wwPDB EM Validation Summary Report

Sep 9, 2026 – 11:58 PM JST

PDB ID	:	6JO6 / pdb_00006jo6
EMDB ID	:	EMD-9854
Title	:	Structure of the green algal photosystem I supercomplex with light-harvesting complex I
Authors	:	Suga, M.; Miyazaki, N.; Takahashi, Y.
Deposited on	:	2019-03-20
Resolution	:	2.90 Å(reported)

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

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

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

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

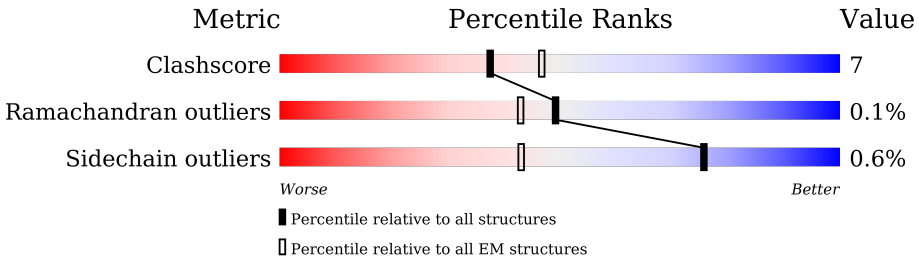
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

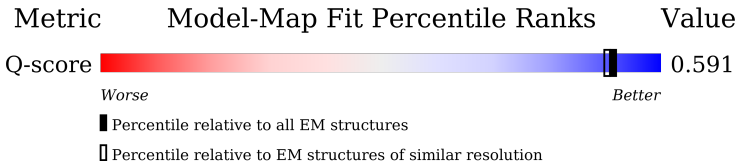
1 Overall quality at a glance

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

The reported resolution of this entry is 2.90 Å.

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





Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	13054 (2.40 - 3.40)

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

Mol	Chain	Length	Quality of chain
1	A	751	86% 12% .
2	B	755	88% 9% .
3	C	81	85% 14% .
4	D	161	75% 14% 11%

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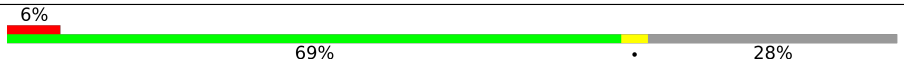
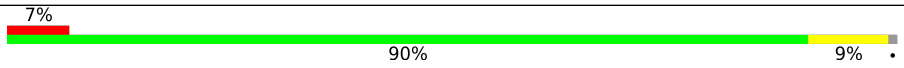
Mol	Chain	Length	Quality of chain
5	E	73	
6	F	165	
7	G	94	
8	I	106	
9	J	41	
10	K	87	
11	L	156	
12	1	194	
12	Z	194	
13	3	268	
14	7	215	
15	8	217	
16	4	236	
17	5	229	
18	6	232	

2 Entry composition (i)

There are 28 unique types of molecules in this entry. The entry contains 45099 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	738	5800	3793	989	996	22	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	732	5822	3824	978	1002	18	0	0

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-16	HIS	-	insertion	UNP P09144
B	-15	HIS	-	insertion	UNP P09144
B	-14	HIS	-	insertion	UNP P09144
B	-13	HIS	-	insertion	UNP P09144
B	-12	HIS	-	insertion	UNP P09144
B	-11	HIS	-	insertion	UNP P09144
B	-10	HIS	-	insertion	UNP P09144
B	-9	HIS	-	insertion	UNP P09144
B	-8	HIS	-	insertion	UNP P09144
B	-7	HIS	-	insertion	UNP P09144
B	-6	HIS	-	insertion	UNP P09144
B	-5	HIS	-	insertion	UNP P09144
B	-4	HIS	-	insertion	UNP P09144
B	-3	HIS	-	insertion	UNP P09144
B	-2	HIS	-	insertion	UNP P09144
B	-1	HIS	-	insertion	UNP P09144
B	0	HIS	-	insertion	UNP P09144
B	1	HIS	-	insertion	UNP P09144
B	2	HIS	-	insertion	UNP P09144
B	3	HIS	-	insertion	UNP P09144

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

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

- Molecule 4 is a protein called Photosystem I reaction center subunit II, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	144	Total	C	N	O	S	0	0
			1132	725	200	200	7		

- Molecule 5 is a protein called Photosystem I reaction center subunit IV, chloroplastic.

Mol	Chain	Residues	Atoms				AltConf	Trace
5	E	61	Total	C	N	O	0	0
			480	306	85	89		

- Molecule 6 is a protein called Photosystem I reaction center subunit F, Photosystem I reaction center subunit III, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	165	Total	C	N	O	S	0	0
			1265	817	213	232	3		

- Molecule 7 is a protein called Photosystem I reaction center subunit V, chloroplastic.

Mol	Chain	Residues	Atoms				AltConf	Trace
7	G	68	Total	C	N	O	0	0
			503	327	87	89		

- Molecule 8 is a protein called Photosystem I reaction center subunit VIII.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	I	37	Total	C	N	O	S	0	0
			281	195	39	46	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	J	39	Total	C	N	O	S	0	0
			320	219	45	55	1		

- Molecule 10 is a protein called Photosystem I reaction center subunit psaK, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	K	45	Total	C	N	O	S	0	0
			297	190	49	56	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
11	L	118	Total	C	N	O	S	0	0
			853	561	136	153	3		

- Molecule 12 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	1	194	Total	C	N	O	S	0	0
			1444	941	240	260	3		
12	Z	192	Total	C	N	O	S	0	0
			1436	937	238	258	3		

- Molecule 13 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	3	202	Total	C	N	O	S	0	0
			1555	1018	252	277	8		

- Molecule 14 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	7	212	Total	C	N	O	S	0	0
			1644	1069	273	296	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
15	8	217	Total	C	N	O	S	0	0
			1649	1073	280	292	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
16	4	203	Total	C	N	O	S	0	0
			1570	1029	254	282	5		

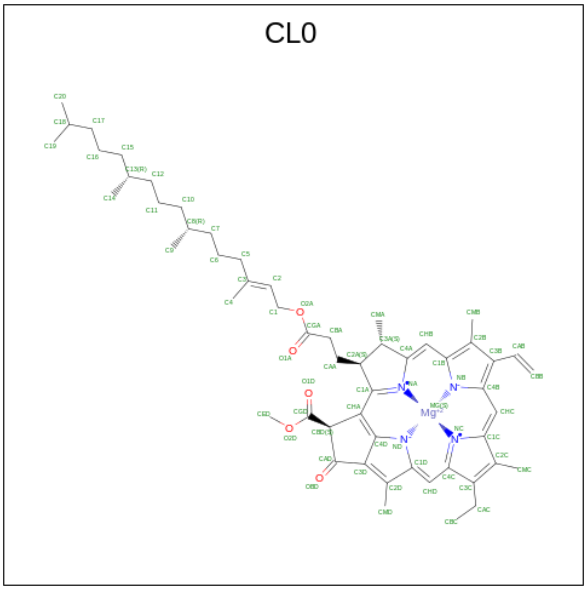
- Molecule 17 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	5	223	Total	C	N	O	S	0	0
			1744	1137	291	308	8		

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

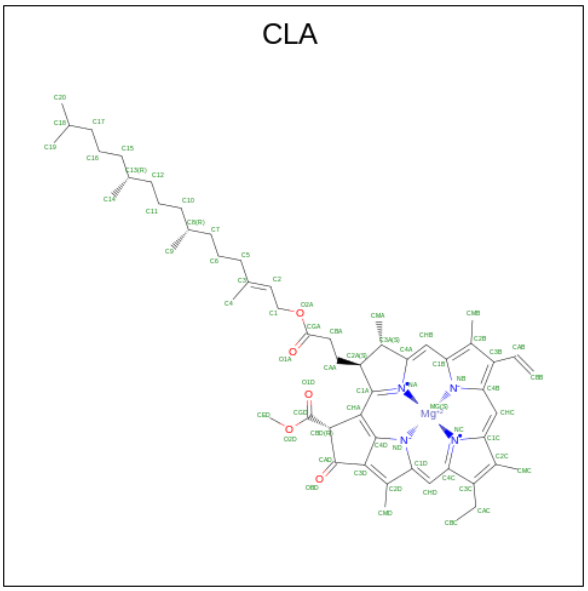
Mol	Chain	Residues	Atoms					AltConf	Trace
18	6	229	Total	C	N	O	S	0	0
			1765	1164	292	303	6		

- Molecule 19 is CHLOROPHYLL A ISOMER (CCD ID: CL0) (formula: $C_{55}H_{72}MgN_4O_5$).



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

- Molecule 20 is CHLOROPHYLL A (CCD ID: CLA) (formula: $C_{55}H_{72}MgN_4O_5$).



Mol	Chain	Residues	Atoms					AltConf
20	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	A	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
20	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	A	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
20	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	A	1	Total	C	Mg	N	O	0
			60	50	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
20	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	A	1	Total	C	Mg	N	O	0
			57	47	1	4	5	
20	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
20	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	A	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
20	A	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
20	A	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
20	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	A	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
20	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	A	1	Total	C	Mg	N	O	0
			50	40	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
20	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
20	A	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
20	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	A	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
20	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
20	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	B	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
20	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
20	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
20	B	1	Total	C	Mg	N	O	0
			57	47	1	4	5	
20	B	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
20	B	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
20	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
20	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	B	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
20	B	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
20	B	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
20	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
20	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	B	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
20	B	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
20	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	B	1	Total	C	Mg	N	O	0
			58	48	1	4	5	
20	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
20	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
20	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
20	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	B	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
20	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	F	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	F	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
20	F	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	G	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
20	G	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
20	J	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
20	K	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
20	K	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
20	L	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	L	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
20	1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	1	1	Total	C	Mg	N	O	0
			57	47	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
20	1	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
20	1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	1	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
20	1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	1	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
20	1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	1	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
20	3	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
20	3	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	3	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	3	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
20	3	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
20	3	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
20	3	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	3	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
20	3	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
20	3	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
20	3	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
20	3	1	Total	C	Mg	N	O	0
			46	36	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
20	3	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
20	7	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	7	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	7	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
20	7	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
20	7	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
20	7	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
20	7	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
20	7	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
20	7	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
20	7	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
20	7	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	7	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
20	7	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
20	7	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
20	8	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	8	1	Total	C	Mg	N	O	0
			62	52	1	4	5	
20	8	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
20	8	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
20	8	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
20	8	1	Total	C	Mg	N	O	0
			50	40	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
20	8	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
20	8	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
20	8	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
20	8	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
20	8	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	8	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
20	8	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
20	Z	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	Z	1	Total	C	Mg	N	O	0
			57	47	1	4	5	
20	Z	1	Total	C	Mg	N	O	0
			57	47	1	4	5	
20	Z	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
20	Z	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	Z	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	Z	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
20	Z	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	Z	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
20	Z	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	Z	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	Z	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
20	4	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
20	4	1	Total	C	Mg	N	O	0
			60	50	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
20	4	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
20	4	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
20	4	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
20	4	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
20	4	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
20	4	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
20	4	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
20	4	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
20	4	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
20	5	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	5	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	5	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
20	5	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
20	5	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
20	5	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
20	5	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
20	5	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
20	5	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
20	5	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
20	5	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
20	5	1	Total	C	Mg	N	O	0
			46	36	1	4	5	

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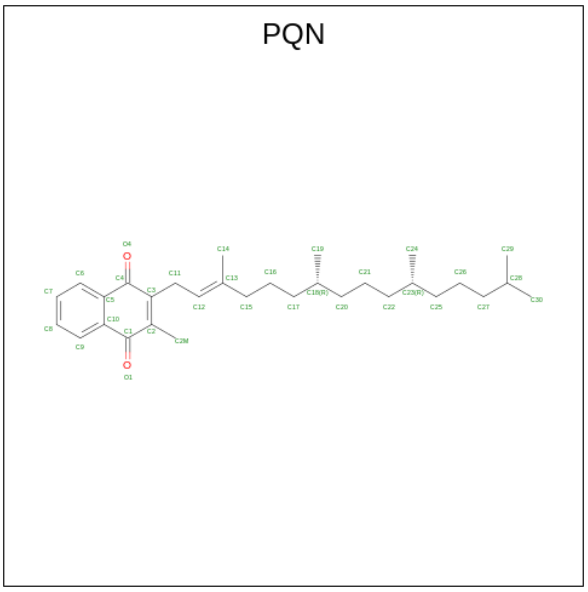
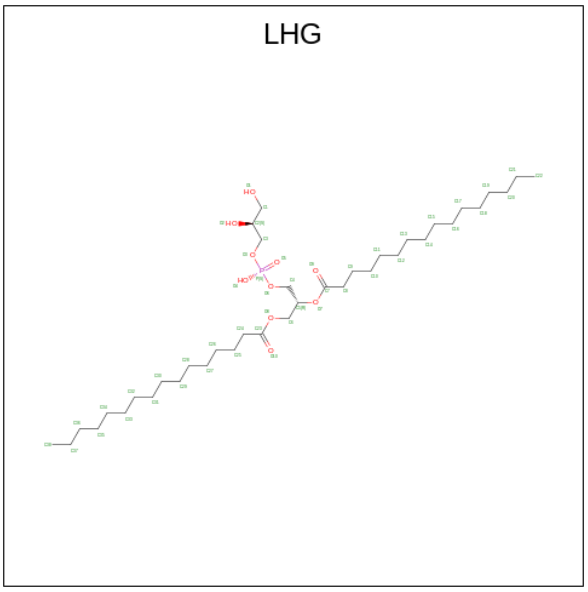
Mol	Chain	Residues	Atoms					AltConf
20	5	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
20	5	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
20	6	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	6	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	6	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
20	6	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	6	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
20	6	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
20	6	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
20	6	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
20	6	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
20	6	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
20	6	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
20	6	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
20	6	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

- Molecule 21 is PHYLLOQUINONE (CCD ID: PQN) (formula: $C_{31}H_{46}O_2$).



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

- Molecule 22 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: $C_{38}H_{75}O_{10}P$).



Mol	Chain	Residues	Atoms				AltConf
22	A	1	Total	C	O	P	0
			49	38	10	1	

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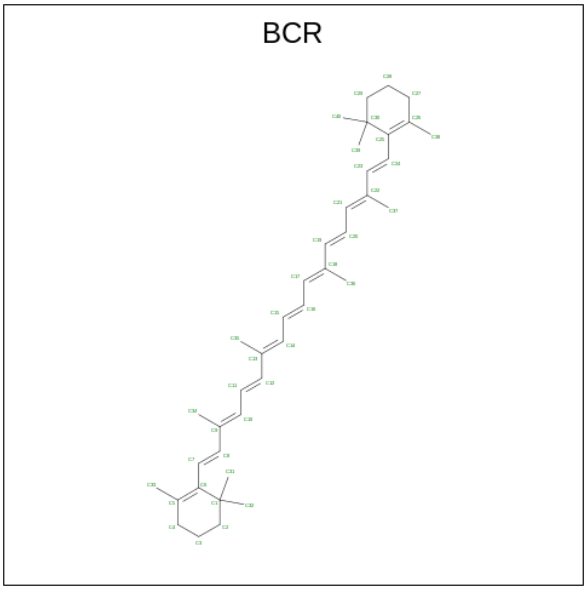
Mol	Chain	Residues	Atoms				AltConf
22	A	1	Total	C	O	P	0
			38	27	10	1	
22	A	1	Total	C	O	P	0
			30	19	10	1	
22	B	1	Total	C	O	P	0
			23	12	10	1	
22	1	1	Total	C	O	P	0
			43	32	10	1	
22	7	1	Total	C	O	P	0
			37	26	10	1	
22	8	1	Total	C	O	P	0
			37	26	10	1	
22	Z	1	Total	C	O	P	0
			43	32	10	1	
22	4	1	Total	C	O	P	0
			49	38	10	1	
22	4	1	Total	C	O	P	0
			32	21	10	1	
22	5	1	Total	C	O	P	0
			37	26	10	1	
22	6	1	Total	C	O	P	0
			49	38	10	1	

- Molecule 23 is BETA-CAROTENE (CCD ID: BCR) (formula: $C_{40}H_{56}$).



Mol	Chain	Residues	Atoms	AltConf
23	A	1	Total C 40 40	0
23	A	1	Total C 40 40	0
23	A	1	Total C 40 40	0
23	A	1	Total C 40 40	0
23	A	1	Total C 40 40	0
23	A	1	Total C 40 40	0
23	B	1	Total C 40 40	0
23	B	1	Total C 40 40	0
23	B	1	Total C 40 40	0
23	B	1	Total C 40 40	0
23	B	1	Total C 40 40	0
23	B	1	Total C 40 40	0
23	B	1	Total C 40 40	0
23	F	1	Total C 40 40	0
23	G	1	Total C 40 40	0
23	I	1	Total C 40 40	0
23	J	1	Total C 40 40	0
23	K	1	Total C 40 40	0
23	K	1	Total C 40 40	0
23	L	1	Total C 40 40	0
23	L	1	Total C 40 40	0
23	3	1	Total C 40 40	0

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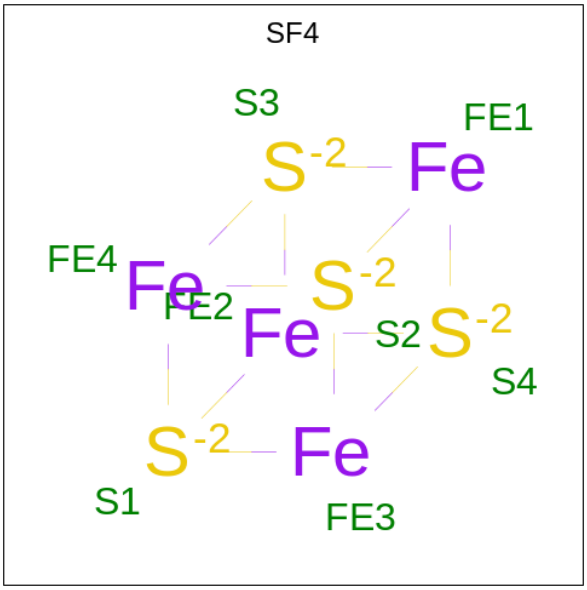
Mol	Chain	Residues	Atoms	AltConf
23	3	1	Total C 40 40	0
23	3	1	Total C 40 40	0
23	7	1	Total C 40 40	0
23	7	1	Total C 40 40	0
23	8	1	Total C 40 40	0
23	4	1	Total C 40 40	0
23	5	1	Total C 40 40	0
23	5	1	Total C 40 40	0
23	6	1	Total C 40 40	0
23	6	1	Total C 40 40	0

- Molecule 24 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



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

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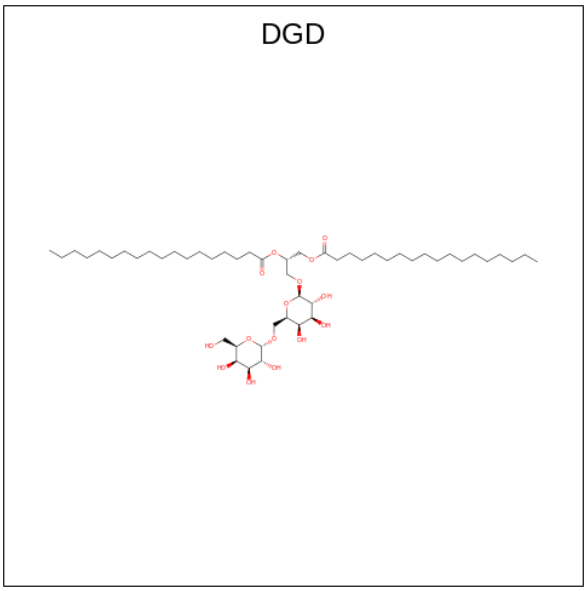
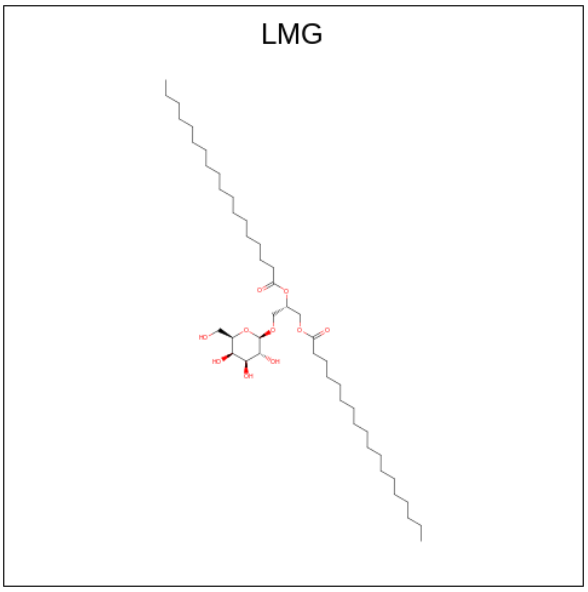
Mol	Chain	Residues	Atoms			AltConf
24	C	1	Total 8	Fe 4	S 4	0
24	C	1	Total 8	Fe 4	S 4	0

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



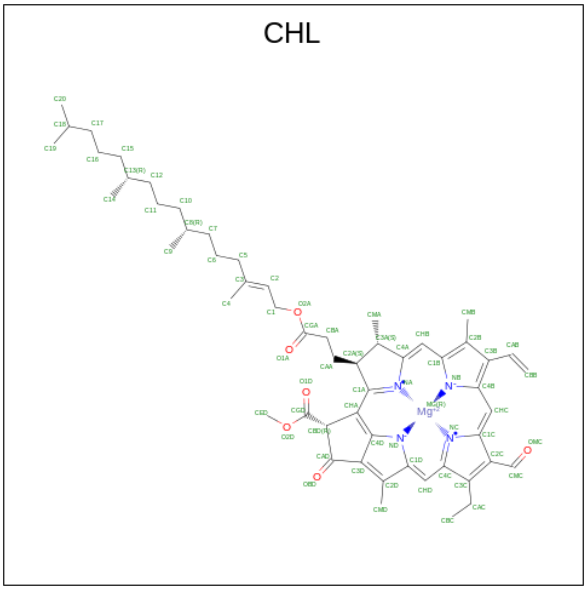
Mol	Chain	Residues	Atoms			AltConf
25	B	1	Total 66	C 51	O 15	0

- Molecule 26 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$).



Mol	Chain	Residues	Atoms			AltConf
26	J	1	Total	C	O	0
			35	25	10	

- Molecule 27 is CHLOROPHYLL B (CCD ID: CHL) (formula: $C_{55}H_{70}MgN_4O_6$).



Mol	Chain	Residues	Atoms					AltConf
27	1	1	Total	C	Mg	N	O	0
			53	42	1	4	6	
27	1	1	Total	C	Mg	N	O	0
			48	37	1	4	6	
27	3	1	Total	C	Mg	N	O	0
			66	55	1	4	6	

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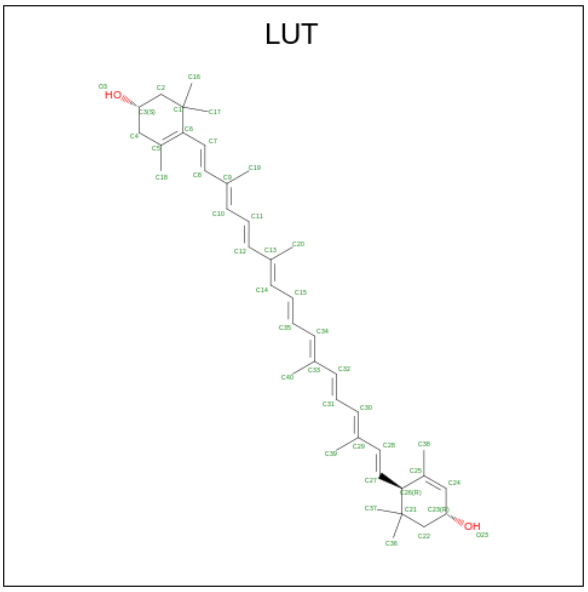
Mol	Chain	Residues	Atoms					AltConf
27	7	1	Total	C	Mg	N	O	0
			54	43	1	4	6	
27	8	1	Total	C	Mg	N	O	0
			56	45	1	4	6	
27	Z	1	Total	C	Mg	N	O	0
			53	42	1	4	6	
27	Z	1	Total	C	Mg	N	O	0
			48	37	1	4	6	
27	4	1	Total	C	Mg	N	O	0
			56	45	1	4	6	
27	4	1	Total	C	Mg	N	O	0
			51	40	1	4	6	
27	4	1	Total	C	Mg	N	O	0
			51	40	1	4	6	
27	4	1	Total	C	Mg	N	O	0
			43	34	1	4	4	
27	5	1	Total	C	Mg	N	O	0
			51	40	1	4	6	
27	5	1	Total	C	Mg	N	O	0
			51	40	1	4	6	
27	5	1	Total	C	Mg	N	O	0
			43	34	1	4	4	
27	6	1	Total	C	Mg	N	O	0
			56	45	1	4	6	
27	6	1	Total	C	Mg	N	O	0
			56	45	1	4	6	
27	6	1	Total	C	Mg	N	O	0
			51	40	1	4	6	
27	6	1	Total	C	Mg	N	O	0
			43	34	1	4	4	

- Molecule 28 is (3R,3'R,6S)-4,5-DIDEHYDRO-5,6-DIHYDRO-BETA,BETA-CAROTENE-3 ,3'-DIOL (CCD ID: LUT) (formula: $C_{40}H_{56}O_2$).



Mol	Chain	Residues	Atoms			AltConf
28	1	1	Total	C	O	0
			42	40	2	
28	1	1	Total	C	O	0
			42	40	2	
28	1	1	Total	C	O	0
			42	40	2	
28	3	1	Total	C	O	0
			42	40	2	
28	3	1	Total	C	O	0
			42	40	2	
28	7	1	Total	C	O	0
			42	40	2	
28	7	1	Total	C	O	0
			42	40	2	
28	8	1	Total	C	O	0
			42	40	2	
28	8	1	Total	C	O	0
			42	40	2	
28	Z	1	Total	C	O	0
			42	40	2	
28	Z	1	Total	C	O	0
			42	40	2	
28	Z	1	Total	C	O	0
			42	40	2	
28	4	1	Total	C	O	0
			42	40	2	
28	4	1	Total	C	O	0
			42	40	2	

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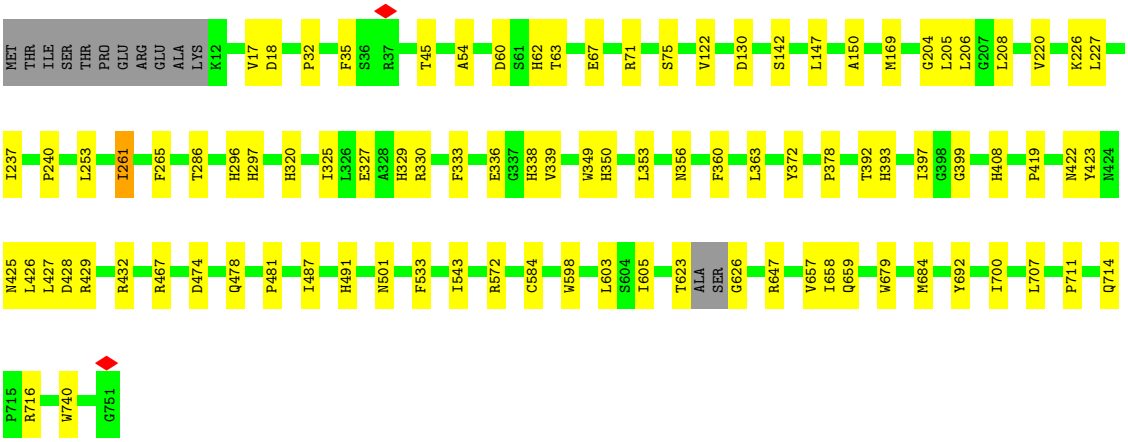
Mol	Chain	Residues	Atoms			AltConf
28	5	1	Total	C	O	0
			42	40	2	
28	5	1	Total	C	O	0
			42	40	2	
28	6	1	Total	C	O	0
			42	40	2	
28	6	1	Total	C	O	0
			42	40	2	

3 Residue-property plots (i)

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

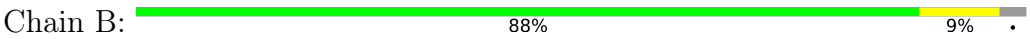
• Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1

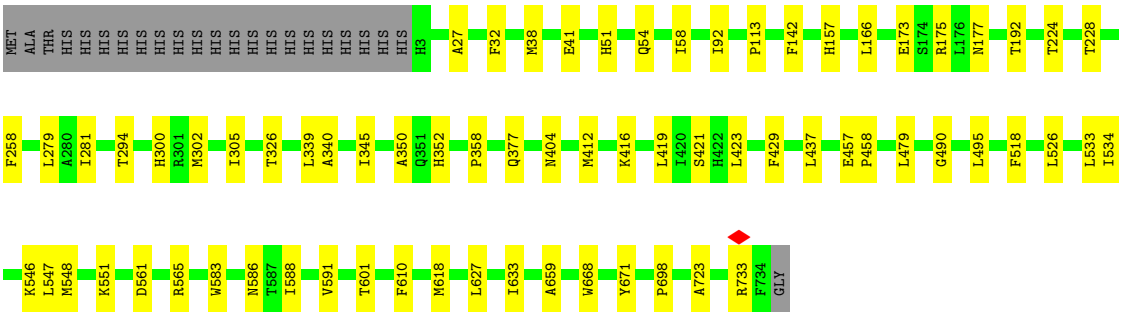
Chain A:



• Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

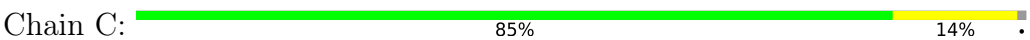
Chain B:

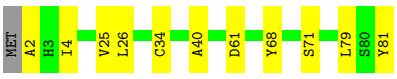




• Molecule 3: Photosystem I iron-sulfur center

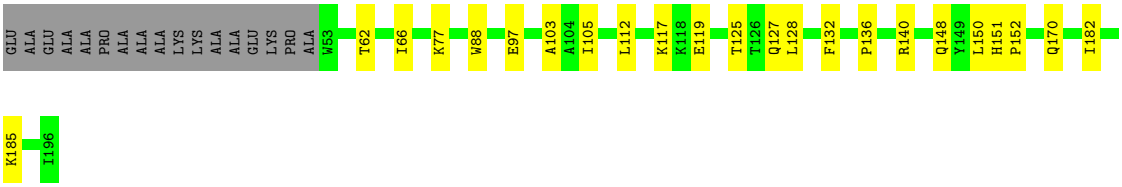
Chain C:





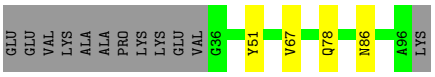
• Molecule 4: Photosystem I reaction center subunit II, chloroplastic

Chain D:



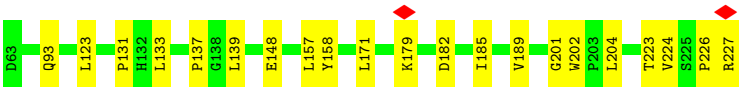
• Molecule 5: Photosystem I reaction center subunit IV, chloroplastic

Chain E:



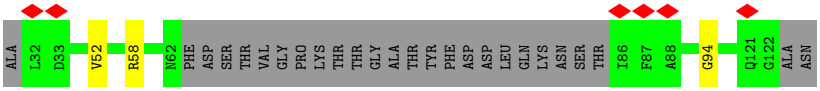
• Molecule 6: Photosystem I reaction center subunit F, Photosystem I reaction center subunit III, chloroplastic

Chain F:



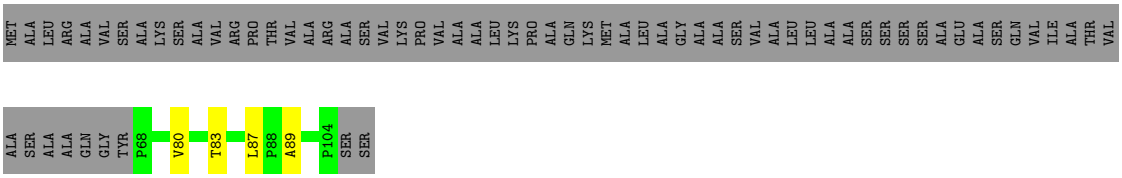
• Molecule 7: Photosystem I reaction center subunit V, chloroplastic

Chain G:



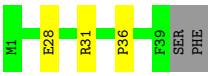
• Molecule 8: Photosystem I reaction center subunit VIII

Chain I:



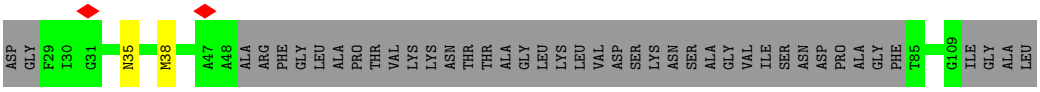
• Molecule 9: Photosystem I reaction center subunit IX

Chain J:



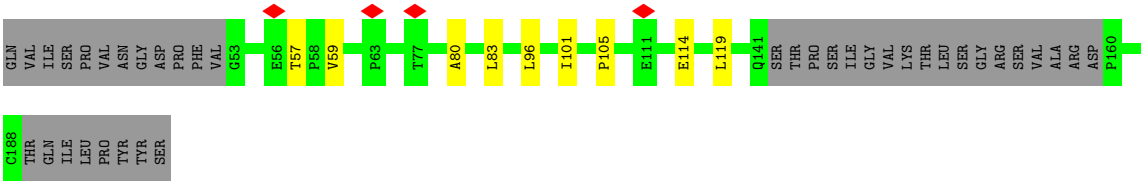
• Molecule 10: Photosystem I reaction center subunit psaK, chloroplastic

Chain K:



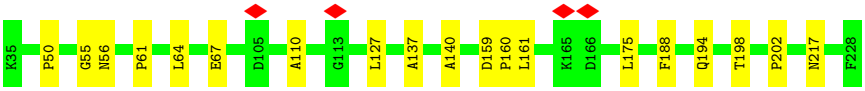
• Molecule 11: Photosystem I reaction center subunit XI

Chain L:



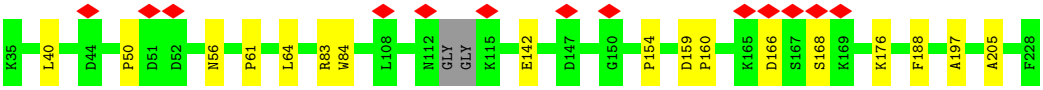
• Molecule 12: Chlorophyll a-b binding protein, chloroplastic

Chain 1:



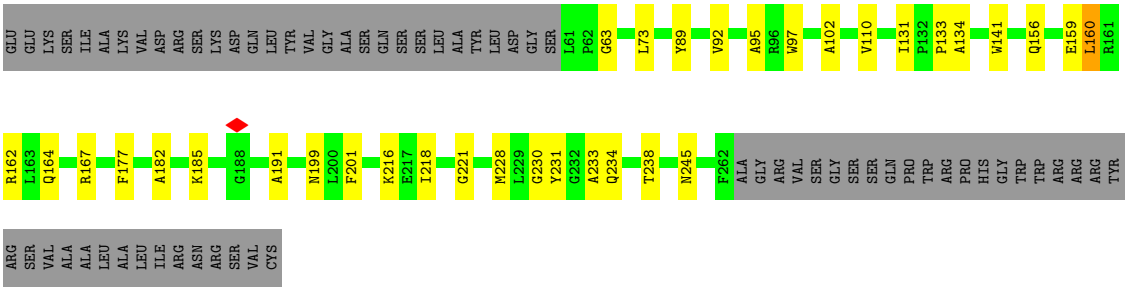
• Molecule 12: Chlorophyll a-b binding protein, chloroplastic

Chain Z:



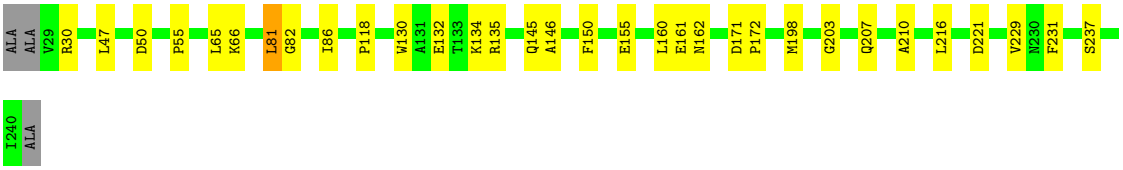
• Molecule 13: Chlorophyll a-b binding protein, chloroplastic

Chain 3:



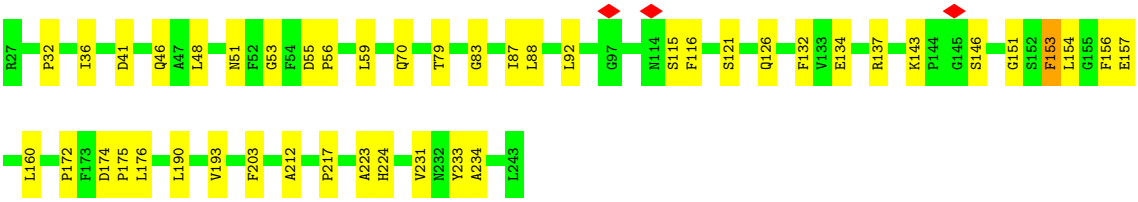
• Molecule 14: Chlorophyll a-b binding protein, chloroplastic

Chain 7:



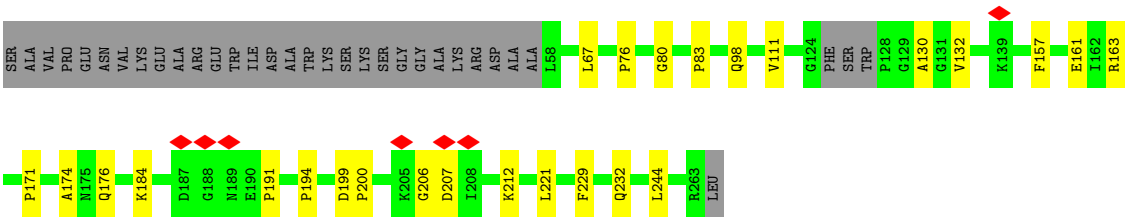
• Molecule 15: Chlorophyll a-b binding protein, chloroplastic

Chain 8:



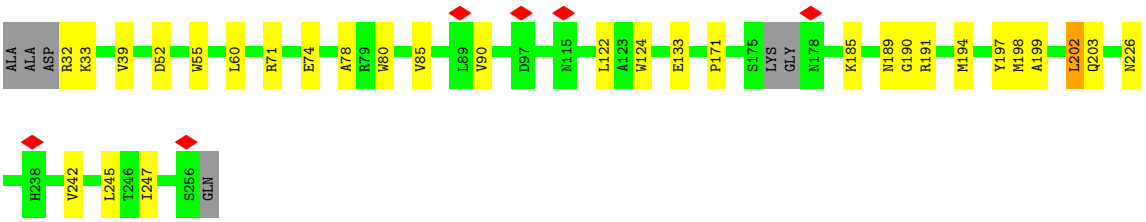
• Molecule 16: Chlorophyll a-b binding protein, chloroplastic

Chain 4:



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

Chain 5:



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

Chain 6:

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	379749	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50.0	Depositor
Minimum defocus (nm)	1600	Depositor
Maximum defocus (nm)	3750	Depositor
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.460	Depositor
Minimum map value	-0.221	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.011	Depositor
Recommended contour level	0.05	Depositor
Map size (Å)	358.4, 358.4, 358.4	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.12, 1.12, 1.12	Depositor

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.31	0/5995	0.68	1/8172 (0.0%)
2	B	0.26	0/6035	0.54	0/8240
3	C	0.26	0/610	0.64	0/826
4	D	0.25	0/1160	0.49	0/1567
5	E	0.19	0/490	0.41	0/667
6	F	0.26	0/1291	0.58	0/1747
7	G	0.18	0/513	0.47	0/696
8	I	0.27	0/293	0.59	0/406
9	J	0.25	0/331	0.56	0/454
10	K	0.18	0/297	0.44	0/401
11	L	0.21	0/874	0.51	0/1194
12	1	0.23	0/1490	0.50	0/2028
12	Z	0.22	0/1481	0.52	0/2015
13	3	0.29	0/1601	0.60	0/2173
14	7	0.26	0/1696	0.57	0/2303
15	8	0.28	0/1700	0.59	0/2315
16	4	0.26	0/1621	0.55	0/2209
17	5	0.23	0/1798	0.52	0/2450
18	6	0.22	0/1827	0.51	0/2497
All	All	0.26	0/31103	0.57	1/42360 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	1
14	7	0	1
16	4	0	1
All	All	0	3

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	261	ILE	N-CA-C	-5.28	107.33	112.29

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
16	4	206	GLY	Peptide
14	7	150	PHE	Peptide
2	B	668	TRP	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5800	0	5646	68	0
2	B	5822	0	5574	51	0
3	C	600	0	581	8	0
4	D	1132	0	1150	14	0
5	E	480	0	476	4	0
6	F	1265	0	1301	15	0
7	G	503	0	496	2	0
8	I	281	0	292	4	0
9	J	320	0	322	3	0
10	K	297	0	319	2	0
11	L	853	0	864	6	0
12	1	1444	0	1396	15	0
12	Z	1436	0	1389	16	0
13	3	1555	0	1522	25	0
14	7	1644	0	1584	27	0
15	8	1649	0	1629	44	0
16	4	1570	0	1527	20	0
17	5	1744	0	1717	34	0
18	6	1765	0	1767	28	0
19	A	65	0	72	1	0
20	1	722	0	735	18	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
20	3	696	0	631	15	0
20	4	576	0	495	19	0
20	5	737	0	638	20	0
20	6	696	0	622	18	0
20	7	741	0	665	20	0
20	8	680	0	593	14	0
20	A	2689	0	2798	114	0
20	B	2480	0	2545	91	0
20	F	175	0	177	7	0
20	G	96	0	72	0	0
20	J	42	0	31	0	0
20	K	91	0	66	4	0
20	L	115	0	111	0	0
20	Z	714	0	716	21	0
21	A	33	0	46	1	0
21	B	33	0	46	1	0
22	1	43	0	56	0	0
22	4	81	0	108	6	0
22	5	37	0	44	1	0
22	6	49	0	73	3	0
22	7	37	0	44	1	0
22	8	37	0	44	0	0
22	A	117	0	153	6	0
22	B	23	0	16	2	0
22	Z	43	0	56	3	0
23	3	120	0	168	12	0
23	4	40	0	56	2	0
23	5	80	0	112	9	0
23	6	80	0	112	8	0
23	7	80	0	112	6	0
23	8	40	0	56	3	0
23	A	240	0	336	20	0
23	B	280	0	392	20	0
23	F	40	0	56	6	0
23	G	40	0	56	4	0
23	I	40	0	56	2	0
23	J	40	0	56	3	0
23	K	80	0	112	2	0
23	L	80	0	112	4	0
24	A	8	0	0	0	0
24	C	16	0	0	0	0
25	B	66	0	96	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
26	J	35	0	40	0	0
27	1	101	0	74	2	0
27	3	66	0	70	3	0
27	4	201	0	150	1	0
27	5	145	0	103	4	0
27	6	206	0	160	5	0
27	7	54	0	43	0	0
27	8	56	0	47	1	0
27	Z	101	0	74	5	0
28	1	126	0	168	14	0
28	3	84	0	112	6	0
28	4	84	0	112	9	0
28	5	84	0	112	8	0
28	6	84	0	112	11	0
28	7	84	0	112	9	0
28	8	84	0	112	14	0
28	Z	126	0	168	11	0
All	All	45099	0	44862	671	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 7.

The worst 5 of 671 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)
15:8:156:PHE:CZ	15:8:172:PRO:HG3	1.95	0.99
17:5:185:LYS:O	17:5:189:ASN:ND2	2.01	0.94
15:8:156:PHE:CE1	15:8:172:PRO:HG3	2.06	0.90
17:5:199:ALA:O	17:5:203:GLN:HG3	1.85	0.77
20:3:610:CLA:HBB1	28:3:621:LUT:H32	1.66	0.77

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	734/751 (98%)	712 (97%)	21 (3%)	1 (0%)	48 77
2	B	730/755 (97%)	706 (97%)	24 (3%)	0	100 100
3	C	78/81 (96%)	73 (94%)	5 (6%)	0	100 100
4	D	142/161 (88%)	134 (94%)	8 (6%)	0	100 100
5	E	59/73 (81%)	54 (92%)	5 (8%)	0	100 100
6	F	163/165 (99%)	158 (97%)	5 (3%)	0	100 100
7	G	64/94 (68%)	63 (98%)	1 (2%)	0	100 100
8	I	35/106 (33%)	34 (97%)	1 (3%)	0	100 100
9	J	37/41 (90%)	35 (95%)	2 (5%)	0	100 100
10	K	41/87 (47%)	41 (100%)	0	0	100 100
11	L	114/156 (73%)	110 (96%)	4 (4%)	0	100 100
12	1	192/194 (99%)	186 (97%)	6 (3%)	0	100 100
12	Z	188/194 (97%)	180 (96%)	8 (4%)	0	100 100
13	3	200/268 (75%)	194 (97%)	6 (3%)	0	100 100
14	7	210/215 (98%)	198 (94%)	12 (6%)	0	100 100
15	8	215/217 (99%)	206 (96%)	9 (4%)	0	100 100
16	4	199/236 (84%)	184 (92%)	14 (7%)	1 (0%)	24 54
17	5	219/229 (96%)	201 (92%)	18 (8%)	0	100 100
18	6	227/232 (98%)	215 (95%)	12 (5%)	0	100 100
All	All	3847/4255 (90%)	3684 (96%)	161 (4%)	2 (0%)	49 77

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	122	VAL
16	4	207	ASP

5.3.2 Protein sidechains (i)

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

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

analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	599/610 (98%)	591 (99%)	8 (1%)	61 86
2	B	596/617 (97%)	595 (100%)	1 (0%)	87 96
3	C	69/70 (99%)	69 (100%)	0	100 100
4	D	121/129 (94%)	120 (99%)	1 (1%)	73 90
5	E	52/62 (84%)	52 (100%)	0	100 100
6	F	127/127 (100%)	127 (100%)	0	100 100
7	G	48/69 (70%)	48 (100%)	0	100 100
8	I	31/76 (41%)	31 (100%)	0	100 100
9	J	35/37 (95%)	35 (100%)	0	100 100
10	K	30/60 (50%)	30 (100%)	0	100 100
11	L	85/119 (71%)	84 (99%)	1 (1%)	63 86
12	1	137/137 (100%)	137 (100%)	0	100 100
12	Z	137/137 (100%)	137 (100%)	0	100 100
13	3	155/209 (74%)	154 (99%)	1 (1%)	78 93
14	7	164/164 (100%)	162 (99%)	2 (1%)	63 86
15	8	163/163 (100%)	162 (99%)	1 (1%)	78 93
16	4	159/185 (86%)	159 (100%)	0	100 100
17	5	181/184 (98%)	179 (99%)	2 (1%)	65 88
18	6	183/185 (99%)	183 (100%)	0	100 100
All	All	3072/3340 (92%)	3055 (99%)	17 (1%)	76 93

5 of 17 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
15	8	153	PHE
17	5	226	ASN
1	A	657	VAL
2	B	479	LEU
4	D	150	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 32 such sidechains are listed below:

Mol	Chain	Res	Type
17	5	142	ASN

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Mol	Chain	Res	Type
17	5	226	ASN
12	1	194	GLN
12	1	56	ASN
18	6	130	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)

285 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	$\#\|Z\| > 2$
28	LUT	Z	619	-	42,43,43	0.72	0	51,60,60	1.71	11 (21%)
20	CLA	5	601	17	69,73,73	2.05	20 (28%)	83,113,113	2.78	29 (34%)
28	LUT	7	621	-	42,43,43	0.74	0	51,60,60	1.55	11 (21%)
28	LUT	Z	617	-	42,43,43	0.77	0	51,60,60	1.61	14 (27%)
27	CHL	4	618	16	47,51,74	2.33	20 (42%)	52,86,114	3.62	24 (46%)
28	LUT	1	618	-	42,43,43	0.74	0	51,60,60	1.58	13 (25%)
20	CLA	A	839	1	69,73,73	2.01	21 (30%)	83,113,113	2.90	31 (37%)
20	CLA	A	827	-	69,73,73	2.04	20 (28%)	83,113,113	2.85	30 (36%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
23	BCR	8	619	-	41,41,41	0.68	0	56,56,56	1.83	13 (23%)
28	LUT	4	620	-	42,43,43	0.73	0	51,60,60	1.54	12 (23%)
20	CLA	7	610	14	64,68,73	2.12	18 (28%)	77,107,113	3.06	33 (42%)
20	CLA	1	604	-	61,65,73	2.19	19 (31%)	73,103,113	2.94	32 (43%)
20	CLA	Z	603	12	61,65,73	2.16	20 (32%)	73,103,113	3.00	32 (43%)
20	CLA	5	603	17	50,54,73	2.35	20 (40%)	60,90,113	3.19	26 (43%)
22	LHG	B	851	20	22,22,48	1.15	2 (9%)	25,28,54	1.24	2 (8%)
20	CLA	B	829	2	69,73,73	2.04	19 (27%)	83,113,113	2.95	33 (39%)
20	CLA	3	610	13	69,73,73	2.03	18 (26%)	83,113,113	2.87	32 (38%)
27	CHL	Z	607	-	52,56,74	2.33	21 (40%)	58,92,114	3.21	24 (41%)
20	CLA	A	821	1	49,53,73	2.39	19 (38%)	59,89,113	3.18	27 (45%)
23	BCR	B	843	-	41,41,41	0.71	0	56,56,56	1.59	9 (16%)
22	LHG	8	620	20	36,36,48	1.03	2 (5%)	39,42,54	1.13	2 (5%)
23	BCR	I	172	-	41,41,41	0.66	0	56,56,56	2.08	15 (26%)
20	CLA	K	4002	-	49,53,73	2.45	20 (40%)	59,89,113	3.27	28 (47%)
28	LUT	1	619	-	42,43,43	0.73	0	51,60,60	1.68	9 (17%)
27	CHL	3	608	-	70,74,74	1.93	19 (27%)	80,114,114	2.95	26 (32%)
20	CLA	4	613	16	60,64,73	2.19	20 (33%)	72,102,113	2.99	30 (41%)
20	CLA	B	833	2	62,66,73	2.13	20 (32%)	74,104,113	3.10	33 (44%)
20	CLA	A	817	-	61,65,73	2.16	20 (32%)	73,103,113	2.96	31 (42%)
20	CLA	B	840	2	69,73,73	2.05	19 (27%)	83,113,113	2.90	28 (33%)
20	CLA	B	822	2	63,67,73	2.15	20 (31%)	75,105,113	2.96	30 (40%)
20	CLA	8	606	-	46,50,73	2.43	20 (43%)	55,85,113	3.31	26 (47%)
20	CLA	3	613	13	59,63,73	2.16	21 (35%)	71,101,113	2.98	29 (40%)
22	LHG	7	625	20	36,36,48	1.03	2 (5%)	39,42,54	1.14	2 (5%)
20	CLA	A	835	1	69,73,73	2.05	20 (28%)	83,113,113	2.90	27 (32%)
20	CLA	1	603	12	69,73,73	2.02	20 (28%)	83,113,113	2.81	29 (34%)
20	CLA	B	837	2	69,73,73	2.01	20 (28%)	83,113,113	2.86	33 (39%)
20	CLA	8	609	15	50,54,73	2.35	20 (40%)	60,90,113	3.28	28 (46%)
20	CLA	F	301	-	69,73,73	2.05	20 (28%)	83,113,113	2.84	32 (38%)
23	BCR	A	849	-	41,41,41	0.75	0	56,56,56	1.74	14 (25%)
20	CLA	A	809	1	69,73,73	2.00	21 (30%)	83,113,113	2.92	31 (37%)
20	CLA	A	837	1	49,53,73	2.45	20 (40%)	59,89,113	3.22	28 (47%)
20	CLA	6	602	18	69,73,73	2.04	20 (28%)	83,113,113	2.83	30 (36%)
28	LUT	1	617	-	42,43,43	0.75	0	51,60,60	1.57	12 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
28	LUT	7	622	-	42,43,43	0.74	0	51,60,60	1.58	10 (19%)
20	CLA	A	818	1	69,73,73	2.01	19 (27%)	83,113,113	2.98	32 (38%)
22	LHG	5	623	20	36,36,48	1.06	2 (5%)	39,42,54	1.12	2 (5%)
20	CLA	A	824	1	55,59,73	2.28	21 (38%)	66,96,113	3.14	26 (39%)
28	LUT	3	622	-	42,43,43	0.79	0	51,60,60	1.71	14 (27%)
27	CHL	1	601	12	57,61,74	2.18	21 (36%)	64,98,114	3.48	28 (43%)
27	CHL	5	618	17	47,51,74	2.35	20 (42%)	52,86,114	3.63	25 (48%)
20	CLA	A	803	-	69,73,73	1.98	20 (28%)	83,113,113	2.93	31 (37%)
20	CLA	6	609	18	54,58,73	2.30	21 (38%)	65,95,113	3.16	28 (43%)
20	CLA	A	838	1	55,59,73	2.27	20 (36%)	66,96,113	3.16	32 (48%)
27	CHL	4	608	-	55,59,74	2.15	20 (36%)	62,96,114	3.27	26 (41%)
20	CLA	6	604	-	69,73,73	2.05	19 (27%)	83,113,113	2.74	29 (34%)
23	BCR	A	852	-	41,41,41	0.72	0	56,56,56	1.91	11 (19%)
20	CLA	5	617	17	50,54,73	2.32	20 (40%)	60,90,113	3.28	27 (45%)
20	CLA	8	612	15	56,60,73	2.24	21 (37%)	67,97,113	3.14	34 (50%)
23	BCR	L	201	-	41,41,41	0.71	0	56,56,56	1.72	10 (17%)
23	BCR	K	4001	-	41,41,41	0.69	0	56,56,56	2.00	15 (26%)
20	CLA	L	204	-	54,58,73	2.34	20 (37%)	65,95,113	3.17	27 (41%)
23	BCR	B	848	-	41,41,41	0.71	0	56,56,56	1.58	10 (17%)
20	CLA	A	810	1	69,73,73	2.00	20 (28%)	83,113,113	2.74	30 (36%)
20	CLA	5	614	17	49,53,73	2.43	20 (40%)	59,89,113	3.27	27 (45%)
23	BCR	L	205	-	41,41,41	0.71	0	56,56,56	1.69	11 (19%)
27	CHL	1	607	-	52,56,74	2.33	21 (40%)	58,92,114	3.14	22 (37%)
20	CLA	F	303	-	49,53,73	2.42	21 (42%)	59,89,113	3.28	27 (45%)
20	CLA	A	811	1	69,73,73	2.00	21 (30%)	83,113,113	2.83	31 (37%)
20	CLA	G	203	7	54,58,73	2.31	20 (37%)	65,95,113	3.22	30 (46%)
23	BCR	B	846	-	41,41,41	0.78	0	56,56,56	1.87	15 (26%)
28	LUT	Z	618	-	42,43,43	0.75	0	51,60,60	1.59	14 (27%)
20	CLA	B	803	-	69,73,73	2.00	19 (27%)	83,113,113	2.83	28 (33%)
23	BCR	J	3003	-	41,41,41	0.72	0	56,56,56	1.73	12 (21%)
20	CLA	5	609	17	54,58,73	2.29	20 (37%)	65,95,113	3.23	30 (46%)
23	BCR	K	4004	-	41,41,41	0.70	0	56,56,56	1.64	10 (17%)
27	CHL	8	607	-	60,64,74	2.13	21 (35%)	68,102,114	3.12	28 (41%)
20	CLA	8	611	22	50,54,73	2.39	21 (42%)	60,90,113	3.16	27 (45%)
28	LUT	5	620	-	42,43,43	0.76	0	51,60,60	1.69	13 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
20	CLA	Z	604	-	61,65,73	2.18	19 (31%)	73,103,113	2.93	30 (41%)
20	CLA	B	852	-	69,73,73	2.06	20 (28%)	83,113,113	2.72	30 (36%)
20	CLA	A	802	-	69,73,73	1.98	20 (28%)	83,113,113	2.83	33 (39%)
20	CLA	7	609	14	54,58,73	2.28	21 (38%)	65,95,113	3.33	33 (50%)
20	CLA	5	616	17	50,54,73	2.37	21 (42%)	60,90,113	3.19	29 (48%)
20	CLA	5	610	17	64,68,73	2.10	20 (31%)	77,107,113	2.95	31 (40%)
27	CHL	6	606	-	60,64,74	2.13	20 (33%)	68,102,114	3.22	28 (41%)
20	CLA	B	804	2	49,53,73	2.38	20 (40%)	59,89,113	3.41	30 (50%)
20	CLA	8	608	-	54,58,73	2.25	19 (35%)	65,95,113	3.17	28 (43%)
21	PQN	A	844	-	34,34,34	1.57	2 (5%)	42,45,45	1.09	3 (7%)
23	BCR	7	624	-	41,41,41	0.66	0	56,56,56	1.78	13 (23%)
20	CLA	3	611	-	45,49,73	2.50	20 (44%)	54,84,113	3.39	28 (51%)
20	CLA	8	613	15	69,73,73	1.98	20 (28%)	83,113,113	2.80	30 (36%)
20	CLA	A	807	1	69,73,73	2.03	21 (30%)	83,113,113	2.87	31 (37%)
20	CLA	B	811	2	58,62,73	2.21	19 (32%)	73,100,113	3.16	32 (43%)
20	CLA	B	826	2	69,73,73	2.01	20 (28%)	83,113,113	2.88	31 (37%)
20	CLA	1	611	22	69,73,73	2.06	20 (28%)	83,113,113	2.78	31 (37%)
23	BCR	B	801	-	41,41,41	0.73	0	56,56,56	1.93	16 (28%)
20	CLA	F	304	6	69,73,73	2.02	21 (30%)	83,113,113	2.88	31 (37%)
20	CLA	A	831	1	69,73,73	1.98	18 (26%)	83,113,113	2.78	28 (33%)
20	CLA	5	602	17	69,73,73	2.03	19 (27%)	83,113,113	2.87	31 (37%)
20	CLA	7	608	-	54,58,73	2.27	19 (35%)	65,95,113	3.12	27 (41%)
20	CLA	Z	602	12	69,73,73	2.03	21 (30%)	83,113,113	2.83	31 (37%)
20	CLA	B	841	22	69,73,73	2.02	20 (28%)	83,113,113	2.84	30 (36%)
20	CLA	A	814	1	69,73,73	1.99	20 (28%)	83,113,113	2.89	30 (36%)
20	CLA	6	603	18	50,54,73	2.36	20 (40%)	60,90,113	3.25	27 (45%)
23	BCR	4	621	-	41,41,41	0.68	0	56,56,56	1.77	13 (23%)
23	BCR	6	625	-	41,41,41	0.66	0	56,56,56	1.99	14 (25%)
28	LUT	8	617	-	42,43,43	0.76	0	51,60,60	1.64	12 (23%)
23	BCR	B	844	-	41,41,41	0.69	0	56,56,56	1.72	12 (21%)
20	CLA	1	613	-	69,73,73	2.03	20 (28%)	83,113,113	2.72	29 (34%)
20	CLA	A	819	1	69,73,73	2.02	20 (28%)	83,113,113	2.82	30 (36%)
28	LUT	6	624	-	42,43,43	0.72	0	51,60,60	1.50	12 (23%)
20	CLA	B	807	2	69,73,73	2.04	20 (28%)	83,113,113	2.85	29 (34%)
20	CLA	B	820	2	60,64,73	2.17	20 (33%)	72,102,113	2.99	30 (41%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
20	CLA	8	603	15	49,53,73	2.37	20 (40%)	59,89,113	3.31	26 (44%)
20	CLA	Z	609	12	69,73,73	2.03	21 (30%)	83,113,113	2.85	31 (37%)
20	CLA	6	613	-	60,64,73	2.19	20 (33%)	72,102,113	2.91	28 (38%)
20	CLA	7	602	14	69,73,73	2.03	20 (28%)	83,113,113	2.86	32 (38%)
20	CLA	B	836	2	64,68,73	2.09	21 (32%)	77,107,113	2.99	31 (40%)
20	CLA	A	833	1	69,73,73	2.01	20 (28%)	83,113,113	2.83	30 (36%)
20	CLA	1	610	12	64,68,73	2.12	20 (31%)	77,107,113	2.99	34 (44%)
20	CLA	B	828	2	69,73,73	2.01	20 (28%)	83,113,113	2.67	28 (33%)
20	CLA	6	622	-	49,53,73	2.39	20 (40%)	59,89,113	3.25	28 (47%)
20	CLA	5	611	22	59,63,73	2.21	21 (35%)	71,101,113	2.97	29 (40%)
20	CLA	B	821	2	50,54,73	2.38	20 (40%)	60,90,113	3.25	26 (43%)
20	CLA	B	815	2	61,65,73	2.17	21 (34%)	73,103,113	3.08	29 (39%)
20	CLA	B	831	2	53,57,73	2.31	20 (37%)	62,93,113	3.25	26 (41%)
20	CLA	3	609	13	54,58,73	2.30	21 (38%)	65,95,113	3.15	32 (49%)
20	CLA	7	603	14	50,54,73	2.38	20 (40%)	60,90,113	3.29	26 (43%)
20	CLA	A	828	1	69,73,73	1.98	19 (27%)	83,113,113	2.92	29 (34%)
20	CLA	Z	616	12	50,54,73	2.41	20 (40%)	60,90,113	3.14	27 (45%)
27	CHL	6	618	18	47,51,74	2.34	20 (42%)	52,86,114	3.61	24 (46%)
20	CLA	3	603	13	69,73,73	2.00	19 (27%)	83,113,113	2.76	31 (37%)
20	CLA	3	604	-	69,73,73	2.03	18 (26%)	83,113,113	2.73	26 (31%)
22	LHG	Z	620	20	42,42,48	0.99	2 (4%)	45,48,54	1.12	4 (8%)
28	LUT	5	624	-	42,43,43	0.77	0	51,60,60	1.55	13 (25%)
23	BCR	B	845	-	41,41,41	0.71	0	56,56,56	1.85	13 (23%)
20	CLA	B	835	-	49,53,73	2.43	21 (42%)	59,89,113	3.13	27 (45%)
20	CLA	7	616	14	50,54,73	2.37	20 (40%)	60,90,113	3.10	26 (43%)
20	CLA	4	609	16	54,58,73	2.29	22 (40%)	65,95,113	3.29	31 (47%)
20	CLA	A	841	1	69,73,73	2.03	20 (28%)	83,113,113	2.90	33 (39%)
20	CLA	A	840	1	69,73,73	2.00	20 (28%)	83,113,113	2.95	31 (37%)
20	CLA	8	614	15	59,63,73	2.20	20 (33%)	71,101,113	2.99	31 (43%)
20	CLA	Z	614	12	69,73,73	2.06	20 (28%)	83,113,113	2.86	28 (33%)
20	CLA	A	805	1,20	59,63,73	2.17	18 (30%)	71,101,113	3.08	30 (42%)
28	LUT	4	619	-	42,43,43	0.73	0	51,60,60	1.61	13 (25%)
20	CLA	3	606	-	46,50,73	2.44	19 (41%)	55,85,113	3.36	25 (45%)
20	CLA	B	818	2	64,68,73	2.08	21 (32%)	77,107,113	2.92	33 (42%)
20	CLA	4	601	16	65,69,73	2.08	20 (30%)	78,108,113	2.88	32 (41%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
20	CLA	6	617	18	50,54,73	2.38	21 (42%)	60,90,113	3.24	27 (45%)
20	CLA	5	604	17	54,58,73	2.31	18 (33%)	65,95,113	3.14	29 (44%)
20	CLA	B	816	2	59,63,73	2.16	20 (33%)	71,101,113	3.09	29 (40%)
20	CLA	1	602	12	69,73,73	2.03	20 (28%)	83,113,113	2.82	30 (36%)
20	CLA	A	806	1	69,73,73	1.97	19 (27%)	83,113,113	2.84	28 (33%)
19	CL0	A	801	1	69,73,73	1.96	19 (27%)	83,113,113	2.91	33 (39%)
20	CLA	A	830	1	69,73,73	1.98	22 (31%)	83,113,113	2.76	29 (34%)
20	CLA	B	838	2	51,55,73	2.31	19 (37%)	61,91,113	3.25	28 (45%)
20	CLA	4	616	16	45,49,73	2.49	20 (44%)	54,84,113	3.51	27 (50%)
20	CLA	B	802	2	69,73,73	1.95	20 (28%)	83,113,113	2.92	31 (37%)
20	CLA	A	836	1	54,58,73	2.29	20 (37%)	65,95,113	3.09	32 (49%)
20	CLA	7	601	14	69,73,73	2.01	20 (28%)	83,113,113	2.87	29 (34%)
20	CLA	K	4003	10	50,54,73	2.39	19 (38%)	60,90,113	3.21	25 (41%)
20	CLA	B	812	2	69,73,73	2.05	21 (30%)	83,113,113	2.78	30 (36%)
20	CLA	A	825	1	59,63,73	2.18	19 (32%)	71,101,113	2.96	29 (40%)
20	CLA	B	810	2	69,73,73	2.04	20 (28%)	83,113,113	2.83	29 (34%)
20	CLA	4	612	16	56,60,73	2.24	20 (35%)	67,97,113	3.13	30 (44%)
22	LHG	1	620	20	42,42,48	0.99	2 (4%)	45,48,54	1.08	3 (6%)
20	CLA	5	613	17	60,64,73	2.20	20 (33%)	72,102,113	2.90	29 (40%)
24	SF4	A	853	2,1	0,12,12	-	-	-		
20	CLA	B	834	2	69,73,73	2.06	21 (30%)	83,113,113	2.77	30 (36%)
27	CHL	7	607	-	58,62,74	2.18	20 (34%)	65,99,114	3.10	25 (38%)
20	CLA	B	830	2	54,58,73	2.27	19 (35%)	65,95,113	3.22	30 (46%)
20	CLA	Z	610	12	64,68,73	2.11	19 (29%)	77,107,113	2.97	32 (41%)
20	CLA	A	813	1	58,62,73	2.22	21 (36%)	69,99,113	3.02	30 (43%)
20	CLA	A	815	1	64,68,73	2.13	20 (31%)	77,107,113	2.93	30 (38%)
20	CLA	A	854	-	69,73,73	1.98	18 (26%)	83,113,113	2.95	33 (39%)
23	BCR	A	850	-	41,41,41	0.72	0	56,56,56	1.90	10 (17%)
20	CLA	4	611	22	59,63,73	2.23	21 (35%)	71,101,113	2.91	30 (42%)
22	LHG	A	846	-	48,48,48	0.91	2 (4%)	51,54,54	1.03	3 (5%)
20	CLA	B	824	-	69,73,73	2.01	20 (28%)	83,113,113	2.83	33 (39%)
20	CLA	3	614	13	49,53,73	2.44	20 (40%)	59,89,113	3.31	27 (45%)
22	LHG	4	623	-	31,31,48	1.15	2 (6%)	34,37,54	1.14	3 (8%)
23	BCR	B	847	-	41,41,41	0.77	0	56,56,56	1.92	14 (25%)
20	CLA	8	610	15	64,68,73	2.10	18 (28%)	77,107,113	3.02	33 (42%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
20	CLA	A	804	1	69,73,73	2.00	21 (30%)	83,113,113	2.97	36 (43%)
20	CLA	8	602	15	66,70,73	2.04	19 (28%)	79,109,113	2.91	29 (36%)
27	CHL	5	608	-	55,59,74	2.19	20 (36%)	62,96,114	3.23	26 (41%)
20	CLA	B	817	2	63,67,73	2.10	19 (30%)	75,105,113	2.95	29 (38%)
20	CLA	1	609	12	69,73,73	2.04	21 (30%)	83,113,113	2.83	29 (34%)
20	CLA	6	610	18	64,68,73	2.15	21 (32%)	77,107,113	2.92	33 (42%)
20	CLA	B	808	2	69,73,73	1.99	21 (30%)	83,113,113	2.84	31 (37%)
20	CLA	B	814	2	64,68,73	2.09	19 (29%)	77,107,113	2.95	31 (40%)
20	CLA	7	604	-	60,64,73	2.15	19 (31%)	72,102,113	2.99	29 (40%)
20	CLA	A	823	1	53,57,73	2.31	20 (37%)	62,93,113	3.19	25 (40%)
22	LHG	A	847	20	37,37,48	1.05	2 (5%)	40,43,54	1.16	3 (7%)
25	DGD	B	850	-	67,67,67	0.80	2 (2%)	81,81,81	1.05	4 (4%)
20	CLA	Z	606	-	56,60,73	2.29	20 (35%)	67,97,113	3.08	30 (44%)
20	CLA	B	839	-	69,73,73	2.03	20 (28%)	83,113,113	2.73	27 (32%)
20	CLA	Z	608	-	69,73,73	2.05	20 (28%)	83,113,113	2.73	29 (34%)
20	CLA	4	602	16	64,68,73	2.12	19 (29%)	77,107,113	2.90	29 (37%)
20	CLA	4	610	16	64,68,73	2.12	19 (29%)	77,107,113	2.88	31 (40%)
20	CLA	8	601	15	69,73,73	2.01	21 (30%)	83,113,113	2.76	31 (37%)
24	SF4	C	101	3	0,12,12	-	-	-		
20	CLA	B	819	-	69,73,73	2.03	17 (24%)	83,113,113	2.66	30 (36%)
20	CLA	A	843	-	69,73,73	2.01	19 (27%)	83,113,113	2.71	28 (33%)
23	BCR	3	717	-	41,41,41	0.73	0	56,56,56	1.82	14 (25%)
20	CLA	5	621	-	50,54,73	2.36	20 (40%)	60,90,113	3.14	29 (48%)
22	LHG	6	619	20	48,48,48	0.93	2 (4%)	51,54,54	1.04	2 (3%)
20	CLA	A	822	-	69,73,73	2.02	19 (27%)	83,113,113	2.67	30 (36%)
23	BCR	A	856	-	41,41,41	0.78	0	56,56,56	1.88	14 (25%)
20	CLA	3	612	13	50,54,73	2.38	21 (42%)	60,90,113	3.31	30 (50%)
20	CLA	7	606	-	46,50,73	2.41	20 (43%)	55,85,113	3.48	27 (49%)
20	CLA	8	616	15	50,54,73	2.37	21 (42%)	60,90,113	3.06	28 (46%)
27	CHL	4	607	-	55,59,74	2.25	20 (36%)	62,96,114	3.32	26 (41%)
20	CLA	B	825	-	69,73,73	2.04	21 (30%)	83,113,113	2.75	28 (33%)
20	CLA	4	604	-	54,58,73	2.33	20 (37%)	65,95,113	3.12	30 (46%)
20	CLA	A	845	22	56,60,73	2.28	20 (35%)	67,97,113	3.16	27 (40%)
27	CHL	Z	601	12	57,61,74	2.22	21 (36%)	64,98,114	3.28	28 (43%)
20	CLA	3	620	-	60,64,73	2.19	19 (31%)	72,102,113	2.92	28 (38%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
20	CLA	A	834	1	69,73,73	2.02	19 (27%)	83,113,113	2.91	32 (38%)
20	CLA	7	612	14	56,60,73	2.23	21 (37%)	67,97,113	3.24	31 (46%)
20	CLA	A	842	1	69,73,73	2.00	19 (27%)	83,113,113	2.90	32 (38%)
21	PQN	B	842	-	34,34,34	1.55	2 (5%)	42,45,45	1.05	2 (4%)
20	CLA	4	603	16	50,54,73	2.35	20 (40%)	60,90,113	3.28	27 (45%)
20	CLA	A	816	1	69,73,73	2.06	20 (28%)	83,113,113	2.80	30 (36%)
20	CLA	6	601	18	69,73,73	2.04	20 (28%)	83,113,113	2.79	31 (37%)
20	CLA	1	616	12	50,54,73	2.39	20 (40%)	60,90,113	3.07	27 (45%)
20	CLA	A	832	1	54,58,73	2.25	20 (37%)	65,95,113	3.07	31 (47%)
23	BCR	3	718	-	41,41,41	0.72	0	56,56,56	1.92	16 (28%)
23	BCR	5	625	-	41,41,41	0.69	0	56,56,56	2.33	20 (35%)
20	CLA	3	607	13	64,68,73	2.13	20 (31%)	77,107,113	2.97	29 (37%)
20	CLA	G	204	7	50,54,73	2.42	20 (40%)	60,90,113	3.24	28 (46%)
28	LUT	8	618	-	42,43,43	0.76	0	51,60,60	1.68	13 (25%)
23	BCR	6	623	-	41,41,41	0.63	0	56,56,56	2.02	16 (28%)
22	LHG	A	855	-	29,29,48	1.20	2 (6%)	32,35,54	1.19	3 (9%)
20	CLA	1	606	-	56,60,73	2.27	20 (35%)	67,97,113	3.09	29 (43%)
20	CLA	L	203	11	69,73,73	2.03	19 (27%)	83,113,113	2.83	29 (34%)
20	CLA	B	805	2	69,73,73	2.05	19 (27%)	83,113,113	2.83	27 (32%)
23	BCR	G	205	-	41,41,41	0.70	0	56,56,56	1.55	13 (23%)
20	CLA	6	616	18	50,54,73	2.43	20 (40%)	60,90,113	3.28	29 (48%)
27	CHL	6	607	-	60,64,74	2.11	21 (35%)	68,102,114	3.18	29 (42%)
23	BCR	A	851	-	41,41,41	0.80	1 (2%)	56,56,56	1.85	13 (23%)
20	CLA	Z	612	-	56,60,73	2.28	20 (35%)	67,97,113	3.09	31 (46%)
23	BCR	A	848	-	41,41,41	0.69	0	56,56,56	1.72	13 (23%)
20	CLA	8	604	-	50,54,73	2.40	20 (40%)	60,90,113	3.18	27 (45%)
20	CLA	6	612	18	56,60,73	2.24	20 (35%)	67,97,113	3.14	29 (43%)
23	BCR	7	623	-	41,41,41	0.70	0	56,56,56	1.99	15 (26%)
20	CLA	B	806	2	69,73,73	1.99	18 (26%)	83,113,113	2.84	32 (38%)
20	CLA	A	812	1,20	69,73,73	2.00	20 (28%)	83,113,113	2.95	31 (37%)
20	CLA	1	612	12	56,60,73	2.23	20 (35%)	67,97,113	3.17	31 (46%)
20	CLA	3	617	13	50,54,73	2.38	20 (40%)	60,90,113	3.25	27 (45%)
23	BCR	F	305	-	41,41,41	0.70	0	56,56,56	1.92	17 (30%)
22	LHG	4	622	20	48,48,48	0.97	2 (4%)	51,54,54	1.11	3 (5%)
20	CLA	B	832	2	69,73,73	2.00	18 (26%)	83,113,113	2.86	30 (36%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
23	BCR	5	622	-	41,41,41	0.65	0	56,56,56	1.84	16 (28%)
20	CLA	B	809	2	69,73,73	1.98	19 (27%)	83,113,113	2.70	30 (36%)
20	CLA	B	827	2	69,73,73	2.01	22 (31%)	83,113,113	2.86	30 (36%)
20	CLA	A	826	-	69,73,73	2.00	18 (26%)	83,113,113	2.75	27 (32%)
23	BCR	3	719	-	41,41,41	0.71	0	56,56,56	1.75	12 (21%)
20	CLA	A	820	1	69,73,73	2.03	22 (31%)	83,113,113	2.87	28 (33%)
20	CLA	7	614	14	47,51,73	2.37	20 (42%)	56,86,113	3.40	28 (50%)
20	CLA	5	606	-	59,63,73	2.22	20 (33%)	71,101,113	2.99	30 (42%)
20	CLA	A	829	1	69,73,73	1.98	20 (28%)	83,113,113	2.87	31 (37%)
20	CLA	6	614	18	49,53,73	2.42	21 (42%)	59,89,113	3.37	28 (47%)
27	CHL	5	607	-	55,59,74	2.25	21 (38%)	62,96,114	3.37	32 (51%)
20	CLA	B	813	2	69,73,73	2.01	20 (28%)	83,113,113	2.79	29 (34%)
20	CLA	Z	611	22	69,73,73	2.06	20 (28%)	83,113,113	2.74	29 (34%)
20	CLA	3	602	13	64,68,73	2.10	22 (34%)	77,107,113	2.96	32 (41%)
20	CLA	6	611	22	59,63,73	2.23	21 (35%)	71,101,113	2.94	28 (39%)
20	CLA	J	3002	9	46,50,73	2.41	19 (41%)	55,85,113	3.39	27 (49%)
20	CLA	5	612	-	56,60,73	2.28	21 (37%)	67,97,113	3.09	28 (41%)
28	LUT	3	621	-	42,43,43	0.77	0	51,60,60	1.61	12 (23%)
20	CLA	A	808	1	69,73,73	2.02	21 (30%)	83,113,113	2.89	31 (37%)
20	CLA	7	613	14	69,73,73	2.00	21 (30%)	83,113,113	2.74	27 (32%)
20	CLA	7	611	22	45,49,73	2.47	21 (46%)	54,84,113	3.51	30 (55%)
20	CLA	1	608	-	69,73,73	2.03	20 (28%)	83,113,113	2.74	29 (34%)
20	CLA	Z	613	-	69,73,73	2.04	20 (28%)	83,113,113	2.70	27 (32%)
20	CLA	B	823	2	64,68,73	2.10	19 (29%)	77,107,113	2.86	31 (40%)
24	SF4	C	102	3	0,12,12	-	-	-		
28	LUT	6	621	-	42,43,43	0.70	0	51,60,60	1.51	11 (21%)
26	LMG	J	3001	-	35,35,55	0.96	0	43,43,63	1.23	6 (13%)
20	CLA	4	614	16	49,53,73	2.40	20 (40%)	59,89,113	3.21	27 (45%)
20	CLA	7	620	-	64,68,73	2.14	20 (31%)	77,107,113	2.89	30 (38%)
27	CHL	4	606	-	60,64,74	2.13	19 (31%)	68,102,114	3.05	25 (36%)
27	CHL	6	608	-	55,59,74	2.20	19 (34%)	62,96,114	3.51	28 (45%)
20	CLA	1	614	12	69,73,73	2.05	21 (30%)	83,113,113	2.83	29 (34%)

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
28	LUT	Z	619	-	-	4/29/67/67	0/2/2/2
20	CLA	5	601	17	-	11/39/115/115	-
28	LUT	7	621	-	-	5/29/67/67	0/2/2/2
28	LUT	Z	617	-	-	4/29/67/67	0/2/2/2
27	CHL	4	618	16	-	6/14/90/117	-
28	LUT	1	618	-	-	2/29/67/67	0/2/2/2
20	CLA	A	839	1	-	12/39/115/115	-
20	CLA	A	827	-	-	8/39/115/115	-
23	BCR	8	619	-	-	8/29/63/63	0/2/2/2
28	LUT	4	620	-	-	2/29/67/67	0/2/2/2
20	CLA	7	610	14	-	7/33/109/115	-
20	CLA	1	604	-	-	10/30/106/115	-
20	CLA	Z	603	12	-	11/30/106/115	-
20	CLA	5	603	17	-	5/17/93/115	-
22	LHG	B	851	20	-	10/26/26/53	-
20	CLA	B	829	2	-	8/39/115/115	-
20	CLA	3	610	13	-	13/39/115/115	-
27	CHL	Z	607	-	-	8/20/96/117	-
20	CLA	A	821	1	-	5/15/91/115	-
23	BCR	B	843	-	-	7/29/63/63	0/2/2/2
22	LHG	8	620	20	-	12/41/41/53	-
23	BCR	I	172	-	-	6/29/63/63	0/2/2/2
20	CLA	K	4002	-	-	7/15/91/115	-
28	LUT	1	619	-	-	2/29/67/67	0/2/2/2
27	CHL	3	608	-	-	17/41/117/117	-
20	CLA	4	613	16	-	13/29/105/115	-
20	CLA	B	833	2	-	9/31/107/115	-
20	CLA	A	817	-	-	4/30/106/115	-
20	CLA	B	840	2	-	10/39/115/115	-
20	CLA	B	822	2	-	14/32/108/115	-
20	CLA	8	606	-	-	4/12/88/115	-
20	CLA	3	613	13	-	18/27/103/115	-
22	LHG	7	625	20	-	9/41/41/53	-
20	CLA	A	835	1	-	14/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	CLA	1	603	12	-	9/39/115/115	-
20	CLA	B	837	2	-	6/39/115/115	-
20	CLA	8	609	15	-	3/17/93/115	-
20	CLA	F	301	-	-	10/39/115/115	-
23	BCR	A	849	-	-	3/29/63/63	0/2/2/2
20	CLA	A	809	1	-	16/39/115/115	-
20	CLA	A	837	1	-	11/15/91/115	-
20	CLA	6	602	18	-	15/39/115/115	-
28	LUT	1	617	-	-	2/29/67/67	0/2/2/2
28	LUT	7	622	-	-	2/29/67/67	0/2/2/2
20	CLA	A	818	1	-	11/39/115/115	-
22	LHG	5	623	20	-	13/41/41/53	-
20	CLA	A	824	1	-	8/23/99/115	-
28	LUT	3	622	-	-	2/29/67/67	0/2/2/2
27	CHL	1	601	12	-	10/26/102/117	-
27	CHL	5	618	17	-	6/14/90/117	-
20	CLA	A	803	-	-	5/39/115/115	-
20	CLA	6	609	18	-	6/21/97/115	-
20	CLA	A	838	1	-	2/23/99/115	-
27	CHL	4	608	-	-	6/23/99/117	-
20	CLA	6	604	-	-	10/39/115/115	-
23	BCR	A	852	-	-	7/29/63/63	0/2/2/2
20	CLA	5	617	17	-	4/17/93/115	-
20	CLA	8	612	15	-	7/24/100/115	-
23	BCR	L	201	-	-	6/29/63/63	0/2/2/2
23	BCR	K	4001	-	-	6/29/63/63	0/2/2/2
20	CLA	L	204	-	-	4/21/97/115	-
23	BCR	B	848	-	-	4/29/63/63	0/2/2/2
20	CLA	A	810	1	-	13/39/115/115	-
20	CLA	5	614	17	-	6/15/91/115	-
23	BCR	L	205	-	-	9/29/63/63	0/2/2/2
27	CHL	1	607	-	-	9/20/96/117	-
20	CLA	F	303	-	-	2/15/91/115	-
20	CLA	A	811	1	-	7/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	CLA	G	203	7	-	3/21/97/115	-
23	BCR	B	846	-	-	7/29/63/63	0/2/2/2
28	LUT	Z	618	-	-	5/29/67/67	0/2/2/2
20	CLA	B	803	-	-	11/39/115/115	-
23	BCR	J	3003	-	-	8/29/63/63	0/2/2/2
20	CLA	5	609	17	-	8/21/97/115	-
23	BCR	K	4004	-	-	6/29/63/63	0/2/2/2
27	CHL	8	607	-	-	13/29/105/117	-
20	CLA	8	611	22	-	7/17/93/115	-
28	LUT	5	620	-	-	2/29/67/67	0/2/2/2
20	CLA	Z	604	-	-	8/30/106/115	-
20	CLA	B	852	-	-	11/39/115/115	-
20	CLA	A	802	-	-	8/39/115/115	-
20	CLA	7	609	14	-	7/21/97/115	-
20	CLA	5	616	17	-	7/17/93/115	-
20	CLA	5	610	17	-	12/33/109/115	-
27	CHL	6	606	-	-	4/29/105/117	-
20	CLA	B	804	2	-	5/15/91/115	-
20	CLA	8	608	-	-	2/21/97/115	-
21	PQN	A	844	-	-	7/23/43/43	0/2/2/2
23	BCR	7	624	-	-	6/29/63/63	0/2/2/2
20	CLA	3	611	-	-	4/10/86/115	-
20	CLA	8	613	15	-	14/39/115/115	-
20	CLA	A	807	1	-	19/39/115/115	-
20	CLA	B	811	2	-	7/25/101/115	-
20	CLA	B	826	2	-	11/39/115/115	-
20	CLA	1	611	22	-	10/39/115/115	-
23	BCR	B	801	-	-	6/29/63/63	0/2/2/2
20	CLA	F	304	6	-	10/39/115/115	-
20	CLA	A	831	1	-	16/39/115/115	-
20	CLA	5	602	17	-	12/39/115/115	-
20	CLA	7	608	-	-	4/21/97/115	-
20	CLA	Z	602	12	-	12/39/115/115	-
20	CLA	B	841	22	-	10/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	CLA	A	814	1	-	19/39/115/115	-
20	CLA	6	603	18	-	5/17/93/115	-
23	BCR	4	621	-	-	11/29/63/63	0/2/2/2
23	BCR	6	625	-	-	7/29/63/63	0/2/2/2
28	LUT	8	617	-	-	3/29/67/67	0/2/2/2
23	BCR	B	844	-	-	8/29/63/63	0/2/2/2
20	CLA	1	613	-	-	14/39/115/115	-
20	CLA	A	819	1	-	13/39/115/115	-
28	LUT	6	624	-	-	3/29/67/67	0/2/2/2
20	CLA	B	807	2	-	11/39/115/115	-
20	CLA	B	820	2	-	10/29/105/115	-
20	CLA	8	603	15	-	4/15/91/115	-
20	CLA	Z	609	12	-	6/39/115/115	-
20	CLA	6	613	-	-	7/29/105/115	-
20	CLA	7	602	14	-	13/39/115/115	-
20	CLA	B	836	2	-	7/33/109/115	-
20	CLA	A	833	1	-	8/39/115/115	-
20	CLA	1	610	12	-	9/33/109/115	-
20	CLA	B	828	2	-	9/39/115/115	-
20	CLA	6	622	-	-	5/15/91/115	-
20	CLA	5	611	22	-	12/27/103/115	-
20	CLA	B	821	2	-	9/17/93/115	-
20	CLA	B	815	2	-	6/30/106/115	-
20	CLA	B	831	2	-	4/20/96/115	-
20	CLA	3	609	13	-	7/21/97/115	-
20	CLA	7	603	14	-	5/17/93/115	-
20	CLA	A	828	1	-	13/39/115/115	-
20	CLA	Z	616	12	-	5/17/93/115	-
27	CHL	6	618	18	-	10/14/90/117	-
20	CLA	3	603	13	-	6/39/115/115	-
20	CLA	3	604	-	-	10/39/115/115	-
22	LHG	Z	620	20	-	17/47/47/53	-
28	LUT	5	624	-	-	3/29/67/67	0/2/2/2
23	BCR	B	845	-	-	10/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	CLA	B	835	-	-	7/15/91/115	-
20	CLA	7	616	14	-	5/17/93/115	-
20	CLA	4	609	16	-	6/21/97/115	-
20	CLA	A	841	1	-	10/39/115/115	-
20	CLA	A	840	1	-	9/39/115/115	-
20	CLA	8	614	15	-	8/27/103/115	-
20	CLA	Z	614	12	-	13/39/115/115	-
20	CLA	A	805	1,20	-	7/27/103/115	-
28	LUT	4	619	-	-	2/29/67/67	0/2/2/2
20	CLA	3	606	-	-	1/12/88/115	-
20	CLA	B	818	2	-	12/33/109/115	-
20	CLA	4	601	16	-	12/35/111/115	-
20	CLA	6	617	18	-	2/17/93/115	-
20	CLA	5	604	17	-	4/21/97/115	-
20	CLA	B	816	2	-	12/27/103/115	-
20	CLA	1	602	12	-	14/39/115/115	-
20	CLA	A	806	1	-	19/39/115/115	-
19	CL0	A	801	1	-	7/39/115/115	-
20	CLA	A	830	1	-	9/39/115/115	-
20	CLA	B	838	2	-	4/18/94/115	-
20	CLA	4	616	16	-	2/10/86/115	-
20	CLA	B	802	2	-	16/39/115/115	-
20	CLA	A	836	1	-	4/21/97/115	-
20	CLA	7	601	14	-	19/39/115/115	-
20	CLA	K	4003	10	-	5/17/93/115	-
20	CLA	B	812	2	-	13/39/115/115	-
20	CLA	A	825	1	-	9/27/103/115	-
20	CLA	B	810	2	-	14/39/115/115	-
20	CLA	4	612	16	-	6/24/100/115	-
22	LHG	1	620	20	-	10/47/47/53	-
20	CLA	5	613	17	-	8/29/105/115	-
24	SF4	A	853	2,1	-	-	0/6/5/5
20	CLA	B	834	2	-	11/39/115/115	-
27	CHL	7	607	-	-	10/27/103/117	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	CLA	B	830	2	-	6/21/97/115	-
20	CLA	Z	610	12	-	14/33/109/115	-
20	CLA	A	813	1	-	8/26/102/115	-
20	CLA	A	815	1	-	10/33/109/115	-
20	CLA	A	854	-	-	12/39/115/115	-
23	BCR	A	850	-	-	4/29/63/63	0/2/2/2
20	CLA	4	611	22	-	10/27/103/115	-
22	LHG	A	846	-	-	14/53/53/53	-
20	CLA	B	824	-	-	13/39/115/115	-
20	CLA	3	614	13	-	4/15/91/115	-
22	LHG	4	623	-	-	10/36/36/53	-
23	BCR	B	847	-	-	9/29/63/63	0/2/2/2
20	CLA	8	610	15	-	9/33/109/115	-
20	CLA	A	804	1	-	10/39/115/115	-
20	CLA	8	602	15	-	11/36/112/115	-
27	CHL	5	608	-	-	9/23/99/117	-
20	CLA	B	817	2	-	13/32/108/115	-
20	CLA	1	609	12	-	11/39/115/115	-
20	CLA	6	610	18	-	11/33/109/115	-
20	CLA	B	808	2	-	10/39/115/115	-
20	CLA	B	814	2	-	7/33/109/115	-
20	CLA	7	604	-	-	8/29/105/115	-
20	CLA	A	823	1	-	13/20/96/115	-
22	LHG	A	847	20	-	10/42/42/53	-
25	DGD	B	850	-	-	12/55/95/95	0/2/2/2
20	CLA	Z	606	-	-	6/24/100/115	-
20	CLA	B	839	-	-	9/39/115/115	-
20	CLA	Z	608	-	-	17/39/115/115	-
20	CLA	4	602	16	-	10/33/109/115	-
20	CLA	4	610	16	-	9/33/109/115	-
20	CLA	8	601	15	-	15/39/115/115	-
24	SF4	C	101	3	-	-	0/6/5/5
20	CLA	B	819	-	-	15/39/115/115	-
20	CLA	A	843	-	-	20/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	BCR	3	717	-	-	8/29/63/63	0/2/2/2
20	CLA	5	621	-	-	5/17/93/115	-
22	LHG	6	619	20	-	17/53/53/53	-
20	CLA	A	822	-	-	13/39/115/115	-
23	BCR	A	856	-	-	8/29/63/63	0/2/2/2
20	CLA	3	612	13	-	2/17/93/115	-
20	CLA	7	606	-	-	7/12/88/115	-
20	CLA	8	616	15	-	4/17/93/115	-
27	CHL	4	607	-	-	12/23/99/117	-
20	CLA	B	825	-	-	8/39/115/115	-
20	CLA	4	604	-	-	6/21/97/115	-
20	CLA	A	845	22	-	13/24/100/115	-
27	CHL	Z	601	12	-	12/26/102/117	-
20	CLA	3	620	-	-	6/29/105/115	-
20	CLA	A	834	1	-	12/39/115/115	-
20	CLA	7	612	14	-	5/24/100/115	-
20	CLA	A	842	1	-	14/39/115/115	-
21	PQN	B	842	-	-	4/23/43/43	0/2/2/2
20	CLA	4	603	16	-	7/17/93/115	-
20	CLA	A	816	1	-	11/39/115/115	-
20	CLA	6	601	18	-	14/39/115/115	-
20	CLA	1	616	12	-	4/17/93/115	-
20	CLA	A	832	1	-	4/21/97/115	-
23	BCR	3	718	-	-	2/29/63/63	0/2/2/2
23	BCR	5	625	-	-	7/29/63/63	0/2/2/2
20	CLA	3	607	13	-	18/33/109/115	-
20	CLA	G	204	7	-	5/17/93/115	-
28	LUT	8	618	-	-	2/29/67/67	0/2/2/2
23	BCR	6	623	-	-	9/29/63/63	0/2/2/2
22	LHG	A	855	-	-	11/34/34/53	-
20	CLA	1	606	-	-	5/24/100/115	-
20	CLA	L	203	11	-	11/39/115/115	-
20	CLA	B	805	2	-	12/39/115/115	-
23	BCR	G	205	-	-	4/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	CLA	6	616	18	-	6/17/93/115	-
27	CHL	6	607	-	-	14/29/105/117	-
23	BCR	A	851	-	-	4/29/63/63	0/2/2/2
20	CLA	Z	612	-	-	8/24/100/115	-
23	BCR	A	848	-	-	4/29/63/63	0/2/2/2
20	CLA	8	604	-	-	7/17/93/115	-
20	CLA	6	612	18	-	5/24/100/115	-
23	BCR	7	623	-	-	8/29/63/63	0/2/2/2
20	CLA	B	806	2	-	14/39/115/115	-
20	CLA	A	812	1,20	-	16/39/115/115	-
20	CLA	1	612	12	-	6/24/100/115	-
20	CLA	3	617	13	-	11/17/93/115	-
23	BCR	F	305	-	-	8/29/63/63	0/2/2/2
22	LHG	4	622	20	-	13/53/53/53	-
20	CLA	B	832	2	-	10/39/115/115	-
23	BCR	5	622	-	-	6/29/63/63	0/2/2/2
20	CLA	B	809	2	-	7/39/115/115	-
20	CLA	B	827	2	-	16/39/115/115	-
20	CLA	A	826	-	-	16/39/115/115	-
23	BCR	3	719	-	-	8/29/63/63	0/2/2/2
20	CLA	A	820	1	-	17/39/115/115	-
20	CLA	7	614	14	-	4/13/89/115	-
20	CLA	5	606	-	-	3/27/103/115	-
20	CLA	A	829	1	-	24/39/115/115	-
20	CLA	6	614	18	-	6/15/91/115	-
27	CHL	5	607	-	-	10/23/99/117	-
20	CLA	B	813	2	-	15/39/115/115	-
20	CLA	Z	611	22	-	12/39/115/115	-
20	CLA	3	602	13	-	11/33/109/115	-
20	CLA	6	611	22	-	9/27/103/115	-
20	CLA	J	3002	9	-	7/12/88/115	-
20	CLA	5	612	-	-	5/24/100/115	-
28	LUT	3	621	-	-	2/29/67/67	0/2/2/2
20	CLA	A	808	1	-	10/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	CLA	7	613	14	-	6/39/115/115	-
20	CLA	7	611	22	-	2/10/86/115	-
20	CLA	1	608	-	-	16/39/115/115	-
20	CLA	Z	613	-	-	13/39/115/115	-
20	CLA	B	823	2	-	9/33/109/115	-
28	LUT	6	621	-	-	4/29/67/67	0/2/2/2
24	SF4	C	102	3	-	-	0/6/5/5
26	LMG	J	3001	-	-	10/30/50/70	0/1/1/1
20	CLA	4	614	16	-	4/15/91/115	-
20	CLA	7	620	-	-	10/33/109/115	-
27	CHL	4	606	-	-	7/29/105/117	-
27	CHL	6	608	-	-	7/23/99/117	-
20	CLA	1	614	12	-	11/39/115/115	-

The worst 5 of 4344 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	A	844	PQN	C3-C2	7.56	1.49	1.35
21	B	842	PQN	C3-C2	7.40	1.48	1.35
20	B	840	CLA	C3C-C2C	6.00	1.49	1.36
20	A	817	CLA	C1D-ND	5.52	1.44	1.37
20	L	204	CLA	C3C-C2C	5.49	1.48	1.36

The worst 5 of 7011 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	6	608	CHL	C4A-NA-C1A	-12.36	101.15	106.71
27	1	601	CHL	C4A-NA-C1A	-11.60	101.49	106.71
27	4	608	CHL	C2D-C1D-ND	10.39	117.76	110.10
27	6	618	CHL	C2D-C1D-ND	10.27	117.67	110.10
20	A	818	CLA	C1D-ND-C4D	-10.24	99.06	106.33

There are no chirality outliers.

5 of 2438 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
20	A	804	CLA	CHA-CBD-CGD-O1D
20	A	804	CLA	CHA-CBD-CGD-O2D
20	A	807	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
20	A	809	CLA	C3A-C2A-CAA-CBA
20	A	812	CLA	C1A-C2A-CAA-CBA

There are no ring outliers.

235 monomers are involved in 499 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
28	Z	619	LUT	3	0
20	5	601	CLA	3	0
28	7	621	LUT	6	0
28	Z	617	LUT	5	0
28	1	618	LUT	5	0
20	A	839	CLA	1	0
20	A	827	CLA	2	0
23	8	619	BCR	3	0
28	4	620	LUT	2	0
20	7	610	CLA	3	0
20	1	604	CLA	1	0
20	Z	603	CLA	2	0
20	5	603	CLA	1	0
22	B	851	LHG	2	0
20	B	829	CLA	6	0
20	3	610	CLA	2	0
20	A	821	CLA	1	0
23	B	843	BCR	5	0
23	I	172	BCR	2	0
20	K	4002	CLA	1	0
28	1	619	LUT	2	0
27	3	608	CHL	3	0
20	4	613	CLA	2	0
20	B	833	CLA	3	0
20	A	817	CLA	3	0
20	B	840	CLA	5	0
20	B	822	CLA	1	0
20	8	606	CLA	1	0
20	3	613	CLA	1	0
22	7	625	LHG	1	0
20	A	835	CLA	1	0
20	1	603	CLA	1	0
20	B	837	CLA	4	0
20	F	301	CLA	3	0
23	A	849	BCR	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
20	A	809	CLA	4	0
20	A	837	CLA	1	0
20	6	602	CLA	1	0
28	1	617	LUT	7	0
28	7	622	LUT	3	0
20	A	818	CLA	3	0
22	5	623	LHG	1	0
20	A	824	CLA	1	0
28	3	622	LUT	3	0
27	1	601	CHL	1	0
27	5	618	CHL	1	0
20	A	803	CLA	2	0
20	6	609	CLA	1	0
20	A	838	CLA	1	0
27	4	608	CHL	1	0
20	6	604	CLA	2	0
23	A	852	BCR	3	0
20	5	617	CLA	1	0
23	L	201	BCR	3	0
23	K	4001	BCR	1	0
23	B	848	BCR	3	0
20	A	810	CLA	3	0
23	L	205	BCR	1	0
27	1	607	CHL	1	0
20	F	303	CLA	2	0
20	A	811	CLA	3	0
23	B	846	BCR	4	0
28	Z	618	LUT	3	0
20	B	803	CLA	3	0
23	J	3003	BCR	3	0
20	5	609	CLA	5	0
23	K	4004	BCR	1	0
27	8	607	CHL	1	0
28	5	620	LUT	4	0
20	Z	604	CLA	1	0
20	A	802	CLA	7	0
20	7	609	CLA	4	0
20	5	610	CLA	1	0
27	6	606	CHL	1	0
21	A	844	PQN	1	0
23	7	624	BCR	1	0
20	8	613	CLA	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
20	A	807	CLA	4	0
20	B	811	CLA	1	0
20	B	826	CLA	2	0
20	1	611	CLA	1	0
23	B	801	BCR	3	0
20	F	304	CLA	2	0
20	A	831	CLA	7	0
20	5	602	CLA	3	0
20	7	608	CLA	1	0
20	Z	602	CLA	4	0
20	B	841	CLA	3	0
20	A	814	CLA	3	0
23	4	621	BCR	2	0
23	6	625	BCR	4	0
28	8	617	LUT	9	0
23	B	844	BCR	3	0
20	1	613	CLA	1	0
20	A	819	CLA	3	0
28	6	624	LUT	4	0
20	B	807	CLA	4	0
20	B	820	CLA	2	0
20	Z	609	CLA	1	0
20	6	613	CLA	3	0
20	7	602	CLA	1	0
20	B	836	CLA	3	0
20	A	833	CLA	2	0
20	1	610	CLA	1	0
20	B	828	CLA	2	0
20	5	611	CLA	1	0
20	B	815	CLA	2	0
20	B	831	CLA	2	0
20	3	609	CLA	2	0
20	A	828	CLA	3	0
20	Z	616	CLA	1	0
27	6	618	CHL	2	0
20	3	603	CLA	2	0
20	3	604	CLA	1	0
22	Z	620	LHG	3	0
28	5	624	LUT	4	0
23	B	845	BCR	1	0
20	B	835	CLA	1	0
20	7	616	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
20	4	609	CLA	2	0
20	A	841	CLA	11	0
20	A	840	CLA	3	0
20	8	614	CLA	2	0
20	A	805	CLA	4	0
28	4	619	LUT	7	0
20	3	606	CLA	1	0
20	B	818	CLA	5	0
20	4	601	CLA	4	0
20	5	604	CLA	1	0
20	B	816	CLA	1	0
20	1	602	CLA	5	0
20	A	806	CLA	7	0
19	A	801	CL0	1	0
20	A	830	CLA	4	0
20	B	838	CLA	2	0
20	B	802	CLA	3	0
20	A	836	CLA	2	0
20	7	601	CLA	5	0
20	K	4003	CLA	3	0
20	B	812	CLA	3	0
20	A	825	CLA	2	0
20	4	612	CLA	4	0
20	5	613	CLA	3	0
20	B	834	CLA	2	0
20	Z	610	CLA	3	0
20	A	813	CLA	1	0
20	A	815	CLA	1	0
20	A	854	CLA	6	0
23	A	850	BCR	4	0
20	4	611	CLA	4	0
22	A	846	LHG	3	0
20	B	824	CLA	3	0
22	4	623	LHG	1	0
23	B	847	BCR	1	0
20	8	610	CLA	2	0
20	A	804	CLA	2	0
20	8	602	CLA	3	0
27	5	608	CHL	2	0
20	B	817	CLA	4	0
20	1	609	CLA	1	0
20	6	610	CLA	5	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
20	B	808	CLA	1	0
20	B	814	CLA	2	0
20	7	604	CLA	2	0
20	A	823	CLA	1	0
22	A	847	LHG	3	0
25	B	850	DGD	2	0
20	B	839	CLA	4	0
20	Z	608	CLA	5	0
20	4	602	CLA	2	0
20	4	610	CLA	1	0
20	8	601	CLA	2	0
20	B	819	CLA	2	0
20	A	843	CLA	5	0
23	3	717	BCR	2	0
22	6	619	LHG	3	0
20	A	822	CLA	2	0
23	A	856	BCR	3	0
20	3	612	CLA	2	0
20	7	606	CLA	1	0
20	8	616	CLA	1	0
20	B	825	CLA	5	0
20	A	845	CLA	1	0
27	Z	601	CHL	5	0
20	A	834	CLA	3	0
20	7	612	CLA	1	0
20	A	842	CLA	2	0
21	B	842	PQN	1	0
20	A	816	CLA	5	0
23	3	718	BCR	4	0
23	5	625	BCR	6	0
20	3	607	CLA	2	0
28	8	618	LUT	5	0
23	6	623	BCR	4	0
20	1	606	CLA	3	0
20	B	805	CLA	8	0
23	G	205	BCR	4	0
20	6	616	CLA	2	0
27	6	607	CHL	2	0
23	A	851	BCR	4	0
20	Z	612	CLA	2	0
23	A	848	BCR	3	0
20	8	604	CLA	1	0

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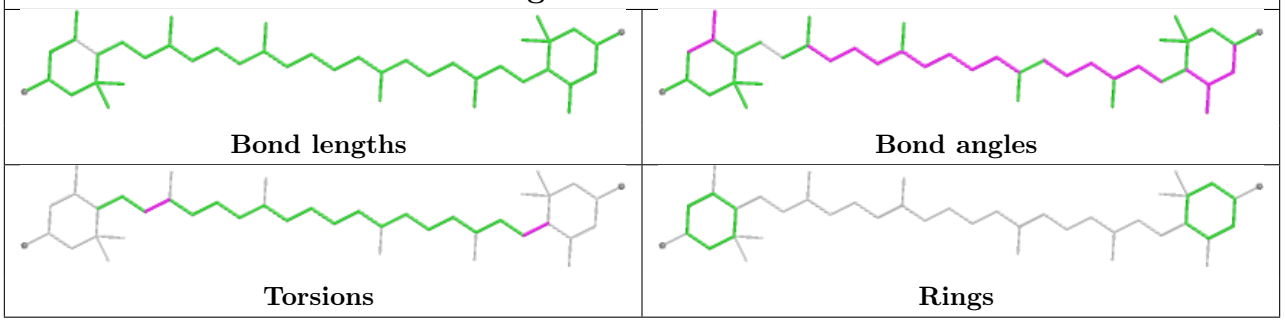
Mol	Chain	Res	Type	Clashes	Symm-Clashes
20	6	612	CLA	1	0
23	7	623	BCR	5	0
20	B	806	CLA	3	0
20	A	812	CLA	7	0
20	1	612	CLA	1	0
20	3	617	CLA	2	0
23	F	305	BCR	6	0
22	4	622	LHG	5	0
20	B	832	CLA	5	0
23	5	622	BCR	3	0
20	B	809	CLA	2	0
20	B	827	CLA	2	0
20	A	826	CLA	1	0
23	3	719	BCR	6	0
20	A	820	CLA	2	0
20	5	606	CLA	1	0
20	A	829	CLA	8	0
20	6	614	CLA	2	0
27	5	607	CHL	2	0
20	B	813	CLA	5	0
20	Z	611	CLA	1	0
20	3	602	CLA	1	0
20	6	611	CLA	2	0
28	3	621	LUT	3	0
20	A	808	CLA	2	0
20	7	613	CLA	3	0
20	1	608	CLA	1	0
20	Z	613	CLA	1	0
20	B	823	CLA	3	0
28	6	621	LUT	7	0
20	7	620	CLA	1	0
20	1	614	CLA	3	0

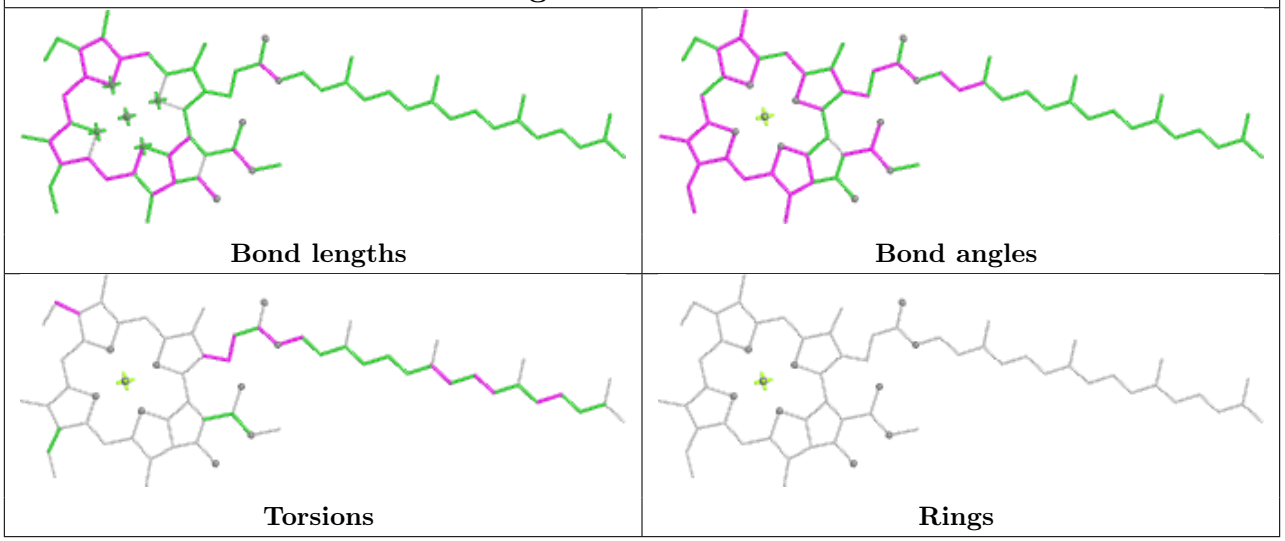
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier.

The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

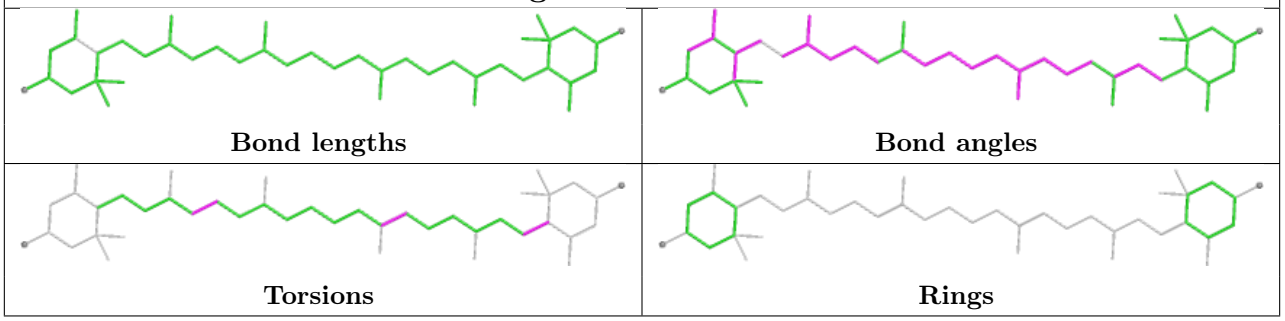
Ligand LUT Z 619



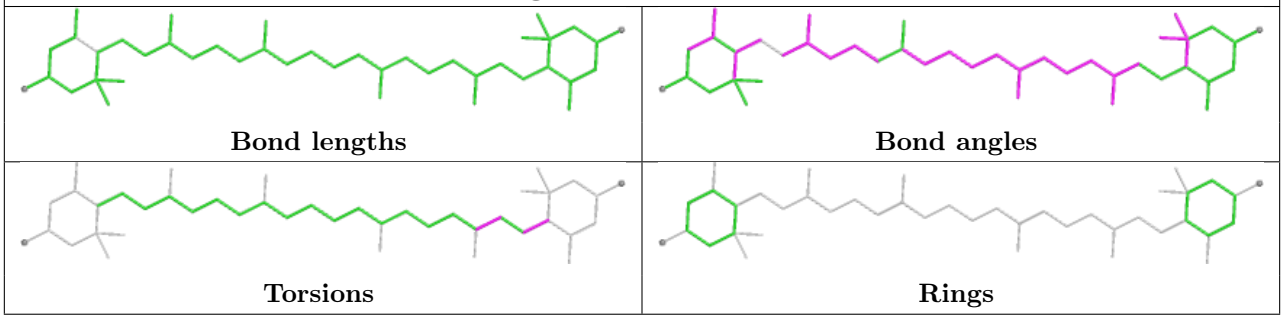
Ligand CLA 5 601



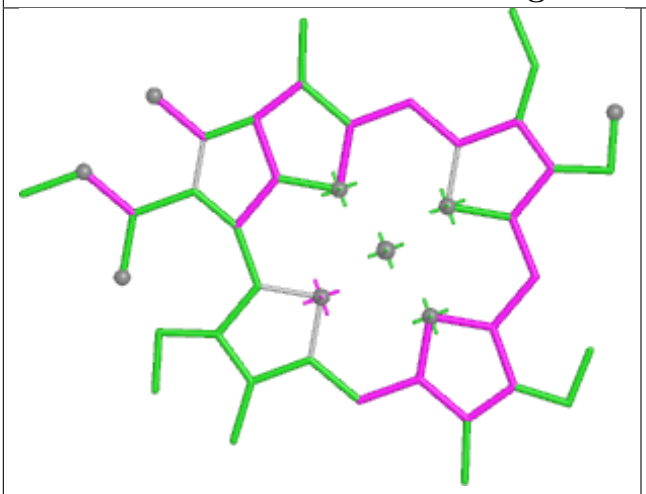
Ligand LUT 7 621



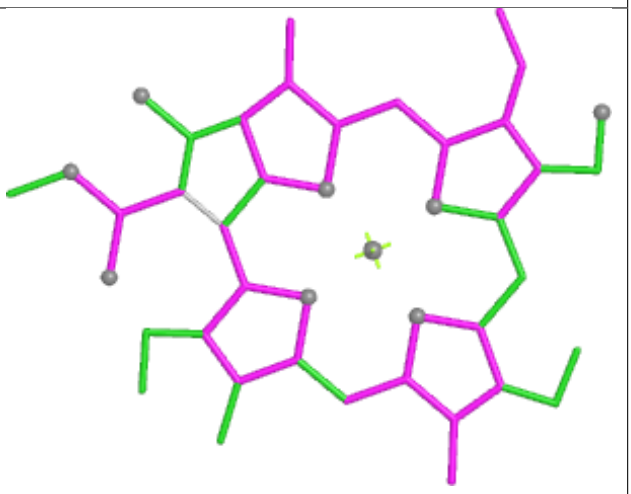
Ligand LUT Z 617



Ligand CHL 4 618



Bond lengths



Bond angles

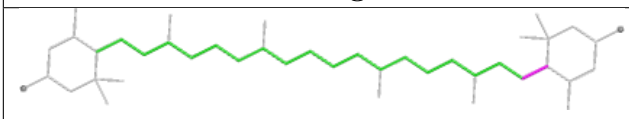
Torsions

Rings

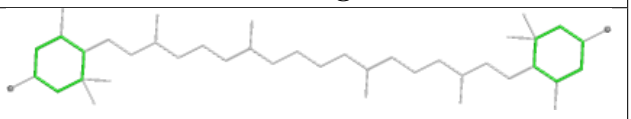
Ligand LUT 1 618

Bond lengths

Bond angles

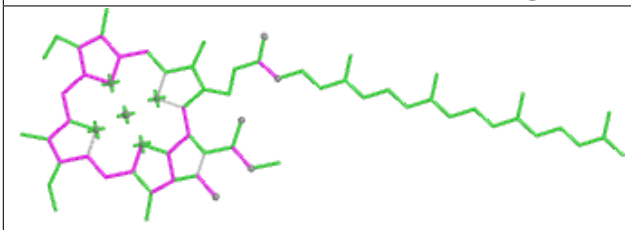


Torsions

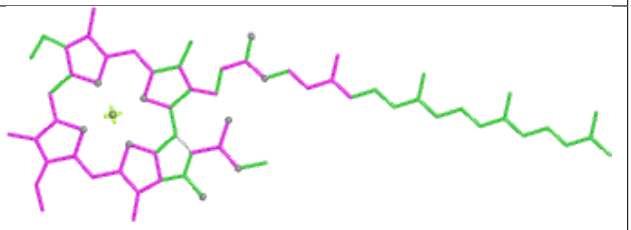


Rings

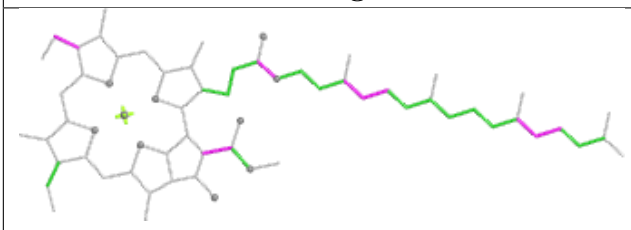
Ligand CLA A 839



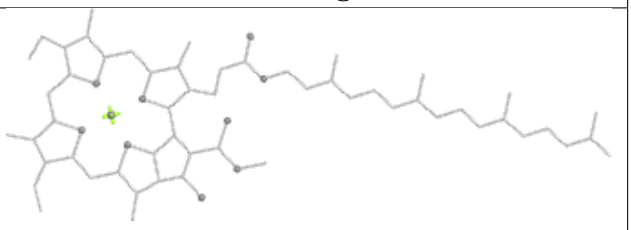
Bond lengths



Bond angles

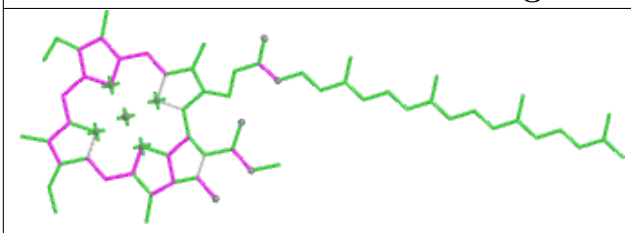


Torsions

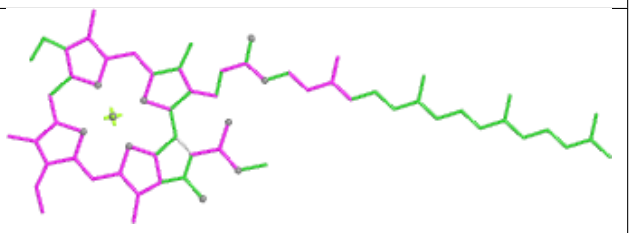


Rings

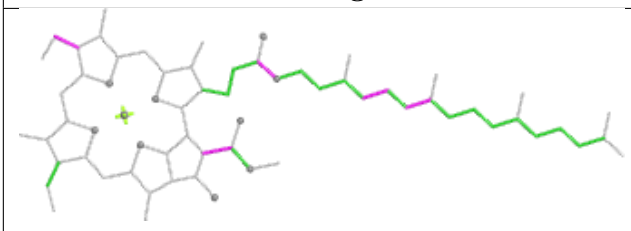
Ligand CLA A 827



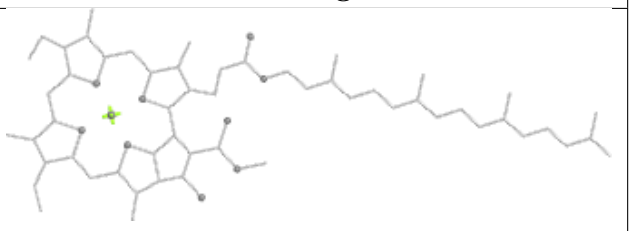
Bond lengths



Bond angles

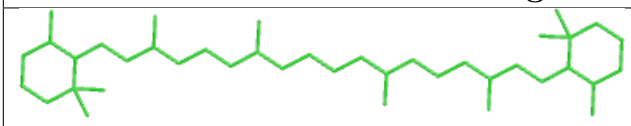


Torsions

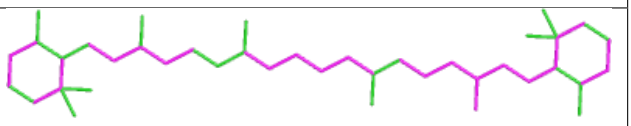


Rings

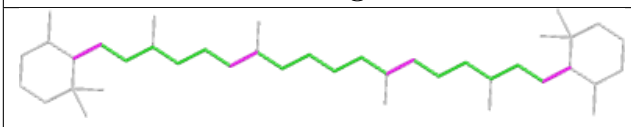
Ligand BCR 8 619



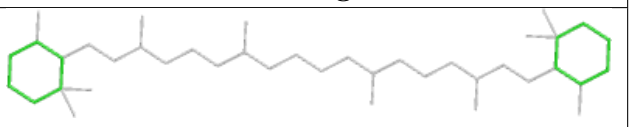
Bond lengths



Bond angles

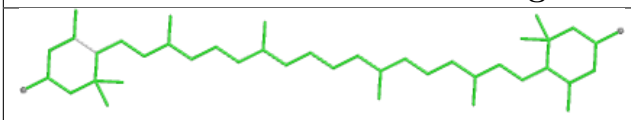


Torsions



Rings

Ligand LUT 4 620



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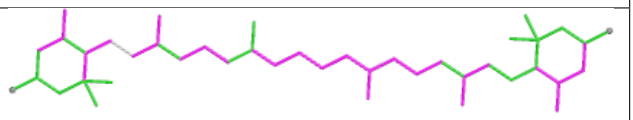

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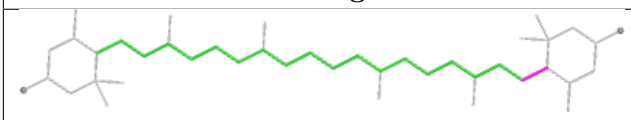

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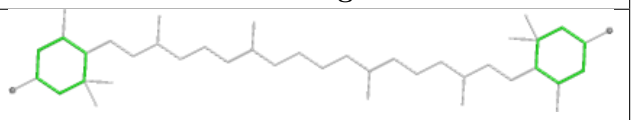
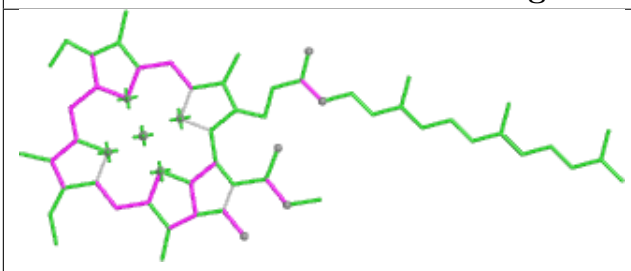


Rings

Ligand CLA 7 610



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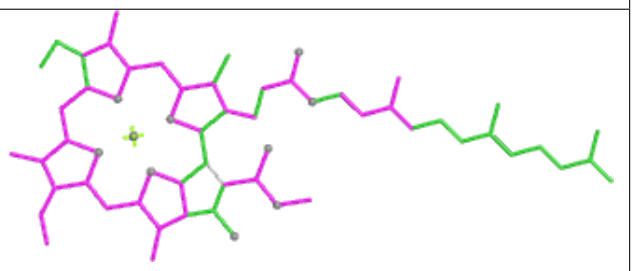
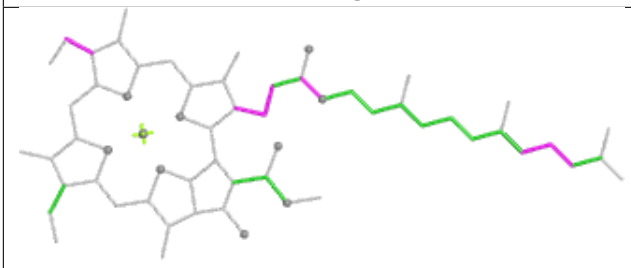


Bond angles



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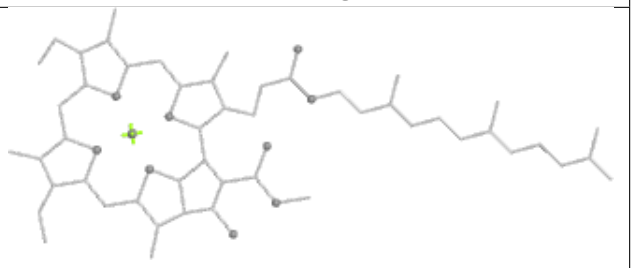
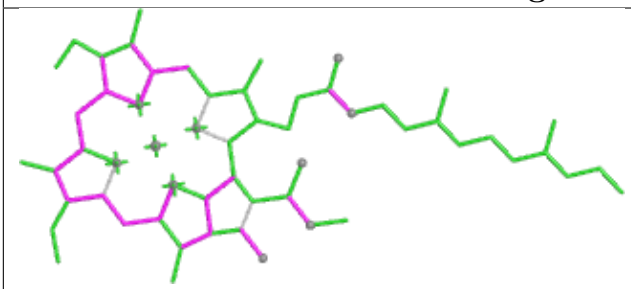


Rings

Ligand CLA 1 604



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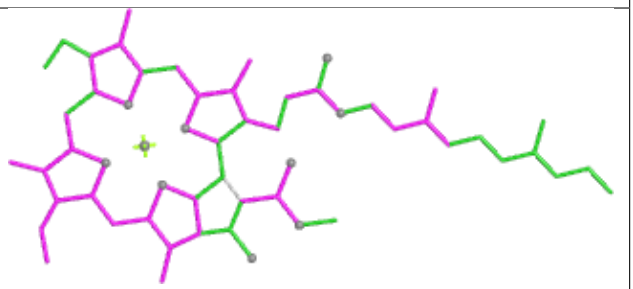
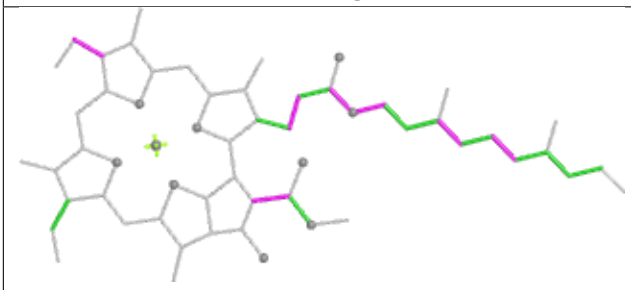


Bond angles



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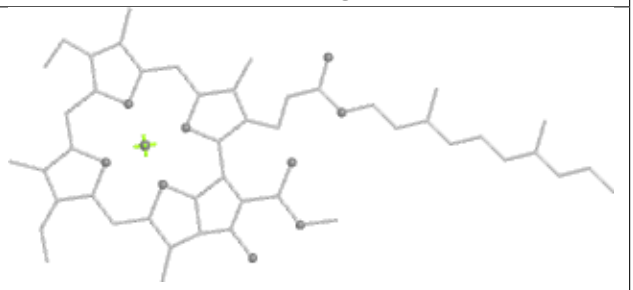
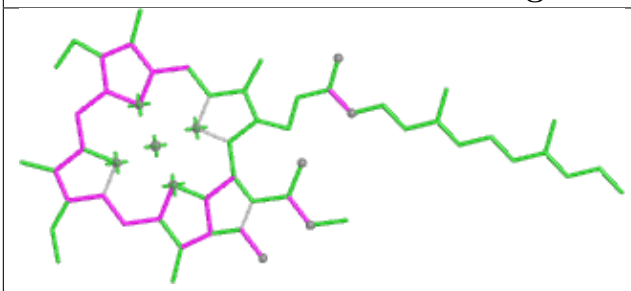


Rings

Ligand CLA Z 603



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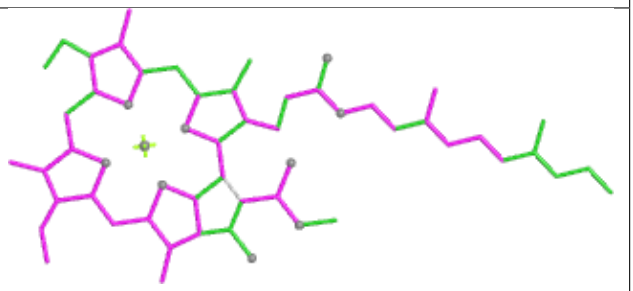
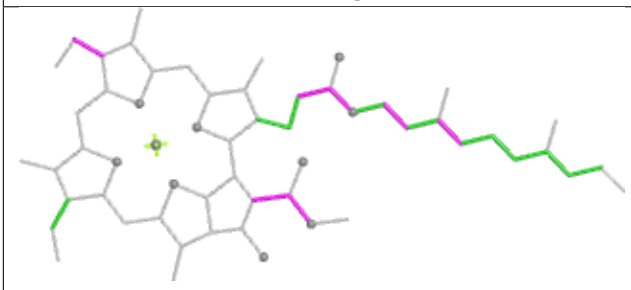


Bond angles



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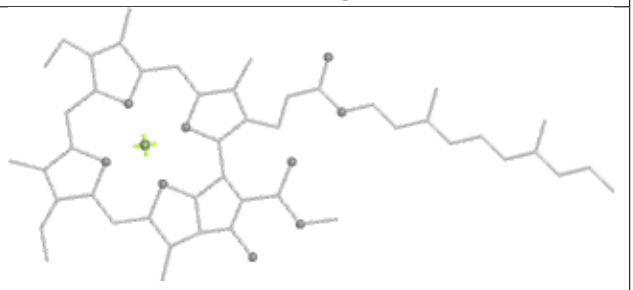
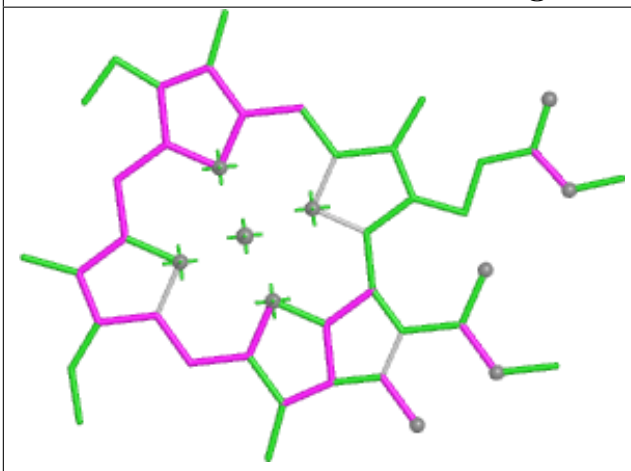


Rings

Ligand CLA 5 603



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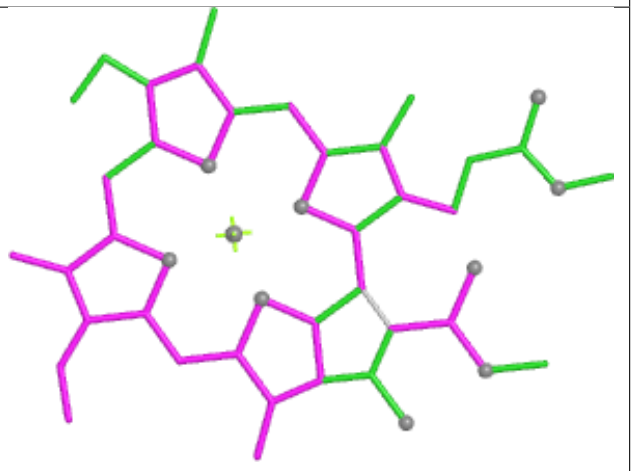

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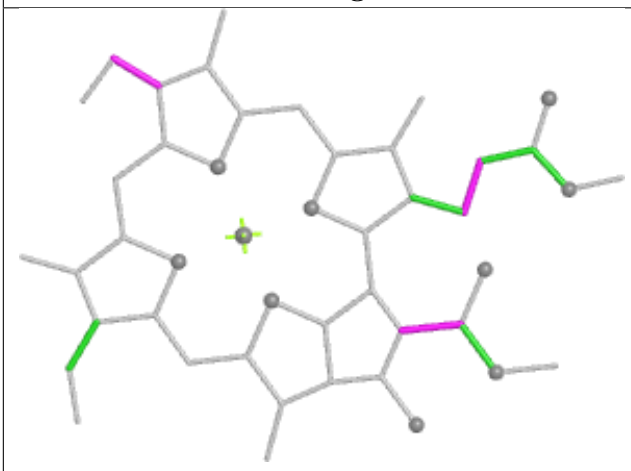

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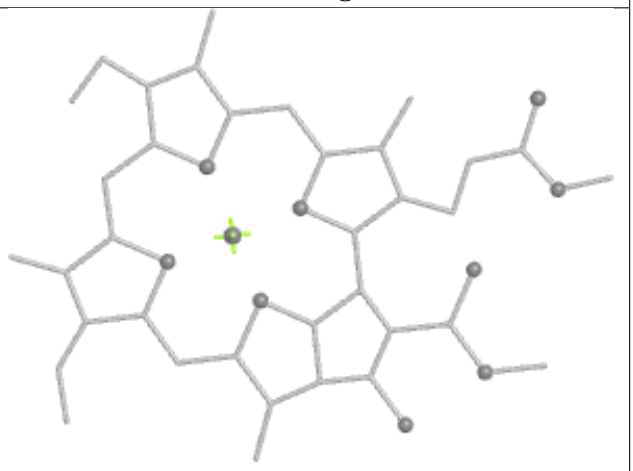
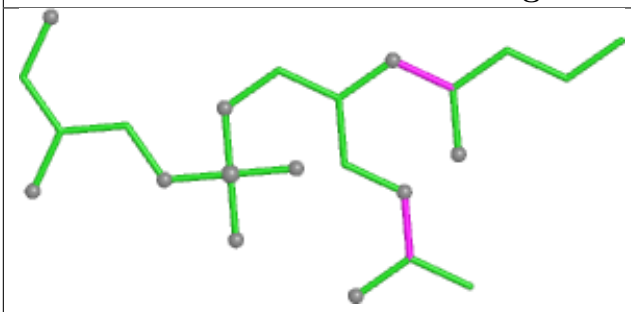


Rings

Ligand LHG B 851



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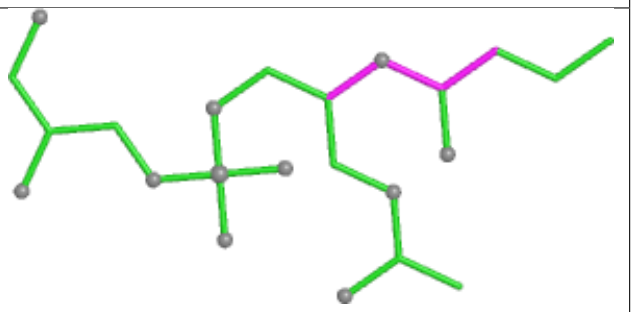

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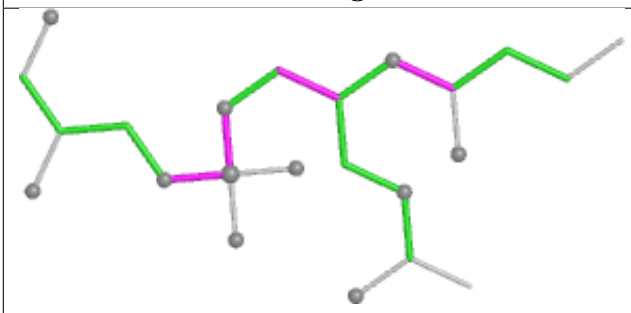

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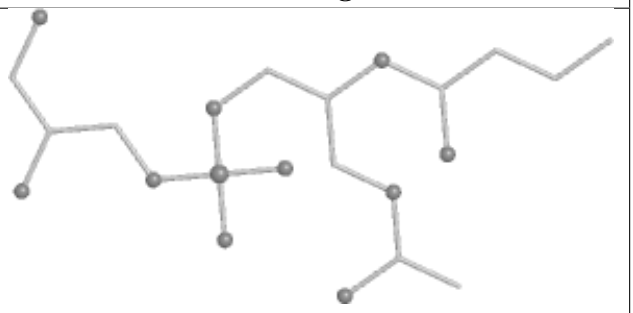
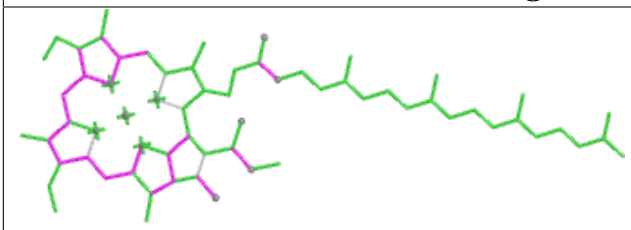


Rings

Ligand CLA B 829



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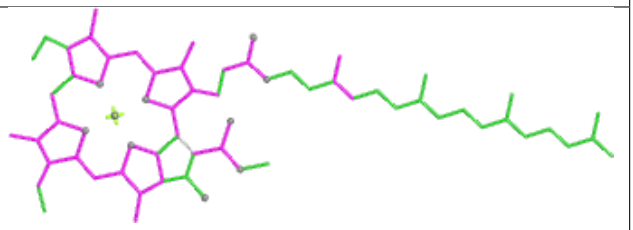

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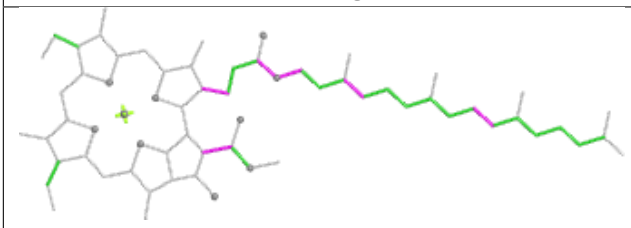

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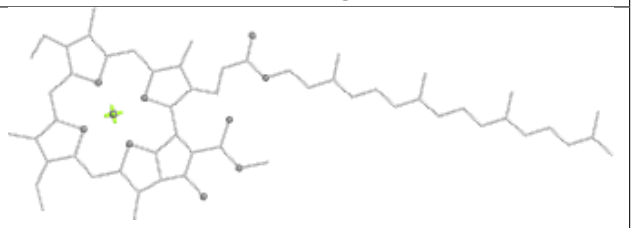
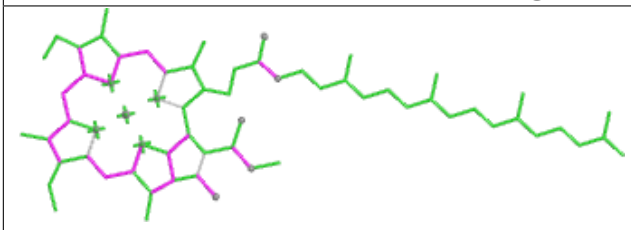


Rings

Ligand CLA 3 610



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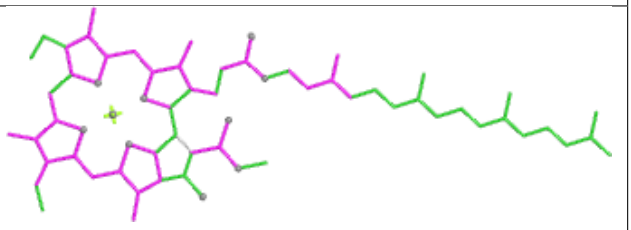
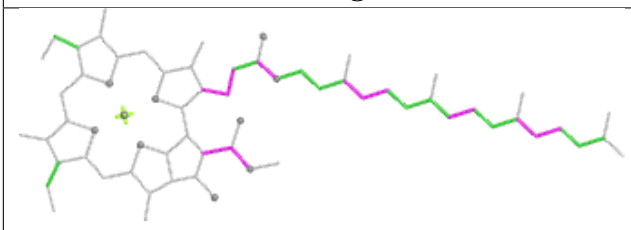


Bond angles



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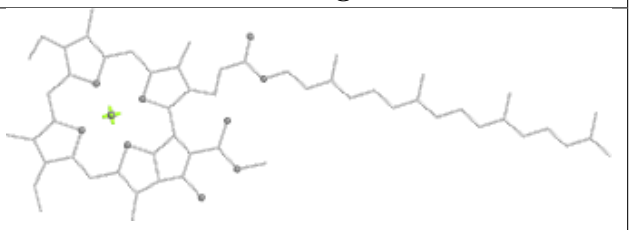
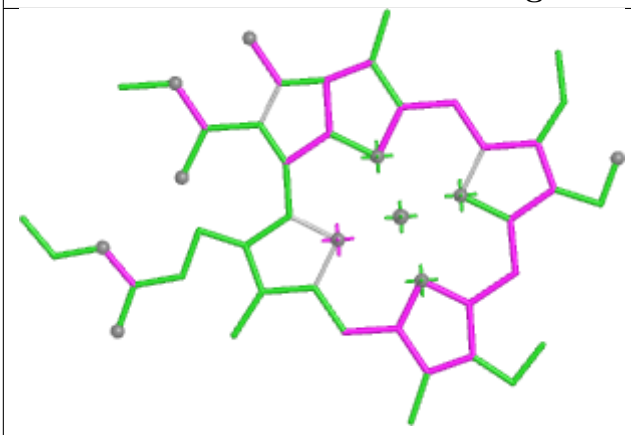


Rings

Ligand CHL Z 607



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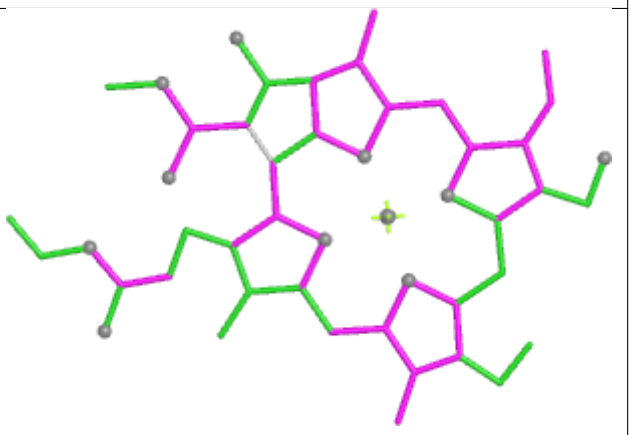
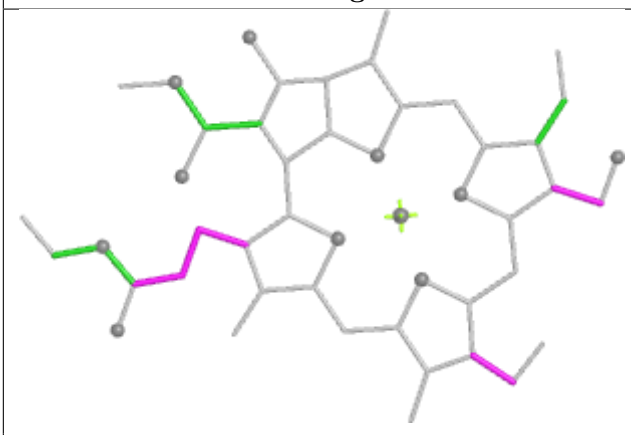


Bond angles



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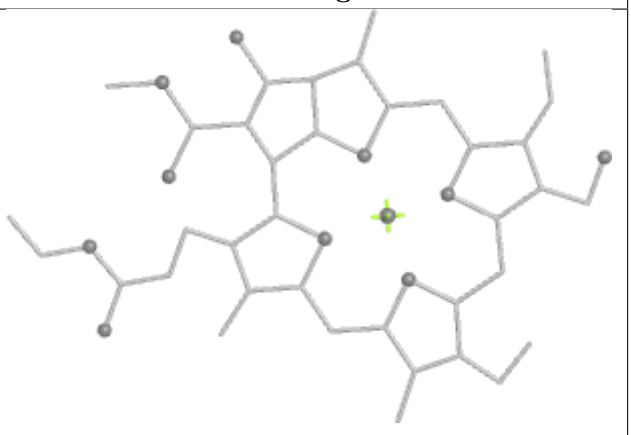
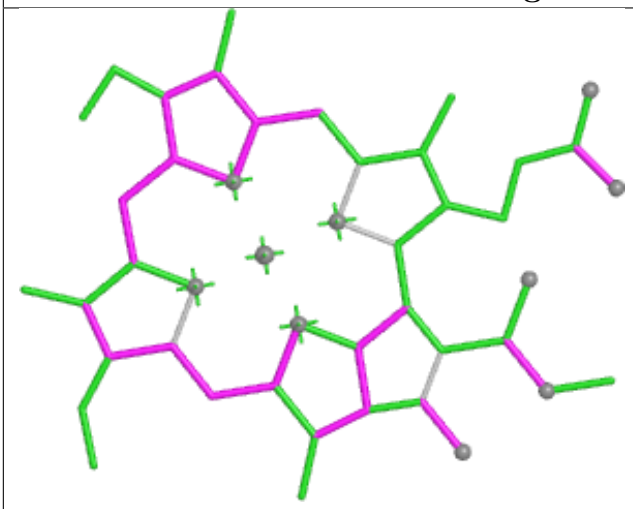


Rings

Ligand CLA A 821



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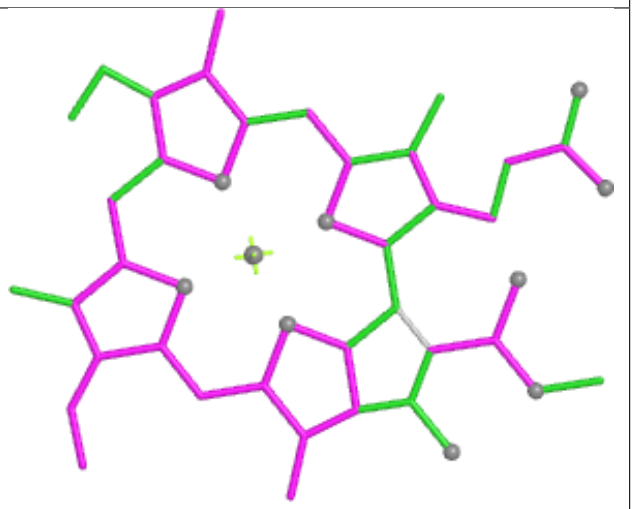
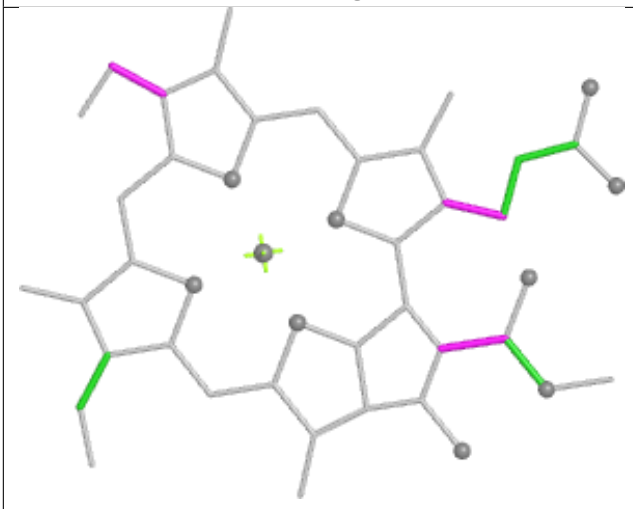


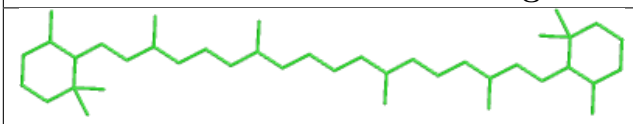
Bond angles



Torsions

Rings

Ligand BCR B 843



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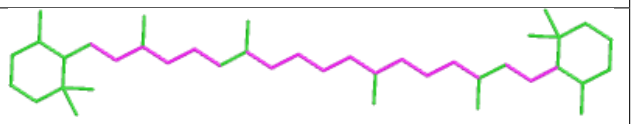
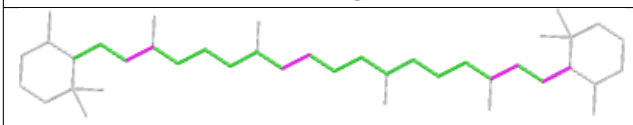
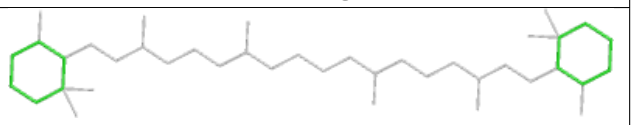


Bond angles

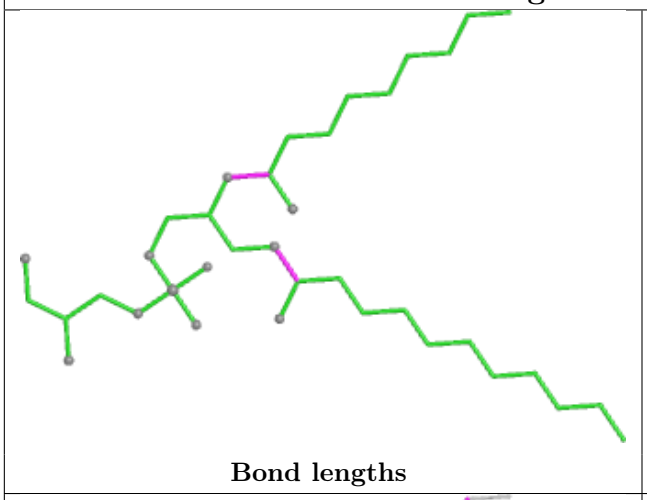


Torsions



Rings

Ligand LHG 8 620



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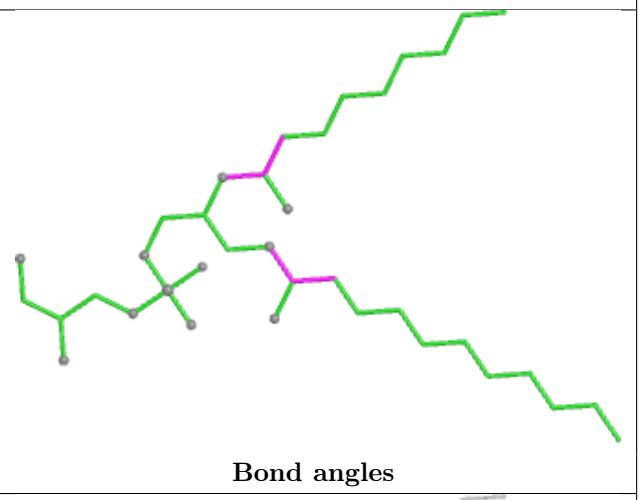
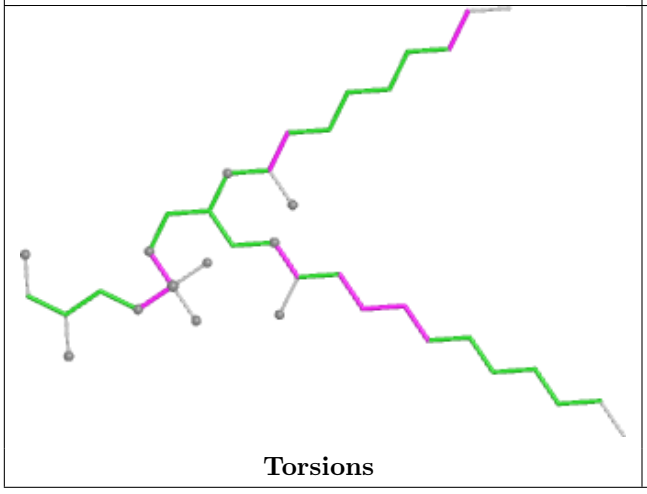
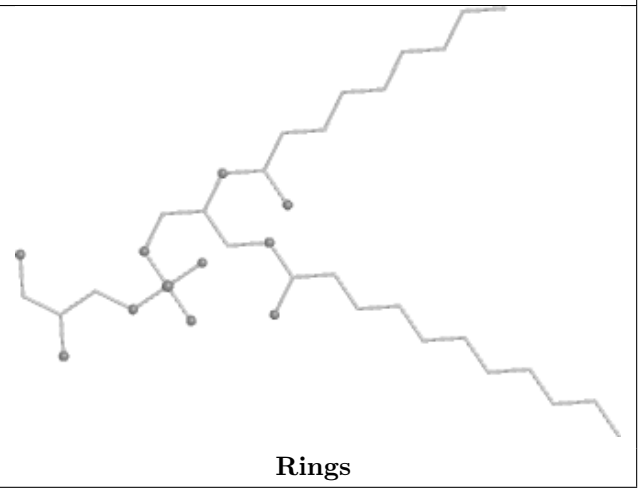


Bond angles

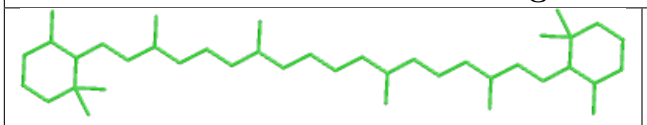


Torsions



Rings

Ligand BCR I 172



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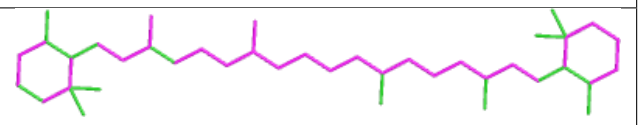
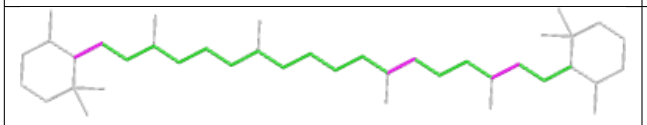


Bond angles



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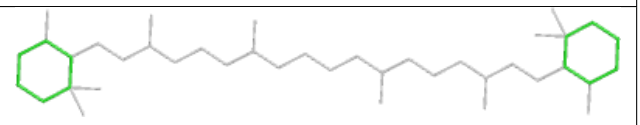
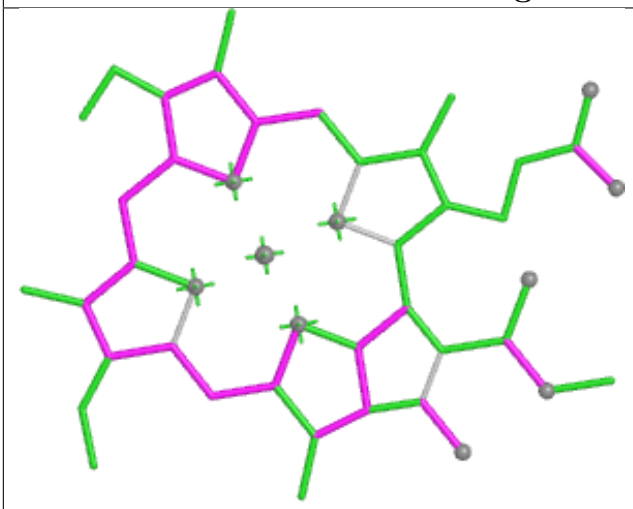
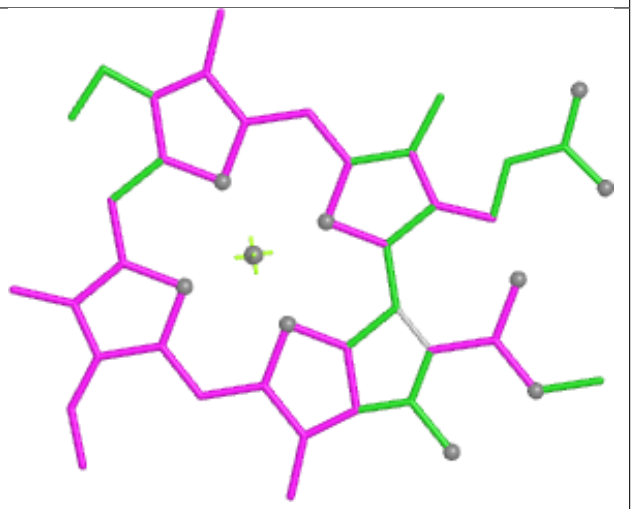


Rings

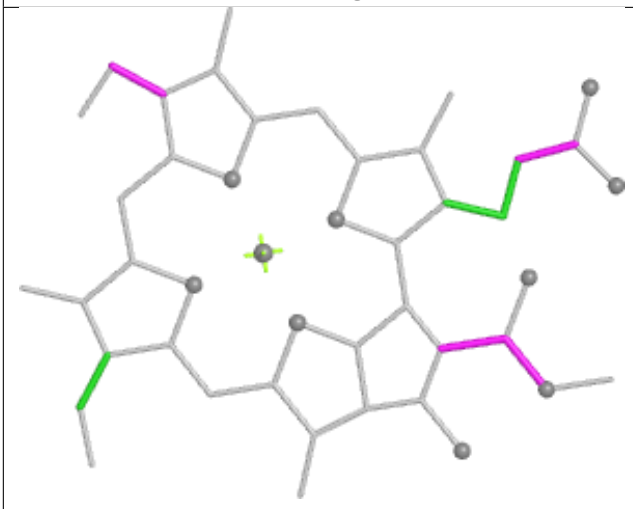
Ligand CLA K 4002



Bond lengths



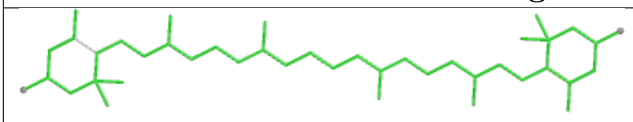
Bond angles



Torsions

Rings

Ligand LUT 1 619



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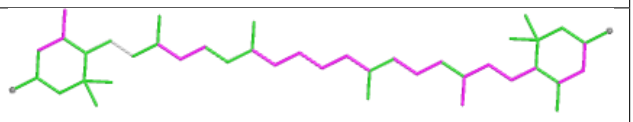

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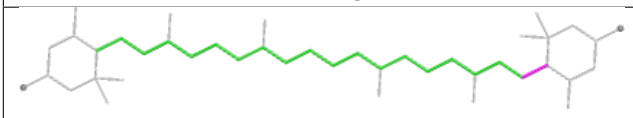
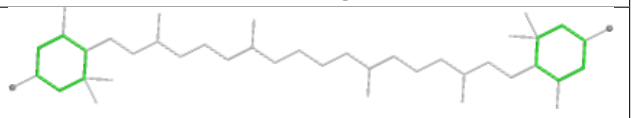
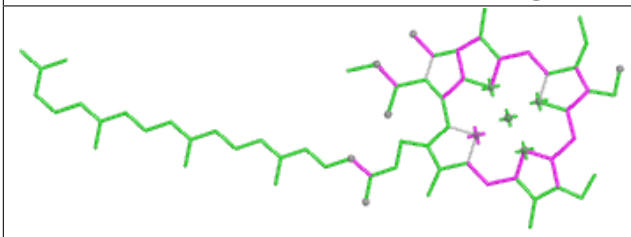
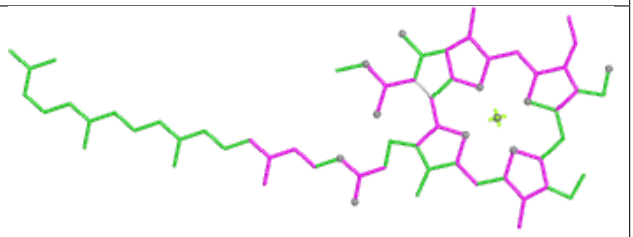
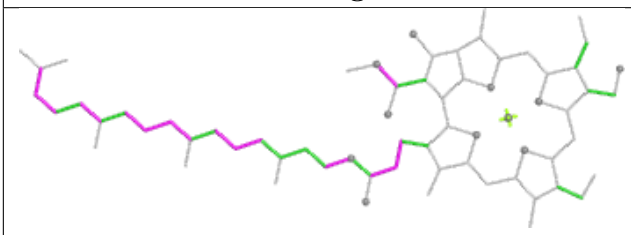
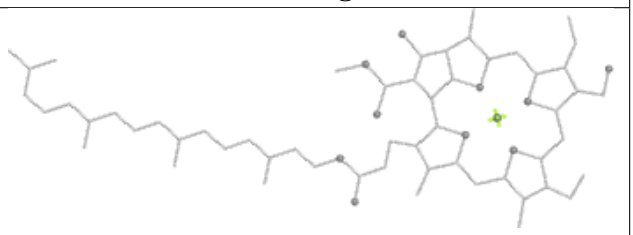
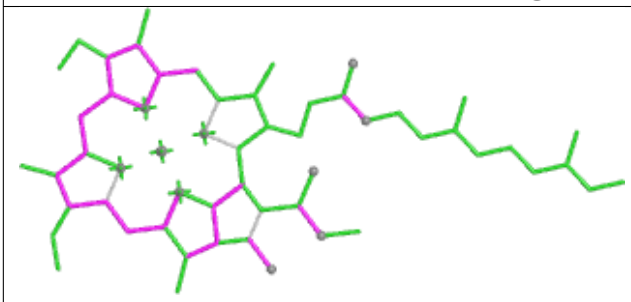
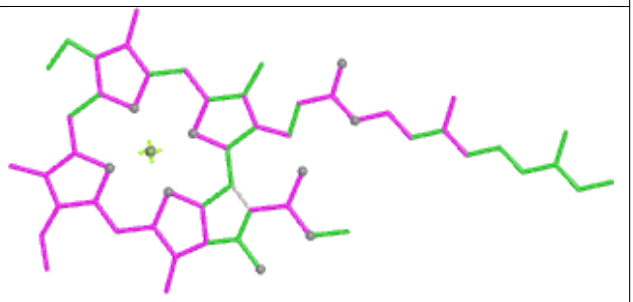
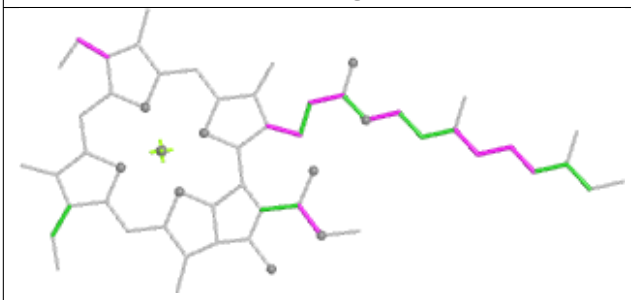
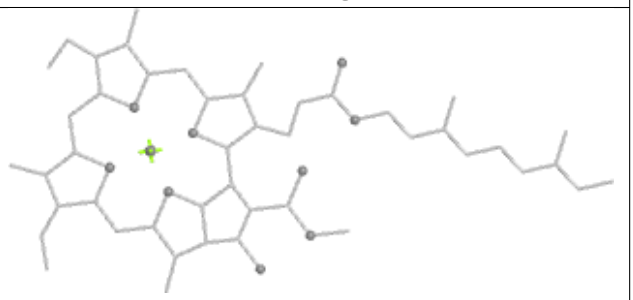


Torsions

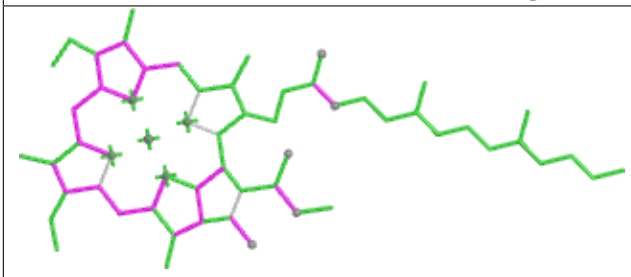


Rings

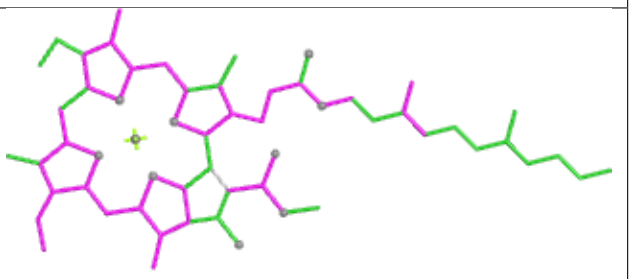
Ligand CHL 3 608	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA 4 613	
 Bond lengths	 Bond angles
 Torsions	 Rings

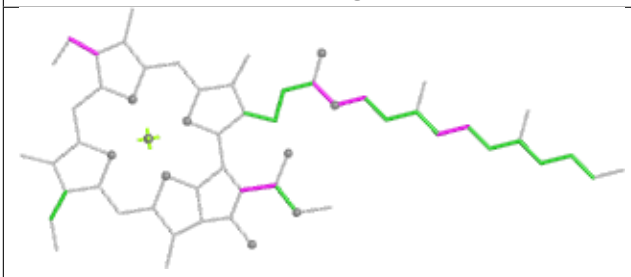
Ligand CLA B 833



Bond lengths



Bond angles



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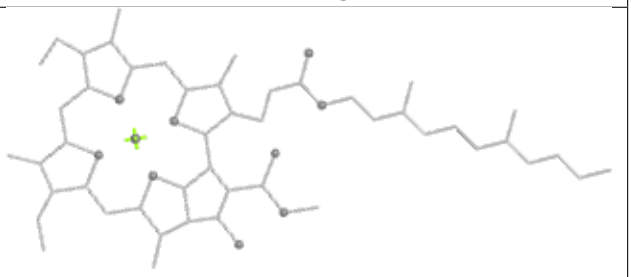
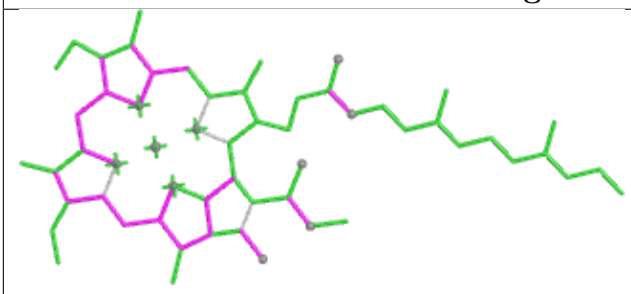


Rings

Ligand CLA A 817



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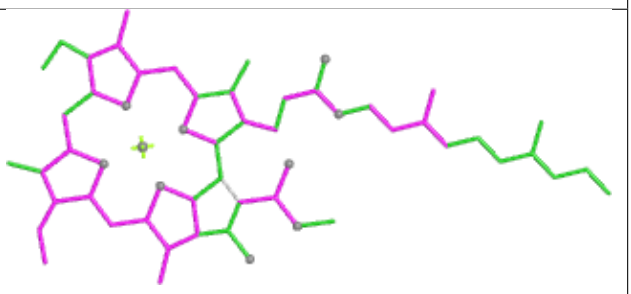

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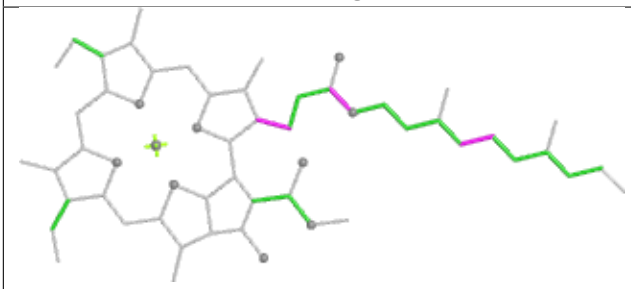

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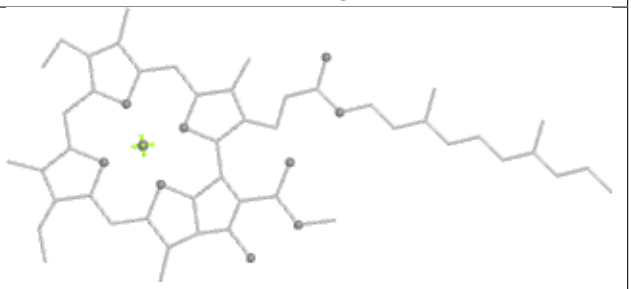
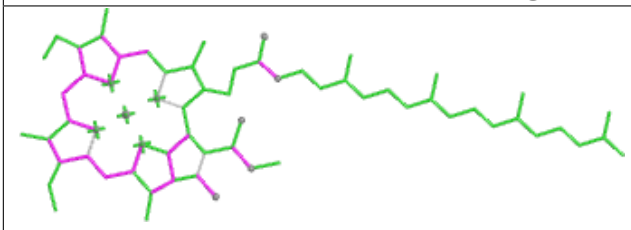


Rings

Ligand CLA B 840



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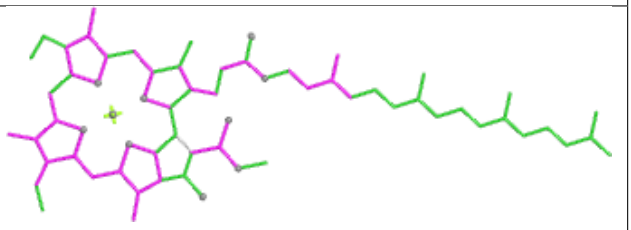
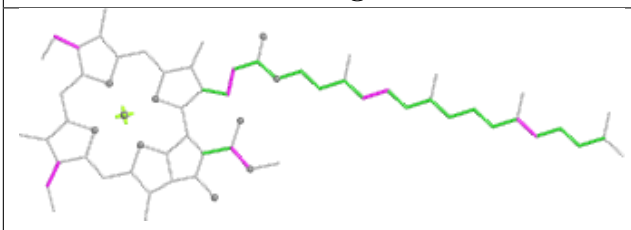


Bond angles



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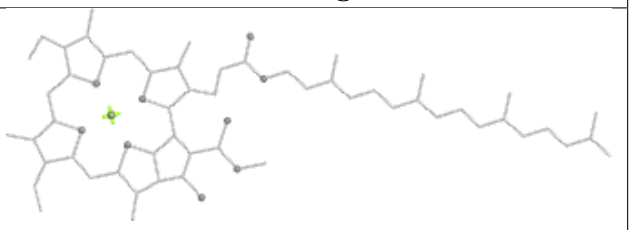
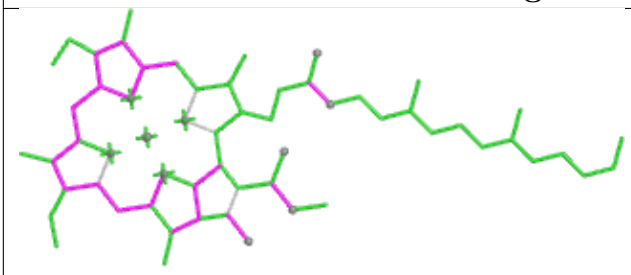


Rings

Ligand CLA B 822



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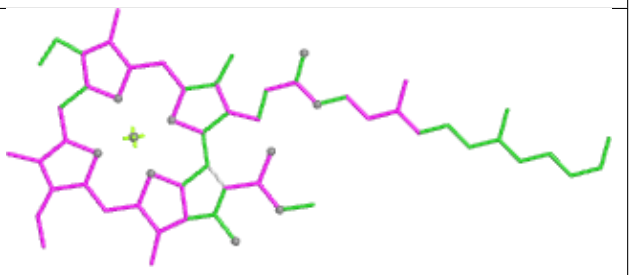

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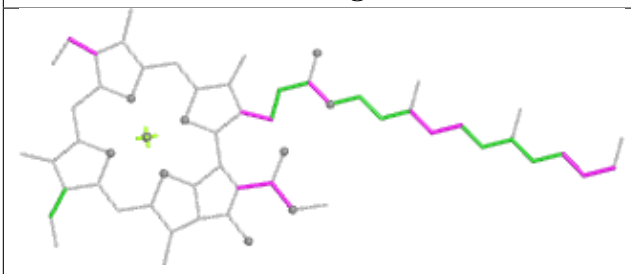

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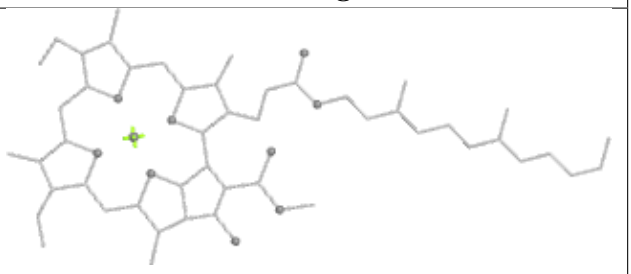
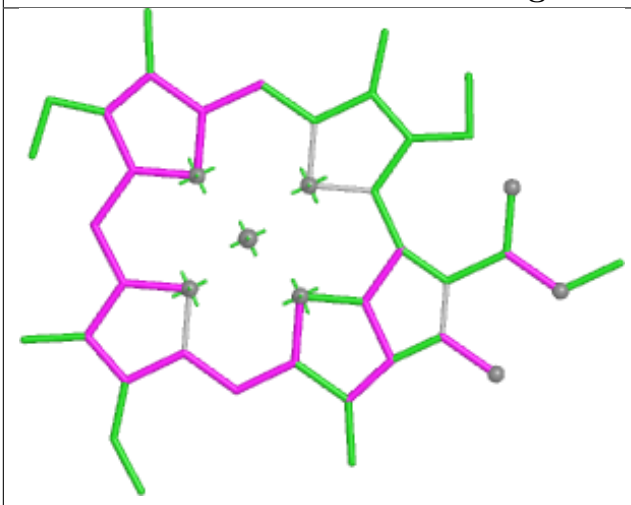


Rings

Ligand CLA 8 606



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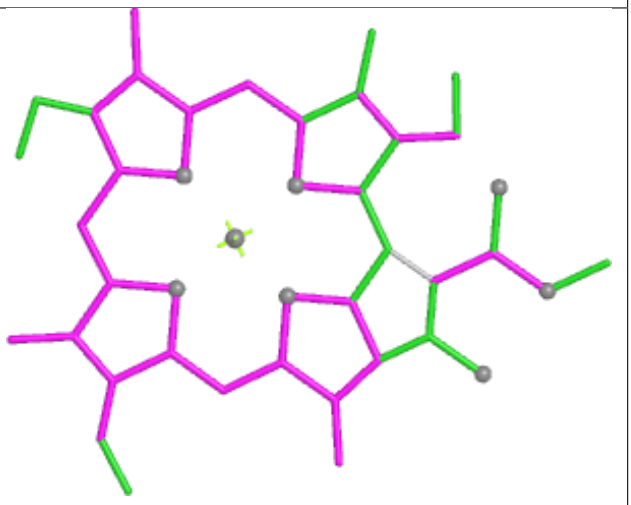
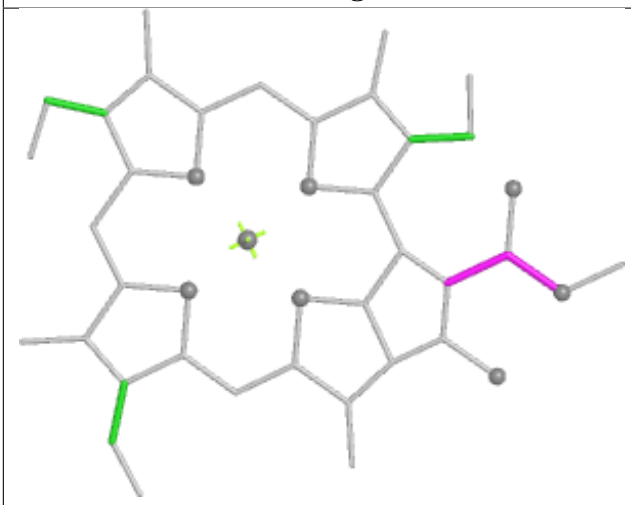


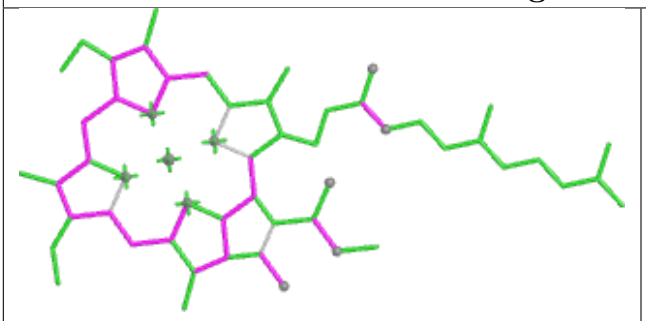
Bond angles



Torsions

Rings

Ligand CLA 3 613



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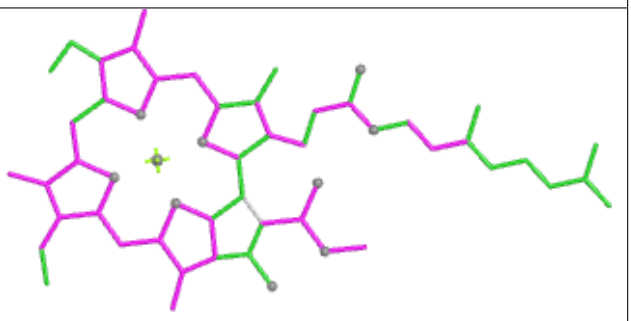

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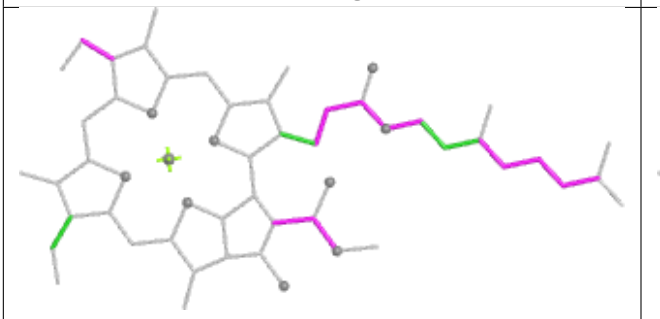

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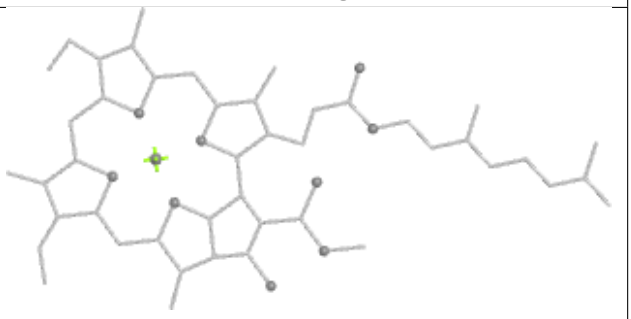
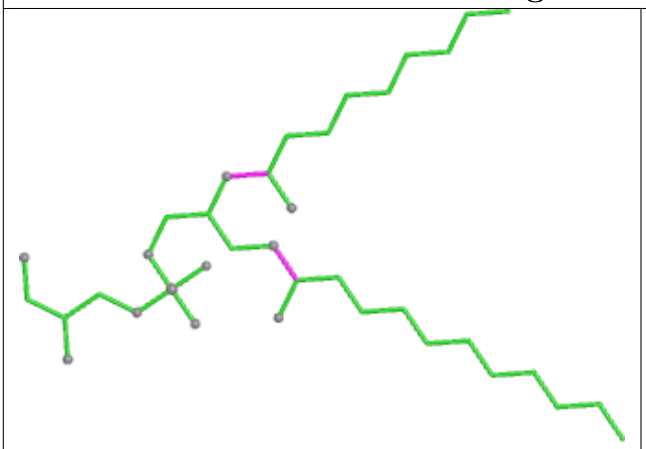


Rings

Ligand LHG 7 625



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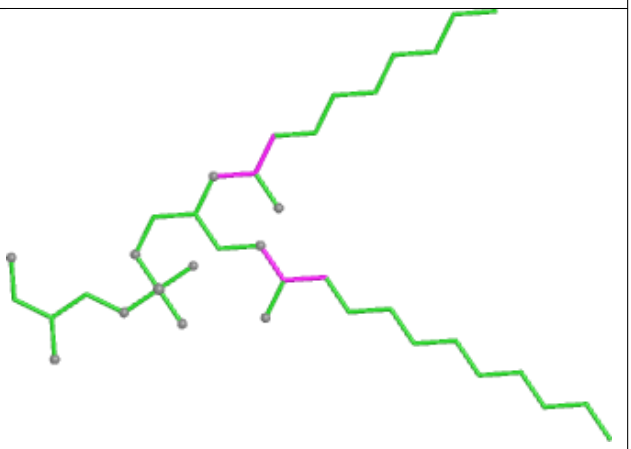
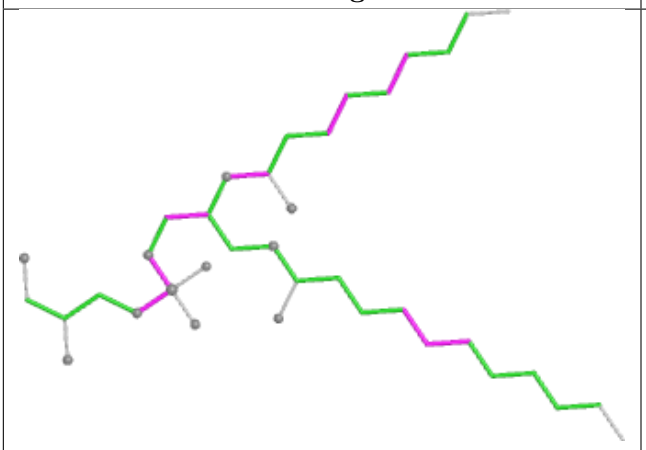


Bond angles



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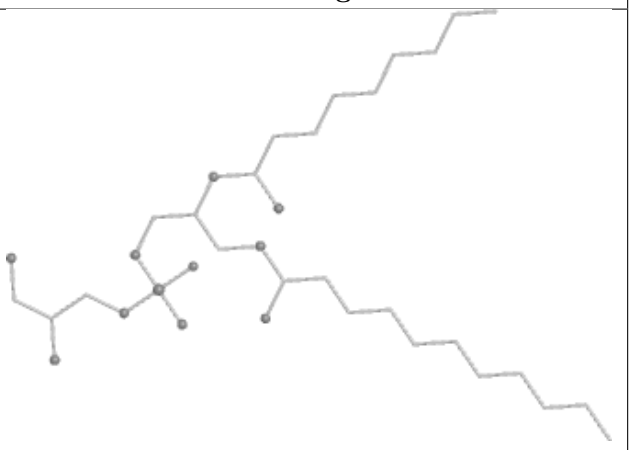
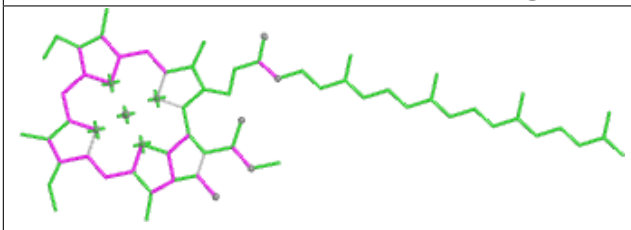


Rings

Ligand CLA A 835



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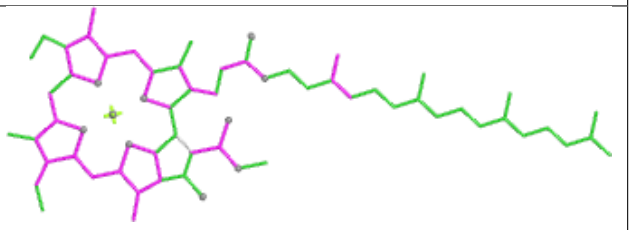

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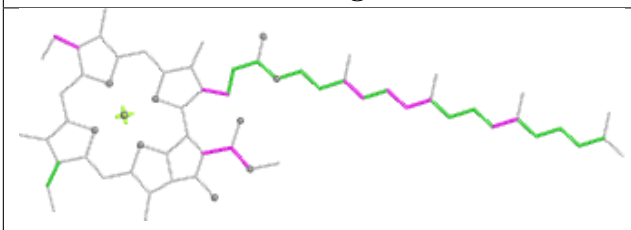

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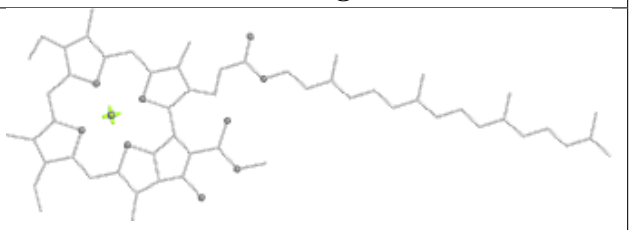
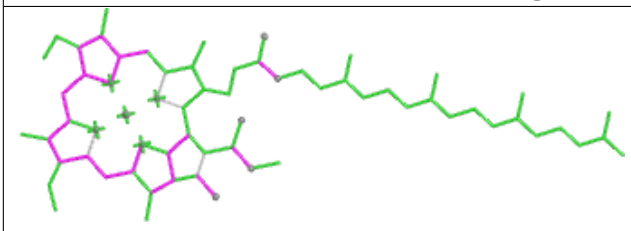


Rings

Ligand CLA 1 603



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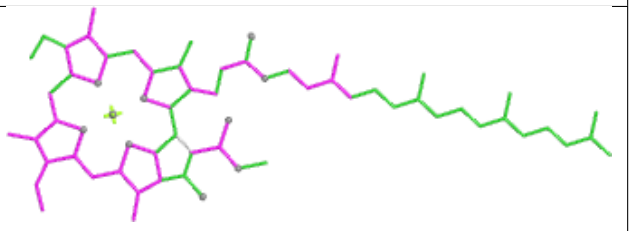

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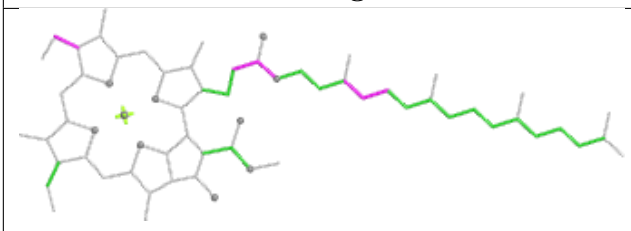

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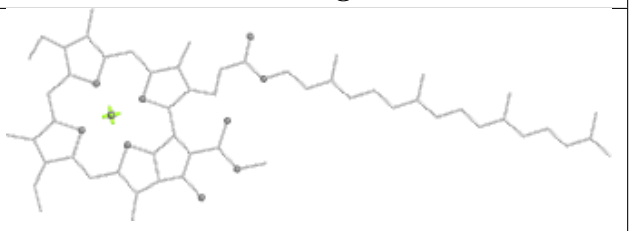
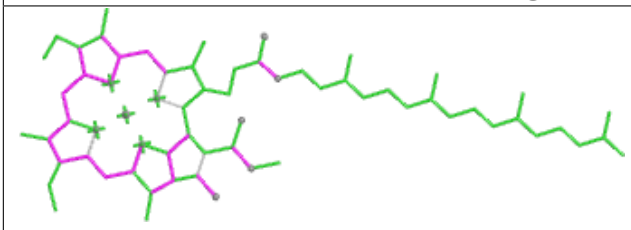


Rings

Ligand CLA B 837



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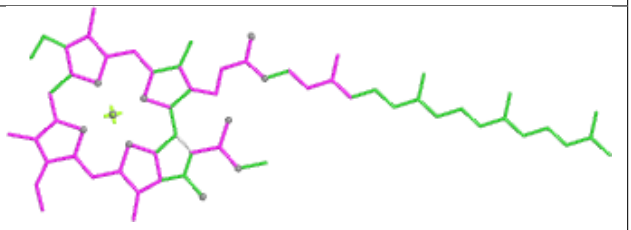
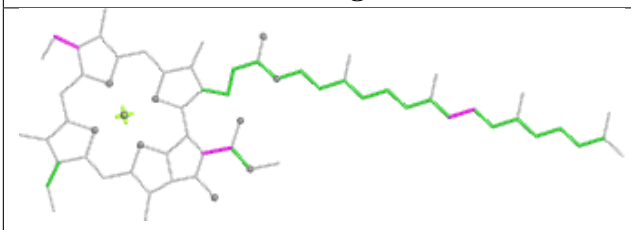


Bond angles



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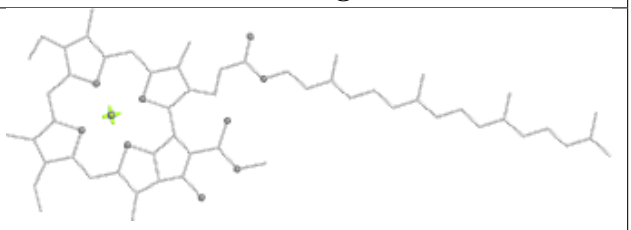
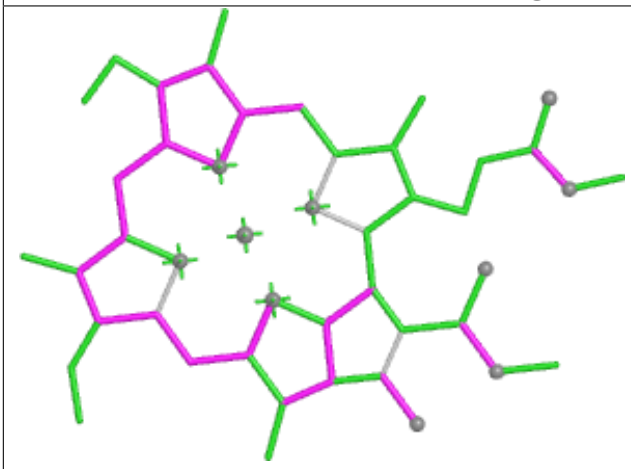
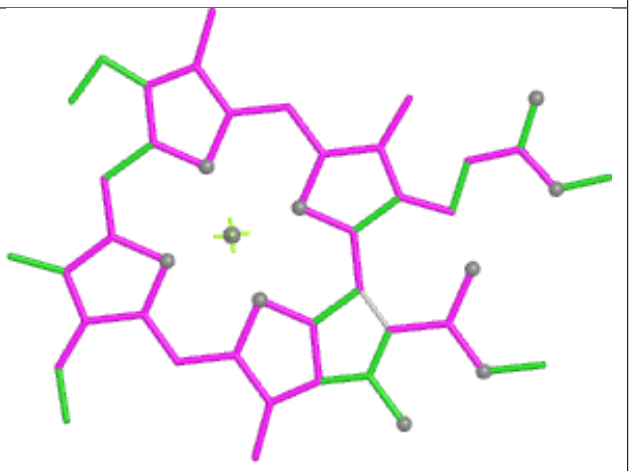
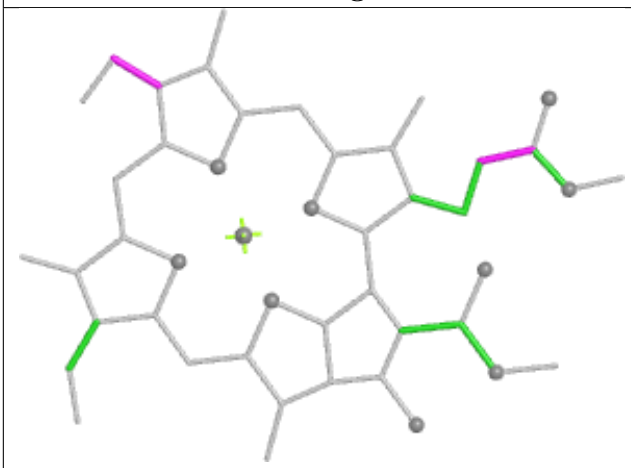
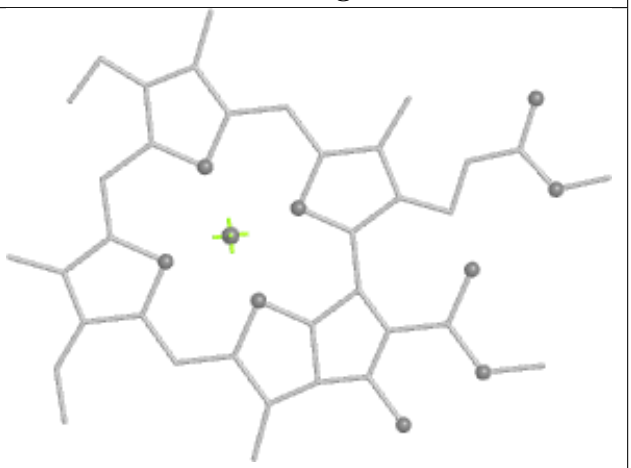
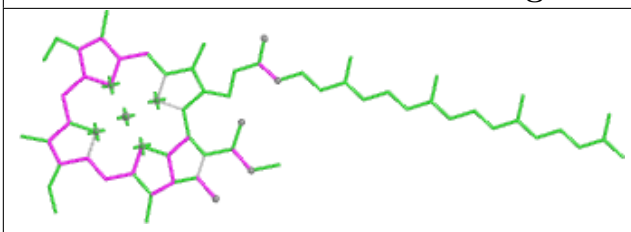
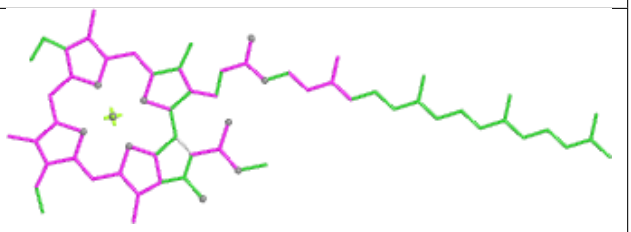
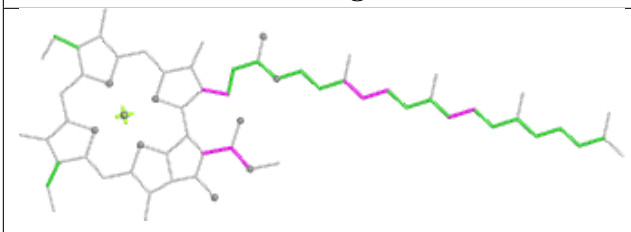
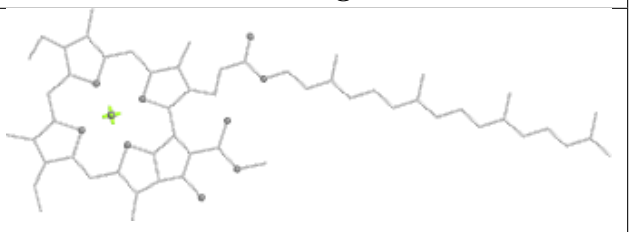
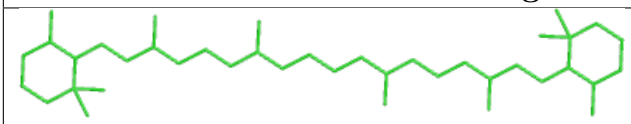


Rings

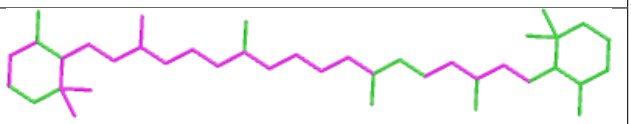
Ligand CLA 8 609	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA F 301	
	
Bond lengths	Bond angles
	
Torsions	Rings

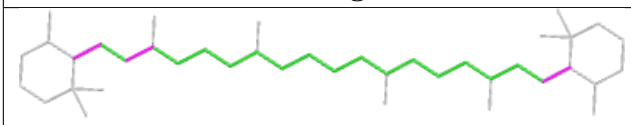
Ligand BCR A 849



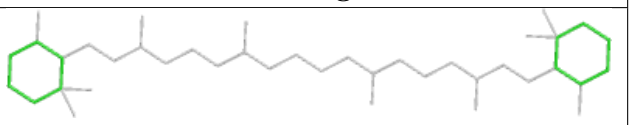
Bond lengths



Bond angles

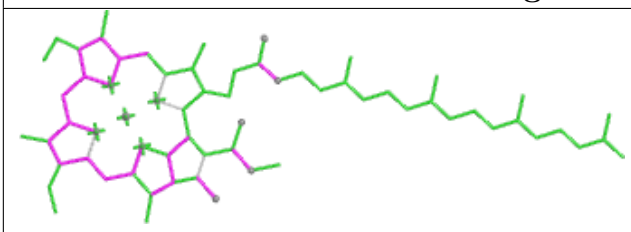


Torsions



Rings

Ligand CLA A 809



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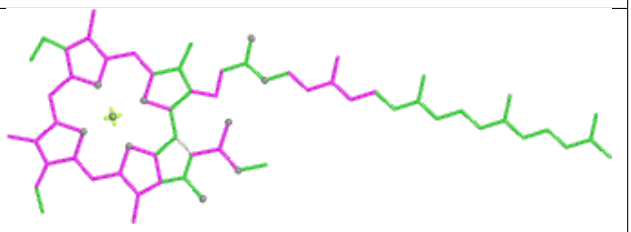

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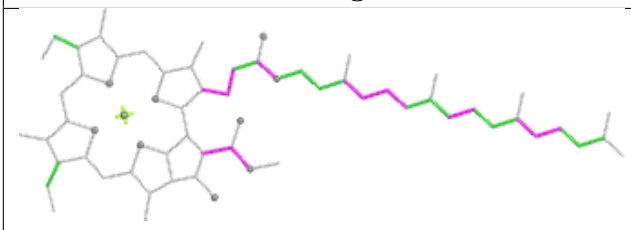

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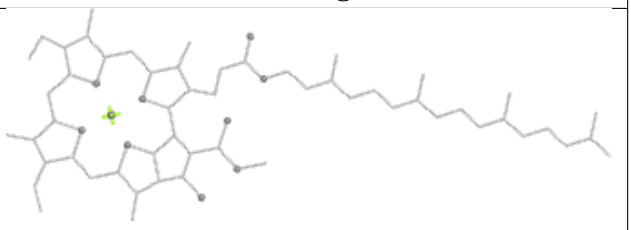
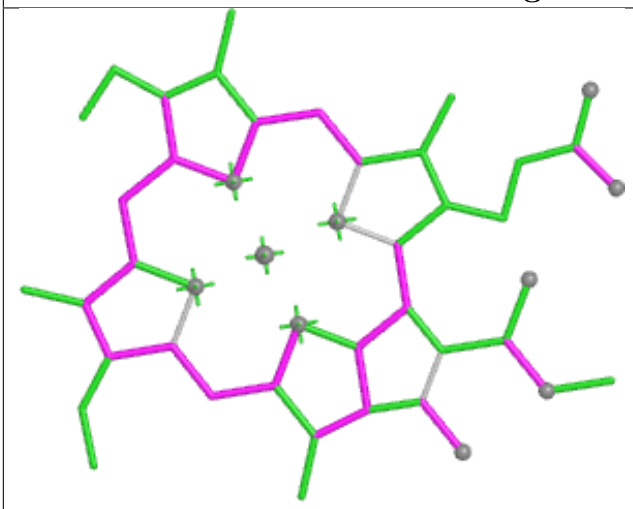


Rings

Ligand CLA A 837



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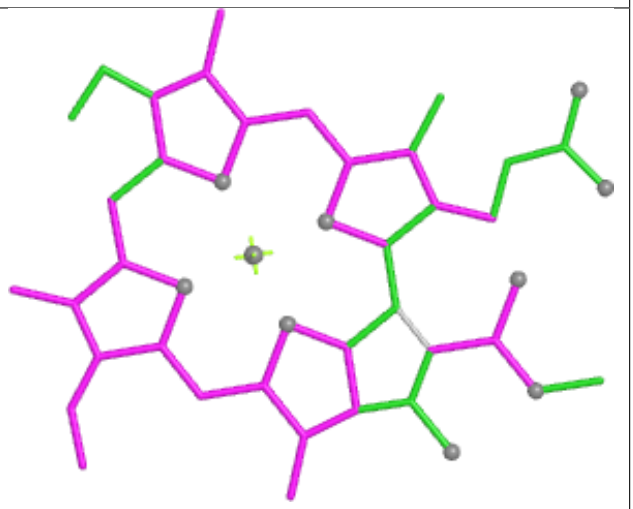
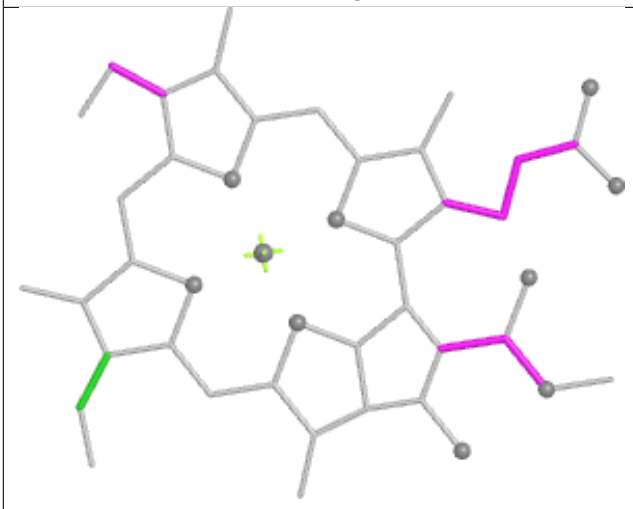


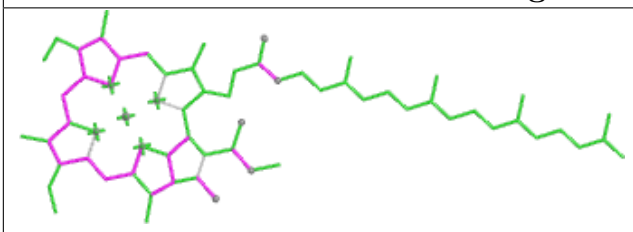
Bond angles



Torsions

Rings

Ligand CLA 6 602



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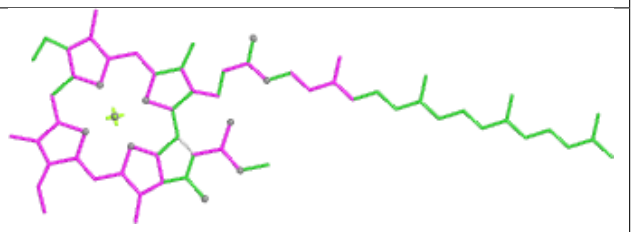
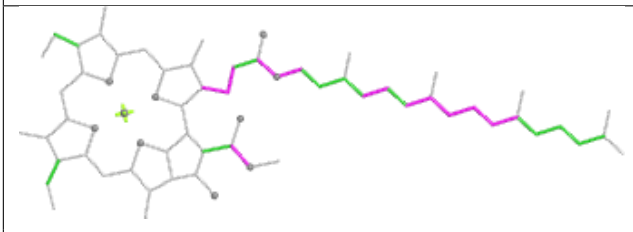


Bond angles



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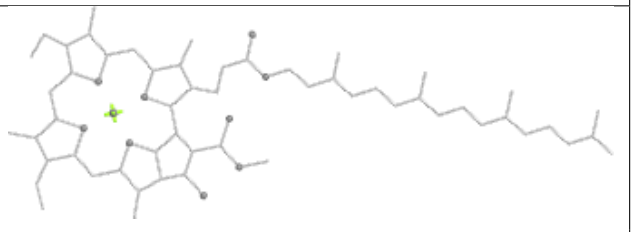
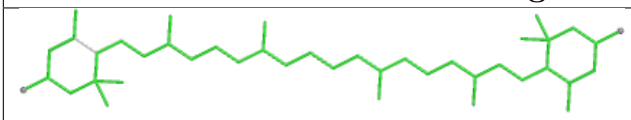


Rings

Ligand LUT 1 617



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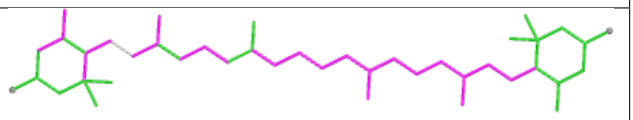
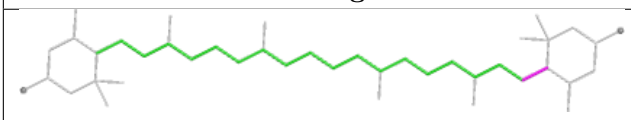


Bond angles



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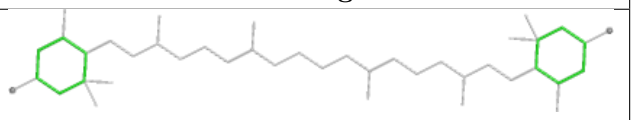
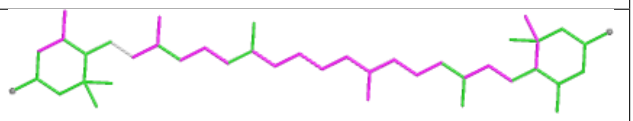


Rings

Ligand LUT 7 622

Bond lengths



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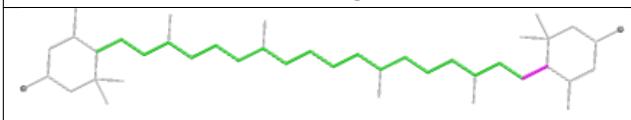

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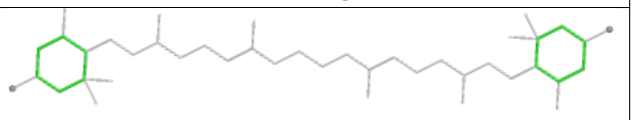
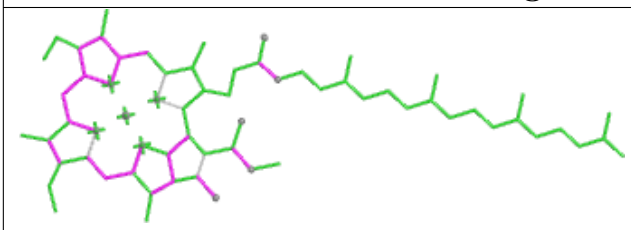


Rings

Ligand CLA A 818



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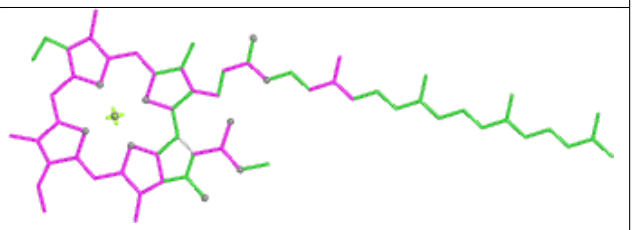
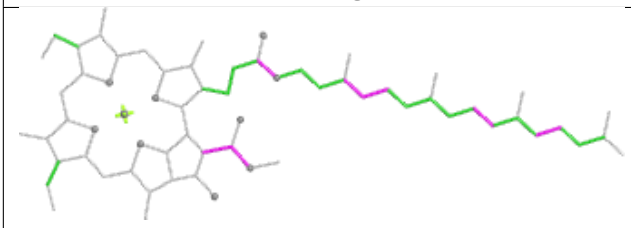


Bond angles



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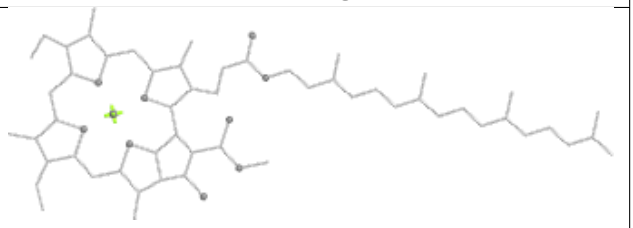
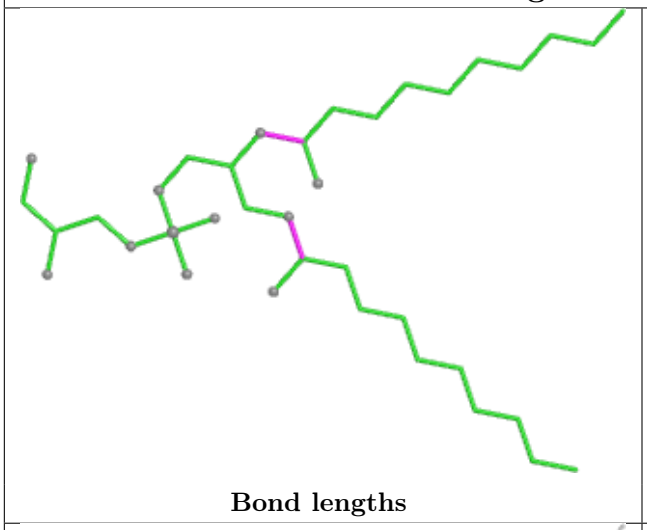


Rings

Ligand LHG 5 623



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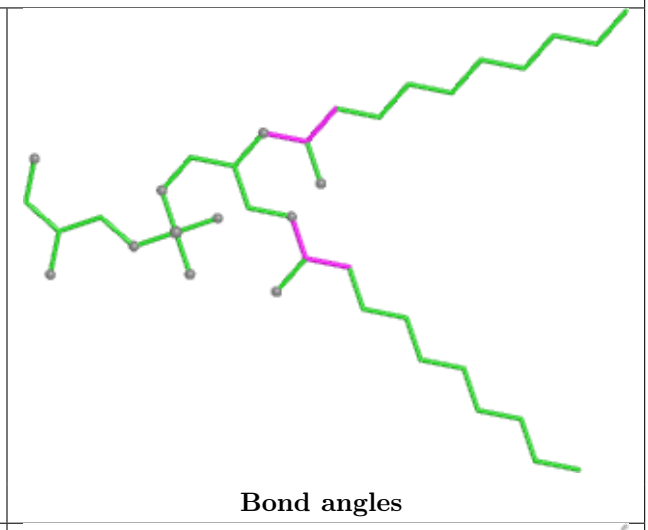

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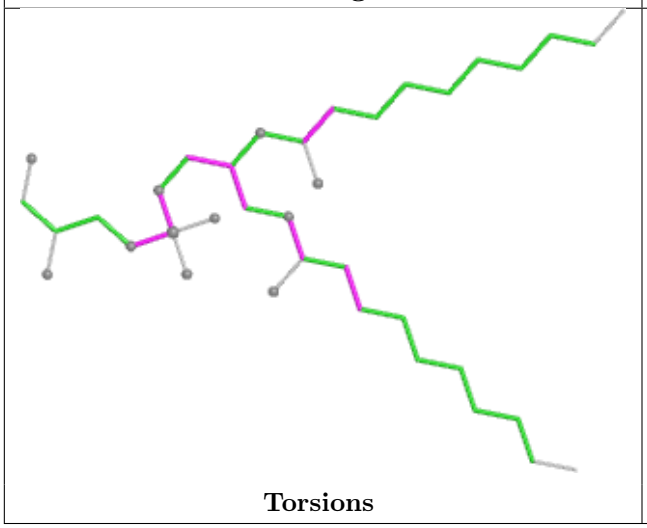

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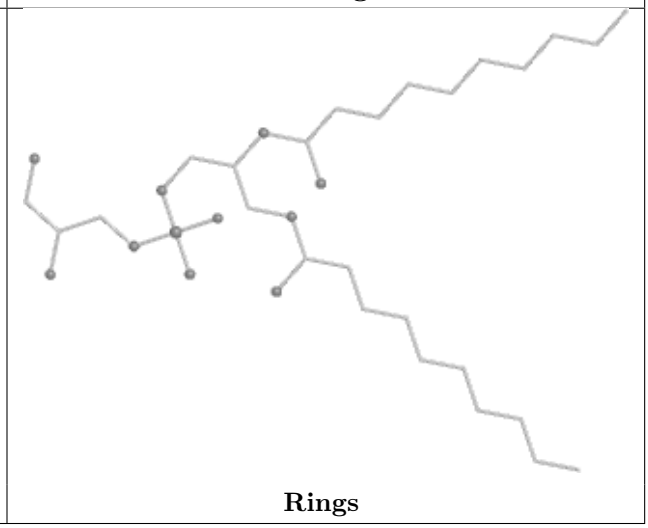
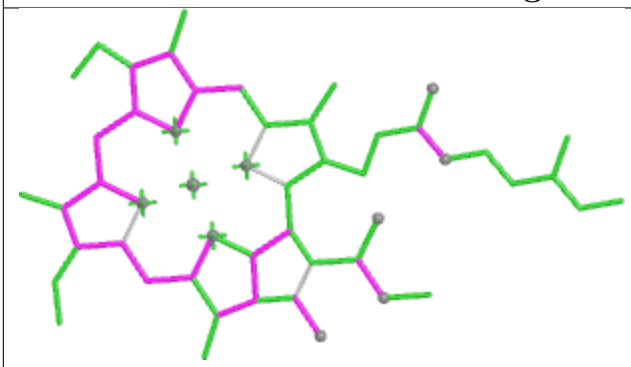


Rings

Ligand CLA A 824



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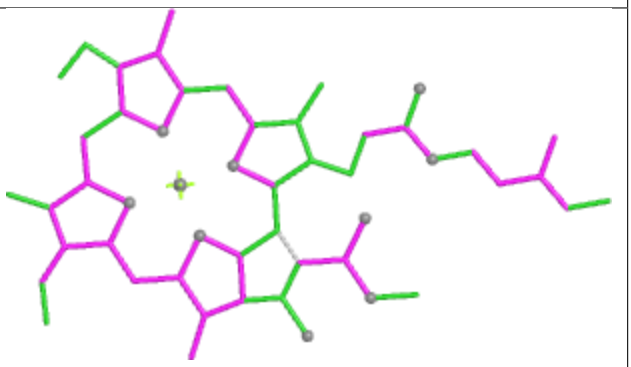

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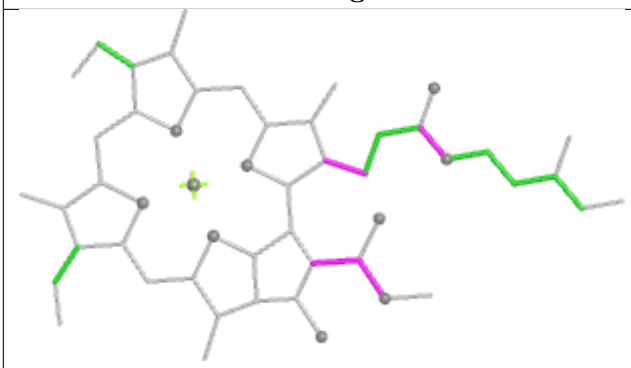

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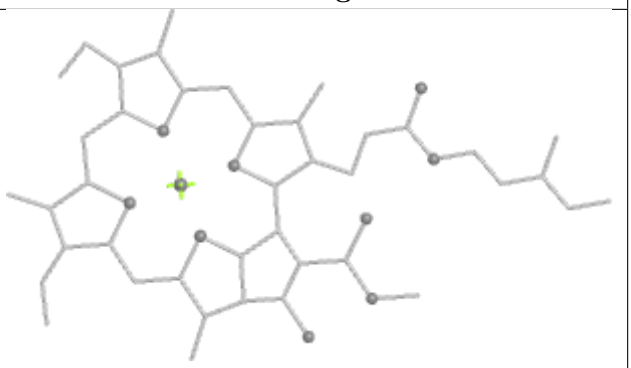
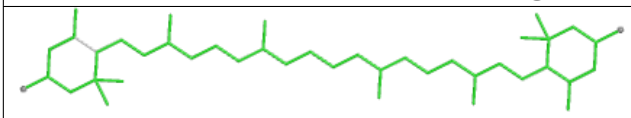


Rings

Ligand LUT 3 622



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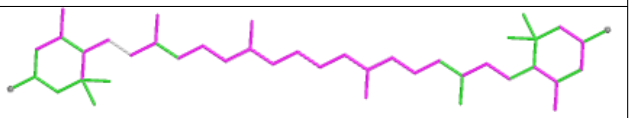
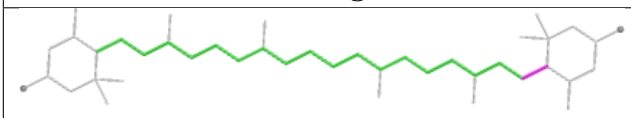


Bond angles



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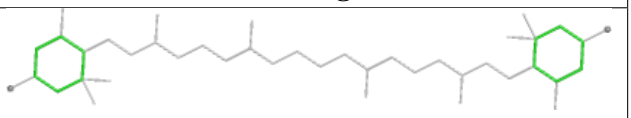
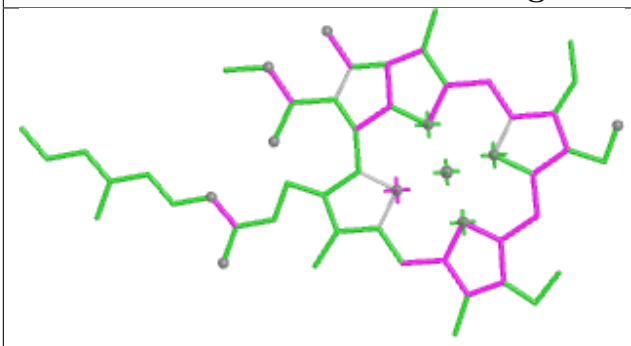


Rings

Ligand CHL 1 601



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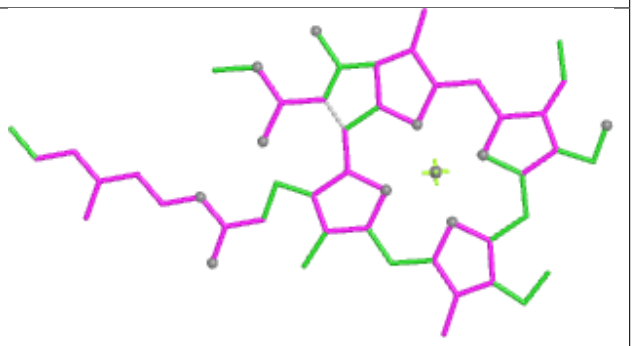
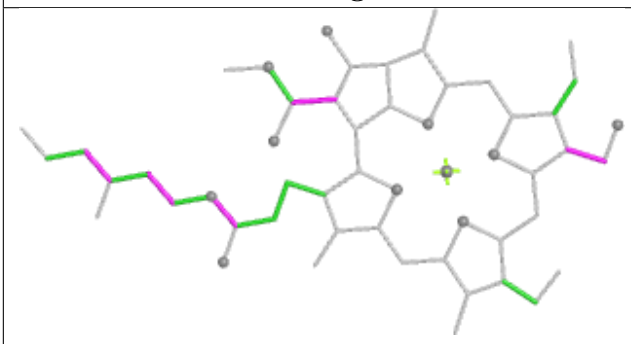


Bond angles



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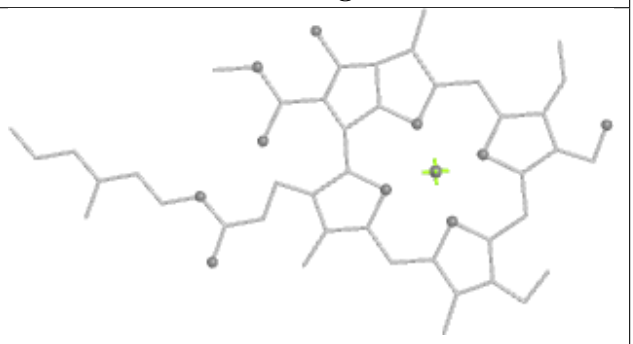
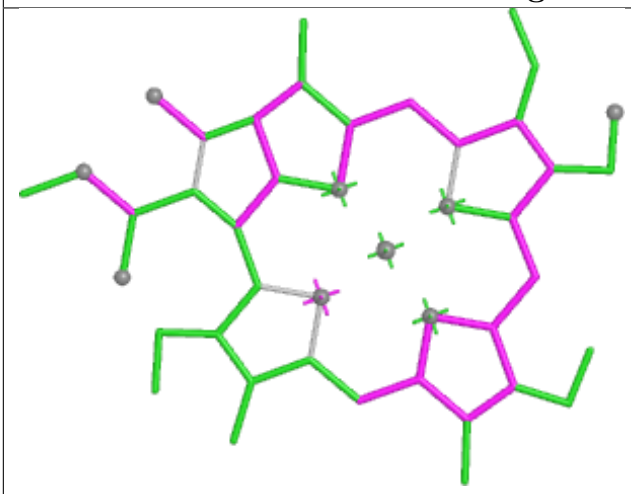


Rings

Ligand CHL 5 618



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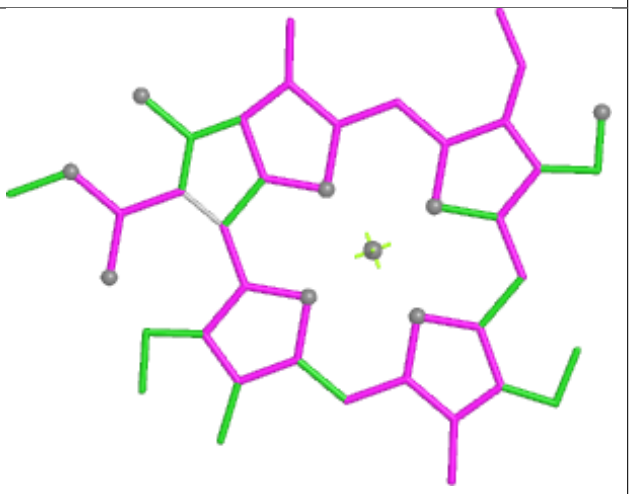
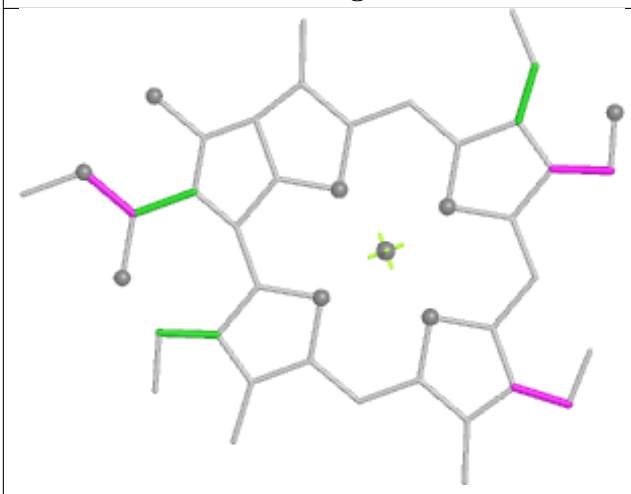


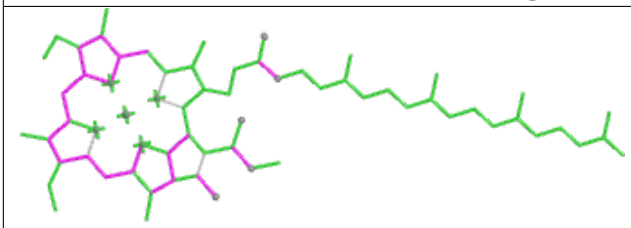
Bond angles



Torsions

Rings

Ligand CLA A 803



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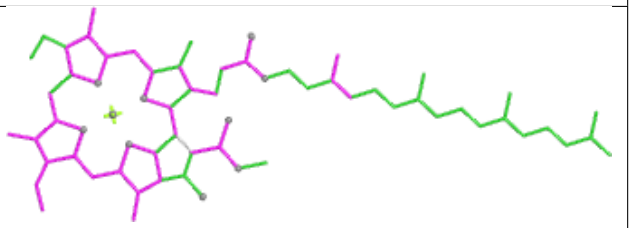
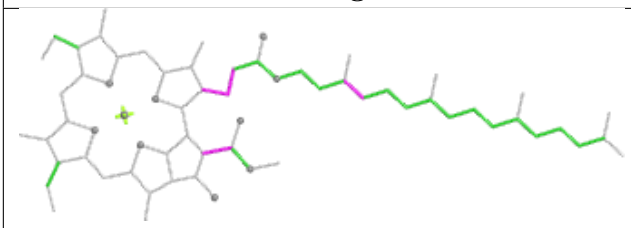
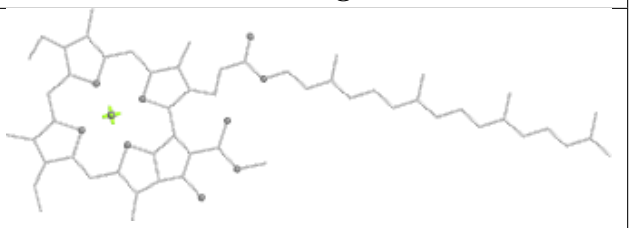


Bond angles

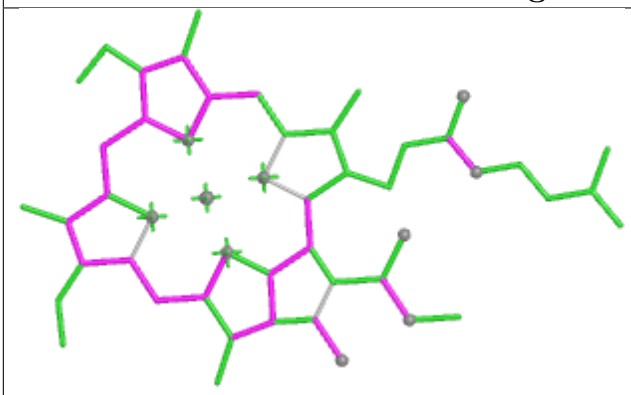


Torsions



Rings

Ligand CLA 6 609



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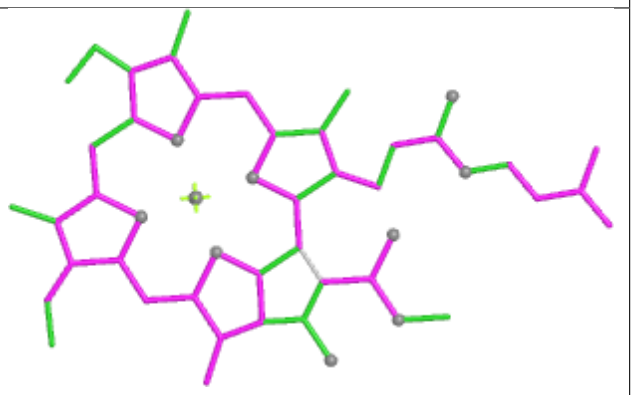
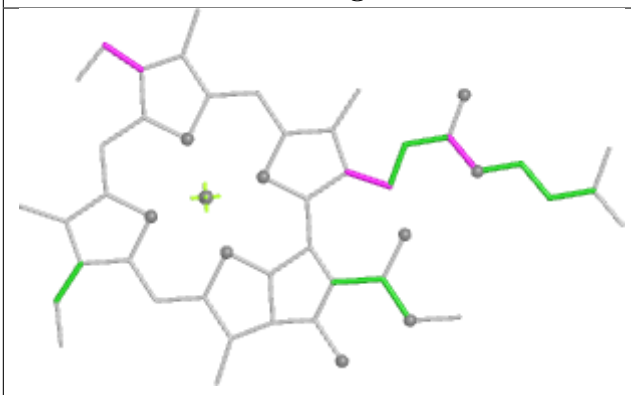
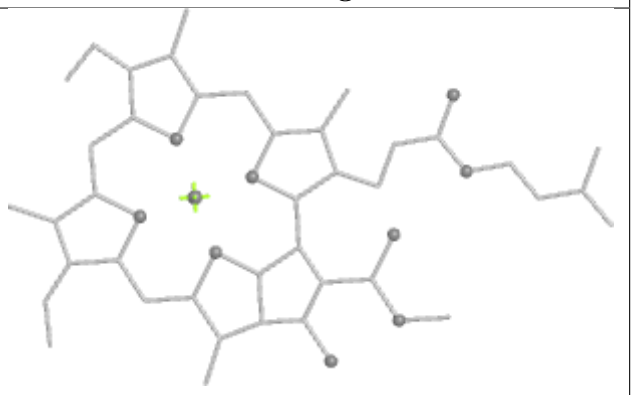


Bond angles

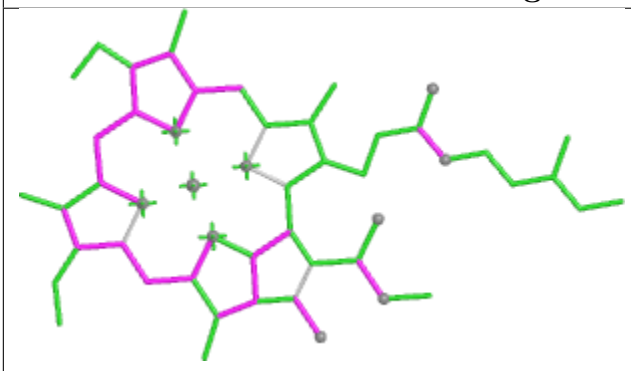


Torsions

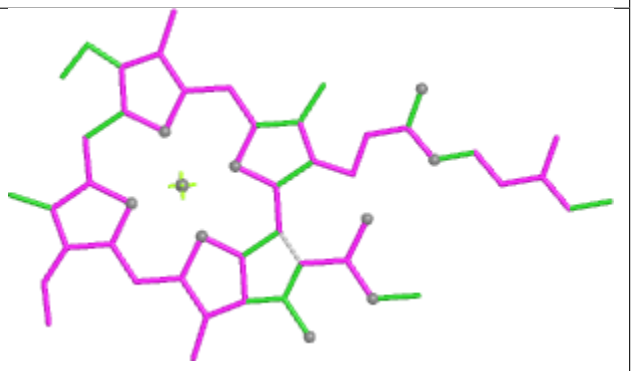


Rings

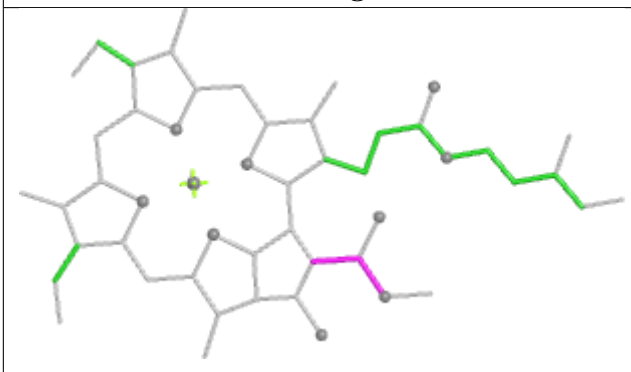
Ligand CLA A 838



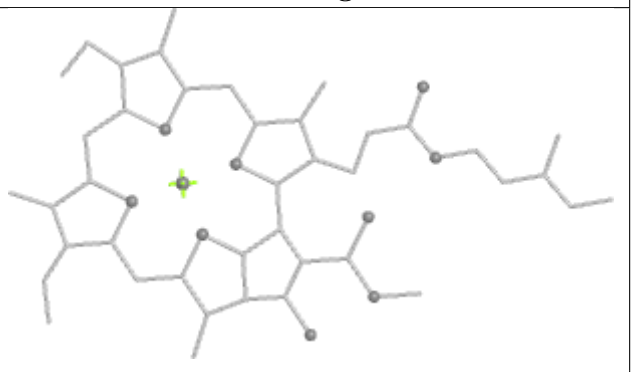
Bond lengths



Bond angles

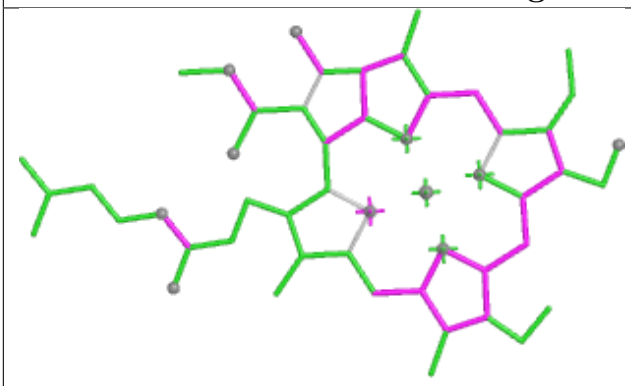


Torsions



Rings

Ligand CHL 4 608



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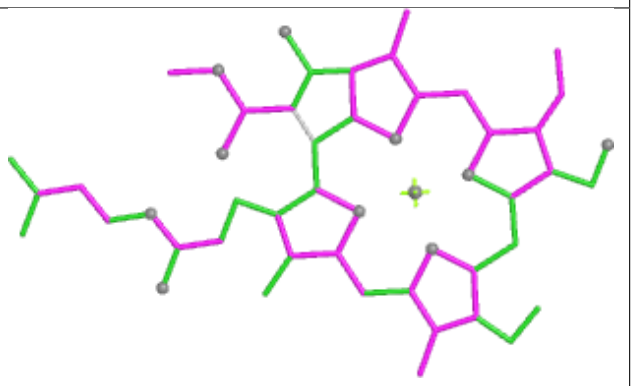

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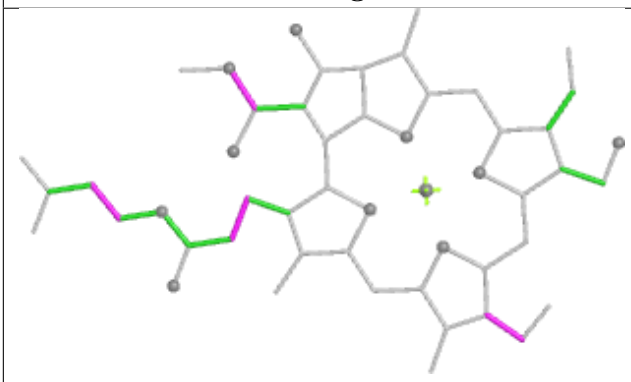

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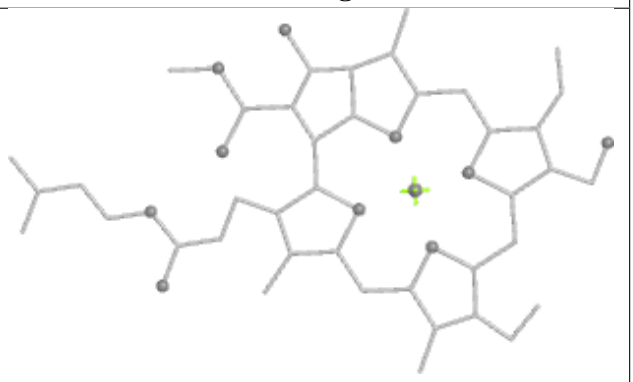
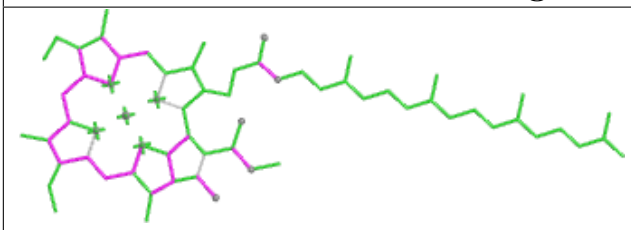


Rings

Ligand CLA 6 604



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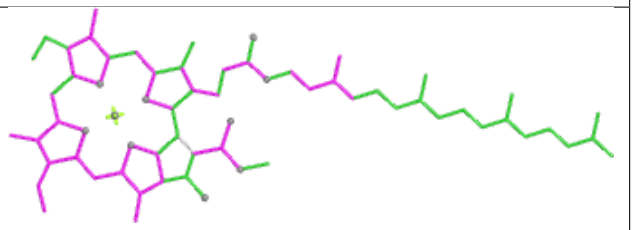
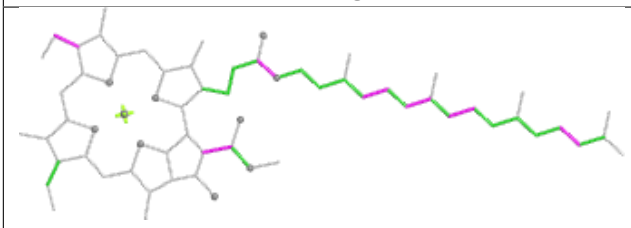


Bond angles



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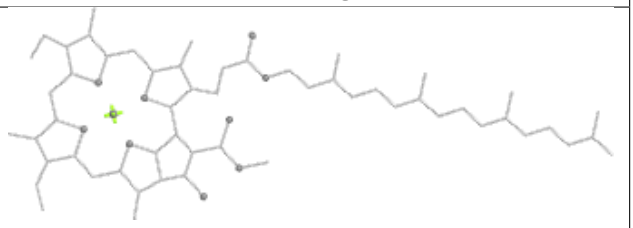
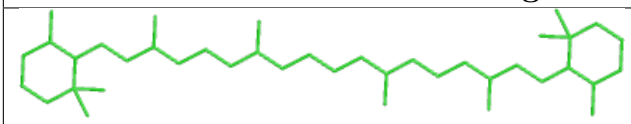


Rings

Ligand BCR A 852



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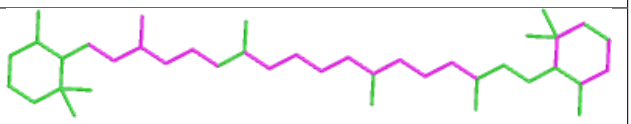
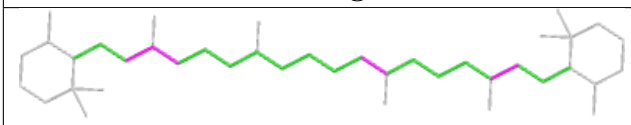


Bond angles



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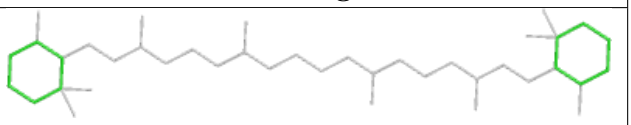
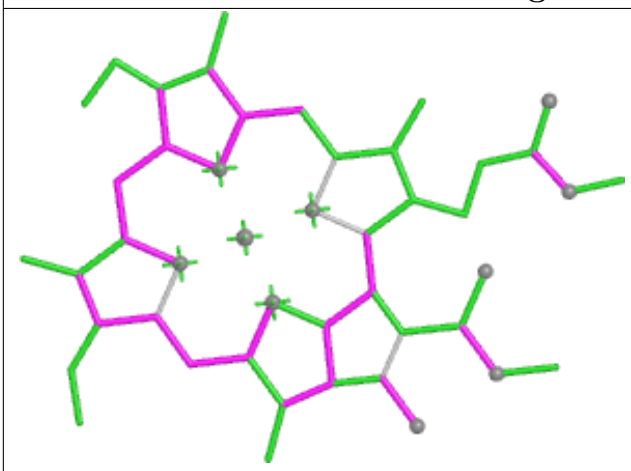


Rings

Ligand CLA 5 617



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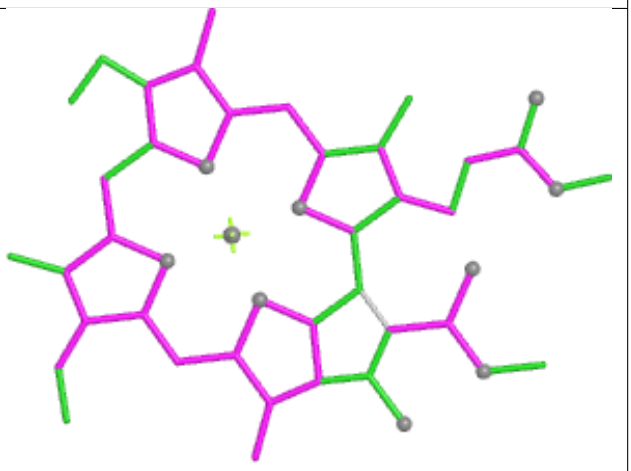
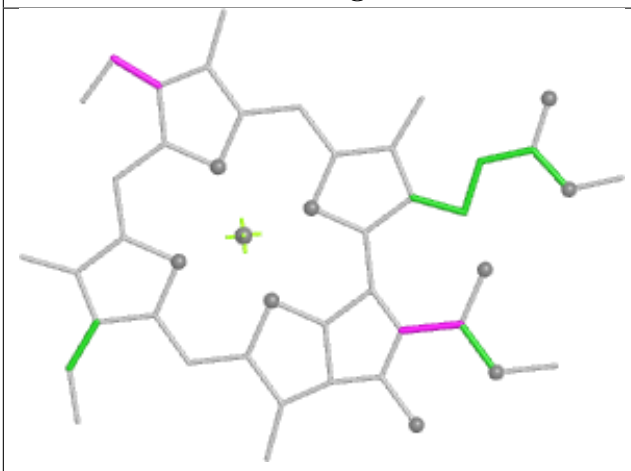


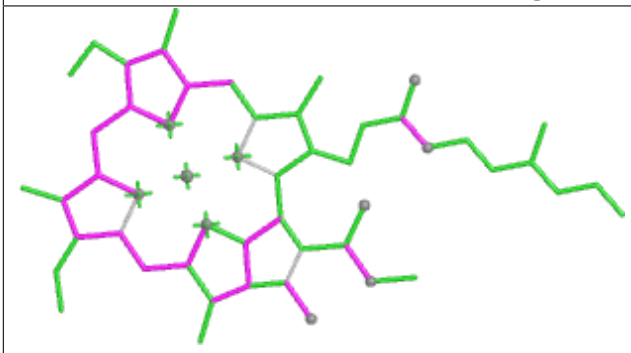
Bond angles



Torsions

Rings

Ligand CLA 8 612



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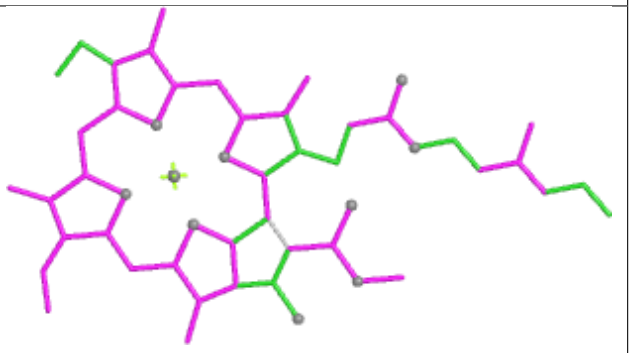

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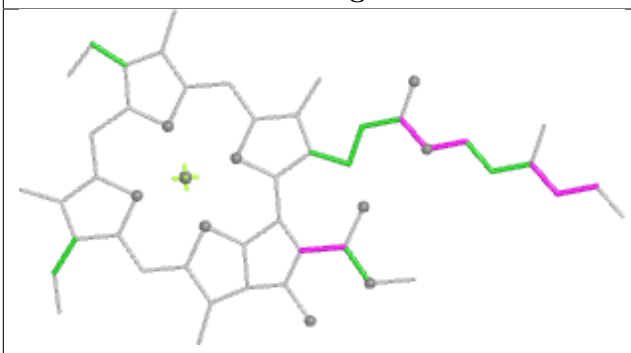

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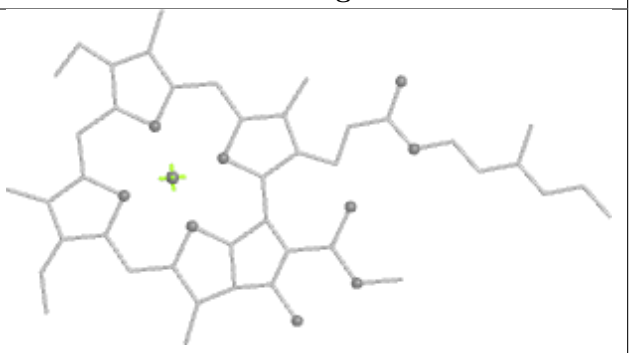
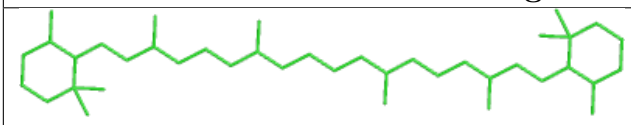


Rings

Ligand BCR L 201



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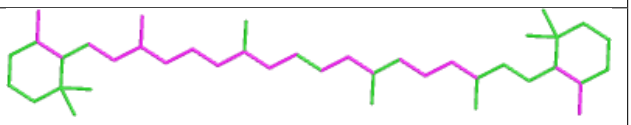
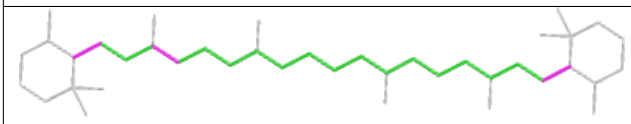


Bond angles



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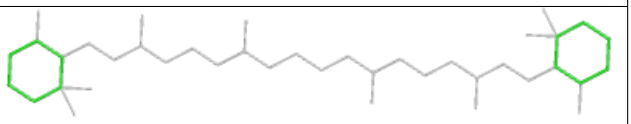
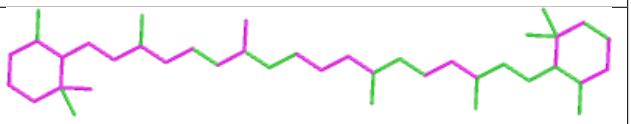


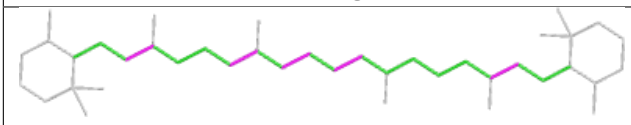
Rings

Ligand BCR K 4001

Bond lengths



Bond angles



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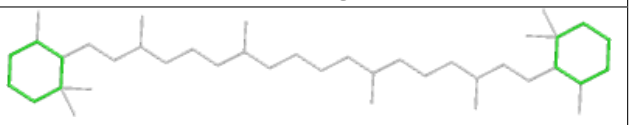
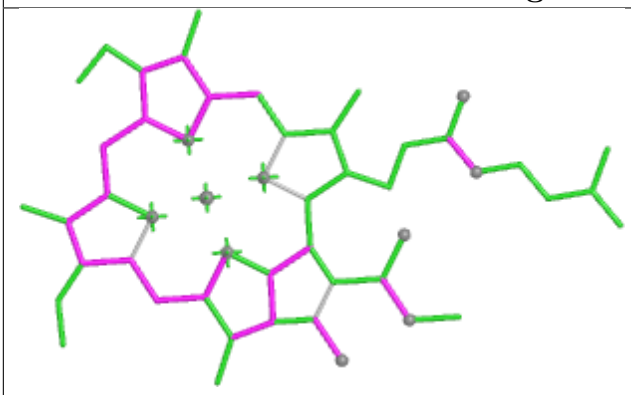


Rings

Ligand CLA L 204



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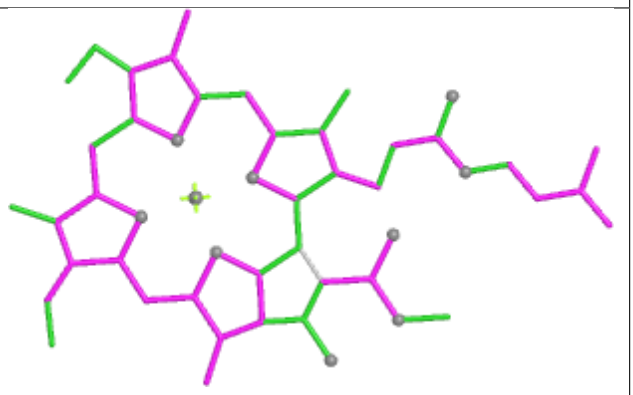
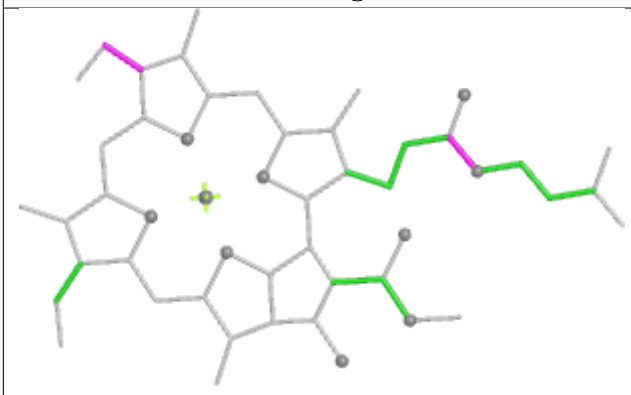


Bond angles



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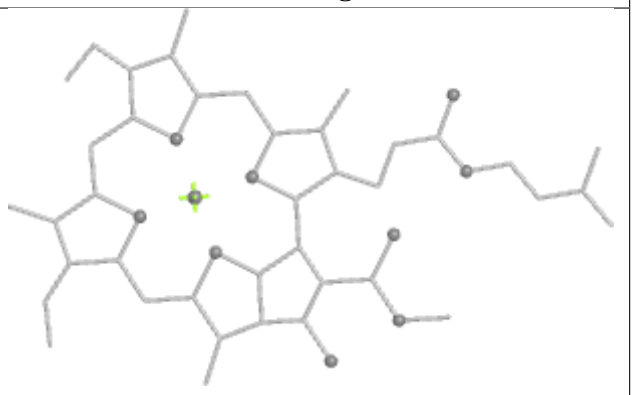
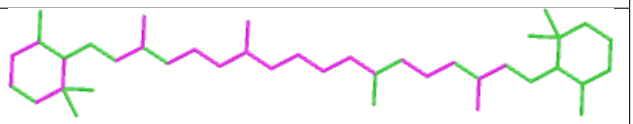


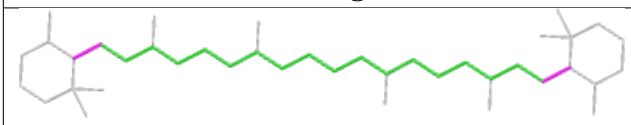
Rings

Ligand BCR B 848

Bond lengths



Bond angles



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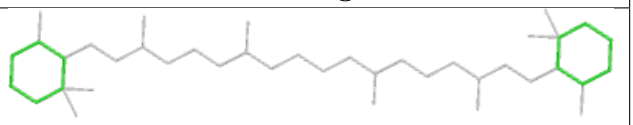
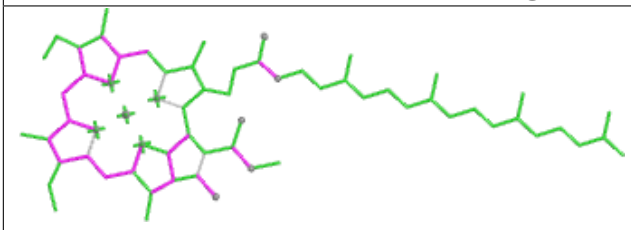


Rings

Ligand CLA A 810



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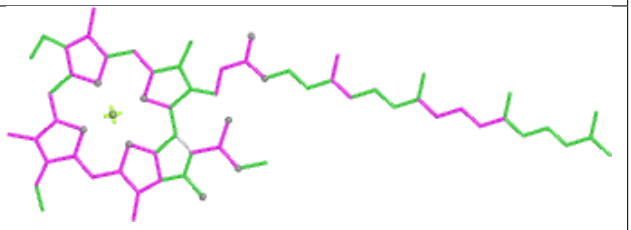

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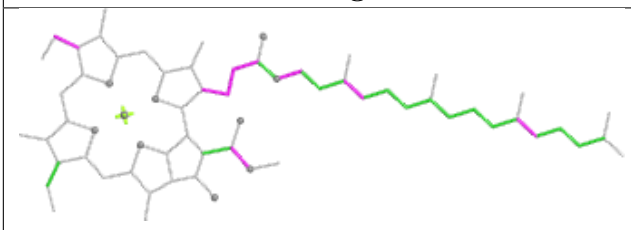

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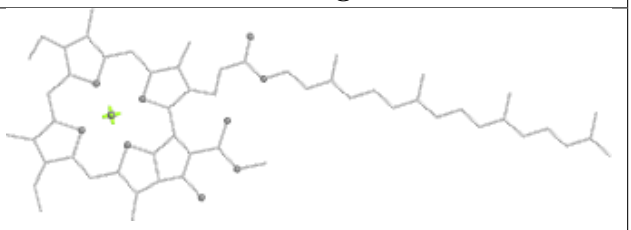
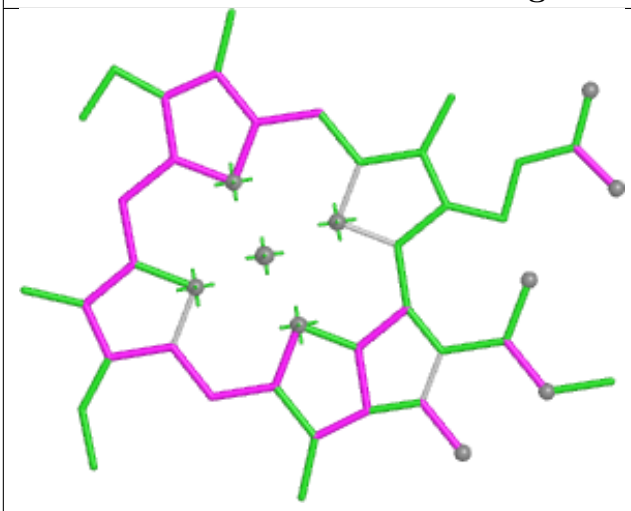


Rings

Ligand CLA 5 614



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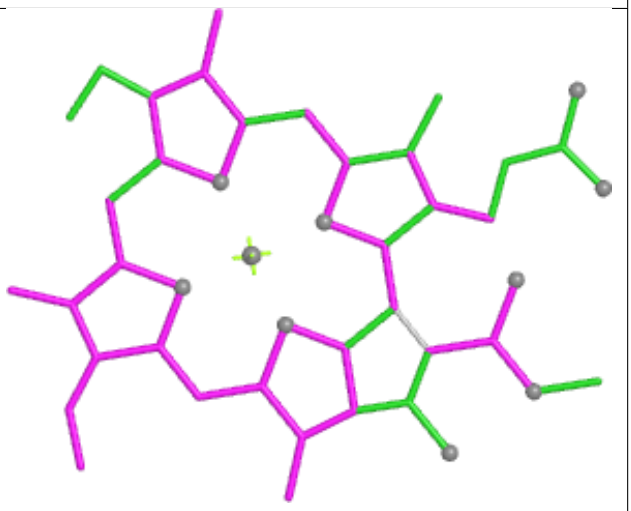

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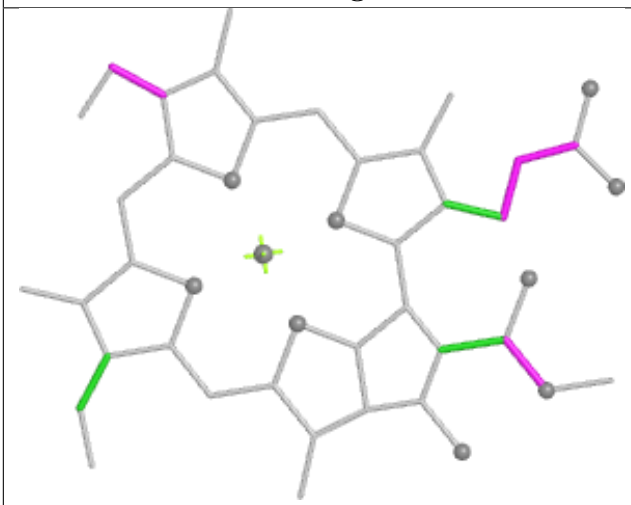

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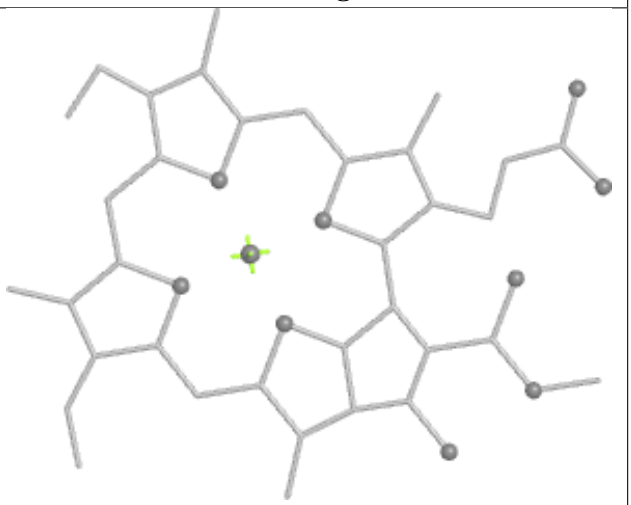
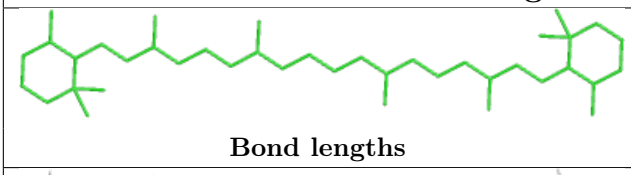
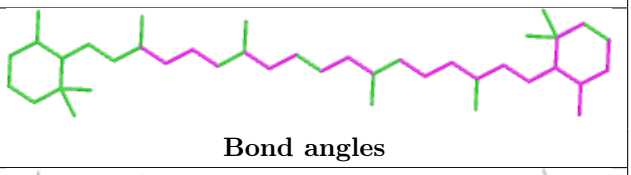


Rings

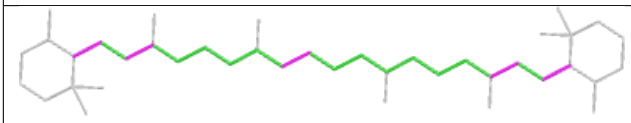
Ligand BCR L 205



Bond lengths



Bond angles



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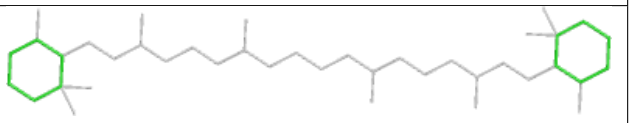
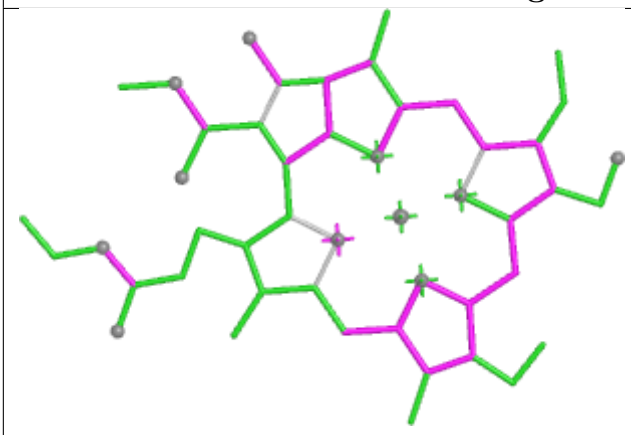


Rings

Ligand CHL 1 607



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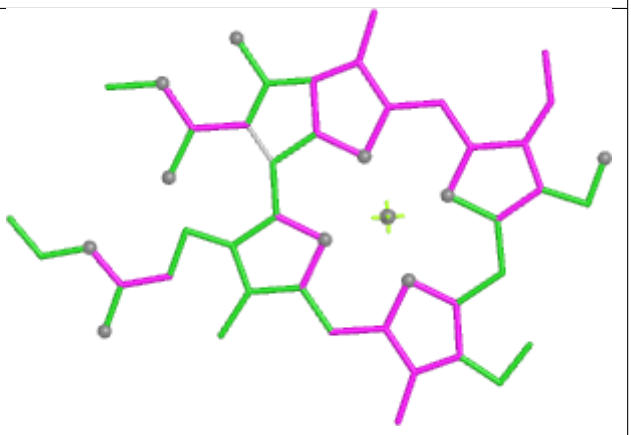
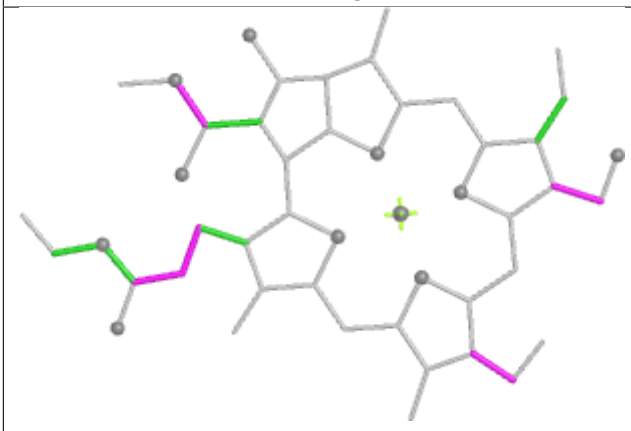
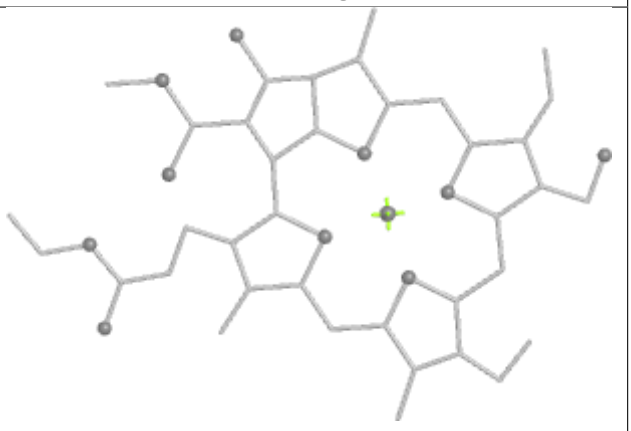


Bond angles

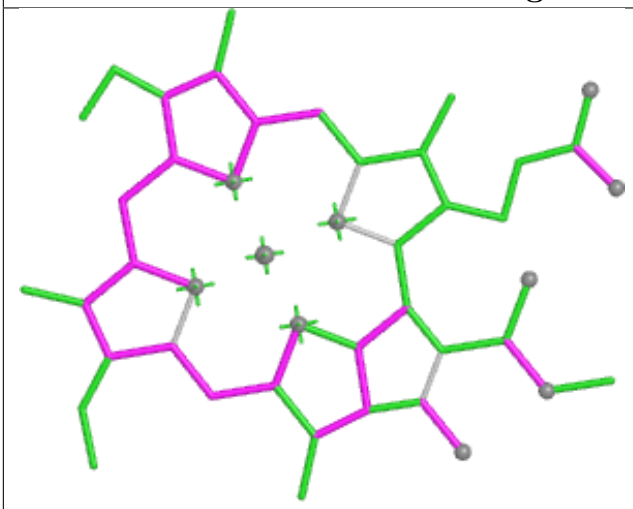


Torsions

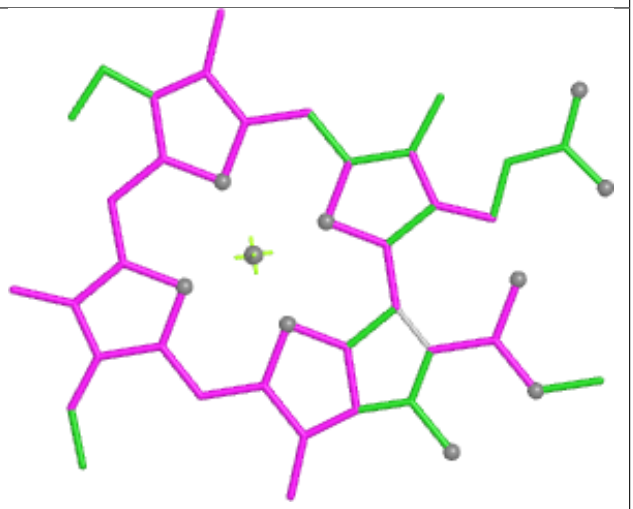


Rings

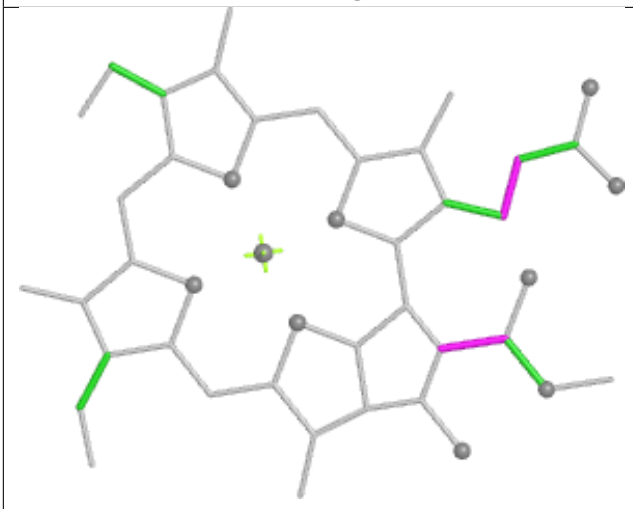
Ligand CLA F 303



Bond lengths



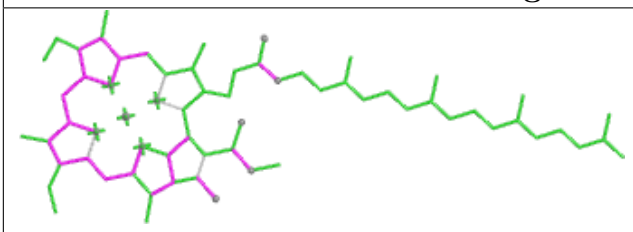
Bond angles



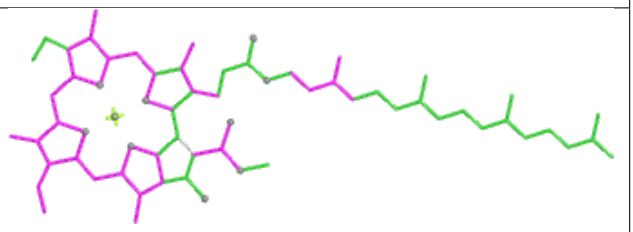
Torsions

Rings

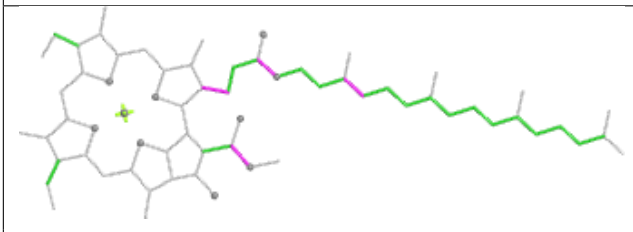
Ligand CLA A 811



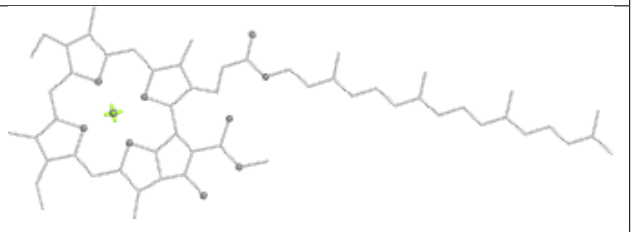
Bond lengths



Bond angles

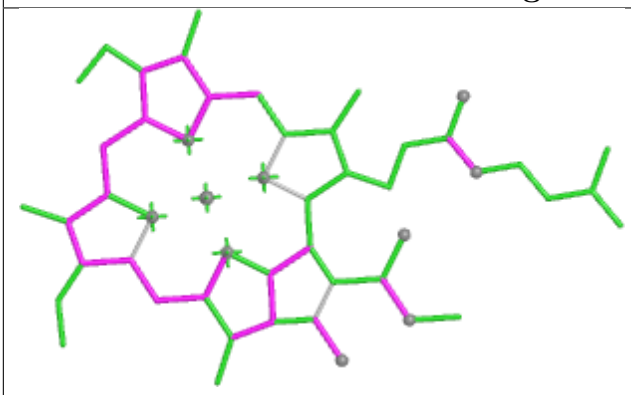


Torsions

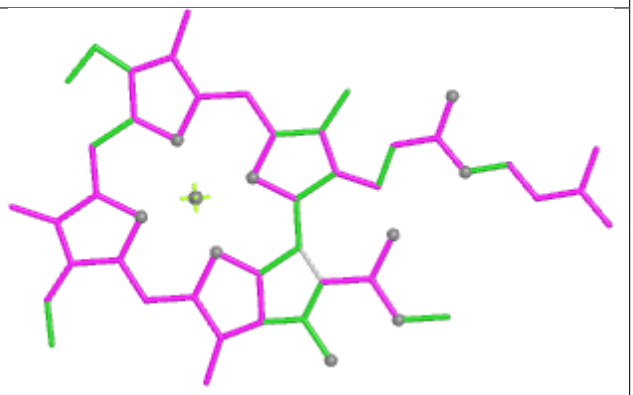


Rings

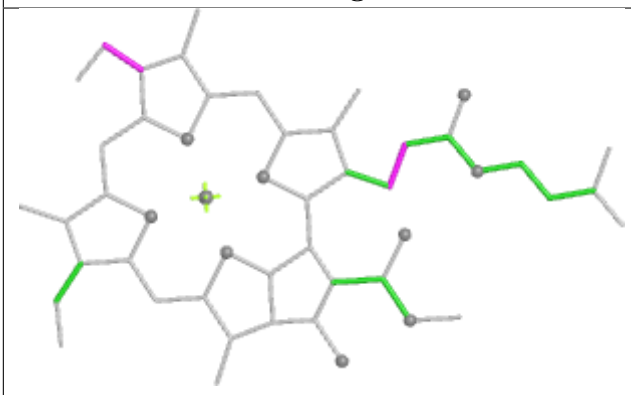
Ligand CLA G 203



Bond lengths



Bond angles



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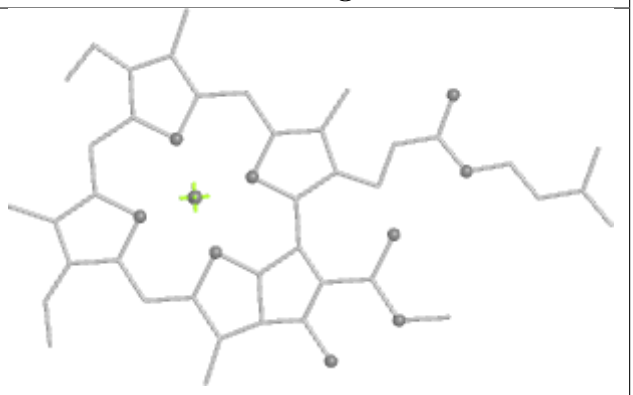
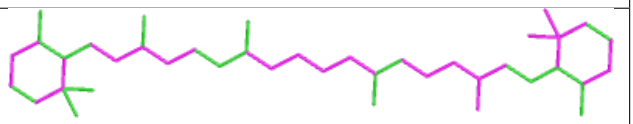


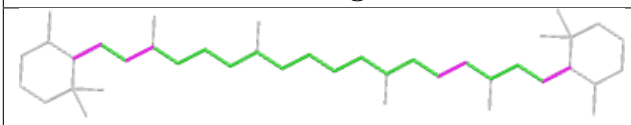
Rings

Ligand BCR B 846

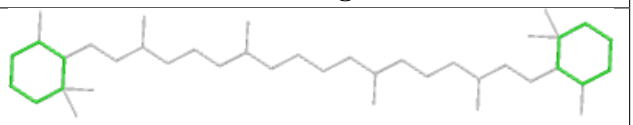
Bond lengths



Bond angles

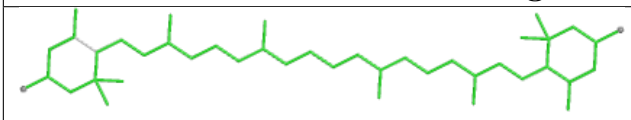


Torsions



Rings

Ligand LUT Z 618



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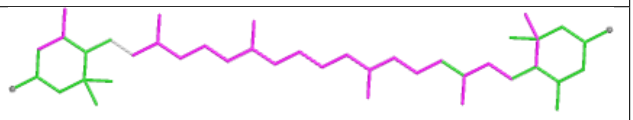
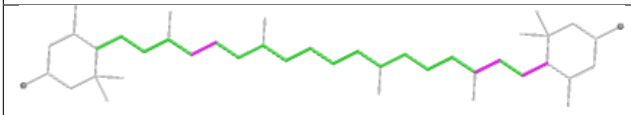


Bond angles



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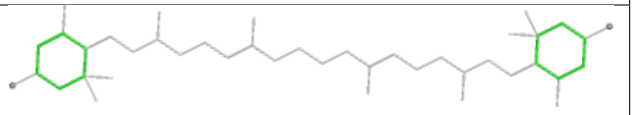
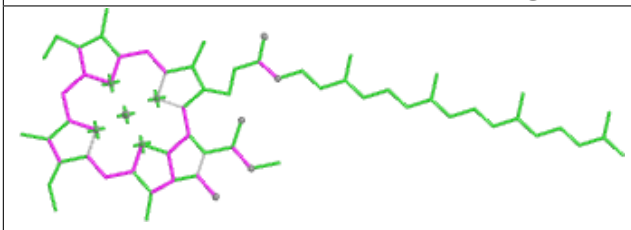


Rings

Ligand CLA B 803



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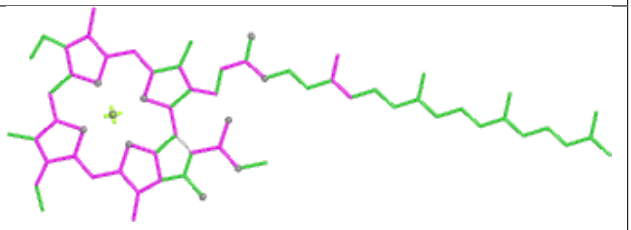
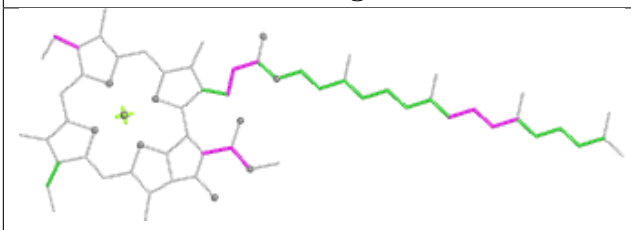


Bond angles



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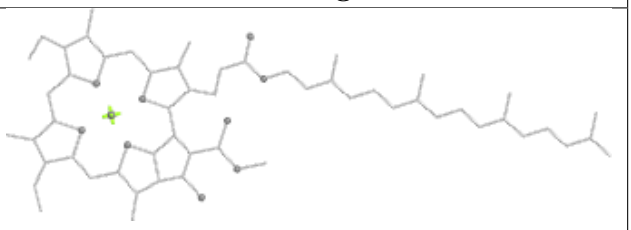
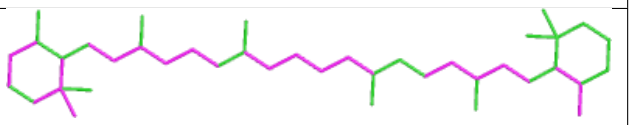


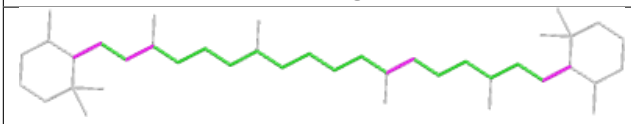
Rings

Ligand BCR J 3003

Bond lengths



Bond angles



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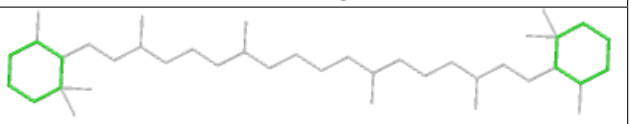
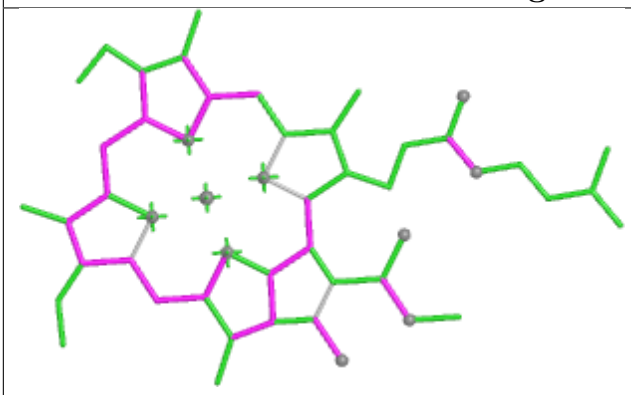
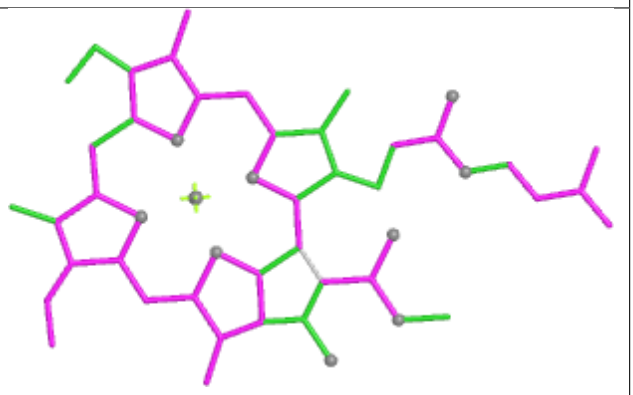


Rings

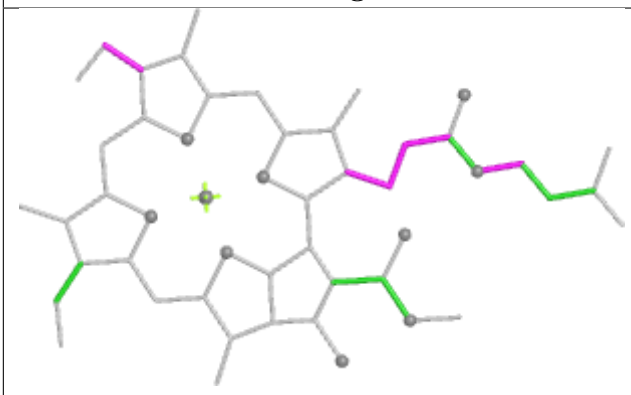
Ligand CLA 5 609



Bond lengths



Bond angles



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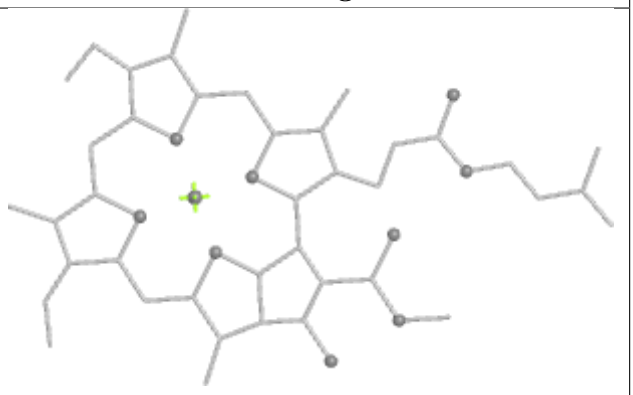
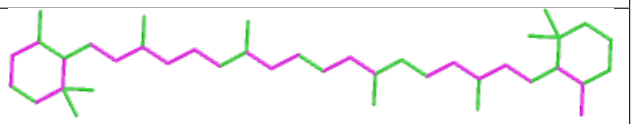


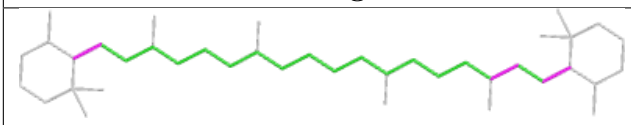
Rings

Ligand BCR K 4004

Bond lengths



Bond angles



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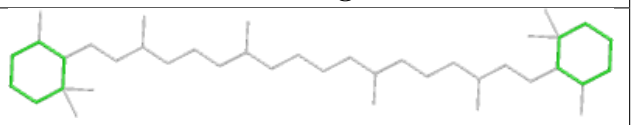
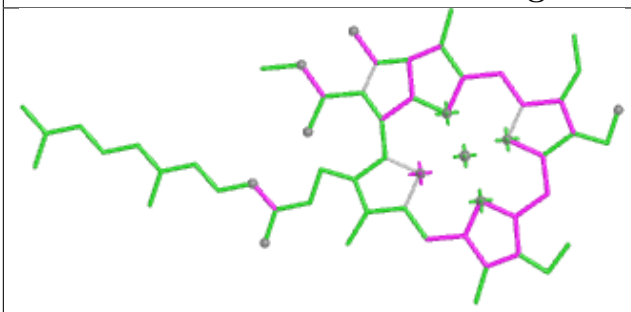


Rings

Ligand CHL 8 607



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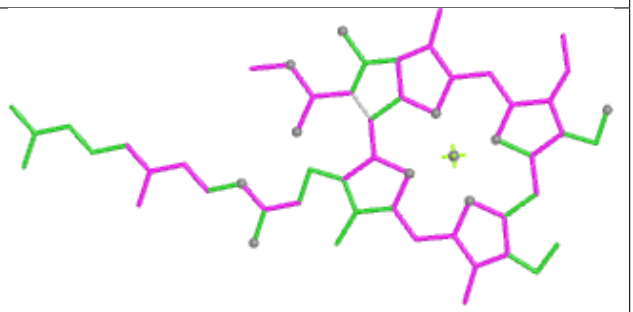
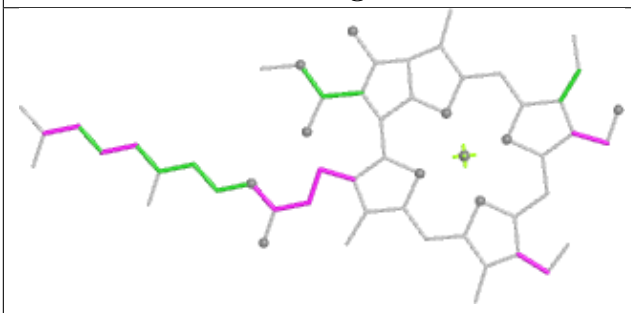


Bond angles



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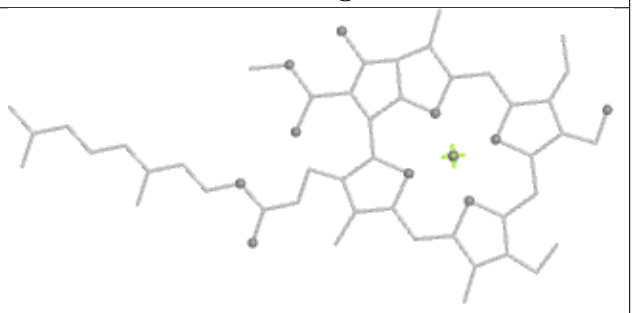
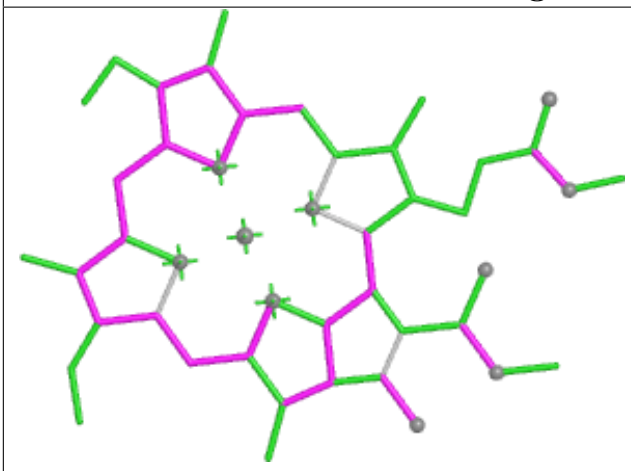


Rings

Ligand CLA 8 611



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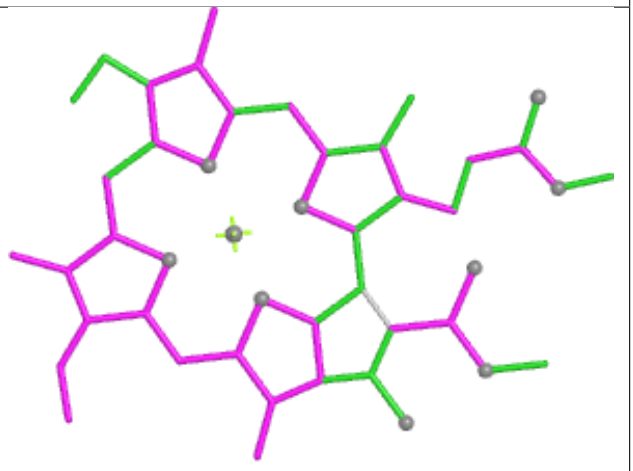
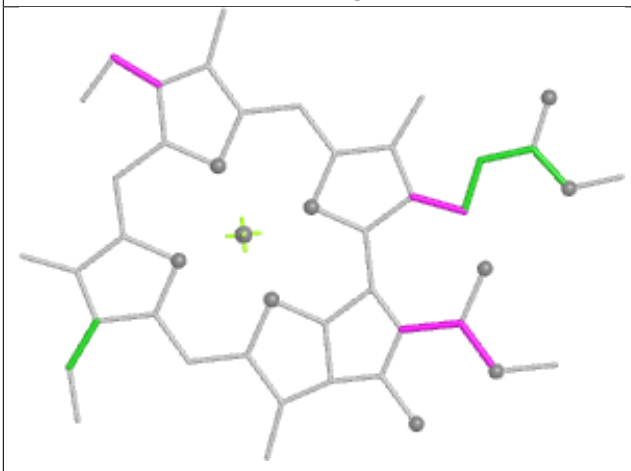


Bond angles



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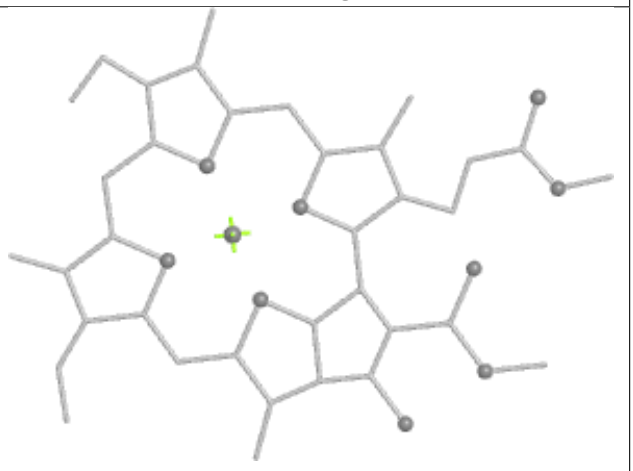
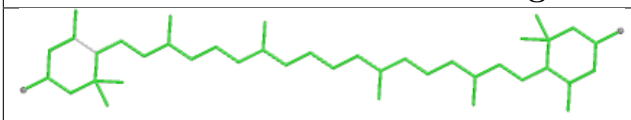
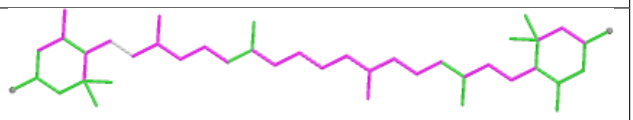


Rings

Ligand LUT 5 620



Bond lengths



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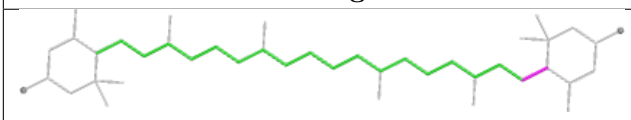

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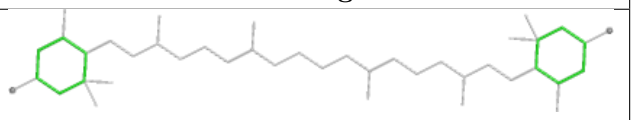
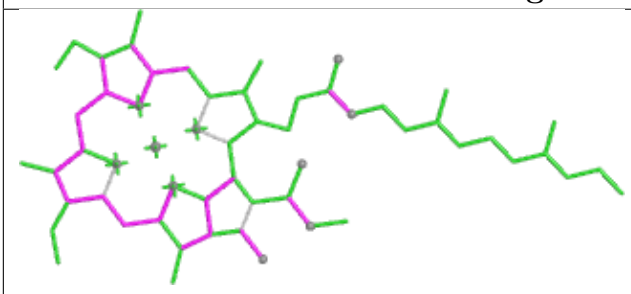


Rings

Ligand CLA Z 604



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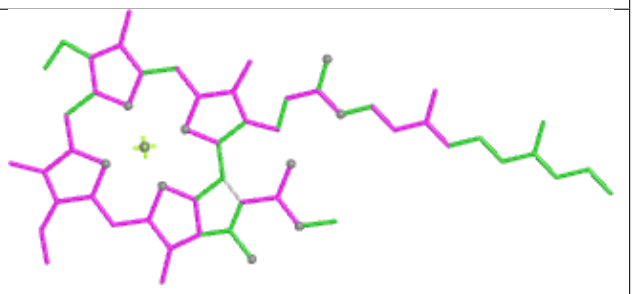
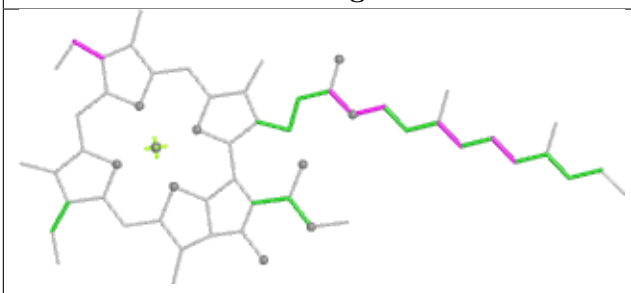


Bond angles



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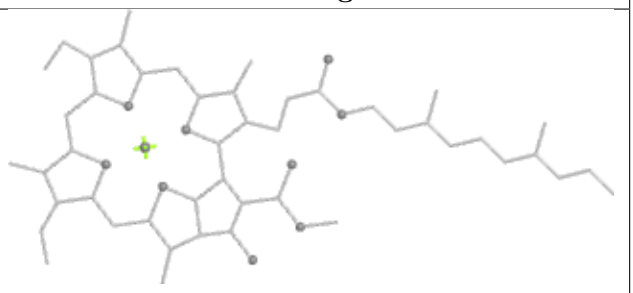
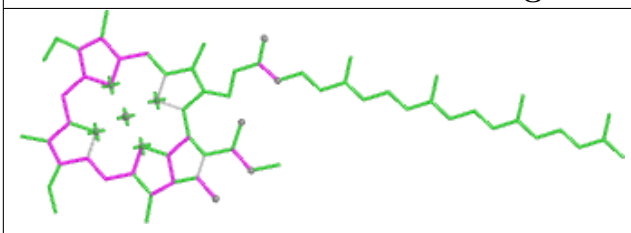


Rings

Ligand CLA B 852



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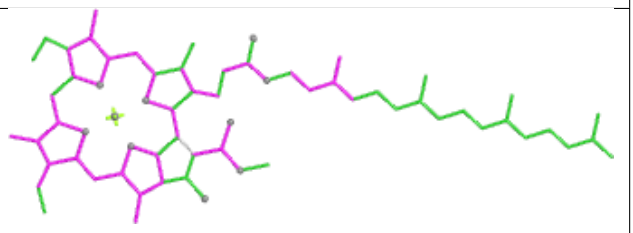
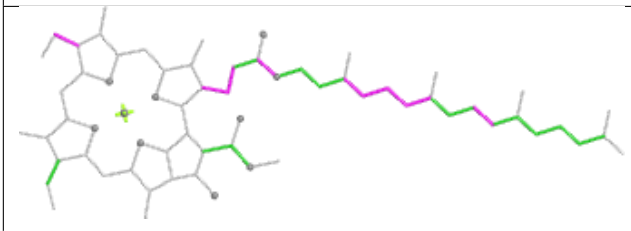


Bond angles



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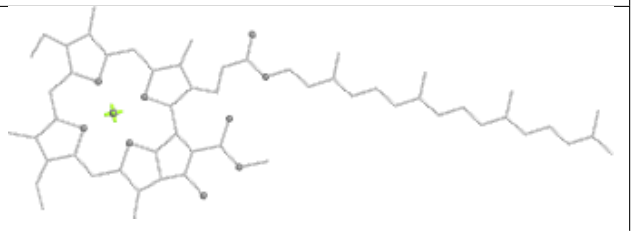
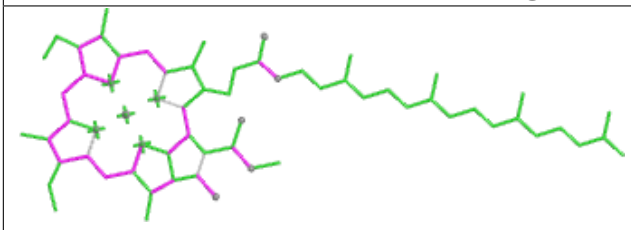
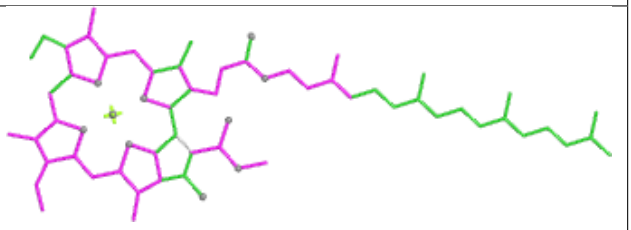


Rings

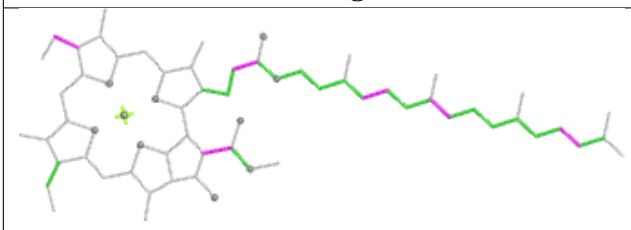
Ligand CLA A 802



Bond lengths



Bond angles



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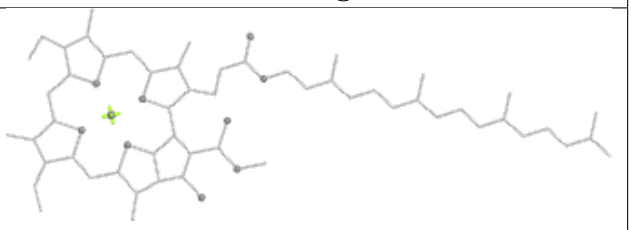
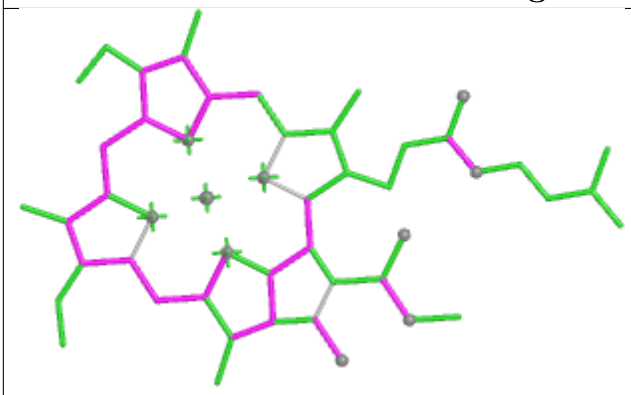
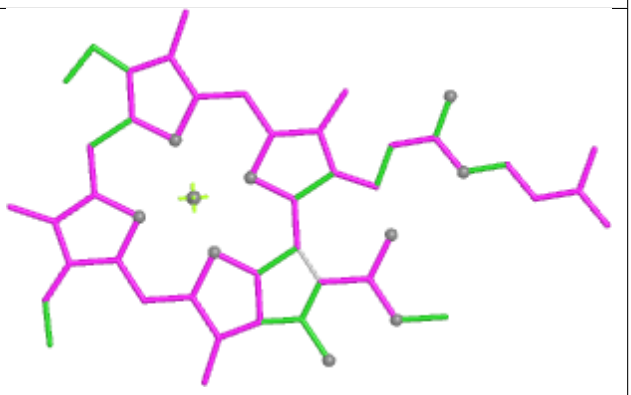


Rings

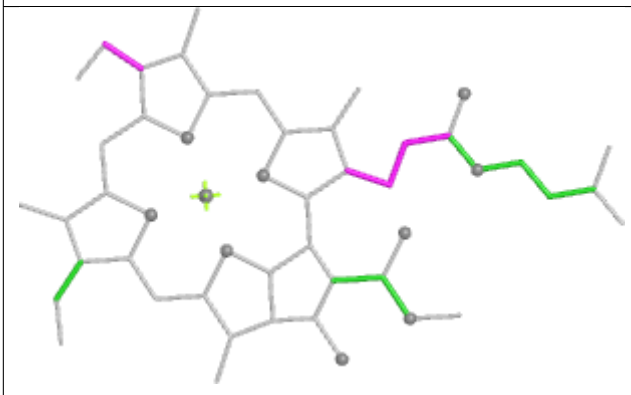
Ligand CLA 7 609



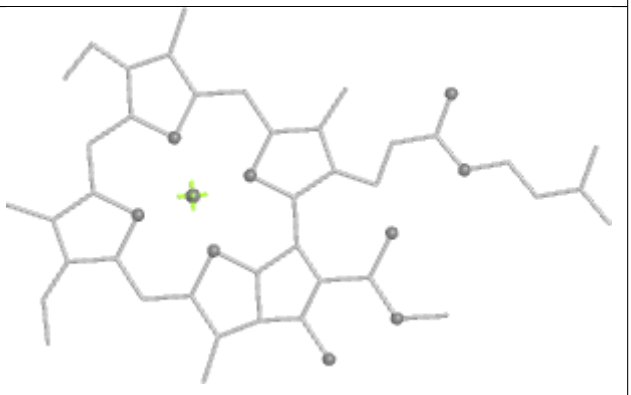
Bond lengths



Bond angles

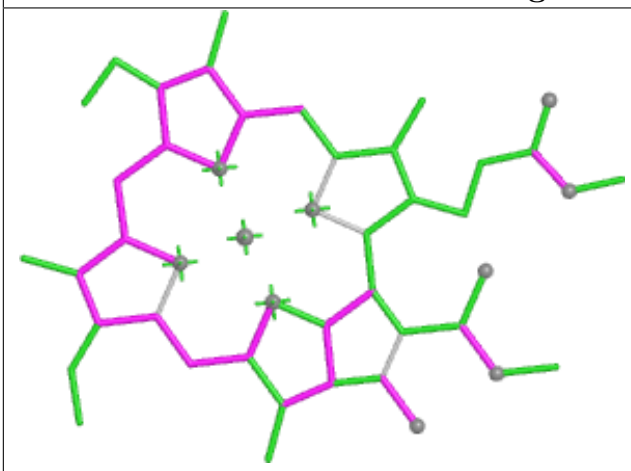


Torsions

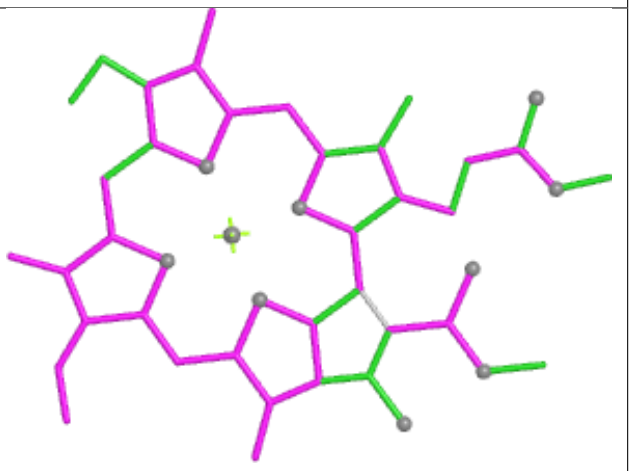


Rings

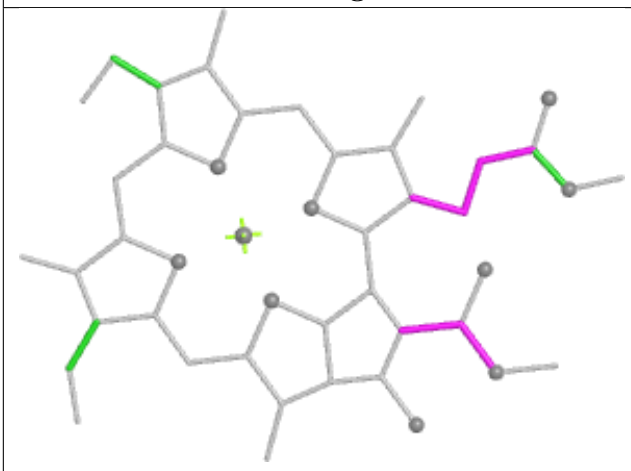
Ligand CLA 5 616



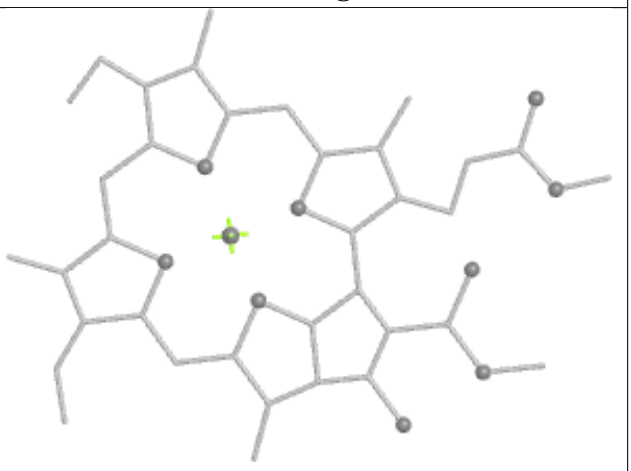
Bond lengths



Bond angles

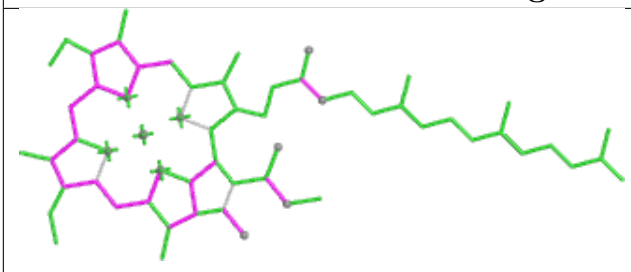


Torsions



Rings

Ligand CLA 5 610



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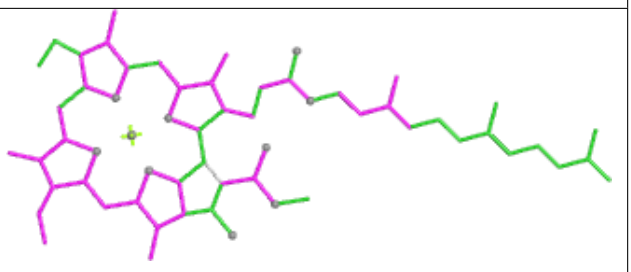
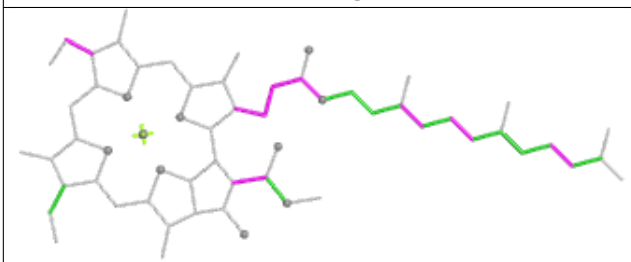


Bond angles



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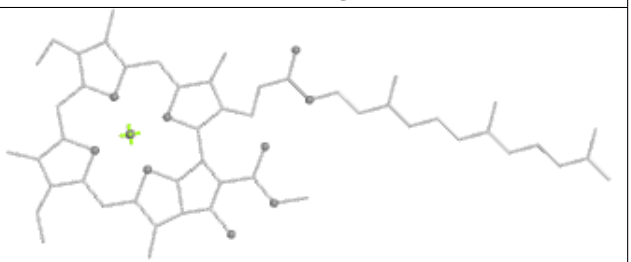
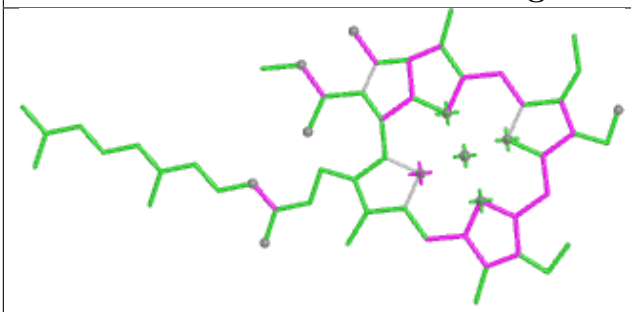


Rings

Ligand CHL 6 606



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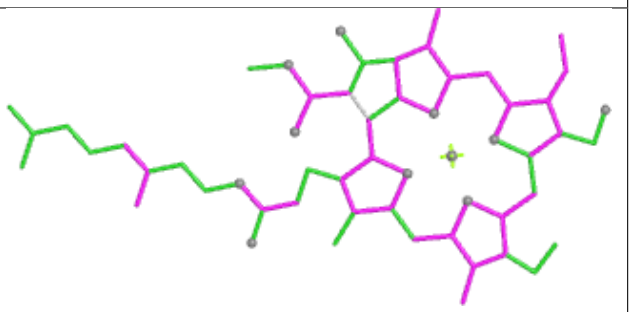
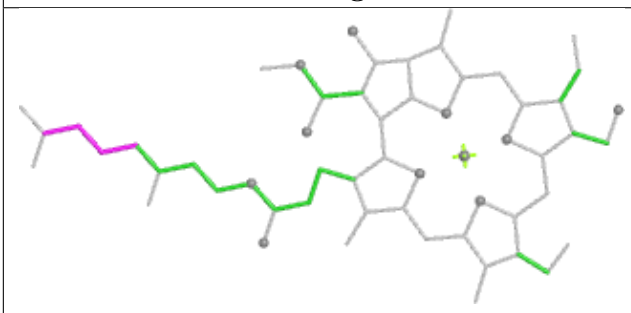


Bond angles



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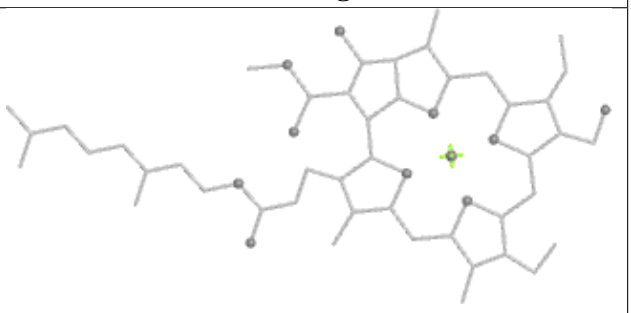
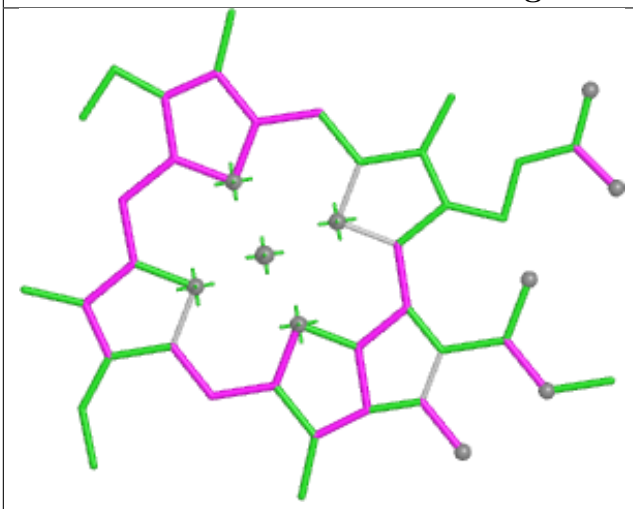


Rings

Ligand CLA B 804



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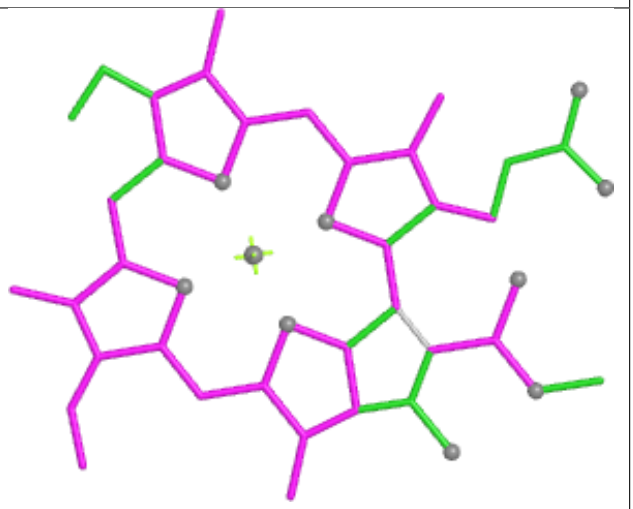
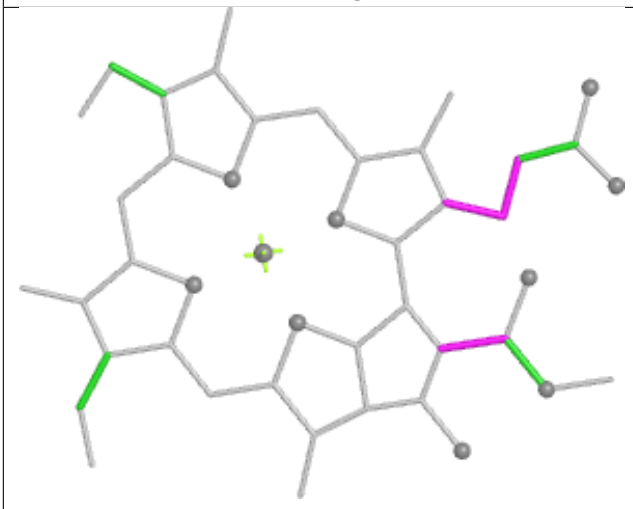


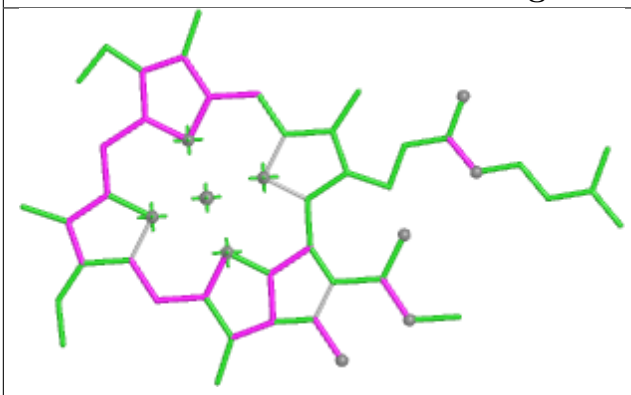
Bond angles



Torsions

Rings

Ligand CLA 8 608



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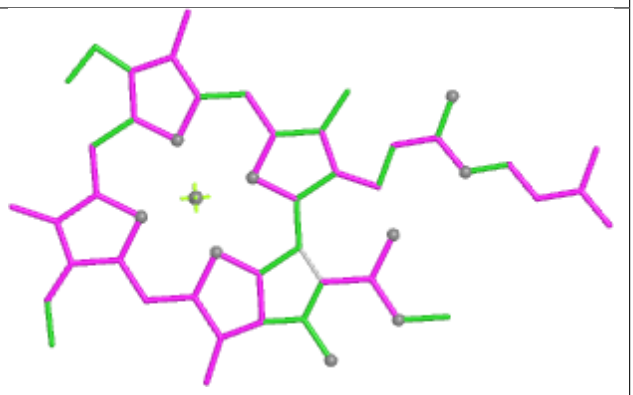

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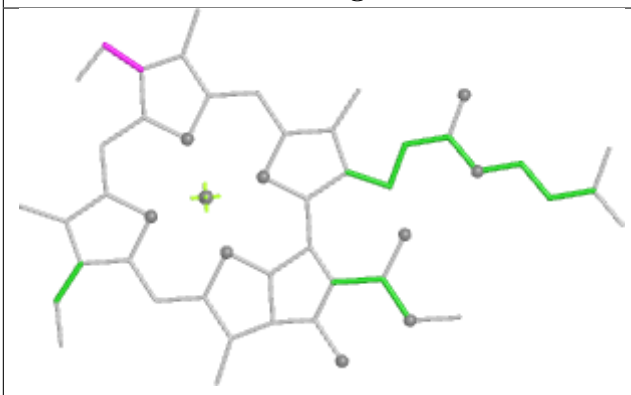

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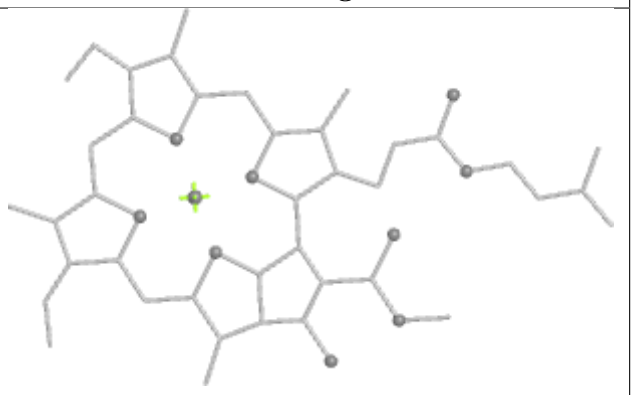
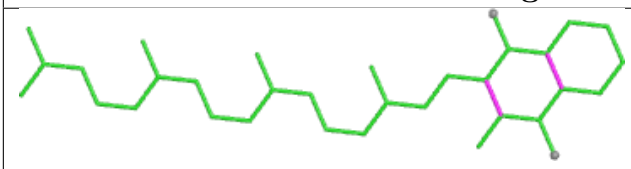


Rings

Ligand PQN A 844



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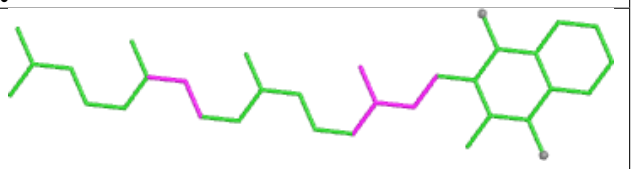

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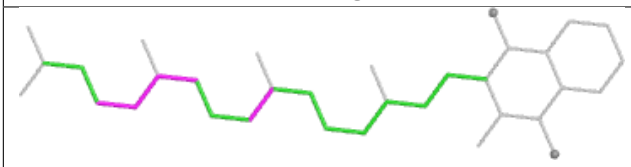

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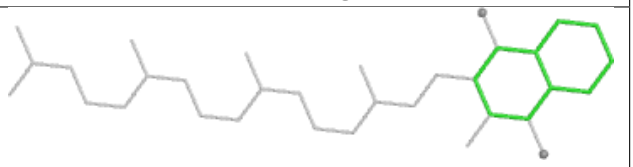
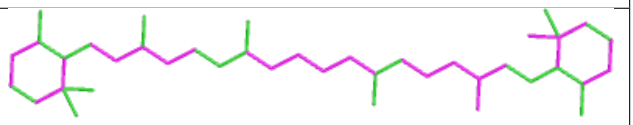


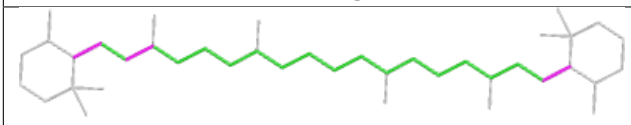
Rings

Ligand BCR 7 624

Bond lengths



Bond angles



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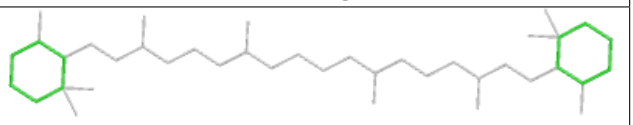
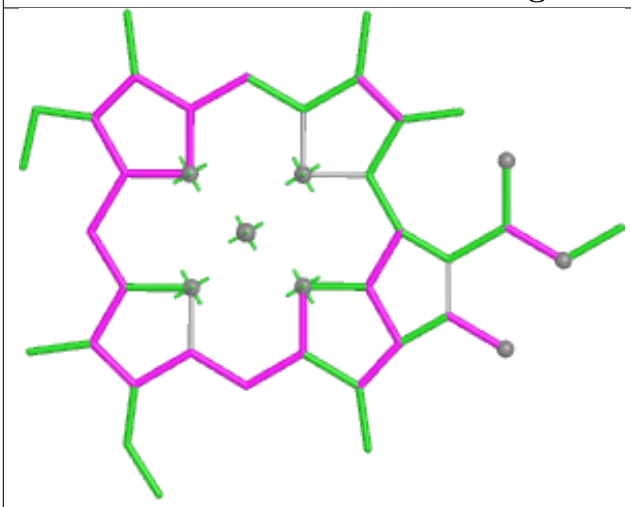


Rings

Ligand CLA 3 611



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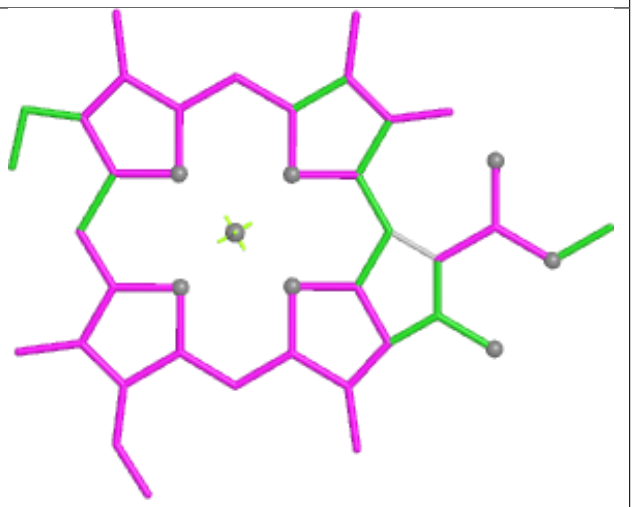
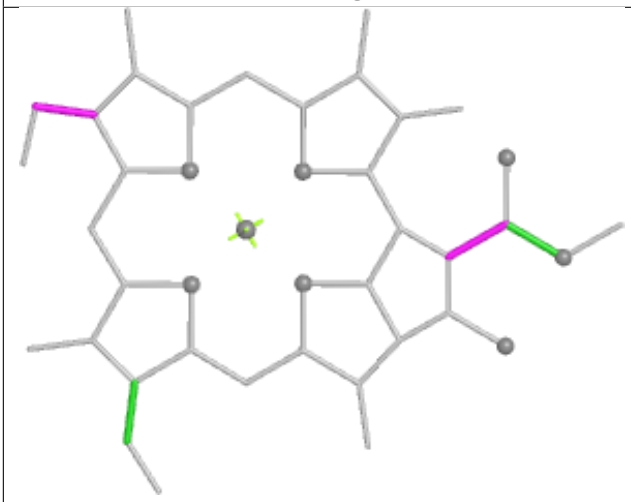


Bond angles



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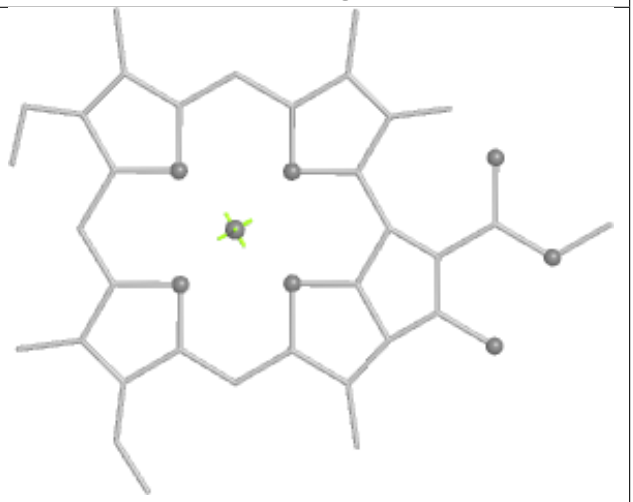
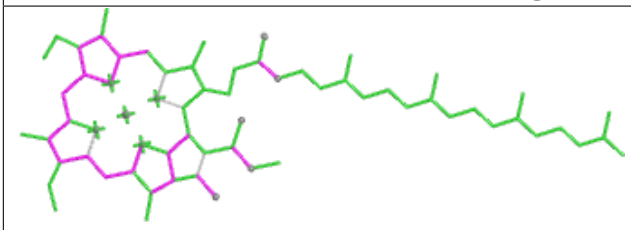


Rings

Ligand CLA 8 613



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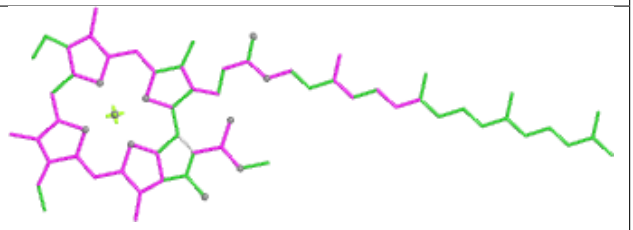
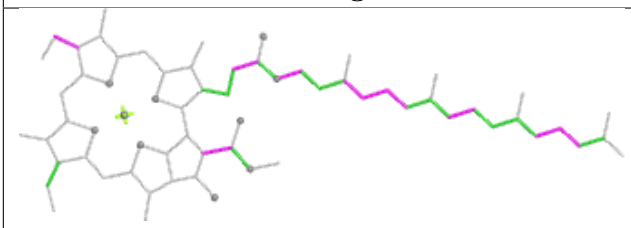
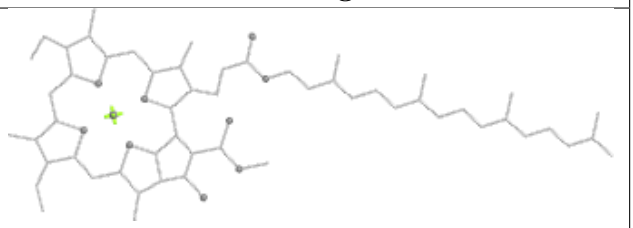


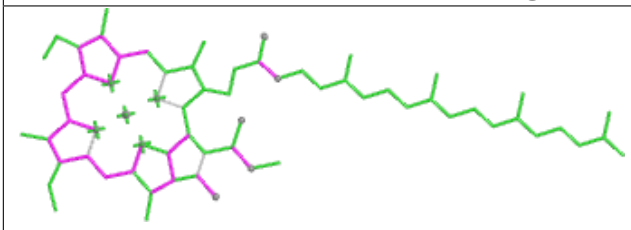
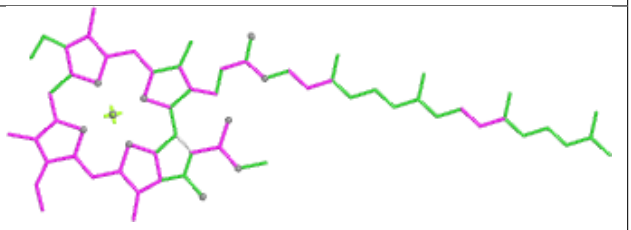
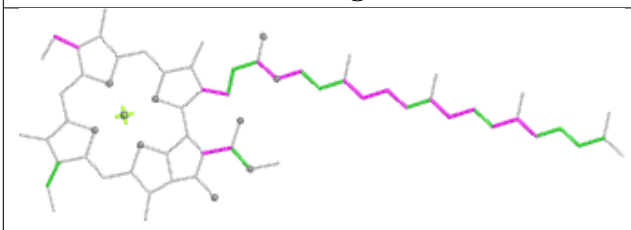
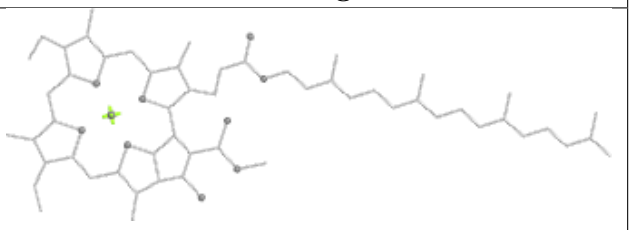
Bond angles

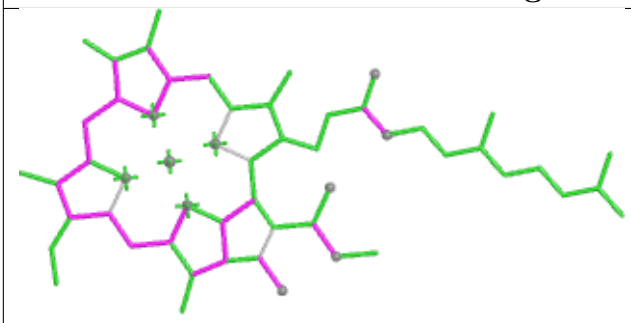
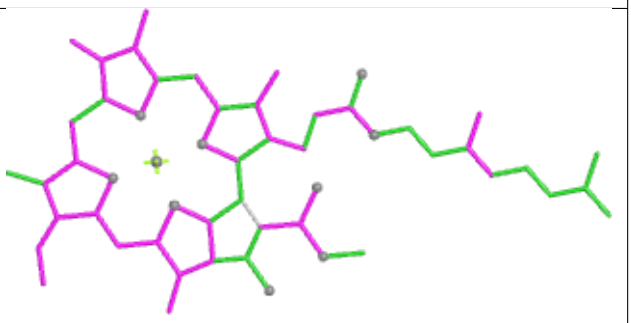
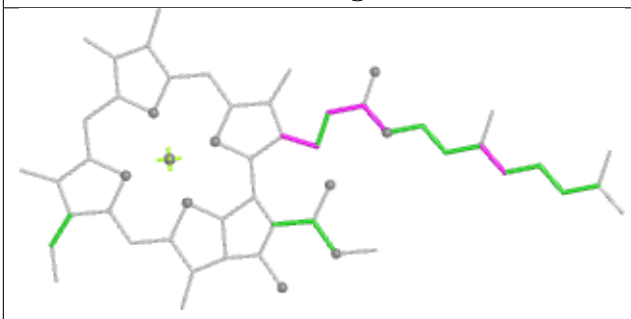
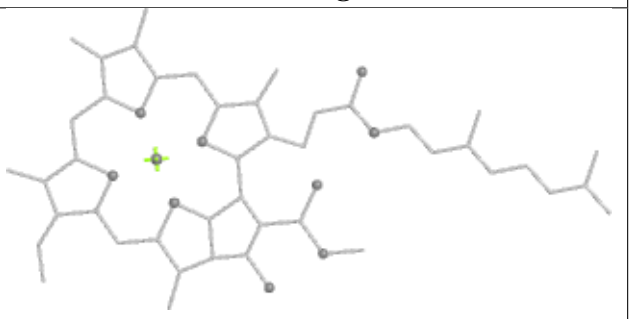


Torsions

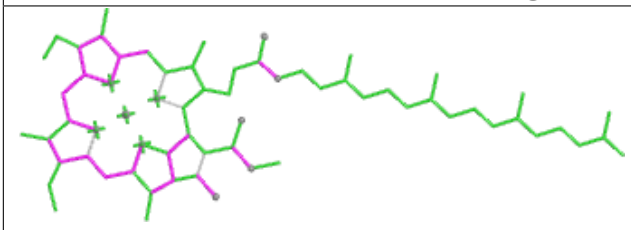


Rings

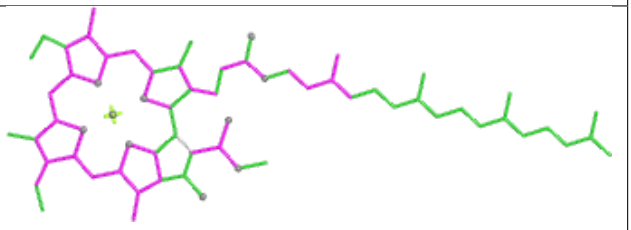
Ligand CLA A 807	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA B 811	
 Bond lengths	 Bond angles
 Torsions	 Rings

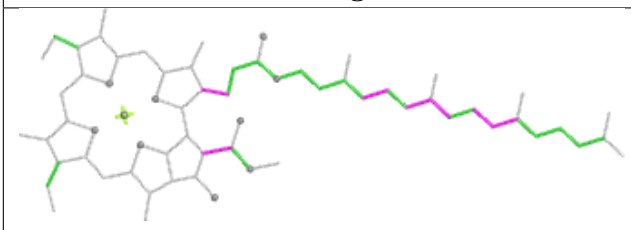
Ligand CLA B 826



Bond lengths



Bond angles



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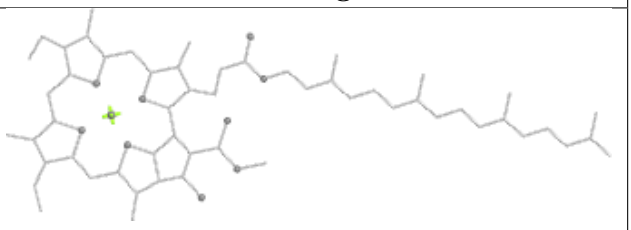
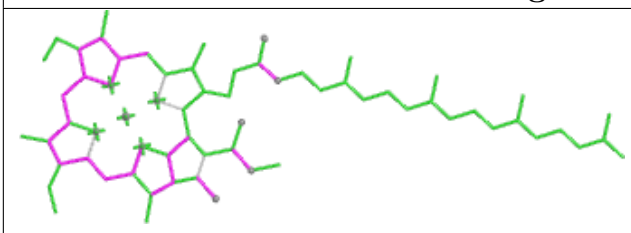


Rings

Ligand CLA 1 611



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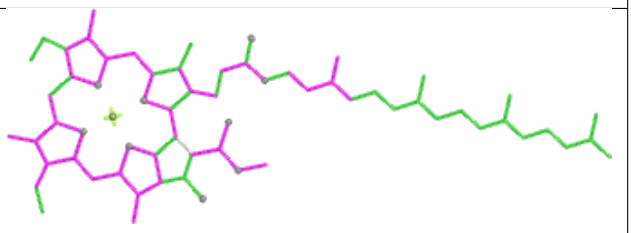
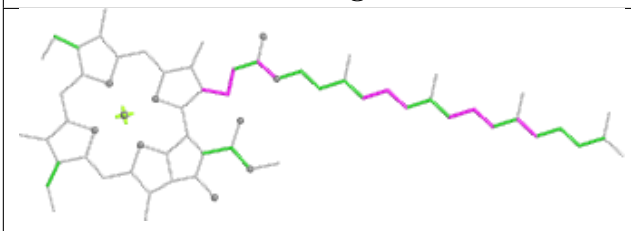


Bond angles



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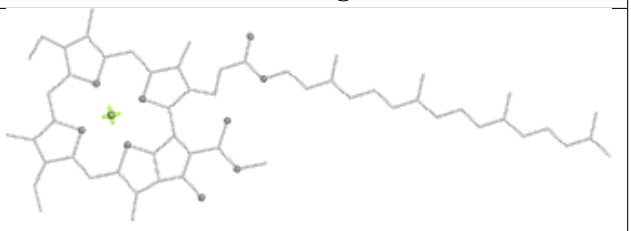
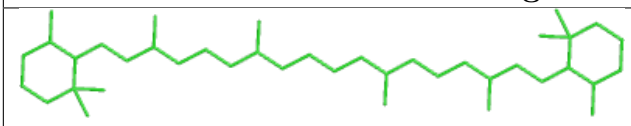


Rings

Ligand BCR B 801



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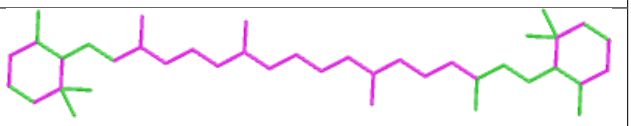
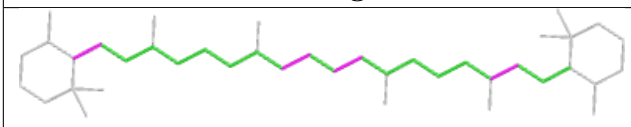


Bond angles



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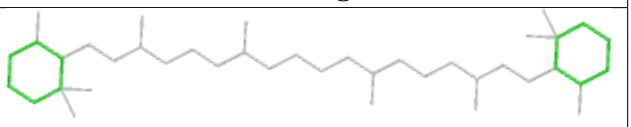
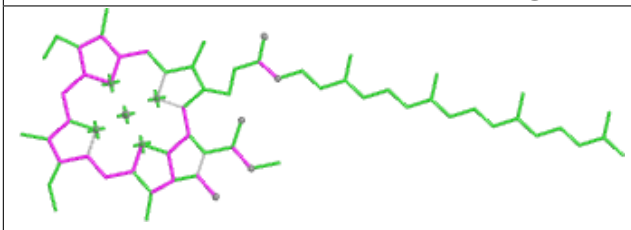
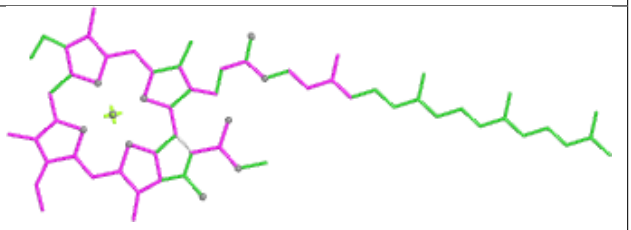


Rings

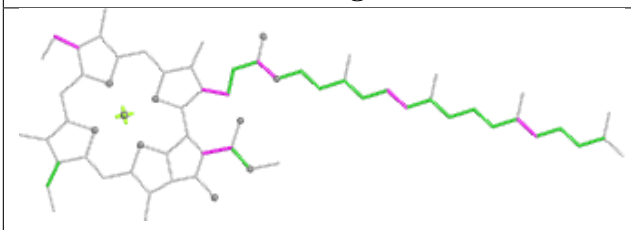
Ligand CLA F 304



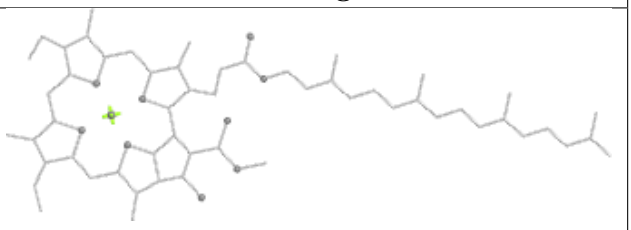
Bond lengths



Bond angles

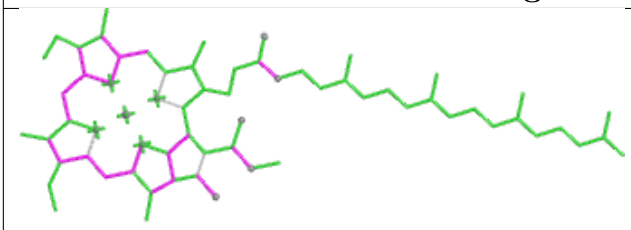


Torsions



Rings

Ligand CLA A 831



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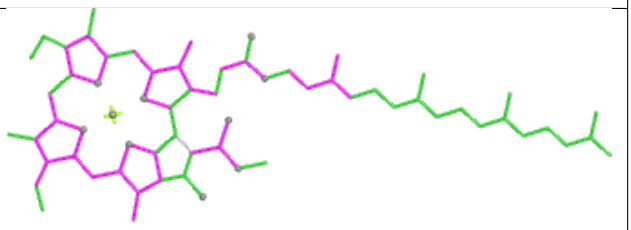
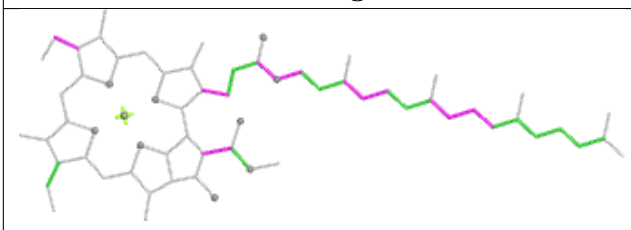
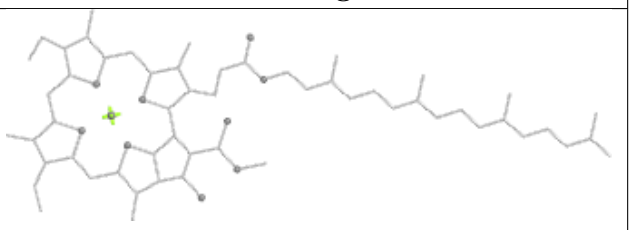


Bond angles

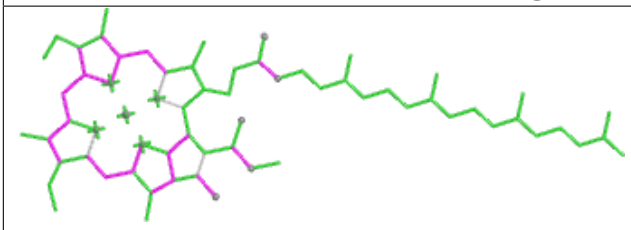


Torsions



Rings

Ligand CLA 5 602



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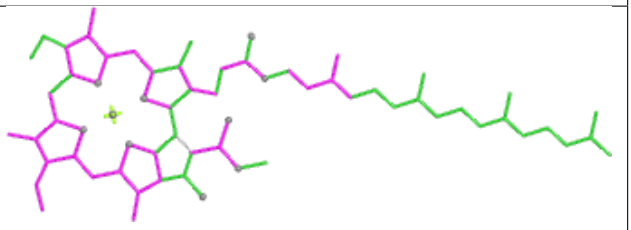
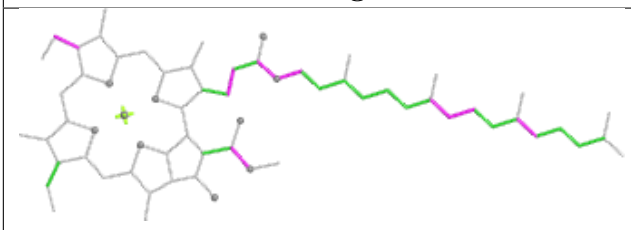


Bond angles



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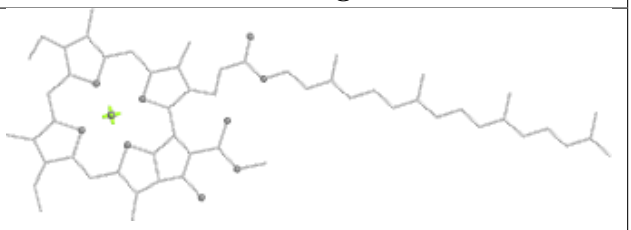
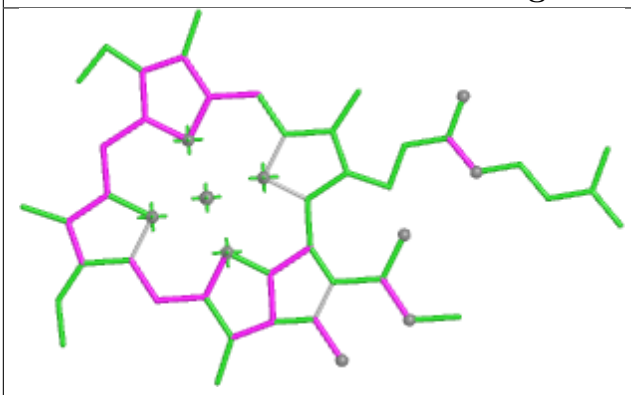


Rings

Ligand CLA 7 608



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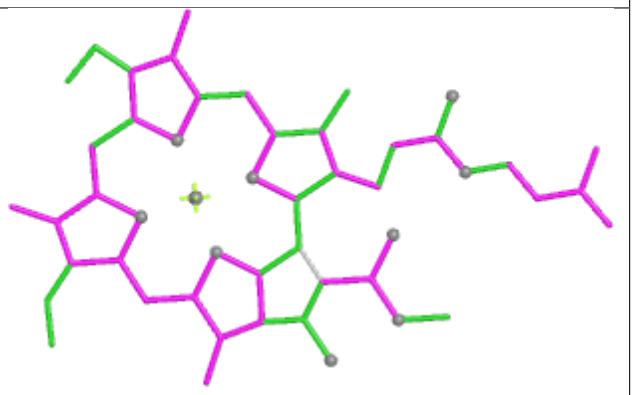

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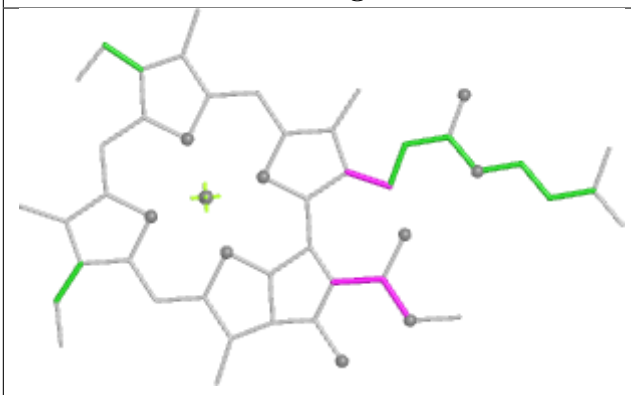

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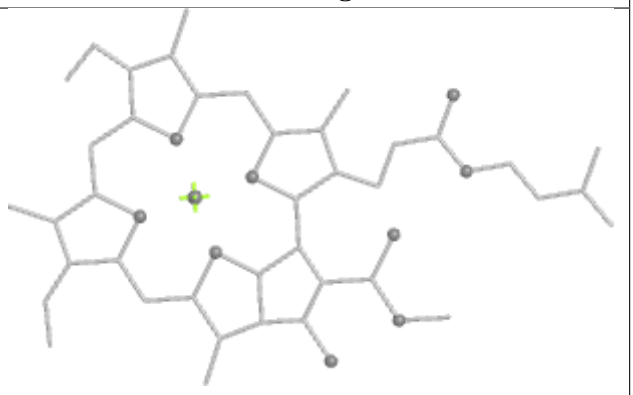
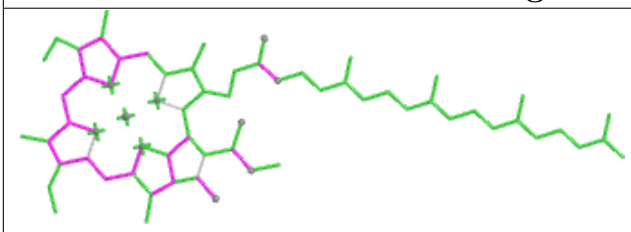


Rings

Ligand CLA Z 602



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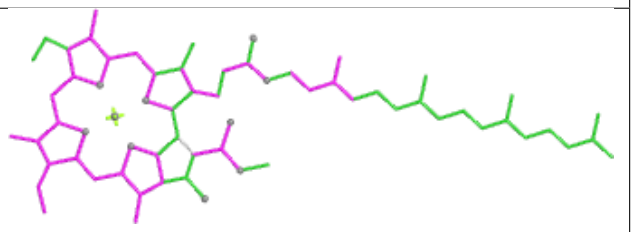
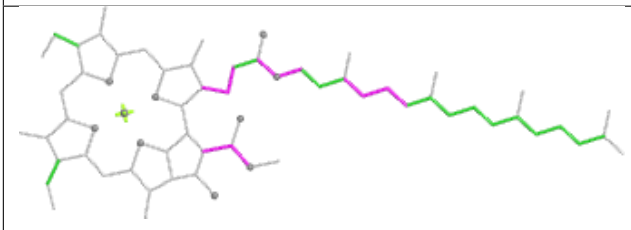


Bond angles



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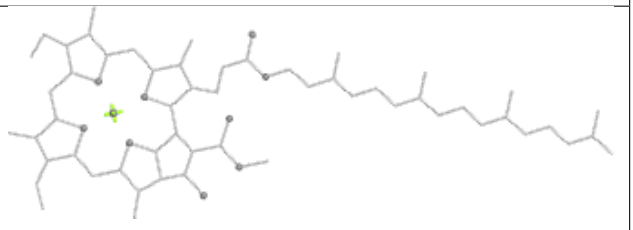
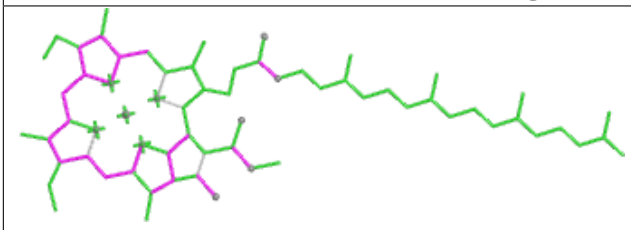


Rings

Ligand CLA B 841



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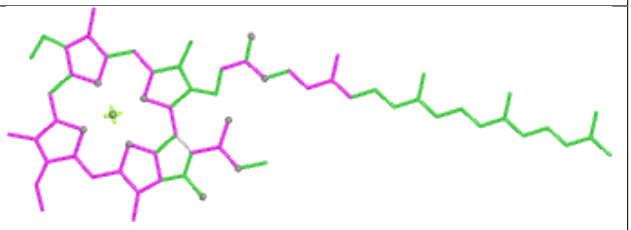
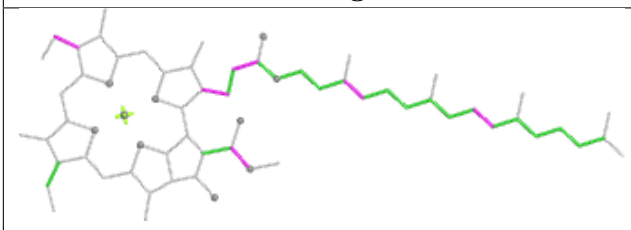


Bond angles



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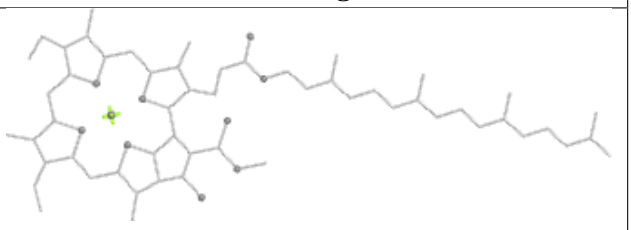
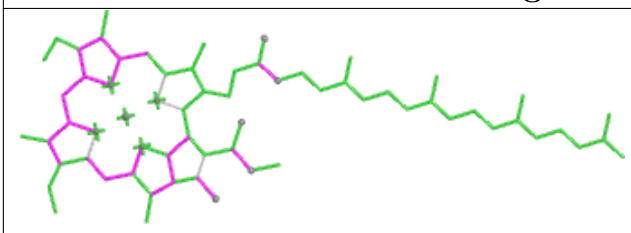


Rings

Ligand CLA A 814



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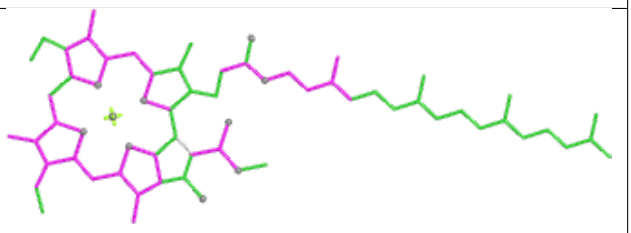
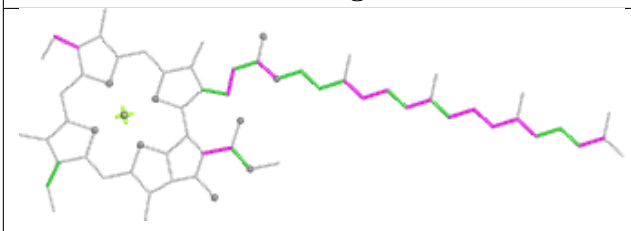


Bond angles



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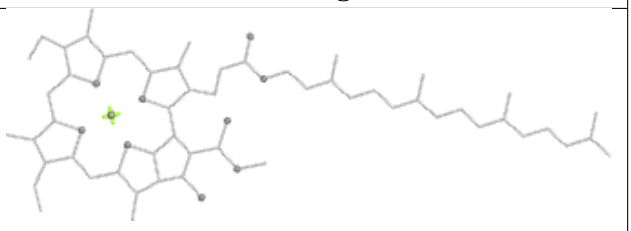
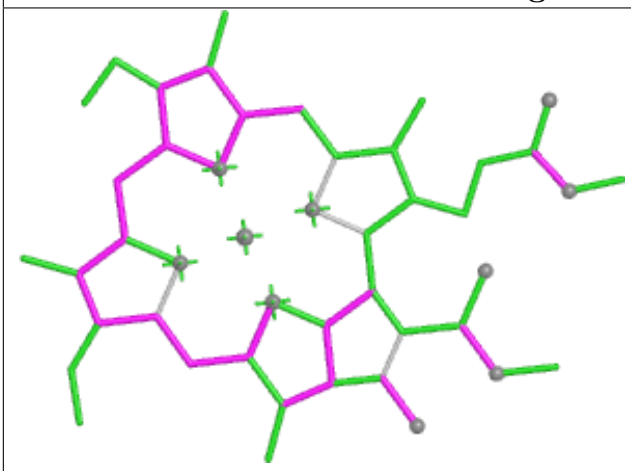


Rings

Ligand CLA 6 603



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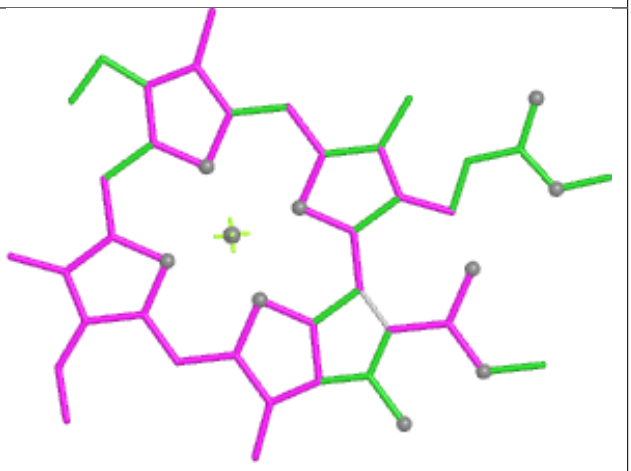
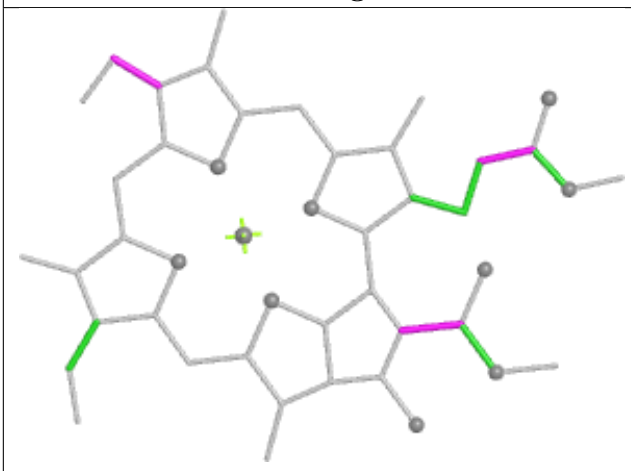


Bond angles



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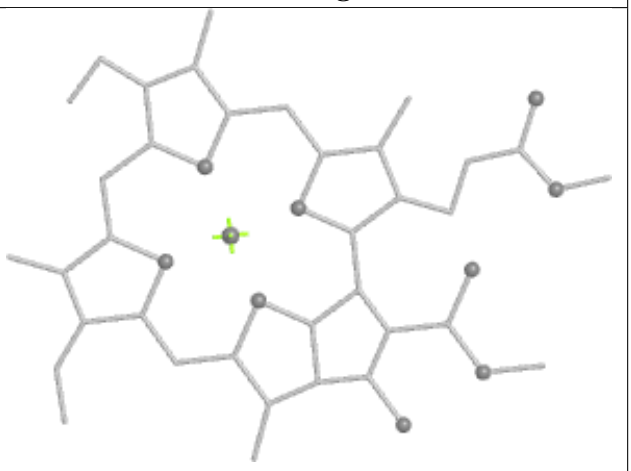
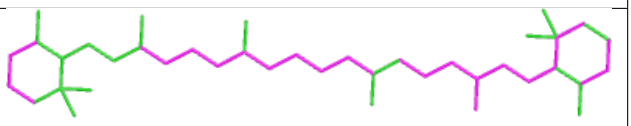


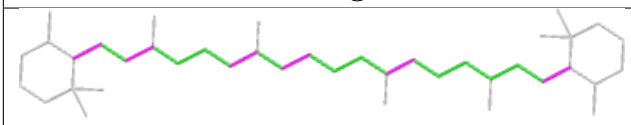
Rings

Ligand BCR 4 621

Bond lengths



Bond angles



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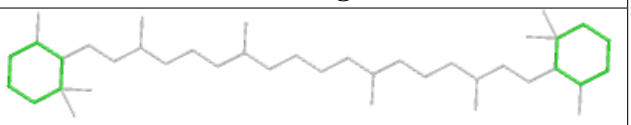
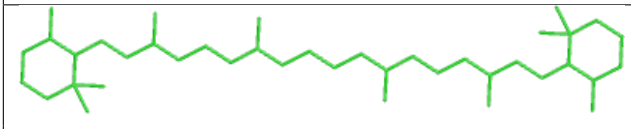


Rings

Ligand BCR 6 625



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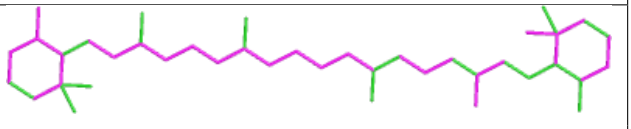
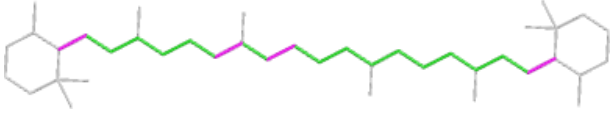
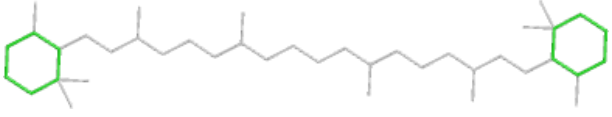


Bond angles

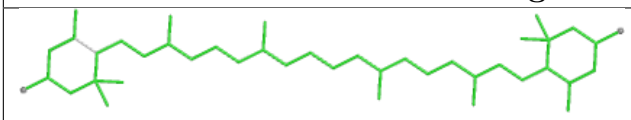


Torsions



Rings

Ligand LUT 8 617



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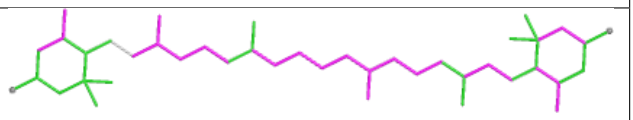
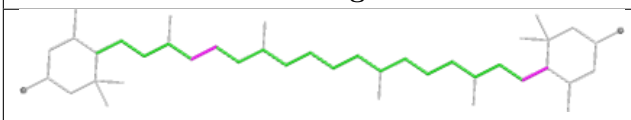


Bond angles



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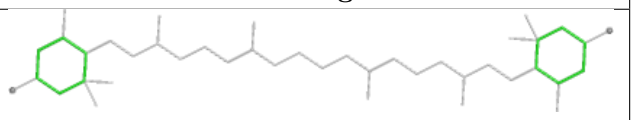
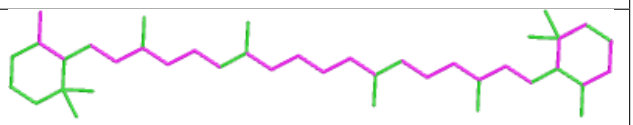


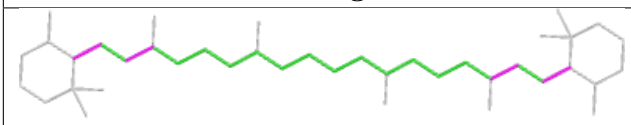
Rings

Ligand BCR B 844

Bond lengths



Bond angles



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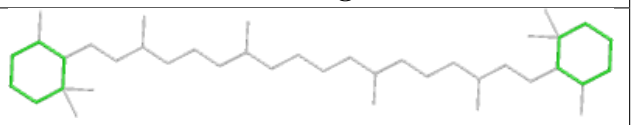
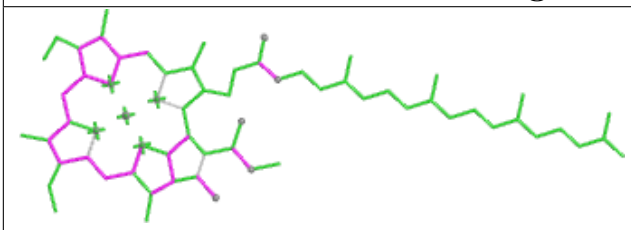


Rings

Ligand CLA 1 613



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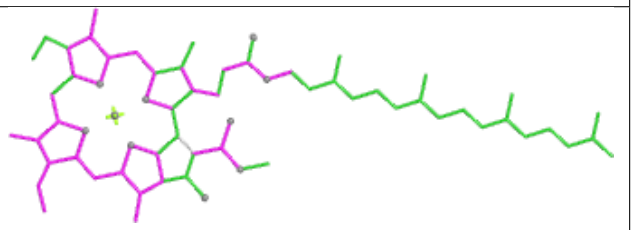
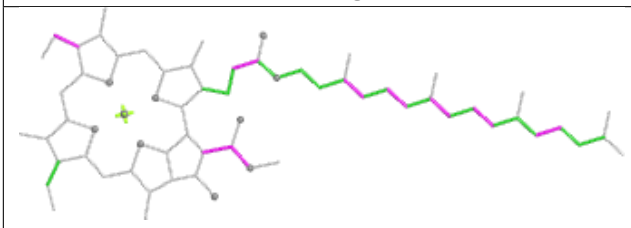


Bond angles



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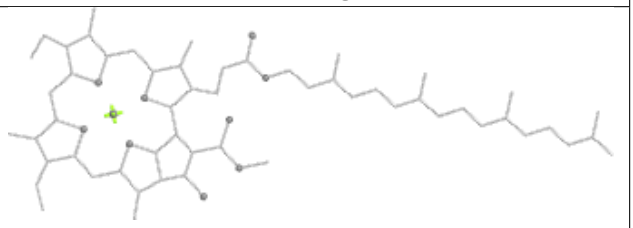
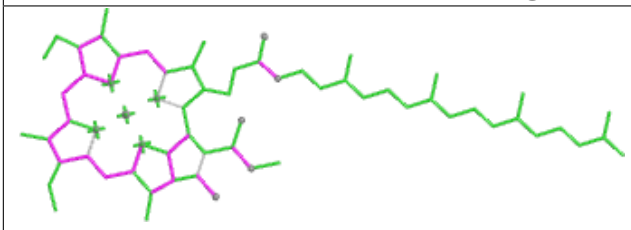
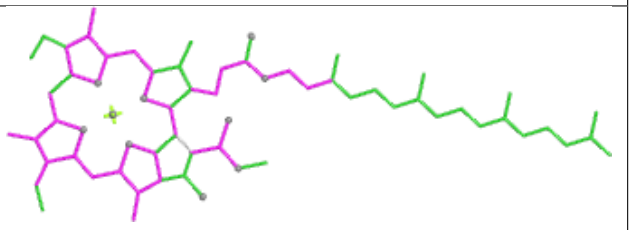


Rings

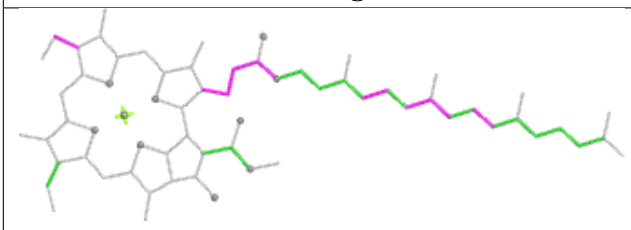
Ligand CLA A 819



Bond lengths



Bond angles



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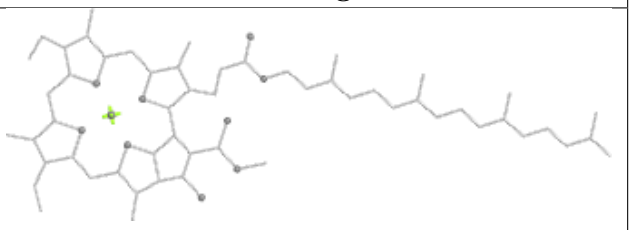
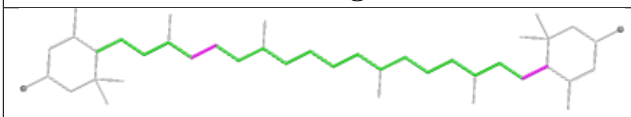


Rings

Ligand LUT 6 624

Bond lengths

Bond angles



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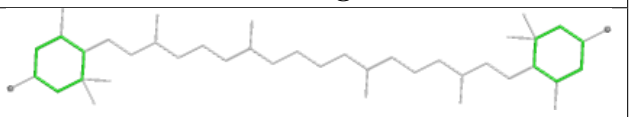
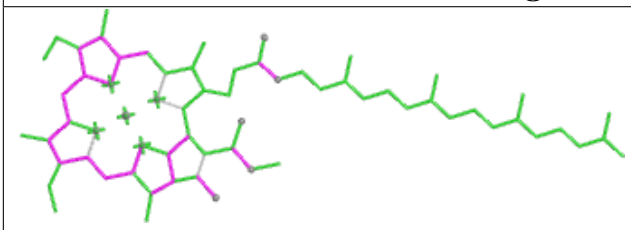
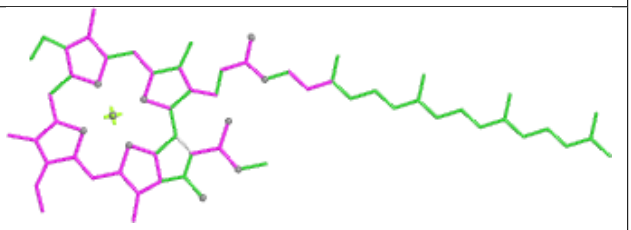


Rings

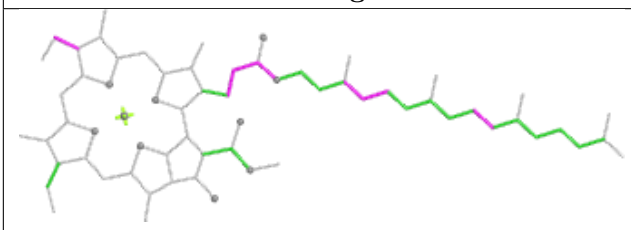
Ligand CLA B 807



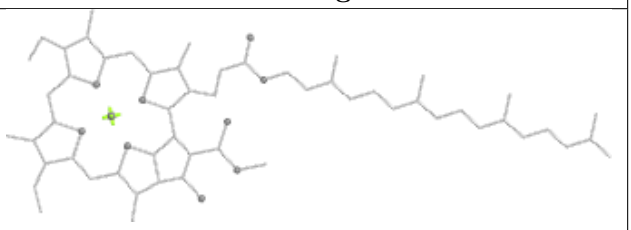
Bond lengths



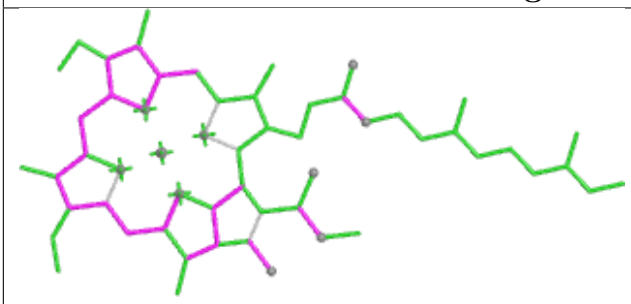
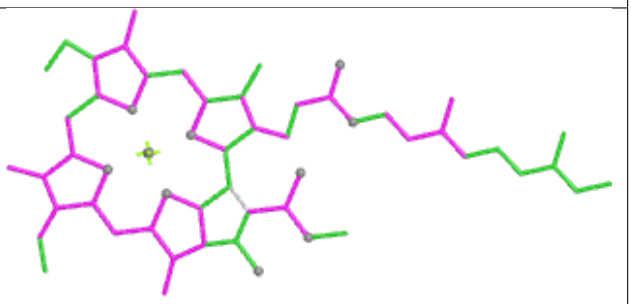
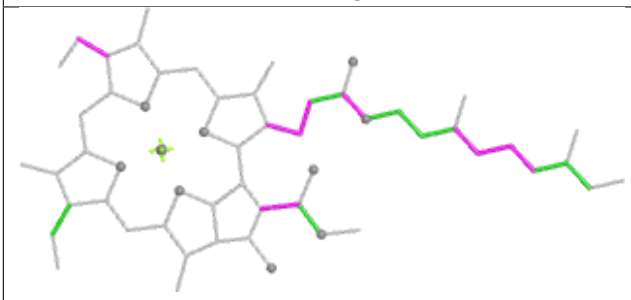
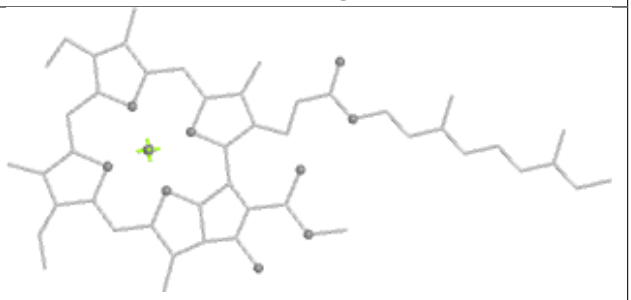
Bond angles



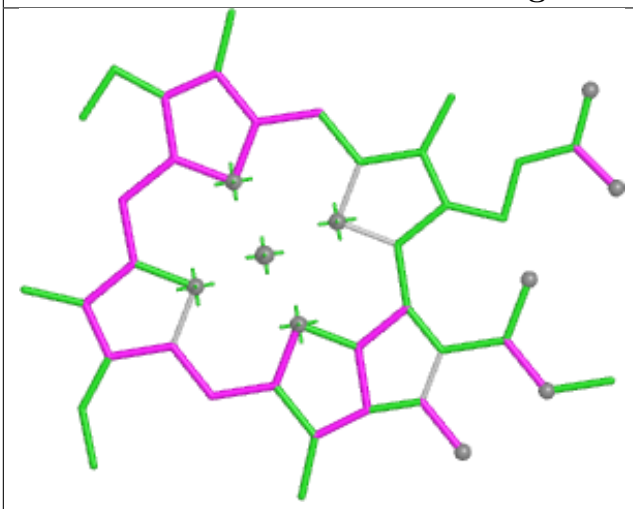
Torsions



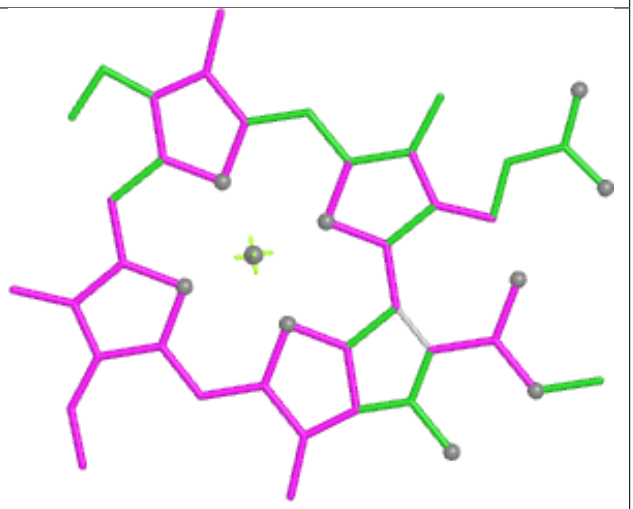
Rings

Ligand CLA B 820	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

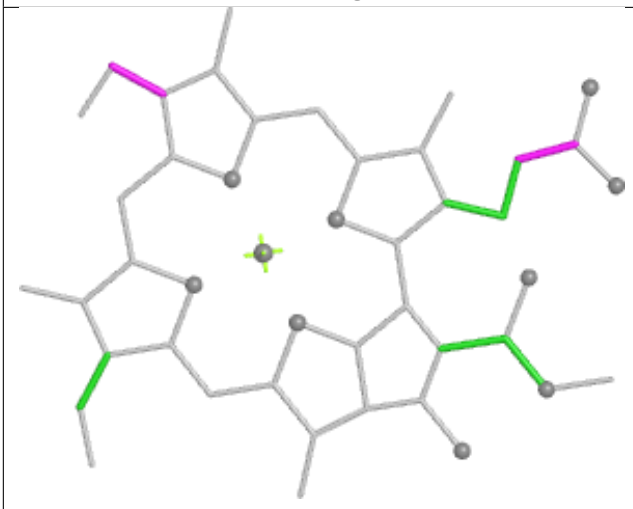
Ligand CLA 8 603



Bond lengths



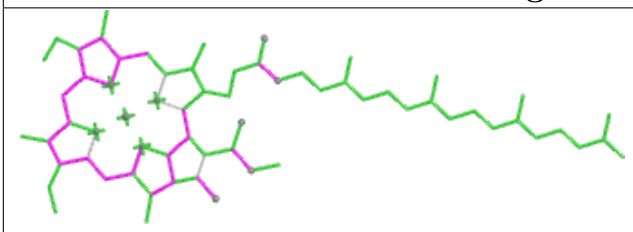
Bond angles



Torsions

Rings

Ligand CLA Z 609



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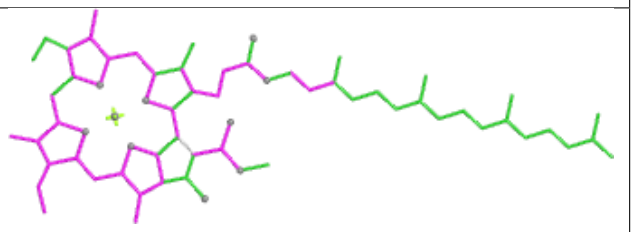

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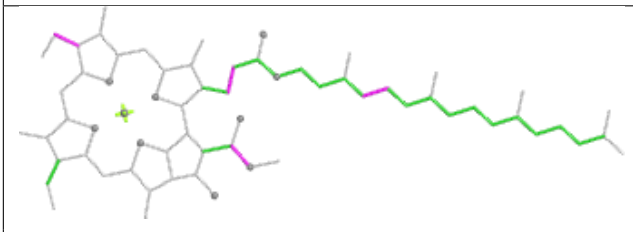
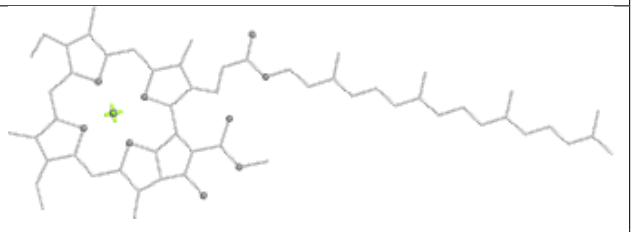


Torsions



Rings

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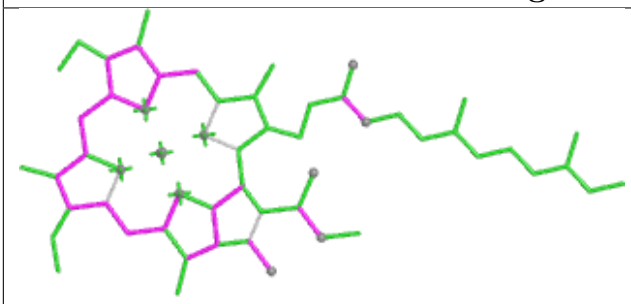
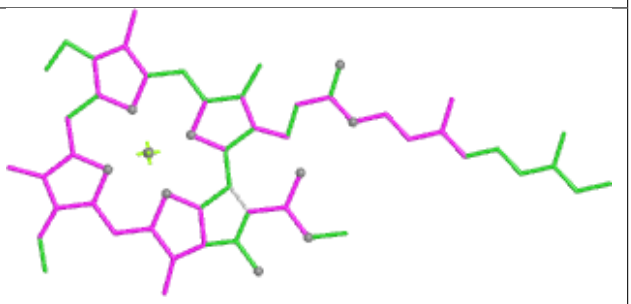
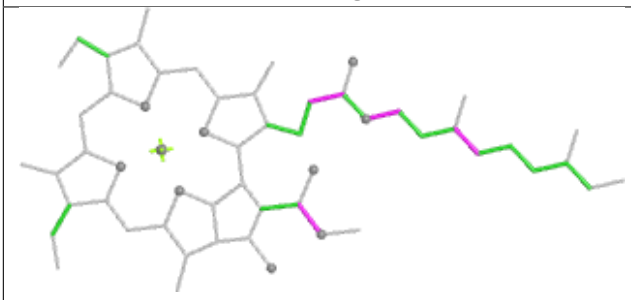
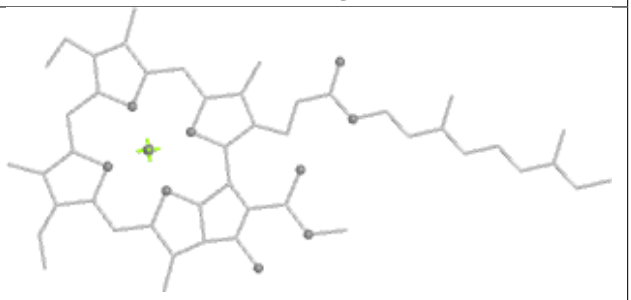
	
Bond lengths	Bond angles
	
Torsions	Rings

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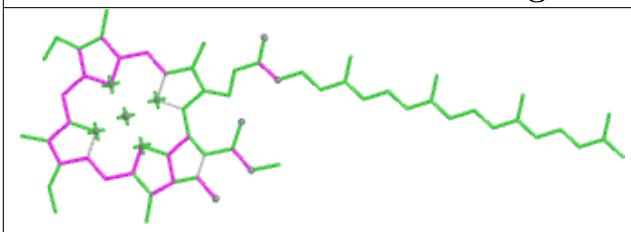
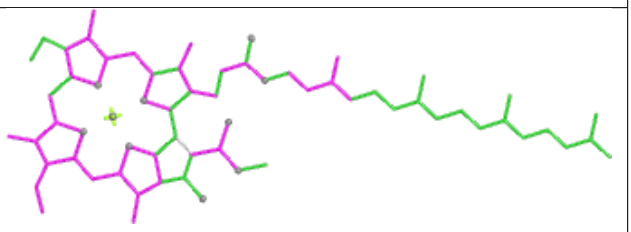
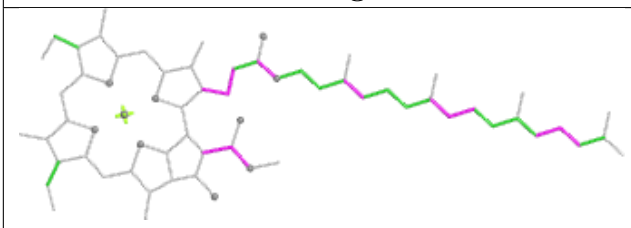
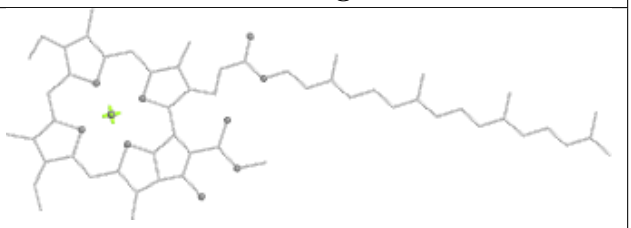
	
Bond lengths	Bond angles
	
Torsions	Rings

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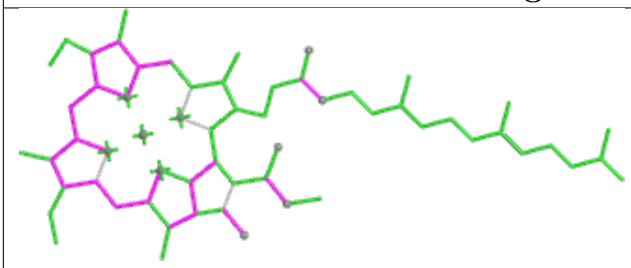
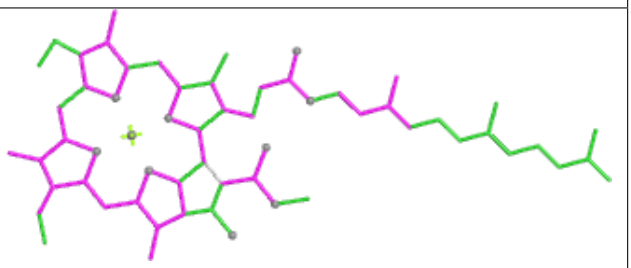
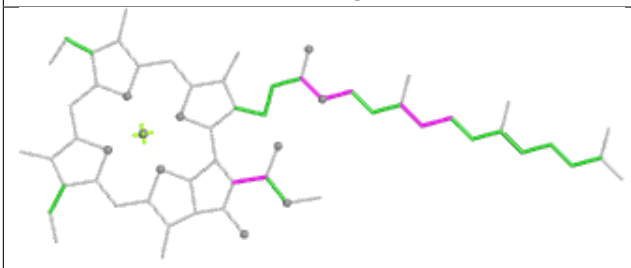
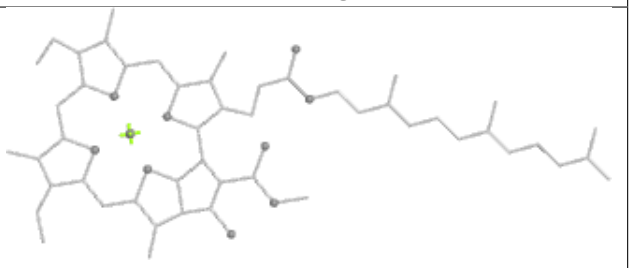
	
Bond lengths	Bond angles
	
Torsions	Rings

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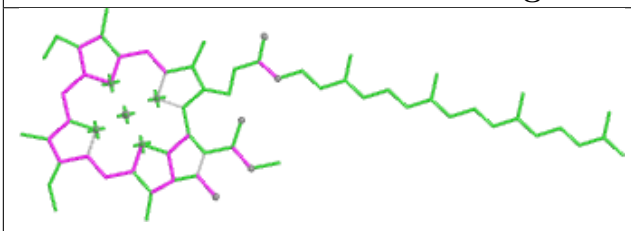
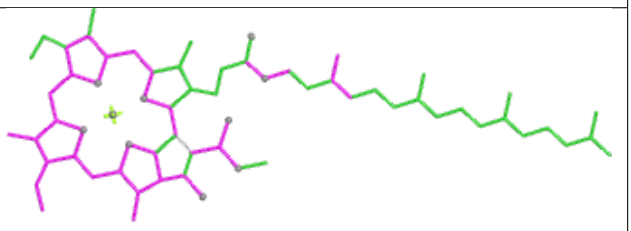
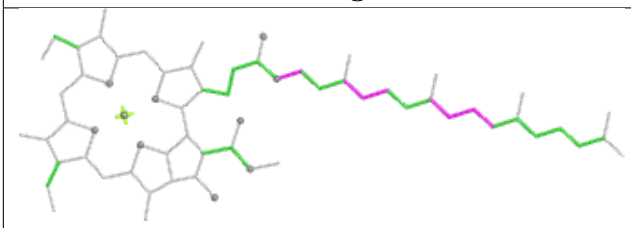
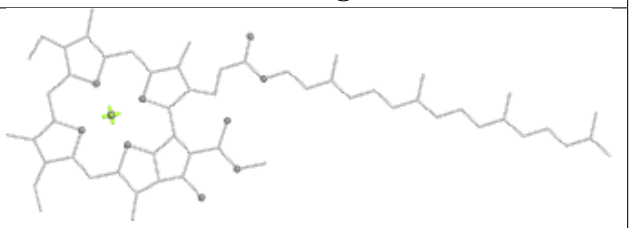
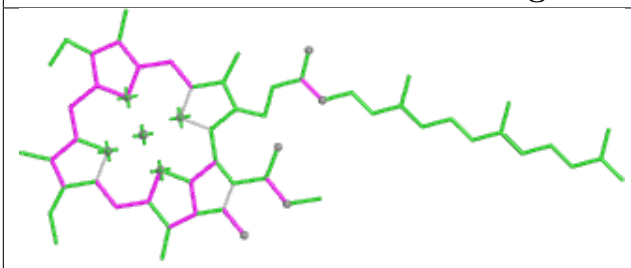
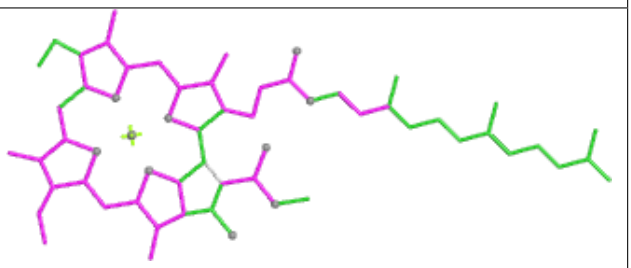
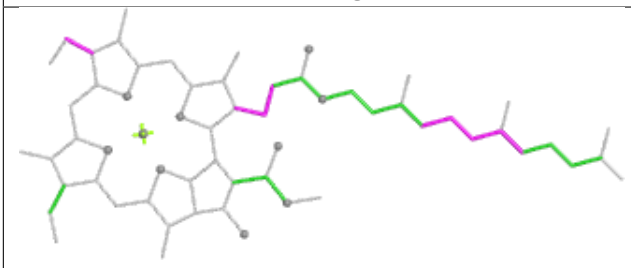
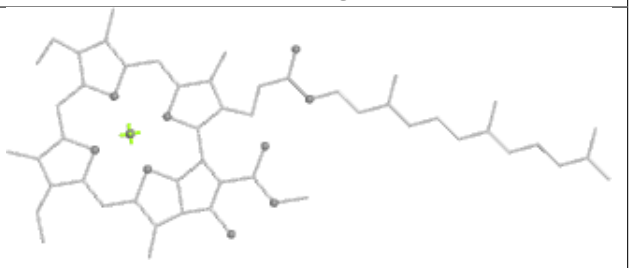
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA 1 610	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

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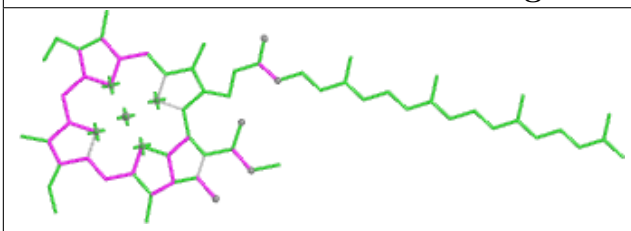
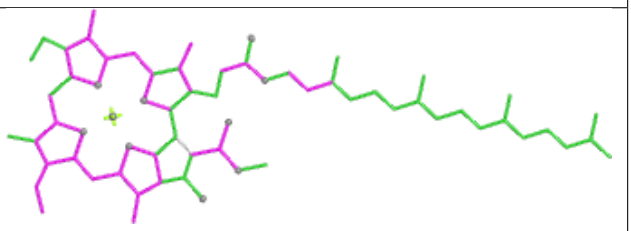
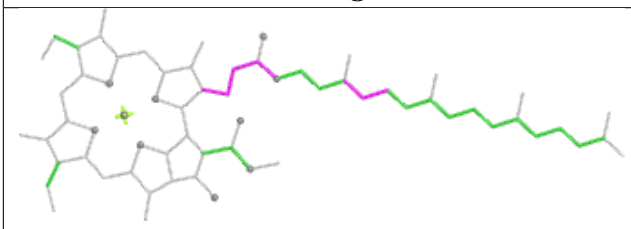
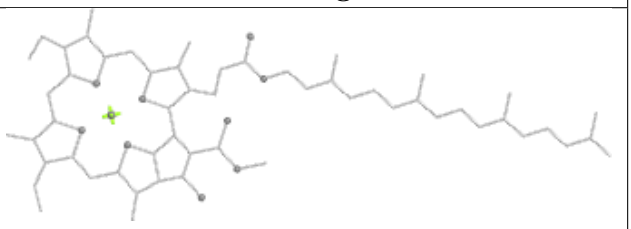
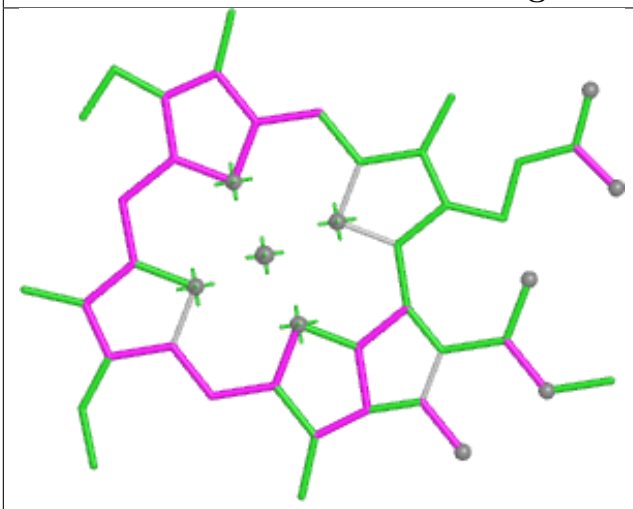
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

Ligand CLA 6 622



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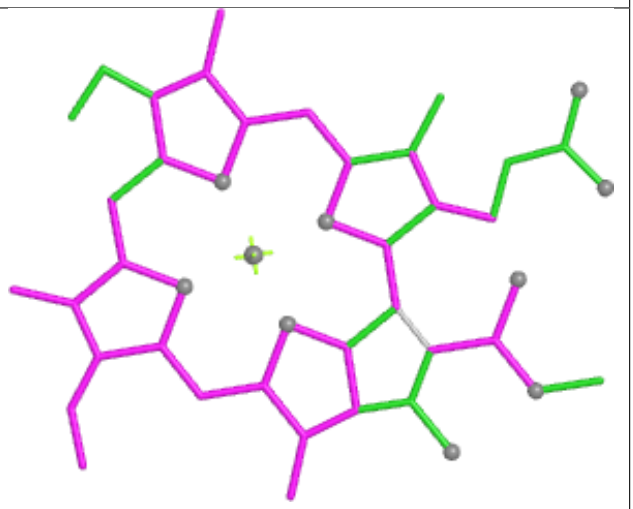
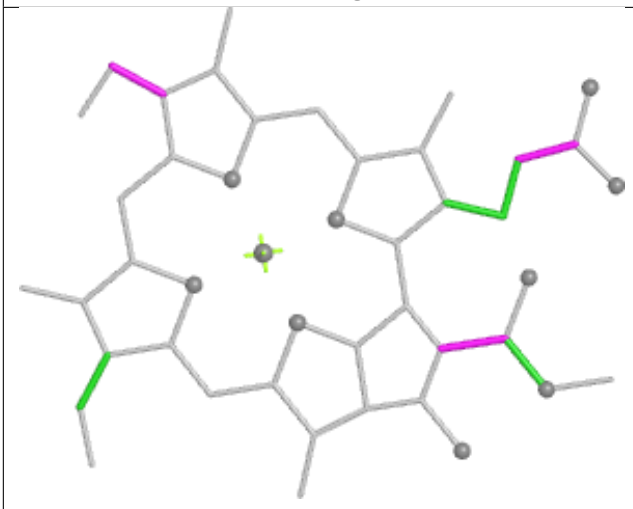


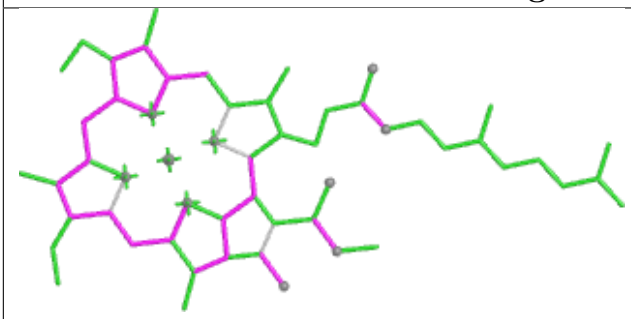
Bond angles



Torsions

Rings

Ligand CLA 5 611



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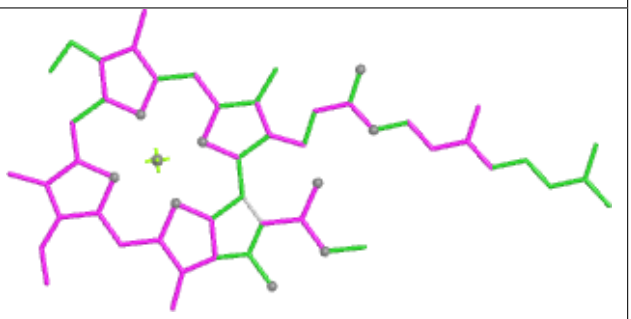
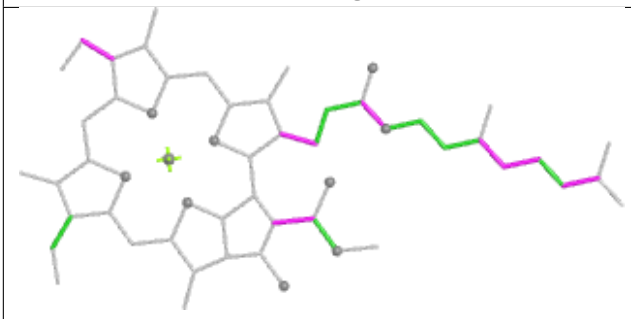


Bond angles



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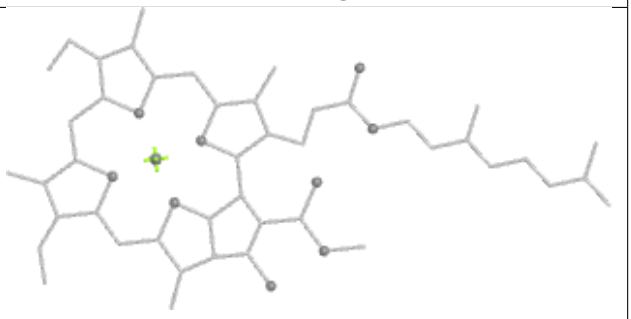
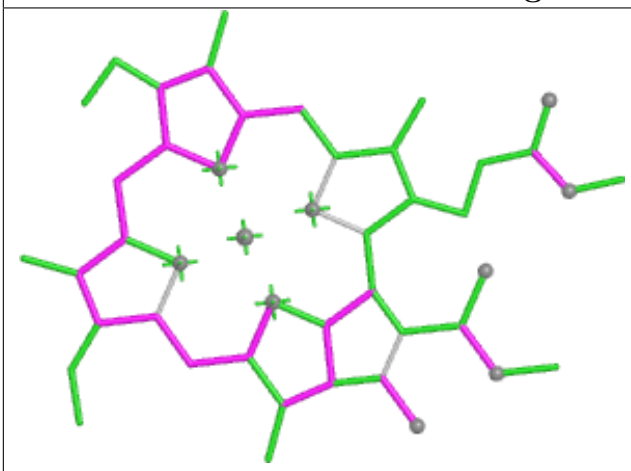


Rings

Ligand CLA B 821



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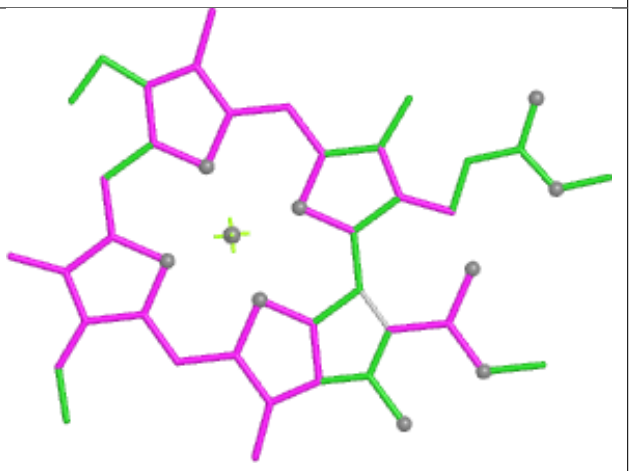
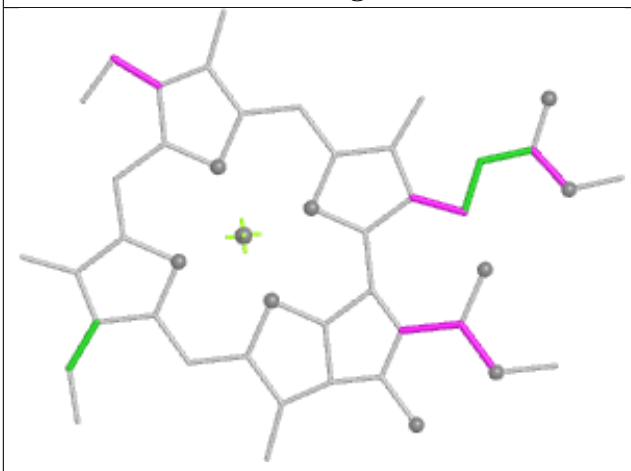


Bond angles



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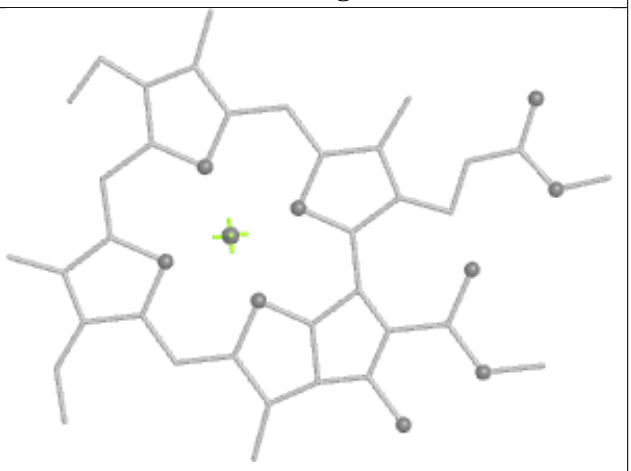
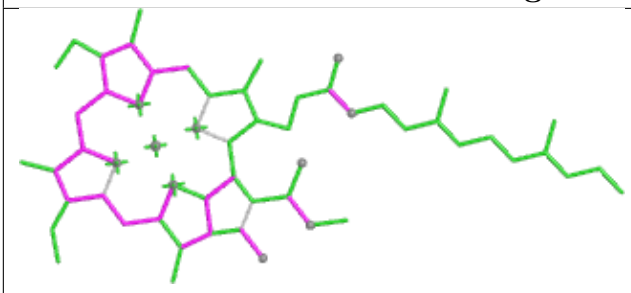


Rings

Ligand CLA B 815



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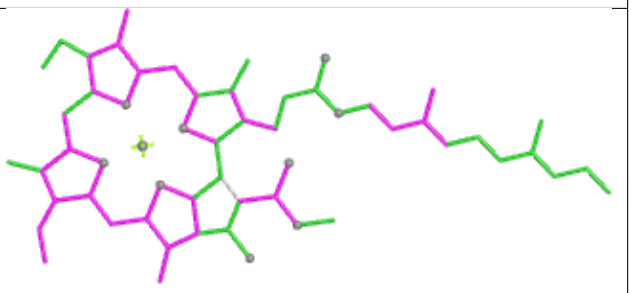
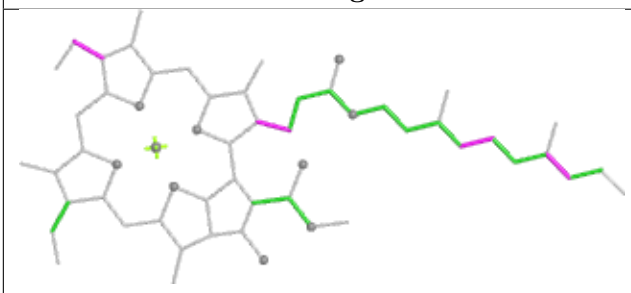


Bond angles



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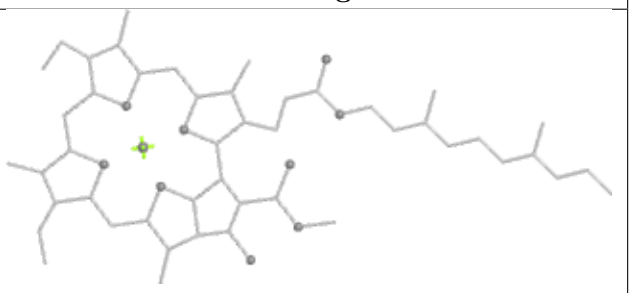
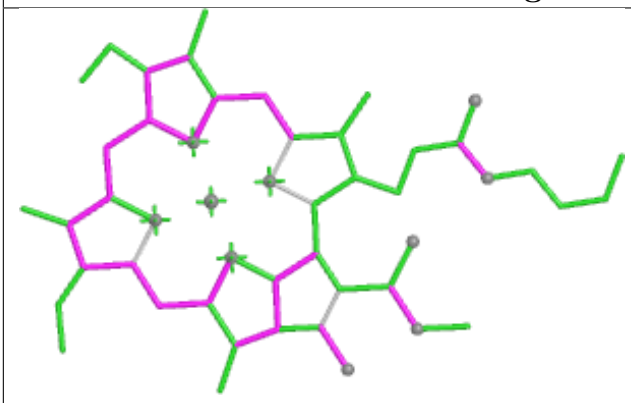
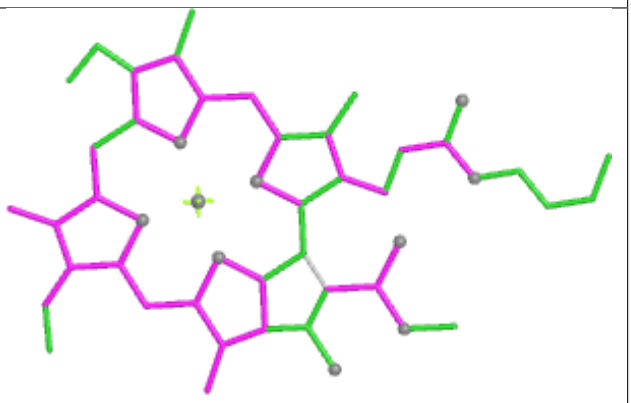


Rings

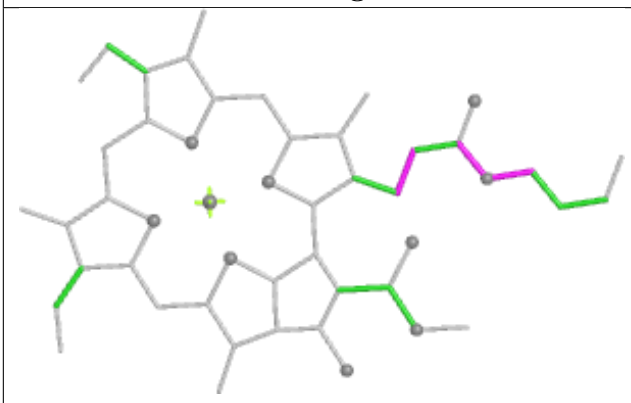
Ligand CLA B 831



Bond lengths



Bond angles



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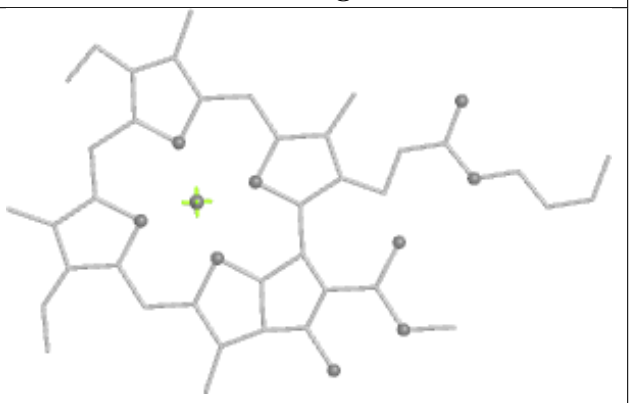
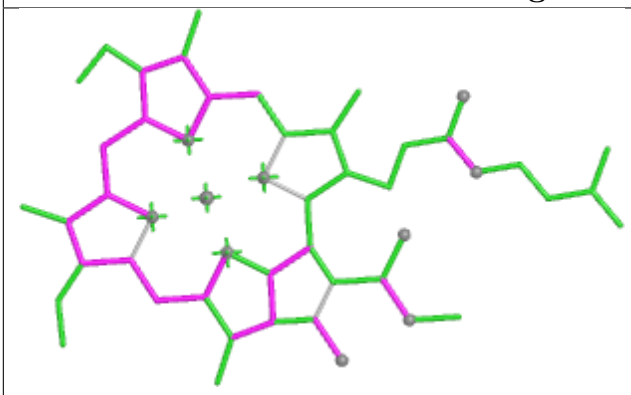
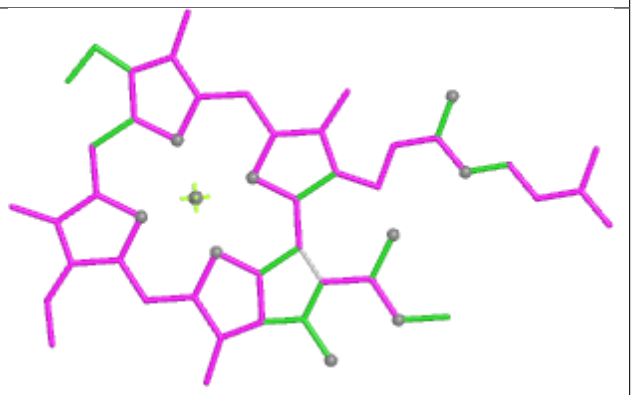


Rings

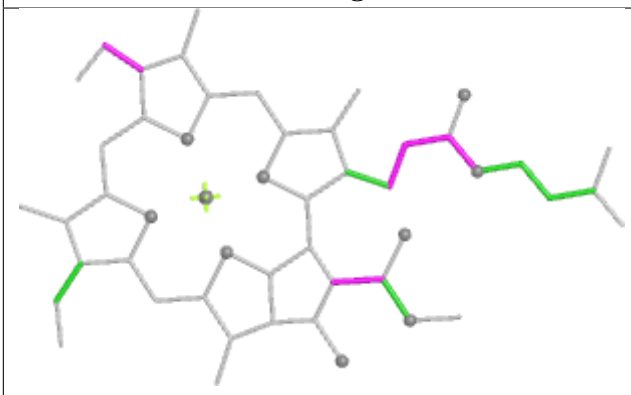
Ligand CLA 3 609



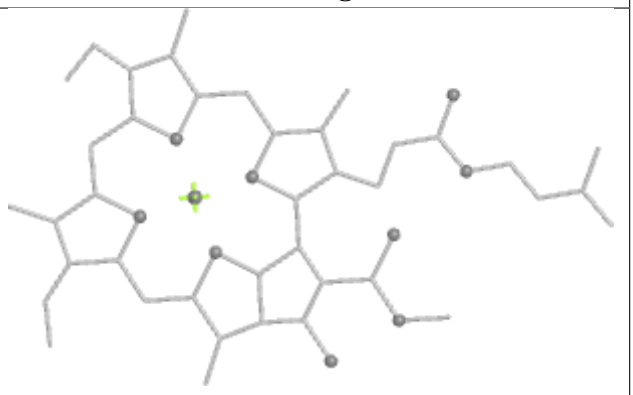
Bond lengths



Bond angles

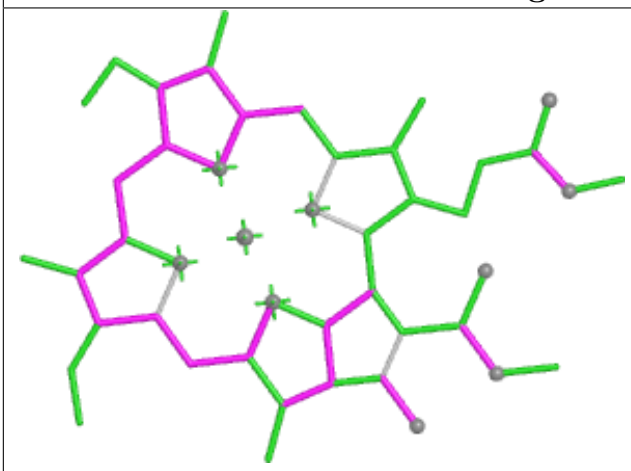


Torsions



Rings

Ligand CLA 7 603



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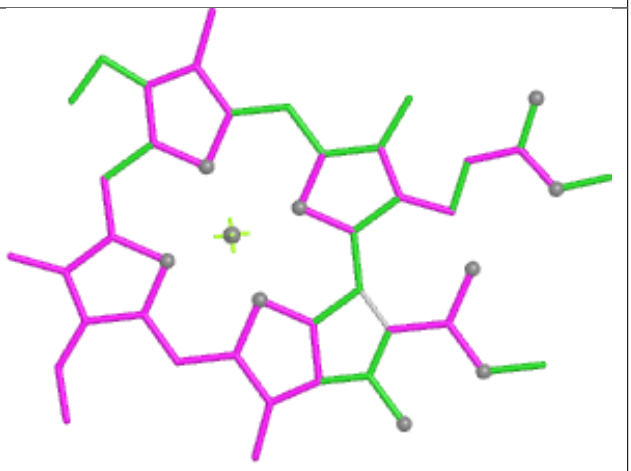
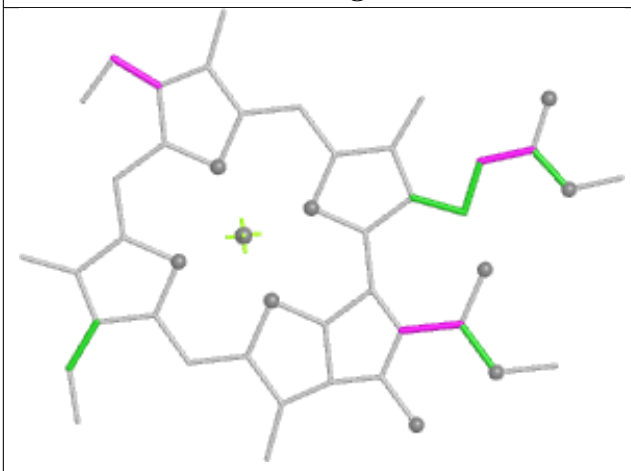


Bond angles



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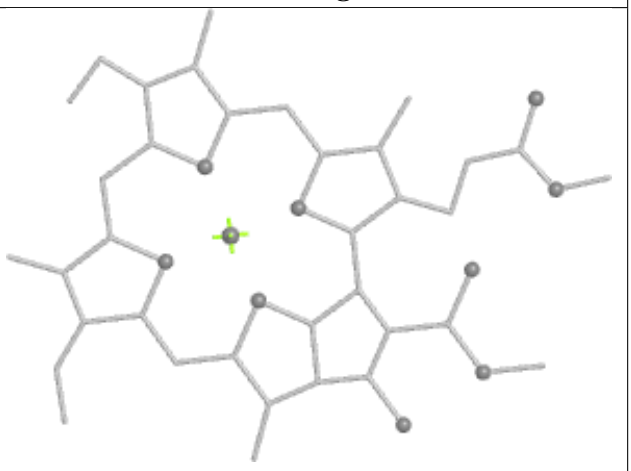
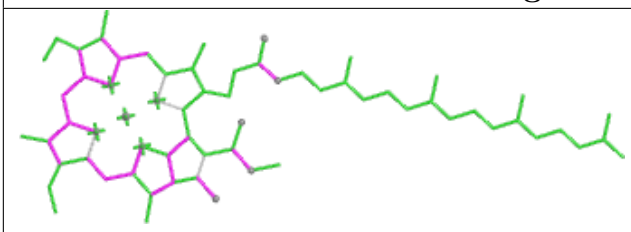


Rings

Ligand CLA A 828



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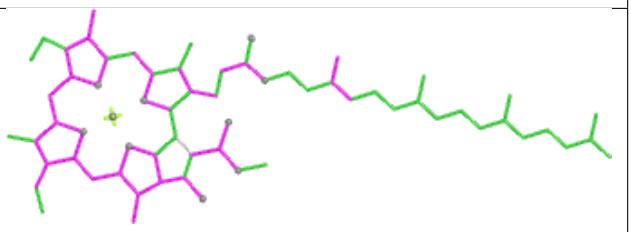

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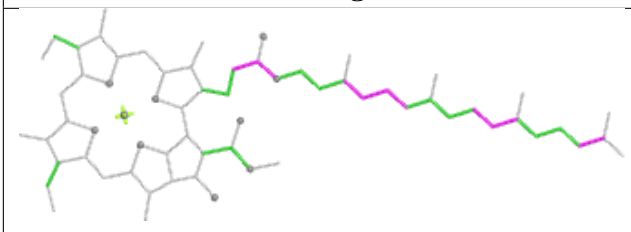

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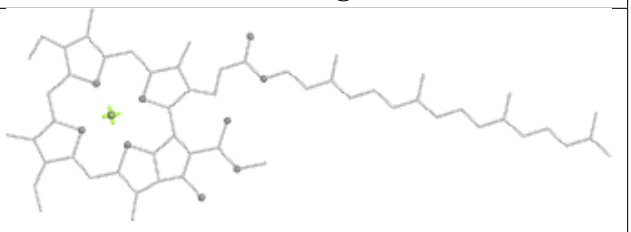
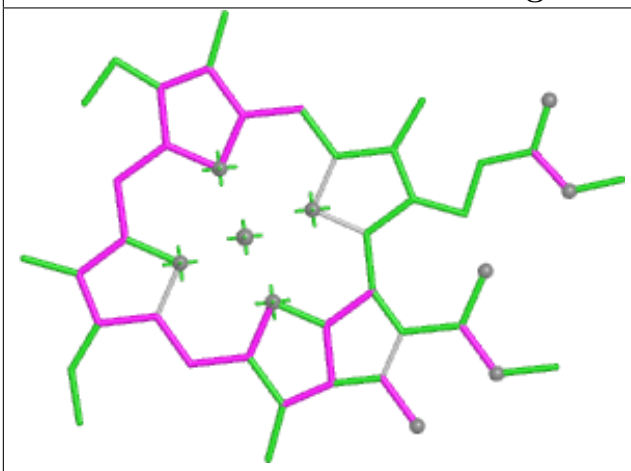


Rings

Ligand CLA Z 616



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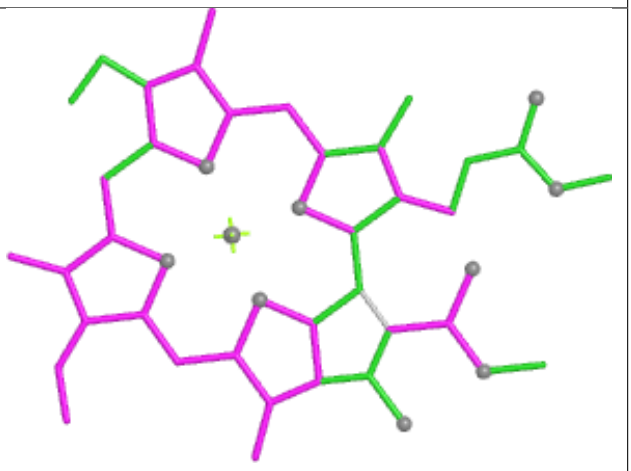
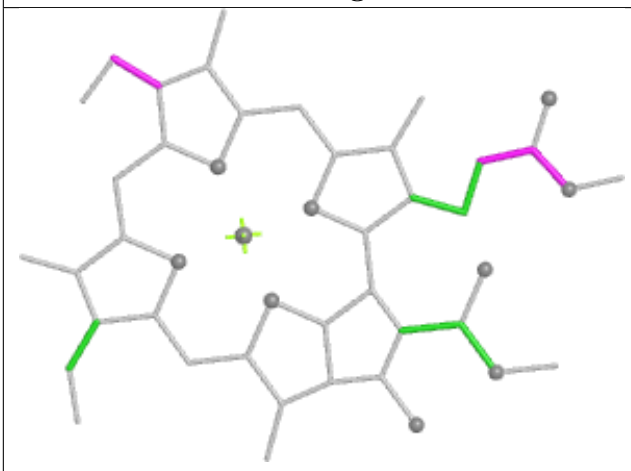


Bond angles



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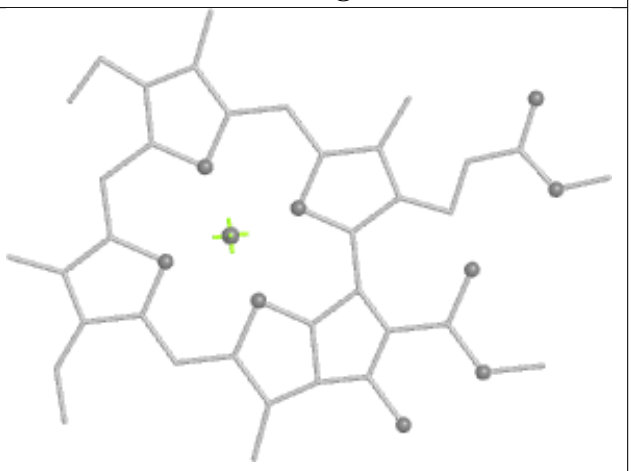
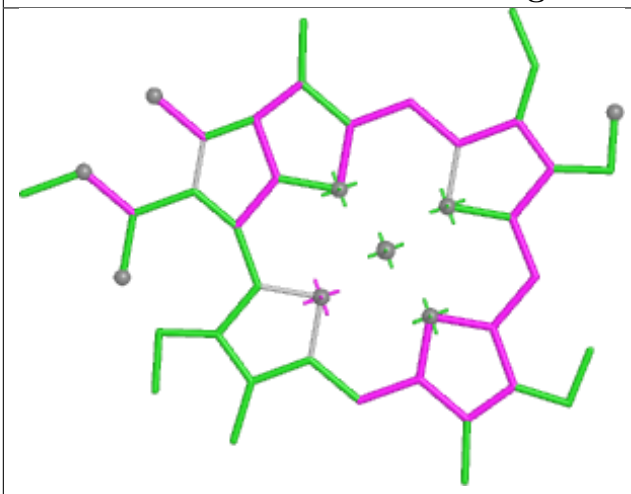


Rings

Ligand CHL 6 618



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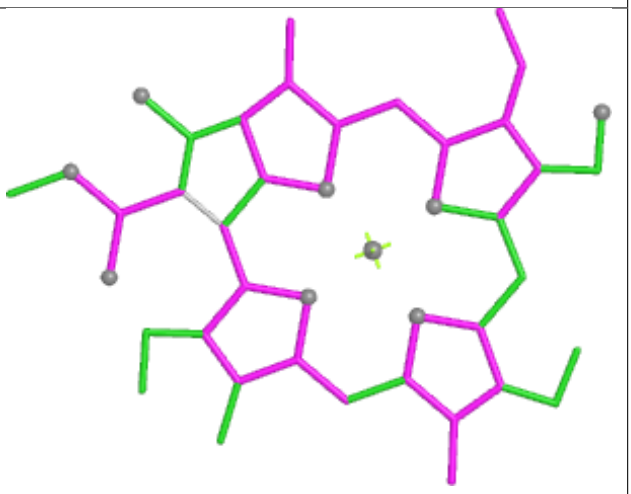
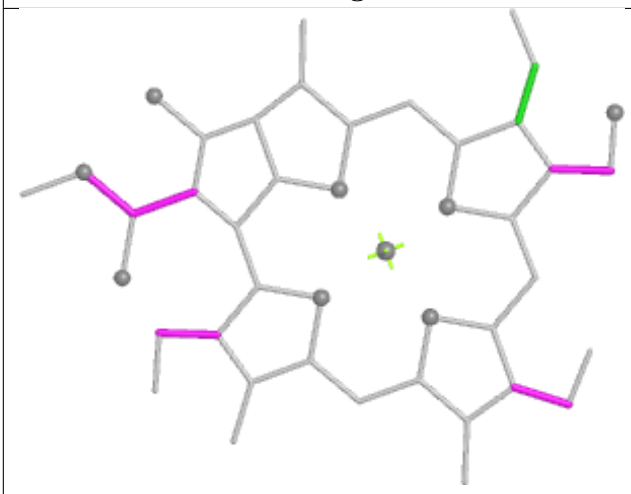


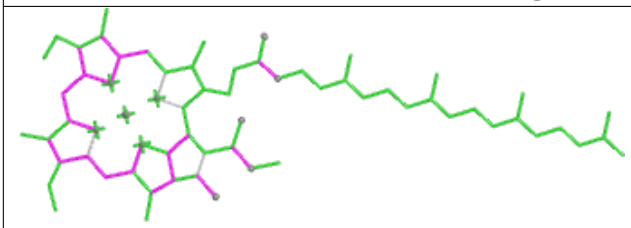
Bond angles



Torsions

Rings

Ligand CLA 3 603



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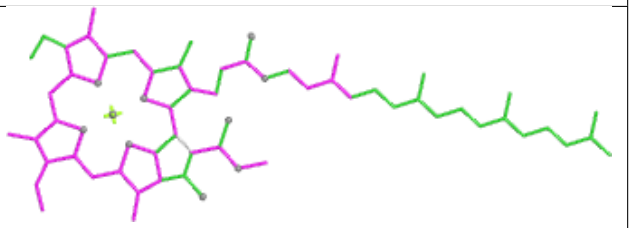

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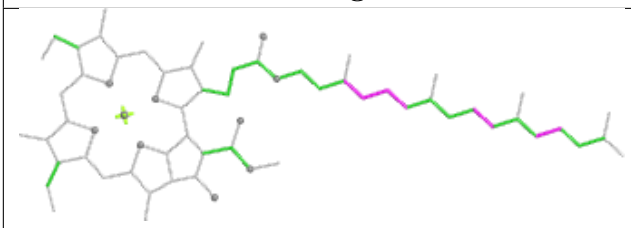

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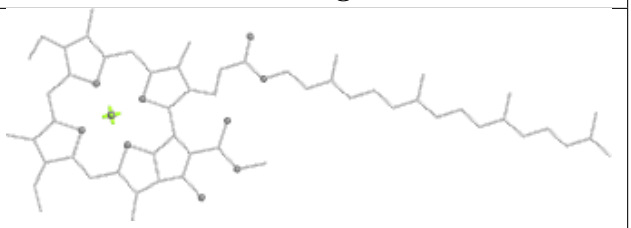
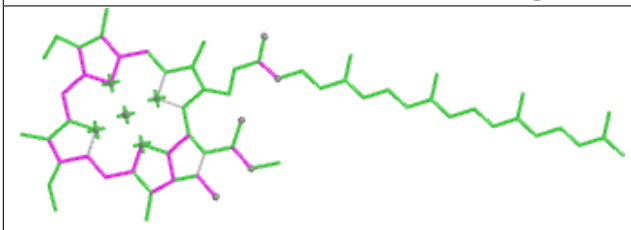


Rings

Ligand CLA 3 604



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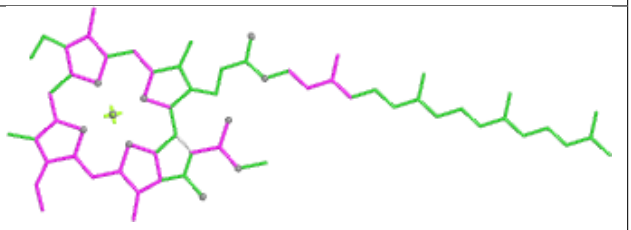
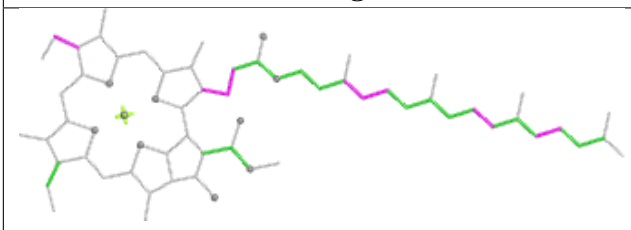


Bond angles



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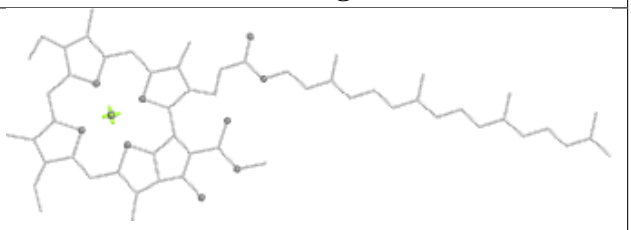
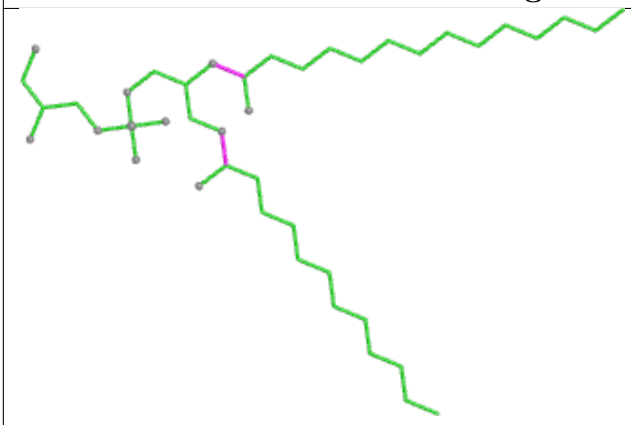


Rings

Ligand LHG Z 620



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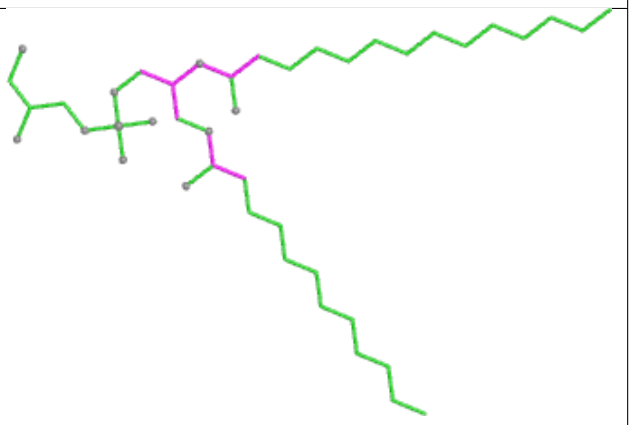
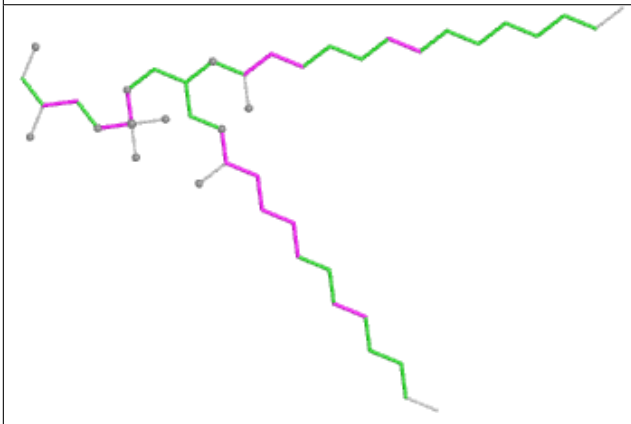


Bond angles



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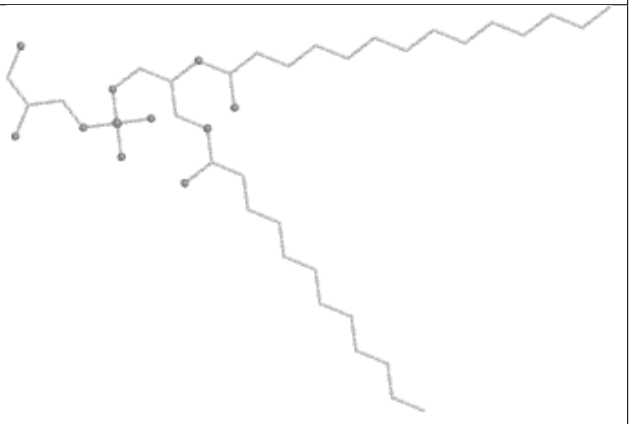
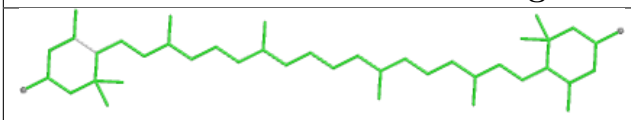
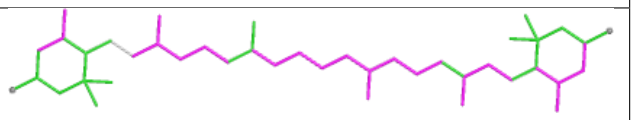
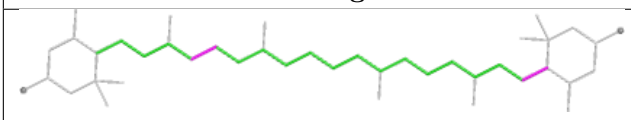
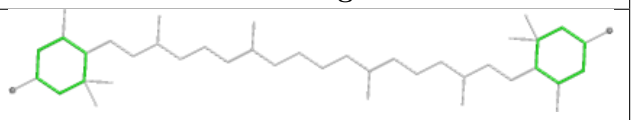
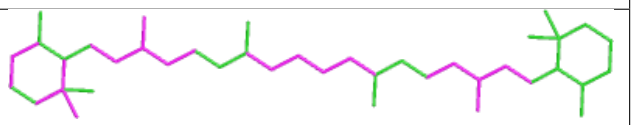
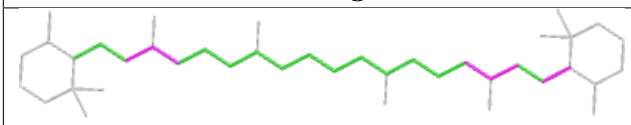
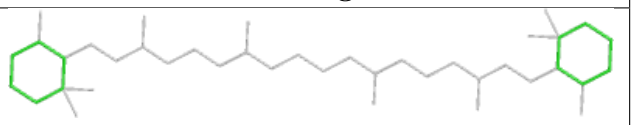
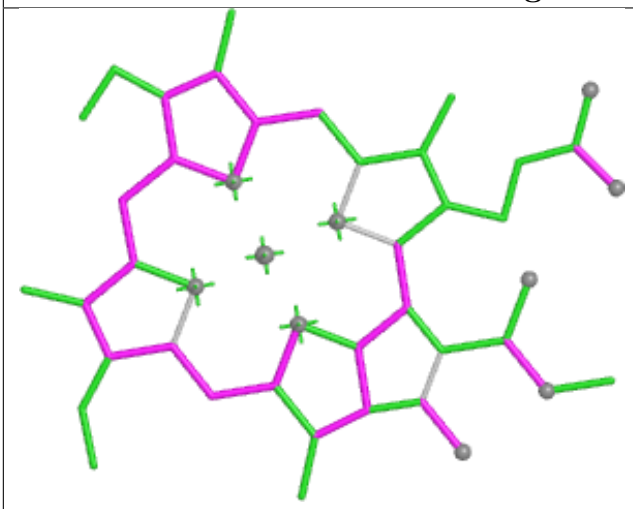


Rings

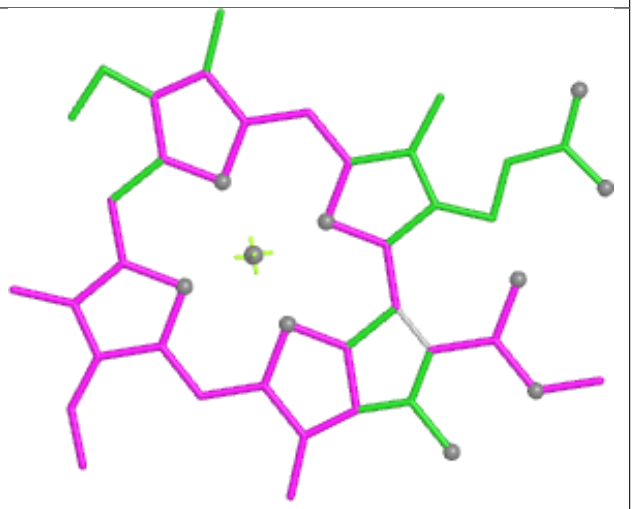
Ligand LUT 5 624	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCR B 845	
	
Bond lengths	Bond angles
	
Torsions	Rings

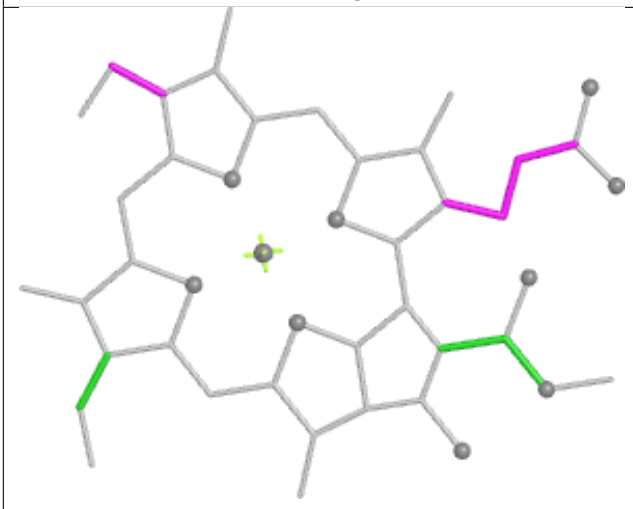
Ligand CLA B 835



Bond lengths



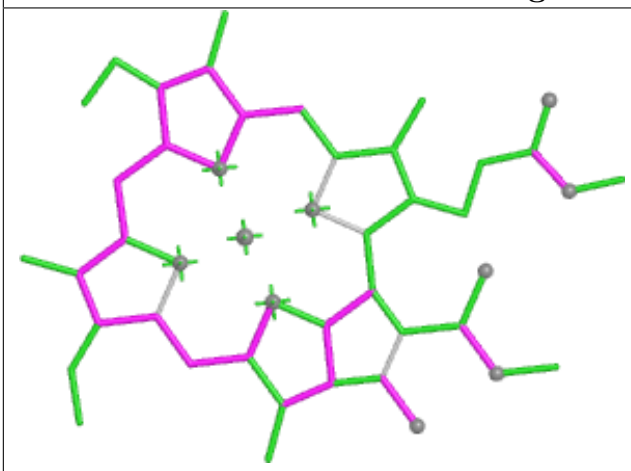
Bond angles



Torsions

Rings

Ligand CLA 7 616



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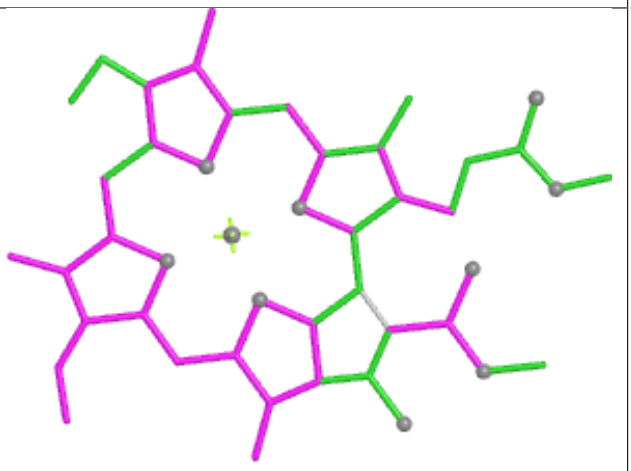
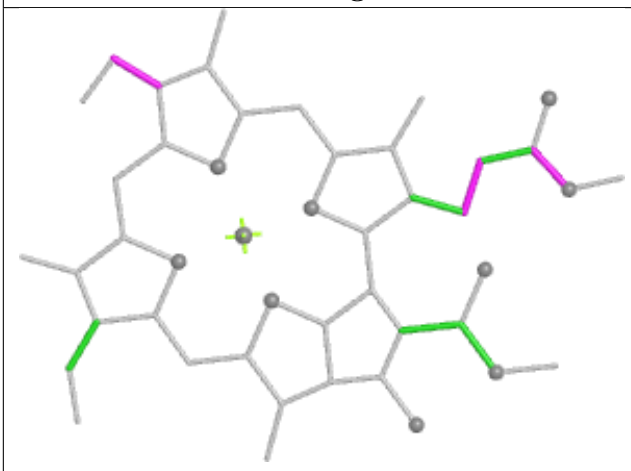


Bond angles



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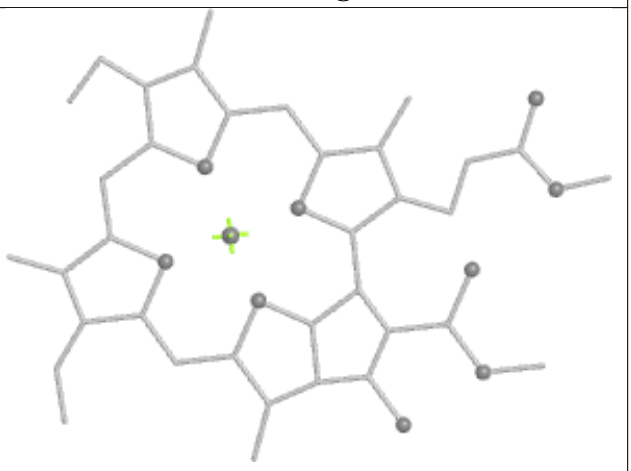
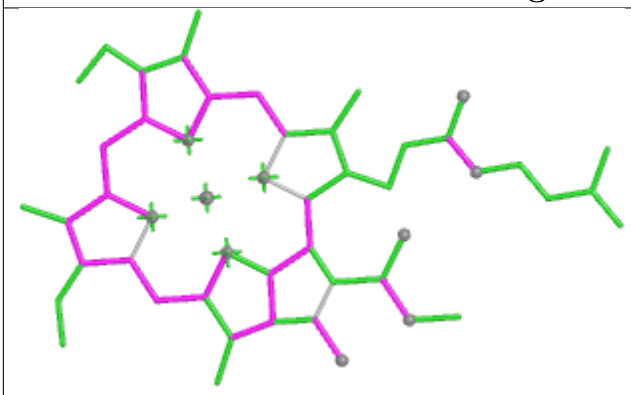


Rings

Ligand CLA 4 609



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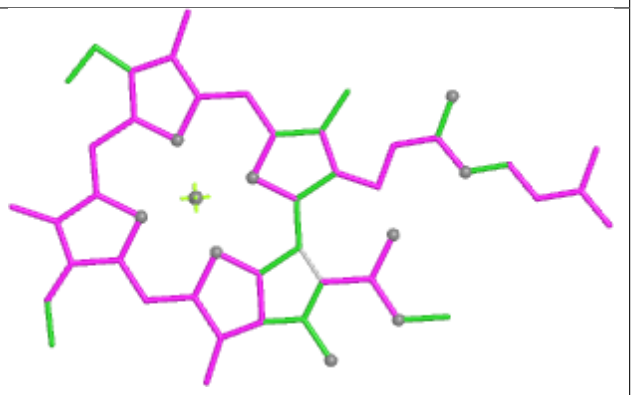
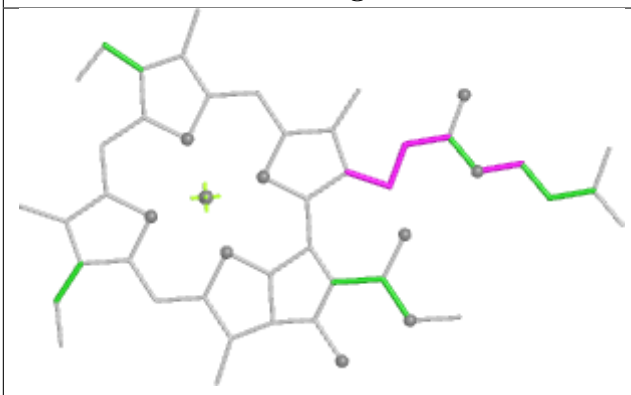


Bond angles



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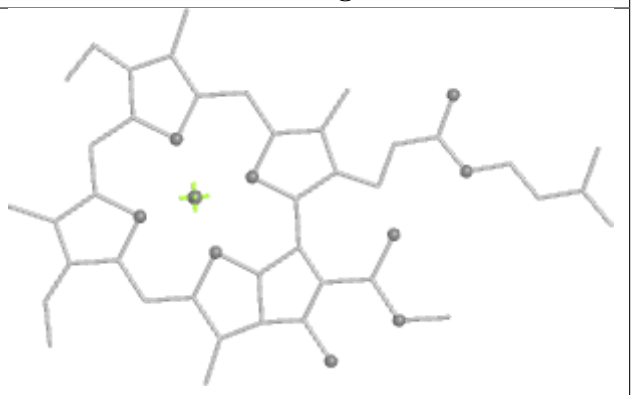
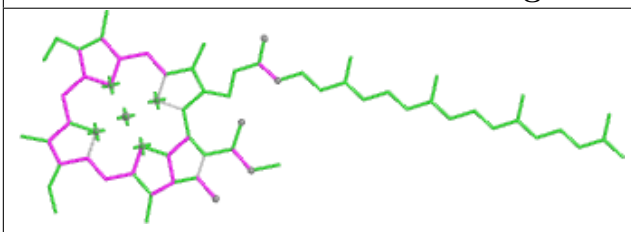


Rings

Ligand CLA A 841



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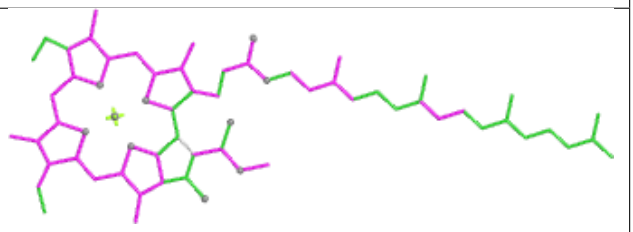
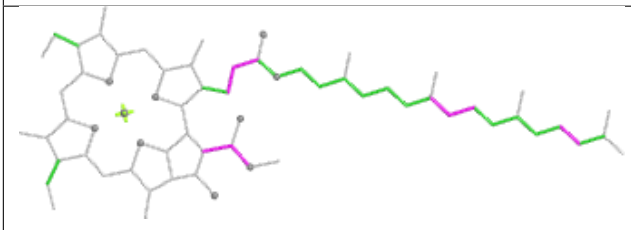


Bond angles



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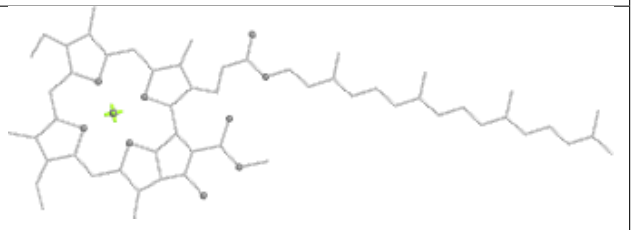
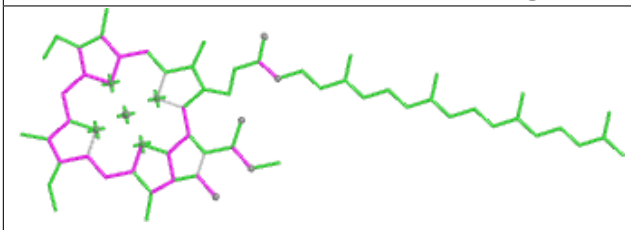
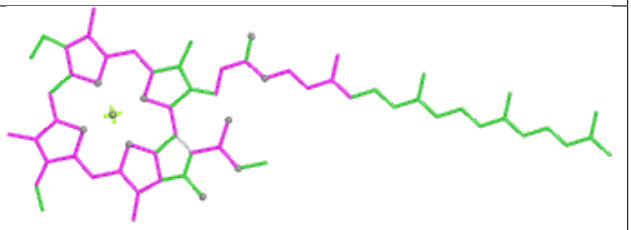


Rings

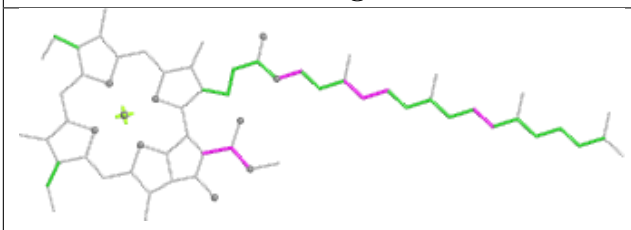
Ligand CLA A 840



Bond lengths



Bond angles



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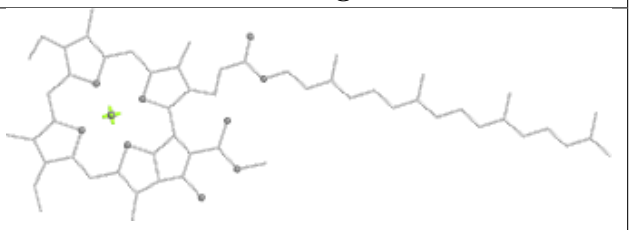
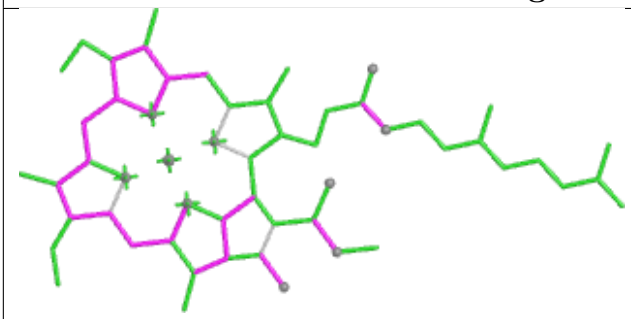
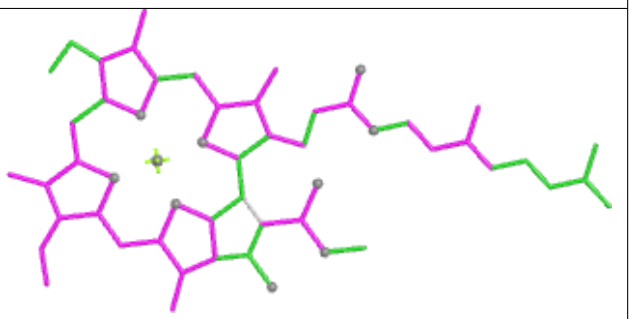


Rings

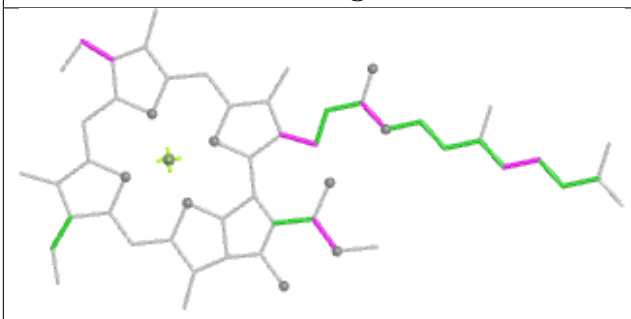
Ligand CLA 8 614



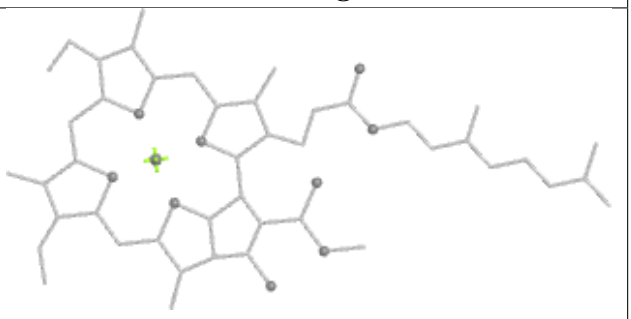
Bond lengths



Bond angles

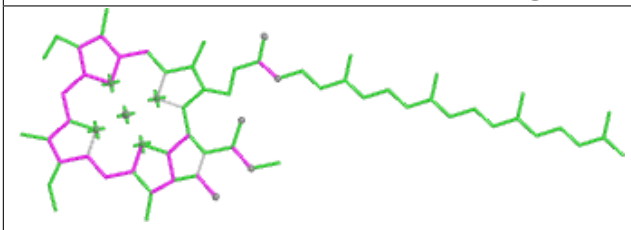


Torsions



Rings

Ligand CLA Z 614



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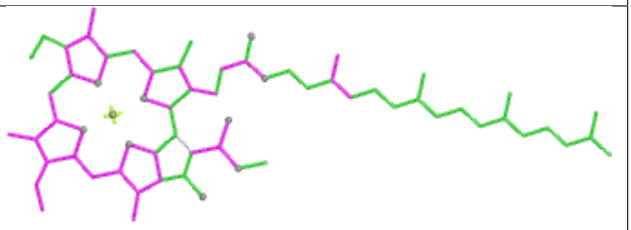

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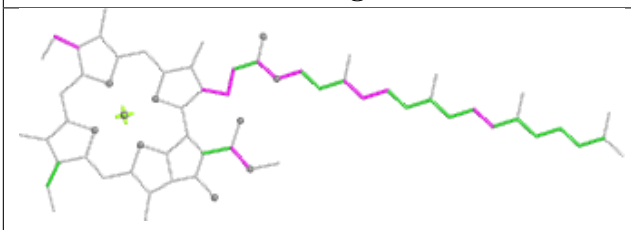

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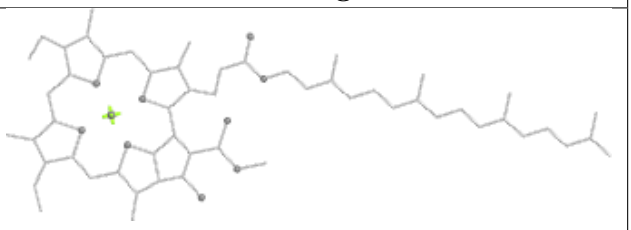
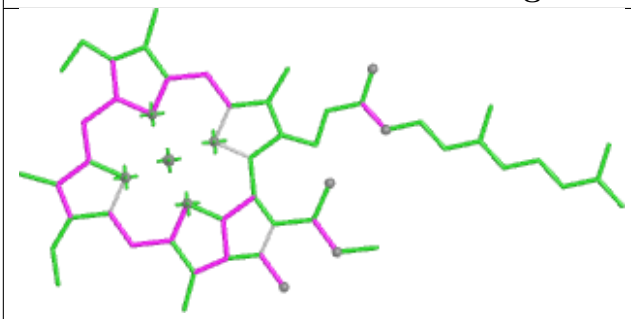


Rings

Ligand CLA A 805



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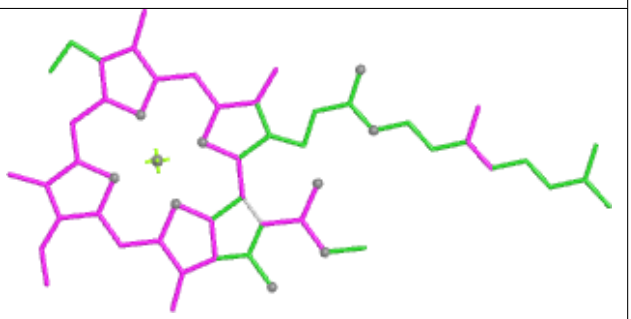

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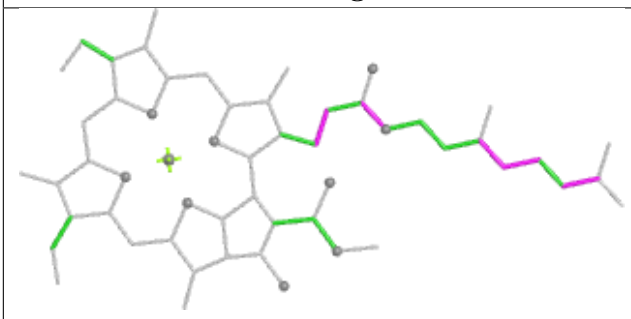

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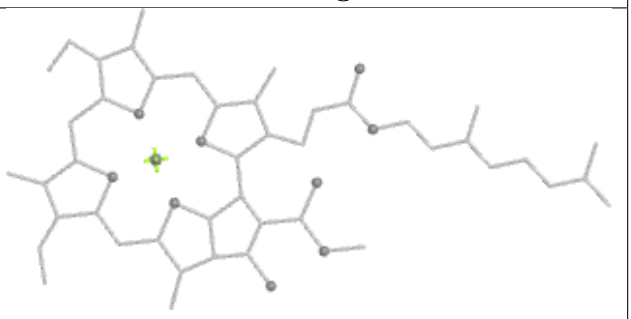
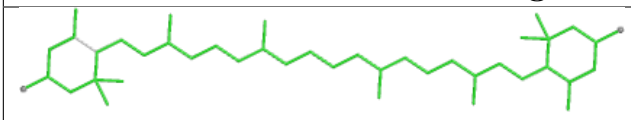


Rings

Ligand LUT 4 619



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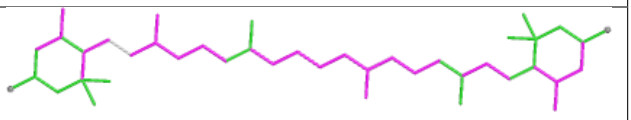

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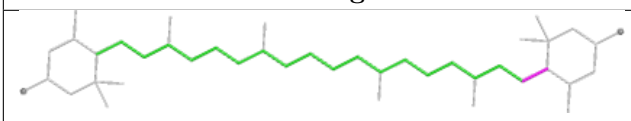

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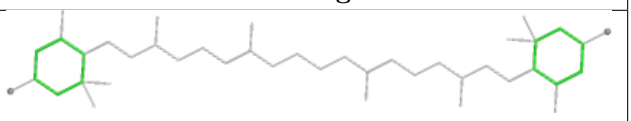
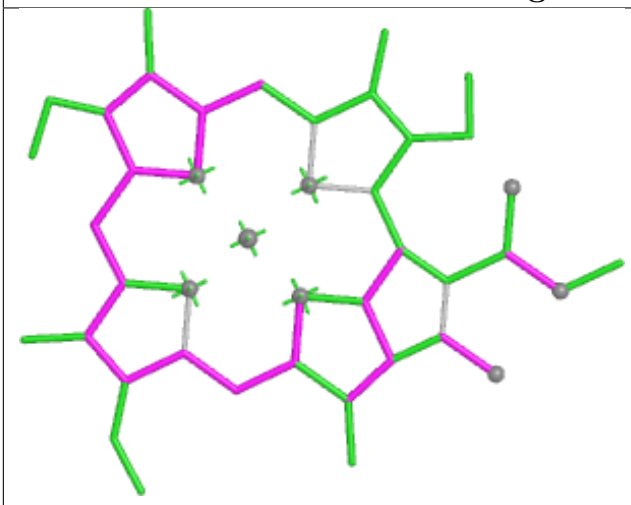


Rings

Ligand CLA 3 606



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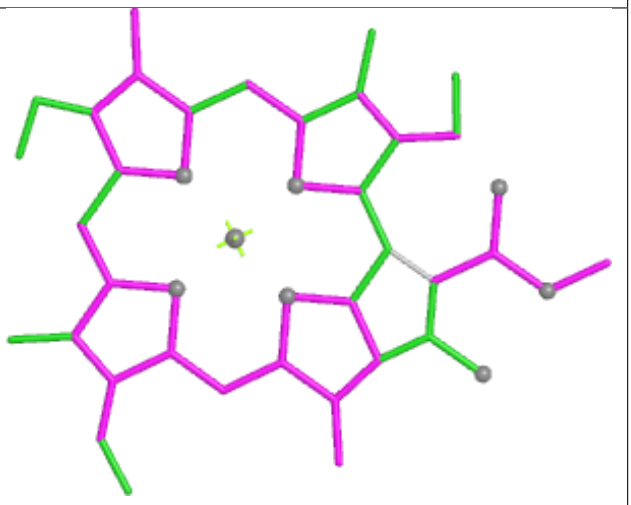
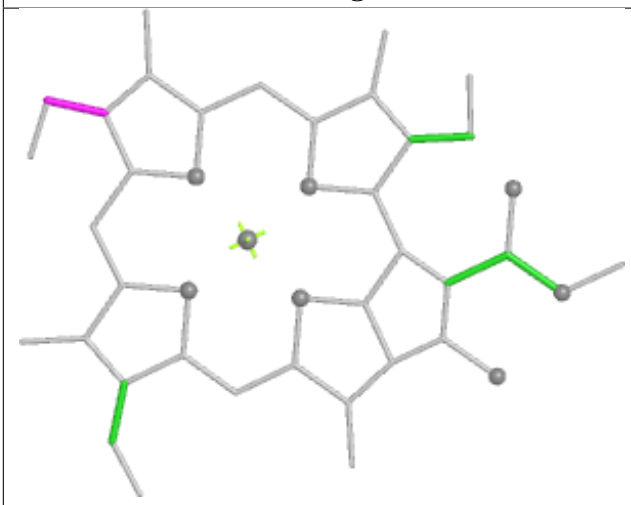


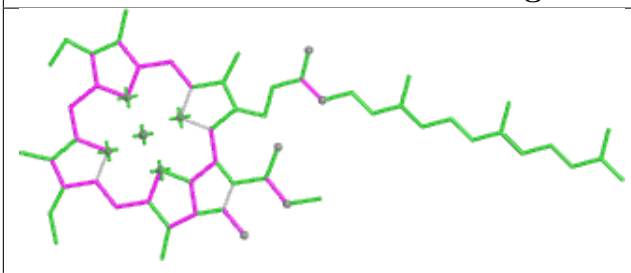
Bond angles



Torsions

Rings

Ligand CLA B 818



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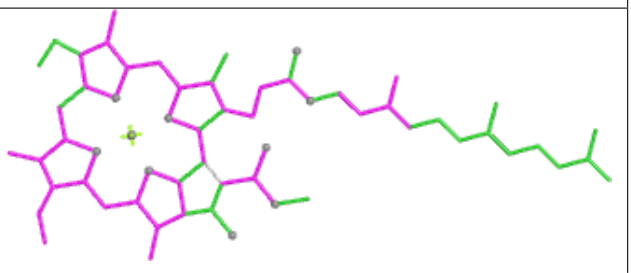

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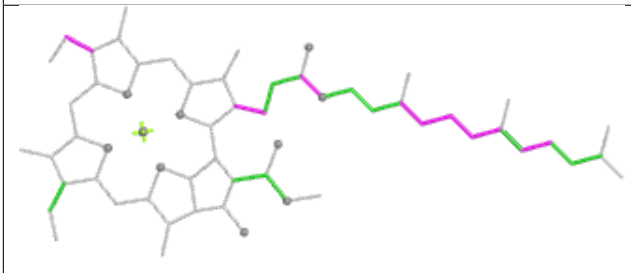

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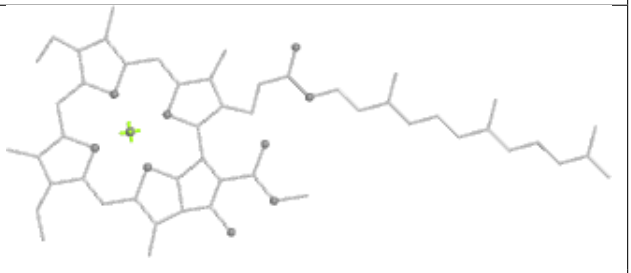
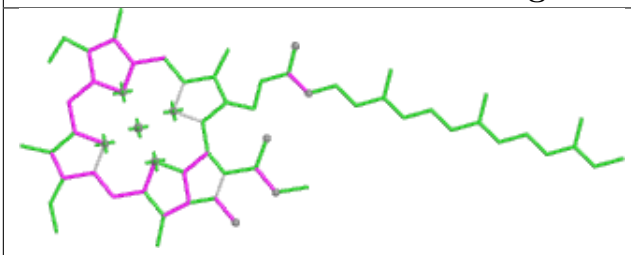


Rings

Ligand CLA 4 601



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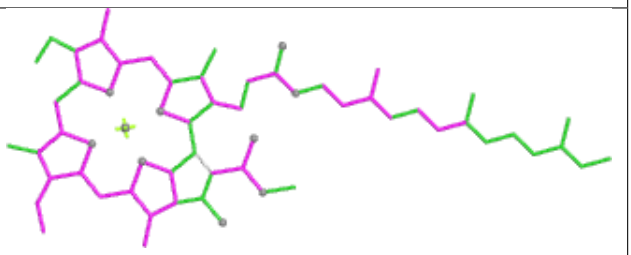
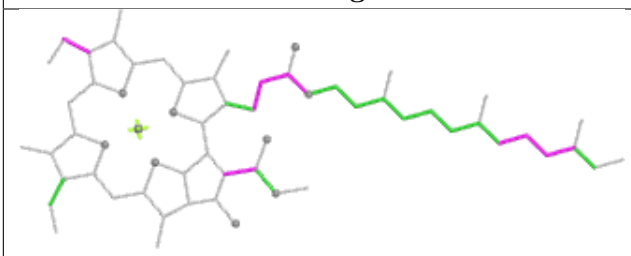


Bond angles



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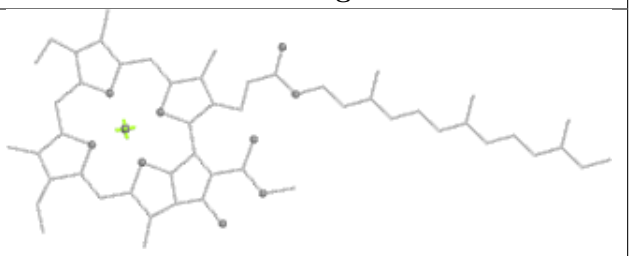
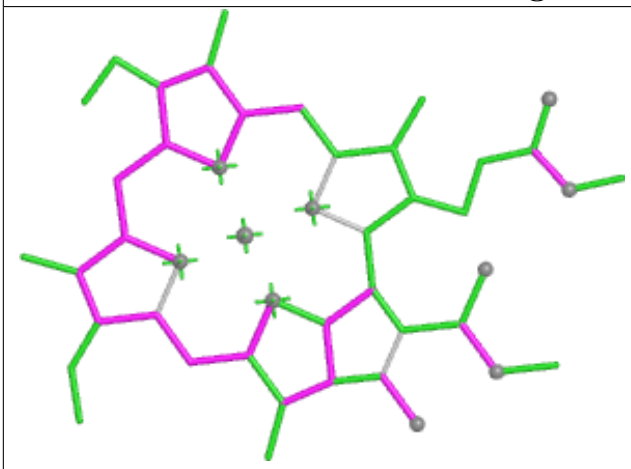


Rings

Ligand CLA 6 617



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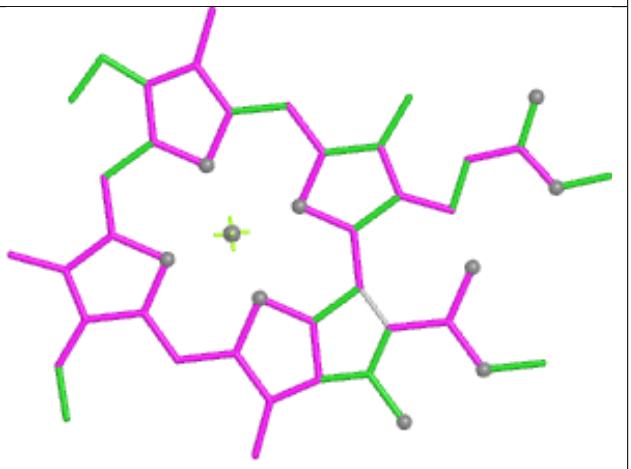

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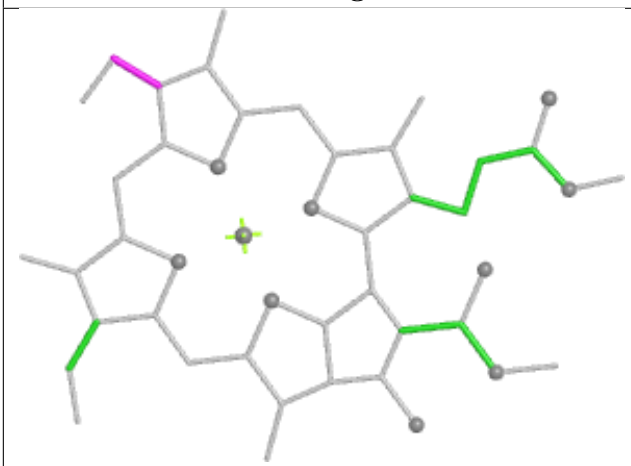
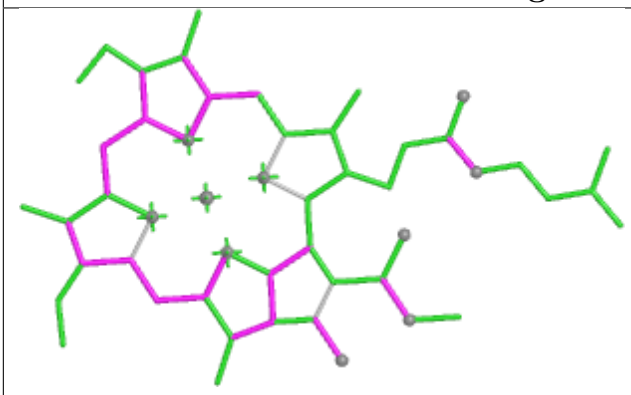


Torsions

Rings

Ligand CLA 5 604



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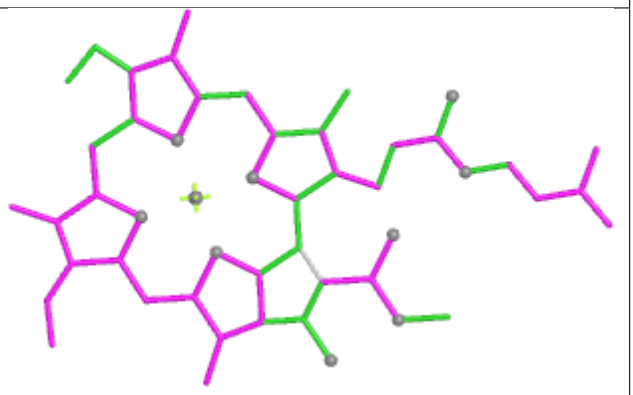

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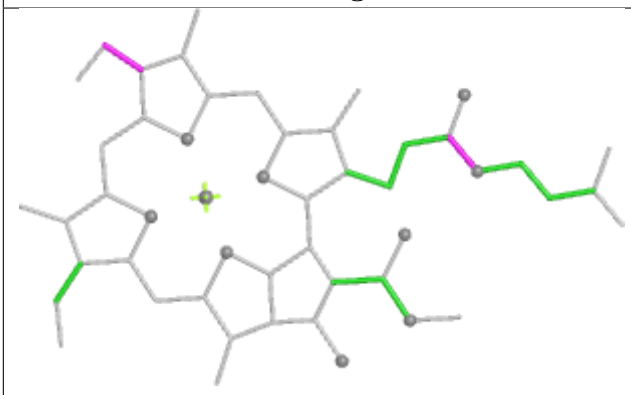
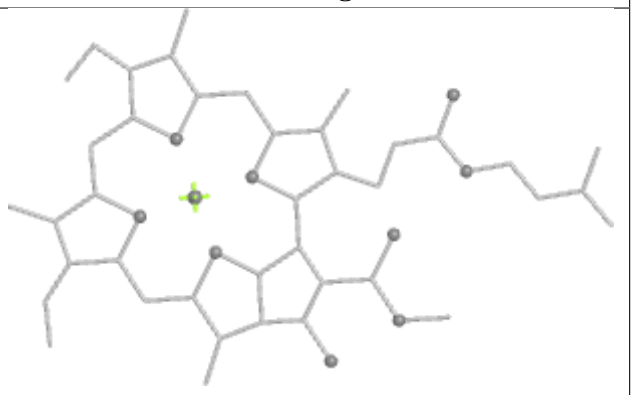
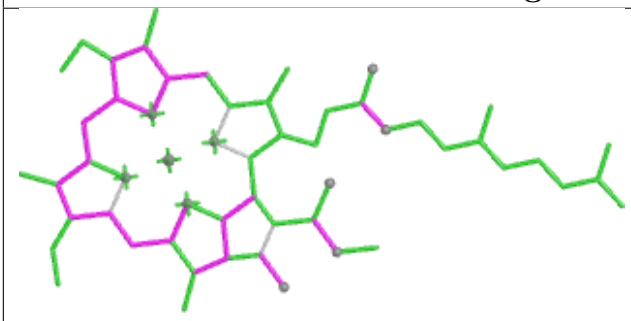


Torsions



Rings

Ligand CLA B 816



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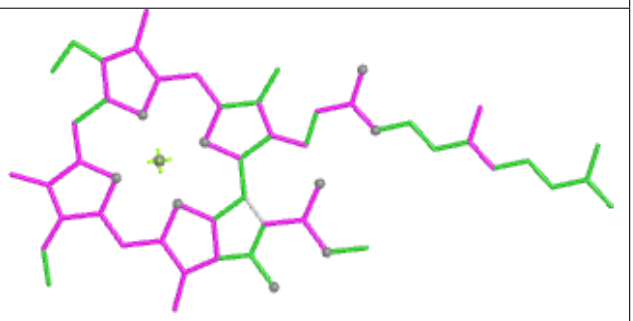
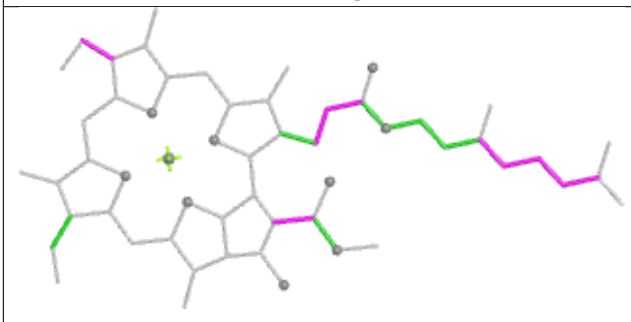


Bond angles



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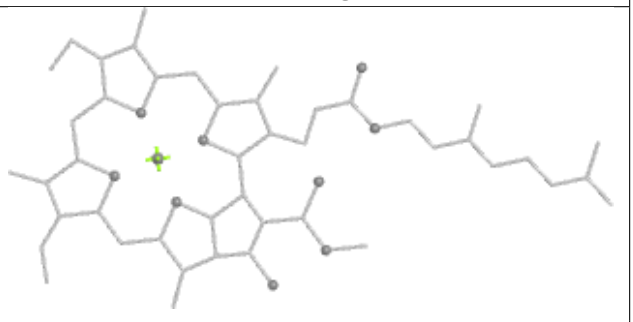
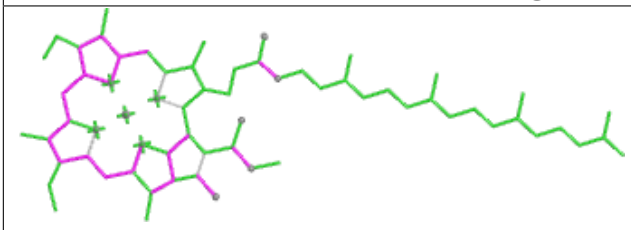


Rings

Ligand CLA 1 602



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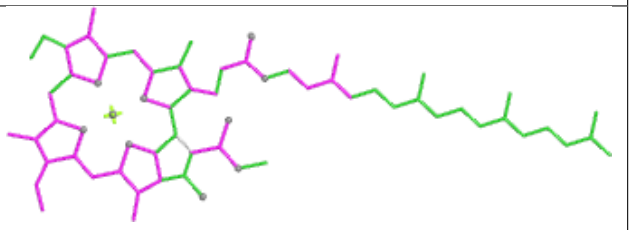

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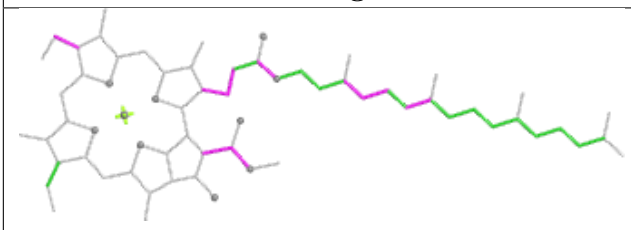

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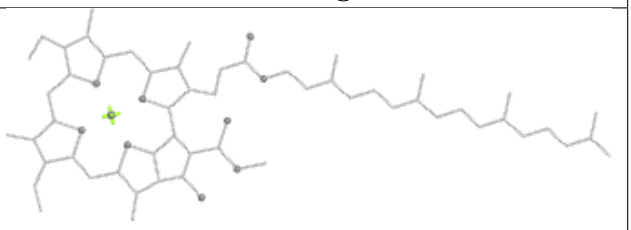
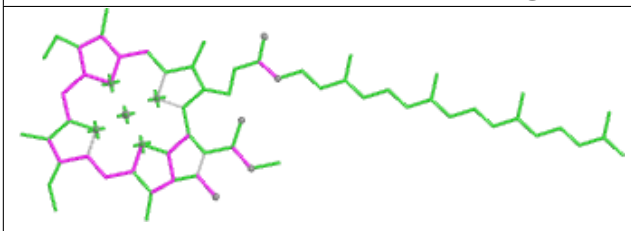


Rings

Ligand CLA A 806



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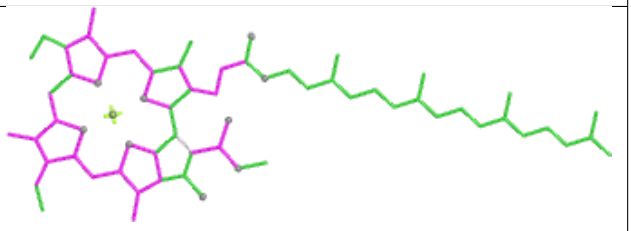

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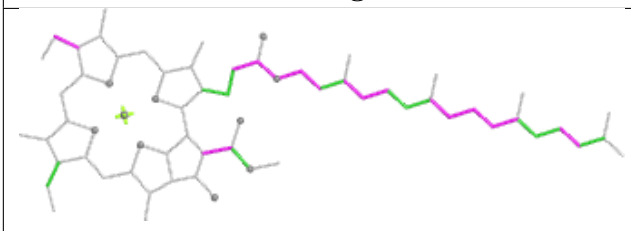

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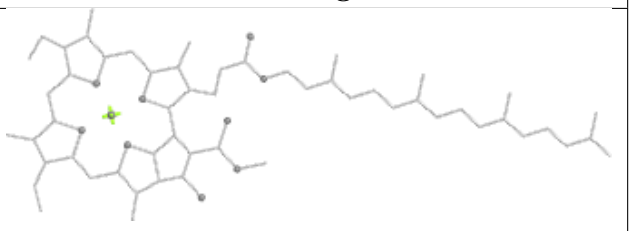
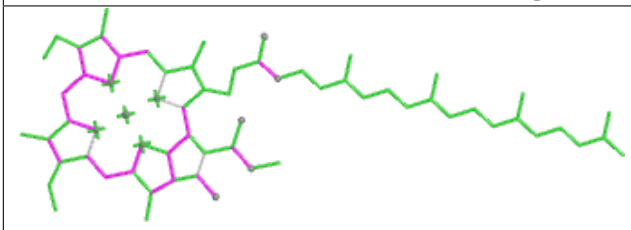


Rings

Ligand CL0 A 801



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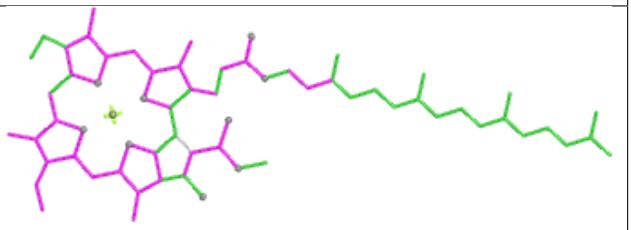
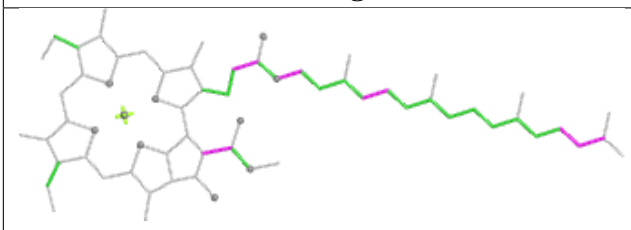


Bond angles



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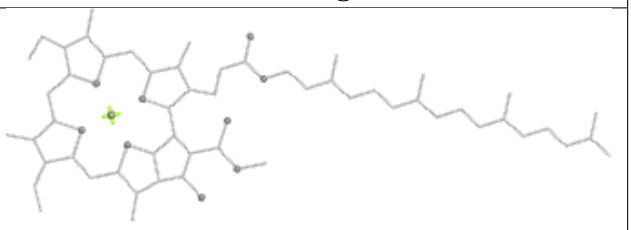
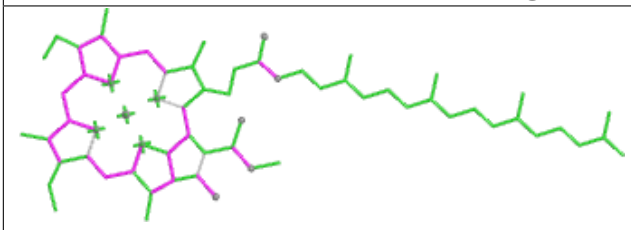


Rings

Ligand CLA A 830



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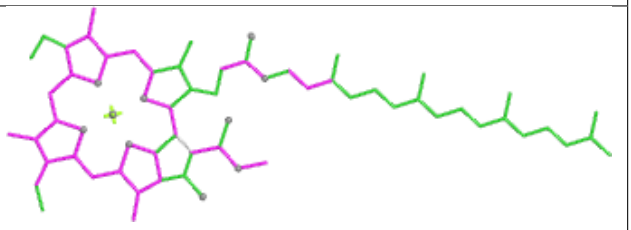
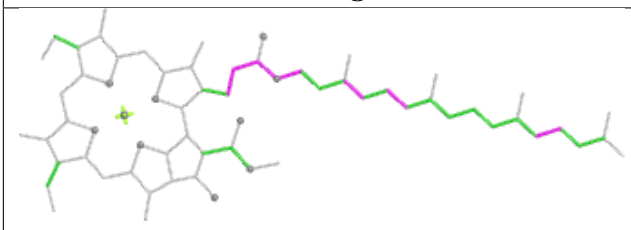


Bond angles



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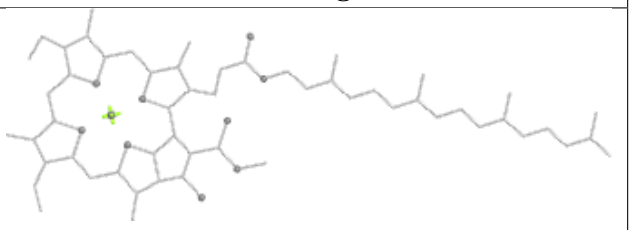
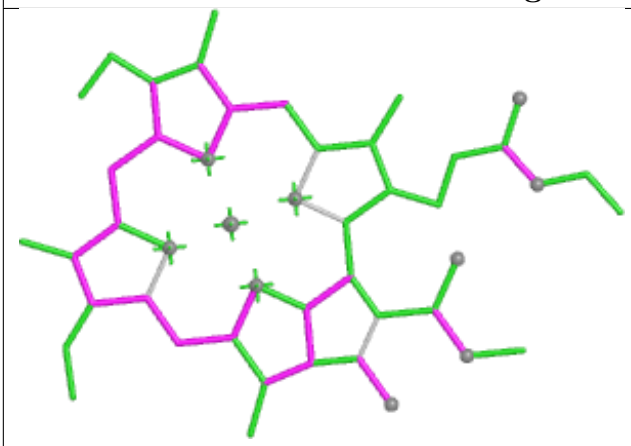
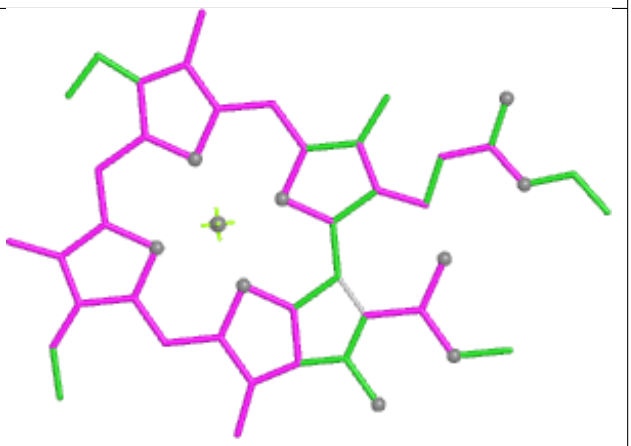


Rings

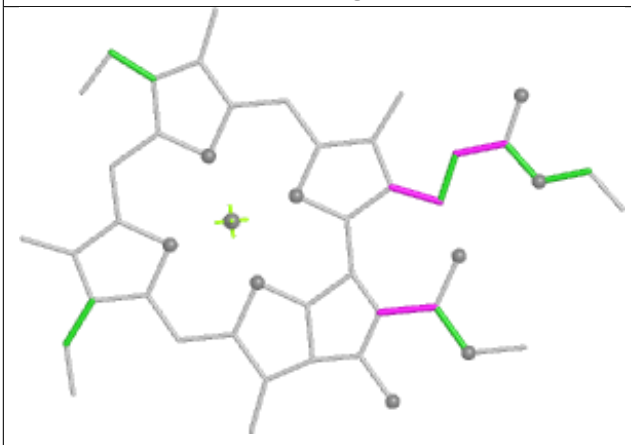
Ligand CLA B 838



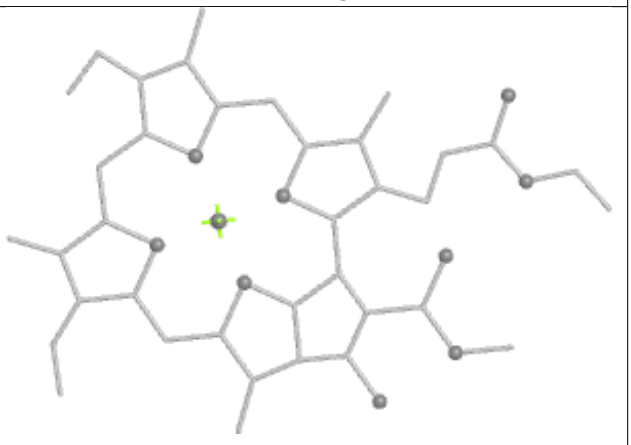
Bond lengths



Bond angles

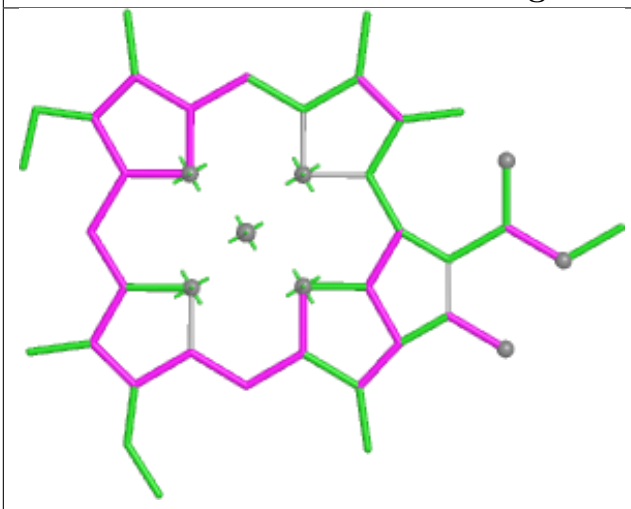


Torsions



Rings

Ligand CLA 4 616



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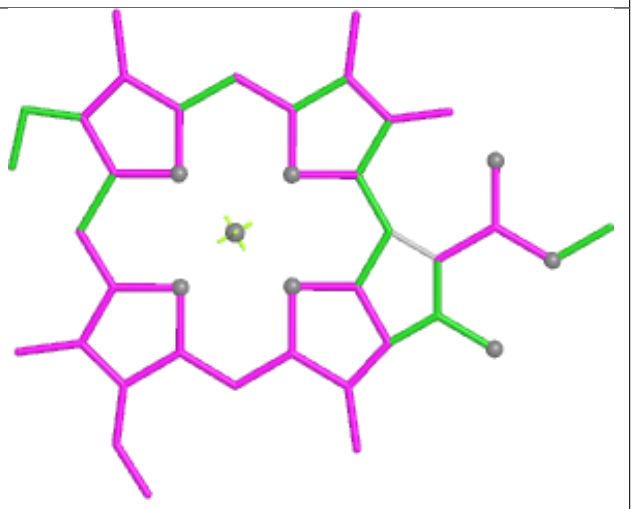
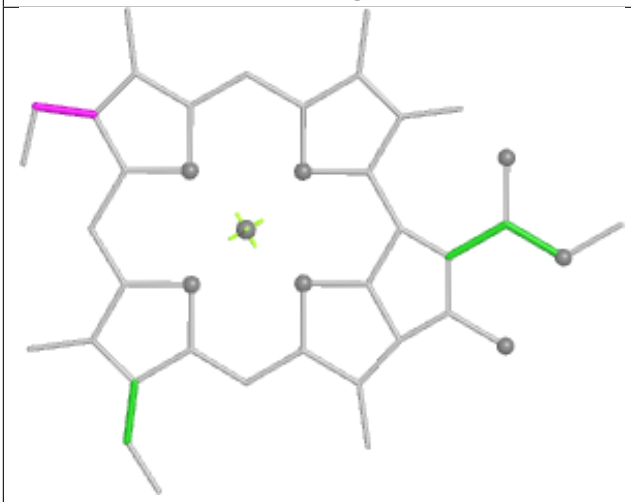


Bond angles



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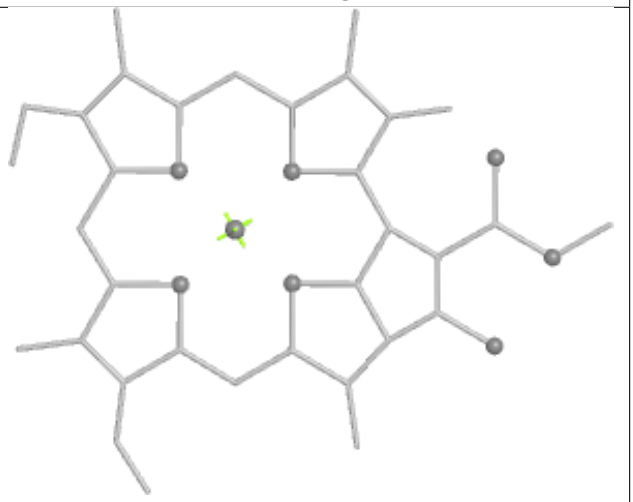
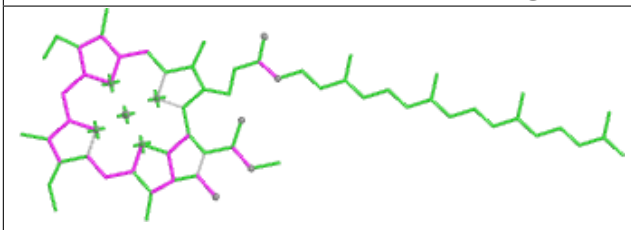


Rings

Ligand CLA B 802



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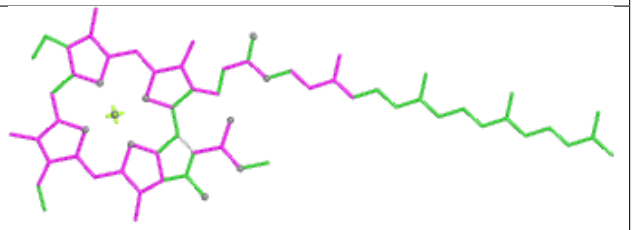

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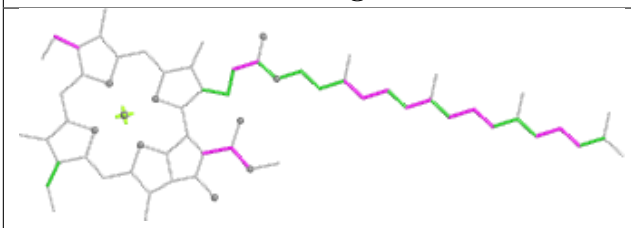

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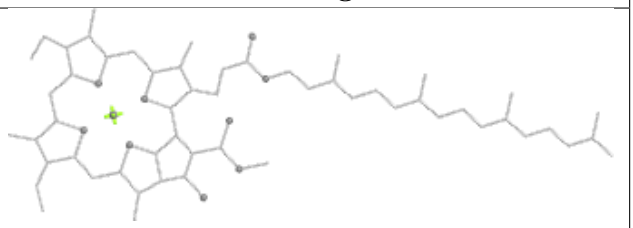
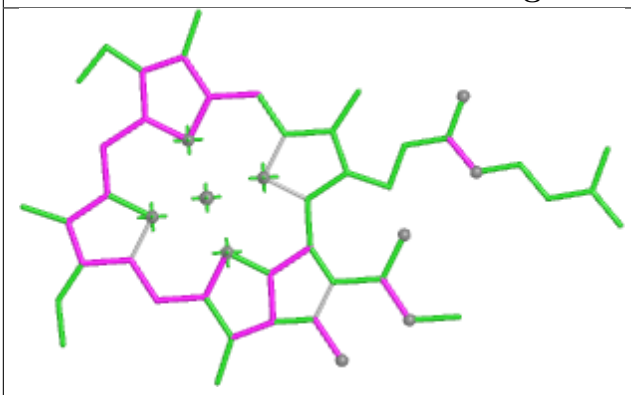


Rings

Ligand CLA A 836



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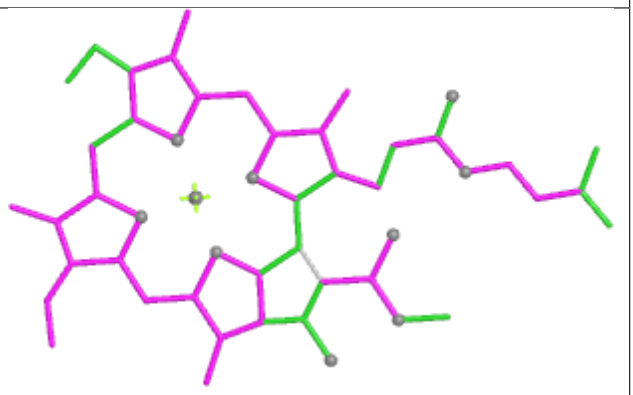

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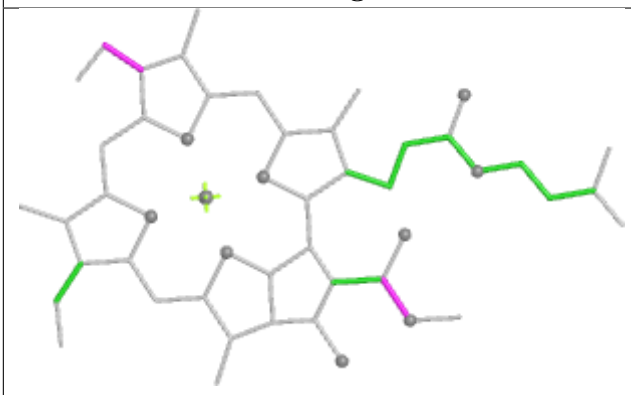

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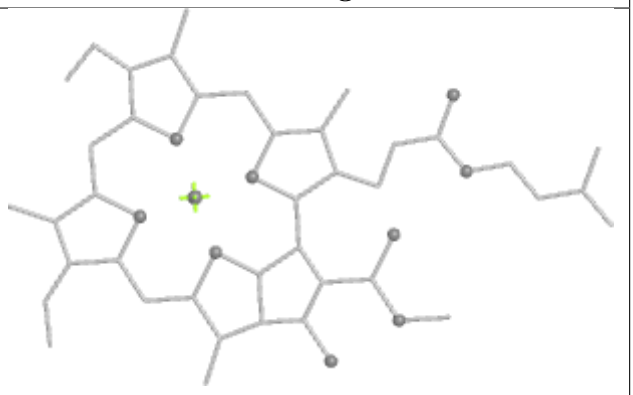
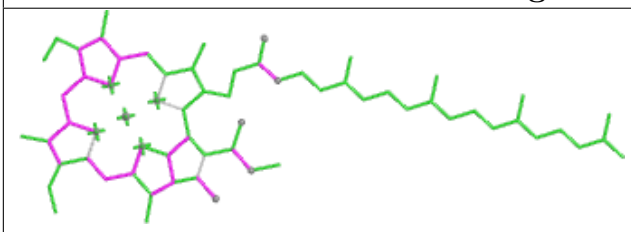


Rings

Ligand CLA 7 601



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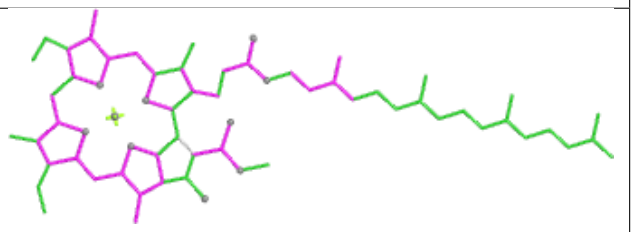
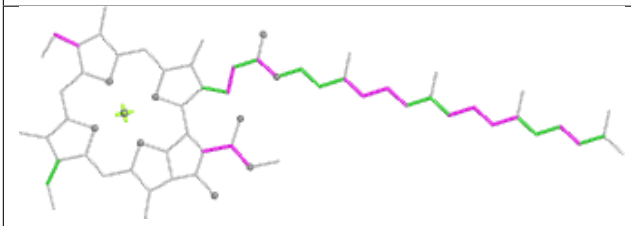


Bond angles



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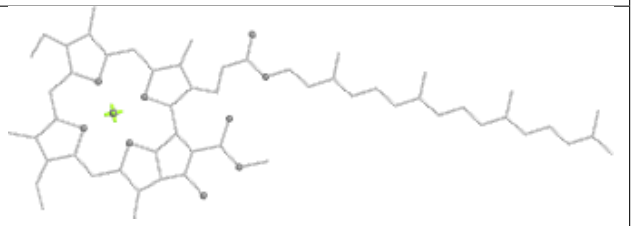
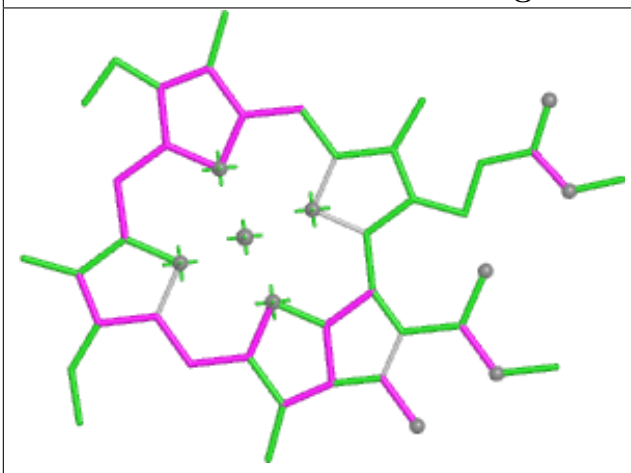


Rings

Ligand CLA K 4003



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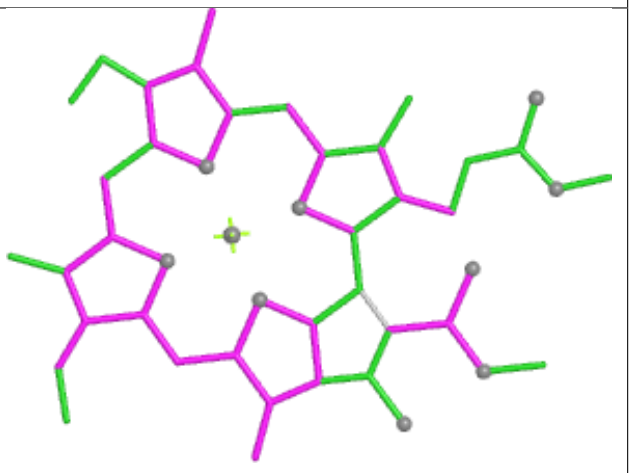

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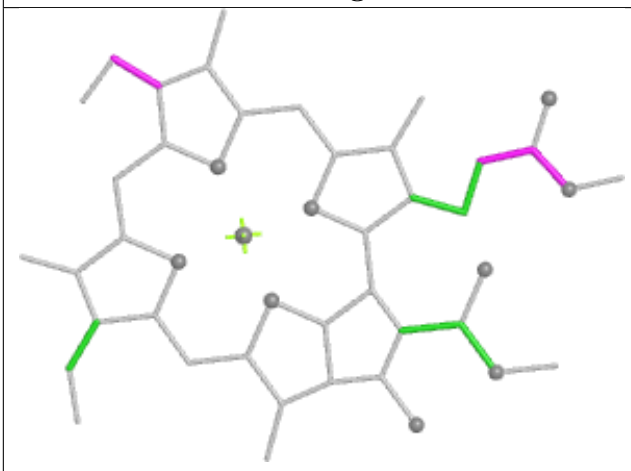

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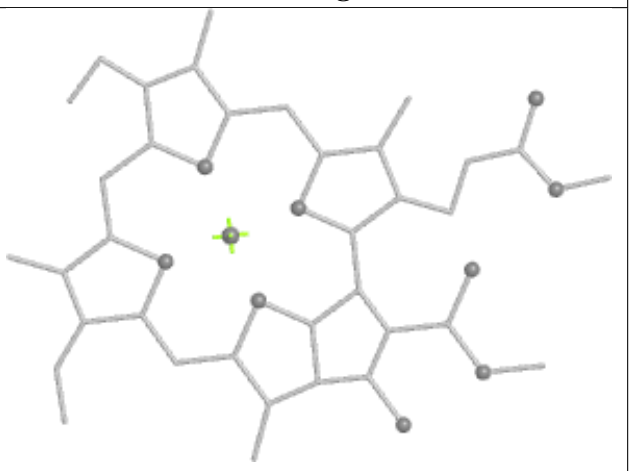
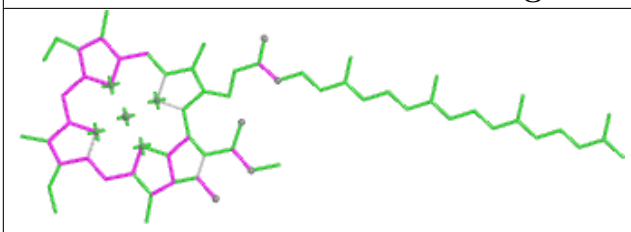


Rings

Ligand CLA B 812



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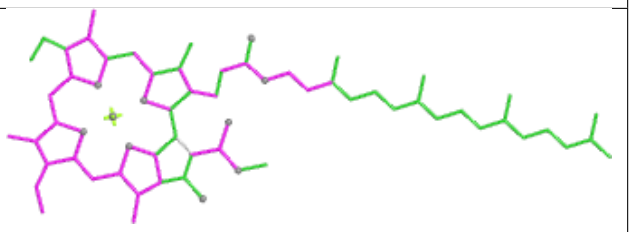
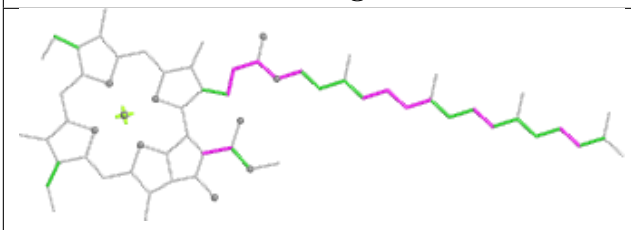


Bond angles



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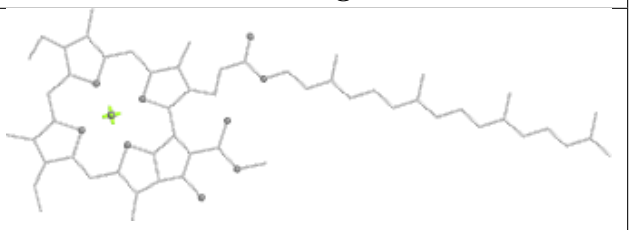
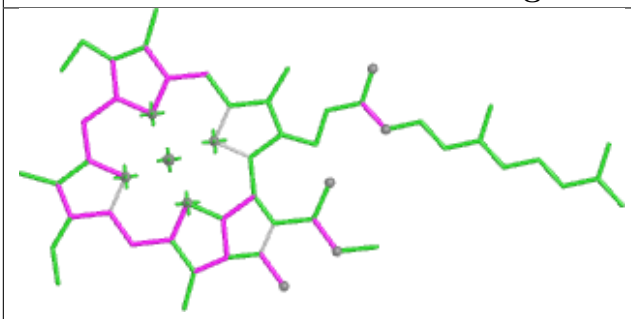


Rings

Ligand CLA A 825



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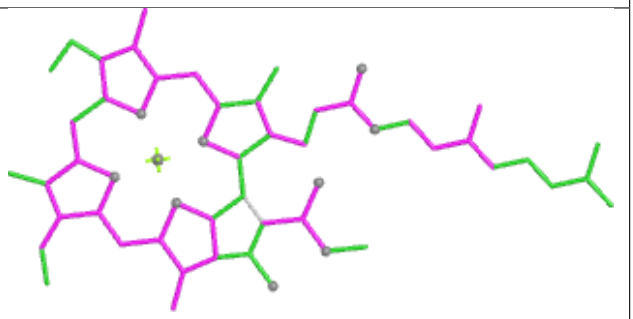
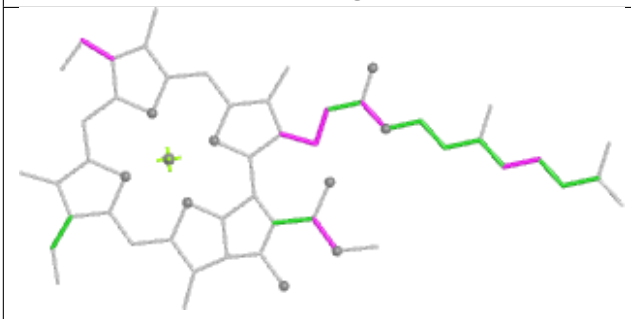


Bond angles



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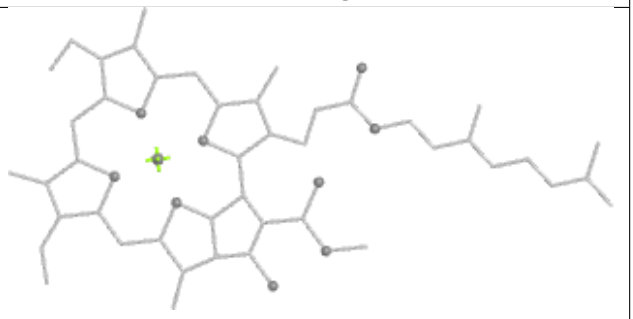
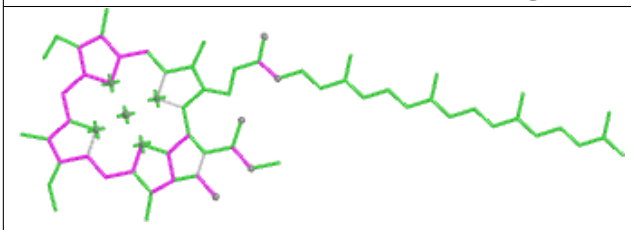


Rings

Ligand CLA B 810



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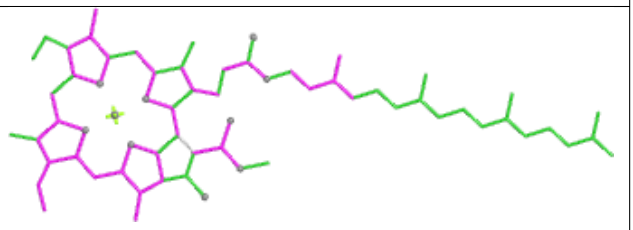

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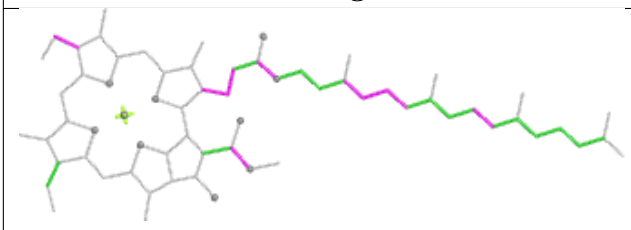

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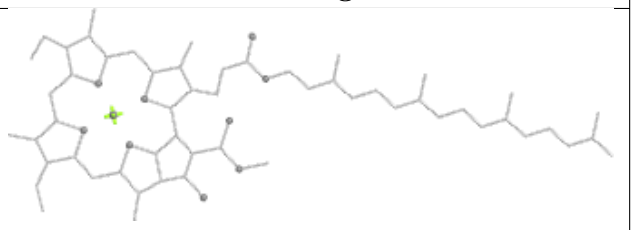
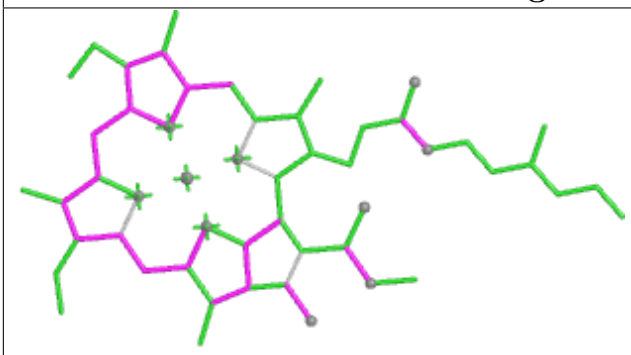


Rings

Ligand CLA 4 612



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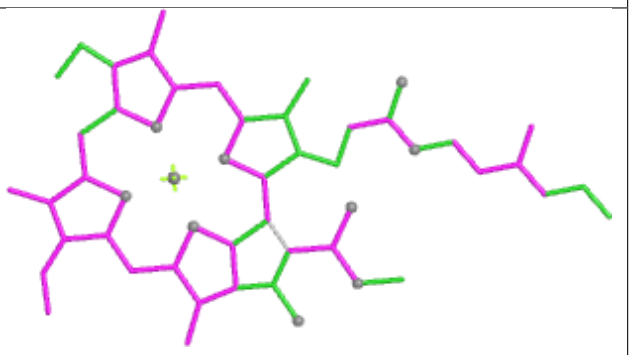
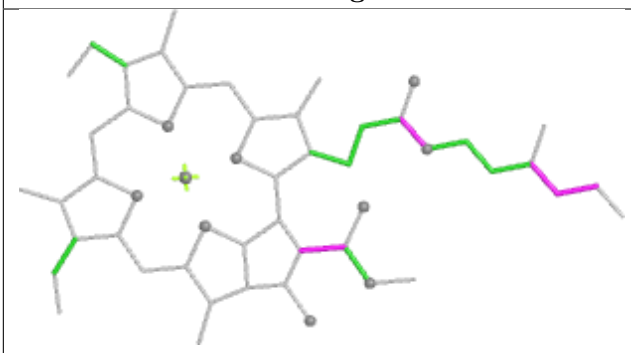


Bond angles



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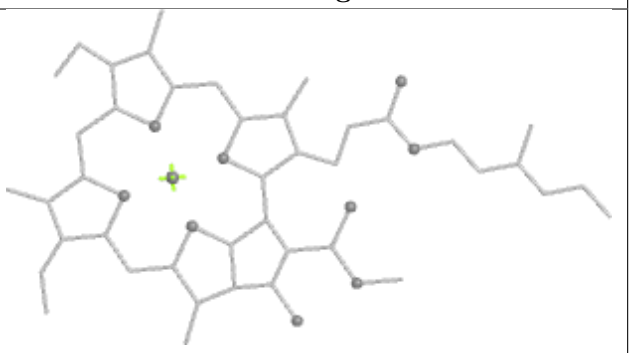
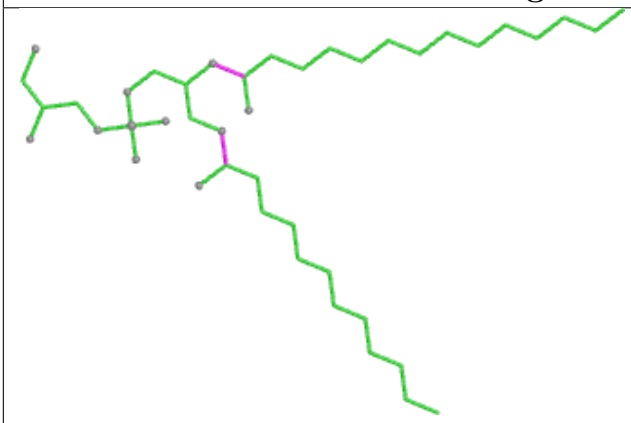


Rings

Ligand LHG 1 620



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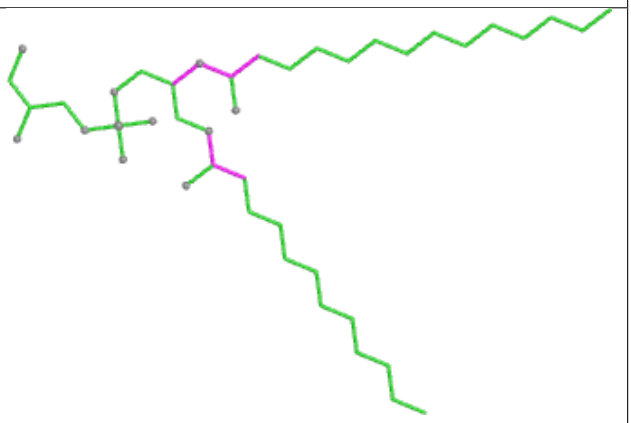

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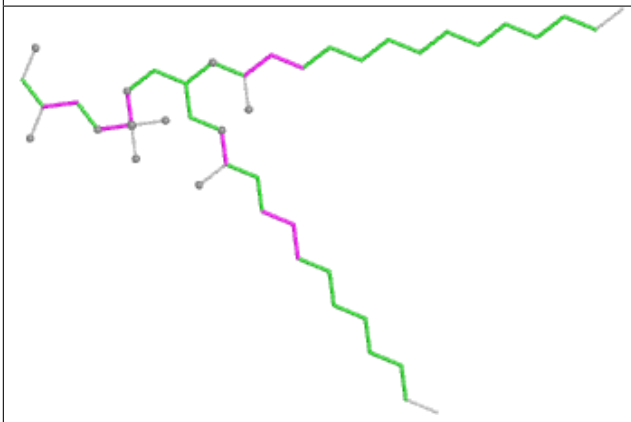

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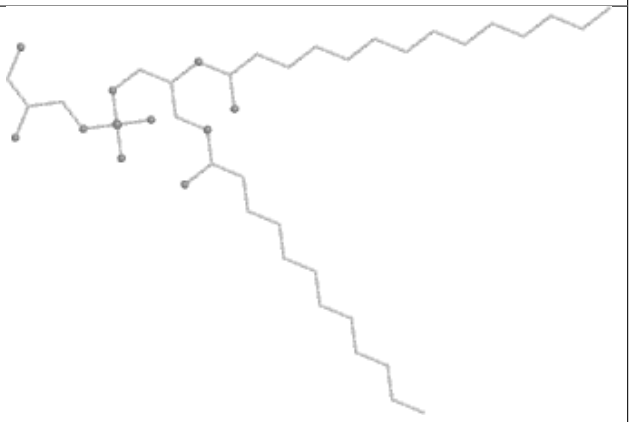
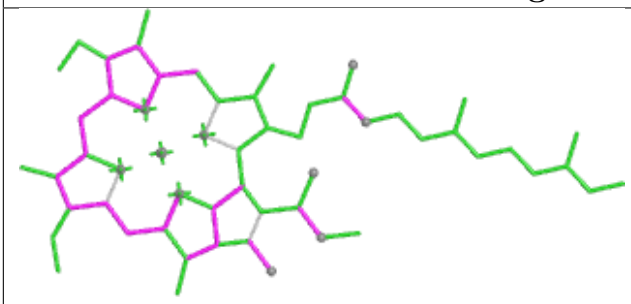
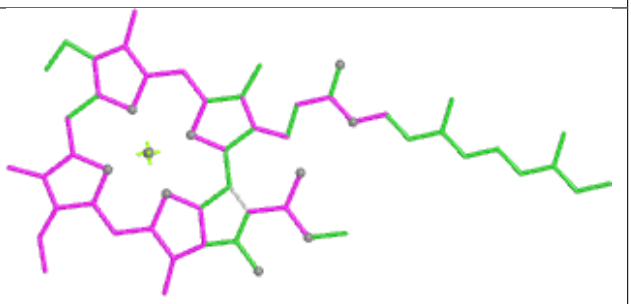
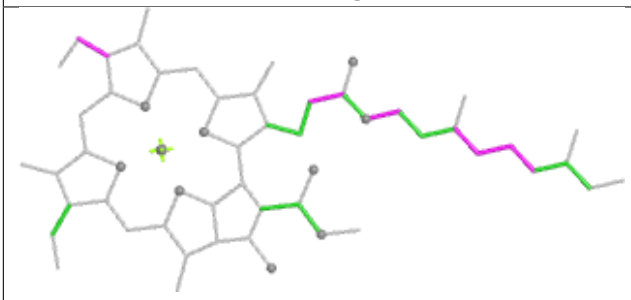
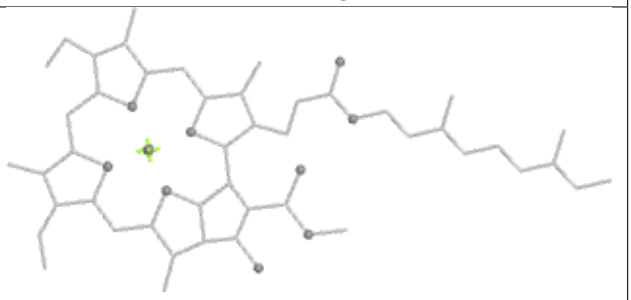
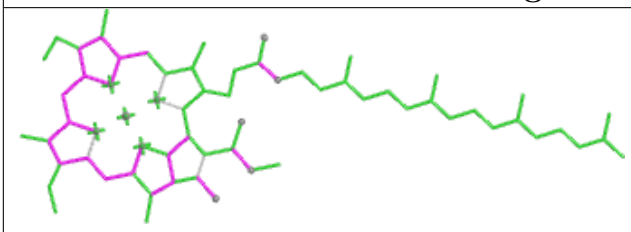
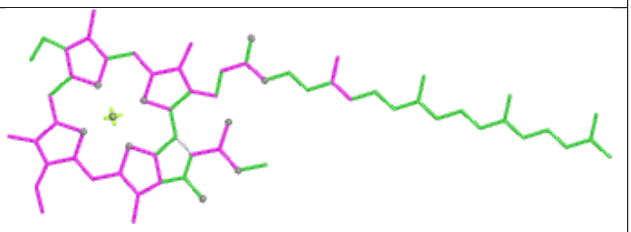
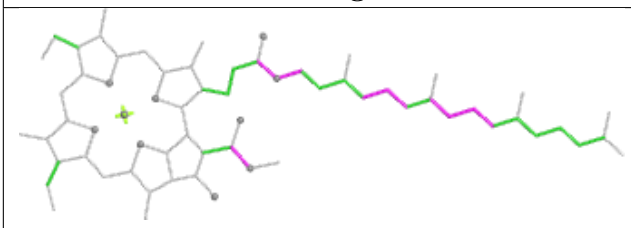
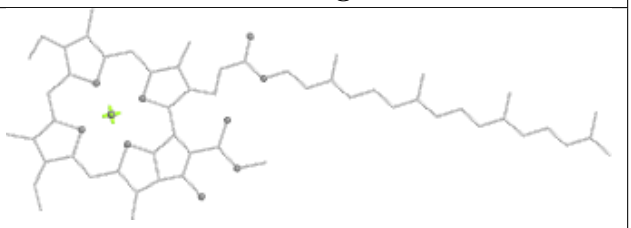
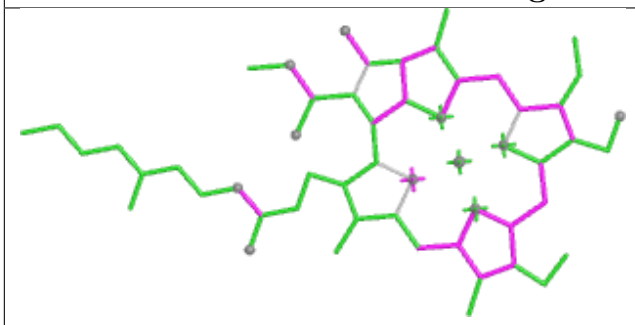


Rings

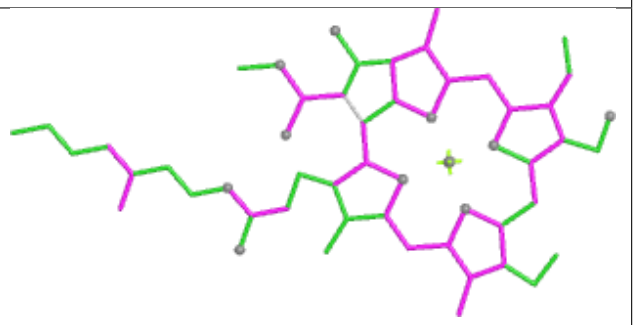
Ligand CLA 5 613	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA B 834	
	
Bond lengths	Bond angles
	
Torsions	Rings

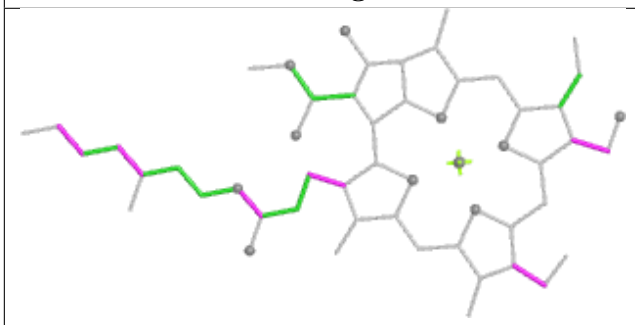
Ligand CHL 7 607



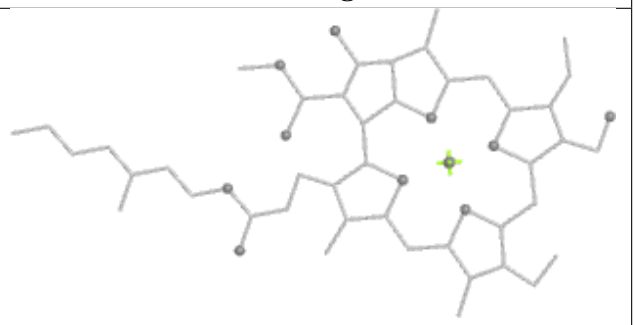
Bond lengths



Bond angles

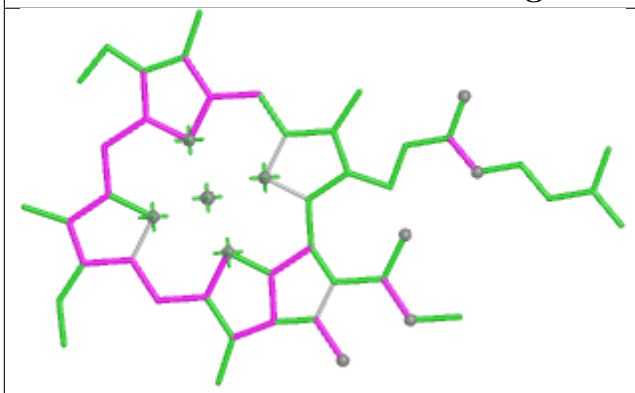


Torsions



Rings

Ligand CLA B 830



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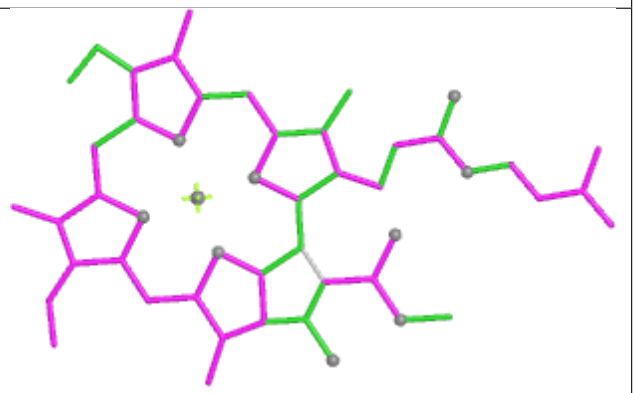
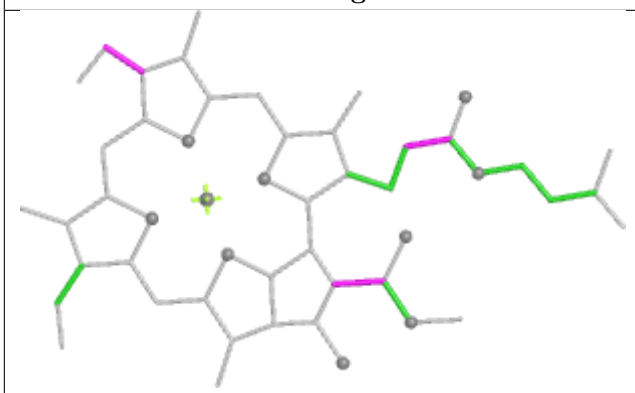
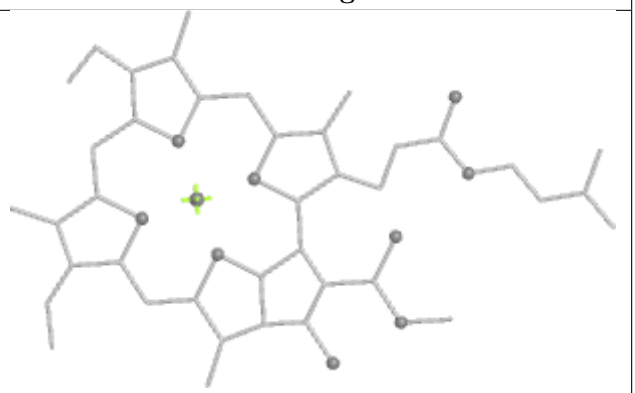


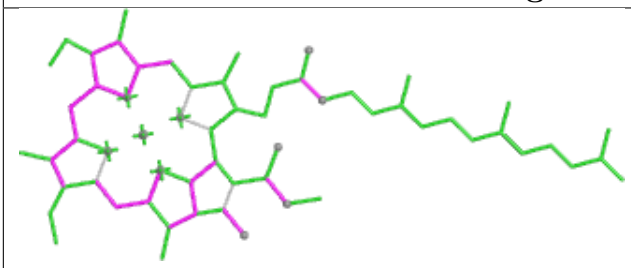
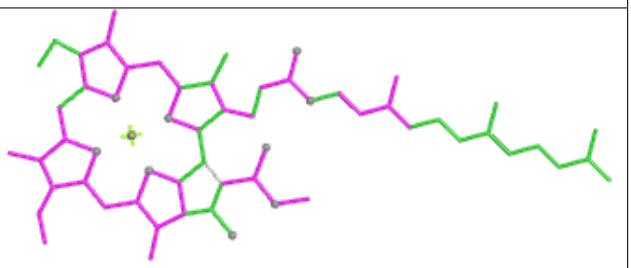
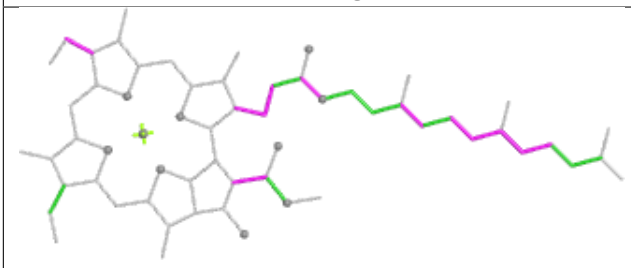
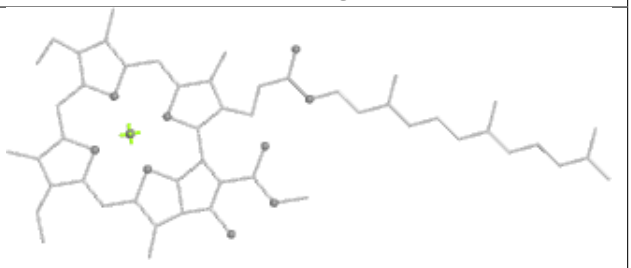
Bond angles

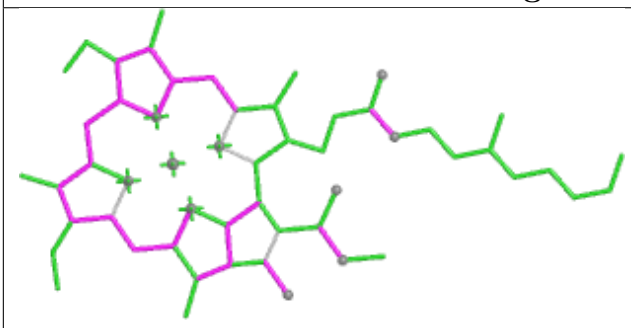
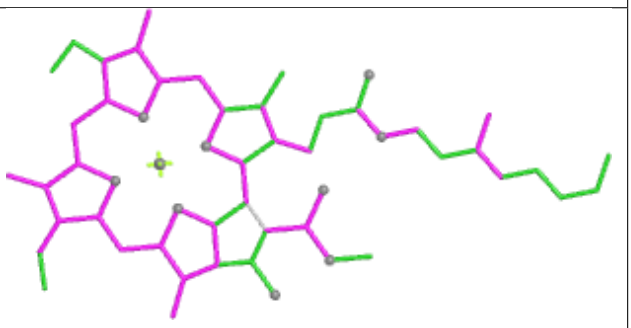
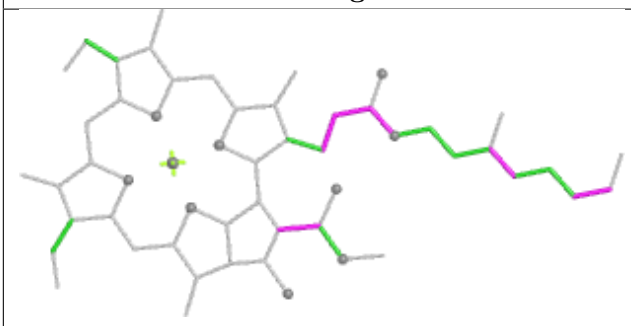
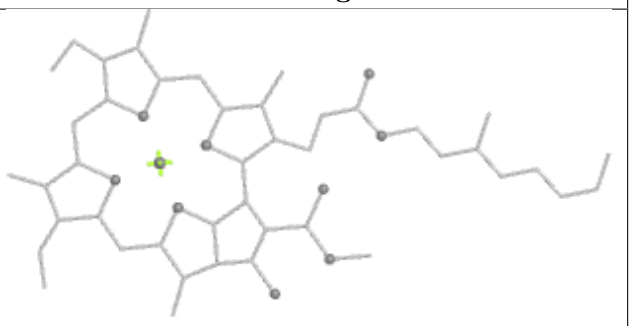


Torsions

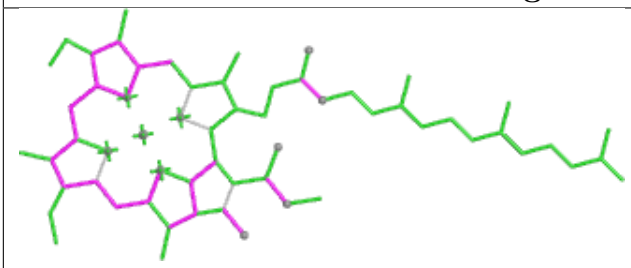


Rings

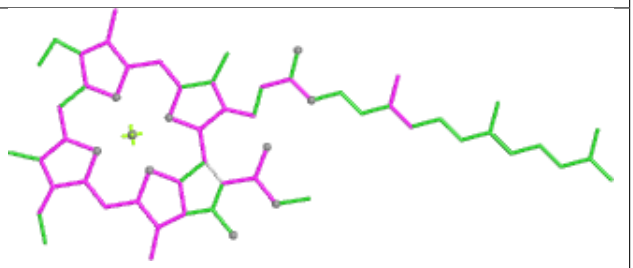
Ligand CLA Z 610	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA A 813	
 Bond lengths	 Bond angles
 Torsions	 Rings

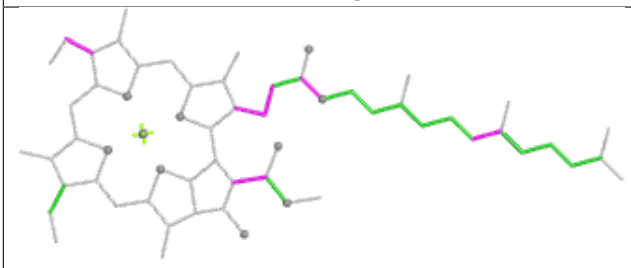
Ligand CLA A 815



Bond lengths



Bond angles



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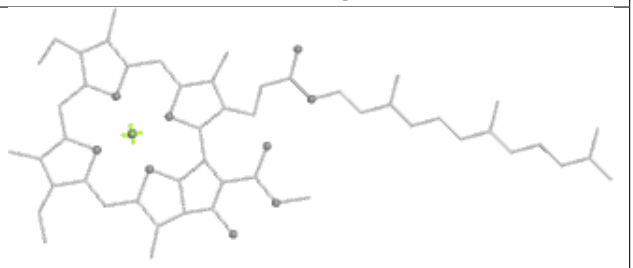
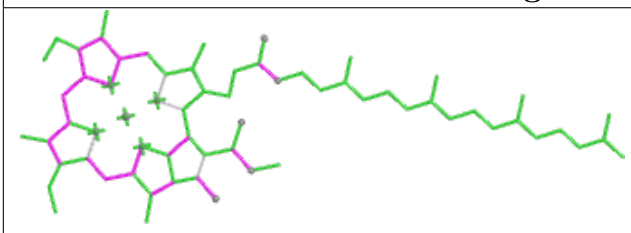


Rings

Ligand CLA A 854



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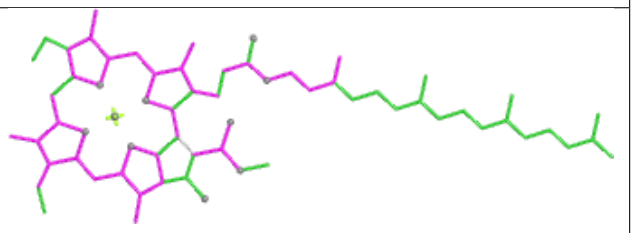
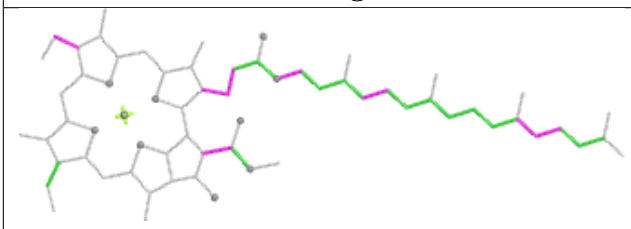


Bond angles



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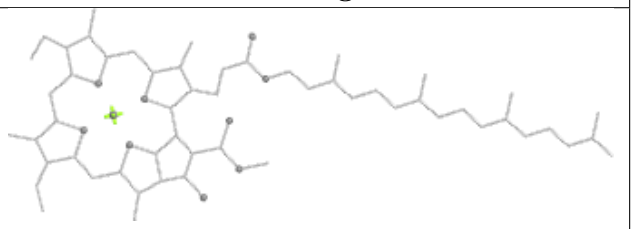
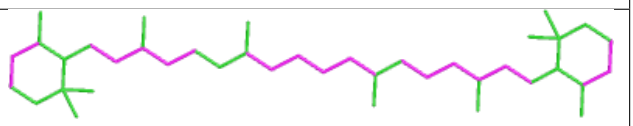


Rings

Ligand BCR A 850

Bond lengths



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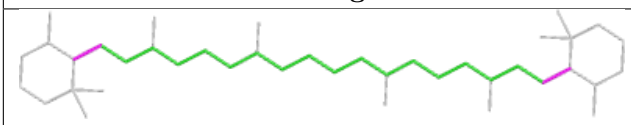

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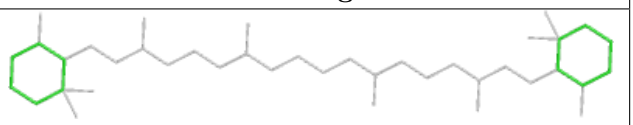
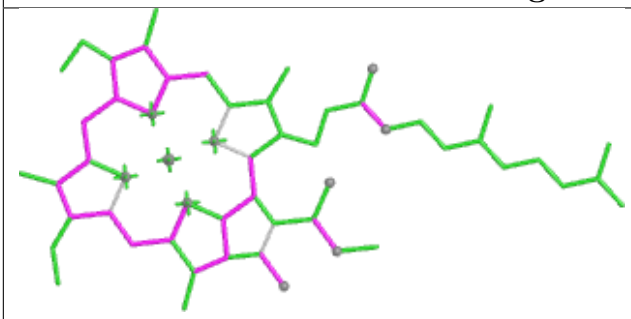


Rings

Ligand CLA 4 611



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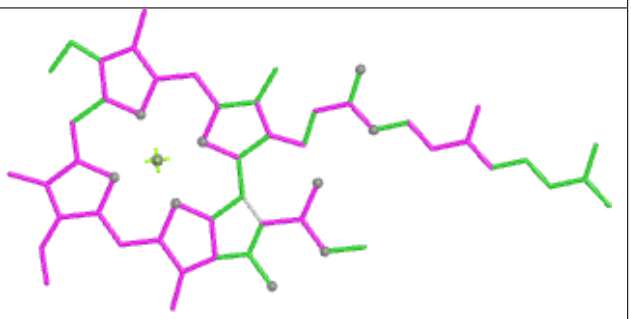
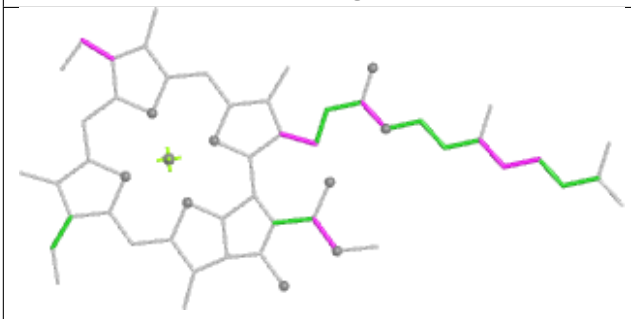


Bond angles



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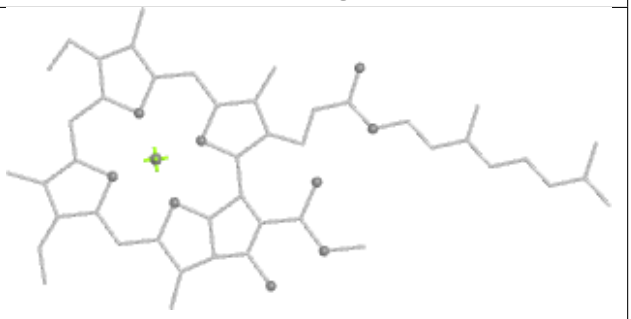
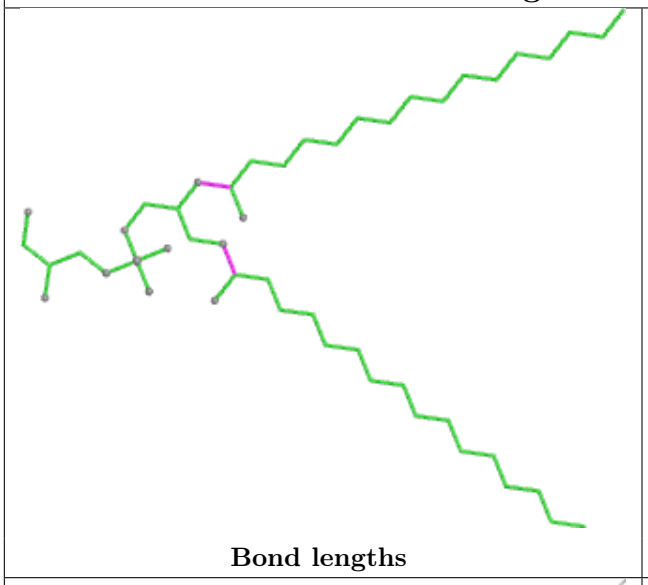


Rings

Ligand LHG A 846



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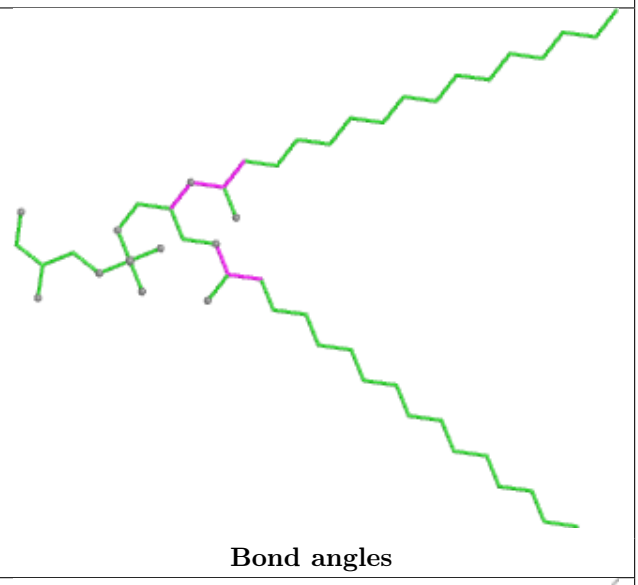
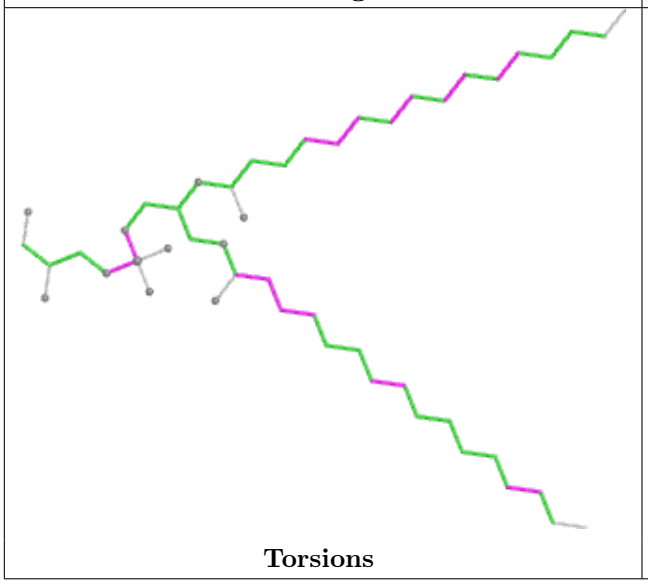


Bond angles



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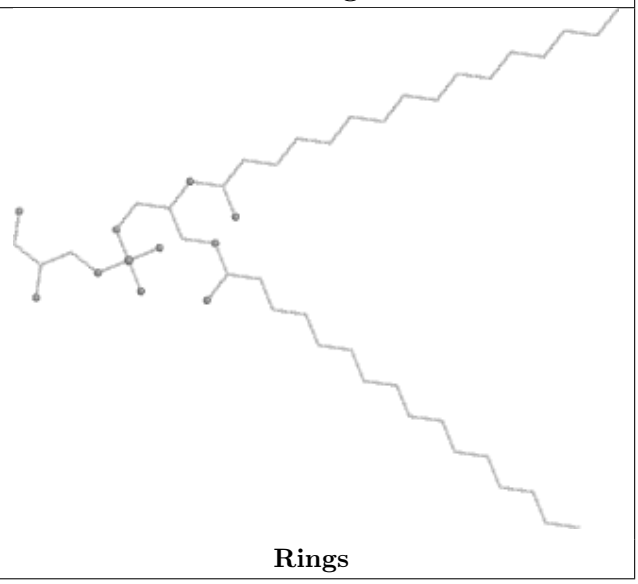
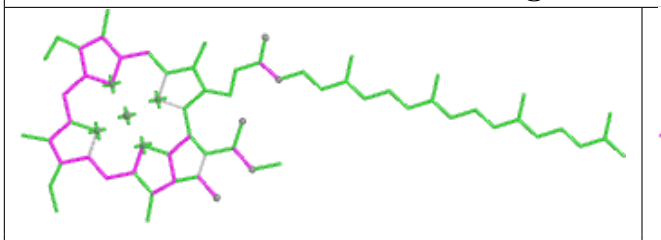


Rings

Ligand CLA B 824



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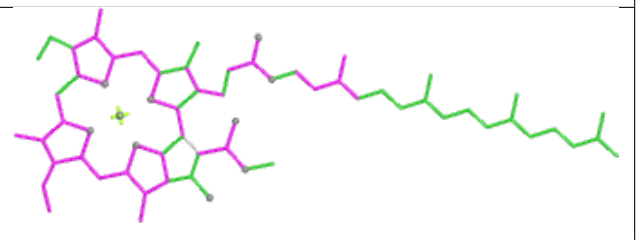
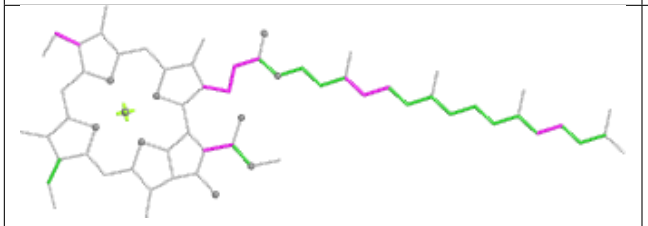


Bond angles



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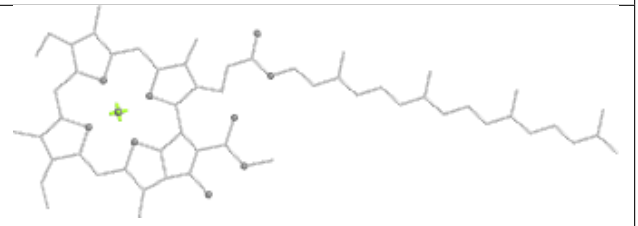
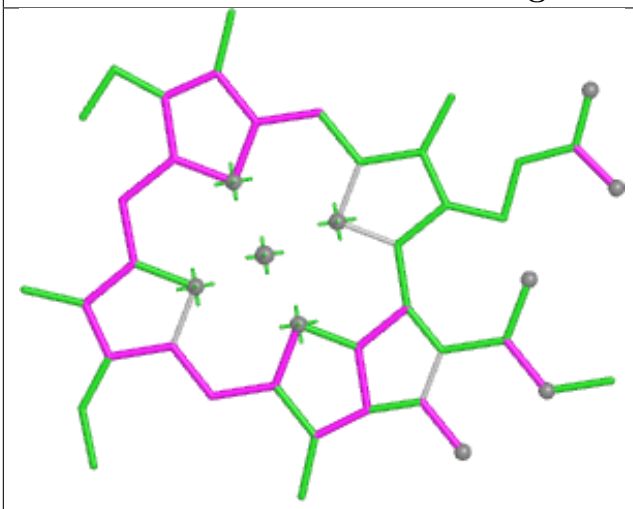


Rings

Ligand CLA 3 614



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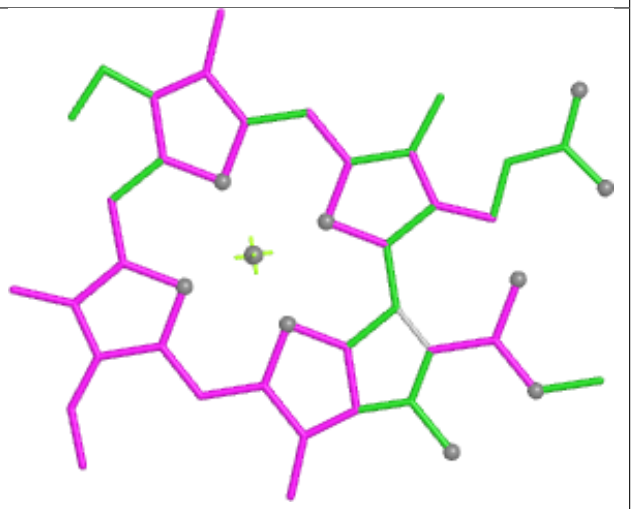
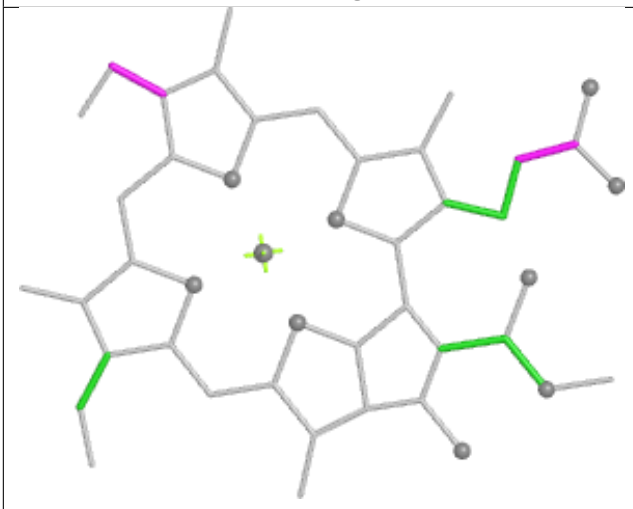


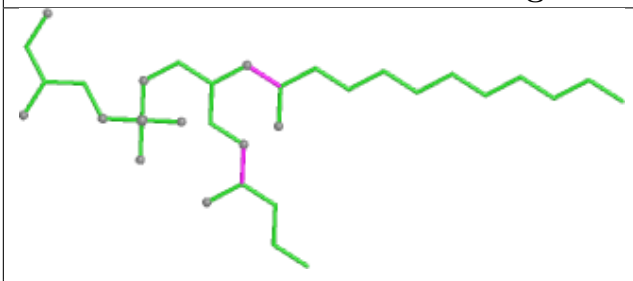
Bond angles



Torsions

Rings

Ligand LHG 4 623



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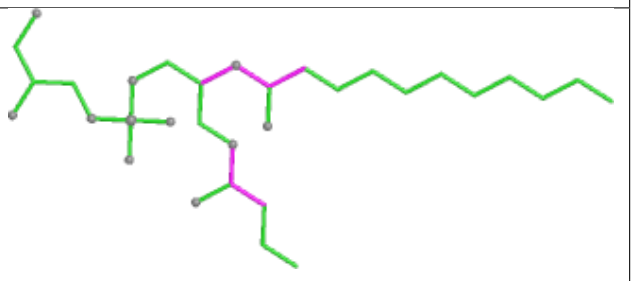

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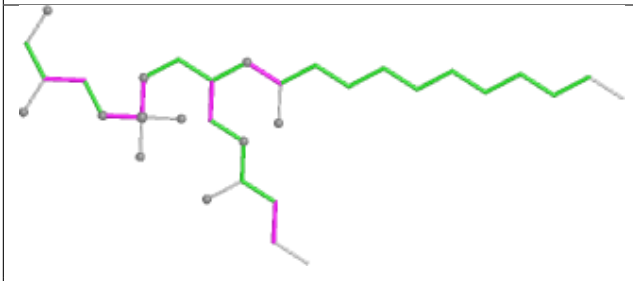

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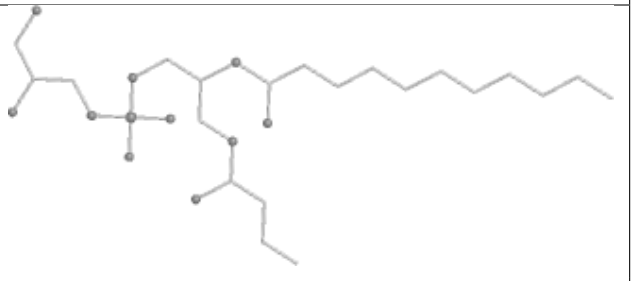
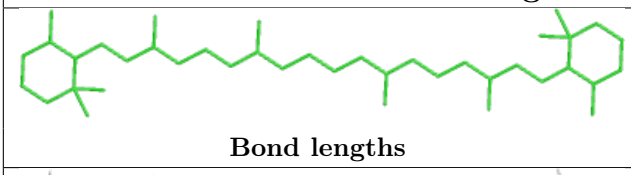


Rings

Ligand BCR B 847



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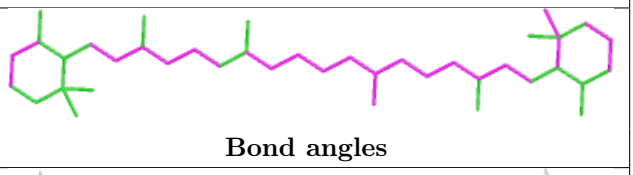

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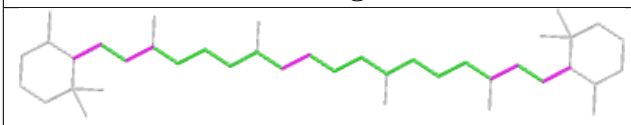

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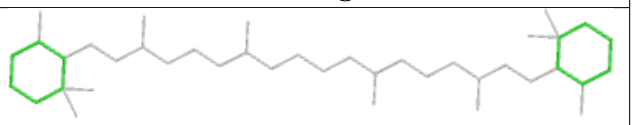
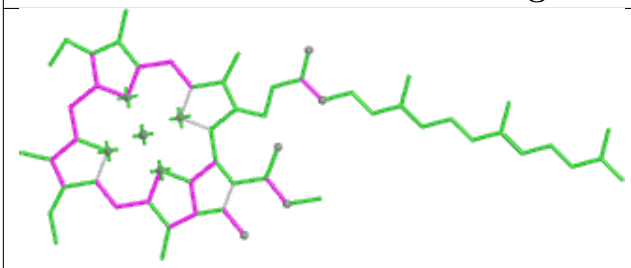


Rings

Ligand CLA 8 610



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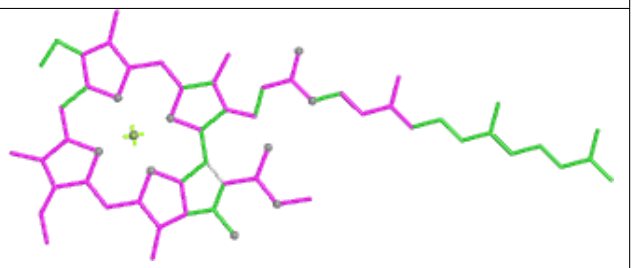

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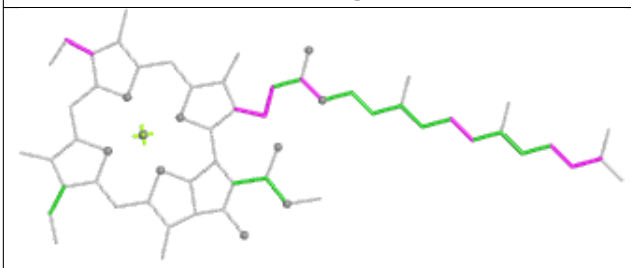

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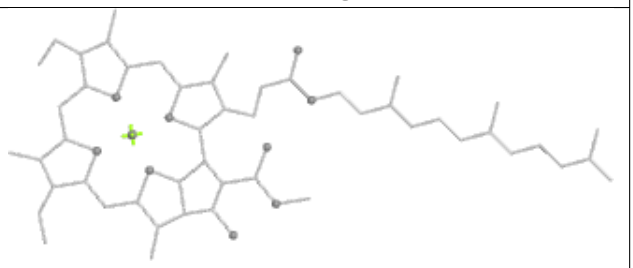
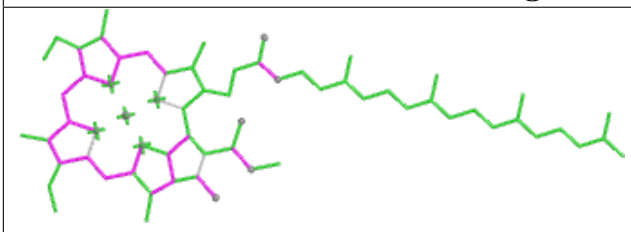


Rings

Ligand CLA A 804



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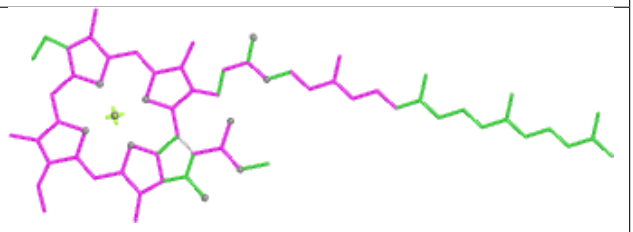
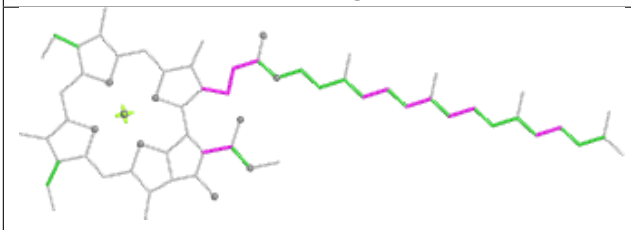


Bond angles



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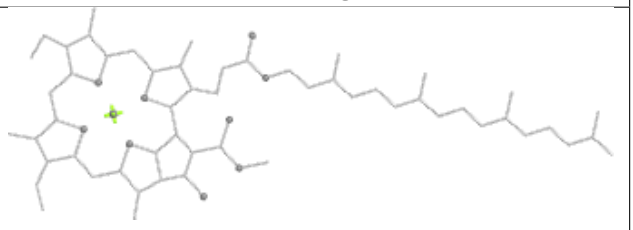
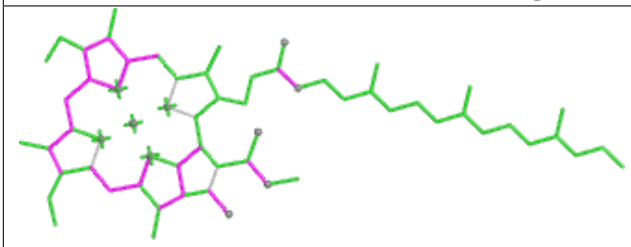
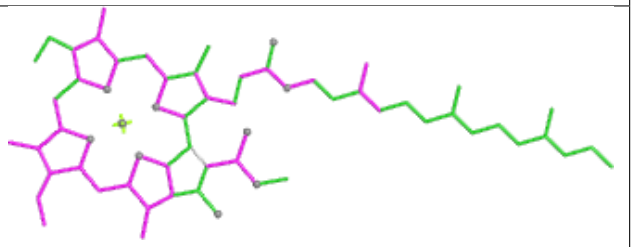


Rings

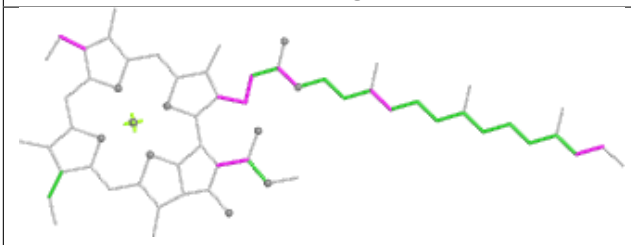
Ligand CLA 8 602



Bond lengths



Bond angles



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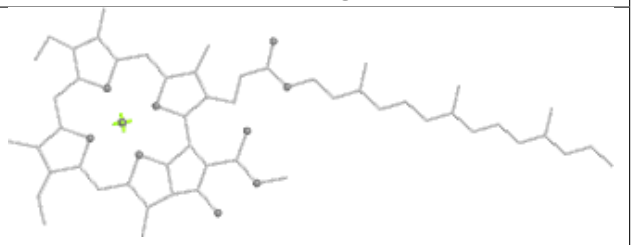
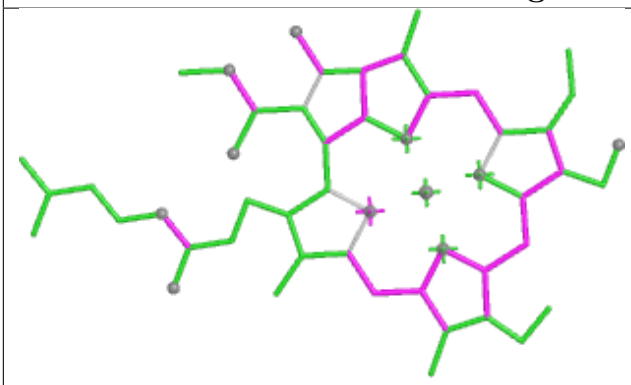
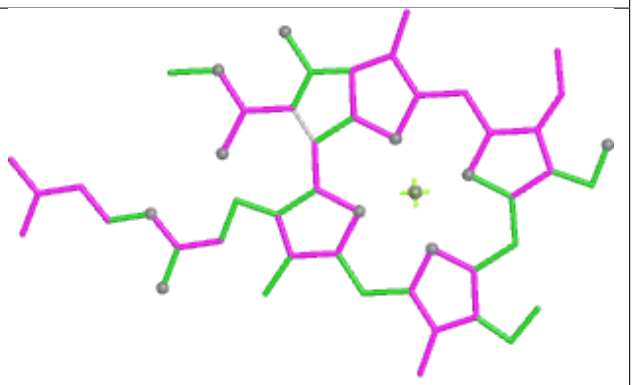


Rings

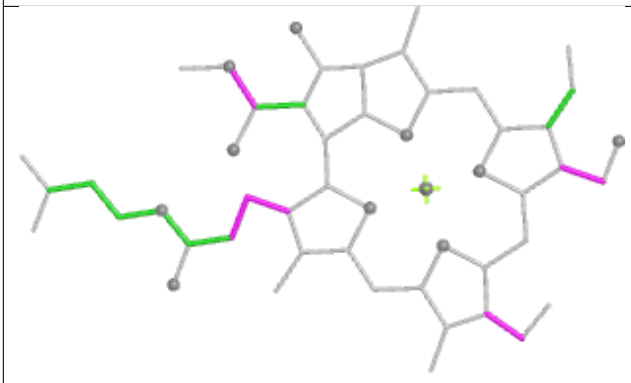
Ligand CHL 5 608



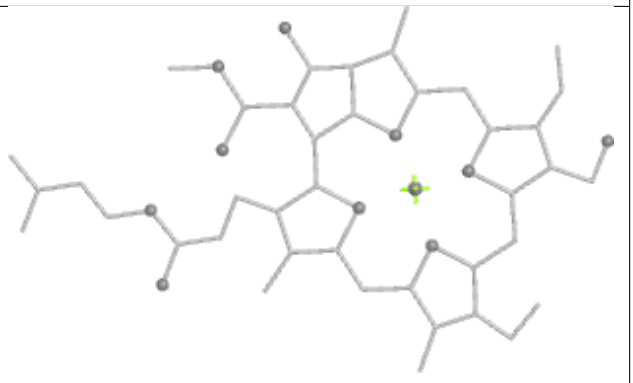
Bond lengths



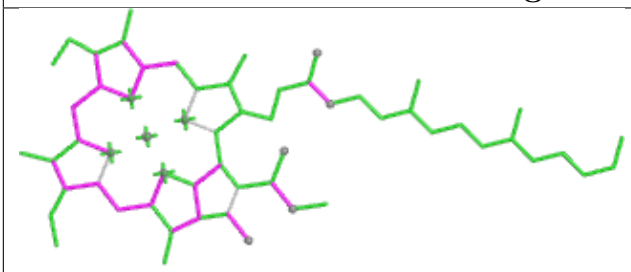
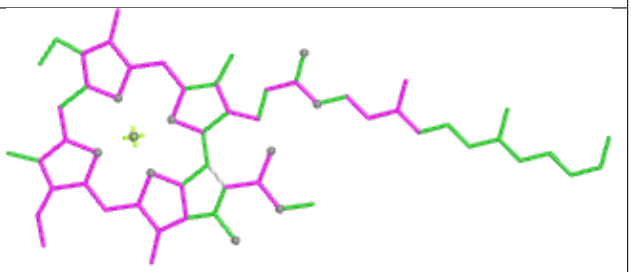
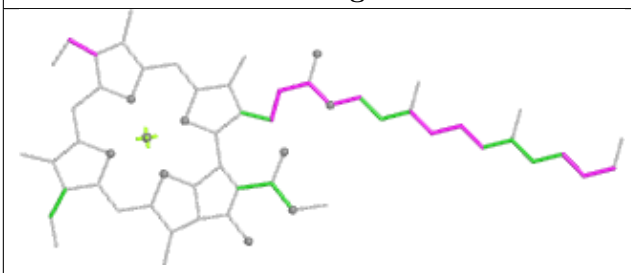
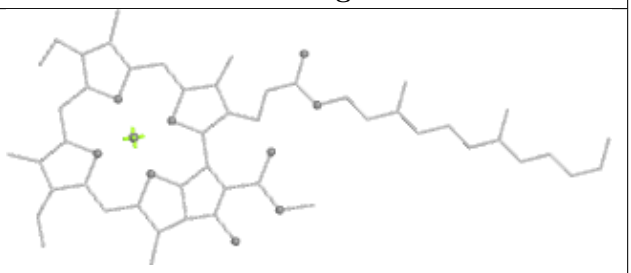
Bond angles

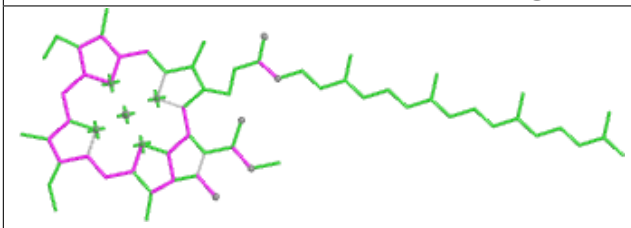
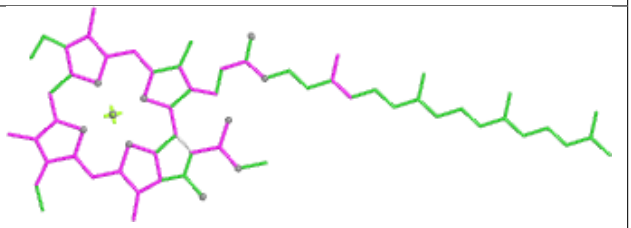
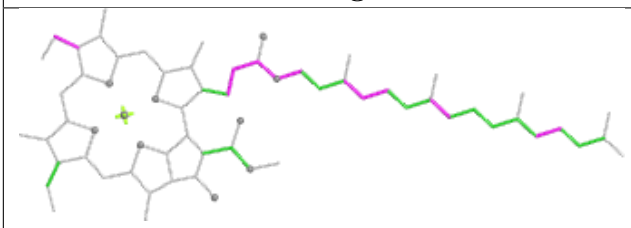
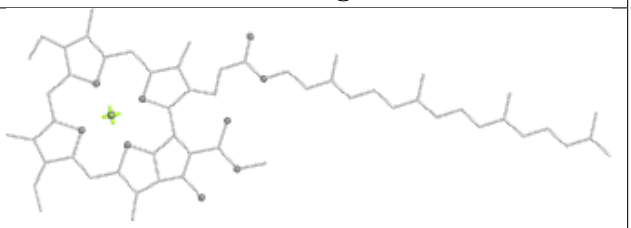


Torsions



Rings

Ligand CLA B 817	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA 1 609	
	
Bond lengths	Bond angles
	
Torsions	Rings

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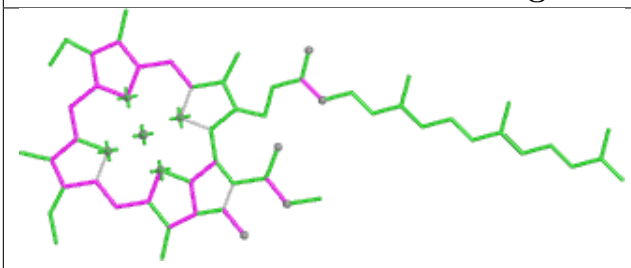
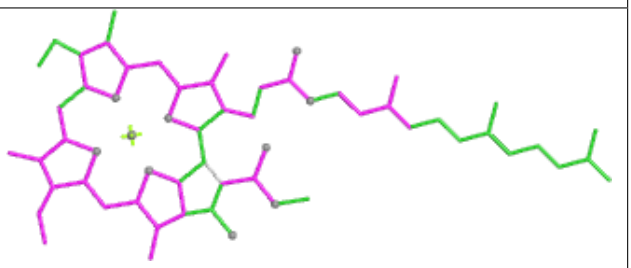
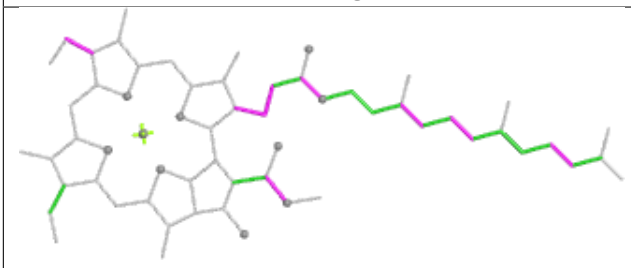
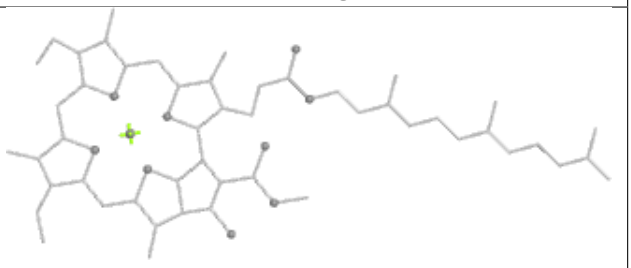
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

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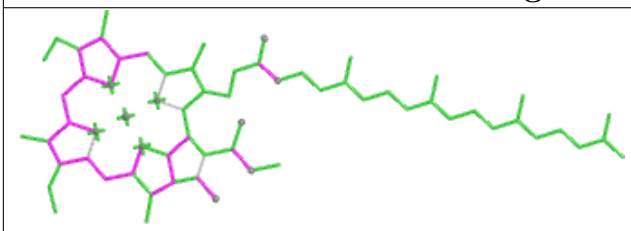
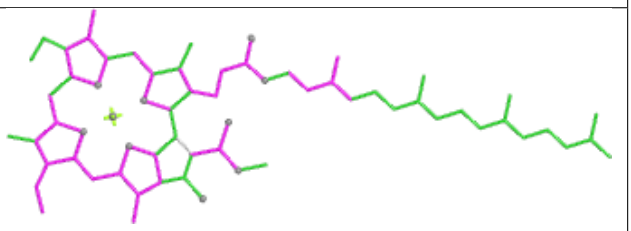
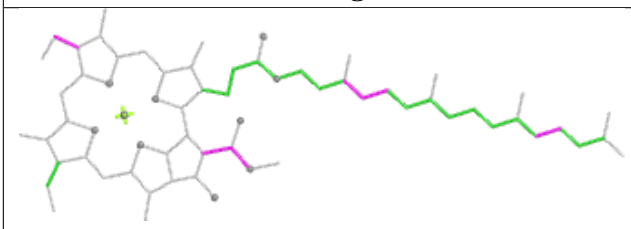
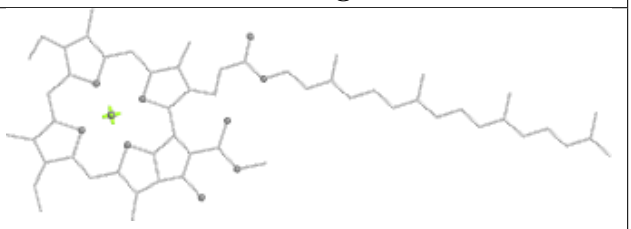
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

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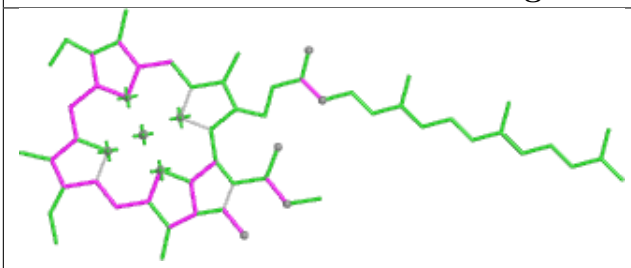
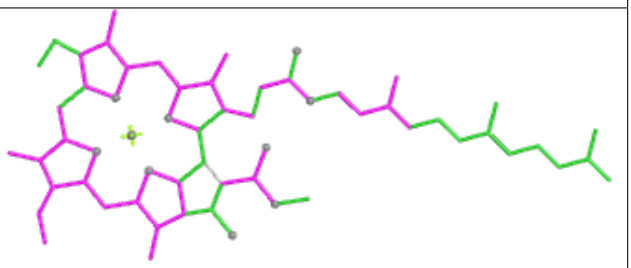
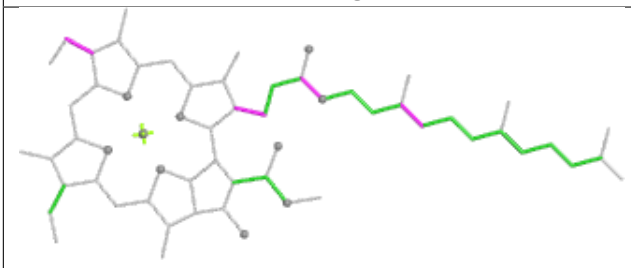
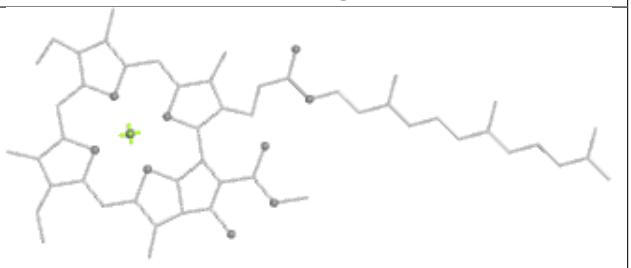
	
Bond lengths	Bond angles
	
Torsions	Rings

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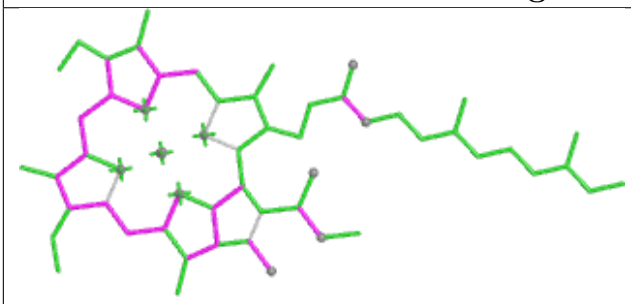
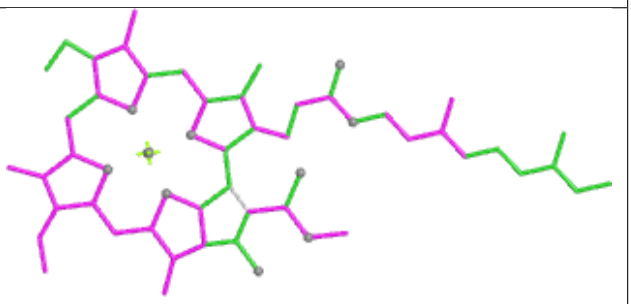
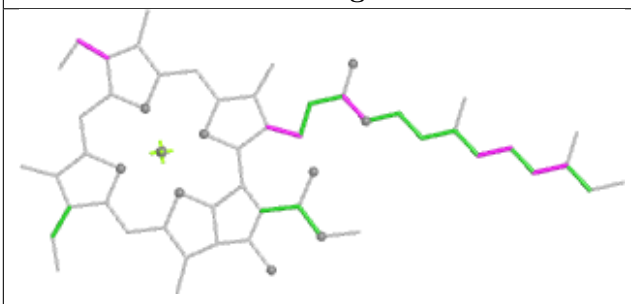
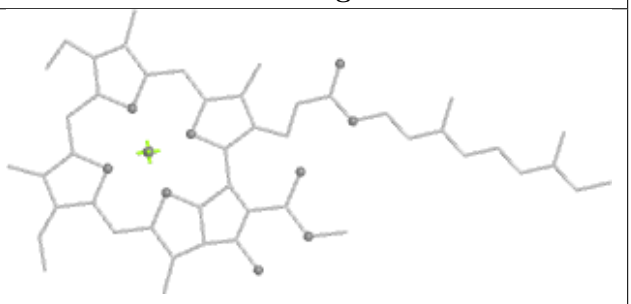
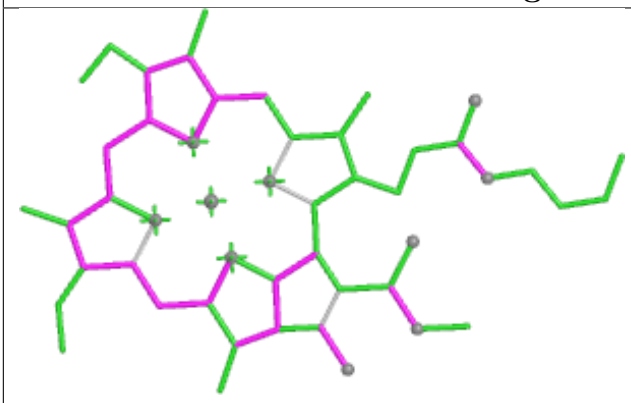
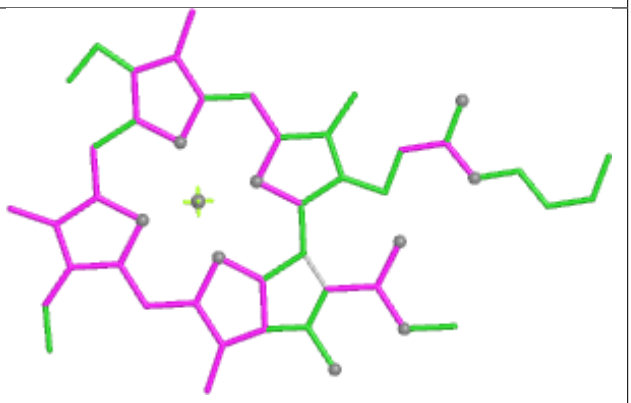
	
Bond lengths	Bond angles
	
Torsions	Rings

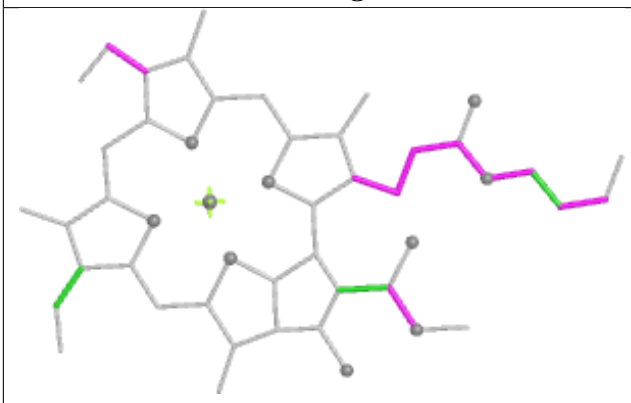
Ligand CLA A 823



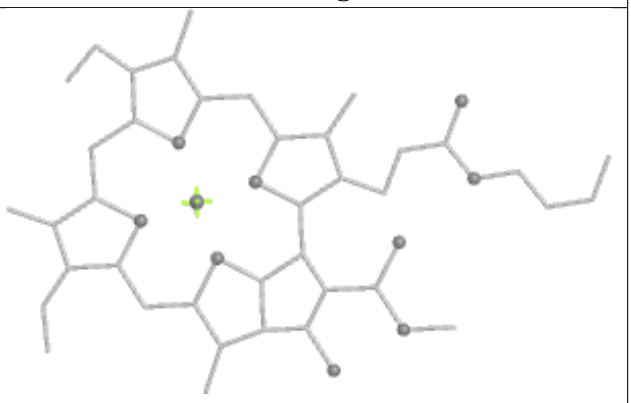
Bond lengths



Bond angles

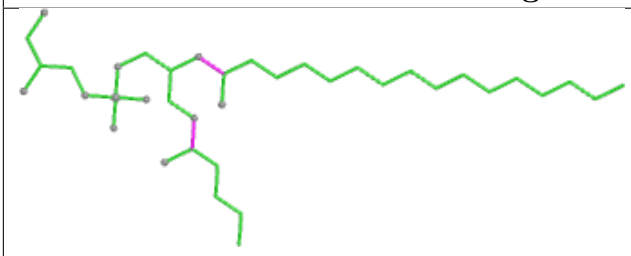


Torsions



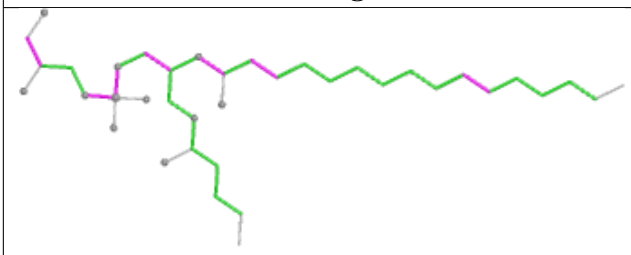
Rings

Ligand LHG A 847

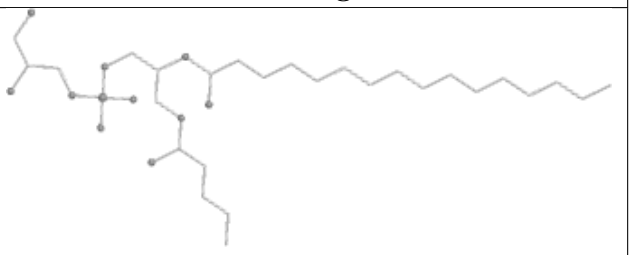


Bond lengths

Bond angles

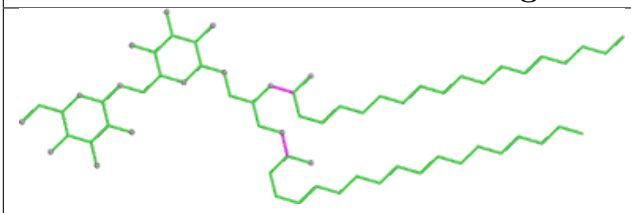


Torsions

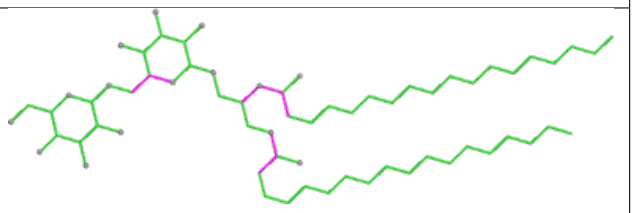


Rings

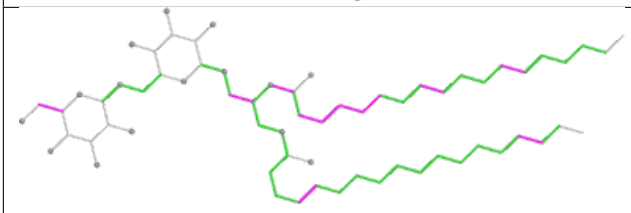
Ligand DGD B 850



Bond lengths



Bond angles



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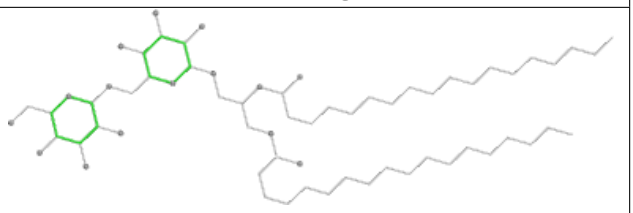
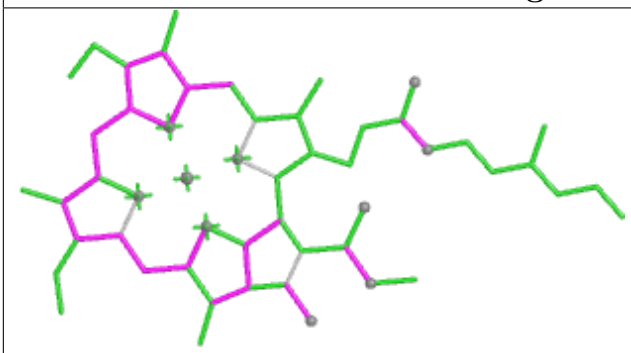


Rings

Ligand CLA Z 606



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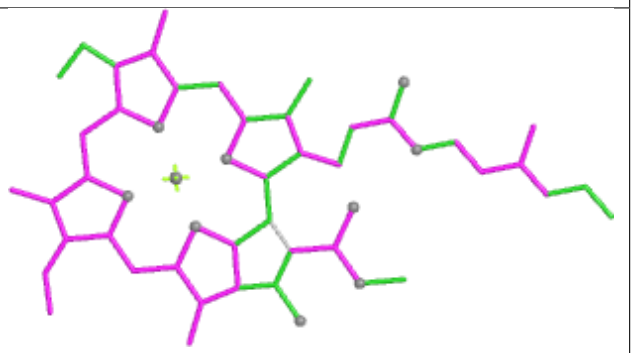
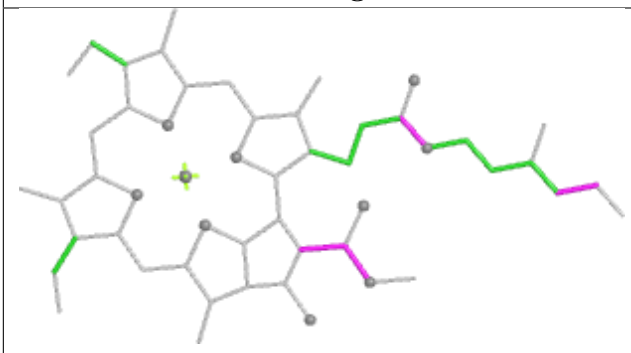
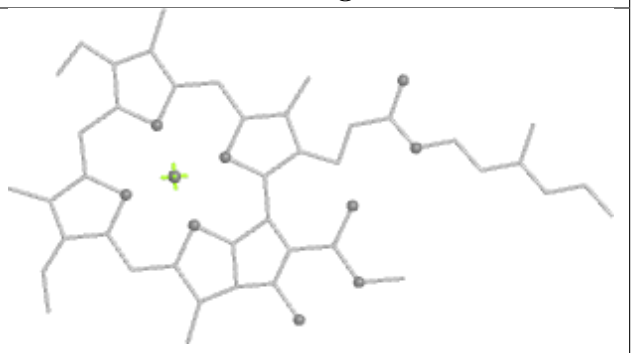


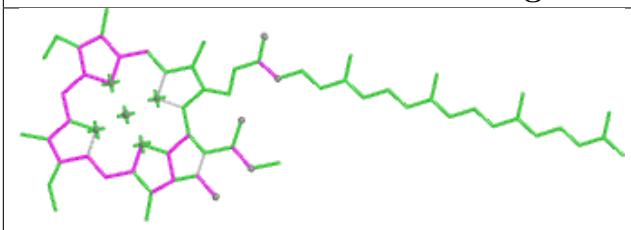
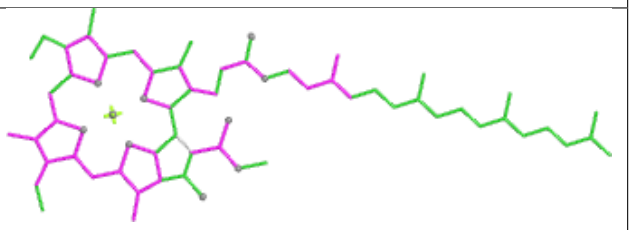
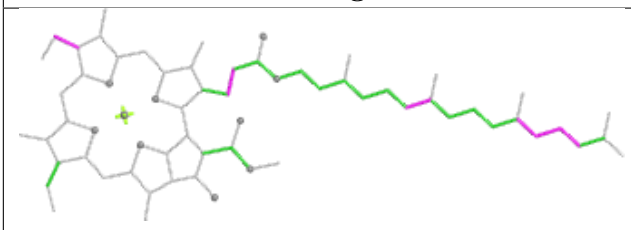
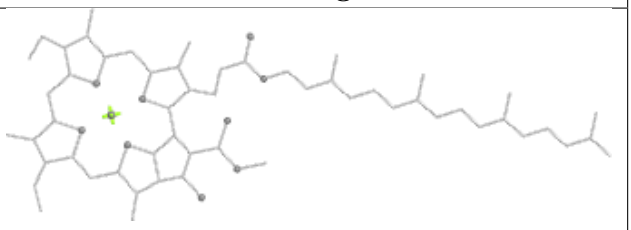
Bond angles



Torsions



Rings

Ligand CLA B 839	
	
Bond lengths	Bond angles
	
Torsions	Rings

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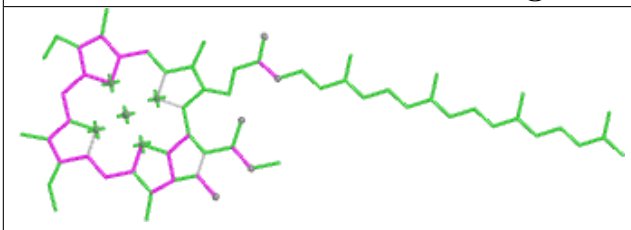
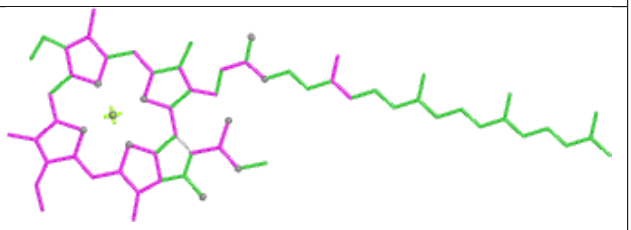
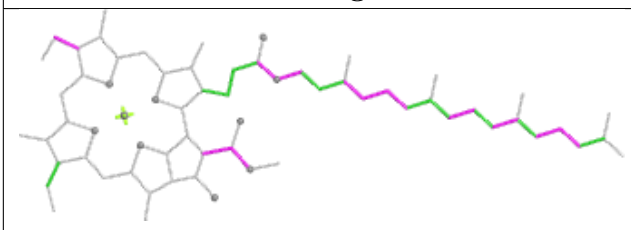
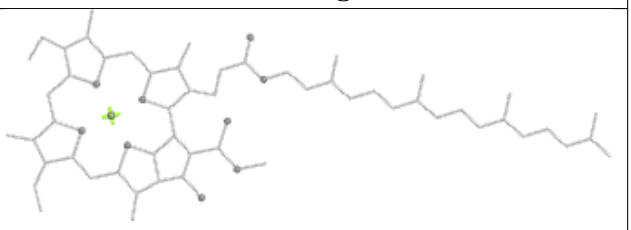
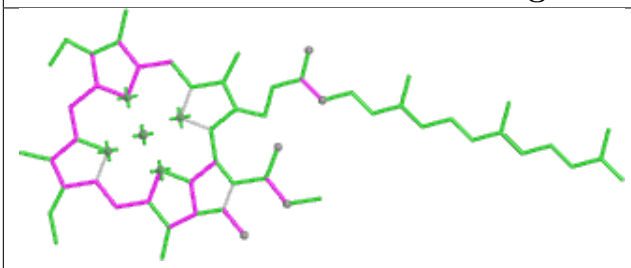
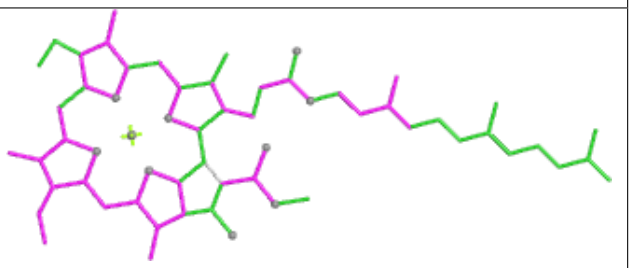
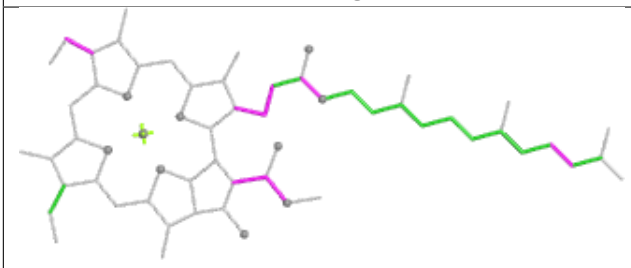
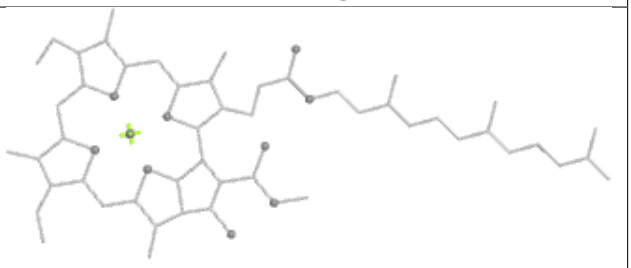
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA 4 602	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

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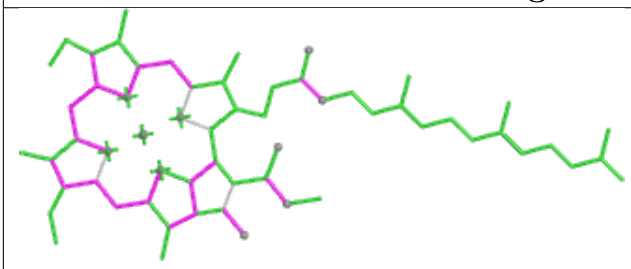
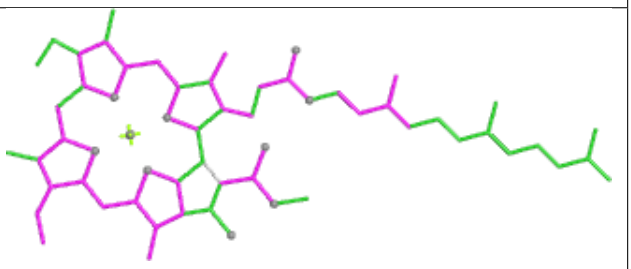
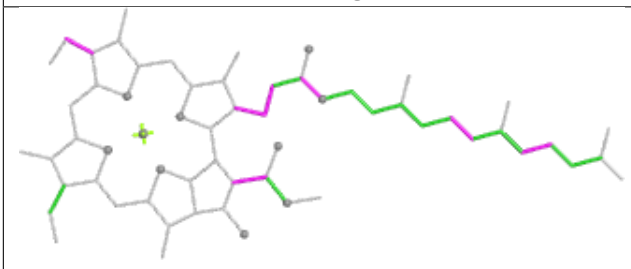
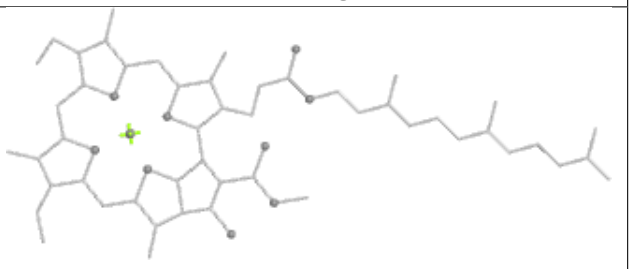
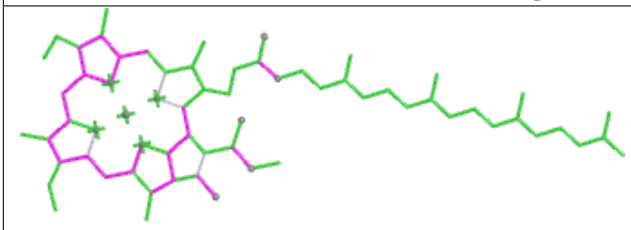
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

Ligand CLA 8 601



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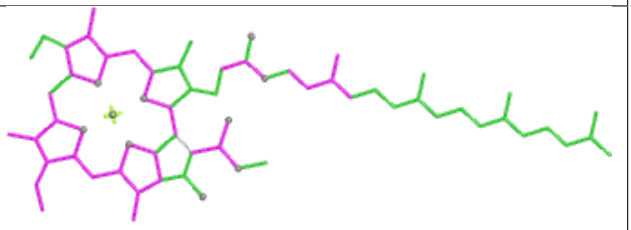

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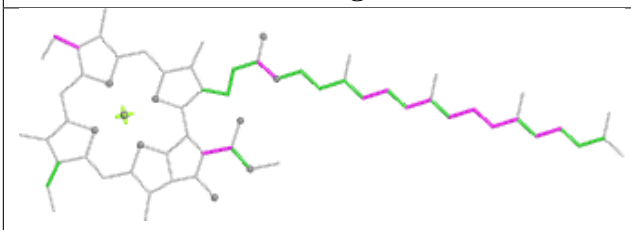

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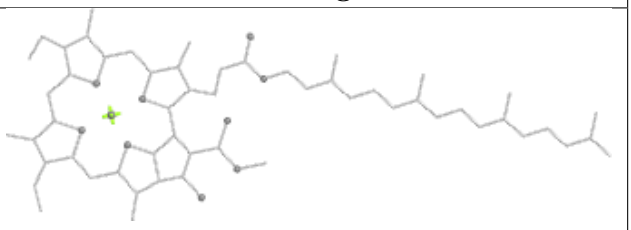
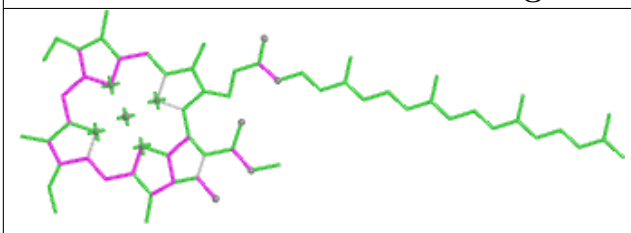


Rings

Ligand CLA B 819



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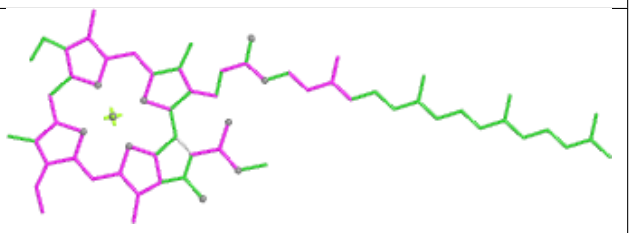

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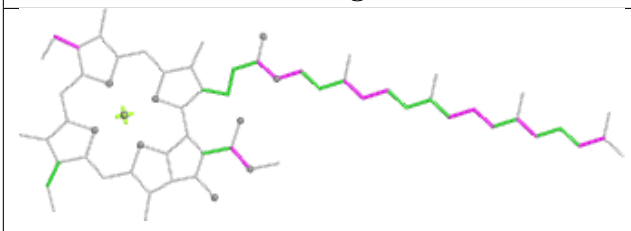

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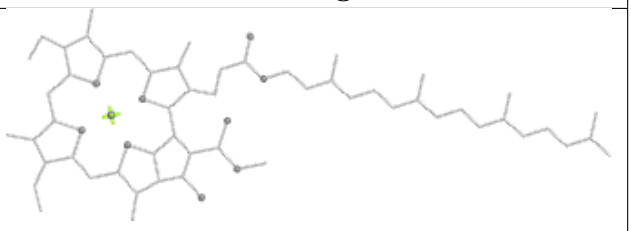
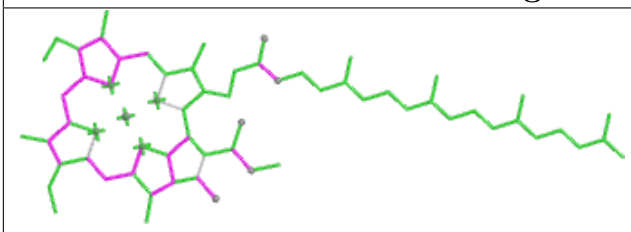


Rings

Ligand CLA A 843



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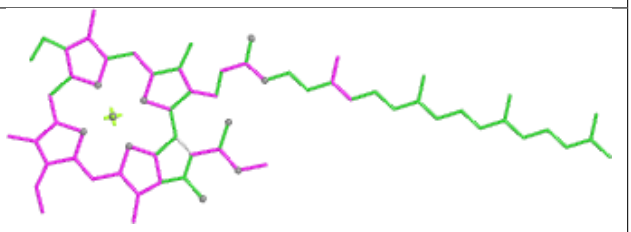

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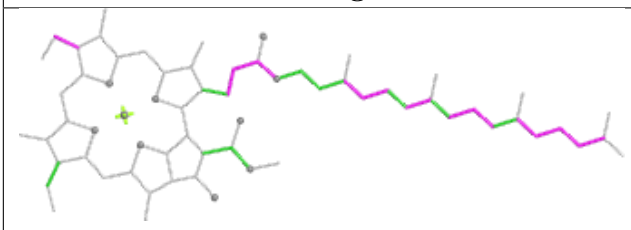

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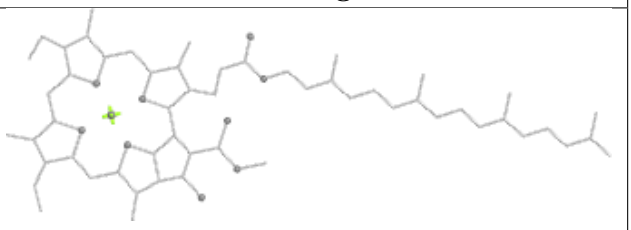
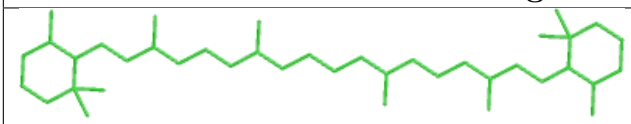


Rings

Ligand BCR 3 717



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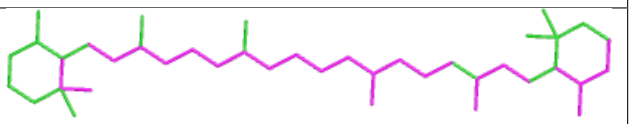

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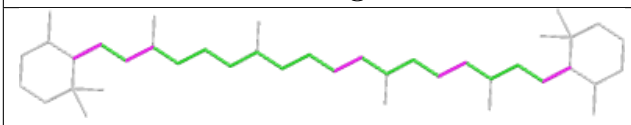

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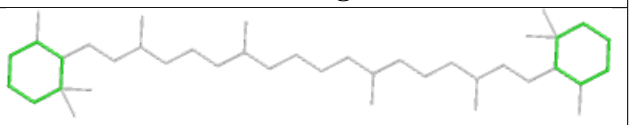
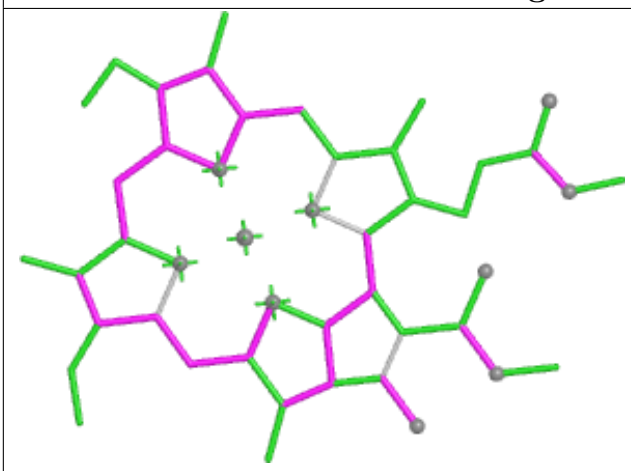


Rings

Ligand CLA 5 621



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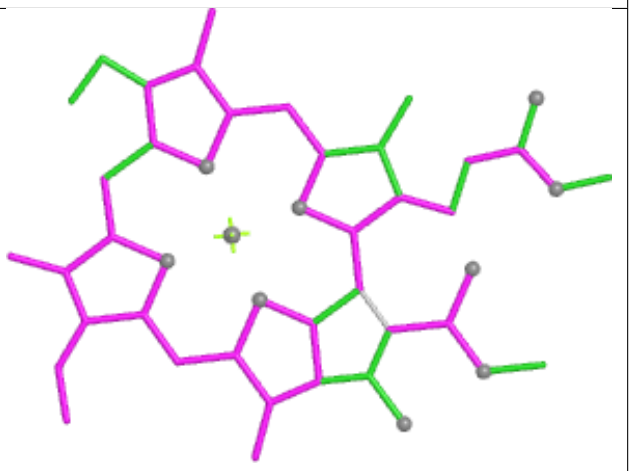

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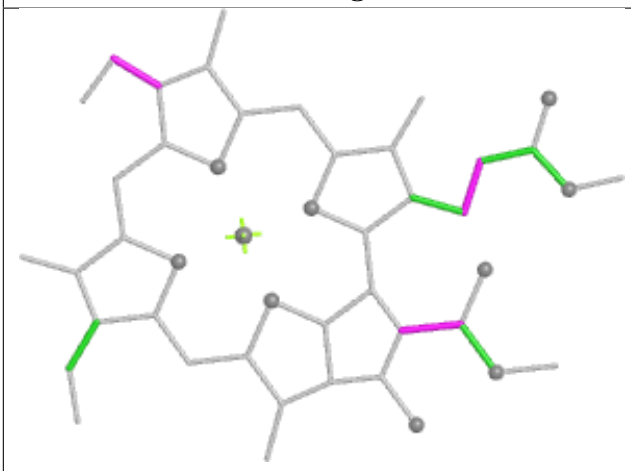
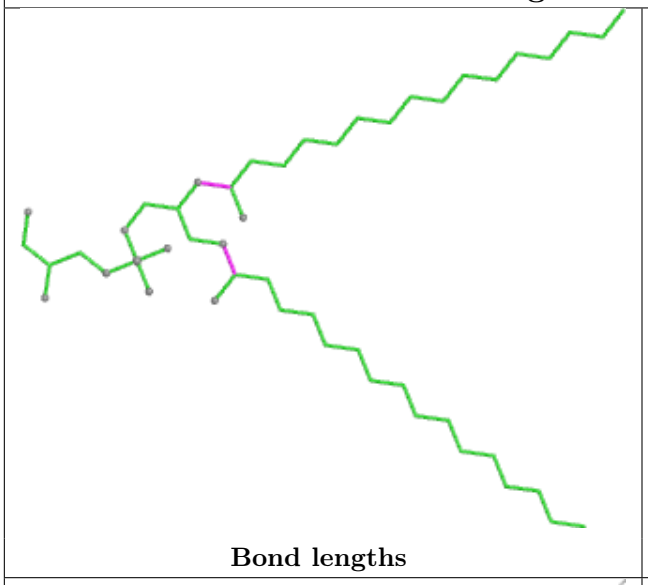


Torsions

Rings

Ligand LHG 6 619



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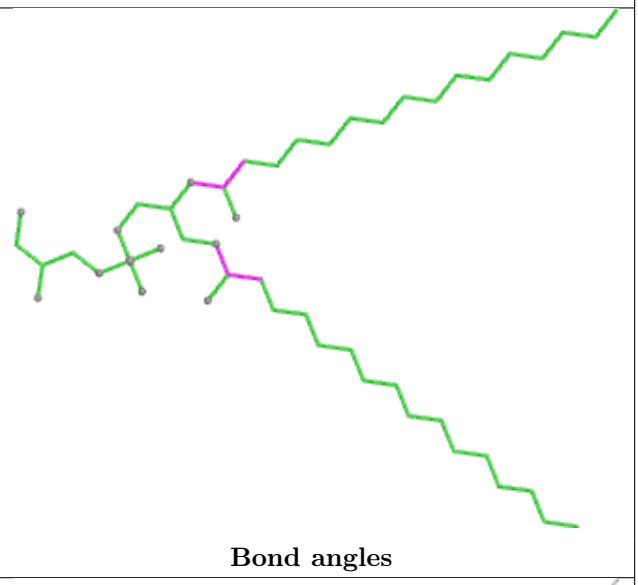

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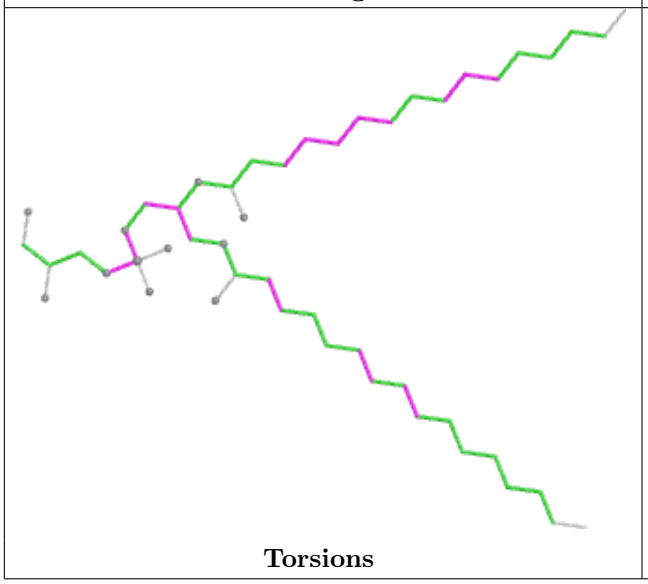

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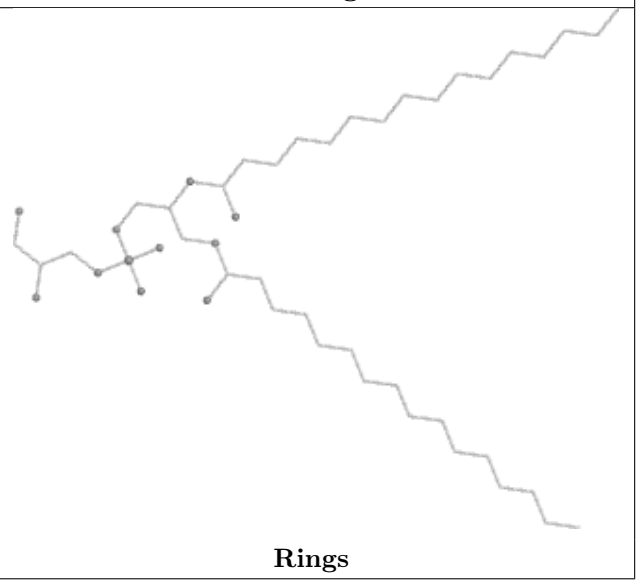
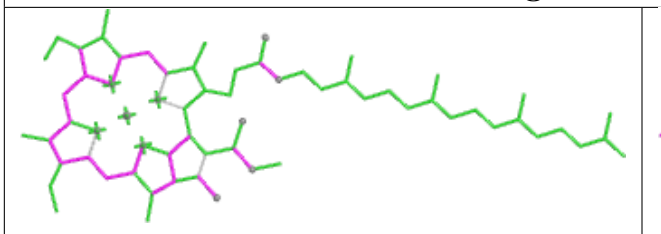


Rings

Ligand CLA A 822



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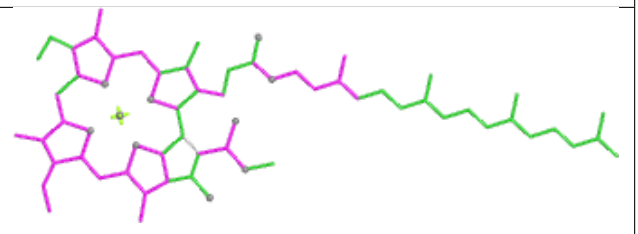

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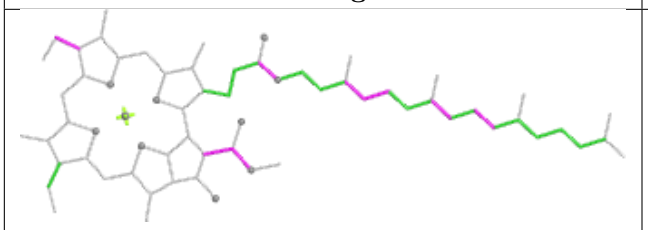

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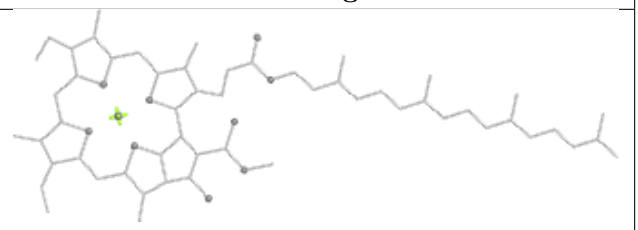
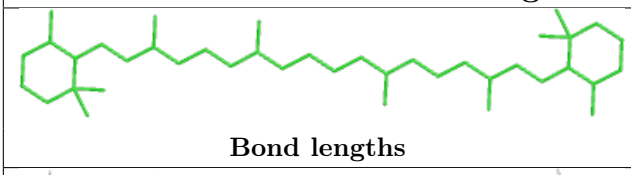


Rings

Ligand BCR A 856



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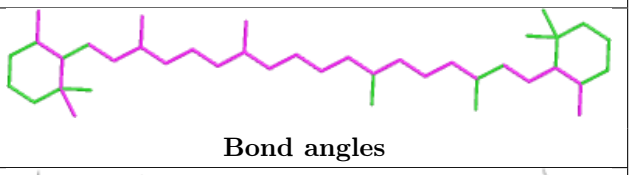

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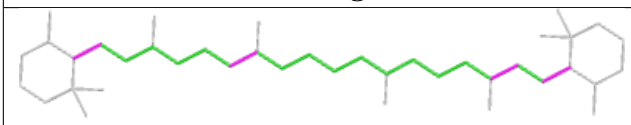

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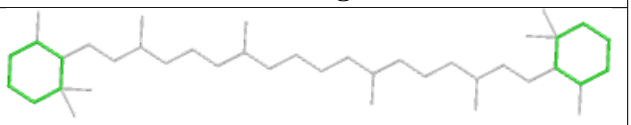
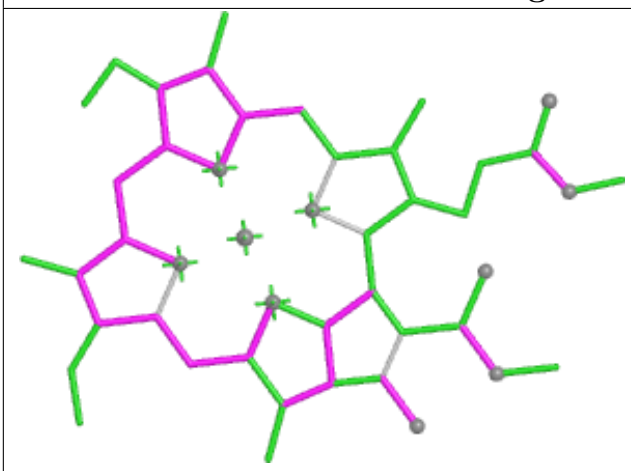


Rings

Ligand CLA 3 612



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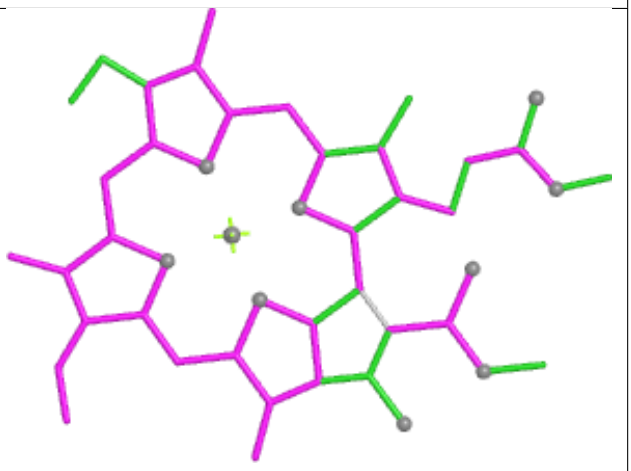

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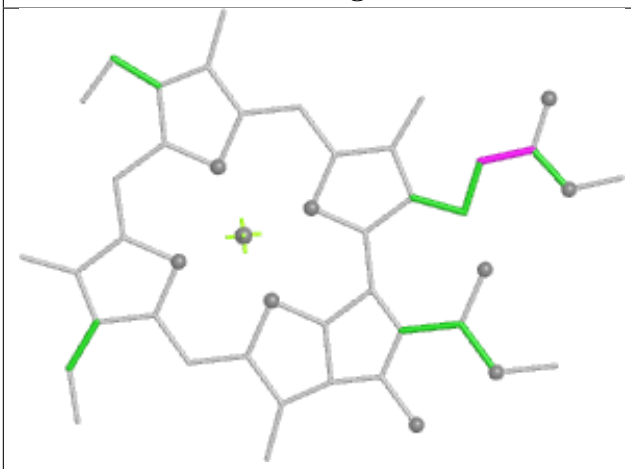
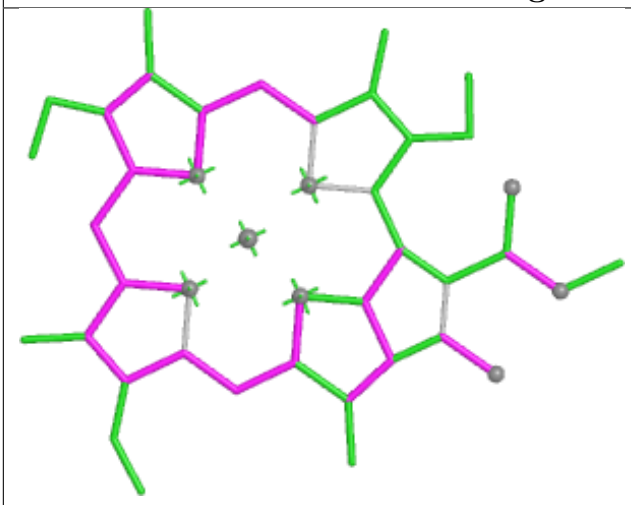


Torsions

Rings

Ligand CLA 7 606



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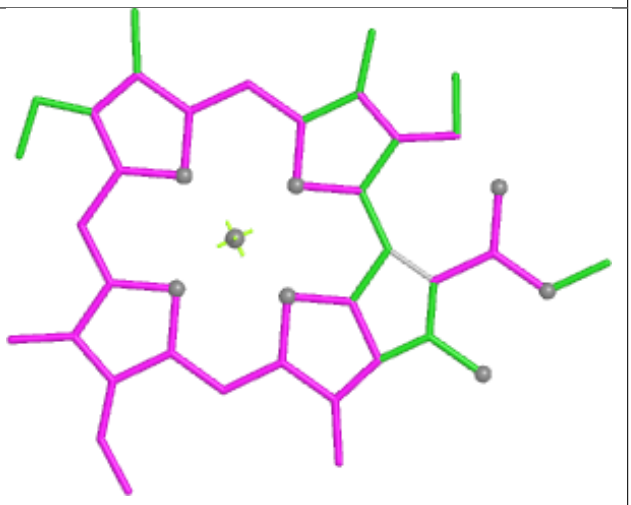
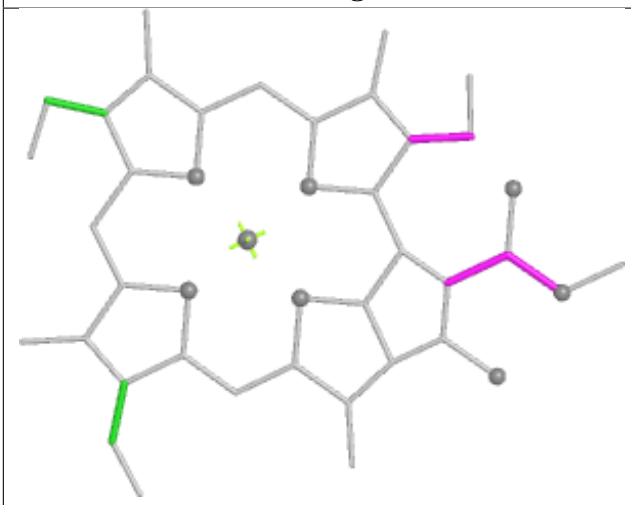


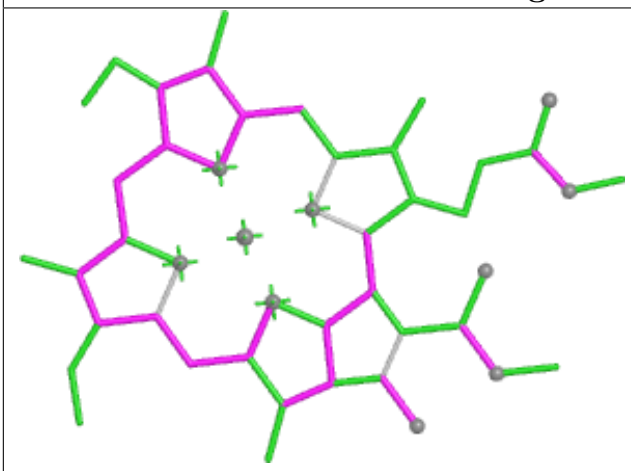
Bond angles



Torsions

Rings

Ligand CLA 8 616



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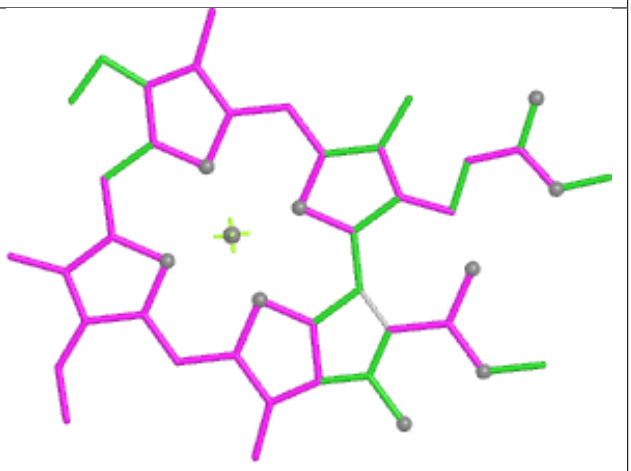

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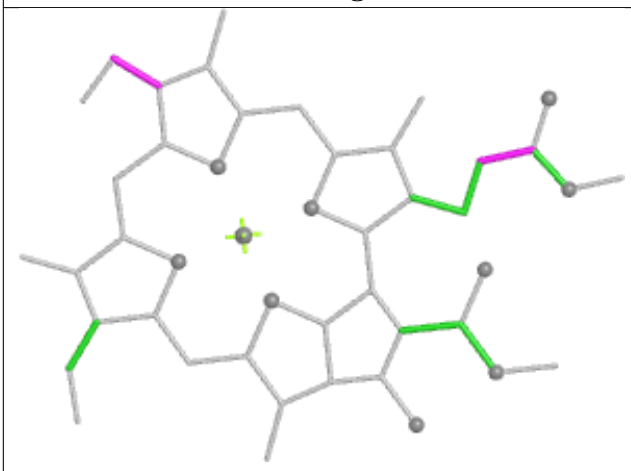

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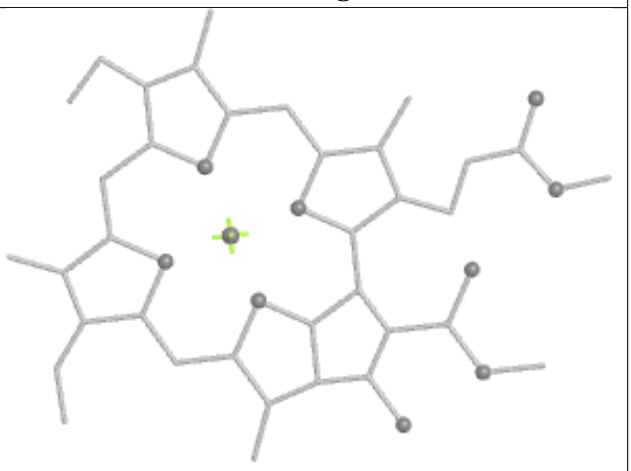
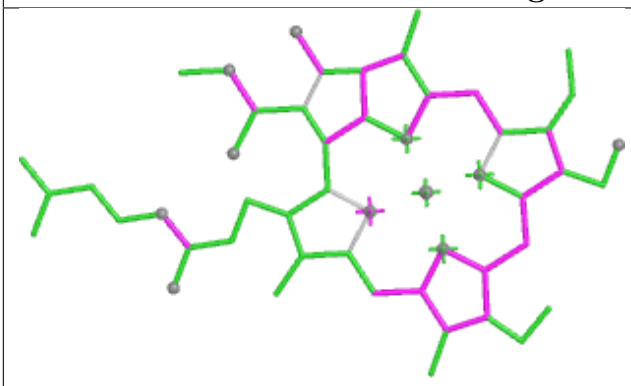


Rings

Ligand CHL 4 607



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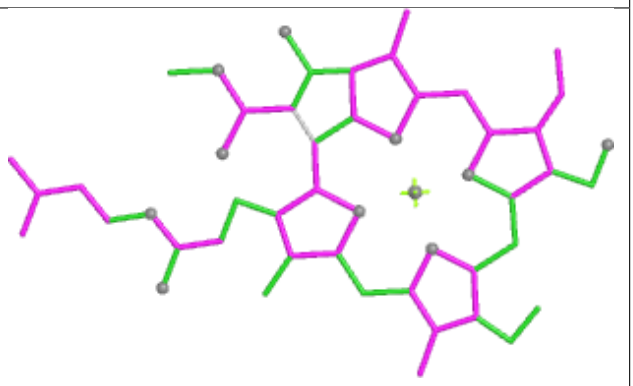
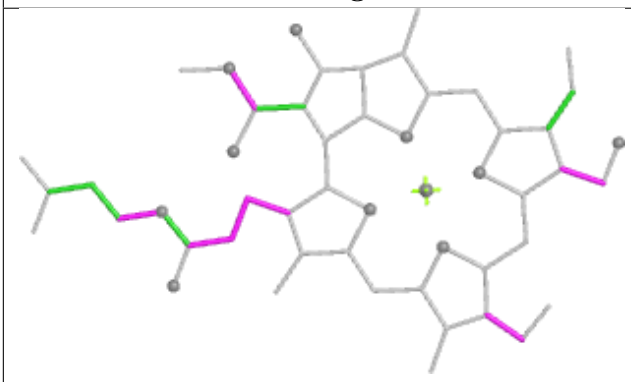


Bond angles



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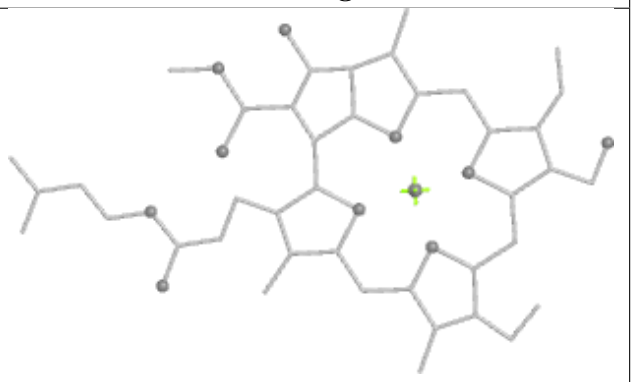
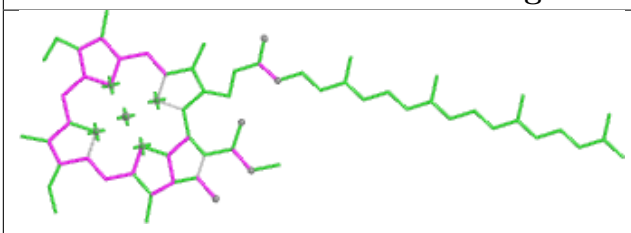


Rings

Ligand CLA B 825



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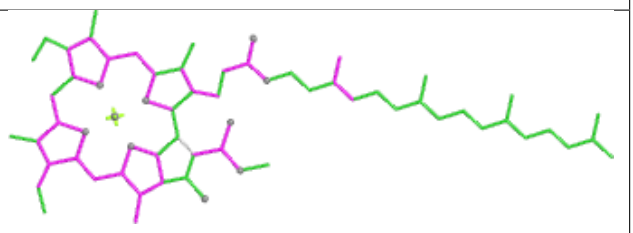
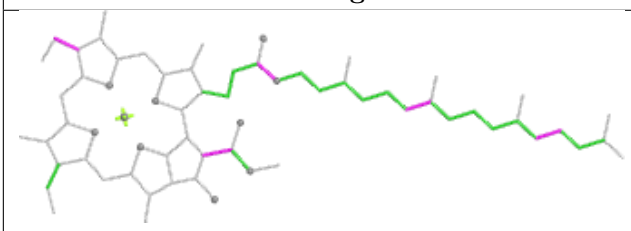


Bond angles



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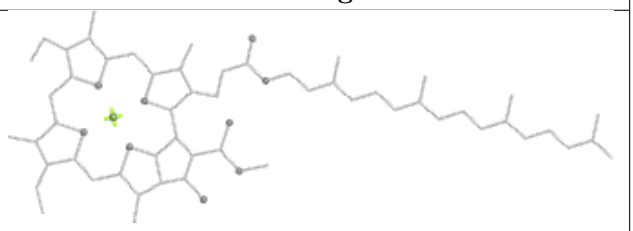
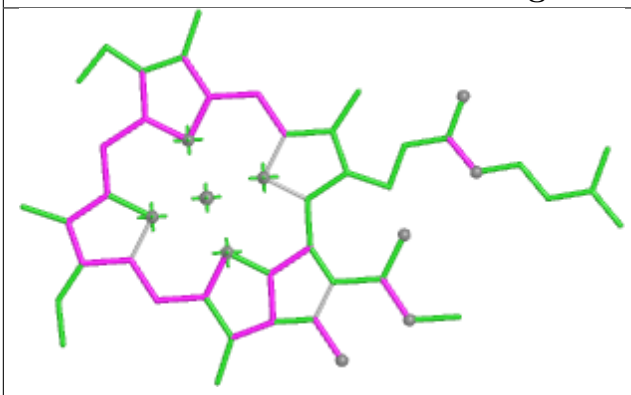


Rings

Ligand CLA 4 604



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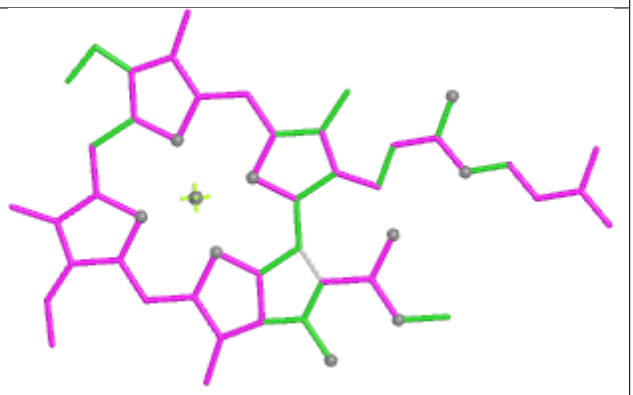
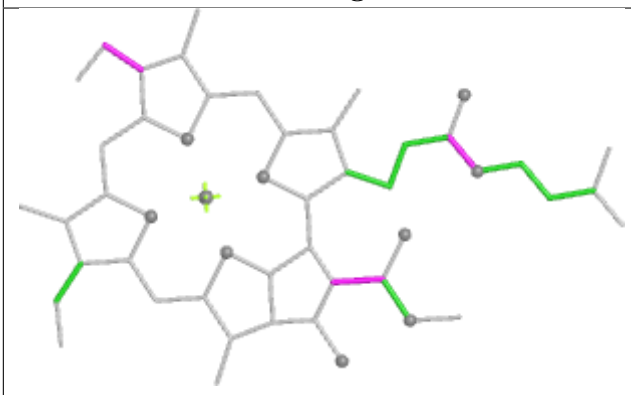


Bond angles



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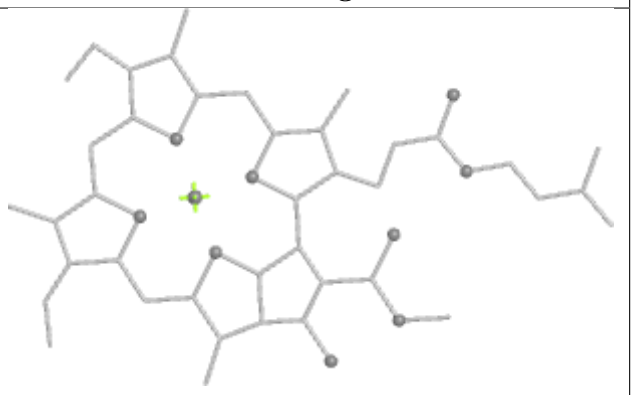
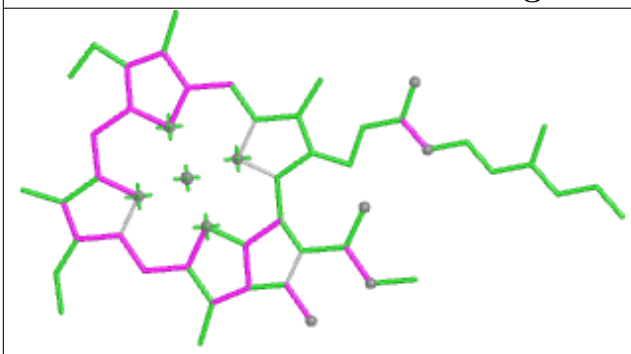
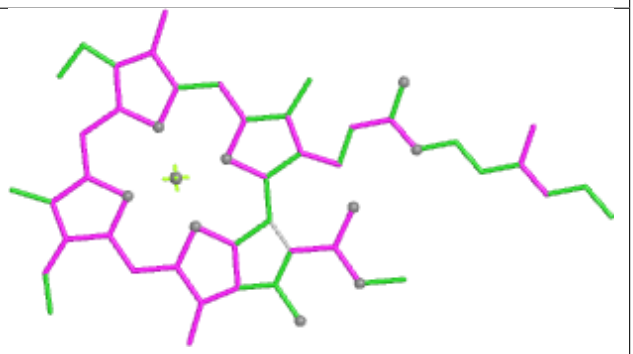


Rings

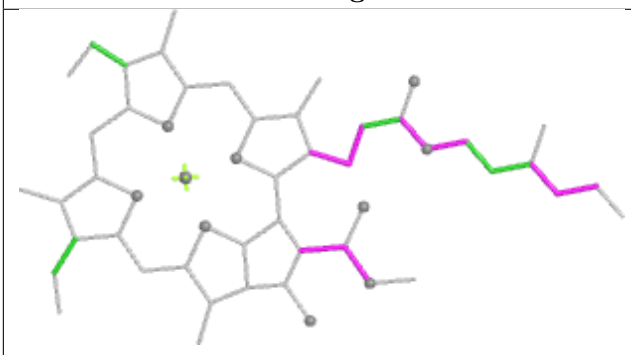
Ligand CLA A 845



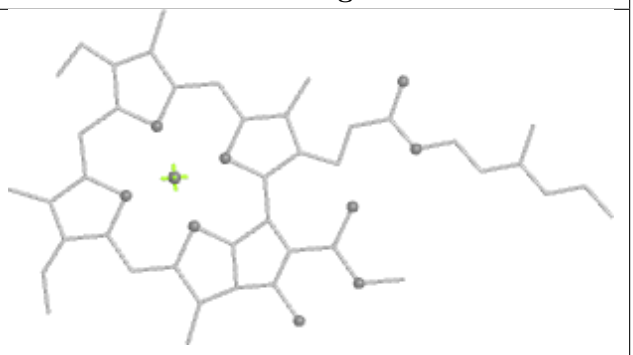
Bond lengths



Bond angles

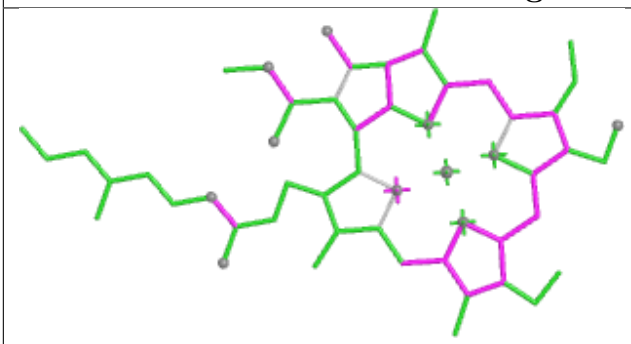


Torsions



Rings

Ligand CHL Z 601



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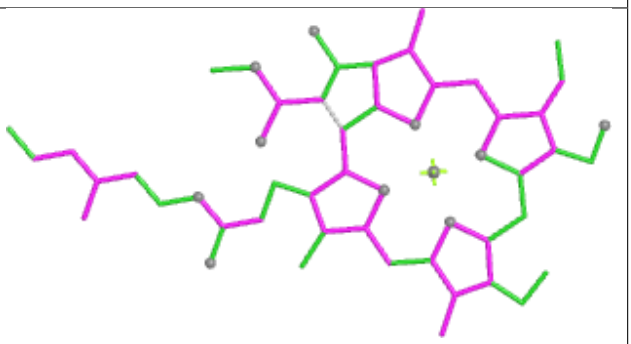

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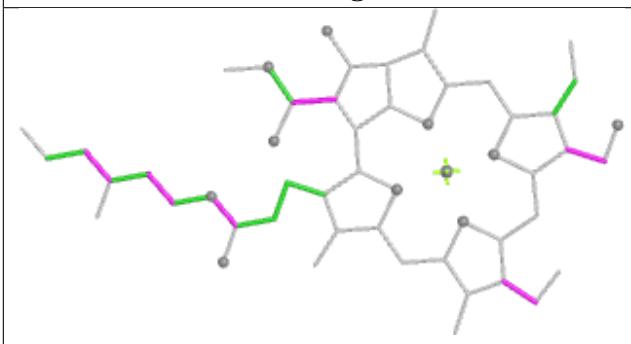

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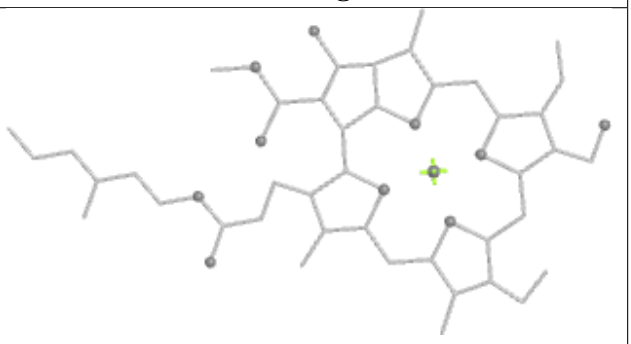
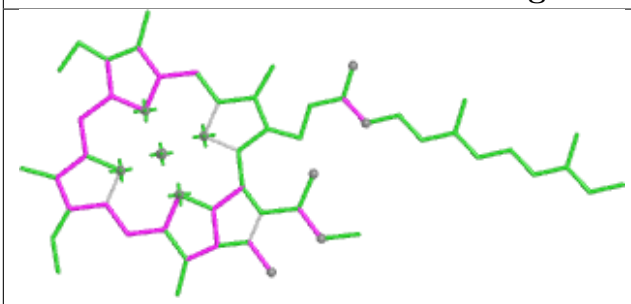


Rings

Ligand CLA 3 620



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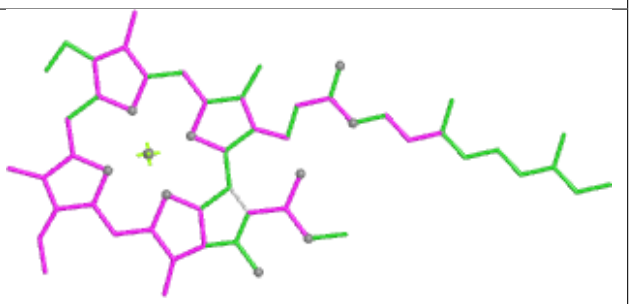

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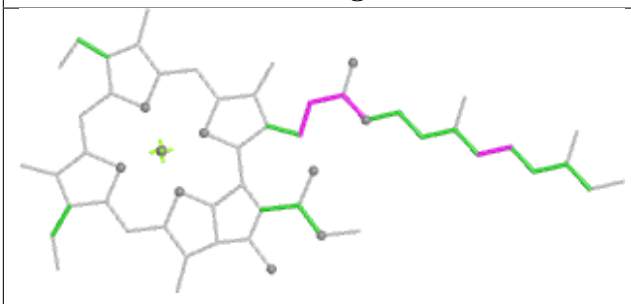

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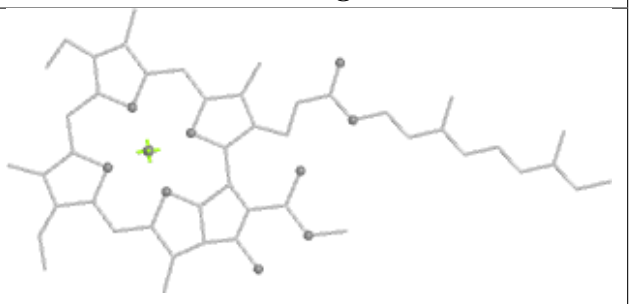
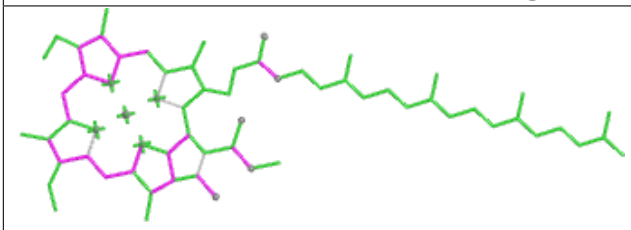


Rings

Ligand CLA A 834



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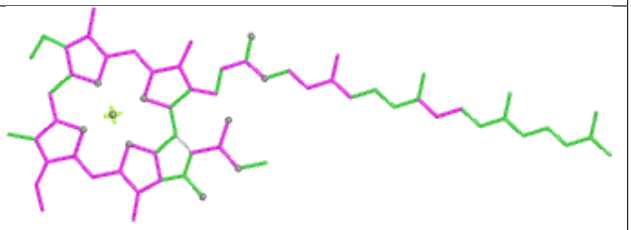
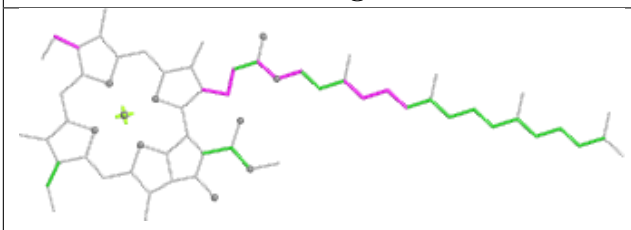


Bond angles



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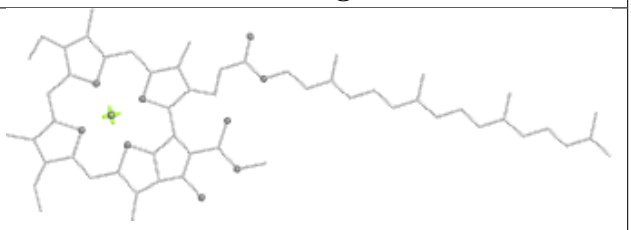
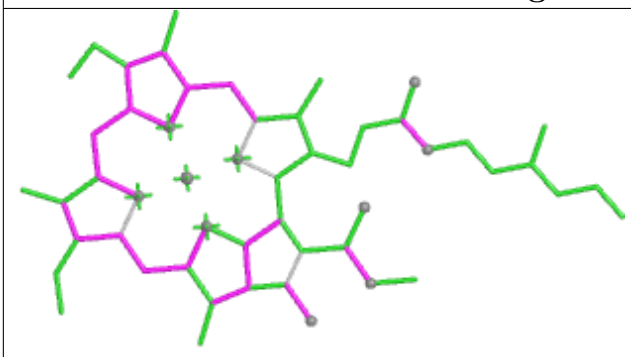


Rings

Ligand CLA 7 612



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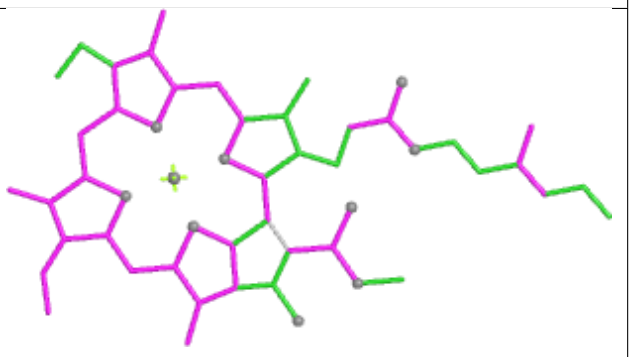

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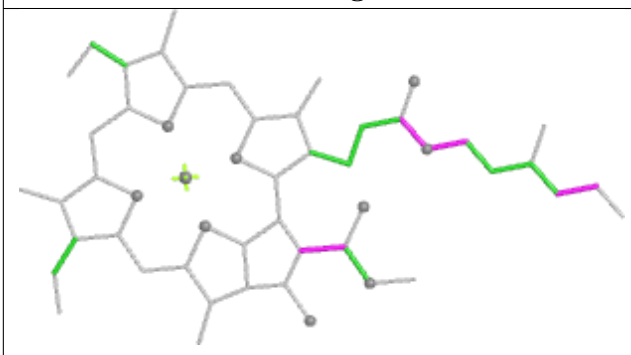

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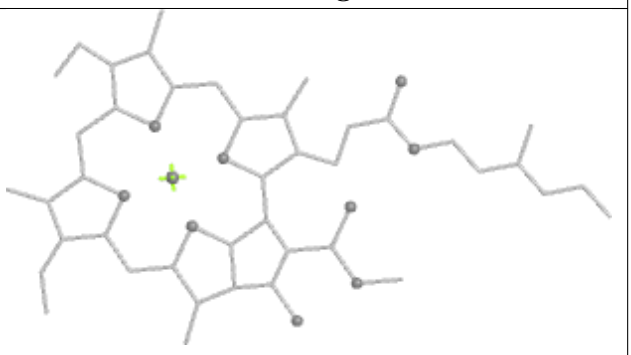
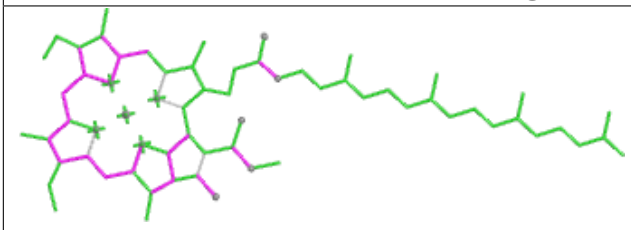


Rings

Ligand CLA A 842



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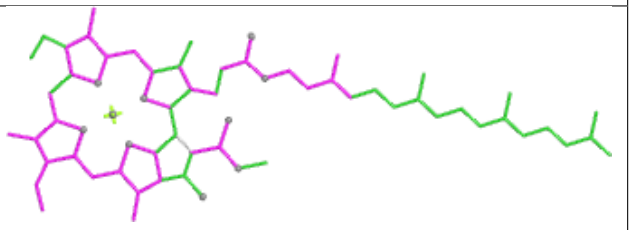
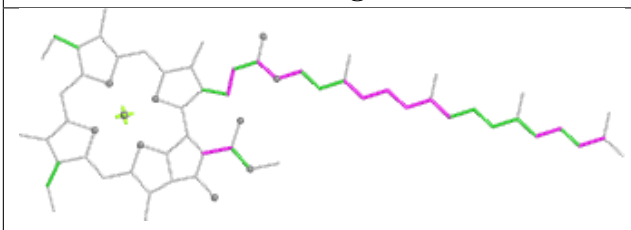


Bond angles



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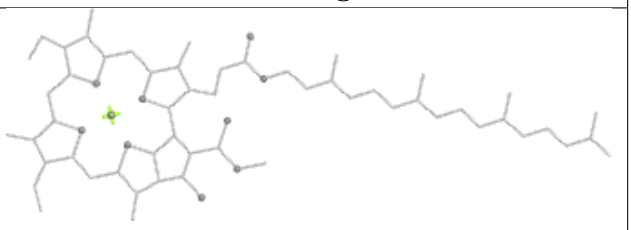
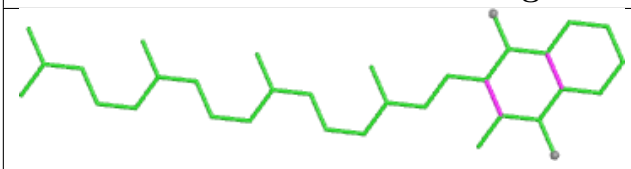


Rings

Ligand PQN B 842



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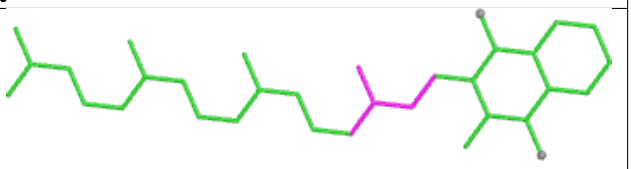
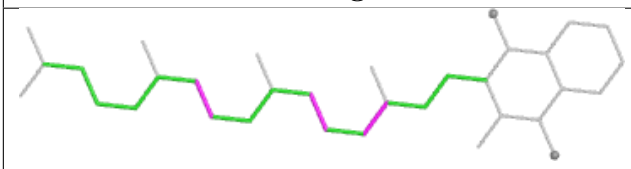


Bond angles



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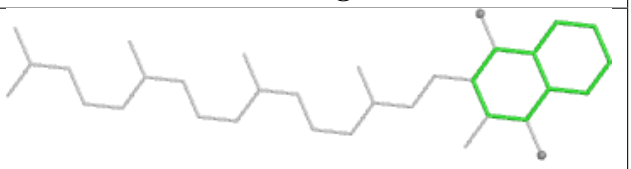
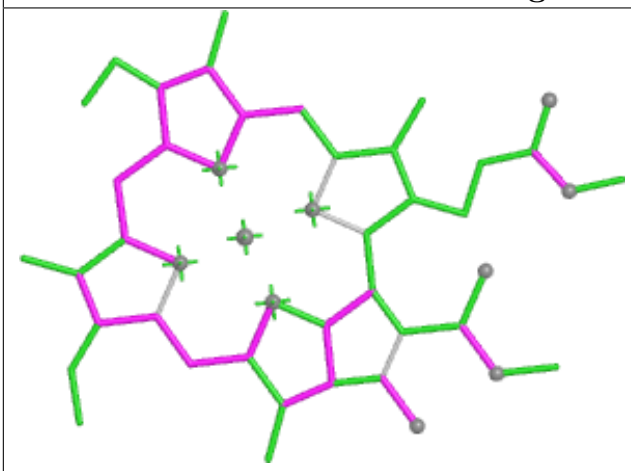


Rings

Ligand CLA 4 603



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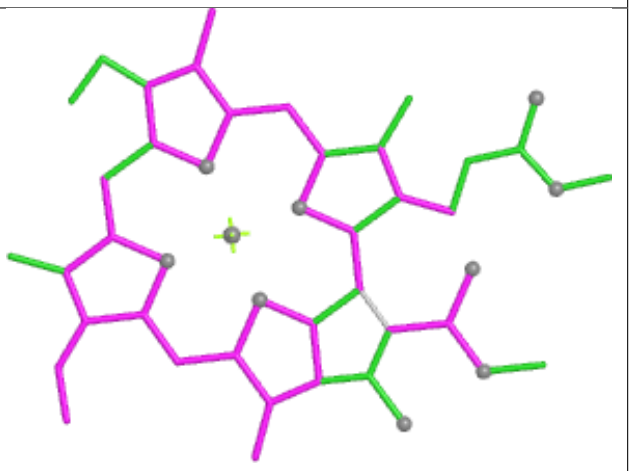
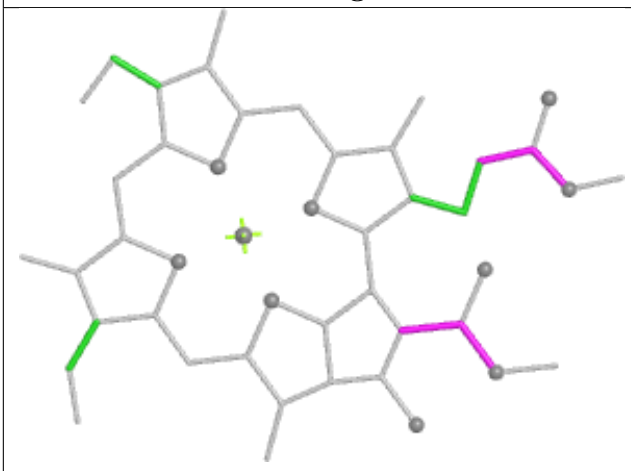


Bond angles



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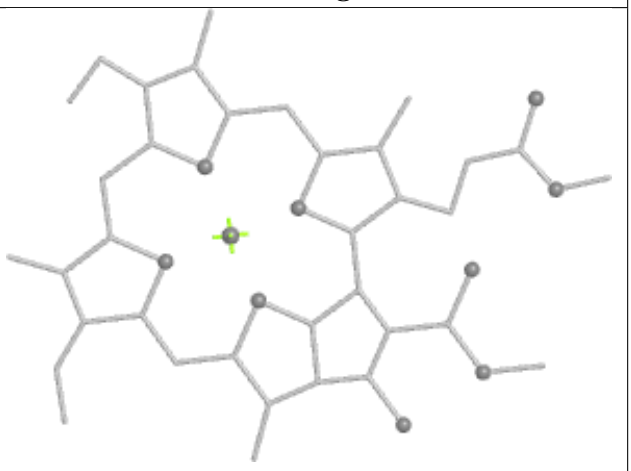
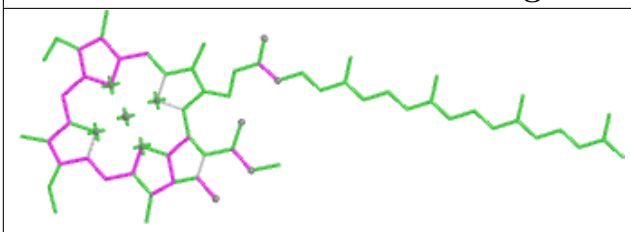


Rings

Ligand CLA A 816



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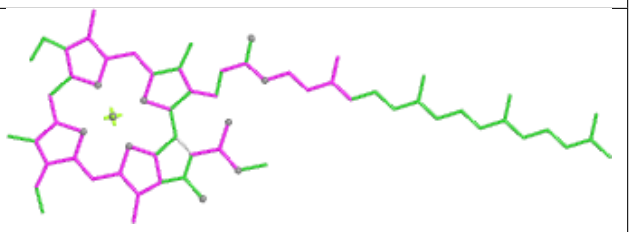

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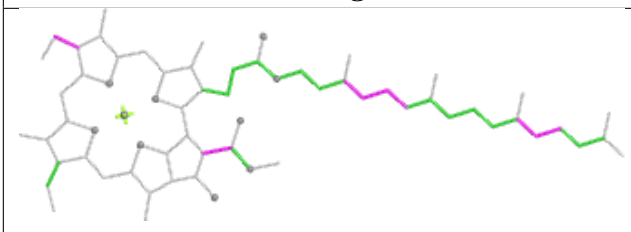

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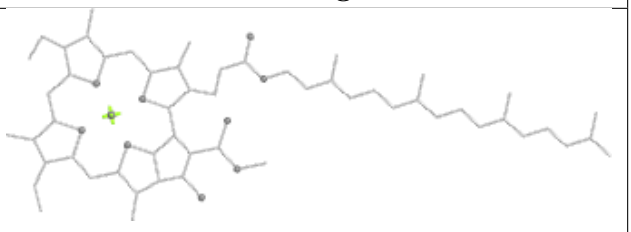
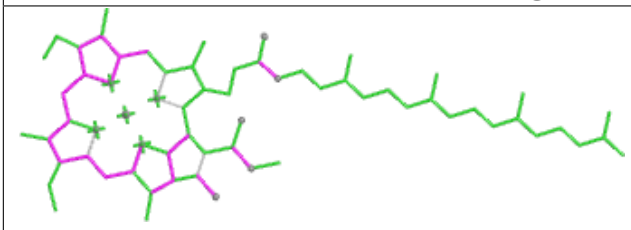


Rings

Ligand CLA 6 601



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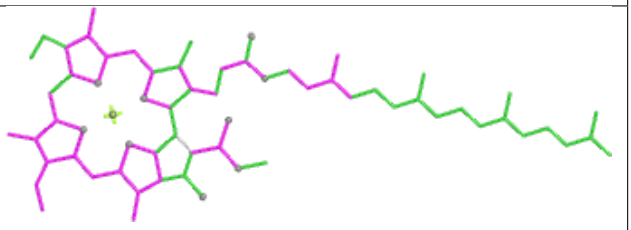

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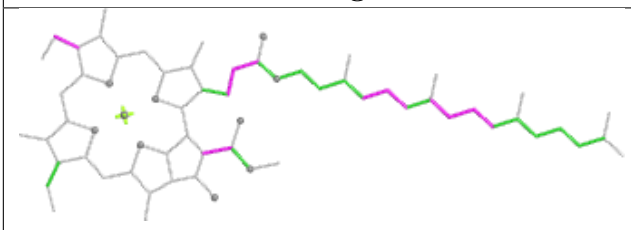

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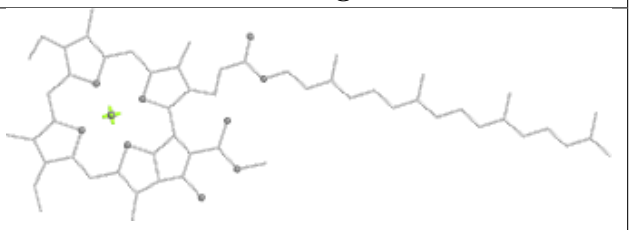
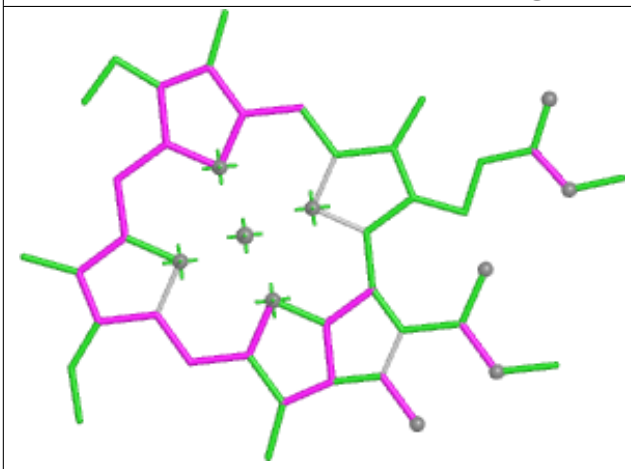


Rings

Ligand CLA 1 616



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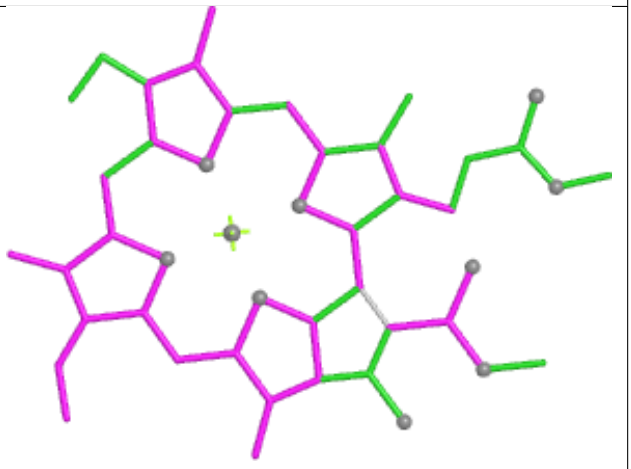

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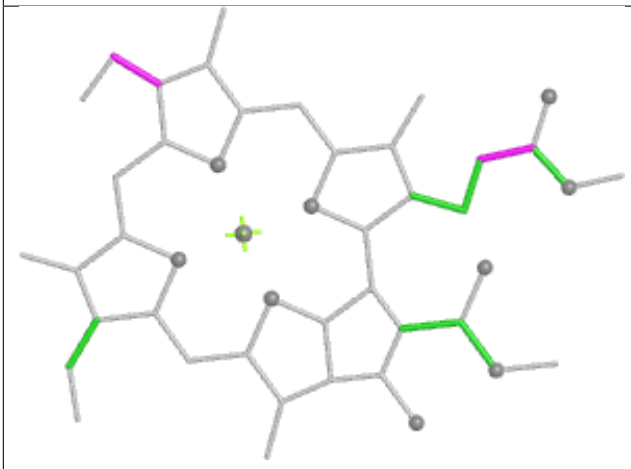

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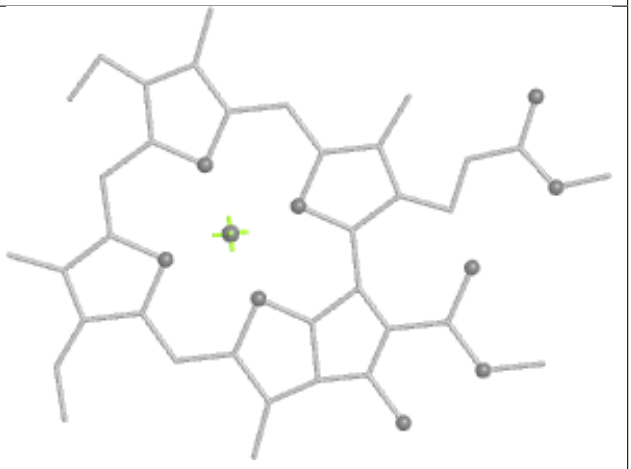
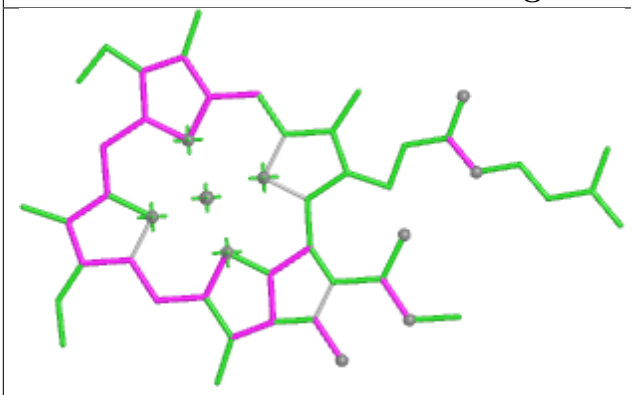


Rings

Ligand CLA A 832



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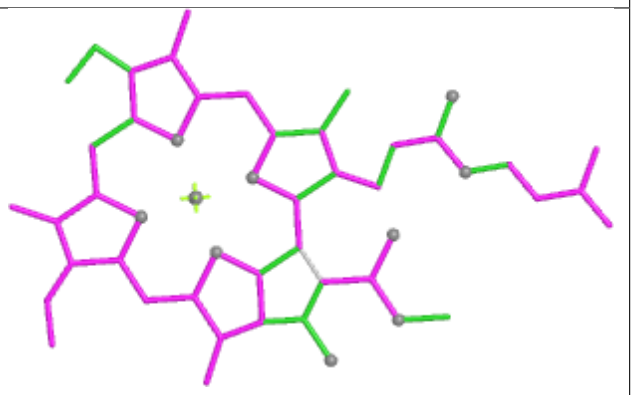
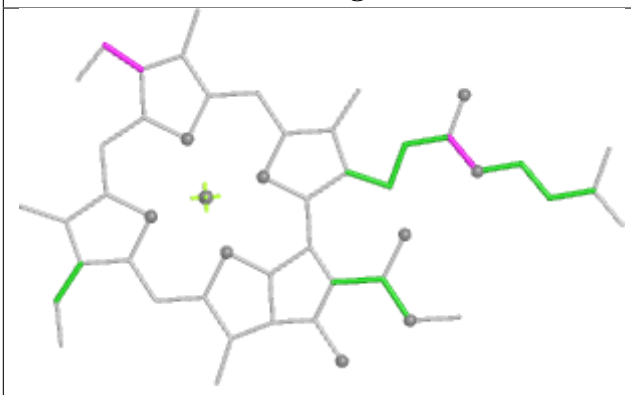


Bond angles



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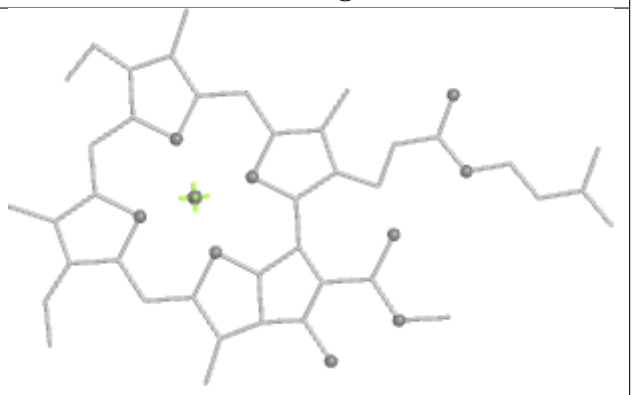
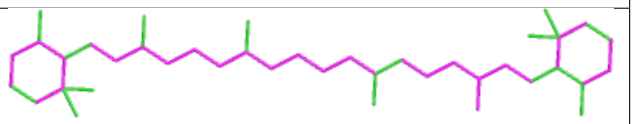


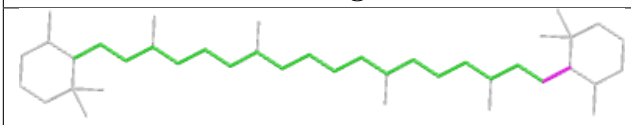
Rings

Ligand BCR 3 718

Bond lengths



Bond angles



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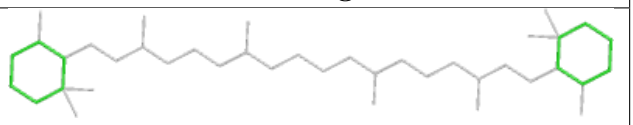
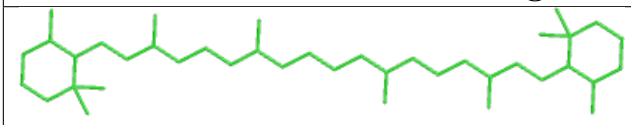


Rings

Ligand BCR 5 625



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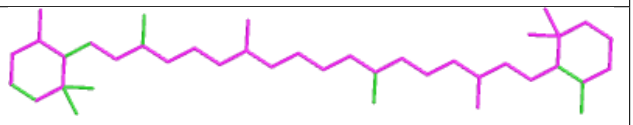
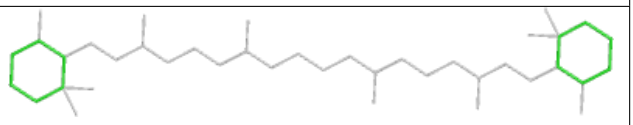


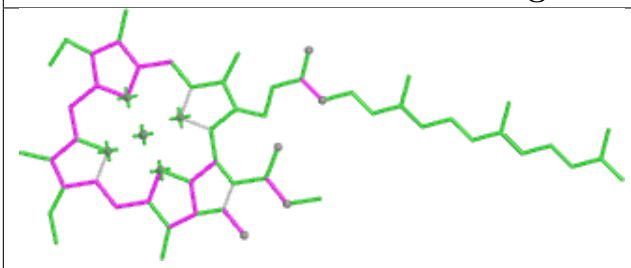
Bond angles

Torsions

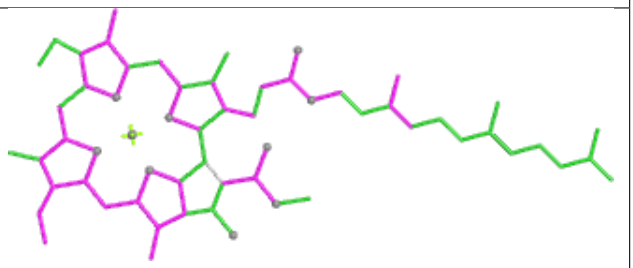


Rings

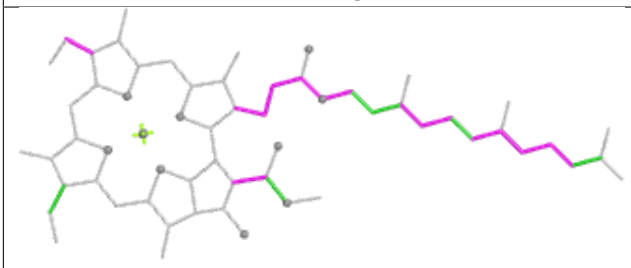
Ligand CLA 3 607



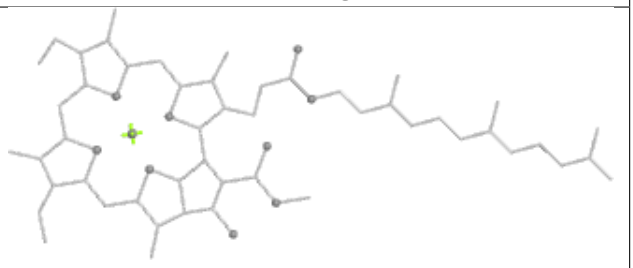
Bond lengths



Bond angles

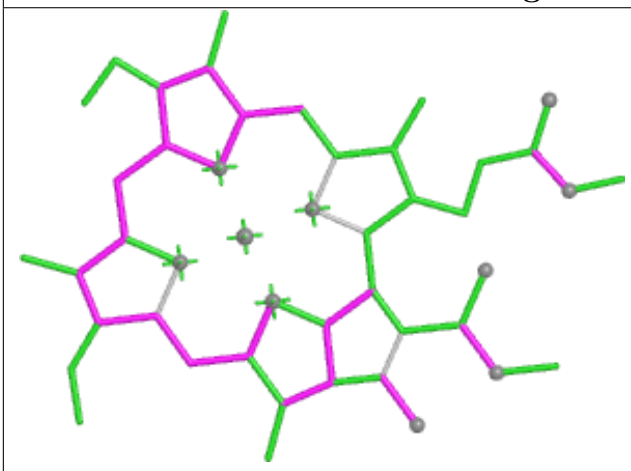


Torsions

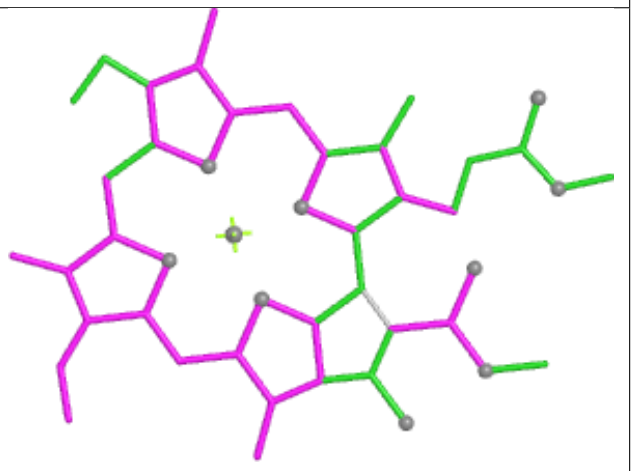


Rings

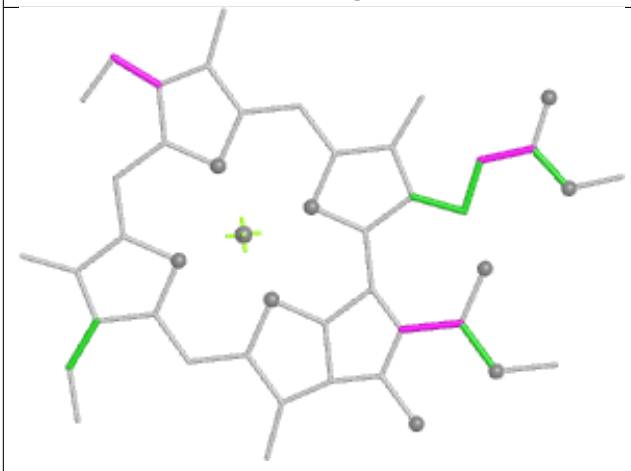
Ligand CLA G 204



Bond lengths



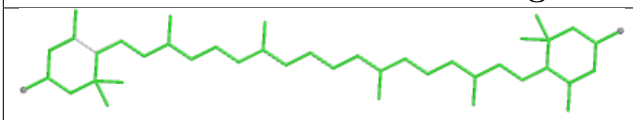
Bond angles



Torsions

Rings

Ligand LUT 8 618



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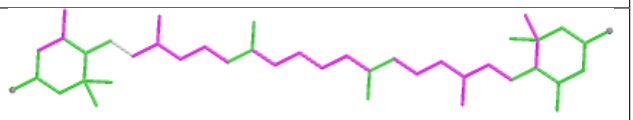
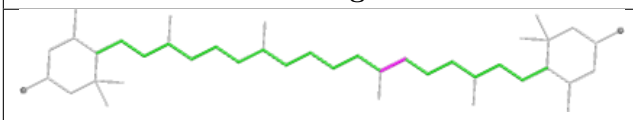


Bond angles



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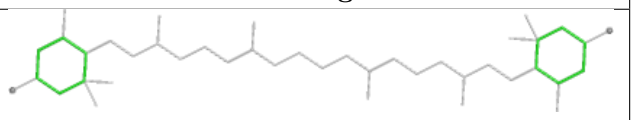
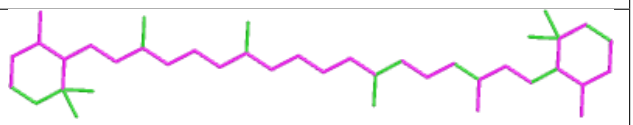


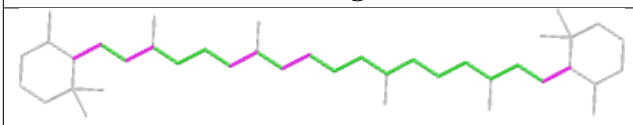
Rings

Ligand BCR 6 623

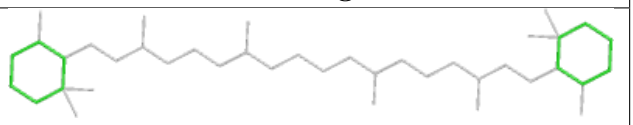
Bond lengths



Bond angles

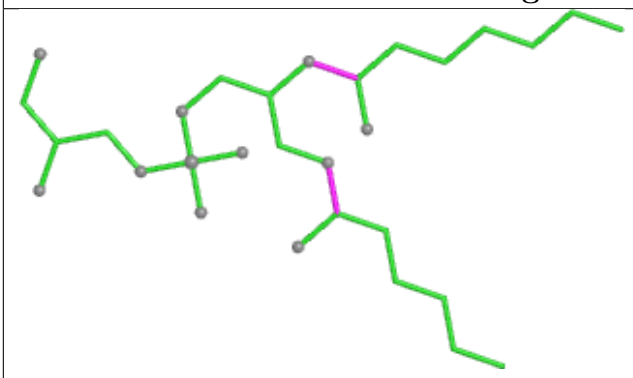


Torsions

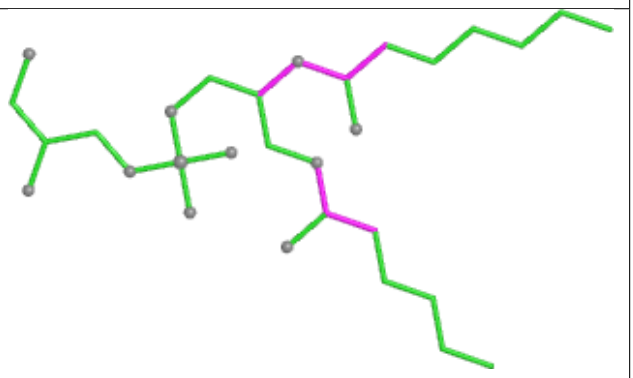


Rings

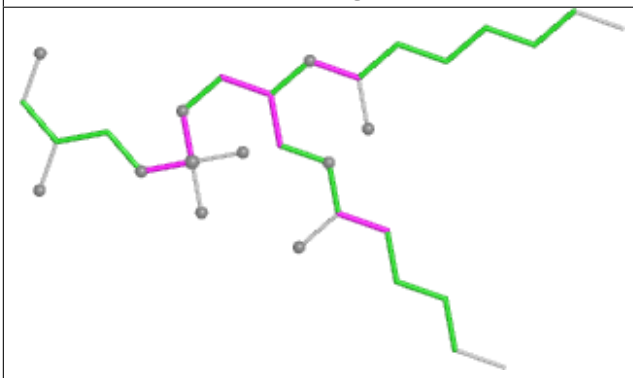
Ligand LHG A 855



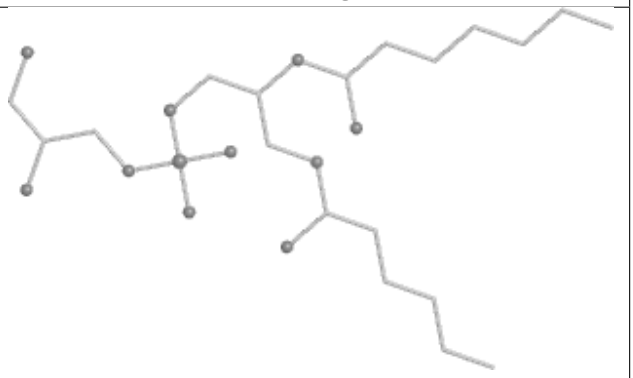
Bond lengths



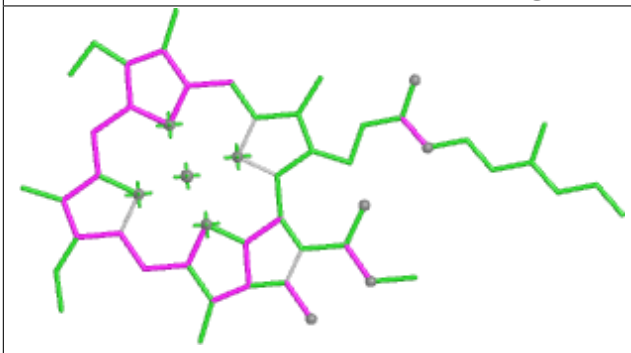
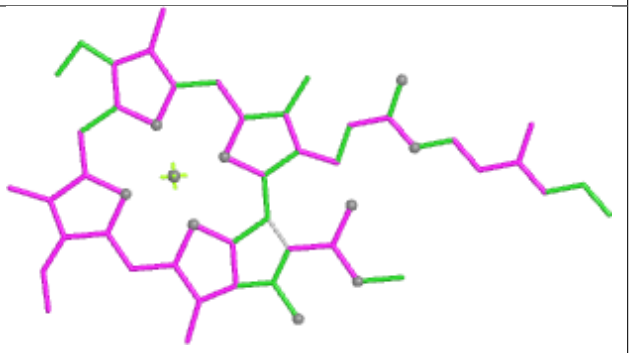
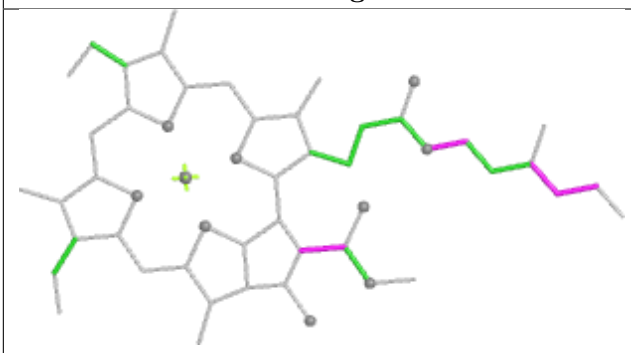
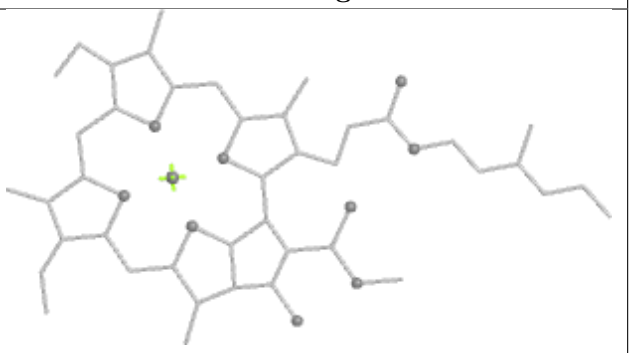
Bond angles

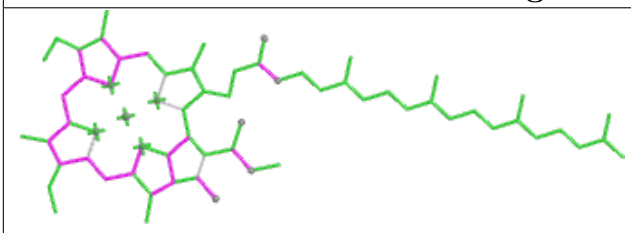
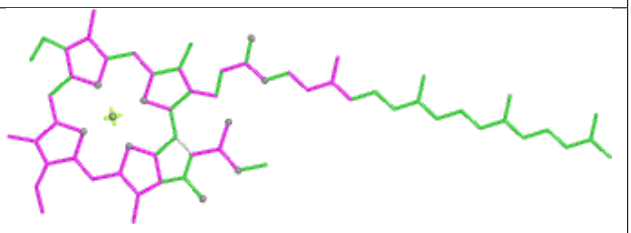
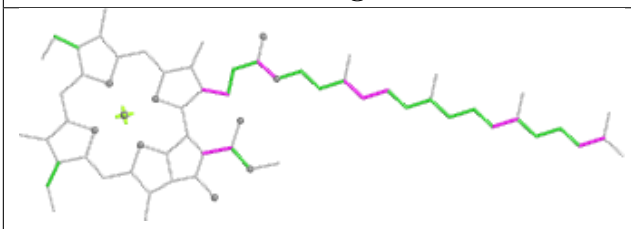
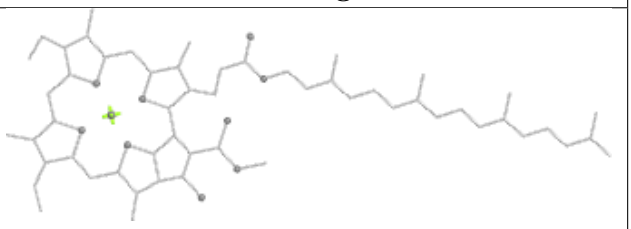


Torsions

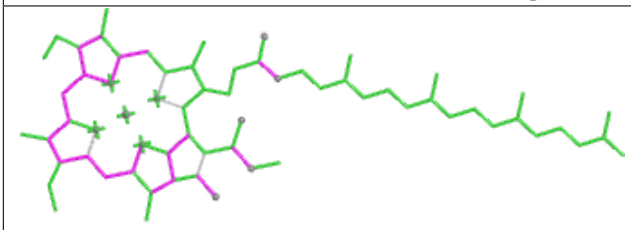


Rings

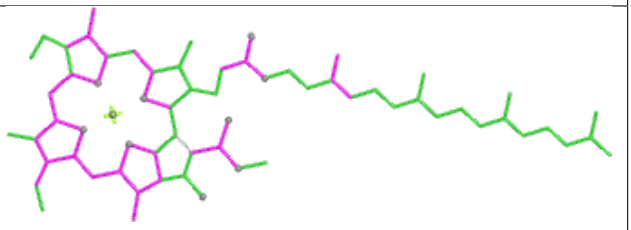
Ligand CLA 1 606	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA L 203	
	
Bond lengths	Bond angles
	
Torsions	Rings

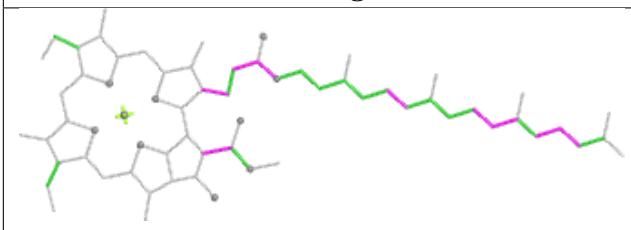
Ligand CLA B 805



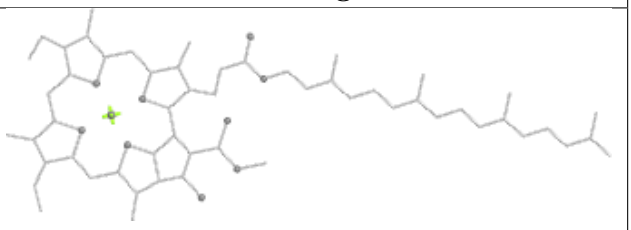
Bond lengths



Bond angles



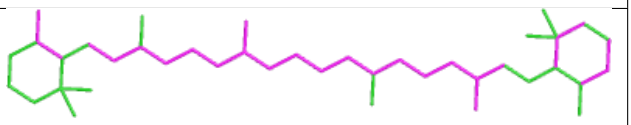
Torsions



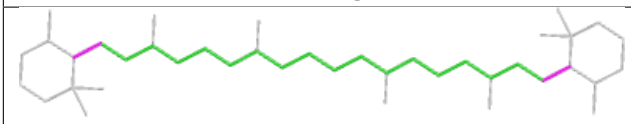
Rings

Ligand BCR G 205

Bond lengths



Bond angles



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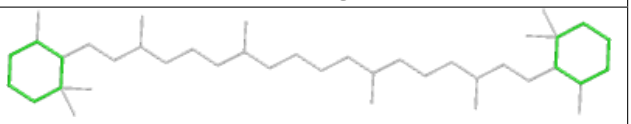
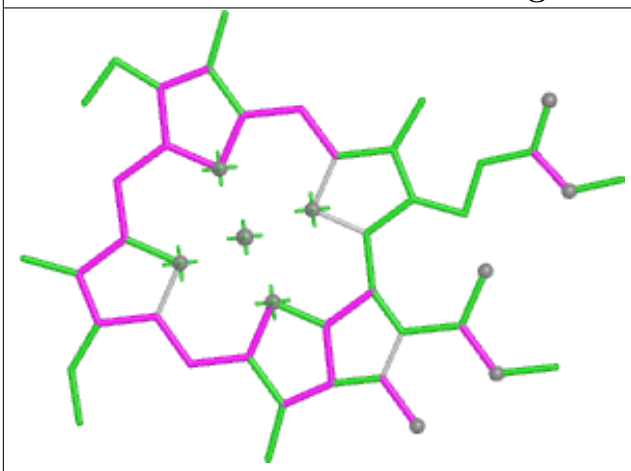
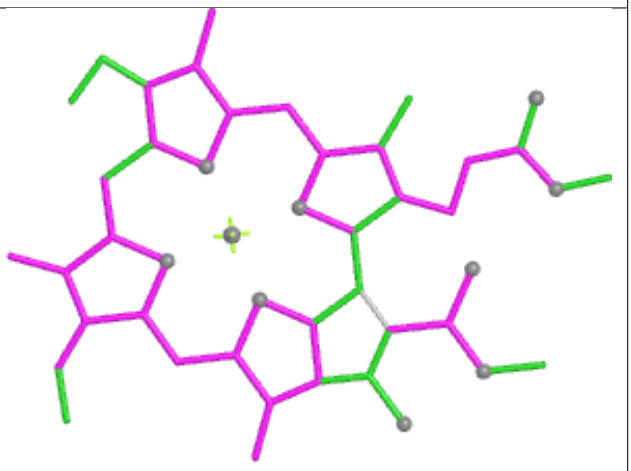


Rings

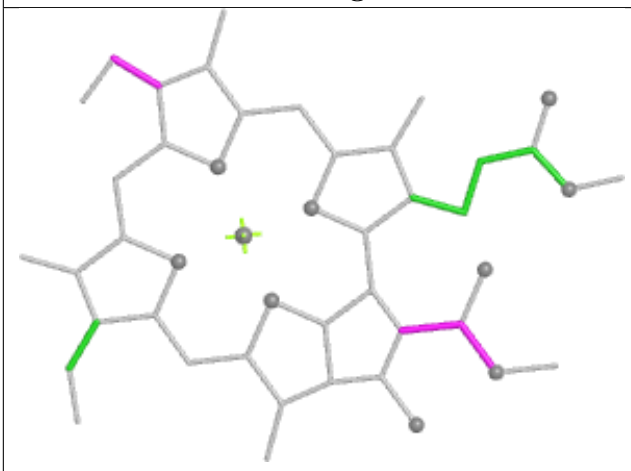
Ligand CLA 6 616



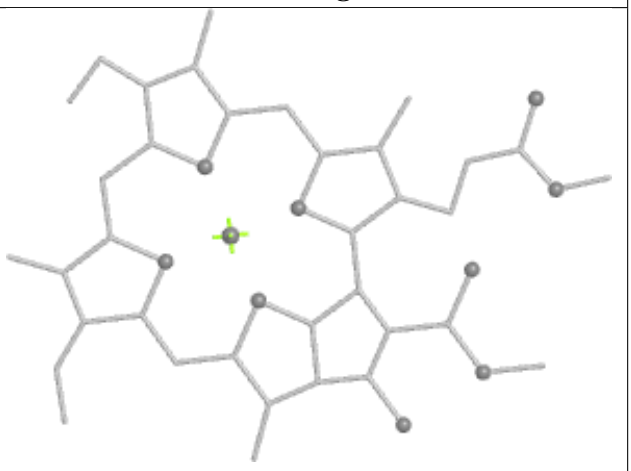
Bond lengths



Bond angles

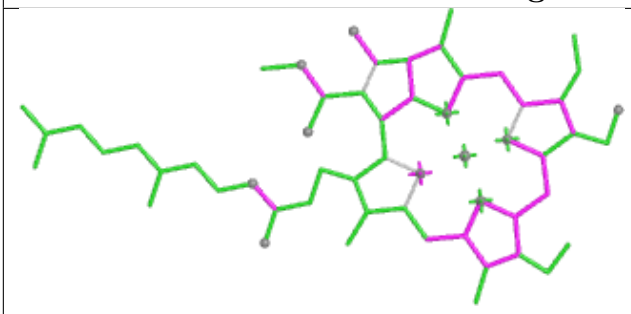


Torsions

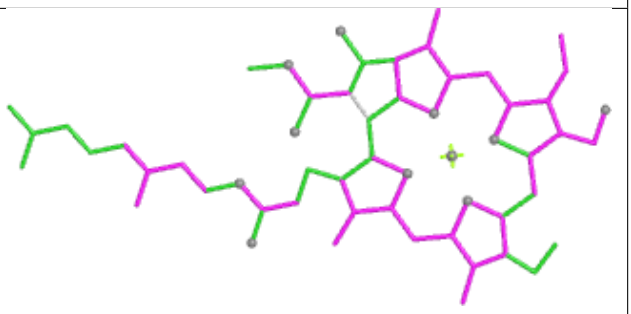


Rings

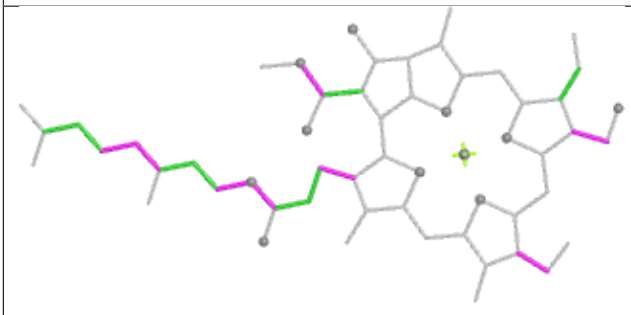
Ligand CHL 6 607



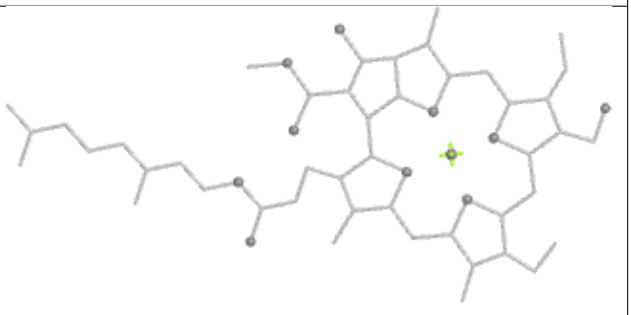
Bond lengths



Bond angles

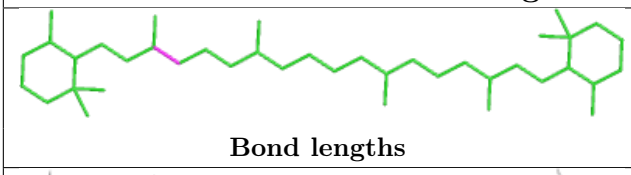


Torsions



Rings

Ligand BCR A 851



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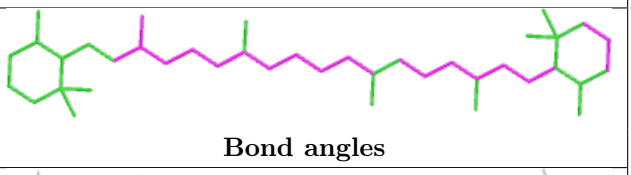
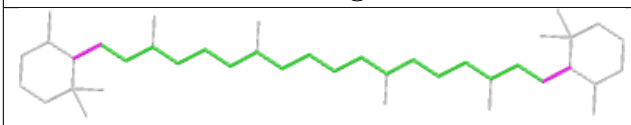
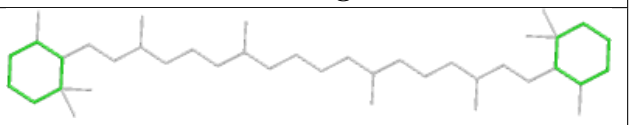


Bond angles

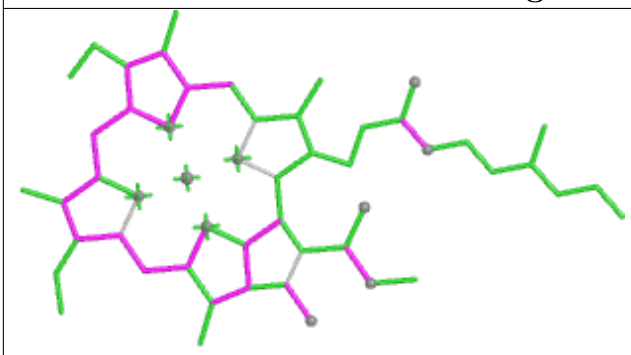


Torsions

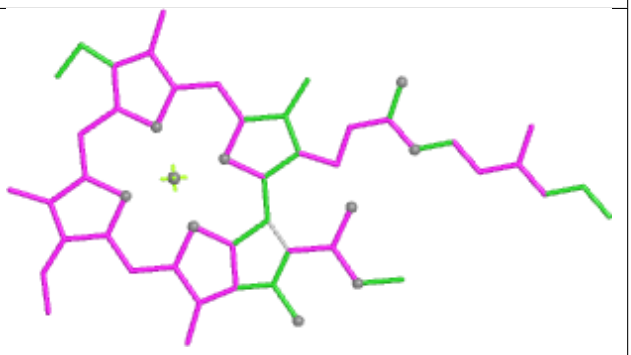


Rings

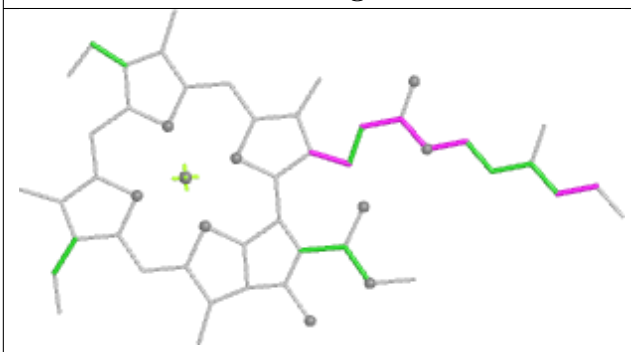
Ligand CLA Z 612



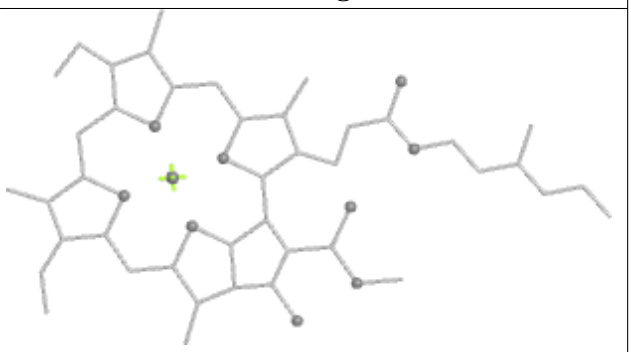
Bond lengths



Bond angles



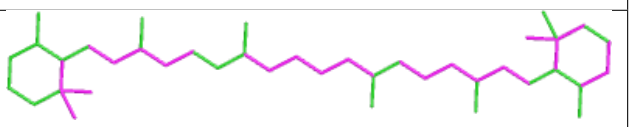
Torsions



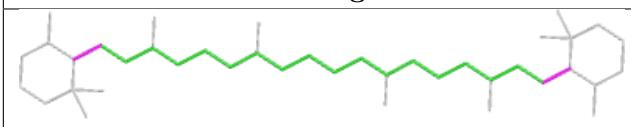
Rings

Ligand BCR A 848

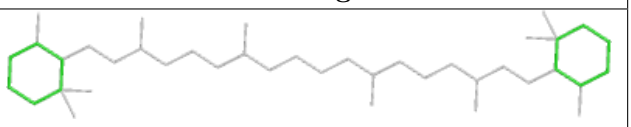
Bond lengths



Bond angles

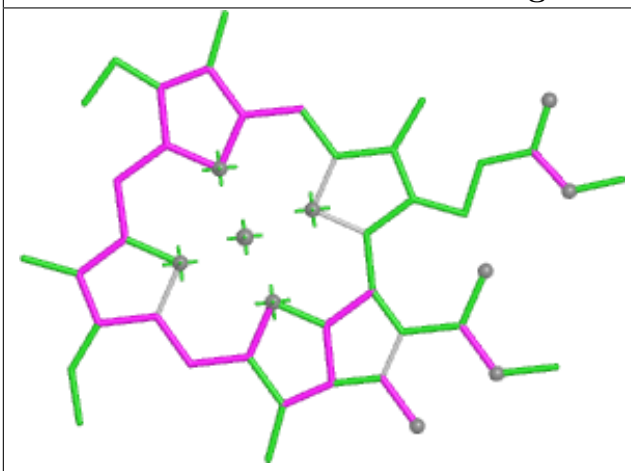


Torsions

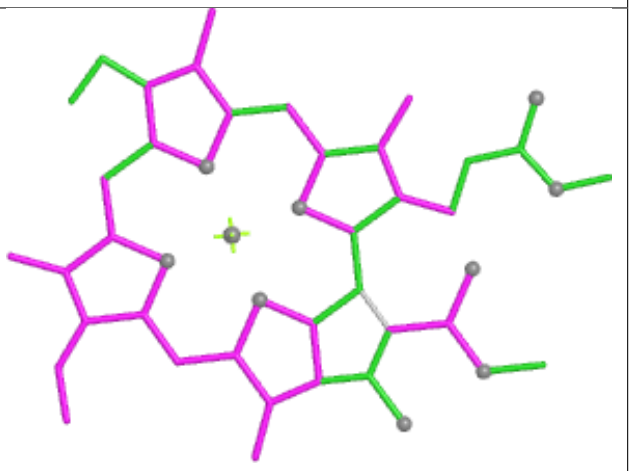


Rings

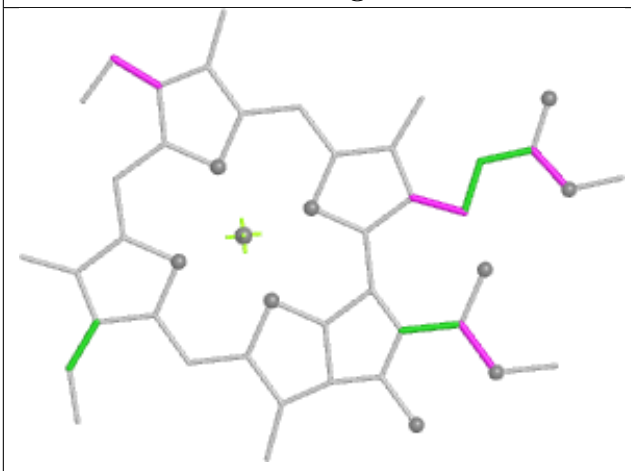
Ligand CLA 8 604



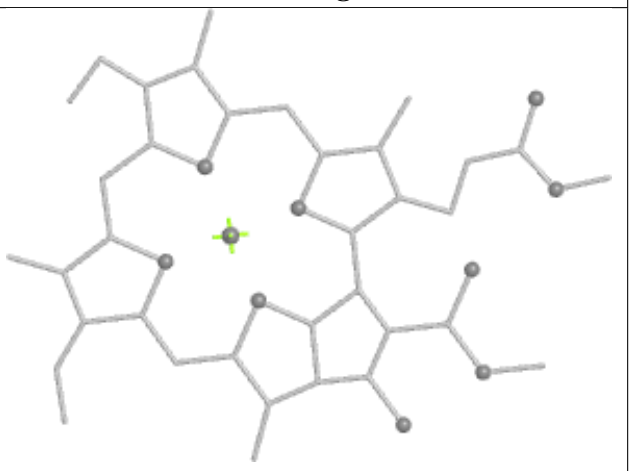
Bond lengths



Bond angles

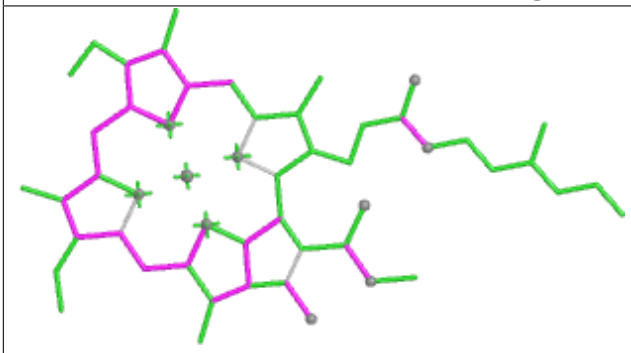


Torsions

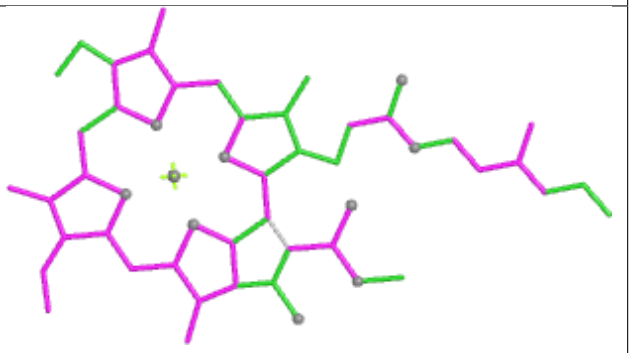


Rings

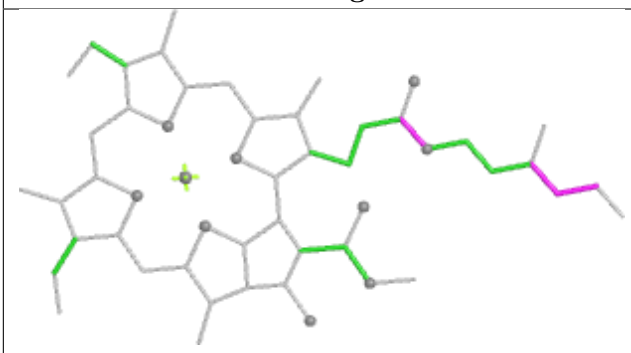
Ligand CLA 6 612



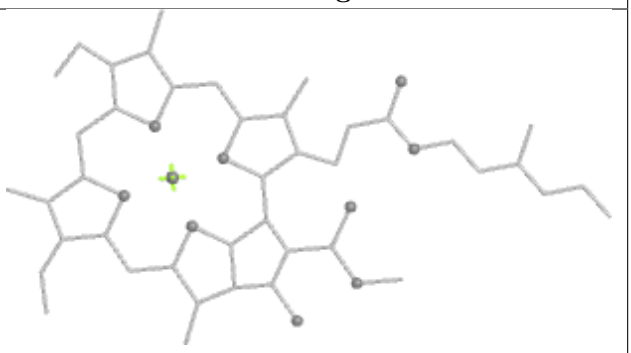
Bond lengths



Bond angles

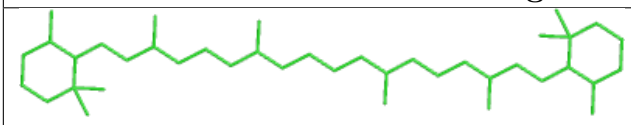


Torsions

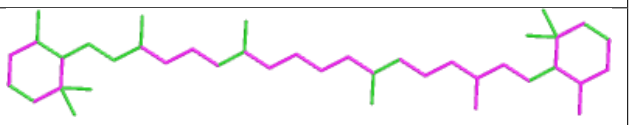


Rings

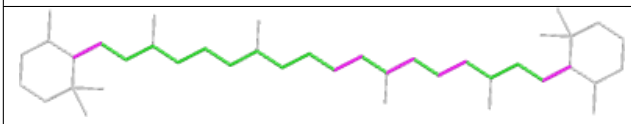
Ligand BCR 7 623



Bond lengths



Bond angles



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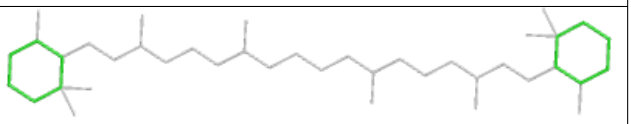
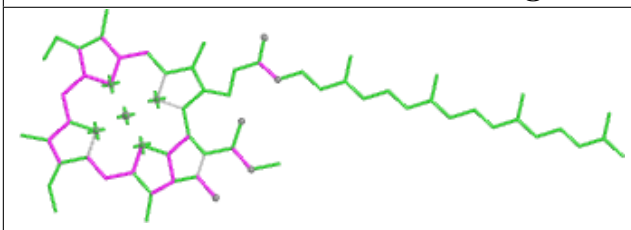
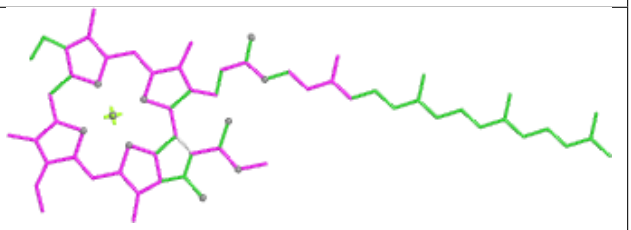


Rings

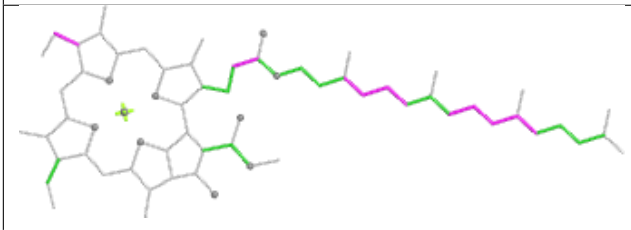
Ligand CLA B 806



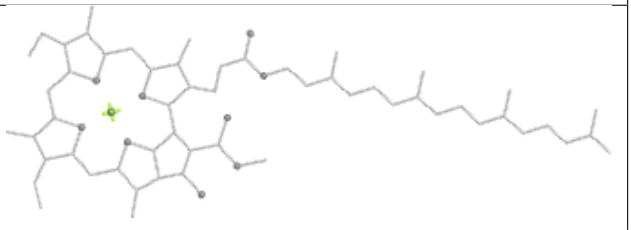
Bond lengths



Bond angles

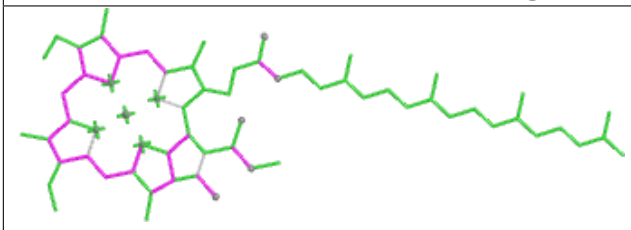


Torsions



Rings

Ligand CLA A 812



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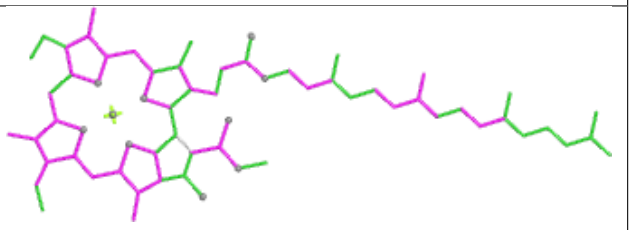
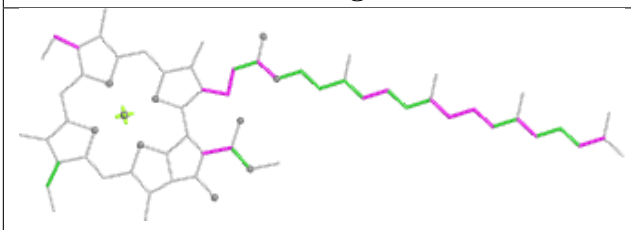


Bond angles



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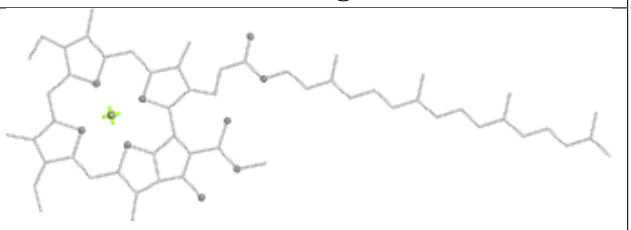
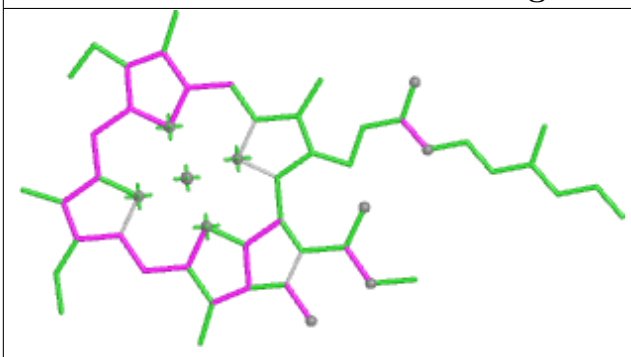


Rings

Ligand CLA 1 612



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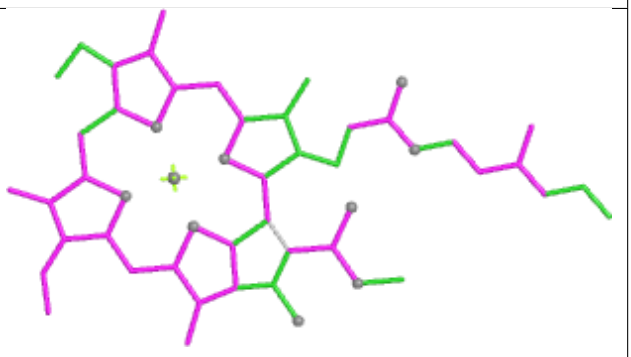
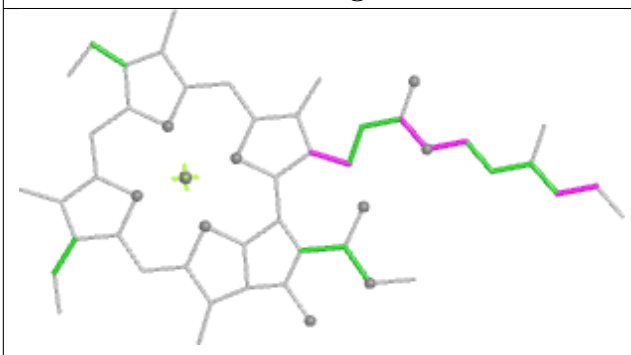


Bond angles



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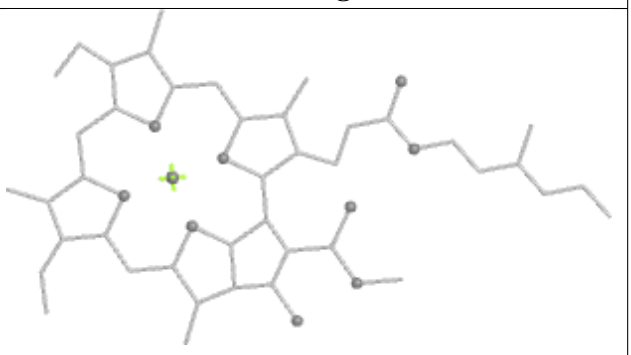
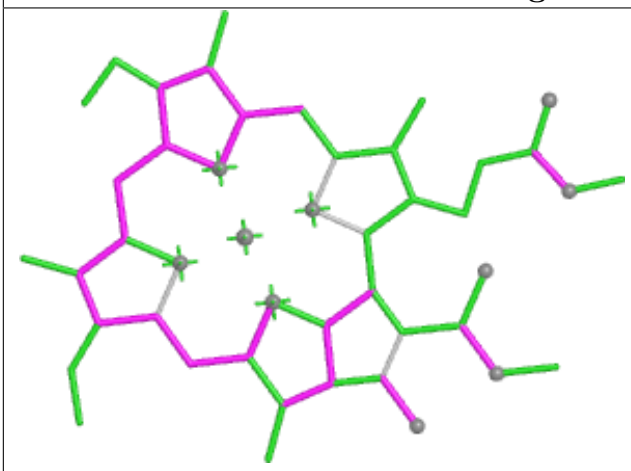


Rings

Ligand CLA 3 617



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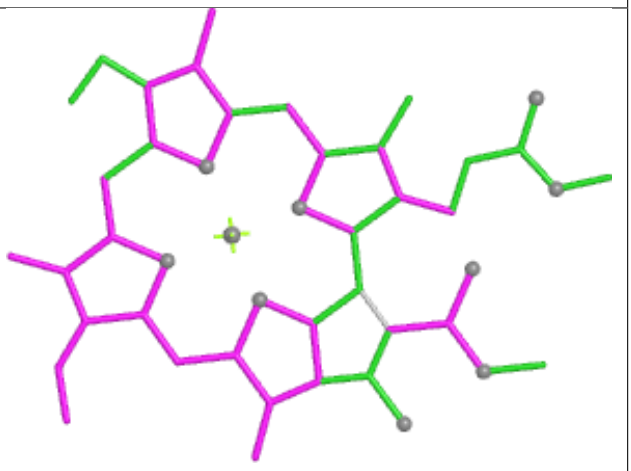
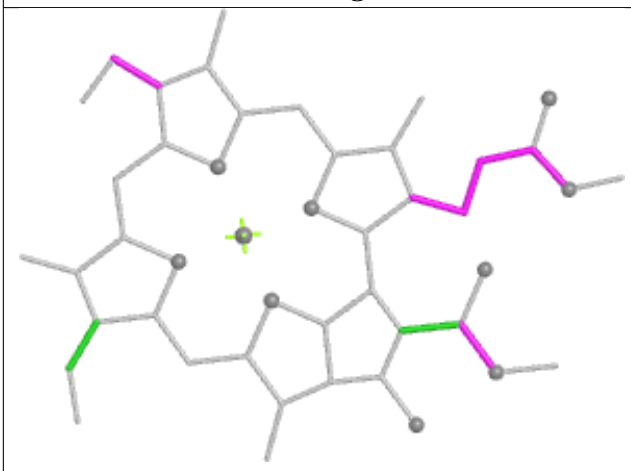


Bond angles



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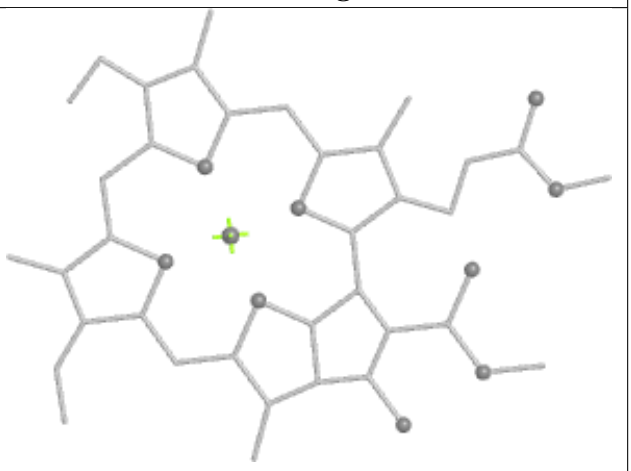
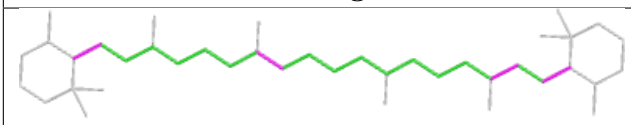


Rings

Ligand BCR F 305

Bond lengths

Bond angles



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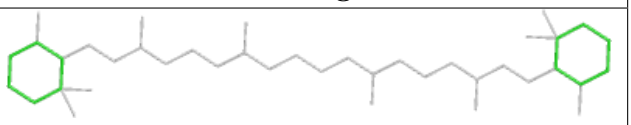
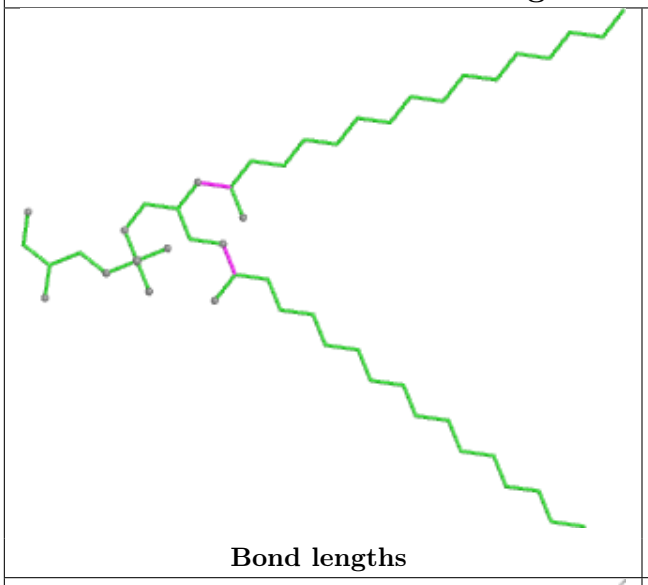
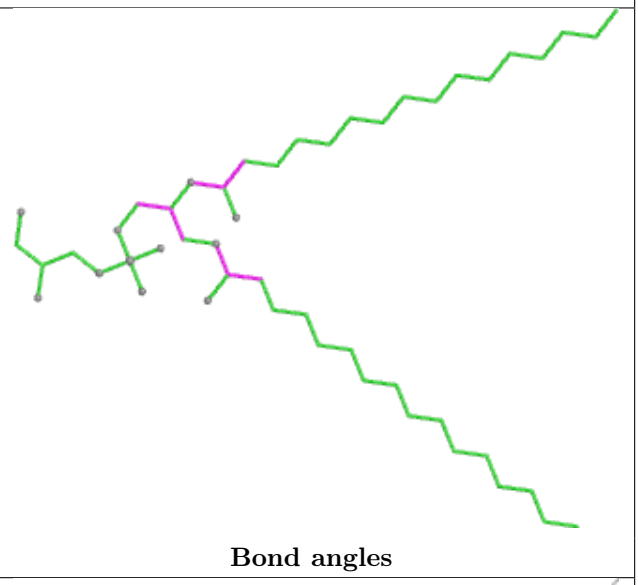


Rings

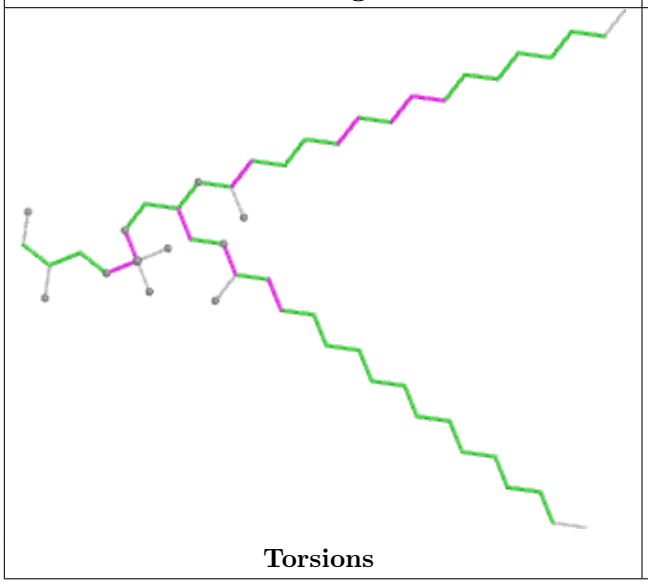
Ligand LHG 4 622



Bond lengths



Bond angles



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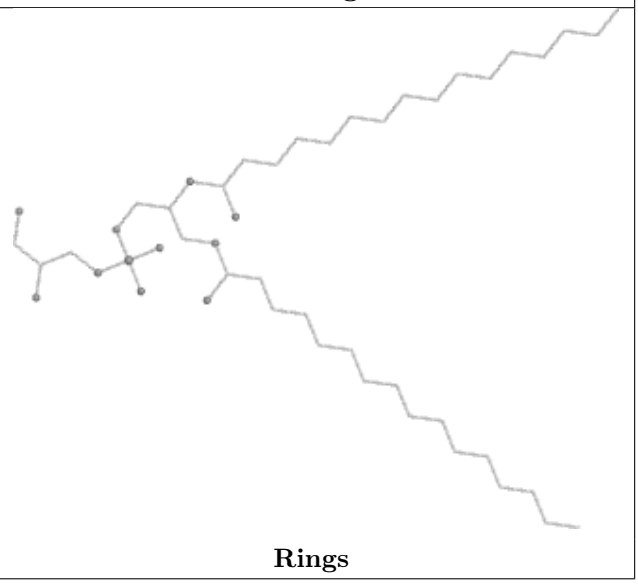
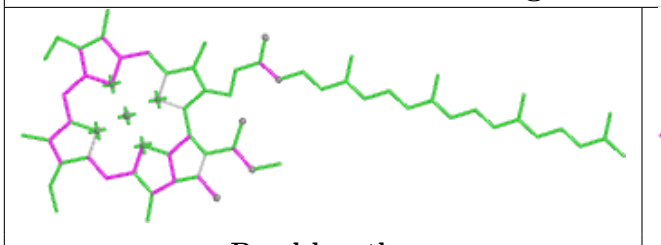


Rings

Ligand CLA B 832



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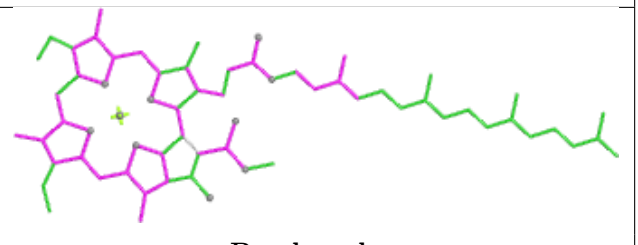
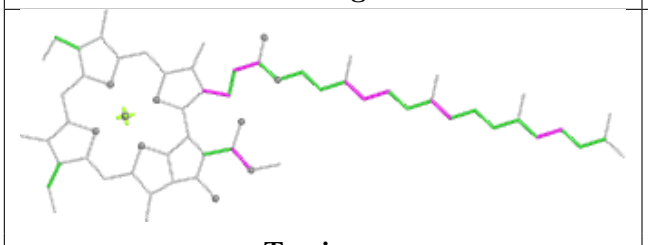


Bond angles



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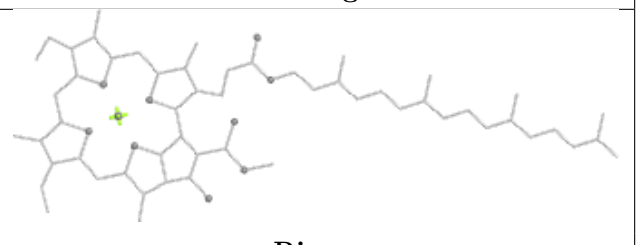
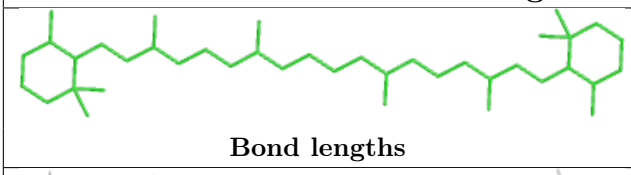


Rings

Ligand BCR 5 622



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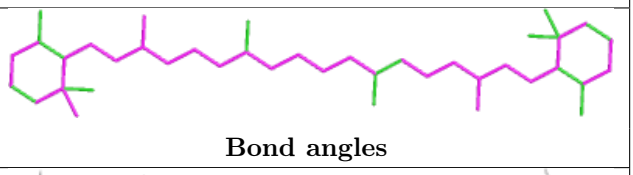
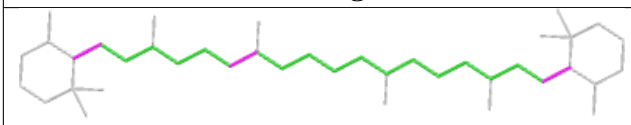
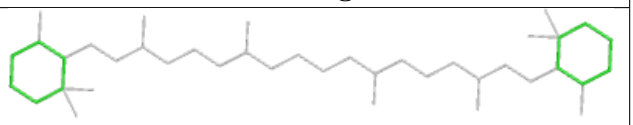


Bond angles

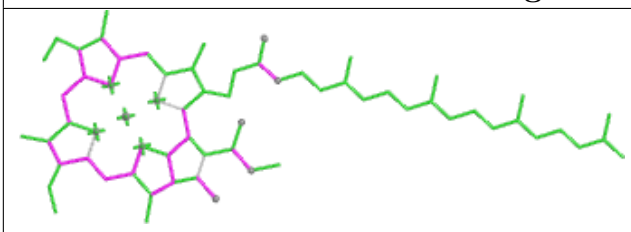


Torsions

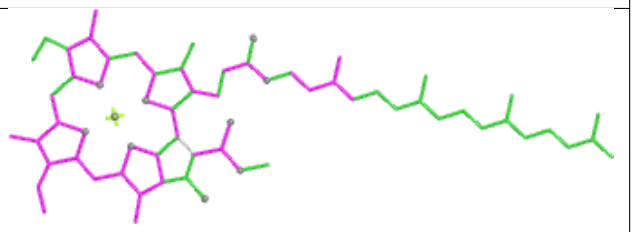


Rings

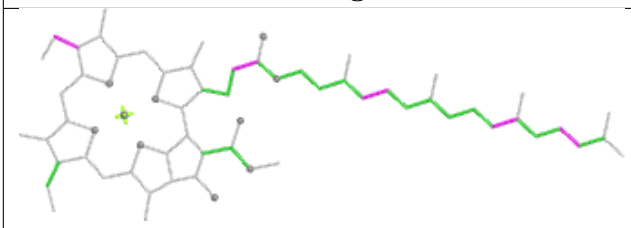
Ligand CLA B 809



Bond lengths



Bond angles



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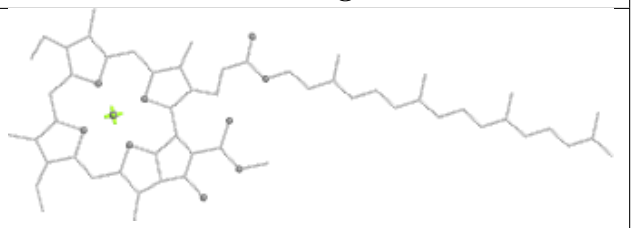
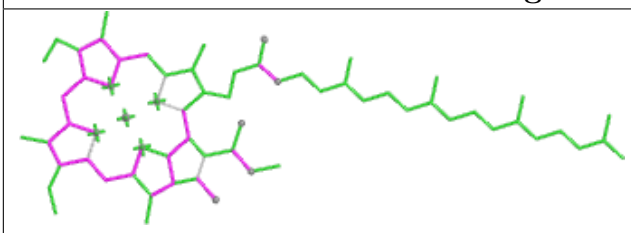


Rings

Ligand CLA B 827



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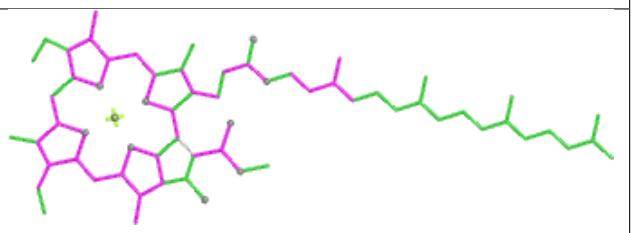
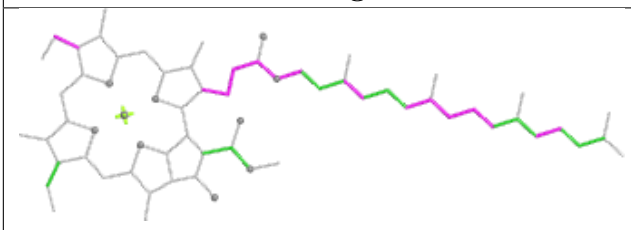
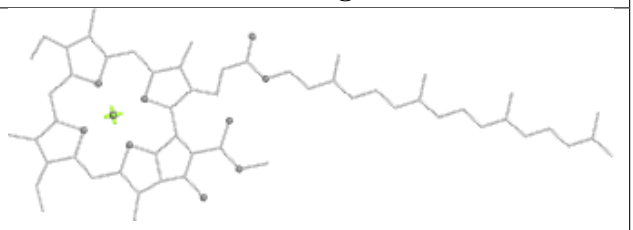


Bond angles

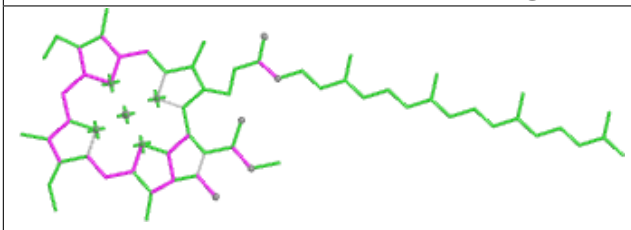


Torsions

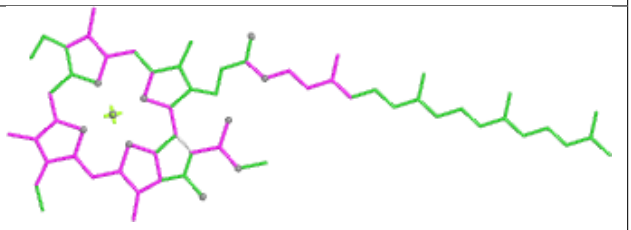


Rings

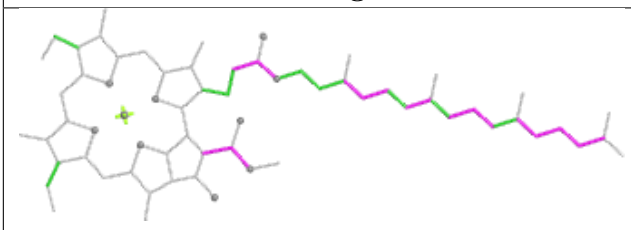
Ligand CLA A 826



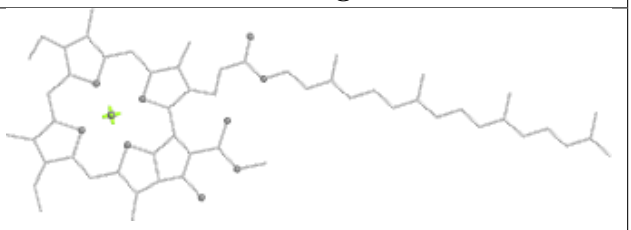
Bond lengths



Bond angles



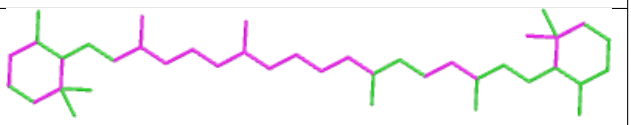
Torsions



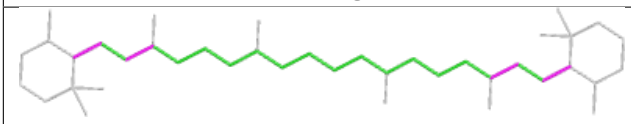
Rings

Ligand BCR 3 719

Bond lengths



Bond angles



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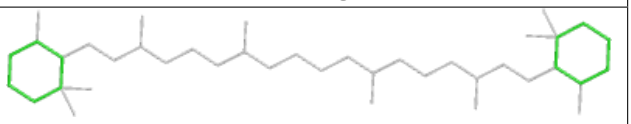
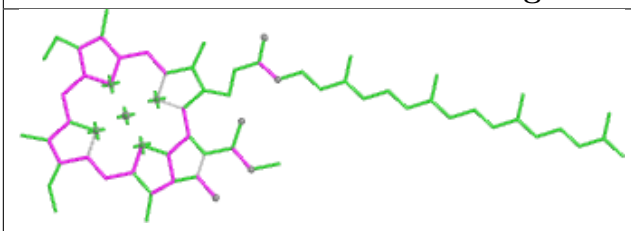
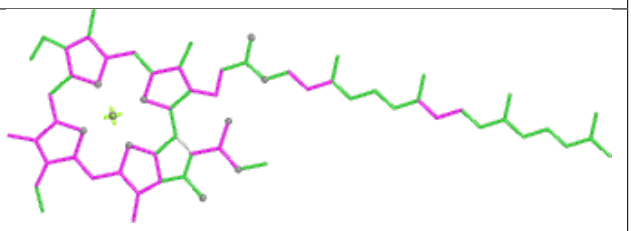


Rings

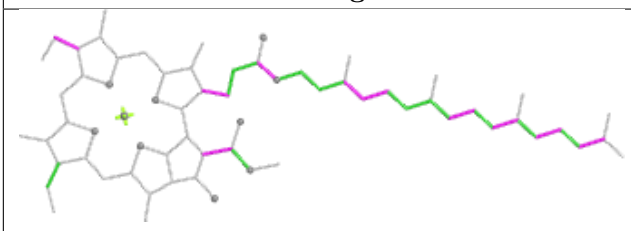
Ligand CLA A 820



Bond lengths



Bond angles



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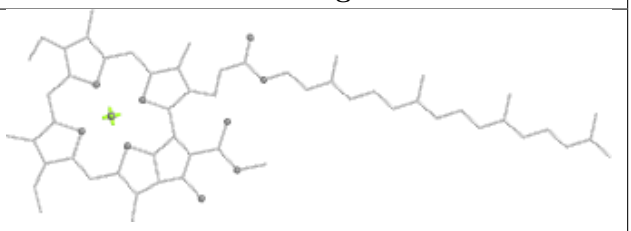
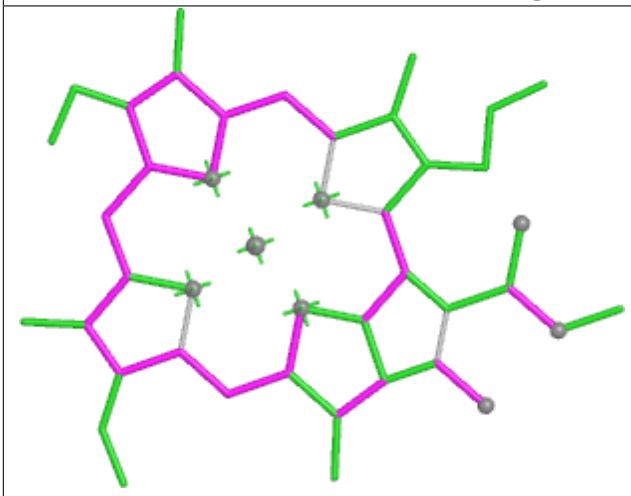
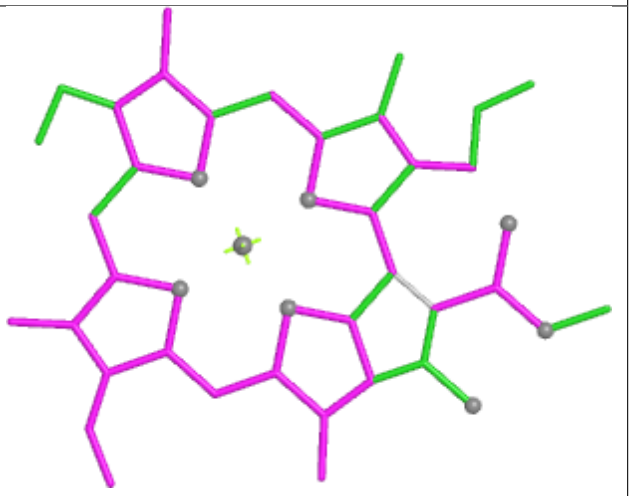


Rings

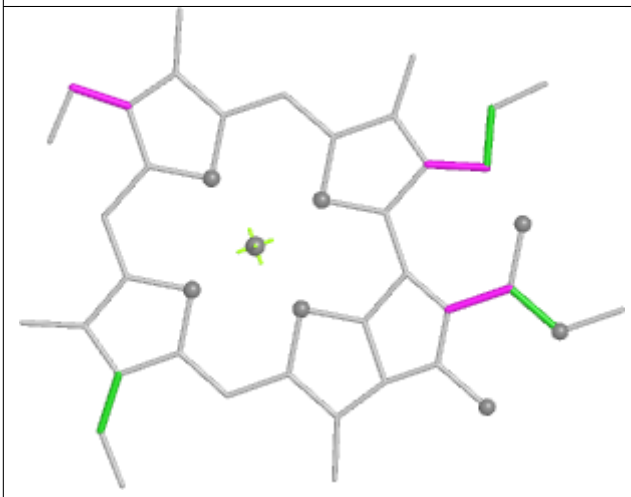
Ligand CLA 7 614



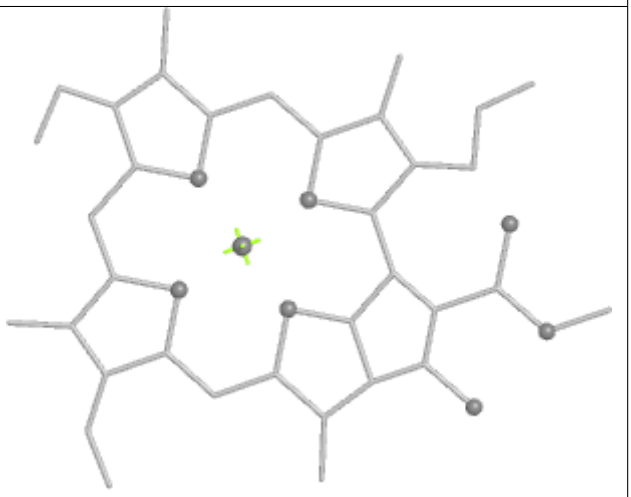
Bond lengths



Bond angles

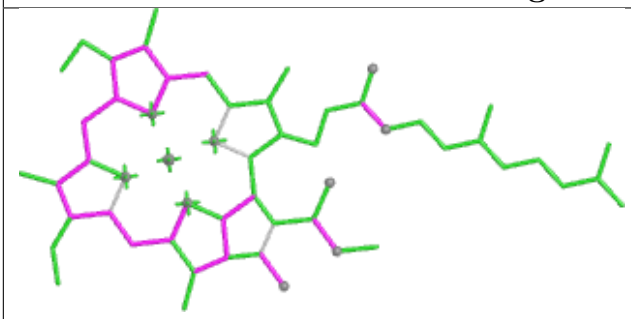


Torsions



Rings

Ligand CLA 5 606



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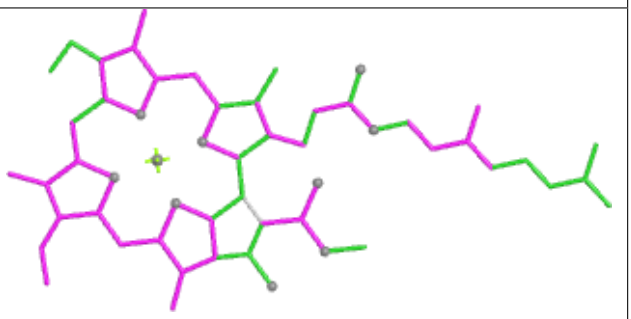

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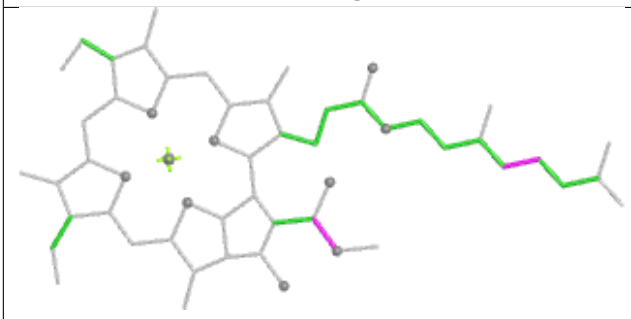

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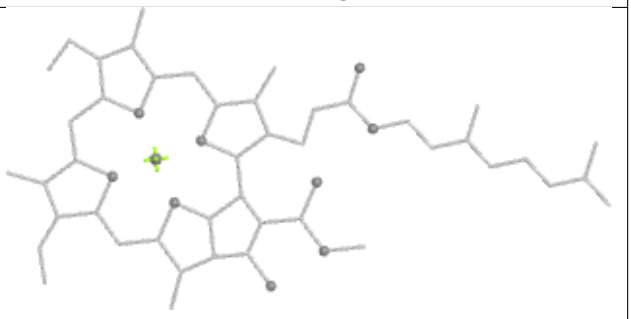
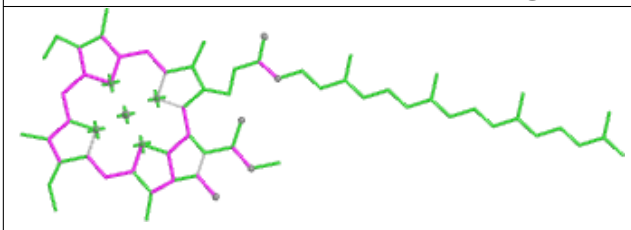


Rings

Ligand CLA A 829



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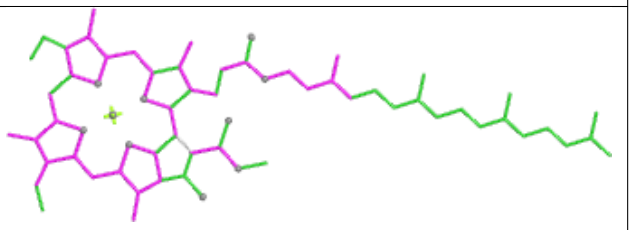

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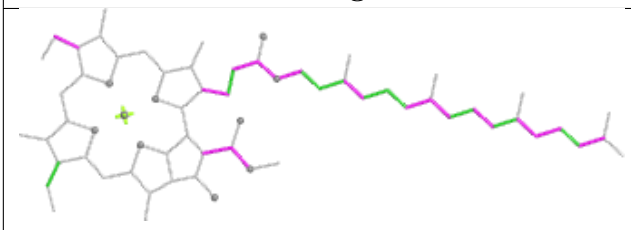

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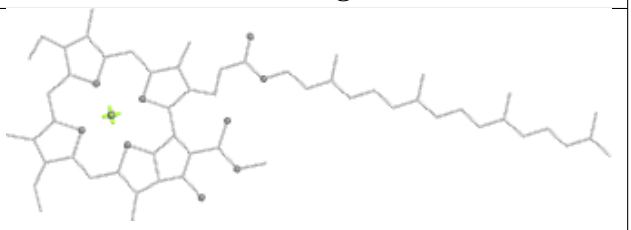
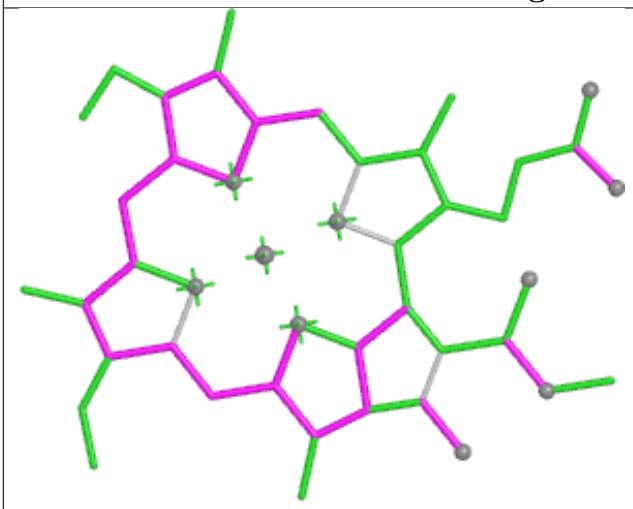


Rings

Ligand CLA 6 614



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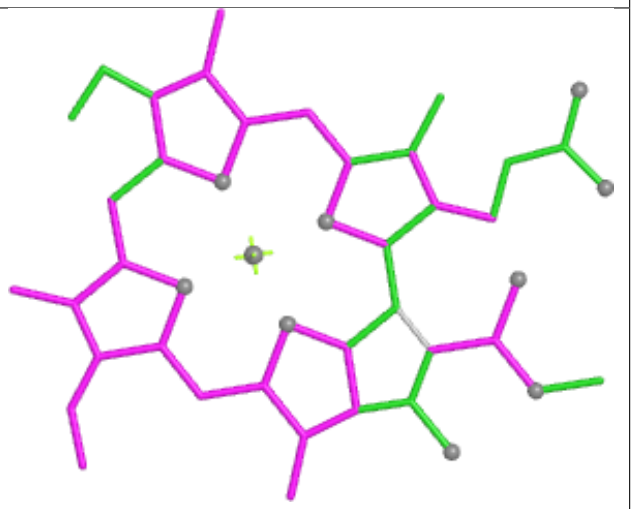

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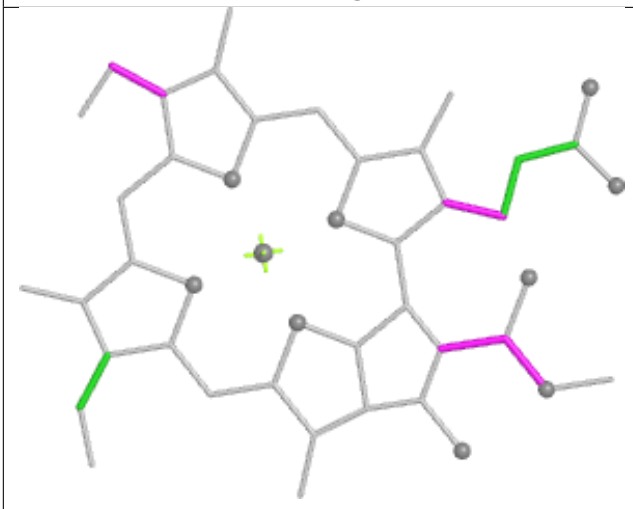
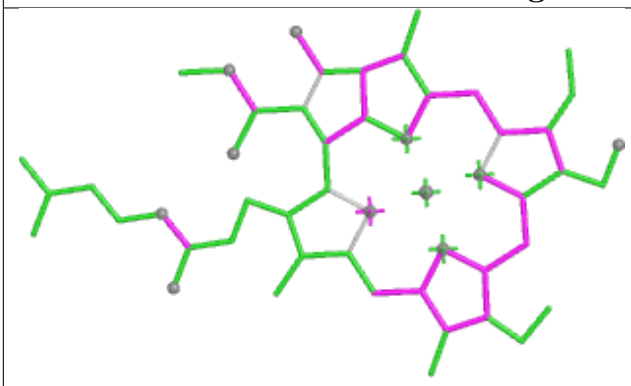


Torsions

Rings

Ligand CHL 5 607



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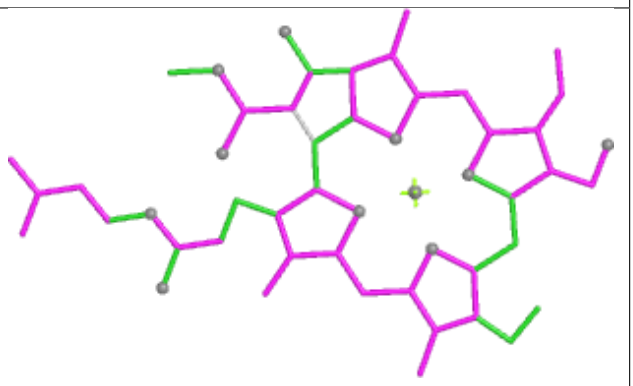
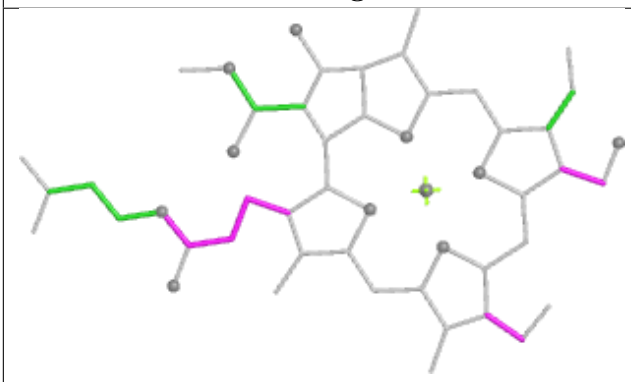


Bond angles



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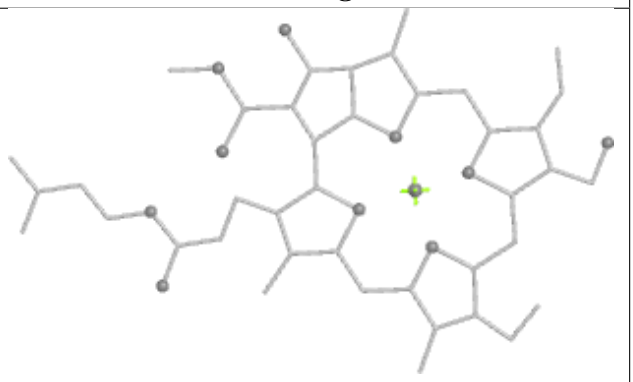
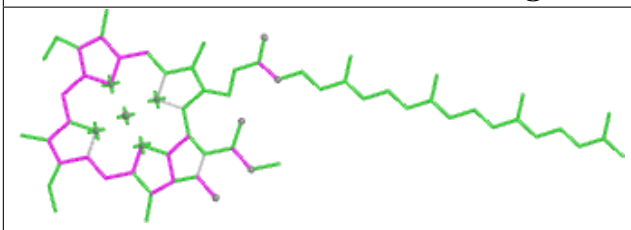


Rings

Ligand CLA B 813



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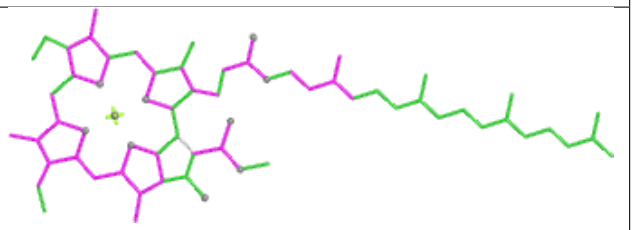

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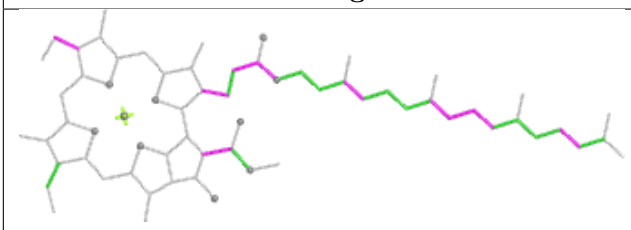

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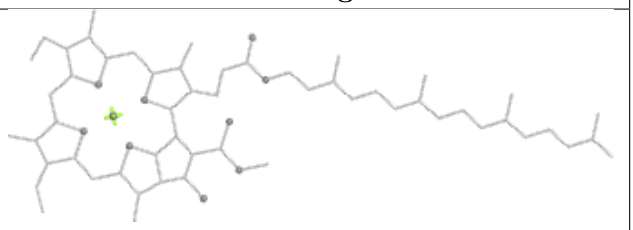
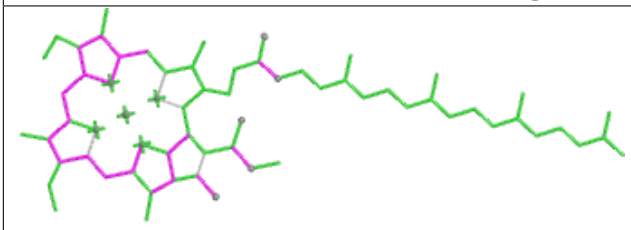
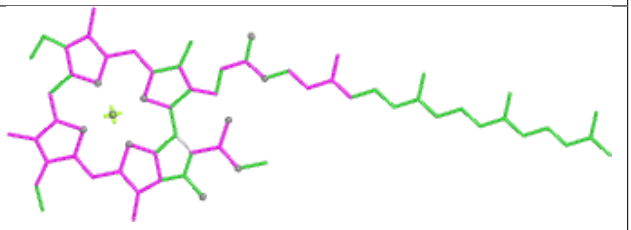
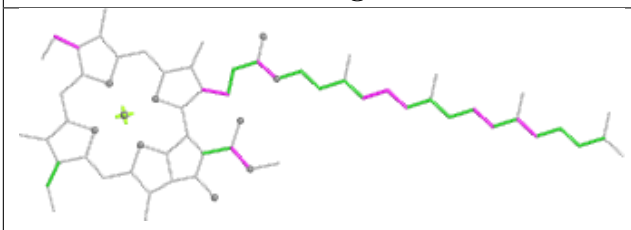
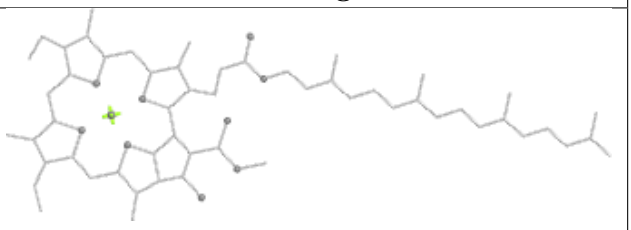


Rings

Ligand CLA Z 611	
 Bond lengths	 Bond angles
 Torsions	 Rings

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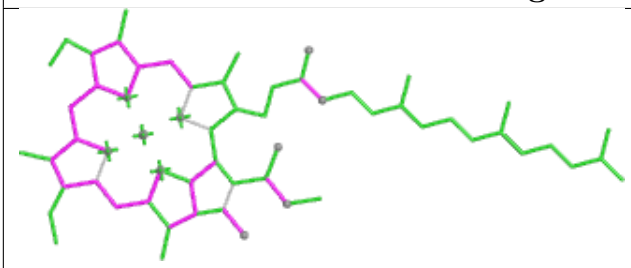
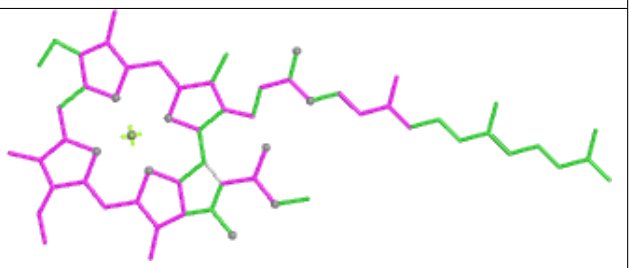
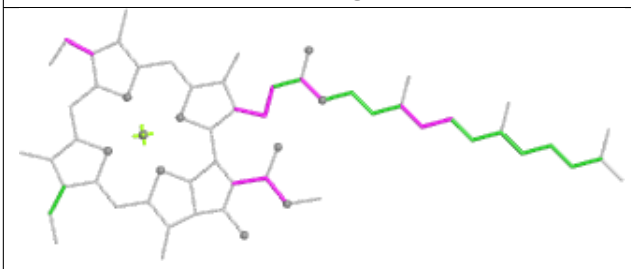
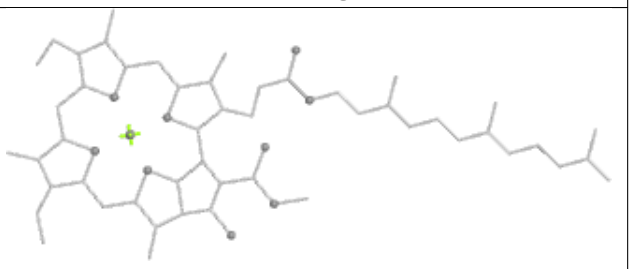
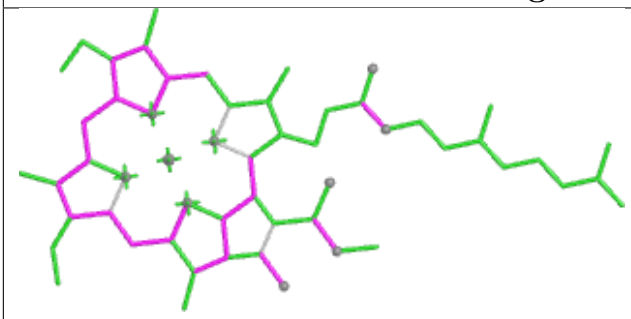
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA 6 611



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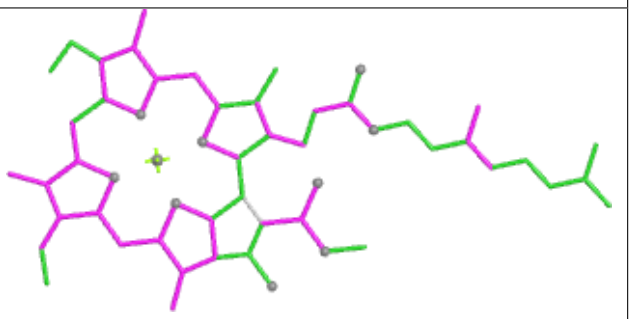
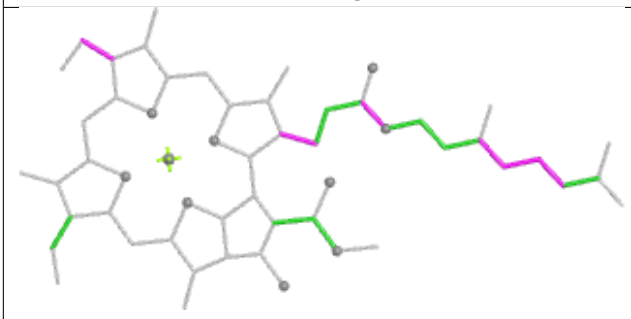


Bond angles



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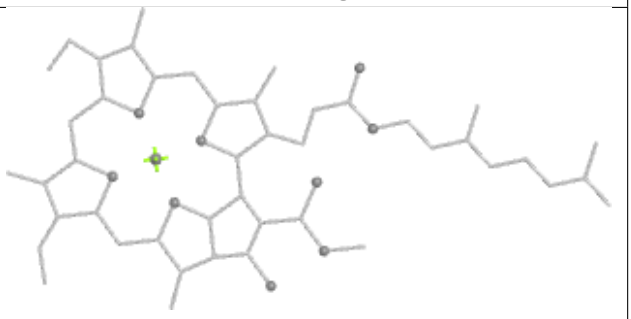
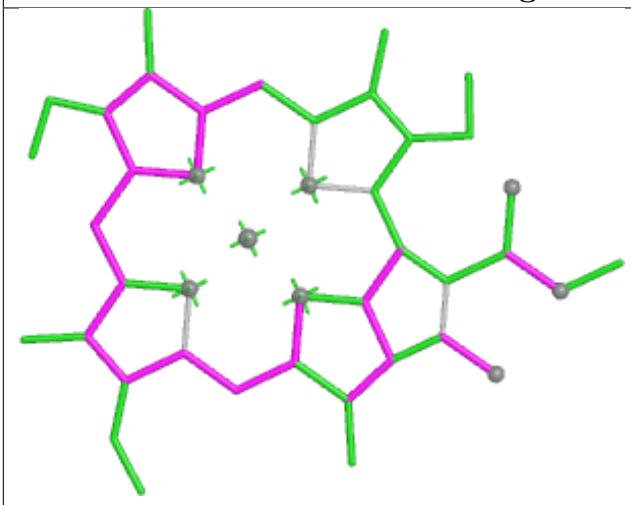


Rings

Ligand CLA J 3002



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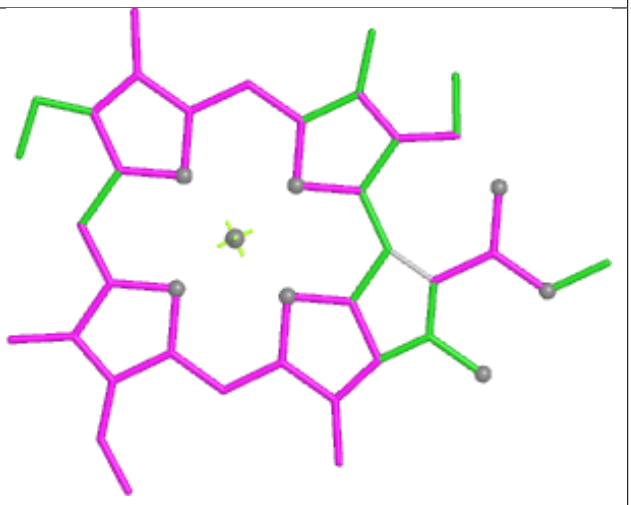

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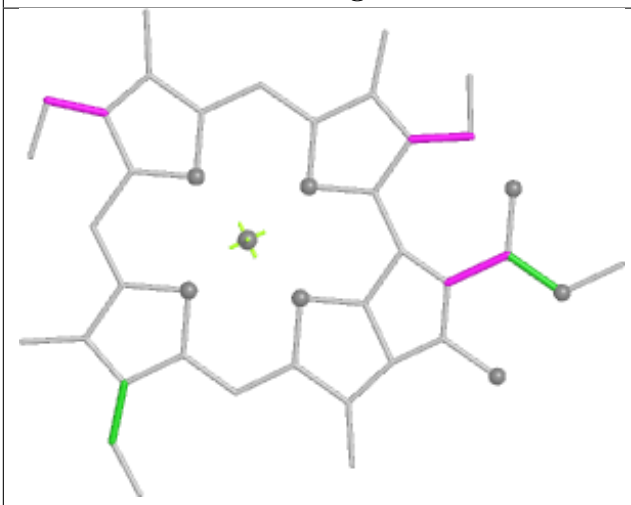
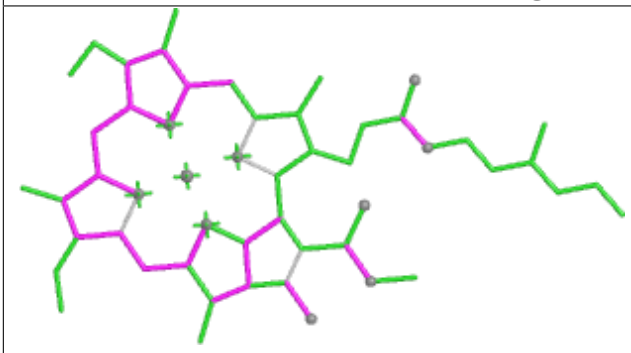


Torsions

Rings

Ligand CLA 5 612



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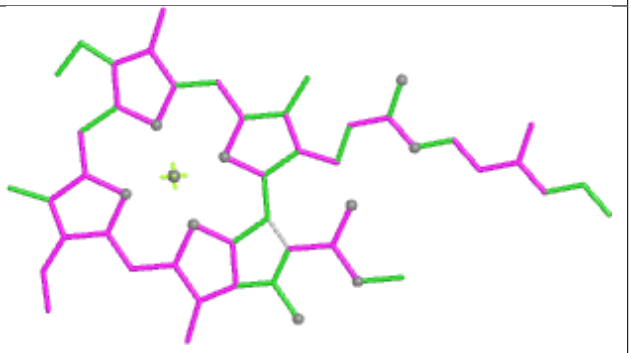

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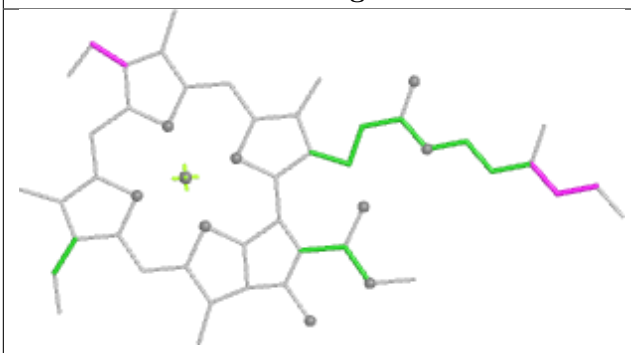

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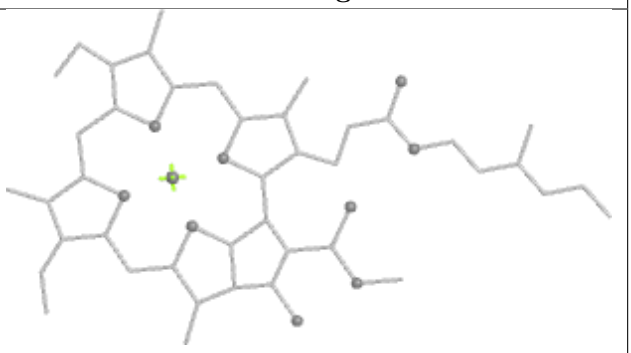
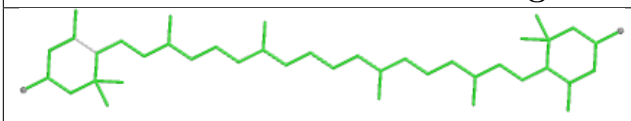


Rings

Ligand LUT 3 621



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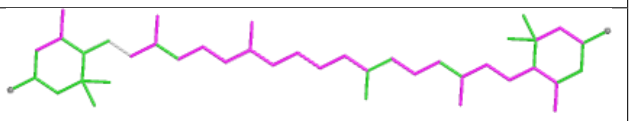

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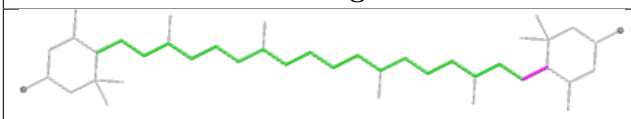

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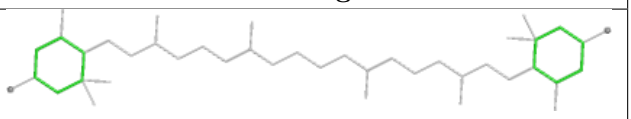
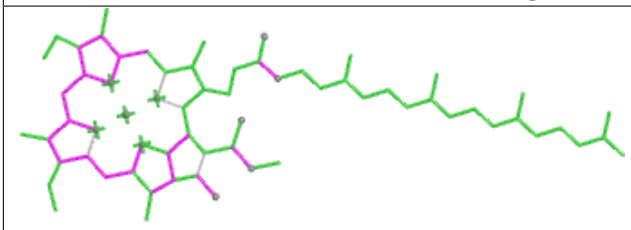


Rings

Ligand CLA A 808



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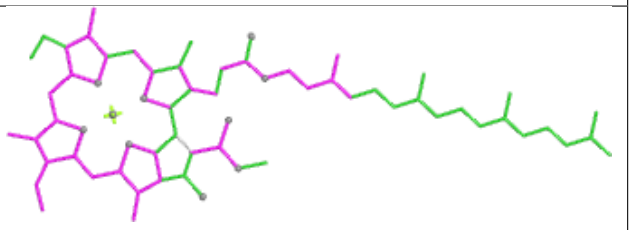

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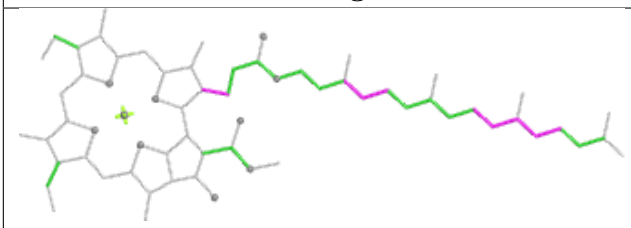

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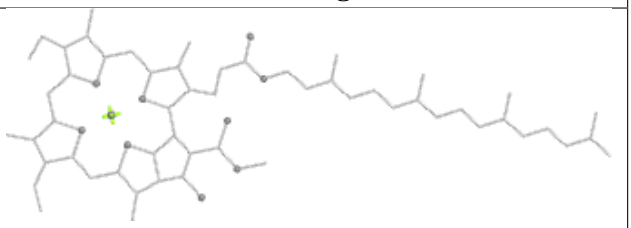
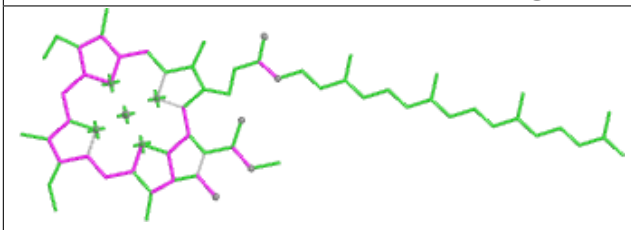


Rings

Ligand CLA 7 613



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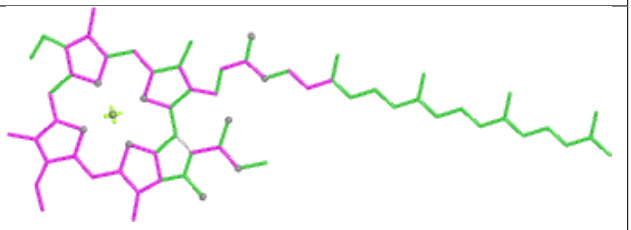
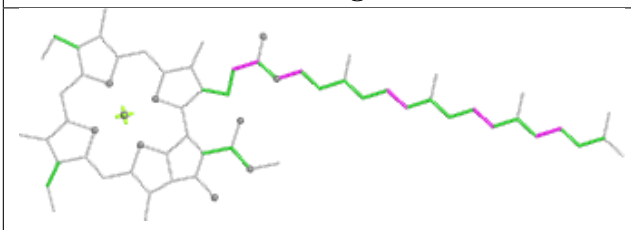


Bond angles



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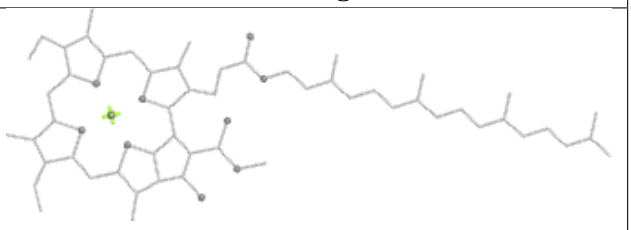
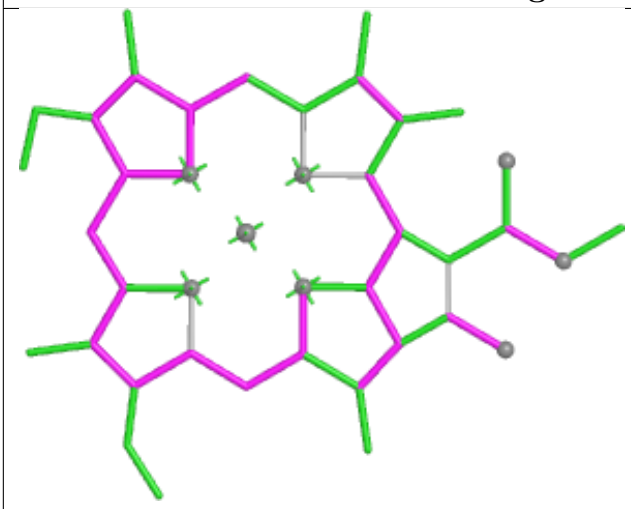


Rings

Ligand CLA 7 611



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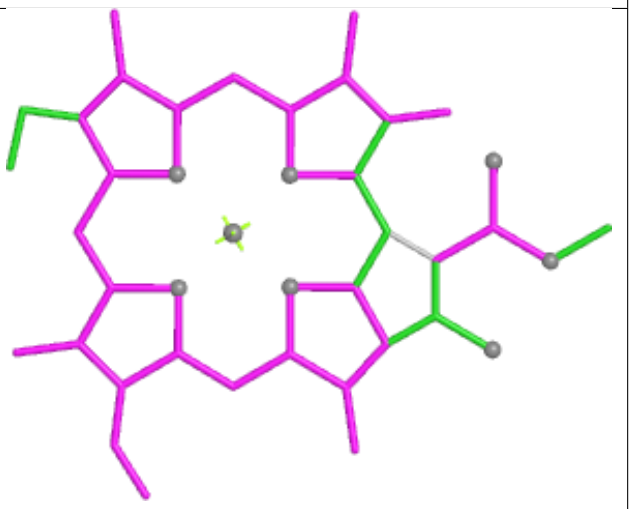
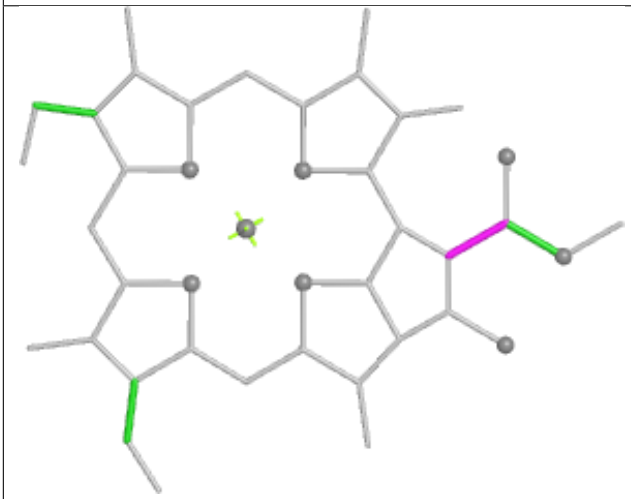
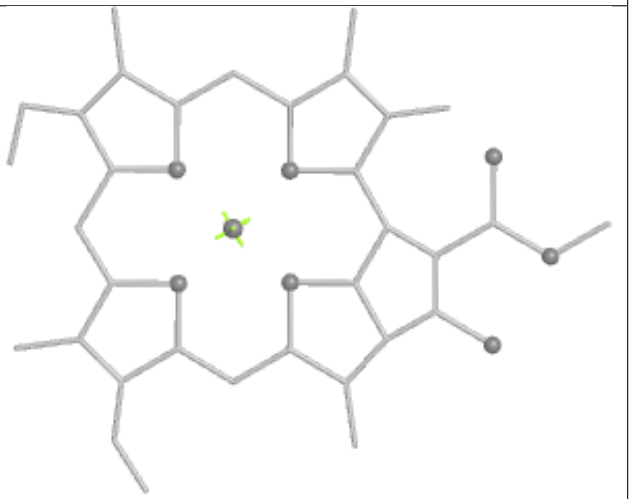


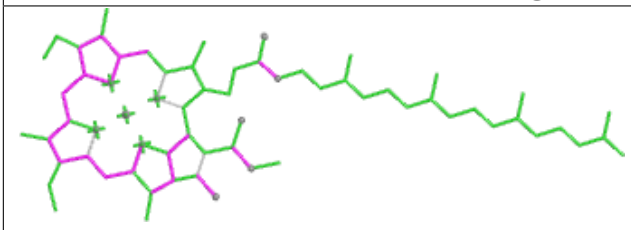
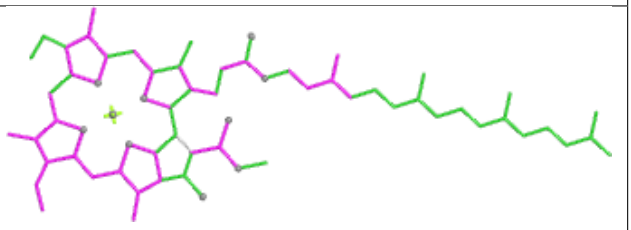
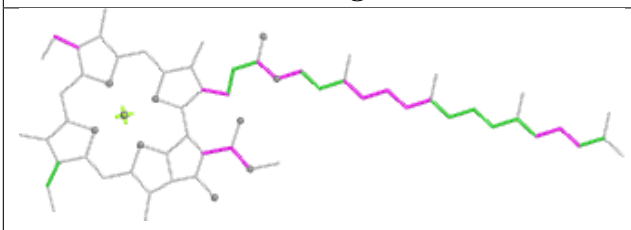
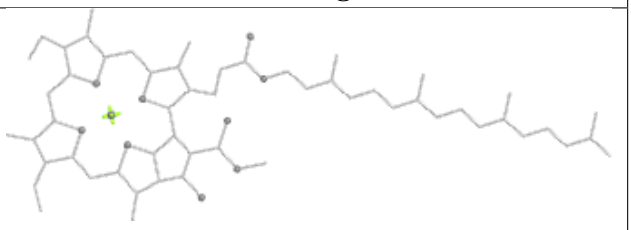
Bond angles

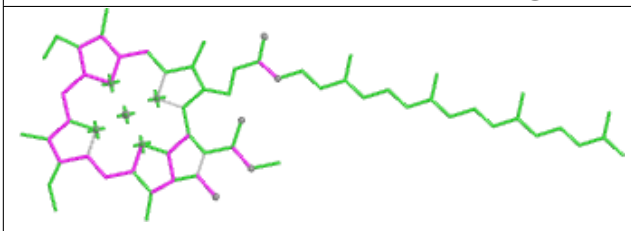
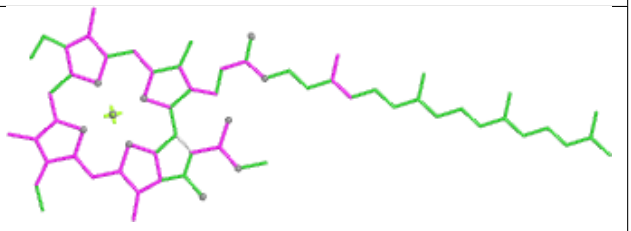
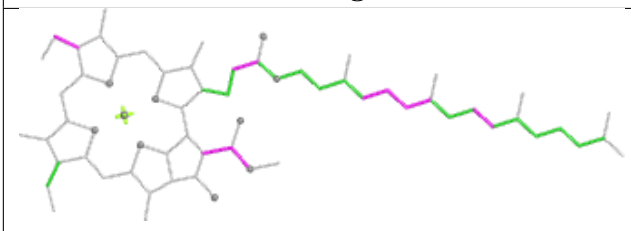
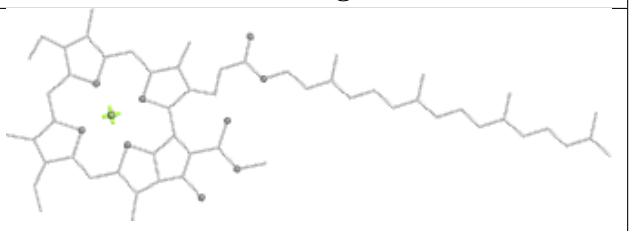


Torsions

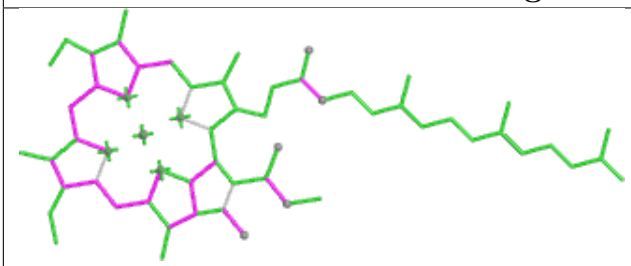


Rings

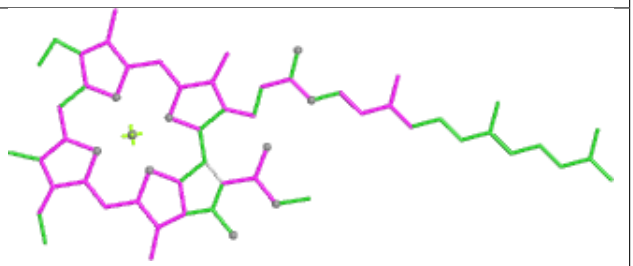
Ligand CLA 1 608	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA Z 613	
 Bond lengths	 Bond angles
 Torsions	 Rings

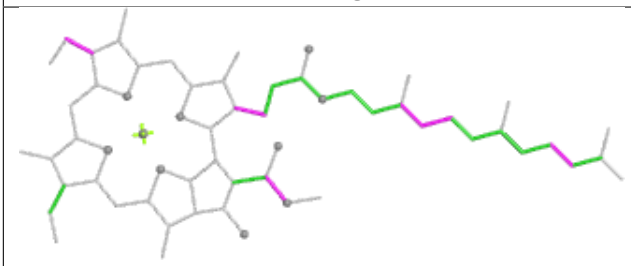
Ligand CLA B 823



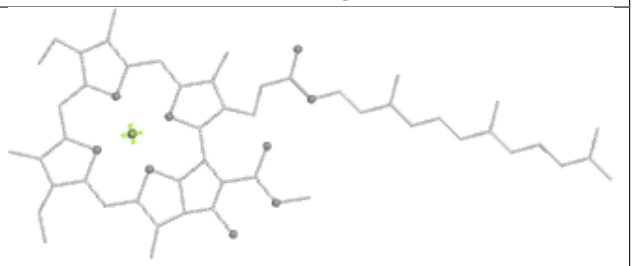
Bond lengths



Bond angles

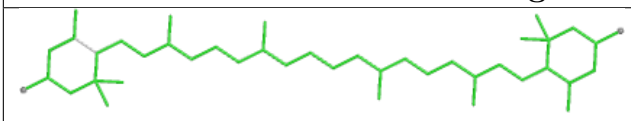


Torsions

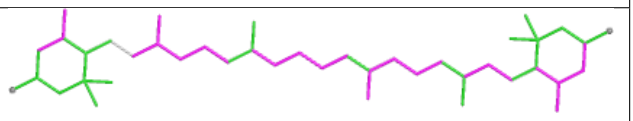


Rings

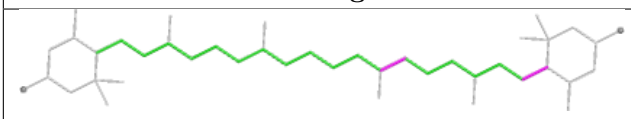
Ligand LUT 6 621



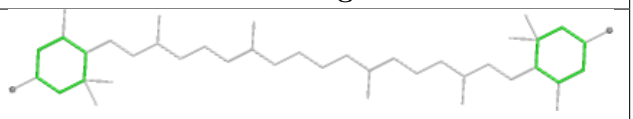
Bond lengths



Bond angles

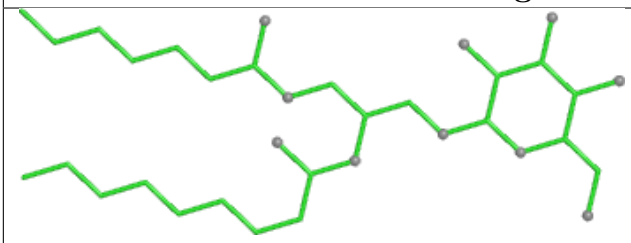


Torsions

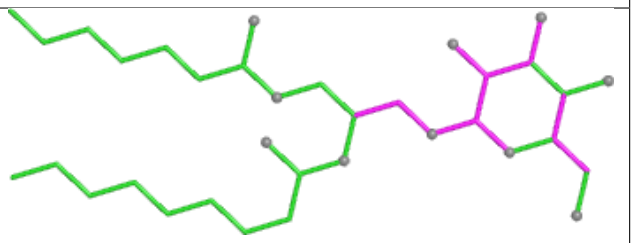


Rings

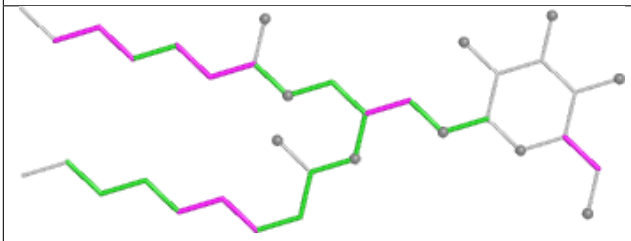
Ligand LMG J 3001



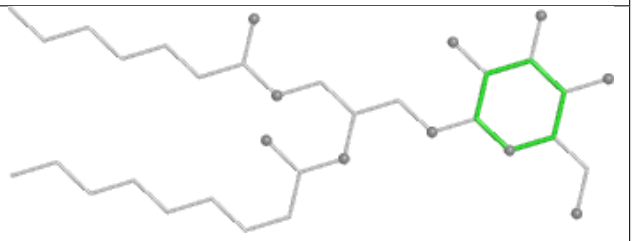
Bond lengths



Bond angles

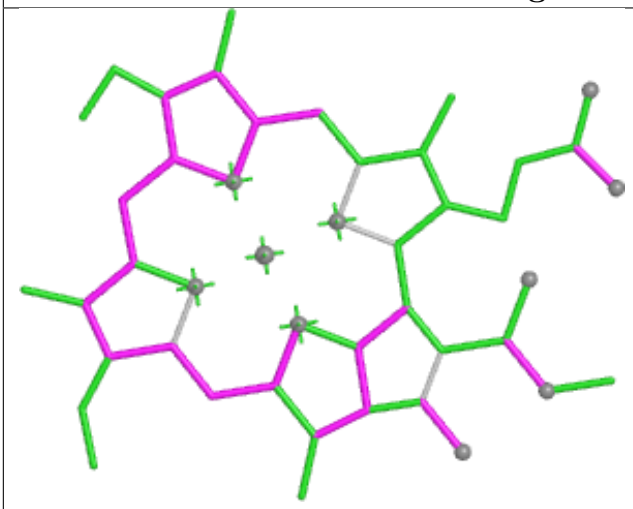


Torsions

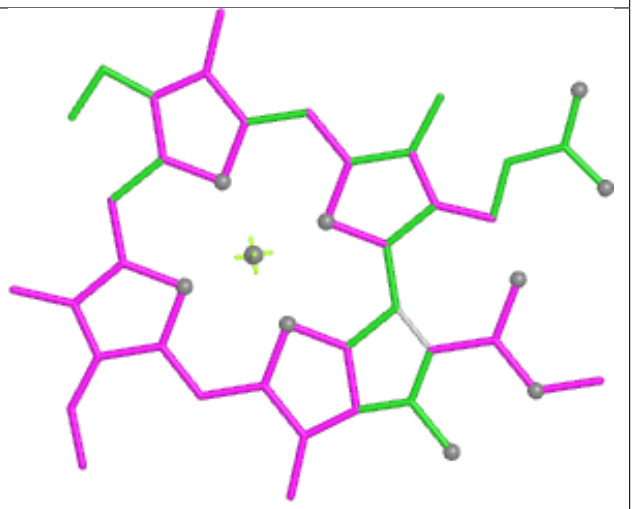


Rings

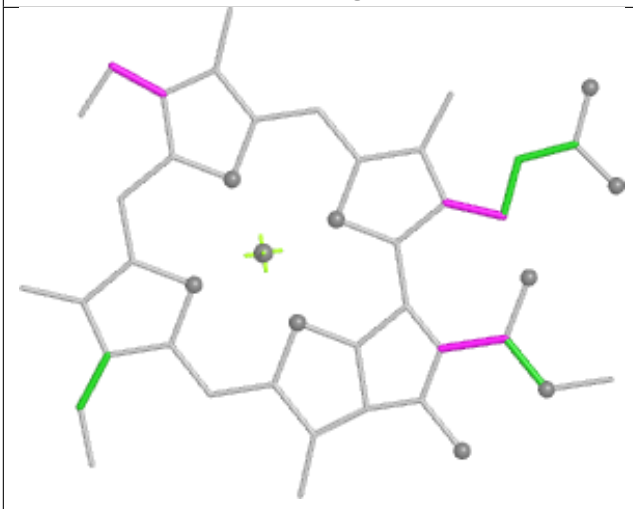
Ligand CLA 4 614



Bond lengths



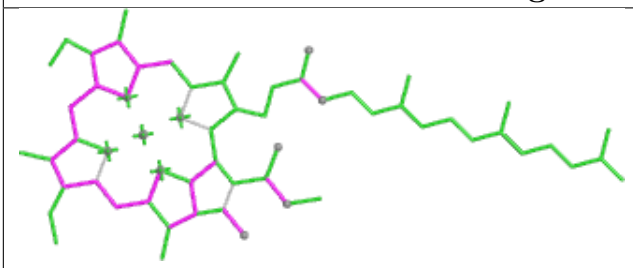
Bond angles



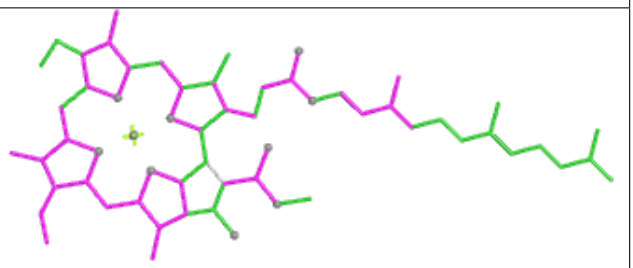
Torsions

Rings

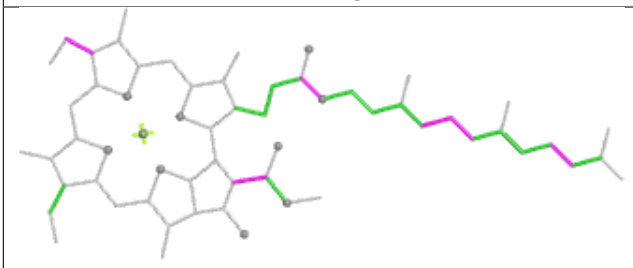
Ligand CLA 7 620



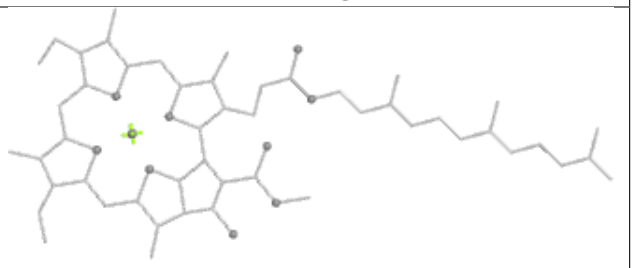
Bond lengths



Bond angles

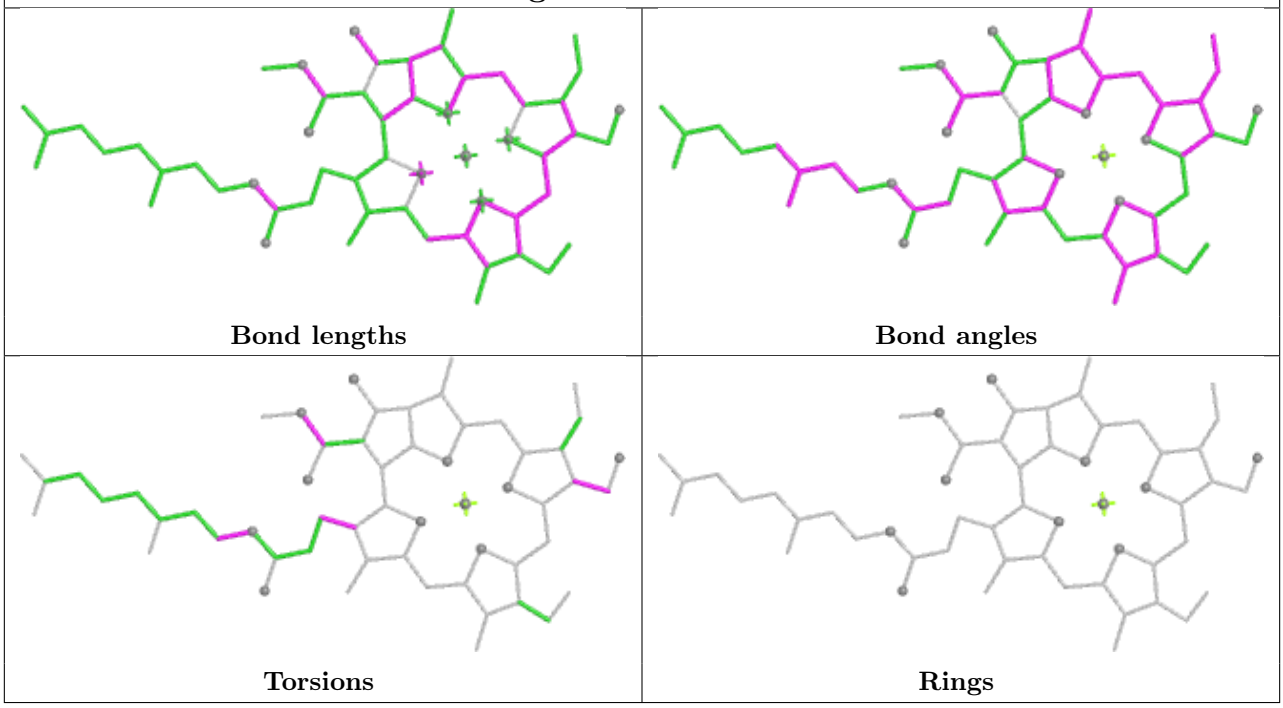


Torsions

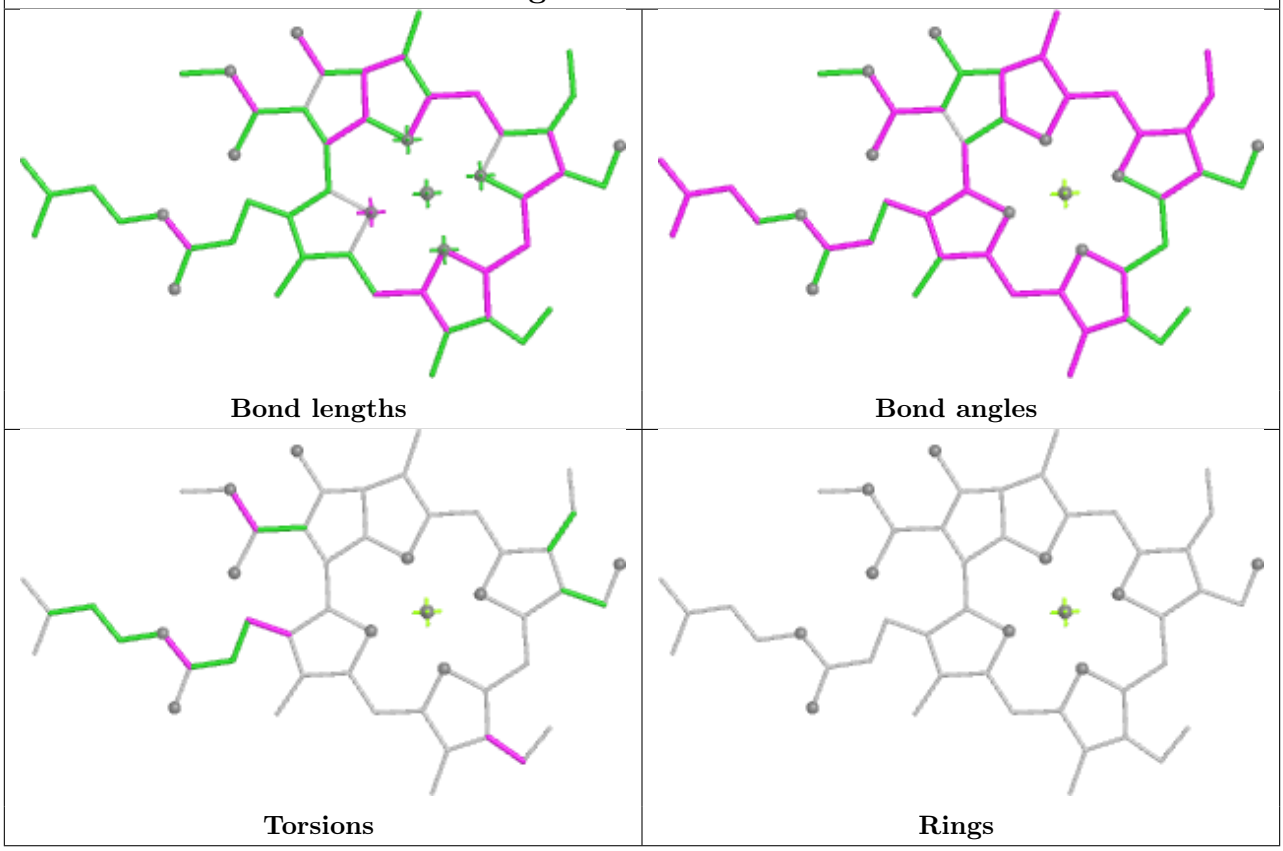


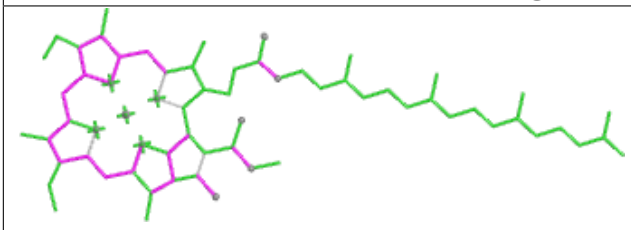
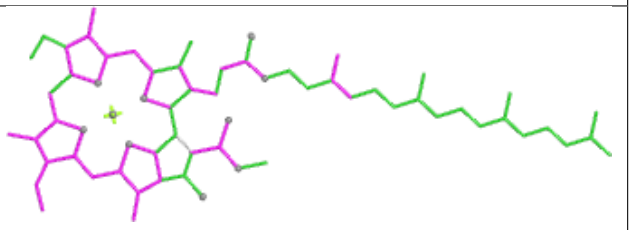
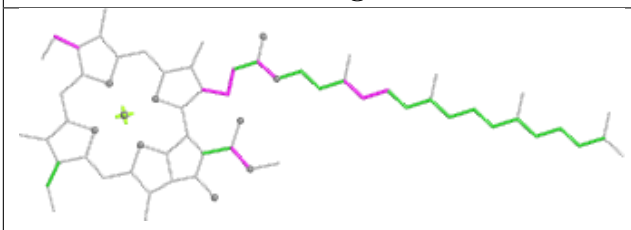
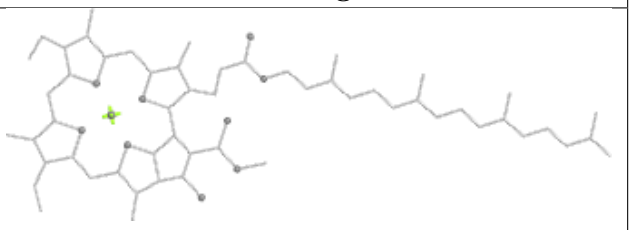
Rings

Ligand CHL 4 606



Ligand CHL 6 608



Ligand CLA 1 614	
 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.

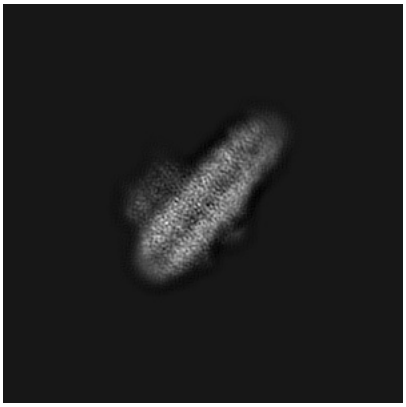
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-9854. These allow visual inspection of the internal detail of the map and identification of artifacts.

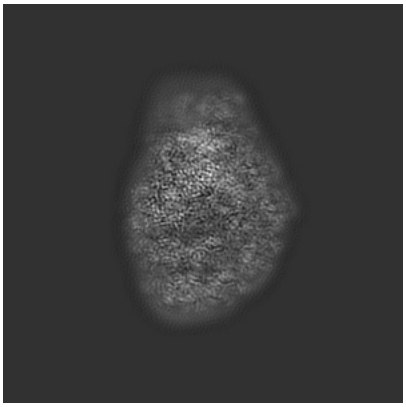
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

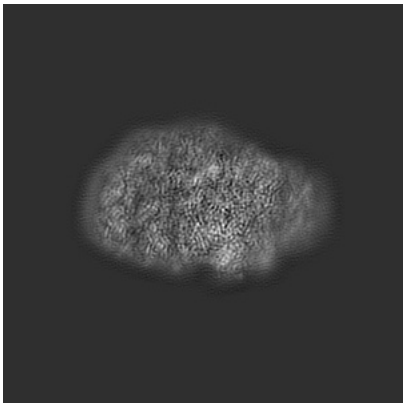
6.1.1 Primary map



X



Y

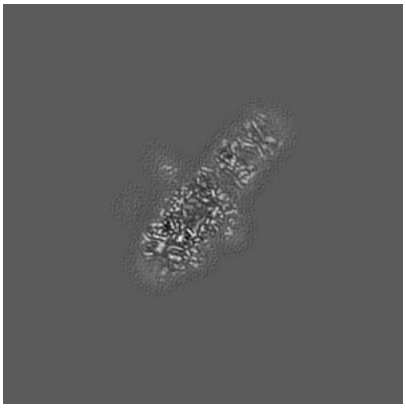


Z

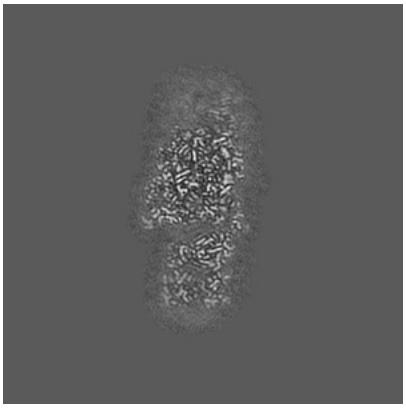
The images above show the map projected in three orthogonal directions.

6.2 Central slices

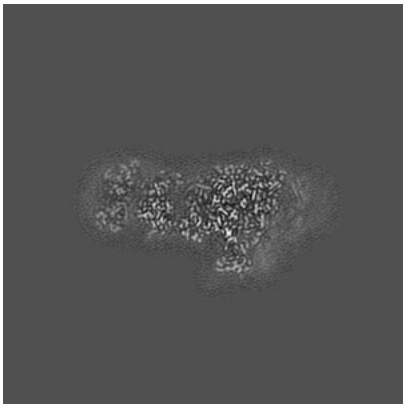
6.2.1 Primary map



X Index: 160



Y Index: 160

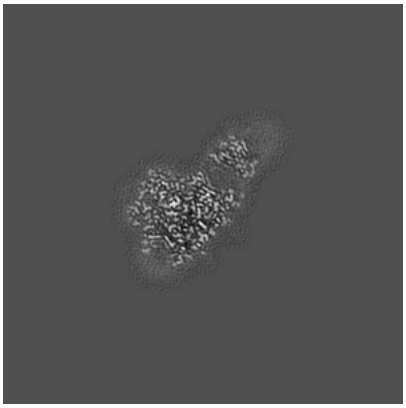


Z Index: 160

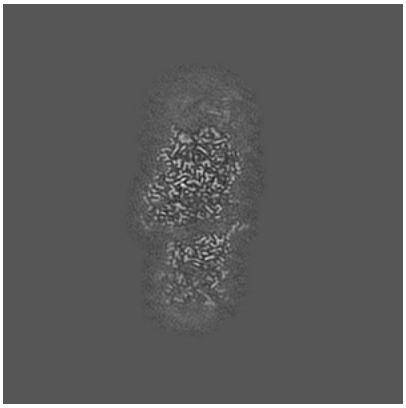
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

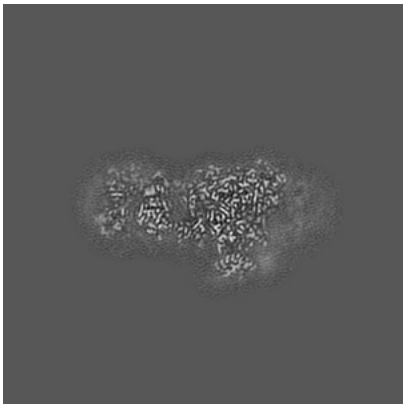
6.3.1 Primary map



X Index: 179



Y Index: 158

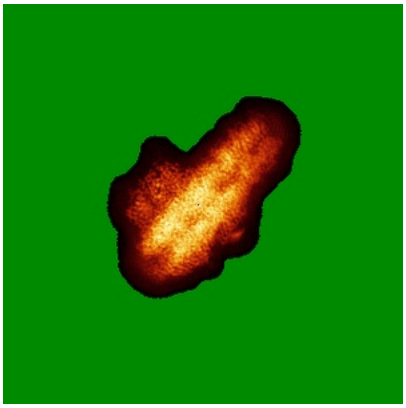


Z Index: 156

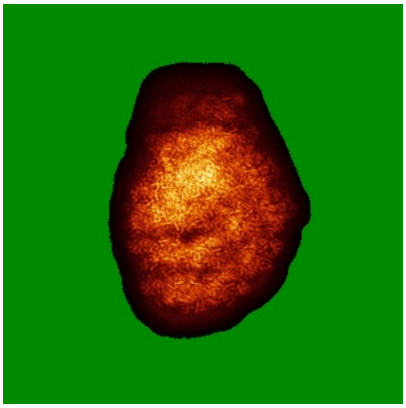
The images above show the largest variance slices of the map in three orthogonal directions.

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

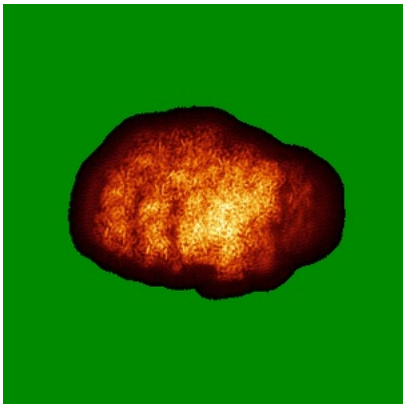
6.4.1 Primary map



X



Y



Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.05. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

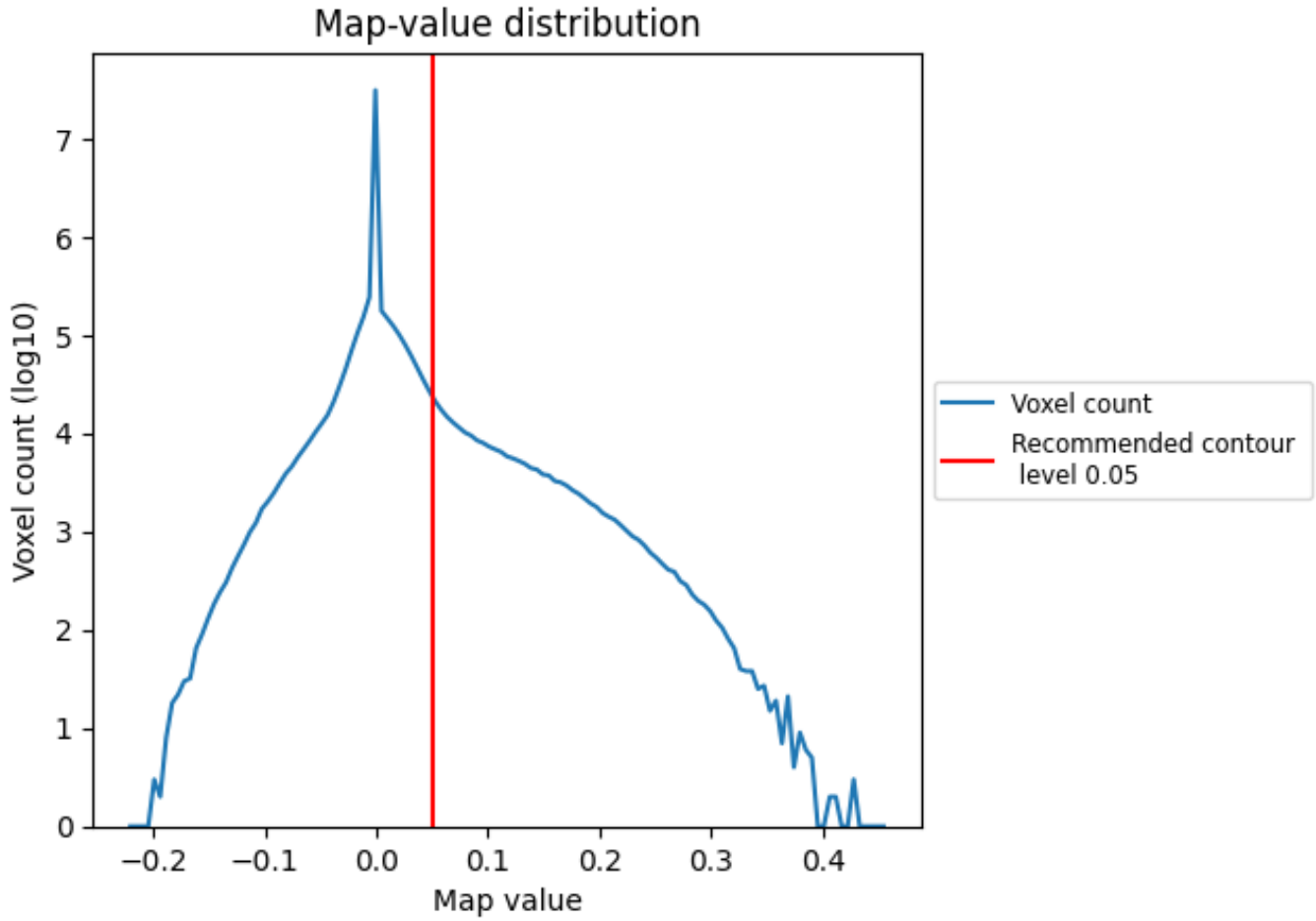
6.6 Mask visualisation (i)

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

7 Map analysis

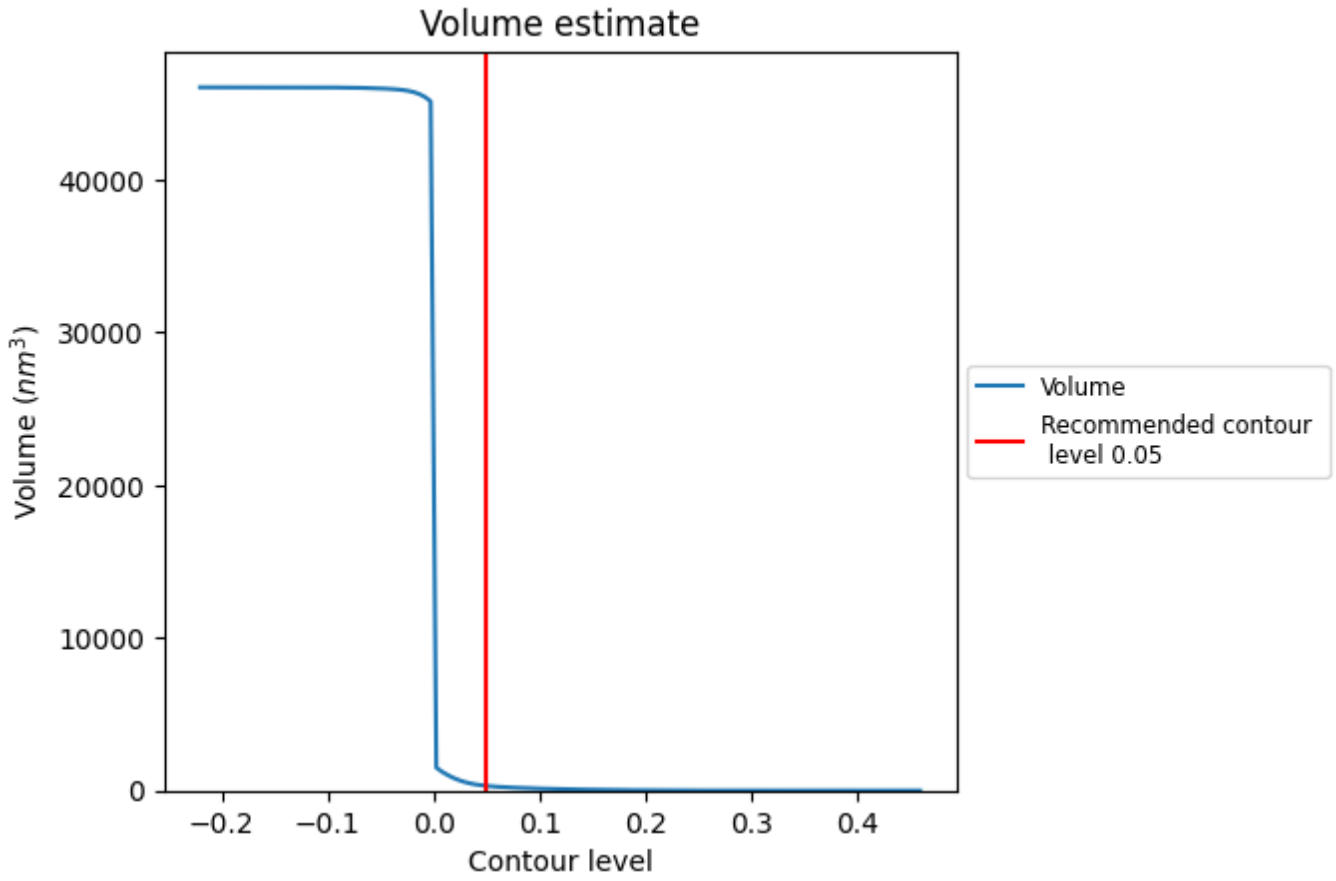
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

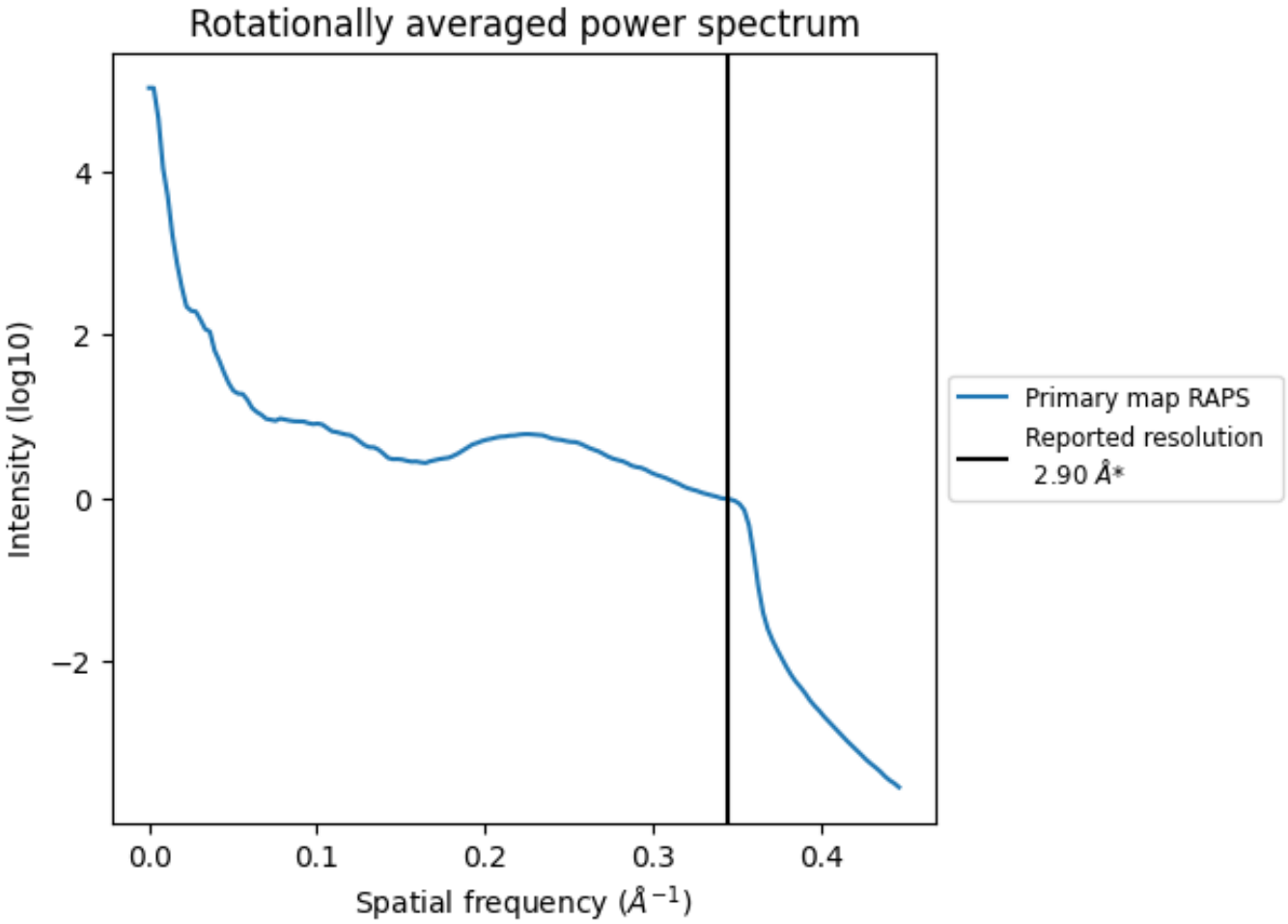
7.2 Volume estimate (i)



The volume at the recommended contour level is 308 nm^3; this corresponds to an approximate mass of 278 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 0.345 $Å^{-1}$

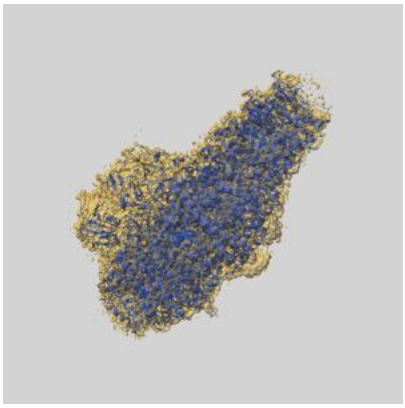
8 Fourier-Shell correlation (i)

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

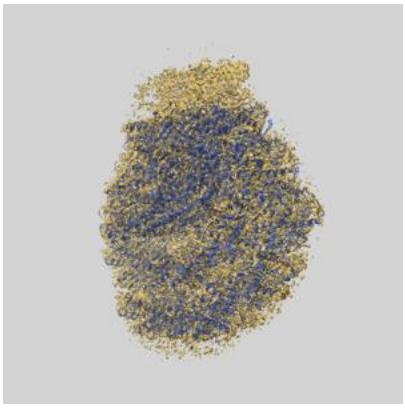
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-9854 and PDB model 6JO6. Per-residue inclusion information can be found in section 3 on page 27.

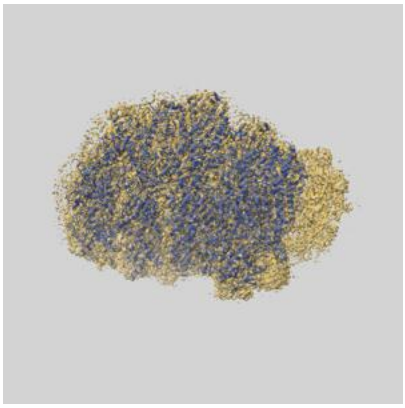
9.1 Map-model overlay



X



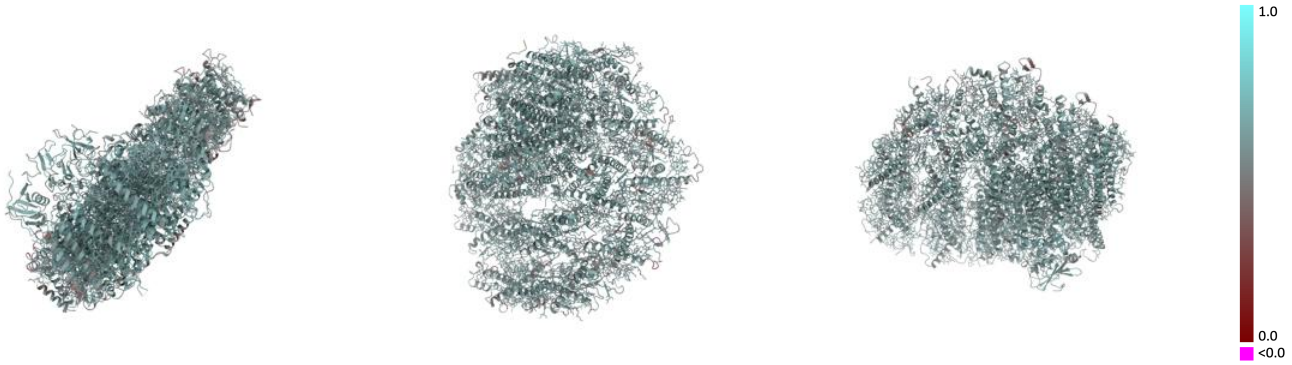
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.05 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.

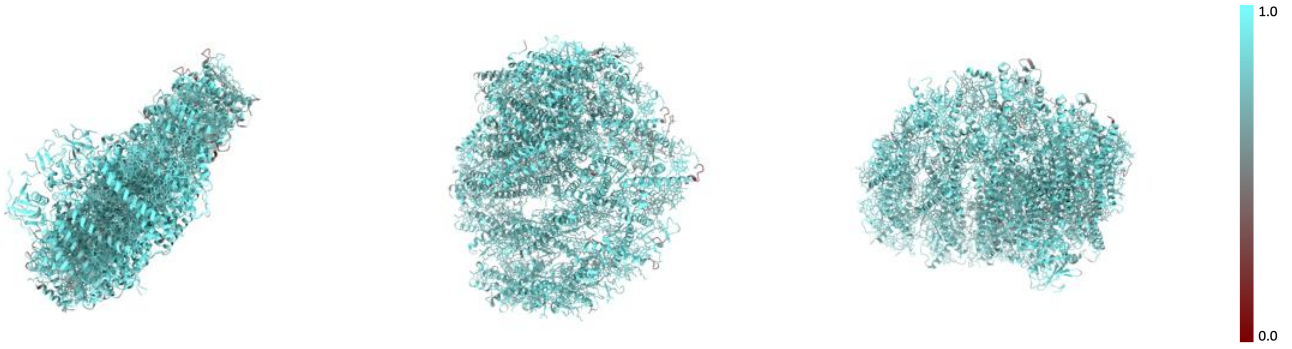
9.2 Q-score mapped to coordinate model (i)



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.

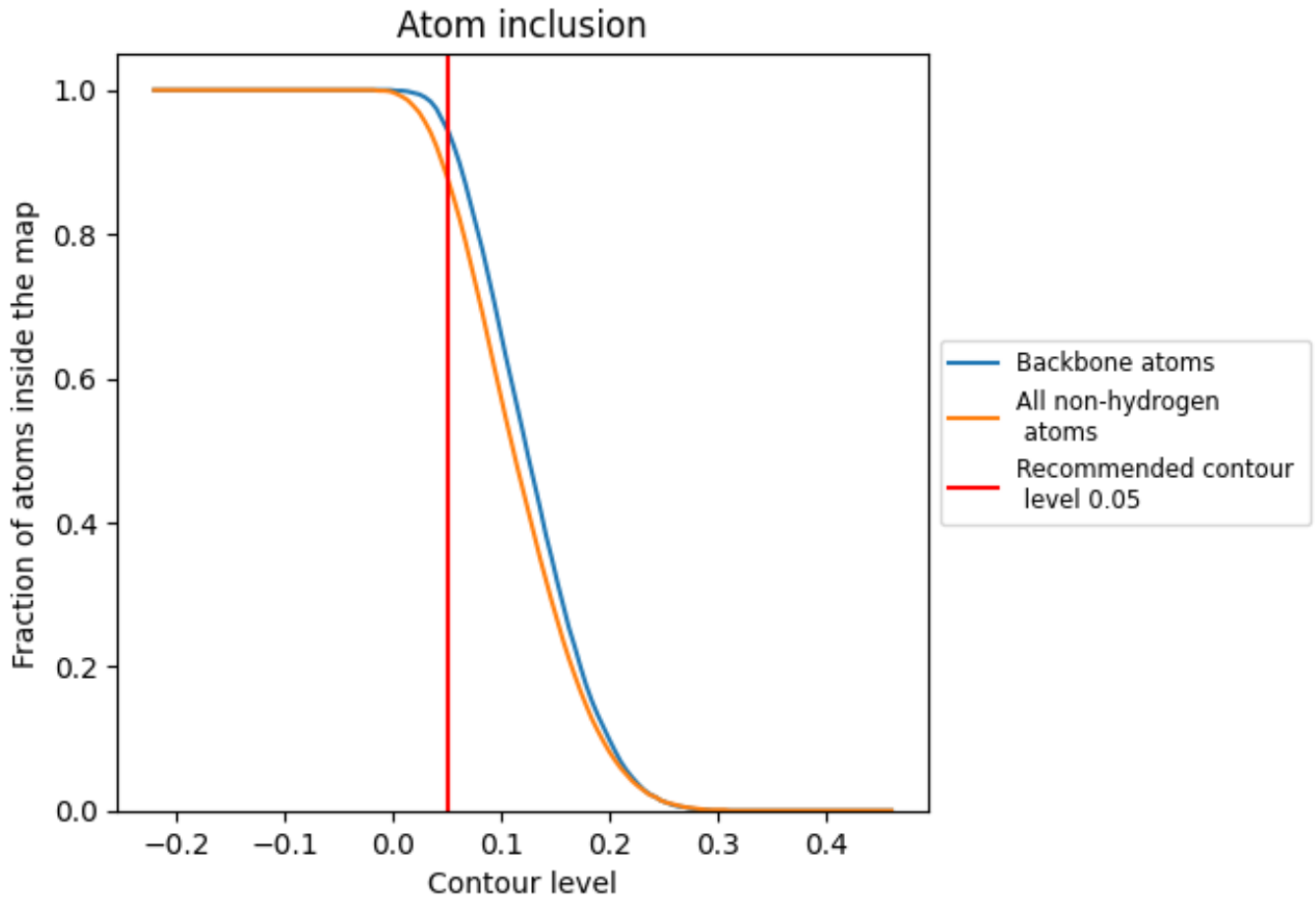
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.05).

9.4 Atom inclusion (i)



At the recommended contour level, 94% of all backbone atoms, 88% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.05) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8790	0.5910
1	0.8390	0.5770
3	0.8870	0.5890
4	0.8400	0.5540
5	0.8450	0.5630
6	0.8420	0.5630
7	0.8790	0.5960
8	0.8880	0.5940
A	0.9260	0.6190
B	0.9190	0.6180
C	0.9440	0.6050
D	0.9050	0.5830
E	0.8990	0.5890
F	0.8650	0.5780
G	0.7770	0.5650
I	0.8460	0.5720
J	0.9040	0.6080
K	0.7800	0.5480
L	0.7830	0.5440
Z	0.7730	0.5450