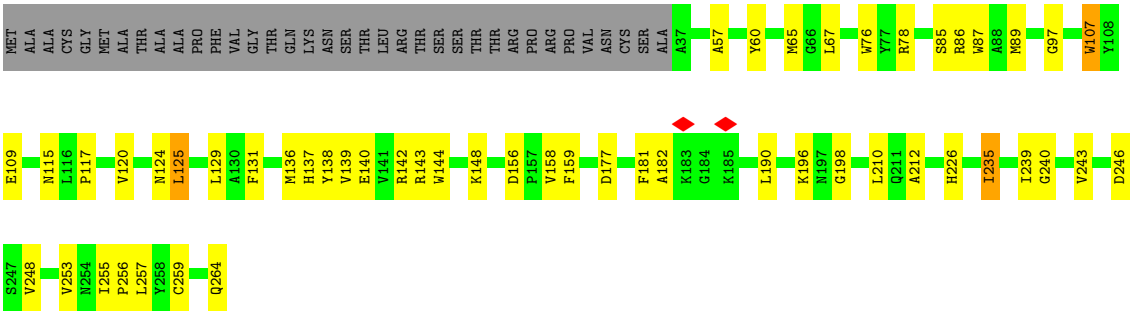
• Molecule 5: Chlorophyll a-b binding protein, chloroplastic

Chain 6:



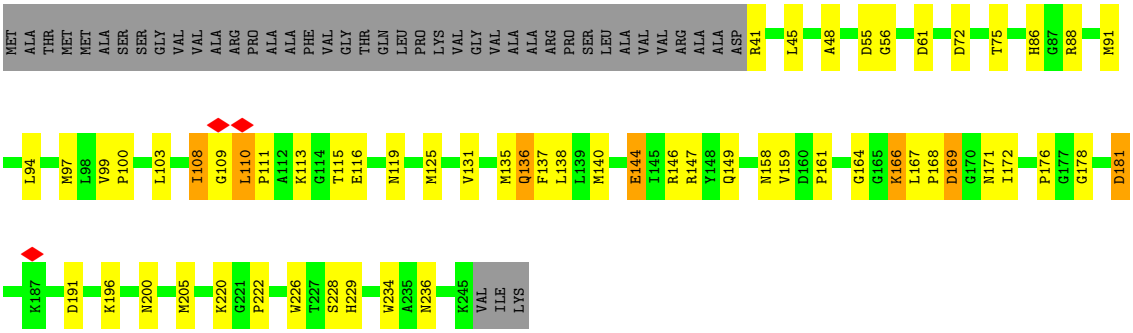
• Molecule 6: Chlorophyll a-b binding protein, chloroplastic

Chain 7:



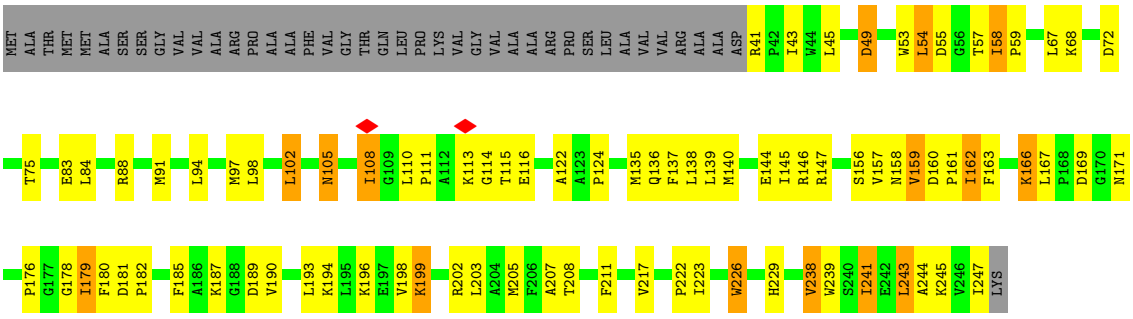
• Molecule 7: Chlorophyll a-b binding protein, chloroplastic

Chain 8:



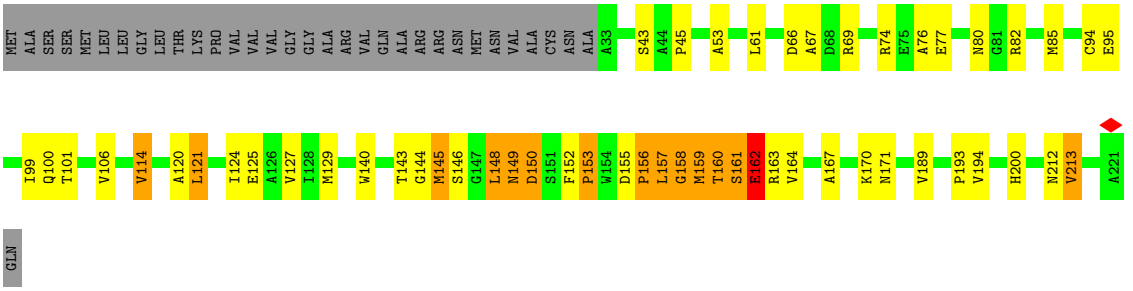
• Molecule 7: Chlorophyll a-b binding protein, chloroplastic

Chain 4:



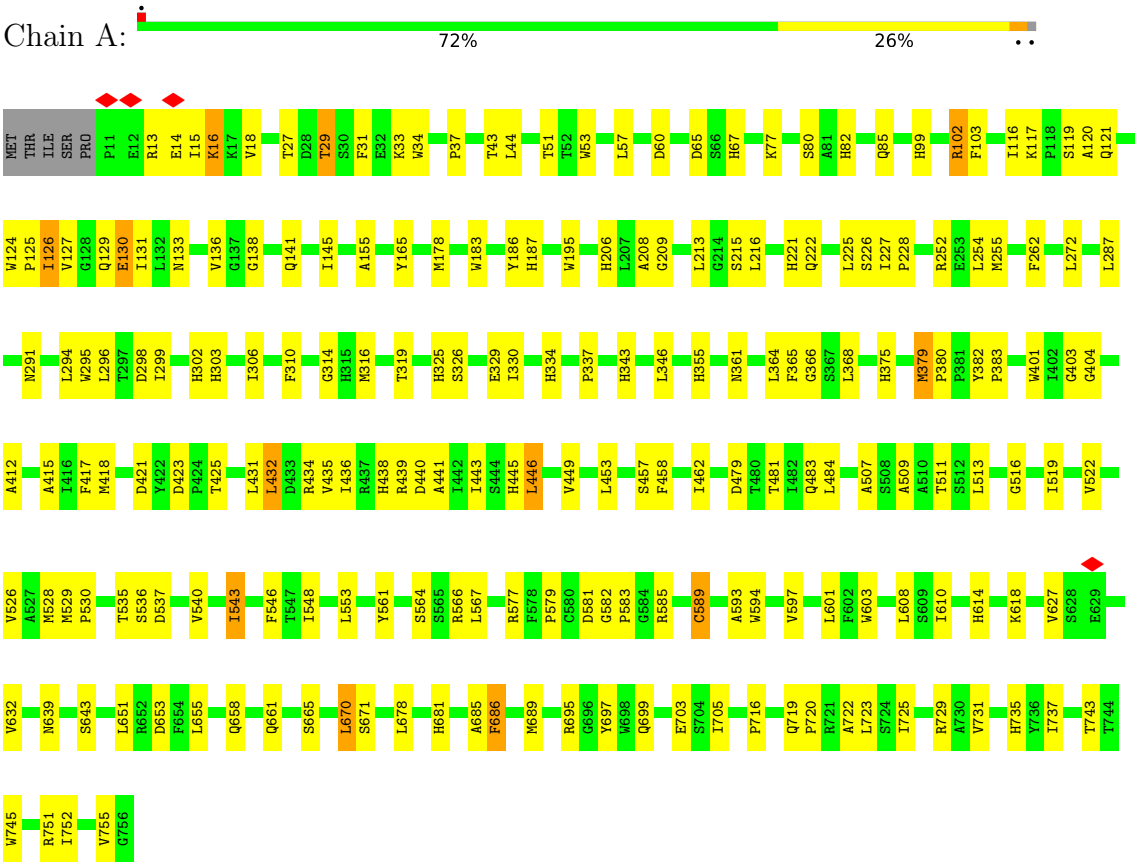
• Molecule 8: Chlorophyll a-b binding protein, chloroplastic

Chain 9:



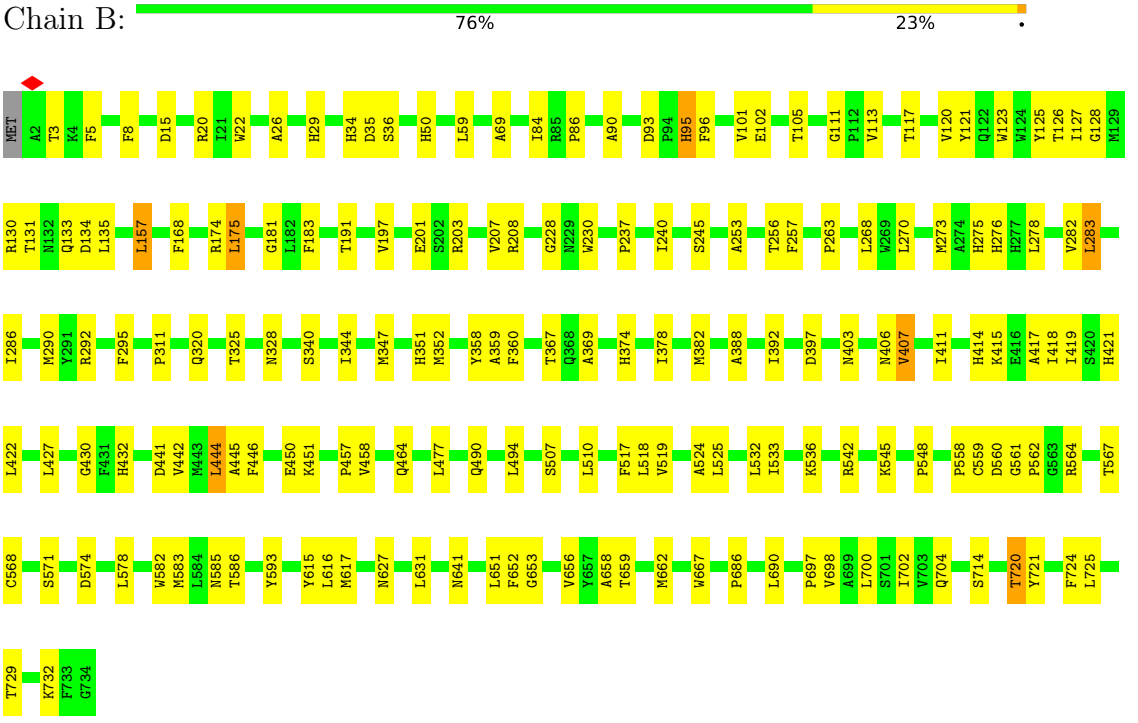
• Molecule 9: Photosystem I P700 chlorophyll a apoprotein A1

Chain A:



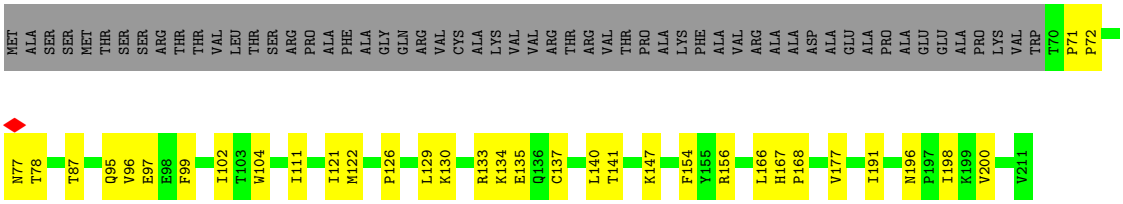
• Molecule 10: photosystem I

Chain B:



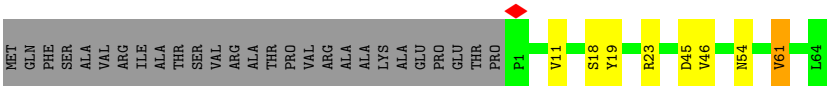
• Molecule 11: Photosystem I reaction center subunit II, chloroplastic

Chain D:



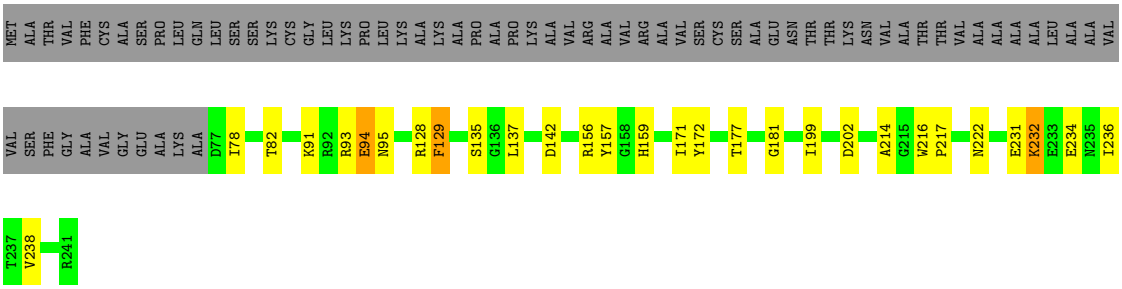
• Molecule 12: PsaE

Chain E:



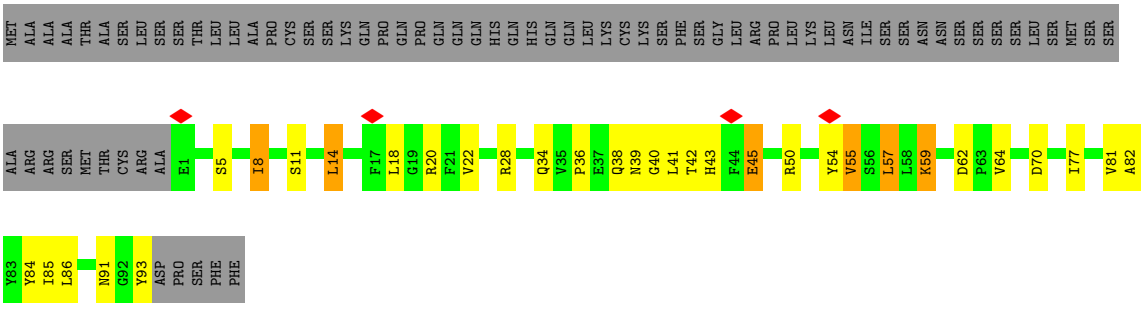
• Molecule 13: Photosystem I reaction center subunit III

Chain F:



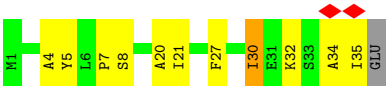
• Molecule 14: PsaG

Chain G:



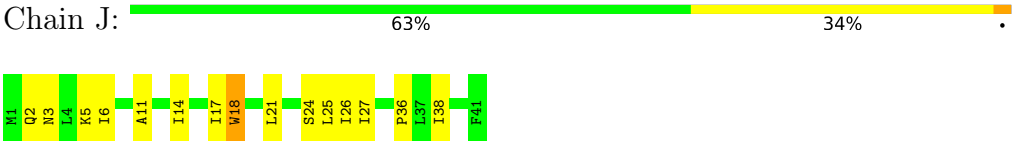
• Molecule 15: Photosystem I reaction center subunit VIII

Chain I:



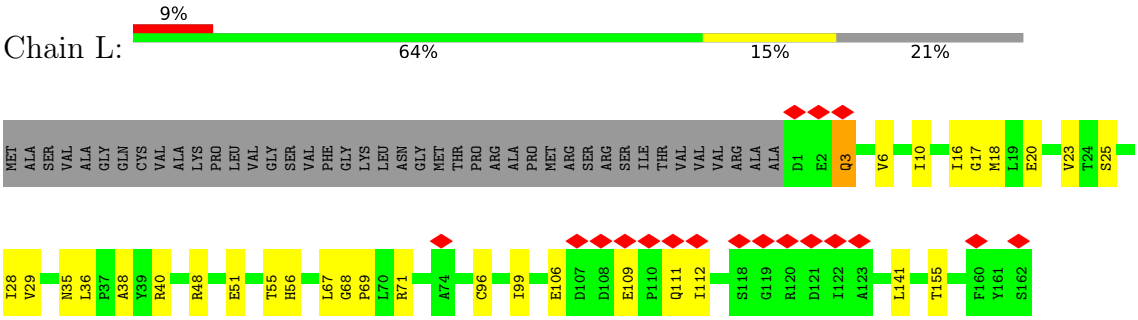
• Molecule 16: Photosystem I reaction center subunit IX

Chain J:



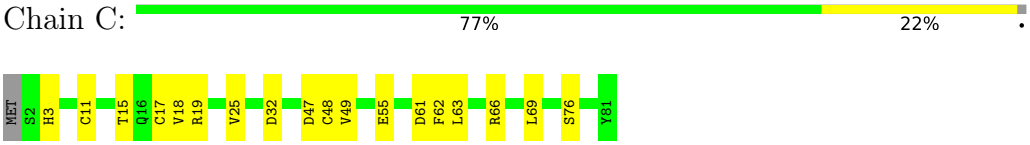
• Molecule 17: PSI subunit V

Chain L:



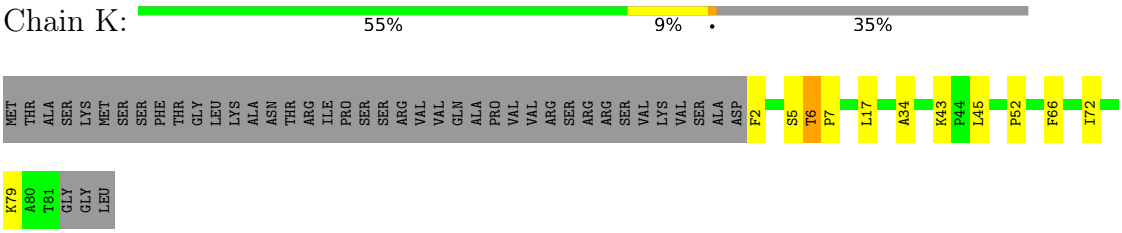
• Molecule 18: Photosystem I iron-sulfur center

Chain C:



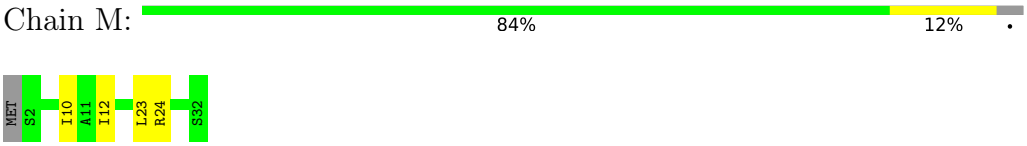
• Molecule 19: PsaK

Chain K:



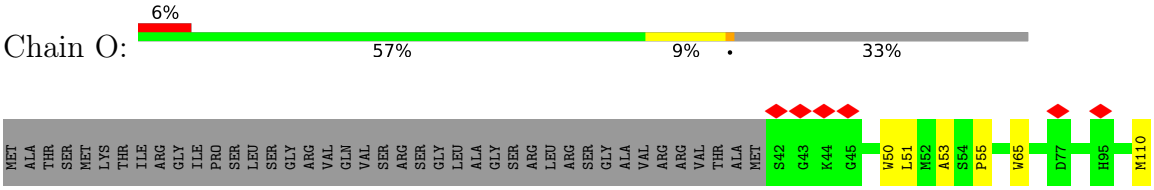
• Molecule 20: Photosystem I reaction center subunit XII

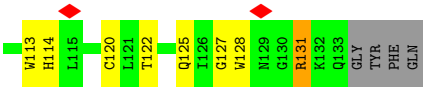
Chain M:



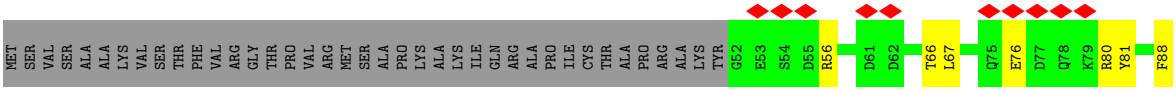
• Molecule 21: PsaO

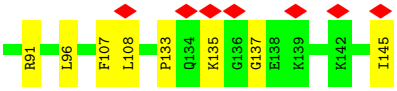
Chain O:





• Molecule 22: PsaH





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	287144	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI MORGAGNI	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	60	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	1.536	Depositor
Minimum map value	-0.386	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.025	Depositor
Recommended contour level	0.203	Depositor
Map size (Å)	532.48, 532.48, 532.48	wwPDB
Map dimensions	512, 512, 512	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: CL0, SF4, DGD, 0IE, PQN, CHL, 0UR, 8CT, LHG, SQD, LMG, 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	0	0.27	0/1685	0.38	0/2285
2	1	0.41	1/1523 (0.1%)	0.45	1/2073 (0.0%)
2	5	0.21	0/1530	0.41	0/2082
3	2	0.47	2/1727 (0.1%)	0.42	2/2351 (0.1%)
4	3	0.25	0/1818	0.32	0/2466
5	6	0.22	0/1862	0.30	0/2542
6	7	0.22	0/1812	0.31	0/2468
7	4	0.34	0/1619	0.62	1/2206 (0.0%)
7	8	0.20	0/1627	0.41	2/2217 (0.1%)
8	9	0.53	0/1492	0.48	1/2036 (0.0%)
9	A	0.42	1/6069 (0.0%)	0.35	1/8267 (0.0%)
10	B	0.37	0/6034	0.35	0/8239
11	D	0.21	0/1135	0.34	0/1533
12	E	0.20	0/521	0.26	0/706
13	F	0.21	0/1298	0.31	0/1748
14	G	0.25	0/743	0.41	0/1010
15	I	0.60	0/269	0.45	0/367
16	J	0.25	0/346	0.37	0/472
17	L	0.22	0/1224	0.34	0/1673
18	C	0.25	0/612	0.37	0/830
19	K	0.20	0/567	0.27	0/769
20	M	0.66	0/241	0.34	0/325
21	O	0.22	0/760	0.32	0/1042
22	H	0.18	0/729	0.34	0/979
All	All	0.34	4/37243 (0.0%)	0.38	8/50686 (0.0%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	2	246	ALA	CA-C	-5.28	1.46	1.52
9	A	689	MET	CA-C	-5.25	1.45	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	1	113	THR	CA-C	-5.14	1.46	1.53
3	2	247	THR	N-CA	-5.12	1.39	1.46

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	4	180	PHE	N-CA-C	-13.95	96.82	112.72
8	9	163	ARG	N-CA-C	-8.43	102.05	111.07
7	8	109	GLY	CA-C-N	6.63	129.47	123.10
7	8	109	GLY	C-N-CA	6.63	129.47	123.10
2	1	108	GLU	N-CA-C	-6.22	104.39	112.23

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	0	1640	0	1609	47	0
2	1	1478	0	1423	55	0
2	5	1484	0	1427	40	0
3	2	1667	0	1562	26	0
4	3	1768	0	1702	45	0
5	6	1797	0	1752	37	0
6	7	1758	0	1701	46	0
7	4	1569	0	1551	67	0
7	8	1574	0	1550	48	0
8	9	1453	0	1404	45	0
9	A	5872	0	5715	162	0
10	B	5824	0	5603	147	0
11	D	1109	0	1124	27	0
12	E	509	0	506	8	0
13	F	1273	0	1290	24	0
14	G	726	0	717	33	0
15	I	262	0	279	10	0
16	J	336	0	355	14	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
17	L	1195	0	1187	25	0
18	C	602	0	591	20	0
19	K	558	0	591	9	0
20	M	238	0	248	4	0
21	O	728	0	699	16	0
22	H	717	0	684	18	0
23	0	215	0	172	14	0
23	1	291	0	262	16	0
23	2	304	0	230	15	0
23	3	240	0	223	10	0
23	4	408	0	308	28	0
23	5	252	0	189	13	0
23	6	486	0	404	28	0
23	7	334	0	280	20	0
23	8	411	0	314	23	0
23	9	193	0	132	5	0
24	0	524	0	459	22	0
24	1	434	0	386	17	0
24	2	389	0	356	8	0
24	3	603	0	554	18	0
24	4	371	0	324	12	0
24	5	409	0	340	13	0
24	6	527	0	456	15	0
24	7	569	0	496	27	0
24	8	364	0	314	10	0
24	9	438	0	403	18	0
24	A	2547	0	2613	127	0
24	B	2368	0	2356	147	0
24	F	92	0	68	4	0
24	G	141	0	105	2	0
24	H	246	0	193	6	0
24	J	42	0	31	2	0
24	K	209	0	176	6	0
24	L	214	0	188	9	0
24	O	220	0	151	10	0
25	0	40	0	0	0	0
25	1	40	0	0	0	0
25	2	40	0	0	0	0
25	3	120	0	0	2	0
25	4	40	0	0	1	0
25	6	80	0	0	0	0
25	7	80	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
25	8	40	0	0	1	0
25	9	40	0	0	0	0
25	A	200	0	0	1	0
25	B	280	0	0	1	0
25	F	80	0	0	1	0
25	G	40	0	0	0	0
25	I	40	0	0	0	0
25	J	80	0	0	1	0
25	K	40	0	0	0	0
25	L	120	0	0	1	0
25	M	40	0	0	0	0
25	O	80	0	0	0	0
26	0	104	0	0	1	0
26	1	104	0	0	1	0
26	2	101	0	0	3	0
26	3	51	0	0	1	0
26	4	101	0	0	3	0
26	5	103	0	0	4	0
26	6	103	0	0	1	0
26	7	51	0	0	2	0
26	8	103	0	0	2	0
26	9	104	0	0	3	0
26	O	52	0	0	2	0
27	0	49	0	74	2	0
27	1	92	0	133	7	0
27	2	64	0	68	2	0
27	3	116	0	144	7	0
27	5	37	0	44	1	0
27	6	37	0	44	5	0
27	7	107	0	127	5	0
27	8	75	0	90	0	0
27	9	47	0	63	5	0
27	A	118	0	152	11	0
27	B	61	0	62	2	0
27	I	46	0	65	4	0
27	L	31	0	32	0	0
28	0	36	0	41	2	0
29	2	36	0	42	0	0
29	3	36	0	42	2	0
29	9	55	0	86	4	0
29	A	73	0	86	7	0
29	J	75	0	93	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
29	M	42	0	54	1	0
29	O	70	0	80	1	0
30	3	44	0	0	0	0
30	7	44	0	0	0	0
31	A	33	0	46	4	0
31	B	33	0	46	1	0
32	A	65	0	72	8	0
33	B	8	0	0	1	0
33	C	16	0	0	0	0
34	B	56	0	70	3	0
All	All	54077	0	49609	1253	0

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

The worst 5 of 1253 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)
2:5:160:PRO:HD2	26:5:314:0UR:C30	1.90	1.01
1:0:147:MET:HB3	1:0:148:PRO:HD2	1.42	1.01
24:A:804:CLA:H11	24:A:805:CLA:HBB1	1.51	0.91
32:A:852:CL0:H15	24:B:804:CLA:HED1	1.52	0.89
9:A:29:THR:HG21	9:A:183:TRP:HE1	1.39	0.88

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	0	211/245 (86%)	192 (91%)	17 (8%)	2 (1%)	14 31
2	1	193/226 (85%)	186 (96%)	6 (3%)	1 (0%)	24 45

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
2	5	193/226 (85%)	177 (92%)	15 (8%)	1 (0%)	24 45
3	2	214/256 (84%)	205 (96%)	9 (4%)	0	100 100
4	3	226/281 (80%)	219 (97%)	7 (3%)	0	100 100
5	6	227/267 (85%)	222 (98%)	5 (2%)	0	100 100
6	7	226/264 (86%)	212 (94%)	12 (5%)	2 (1%)	14 31
7	4	205/248 (83%)	176 (86%)	28 (14%)	1 (0%)	24 45
7	8	203/248 (82%)	187 (92%)	14 (7%)	2 (1%)	12 28
8	9	187/222 (84%)	168 (90%)	12 (6%)	7 (4%)	2 5
9	A	744/751 (99%)	711 (96%)	32 (4%)	1 (0%)	48 71
10	B	731/734 (100%)	707 (97%)	24 (3%)	0	100 100
11	D	140/198 (71%)	134 (96%)	6 (4%)	0	100 100
12	E	62/91 (68%)	60 (97%)	2 (3%)	0	100 100
13	F	163/236 (69%)	155 (95%)	8 (5%)	0	100 100
14	G	91/167 (54%)	85 (93%)	6 (7%)	0	100 100
15	I	33/36 (92%)	30 (91%)	3 (9%)	0	100 100
16	J	39/41 (95%)	39 (100%)	0	0	100 100
17	L	160/204 (78%)	157 (98%)	3 (2%)	0	100 100
18	C	78/81 (96%)	75 (96%)	3 (4%)	0	100 100
19	K	78/123 (63%)	78 (100%)	0	0	100 100
20	M	29/32 (91%)	29 (100%)	0	0	100 100
21	O	90/137 (66%)	85 (94%)	5 (6%)	0	100 100
22	H	92/133 (69%)	82 (89%)	10 (11%)	0	100 100
All	All	4615/5447 (85%)	4371 (95%)	227 (5%)	17 (0%)	31 51

5 of 17 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	0	148	PRO
6	7	125	LEU
7	8	108	ILE
8	9	153	PRO
1	0	149	PHE

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	0	167/194 (86%)	162 (97%)	5 (3%)	36	63
2	1	148/175 (85%)	139 (94%)	9 (6%)	17	37
2	5	149/175 (85%)	144 (97%)	5 (3%)	32	59
3	2	166/197 (84%)	163 (98%)	3 (2%)	51	76
4	3	186/225 (83%)	183 (98%)	3 (2%)	55	78
5	6	188/216 (87%)	181 (96%)	7 (4%)	30	56
6	7	181/209 (87%)	176 (97%)	5 (3%)	38	65
7	4	158/189 (84%)	133 (84%)	25 (16%)	2	6
7	8	159/189 (84%)	150 (94%)	9 (6%)	18	40
8	9	147/173 (85%)	136 (92%)	11 (8%)	12	28
9	A	609/614 (99%)	591 (97%)	18 (3%)	36	63
10	B	600/601 (100%)	586 (98%)	14 (2%)	44	71
11	D	119/162 (74%)	117 (98%)	2 (2%)	53	77
12	E	56/77 (73%)	54 (96%)	2 (4%)	31	57
13	F	129/180 (72%)	123 (95%)	6 (5%)	23	47
14	G	79/145 (54%)	71 (90%)	8 (10%)	7	16
15	I	27/28 (96%)	26 (96%)	1 (4%)	30	56
16	J	38/38 (100%)	36 (95%)	2 (5%)	20	43
17	L	124/157 (79%)	119 (96%)	5 (4%)	28	53
18	C	68/69 (99%)	66 (97%)	2 (3%)	37	64
19	K	58/94 (62%)	55 (95%)	3 (5%)	21	43
20	M	26/27 (96%)	26 (100%)	0	100	100
21	O	76/111 (68%)	75 (99%)	1 (1%)	61	81
22	H	69/103 (67%)	69 (100%)	0	100	100
All	All	3727/4348 (86%)	3581 (96%)	146 (4%)	30	54

5 of 146 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
18	C	11	CYS
7	4	238	VAL
19	K	45	LEU
7	4	113	LYS
8	9	145	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 34 such sidechains are listed below:

Mol	Chain	Res	Type
17	L	35	ASN
18	C	3	HIS
21	O	129	ASN
8	9	215	ASN
8	9	86	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)

352 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	$\#\|Z\|>2$
24	CLA	G	101	14	54,58,73	1.31	9 (16%)	64,95,113	1.41	6 (9%)
23	CHL	1	306	-	60,74,74	3.22	19 (31%)	58,114,114	2.53	18 (31%)
34	DGD	B	849	-	57,57,67	0.88	2 (3%)	71,71,81	1.18	5 (7%)
27	LHG	7	324	-	38,38,48	1.27	6 (15%)	41,44,54	1.00	2 (4%)
24	CLA	9	302	-	69,73,73	1.16	9 (13%)	82,113,113	1.26	5 (6%)
23	CHL	7	302	6	58,72,74	3.14	19 (32%)	55,111,114	2.84	17 (30%)
24	CLA	7	309	-	63,67,73	1.20	9 (14%)	74,105,113	1.33	7 (9%)
25	8CT	3	317	-	40,41,41	4.79	23 (57%)	51,56,56	2.60	17 (33%)
24	CLA	A	819	9	59,63,73	1.24	9 (15%)	70,101,113	1.36	5 (7%)
24	CLA	A	837	9	60,64,73	1.24	9 (15%)	71,102,113	1.32	6 (8%)
24	CLA	3	312	4	59,63,73	1.24	9 (15%)	70,101,113	1.32	5 (7%)
24	CLA	5	310	-	49,53,73	1.38	8 (16%)	58,89,113	1.44	4 (6%)
24	CLA	8	310	-	64,68,73	1.20	9 (14%)	76,107,113	1.32	7 (9%)
24	CLA	7	311	6	56,60,73	1.29	9 (16%)	65,97,113	1.38	6 (9%)
23	CHL	7	306	-	55,69,74	3.32	19 (34%)	51,107,114	2.73	18 (35%)
24	CLA	7	303	6	49,53,73	1.38	9 (18%)	58,89,113	1.42	4 (6%)
24	CLA	8	311	27	50,54,73	1.34	9 (18%)	59,90,113	1.35	4 (6%)
23	CHL	7	305	-	42,56,74	3.76	19 (45%)	36,92,114	3.29	17 (47%)
24	CLA	B	809	10	69,73,73	1.16	9 (13%)	82,113,113	1.28	6 (7%)
24	CLA	1	311	2	69,73,73	1.15	9 (13%)	82,113,113	1.31	6 (7%)
24	CLA	B	818	10	63,67,73	1.20	9 (14%)	74,105,113	1.36	7 (9%)
24	CLA	A	853	-	69,73,73	1.14	9 (13%)	82,113,113	1.35	9 (10%)
23	CHL	7	301	6	57,71,74	3.30	19 (33%)	54,110,114	2.66	18 (33%)
24	CLA	A	822	9	55,59,73	1.32	9 (16%)	64,96,113	1.39	6 (9%)
31	PQN	A	841	-	34,34,34	1.53	2 (5%)	43,45,45	1.31	5 (11%)
24	CLA	A	818	9	69,73,73	1.15	9 (13%)	82,113,113	1.31	9 (10%)
24	CLA	A	826	9	69,73,73	1.16	9 (13%)	82,113,113	1.33	9 (10%)
24	CLA	B	827	-	69,73,73	1.15	9 (13%)	82,113,113	1.34	7 (8%)
24	CLA	1	313	-	50,54,73	1.33	9 (18%)	59,90,113	1.41	4 (6%)
31	PQN	B	842	-	34,34,34	1.57	2 (5%)	43,45,45	1.13	3 (6%)
24	CLA	A	825	-	69,73,73	1.14	9 (13%)	82,113,113	1.28	7 (8%)
23	CHL	2	312	3	45,59,74	3.63	19 (42%)	40,96,114	3.06	17 (42%)
23	CHL	3	301	-	55,69,74	3.29	19 (34%)	52,108,114	2.88	19 (36%)
24	CLA	B	815	10	59,63,73	1.24	9 (15%)	70,101,113	1.36	8 (11%)
25	8CT	B	846	-	40,41,41	4.90	23 (57%)	51,56,56	3.31	22 (43%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
27	LHG	8	320	24	43,43,48	1.20	6 (13%)	46,49,54	0.94	2 (4%)
23	CHL	6	308	5	54,68,74	3.34	19 (35%)	50,106,114	2.76	17 (34%)
24	CLA	B	814	10	69,73,73	1.15	9 (13%)	82,113,113	1.29	6 (7%)
24	CLA	H	204	-	51,55,73	1.33	9 (17%)	60,91,113	1.43	5 (8%)
24	CLA	B	813	10	59,63,73	1.25	9 (15%)	70,101,113	1.34	5 (7%)
25	8CT	2	314	-	40,41,41	4.79	23 (57%)	51,56,56	3.05	19 (37%)
24	CLA	8	304	7	50,54,73	1.35	9 (18%)	59,90,113	1.37	4 (6%)
27	LHG	A	850	-	41,41,48	1.24	6 (14%)	44,47,54	1.04	3 (6%)
24	CLA	A	802	9	69,73,73	1.15	9 (13%)	82,113,113	1.31	7 (8%)
25	8CT	0	314	-	40,41,41	4.80	23 (57%)	51,56,56	2.82	18 (35%)
25	8CT	A	845	-	40,41,41	4.73	23 (57%)	51,56,56	3.14	20 (39%)
24	CLA	A	834	9	61,65,73	1.23	8 (13%)	72,103,113	1.37	5 (6%)
24	CLA	3	306	4	51,55,73	1.32	9 (17%)	60,91,113	1.40	5 (8%)
26	0UR	4	317	-	49,52,58	0.99	2 (4%)	58,71,77	2.19	21 (36%)
24	CLA	B	817	10	64,68,73	1.17	9 (14%)	76,107,113	1.45	9 (11%)
24	CLA	0	319	-	50,54,73	1.33	9 (18%)	59,90,113	1.39	4 (6%)
24	CLA	3	315	-	56,60,73	1.28	9 (16%)	65,97,113	1.48	7 (10%)
23	CHL	5	306	-	41,55,74	3.95	20 (48%)	35,91,114	3.04	16 (45%)
24	CLA	A	820	-	69,73,73	1.15	9 (13%)	82,113,113	1.27	7 (8%)
24	CLA	A	828	9	69,73,73	1.16	9 (13%)	82,113,113	1.30	6 (7%)
25	8CT	K	105	-	40,41,41	4.75	23 (57%)	51,56,56	3.31	23 (45%)
23	CHL	8	309	-	41,55,74	3.84	19 (46%)	35,91,114	3.20	17 (48%)
26	0UR	1	315	-	50,53,58	0.97	1 (2%)	59,72,77	1.76	17 (28%)
24	CLA	B	806	-	69,73,73	1.15	10 (14%)	82,113,113	1.34	7 (8%)
24	CLA	1	302	2	60,64,73	1.25	9 (15%)	71,102,113	1.39	5 (7%)
27	LHG	3	324	-	42,42,48	1.20	6 (14%)	45,47,54	1.06	4 (8%)
24	CLA	A	806	9	57,61,73	1.26	9 (15%)	65,97,113	1.43	8 (12%)
29	LMG	O	203	-	31,31,55	0.92	0	39,39,63	1.25	5 (12%)
25	8CT	4	316	-	40,41,41	4.77	23 (57%)	51,56,56	3.00	19 (37%)
27	LHG	3	322	-	35,35,48	1.31	6 (17%)	38,41,54	1.07	2 (5%)
23	CHL	5	305	-	42,56,74	3.95	18 (42%)	36,92,114	2.83	13 (36%)
25	8CT	B	843	-	40,41,41	4.88	23 (57%)	51,56,56	2.79	19 (37%)
23	CHL	6	302	5	58,72,74	3.15	18 (31%)	55,111,114	2.98	19 (34%)
24	CLA	5	303	-	56,60,73	1.29	7 (12%)	65,97,113	1.34	4 (6%)
24	CLA	A	812	9	69,73,73	1.15	9 (13%)	82,113,113	1.30	7 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
24	CLA	A	824	-	69,73,73	1.15	9 (13%)	82,113,113	1.31	8 (9%)
24	CLA	4	303	7	49,53,73	1.36	9 (18%)	58,89,113	1.42	4 (6%)
24	CLA	6	314	-	49,53,73	1.35	9 (18%)	58,89,113	1.44	5 (8%)
24	CLA	L	202	17	67,71,73	1.17	9 (13%)	79,110,113	1.32	5 (6%)
24	CLA	B	810	10	66,70,73	1.16	9 (13%)	78,109,113	1.32	7 (8%)
24	CLA	O	209	-	55,59,73	1.31	9 (16%)	64,96,113	1.33	5 (7%)
27	LHG	0	317	-	48,48,48	1.13	6 (12%)	51,54,54	0.94	2 (3%)
25	8CT	J	104	-	40,41,41	4.80	23 (57%)	51,56,56	3.45	22 (43%)
24	CLA	4	304	-	64,68,73	1.19	8 (12%)	76,107,113	1.27	5 (6%)
30	0IE	7	321	-	42,45,45	1.16	5 (11%)	51,63,63	1.49	11 (21%)
24	CLA	H	202	10	59,63,73	1.24	9 (15%)	70,101,113	1.36	8 (11%)
24	CLA	K	101	-	64,68,73	1.20	9 (14%)	76,107,113	1.30	6 (7%)
24	CLA	B	829	-	69,73,73	1.16	9 (13%)	82,113,113	1.22	4 (4%)
23	CHL	3	302	4	56,70,74	3.24	19 (33%)	53,109,114	2.86	19 (35%)
23	CHL	5	304	-	40,54,74	3.98	19 (47%)	34,90,114	3.21	15 (44%)
24	CLA	4	311	-	52,56,73	1.32	9 (17%)	61,92,113	1.41	5 (8%)
23	CHL	4	307	-	45,59,74	3.63	19 (42%)	40,96,114	3.19	17 (42%)
24	CLA	B	840	10	69,73,73	1.16	7 (10%)	82,113,113	1.30	5 (6%)
23	CHL	8	307	-	45,59,74	3.71	18 (40%)	40,96,114	3.02	19 (47%)
24	CLA	5	307	-	50,54,73	1.36	9 (18%)	59,90,113	1.36	4 (6%)
24	CLA	0	310	-	51,55,73	1.33	9 (17%)	60,91,113	1.46	5 (8%)
24	CLA	B	819	10	64,68,73	1.19	9 (14%)	76,107,113	1.32	7 (9%)
24	CLA	3	304	-	69,73,73	1.16	9 (13%)	82,113,113	1.34	6 (7%)
26	0UR	2	315	-	49,52,58	1.02	2 (4%)	58,71,77	2.17	19 (32%)
24	CLA	3	314	4	50,54,73	1.34	9 (18%)	59,90,113	1.41	4 (6%)
25	8CT	B	848	-	40,41,41	4.81	23 (57%)	51,56,56	2.63	19 (37%)
24	CLA	4	314	7	49,53,73	1.35	9 (18%)	58,89,113	1.41	5 (8%)
26	0UR	1	316	-	50,53,58	1.01	1 (2%)	59,72,77	1.88	12 (20%)
23	CHL	3	307	-	60,74,74	3.06	19 (31%)	58,114,114	2.90	18 (31%)
24	CLA	F	302	13	51,55,73	1.34	9 (17%)	60,91,113	1.39	5 (8%)
27	LHG	B	852	-	37,37,48	1.29	6 (16%)	40,43,54	1.16	4 (10%)
24	CLA	5	311	2	60,64,73	1.24	9 (15%)	71,102,113	1.34	4 (5%)
24	CLA	6	309	5	62,66,73	1.22	9 (14%)	73,104,113	1.33	8 (10%)
25	8CT	J	101	-	40,41,41	4.75	23 (57%)	51,56,56	2.87	18 (35%)
24	CLA	5	308	-	64,68,73	1.21	9 (14%)	76,107,113	1.29	7 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
24	CLA	5	309	27	49,53,73	1.37	9 (18%)	58,89,113	1.40	4 (6%)
23	CHL	6	306	-	45,59,74	3.61	19 (42%)	40,96,114	3.26	19 (47%)
25	8CT	L	207	-	40,41,41	4.80	23 (57%)	51,56,56	2.63	20 (39%)
24	CLA	6	312	5	60,64,73	1.23	9 (15%)	71,102,113	1.33	5 (7%)
24	CLA	A	835	-	55,59,73	1.27	9 (16%)	64,96,113	1.42	8 (12%)
23	CHL	6	315	5	37,51,74	4.03	17 (45%)	30,86,114	3.31	14 (46%)
23	CHL	2	307	-	41,55,74	3.82	19 (46%)	35,91,114	3.10	15 (42%)
24	CLA	A	805	-	69,73,73	1.16	9 (13%)	82,113,113	1.31	6 (7%)
27	LHG	I	102	-	45,45,48	1.17	5 (11%)	48,51,54	0.98	3 (6%)
24	CLA	0	309	-	45,49,73	1.39	9 (20%)	54,84,113	1.47	5 (9%)
24	CLA	B	826	-	53,56,73	1.41	11 (20%)	63,89,113	2.42	11 (17%)
24	CLA	B	811	10	69,73,73	1.15	9 (13%)	82,113,113	1.35	7 (8%)
24	CLA	7	315	6	52,56,73	1.31	9 (17%)	61,92,113	1.41	5 (8%)
24	CLA	A	816	9	65,69,73	1.17	9 (13%)	77,108,113	1.35	6 (7%)
24	CLA	3	309	4	69,73,73	1.15	9 (13%)	82,113,113	1.30	7 (8%)
24	CLA	6	303	5	56,60,73	1.29	8 (14%)	65,97,113	1.38	5 (7%)
24	CLA	A	829	9	69,73,73	1.17	10 (14%)	82,113,113	1.42	9 (10%)
24	CLA	0	312	1	50,54,73	1.34	8 (16%)	59,90,113	1.36	4 (6%)
24	CLA	B	835	-	49,53,73	1.36	9 (18%)	58,89,113	1.46	4 (6%)
23	CHL	8	301	2	46,60,74	3.74	19 (41%)	40,97,114	2.94	16 (40%)
24	CLA	9	310	8	56,60,73	1.29	9 (16%)	65,97,113	1.38	6 (9%)
26	0UR	5	314	-	49,52,58	0.97	1 (2%)	58,71,77	1.82	13 (22%)
25	8CT	A	847	-	40,41,41	4.70	23 (57%)	51,56,56	3.21	23 (45%)
23	CHL	1	301	-	58,72,74	3.19	19 (32%)	55,111,114	2.82	20 (36%)
23	CHL	6	301	5	55,69,74	3.30	19 (34%)	52,108,114	2.77	18 (34%)
24	CLA	A	808	9	69,73,73	1.15	9 (13%)	82,113,113	1.32	6 (7%)
24	CLA	6	311	5	52,56,73	1.33	9 (17%)	61,92,113	1.38	5 (8%)
29	LMG	9	317	-	55,55,55	0.70	1 (1%)	63,63,63	1.39	9 (14%)
24	CLA	B	837	-	69,73,73	1.14	9 (13%)	82,113,113	1.31	7 (8%)
24	CLA	2	310	3	52,56,73	1.30	8 (15%)	61,92,113	1.45	6 (9%)
24	CLA	6	316	5	69,73,73	1.15	9 (13%)	82,113,113	1.32	7 (8%)
25	8CT	L	204	-	40,41,41	4.76	23 (57%)	51,56,56	3.02	19 (37%)
26	0UR	6	321	-	50,53,58	1.02	2 (4%)	59,72,77	1.75	13 (22%)
23	CHL	3	305	-	45,59,74	3.64	19 (42%)	40,96,114	3.14	17 (42%)
33	SF4	C	102	18	0,12,12	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
23	CHL	2	304	-	37,51,74	3.93	18 (48%)	30,86,114	3.72	15 (50%)
24	CLA	A	838	9	69,73,73	1.15	9 (13%)	82,113,113	1.32	6 (7%)
24	CLA	6	318	-	55,59,73	1.30	9 (16%)	64,96,113	1.32	5 (7%)
23	CHL	0	301	1	46,60,74	3.61	19 (41%)	40,97,114	3.06	17 (42%)
24	CLA	0	307	-	64,68,73	1.21	9 (14%)	76,107,113	1.27	5 (6%)
24	CLA	A	827	9	69,73,73	1.14	9 (13%)	82,113,113	1.29	8 (9%)
23	CHL	0	306	-	42,56,74	3.89	18 (42%)	36,92,114	3.32	14 (38%)
24	CLA	3	311	4	50,54,73	1.35	9 (18%)	59,90,113	1.47	5 (8%)
24	CLA	K	102	19	57,61,73	1.25	9 (15%)	67,98,113	1.39	7 (10%)
27	LHG	1	318	-	42,42,48	1.22	6 (14%)	45,48,54	0.98	2 (4%)
24	CLA	1	309	27	67,71,73	1.17	9 (13%)	79,110,113	1.28	4 (5%)
23	CHL	5	312	2	41,55,74	4.04	18 (43%)	35,91,114	3.02	14 (40%)
23	CHL	8	308	-	45,59,74	3.66	19 (42%)	40,96,114	3.08	17 (42%)
23	CHL	0	305	-	45,59,74	3.74	18 (40%)	40,96,114	3.07	19 (47%)
24	CLA	B	838	10	51,55,73	1.30	8 (15%)	60,91,113	1.41	6 (10%)
24	CLA	L	206	-	51,55,73	1.34	9 (17%)	60,91,113	1.37	5 (8%)
27	LHG	5	316	24	36,36,48	1.29	6 (16%)	39,42,54	1.09	3 (7%)
25	8CT	B	845	-	40,41,41	4.76	23 (57%)	51,56,56	3.28	22 (43%)
24	CLA	A	814	9	69,73,73	1.15	9 (13%)	82,113,113	1.33	6 (7%)
24	CLA	9	304	-	55,59,73	1.29	8 (14%)	64,96,113	1.37	5 (7%)
27	LHG	3	320	-	35,35,48	1.32	6 (17%)	38,41,54	1.14	2 (5%)
32	CL0	A	852	9	58,73,73	2.15	13 (22%)	60,113,113	1.55	11 (18%)
24	CLA	1	303	-	56,60,73	1.28	9 (16%)	65,97,113	1.33	6 (9%)
23	CHL	4	306	-	42,56,74	3.84	19 (45%)	36,92,114	3.25	16 (44%)
24	CLA	G	102	14	49,53,73	1.36	9 (18%)	58,89,113	1.45	4 (6%)
23	CHL	4	315	2	48,62,74	3.55	19 (39%)	43,99,114	3.10	17 (39%)
24	CLA	B	841	27	69,73,73	1.15	8 (11%)	82,113,113	1.30	6 (7%)
26	0UR	2	316	-	48,51,58	1.01	1 (2%)	57,70,77	1.99	13 (22%)
24	CLA	0	311	1	69,73,73	1.16	9 (13%)	82,113,113	1.26	5 (6%)
27	LHG	6	322	24	36,36,48	1.29	5 (13%)	39,42,54	1.06	2 (5%)
24	CLA	B	804	-	69,73,73	1.14	9 (13%)	82,113,113	1.25	7 (8%)
24	CLA	6	310	27	64,68,73	1.21	9 (14%)	76,107,113	1.30	5 (6%)
24	CLA	B	839	-	69,73,73	1.15	9 (13%)	82,113,113	1.28	5 (6%)
24	CLA	F	303	-	49,53,73	1.36	9 (18%)	58,89,113	1.43	4 (6%)
23	CHL	6	323	7	55,69,74	3.35	19 (34%)	52,108,114	2.89	19 (36%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
25	8CT	3	323	-	40,41,41	4.76	23 (57%)	51,56,56	3.69	24 (47%)
26	0UR	0	316	-	50,53,58	0.98	1 (2%)	59,72,77	1.96	18 (30%)
26	0UR	O	207	-	50,53,58	0.99	2 (4%)	59,72,77	1.97	16 (27%)
24	CLA	O	204	-	45,49,73	1.40	9 (20%)	54,84,113	1.51	5 (9%)
24	CLA	4	310	27	64,68,73	1.20	9 (14%)	76,107,113	1.29	5 (6%)
24	CLA	1	308	2	59,63,73	1.25	9 (15%)	70,101,113	1.31	6 (8%)
24	CLA	7	304	-	59,63,73	1.25	9 (15%)	70,101,113	1.36	7 (10%)
24	CLA	B	822	10	64,68,73	1.20	8 (12%)	76,107,113	1.34	5 (6%)
27	LHG	A	842	-	48,48,48	1.11	5 (10%)	51,54,54	1.00	3 (5%)
23	CHL	1	312	2	56,70,74	3.30	19 (33%)	53,109,114	2.70	17 (32%)
26	0UR	6	320	-	49,52,58	1.00	2 (4%)	58,71,77	1.92	15 (25%)
25	8CT	3	316	-	40,41,41	4.78	23 (57%)	51,56,56	3.09	18 (35%)
23	CHL	7	307	-	45,59,74	3.64	19 (42%)	40,96,114	2.86	16 (40%)
23	CHL	2	306	-	45,59,74	3.58	19 (42%)	40,96,114	3.44	19 (47%)
23	CHL	8	314	7	50,64,74	3.45	19 (38%)	46,102,114	2.94	17 (36%)
24	CLA	9	308	-	64,68,73	1.20	9 (14%)	76,107,113	1.32	8 (10%)
24	CLA	7	308	-	69,73,73	1.15	9 (13%)	82,113,113	1.25	5 (6%)
23	CHL	2	305	-	42,56,74	3.82	19 (45%)	36,92,114	3.23	16 (44%)
24	CLA	6	304	-	50,54,73	1.36	9 (18%)	59,90,113	1.41	4 (6%)
24	CLA	0	308	-	64,68,73	1.20	8 (12%)	76,107,113	1.32	7 (9%)
33	SF4	C	101	-	0,12,12	-	-	-		
23	CHL	4	313	7	45,59,74	3.63	19 (42%)	40,96,114	3.20	18 (45%)
25	8CT	7	318	-	40,41,41	4.73	23 (57%)	51,56,56	2.70	19 (37%)
23	CHL	6	307	-	45,59,74	3.62	19 (42%)	40,96,114	3.14	18 (45%)
24	CLA	A	848	-	69,73,73	1.16	8 (11%)	82,113,113	1.29	6 (7%)
24	CLA	A	836	9	65,69,73	1.18	9 (13%)	77,108,113	1.35	7 (9%)
23	CHL	0	302	1	58,72,74	3.20	19 (32%)	55,111,114	2.74	18 (32%)
25	8CT	9	313	-	40,41,41	4.80	23 (57%)	51,56,56	2.77	19 (37%)
26	0UR	3	318	-	49,52,58	1.03	1 (2%)	58,71,77	2.13	21 (36%)
23	CHL	5	301	2	58,72,74	3.18	19 (32%)	55,111,114	2.79	18 (32%)
24	CLA	2	313	3	49,53,73	1.37	9 (18%)	58,89,113	1.42	4 (6%)
25	8CT	6	324	-	40,41,41	4.84	23 (57%)	51,56,56	2.59	17 (33%)
24	CLA	0	304	-	56,60,73	1.30	9 (16%)	65,97,113	1.37	6 (9%)
24	CLA	J	103	16	46,50,73	1.38	9 (19%)	53,85,113	1.44	4 (7%)
25	8CT	O	202	-	40,41,41	4.73	23 (57%)	51,56,56	2.84	23 (45%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
33	SF4	B	803	-	0,12,12	-	-	-		
29	LMG	A	854	-	37,37,55	0.88	1 (2%)	45,45,63	1.26	4 (8%)
24	CLA	B	830	10	60,64,73	1.28	10 (16%)	71,102,113	1.44	9 (12%)
24	CLA	O	201	27	56,60,73	1.27	9 (16%)	65,97,113	1.41	8 (12%)
24	CLA	A	832	9	69,73,73	1.14	9 (13%)	82,113,113	1.29	5 (6%)
24	CLA	O	205	21	41,46,73	1.48	9 (21%)	47,80,113	1.50	5 (10%)
24	CLA	H	203	22	51,55,73	1.33	9 (17%)	60,91,113	1.38	4 (6%)
24	CLA	9	309	27	45,49,73	1.40	9 (20%)	54,84,113	1.46	5 (9%)
23	CHL	8	303	7	58,72,74	3.18	19 (32%)	55,111,114	2.79	19 (34%)
24	CLA	B	802	10	69,73,73	1.15	9 (13%)	82,113,113	1.26	6 (7%)
24	CLA	B	816	10	64,68,73	1.19	9 (14%)	76,107,113	1.35	7 (9%)
25	8CT	O	208	-	40,41,41	4.79	23 (57%)	51,56,56	2.64	19 (37%)
24	CLA	2	309	27	64,68,73	1.19	9 (14%)	76,107,113	1.28	5 (6%)
25	8CT	B	844	-	40,41,41	4.85	23 (57%)	51,56,56	2.73	22 (43%)
24	CLA	A	840	-	69,73,73	1.16	9 (13%)	82,113,113	1.32	6 (7%)
27	LHG	8	302	-	30,30,48	1.38	6 (20%)	33,36,54	1.12	2 (6%)
25	8CT	I	101	-	40,41,41	4.72	23 (57%)	51,56,56	2.84	18 (35%)
24	CLA	A	830	9	54,58,73	1.29	9 (16%)	64,95,113	1.44	6 (9%)
25	8CT	B	850	-	40,41,41	4.76	23 (57%)	51,56,56	2.52	17 (33%)
24	CLA	H	205	-	55,59,73	1.30	9 (16%)	64,96,113	1.38	6 (9%)
24	CLA	B	825	-	69,73,73	1.16	9 (13%)	82,113,113	1.31	6 (7%)
26	0UR	9	314	-	50,53,58	0.96	1 (2%)	59,72,77	1.76	16 (27%)
24	CLA	1	307	-	49,53,73	1.37	9 (18%)	58,89,113	1.43	4 (6%)
24	CLA	B	812	10	56,60,73	1.27	8 (14%)	65,97,113	1.41	7 (10%)
30	0IE	3	319	-	42,45,45	1.16	5 (11%)	51,63,63	1.51	11 (21%)
29	LMG	2	318	-	36,36,55	0.89	1 (2%)	44,44,63	1.24	5 (11%)
24	CLA	3	308	-	69,73,73	1.15	9 (13%)	82,113,113	1.29	6 (7%)
25	8CT	B	847	-	40,41,41	4.75	23 (57%)	51,56,56	3.17	20 (39%)
24	CLA	B	808	10	69,73,73	1.15	9 (13%)	82,113,113	1.34	9 (10%)
26	0UR	5	315	-	50,53,58	0.98	1 (2%)	59,72,77	1.96	14 (23%)
27	LHG	7	323	-	37,37,48	1.22	6 (16%)	40,43,54	1.06	2 (5%)
23	CHL	9	312	8	41,55,74	3.85	18 (43%)	35,91,114	3.34	16 (45%)
24	CLA	A	815	-	49,53,73	1.39	9 (18%)	58,89,113	1.46	4 (6%)
25	8CT	1	314	-	40,41,41	4.83	23 (57%)	51,56,56	2.75	19 (37%)
29	LMG	M	101	-	42,42,55	0.79	0	50,50,63	1.31	7 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
24	CLA	8	305	-	69,73,73	1.16	8 (11%)	82,113,113	1.24	6 (7%)
25	8CT	A	846	-	40,41,41	4.71	23 (57%)	51,56,56	3.07	21 (41%)
25	8CT	F	301	-	40,41,41	4.78	23 (57%)	51,56,56	2.63	20 (39%)
24	CLA	2	303	-	64,68,73	1.20	9 (14%)	76,107,113	1.28	5 (6%)
24	CLA	A	821	-	53,57,73	1.29	9 (16%)	61,93,113	1.39	5 (8%)
23	CHL	6	313	5	46,60,74	3.62	19 (41%)	40,97,114	3.26	19 (47%)
24	CLA	6	317	-	50,54,73	1.34	9 (18%)	59,90,113	1.40	4 (6%)
29	LMG	3	321	-	36,36,55	0.86	0	44,44,63	1.26	5 (11%)
24	CLA	B	831	10	54,58,73	1.30	9 (16%)	64,95,113	1.39	5 (7%)
24	CLA	2	302	3	60,64,73	1.25	9 (15%)	71,102,113	1.35	5 (7%)
24	CLA	L	203	-	50,54,73	1.34	9 (18%)	59,90,113	1.38	4 (6%)
25	8CT	G	104	-	40,41,41	4.81	23 (57%)	51,56,56	3.09	20 (39%)
24	CLA	A	831	9	69,73,73	1.16	9 (13%)	82,113,113	1.27	5 (6%)
24	CLA	A	807	9	69,73,73	1.13	9 (13%)	82,113,113	1.29	6 (7%)
24	CLA	0	303	1	66,70,73	1.19	9 (13%)	78,109,113	1.27	4 (5%)
24	CLA	7	316	-	49,53,73	1.38	7 (14%)	58,89,113	1.47	5 (8%)
24	CLA	1	310	2	56,60,73	1.28	9 (16%)	65,97,113	1.40	6 (9%)
24	CLA	3	303	-	59,63,73	1.24	9 (15%)	70,101,113	1.35	8 (11%)
24	CLA	A	810	9	69,73,73	1.14	8 (11%)	82,113,113	1.26	4 (4%)
26	0UR	4	318	-	48,51,58	0.99	1 (2%)	57,70,77	1.73	13 (22%)
24	CLA	B	801	10	62,66,73	1.21	8 (12%)	73,104,113	1.38	7 (9%)
24	CLA	4	312	7	57,61,73	1.27	9 (15%)	67,98,113	1.35	4 (5%)
23	CHL	1	304	-	45,59,74	3.65	19 (42%)	40,96,114	3.26	17 (42%)
27	LHG	B	851	24	22,22,48	1.33	3 (13%)	25,28,54	1.08	1 (4%)
25	8CT	A	844	-	40,41,41	4.76	23 (57%)	51,56,56	2.93	19 (37%)
25	8CT	7	319	-	40,41,41	4.74	23 (57%)	51,56,56	2.77	20 (39%)
24	CLA	A	823	9	59,63,73	1.24	9 (15%)	70,101,113	1.32	5 (7%)
24	CLA	8	315	-	49,53,73	1.37	9 (18%)	58,89,113	1.42	4 (6%)
24	CLA	B	805	10	69,73,73	1.14	9 (13%)	82,113,113	1.25	6 (7%)
24	CLA	B	834	10	65,69,73	1.19	9 (13%)	77,108,113	1.26	4 (5%)
24	CLA	B	821	10	54,58,73	1.28	9 (16%)	64,95,113	1.45	8 (12%)
29	LMG	A	851	-	36,36,55	0.90	1 (2%)	44,44,63	1.31	5 (11%)
27	LHG	7	322	24	29,29,48	1.41	6 (20%)	32,35,54	1.11	2 (6%)
29	LMG	J	105	-	46,46,55	0.88	2 (4%)	54,54,63	1.36	7 (12%)
24	CLA	8	312	7	50,54,73	1.36	9 (18%)	59,90,113	1.39	4 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
24	CLA	5	313	2	50,54,73	1.36	9 (18%)	59,90,113	1.35	4 (6%)
24	CLA	G	103	14	50,54,73	1.35	8 (16%)	59,90,113	1.38	4 (6%)
24	CLA	A	813	9	61,65,73	1.22	8 (13%)	72,103,113	1.34	6 (8%)
27	LHG	1	317	24	48,48,48	1.14	5 (10%)	51,54,54	0.98	2 (3%)
23	CHL	7	313	6	41,55,74	3.90	19 (46%)	35,91,114	3.03	16 (45%)
23	CHL	9	301	8	41,55,74	3.85	19 (46%)	35,91,114	3.19	15 (42%)
24	CLA	3	310	-	66,70,73	1.18	9 (13%)	78,109,113	1.28	5 (6%)
24	CLA	K	104	19	54,58,73	1.30	9 (16%)	64,95,113	1.39	6 (9%)
25	8CT	A	849	-	40,41,41	4.78	23 (57%)	51,56,56	2.92	21 (41%)
24	CLA	A	803	9	59,63,73	1.22	9 (15%)	70,101,113	1.39	6 (8%)
24	CLA	K	103	19	50,54,73	1.35	9 (18%)	59,90,113	1.43	4 (6%)
24	CLA	A	839	9	69,73,73	1.14	9 (13%)	82,113,113	1.32	6 (7%)
26	0UR	8	319	-	50,53,58	0.99	1 (2%)	59,72,77	1.96	13 (22%)
24	CLA	7	312	6	59,63,73	1.25	9 (15%)	70,101,113	1.33	4 (5%)
24	CLA	2	308	3	64,68,73	1.19	9 (14%)	76,107,113	1.31	8 (10%)
25	8CT	F	304	-	40,41,41	4.77	23 (57%)	51,56,56	2.76	17 (33%)
27	LHG	2	317	24	31,31,48	1.38	5 (16%)	34,37,54	1.13	3 (8%)
26	0UR	8	318	-	49,52,58	0.97	1 (2%)	58,71,77	1.83	17 (29%)
24	CLA	A	804	9	69,73,73	1.17	9 (13%)	82,113,113	1.29	5 (6%)
27	LHG	A	843	24	26,26,48	1.29	4 (15%)	29,32,54	1.20	2 (6%)
24	CLA	9	303	8	52,56,73	1.32	8 (15%)	61,92,113	1.42	5 (8%)
24	CLA	B	820	-	60,64,73	1.24	9 (15%)	71,102,113	1.35	5 (7%)
23	CHL	4	302	7	47,61,74	3.53	19 (40%)	41,98,114	3.14	19 (46%)
24	CLA	7	317	6	64,68,73	1.19	9 (14%)	76,107,113	1.32	6 (7%)
24	CLA	B	824	10	64,68,73	1.21	9 (14%)	76,107,113	1.28	6 (7%)
27	LHG	9	316	24	45,45,48	1.18	6 (13%)	47,50,54	0.97	2 (4%)
26	0UR	0	315	-	50,53,58	0.96	1 (2%)	59,72,77	1.76	13 (22%)
24	CLA	B	836	10	64,68,73	1.20	9 (14%)	76,107,113	1.34	8 (10%)
24	CLA	7	310	27	41,45,73	1.44	8 (19%)	50,78,113	1.41	5 (10%)
24	CLA	A	801	-	69,73,73	1.16	9 (13%)	82,113,113	1.24	4 (4%)
24	CLA	A	811	9	58,62,73	1.27	9 (15%)	68,99,113	1.32	6 (8%)
29	LMG	O	210	-	39,39,55	0.81	1 (2%)	47,47,63	1.27	5 (10%)
26	0UR	7	320	-	49,52,58	1.00	1 (2%)	58,71,77	2.14	18 (31%)
24	CLA	B	833	10	59,63,73	1.26	9 (15%)	70,101,113	1.37	8 (11%)
24	CLA	L	201	9	62,66,73	1.21	9 (14%)	73,104,113	1.37	7 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
24	CLA	8	313	7	60,64,73	1.24	9 (15%)	71,102,113	1.33	4 (5%)
24	CLA	9	311	8	60,64,73	1.23	9 (15%)	71,102,113	1.32	5 (7%)
24	CLA	9	307	-	69,73,73	1.15	9 (13%)	82,113,113	1.28	5 (6%)
25	8CT	6	319	-	40,41,41	4.80	23 (57%)	51,56,56	3.46	21 (41%)
24	CLA	H	201	17	50,54,73	1.34	9 (18%)	59,90,113	1.43	4 (6%)
24	CLA	A	817	9	69,73,73	1.14	7 (10%)	82,113,113	1.32	9 (10%)
24	CLA	5	302	2	63,67,73	1.22	8 (12%)	74,105,113	1.35	5 (6%)
23	CHL	9	305	-	45,59,74	3.63	19 (42%)	40,96,114	3.17	17 (42%)
23	CHL	6	305	-	37,51,74	3.96	18 (48%)	30,86,114	3.57	14 (46%)
24	CLA	0	313	1	49,53,73	1.40	8 (16%)	58,89,113	1.46	4 (6%)
28	SQD	0	318	-	36,36,54	1.20	4 (11%)	43,44,65	1.46	6 (13%)
23	CHL	8	316	-	37,51,74	4.10	17 (45%)	30,86,114	3.27	13 (43%)
24	CLA	A	833	9	50,54,73	1.32	8 (16%)	59,90,113	1.43	4 (6%)
25	8CT	L	205	-	40,41,41	4.79	23 (57%)	51,56,56	2.83	19 (37%)
24	CLA	7	314	6	51,55,73	1.33	9 (17%)	60,91,113	1.42	5 (8%)
24	CLA	3	313	4	49,53,73	1.37	9 (18%)	58,89,113	1.43	4 (6%)
23	CHL	1	305	-	42,56,74	3.85	19 (45%)	36,92,114	2.98	17 (47%)
23	CHL	2	301	3	58,72,74	3.17	19 (32%)	55,111,114	2.79	20 (36%)
24	CLA	4	309	-	64,68,73	1.21	8 (12%)	76,107,113	1.23	6 (7%)
24	CLA	B	832	-	69,73,73	1.16	9 (13%)	82,113,113	1.34	8 (9%)
27	LHG	L	208	-	30,30,48	1.37	6 (20%)	33,36,54	1.15	2 (6%)
24	CLA	B	823	-	56,60,73	1.29	9 (16%)	65,97,113	3.60	8 (12%)
29	LMG	J	102	-	29,29,55	0.97	1 (3%)	37,37,63	1.28	4 (10%)
24	CLA	B	828	-	64,68,73	1.19	9 (14%)	76,107,113	1.27	5 (6%)
23	CHL	4	301	7	55,69,74	3.32	19 (34%)	52,108,114	2.92	17 (32%)
27	LHG	2	319	24	31,31,48	1.37	5 (16%)	34,37,54	1.16	3 (8%)
23	CHL	4	308	-	41,55,74	3.83	19 (46%)	35,91,114	3.17	16 (45%)
24	CLA	B	807	10	49,53,73	1.35	9 (18%)	58,89,113	1.51	7 (12%)
24	CLA	O	206	-	41,46,73	1.59	9 (21%)	51,81,113	1.53	7 (13%)
25	8CT	8	317	-	40,41,41	4.81	23 (57%)	51,56,56	2.76	19 (37%)
24	CLA	2	311	3	64,68,73	1.18	8 (12%)	76,107,113	1.34	6 (7%)
25	8CT	M	102	-	40,41,41	4.76	23 (57%)	51,56,56	2.90	19 (37%)
26	0UR	9	315	-	50,53,58	1.01	2 (4%)	59,72,77	1.87	17 (28%)
23	CHL	9	306	-	42,56,74	3.80	19 (45%)	36,92,114	3.36	16 (44%)
23	CHL	8	306	-	41,55,74	3.85	19 (46%)	35,91,114	3.20	16 (45%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
23	CHL	4	305	-	37,51,74	3.97	18 (48%)	30,86,114	3.63	14 (46%)
24	CLA	A	809	9	69,73,73	1.17	9 (13%)	82,113,113	1.29	5 (6%)

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
24	CLA	G	101	14	1/1/12/20	7/21/97/115	-
23	CHL	1	306	-	3/3/20/26	22/39/137/137	-
34	DGD	B	849	-	-	27/45/85/95	0/2/2/2
27	LHG	7	324	-	-	20/43/43/53	-
24	CLA	9	302	-	1/1/15/20	15/39/115/115	-
23	CHL	7	302	6	3/3/19/26	16/37/135/137	-
24	CLA	7	309	-	1/1/13/20	11/32/108/115	-
25	8CT	3	317	-	-	9/29/63/63	0/2/2/2
24	CLA	A	819	9	1/1/13/20	8/27/103/115	-
24	CLA	A	837	9	1/1/13/20	3/29/105/115	-
24	CLA	3	312	4	1/1/13/20	5/27/103/115	-
24	CLA	5	310	-	1/1/11/20	8/15/91/115	-
24	CLA	8	310	-	1/1/14/20	6/33/109/115	-
24	CLA	7	311	6	1/1/12/20	8/24/100/115	-
23	CHL	7	306	-	3/3/18/26	17/33/131/137	-
24	CLA	7	303	6	1/1/11/20	6/15/91/115	-
24	CLA	8	311	27	1/1/11/20	4/17/93/115	-
23	CHL	7	305	-	3/3/16/26	7/18/116/137	-
24	CLA	B	809	10	1/1/15/20	11/39/115/115	-
24	CLA	1	311	2	1/1/15/20	12/39/115/115	-
24	CLA	B	818	10	1/1/13/20	8/32/108/115	-
24	CLA	A	853	-	1/1/15/20	10/39/115/115	-
23	CHL	7	301	6	3/3/19/26	14/36/134/137	-
24	CLA	A	822	9	1/1/12/20	4/23/99/115	-
31	PQN	A	841	-	-	7/23/43/43	0/2/2/2
24	CLA	A	818	9	1/1/15/20	18/39/115/115	-
24	CLA	A	826	9	1/1/15/20	2/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CLA	B	827	-	1/1/15/20	10/39/115/115	-
24	CLA	1	313	-	1/1/11/20	4/17/93/115	-
31	PQN	B	842	-	-	6/23/43/43	0/2/2/2
24	CLA	A	825	-	1/1/15/20	10/39/115/115	-
23	CHL	2	312	3	3/3/17/26	3/21/119/137	-
23	CHL	3	301	-	3/3/19/26	9/33/131/137	-
24	CLA	B	815	10	1/1/13/20	3/27/103/115	-
25	8CT	B	846	-	-	13/29/63/63	0/2/2/2
27	LHG	8	320	24	-	30/48/48/53	-
23	CHL	6	308	5	3/3/18/26	8/32/130/137	-
24	CLA	B	814	10	1/1/15/20	15/39/115/115	-
24	CLA	H	204	-	1/1/11/20	3/18/94/115	-
24	CLA	B	813	10	1/1/13/20	10/27/103/115	-
25	8CT	2	314	-	-	12/29/63/63	0/2/2/2
24	CLA	8	304	7	1/1/11/20	6/17/93/115	-
27	LHG	A	850	-	-	26/46/46/53	-
24	CLA	A	802	9	1/1/15/20	9/39/115/115	-
25	8CT	0	314	-	-	5/29/63/63	0/2/2/2
25	8CT	A	845	-	-	10/29/63/63	0/2/2/2
24	CLA	A	834	9	1/1/13/20	12/30/106/115	-
24	CLA	3	306	4	1/1/11/20	5/18/94/115	-
26	0UR	4	317	-	-	9/41/80/86	0/2/2/2
24	CLA	B	817	10	1/1/14/20	18/33/109/115	-
24	CLA	0	319	-	1/1/11/20	1/17/93/115	-
24	CLA	3	315	-	1/1/12/20	5/24/100/115	-
23	CHL	5	306	-	3/3/16/26	7/17/115/137	-
24	CLA	A	820	-	1/1/15/20	10/39/115/115	-
24	CLA	A	828	9	1/1/15/20	13/39/115/115	-
25	8CT	K	105	-	-	12/29/63/63	0/2/2/2
23	CHL	8	309	-	3/3/16/26	2/17/115/137	-
26	0UR	1	315	-	-	3/42/81/86	0/2/2/2
24	CLA	B	806	-	1/1/15/20	11/39/115/115	-
24	CLA	1	302	2	1/1/13/20	14/29/105/115	-
27	LHG	3	324	-	-	23/46/46/53	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CLA	A	806	9	1/1/12/20	4/23/99/115	-
29	LMG	O	203	-	-	13/26/46/70	0/1/1/1
25	8CT	4	316	-	-	8/29/63/63	0/2/2/2
27	LHG	3	322	-	-	18/40/40/53	-
23	CHL	5	305	-	3/3/16/26	11/18/116/137	-
25	8CT	B	843	-	-	14/29/63/63	0/2/2/2
23	CHL	6	302	5	3/3/19/26	19/37/135/137	-
24	CLA	5	303	-	1/1/12/20	8/24/100/115	-
24	CLA	A	812	9	1/1/15/20	7/39/115/115	-
24	CLA	A	824	-	1/1/15/20	8/39/115/115	-
24	CLA	4	303	7	1/1/11/20	4/15/91/115	-
24	CLA	6	314	-	1/1/11/20	2/15/91/115	-
24	CLA	L	202	17	1/1/14/20	19/37/113/115	-
24	CLA	B	810	10	1/1/14/20	6/36/112/115	-
24	CLA	O	209	-	1/1/12/20	9/23/99/115	-
27	LHG	0	317	-	-	30/53/53/53	-
25	8CT	J	104	-	-	8/29/63/63	0/2/2/2
24	CLA	4	304	-	1/1/14/20	8/33/109/115	-
30	0IE	7	321	-	-	2/33/72/72	0/2/2/2
24	CLA	H	202	10	1/1/13/20	7/27/103/115	-
24	CLA	K	101	-	1/1/14/20	10/33/109/115	-
24	CLA	B	829	-	1/1/15/20	9/39/115/115	-
23	CHL	3	302	4	3/3/19/26	18/35/133/137	-
23	CHL	5	304	-	3/3/16/26	9/15/113/137	-
24	CLA	4	311	-	1/1/11/20	4/19/95/115	-
23	CHL	4	307	-	3/3/17/26	10/21/119/137	-
24	CLA	B	840	10	1/1/15/20	10/39/115/115	-
23	CHL	8	307	-	3/3/17/26	13/21/119/137	-
24	CLA	5	307	-	1/1/11/20	7/17/93/115	-
24	CLA	0	310	-	1/1/11/20	8/18/94/115	-
24	CLA	B	819	10	1/1/14/20	14/33/109/115	-
24	CLA	3	304	-	1/1/15/20	7/39/115/115	-
26	0UR	2	315	-	-	7/41/80/86	0/2/2/2
24	CLA	3	314	4	1/1/11/20	0/17/93/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	8CT	B	848	-	-	9/29/63/63	0/2/2/2
24	CLA	4	314	7	1/1/11/20	4/15/91/115	-
26	0UR	1	316	-	-	10/42/81/86	0/2/2/2
23	CHL	3	307	-	3/3/20/26	26/39/137/137	-
24	CLA	F	302	13	1/1/11/20	4/18/94/115	-
27	LHG	B	852	-	-	27/42/42/53	-
24	CLA	5	311	2	1/1/13/20	10/29/105/115	-
24	CLA	6	309	5	1/1/13/20	2/31/107/115	-
25	8CT	J	101	-	-	11/29/63/63	0/2/2/2
24	CLA	5	308	-	1/1/14/20	8/33/109/115	-
24	CLA	5	309	27	1/1/11/20	5/15/91/115	-
23	CHL	6	306	-	3/3/17/26	7/21/119/137	-
25	8CT	L	207	-	-	9/29/63/63	0/2/2/2
24	CLA	6	312	5	1/1/13/20	7/29/105/115	-
24	CLA	A	835	-	1/1/12/20	8/23/99/115	-
23	CHL	6	315	5	3/3/15/26	4/12/110/137	-
23	CHL	2	307	-	3/3/16/26	4/17/115/137	-
24	CLA	A	805	-	1/1/15/20	19/39/115/115	-
27	LHG	I	102	-	-	20/50/50/53	-
24	CLA	0	309	-	1/1/10/20	2/10/86/115	-
24	CLA	B	826	-	1/1/10/20	1/23/87/115	-
24	CLA	B	811	10	1/1/15/20	9/39/115/115	-
24	CLA	7	315	6	1/1/12/20	2/15/91/115	-
24	CLA	A	816	9	1/1/14/20	16/35/111/115	-
24	CLA	3	309	4	1/1/15/20	12/39/115/115	-
24	CLA	6	303	5	1/1/12/20	6/24/100/115	-
24	CLA	A	829	9	1/1/15/20	12/39/115/115	-
24	CLA	0	312	1	1/1/11/20	10/17/93/115	-
24	CLA	B	835	-	1/1/11/20	0/15/91/115	-
23	CHL	8	301	2	3/3/17/26	10/23/121/137	-
24	CLA	9	310	8	1/1/12/20	6/24/100/115	-
26	0UR	5	314	-	-	11/41/80/86	0/2/2/2
25	8CT	A	847	-	-	10/29/63/63	0/2/2/2
23	CHL	1	301	-	3/3/19/26	16/37/135/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CHL	6	301	5	3/3/19/26	14/33/131/137	-
24	CLA	A	808	9	1/1/15/20	9/39/115/115	-
24	CLA	6	311	5	1/1/11/20	3/19/95/115	-
29	LMG	9	317	-	-	31/50/70/70	0/1/1/1
24	CLA	B	837	-	1/1/15/20	4/39/115/115	-
24	CLA	2	310	3	1/1/11/20	5/19/95/115	-
24	CLA	6	316	5	1/1/15/20	15/39/115/115	-
25	8CT	L	204	-	-	7/29/63/63	0/2/2/2
26	0UR	6	321	-	-	11/42/81/86	0/2/2/2
23	CHL	3	305	-	3/3/17/26	4/21/119/137	-
33	SF4	C	102	18	-	-	0/6/5/5
23	CHL	2	304	-	3/3/15/26	0/12/110/137	-
24	CLA	A	838	9	1/1/15/20	12/39/115/115	-
24	CLA	6	318	-	1/1/12/20	10/23/99/115	-
23	CHL	0	301	1	3/3/17/26	12/23/121/137	-
24	CLA	0	307	-	1/1/14/20	12/33/109/115	-
24	CLA	A	827	9	1/1/15/20	18/39/115/115	-
23	CHL	0	306	-	3/3/16/26	8/18/116/137	-
24	CLA	3	311	4	1/1/11/20	1/17/93/115	-
24	CLA	K	102	19	1/1/12/20	11/25/101/115	-
27	LHG	1	318	-	-	17/47/47/53	-
24	CLA	1	309	27	1/1/14/20	11/37/113/115	-
23	CHL	5	312	2	3/3/16/26	9/17/115/137	-
23	CHL	8	308	-	3/3/17/26	9/21/119/137	-
23	CHL	0	305	-	3/3/17/26	7/21/119/137	-
24	CLA	B	838	10	1/1/11/20	2/18/94/115	-
24	CLA	L	206	-	1/1/11/20	7/18/94/115	-
27	LHG	5	316	24	-	13/41/41/53	-
25	8CT	B	845	-	-	10/29/63/63	0/2/2/2
24	CLA	A	814	9	1/1/15/20	8/39/115/115	-
24	CLA	9	304	-	1/1/12/20	0/23/99/115	-
32	CL0	A	852	9	3/3/20/25	10/37/135/135	-
27	LHG	3	320	-	-	15/40/40/53	-
24	CLA	1	303	-	1/1/12/20	3/24/100/115	-
23	CHL	4	306	-	3/3/16/26	6/18/116/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CLA	G	102	14	1/1/11/20	4/15/91/115	-
23	CHL	4	315	2	3/3/17/26	11/25/123/137	-
24	CLA	B	841	27	1/1/15/20	8/39/115/115	-
26	0UR	2	316	-	-	11/40/79/86	0/2/2/2
24	CLA	0	311	1	1/1/15/20	12/39/115/115	-
27	LHG	6	322	24	-	17/41/41/53	-
24	CLA	B	804	-	1/1/15/20	13/39/115/115	-
24	CLA	6	310	27	1/1/14/20	11/33/109/115	-
24	CLA	B	839	-	1/1/15/20	8/39/115/115	-
24	CLA	F	303	-	1/1/11/20	6/15/91/115	-
23	CHL	6	323	7	3/3/19/26	5/33/131/137	-
25	8CT	3	323	-	-	7/29/63/63	0/2/2/2
26	0UR	0	316	-	-	12/42/81/86	0/2/2/2
26	0UR	O	207	-	-	5/42/81/86	0/2/2/2
24	CLA	O	204	-	1/1/10/20	6/10/86/115	-
24	CLA	4	310	27	1/1/14/20	14/33/109/115	-
24	CLA	1	308	2	1/1/13/20	6/27/103/115	-
24	CLA	7	304	-	1/1/13/20	7/27/103/115	-
24	CLA	B	822	10	1/1/14/20	11/33/109/115	-
27	LHG	A	842	-	-	19/53/53/53	-
23	CHL	1	312	2	3/3/19/26	21/35/133/137	-
26	0UR	6	320	-	-	11/41/80/86	0/2/2/2
25	8CT	3	316	-	-	9/29/63/63	0/2/2/2
23	CHL	7	307	-	3/3/17/26	4/21/119/137	-
23	CHL	2	306	-	3/3/17/26	6/21/119/137	-
23	CHL	8	314	7	3/3/18/26	9/27/125/137	-
24	CLA	9	308	-	1/1/14/20	7/33/109/115	-
24	CLA	7	308	-	1/1/15/20	15/39/115/115	-
23	CHL	2	305	-	3/3/16/26	5/18/116/137	-
24	CLA	6	304	-	1/1/11/20	6/17/93/115	-
24	CLA	0	308	-	1/1/14/20	9/33/109/115	-
33	SF4	C	101	-	-	-	0/6/5/5
23	CHL	4	313	7	3/3/17/26	5/21/119/137	-
25	8CT	7	318	-	-	15/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CHL	6	307	-	3/3/17/26	7/21/119/137	-
24	CLA	A	848	-	1/1/15/20	12/39/115/115	-
24	CLA	A	836	9	1/1/14/20	12/35/111/115	-
23	CHL	0	302	1	3/3/19/26	14/37/135/137	-
25	8CT	9	313	-	-	11/29/63/63	0/2/2/2
26	0UR	3	318	-	-	9/41/80/86	0/2/2/2
23	CHL	5	301	2	3/3/19/26	18/37/135/137	-
24	CLA	2	313	3	1/1/11/20	5/15/91/115	-
25	8CT	6	324	-	-	11/29/63/63	0/2/2/2
24	CLA	0	304	-	1/1/12/20	4/24/100/115	-
24	CLA	J	103	16	1/1/10/20	3/12/88/115	-
25	8CT	O	202	-	-	7/29/63/63	0/2/2/2
33	SF4	B	803	-	-	-	0/6/5/5
29	LMG	A	854	-	-	15/32/52/70	0/1/1/1
24	CLA	B	830	10	1/1/13/20	7/29/105/115	-
24	CLA	O	201	27	1/1/12/20	6/24/100/115	-
24	CLA	A	832	9	1/1/15/20	12/39/115/115	-
24	CLA	O	205	21	1/1/9/20	2/6/78/115	-
24	CLA	H	203	22	1/1/11/20	6/18/94/115	-
24	CLA	9	309	27	1/1/10/20	4/10/86/115	-
23	CHL	8	303	7	3/3/19/26	17/37/135/137	-
24	CLA	B	802	10	1/1/15/20	13/39/115/115	-
24	CLA	B	816	10	1/1/14/20	8/33/109/115	-
25	8CT	O	208	-	-	6/29/63/63	0/2/2/2
24	CLA	2	309	27	1/1/14/20	14/33/109/115	-
25	8CT	B	844	-	-	11/29/63/63	0/2/2/2
24	CLA	A	840	-	1/1/15/20	10/39/115/115	-
27	LHG	8	302	-	-	12/35/35/53	-
25	8CT	I	101	-	-	8/29/63/63	0/2/2/2
24	CLA	A	830	9	1/1/12/20	3/21/97/115	-
25	8CT	B	850	-	-	13/29/63/63	0/2/2/2
24	CLA	H	205	-	1/1/12/20	9/23/99/115	-
24	CLA	B	825	-	1/1/15/20	7/39/115/115	-
26	0UR	9	314	-	-	3/42/81/86	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CLA	1	307	-	1/1/11/20	6/15/91/115	-
24	CLA	B	812	10	1/1/12/20	4/24/100/115	-
30	0IE	3	319	-	-	2/33/72/72	0/2/2/2
29	LMG	2	318	-	-	14/31/51/70	0/1/1/1
24	CLA	3	308	-	1/1/15/20	16/39/115/115	-
25	8CT	B	847	-	-	9/29/63/63	0/2/2/2
24	CLA	B	808	10	1/1/15/20	10/39/115/115	-
26	0UR	5	315	-	-	10/42/81/86	0/2/2/2
27	LHG	7	323	-	-	20/42/42/53	-
23	CHL	9	312	8	3/3/16/26	9/17/115/137	-
24	CLA	A	815	-	1/1/11/20	5/15/91/115	-
25	8CT	1	314	-	-	8/29/63/63	0/2/2/2
29	LMG	M	101	-	-	23/37/57/70	0/1/1/1
24	CLA	8	305	-	1/1/15/20	10/39/115/115	-
25	8CT	A	846	-	-	7/29/63/63	0/2/2/2
25	8CT	F	301	-	-	14/29/63/63	0/2/2/2
24	CLA	2	303	-	1/1/14/20	11/33/109/115	-
24	CLA	A	821	-	1/1/11/20	5/20/96/115	-
23	CHL	6	313	5	3/3/17/26	6/23/121/137	-
24	CLA	6	317	-	1/1/11/20	11/17/93/115	-
29	LMG	3	321	-	-	16/31/51/70	0/1/1/1
24	CLA	B	831	10	1/1/12/20	7/21/97/115	-
24	CLA	2	302	3	1/1/13/20	9/29/105/115	-
24	CLA	L	203	-	1/1/11/20	6/17/93/115	-
25	8CT	G	104	-	-	13/29/63/63	0/2/2/2
24	CLA	A	831	9	1/1/15/20	10/39/115/115	-
24	CLA	A	807	9	1/1/15/20	21/39/115/115	-
24	CLA	0	303	1	1/1/14/20	10/36/112/115	-
24	CLA	7	316	-	1/1/11/20	13/15/91/115	-
24	CLA	1	310	2	1/1/12/20	6/24/100/115	-
24	CLA	3	303	-	1/1/13/20	7/27/103/115	-
24	CLA	A	810	9	1/1/15/20	12/39/115/115	-
26	0UR	4	318	-	-	13/40/79/86	0/2/2/2
24	CLA	B	801	10	1/1/13/20	13/31/107/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CLA	4	312	7	1/1/12/20	6/25/101/115	-
23	CHL	1	304	-	3/3/17/26	7/21/119/137	-
27	LHG	B	851	24	-	17/26/26/53	-
25	8CT	A	844	-	-	4/29/63/63	0/2/2/2
25	8CT	7	319	-	-	10/29/63/63	0/2/2/2
24	CLA	A	823	9	1/1/13/20	8/27/103/115	-
24	CLA	8	315	-	1/1/11/20	9/15/91/115	-
24	CLA	B	805	10	1/1/15/20	9/39/115/115	-
24	CLA	B	834	10	1/1/14/20	15/35/111/115	-
24	CLA	B	821	10	1/1/12/20	0/21/97/115	-
29	LMG	A	851	-	-	13/31/51/70	0/1/1/1
27	LHG	7	322	24	-	10/34/34/53	-
29	LMG	J	105	-	-	15/41/61/70	0/1/1/1
24	CLA	8	312	7	1/1/11/20	8/17/93/115	-
24	CLA	5	313	2	1/1/11/20	9/17/93/115	-
24	CLA	G	103	14	1/1/11/20	5/17/93/115	-
24	CLA	A	813	9	1/1/13/20	10/30/106/115	-
27	LHG	1	317	24	-	21/53/53/53	-
23	CHL	7	313	6	3/3/16/26	9/17/115/137	-
23	CHL	9	301	8	3/3/16/26	8/17/115/137	-
24	CLA	3	310	-	1/1/14/20	13/36/112/115	-
24	CLA	K	104	19	1/1/12/20	11/21/97/115	-
25	8CT	A	849	-	-	10/29/63/63	0/2/2/2
24	CLA	A	803	9	1/1/13/20	8/27/103/115	-
24	CLA	K	103	19	1/1/11/20	5/17/93/115	-
24	CLA	A	839	9	1/1/15/20	17/39/115/115	-
26	0UR	8	319	-	-	8/42/81/86	0/2/2/2
24	CLA	7	312	6	1/1/13/20	10/27/103/115	-
24	CLA	2	308	3	1/1/14/20	3/33/109/115	-
25	8CT	F	304	-	-	9/29/63/63	0/2/2/2
27	LHG	2	317	24	-	17/36/36/53	-
26	0UR	8	318	-	-	7/41/80/86	0/2/2/2
24	CLA	A	804	9	1/1/15/20	13/39/115/115	-
27	LHG	A	843	24	-	17/31/31/53	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CLA	9	303	8	1/1/11/20	5/19/95/115	-
24	CLA	B	820	-	1/1/13/20	10/29/105/115	-
23	CHL	4	302	7	3/3/17/26	13/24/122/137	-
24	CLA	7	317	6	1/1/14/20	9/33/109/115	-
24	CLA	B	824	10	1/1/14/20	8/33/109/115	-
27	LHG	9	316	24	-	18/48/48/53	-
26	0UR	0	315	-	-	3/42/81/86	0/2/2/2
24	CLA	B	836	10	1/1/14/20	11/33/109/115	-
24	CLA	7	310	27	1/1/8/20	2/4/76/115	-
24	CLA	A	801	-	1/1/15/20	4/39/115/115	-
24	CLA	A	811	9	1/1/12/20	1/26/102/115	-
29	LMG	O	210	-	-	10/34/54/70	0/1/1/1
26	0UR	7	320	-	-	9/41/80/86	0/2/2/2
24	CLA	B	833	10	1/1/13/20	9/27/103/115	-
24	CLA	L	201	9	1/1/13/20	7/31/107/115	-
24	CLA	8	313	7	1/1/13/20	8/29/105/115	-
24	CLA	9	311	8	1/1/13/20	6/29/105/115	-
24	CLA	9	307	-	1/1/15/20	12/39/115/115	-
25	8CT	6	319	-	-	8/29/63/63	0/2/2/2
24	CLA	H	201	17	1/1/11/20	5/17/93/115	-
24	CLA	A	817	9	1/1/15/20	12/39/115/115	-
24	CLA	5	302	2	1/1/13/20	13/32/108/115	-
23	CHL	9	305	-	3/3/17/26	7/21/119/137	-
23	CHL	6	305	-	3/3/15/26	0/12/110/137	-
24	CLA	0	313	1	1/1/11/20	11/15/91/115	-
28	SQD	0	318	-	-	17/31/51/69	0/1/1/1
23	CHL	8	316	-	3/3/15/26	4/12/110/137	-
24	CLA	A	833	9	1/1/11/20	0/17/93/115	-
25	8CT	L	205	-	-	8/29/63/63	0/2/2/2
24	CLA	7	314	6	1/1/11/20	8/18/94/115	-
24	CLA	3	313	4	1/1/11/20	7/15/91/115	-
23	CHL	1	305	-	3/3/16/26	7/18/116/137	-
23	CHL	2	301	3	3/3/19/26	26/37/135/137	-
24	CLA	4	309	-	1/1/14/20	5/33/109/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CLA	B	832	-	1/1/15/20	8/39/115/115	-
27	LHG	L	208	-	-	13/35/35/53	-
24	CLA	B	823	-	1/1/12/20	10/24/100/115	-
29	LMG	J	102	-	-	12/24/44/70	0/1/1/1
24	CLA	B	828	-	1/1/14/20	6/33/109/115	-
23	CHL	4	301	7	3/3/19/26	16/33/131/137	-
27	LHG	2	319	24	-	12/36/36/53	-
23	CHL	4	308	-	3/3/16/26	3/17/115/137	-
24	CLA	B	807	10	1/1/11/20	5/15/91/115	-
24	CLA	O	206	-	1/1/10/20	1/4/80/115	-
25	8CT	8	317	-	-	10/29/63/63	0/2/2/2
24	CLA	2	311	3	1/1/14/20	10/33/109/115	-
25	8CT	M	102	-	-	8/29/63/63	0/2/2/2
26	0UR	9	315	-	-	8/42/81/86	0/2/2/2
23	CHL	9	306	-	3/3/16/26	7/18/116/137	-
23	CHL	8	306	-	3/3/16/26	6/17/115/137	-
23	CHL	4	305	-	3/3/15/26	0/12/110/137	-
24	CLA	A	809	9	1/1/15/20	3/39/115/115	-

The worst 5 of 3884 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	J	104	8CT	C02-C03	14.90	1.59	1.34
25	B	844	8CT	C02-C03	14.87	1.59	1.34
25	6	324	8CT	C02-C03	14.86	1.59	1.34
25	A	844	8CT	C02-C03	14.78	1.59	1.34
25	G	104	8CT	C02-C03	14.77	1.59	1.34

The worst 5 of 3319 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	B	823	CLA	O2A-CGA-O1A	-19.95	73.72	123.63
24	B	823	CLA	O2A-CGA-CBA	15.01	157.60	111.83
25	K	105	8CT	C33-C32-C31	-11.86	113.51	124.83
25	G	104	8CT	C33-C32-C31	-11.78	113.58	124.83
24	B	826	CLA	CHA-C4D-ND	11.50	135.06	125.22

5 of 373 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
23	0	301	CHL	NC
23	0	301	CHL	ND
23	0	301	CHL	NA
23	0	302	CHL	NC
23	0	302	CHL	ND

5 of 3316 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
23	0	301	CHL	C3A-C2A-CAA-CBA
23	0	301	CHL	C1C-C2C-CMC-OMC
23	0	301	CHL	C3C-C2C-CMC-OMC
23	0	301	CHL	C2-C3-C5-C6
23	0	301	CHL	C4-C3-C5-C6

There are no ring outliers.

268 monomers are involved in 685 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	1	306	CHL	4	0
34	B	849	DGD	3	0
24	9	302	CLA	4	0
23	7	302	CHL	3	0
24	7	309	CLA	3	0
24	A	837	CLA	3	0
24	3	312	CLA	2	0
24	5	310	CLA	2	0
24	8	310	CLA	1	0
23	7	306	CHL	4	0
23	7	305	CHL	4	0
24	B	809	CLA	10	0
24	1	311	CLA	8	0
24	B	818	CLA	11	0
24	A	853	CLA	8	0
23	7	301	CHL	3	0
31	A	841	PQN	4	0
24	A	818	CLA	4	0
24	A	826	CLA	3	0
24	B	827	CLA	4	0
31	B	842	PQN	1	0
24	A	825	CLA	2	0
23	2	312	CHL	6	0
23	3	301	CHL	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	6	308	CHL	3	0
24	B	814	CLA	7	0
24	H	204	CLA	1	0
24	B	813	CLA	4	0
27	A	850	LHG	3	0
24	A	802	CLA	3	0
24	3	306	CLA	2	0
26	4	317	0UR	3	0
24	B	817	CLA	8	0
24	3	315	CLA	1	0
23	5	306	CHL	2	0
24	A	820	CLA	6	0
24	A	828	CLA	4	0
23	8	309	CHL	2	0
26	1	315	0UR	1	0
24	B	806	CLA	6	0
24	1	302	CLA	2	0
27	3	324	LHG	3	0
24	A	806	CLA	2	0
25	4	316	8CT	1	0
27	3	322	LHG	3	0
23	5	305	CHL	1	0
23	6	302	CHL	2	0
24	5	303	CLA	2	0
24	A	812	CLA	7	0
24	A	824	CLA	5	0
24	L	202	CLA	5	0
24	B	810	CLA	4	0
24	O	209	CLA	1	0
27	0	317	LHG	2	0
25	J	104	8CT	1	0
24	4	304	CLA	1	0
24	H	202	CLA	3	0
24	B	829	CLA	3	0
23	3	302	CHL	3	0
23	5	304	CHL	4	0
24	4	311	CLA	4	0
23	4	307	CHL	3	0
24	B	840	CLA	1	0
23	8	307	CHL	1	0
24	5	307	CLA	2	0
24	0	310	CLA	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	B	819	CLA	4	0
24	3	304	CLA	1	0
26	2	315	0UR	3	0
24	3	314	CLA	3	0
24	4	314	CLA	1	0
23	3	307	CHL	5	0
24	F	302	CLA	1	0
27	B	852	LHG	1	0
24	5	311	CLA	3	0
24	6	309	CLA	1	0
24	5	308	CLA	3	0
23	6	306	CHL	2	0
24	6	312	CLA	3	0
24	A	835	CLA	1	0
23	6	315	CHL	1	0
23	2	307	CHL	1	0
24	A	805	CLA	5	0
27	I	102	LHG	4	0
24	0	309	CLA	2	0
24	B	826	CLA	3	0
24	B	811	CLA	8	0
24	A	816	CLA	2	0
24	3	309	CLA	4	0
24	6	303	CLA	1	0
24	A	829	CLA	5	0
24	0	312	CLA	2	0
24	B	835	CLA	1	0
23	8	301	CHL	6	0
24	9	310	CLA	2	0
26	5	314	0UR	4	0
25	A	847	8CT	1	0
23	1	301	CHL	4	0
23	6	301	CHL	9	0
24	A	808	CLA	7	0
24	6	311	CLA	1	0
29	9	317	LMG	4	0
24	B	837	CLA	3	0
24	6	316	CLA	4	0
25	L	204	8CT	1	0
26	6	321	0UR	1	0
23	3	305	CHL	1	0
24	A	838	CLA	6	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	0	301	CHL	6	0
24	0	307	CLA	1	0
24	A	827	CLA	7	0
23	0	306	CHL	5	0
24	K	102	CLA	3	0
27	1	318	LHG	2	0
23	5	312	CHL	1	0
23	8	308	CHL	4	0
23	0	305	CHL	5	0
24	B	838	CLA	4	0
27	5	316	LHG	1	0
24	A	814	CLA	2	0
27	3	320	LHG	1	0
32	A	852	CL0	8	0
24	1	303	CLA	1	0
23	4	306	CHL	2	0
24	G	102	CLA	1	0
23	4	315	CHL	7	0
24	B	841	CLA	4	0
24	0	311	CLA	6	0
27	6	322	LHG	5	0
24	B	804	CLA	9	0
24	6	310	CLA	3	0
24	B	839	CLA	5	0
24	F	303	CLA	3	0
23	6	323	CHL	4	0
25	3	323	8CT	1	0
26	O	207	0UR	2	0
24	O	204	CLA	1	0
24	4	310	CLA	2	0
24	1	308	CLA	2	0
24	7	304	CLA	5	0
24	B	822	CLA	4	0
27	A	842	LHG	5	0
23	1	312	CHL	3	0
25	3	316	8CT	1	0
23	7	307	CHL	6	0
23	2	306	CHL	3	0
23	8	314	CHL	3	0
24	9	308	CLA	4	0
24	7	308	CLA	8	0
23	2	305	CHL	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	6	304	CLA	2	0
24	0	308	CLA	2	0
23	4	313	CHL	3	0
23	6	307	CHL	3	0
24	A	848	CLA	4	0
24	A	836	CLA	3	0
23	0	302	CHL	3	0
26	3	318	0UR	1	0
23	5	301	CHL	5	0
24	2	313	CLA	1	0
24	J	103	CLA	2	0
33	B	803	SF4	1	0
29	A	854	LMG	3	0
24	B	830	CLA	6	0
24	O	201	CLA	4	0
23	8	303	CHL	1	0
24	B	802	CLA	5	0
24	B	816	CLA	2	0
24	2	309	CLA	3	0
24	A	840	CLA	4	0
24	A	830	CLA	3	0
24	B	825	CLA	4	0
26	9	314	0UR	2	0
24	1	307	CLA	2	0
24	B	812	CLA	1	0
24	3	308	CLA	1	0
25	B	847	8CT	1	0
24	B	808	CLA	6	0
27	7	323	LHG	3	0
23	9	312	CHL	1	0
24	A	815	CLA	1	0
29	M	101	LMG	1	0
24	8	305	CLA	3	0
25	F	301	8CT	1	0
24	A	821	CLA	2	0
23	6	313	CHL	2	0
29	3	321	LMG	2	0
24	B	831	CLA	3	0
24	L	203	CLA	2	0
24	A	831	CLA	4	0
24	A	807	CLA	7	0
24	0	303	CLA	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	7	316	CLA	6	0
24	1	310	CLA	2	0
24	3	303	CLA	3	0
24	A	810	CLA	6	0
24	B	801	CLA	1	0
24	4	312	CLA	2	0
23	1	304	CHL	3	0
27	B	851	LHG	1	0
24	A	823	CLA	1	0
24	8	315	CLA	2	0
24	B	805	CLA	4	0
24	B	834	CLA	7	0
29	A	851	LMG	4	0
27	7	322	LHG	2	0
29	J	105	LMG	2	0
24	8	312	CLA	2	0
24	5	313	CLA	1	0
24	G	103	CLA	1	0
24	A	813	CLA	4	0
27	1	317	LHG	5	0
23	9	301	CHL	1	0
24	K	104	CLA	2	0
24	A	803	CLA	1	0
24	K	103	CLA	1	0
24	A	839	CLA	5	0
24	7	312	CLA	5	0
24	2	308	CLA	2	0
27	2	317	LHG	2	0
26	8	318	0UR	2	0
24	A	804	CLA	2	0
27	A	843	LHG	3	0
24	9	303	CLA	1	0
24	B	820	CLA	4	0
23	4	302	CHL	2	0
24	7	317	CLA	1	0
24	B	824	CLA	5	0
27	9	316	LHG	5	0
26	0	315	0UR	1	0
24	B	836	CLA	3	0
24	A	801	CLA	2	0
24	A	811	CLA	2	0
29	O	210	LMG	1	0

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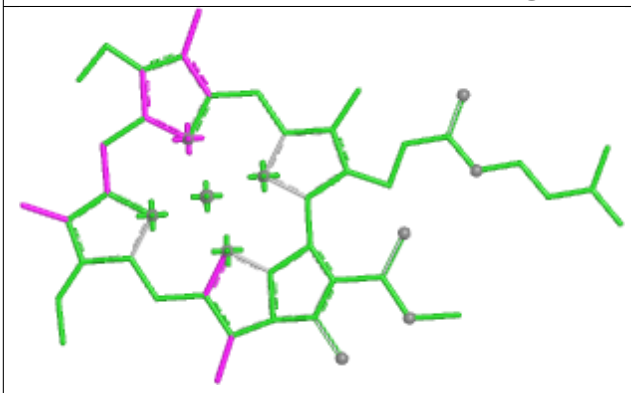
Mol	Chain	Res	Type	Clashes	Symm-Clashes
26	7	320	0UR	2	0
24	B	833	CLA	6	0
24	L	201	CLA	3	0
24	8	313	CLA	3	0
24	9	311	CLA	2	0
24	9	307	CLA	6	0
24	H	201	CLA	2	0
24	A	817	CLA	8	0
24	5	302	CLA	3	0
23	9	305	CHL	1	0
23	6	305	CHL	2	0
24	0	313	CLA	4	0
28	0	318	SQD	2	0
23	8	316	CHL	3	0
24	7	314	CLA	1	0
24	3	313	CLA	1	0
23	1	305	CHL	2	0
23	2	301	CHL	3	0
24	4	309	CLA	5	0
24	B	832	CLA	3	0
24	B	823	CLA	4	0
29	J	102	LMG	1	0
24	B	828	CLA	3	0
23	4	301	CHL	7	0
23	4	308	CHL	2	0
24	B	807	CLA	1	0
24	O	206	CLA	4	0
25	8	317	8CT	1	0
24	2	311	CLA	2	0
26	9	315	0UR	1	0
23	9	306	CHL	2	0
23	8	306	CHL	3	0
23	4	305	CHL	3	0
24	A	809	CLA	4	0

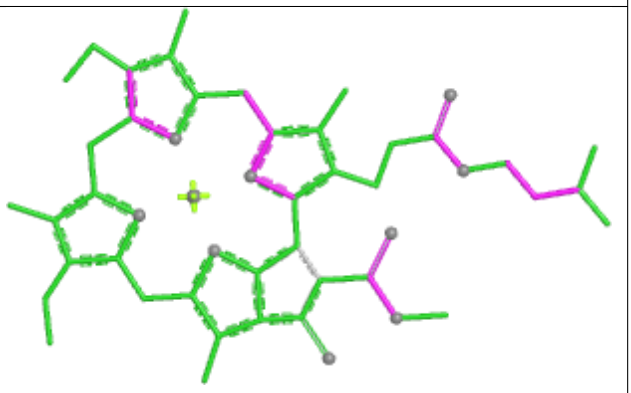
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

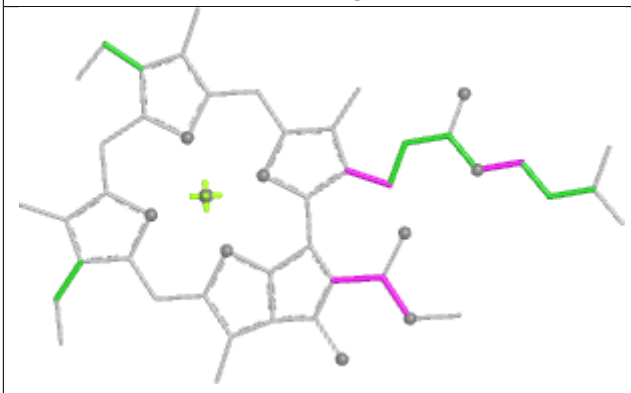
Ligand CLA G 101



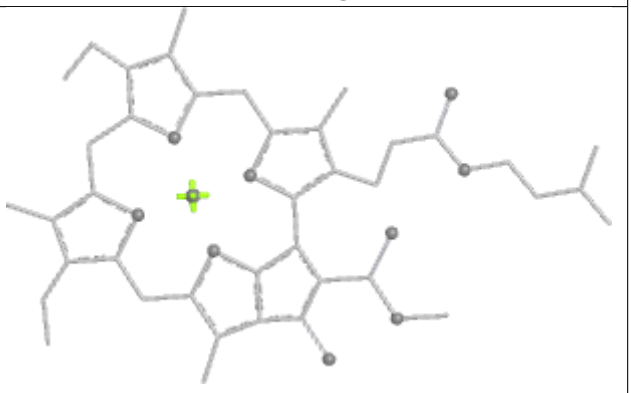
Bond lengths



Bond angles

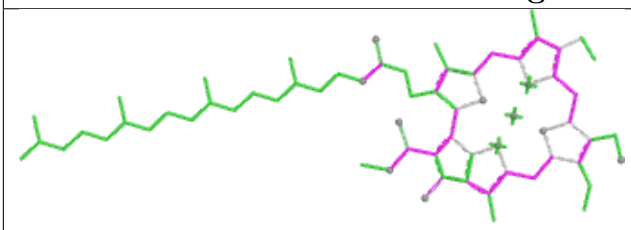


Torsions



Rings

Ligand CHL 1 306



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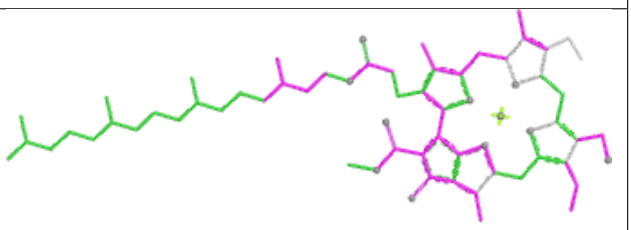

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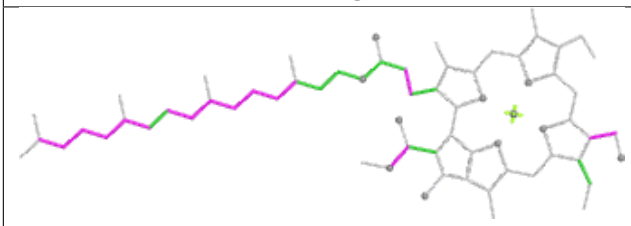
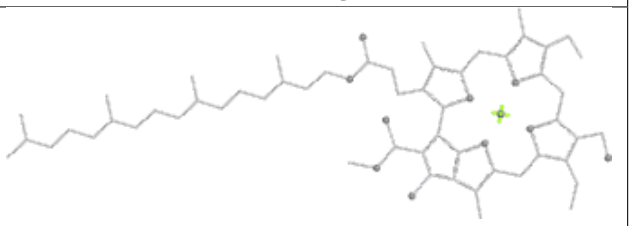
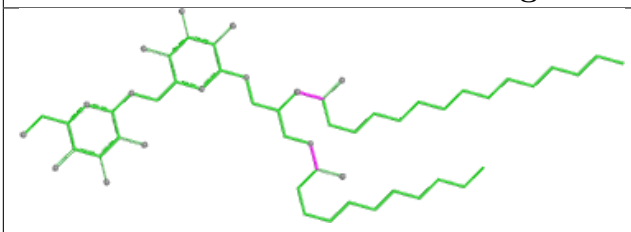


Torsions

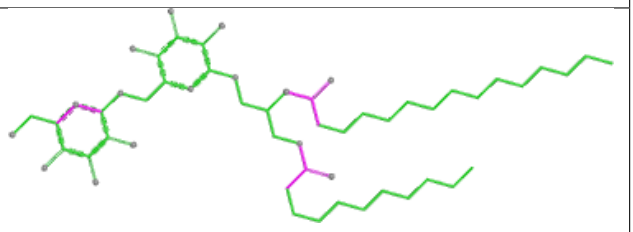


Rings

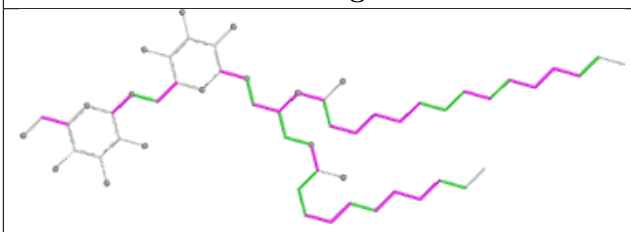
Ligand DGD B 849



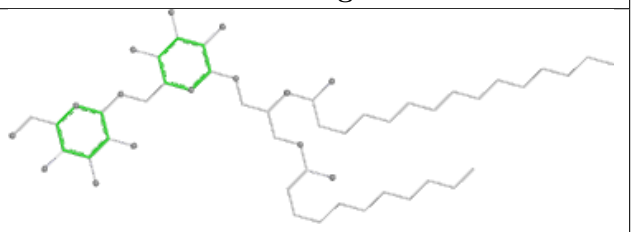
Bond lengths



Bond angles

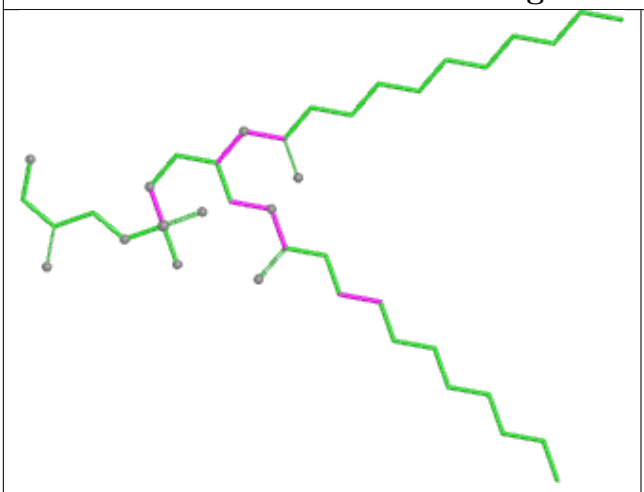


Torsions

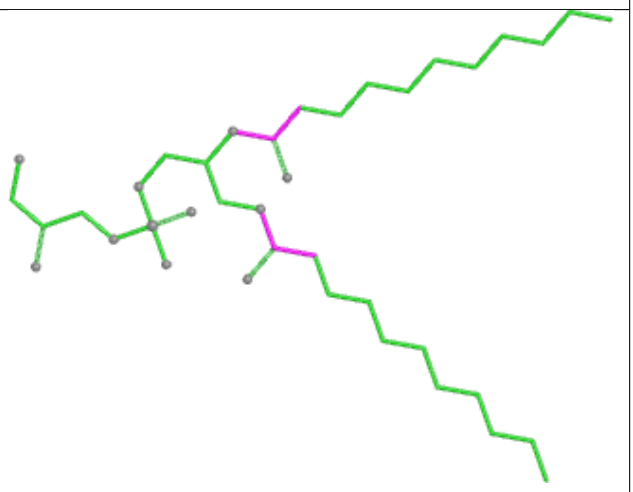


Rings

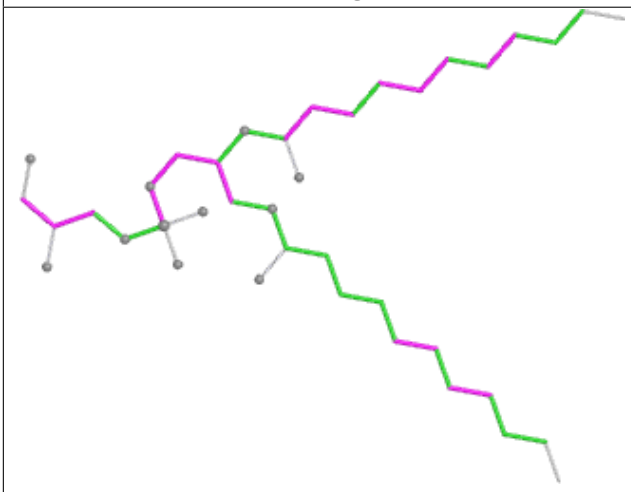
Ligand LHG 7 324



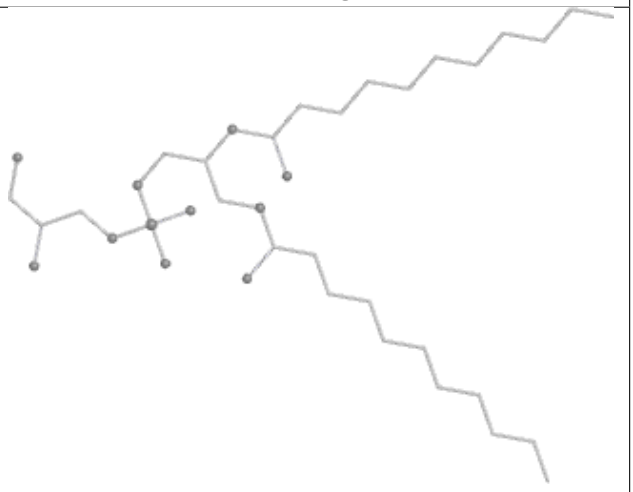
Bond lengths



Bond angles

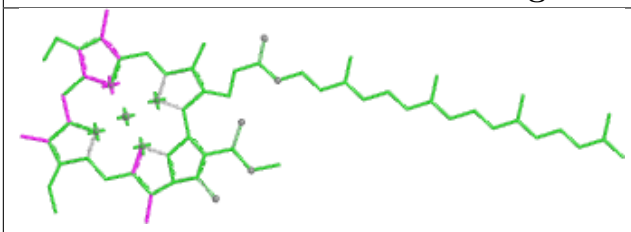


Torsions

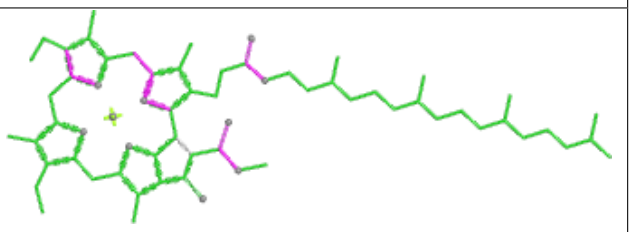


Rings

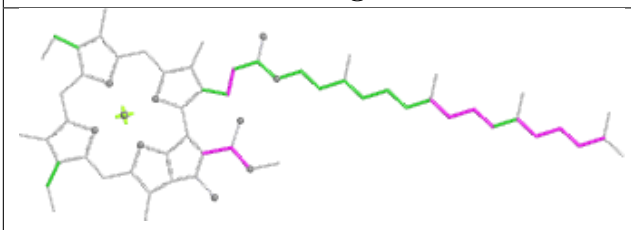
Ligand CLA 9 302



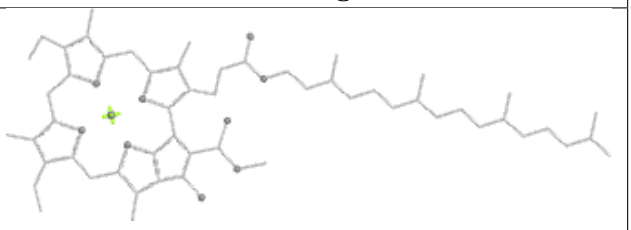
Bond lengths



Bond angles

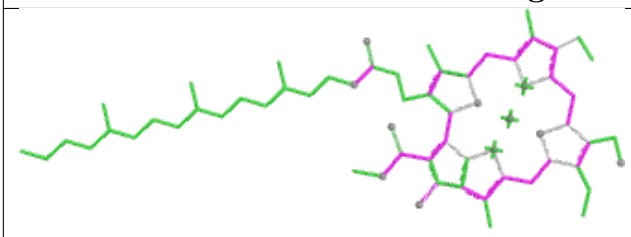


Torsions

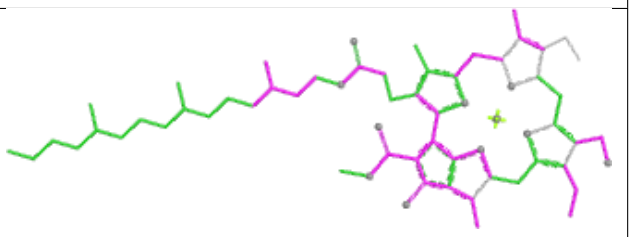


Rings

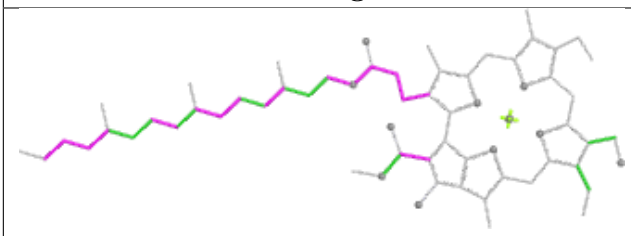
Ligand CHL 7 302



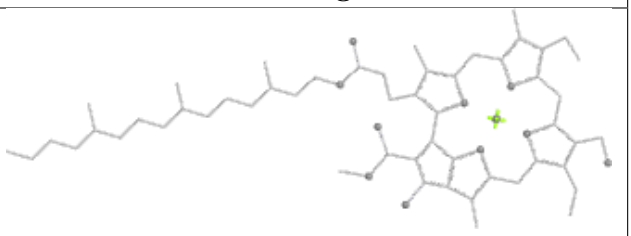
Bond lengths



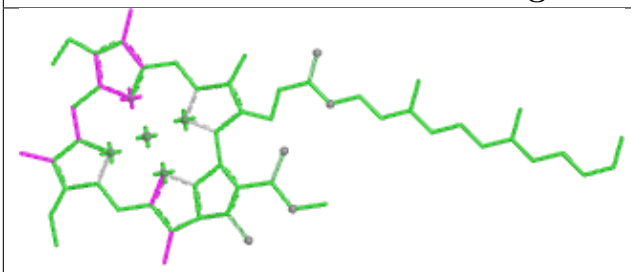
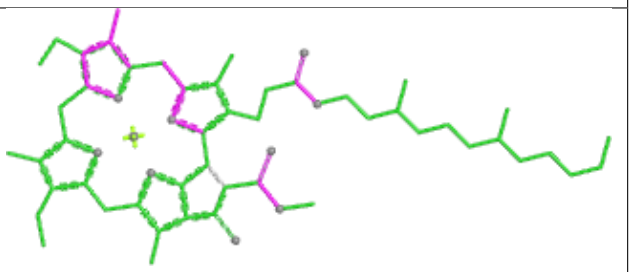
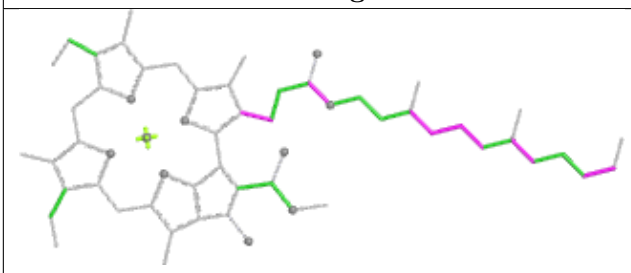
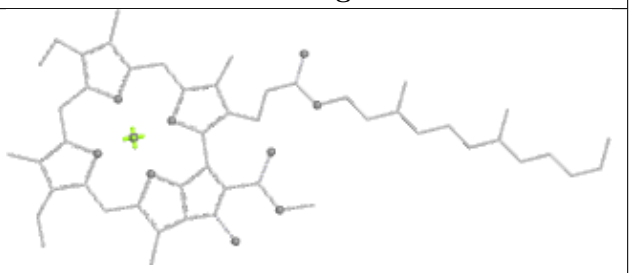
Bond angles

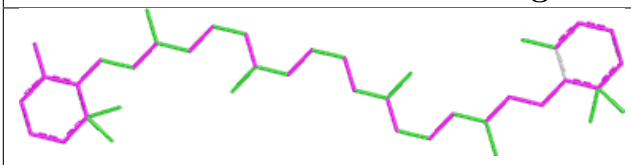
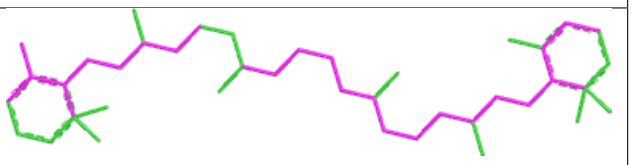
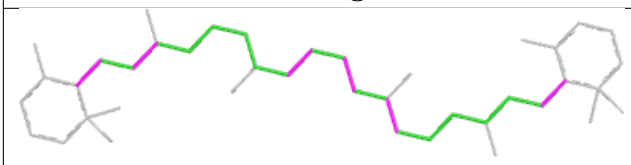
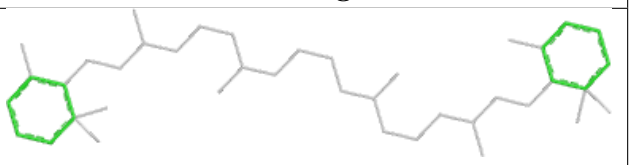


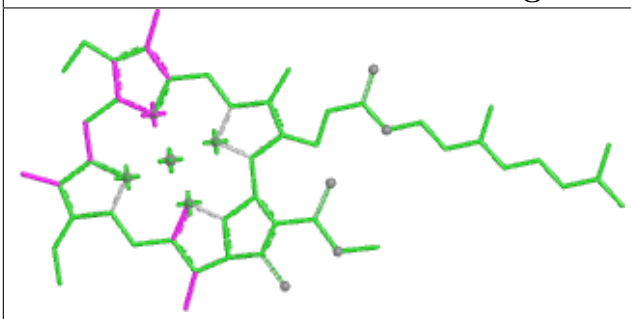
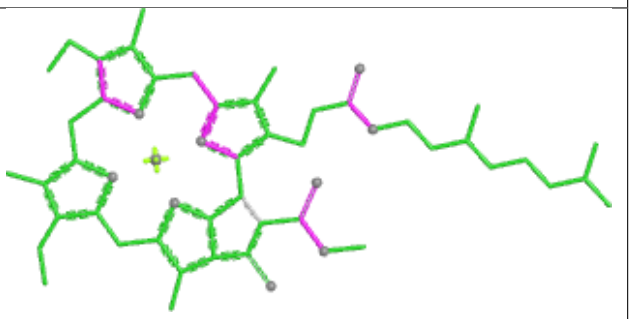
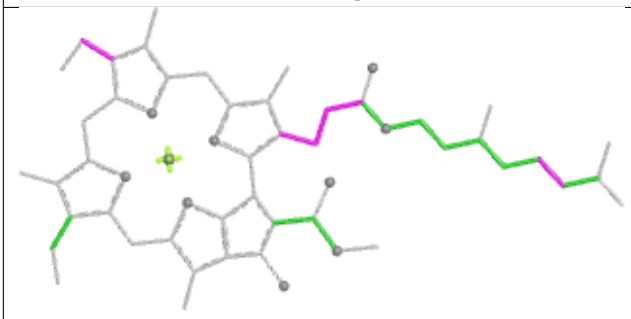
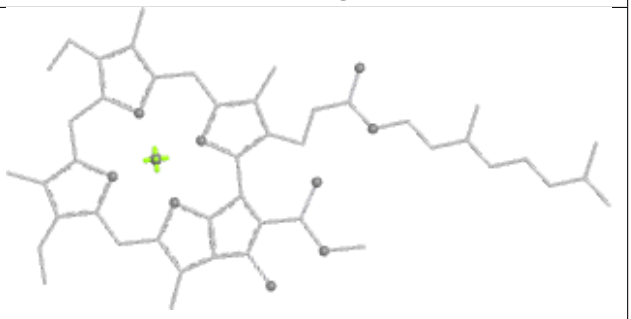
Torsions



Rings

Ligand CLA 7 309	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand 8CT 3 317	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA A 819	
 Bond lengths	 Bond angles
 Torsions	 Rings

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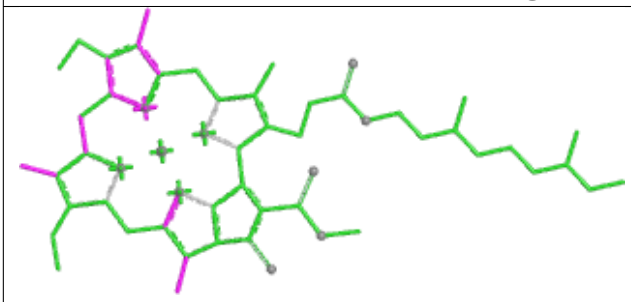
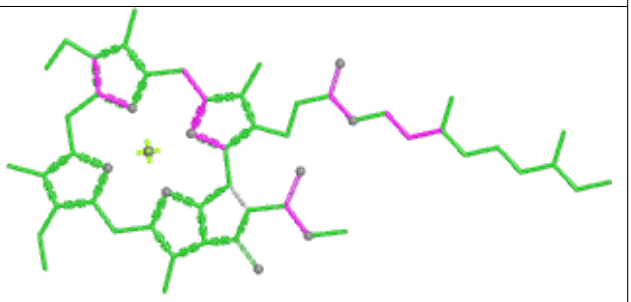
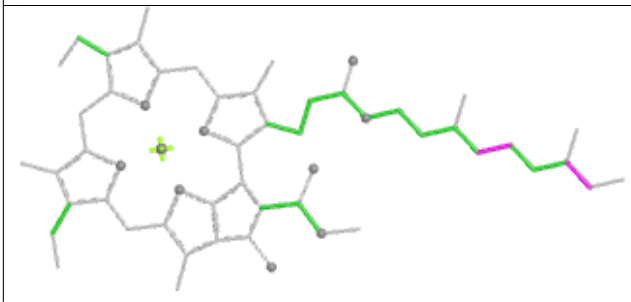
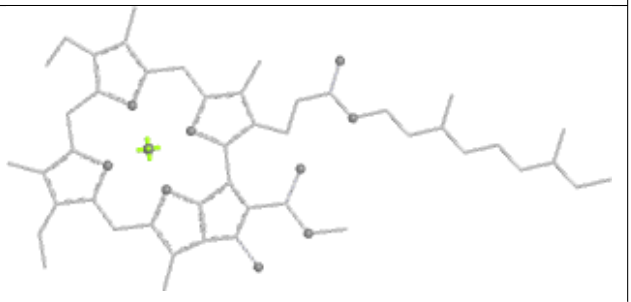
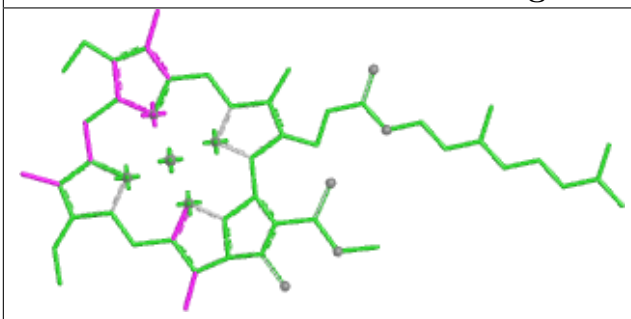
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA 3 312



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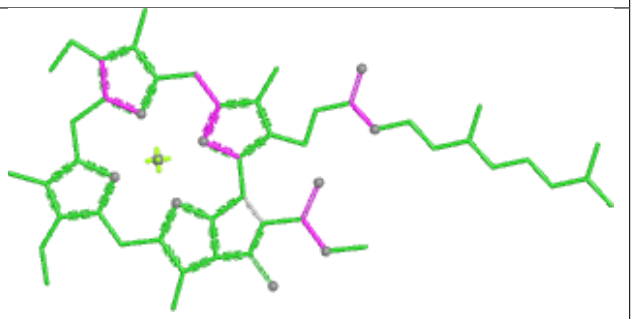

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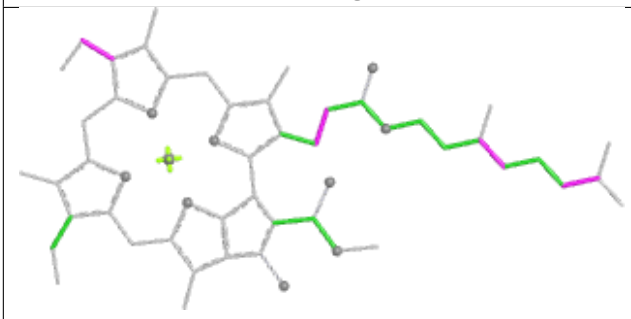

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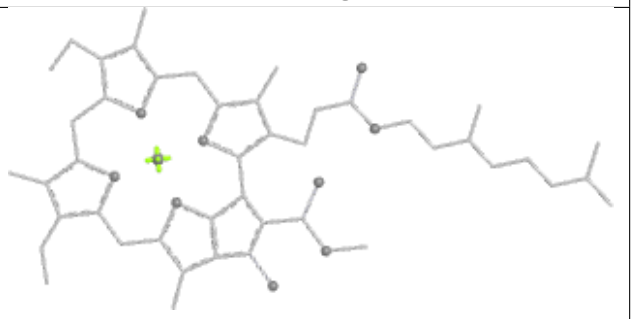
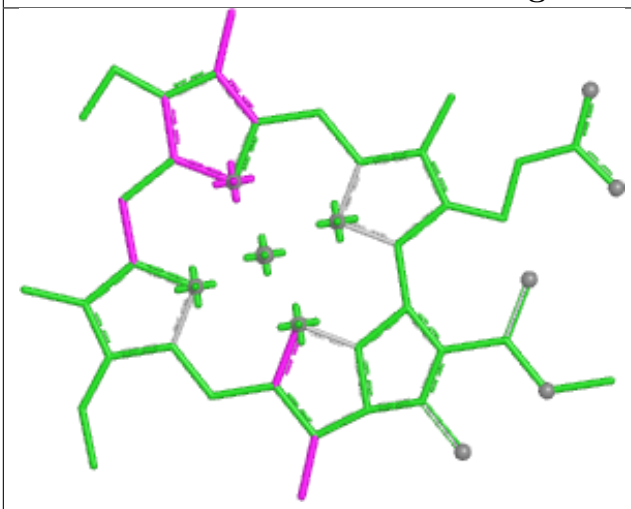


Rings

Ligand CLA 5 310



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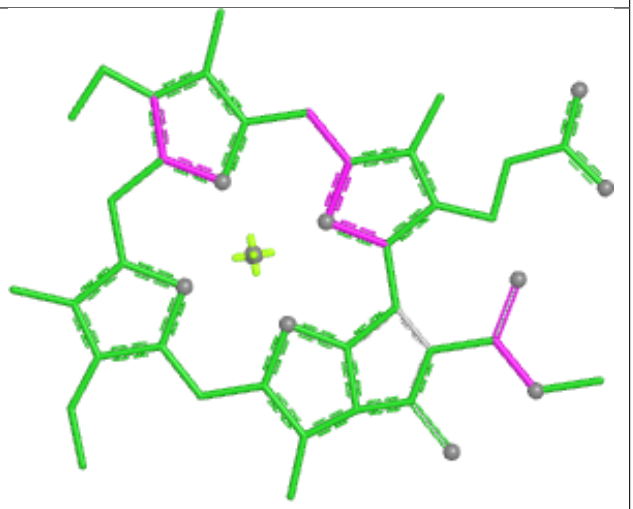

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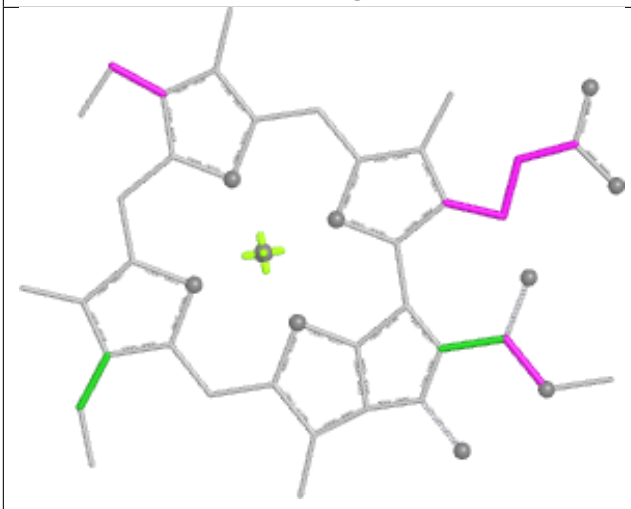
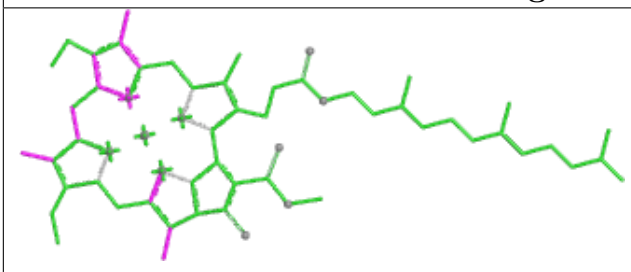


Torsions

Rings

Ligand CLA 8 310



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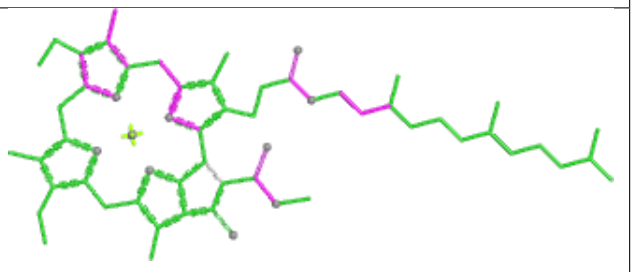

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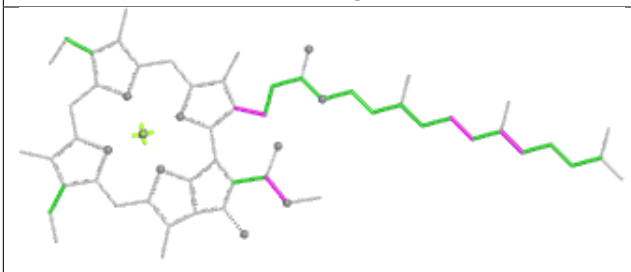

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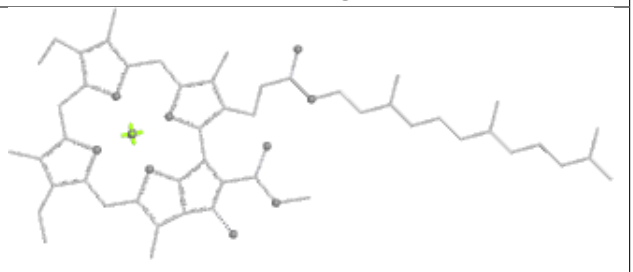
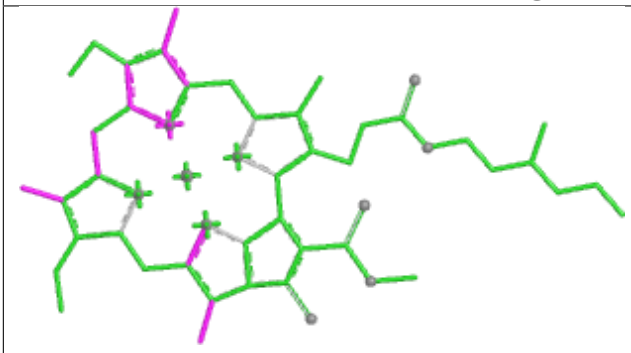


Rings

Ligand CLA 7 311



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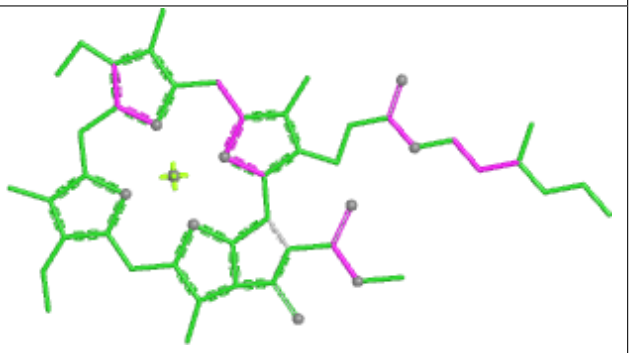

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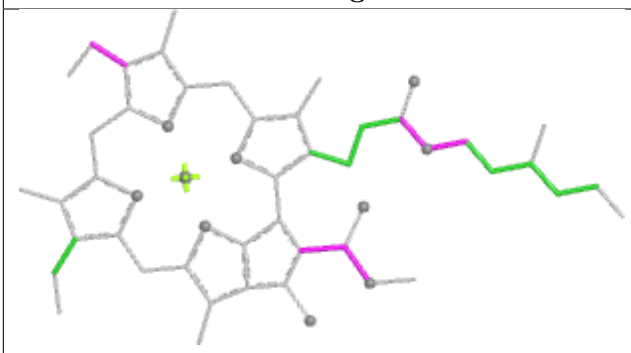

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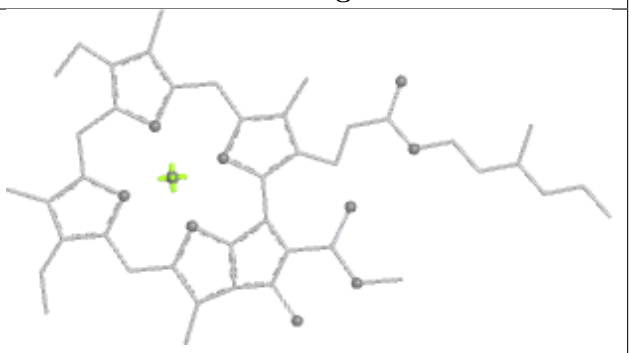
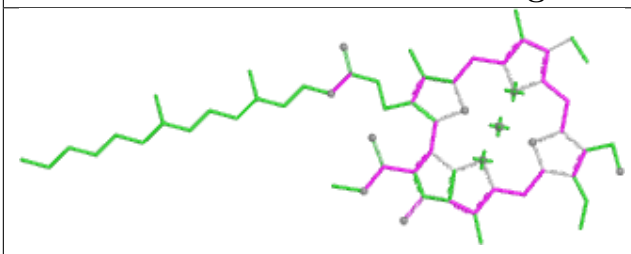


Rings

Ligand CHL 7 306



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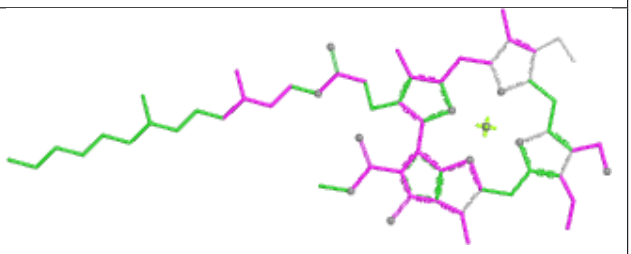

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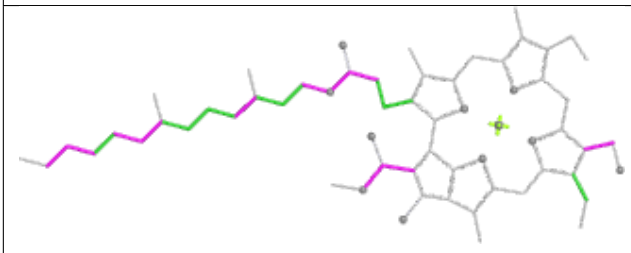

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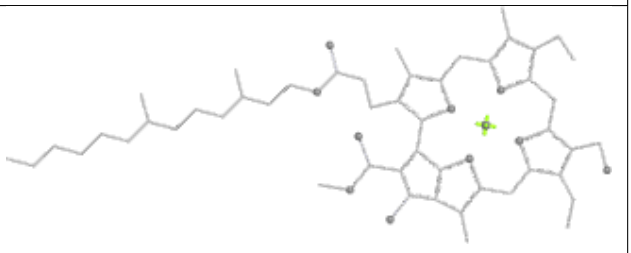
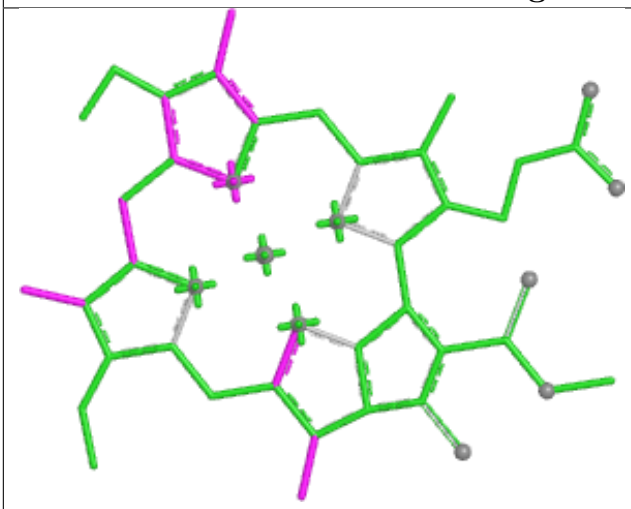


Rings

Ligand CLA 7 303



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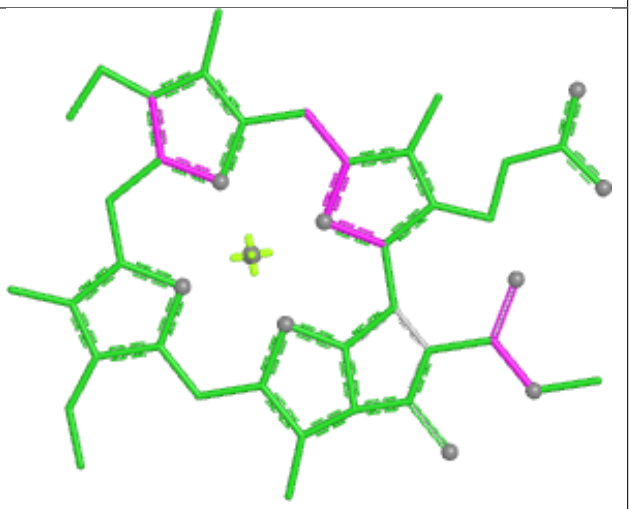

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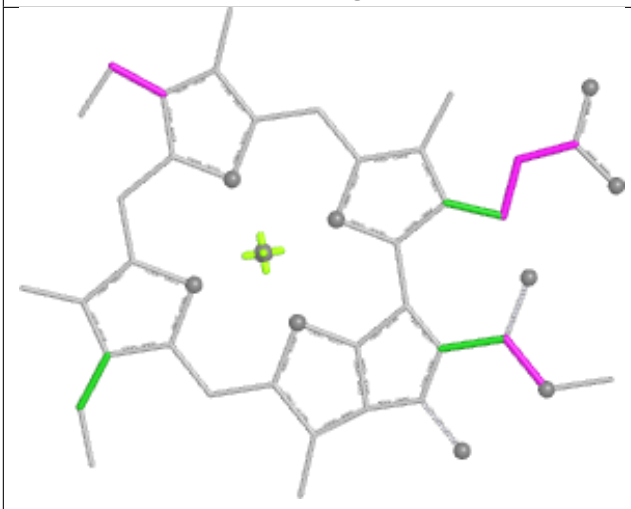
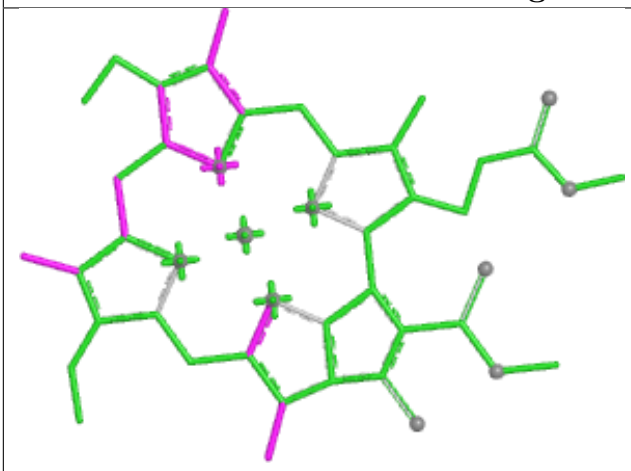


Torsions

Rings

Ligand CLA 8 311



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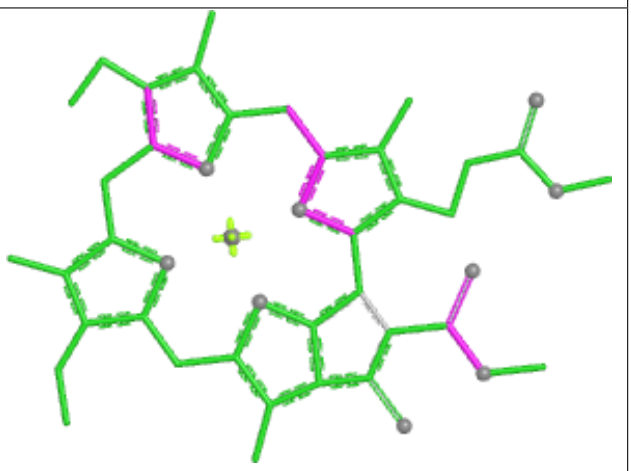

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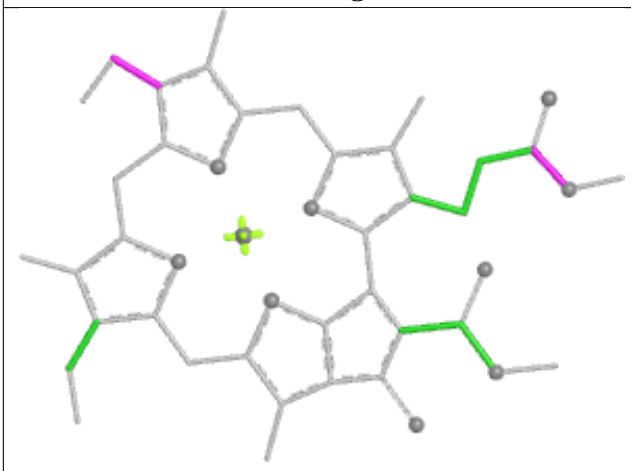

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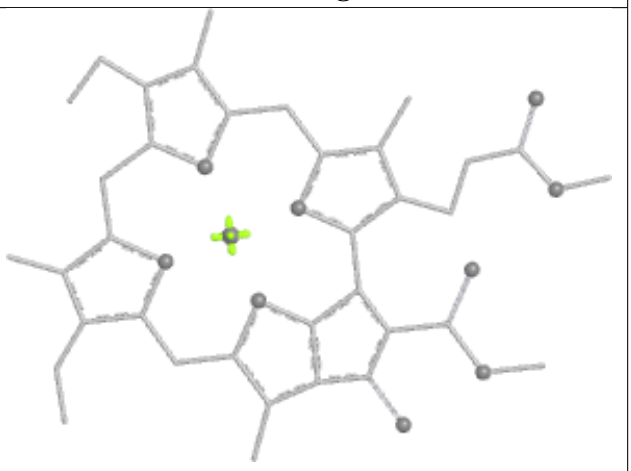
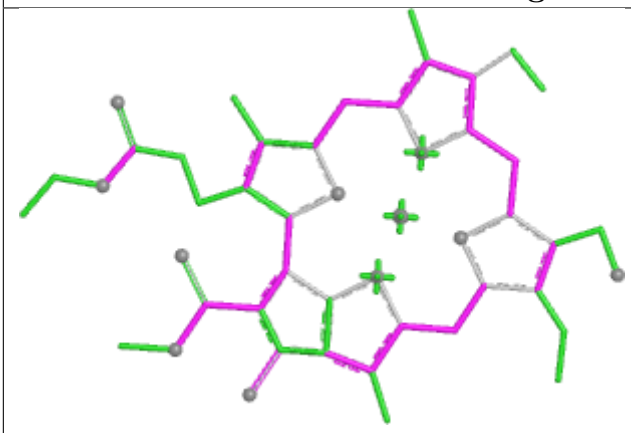


Rings

Ligand CHL 7 305



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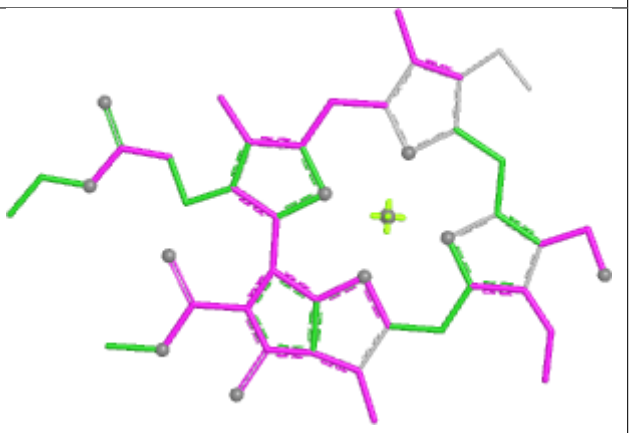

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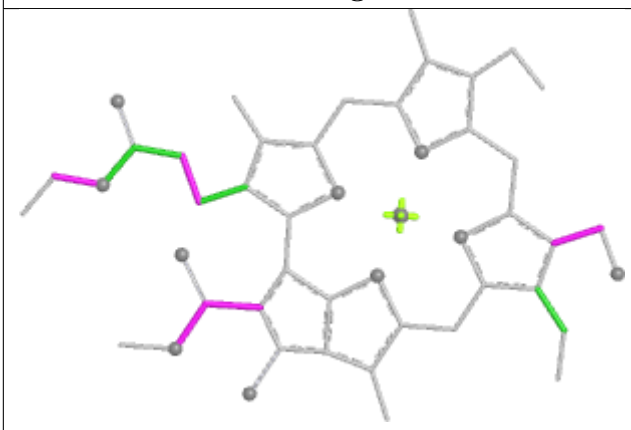
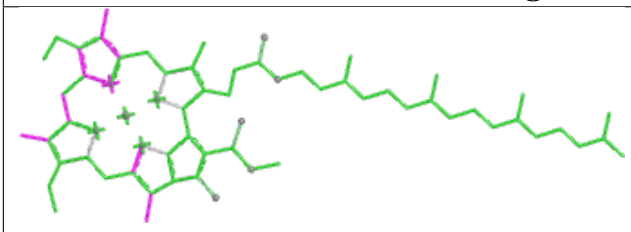


Torsions

Rings

Ligand CLA B 809



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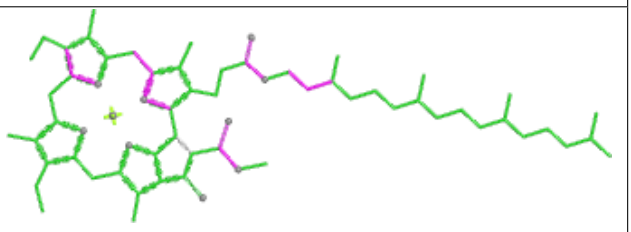

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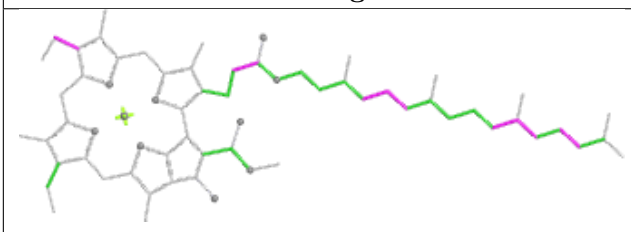

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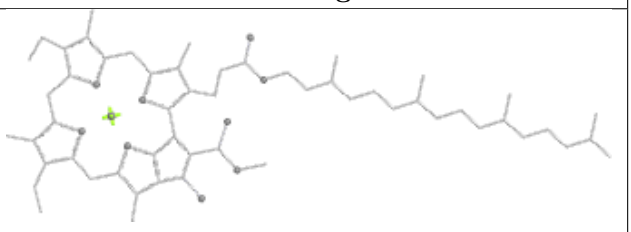
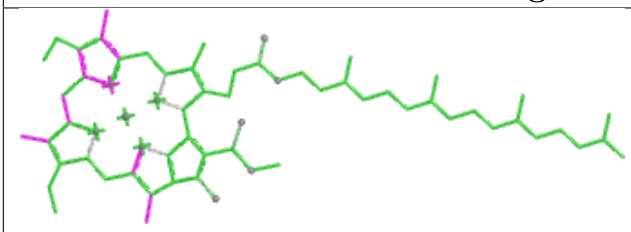


Rings

Ligand CLA 1 311



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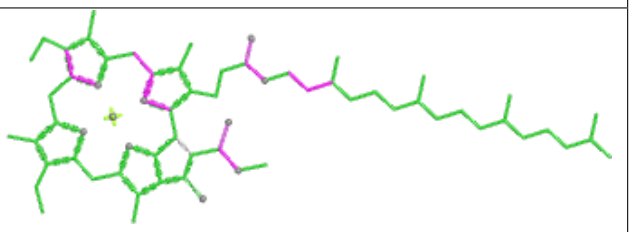
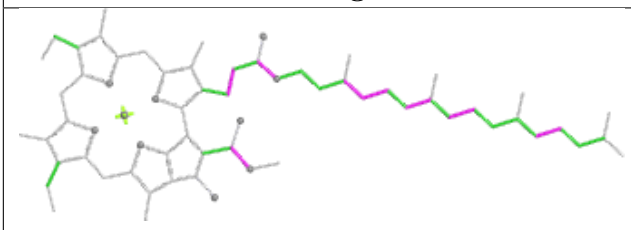
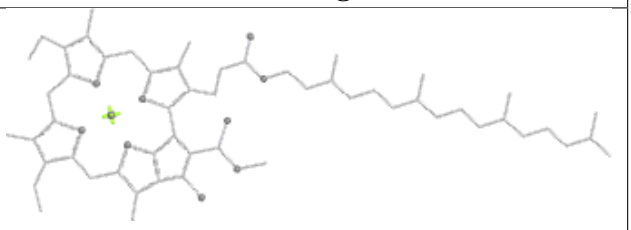


Bond angles

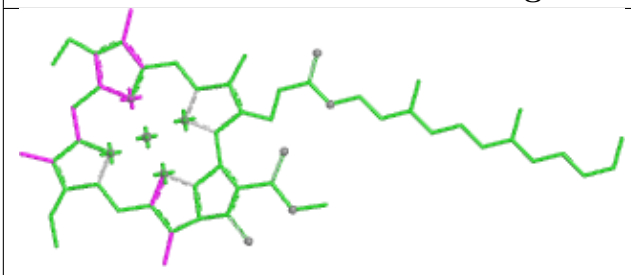


Torsions

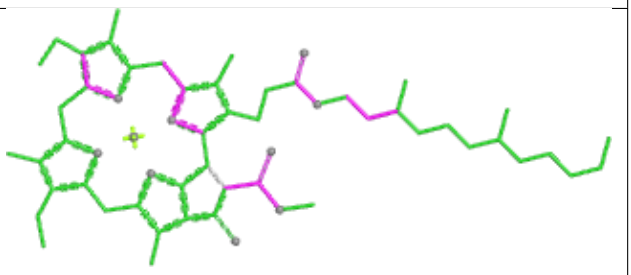


Rings

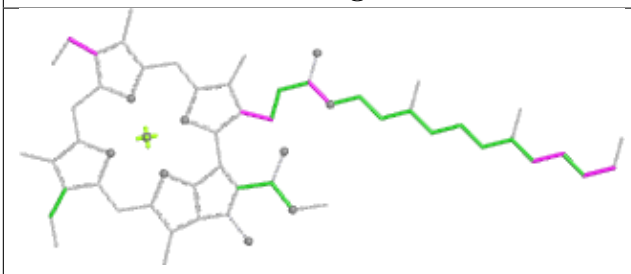
Ligand CLA B 818



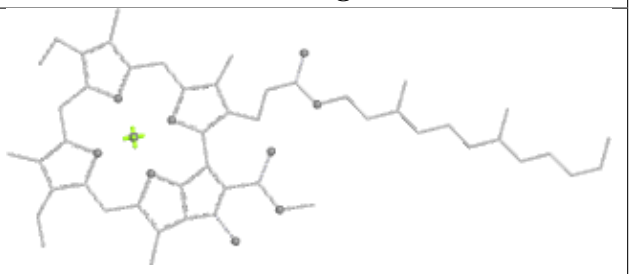
Bond lengths



Bond angles

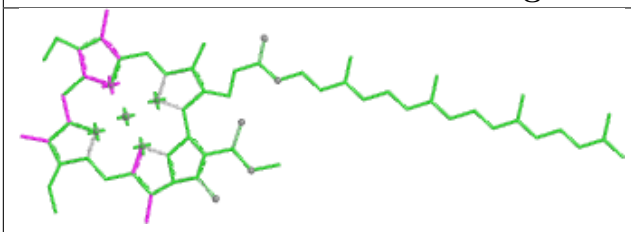


Torsions



Rings

Ligand CLA A 853



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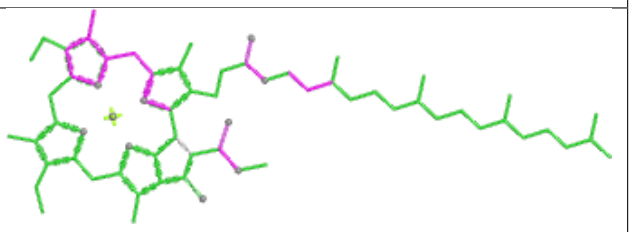

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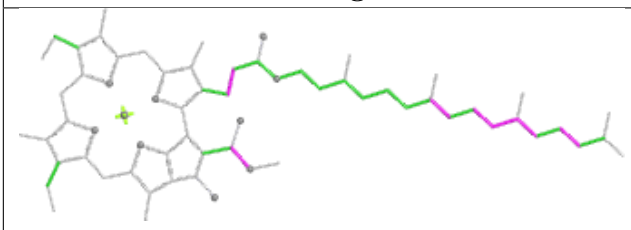

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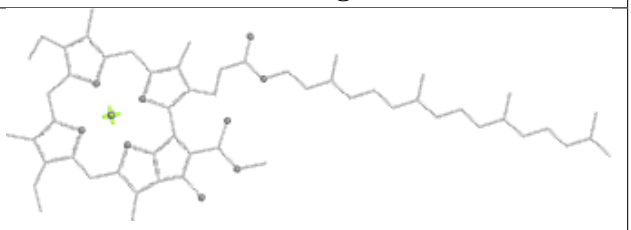
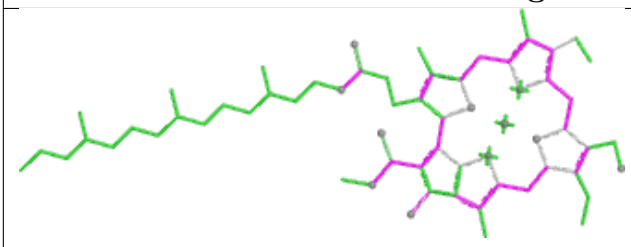


Rings

Ligand CHL 7 301



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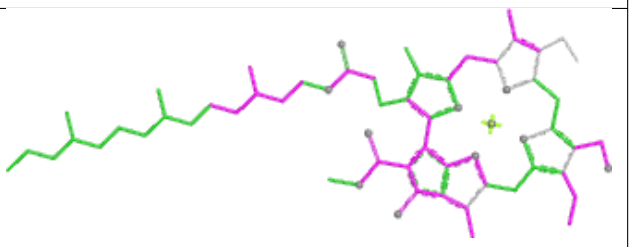
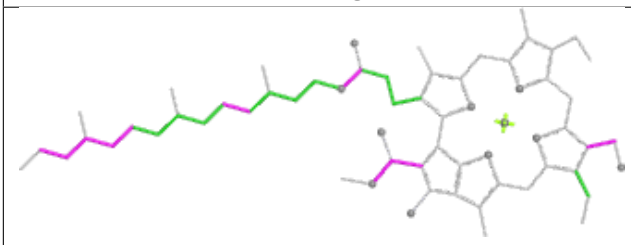


Bond angles



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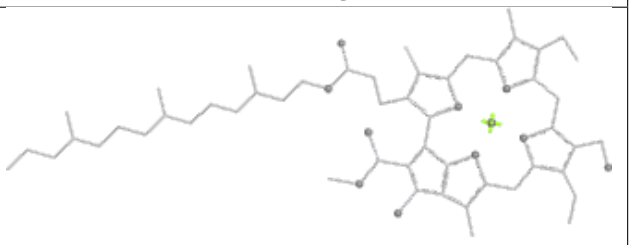
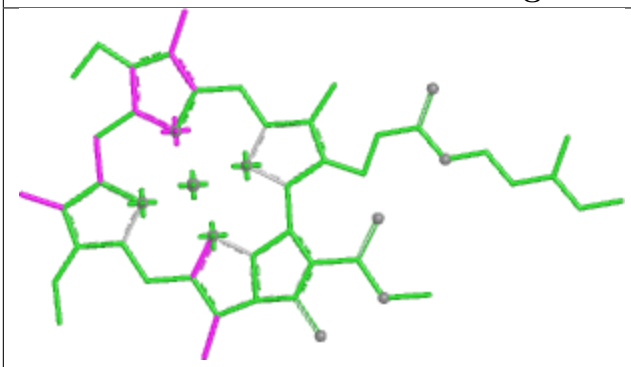


Rings

Ligand CLA A 822



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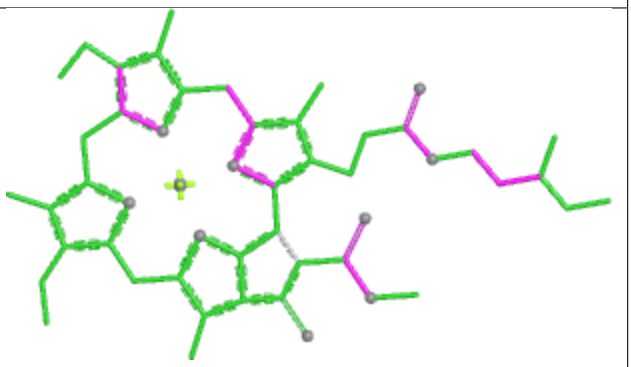
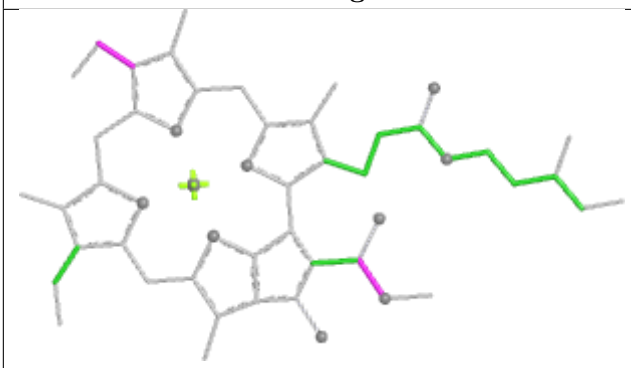


Bond angles



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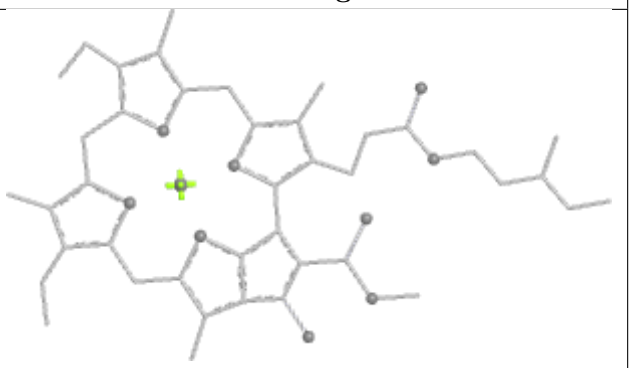
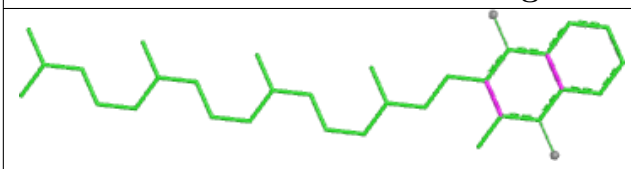


Rings

Ligand PQN A 841



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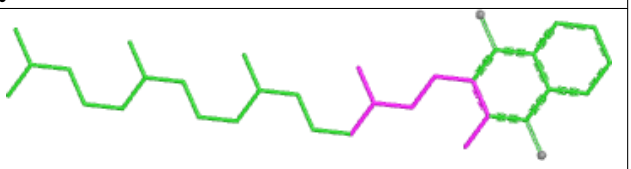
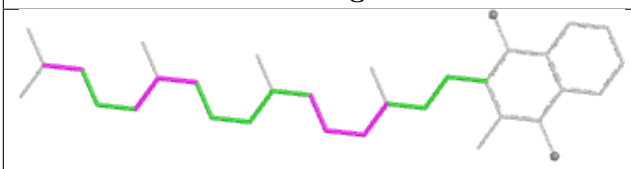


Bond angles



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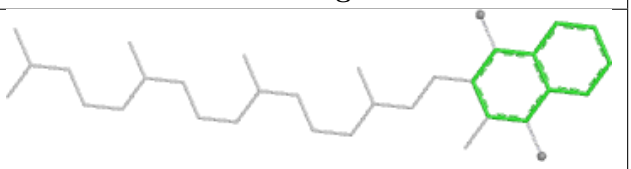
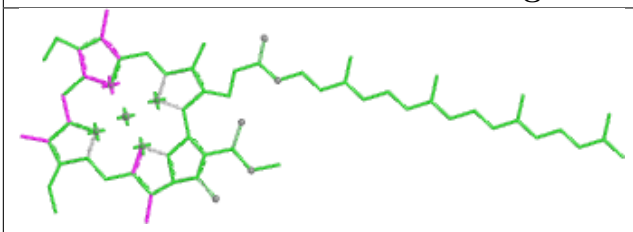


Rings

Ligand CLA A 818



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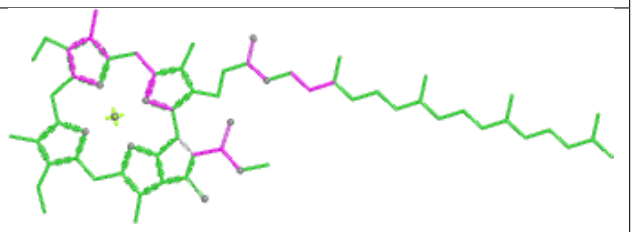

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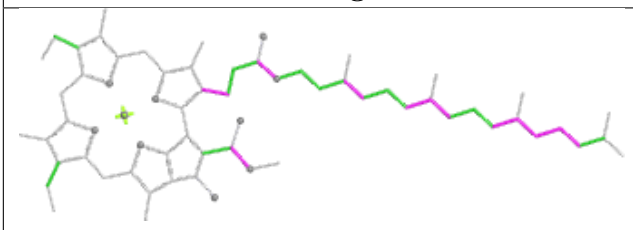

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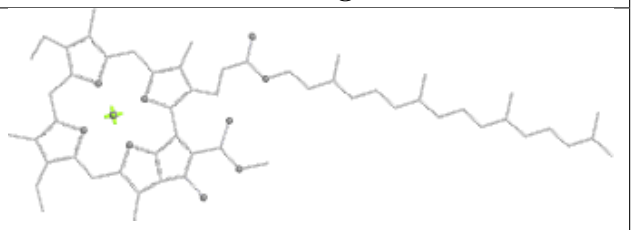
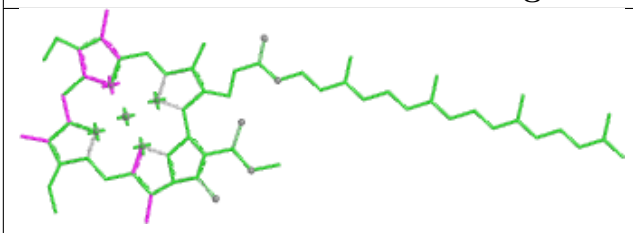


Rings

Ligand CLA A 826



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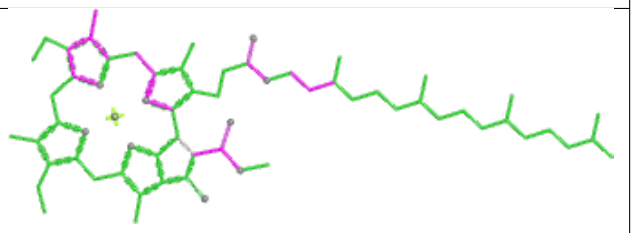

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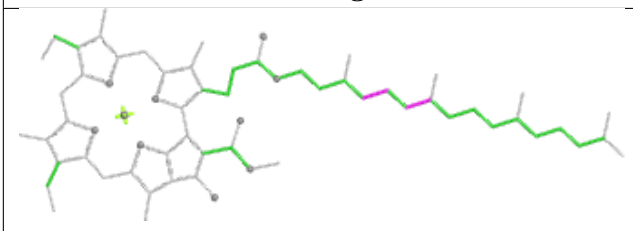

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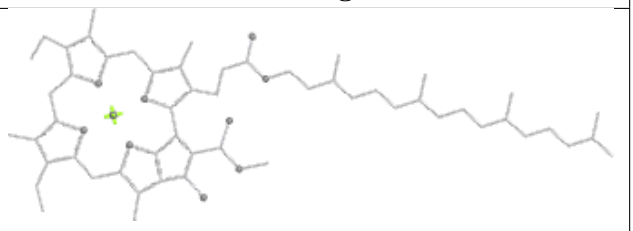
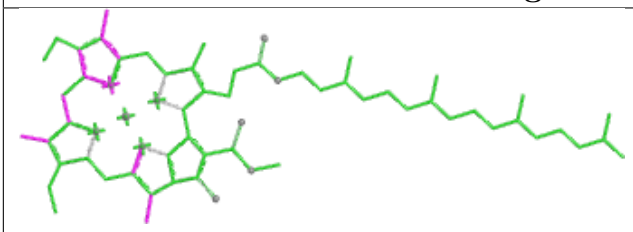


Rings

Ligand CLA B 827



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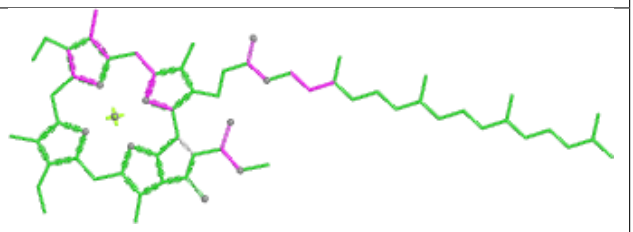
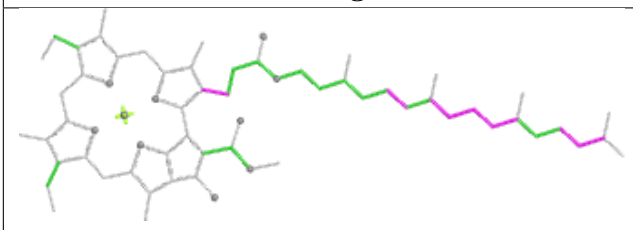


Bond angles



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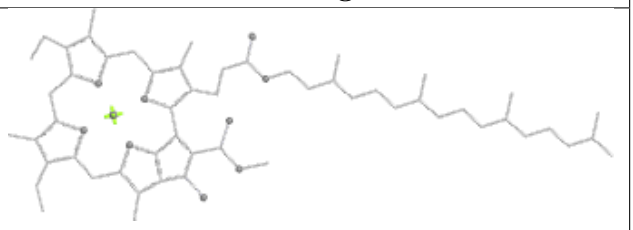
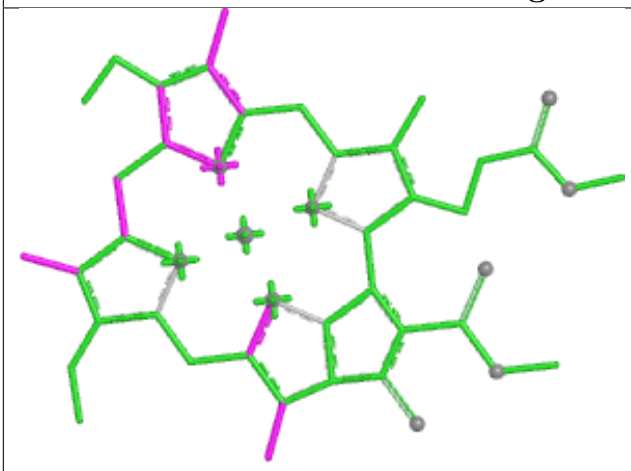


Rings

Ligand CLA 1 313



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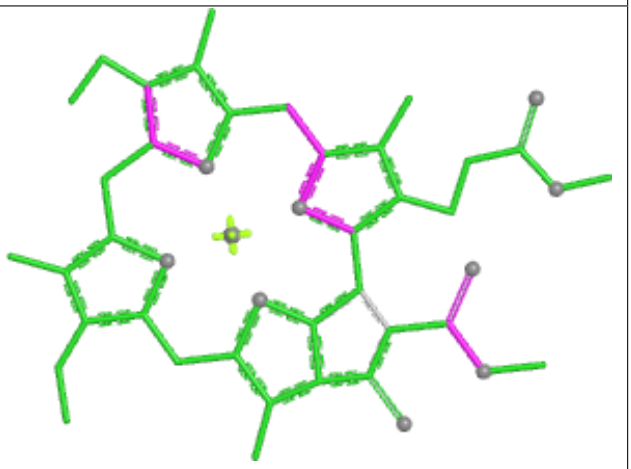

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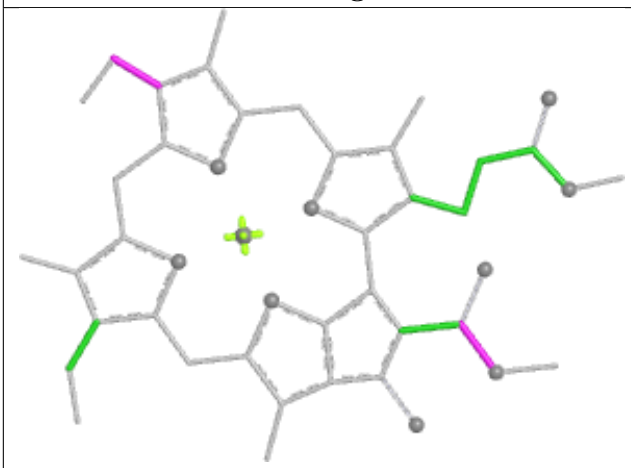

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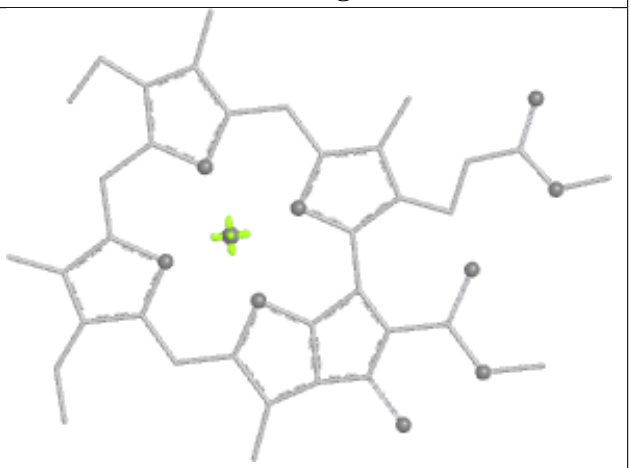
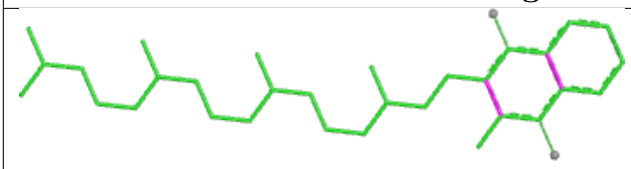


Rings

Ligand PQN B 842



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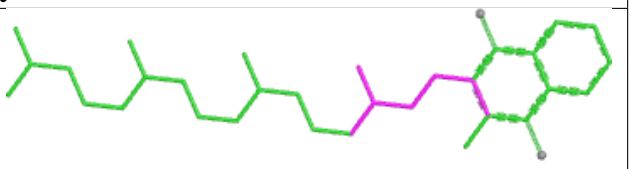
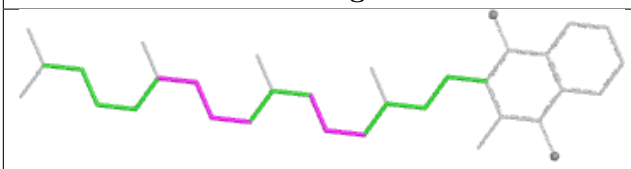


Bond angles



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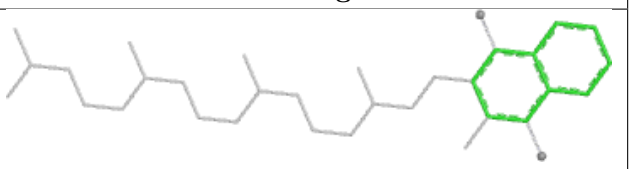
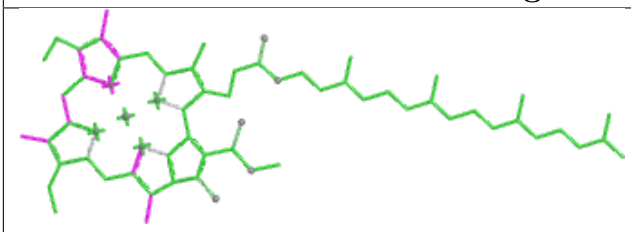


Rings

Ligand CLA A 825



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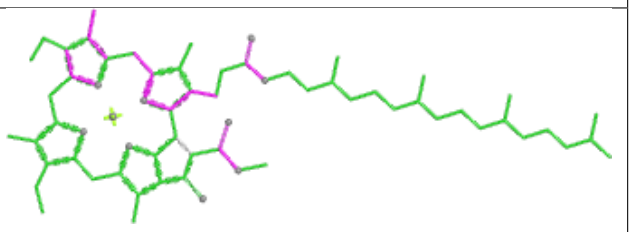
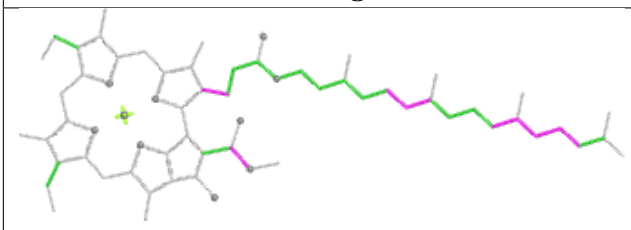


Bond angles



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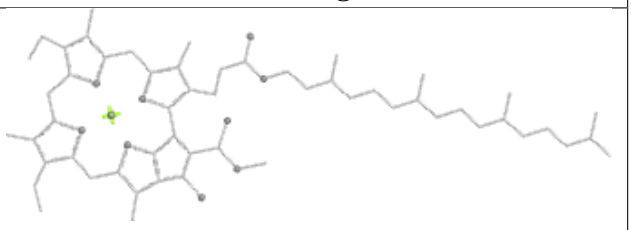
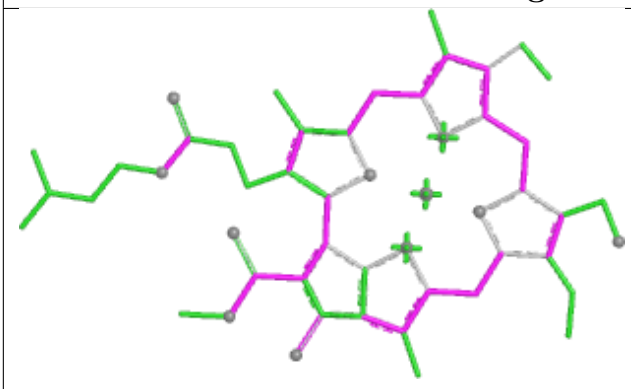


Rings

Ligand CHL 2 312



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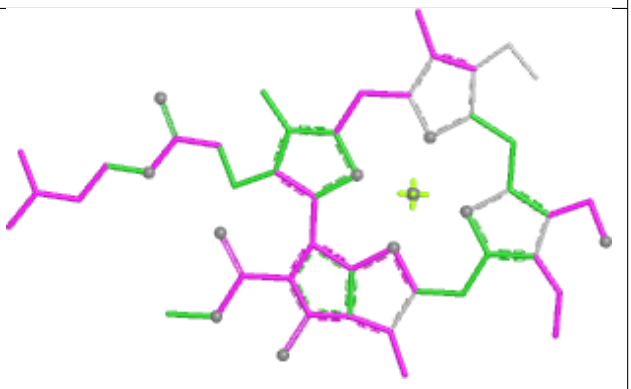
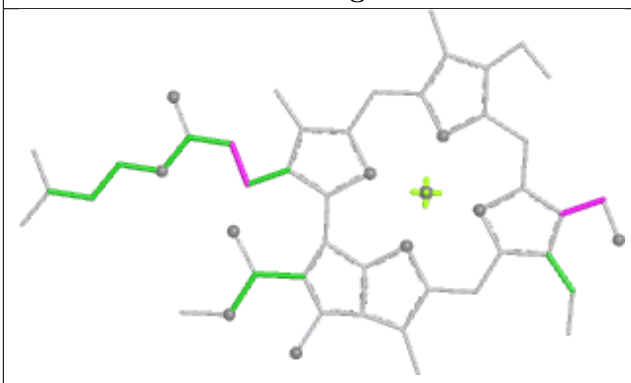


Bond angles



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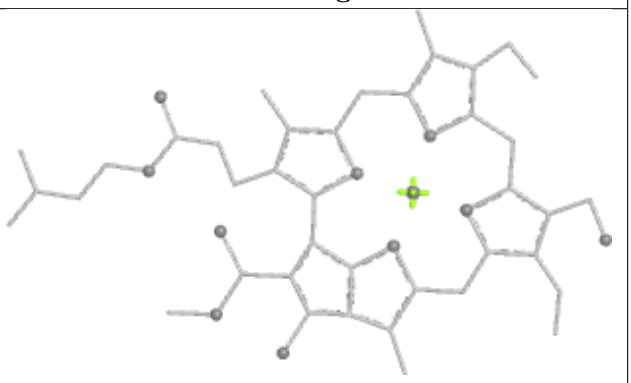
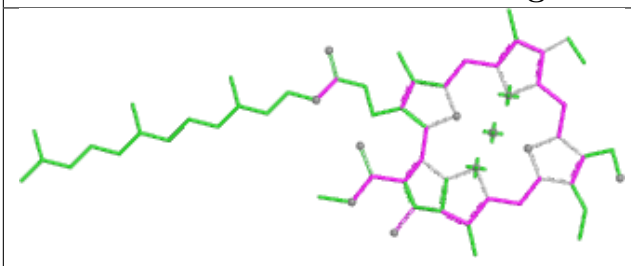
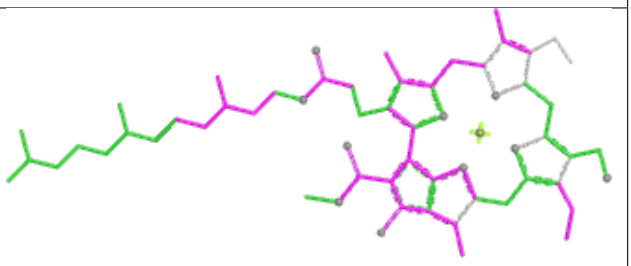
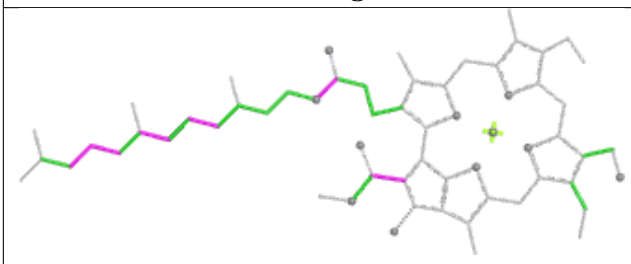
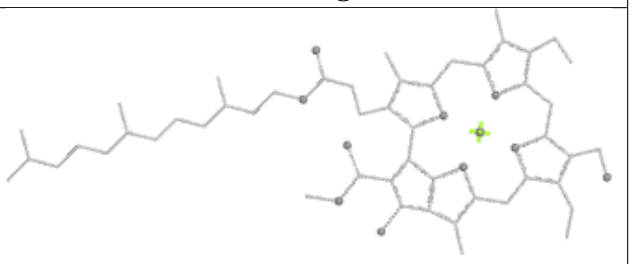
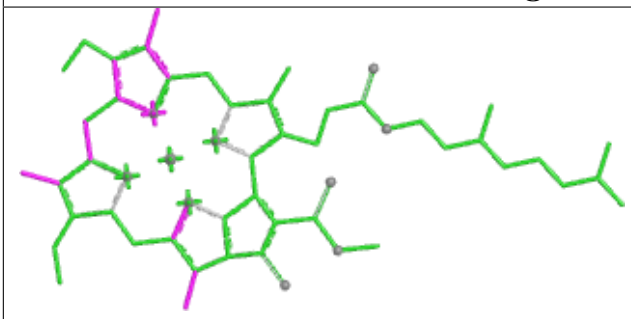
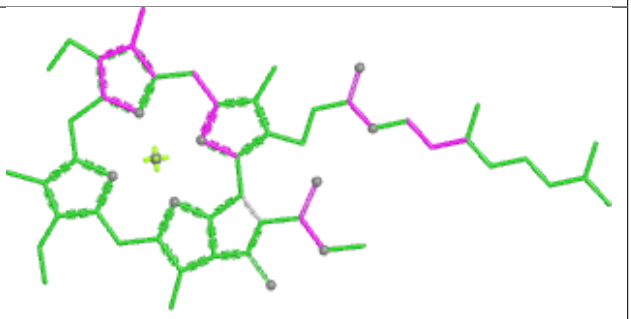
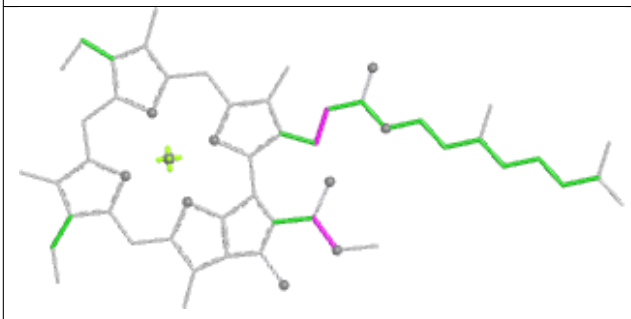
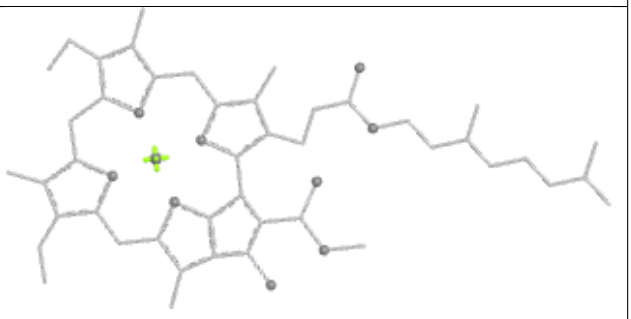
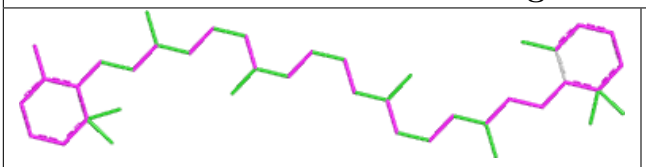


Rings

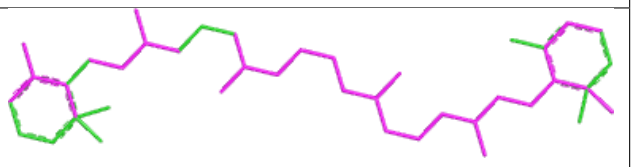
Ligand CHL 3 301	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA B 815	
 Bond lengths	 Bond angles
 Torsions	 Rings

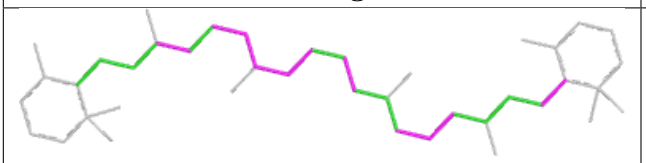
Ligand 8CT B 846



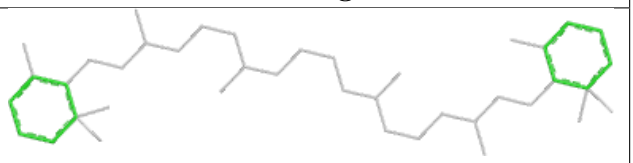
Bond lengths



Bond angles

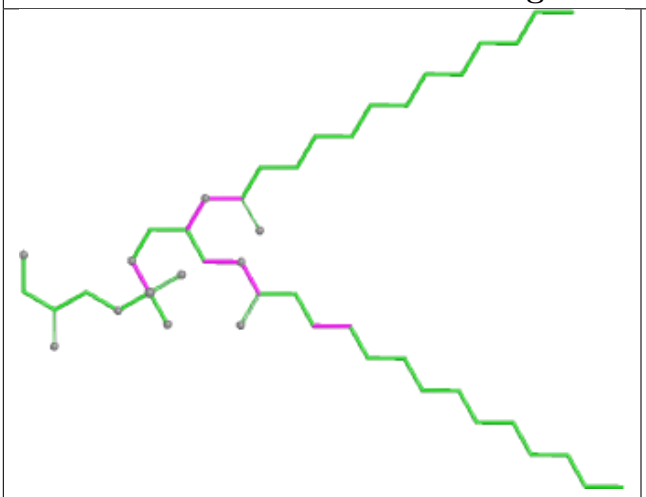


Torsions



Rings

Ligand LHG 8 320



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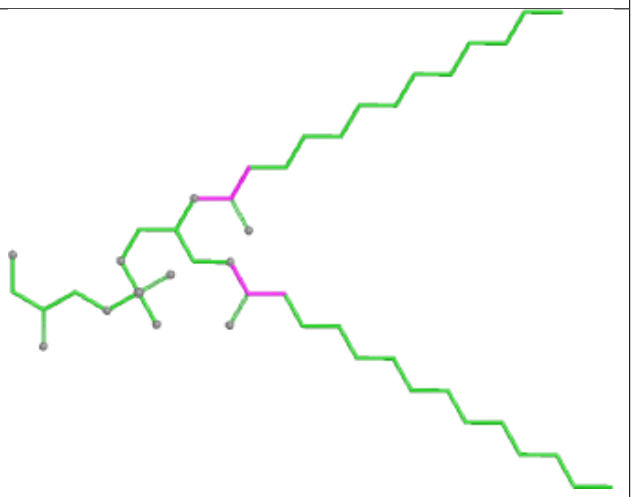

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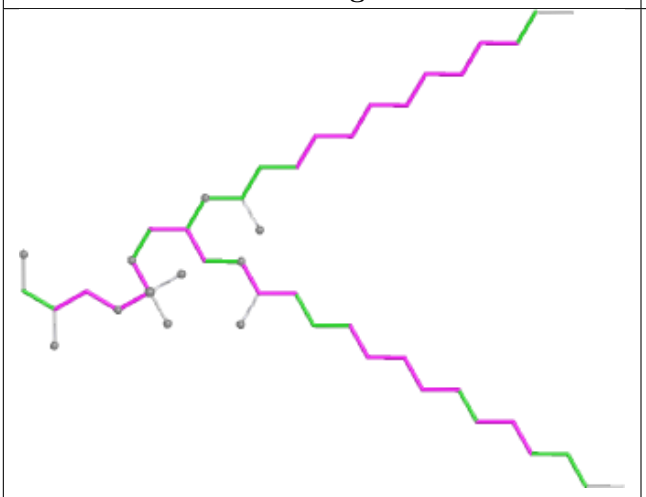

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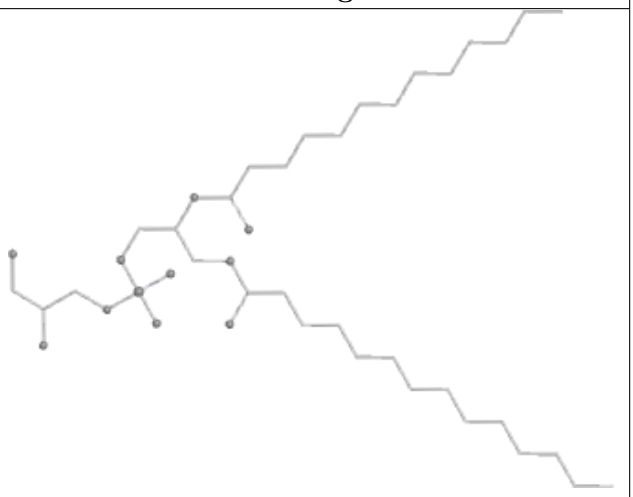
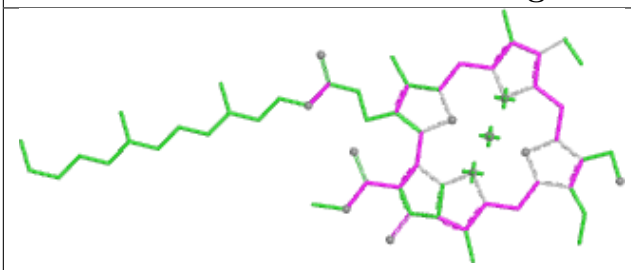


Rings

Ligand CHL 6 308



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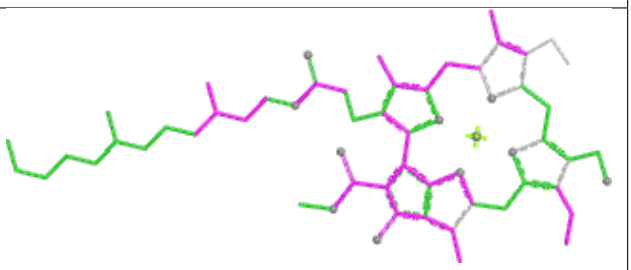

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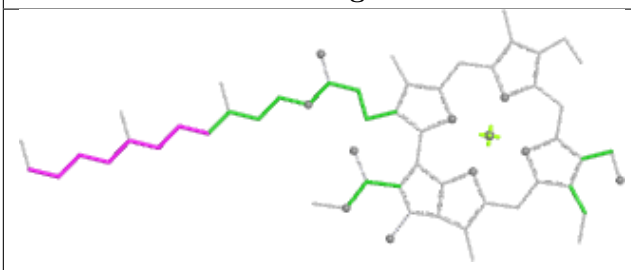

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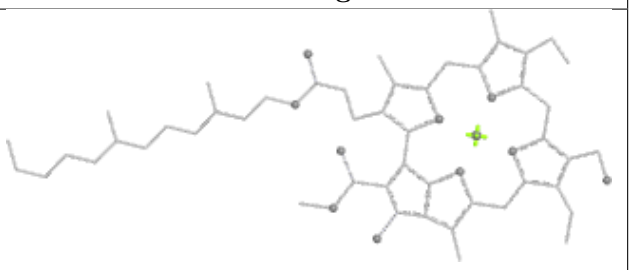
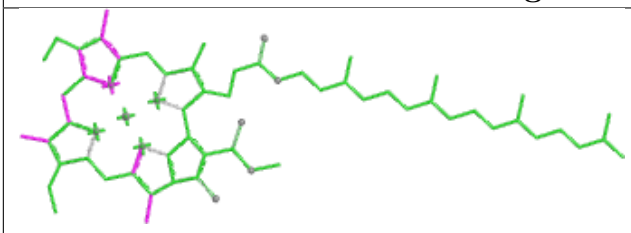


Rings

Ligand CLA B 814



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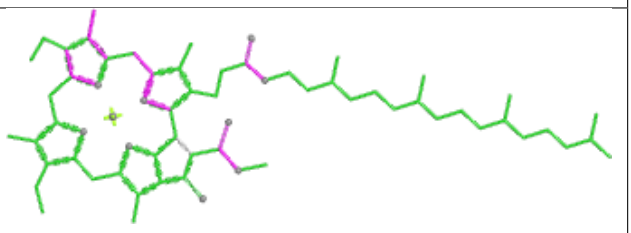

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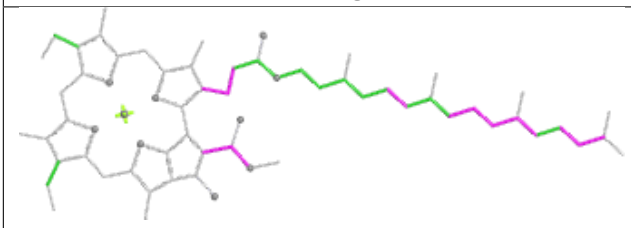

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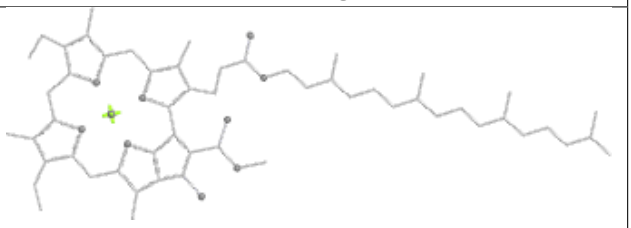
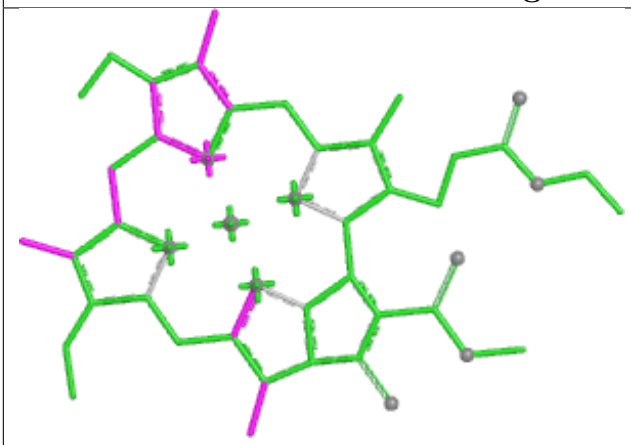


Rings

Ligand CLA H 204



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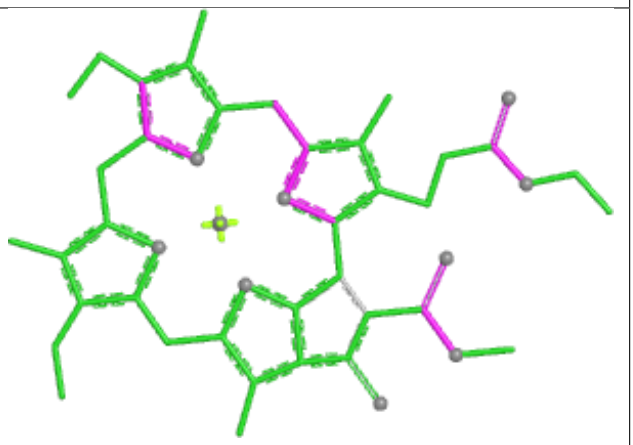

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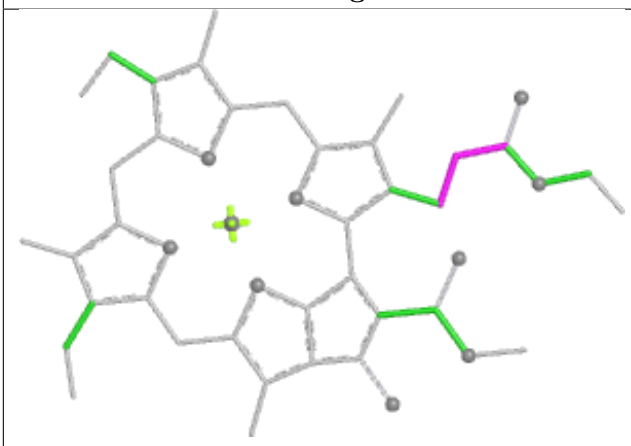

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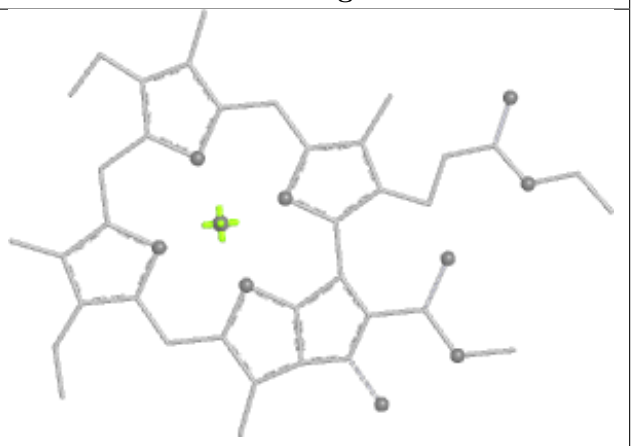
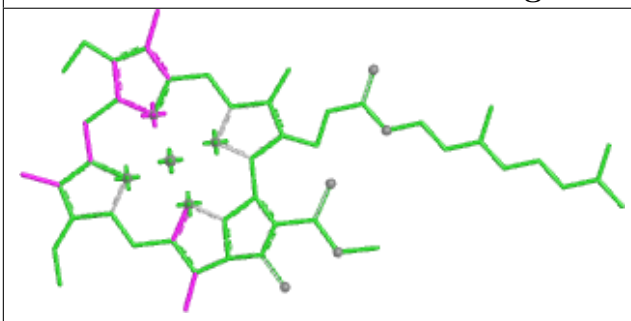


Rings

Ligand CLA B 813



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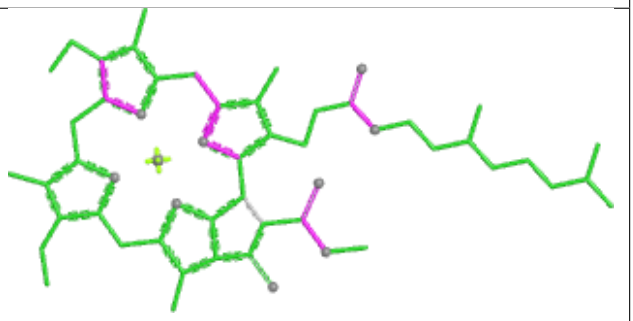

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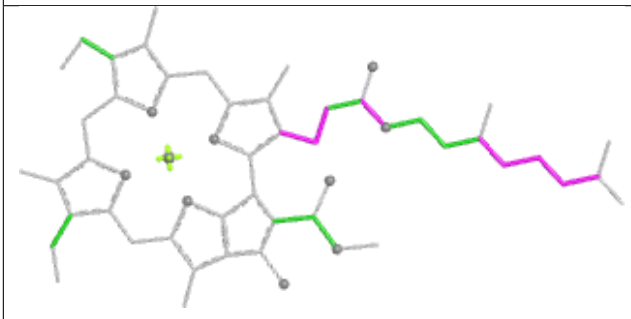

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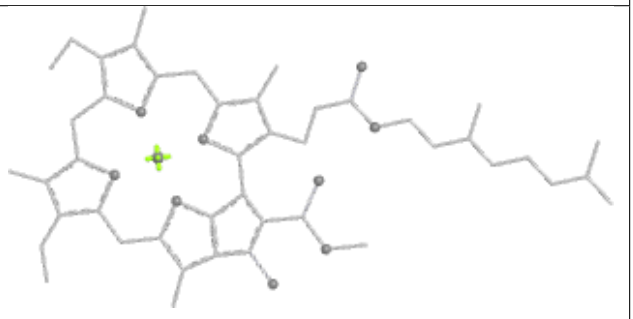
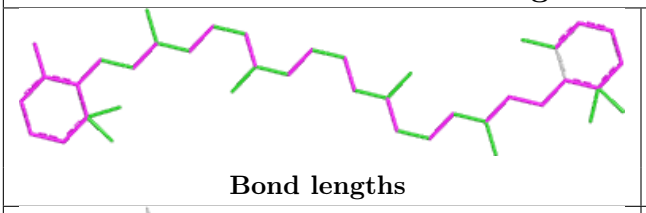


Rings

Ligand 8CT 2 314



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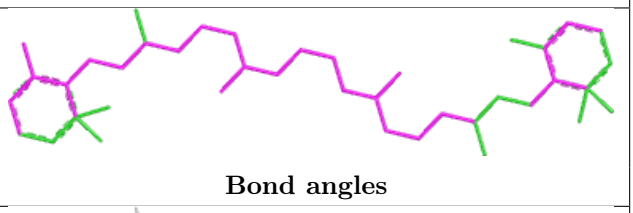

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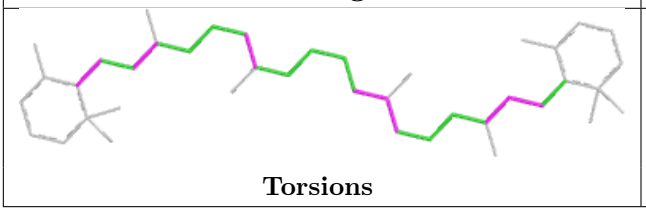

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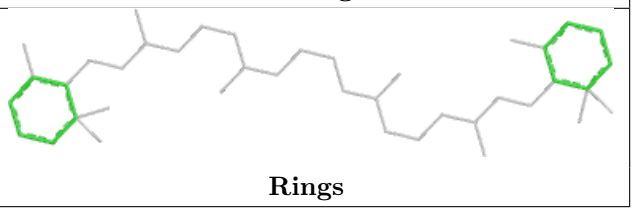
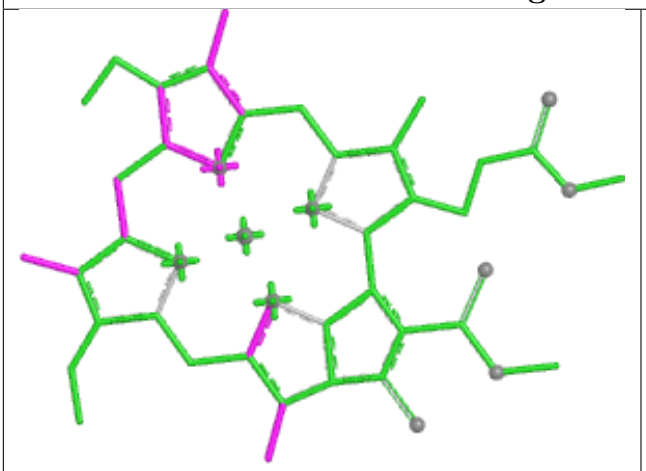


Rings

Ligand CLA 8 304



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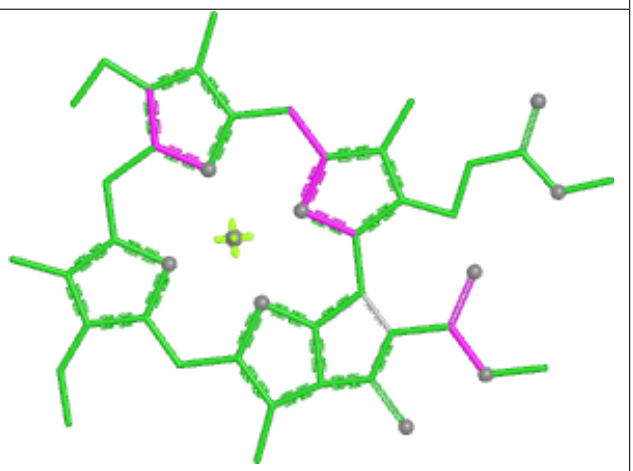

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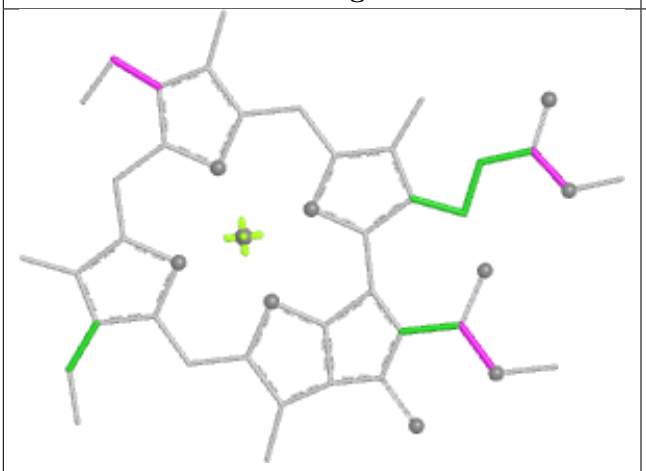

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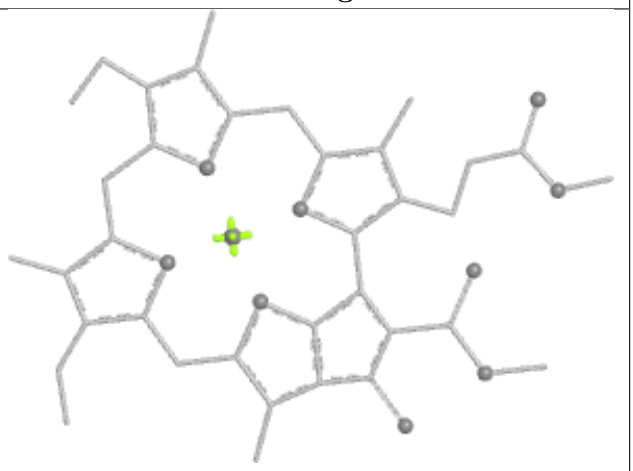
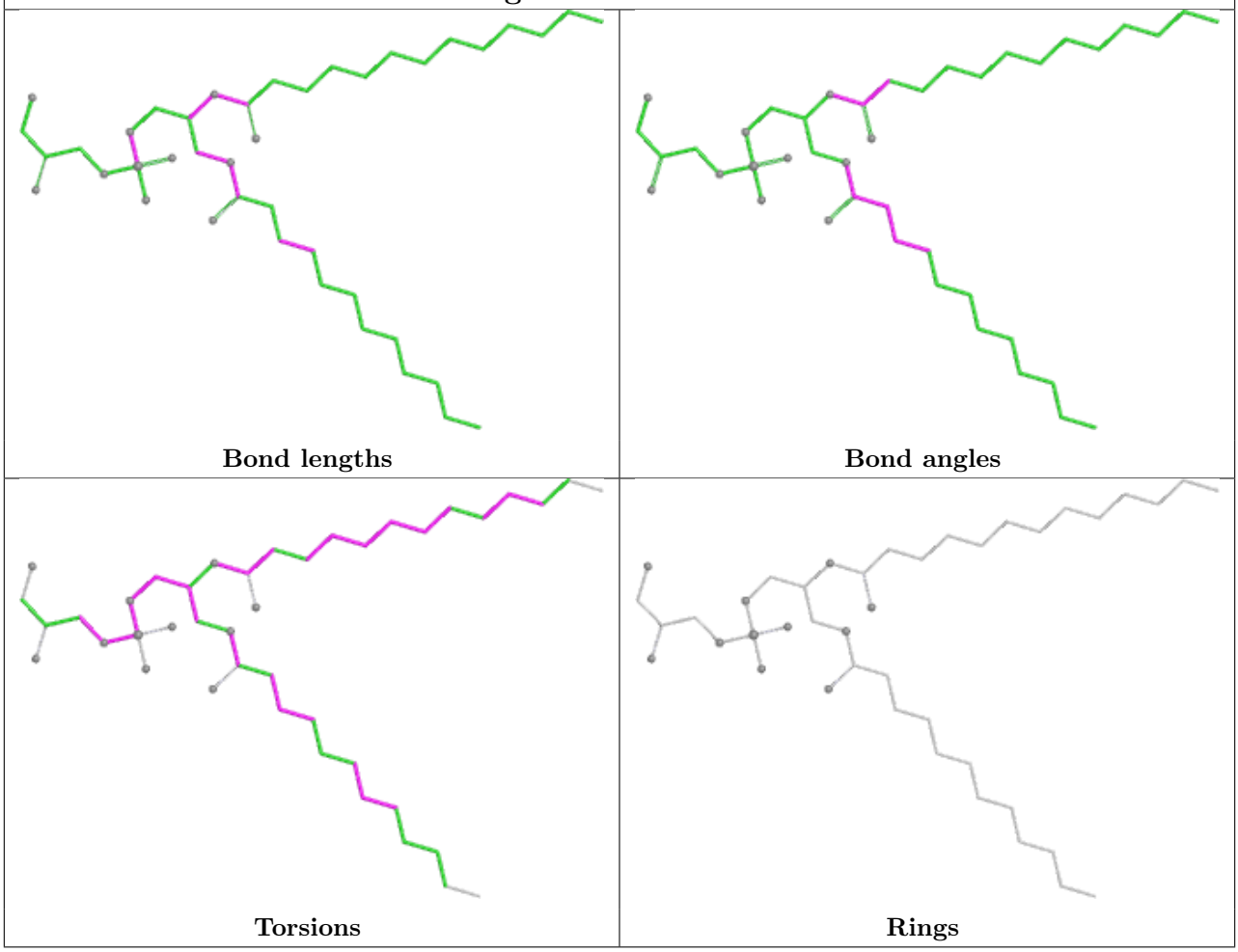


Rings

Ligand LHG A 850



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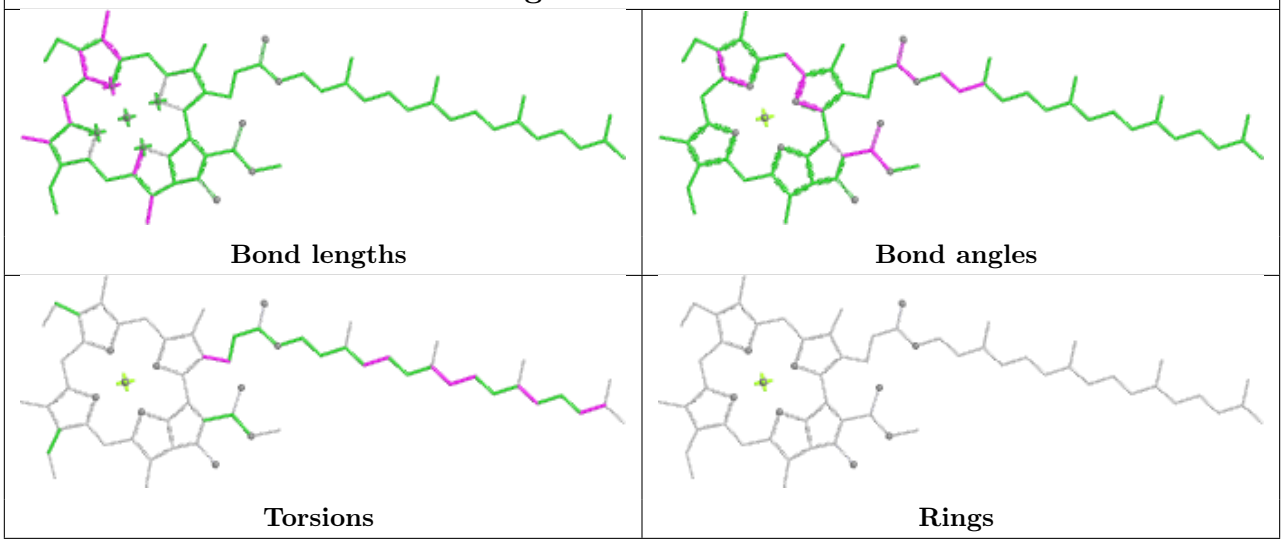
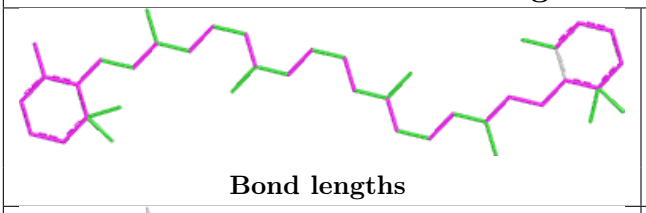


Ligand 8CT 0 314



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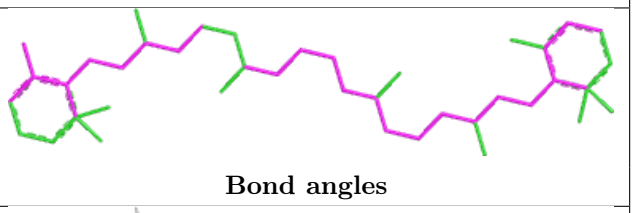

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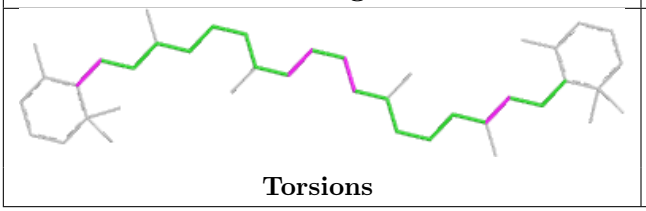

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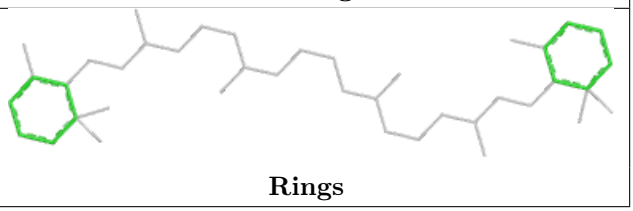
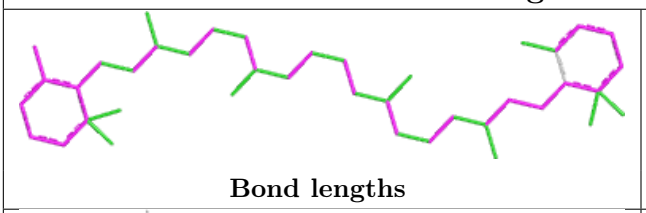


Rings

Ligand 8CT A 845



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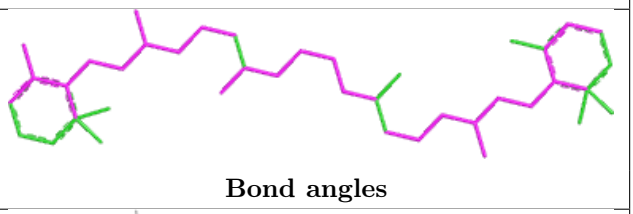

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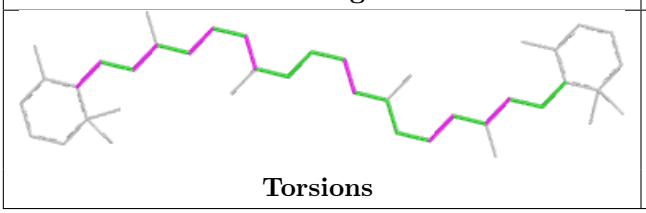

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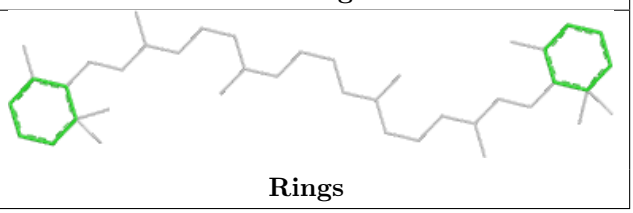
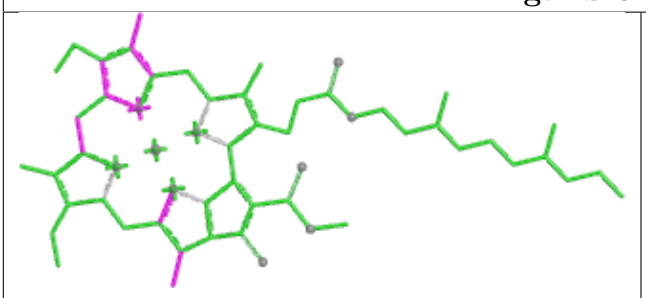


Rings

Ligand CLA A 834



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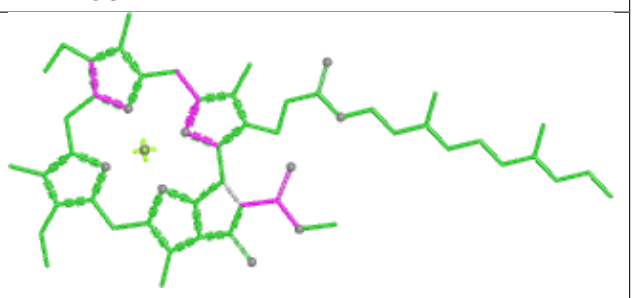

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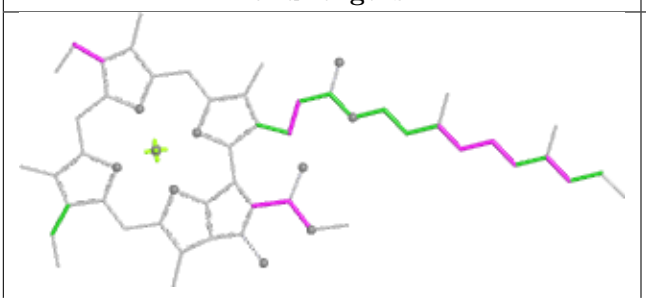

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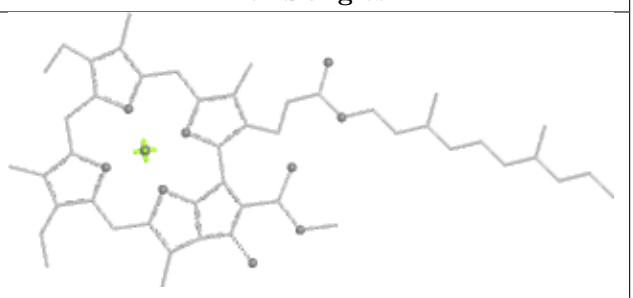
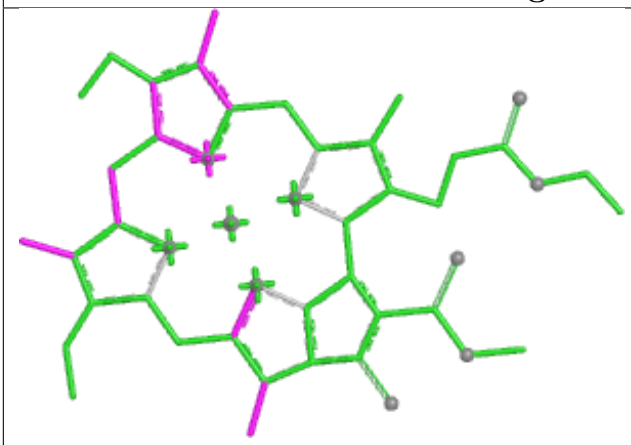
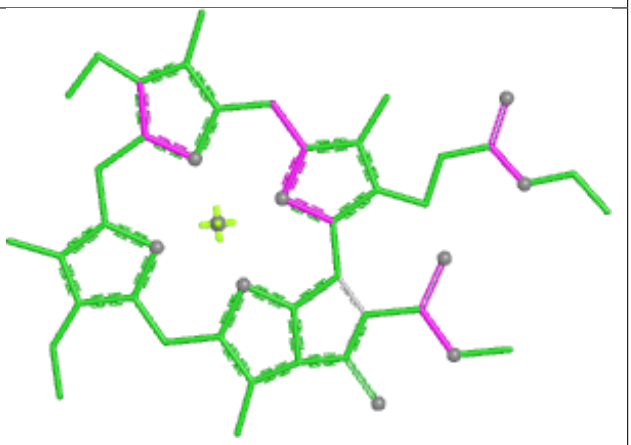


Rings

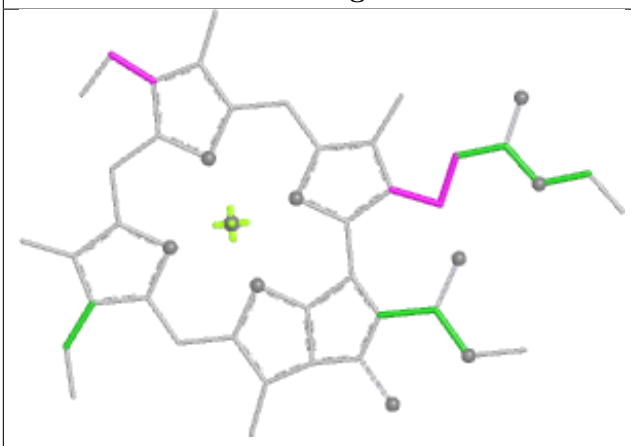
Ligand CLA 3 306



Bond lengths



Bond angles



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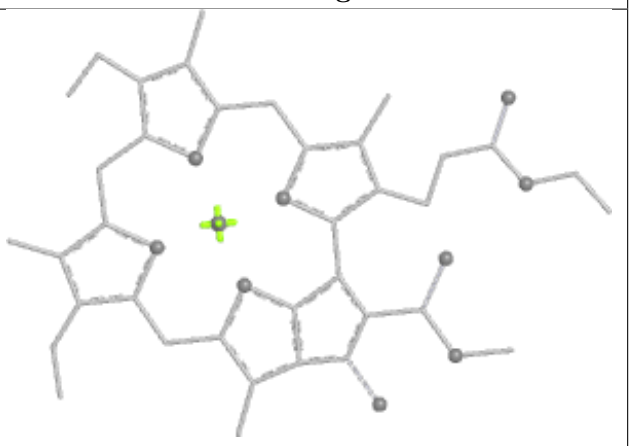
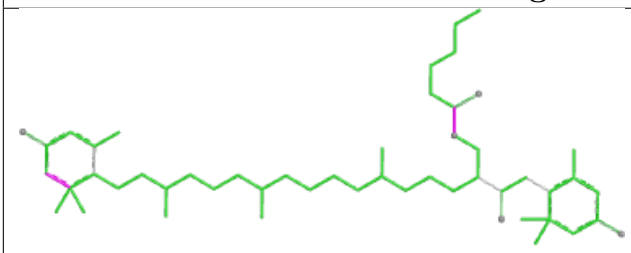


Rings

Ligand 0UR 4 317



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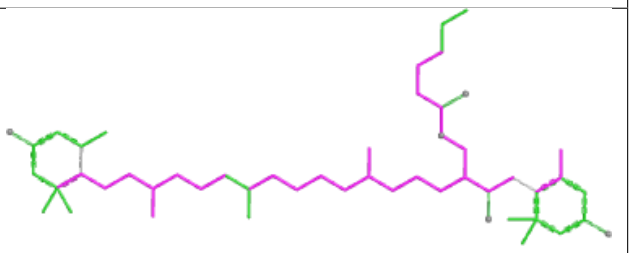
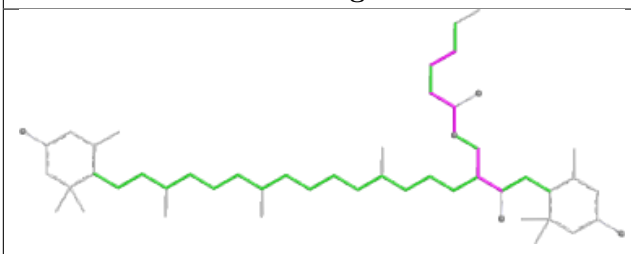
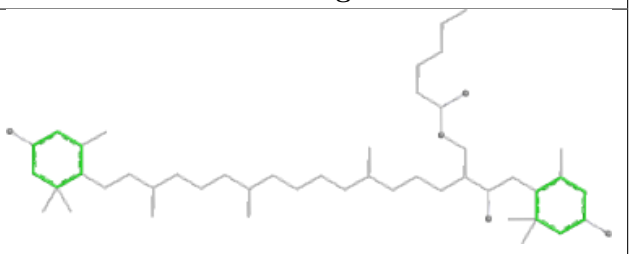


Bond angles

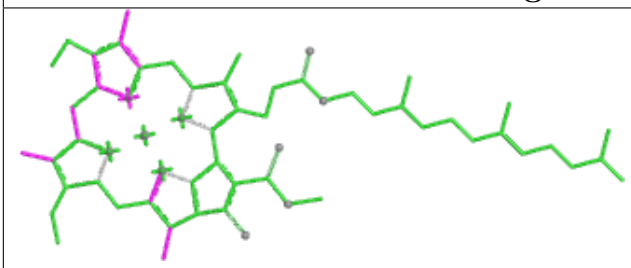


Torsions



Rings

Ligand CLA B 817



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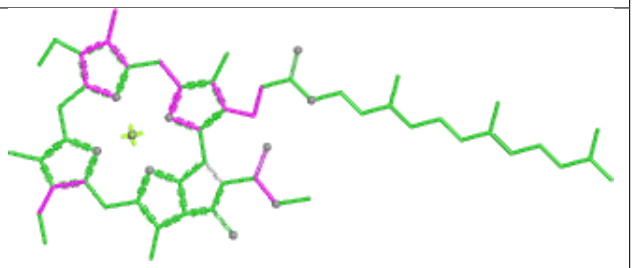
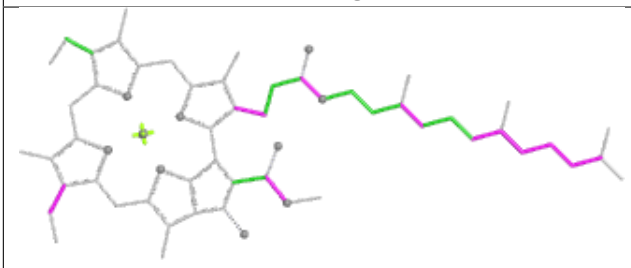


Bond angles



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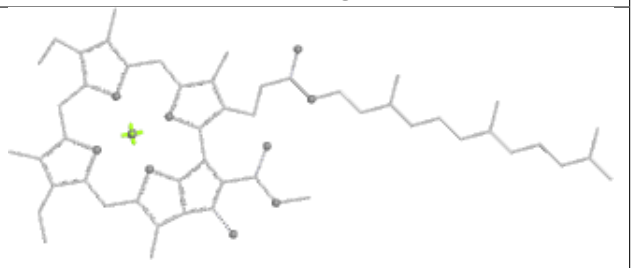
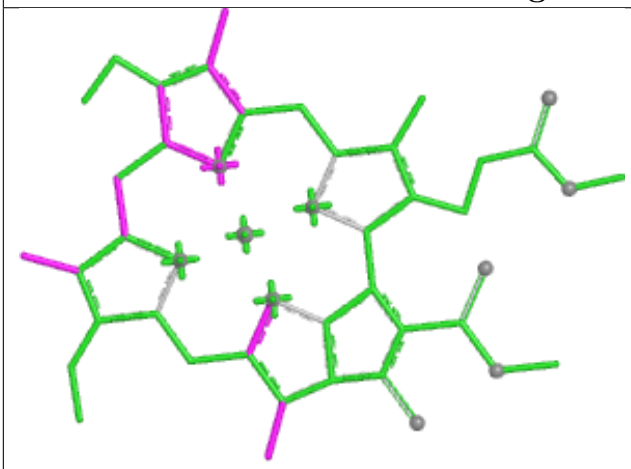


Rings

Ligand CLA 0 319



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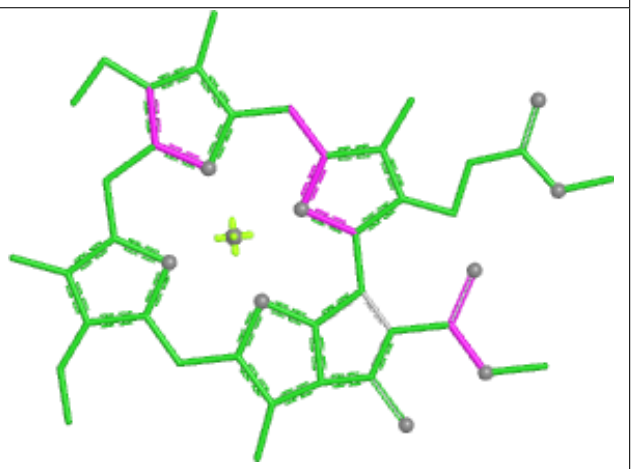
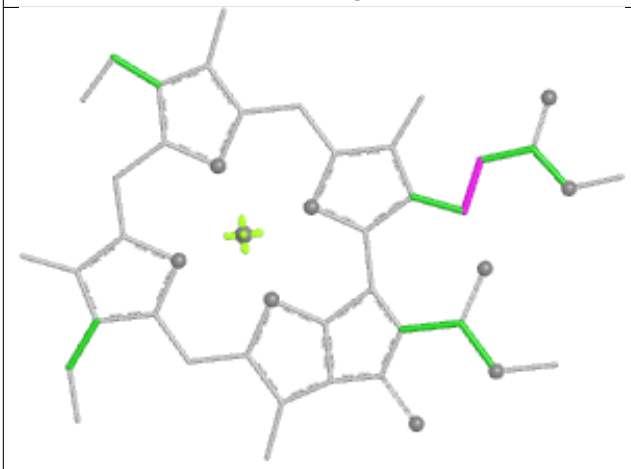
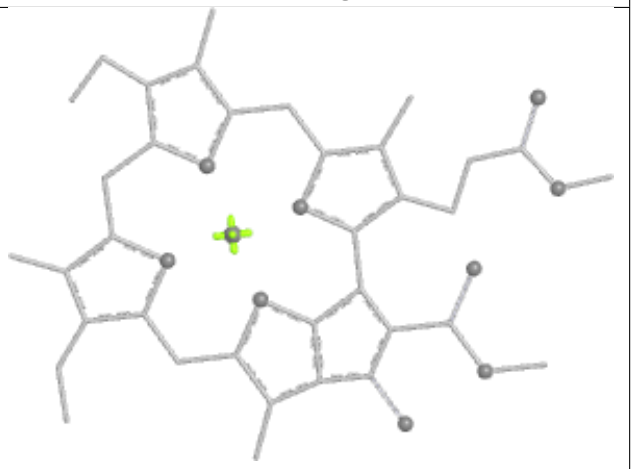


Bond angles

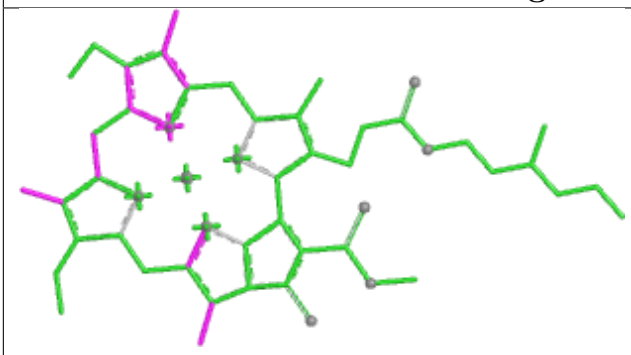


Torsions



Rings

Ligand CLA 3 315



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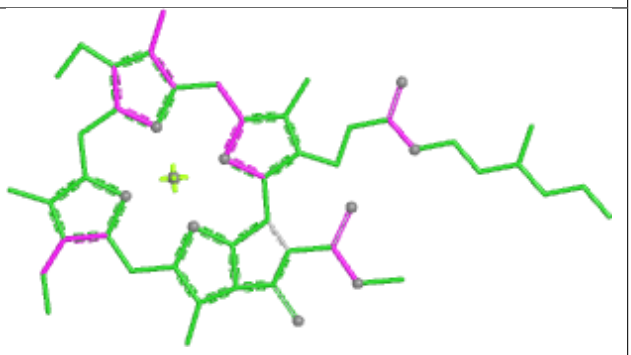
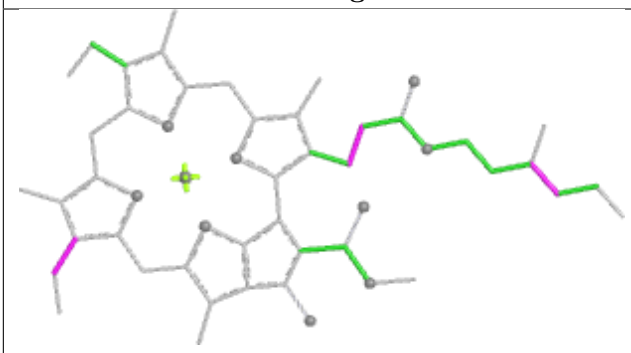


Bond angles



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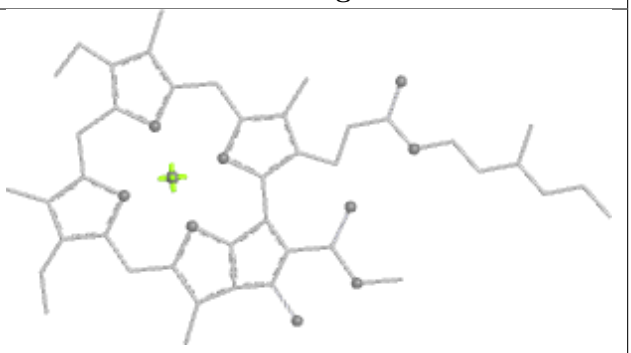
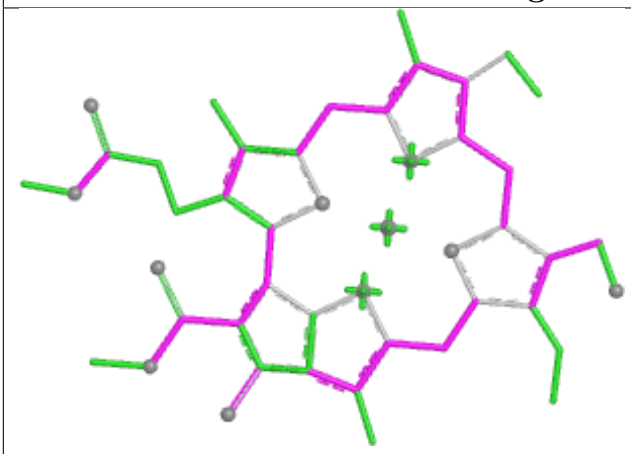


Rings

Ligand CHL 5 306



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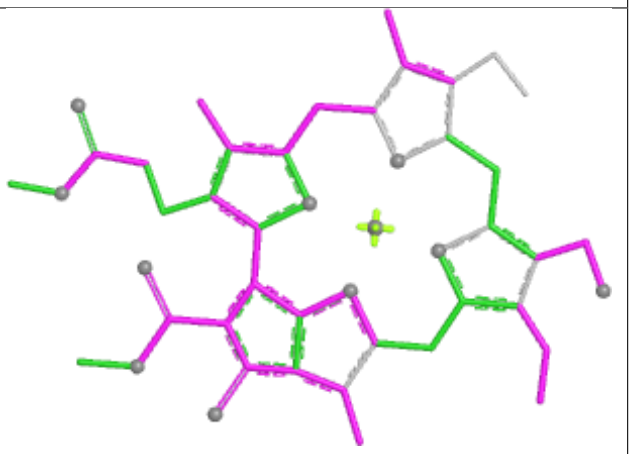
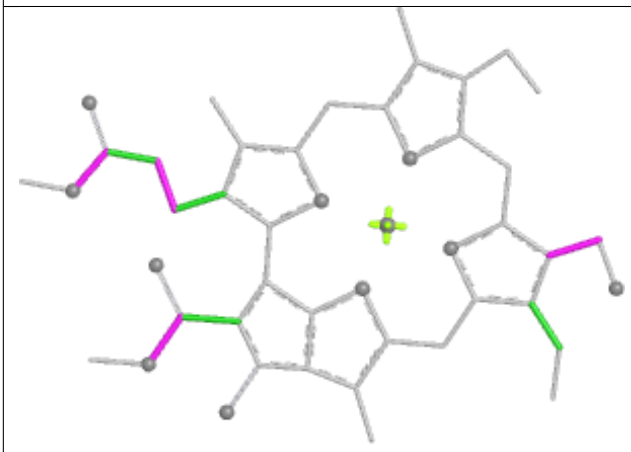


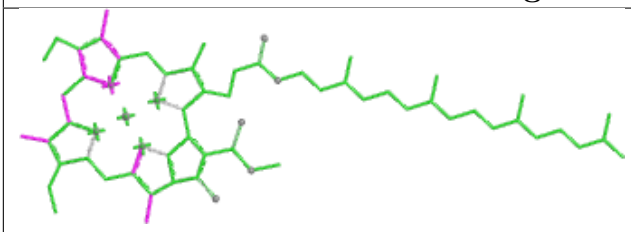
Bond angles



Torsions

Rings

Ligand CLA A 820



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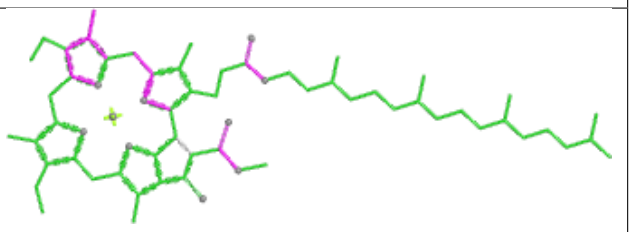
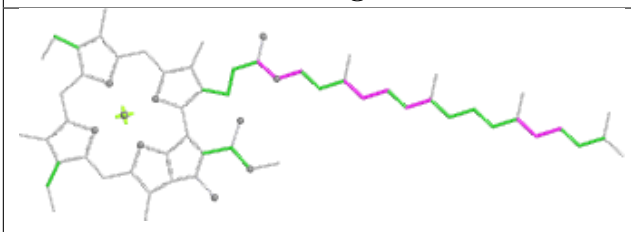


Bond angles



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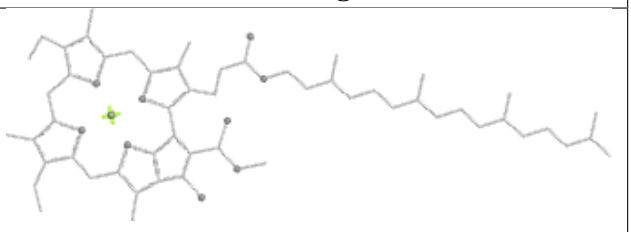
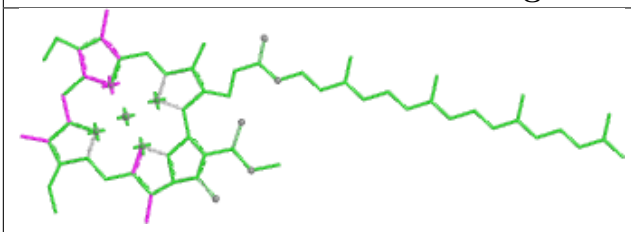


Rings

Ligand CLA A 828



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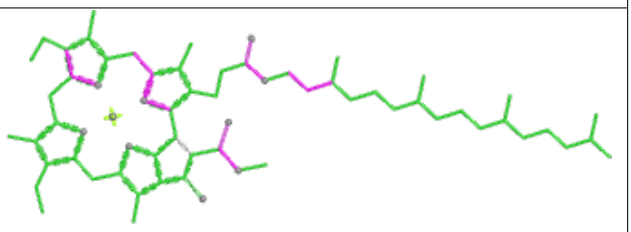
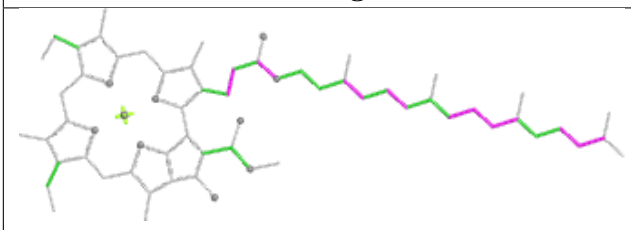


Bond angles



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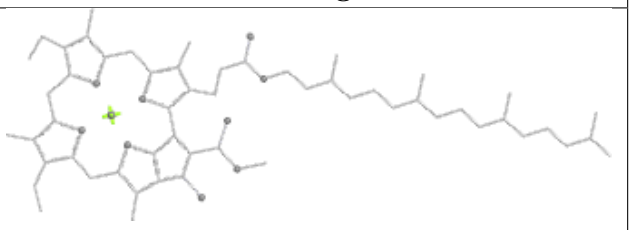
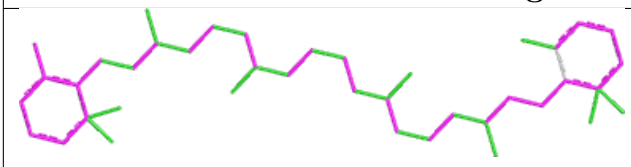


Rings

Ligand 8CT K 105



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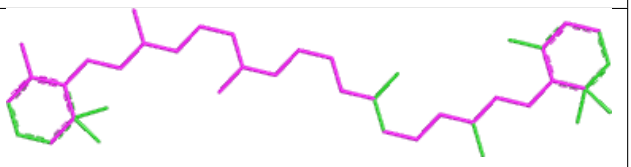

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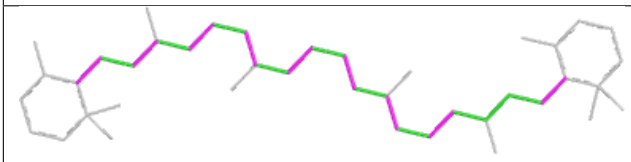

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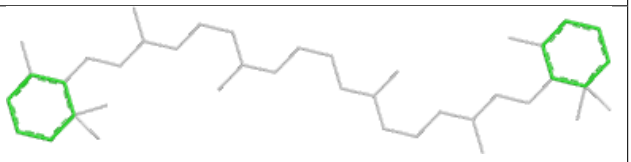
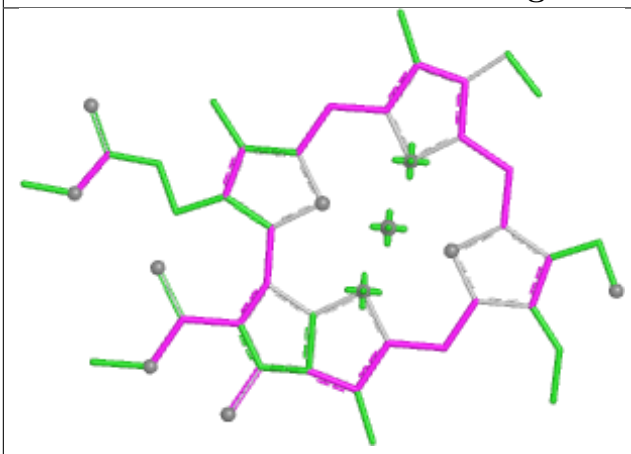


Rings

Ligand CHL 8 309



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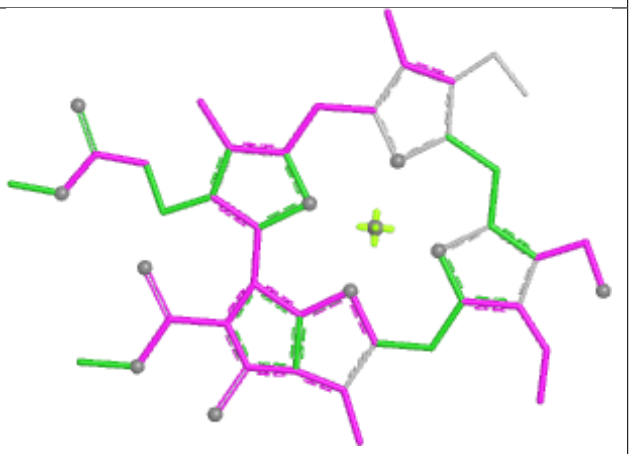
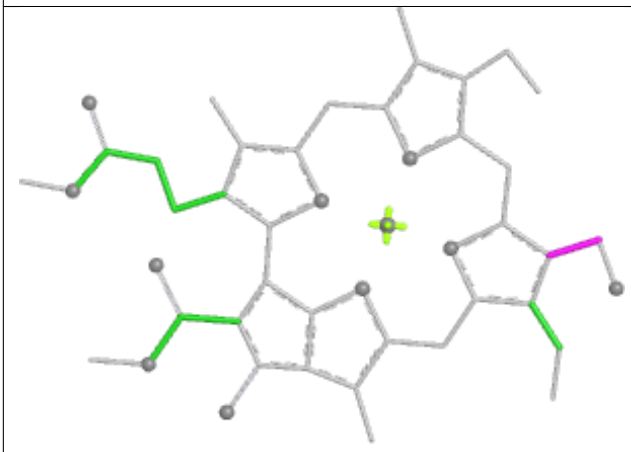


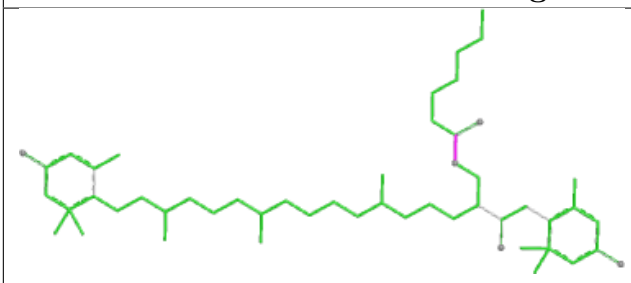
Bond angles



Torsions

Rings

Ligand 0UR 1 315



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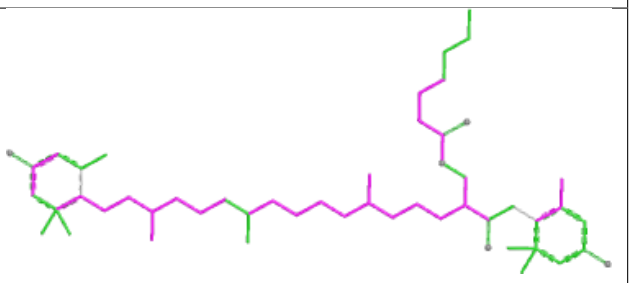
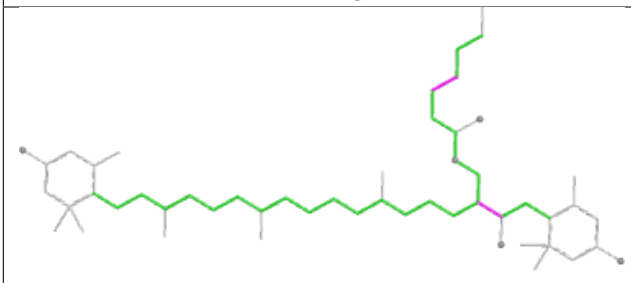


Bond angles



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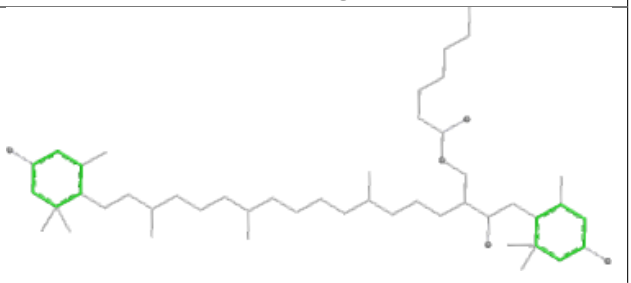
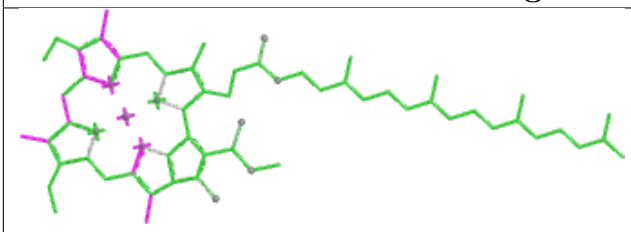


Rings

Ligand CLA B 806



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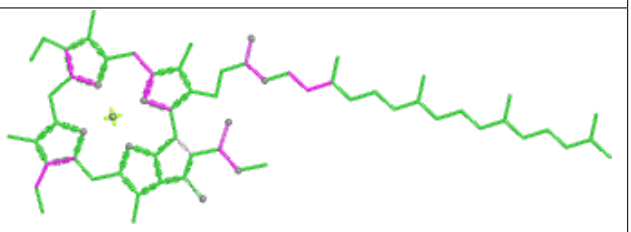

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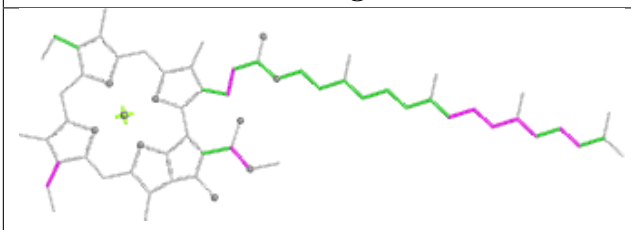

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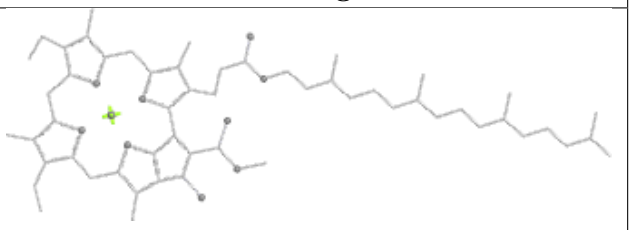
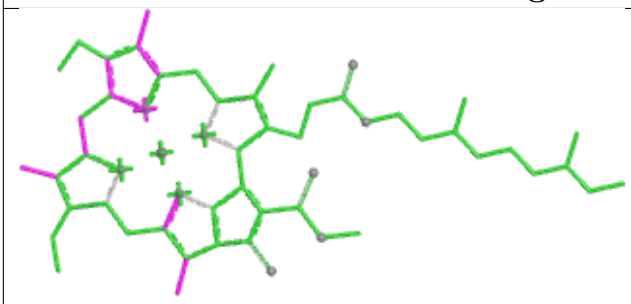


Rings

Ligand CLA 1 302



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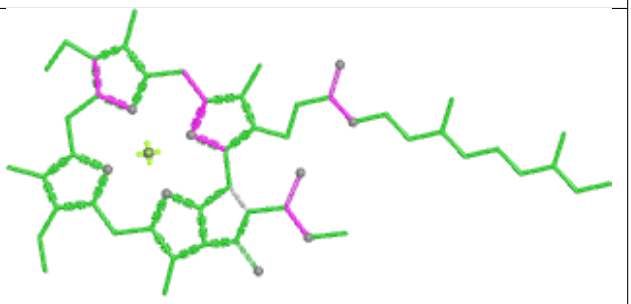

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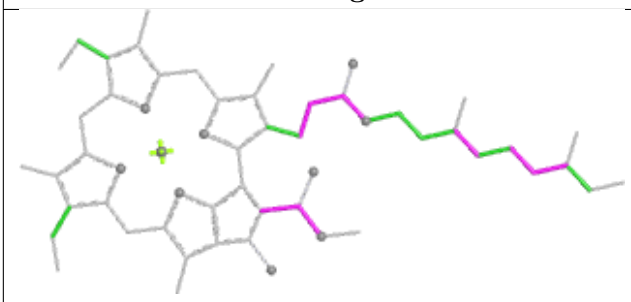

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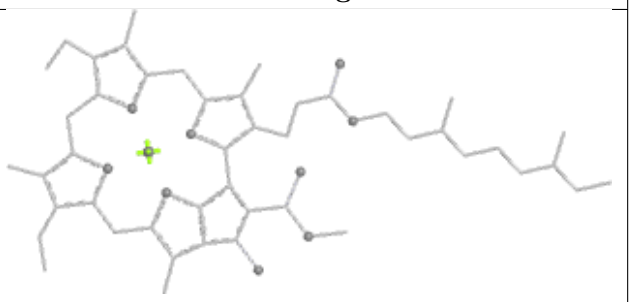
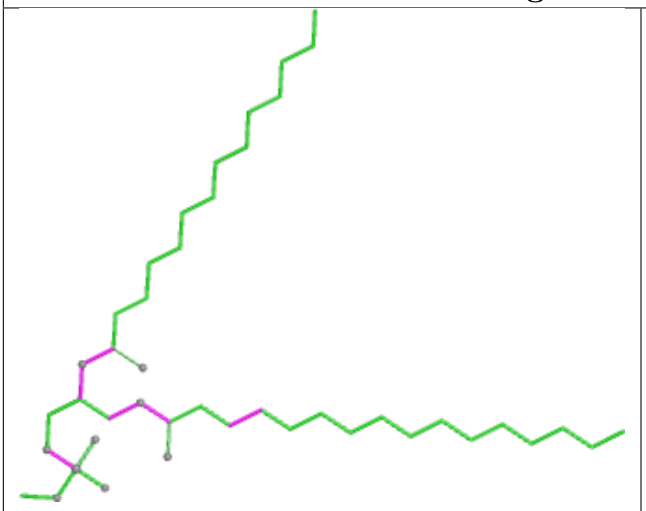


Rings

Ligand LHG 3 324



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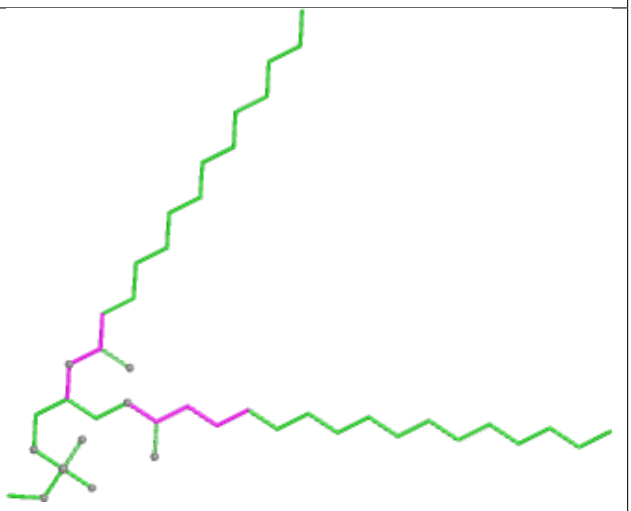
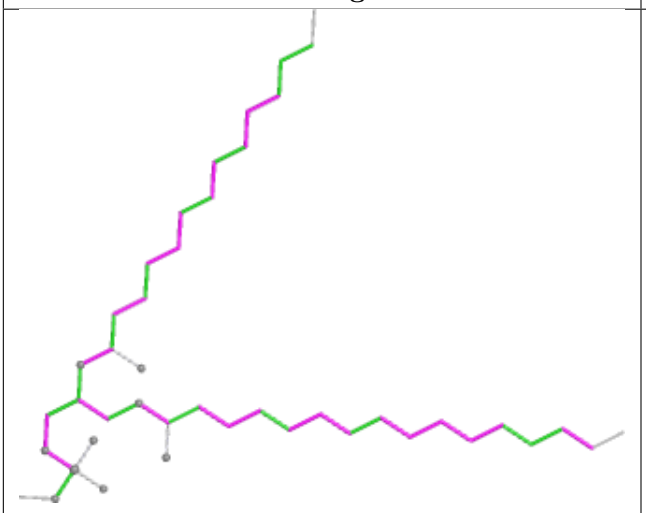


Bond angles



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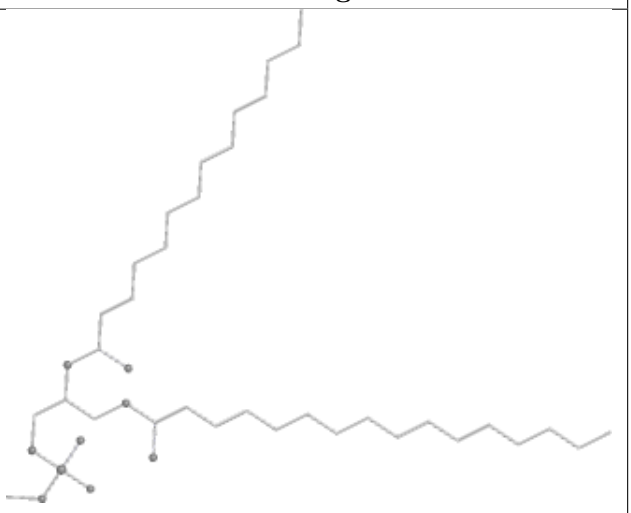
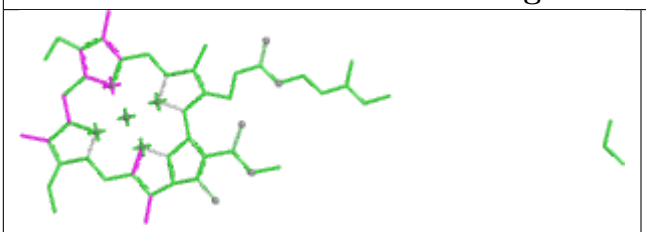


Rings

Ligand CLA A 806



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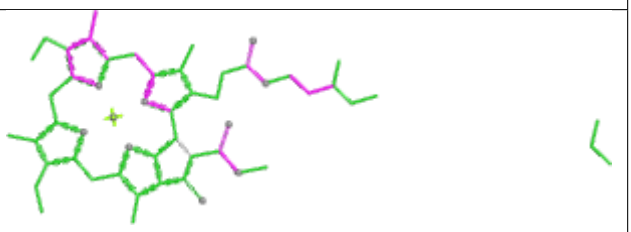
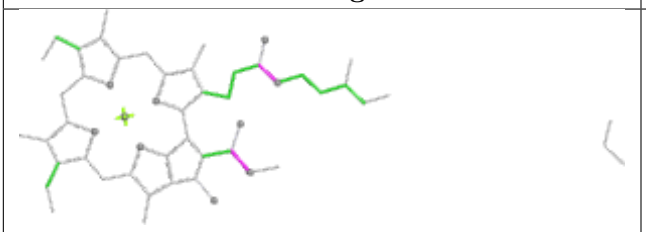


Bond angles



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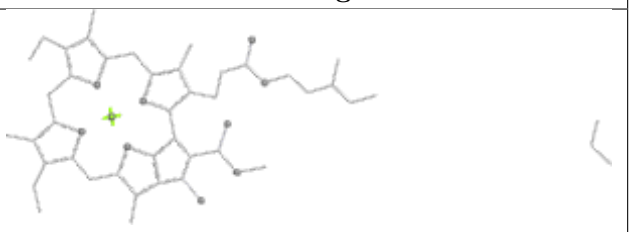
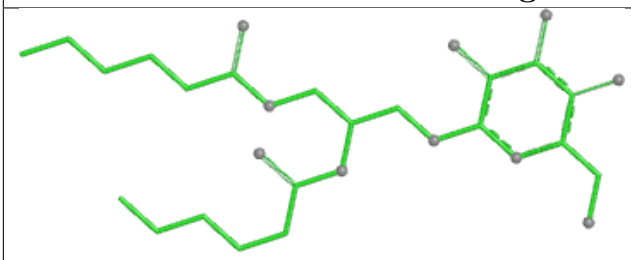


Rings

Ligand LMG O 203



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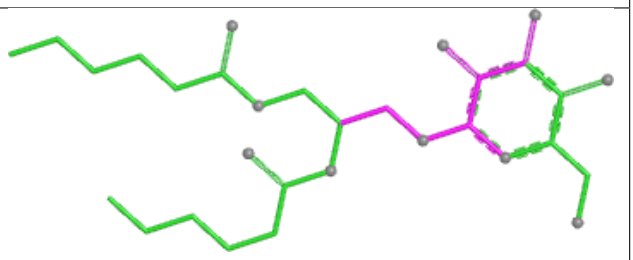
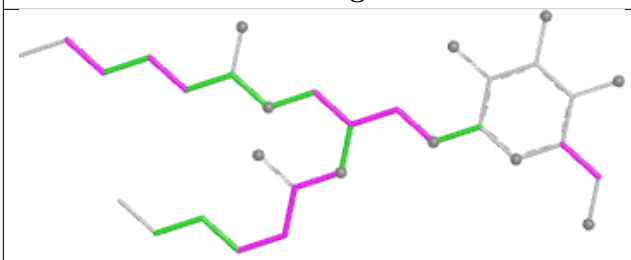
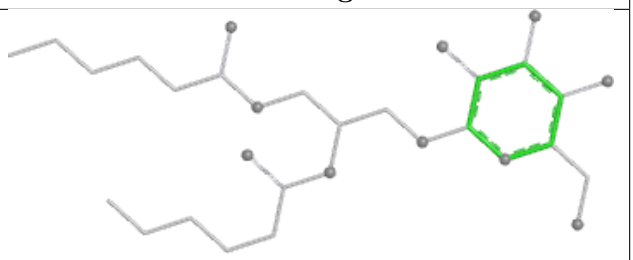


Bond angles

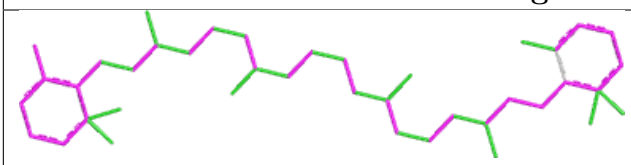


Torsions

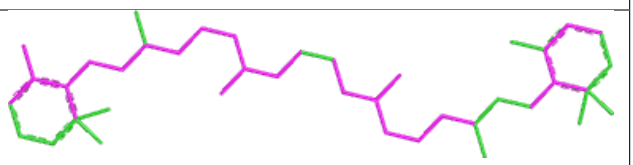


Rings

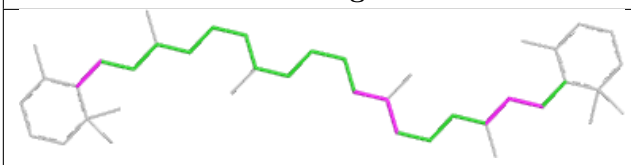
Ligand 8CT 4 316



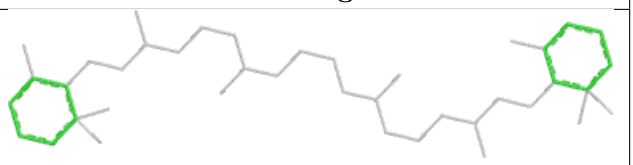
Bond lengths



Bond angles

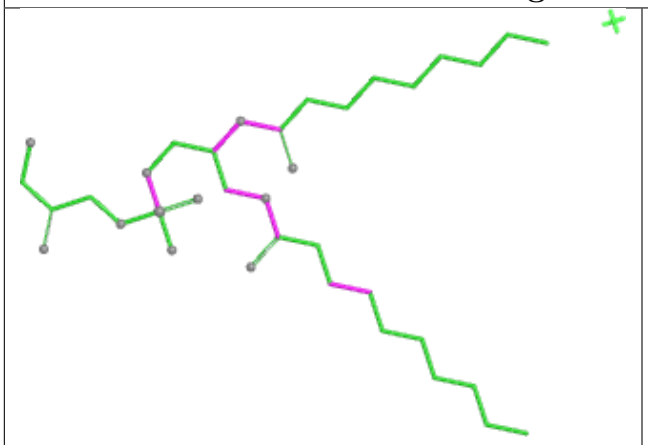


Torsions



Rings

Ligand LHG 3 322



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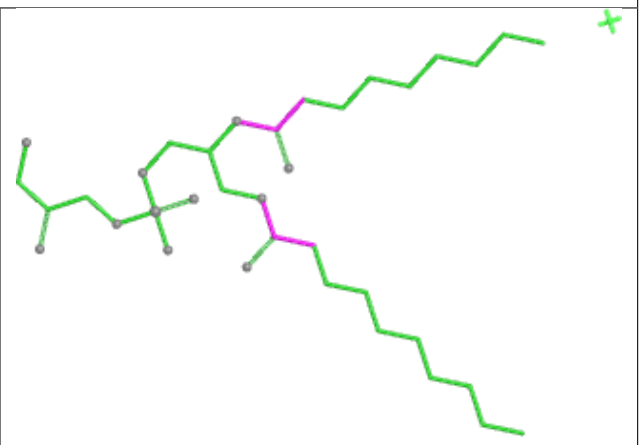
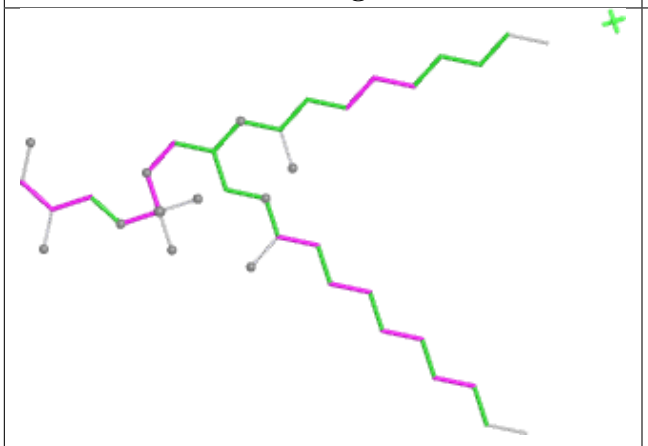


Bond angles



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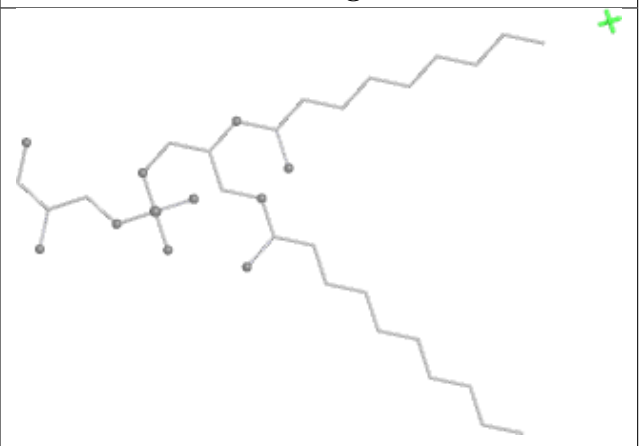
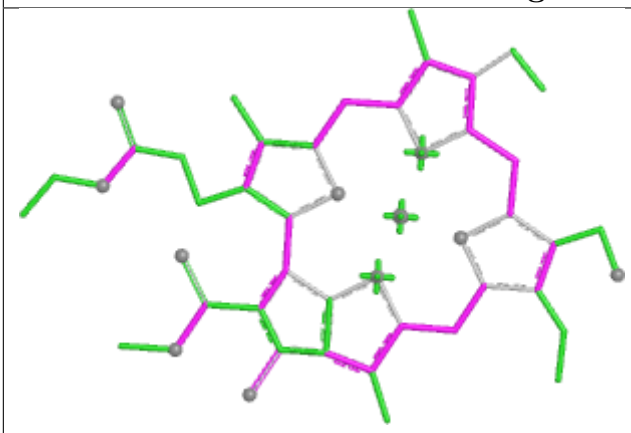


Rings

Ligand CHL 5 305



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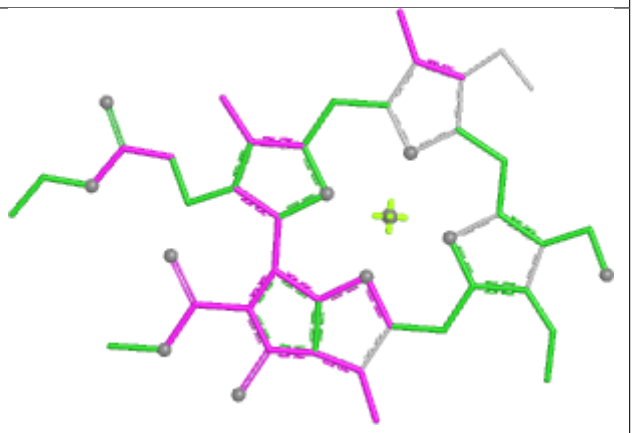
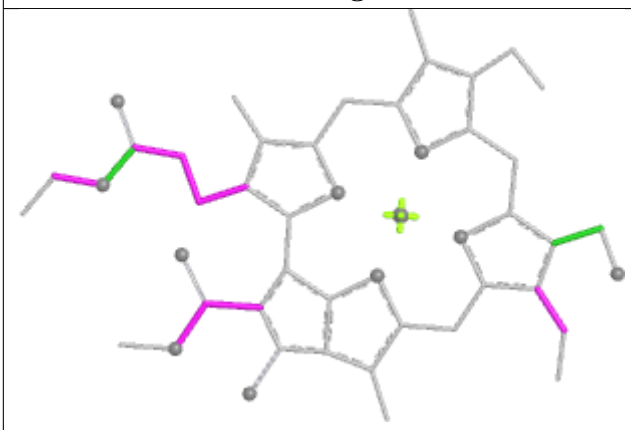


Bond angles



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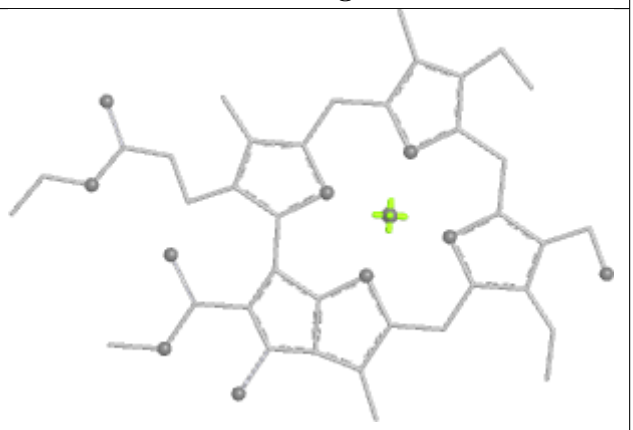
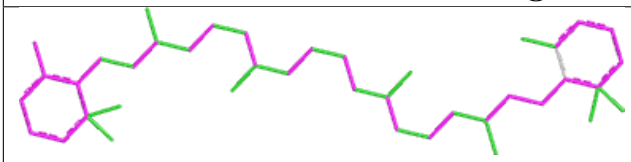


Rings

Ligand 8CT B 843



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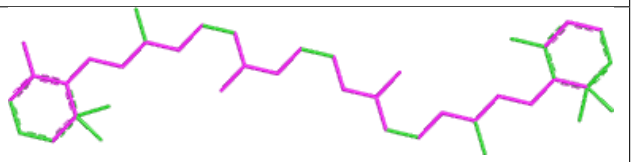
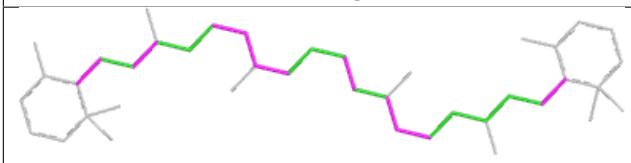


Bond angles



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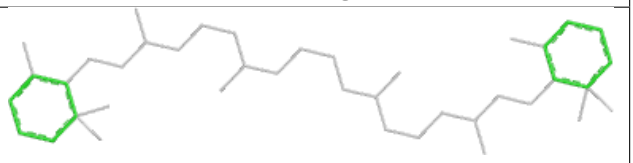
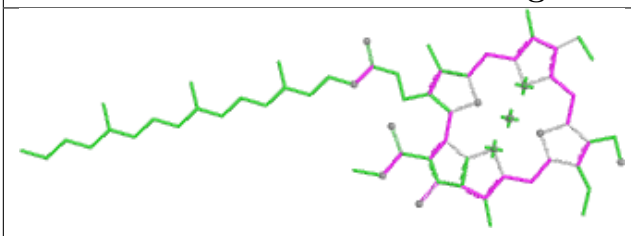


Rings

Ligand CHL 6 302



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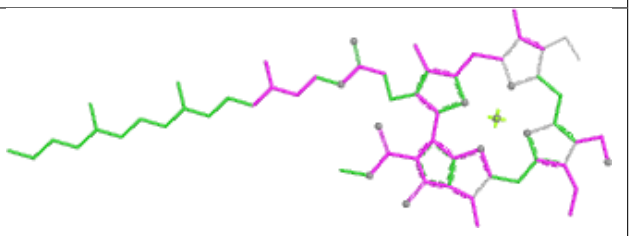
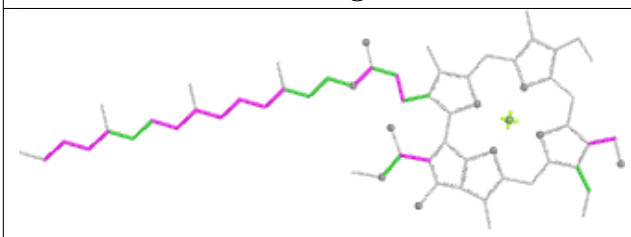


Bond angles



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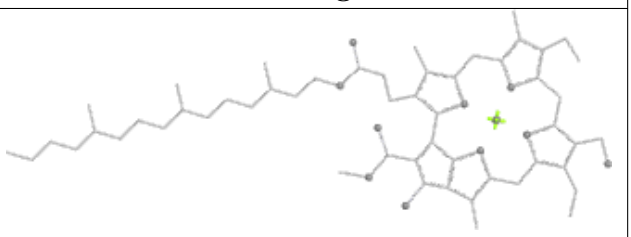
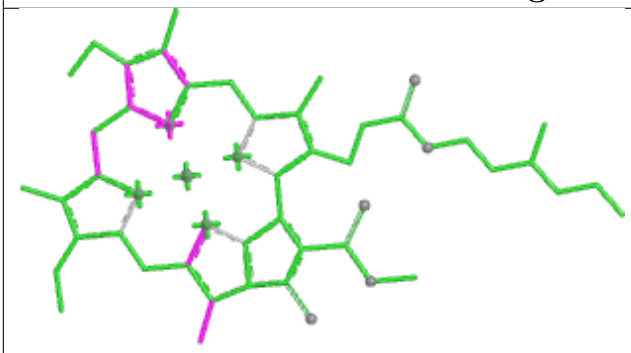


Rings

Ligand CLA 5 303



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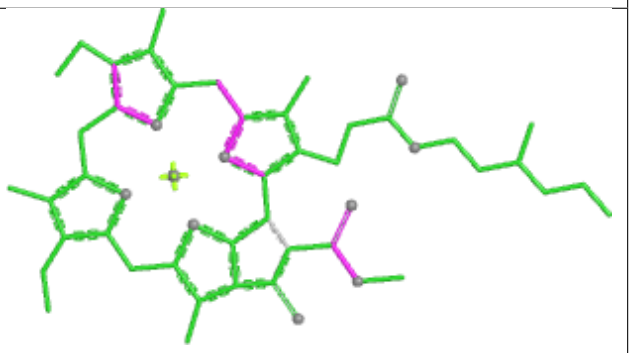

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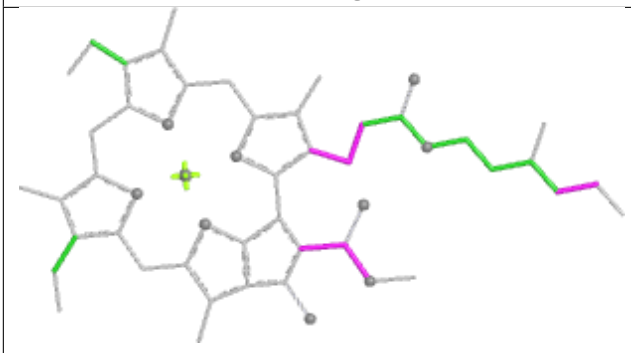

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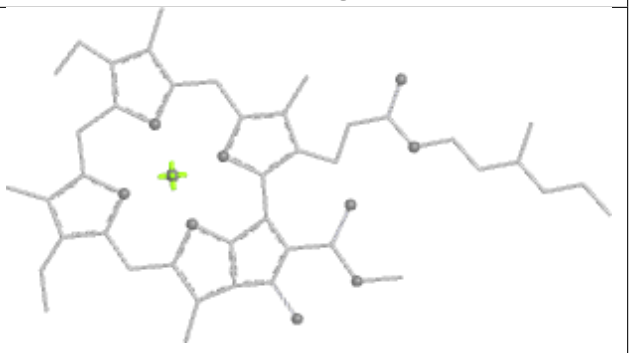
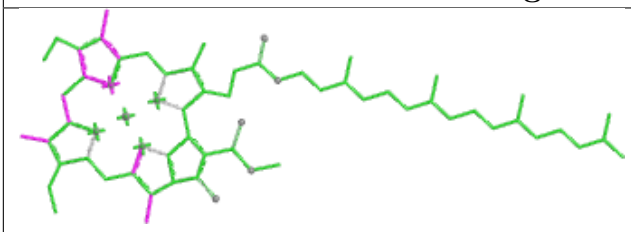


Rings

Ligand CLA A 812



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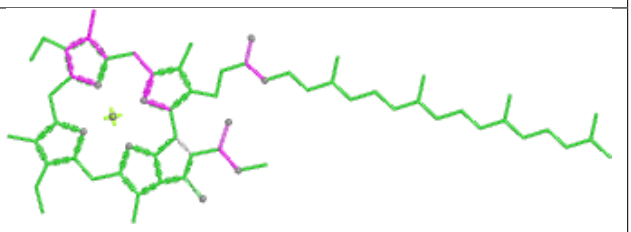

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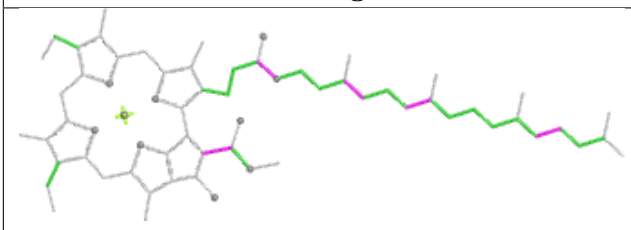

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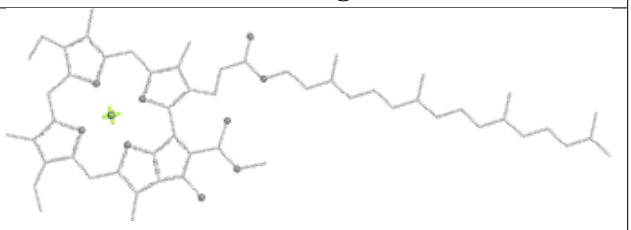
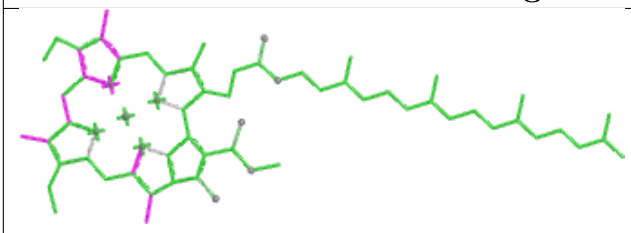


Rings

Ligand CLA A 824



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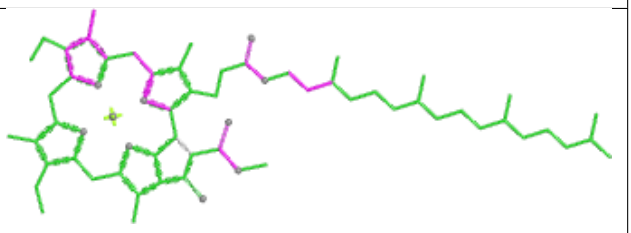
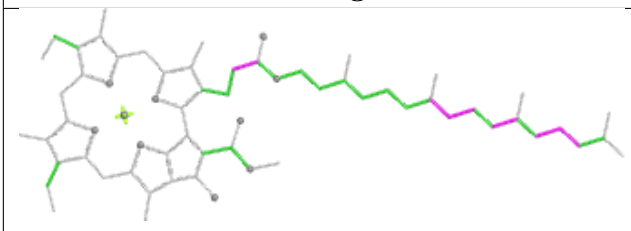


Bond angles



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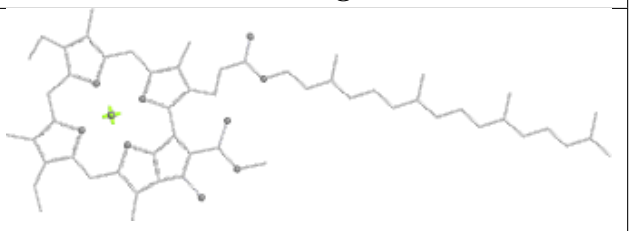
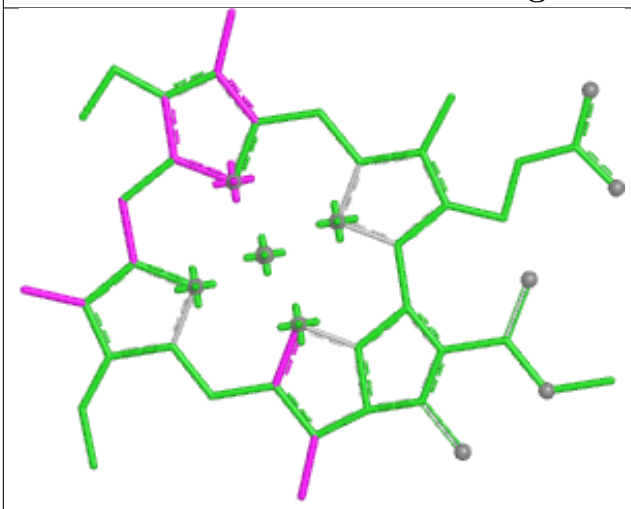


Rings

Ligand CLA 4 303



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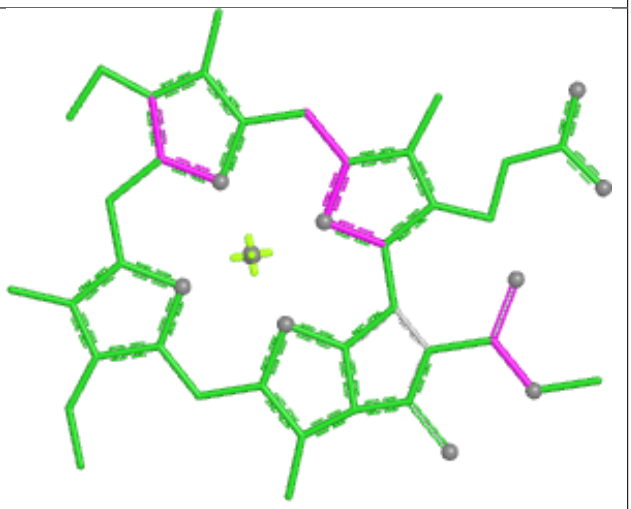

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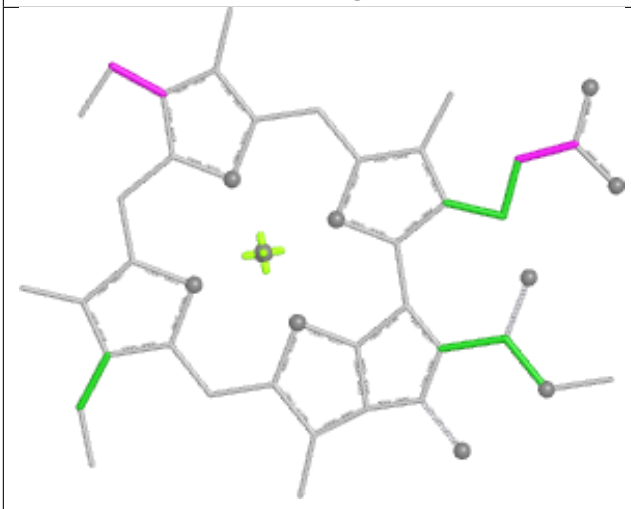
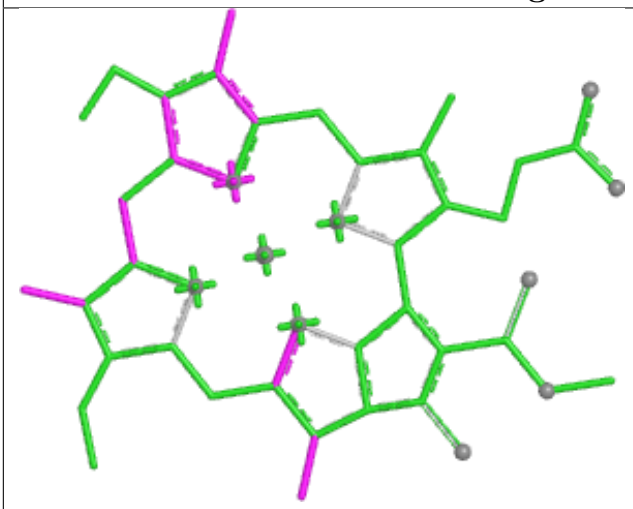


Torsions

Rings

Ligand CLA 6 314



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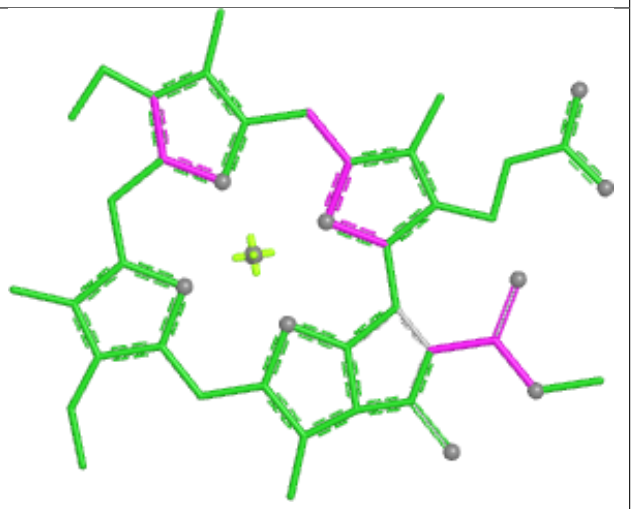

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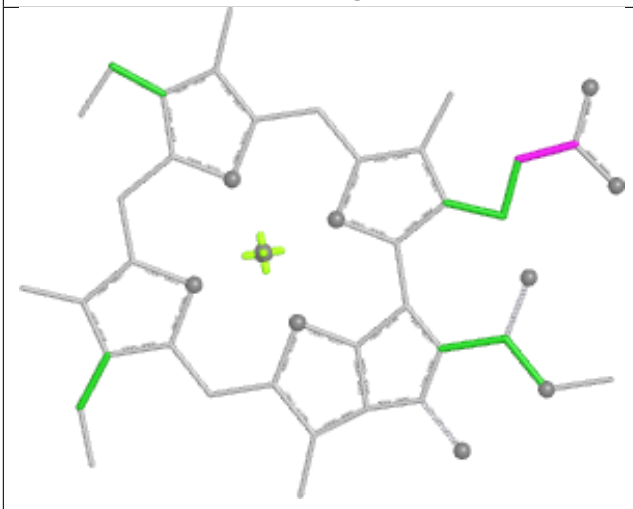
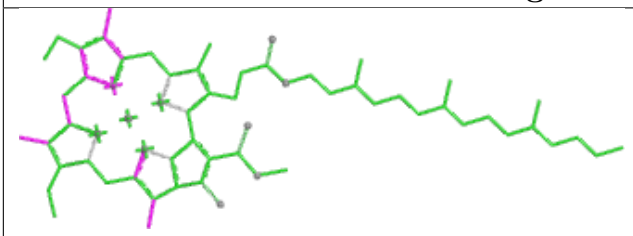


Torsions

Rings

Ligand CLA L 202



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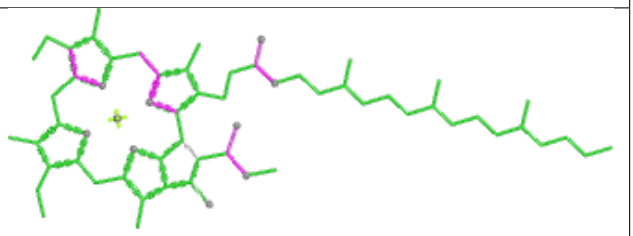
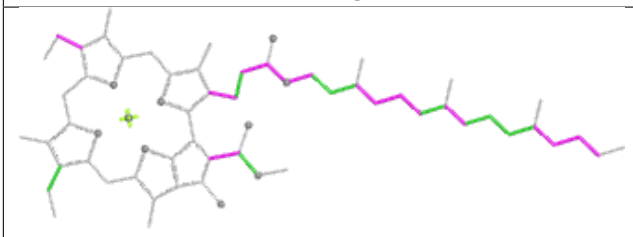


Bond angles



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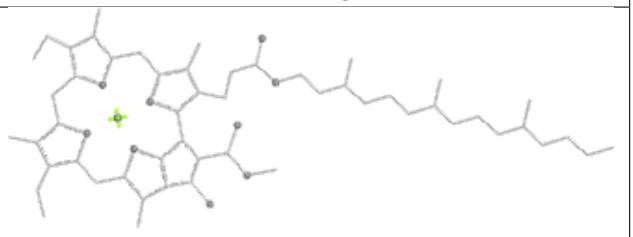
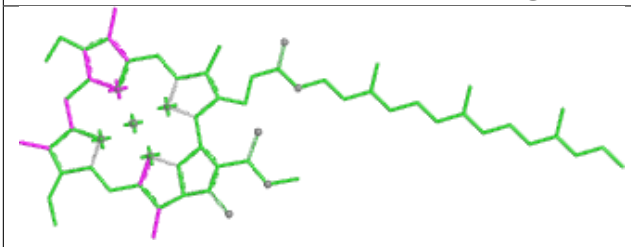
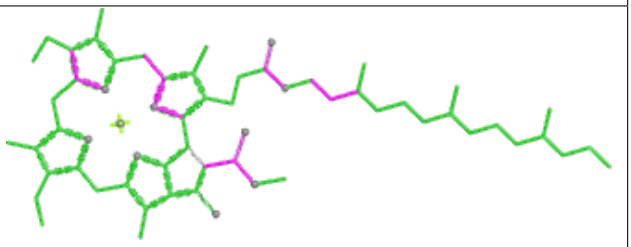
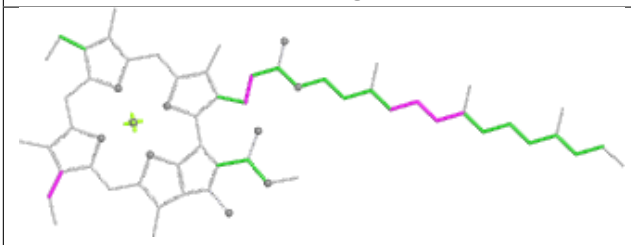
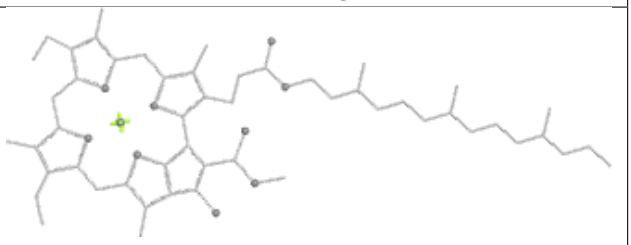
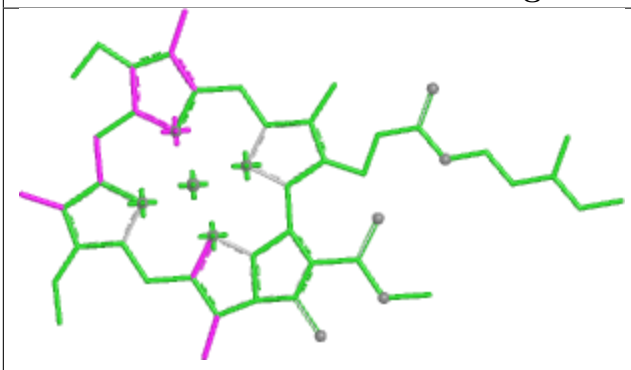
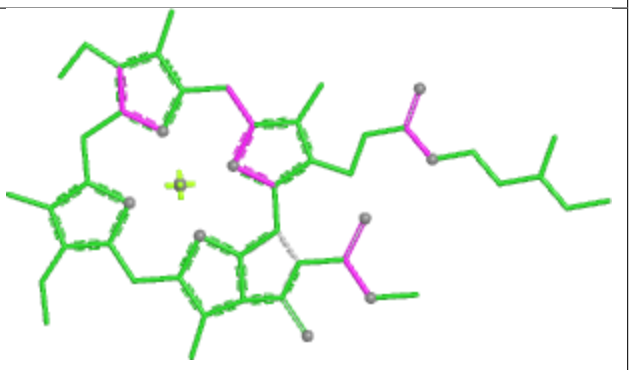
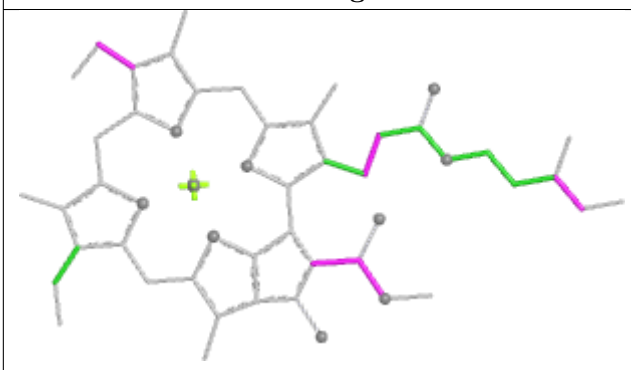
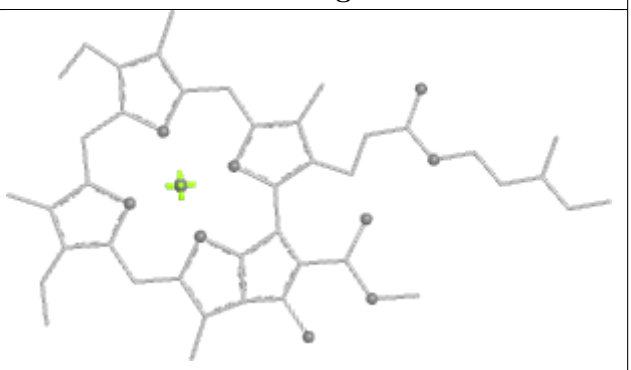
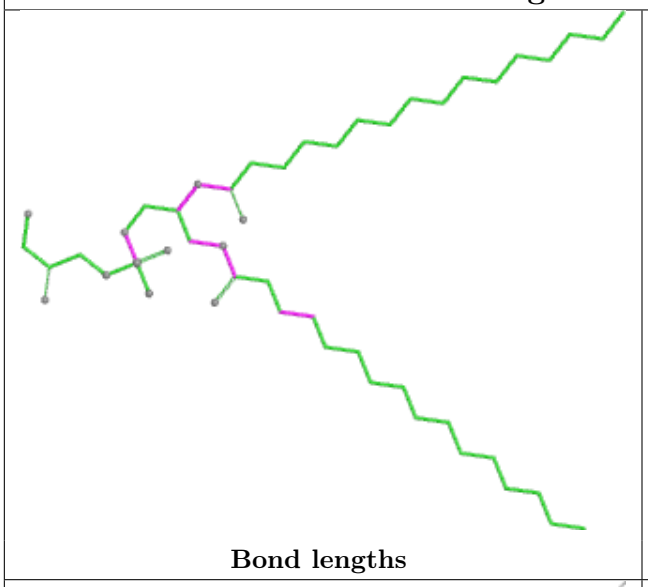


Rings

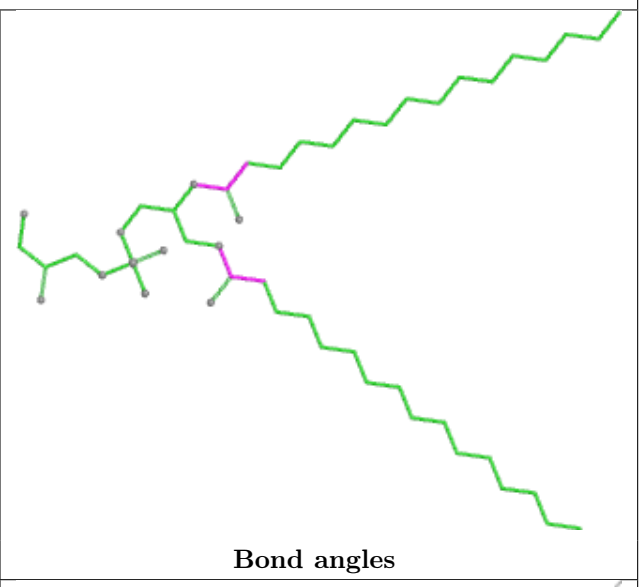
Ligand CLA B 810	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA O 209	
	
Bond lengths	Bond angles
	
Torsions	Rings

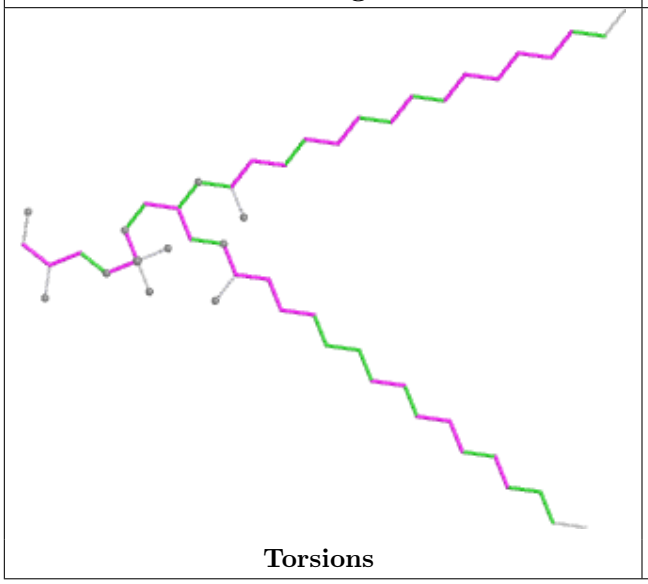
Ligand LHG 0 317



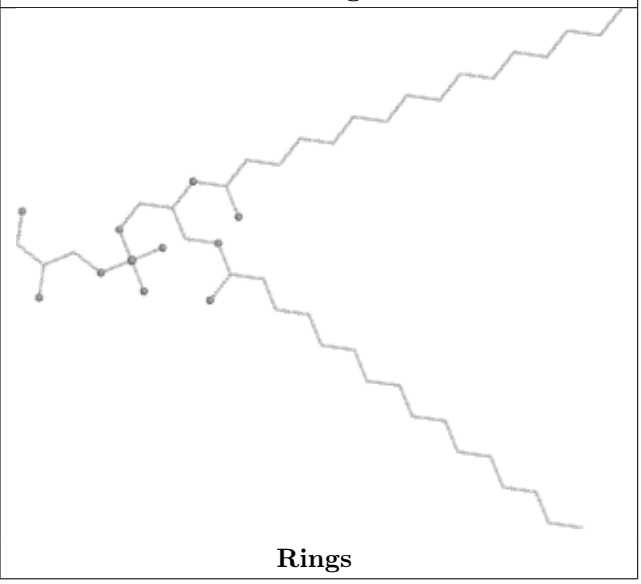
Bond lengths



Bond angles

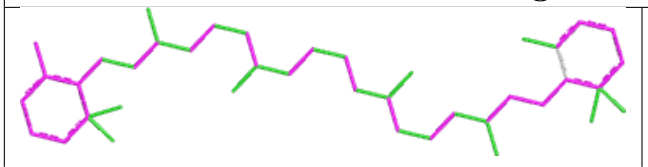


Torsions

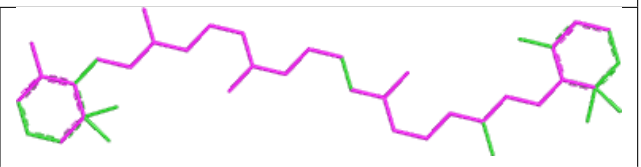


Rings

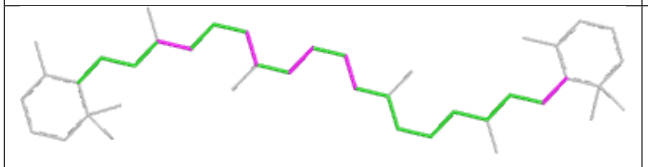
Ligand 8CT J 104



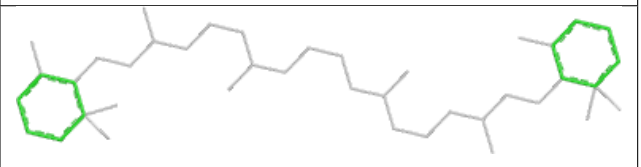
Bond lengths



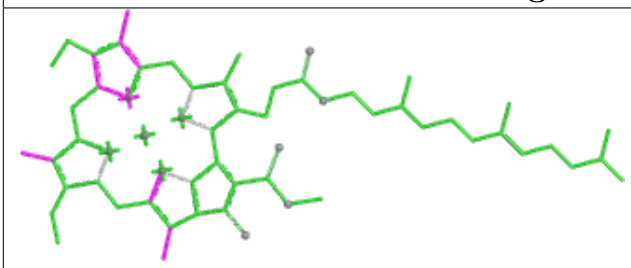
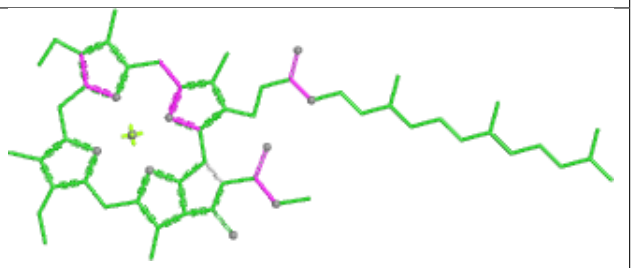
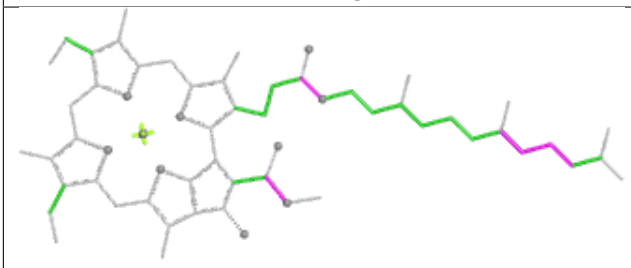
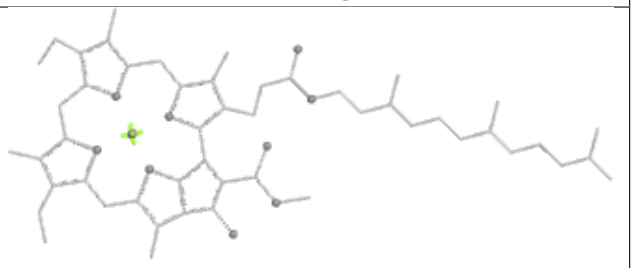
Bond angles

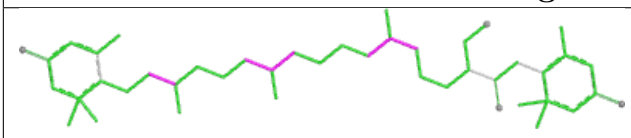
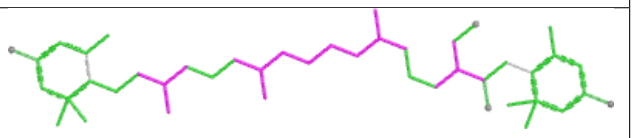
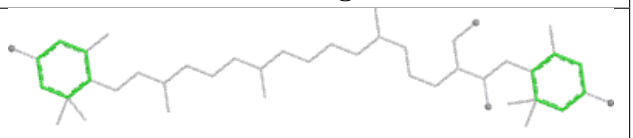


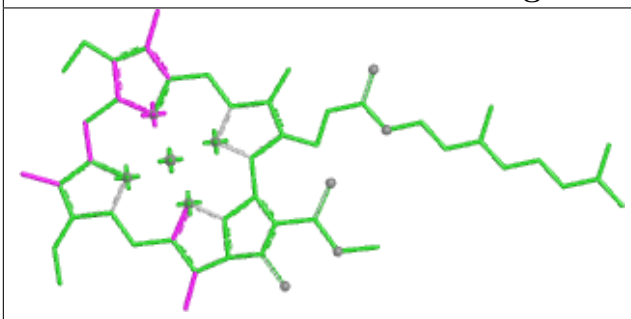
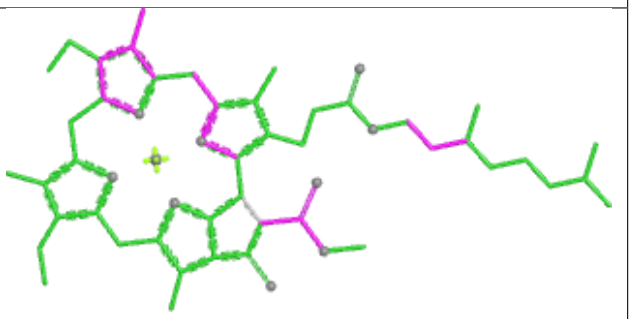
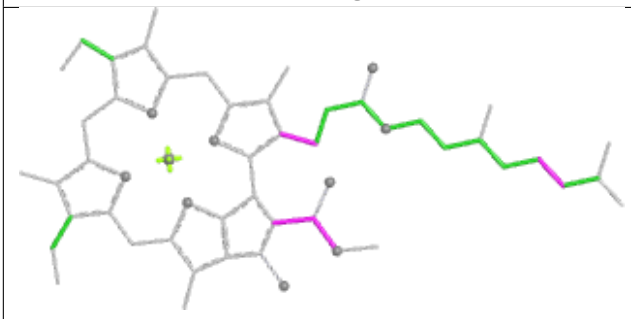
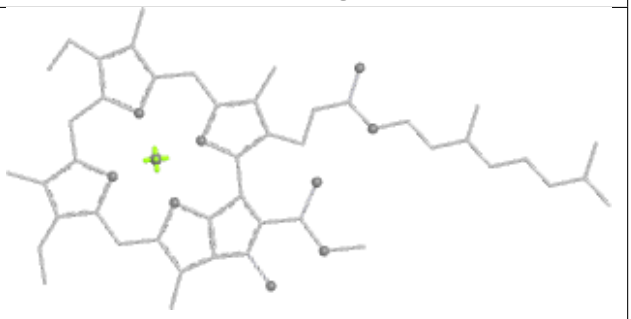
Torsions

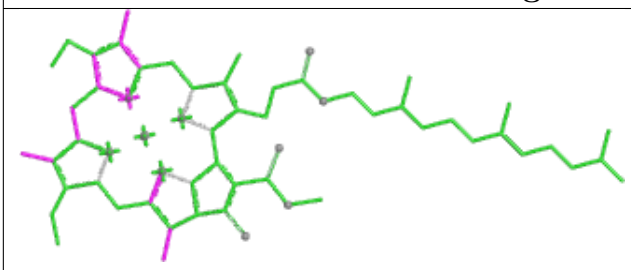
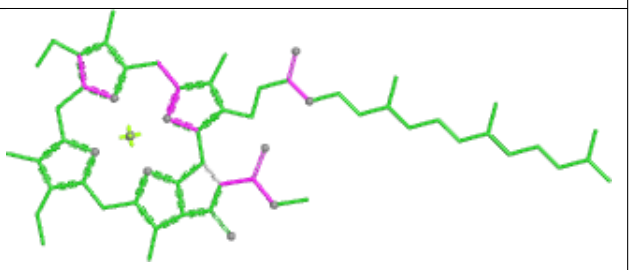


Rings

Ligand CLA 4 304	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand 0IE 7 321	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA H 202	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA K 101	
	
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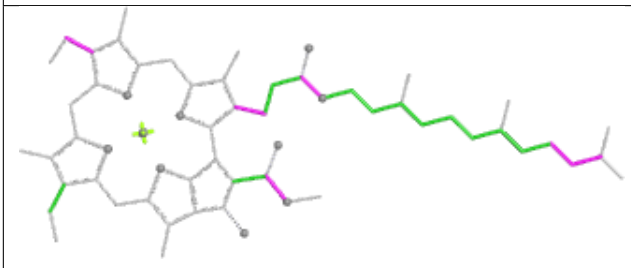
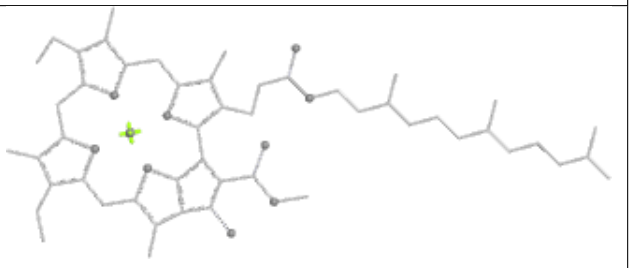
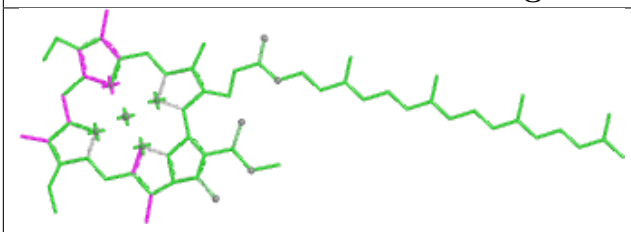
	
Torsions	Rings

Ligand CLA B 829



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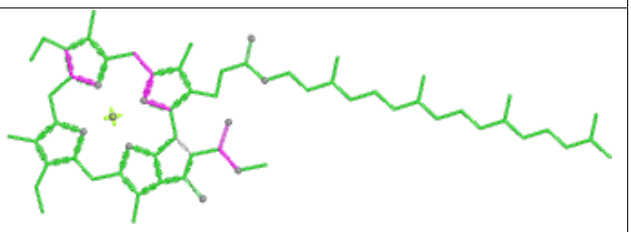
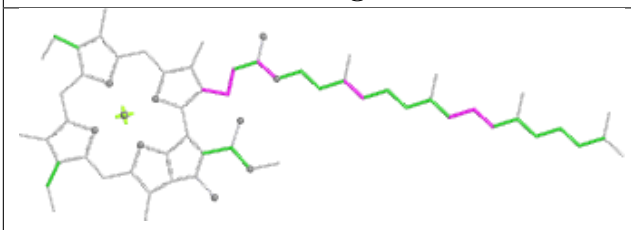
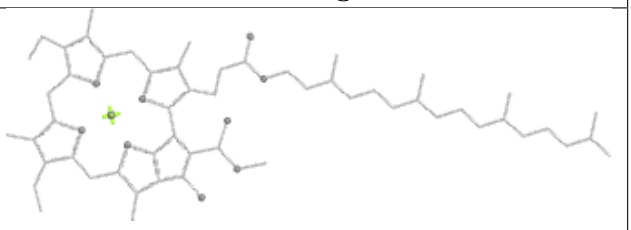


Bond angles

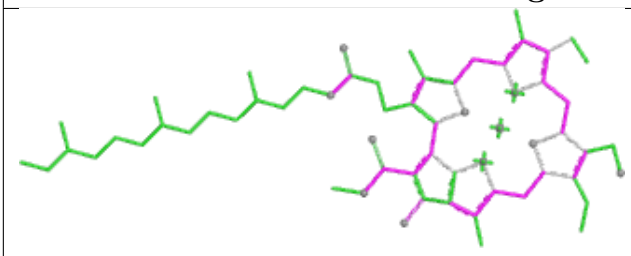


Torsions

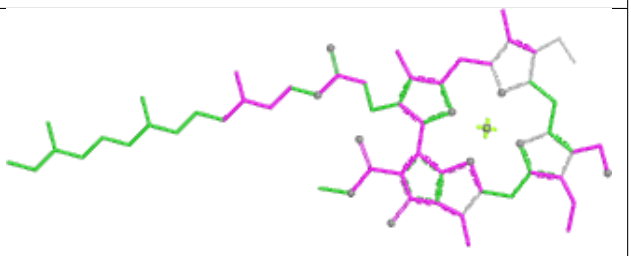


Rings

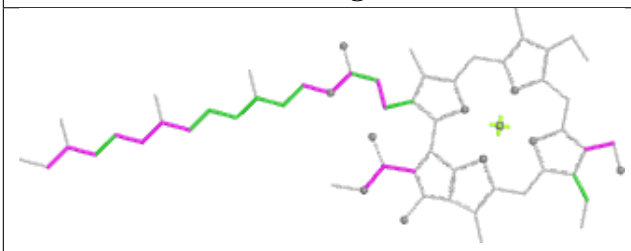
Ligand CHL 3 302



Bond lengths



Bond angles



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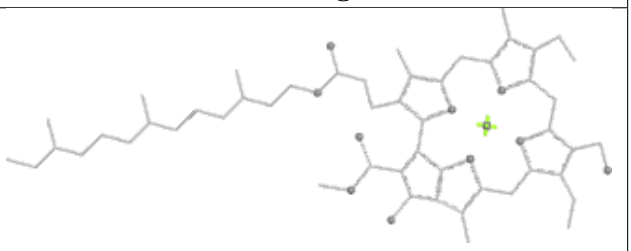
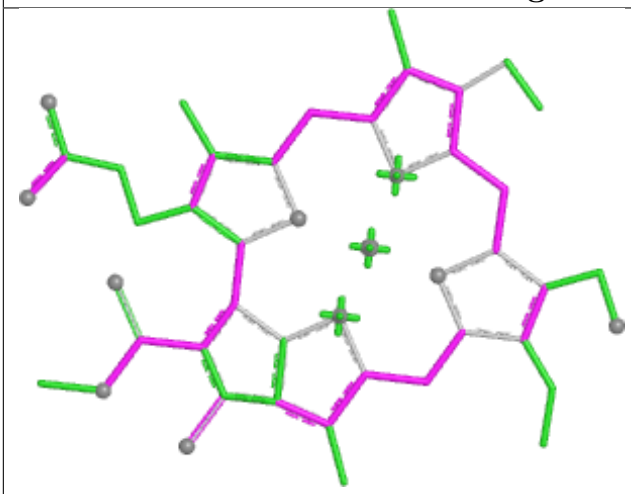


Rings

Ligand CHL 5 304



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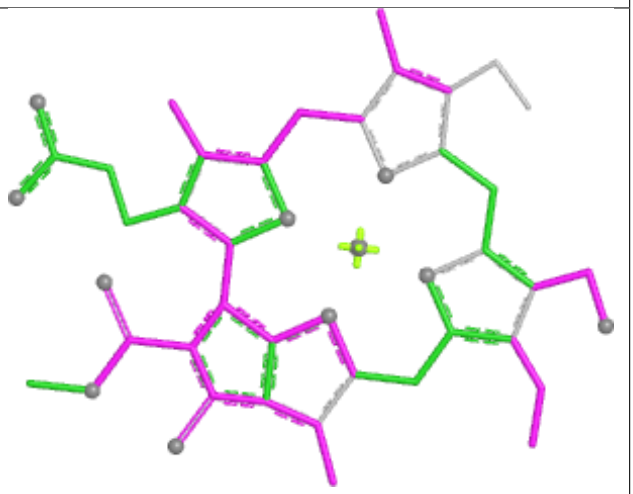

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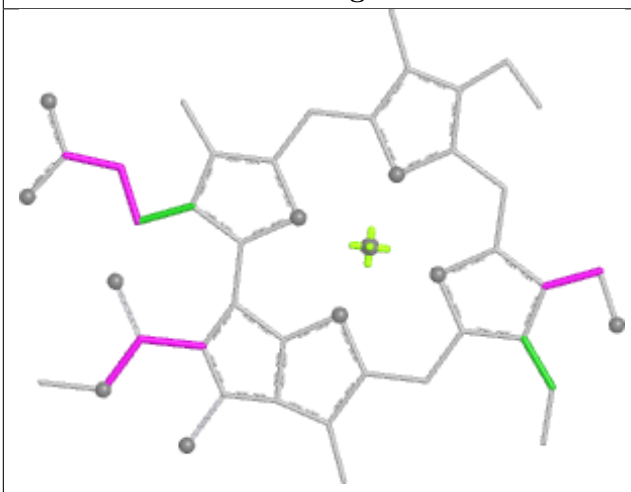

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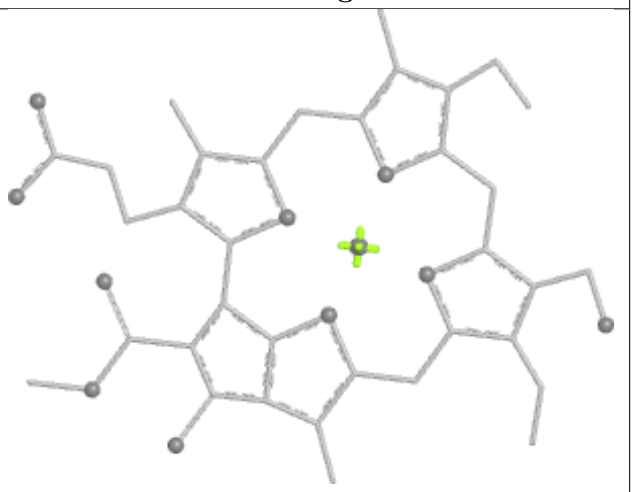
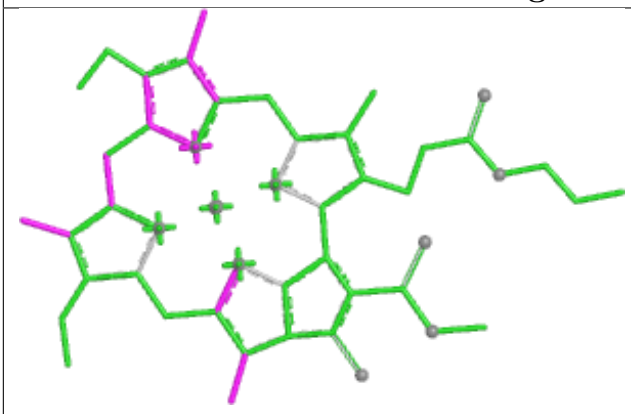


Rings

Ligand CLA 4 311



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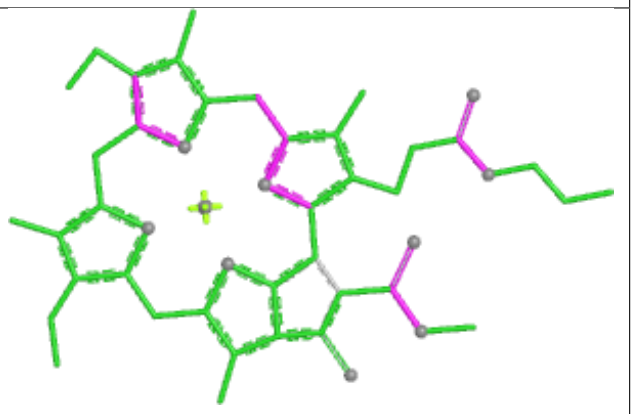
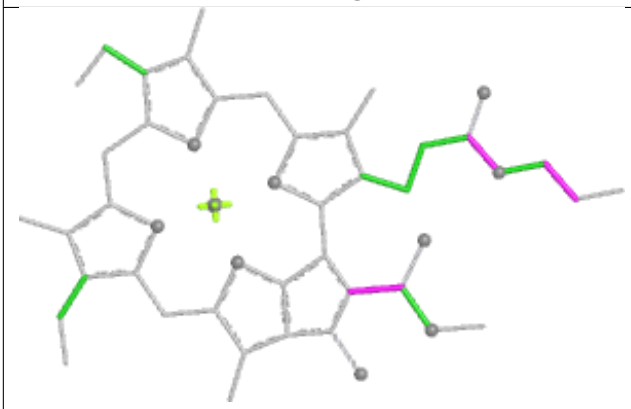


Bond angles



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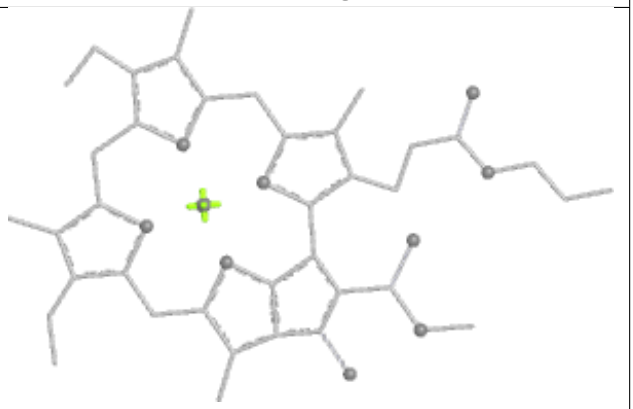
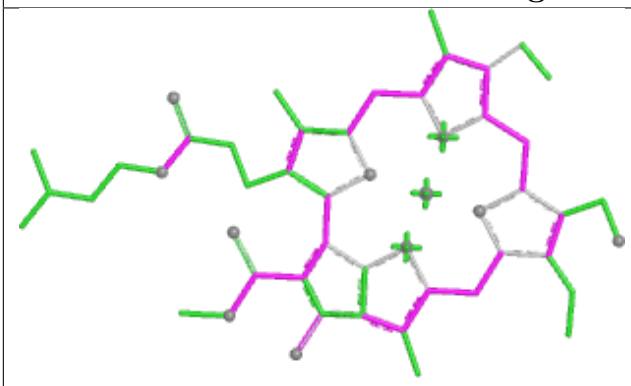


Rings

Ligand CHL 4 307



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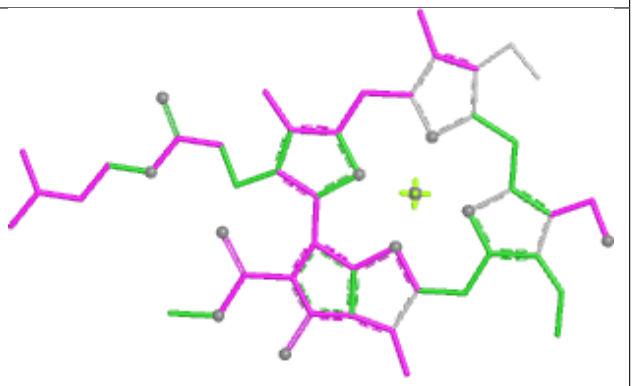
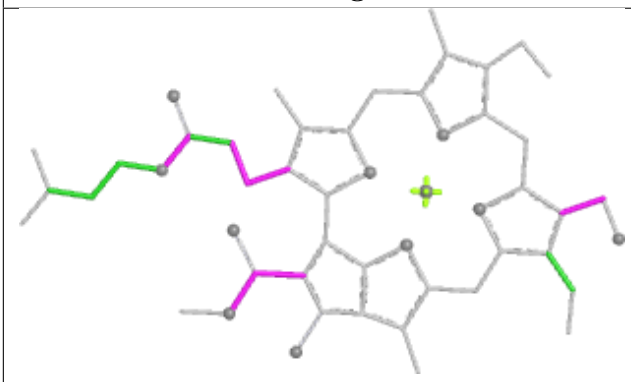


Bond angles



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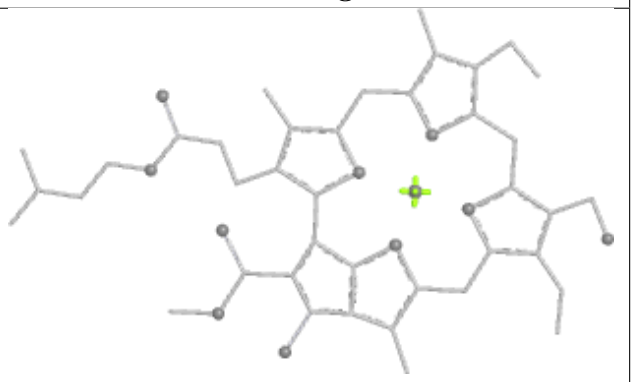
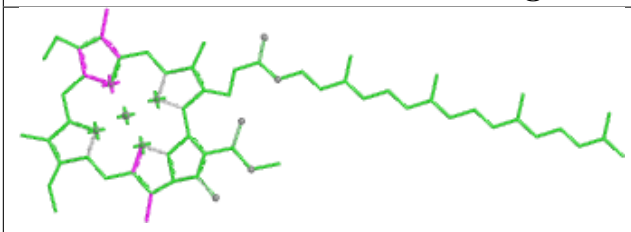


Rings

Ligand CLA B 840



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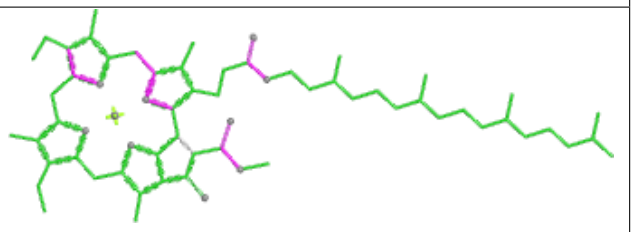
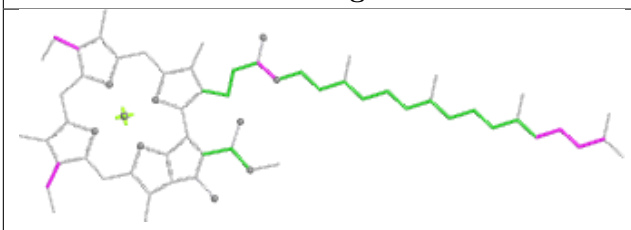


Bond angles



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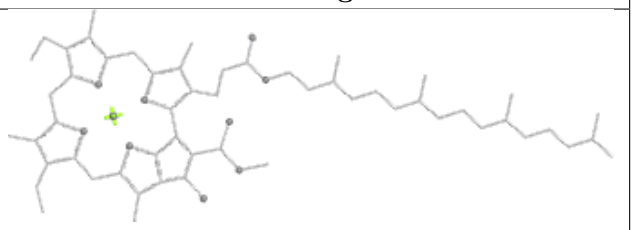
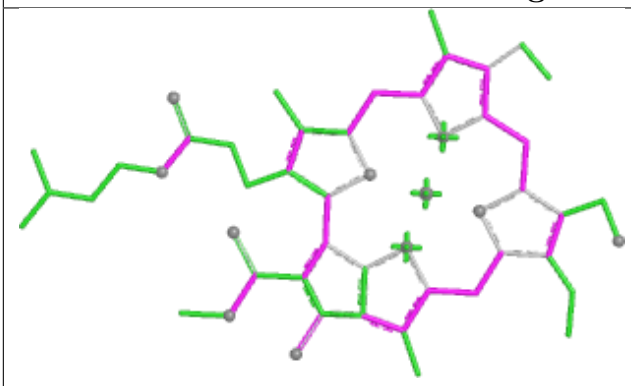


Rings

Ligand CHL 8 307



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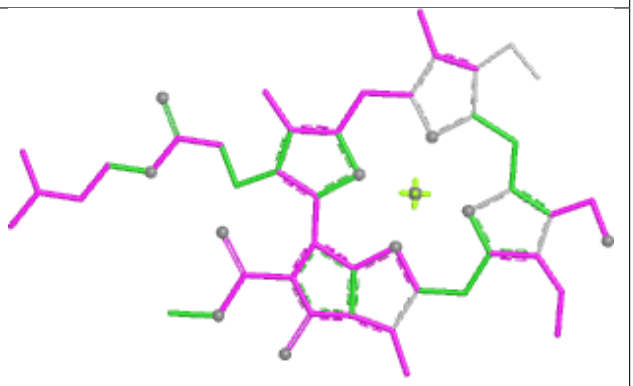
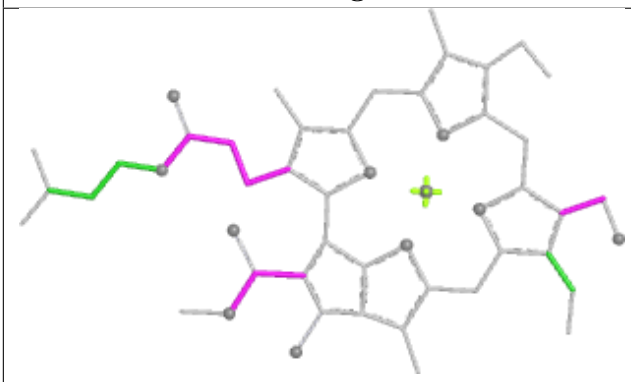
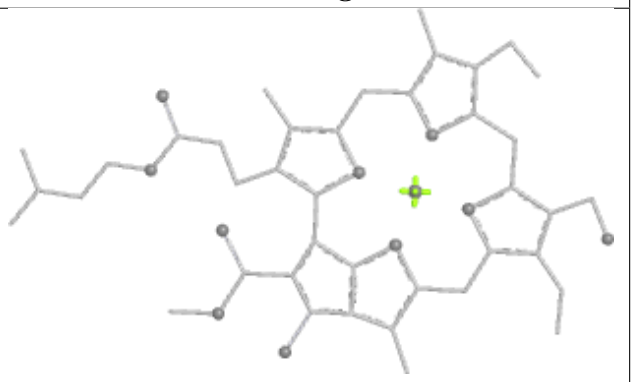


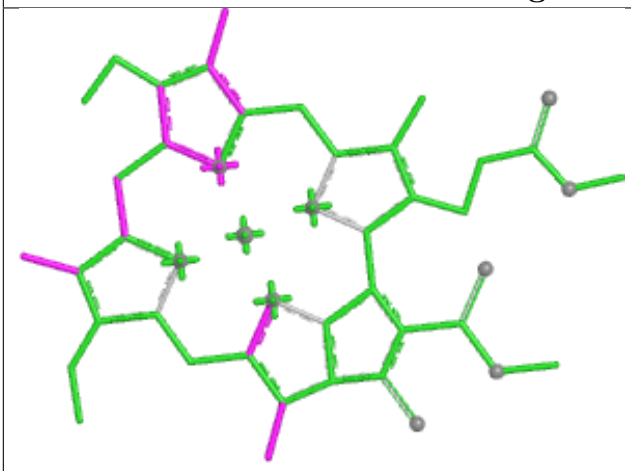
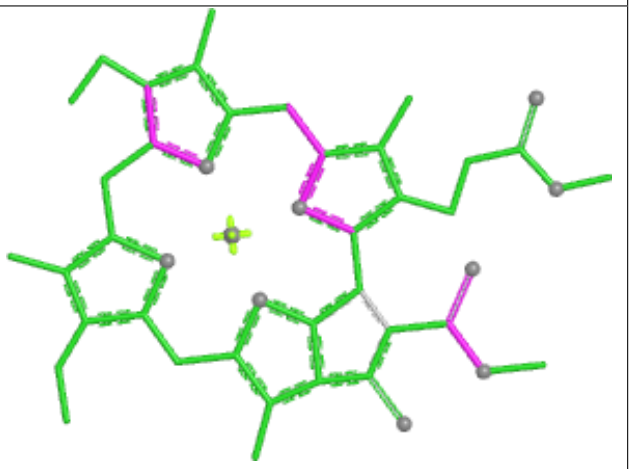
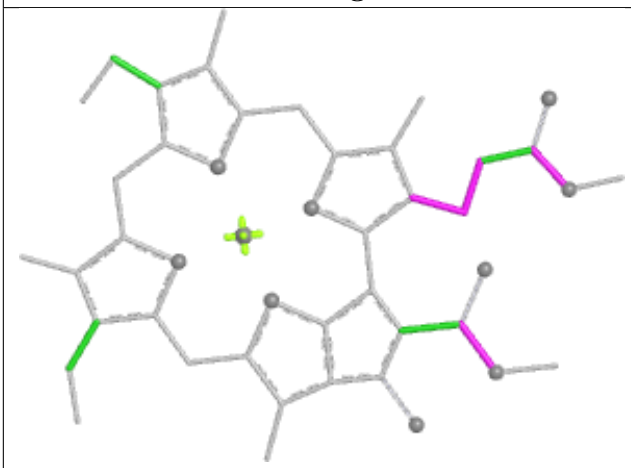
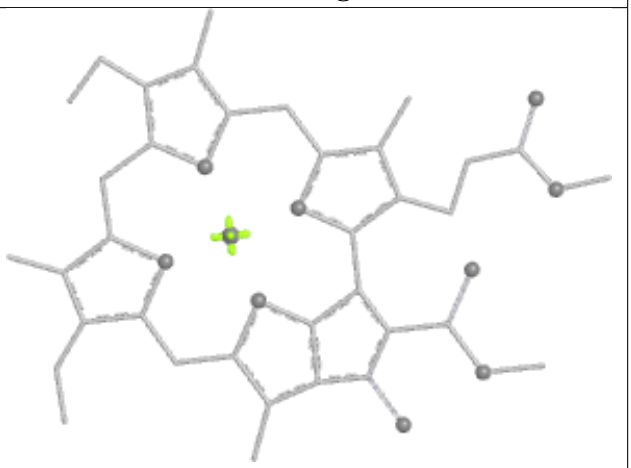
Bond angles



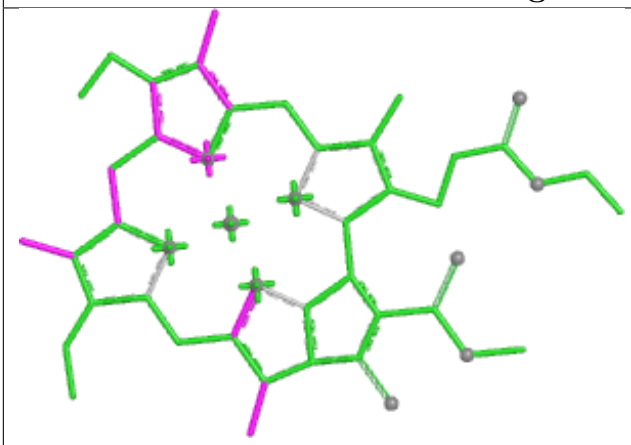
Torsions



Rings

Ligand CLA 5 307	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

Ligand CLA 0 310



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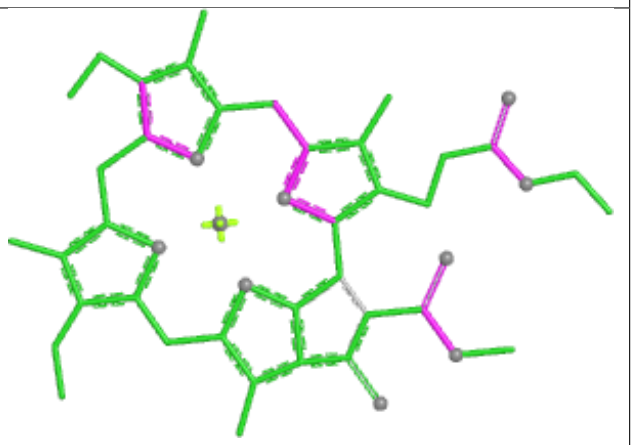
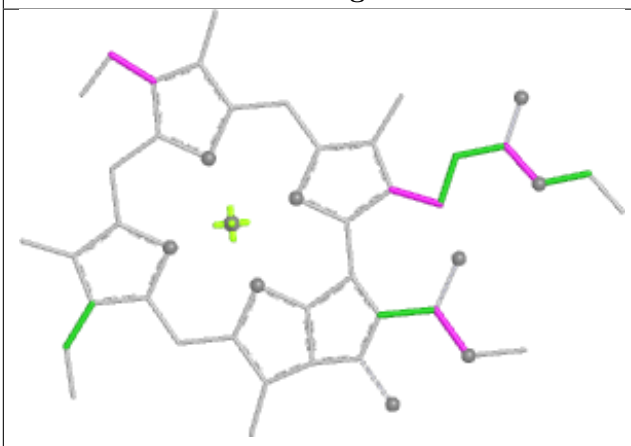
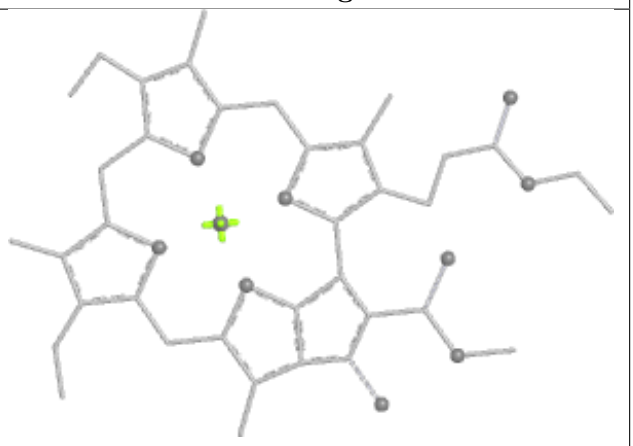


Bond angles

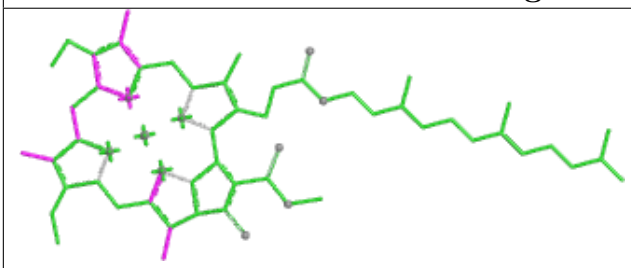


Torsions

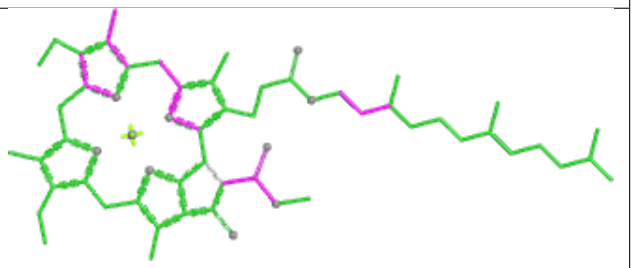


Rings

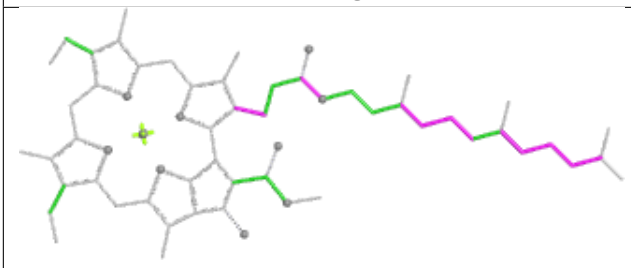
Ligand CLA B 819



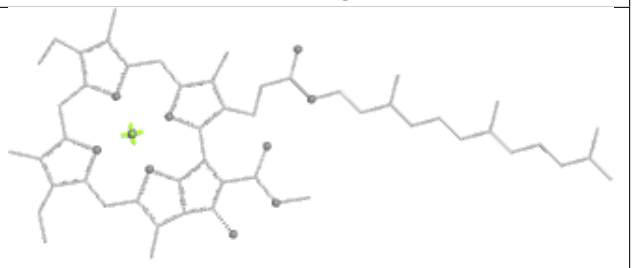
Bond lengths



Bond angles

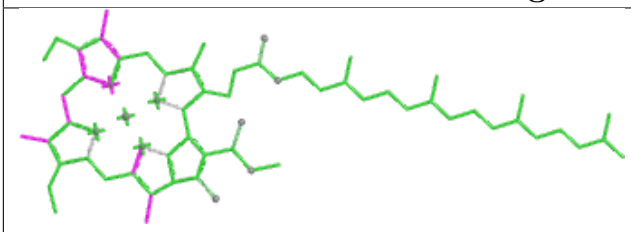


Torsions



Rings

Ligand CLA 3 304



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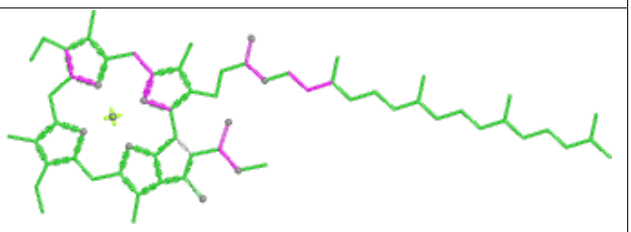
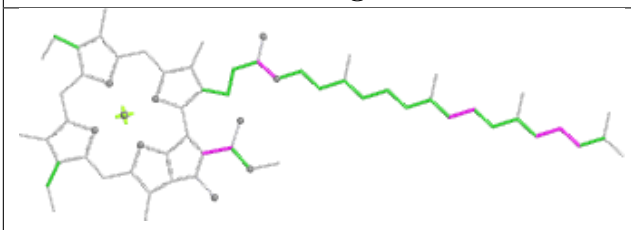


Bond angles



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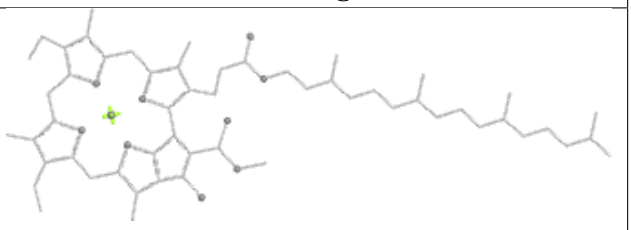
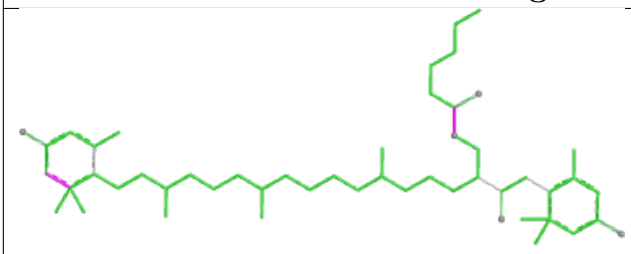


Rings

Ligand 0UR 2 315



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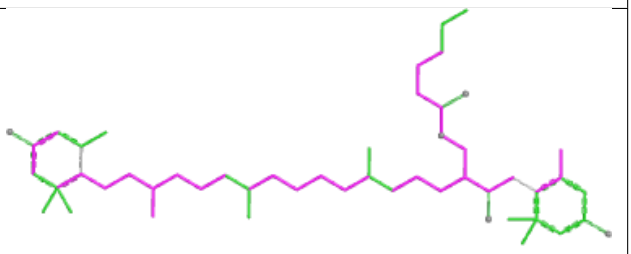

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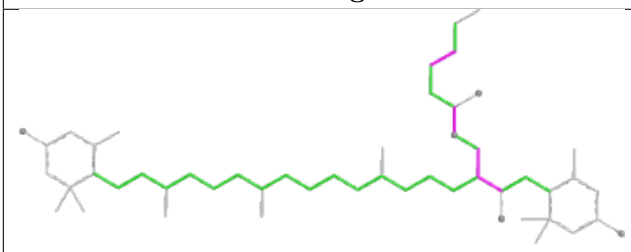

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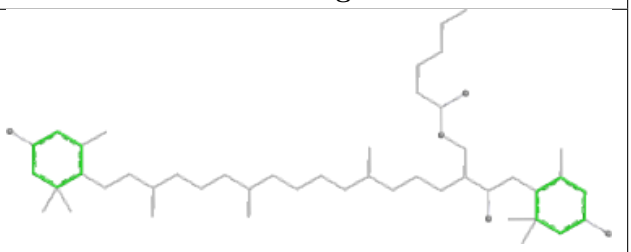
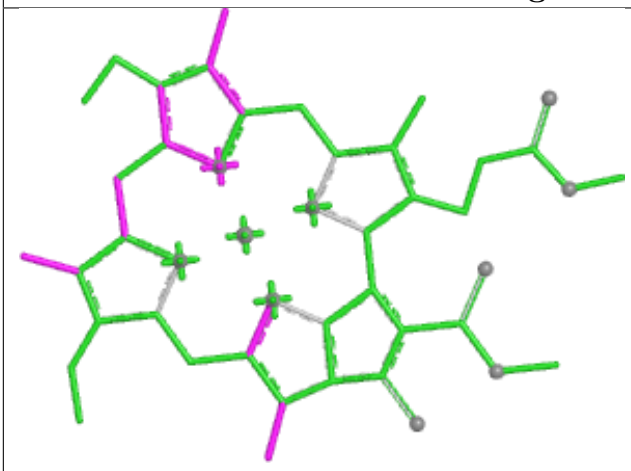


Rings

Ligand CLA 3 314



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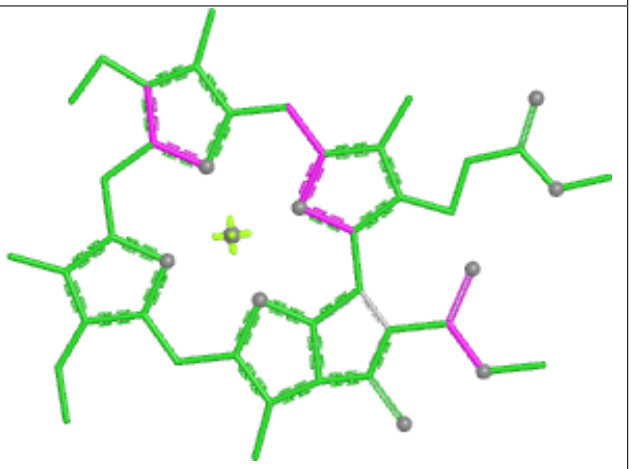
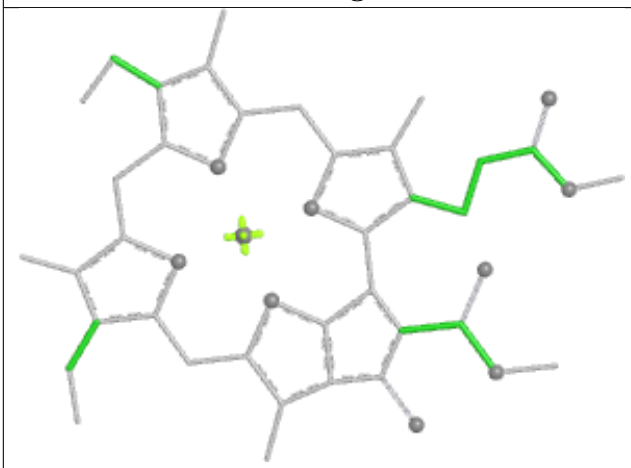


Bond angles



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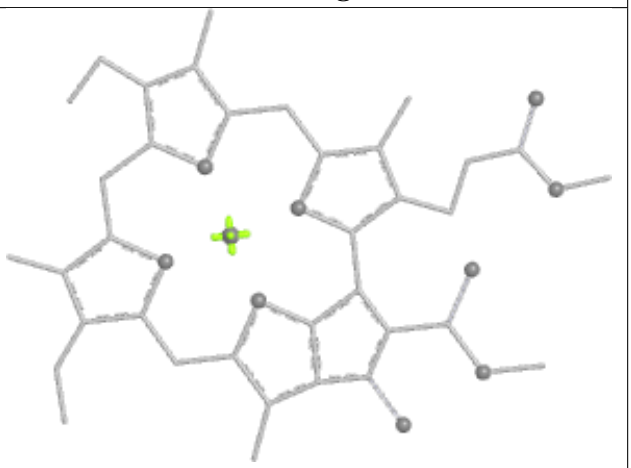
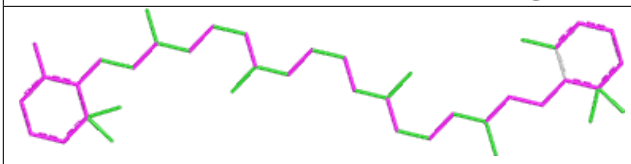


Rings

Ligand 8CT B 848



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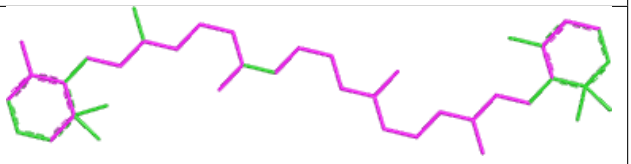

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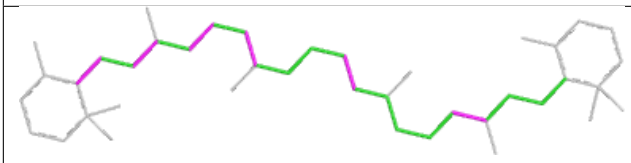

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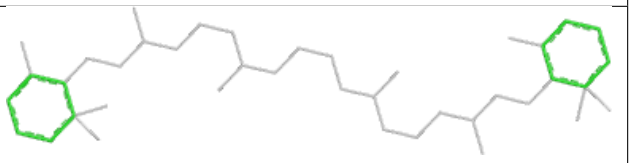
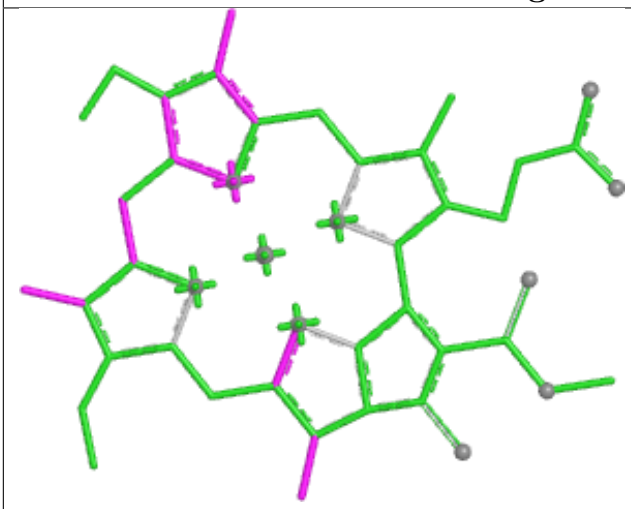


Rings

Ligand CLA 4 314



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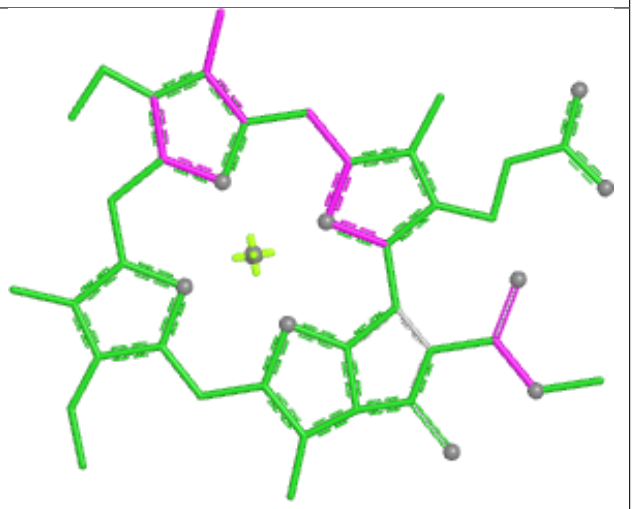

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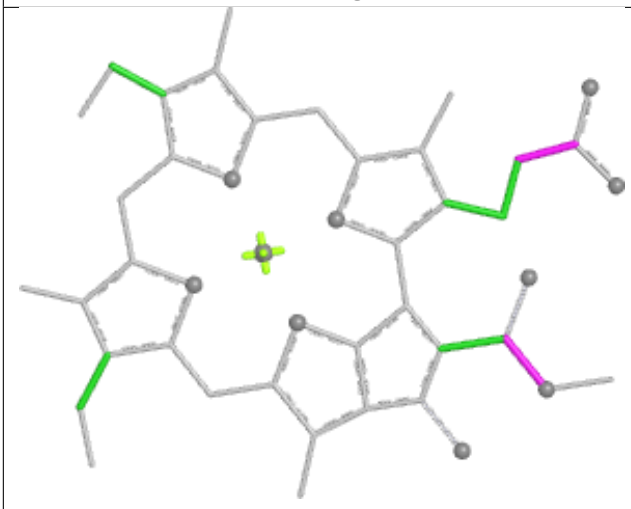
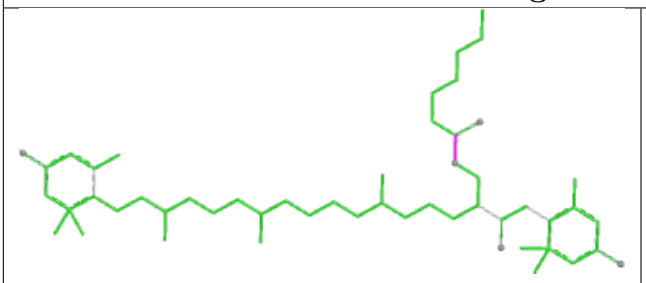


Torsions

Rings

Ligand 0UR 1 316



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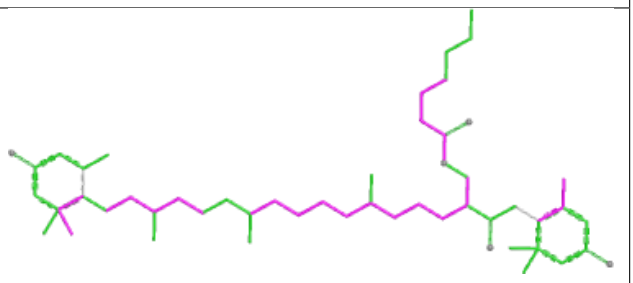
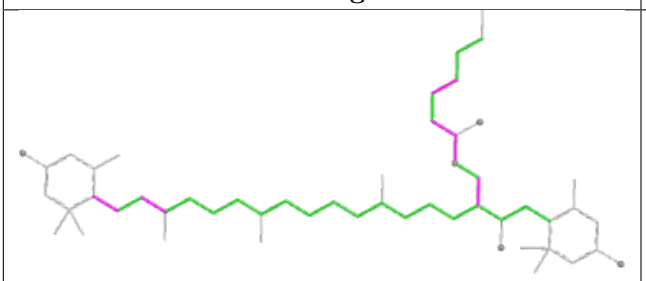


Bond angles



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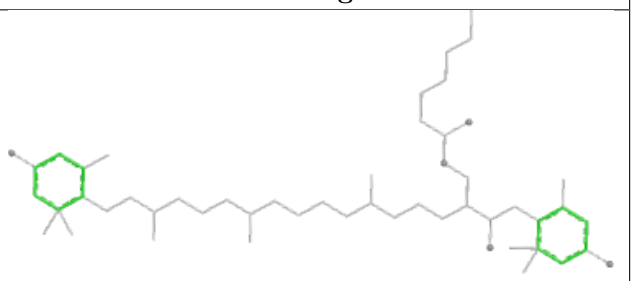
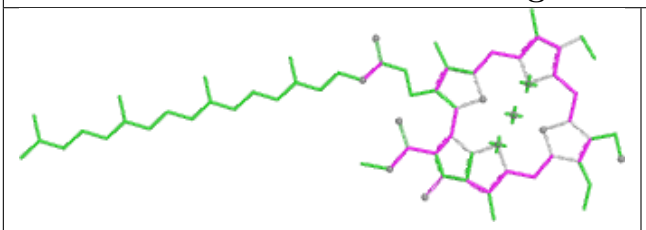


Rings

Ligand CHL 3 307



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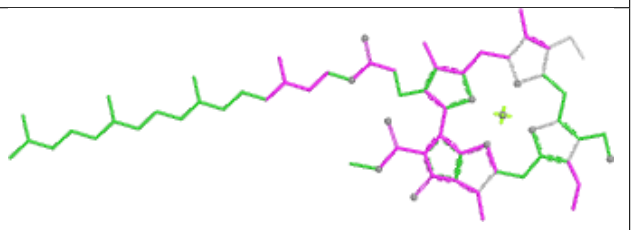

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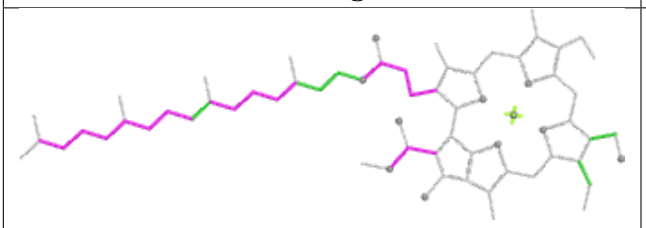

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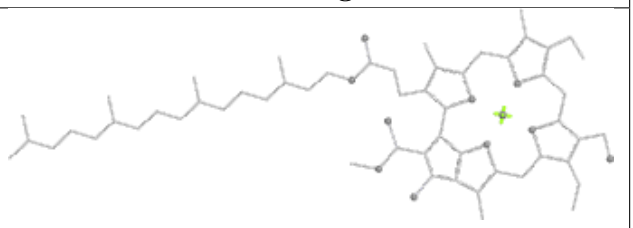
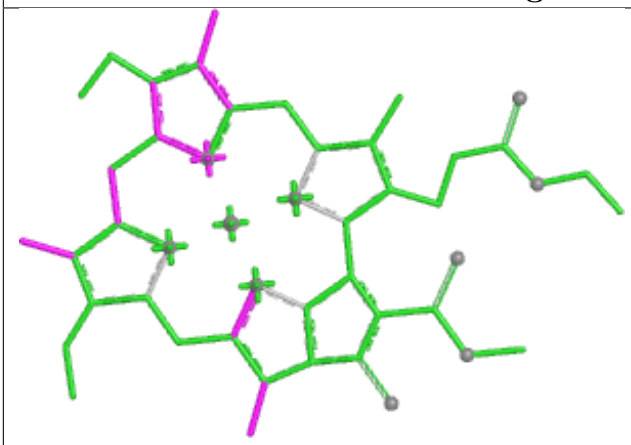


Rings

Ligand CLA F 302



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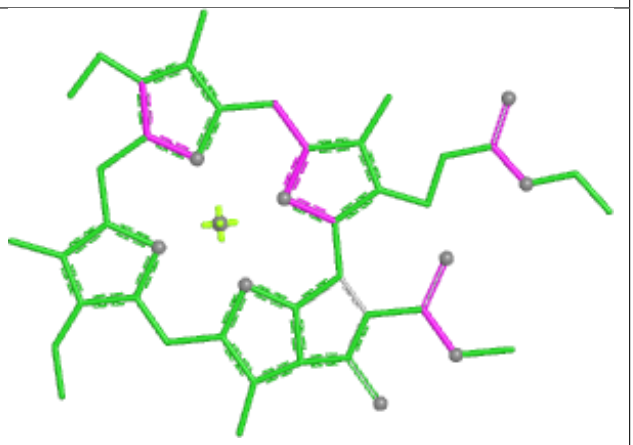
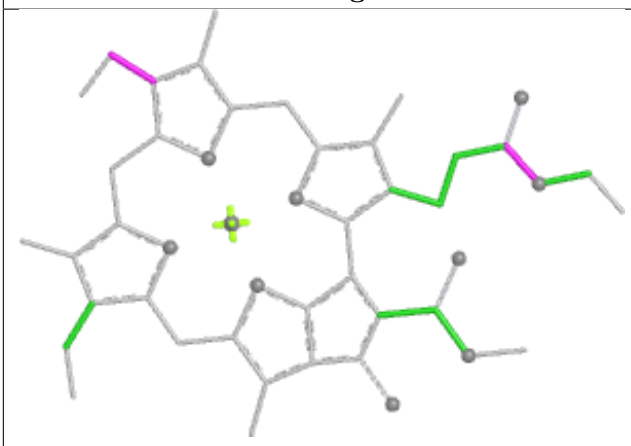


Bond angles



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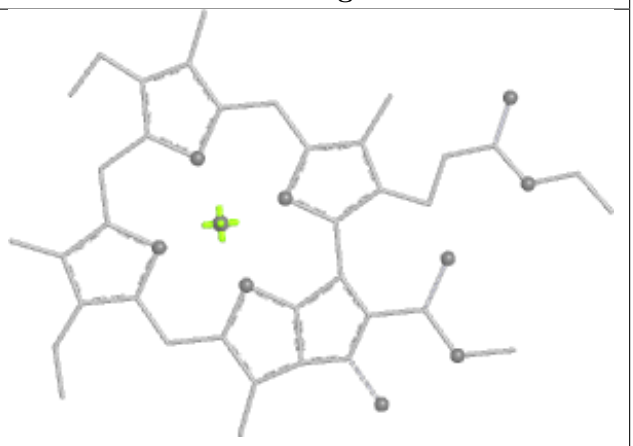
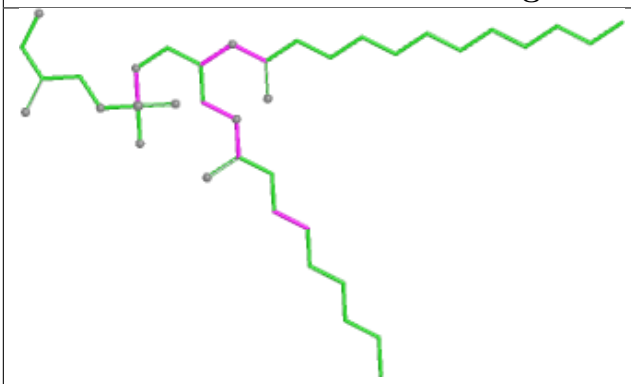


Rings

Ligand LHG B 852



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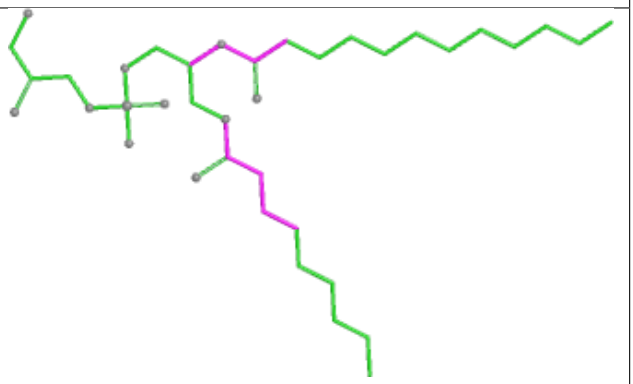

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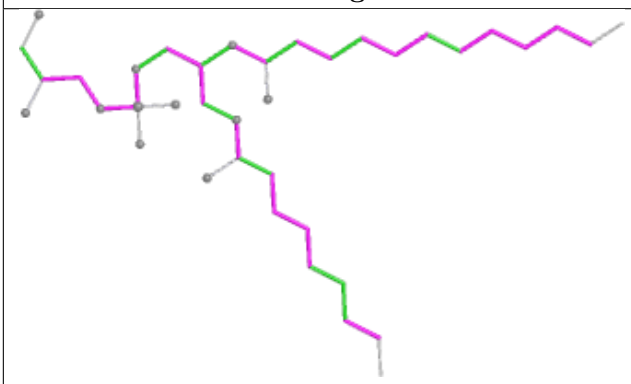

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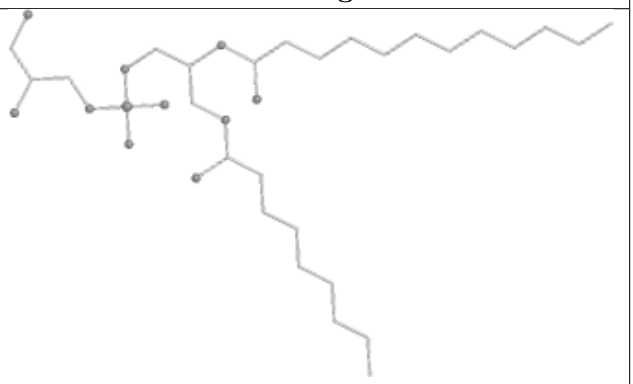
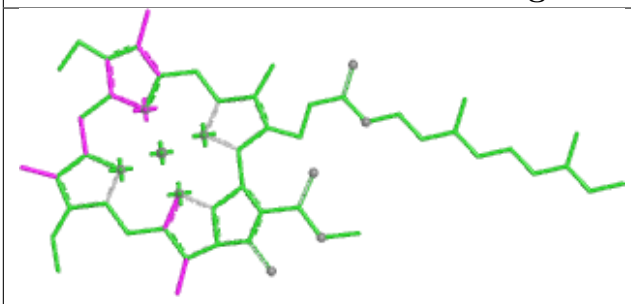


Rings

Ligand CLA 5 311



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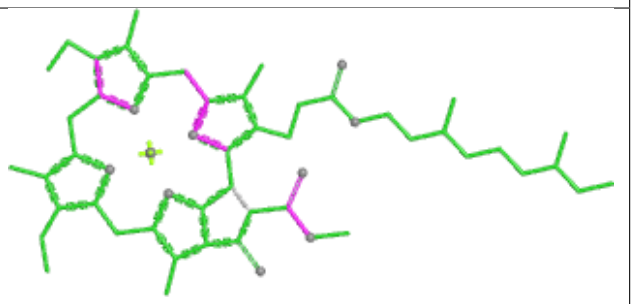

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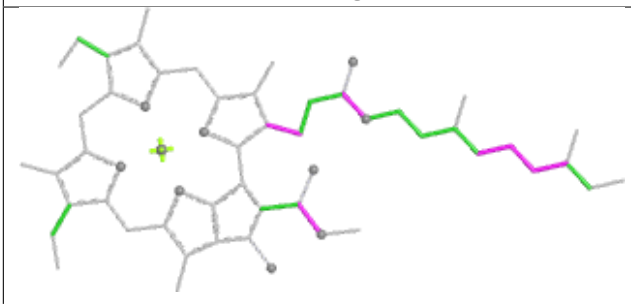

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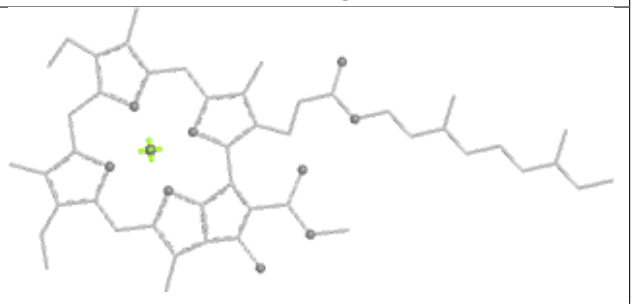
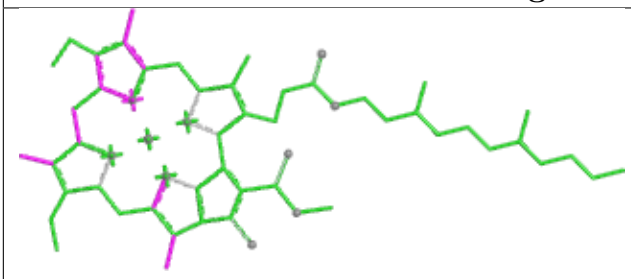


Rings

Ligand CLA 6 309



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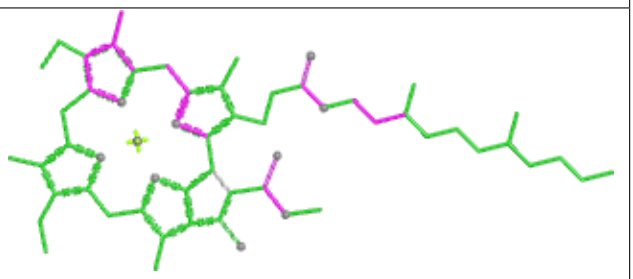

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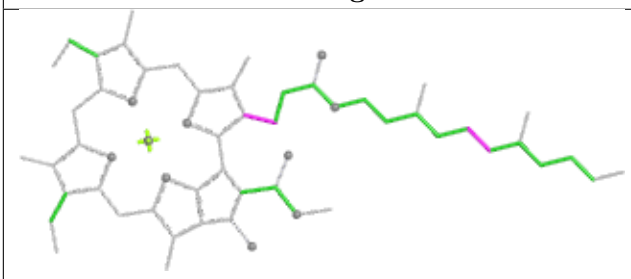

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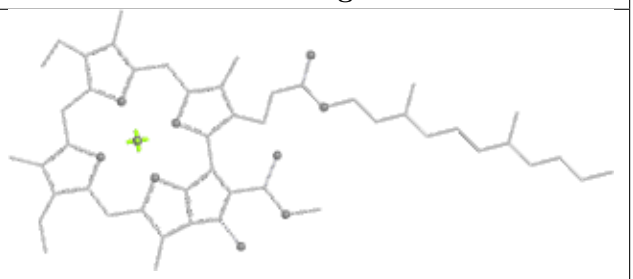
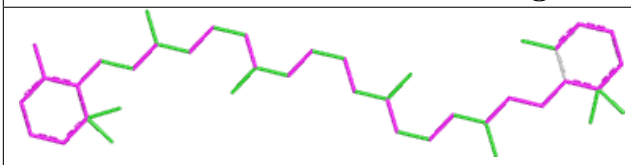


Rings

Ligand 8CT J 101



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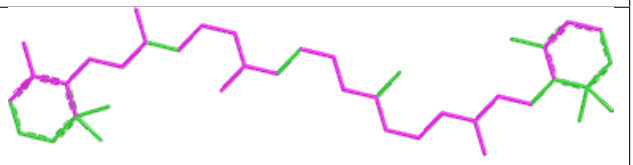
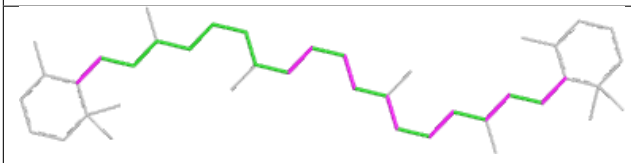


Bond angles



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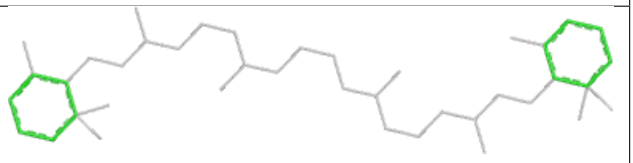
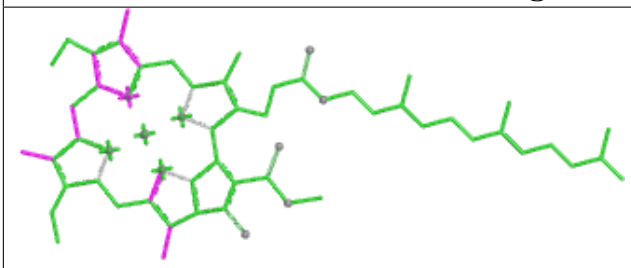


Rings

Ligand CLA 5 308



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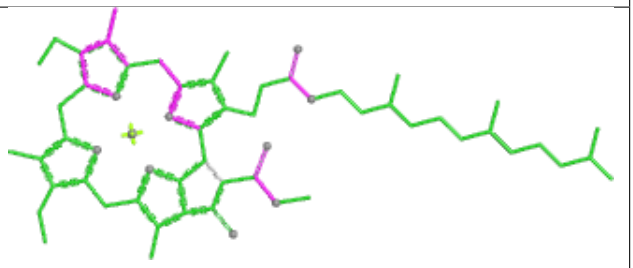
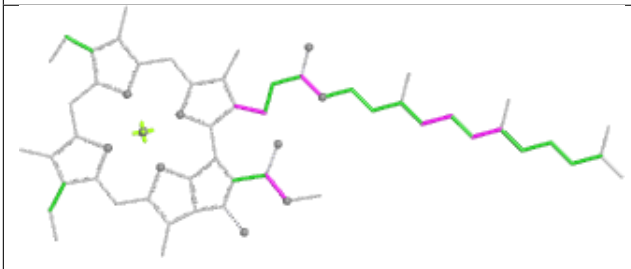


Bond angles



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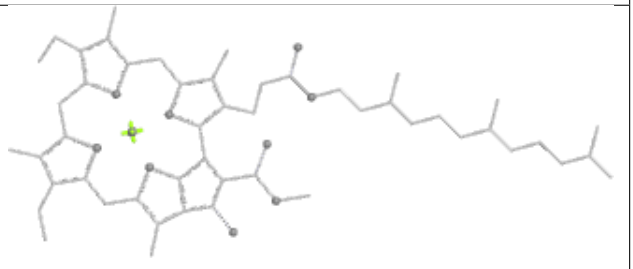
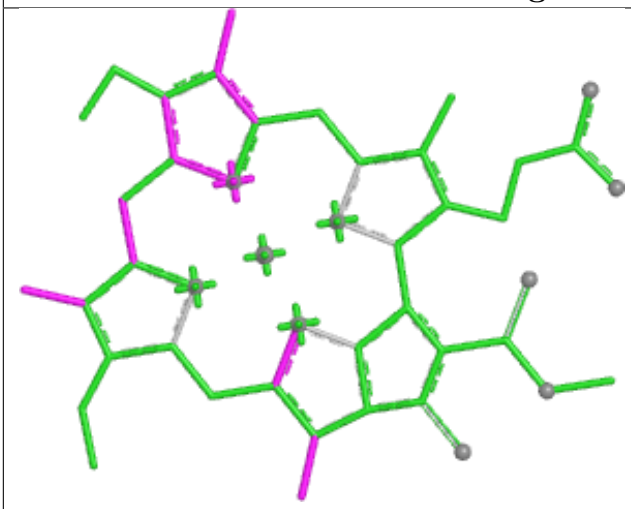
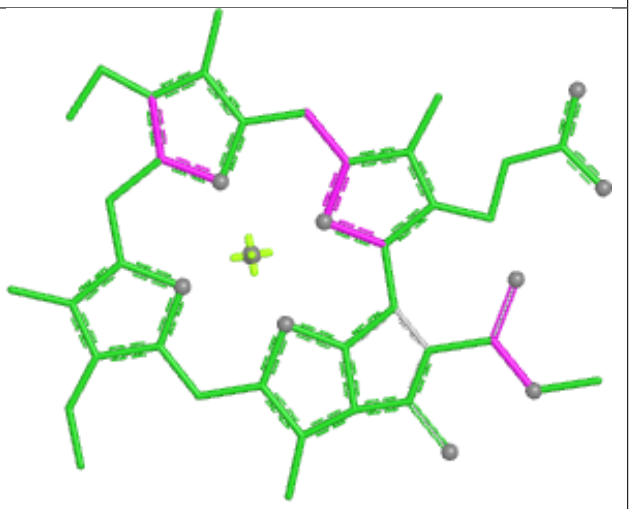


Rings

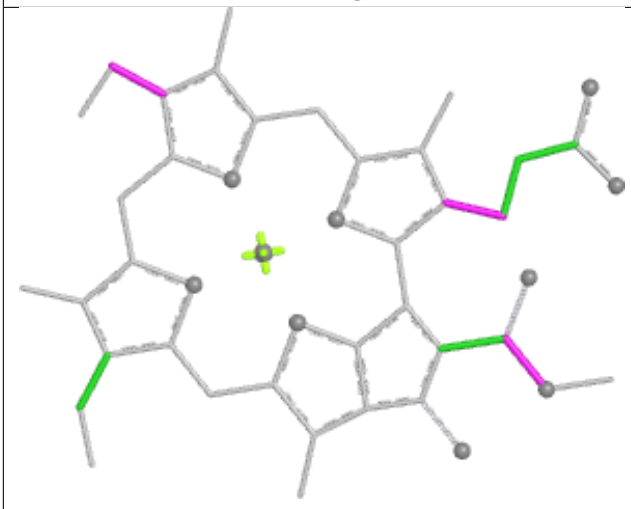
Ligand CLA 5 309



Bond lengths



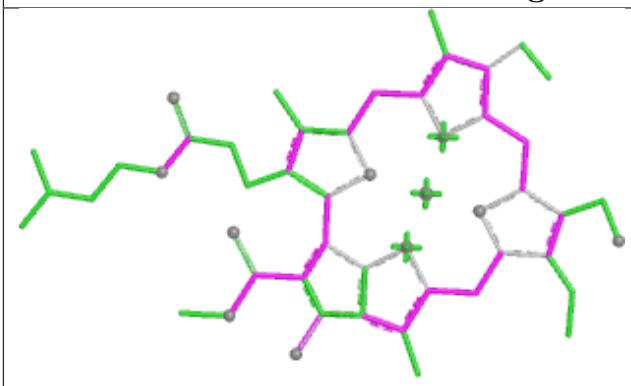
Bond angles



Torsions

Rings

Ligand CHL 6 306



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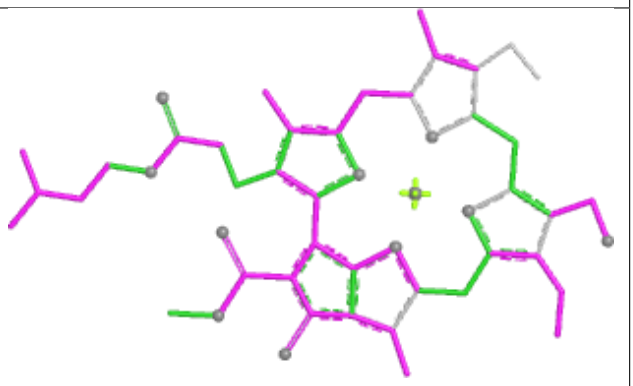
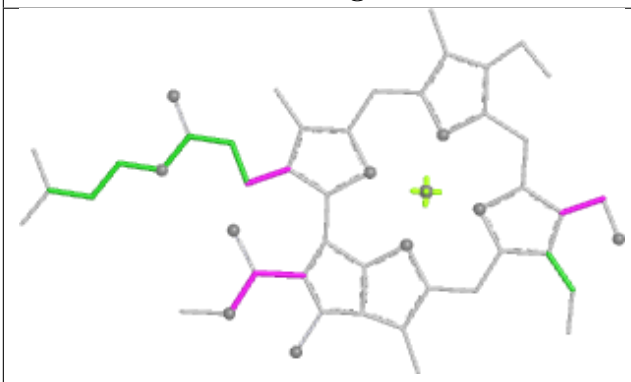
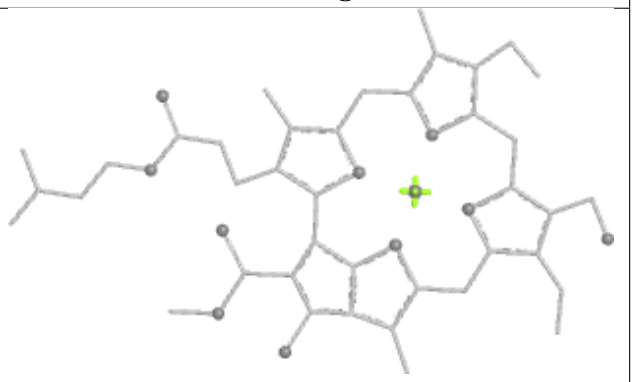


Bond angles

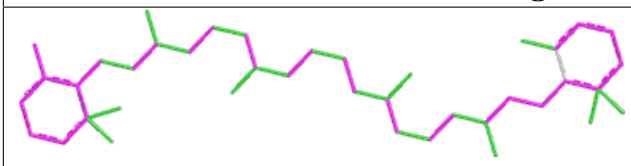


Torsions

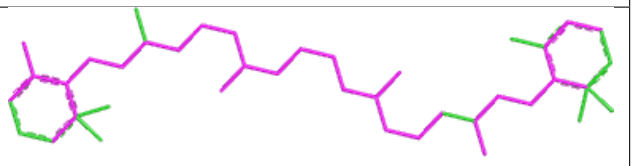


Rings

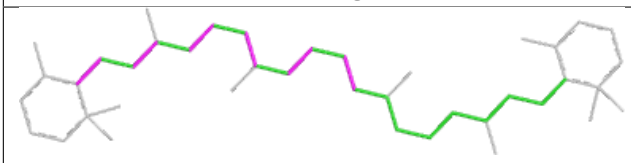
Ligand 8CT L 207



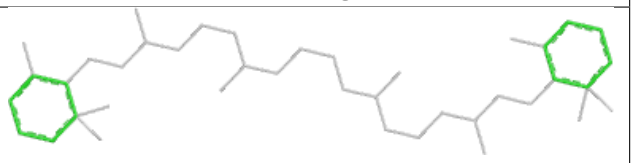
Bond lengths



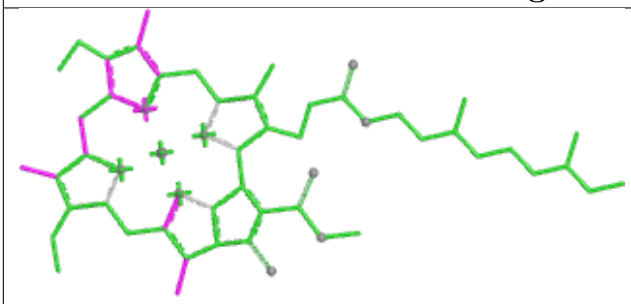
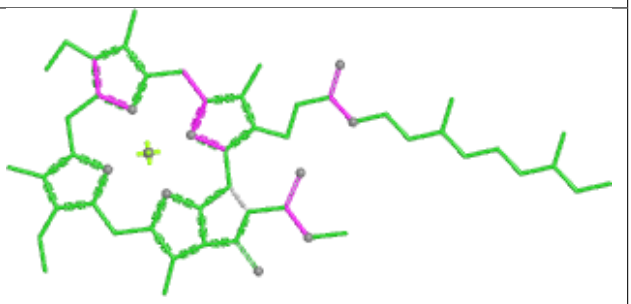
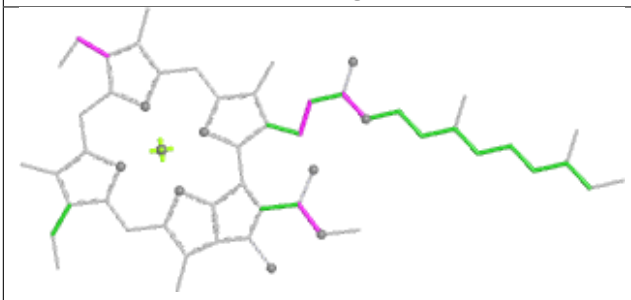
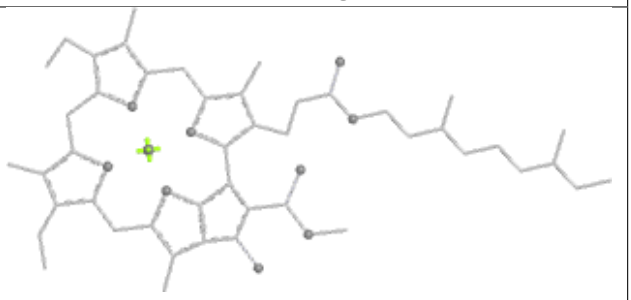
Bond angles

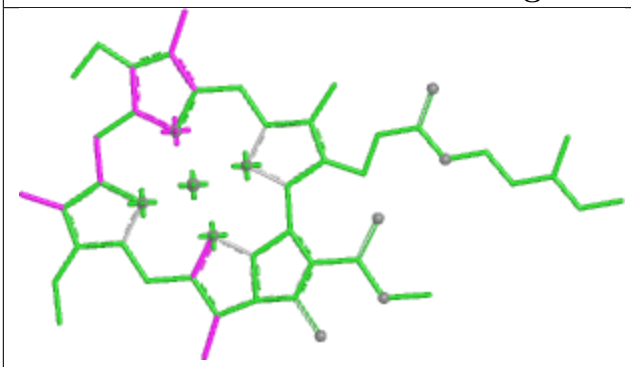
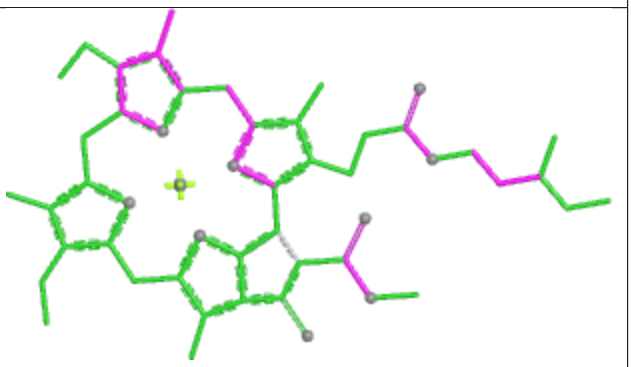
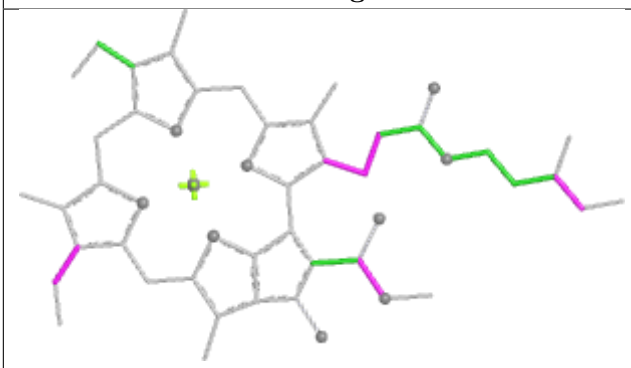
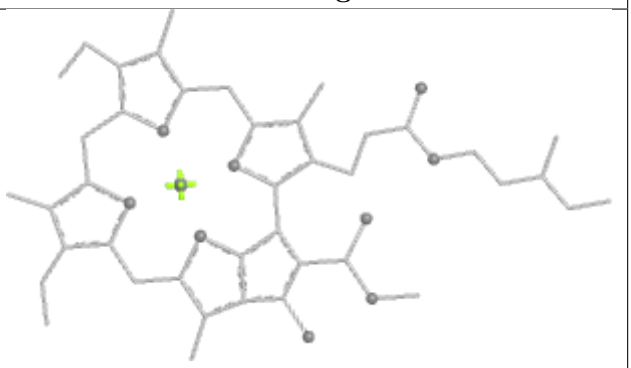


Torsions

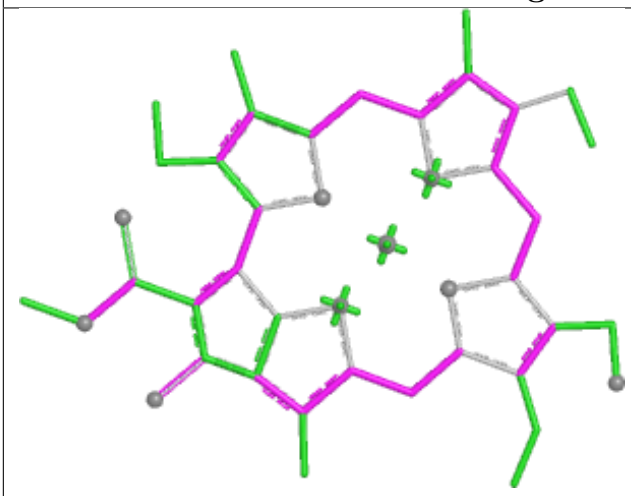


Rings

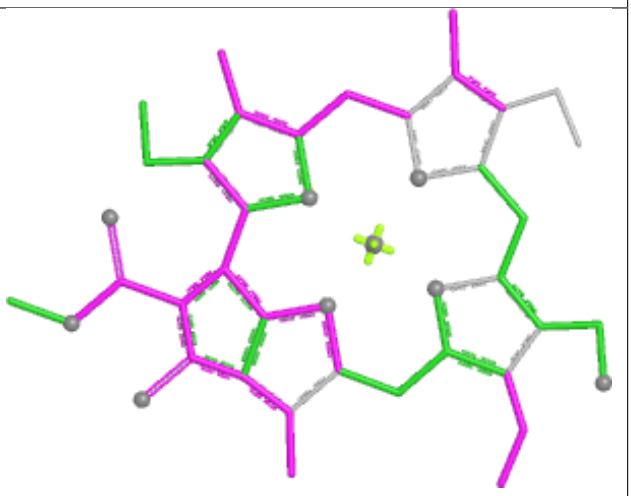
Ligand CLA 6 312	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA A 835	
	
Bond lengths	Bond angles
	
Torsions	Rings

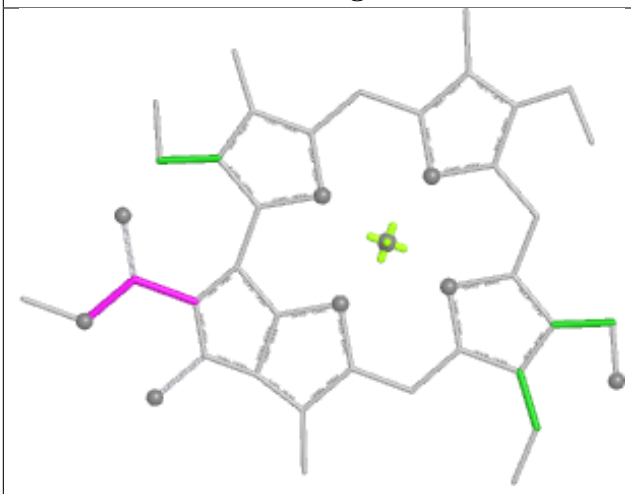
Ligand CHL 6 315



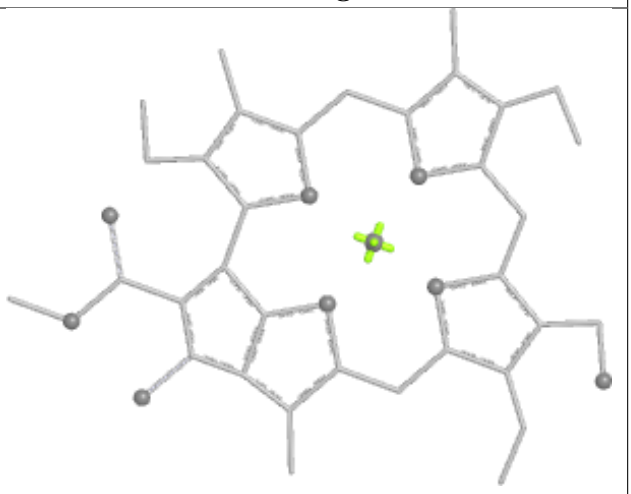
Bond lengths



Bond angles

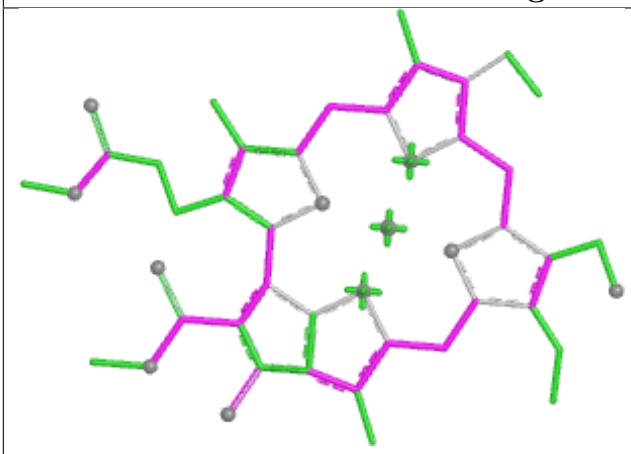


Torsions



Rings

Ligand CHL 2 307



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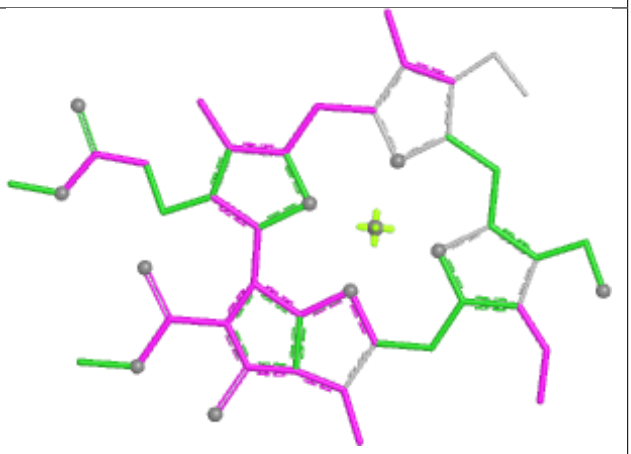
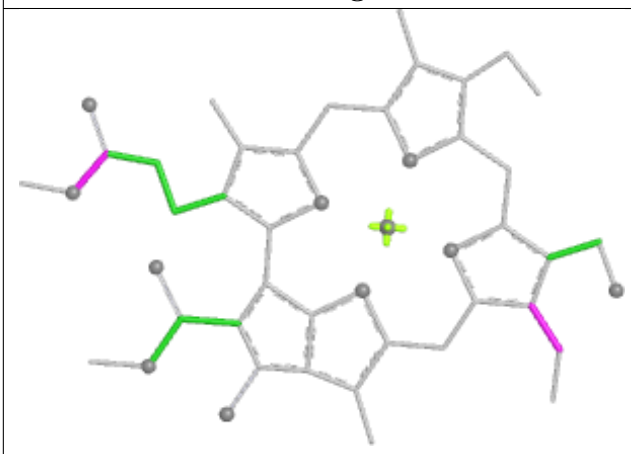


Bond angles



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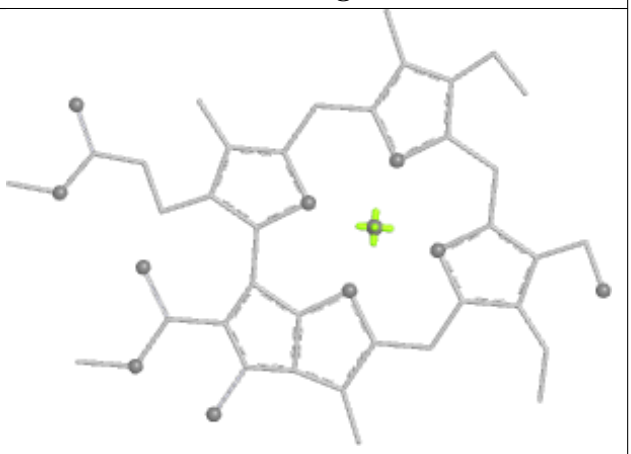
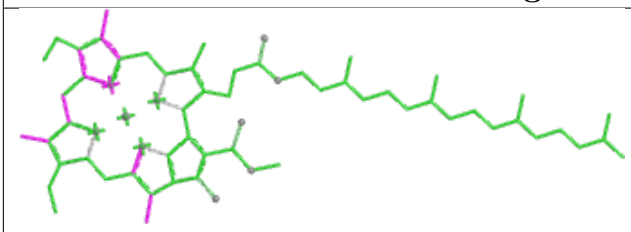


Rings

Ligand CLA A 805



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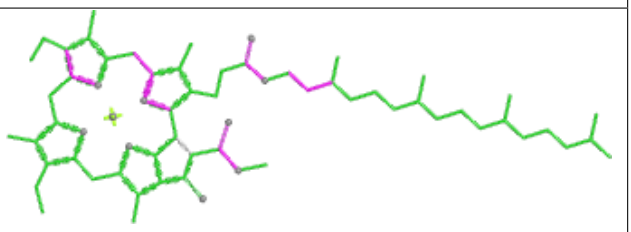
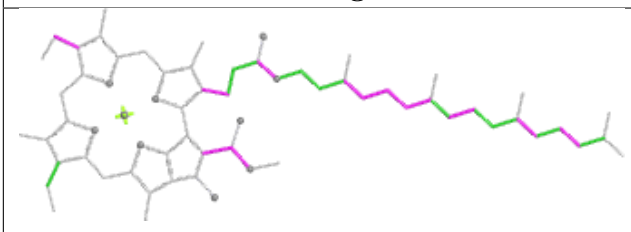


Bond angles



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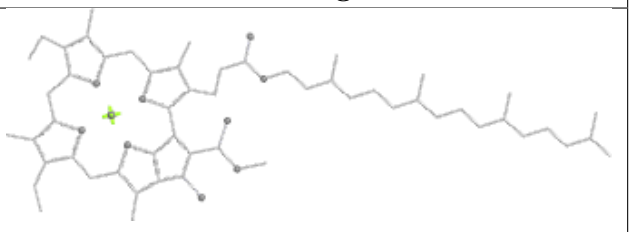
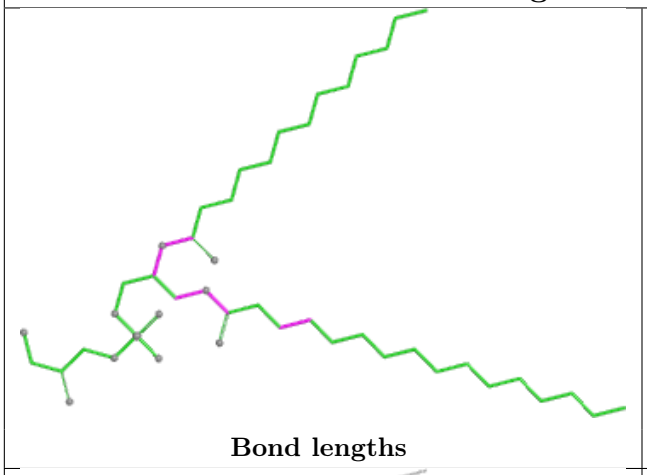
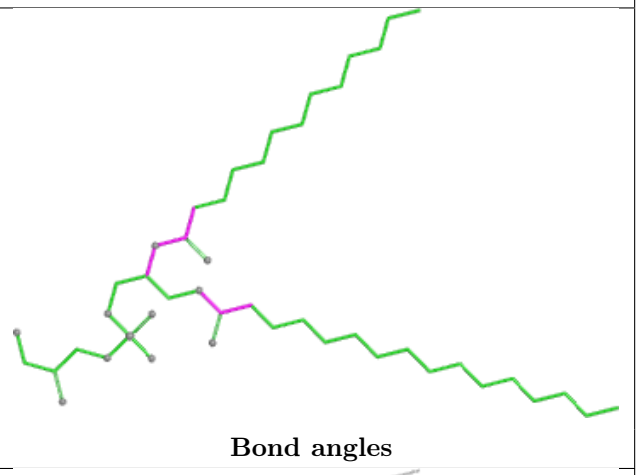


Rings

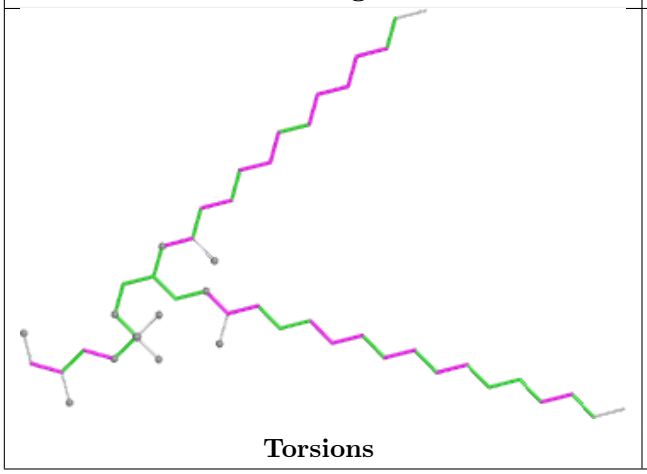
Ligand LHG I 102



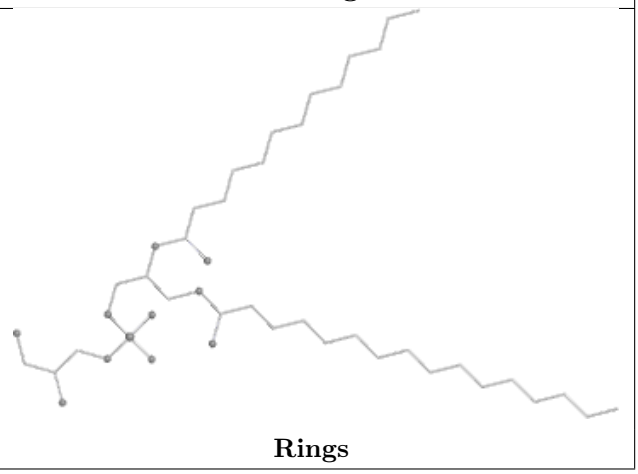
Bond lengths



Bond angles

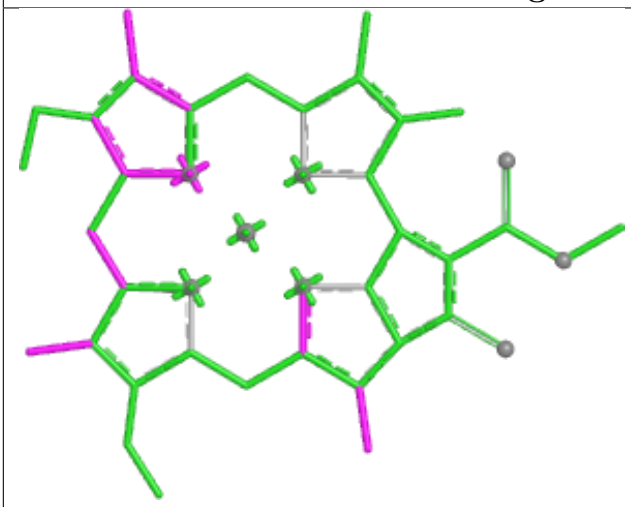


Torsions



Rings

Ligand CLA 0 309



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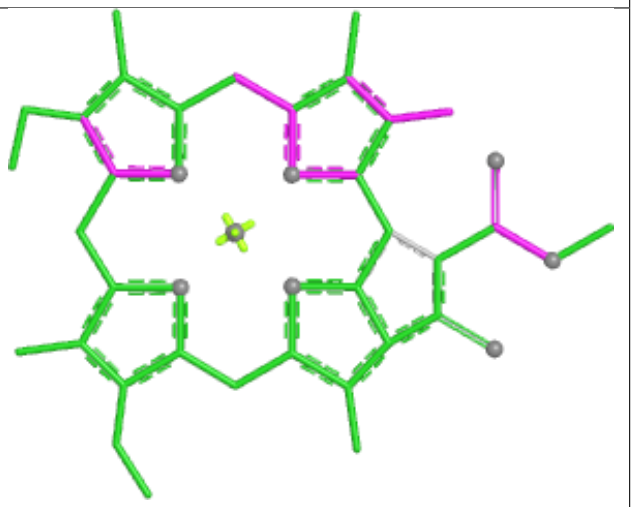
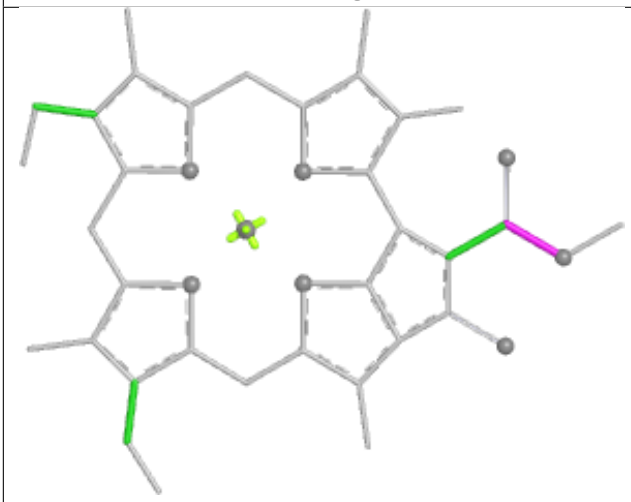


Bond angles



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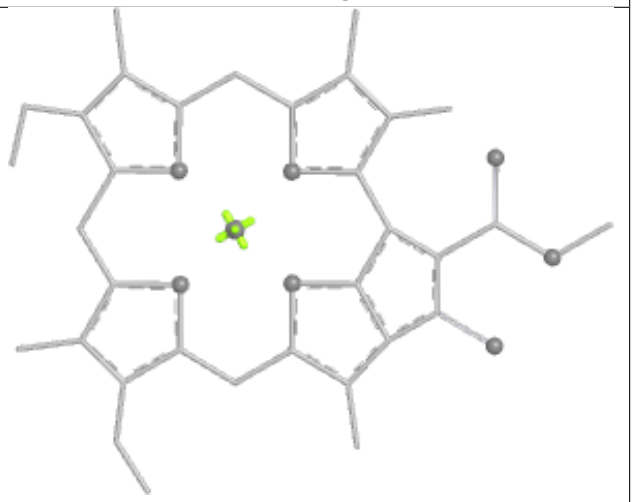
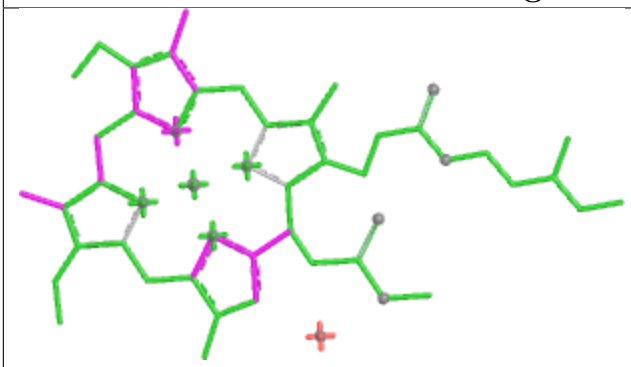


Rings

Ligand CLA B 826



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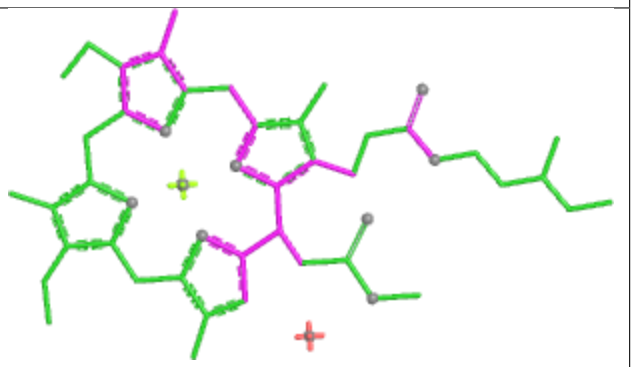
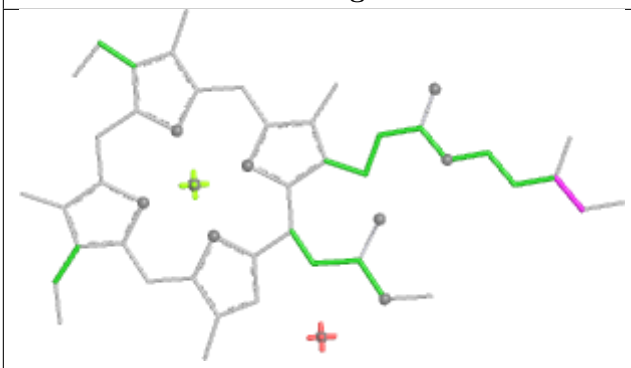
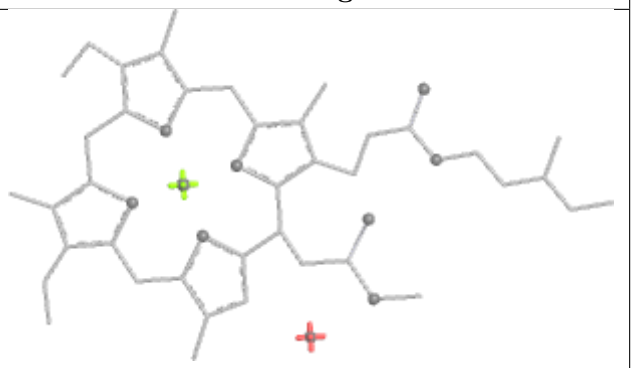


Bond angles

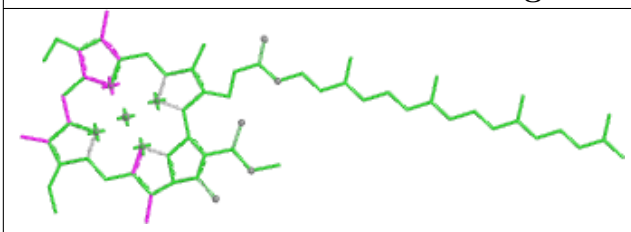


Torsions



Rings

Ligand CLA B 811



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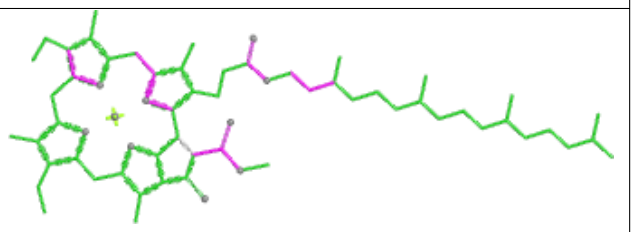
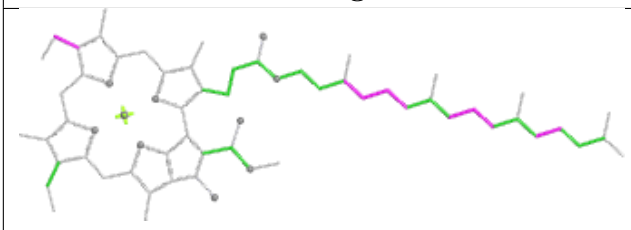
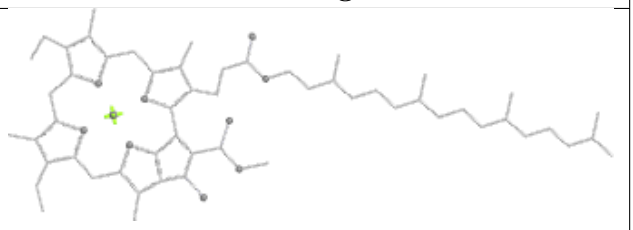


Bond angles

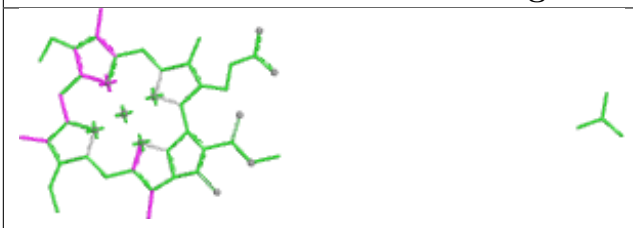


Torsions

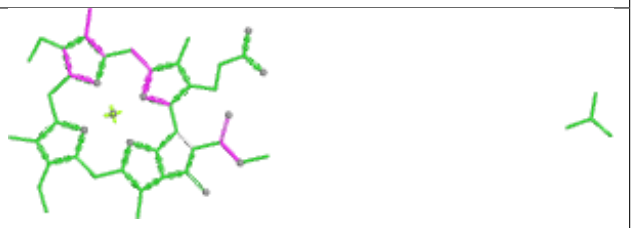


Rings

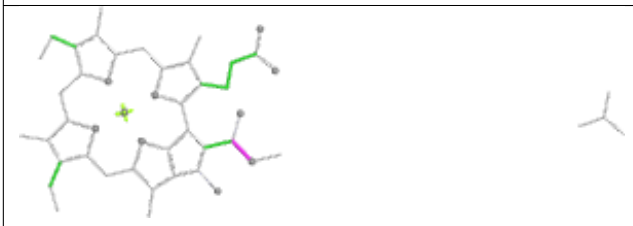
Ligand CLA 7 315



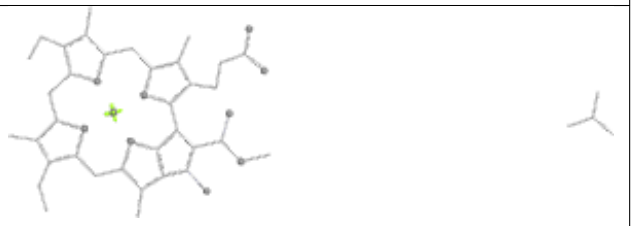
Bond lengths



Bond angles

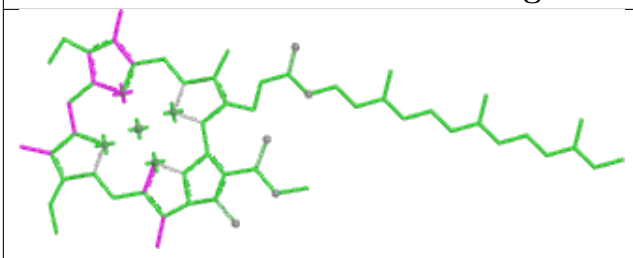


Torsions

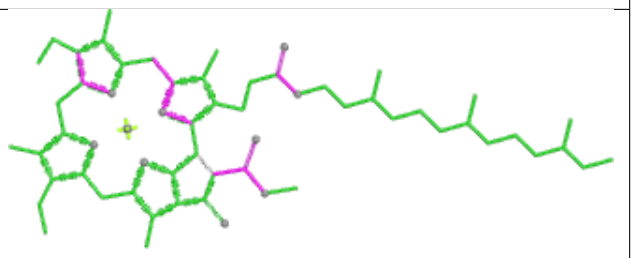


Rings

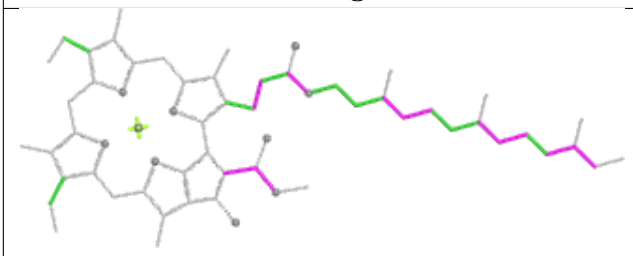
Ligand CLA A 816



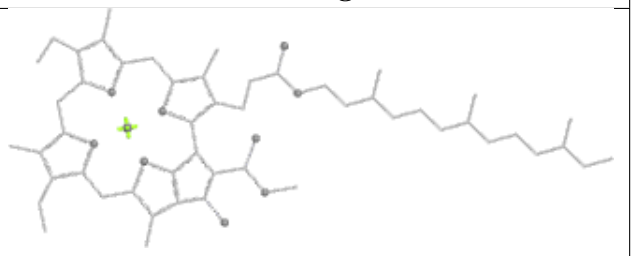
Bond lengths



Bond angles

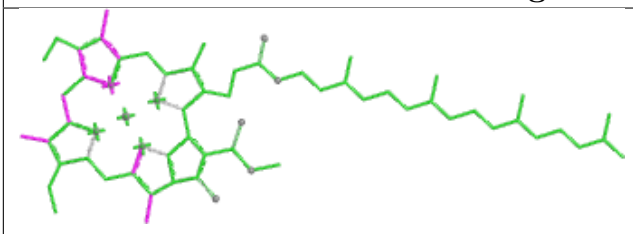


Torsions

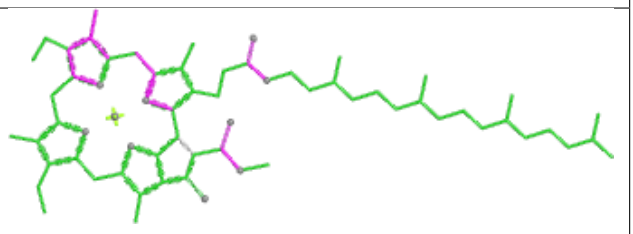


Rings

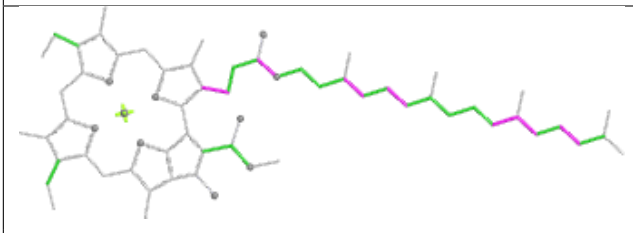
Ligand CLA 3 309



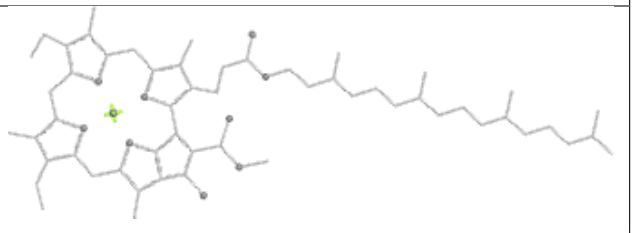
Bond lengths



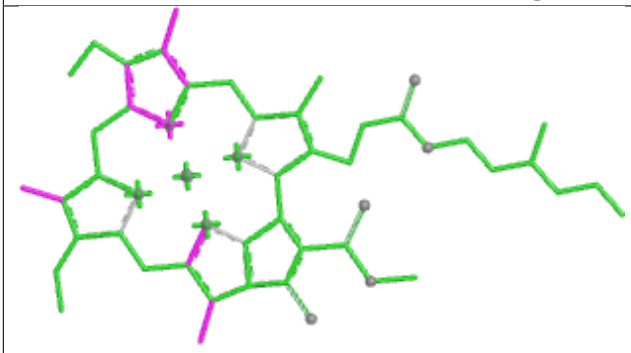
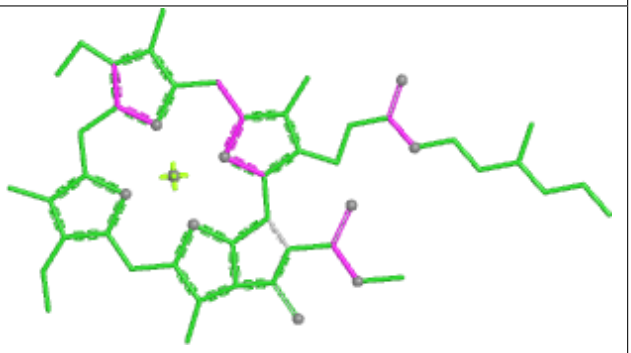
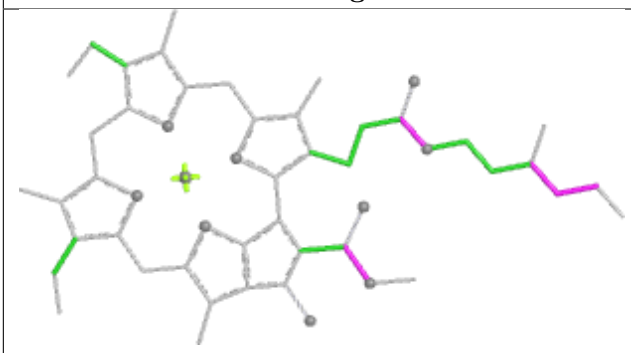
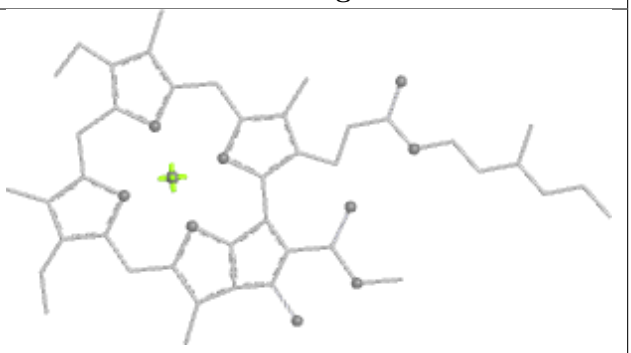
Bond angles

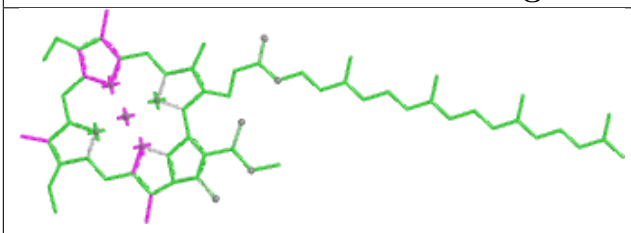
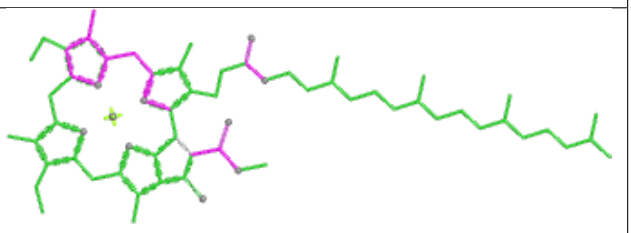
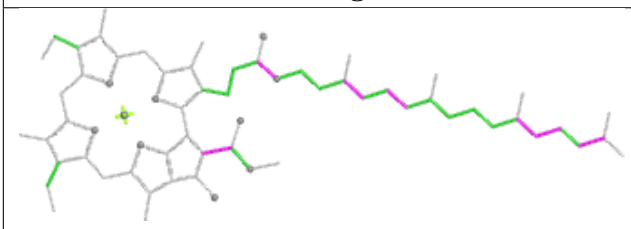
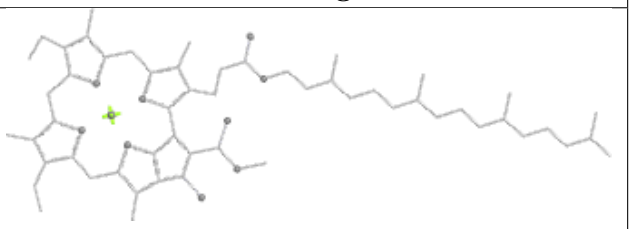


Torsions

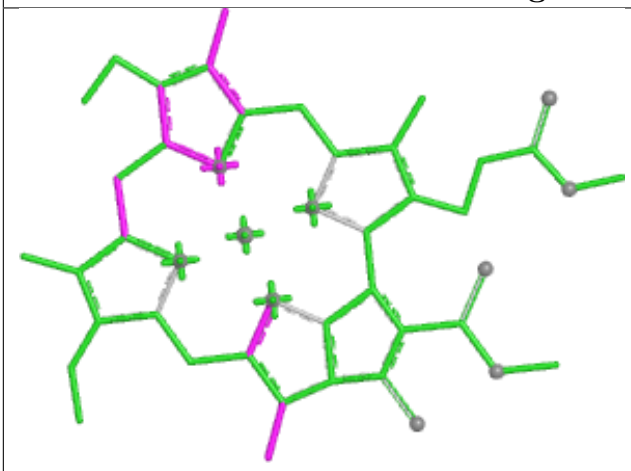


Rings

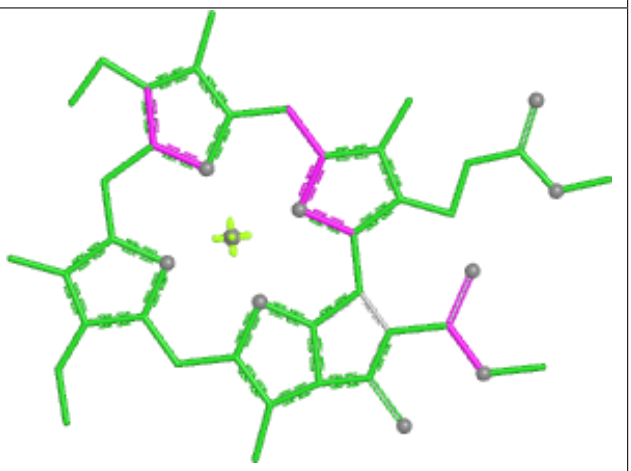
Ligand CLA 6 303	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA A 829	
 Bond lengths	 Bond angles
 Torsions	 Rings

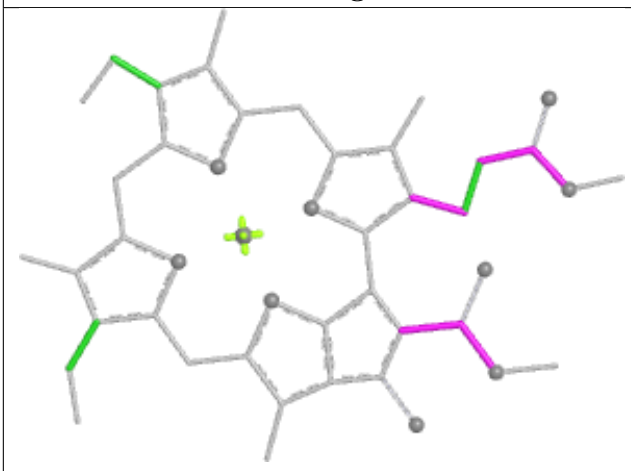
Ligand CLA 0 312



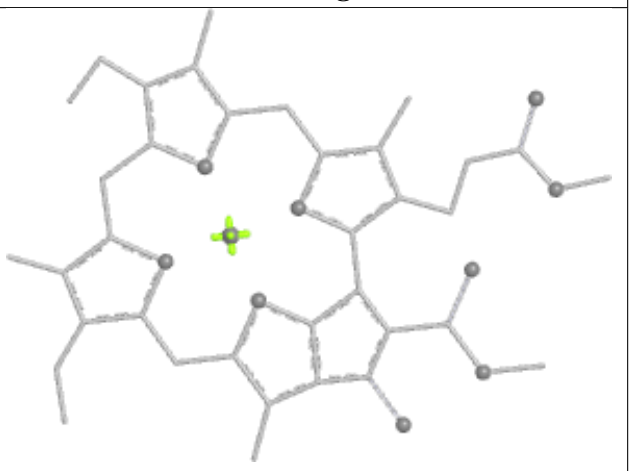
Bond lengths



Bond angles

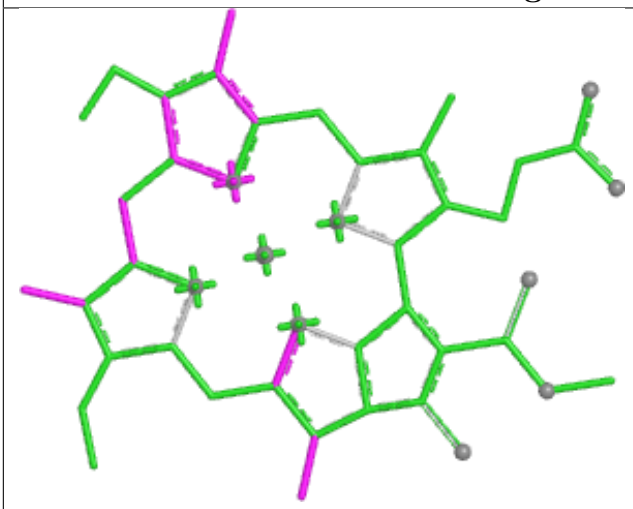


Torsions

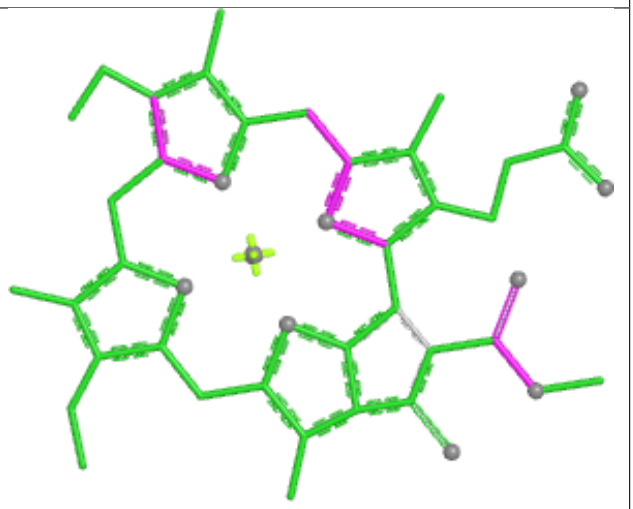


Rings

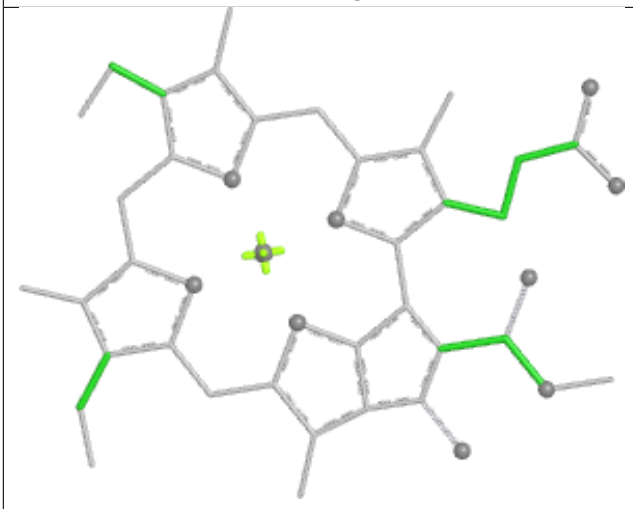
Ligand CLA B 835



Bond lengths



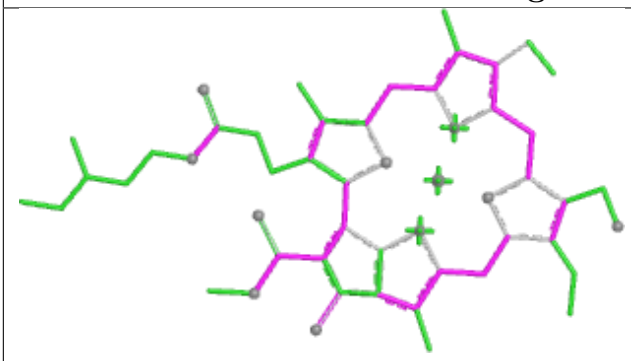
Bond angles



Torsions

Rings

Ligand CHL 8 301



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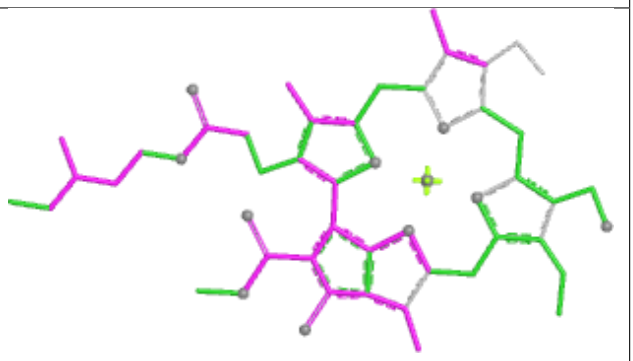
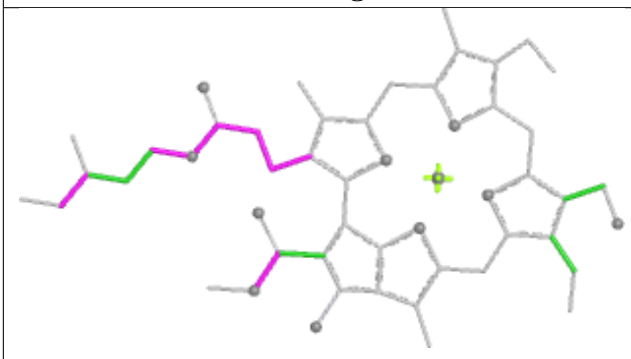
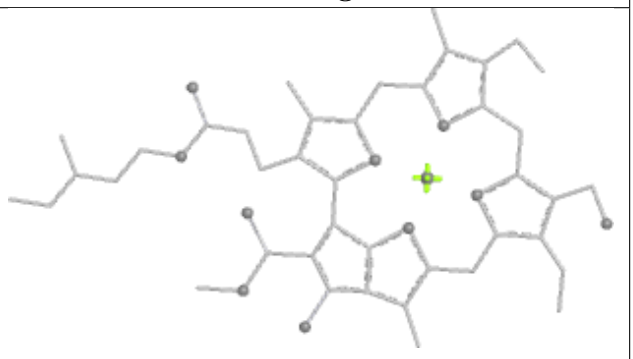


Bond angles

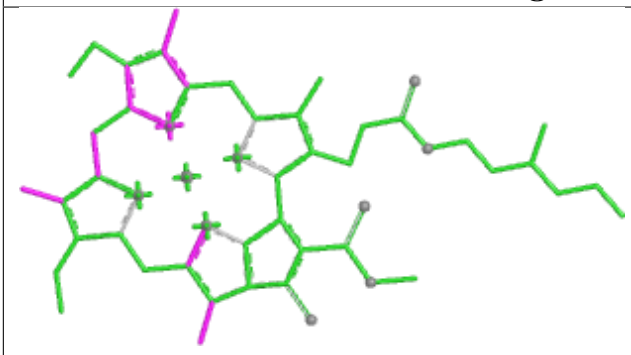


Torsions

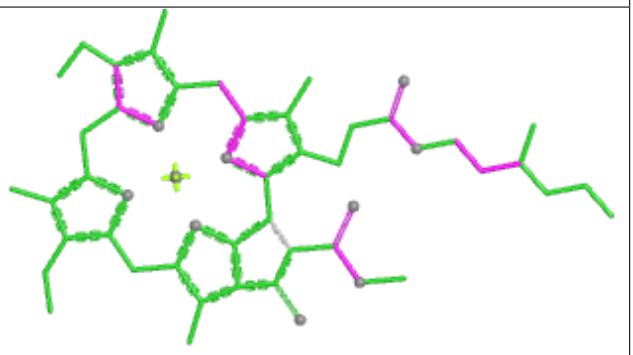


Rings

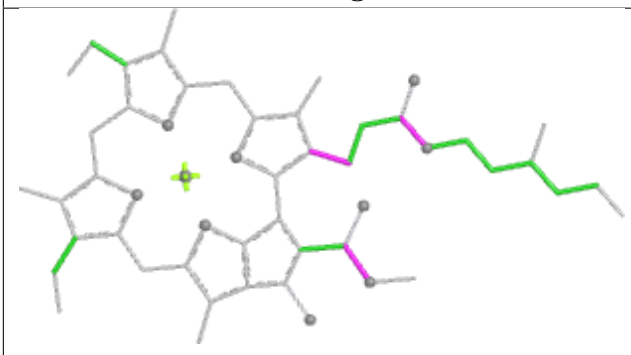
Ligand CLA 9 310



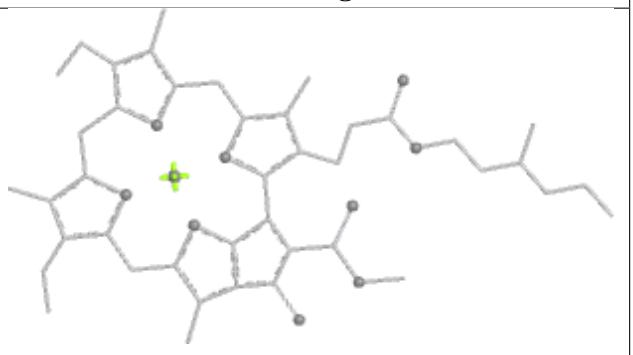
Bond lengths



Bond angles

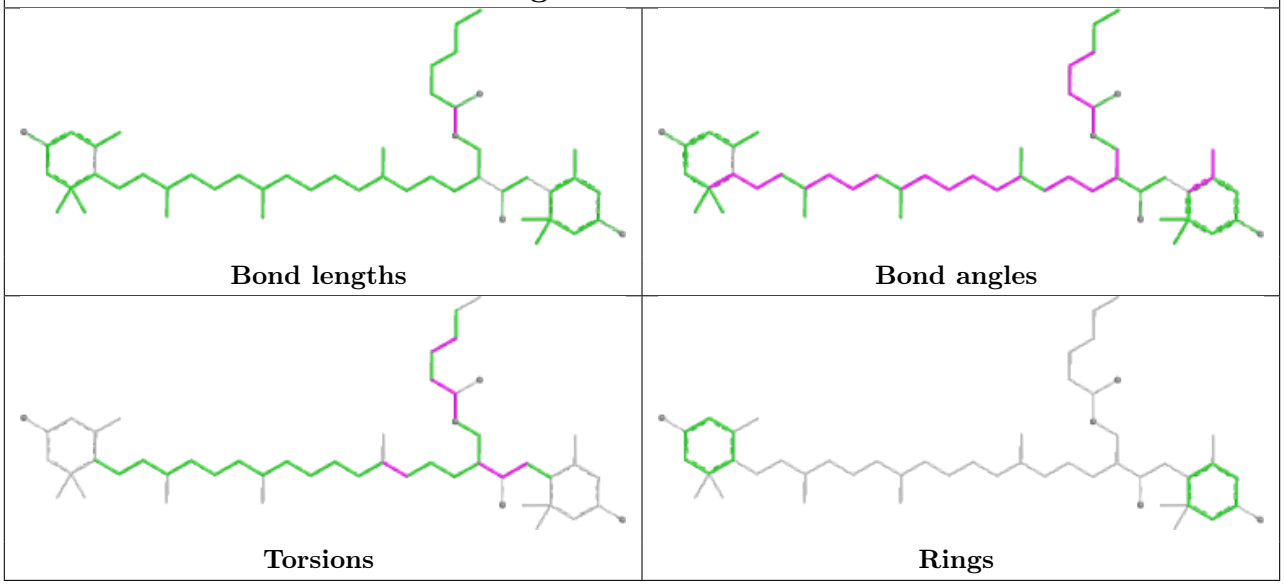


Torsions

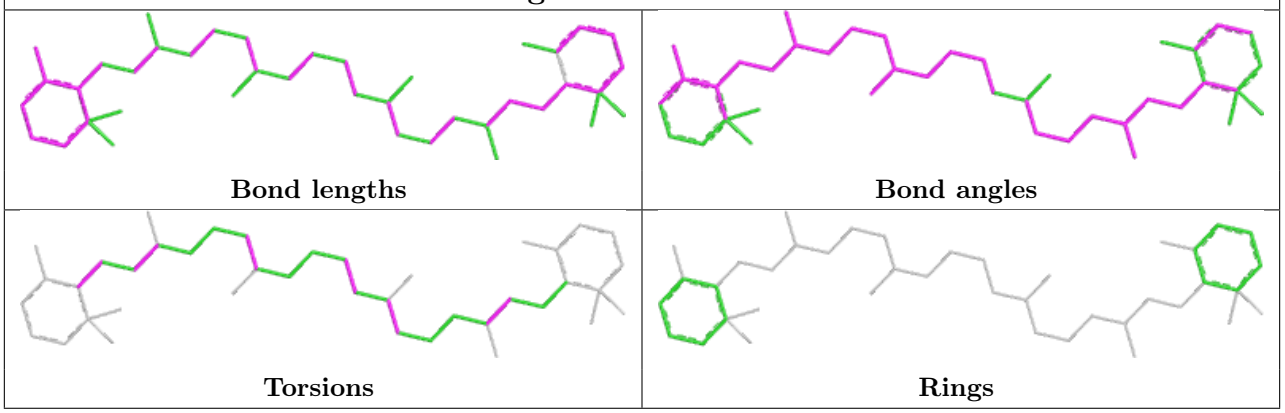


Rings

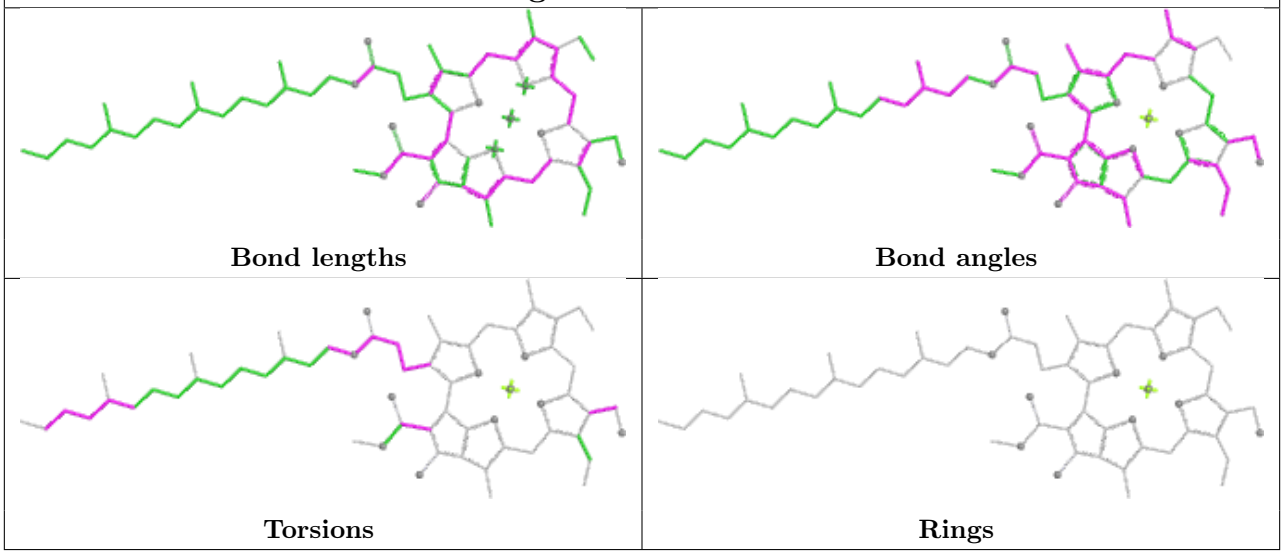
Ligand 0UR 5 314



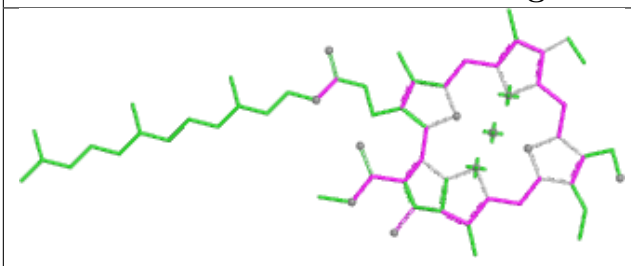
Ligand 8CT A 847



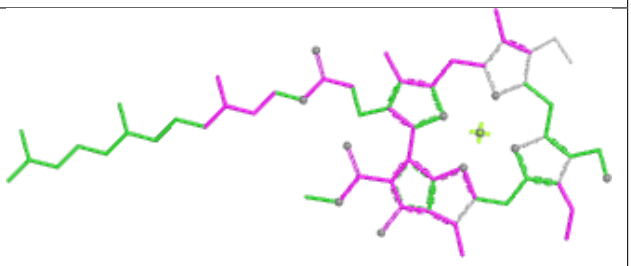
Ligand CHL 1 301



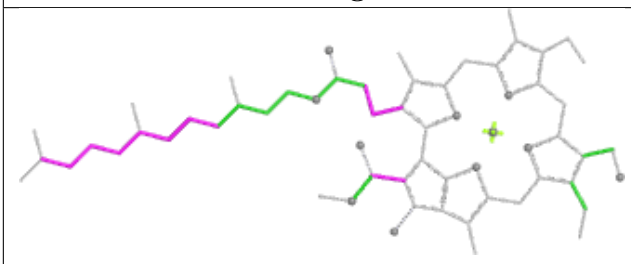
Ligand CHL 6 301



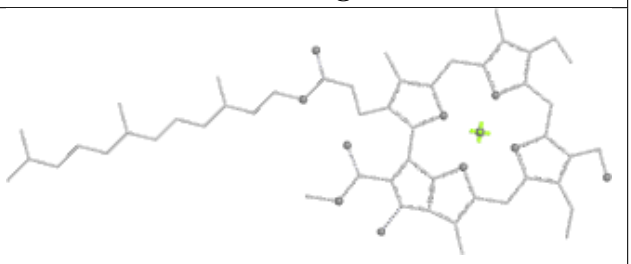
Bond lengths



Bond angles

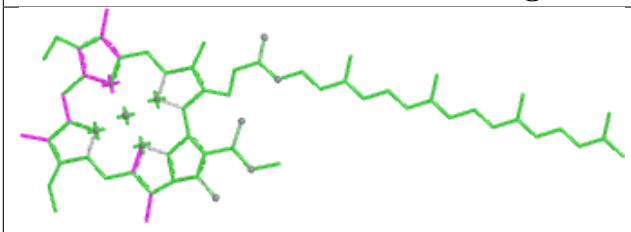


Torsions

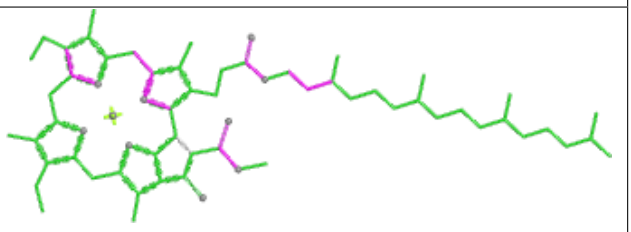


Rings

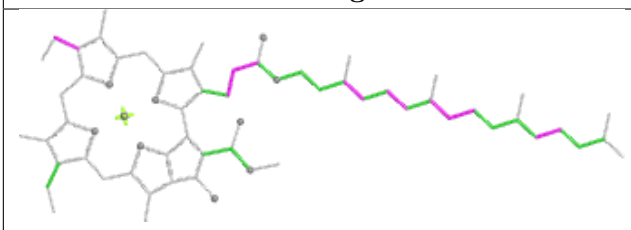
Ligand CLA A 808



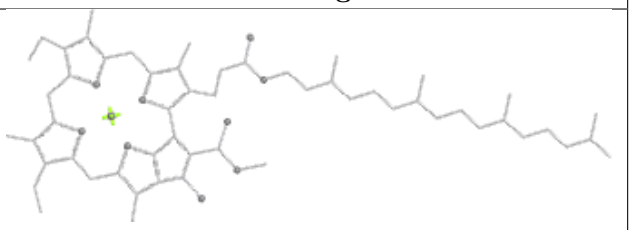
Bond lengths



Bond angles

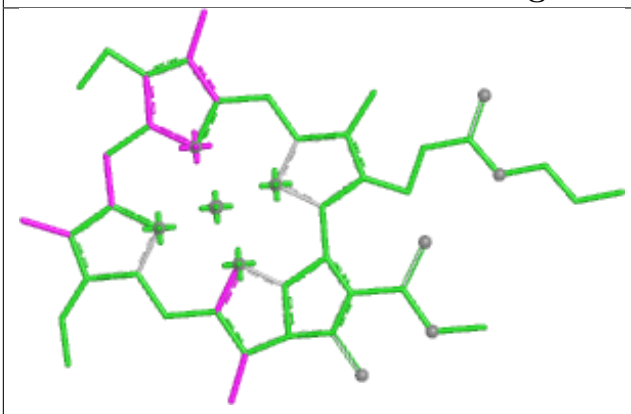


Torsions



Rings

Ligand CLA 6 311



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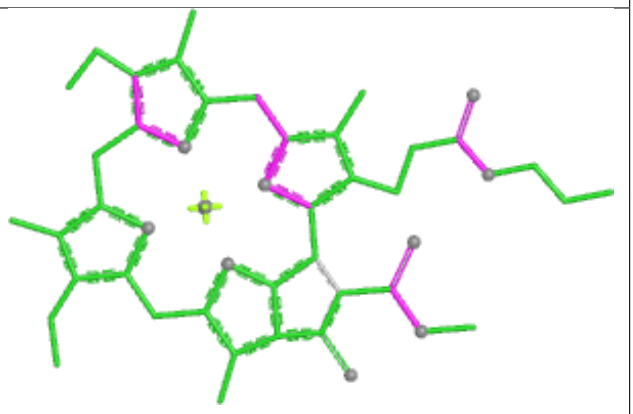
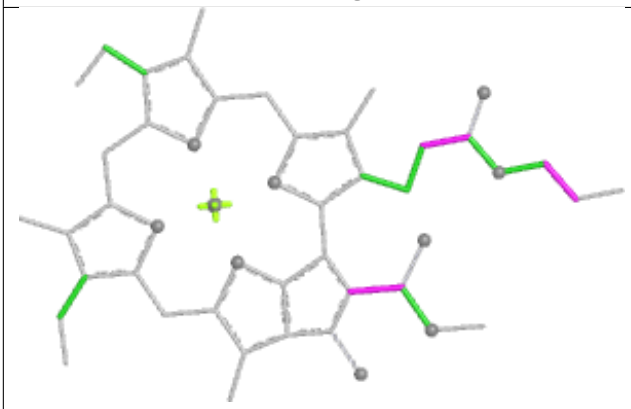


Bond angles



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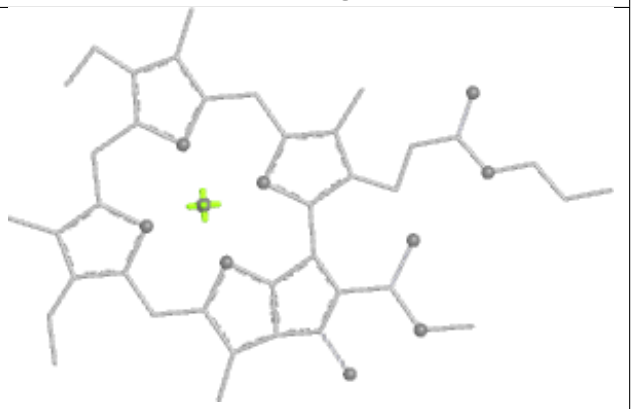
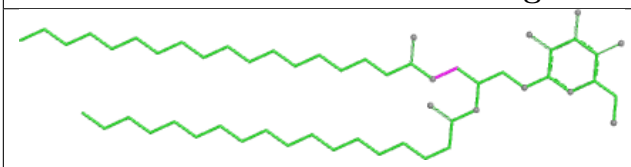


Rings

Ligand LMG 9 317



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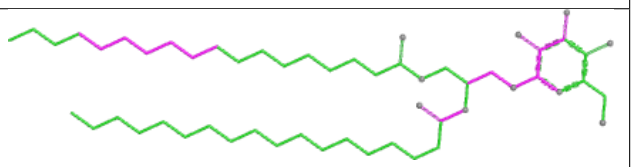
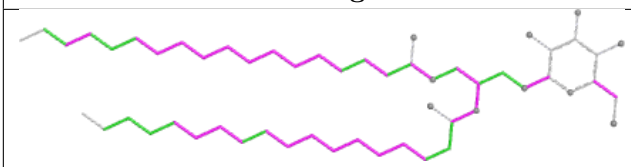


Bond angles



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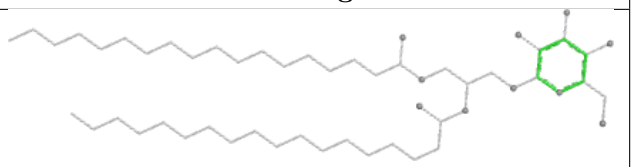
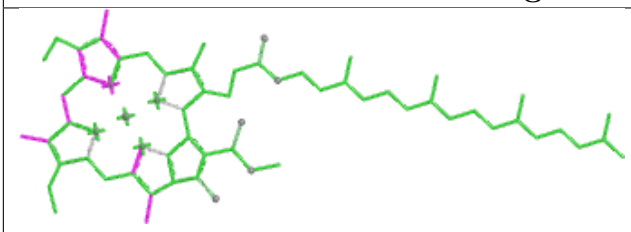


Rings

Ligand CLA B 837



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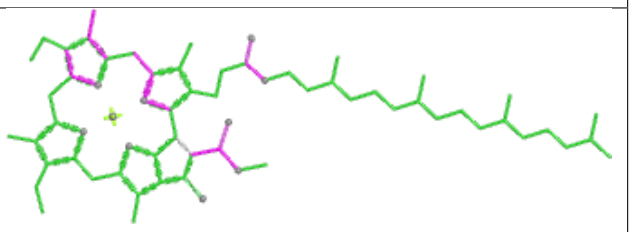
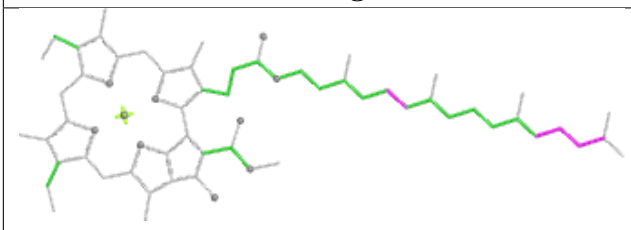


Bond angles



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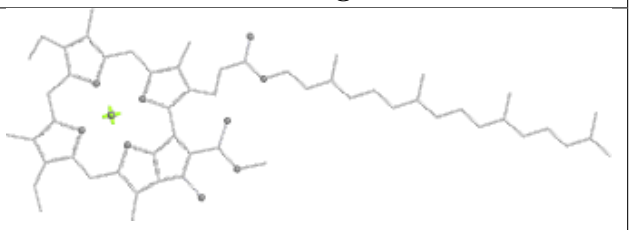
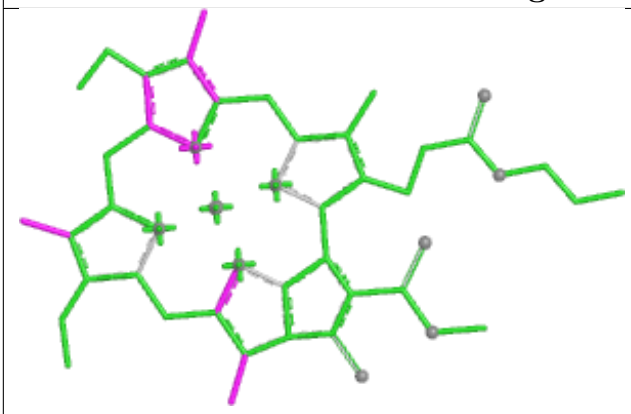
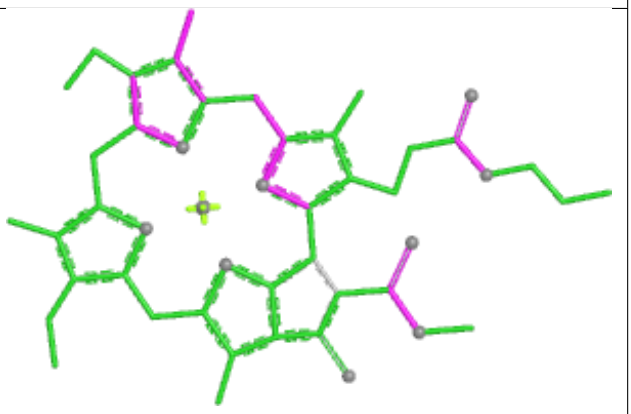


Rings

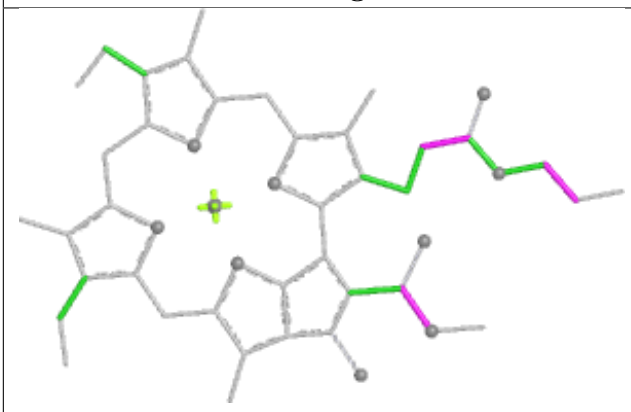
Ligand CLA 2 310



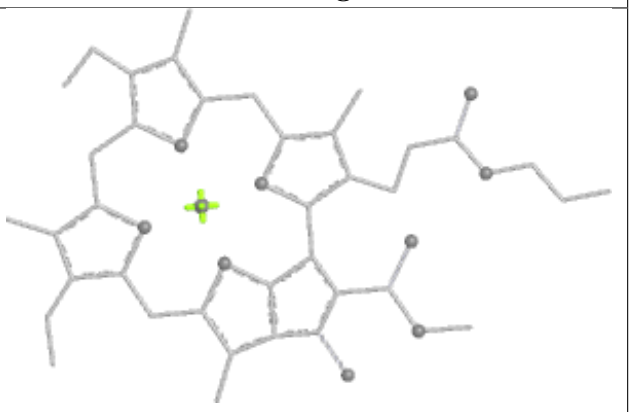
Bond lengths



Bond angles

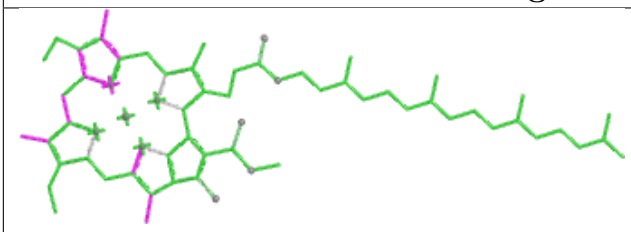


Torsions

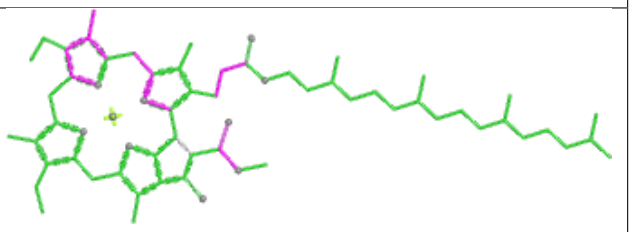


Rings

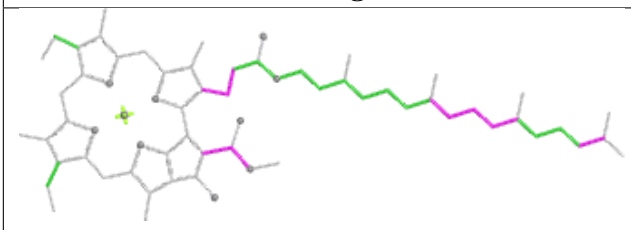
Ligand CLA 6 316



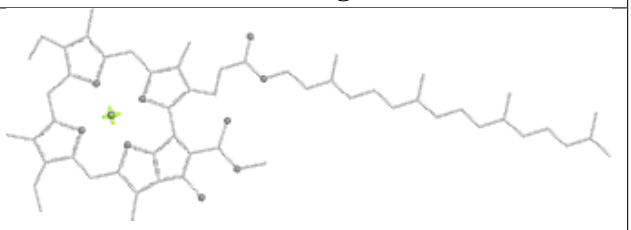
Bond lengths



Bond angles

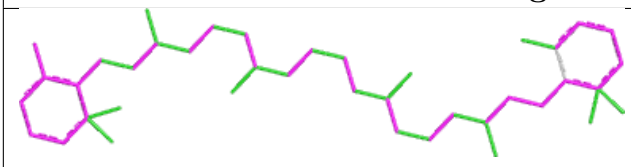


Torsions

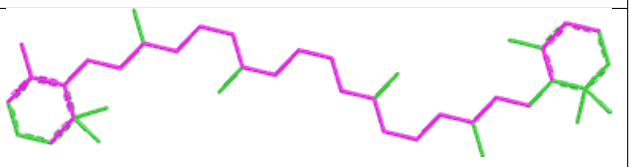


Rings

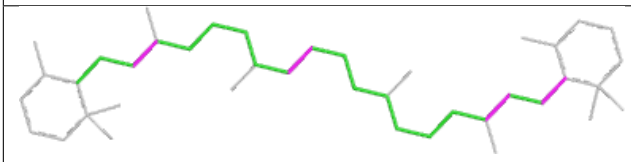
Ligand 8CT L 204



Bond lengths



Bond angles



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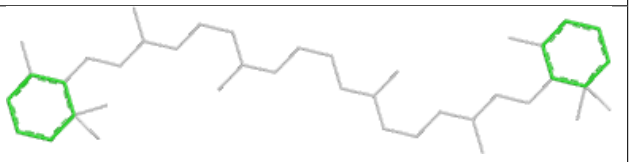
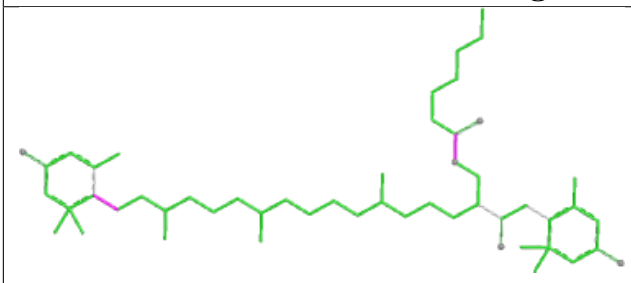


Rings

Ligand 0UR 6 321



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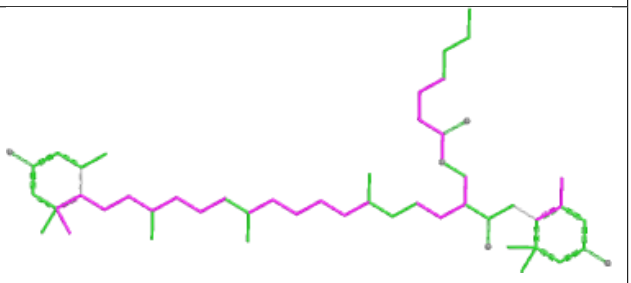
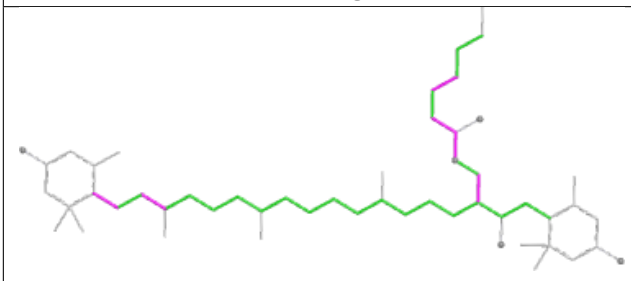


Bond angles



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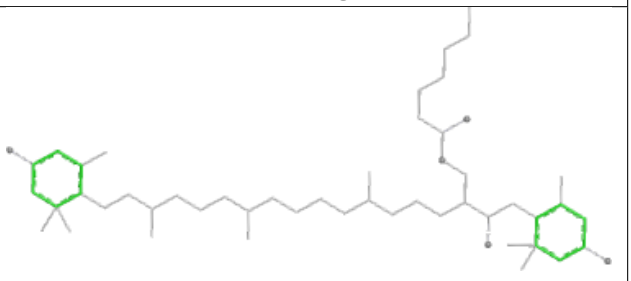
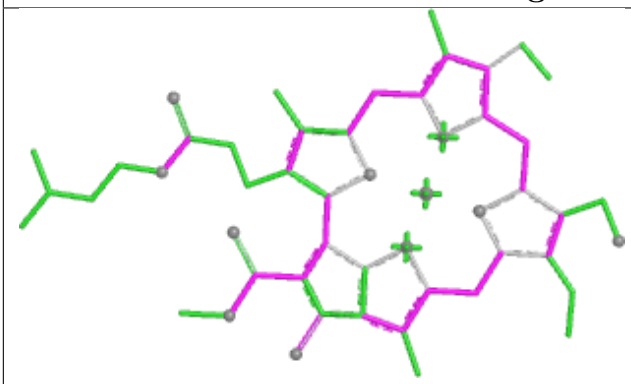


Rings

Ligand CHL 3 305



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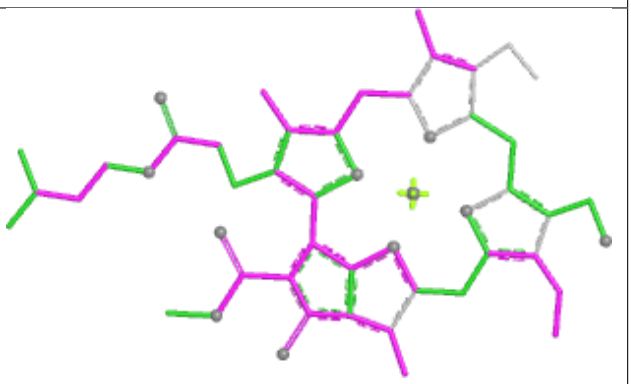
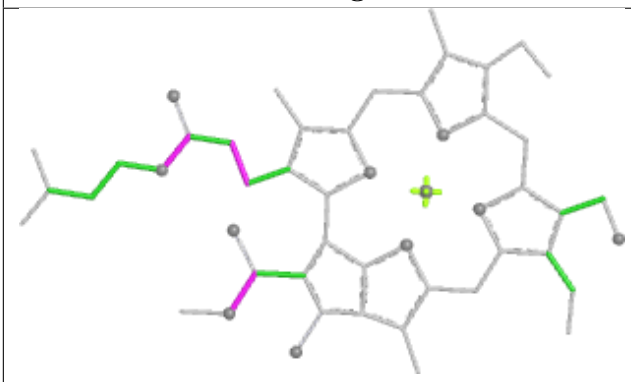
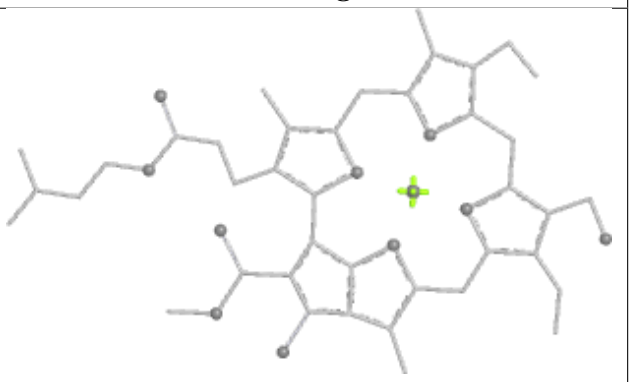


Bond angles

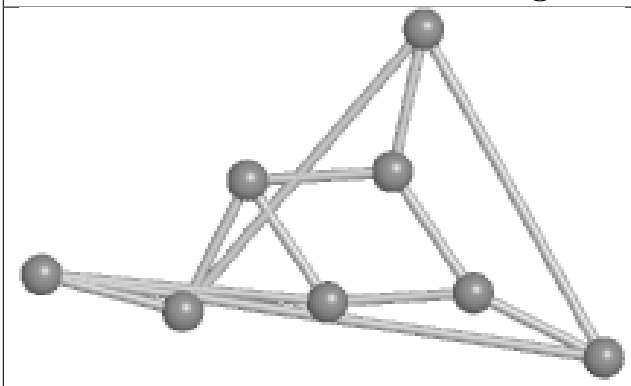


Torsions



Rings

Ligand SF4 C 102



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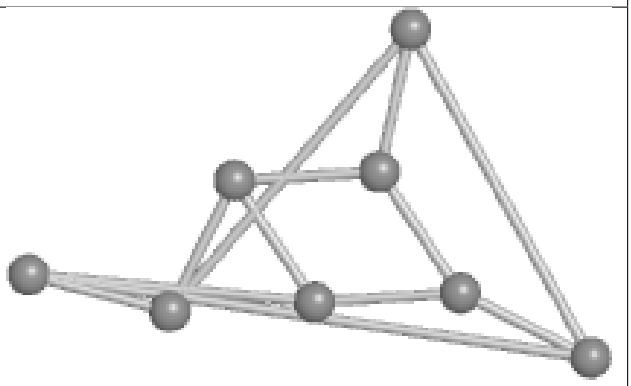
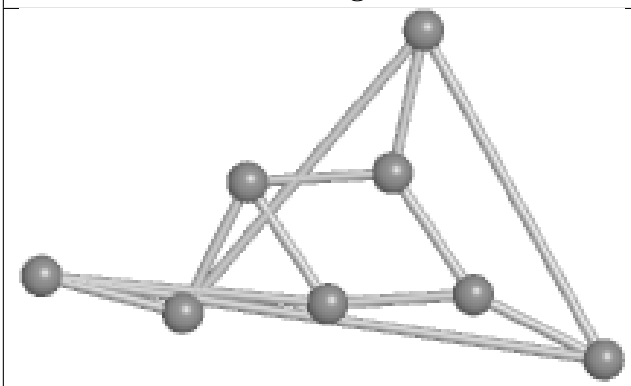


Bond angles



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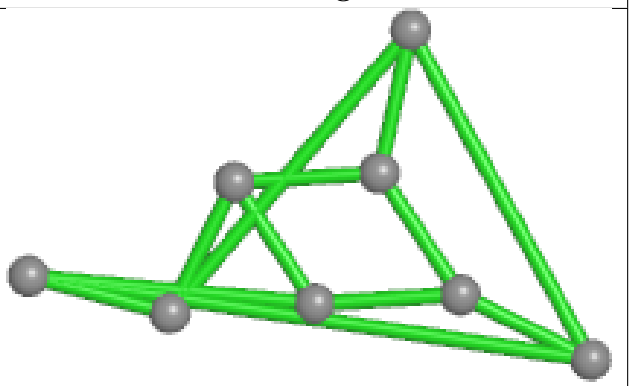
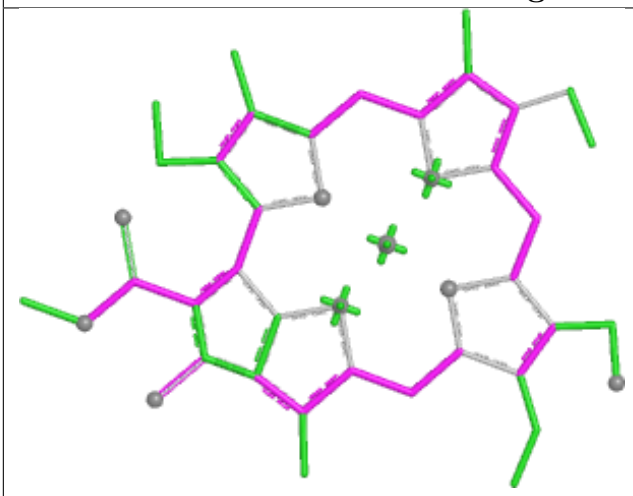


Rings

Ligand CHL 2 304



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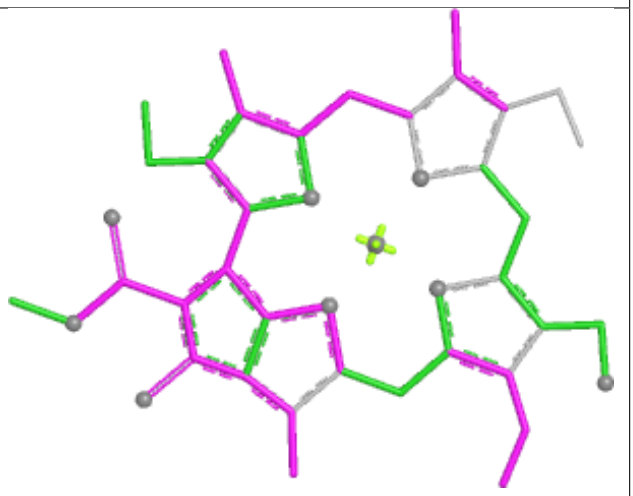
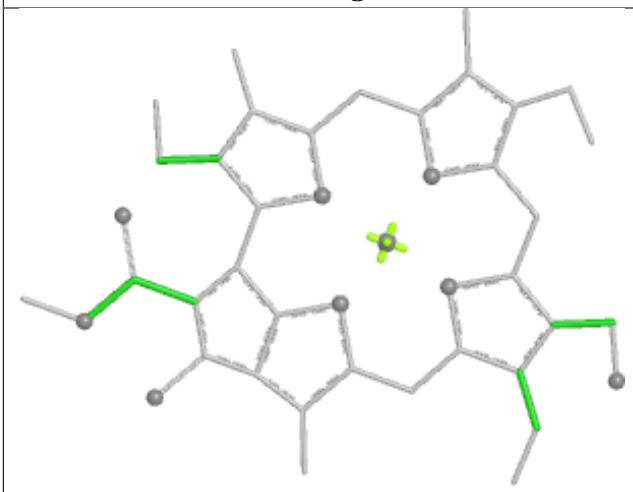


Bond angles



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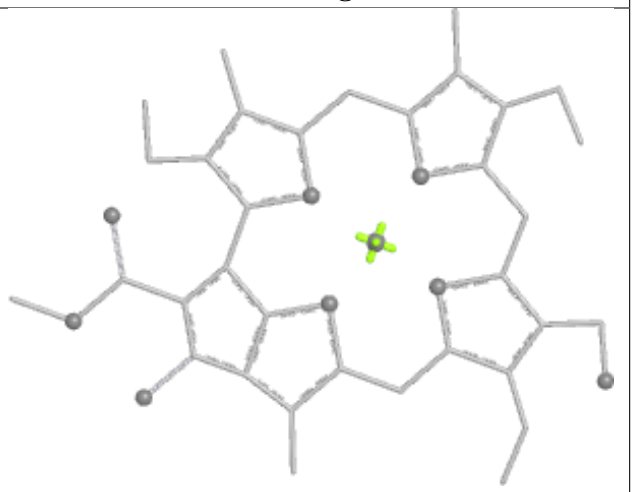
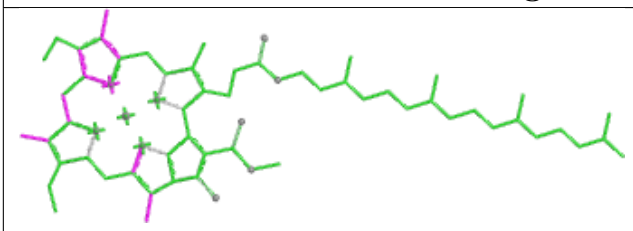


Rings

Ligand CLA A 838



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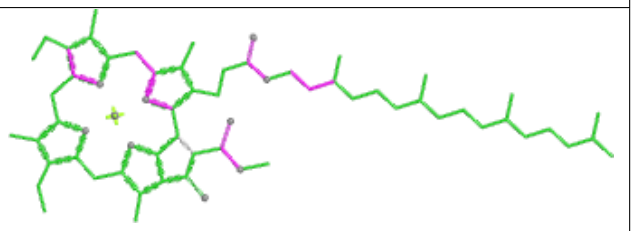
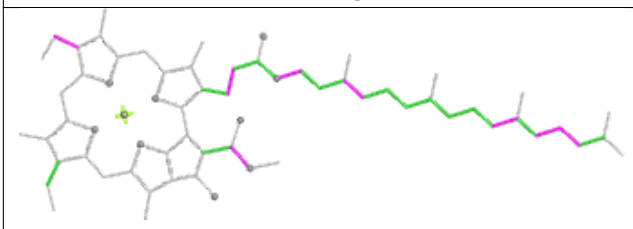


Bond angles



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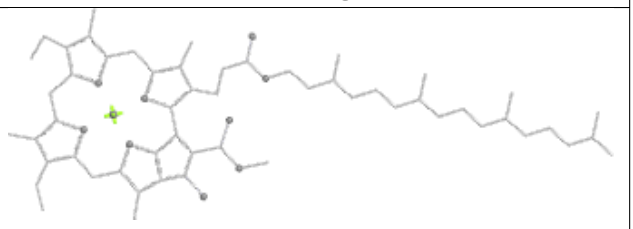
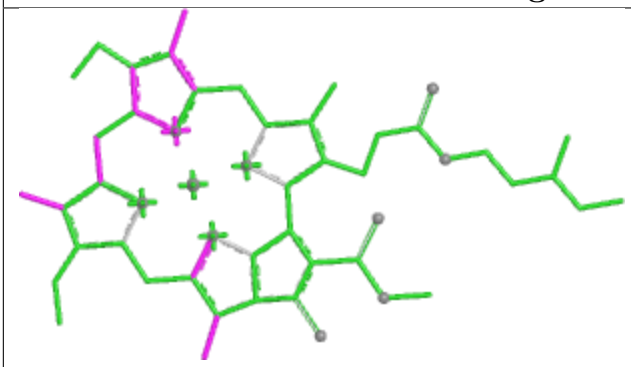


Rings

Ligand CLA 6 318



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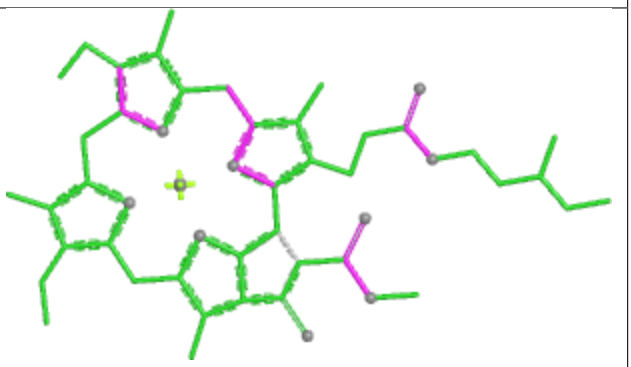
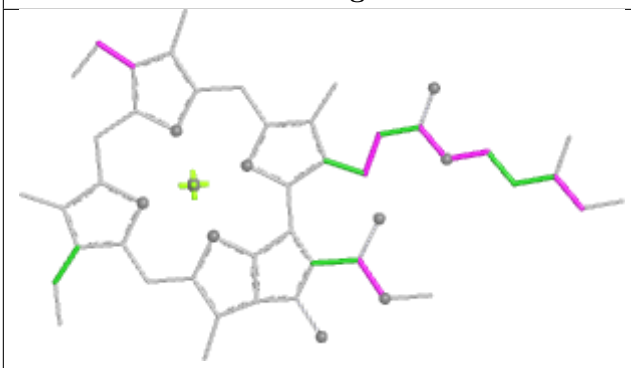


Bond angles



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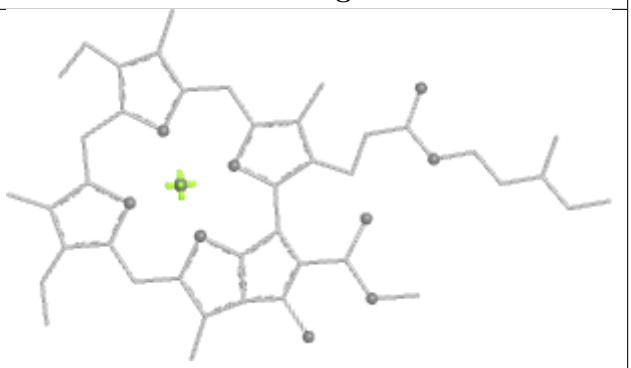
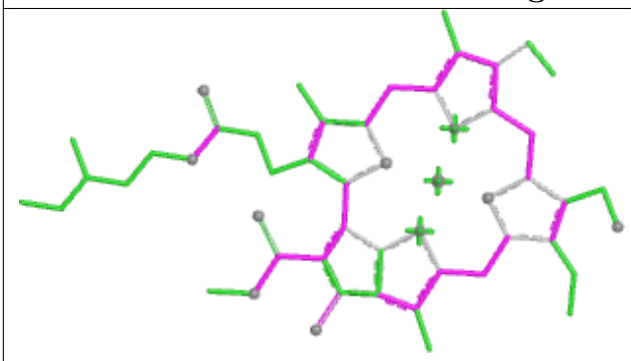


Rings

Ligand CHL 0 301



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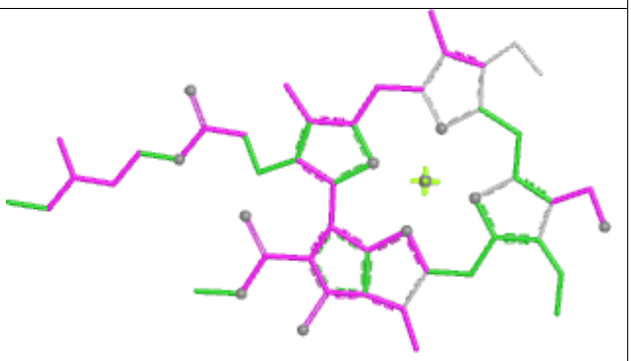
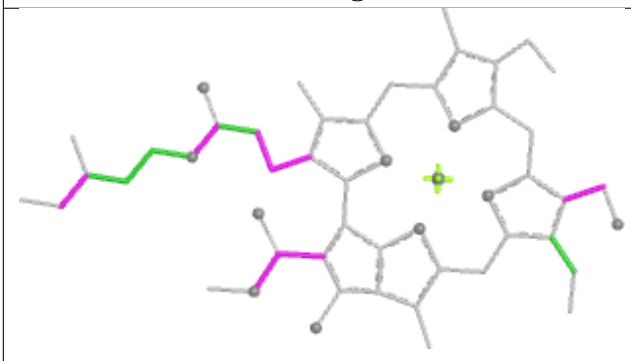
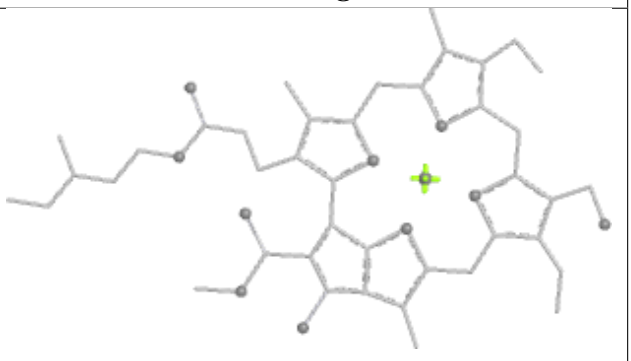


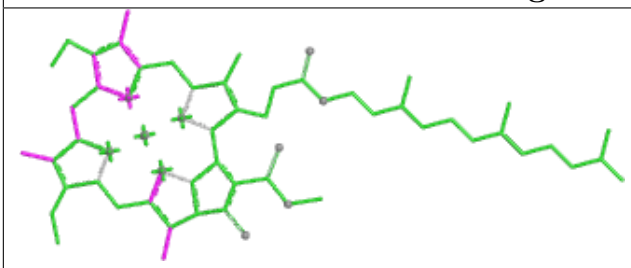
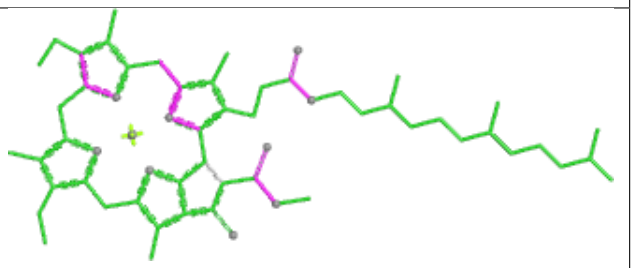
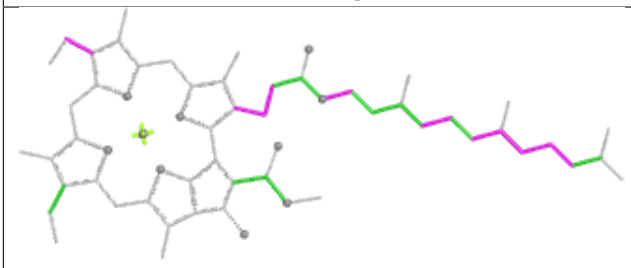
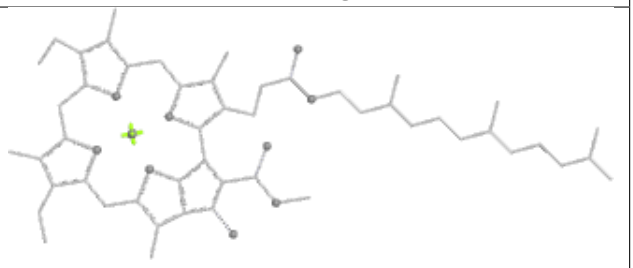
Bond angles

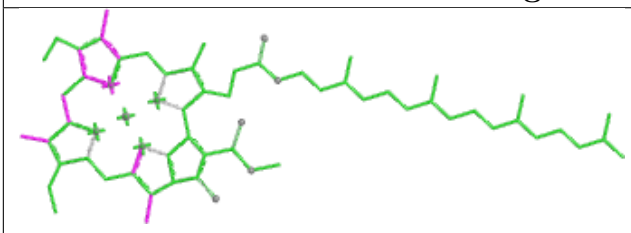
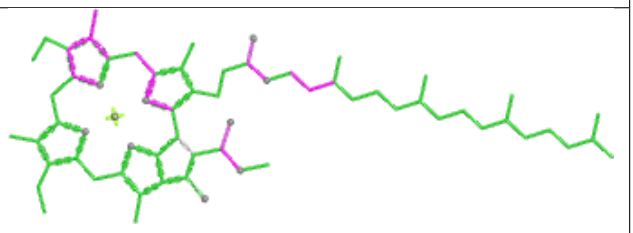
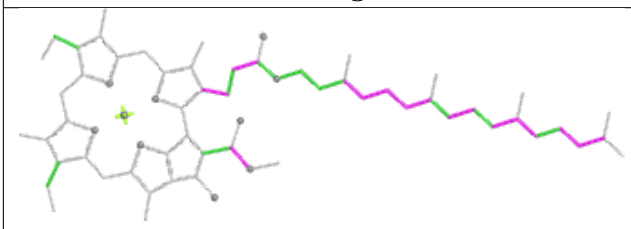
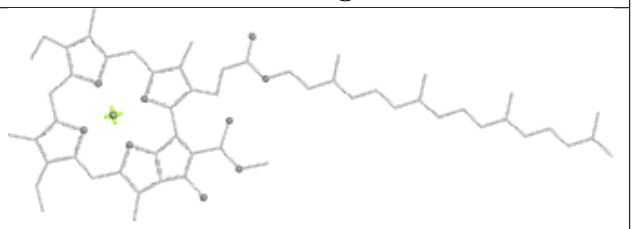


Torsions

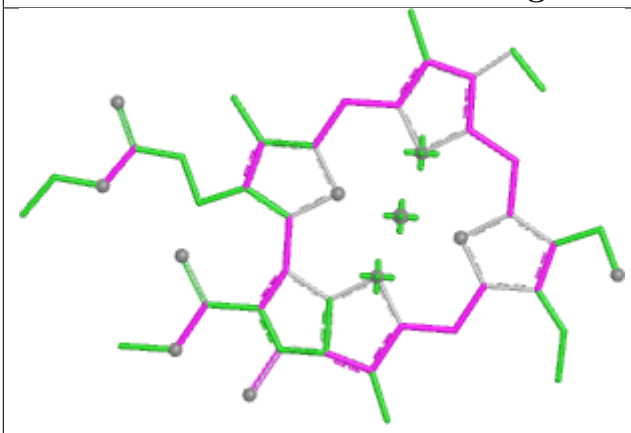


Rings

Ligand CLA 0 307	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA A 827	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CHL 0 306



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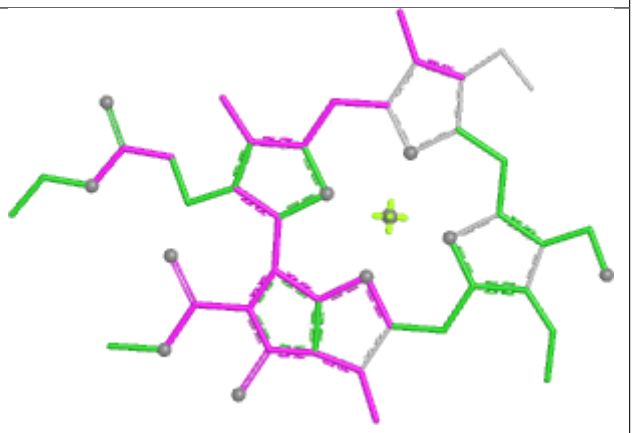
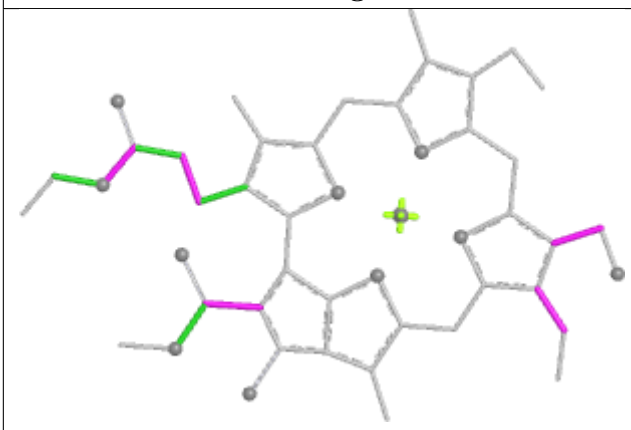
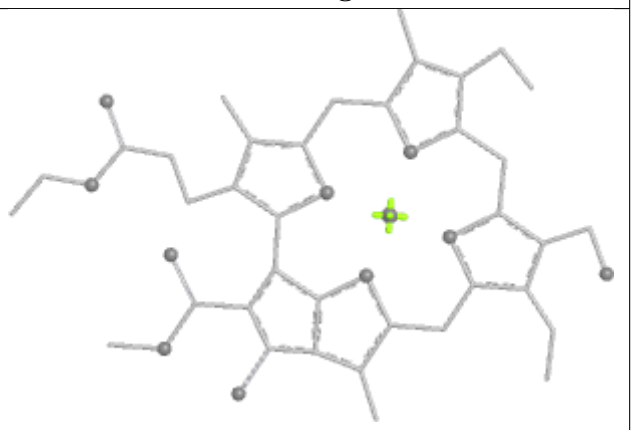


Bond angles

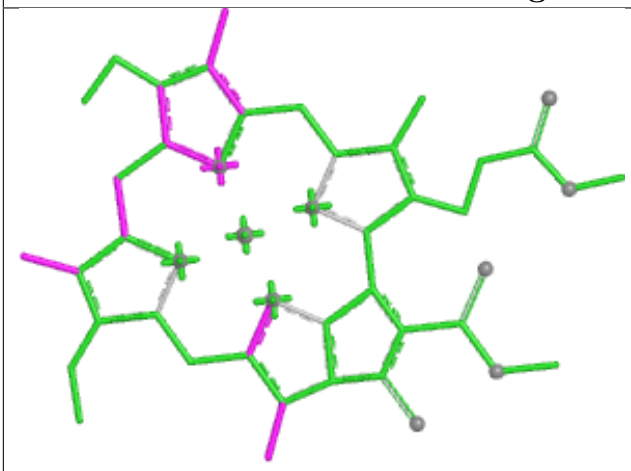


Torsions



Rings

Ligand CLA 3 311



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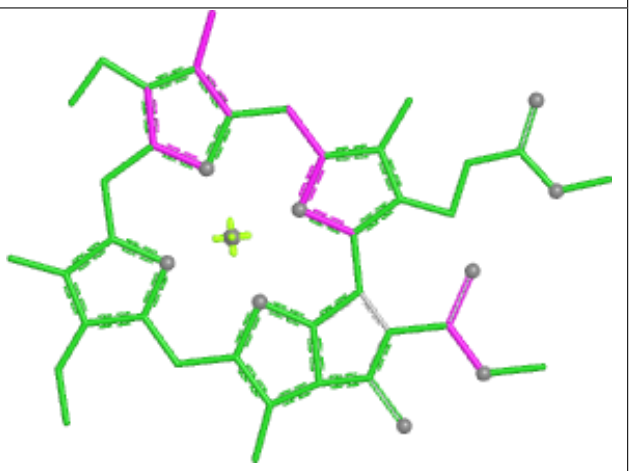
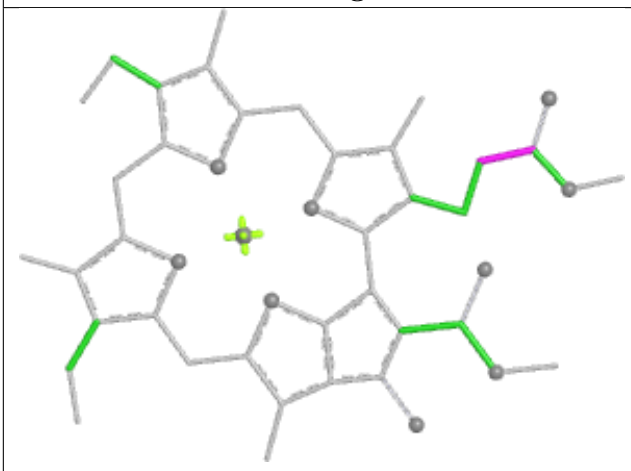


Bond angles



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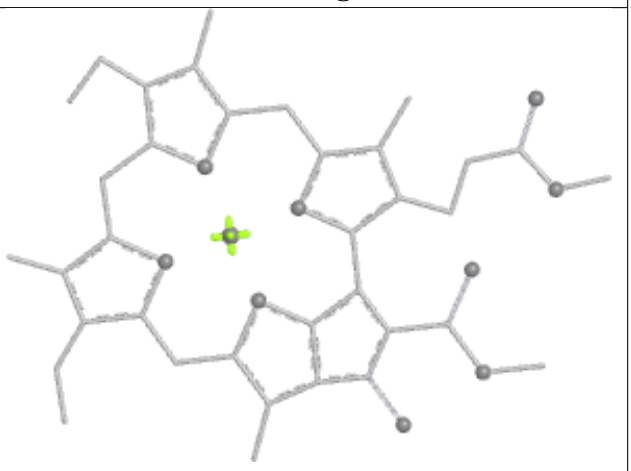
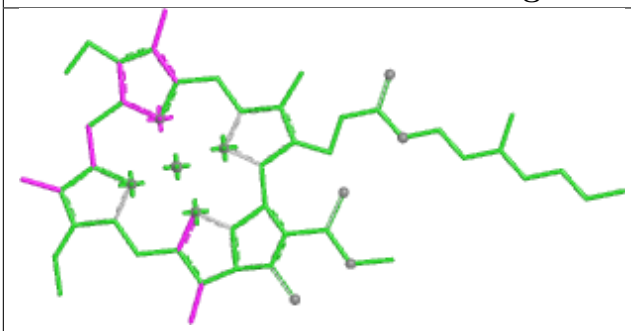
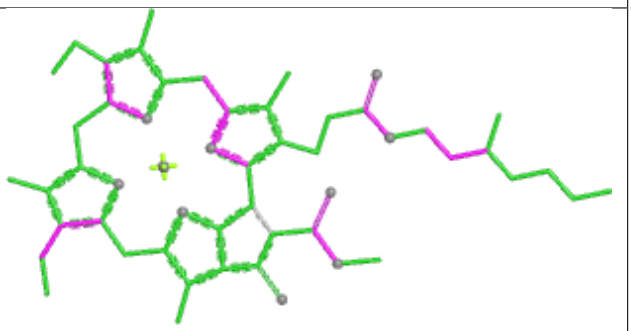


Rings

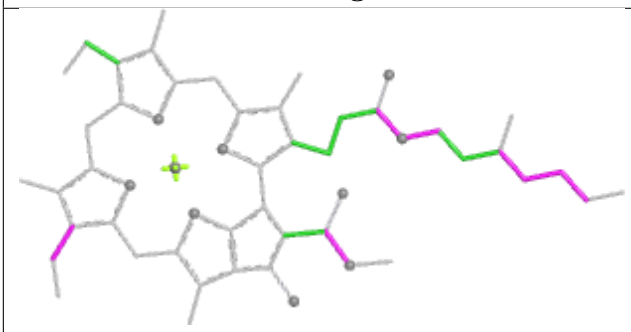
Ligand CLA K 102



Bond lengths



Bond angles



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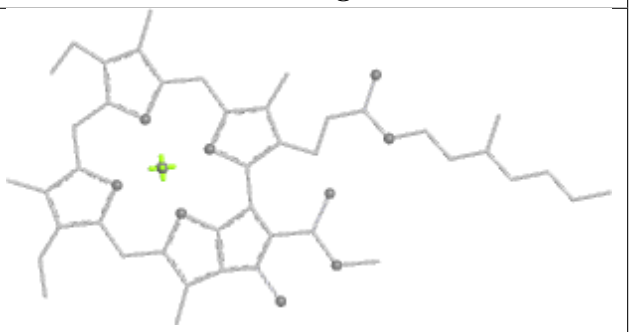
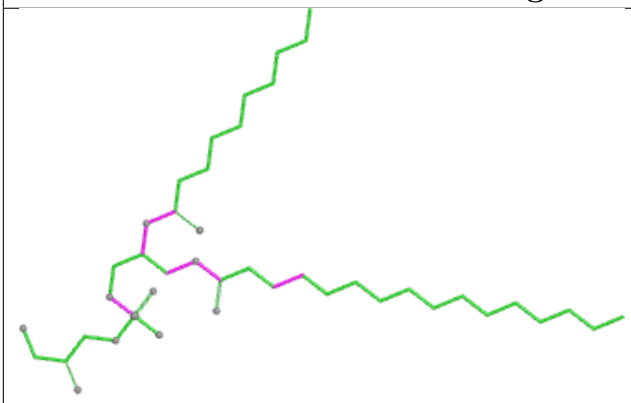
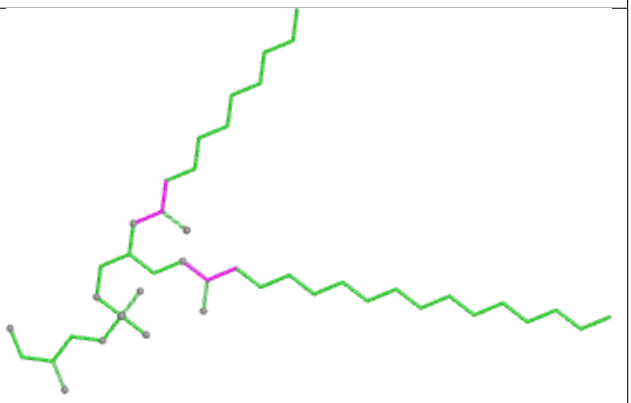


Rings

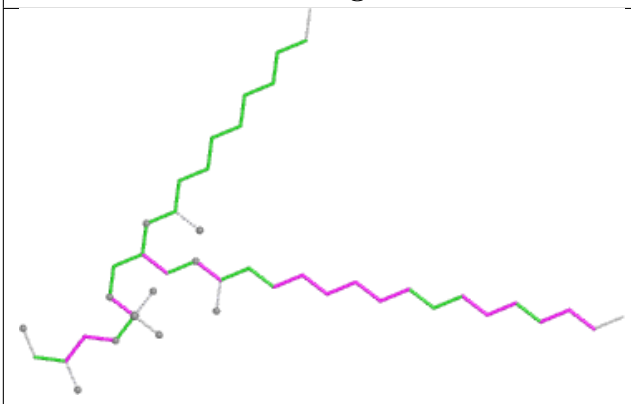
Ligand LHG 1 318



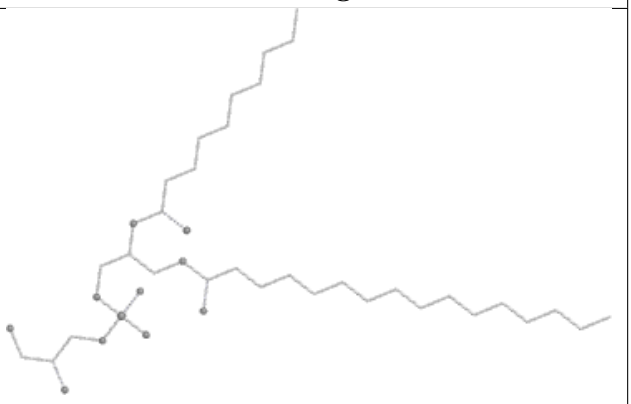
Bond lengths



Bond angles

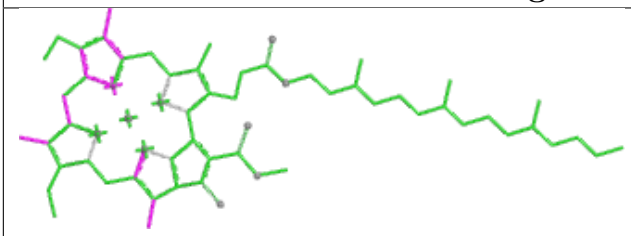


Torsions



Rings

Ligand CLA 1 309



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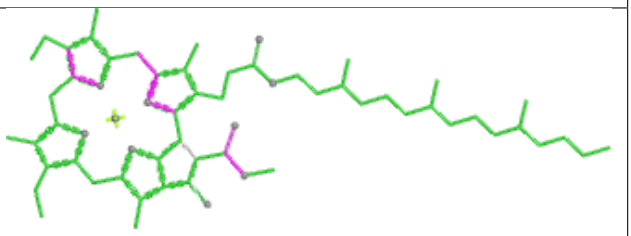
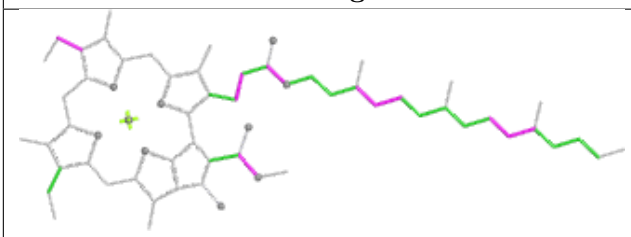
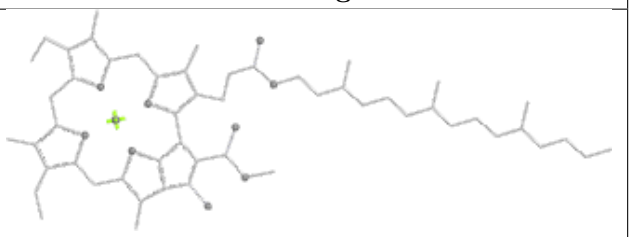


Bond angles

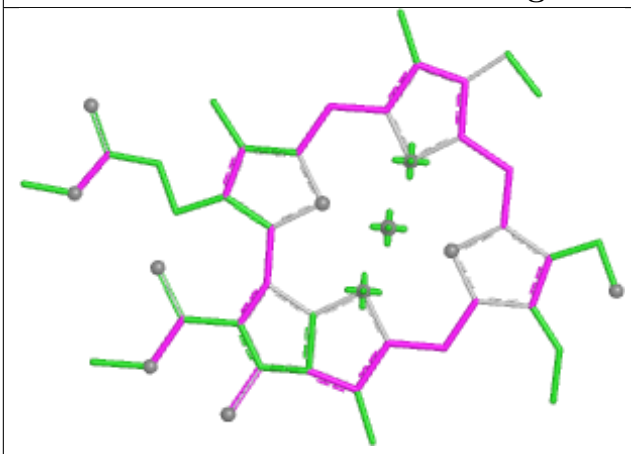


Torsions



Rings

Ligand CHL 5 312



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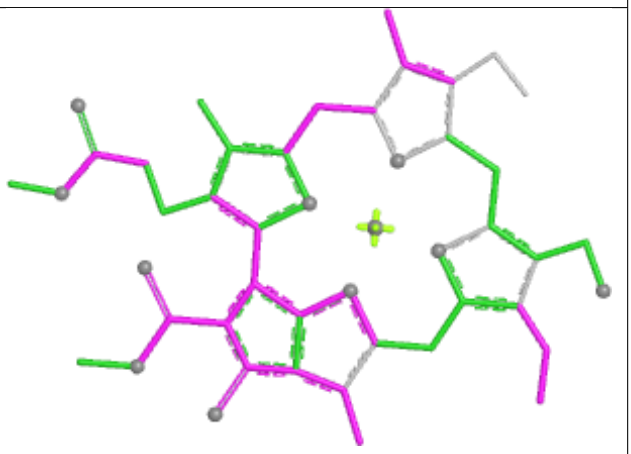
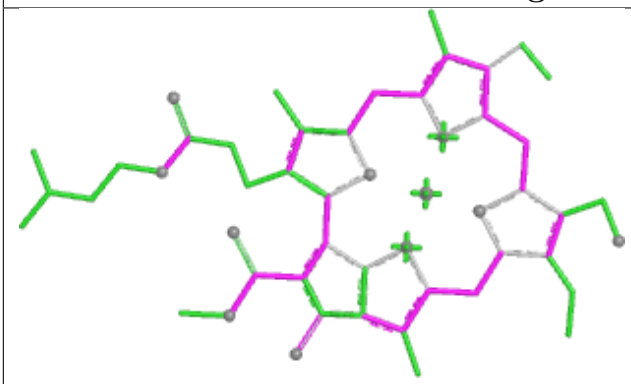


Bond angles

Torsions

Rings

Ligand CHL 8 308



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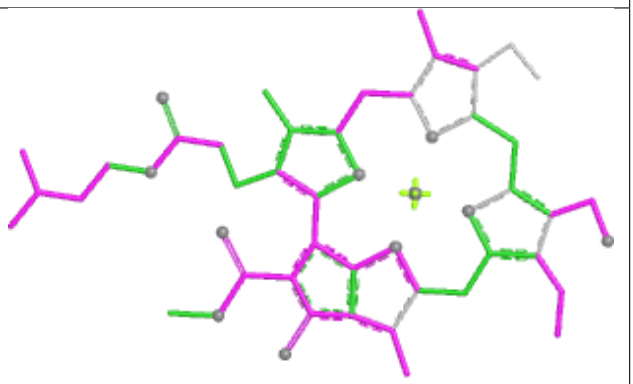
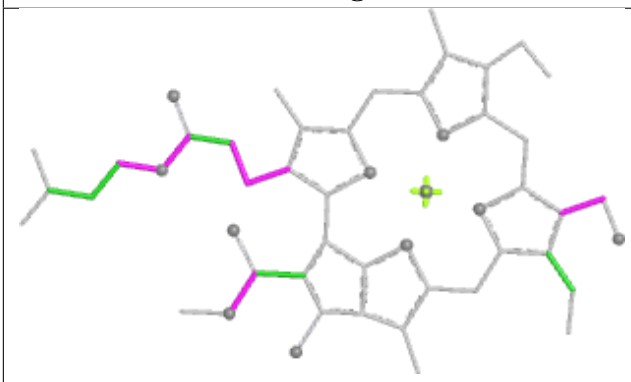
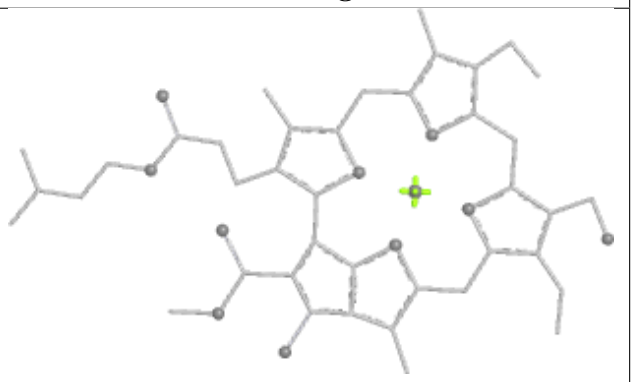


Bond angles

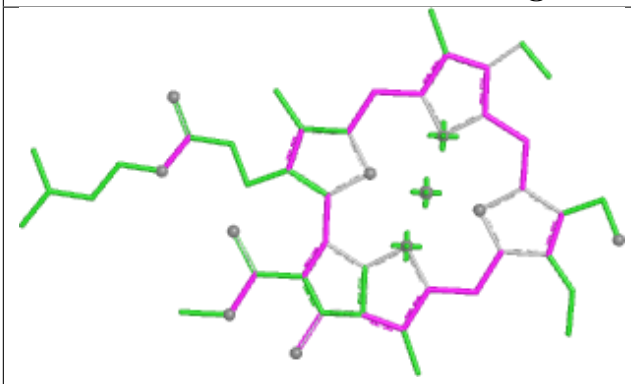


Torsions



Rings

Ligand CHL 0 305



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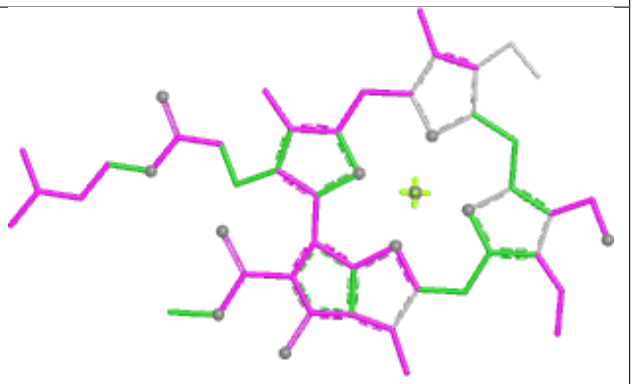
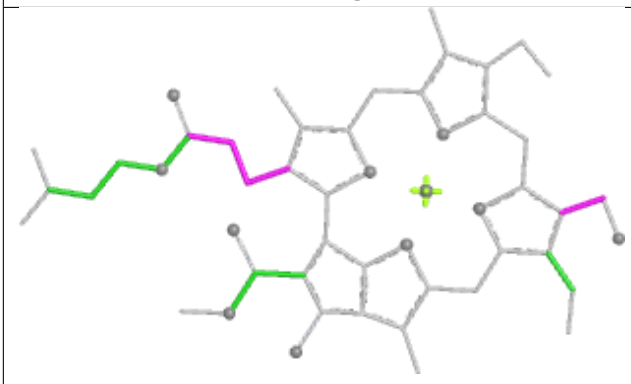


Bond angles



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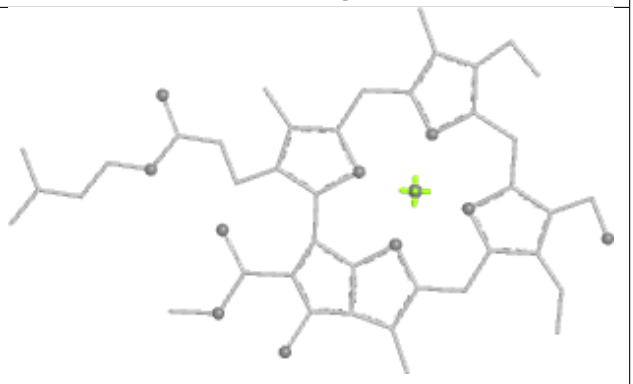
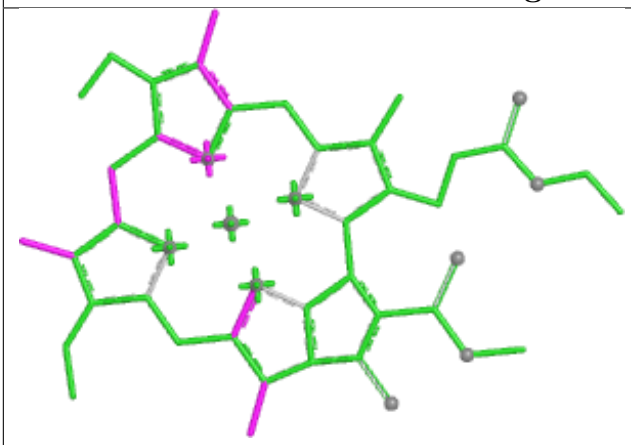


Rings

Ligand CLA B 838



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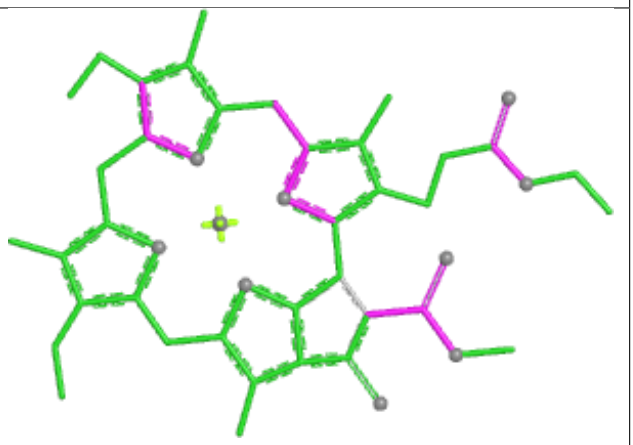
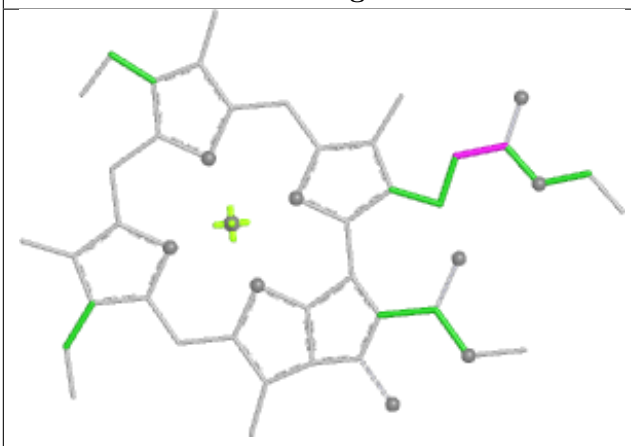


Bond angles



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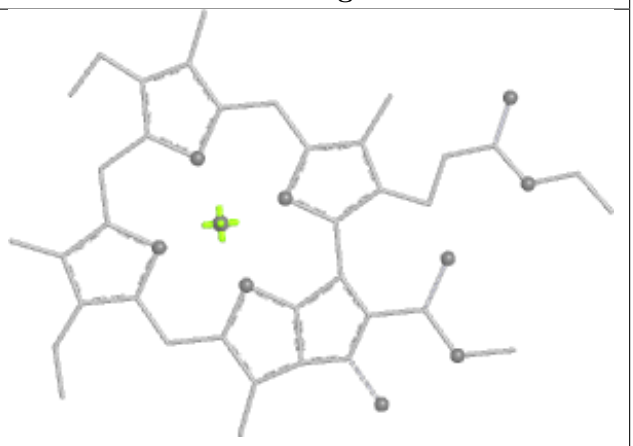
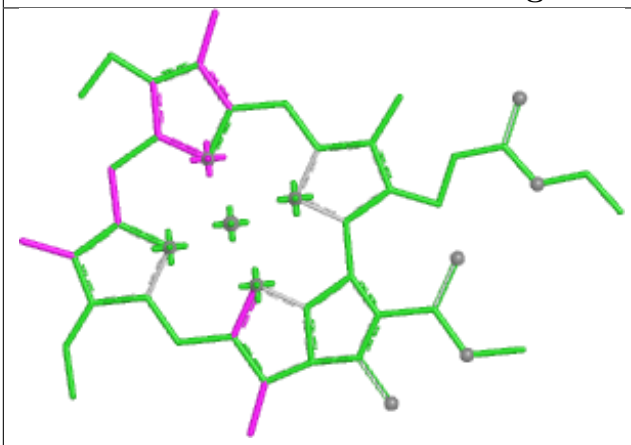


Rings

Ligand CLA L 206



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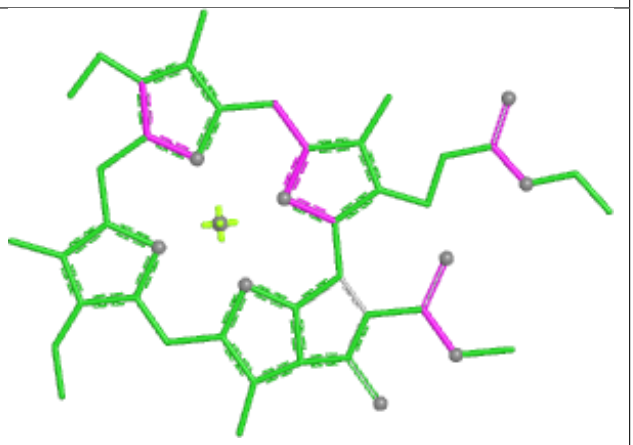
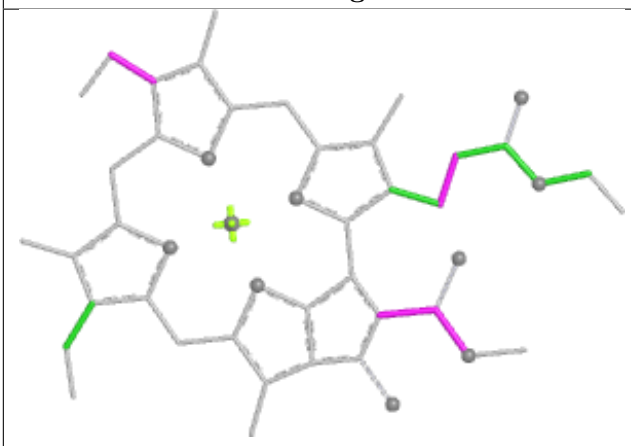
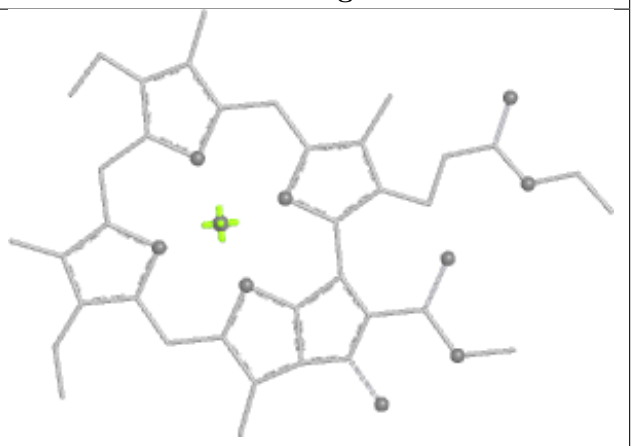


Bond angles

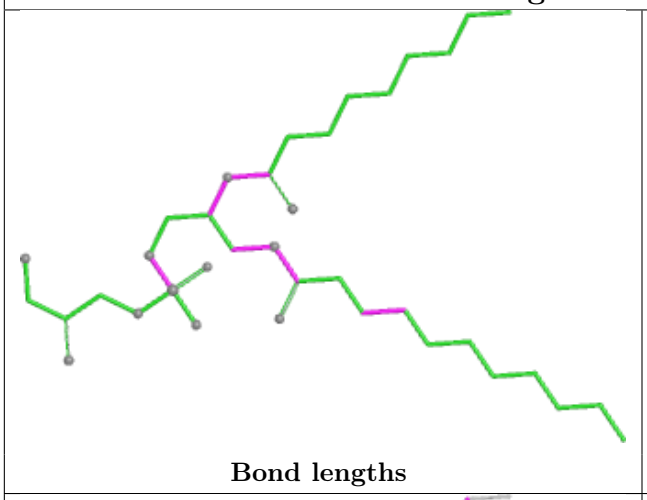


Torsions



Rings

Ligand LHG 5 316



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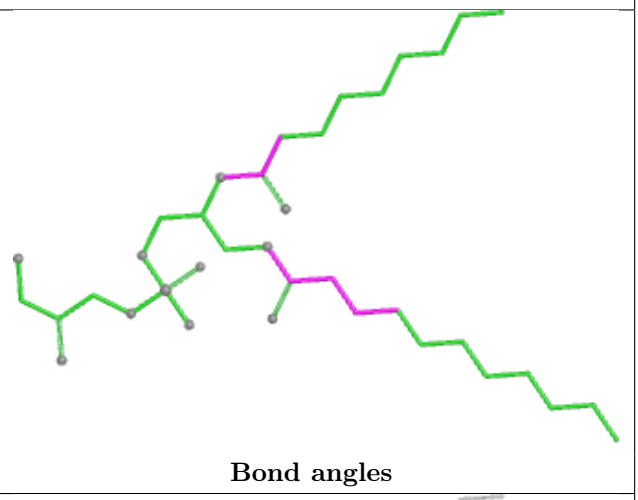
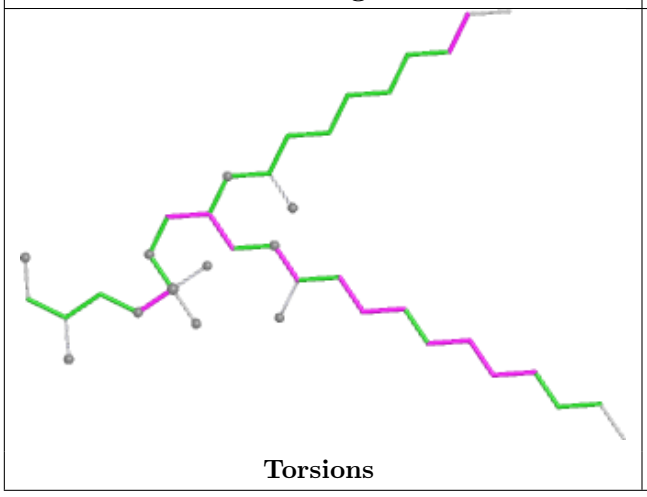
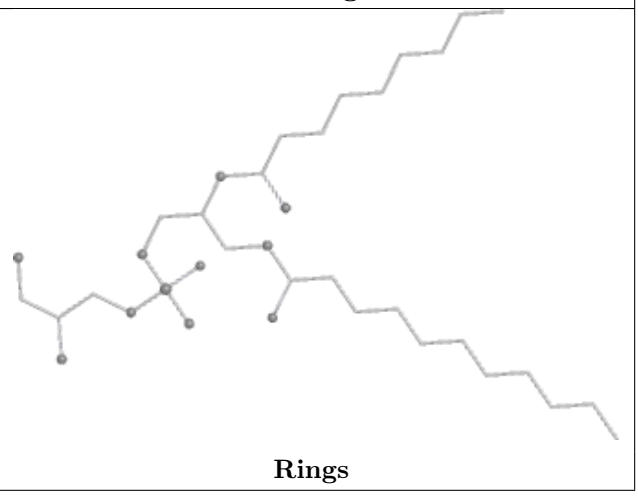


Bond angles

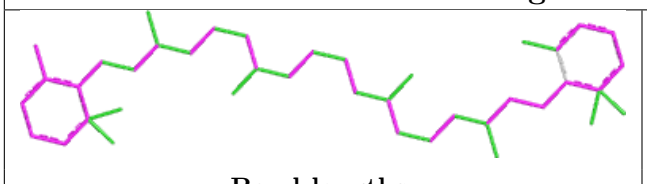


Torsions

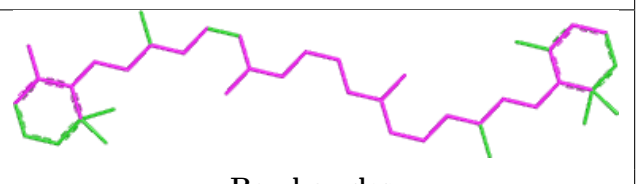


Rings

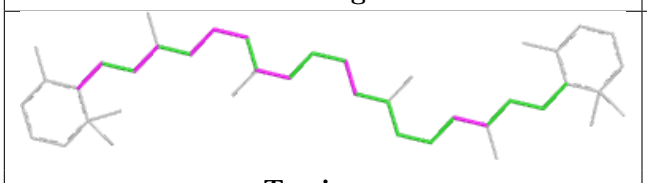
Ligand 8CT B 845



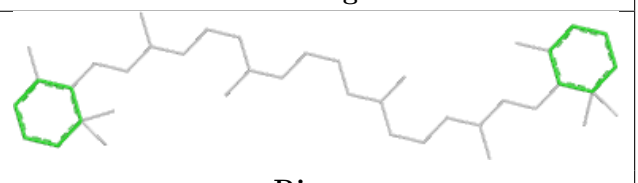
Bond lengths



Bond angles

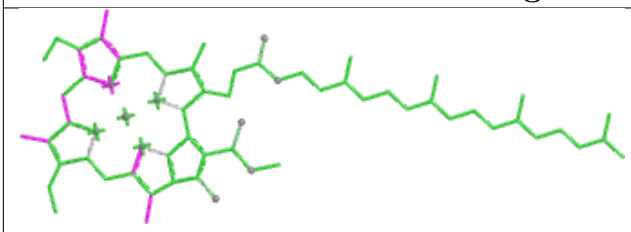


Torsions

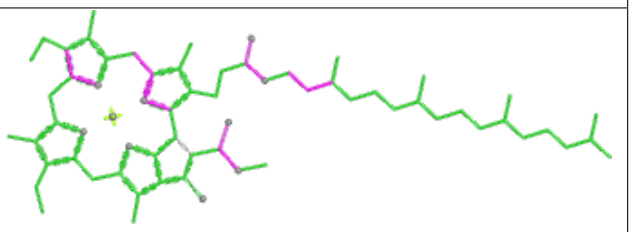


Rings

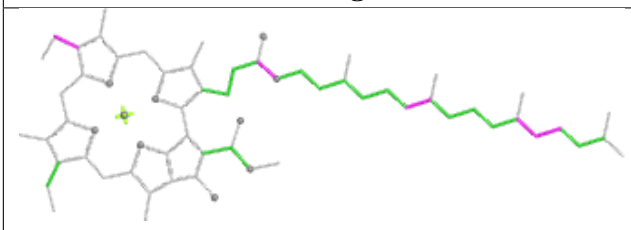
Ligand CLA A 814



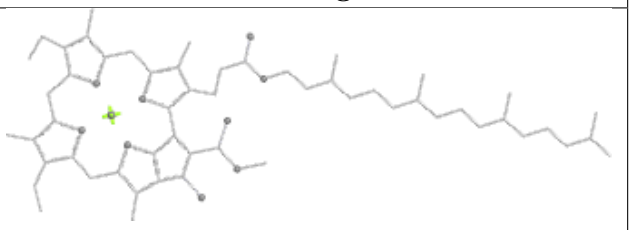
Bond lengths



Bond angles

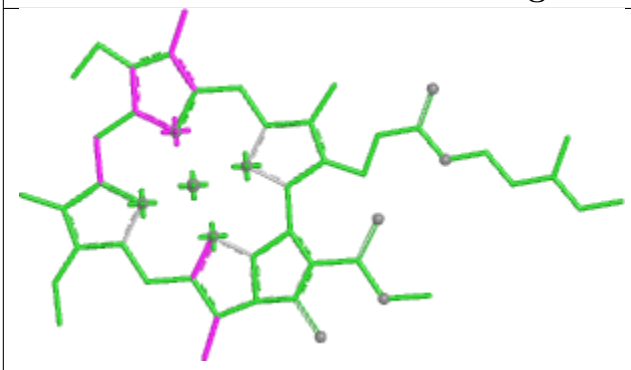


Torsions



Rings

Ligand CLA 9 304



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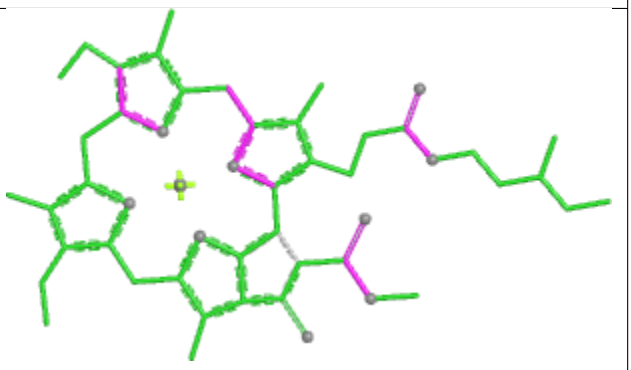
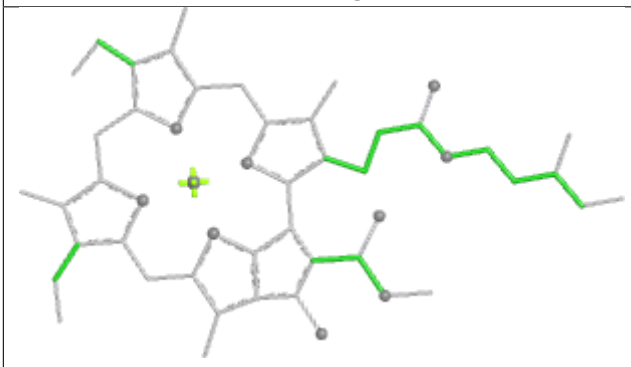
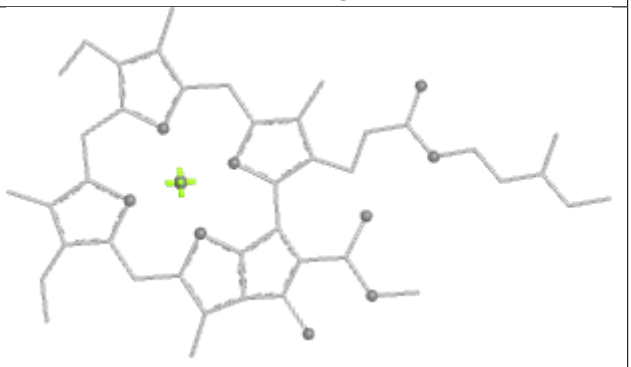


Bond angles

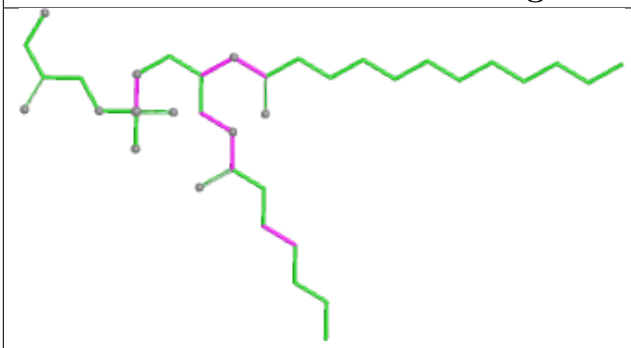


Torsions



Rings

Ligand LHG 3 320



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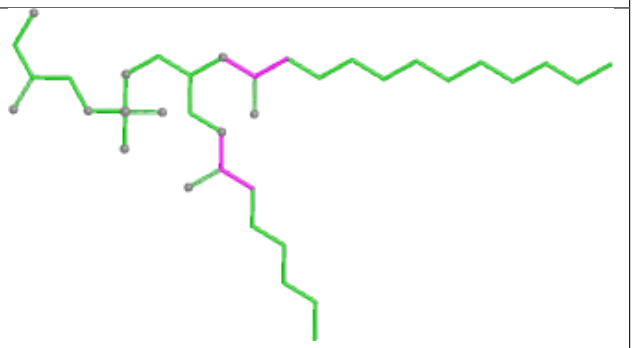
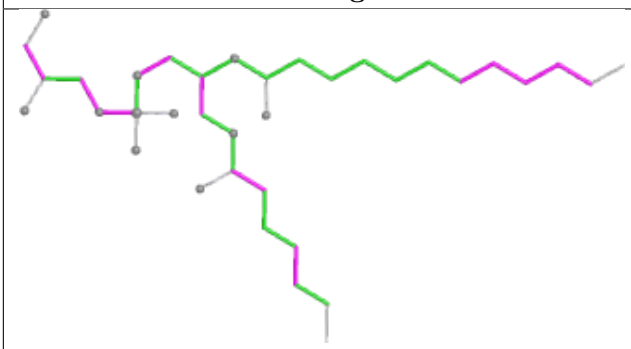
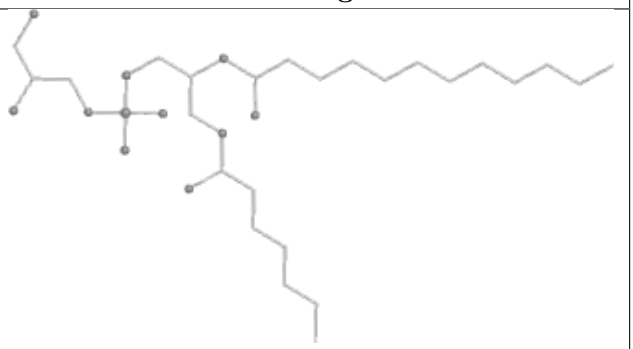


Bond angles

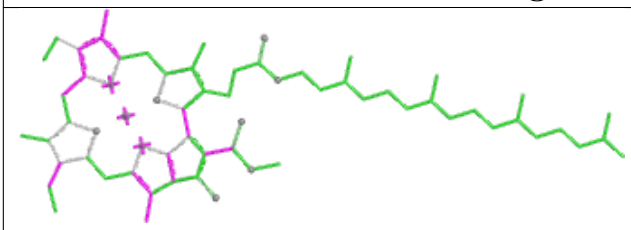


Torsions



Rings

Ligand CL0 A 852



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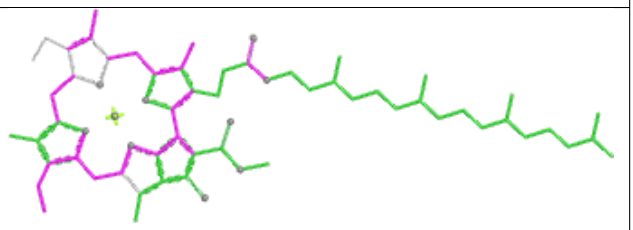
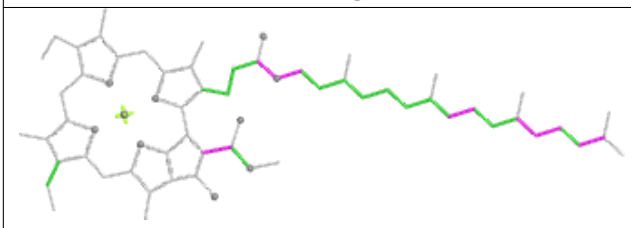
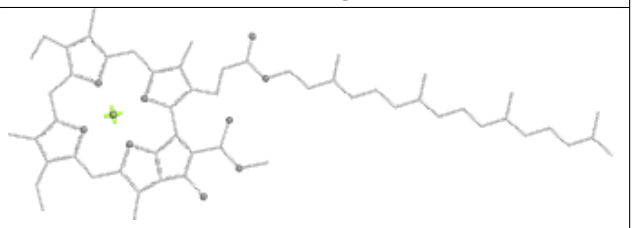


Bond angles

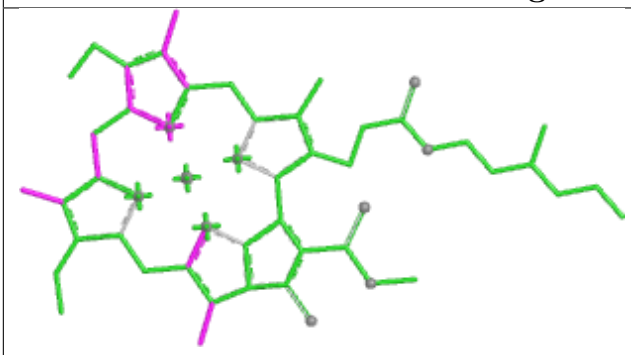


Torsions



Rings

Ligand CLA 1 303



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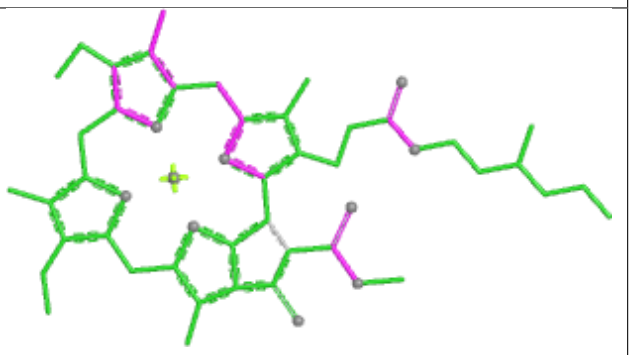
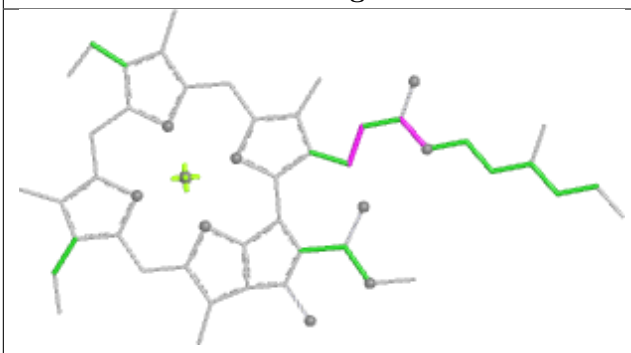


Bond angles



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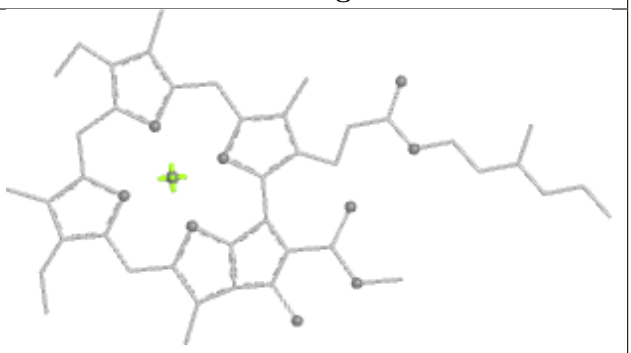
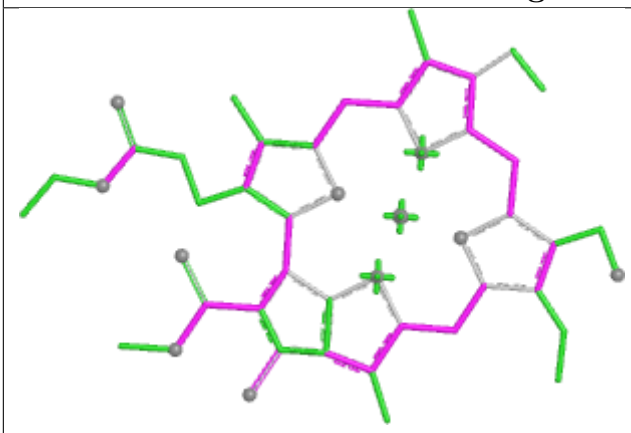


Rings

Ligand CHL 4 306



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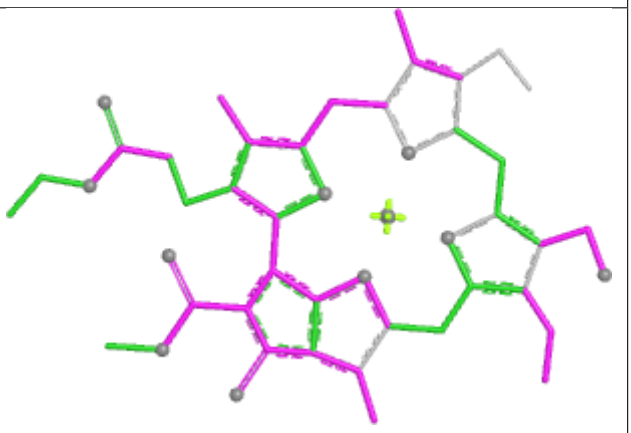
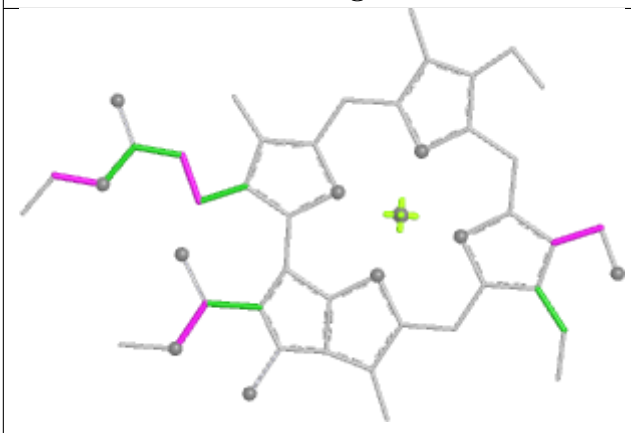
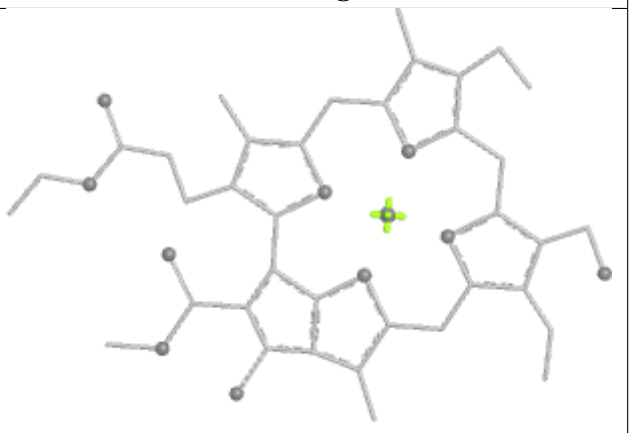


Bond angles

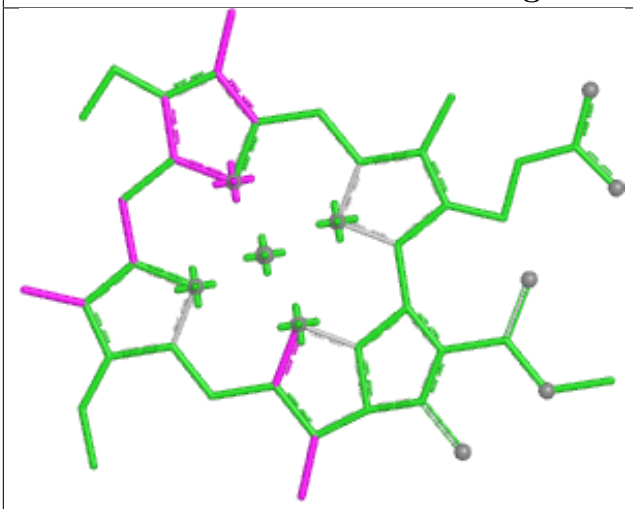


Torsions



Rings

Ligand CLA G 102



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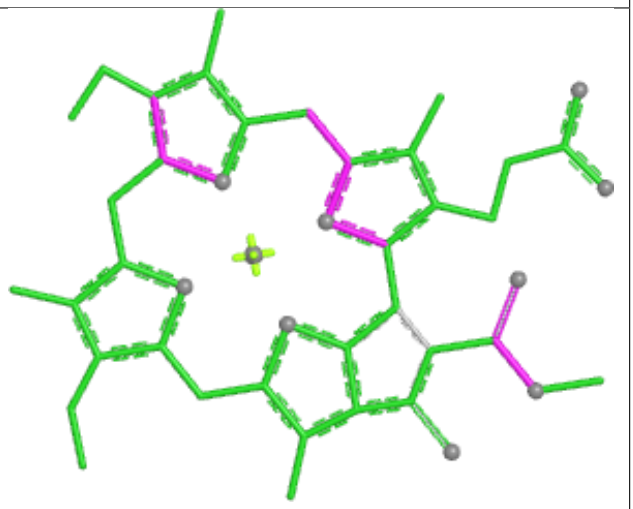
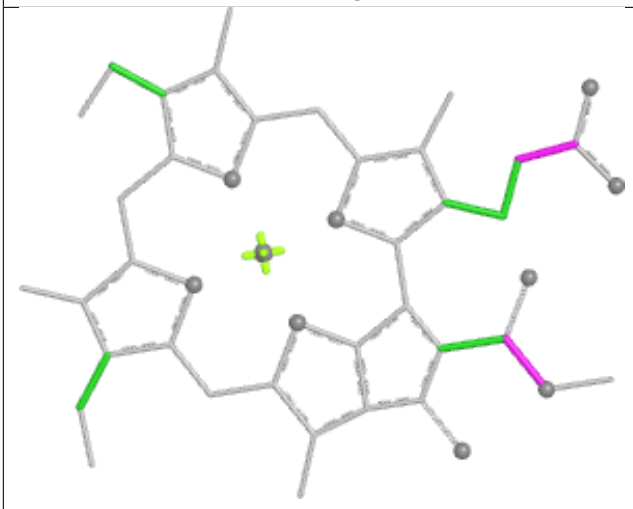


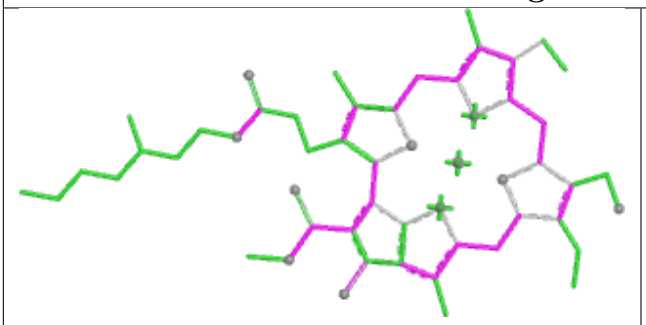
Bond angles



Torsions

Rings

Ligand CHL 4 315



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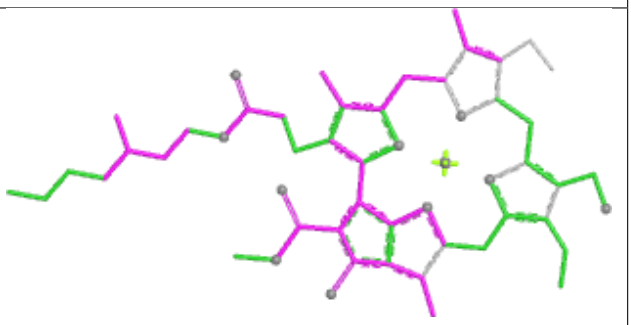
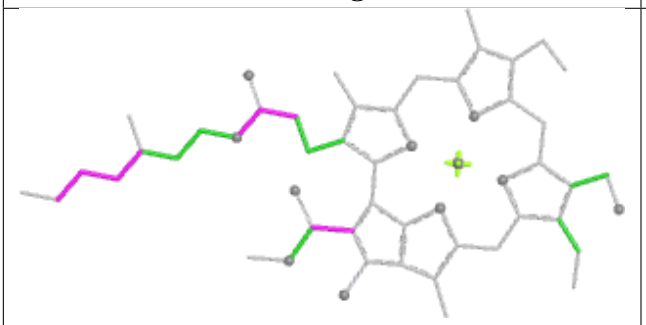
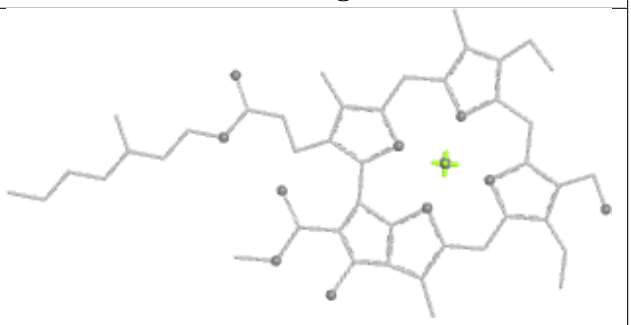


Bond angles

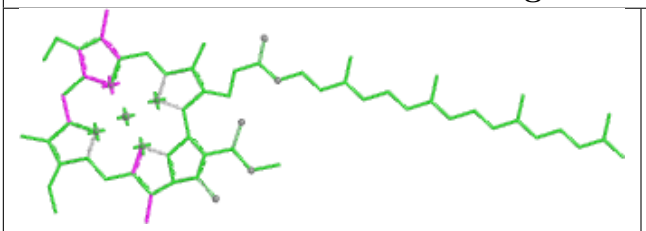


Torsions



Rings

Ligand CLA B 841



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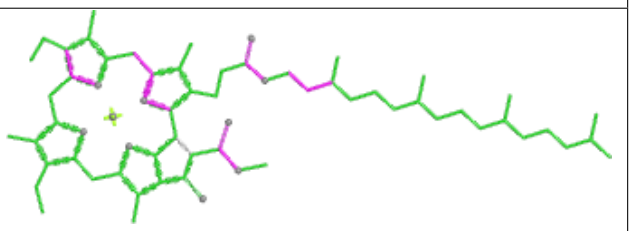
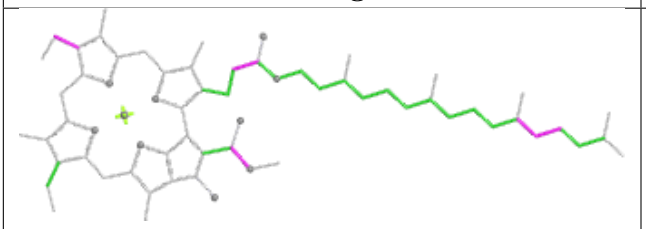
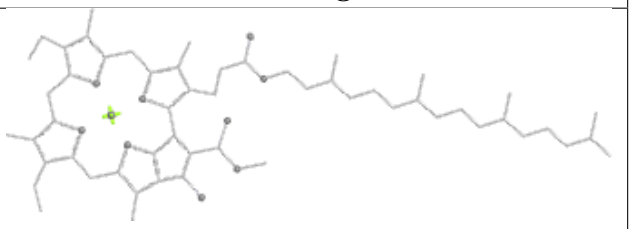


Bond angles

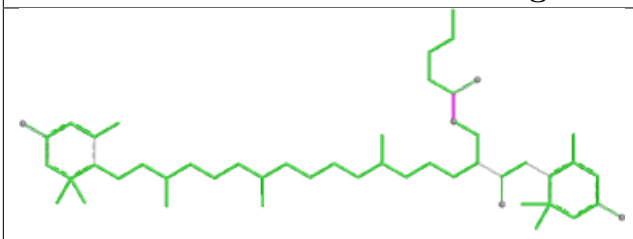


Torsions



Rings

Ligand 0UR 2 316



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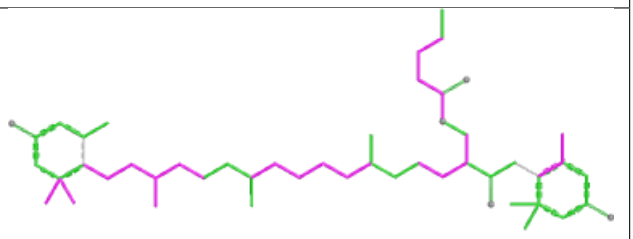

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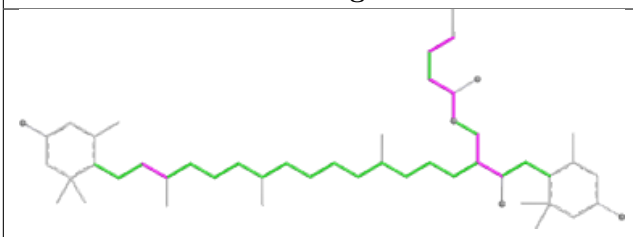

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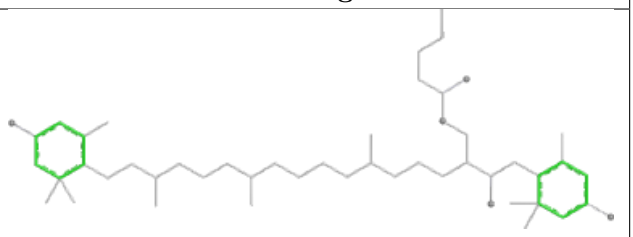
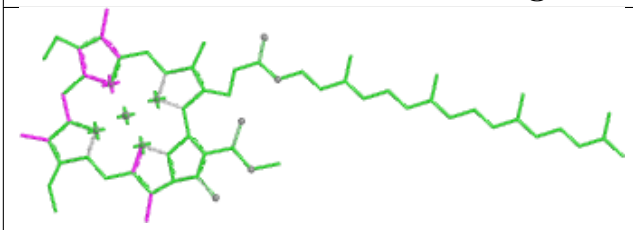


Rings

Ligand CLA 0 311



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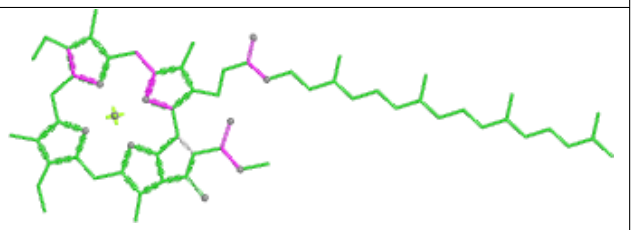

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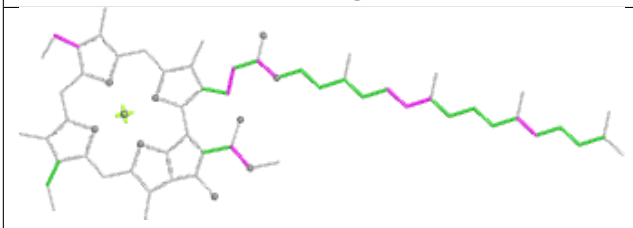

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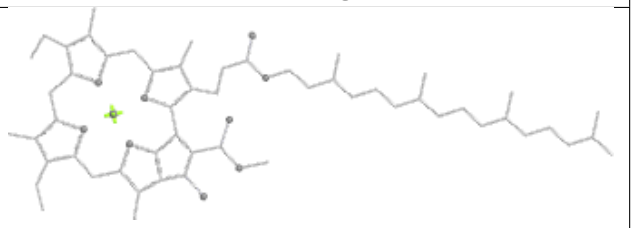
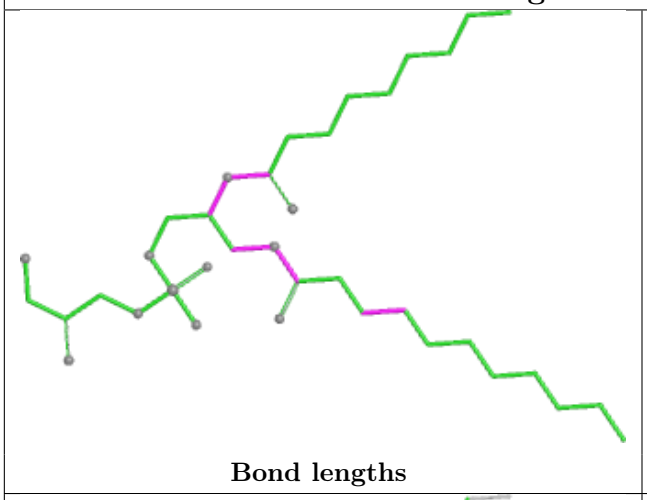


Rings

Ligand LHG 6 322



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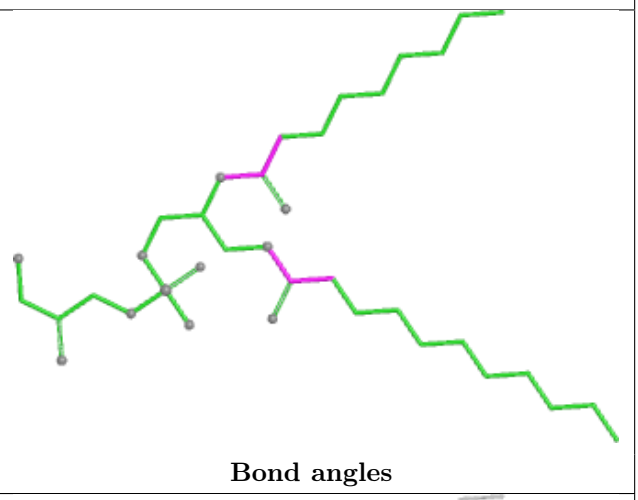
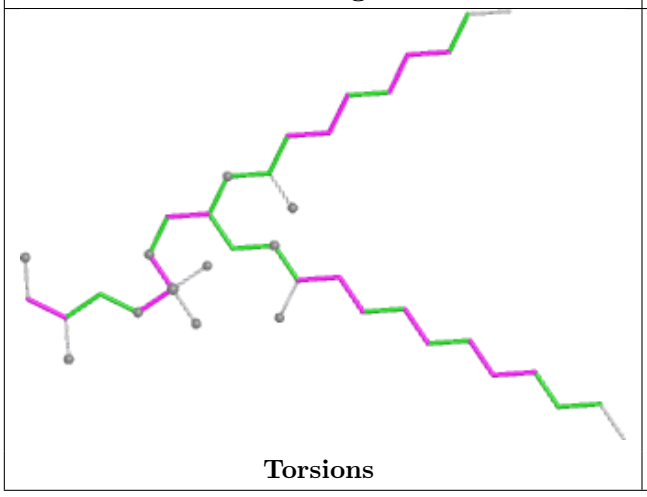


Bond angles



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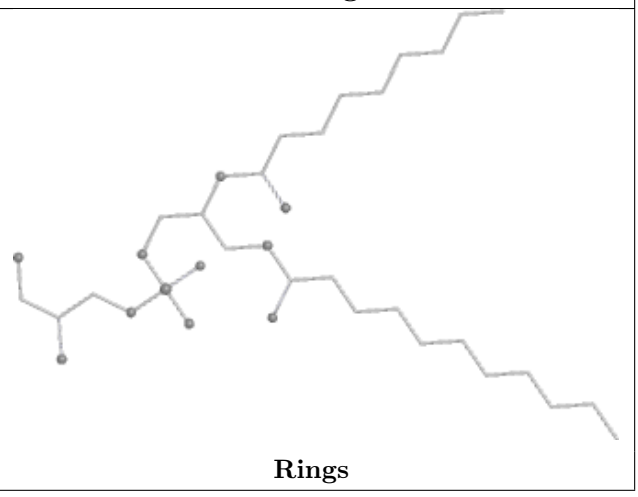
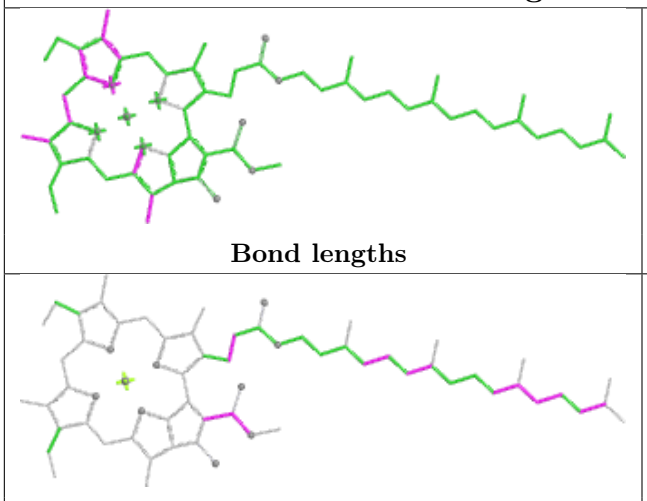


Rings

Ligand CLA B 804



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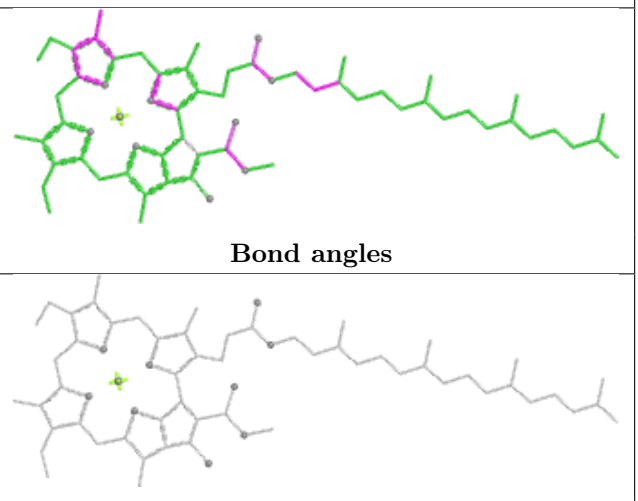
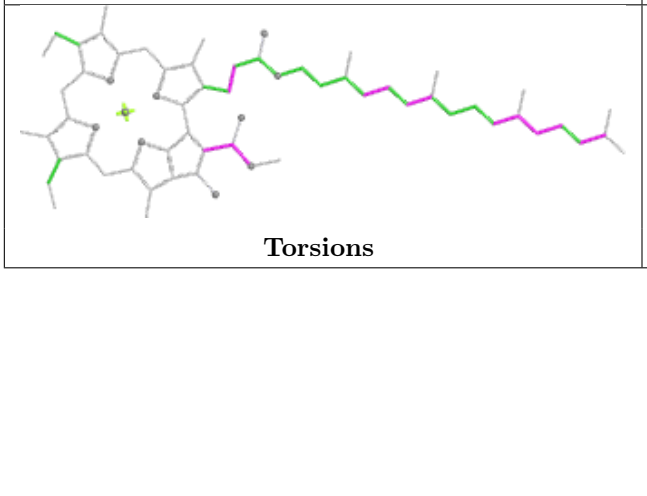
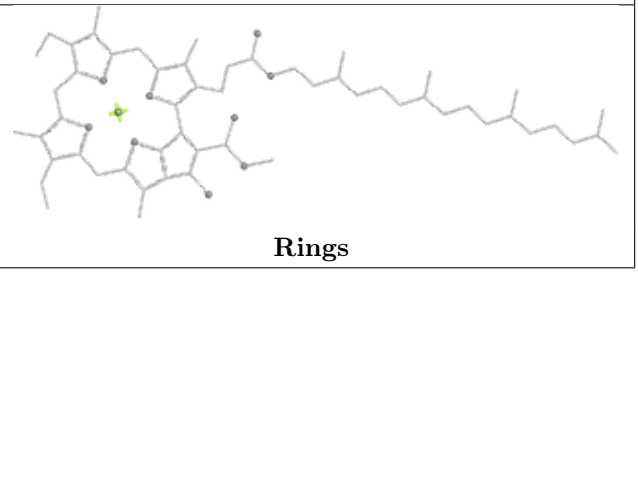


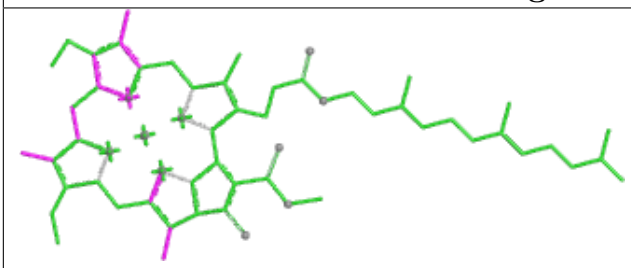
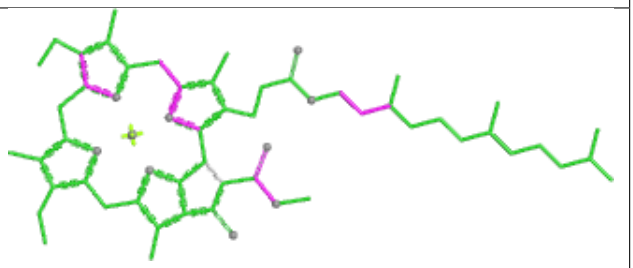
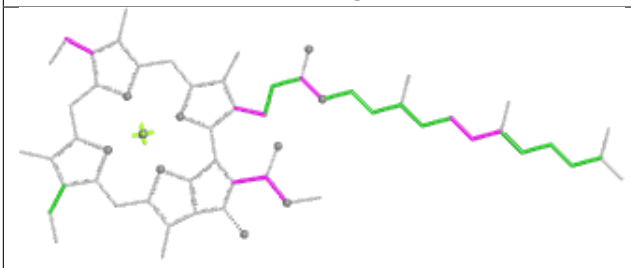
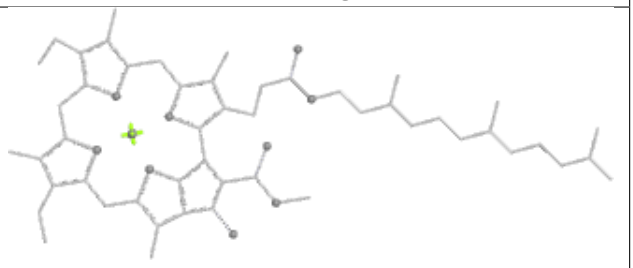
Bond angles

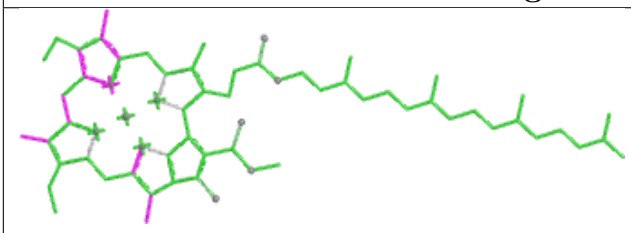
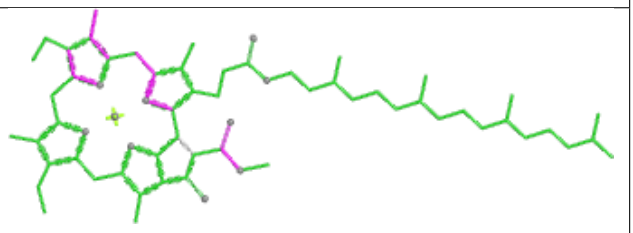
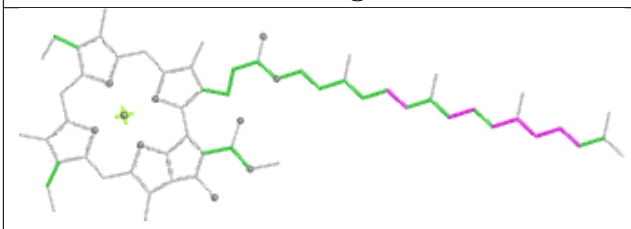
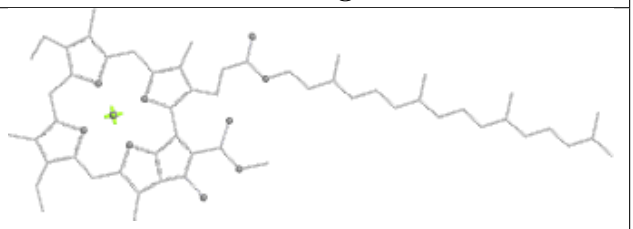


Torsions

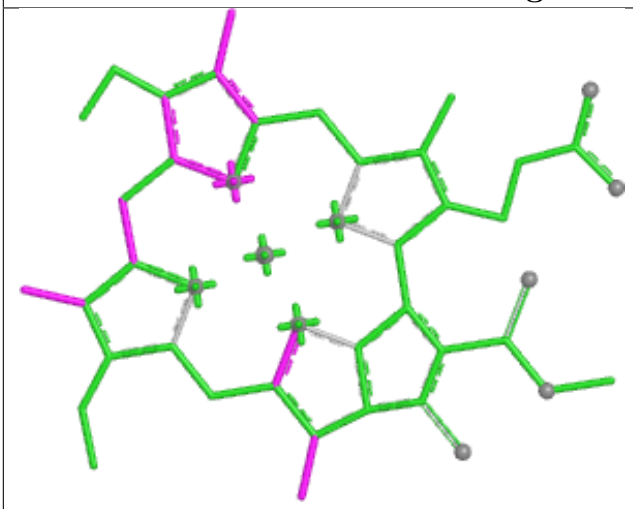


Rings

Ligand CLA 6 310	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

Ligand CLA B 839	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

Ligand CLA F 303



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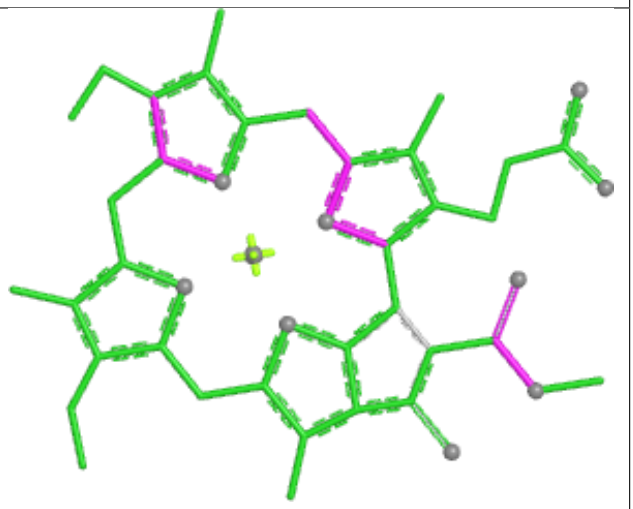
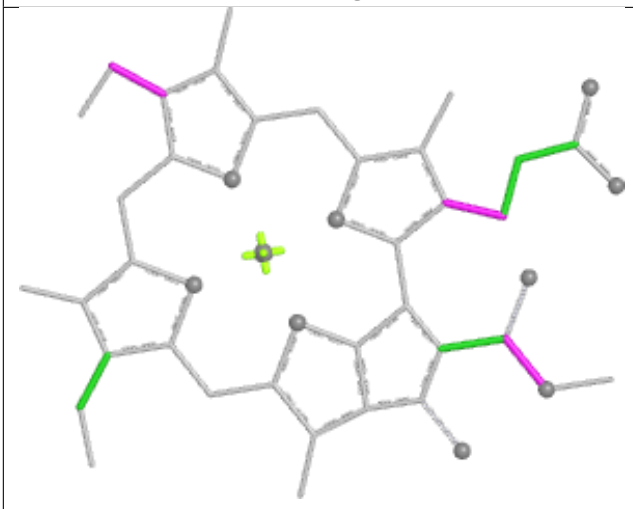


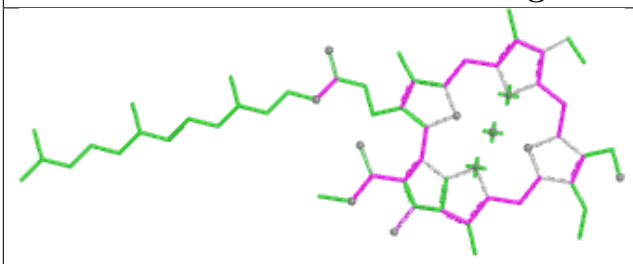
Bond angles



Torsions

Rings

Ligand CHL 6 323



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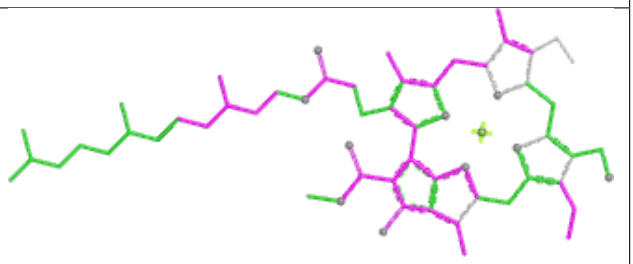
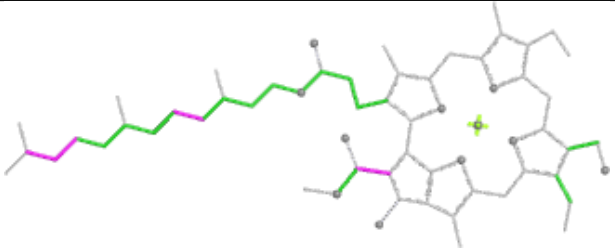
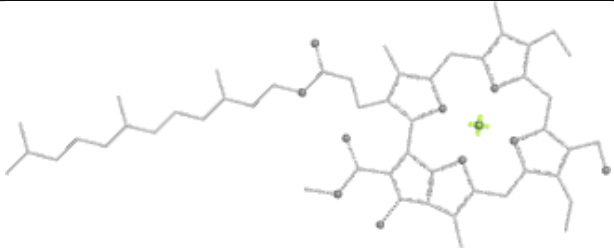


Bond angles

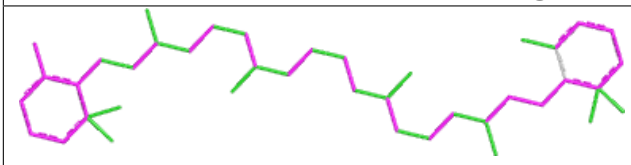


Torsions



Rings

Ligand 8CT 3 323



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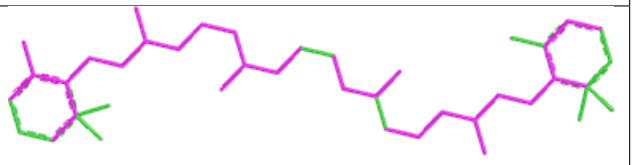
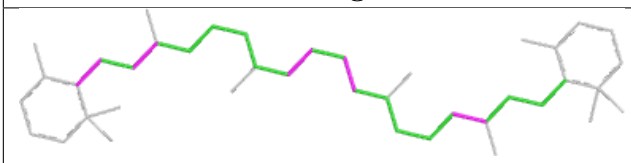
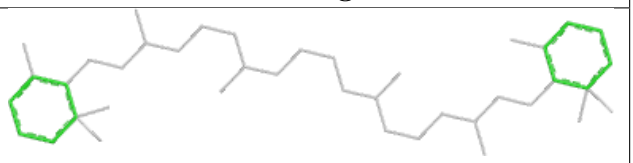


Bond angles

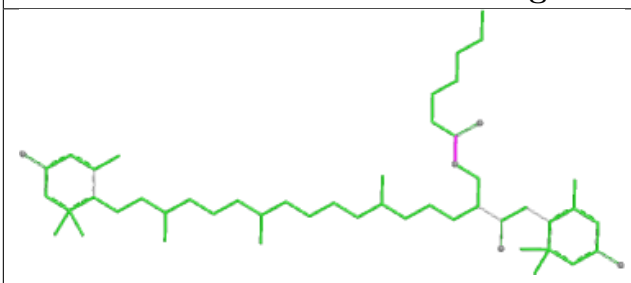


Torsions



Rings

Ligand 0UR 0 316



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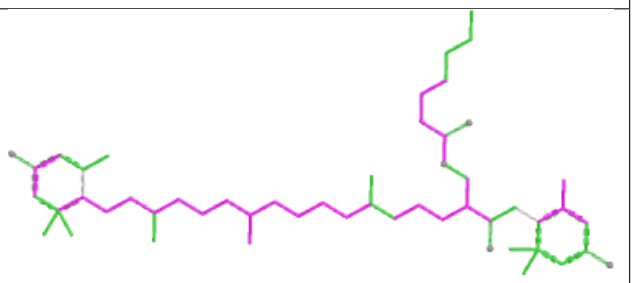
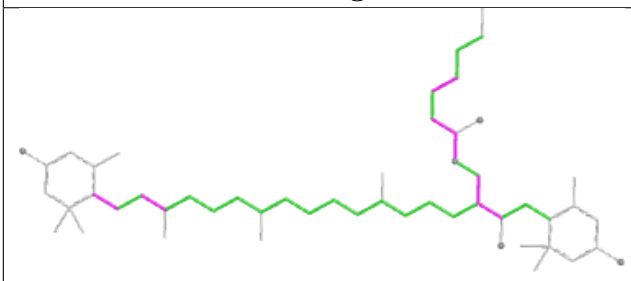
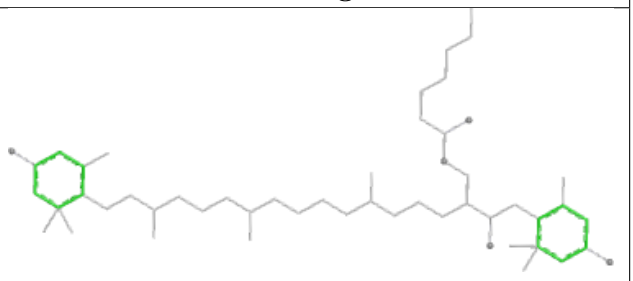


Bond angles

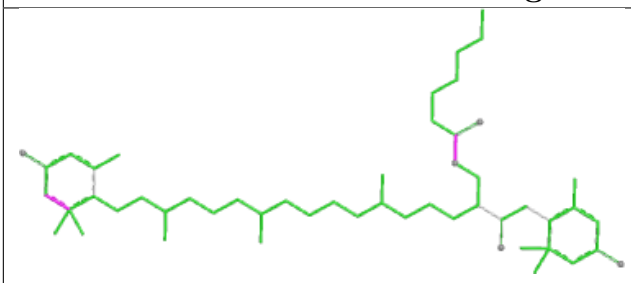


Torsions



Rings

Ligand 0UR O 207



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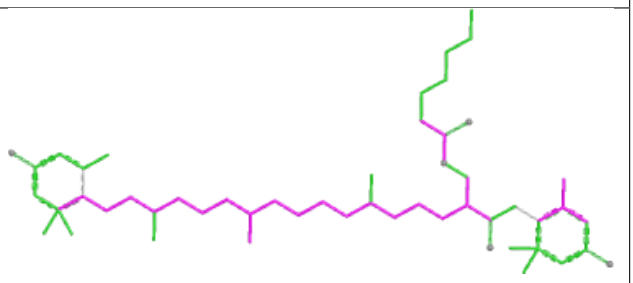
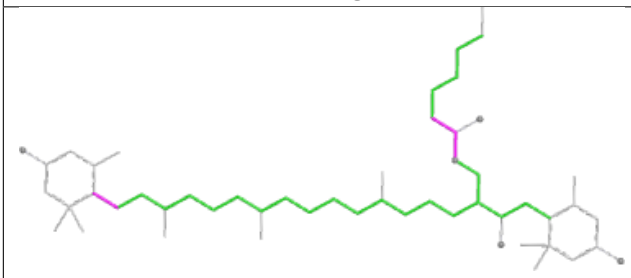
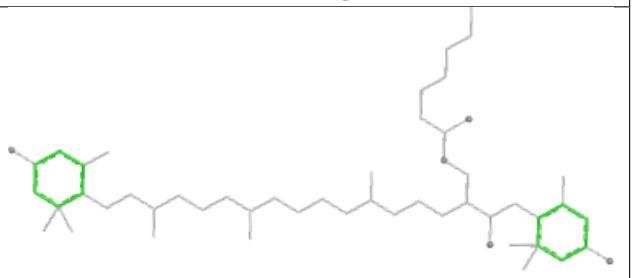


Bond angles

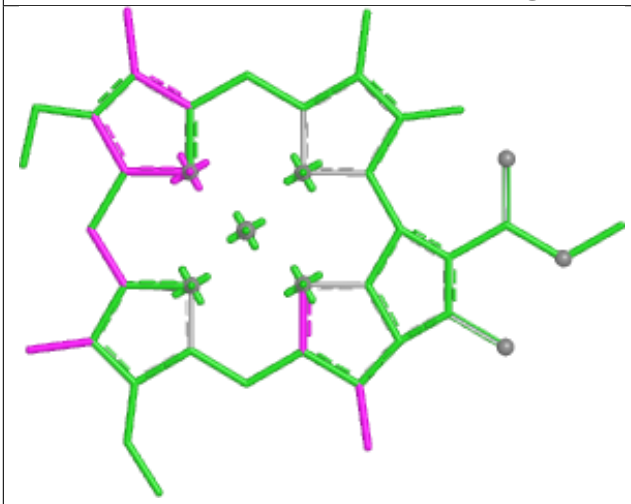


Torsions

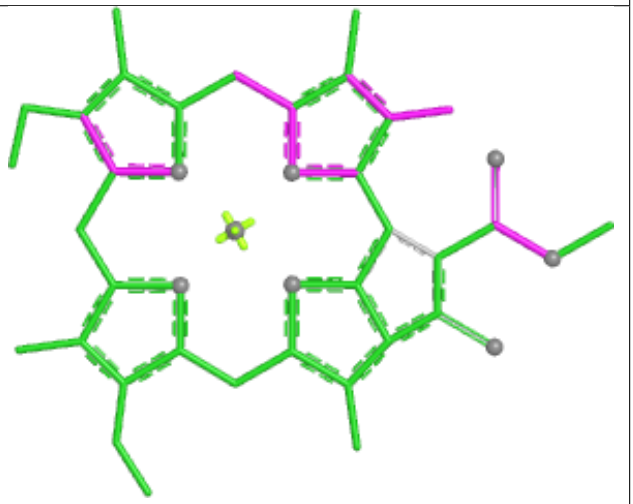


Rings

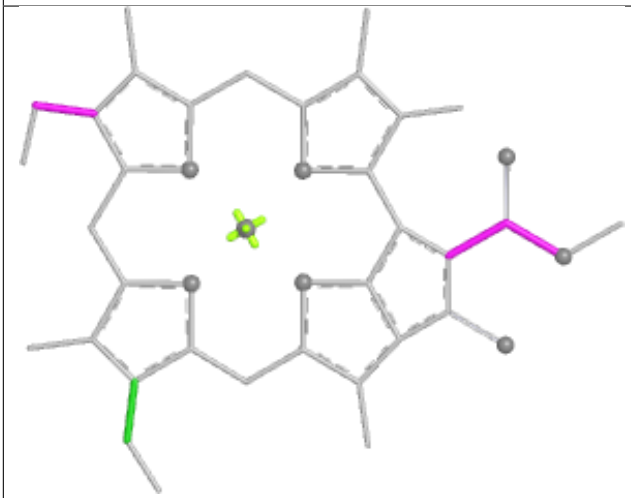
Ligand CLA O 204



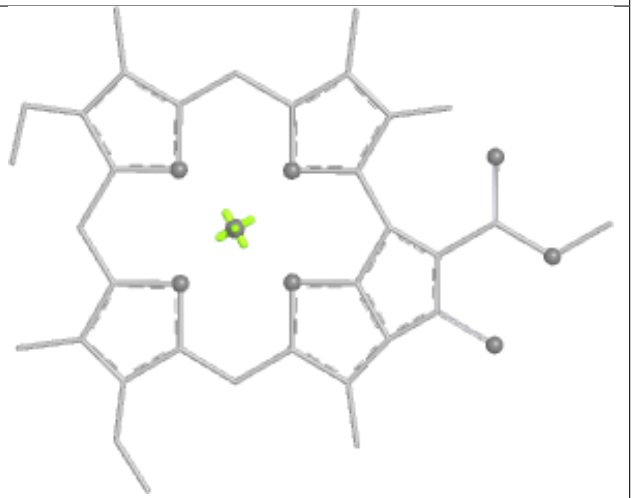
Bond lengths



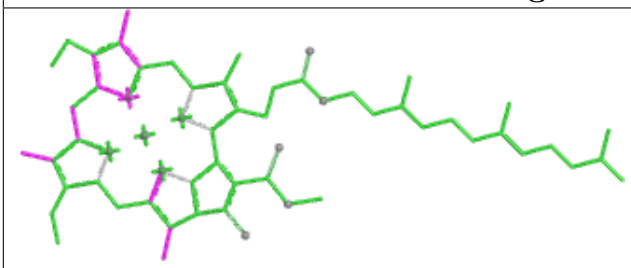
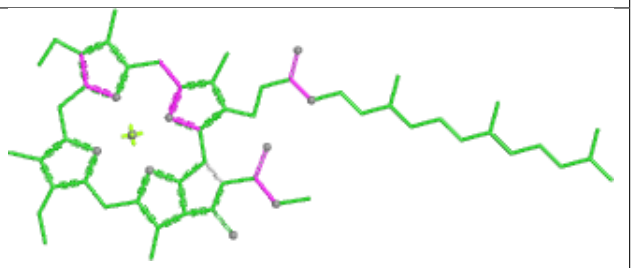
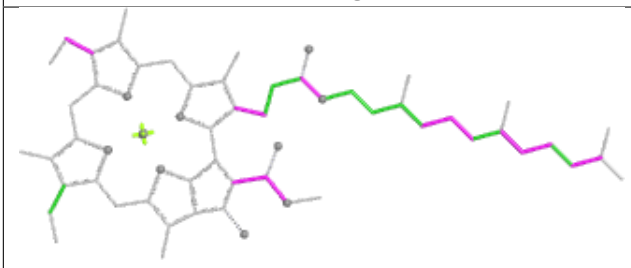
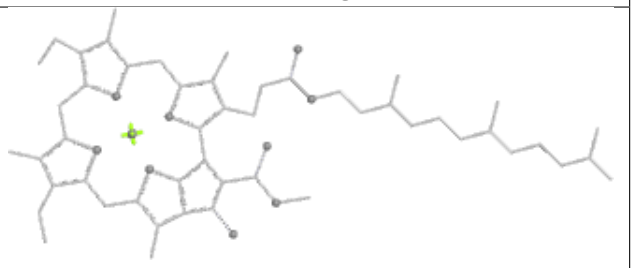
Bond angles

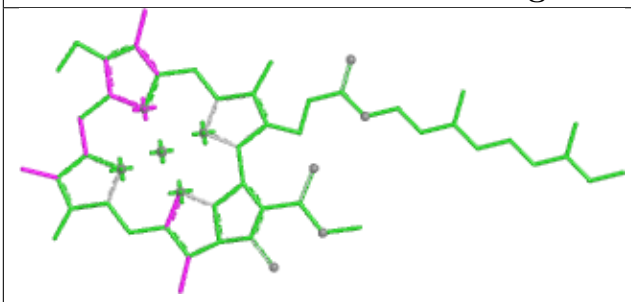
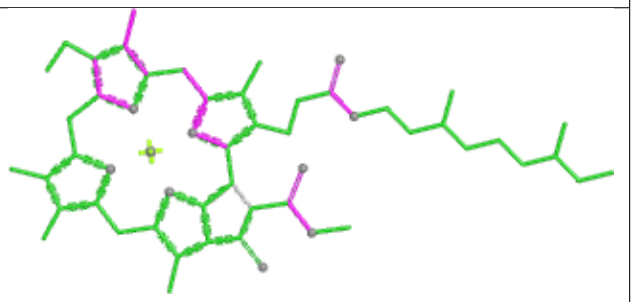


Torsions



Rings

Ligand CLA 4 310	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

Ligand CLA 1 308	
	
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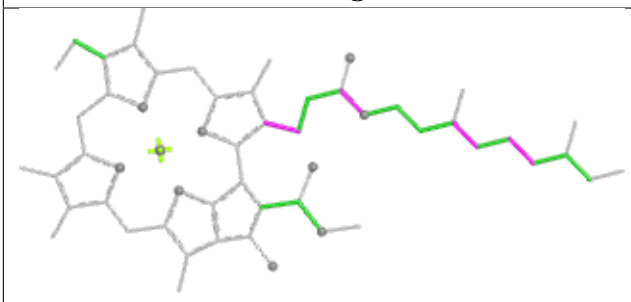
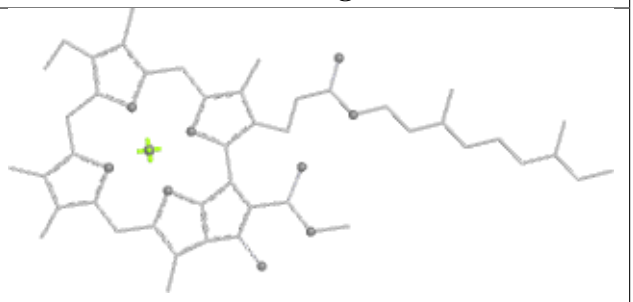
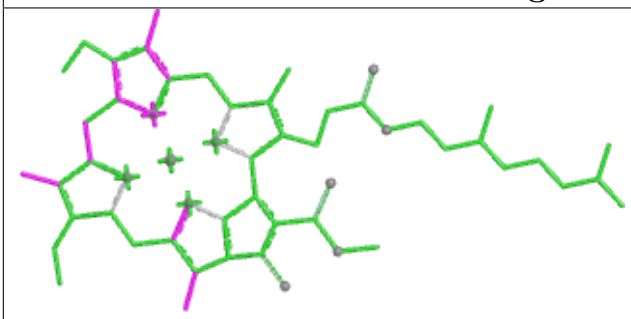
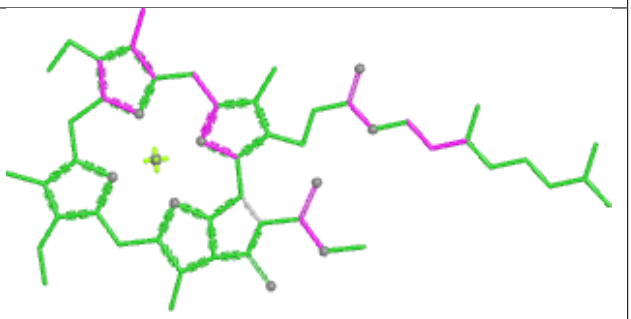
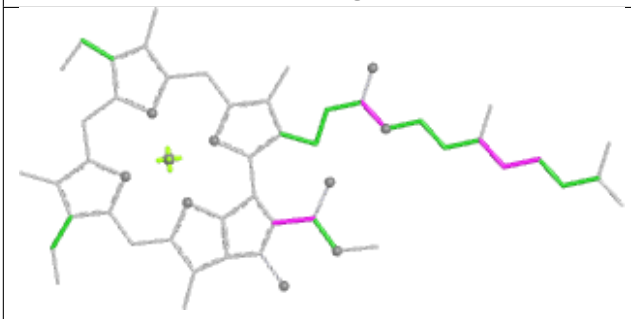
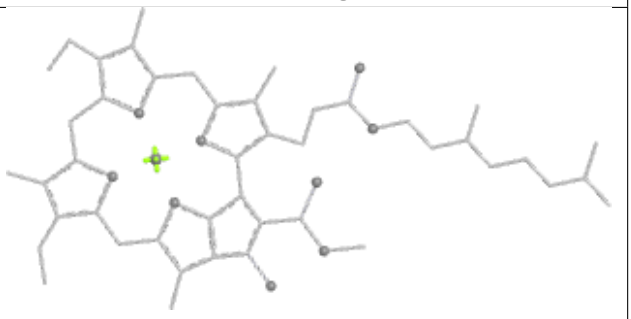
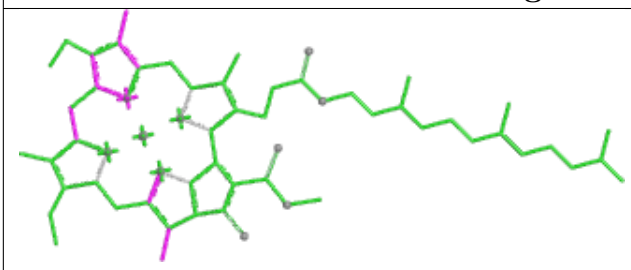
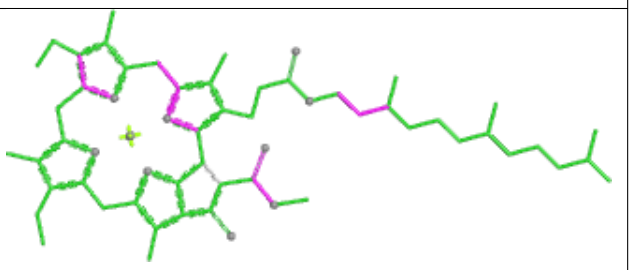
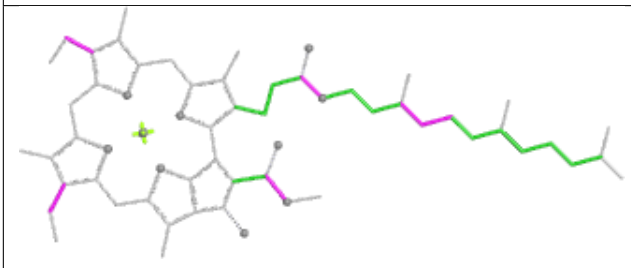
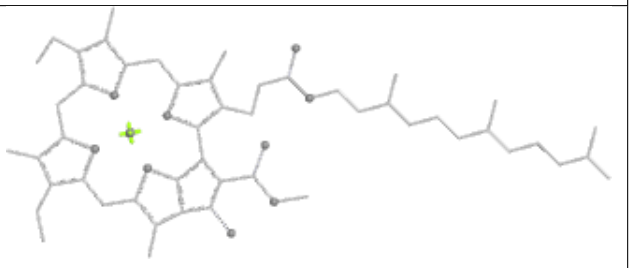
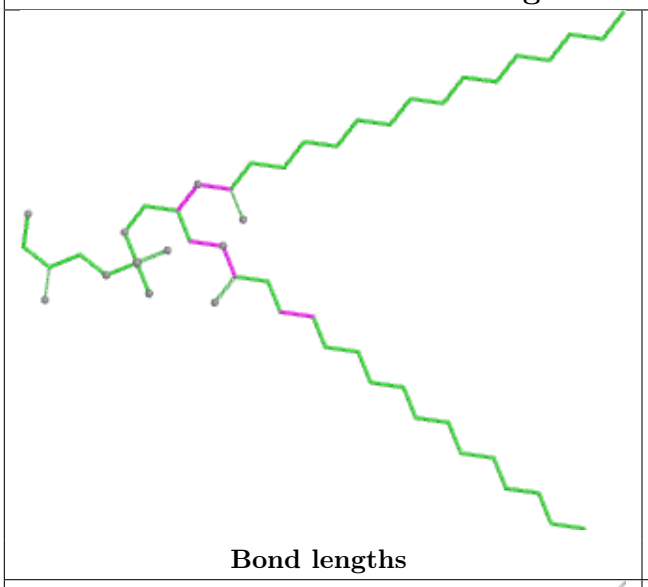
	
Torsions	**Rings**

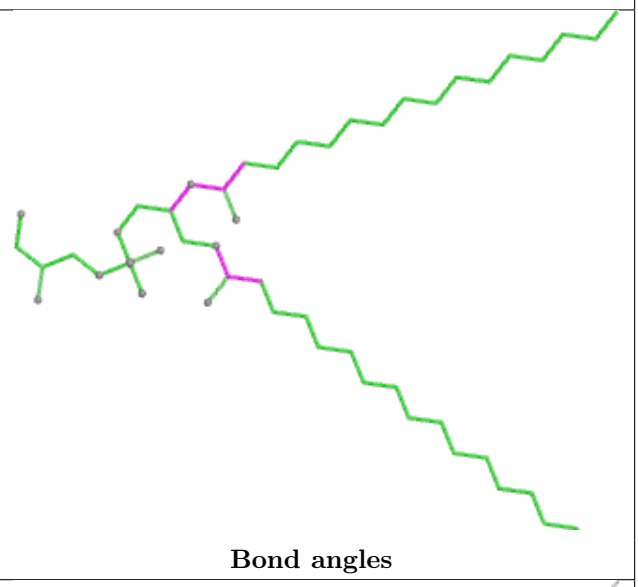
Ligand CLA 7 304	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA B 822	
	
Bond lengths	Bond angles
	
Torsions	Rings

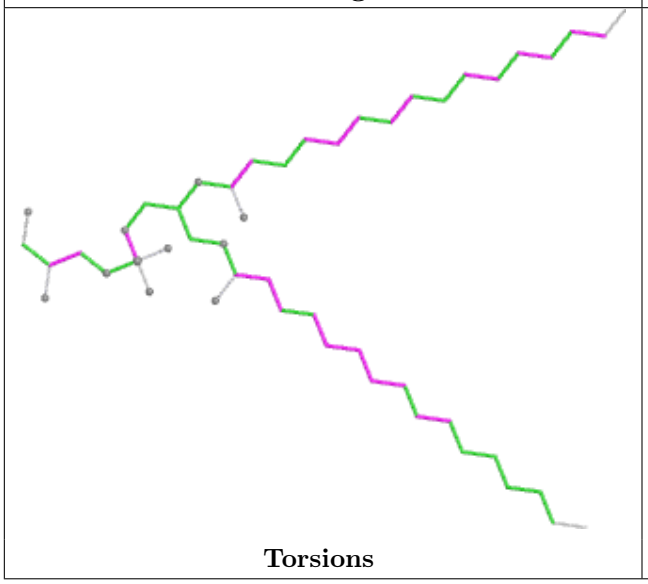
Ligand LHG A 842



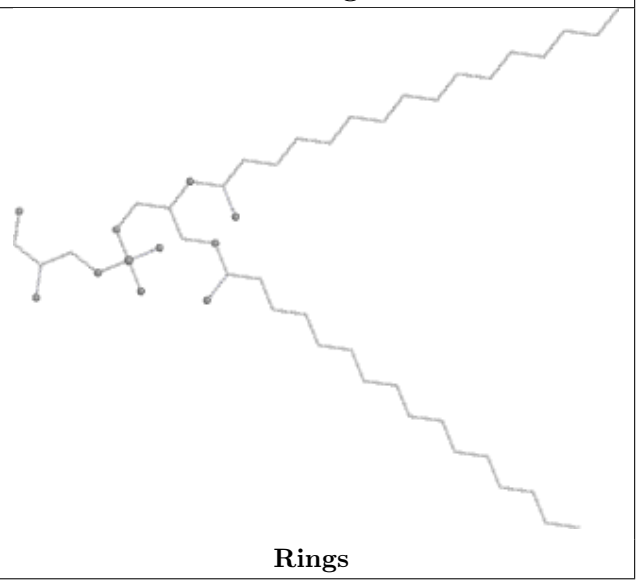
Bond lengths



Bond angles

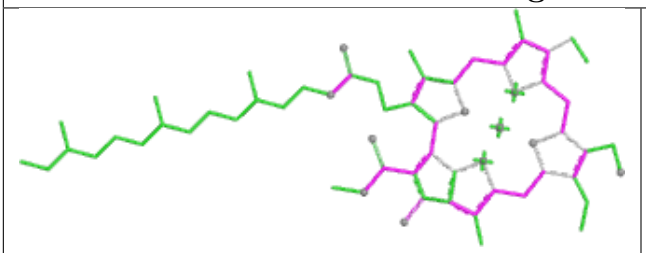


Torsions



Rings

Ligand CHL 1 312



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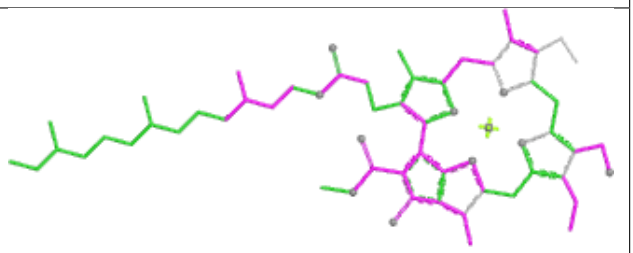
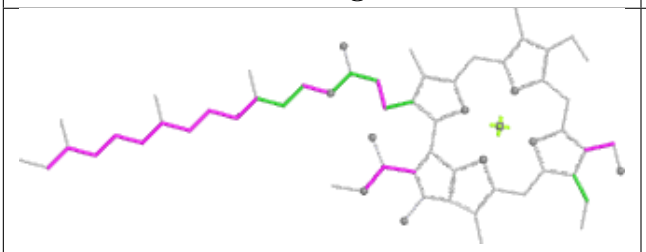


Bond angles



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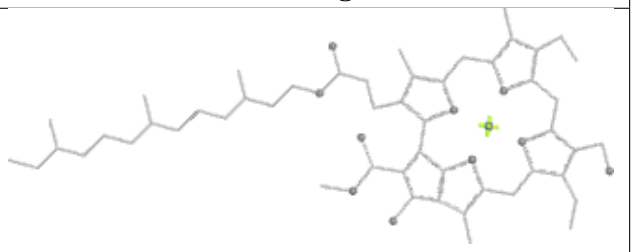
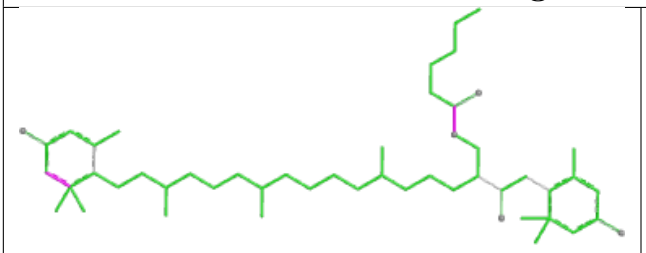


Rings

Ligand 0UR 6 320



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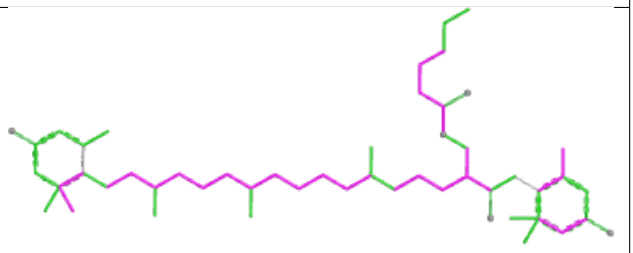
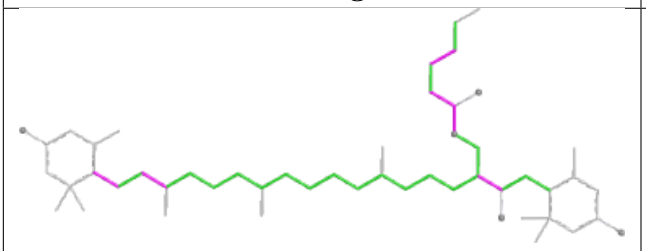


Bond angles



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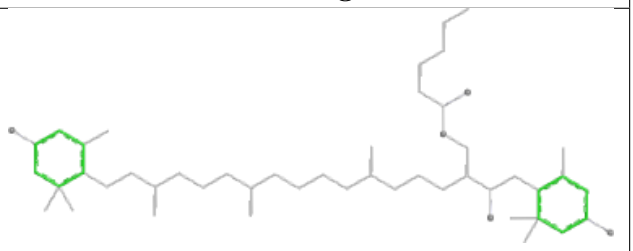
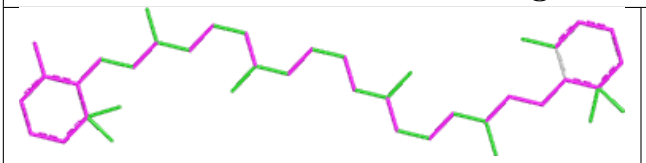


Rings

Ligand 8CT 3 316



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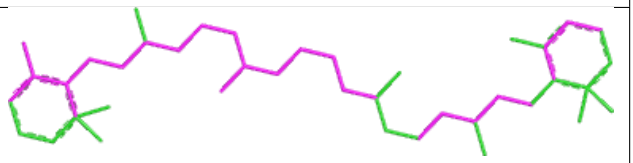
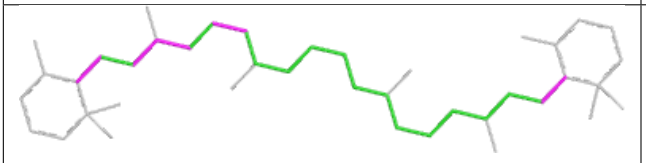


Bond angles



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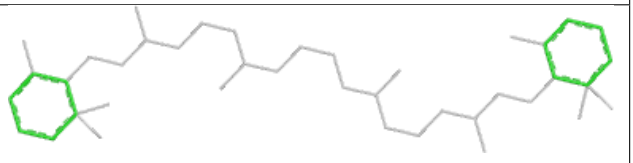
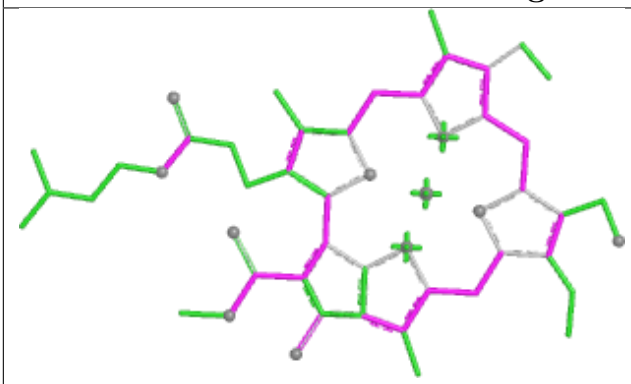


Rings

Ligand CHL 7 307



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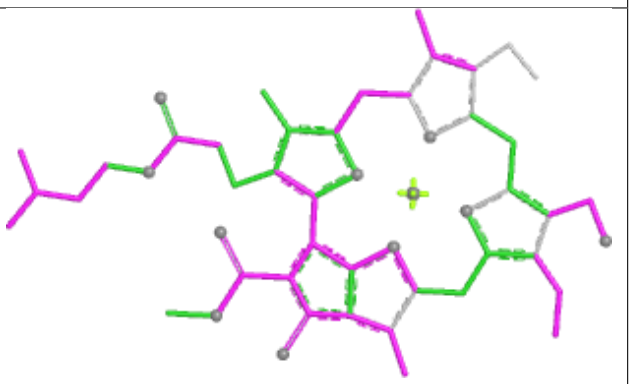
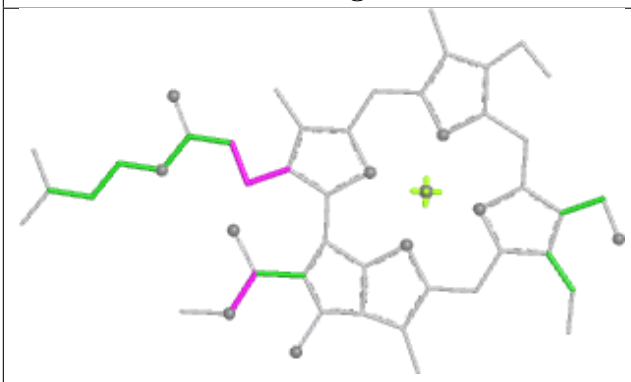


Bond angles



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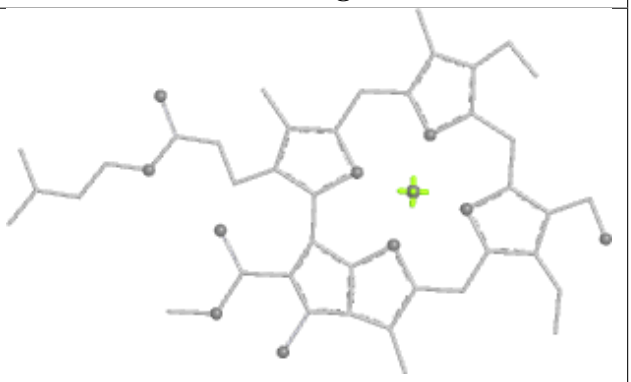
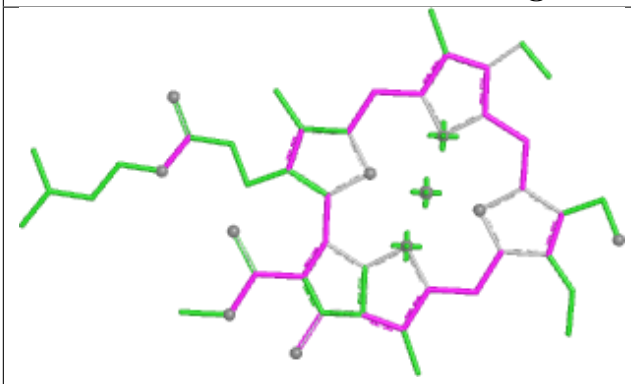


Rings

Ligand CHL 2 306



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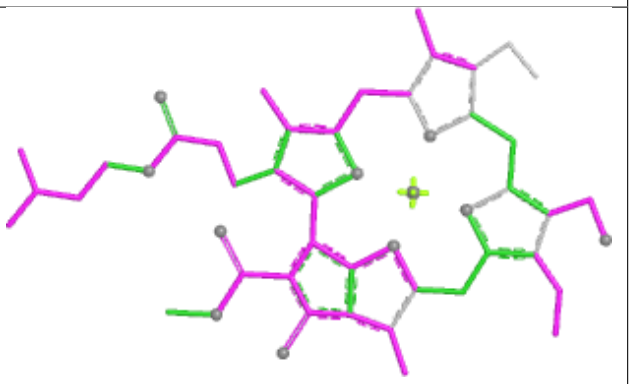
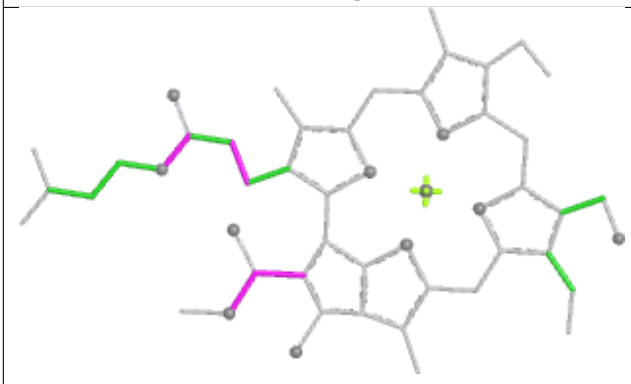


Bond angles



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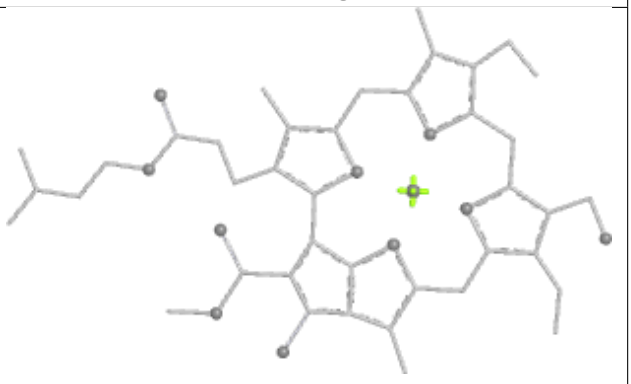

Rings

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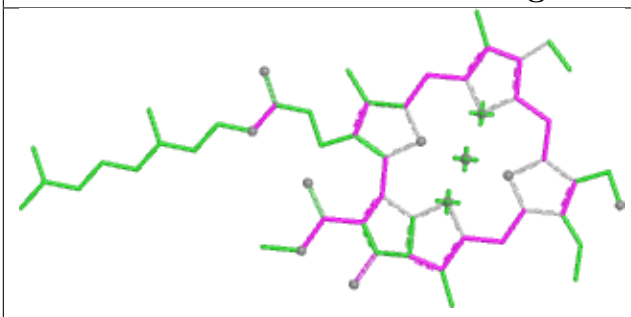
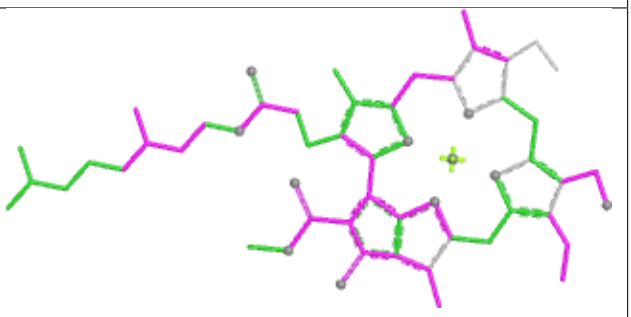
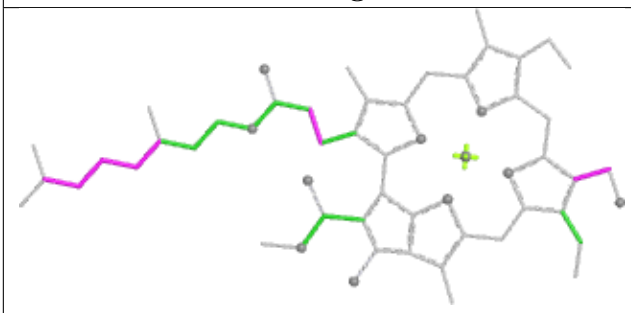
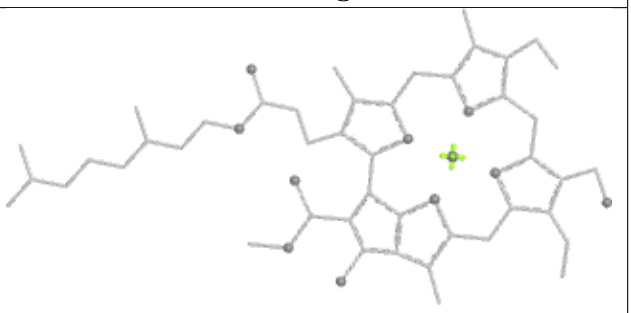
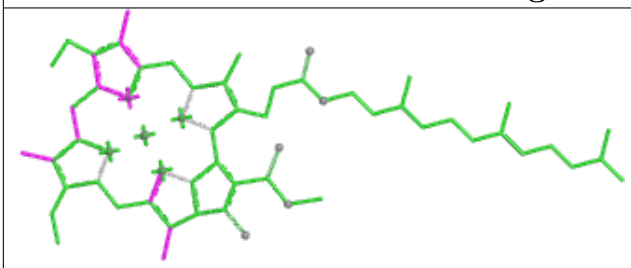
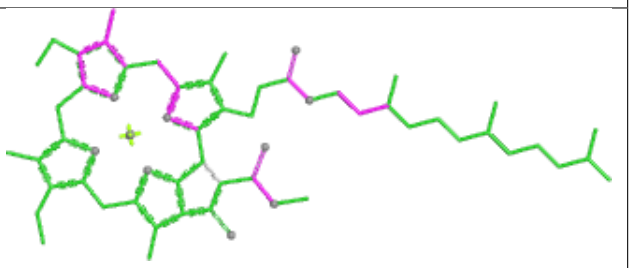
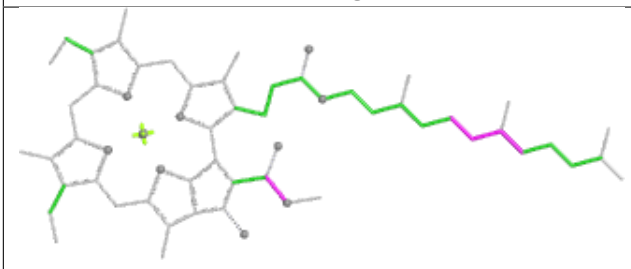
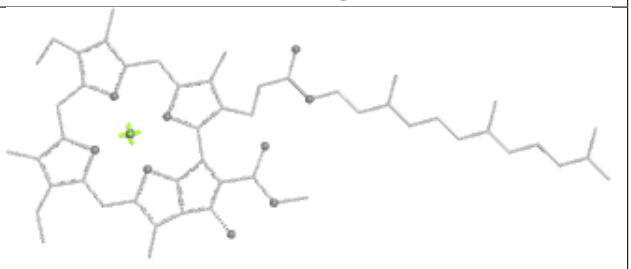
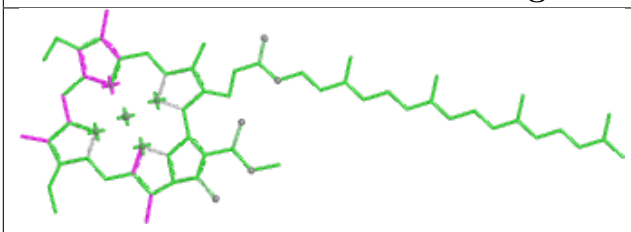
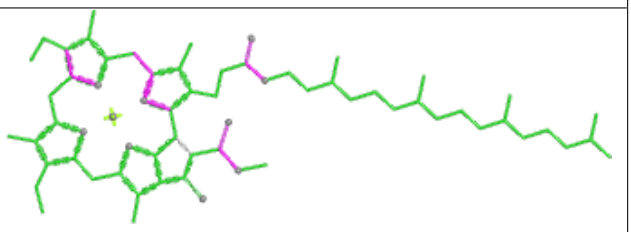
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA 9 308	
	
Bond lengths	Bond angles
	
Torsions	Rings

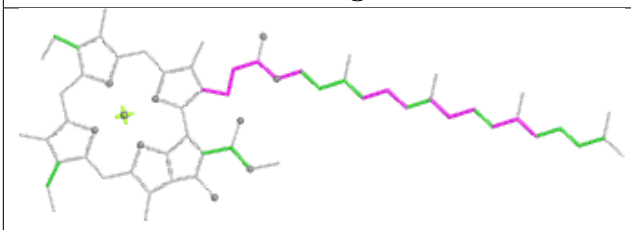
Ligand CLA 7 308



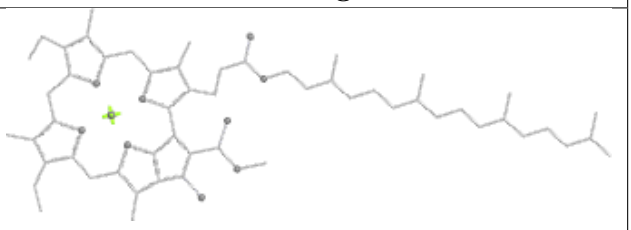
Bond lengths



Bond angles

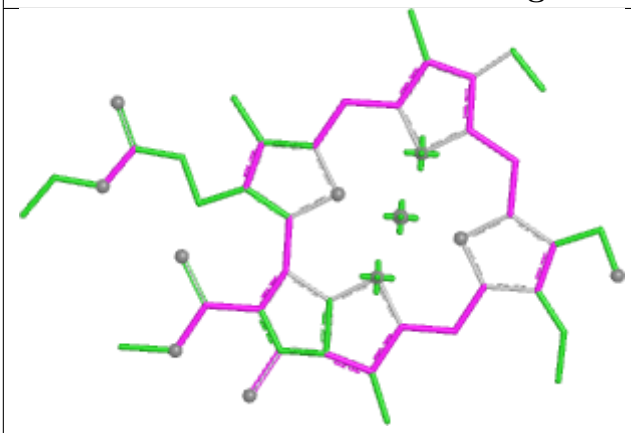


Torsions

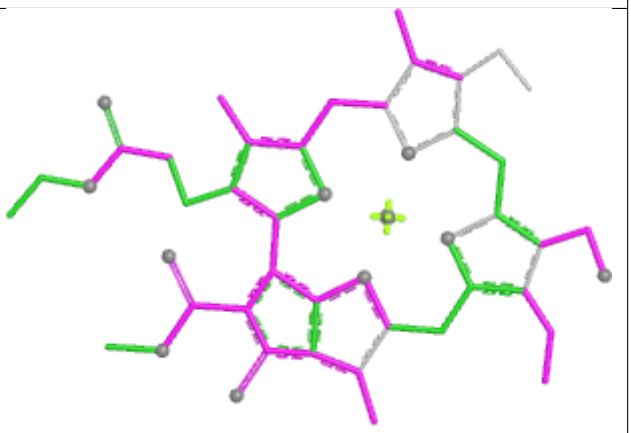


Rings

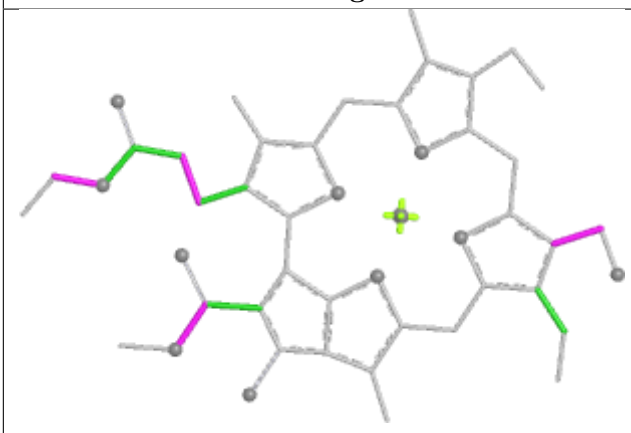
Ligand CHL 2 305



Bond lengths



Bond angles



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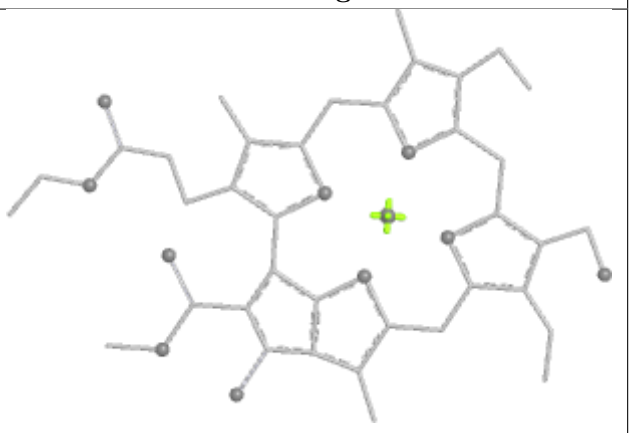
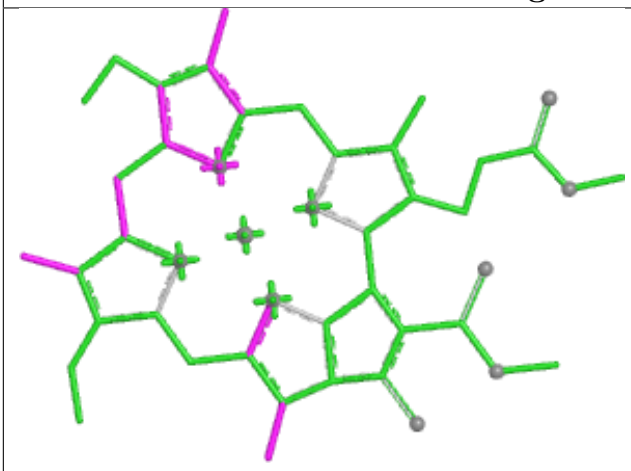


Rings

Ligand CLA 6 304



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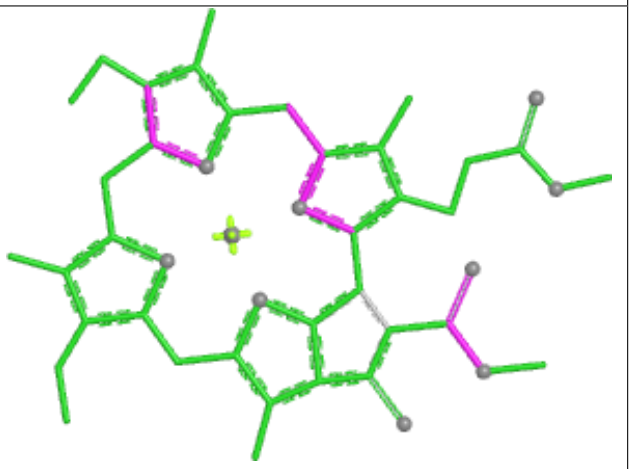

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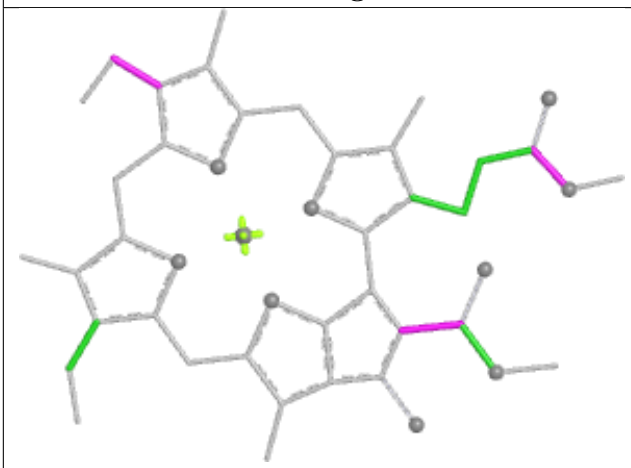

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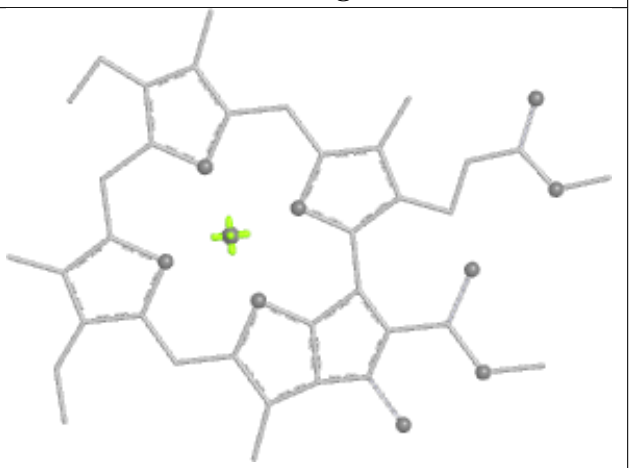
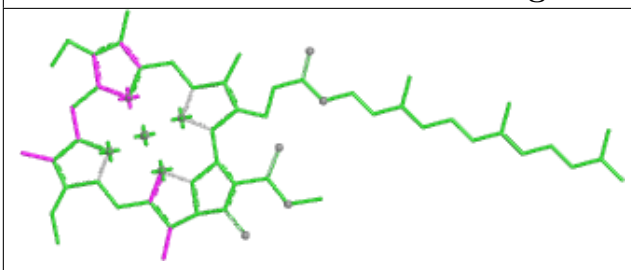


Rings

Ligand CLA 0 308



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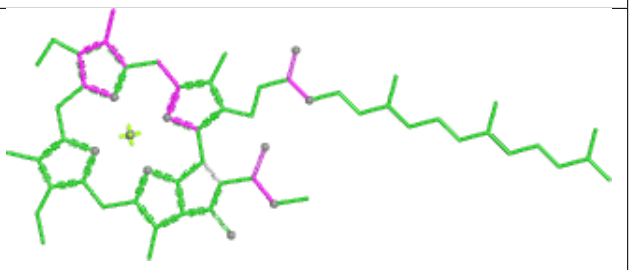
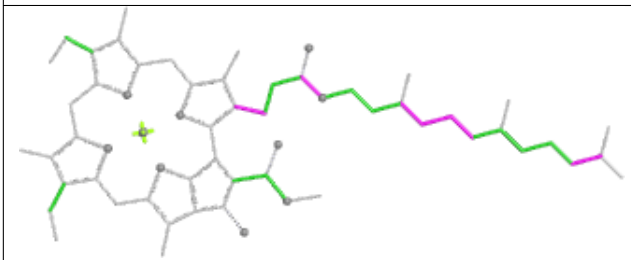


Bond angles



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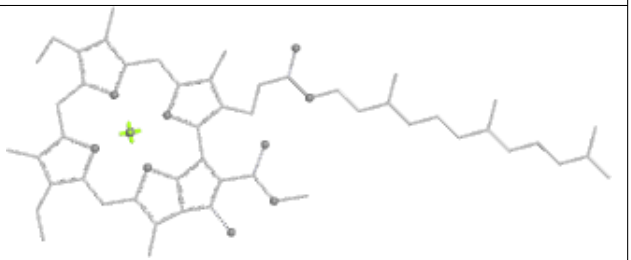
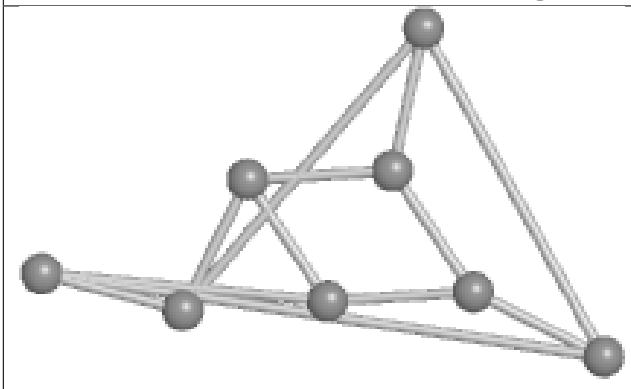


Rings

Ligand SF4 C 101



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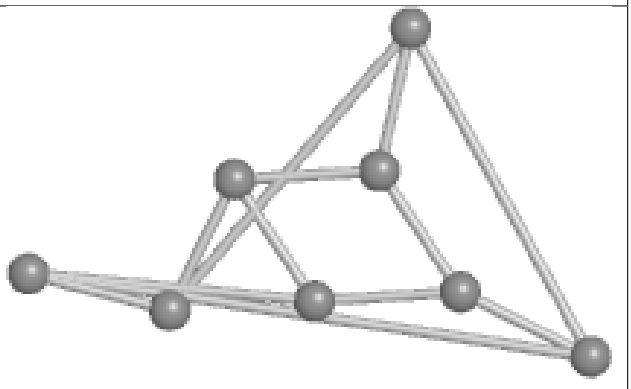
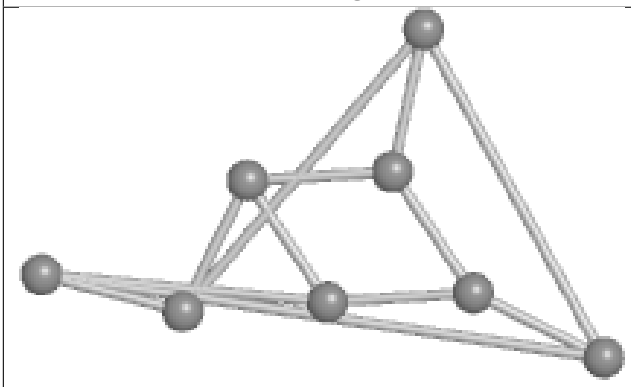


Bond angles



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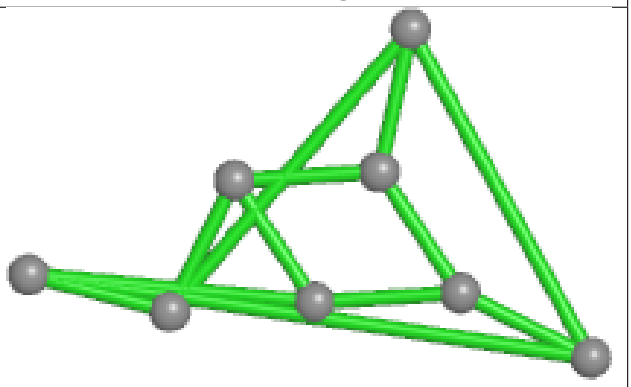
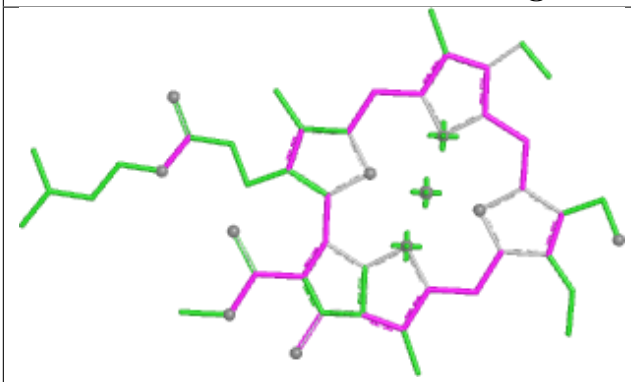


Rings

Ligand CHL 4 313



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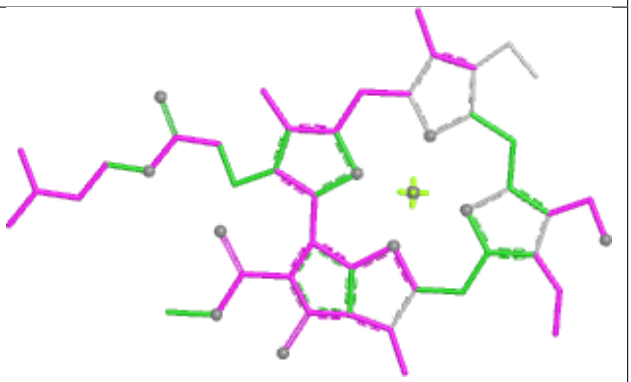

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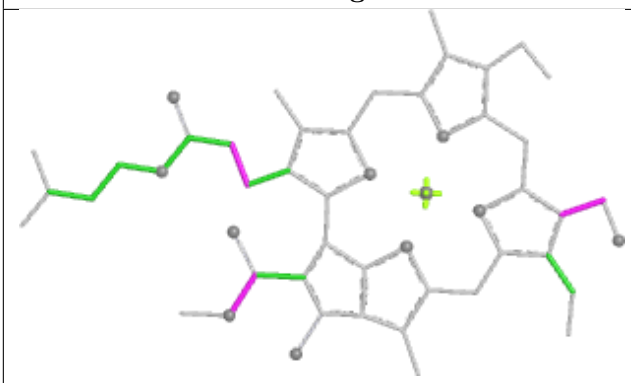

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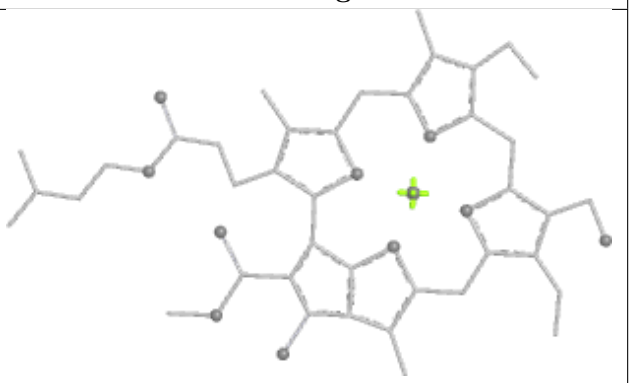
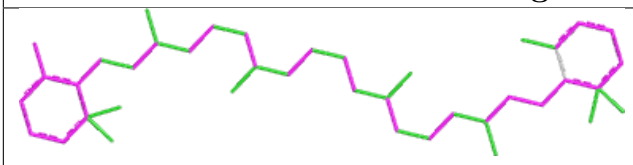


Rings

Ligand 8CT 7 318



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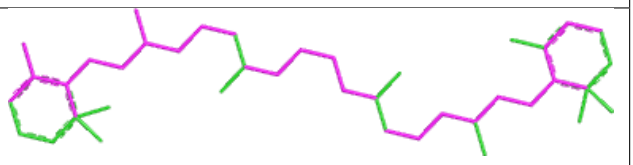

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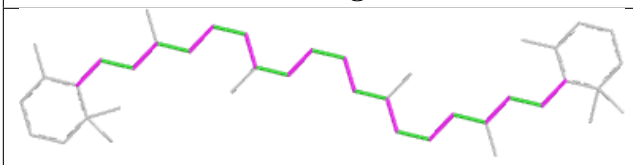

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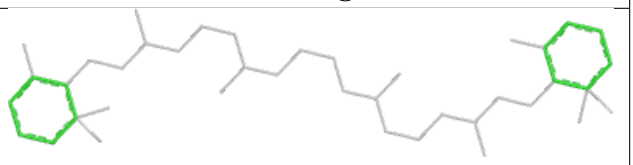
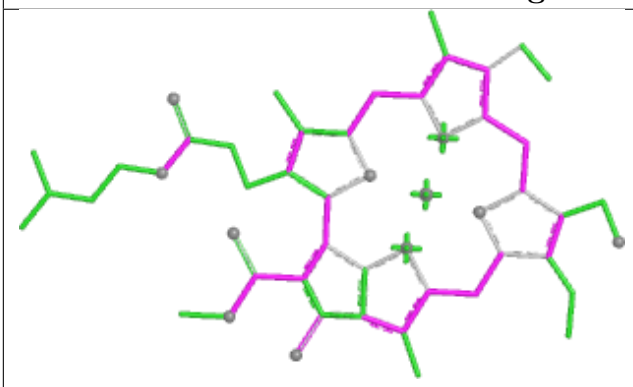


Rings

Ligand CHL 6 307



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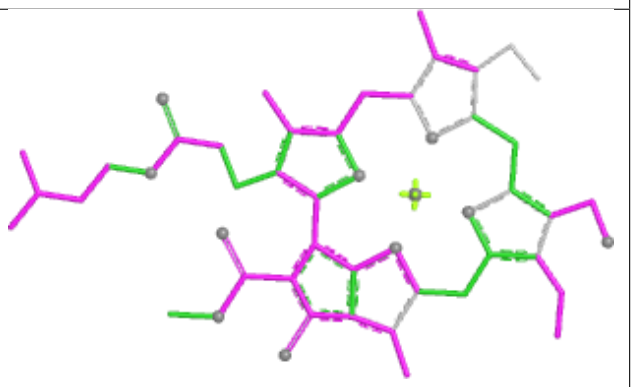

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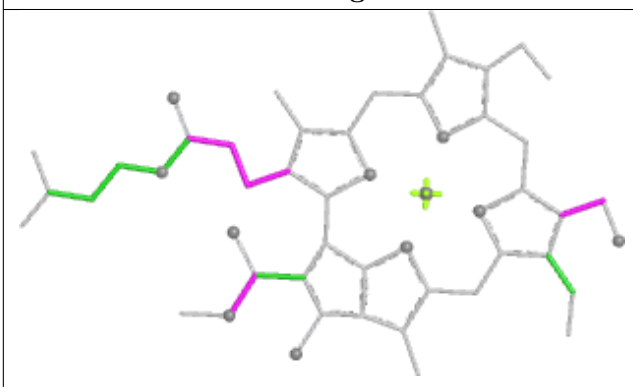

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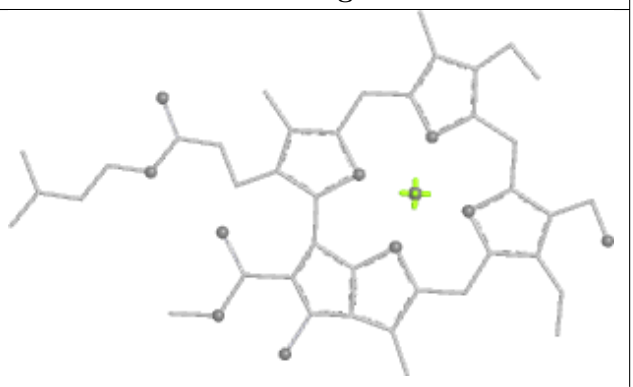
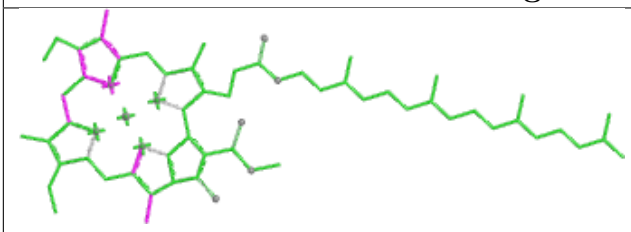


Rings

Ligand CLA A 848



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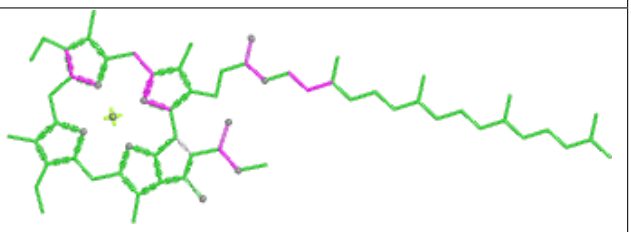
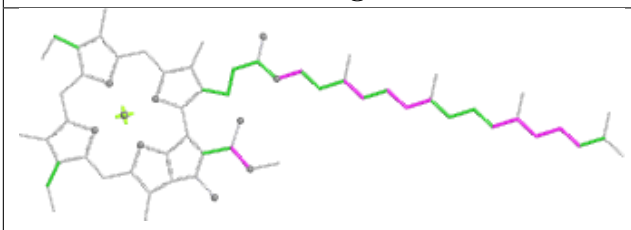


Bond angles



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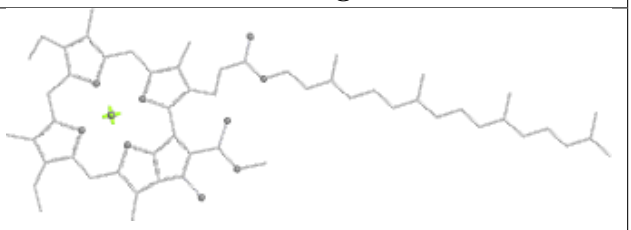
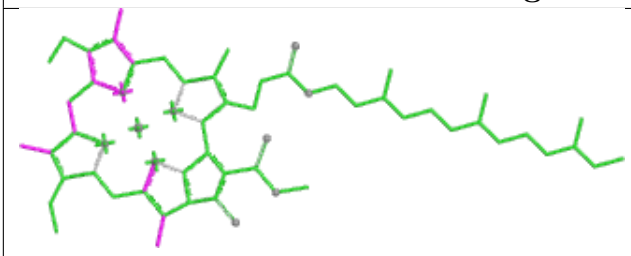


Rings

Ligand CLA A 836



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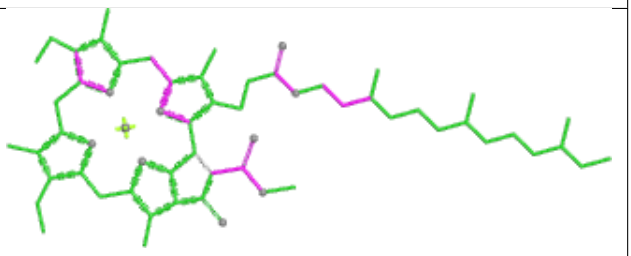
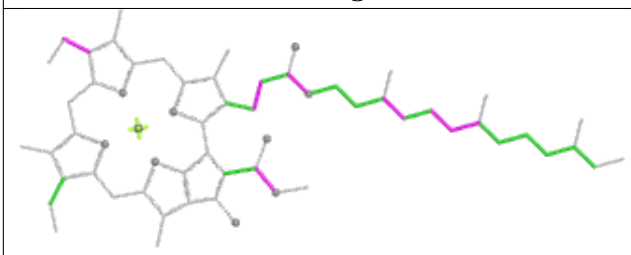


Bond angles



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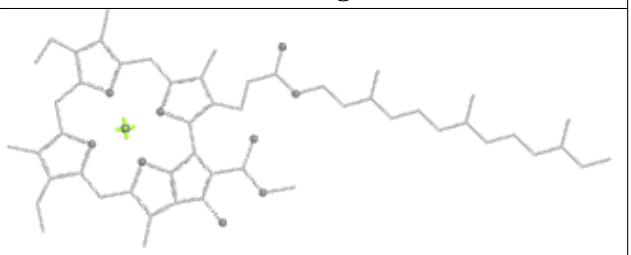
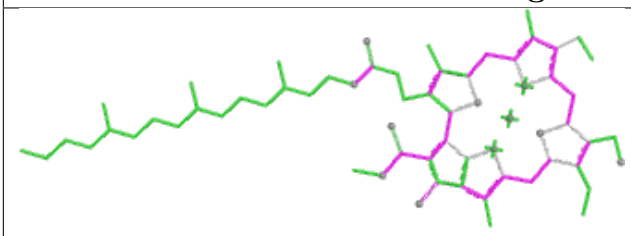


Rings

Ligand CHL 0 302



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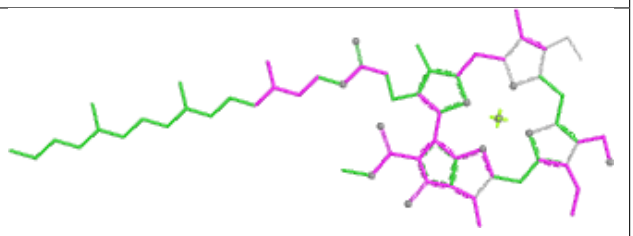
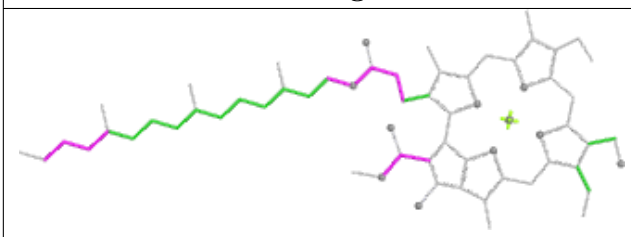


Bond angles



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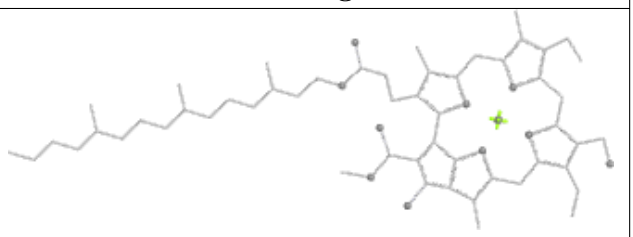
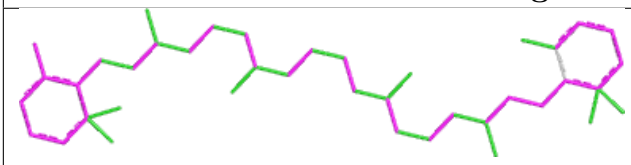


Rings

Ligand 8CT 9 313



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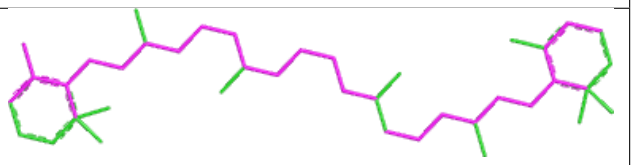
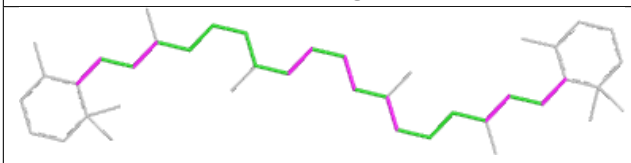


Bond angles



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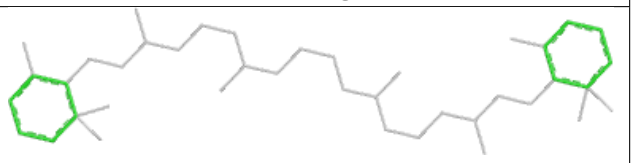
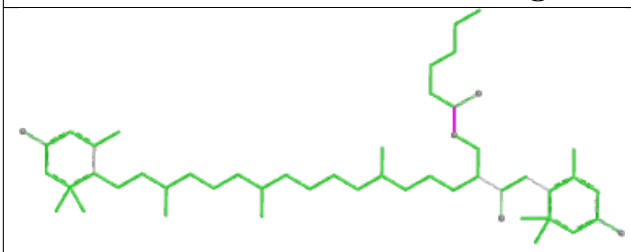


Rings

Ligand 0UR 3 318



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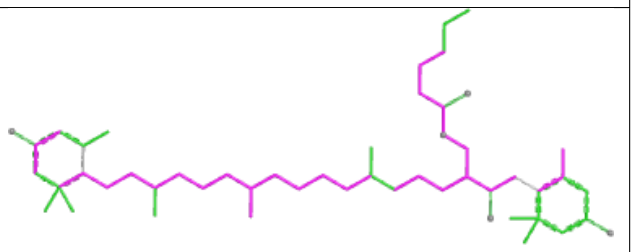
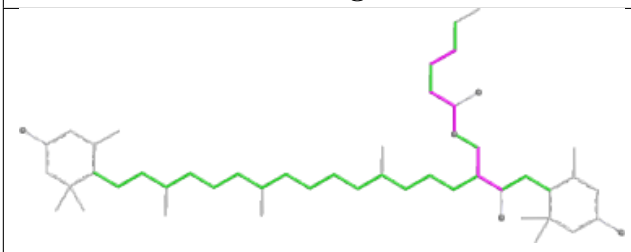


Bond angles



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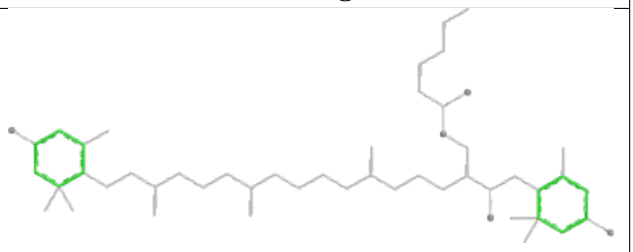
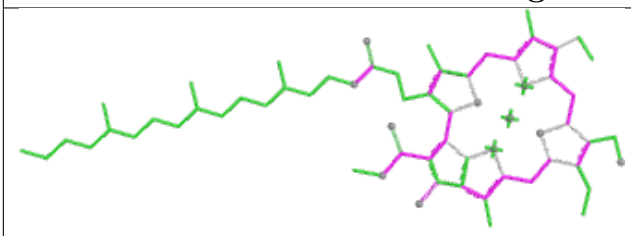


Rings

Ligand CHL 5 301



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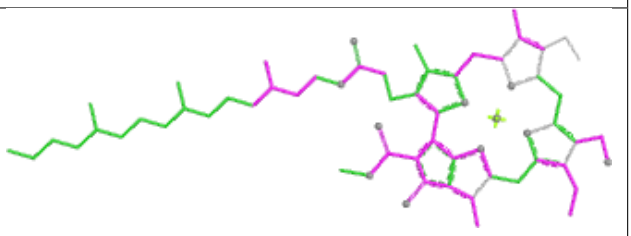
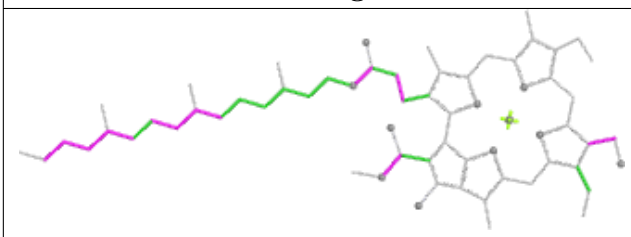


Bond angles



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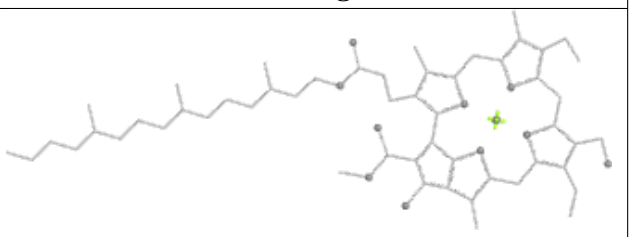
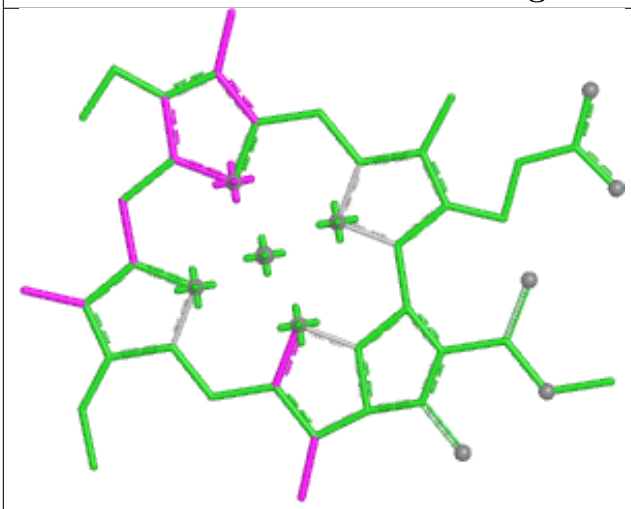
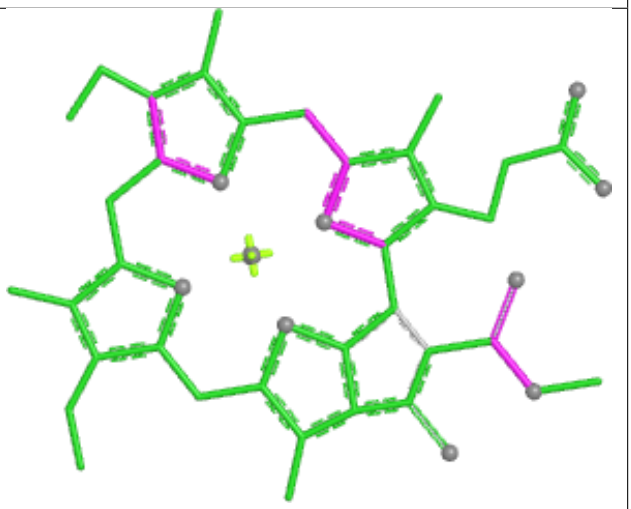


Rings

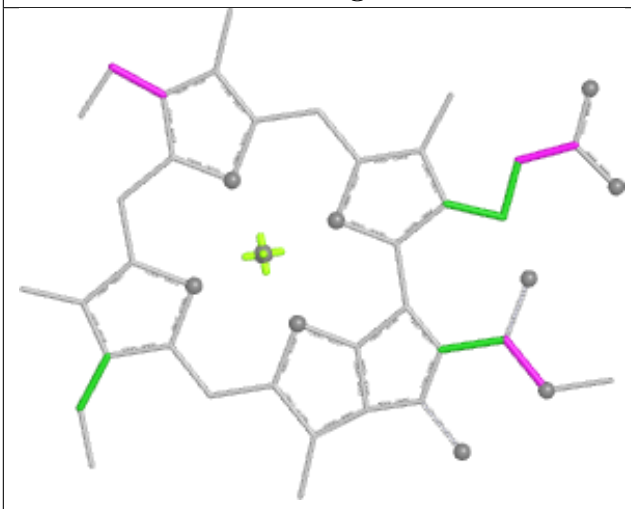
Ligand CLA 2 313



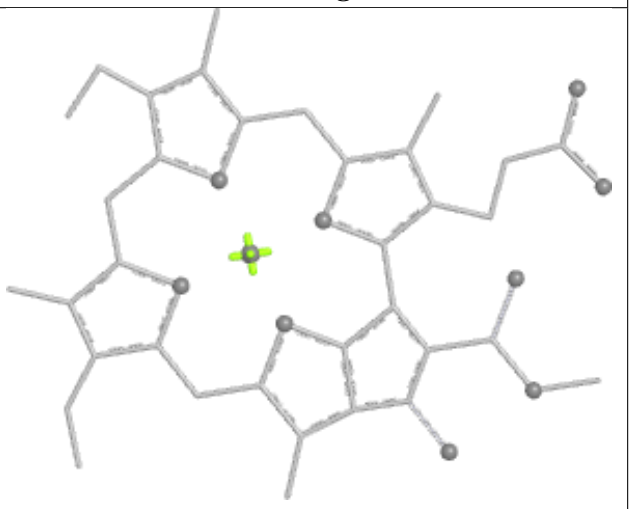
Bond lengths



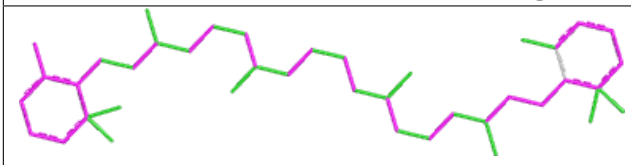
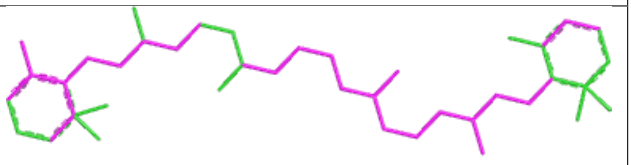
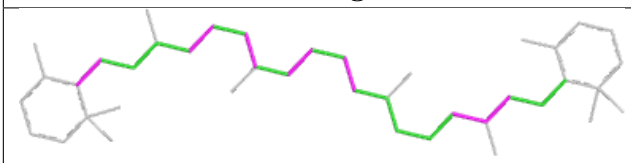
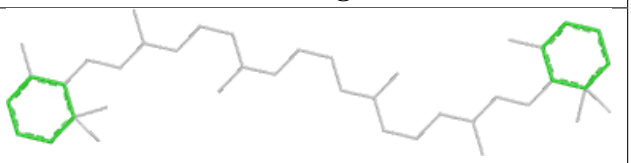
Bond angles

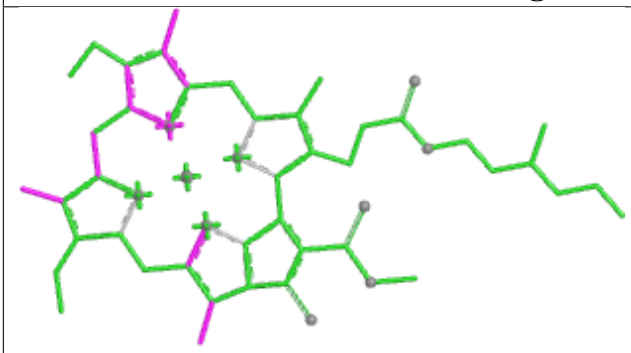
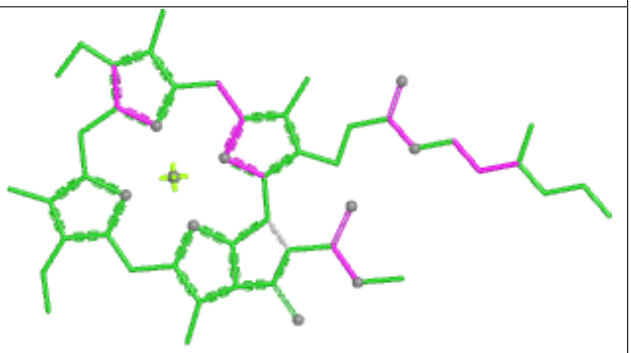
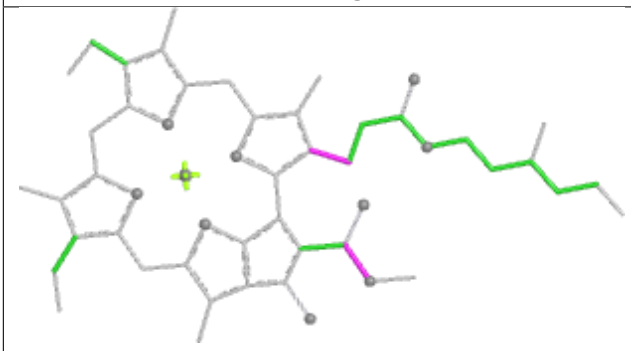
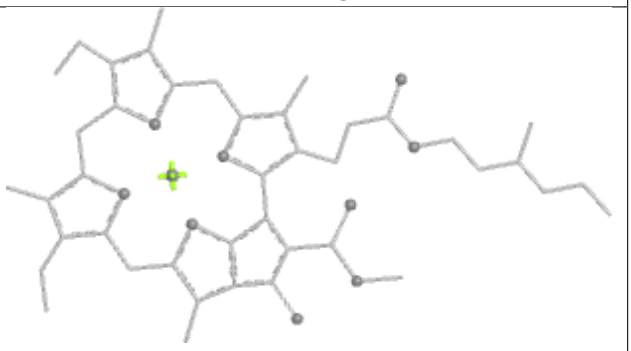


Torsions

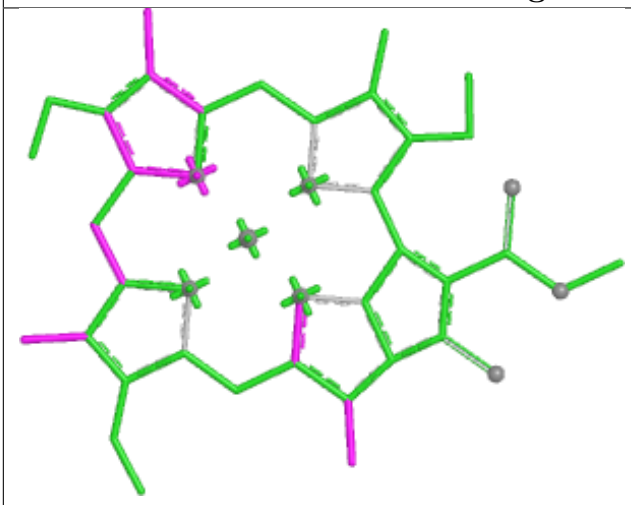


Rings

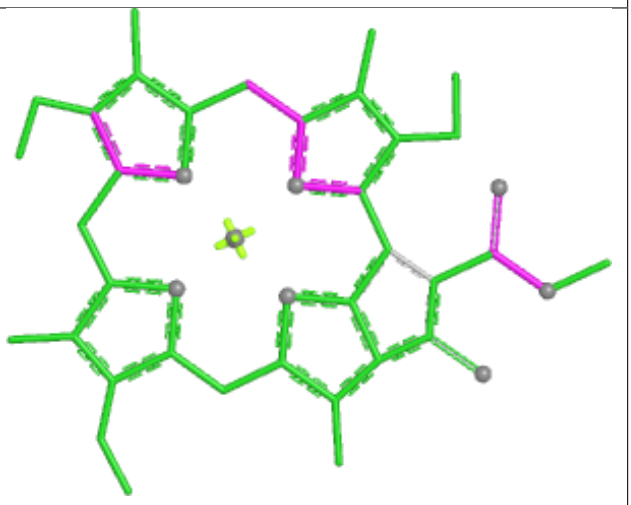
Ligand 8CT 6 324	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA 0 304	
 Bond lengths	 Bond angles
 Torsions	 Rings

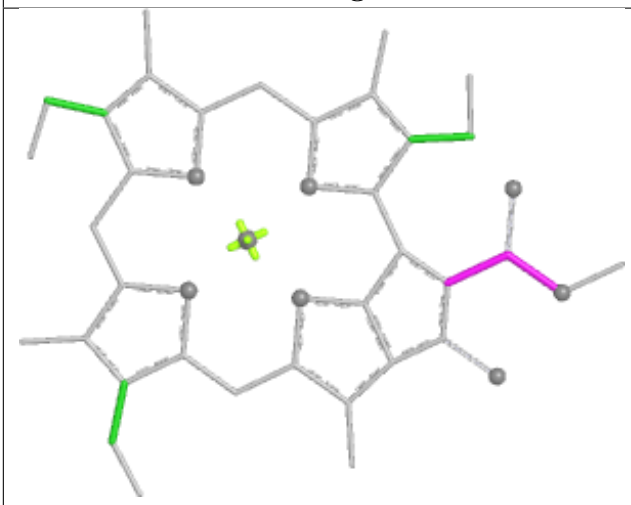
Ligand CLA J 103



Bond lengths



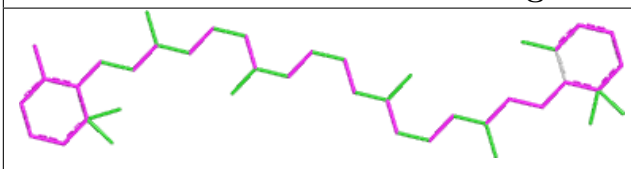
Bond angles



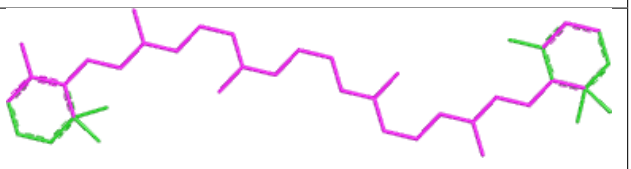
Torsions

Rings

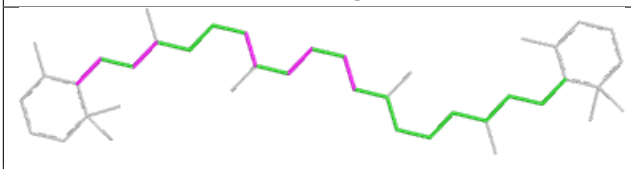
Ligand 8CT O 202



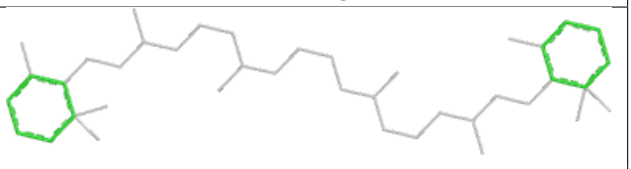
Bond lengths



Bond angles

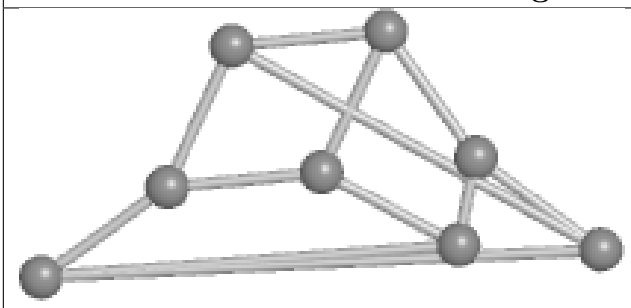


Torsions



Rings

Ligand SF4 B 803



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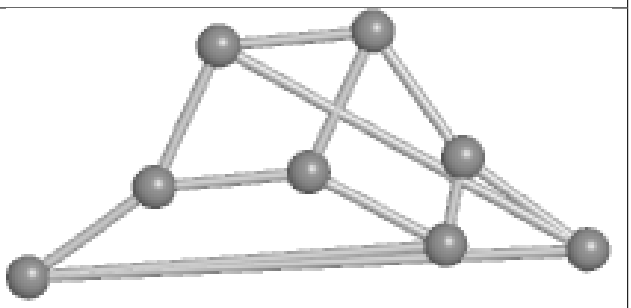
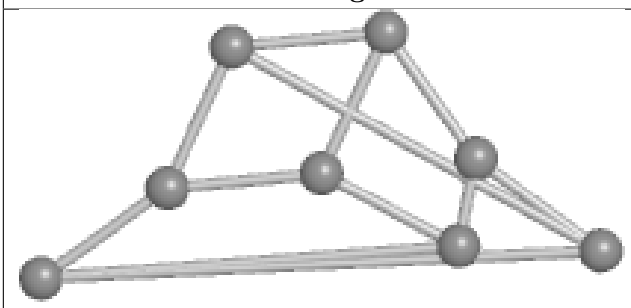
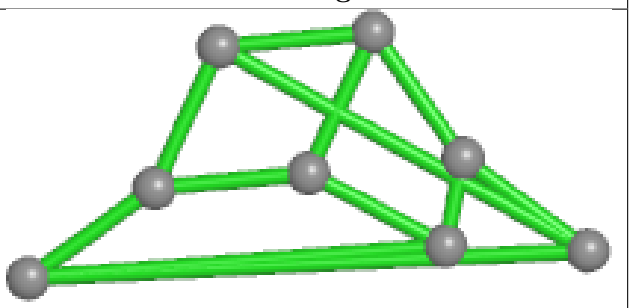


Bond angles

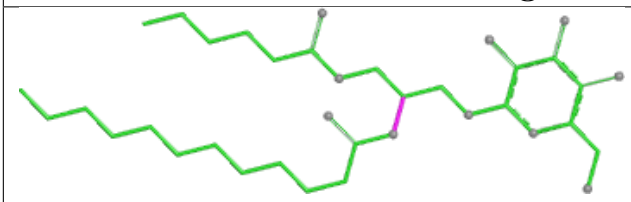


Torsions

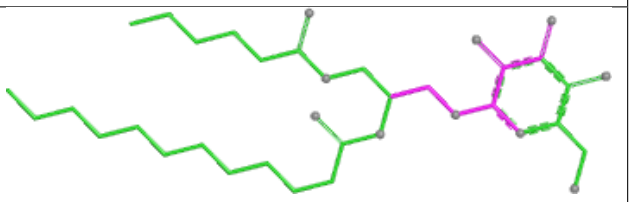


Rings

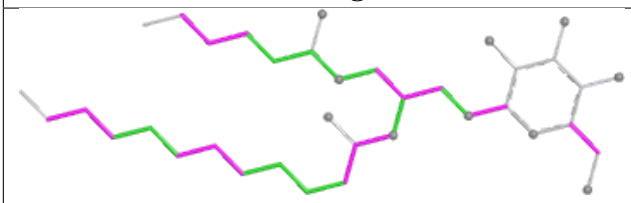
Ligand LMG A 854



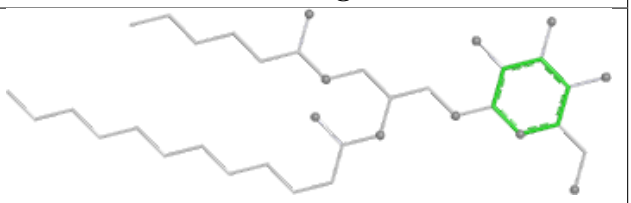
Bond lengths



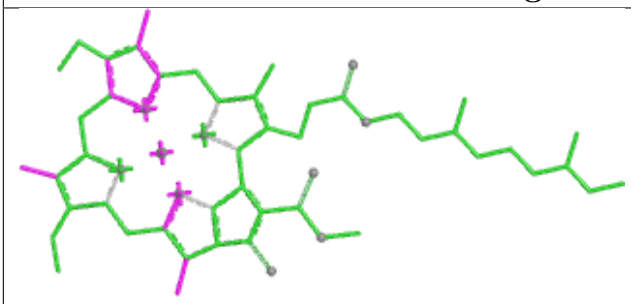
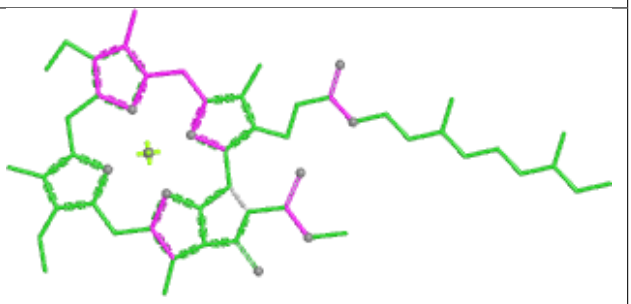
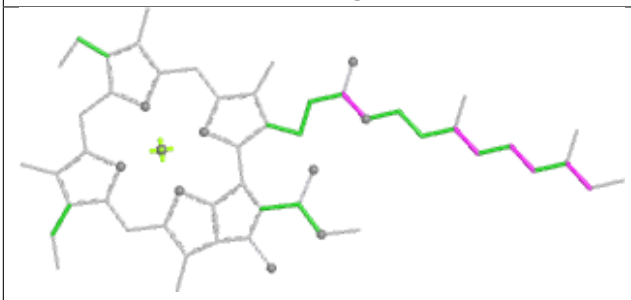
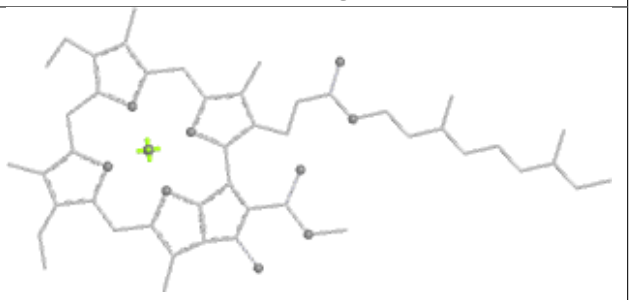
Bond angles

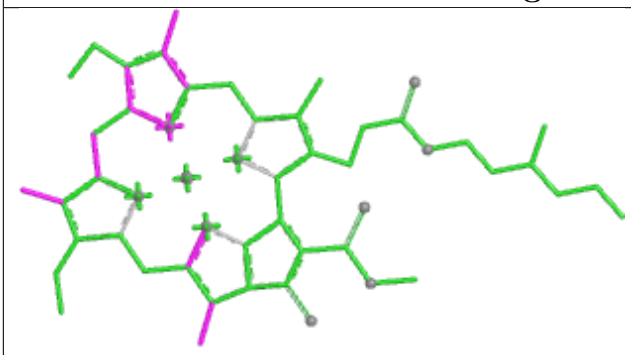
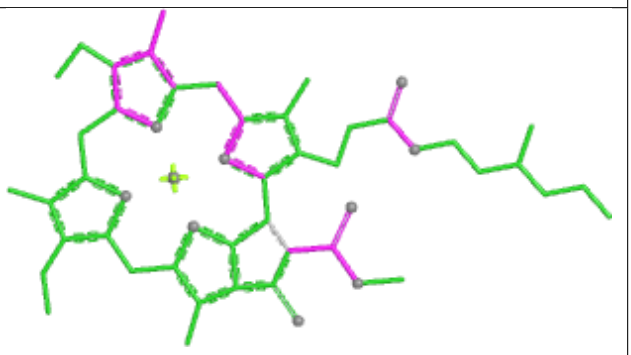
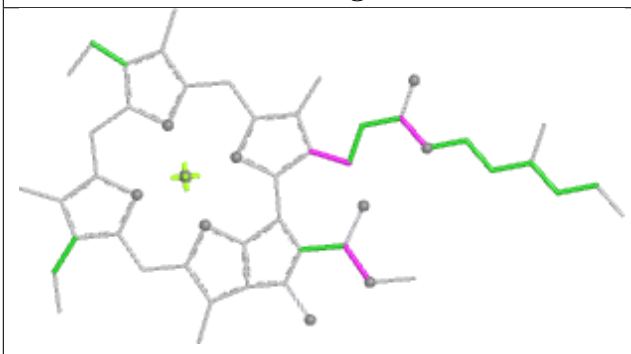
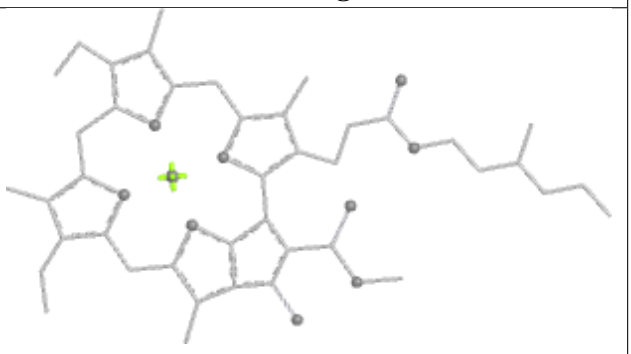


Torsions

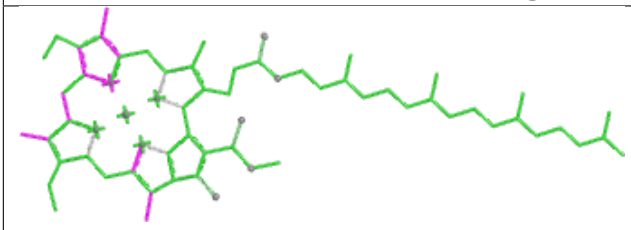


Rings

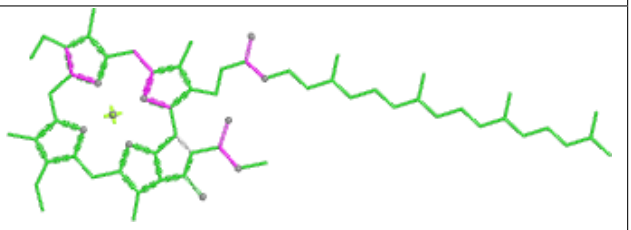
Ligand CLA B 830	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA O 201	
	
Bond lengths	Bond angles
	
Torsions	Rings

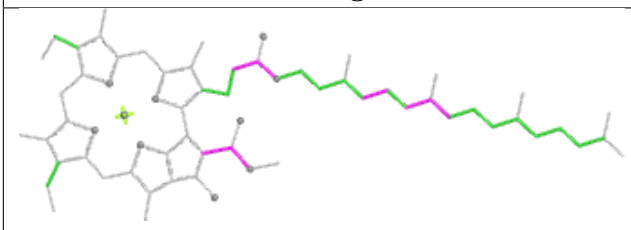
Ligand CLA A 832



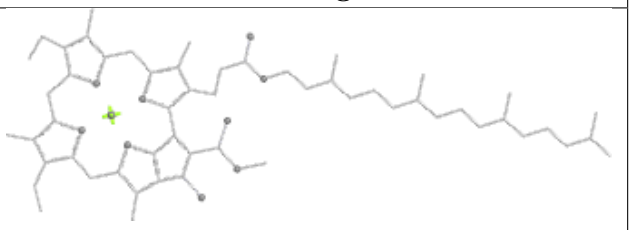
Bond lengths



Bond angles

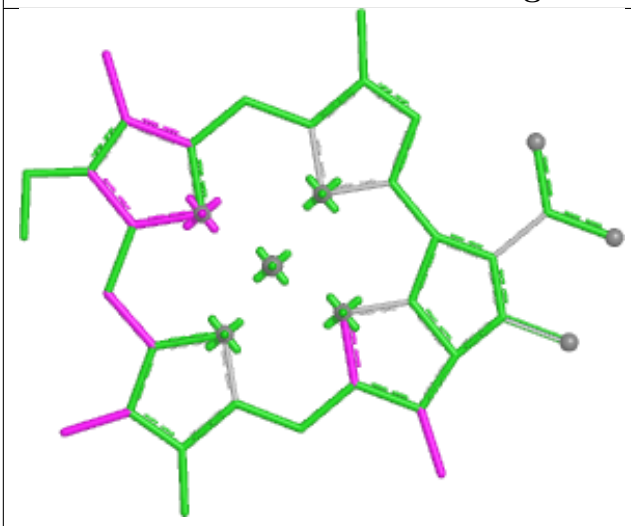


Torsions



Rings

Ligand CLA O 205



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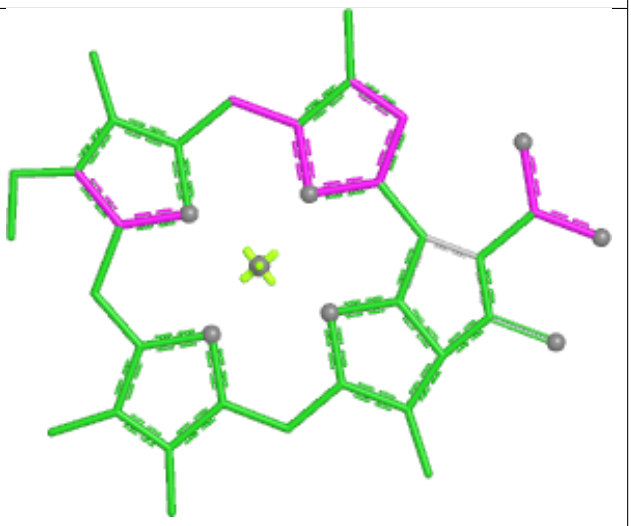
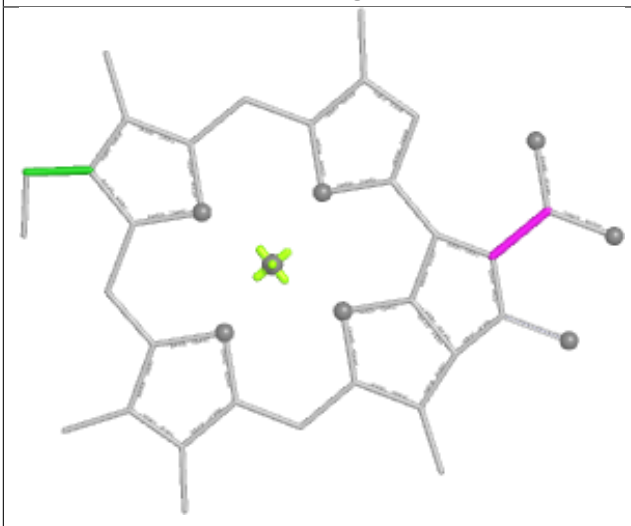
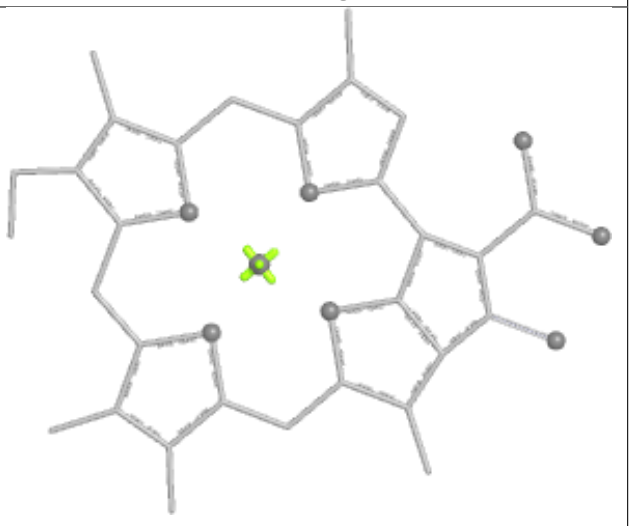


Bond angles

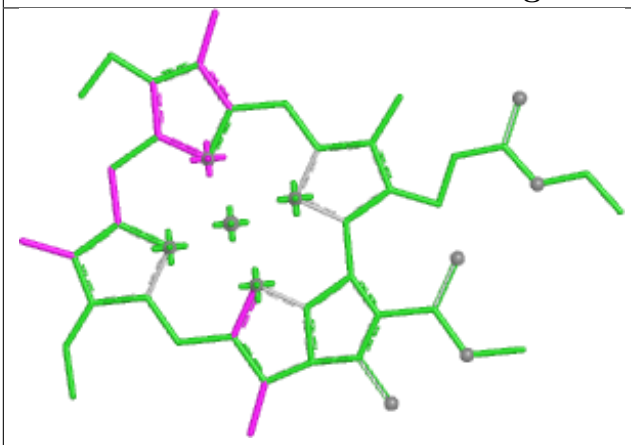


Torsions



Rings

Ligand CLA H 203



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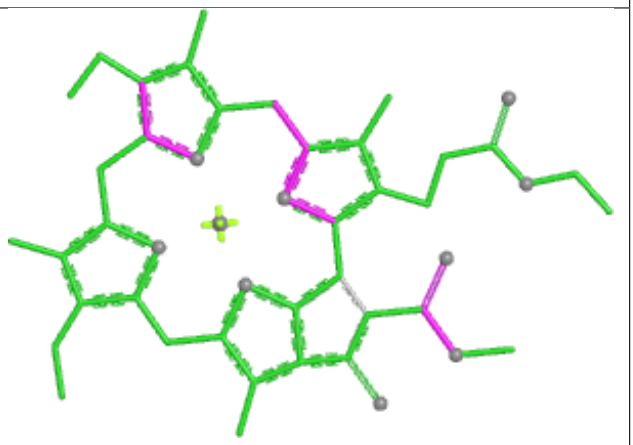
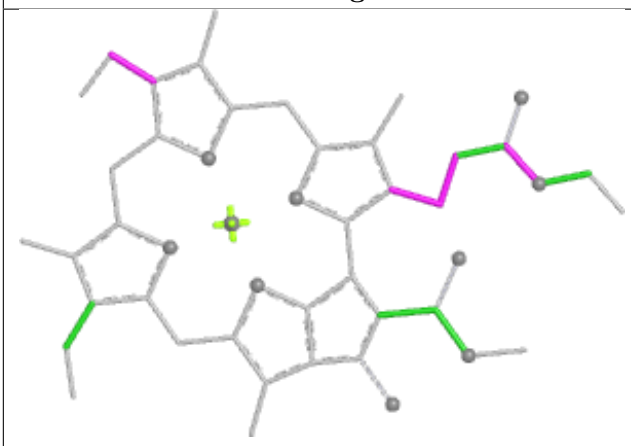
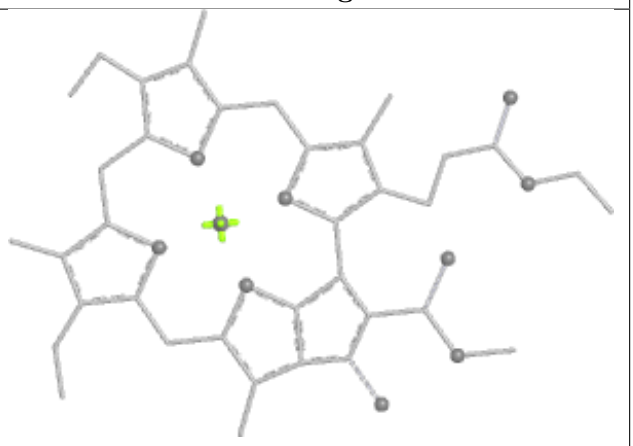


Bond angles

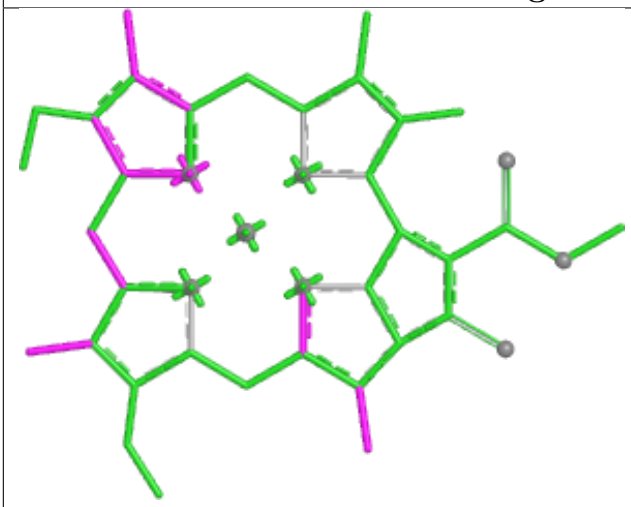


Torsions

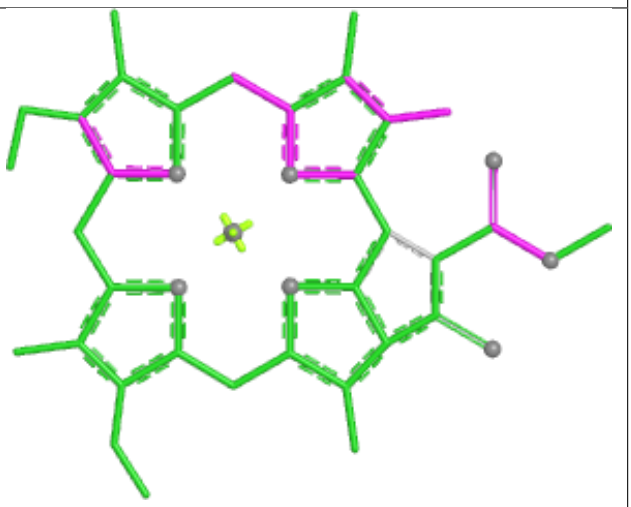


Rings

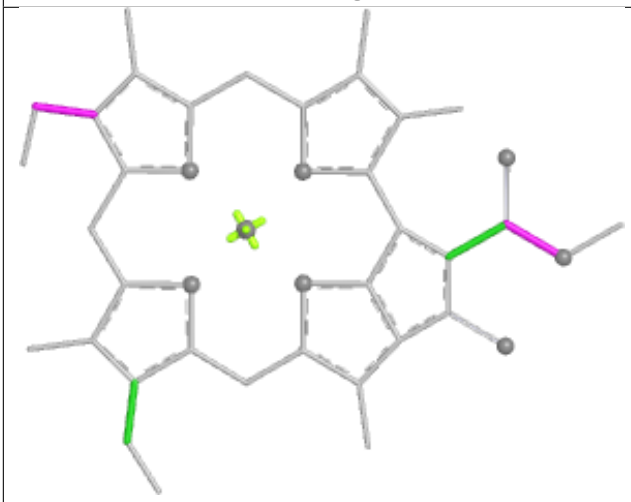
Ligand CLA 9 309



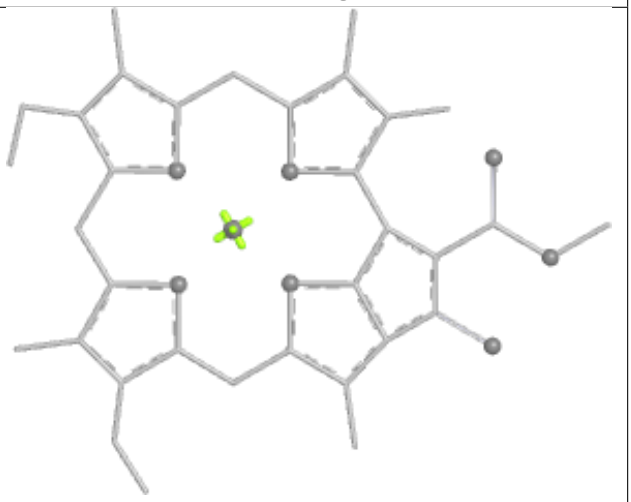
Bond lengths



Bond angles

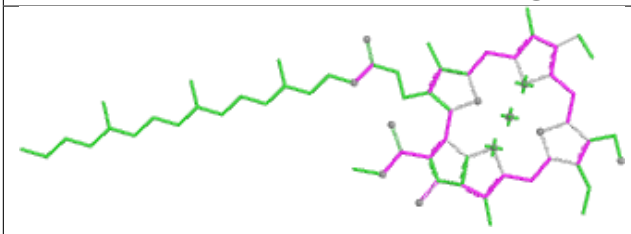


Torsions



Rings

Ligand CHL 8 303



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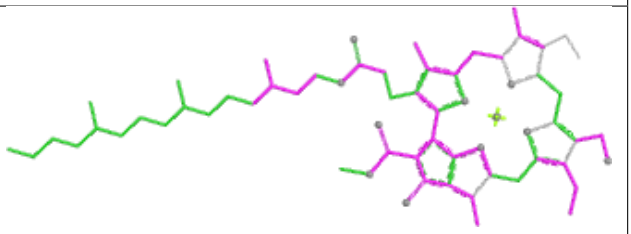
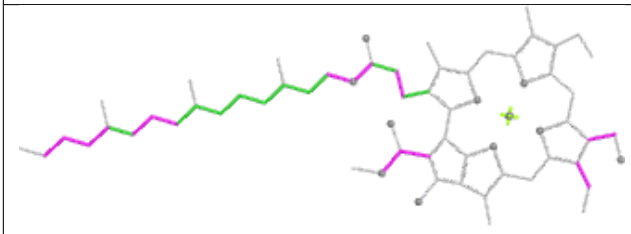
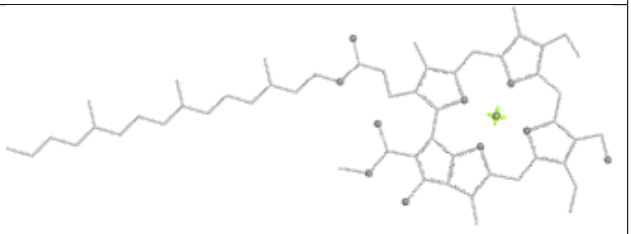


Bond angles

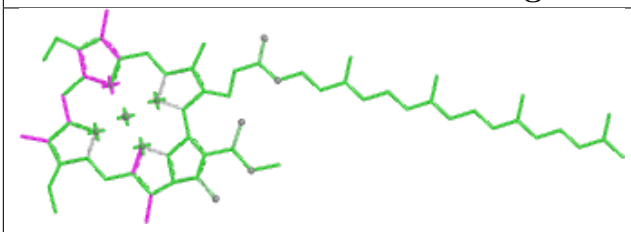


Torsions

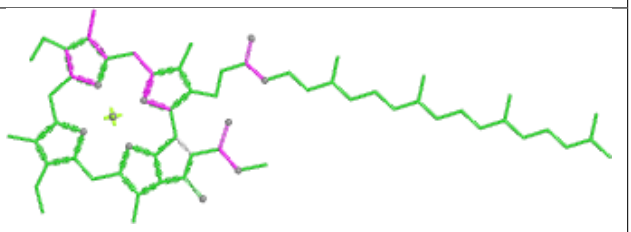


Rings

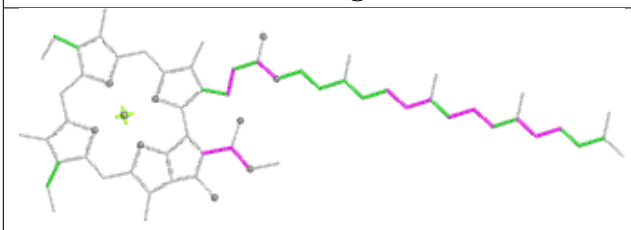
Ligand CLA B 802



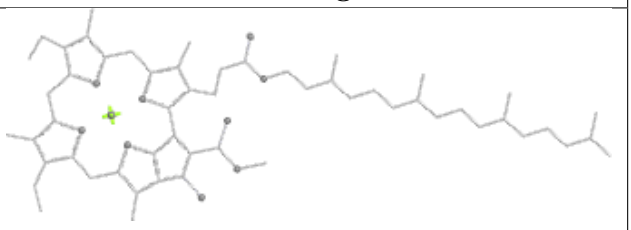
Bond lengths



Bond angles

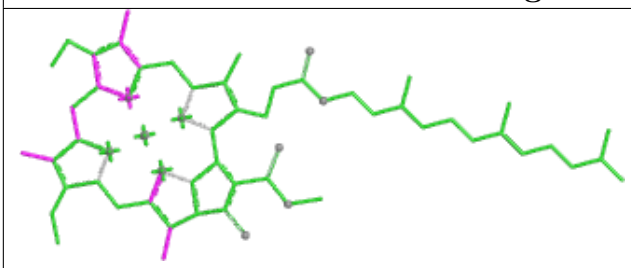


Torsions

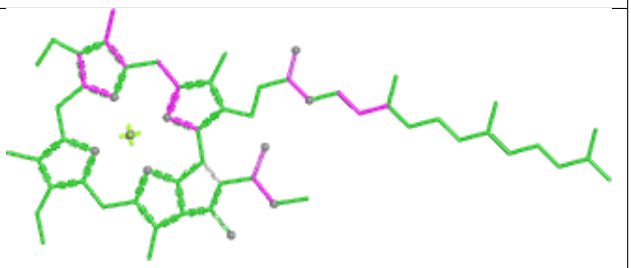


Rings

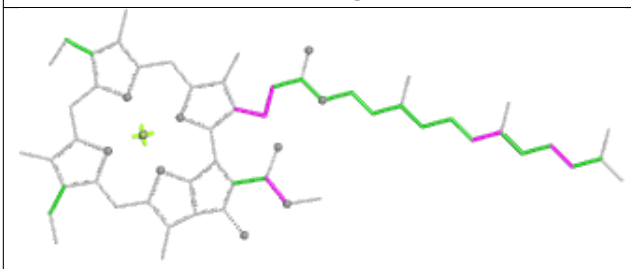
Ligand CLA B 816



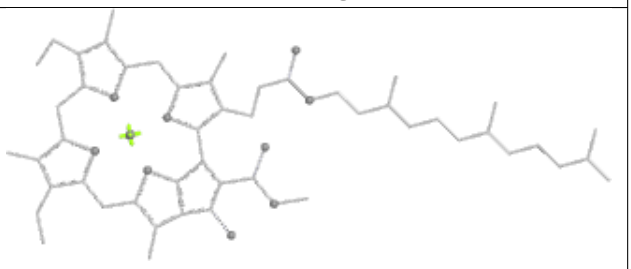
Bond lengths



Bond angles

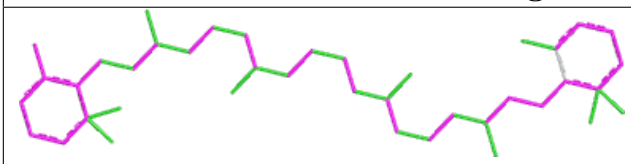


Torsions

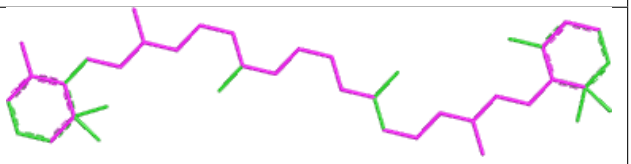


Rings

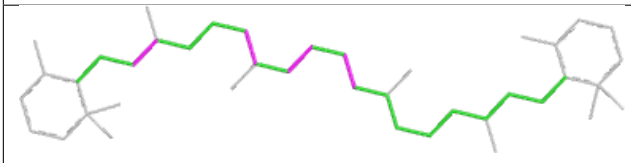
Ligand 8CT O 208



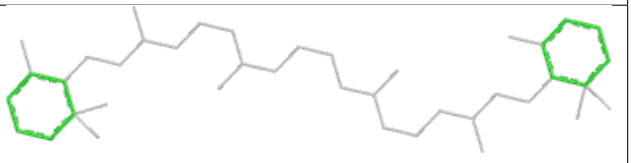
Bond lengths



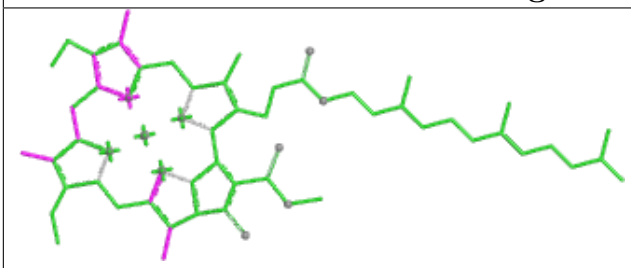
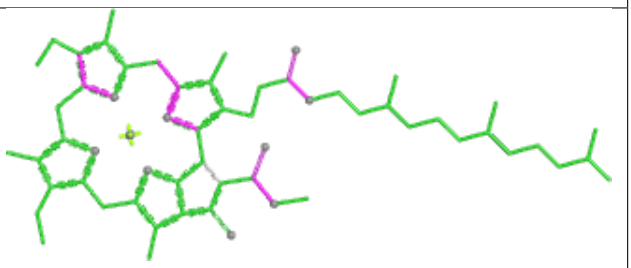
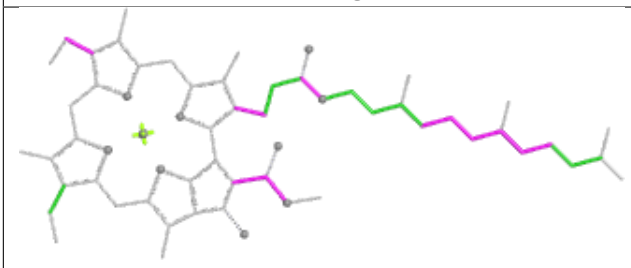
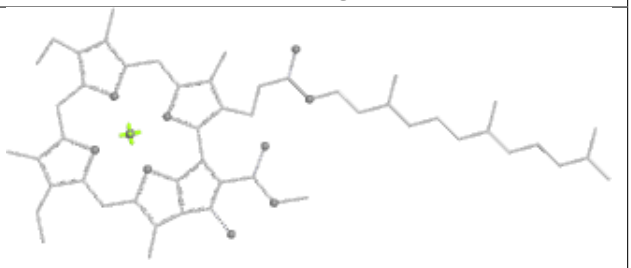
Bond angles

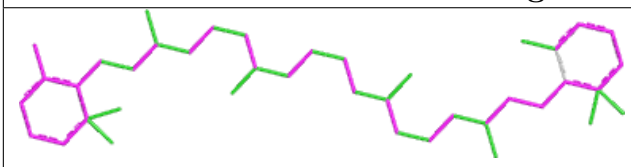
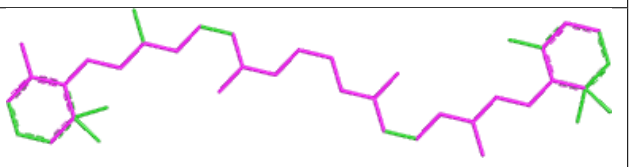
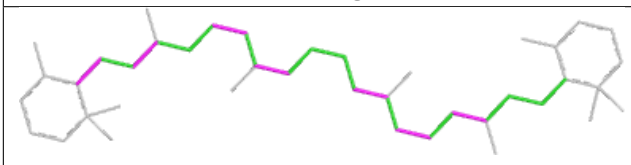
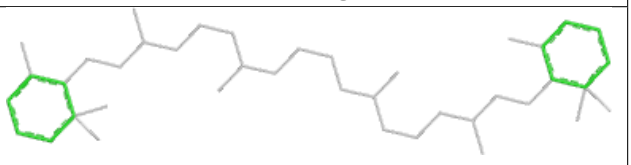


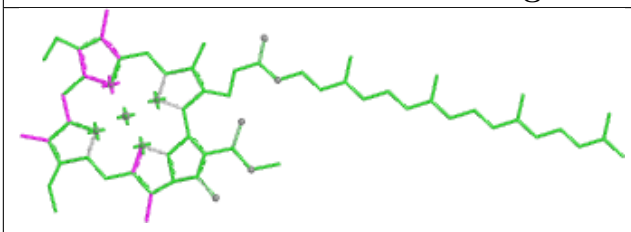
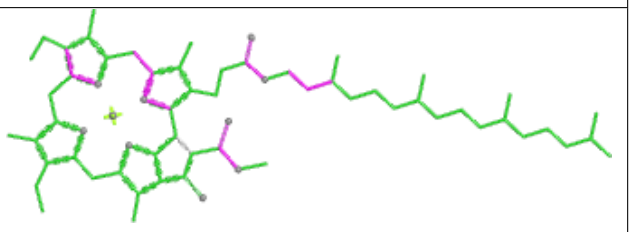
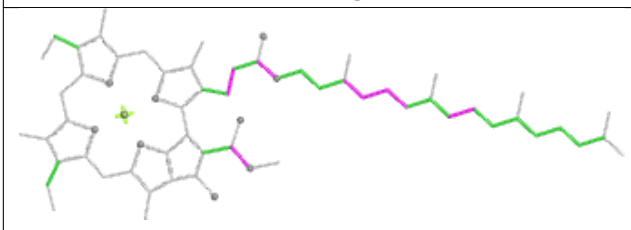
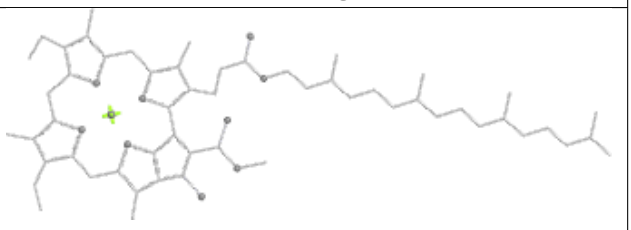
Torsions



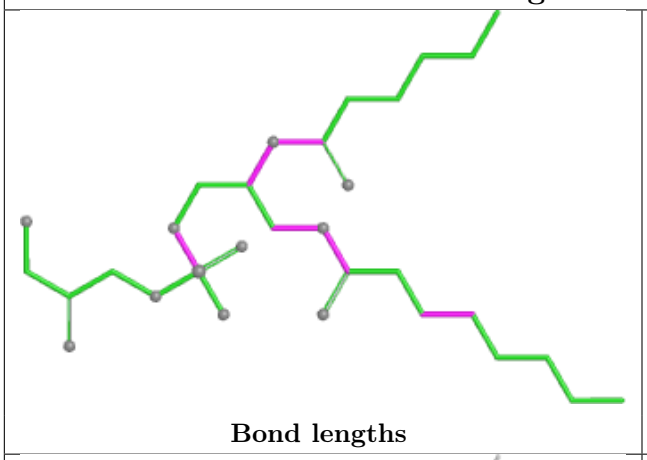
Rings

Ligand CLA 2 309	
	
Bond lengths	Bond angles
	
Torsions	Rings

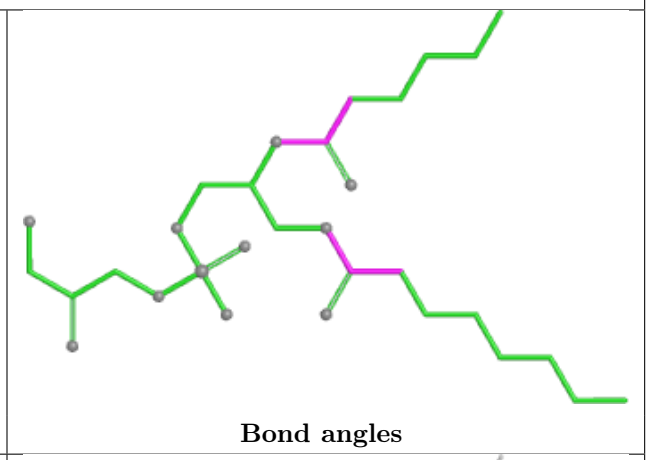
Ligand 8CT B 844	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA A 840	
	
Bond lengths	Bond angles
	
Torsions	Rings

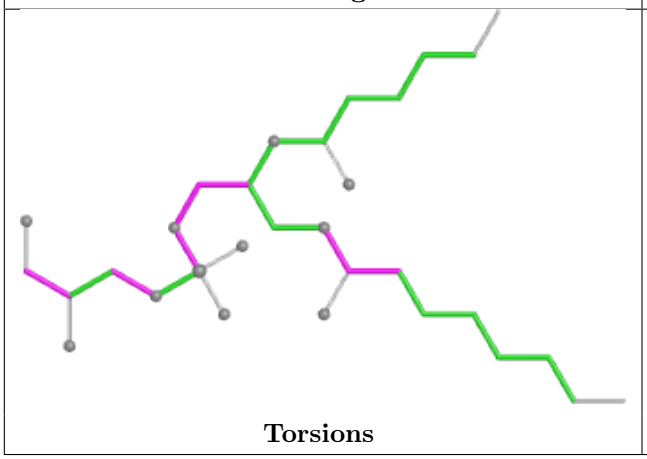
Ligand LHG 8 302



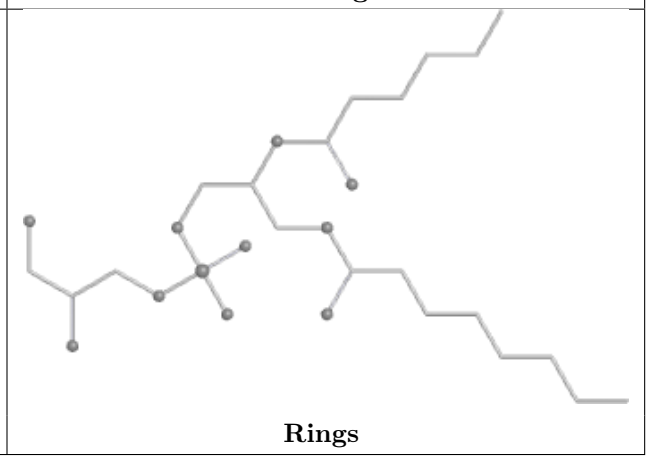
Bond lengths



Bond angles

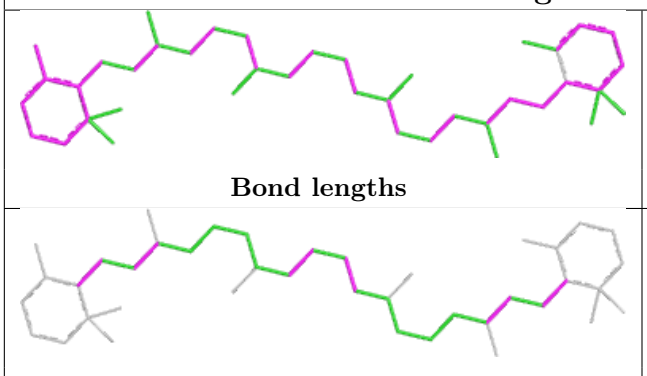


Torsions



Rings

Ligand 8CT I 101



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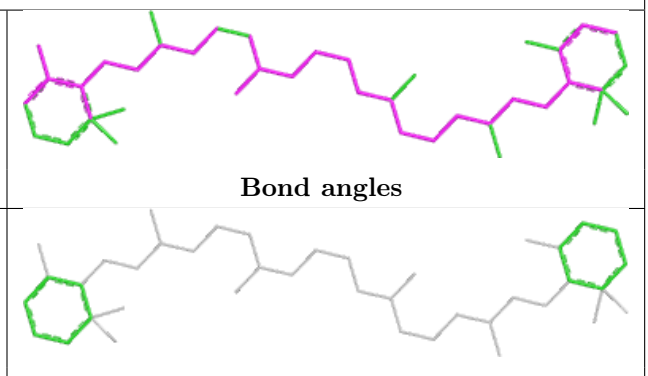
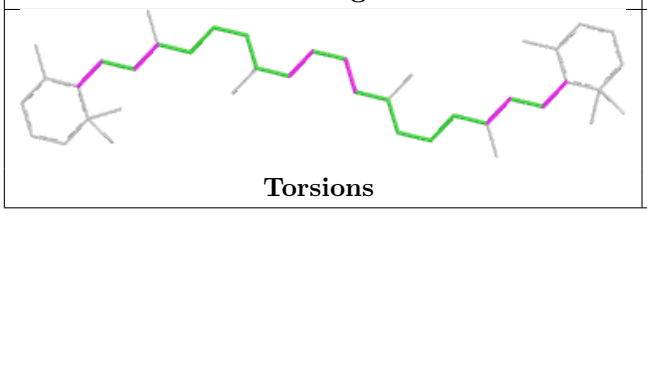


Bond angles



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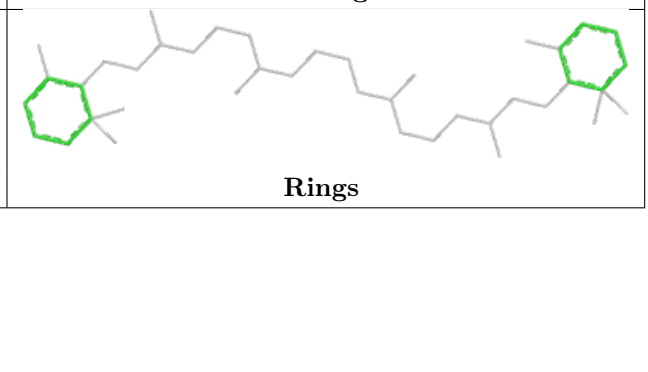
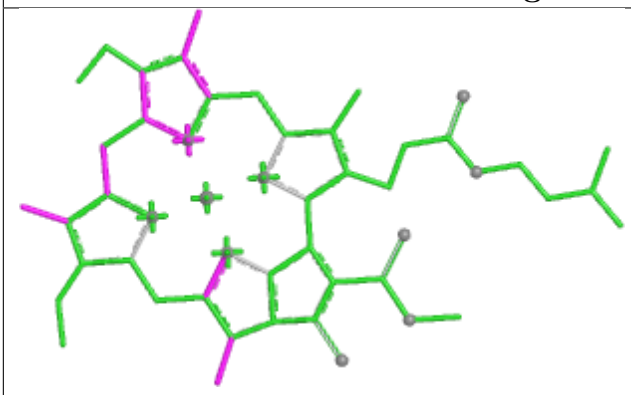
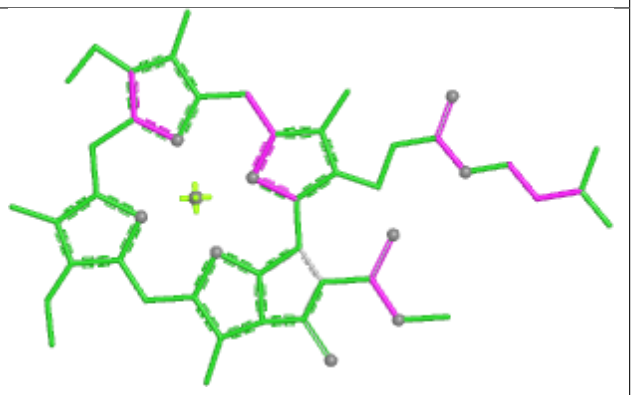


Rings

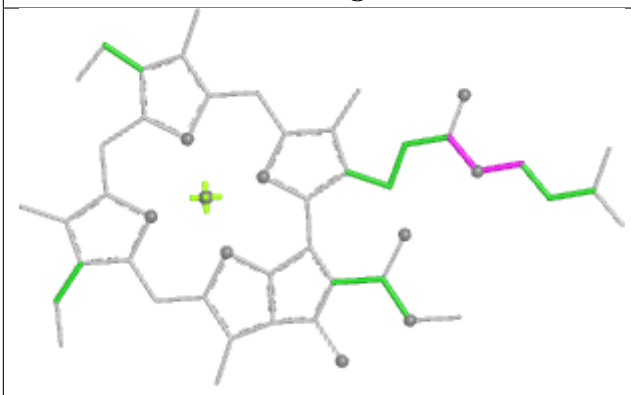
Ligand CLA A 830



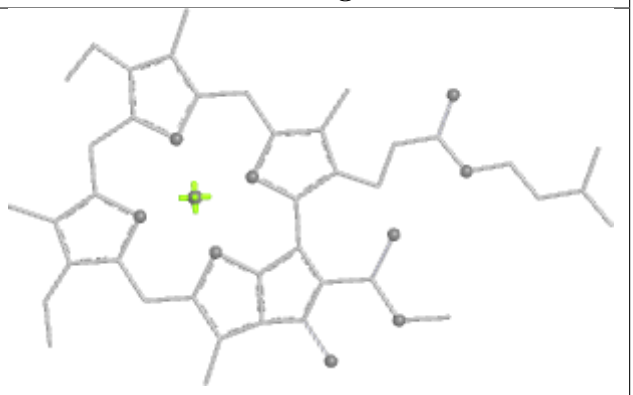
Bond lengths



Bond angles

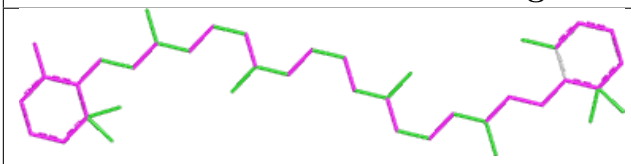


Torsions

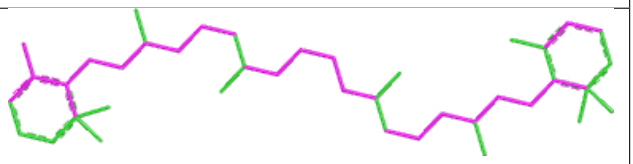


Rings

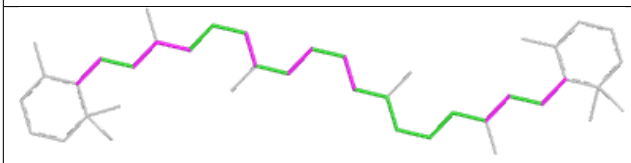
Ligand 8CT B 850



Bond lengths



Bond angles



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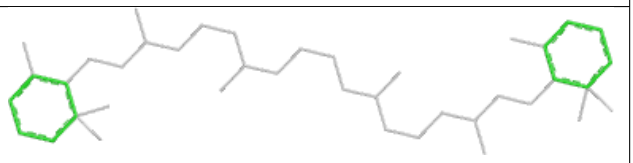
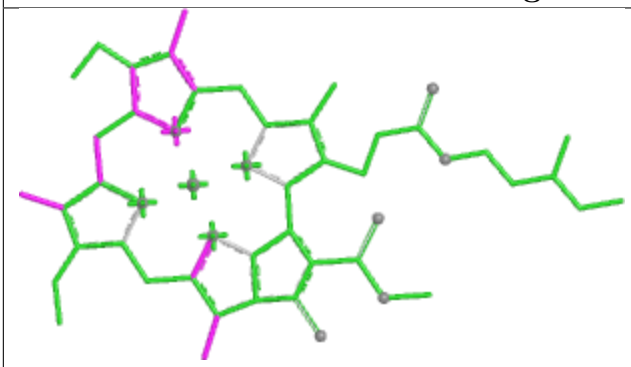


Rings

Ligand CLA H 205



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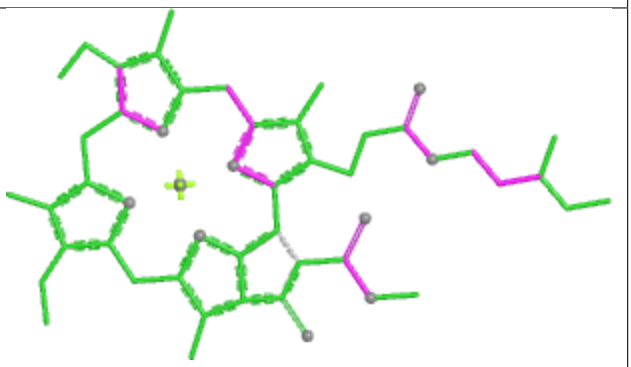
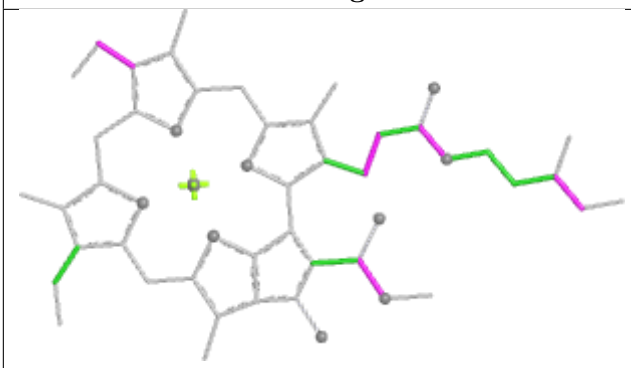
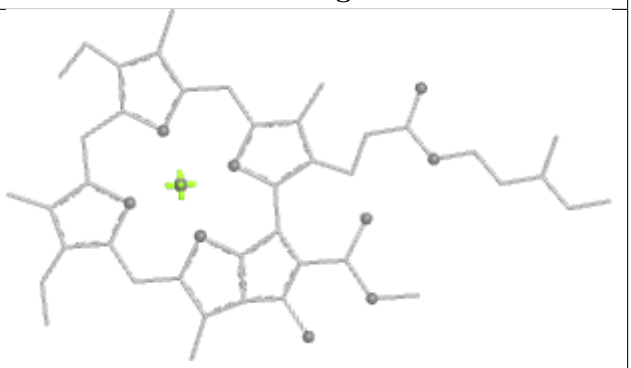


Bond angles

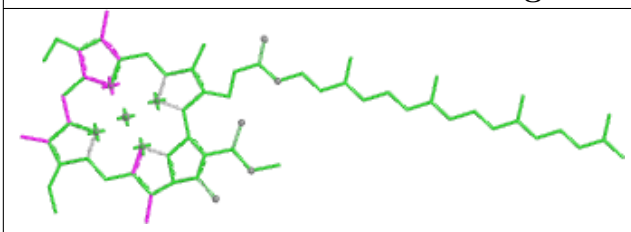


Torsions



Rings

Ligand CLA B 825



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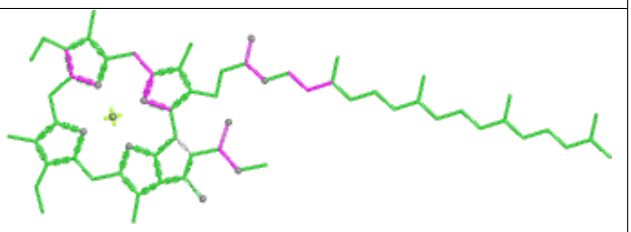
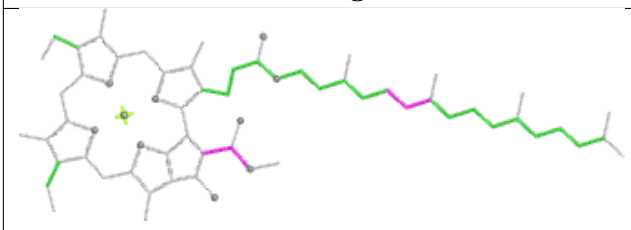


Bond angles



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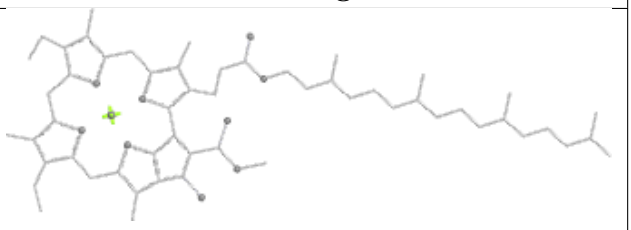
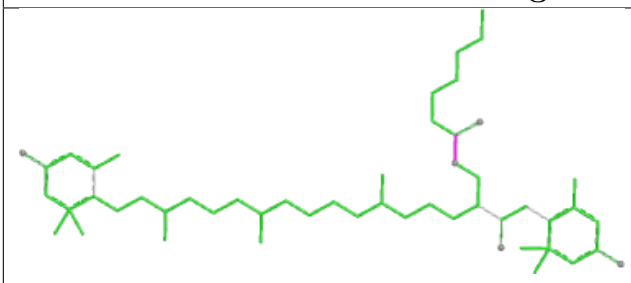
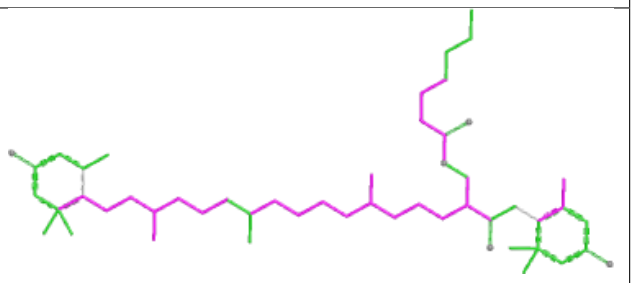


Rings

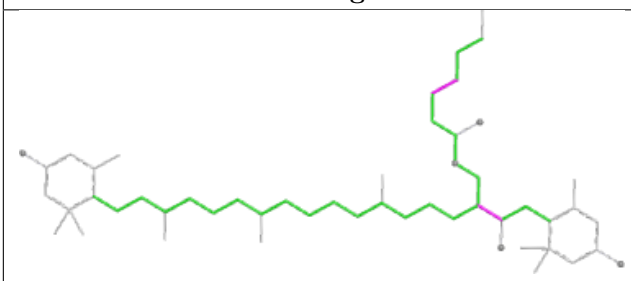
Ligand 0UR 9 314



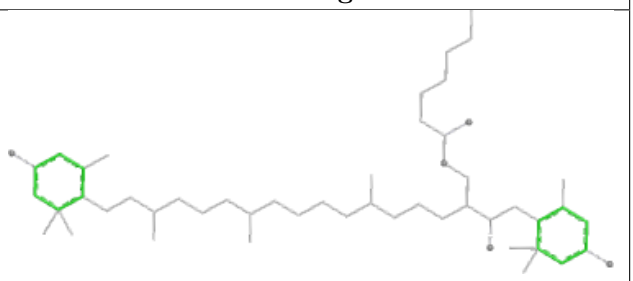
Bond lengths



Bond angles

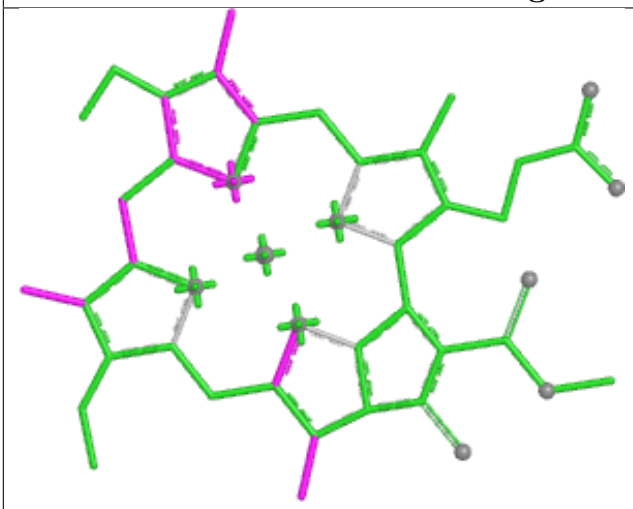


Torsions

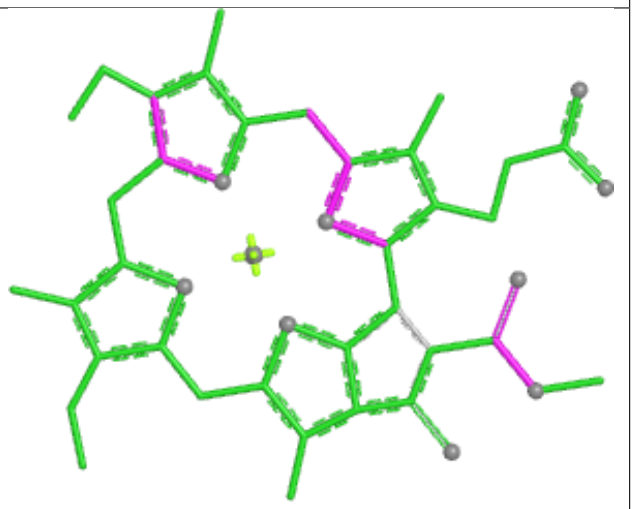


Rings

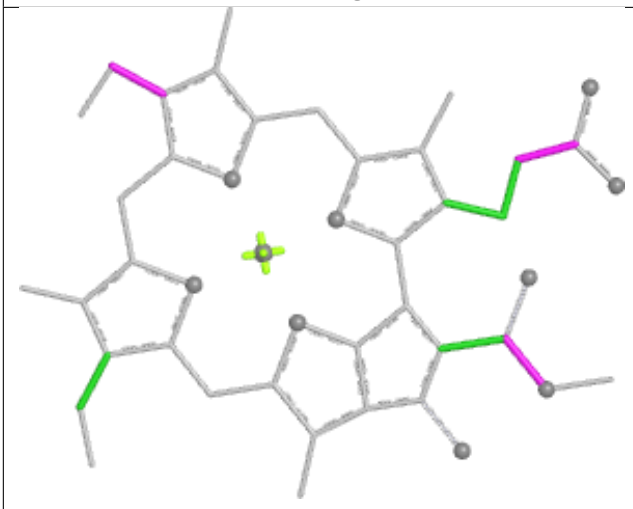
Ligand CLA 1 307



Bond lengths



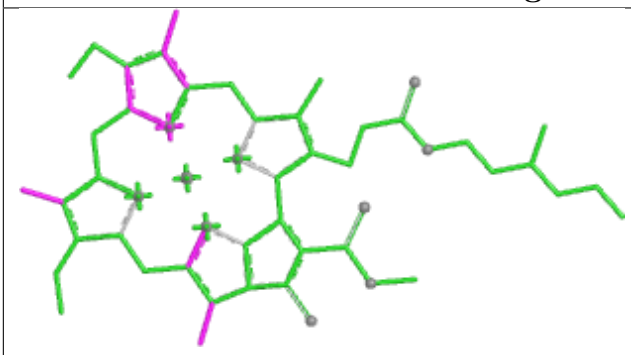
Bond angles



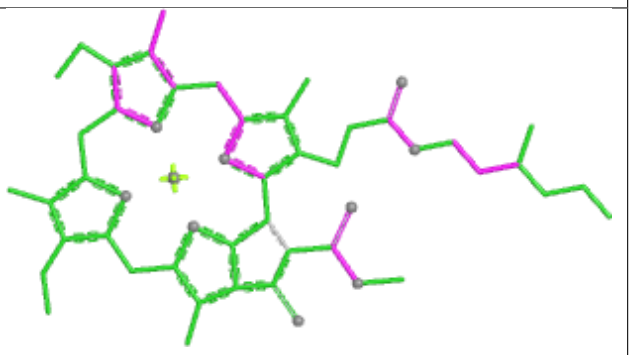
Torsions

Rings

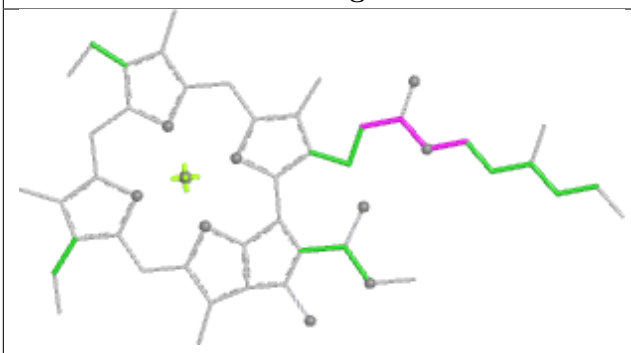
Ligand CLA B 812



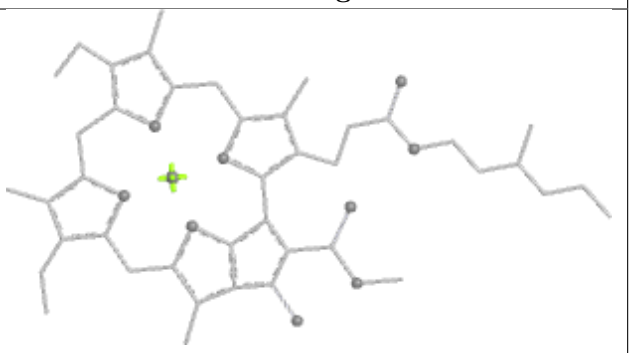
Bond lengths



Bond angles

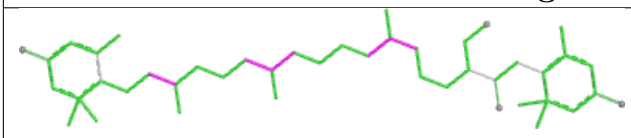


Torsions



Rings

Ligand 0IE 3 319



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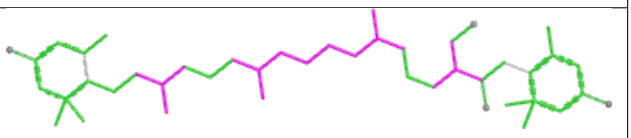

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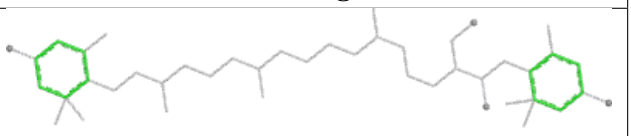
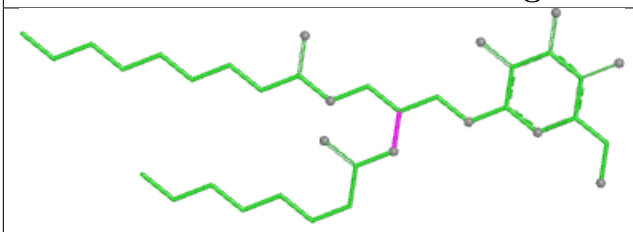
Torsions



Rings

Ligand LMG 2 318



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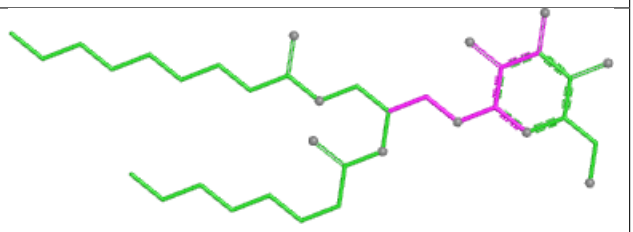

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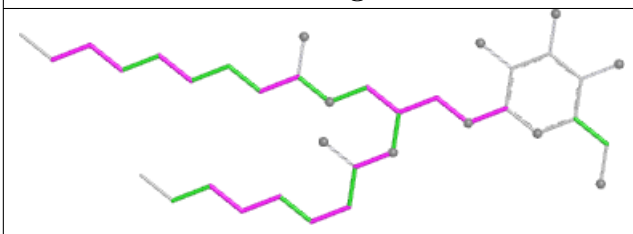

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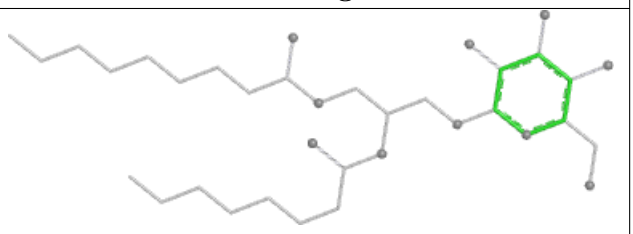
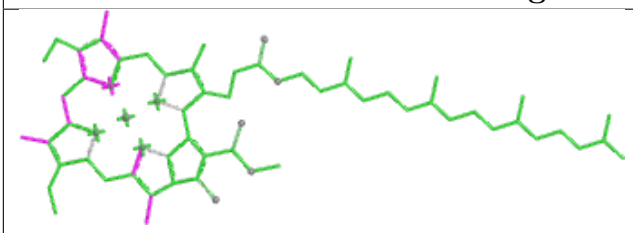


Rings

Ligand CLA 3 308



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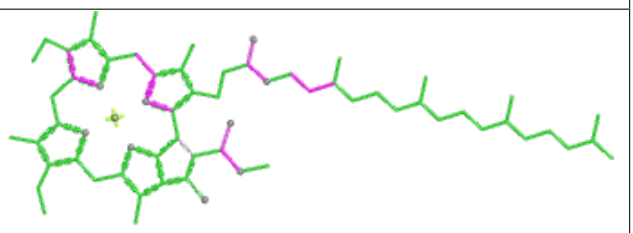
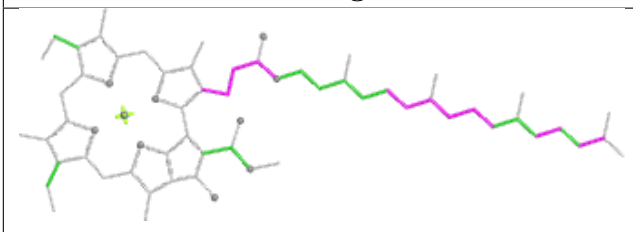
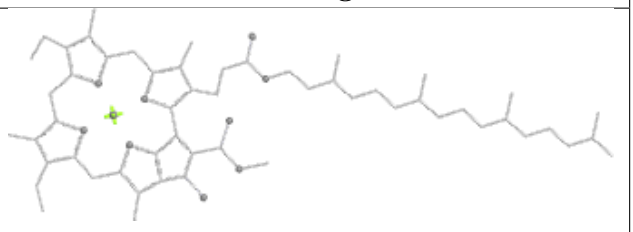


Bond angles

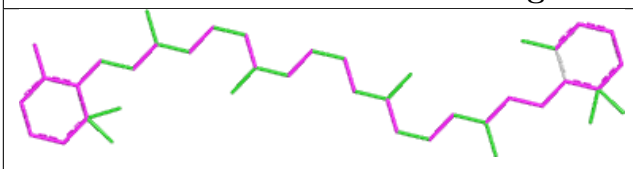


Torsions



Rings

Ligand 8CT B 847



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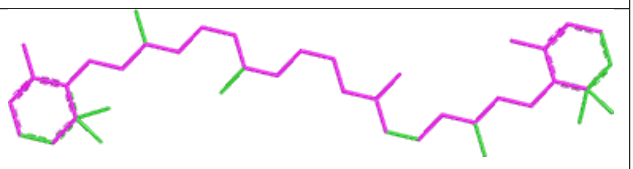

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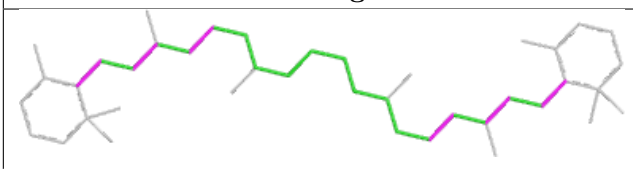

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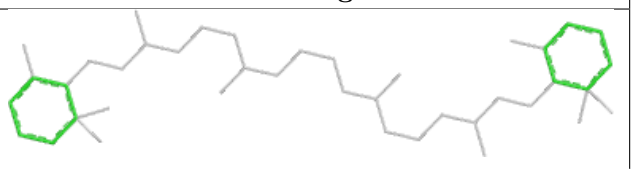
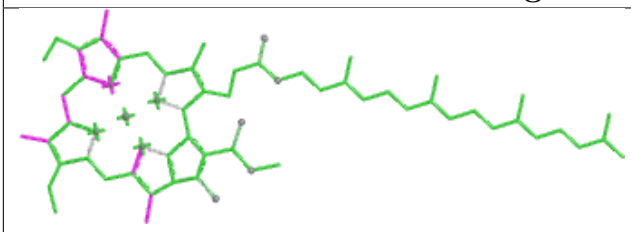


Rings

Ligand CLA B 808



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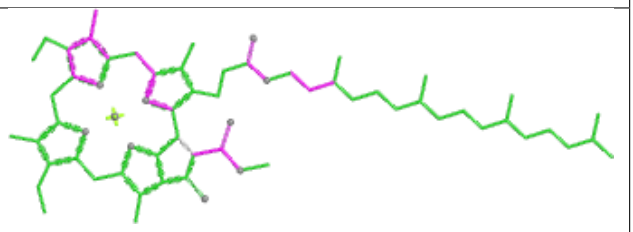

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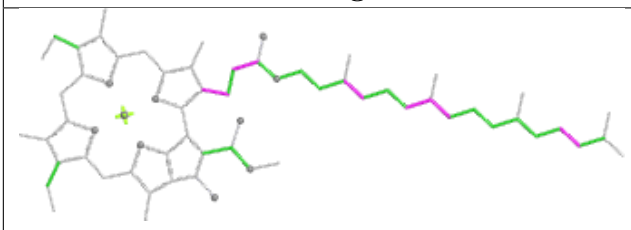

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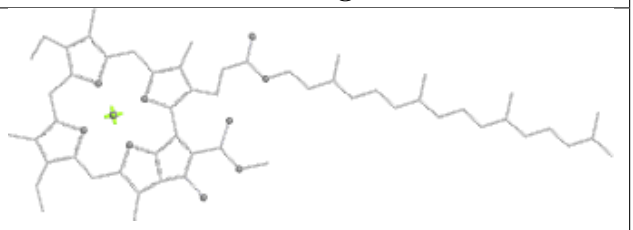
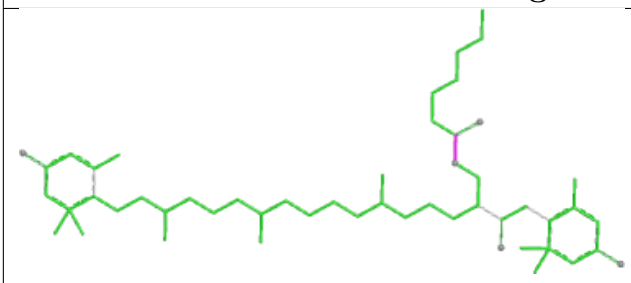


Rings

Ligand 0UR 5 315



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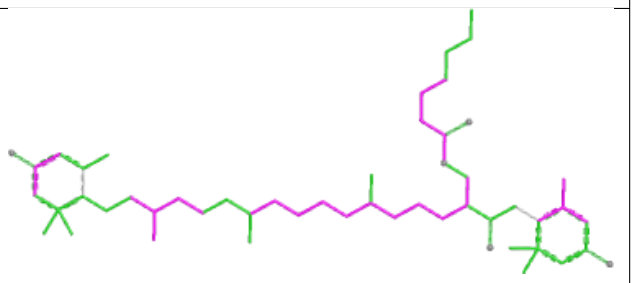

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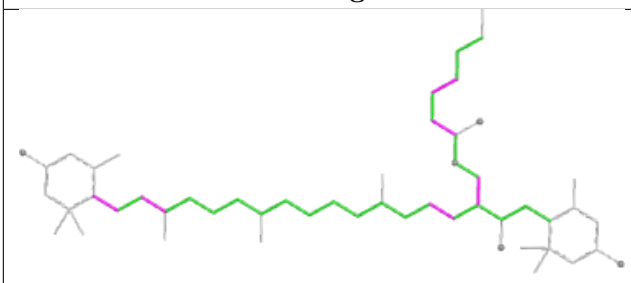

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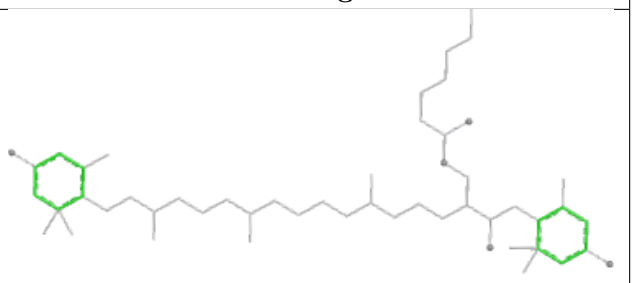
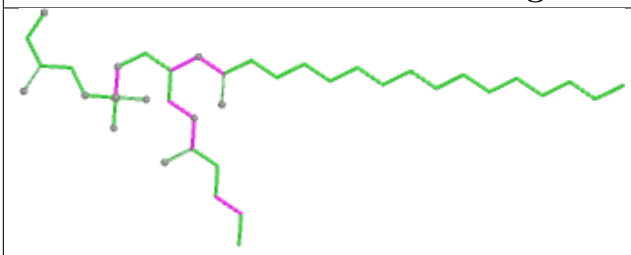


Rings

Ligand LHG 7 323



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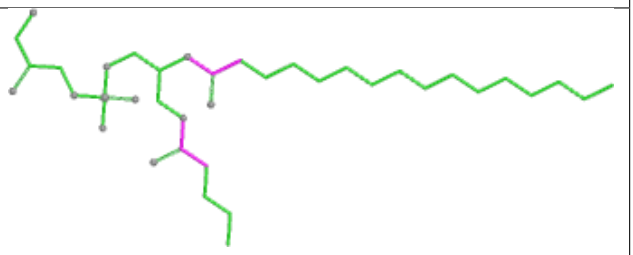

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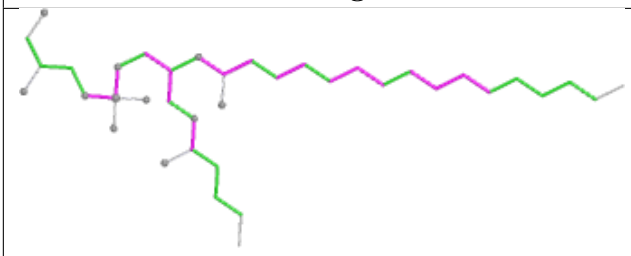

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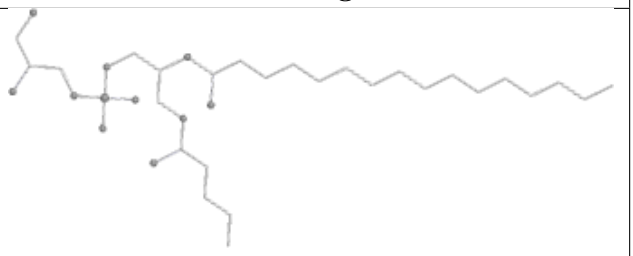
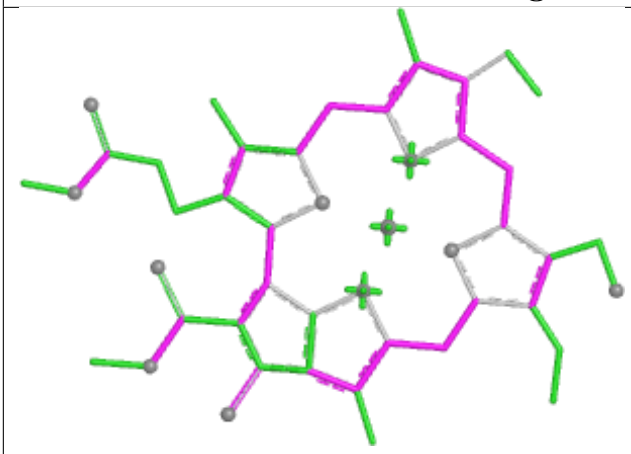


Rings

Ligand CHL 9 312



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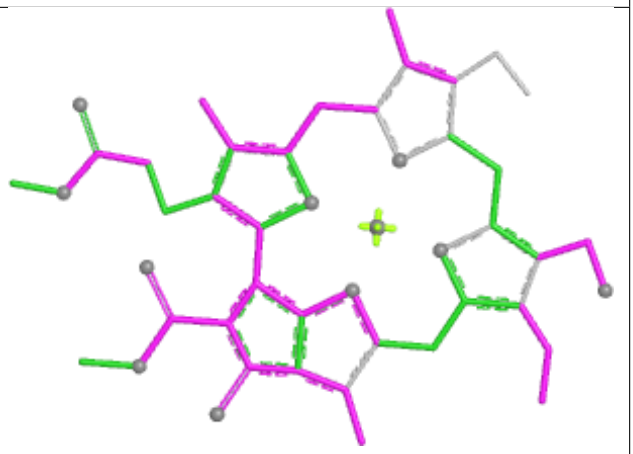
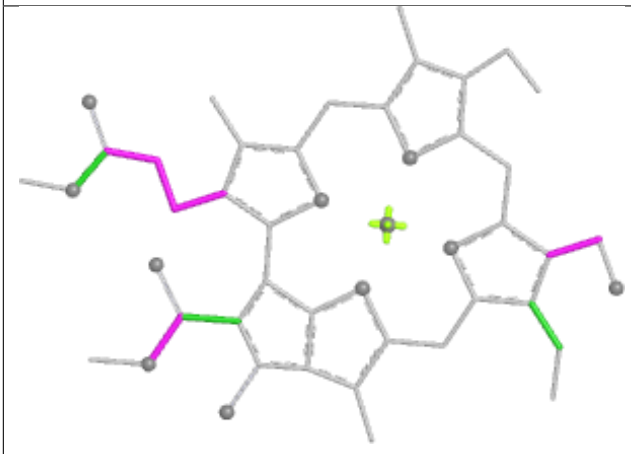


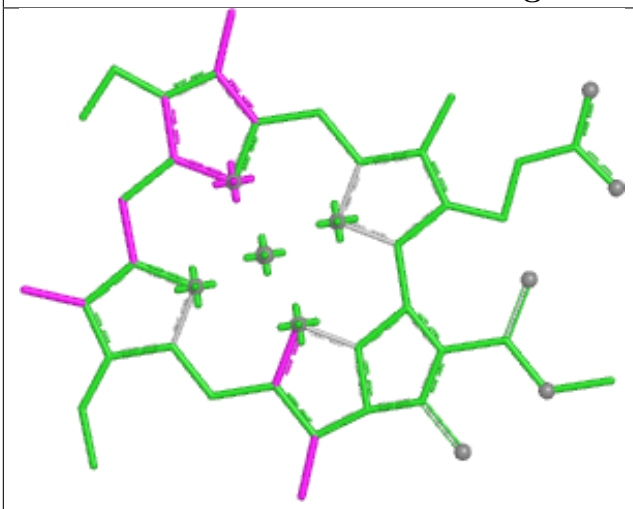
Bond angles



Torsions

Rings

Ligand CLA A 815



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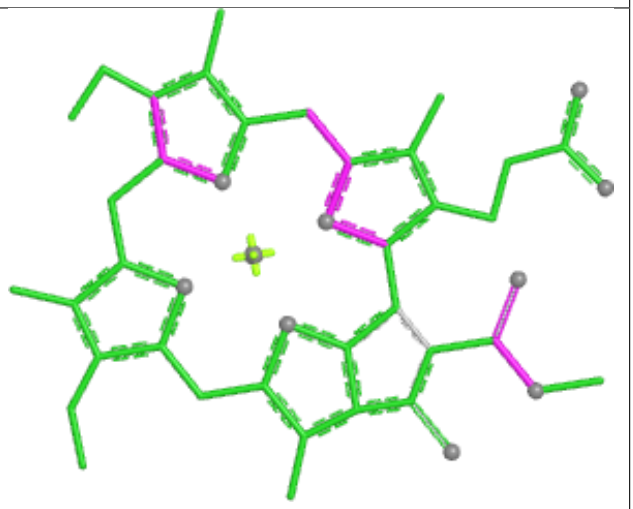

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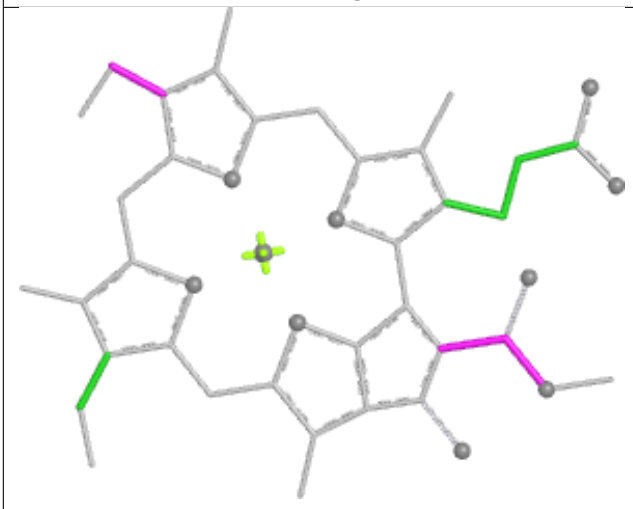
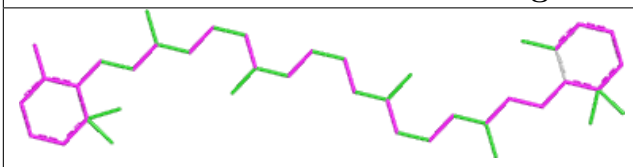


Torsions

Rings

Ligand 8CT 1 314



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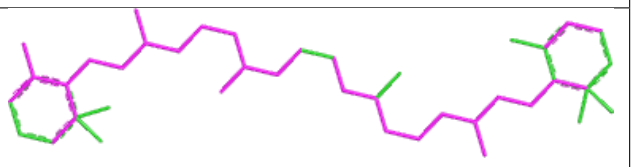

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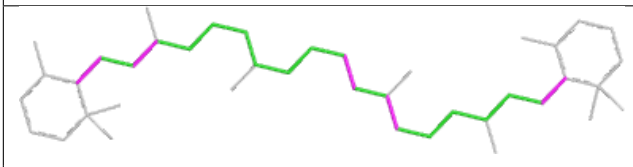

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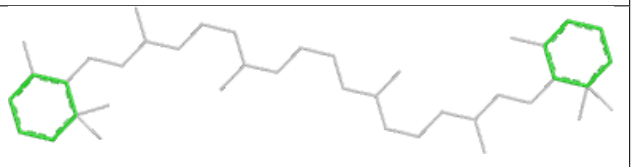
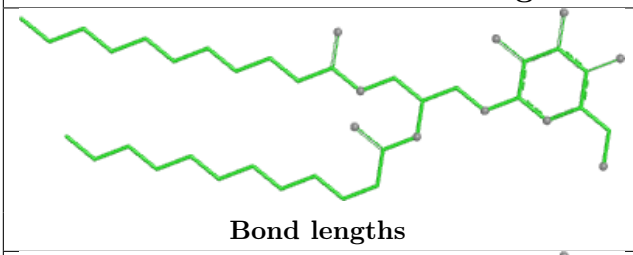


Rings

Ligand LMG M 101



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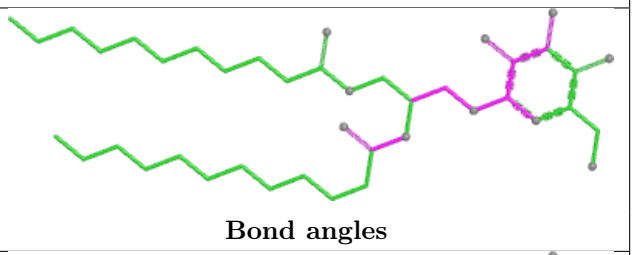

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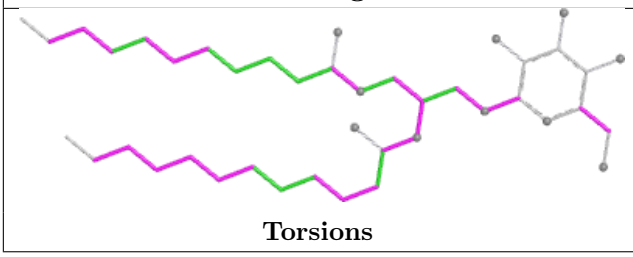

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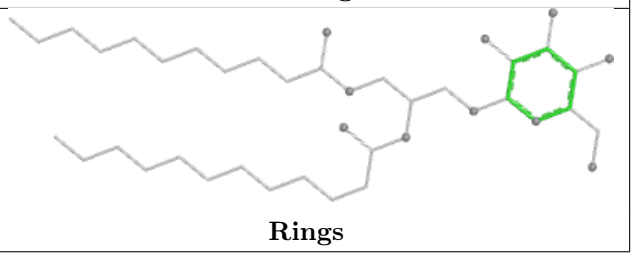
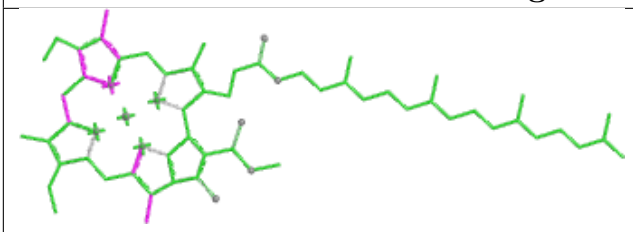


Rings

Ligand CLA 8 305



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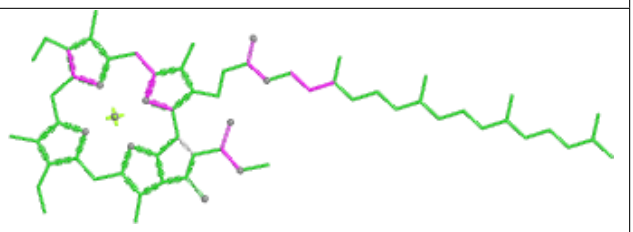

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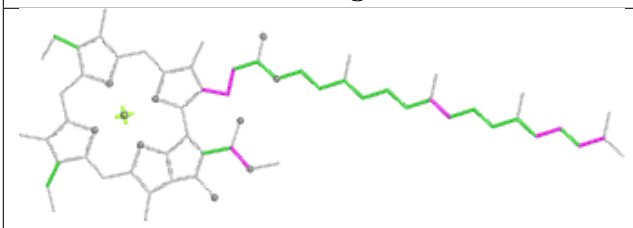

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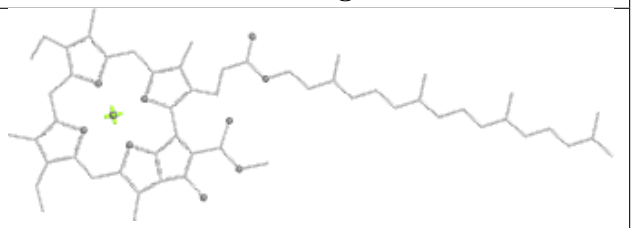
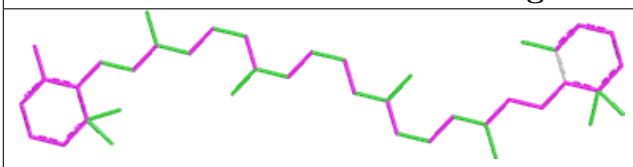


Rings

Ligand 8CT A 846



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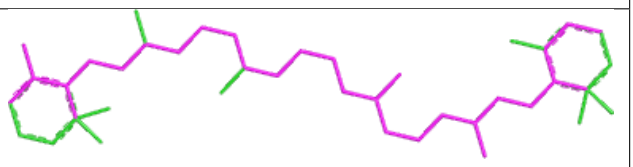
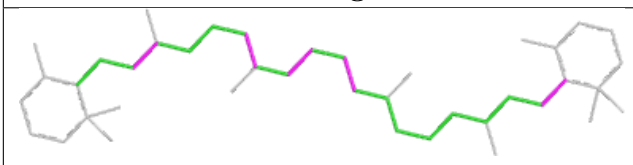
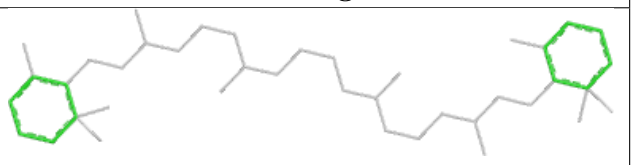


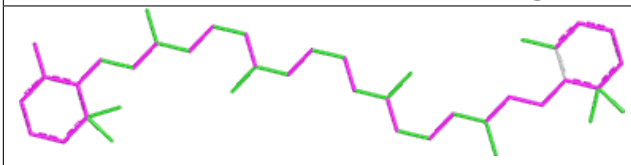
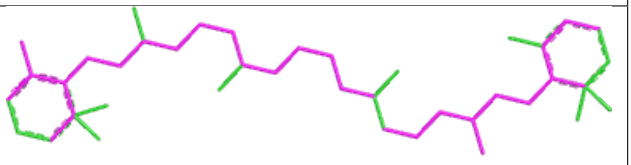
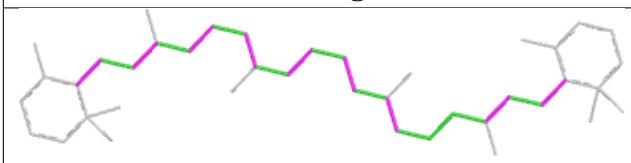
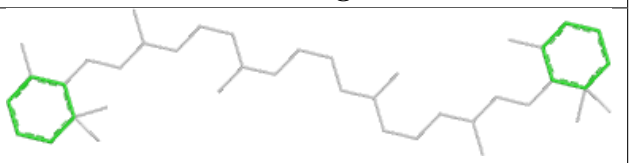
Bond angles

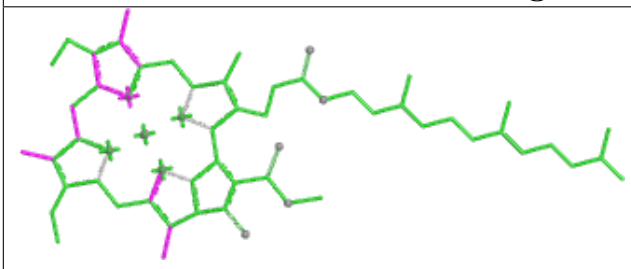
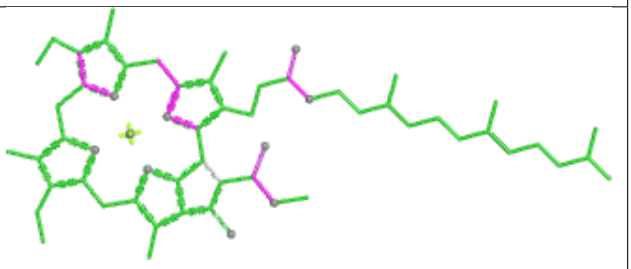
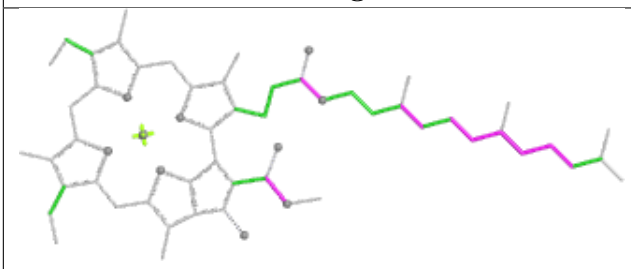
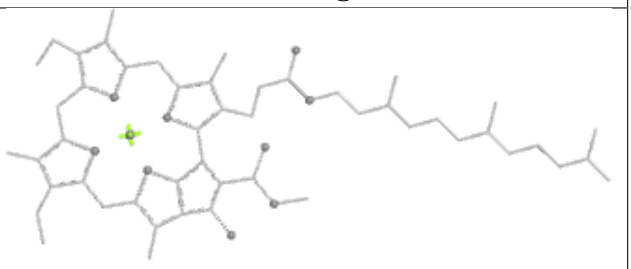


Torsions

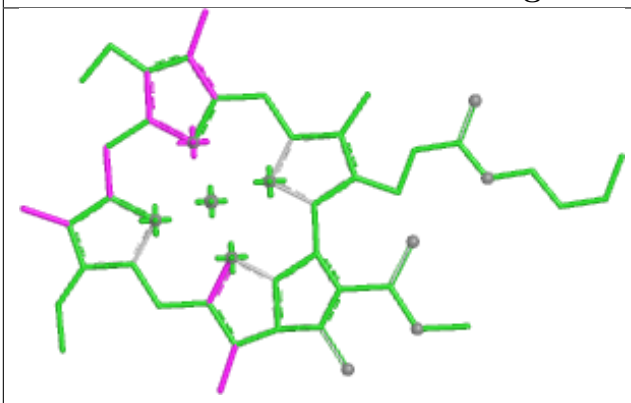


Rings

Ligand 8CT F 301	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA 2 303	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA A 821



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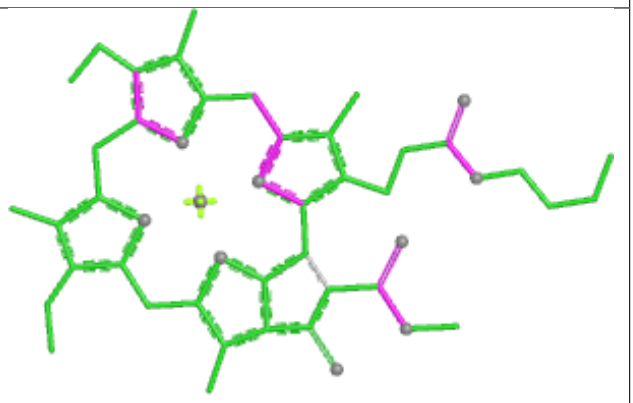
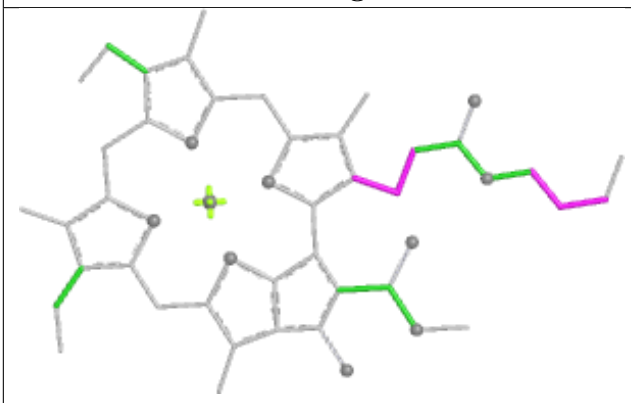


Bond angles



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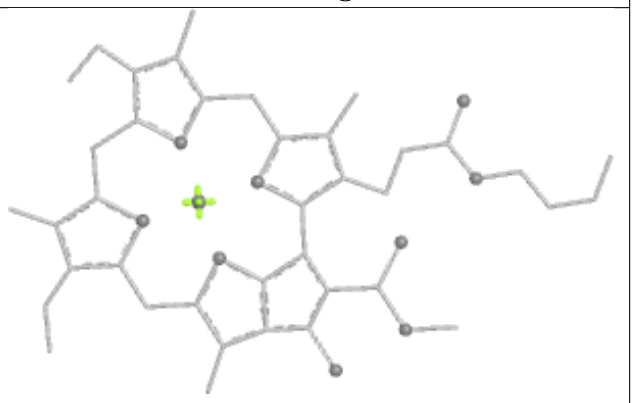
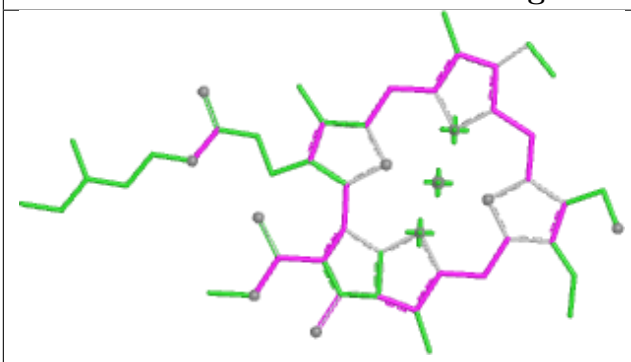


Rings

Ligand CHL 6 313



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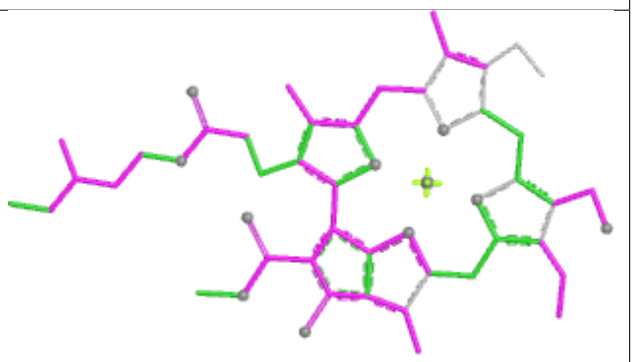

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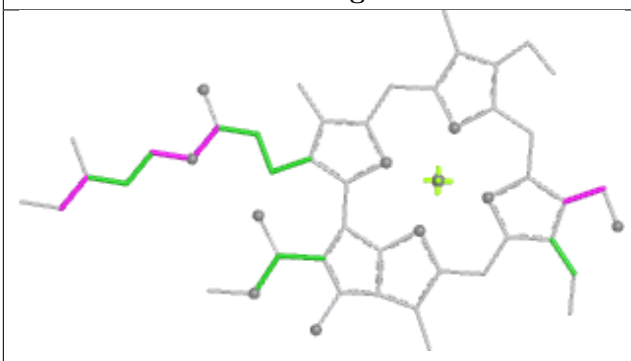

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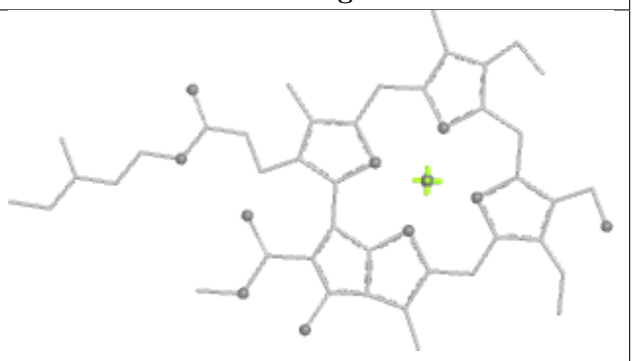
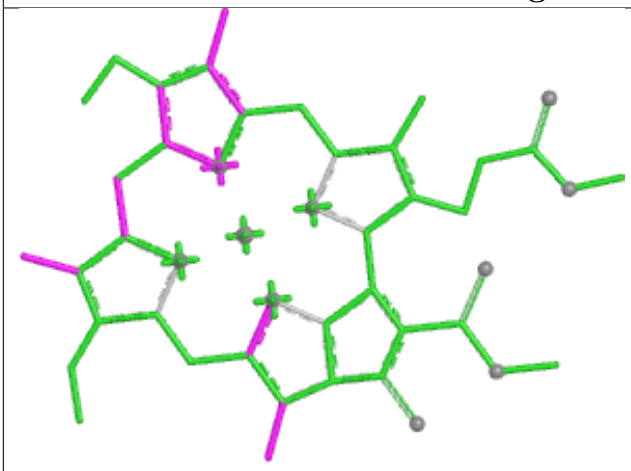


Rings

Ligand CLA 6 317



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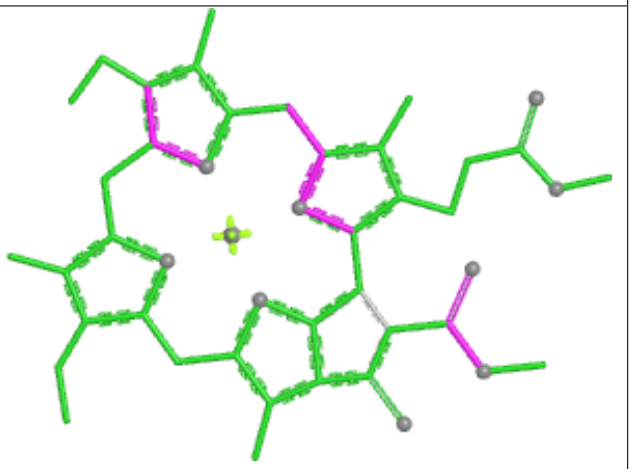

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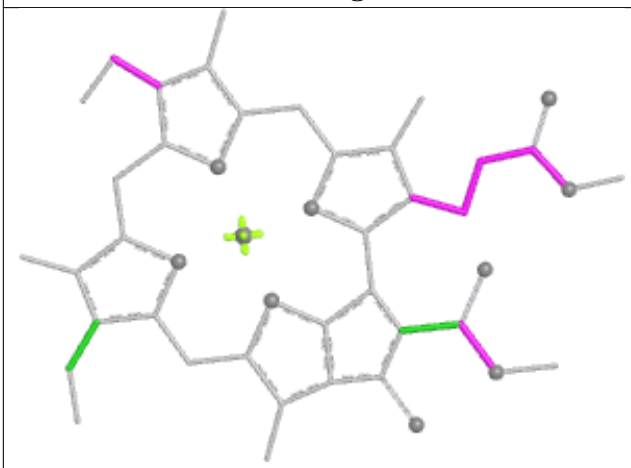

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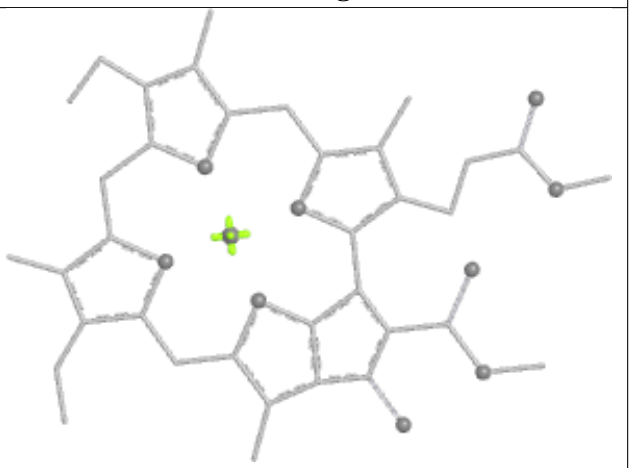
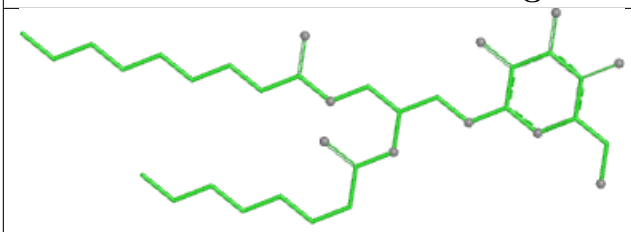


Rings

Ligand LMG 3 321



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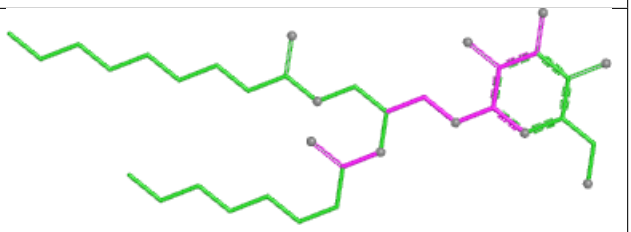

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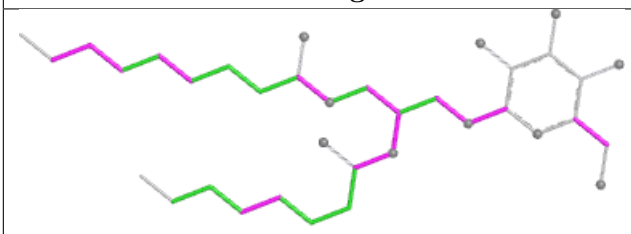

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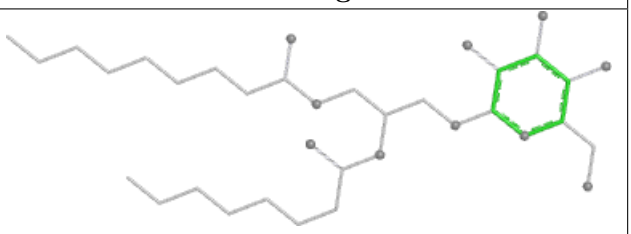
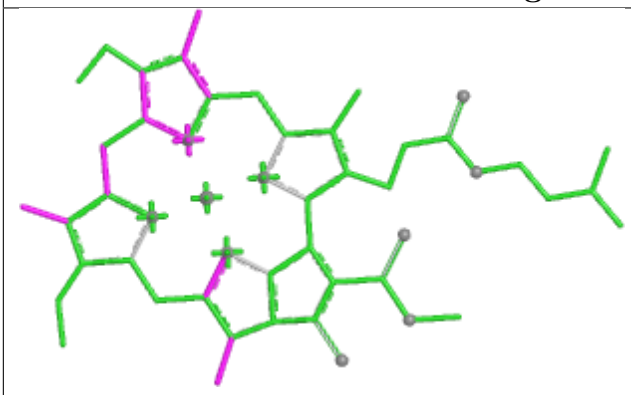


Rings

Ligand CLA B 831



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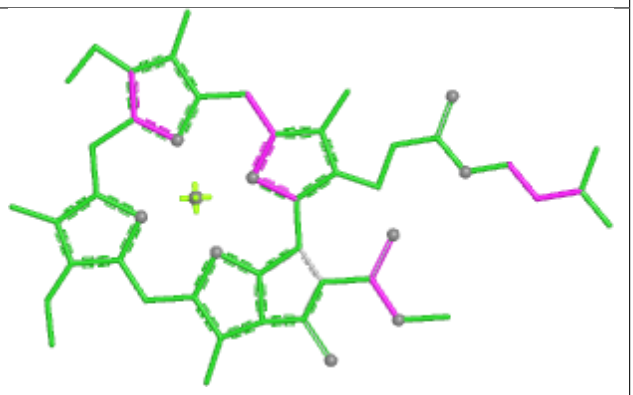

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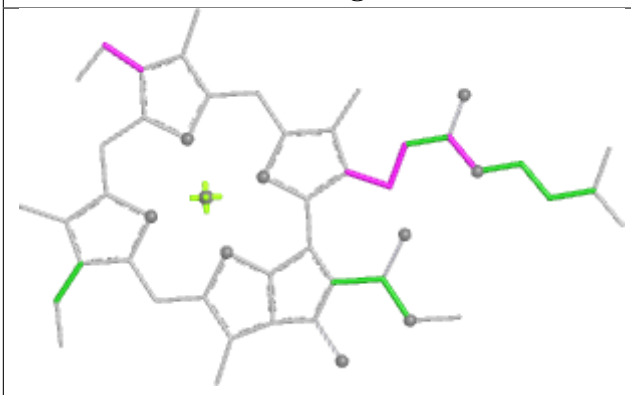

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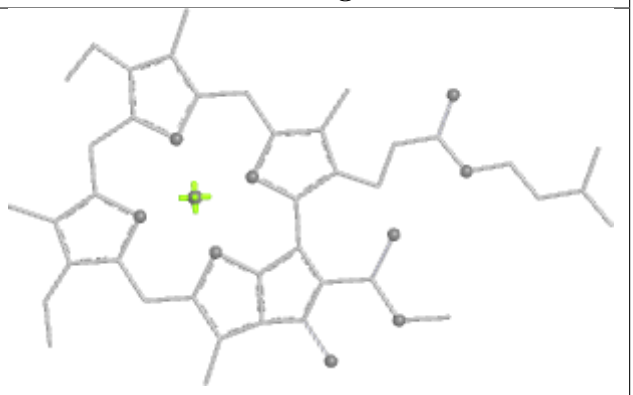
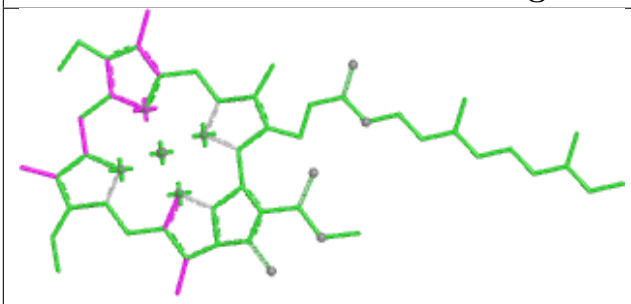


Rings

Ligand CLA 2 302



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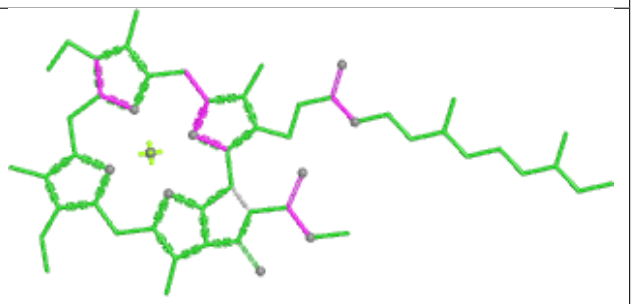

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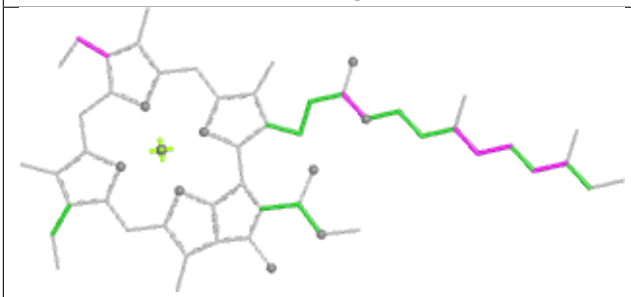

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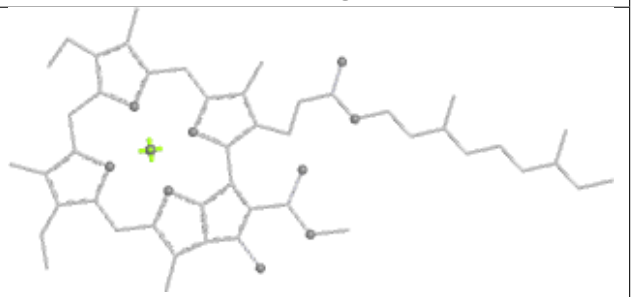
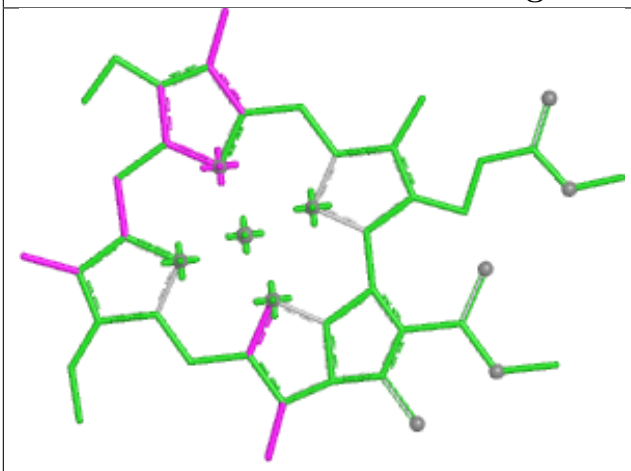


Rings

Ligand CLA L 203



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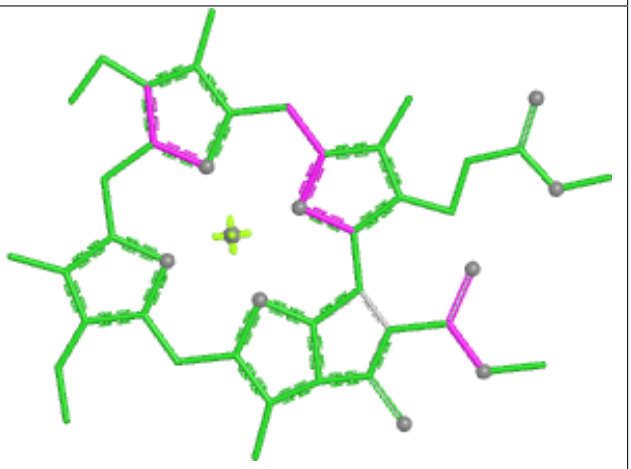

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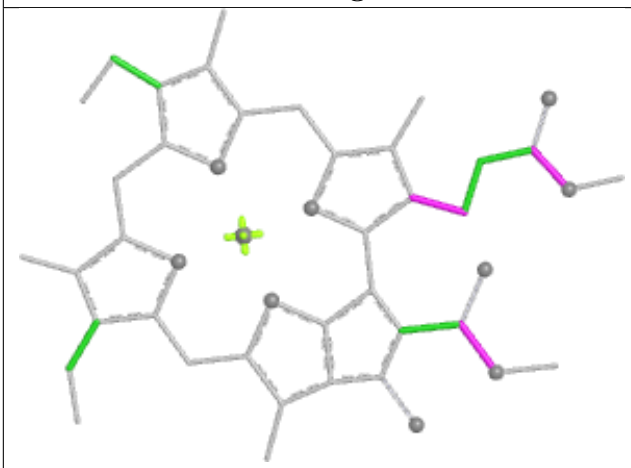

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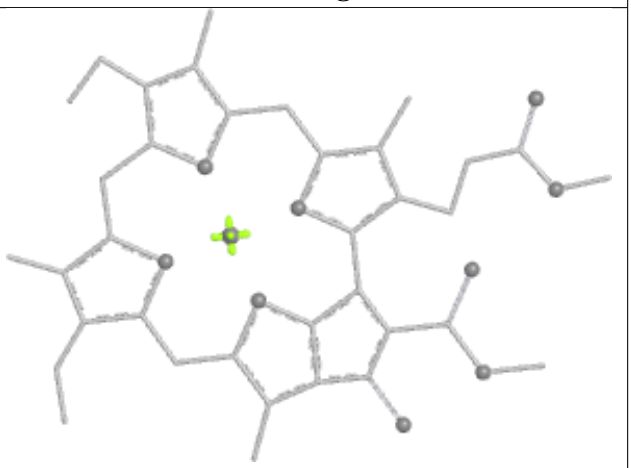
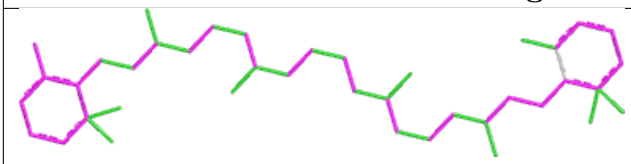


Rings

Ligand 8CT G 104



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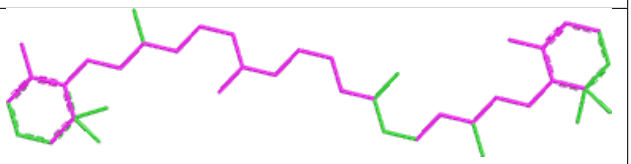

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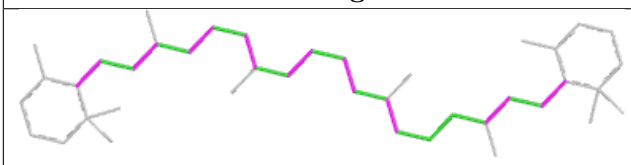

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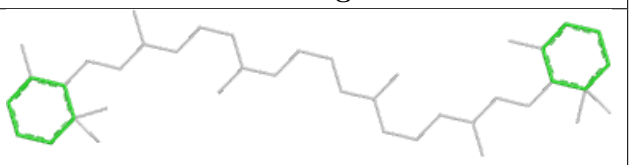
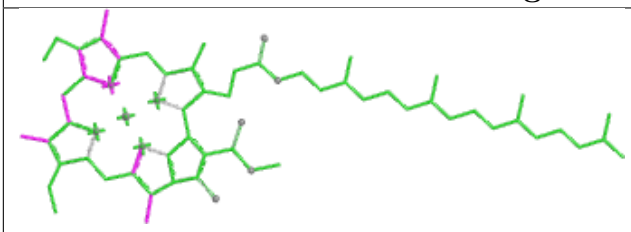


Rings

Ligand CLA A 831



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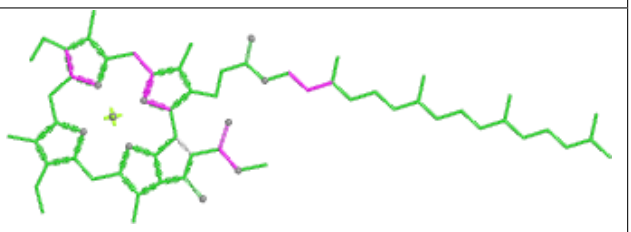

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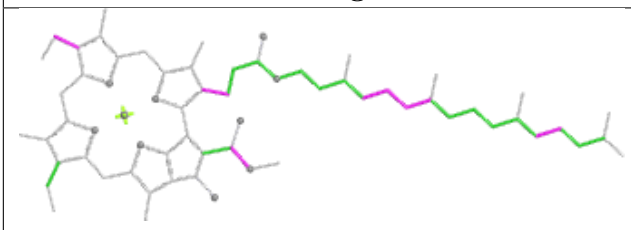

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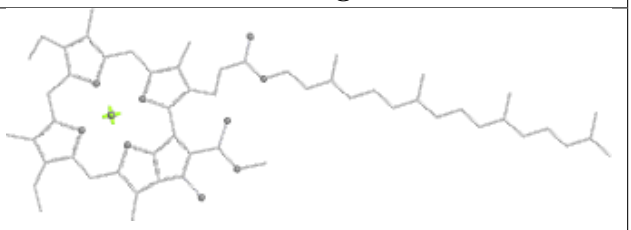
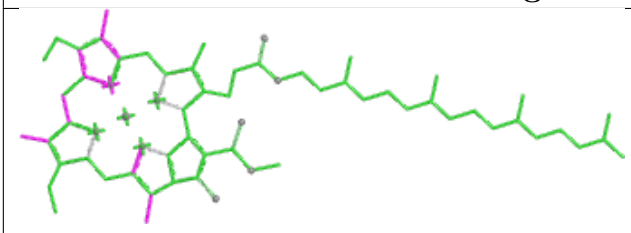


Rings

Ligand CLA A 807



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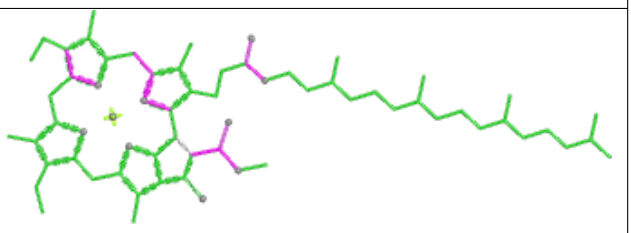
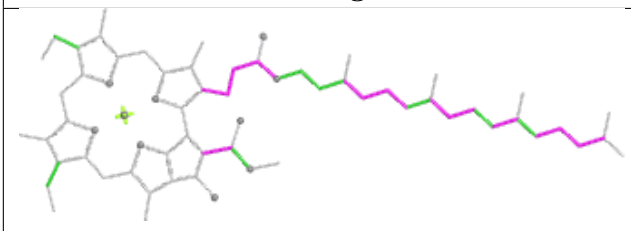


Bond angles



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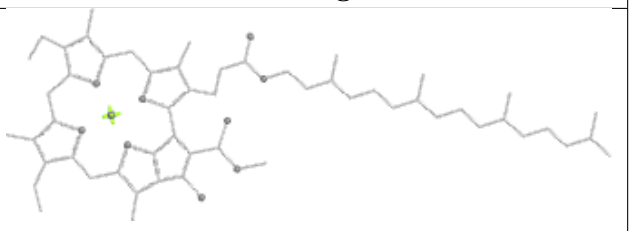
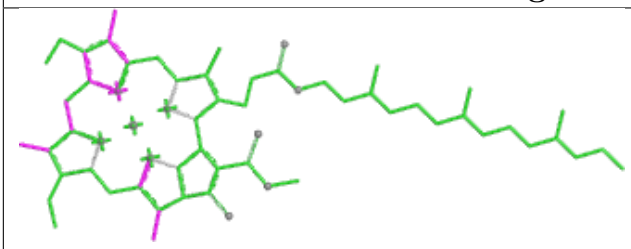


Rings

Ligand CLA 0 303



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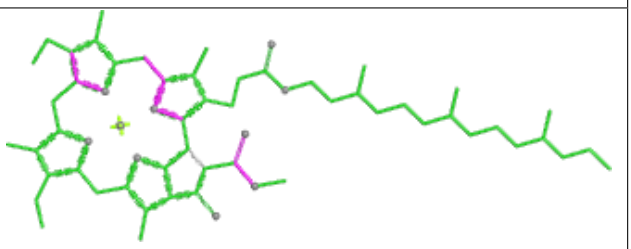
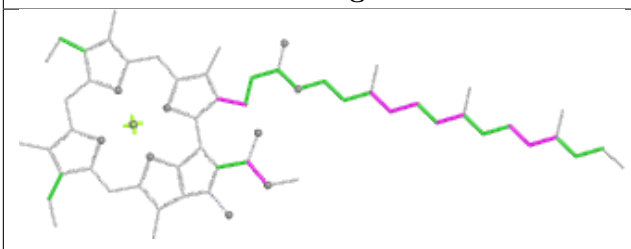


Bond angles



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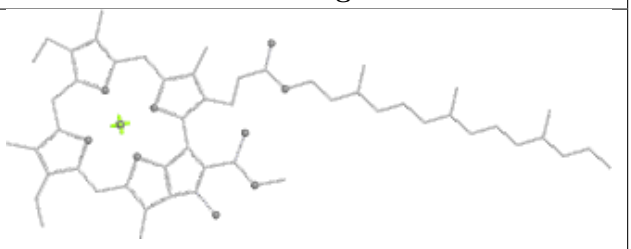
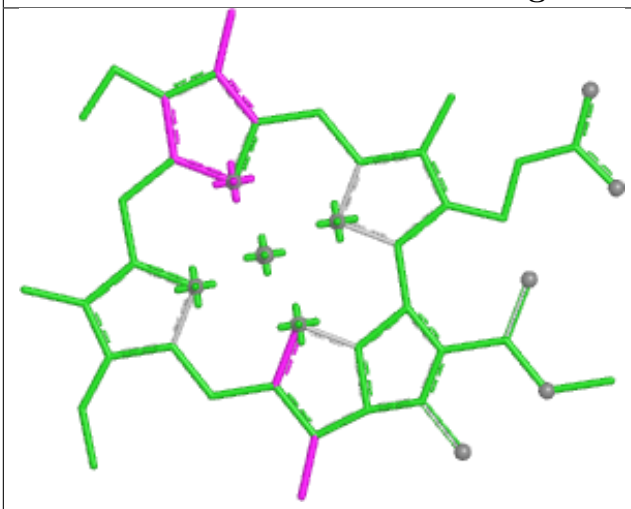


Rings

Ligand CLA 7 316



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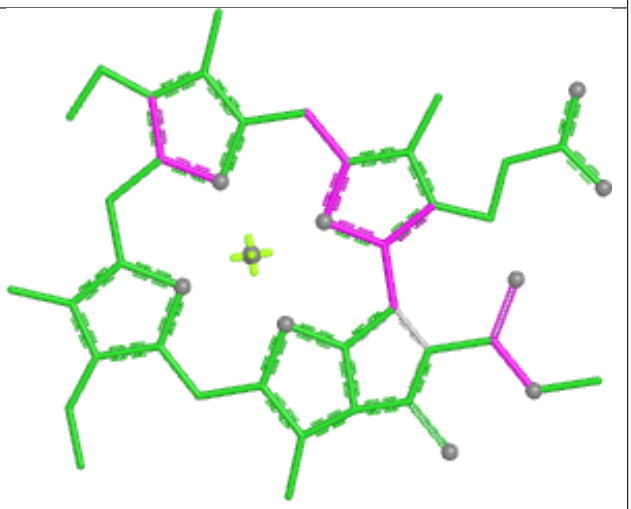
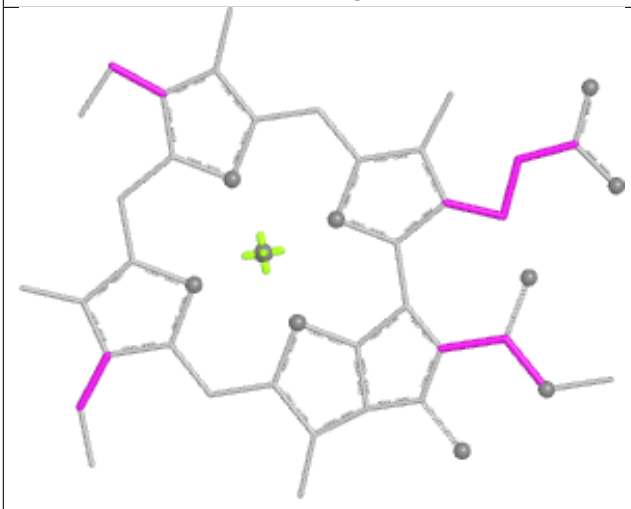


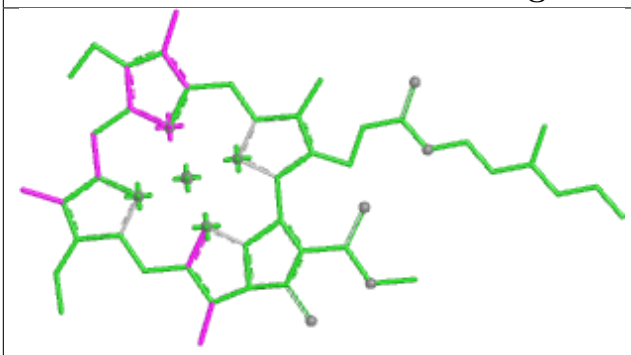
Bond angles



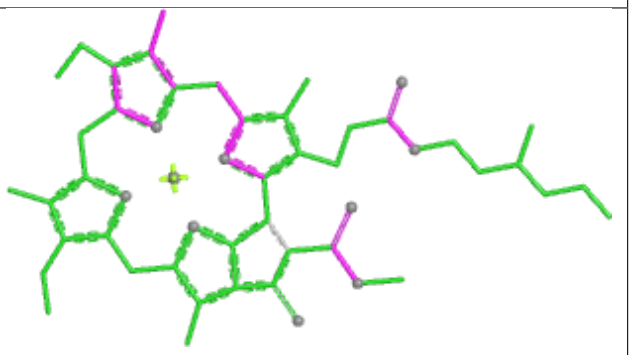
Torsions

Rings

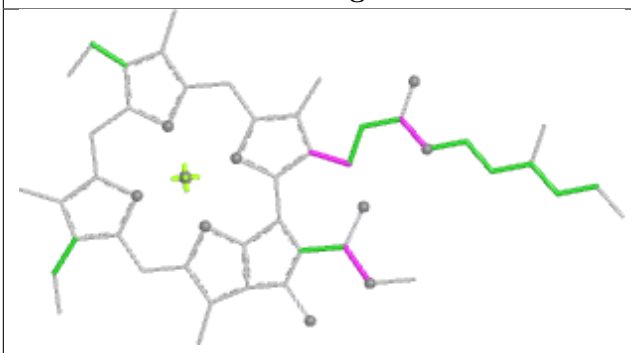
Ligand CLA 1 310



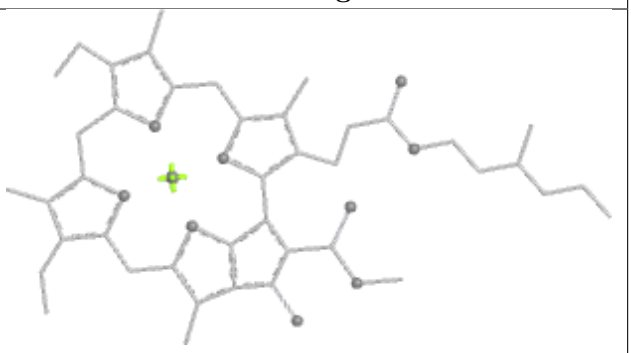
Bond lengths



Bond angles

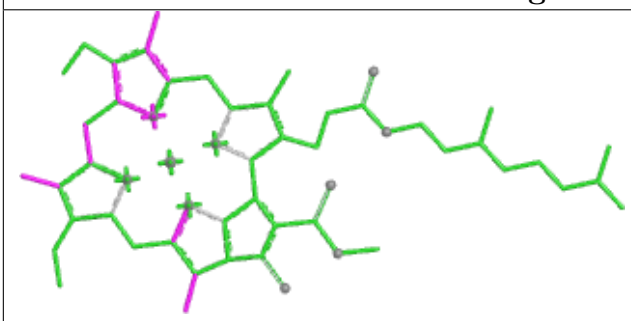


Torsions



Rings

Ligand CLA 3 303



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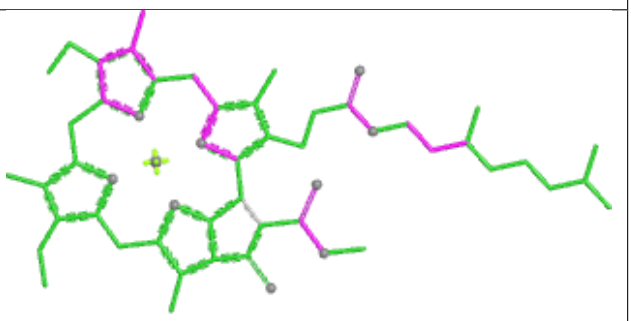

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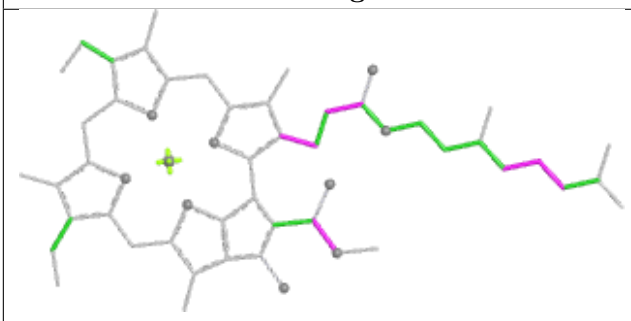

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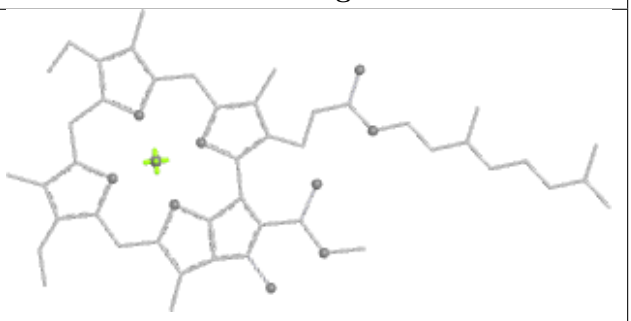
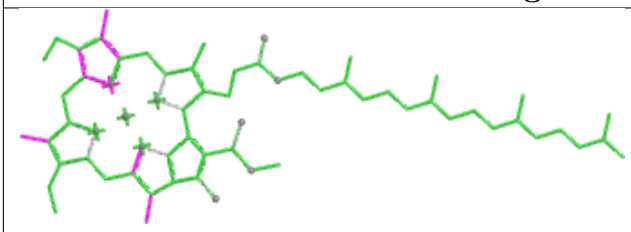


Rings

Ligand CLA A 810



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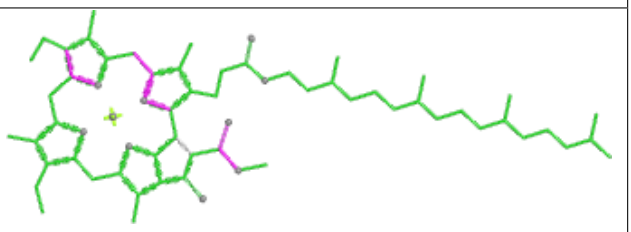

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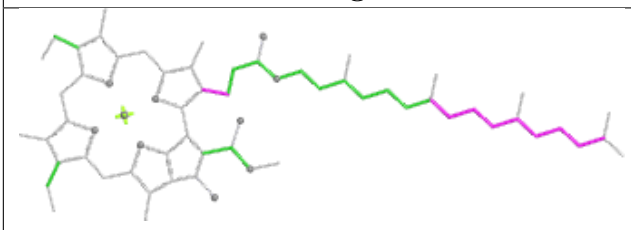

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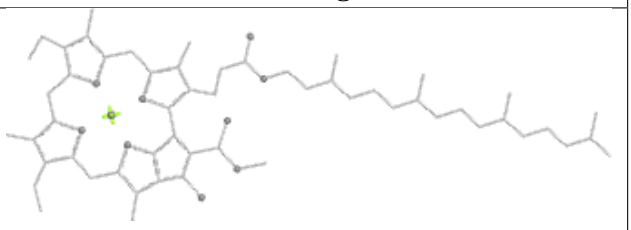
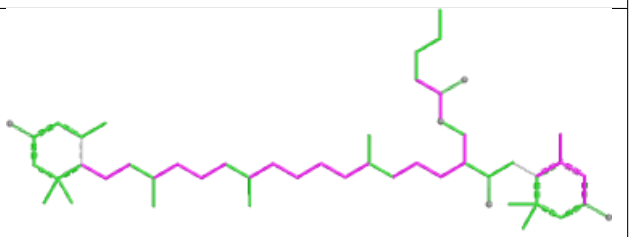


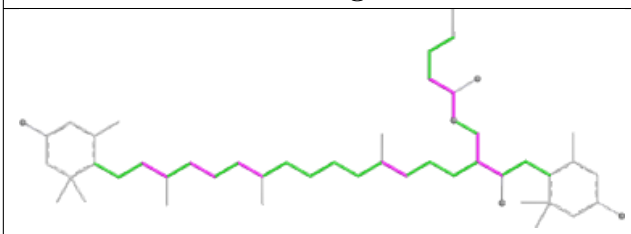
Rings

Ligand 0UR 4 318

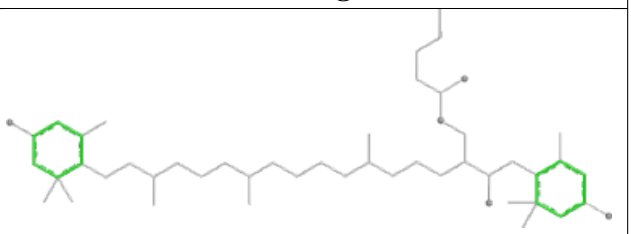
Bond lengths



Bond angles

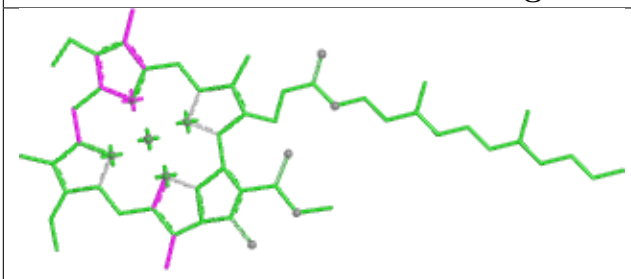


Torsions



Rings

Ligand CLA B 801



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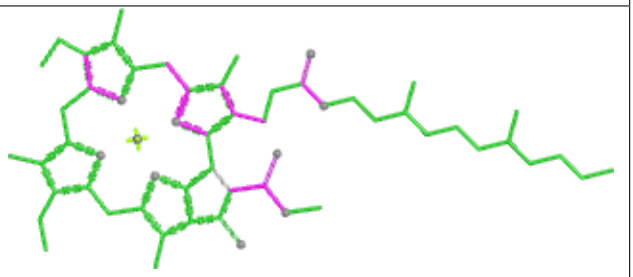
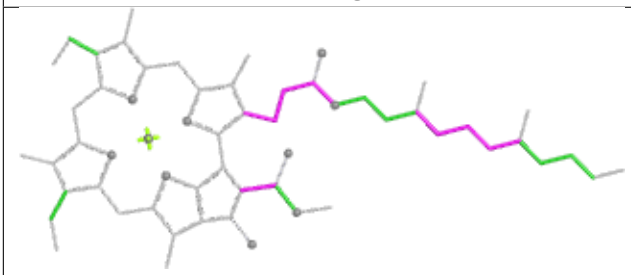


Bond angles



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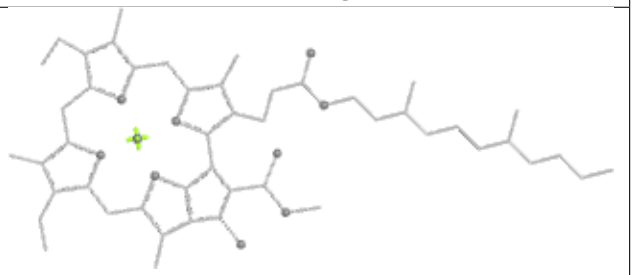
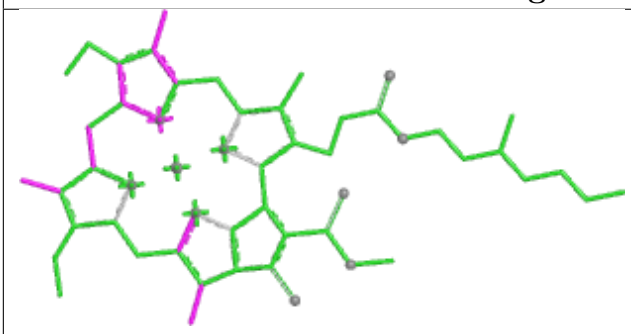


Rings

Ligand CLA 4 312



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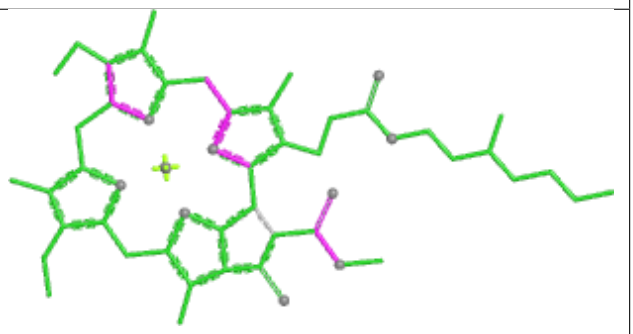

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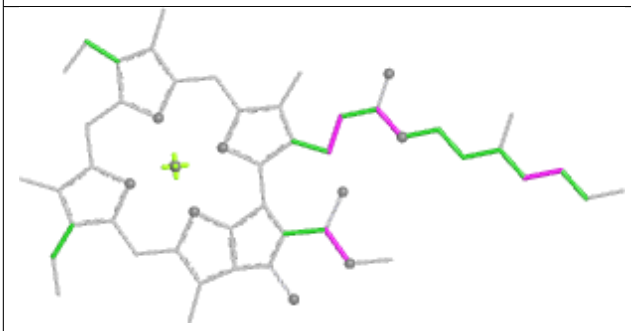

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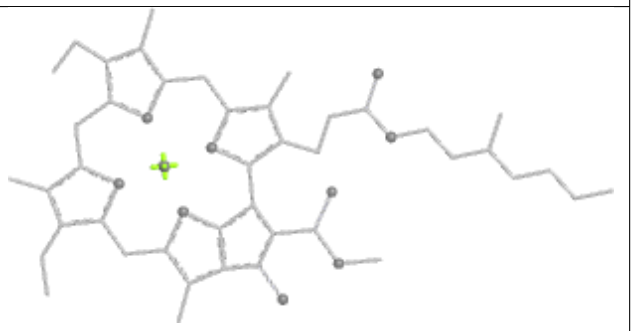
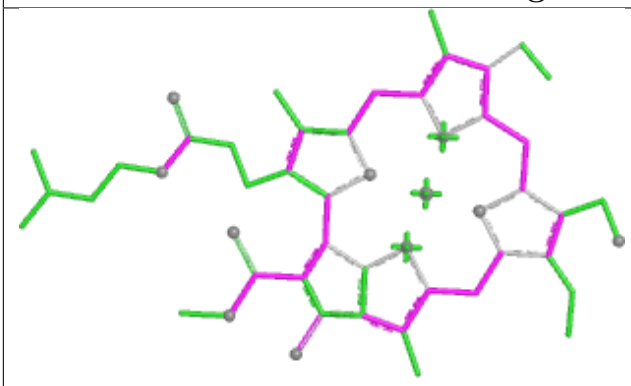


Rings

Ligand CHL 1 304



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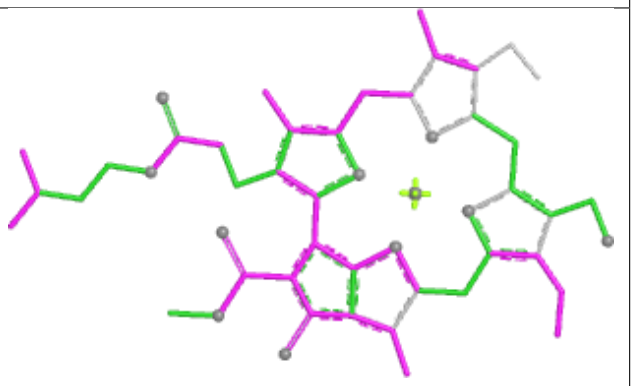
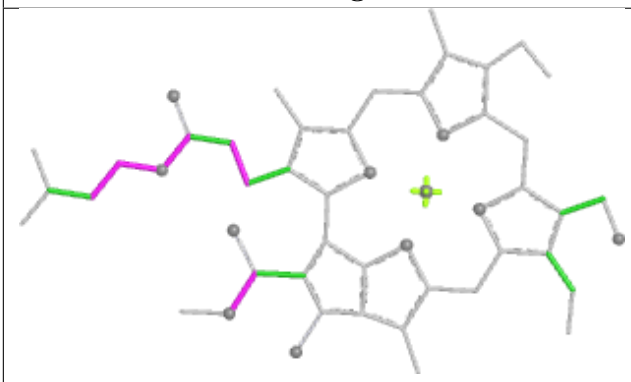


Bond angles



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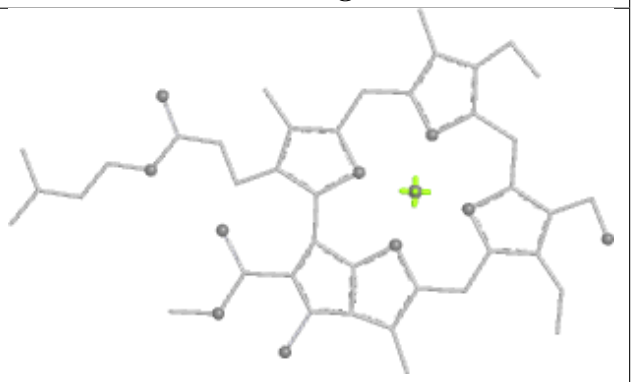
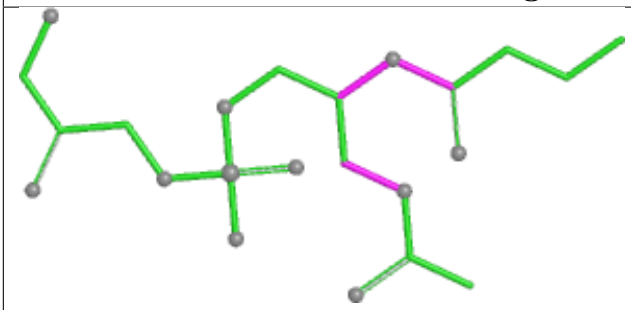


Rings

Ligand LHG B 851



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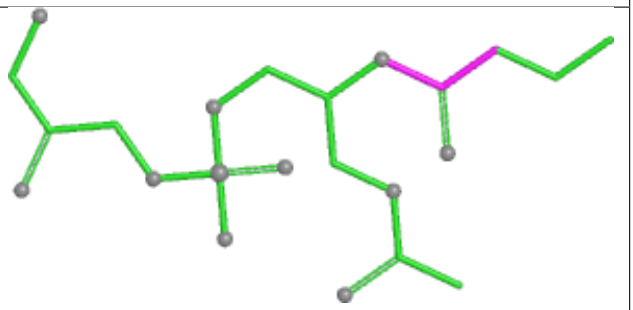

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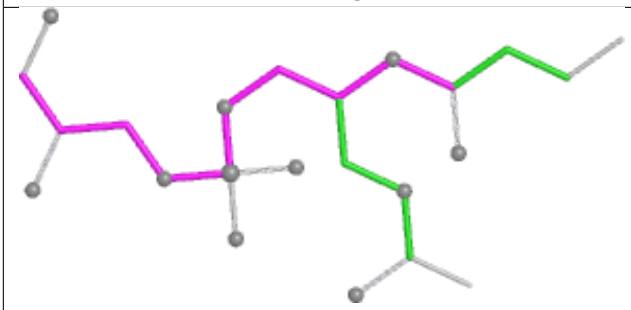

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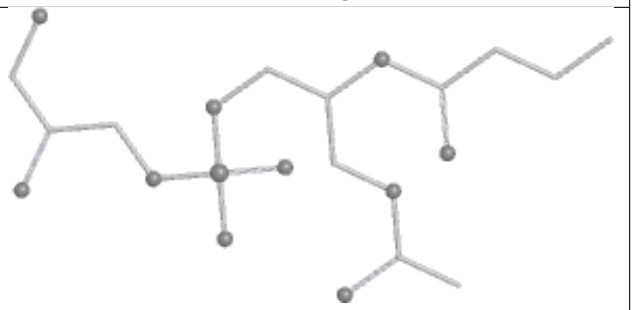
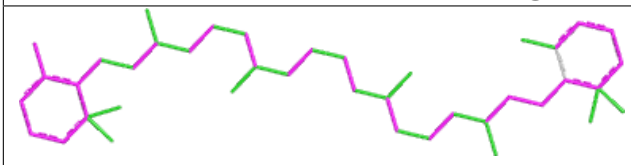


Rings

Ligand 8CT A 844



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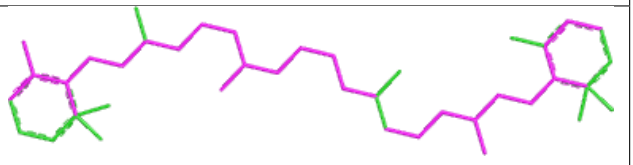
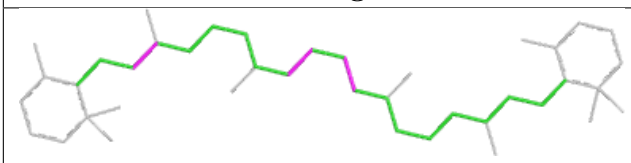


Bond angles



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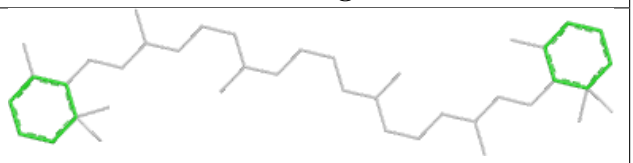
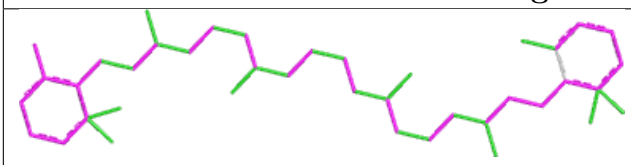


Rings

Ligand 8CT 7 319



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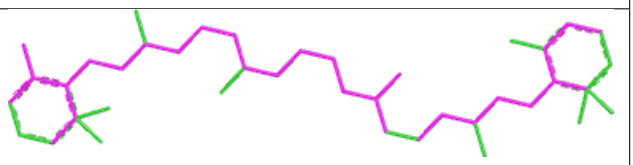
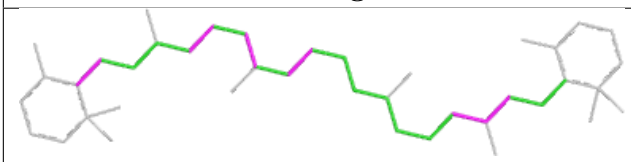


Bond angles



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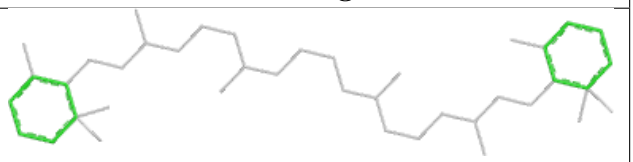
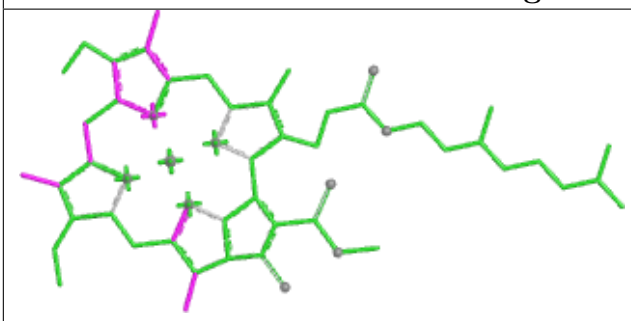


Rings

Ligand CLA A 823



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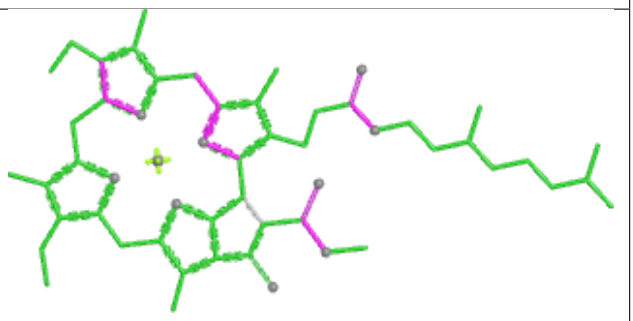
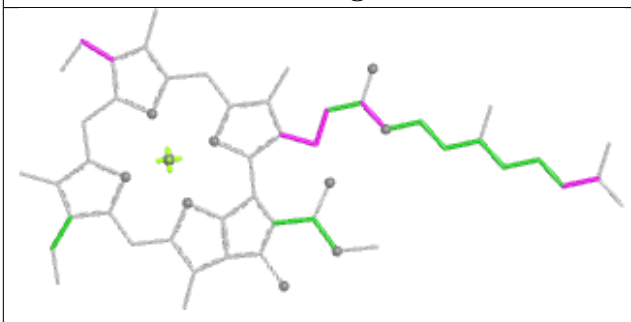


Bond angles



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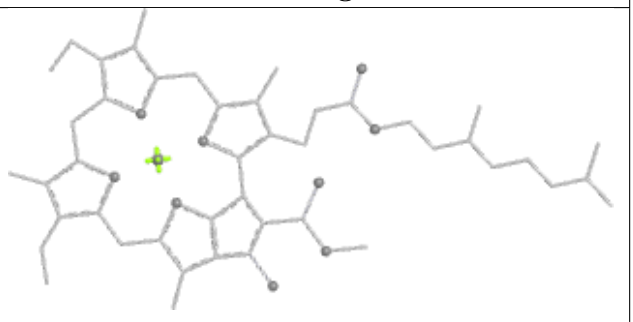
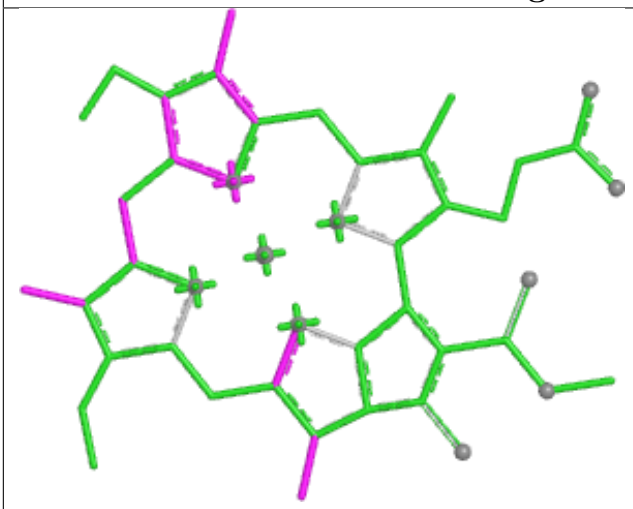


Rings

Ligand CLA 8 315



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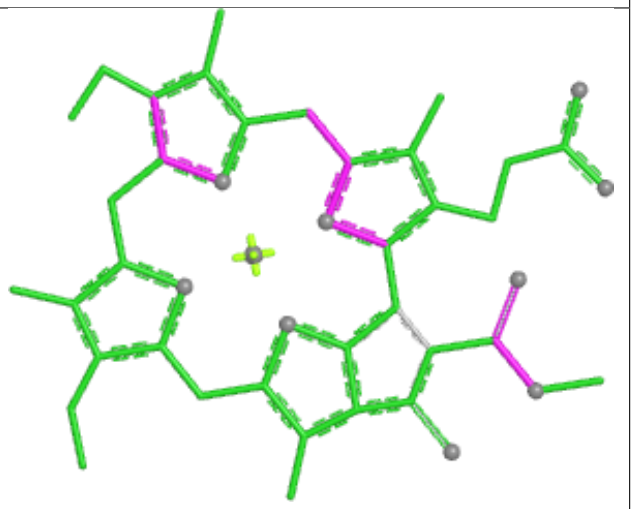
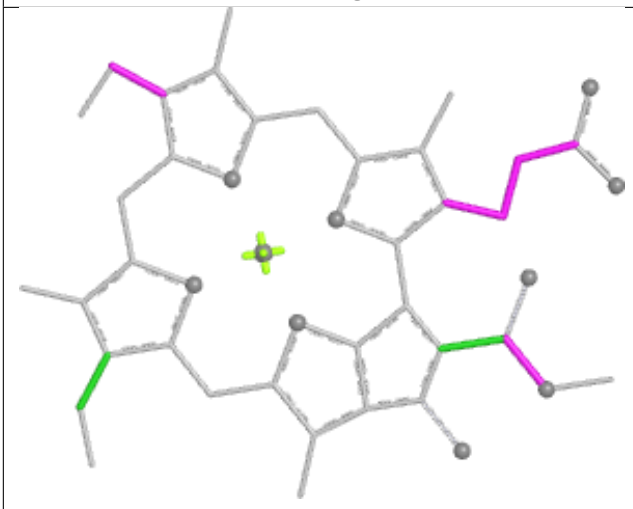


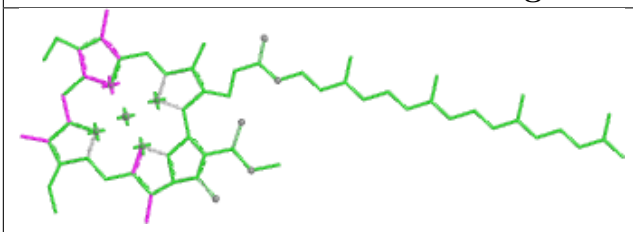
Bond angles



Torsions

Rings

Ligand CLA B 805



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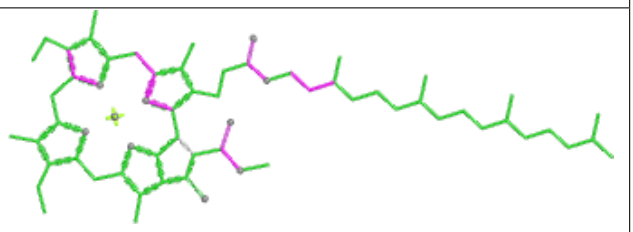
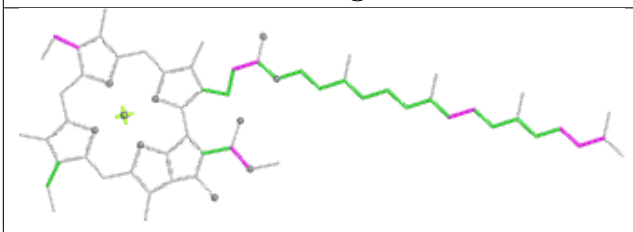
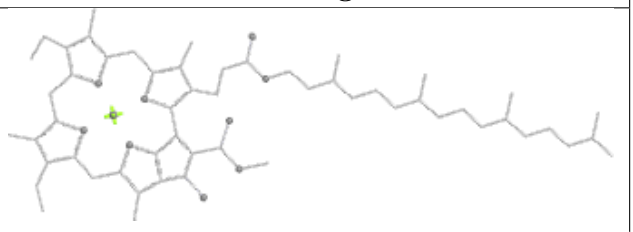


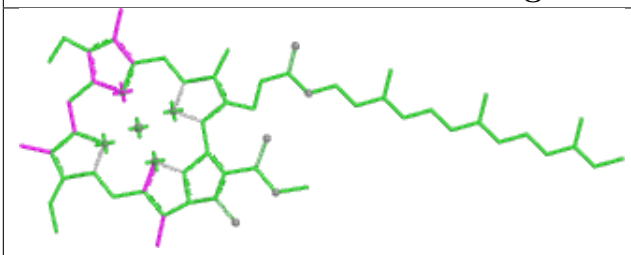
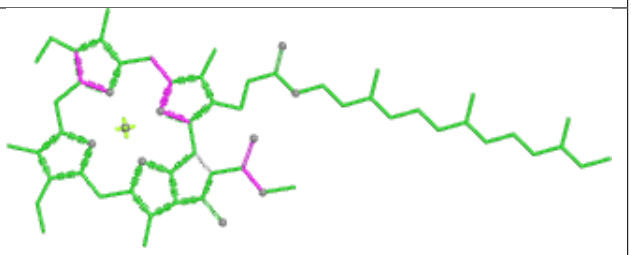
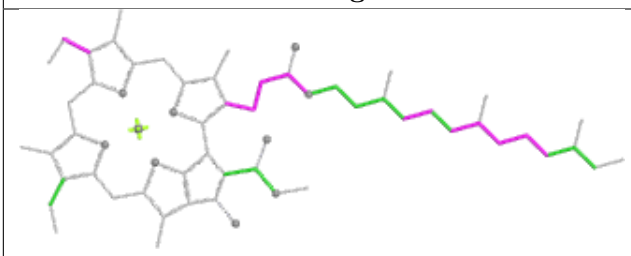
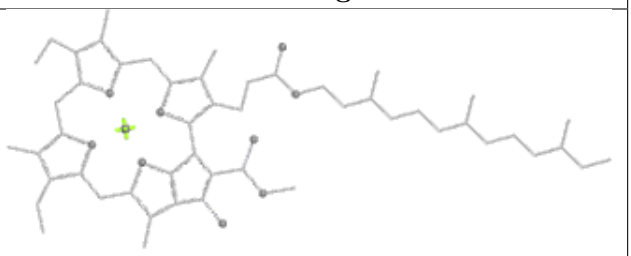
Bond angles



Torsions



Rings

Ligand CLA B 834	
 Bond lengths	 Bond angles
 Torsions	 Rings

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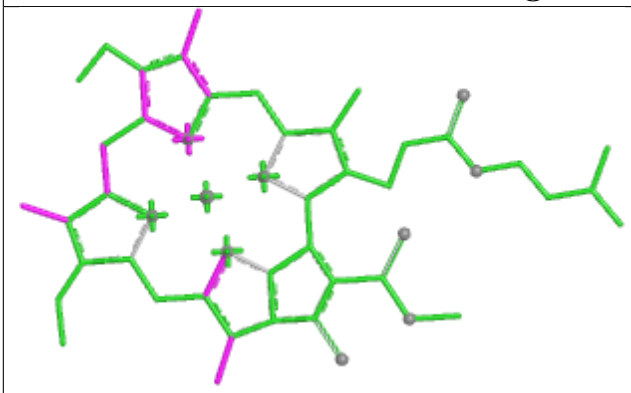
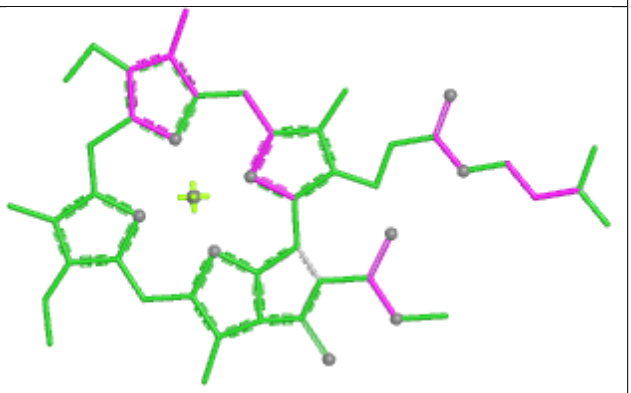
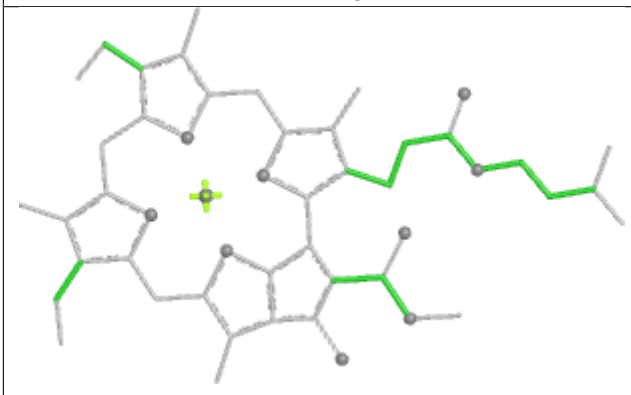
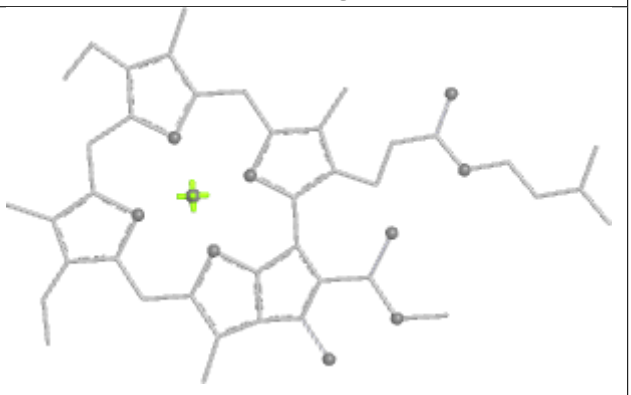
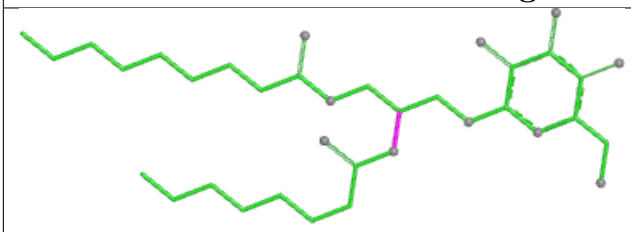
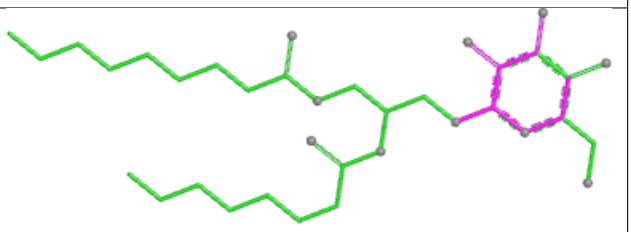
 Bond lengths	 Bond angles
 Torsions	 Rings

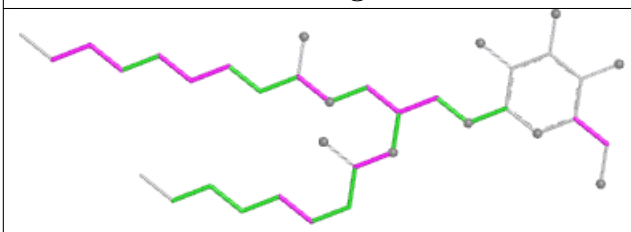
Ligand LMG A 851



Bond lengths



Bond angles



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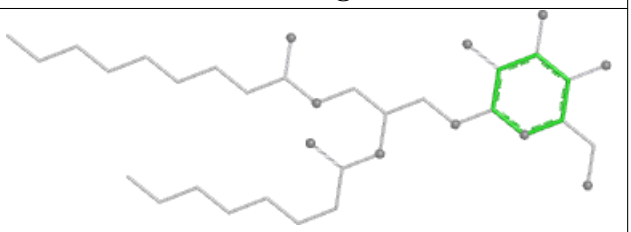
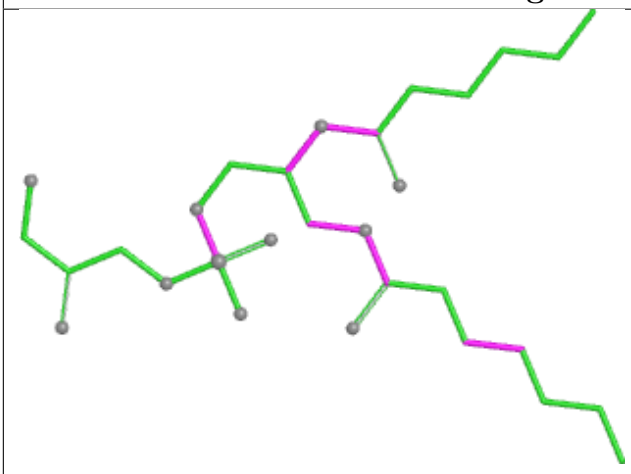


Rings

Ligand LHG 7 322



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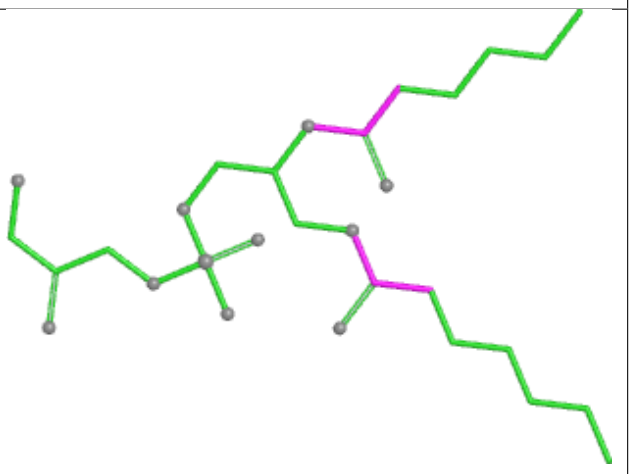

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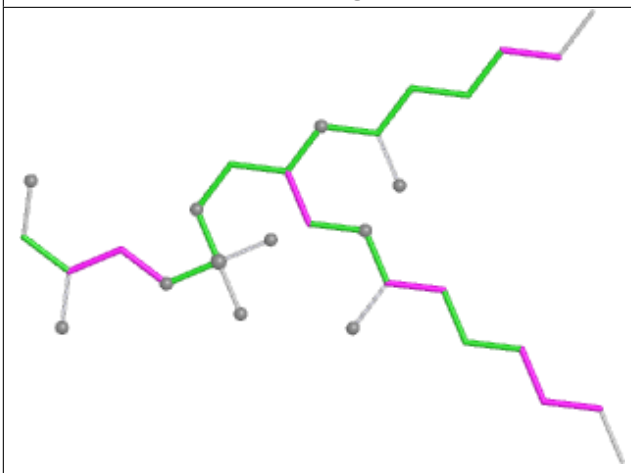

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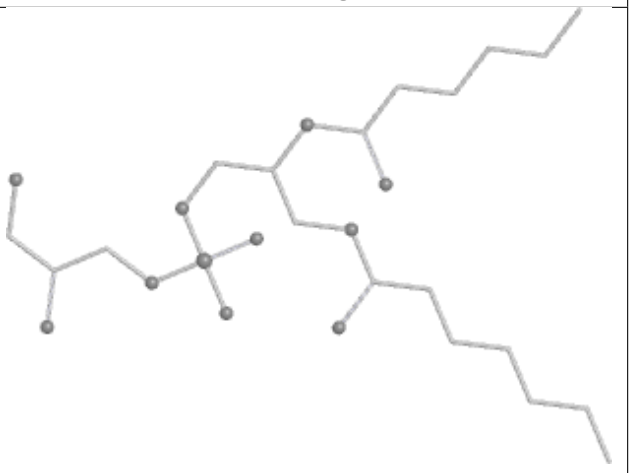
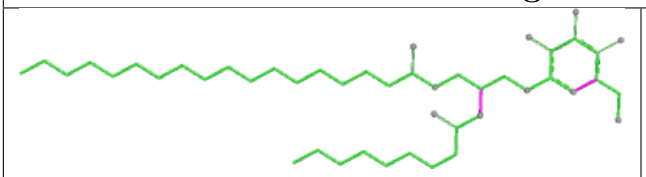


Rings

Ligand LMG J 105



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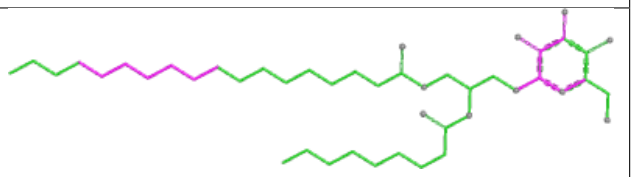

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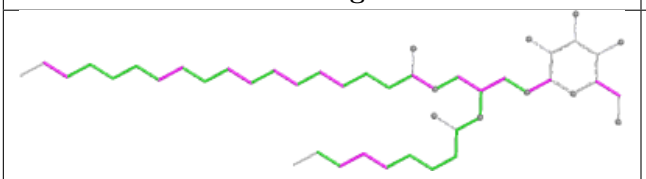

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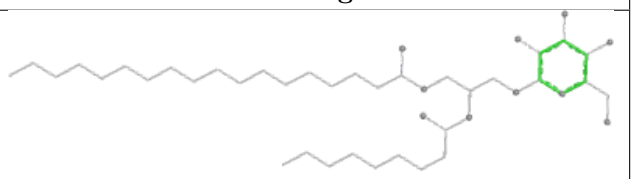
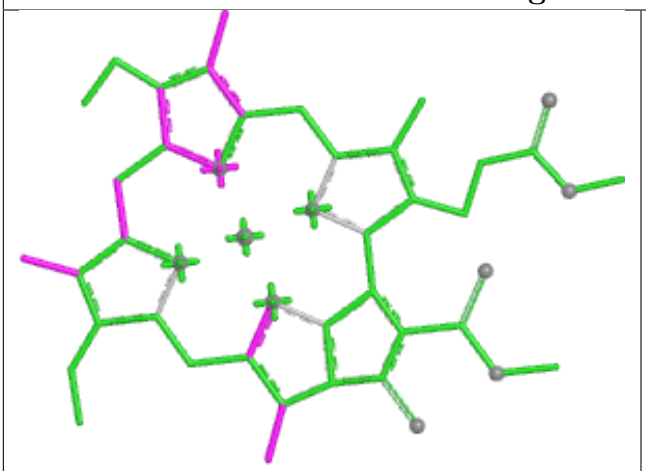


Rings

Ligand CLA 8 312



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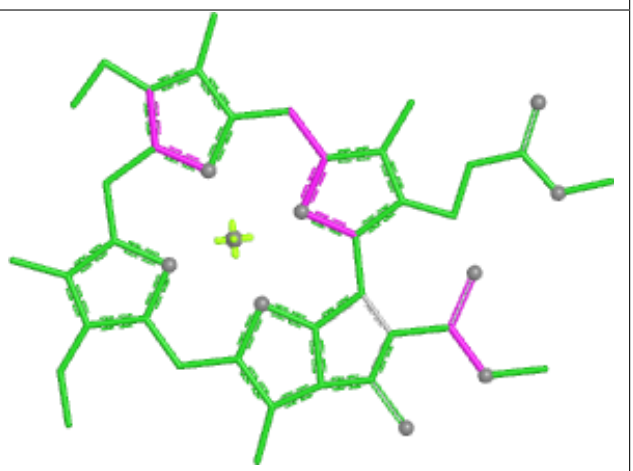

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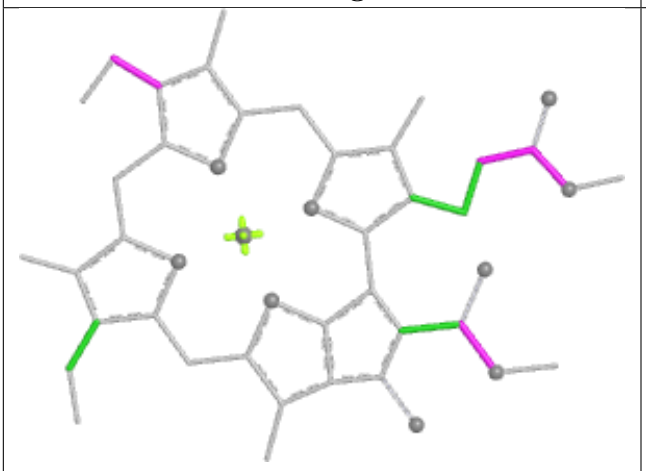

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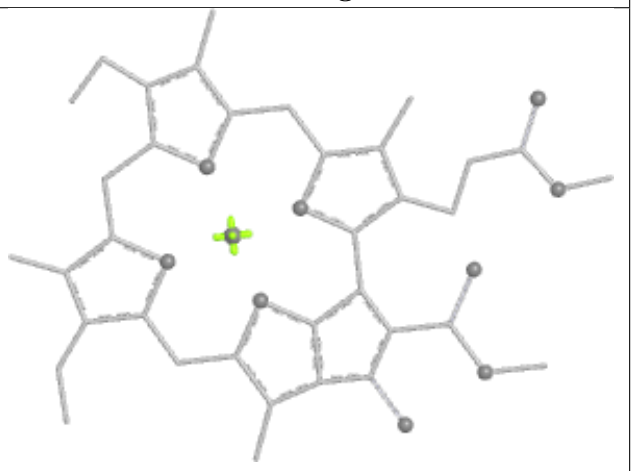
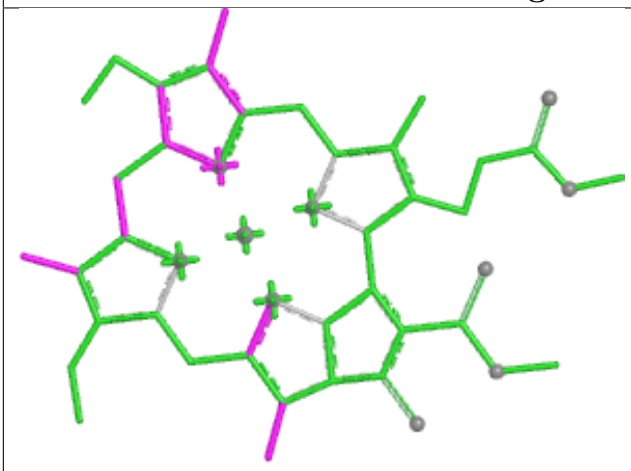


Rings

Ligand CLA 5 313



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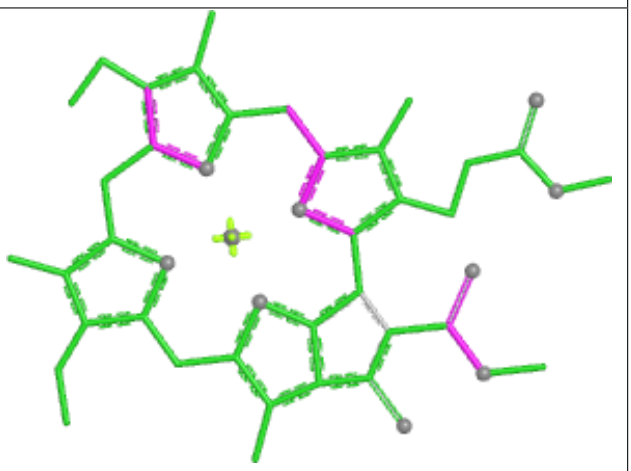
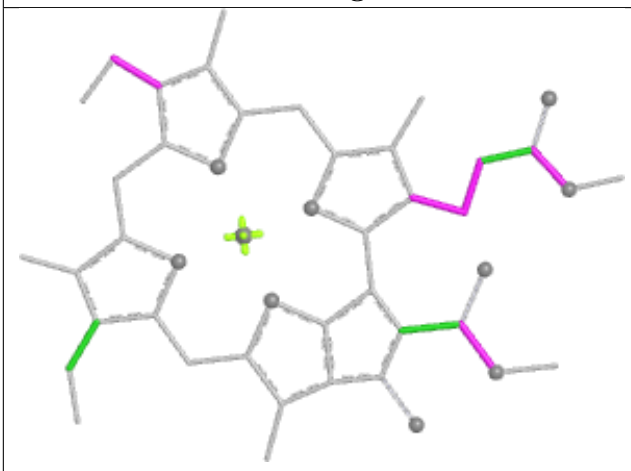


Bond angles



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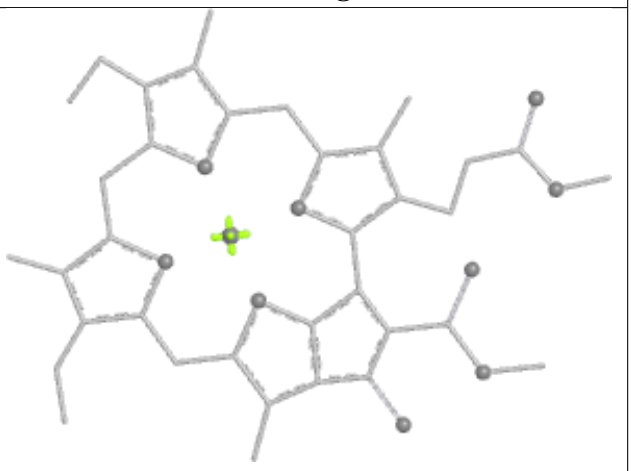
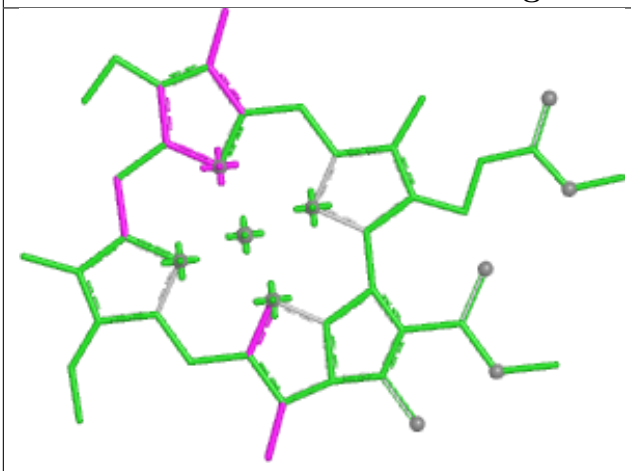


Rings

Ligand CLA G 103



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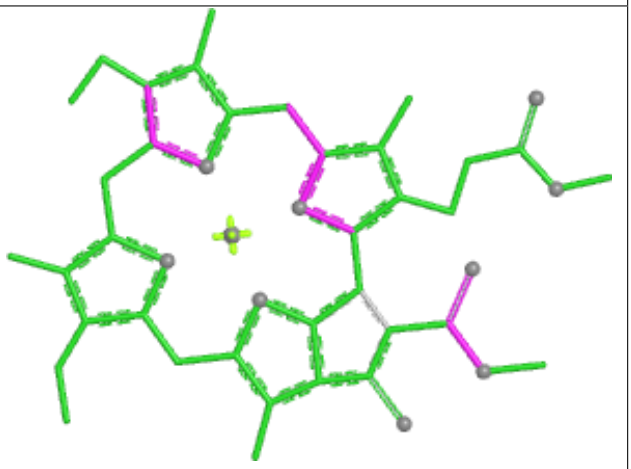

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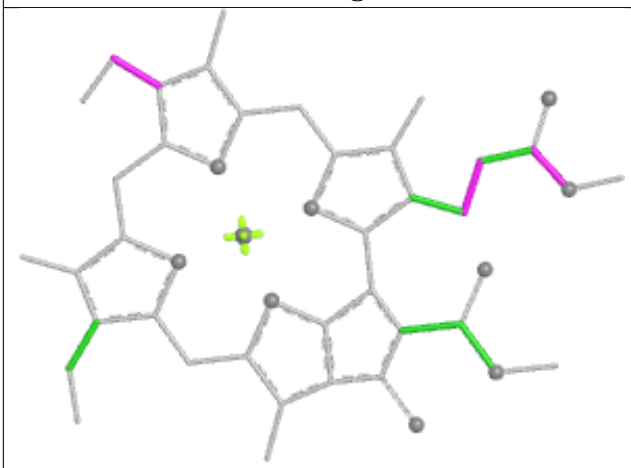

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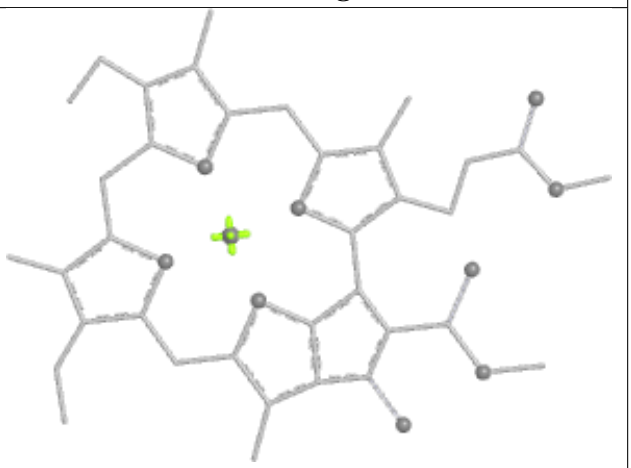
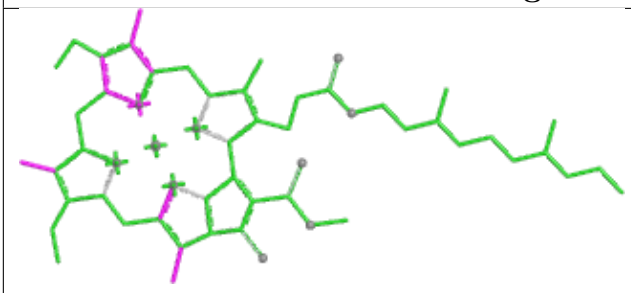


Rings

Ligand CLA A 813



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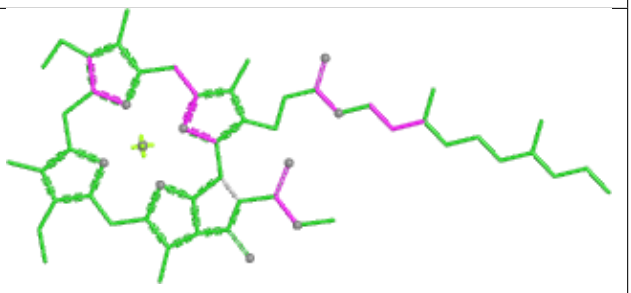

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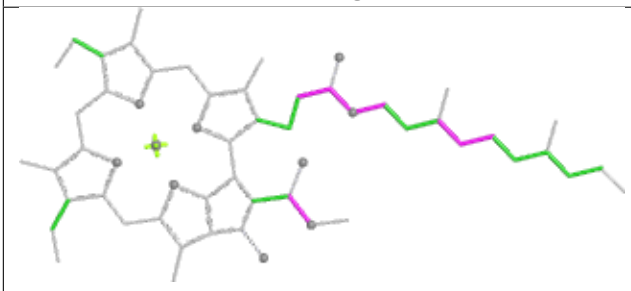

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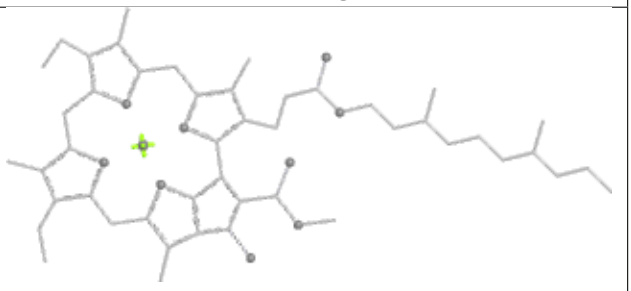
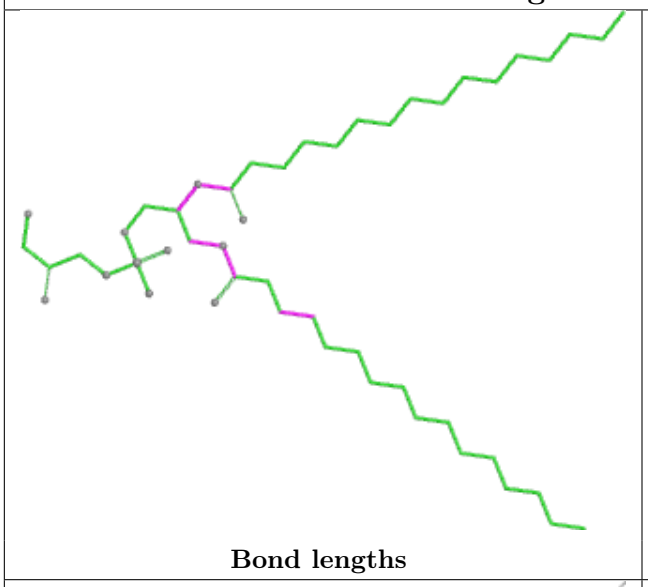


Rings

Ligand LHG 1 317



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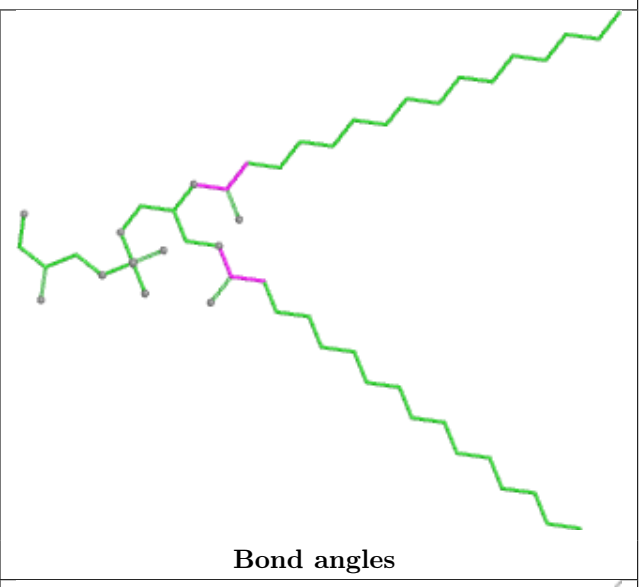

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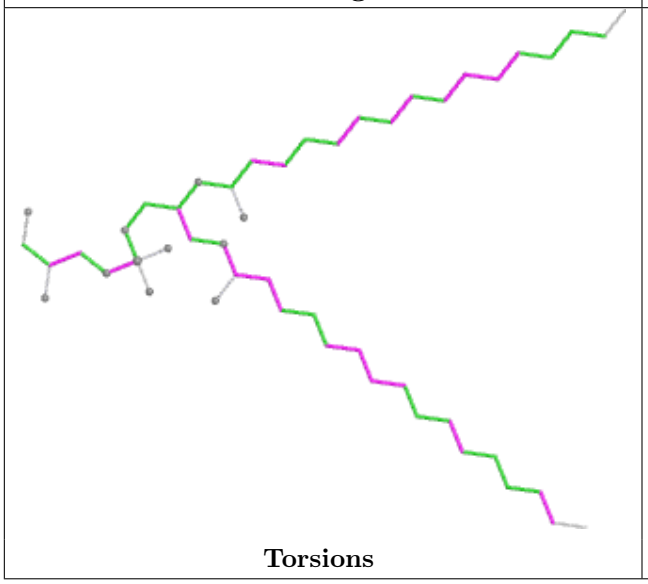

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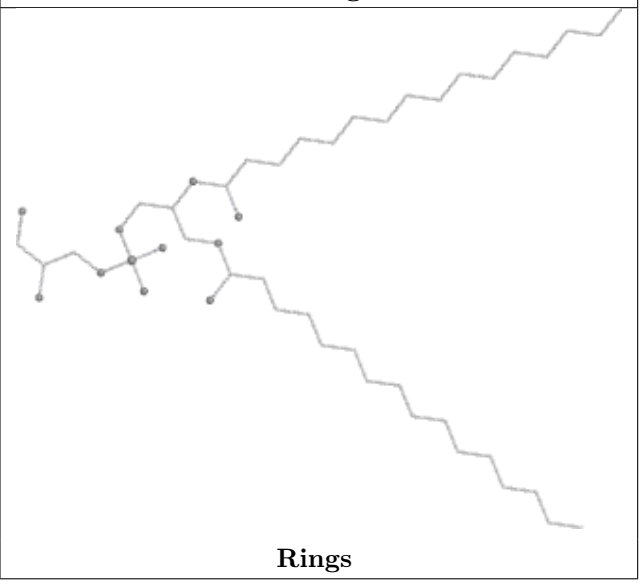
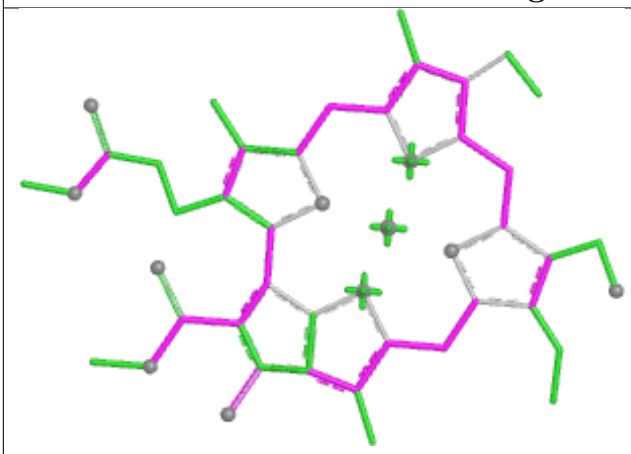


Rings

Ligand CHL 7 313



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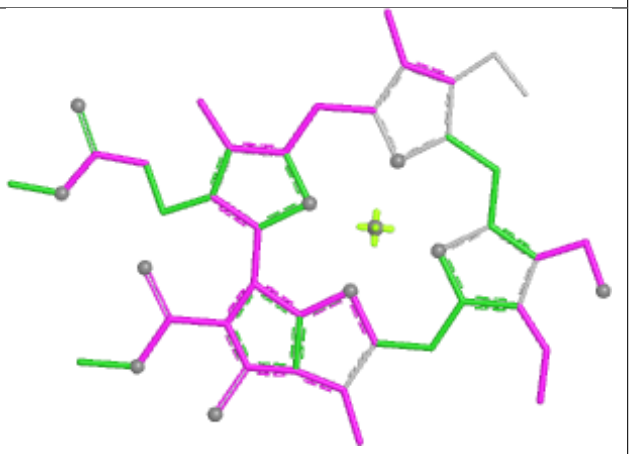

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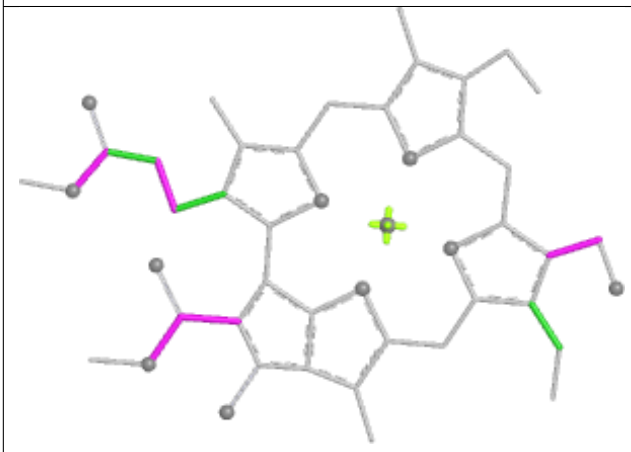
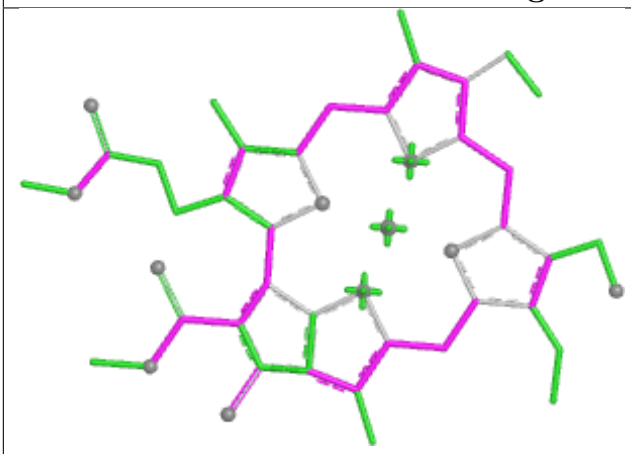


Torsions

Rings

Ligand CHL 9 301



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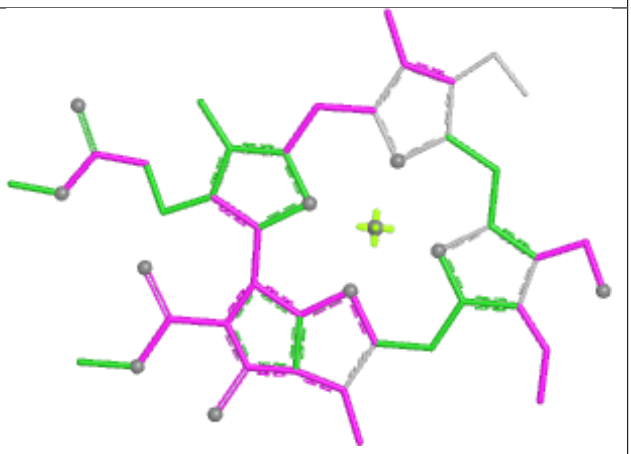

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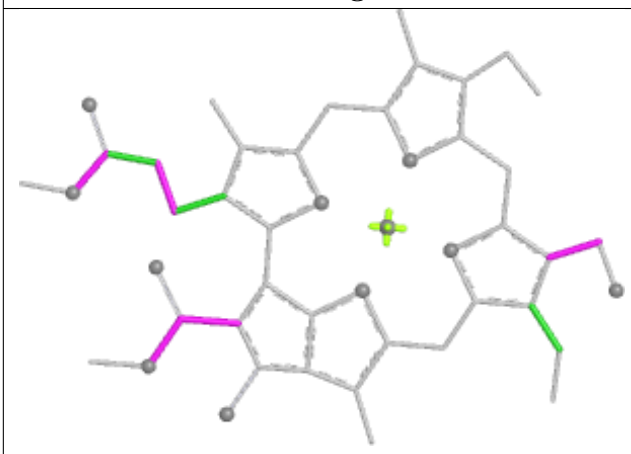

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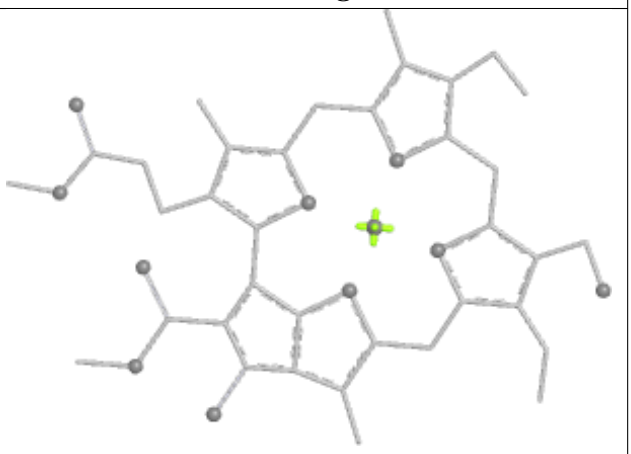
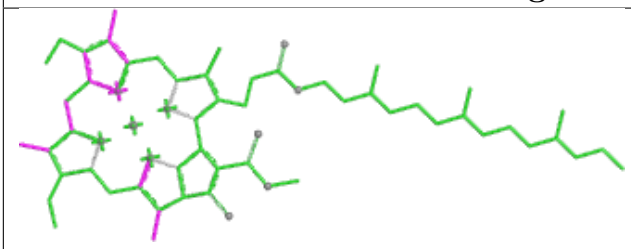


Rings

Ligand CLA 3 310



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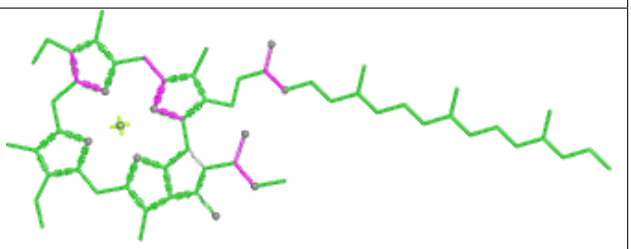

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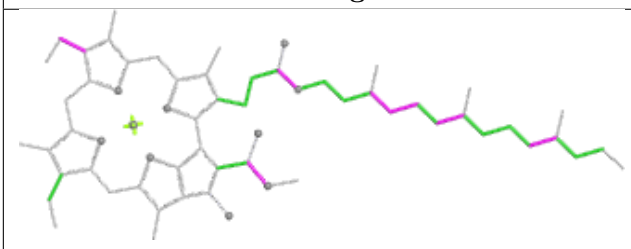

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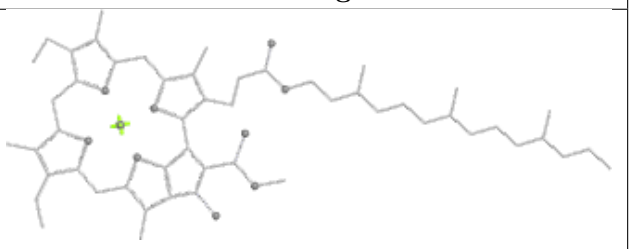
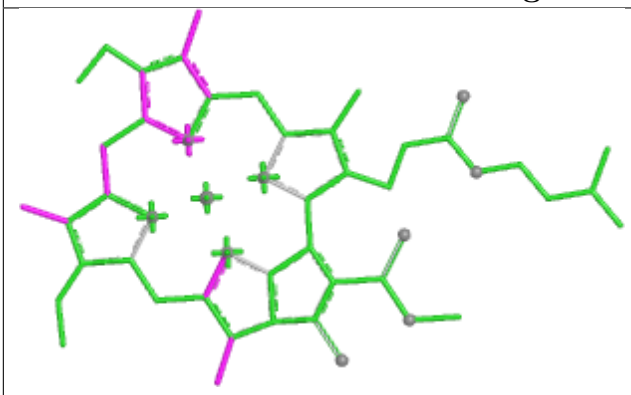


Rings

Ligand CLA K 104



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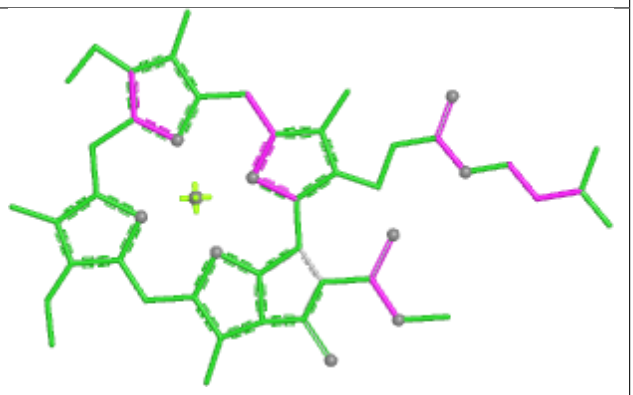

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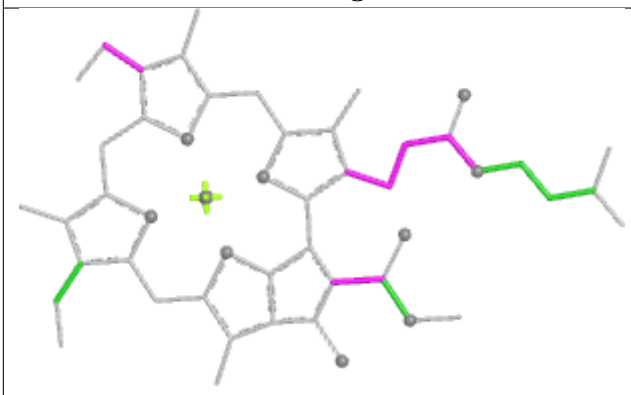

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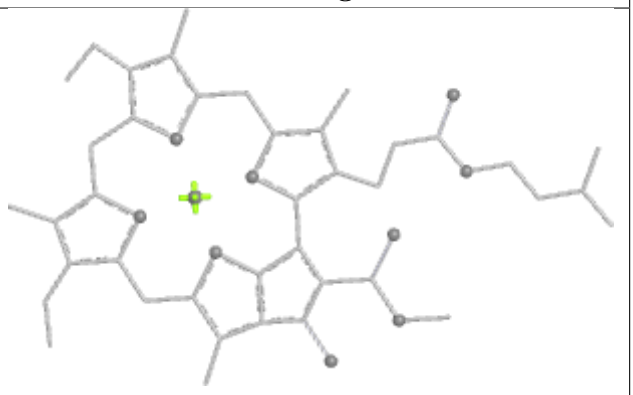
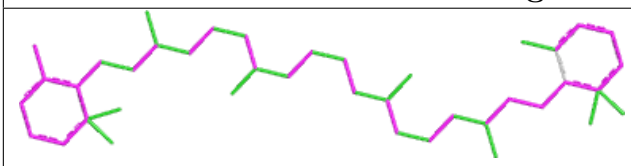


Rings

Ligand 8CT A 849



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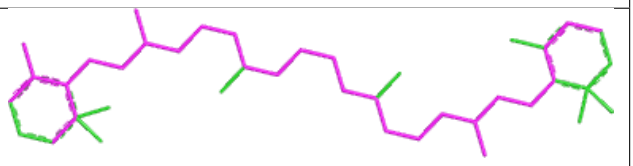
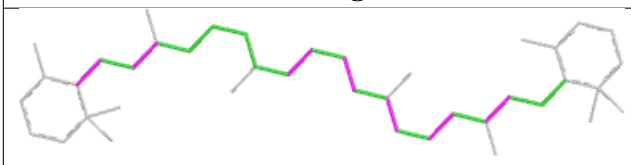


Bond angles



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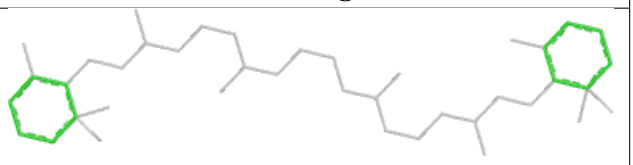
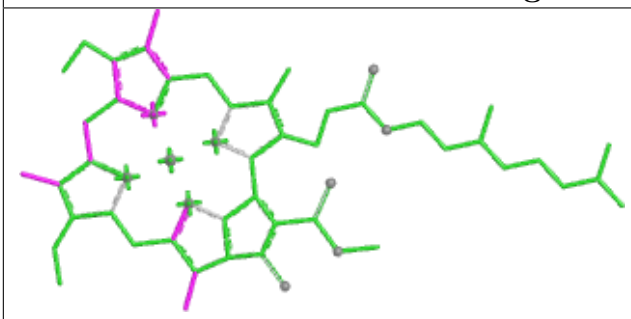
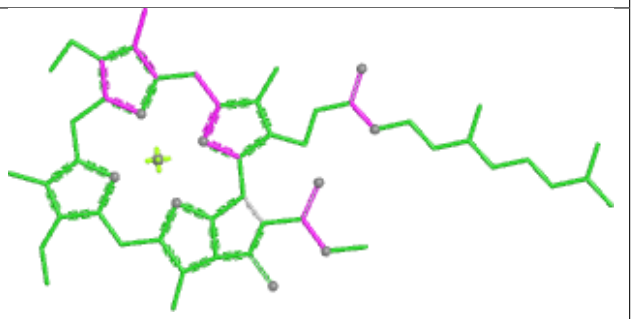


Rings

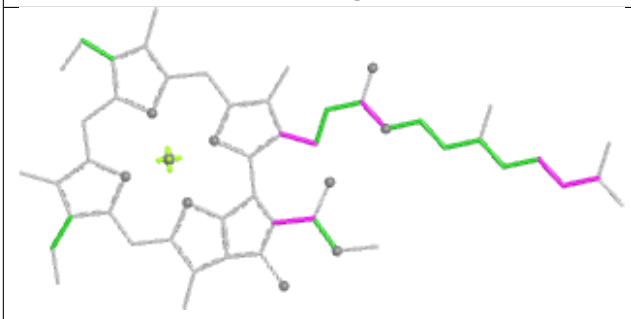
Ligand CLA A 803



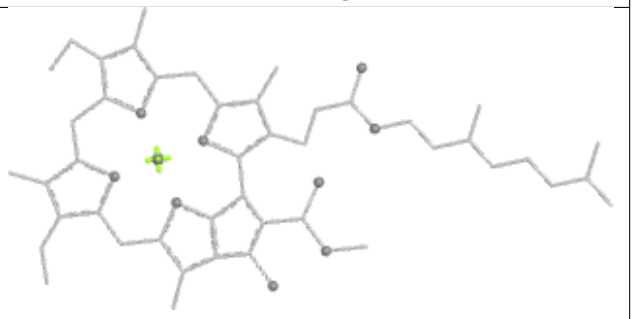
Bond lengths



Bond angles

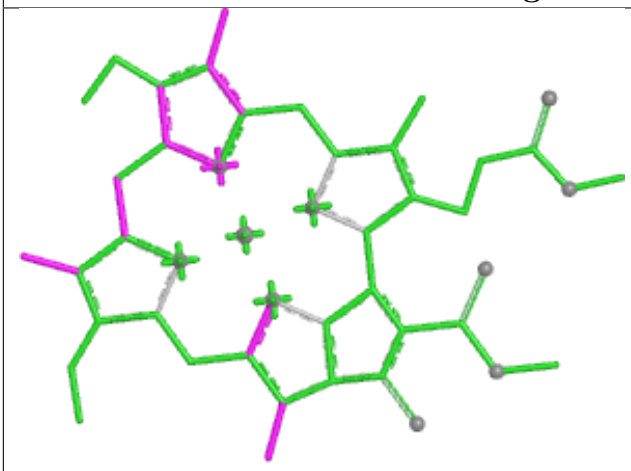


Torsions

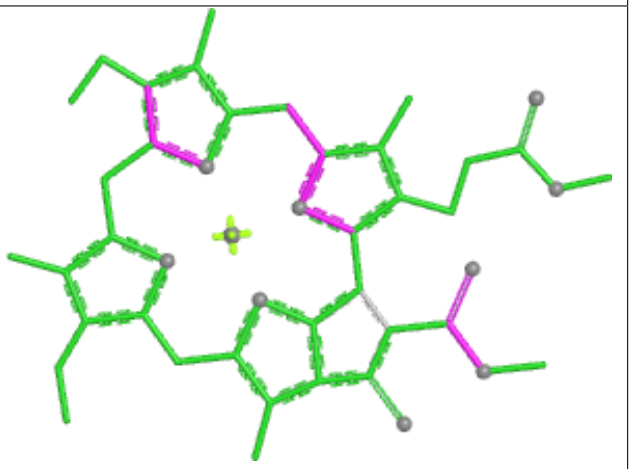


Rings

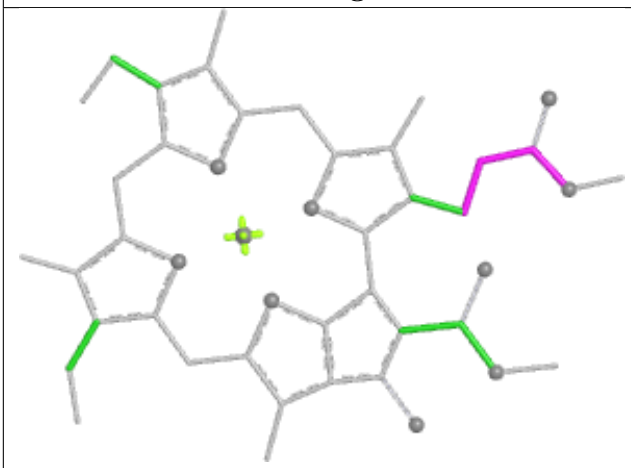
Ligand CLA K 103



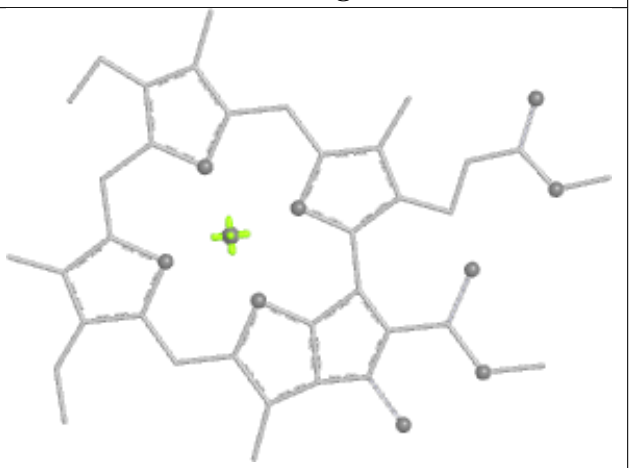
Bond lengths



Bond angles

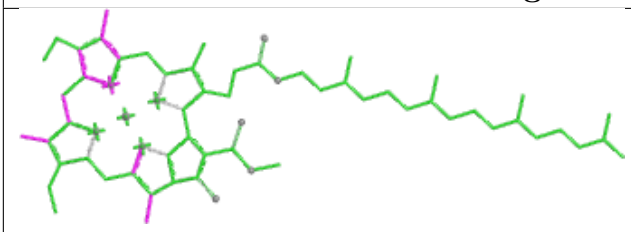


Torsions

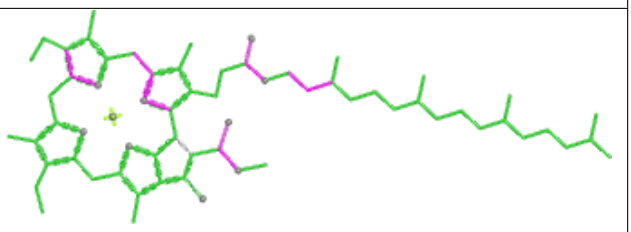


Rings

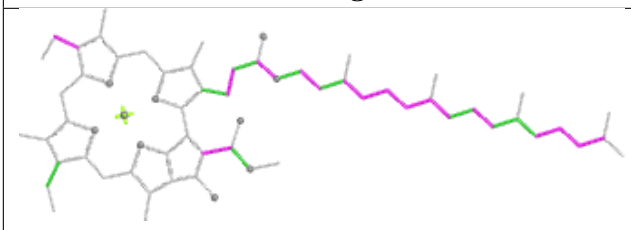
Ligand CLA A 839



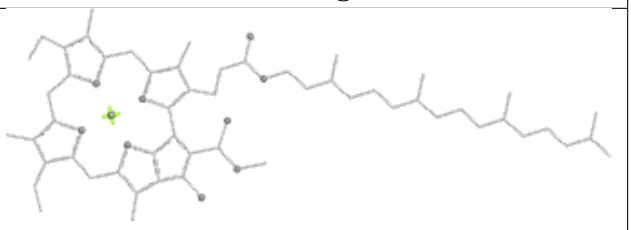
Bond lengths



Bond angles

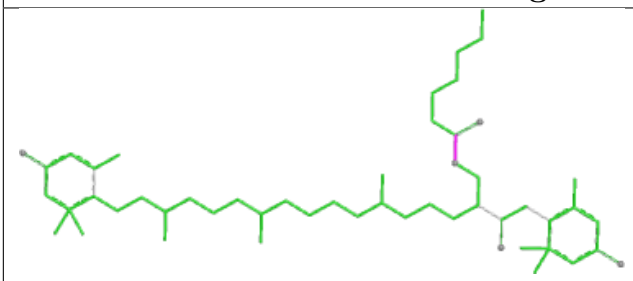


Torsions



Rings

Ligand 0UR 8 319



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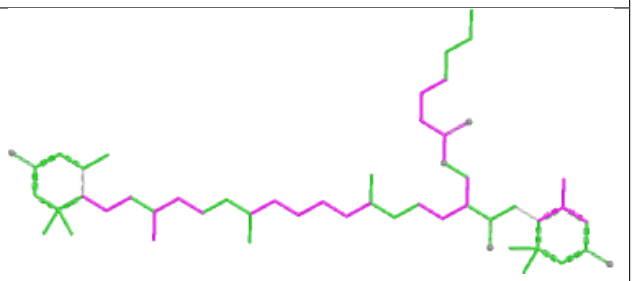
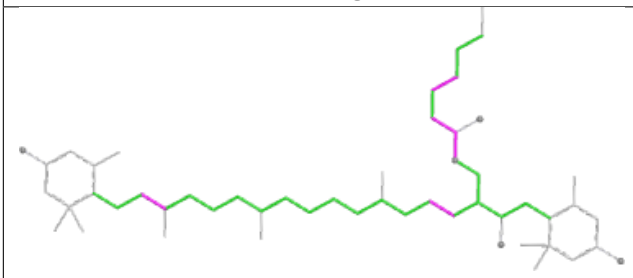
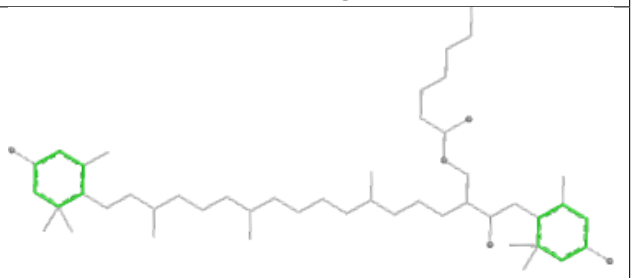


Bond angles

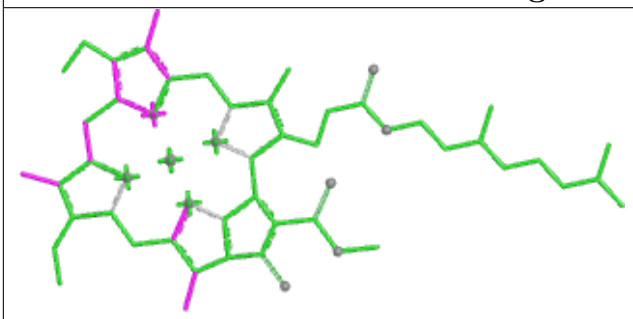


Torsions

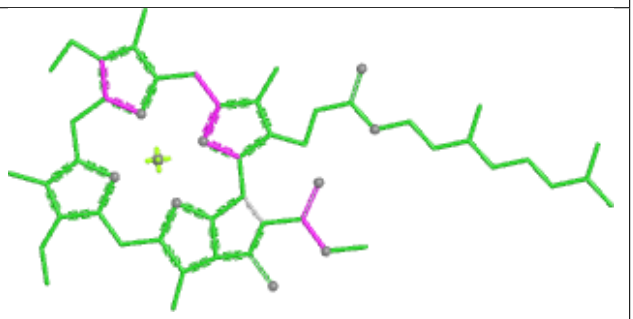


Rings

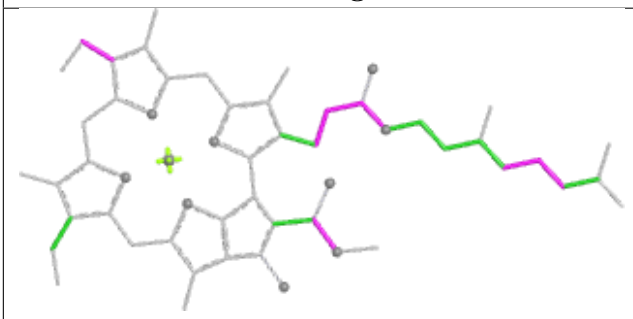
Ligand CLA 7 312



Bond lengths



Bond angles



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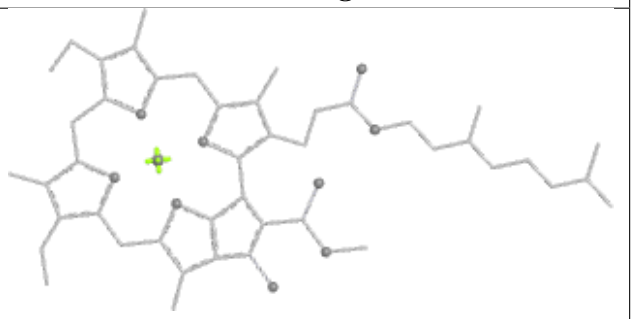
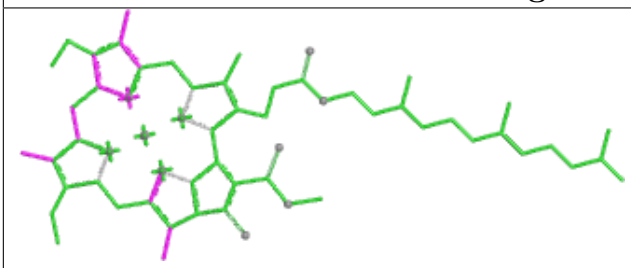
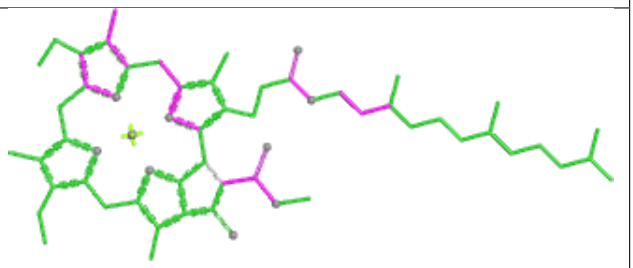
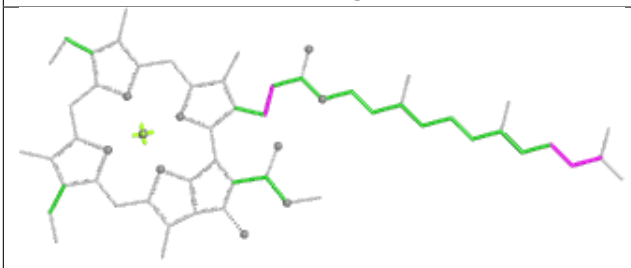
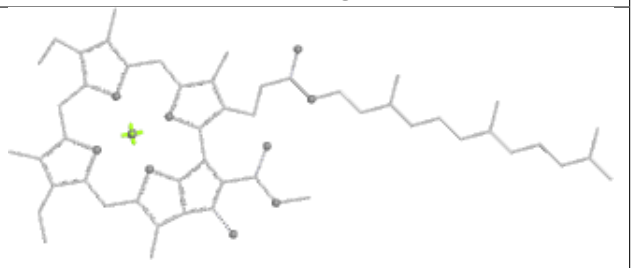
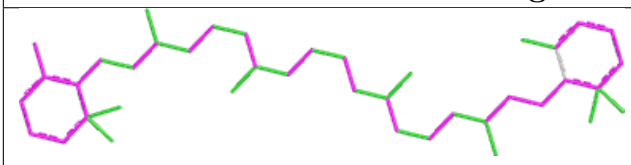
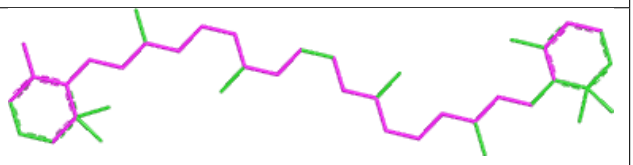
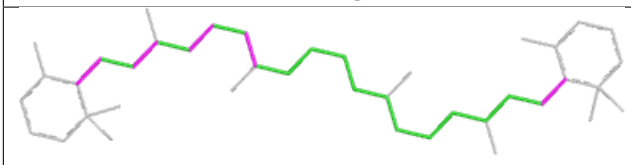
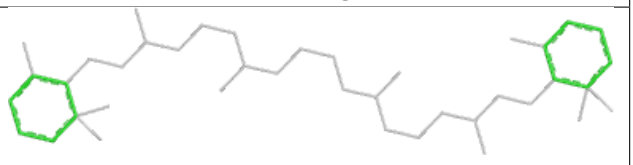
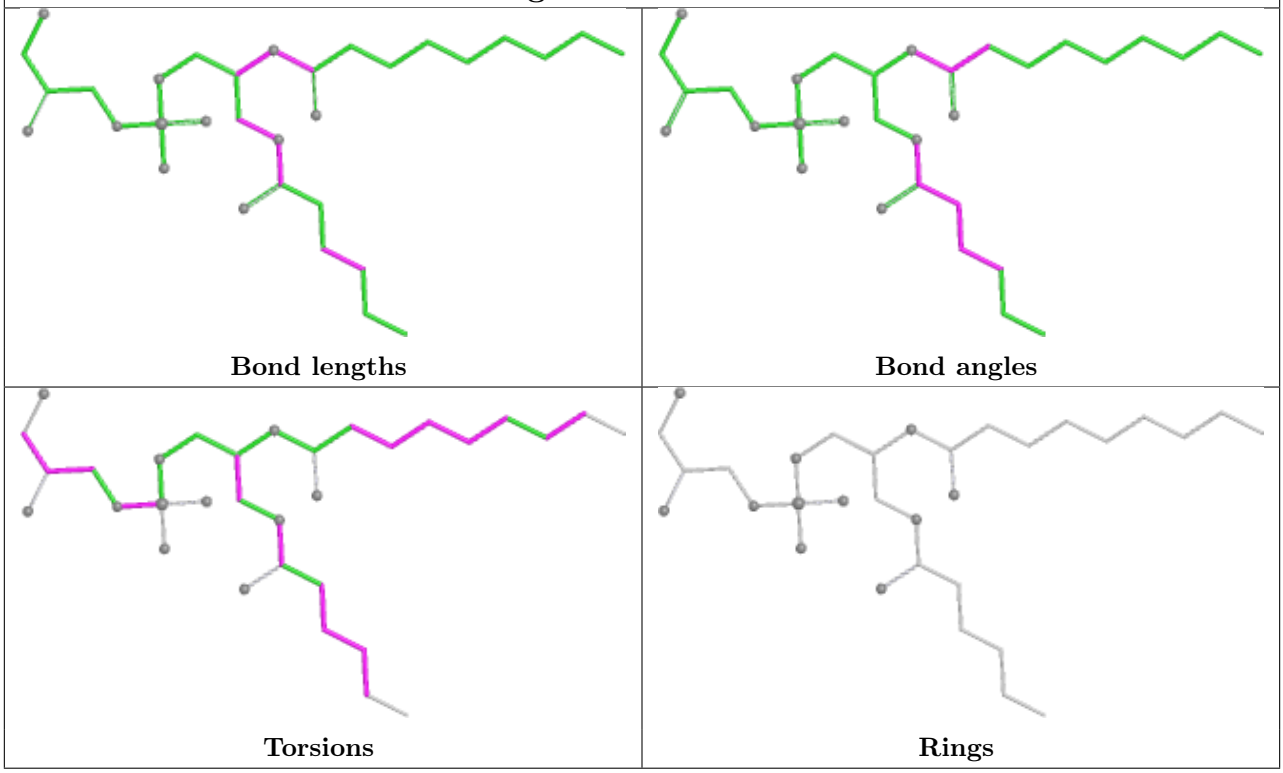


Rings

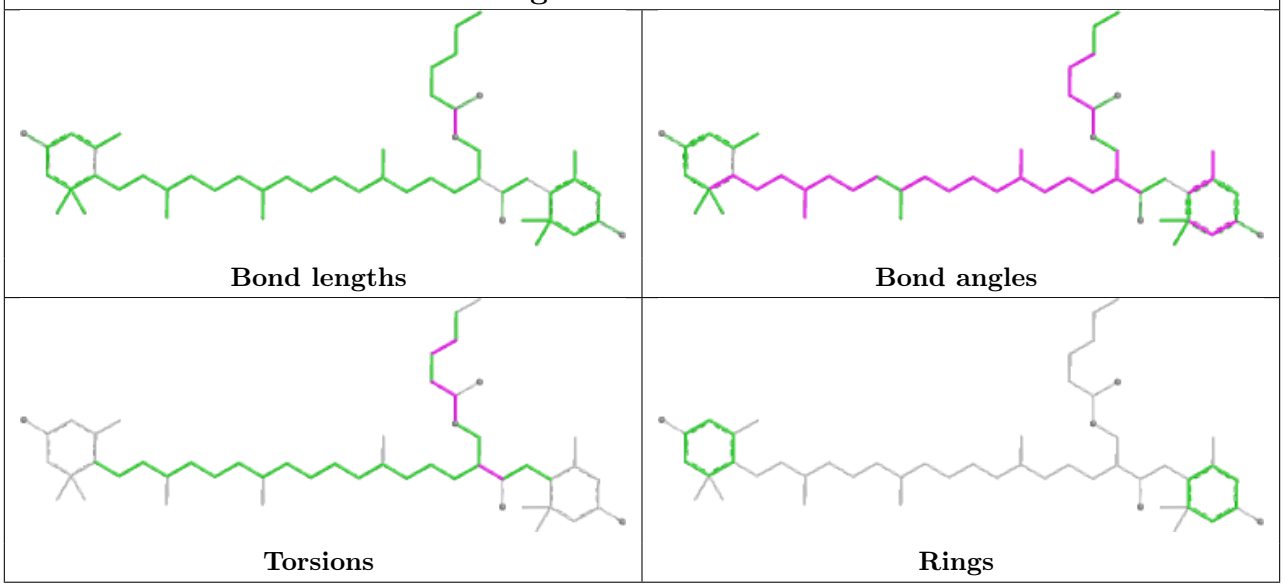
Ligand CLA 2 308	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand 8CT F 304	
	
Bond lengths	Bond angles
	
Torsions	Rings

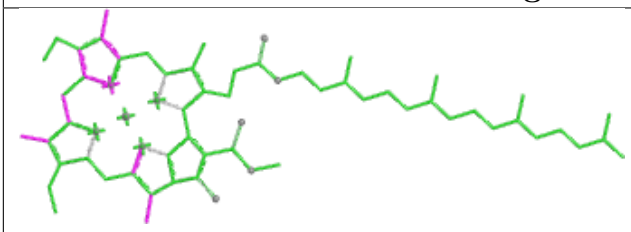
Ligand LHG 2 317



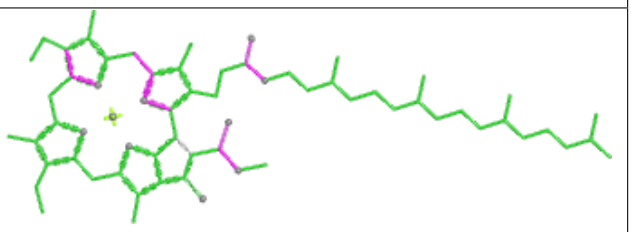
Ligand 0UR 8 318



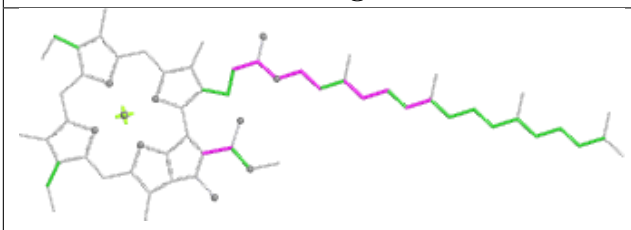
Ligand CLA A 804



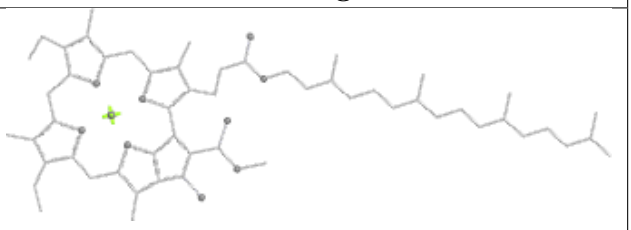
Bond lengths



Bond angles

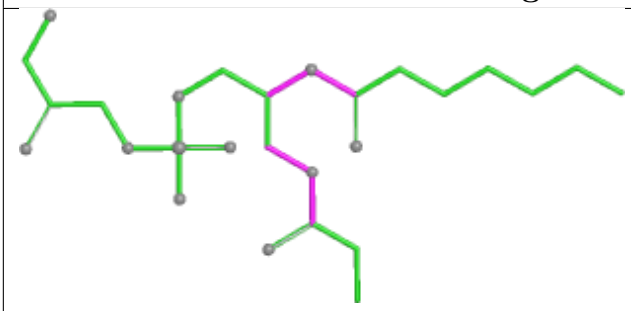


Torsions

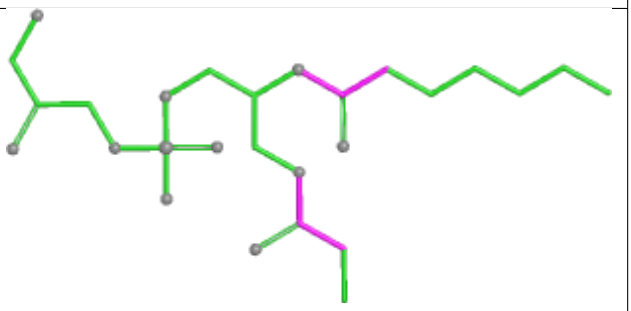


Rings

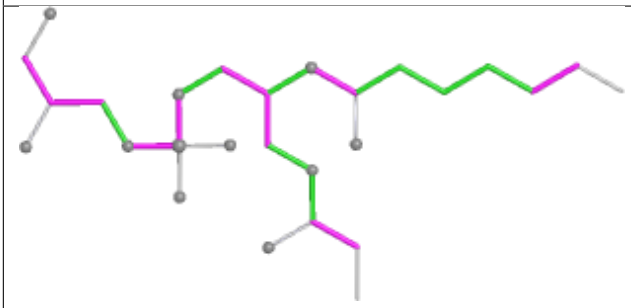
Ligand LHG A 843



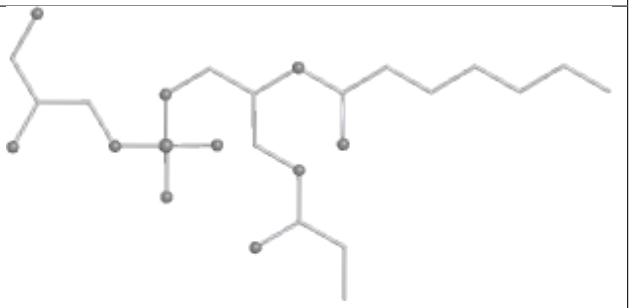
Bond lengths



Bond angles

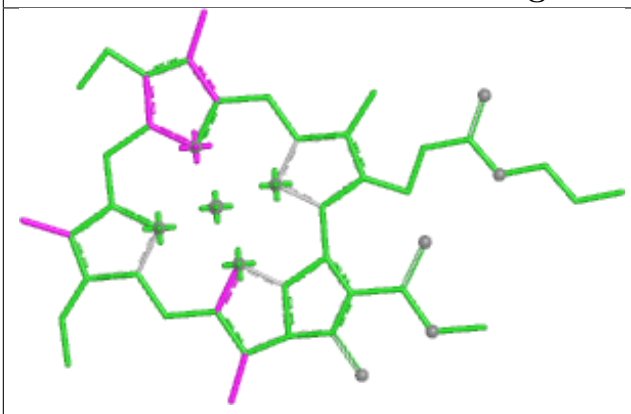


Torsions

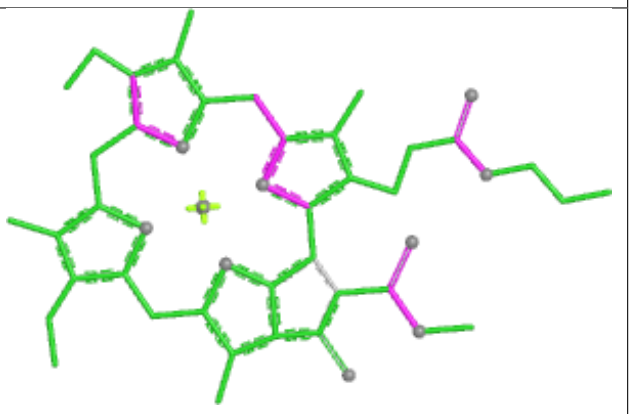


Rings

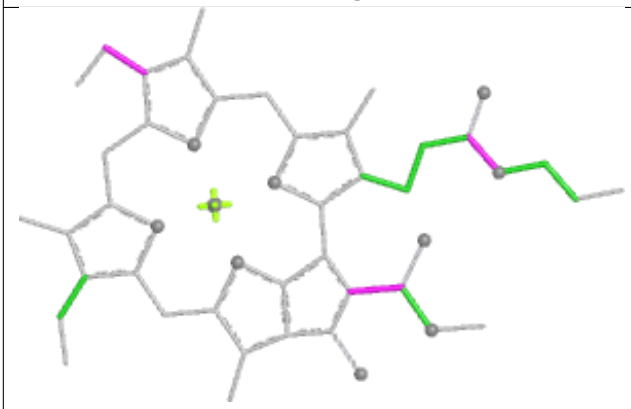
Ligand CLA 9 303



Bond lengths



Bond angles



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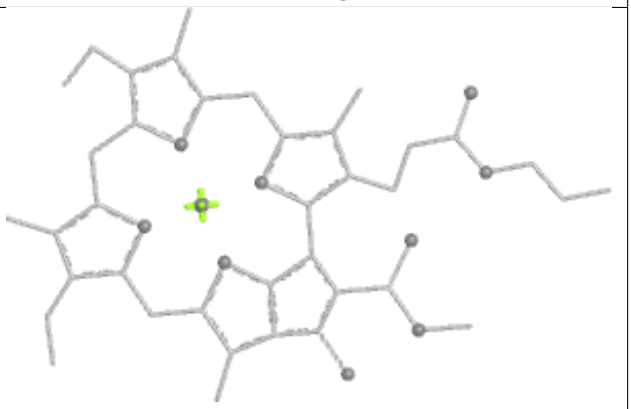
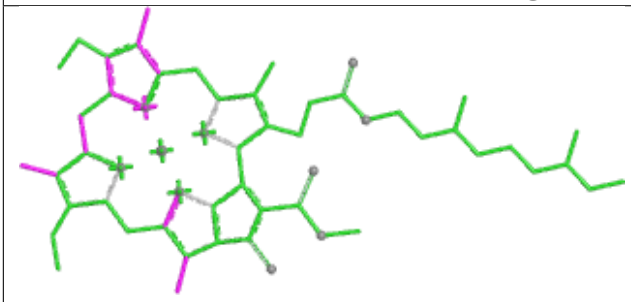
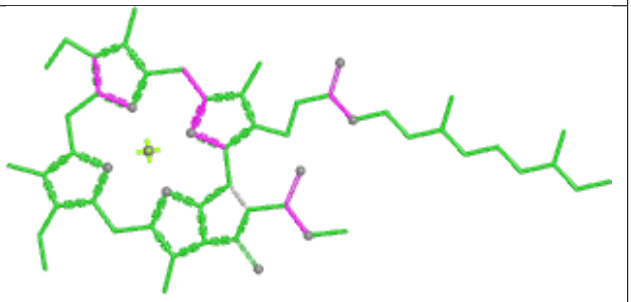


Rings

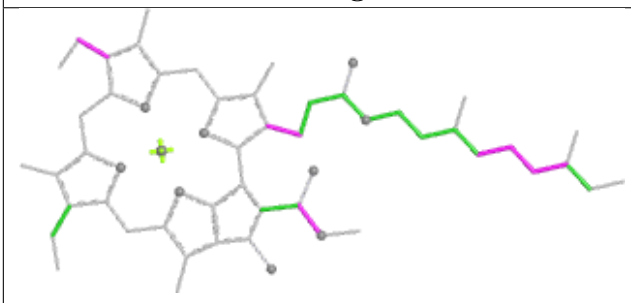
Ligand CLA B 820



Bond lengths



Bond angles



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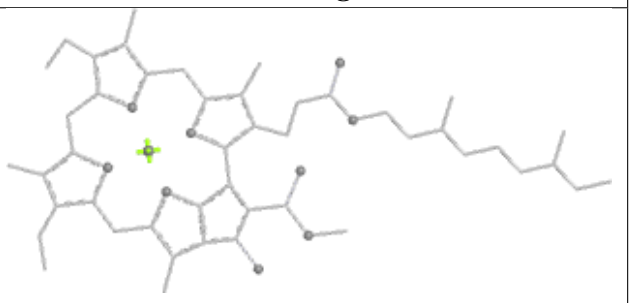
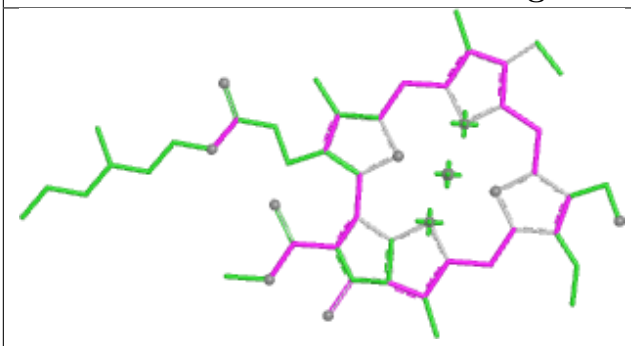
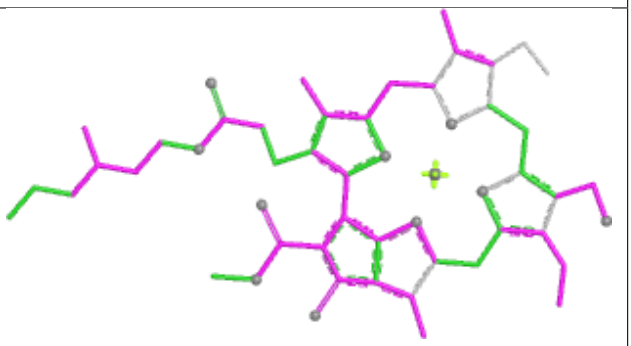


Rings

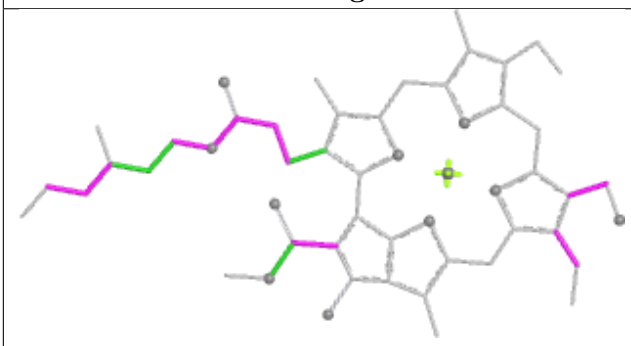
Ligand CHL 4 302



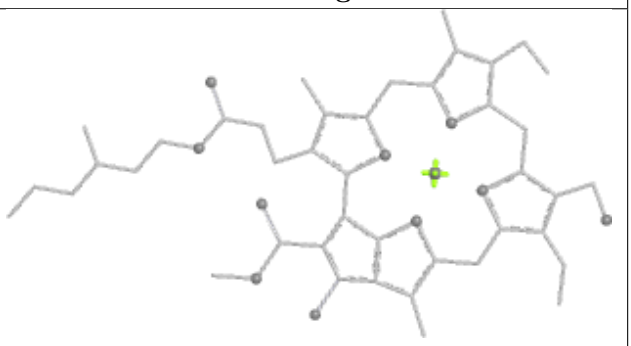
Bond lengths



Bond angles

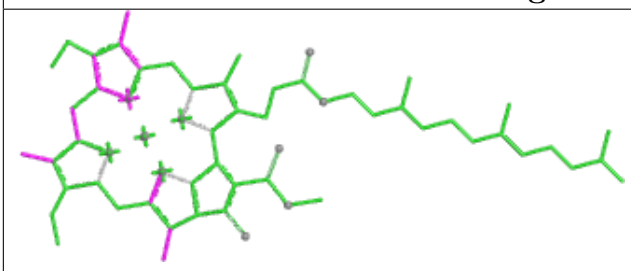


Torsions

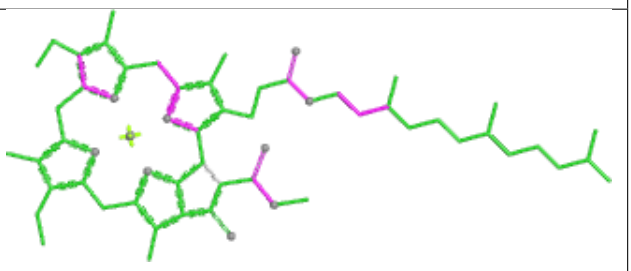


Rings

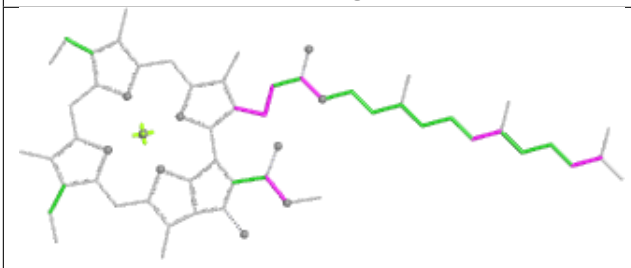
Ligand CLA 7 317



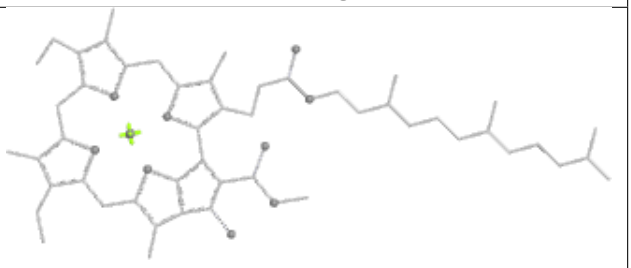
Bond lengths



Bond angles

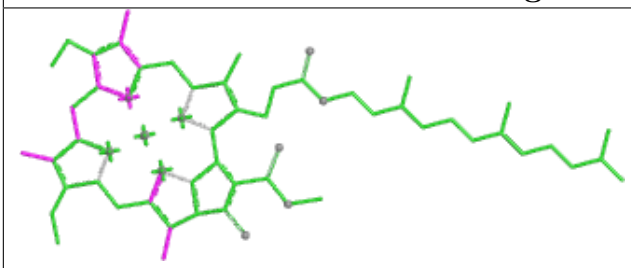


Torsions

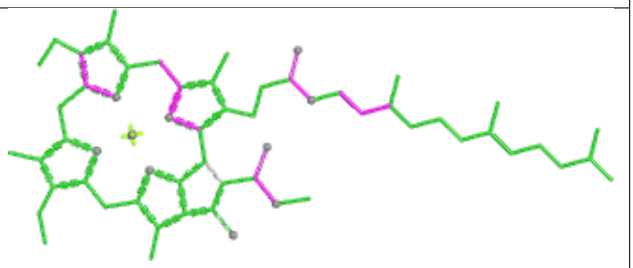


Rings

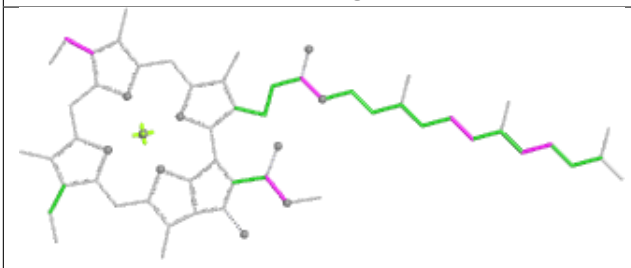
Ligand CLA B 824



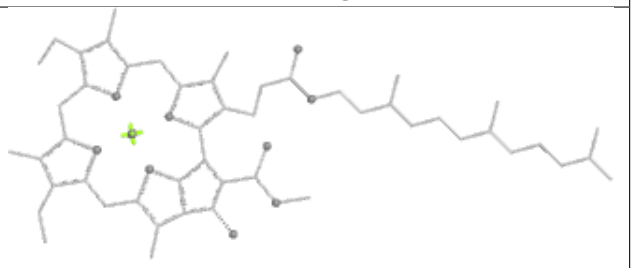
Bond lengths



Bond angles

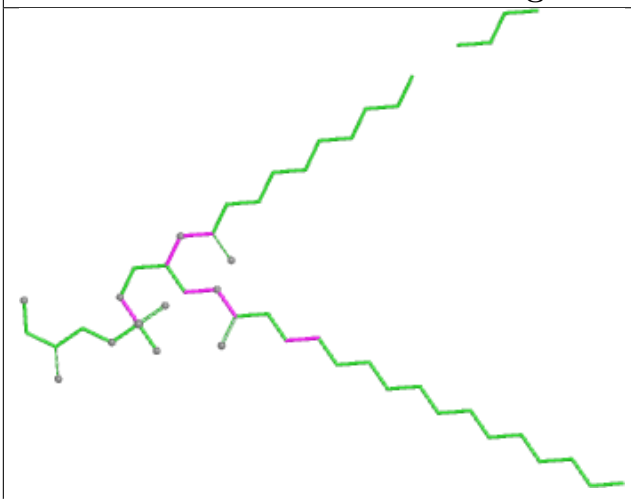


Torsions

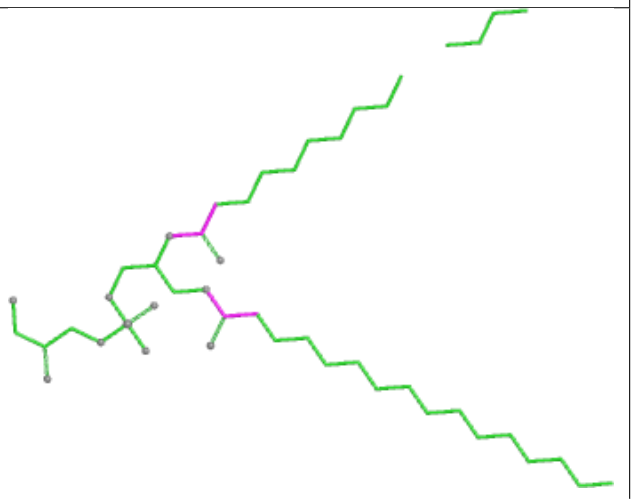


Rings

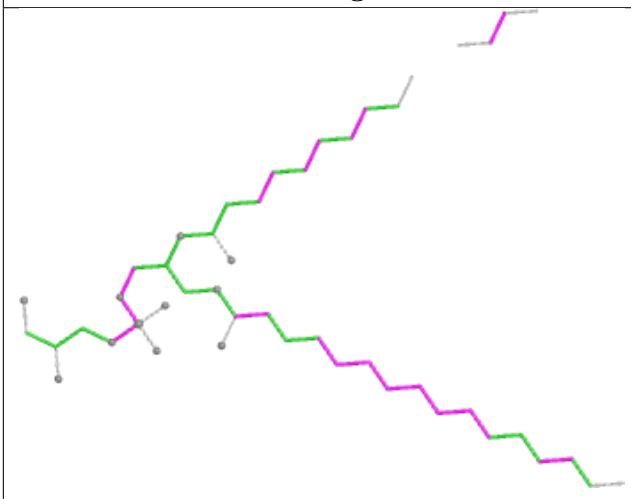
Ligand LHG 9 316



Bond lengths



Bond angles



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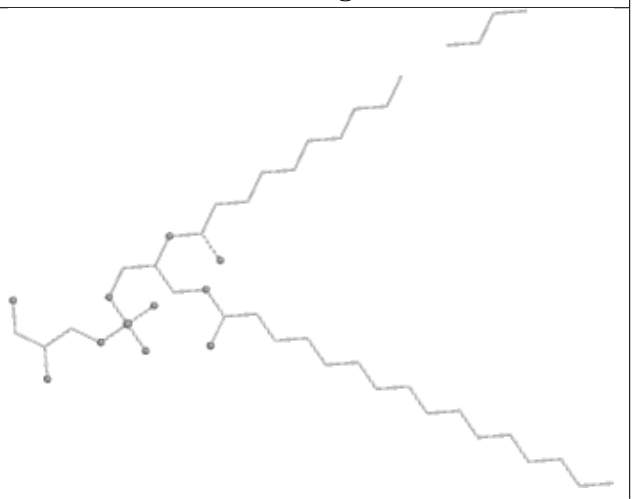
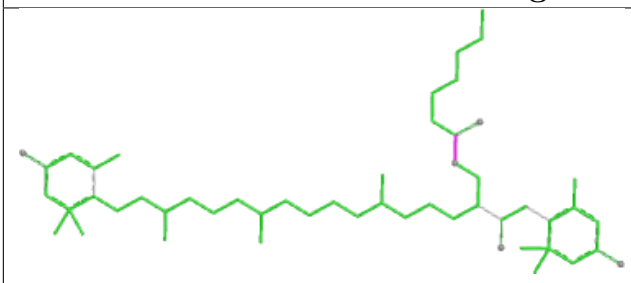


Rings

Ligand 0UR 0 315



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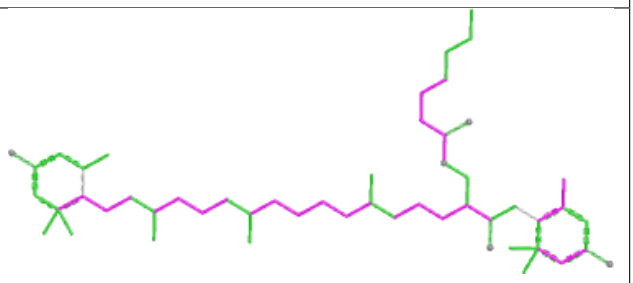
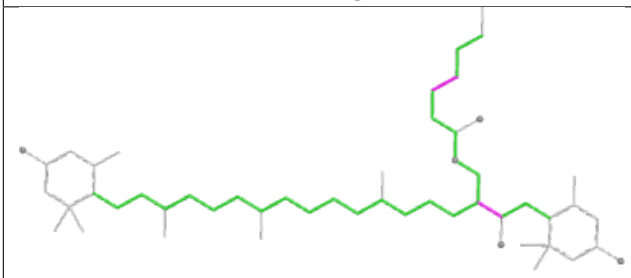
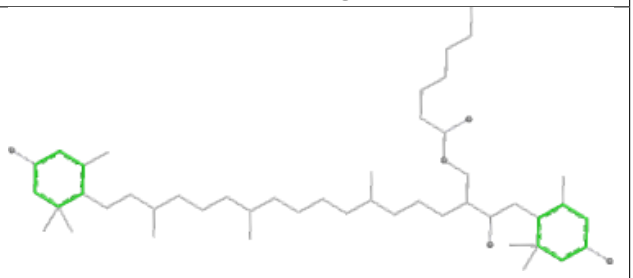


Bond angles

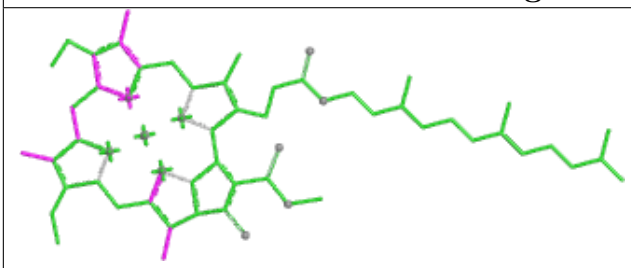


Torsions



Rings

Ligand CLA B 836



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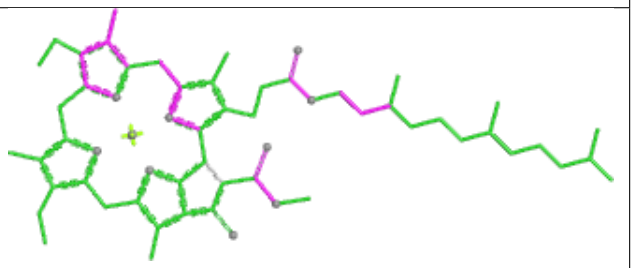
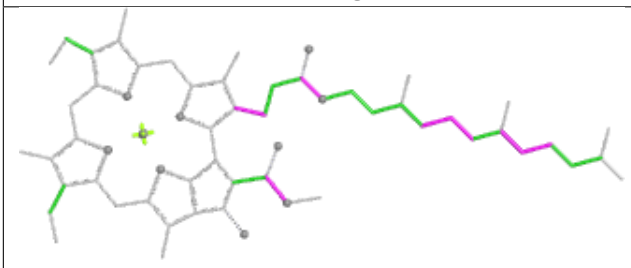


Bond angles



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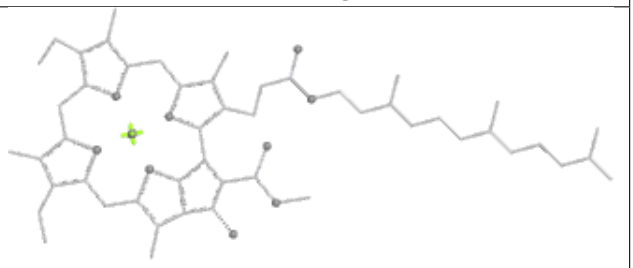
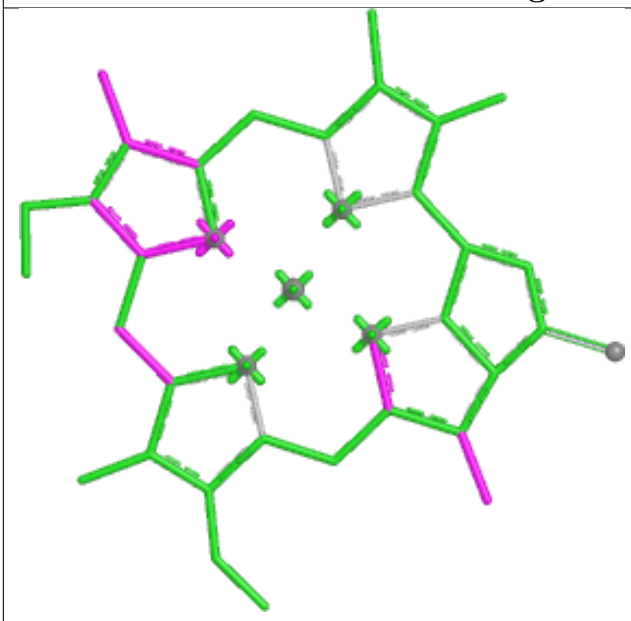
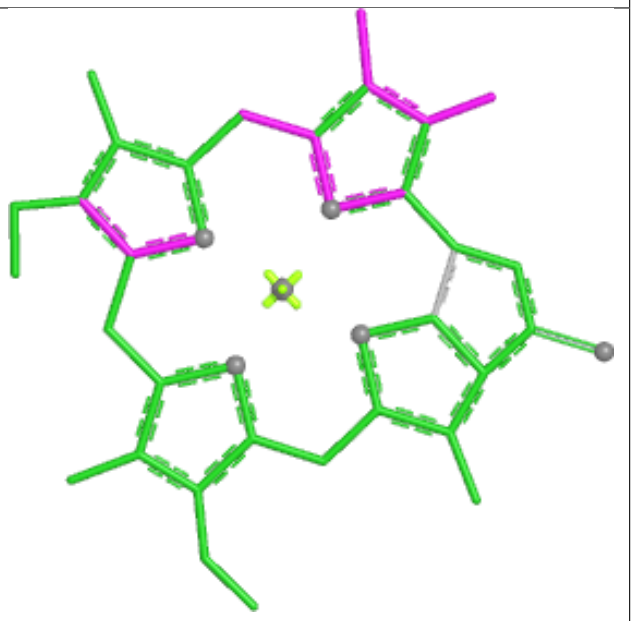


Rings

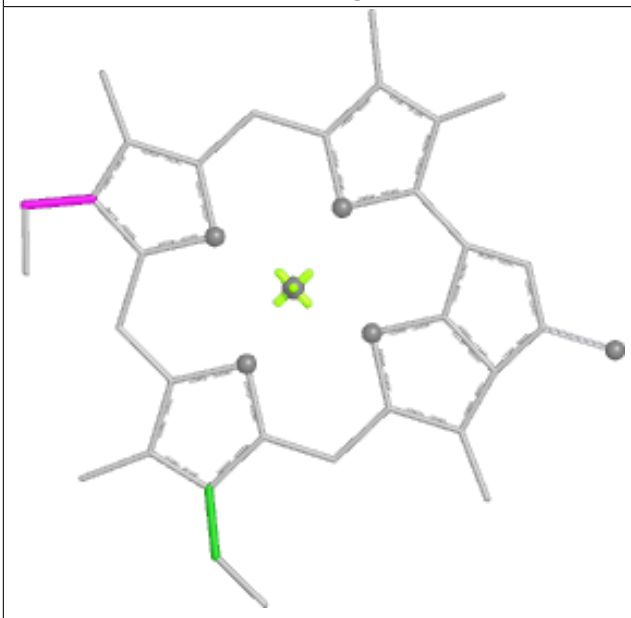
Ligand CLA 7 310



Bond lengths



Bond angles



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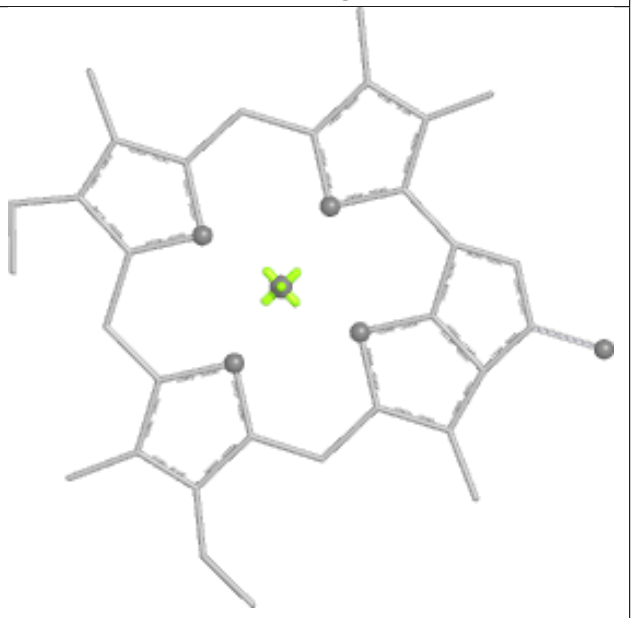
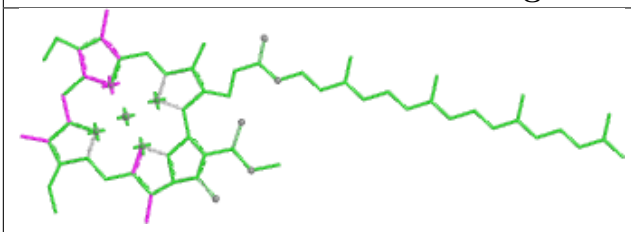
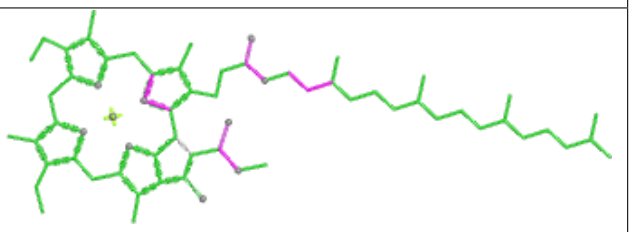
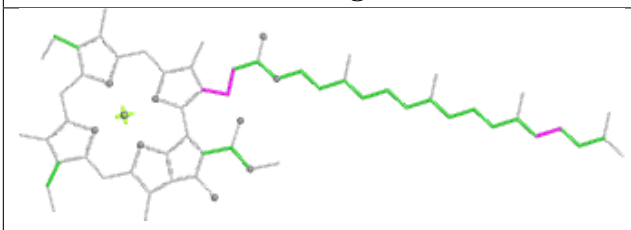
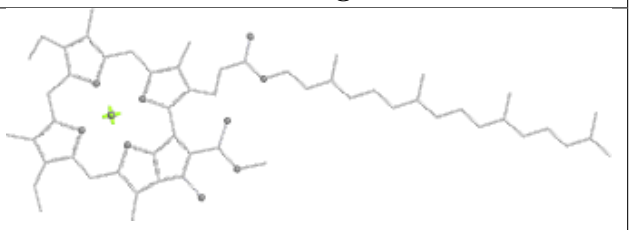
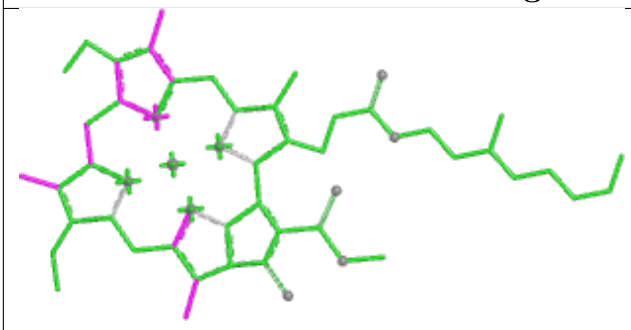
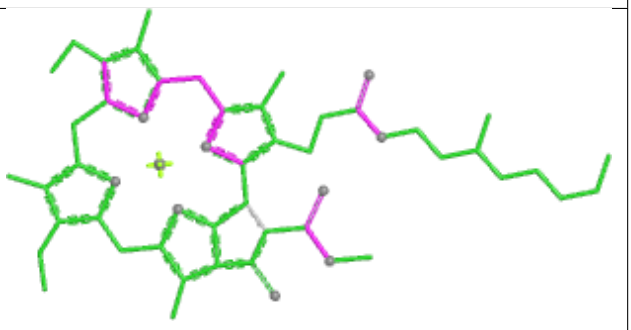
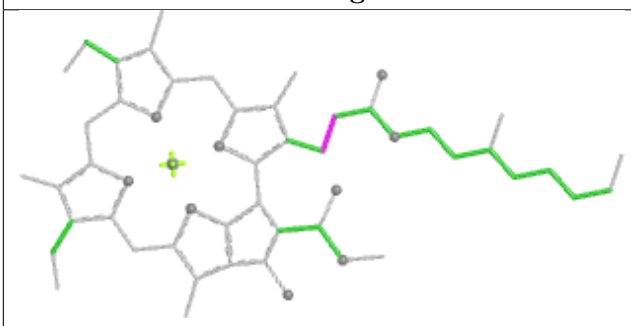
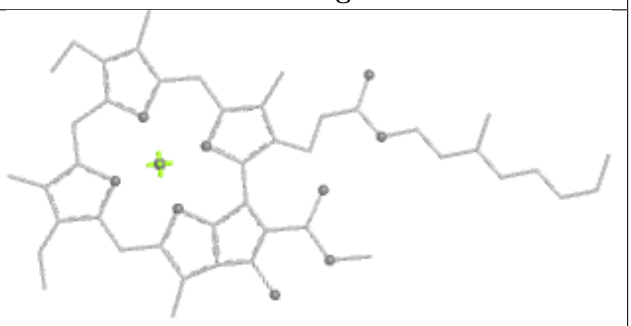
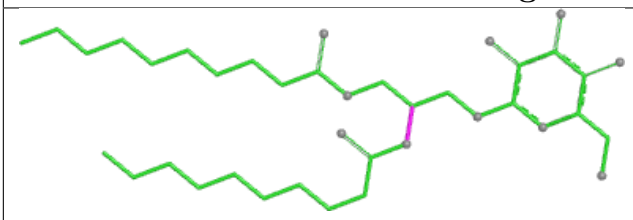


Rings

Ligand CLA A 801	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA A 811	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand LMG O 210



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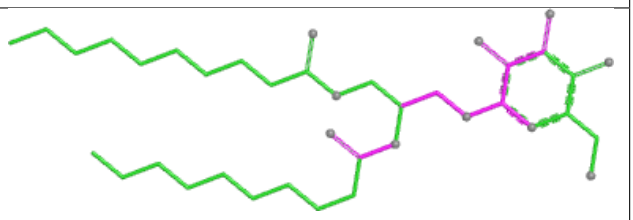
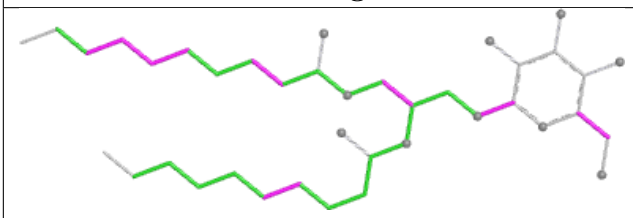
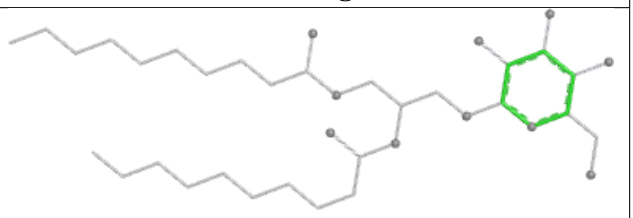


Bond angles

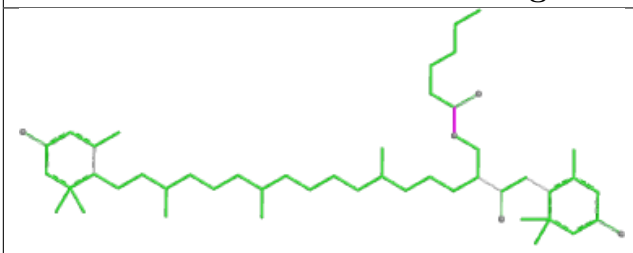


Torsions

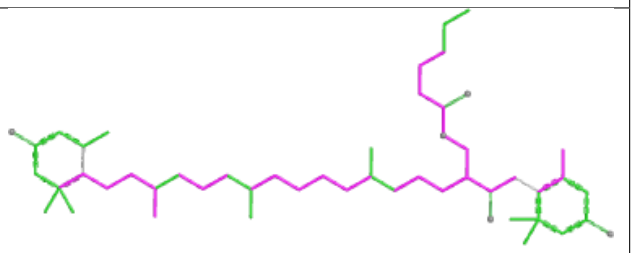


Rings

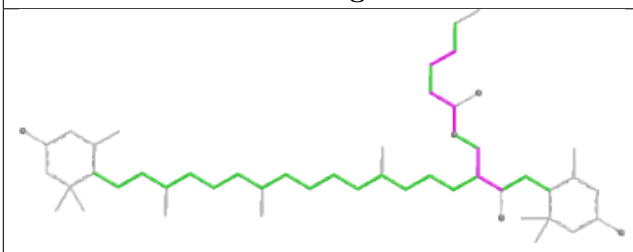
Ligand 0UR 7 320



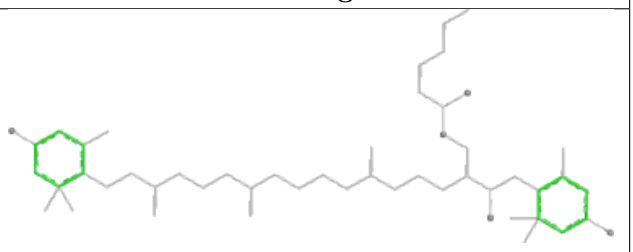
Bond lengths



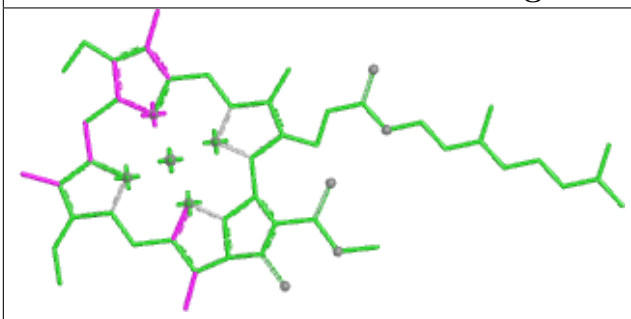
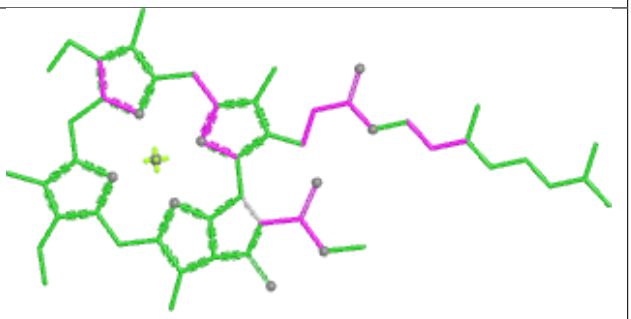
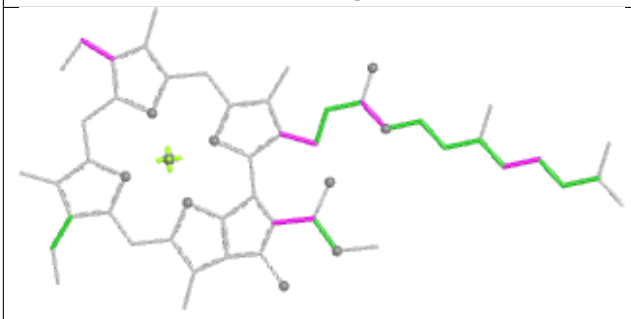
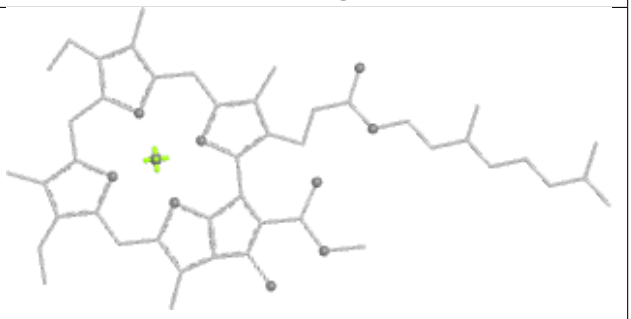
Bond angles

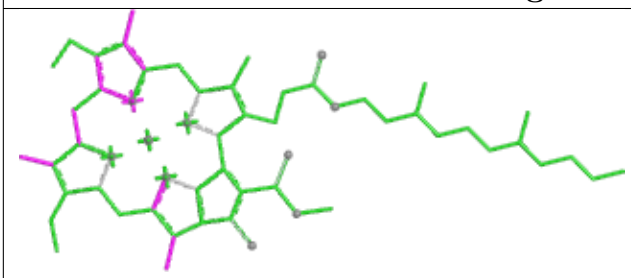
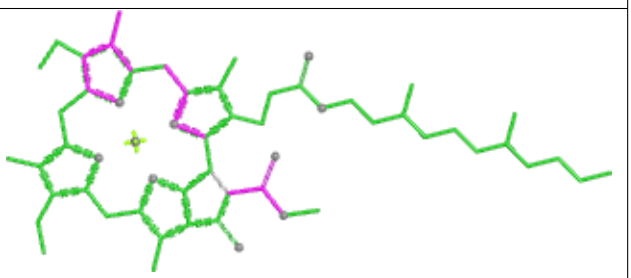
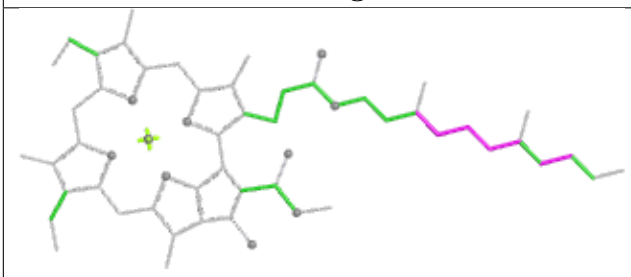
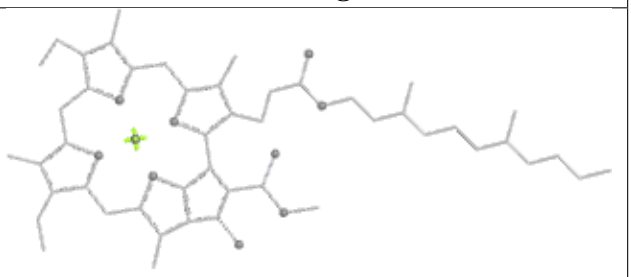


Torsions



Rings

Ligand CLA B 833	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA L 201	
 Bond lengths	 Bond angles
 Torsions	 Rings

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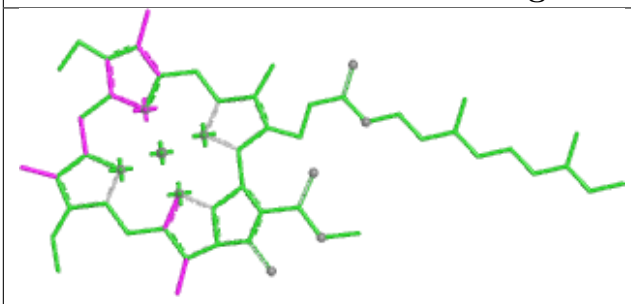
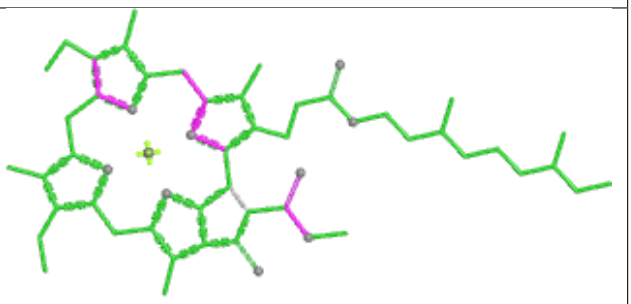
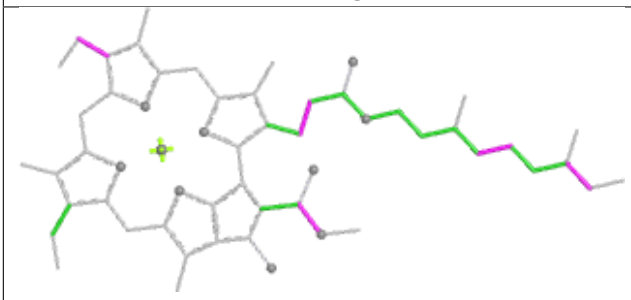
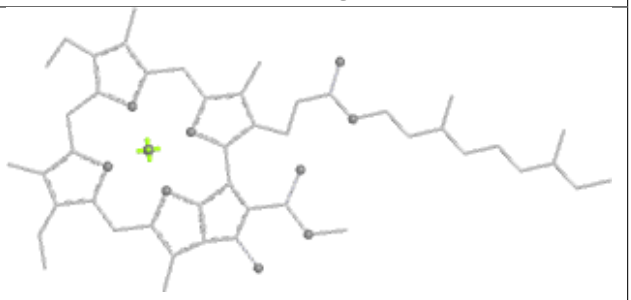
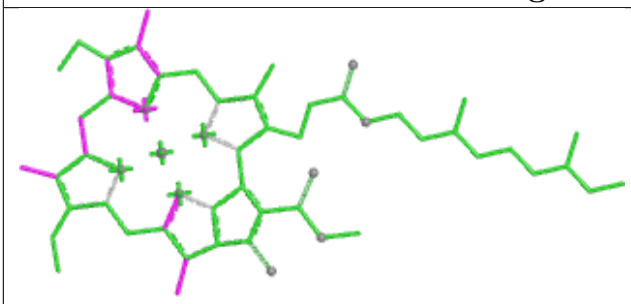
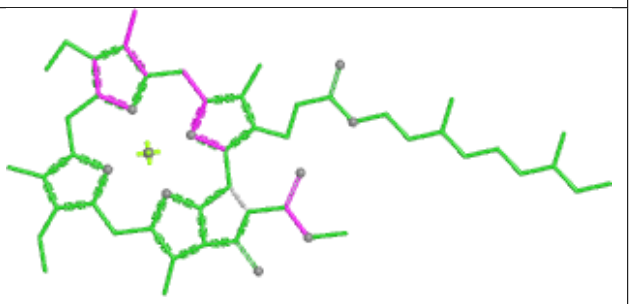
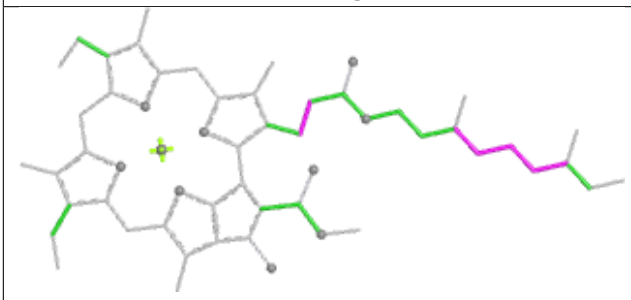
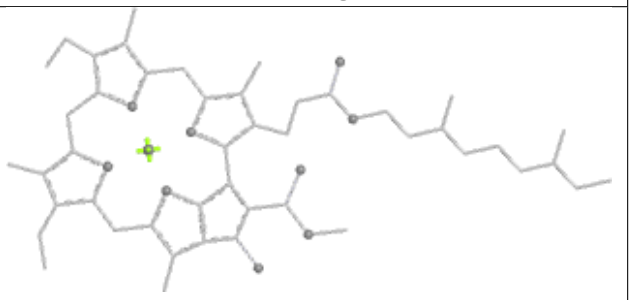
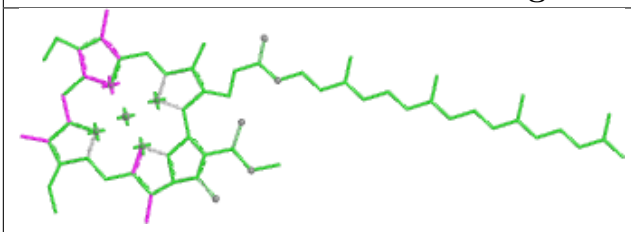
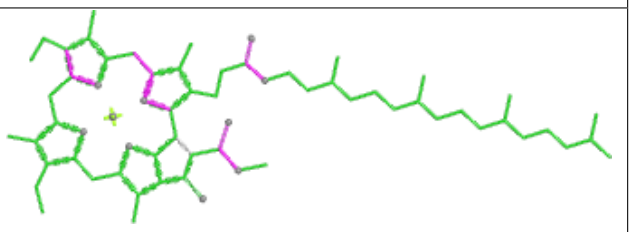
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA 9 311	
	
Bond lengths	Bond angles
	
Torsions	Rings

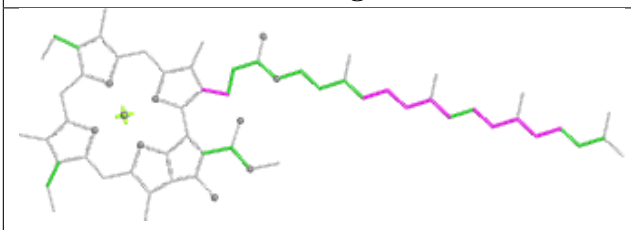
Ligand CLA 9 307



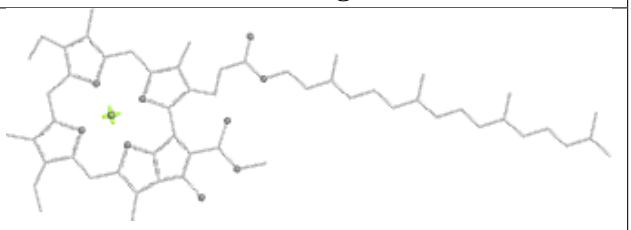
Bond lengths



Bond angles

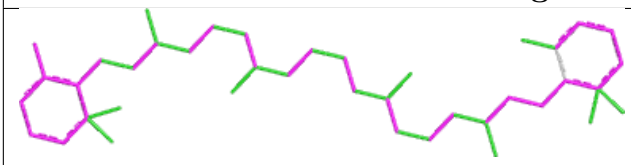


Torsions

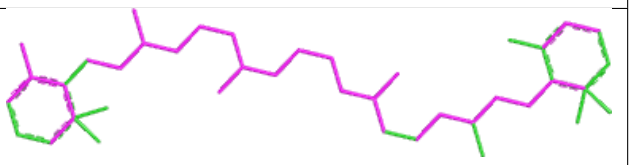


Rings

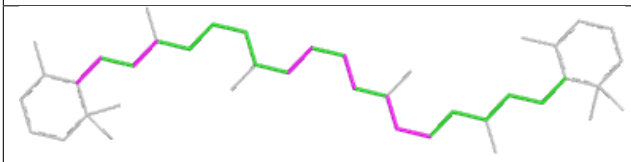
Ligand 8CT 6 319



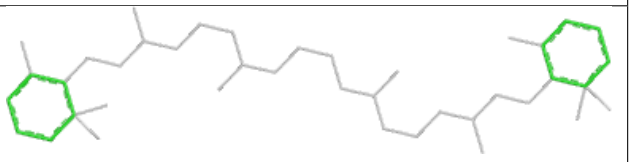
Bond lengths



Bond angles

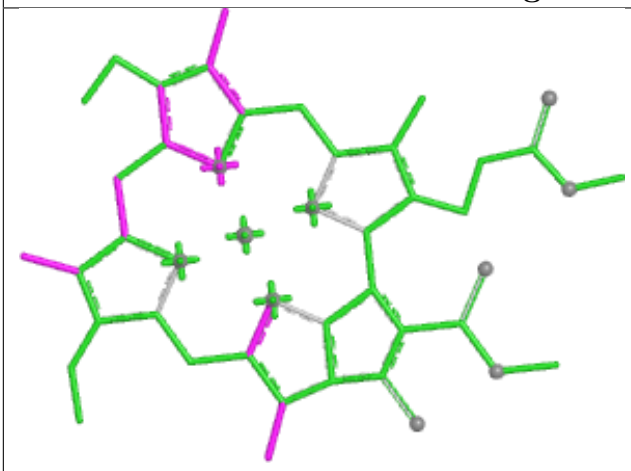


Torsions



Rings

Ligand CLA H 201



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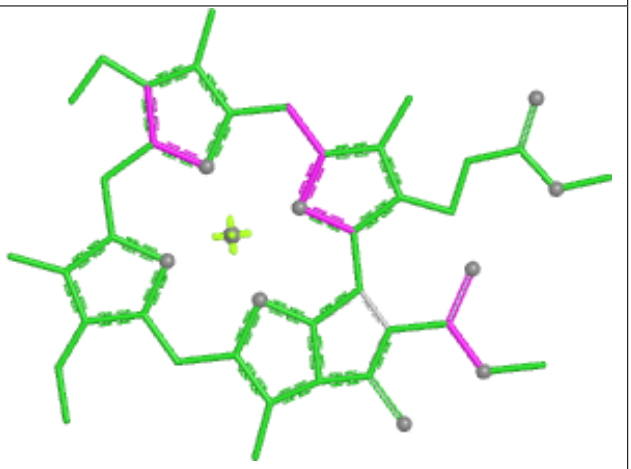

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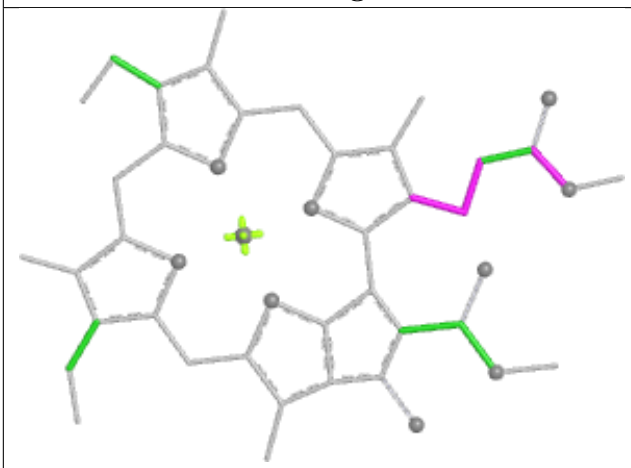

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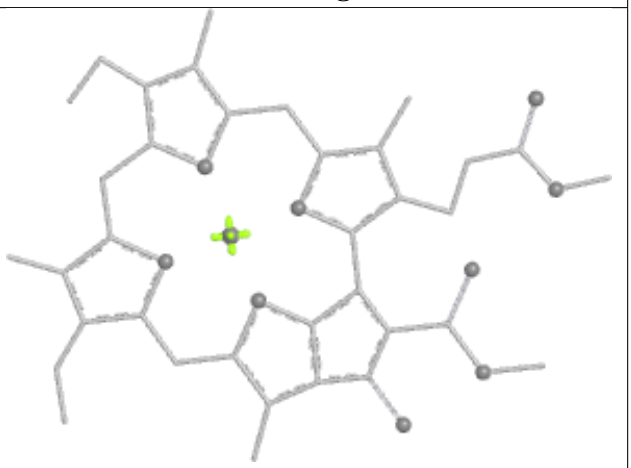
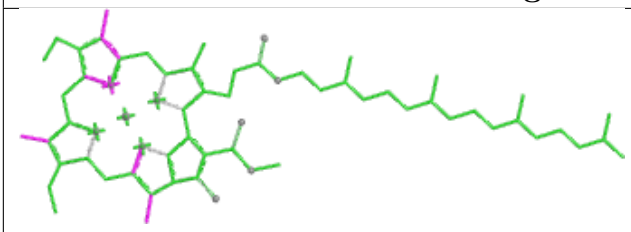


Rings

Ligand CLA A 817



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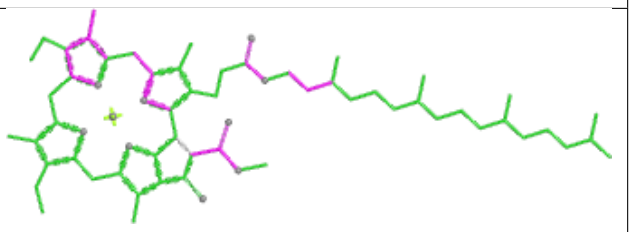

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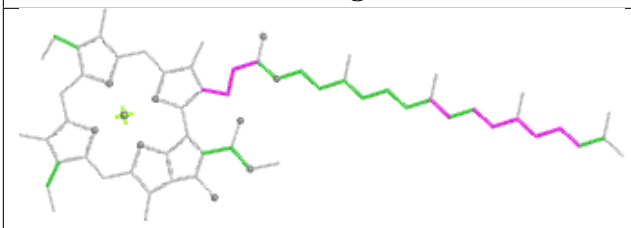

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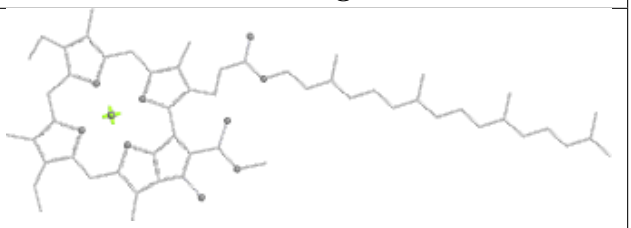
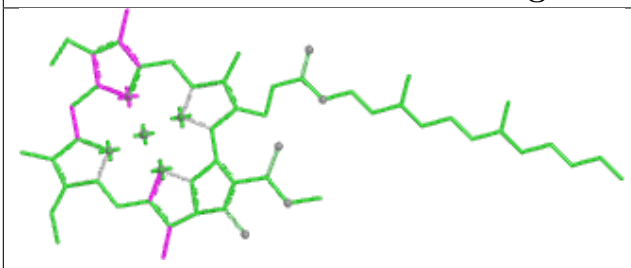


Rings

Ligand CLA 5 302



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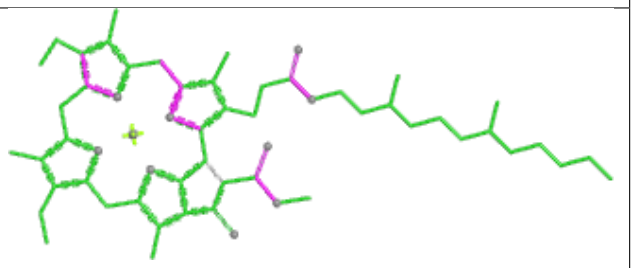
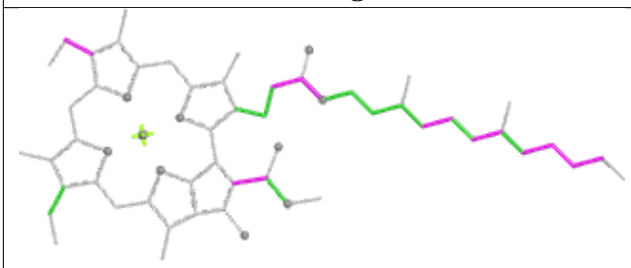


Bond angles



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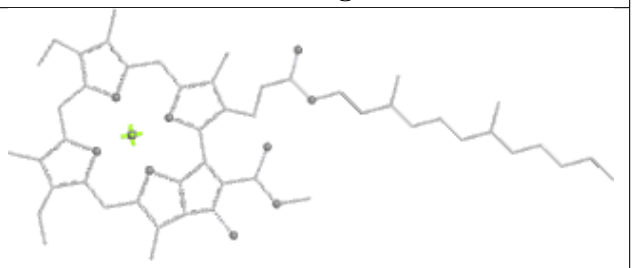
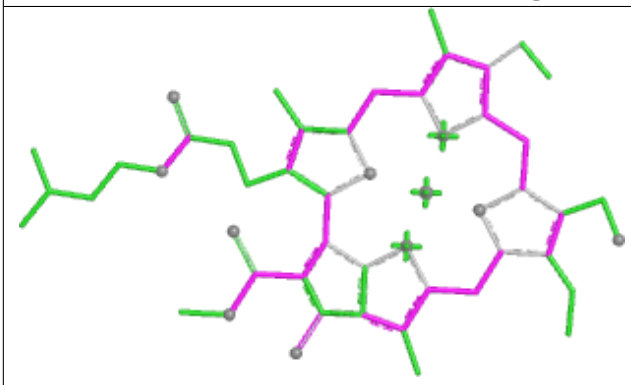


Rings

Ligand CHL 9 305



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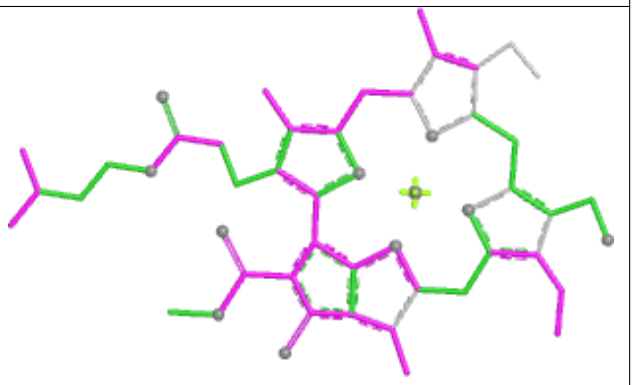
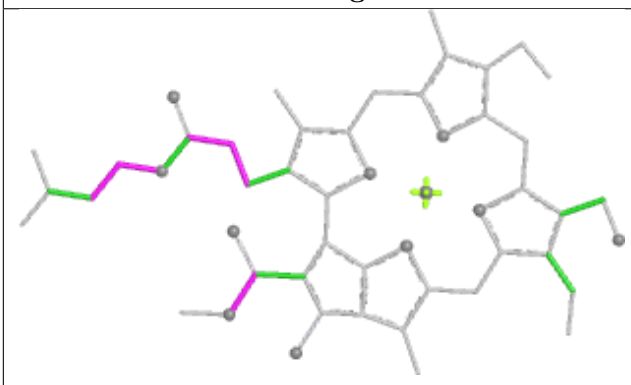


Bond angles



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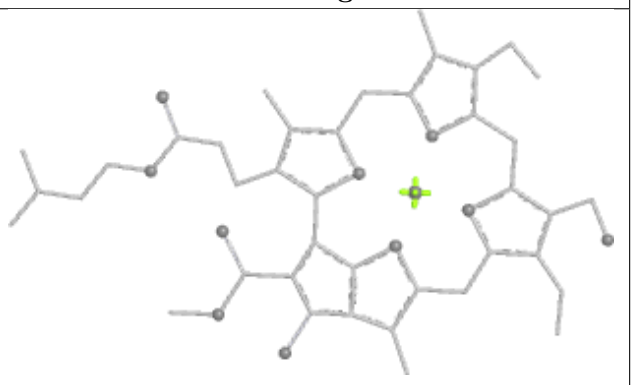
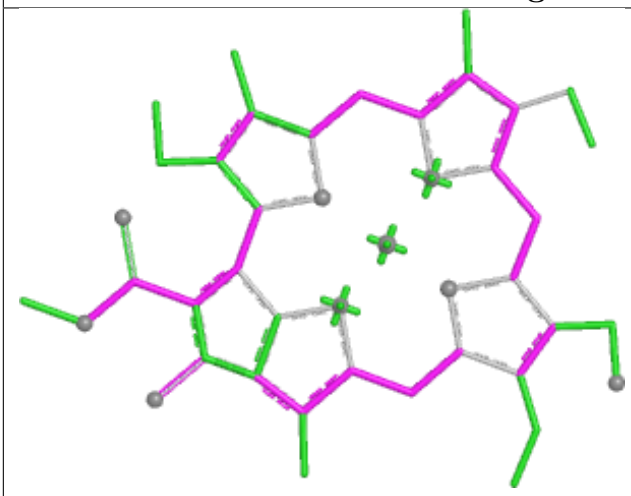


Rings

Ligand CHL 6 305



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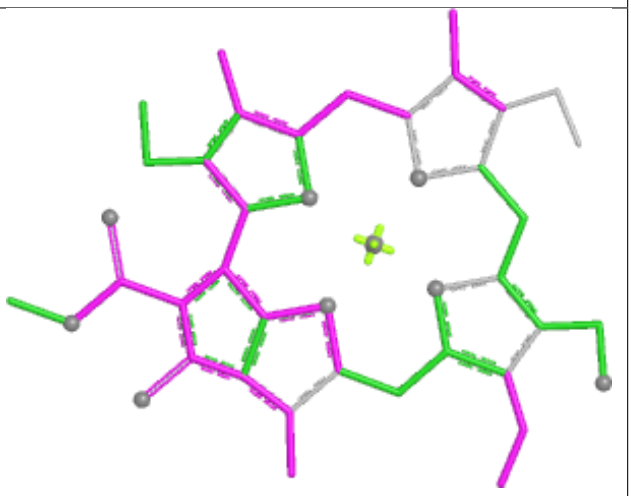

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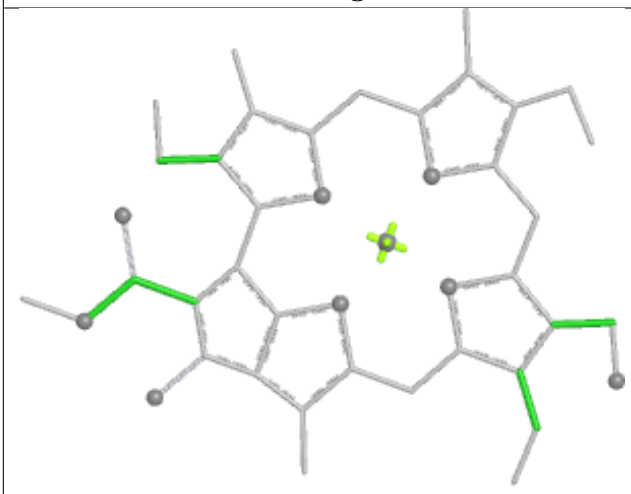

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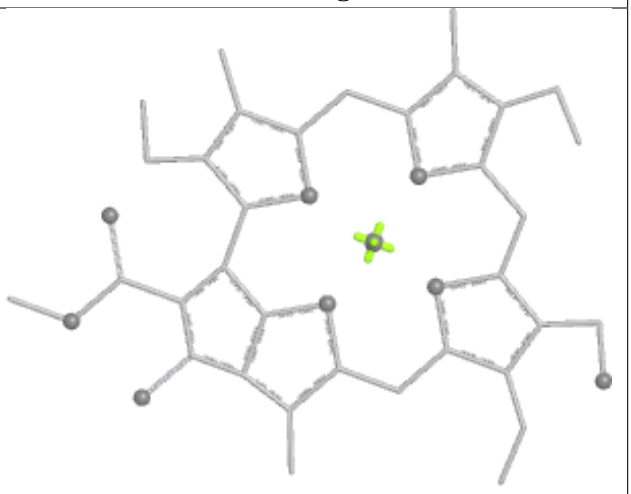
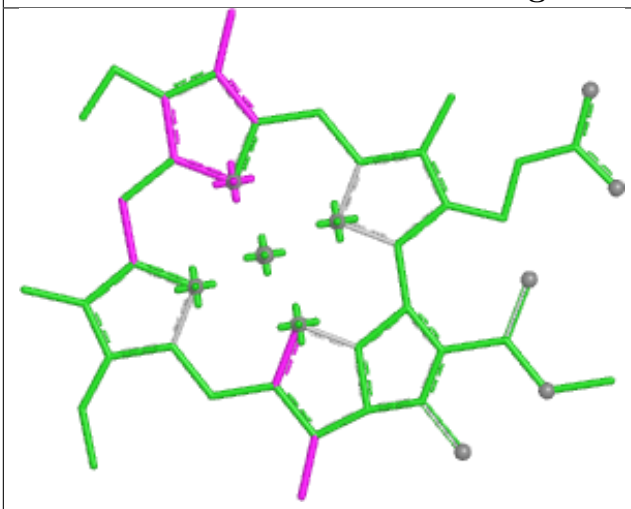


Rings

Ligand CLA 0 313



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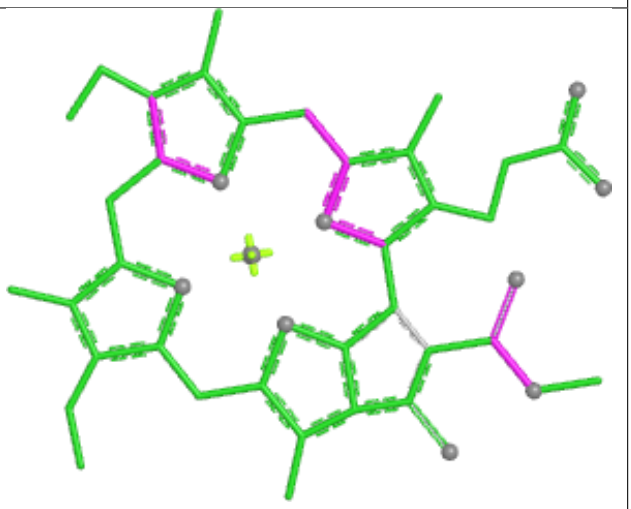

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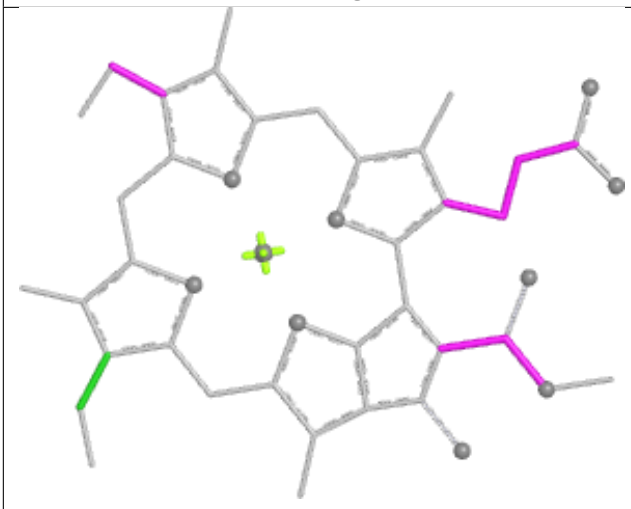
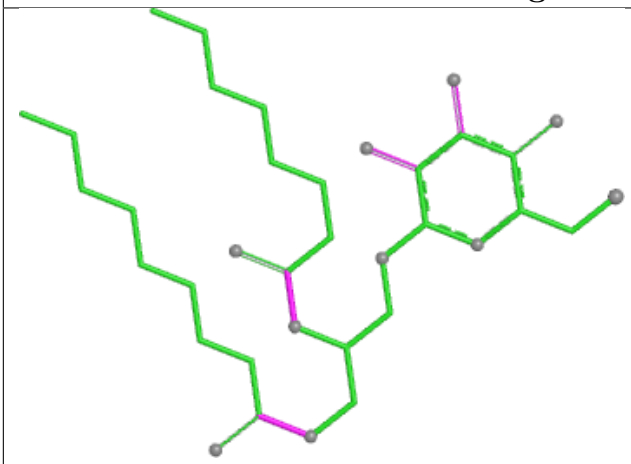


Torsions

Rings

Ligand SQD 0 318



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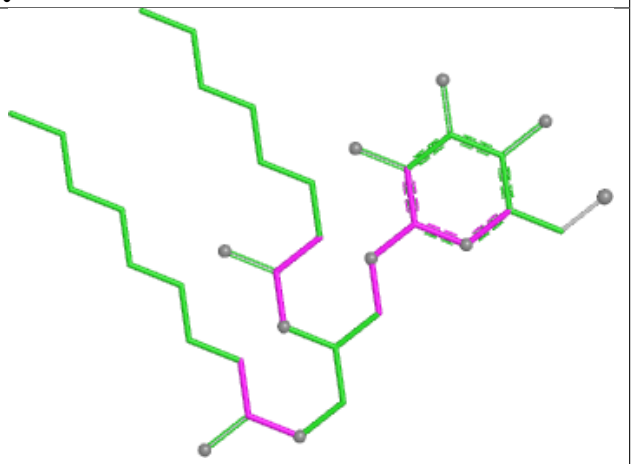

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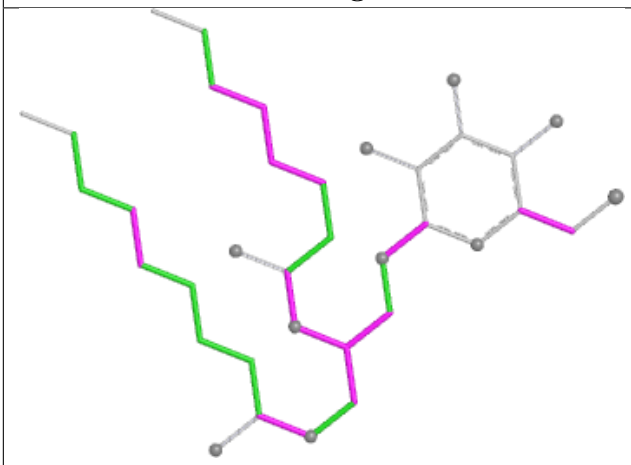

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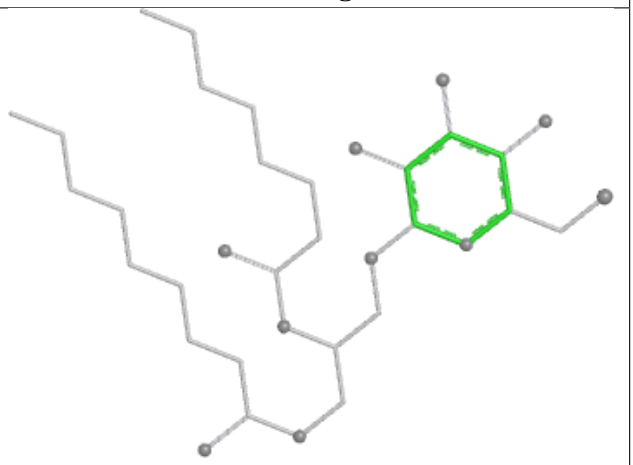
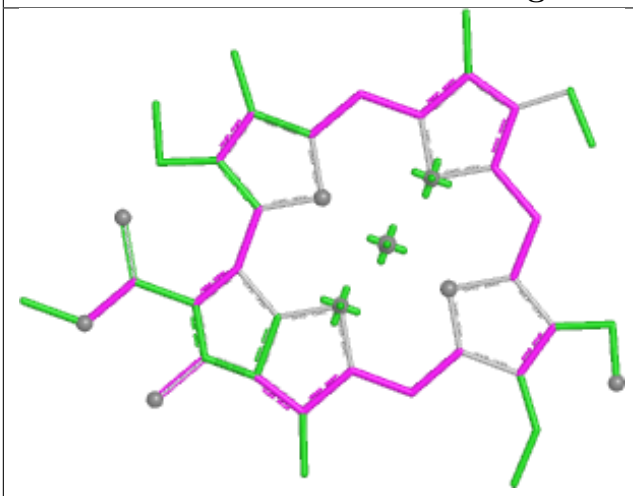


Rings

Ligand CHL 8 316



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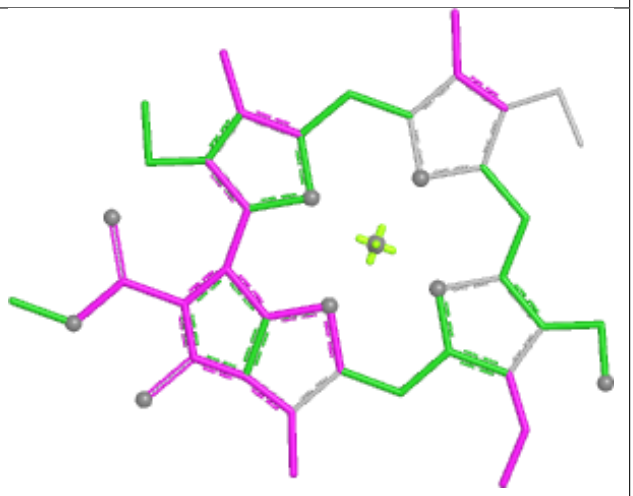
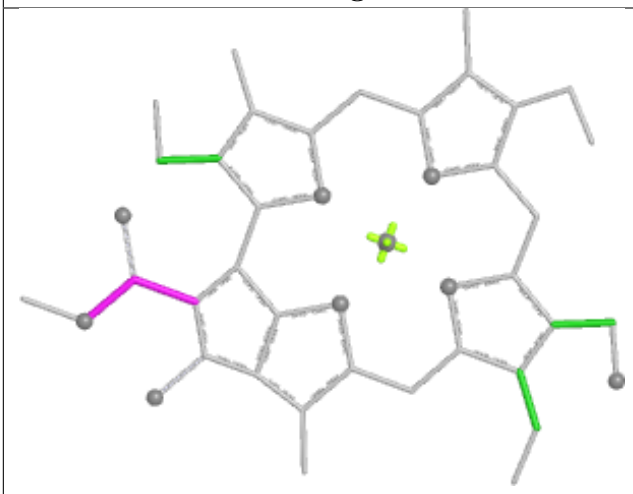


Bond angles



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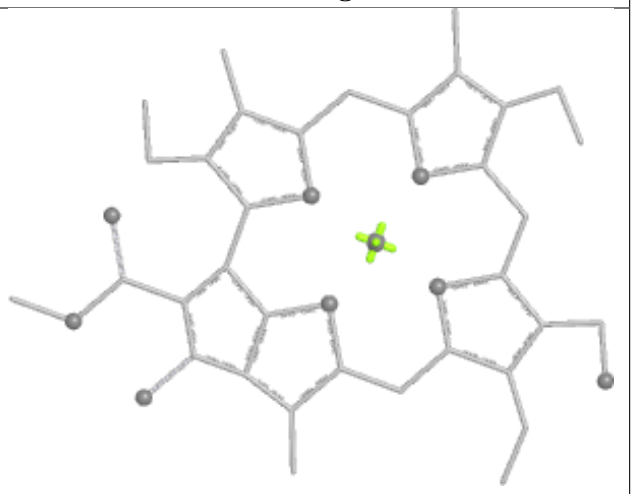
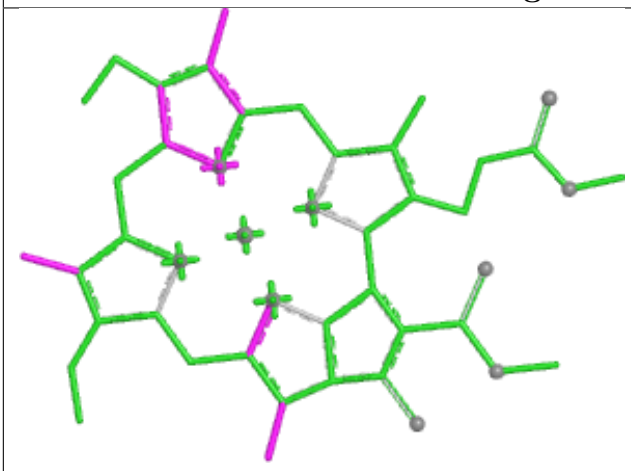


Rings

Ligand CLA A 833



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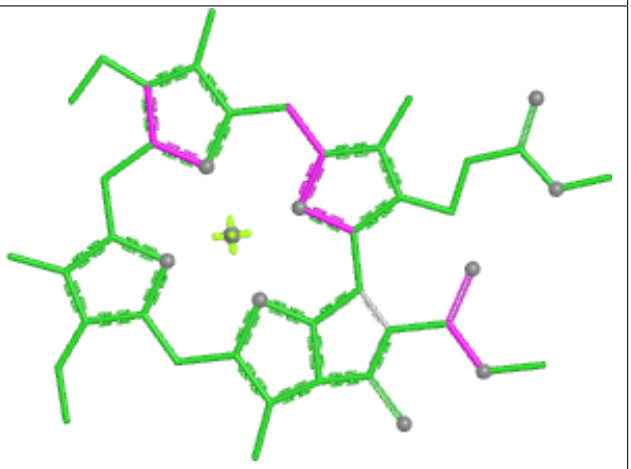
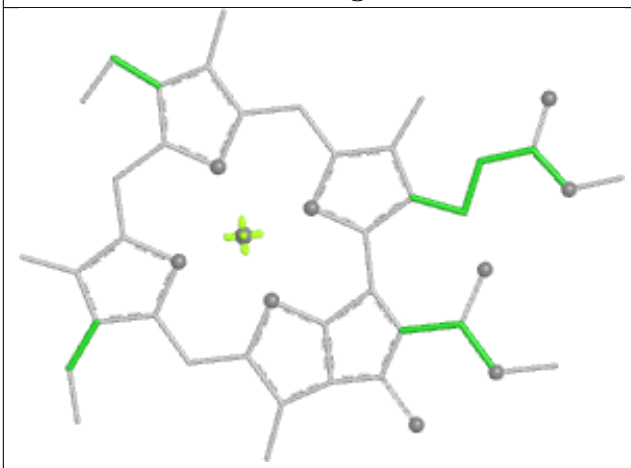
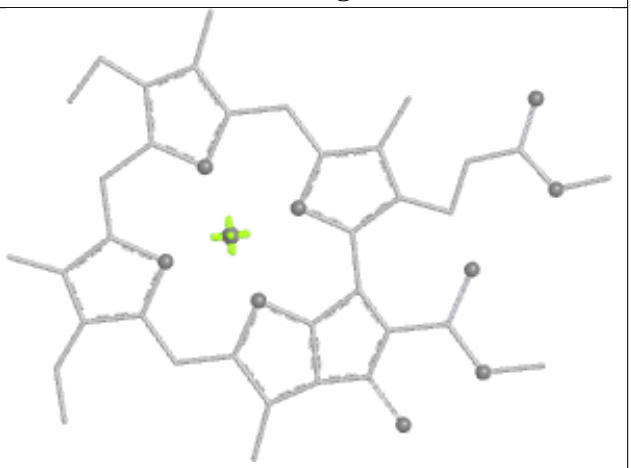


Bond angles

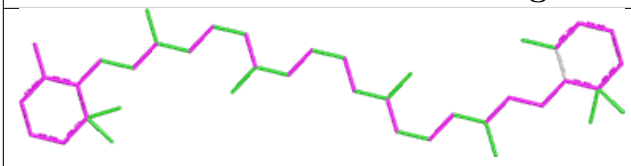


Torsions



Rings

Ligand 8CT L 205



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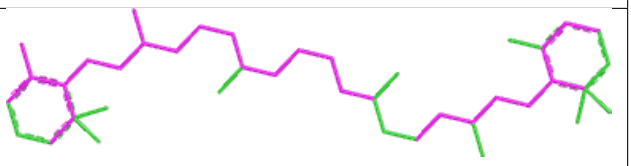

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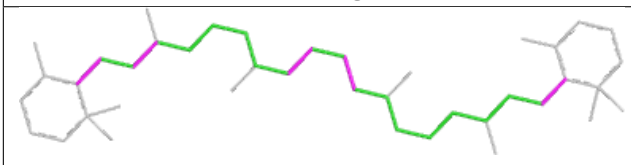

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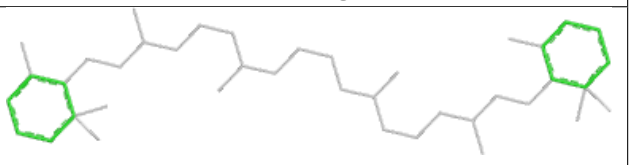
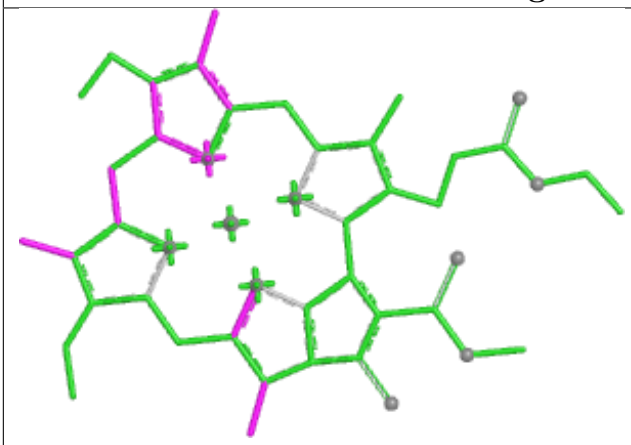


Rings

Ligand CLA 7 314



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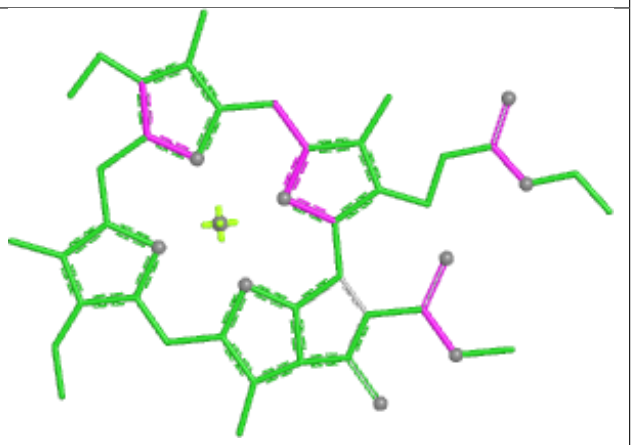
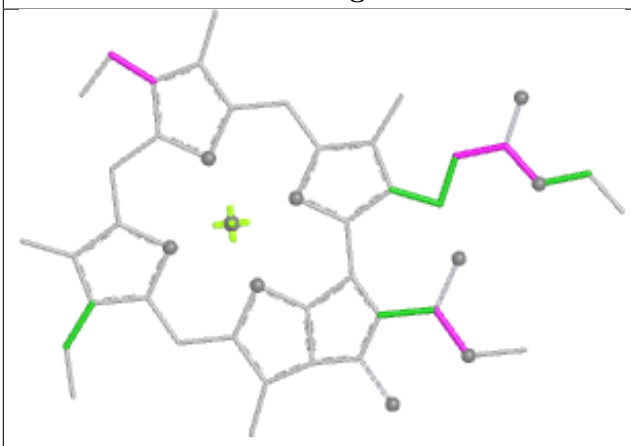
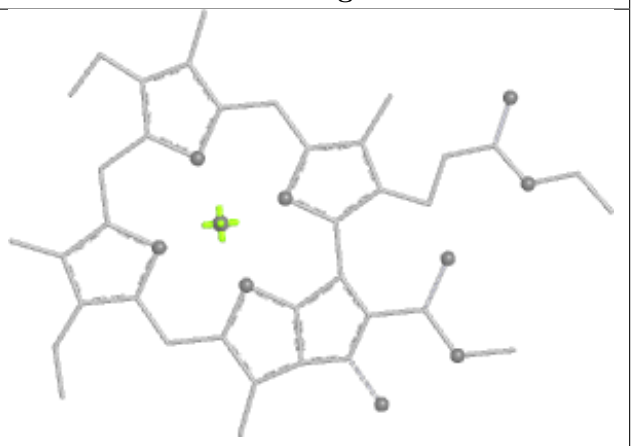


Bond angles

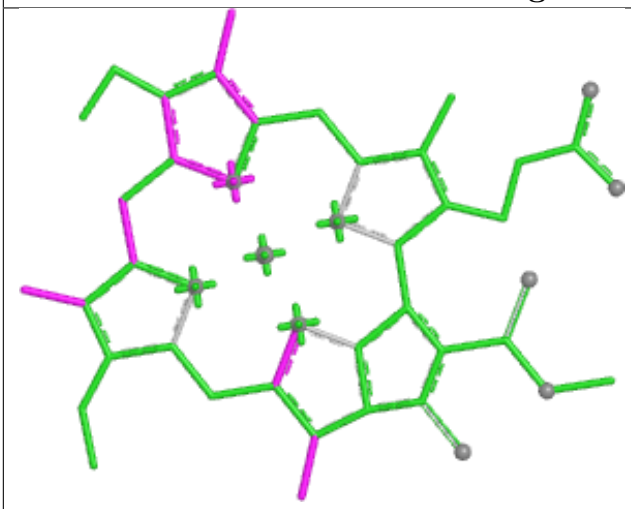


Torsions



Rings

Ligand CLA 3 313



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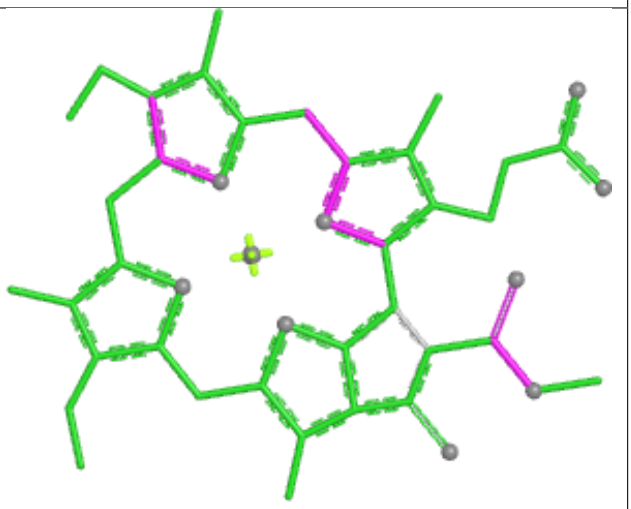
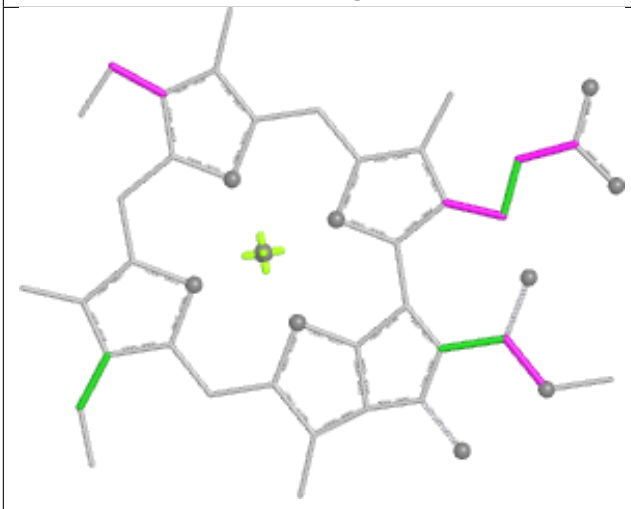


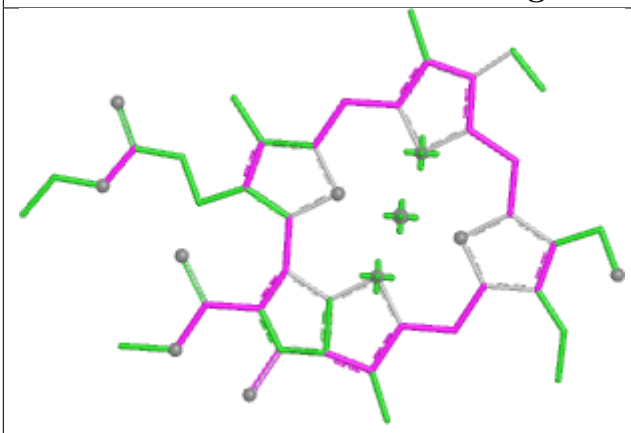
Bond angles



Torsions

Rings

Ligand CHL 1 305



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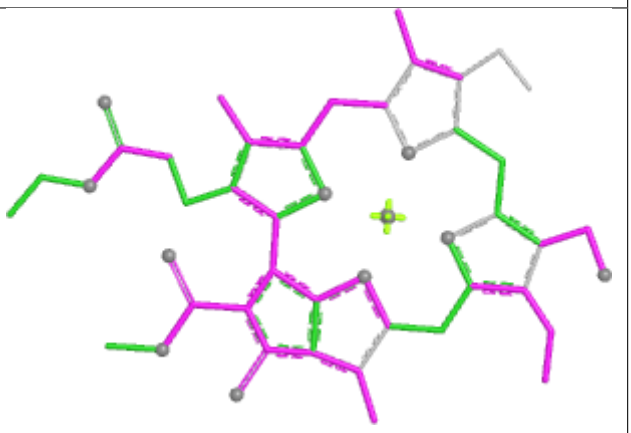
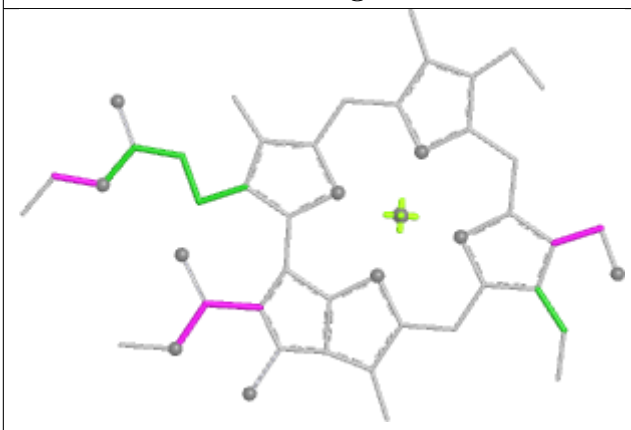


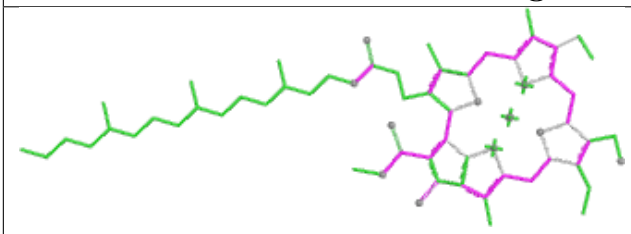
Bond angles



Torsions

Rings

Ligand CHL 2 301



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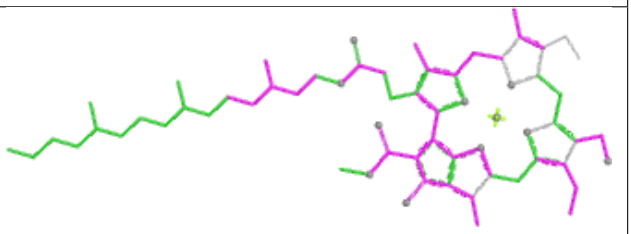
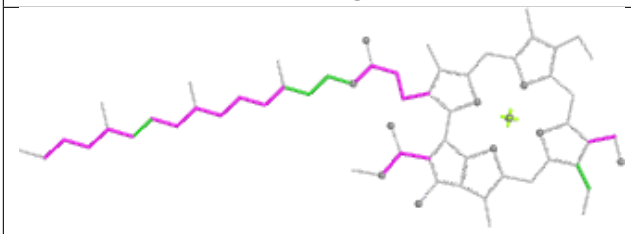
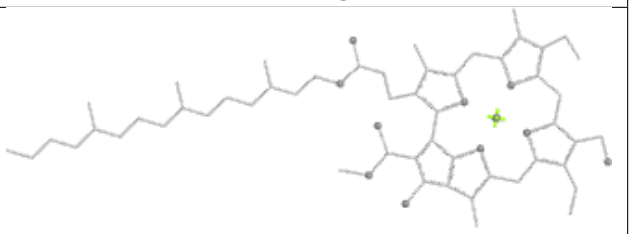


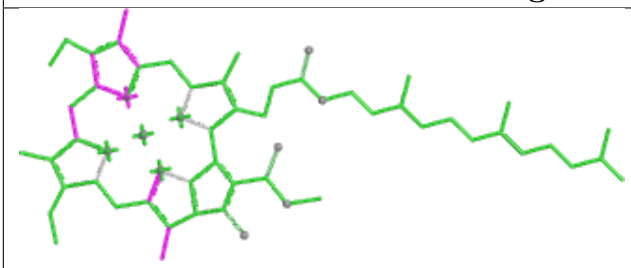
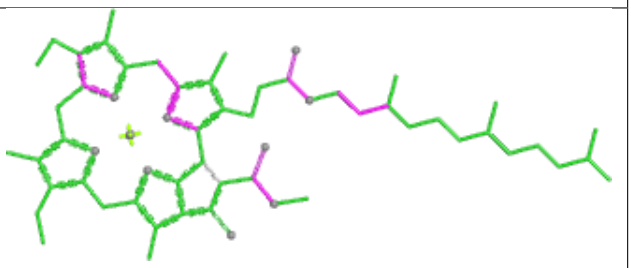
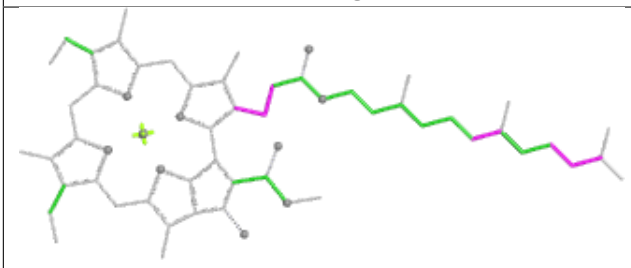
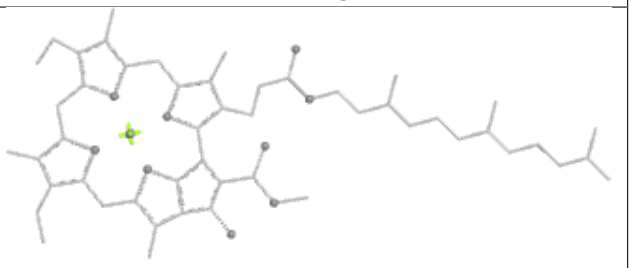
Bond angles

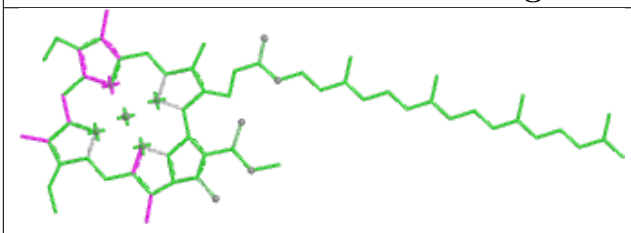
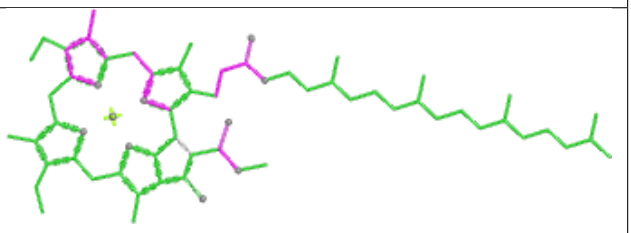
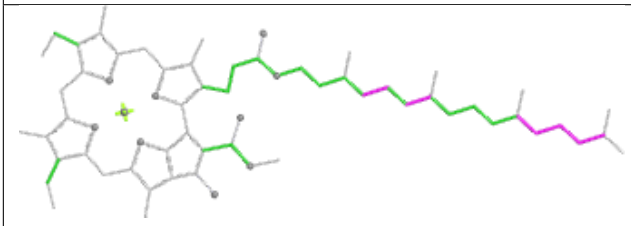
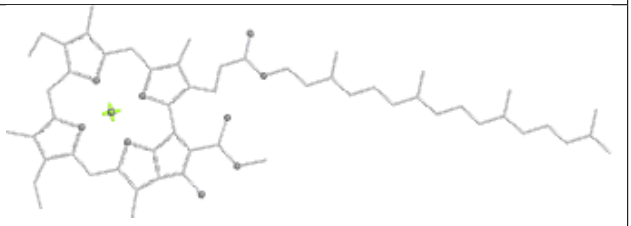


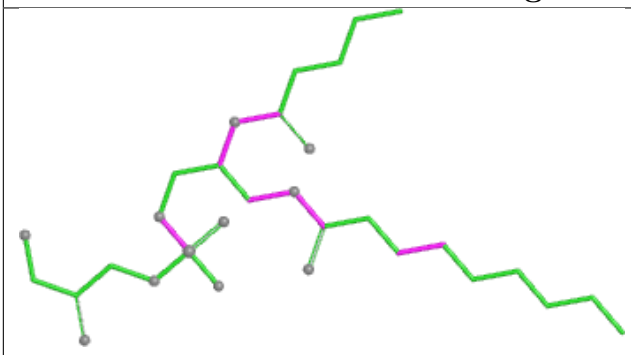
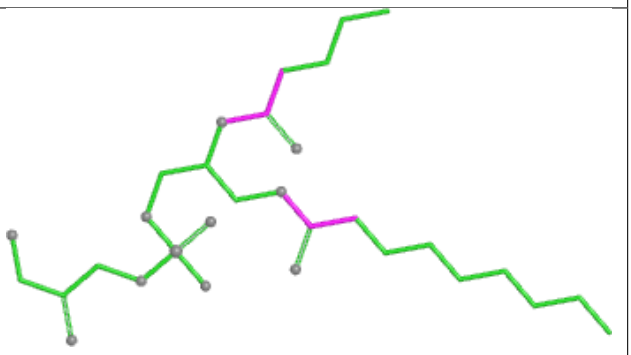
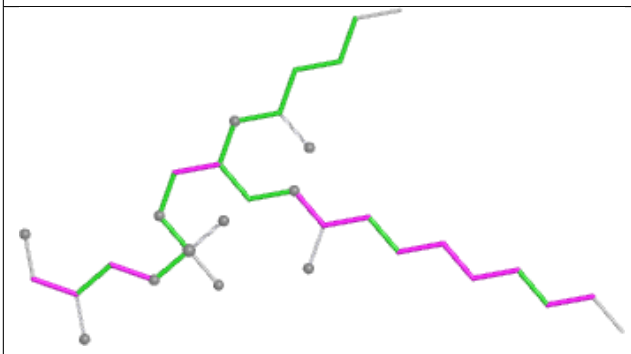
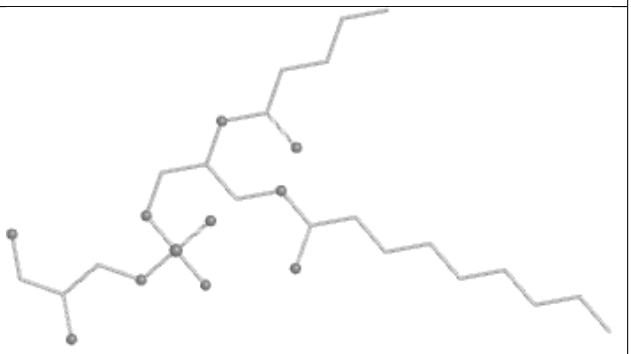
Torsions

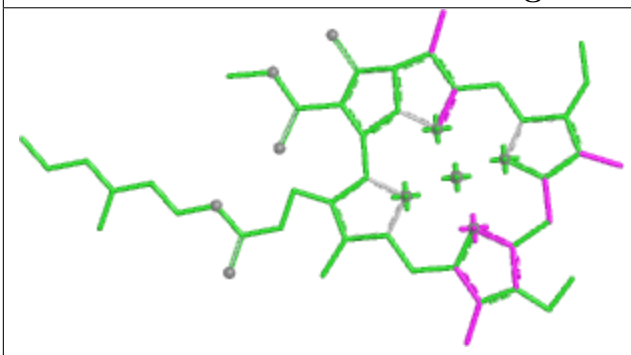
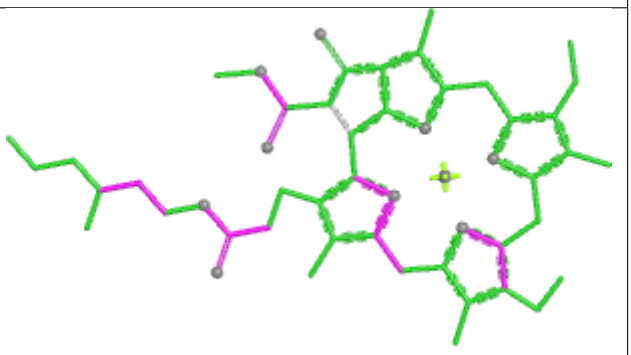
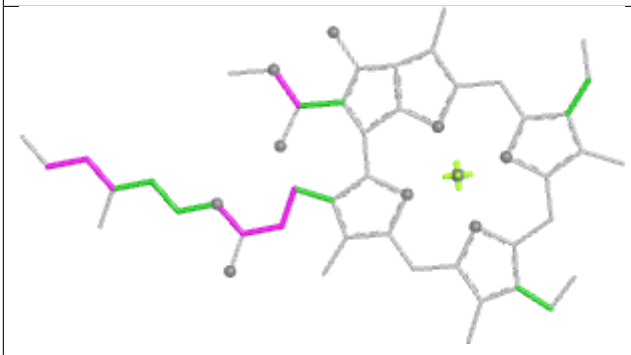
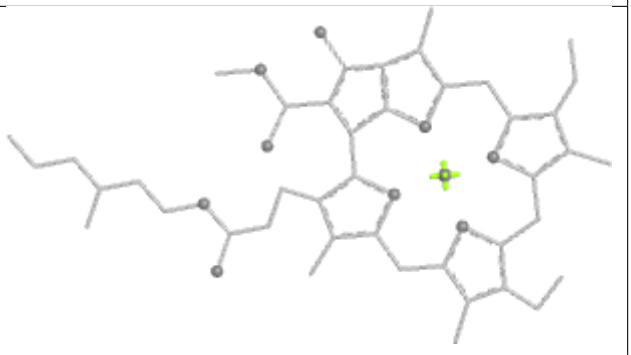


Rings

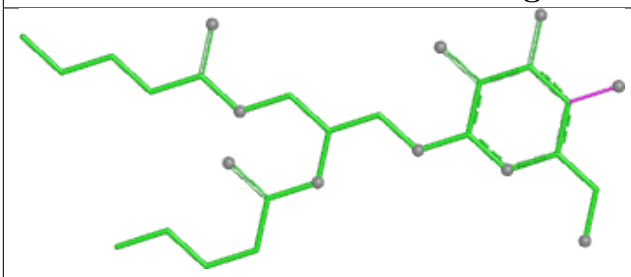
Ligand CLA 4 309	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA B 832	
 Bond lengths	 Bond angles
 Torsions	 Rings

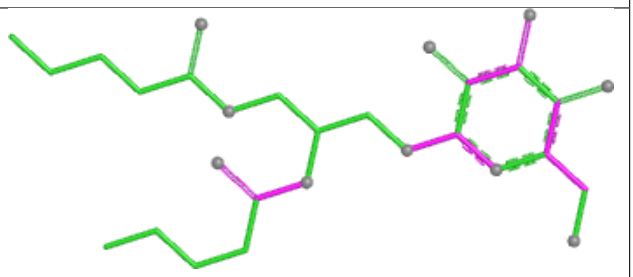
Ligand LHG L 208	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA B 823	
 Bond lengths	 Bond angles
 Torsions	 Rings

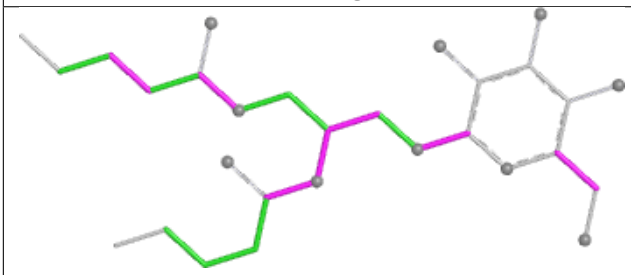
Ligand LMG J 102



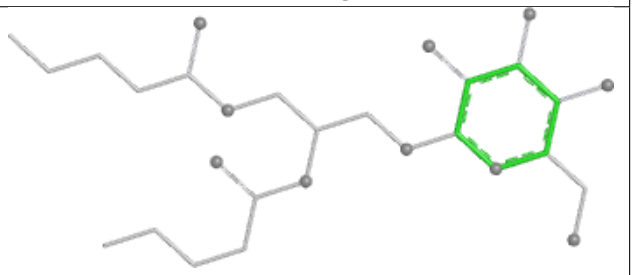
Bond lengths



Bond angles

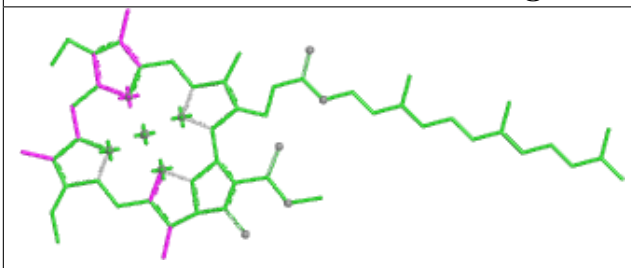


Torsions



Rings

Ligand CLA B 828



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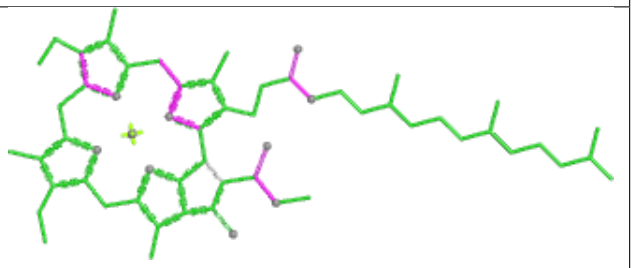
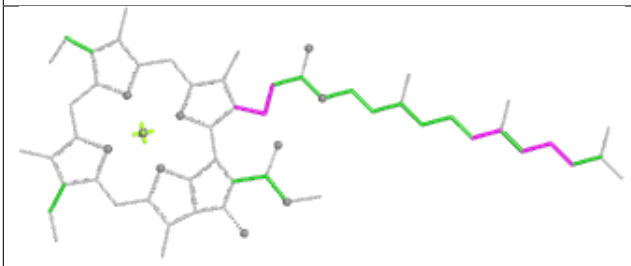


Bond angles



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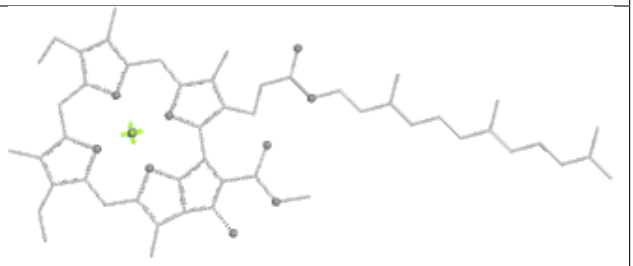
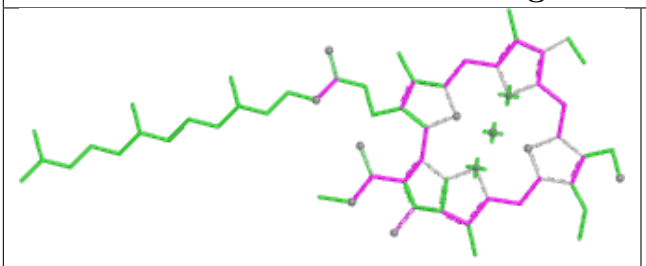


Rings

Ligand CHL 4 301



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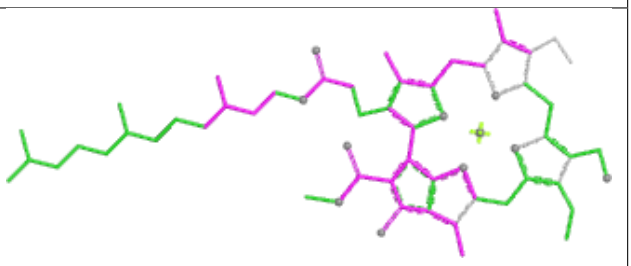
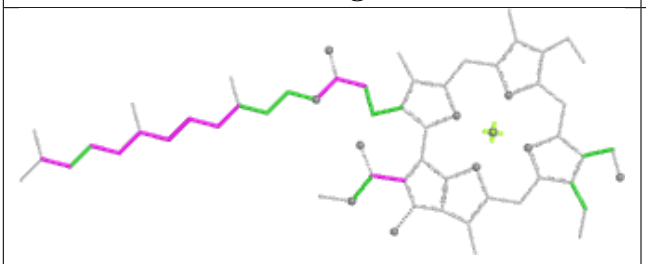


Bond angles



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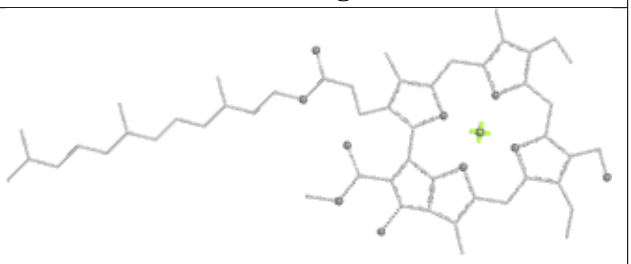
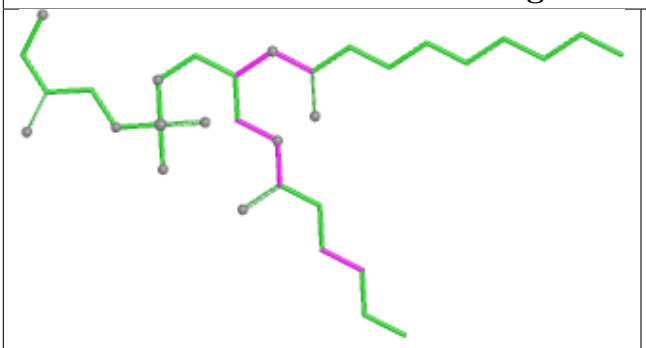


Rings

Ligand LHG 2 319



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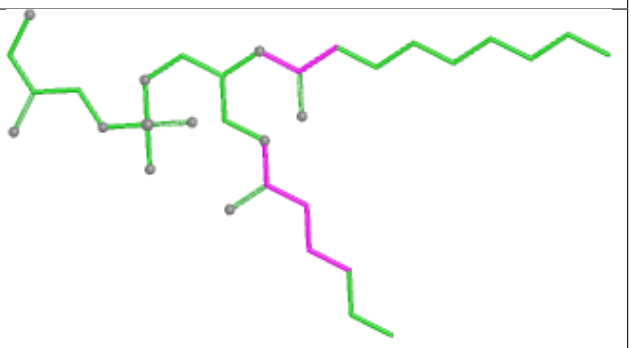
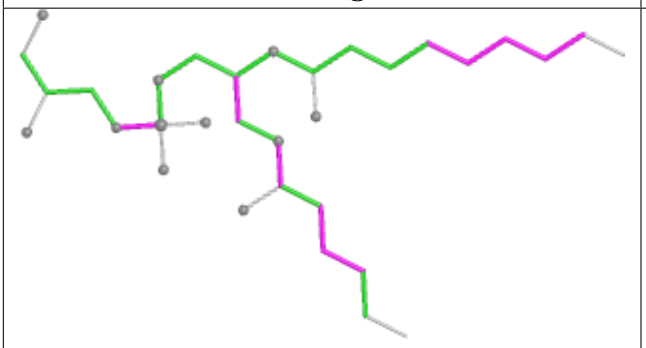
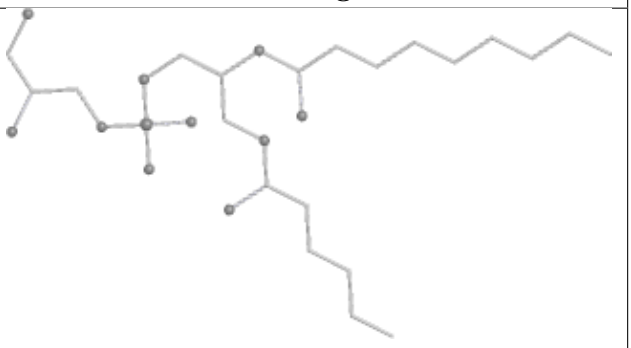


Bond angles

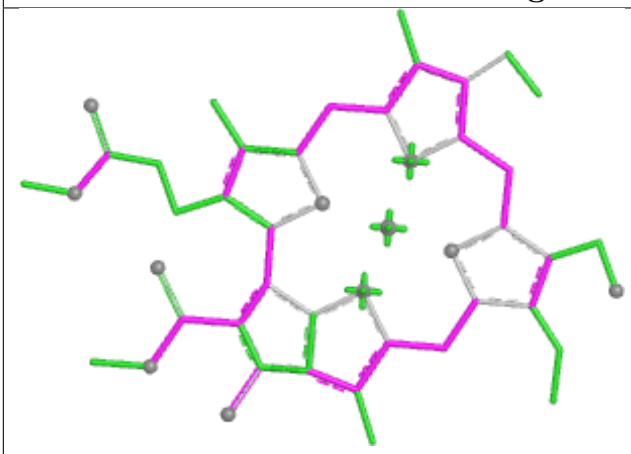


Torsions



Rings

Ligand CHL 4 308



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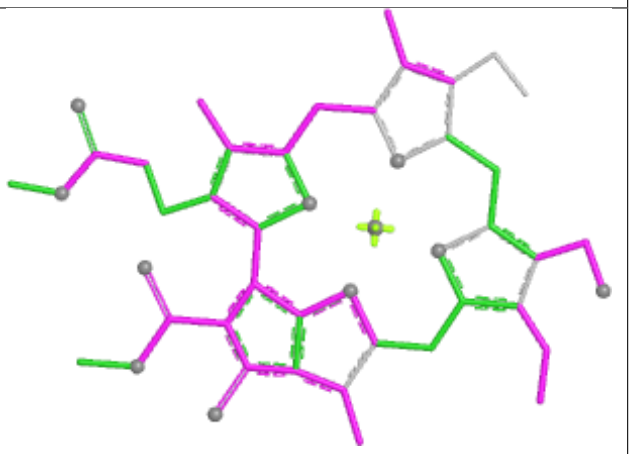

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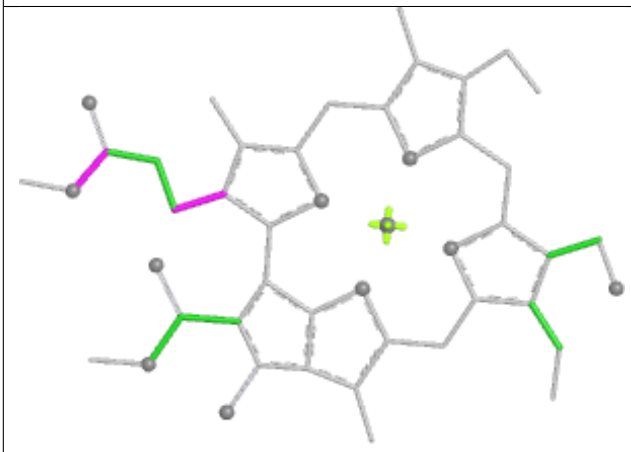
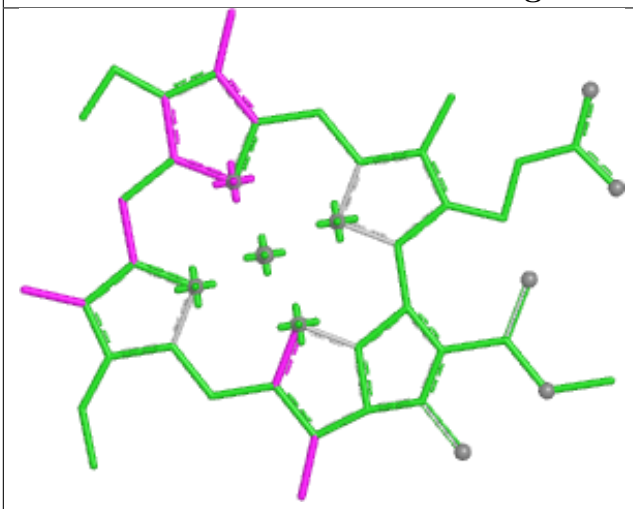


Torsions

Rings

Ligand CLA B 807



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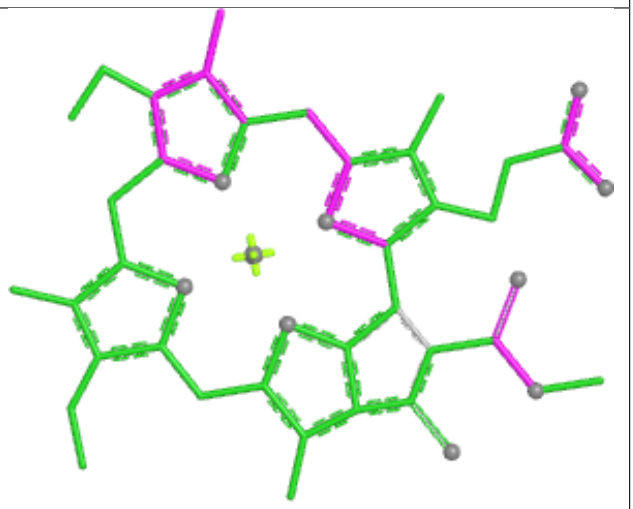

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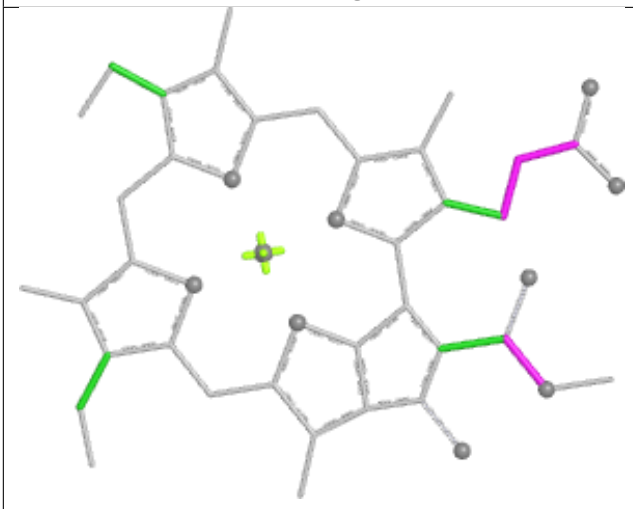
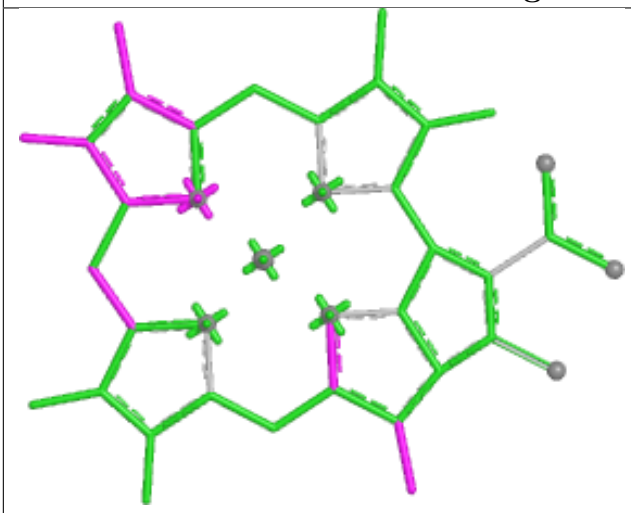


Torsions

Rings

Ligand CLA O 206



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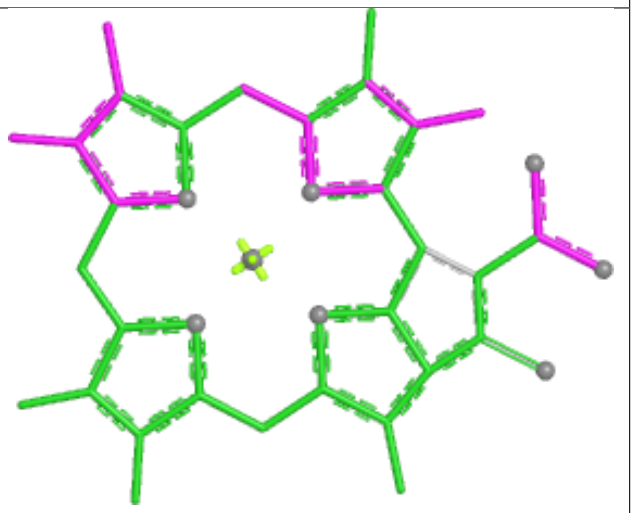

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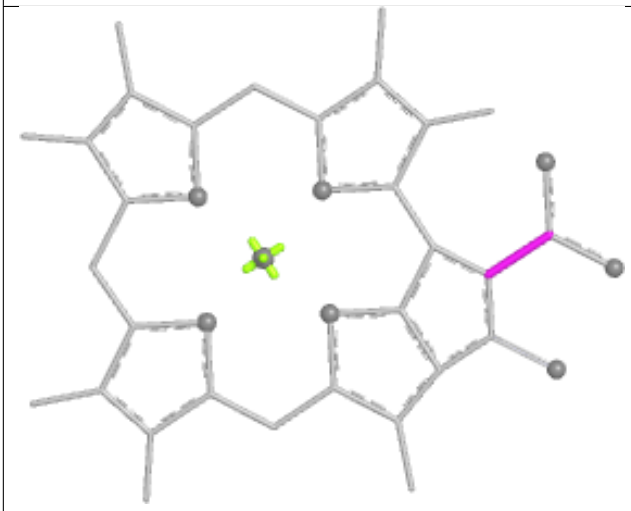

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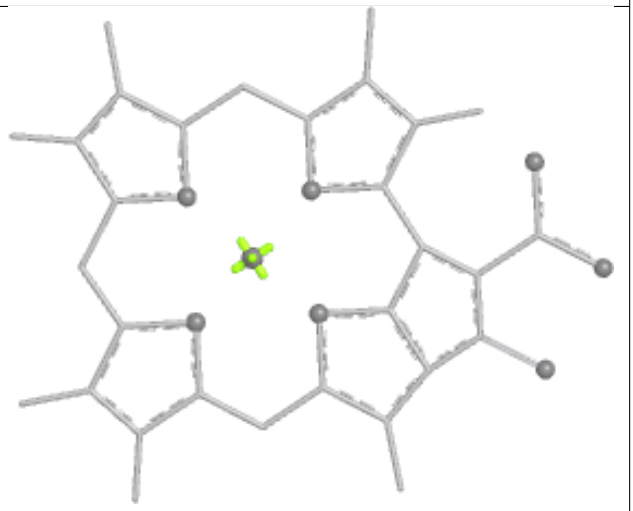
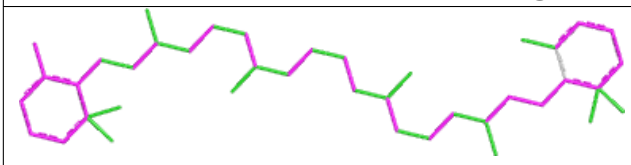


Rings

Ligand 8CT 8 317



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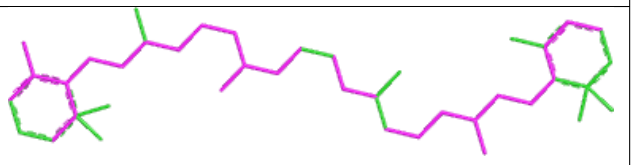
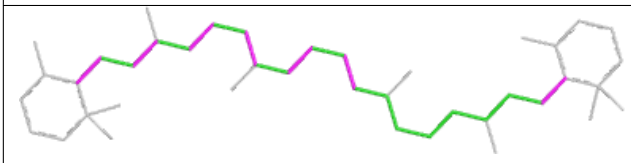


Bond angles



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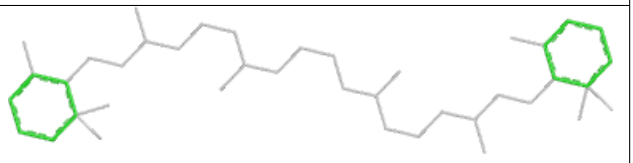
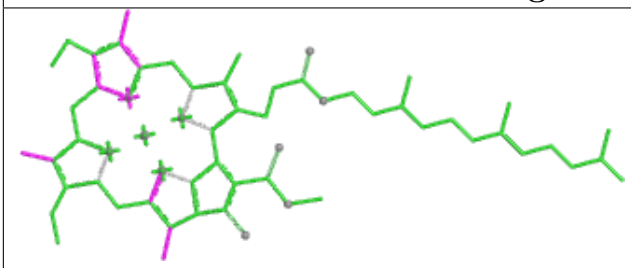


Rings

Ligand CLA 2 311



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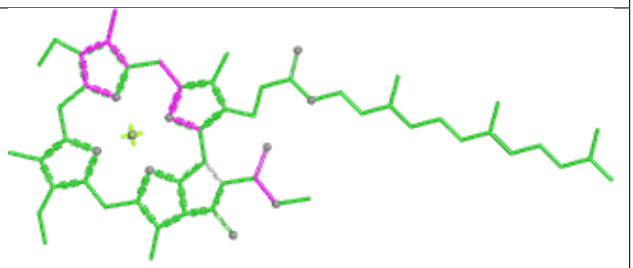
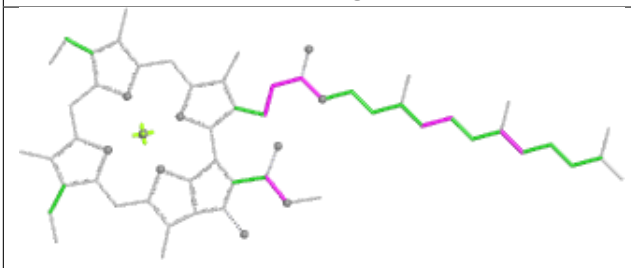


Bond angles



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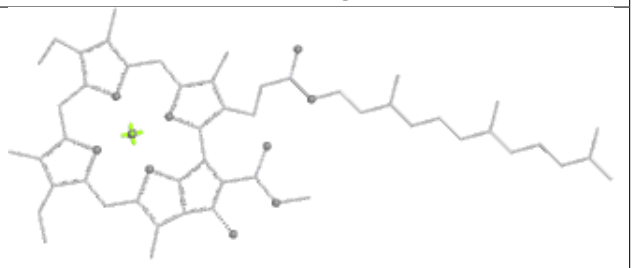
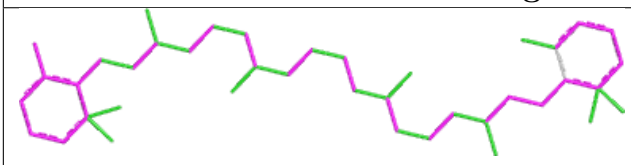


Rings

Ligand 8CT M 102



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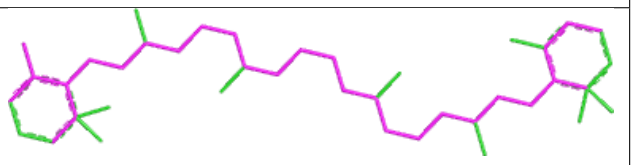
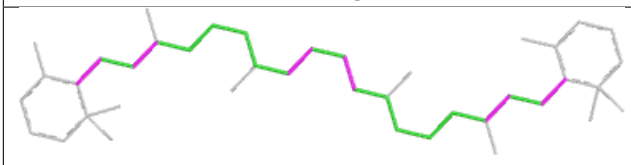
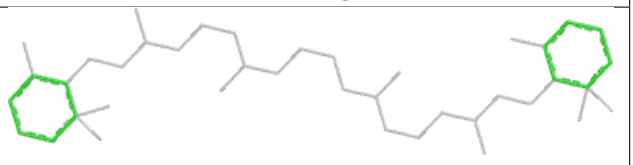


Bond angles

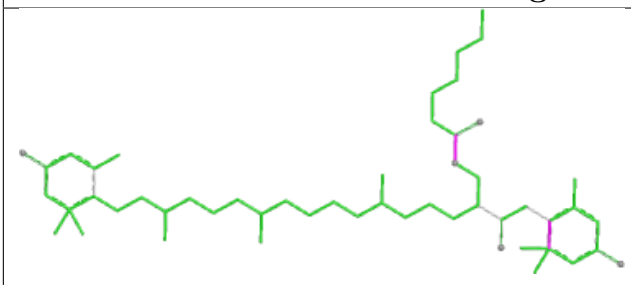


Torsions

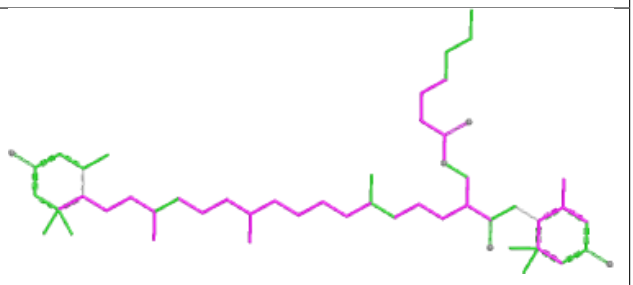


Rings

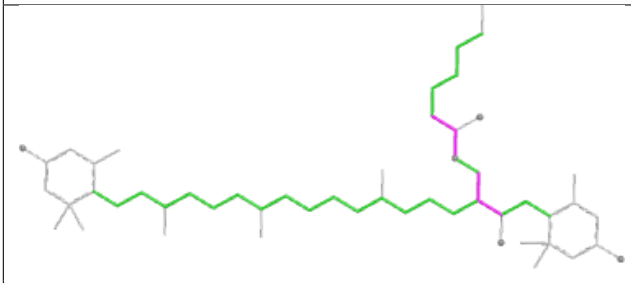
Ligand 0UR 9 315



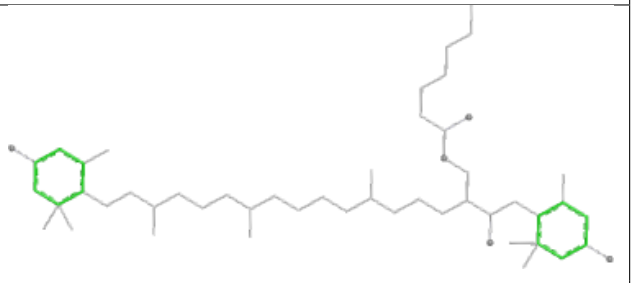
Bond lengths



Bond angles

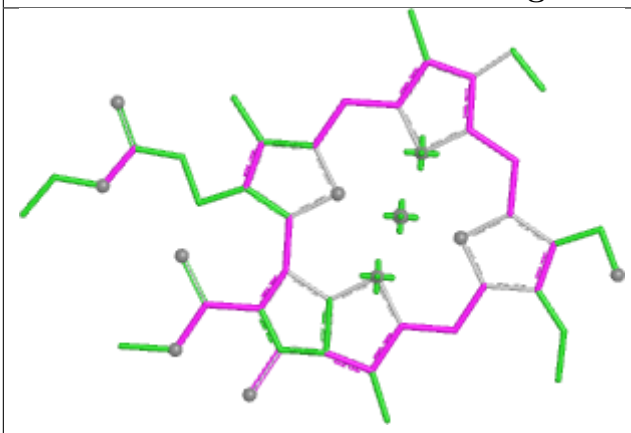


Torsions

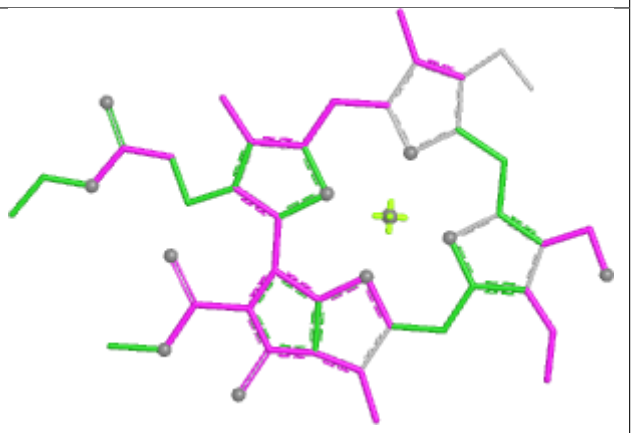


Rings

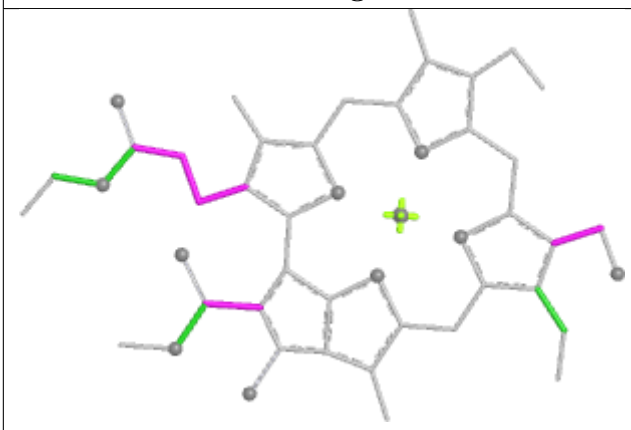
Ligand CHL 9 306



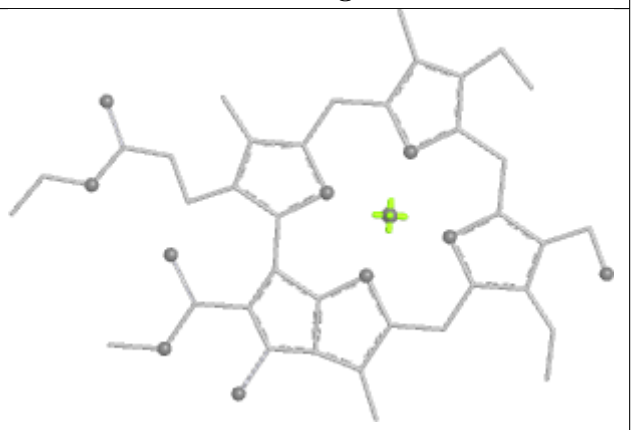
Bond lengths



Bond angles

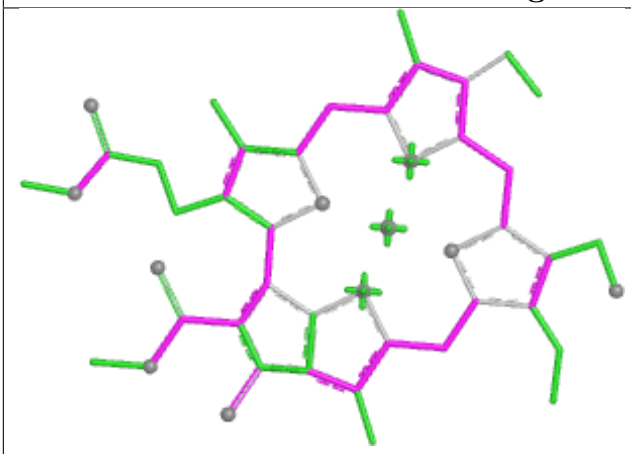


Torsions

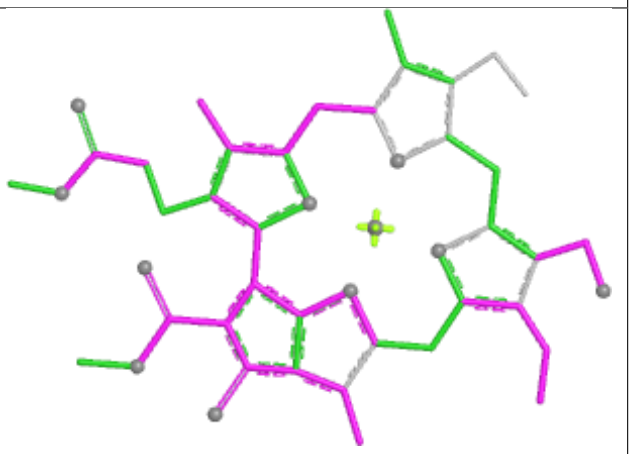


Rings

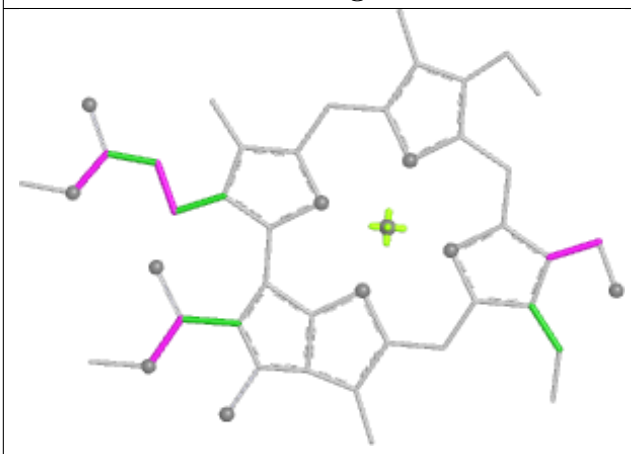
Ligand CHL 8 306



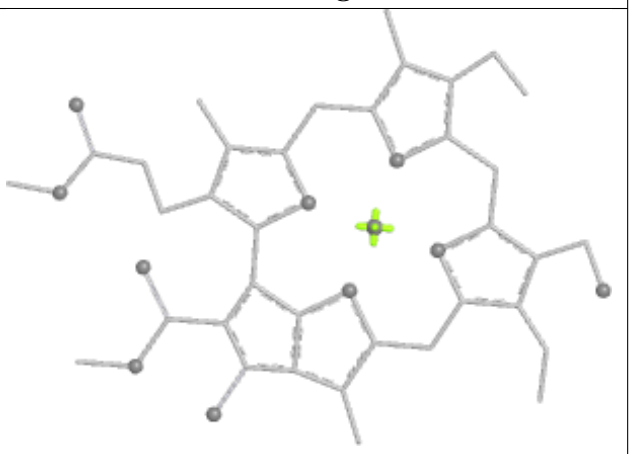
Bond lengths



Bond angles

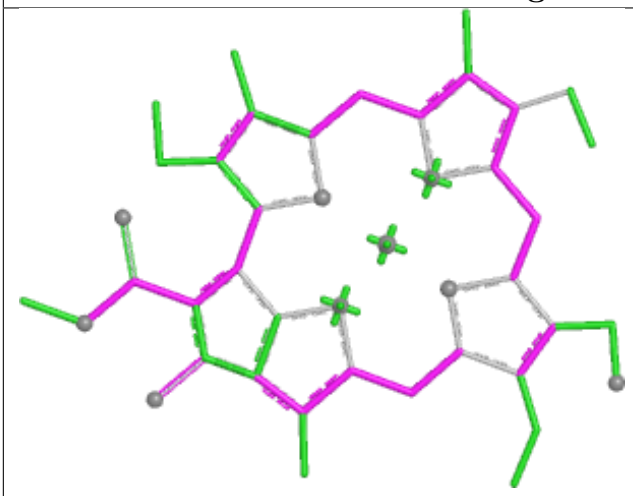


Torsions

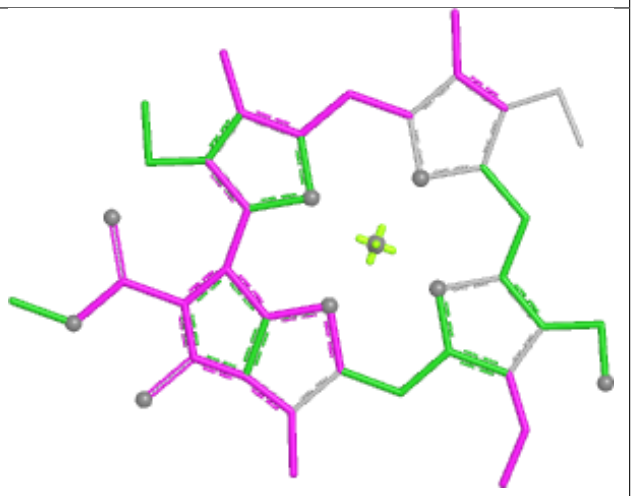


Rings

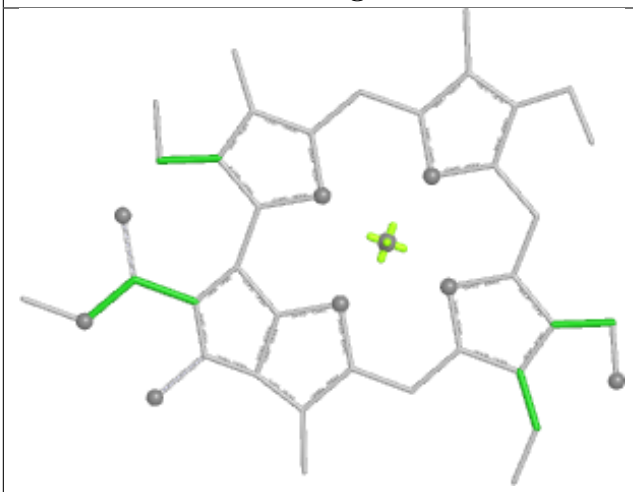
Ligand CHL 4 305



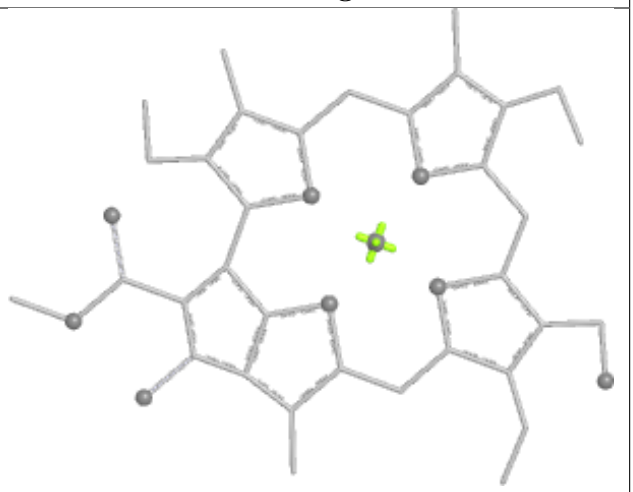
Bond lengths



Bond angles

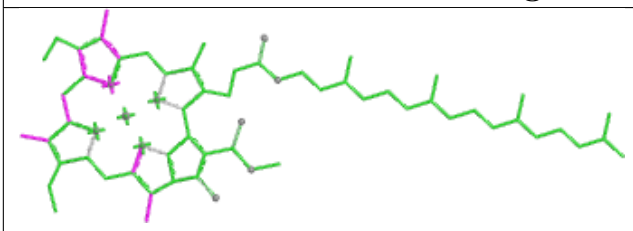


Torsions

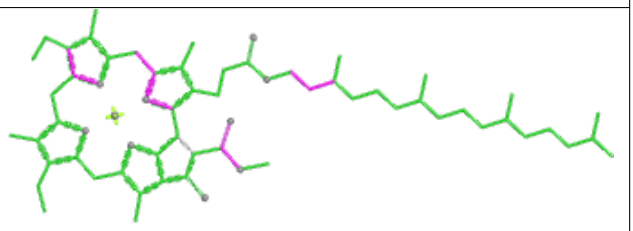


Rings

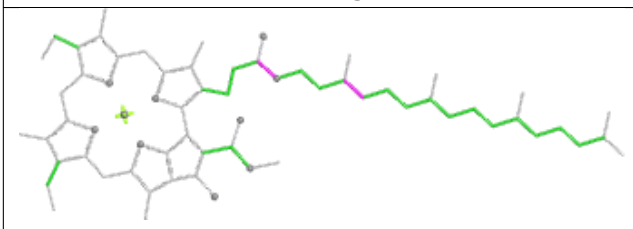
Ligand CLA A 809



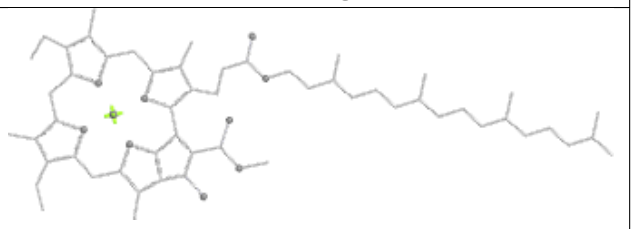
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

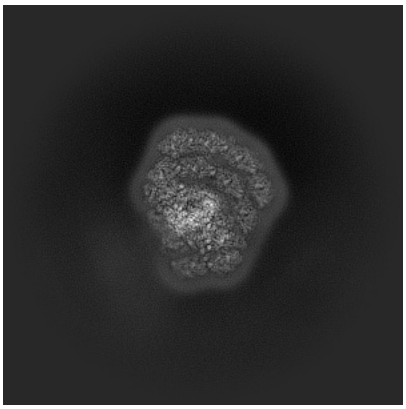
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-61973. These allow visual inspection of the internal detail of the map and identification of artifacts.

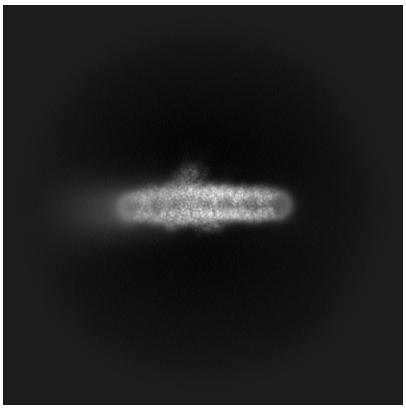
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

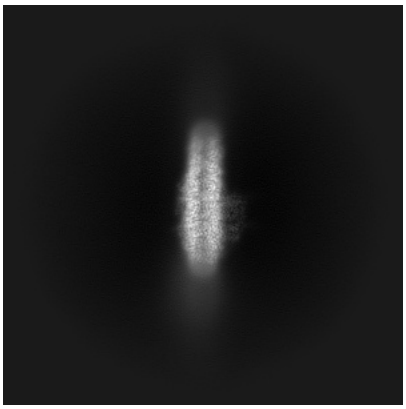
6.1.1 Primary map



X

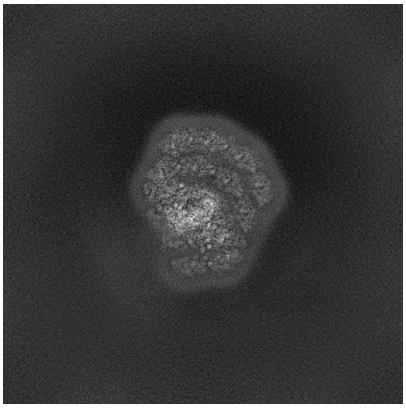


Y

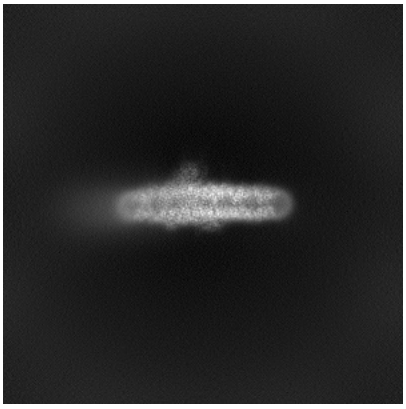


Z

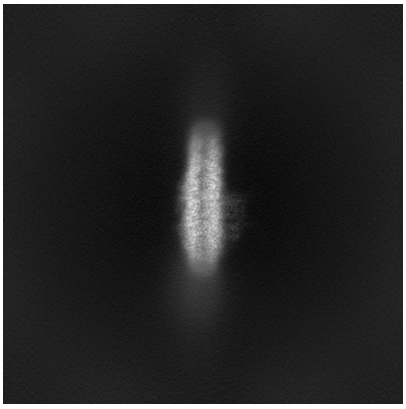
6.1.2 Raw map



X



Y

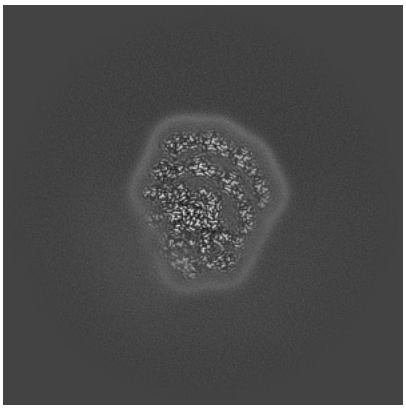


Z

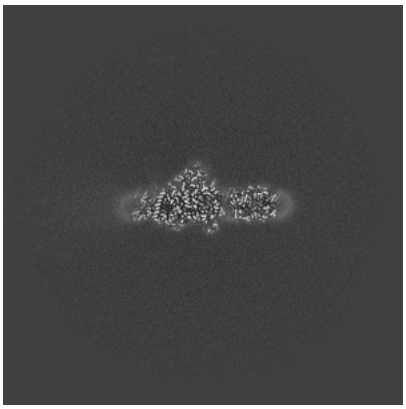
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

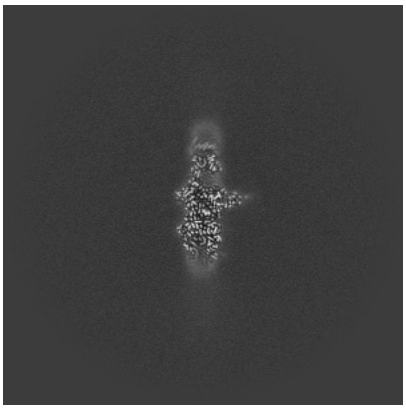
6.2.1 Primary map



X Index: 256

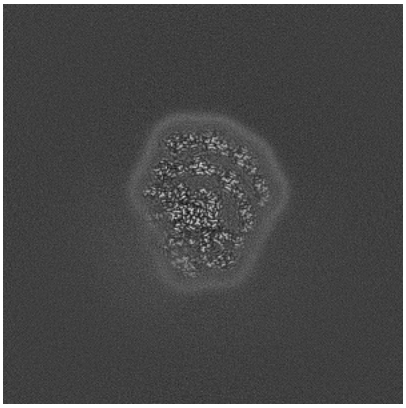


Y Index: 256

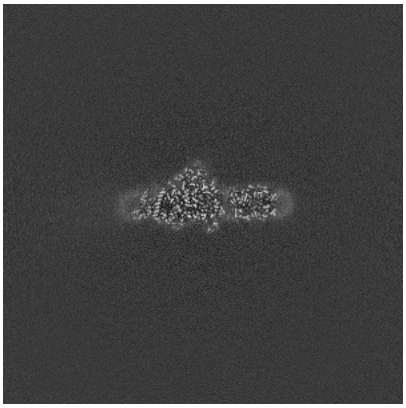


Z Index: 256

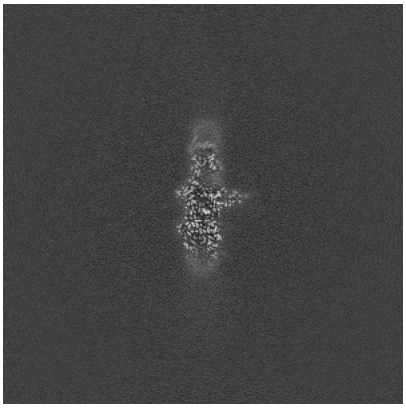
6.2.2 Raw map



X Index: 256



Y Index: 256

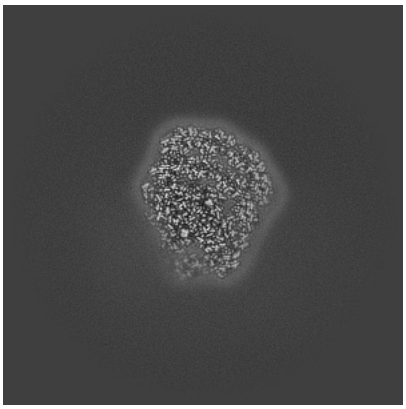


Z Index: 256

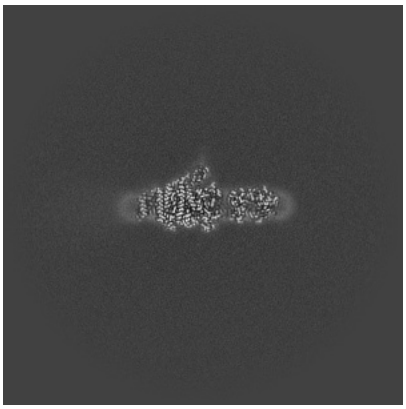
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

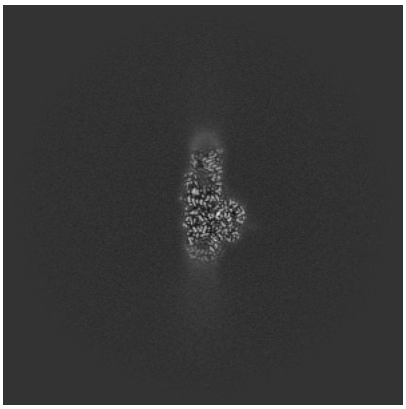
6.3.1 Primary map



X Index: 268

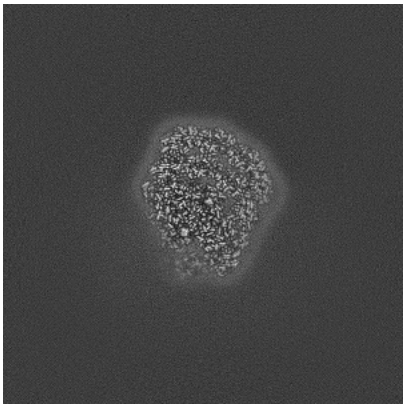


Y Index: 263

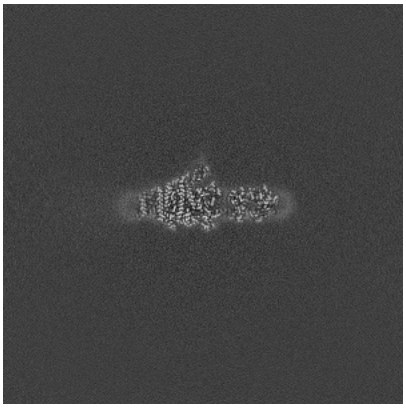


Z Index: 238

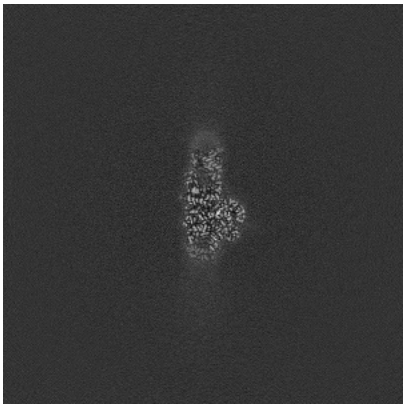
6.3.2 Raw map



X Index: 268



Y Index: 263

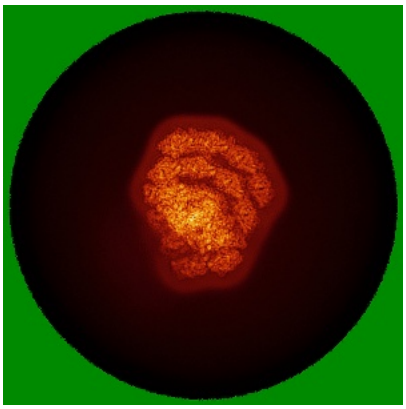


Z Index: 238

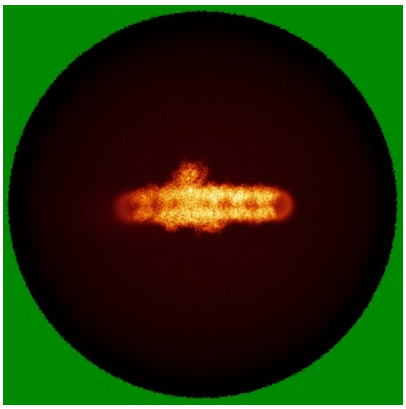
The images above show the largest variance slices of the map in three orthogonal directions.

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

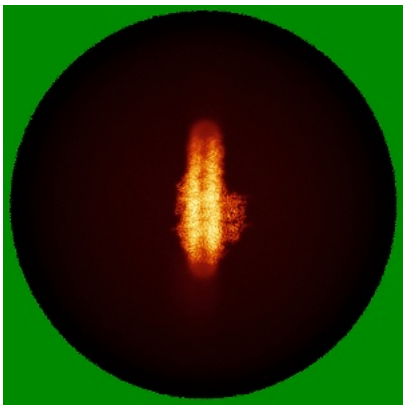
6.4.1 Primary map



X

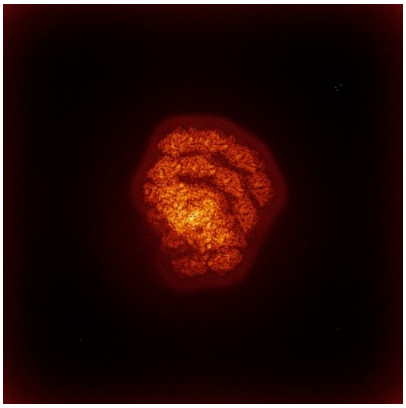


Y

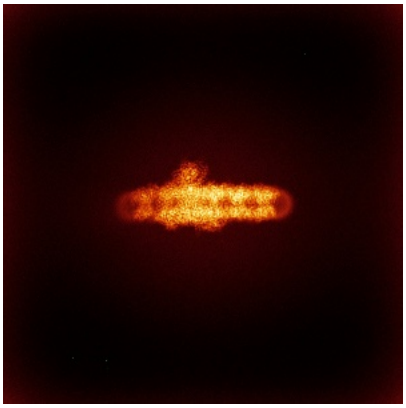


Z

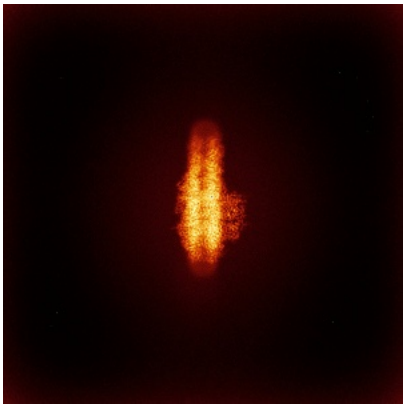
6.4.2 Raw map



X



Y

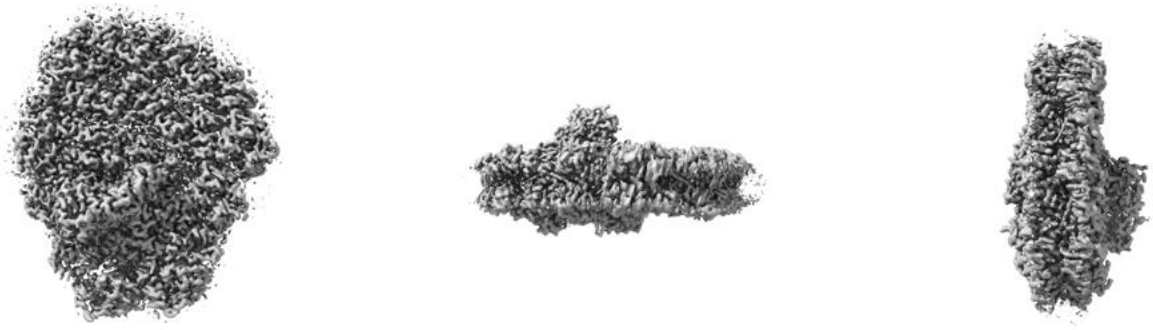


Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.203. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map

X Y Z

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

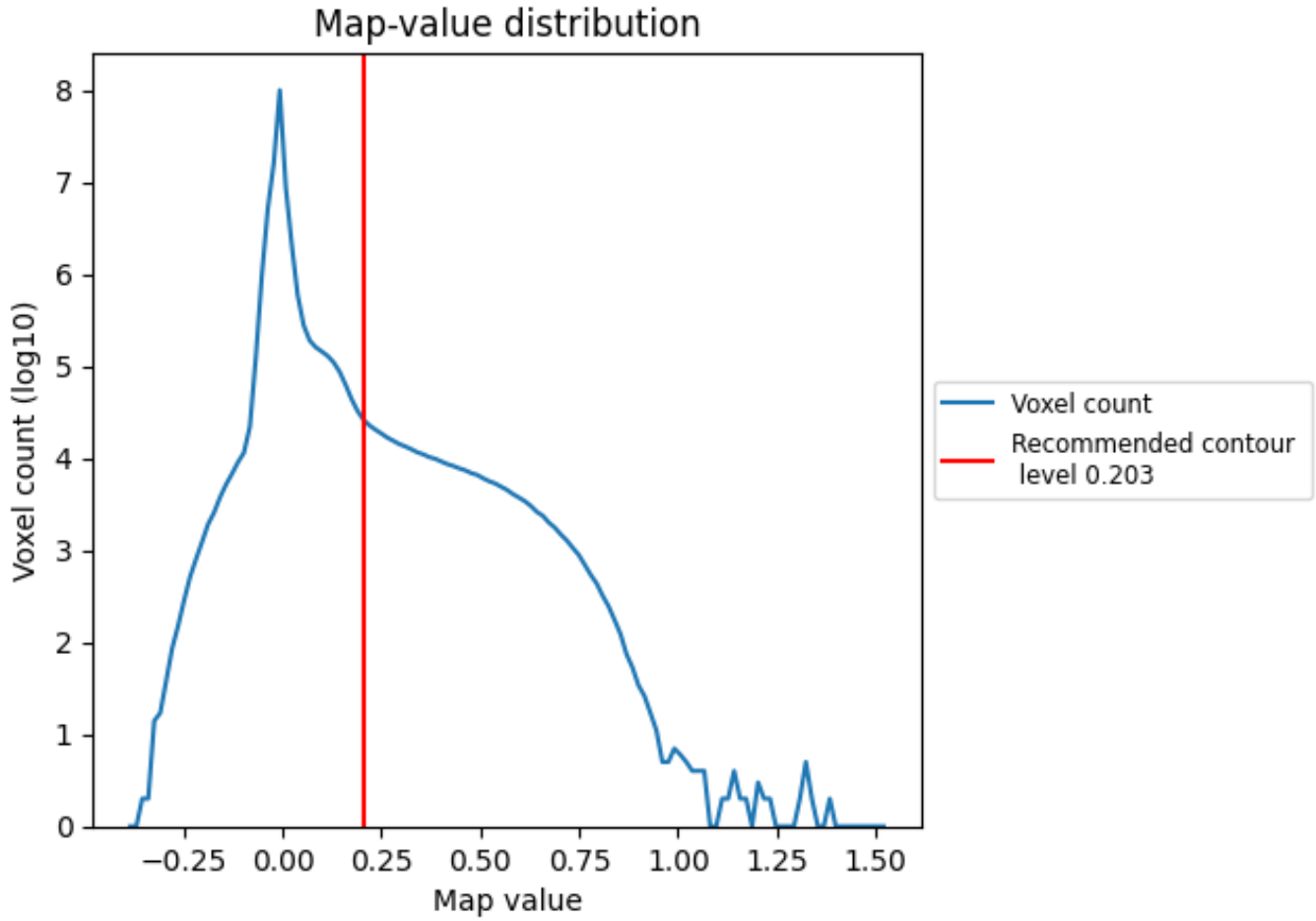
6.6 Mask visualisation (i)

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

7 Map analysis

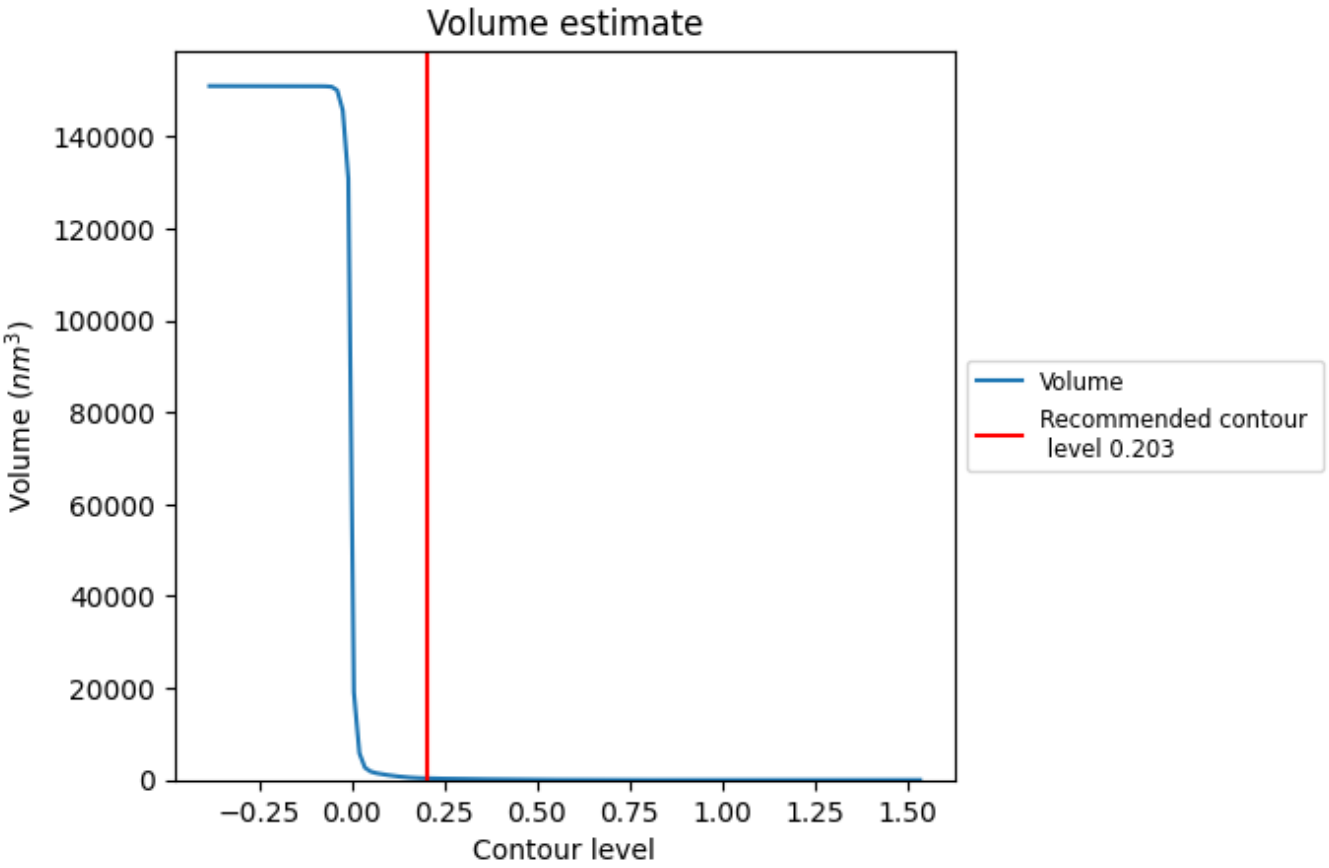
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

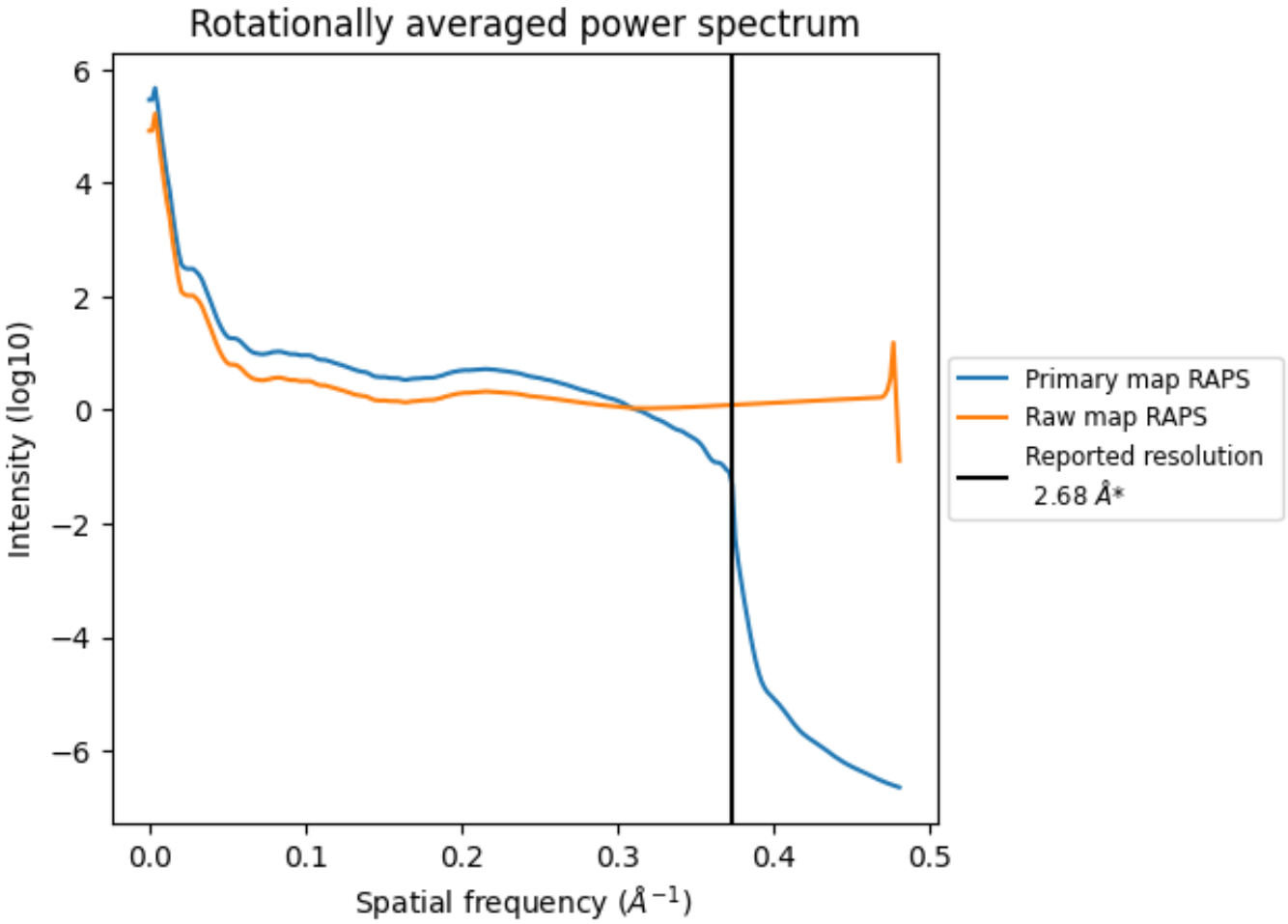
7.2 Volume estimate (i)



The volume at the recommended contour level is 356 nm^3; this corresponds to an approximate mass of 322 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum (i)

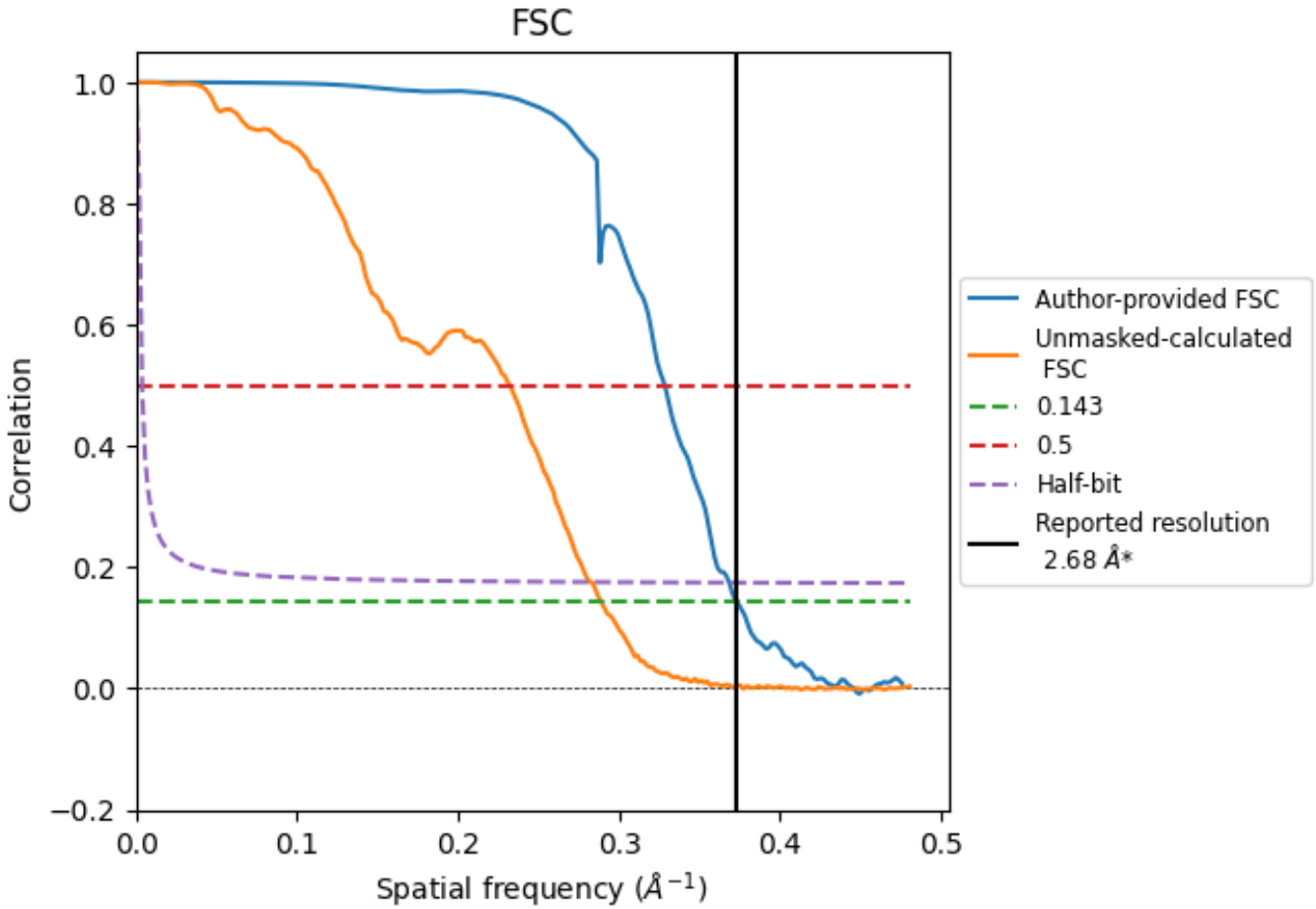


*Reported resolution corresponds to spatial frequency of 0.373 Å^{-1}

8 Fourier-Shell correlation

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

8.1 FSC



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

8.2 Resolution estimates (i)

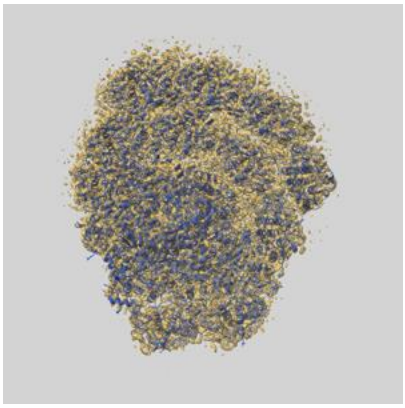
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.68	-	-
Author-provided FSC curve	2.68	3.04	2.71
Unmasked-calculated*	3.46	4.30	3.54

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.46 differs from the reported value 2.68 by more than 10 %

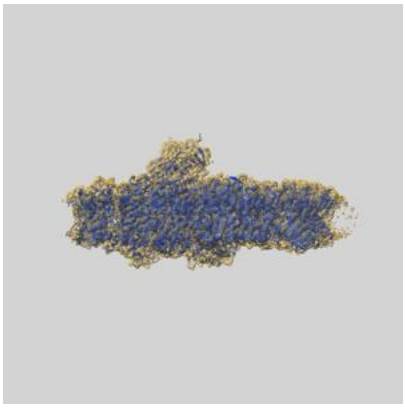
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-61973 and PDB model 9K1E. Per-residue inclusion information can be found in section 3 on page 37.

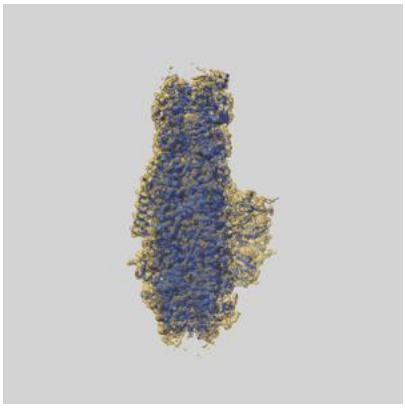
9.1 Map-model overlay



X



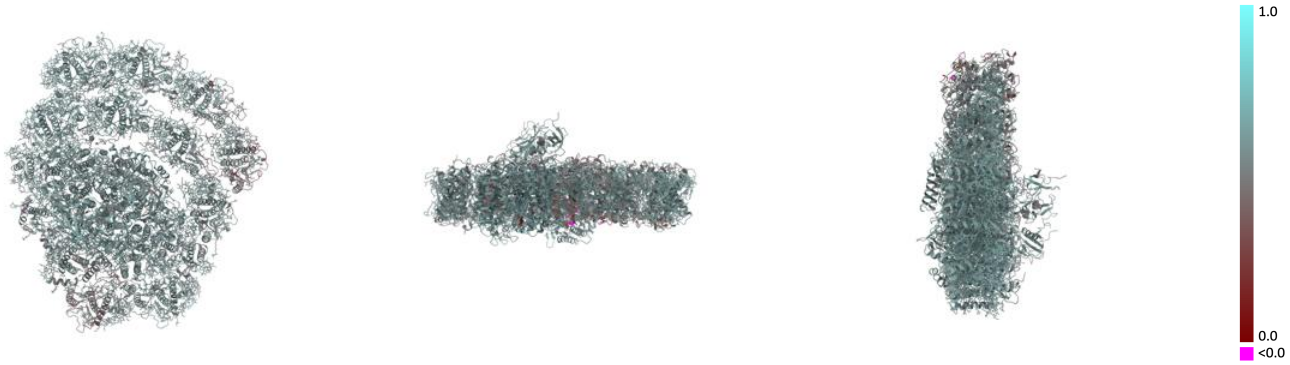
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.203 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

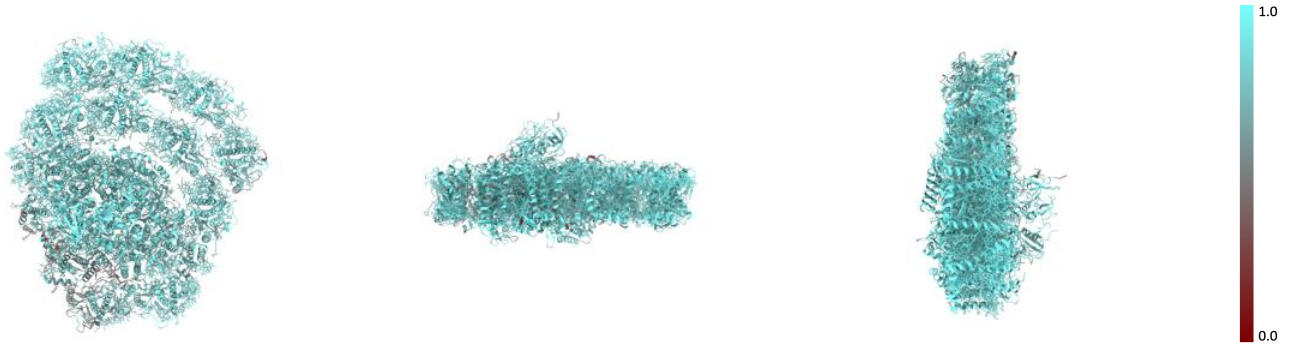
9.2 Q-score mapped to coordinate model



X Y Z

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

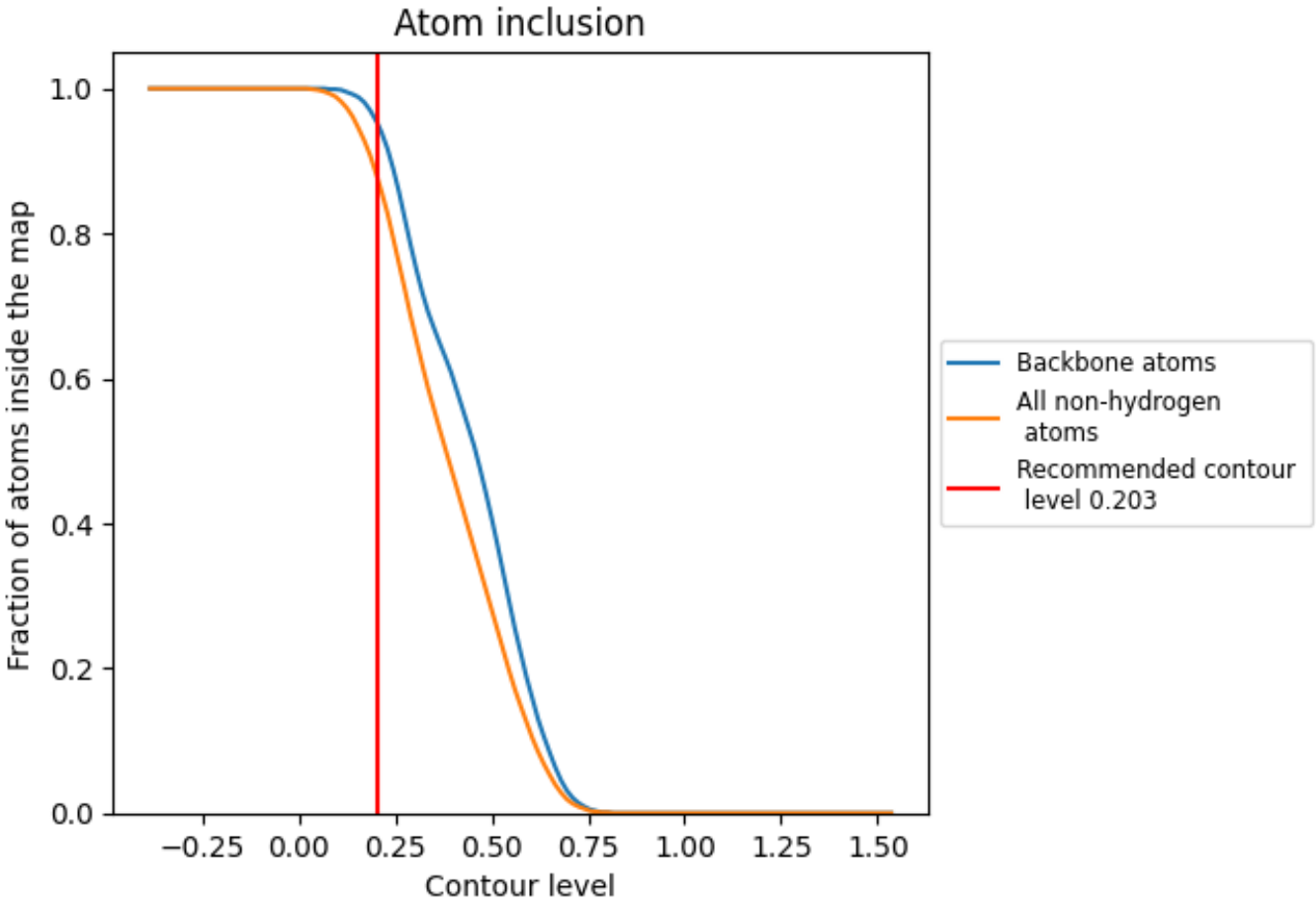
9.3 Atom inclusion mapped to coordinate model



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.203).

9.4 Atom inclusion (i)



At the recommended contour level, 95% of all backbone atoms, 88% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.203) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8780	0.5690
0	0.6840	0.4860
1	0.8580	0.5500
2	0.9240	0.5870
3	0.9240	0.5890
4	0.8710	0.5440
5	0.7850	0.4690
6	0.9090	0.5720
7	0.9070	0.5760
8	0.8660	0.5350
9	0.8650	0.5600
A	0.9370	0.6050
B	0.9420	0.6030
C	0.9600	0.5880
D	0.9110	0.5820
E	0.8580	0.5600
F	0.9030	0.5700
G	0.7840	0.5290
H	0.6250	0.5400
I	0.8210	0.5660
J	0.9140	0.5760
K	0.8720	0.5610
L	0.7190	0.5500
M	0.8900	0.5810
O	0.6960	0.5340