wwPDB EM Validation Summary Report

Jun 17, 2025 – 11:17 AM EDT

PDB ID	:	9MGZ / pdb_00009mgz
EMDB ID	:	EMD-48264
Title	:	Dunaliella tertiolecta PSI-LHCI-TIDI1 supercomplex
Authors	:	Liu, H.W.; Khera, R.; Iwai, M.; Merchant, S.S.
Deposited on	:	2024-12-11
Resolution	:	2.80 Å(reported)
Based on initial model	:	6SL5

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

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

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

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

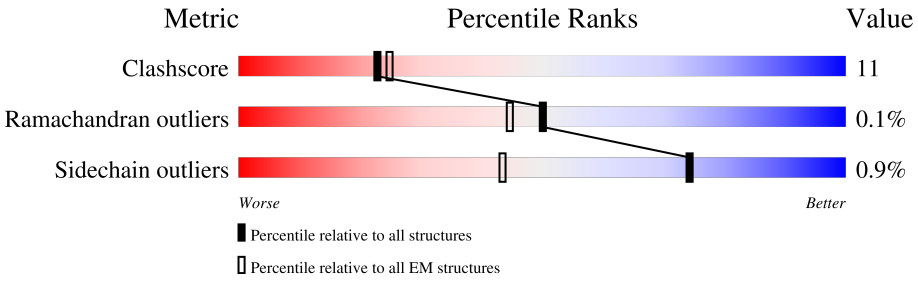
EMDB validation analysis	:	0.0.1.dev118
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4-5-2 with Phenix2.0rc1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.44

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 2.80 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	1	228	48% 71% 15% 14%
1	a	228	10% 73% 13% 14%
2	3	286	5% 61% 17% 21%
3	7	255	• 67% 18% 15%
3	c	255	19% 63% 18% • 18%
4	8	254	6% 79% 9% • 11%
4	b	254	21% 78% 10% 12%
5	A	751	76% 23% •

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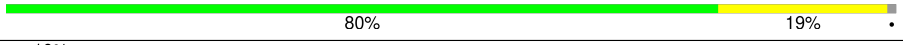
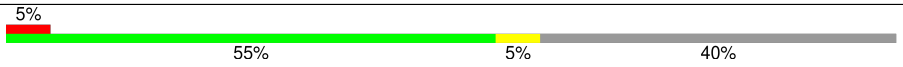
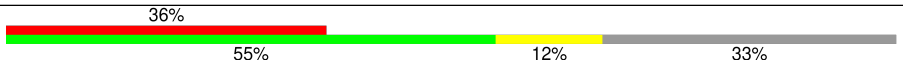
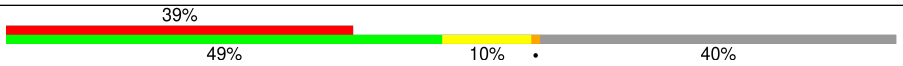
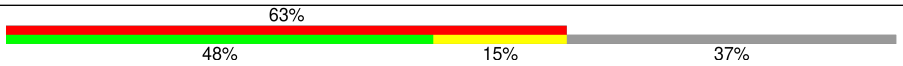
Mol	Chain	Length	Quality of chain
6	B	735	
7	C	81	
8	D	193	
9	E	111	
10	F	227	
11	J	41	
12	K	123	
13	T	350	
14	L	198	
15	I	108	

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
16	CHL	1	601	X	-	-	-
16	CHL	1	606	X	-	-	-
16	CHL	3	301	X	-	-	-
16	CHL	3	322	X	-	-	-
16	CHL	7	305	X	-	-	-
16	CHL	7	306	X	-	-	-
16	CHL	7	307	X	-	-	-
16	CHL	8	306	X	-	-	-
16	CHL	8	307	X	-	-	-
16	CHL	8	308	X	-	-	-
16	CHL	T	401	X	-	-	-
16	CHL	T	416	X	-	-	-
16	CHL	a	601	X	-	-	-
16	CHL	a	606	X	-	-	-
16	CHL	b	605	X	-	-	-
16	CHL	b	606	X	-	-	-
16	CHL	b	607	X	-	-	-
16	CHL	c	304	X	-	-	-
16	CHL	c	305	X	-	-	-
16	CHL	c	306	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
17	CLA	1	602	X	-	-	-
17	CLA	1	603	X	-	-	-
17	CLA	1	604	X	-	-	-
17	CLA	1	605	X	-	-	-
17	CLA	1	607	X	-	-	-
17	CLA	1	608	X	-	-	-
17	CLA	1	609	X	-	-	-
17	CLA	1	610	X	-	-	-
17	CLA	1	611	X	-	-	-
17	CLA	1	612	X	-	-	-
17	CLA	1	613	X	-	-	-
17	CLA	1	614	X	-	-	-
17	CLA	3	302	X	-	-	-
17	CLA	3	303	X	-	-	-
17	CLA	3	304	X	-	-	-
17	CLA	3	305	X	-	-	-
17	CLA	3	306	X	-	-	-
17	CLA	3	307	X	-	-	-
17	CLA	3	308	X	-	-	-
17	CLA	3	309	X	-	-	-
17	CLA	3	310	X	-	-	-
17	CLA	3	311	X	-	-	-
17	CLA	3	312	X	-	-	-
17	CLA	3	313	X	-	-	-
17	CLA	3	314	X	-	-	-
17	CLA	3	323	X	-	-	-
17	CLA	3	324	X	-	-	-
17	CLA	7	302	X	-	-	-
17	CLA	7	303	X	-	-	-
17	CLA	7	304	X	-	-	-
17	CLA	7	308	X	-	-	-
17	CLA	7	309	X	-	-	-
17	CLA	7	310	X	-	-	-
17	CLA	7	311	X	-	-	-
17	CLA	7	312	X	-	-	-
17	CLA	7	313	X	-	-	-
17	CLA	7	314	X	-	-	-
17	CLA	8	302	X	-	-	-
17	CLA	8	303	X	-	-	-
17	CLA	8	304	X	-	-	-
17	CLA	8	305	X	-	-	-
17	CLA	8	309	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
17	CLA	8	310	X	-	-	-
17	CLA	8	311	X	-	-	-
17	CLA	8	312	X	-	-	-
17	CLA	8	313	X	-	-	-
17	CLA	8	314	X	-	-	-
17	CLA	8	315	X	-	-	-
17	CLA	A	5004	X	-	-	-
17	CLA	A	5005	X	-	-	-
17	CLA	A	5006	X	-	-	-
17	CLA	A	5007	X	-	-	-
17	CLA	A	5008	X	-	-	-
17	CLA	A	5009	X	-	-	-
17	CLA	A	5010	X	-	-	-
17	CLA	A	5011	X	-	-	-
17	CLA	A	5012	X	-	-	-
17	CLA	A	5013	X	-	-	-
17	CLA	A	5015	X	-	-	-
17	CLA	A	5016	X	-	-	-
17	CLA	A	5017	X	-	-	-
17	CLA	A	5018	X	-	-	-
17	CLA	A	5019	X	-	-	-
17	CLA	A	5020	X	-	-	-
17	CLA	A	5021	X	-	-	-
17	CLA	A	5022	X	-	-	-
17	CLA	A	5023	X	-	-	-
17	CLA	A	5024	X	-	-	-
17	CLA	A	5025	X	-	-	-
17	CLA	A	5026	X	-	-	-
17	CLA	A	5027	X	-	-	-
17	CLA	A	5028	X	-	-	-
17	CLA	A	5029	X	-	-	-
17	CLA	A	5030	X	-	-	-
17	CLA	A	5031	X	-	-	-
17	CLA	A	5032	X	-	-	-
17	CLA	A	5033	X	-	-	-
17	CLA	A	5034	X	-	-	-
17	CLA	A	5035	X	-	-	-
17	CLA	A	5036	X	-	-	-
17	CLA	A	5037	X	-	-	-
17	CLA	A	5038	X	-	-	-
17	CLA	A	5039	X	-	-	-
17	CLA	A	5040	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
17	CLA	A	5041	X	-	-	-
17	CLA	A	5042	X	-	-	-
17	CLA	A	5043	X	-	-	-
17	CLA	A	5044	X	-	-	-
17	CLA	B	802	X	-	-	-
17	CLA	B	803	X	-	-	-
17	CLA	B	804	X	-	-	-
17	CLA	B	805	X	-	-	-
17	CLA	B	806	X	-	-	-
17	CLA	B	807	X	-	-	-
17	CLA	B	808	X	-	-	-
17	CLA	B	809	X	-	-	-
17	CLA	B	810	X	-	-	-
17	CLA	B	811	X	-	-	-
17	CLA	B	812	X	-	-	-
17	CLA	B	813	X	-	-	-
17	CLA	B	814	X	-	-	-
17	CLA	B	815	X	-	-	-
17	CLA	B	816	X	-	-	-
17	CLA	B	817	X	-	-	-
17	CLA	B	818	X	-	-	-
17	CLA	B	819	X	-	-	-
17	CLA	B	820	X	-	-	-
17	CLA	B	821	X	-	-	-
17	CLA	B	822	X	-	-	-
17	CLA	B	823	X	-	-	-
17	CLA	B	824	X	-	-	-
17	CLA	B	825	X	-	-	-
17	CLA	B	826	X	-	-	-
17	CLA	B	827	X	-	-	-
17	CLA	B	828	X	-	-	-
17	CLA	B	829	X	-	-	-
17	CLA	B	830	X	-	-	-
17	CLA	B	831	X	-	-	-
17	CLA	B	832	X	-	-	-
17	CLA	B	833	X	-	-	-
17	CLA	B	834	X	-	-	-
17	CLA	B	835	X	-	-	-
17	CLA	B	836	X	-	-	-
17	CLA	B	837	X	-	-	-
17	CLA	B	838	X	-	-	-
17	CLA	B	839	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
17	CLA	B	840	X	-	-	-
17	CLA	B	841	X	-	-	-
17	CLA	F	5004	X	-	-	-
17	CLA	F	5006	X	-	-	-
17	CLA	F	5007	X	-	-	-
17	CLA	F	5008	X	-	-	-
17	CLA	F	5009	X	-	-	-
17	CLA	J	102	X	-	-	-
17	CLA	K	201	X	-	-	-
17	CLA	K	202	X	-	-	-
17	CLA	K	203	X	-	-	-
17	CLA	K	204	X	-	-	-
17	CLA	L	201	X	-	-	-
17	CLA	L	202	X	-	-	-
17	CLA	T	402	X	-	-	-
17	CLA	T	403	X	-	-	-
17	CLA	T	404	X	-	-	-
17	CLA	T	405	X	-	-	-
17	CLA	T	406	X	-	-	-
17	CLA	T	407	X	-	-	-
17	CLA	T	408	X	-	-	-
17	CLA	T	409	X	-	-	-
17	CLA	T	411	X	-	-	-
17	CLA	T	412	X	-	-	-
17	CLA	a	602	X	-	-	-
17	CLA	a	603	X	-	-	-
17	CLA	a	604	X	-	-	-
17	CLA	a	605	X	-	-	-
17	CLA	a	607	X	-	-	-
17	CLA	a	608	X	-	-	-
17	CLA	a	609	X	-	-	-
17	CLA	a	610	X	-	-	-
17	CLA	a	611	X	-	-	-
17	CLA	a	612	X	-	-	-
17	CLA	a	613	X	-	-	-
17	CLA	a	614	X	-	-	-
17	CLA	b	601	X	-	-	-
17	CLA	b	602	X	-	-	-
17	CLA	b	603	X	-	-	-
17	CLA	b	604	X	-	-	-
17	CLA	b	608	X	-	-	-
17	CLA	b	609	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
17	CLA	b	610	X	-	-	-
17	CLA	b	611	X	-	-	-
17	CLA	b	612	X	-	-	-
17	CLA	b	613	X	-	-	-
17	CLA	b	614	X	-	-	-
17	CLA	c	301	X	-	-	-
17	CLA	c	302	X	-	-	-
17	CLA	c	303	X	-	-	-
17	CLA	c	307	X	-	-	-
17	CLA	c	308	X	-	-	-
17	CLA	c	309	X	-	-	-
17	CLA	c	310	X	-	-	-
17	CLA	c	311	X	-	-	-
17	CLA	c	312	X	-	-	-
18	LUT	1	615	X	-	-	-
18	LUT	3	315	X	-	-	-
18	LUT	7	315	X	-	-	-
18	LUT	8	316	X	-	-	-
18	LUT	T	413	X	-	-	-
18	LUT	a	615	X	-	-	-
18	LUT	b	615	X	-	-	-
18	LUT	c	314	X	-	-	-
27	CL0	A	5003	X	-	-	-

2 Entry composition (i)

There are 30 unique types of molecules in this entry. The entry contains 44202 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	1	197	Total	C	N	O	S	0	0
			1505	965	255	278	7		
1	a	197	Total	C	N	O	S	0	0
			1505	965	255	278	7		

- Molecule 2 is a protein called LHCA3.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	3	226	Total	C	N	O	S	0	0
			1719	1120	282	312	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	7	217	Total	C	N	O	S	0	0
			1669	1078	281	304	6		
3	c	209	Total	C	N	O	S	0	0
			1607	1037	271	293	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	8	226	Total	C	N	O	S	0	0
			1721	1108	286	320	7		
4	b	224	Total	C	N	O	S	0	0
			1710	1102	284	317	7		

- Molecule 5 is a protein called Photosystem I P700 chlorophyll a apoprotein A1.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	A	740	Total	C	N	O	S	0	0
			5808	3795	993	1002	18		

- Molecule 6 is a protein called Photosystem I P700 chlorophyll a apoprotein A2.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	B	734	Total	C	N	O	S	0	0
			5814	3816	975	1010	13		

- Molecule 7 is a protein called Photosystem I iron-sulfur center.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	C	80	Total	C	N	O	S	0	0
			600	370	104	115	11		

- Molecule 8 is a protein called Photosystem I reaction center subunit II, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	D	143	Total	C	N	O	S	0	0
			1133	727	193	207	6		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
9	E	67	Total	C	N	O	0	0
			535	340	94	101		

- Molecule 10 is a protein called PSAF1.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	F	165	Total	C	N	O	S	0	0
			1300	836	225	237	2		

- Molecule 11 is a protein called Photosystem I reaction center subunit IX.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	J	41	Total	C	N	O	S	0	0
			327	223	47	56	1		

- Molecule 12 is a protein called PSI-K.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	K	83	Total	C	N	O	S	0	0
			579	370	101	105	3		

- Molecule 13 is a protein called TIDI1.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	T	210	Total	C	N	O	S	0	0
			1639	1062	271	298	8		

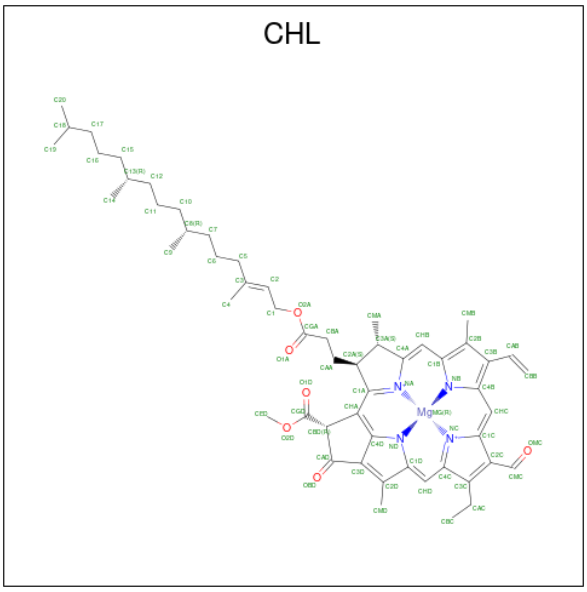
- Molecule 14 is a protein called PSAL1.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	L	124	Total	C	N	O	S	0	0
			894	582	147	160	5		

- 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
			274	191	40	42	1		

- Molecule 16 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
16	1	1	Total	C	Mg	N	O	0
			51	40	1	4	6	
16	1	1	Total	C	Mg	N	O	0
			47	36	1	4	6	
16	3	1	Total	C	Mg	N	O	0
			62	51	1	4	6	
16	3	1	Total	C	Mg	N	O	0
			61	50	1	4	6	

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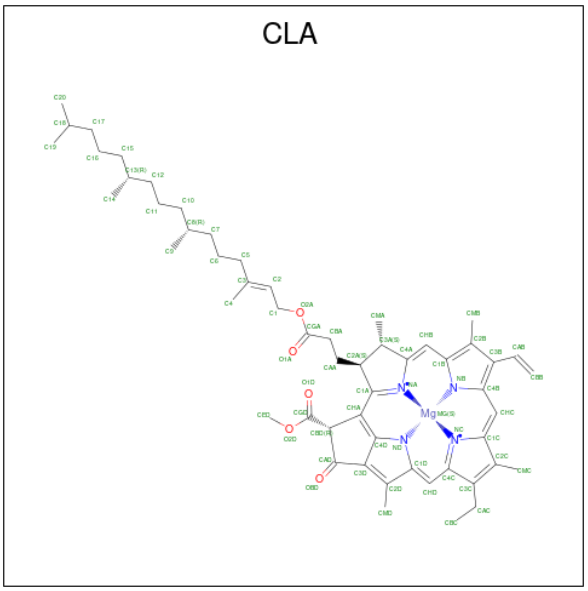
Mol	Chain	Residues	Atoms					AltConf
16	7	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
16	7	1	Total	C	Mg	N	O	0
			47	36	1	4	6	
16	7	1	Total	C	Mg	N	O	0
			48	37	1	4	6	
16	8	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
16	8	1	Total	C	Mg	N	O	0
			47	36	1	4	6	
16	8	1	Total	C	Mg	N	O	0
			51	40	1	4	6	
16	T	1	Total	C	Mg	N	O	0
			51	40	1	4	6	
16	T	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
16	a	1	Total	C	Mg	N	O	0
			47	36	1	4	6	
16	a	1	Total	C	Mg	N	O	0
			47	36	1	4	6	
16	b	1	Total	C	Mg	N	O	0
			47	36	1	4	6	
16	b	1	Total	C	Mg	N	O	0
			47	36	1	4	6	
16	b	1	Total	C	Mg	N	O	0
			51	40	1	4	6	
16	c	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
16	c	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
16	c	1	Total	C	Mg	N	O	0
			48	37	1	4	6	

- Molecule 17 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
17	1	1	Total 55	C 45	Mg 1	N 4	O 5	0
17	1	1	Total 45	C 35	Mg 1	N 4	O 5	0
17	1	1	Total 50	C 40	Mg 1	N 4	O 5	0
17	1	1	Total 45	C 35	Mg 1	N 4	O 5	0
17	1	1	Total 65	C 55	Mg 1	N 4	O 5	0
17	1	1	Total 45	C 35	Mg 1	N 4	O 5	0
17	1	1	Total 65	C 55	Mg 1	N 4	O 5	0
17	1	1	Total 46	C 36	Mg 1	N 4	O 5	0
17	1	1	Total 46	C 36	Mg 1	N 4	O 5	0
17	1	1	Total 60	C 50	Mg 1	N 4	O 5	0
17	1	1	Total 46	C 36	Mg 1	N 4	O 5	0
17	1	1	Total 46	C 36	Mg 1	N 4	O 5	0
17	3	1	Total 65	C 55	Mg 1	N 4	O 5	0
17	3	1	Total 46	C 36	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
17	3	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
17	3	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
17	3	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
17	3	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	3	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
17	3	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
17	3	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
17	3	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
17	3	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
17	3	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
17	3	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
17	3	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
17	3	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
17	7	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
17	7	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
17	7	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
17	7	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
17	7	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
17	7	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
17	7	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
17	7	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
17	7	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
17	7	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
17	8	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
17	8	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
17	8	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
17	8	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
17	8	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
17	8	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
17	8	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
17	8	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
17	8	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
17	8	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
17	8	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
17	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	A	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
17	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	A	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
17	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
17	A	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
17	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	A	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
17	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	A	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
17	A	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
17	A	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
17	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	A	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
17	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	A	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
17	A	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
17	A	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
17	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	A	1	Total	C	Mg	N	O	0
			57	47	1	4	5	
17	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
17	A	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
17	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	A	1	Total	C	Mg	N	O	0
			64	54	1	4	5	
17	A	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
17	A	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
17	A	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
17	A	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
17	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	A	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
17	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
17	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	B	1	Total	C	Mg	N	O	0
			48	38	1	4	5	
17	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	B	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
17	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
17	B	1	Total	C	Mg	N	O	0
			55	45	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
17	B	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
17	B	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
17	B	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
17	B	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
17	B	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
17	B	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
17	B	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
17	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
17	B	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
17	B	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
17	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
17	B	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
17	B	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
17	B	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
17	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
17	B	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
17	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	B	1	Total	C	Mg	N	O	0
			55	45	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
17	B	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
17	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
17	B	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
17	B	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
17	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
17	B	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
17	B	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
17	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	F	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	F	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
17	F	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
17	F	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
17	F	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
17	J	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
17	K	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
17	K	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
17	K	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
17	K	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
17	T	1	Total	C	Mg	N	O	0
			50	40	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
17	T	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
17	T	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
17	T	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
17	T	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
17	T	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
17	T	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
17	T	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
17	T	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
17	T	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
17	T	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
17	a	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
17	a	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
17	a	1	Total	C	Mg	N	O	0
			48	38	1	4	5	
17	a	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
17	a	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
17	a	1	Total	C	Mg	N	O	0
			45	36	1	4	4	
17	a	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
17	a	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
17	a	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
17	a	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
17	a	1	Total	C	Mg	N	O	0
			46	36	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
17	a	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
17	b	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
17	b	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
17	b	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
17	b	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
17	b	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
17	b	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
17	b	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
17	b	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
17	b	1	Total	C	Mg	N	O	0
			48	38	1	4	5	
17	b	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
17	b	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
17	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	c	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
17	c	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
17	c	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
17	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	c	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
17	c	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
17	c	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
17	c	1	Total	C	Mg	N	O	0
			50	40	1	4	5	

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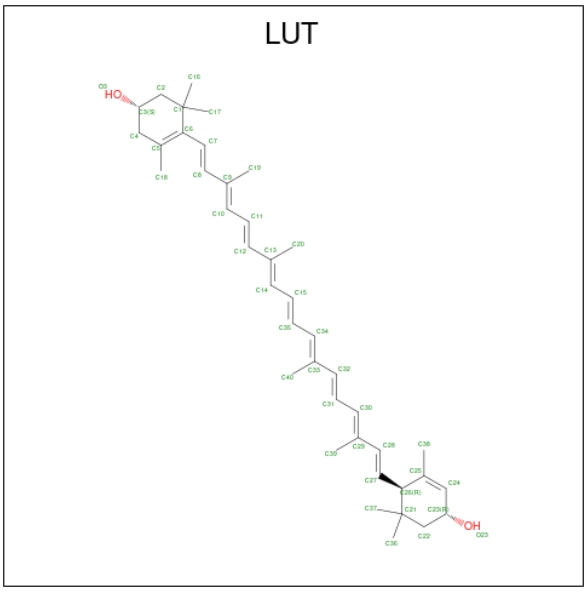
Mol	Chain	Residues	Atoms					AltConf
17	c	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
17	L	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
17	L	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

- Molecule 18 is (3R,3'R,6S)-4,5-DIDEHYDRO-5,6-DIHYDRO-BETA,BETA-CAROTENE-3,3'-DIOL (CCD ID: LUT) (formula: $C_{40}H_{56}O_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
18	1	1	Total	C	O	0
			42	40	2	
18	3	1	Total	C	O	0
			42	40	2	
18	7	1	Total	C	O	0
			42	40	2	
18	8	1	Total	C	O	0
			42	40	2	
18	T	1	Total	C	O	0
			42	40	2	
18	a	1	Total	C	O	0
			42	40	2	
18	b	1	Total	C	O	0
			42	40	2	

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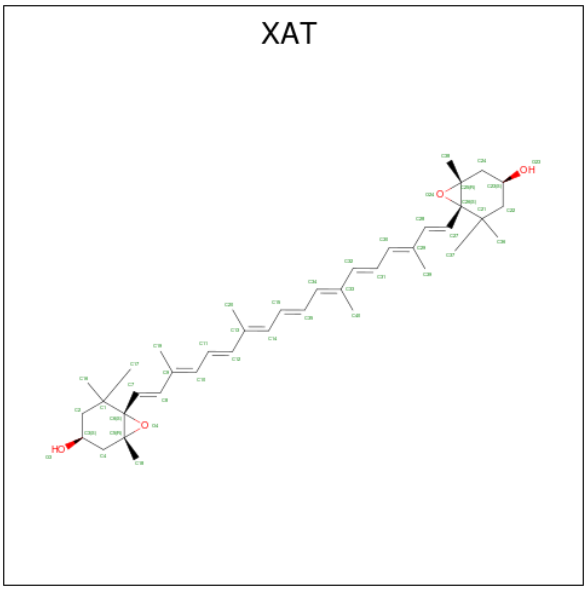
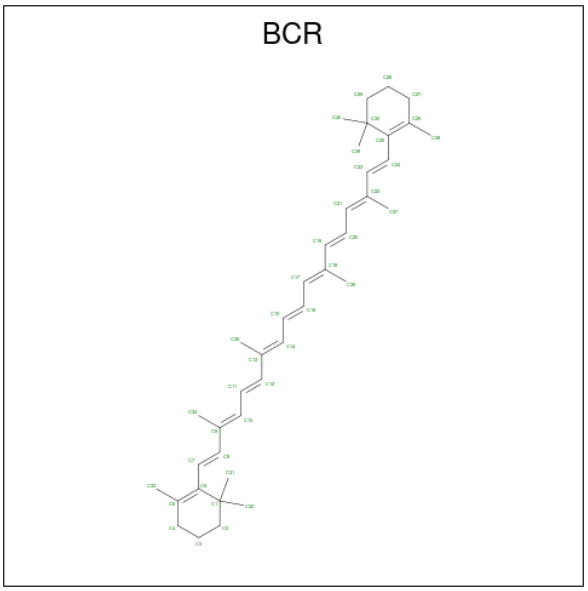
Mol	Chain	Residues	Atoms			AltConf
18	c	1	Total	C	O	0
			42	40	2	

- Molecule 19 is (3S,5R,6S,3'S,5'R,6'S)-5,6,5',6'-DIEPOXY-5,6,5',6'- TETRAHYDRO-BETA ,BETA-CAROTENE-3,3'-DIOL (CCD ID: XAT) (formula: $C_{40}H_{56}O_4$).



Mol	Chain	Residues	Atoms			AltConf
19	1	1	Total	C	O	0
			44	40	4	
19	3	1	Total	C	O	0
			44	40	4	
19	7	1	Total	C	O	0
			44	40	4	
19	8	1	Total	C	O	0
			44	40	4	
19	T	1	Total	C	O	0
			44	40	4	
19	a	1	Total	C	O	0
			44	40	4	
19	b	1	Total	C	O	0
			44	40	4	
19	c	1	Total	C	O	0
			44	40	4	

- Molecule 20 is BETA-CAROTENE (CCD ID: BCR) (formula: $C_{40}H_{56}$).



Mol	Chain	Residues	Atoms	AltConf
20	1	1	Total C 40 40	0
20	3	1	Total C 40 40	0
20	3	1	Total C 40 40	0
20	3	1	Total C 40 40	0
20	7	1	Total C 40 40	0
20	8	1	Total C 40 40	0
20	A	1	Total C 40 40	0
20	A	1	Total C 40 40	0
20	A	1	Total C 40 40	0
20	A	1	Total C 40 40	0
20	A	1	Total C 40 40	0
20	A	1	Total C 40 40	0
20	B	1	Total C 40 40	0
20	B	1	Total C 40 40	0

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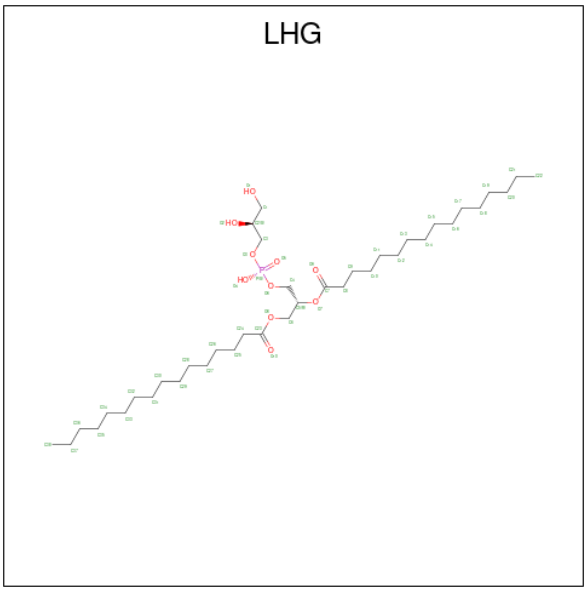
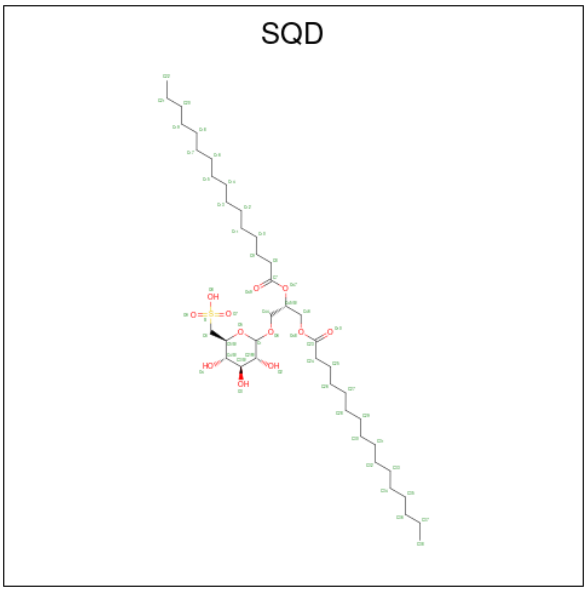
Mol	Chain	Residues	Atoms	AltConf
20	B	1	Total C 40 40	0
20	B	1	Total C 40 40	0
20	B	1	Total C 40 40	0
20	B	1	Total C 40 40	0
20	B	1	Total C 40 40	0
20	F	1	Total C 40 40	0
20	F	1	Total C 40 40	0
20	J	1	Total C 40 40	0
20	J	1	Total C 40 40	0
20	K	1	Total C 40 40	0
20	T	1	Total C 40 40	0
20	a	1	Total C 40 40	0
20	b	1	Total C 40 40	0
20	c	1	Total C 40 40	0
20	L	1	Total C 40 40	0
20	L	1	Total C 40 40	0
20	I	1	Total C 40 40	0

- Molecule 21 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: $C_{38}H_{75}O_{10}P$) (labeled as "Ligand of Interest" by depositor).



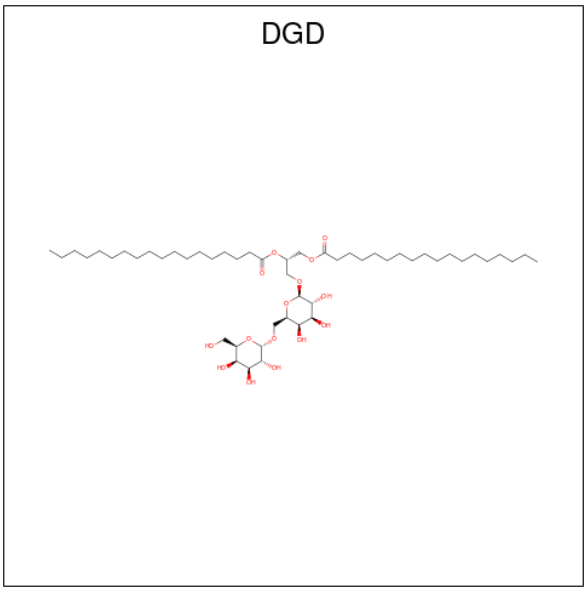
Mol	Chain	Residues	Atoms				AltConf
21	1	1	Total	C	O	P	0
			27	16	10	1	
21	1	1	Total	C	O	P	0
			31	20	10	1	
21	7	1	Total	C	O	P	0
			34	23	10	1	
21	8	1	Total	C	O	P	0
			30	19	10	1	
21	A	1	Total	C	O	P	0
			36	25	10	1	
21	A	1	Total	C	O	P	0
			49	38	10	1	
21	A	1	Total	C	O	P	0
			30	20	9	1	
21	F	1	Total	C	O	P	0
			31	20	10	1	
21	a	1	Total	C	O	P	0
			23	13	9	1	
21	a	1	Total	C	O	P	0
			23	12	10	1	
21	b	1	Total	C	O	P	0
			21	10	10	1	
21	c	1	Total	C	O	P	0
			28	17	10	1	

- Molecule 22 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
22	3	1	Total	C	O	S	0
			35	22	12	1	

- Molecule 23 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
23	3	1	Total	C	O	0
			50	35	15	
23	8	1	Total	C	O	0
			39	24	15	

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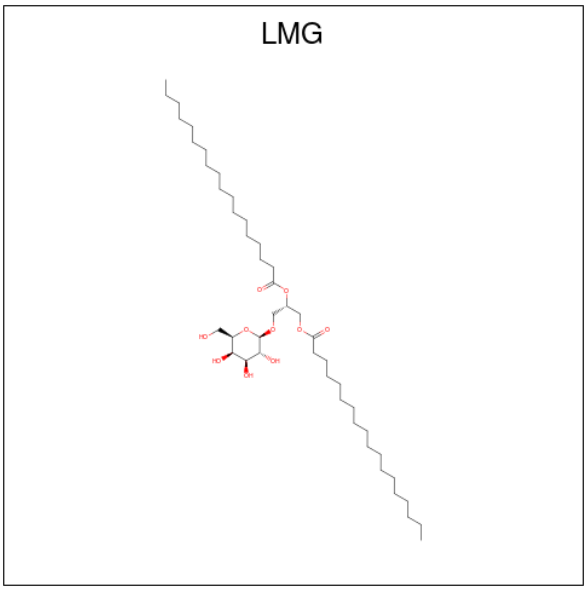
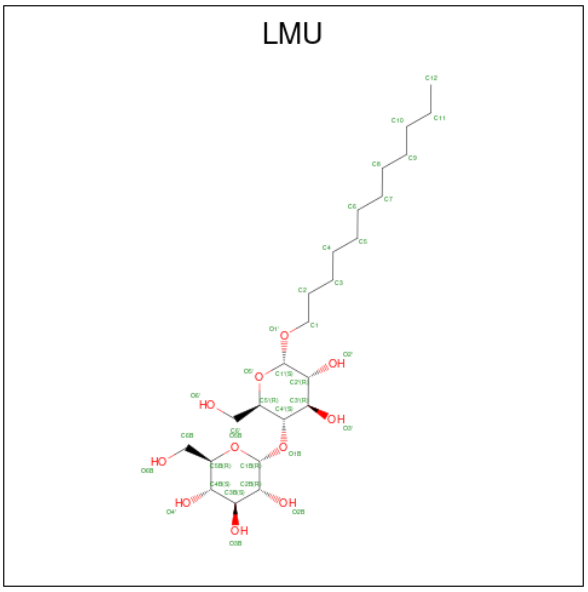
Mol	Chain	Residues	Atoms			AltConf
23	B	1	Total	C	O	0
			61	46	15	

- Molecule 24 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$) (labeled as "Ligand of Interest" by depositor).



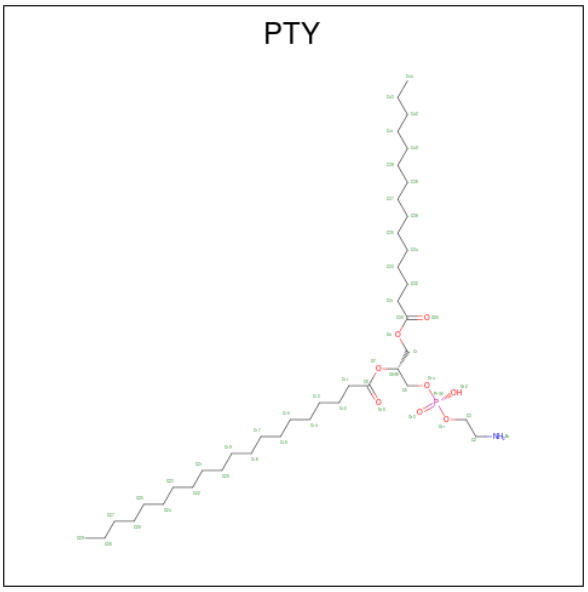
Mol	Chain	Residues	Atoms			AltConf
24	7	1	Total	C	O	0
			50	40	10	
24	A	1	Total	C	O	0
			32	22	10	
24	F	1	Total	C	O	0
			29	19	10	

- Molecule 25 is DODECYL-ALPHA-D-MALTOSIDE (CCD ID: LMU) (formula: $C_{24}H_{46}O_{11}$).



Mol	Chain	Residues	Atoms			AltConf
25	7	1	Total 35	C 24	O 11	0
25	A	1	Total 35	C 24	O 11	0

- Molecule 26 is PHOSPHATIDYLETHANOLAMINE (CCD ID: PTY) (formula: $C_{40}H_{80}NO_8P$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
26	8	1	Total 21	C 11	N 1	O 8	P 1	0

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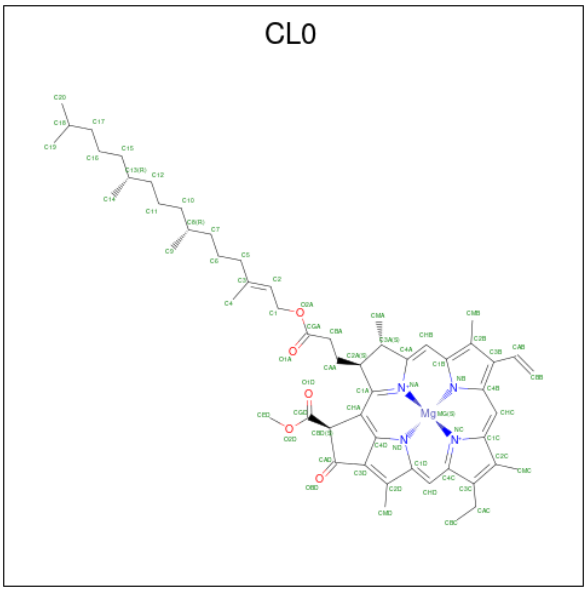
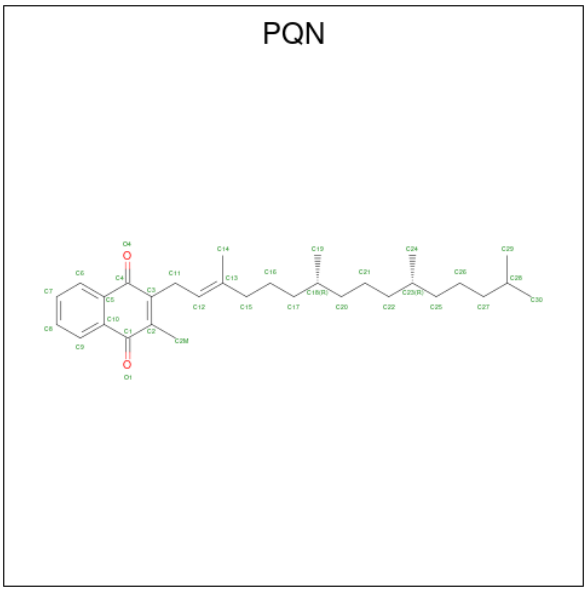
Mol	Chain	Residues	Atoms					AltConf
26	8	1	Total	C	N	O	P	0
			21	11	1	8	1	
26	F	1	Total	C	N	O	P	0
			33	23	1	8	1	
26	F	1	Total	C	N	O	P	0
			18	8	1	8	1	

- Molecule 27 is CHLOROPHYLL A ISOMER (CCD ID: CL0) (formula: $C_{55}H_{72}MgN_4O_5$) (labeled as "Ligand of Interest" by depositor).



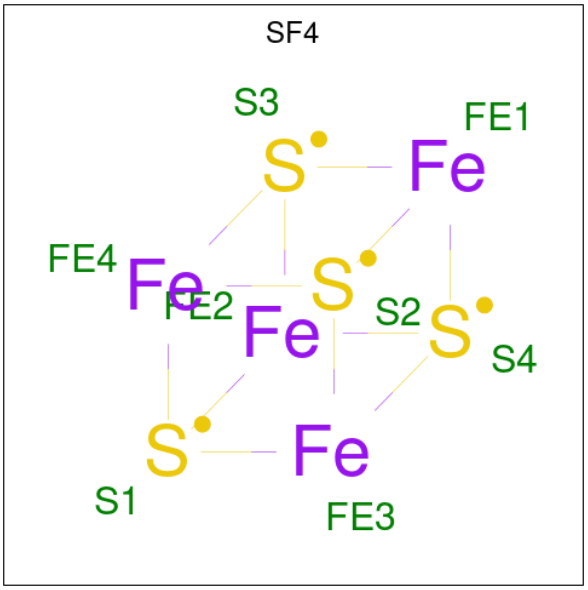
Mol	Chain	Residues	Atoms					AltConf
27	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

- Molecule 28 is PHYLLOQUINONE (CCD ID: PQN) (formula: $C_{31}H_{46}O_2$).



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

- Molecule 29 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



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

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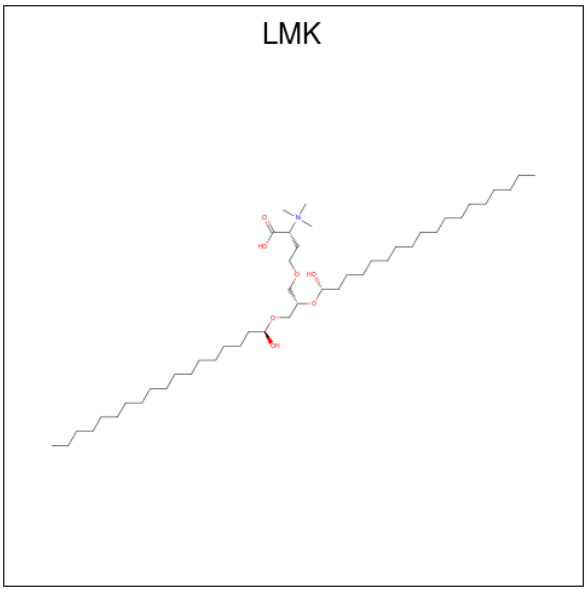
Mol	Chain	Residues	Atoms			AltConf
			Total	Fe	S	
29	C	1	8	4	4	0

- Molecule 30 is trimethyl-[(2 {R})-1-oxidanyl-1-oxidanylidene-4-[(2 {S})-2-[(1 {S})-1-oxidanyloctadecoxy]-3-[(1 {R})-1-oxidanyloctadecoxy]propoxy]butan-2-yl]azanium (CCD ID: LMK) (formula: $C_{46}H_{94}NO_7$) (labeled as "Ligand of Interest" by depositor).



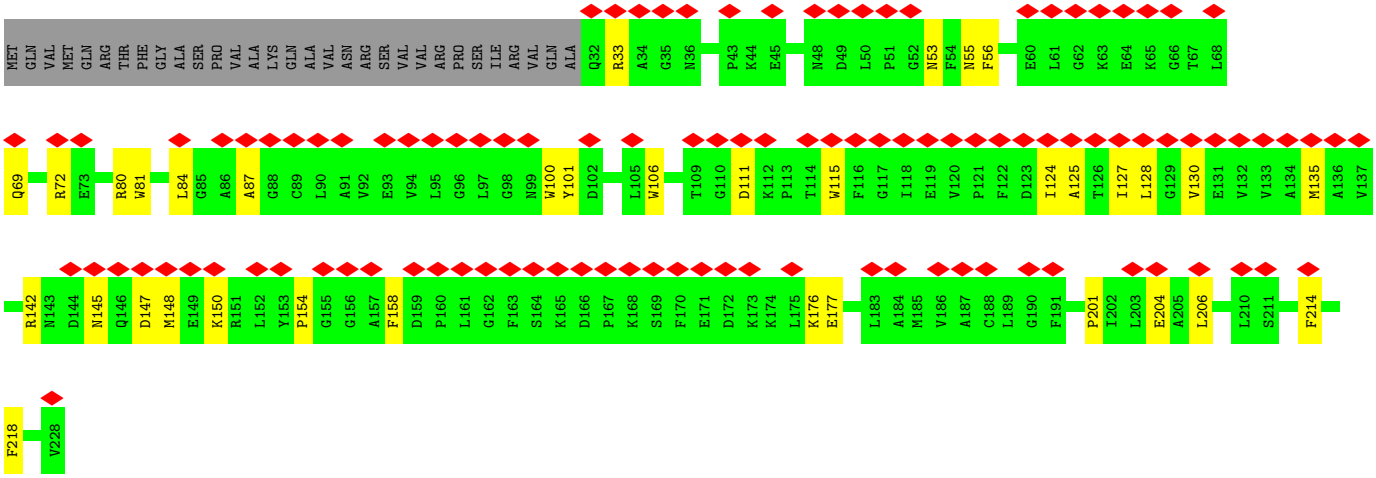
Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
30	J	1	35	27	1	7	0

3 Residue-property plots

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.

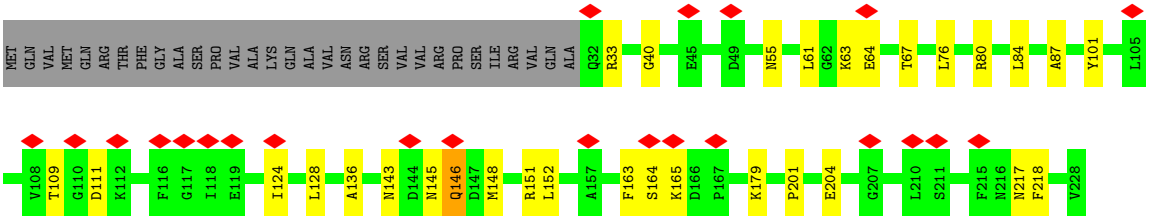
• Molecule 1: Chlorophyll a-b binding protein, chloroplastic

Chain 1:



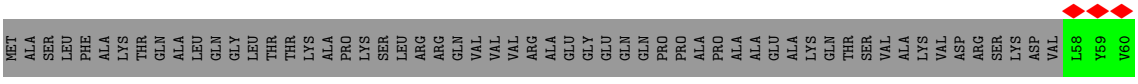
• Molecule 1: Chlorophyll a-b binding protein, chloroplastic

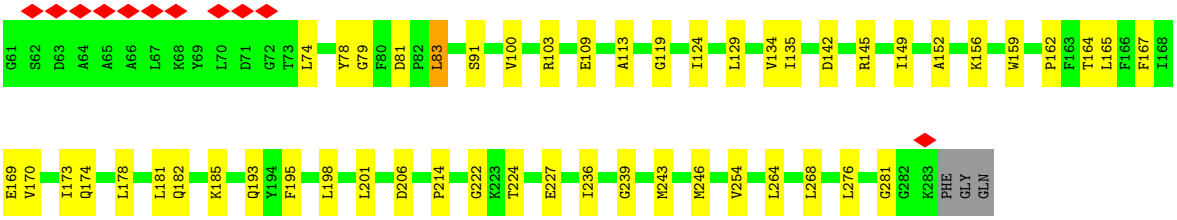
Chain a:



• Molecule 2: LHCA3

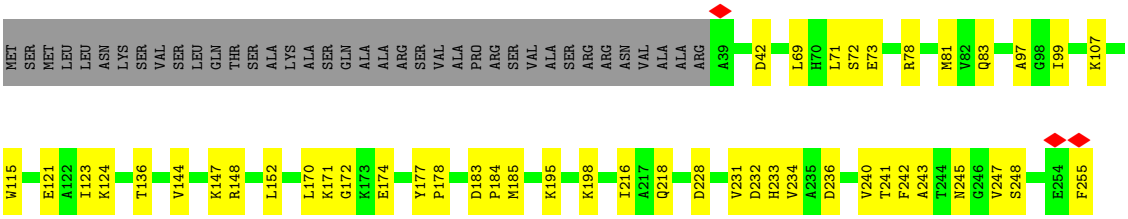
Chain 3:





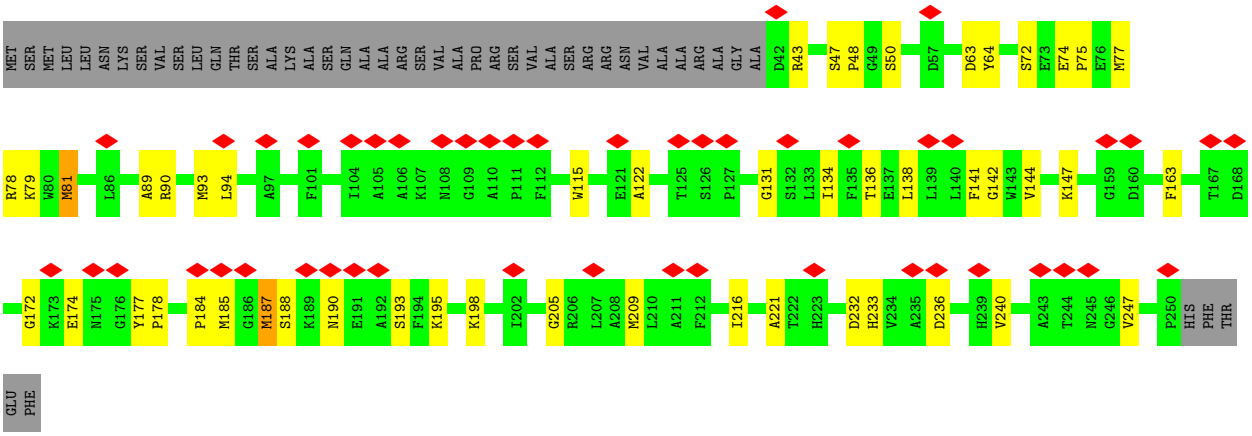
• Molecule 3: Chlorophyll a-b binding protein, chloroplastic

Chain 7:



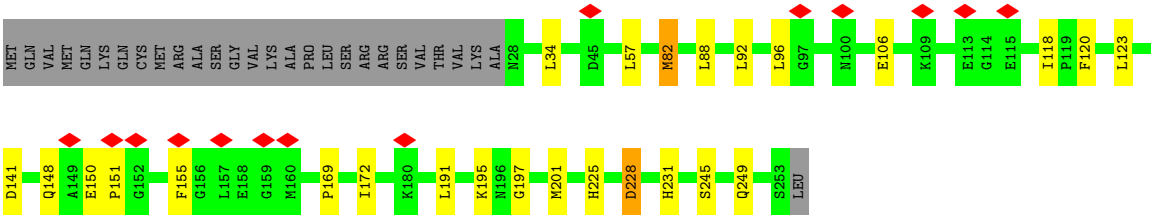
• Molecule 3: Chlorophyll a-b binding protein, chloroplastic

Chain c:



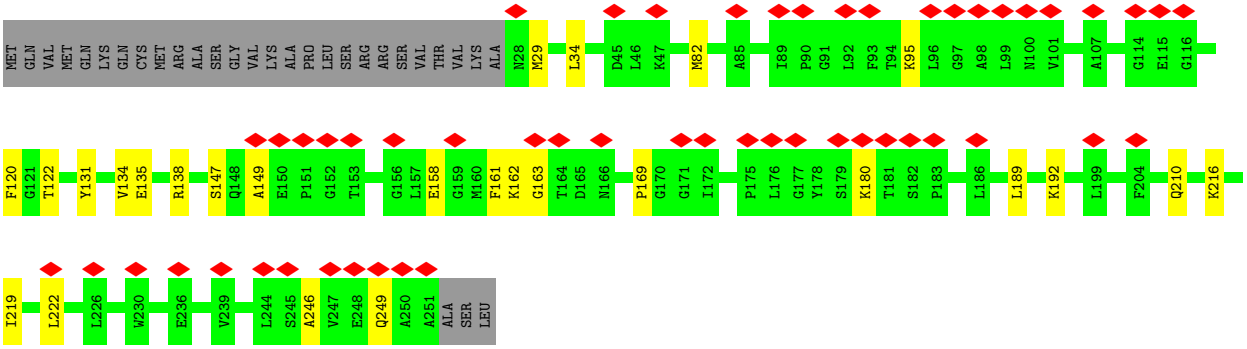
• Molecule 4: Chlorophyll a-b binding protein, chloroplastic

Chain 8:



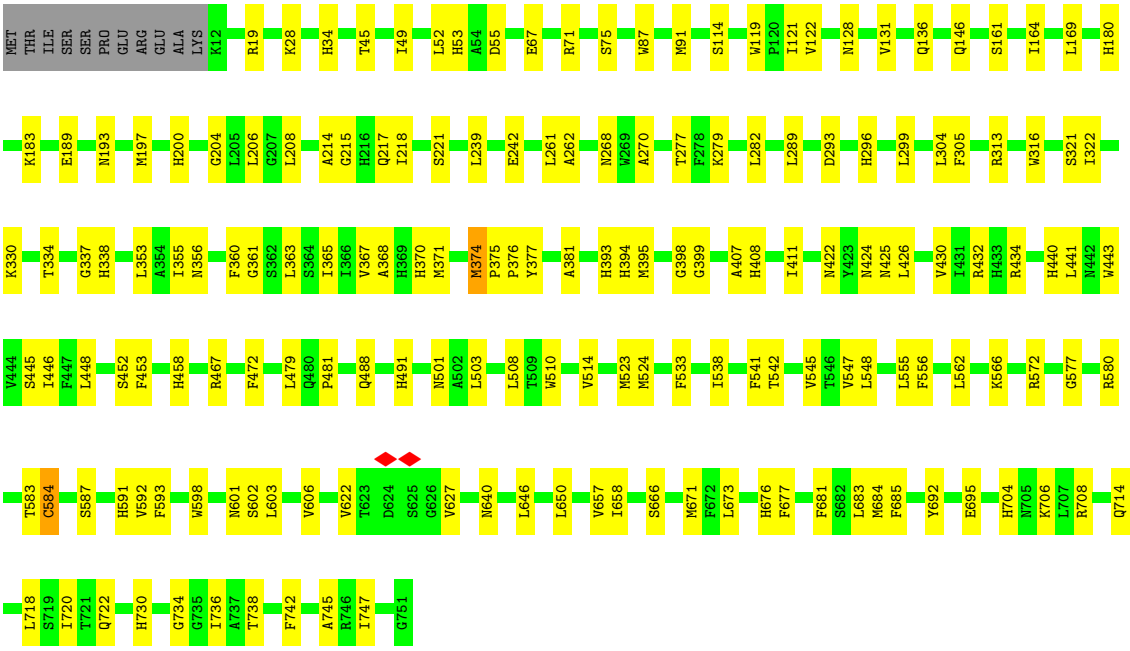
• Molecule 4: Chlorophyll a-b binding protein, chloroplastic

Chain b:



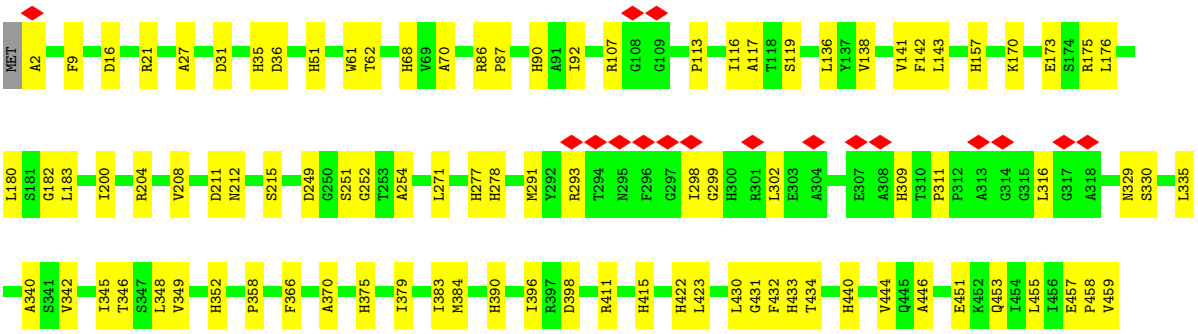
• Molecule 5: Photosystem I P700 chlorophyll a apoprotein A1

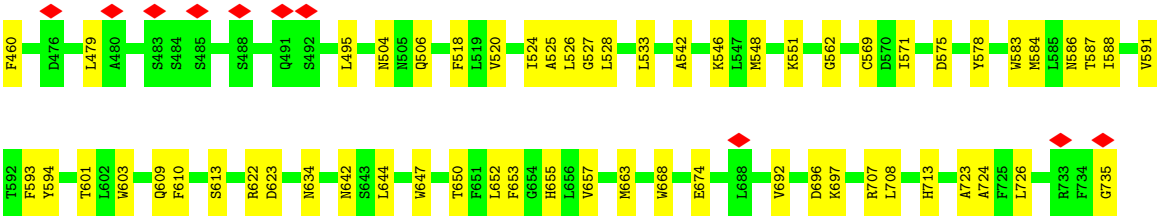
Chain A:



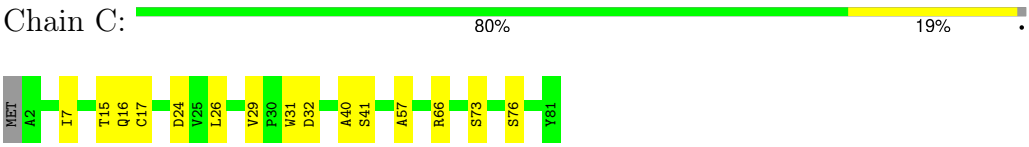
• Molecule 6: Photosystem I P700 chlorophyll a apoprotein A2

Chain B:

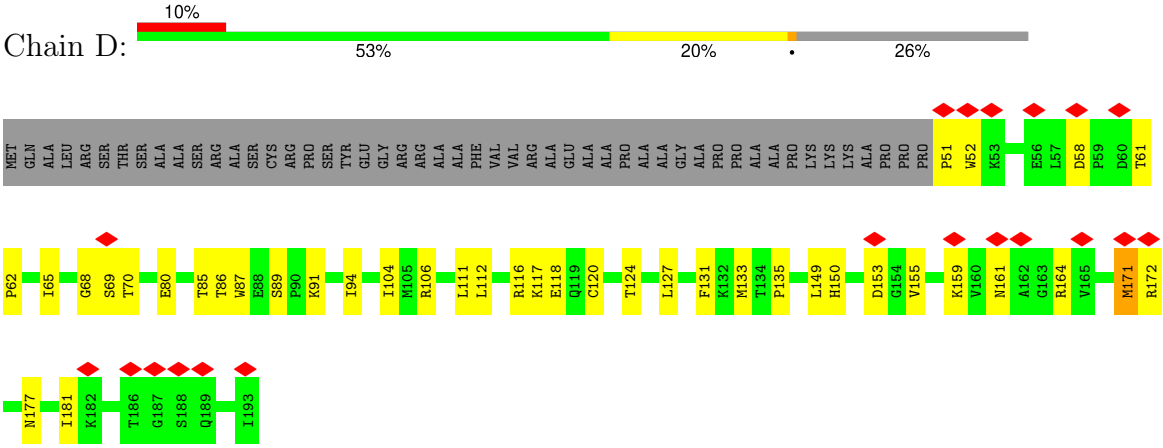




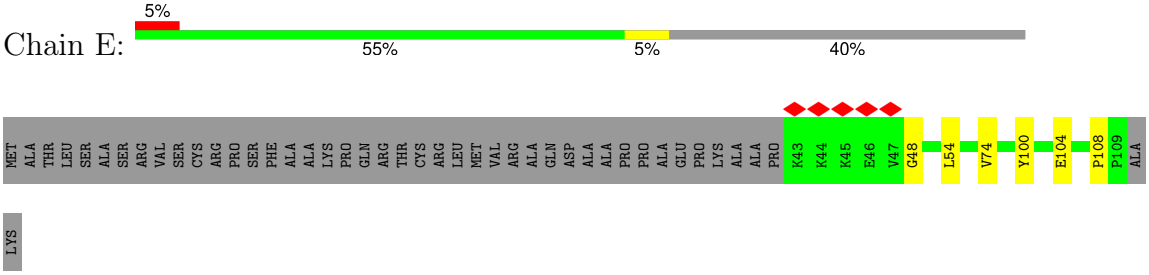
• Molecule 7: Photosystem I iron-sulfur center



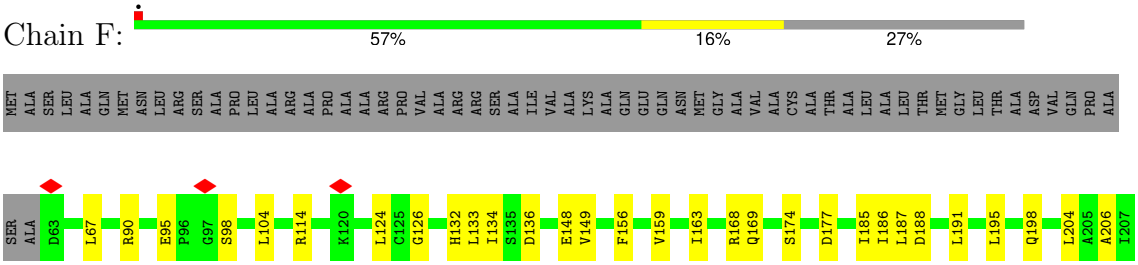
• Molecule 8: Photosystem I reaction center subunit II, chloroplastic



• Molecule 9: Photosystem I reaction center subunit IV

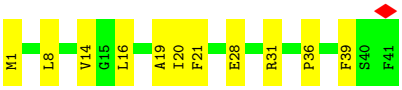


• Molecule 10: PSAF1



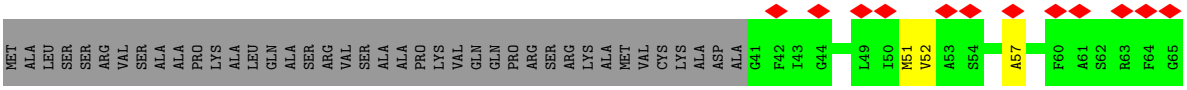
• Molecule 11: Photosystem I reaction center subunit IX

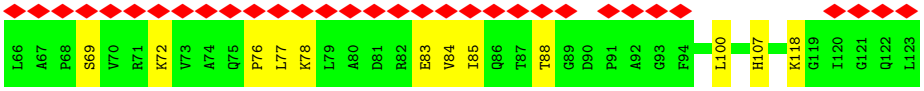
Chain J:



• Molecule 12: PSI-K

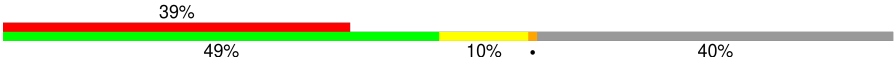
Chain K:

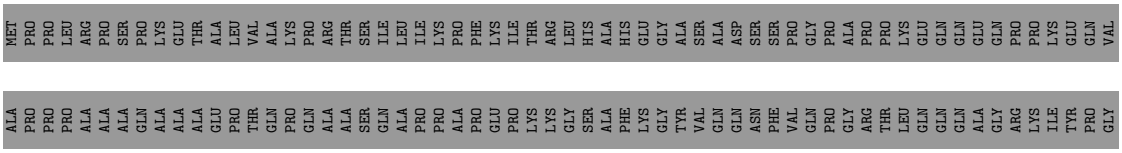


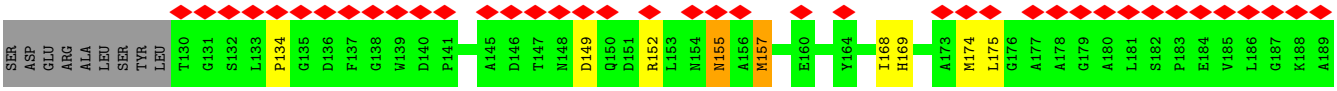


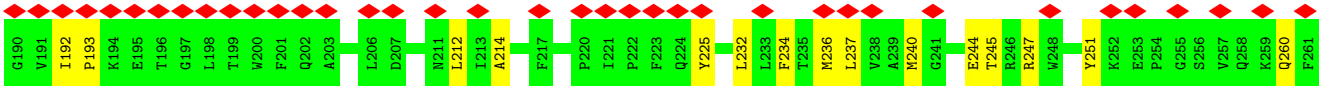
• Molecule 13: TIDI1

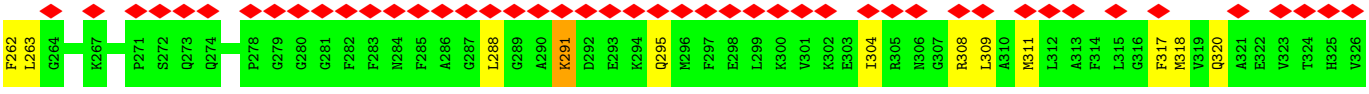
Chain T:

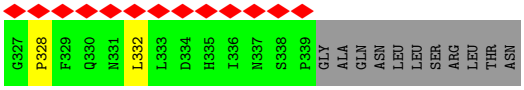






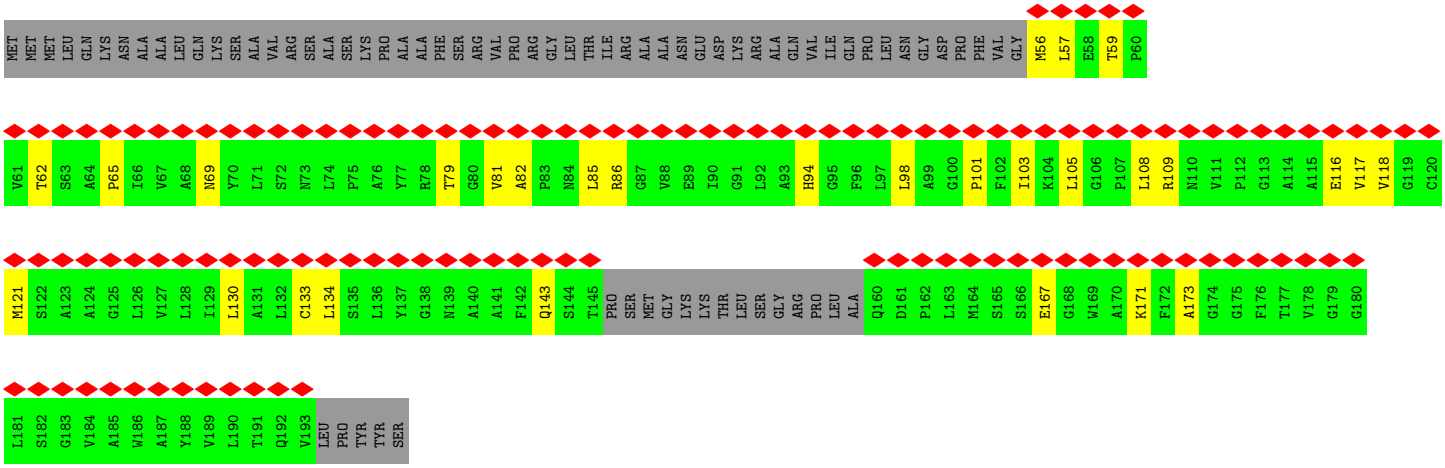




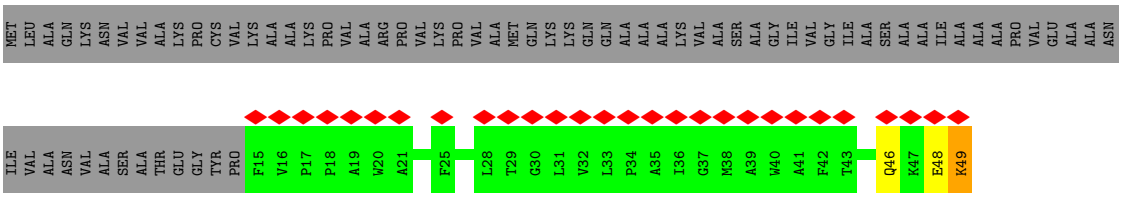


• Molecule 14: PSAL1

Chain L:



• Molecule 15: Photosystem I reaction center subunit VIII



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	217073	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	60	Depositor
Minimum defocus (nm)	900	Depositor
Maximum defocus (nm)	2100	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.083	Depositor
Minimum map value	-0.018	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.0151	Depositor
Map size (Å)	503.99997, 503.99997, 503.99997	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.05, 1.05, 1.05	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: BCR, LHG, LMG, SQD, SF4, LUT, LMU, CHL, XAT, LMK, DGD, PTY, CL0, CLA, PQN

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	1	0.19	0/1544	0.40	0/2093
1	a	0.16	0/1544	0.43	0/2093
2	3	0.16	0/1768	0.40	0/2402
3	7	0.14	0/1722	0.36	0/2339
3	c	0.16	0/1657	0.41	1/2251 (0.0%)
4	8	0.15	0/1770	0.38	1/2401 (0.0%)
4	b	0.14	0/1759	0.33	0/2386
5	A	0.14	0/6004	0.30	0/8190
6	B	0.14	0/6026	0.33	0/8235
7	C	0.11	0/610	0.30	0/828
8	D	0.13	0/1163	0.41	1/1571 (0.1%)
9	E	0.19	0/547	0.37	0/743
10	F	0.16	0/1329	0.36	0/1797
11	J	0.18	0/338	0.46	0/461
12	K	0.19	0/587	0.52	0/795
13	T	0.18	0/1688	0.47	0/2292
14	L	0.18	0/914	0.39	0/1248
15	I	0.19	0/286	0.41	0/394
All	All	0.15	0/31256	0.37	3/42519 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	8	82	MET	CB-CG-SD	5.25	128.45	112.70
3	c	81	MET	CB-CG-SD	5.23	128.40	112.70
8	D	171	MET	CB-CG-SD	5.06	127.89	112.70

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1	1505	0	1470	31	0
1	a	1505	0	1469	35	0
2	3	1719	0	1671	48	0
3	7	1669	0	1615	35	0
3	c	1607	0	1563	49	0
4	8	1721	0	1662	22	0
4	b	1710	0	1652	21	0
5	A	5808	0	5637	148	0
6	B	5814	0	5560	132	0
7	C	600	0	582	15	0
8	D	1133	0	1138	31	0
9	E	535	0	534	3	0
10	F	1300	0	1322	26	0
11	J	327	0	328	12	0
12	K	579	0	608	14	0
13	T	1639	0	1590	29	0
14	L	894	0	908	27	0
15	I	274	0	282	3	0
16	1	98	0	68	4	0
16	3	123	0	114	16	0
16	7	141	0	95	10	0
16	8	144	0	99	10	0
16	T	97	0	68	11	0
16	a	94	0	62	3	0
16	b	145	0	99	12	0
16	c	144	0	101	22	0
17	1	614	0	522	23	0
17	3	773	0	655	27	0
17	7	510	0	423	18	0
17	8	546	0	431	18	0
17	A	2453	0	2473	140	0
17	B	2252	0	2113	107	0
17	F	263	0	230	8	0
17	J	49	0	39	3	0
17	K	181	0	132	7	0
17	L	110	0	101	4	0
17	T	531	0	401	13	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
17	a	578	0	441	15	0
17	b	551	0	440	14	0
17	c	526	0	457	27	0
18	1	42	0	56	6	0
18	3	42	0	56	3	0
18	7	42	0	56	3	0
18	8	42	0	56	1	0
18	T	42	0	47	4	0
18	a	42	0	56	4	0
18	b	42	0	56	1	0
18	c	42	0	56	0	0
19	1	44	0	56	1	0
19	3	44	0	56	4	0
19	7	44	0	56	6	0
19	8	44	0	56	1	0
19	T	44	0	56	2	0
19	a	44	0	56	1	0
19	b	44	0	56	0	0
19	c	44	0	55	1	0
20	1	40	0	54	8	0
20	3	120	0	163	9	0
20	7	40	0	56	3	0
20	8	40	0	56	5	0
20	A	240	0	336	24	0
20	B	280	0	391	21	0
20	F	80	0	112	9	0
20	I	40	0	53	2	0
20	J	80	0	112	6	0
20	K	40	0	55	5	0
20	L	80	0	110	6	0
20	T	40	0	56	3	0
20	a	40	0	56	4	0
20	b	40	0	56	6	0
20	c	40	0	56	2	0
21	1	58	0	56	2	0
21	7	34	0	37	0	0
21	8	30	0	30	2	0
21	A	115	0	143	9	0
21	F	31	0	31	0	0
21	a	46	0	29	2	0
21	b	21	0	12	0	0
21	c	28	0	25	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
22	3	35	0	33	5	0
23	3	50	0	56	1	0
23	8	39	0	36	2	0
23	B	61	0	83	8	0
24	7	50	0	73	5	0
24	A	32	0	27	2	0
24	F	29	0	28	1	0
25	7	35	0	46	3	0
25	A	35	0	46	1	0
26	8	42	0	30	0	0
26	F	51	0	49	0	0
27	A	65	0	72	8	0
28	A	33	0	46	2	0
28	B	33	0	46	3	0
29	A	8	0	0	0	0
29	C	16	0	0	1	0
30	J	35	0	0	0	0
All	All	44202	0	42797	957	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 11.

The worst 5 of 957 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)
14:L:81:VAL:CG1	14:L:85:LEU:HD12	1.67	1.23
1:a:76:LEU:HD12	1:a:152:LEU:CD2	1.71	1.20
5:A:646:LEU:HD22	6:B:652:LEU:HD21	1.24	1.18
1:a:76:LEU:CD1	1:a:152:LEU:HD22	1.73	1.17
1:1:201:PRO:HD2	1:1:204:GLU:OE1	1.43	1.16

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	1	195/228 (86%)	187 (96%)	7 (4%)	1 (0%)	25 56
1	a	195/228 (86%)	184 (94%)	9 (5%)	2 (1%)	13 39
2	3	224/286 (78%)	213 (95%)	11 (5%)	0	100 100
3	7	215/255 (84%)	206 (96%)	9 (4%)	0	100 100
3	c	207/255 (81%)	201 (97%)	6 (3%)	0	100 100
4	8	224/254 (88%)	221 (99%)	3 (1%)	0	100 100
4	b	222/254 (87%)	217 (98%)	5 (2%)	0	100 100
5	A	738/751 (98%)	715 (97%)	23 (3%)	0	100 100
6	B	732/735 (100%)	711 (97%)	21 (3%)	0	100 100
7	C	78/81 (96%)	75 (96%)	3 (4%)	0	100 100
8	D	141/193 (73%)	131 (93%)	10 (7%)	0	100 100
9	E	65/111 (59%)	62 (95%)	3 (5%)	0	100 100
10	F	163/227 (72%)	154 (94%)	9 (6%)	0	100 100
11	J	39/41 (95%)	38 (97%)	1 (3%)	0	100 100
12	K	81/123 (66%)	72 (89%)	9 (11%)	0	100 100
13	T	208/350 (59%)	200 (96%)	8 (4%)	0	100 100
14	L	120/198 (61%)	118 (98%)	2 (2%)	0	100 100
15	I	33/108 (31%)	33 (100%)	0	0	100 100
All	All	3880/4678 (83%)	3738 (96%)	139 (4%)	3 (0%)	50 77

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	a	146	GLN
1	a	64	GLU
1	1	55	ASN

5.3.2 Protein sidechains (i)

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

The Analysed column shows the number of residues for which the sidechain conformation was

analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	1	153/179 (86%)	153 (100%)	0	100 100
1	a	153/179 (86%)	153 (100%)	0	100 100
2	3	170/217 (78%)	169 (99%)	1 (1%)	84 95
3	7	171/201 (85%)	168 (98%)	3 (2%)	54 83
3	c	166/201 (83%)	165 (99%)	1 (1%)	84 95
4	8	173/197 (88%)	172 (99%)	1 (1%)	84 95
4	b	172/197 (87%)	168 (98%)	4 (2%)	45 78
5	A	599/609 (98%)	596 (100%)	3 (0%)	86 95
6	B	595/596 (100%)	592 (100%)	3 (0%)	86 95
7	C	68/69 (99%)	68 (100%)	0	100 100
8	D	123/156 (79%)	123 (100%)	0	100 100
9	E	60/93 (64%)	60 (100%)	0	100 100
10	F	136/177 (77%)	135 (99%)	1 (1%)	81 94
11	J	36/36 (100%)	36 (100%)	0	100 100
12	K	58/88 (66%)	58 (100%)	0	100 100
13	T	169/280 (60%)	161 (95%)	8 (5%)	22 54
14	L	91/150 (61%)	90 (99%)	1 (1%)	70 90
15	I	28/76 (37%)	27 (96%)	1 (4%)	30 64
All	All	3121/3701 (84%)	3094 (99%)	27 (1%)	74 92

5 of 27 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
13	T	174	MET
13	T	291	LYS
3	c	187	MET
13	T	240	MET
13	T	317	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 38 such sidechains are listed below:

Mol	Chain	Res	Type
4	b	30	ASN
14	L	69	ASN

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Mol	Chain	Res	Type
4	b	140	GLN
3	c	154	ASN
15	I	46	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

284 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
26	PTY	F	5003	-	17,17,49	0.70	0	18,21,54	0.60	0
17	CLA	A	5038	5	48,58,73	1.54	6 (12%)	56,95,113	1.55	7 (12%)
17	CLA	b	604	-	48,58,73	1.56	6 (12%)	56,95,113	1.55	7 (12%)
16	CHL	c	305	-	48,58,74	1.20	5 (10%)	50,94,114	2.20	8 (16%)
17	CLA	B	835	-	48,58,73	1.55	6 (12%)	56,95,113	1.54	8 (14%)
20	BCR	T	415	-	41,41,41	0.12	0	56,56,56	0.28	0
16	CHL	T	401	13	49,59,74	1.40	4 (8%)	53,96,114	2.50	11 (20%)
17	CLA	A	5021	5	48,58,73	1.50	6 (12%)	56,95,113	1.42	8 (14%)
17	CLA	b	614	4	44,54,73	1.61	5 (11%)	51,90,113	1.40	6 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
17	CLA	A	5011	5	63,73,73	1.33	6 (9%)	74,113,113	1.23	8 (10%)
16	CHL	8	308	-	49,59,74	1.30	4 (8%)	53,96,114	2.52	7 (13%)
17	CLA	1	608	-	43,53,73	1.63	5 (11%)	50,89,113	1.48	6 (12%)
17	CLA	8	302	4	44,54,73	1.58	5 (11%)	51,90,113	1.55	7 (13%)
17	CLA	7	313	3	48,58,73	1.54	5 (10%)	56,95,113	1.43	8 (14%)
17	CLA	3	302	2	63,73,73	1.36	7 (11%)	74,113,113	1.32	6 (8%)
17	CLA	1	614	1	44,54,73	1.60	5 (11%)	51,90,113	1.50	6 (11%)
17	CLA	3	306	-	53,63,73	1.44	6 (11%)	62,101,113	1.37	8 (12%)
19	XAT	c	315	-	41,47,47	0.16	0	54,74,74	0.76	2 (3%)
16	CHL	T	416	-	44,54,74	1.42	5 (11%)	47,90,114	2.28	8 (17%)
17	CLA	T	409	-	50,60,73	1.54	5 (10%)	57,97,113	1.62	10 (17%)
17	CLA	3	323	5	53,63,73	1.44	5 (9%)	62,101,113	1.36	7 (11%)
17	CLA	B	802	6	63,73,73	1.37	7 (11%)	74,113,113	1.15	7 (9%)
23	DGD	B	848	-	62,62,67	0.18	0	76,76,81	0.23	0
17	CLA	a	608	1	43,53,73	1.62	5 (11%)	49,88,113	1.59	7 (14%)
21	LHG	A	5055	17	29,29,48	0.37	0	33,35,54	0.33	0
17	CLA	A	5025	5	58,68,73	1.40	6 (10%)	68,107,113	1.34	7 (10%)
21	LHG	a	619	17	22,22,48	0.40	0	25,28,54	0.38	0
17	CLA	7	308	3	44,54,73	1.59	4 (9%)	51,90,113	1.50	6 (11%)
17	CLA	B	815	-	48,58,73	1.52	5 (10%)	56,95,113	1.49	8 (14%)
17	CLA	B	839	6	63,73,73	1.35	7 (11%)	74,113,113	1.22	8 (10%)
17	CLA	B	806	6	63,73,73	1.34	7 (11%)	74,113,113	1.22	6 (8%)
18	LUT	T	413	-	42,43,43	0.37	0	51,60,60	0.63	2 (3%)
17	CLA	c	309	21	58,68,73	1.40	5 (8%)	68,107,113	1.38	8 (11%)
17	CLA	A	5027	-	55,65,73	1.49	6 (10%)	64,103,113	1.30	8 (12%)
17	CLA	A	5019	5	59,69,73	1.43	7 (11%)	69,108,113	1.38	6 (8%)
17	CLA	B	823	6	48,58,73	1.52	4 (8%)	56,95,113	1.35	7 (12%)
17	CLA	B	829	6	63,73,73	1.38	5 (7%)	74,113,113	1.25	7 (9%)
17	CLA	B	820	-	53,63,73	1.49	5 (9%)	62,101,113	1.42	7 (11%)
16	CHL	c	304	-	44,54,74	1.33	4 (9%)	47,90,114	2.21	4 (8%)
17	CLA	A	5020	5	63,73,73	1.33	6 (9%)	74,113,113	1.30	8 (10%)
20	BCR	b	617	-	41,41,41	0.14	0	56,56,56	0.37	0
26	PTY	F	5002	-	32,32,49	0.56	0	35,37,54	0.45	0
17	CLA	8	313	4	49,59,73	1.63	6 (12%)	56,96,113	1.36	7 (12%)
17	CLA	B	812	6	44,54,73	1.60	5 (11%)	51,90,113	1.43	6 (11%)
17	CLA	b	609	4	58,68,73	1.36	6 (10%)	68,107,113	1.22	6 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
18	LUT	b	615	-	42,43,43	0.23	0	51,60,60	0.42	0
20	BCR	B	846	-	41,41,41	0.15	0	56,56,56	0.21	0
17	CLA	F	5007	-	45,55,73	1.56	6 (13%)	52,91,113	1.33	7 (13%)
16	CHL	7	306	-	45,55,74	1.21	5 (11%)	48,91,114	2.46	9 (18%)
17	CLA	8	312	4	48,58,73	1.60	8 (16%)	56,95,113	1.54	9 (16%)
17	CLA	A	5004	-	63,73,73	1.32	6 (9%)	74,113,113	1.21	6 (8%)
17	CLA	T	406	-	48,58,73	1.54	5 (10%)	56,95,113	1.47	8 (14%)
17	CLA	A	5017	-	53,63,73	1.48	5 (9%)	62,101,113	1.47	7 (11%)
16	CHL	3	301	2	60,70,74	1.20	4 (6%)	66,109,114	1.91	8 (12%)
20	BCR	L	204	-	41,41,41	0.14	0	56,56,56	0.24	0
25	LMU	A	5054	-	36,36,36	0.13	0	47,47,47	0.19	0
17	CLA	7	304	-	48,58,73	1.60	6 (12%)	56,95,113	1.51	8 (14%)
20	BCR	3	319	-	41,41,41	0.19	0	56,56,56	0.29	0
29	SF4	C	101	7	0,12,12	-	-	-		
17	CLA	A	5018	5	58,68,73	1.39	6 (10%)	68,107,113	1.31	6 (8%)
17	CLA	b	602	4	58,68,73	1.37	5 (8%)	68,107,113	1.25	7 (10%)
17	CLA	c	307	3	48,58,73	1.48	6 (12%)	56,95,113	1.84	9 (16%)
17	CLA	3	303	-	44,54,73	1.59	5 (11%)	51,90,113	1.50	6 (11%)
20	BCR	B	843	-	41,41,41	0.16	0	56,56,56	0.31	0
17	CLA	B	841	-	63,73,73	1.34	5 (7%)	74,113,113	1.27	7 (9%)
17	CLA	T	402	13	48,58,73	1.53	6 (12%)	56,95,113	1.47	8 (14%)
17	CLA	B	803	-	63,73,73	1.30	6 (9%)	74,113,113	1.27	6 (8%)
17	CLA	B	810	6	53,63,73	1.47	5 (9%)	62,101,113	1.42	6 (9%)
17	CLA	F	5009	10	44,54,73	1.61	5 (11%)	51,90,113	1.58	6 (11%)
17	CLA	A	5043	21	43,53,73	1.59	6 (13%)	50,89,113	1.48	7 (14%)
17	CLA	a	611	1	44,54,73	1.61	6 (13%)	51,90,113	1.60	8 (15%)
17	CLA	c	303	-	48,58,73	1.54	5 (10%)	56,95,113	1.45	7 (12%)
21	LHG	A	5002	-	35,35,48	0.35	0	38,41,54	0.37	0
29	SF4	C	102	7	0,12,12	-	-	-		
16	CHL	b	606	-	45,55,74	1.26	5 (11%)	48,91,114	2.22	9 (18%)
17	CLA	A	5007	17	58,68,73	1.37	4 (6%)	68,107,113	1.24	6 (8%)
17	CLA	B	833	6	58,68,73	1.40	5 (8%)	68,107,113	1.32	7 (10%)
17	CLA	8	310	4	58,68,73	1.35	5 (8%)	68,107,113	1.25	6 (8%)
17	CLA	7	310	21	44,54,73	1.59	4 (9%)	51,90,113	1.37	6 (11%)
17	CLA	7	312	3	63,73,73	1.40	6 (9%)	74,113,113	1.35	8 (10%)
17	CLA	A	5039	5	53,63,73	1.44	5 (9%)	62,101,113	1.35	8 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
19	XAT	T	414	-	41,47,47	0.15	0	54,74,74	0.72	1 (1%)
17	CLA	K	203	12	43,53,73	1.64	6 (13%)	50,89,113	1.40	6 (12%)
17	CLA	T	405	13	43,53,73	1.62	5 (11%)	50,89,113	1.46	7 (14%)
17	CLA	A	5044	-	63,73,73	1.30	5 (7%)	74,113,113	1.27	7 (9%)
17	CLA	B	838	-	53,63,73	1.50	7 (13%)	62,101,113	1.41	7 (11%)
18	LUT	1	615	-	42,43,43	0.20	0	51,60,60	1.47	8 (15%)
17	CLA	c	302	3	44,54,73	1.57	6 (13%)	51,90,113	1.40	6 (11%)
21	LHG	8	321	17	29,29,48	0.37	0	32,35,54	0.35	0
17	CLA	c	301	3	63,73,73	1.34	5 (7%)	74,113,113	1.22	8 (10%)
16	CHL	3	322	-	59,69,74	1.42	4 (6%)	65,108,114	1.90	7 (10%)
19	XAT	b	616	-	41,47,47	0.14	0	54,74,74	0.79	2 (3%)
20	BCR	A	5047	-	41,41,41	0.17	0	56,56,56	0.32	0
17	CLA	B	821	-	41,51,73	1.63	5 (12%)	47,86,113	1.42	6 (12%)
17	CLA	7	311	3	44,54,73	1.62	6 (13%)	51,90,113	1.58	8 (15%)
20	BCR	J	103	-	41,41,41	0.15	0	56,56,56	0.27	0
17	CLA	L	201	14	63,73,73	1.31	6 (9%)	74,113,113	1.18	7 (9%)
17	CLA	A	5033	5	53,63,73	1.46	5 (9%)	62,101,113	1.30	7 (11%)
17	CLA	B	809	6	58,68,73	1.41	5 (8%)	68,107,113	1.31	7 (10%)
17	CLA	A	5041	5	63,73,73	1.31	5 (7%)	74,113,113	1.29	8 (10%)
17	CLA	1	603	1	43,53,73	1.65	6 (13%)	50,89,113	1.53	6 (12%)
17	CLA	1	604	-	48,58,73	1.51	5 (10%)	56,95,113	1.44	7 (12%)
17	CLA	B	832	6	53,63,73	1.46	6 (11%)	62,101,113	1.30	9 (14%)
17	CLA	T	407	13	48,58,73	1.51	6 (12%)	56,95,113	1.37	8 (14%)
19	XAT	3	316	-	41,47,47	0.14	0	54,74,74	0.78	2 (3%)
21	LHG	A	5053	-	48,48,48	0.29	0	51,54,54	0.29	0
24	LMG	F	5011	-	29,29,55	0.20	0	37,37,63	0.15	0
17	CLA	F	5004	6	63,73,73	1.46	9 (14%)	74,113,113	1.49	8 (10%)
21	LHG	c	317	17	27,27,48	0.37	0	30,33,54	0.35	0
17	CLA	b	612	4	46,56,73	1.65	6 (13%)	53,92,113	1.41	7 (13%)
21	LHG	b	618	17	20,20,48	0.39	0	23,26,54	0.39	0
17	CLA	T	410	13	48,58,73	1.53	5 (10%)	56,95,113	1.46	8 (14%)
19	XAT	1	616	-	41,47,47	0.15	0	54,74,74	0.97	3 (5%)
17	CLA	3	310	2	44,54,73	1.61	6 (13%)	51,90,113	1.55	6 (11%)
17	CLA	3	312	2	44,54,73	1.56	6 (13%)	51,90,113	1.35	6 (11%)
17	CLA	B	819	-	58,68,73	1.44	6 (10%)	68,107,113	1.36	6 (8%)
20	BCR	L	203	-	41,41,41	0.14	0	56,56,56	0.36	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
17	CLA	F	5008	10	43,53,73	1.62	5 (11%)	50,89,113	1.44	6 (12%)
17	CLA	c	312	3	48,58,73	1.57	6 (12%)	56,95,113	1.38	8 (14%)
16	CHL	a	601	-	45,55,74	1.49	5 (11%)	48,91,114	2.03	8 (16%)
17	CLA	A	5012	5	53,63,73	1.48	7 (13%)	62,101,113	1.48	9 (14%)
17	CLA	B	822	6	43,53,73	1.61	5 (11%)	50,89,113	1.52	6 (12%)
17	CLA	B	811	6	48,58,73	1.57	5 (10%)	56,95,113	1.41	7 (12%)
17	CLA	K	202	-	44,54,73	1.58	5 (11%)	51,90,113	1.37	7 (13%)
17	CLA	A	5026	-	63,73,73	1.37	6 (9%)	74,113,113	1.41	6 (8%)
27	CL0	A	5003	5	63,73,73	1.17	4 (6%)	74,113,113	1.88	8 (10%)
19	XAT	7	316	-	41,47,47	0.18	0	54,74,74	0.85	3 (5%)
21	LHG	7	318	17	33,33,48	0.35	0	36,39,54	0.34	0
17	CLA	7	314	3	44,54,73	1.57	5 (11%)	51,90,113	1.45	6 (11%)
17	CLA	1	607	-	63,73,73	1.34	5 (7%)	74,113,113	1.22	7 (9%)
17	CLA	3	305	2	48,58,73	1.50	6 (12%)	56,95,113	1.41	8 (14%)
16	CHL	8	306	-	44,54,74	1.76	4 (9%)	47,90,114	1.83	7 (14%)
17	CLA	B	824	-	48,58,73	1.53	7 (14%)	56,95,113	1.64	8 (14%)
17	CLA	1	609	1	63,73,73	1.32	6 (9%)	74,113,113	1.33	6 (8%)
17	CLA	F	5006	-	58,68,73	1.37	5 (8%)	68,107,113	1.24	7 (10%)
17	CLA	b	603	4	48,58,73	1.57	7 (14%)	56,95,113	1.55	7 (12%)
17	CLA	b	611	4	48,58,73	1.59	6 (12%)	56,95,113	1.54	9 (16%)
17	CLA	c	311	-	48,58,73	1.56	5 (10%)	56,95,113	1.45	7 (12%)
20	BCR	A	5051	-	41,41,41	0.14	0	56,56,56	0.25	0
17	CLA	A	5013	17,5	63,73,73	1.29	5 (7%)	74,113,113	1.24	9 (12%)
17	CLA	8	315	4	43,53,73	1.63	5 (11%)	50,89,113	1.42	6 (12%)
20	BCR	B	847	-	41,41,41	0.12	0	56,56,56	0.35	0
17	CLA	a	609	1	58,68,73	1.38	6 (10%)	68,107,113	1.22	7 (10%)
17	CLA	A	5016	5	63,73,73	1.36	7 (11%)	74,113,113	1.40	9 (12%)
17	CLA	A	5037	5	48,58,73	1.55	6 (12%)	56,95,113	1.44	8 (14%)
17	CLA	a	612	-	48,58,73	1.55	6 (12%)	56,95,113	1.41	7 (12%)
17	CLA	7	309	3	44,54,73	1.53	6 (13%)	51,90,113	1.31	5 (9%)
17	CLA	B	826	6	63,73,73	1.39	6 (9%)	74,113,113	1.37	7 (9%)
18	LUT	3	315	-	42,43,43	0.20	0	51,60,60	0.35	0
17	CLA	A	5031	5	63,73,73	1.38	6 (9%)	74,113,113	1.29	6 (8%)
17	CLA	c	313	3	43,53,73	1.63	5 (11%)	50,89,113	1.50	6 (12%)
21	LHG	a	618	-	22,22,48	0.45	0	25,27,54	0.46	0
20	BCR	7	317	-	41,41,41	0.16	0	56,56,56	0.43	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
20	BCR	c	316	-	41,41,41	0.14	0	56,56,56	0.58	2 (3%)
17	CLA	7	302	3	58,68,73	1.38	6 (10%)	68,107,113	1.20	5 (7%)
26	PTY	8	320	-	20,20,49	0.66	0	21,24,54	0.55	0
24	LMG	7	301	-	50,50,55	0.18	0	58,58,63	0.15	0
20	BCR	F	5010	-	41,41,41	0.15	0	56,56,56	0.33	0
25	LMU	7	319	-	36,36,36	0.12	0	47,47,47	0.15	0
18	LUT	8	316	-	42,43,43	0.26	0	51,60,60	0.45	0
16	CHL	a	606	-	45,55,74	1.38	5 (11%)	48,91,114	2.28	12 (25%)
20	BCR	a	617	-	41,41,41	0.18	0	56,56,56	0.34	0
16	CHL	b	605	-	45,55,74	1.35	4 (8%)	48,91,114	2.25	8 (16%)
21	LHG	1	619	-	30,30,48	0.36	0	33,36,54	0.34	0
17	CLA	1	605	-	43,53,73	1.72	5 (11%)	50,89,113	1.59	6 (12%)
17	CLA	B	828	-	53,63,73	1.56	6 (11%)	62,101,113	1.44	6 (9%)
18	LUT	a	615	-	42,43,43	0.17	0	51,60,60	1.17	6 (11%)
16	CHL	1	601	-	49,59,74	1.45	4 (8%)	53,96,114	1.82	9 (16%)
17	CLA	1	602	1	53,63,73	1.45	5 (9%)	62,101,113	1.44	9 (14%)
17	CLA	B	807	6	53,63,73	1.44	5 (9%)	62,101,113	1.33	7 (11%)
17	CLA	1	611	1	44,54,73	1.63	8 (18%)	51,90,113	1.59	8 (15%)
17	CLA	1	612	-	58,68,73	1.41	5 (8%)	68,107,113	1.32	8 (11%)
17	CLA	8	303	4	48,58,73	1.50	5 (10%)	56,95,113	1.31	7 (12%)
17	CLA	a	605	-	43,53,73	1.62	6 (13%)	50,89,113	1.45	6 (12%)
17	CLA	A	5009	5	63,73,73	1.35	7 (11%)	74,113,113	1.39	8 (10%)
17	CLA	B	840	-	63,73,73	1.34	5 (7%)	74,113,113	1.35	6 (8%)
19	XAT	8	317	-	41,47,47	0.15	0	54,74,74	0.88	1 (1%)
16	CHL	b	607	-	49,59,74	1.30	5 (10%)	53,96,114	2.22	8 (15%)
17	CLA	3	324	5	53,63,73	1.47	6 (11%)	62,101,113	1.33	6 (9%)
17	CLA	a	614	1	44,54,73	1.59	5 (11%)	51,90,113	1.53	6 (11%)
17	CLA	c	310	3	43,53,73	1.66	7 (16%)	50,89,113	1.63	7 (14%)
16	CHL	7	305	-	44,54,74	1.60	4 (9%)	47,90,114	1.48	8 (17%)
17	CLA	B	837	6	48,58,73	1.52	5 (10%)	56,95,113	1.42	8 (14%)
17	CLA	A	5015	-	53,63,73	1.42	5 (9%)	62,101,113	1.51	7 (11%)
17	CLA	a	610	21	44,54,73	1.60	5 (11%)	51,90,113	1.39	6 (11%)
17	CLA	b	608	-	43,53,73	1.63	5 (11%)	50,89,113	1.47	7 (14%)
17	CLA	A	5036	5	62,72,73	1.35	5 (8%)	72,111,113	1.30	6 (8%)
17	CLA	c	308	3	63,73,73	1.31	6 (9%)	74,113,113	1.30	7 (9%)
17	CLA	a	613	1	44,54,73	1.58	5 (11%)	51,90,113	1.34	6 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
17	CLA	B	813	6	48,58,73	1.54	4 (8%)	56,95,113	1.51	8 (14%)
17	CLA	A	5040	-	58,68,73	1.39	6 (10%)	68,107,113	1.26	6 (8%)
28	PQN	B	842	-	34,34,34	0.29	0	43,45,45	0.51	1 (2%)
17	CLA	b	601	4	44,54,73	1.59	5 (11%)	51,90,113	1.42	6 (11%)
17	CLA	A	5024	5	58,68,73	1.38	5 (8%)	68,107,113	1.22	6 (8%)
17	CLA	A	5029	5	63,73,73	1.29	5 (7%)	74,113,113	1.40	7 (9%)
17	CLA	A	5030	-	63,73,73	1.33	6 (9%)	74,113,113	1.30	7 (9%)
23	DGD	8	301	-	40,40,67	0.27	0	54,54,81	0.47	0
17	CLA	B	804	6	46,56,73	1.54	6 (13%)	53,92,113	1.28	7 (13%)
20	BCR	A	5050	-	41,41,41	0.17	0	56,56,56	0.29	0
17	CLA	8	314	4	44,54,73	1.60	5 (11%)	51,90,113	1.44	6 (11%)
17	CLA	K	201	-	43,53,73	1.66	6 (13%)	50,89,113	1.50	6 (12%)
17	CLA	3	314	2	44,54,73	1.59	6 (13%)	51,90,113	1.44	6 (11%)
17	CLA	B	825	-	48,58,73	1.56	7 (14%)	56,95,113	1.33	8 (14%)
17	CLA	L	202	-	43,53,73	1.68	6 (13%)	50,89,113	1.46	4 (8%)
17	CLA	a	603	-	43,53,73	1.64	5 (11%)	50,89,113	1.58	6 (12%)
17	CLA	B	830	6	63,73,73	1.36	5 (7%)	74,113,113	1.30	8 (10%)
16	CHL	c	306	-	46,56,74	1.52	4 (8%)	49,92,114	2.00	6 (12%)
17	CLA	A	5005	-	63,73,73	1.28	6 (9%)	74,113,113	1.31	5 (6%)
20	BCR	F	5005	-	41,41,41	0.15	0	56,56,56	0.26	0
20	BCR	I	4001	-	41,41,41	0.17	0	56,56,56	0.26	0
17	CLA	3	304	-	44,54,73	1.59	6 (13%)	51,90,113	1.45	6 (11%)
17	CLA	3	309	2	44,54,73	1.58	5 (11%)	51,90,113	1.29	6 (11%)
17	CLA	B	817	6	53,63,73	1.46	5 (9%)	62,101,113	1.31	7 (11%)
17	CLA	8	305	-	44,54,73	1.64	7 (15%)	51,90,113	1.60	6 (11%)
17	CLA	A	5042	5	58,68,73	1.40	6 (10%)	68,107,113	1.32	7 (10%)
19	XAT	a	616	-	41,47,47	0.15	0	54,74,74	0.77	2 (3%)
17	CLA	b	613	4	44,54,73	1.57	5 (11%)	51,90,113	1.33	7 (13%)
17	CLA	3	308	2	53,63,73	1.43	5 (9%)	62,101,113	1.26	8 (12%)
17	CLA	A	5010	-	48,58,73	1.56	8 (16%)	56,95,113	1.50	8 (14%)
20	BCR	B	845	-	41,41,41	0.28	0	56,56,56	0.91	3 (5%)
29	SF4	A	5046	6,5	0,12,12	-	-	-		
17	CLA	A	5022	-	63,73,73	1.33	5 (7%)	74,113,113	1.29	6 (8%)
20	BCR	A	5049	-	41,41,41	0.29	0	56,56,56	0.83	2 (3%)
21	LHG	1	618	17	26,26,48	0.40	0	29,32,54	0.43	0
17	CLA	B	834	-	48,58,73	1.52	5 (10%)	56,95,113	1.46	8 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
20	BCR	3	317	-	41,41,41	0.14	0	56,56,56	0.32	0
17	CLA	T	411	-	44,54,73	1.59	5 (11%)	51,90,113	1.37	6 (11%)
21	LHG	F	5001	-	30,30,48	0.37	0	33,36,54	0.32	0
20	BCR	A	5048	-	41,41,41	0.29	0	56,56,56	0.58	0
17	CLA	1	613	1	44,54,73	1.59	5 (11%)	51,90,113	1.49	6 (11%)
17	CLA	A	5014	-	63,73,73	1.33	6 (9%)	74,113,113	1.37	7 (9%)
17	CLA	a	607	-	44,54,73	1.63	7 (15%)	51,90,113	1.55	6 (11%)
22	SQD	3	320	-	33,35,54	0.27	0	43,46,65	0.52	0
18	LUT	c	314	-	42,43,43	0.40	1 (2%)	51,60,60	0.59	0
17	CLA	K	204	-	43,53,73	1.62	5 (11%)	50,89,113	1.39	6 (12%)
17	CLA	8	311	21	53,63,73	1.48	6 (11%)	62,101,113	1.34	7 (11%)
17	CLA	a	602	1	53,63,73	1.45	6 (11%)	62,101,113	1.31	7 (11%)
16	CHL	7	307	-	46,56,74	1.47	4 (8%)	49,92,114	2.00	6 (12%)
20	BCR	1	617	-	41,41,41	0.24	0	56,56,56	0.46	0
17	CLA	7	303	3	53,63,73	1.49	7 (13%)	62,101,113	1.37	7 (11%)
17	CLA	A	5034	5	63,73,73	1.35	4 (6%)	74,113,113	1.33	8 (10%)
17	CLA	b	610	21	48,58,73	1.53	5 (10%)	56,95,113	1.39	7 (12%)
17	CLA	B	827	-	58,68,73	1.37	5 (8%)	68,107,113	1.28	6 (8%)
17	CLA	B	836	6	58,68,73	1.38	5 (8%)	68,107,113	1.35	7 (10%)
20	BCR	A	5052	-	41,41,41	0.17	0	56,56,56	0.36	0
17	CLA	8	309	4	44,54,73	1.62	5 (11%)	51,90,113	1.46	6 (11%)
16	CHL	8	307	-	45,55,74	1.25	5 (11%)	48,91,114	2.15	7 (14%)
16	CHL	1	606	-	45,55,74	1.42	5 (11%)	48,91,114	2.24	9 (18%)
17	CLA	B	814	-	48,58,73	1.56	7 (14%)	56,95,113	1.47	7 (12%)
30	LMK	J	101	-	34,34,53	0.44	0	34,41,60	0.56	1 (2%)
20	BCR	B	844	-	41,41,41	0.21	0	56,56,56	0.44	0
17	CLA	B	818	6	63,73,73	1.33	6 (9%)	74,113,113	1.28	8 (10%)
17	CLA	T	403	-	48,58,73	1.54	8 (16%)	56,95,113	1.44	9 (16%)
26	PTY	8	319	-	20,20,49	0.69	0	23,25,54	0.51	0
28	PQN	A	5045	-	34,34,34	0.27	0	43,45,45	0.57	1 (2%)
20	BCR	B	801	-	41,41,41	0.15	0	56,56,56	0.35	0
20	BCR	J	104	-	41,41,41	0.16	0	56,56,56	0.33	0
17	CLA	B	805	-	63,73,73	1.30	5 (7%)	74,113,113	1.40	7 (9%)
17	CLA	3	313	-	40,50,73	1.66	5 (12%)	45,85,113	1.40	6 (13%)
23	DGD	3	321	-	51,51,67	0.17	0	65,65,81	0.16	0
20	BCR	8	318	-	41,41,41	0.17	0	56,56,56	0.53	0
17	CLA	3	307	2	63,73,73	1.33	5 (7%)	74,113,113	1.21	8 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
17	CLA	a	604	-	47,56,73	1.55	7 (14%)	54,92,113	1.44	8 (14%)
20	BCR	K	205	-	41,41,41	0.27	0	56,56,56	0.76	2 (3%)
20	BCR	3	318	-	41,41,41	0.14	0	56,56,56	0.32	0
17	CLA	A	5028	5	63,73,73	1.36	7 (11%)	74,113,113	1.36	7 (9%)
17	CLA	B	808	6	63,73,73	1.33	7 (11%)	74,113,113	1.24	7 (9%)
17	CLA	3	311	-	53,63,73	1.48	5 (9%)	62,101,113	1.40	7 (11%)
17	CLA	A	5008	5	63,73,73	1.31	6 (9%)	74,113,113	1.26	8 (10%)
17	CLA	B	816	6	48,58,73	1.54	6 (12%)	56,95,113	1.47	8 (14%)
17	CLA	T	408	13	48,58,73	1.52	6 (12%)	56,95,113	1.38	8 (14%)
17	CLA	8	304	4	49,59,73	1.56	6 (12%)	56,96,113	1.56	8 (14%)
17	CLA	A	5006	5	63,73,73	1.34	6 (9%)	74,113,113	1.31	8 (10%)
17	CLA	A	5023	5	44,54,73	1.60	6 (13%)	51,90,113	1.50	6 (11%)
17	CLA	B	831	6	53,63,73	1.47	6 (11%)	62,101,113	1.36	8 (12%)
18	LUT	7	315	-	42,43,43	0.38	1 (2%)	51,60,60	0.52	1 (1%)
17	CLA	1	610	21	44,54,73	1.58	5 (11%)	51,90,113	1.40	6 (11%)
17	CLA	A	5035	5	63,73,73	1.33	6 (9%)	74,113,113	1.28	7 (9%)
17	CLA	J	102	11	47,57,73	1.54	5 (10%)	53,93,113	1.51	7 (13%)
17	CLA	T	404	-	44,54,73	1.58	5 (11%)	51,90,113	1.37	7 (13%)
20	BCR	B	849	-	41,41,41	0.22	0	56,56,56	1.03	4 (7%)
17	CLA	A	5032	5	43,53,73	1.64	6 (13%)	50,89,113	1.49	6 (12%)
24	LMG	A	5001	-	32,32,55	0.23	0	40,40,63	0.25	0
17	CLA	T	412	-	40,50,73	1.66	5 (12%)	45,85,113	1.34	6 (13%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	PTY	F	5003	-	-	10/19/19/53	-
17	CLA	A	5038	5	1/1/12/20	7/19/97/115	-
17	CLA	b	604	-	1/1/12/20	6/19/97/115	-
16	CHL	c	305	-	1/1/16/26	12/20/118/137	-
17	CLA	B	835	-	1/1/12/20	7/19/97/115	-
20	BCR	T	415	-	-	4/29/63/63	0/2/2/2
16	CHL	T	401	13	2/2/17/26	8/21/119/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	CLA	A	5021	5	1/1/12/20	3/19/97/115	-
17	CLA	b	614	4	1/1/11/20	5/15/93/115	-
17	CLA	A	5011	5	1/1/15/20	12/37/115/115	-
16	CHL	8	308	-	2/2/17/26	8/21/119/137	-
17	CLA	1	608	-	1/1/11/20	6/13/91/115	-
17	CLA	8	302	4	1/1/11/20	3/15/93/115	-
17	CLA	7	313	3	1/1/12/20	3/19/97/115	-
17	CLA	3	302	2	1/1/15/20	5/37/115/115	-
17	CLA	1	614	1	1/1/11/20	7/15/93/115	-
17	CLA	3	306	-	1/1/13/20	6/25/103/115	-
19	XAT	c	315	-	-	3/31/93/93	0/4/4/4
16	CHL	T	416	-	2/2/16/26	8/15/113/137	-
17	CLA	T	409	-	1/1/12/20	11/22/100/115	-
17	CLA	3	323	5	1/1/13/20	8/25/103/115	-
17	CLA	B	802	6	1/1/15/20	13/37/115/115	-
23	DGD	B	848	-	-	4/50/90/95	0/2/2/2
17	CLA	a	608	1	1/1/10/20	5/13/91/115	-
21	LHG	A	5055	17	-	3/33/33/53	-
17	CLA	A	5025	5	1/1/14/20	7/31/109/115	-
21	LHG	a	619	17	-	6/26/26/53	-
17	CLA	7	308	3	1/1/11/20	4/15/93/115	-
17	CLA	B	815	-	1/1/12/20	4/19/97/115	-
17	CLA	B	839	6	1/1/15/20	8/37/115/115	-
17	CLA	B	806	6	1/1/15/20	15/37/115/115	-
18	LUT	T	413	-	3/3/12/27	3/29/67/67	0/2/2/2
17	CLA	c	309	21	1/1/14/20	9/31/109/115	-
17	CLA	A	5027	-	1/1/13/20	7/28/106/115	-
17	CLA	A	5019	5	1/1/14/20	8/33/111/115	-
17	CLA	B	823	6	1/1/12/20	7/19/97/115	-
17	CLA	B	829	6	1/1/15/20	15/37/115/115	-
17	CLA	B	820	-	1/1/13/20	8/25/103/115	-
16	CHL	c	304	-	1/1/16/26	7/15/113/137	-
17	CLA	A	5020	5	1/1/15/20	11/37/115/115	-
20	BCR	b	617	-	-	4/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	PTY	F	5002	-	-	6/36/36/53	-
17	CLA	8	313	4	1/1/12/20	6/21/99/115	-
17	CLA	B	812	6	1/1/11/20	4/15/93/115	-
17	CLA	b	609	4	1/1/14/20	9/31/109/115	-
18	LUT	b	615	-	3/3/12/27	2/29/67/67	0/2/2/2
20	BCR	B	846	-	-	2/29/63/63	0/2/2/2
17	CLA	F	5007	-	1/1/11/20	7/16/94/115	-
16	CHL	7	306	-	2/2/16/26	7/17/115/137	-
17	CLA	8	312	4	1/1/12/20	6/19/97/115	-
17	CLA	A	5004	-	1/1/15/20	13/37/115/115	-
17	CLA	T	406	-	1/1/12/20	8/19/97/115	-
17	CLA	A	5017	-	1/1/13/20	10/25/103/115	-
16	CHL	3	301	2	2/2/19/26	19/35/133/137	-
20	BCR	L	204	-	-	4/29/63/63	0/2/2/2
25	LMU	A	5054	-	-	5/21/61/61	0/2/2/2
17	CLA	7	304	-	1/1/12/20	5/19/97/115	-
20	BCR	3	319	-	-	4/29/63/63	0/2/2/2
29	SF4	C	101	7	-	-	0/6/5/5
17	CLA	A	5018	5	1/1/14/20	11/31/109/115	-
17	CLA	b	602	4	1/1/14/20	9/31/109/115	-
17	CLA	c	307	3	1/1/12/20	4/19/97/115	-
17	CLA	3	303	-	1/1/11/20	6/15/93/115	-
20	BCR	B	843	-	-	5/29/63/63	0/2/2/2
17	CLA	B	841	-	1/1/15/20	11/37/115/115	-
17	CLA	T	402	13	1/1/12/20	4/19/97/115	-
17	CLA	B	803	-	1/1/15/20	16/37/115/115	-
17	CLA	B	810	6	1/1/13/20	11/25/103/115	-
17	CLA	F	5009	10	1/1/11/20	3/15/93/115	-
17	CLA	A	5043	21	1/1/11/20	6/13/91/115	-
17	CLA	a	611	1	1/1/11/20	6/15/93/115	-
17	CLA	c	303	-	1/1/12/20	4/19/97/115	-
21	LHG	A	5002	-	-	8/40/40/53	-
29	SF4	C	102	7	-	-	0/6/5/5
16	CHL	b	606	-	1/1/16/26	6/17/115/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	CLA	A	5007	17	1/1/14/20	9/31/109/115	-
17	CLA	B	833	6	1/1/14/20	9/31/109/115	-
17	CLA	8	310	4	1/1/14/20	9/31/109/115	-
17	CLA	7	310	21	1/1/11/20	5/15/93/115	-
17	CLA	7	312	3	1/1/15/20	11/37/115/115	-
17	CLA	A	5039	5	1/1/13/20	3/25/103/115	-
19	XAT	T	414	-	-	1/31/93/93	0/4/4/4
17	CLA	K	203	12	1/1/11/20	8/13/91/115	-
17	CLA	T	405	13	1/1/11/20	4/13/91/115	-
17	CLA	A	5044	-	1/1/15/20	12/37/115/115	-
17	CLA	B	838	-	1/1/13/20	7/25/103/115	-
18	LUT	1	615	-	3/3/12/27	10/29/67/67	0/2/2/2
17	CLA	c	302	3	1/1/11/20	2/15/93/115	-
21	LHG	8	321	17	-	9/34/34/53	-
17	CLA	c	301	3	1/1/15/20	12/37/115/115	-
16	CHL	3	322	-	3/3/19/26	17/33/131/137	-
19	XAT	b	616	-	-	0/31/93/93	0/4/4/4
20	BCR	A	5047	-	-	4/29/63/63	0/2/2/2
17	CLA	B	821	-	1/1/10/20	6/11/89/115	-
17	CLA	7	311	3	1/1/11/20	5/15/93/115	-
20	BCR	J	103	-	-	4/29/63/63	0/2/2/2
17	CLA	L	201	14	1/1/15/20	8/37/115/115	-
17	CLA	A	5033	5	1/1/13/20	3/25/103/115	-
17	CLA	B	809	6	1/1/14/20	10/31/109/115	-
17	CLA	A	5041	5	1/1/15/20	6/37/115/115	-
17	CLA	1	603	1	1/1/11/20	4/13/91/115	-
17	CLA	1	604	-	1/1/12/20	7/19/97/115	-
17	CLA	B	832	6	1/1/13/20	6/25/103/115	-
17	CLA	T	407	13	1/1/12/20	9/19/97/115	-
19	XAT	3	316	-	-	3/31/93/93	0/4/4/4
21	LHG	A	5053	-	-	11/53/53/53	-
24	LMG	F	5011	-	-	3/24/44/70	0/1/1/1
17	CLA	F	5004	6	1/1/15/20	12/37/115/115	-
21	LHG	c	317	17	-	3/32/32/53	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	CLA	b	612	4	1/1/11/20	6/17/95/115	-
21	LHG	b	618	17	-	7/23/23/53	-
17	CLA	T	410	13	-	5/19/97/115	-
19	XAT	1	616	-	-	2/31/93/93	0/4/4/4
17	CLA	3	310	2	1/1/11/20	6/15/93/115	-
17	CLA	3	312	2	1/1/11/20	8/15/93/115	-
17	CLA	B	819	-	1/1/14/20	7/31/109/115	-
20	BCR	L	203	-	-	4/29/63/63	0/2/2/2
17	CLA	F	5008	10	1/1/11/20	3/13/91/115	-
17	CLA	c	312	3	1/1/12/20	5/19/97/115	-
16	CHL	a	601	-	2/2/16/26	7/17/115/137	-
17	CLA	A	5012	5	1/1/13/20	5/25/103/115	-
17	CLA	B	822	6	1/1/11/20	3/13/91/115	-
17	CLA	B	811	6	1/1/12/20	6/19/97/115	-
17	CLA	K	202	-	1/1/11/20	5/15/93/115	-
17	CLA	A	5026	-	1/1/15/20	11/37/115/115	-
27	CL0	A	5003	5	1/1/20/25	15/37/135/135	-
19	XAT	7	316	-	-	4/31/93/93	0/4/4/4
21	LHG	7	318	17	-	2/38/38/53	-
17	CLA	7	314	3	1/1/11/20	5/15/93/115	-
17	CLA	1	607	-	1/1/15/20	11/37/115/115	-
17	CLA	3	305	2	1/1/12/20	4/19/97/115	-
16	CHL	8	306	-	1/1/16/26	9/15/113/137	-
17	CLA	B	824	-	1/1/12/20	9/19/97/115	-
17	CLA	1	609	1	1/1/15/20	9/37/115/115	-
17	CLA	F	5006	-	1/1/14/20	6/31/109/115	-
17	CLA	b	603	4	1/1/12/20	8/19/97/115	-
17	CLA	b	611	4	1/1/12/20	8/19/97/115	-
17	CLA	c	311	-	1/1/12/20	4/19/97/115	-
20	BCR	A	5051	-	-	2/29/63/63	0/2/2/2
17	CLA	A	5013	17,5	1/1/15/20	13/37/115/115	-
17	CLA	8	315	4	1/1/11/20	6/13/91/115	-
20	BCR	B	847	-	-	2/29/63/63	0/2/2/2
17	CLA	a	609	1	1/1/14/20	9/31/109/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	CLA	A	5016	5	1/1/15/20	16/37/115/115	-
17	CLA	A	5037	5	1/1/12/20	7/19/97/115	-
17	CLA	a	612	-	1/1/12/20	6/19/97/115	-
17	CLA	7	309	3	1/1/11/20	5/15/93/115	-
17	CLA	B	826	6	1/1/15/20	7/37/115/115	-
18	LUT	3	315	-	3/3/12/27	3/29/67/67	0/2/2/2
17	CLA	A	5031	5	1/1/15/20	7/37/115/115	-
17	CLA	c	313	3	-	4/13/91/115	-
21	LHG	a	618	-	-	14/26/26/53	-
20	BCR	7	317	-	-	4/29/63/63	0/2/2/2
20	BCR	c	316	-	-	9/29/63/63	0/2/2/2
17	CLA	7	302	3	1/1/14/20	11/31/109/115	-
26	PTY	8	320	-	-	8/23/23/53	-
24	LMG	7	301	-	-	12/45/65/70	0/1/1/1
20	BCR	F	5010	-	-	4/29/63/63	0/2/2/2
25	LMU	7	319	-	-	9/21/61/61	0/2/2/2
18	LUT	8	316	-	3/3/12/27	2/29/67/67	0/2/2/2
16	CHL	a	606	-	2/2/16/26	4/17/115/137	-
20	BCR	a	617	-	-	5/29/63/63	0/2/2/2
16	CHL	b	605	-	1/1/16/26	8/17/115/137	-
21	LHG	1	619	-	-	7/35/35/53	-
17	CLA	1	605	-	1/1/11/20	4/13/91/115	-
17	CLA	B	828	-	1/1/13/20	10/25/103/115	-
18	LUT	a	615	-	3/3/12/27	9/29/67/67	0/2/2/2
16	CHL	1	601	-	1/1/17/26	9/21/119/137	-
17	CLA	1	602	1	1/1/13/20	13/25/103/115	-
17	CLA	B	807	6	1/1/13/20	9/25/103/115	-
17	CLA	1	611	1	1/1/11/20	6/15/93/115	-
17	CLA	1	612	-	1/1/14/20	9/31/109/115	-
17	CLA	8	303	4	1/1/12/20	6/19/97/115	-
17	CLA	a	605	-	1/1/11/20	4/13/91/115	-
17	CLA	A	5009	5	1/1/15/20	13/37/115/115	-
17	CLA	B	840	-	1/1/15/20	9/37/115/115	-
19	XAT	8	317	-	-	0/31/93/93	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	CHL	b	607	-	2/2/17/26	6/21/119/137	-
17	CLA	3	324	5	1/1/13/20	4/25/103/115	-
17	CLA	a	614	1	1/1/11/20	6/15/93/115	-
17	CLA	c	310	3	1/1/11/20	5/13/91/115	-
16	CHL	7	305	-	1/1/16/26	5/15/113/137	-
17	CLA	B	837	6	1/1/12/20	6/19/97/115	-
17	CLA	A	5015	-	1/1/13/20	6/25/103/115	-
17	CLA	a	610	21	1/1/11/20	6/15/93/115	-
17	CLA	b	608	-	1/1/11/20	4/13/91/115	-
17	CLA	A	5036	5	1/1/15/20	7/37/115/115	-
17	CLA	c	308	3	1/1/15/20	14/37/115/115	-
17	CLA	a	613	1	1/1/11/20	4/15/93/115	-
17	CLA	B	813	6	1/1/12/20	7/19/97/115	-
17	CLA	A	5040	-	1/1/14/20	8/31/109/115	-
28	PQN	B	842	-	-	1/23/43/43	0/2/2/2
17	CLA	b	601	4	1/1/11/20	7/15/93/115	-
17	CLA	A	5024	5	1/1/14/20	14/31/109/115	-
17	CLA	A	5029	5	1/1/15/20	11/37/115/115	-
17	CLA	A	5030	-	1/1/15/20	8/37/115/115	-
23	DGD	8	301	-	-	14/28/68/95	0/2/2/2
17	CLA	B	804	6	1/1/11/20	7/17/95/115	-
20	BCR	A	5050	-	-	2/29/63/63	0/2/2/2
17	CLA	8	314	4	1/1/11/20	7/15/93/115	-
17	CLA	K	201	-	1/1/11/20	5/13/91/115	-
17	CLA	3	314	2	1/1/11/20	6/15/93/115	-
17	CLA	B	825	-	1/1/12/20	4/19/97/115	-
17	CLA	L	202	-	1/1/11/20	4/13/91/115	-
17	CLA	a	603	-	1/1/11/20	6/13/91/115	-
17	CLA	B	830	6	1/1/15/20	10/37/115/115	-
16	CHL	c	306	-	1/1/16/26	4/18/116/137	-
17	CLA	A	5005	-	1/1/15/20	3/37/115/115	-
20	BCR	F	5005	-	-	0/29/63/63	0/2/2/2
20	BCR	I	4001	-	-	2/29/63/63	0/2/2/2
17	CLA	3	304	-	1/1/11/20	6/15/93/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	CLA	3	309	2	1/1/11/20	7/15/93/115	-
17	CLA	B	817	6	1/1/13/20	7/25/103/115	-
17	CLA	8	305	-	1/1/11/20	7/15/93/115	-
17	CLA	A	5042	5	1/1/14/20	6/31/109/115	-
19	XAT	a	616	-	-	3/31/93/93	0/4/4/4
17	CLA	b	613	4	1/1/11/20	5/15/93/115	-
17	CLA	3	308	2	1/1/13/20	8/25/103/115	-
17	CLA	A	5010	-	1/1/12/20	5/19/97/115	-
20	BCR	B	845	-	-	9/29/63/63	0/2/2/2
29	SF4	A	5046	6,5	-	-	0/6/5/5
17	CLA	A	5022	-	1/1/15/20	12/37/115/115	-
20	BCR	A	5049	-	-	3/29/63/63	0/2/2/2
21	LHG	1	618	17	-	11/31/31/53	-
17	CLA	B	834	-	1/1/12/20	11/19/97/115	-
20	BCR	3	317	-	-	4/29/63/63	0/2/2/2
17	CLA	T	411	-	1/1/11/20	8/15/93/115	-
21	LHG	F	5001	-	-	11/35/35/53	-
20	BCR	A	5048	-	-	7/29/63/63	0/2/2/2
17	CLA	1	613	1	1/1/11/20	5/15/93/115	-
17	CLA	A	5014	-	-	12/37/115/115	-
17	CLA	a	607	-	1/1/11/20	2/15/93/115	-
22	SQD	3	320	-	-	11/30/50/69	0/1/1/1
18	LUT	c	314	-	3/3/12/27	5/29/67/67	0/2/2/2
17	CLA	K	204	-	1/1/11/20	7/13/91/115	-
17	CLA	8	311	21	1/1/13/20	4/25/103/115	-
17	CLA	a	602	1	1/1/13/20	4/25/103/115	-
16	CHL	7	307	-	2/2/16/26	6/18/116/137	-
20	BCR	1	617	-	-	5/29/63/63	0/2/2/2
17	CLA	7	303	3	1/1/13/20	2/25/103/115	-
17	CLA	A	5034	5	1/1/15/20	6/37/115/115	-
17	CLA	b	610	21	1/1/12/20	6/19/97/115	-
17	CLA	B	827	-	1/1/14/20	10/31/109/115	-
17	CLA	B	836	6	1/1/14/20	5/31/109/115	-
20	BCR	A	5052	-	-	5/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	CLA	8	309	4	1/1/11/20	3/15/93/115	-
16	CHL	8	307	-	1/1/16/26	7/17/115/137	-
16	CHL	1	606	-	2/2/16/26	2/17/115/137	-
17	CLA	B	814	-	1/1/12/20	10/19/97/115	-
30	LMK	J	101	-	-	3/41/41/60	-
20	BCR	B	844	-	-	2/29/63/63	0/2/2/2
17	CLA	B	818	6	1/1/15/20	12/37/115/115	-
17	CLA	T	403	-	1/1/12/20	8/19/97/115	-
26	PTY	8	319	-	-	9/23/23/53	-
28	PQN	A	5045	-	-	2/23/43/43	0/2/2/2
20	BCR	B	801	-	-	2/29/63/63	0/2/2/2
20	BCR	J	104	-	-	2/29/63/63	0/2/2/2
17	CLA	B	805	-	1/1/15/20	9/37/115/115	-
17	CLA	3	313	-	1/1/10/20	3/10/88/115	-
23	DGD	3	321	-	-	10/39/79/95	0/2/2/2
20	BCR	8	318	-	-	6/29/63/63	0/2/2/2
17	CLA	3	307	2	1/1/15/20	11/37/115/115	-
17	CLA	a	604	-	1/1/12/20	8/17/95/115	-
20	BCR	K	205	-	-	10/29/63/63	0/2/2/2
20	BCR	3	318	-	-	4/29/63/63	0/2/2/2
17	CLA	A	5028	5	1/1/15/20	14/37/115/115	-
17	CLA	B	808	6	1/1/15/20	18/37/115/115	-
17	CLA	3	311	-	1/1/13/20	8/25/103/115	-
17	CLA	A	5008	5	1/1/15/20	13/37/115/115	-
17	CLA	B	816	6	1/1/12/20	4/19/97/115	-
17	CLA	T	408	13	1/1/12/20	5/19/97/115	-
17	CLA	8	304	4	1/1/12/20	8/21/99/115	-
17	CLA	A	5006	5	1/1/15/20	15/37/115/115	-
17	CLA	A	5023	5	1/1/11/20	5/15/93/115	-
17	CLA	B	831	6	1/1/13/20	8/25/103/115	-
18	LUT	7	315	-	3/3/12/27	2/29/67/67	0/2/2/2
17	CLA	1	610	21	1/1/11/20	7/15/93/115	-
17	CLA	A	5035	5	1/1/15/20	13/37/115/115	-
17	CLA	J	102	11	1/1/11/20	5/18/96/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	CLA	T	404	-	1/1/11/20	8/15/93/115	-
20	BCR	B	849	-	-	6/29/63/63	0/2/2/2
17	CLA	A	5032	5	1/1/11/20	4/13/91/115	-
24	LMG	A	5001	-	-	4/26/46/70	0/1/1/1
17	CLA	T	412	-	1/1/10/20	2/10/88/115	-

The worst 5 of 1140 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	8	306	CHL	MG-NA	7.52	2.24	2.06
16	3	322	CHL	MG-NA	7.12	2.23	2.06
16	8	306	CHL	MG-NC	7.00	2.22	2.06
17	A	5031	CLA	CHB-C4A	6.85	1.39	1.33
17	B	829	CLA	CHB-C4A	6.67	1.39	1.33

The worst 5 of 1505 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	8	308	CHL	C4A-NA-C1A	15.65	113.82	106.68
16	T	401	CHL	C4A-NA-C1A	15.40	113.71	106.68
16	7	306	CHL	C4A-NA-C1A	14.52	113.31	106.68
16	b	607	CHL	C4A-NA-C1A	13.23	112.72	106.68
27	A	5003	CL0	C4A-NA-C1A	13.04	112.63	106.68

5 of 239 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
16	1	601	CHL	ND
16	1	606	CHL	ND
16	1	606	CHL	NA
16	3	301	CHL	C8
16	3	301	CHL	NC

5 of 1918 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
16	1	601	CHL	C1A-C2A-CAA-CBA
16	1	601	CHL	C3A-C2A-CAA-CBA
16	1	601	CHL	C1C-C2C-CMC-OMC
16	1	601	CHL	C3C-C2C-CMC-OMC
16	1	601	CHL	CHA-CBD-CGD-O1D

There are no ring outliers.

247 monomers are involved in 585 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	b	604	CLA	2	0
16	c	305	CHL	4	0
20	T	415	BCR	3	0
16	T	401	CHL	4	0
17	A	5021	CLA	1	0
17	b	614	CLA	1	0
17	A	5011	CLA	6	0
16	8	308	CHL	4	0
17	1	608	CLA	2	0
17	8	302	CLA	3	0
17	7	313	CLA	2	0
17	3	302	CLA	4	0
17	1	614	CLA	1	0
17	3	306	CLA	2	0
19	c	315	XAT	1	0
16	T	416	CHL	7	0
17	T	409	CLA	1	0
17	3	323	CLA	3	0
17	B	802	CLA	7	0
23	B	848	DGD	8	0
17	a	608	CLA	2	0
21	A	5055	LHG	2	0
17	A	5025	CLA	6	0
21	a	619	LHG	1	0
17	7	308	CLA	2	0
17	B	839	CLA	6	0
17	B	806	CLA	5	0
18	T	413	LUT	4	0
17	c	309	CLA	1	0
17	A	5027	CLA	1	0
17	A	5019	CLA	8	0
17	B	823	CLA	1	0
17	B	829	CLA	7	0
17	B	820	CLA	2	0
16	c	304	CHL	7	0
17	A	5020	CLA	4	0
20	b	617	BCR	6	0
17	8	313	CLA	2	0
17	B	812	CLA	1	0
17	b	609	CLA	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	b	615	LUT	1	0
20	B	846	BCR	4	0
17	F	5007	CLA	2	0
16	7	306	CHL	4	0
17	8	312	CLA	1	0
17	A	5004	CLA	11	0
17	T	406	CLA	2	0
17	A	5017	CLA	7	0
16	3	301	CHL	10	0
20	L	204	BCR	4	0
25	A	5054	LMU	1	0
17	7	304	CLA	1	0
20	3	319	BCR	2	0
17	A	5018	CLA	6	0
17	b	602	CLA	3	0
17	c	307	CLA	5	0
20	B	843	BCR	2	0
17	B	841	CLA	3	0
17	T	402	CLA	1	0
17	B	803	CLA	8	0
17	B	810	CLA	2	0
17	F	5009	CLA	1	0
17	A	5043	CLA	1	0
17	a	611	CLA	1	0
17	c	303	CLA	3	0
21	A	5002	LHG	2	0
29	C	102	SF4	1	0
16	b	606	CHL	3	0
17	A	5007	CLA	3	0
17	B	833	CLA	1	0
17	8	310	CLA	2	0
17	7	312	CLA	6	0
19	T	414	XAT	2	0
17	K	203	CLA	3	0
17	T	405	CLA	1	0
17	A	5044	CLA	7	0
17	B	838	CLA	2	0
18	1	615	LUT	6	0
17	c	302	CLA	1	0
21	8	321	LHG	2	0
17	c	301	CLA	7	0
16	3	322	CHL	6	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
20	A	5047	BCR	2	0
17	B	821	CLA	2	0
20	J	103	BCR	2	0
17	L	201	CLA	4	0
17	A	5033	CLA	4	0
17	B	809	CLA	5	0
17	A	5041	CLA	2	0
17	1	604	CLA	6	0
17	B	832	CLA	4	0
19	3	316	XAT	4	0
21	A	5053	LHG	5	0
24	F	5011	LMG	1	0
17	F	5004	CLA	4	0
21	c	317	LHG	1	0
17	b	612	CLA	1	0
17	T	410	CLA	1	0
19	1	616	XAT	1	0
17	3	312	CLA	1	0
17	B	819	CLA	3	0
20	L	203	BCR	2	0
17	c	312	CLA	2	0
16	a	601	CHL	2	0
17	A	5012	CLA	2	0
17	B	822	CLA	2	0
17	B	811	CLA	2	0
17	K	202	CLA	1	0
17	A	5026	CLA	3	0
27	A	5003	CL0	8	0
19	7	316	XAT	6	0
17	1	607	CLA	3	0
17	3	305	CLA	4	0
16	8	306	CHL	4	0
17	1	609	CLA	3	0
17	F	5006	CLA	1	0
17	b	611	CLA	2	0
17	c	311	CLA	1	0
20	A	5051	BCR	3	0
17	A	5013	CLA	6	0
17	8	315	CLA	1	0
20	B	847	BCR	2	0
17	a	609	CLA	2	0
17	A	5016	CLA	7	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	A	5037	CLA	2	0
17	a	612	CLA	2	0
17	7	309	CLA	1	0
17	B	826	CLA	5	0
18	3	315	LUT	3	0
17	A	5031	CLA	2	0
17	c	313	CLA	3	0
21	a	618	LHG	1	0
20	7	317	BCR	3	0
20	c	316	BCR	2	0
17	7	302	CLA	4	0
24	7	301	LMG	5	0
20	F	5010	BCR	4	0
25	7	319	LMU	3	0
18	8	316	LUT	1	0
16	a	606	CHL	1	0
20	a	617	BCR	4	0
16	b	605	CHL	6	0
21	1	619	LHG	1	0
17	1	605	CLA	5	0
17	B	828	CLA	5	0
18	a	615	LUT	4	0
16	1	601	CHL	2	0
17	B	807	CLA	4	0
17	1	611	CLA	1	0
17	1	612	CLA	2	0
17	8	303	CLA	3	0
17	a	605	CLA	1	0
17	A	5009	CLA	3	0
17	B	840	CLA	2	0
19	8	317	XAT	1	0
16	b	607	CHL	4	0
17	3	324	CLA	3	0
16	7	305	CHL	4	0
17	B	837	CLA	2	0
17	A	5015	CLA	2	0
17	A	5036	CLA	5	0
17	c	308	CLA	4	0
17	a	613	CLA	1	0
17	B	813	CLA	4	0
17	A	5040	CLA	1	0
28	B	842	PQN	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	b	601	CLA	3	0
17	A	5024	CLA	1	0
17	A	5029	CLA	9	0
17	A	5030	CLA	5	0
23	8	301	DGD	2	0
17	B	804	CLA	1	0
20	A	5050	BCR	5	0
17	8	314	CLA	1	0
17	K	201	CLA	1	0
17	3	314	CLA	1	0
17	B	825	CLA	3	0
17	B	830	CLA	3	0
16	c	306	CHL	14	0
17	A	5005	CLA	6	0
20	F	5005	BCR	5	0
20	I	4001	BCR	2	0
17	3	304	CLA	1	0
17	3	309	CLA	1	0
17	B	817	CLA	4	0
17	8	305	CLA	3	0
17	A	5042	CLA	4	0
19	a	616	XAT	1	0
17	b	613	CLA	1	0
17	3	308	CLA	1	0
17	A	5010	CLA	3	0
20	B	845	BCR	3	0
17	A	5022	CLA	4	0
20	A	5049	BCR	4	0
21	1	618	LHG	1	0
20	3	317	BCR	3	0
20	A	5048	BCR	6	0
17	1	613	CLA	1	0
17	A	5014	CLA	8	0
17	a	607	CLA	1	0
22	3	320	SQD	5	0
17	K	204	CLA	2	0
17	8	311	CLA	2	0
17	a	602	CLA	1	0
16	7	307	CHL	4	0
20	1	617	BCR	8	0
17	7	303	CLA	2	0
17	A	5034	CLA	2	0

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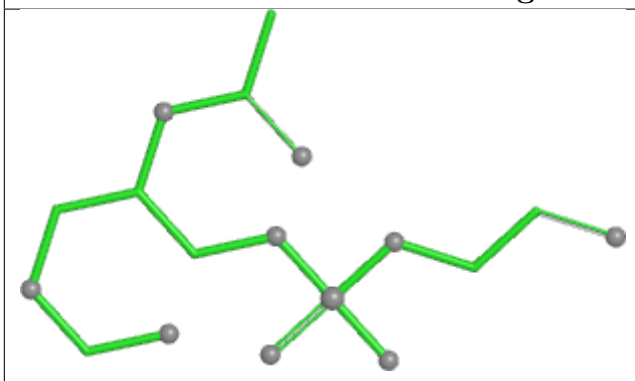
Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	b	610	CLA	1	0
17	B	827	CLA	5	0
17	B	836	CLA	4	0
20	A	5052	BCR	7	0
17	8	309	CLA	1	0
16	8	307	CHL	2	0
16	1	606	CHL	2	0
17	B	814	CLA	1	0
20	B	844	BCR	2	0
17	B	818	CLA	9	0
17	T	403	CLA	2	0
28	A	5045	PQN	2	0
20	B	801	BCR	3	0
20	J	104	BCR	4	0
17	B	805	CLA	2	0
23	3	321	DGD	1	0
20	8	318	BCR	5	0
17	3	307	CLA	7	0
17	a	604	CLA	4	0
20	K	205	BCR	5	0
20	3	318	BCR	4	0
17	A	5028	CLA	6	0
17	B	808	CLA	3	0
17	3	311	CLA	2	0
17	A	5008	CLA	5	0
17	B	816	CLA	1	0
17	T	408	CLA	1	0
17	8	304	CLA	1	0
17	A	5006	CLA	2	0
17	B	831	CLA	1	0
18	7	315	LUT	3	0
17	1	610	CLA	1	0
17	A	5035	CLA	5	0
17	J	102	CLA	3	0
17	T	404	CLA	3	0
20	B	849	BCR	5	0
17	A	5032	CLA	3	0
24	A	5001	LMG	2	0
17	T	412	CLA	2	0

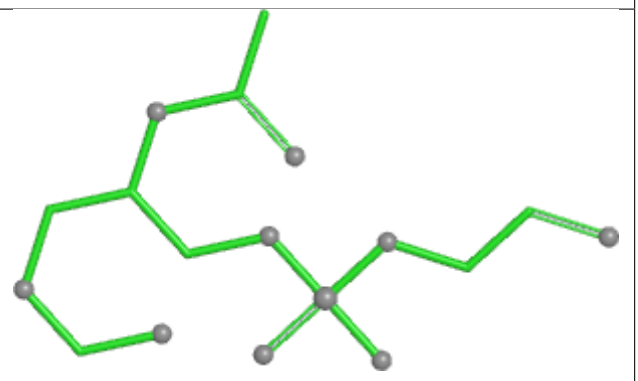
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will

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.

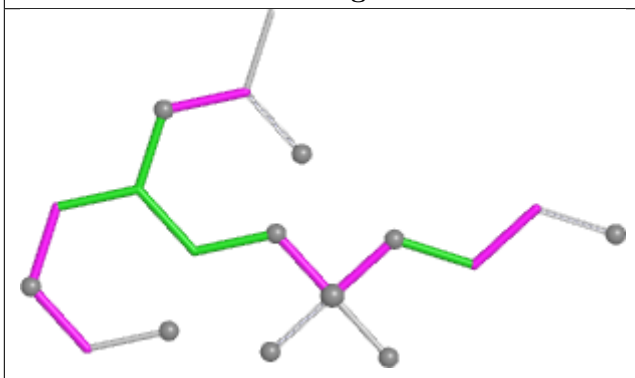
Ligand PTY F 5003



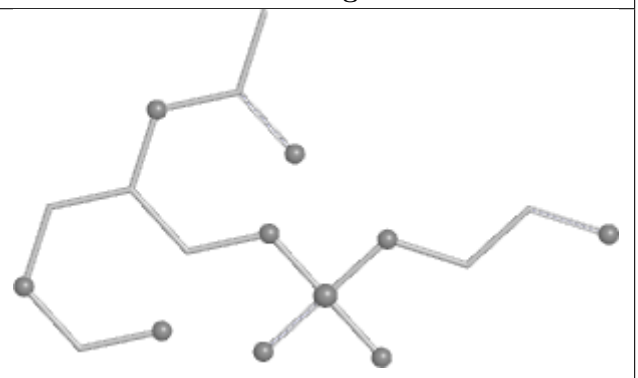
Bond lengths



Bond angles

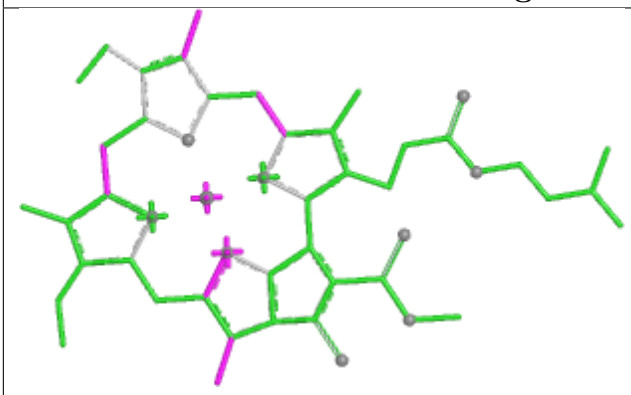


Torsions

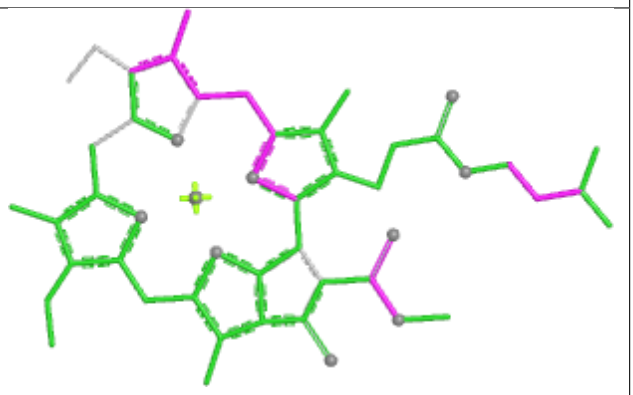


Rings

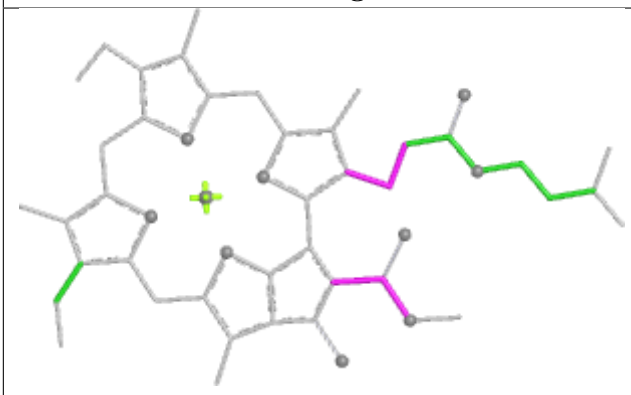
Ligand CLA A 5038



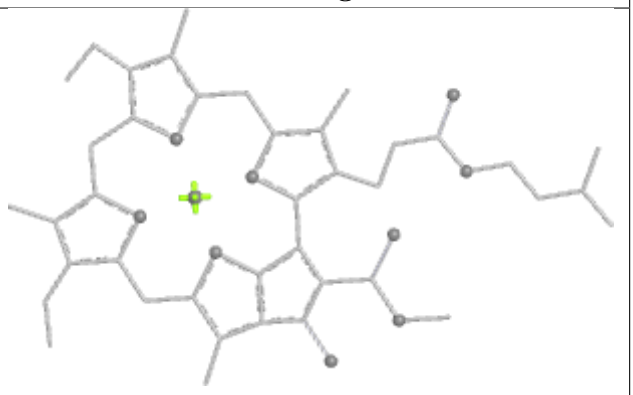
Bond lengths



Bond angles

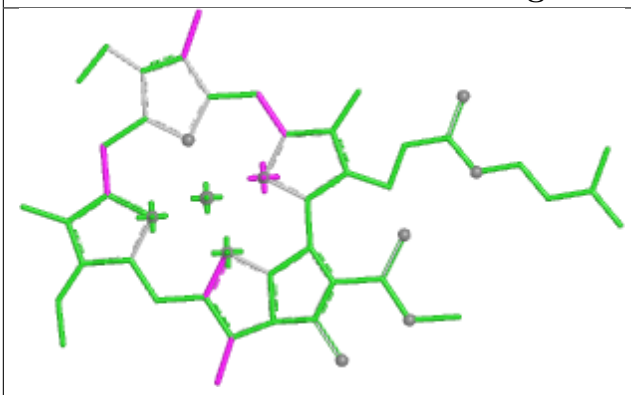


Torsions

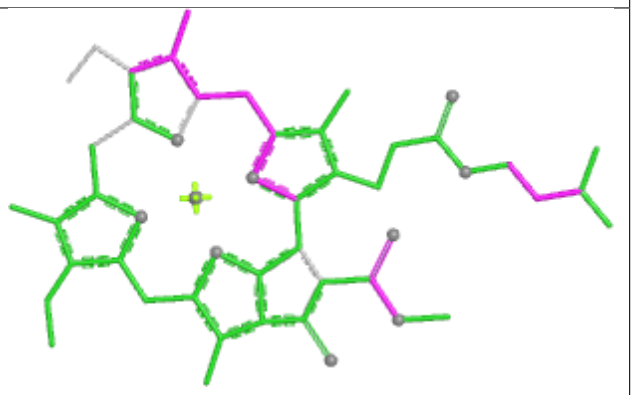


Rings

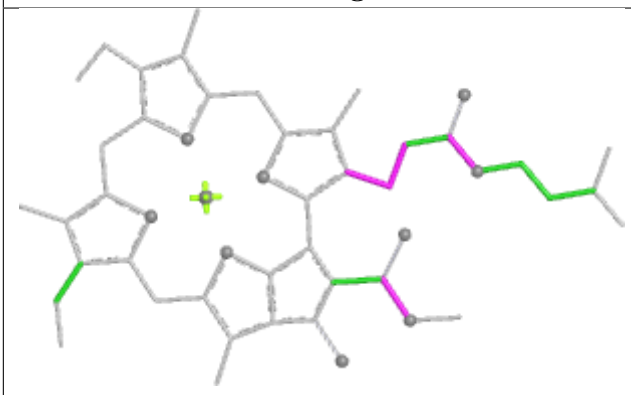
Ligand CLA b 604



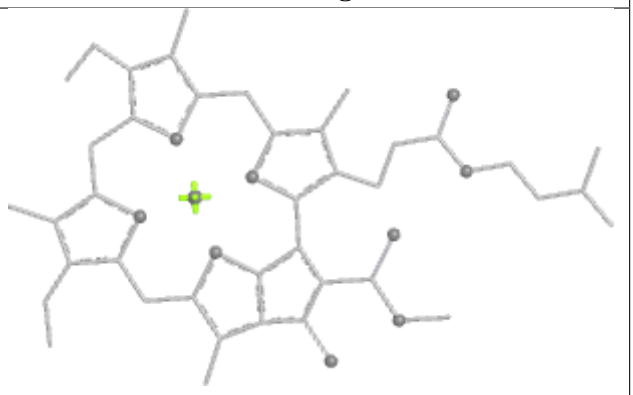
Bond lengths



Bond angles

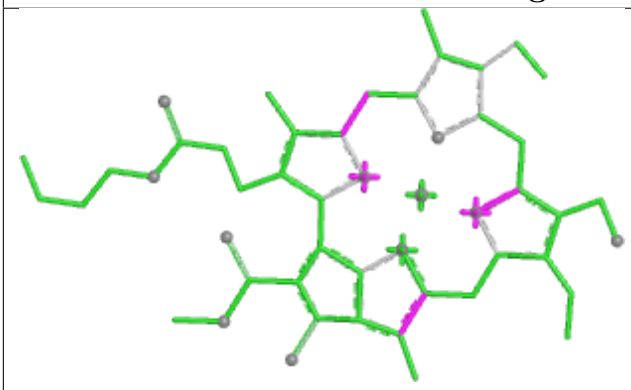


Torsions

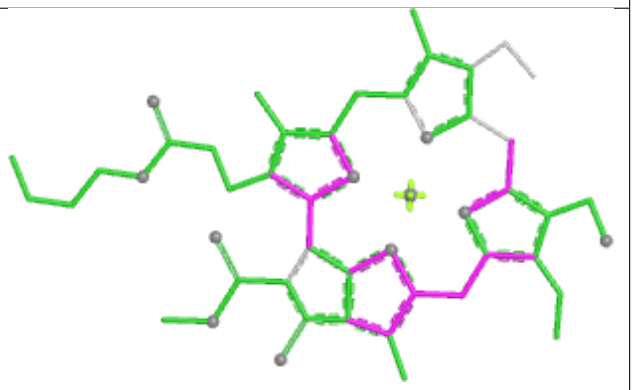


Rings

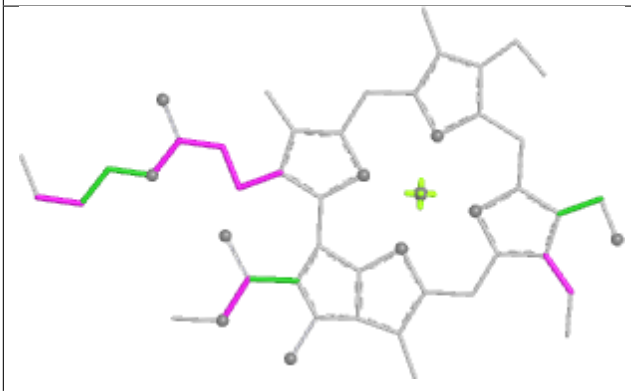
Ligand CHL c 305



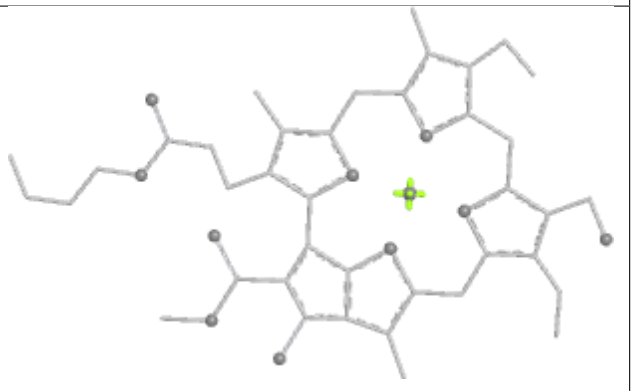
Bond lengths



Bond angles

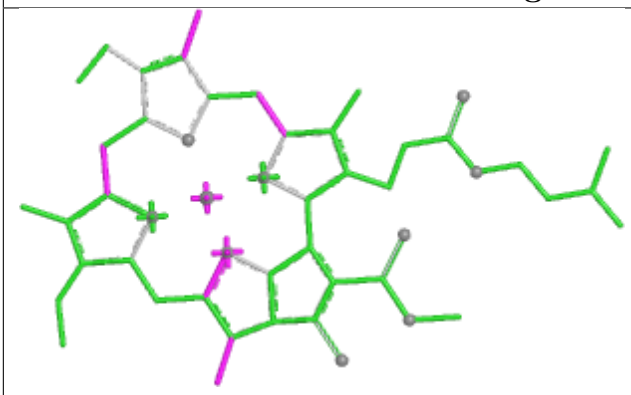


Torsions

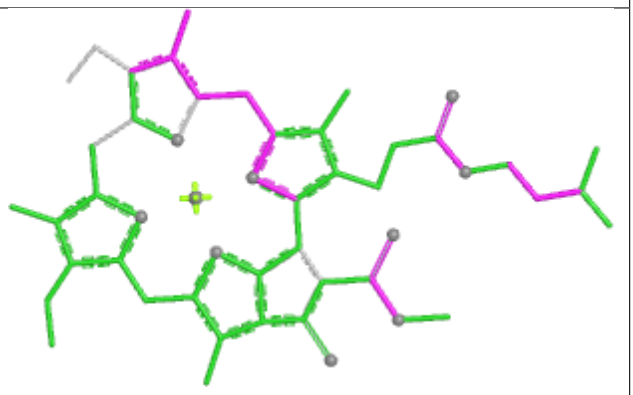


Rings

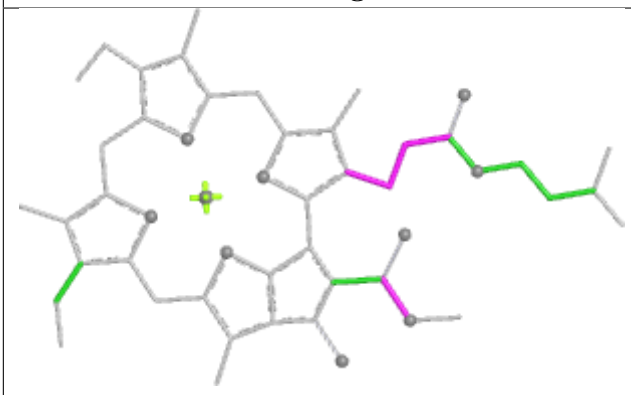
Ligand CLA B 835



Bond lengths



Bond angles



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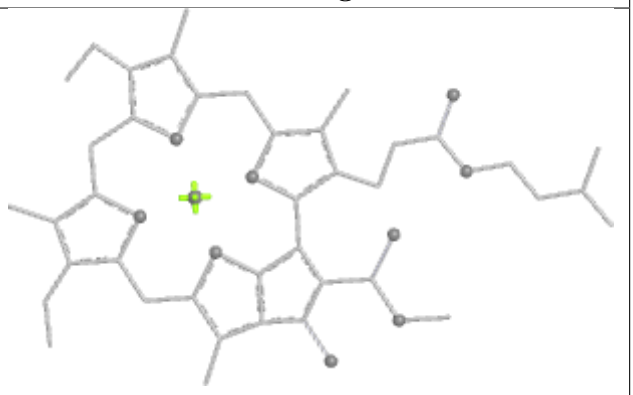
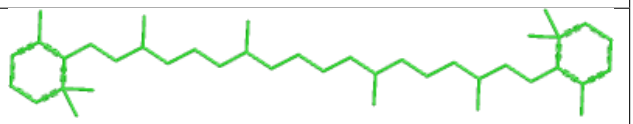


Rings

Ligand BCR T 415

Bond lengths



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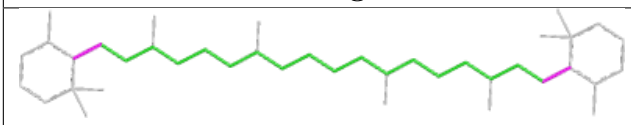

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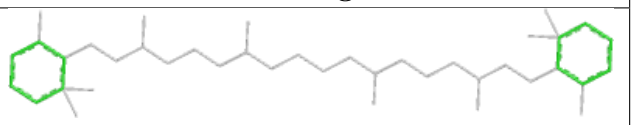
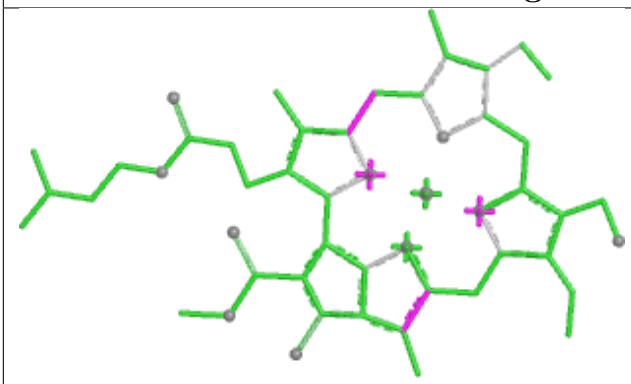
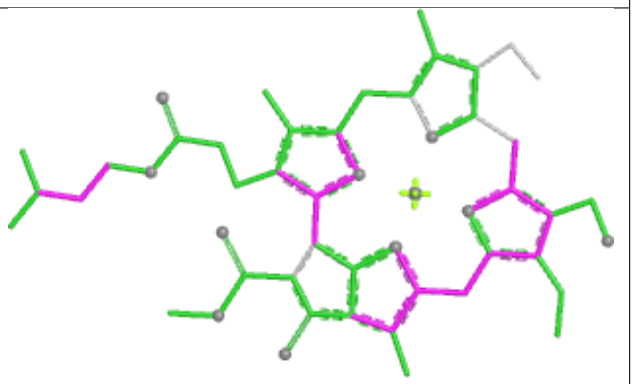


Rings

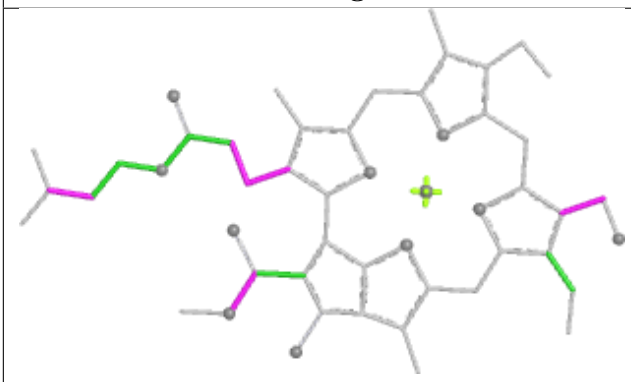
Ligand CHL T 401



Bond lengths



Bond angles



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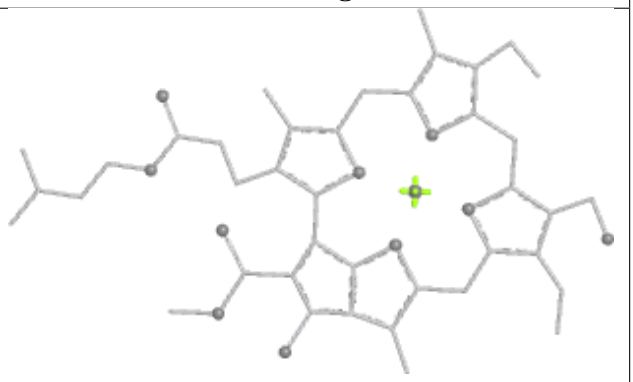
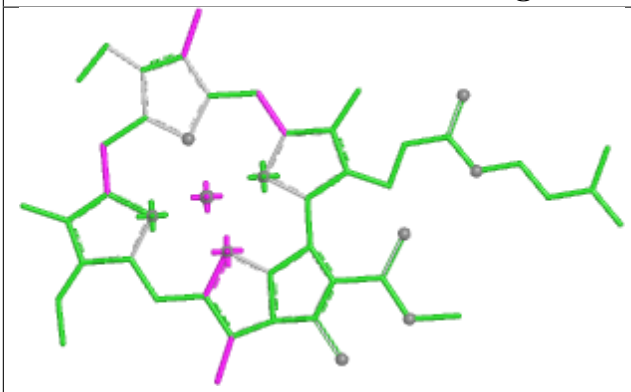
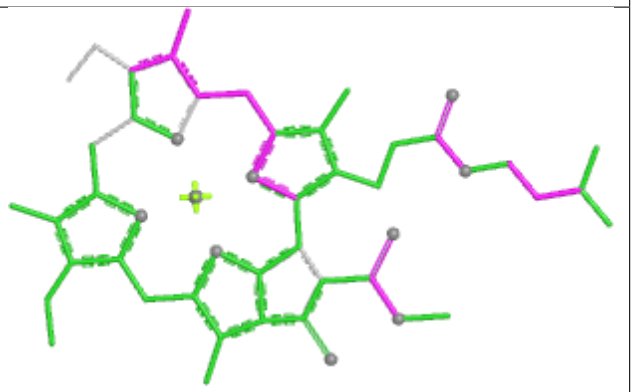


Rings

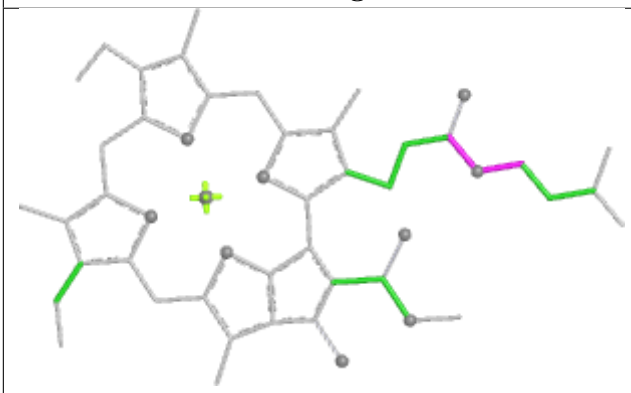
Ligand CLA A 5021



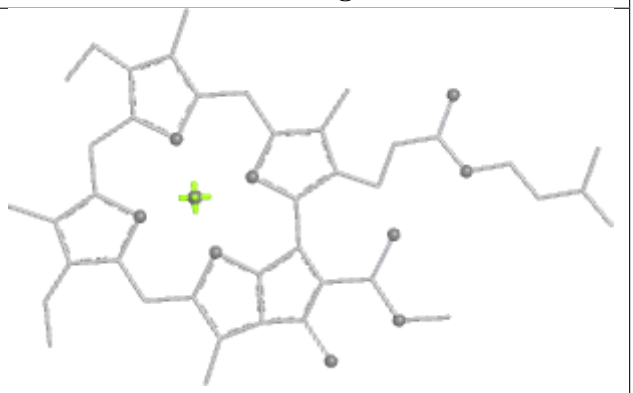
Bond lengths



Bond angles

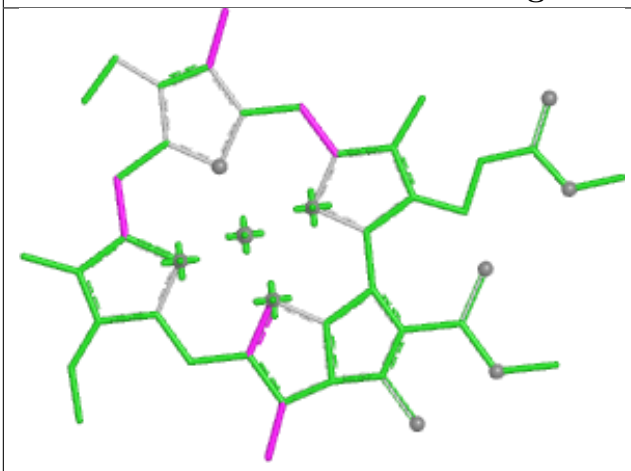


Torsions

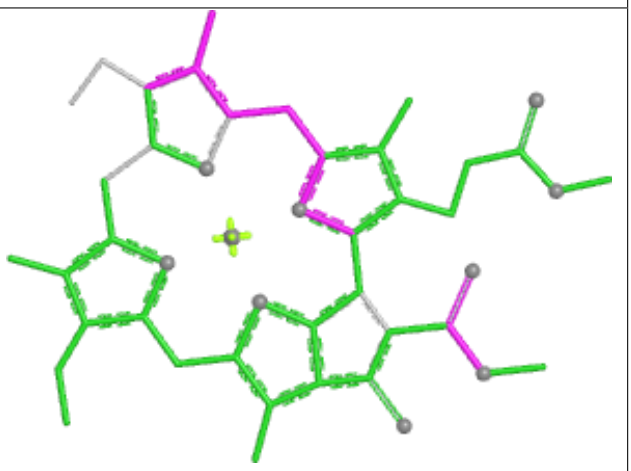


Rings

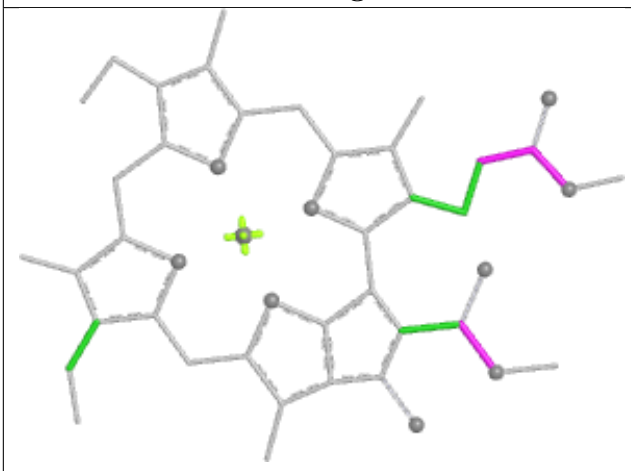
Ligand CLA b 614



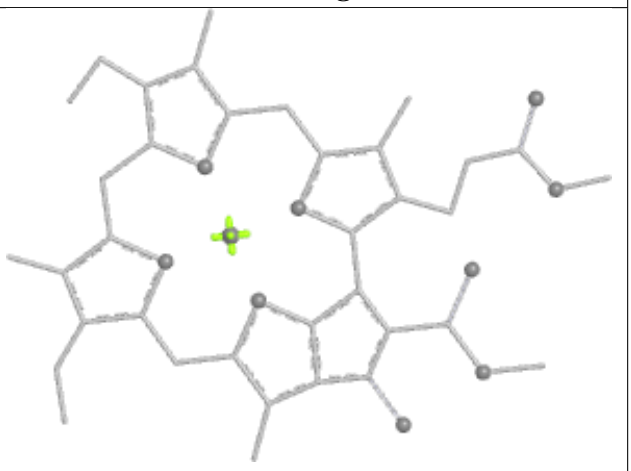
Bond lengths



Bond angles

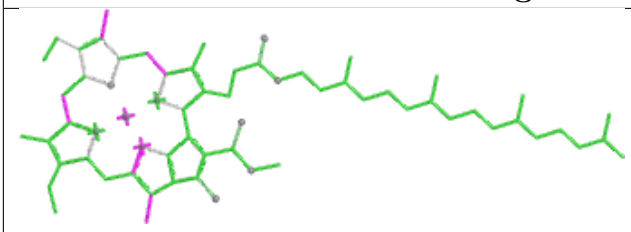


Torsions

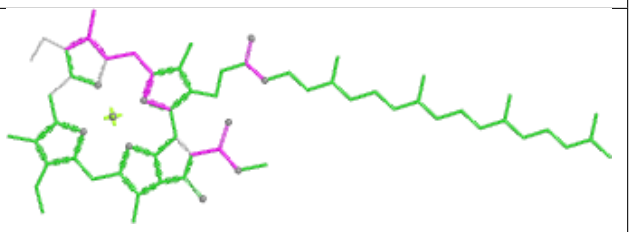


Rings

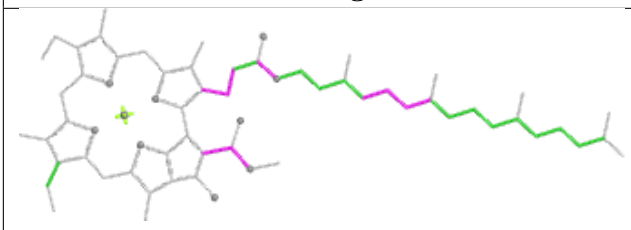
Ligand CLA A 5011



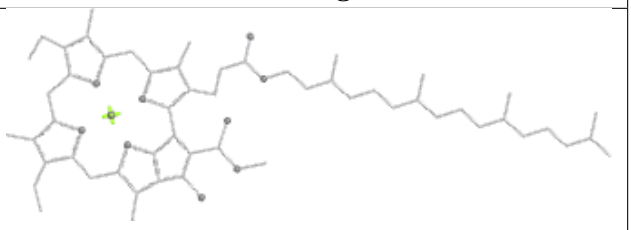
Bond lengths



Bond angles

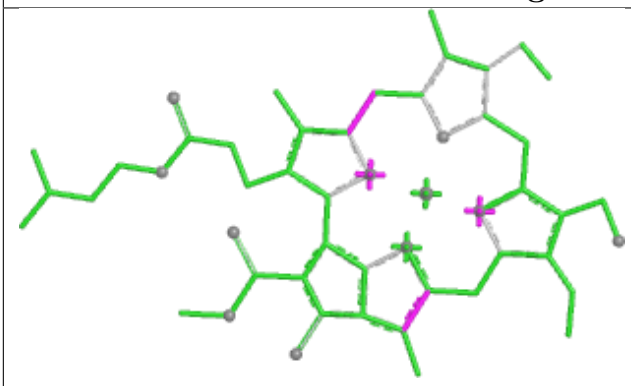


Torsions



Rings

Ligand CHL 8 308



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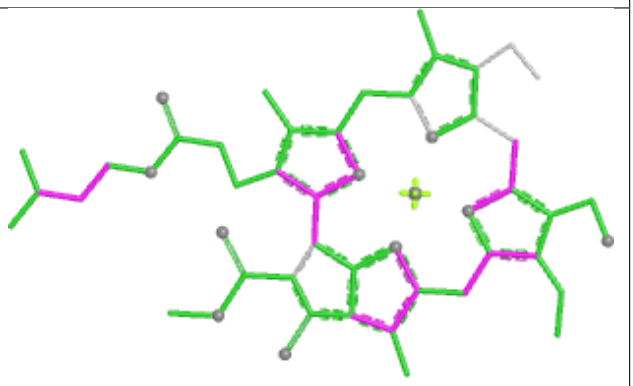
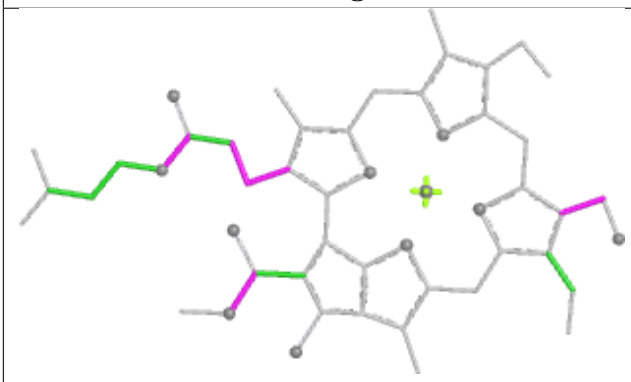
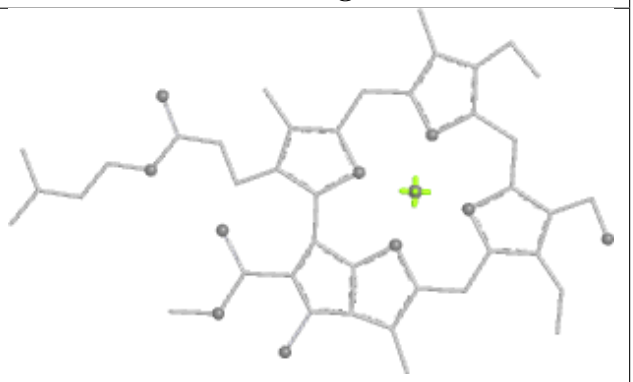


Bond angles

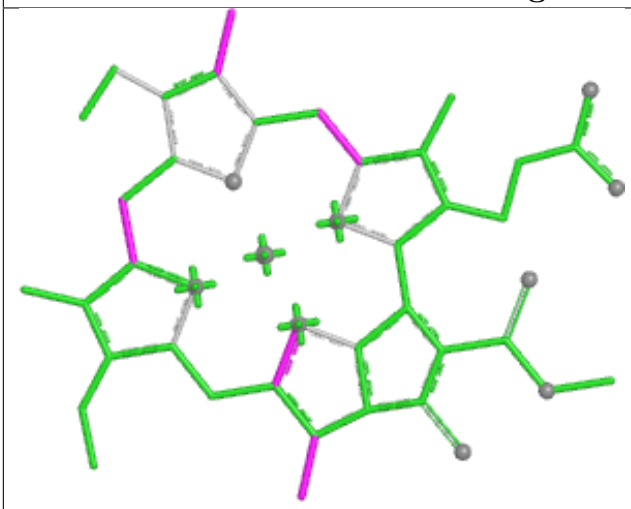


Torsions

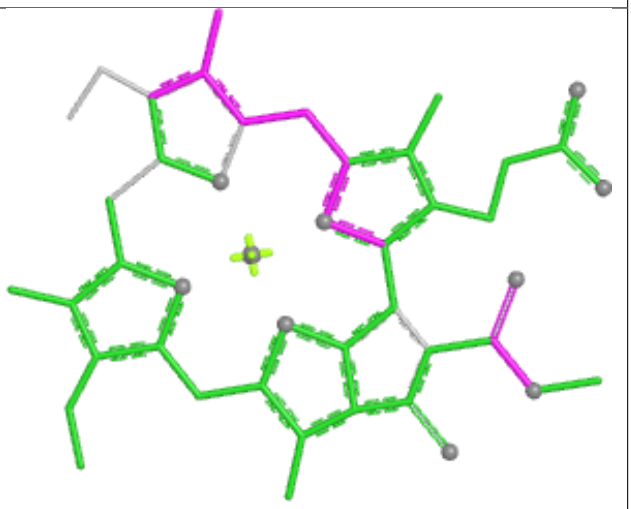


Rings

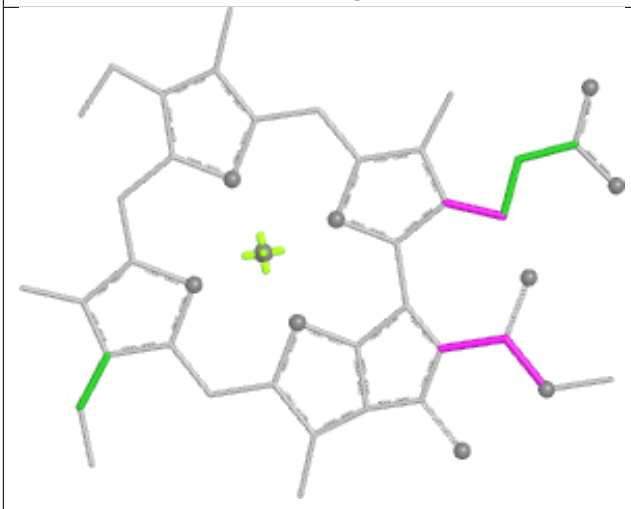
Ligand CLA 1 608



Bond lengths



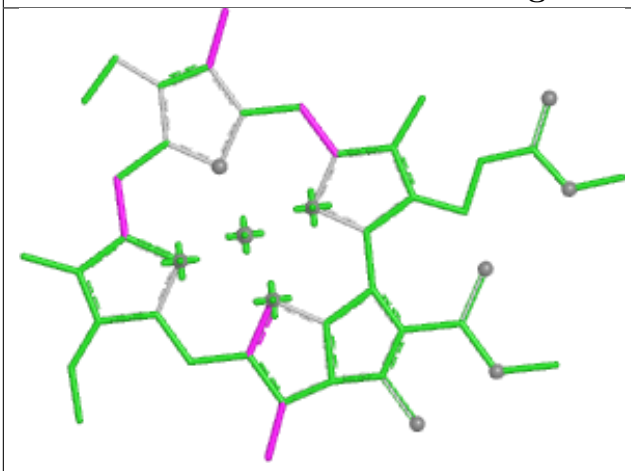
Bond angles



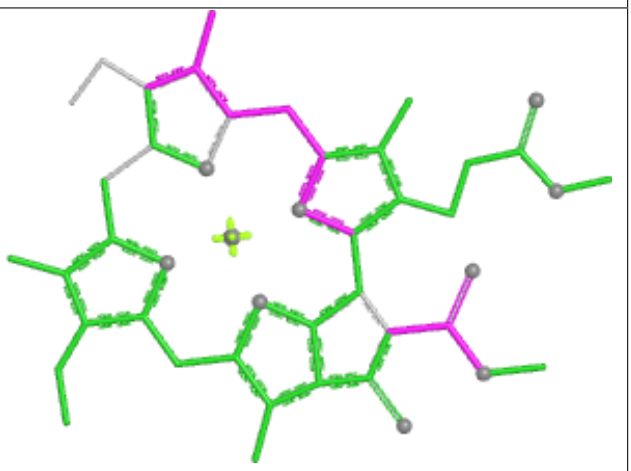
Torsions

Rings

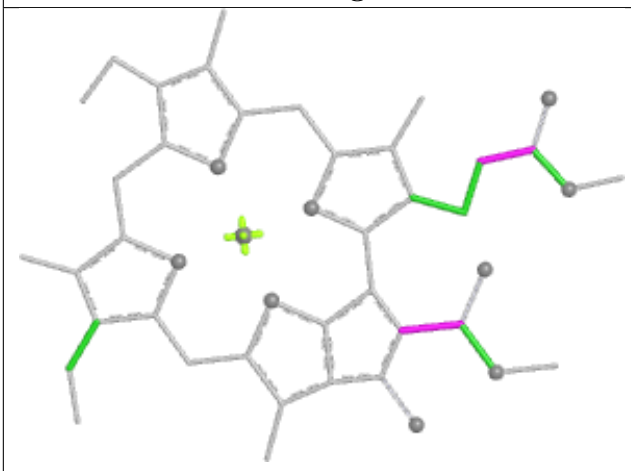
Ligand CLA 8 302



Bond lengths



Bond angles



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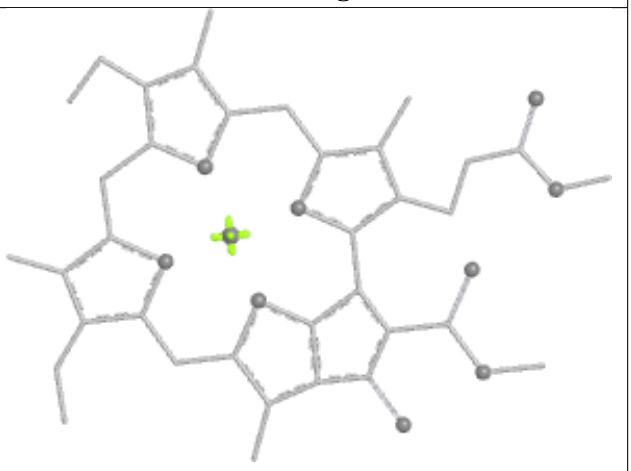
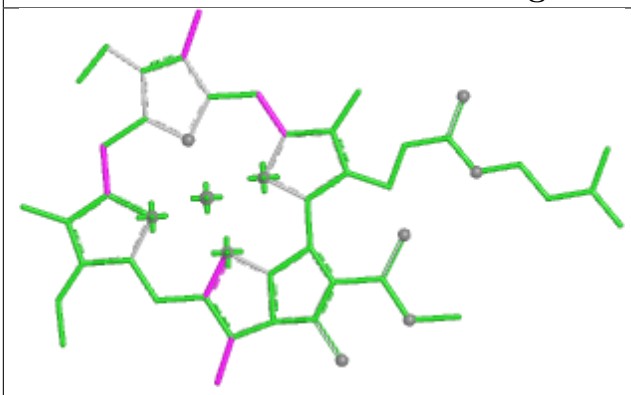


Rings

Ligand CLA 7 313



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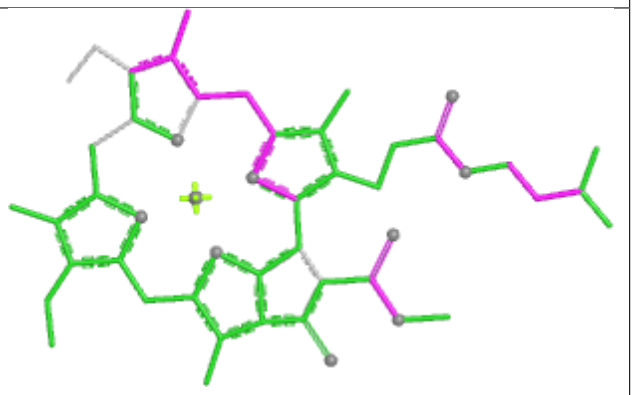
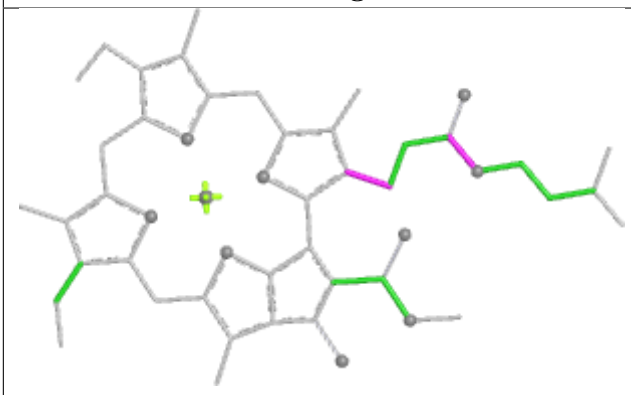


Bond angles



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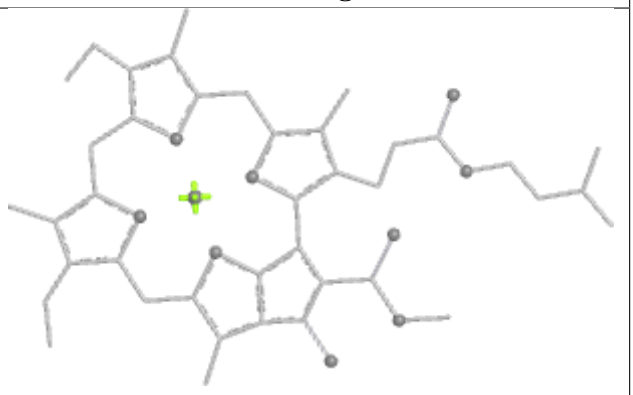
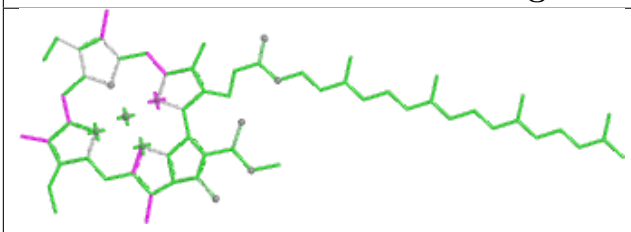
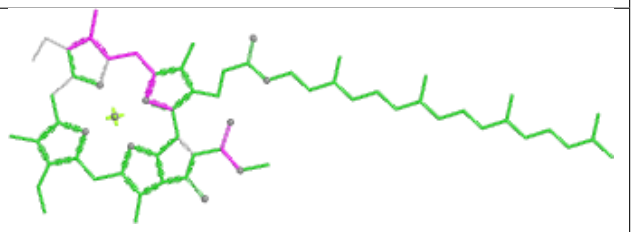


Rings

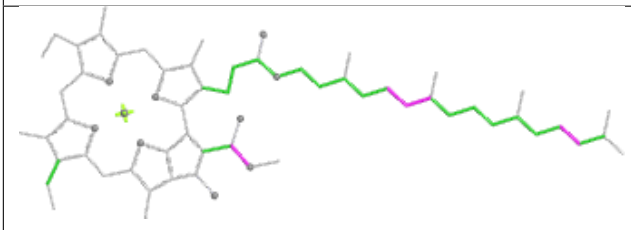
Ligand CLA 3 302



Bond lengths



Bond angles



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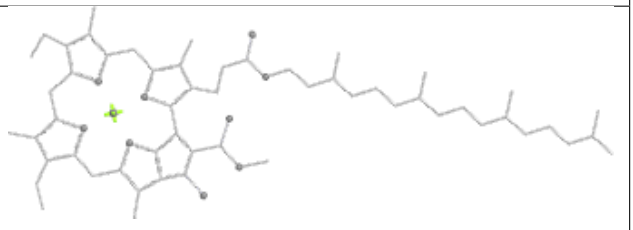
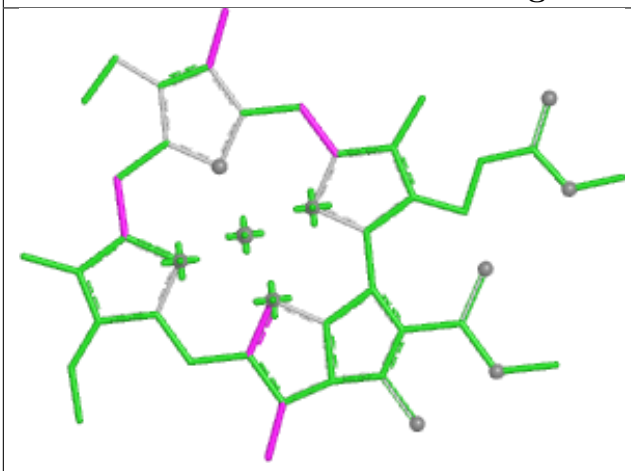


Rings

Ligand CLA 1 614



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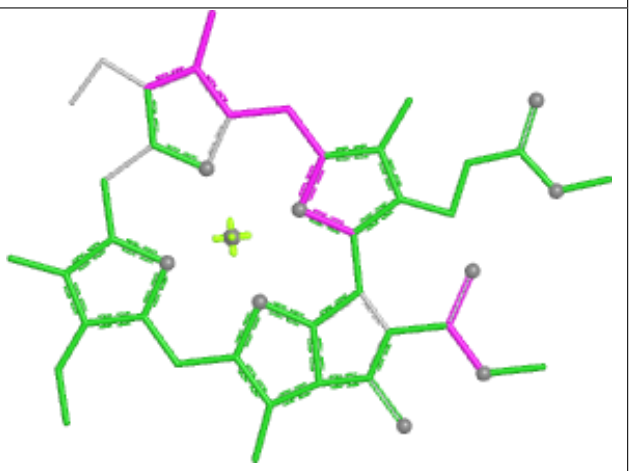
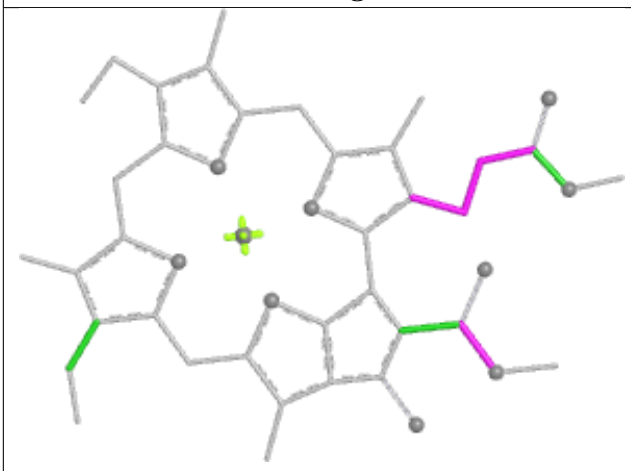
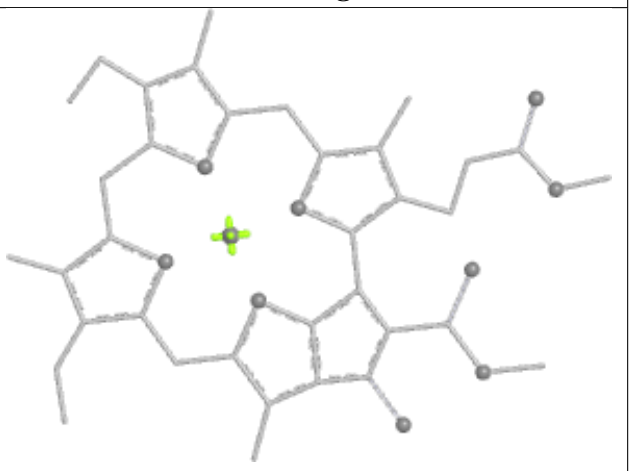


Bond angles

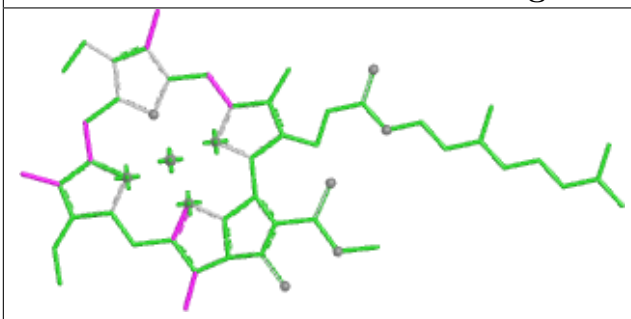


Torsions



Rings

Ligand CLA 3 306



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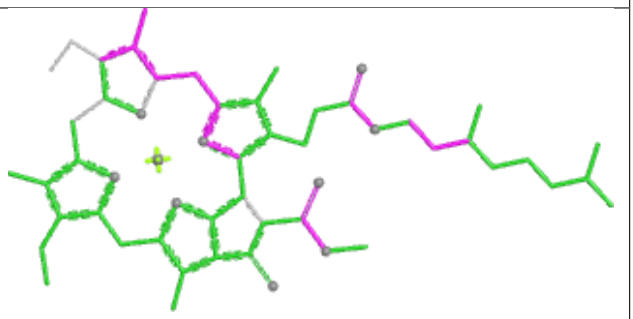
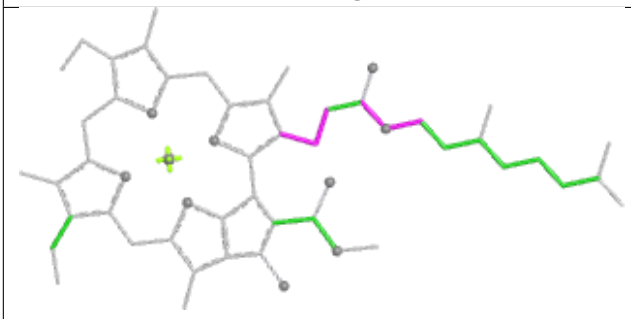
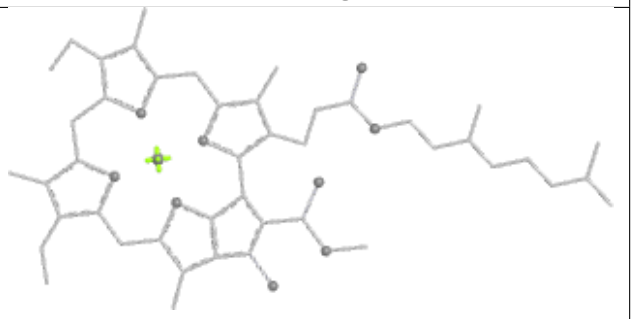


Bond angles

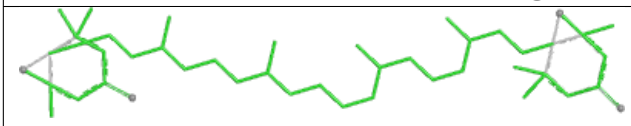


Torsions

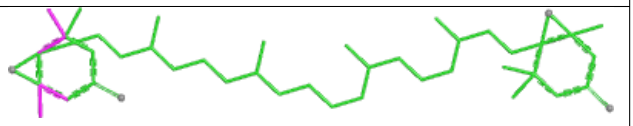


Rings

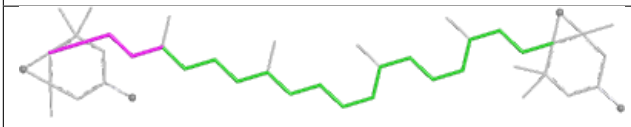
Ligand XAT c 315



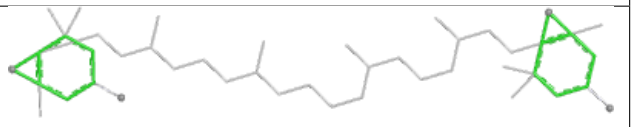
Bond lengths



Bond angles

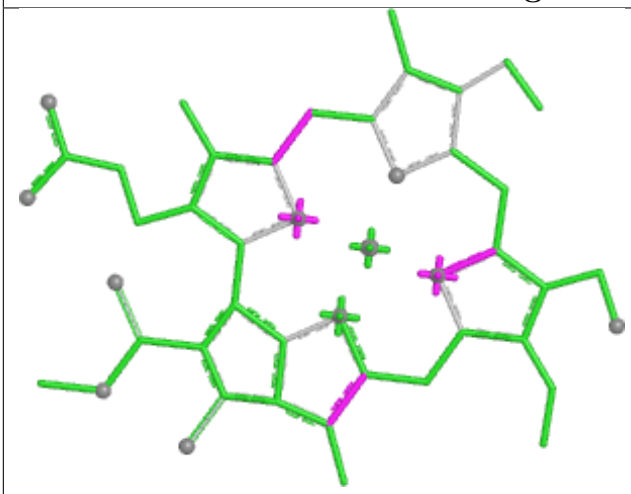


Torsions

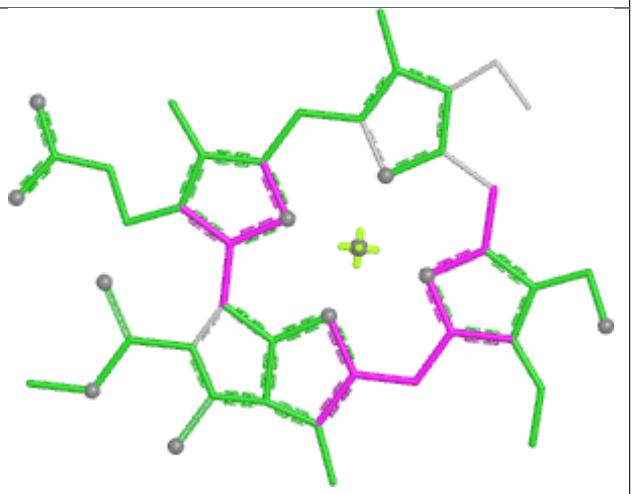


Rings

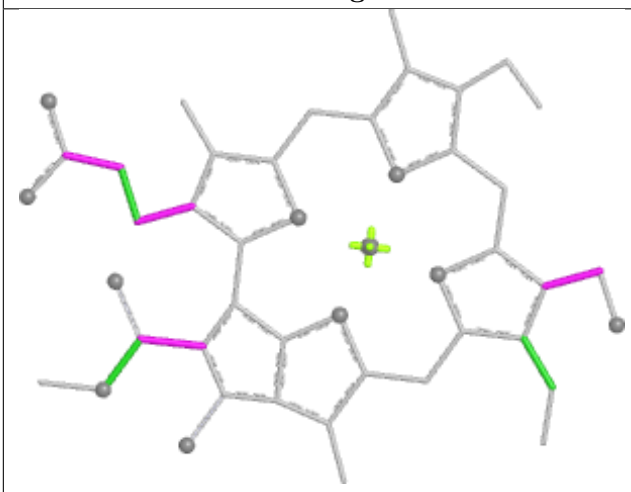
Ligand CHL T 416



Bond lengths



Bond angles



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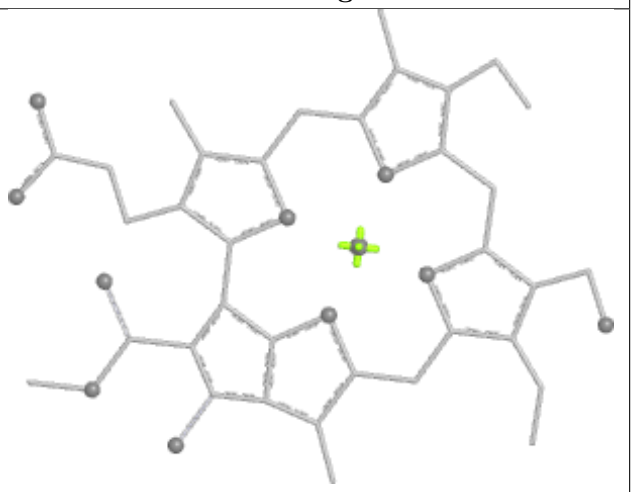
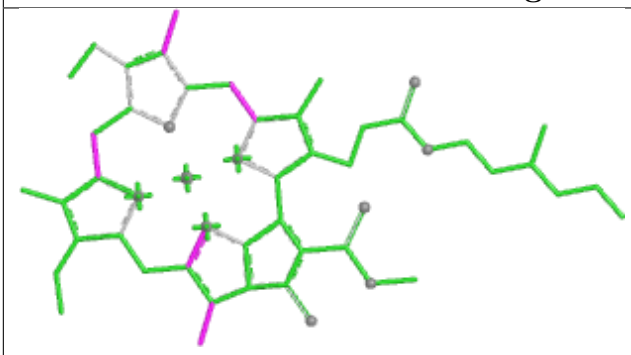
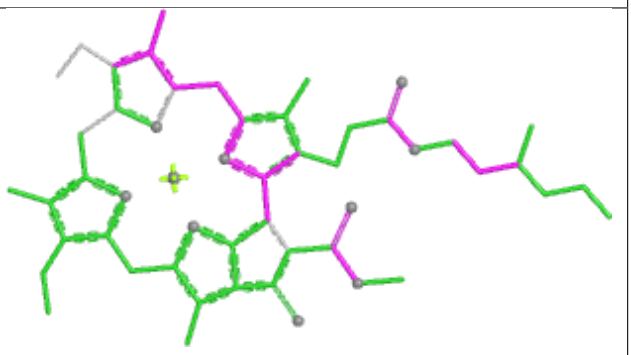


Rings

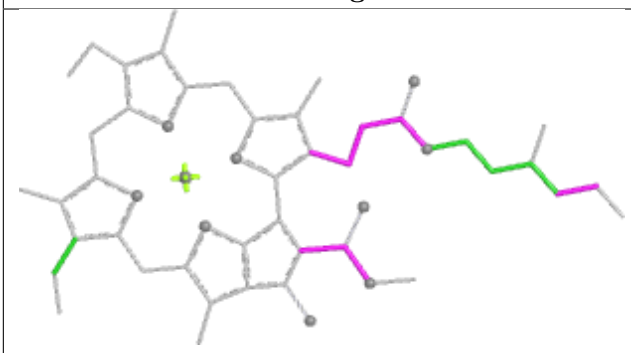
Ligand CLA T 409



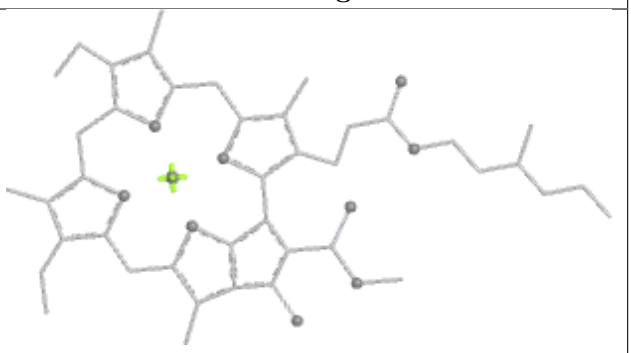
Bond lengths



Bond angles

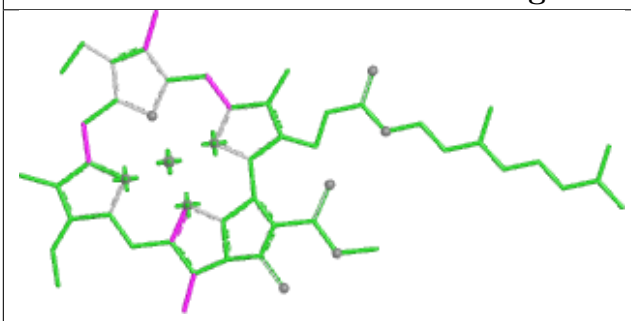


Torsions

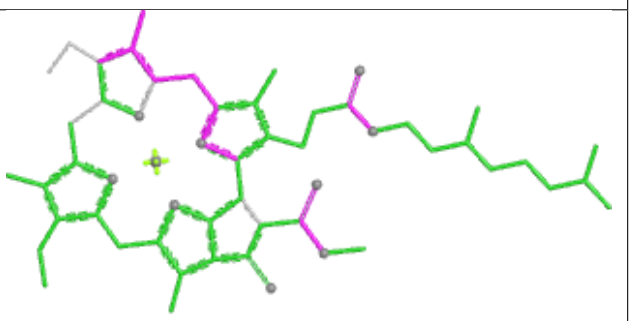


Rings

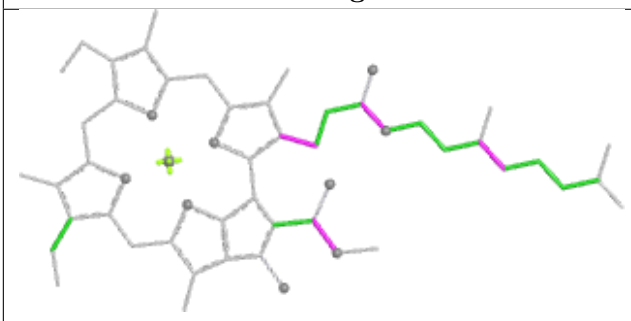
Ligand CLA 3 323



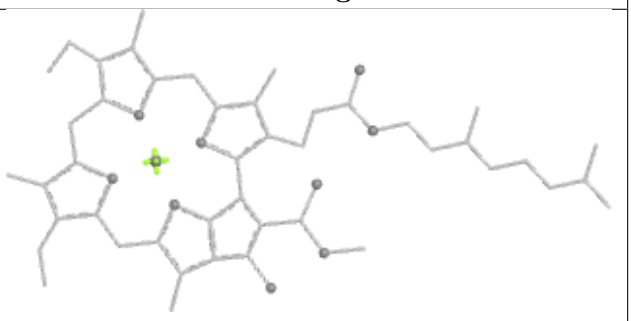
Bond lengths



Bond angles

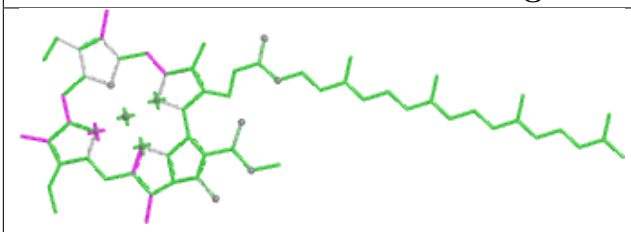


Torsions

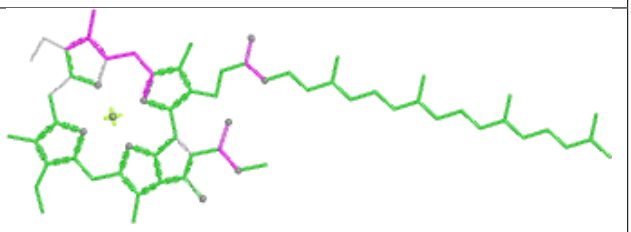


Rings

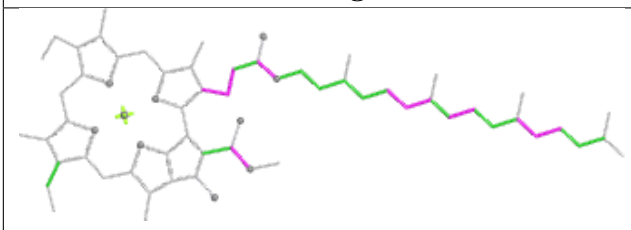
Ligand CLA B 802



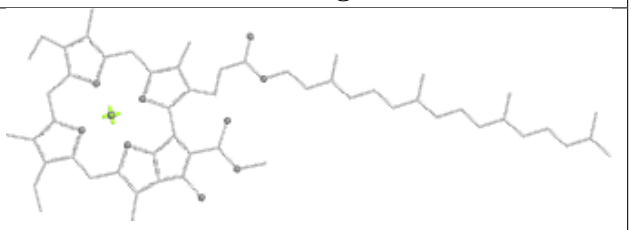
Bond lengths



Bond angles

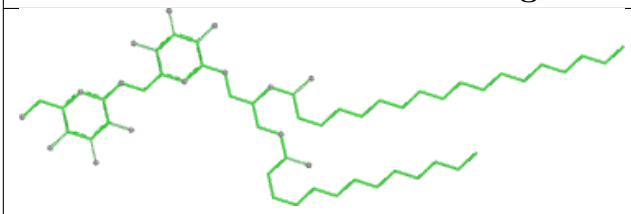


Torsions

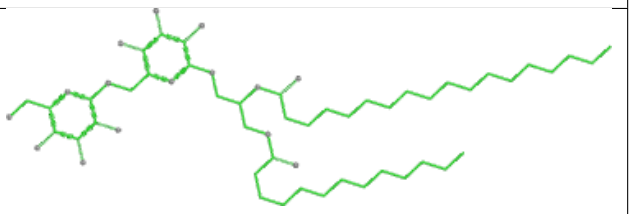


Rings

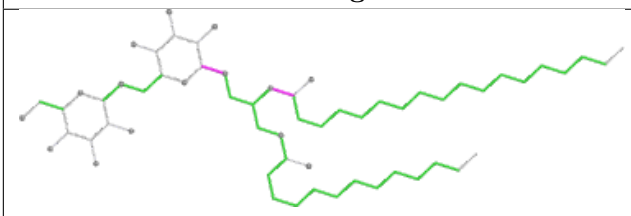
Ligand DGD B 848



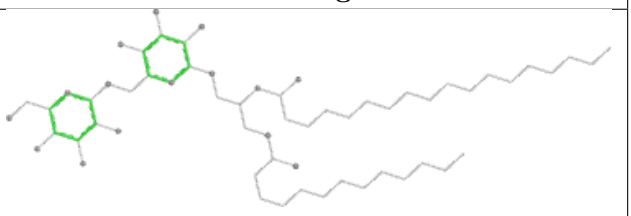
Bond lengths



Bond angles

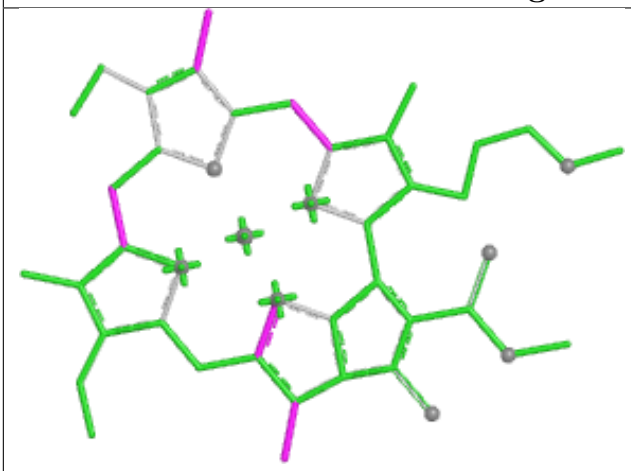


Torsions

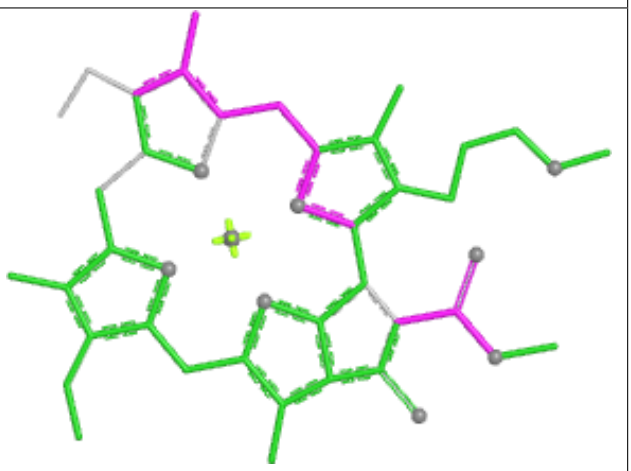


Rings

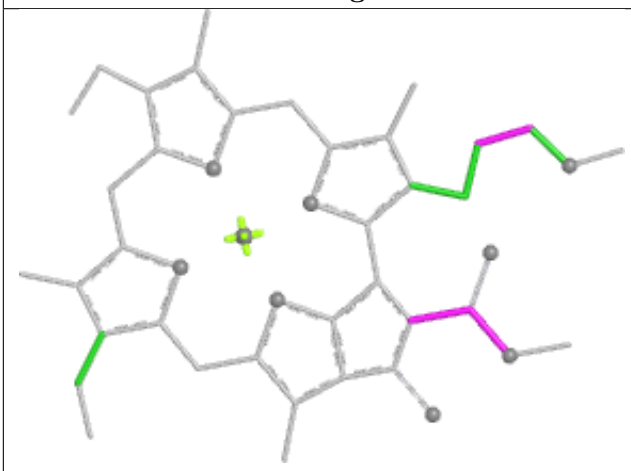
Ligand CLA a 608



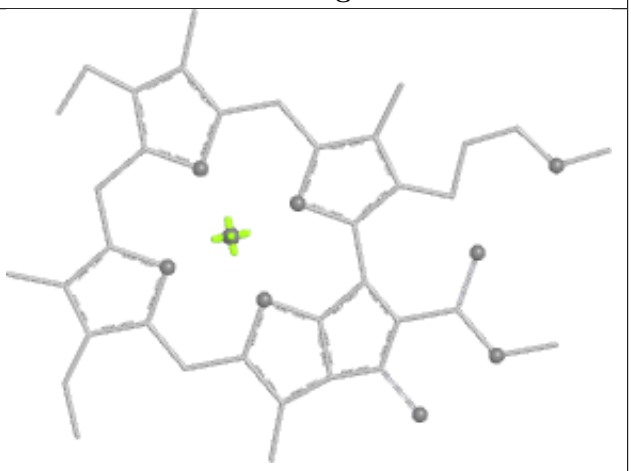
Bond lengths



Bond angles

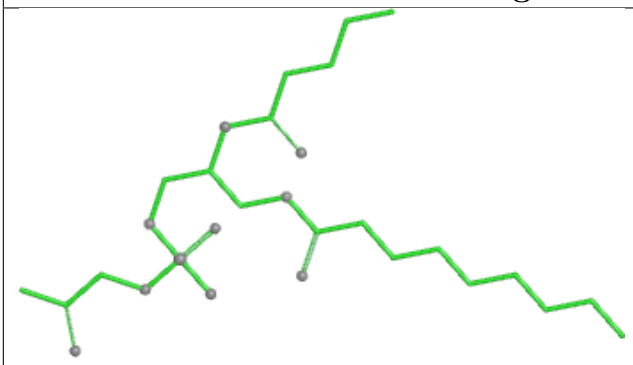


Torsions

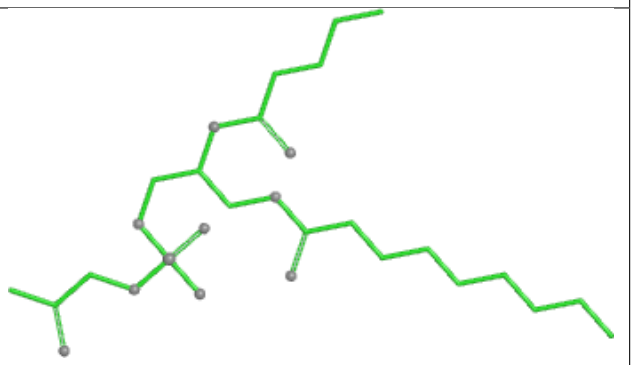


Rings

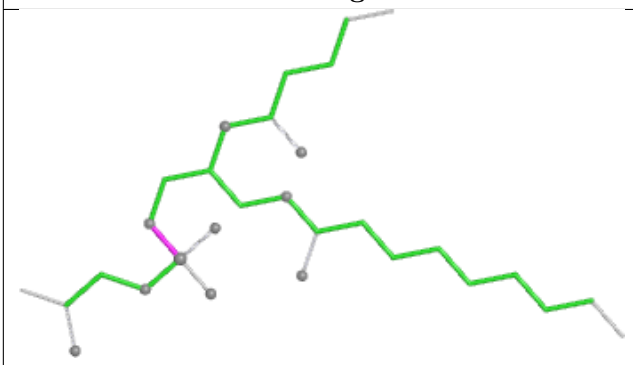
Ligand LHG A 5055



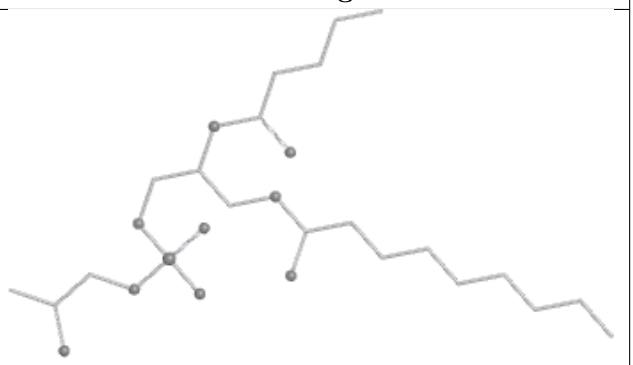
Bond lengths



Bond angles

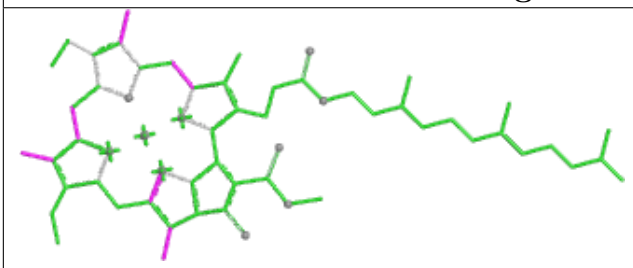


Torsions

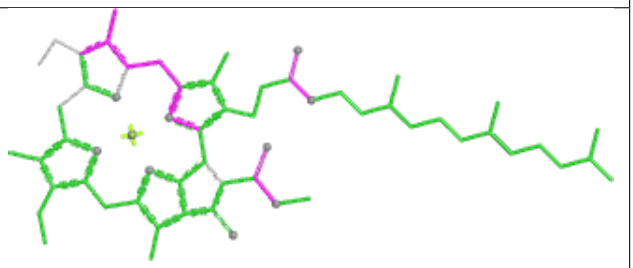


Rings

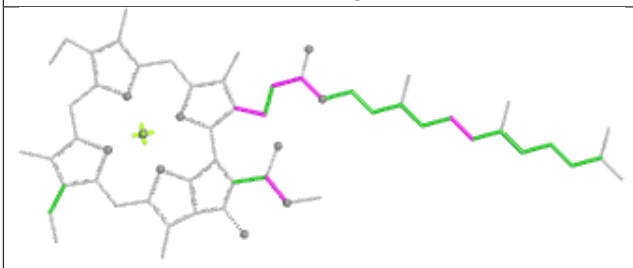
Ligand CLA A 5025



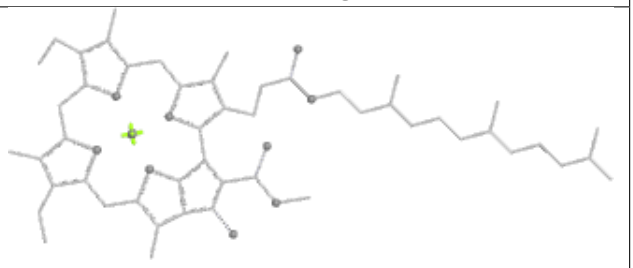
Bond lengths



Bond angles

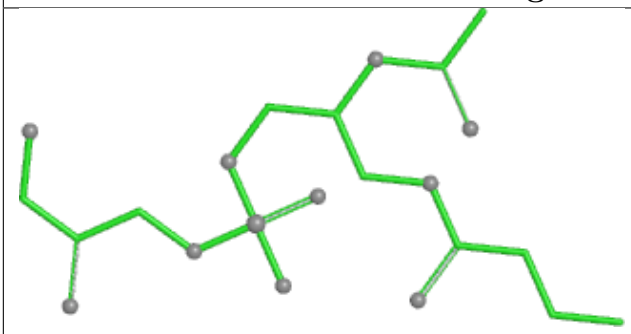


Torsions

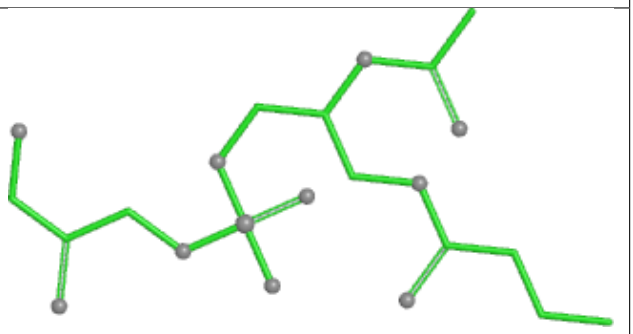


Rings

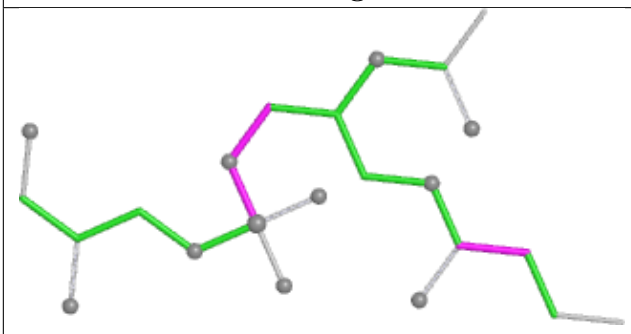
Ligand LHG a 619



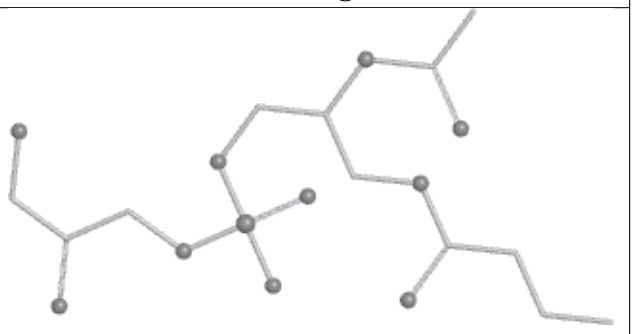
Bond lengths



Bond angles

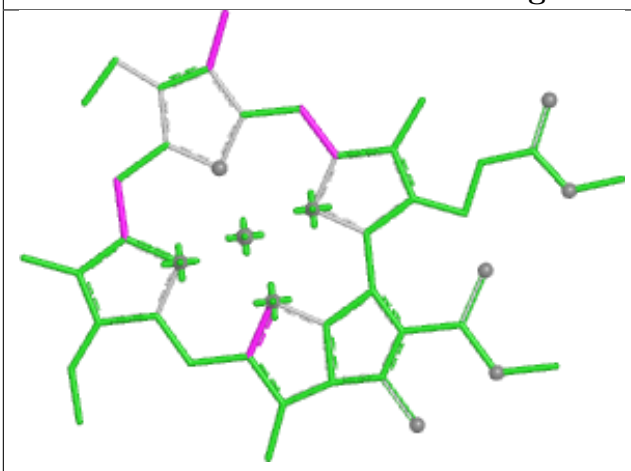


Torsions

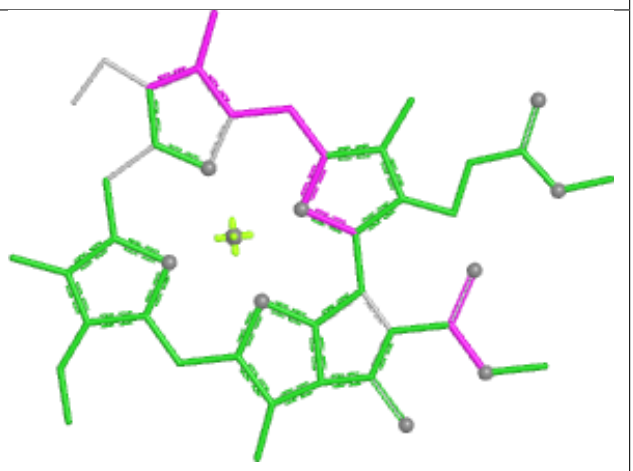


Rings

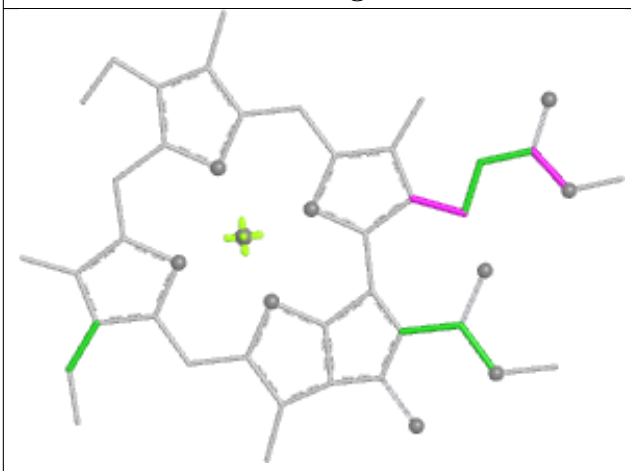
Ligand CLA 7 308



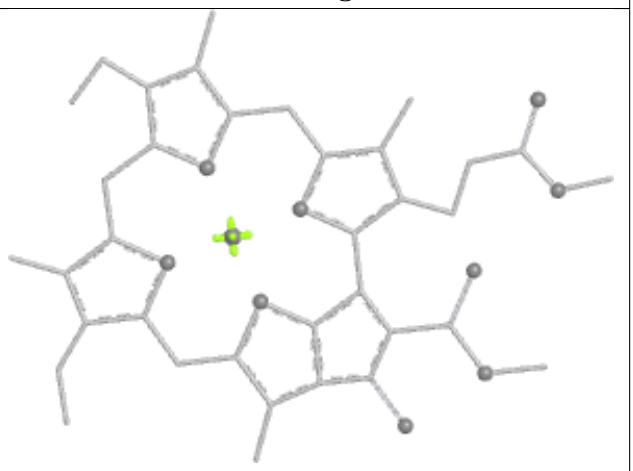
Bond lengths



Bond angles

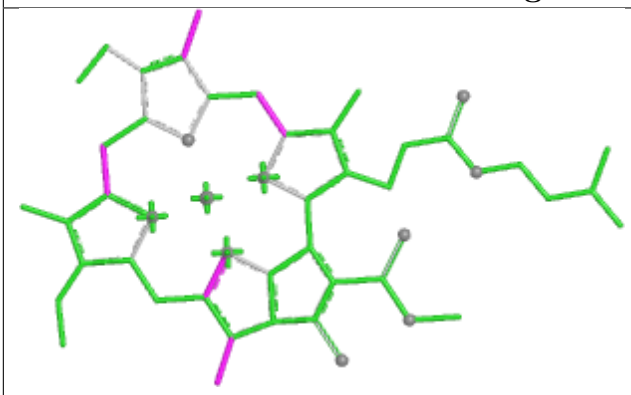


Torsions

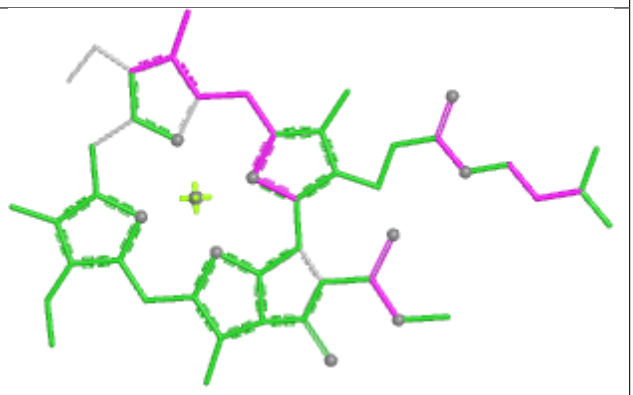


Rings

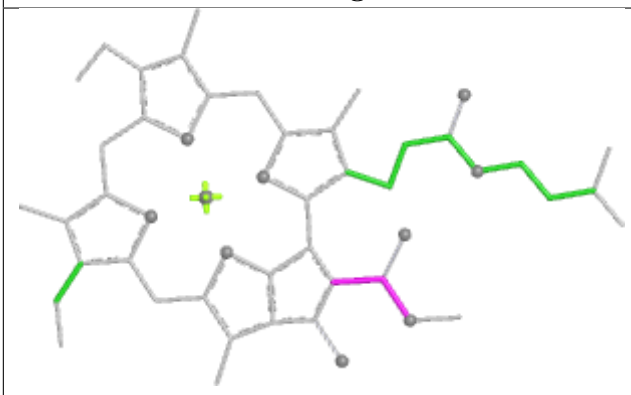
Ligand CLA B 815



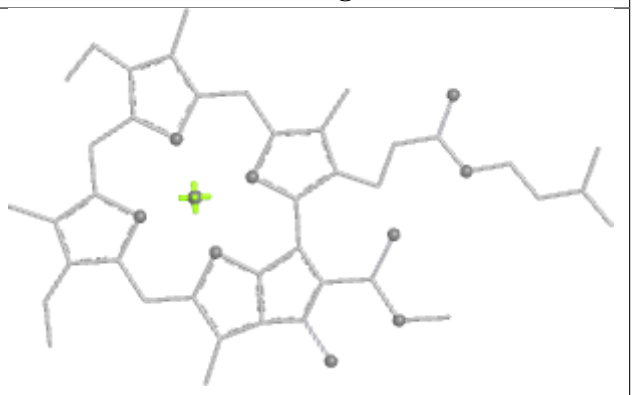
Bond lengths



Bond angles

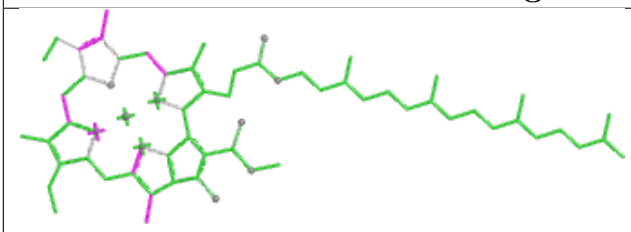


Torsions

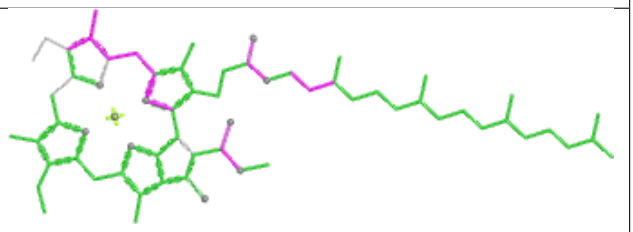


Rings

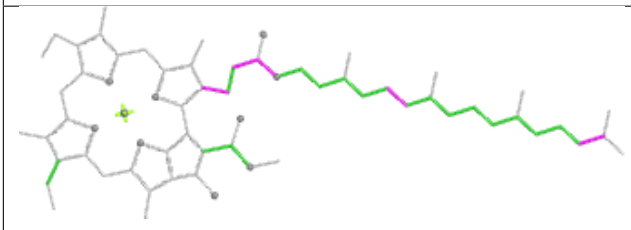
Ligand CLA B 839



Bond lengths



Bond angles



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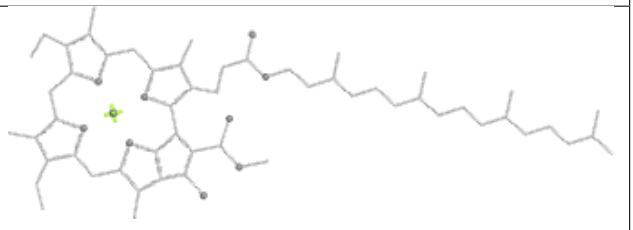
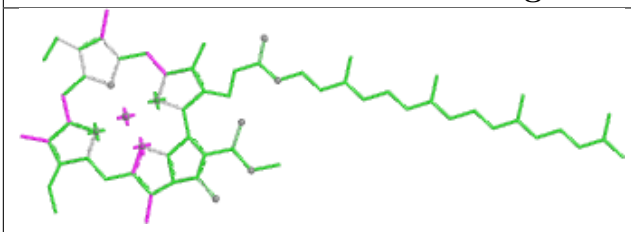
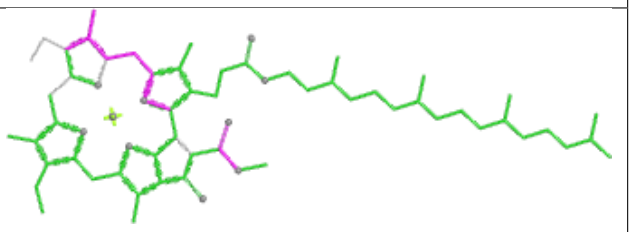


Rings

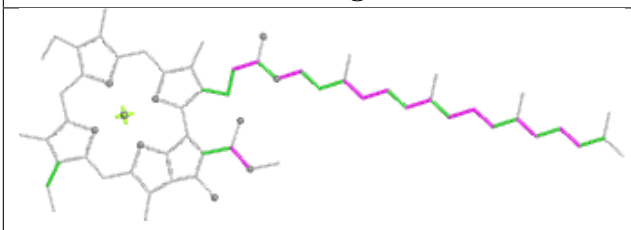
Ligand CLA B 806



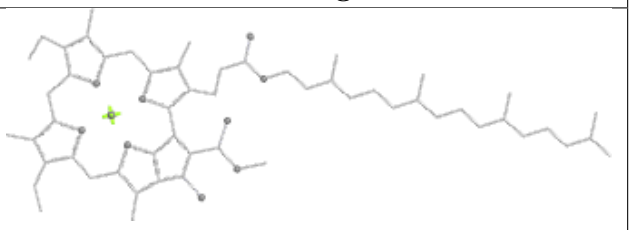
Bond lengths



Bond angles



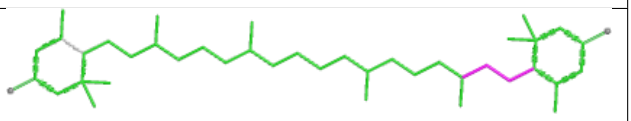
Torsions



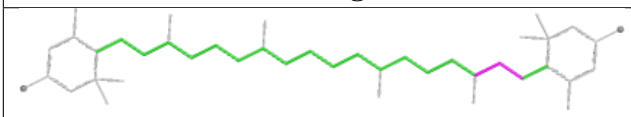
Rings

Ligand LUT T 413

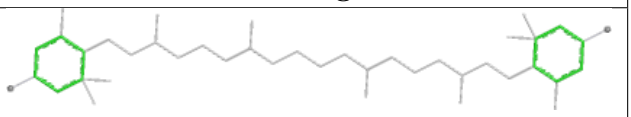
Bond lengths



Bond angles

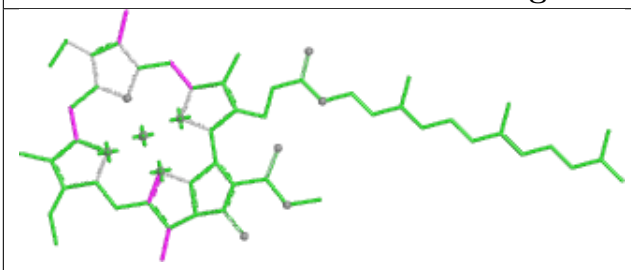


Torsions

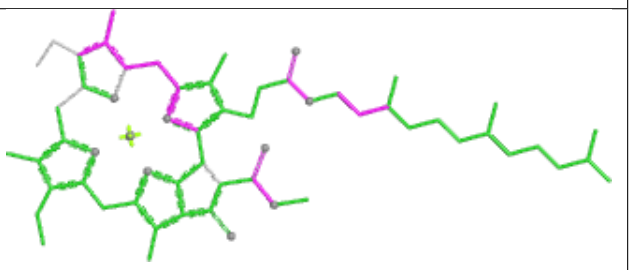


Rings

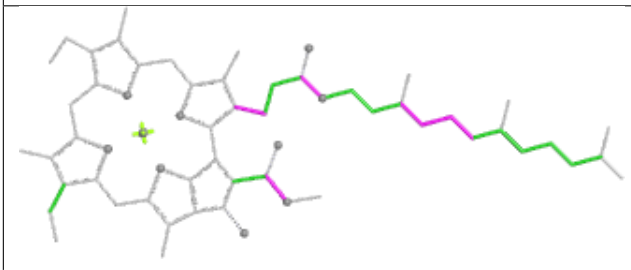
Ligand CLA c 309



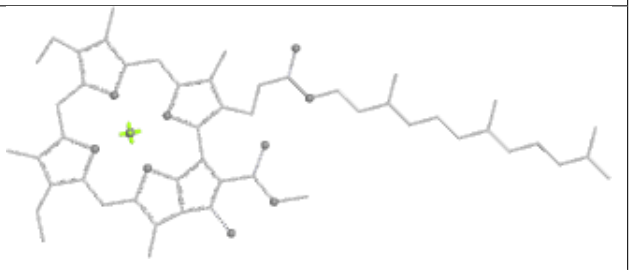
Bond lengths



Bond angles

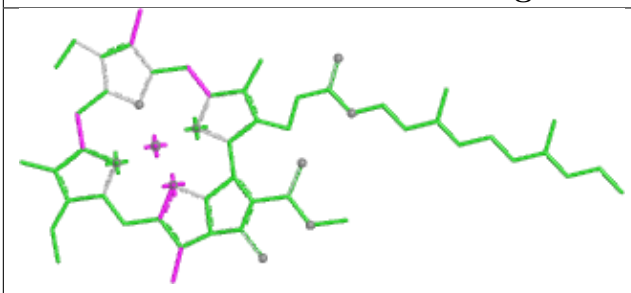


Torsions

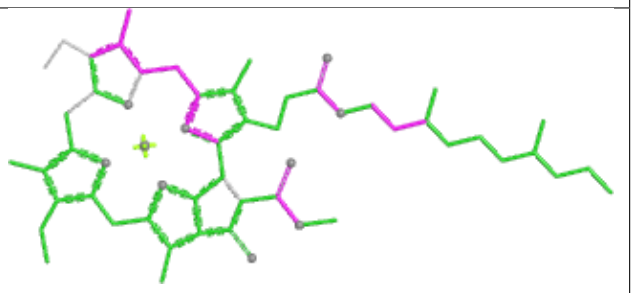


Rings

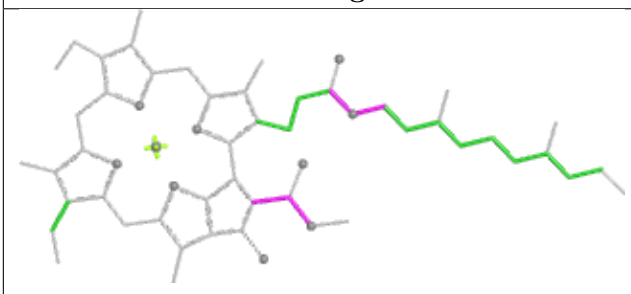
Ligand CLA A 5027



Bond lengths



Bond angles



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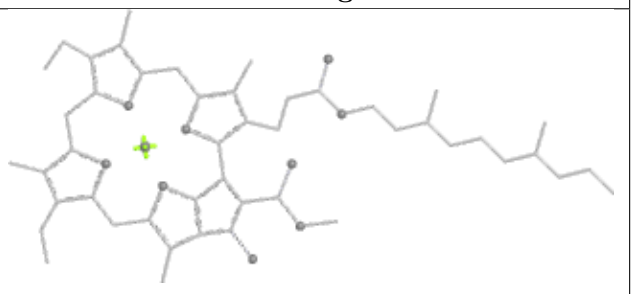
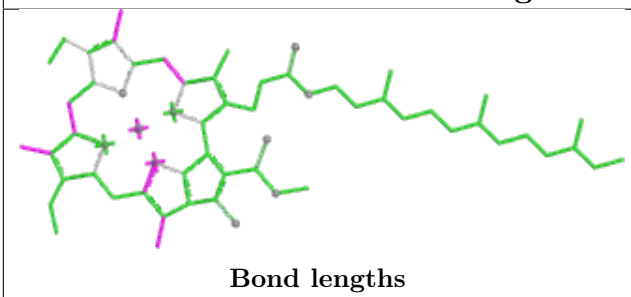
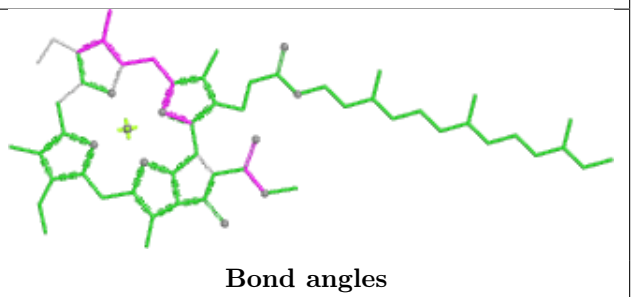


Rings

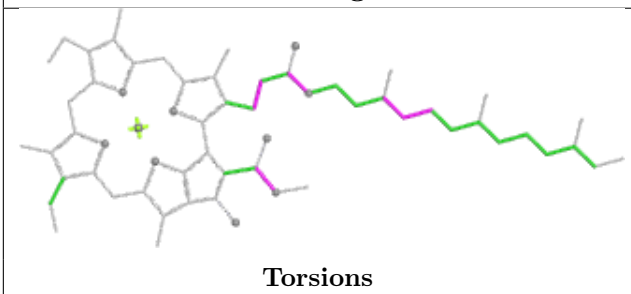
Ligand CLA A 5019



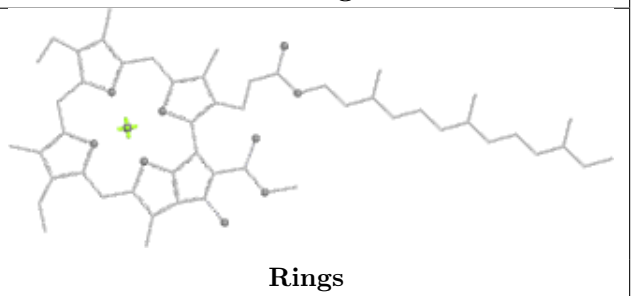
Bond lengths



Bond angles

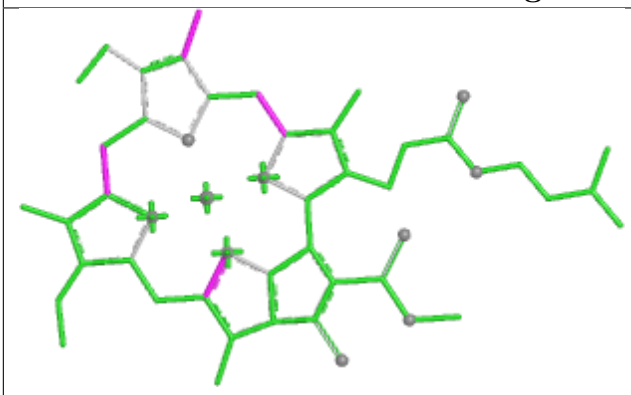


Torsions

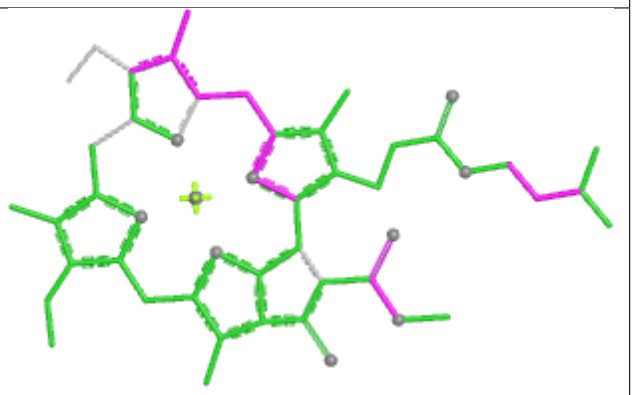


Rings

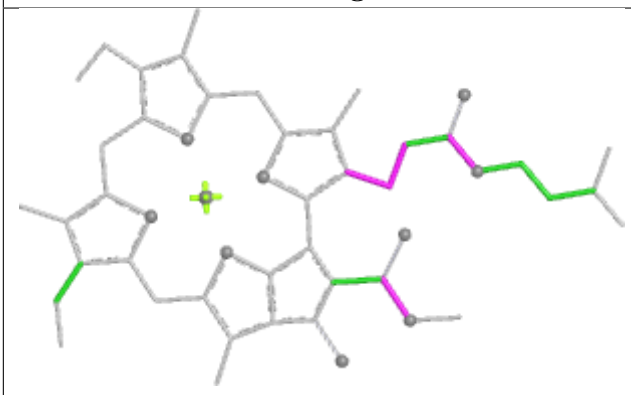
Ligand CLA B 823



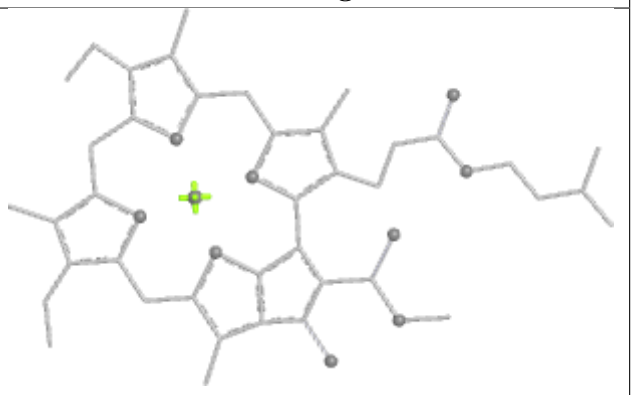
Bond lengths



Bond angles

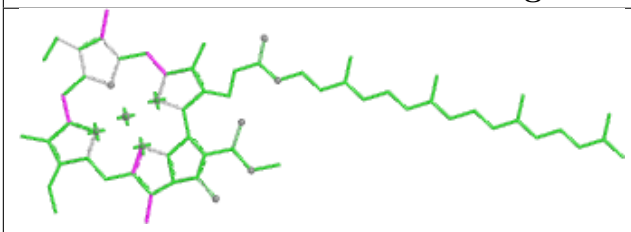


Torsions

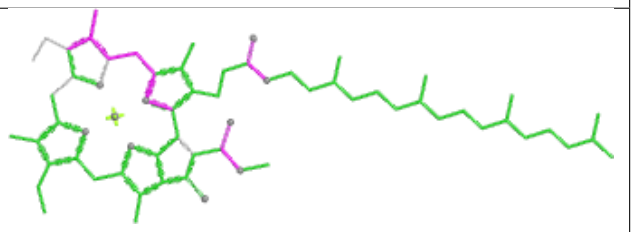


Rings

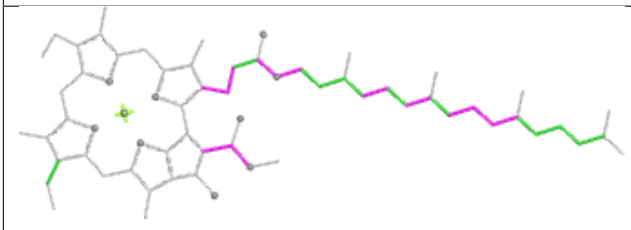
Ligand CLA B 829



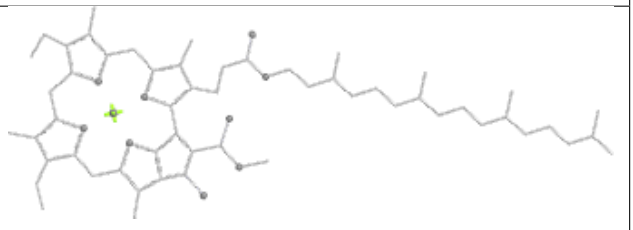
Bond lengths



Bond angles

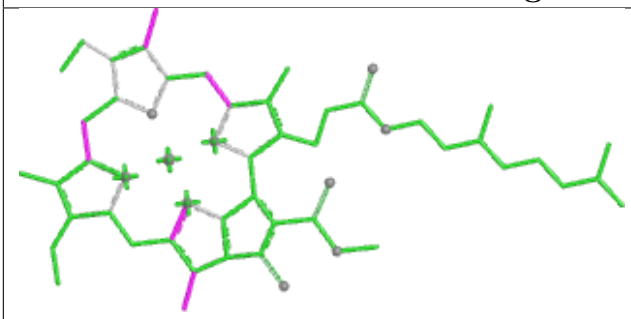


Torsions

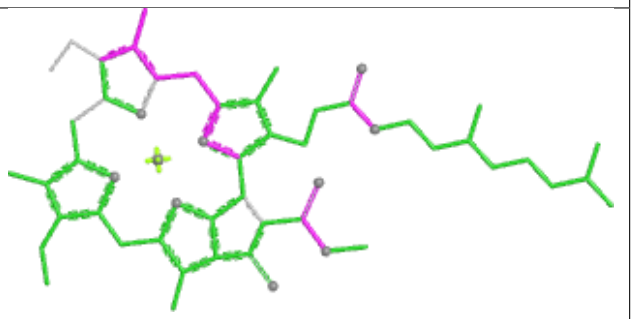


Rings

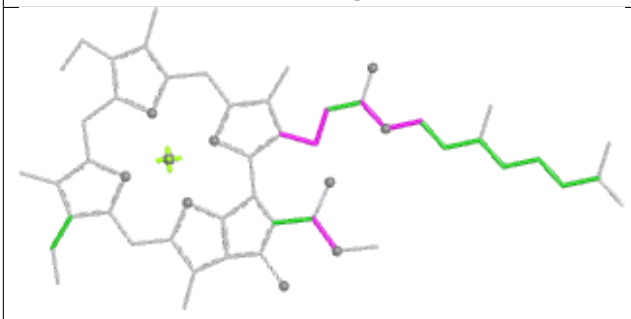
Ligand CLA B 820



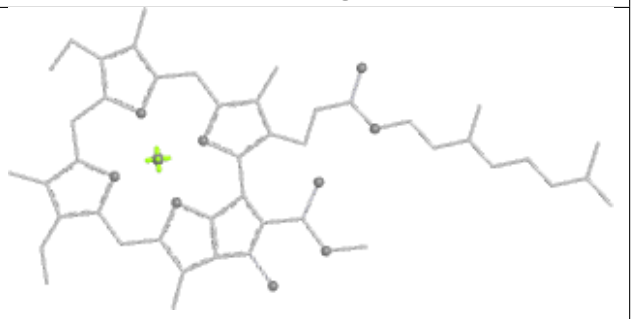
Bond lengths



Bond angles

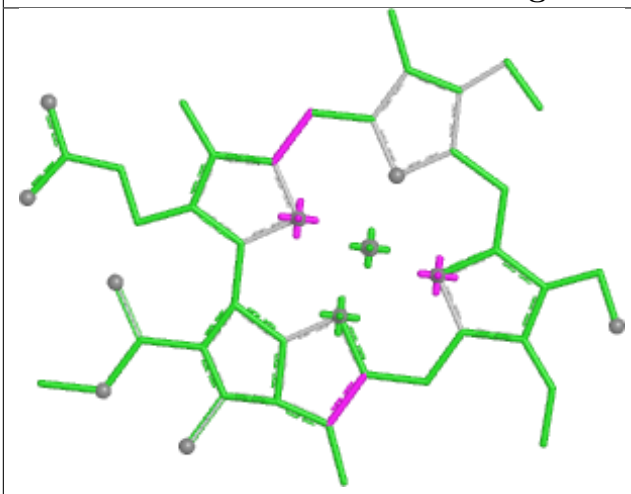


Torsions

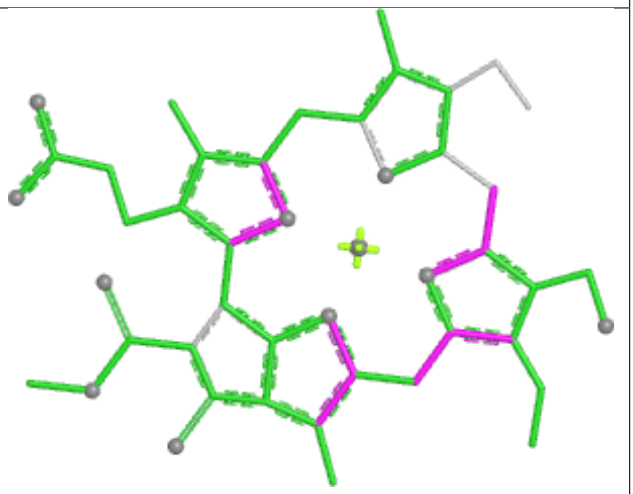


Rings

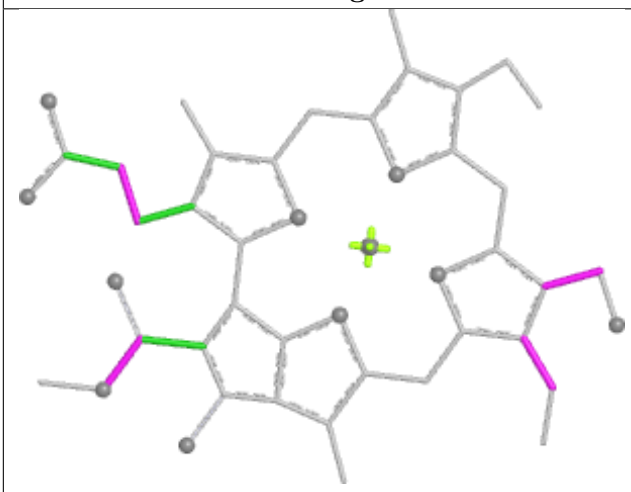
Ligand CHL c 304



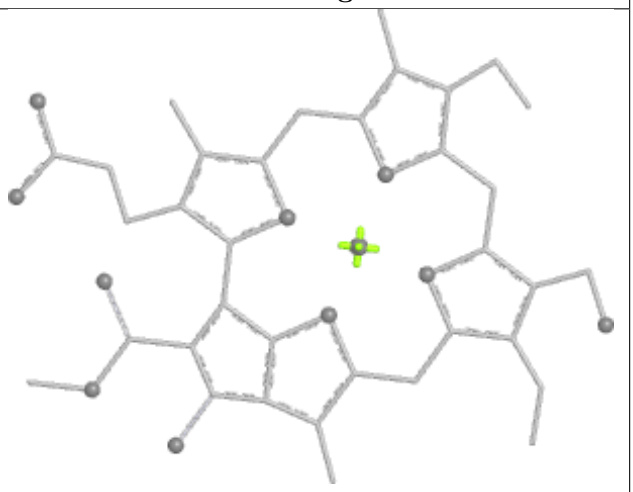
Bond lengths



Bond angles

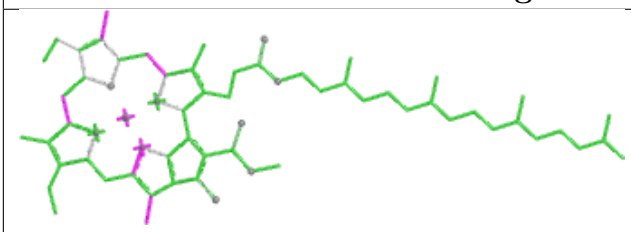


Torsions

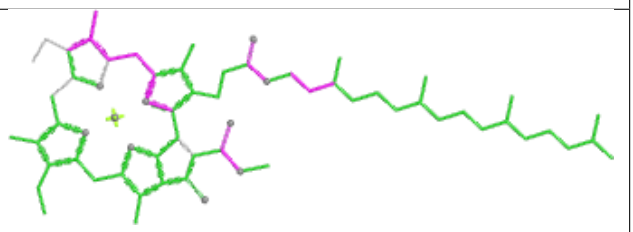


Rings

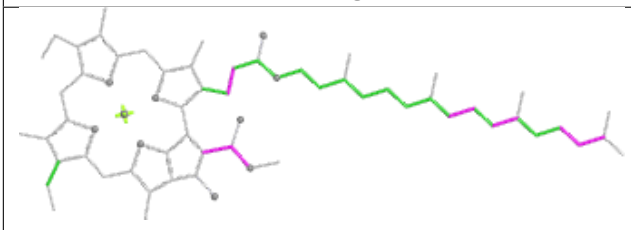
Ligand CLA A 5020



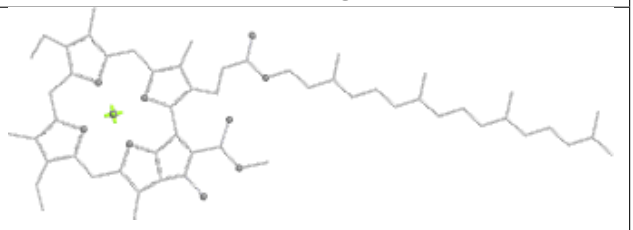
Bond lengths



Bond angles

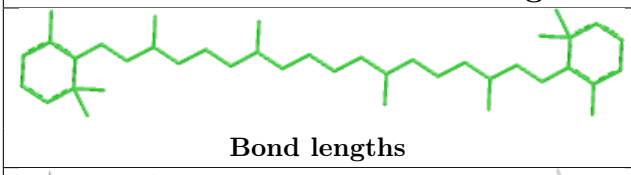


Torsions

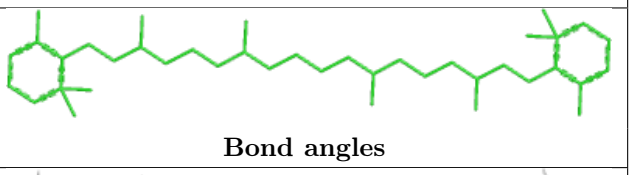


Rings

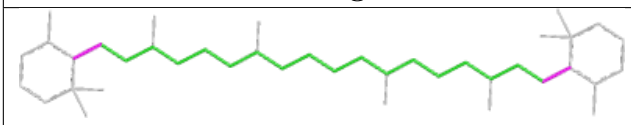
Ligand BCR b 617



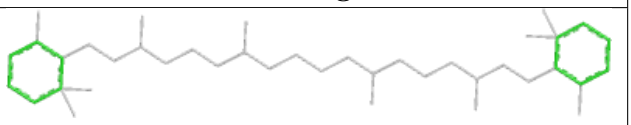
Bond lengths



Bond angles

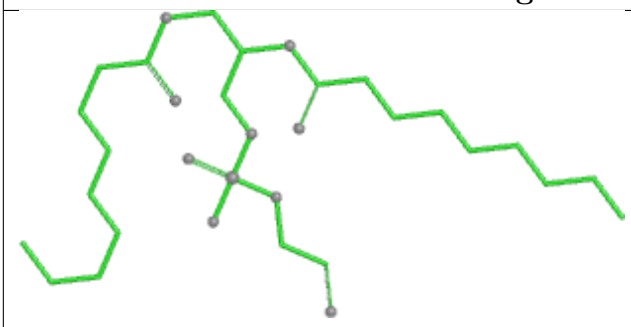


Torsions

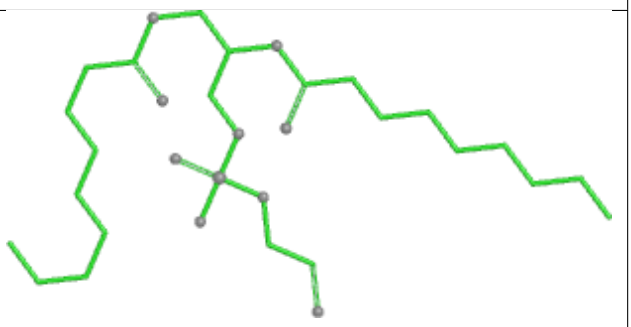


Rings

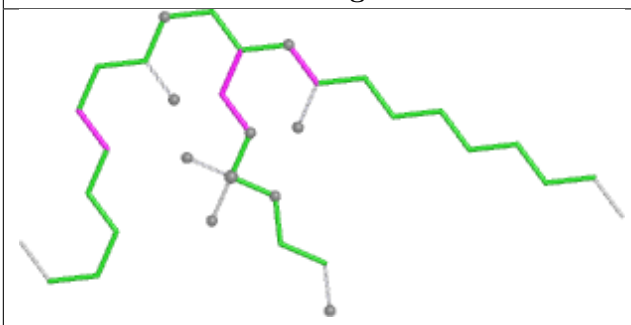
Ligand PTY F 5002



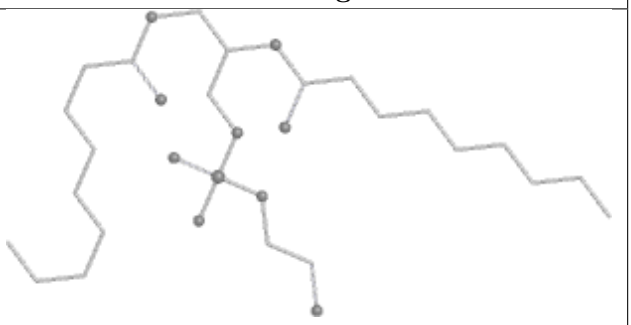
Bond lengths



Bond angles

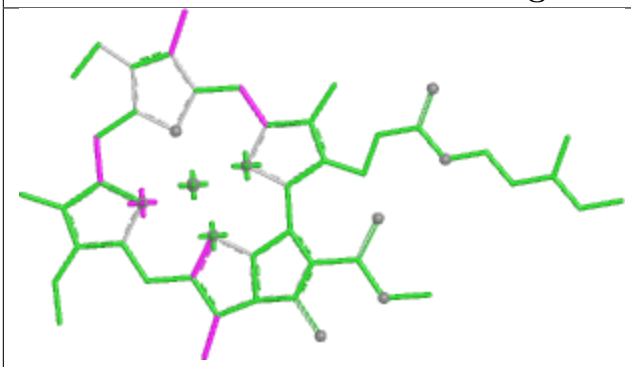


Torsions



Rings

Ligand CLA 8 313



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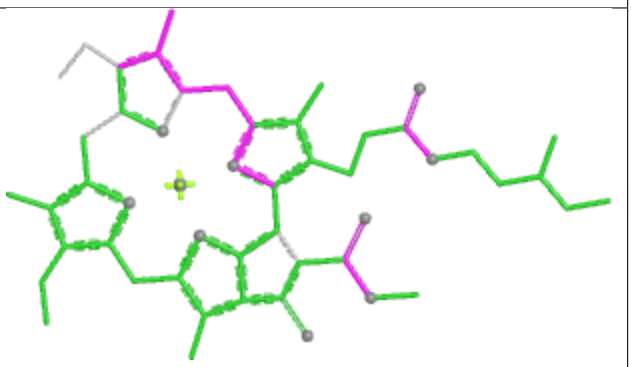
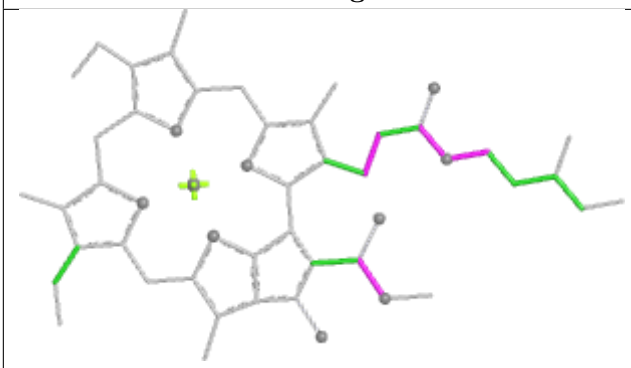


Bond angles



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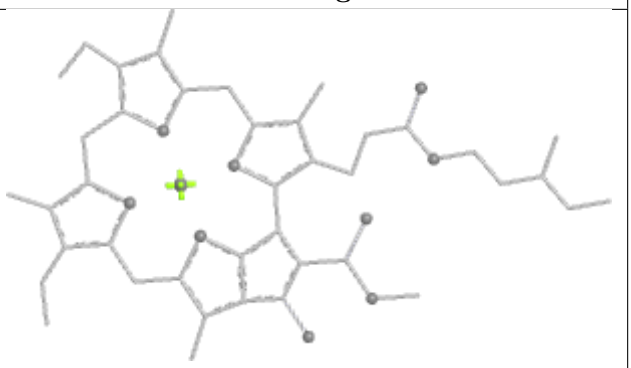
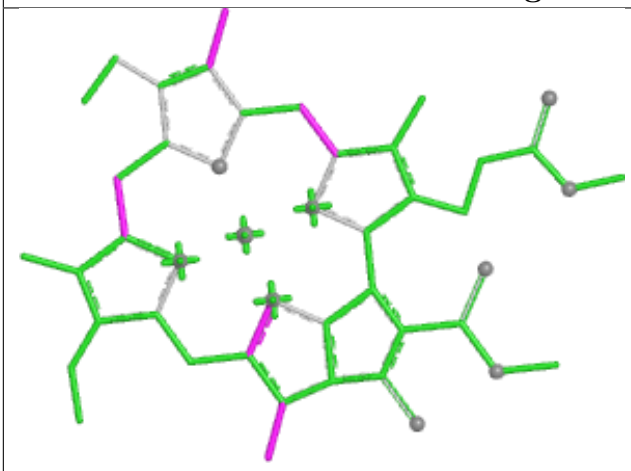
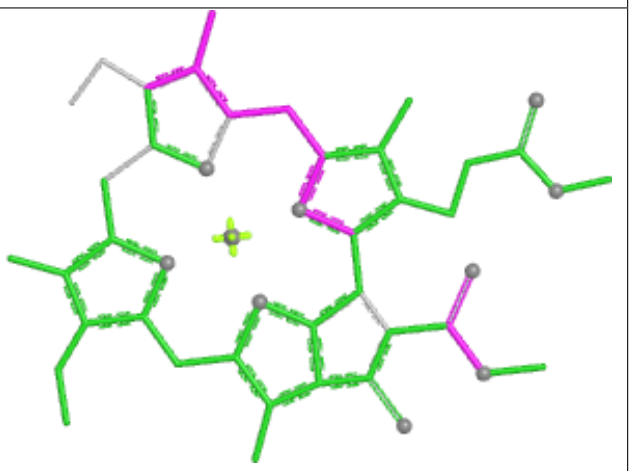


Rings

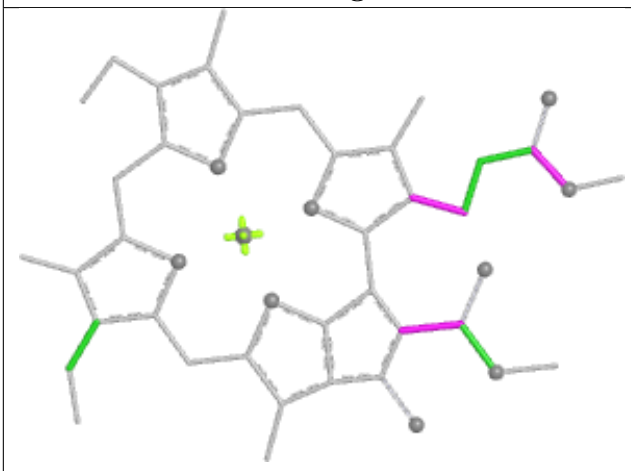
Ligand CLA B 812



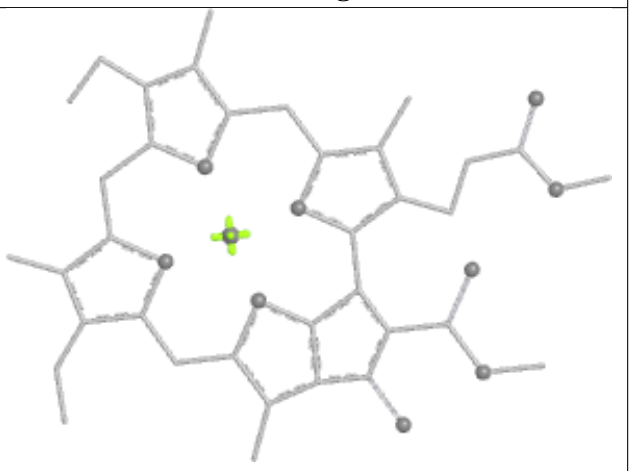
Bond lengths



Bond angles

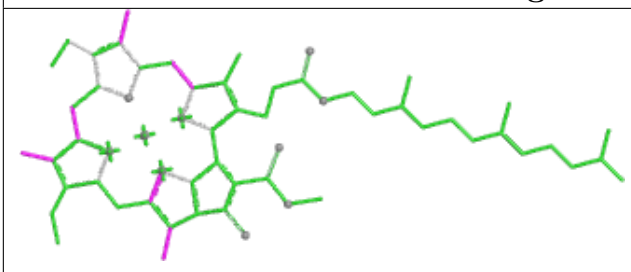


Torsions

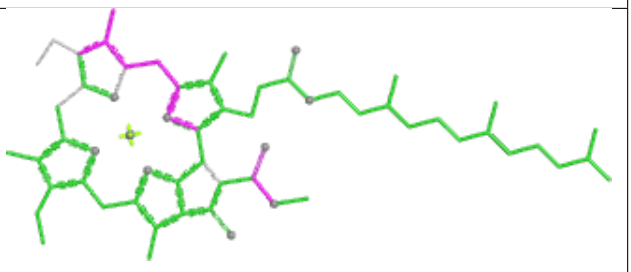


Rings

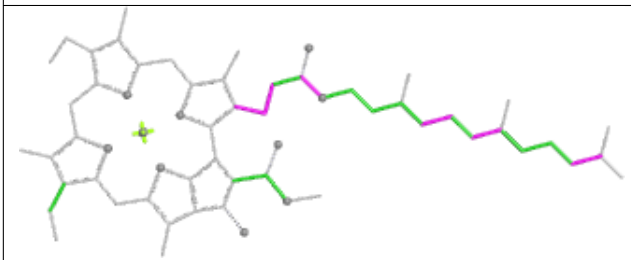
Ligand CLA b 609



Bond lengths



Bond angles



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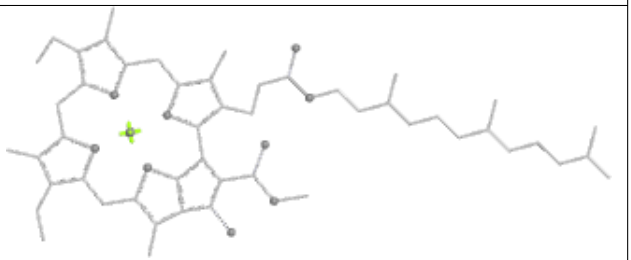
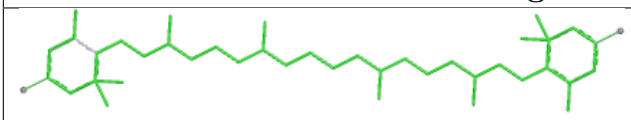
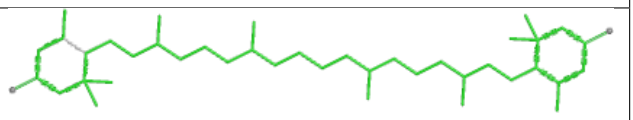


Rings

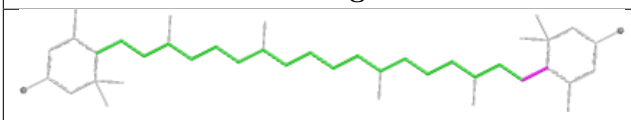
Ligand LUT b 615



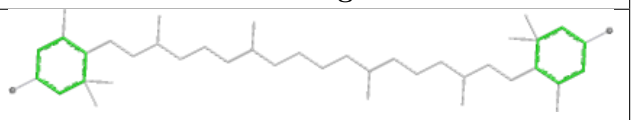
Bond lengths



Bond angles



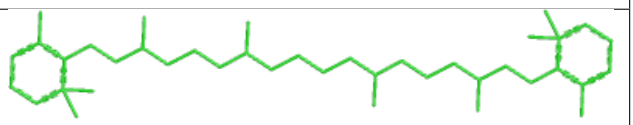
Torsions



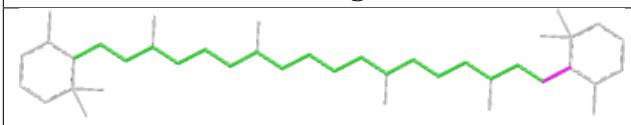
Rings

Ligand BCR B 846

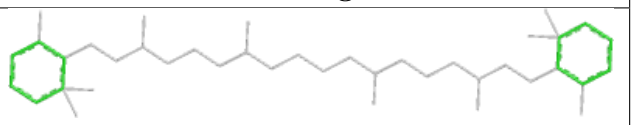
Bond lengths



Bond angles

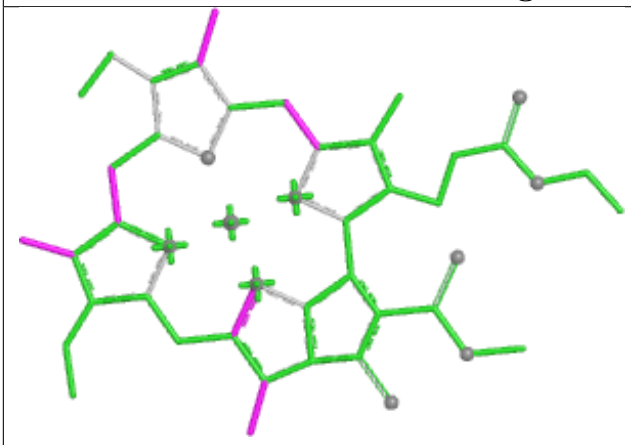


Torsions

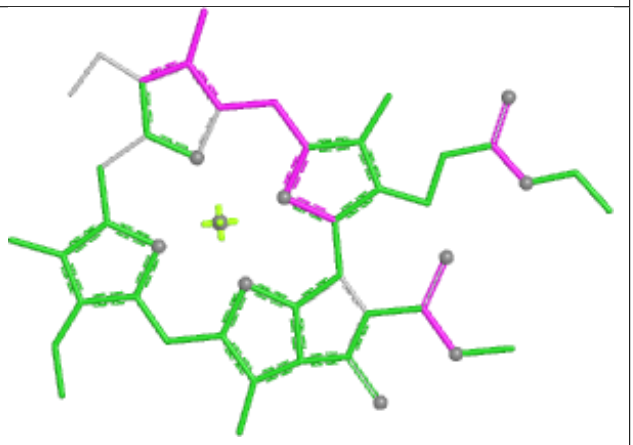


Rings

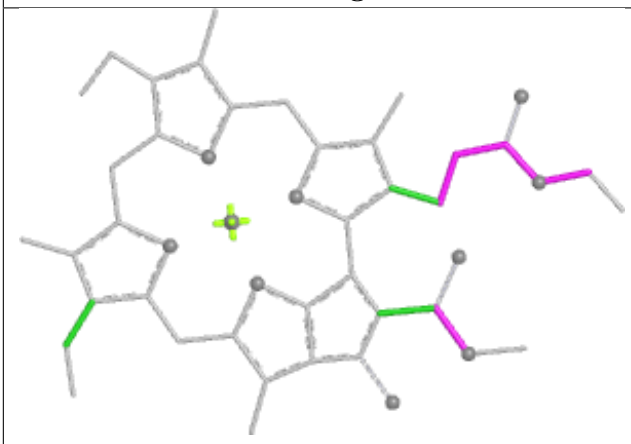
Ligand CLA F 5007



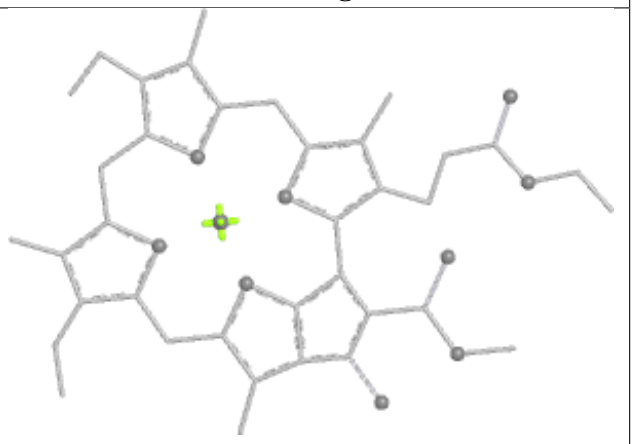
Bond lengths



Bond angles

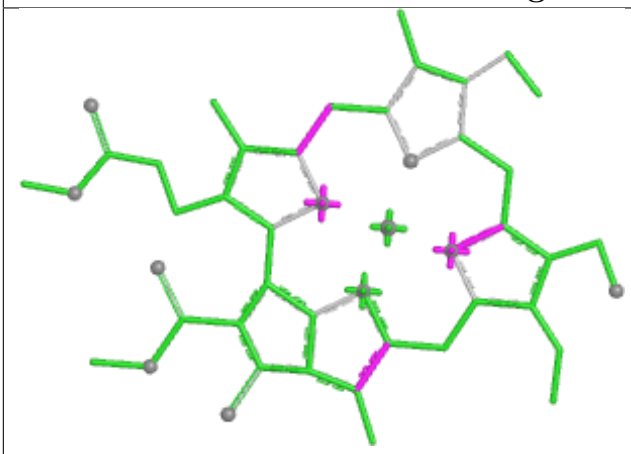


Torsions

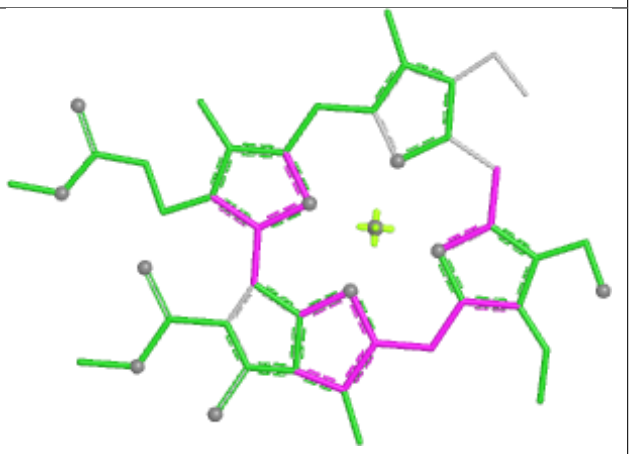


Rings

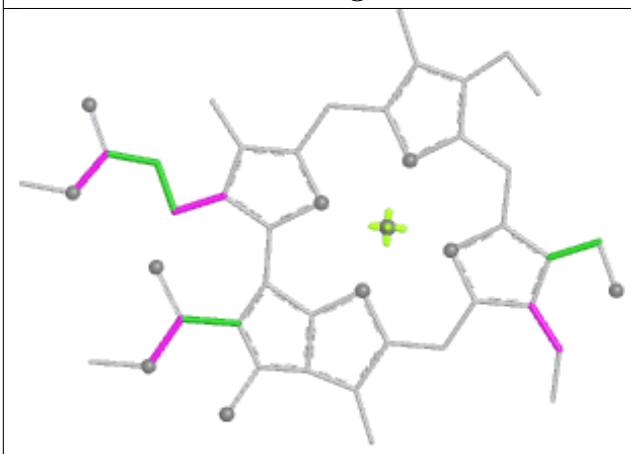
Ligand CHL 7 306



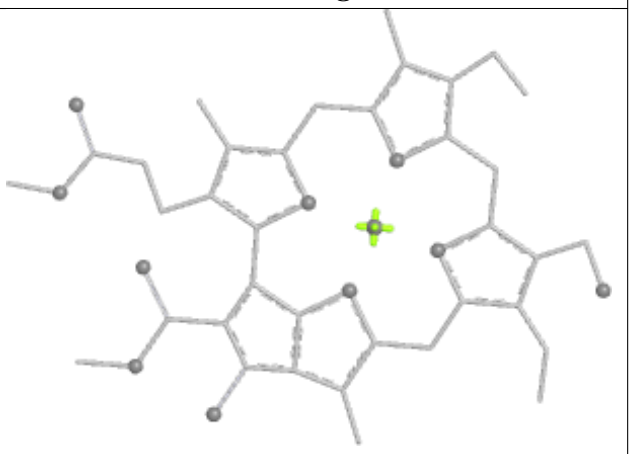
Bond lengths



Bond angles

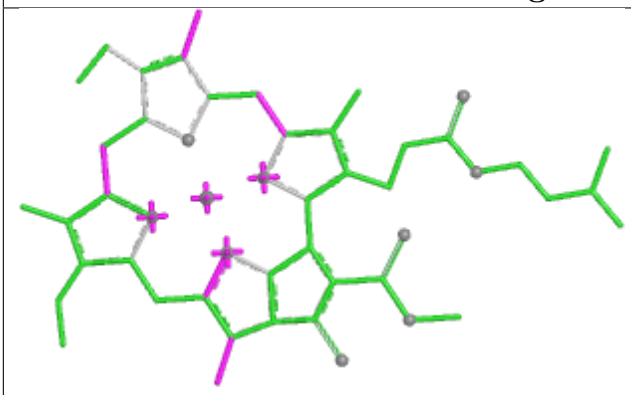


Torsions



Rings

Ligand CLA 8 312



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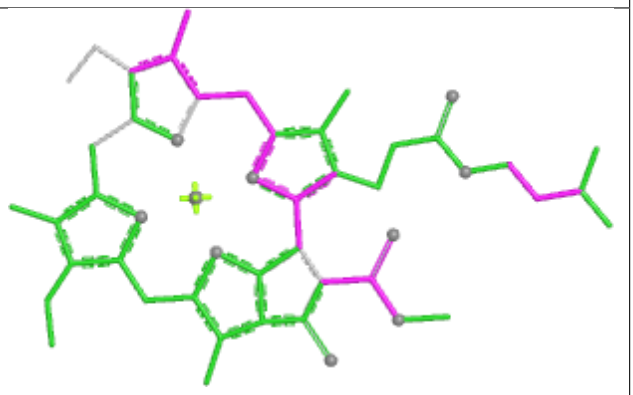
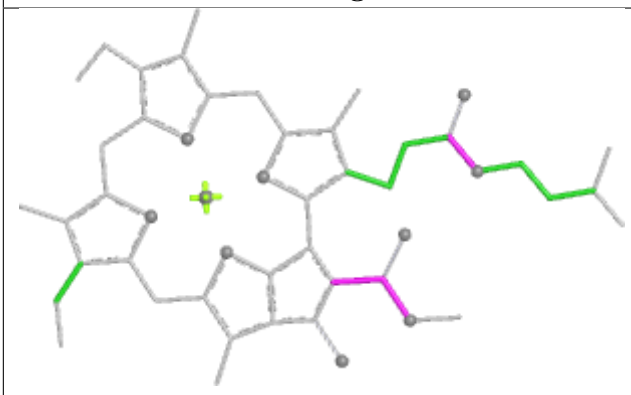
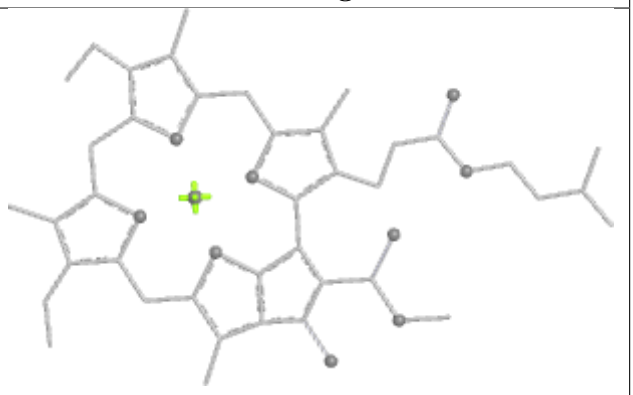


Bond angles

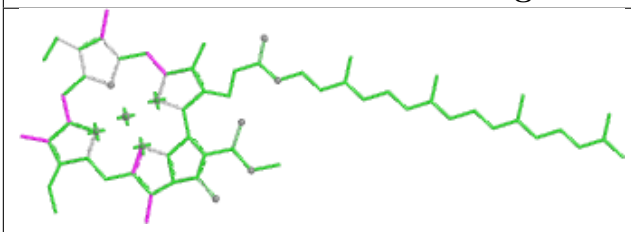


Torsions

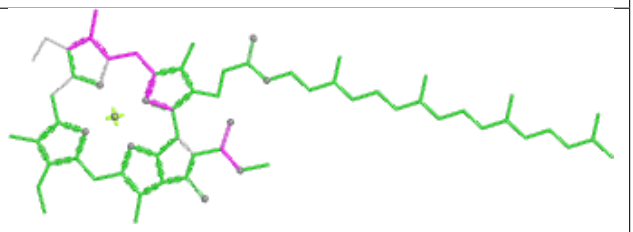


Rings

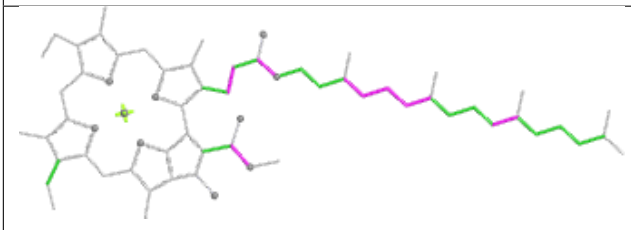
Ligand CLA A 5004



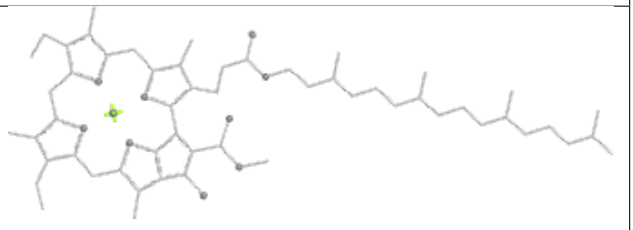
Bond lengths



Bond angles

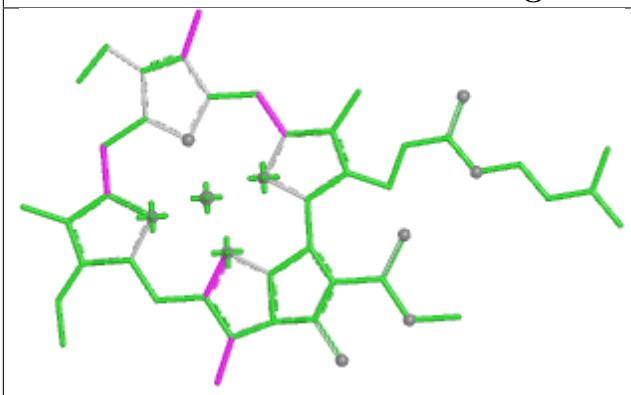


Torsions

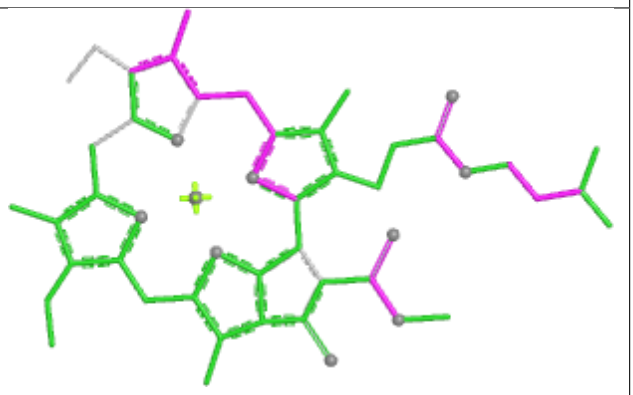


Rings

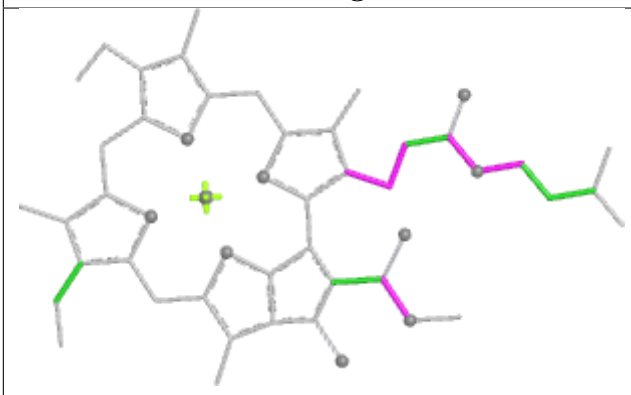
Ligand CLA T 406



Bond lengths



Bond angles



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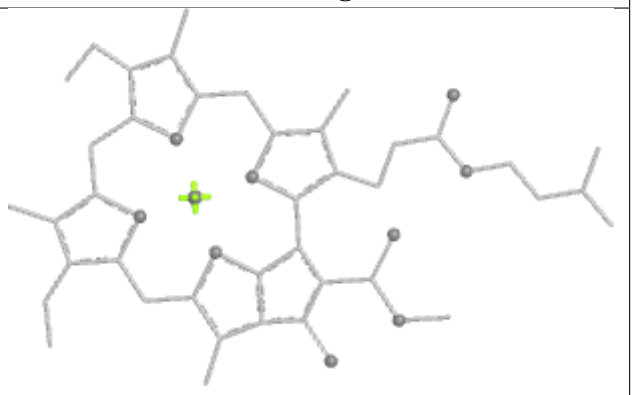
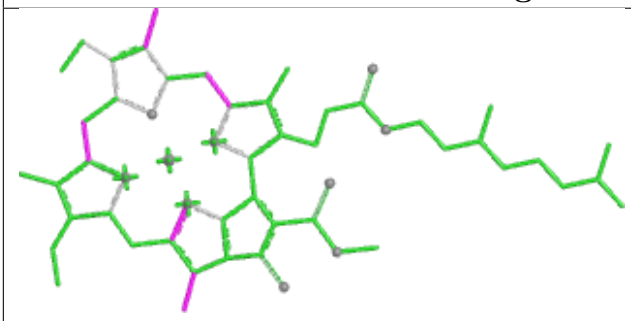
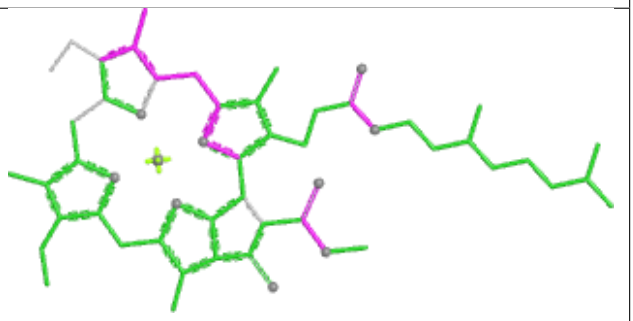


Rings

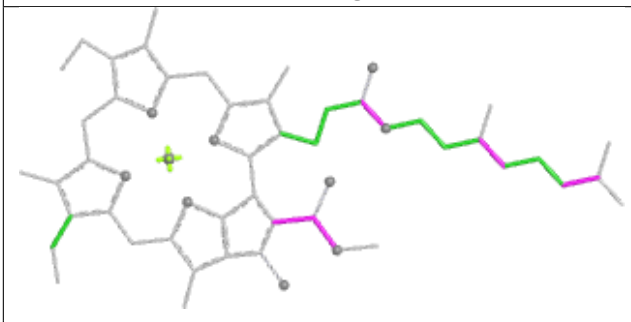
Ligand CLA A 5017



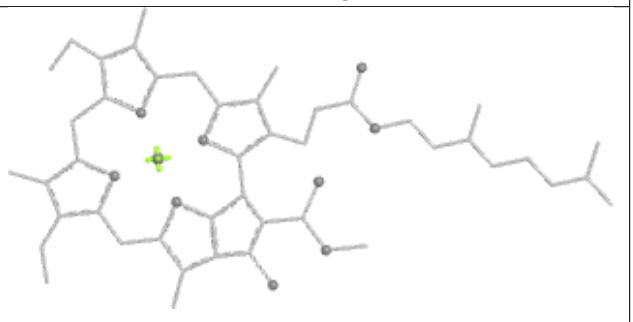
Bond lengths



Bond angles

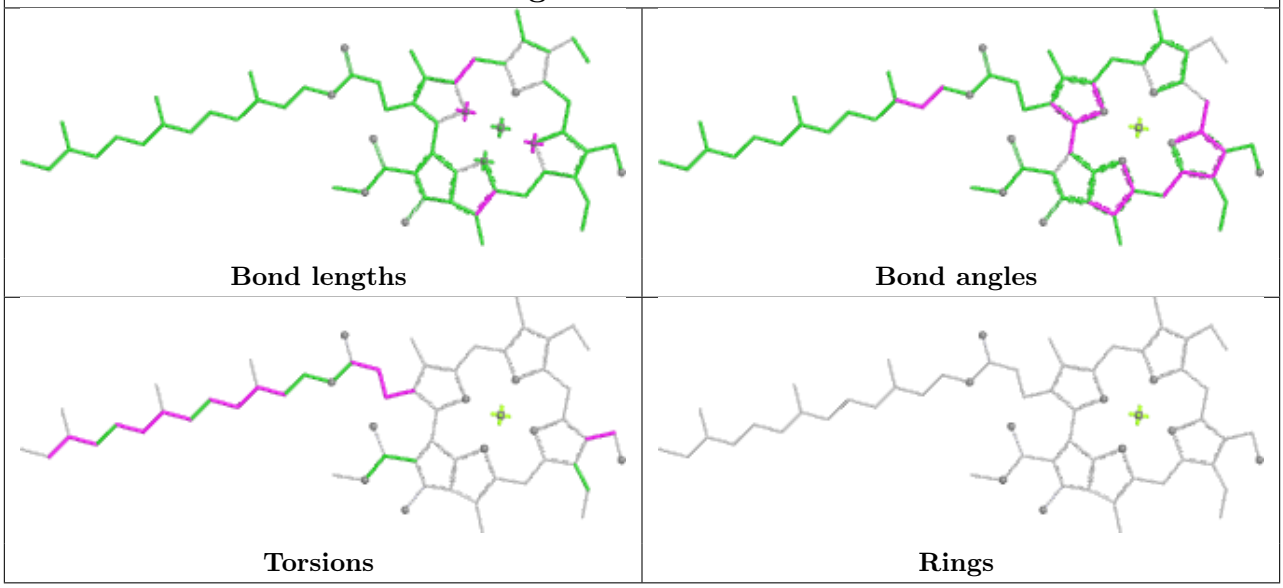


Torsions

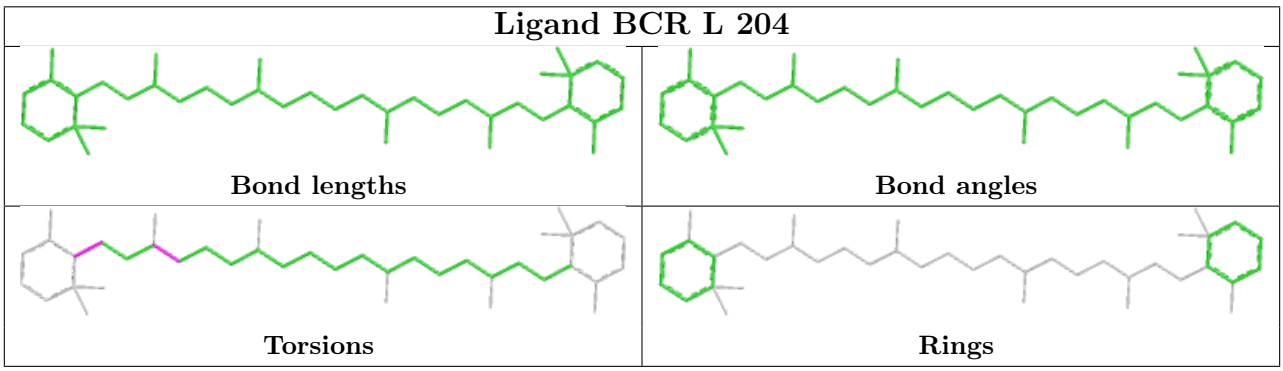


Rings

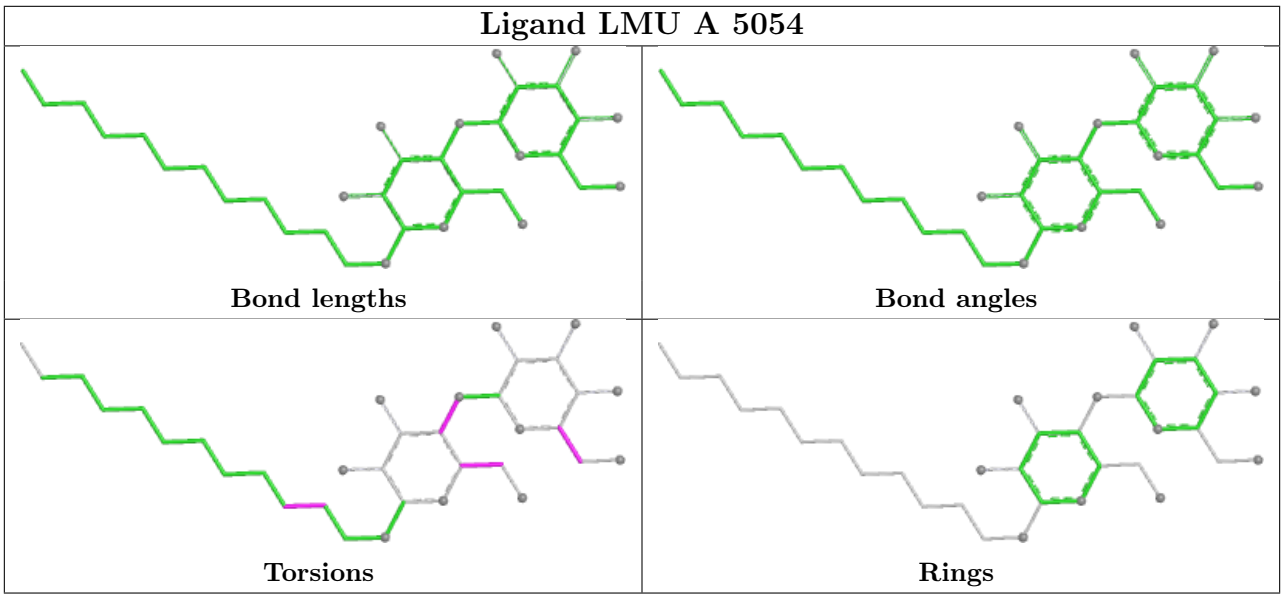
Ligand CHL 3 301



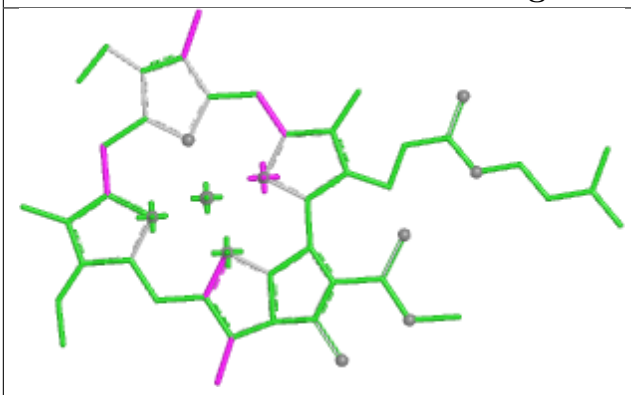
Ligand BCR L 204



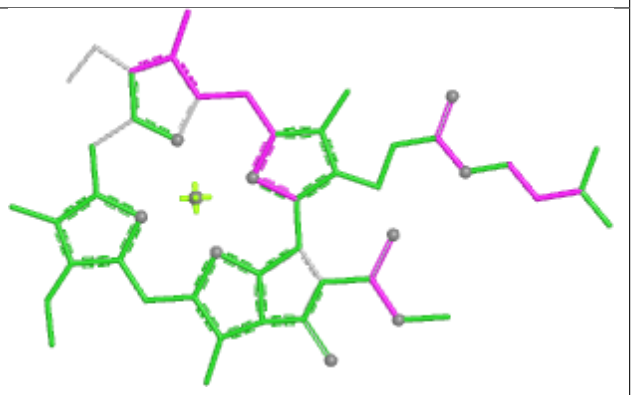
Ligand LMU A 5054



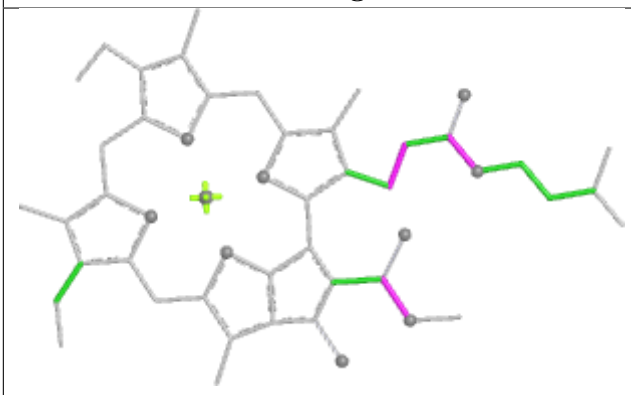
Ligand CLA 7 304



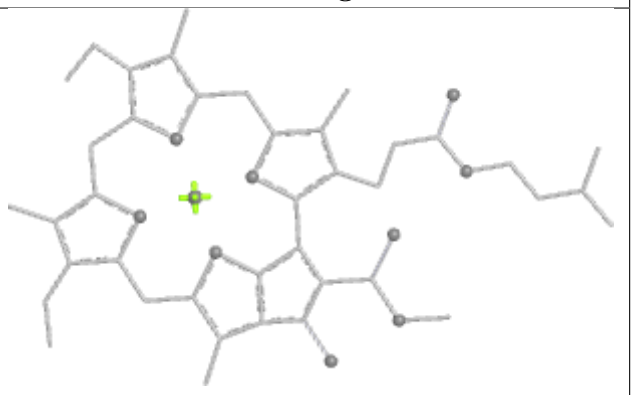
Bond lengths



Bond angles



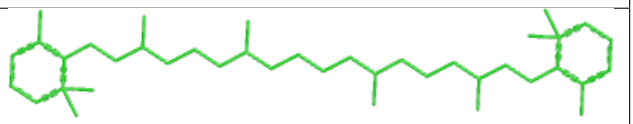
Torsions



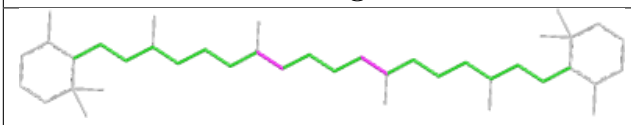
Rings

Ligand BCR 3 319

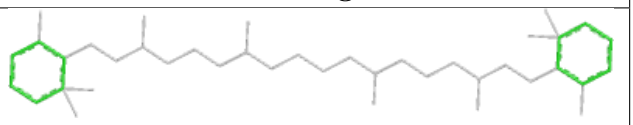
Bond lengths



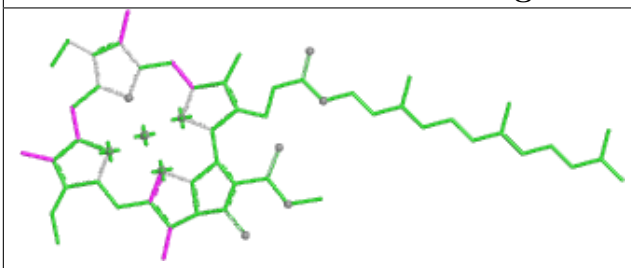
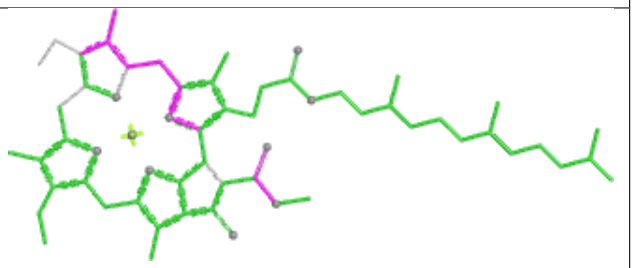
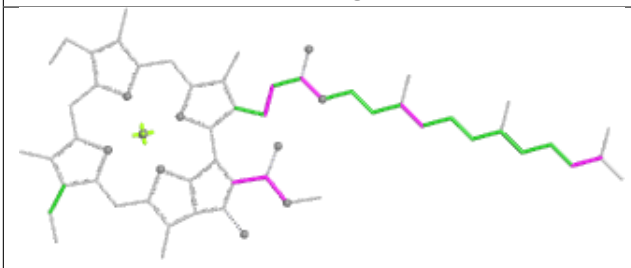
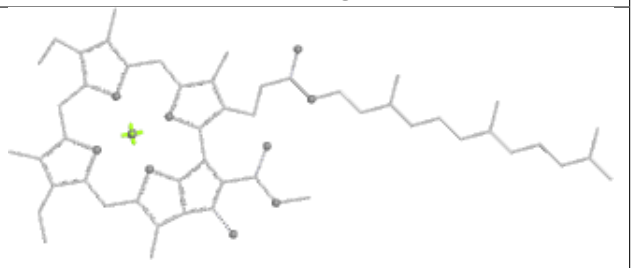
Bond angles

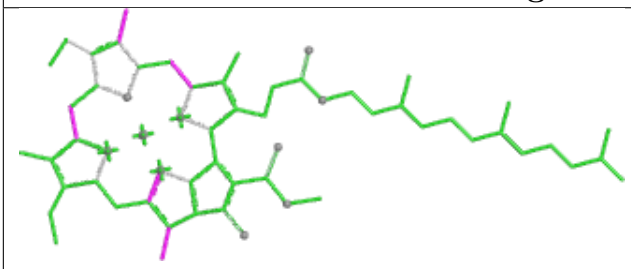
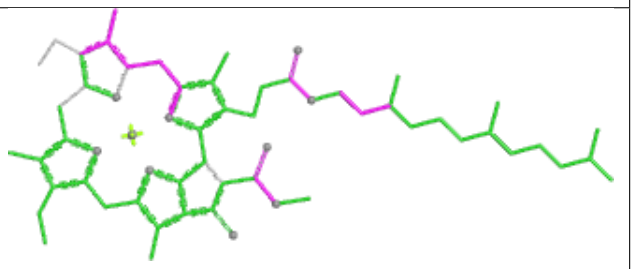
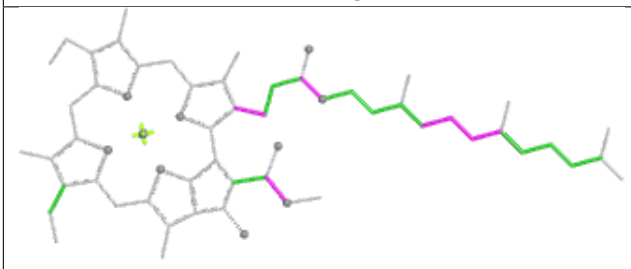
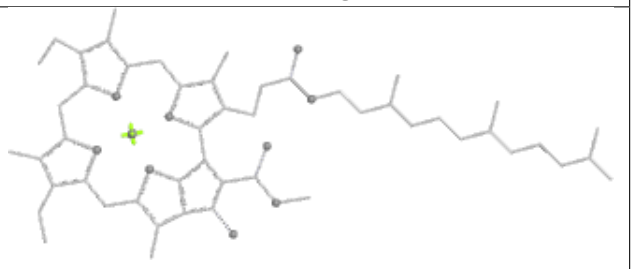


Torsions

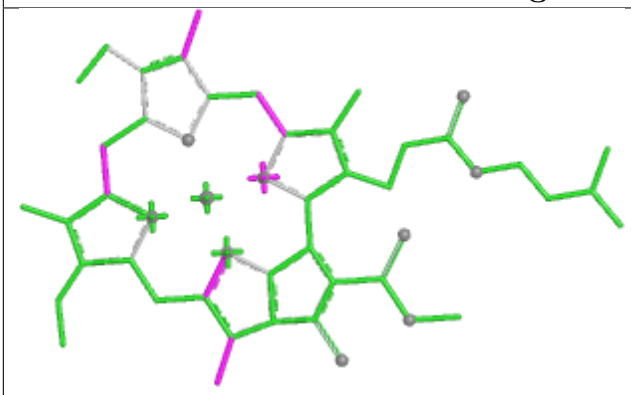


Rings

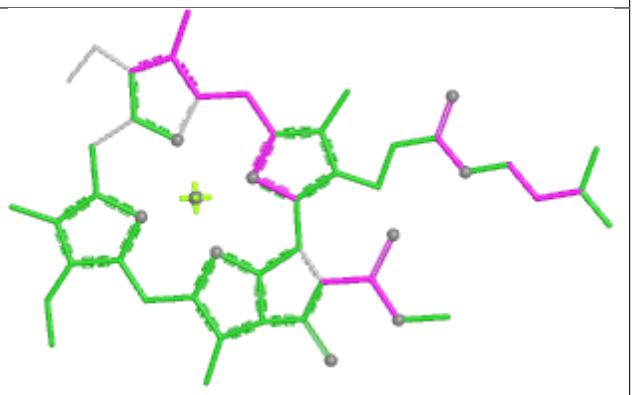
Ligand CLA A 5018	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

Ligand CLA b 602	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

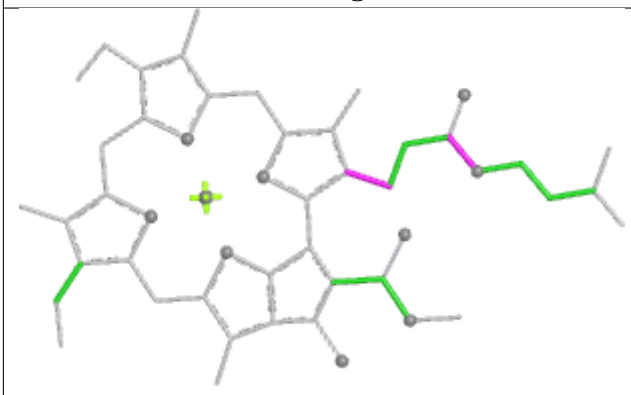
Ligand CLA c 307



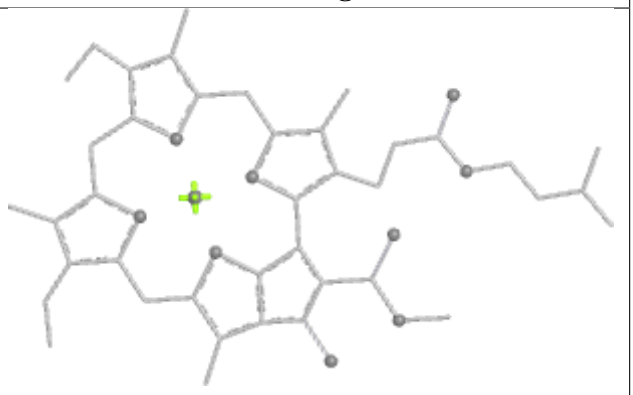
Bond lengths



Bond angles

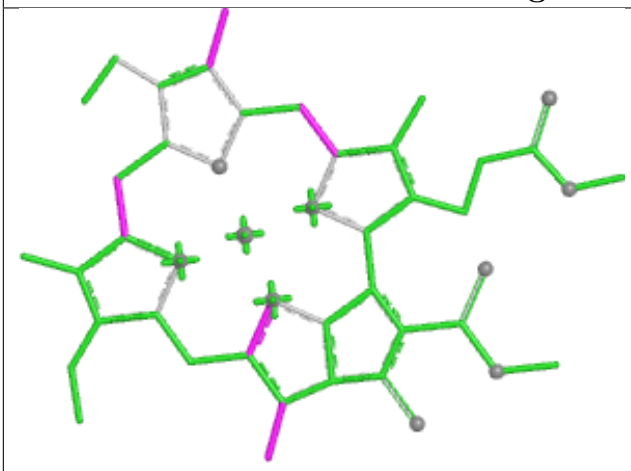


Torsions

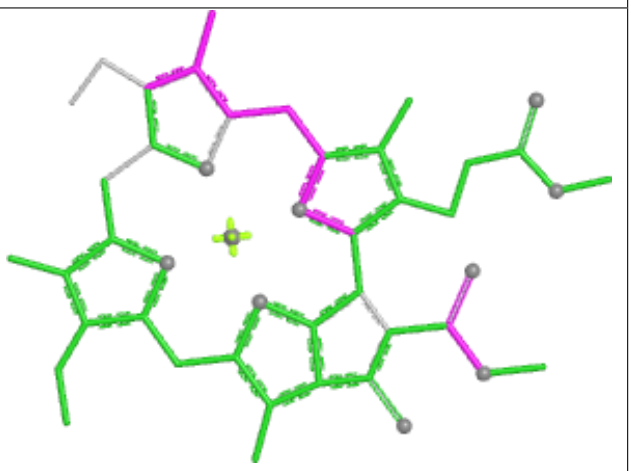


Rings

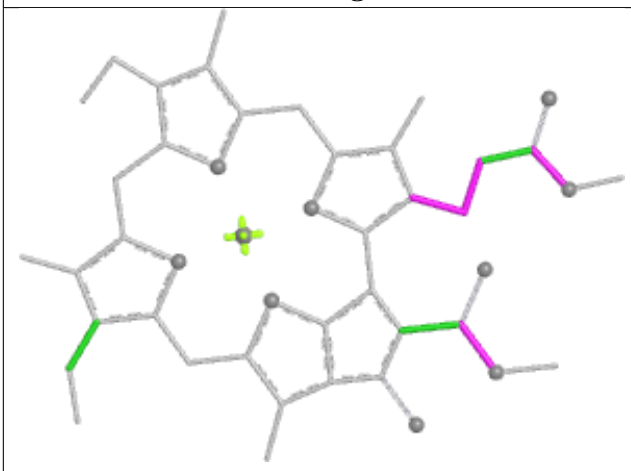
Ligand CLA 3 303



Bond lengths



Bond angles



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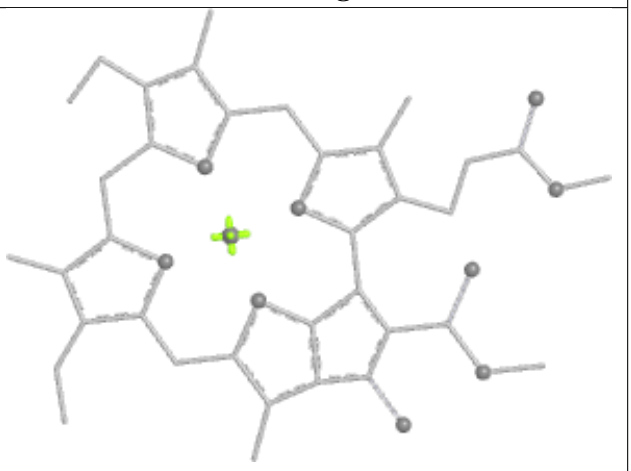
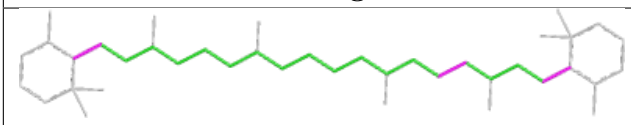


Rings

Ligand BCR B 843

Bond lengths

Bond angles



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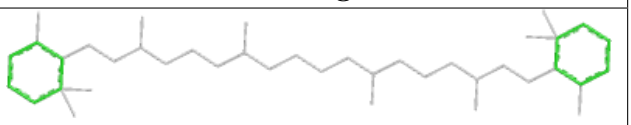
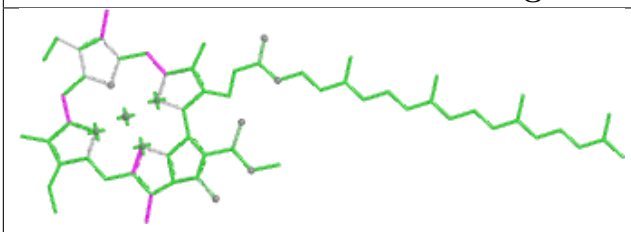
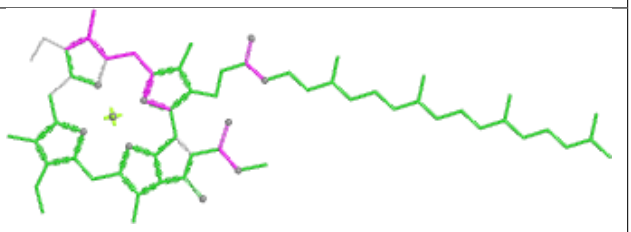


Rings

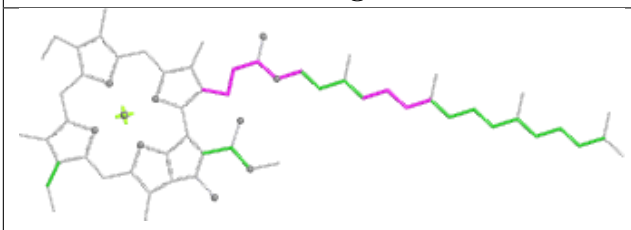
Ligand CLA B 841



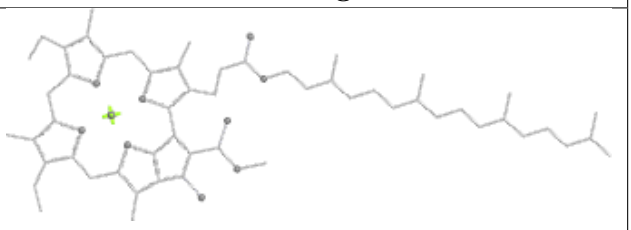
Bond lengths



Bond angles

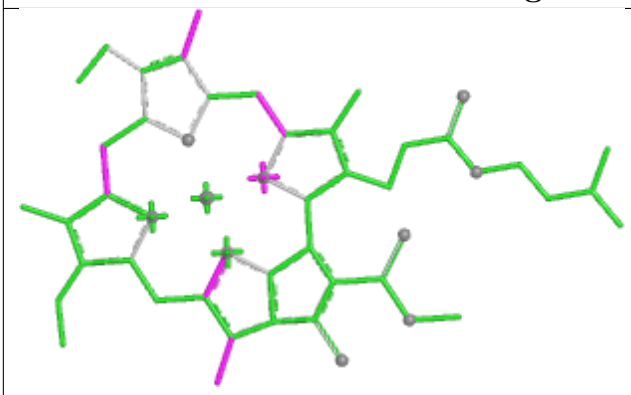


Torsions

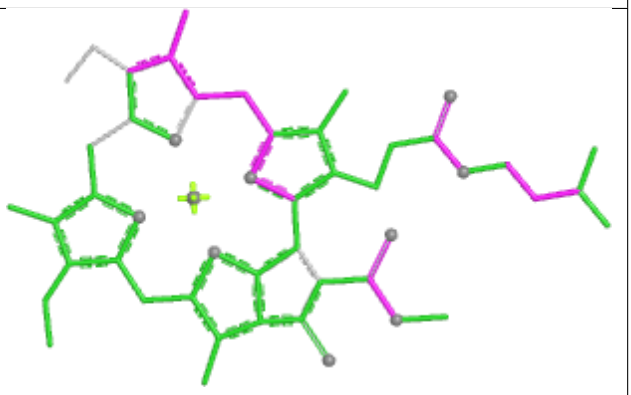


Rings

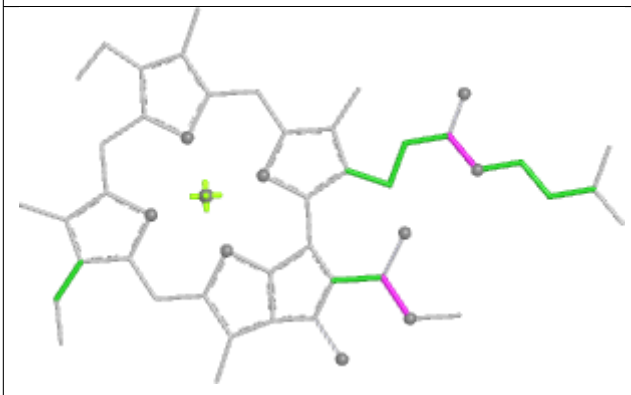
Ligand CLA T 402



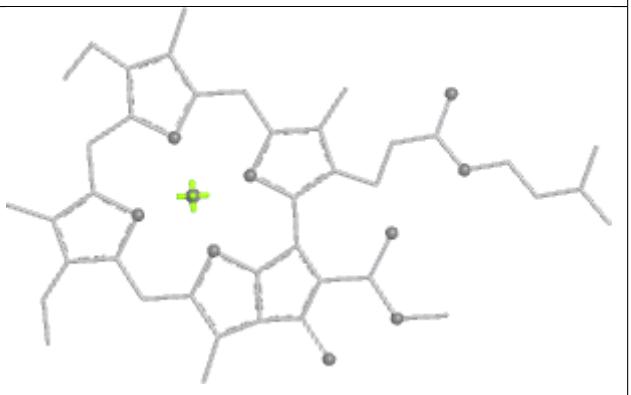
Bond lengths



Bond angles

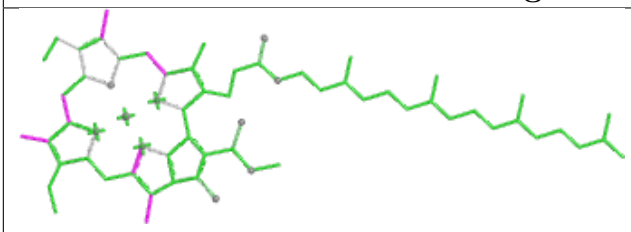


Torsions

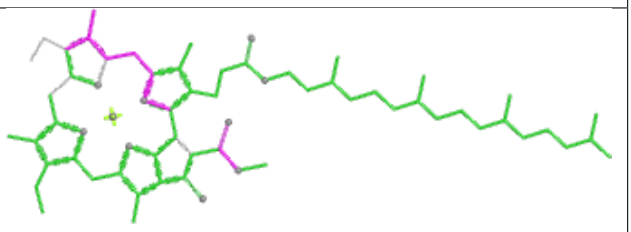


Rings

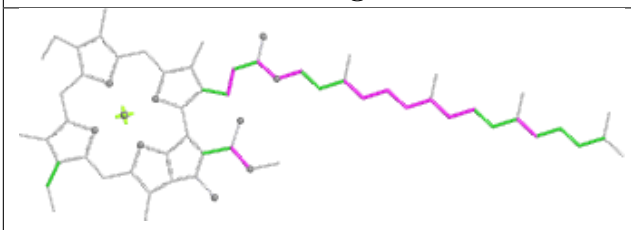
Ligand CLA B 803



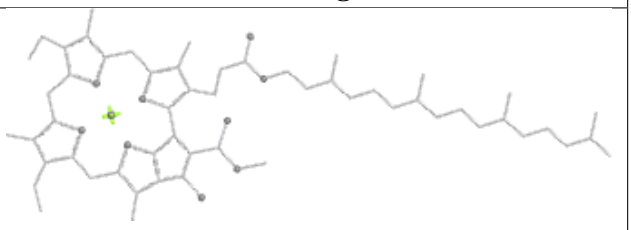
Bond lengths



Bond angles

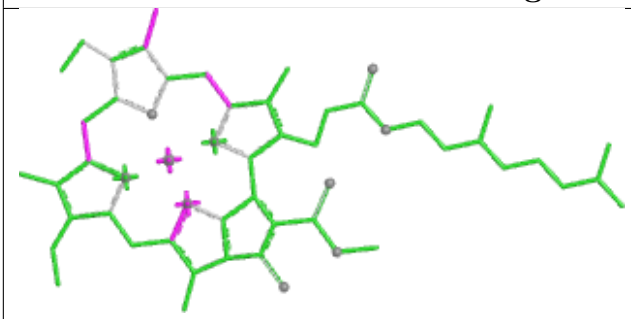


Torsions

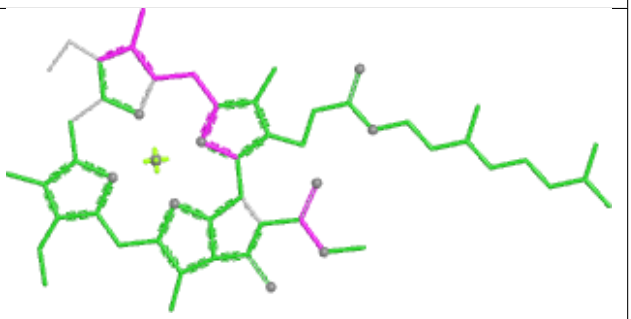


Rings

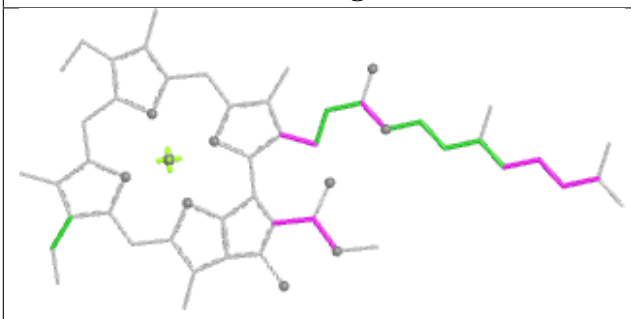
Ligand CLA B 810



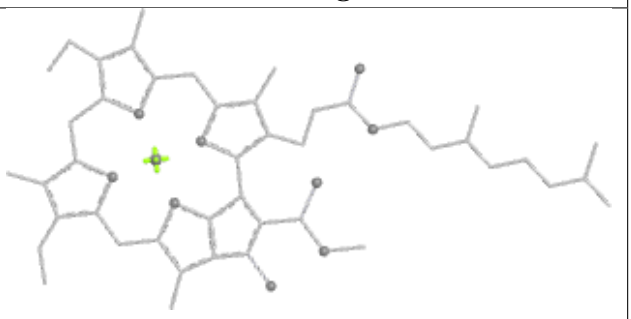
Bond lengths



Bond angles

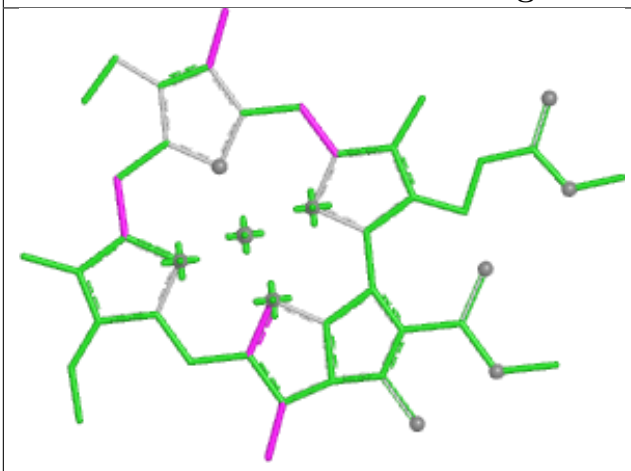


Torsions

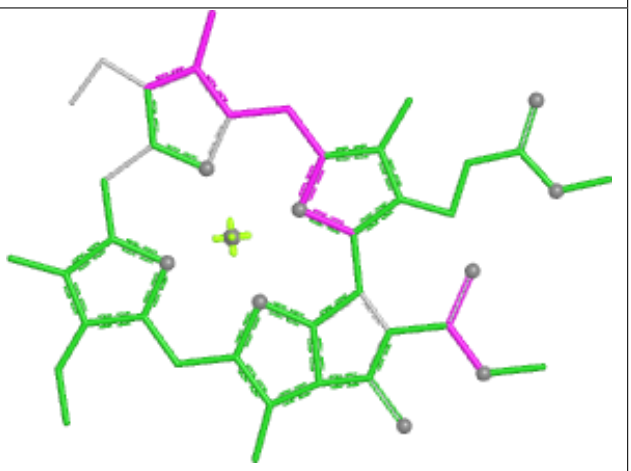


Rings

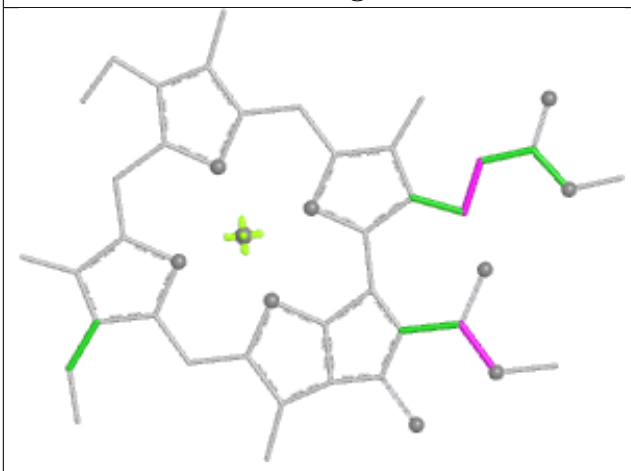
Ligand CLA F 5009



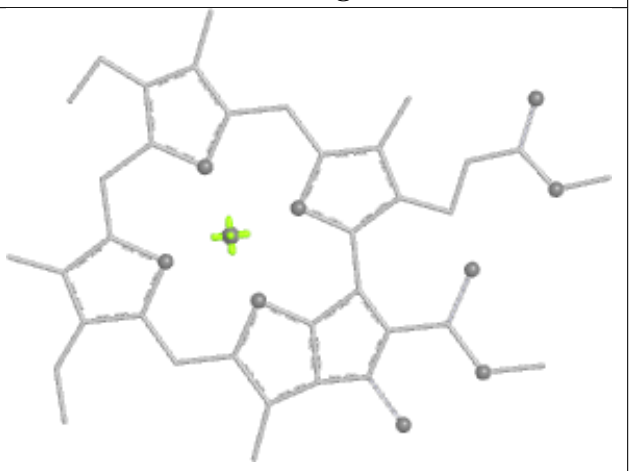
Bond lengths



Bond angles

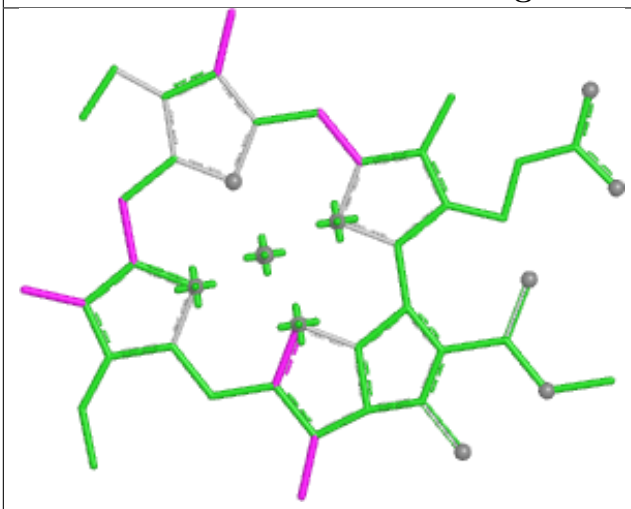


Torsions

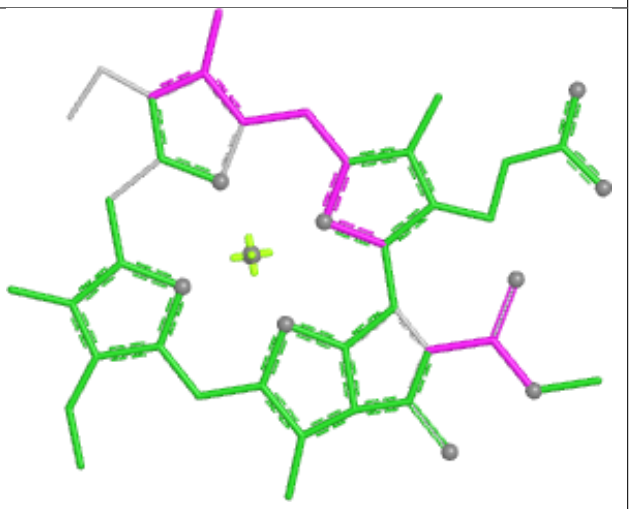


Rings

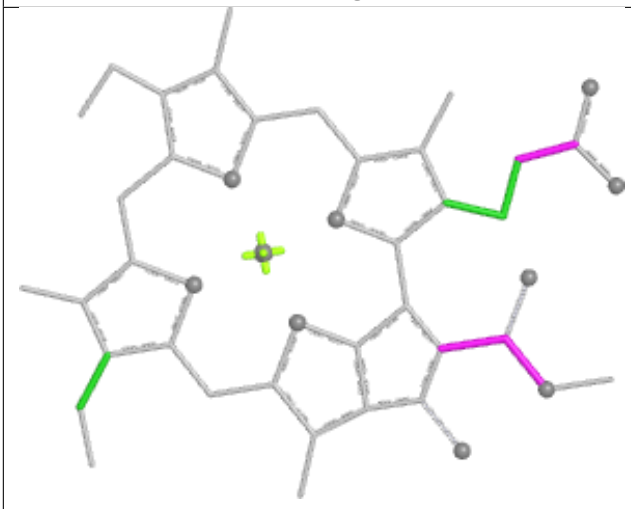
Ligand CLA A 5043



Bond lengths



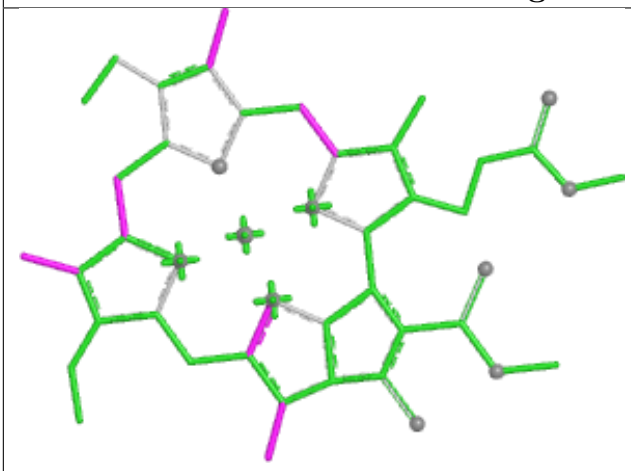
Bond angles



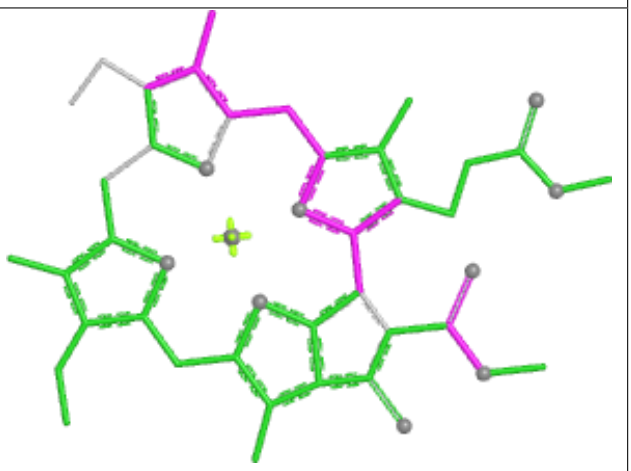
Torsions

Rings

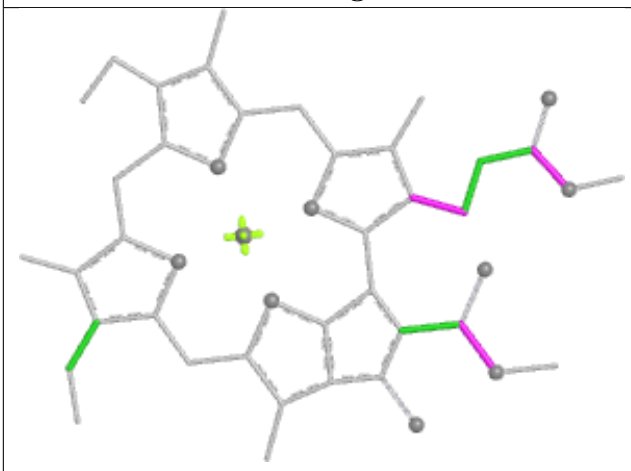
Ligand CLA a 611



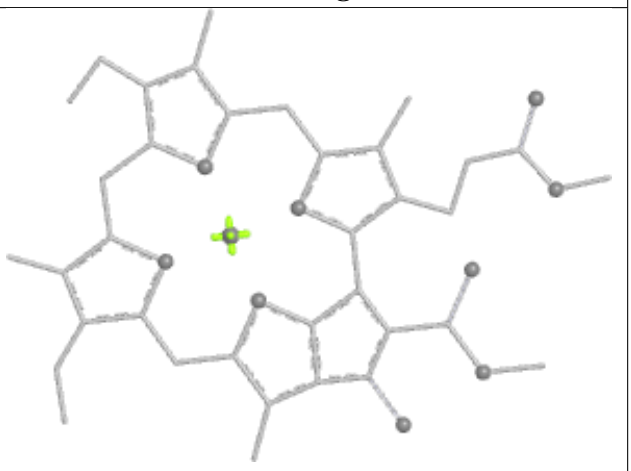
Bond lengths



Bond angles

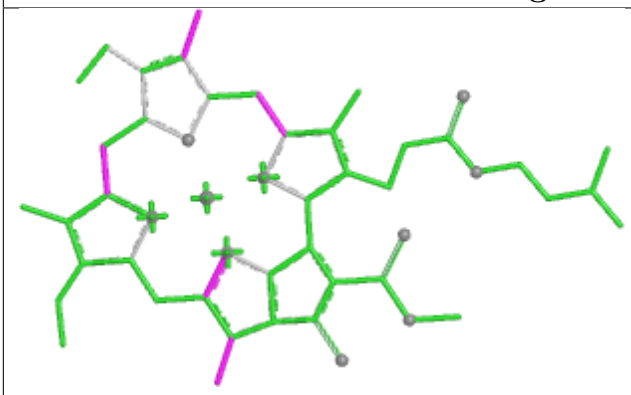


Torsions

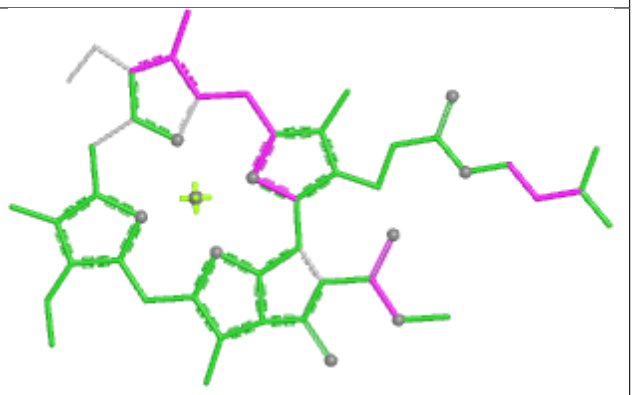


Rings

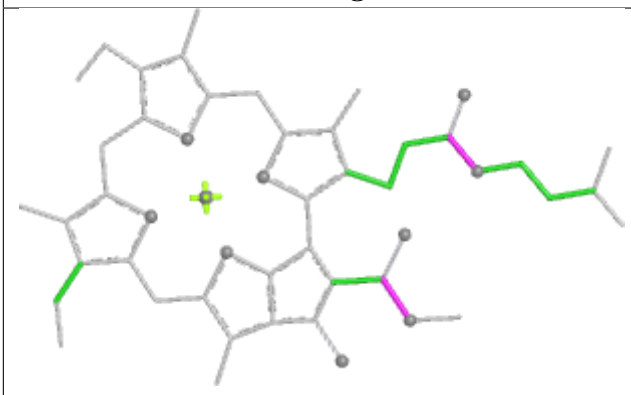
Ligand CLA c 303



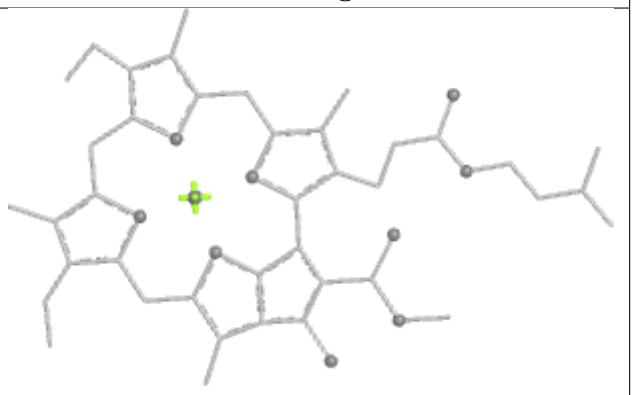
Bond lengths



Bond angles

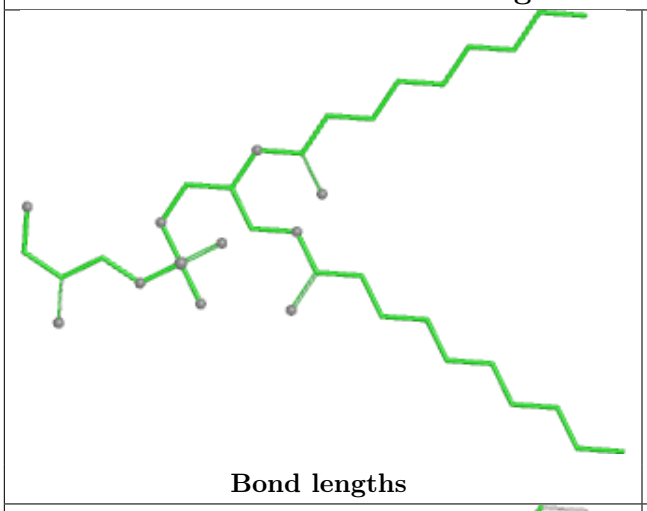


Torsions

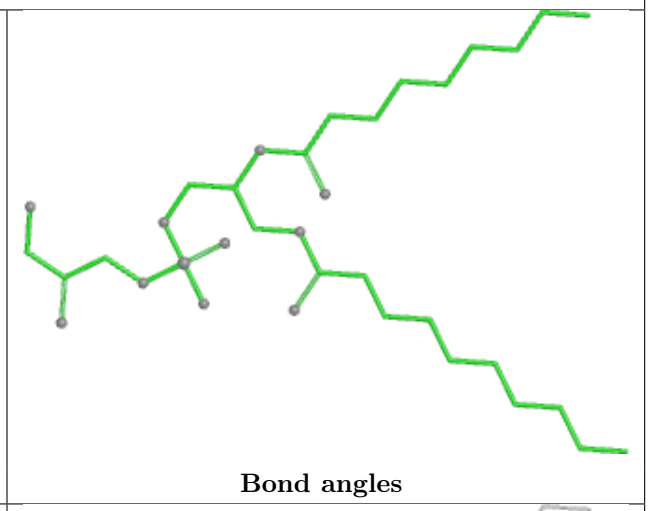


Rings

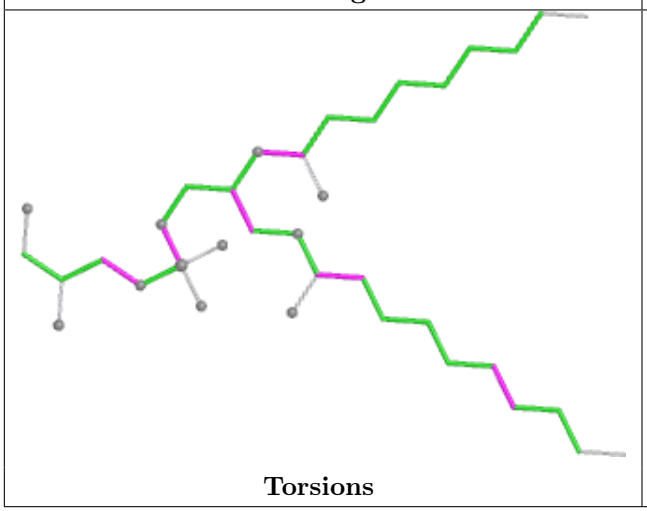
Ligand LHG A 5002



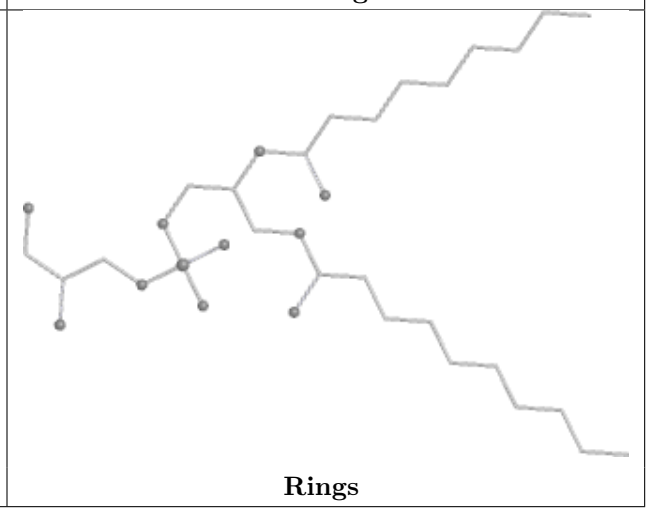
Bond lengths



Bond angles

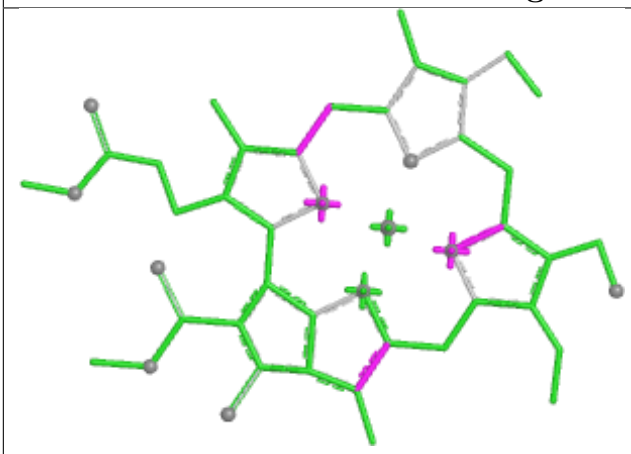


Torsions

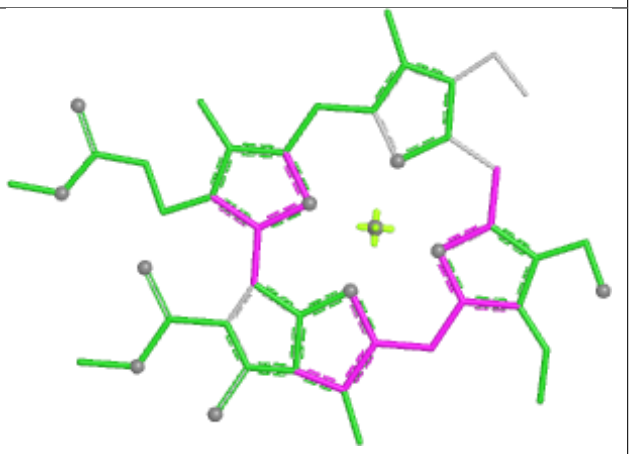


Rings

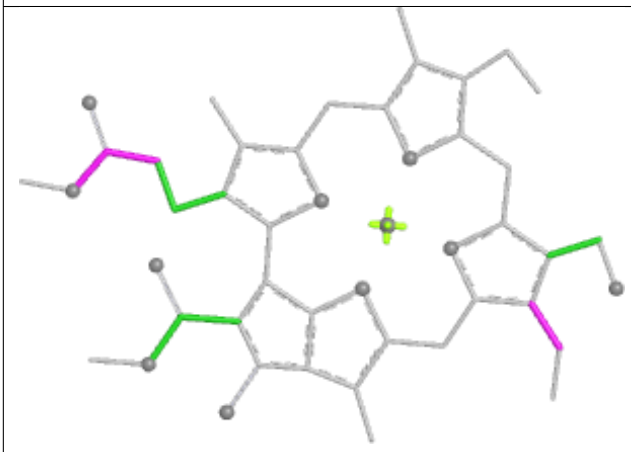
Ligand CHL b 606



Bond lengths



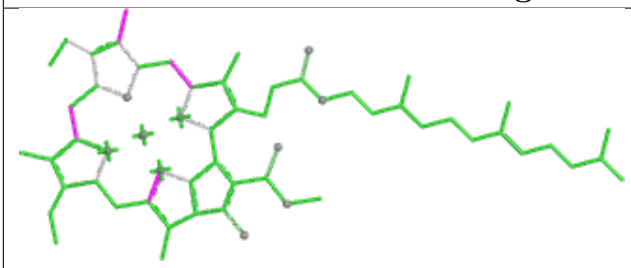
Bond angles



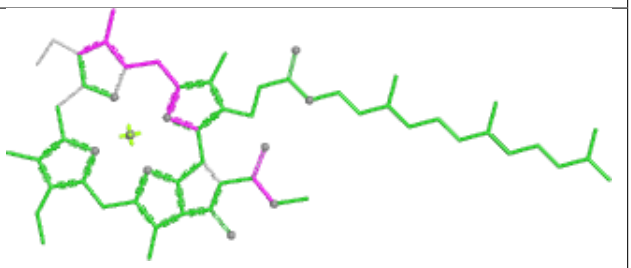
Torsions

Rings

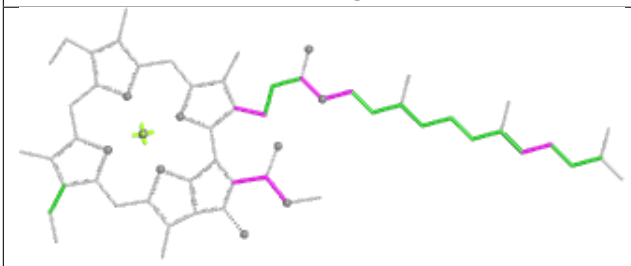
Ligand CLA A 5007



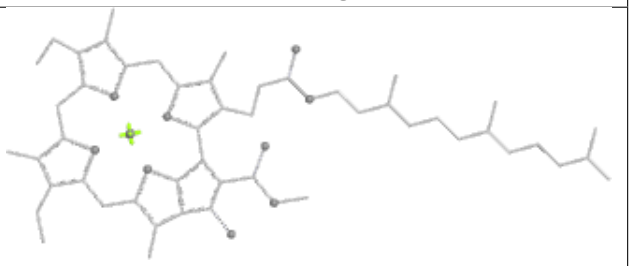
Bond lengths



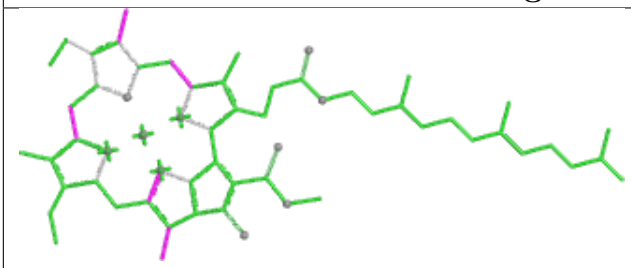
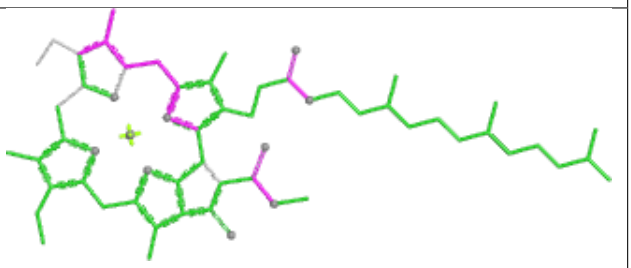
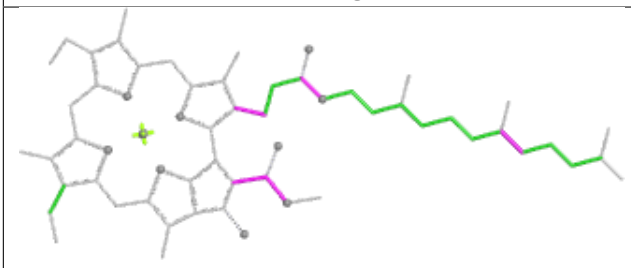
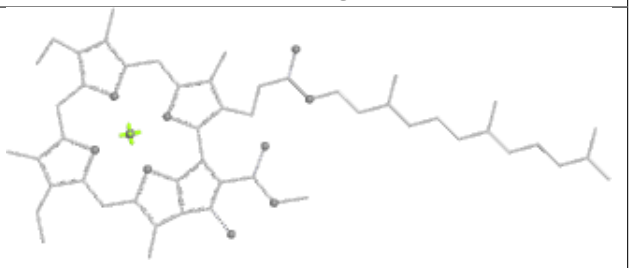
Bond angles

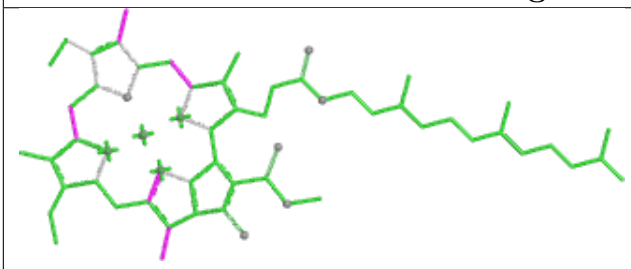
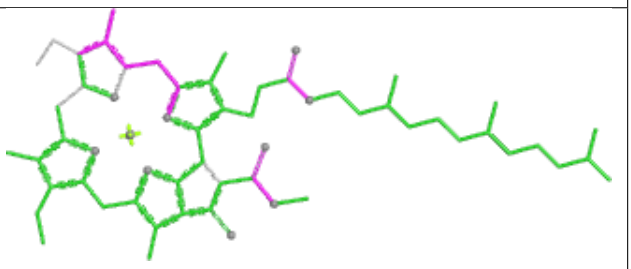
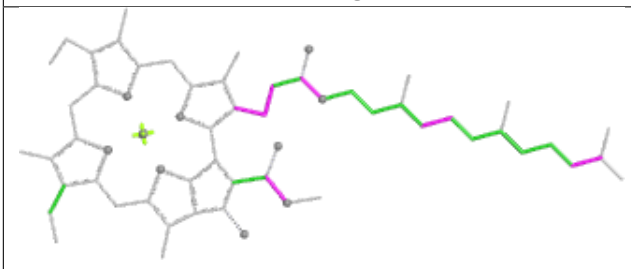
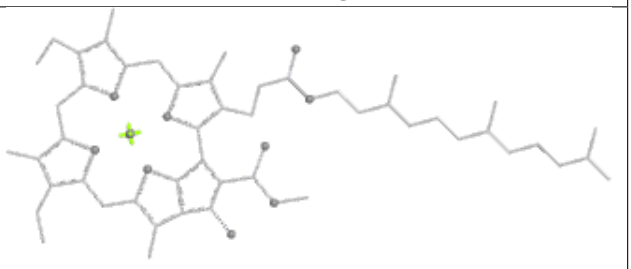


Torsions

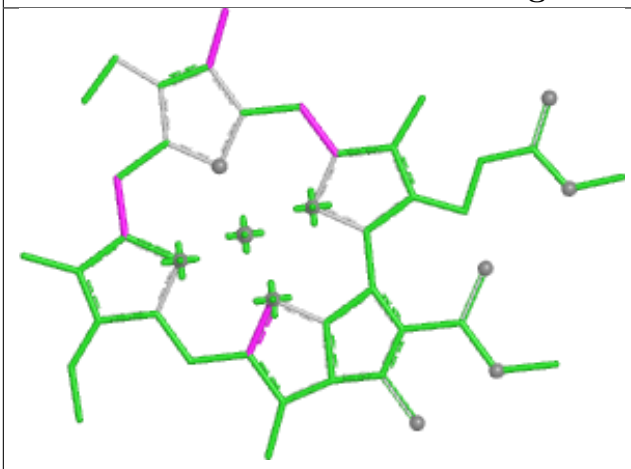


Rings

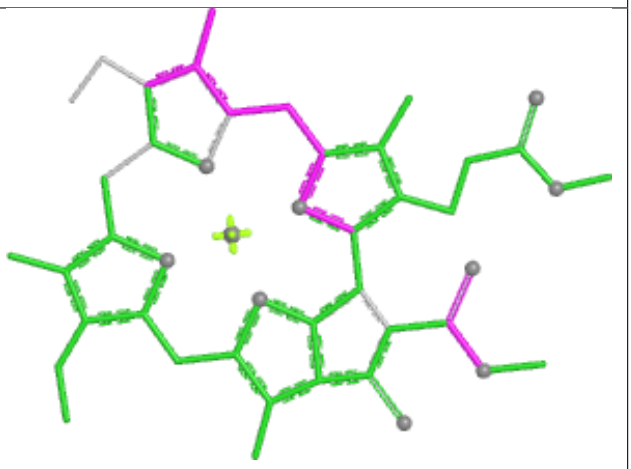
Ligand CLA B 833	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

Ligand CLA 8 310	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

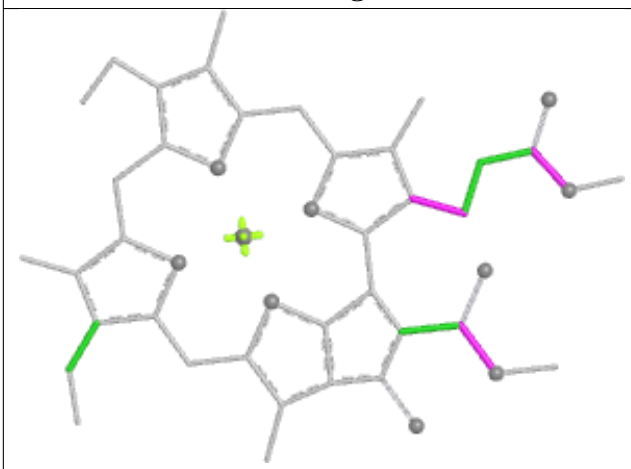
Ligand CLA 7 310



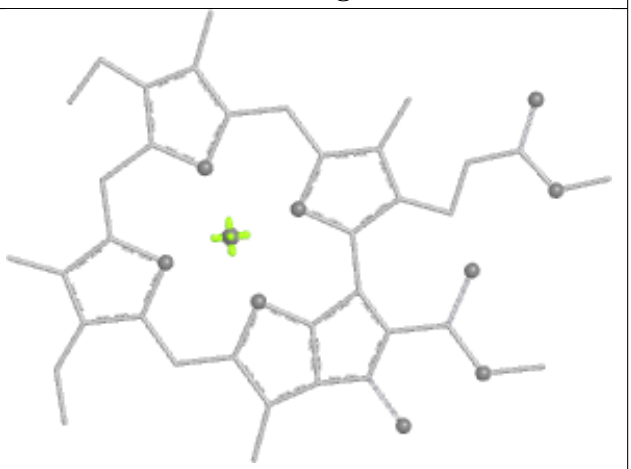
Bond lengths



Bond angles

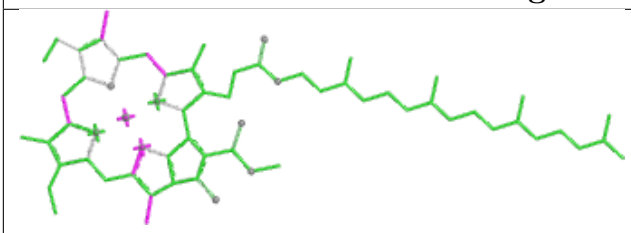


Torsions

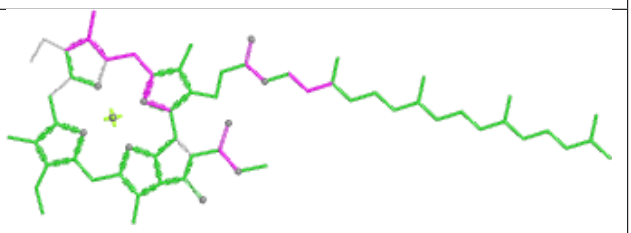


Rings

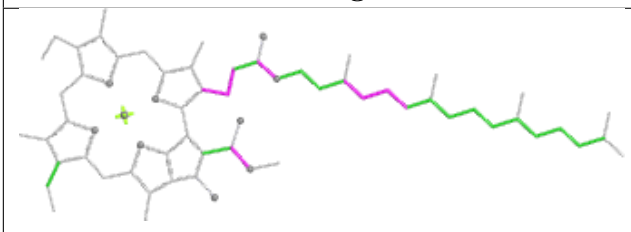
Ligand CLA 7 312



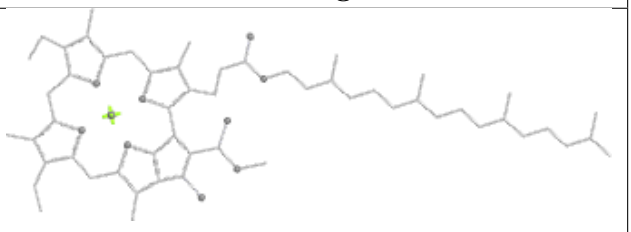
Bond lengths



Bond angles

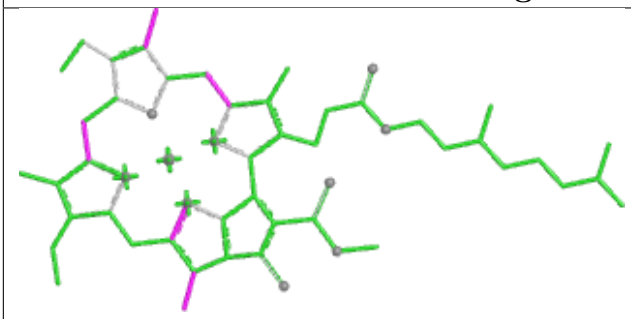


Torsions

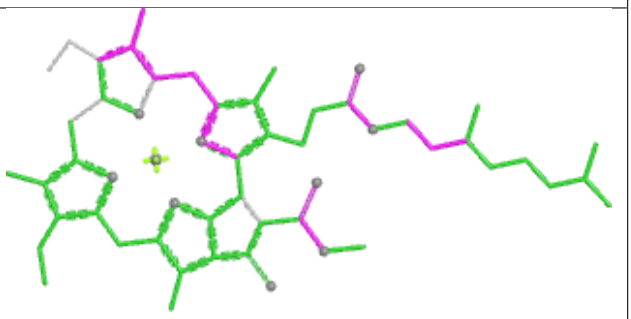


Rings

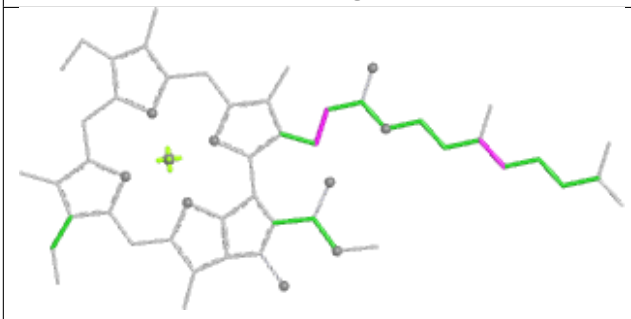
Ligand CLA A 5039



Bond lengths



Bond angles



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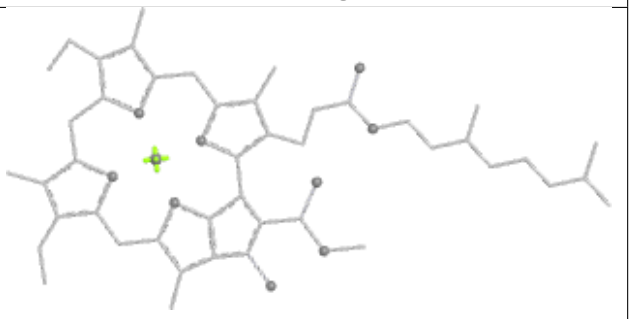
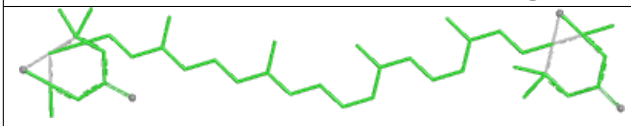
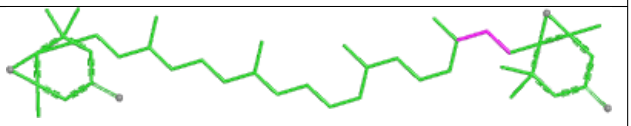


Rings

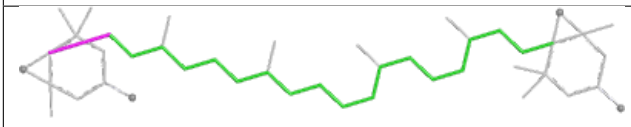
Ligand XAT T 414



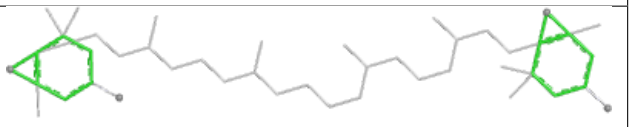
Bond lengths



Bond angles

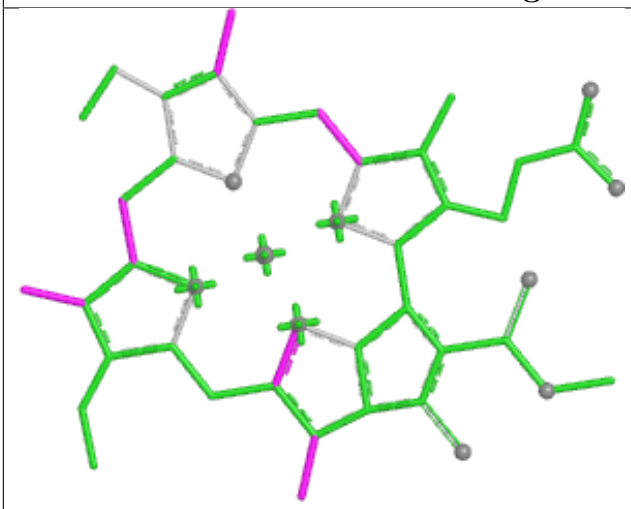


Torsions

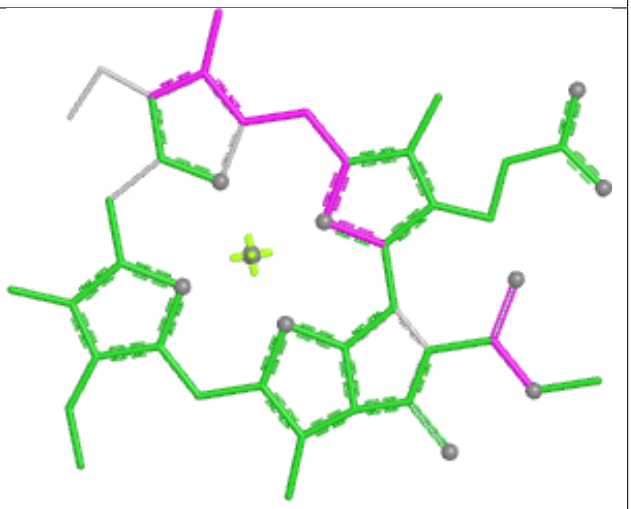


Rings

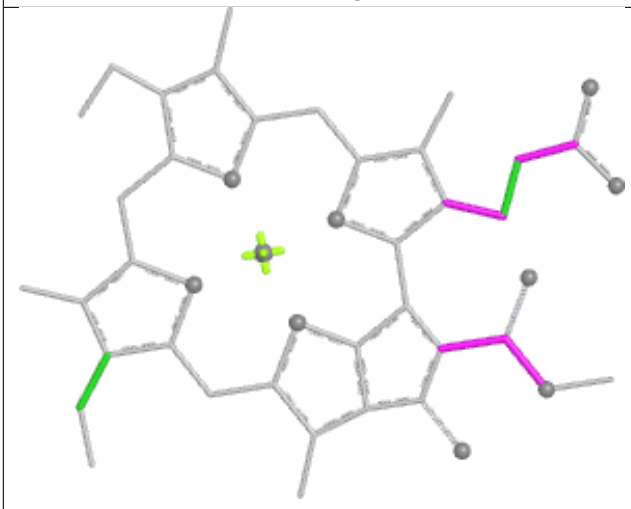
Ligand CLA K 203



Bond lengths



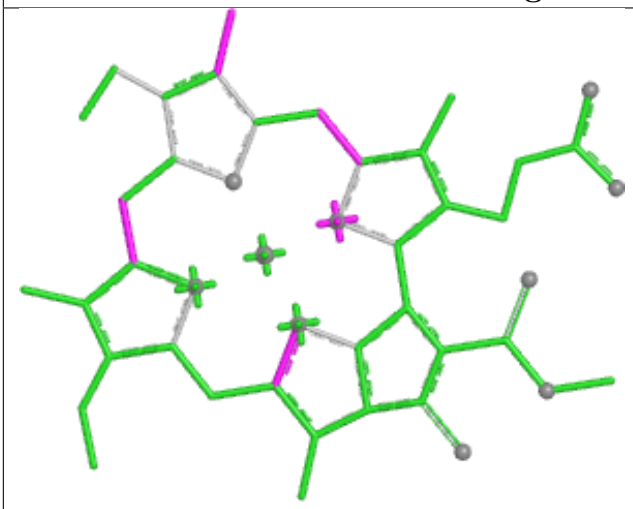
Bond angles



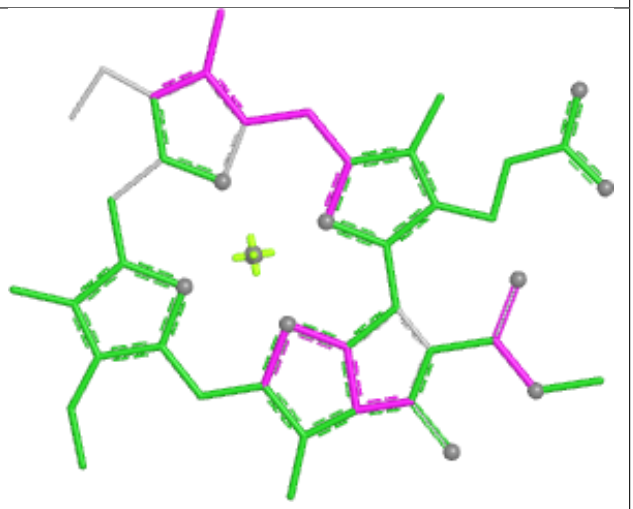
Torsions

Rings

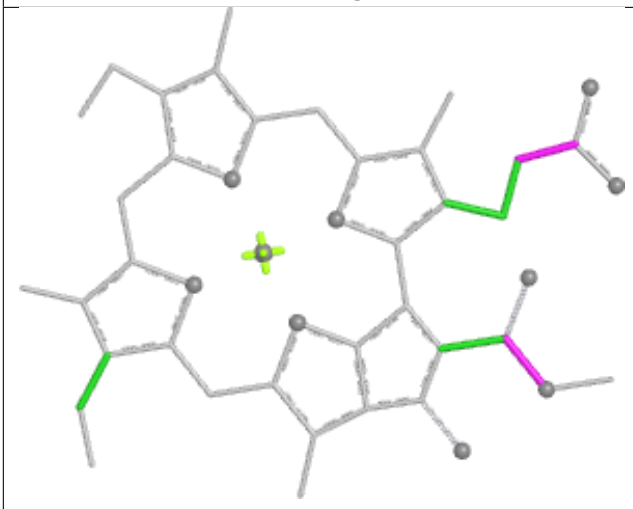
Ligand CLA T 405



Bond lengths



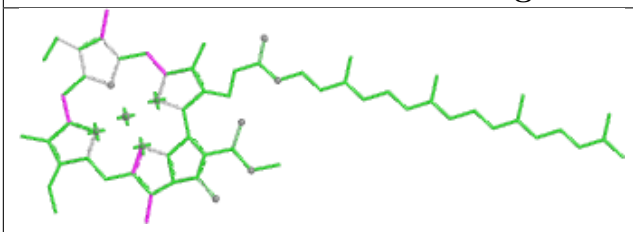
Bond angles



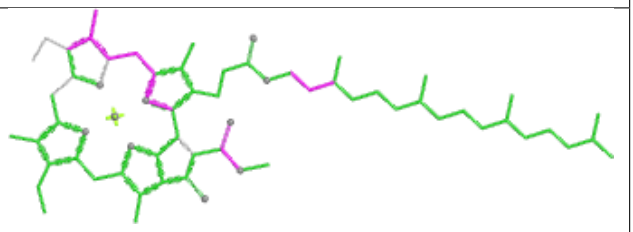
Torsions

Rings

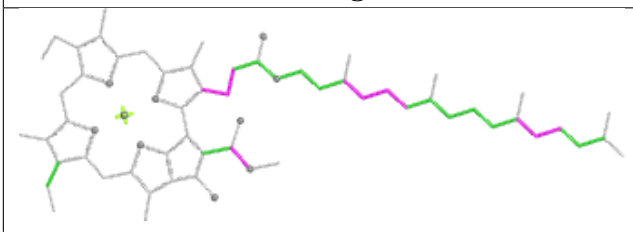
Ligand CLA A 5044



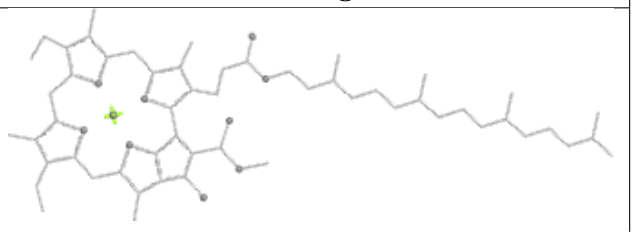
Bond lengths



Bond angles

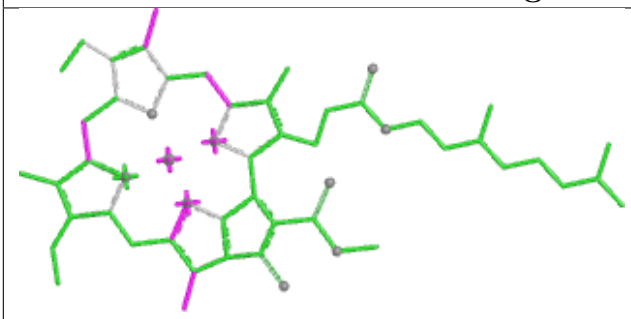


Torsions

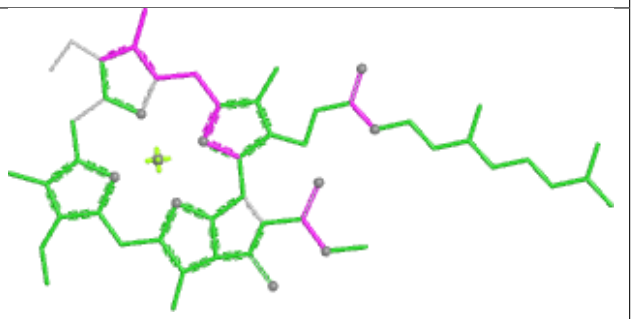


Rings

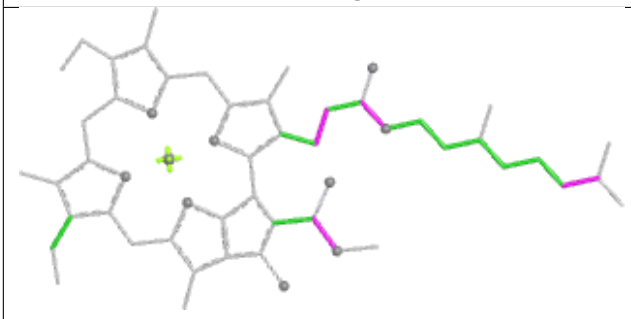
Ligand CLA B 838



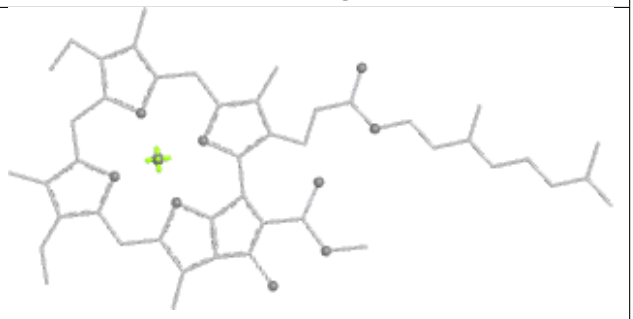
Bond lengths



Bond angles

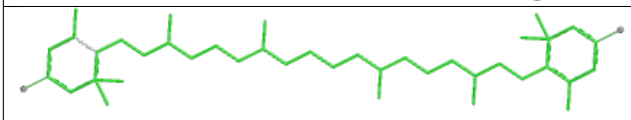


Torsions

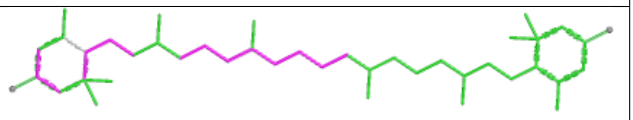


Rings

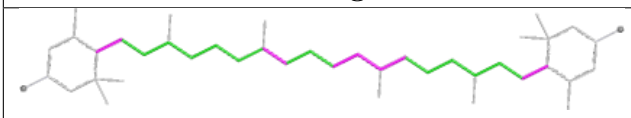
Ligand LUT 1 615



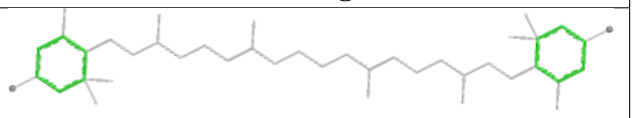
Bond lengths



Bond angles

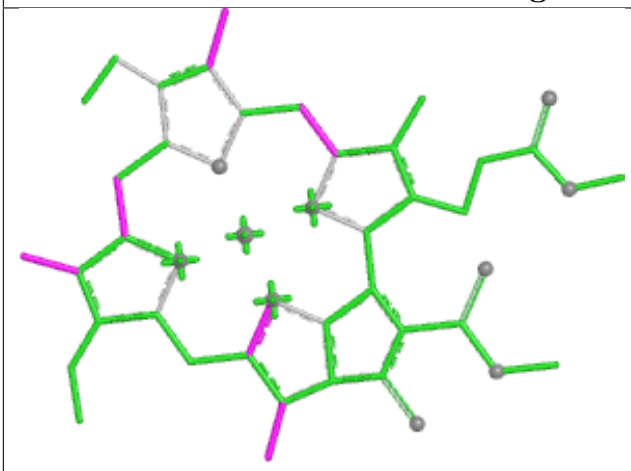


Torsions

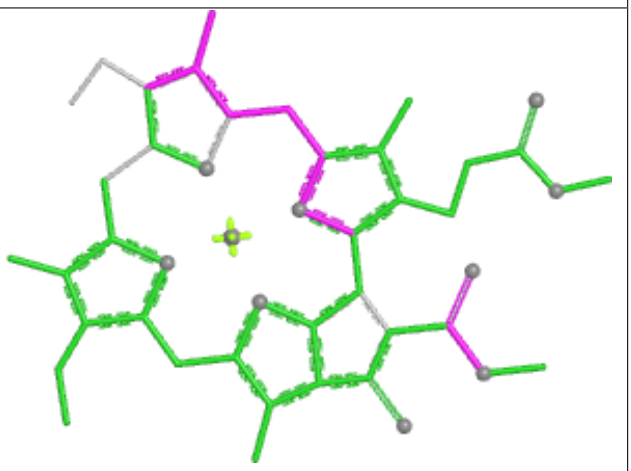


Rings

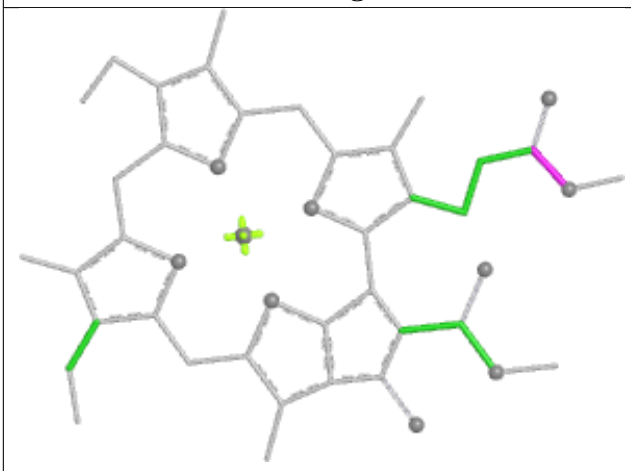
Ligand CLA c 302



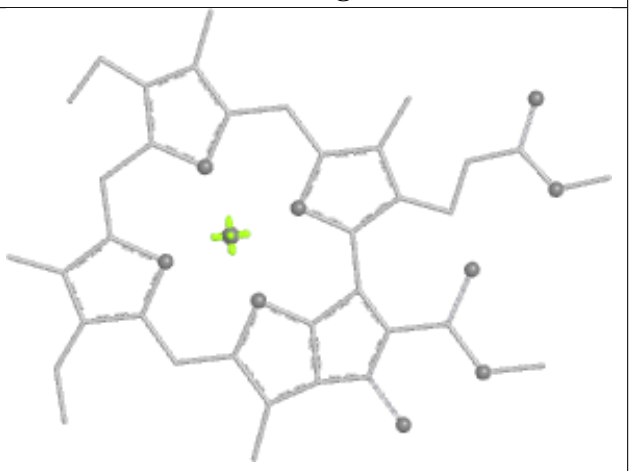
Bond lengths



Bond angles

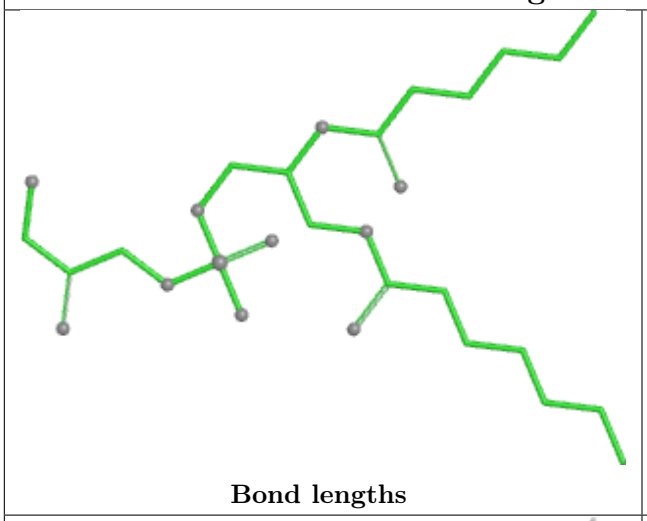


Torsions

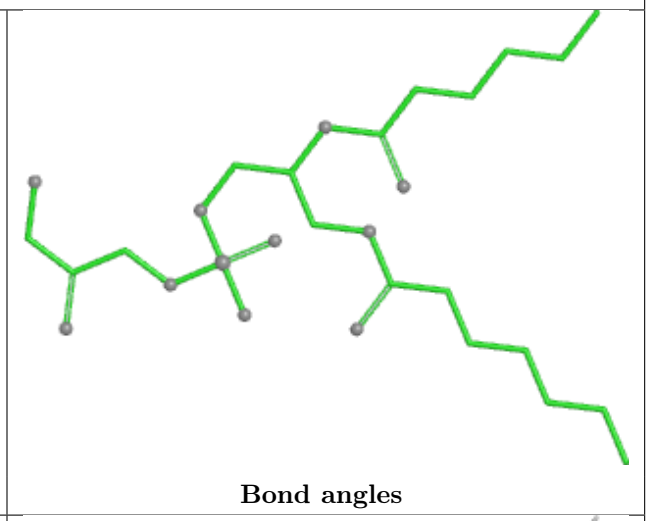


Rings

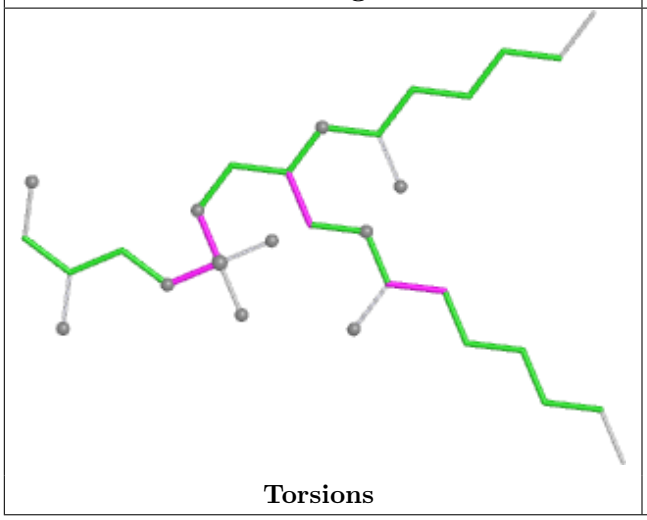
Ligand LHG 8 321



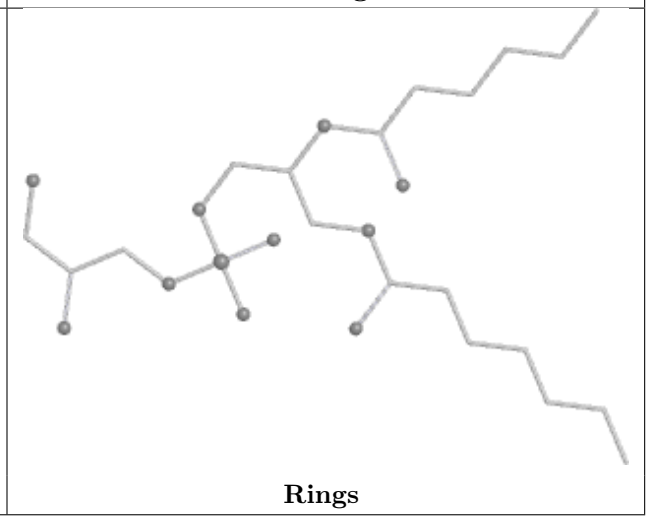
Bond lengths



Bond angles

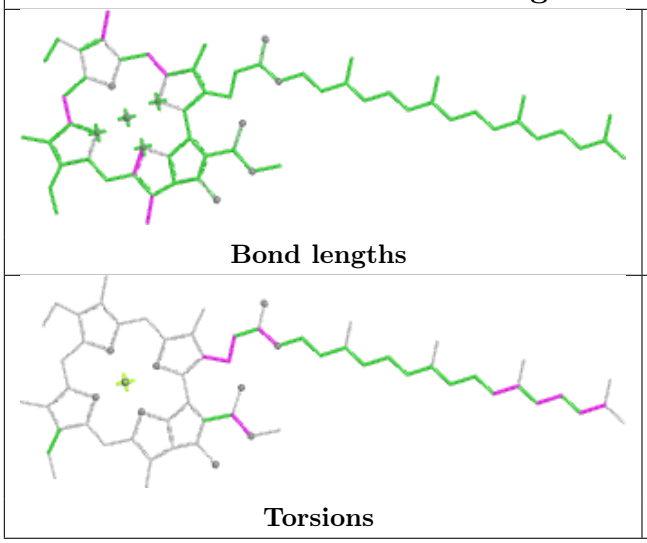


Torsions



Rings

Ligand CLA c 301



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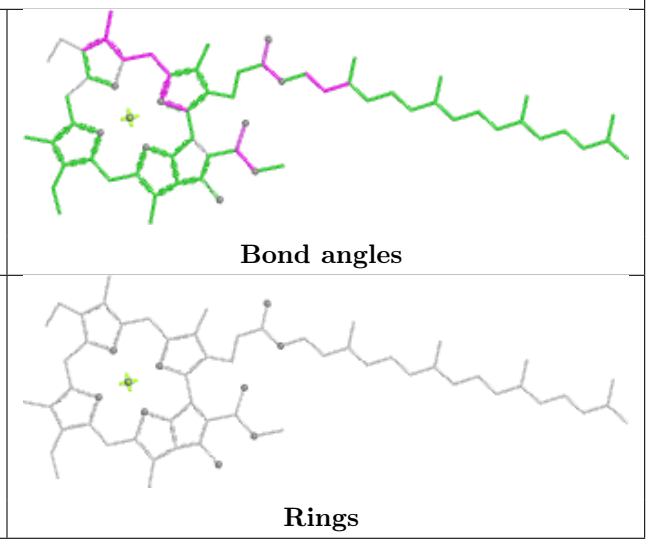
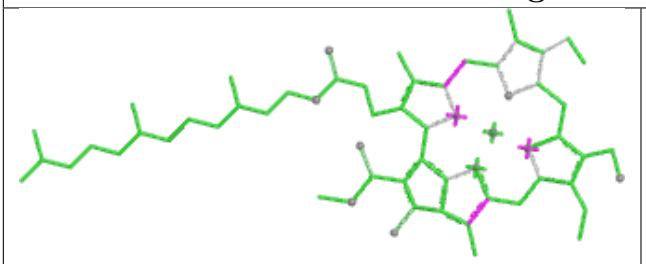


Bond angles

Torsions

Rings

Ligand CHL 3 322



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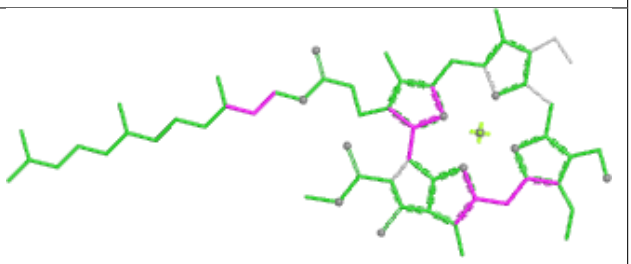
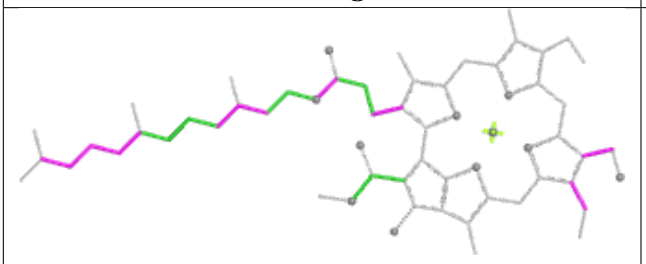
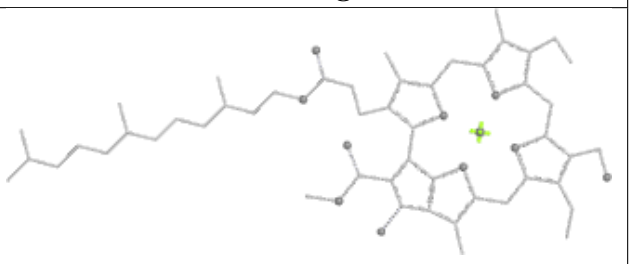


Bond angles

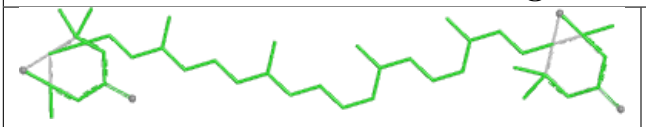


Torsions



Rings

Ligand XAT b 616



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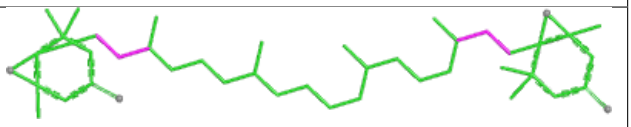
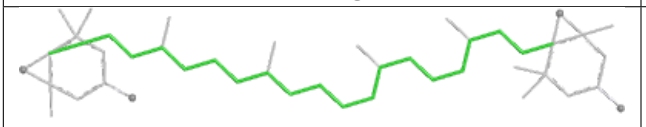
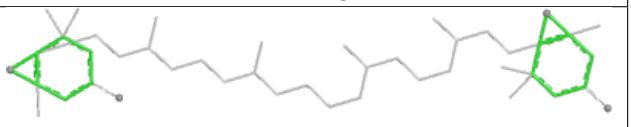


Bond angles

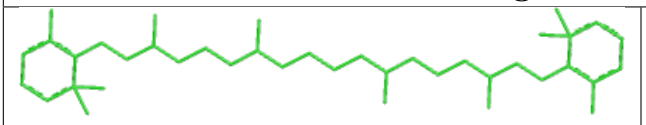


Torsions



Rings

Ligand BCR A 5047



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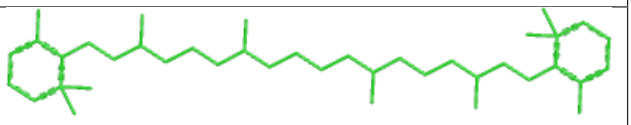
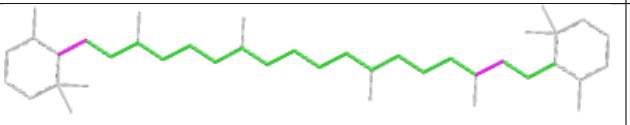
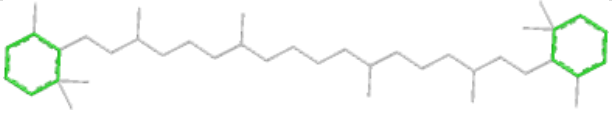


Bond angles

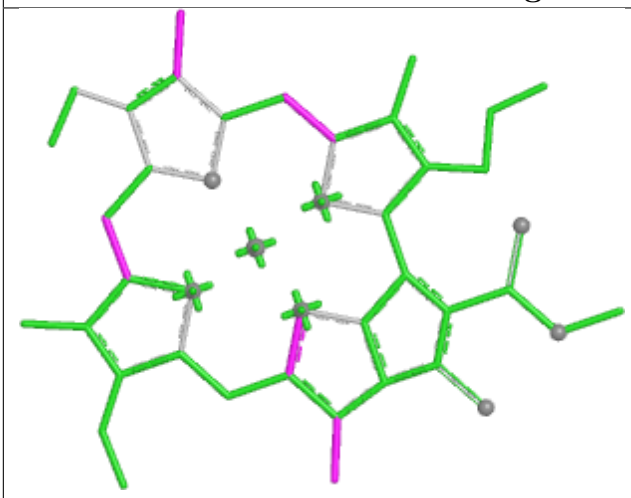


Torsions



Rings

Ligand CLA B 821



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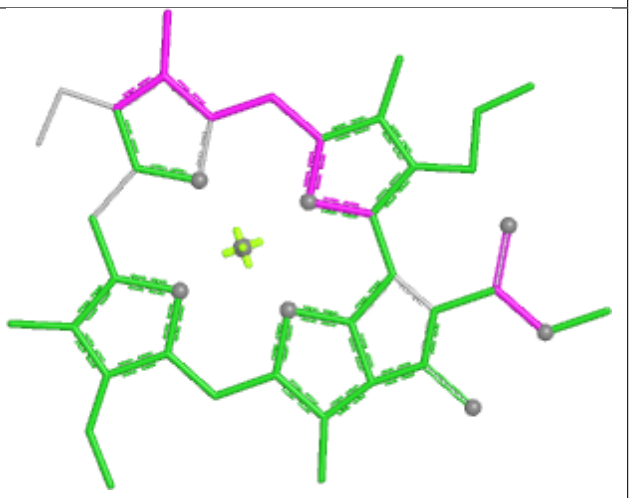
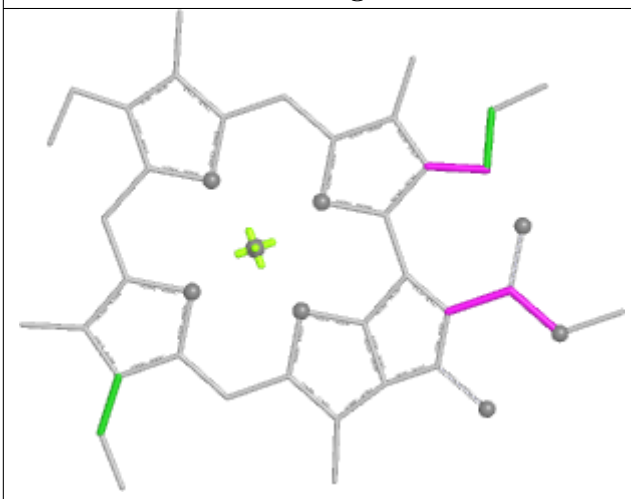


Bond angles



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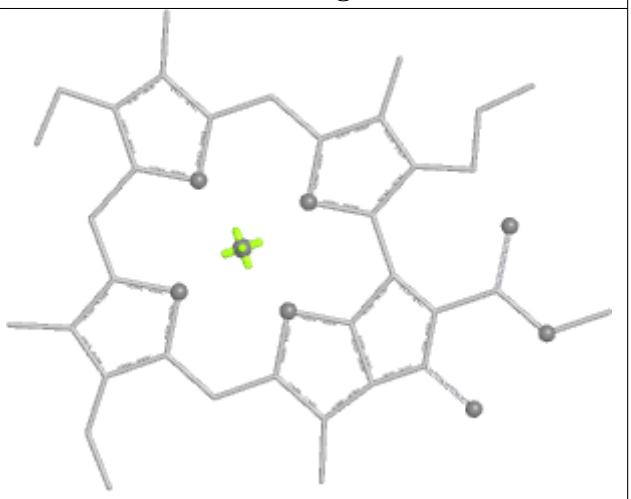
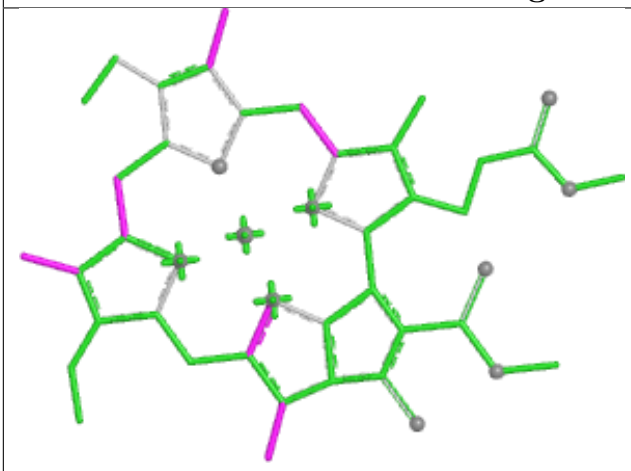


Rings

Ligand CLA 7 311



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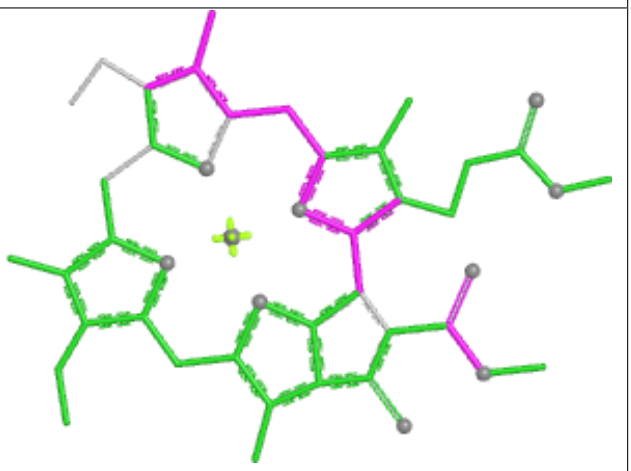
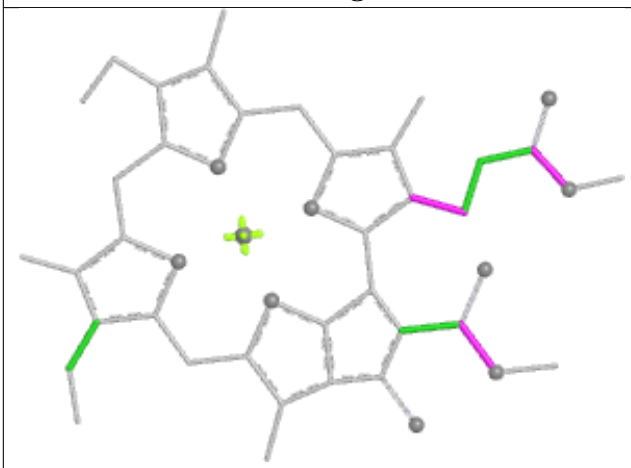
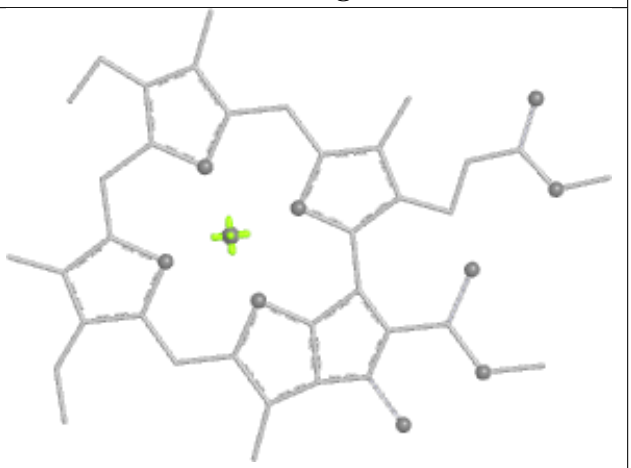


Bond angles



Torsions

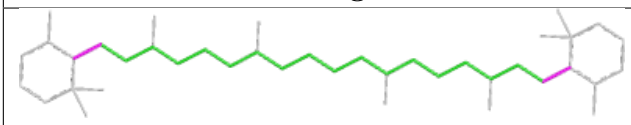


Rings

Ligand BCR J 103

Bond lengths

Bond angles



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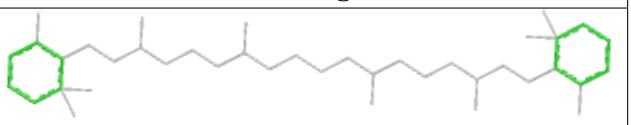
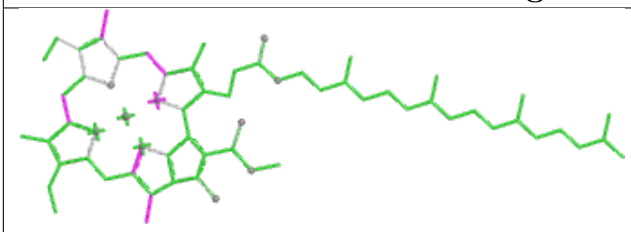


Rings

Ligand CLA L 201



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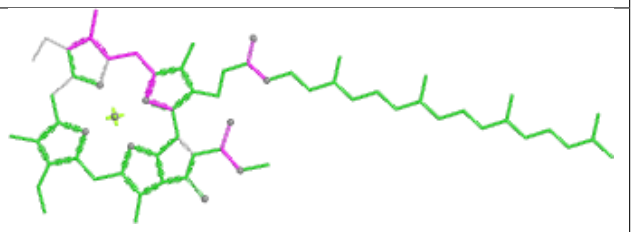
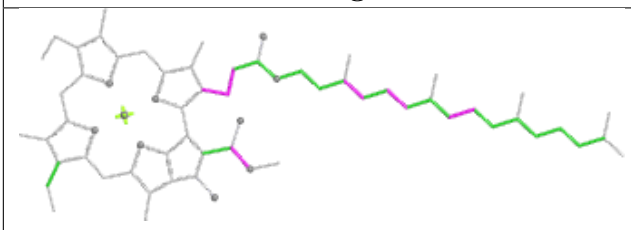


Bond angles



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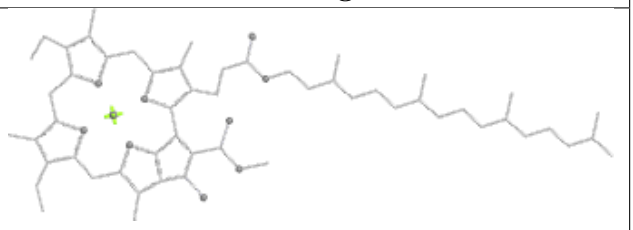
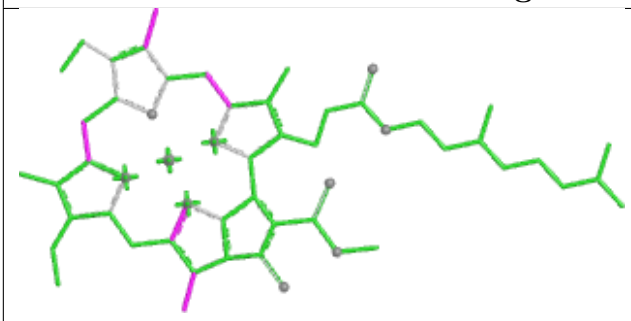
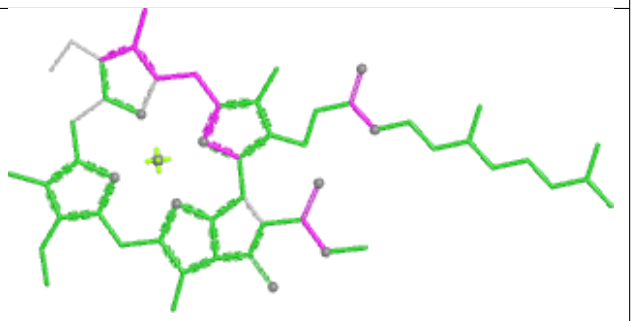


Rings

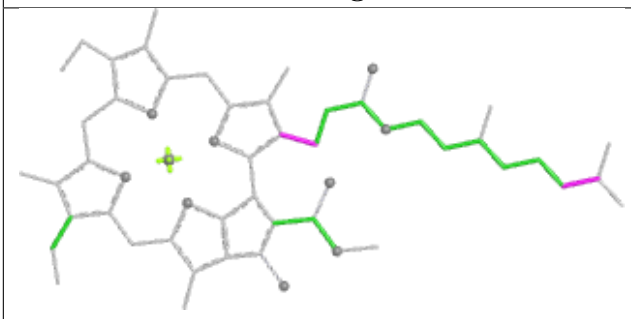
Ligand CLA A 5033



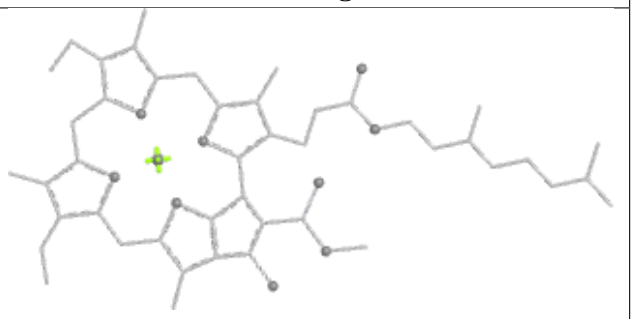
Bond lengths



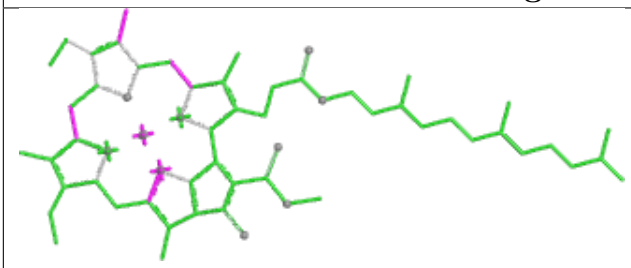
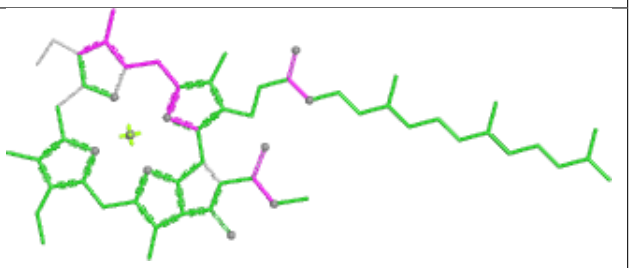
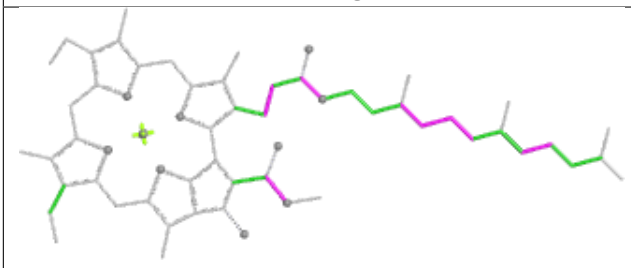
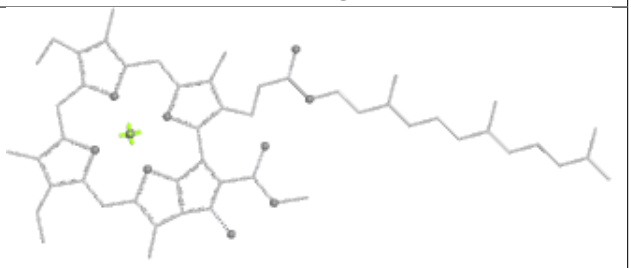
Bond angles

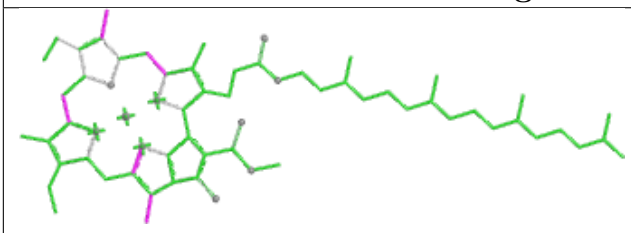
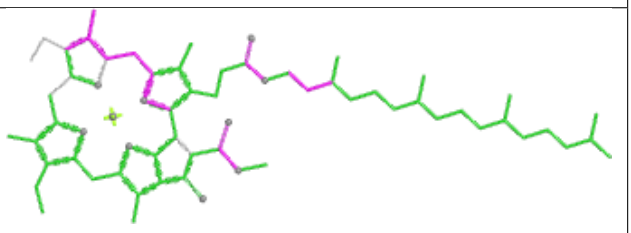
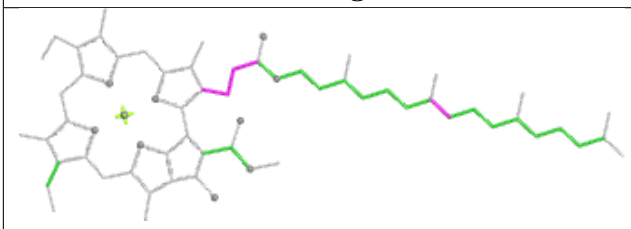
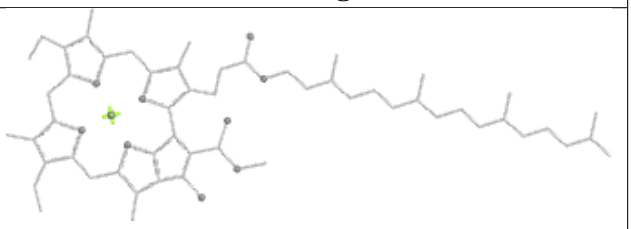


Torsions

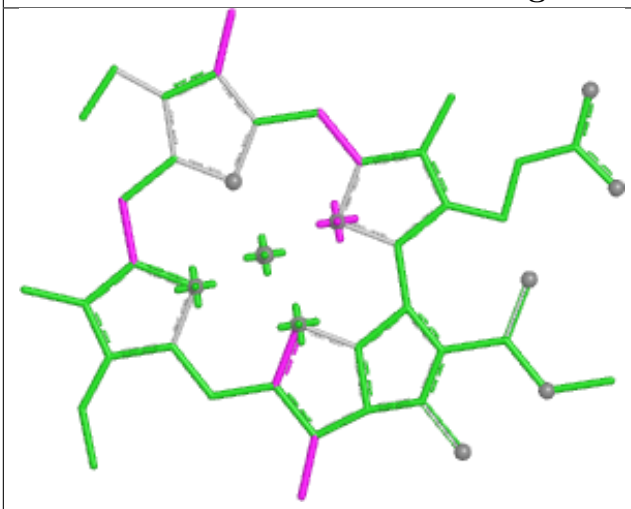


Rings

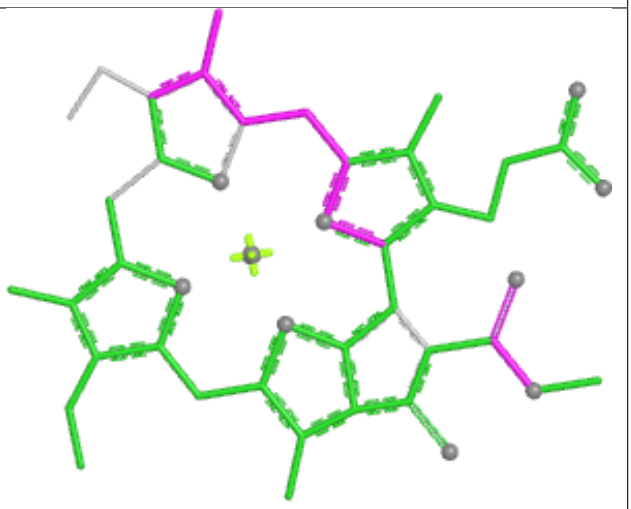
Ligand CLA B 809	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

Ligand CLA A 5041	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

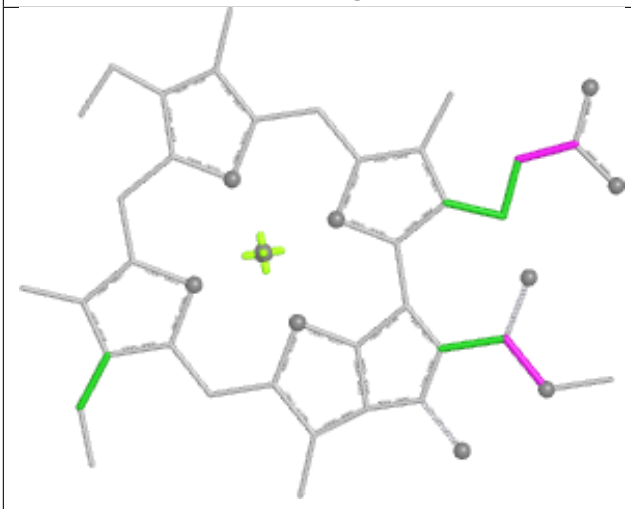
Ligand CLA 1 603



Bond lengths



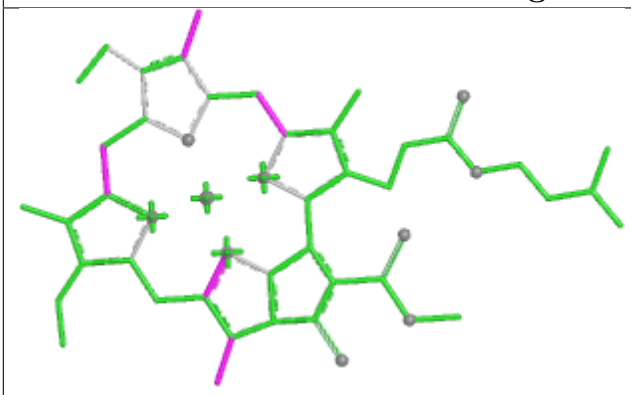
Bond angles



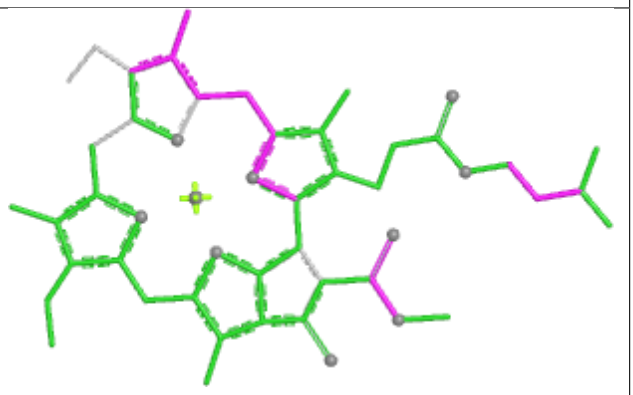
Torsions

Rings

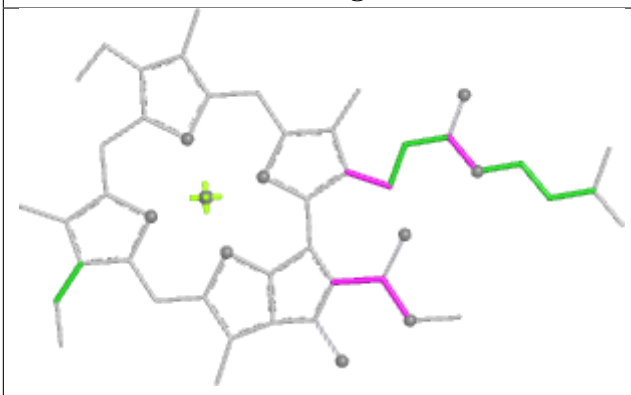
Ligand CLA 1 604



Bond lengths



Bond angles



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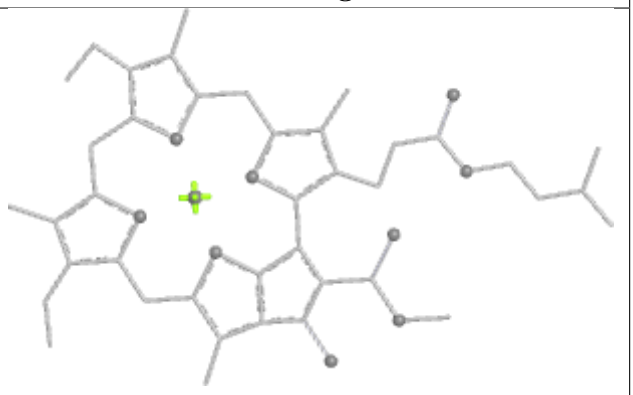
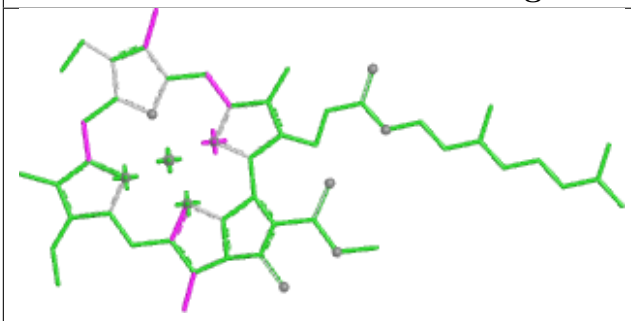
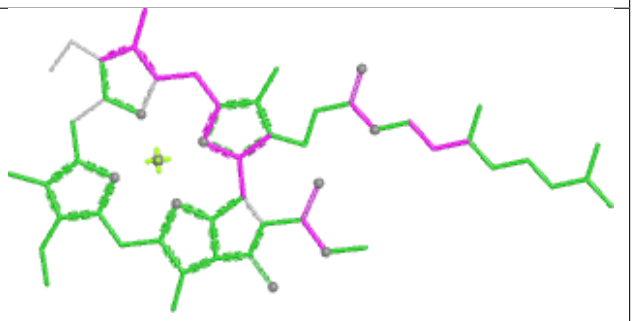


Rings

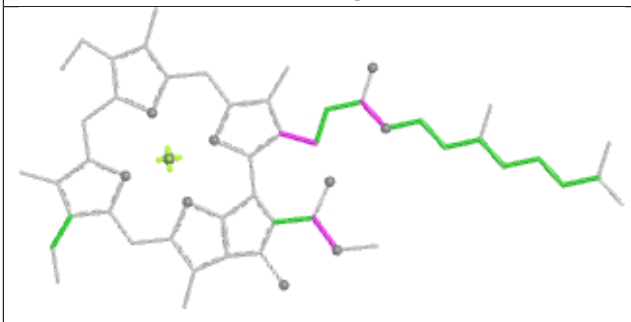
Ligand CLA B 832



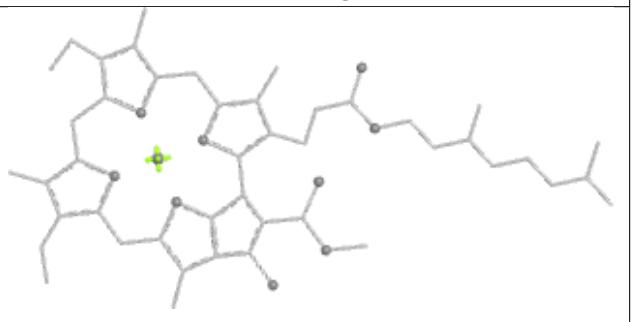
Bond lengths



Bond angles

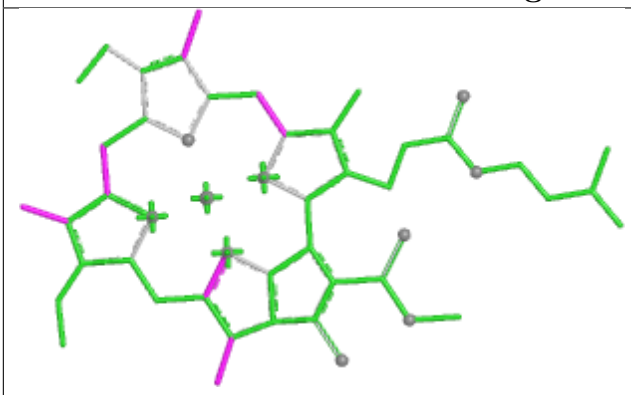


Torsions

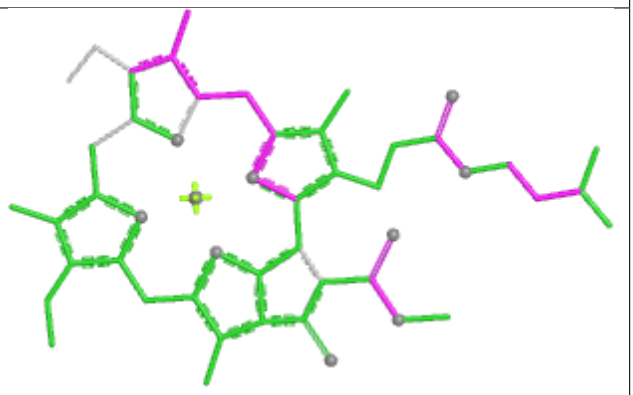


Rings

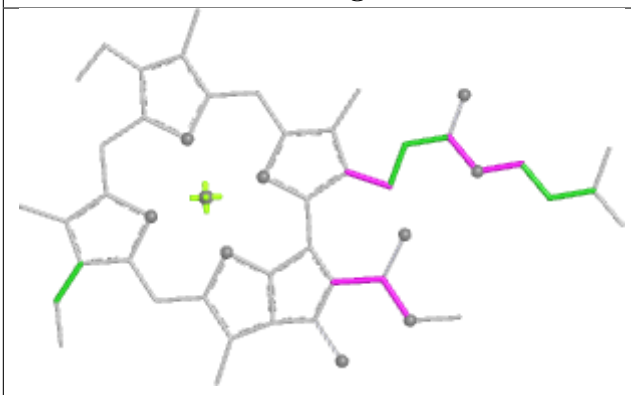
Ligand CLA T 407



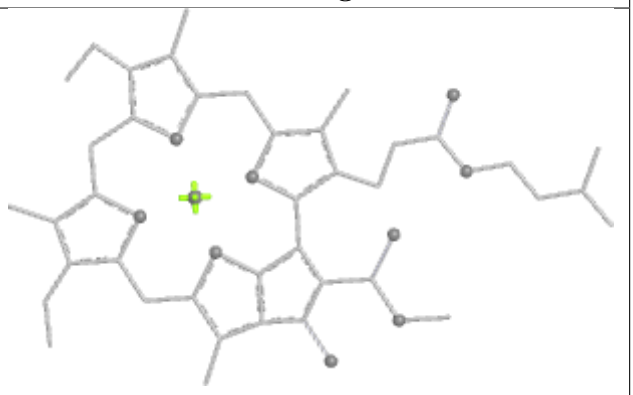
Bond lengths



Bond angles

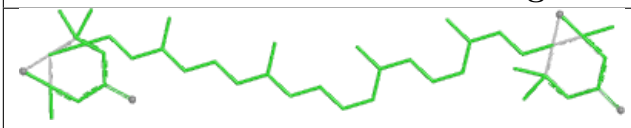


Torsions

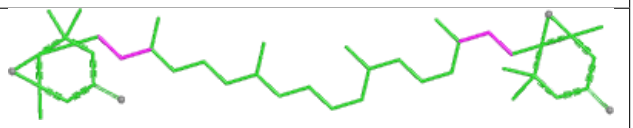


Rings

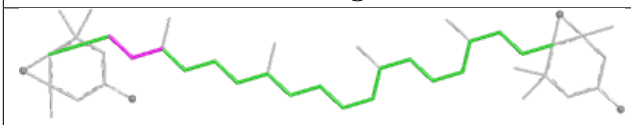
Ligand XAT 3 316



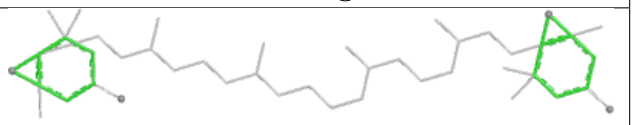
Bond lengths



Bond angles

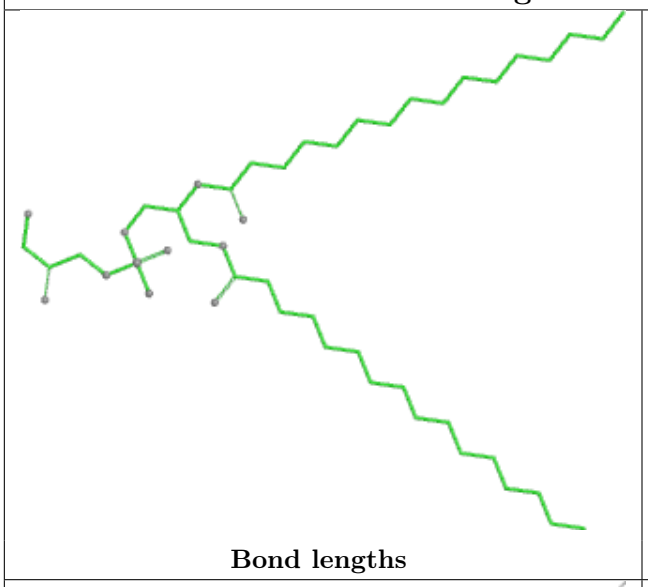


Torsions



Rings

Ligand LHG A 5053



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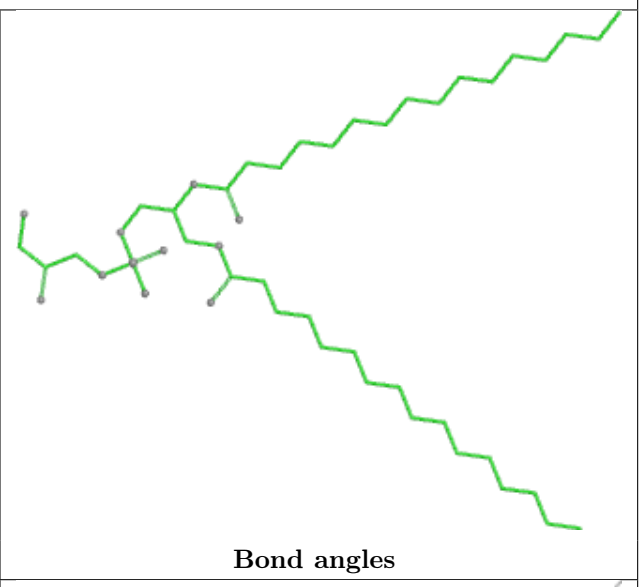
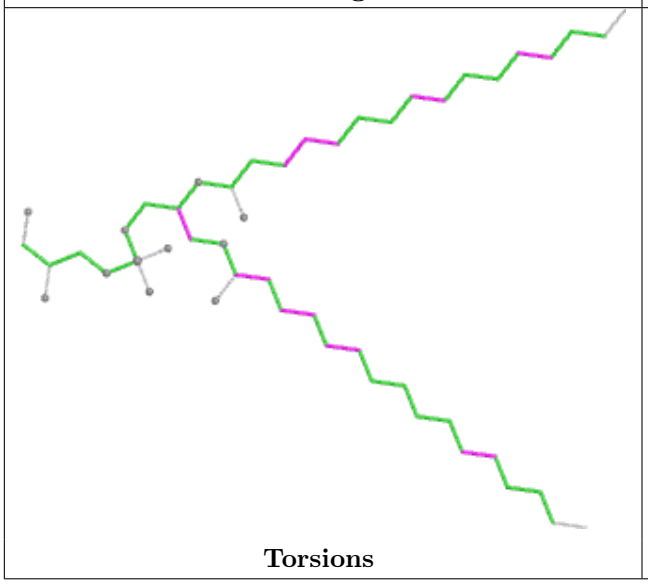
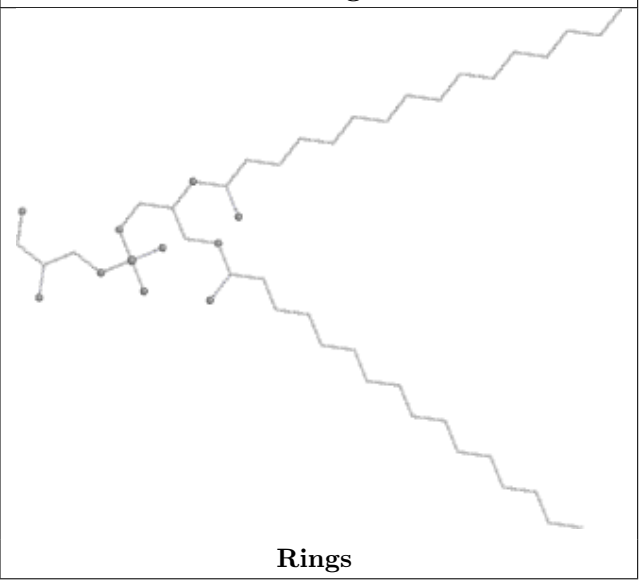


Bond angles

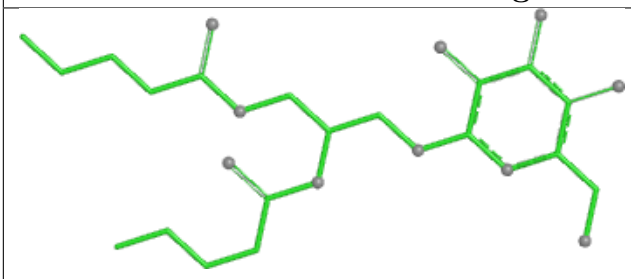


Torsions

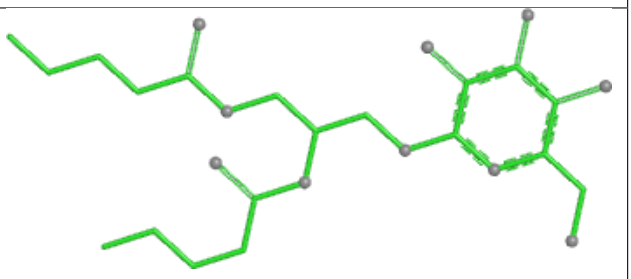


Rings

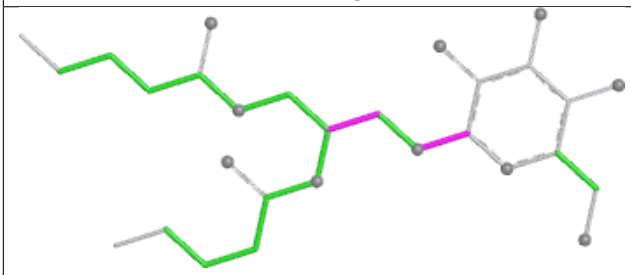
Ligand LMG F 5011



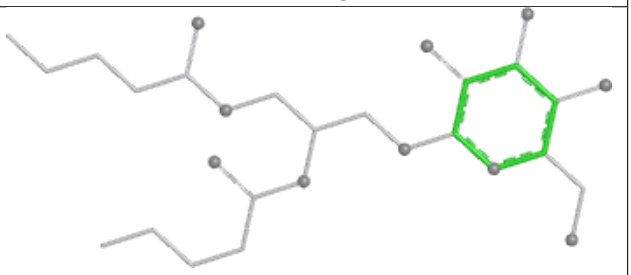
Bond lengths



Bond angles

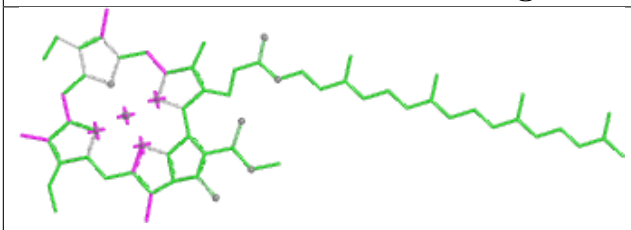


Torsions



Rings

Ligand CLA F 5004



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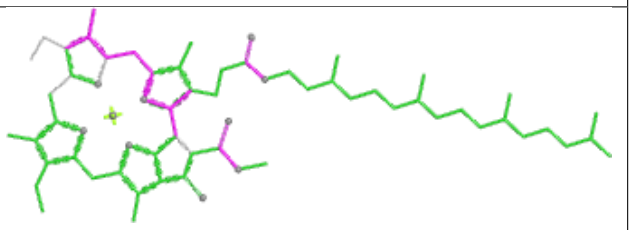
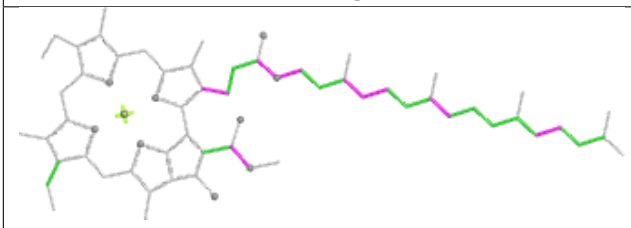
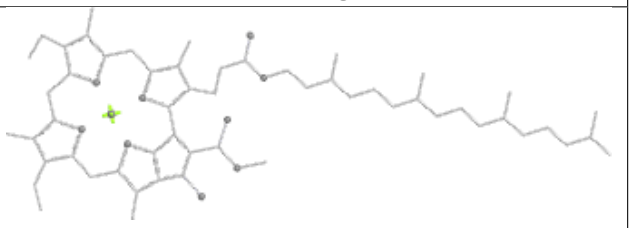


Bond angles

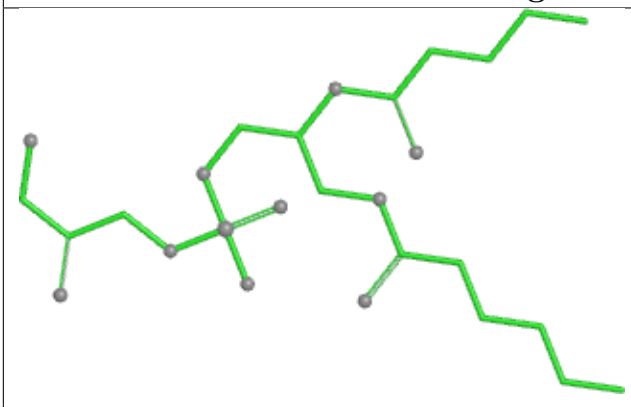


Torsions

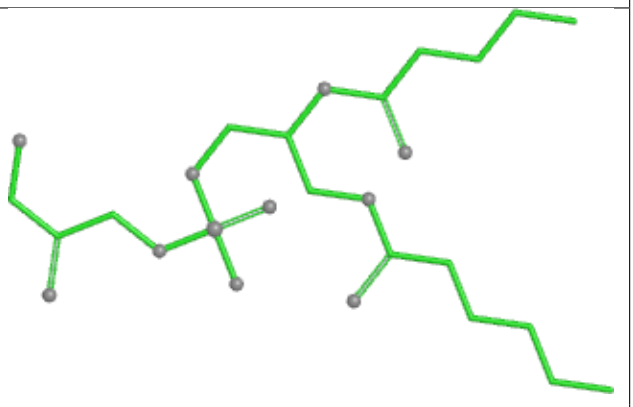


Rings

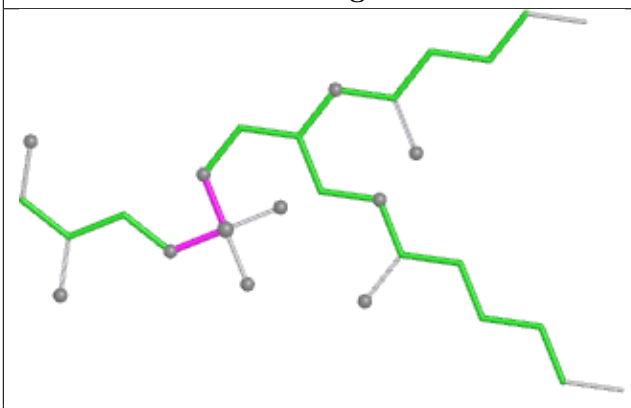
Ligand LHG c 317



Bond lengths



Bond angles



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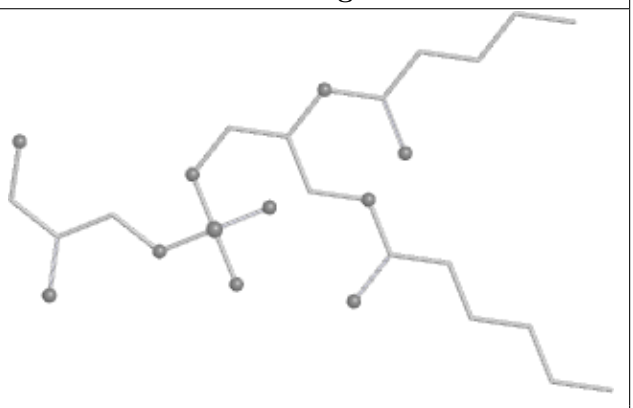
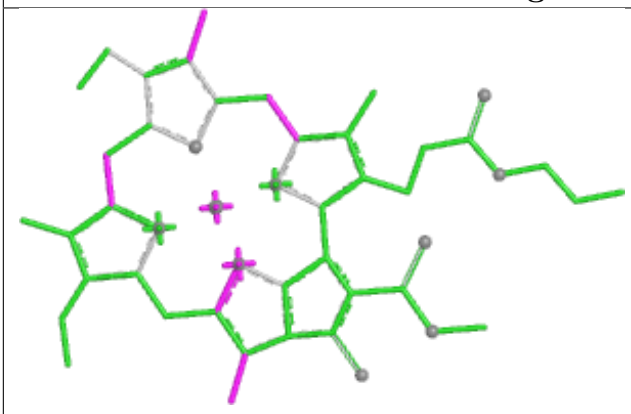


Rings

Ligand CLA b 612



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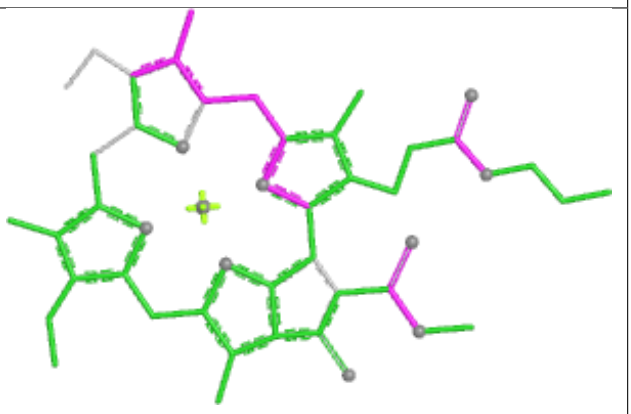
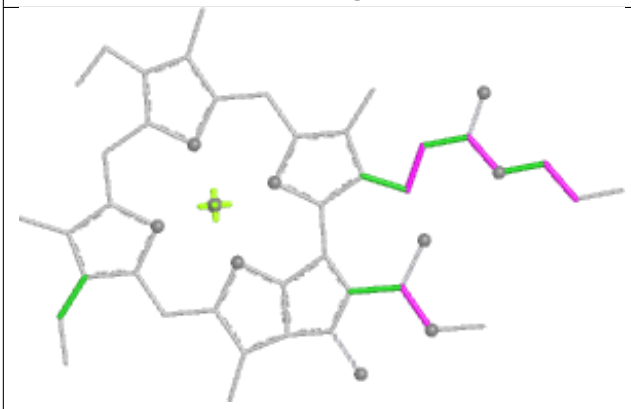


Bond angles



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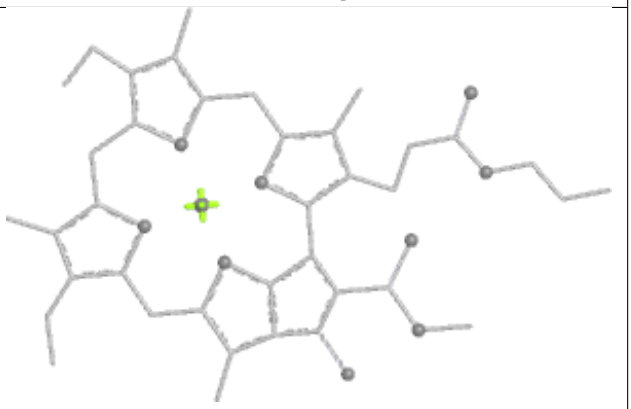
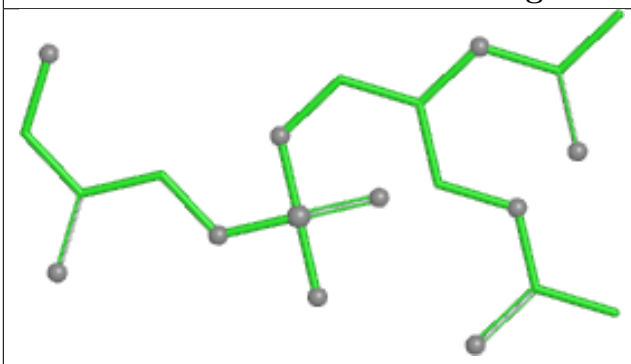
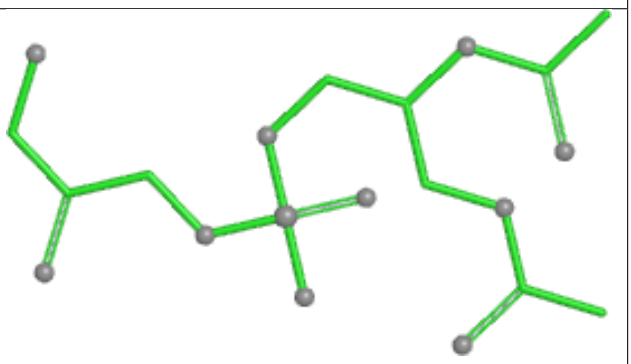


Rings

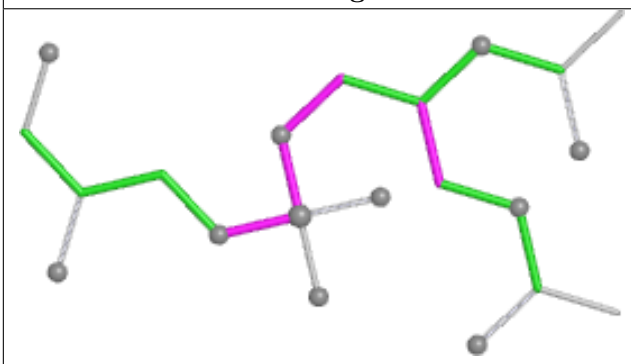
Ligand LHG b 618



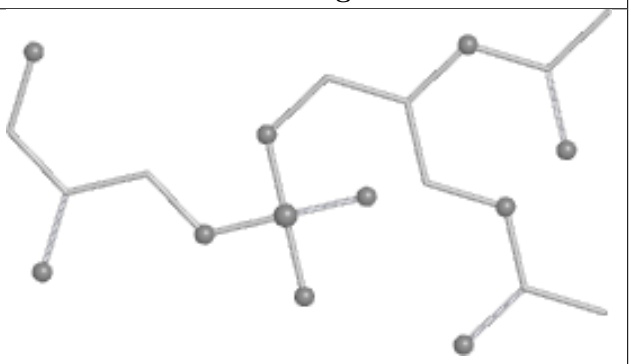
Bond lengths



Bond angles

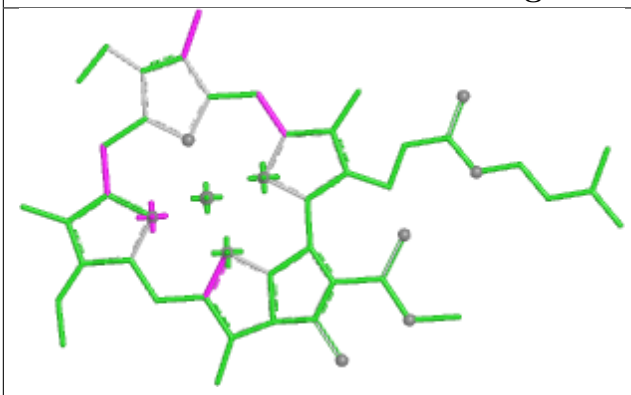


Torsions

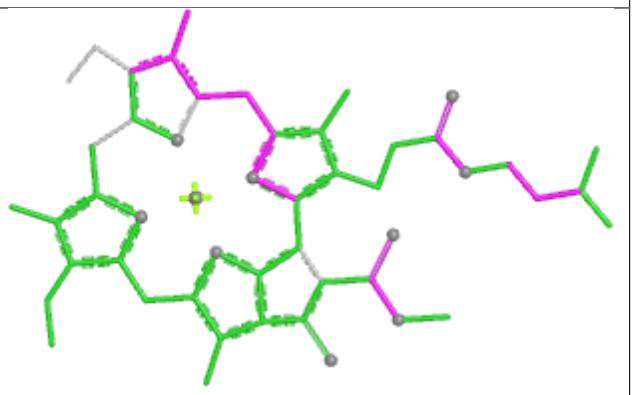


Rings

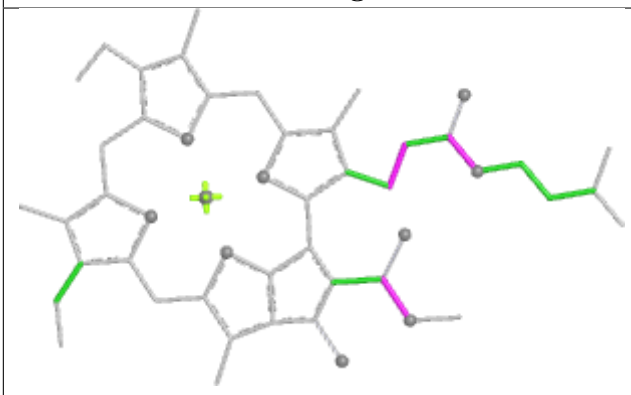
Ligand CLA T 410



Bond lengths



Bond angles



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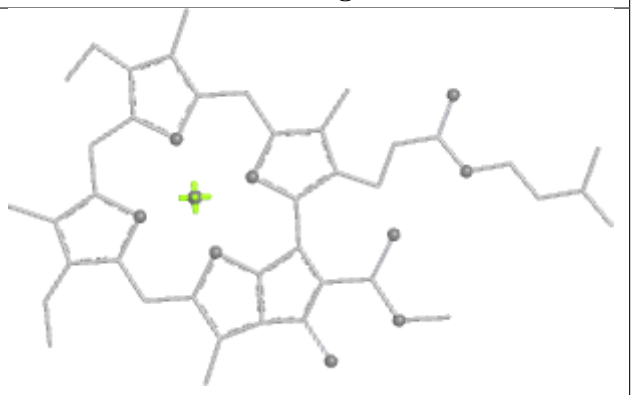
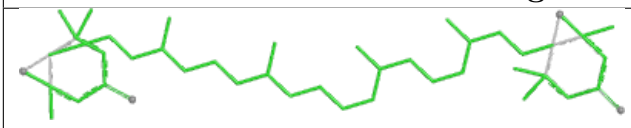


Rings

Ligand XAT 1 616



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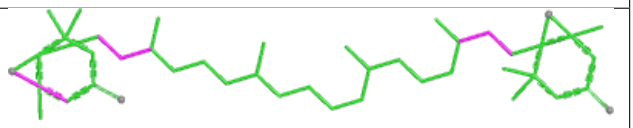
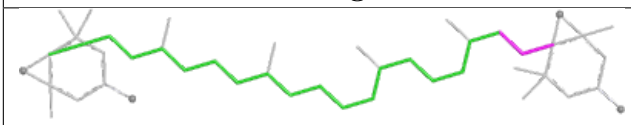
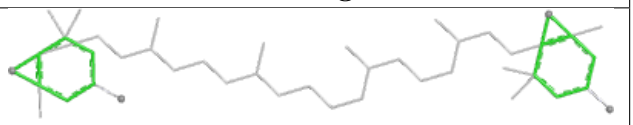


Bond angles

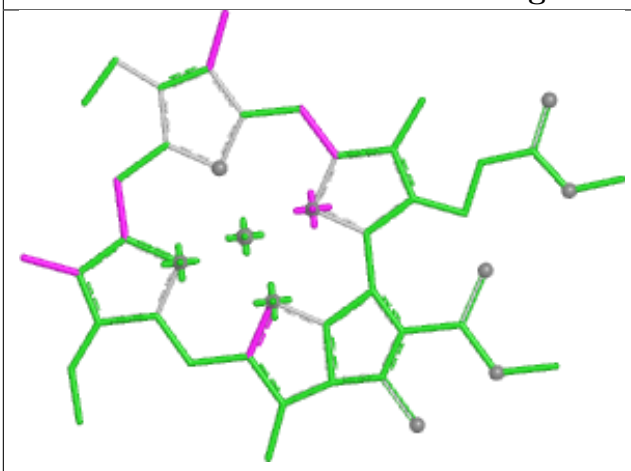


Torsions

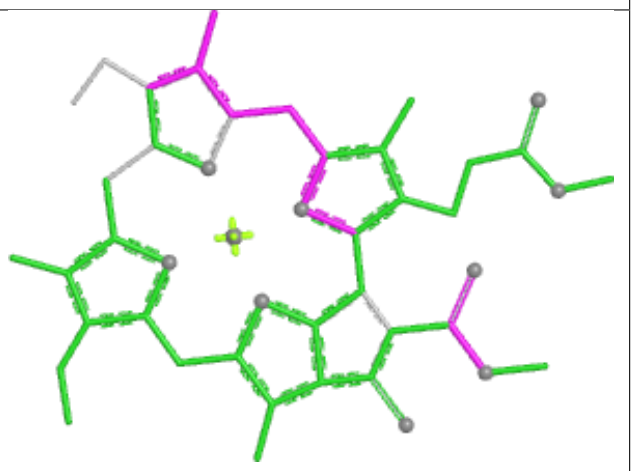


Rings

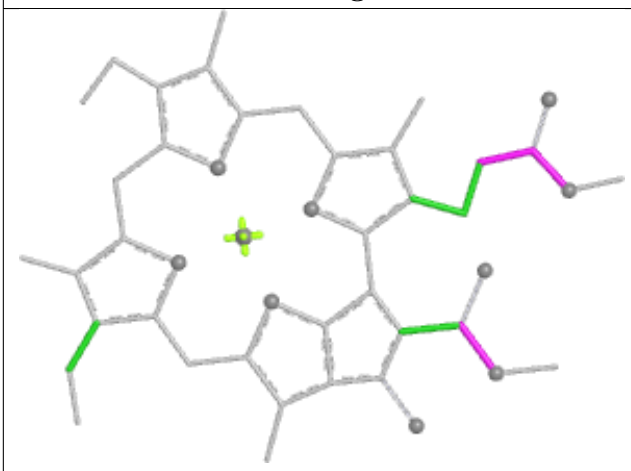
Ligand CLA 3 310



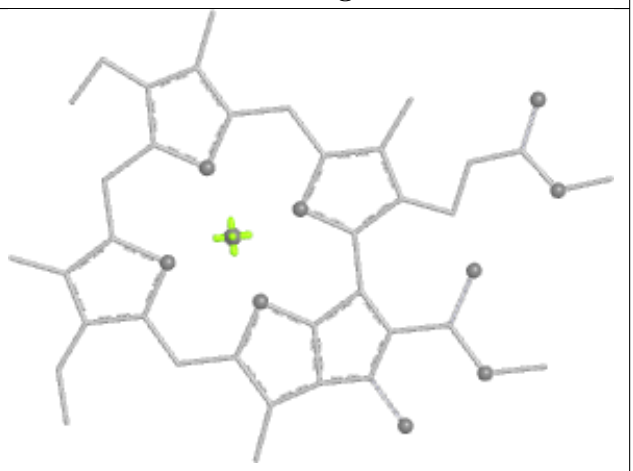
Bond lengths



Bond angles

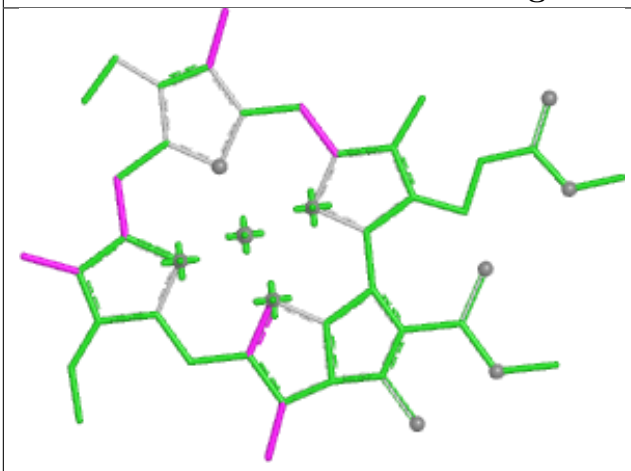


Torsions



Rings

Ligand CLA 3 312



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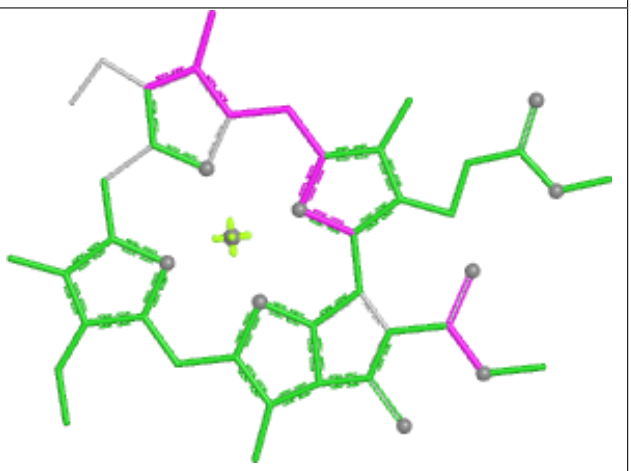
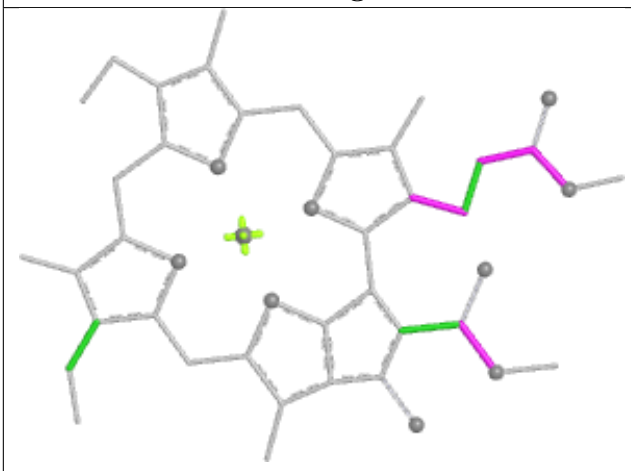


Bond angles



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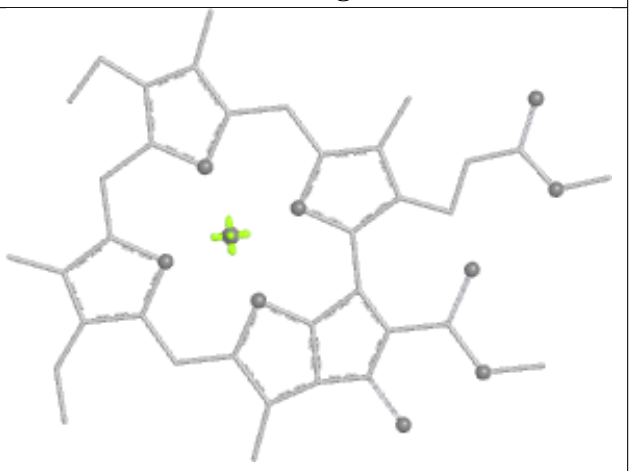
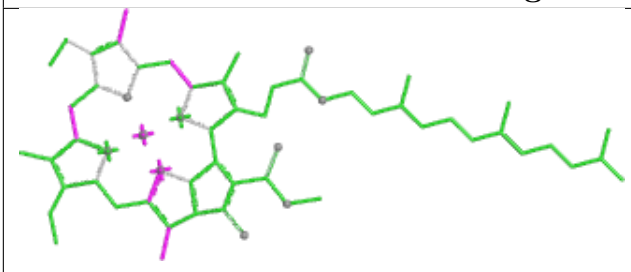
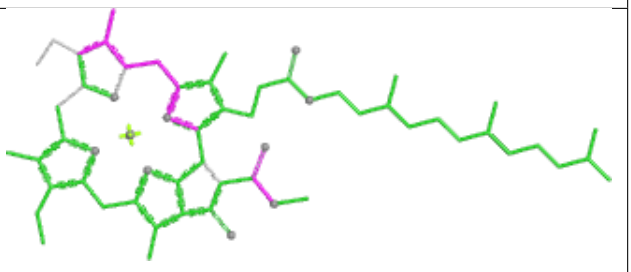


Rings

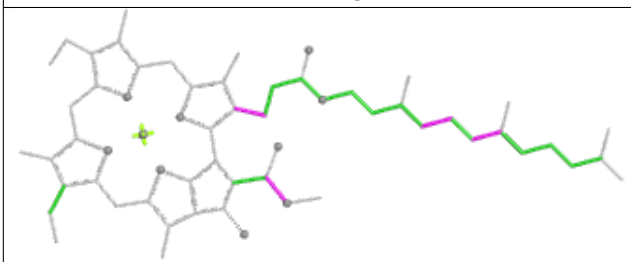
Ligand CLA B 819



Bond lengths



Bond angles



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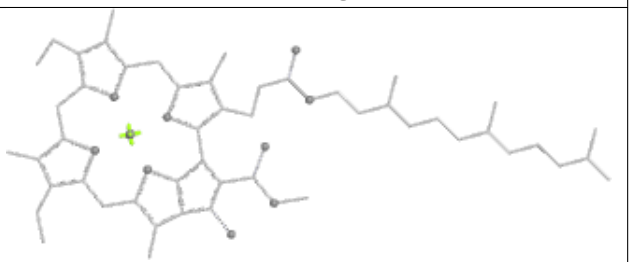
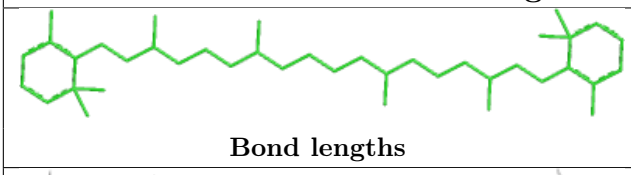
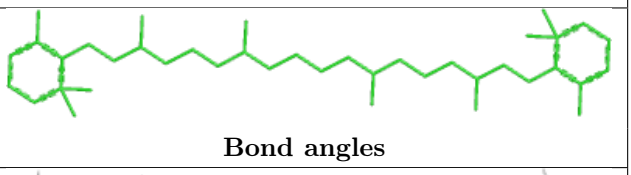


Rings

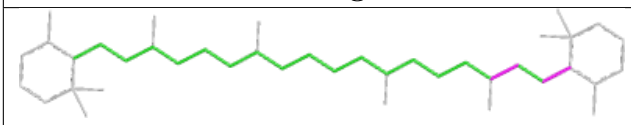
Ligand BCR L 203



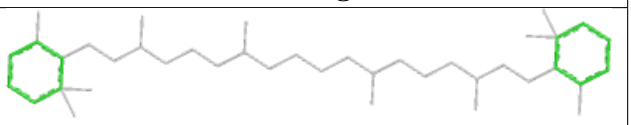
Bond lengths



Bond angles

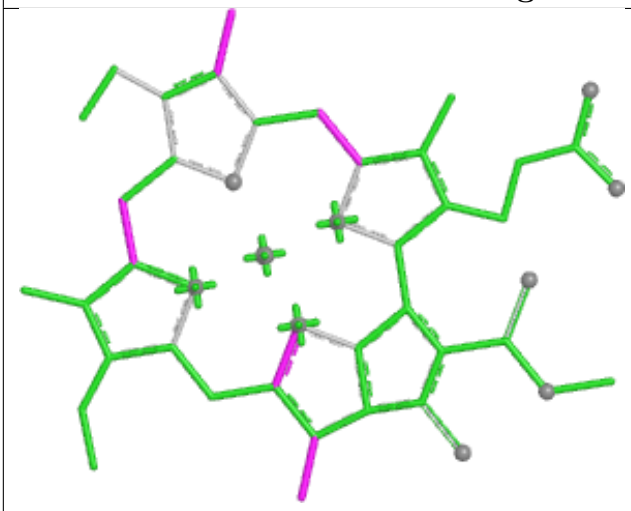


Torsions

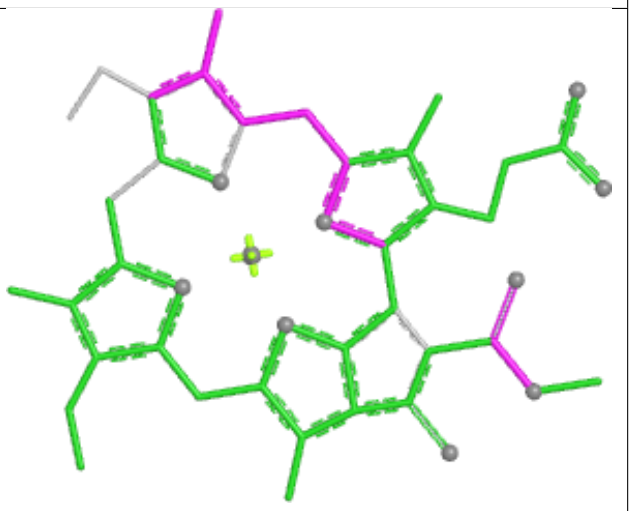


Rings

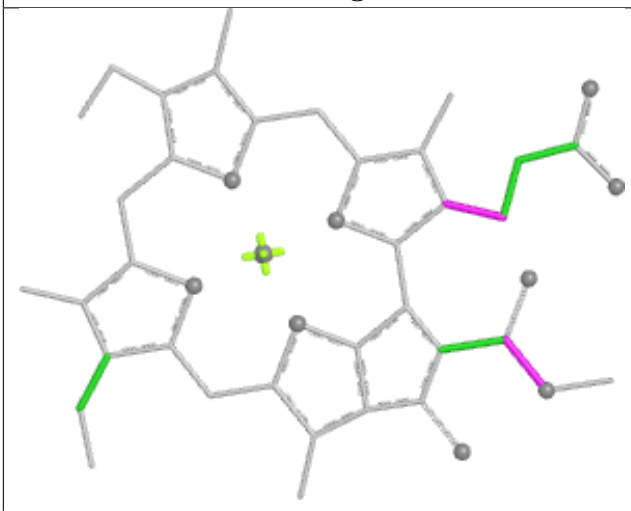
Ligand CLA F 5008



Bond lengths



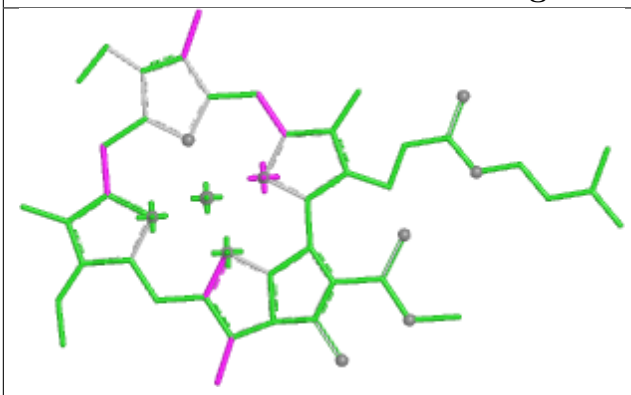
Bond angles



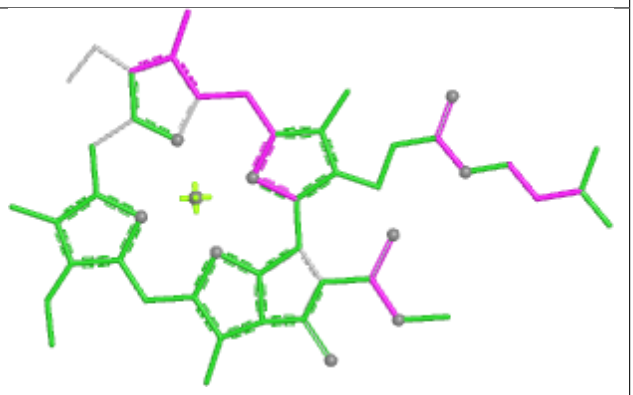
Torsions

Rings

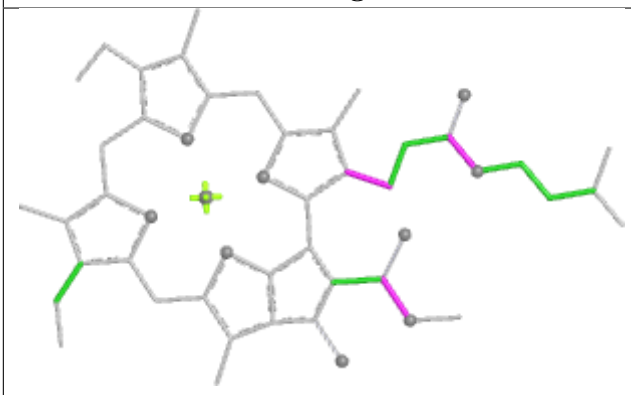
Ligand CLA c 312



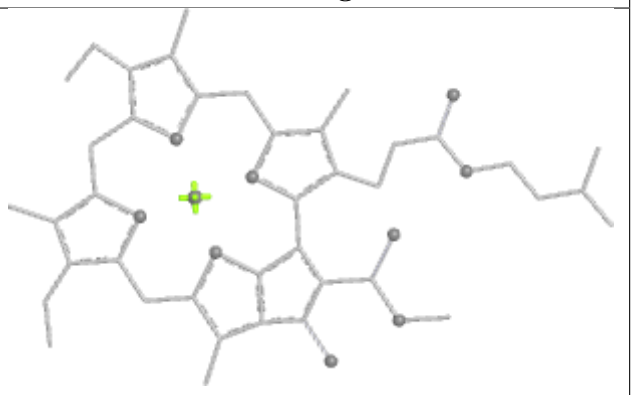
Bond lengths



Bond angles

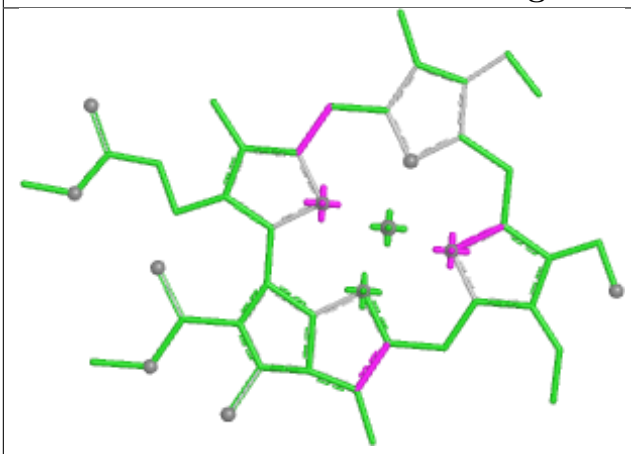


Torsions

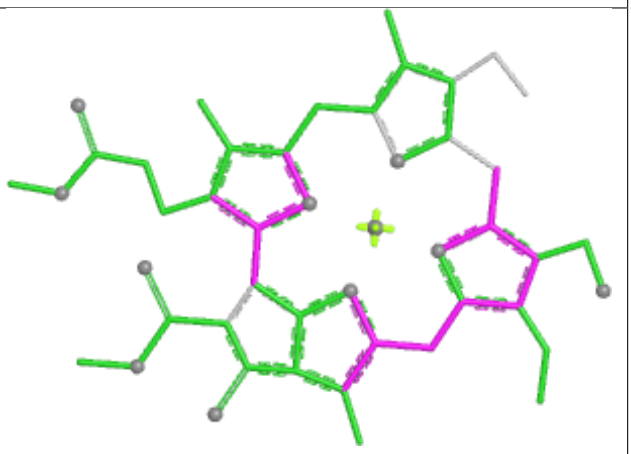


Rings

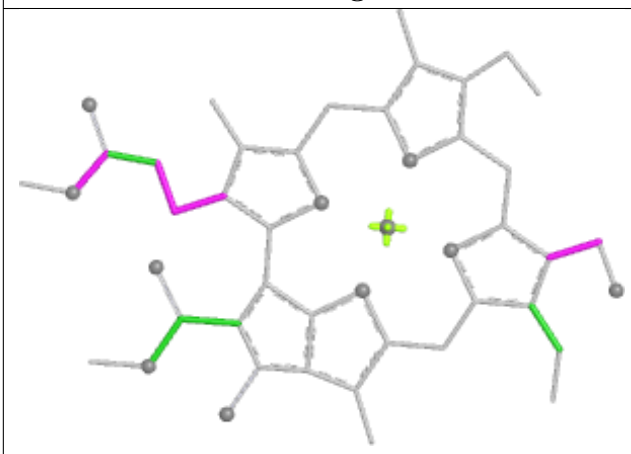
Ligand CHL a 601



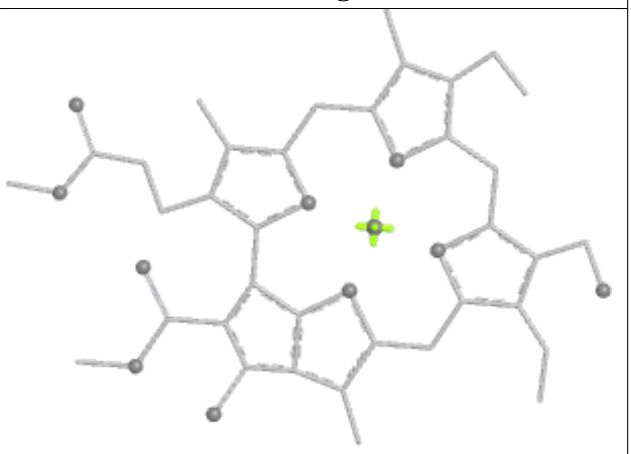
Bond lengths



Bond angles

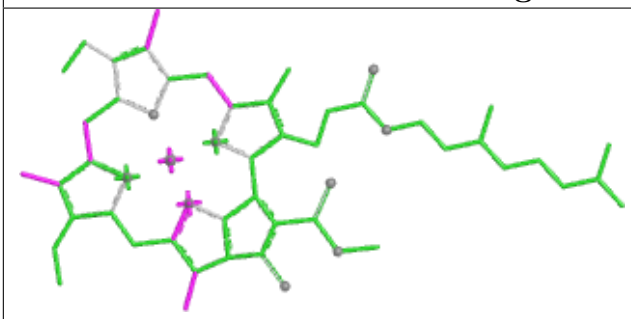


Torsions

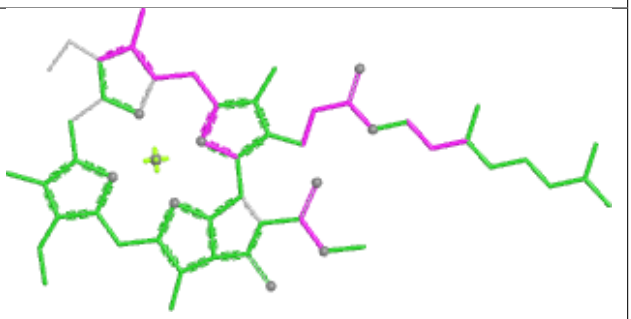


Rings

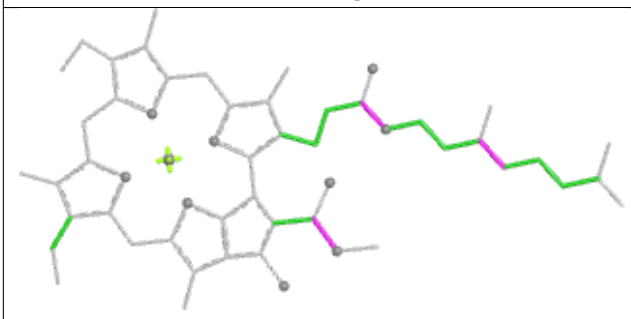
Ligand CLA A 5012



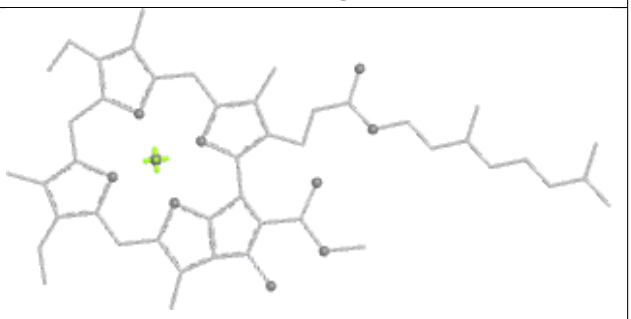
Bond lengths



Bond angles

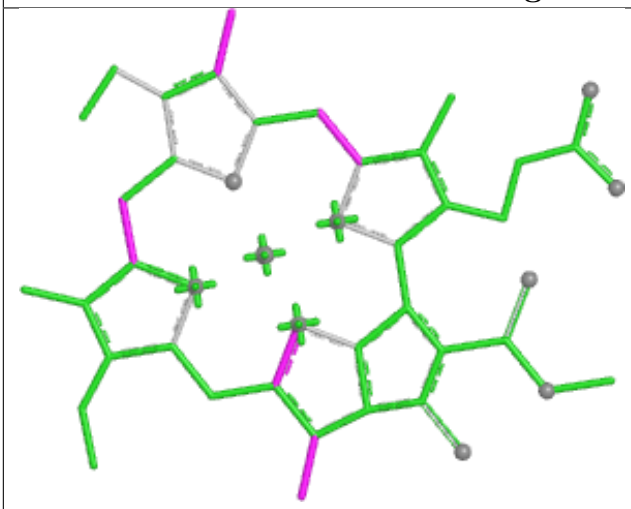


Torsions

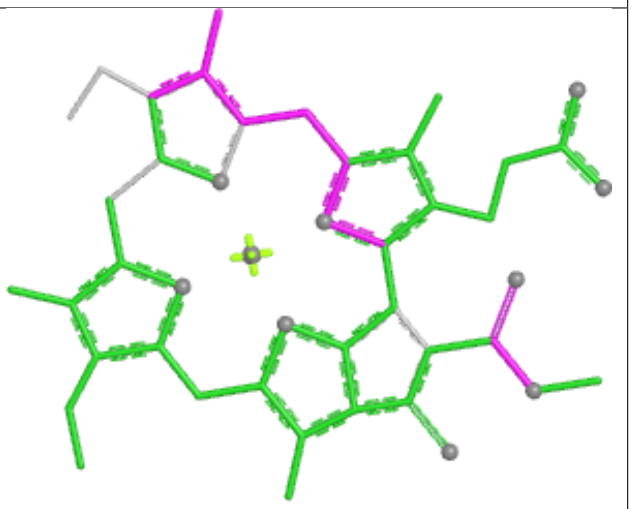


Rings

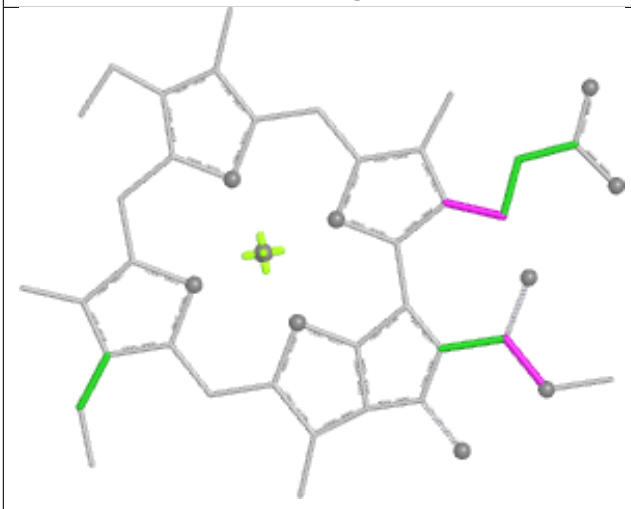
Ligand CLA B 822



Bond lengths



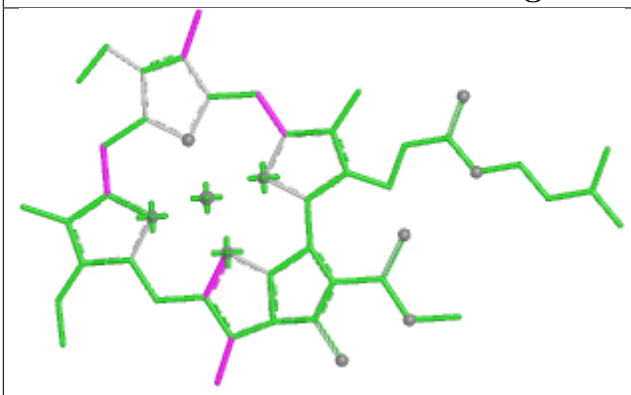
Bond angles



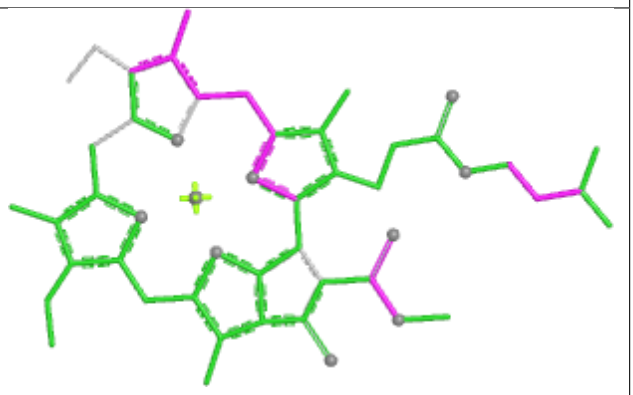
Torsions

Rings

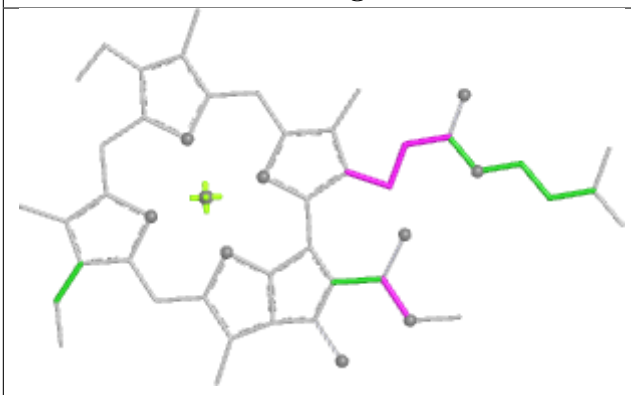
Ligand CLA B 811



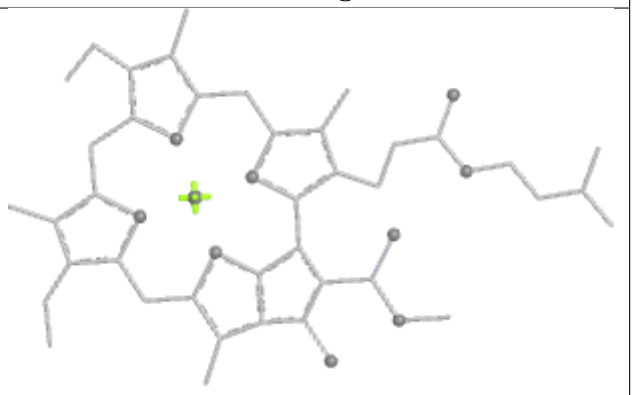
Bond lengths



Bond angles

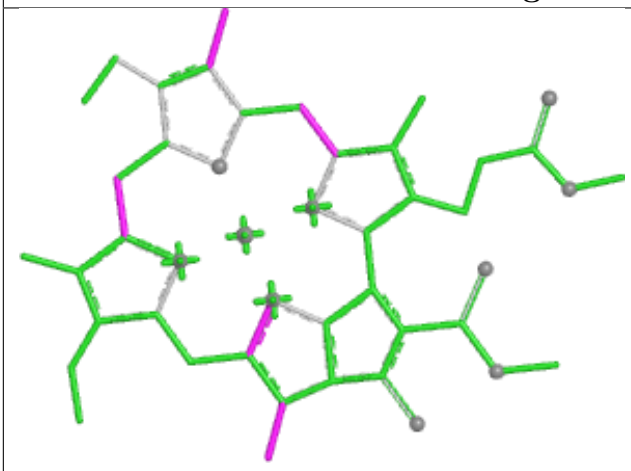


Torsions

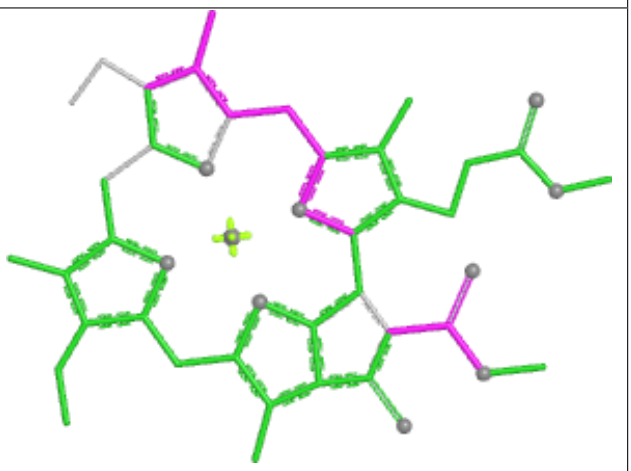


Rings

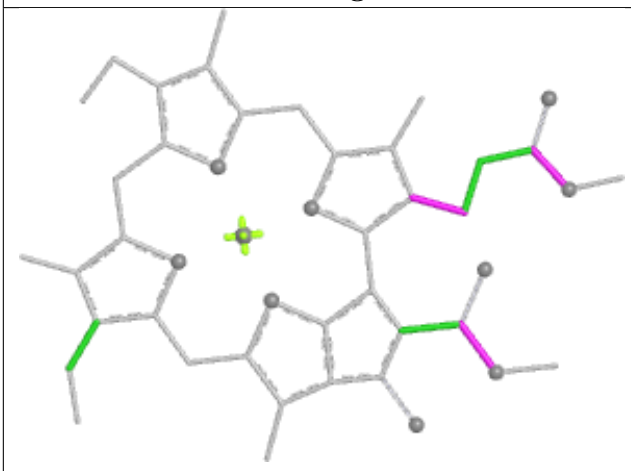
Ligand CLA K 202



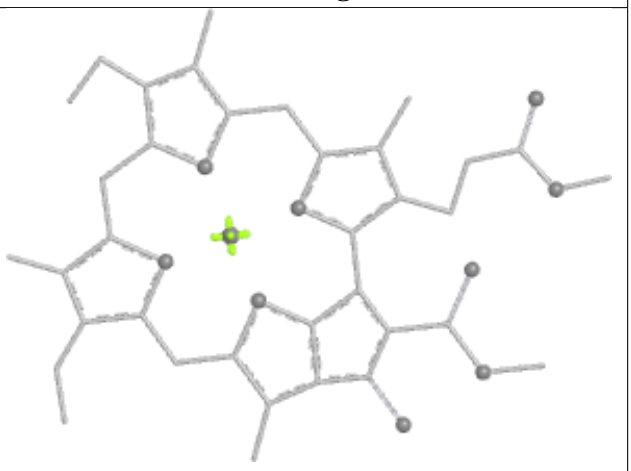
Bond lengths



Bond angles

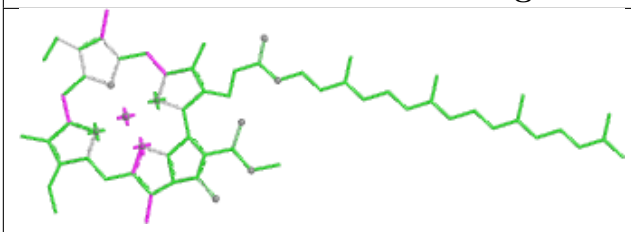


Torsions

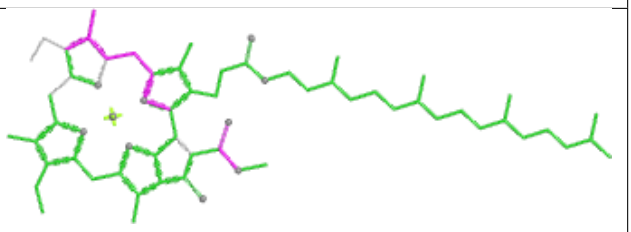


Rings

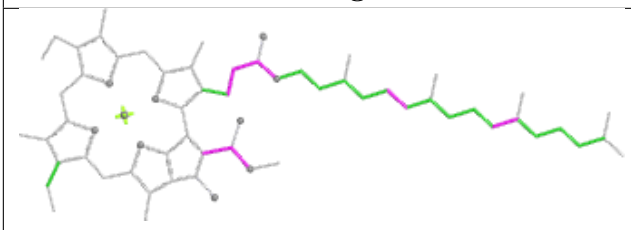
Ligand CLA A 5026



Bond lengths



Bond angles



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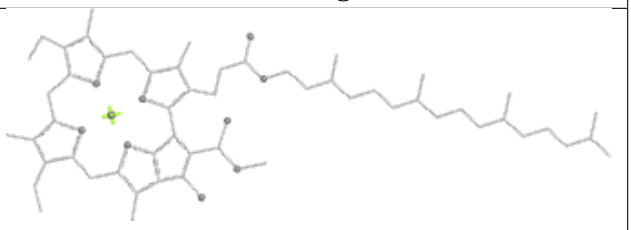
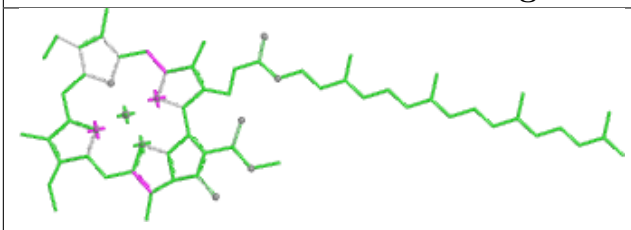
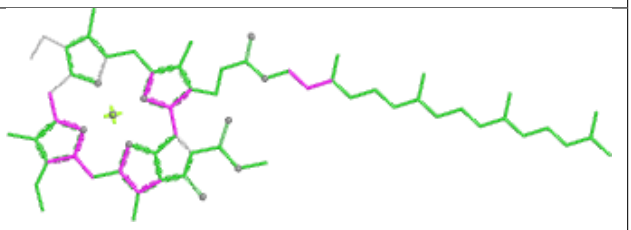


Rings

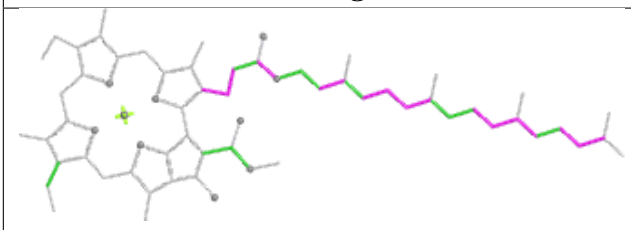
Ligand CL0 A 5003



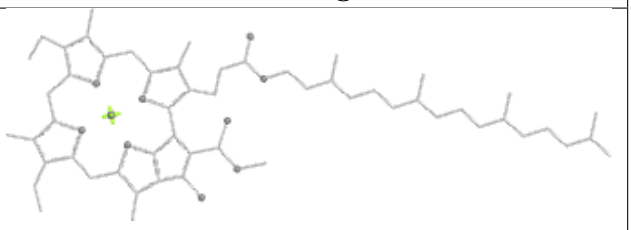
Bond lengths



Bond angles

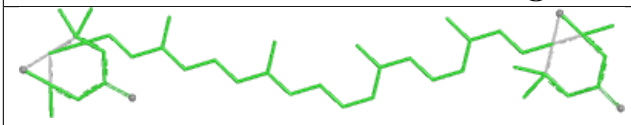


Torsions



Rings

Ligand XAT 7 316



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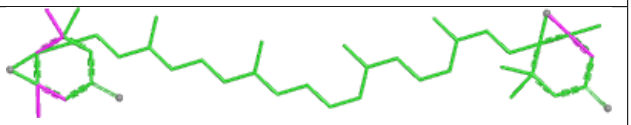
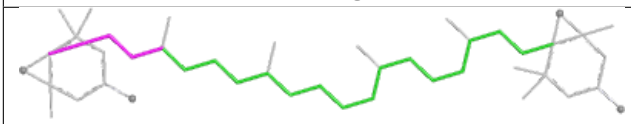


Bond angles



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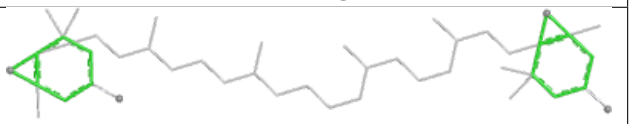
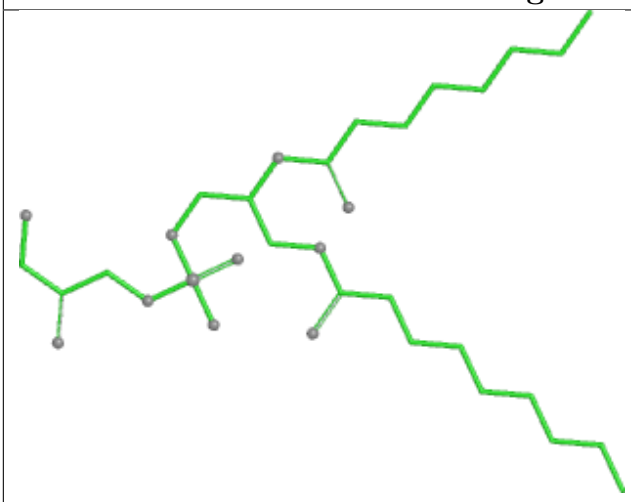


Rings

Ligand LHG 7 318



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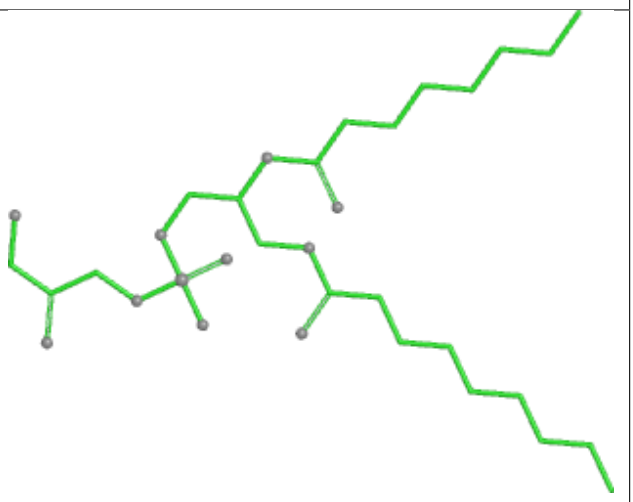
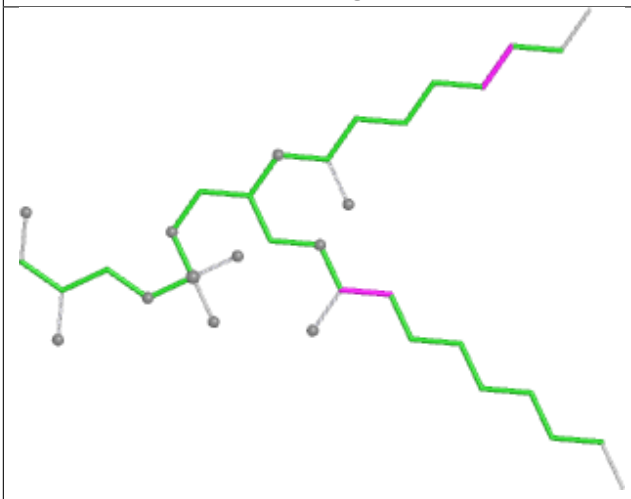
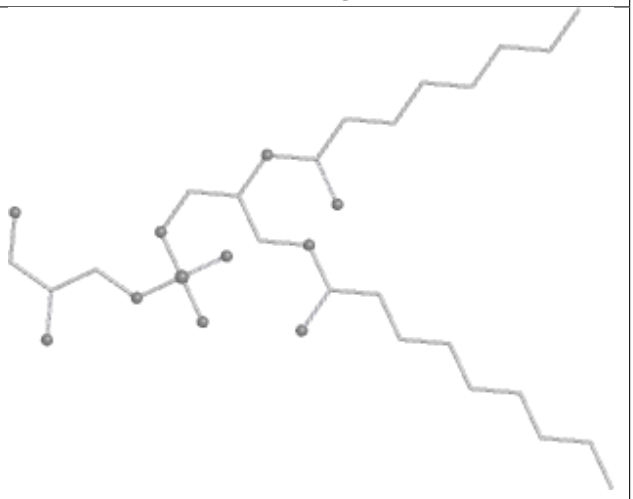


Bond angles

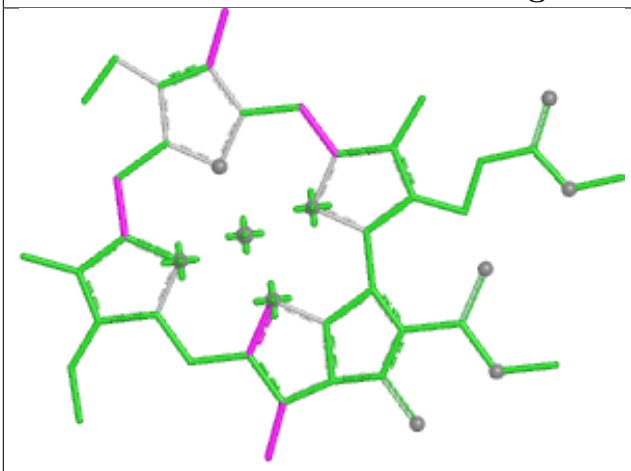


Torsions

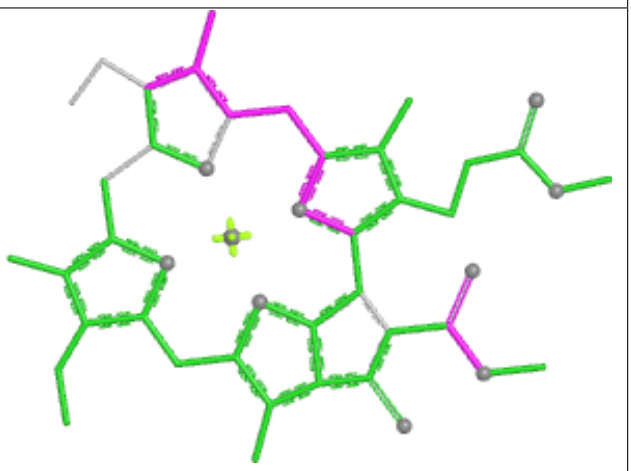


Rings

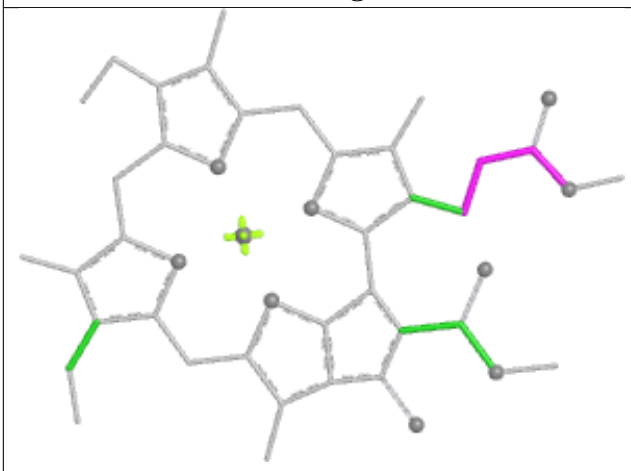
Ligand CLA 7 314



Bond lengths



Bond angles



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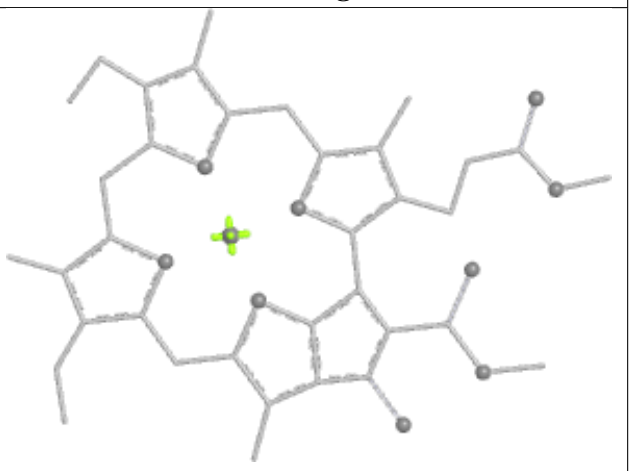
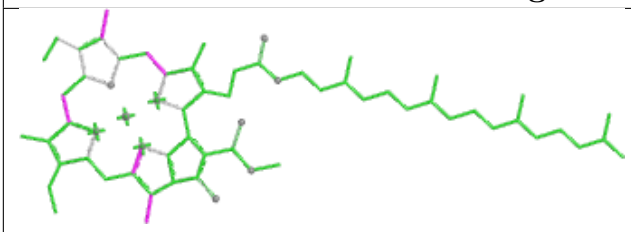
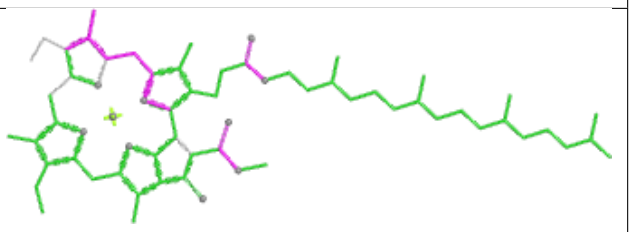


Rings

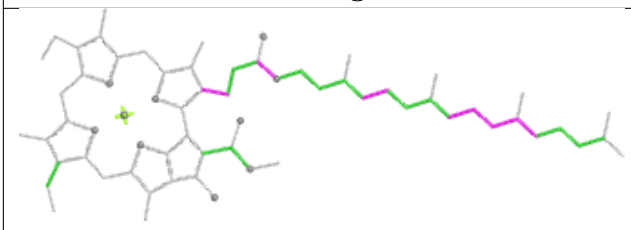
Ligand CLA 1 607



Bond lengths



Bond angles



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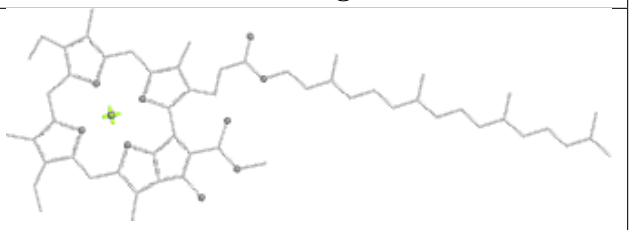
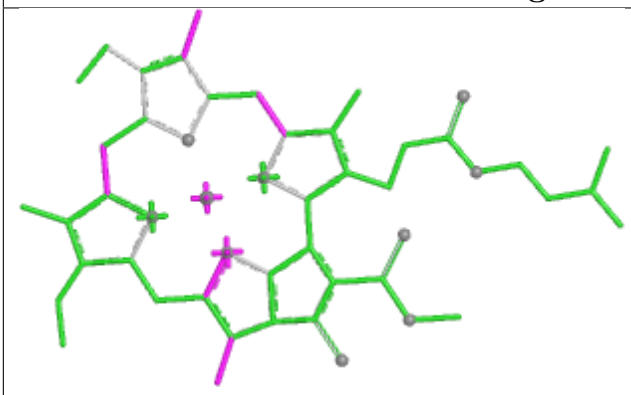


Rings

Ligand CLA 3 305



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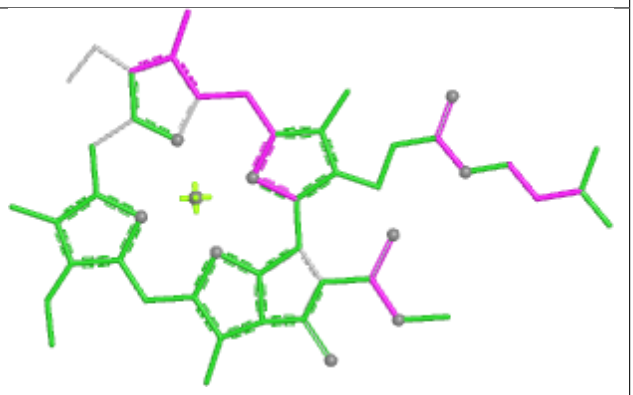
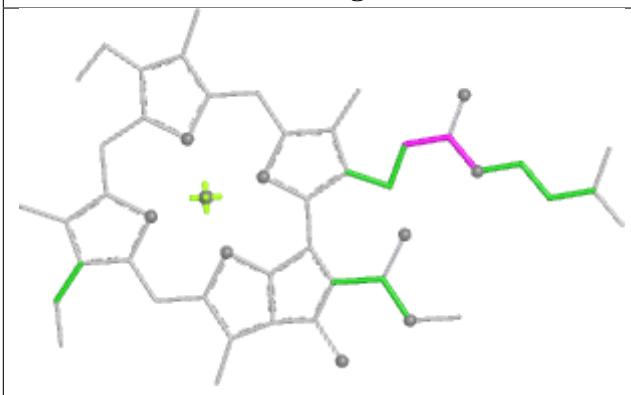
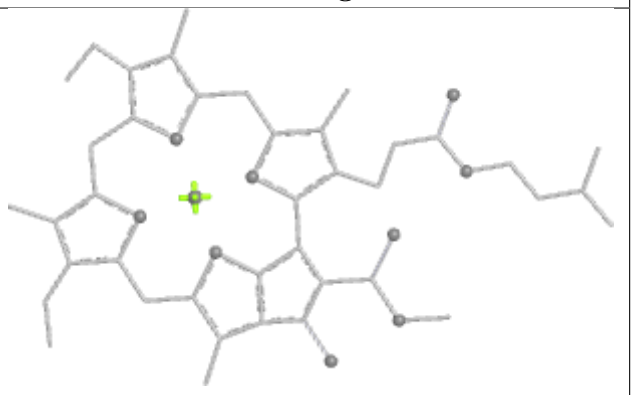


Bond angles

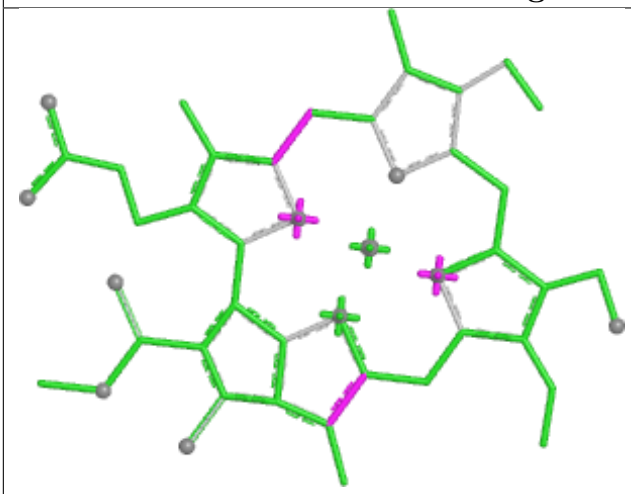


Torsions

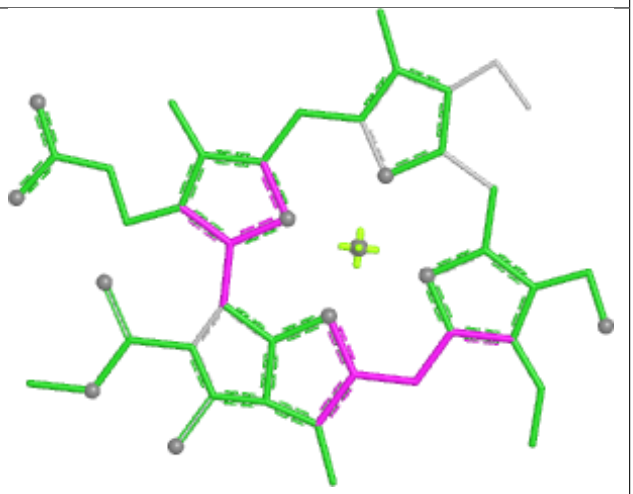


Rings

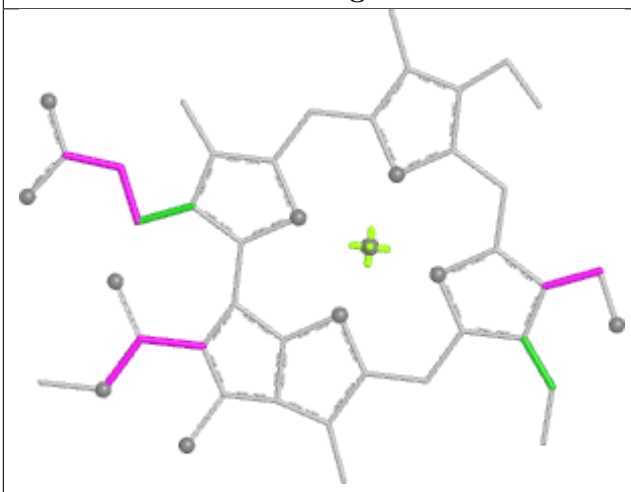
Ligand CHL 8 306



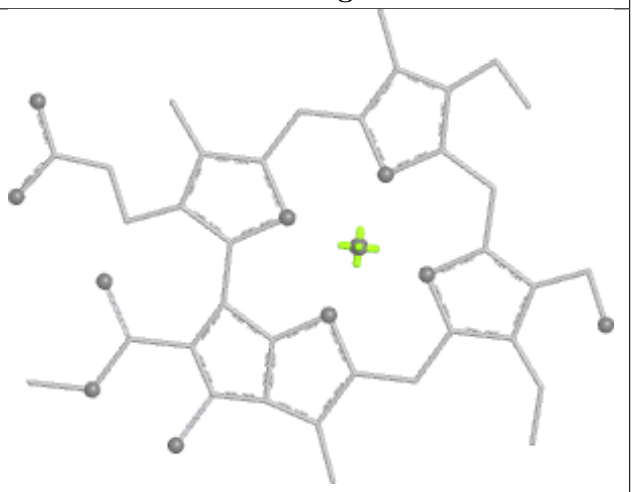
Bond lengths



Bond angles

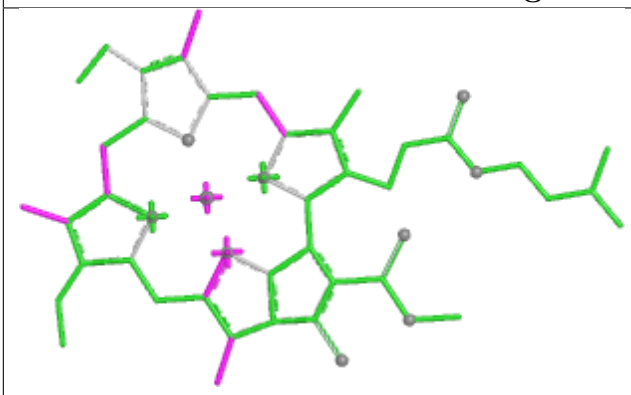


Torsions

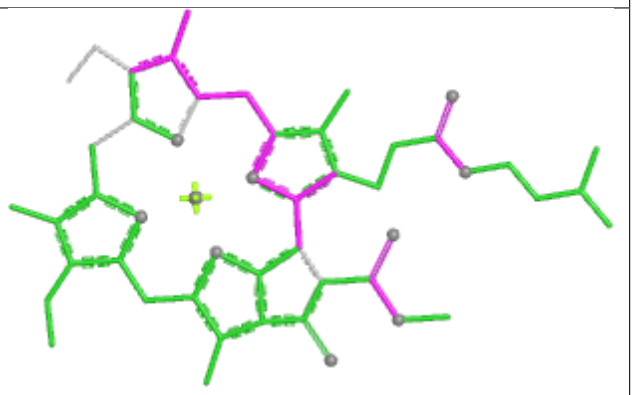


Rings

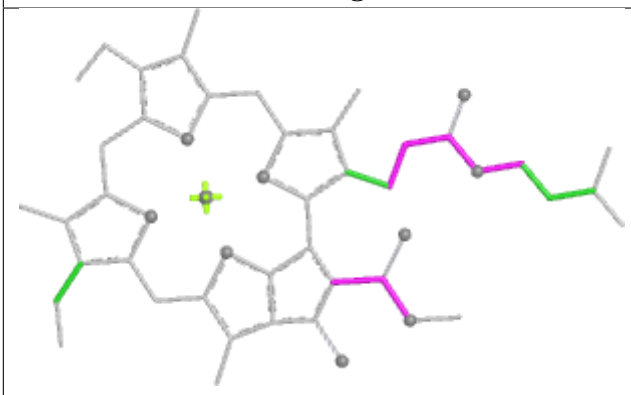
Ligand CLA B 824



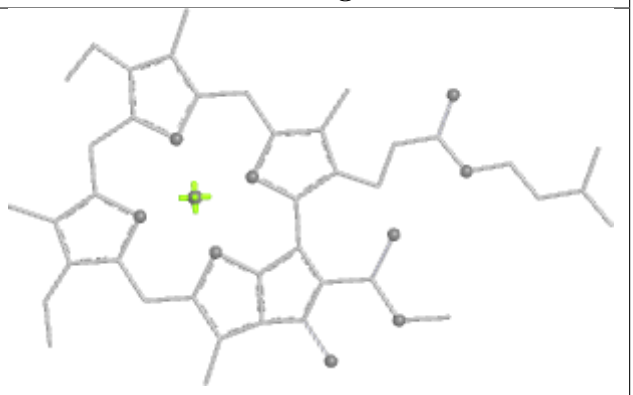
Bond lengths



Bond angles

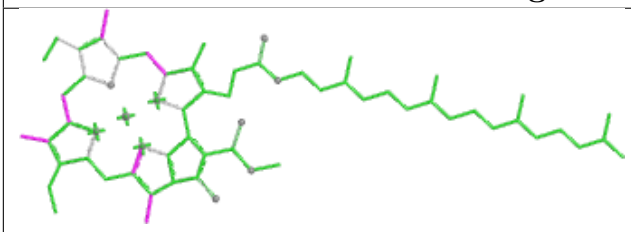


Torsions

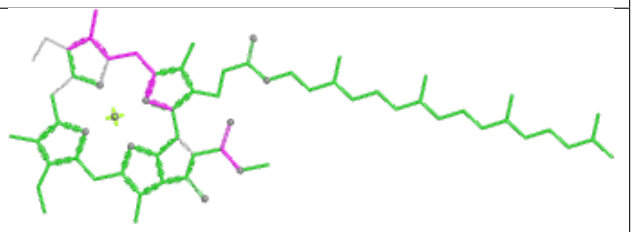


Rings

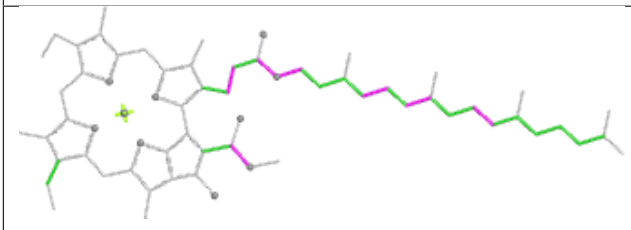
Ligand CLA 1 609



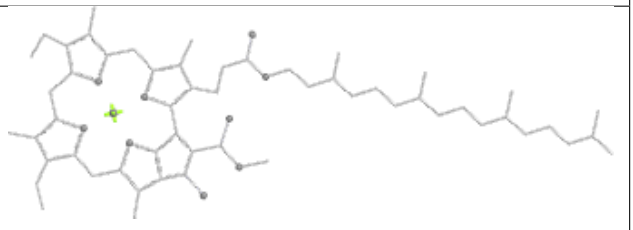
Bond lengths



Bond angles

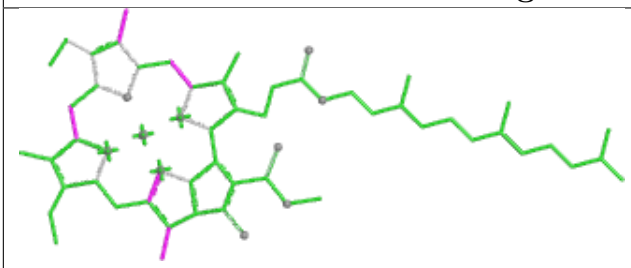


Torsions

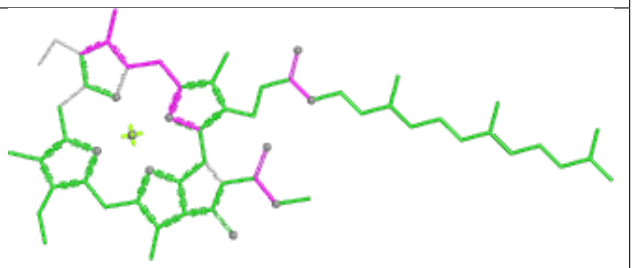


Rings

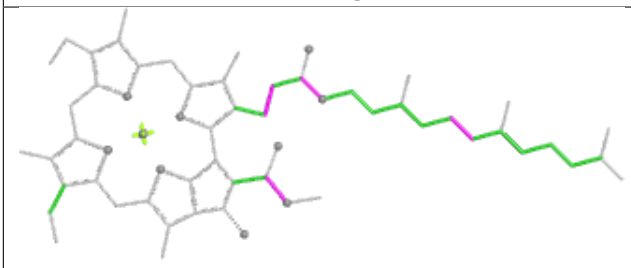
Ligand CLA F 5006



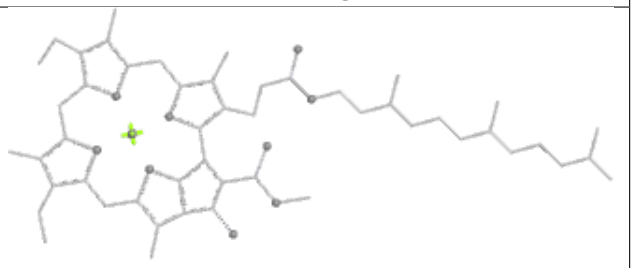
Bond lengths



Bond angles

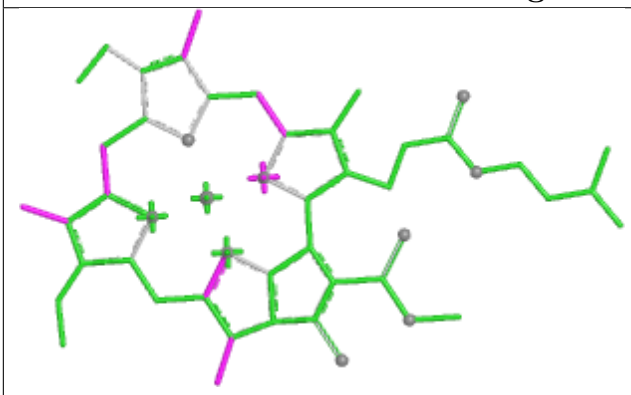


Torsions

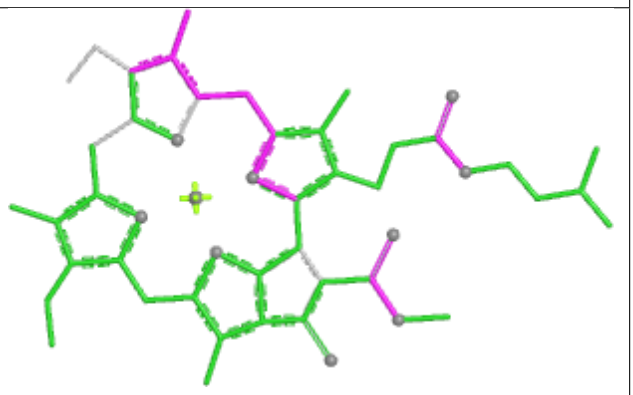


Rings

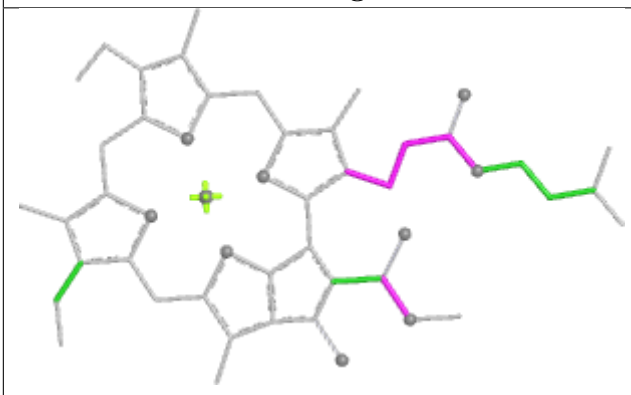
Ligand CLA b 603



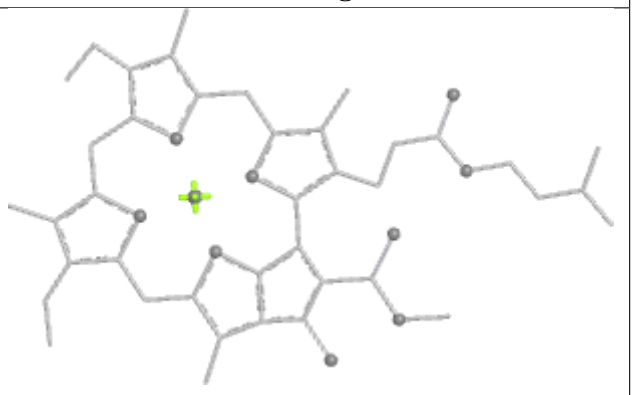
Bond lengths



Bond angles

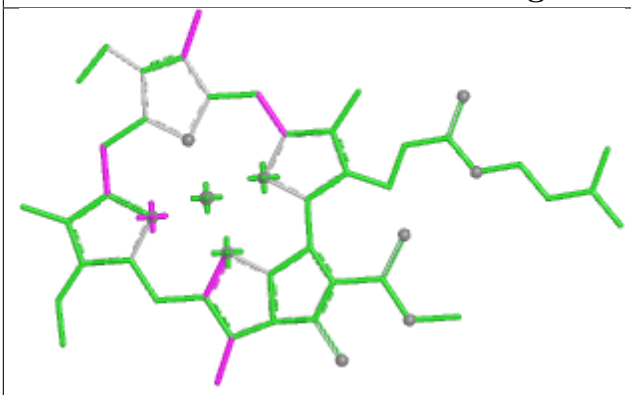


Torsions

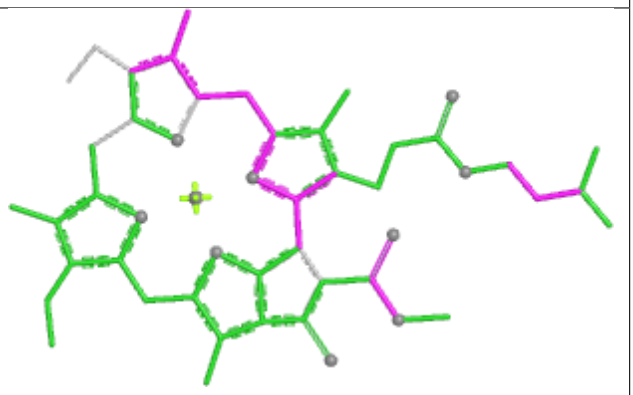


Rings

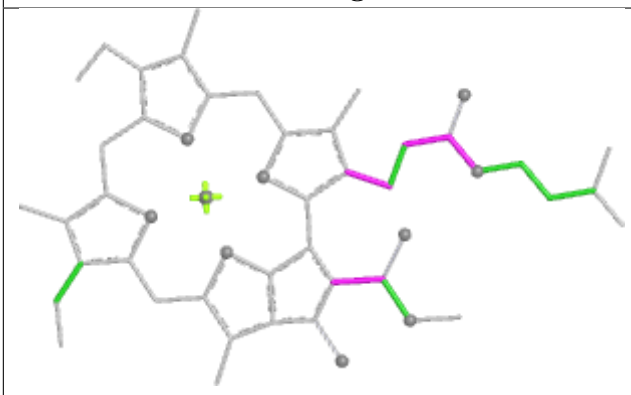
Ligand CLA b 611



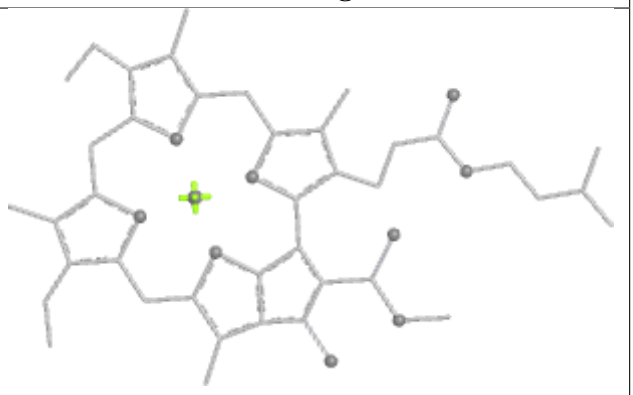
Bond lengths



Bond angles

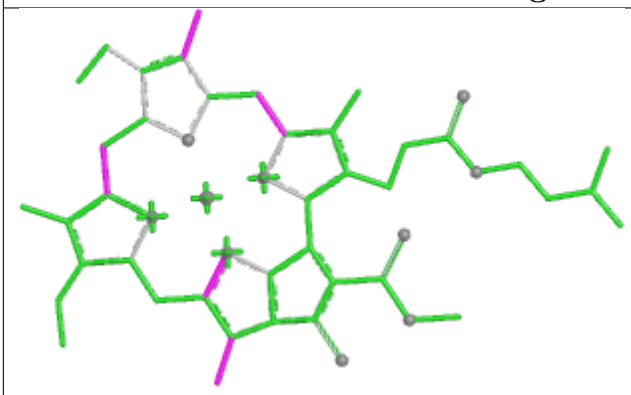


Torsions

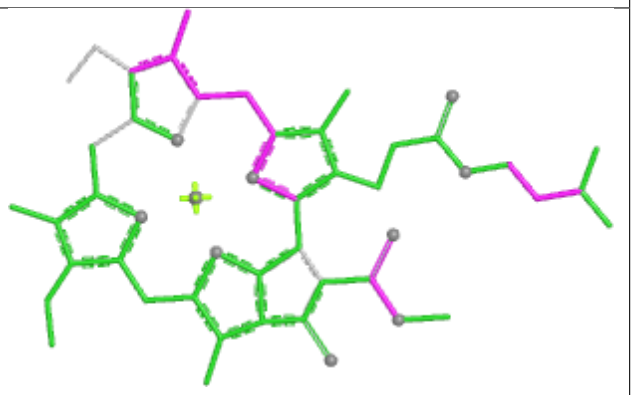


Rings

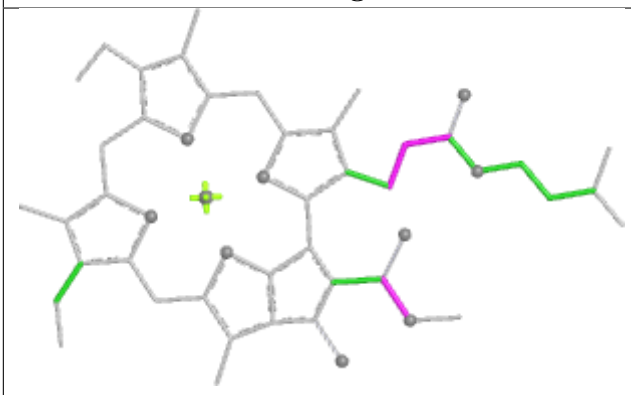
Ligand CLA c 311



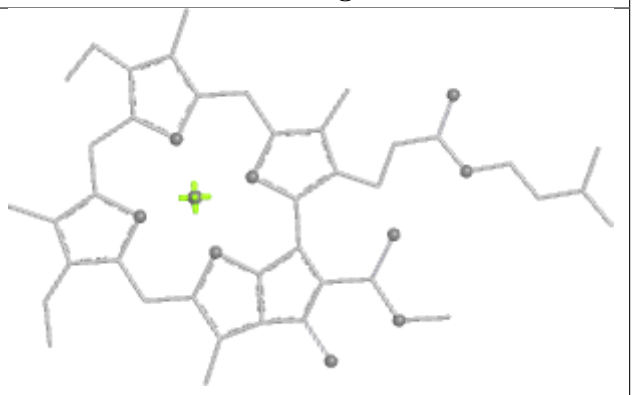
Bond lengths



Bond angles



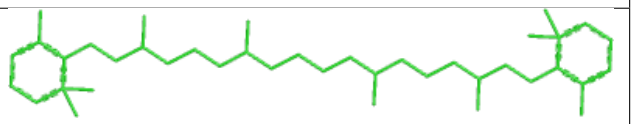
Torsions



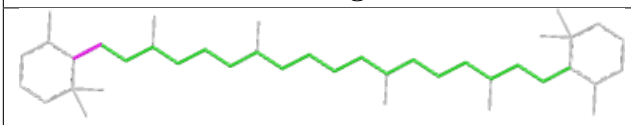
Rings

Ligand BCR A 5051

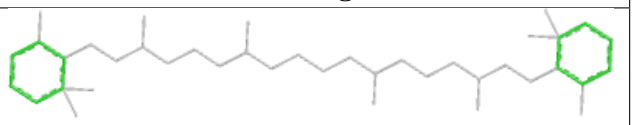
Bond lengths



Bond angles

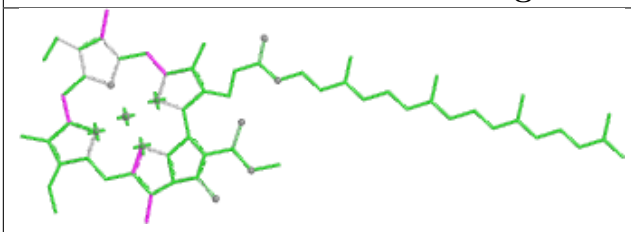


Torsions

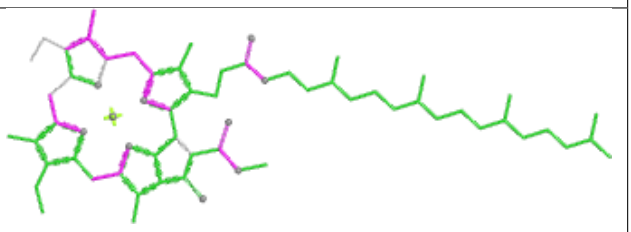


Rings

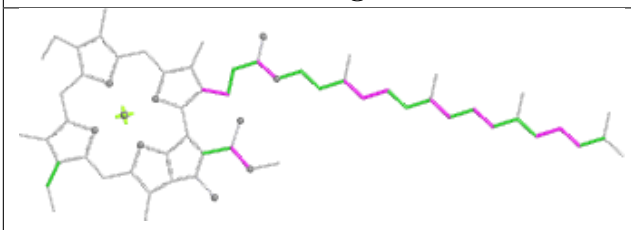
Ligand CLA A 5013



Bond lengths



Bond angles



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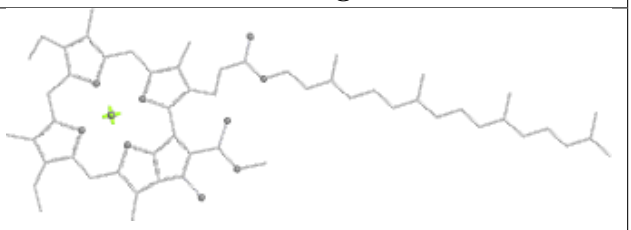
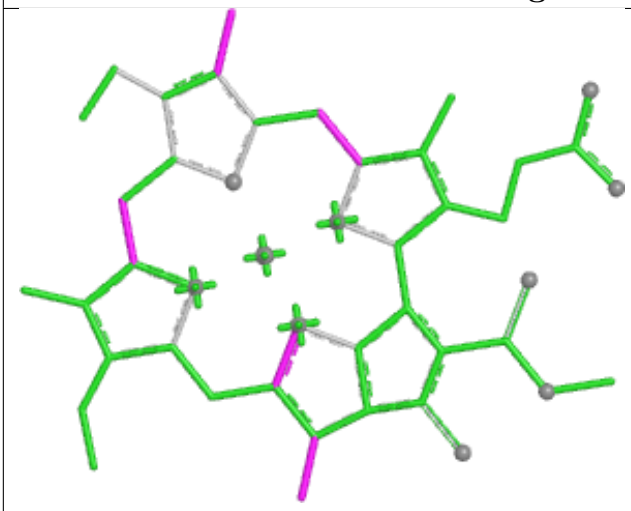
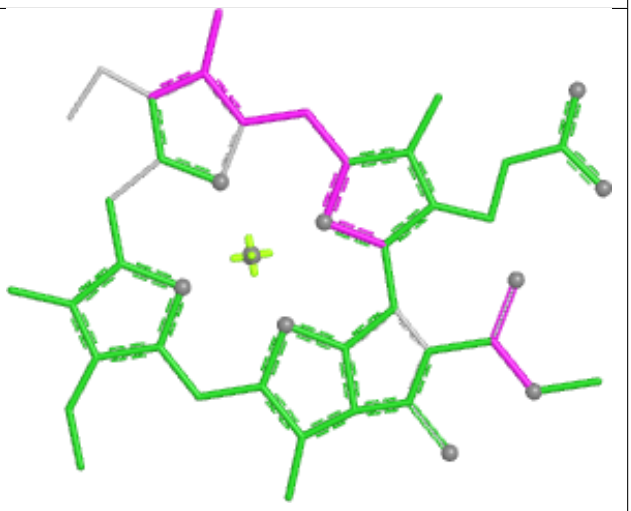


Rings

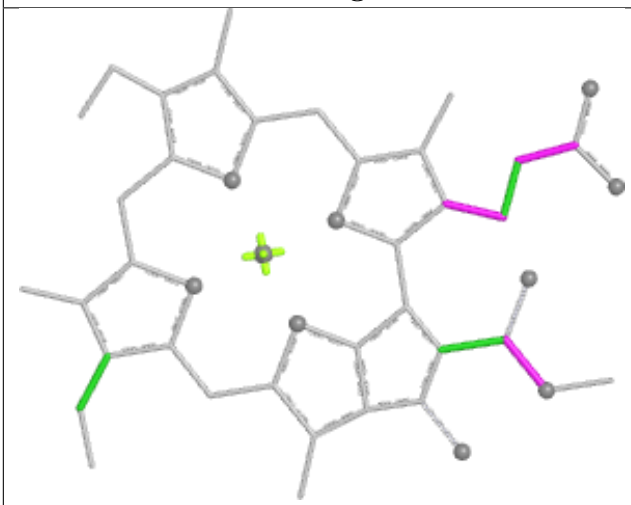
Ligand CLA 8 315



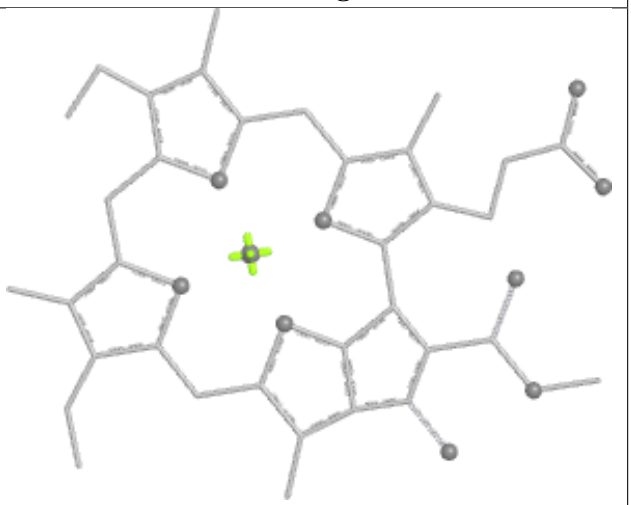
Bond lengths



Bond angles

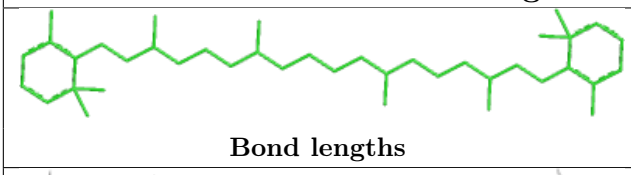


Torsions

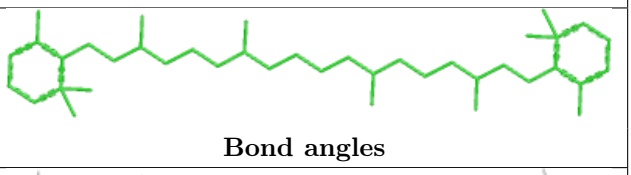


Rings

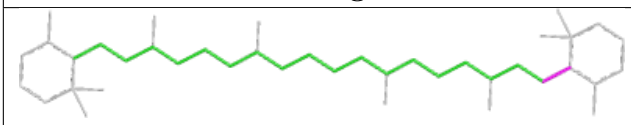
Ligand BCR B 847



Bond lengths



Bond angles



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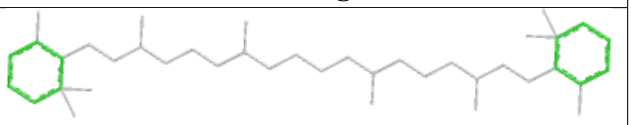
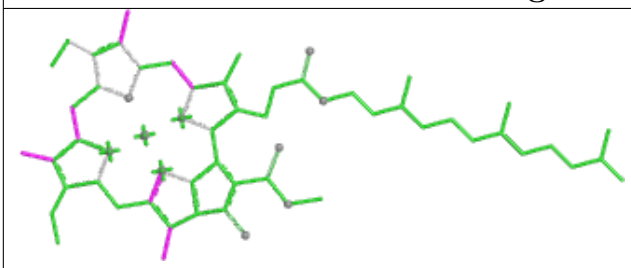
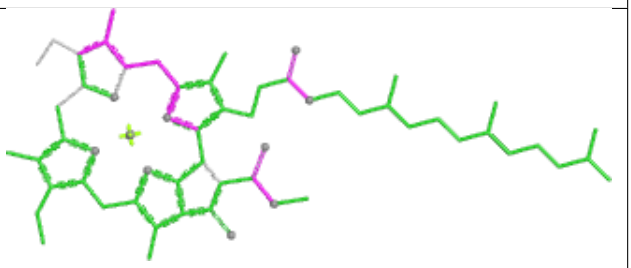


Rings

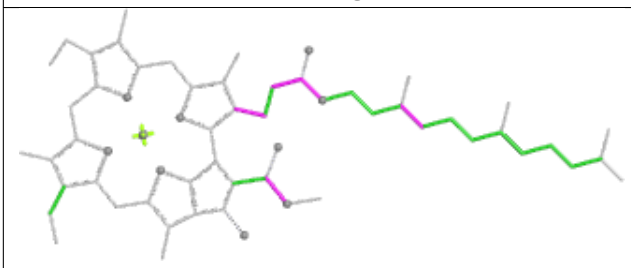
Ligand CLA a 609



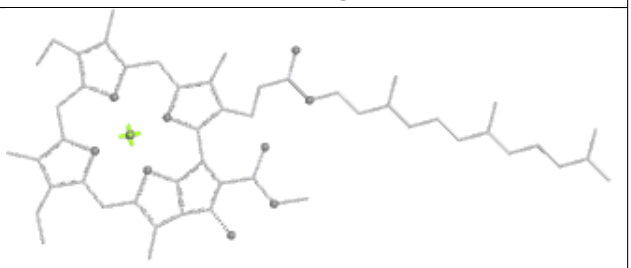
Bond lengths



Bond angles

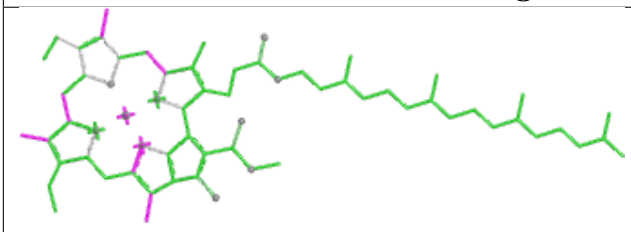


Torsions

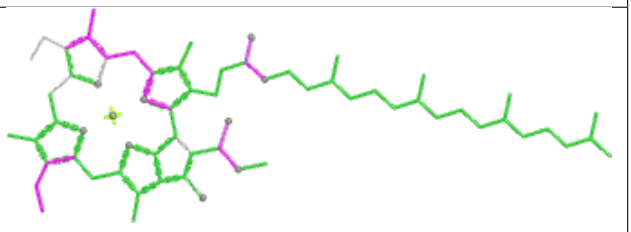


Rings

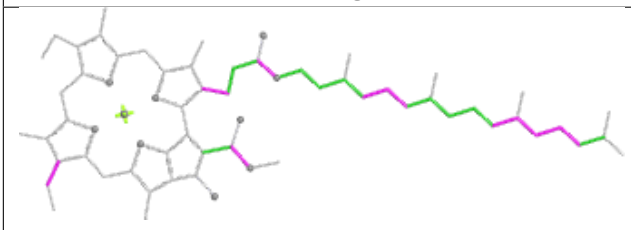
Ligand CLA A 5016



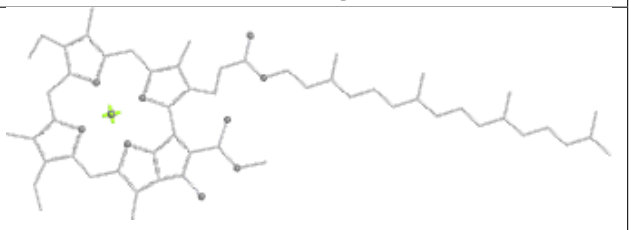
Bond lengths



Bond angles

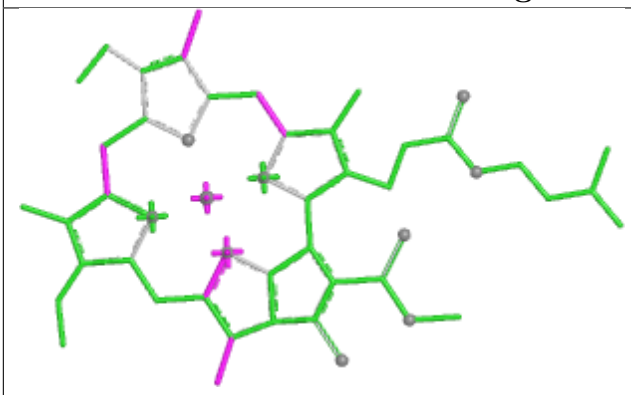


Torsions

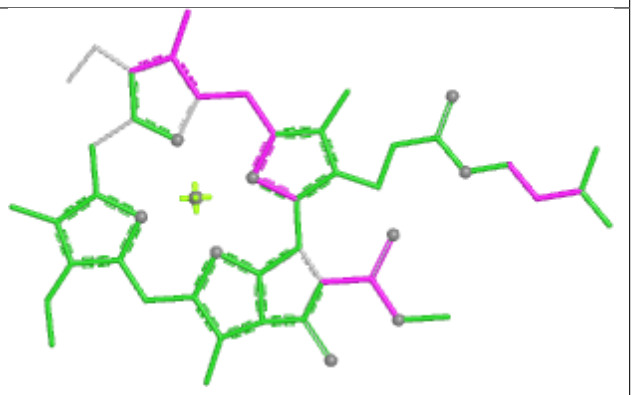


Rings

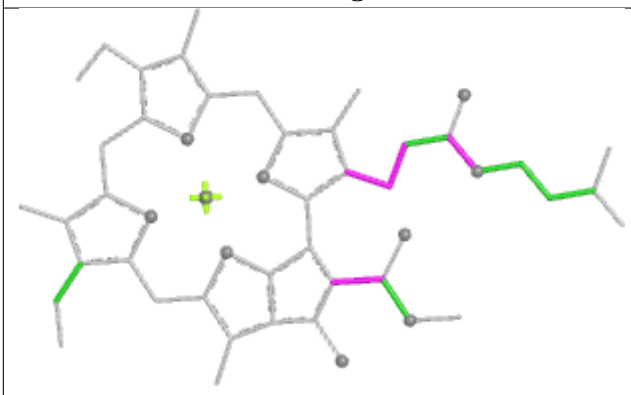
Ligand CLA A 5037



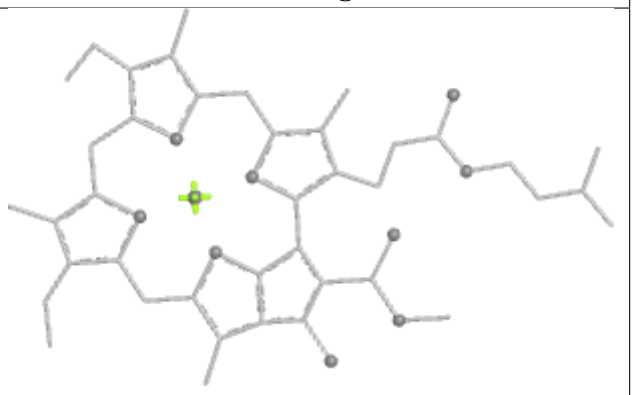
Bond lengths



Bond angles

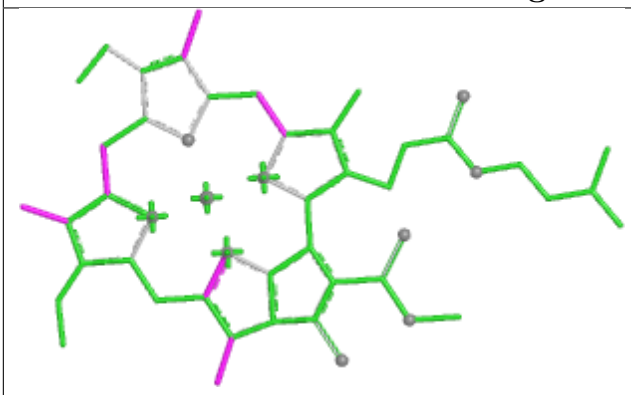


Torsions



Rings

Ligand CLA a 612



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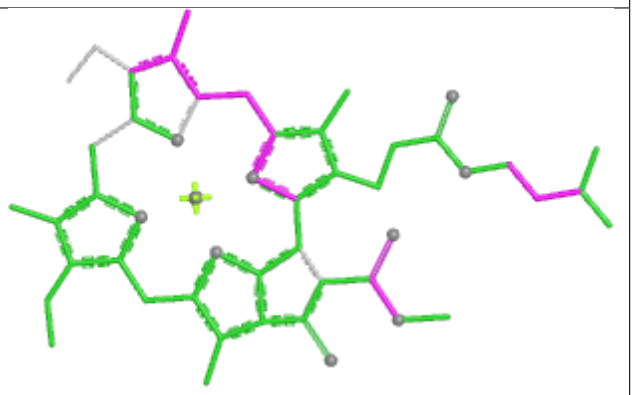
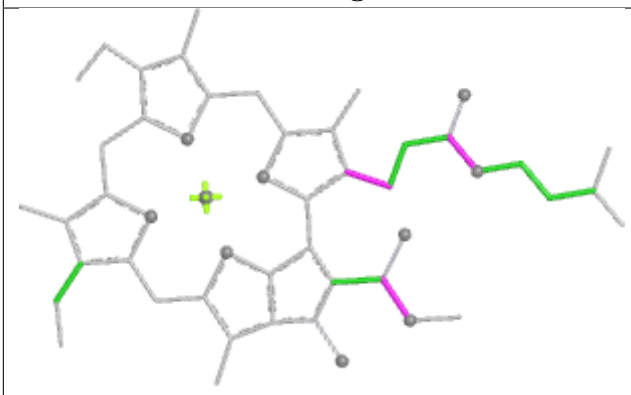
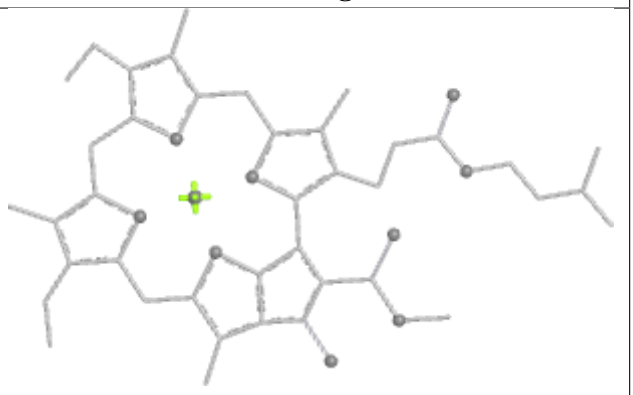


Bond angles

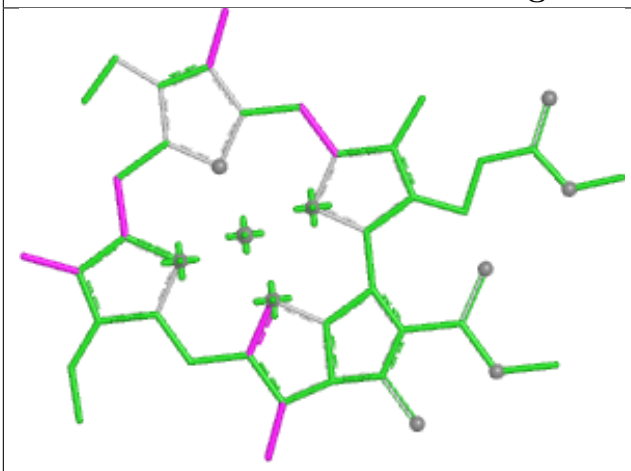


Torsions

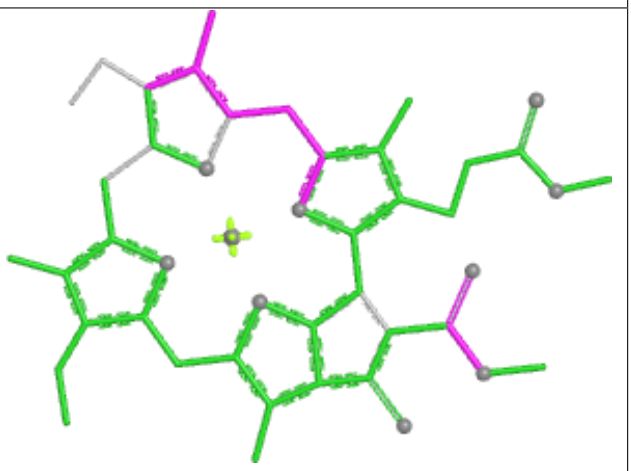


Rings

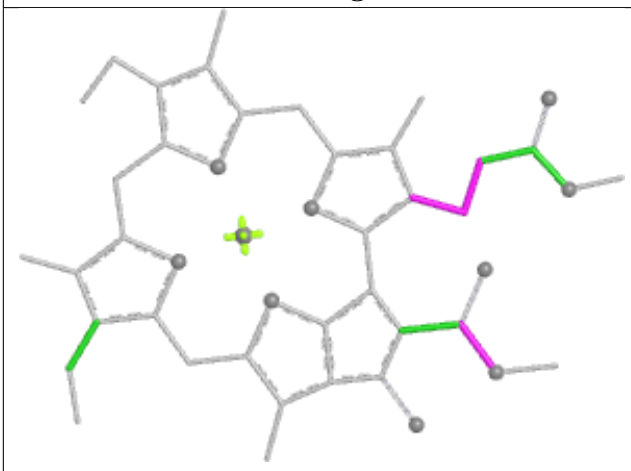
Ligand CLA 7 309



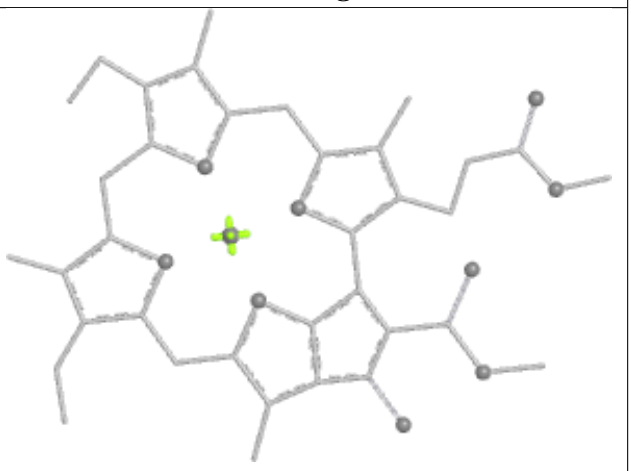
Bond lengths



Bond angles

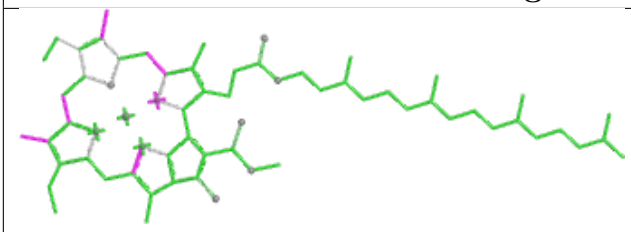


Torsions

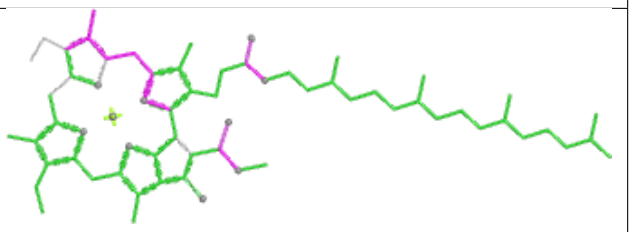


Rings

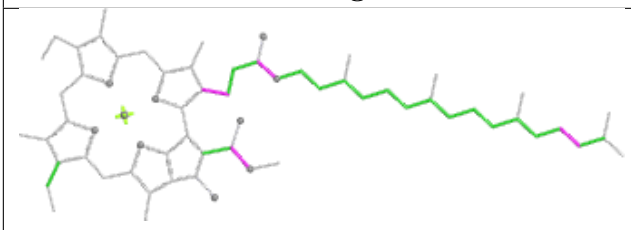
Ligand CLA B 826



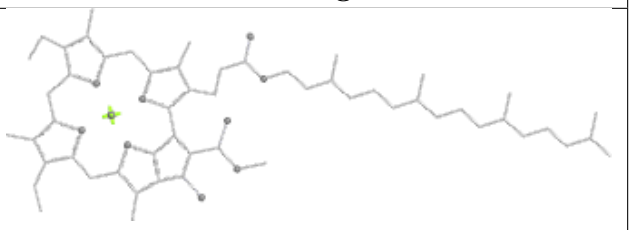
Bond lengths



Bond angles

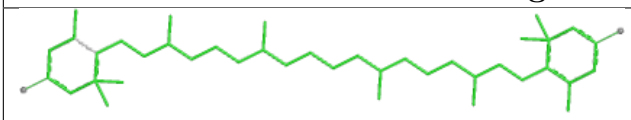


Torsions

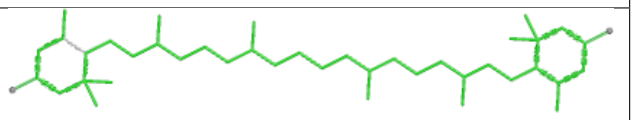


Rings

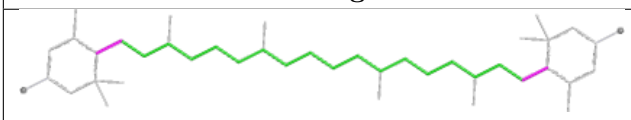
Ligand LUT 3 315



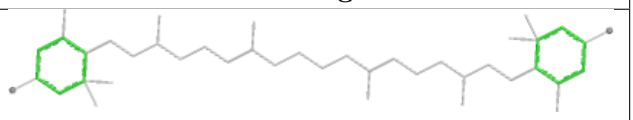
Bond lengths



Bond angles

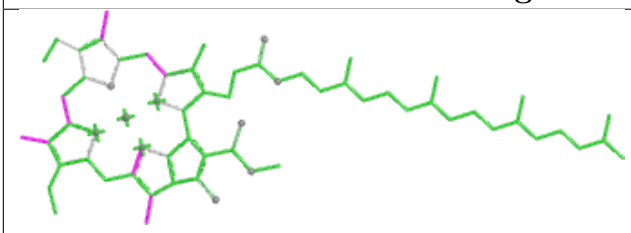


Torsions

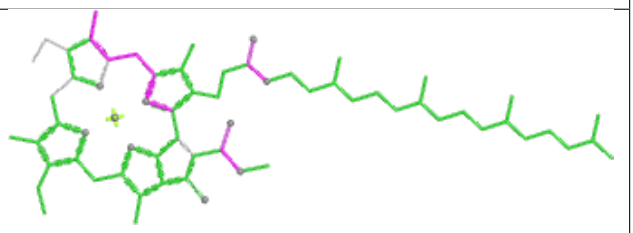


Rings

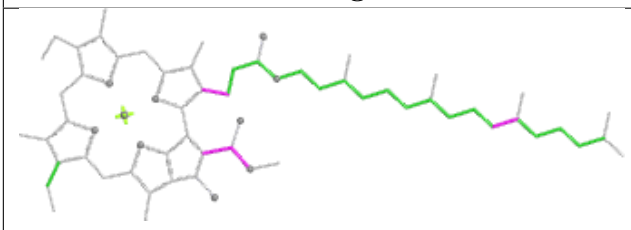
Ligand CLA A 5031



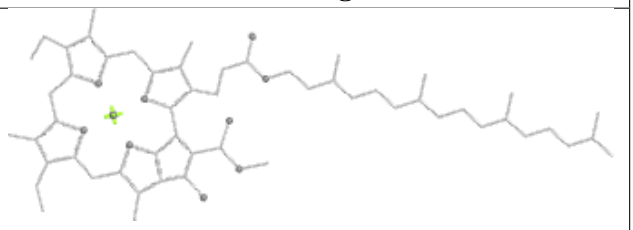
Bond lengths



Bond angles

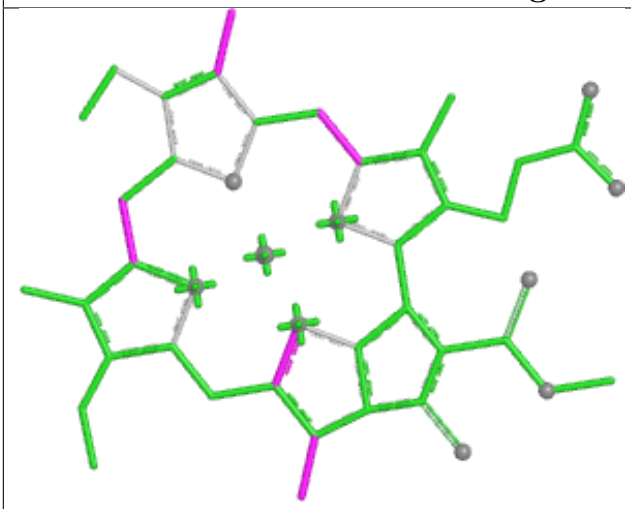


Torsions

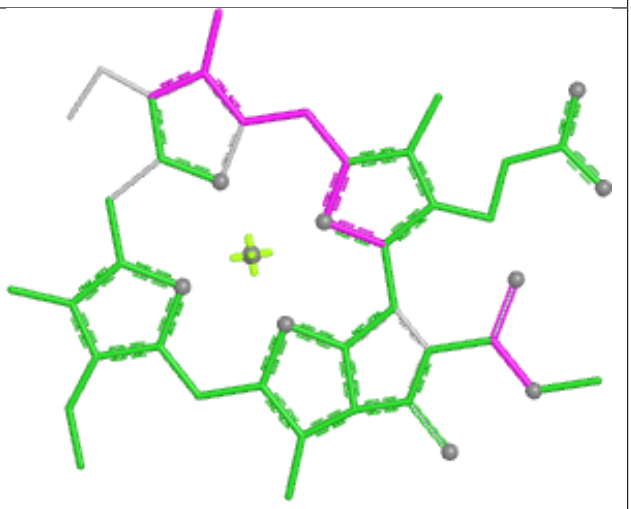


Rings

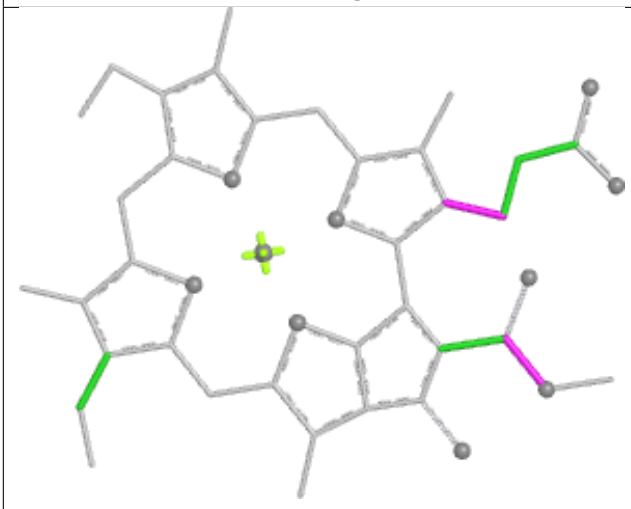
Ligand CLA c 313



Bond lengths



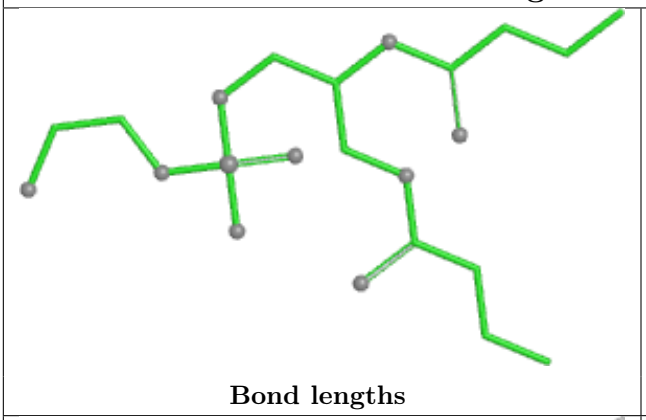
Bond angles



Torsions

Rings

Ligand LHG a 618



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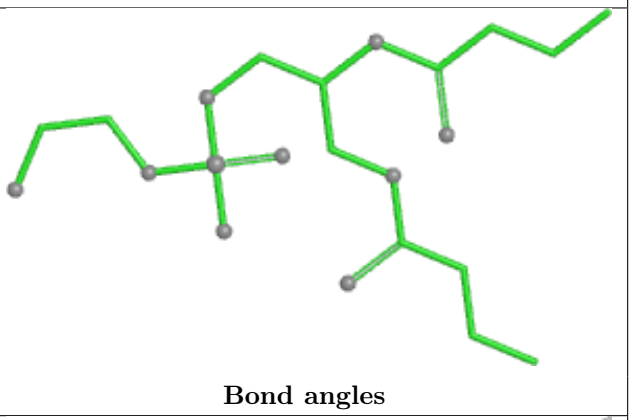
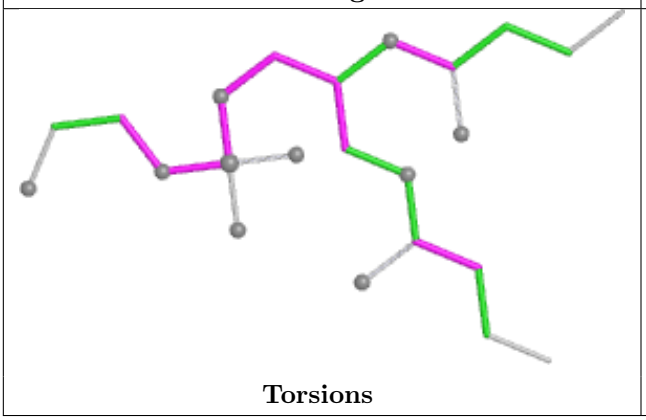


Bond angles



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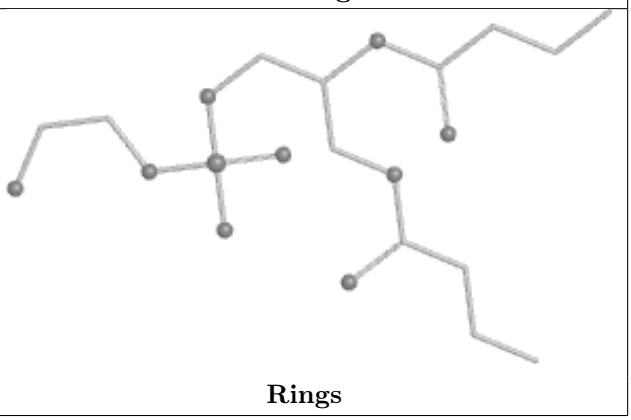
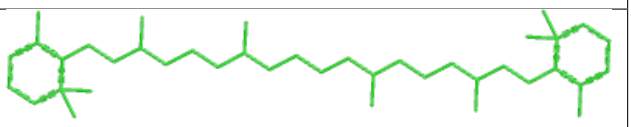


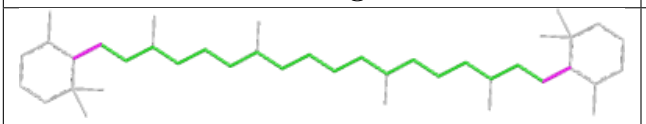
Rings

Ligand BCR 7 317

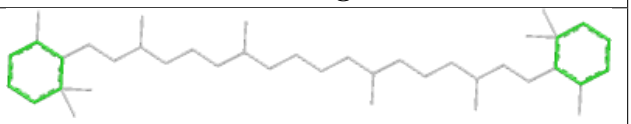
Bond lengths



Bond angles

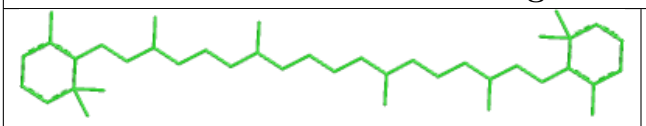


Torsions

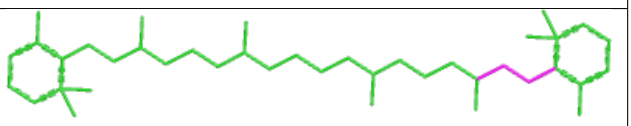


Rings

Ligand BCR c 316

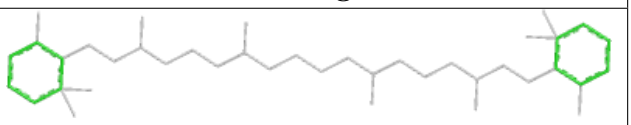


Bond lengths



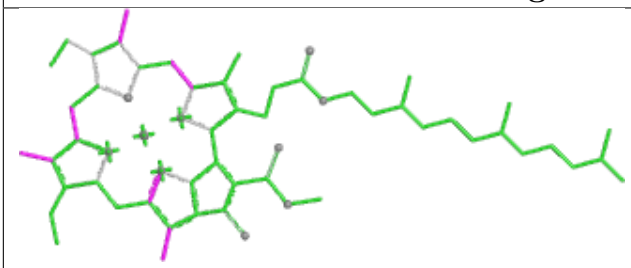
Bond angles

Torsions

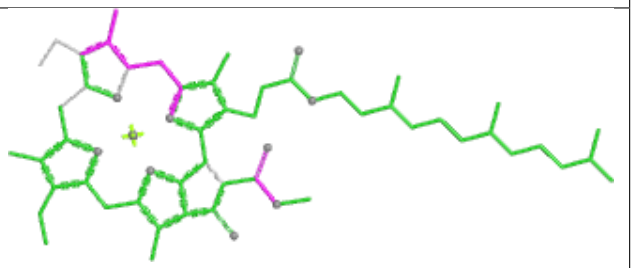


Rings

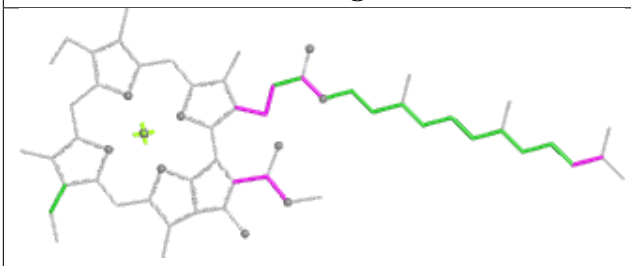
Ligand CLA 7 302



Bond lengths



Bond angles



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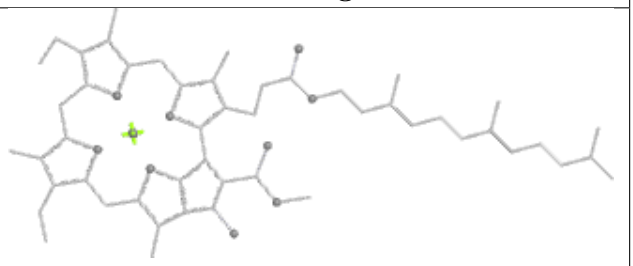
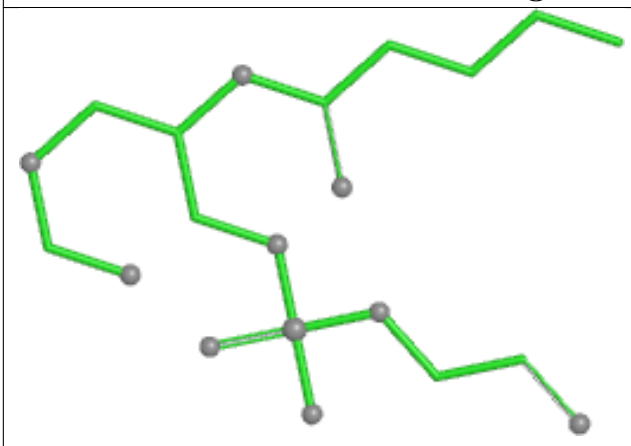
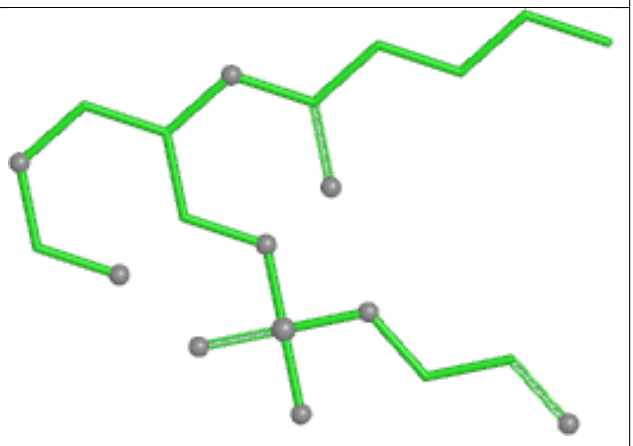


Rings

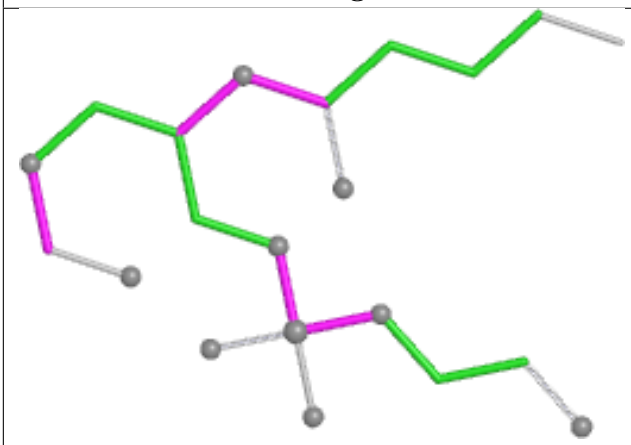
Ligand PTY 8 320



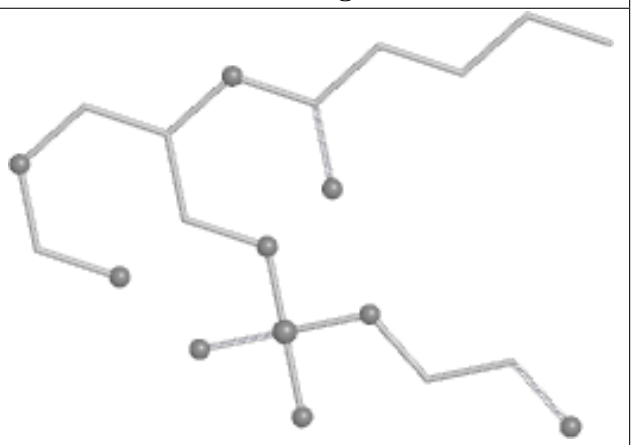
Bond lengths



Bond angles

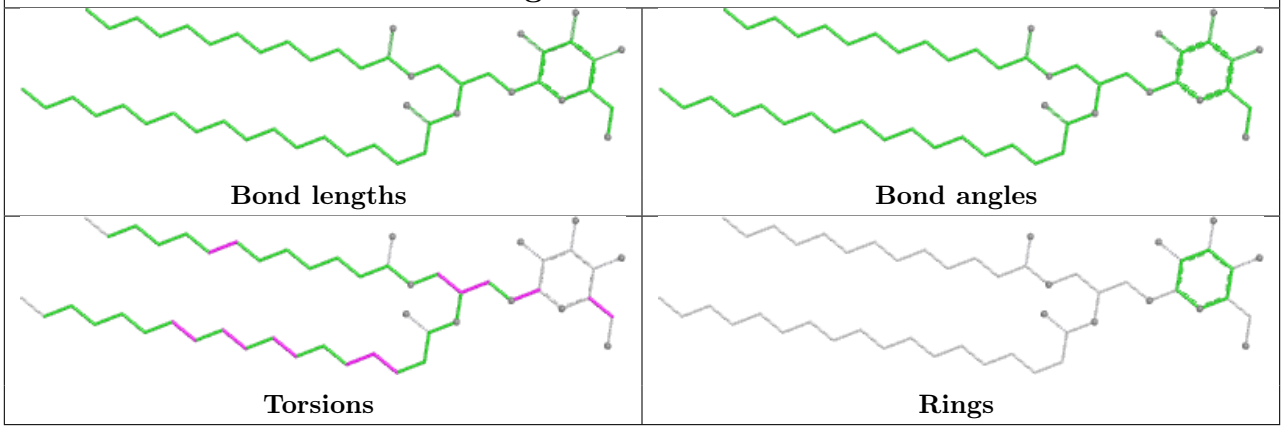


Torsions

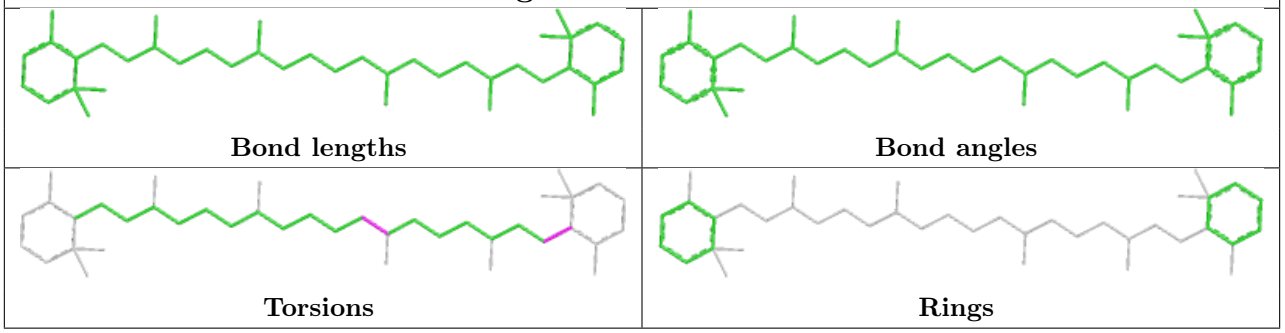


Rings

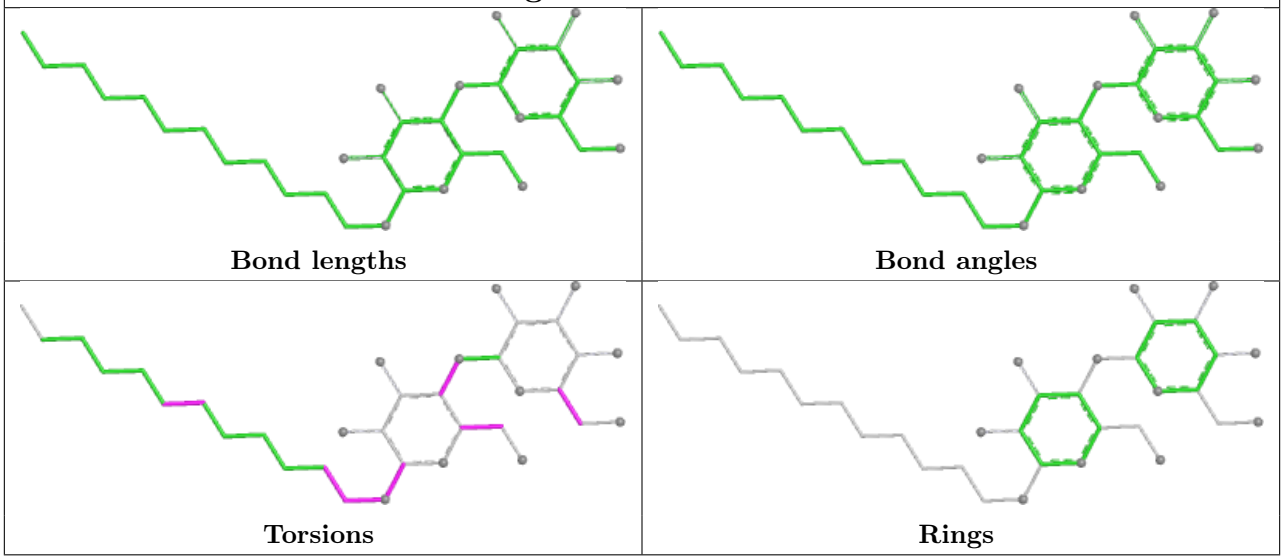
Ligand LMG 7 301



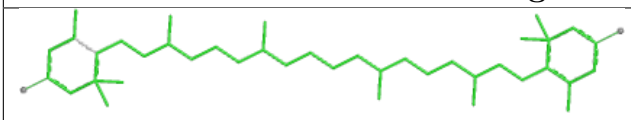
Ligand BCR F 5010



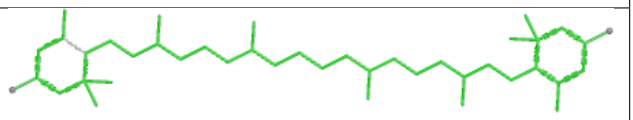
Ligand LMU 7 319



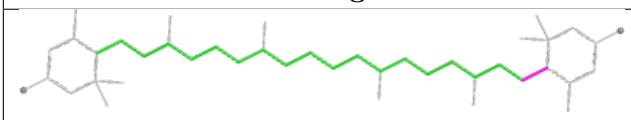
Ligand LUT 8 316



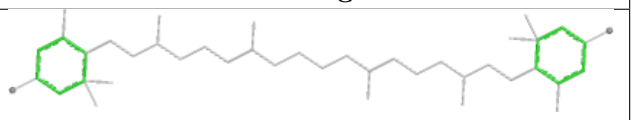
Bond lengths



Bond angles

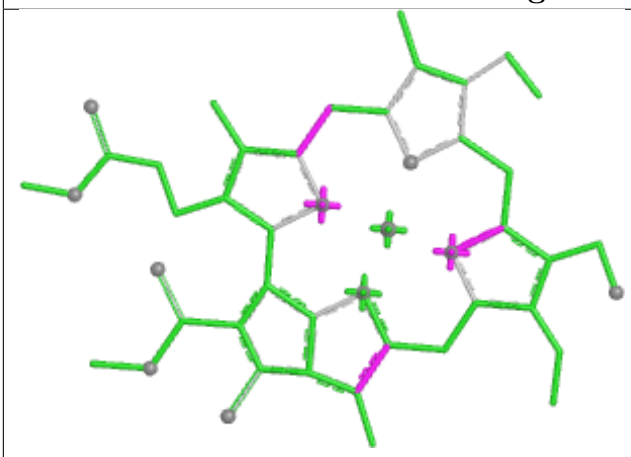


Torsions

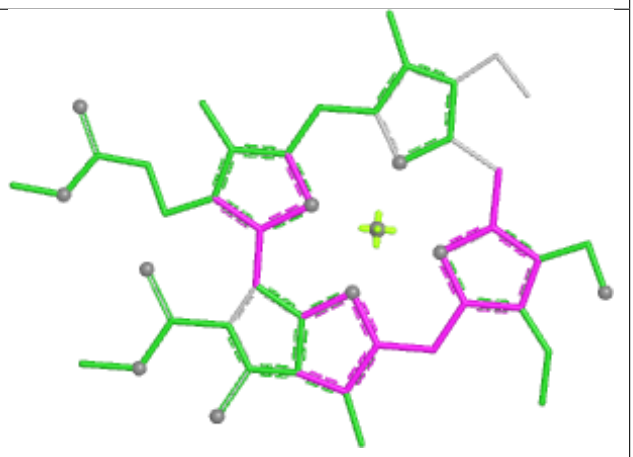


Rings

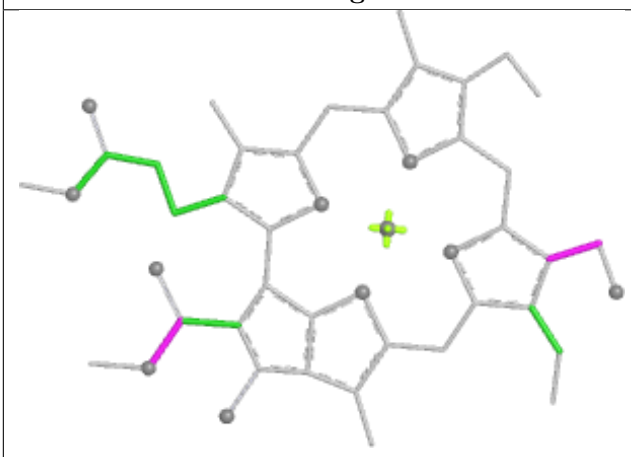
Ligand CHL a 606



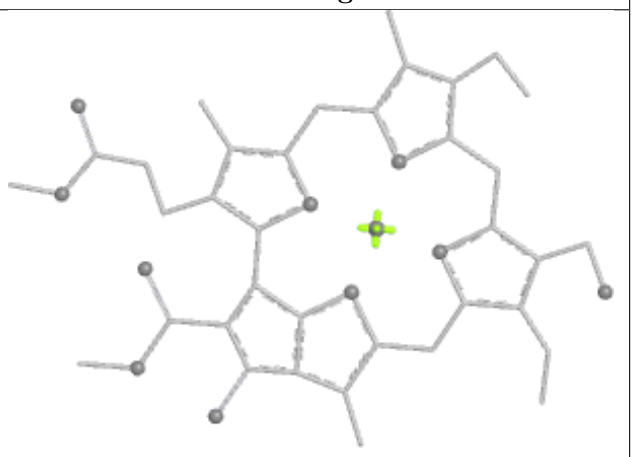
Bond lengths



Bond angles



Torsions

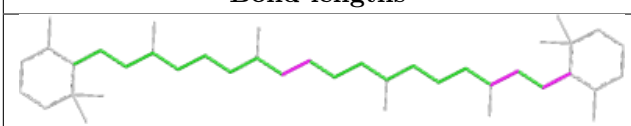


Rings

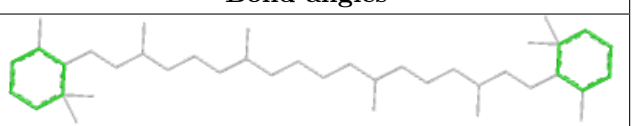
Ligand BCR a 617

Bond lengths

Bond angles

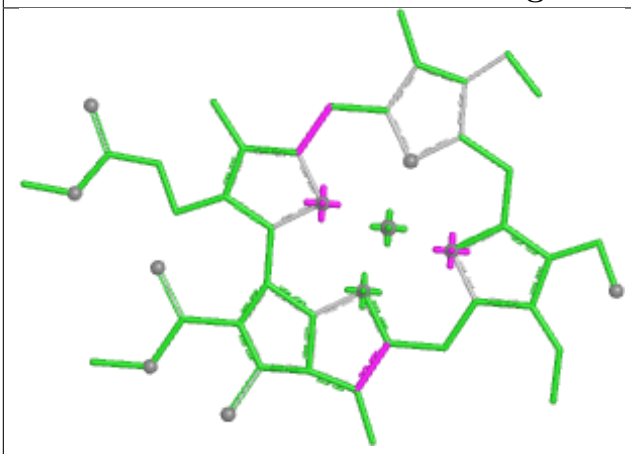


Torsions

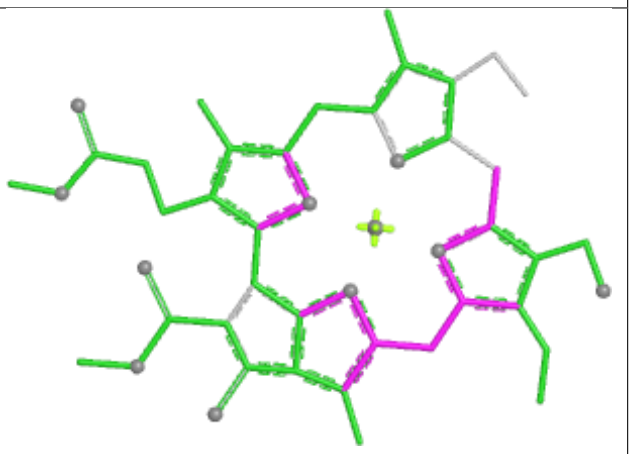


Rings

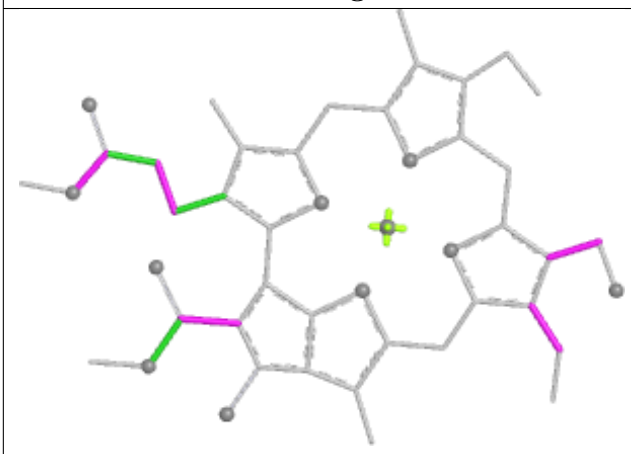
Ligand CHL b 605



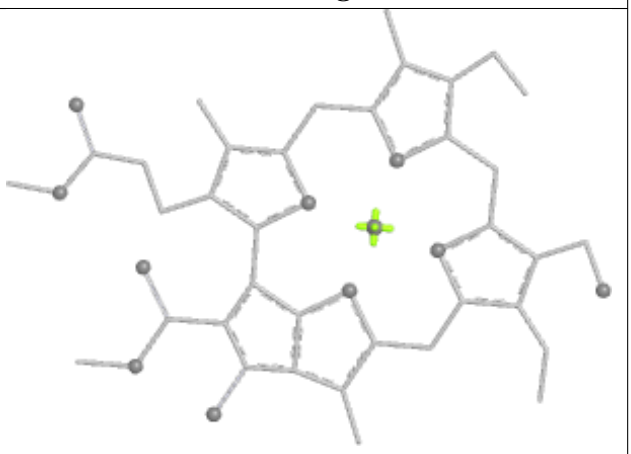
Bond lengths



Bond angles

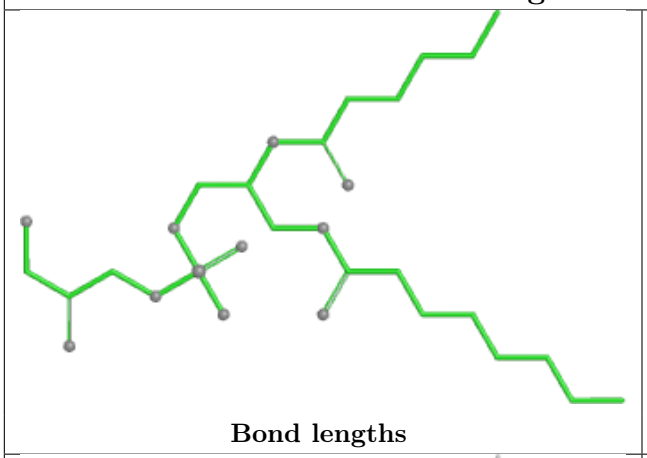


Torsions

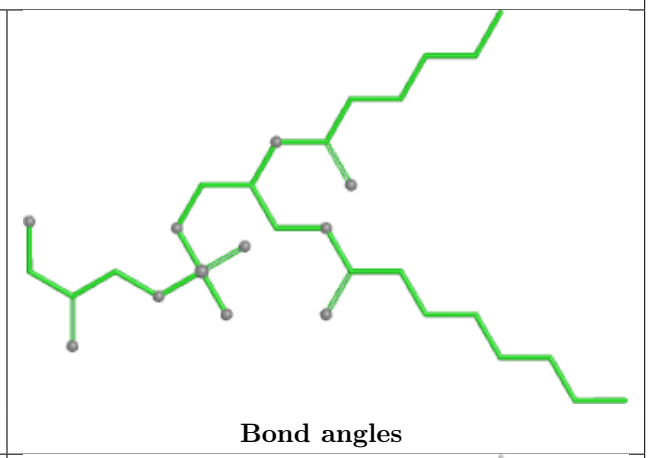


Rings

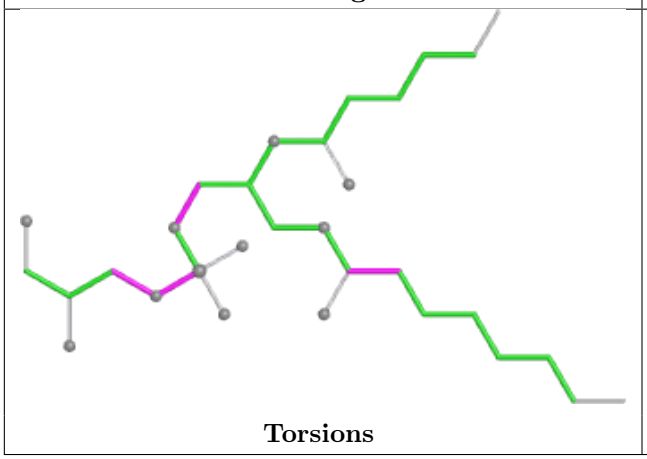
Ligand LHG 1 619



Bond lengths



Bond angles



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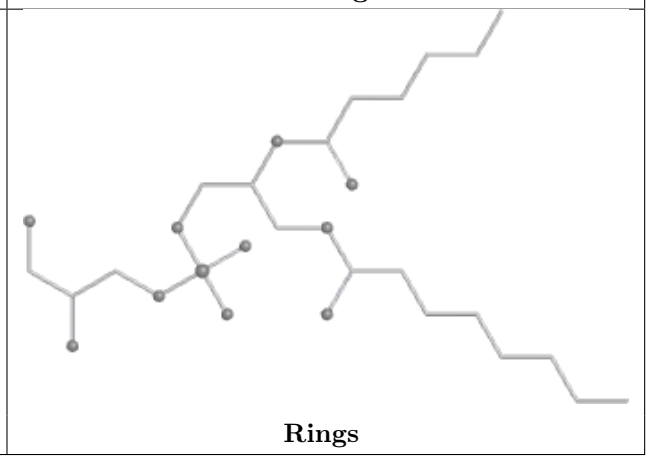
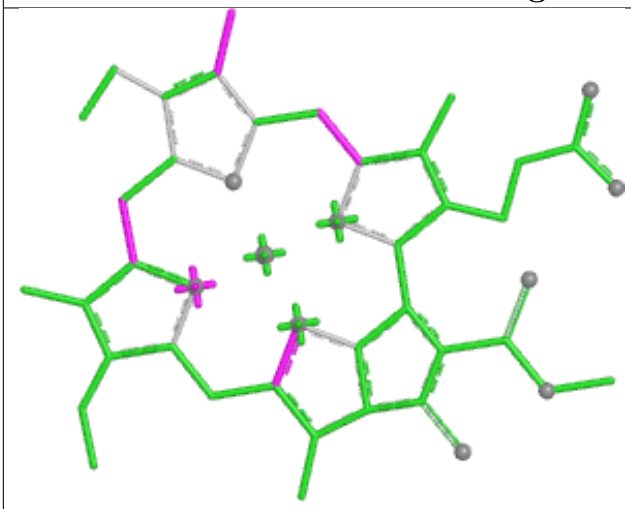
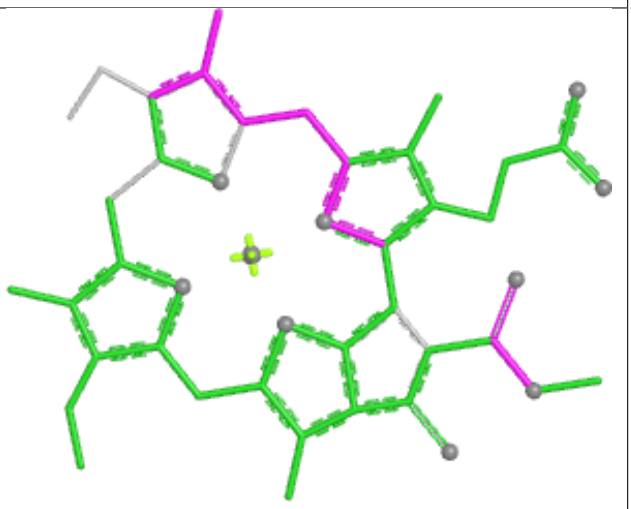


Rings

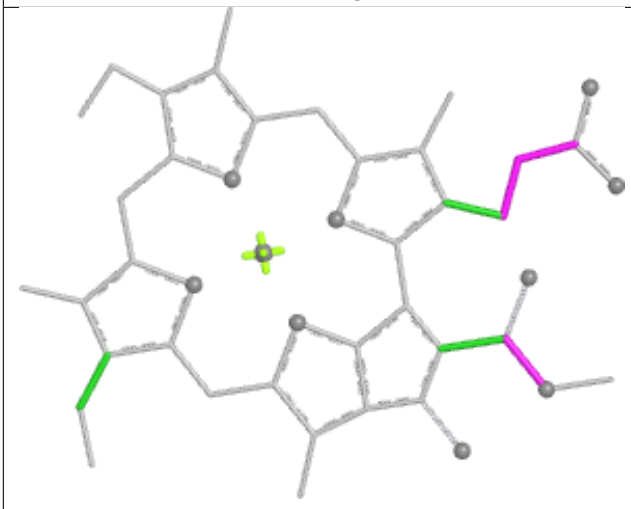
Ligand CLA 1 605



Bond lengths



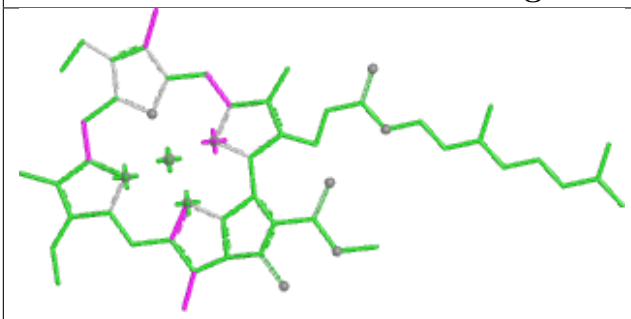
Bond angles



Torsions

Rings

Ligand CLA B 828



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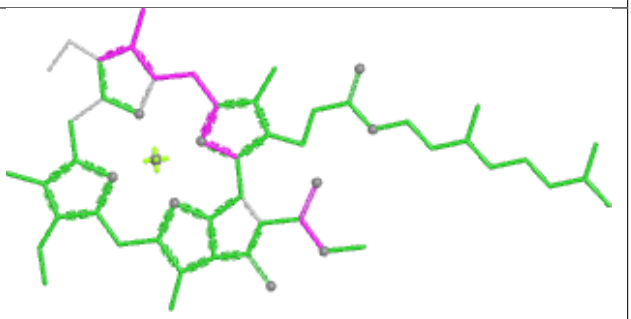
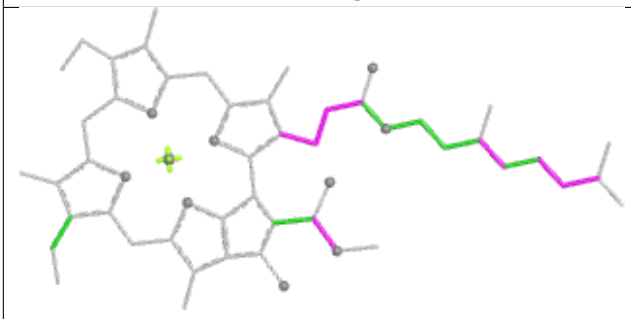
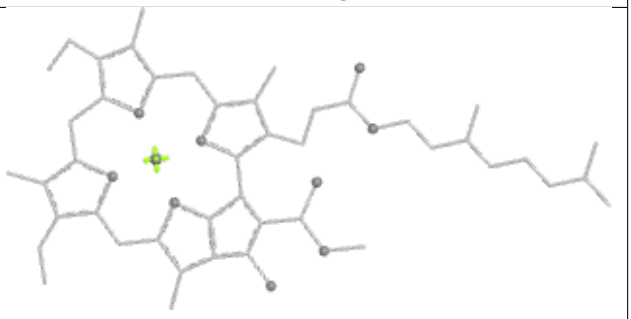


Bond angles

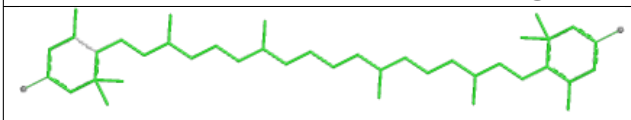


Torsions

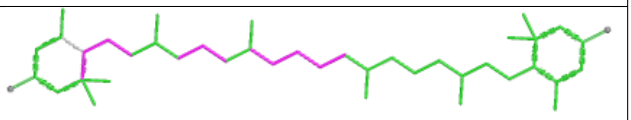


Rings

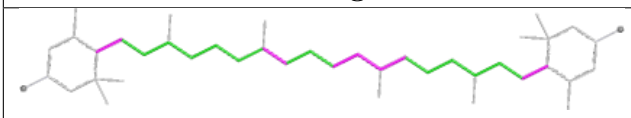
Ligand LUT a 615



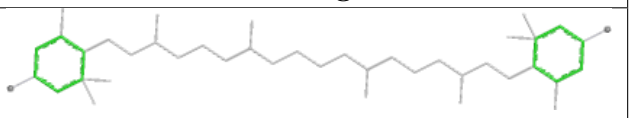
Bond lengths



Bond angles

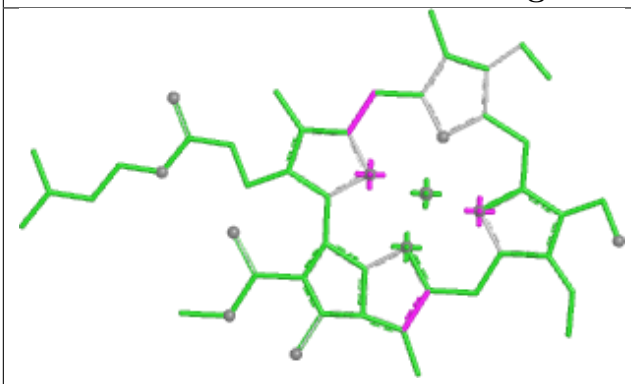


Torsions

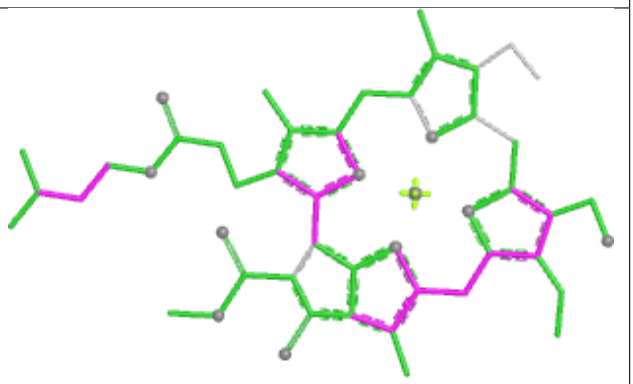


Rings

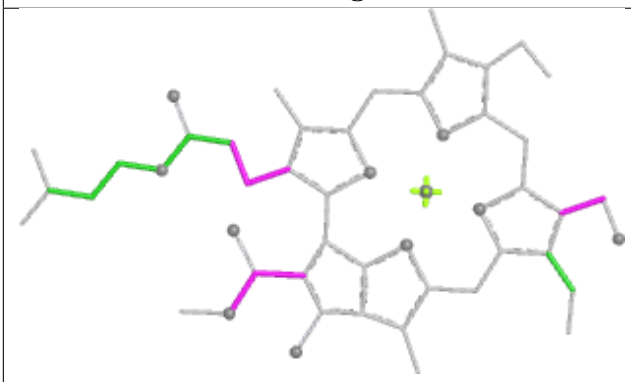
Ligand CHL 1 601



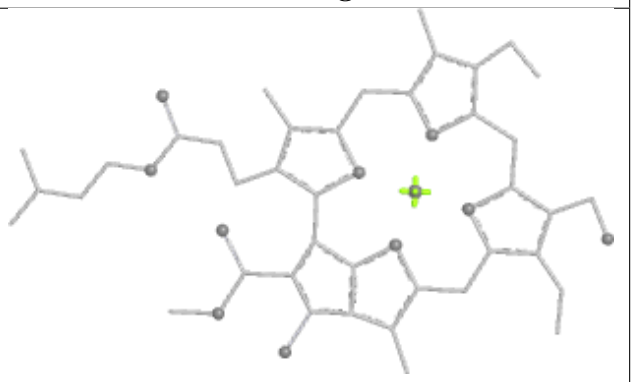
Bond lengths



Bond angles

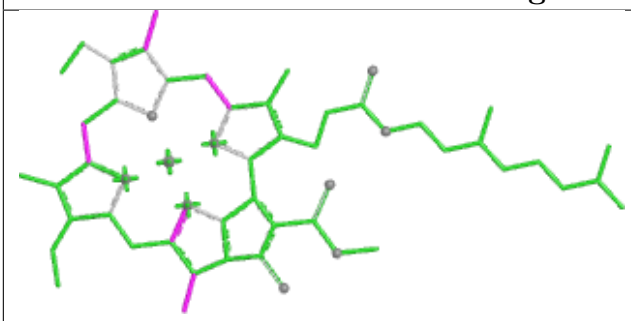


Torsions

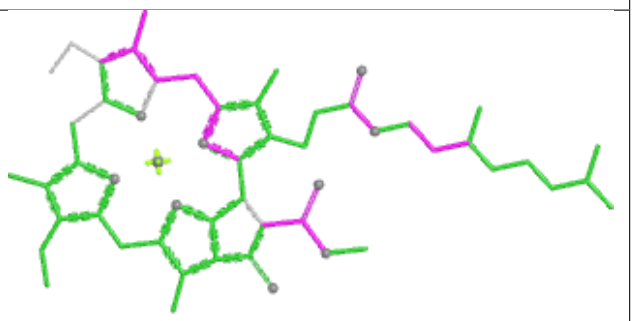


Rings

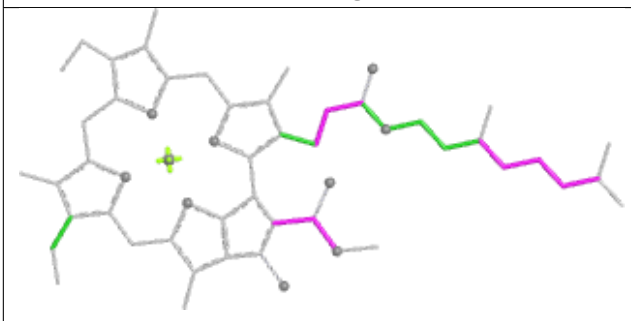
Ligand CLA 1 602



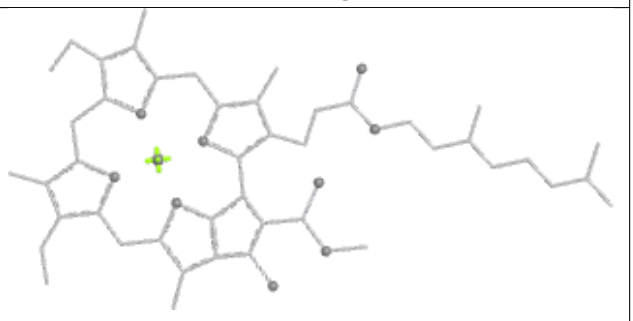
Bond lengths



Bond angles

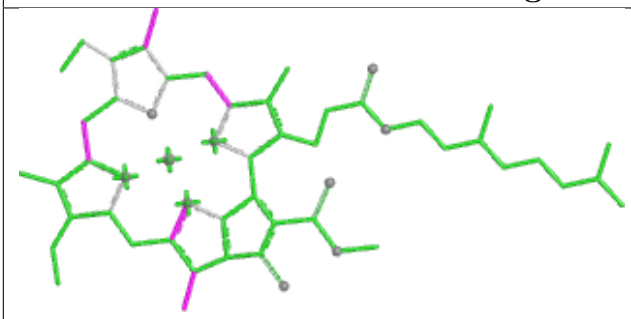


Torsions

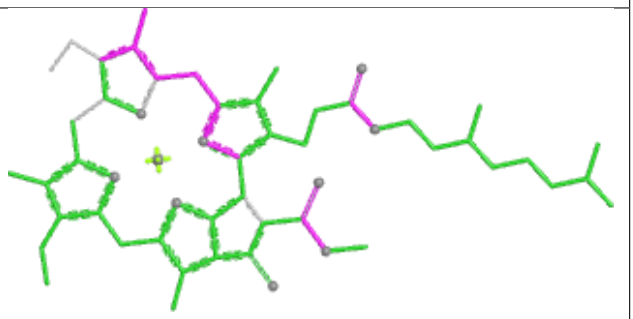


Rings

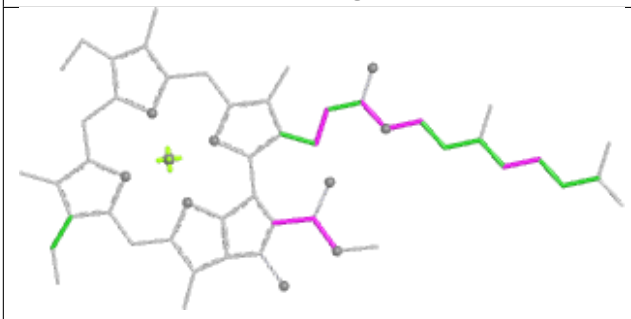
Ligand CLA B 807



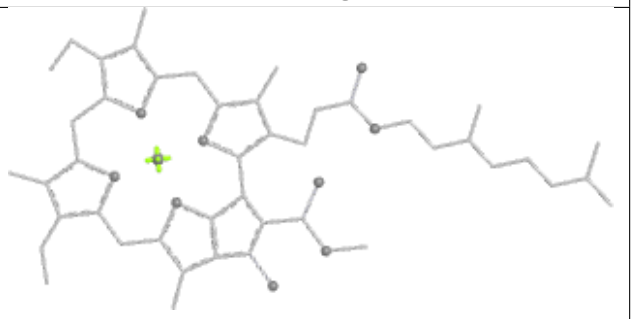
Bond lengths



Bond angles

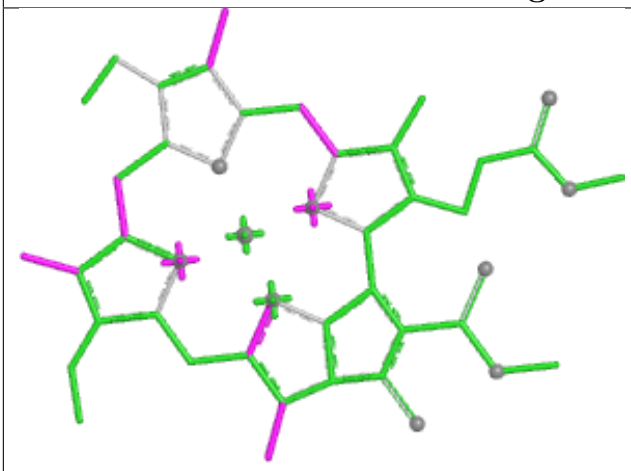


Torsions

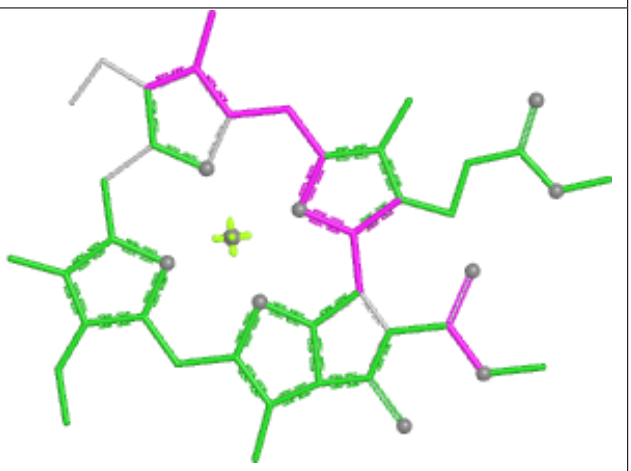


Rings

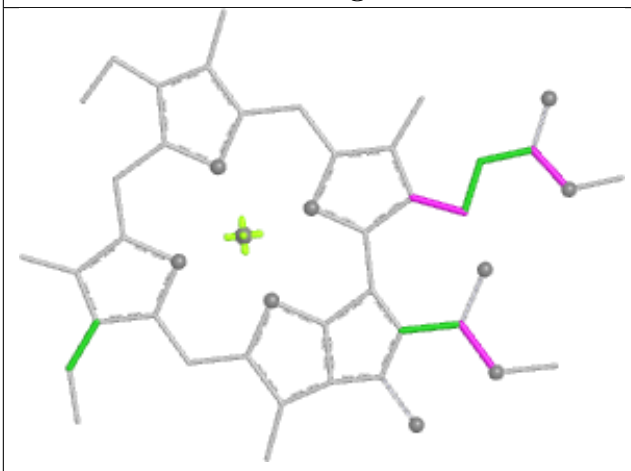
Ligand CLA 1 611



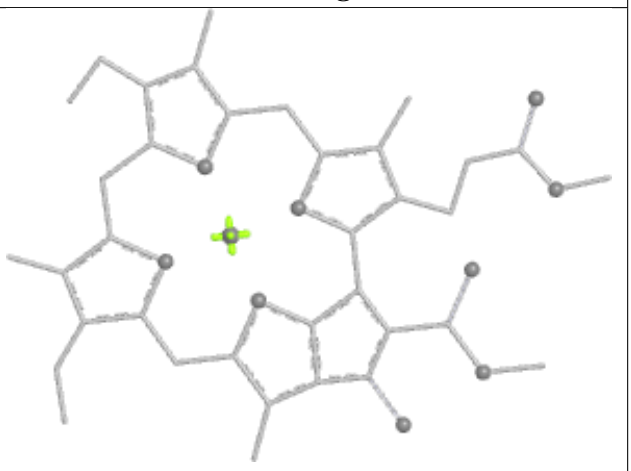
Bond lengths



Bond angles

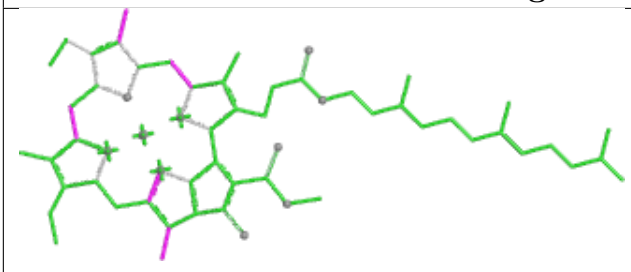


Torsions

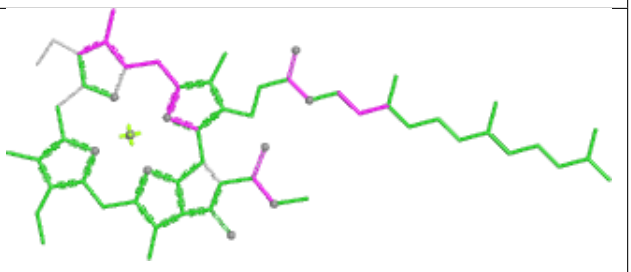


Rings

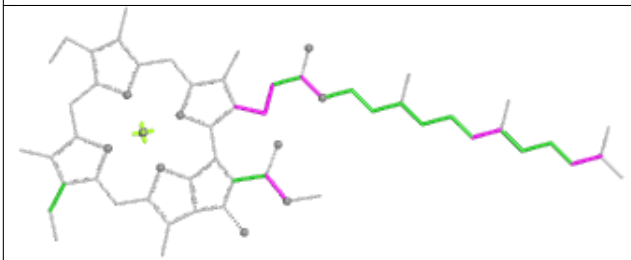
Ligand CLA 1 612



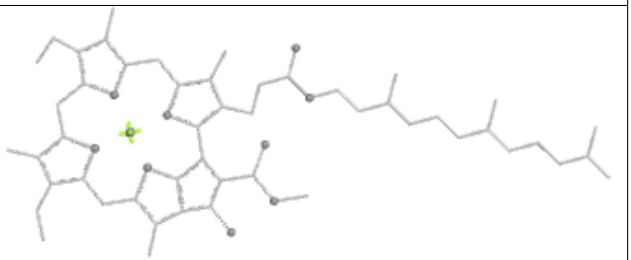
Bond lengths



Bond angles

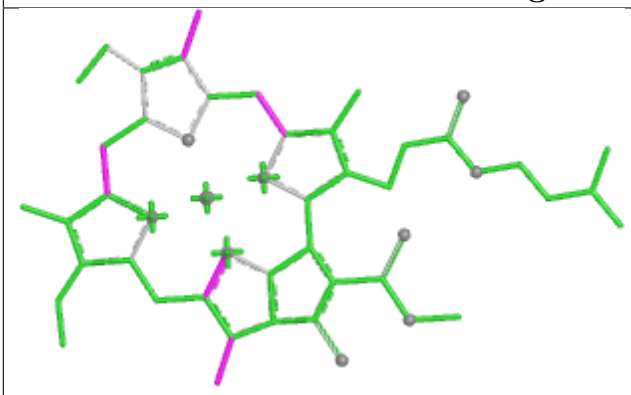


Torsions



Rings

Ligand CLA 8 303



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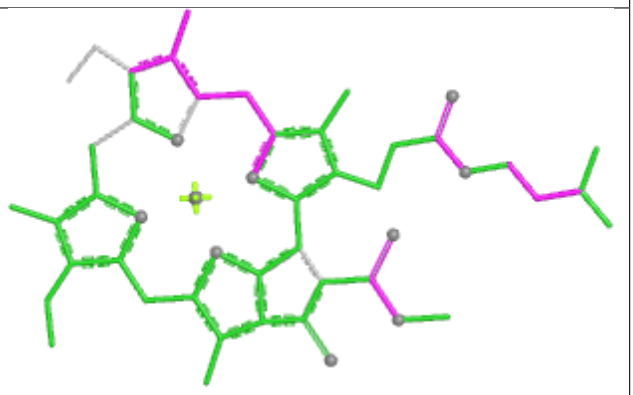
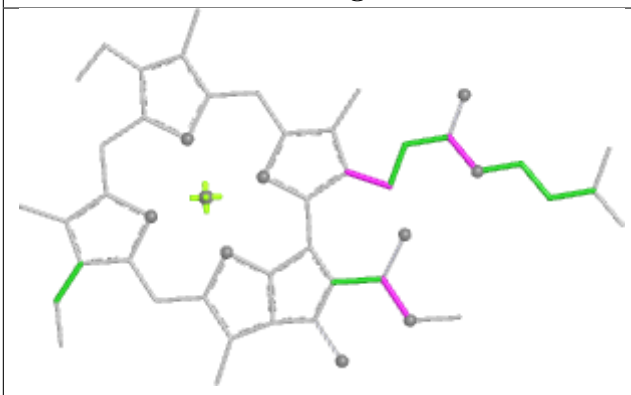
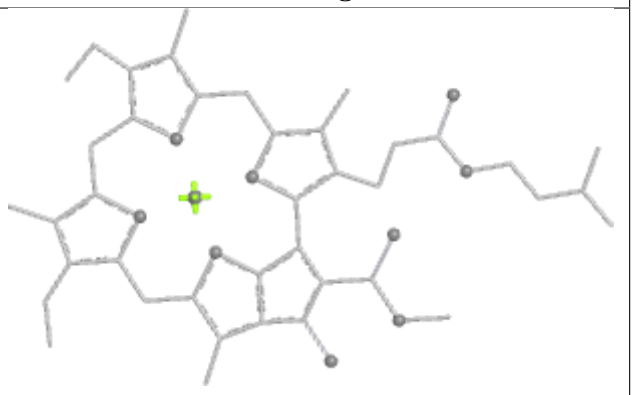


Bond angles

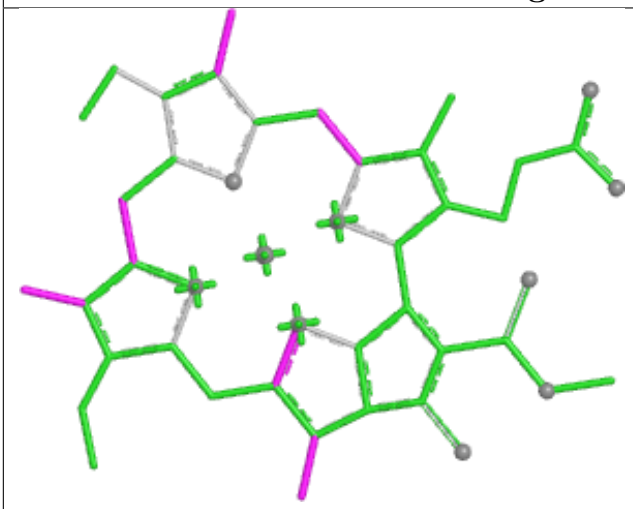


Torsions

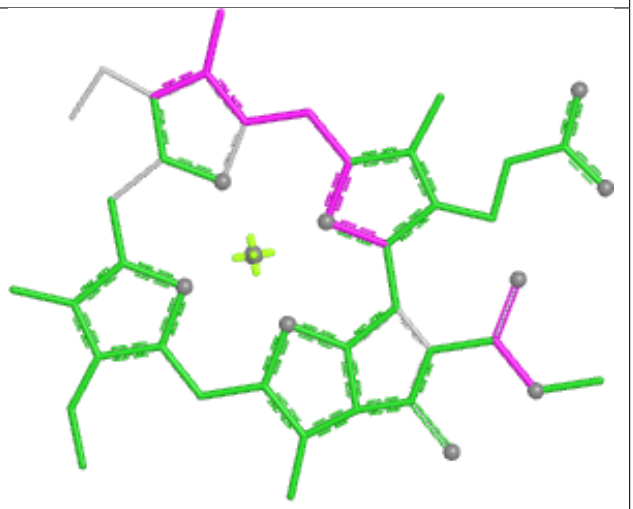


Rings

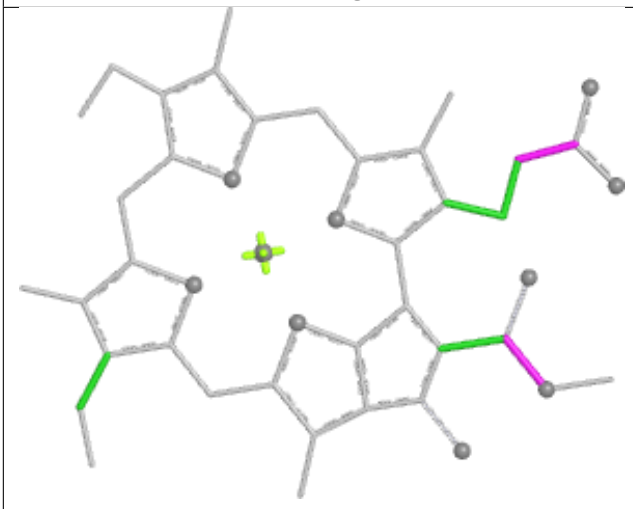
Ligand CLA a 605



Bond lengths



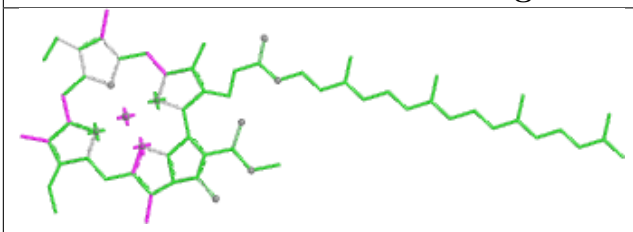
Bond angles



Torsions

Rings

Ligand CLA A 5009



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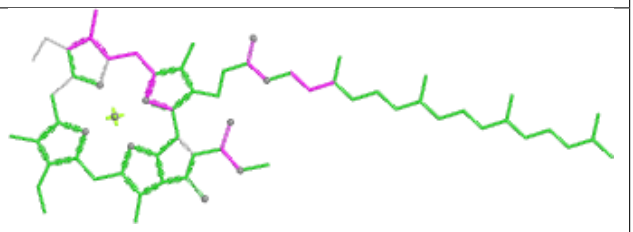
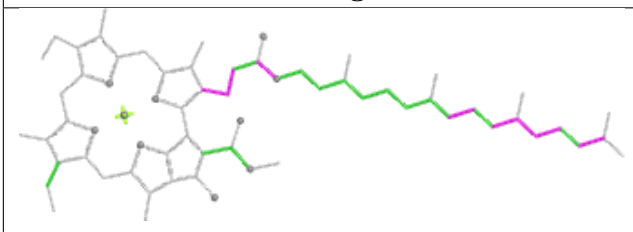


Bond angles



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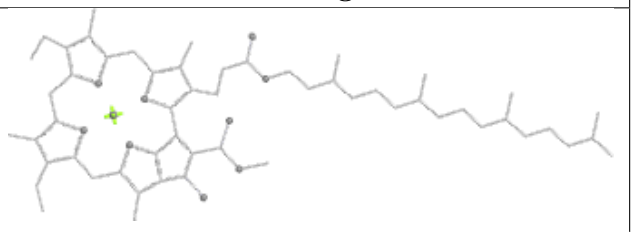
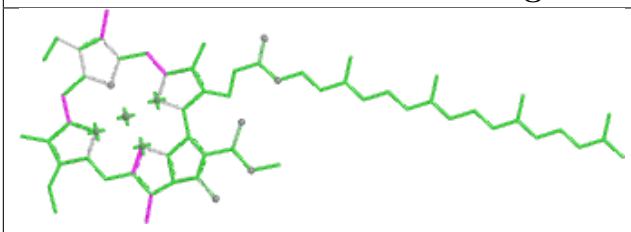
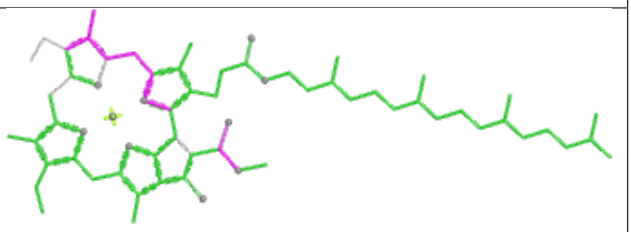


Rings

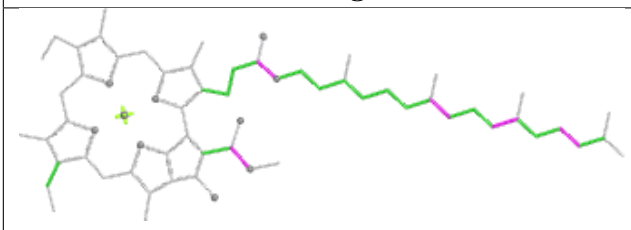
Ligand CLA B 840



Bond lengths



Bond angles



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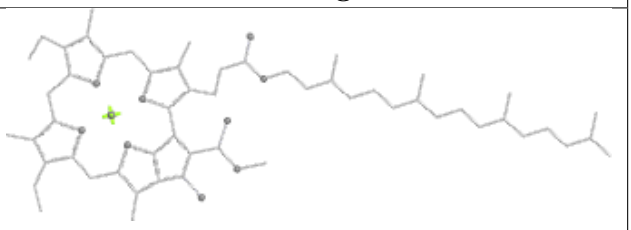
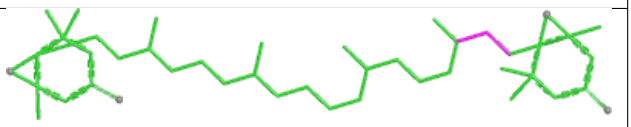


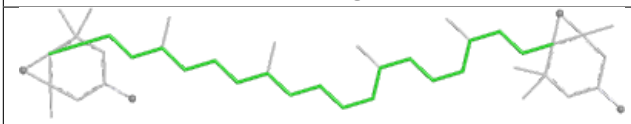
Rings

Ligand XAT 8 317

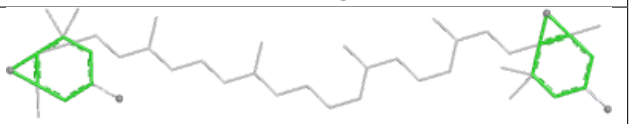
Bond lengths



Bond angles

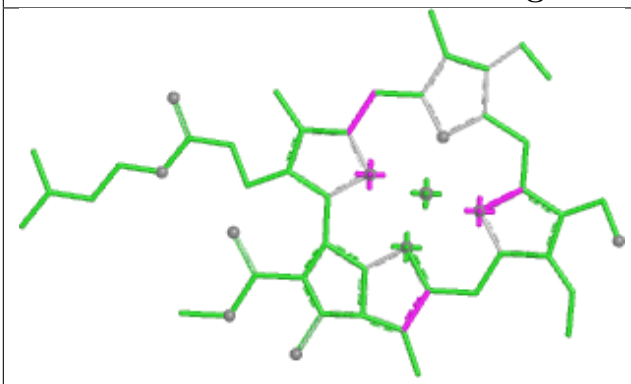


Torsions

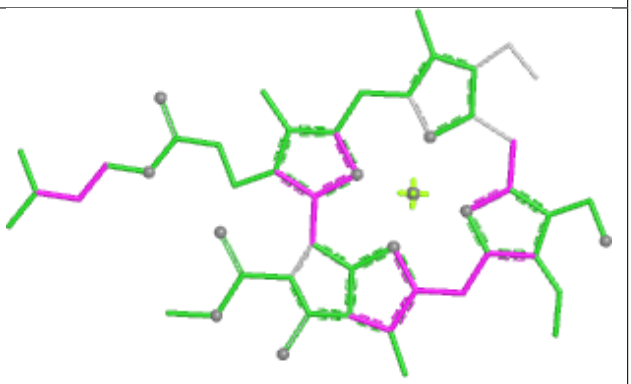


Rings

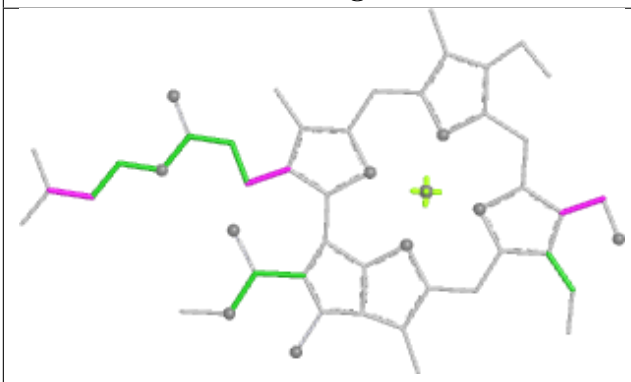
Ligand CHL b 607



Bond lengths



Bond angles



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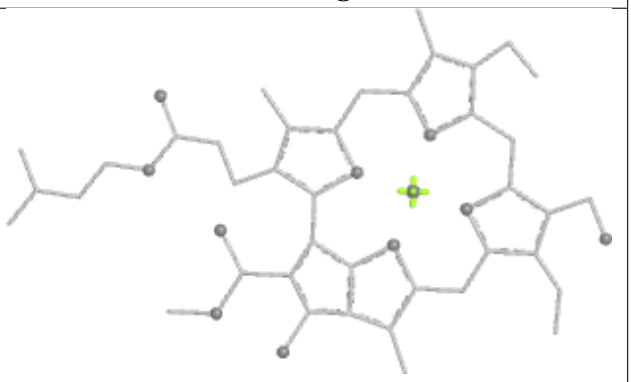
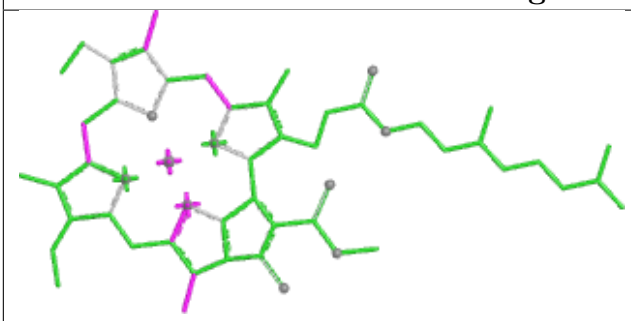
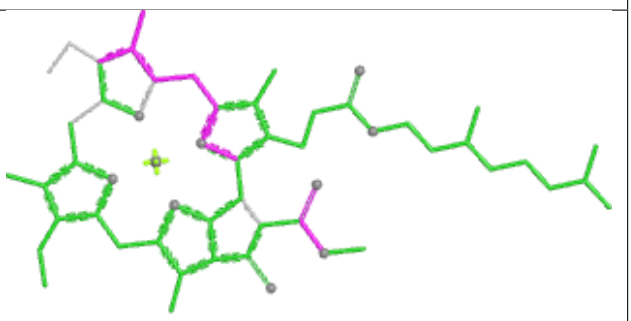


Rings

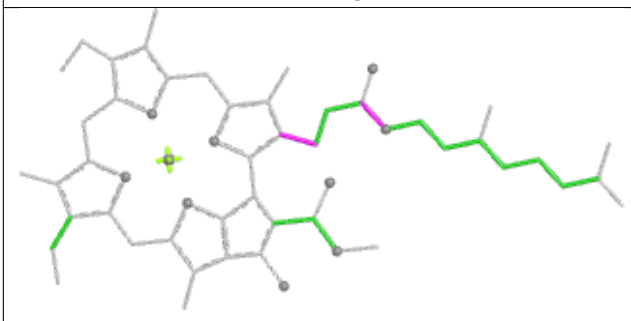
Ligand CLA 3 324



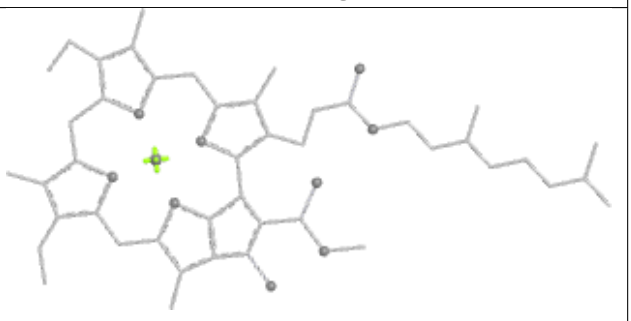
Bond lengths



Bond angles

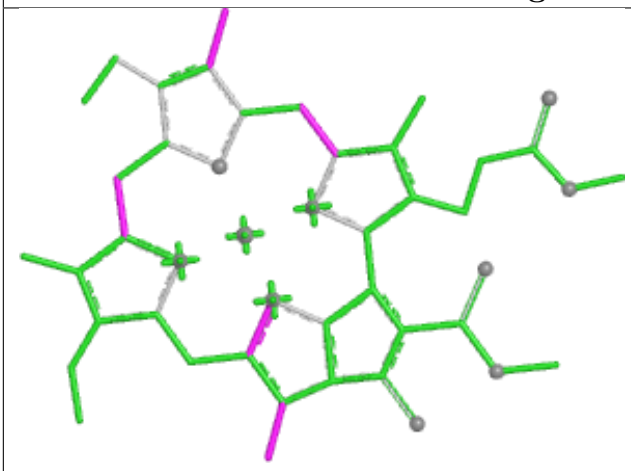


Torsions

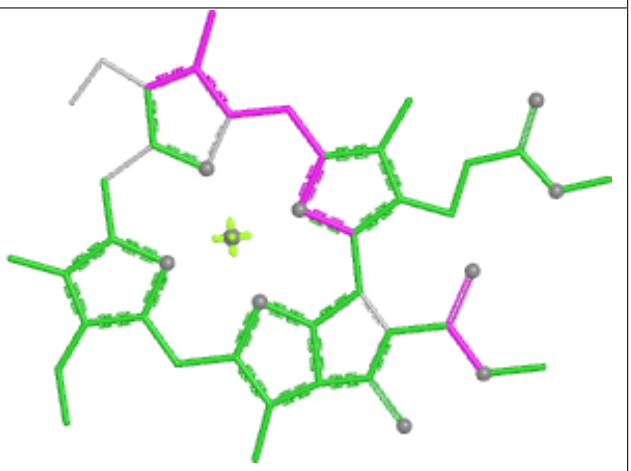


Rings

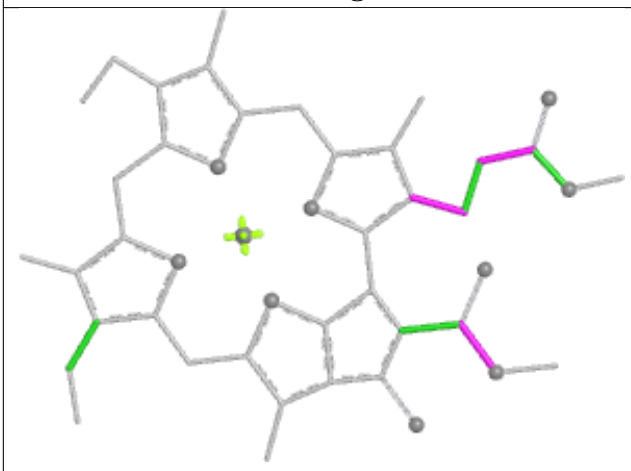
Ligand CLA a 614



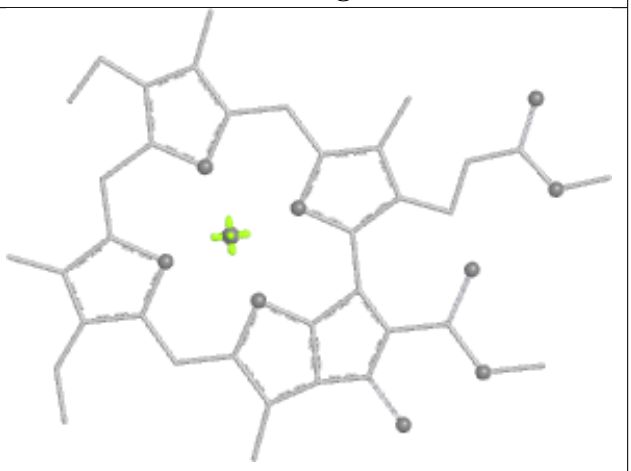
Bond lengths



Bond angles

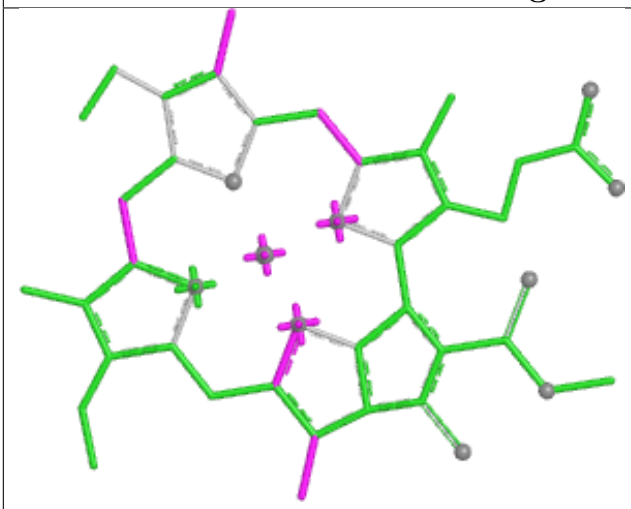


Torsions

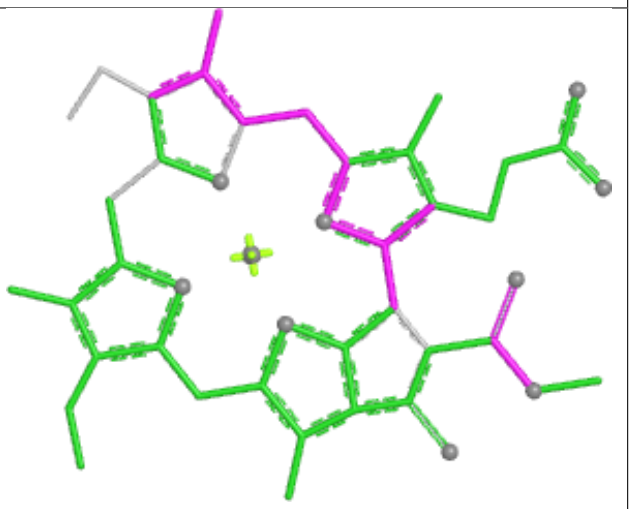


Rings

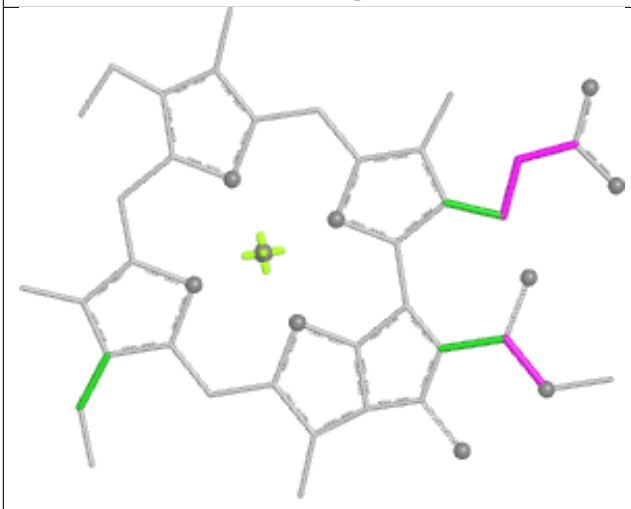
Ligand CLA c 310



Bond lengths



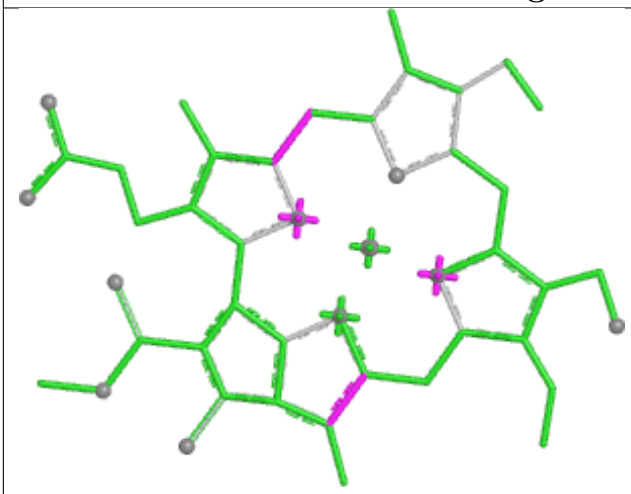
Bond angles



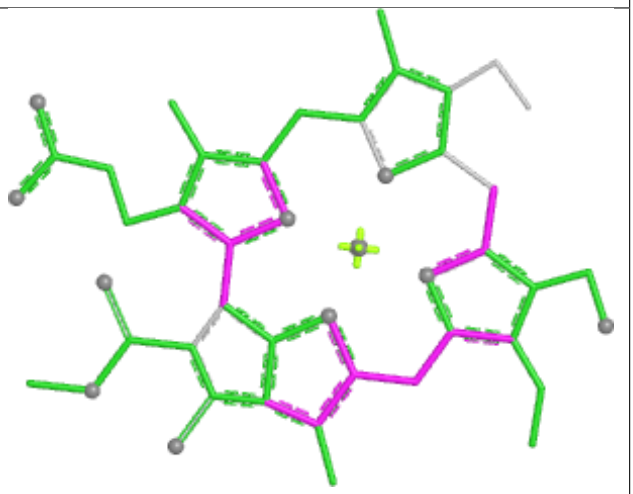
Torsions

Rings

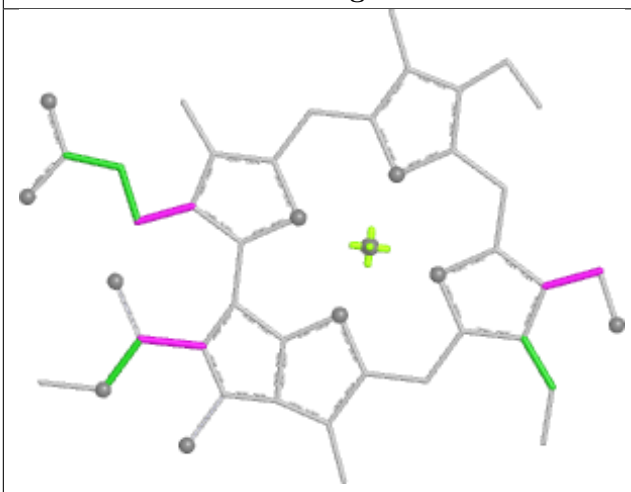
Ligand CHL 7 305



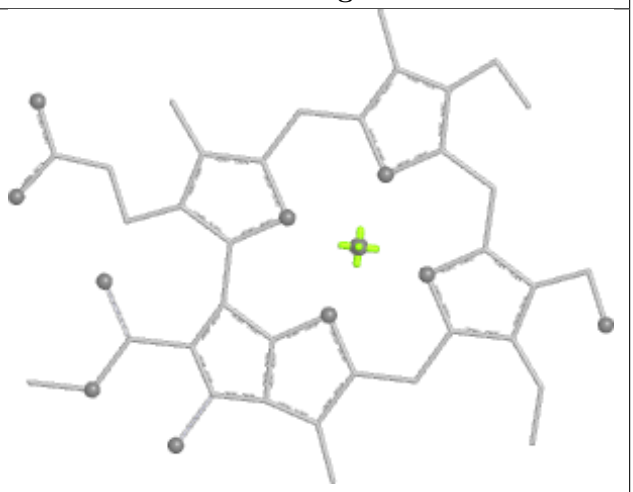
Bond lengths



Bond angles

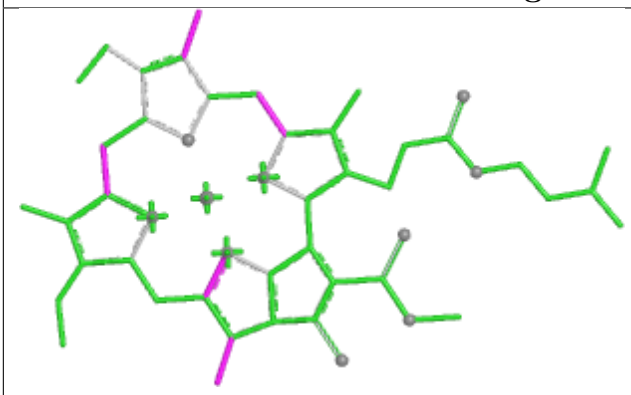


Torsions

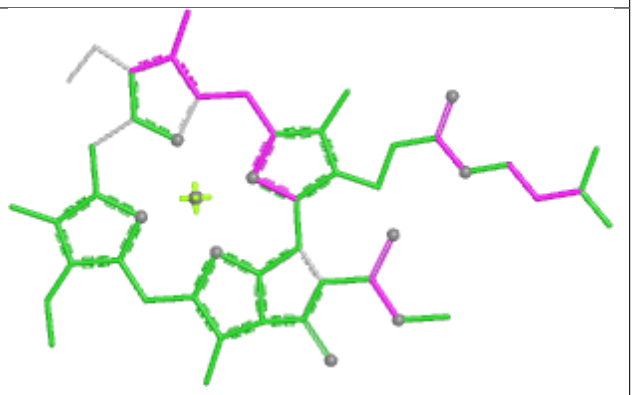


Rings

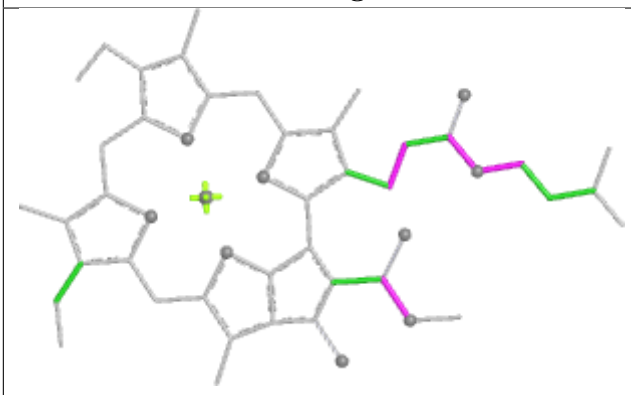
Ligand CLA B 837



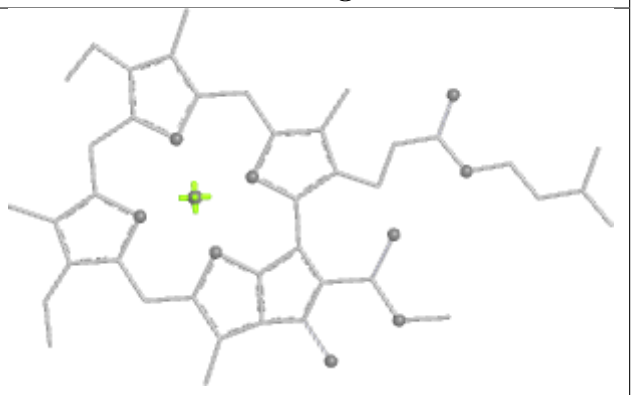
Bond lengths



Bond angles

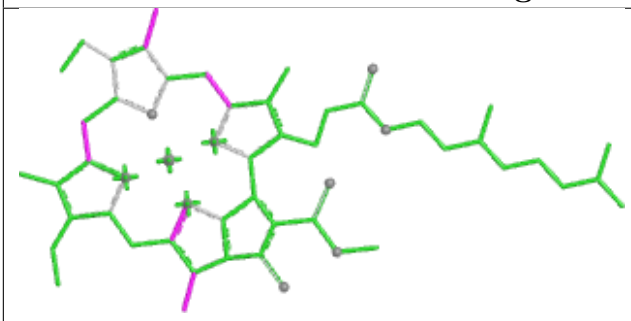


Torsions

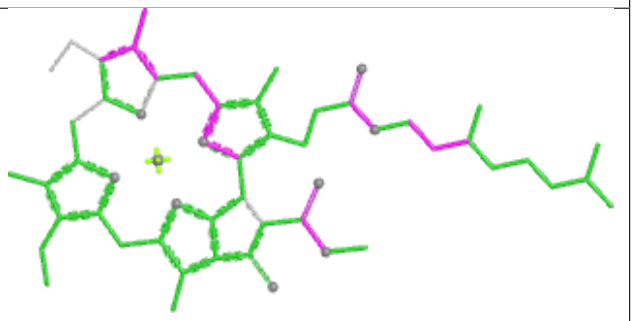


Rings

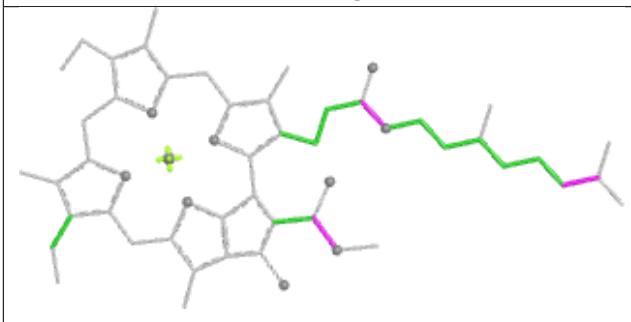
Ligand CLA A 5015



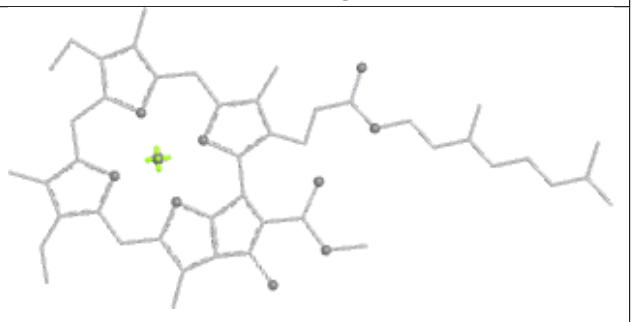
Bond lengths



Bond angles

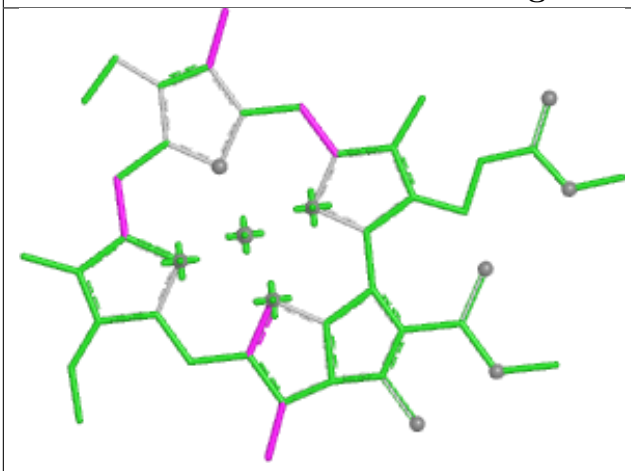


Torsions

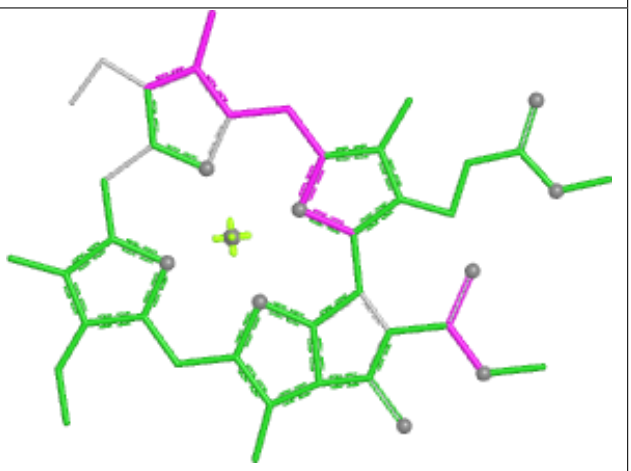


Rings

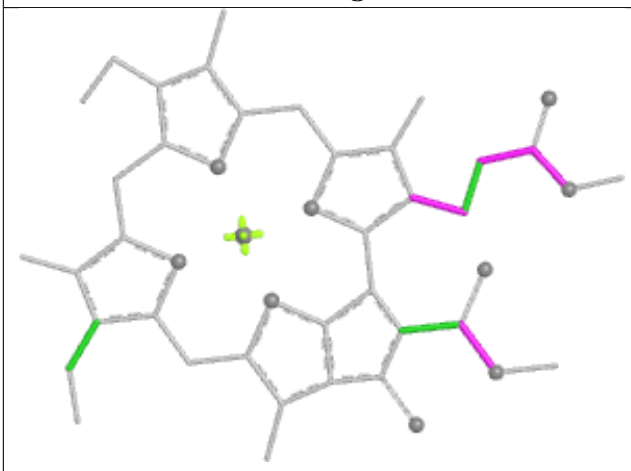
Ligand CLA a 610



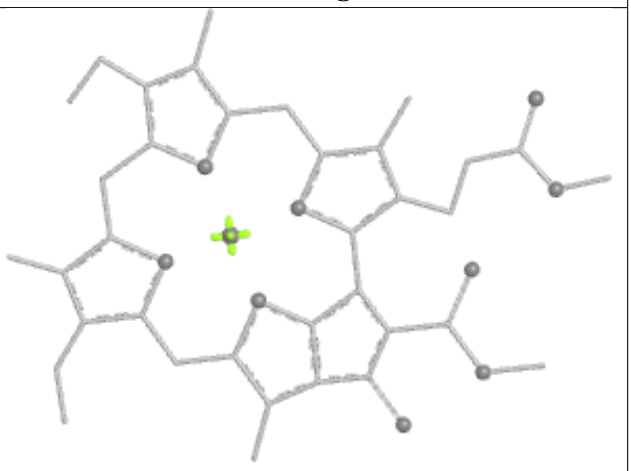
Bond lengths



Bond angles

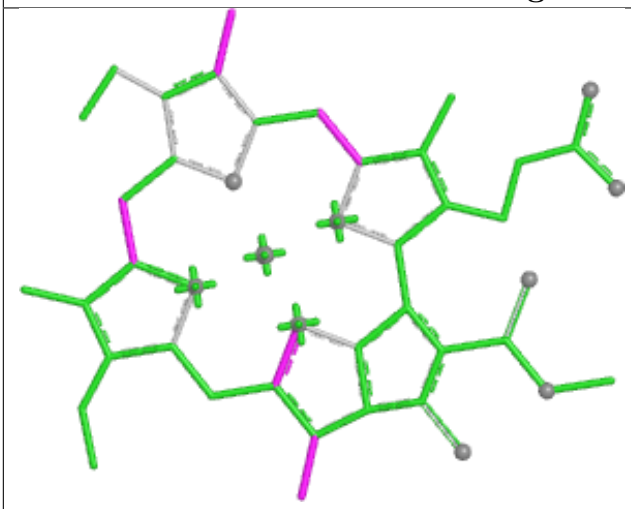


Torsions

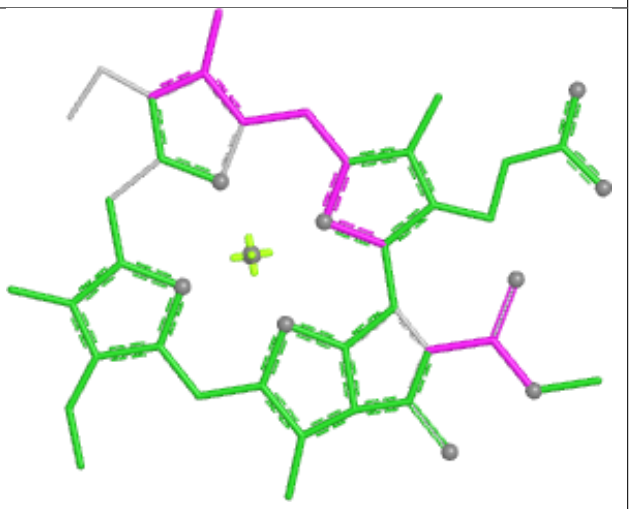


Rings

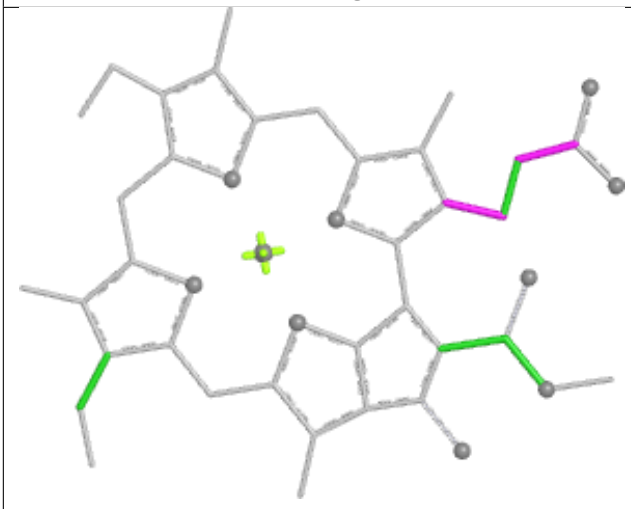
Ligand CLA b 608



Bond lengths



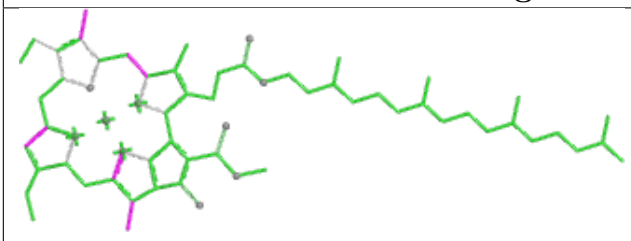
Bond angles



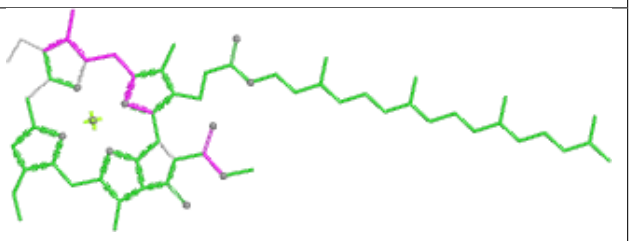
Torsions

Rings

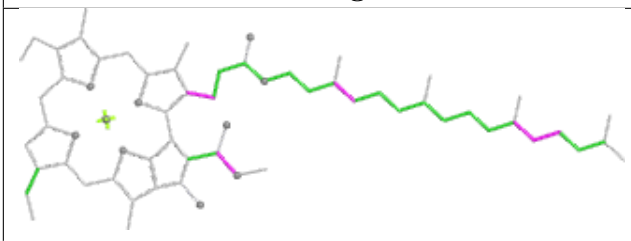
Ligand CLA A 5036



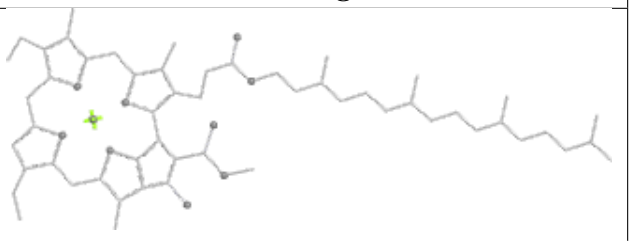
Bond lengths



Bond angles

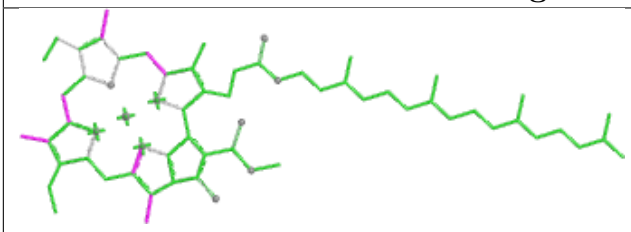


Torsions



Rings

Ligand CLA c 308



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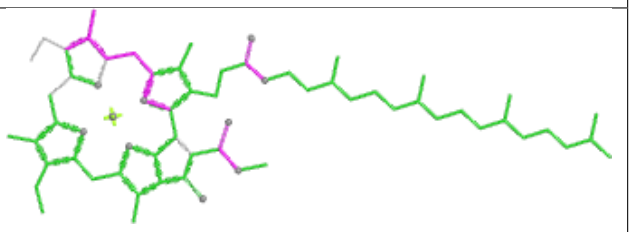
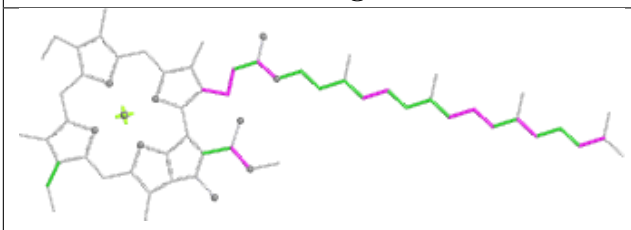


Bond angles



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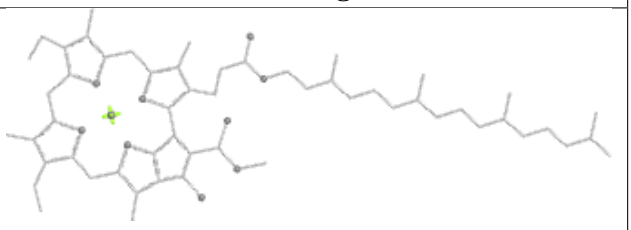
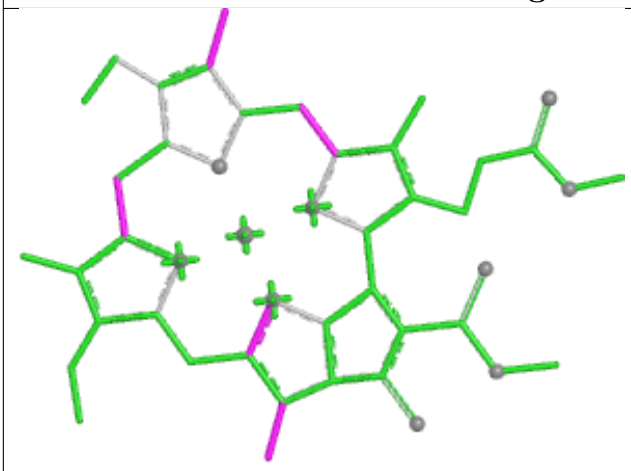
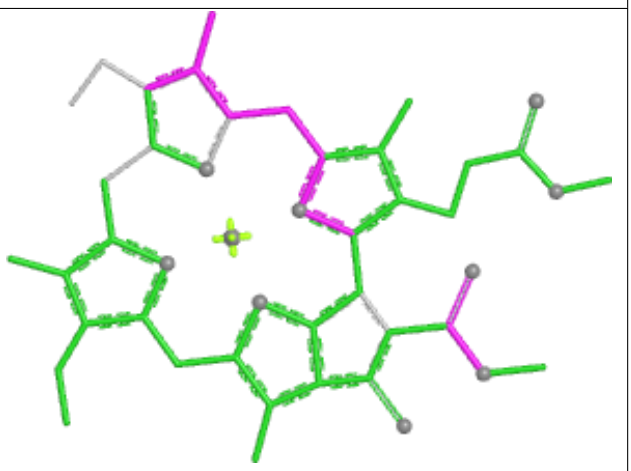


Rings

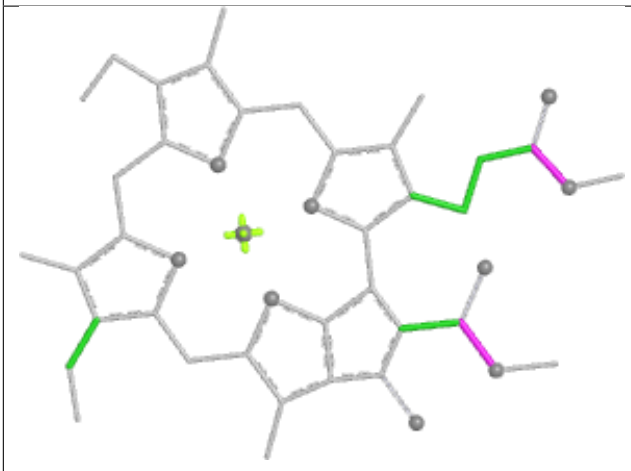
Ligand CLA a 613



Bond lengths



Bond angles



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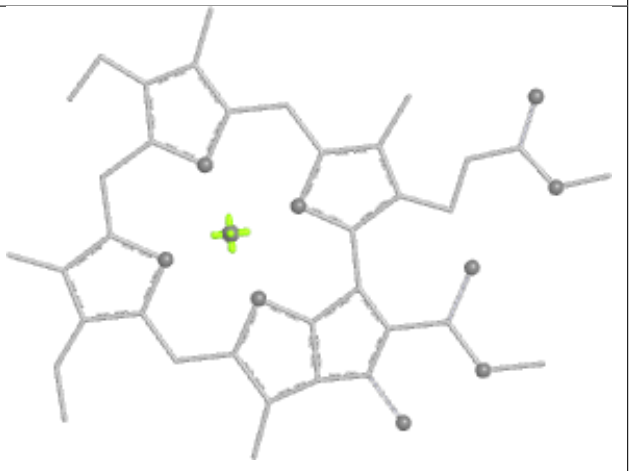
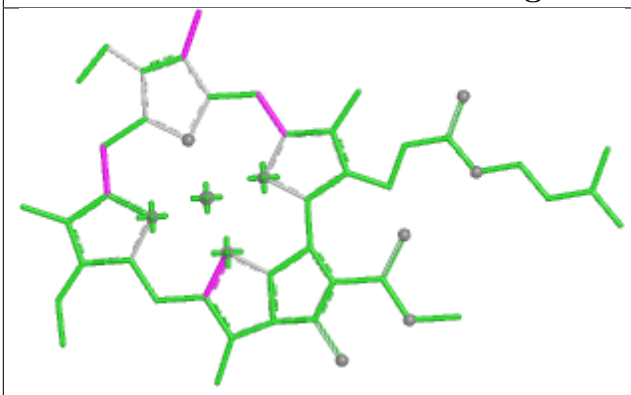
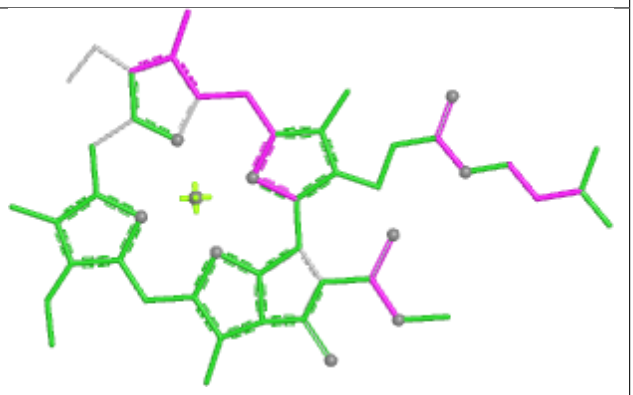


Rings

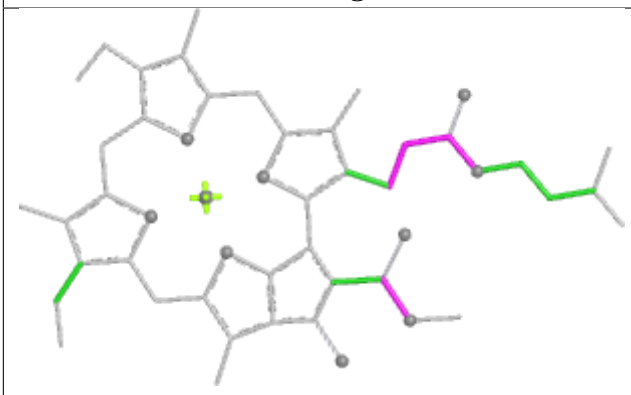
Ligand CLA B 813



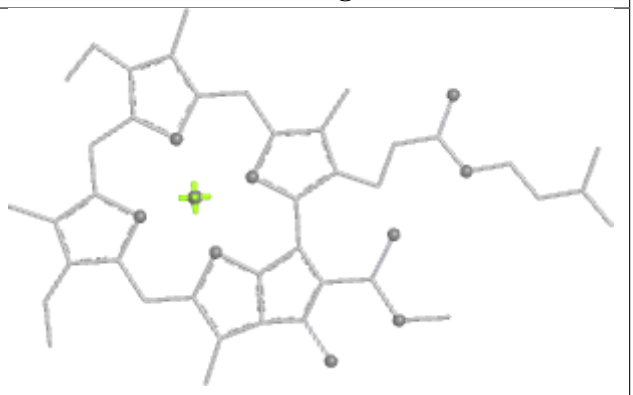
Bond lengths



Bond angles

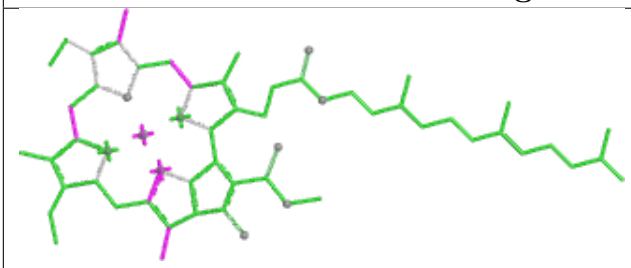


Torsions

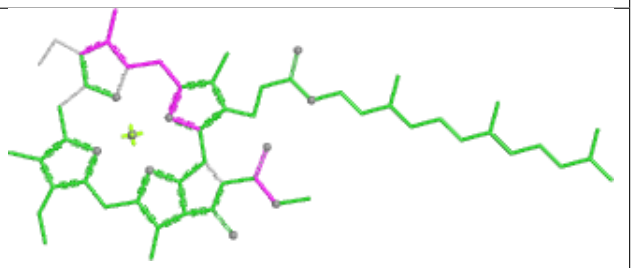


Rings

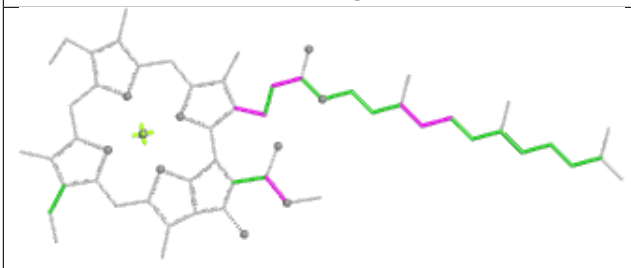
Ligand CLA A 5040



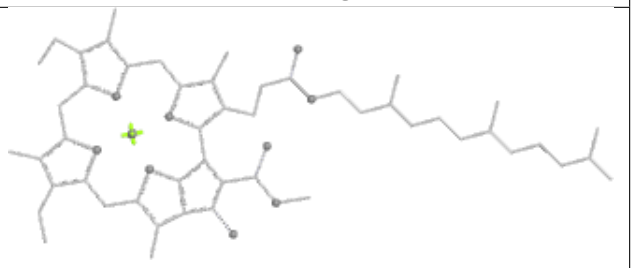
Bond lengths



Bond angles

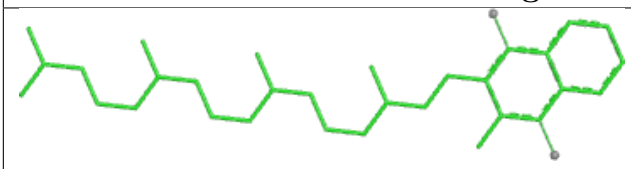


Torsions

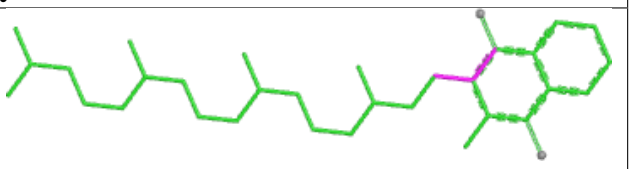


Rings

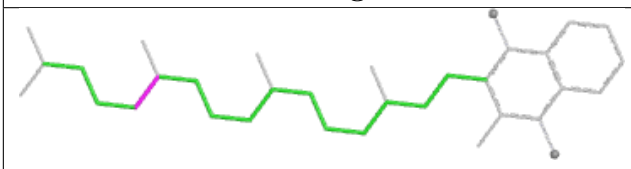
Ligand PQN B 842



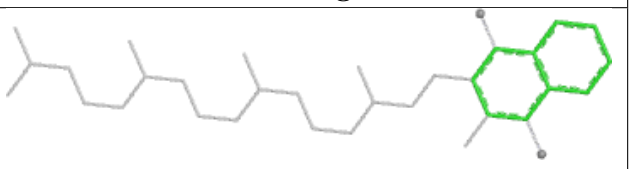
Bond lengths



Bond angles

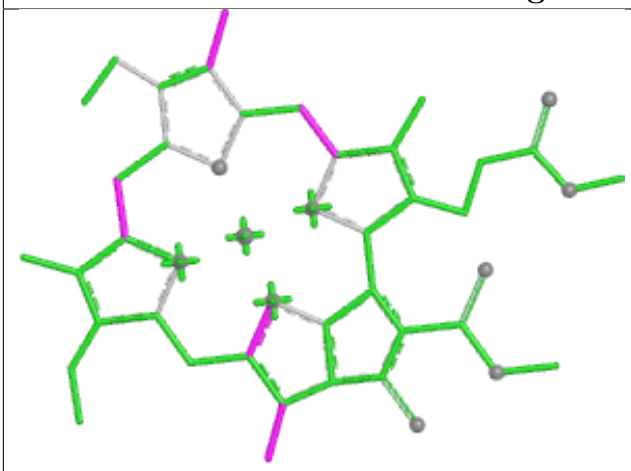


Torsions

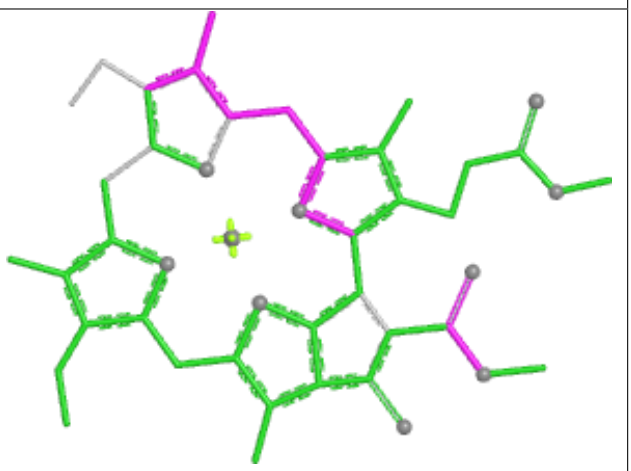


Rings

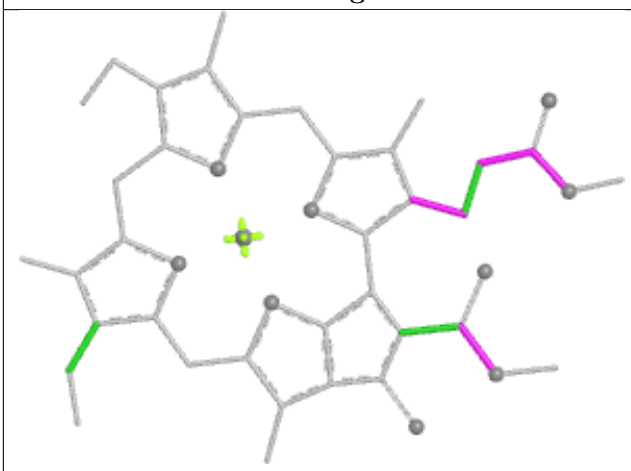
Ligand CLA b 601



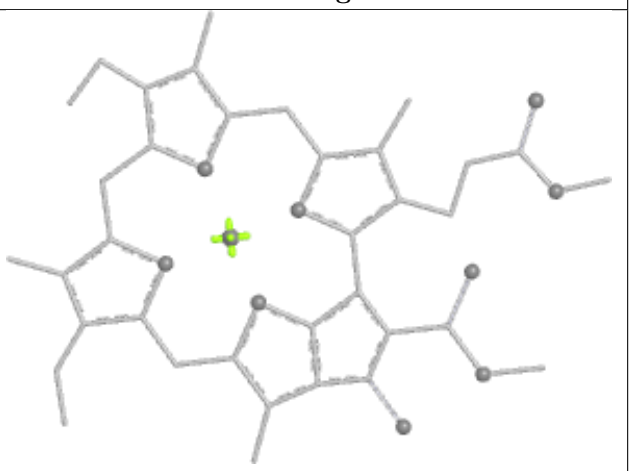
Bond lengths



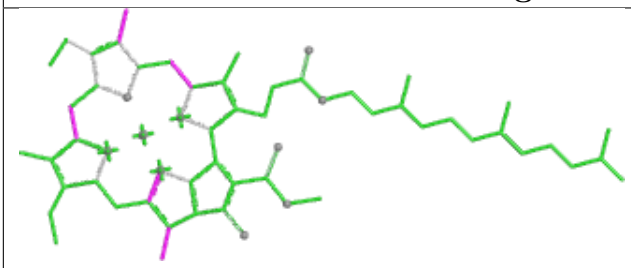
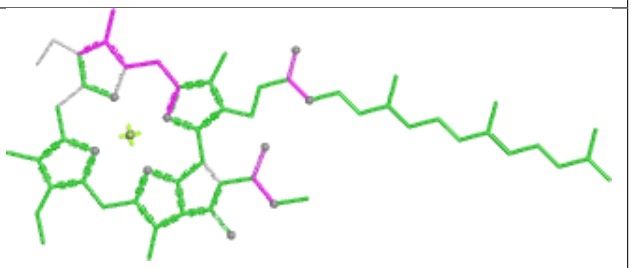
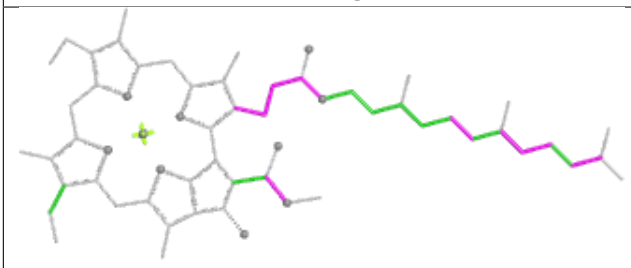
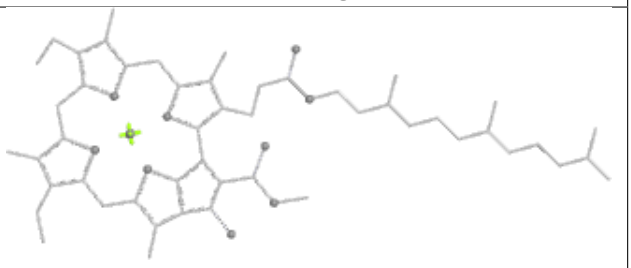
Bond angles

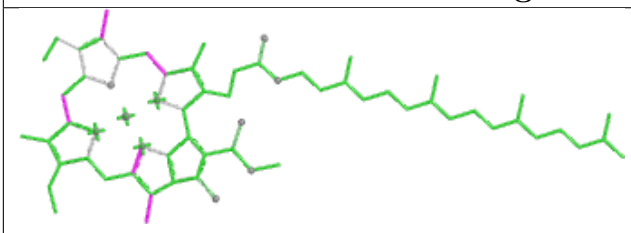
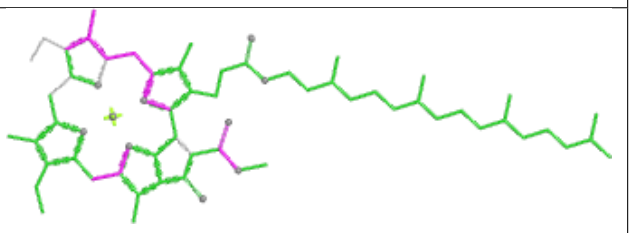
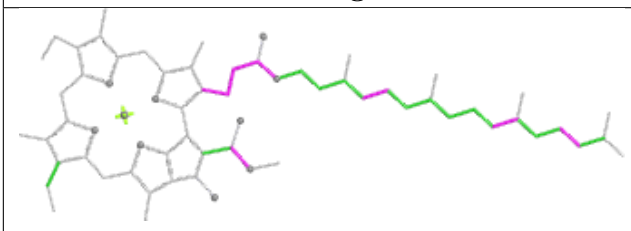
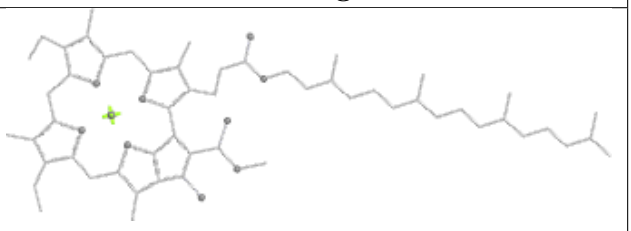


Torsions

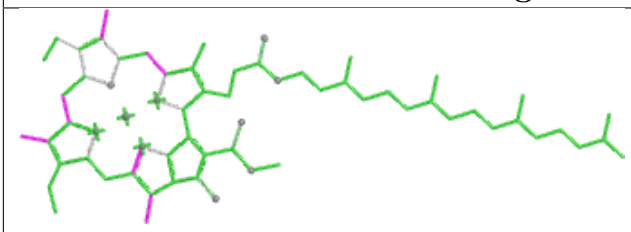


Rings

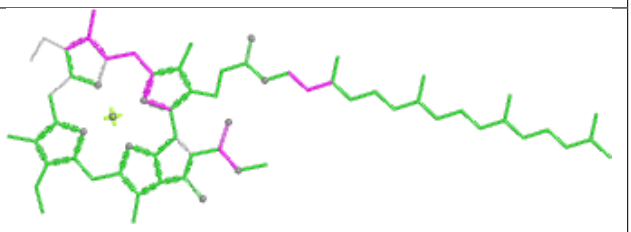
Ligand CLA A 5024	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA A 5029	
	
Bond lengths	Bond angles
	
Torsions	Rings

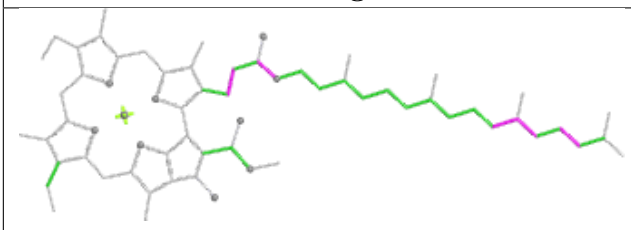
Ligand CLA A 5030



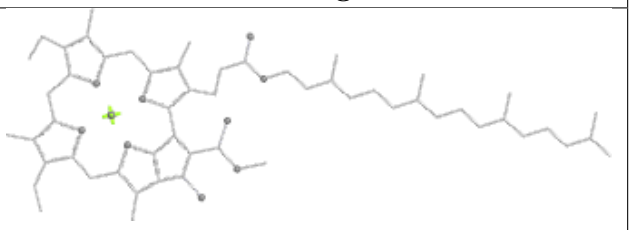
Bond lengths



Bond angles

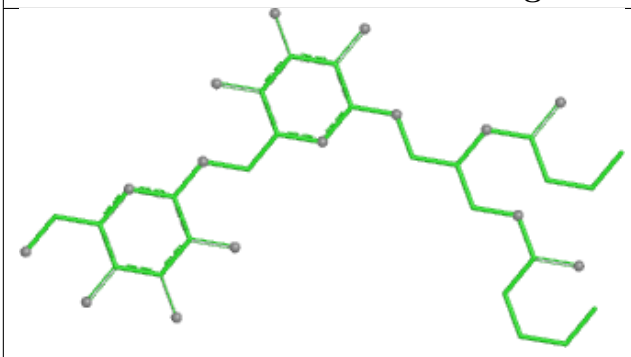


Torsions

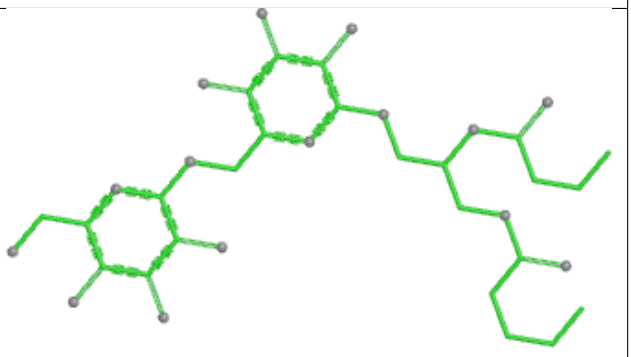


Rings

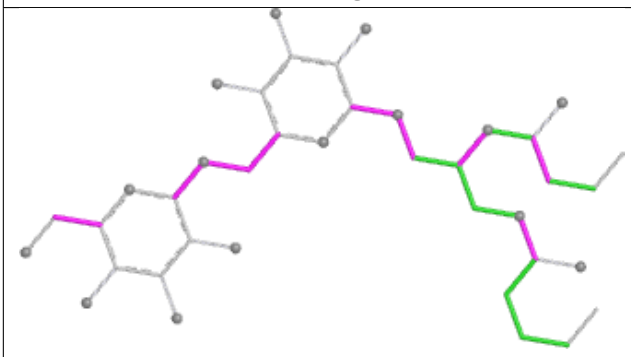
Ligand DGD 8 301



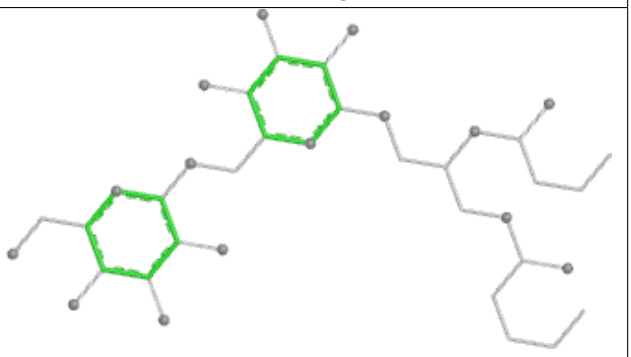
Bond lengths



Bond angles

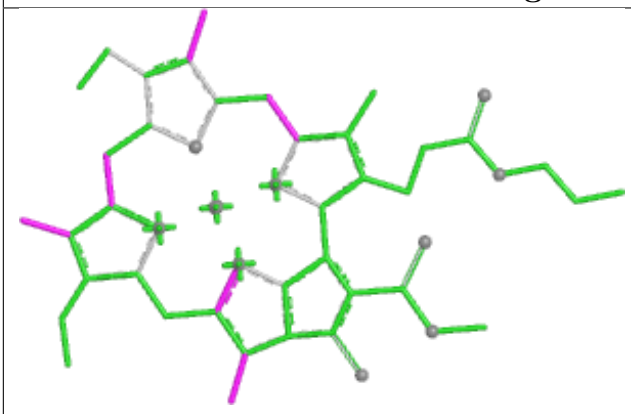


Torsions

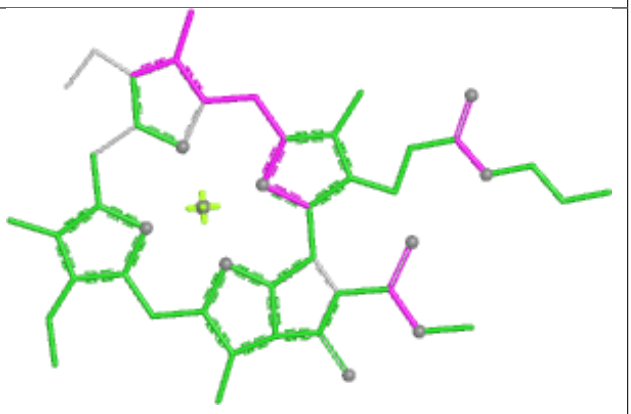


Rings

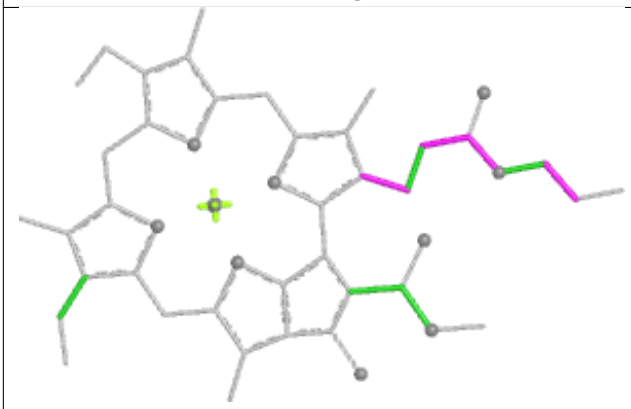
Ligand CLA B 804



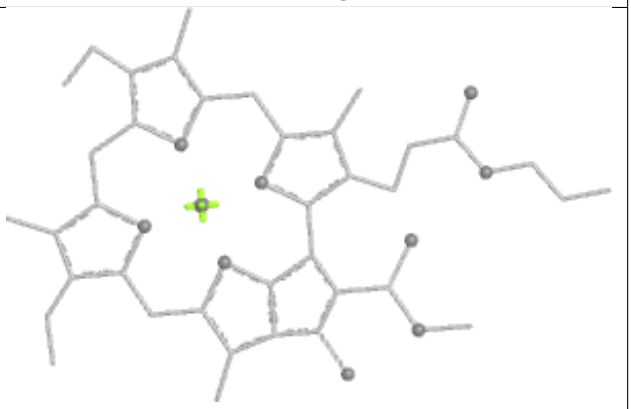
Bond lengths



Bond angles

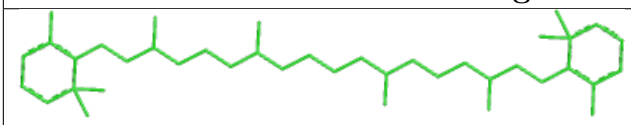


Torsions

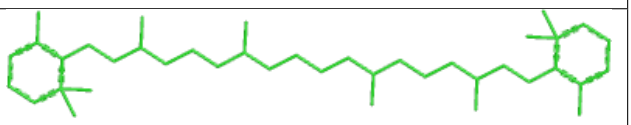


Rings

Ligand BCR A 5050

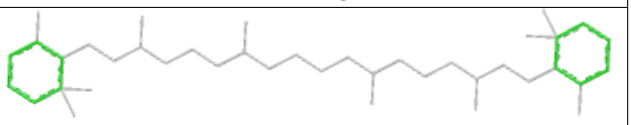


Bond lengths



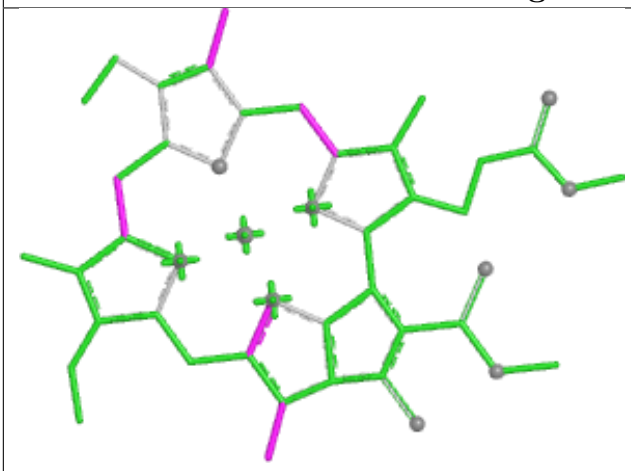
Bond angles

Torsions



Rings

Ligand CLA 8 314



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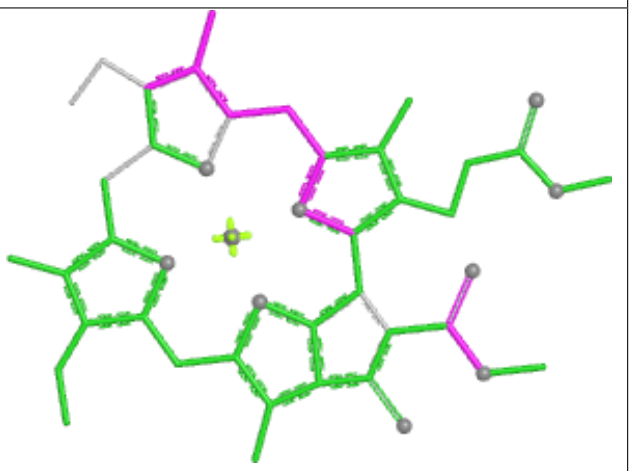
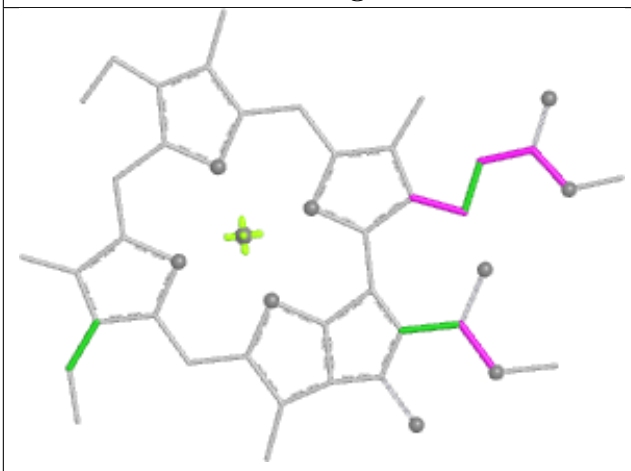


Bond angles



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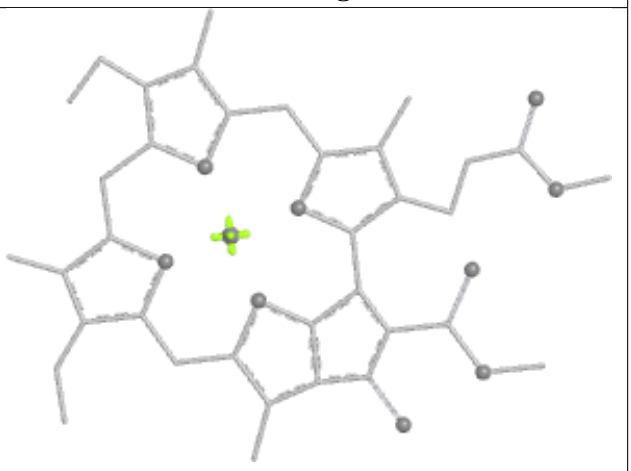
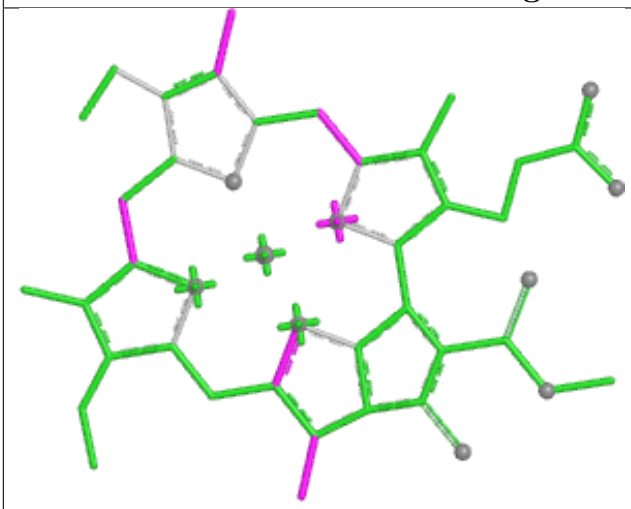


Rings

Ligand CLA K 201



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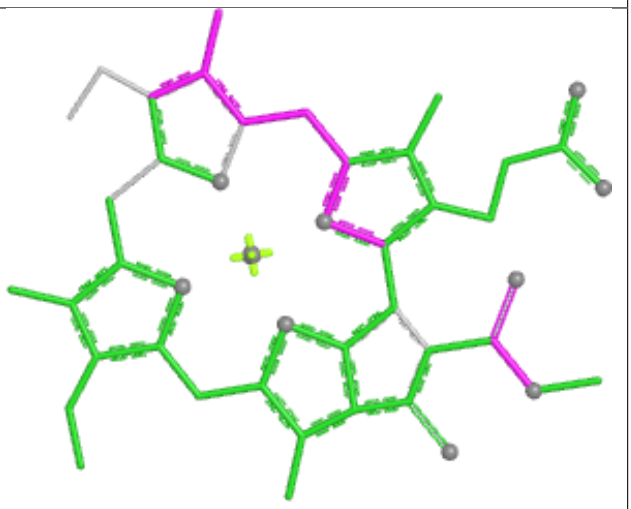
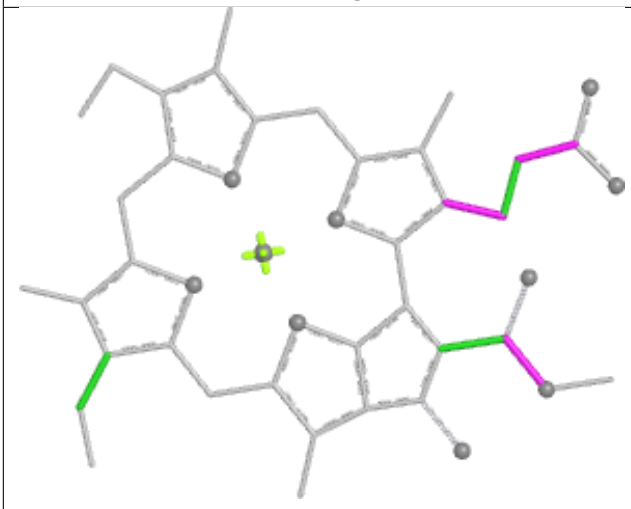


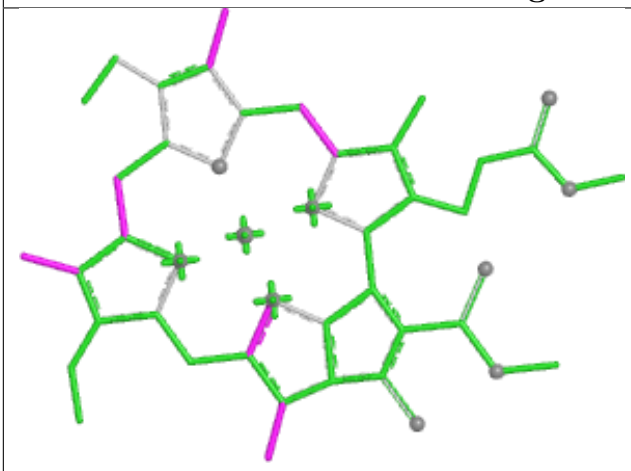
Bond angles



Torsions

Rings

Ligand CLA 3 314



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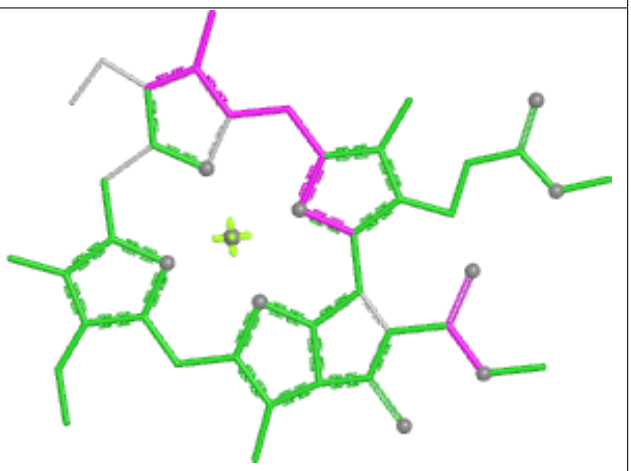
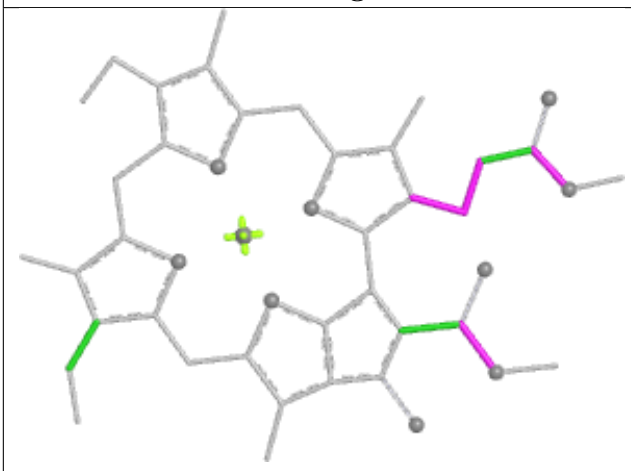


Bond angles



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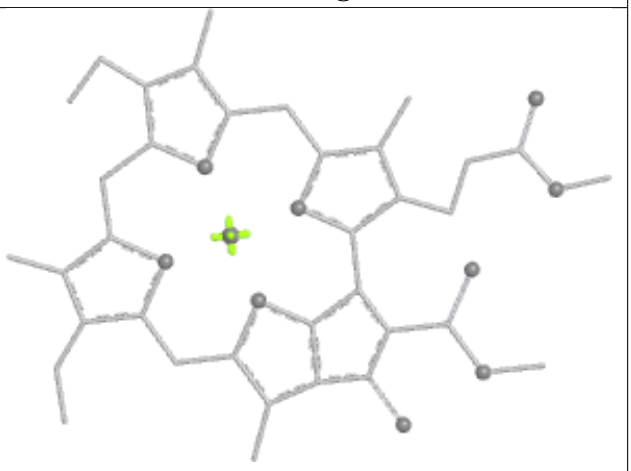
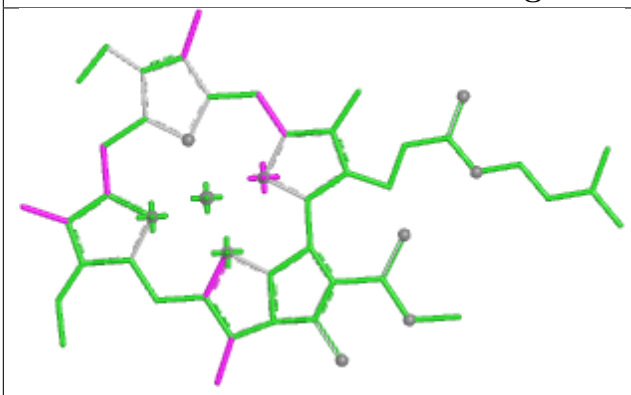


Rings

Ligand CLA B 825



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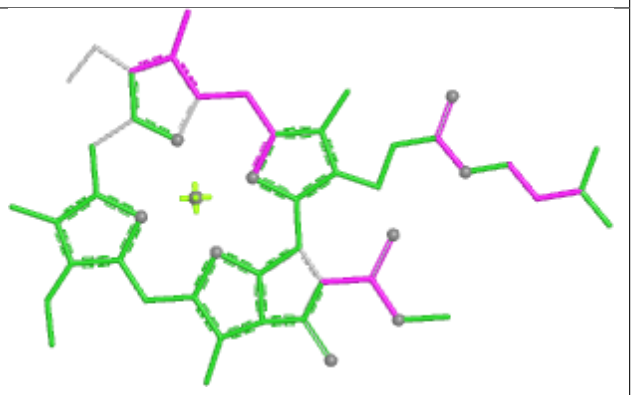
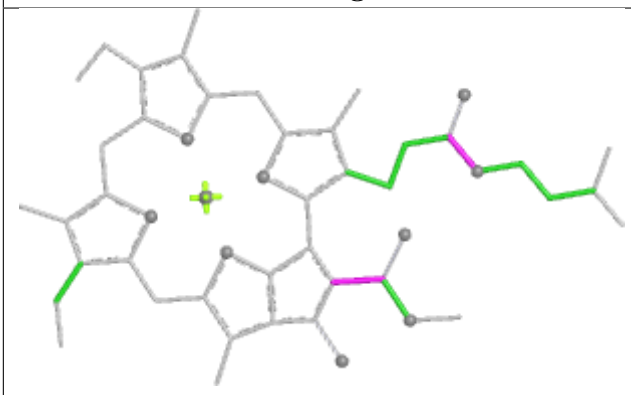


Bond angles



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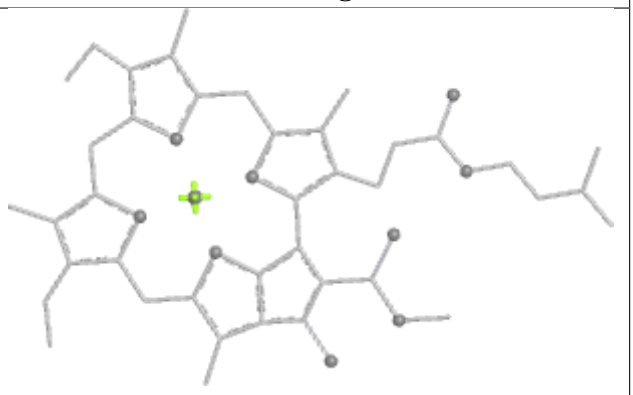
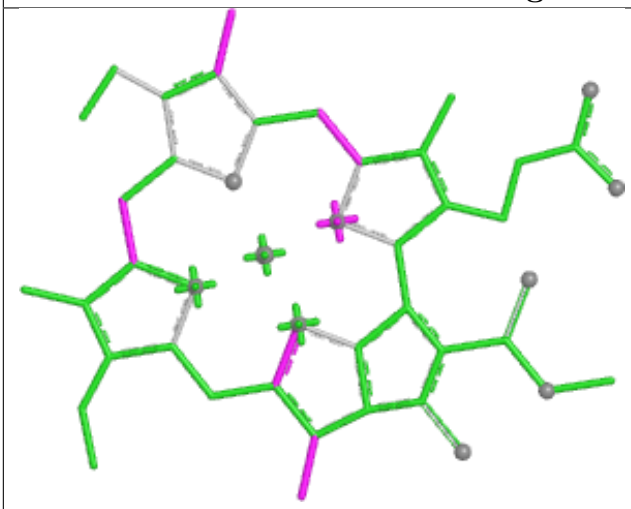


Rings

Ligand CLA L 202



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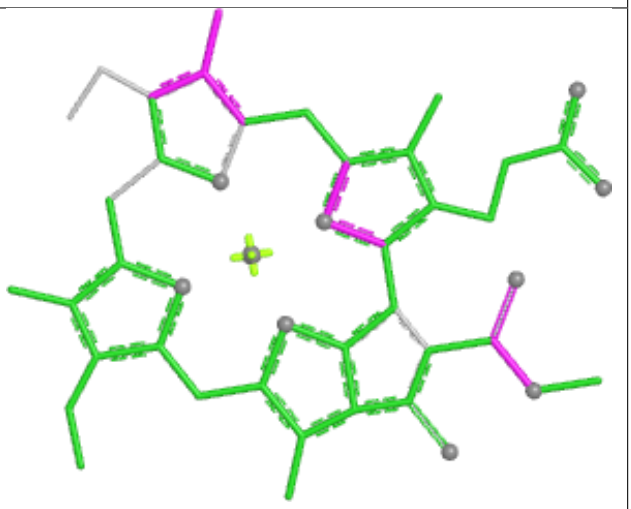
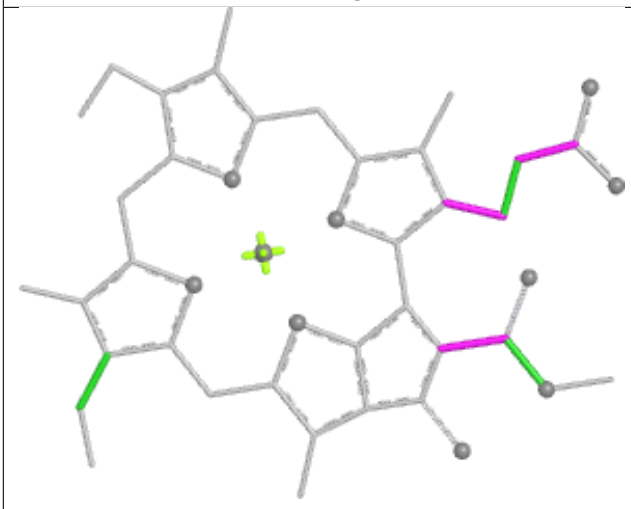


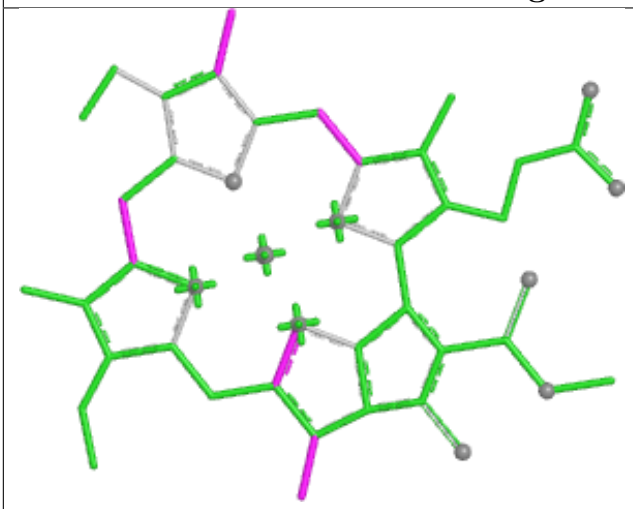
Bond angles



Torsions

Rings

Ligand CLA a 603



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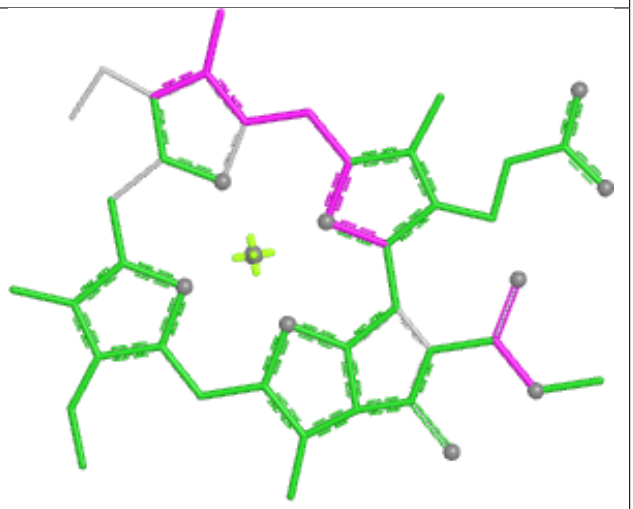
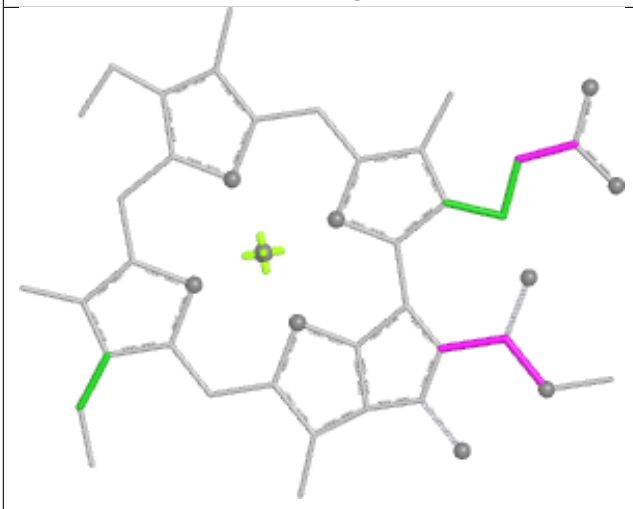


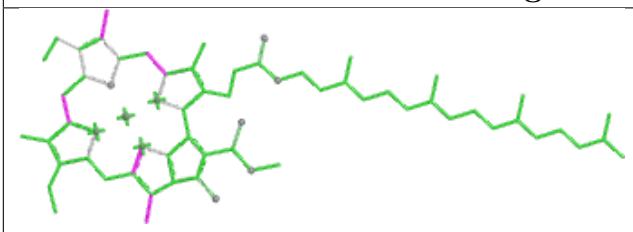
Bond angles



Torsions

Rings

Ligand CLA B 830



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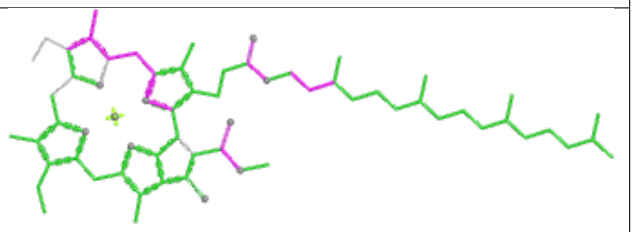
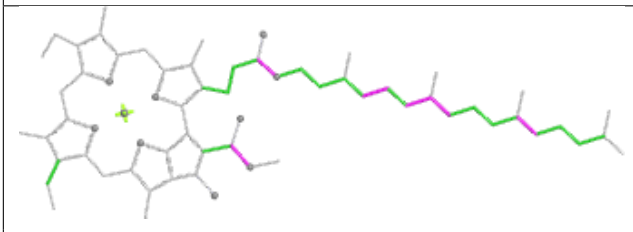
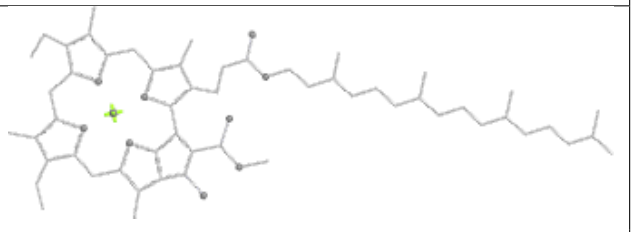


Bond angles

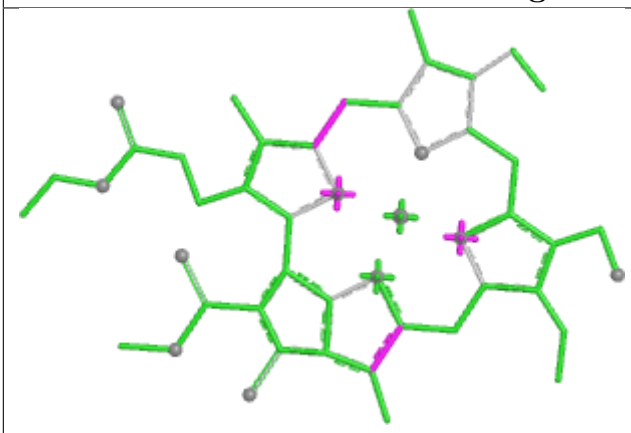


Torsions



Rings

Ligand CHL c 306



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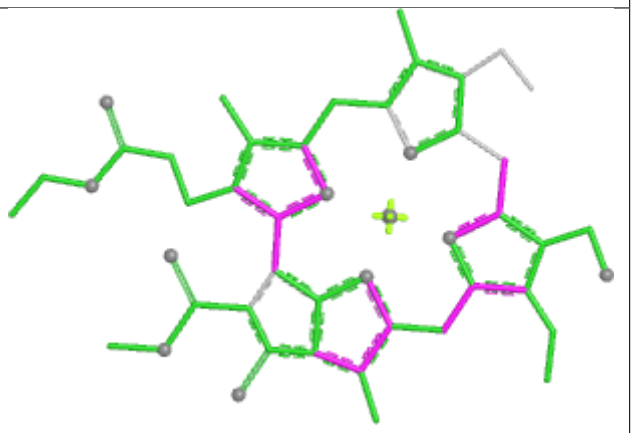
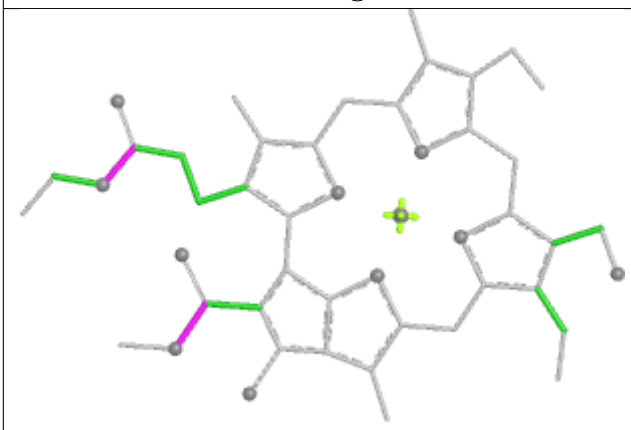
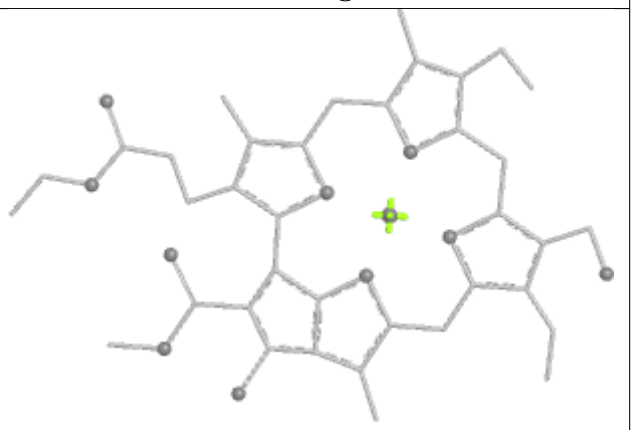


Bond angles

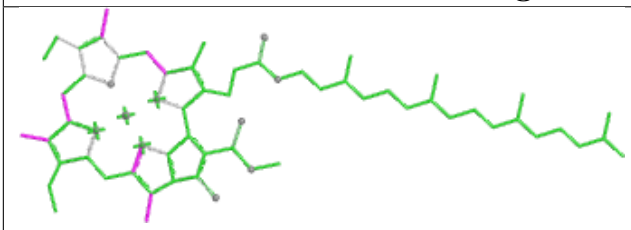


Torsions



Rings

Ligand CLA A 5005



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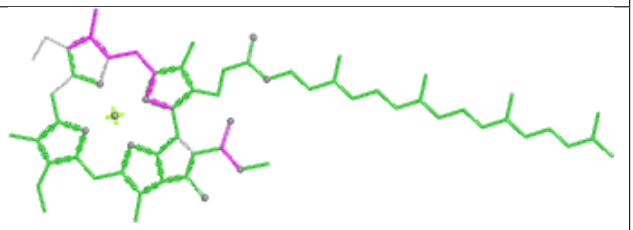
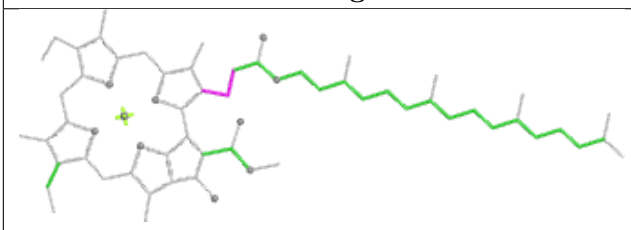
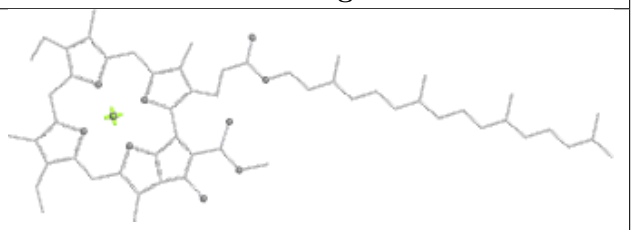


Bond angles

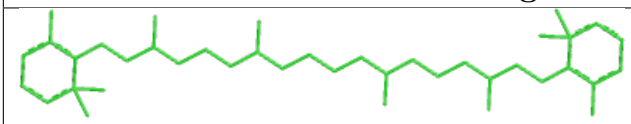


Torsions



Rings

Ligand BCR I 4001



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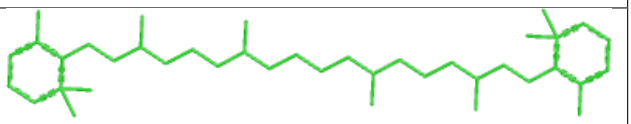
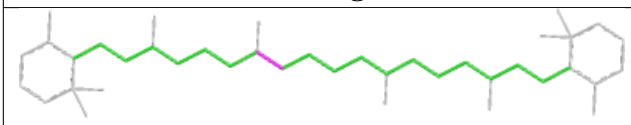
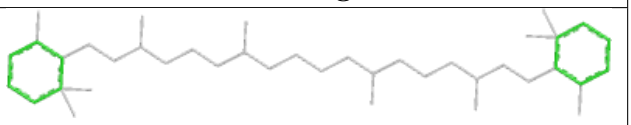


Bond angles

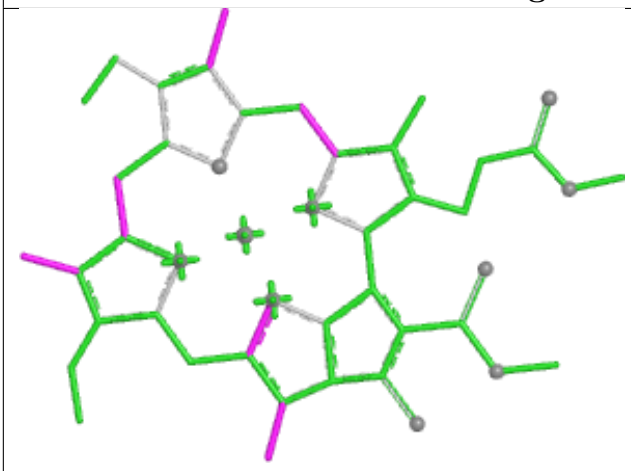


Torsions



Rings

Ligand CLA 3 304



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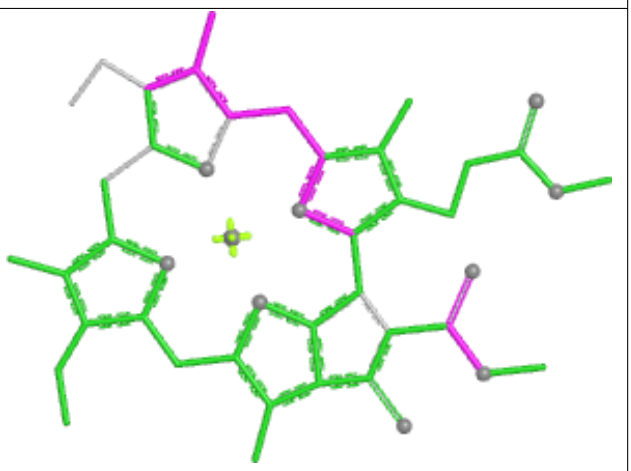
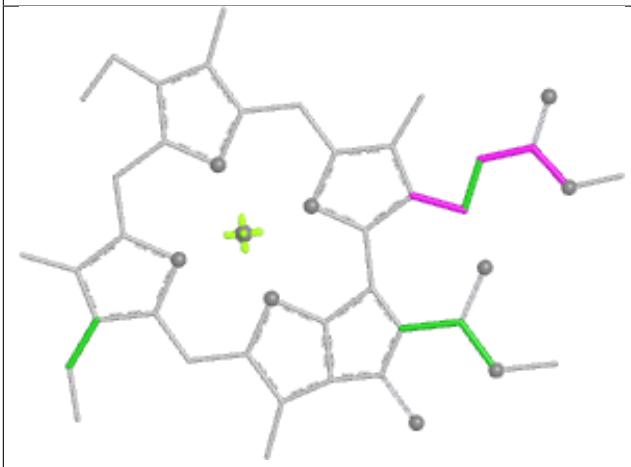


Bond angles



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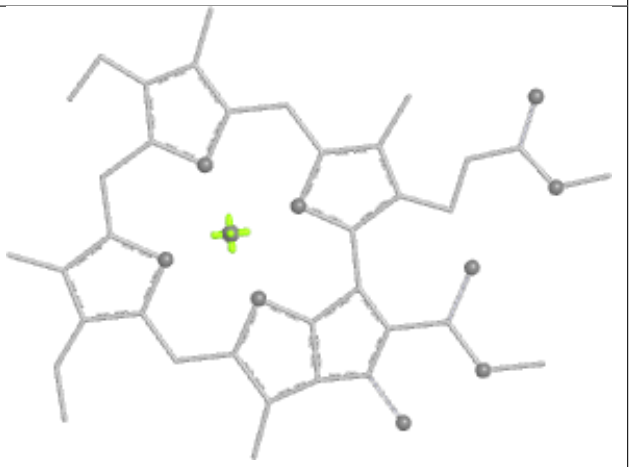
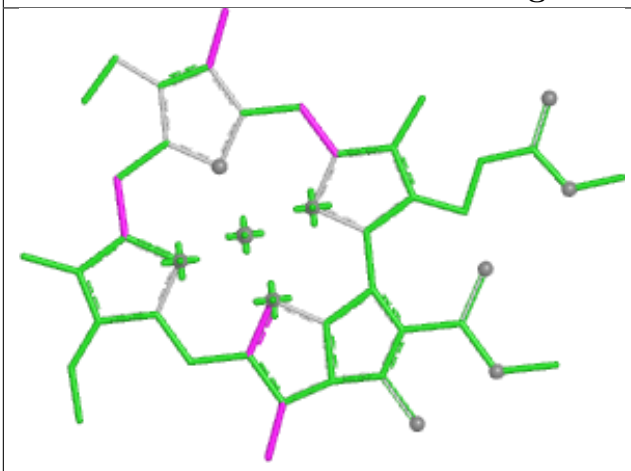


Rings

Ligand CLA 3 309



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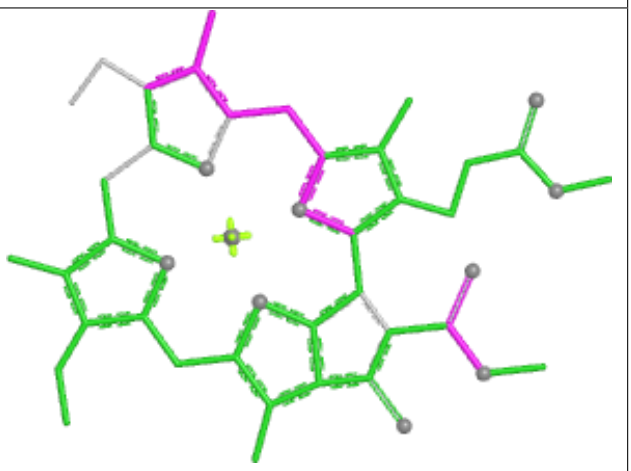
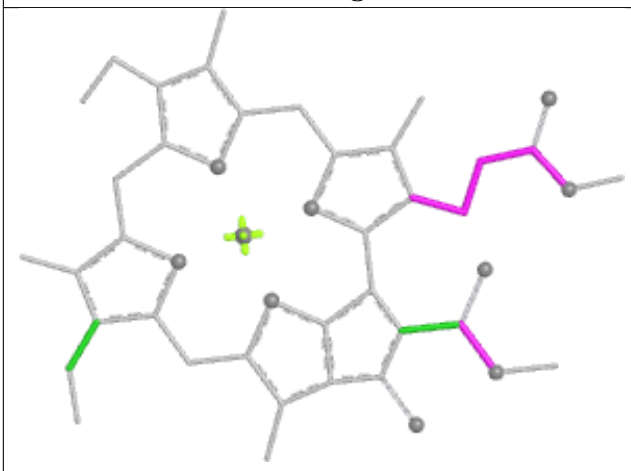


Bond angles



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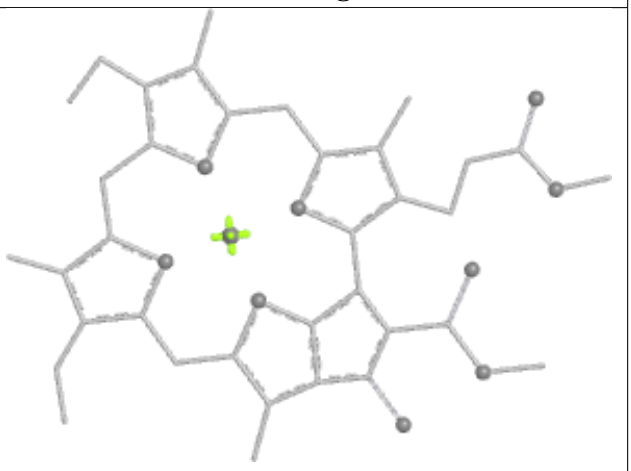
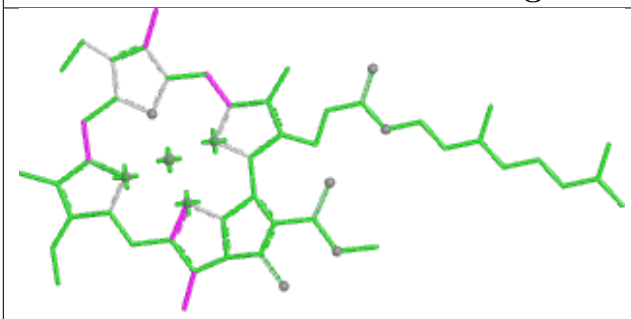


Rings

Ligand CLA B 817



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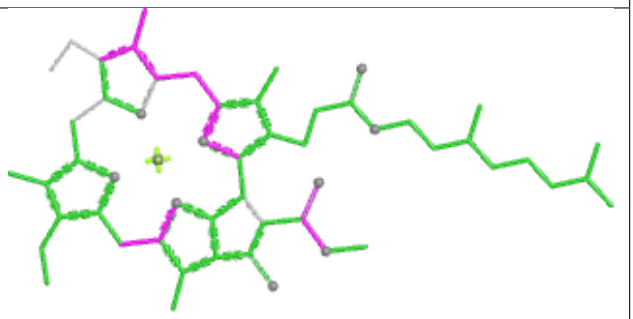
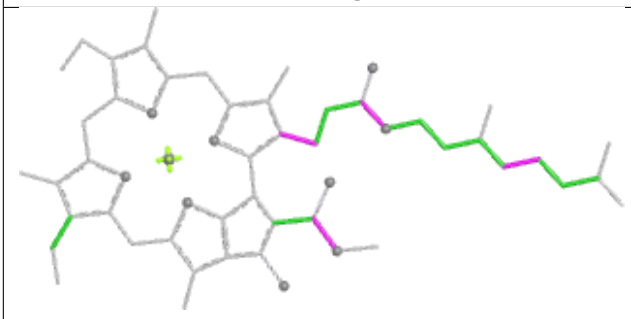
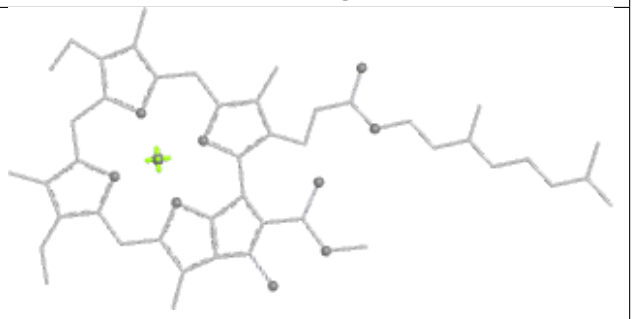


Bond angles

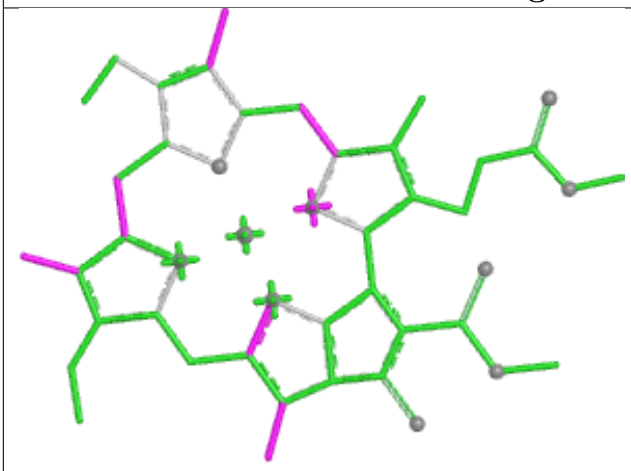


Torsions

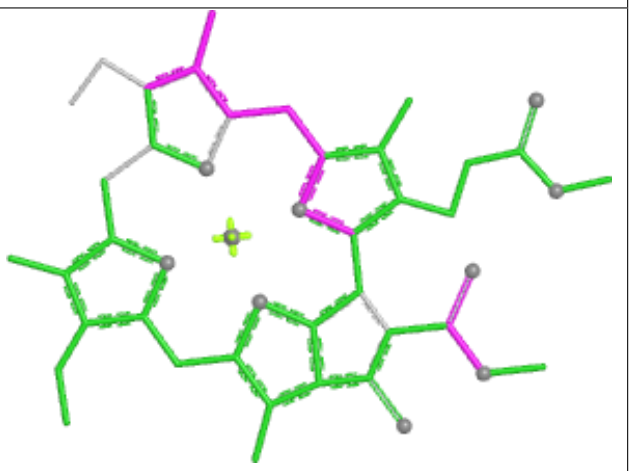


Rings

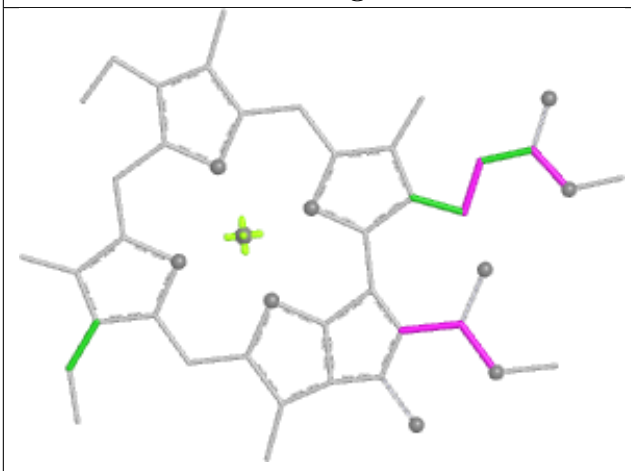
Ligand CLA 8 305



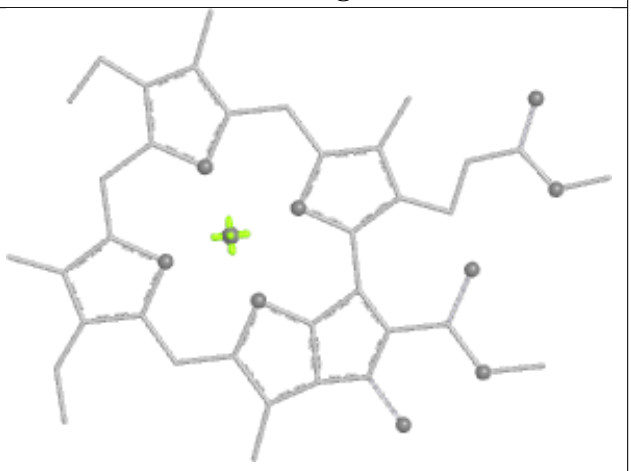
Bond lengths



Bond angles

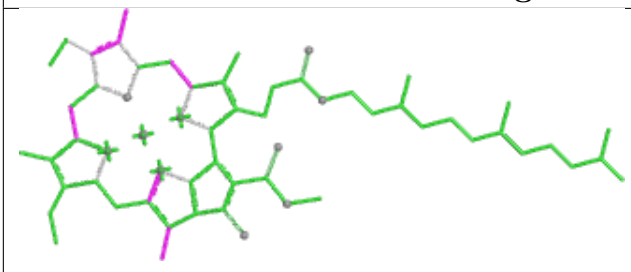


Torsions

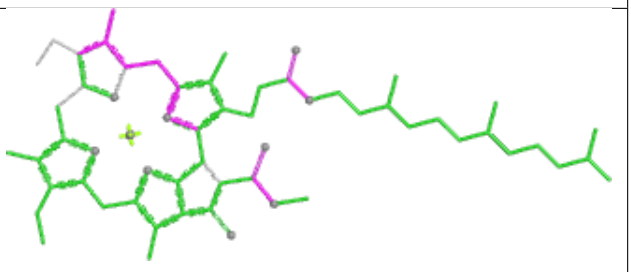


Rings

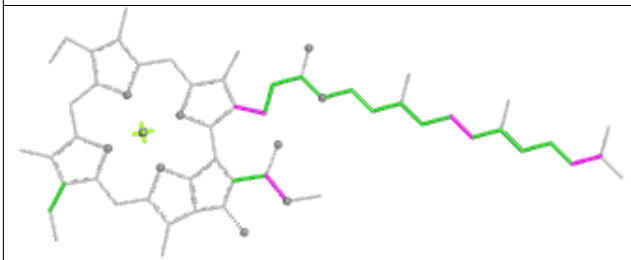
Ligand CLA A 5042



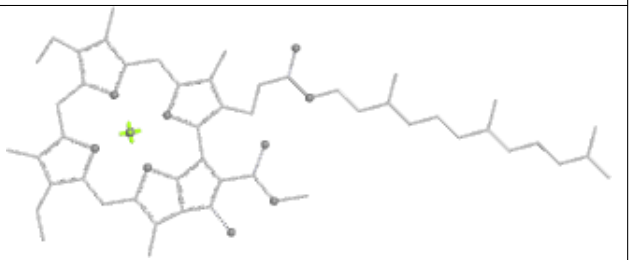
Bond lengths



Bond angles

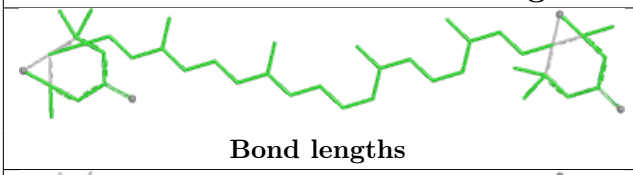


Torsions

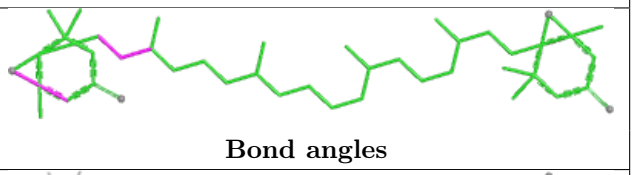


Rings

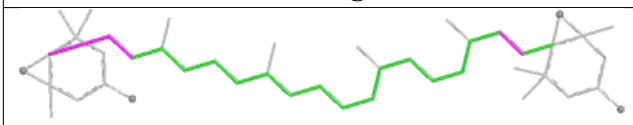
Ligand XAT a 616



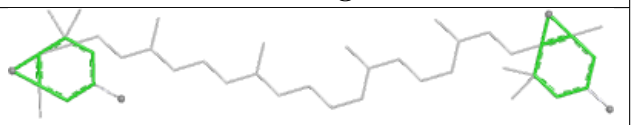
Bond lengths



Bond angles

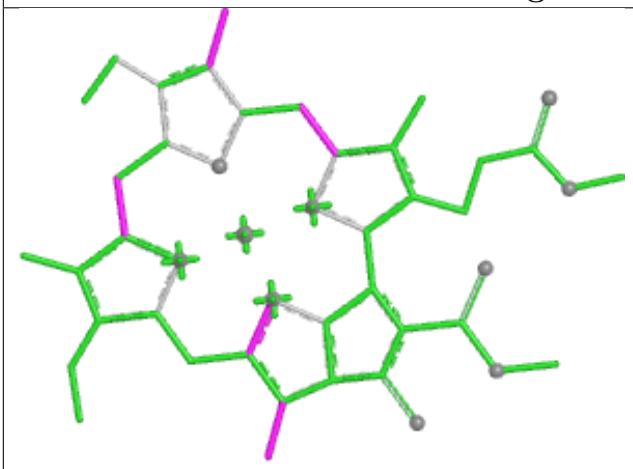


Torsions



Rings

Ligand CLA b 613



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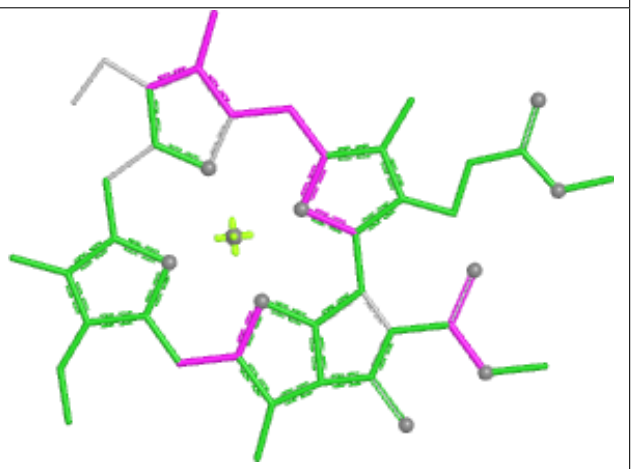
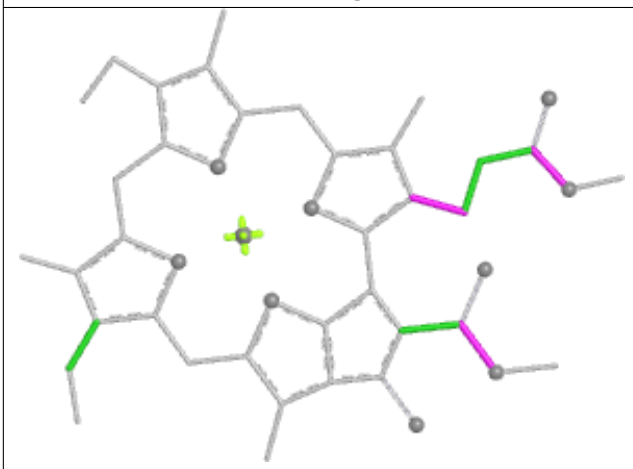
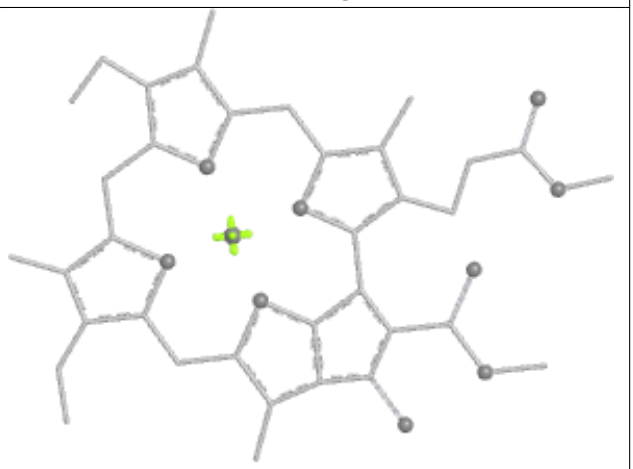


Bond angles

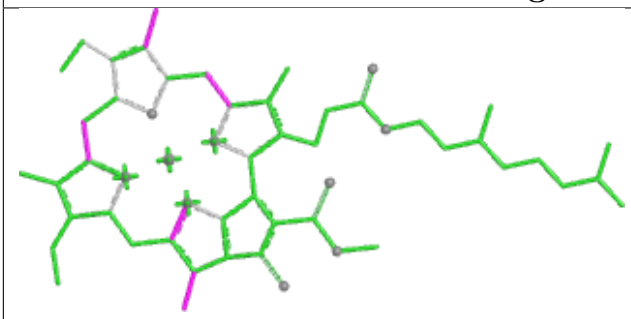


Torsions

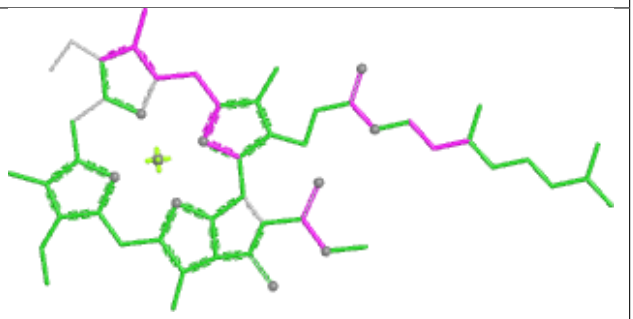


Rings

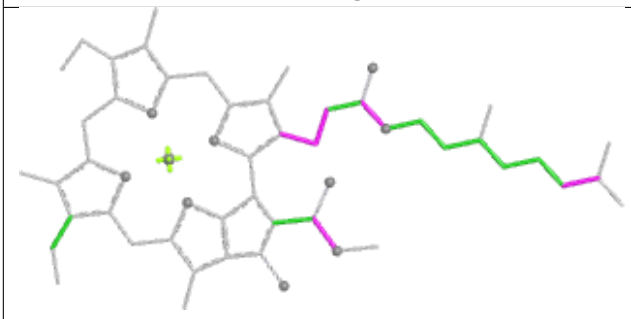
Ligand CLA 3 308



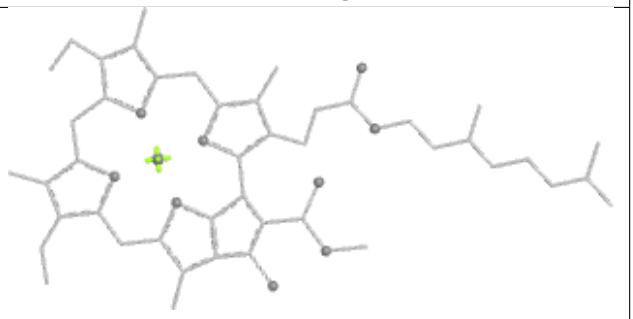
Bond lengths



Bond angles

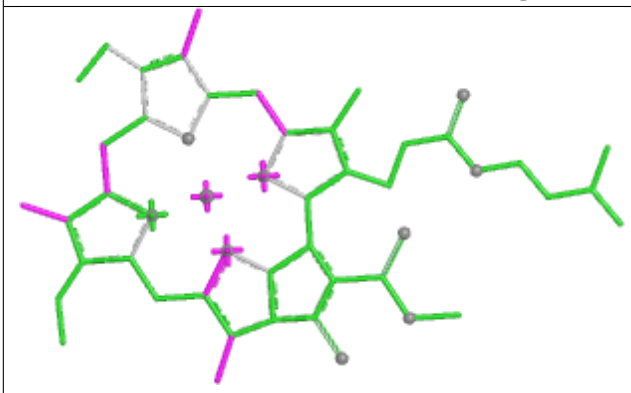


Torsions

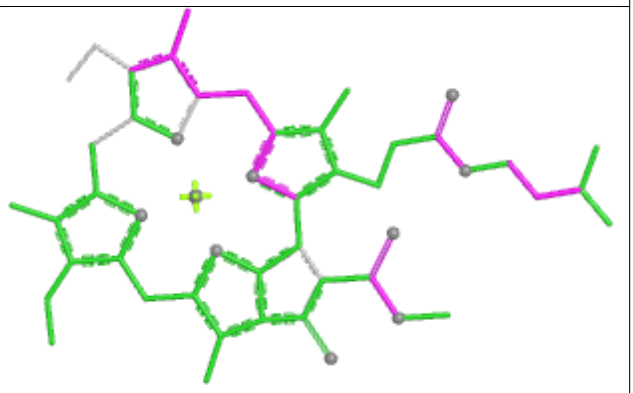


Rings

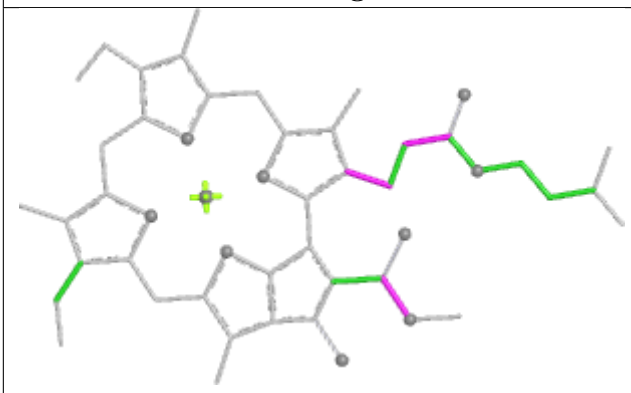
Ligand CLA A 5010



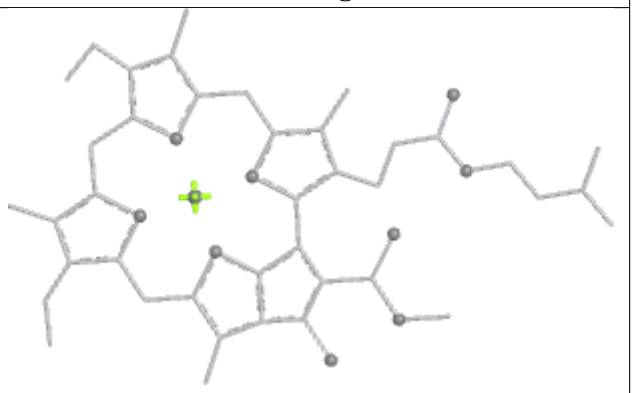
Bond lengths



Bond angles

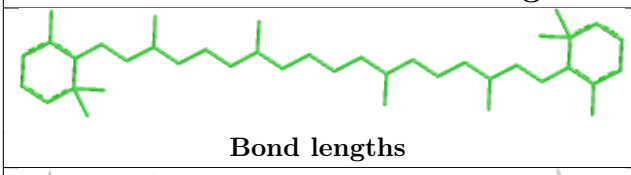


Torsions

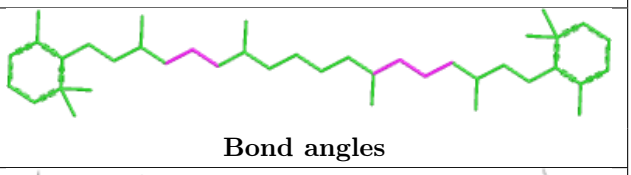


Rings

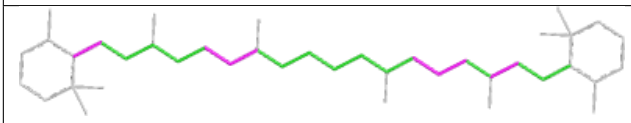
Ligand BCR B 845



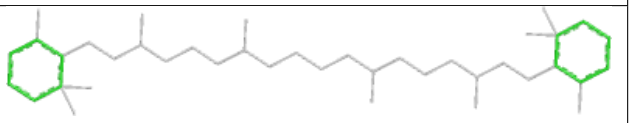
Bond lengths



Bond angles

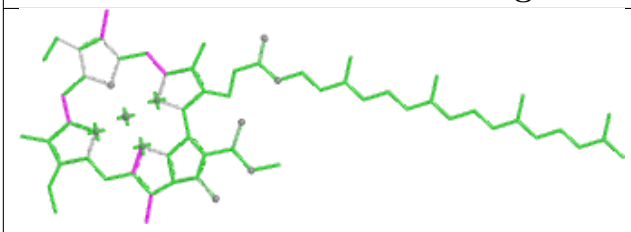


Torsions



Rings

Ligand CLA A 5022



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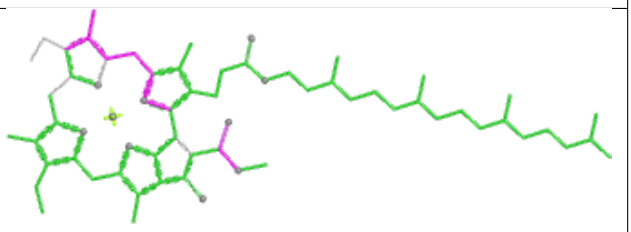
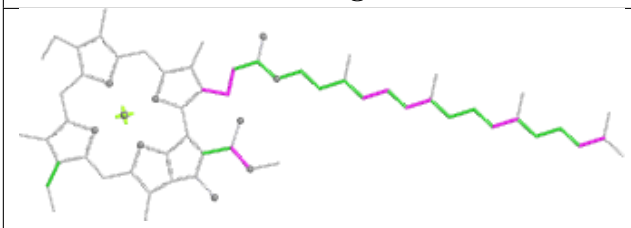
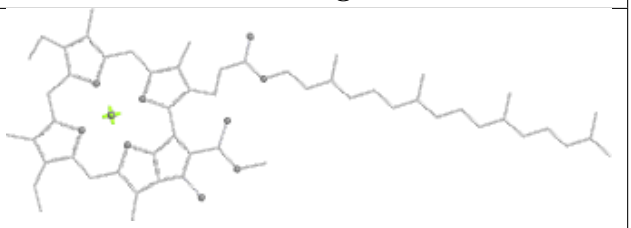


Bond angles

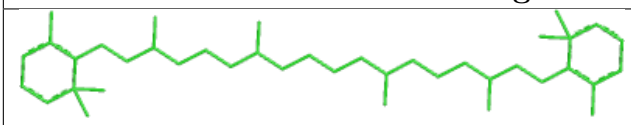


Torsions

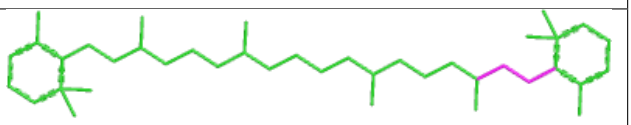


Rings

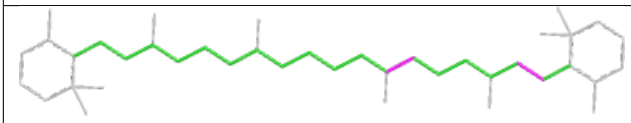
Ligand BCR A 5049



Bond lengths



Bond angles



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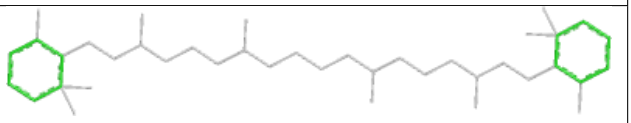
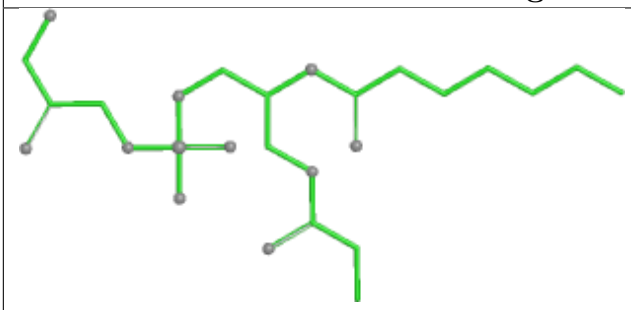
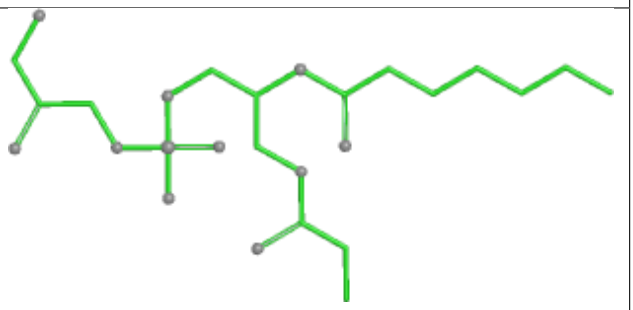


Rings

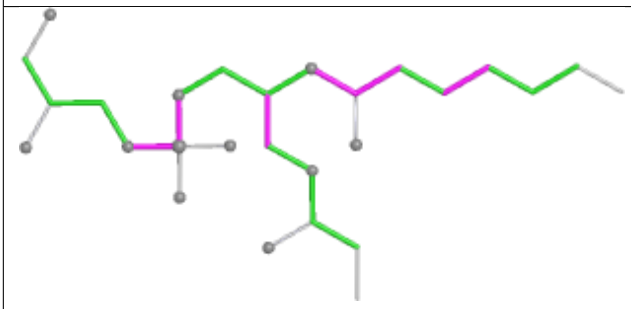
Ligand LHG 1 618



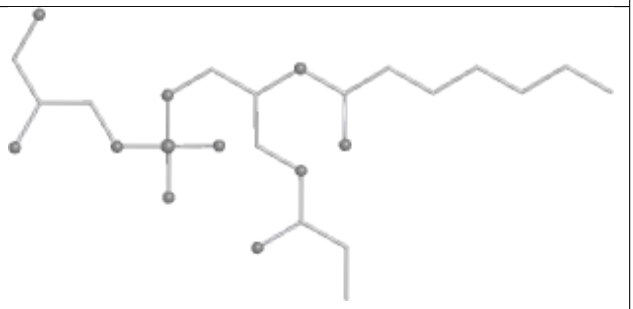
Bond lengths



Bond angles

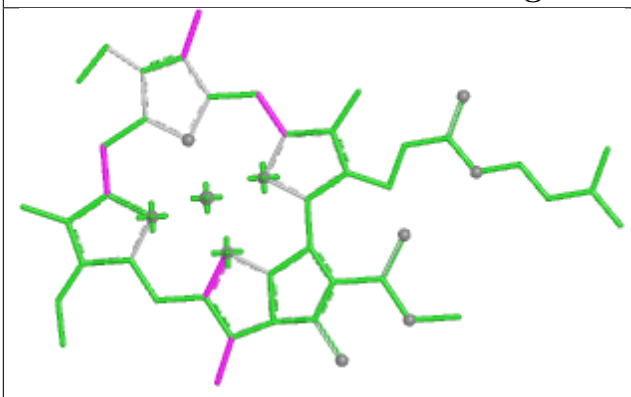


Torsions

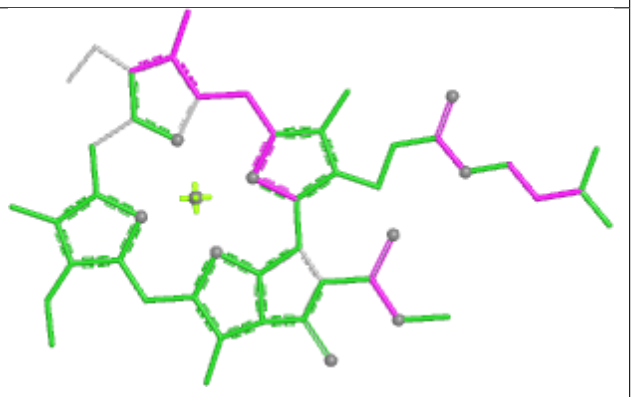


Rings

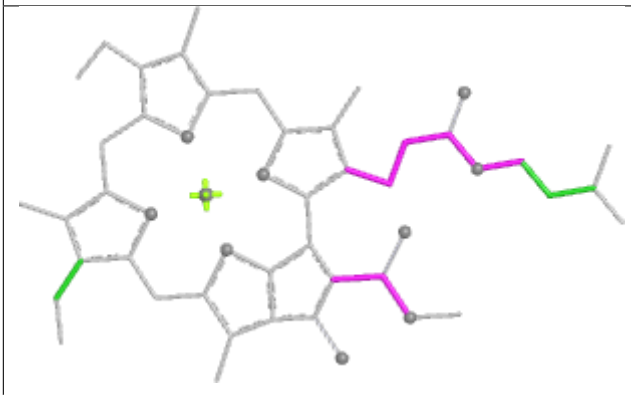
Ligand CLA B 834



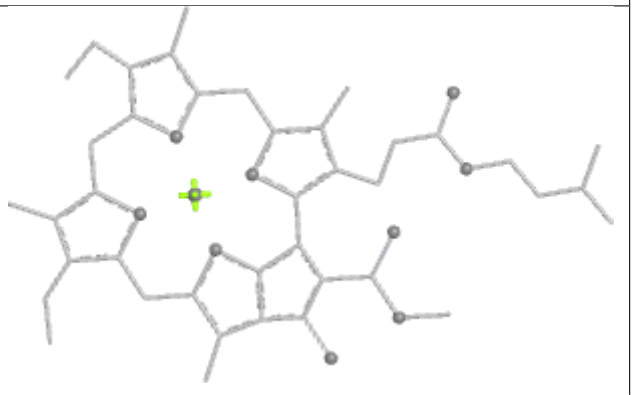
Bond lengths



Bond angles

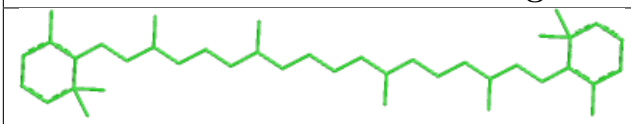


Torsions

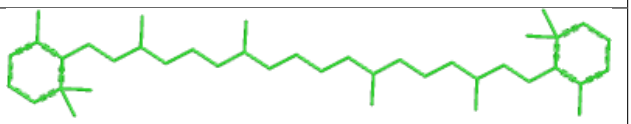


Rings

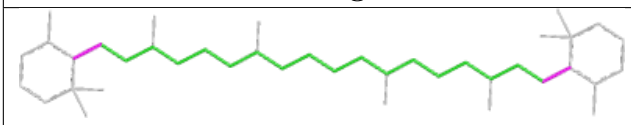
Ligand BCR 3 317



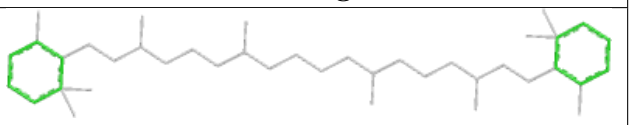
Bond lengths



Bond angles

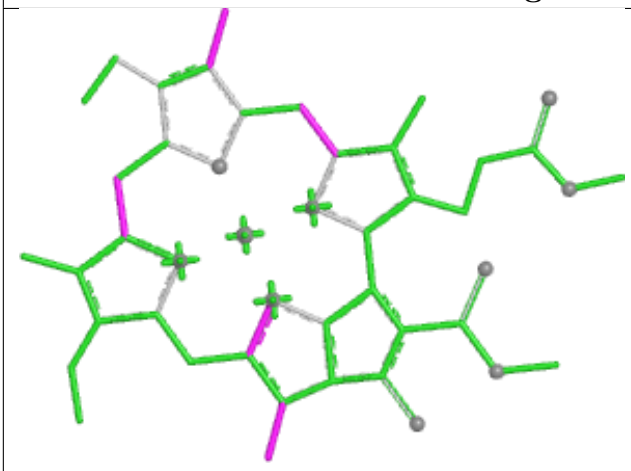


Torsions

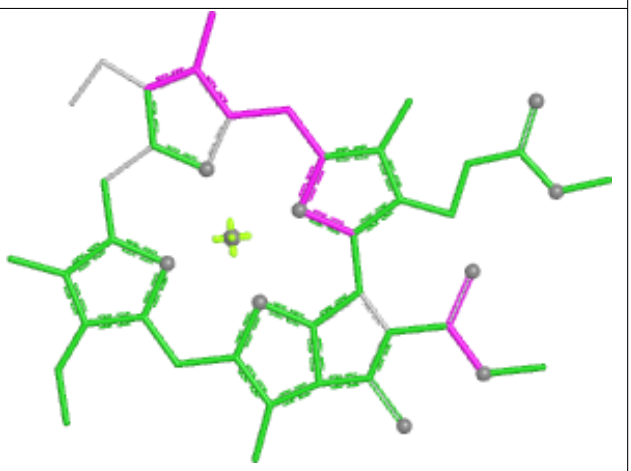


Rings

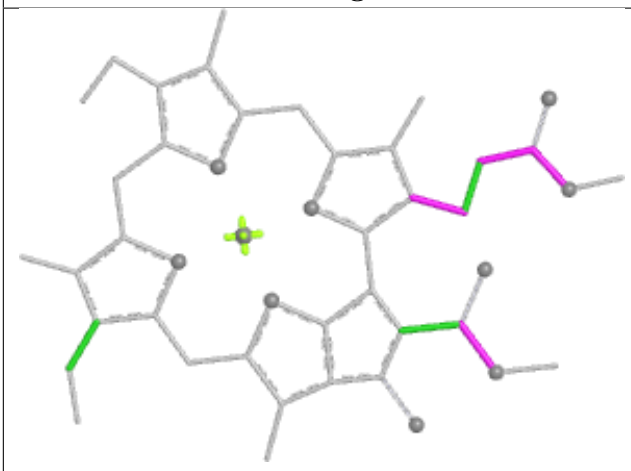
Ligand CLA T 411



Bond lengths



Bond angles



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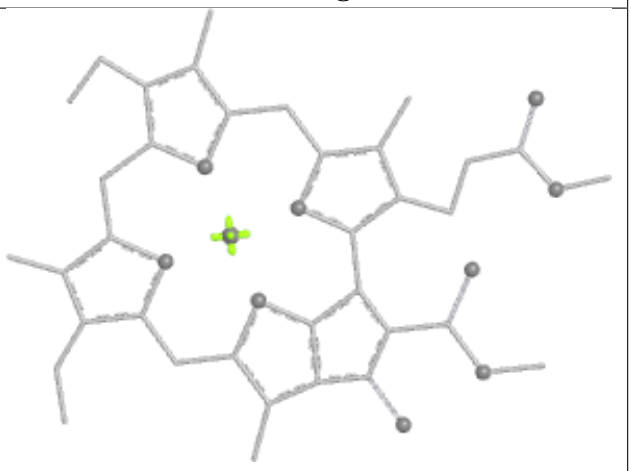
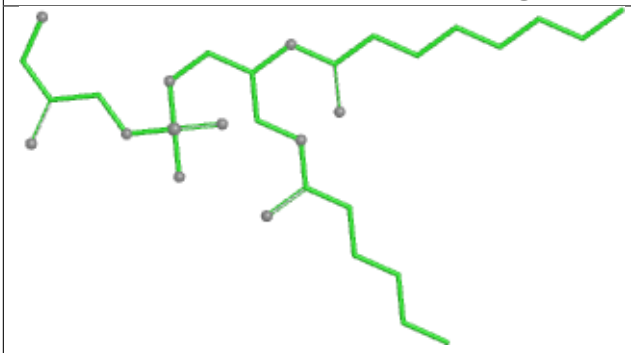
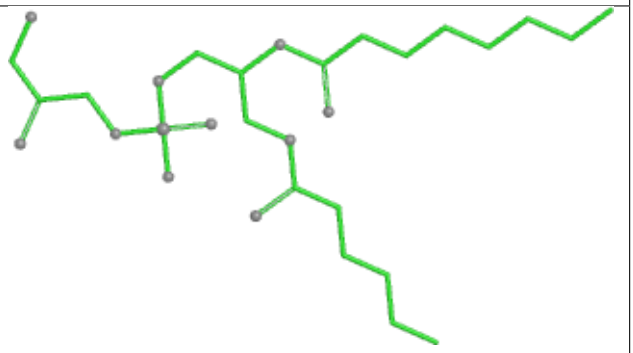


Rings

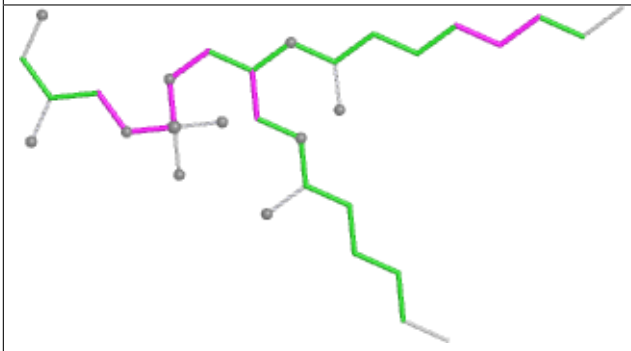
Ligand LHG F 5001



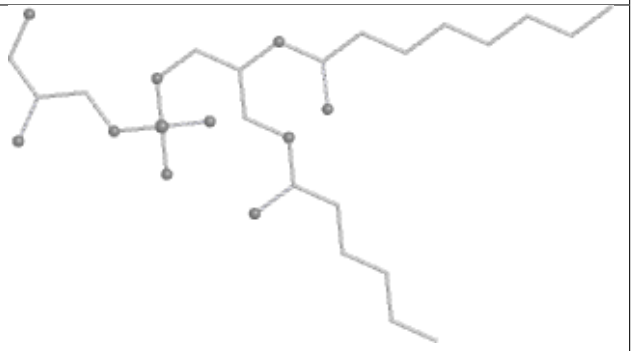
Bond lengths



Bond angles

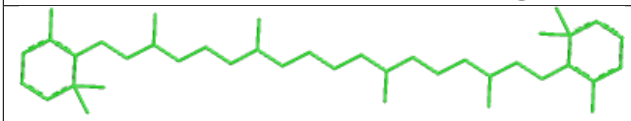


Torsions

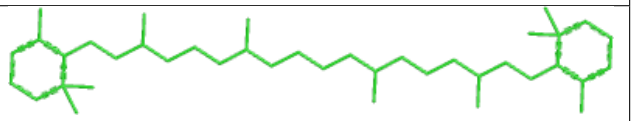


Rings

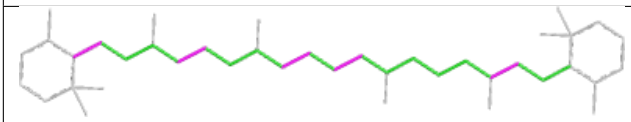
Ligand BCR A 5048



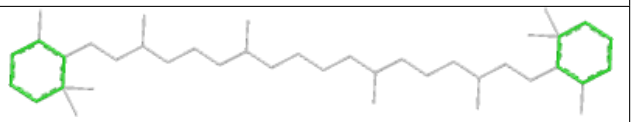
Bond lengths



Bond angles

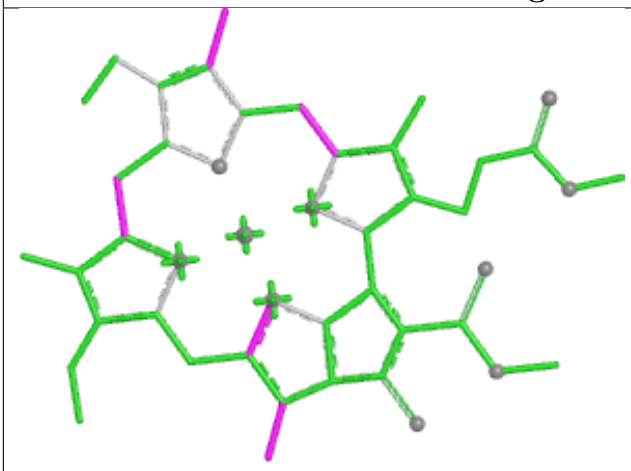


Torsions

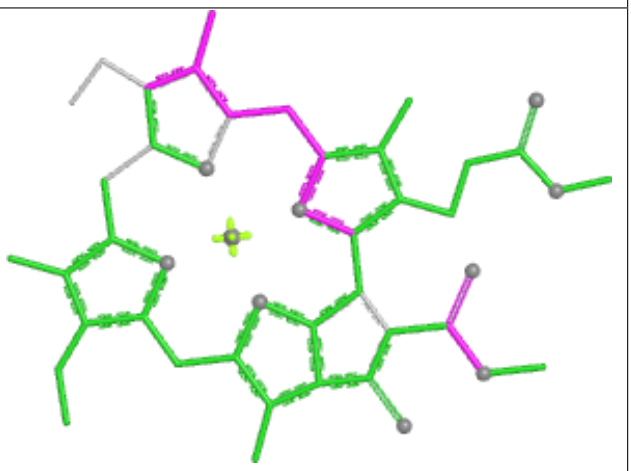


Rings

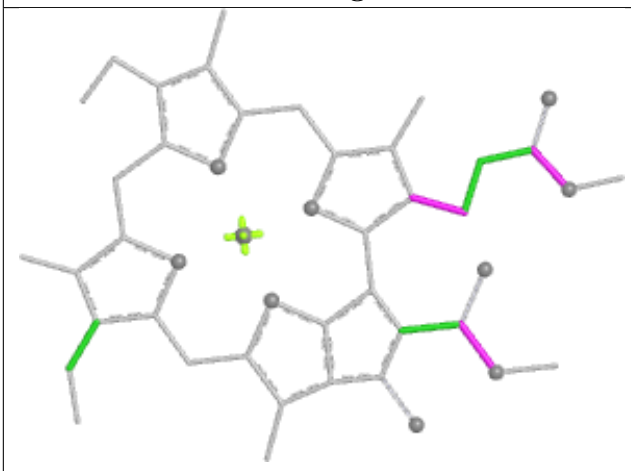
Ligand CLA 1 613



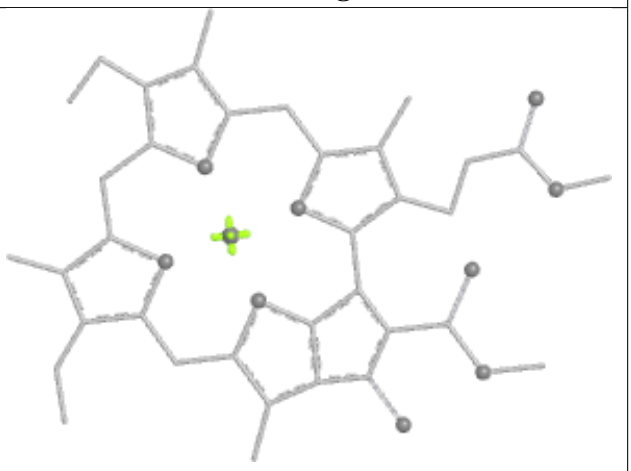
Bond lengths



Bond angles

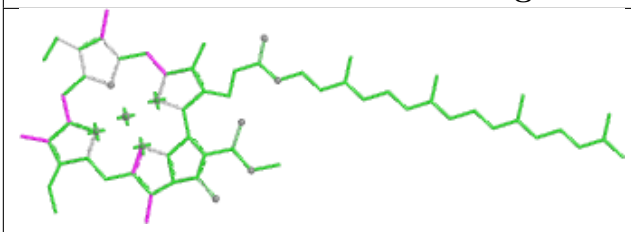


Torsions

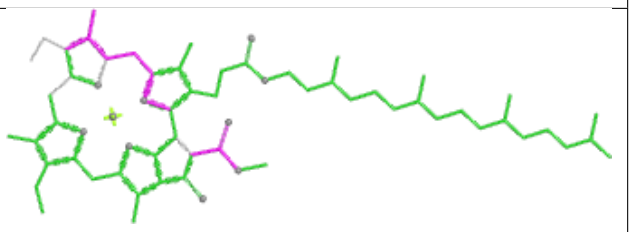


Rings

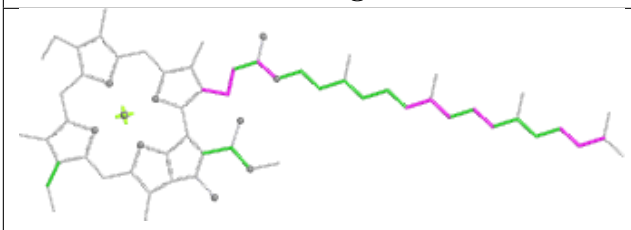
Ligand CLA A 5014



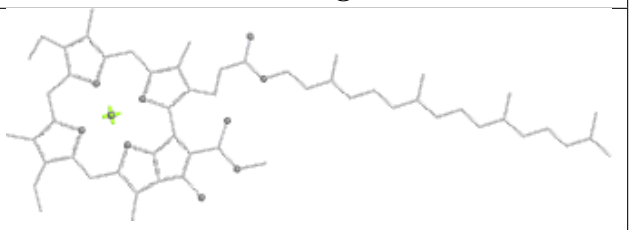
Bond lengths



Bond angles

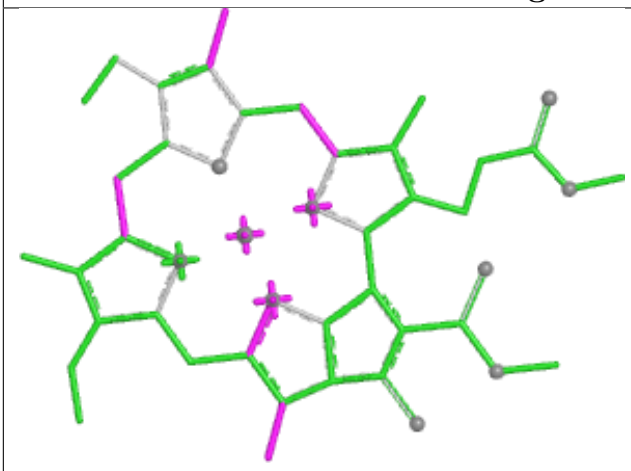


Torsions

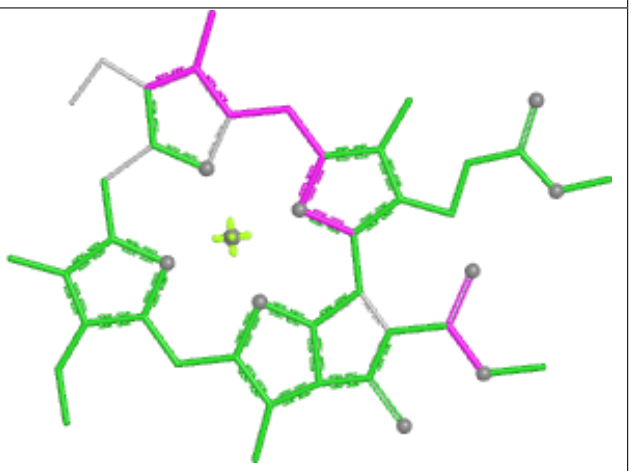


Rings

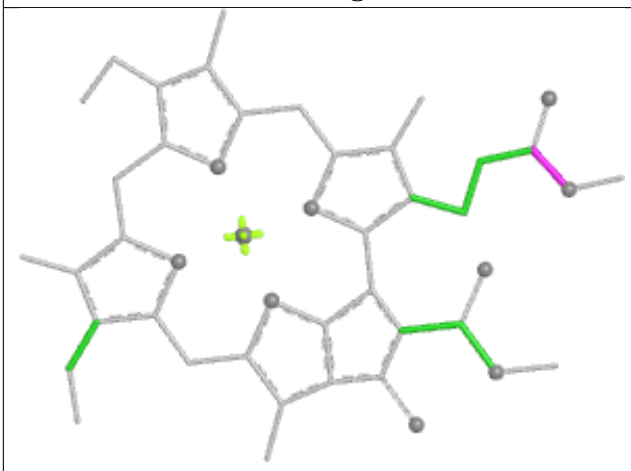
Ligand CLA a 607



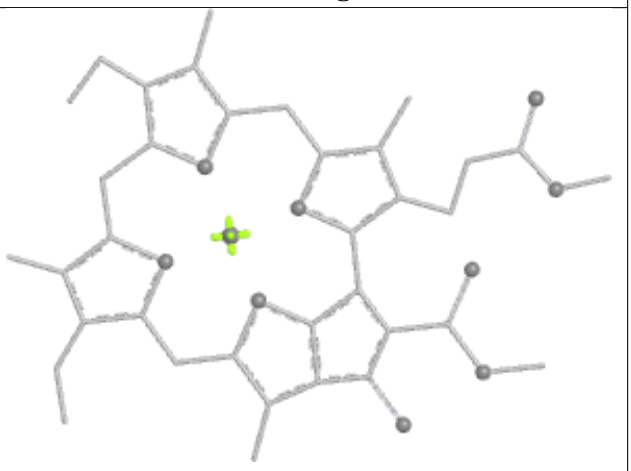
Bond lengths



Bond angles

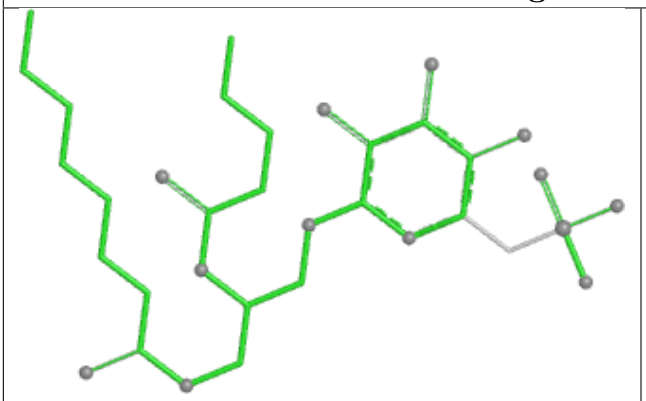


Torsions

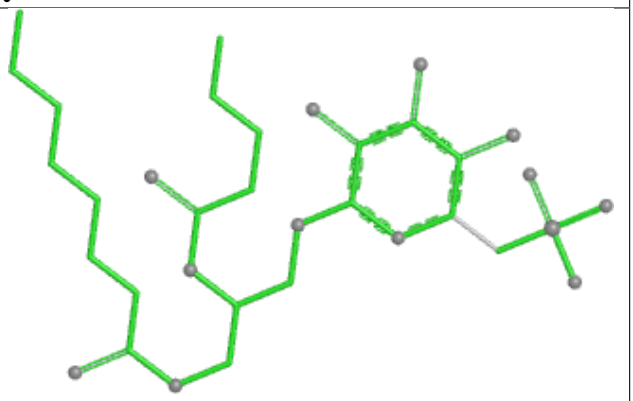


Rings

Ligand SQD 3 320



Bond lengths



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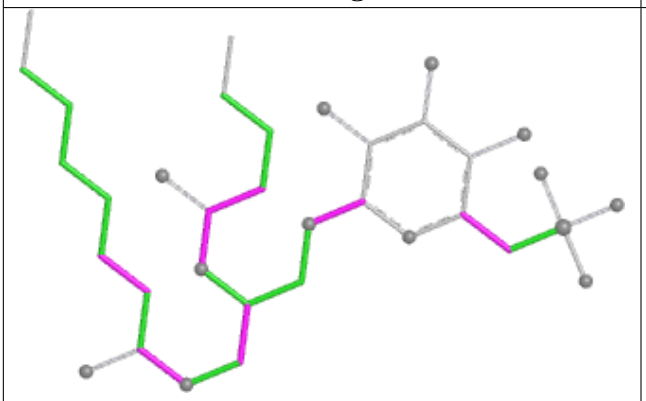
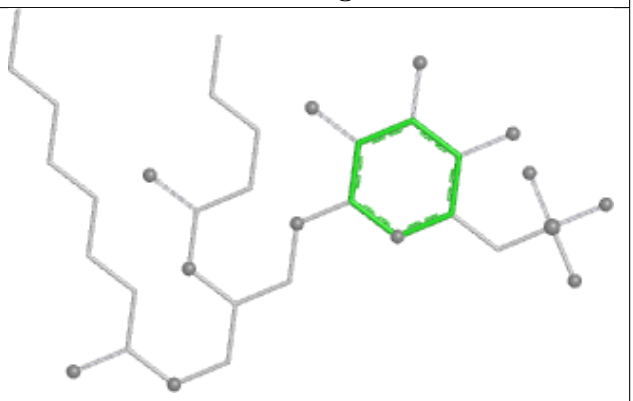


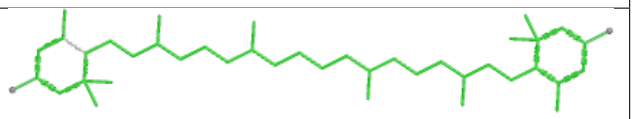
Torsions



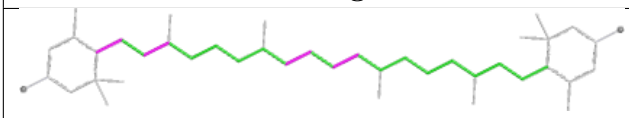
Rings

Ligand LUT c 314

Bond lengths



Bond angles



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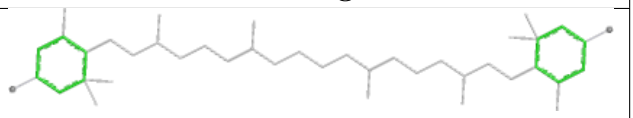
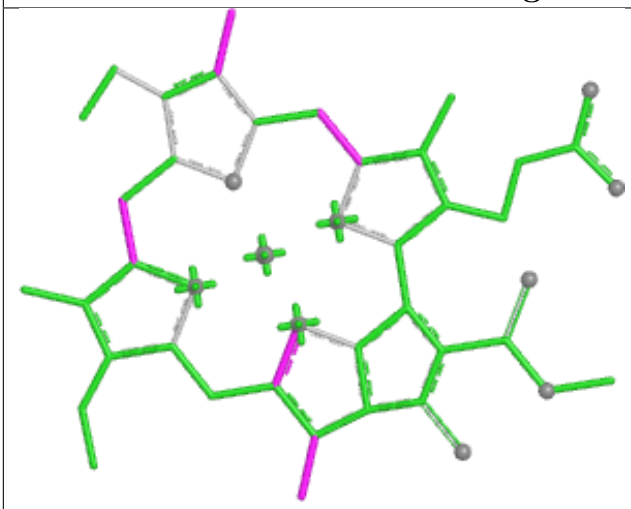
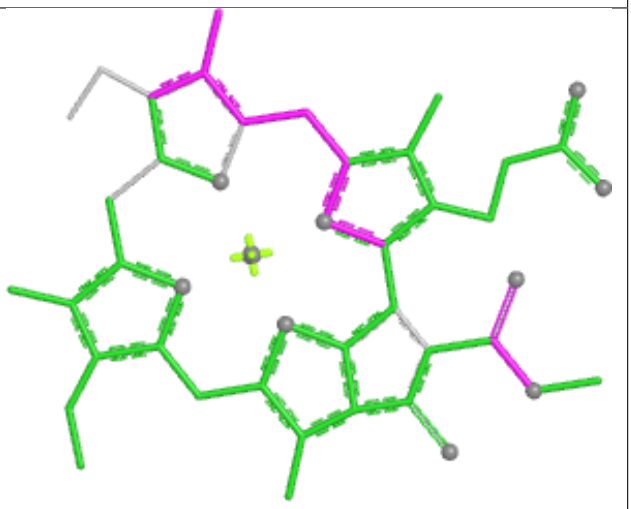


Rings

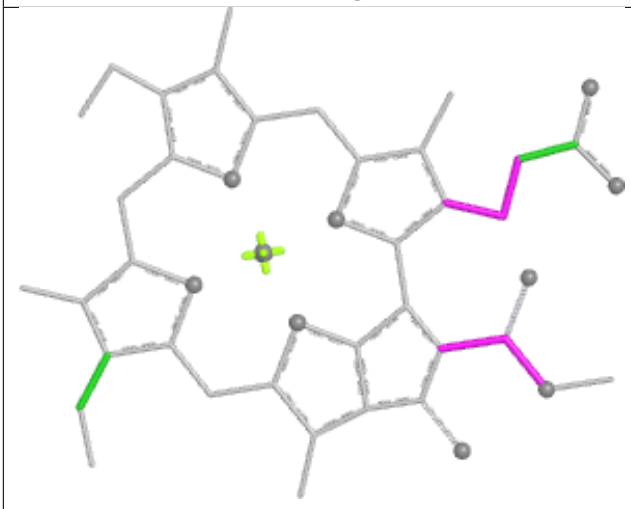
Ligand CLA K 204



Bond lengths



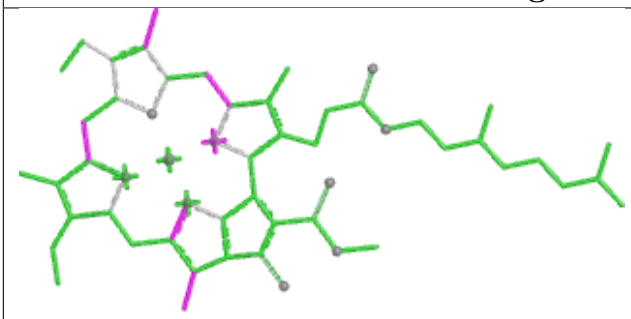
Bond angles



Torsions

Rings

Ligand CLA 8 311



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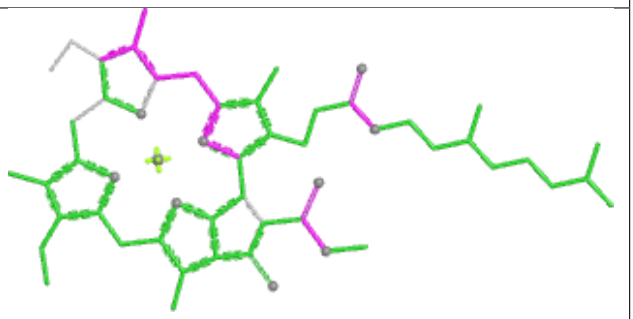
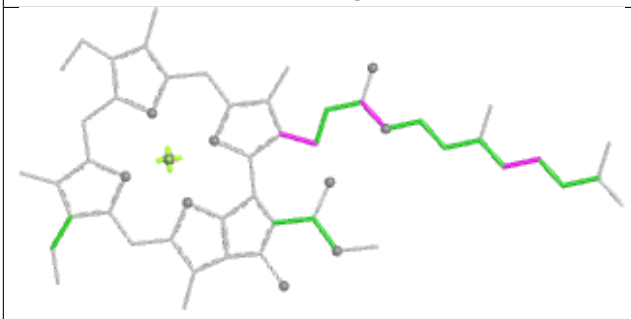


Bond angles



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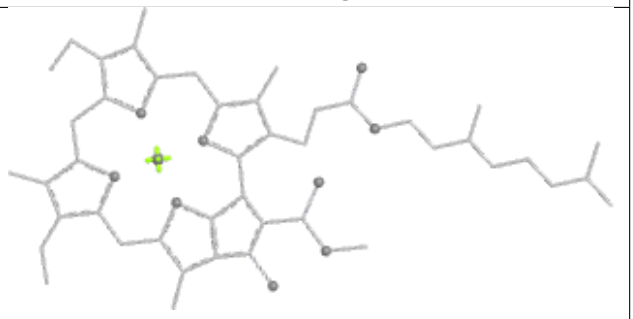
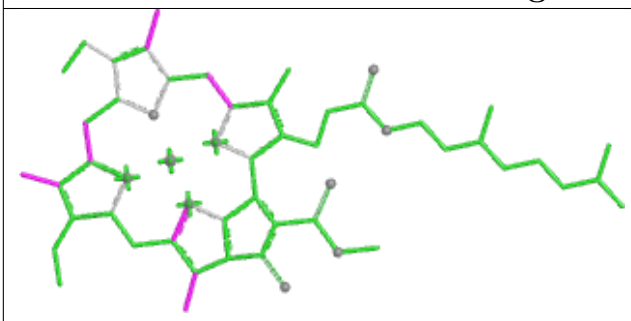


Rings

Ligand CLA a 602



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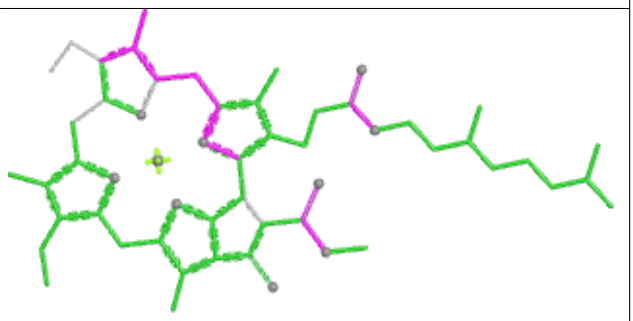
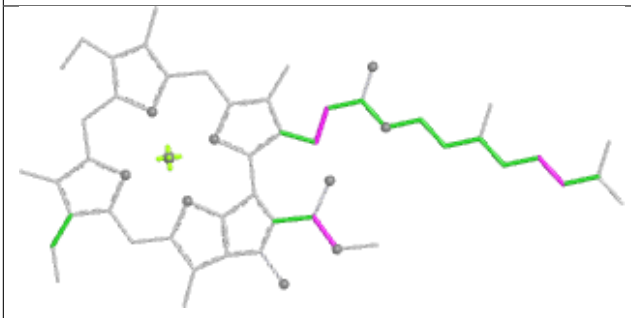


Bond angles



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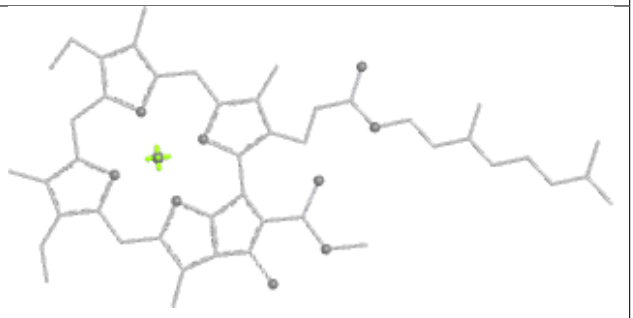
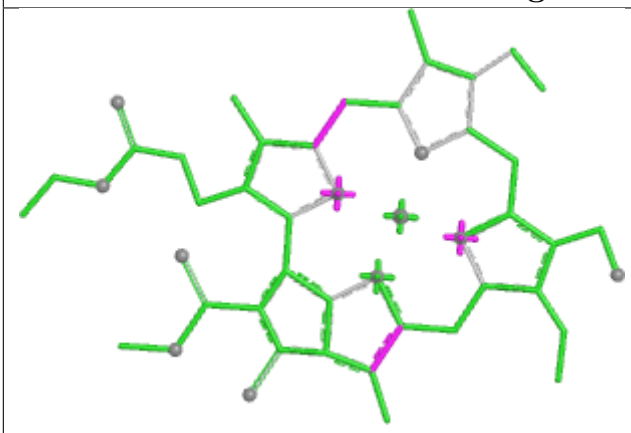
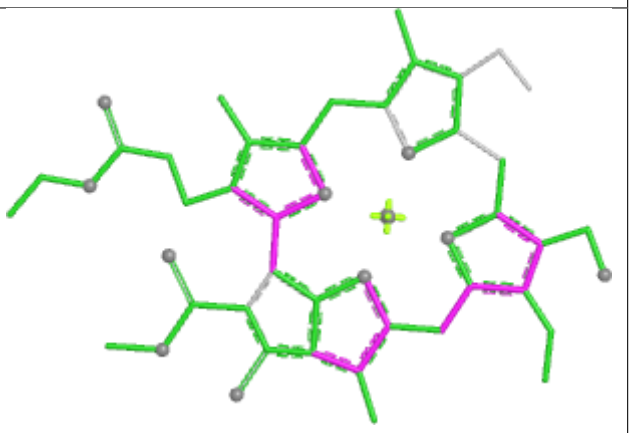


Rings

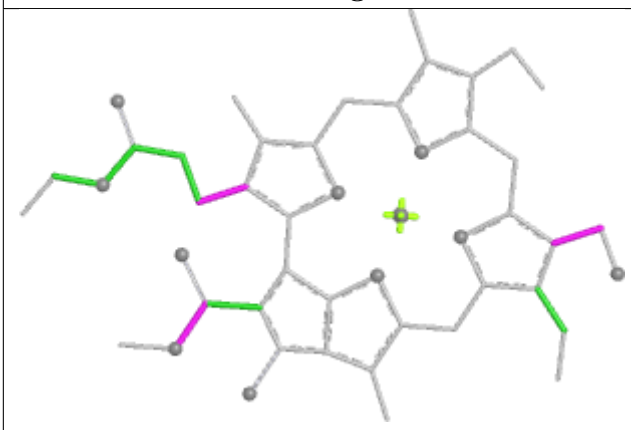
Ligand CHL 7 307



Bond lengths



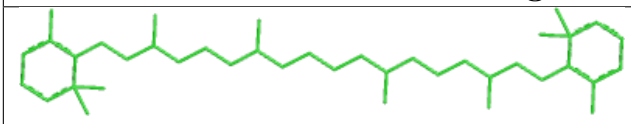
Bond angles



Torsions

Rings

Ligand BCR 1 617



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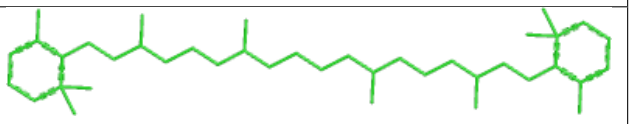
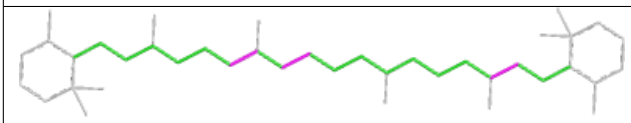


Bond angles



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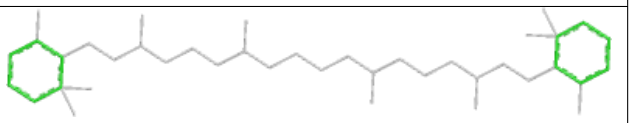
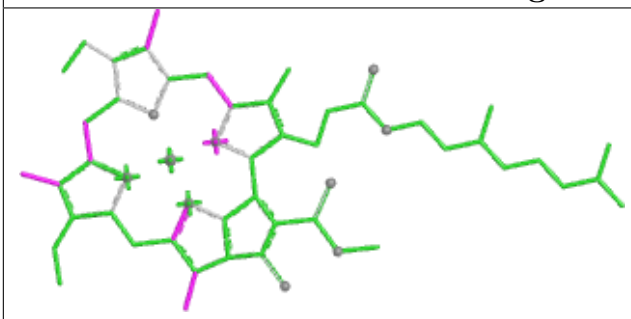
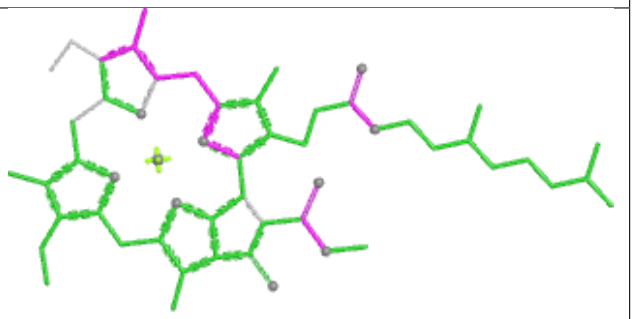


Rings

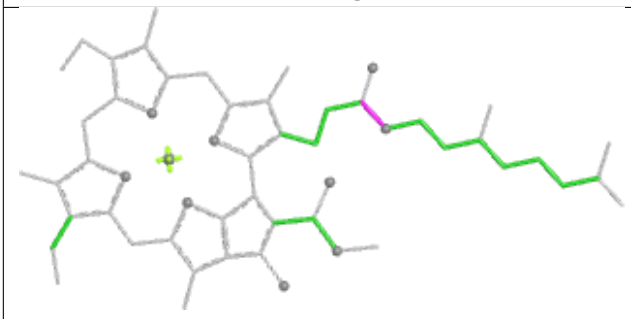
Ligand CLA 7 303



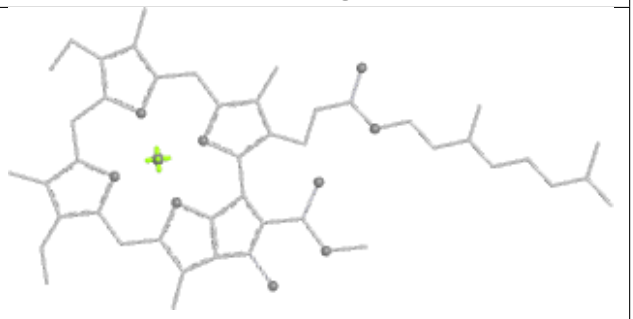
Bond lengths



Bond angles

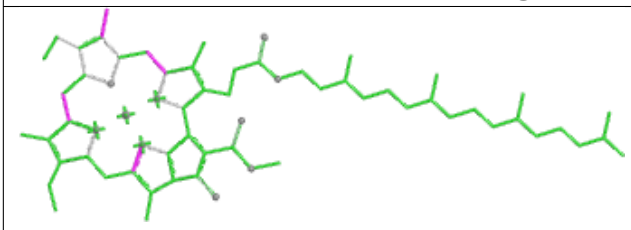


Torsions

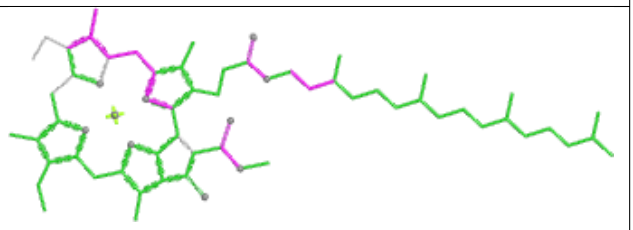


Rings

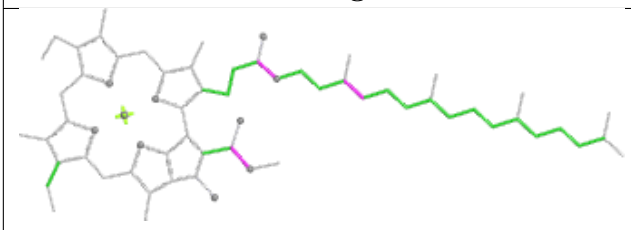
Ligand CLA A 5034



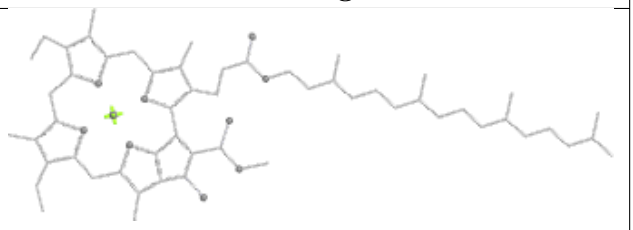
Bond lengths



Bond angles

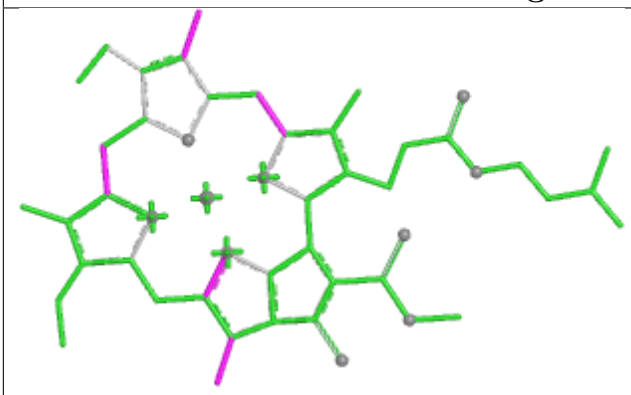


Torsions



Rings

Ligand CLA b 610



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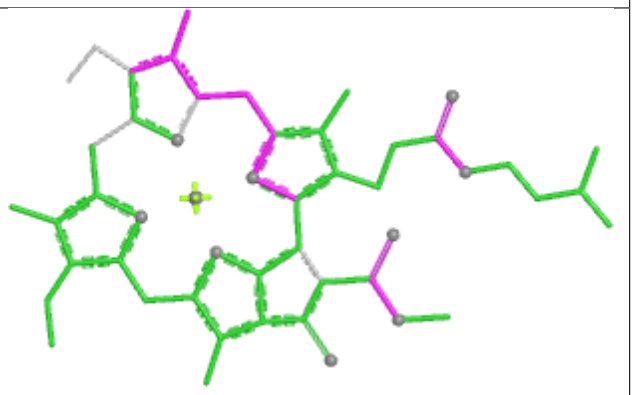
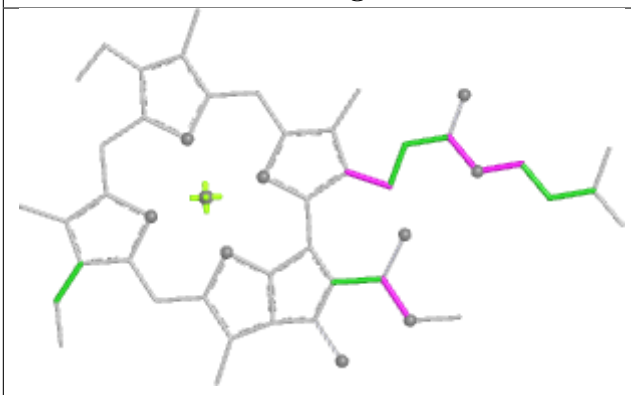


Bond angles



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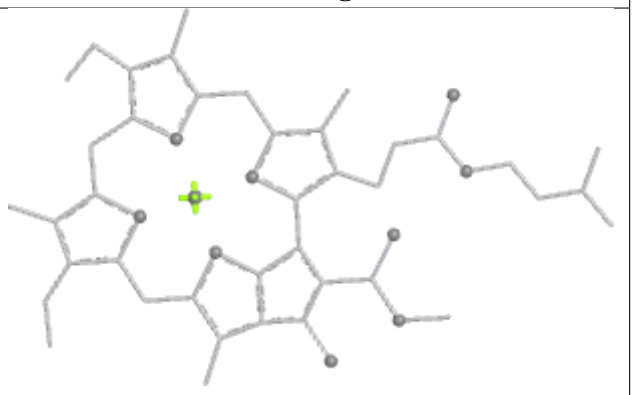
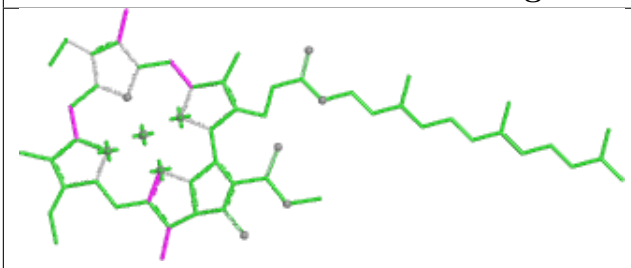
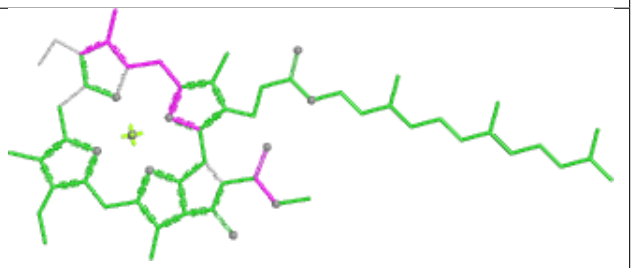


Rings

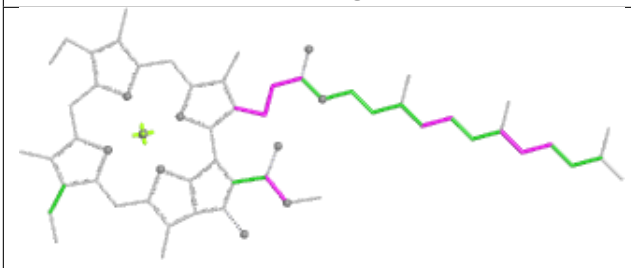
Ligand CLA B 827



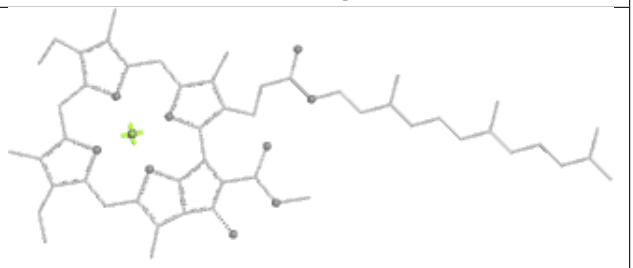
Bond lengths



Bond angles

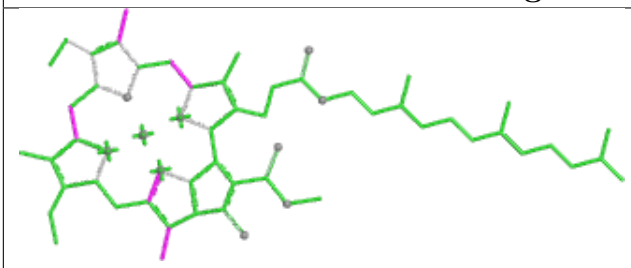


Torsions

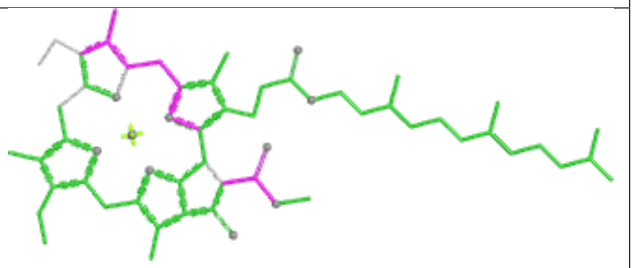


Rings

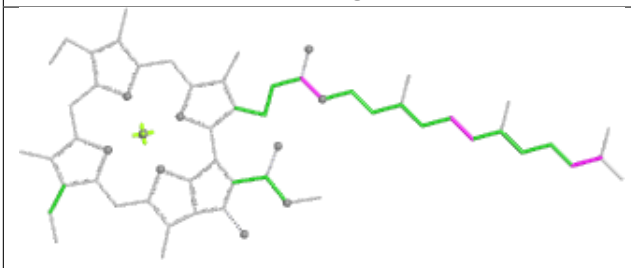
Ligand CLA B 836



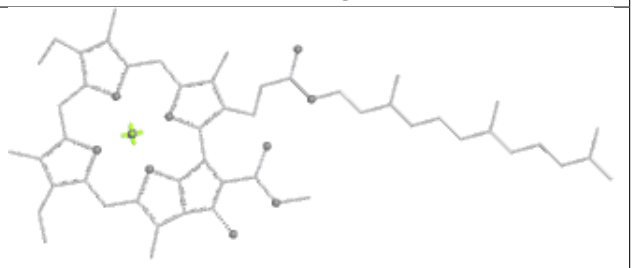
Bond lengths



Bond angles

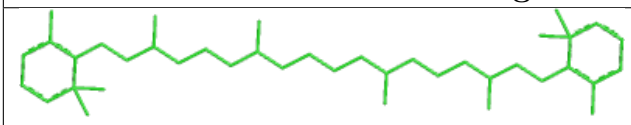


Torsions

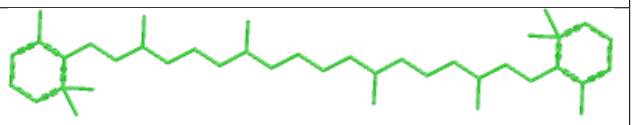


Rings

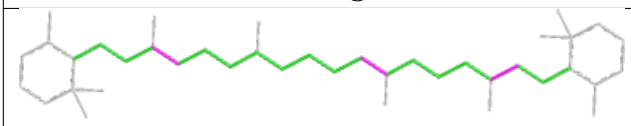
Ligand BCR A 5052



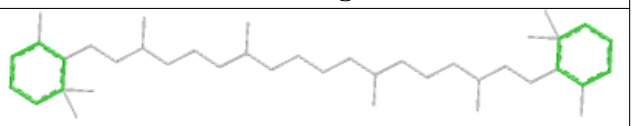
Bond lengths



Bond angles

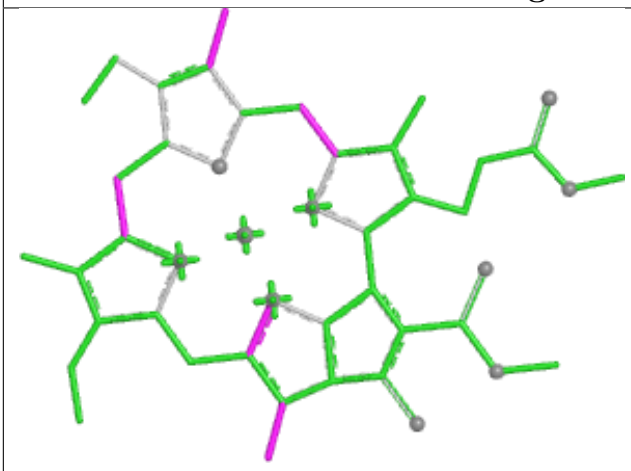


Torsions

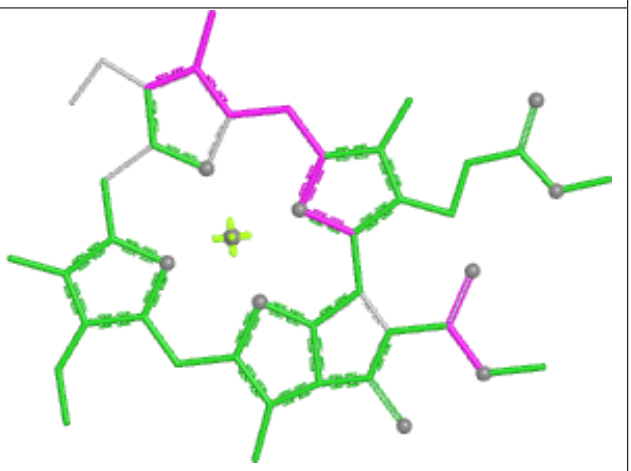


Rings

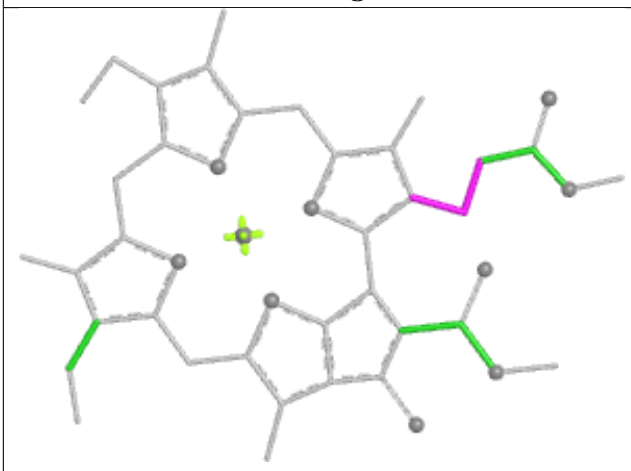
Ligand CLA 8 309



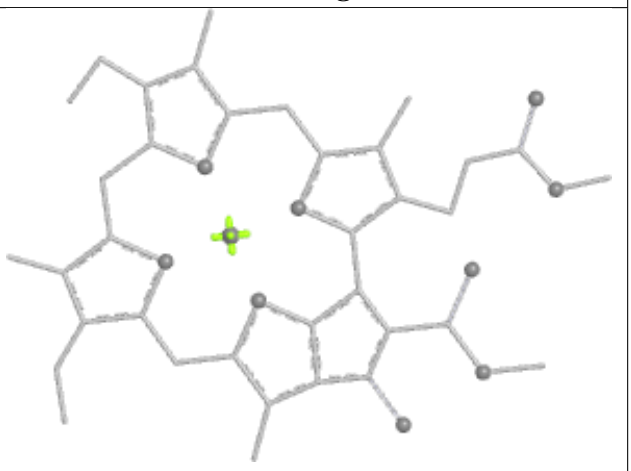
Bond lengths



Bond angles

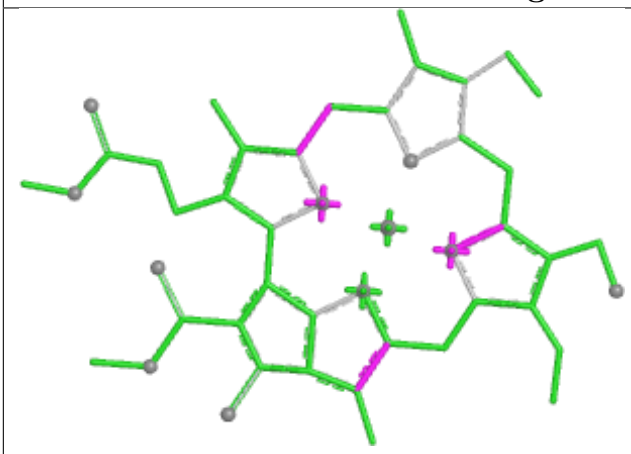


Torsions

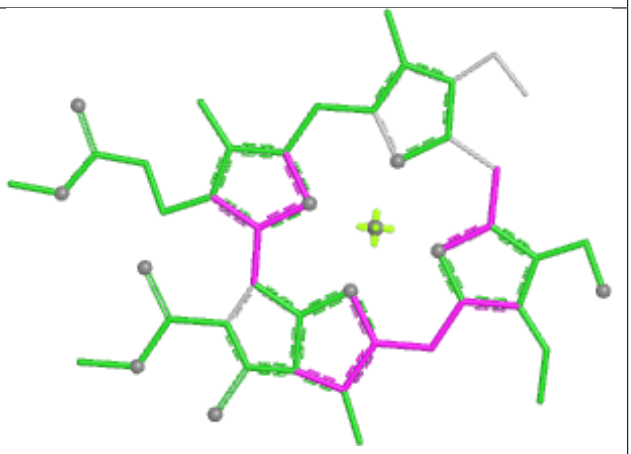


Rings

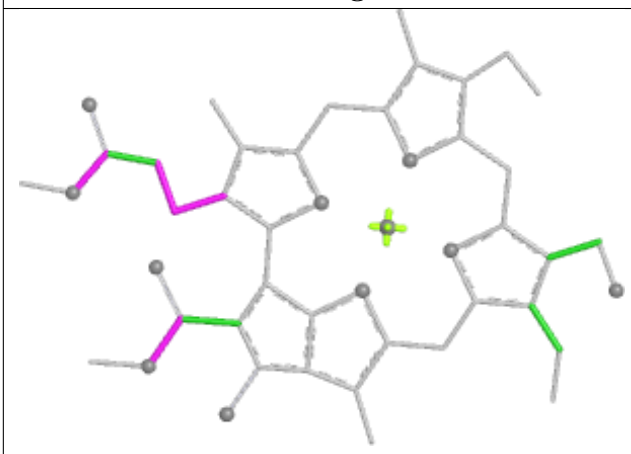
Ligand CHL 8 307



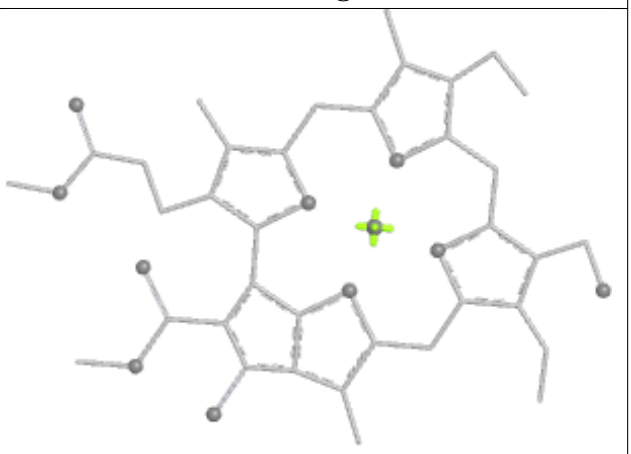
Bond lengths



Bond angles

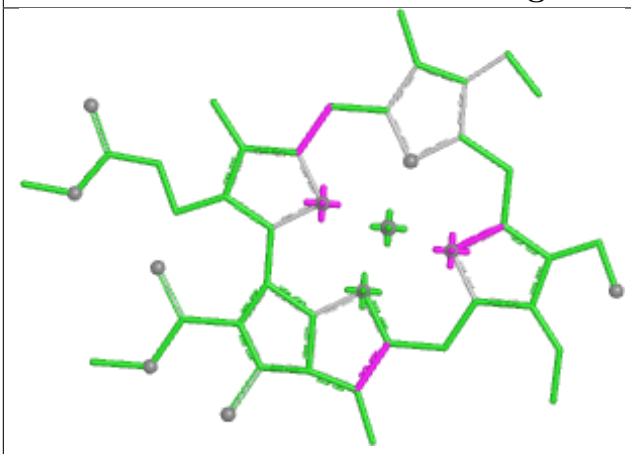


Torsions

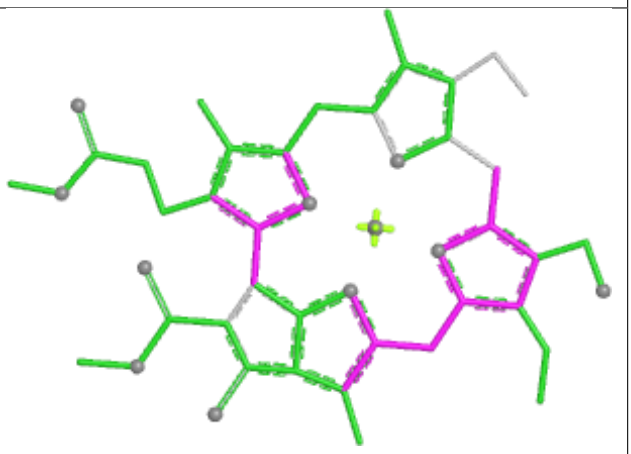


Rings

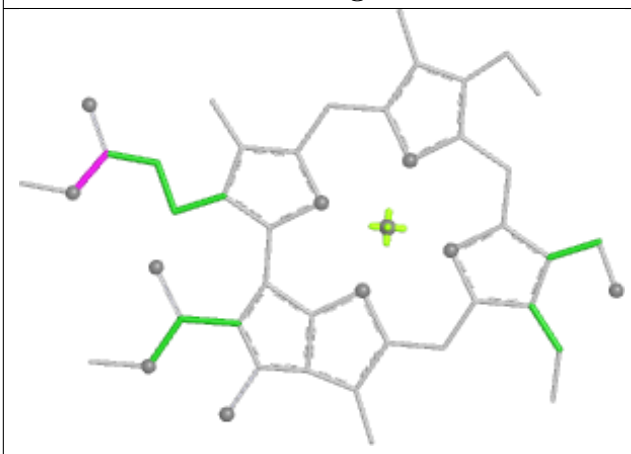
Ligand CHL 1 606



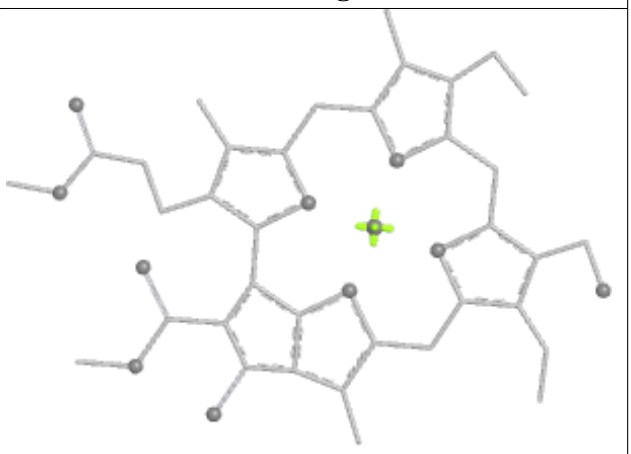
Bond lengths



Bond angles

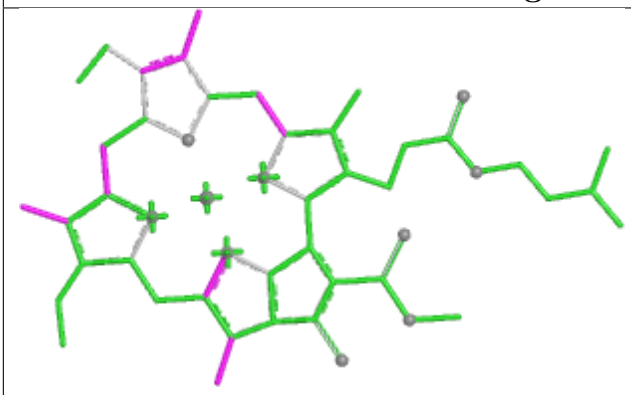


Torsions

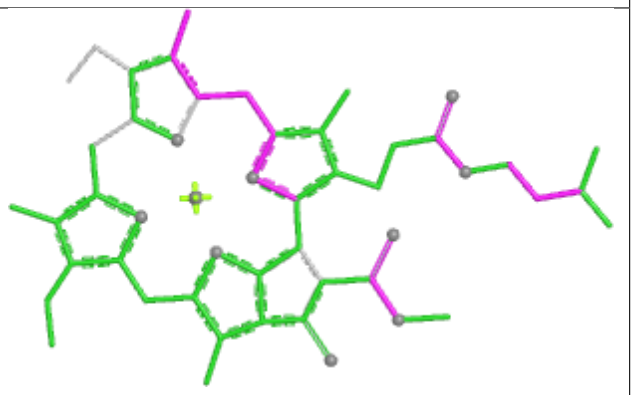


Rings

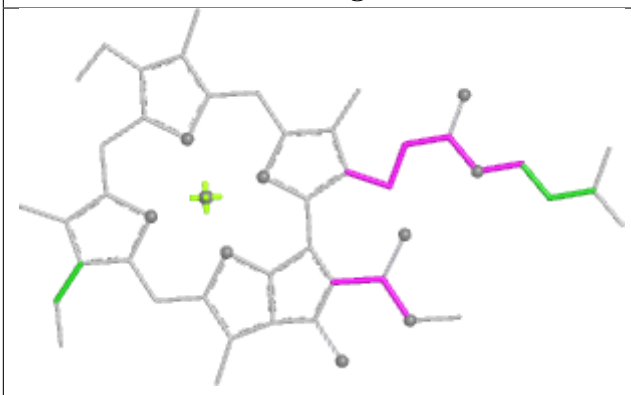
Ligand CLA B 814



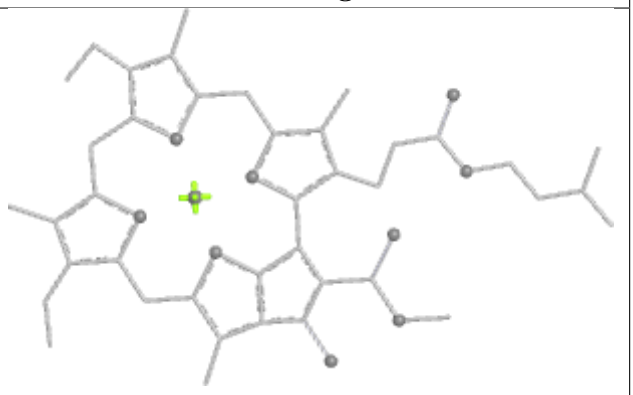
Bond lengths



Bond angles

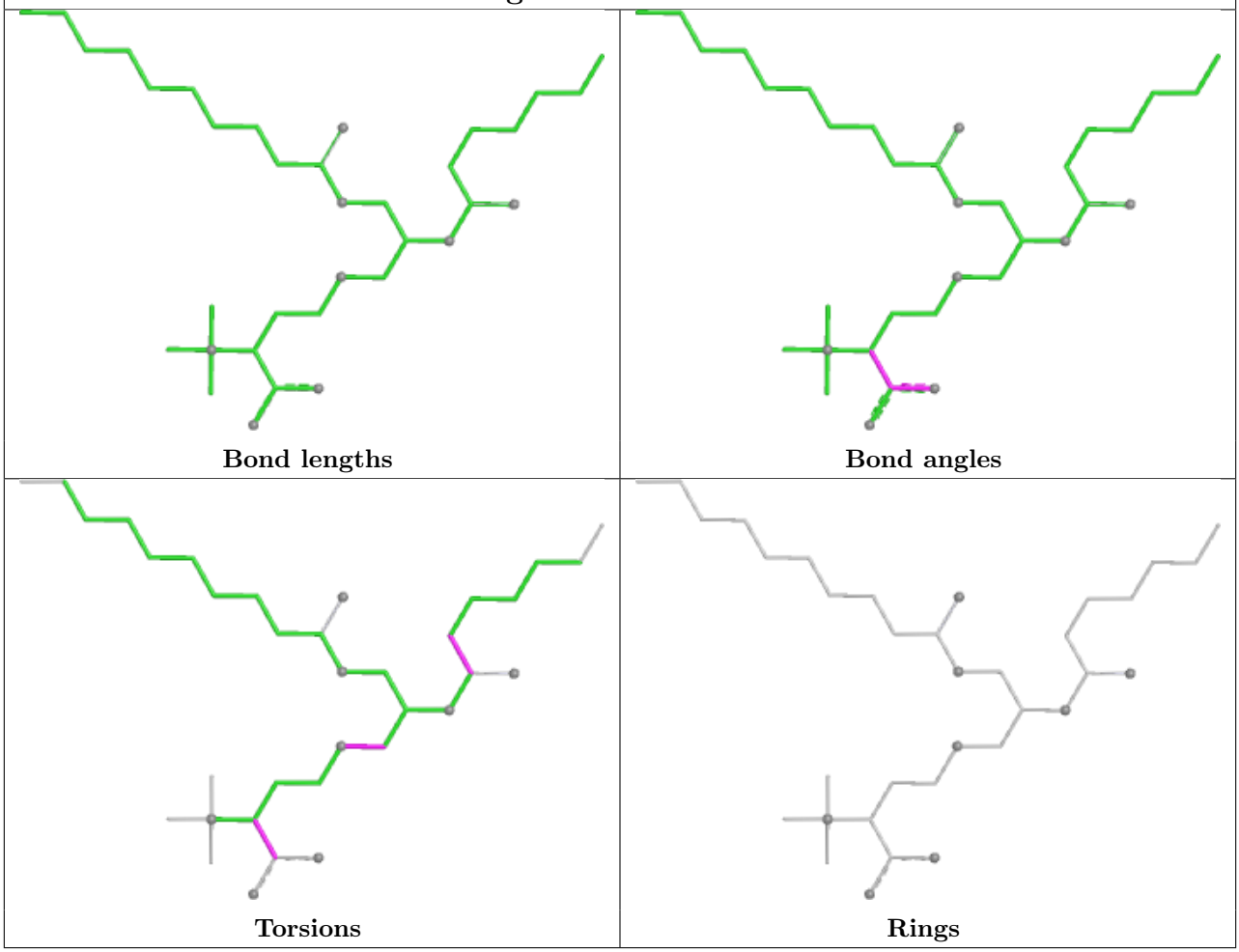


Torsions

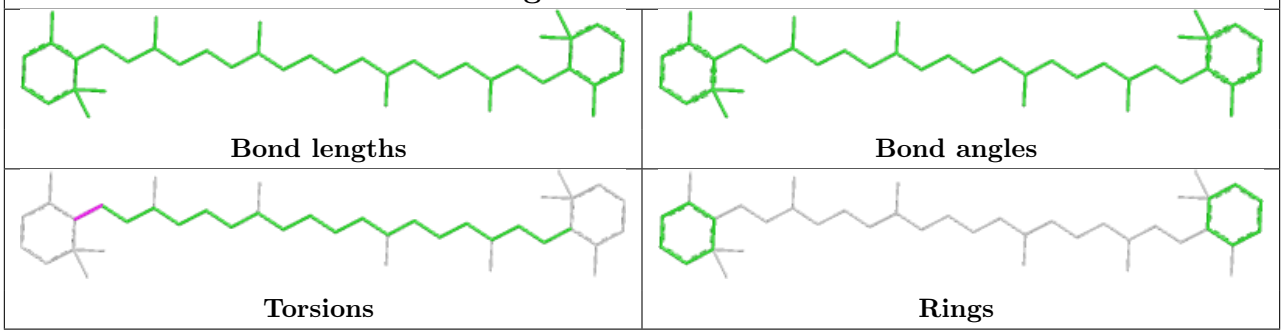


Rings

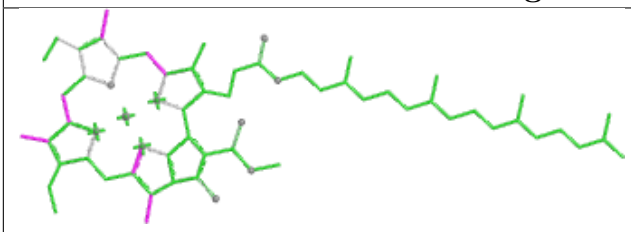
Ligand LMK J 101



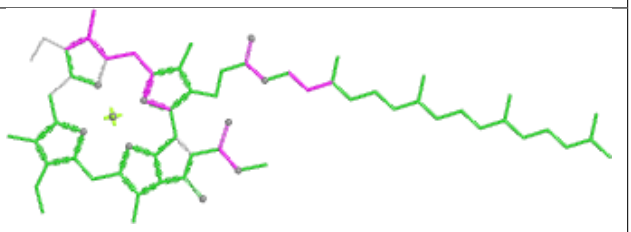
Ligand BCR B 844



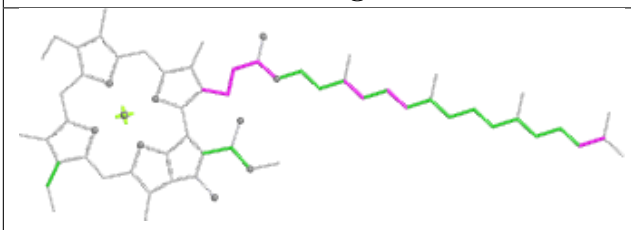
Ligand CLA B 818



Bond lengths



Bond angles



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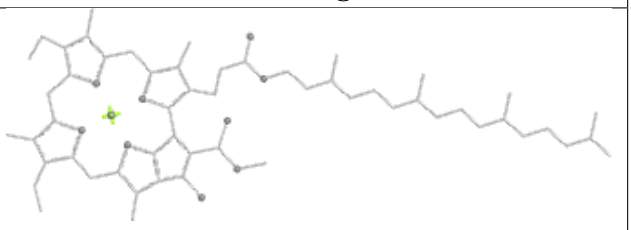
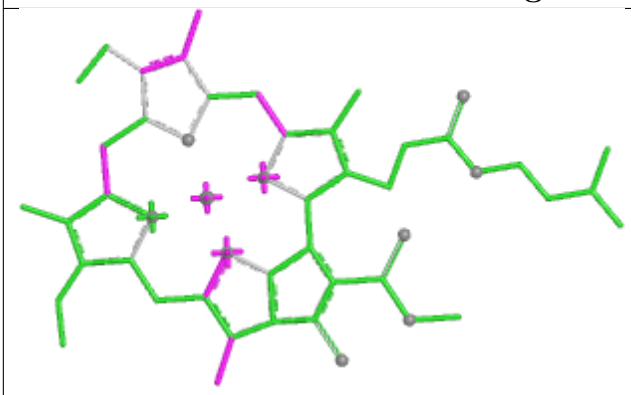
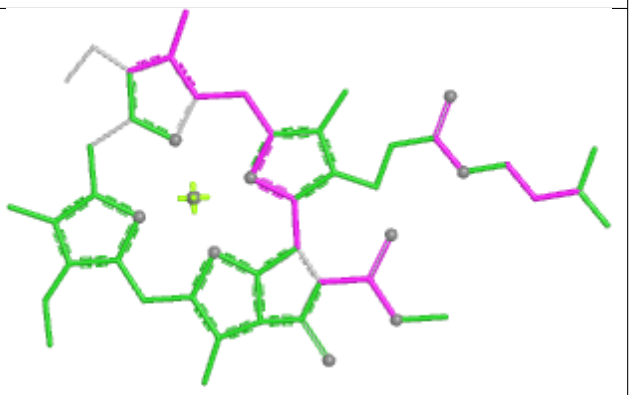


Rings

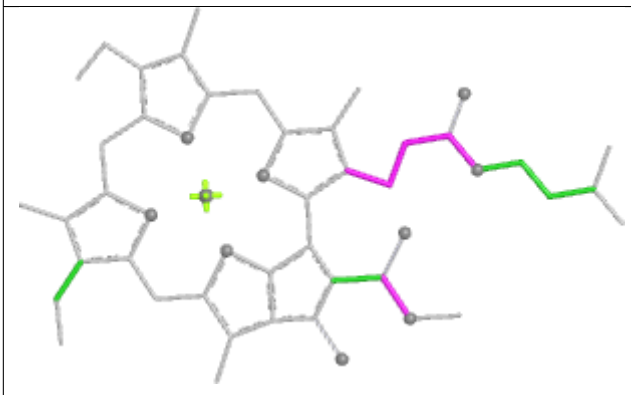
Ligand CLA T 403



Bond lengths



Bond angles



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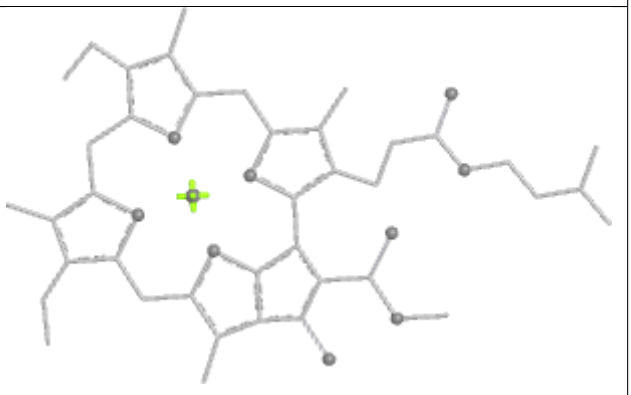
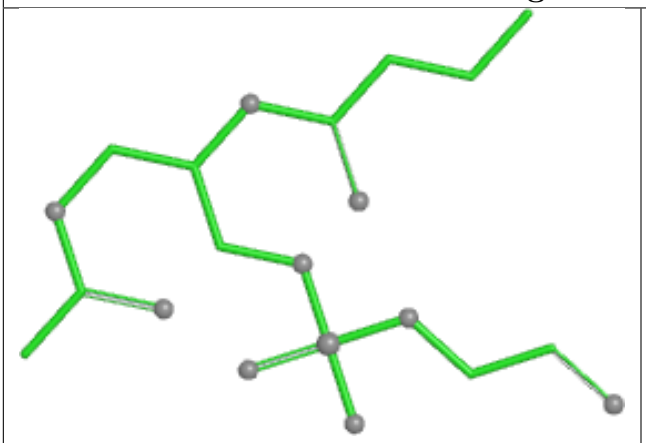
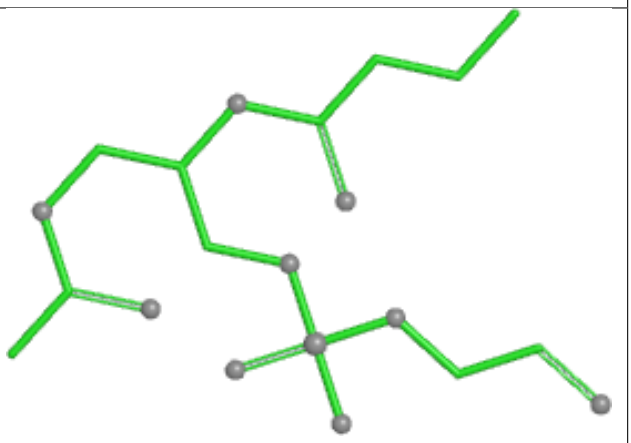


Rings

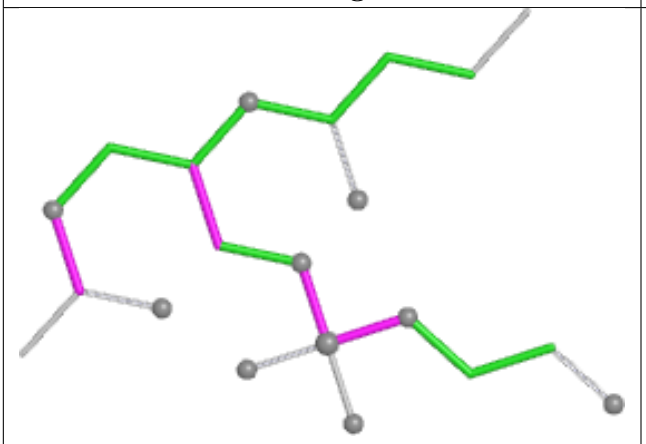
Ligand PTY 8 319



Bond lengths



Bond angles



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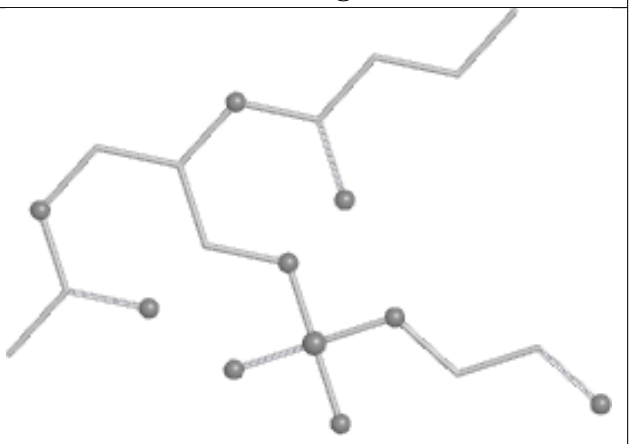
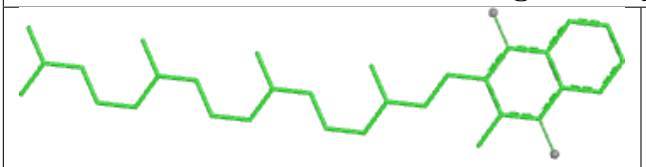
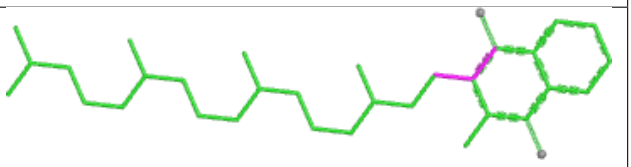


Rings

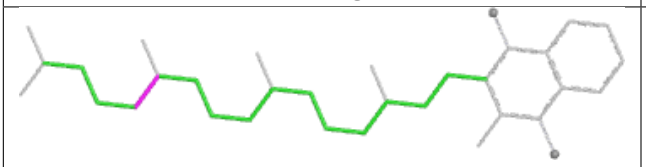
Ligand PQN A 5045



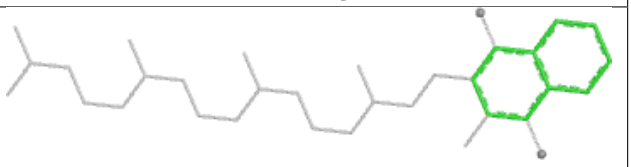
Bond lengths



Bond angles

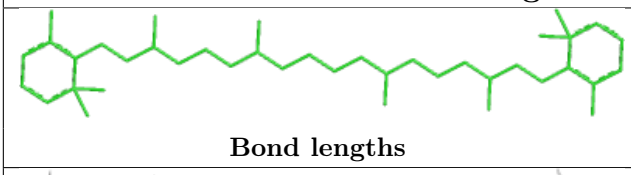


Torsions

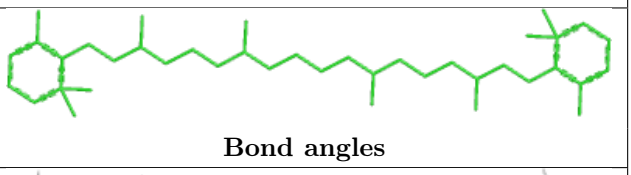


Rings

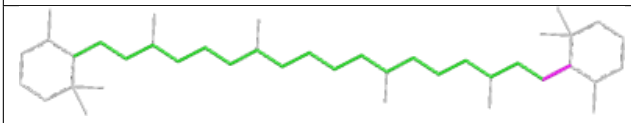
Ligand BCR B 801



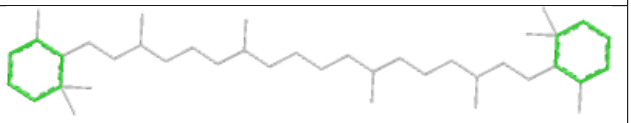
Bond lengths



Bond angles



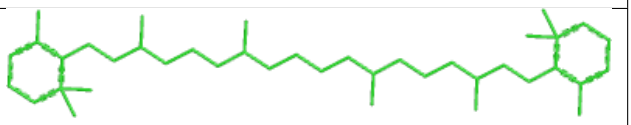
Torsions



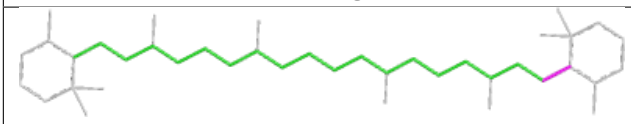
Rings

Ligand BCR J 104

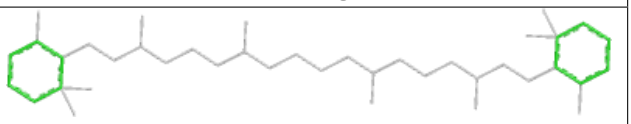
Bond lengths



Bond angles

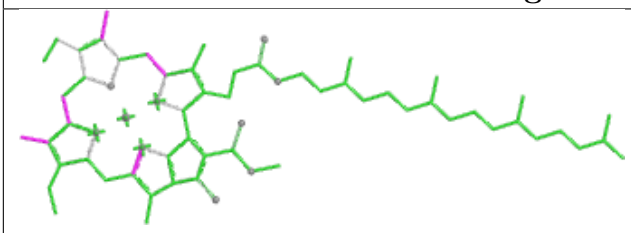


Torsions

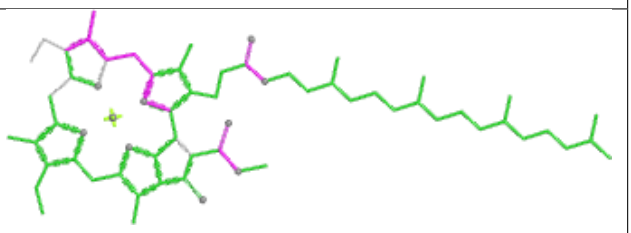


Rings

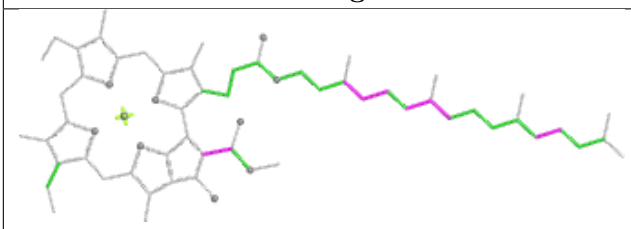
Ligand CLA B 805



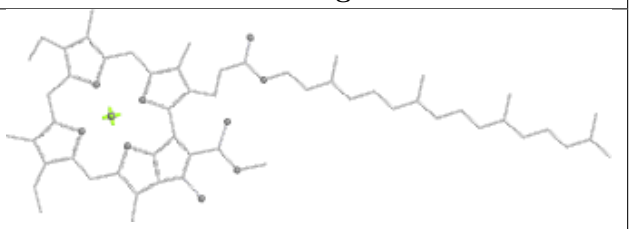
Bond lengths



Bond angles

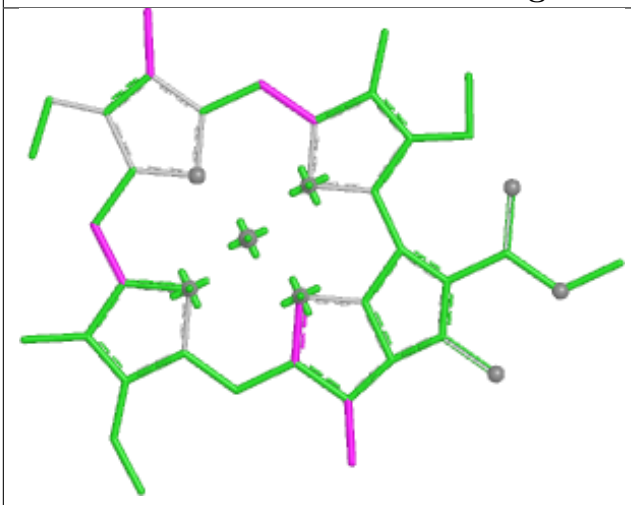


Torsions

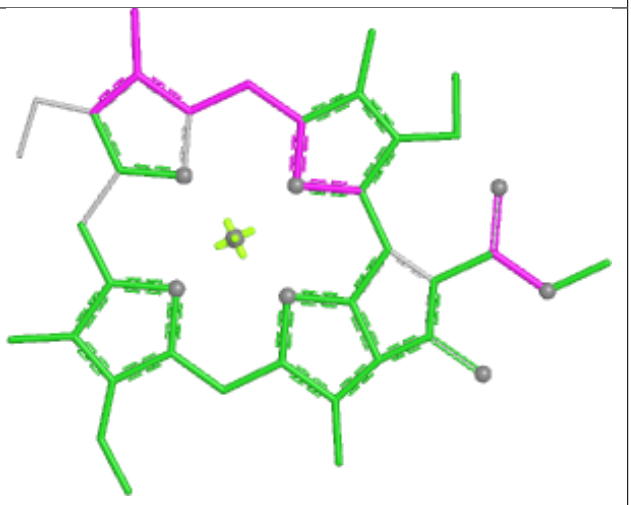


Rings

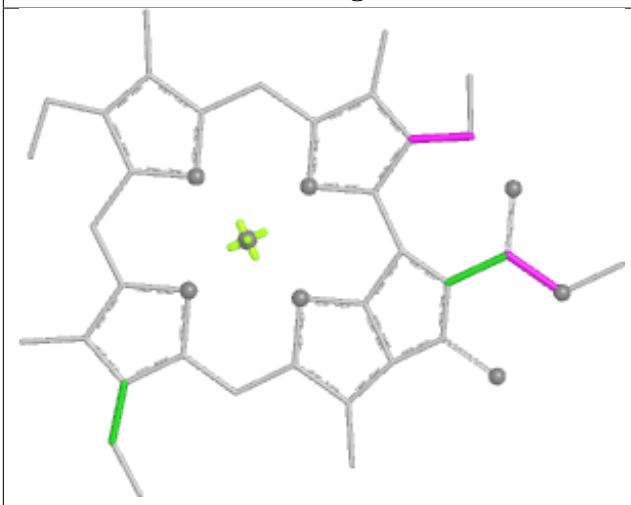
Ligand CLA 3 313



Bond lengths



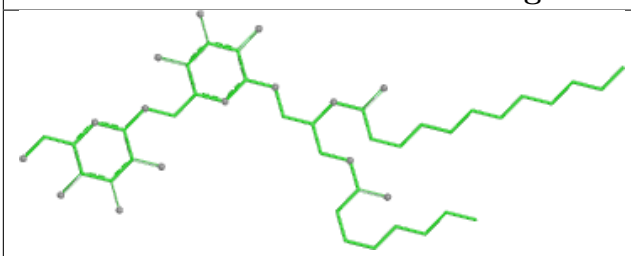
Bond angles



Torsions

Rings

Ligand DGD 3 321



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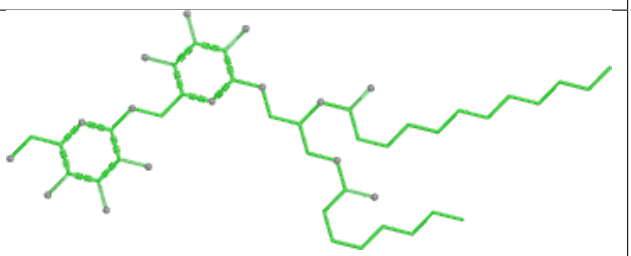
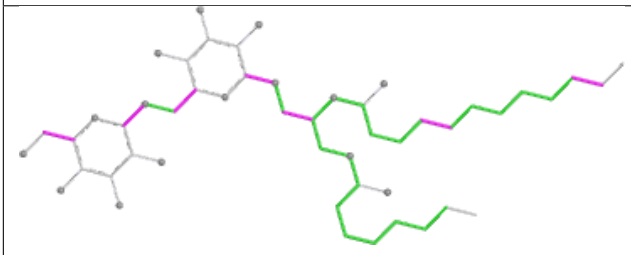
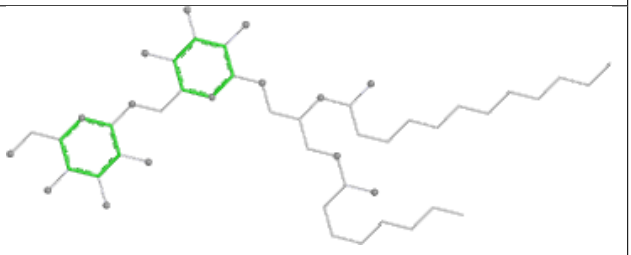


Bond angles

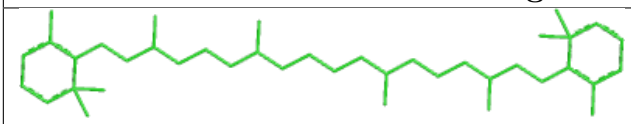


Torsions



Rings

Ligand BCR 8 318



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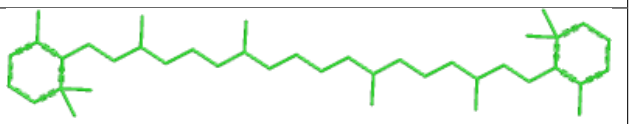
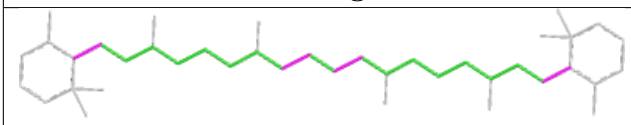
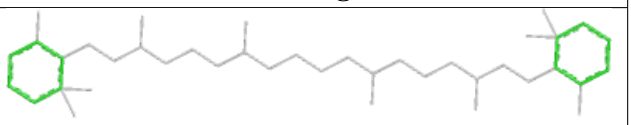


Bond angles

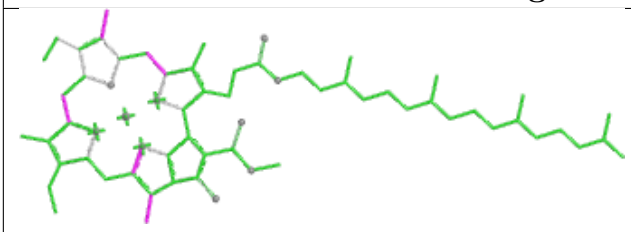


Torsions

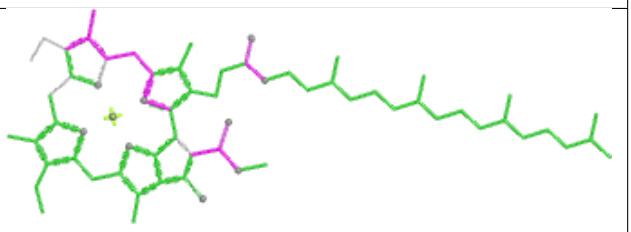


Rings

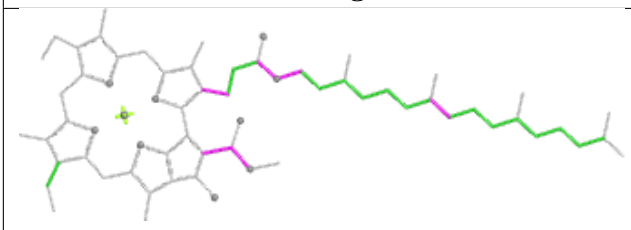
Ligand CLA 3 307



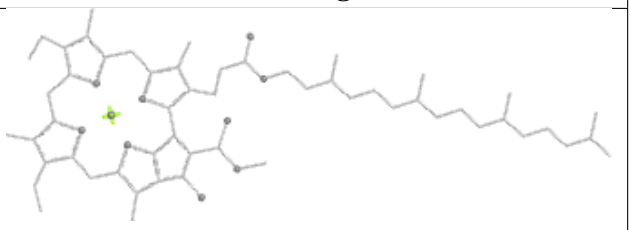
Bond lengths



Bond angles

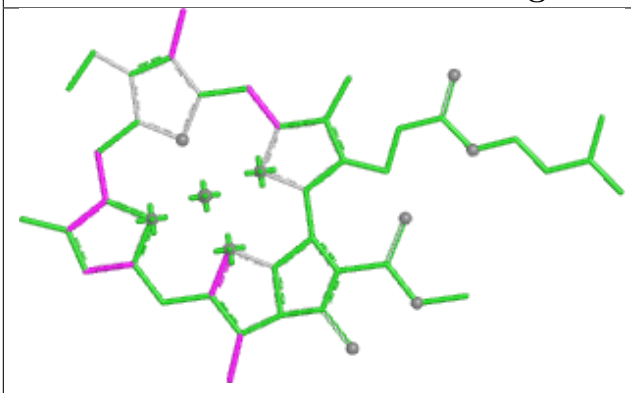


Torsions

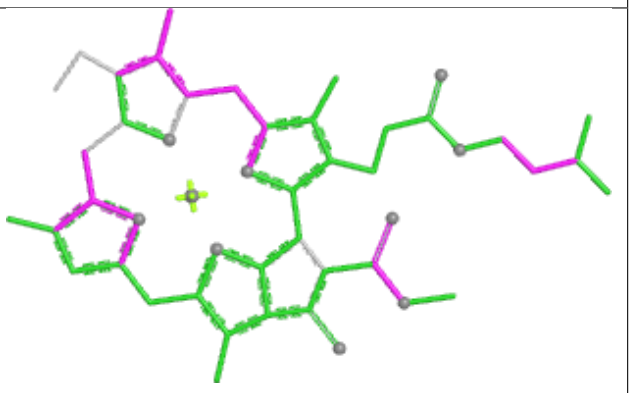


Rings

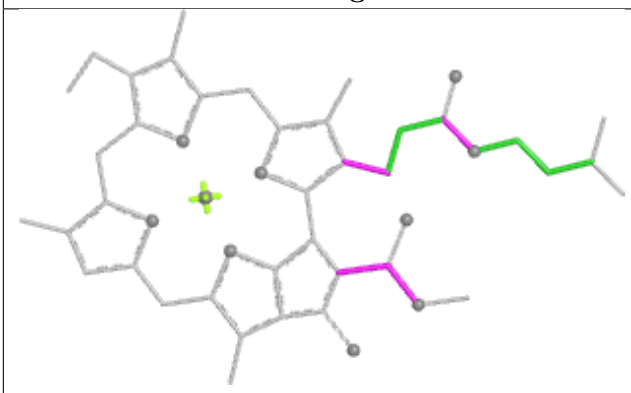
Ligand CLA a 604



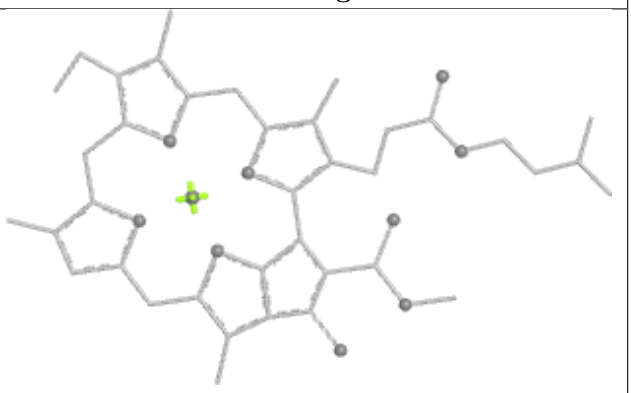
Bond lengths



Bond angles

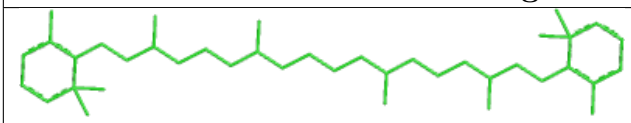


Torsions

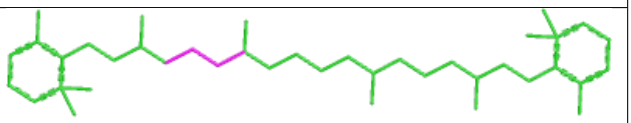


Rings

Ligand BCR K 205

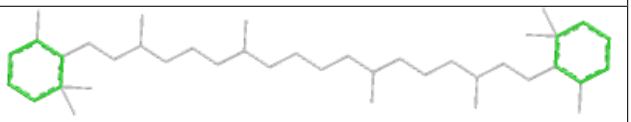


Bond lengths



Bond angles

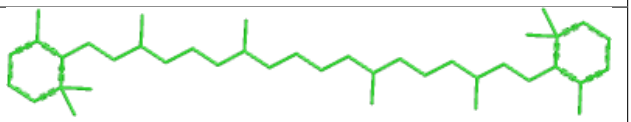
Torsions



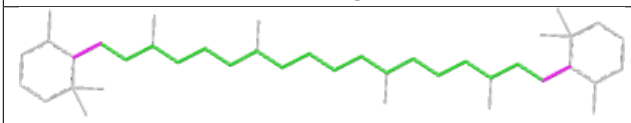
Rings

Ligand BCR 3 318

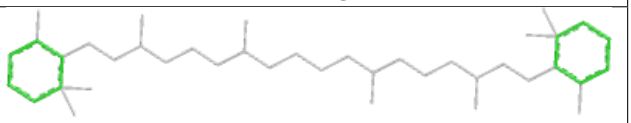
Bond lengths



Bond angles

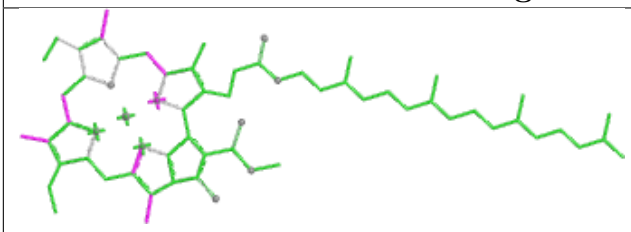


Torsions

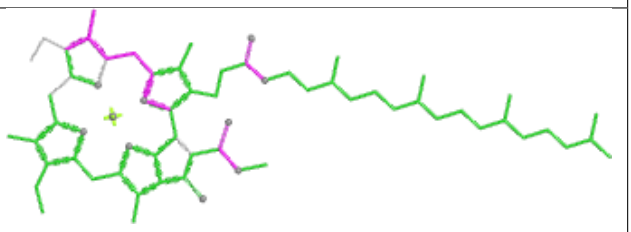


Rings

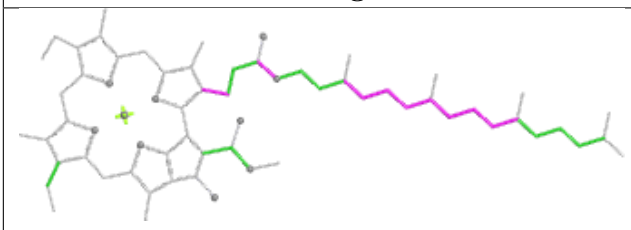
Ligand CLA A 5028



Bond lengths



Bond angles



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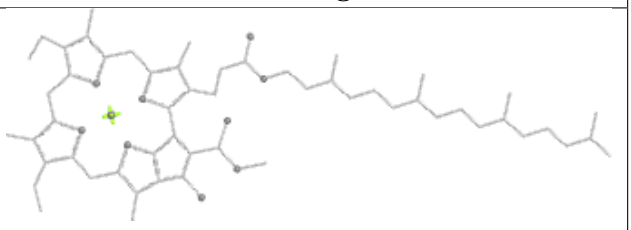
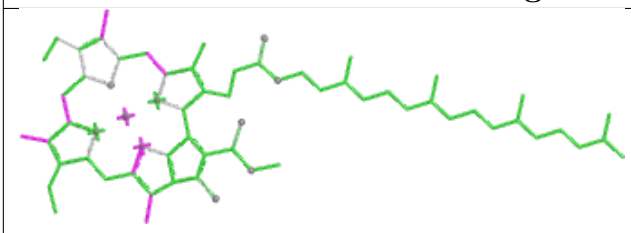
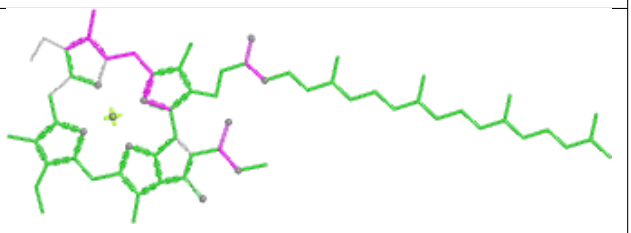


Rings

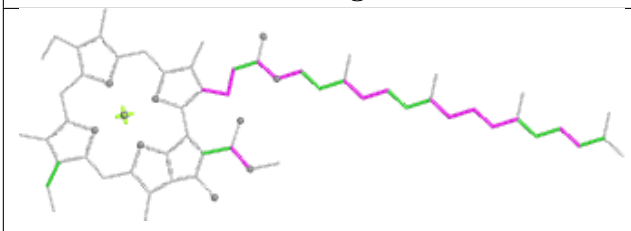
Ligand CLA B 808



Bond lengths



Bond angles



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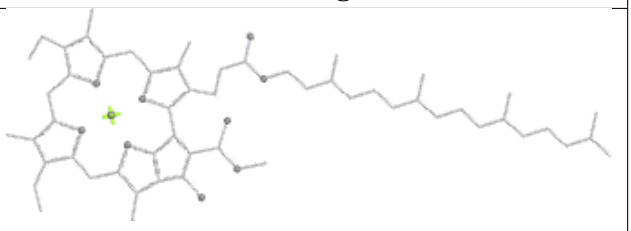
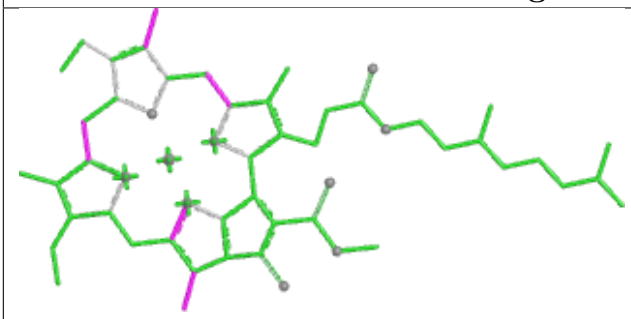
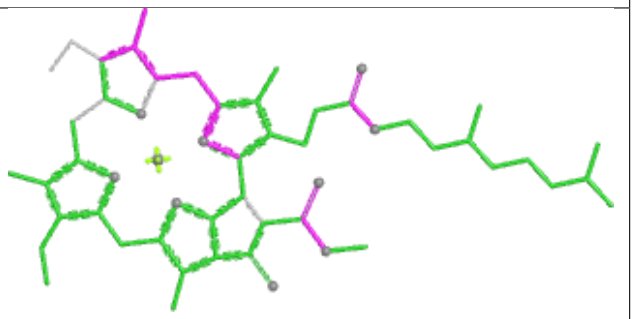


Rings

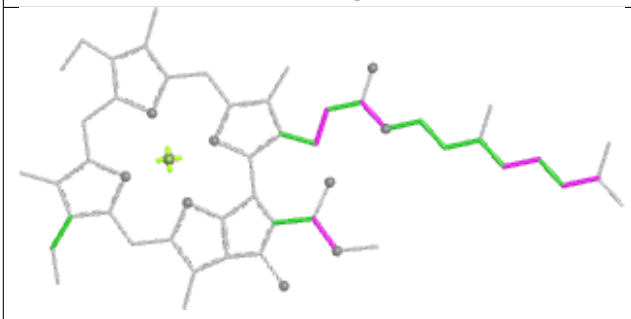
Ligand CLA 3 311



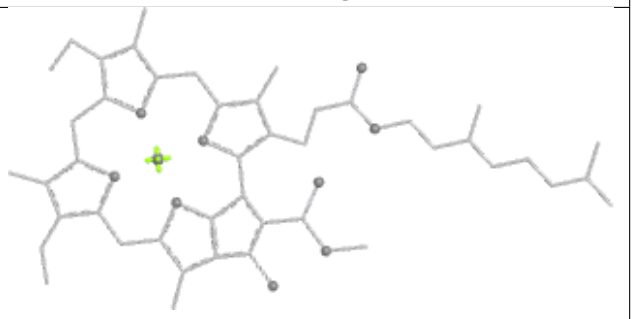
Bond lengths



Bond angles

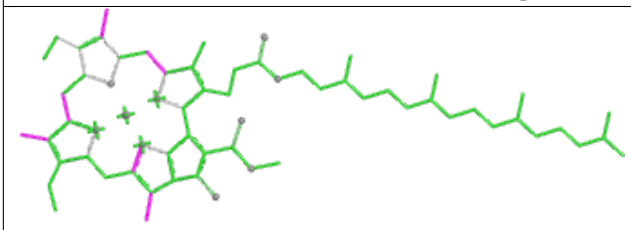


Torsions

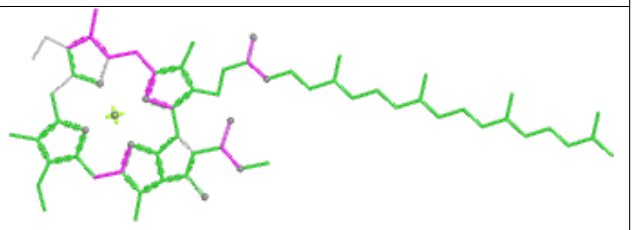


Rings

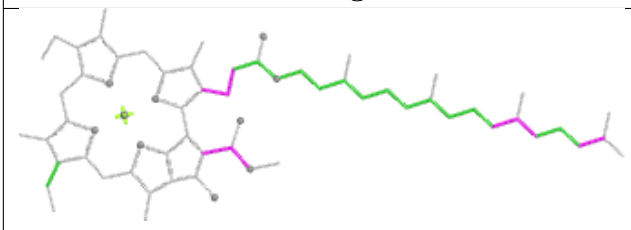
Ligand CLA A 5008



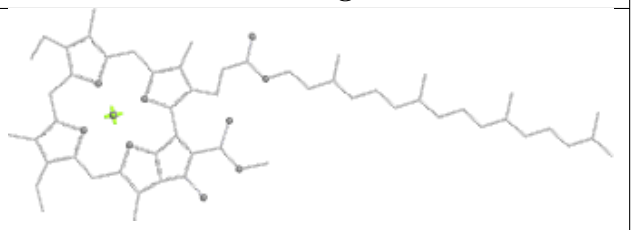
Bond lengths



Bond angles

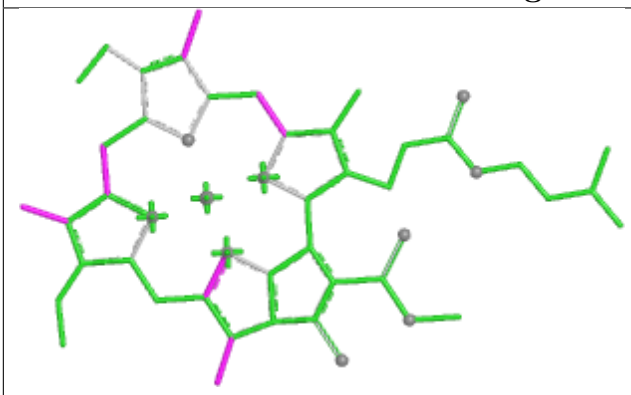


Torsions

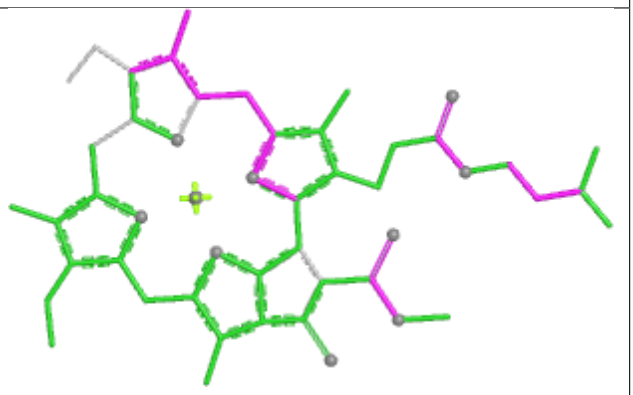


Rings

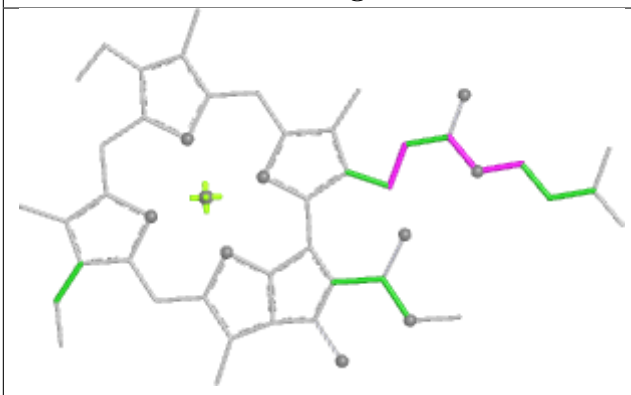
Ligand CLA B 816



Bond lengths



Bond angles



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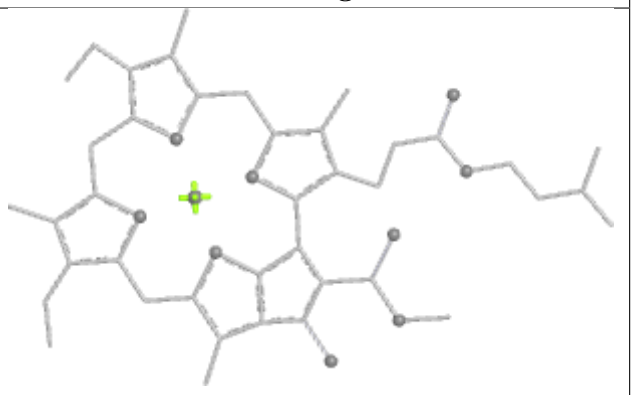
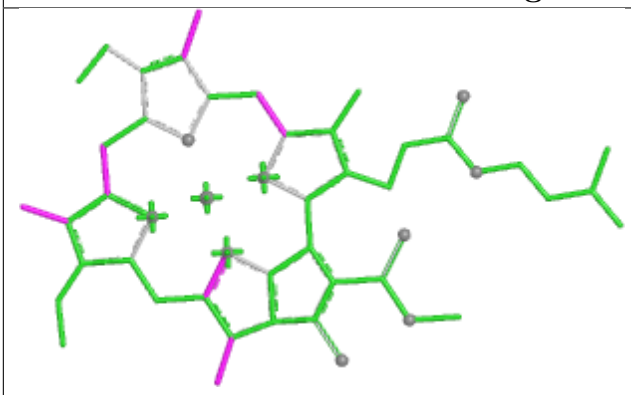


Rings

Ligand CLA T 408



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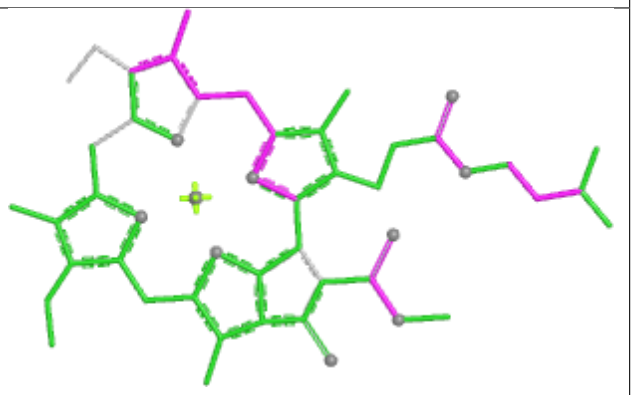
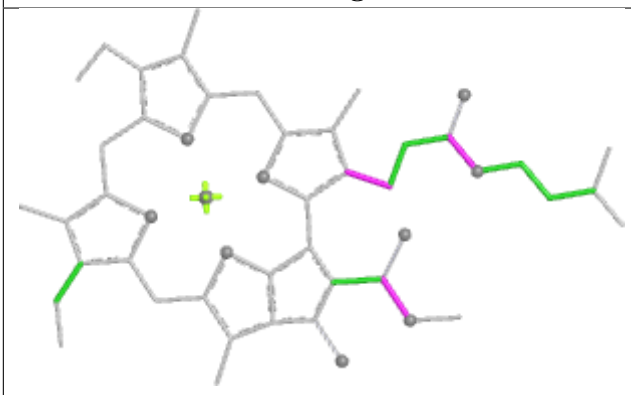


Bond angles



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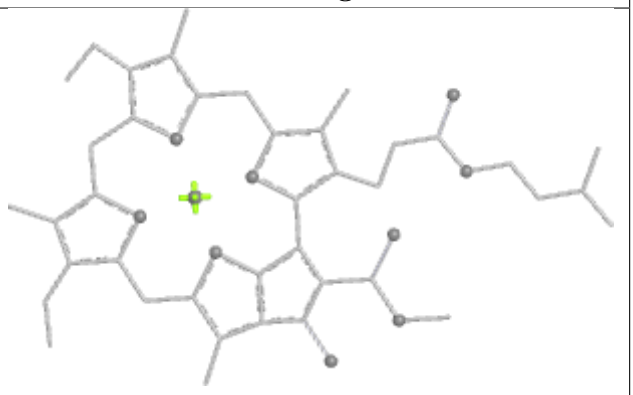
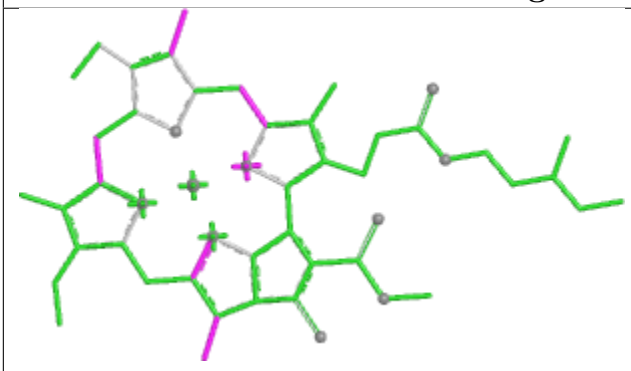
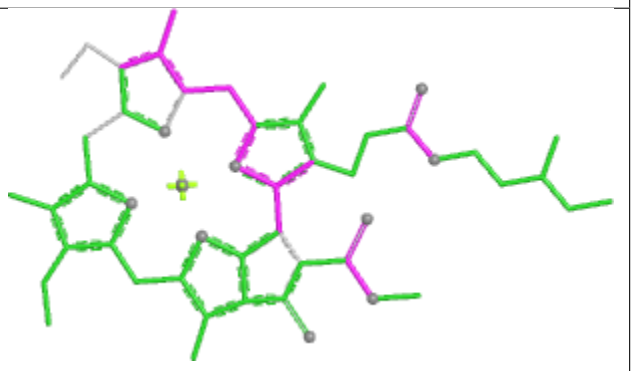


Rings

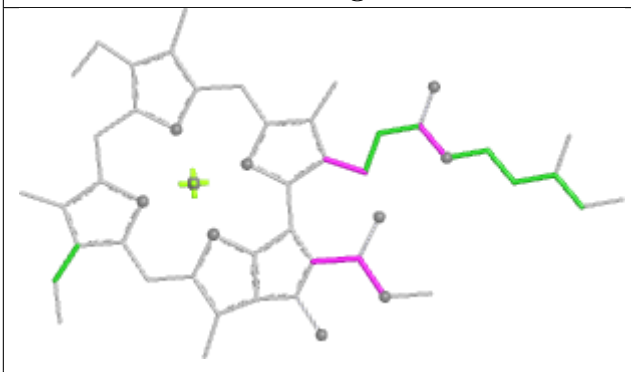
Ligand CLA 8 304



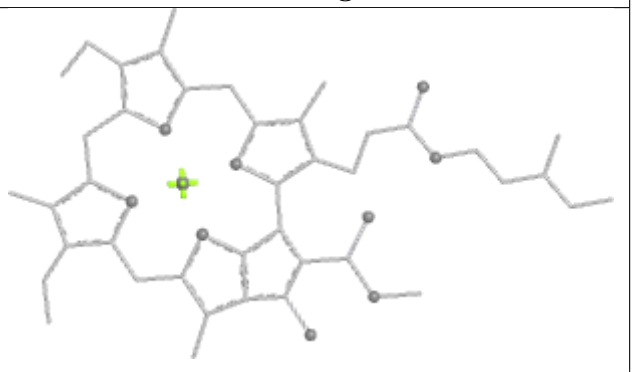
Bond lengths



Bond angles

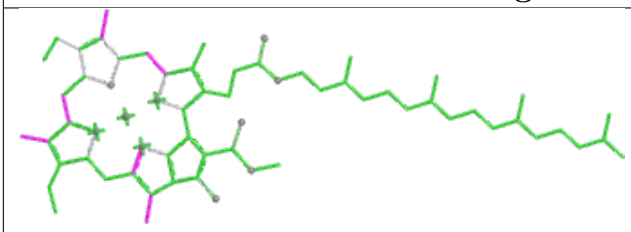


Torsions

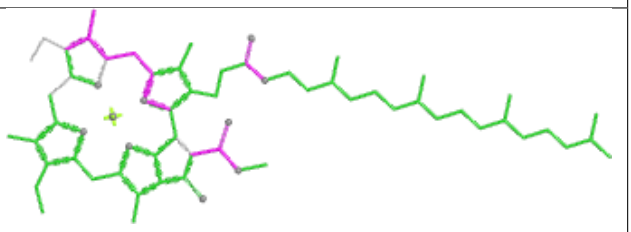


Rings

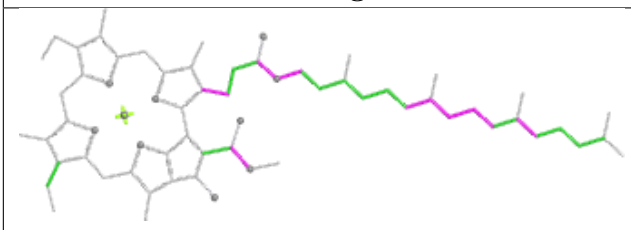
Ligand CLA A 5006



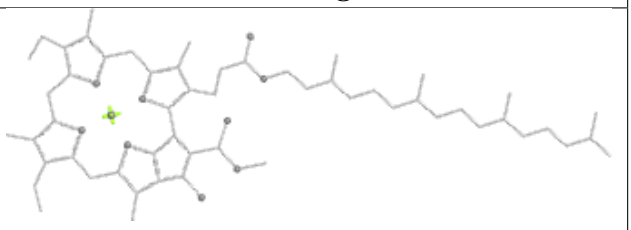
Bond lengths



Bond angles

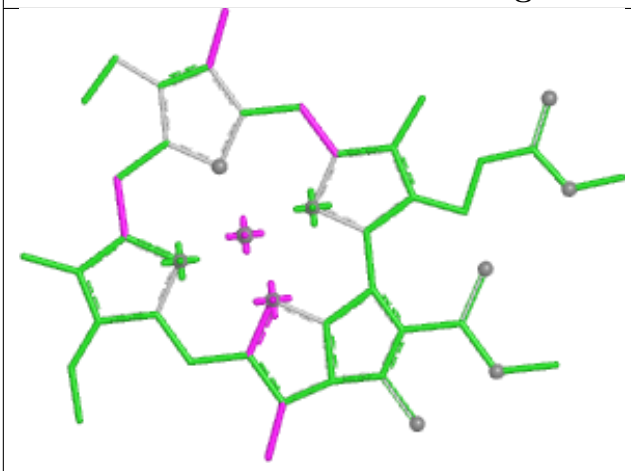


Torsions

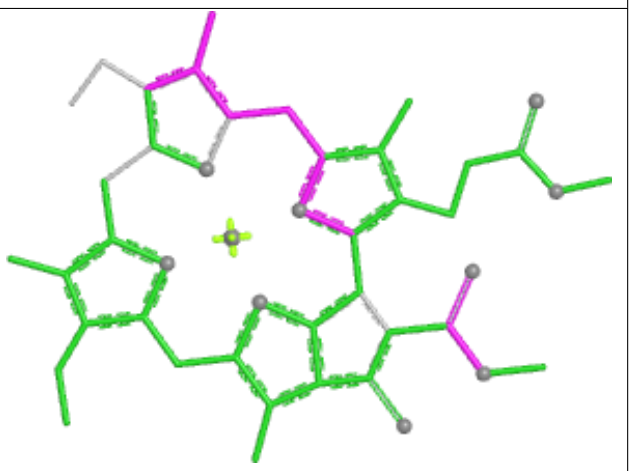


Rings

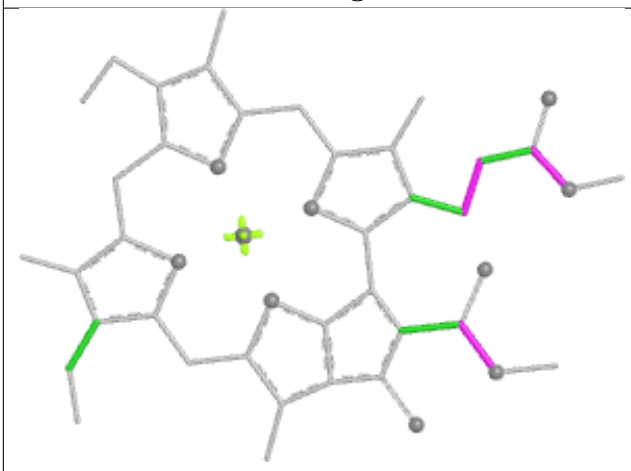
Ligand CLA A 5023



Bond lengths



Bond angles



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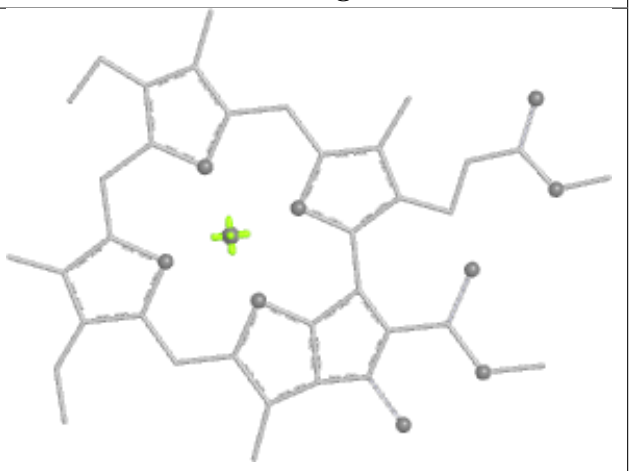
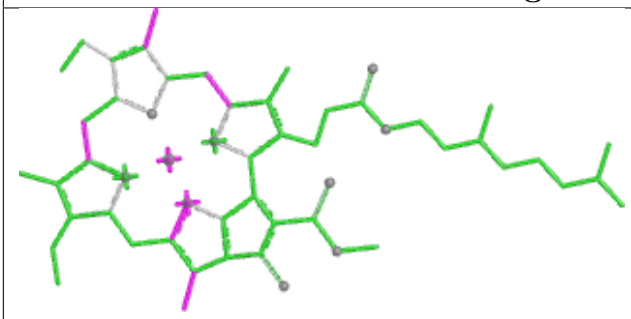
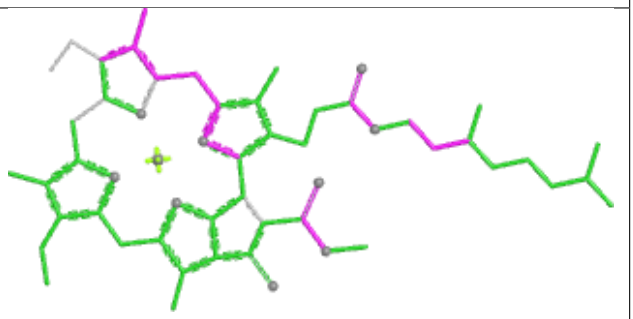


Rings

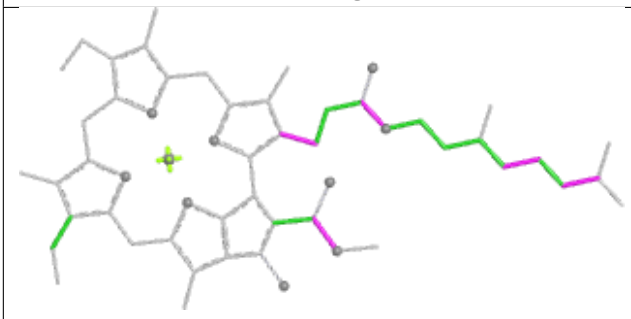
Ligand CLA B 831



Bond lengths



Bond angles



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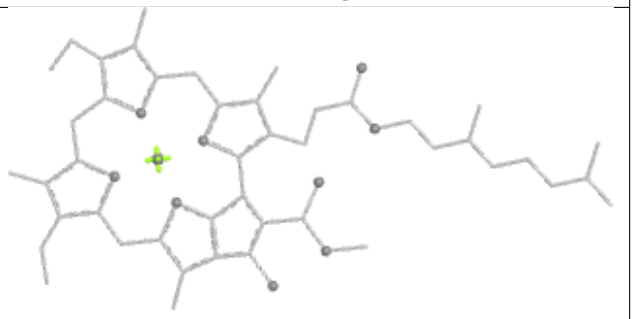
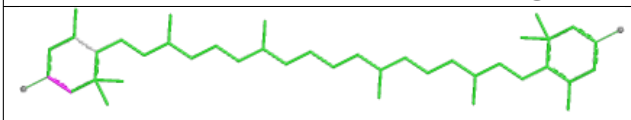
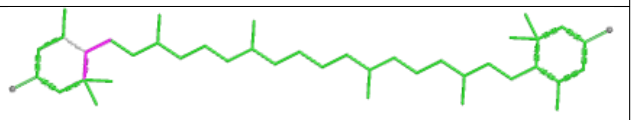


Rings

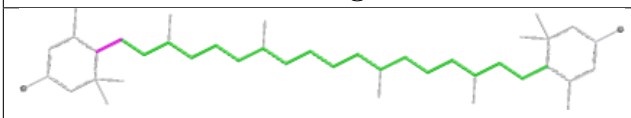
Ligand LUT 7 315



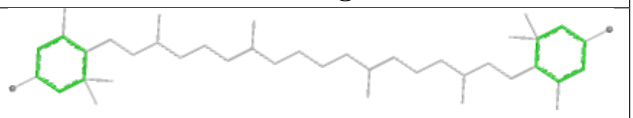
Bond lengths



Bond angles

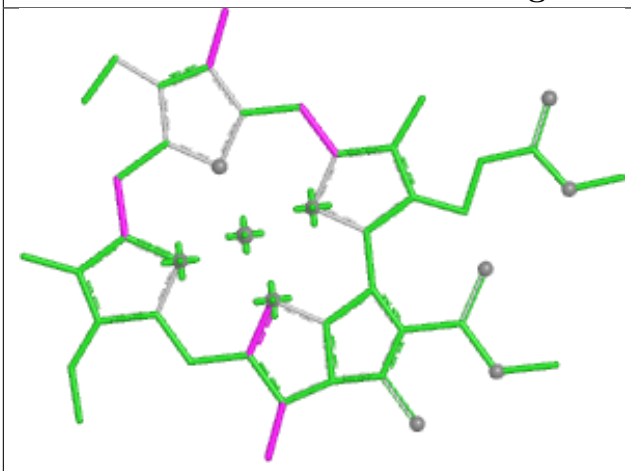


Torsions

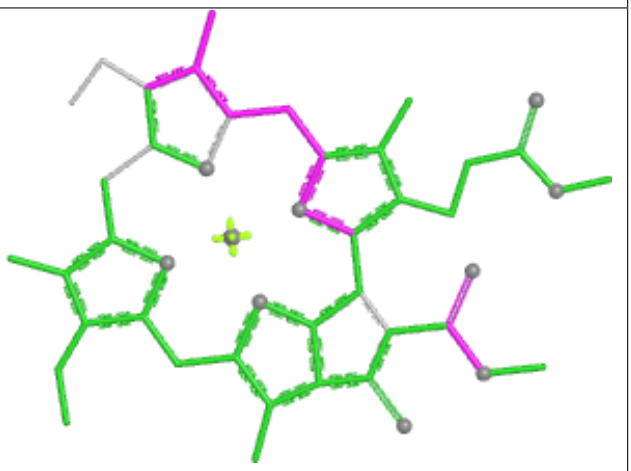


Rings

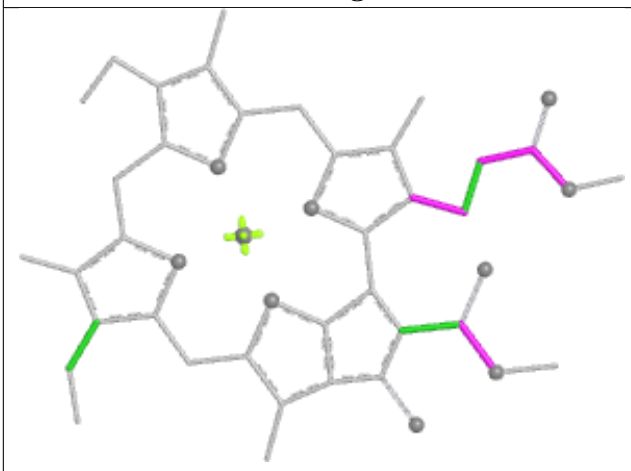
Ligand CLA 1 610



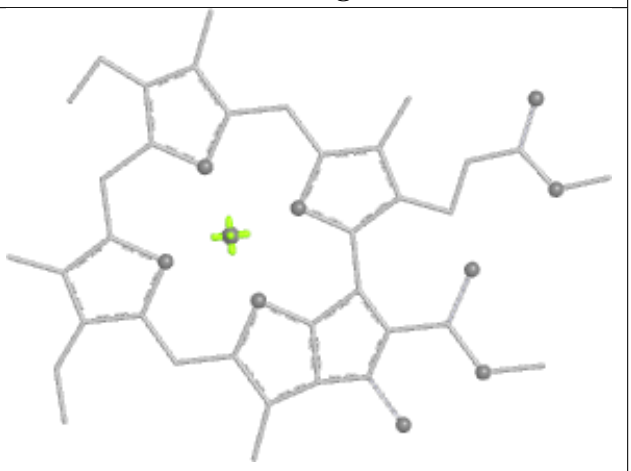
Bond lengths



Bond angles

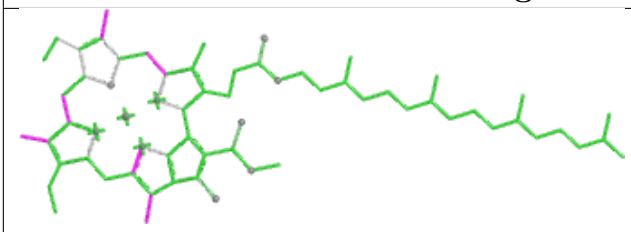


Torsions

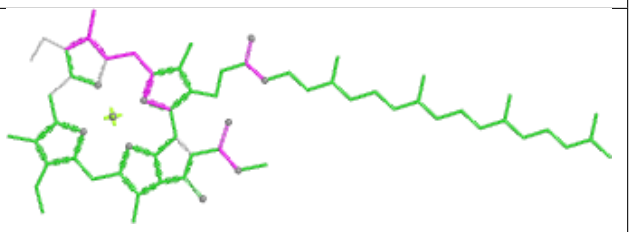


Rings

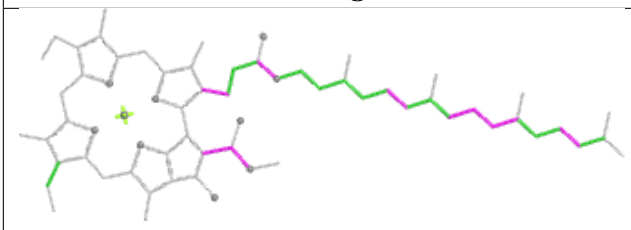
Ligand CLA A 5035



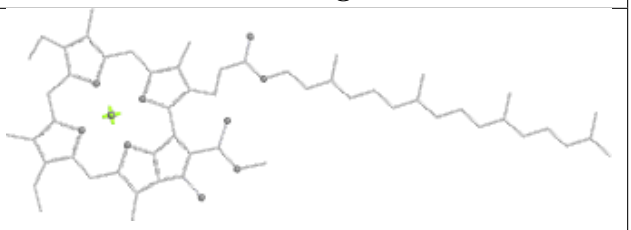
Bond lengths



Bond angles

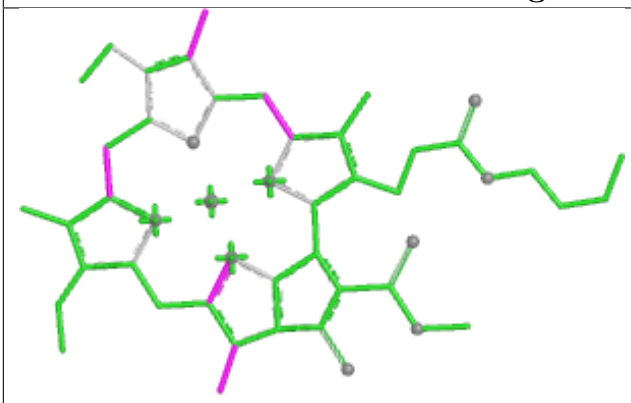


Torsions

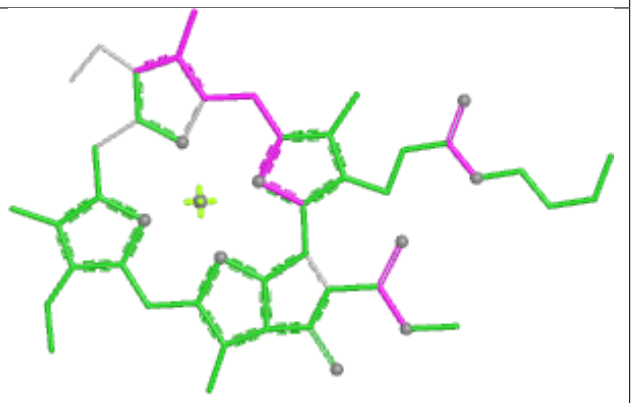


Rings

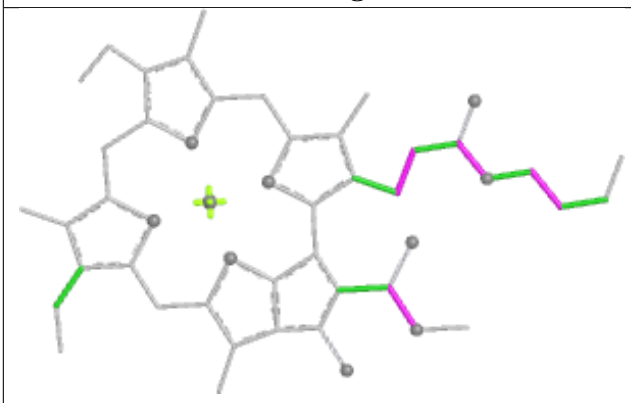
Ligand CLA J 102



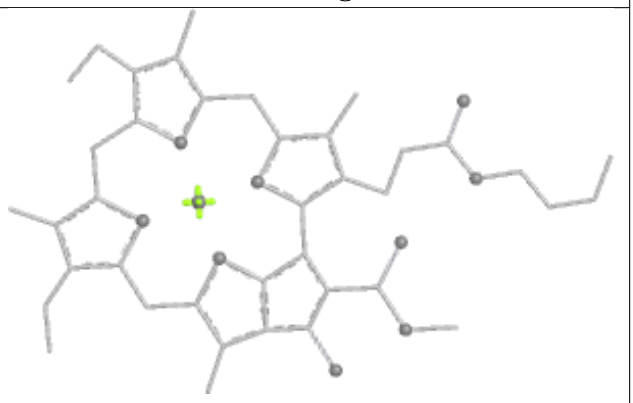
Bond lengths



Bond angles

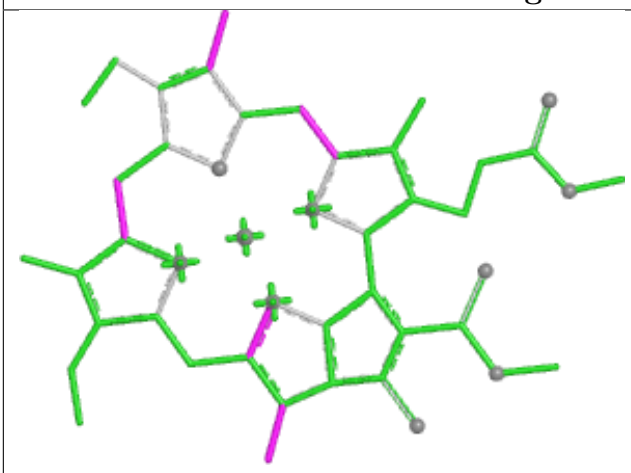


Torsions

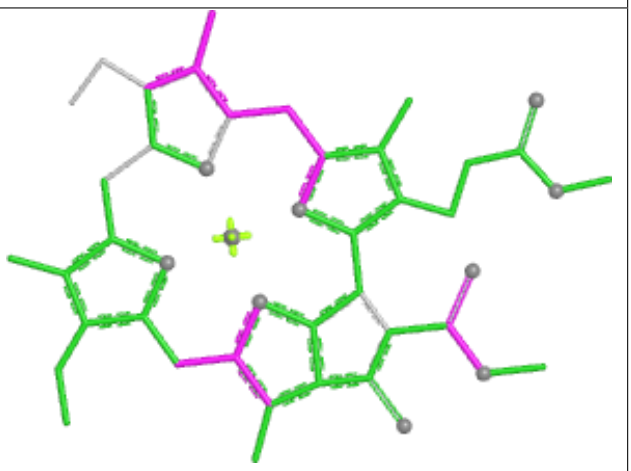


Rings

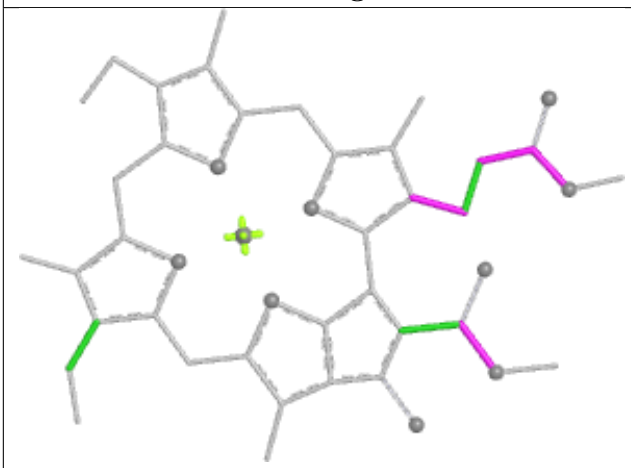
Ligand CLA T 404



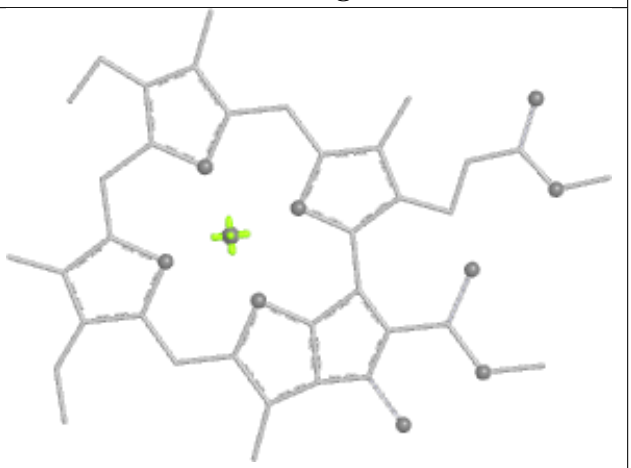
Bond lengths



Bond angles



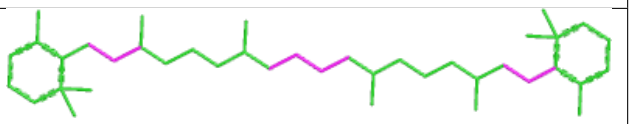
Torsions



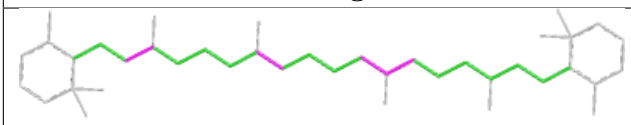
Rings

Ligand BCR B 849

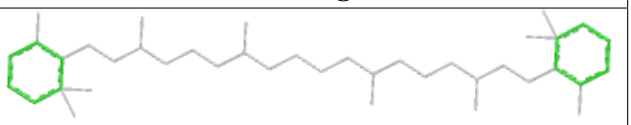
Bond lengths



Bond angles

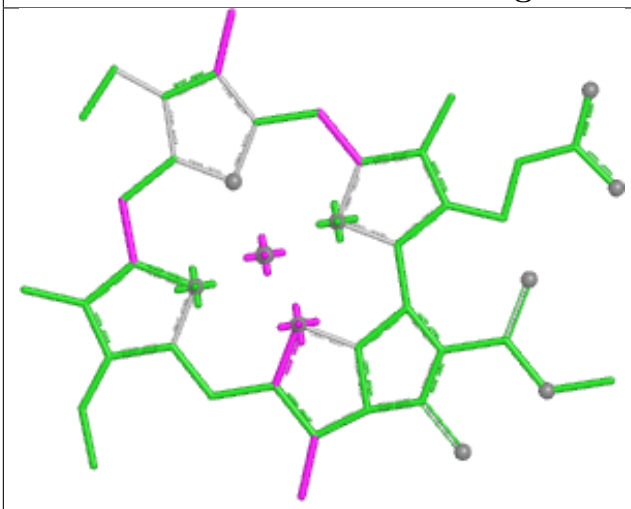


Torsions

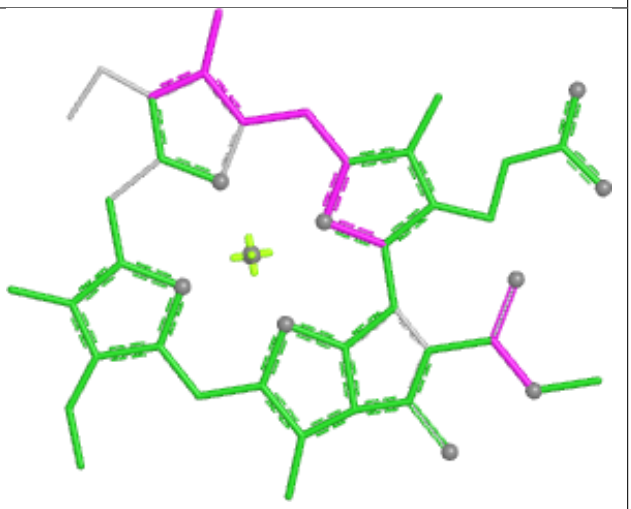


Rings

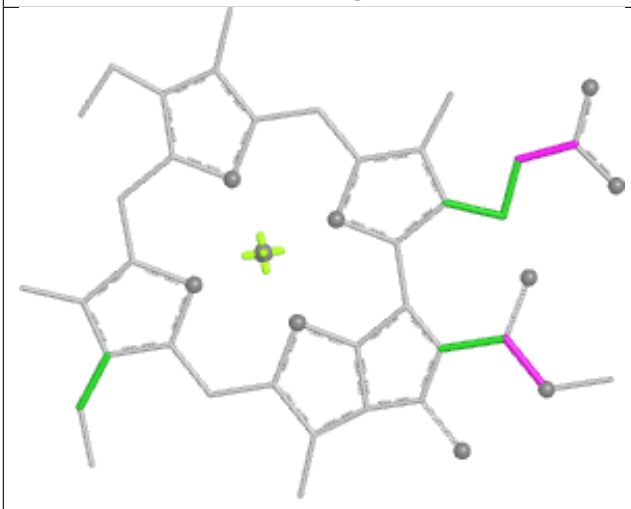
Ligand CLA A 5032



Bond lengths



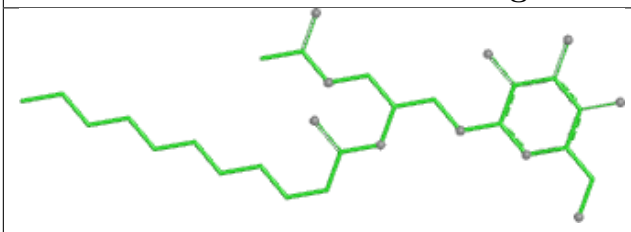
Bond angles



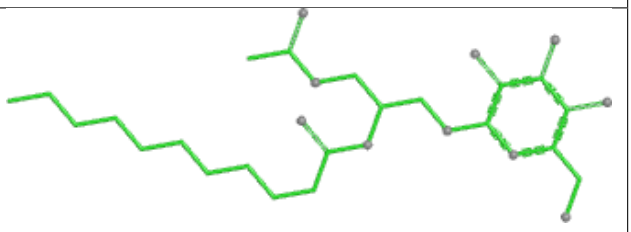
Torsions

Rings

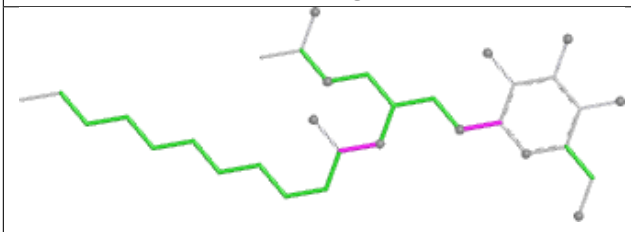
Ligand LMG A 5001



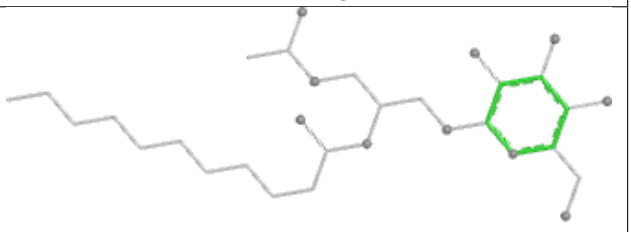
Bond lengths



Bond angles

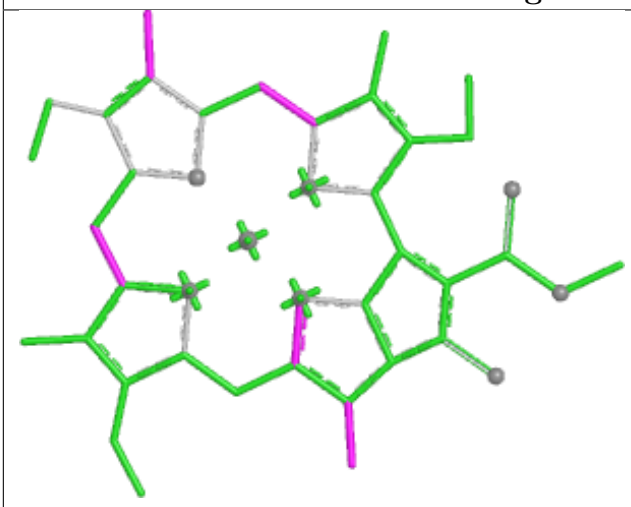


Torsions

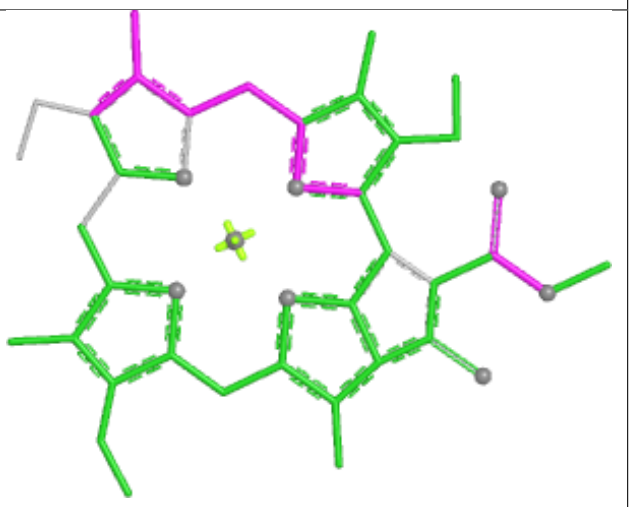


Rings

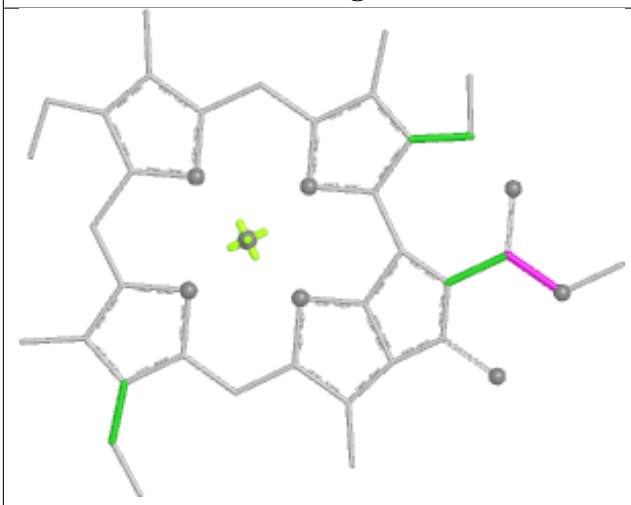
Ligand CLA T 412



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.

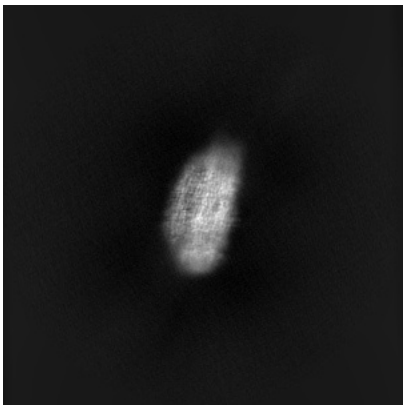
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-48264. These allow visual inspection of the internal detail of the map and identification of artifacts.

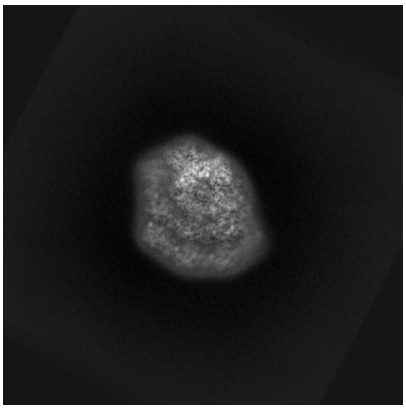
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

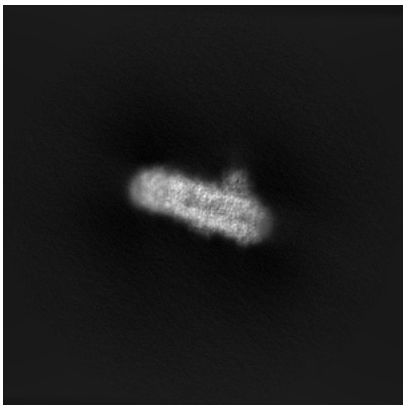
6.1.1 Primary map



X

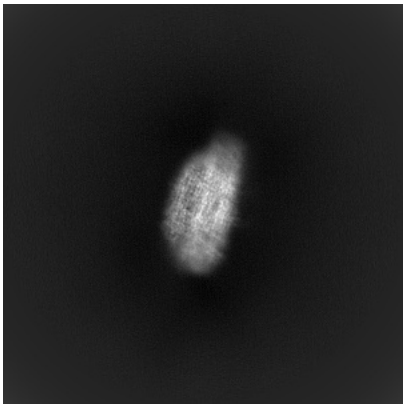


Y

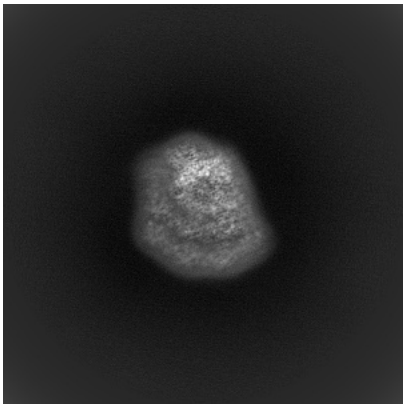


Z

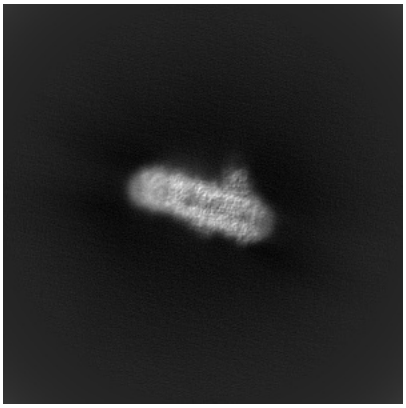
6.1.2 Raw map



X



Y

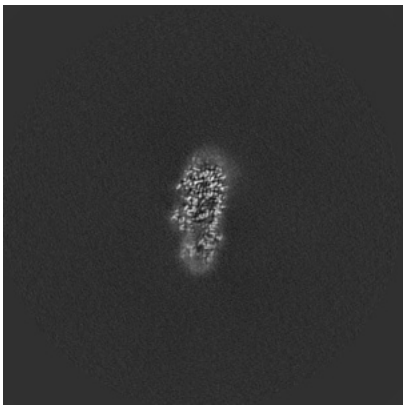


Z

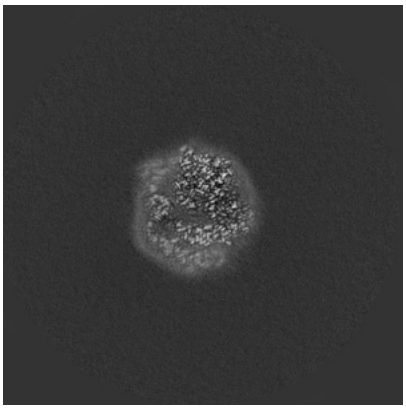
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

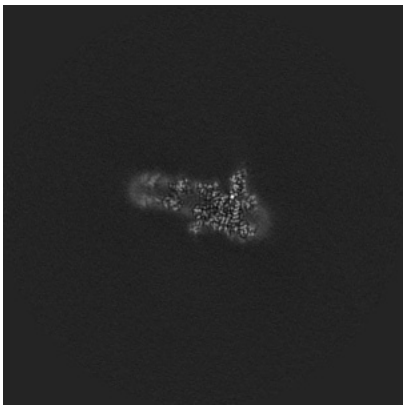
6.2.1 Primary map



X Index: 240

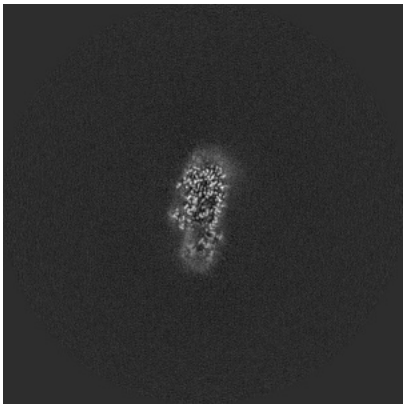


Y Index: 240

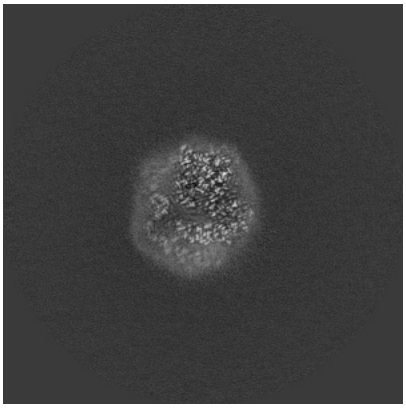


Z Index: 240

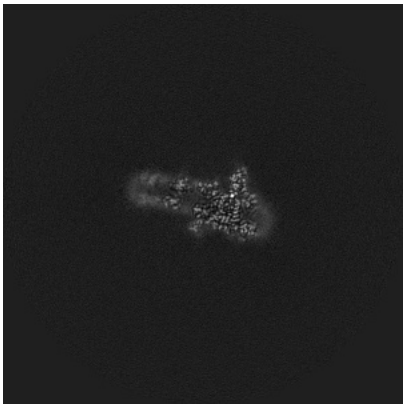
6.2.2 Raw map



X Index: 240



Y Index: 240

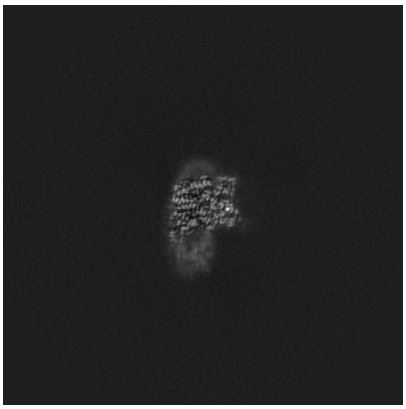


Z Index: 240

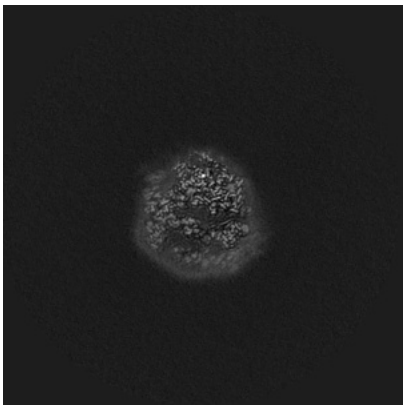
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

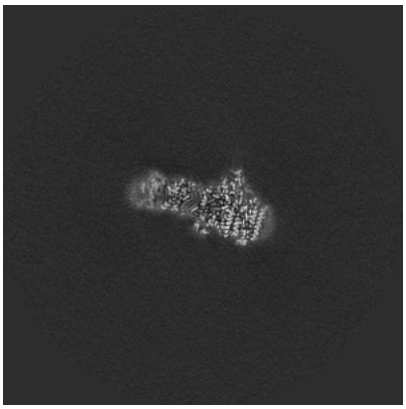
6.3.1 Primary map



X Index: 277

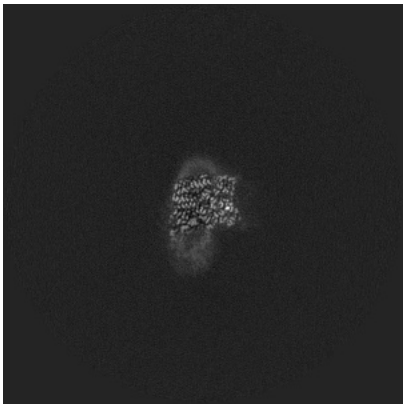


Y Index: 249

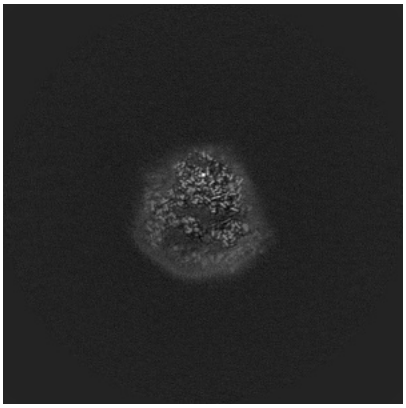


Z Index: 228

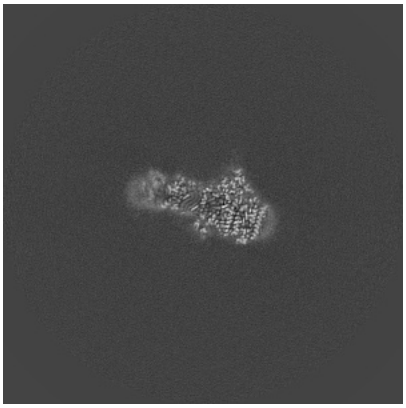
6.3.2 Raw map



X Index: 277



Y Index: 249

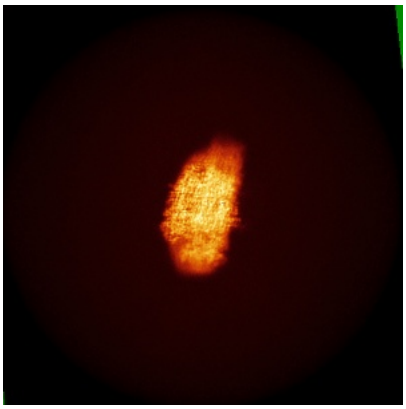


Z Index: 228

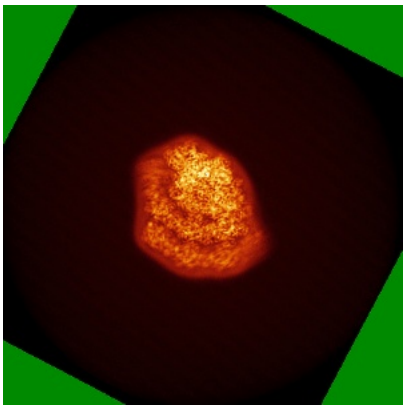
The images above show the largest variance slices of the map in three orthogonal directions.

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

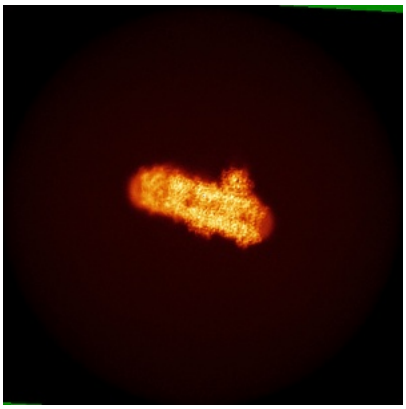
6.4.1 Primary map



X

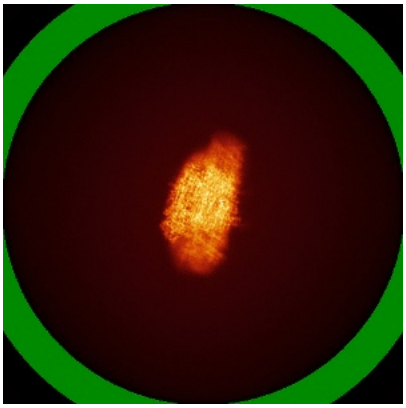


Y

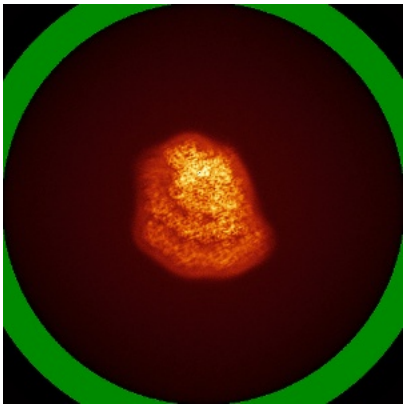


Z

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 0.0151. 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.

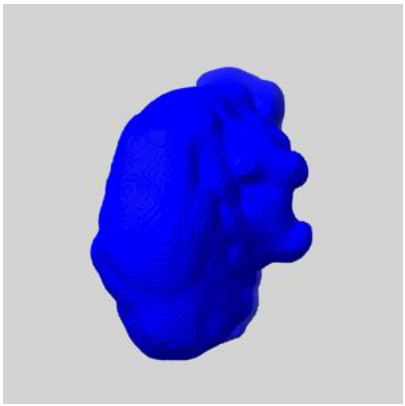
6.6 Mask visualisation

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

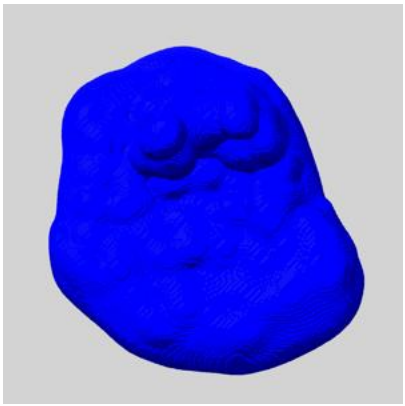
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

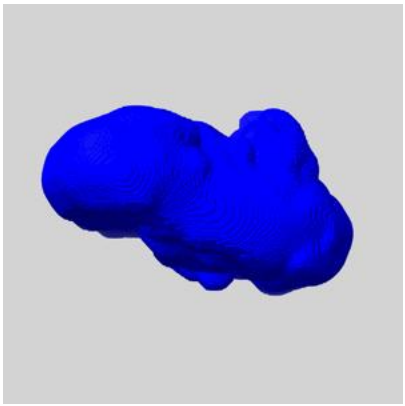
6.6.1 emd_48264_msk_1.map



X



Y

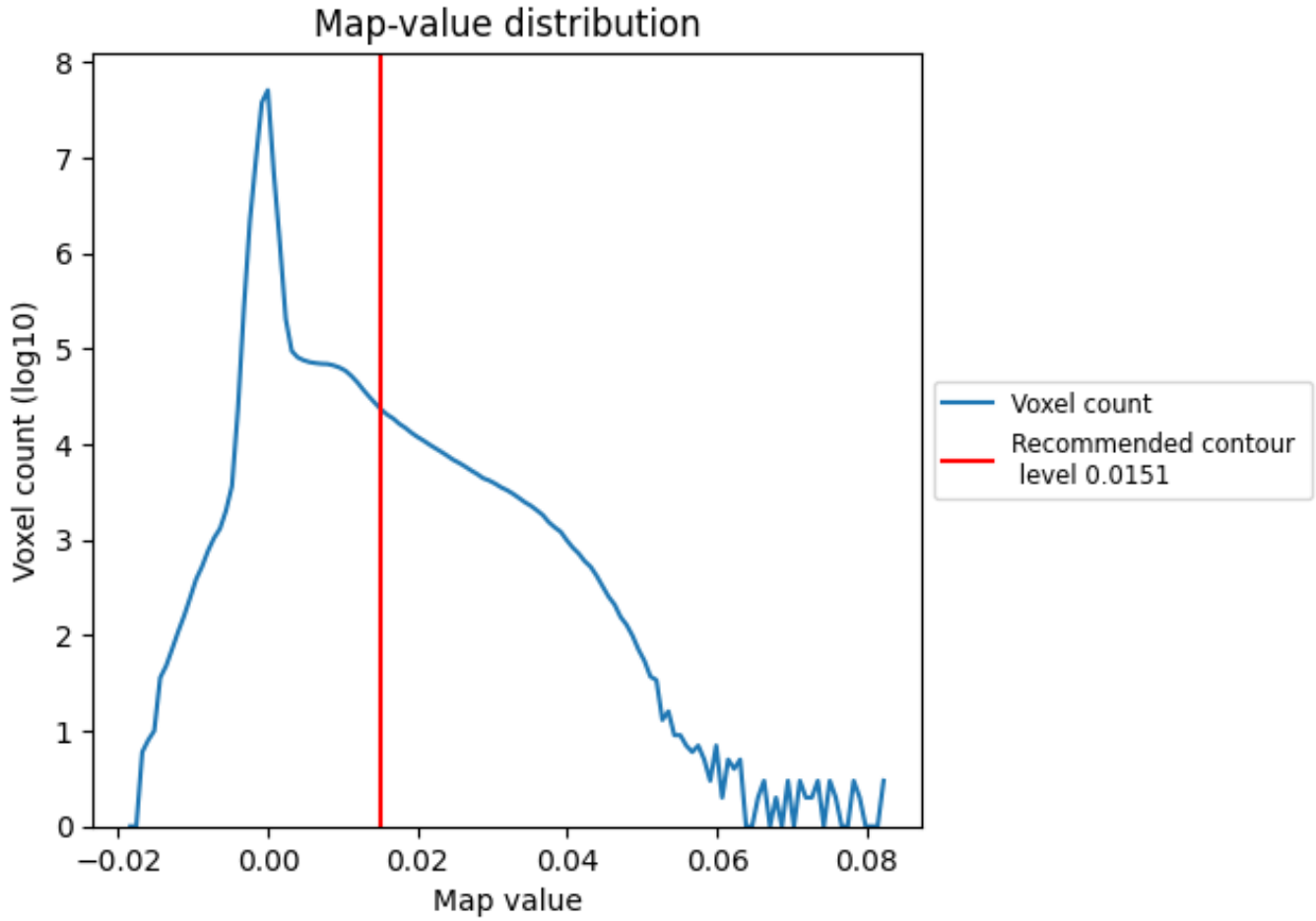


Z

7 Map analysis

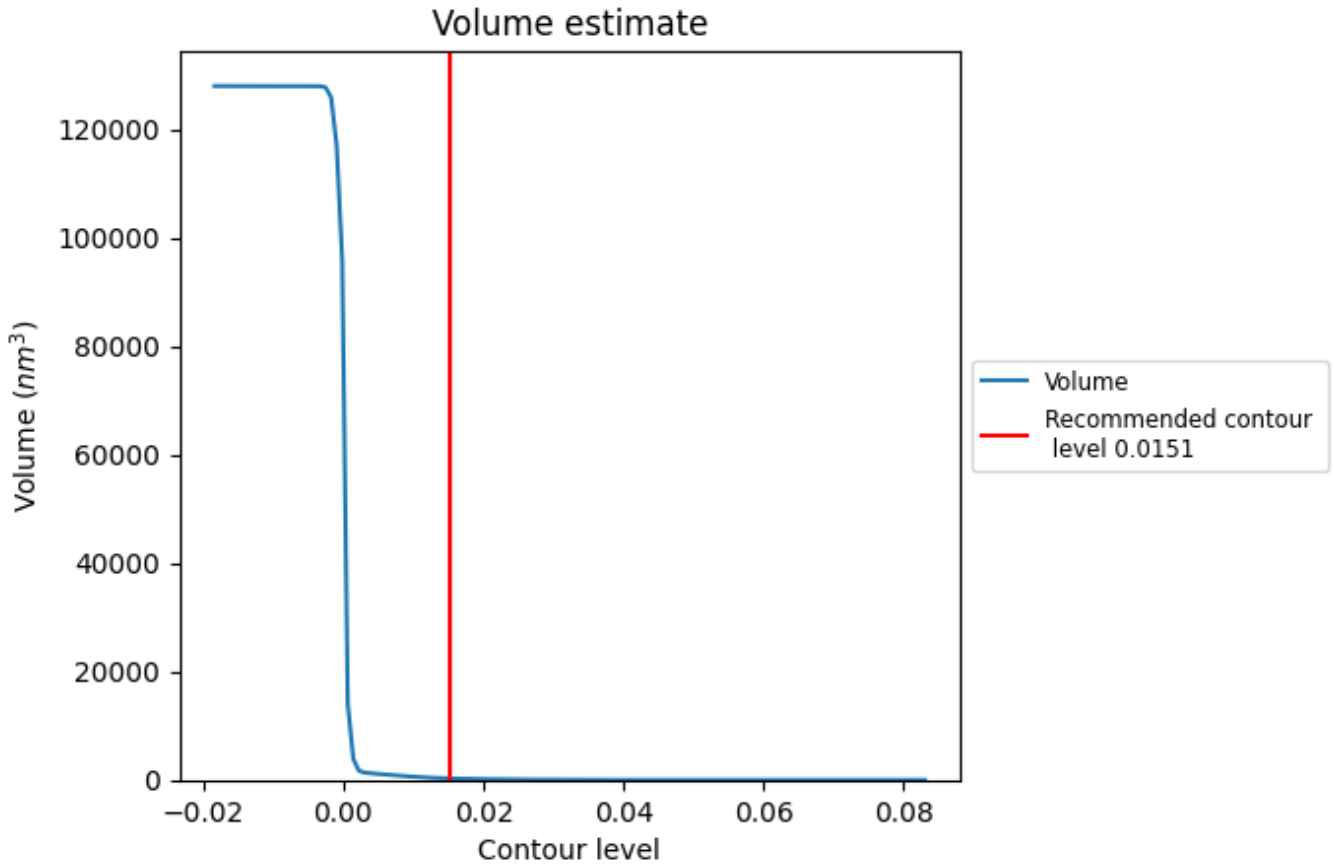
This section contains the results of statistical analysis of the map.

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.

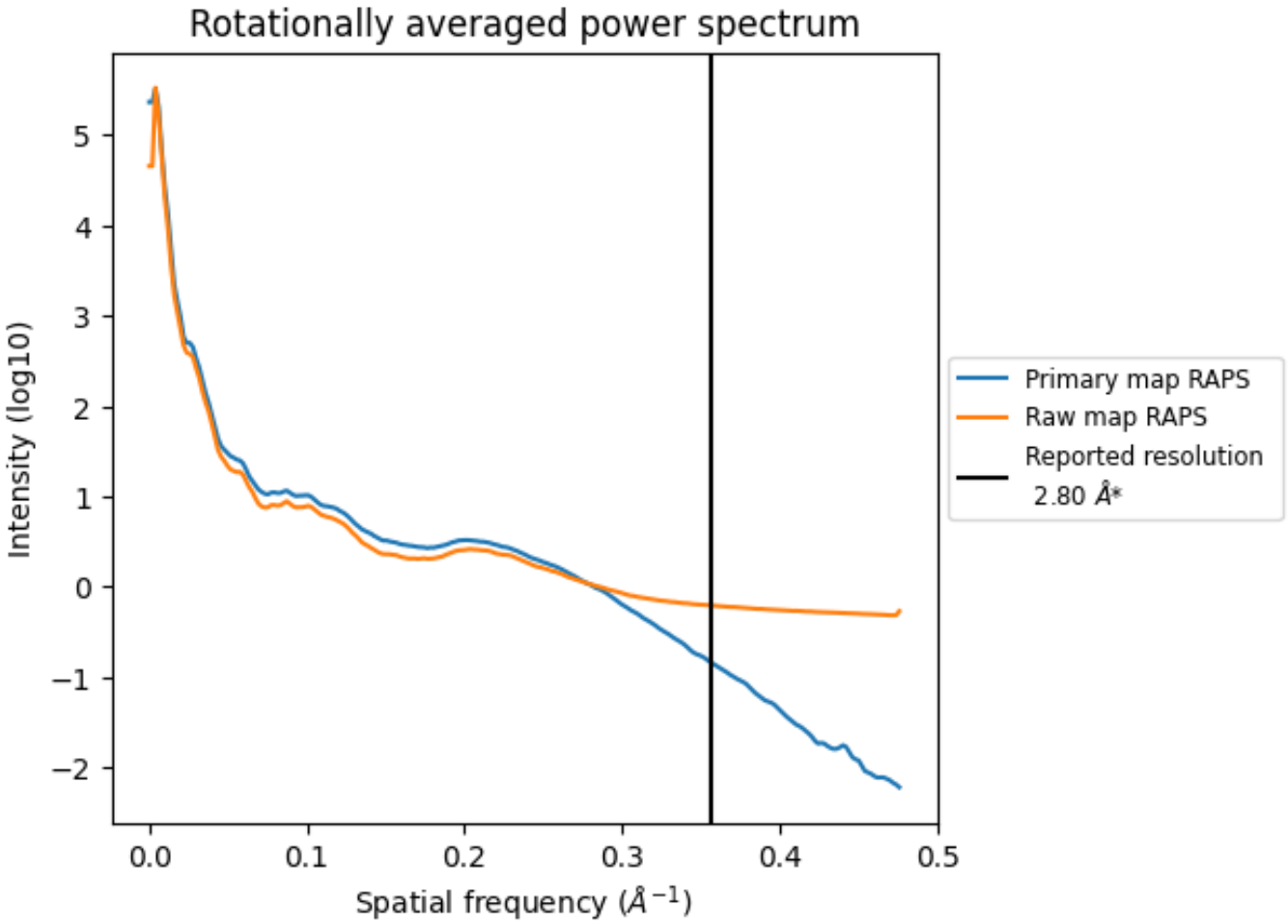
7.2 Volume estimate (i)



The volume at the recommended contour level is 278 nm^3; this corresponds to an approximate mass of 251 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)

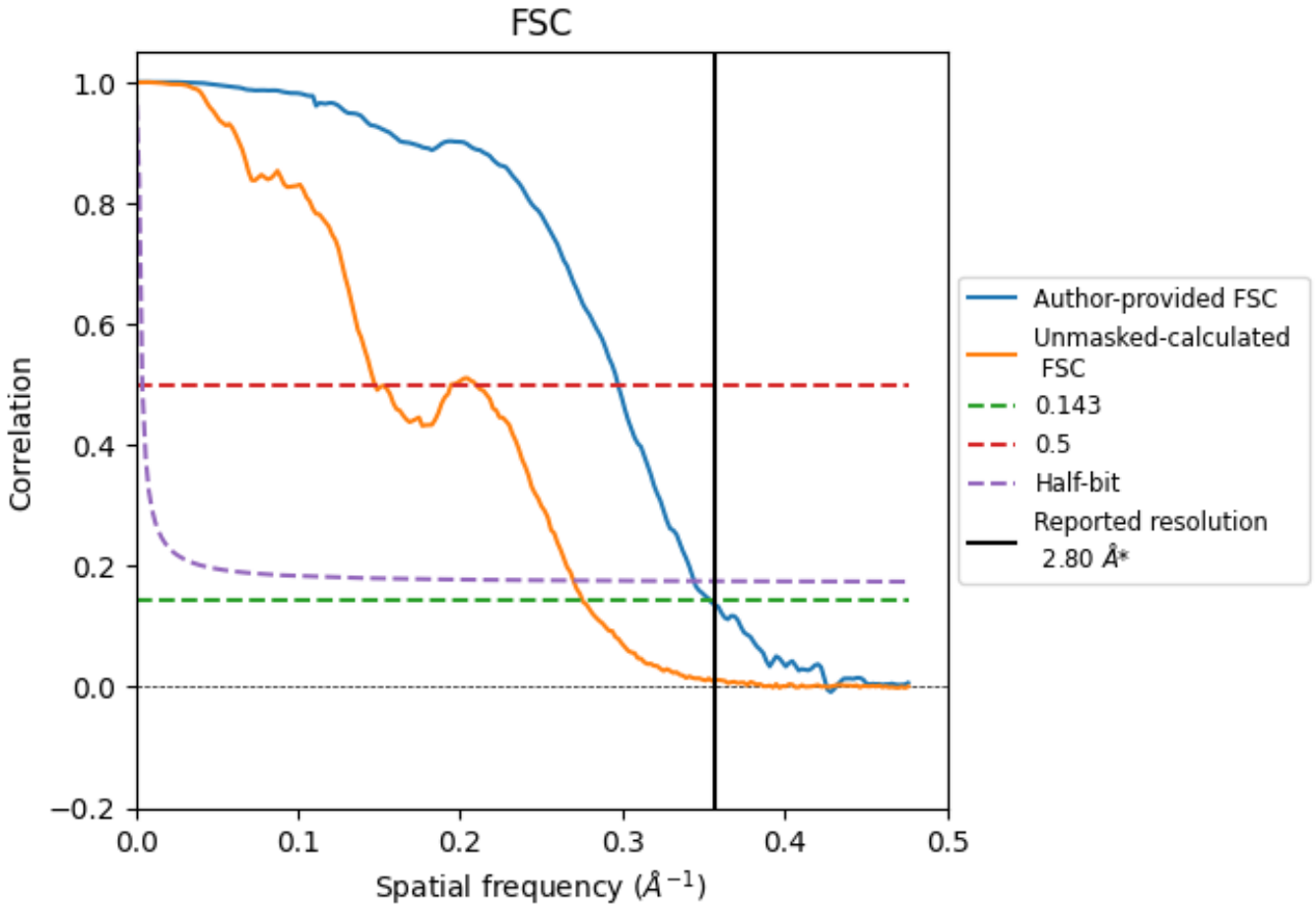


*Reported resolution corresponds to spatial frequency of 0.357 Å^{-1}

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 0.357 Å^{-1}

8.2 Resolution estimates (i)

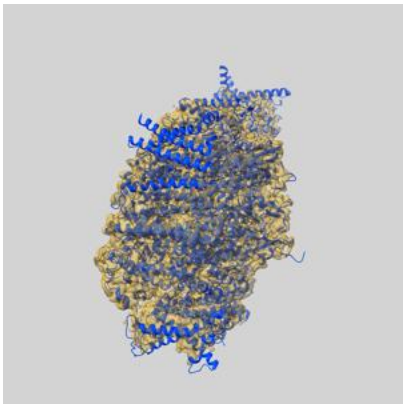
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.80	-	-
Author-provided FSC curve	2.83	3.36	2.91
Unmasked-calculated*	3.63	6.78	3.71

*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 3.63 differs from the reported value 2.8 by more than 10 %

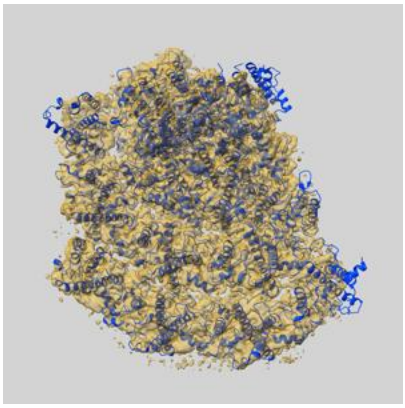
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-48264 and PDB model 9MGZ. Per-residue inclusion information can be found in section 3 on page 33.

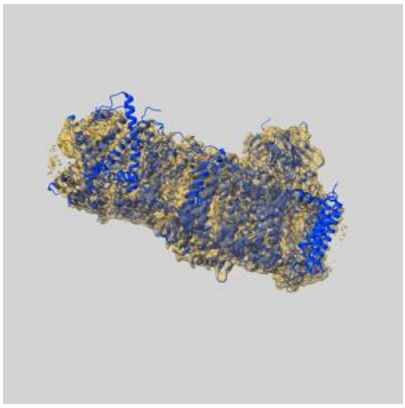
9.1 Map-model overlay



X



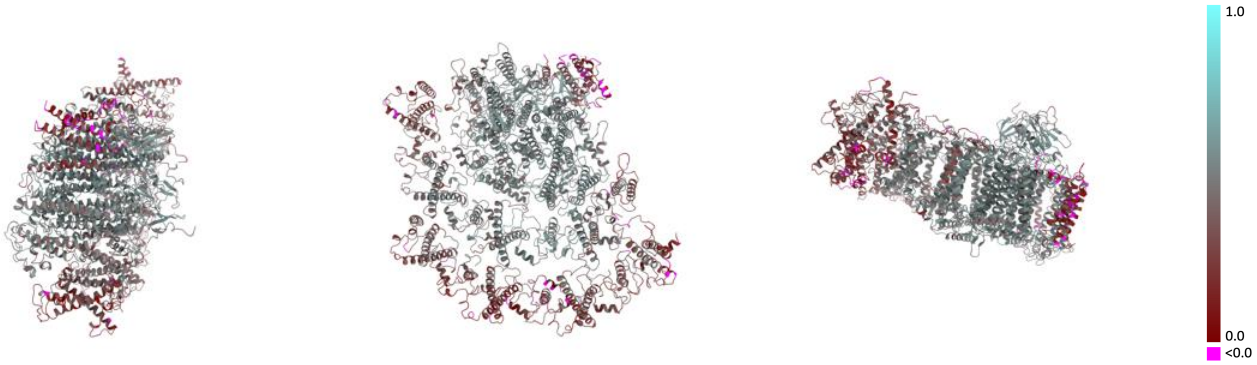
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0151 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

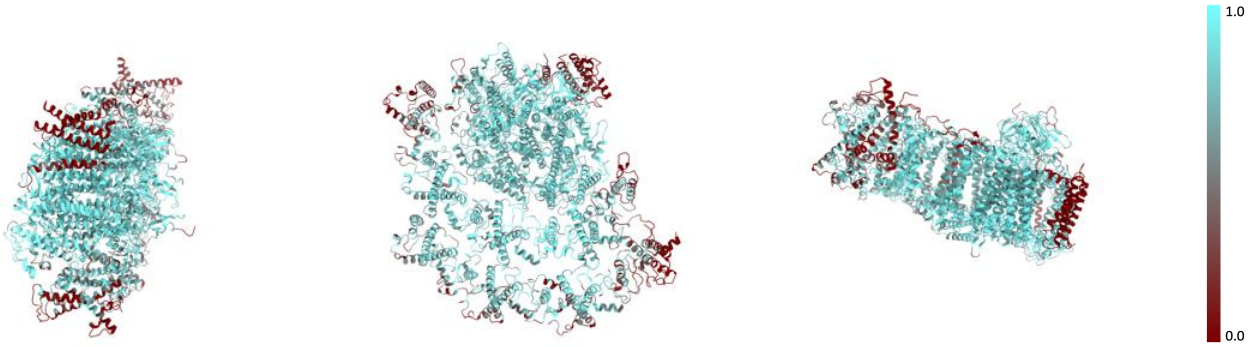
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

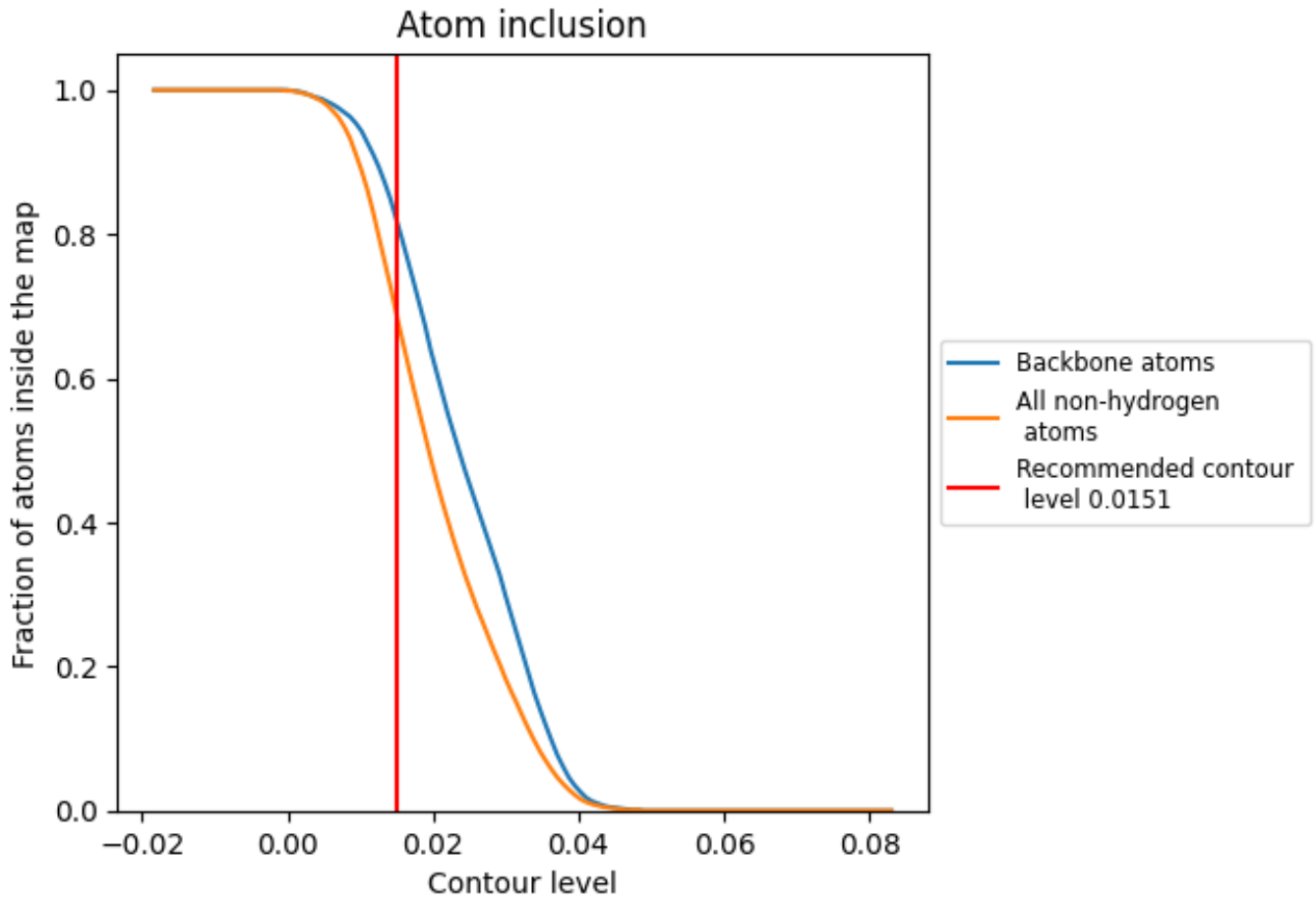
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0151).

9.4 Atom inclusion (i)



At the recommended contour level, 82% of all backbone atoms, 68% 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 (0.0151) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6830	0.4200
1	0.3730	0.2550
3	0.7700	0.4760
7	0.7960	0.4870
8	0.7280	0.4340
A	0.8310	0.5250
B	0.7930	0.4920
C	0.9220	0.5250
D	0.7140	0.4830
E	0.7810	0.4970
F	0.7440	0.4650
I	0.1160	0.2330
J	0.7660	0.4970
K	0.3510	0.3060
L	0.0170	0.1430
T	0.2980	0.2780
a	0.6690	0.3280
b	0.5940	0.2330
c	0.6130	0.2830