wwPDB EM Validation Summary Report (i)

Sep 15, 2026 – 07:42 AM JST

PDB ID	:	8ZET / pdb_00008zet
EMDB ID	:	EMD-60044
Title	:	Tp-PSI-FCPI-S in Thalassiosira pseudonana
Authors	:	Feng, Y.; Li, Z.; Shen, J.R.; Wang, W.
Deposited on	:	2024-05-06
Resolution	:	3.20 Å(reported)

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

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

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

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

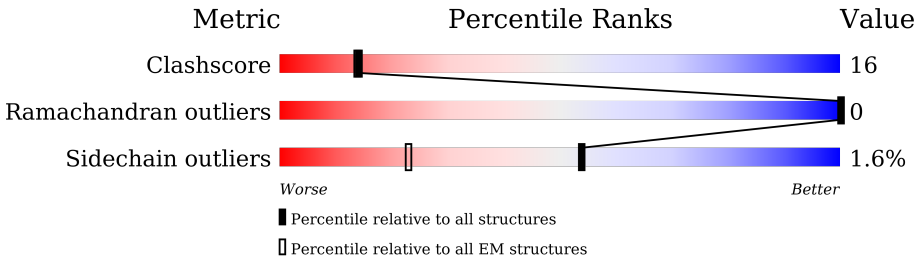
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using 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

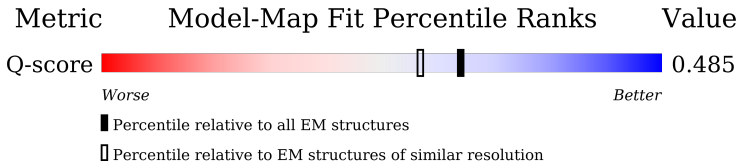
1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.20 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	15020 (2.70 - 3.70)

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	743	80% 20%
2	b	732	77% 23%
3	c	80	78% 22%
4	d	132	73% 27%

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Mol	Chain	Length	Quality of chain
5	e	62	71% 27%
6	f	160	76% 24%
7	g	131	64% 34%
8	i	33	64% 36%
9	j	40	70% 22% 8%
10	l	146	74% 25%
11	m	29	72% 28%
12	r	89	67% 33%
13	B	165	69% 26% 5%
14	C	170	68% 29%
15	D	164	73% 25%
16	E	185	72% 28%
17	H	168	70% 30%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
24	SF4	c	102	-	-	X	-

2 Entry composition (i)

There are 29 unique types of molecules in this entry. The entry contains 36577 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	743	5852	3822	992	1009	29	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	5824	3827	982	996	19	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	c	80	599	368	103	118	10	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	d	132	1040	665	177	195	3	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	e	62	503	317	89	96	1	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	f	160	1242	795	211	233	3	0	0

- Molecule 7 is a protein called Photosystem I reaction center subunit Psa29.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	g	131	Total	C	N	O	S	0	0
			981	619	154	204	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	i	33	Total	C	N	O	S	0	0
			256	177	34	44	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	j	40	Total	C	N	O	S	0	0
			332	224	48	57	3		

- Molecule 10 is a protein called Photosystem I reaction center subunit XI.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	l	146	Total	C	N	O	S	0	0
			1095	722	178	193	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
11	m	29	Total	C	N	O	S	0	0
			220	147	33	38	2		

- Molecule 12 is a protein called Tp-PsaR.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	r	89	Total	C	N	O	S	0	0
			683	443	112	121	7		

- Molecule 13 is a protein called Fucoxanthin chlorophyll a/c-binding protein Lhcq8.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	B	165	Total	C	N	O	S	0	0
			1285	833	204	240	8		

- Molecule 14 is a protein called Fucoxanthin chl a/c light-harvesting protein, major type.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	C	170	Total	C	N	O	S	0	0
			1302	841	213	240	8		

- Molecule 15 is a protein called Pt17531-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	D	164	Total	C	N	O	S	0	0
			1271	819	208	234	10		

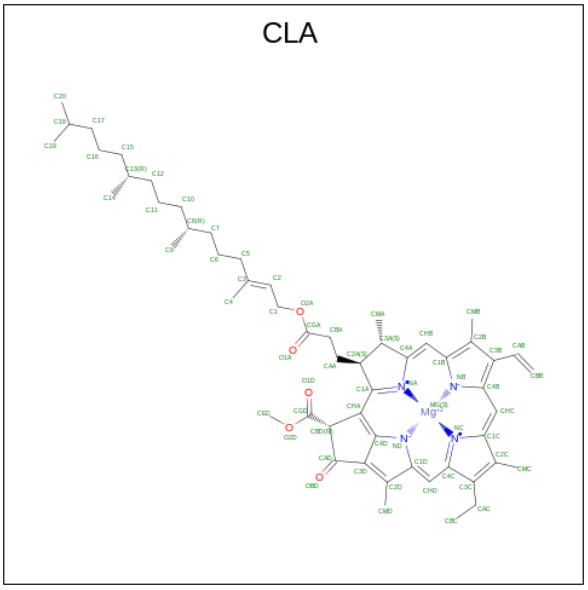
- Molecule 16 is a protein called Tp-RedCAP.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	E	185	Total	C	N	O	S	0	0
			1413	902	235	262	14		

- Molecule 17 is a protein called Fucoxanthin chl a/c light-harvesting protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	H	168	Total	C	N	O	S	0	0
			1300	834	214	242	10		

- Molecule 18 is CHLOROPHYLL A (CCD ID: CLA) (formula: $C_{55}H_{72}MgN_4O_5$) (labeled as "Ligand of Interest" by depositor).



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

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Mol	Chain	Residues	Atoms					AltConf
18	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	a	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
18	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	a	1	Total	C	Mg	N	O	0
			62	52	1	4	5	
18	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	a	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
18	a	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
18	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	a	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
18	a	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
18	a	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
18	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	a	1	Total	C	Mg	N	O	0
			50	40	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
18	a	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
18	a	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
18	a	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
18	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	a	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
18	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	a	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
18	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	a	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
18	a	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
18	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
18	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	b	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
18	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	b	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
18	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	b	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
18	b	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
18	b	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
18	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	b	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
18	b	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
18	b	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
18	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	b	1	Total	C	Mg	N	O	0
			50	40	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
18	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	b	1	Total	C	Mg	N	O	0
			58	48	1	4	5	
18	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	b	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
18	b	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
18	b	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
18	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	b	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
18	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	b	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
18	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	b	1	Total	C	Mg	N	O	0
			62	52	1	4	5	
18	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	b	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
18	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
18	f	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	f	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	f	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
18	i	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
18	j	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
18	l	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
18	l	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	l	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
18	r	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
18	B	1	Total	C	Mg	N	O	0
			57	49	1	4	3	
18	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	B	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
18	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	B	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
18	C	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
18	C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	C	1	Total	C	Mg	N	O	0
			62	52	1	4	5	
18	C	1	Total	C	Mg	N	O	0
			46	36	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
18	C	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
18	C	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
18	C	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
18	C	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
18	C	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
18	C	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
18	C	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
18	D	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
18	D	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	D	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
18	D	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
18	D	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
18	D	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
18	D	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	D	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
18	D	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
18	D	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
18	D	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
18	E	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	E	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	E	1	Total	C	Mg	N	O	0
			46	36	1	4	5	

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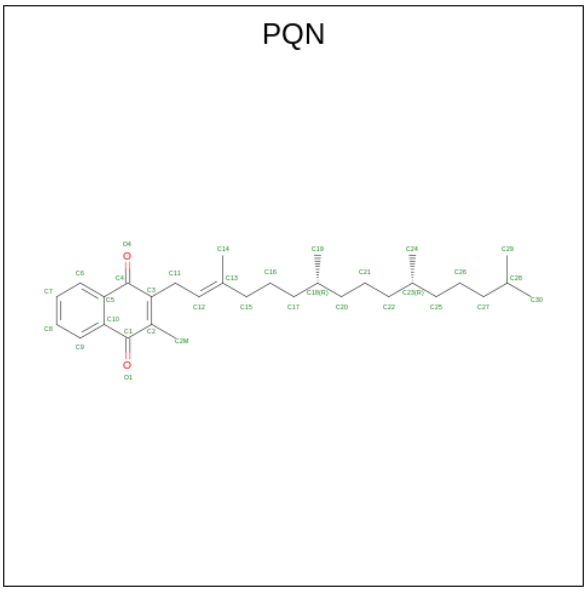
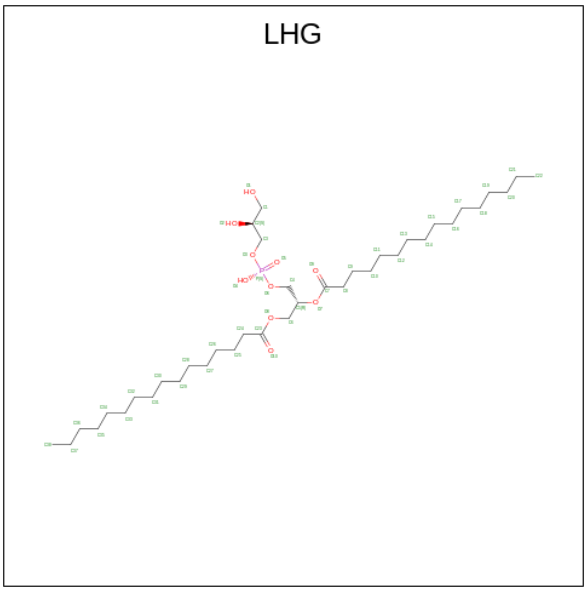
Mol	Chain	Residues	Atoms					AltConf
18	E	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	E	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
18	E	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
18	E	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	E	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
18	H	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
18	H	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	H	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	H	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	H	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
18	H	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
18	H	1	Total	C	Mg	N	O	0
			57	47	1	4	5	
18	H	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	H	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	H	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

- Molecule 19 is PHYLLOQUINONE (CCD ID: PQN) (formula: $C_{31}H_{46}O_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
19	a	1	Total	C	O	0
			33	31	2	
19	b	1	Total	C	O	0
			33	31	2	

- Molecule 20 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: $C_{38}H_{75}O_{10}P$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
20	a	1	Total	C	O	P	0
			49	38	10	1	

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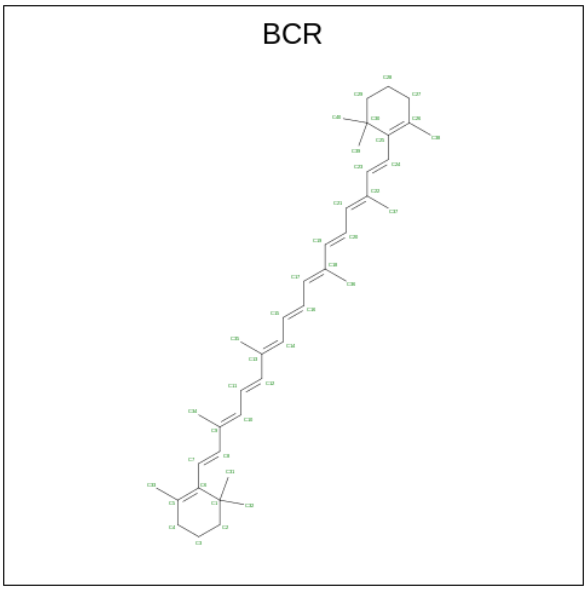
Mol	Chain	Residues	Atoms				AltConf
20	a	1	Total	C	O	P	0
			27	16	10	1	
20	a	1	Total	C	O	P	0
			33	22	10	1	
20	b	1	Total	C	O	P	0
			49	38	10	1	
20	j	1	Total	C	O	P	0
			49	38	10	1	
20	B	1	Total	C	O	P	0
			42	31	10	1	
20	D	1	Total	C	O	P	0
			49	38	10	1	
20	E	1	Total	C	O	P	0
			49	38	10	1	
20	E	1	Total	C	O	P	0
			42	31	10	1	
20	H	1	Total	C	O	P	0
			35	24	10	1	

- Molecule 21 is BETA-CAROTENE (CCD ID: BCR) (formula: $C_{40}H_{56}$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms		AltConf
21	a	1	Total	C	0
			40	40	
21	a	1	Total	C	0
			40	40	

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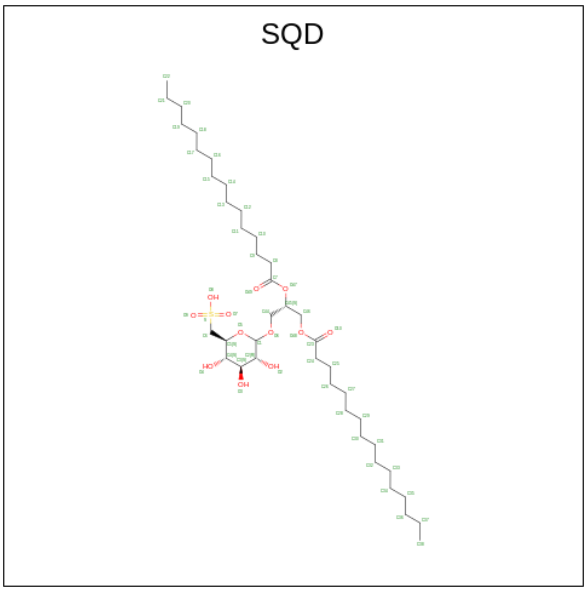
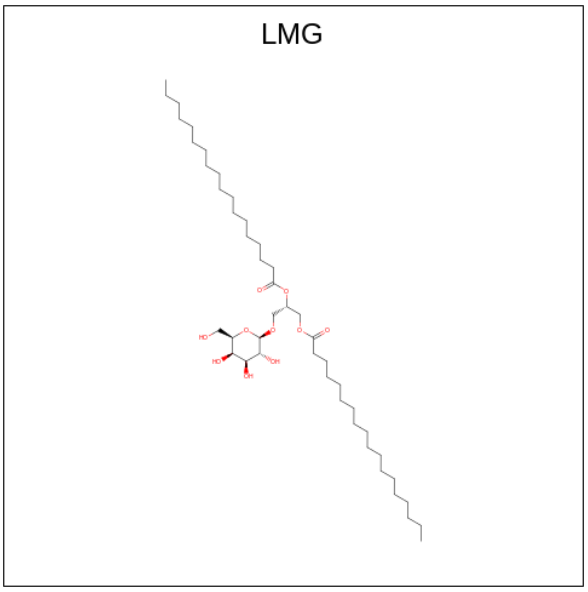
Mol	Chain	Residues	Atoms	AltConf
21	a	1	Total C 40 40	0
21	a	1	Total C 40 40	0
21	a	1	Total C 40 40	0
21	b	1	Total C 40 40	0
21	b	1	Total C 40 40	0
21	b	1	Total C 40 40	0
21	b	1	Total C 40 40	0
21	f	1	Total C 40 40	0
21	f	1	Total C 40 40	0
21	i	1	Total C 40 40	0
21	i	1	Total C 40 40	0
21	j	1	Total C 40 40	0
21	j	1	Total C 40 40	0
21	l	1	Total C 40 40	0
21	l	1	Total C 40 40	0
21	m	1	Total C 40 40	0
21	r	1	Total C 40 40	0
21	E	1	Total C 40 40	0
21	E	1	Total C 40 40	0

- Molecule 22 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (CCD ID: SQD) (formula: $C_{41}H_{78}O_{12}S$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
22	a	1	Total	C	O	S	0
			33	23	9	1	

- Molecule 23 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
23	a	1	Total	C	O	0
			33	23	10	
23	j	1	Total	C	O	0
			37	27	10	

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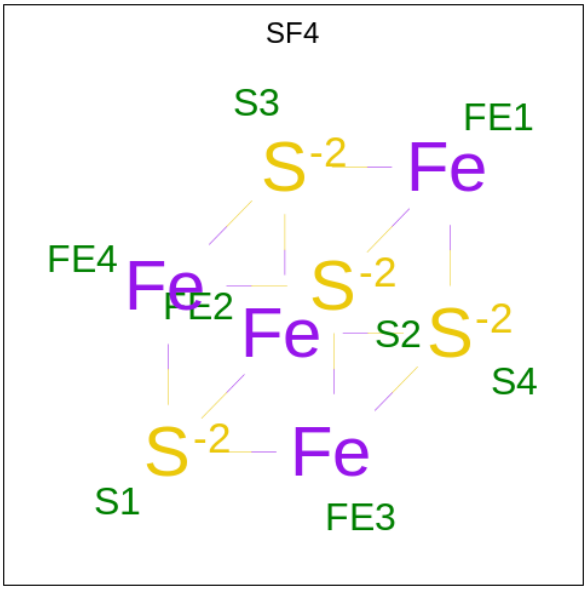
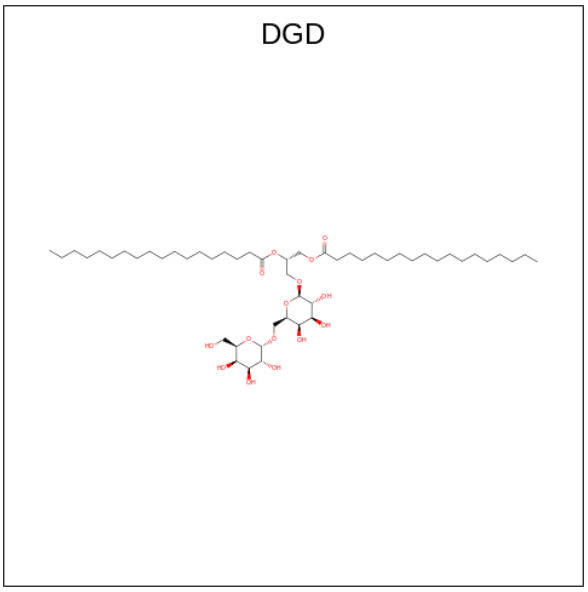
Mol	Chain	Residues	Atoms	AltConf
23	l	1	Total C O 40 30 10	0
23	C	1	Total C O 31 21 10	0
23	C	1	Total C O 44 34 10	0
23	D	1	Total C O 46 36 10	0
23	E	1	Total C O 43 33 10	0

- Molecule 24 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4) (labeled as "Ligand of Interest" by depositor).



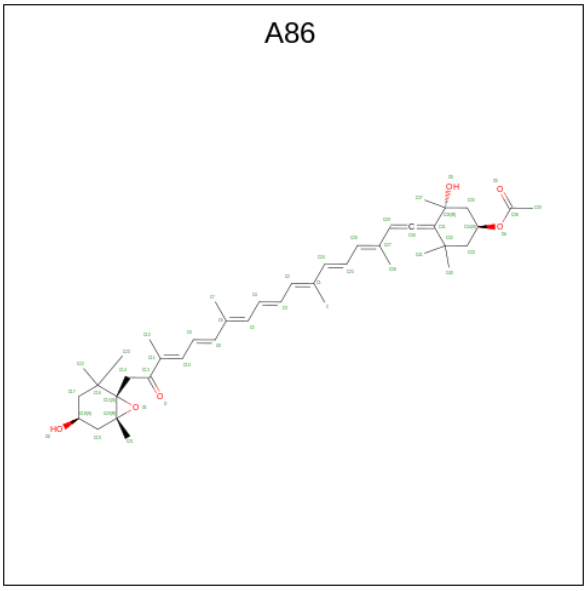
Mol	Chain	Residues	Atoms	AltConf
24	b	1	Total Fe S 8 4 4	0
24	c	1	Total Fe S 8 4 4	0
24	c	1	Total Fe S 8 4 4	0

- Molecule 25 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: $C_{51}H_{96}O_{15}$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
25	b	1	Total	C	O	0
			60	45	15	

- Molecule 26 is (3S,3'S,5R,5'R,6S,6'R,8'R)-3,5'-dihydroxy-8-oxo-6',7'-didehydro-5,5',6,6',7,8-hexahydro-5,6-epoxy-beta,beta-caroten-3'- yl acetate (CCD ID: A86) (formula: $C_{42}H_{58}O_6$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
26	b	1	Total	C	O	0
			48	42	6	
26	m	1	Total	C	O	0
			48	42	6	

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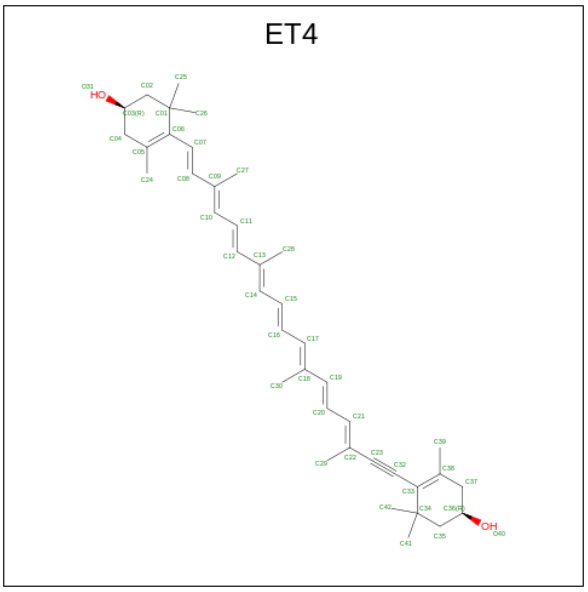
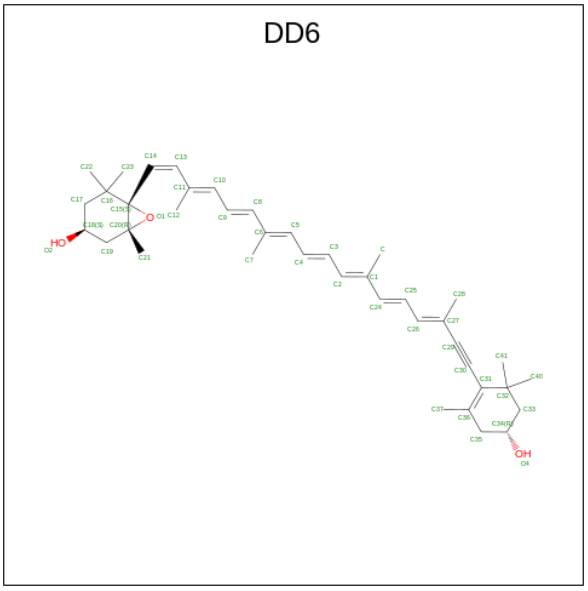
Mol	Chain	Residues	Atoms	AltConf
26	r	1	Total C O 48 42 6	0
26	B	1	Total C O 48 42 6	0
26	B	1	Total C O 48 42 6	0
26	B	1	Total C O 48 42 6	0
26	B	1	Total C O 48 42 6	0
26	C	1	Total C O 48 42 6	0
26	C	1	Total C O 48 42 6	0
26	C	1	Total C O 48 42 6	0
26	D	1	Total C O 48 42 6	0
26	D	1	Total C O 48 42 6	0
26	D	1	Total C O 48 42 6	0
26	E	1	Total C O 48 42 6	0
26	H	1	Total C O 48 42 6	0
26	H	1	Total C O 48 42 6	0
26	H	1	Total C O 48 42 6	0

- Molecule 27 is (1 {R})-3,5,5-trimethyl-4-[(1 {E},3 {E},5 {E},7 {E},9 {E},11 {E},13 {E},15 {E})-3,7,12,16-tetramethyl-18-[(4 {R})-2,6,6-trimethyl-4-oxidanyl-cyclohexen-1-yl]octadeca-1,3,5,7,9,11,13,15-octaen-17-ynyl]cyclohex-3-en-1-ol (CCD ID: ET4) (formula: $C_{40}H_{54}O_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
27	l	1	Total	C	O	0
			42	40	2	

- Molecule 28 is (3S,3'R,5R,6S,7cis)-7',8'-didehydro-5,6-dihydro-5,6-epoxy-beta,beta-carotene-3,3'-diol (CCD ID: DD6) (formula: $C_{40}H_{54}O_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
28	B	1	Total	C	O	0
			43	40	3	
28	C	1	Total	C	O	0
			43	40	3	

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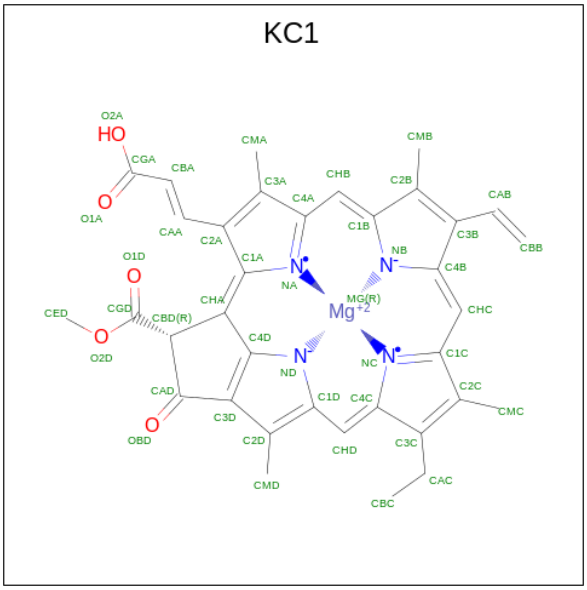
Mol	Chain	Residues	Atoms	AltConf
28	D	1	Total C O 43 40 3	0
28	E	1	Total C O 43 40 3	0
28	E	1	Total C O 43 40 3	0
28	E	1	Total C O 43 40 3	0
28	E	1	Total C O 43 40 3	0
28	H	1	Total C O 43 40 3	0

- Molecule 29 is Chlorophyll c1 (CCD ID: KC1) (formula: $C_{35}H_{30}MgN_4O_5$) (labeled as "Ligand of Interest" by depositor).



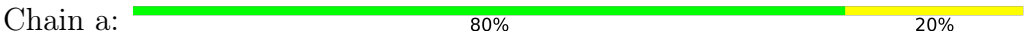
Mol	Chain	Residues	Atoms	AltConf
29	B	1	Total C Mg N O 45 35 1 4 5	0
29	C	1	Total C Mg N O 45 35 1 4 5	0
29	C	1	Total C Mg N O 45 35 1 4 5	0
29	H	1	Total C Mg N O 45 35 1 4 5	0

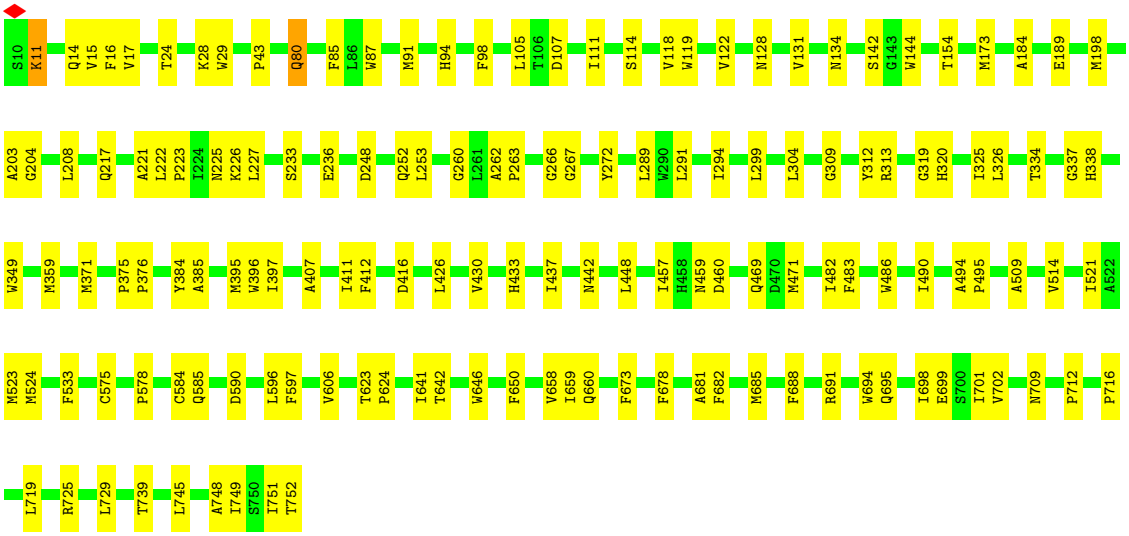
3 Residue-property plots (i)

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:

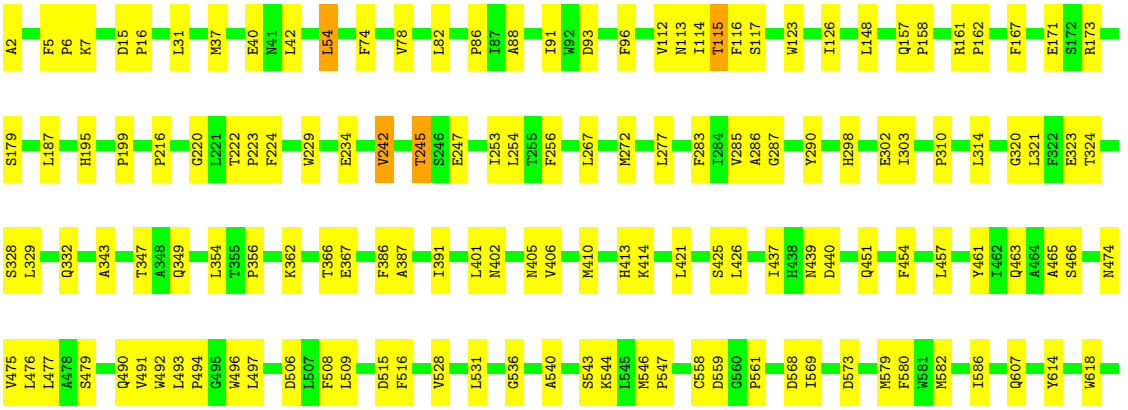


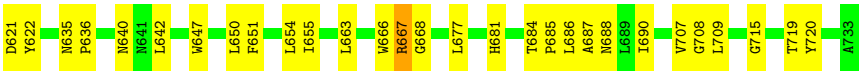


• Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

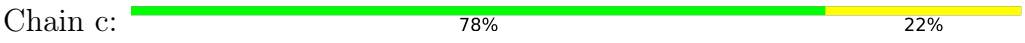
Chain b:

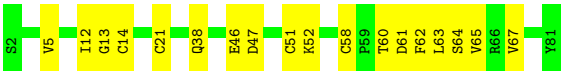






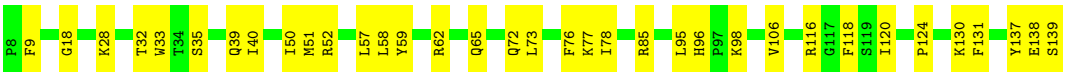
• Molecule 3: Photosystem I iron-sulfur center





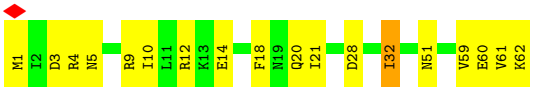
• Molecule 4: Photosystem I reaction center subunit II





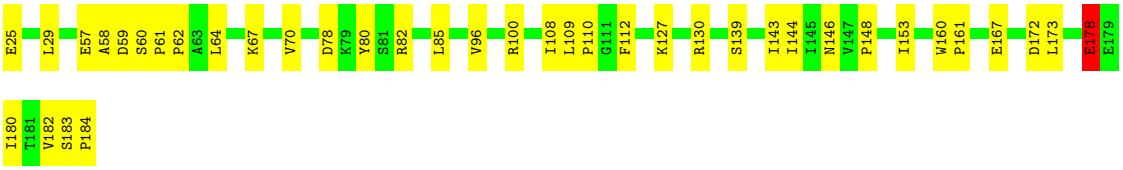
• Molecule 5: Photosystem I reaction center subunit IV





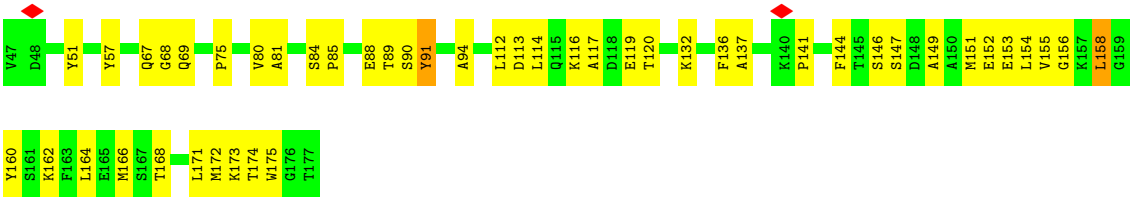
• Molecule 6: Photosystem I reaction center subunit III





• Molecule 7: Photosystem I reaction center subunit Psa29





• Molecule 8: Photosystem I reaction center subunit VIII

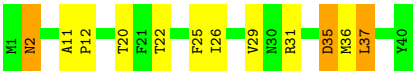




• Molecule 9: Photosystem I reaction center subunit IX

Chain j:

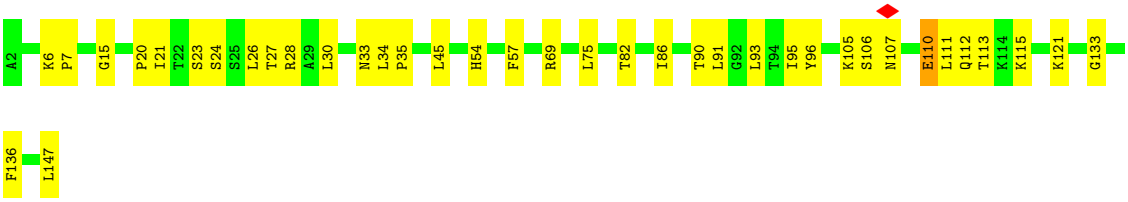




• Molecule 10: Photosystem I reaction center subunit XI

Chain l:

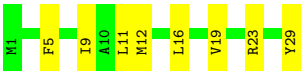




• Molecule 11: Photosystem I reaction center subunit XII

Chain m:

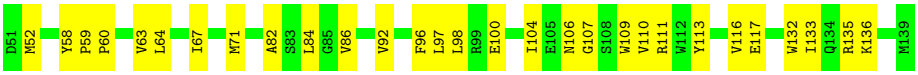




• Molecule 12: Tp-PsaR

Chain r:

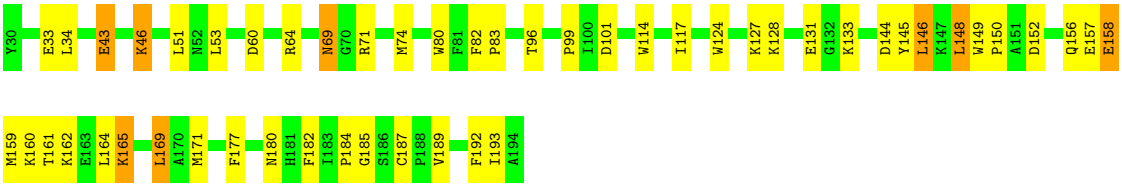




• Molecule 13: Fucoxanthin chlorophyll a/c-binding protein Lhcq8

Chain B:

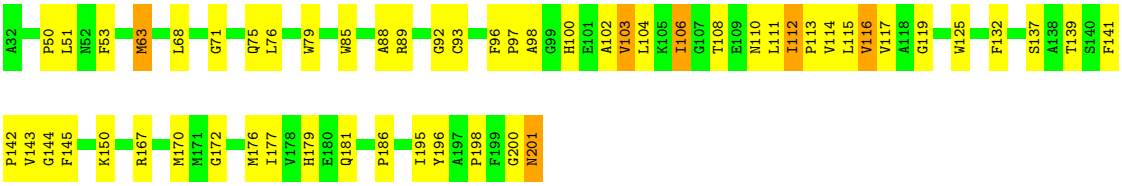




• Molecule 14: Fucoxanthin chl a/c light-harvesting protein, major type

Chain C:

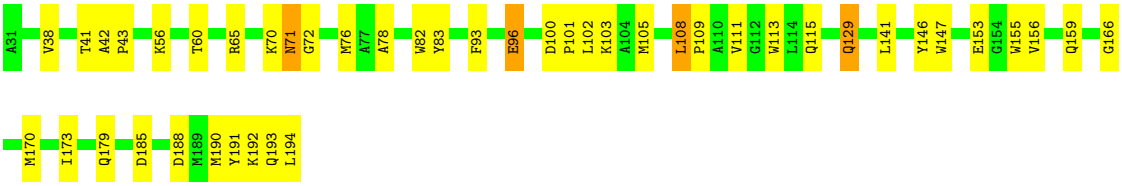




• Molecule 15: Pt17531-like protein

Chain D:

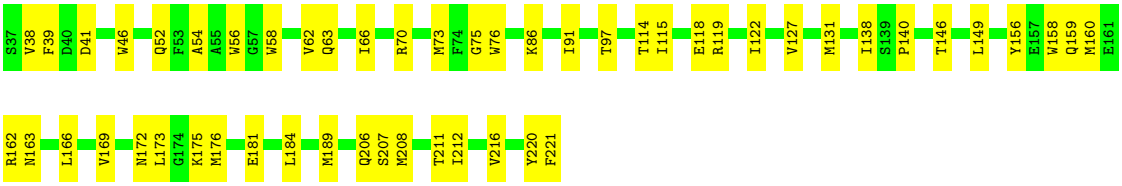




• Molecule 16: Tp-RedCAP

Chain E:

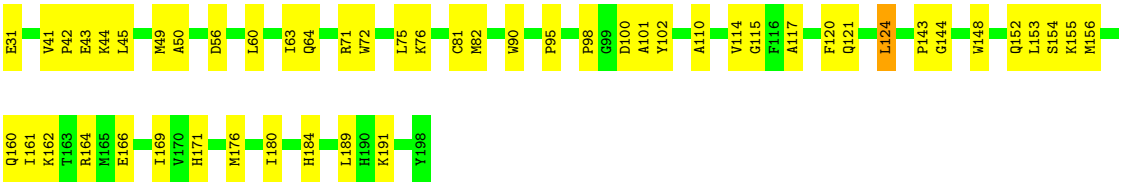




• Molecule 17: Fucoxanthin chl a/c light-harvesting protein

Chain H:





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	52772	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	60	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOCONTINUUM (6k x 4k)	Depositor
Maximum map value	1.370	Depositor
Minimum map value	-0.381	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.019	Depositor
Recommended contour level	0.08	Depositor
Map size (Å)	563.2, 563.2, 563.2	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.1, 1.1, 1.1	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: KC1, PQN, DGD, ET4, LHG, SF4, SQD, A86, BCR, LMG, DD6, CLA

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	a	0.53	0/6049	0.67	2/8234 (0.0%)
2	b	0.53	0/6034	0.66	1/8236 (0.0%)
3	c	0.52	0/609	0.80	1/826 (0.1%)
4	d	0.47	0/1067	0.72	0/1441
5	e	0.43	0/511	0.72	0/690
6	f	0.53	0/1271	0.73	3/1727 (0.2%)
7	g	0.43	0/1003	0.68	1/1354 (0.1%)
8	i	0.51	0/264	0.73	0/360
9	j	0.52	0/342	0.78	2/463 (0.4%)
10	l	0.54	0/1123	0.67	1/1523 (0.1%)
11	m	0.56	0/222	0.56	0/300
12	r	0.48	0/704	0.60	0/957
13	B	0.53	0/1324	0.66	0/1804
14	C	0.50	0/1339	0.68	1/1813 (0.1%)
15	D	0.51	0/1304	0.64	0/1771
16	E	0.52	0/1450	0.67	0/1974
17	H	0.51	0/1334	0.65	1/1809 (0.1%)
All	All	0.52	0/25950	0.67	13/35282 (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
4	d	0	1

There are no bond length outliers.

The worst 5 of 13 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	b	667	ARG	N-CA-C	8.65	120.33	111.07
7	g	156	GLY	N-CA-C	-8.09	103.12	112.50
6	f	58	ALA	CB-CA-C	-6.27	109.33	116.54
1	a	266	GLY	N-CA-C	-6.25	102.80	112.85
1	a	122	VAL	N-CA-C	6.09	122.02	109.34

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	d	96	HIS	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	5852	0	5682	113	0
2	b	5824	0	5643	143	0
3	c	599	0	582	18	0
4	d	1040	0	1027	26	0
5	e	503	0	500	18	0
6	f	1242	0	1239	34	0
7	g	981	0	922	40	0
8	i	256	0	259	13	0
9	j	332	0	331	19	0
10	l	1095	0	1116	37	0
11	m	220	0	241	8	0
12	r	683	0	675	26	0
13	B	1285	0	1239	61	0
14	C	1302	0	1243	69	0
15	D	1271	0	1227	41	0
16	E	1413	0	1365	47	0
17	H	1300	0	1262	44	0
18	B	469	0	479	33	0
18	C	547	0	472	60	0
18	D	568	0	501	34	0
18	E	462	0	454	21	0
18	H	587	0	583	54	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
18	a	2671	0	2759	134	0
18	b	2492	0	2569	138	0
18	f	175	0	177	3	0
18	i	60	0	59	1	0
18	j	41	0	29	1	0
18	l	159	0	144	10	0
18	r	45	0	33	2	0
19	a	33	0	46	1	0
19	b	33	0	46	4	0
20	B	42	0	54	3	0
20	D	49	0	74	6	0
20	E	91	0	131	5	0
20	H	35	0	43	0	0
20	a	109	0	134	6	0
20	b	49	0	74	5	0
20	j	49	0	74	5	0
21	E	80	0	112	9	0
21	a	200	0	280	31	0
21	b	160	0	224	19	0
21	f	80	0	112	6	0
21	i	80	0	112	14	0
21	j	80	0	112	17	0
21	l	80	0	112	11	0
21	m	40	0	56	5	0
21	r	40	0	56	2	0
22	a	33	0	39	7	0
23	C	75	0	88	1	0
23	D	46	0	61	1	0
23	E	43	0	55	5	0
23	a	33	0	33	2	0
23	j	37	0	42	0	0
23	l	40	0	49	1	0
24	b	8	0	0	1	0
24	c	16	0	0	6	0
25	b	60	0	81	0	0
26	B	192	0	0	7	0
26	C	144	0	0	5	0
26	D	144	0	0	3	0
26	E	48	0	0	0	0
26	H	144	0	0	17	0
26	b	48	0	0	4	0
26	m	48	0	0	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
26	r	48	0	0	1	0
27	l	42	0	0	0	0
28	B	43	0	0	0	0
28	C	43	0	0	1	0
28	D	43	0	0	3	0
28	E	172	0	0	2	0
28	H	43	0	0	3	0
29	B	45	0	0	5	0
29	C	90	0	0	4	0
29	H	45	0	0	1	0
All	All	36577	0	35112	1118	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 16.

The worst 5 of 1118 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)
26:H:302:A86:C1	18:H:309:CLA:CMD	2.27	1.12
26:H:302:A86:C1	18:H:309:CLA:HMD1	1.82	1.10
18:a:807:CLA:H202	21:j:105:BCR:H392	1.33	1.05
13:B:165:LYS:CB	18:B:306:CLA:HMD2	1.86	1.05
13:B:165:LYS:HB3	18:B:306:CLA:CMD	1.88	1.02

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	741/743 (100%)	723 (98%)	18 (2%)	0	100	100
2	b	730/732 (100%)	713 (98%)	17 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	c	78/80 (98%)	74 (95%)	4 (5%)	0	100	100
4	d	130/132 (98%)	126 (97%)	4 (3%)	0	100	100
5	e	60/62 (97%)	58 (97%)	2 (3%)	0	100	100
6	f	158/160 (99%)	152 (96%)	6 (4%)	0	100	100
7	g	129/131 (98%)	121 (94%)	8 (6%)	0	100	100
8	i	31/33 (94%)	30 (97%)	1 (3%)	0	100	100
9	j	38/40 (95%)	36 (95%)	2 (5%)	0	100	100
10	l	144/146 (99%)	138 (96%)	6 (4%)	0	100	100
11	m	27/29 (93%)	26 (96%)	1 (4%)	0	100	100
12	r	87/89 (98%)	86 (99%)	1 (1%)	0	100	100
13	B	163/165 (99%)	157 (96%)	6 (4%)	0	100	100
14	C	168/170 (99%)	165 (98%)	3 (2%)	0	100	100
15	D	162/164 (99%)	156 (96%)	6 (4%)	0	100	100
16	E	183/185 (99%)	180 (98%)	3 (2%)	0	100	100
17	H	166/168 (99%)	162 (98%)	4 (2%)	0	100	100
All	All	3195/3229 (99%)	3103 (97%)	92 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	603/603 (100%)	598 (99%)	5 (1%)	73	82
2	b	597/597 (100%)	591 (99%)	6 (1%)	68	80
3	c	69/69 (100%)	68 (99%)	1 (1%)	59	77
4	d	111/111 (100%)	111 (100%)	0	100	100
5	e	55/55 (100%)	52 (94%)	3 (6%)	19	52
6	f	132/132 (100%)	130 (98%)	2 (2%)	57	76

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
7	g	98/98 (100%)	95 (97%)	3 (3%)	35 66
8	i	28/28 (100%)	28 (100%)	0	100 100
9	j	36/36 (100%)	34 (94%)	2 (6%)	19 52
10	l	113/113 (100%)	113 (100%)	0	100 100
11	m	22/22 (100%)	22 (100%)	0	100 100
12	r	72/72 (100%)	72 (100%)	0	100 100
13	B	133/133 (100%)	124 (93%)	9 (7%)	14 46
14	C	129/130 (99%)	123 (95%)	6 (5%)	23 57
15	D	128/128 (100%)	124 (97%)	4 (3%)	35 66
16	E	144/144 (100%)	144 (100%)	0	100 100
17	H	136/136 (100%)	135 (99%)	1 (1%)	76 83
All	All	2606/2607 (100%)	2564 (98%)	42 (2%)	54 75

5 of 42 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
13	B	164	LEU
14	C	116	VAL
13	B	165	LYS
14	C	68	LEU
15	D	71	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 44 such sidechains are listed below:

Mol	Chain	Res	Type
9	j	2	ASN
14	C	52	ASN
10	l	9	ASN
13	B	69	ASN
15	D	71	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

217 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	$\#\|Z\| > 2$
23	LMG	l	207	-	40,40,55	1.22	4 (10%)	48,48,63	1.76	4 (8%)
18	CLA	a	802	-	69,73,73	1.25	9 (13%)	83,113,113	1.29	7 (8%)
18	CLA	f	202	-	69,73,73	1.24	8 (11%)	83,113,113	1.31	7 (8%)
18	CLA	C	306	23	49,53,73	1.49	9 (18%)	59,89,113	1.46	4 (6%)
21	BCR	l	201	-	41,41,41	1.00	2 (4%)	56,56,56	2.04	16 (28%)
29	KC1	C	313	-	49,53,53	1.40	6 (12%)	63,89,89	2.05	14 (22%)
20	LHG	D	201	-	48,48,48	1.08	4 (8%)	51,54,54	1.03	2 (3%)
18	CLA	a	806	1	69,73,73	1.25	9 (13%)	83,113,113	1.29	4 (4%)
18	CLA	a	826	1	69,73,73	1.27	8 (11%)	83,113,113	1.32	6 (7%)
18	CLA	D	211	15	50,54,73	1.47	9 (18%)	60,90,113	1.43	4 (6%)
18	CLA	D	210	-	60,64,73	1.35	11 (18%)	72,102,113	1.46	8 (11%)
18	CLA	a	839	1	69,73,73	1.23	9 (13%)	83,113,113	1.31	6 (7%)
21	BCR	f	205	-	41,41,41	0.72	0	56,56,56	1.96	16 (28%)
29	KC1	H	312	17	49,53,53	1.70	9 (18%)	63,89,89	2.12	14 (22%)
18	CLA	a	815	1	69,73,73	1.24	9 (13%)	83,113,113	1.28	9 (10%)
18	CLA	b	813	2	59,63,73	1.36	9 (15%)	71,101,113	1.36	5 (7%)
26	A86	E	302	-	44,50,50	1.45	6 (13%)	51,76,76	2.82	23 (45%)
21	BCR	b	832	-	41,41,41	0.70	0	56,56,56	1.92	14 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
18	CLA	f	203	-	69,73,73	1.24	7 (10%)	83,113,113	1.29	5 (6%)
18	CLA	a	808	1	69,73,73	1.26	10 (14%)	83,113,113	1.29	5 (6%)
18	CLA	a	822	1	54,58,73	1.40	8 (14%)	65,95,113	1.43	5 (7%)
18	CLA	E	316	-	60,64,73	1.33	8 (13%)	72,102,113	1.36	6 (8%)
18	CLA	C	309	-	66,70,73	1.28	11 (16%)	79,109,113	1.50	10 (12%)
21	BCR	j	105	-	41,41,41	0.72	0	56,56,56	2.09	13 (23%)
18	CLA	b	824	-	69,73,73	1.31	10 (14%)	83,113,113	1.49	6 (7%)
18	CLA	a	821	1	69,73,73	1.25	8 (11%)	83,113,113	1.30	7 (8%)
18	CLA	b	840	2	65,69,73	1.27	10 (15%)	78,108,113	1.35	6 (7%)
18	CLA	a	804	18,1	59,63,73	1.36	9 (15%)	71,101,113	1.35	8 (11%)
23	LMG	j	103	-	37,37,55	1.59	5 (13%)	45,45,63	3.61	8 (17%)
18	CLA	a	820	1	69,73,73	1.25	8 (11%)	83,113,113	1.32	8 (9%)
18	CLA	b	816	2	59,63,73	1.34	9 (15%)	71,101,113	1.33	5 (7%)
18	CLA	E	311	16	50,54,73	1.46	9 (18%)	60,90,113	1.39	5 (8%)
18	CLA	a	816	1	49,53,73	1.49	9 (18%)	59,89,113	1.44	4 (6%)
18	CLA	B	310	13	50,54,73	1.46	8 (16%)	60,90,113	1.40	4 (6%)
20	LHG	b	835	18	48,48,48	1.09	3 (6%)	51,54,54	1.03	3 (5%)
18	CLA	b	843	2	69,73,73	1.28	10 (14%)	83,113,113	1.37	9 (10%)
18	CLA	a	853	1	59,63,73	1.36	9 (15%)	71,101,113	1.38	8 (11%)
26	A86	B	301	-	44,50,50	1.30	4 (9%)	51,76,76	2.80	18 (35%)
18	CLA	b	837	2	64,68,73	1.31	10 (15%)	77,107,113	1.46	8 (10%)
29	KC1	C	308	14	49,53,53	1.39	7 (14%)	63,89,89	2.06	13 (20%)
24	SF4	c	101	3	0,12,12	-	-	-		
18	CLA	E	310	16	69,73,73	1.25	9 (13%)	83,113,113	1.27	5 (6%)
18	CLA	l	203	10	69,73,73	1.28	11 (15%)	83,113,113	1.49	10 (12%)
21	BCR	b	839	-	41,41,41	1.01	2 (4%)	56,56,56	2.04	21 (37%)
24	SF4	c	102	3	0,12,12	-	-	-		
18	CLA	H	306	17	69,73,73	1.28	11 (15%)	83,113,113	1.32	9 (10%)
18	CLA	i	101	-	64,68,73	1.30	9 (14%)	77,107,113	1.33	9 (11%)
18	CLA	C	317	-	46,50,73	1.61	10 (21%)	55,85,113	1.63	8 (14%)
18	CLA	a	855	1	69,73,73	1.24	8 (11%)	83,113,113	1.32	8 (9%)
18	CLA	B	307	13	69,73,73	1.25	10 (14%)	83,113,113	1.28	5 (6%)
18	CLA	b	844	2	66,70,73	1.26	9 (13%)	79,109,113	1.34	5 (6%)
18	CLA	C	316	14	45,49,73	1.52	12 (26%)	54,84,113	1.56	9 (16%)
18	CLA	l	205	-	49,53,73	1.47	8 (16%)	59,89,113	1.46	5 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
18	CLA	a	846	-	69,73,73	1.24	9 (13%)	83,113,113	1.27	6 (7%)
28	DD6	E	307	-	39,45,45	2.13	3 (7%)	52,67,67	3.02	23 (44%)
20	LHG	B	315	-	41,41,48	0.98	2 (4%)	44,47,54	1.08	3 (6%)
26	A86	B	305	-	44,50,50	1.49	7 (15%)	51,76,76	3.13	26 (50%)
18	CLA	b	818	2	69,73,73	1.25	9 (13%)	83,113,113	1.28	5 (6%)
18	CLA	b	805	2	69,73,73	1.25	8 (11%)	83,113,113	1.35	5 (6%)
18	CLA	a	841	-	69,73,73	1.30	11 (15%)	83,113,113	1.34	6 (7%)
18	CLA	f	204	6	49,53,73	1.49	9 (18%)	59,89,113	1.45	4 (6%)
18	CLA	a	814	1	69,73,73	1.25	9 (13%)	83,113,113	1.29	6 (7%)
18	CLA	a	810	1	69,73,73	1.24	9 (13%)	83,113,113	1.29	6 (7%)
18	CLA	C	312	14	65,69,73	1.31	11 (16%)	78,108,113	1.40	6 (7%)
18	CLA	b	838	-	69,73,73	1.25	10 (14%)	83,113,113	1.31	5 (6%)
26	A86	H	302	-	44,50,50	1.61	8 (18%)	51,76,76	3.41	23 (45%)
28	DD6	E	308	-	39,45,45	1.99	3 (7%)	52,67,67	1.78	13 (25%)
18	CLA	b	849	-	69,73,73	1.26	9 (13%)	83,113,113	1.32	5 (6%)
18	CLA	H	307	17	69,73,73	1.27	11 (15%)	83,113,113	1.50	13 (15%)
18	CLA	a	811	1	54,58,73	1.39	8 (14%)	65,95,113	1.45	6 (9%)
18	CLA	D	214	15	60,64,73	1.35	10 (16%)	72,102,113	1.39	6 (8%)
21	BCR	a	833	-	41,41,41	0.93	1 (2%)	56,56,56	1.92	20 (35%)
18	CLA	a	823	1	49,53,73	1.47	8 (16%)	59,89,113	1.44	5 (8%)
20	LHG	E	317	-	41,41,48	1.00	2 (4%)	44,47,54	1.20	4 (9%)
18	CLA	C	310	14	50,54,73	1.43	9 (18%)	60,90,113	1.44	6 (10%)
18	CLA	H	315	17	49,53,73	1.47	7 (14%)	59,89,113	1.47	4 (6%)
18	CLA	B	311	13	69,73,73	1.24	9 (13%)	83,113,113	1.29	7 (8%)
20	LHG	H	316	-	34,34,48	1.12	3 (8%)	37,40,54	0.97	2 (5%)
18	CLA	b	826	2	64,68,73	1.30	8 (12%)	77,107,113	1.37	8 (10%)
21	BCR	a	845	-	41,41,41	0.98	2 (4%)	56,56,56	1.94	20 (35%)
18	CLA	a	830	20	56,60,73	1.39	10 (17%)	67,97,113	1.38	5 (7%)
18	CLA	C	307	14	69,73,73	1.28	10 (14%)	83,113,113	1.36	9 (10%)
18	CLA	b	806	2	69,73,73	1.26	7 (10%)	83,113,113	1.28	5 (6%)
18	CLA	E	313	16	59,63,73	1.35	9 (15%)	71,101,113	1.40	7 (9%)
28	DD6	C	303	-	39,45,45	2.20	5 (12%)	52,67,67	2.32	18 (34%)
18	CLA	b	814	-	69,73,73	1.26	9 (13%)	83,113,113	1.32	9 (10%)
18	CLA	b	830	20	69,73,73	1.25	8 (11%)	83,113,113	1.29	6 (7%)
18	CLA	C	318	14	46,50,73	1.51	10 (21%)	55,85,113	1.50	6 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
21	BCR	i	102	-	41,41,41	0.75	0	56,56,56	1.94	17 (30%)
18	CLA	b	822	2	69,73,73	1.25	8 (11%)	83,113,113	1.32	7 (8%)
18	CLA	b	811	2	64,68,73	1.31	10 (15%)	77,107,113	1.42	7 (9%)
18	CLA	a	812	-	49,53,73	1.49	9 (18%)	59,89,113	1.47	4 (6%)
18	CLA	b	815	2	50,54,73	1.46	8 (16%)	60,90,113	1.47	4 (6%)
18	CLA	a	854	-	69,73,73	1.29	9 (13%)	83,113,113	1.46	10 (12%)
18	CLA	B	306	13	62,65,73	1.32	11 (17%)	74,102,113	1.27	5 (6%)
18	CLA	b	842	2	69,73,73	1.25	8 (11%)	83,113,113	1.30	6 (7%)
26	A86	C	305	-	44,50,50	1.53	7 (15%)	51,76,76	3.11	24 (47%)
18	CLA	a	827	1	69,73,73	1.24	7 (10%)	83,113,113	1.32	5 (6%)
26	A86	b	847	-	44,50,50	1.41	6 (13%)	51,76,76	2.22	13 (25%)
18	CLA	a	817	1	53,57,73	1.42	8 (15%)	62,93,113	1.44	6 (9%)
26	A86	C	302	-	44,50,50	1.50	6 (13%)	51,76,76	2.99	22 (43%)
26	A86	B	304	-	44,50,50	1.52	7 (15%)	51,76,76	2.80	18 (35%)
18	CLA	a	818	1	55,59,73	1.43	11 (20%)	66,96,113	1.56	7 (10%)
18	CLA	a	825	1	64,68,73	1.34	11 (17%)	77,107,113	1.48	8 (10%)
18	CLA	b	821	2	54,58,73	1.40	9 (16%)	65,95,113	1.38	6 (9%)
18	CLA	a	837	1	64,68,73	1.36	9 (14%)	77,107,113	1.53	10 (12%)
18	CLA	a	828	1	69,73,73	1.24	8 (11%)	83,113,113	1.28	6 (7%)
20	LHG	a	832	18	26,26,48	1.29	5 (19%)	29,32,54	1.19	2 (6%)
21	BCR	i	103	-	41,41,41	0.70	0	56,56,56	2.04	13 (23%)
18	CLA	B	312	13	69,73,73	1.24	7 (10%)	83,113,113	1.30	5 (6%)
18	CLA	H	310	-	64,68,73	1.30	10 (15%)	77,107,113	1.47	8 (10%)
21	BCR	f	201	-	41,41,41	0.94	1 (2%)	56,56,56	1.94	18 (32%)
23	LMG	a	851	-	33,33,55	1.62	5 (15%)	41,41,63	3.61	8 (19%)
20	LHG	j	102	-	48,48,48	1.11	6 (12%)	51,54,54	0.91	2 (3%)
18	CLA	D	215	-	45,49,73	1.51	8 (17%)	54,84,113	1.48	5 (9%)
19	PQN	b	831	-	34,34,34	1.58	2 (5%)	42,45,45	1.17	3 (7%)
26	A86	D	204	-	44,50,50	1.54	8 (18%)	51,76,76	3.73	22 (43%)
26	A86	r	203	-	44,50,50	1.50	7 (15%)	51,76,76	3.78	27 (52%)
18	CLA	a	847	1	69,73,73	1.25	9 (13%)	83,113,113	1.29	5 (6%)
18	CLA	b	823	2	62,66,73	1.31	9 (14%)	74,104,113	1.37	6 (8%)
22	SQD	a	849	-	31,32,54	3.14	8 (25%)	34,36,65	2.91	9 (26%)
26	A86	m	102	-	44,50,50	1.36	4 (9%)	51,76,76	3.28	25 (49%)
18	CLA	E	314	16	49,53,73	1.50	12 (24%)	59,89,113	1.50	8 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
21	BCR	b	833	-	41,41,41	0.71	0	56,56,56	3.25	21 (37%)
26	A86	D	206	-	44,50,50	1.46	6 (13%)	51,76,76	3.10	21 (41%)
18	CLA	b	825	-	49,53,73	1.50	9 (18%)	59,89,113	1.45	5 (8%)
23	LMG	C	319	18	44,44,55	1.32	7 (15%)	52,52,63	1.86	4 (7%)
18	CLA	D	213	15	69,73,73	1.25	9 (13%)	83,113,113	1.28	6 (7%)
18	CLA	l	202	10	53,57,73	1.45	10 (18%)	62,93,113	1.51	8 (12%)
18	CLA	E	309	16	69,73,73	1.25	9 (13%)	83,113,113	1.30	7 (8%)
21	BCR	a	850	-	41,41,41	1.03	2 (4%)	56,56,56	1.82	13 (23%)
18	CLA	a	848	1	60,64,73	1.34	9 (15%)	72,102,113	1.34	4 (5%)
18	CLA	b	808	2	69,73,73	1.24	9 (13%)	83,113,113	1.30	5 (6%)
20	LHG	E	301	-	48,48,48	1.11	6 (12%)	51,54,54	1.04	3 (5%)
28	DD6	B	303	-	39,45,45	2.32	7 (17%)	52,67,67	2.91	20 (38%)
18	CLA	b	803	2	69,73,73	1.30	11 (15%)	83,113,113	1.36	8 (9%)
20	LHG	a	831	-	48,48,48	1.11	3 (6%)	51,54,54	1.00	3 (5%)
18	CLA	D	209	15	53,57,73	1.43	10 (18%)	62,93,113	1.42	5 (8%)
18	CLA	a	803	1	69,73,73	1.28	12 (17%)	83,113,113	1.51	10 (12%)
18	CLA	b	848	2	58,62,73	1.35	9 (15%)	69,99,113	1.33	4 (5%)
18	CLA	a	843	-	69,73,73	1.24	8 (11%)	83,113,113	1.33	7 (8%)
18	CLA	j	104	9	45,49,73	1.51	8 (17%)	54,84,113	1.54	5 (9%)
26	A86	C	304	-	44,50,50	1.44	5 (11%)	51,76,76	2.68	16 (31%)
18	CLA	H	314	17	69,73,73	1.28	11 (15%)	83,113,113	1.41	12 (14%)
18	CLA	a	824	1	55,59,73	1.38	8 (14%)	66,96,113	1.43	6 (9%)
18	CLA	b	812	2	63,67,73	1.30	8 (12%)	75,105,113	1.33	6 (8%)
29	KC1	B	313	-	49,53,53	1.61	9 (18%)	63,89,89	2.17	13 (20%)
18	CLA	b	817	2	64,68,73	1.30	9 (14%)	77,107,113	1.31	5 (6%)
18	CLA	b	809	2	59,63,73	1.37	9 (15%)	71,101,113	1.38	5 (7%)
18	CLA	a	842	-	69,73,73	1.27	10 (14%)	83,113,113	1.41	9 (10%)
18	CLA	C	311	14	64,68,73	1.33	10 (15%)	77,107,113	1.37	8 (10%)
18	CLA	b	801	-	69,73,73	1.29	10 (14%)	83,113,113	1.46	7 (8%)
18	CLA	b	807	2	69,73,73	1.24	8 (11%)	83,113,113	1.25	5 (6%)
18	CLA	C	315	14	46,50,73	1.52	7 (15%)	55,85,113	1.44	4 (7%)
18	CLA	H	308	17	69,73,73	1.26	11 (15%)	83,113,113	1.44	9 (10%)
26	A86	D	203	-	44,50,50	1.34	4 (9%)	51,76,76	3.58	21 (41%)
18	CLA	H	309	17	50,54,73	1.45	9 (18%)	60,90,113	1.42	5 (8%)
28	DD6	H	303	-	39,45,45	2.48	11 (28%)	52,67,67	2.56	20 (38%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
18	CLA	D	207	-	65,69,73	1.31	10 (15%)	78,108,113	1.42	8 (10%)
18	CLA	a	838	1	69,73,73	1.24	7 (10%)	83,113,113	1.29	6 (7%)
21	BCR	l	204	-	41,41,41	0.86	0	56,56,56	2.07	15 (26%)
28	DD6	E	303	-	39,45,45	1.99	2 (5%)	52,67,67	1.91	10 (19%)
20	LHG	a	835	-	32,32,48	1.28	5 (15%)	35,38,54	1.17	2 (5%)
18	CLA	b	829	2	69,73,73	1.29	11 (15%)	83,113,113	1.46	10 (12%)
21	BCR	a	834	-	41,41,41	0.73	0	56,56,56	1.97	14 (25%)
18	CLA	b	828	-	69,73,73	1.25	9 (13%)	83,113,113	1.31	8 (9%)
18	CLA	a	840	-	69,73,73	1.32	10 (14%)	83,113,113	1.38	8 (9%)
18	CLA	b	810	2	69,73,73	1.25	10 (14%)	83,113,113	1.31	5 (6%)
18	CLA	D	217	-	45,49,73	1.52	8 (17%)	54,84,113	1.51	8 (14%)
18	CLA	b	827	2	51,55,73	1.45	10 (19%)	61,91,113	1.42	5 (8%)
18	CLA	a	819	1	69,73,73	1.25	9 (13%)	83,113,113	1.31	5 (6%)
18	CLA	b	850	2	69,73,73	1.25	7 (10%)	83,113,113	1.29	5 (6%)
18	CLA	a	844	1	69,73,73	1.26	7 (10%)	83,113,113	1.30	5 (6%)
24	SF4	b	802	2	0,12,12	-	-	-		
21	BCR	a	852	-	41,41,41	0.71	0	56,56,56	2.16	19 (33%)
18	CLA	b	820	2	69,73,73	1.26	10 (14%)	83,113,113	1.50	9 (10%)
18	CLA	D	216	15	50,54,73	1.47	10 (20%)	60,90,113	1.44	7 (11%)
27	ET4	l	206	-	41,43,43	1.45	7 (17%)	54,60,60	2.28	19 (35%)
21	BCR	E	306	-	41,41,41	0.71	0	56,56,56	2.02	16 (28%)
21	BCR	E	305	-	41,41,41	0.70	0	56,56,56	1.87	17 (30%)
18	CLA	a	836	1	69,73,73	1.23	8 (11%)	83,113,113	1.26	5 (6%)
18	CLA	E	312	16	69,73,73	1.32	11 (15%)	83,113,113	1.36	7 (8%)
18	CLA	a	805	1	69,73,73	1.23	9 (13%)	83,113,113	1.33	5 (6%)
18	CLA	b	841	2	69,73,73	1.25	8 (11%)	83,113,113	1.28	6 (7%)
18	CLA	H	311	17	61,65,73	1.35	11 (18%)	73,103,113	1.43	6 (8%)
28	DD6	D	205	-	39,45,45	2.22	6 (15%)	52,67,67	3.22	26 (50%)
18	CLA	r	202	12	49,53,73	1.48	7 (14%)	59,89,113	1.43	7 (11%)
23	LMG	D	202	-	46,46,55	1.84	7 (15%)	54,54,63	1.36	5 (9%)
18	CLA	C	314	14	45,49,73	1.54	12 (26%)	54,84,113	1.52	7 (12%)
25	DGD	b	834	-	61,61,67	0.85	2 (3%)	75,75,81	1.10	4 (5%)
18	CLA	H	305	-	58,62,73	1.38	10 (17%)	69,99,113	1.50	6 (8%)
26	A86	B	302	-	44,50,50	1.62	9 (20%)	51,76,76	3.40	23 (45%)
18	CLA	a	809	18,1	66,70,73	1.26	7 (10%)	79,109,113	1.29	5 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
18	CLA	b	819	2	69,73,73	1.24	9 (13%)	83,113,113	1.26	5 (6%)
18	CLA	a	813	1	69,73,73	1.27	11 (15%)	83,113,113	1.49	11 (13%)
18	CLA	a	801	1	69,73,73	1.36	11 (15%)	83,113,113	1.35	9 (10%)
18	CLA	D	208	15	69,73,73	1.30	12 (17%)	83,113,113	1.47	10 (12%)
23	LMG	C	301	-	31,31,55	1.61	6 (19%)	39,39,63	3.02	7 (17%)
18	CLA	b	846	2	69,73,73	1.25	9 (13%)	83,113,113	1.26	5 (6%)
18	CLA	B	308	13	69,73,73	1.25	9 (13%)	83,113,113	1.28	5 (6%)
19	PQN	a	829	-	34,34,34	1.59	2 (5%)	42,45,45	1.07	2 (4%)
21	BCR	m	101	-	41,41,41	0.67	0	56,56,56	2.14	16 (28%)
18	CLA	a	807	1	69,73,73	1.29	12 (17%)	83,113,113	1.47	10 (12%)
28	DD6	E	304	-	39,45,45	2.53	8 (20%)	52,67,67	3.42	16 (30%)
18	CLA	E	315	16	69,73,73	1.26	9 (13%)	83,113,113	1.29	6 (7%)
26	A86	H	304	-	44,50,50	1.46	5 (11%)	51,76,76	2.89	24 (47%)
18	CLA	B	314	13	45,49,73	1.53	11 (24%)	54,84,113	1.53	8 (14%)
21	BCR	b	836	-	41,41,41	0.74	0	56,56,56	2.00	18 (32%)
23	LMG	E	318	-	43,43,55	2.06	7 (16%)	51,51,63	1.98	7 (13%)
18	CLA	b	845	-	69,73,73	1.24	9 (13%)	83,113,113	1.28	6 (7%)
21	BCR	j	101	-	41,41,41	0.70	0	56,56,56	2.06	14 (25%)
18	CLA	B	309	-	69,73,73	1.24	9 (13%)	83,113,113	1.31	4 (4%)
18	CLA	b	804	2	49,53,73	1.52	12 (24%)	59,89,113	1.53	6 (10%)
26	A86	H	301	-	44,50,50	1.51	8 (18%)	51,76,76	3.17	24 (47%)
21	BCR	r	201	-	41,41,41	0.71	0	56,56,56	1.75	15 (26%)
18	CLA	H	313	17	69,73,73	1.27	12 (17%)	83,113,113	1.44	8 (9%)
18	CLA	D	212	15	46,50,73	1.49	9 (19%)	55,85,113	1.44	4 (7%)

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
23	LMG	l	207	-	-	16/35/55/70	0/1/1/1
18	CLA	a	802	-	-	10/39/115/115	-
18	CLA	f	202	-	-	10/39/115/115	-
18	CLA	C	306	23	-	6/15/91/115	-
21	BCR	l	201	-	-	6/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	KC1	C	313	-	-	7/15/71/71	-
20	LHG	D	201	-	-	32/53/53/53	-
18	CLA	a	806	1	-	13/39/115/115	-
18	CLA	a	826	1	-	14/39/115/115	-
18	CLA	D	211	15	-	11/17/93/115	-
18	CLA	D	210	-	-	6/29/105/115	-
18	CLA	a	839	1	-	11/39/115/115	-
21	BCR	f	205	-	-	2/29/63/63	0/2/2/2
29	KC1	H	312	17	-	9/15/71/71	-
18	CLA	a	815	1	-	15/39/115/115	-
18	CLA	b	813	2	-	14/27/103/115	-
26	A86	E	302	-	-	5/34/90/90	0/3/3/3
21	BCR	b	832	-	-	0/29/63/63	0/2/2/2
18	CLA	f	203	-	-	12/39/115/115	-
18	CLA	a	808	1	-	12/39/115/115	-
18	CLA	a	822	1	-	7/21/97/115	-
18	CLA	E	316	-	-	7/29/105/115	-
18	CLA	C	309	-	-	14/36/112/115	-
21	BCR	j	105	-	-	5/29/63/63	0/2/2/2
18	CLA	b	824	-	-	17/39/115/115	-
18	CLA	a	821	1	-	12/39/115/115	-
18	CLA	b	840	2	-	12/35/111/115	-
18	CLA	a	804	18,1	-	6/27/103/115	-
23	LMG	j	103	-	-	16/32/52/70	0/1/1/1
18	CLA	a	820	1	-	8/39/115/115	-
18	CLA	b	816	2	-	5/27/103/115	-
18	CLA	E	311	16	-	8/17/93/115	-
18	CLA	a	816	1	-	9/15/91/115	-
18	CLA	B	310	13	-	7/17/93/115	-
20	LHG	b	835	18	-	32/53/53/53	-
18	CLA	b	843	2	-	18/39/115/115	-
18	CLA	a	853	1	-	12/27/103/115	-
26	A86	B	301	-	-	12/34/90/90	0/3/3/3
18	CLA	b	837	2	-	14/33/109/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	KC1	C	308	14	-	7/15/71/71	-
24	SF4	c	101	3	-	-	0/6/5/5
18	CLA	E	310	16	-	14/39/115/115	-
18	CLA	l	203	10	-	18/39/115/115	-
21	BCR	b	839	-	-	6/29/63/63	0/2/2/2
24	SF4	c	102	3	-	-	0/6/5/5
18	CLA	H	306	17	-	12/39/115/115	-
18	CLA	i	101	-	-	11/33/109/115	-
18	CLA	C	317	-	-	10/12/88/115	-
18	CLA	a	855	1	-	14/39/115/115	-
18	CLA	B	307	13	-	9/39/115/115	-
18	CLA	b	844	2	-	12/36/112/115	-
18	CLA	C	316	14	-	5/10/86/115	-
18	CLA	l	205	-	-	4/15/91/115	-
18	CLA	a	846	-	-	10/39/115/115	-
28	DD6	E	307	-	-	10/26/80/80	0/3/3/3
20	LHG	B	315	-	-	25/46/46/53	-
26	A86	B	305	-	-	4/34/90/90	0/3/3/3
18	CLA	b	818	2	-	9/39/115/115	-
18	CLA	b	805	2	-	15/39/115/115	-
18	CLA	a	841	-	-	22/39/115/115	-
18	CLA	f	204	6	-	5/15/91/115	-
18	CLA	a	814	1	-	9/39/115/115	-
18	CLA	a	810	1	-	9/39/115/115	-
18	CLA	C	312	14	-	12/35/111/115	-
18	CLA	b	838	-	-	7/39/115/115	-
26	A86	H	302	-	-	5/34/90/90	0/3/3/3
28	DD6	E	308	-	-	1/26/80/80	0/3/3/3
18	CLA	b	849	-	-	16/39/115/115	-
18	CLA	H	307	17	-	15/39/115/115	-
18	CLA	a	811	1	-	8/21/97/115	-
18	CLA	D	214	15	-	9/29/105/115	-
21	BCR	a	833	-	-	0/29/63/63	0/2/2/2
18	CLA	a	823	1	-	11/15/91/115	-
20	LHG	E	317	-	-	6/46/46/53	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	CLA	C	310	14	-	8/17/93/115	-
18	CLA	H	315	17	-	6/15/91/115	-
18	CLA	B	311	13	-	13/39/115/115	-
20	LHG	H	316	-	-	19/38/38/53	-
18	CLA	b	826	2	-	9/33/109/115	-
21	BCR	a	845	-	-	2/29/63/63	0/2/2/2
18	CLA	a	830	20	-	8/24/100/115	-
18	CLA	C	307	14	-	8/39/115/115	-
18	CLA	b	806	2	-	17/39/115/115	-
18	CLA	E	313	16	-	11/27/103/115	-
28	DD6	C	303	-	-	5/26/80/80	0/3/3/3
18	CLA	b	814	-	-	11/39/115/115	-
18	CLA	b	830	20	-	9/39/115/115	-
18	CLA	C	318	14	-	7/12/88/115	-
21	BCR	i	102	-	-	0/29/63/63	0/2/2/2
18	CLA	b	822	2	-	18/39/115/115	-
18	CLA	b	811	2	-	9/33/109/115	-
18	CLA	a	812	-	-	6/15/91/115	-
18	CLA	b	815	2	-	5/17/93/115	-
18	CLA	a	854	-	-	16/39/115/115	-
18	CLA	B	306	13	-	18/29/101/115	-
18	CLA	b	842	2	-	16/39/115/115	-
26	A86	C	305	-	-	4/34/90/90	0/3/3/3
18	CLA	a	827	1	-	10/39/115/115	-
26	A86	b	847	-	-	17/34/90/90	0/3/3/3
18	CLA	a	817	1	-	12/20/96/115	-
26	A86	C	302	-	-	5/34/90/90	0/3/3/3
26	A86	B	304	-	-	3/34/90/90	0/3/3/3
18	CLA	a	818	1	-	5/23/99/115	-
18	CLA	a	825	1	-	14/33/109/115	-
18	CLA	b	821	2	-	10/21/97/115	-
18	CLA	a	837	1	-	14/33/109/115	-
18	CLA	a	828	1	-	13/39/115/115	-
20	LHG	a	832	18	-	12/31/31/53	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	BCR	i	103	-	-	4/29/63/63	0/2/2/2
18	CLA	B	312	13	-	13/39/115/115	-
18	CLA	H	310	-	-	9/33/109/115	-
21	BCR	f	201	-	-	9/29/63/63	0/2/2/2
23	LMG	a	851	-	-	16/28/48/70	0/1/1/1
20	LHG	j	102	-	-	20/53/53/53	-
18	CLA	D	215	-	-	4/10/86/115	-
19	PQN	b	831	-	-	3/23/43/43	0/2/2/2
26	A86	D	204	-	-	4/34/90/90	0/3/3/3
26	A86	r	203	-	-	6/34/90/90	0/3/3/3
18	CLA	a	847	1	-	15/39/115/115	-
18	CLA	b	823	2	-	13/31/107/115	-
22	SQD	a	849	-	-	18/33/33/69	-
26	A86	m	102	-	-	7/34/90/90	0/3/3/3
18	CLA	E	314	16	-	4/15/91/115	-
21	BCR	b	833	-	-	6/29/63/63	0/2/2/2
26	A86	D	206	-	-	6/34/90/90	0/3/3/3
18	CLA	b	825	-	-	6/15/91/115	-
23	LMG	C	319	18	-	19/39/59/70	0/1/1/1
18	CLA	D	213	15	-	10/39/115/115	-
18	CLA	l	202	10	-	8/20/96/115	-
18	CLA	E	309	16	-	14/39/115/115	-
21	BCR	a	850	-	-	4/29/63/63	0/2/2/2
18	CLA	a	848	1	-	11/29/105/115	-
18	CLA	b	808	2	-	12/39/115/115	-
20	LHG	E	301	-	-	35/53/53/53	-
28	DD6	B	303	-	-	0/26/80/80	0/3/3/3
18	CLA	b	803	2	-	18/39/115/115	-
20	LHG	a	831	-	-	26/53/53/53	-
18	CLA	D	209	15	-	11/20/96/115	-
18	CLA	a	803	1	-	13/39/115/115	-
18	CLA	b	848	2	-	10/26/102/115	-
18	CLA	a	843	-	-	12/39/115/115	-
18	CLA	j	104	9	-	4/10/86/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	A86	C	304	-	-	3/34/90/90	0/3/3/3
18	CLA	H	314	17	-	15/39/115/115	-
18	CLA	a	824	1	-	10/23/99/115	-
18	CLA	b	812	2	-	9/32/108/115	-
29	KC1	B	313	-	-	8/15/71/71	-
18	CLA	b	817	2	-	19/33/109/115	-
18	CLA	b	809	2	-	5/27/103/115	-
18	CLA	a	842	-	-	10/39/115/115	-
18	CLA	C	311	14	-	14/33/109/115	-
18	CLA	b	801	-	-	9/39/115/115	-
18	CLA	b	807	2	-	11/39/115/115	-
18	CLA	C	315	14	-	6/12/88/115	-
18	CLA	H	308	17	-	12/39/115/115	-
26	A86	D	203	-	-	9/34/90/90	0/3/3/3
18	CLA	H	309	17	-	10/17/93/115	-
28	DD6	H	303	-	-	3/26/80/80	0/3/3/3
18	CLA	D	207	-	-	12/35/111/115	-
18	CLA	a	838	1	-	12/39/115/115	-
21	BCR	l	204	-	-	8/29/63/63	0/2/2/2
28	DD6	E	303	-	-	3/26/80/80	0/3/3/3
20	LHG	a	835	-	-	20/36/36/53	-
18	CLA	b	829	2	-	14/39/115/115	-
21	BCR	a	834	-	-	4/29/63/63	0/2/2/2
18	CLA	b	828	-	-	11/39/115/115	-
18	CLA	a	840	-	-	13/39/115/115	-
18	CLA	b	810	2	-	10/39/115/115	-
18	CLA	D	217	-	-	5/10/86/115	-
18	CLA	b	827	2	-	7/18/94/115	-
18	CLA	a	819	1	-	4/39/115/115	-
18	CLA	b	850	2	-	12/39/115/115	-
18	CLA	a	844	1	-	19/39/115/115	-
24	SF4	b	802	2	-	-	0/6/5/5
21	BCR	a	852	-	-	8/29/63/63	0/2/2/2
18	CLA	b	820	2	-	17/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	CLA	D	216	15	-	5/17/93/115	-
27	ET4	l	206	-	-	3/25/67/67	0/2/2/2
21	BCR	E	306	-	-	0/29/63/63	0/2/2/2
21	BCR	E	305	-	-	2/29/63/63	0/2/2/2
18	CLA	a	836	1	-	13/39/115/115	-
18	CLA	E	312	16	-	11/39/115/115	-
18	CLA	a	805	1	-	15/39/115/115	-
18	CLA	b	841	2	-	9/39/115/115	-
18	CLA	H	311	17	-	8/30/106/115	-
28	DD6	D	205	-	-	3/26/80/80	0/3/3/3
18	CLA	r	202	12	-	12/15/91/115	-
23	LMG	D	202	-	-	17/41/61/70	0/1/1/1
18	CLA	C	314	14	-	5/10/86/115	-
25	DGD	b	834	-	-	27/49/89/95	0/2/2/2
18	CLA	H	305	-	-	10/26/102/115	-
26	A86	B	302	-	-	5/34/90/90	0/3/3/3
18	CLA	a	809	18,1	-	14/36/112/115	-
18	CLA	b	819	2	-	16/39/115/115	-
18	CLA	a	813	1	-	24/39/115/115	-
18	CLA	a	801	1	-	17/39/115/115	-
18	CLA	D	208	15	-	15/39/115/115	-
23	LMG	C	301	-	-	14/26/46/70	0/1/1/1
18	CLA	b	846	2	-	14/39/115/115	-
18	CLA	B	308	13	-	11/39/115/115	-
19	PQN	a	829	-	-	2/23/43/43	0/2/2/2
21	BCR	m	101	-	-	7/29/63/63	0/2/2/2
18	CLA	a	807	1	-	9/39/115/115	-
28	DD6	E	304	-	-	6/26/80/80	0/3/3/3
18	CLA	E	315	16	-	12/39/115/115	-
26	A86	H	304	-	-	4/34/90/90	0/3/3/3
18	CLA	B	314	13	-	2/10/86/115	-
21	BCR	b	836	-	-	5/29/63/63	0/2/2/2
23	LMG	E	318	-	-	21/38/58/70	0/1/1/1
18	CLA	b	845	-	-	14/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	BCR	j	101	-	-	4/29/63/63	0/2/2/2
18	CLA	B	309	-	-	12/39/115/115	-
18	CLA	b	804	2	-	3/15/91/115	-
26	A86	H	301	-	-	5/34/90/90	0/3/3/3
21	BCR	r	201	-	-	4/29/63/63	0/2/2/2
18	CLA	H	313	17	-	18/39/115/115	-
18	CLA	D	212	15	-	3/12/88/115	-

The worst 5 of 1610 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	a	849	SQD	C6-S	-12.47	1.59	1.77
23	E	318	LMG	O2-C2	-10.74	1.17	1.43
23	D	202	LMG	O2-C2	-9.35	1.21	1.43
28	H	303	DD6	C29-C27	-9.22	1.24	1.42
28	C	303	DD6	C29-C27	-9.14	1.25	1.42

The worst 5 of 1943 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	j	103	LMG	O2-C2-C1	-21.31	58.28	110.05
23	a	851	LMG	O2-C2-C1	-18.81	64.35	110.05
28	E	304	DD6	C21-C20-C15	-16.18	95.14	122.26
26	r	203	A86	O1-C20-C19	-15.79	101.52	113.38
23	C	301	LMG	O2-C2-C1	15.25	147.09	110.05

There are no chirality outliers.

5 of 2205 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
18	a	801	CLA	CBD-CGD-O2D-CED
18	a	801	CLA	O1D-CGD-O2D-CED
18	a	802	CLA	CHA-CBD-CGD-O1D
18	a	802	CLA	CHA-CBD-CGD-O2D
18	a	803	CLA	CHA-CBD-CGD-O1D

There are no ring outliers.

188 monomers are involved in 609 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	l	207	LMG	1	0
18	a	802	CLA	12	0
18	f	202	CLA	1	0
21	l	201	BCR	3	0
20	D	201	LHG	6	0
18	a	806	CLA	4	0
18	a	826	CLA	1	0
18	D	211	CLA	2	0
18	D	210	CLA	1	0
18	a	839	CLA	1	0
21	f	205	BCR	2	0
29	H	312	KC1	1	0
18	a	815	CLA	6	0
18	b	813	CLA	18	0
21	b	832	BCR	3	0
18	f	203	CLA	1	0
18	a	808	CLA	5	0
18	E	316	CLA	6	0
18	C	309	CLA	6	0
21	j	105	BCR	11	0
18	b	824	CLA	5	0
18	a	821	CLA	1	0
18	b	840	CLA	3	0
18	a	804	CLA	7	0
18	a	820	CLA	2	0
18	E	311	CLA	1	0
18	a	816	CLA	1	0
20	b	835	LHG	5	0
18	b	843	CLA	5	0
26	B	301	A86	2	0
18	b	837	CLA	2	0
29	C	308	KC1	4	0
24	c	101	SF4	1	0
18	E	310	CLA	1	0
18	l	203	CLA	6	0
21	b	839	BCR	9	0
24	c	102	SF4	5	0
18	H	306	CLA	8	0
18	i	101	CLA	1	0
18	C	317	CLA	8	0
18	a	855	CLA	5	0
18	B	307	CLA	4	0
18	b	844	CLA	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	C	316	CLA	10	0
18	a	846	CLA	1	0
28	E	307	DD6	1	0
20	B	315	LHG	3	0
18	b	818	CLA	3	0
18	b	805	CLA	4	0
18	a	841	CLA	7	0
18	f	204	CLA	1	0
18	a	814	CLA	2	0
18	a	810	CLA	3	0
18	C	312	CLA	10	0
18	b	838	CLA	4	0
26	H	302	A86	17	0
18	b	849	CLA	5	0
18	H	307	CLA	4	0
18	a	811	CLA	1	0
18	D	214	CLA	5	0
21	a	833	BCR	17	0
18	a	823	CLA	1	0
20	E	317	LHG	2	0
18	C	310	CLA	3	0
18	B	311	CLA	4	0
21	a	845	BCR	4	0
18	a	830	CLA	3	0
18	C	307	CLA	6	0
18	b	806	CLA	3	0
18	E	313	CLA	2	0
28	C	303	DD6	1	0
18	b	814	CLA	7	0
18	b	830	CLA	1	0
18	C	318	CLA	11	0
21	i	102	BCR	9	0
18	b	822	CLA	3	0
18	b	811	CLA	1	0
18	a	854	CLA	3	0
18	B	306	CLA	13	0
18	b	842	CLA	6	0
26	C	305	A86	4	0
18	a	827	CLA	3	0
26	b	847	A86	4	0
18	a	817	CLA	1	0
26	B	304	A86	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	a	818	CLA	2	0
18	a	825	CLA	5	0
18	b	821	CLA	3	0
18	a	837	CLA	5	0
18	a	828	CLA	2	0
20	a	832	LHG	3	0
21	i	103	BCR	5	0
18	B	312	CLA	7	0
18	H	310	CLA	3	0
21	f	201	BCR	4	0
23	a	851	LMG	2	0
20	j	102	LHG	5	0
18	D	215	CLA	5	0
19	b	831	PQN	4	0
26	r	203	A86	1	0
18	a	847	CLA	3	0
18	b	823	CLA	7	0
22	a	849	SQD	7	0
26	m	102	A86	5	0
21	b	833	BCR	3	0
18	b	825	CLA	3	0
23	C	319	LMG	1	0
18	D	213	CLA	2	0
18	l	202	CLA	4	0
18	E	309	CLA	5	0
21	a	850	BCR	4	0
18	a	848	CLA	5	0
18	b	808	CLA	2	0
20	E	301	LHG	3	0
18	b	803	CLA	4	0
20	a	831	LHG	2	0
18	D	209	CLA	3	0
18	a	803	CLA	12	0
18	b	848	CLA	3	0
18	j	104	CLA	1	0
26	C	304	A86	1	0
18	H	314	CLA	5	0
18	b	812	CLA	2	0
29	B	313	KC1	5	0
18	b	817	CLA	6	0
18	b	809	CLA	2	0
18	a	842	CLA	5	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	C	311	CLA	6	0
18	b	801	CLA	10	0
18	b	807	CLA	3	0
18	C	315	CLA	2	0
18	H	308	CLA	4	0
26	D	203	A86	3	0
18	H	309	CLA	16	0
28	H	303	DD6	3	0
18	D	207	CLA	3	0
18	a	838	CLA	2	0
21	l	204	BCR	8	0
20	a	835	LHG	1	0
18	b	829	CLA	6	0
21	a	834	BCR	4	0
18	b	828	CLA	1	0
18	a	840	CLA	2	0
18	b	810	CLA	2	0
18	D	217	CLA	3	0
18	b	827	CLA	2	0
18	a	819	CLA	1	0
18	b	850	CLA	6	0
18	a	844	CLA	5	0
24	b	802	SF4	1	0
21	a	852	BCR	14	0
18	b	820	CLA	5	0
18	D	216	CLA	4	0
21	E	306	BCR	7	0
21	E	305	BCR	2	0
18	a	836	CLA	3	0
18	E	312	CLA	7	0
18	a	805	CLA	2	0
18	b	841	CLA	3	0
18	H	311	CLA	6	0
28	D	205	DD6	3	0
18	r	202	CLA	2	0
23	D	202	LMG	1	0
18	C	314	CLA	3	0
18	H	305	CLA	3	0
26	B	302	A86	3	0
18	a	809	CLA	4	0
18	b	819	CLA	4	0
18	a	813	CLA	8	0

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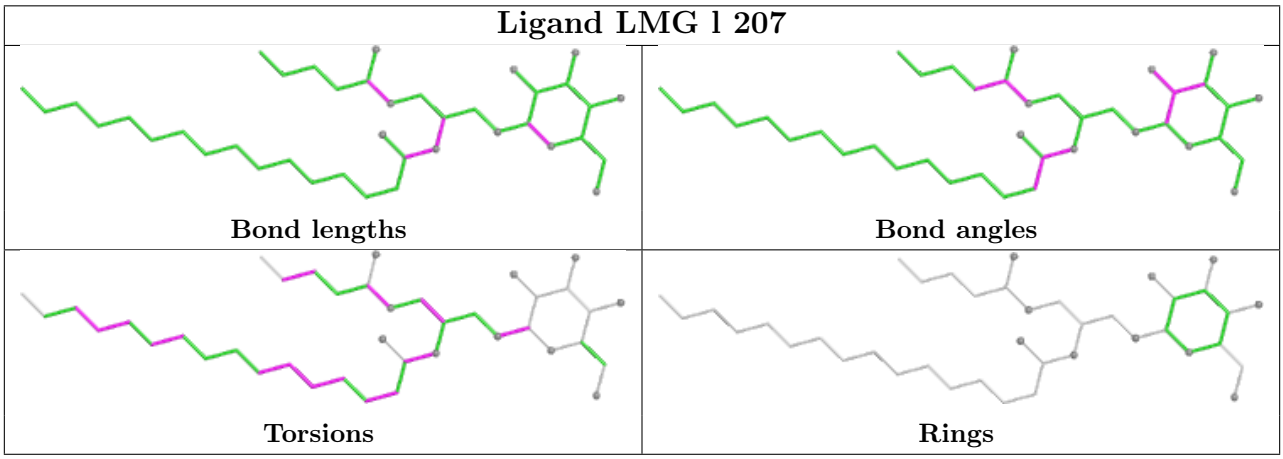
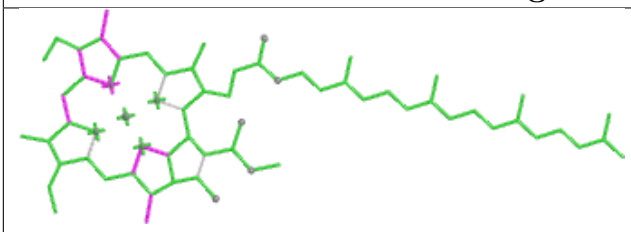
Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	a	801	CLA	3	0
18	D	208	CLA	9	0
18	b	846	CLA	2	0
18	B	308	CLA	1	0
19	a	829	PQN	1	0
21	m	101	BCR	5	0
18	a	807	CLA	14	0
28	E	304	DD6	1	0
18	E	315	CLA	3	0
18	B	314	CLA	3	0
21	b	836	BCR	4	0
23	E	318	LMG	5	0
18	b	845	CLA	7	0
21	j	101	BCR	6	0
18	B	309	CLA	2	0
18	b	804	CLA	1	0
21	r	201	BCR	2	0
18	H	313	CLA	6	0
18	D	212	CLA	1	0

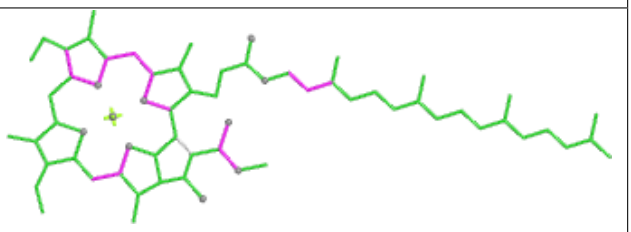
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



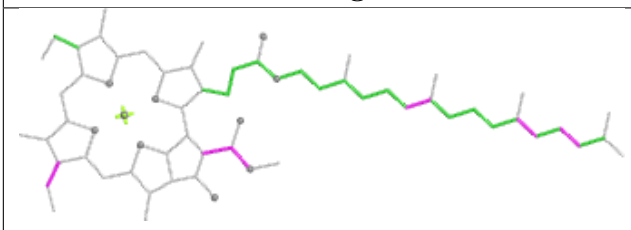
Ligand CLA a 802



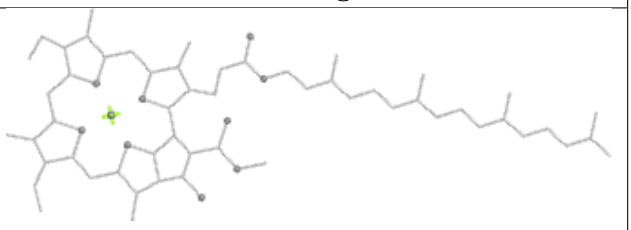
Bond lengths



Bond angles

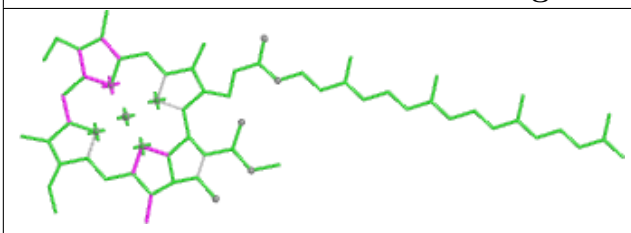


Torsions

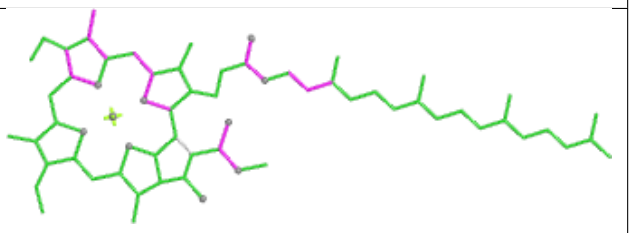


Rings

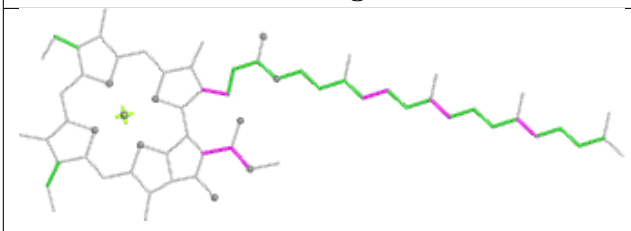
Ligand CLA f 202



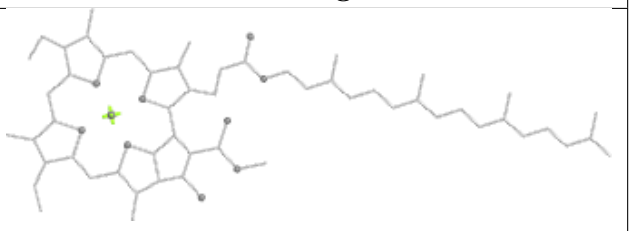
Bond lengths



Bond angles

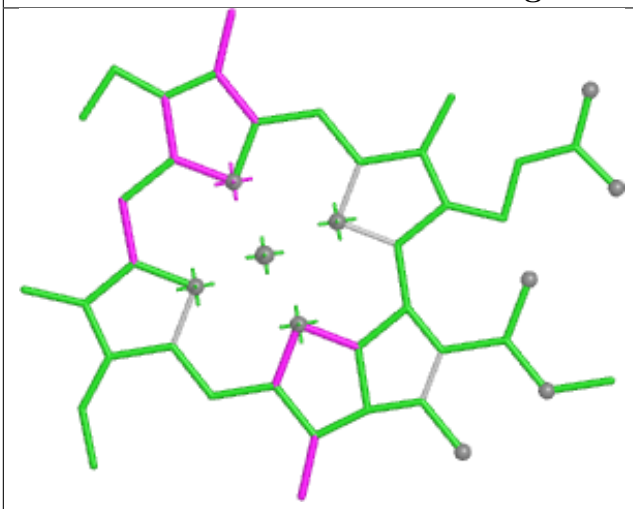


Torsions

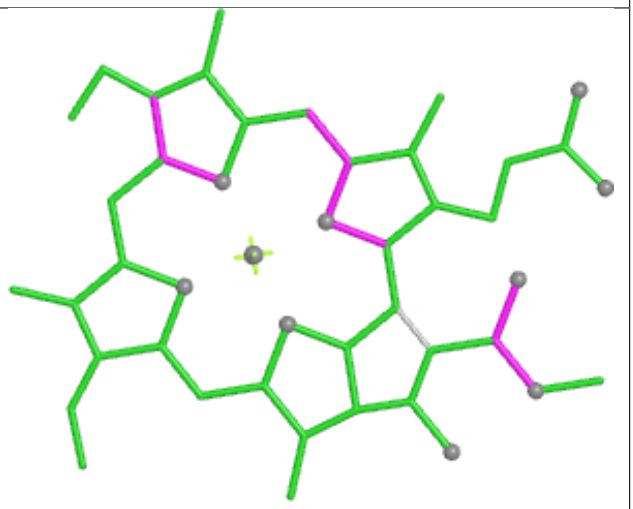


Rings

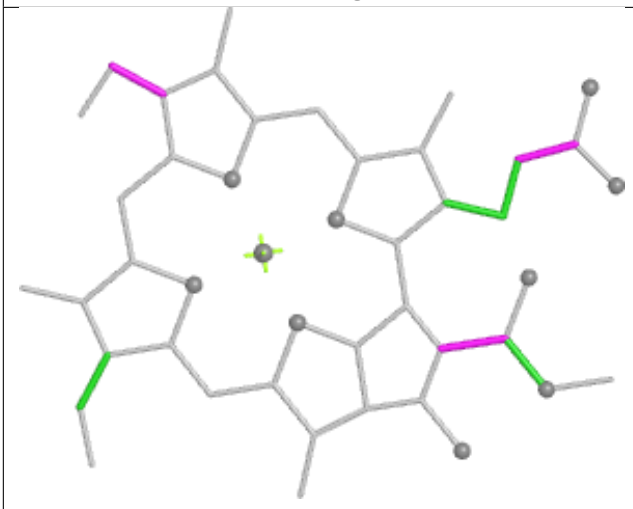
Ligand CLA C 306



Bond lengths



Bond angles

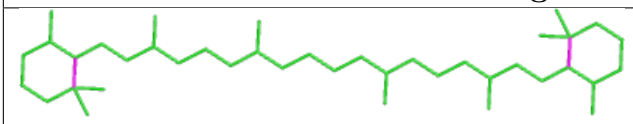


Torsions

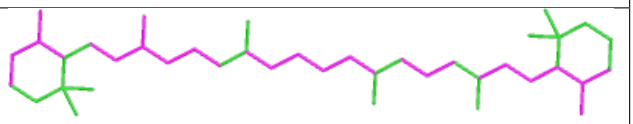


Rings

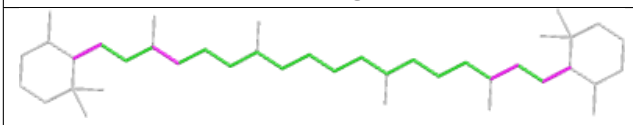
Ligand BCR l 201



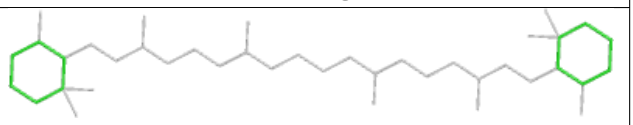
Bond lengths



Bond angles

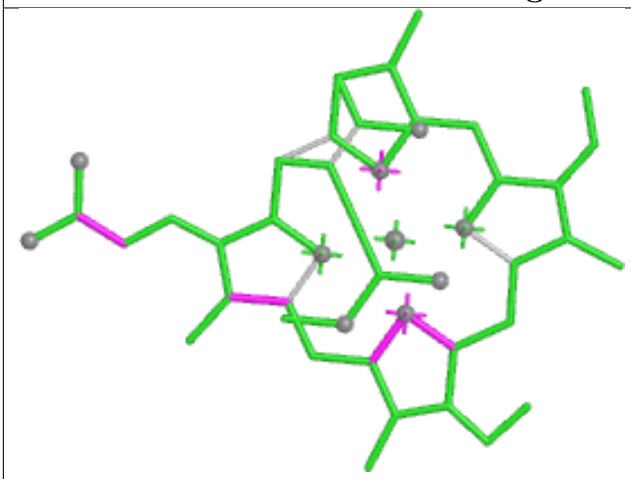


Torsions

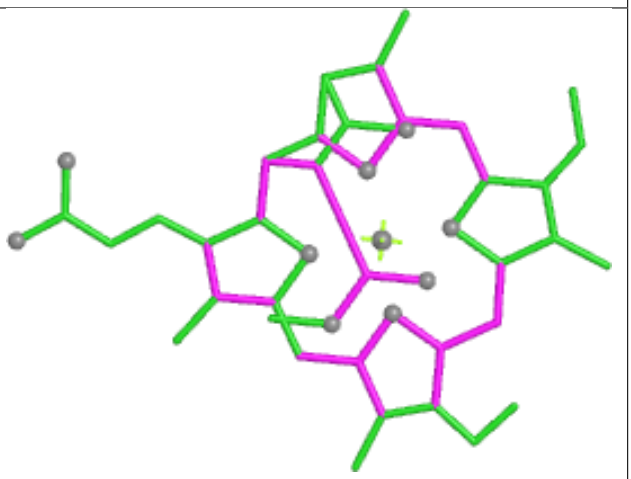


Rings

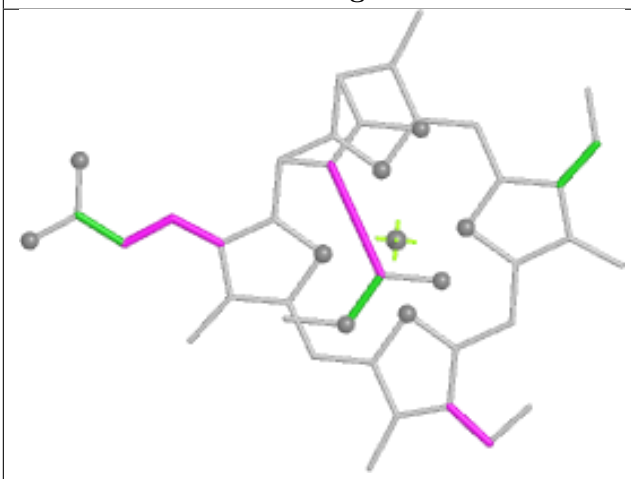
Ligand KC1 C 313



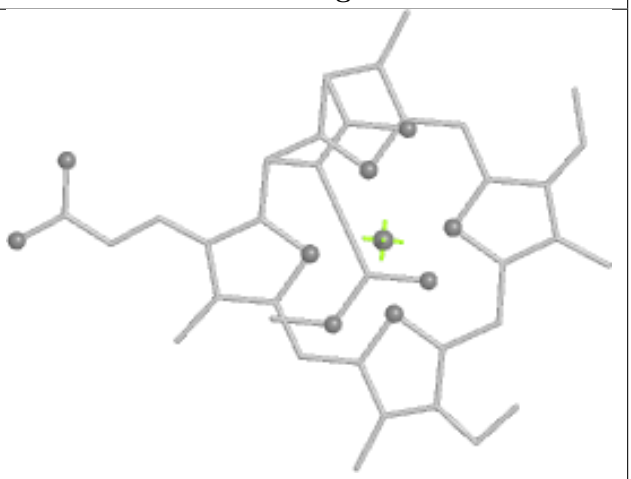
Bond lengths



Bond angles

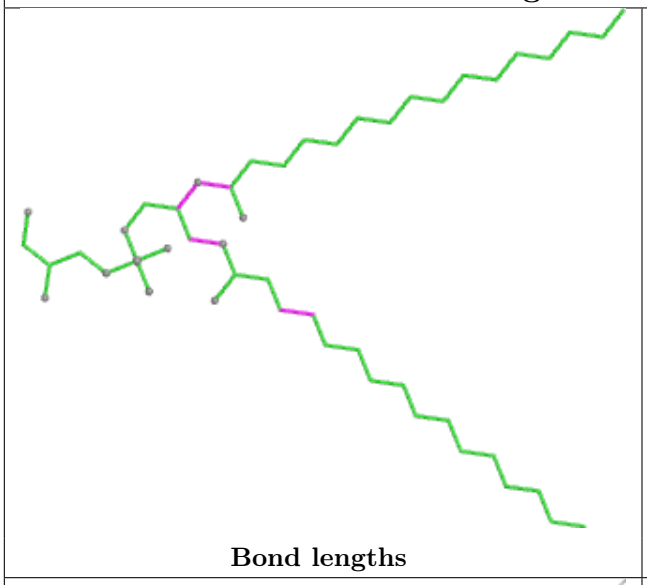


Torsions

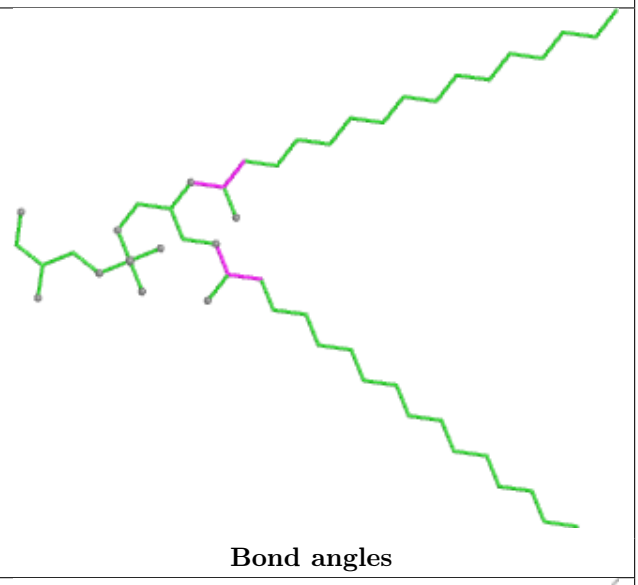


Rings

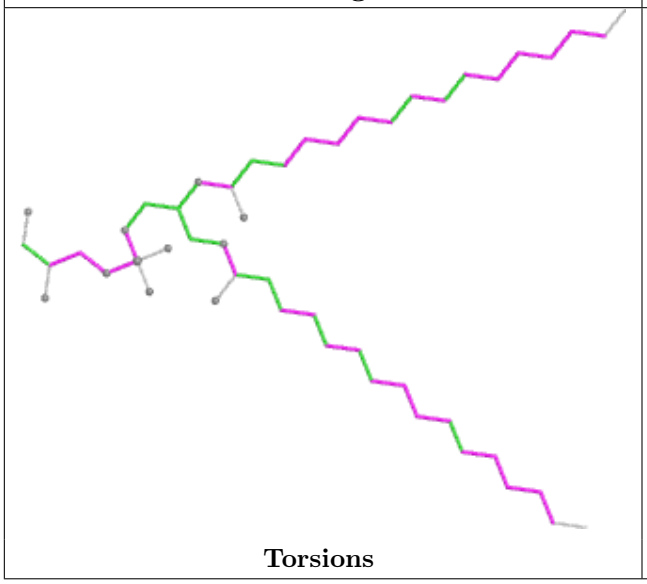
Ligand LHG D 201



Bond lengths



Bond angles



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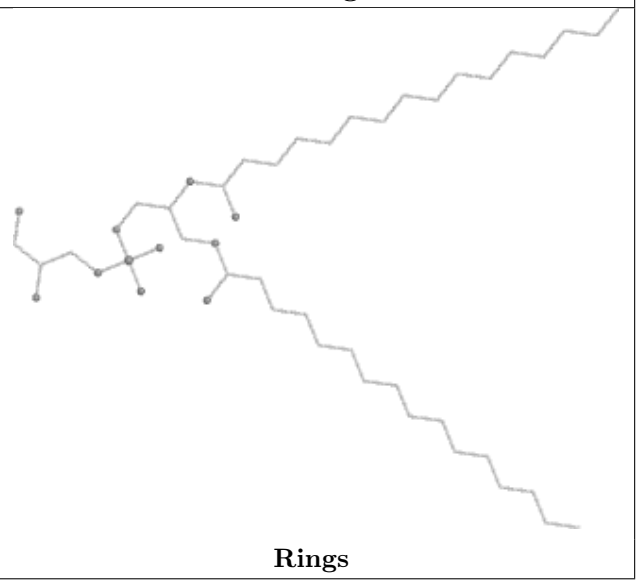
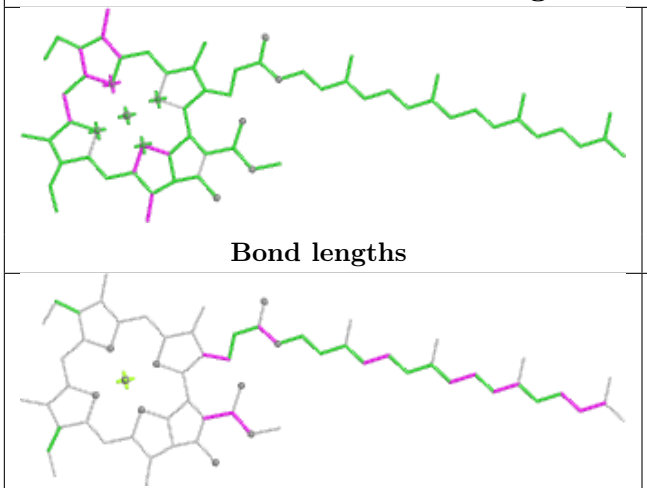


Rings

Ligand CLA a 806



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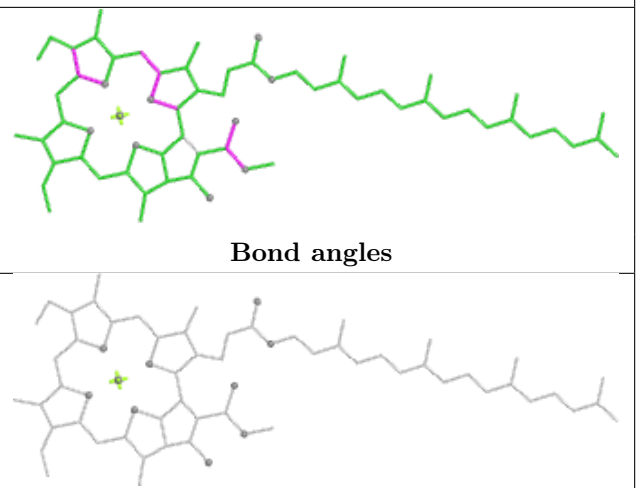
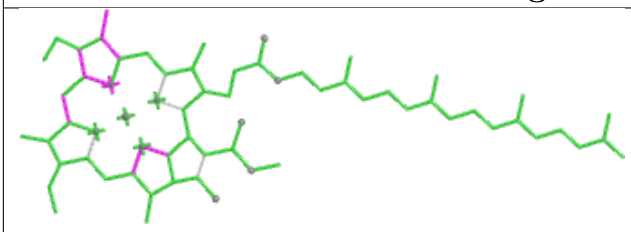


Bond angles

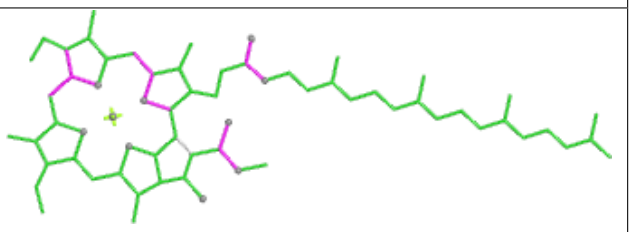
Torsions

Rings

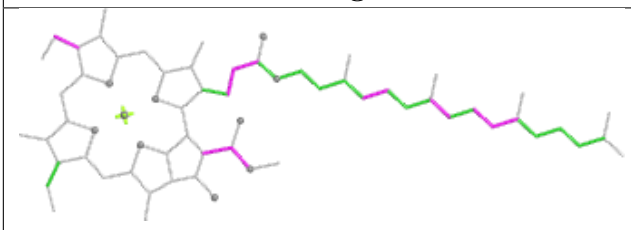
Ligand CLA a 826



Bond lengths



Bond angles



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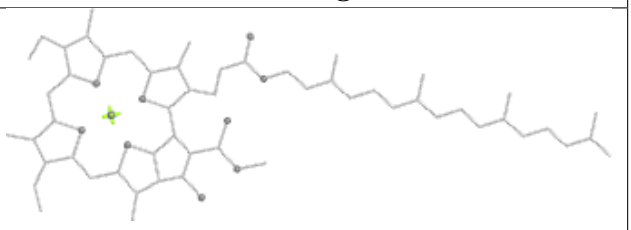
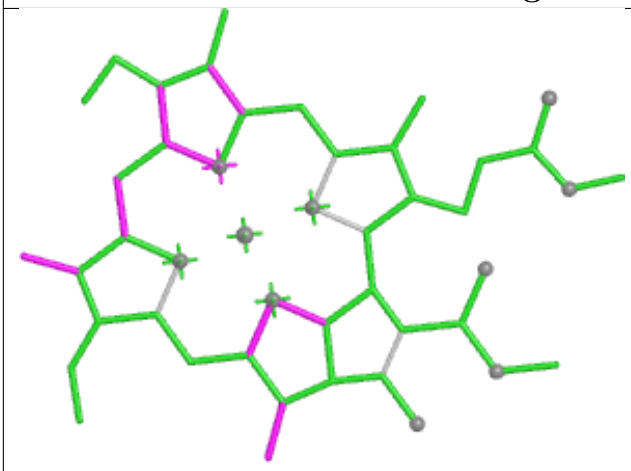


Rings

Ligand CLA D 211



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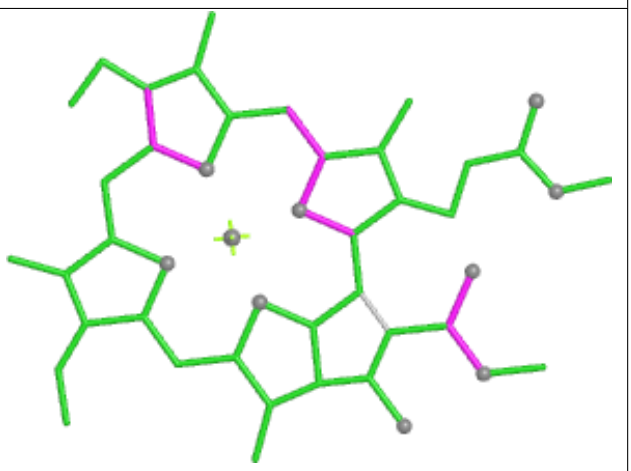
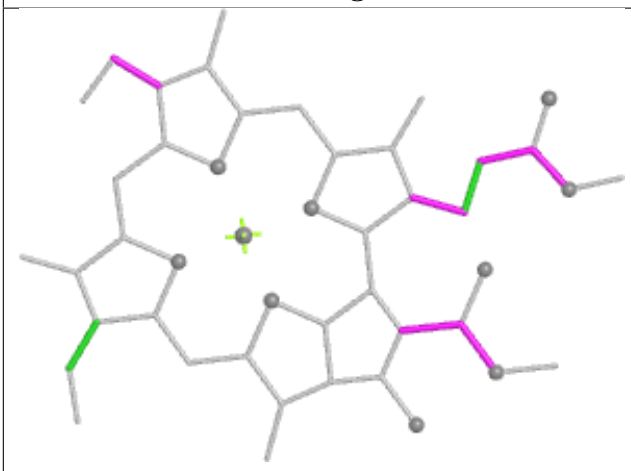


Bond angles

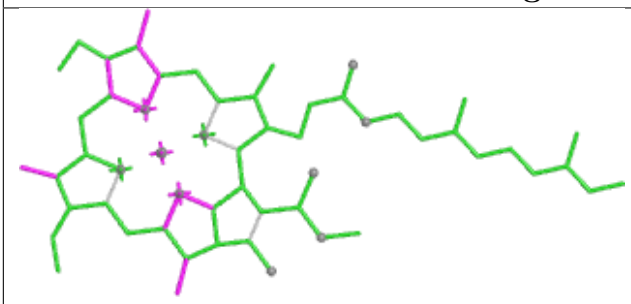


Torsions



Rings

Ligand CLA D 210



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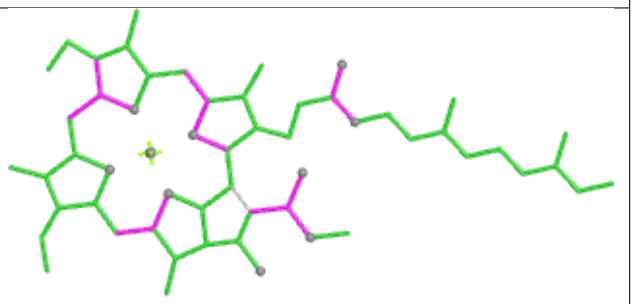
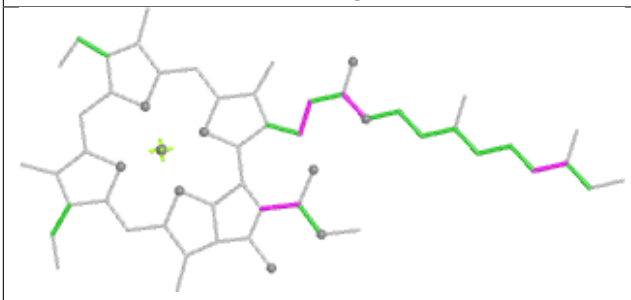


Bond angles



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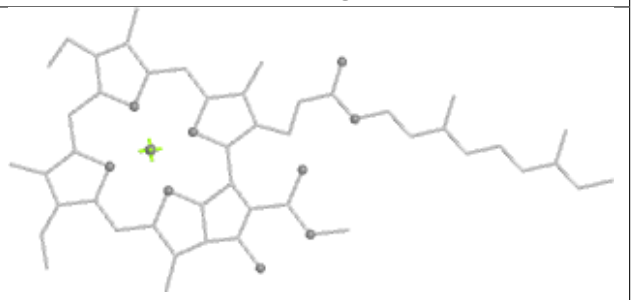
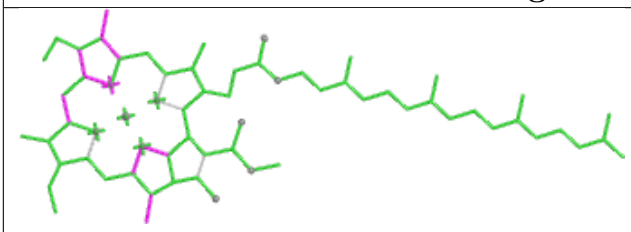


Rings

Ligand CLA a 839



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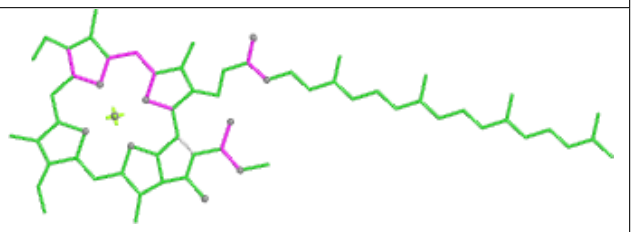
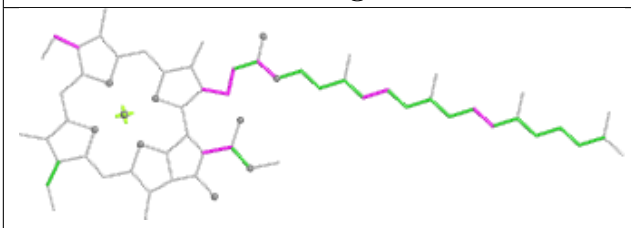


Bond angles



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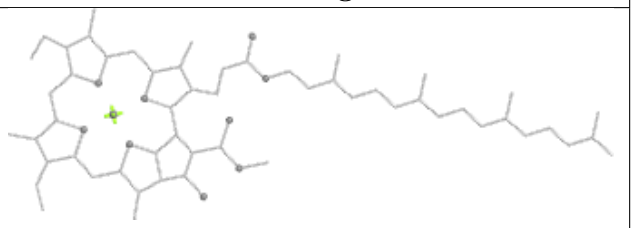
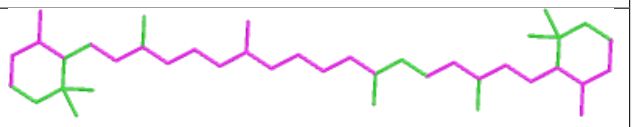


Rings

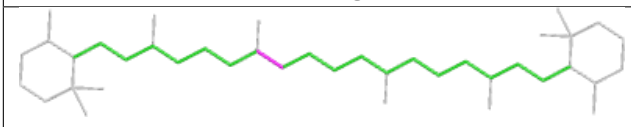
Ligand BCR f 205



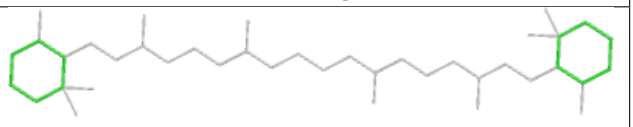
Bond lengths



Bond angles

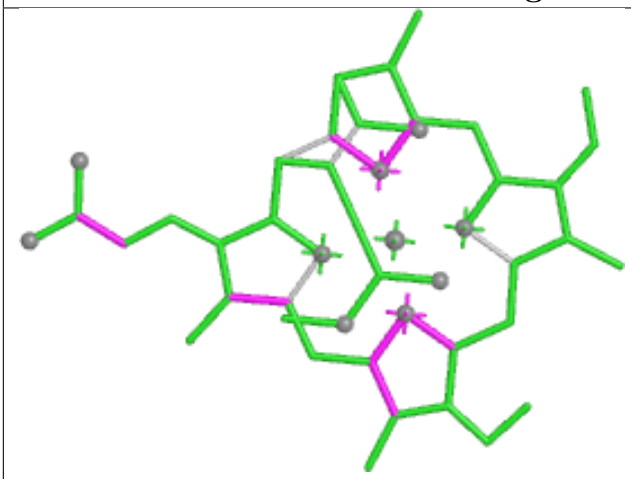


Torsions



Rings

Ligand KC1 H 312



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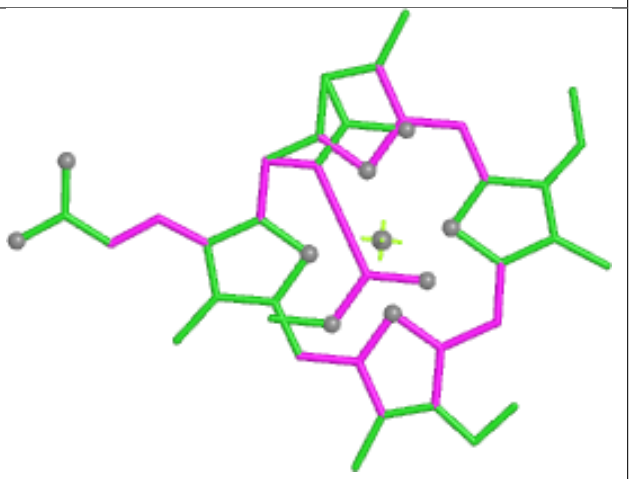
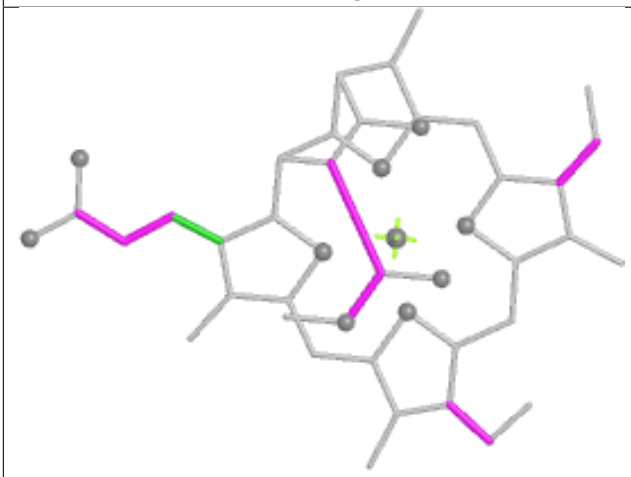


Bond angles



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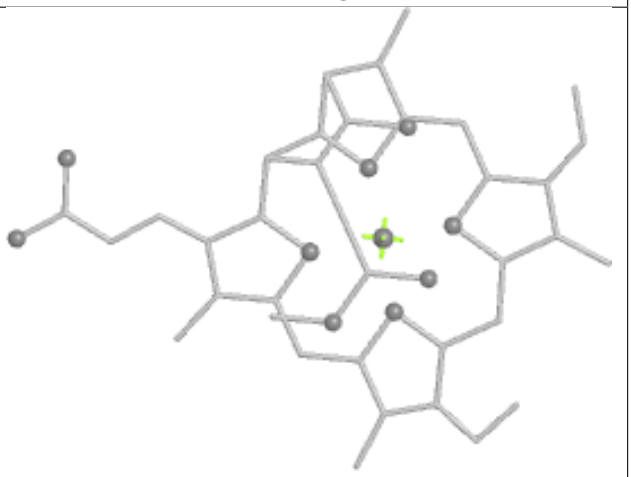
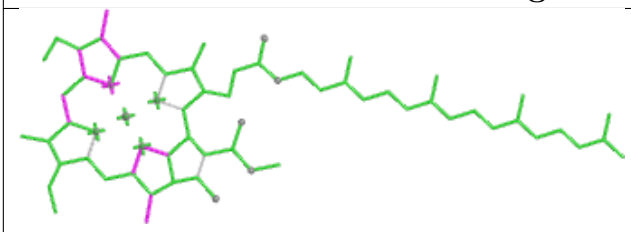


Rings

Ligand CLA a 815



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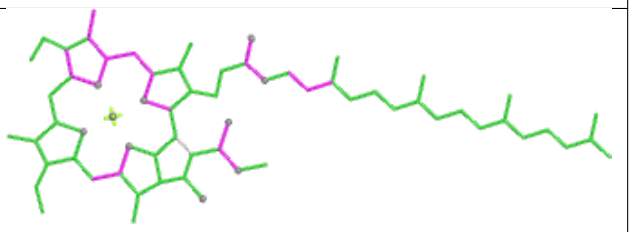
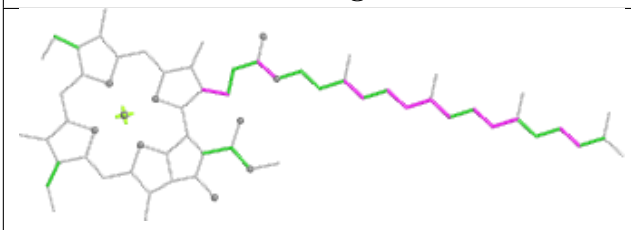


Bond angles



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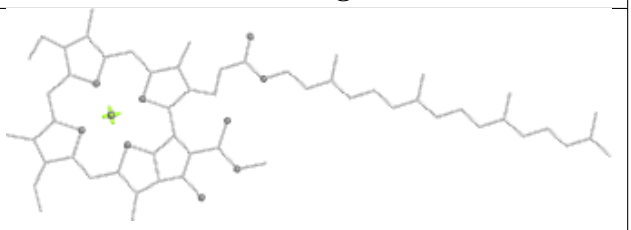
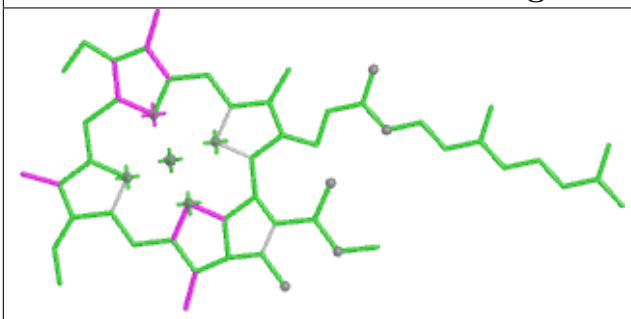
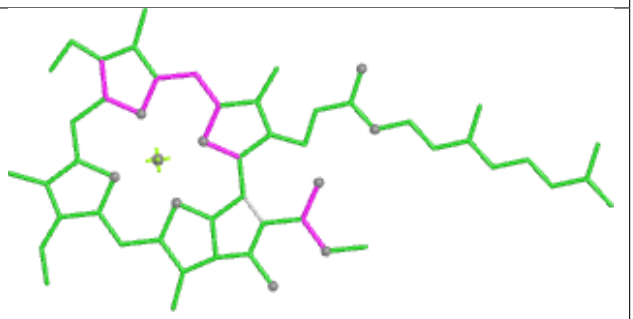


Rings

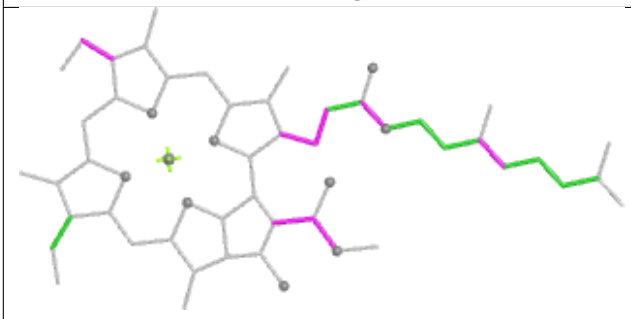
Ligand CLA b 813



Bond lengths



Bond angles



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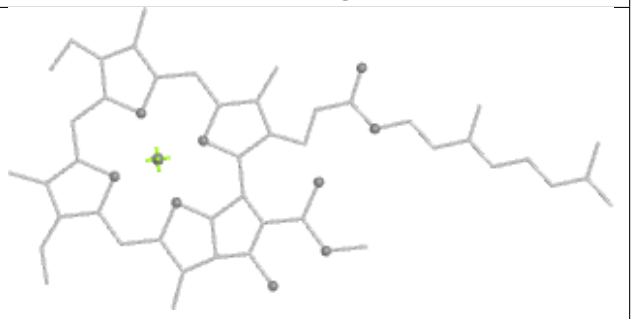
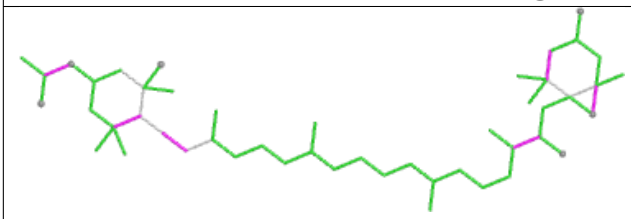
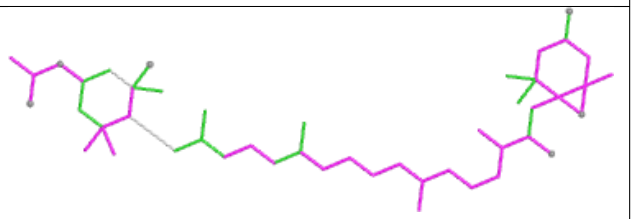


Rings

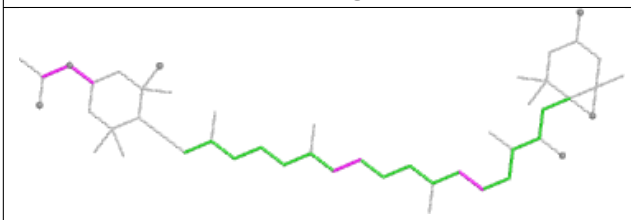
Ligand A86 E 302



Bond lengths



Bond angles



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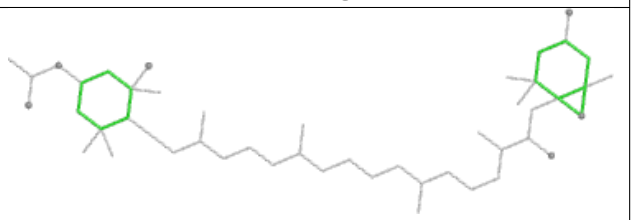
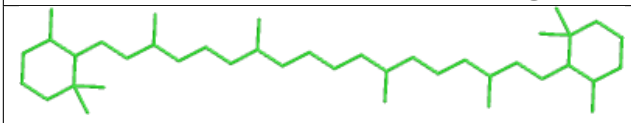
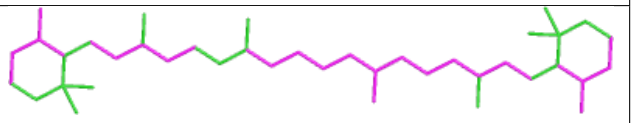


Rings

Ligand BCR b 832



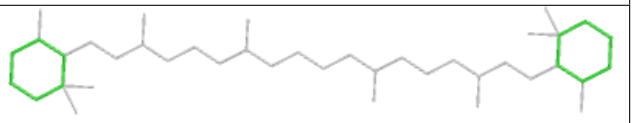
Bond lengths



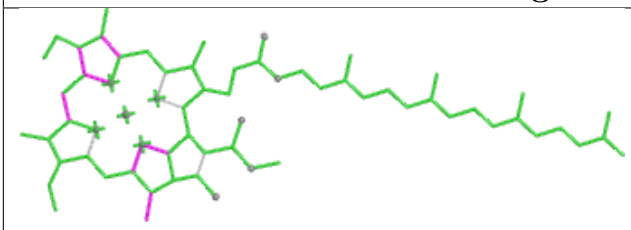
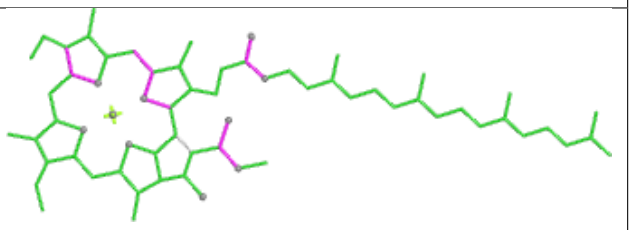
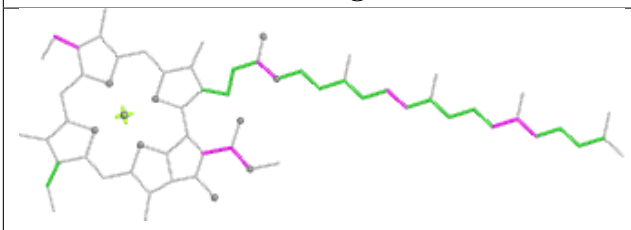
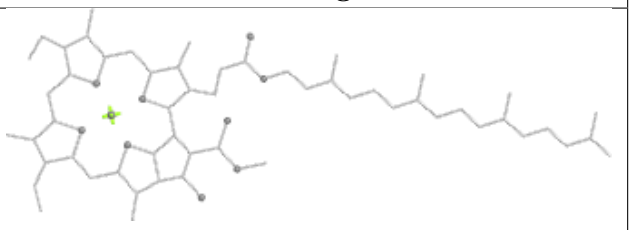
Bond angles

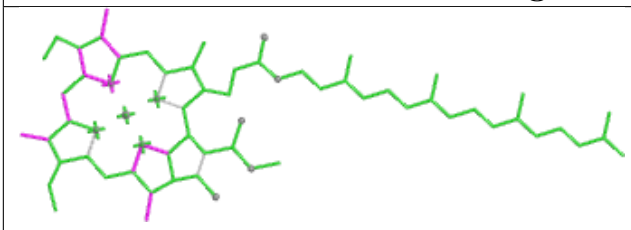
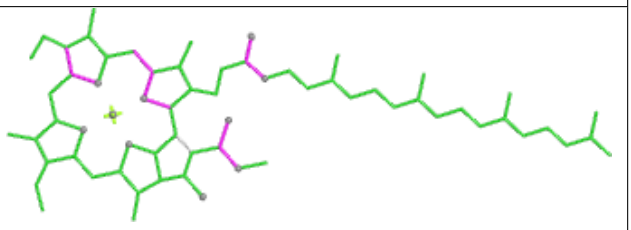
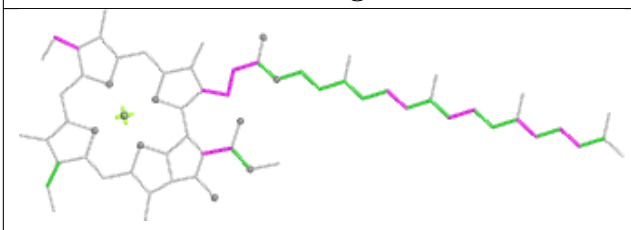
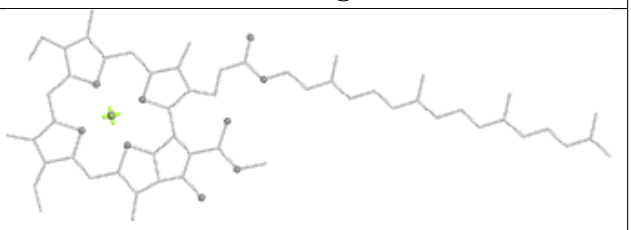


Torsions

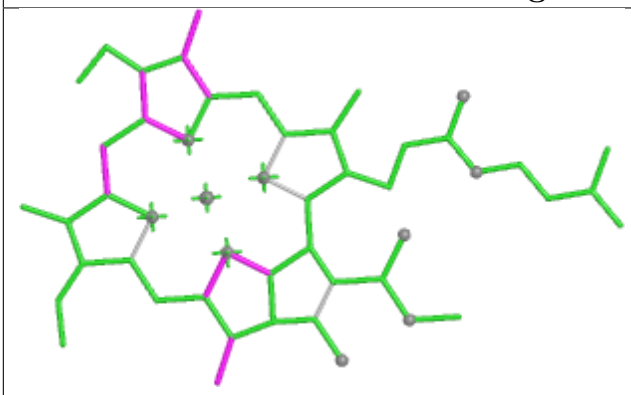


Rings

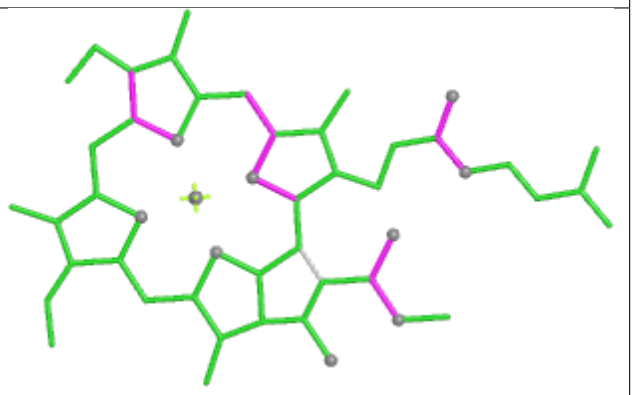
Ligand CLA f 203	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA a 808	
	
Bond lengths	Bond angles
	
Torsions	Rings

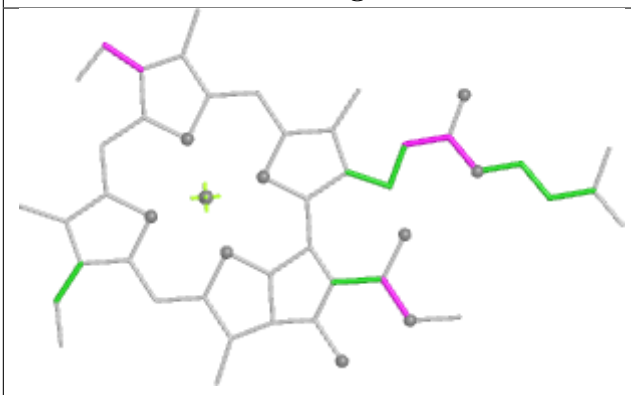
Ligand CLA a 822



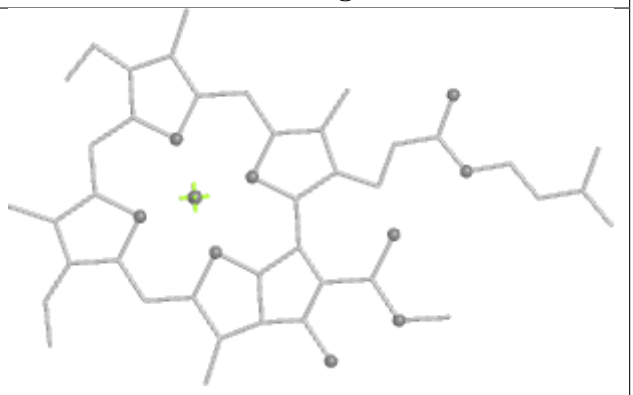
Bond lengths



Bond angles

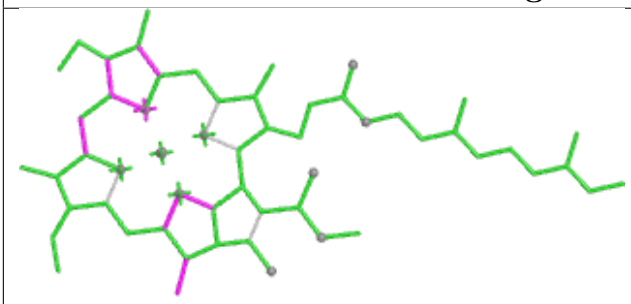


Torsions

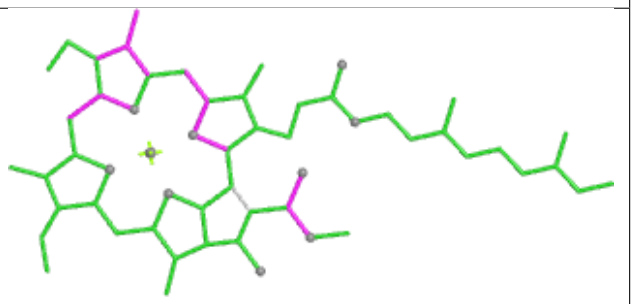


Rings

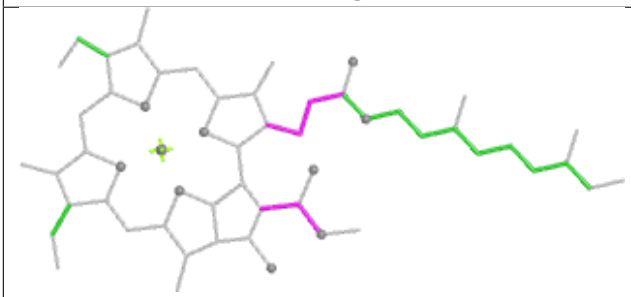
Ligand CLA E 316



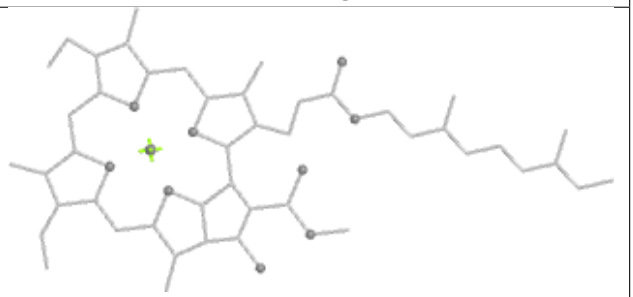
Bond lengths



Bond angles

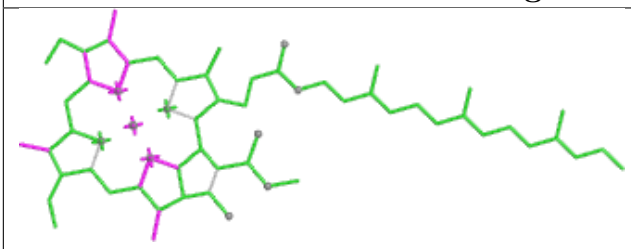


Torsions



Rings

Ligand CLA C 309



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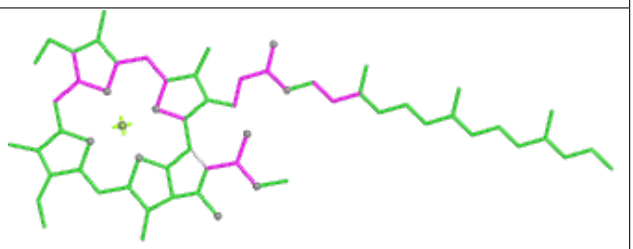

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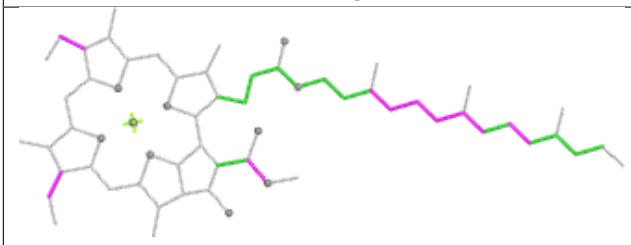

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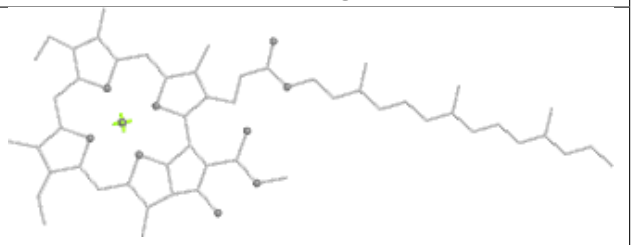
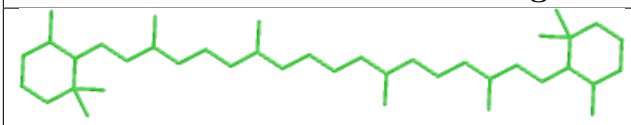


Rings

Ligand BCR j 105



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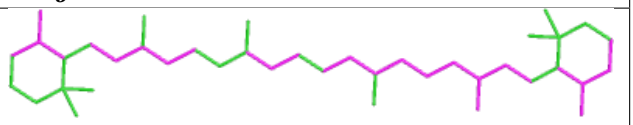
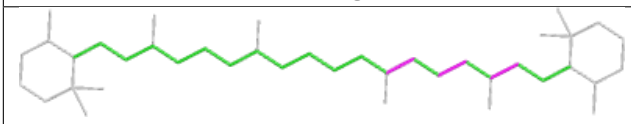


Bond angles



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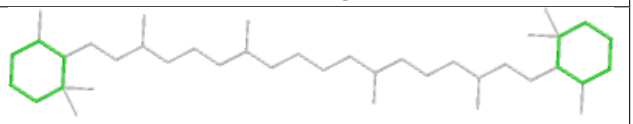
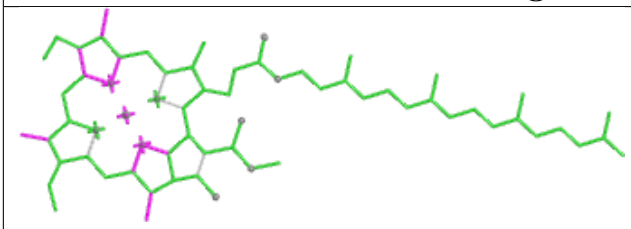


Rings

Ligand CLA b 824



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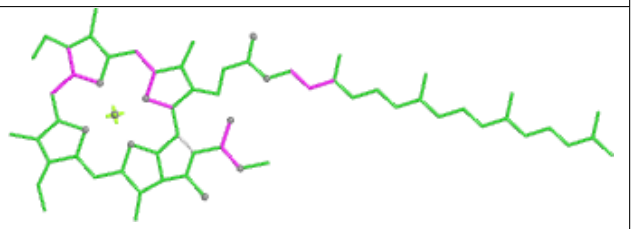
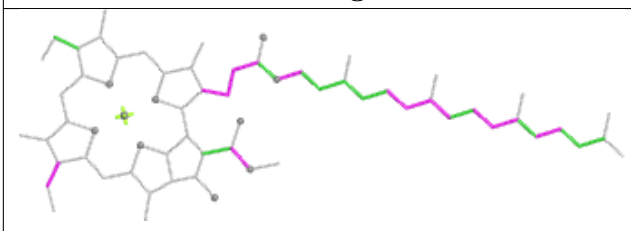


Bond angles



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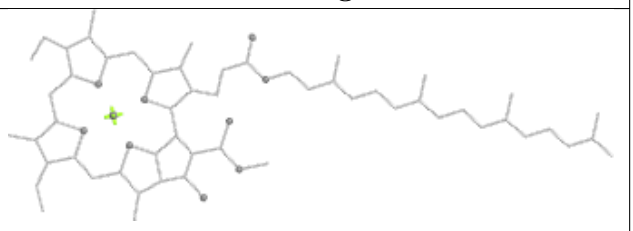
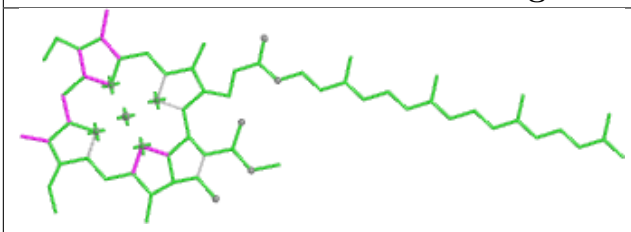


Rings

Ligand CLA a 821



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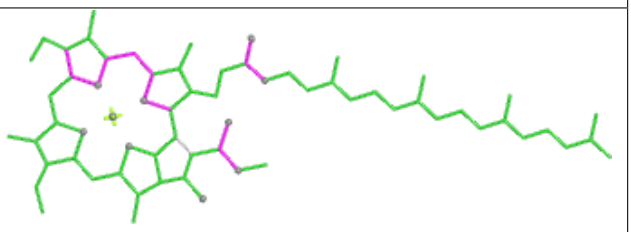
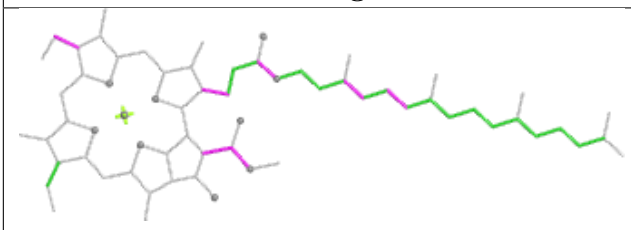


Bond angles



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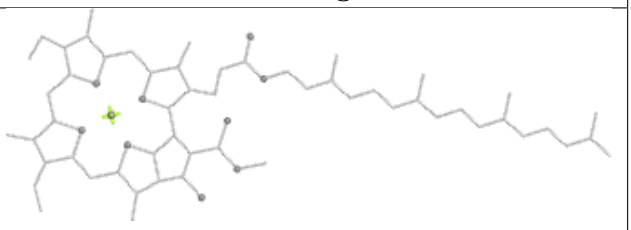
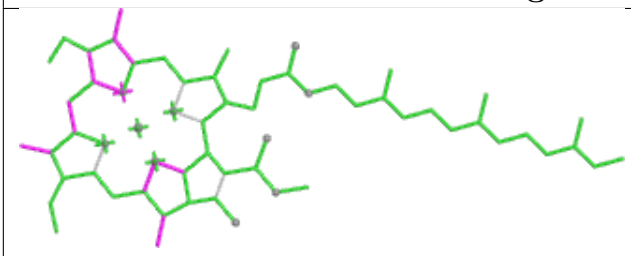


Rings

Ligand CLA b 840



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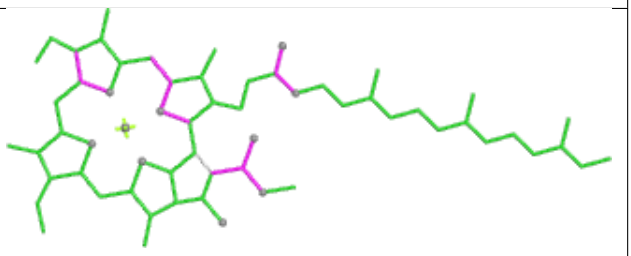
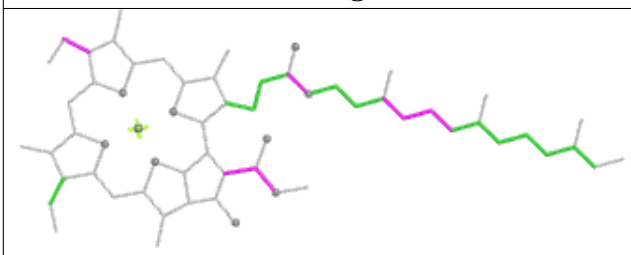


Bond angles



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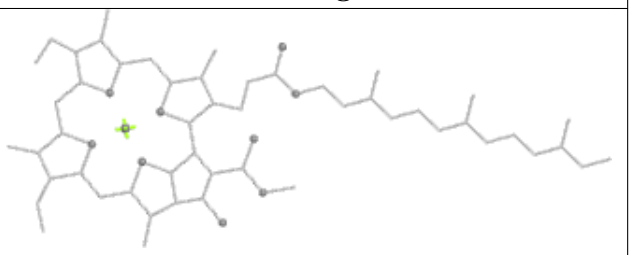
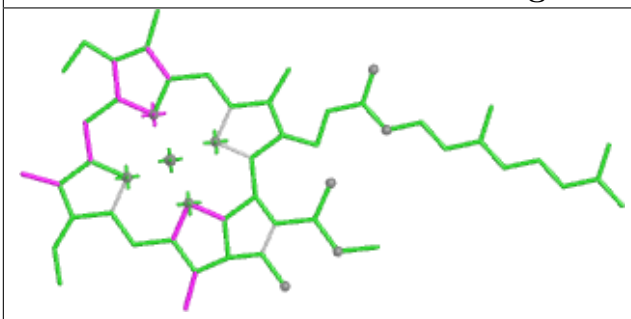


Rings

Ligand CLA a 804



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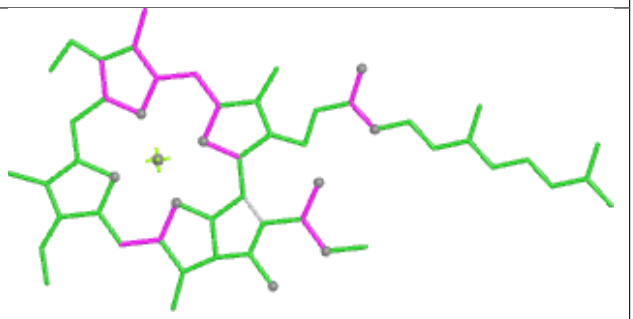
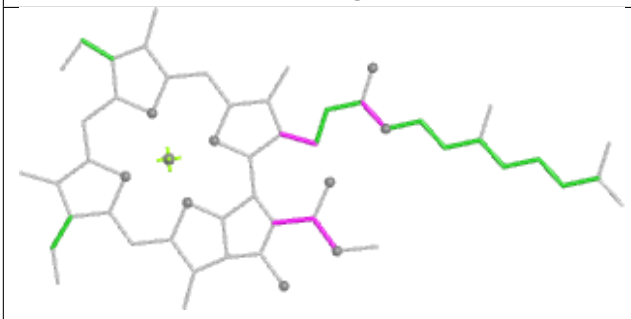


Bond angles



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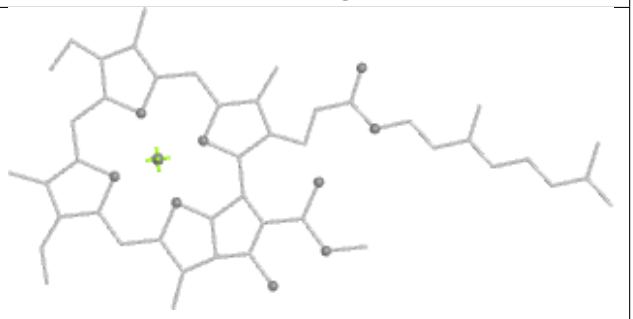
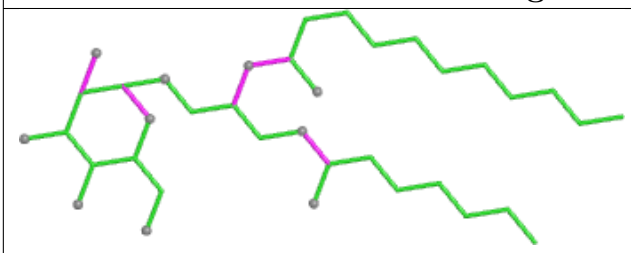


Rings

Ligand LMG j 103



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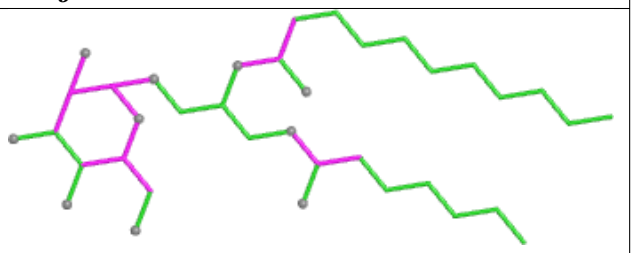
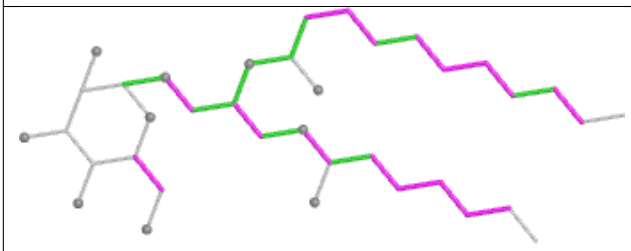


Bond angles



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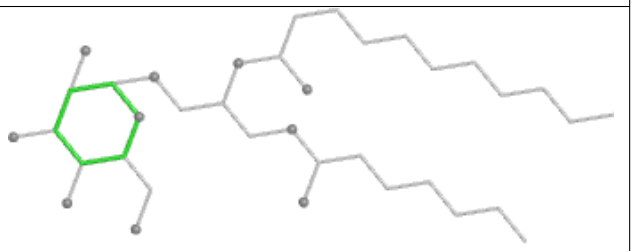
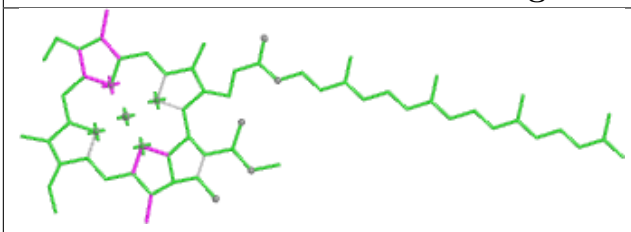


Rings

Ligand CLA a 820



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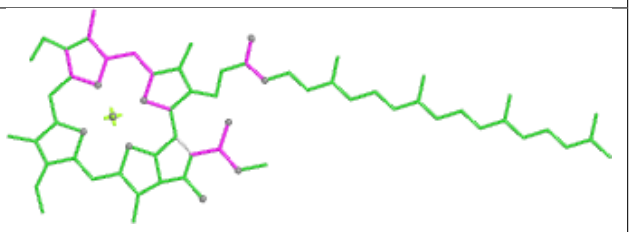
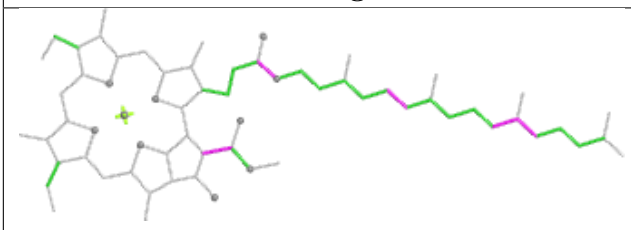


Bond angles



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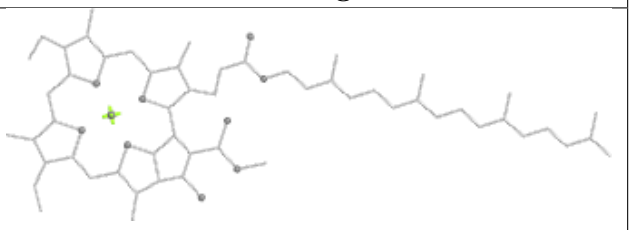
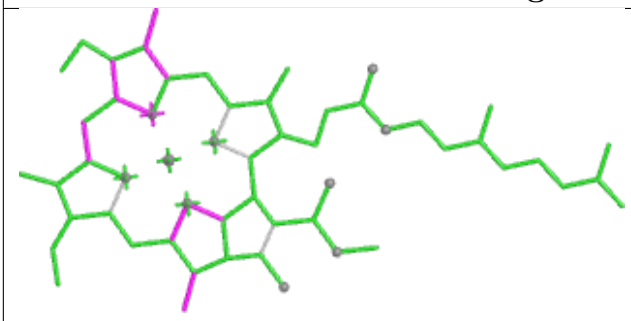
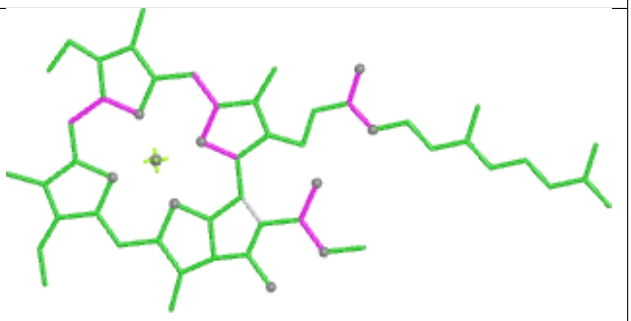


Rings

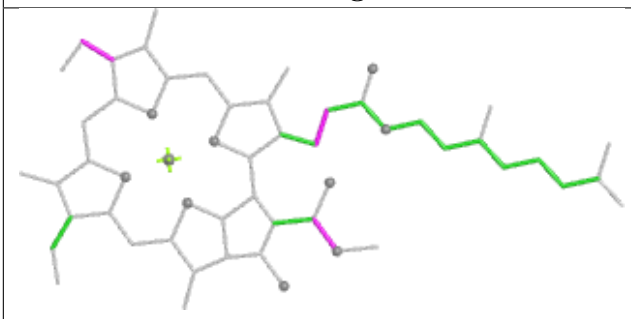
Ligand CLA b 816



Bond lengths



Bond angles



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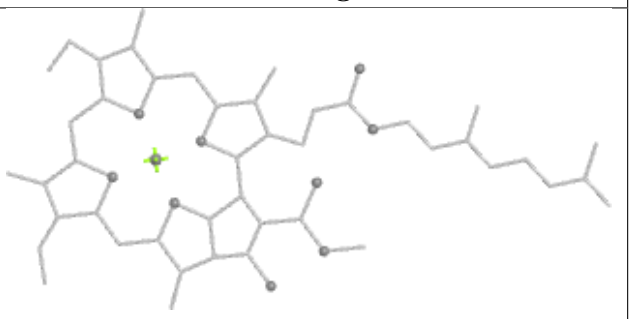
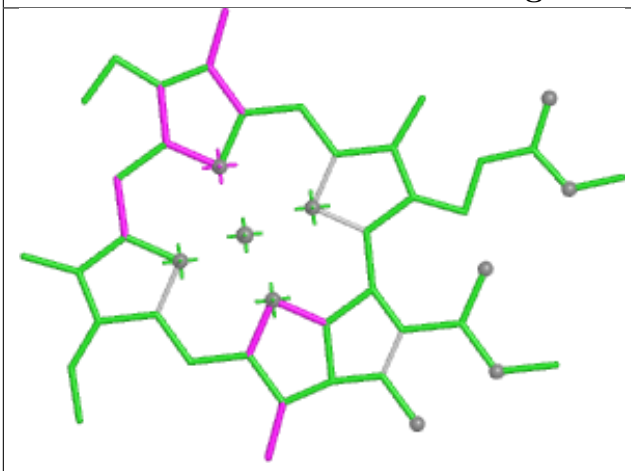


Rings

Ligand CLA E 311



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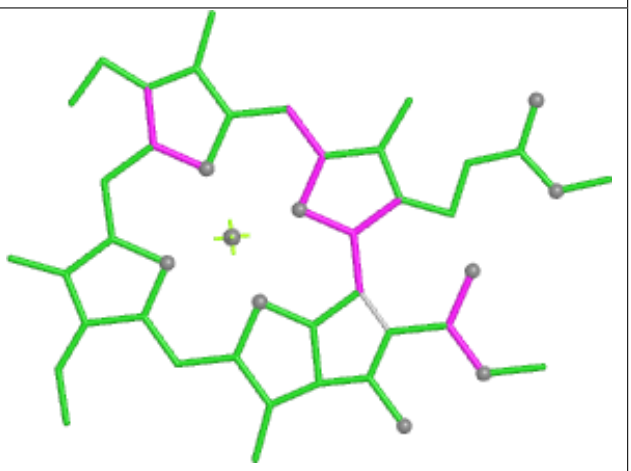
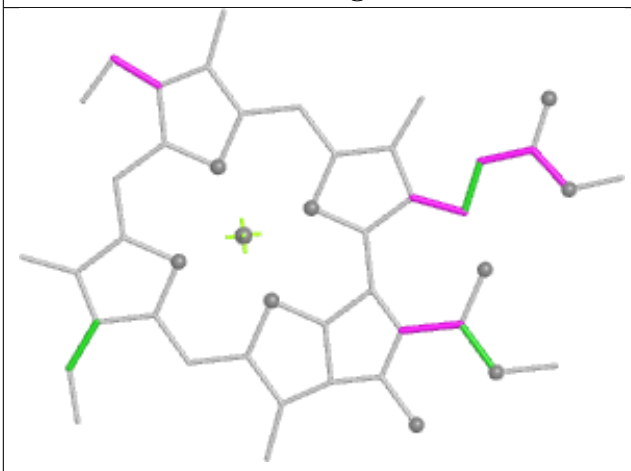


Bond angles



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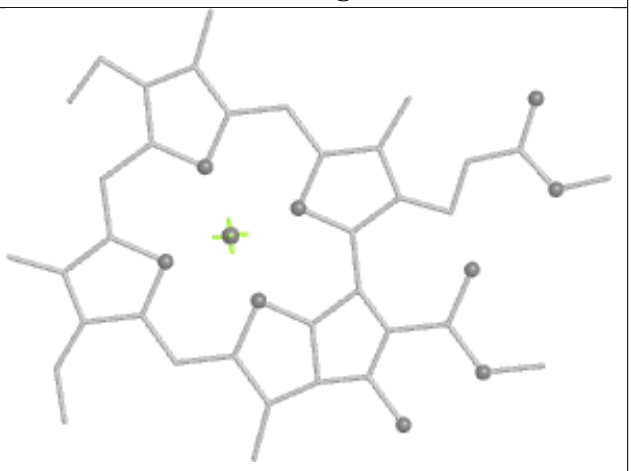
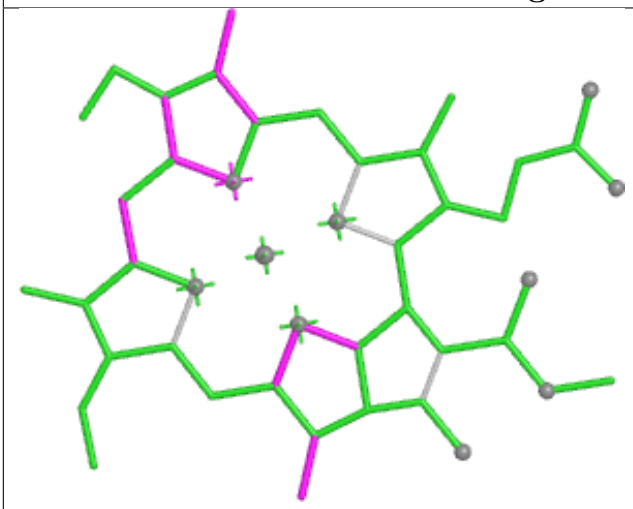


Rings

Ligand CLA a 816



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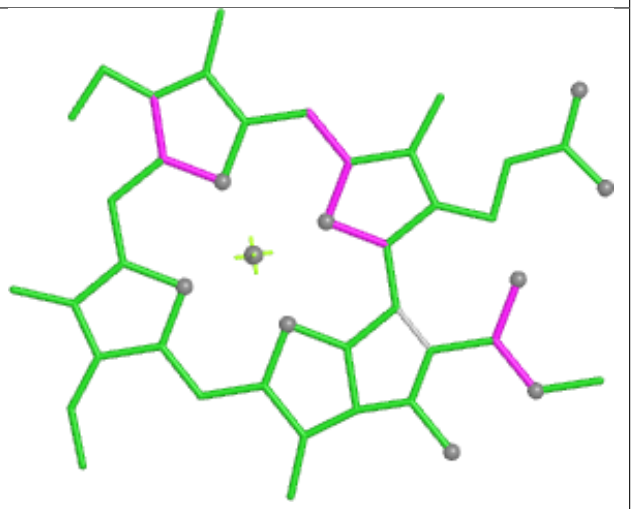
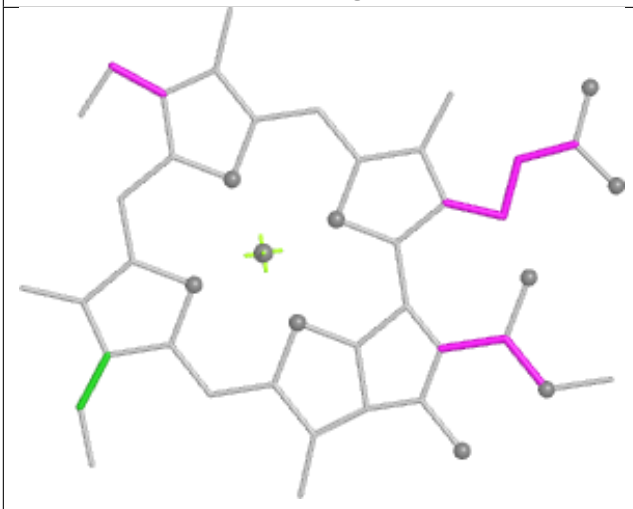


Bond angles

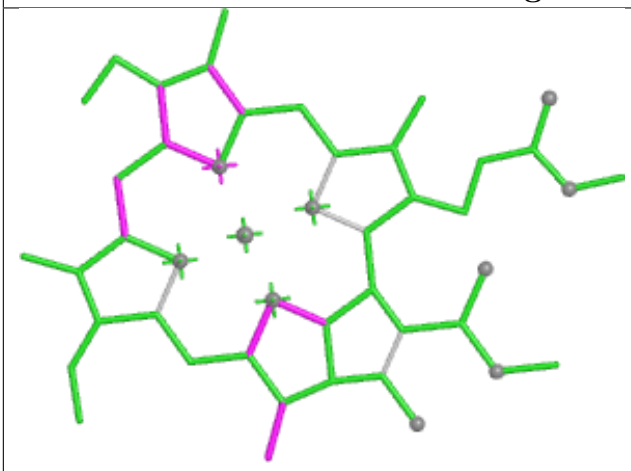


Torsions



Rings

Ligand CLA B 310



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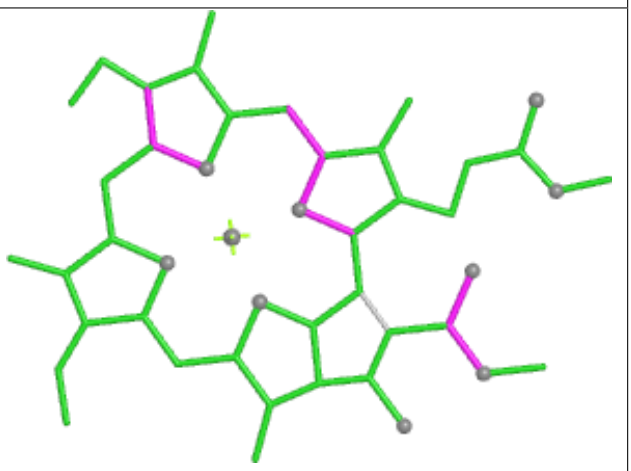
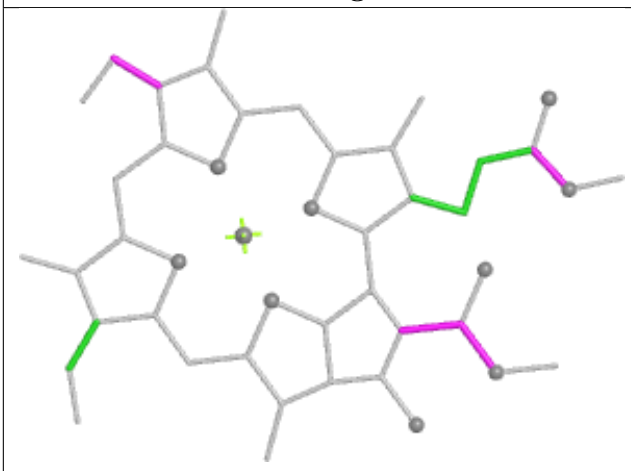


Bond angles



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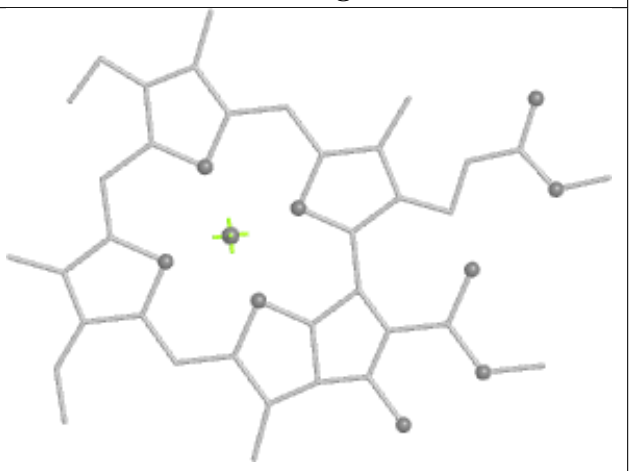
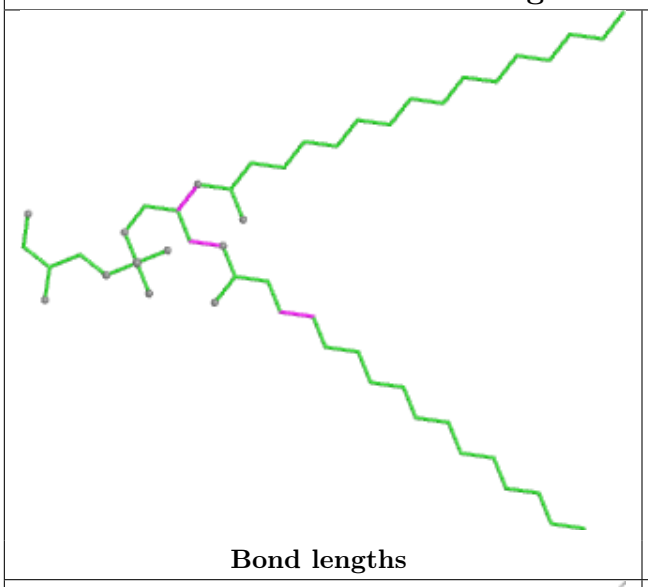


Rings

Ligand LHG b 835



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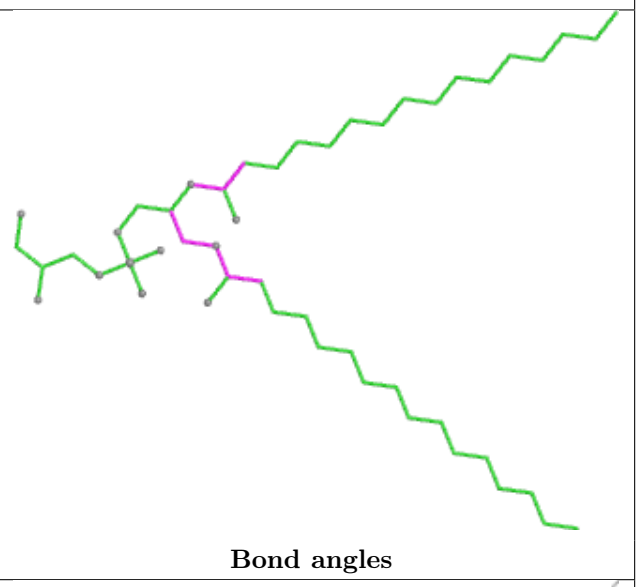
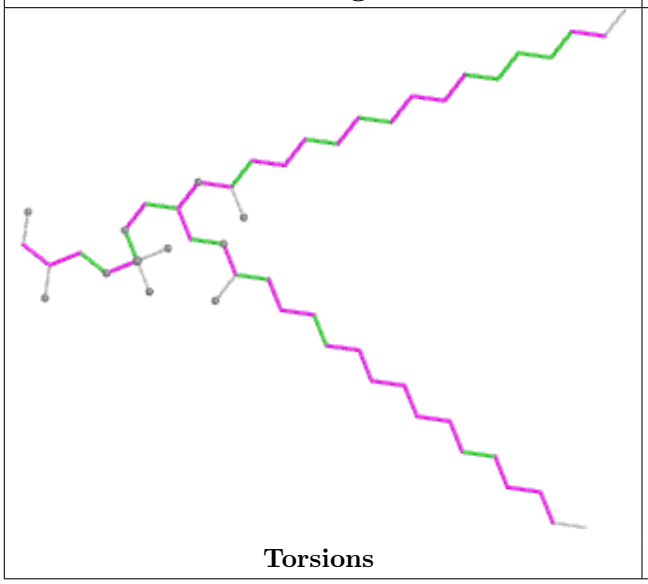


Bond angles



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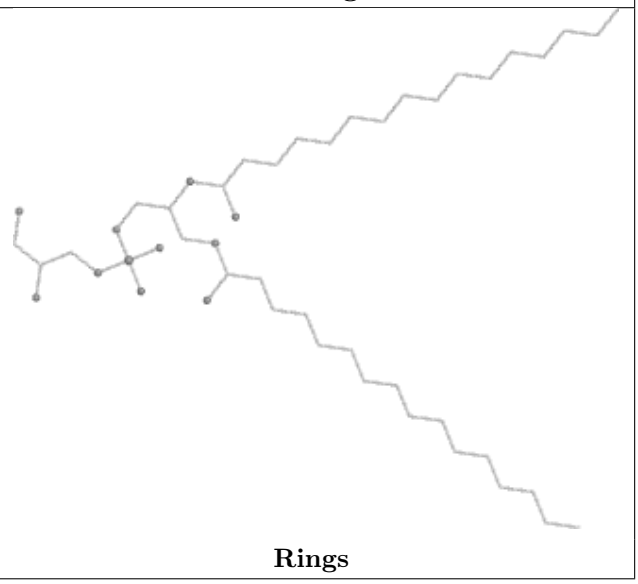
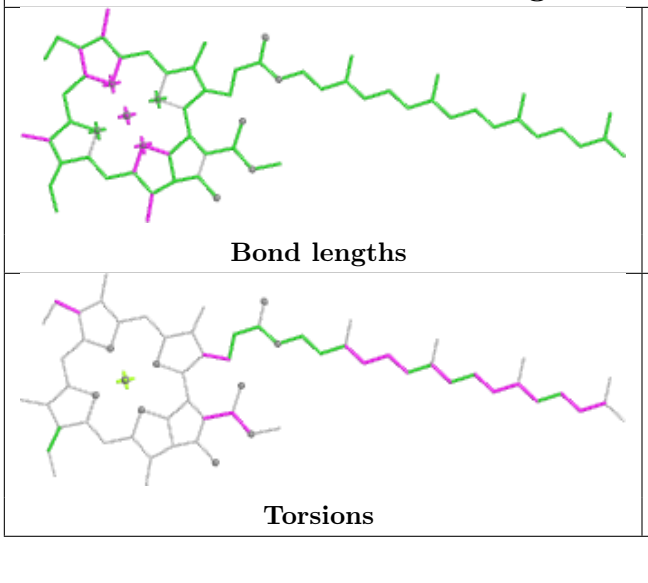
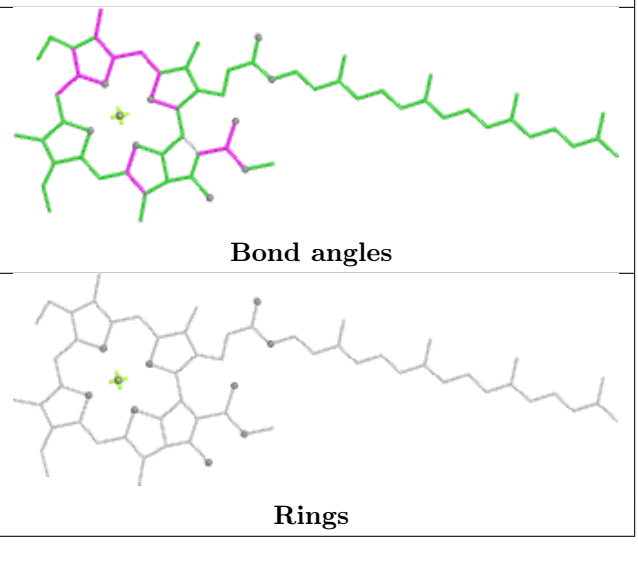


Rings

Ligand CLA b 843



Bond lengths

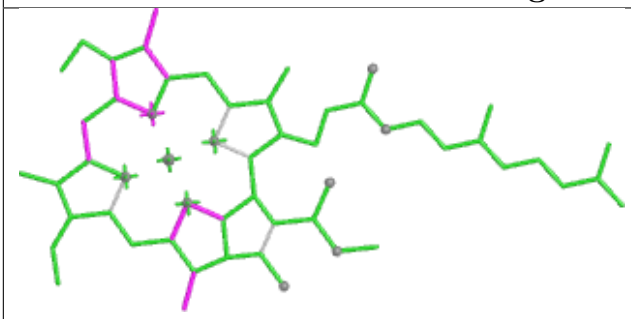


Bond angles

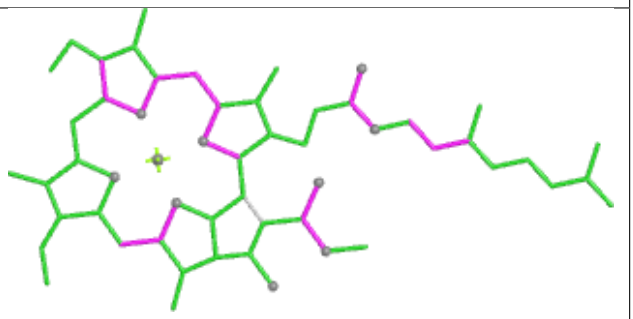
Torsions

Rings

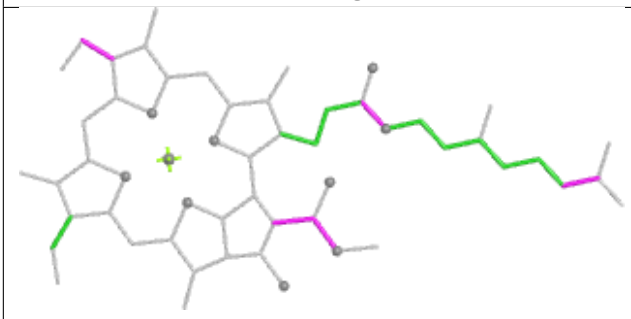
Ligand CLA a 853



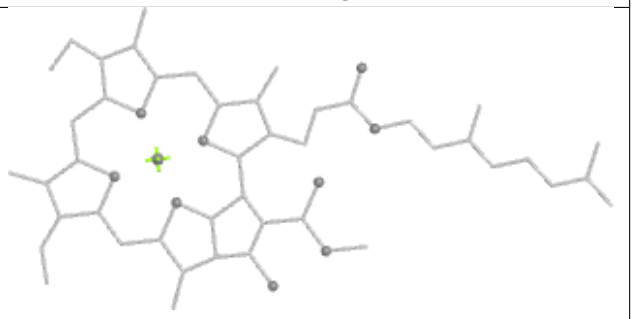
Bond lengths



Bond angles

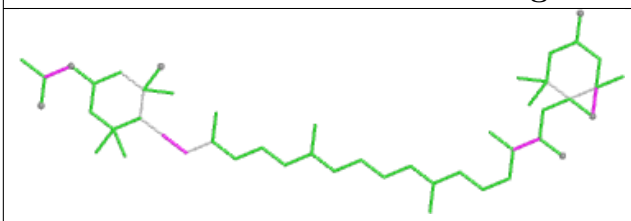


Torsions



Rings

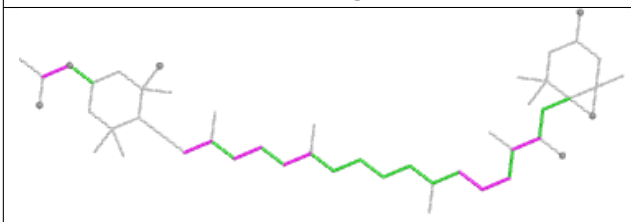
Ligand A86 B 301



Bond lengths



Bond angles



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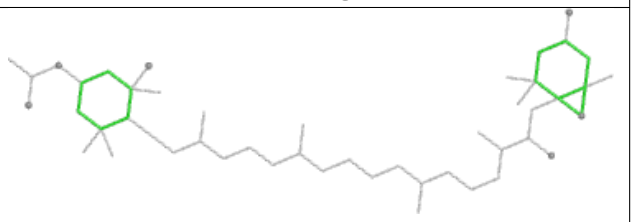
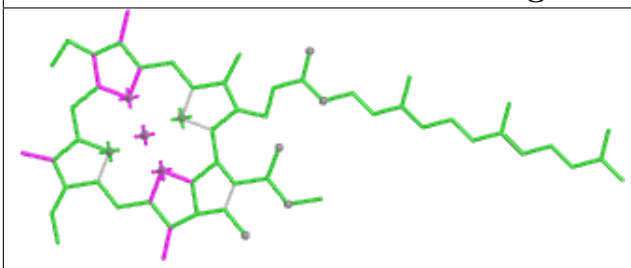


Rings

Ligand CLA b 837



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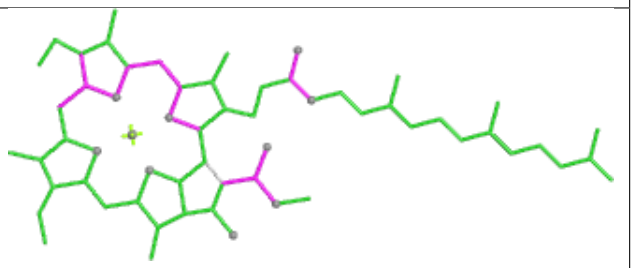
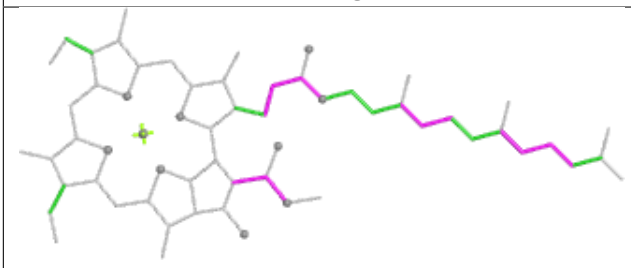


Bond angles



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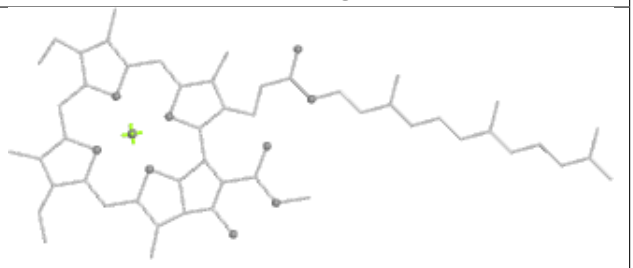
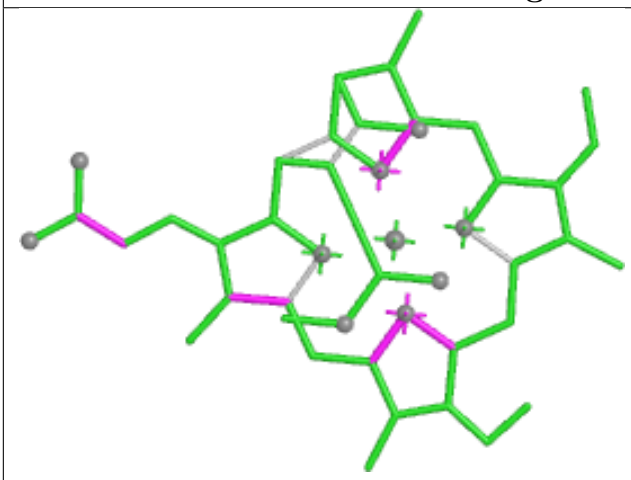


Rings

Ligand KC1 C 308



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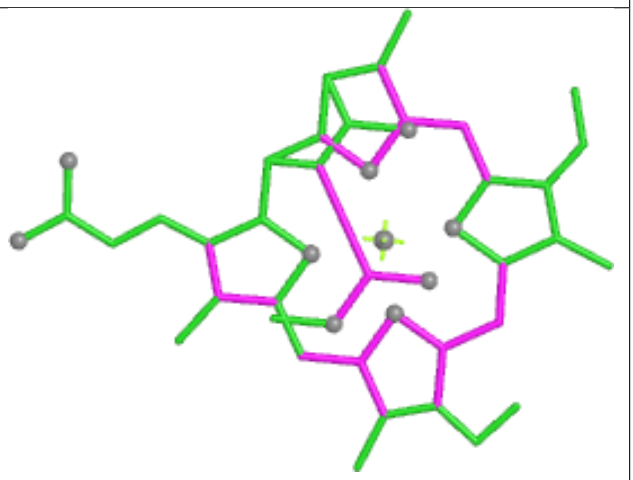
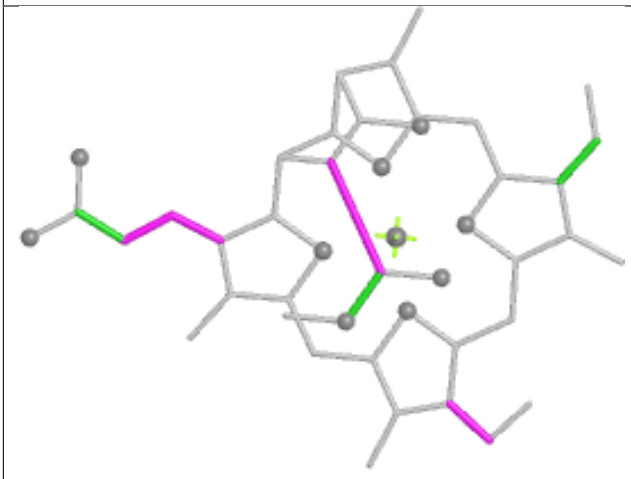


Bond angles



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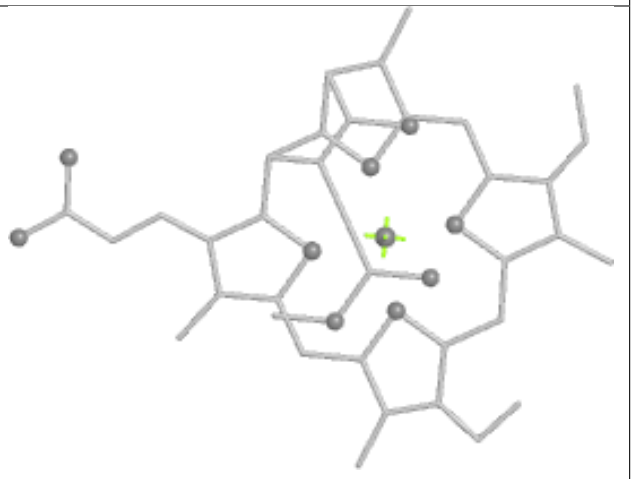
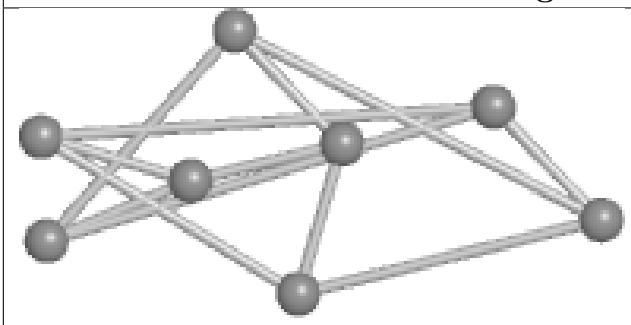


Rings

Ligand SF4 c 101



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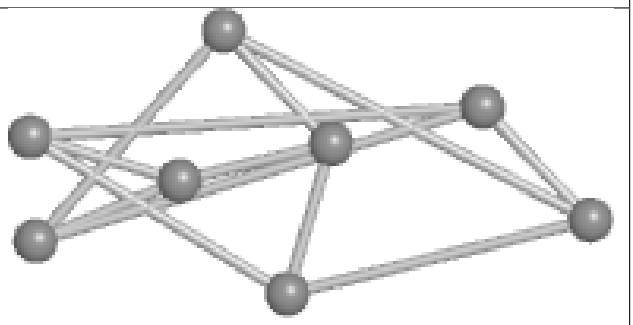

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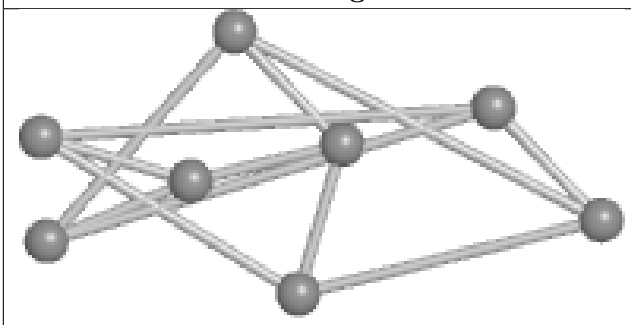

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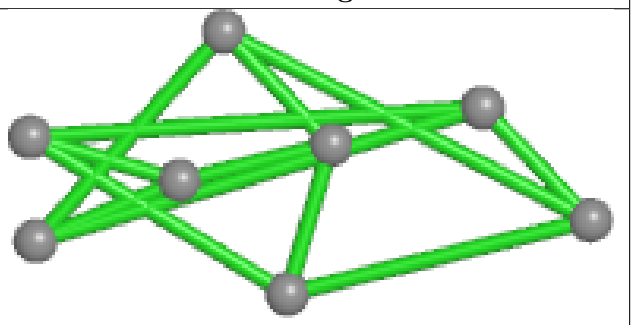
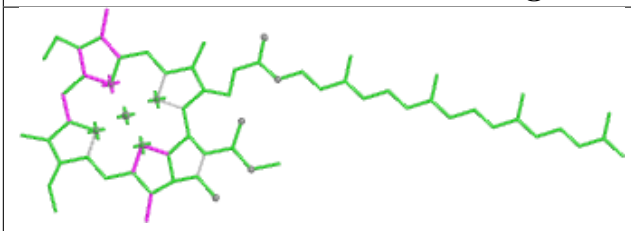


Rings

Ligand CLA E 310



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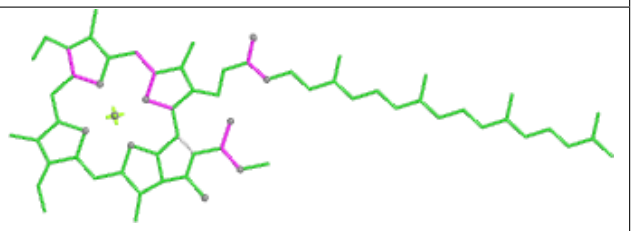
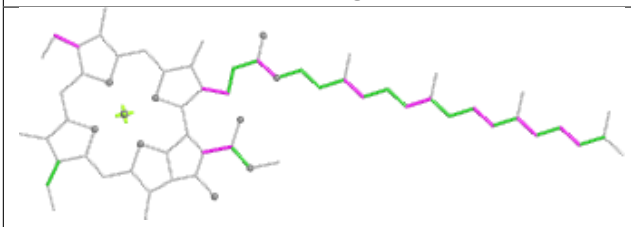


Bond angles



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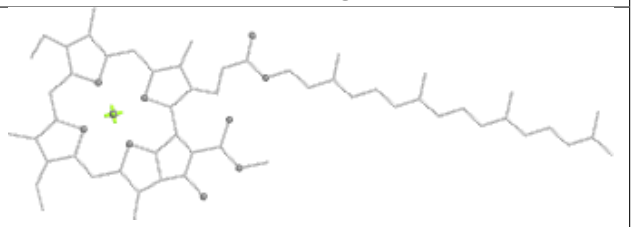
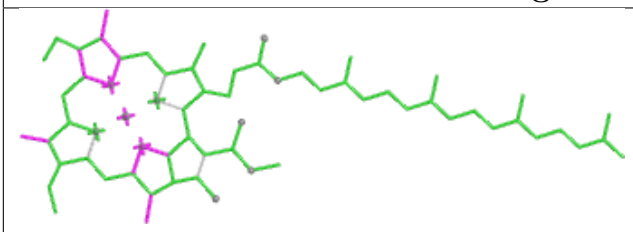


Rings

Ligand CLA l 203



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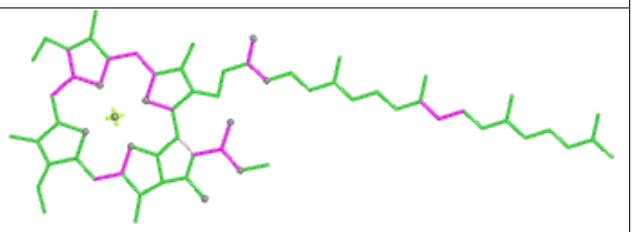
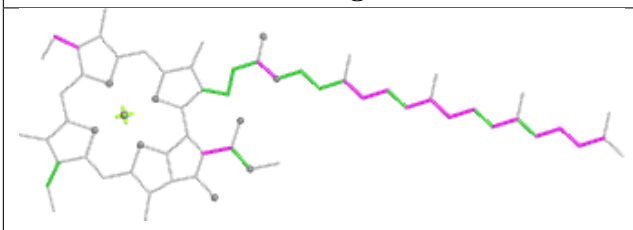


Bond angles



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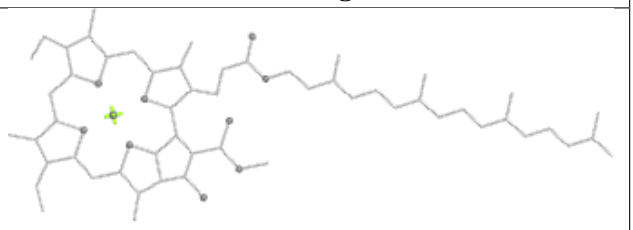
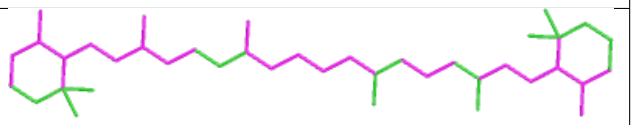


Rings

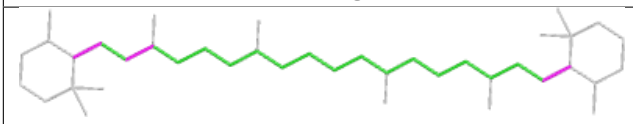
Ligand BCR b 839



Bond lengths



Bond angles



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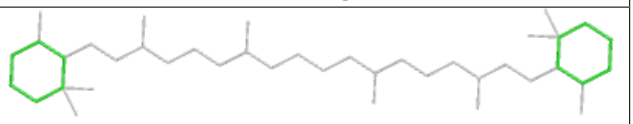
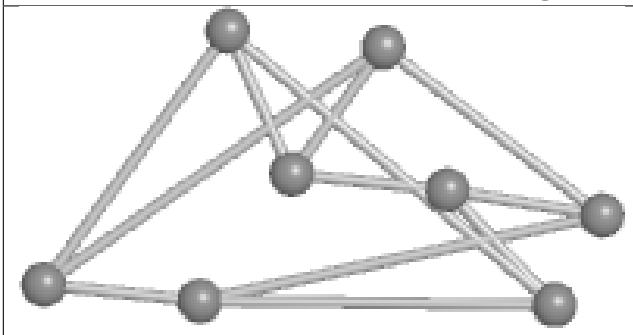


Rings

Ligand SF4 c 102



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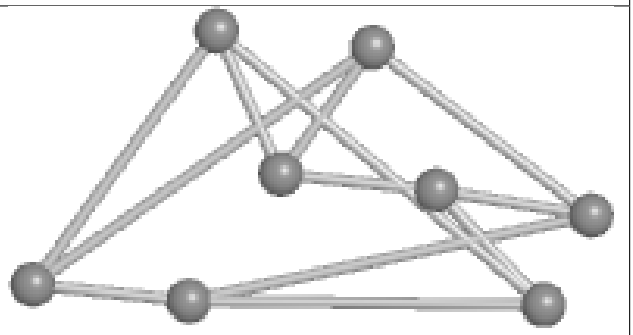

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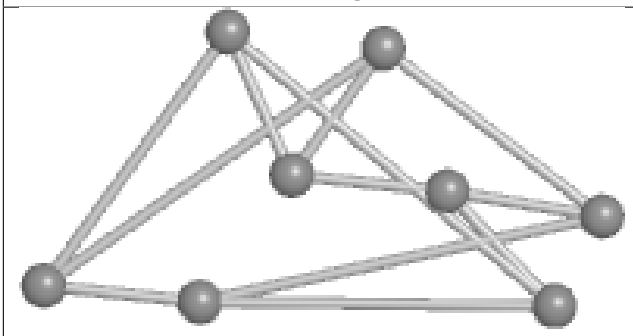

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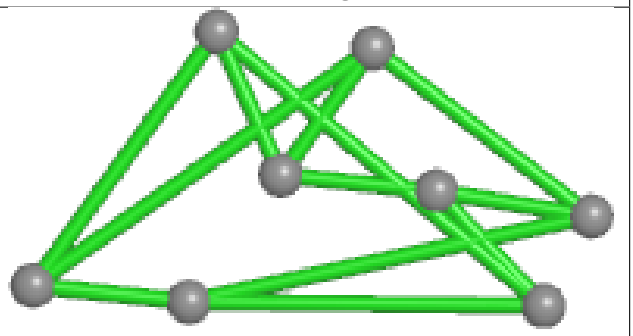
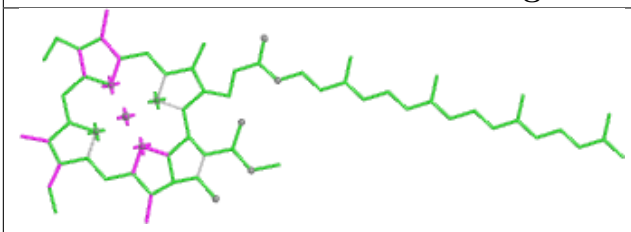


Rings

Ligand CLA H 306



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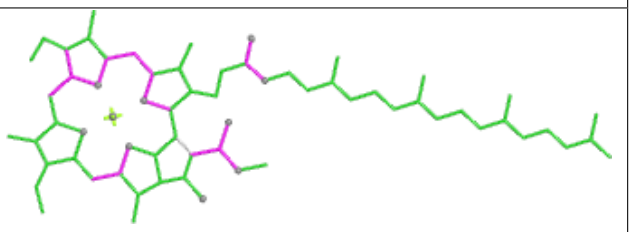
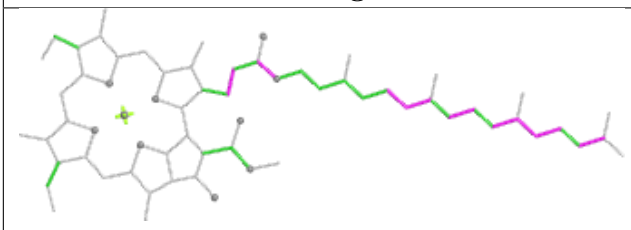


Bond angles



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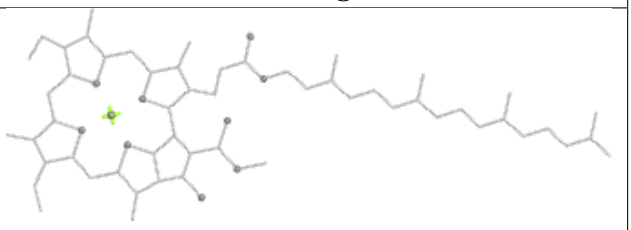
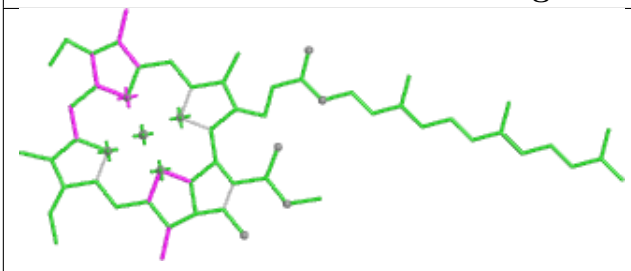


Rings

Ligand CLA i 101



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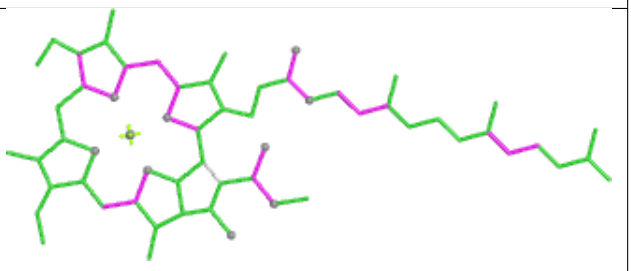
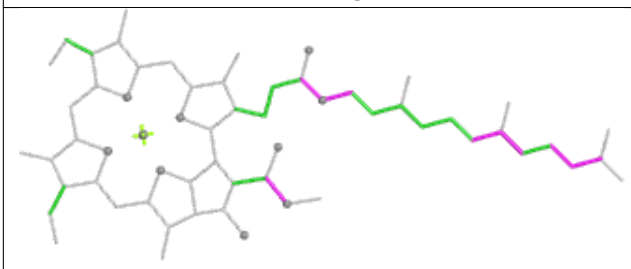


Bond angles



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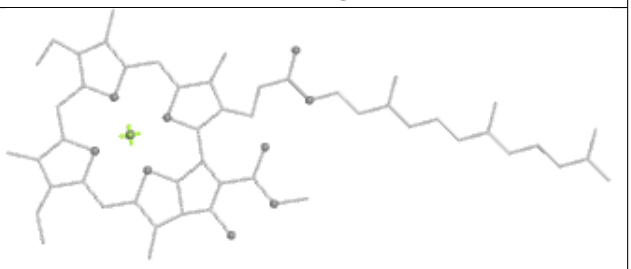
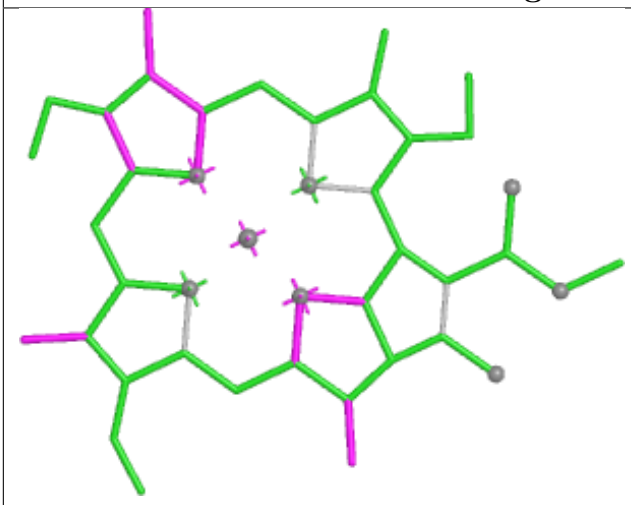


Rings

Ligand CLA C 317



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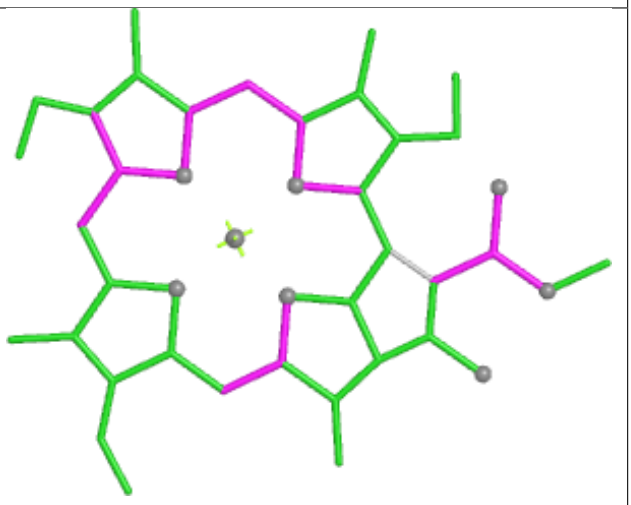
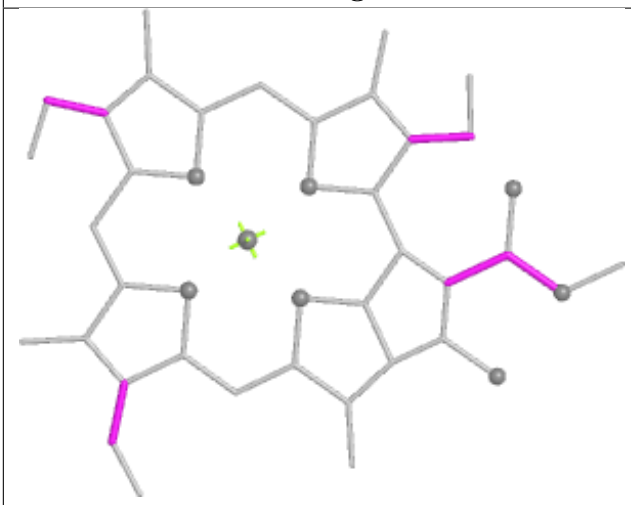


Bond angles

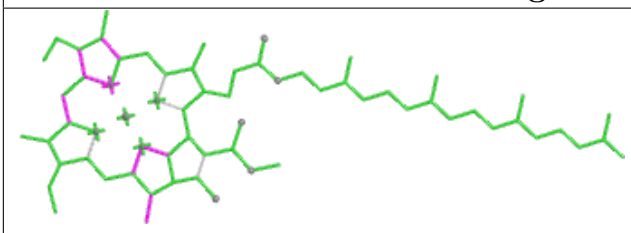


Torsions



Rings

Ligand CLA a 855



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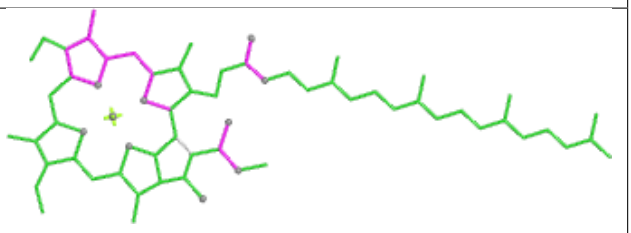

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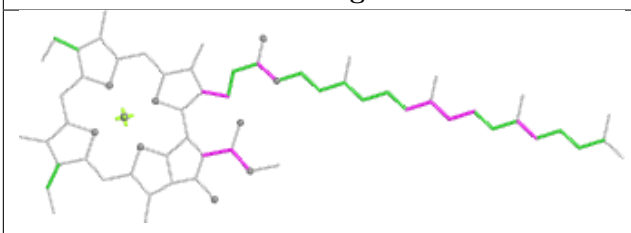

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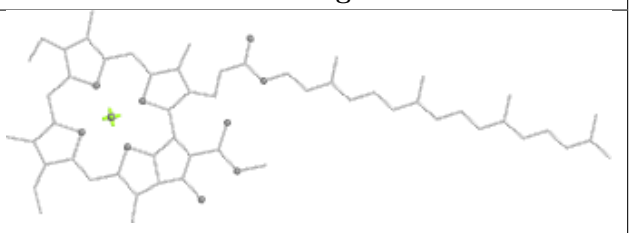
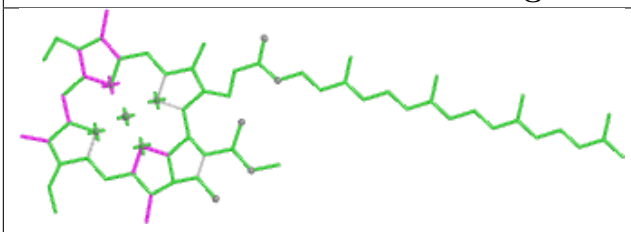
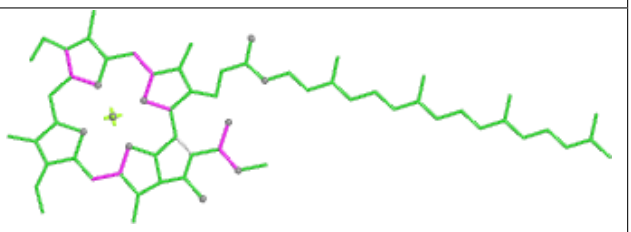
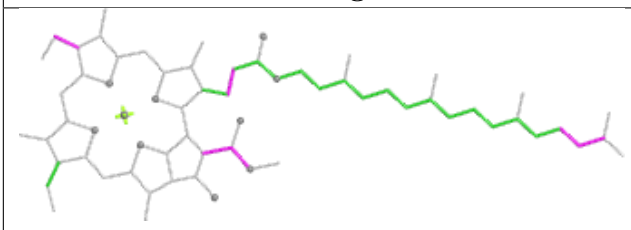
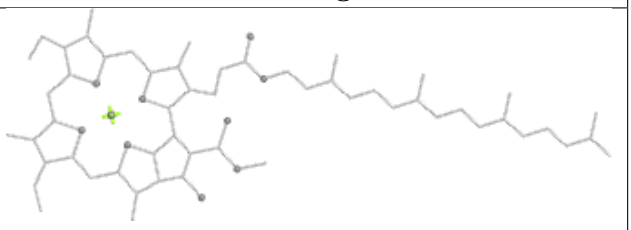
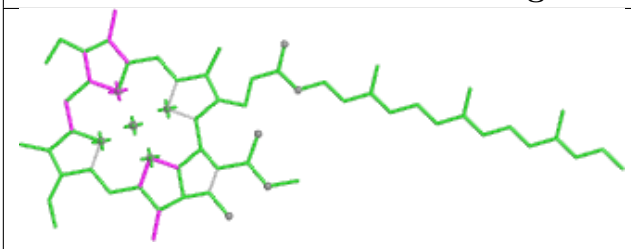
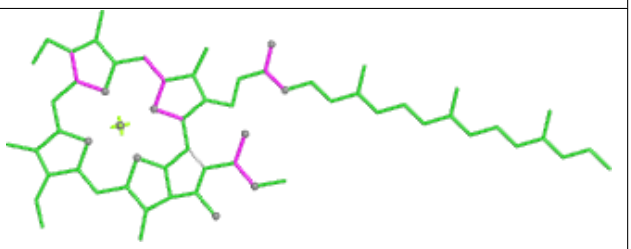
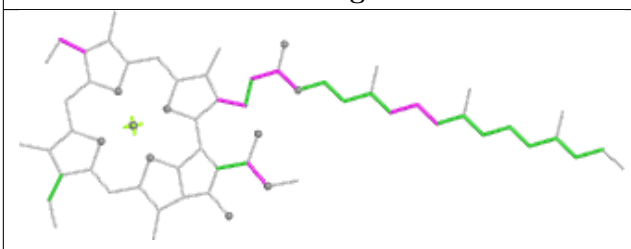
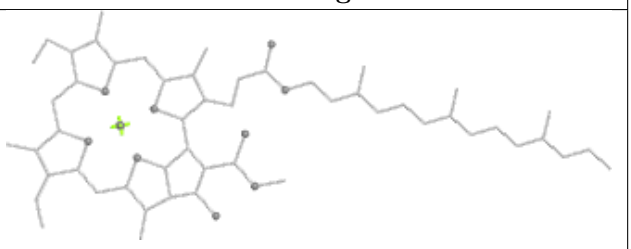
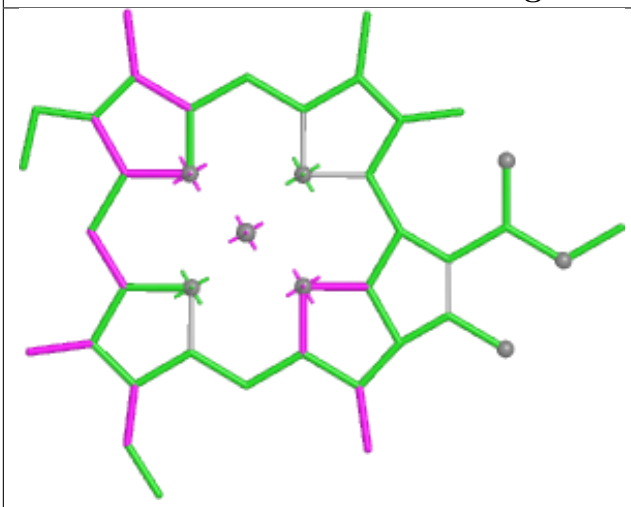


Rings

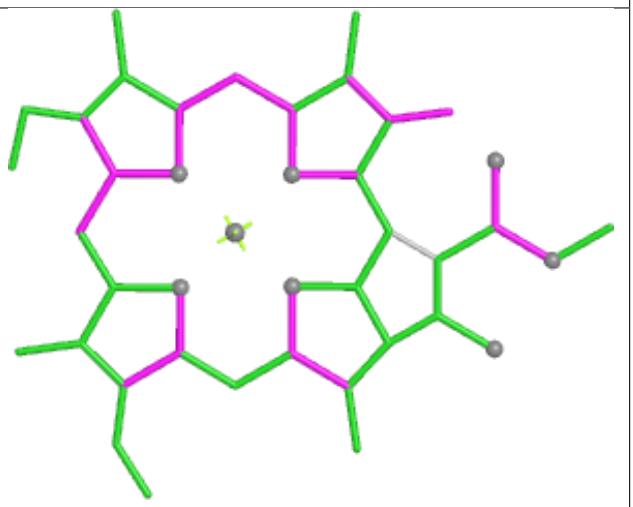
Ligand CLA B 307	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA b 844	
	
Bond lengths	Bond angles
	
Torsions	Rings

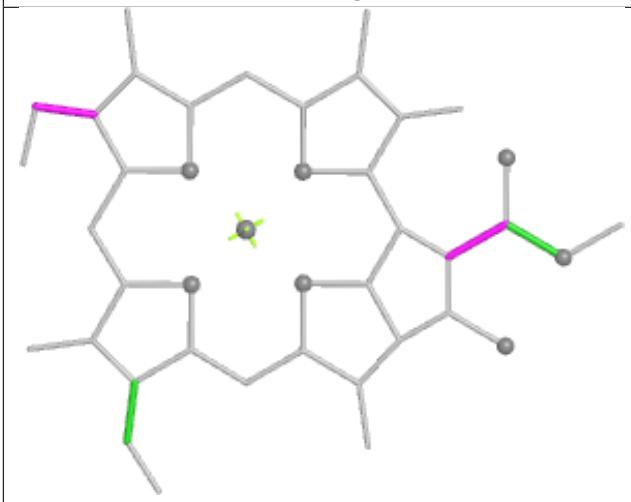
Ligand CLA C 316



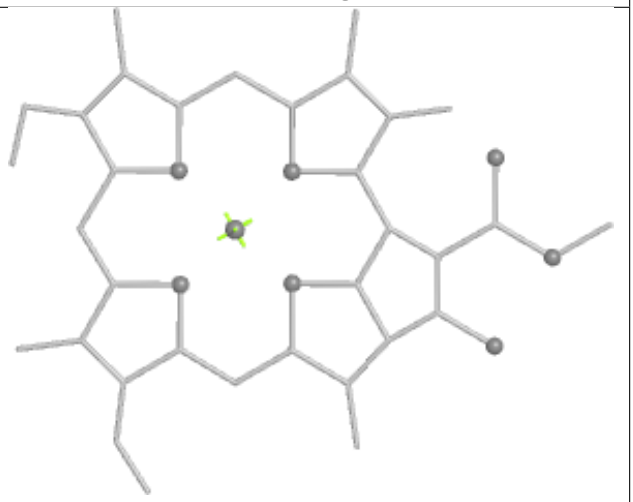
Bond lengths



Bond angles

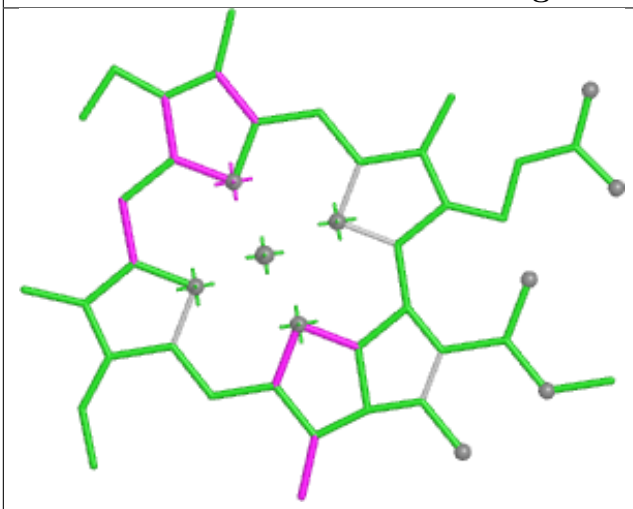


Torsions

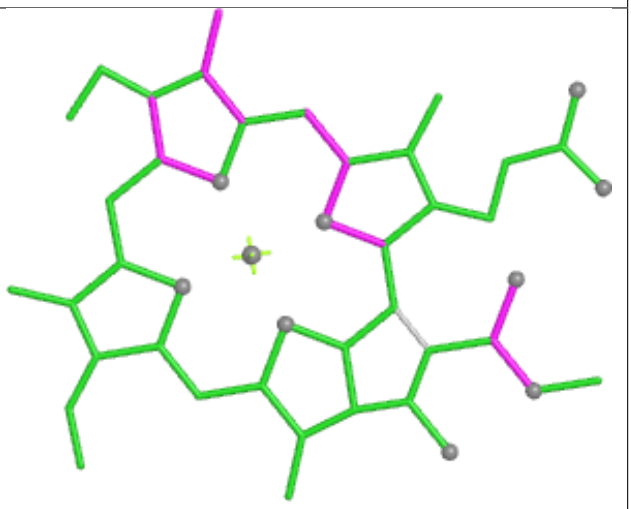


Rings

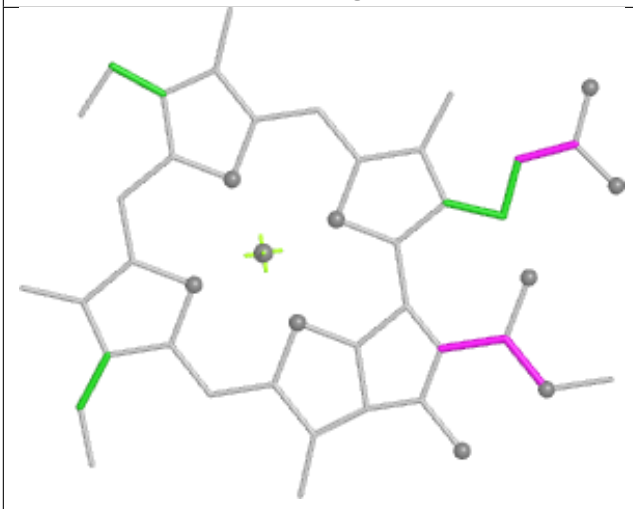
Ligand CLA l 205



Bond lengths



Bond angles

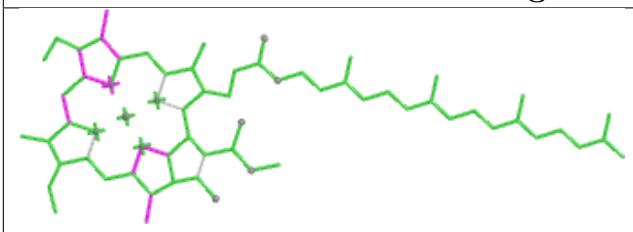


Torsions



Rings

Ligand CLA a 846



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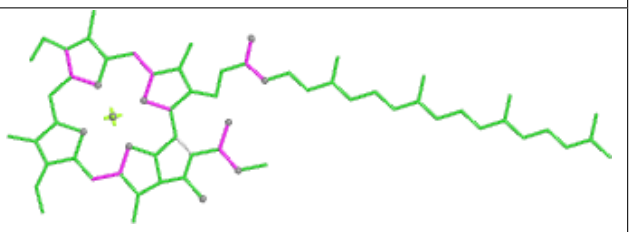
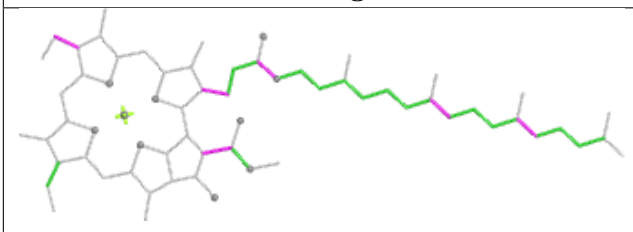


Bond angles



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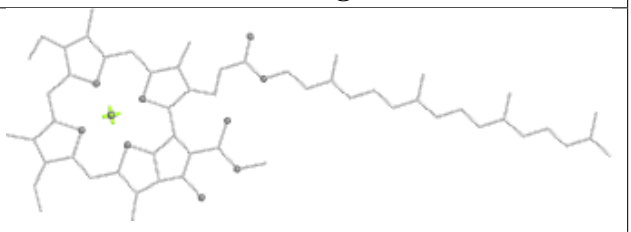
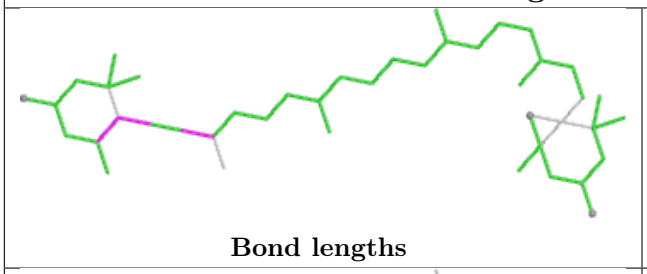


Rings

Ligand DD6 E 307



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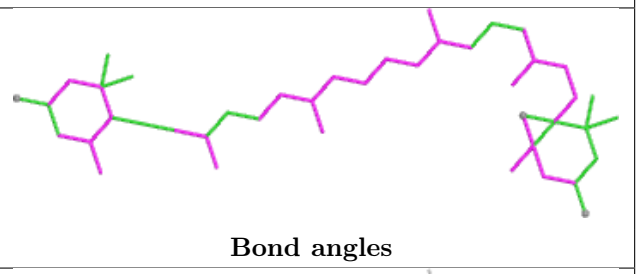
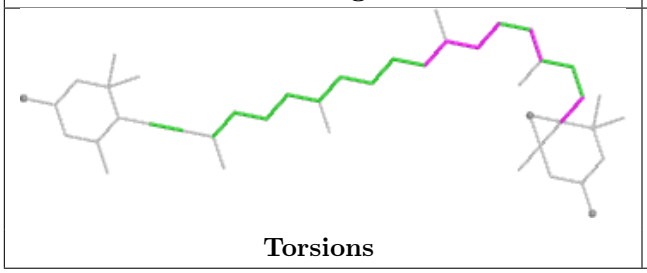


Bond angles



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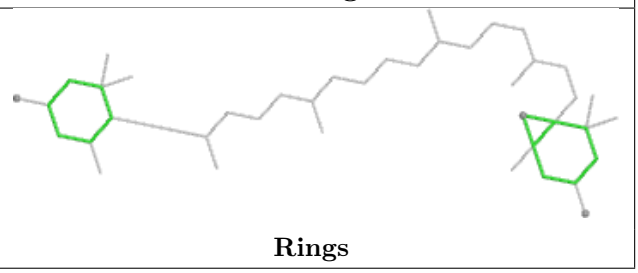
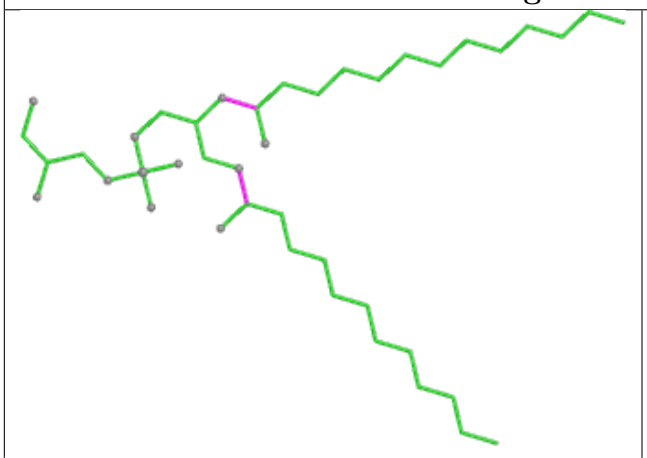


Rings

Ligand LHG B 315



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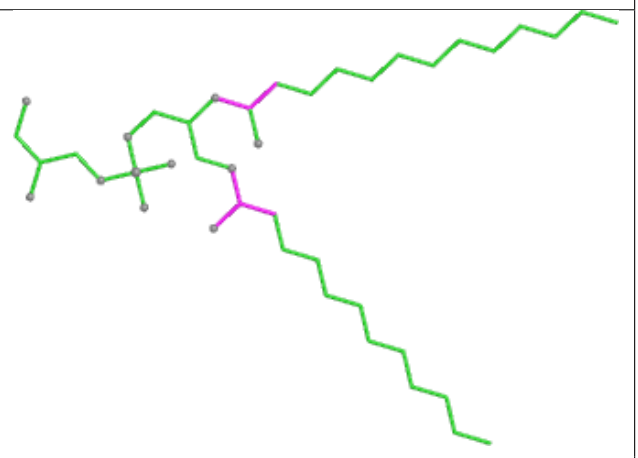
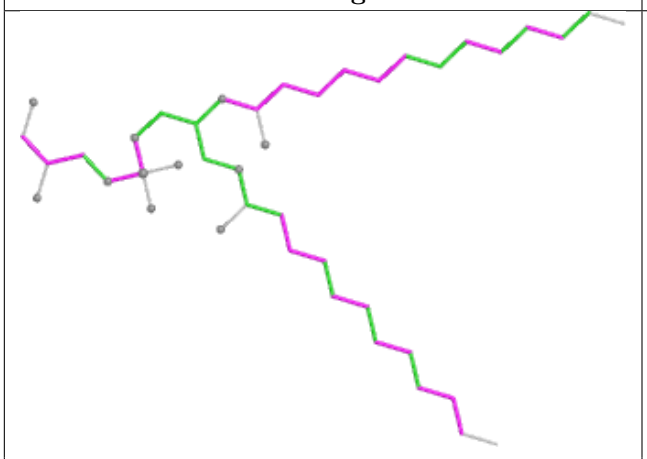


Bond angles



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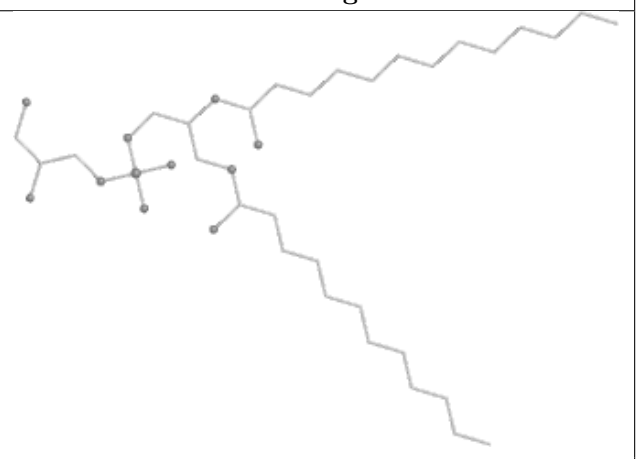
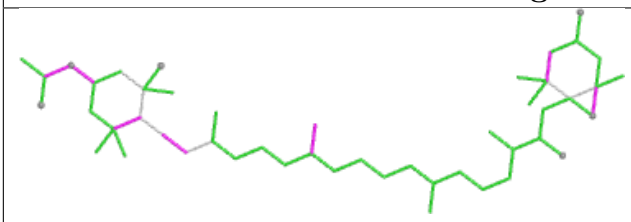


Rings

Ligand A86 B 305



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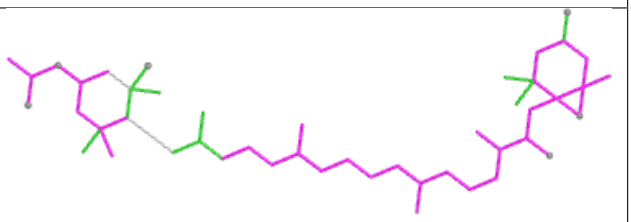
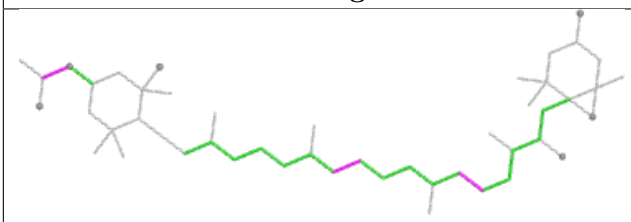


Bond angles



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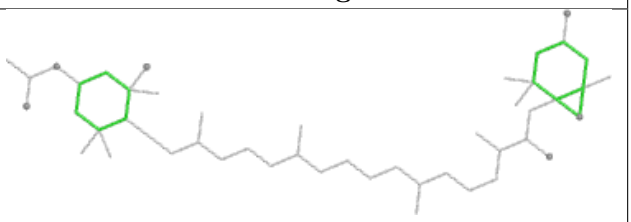
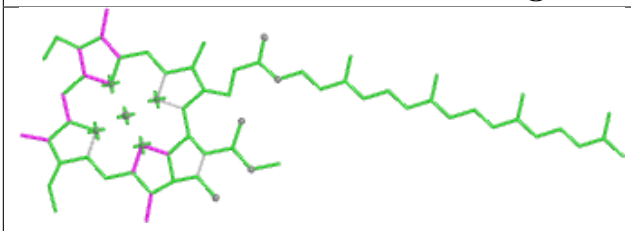


Rings

Ligand CLA b 818



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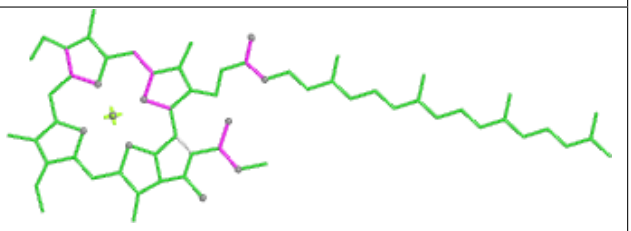
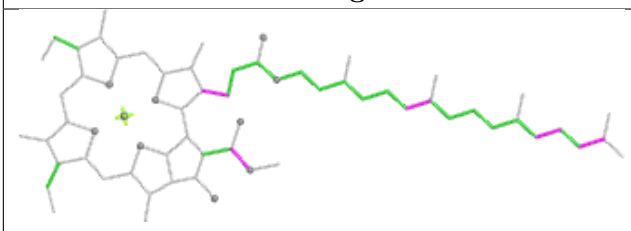


Bond angles



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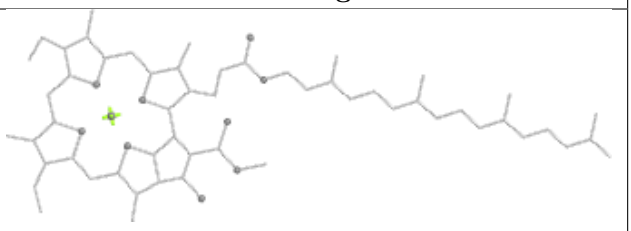
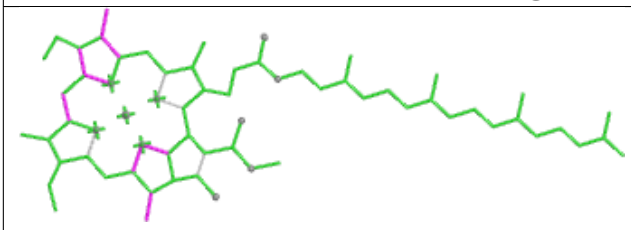


Rings

Ligand CLA b 805



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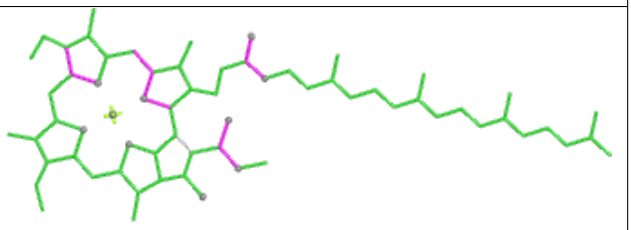
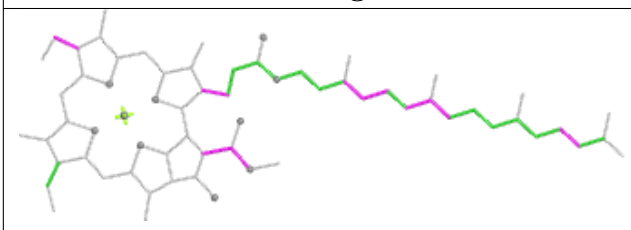


Bond angles



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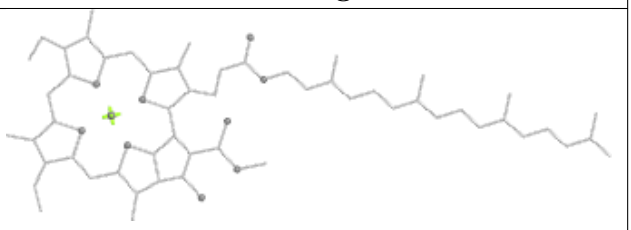
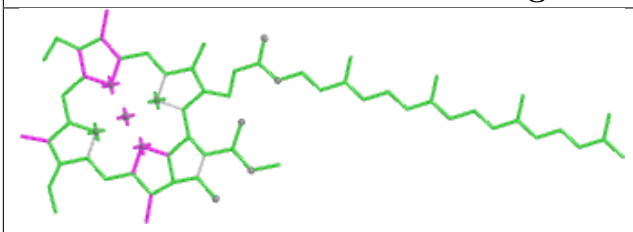


Rings

Ligand CLA a 841



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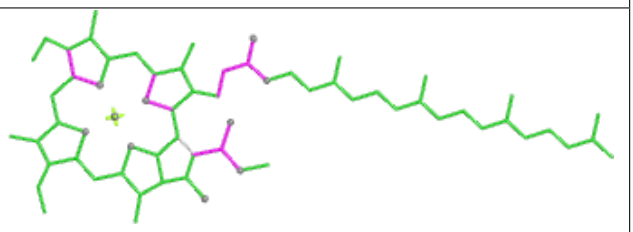
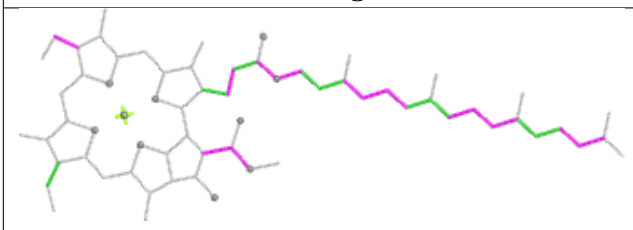


Bond angles



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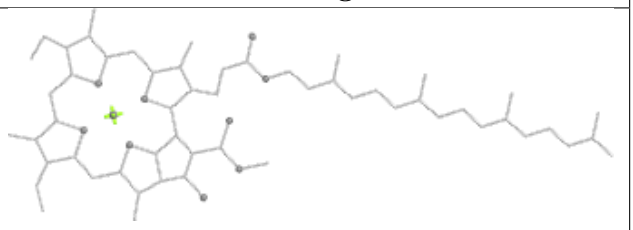
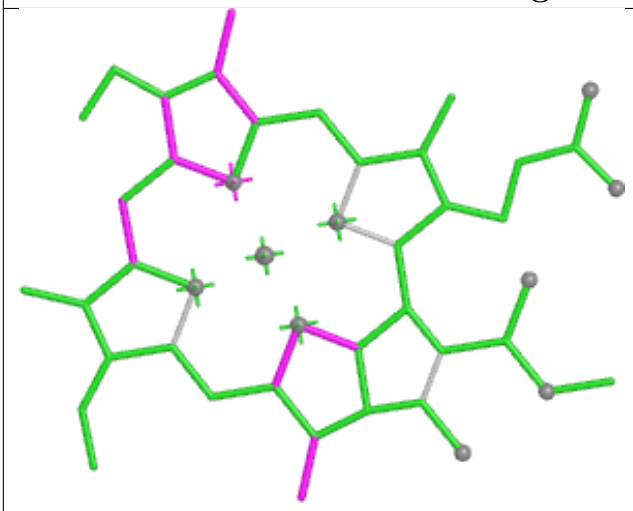


Rings

Ligand CLA f 204



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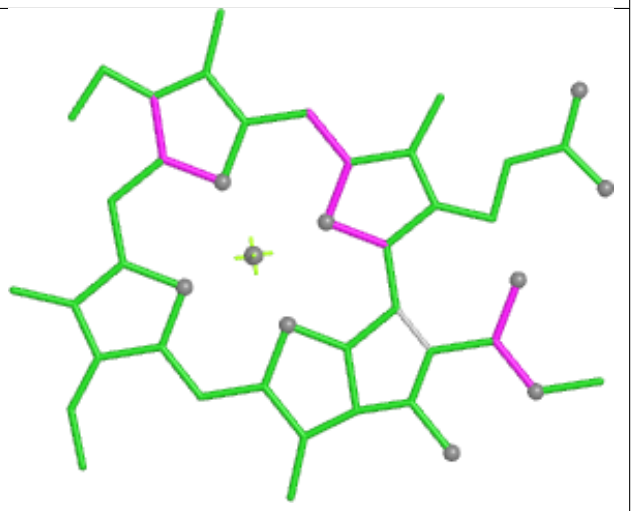
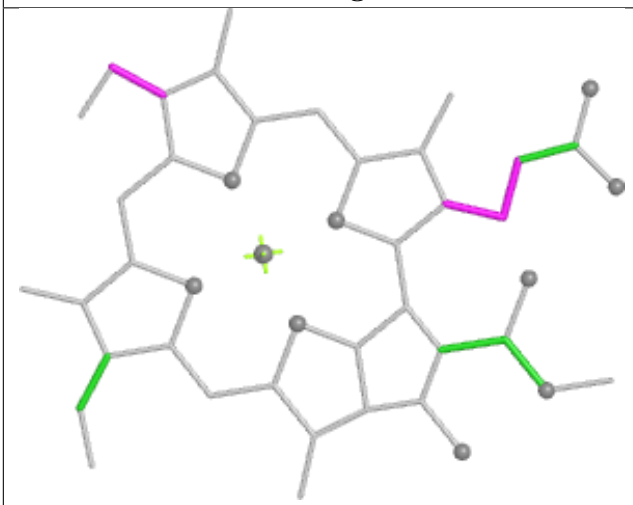


Bond angles



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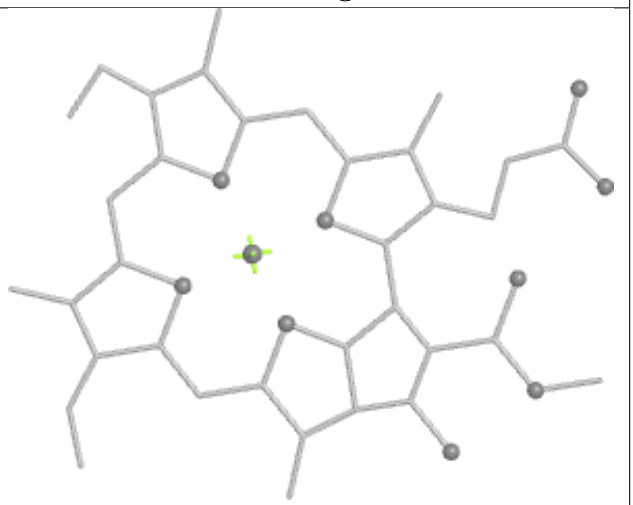
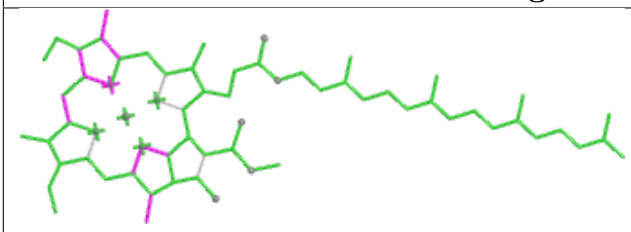


Rings

Ligand CLA a 814



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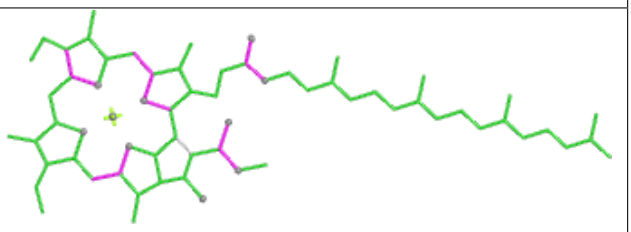
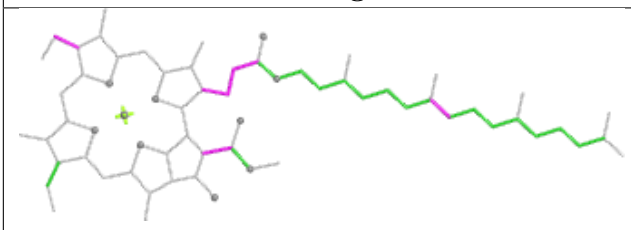


Bond angles



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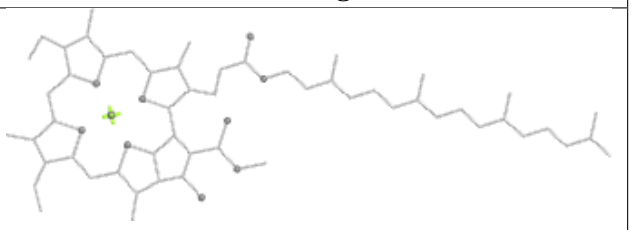
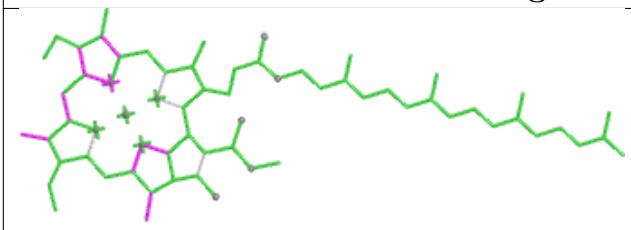


Rings

Ligand CLA a 810



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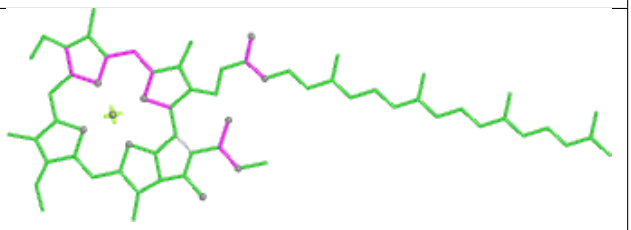
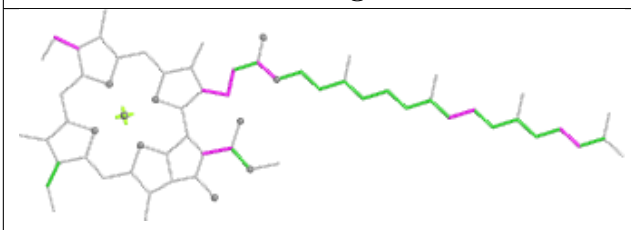


Bond angles



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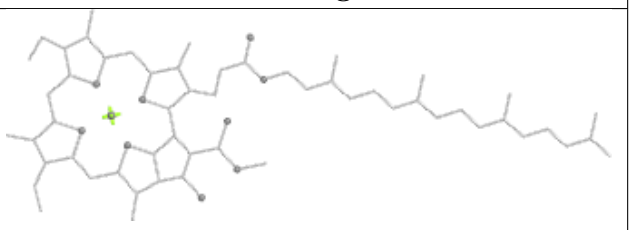
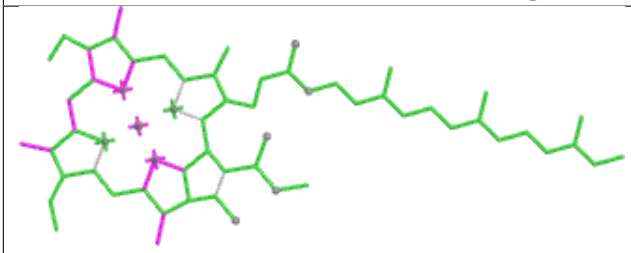


Rings

Ligand CLA C 312



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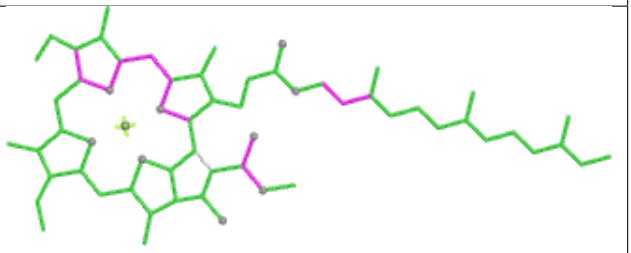
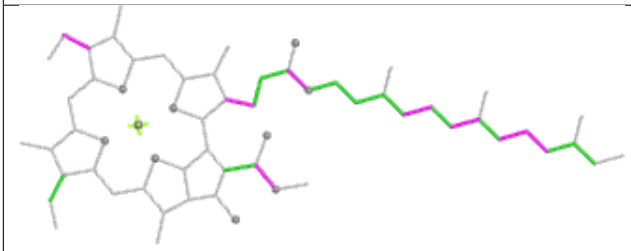


Bond angles



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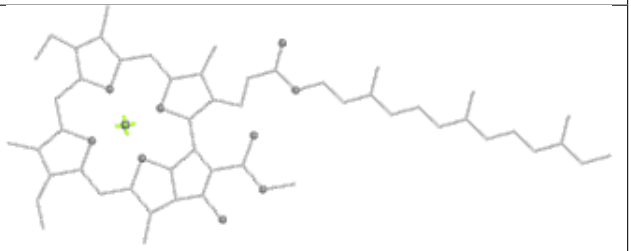
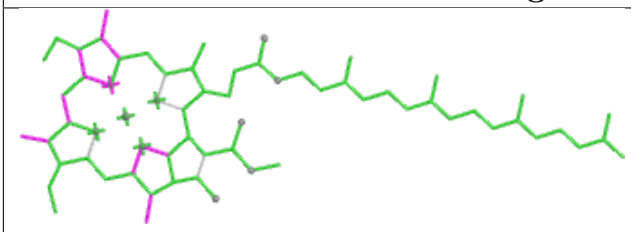
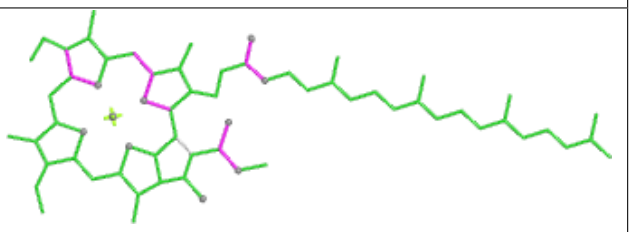


Rings

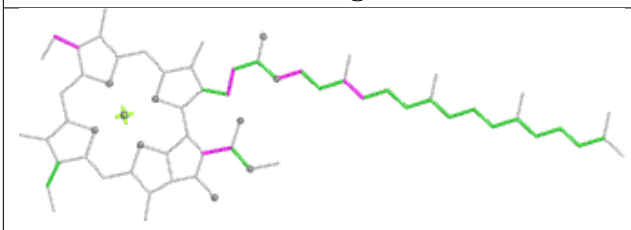
Ligand CLA b 838



Bond lengths



Bond angles



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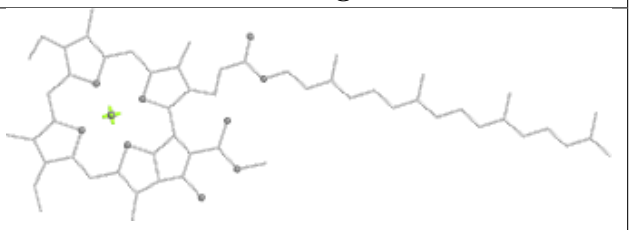
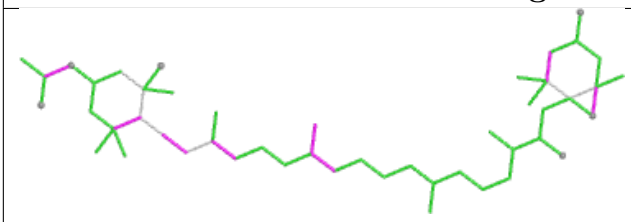
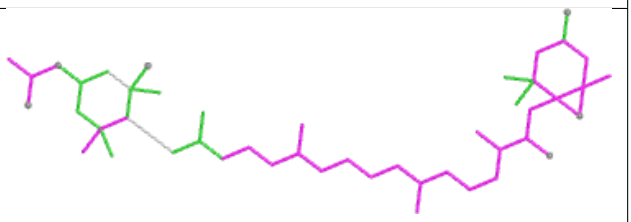


Rings

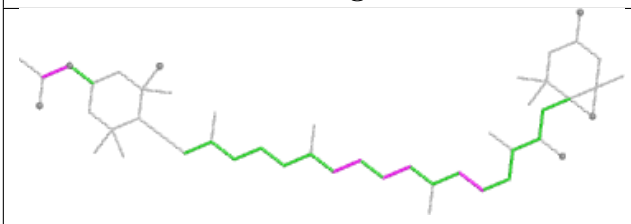
Ligand A86 H 302



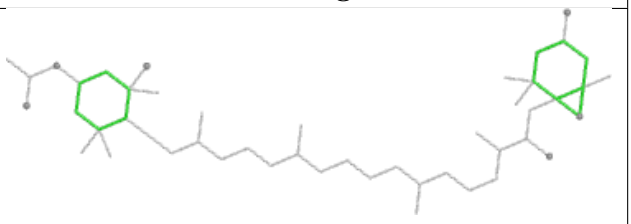
Bond lengths



Bond angles

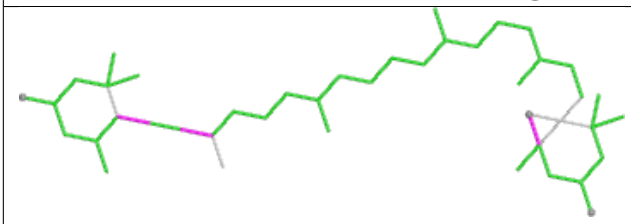


Torsions

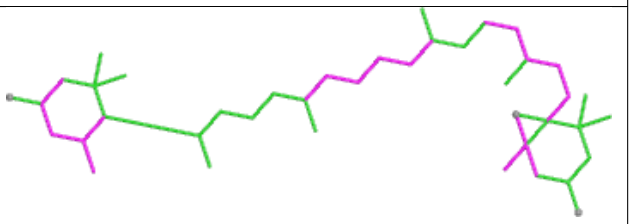


Rings

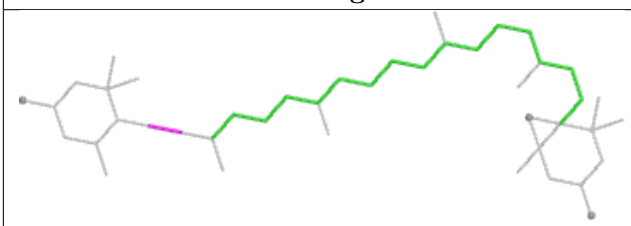
Ligand DD6 E 308



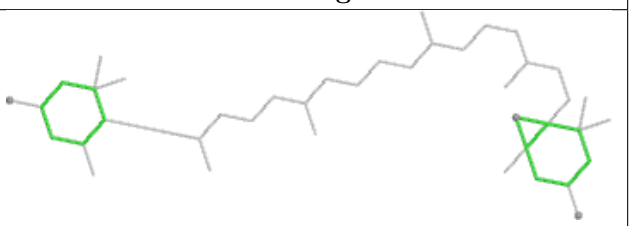
Bond lengths



Bond angles

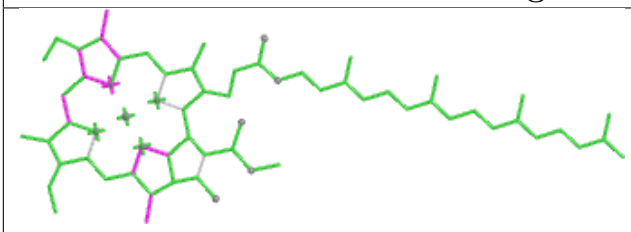


Torsions

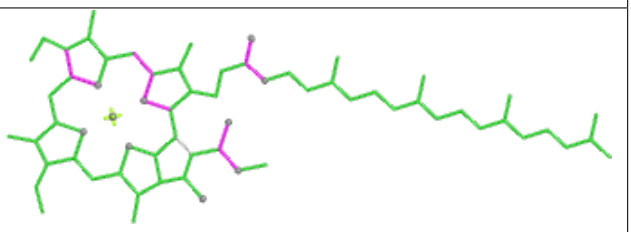


Rings

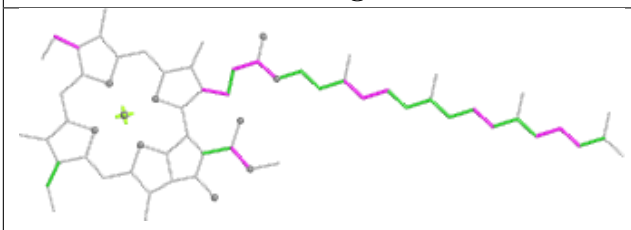
Ligand CLA b 849



Bond lengths



Bond angles



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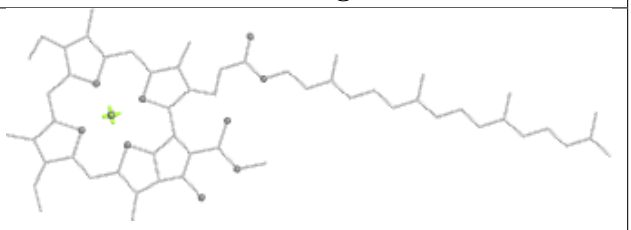
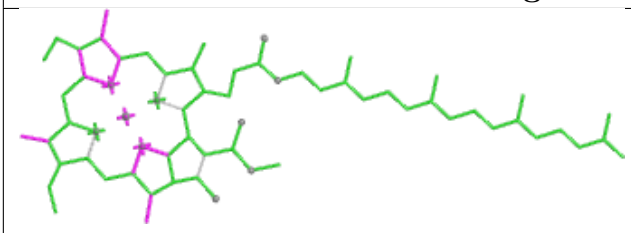


Rings

Ligand CLA H 307



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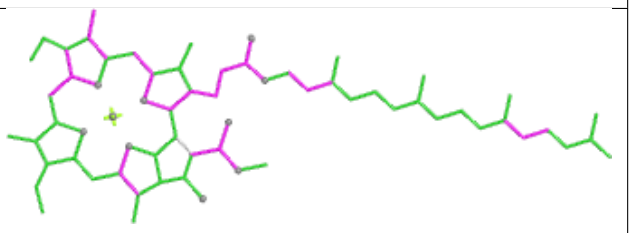
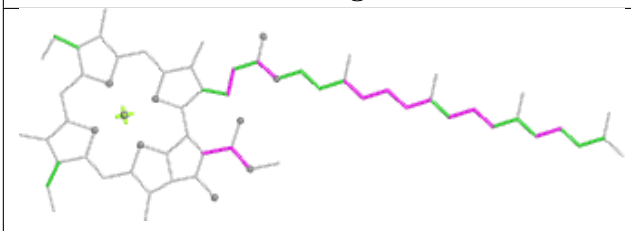


Bond angles



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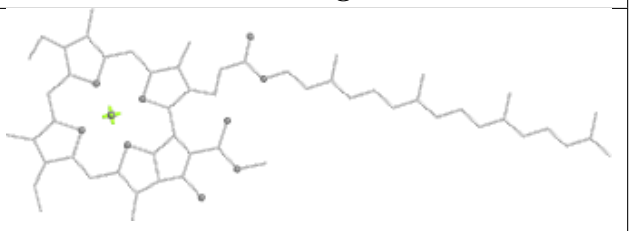
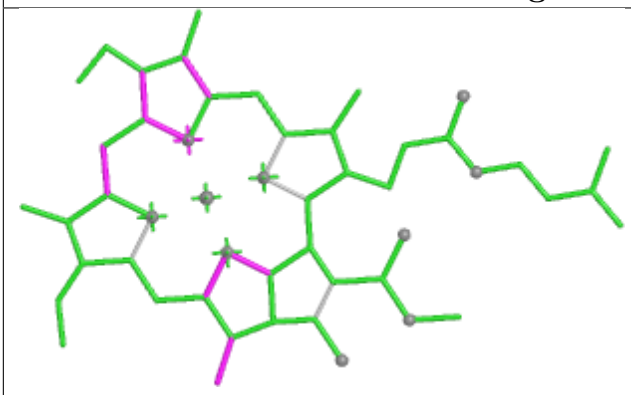


Rings

Ligand CLA a 811



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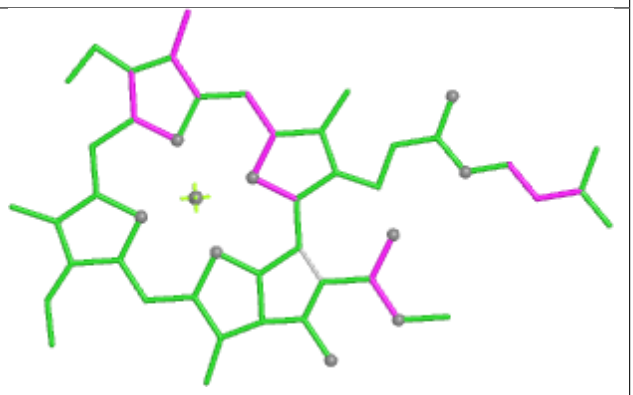

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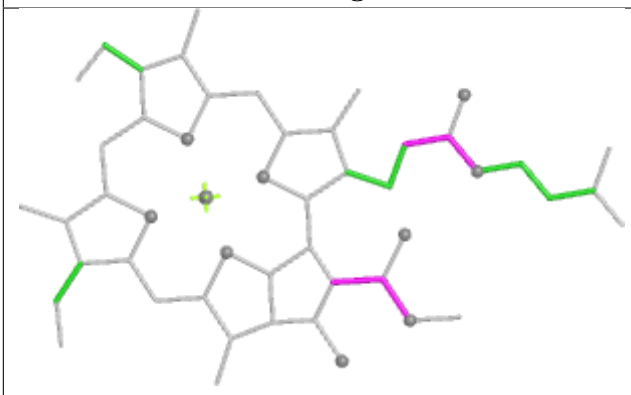

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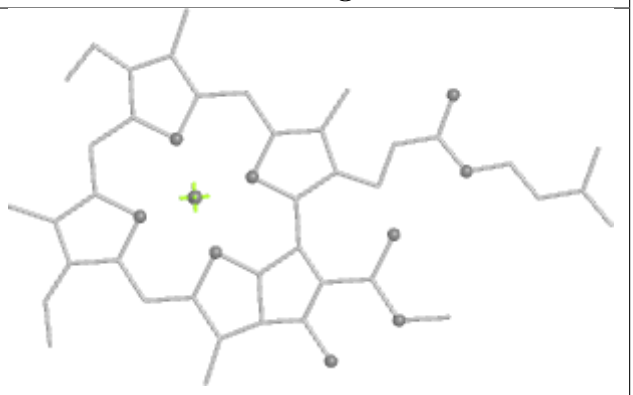
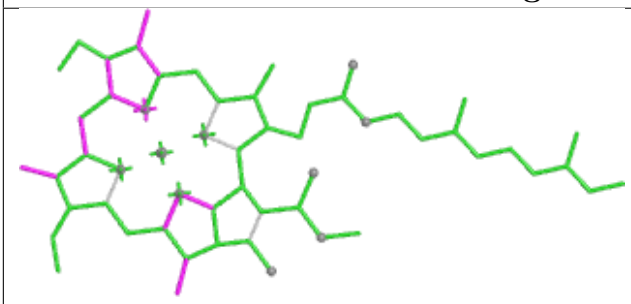


Rings

Ligand CLA D 214



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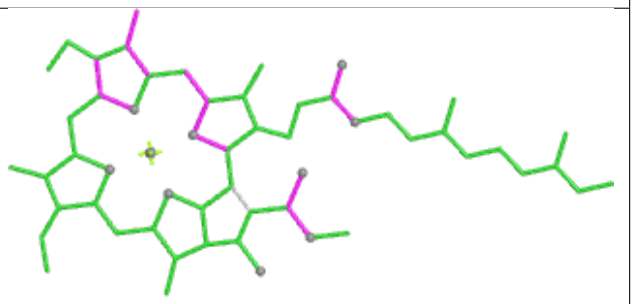
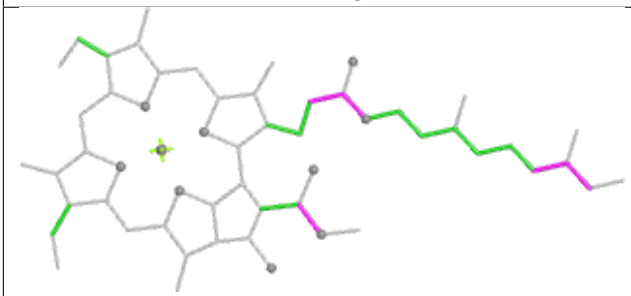


Bond angles



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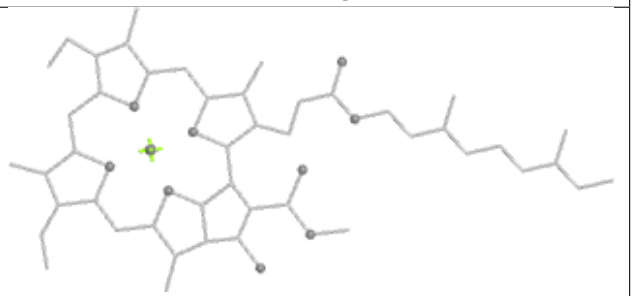
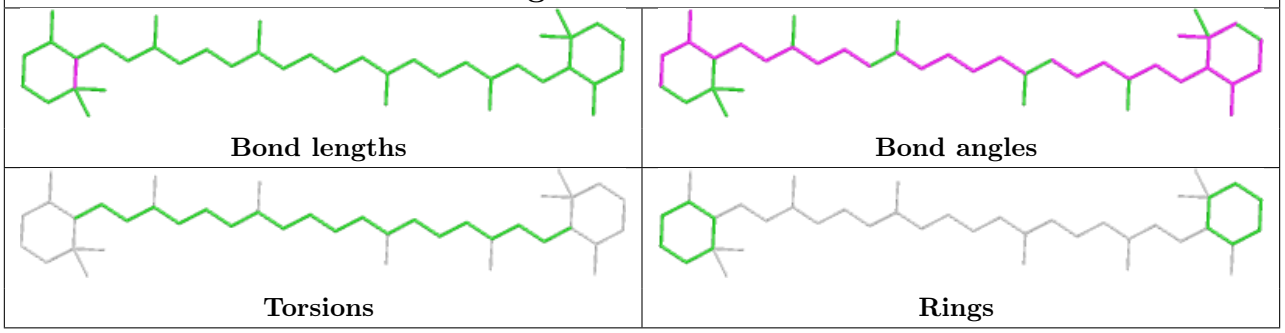


Rings

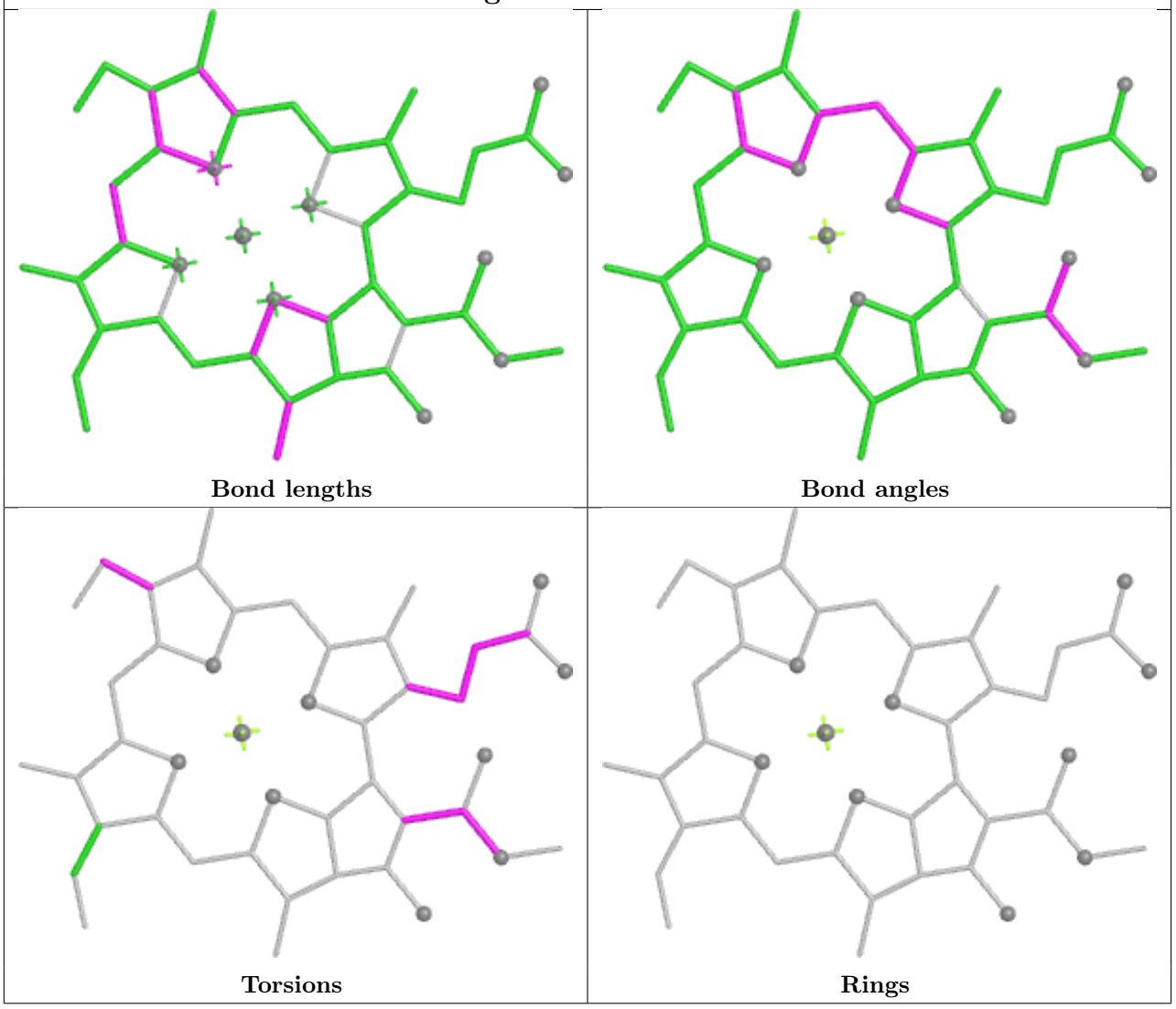
Ligand BCR a 833



Bond lengths | Bond angles

Torsions | Rings

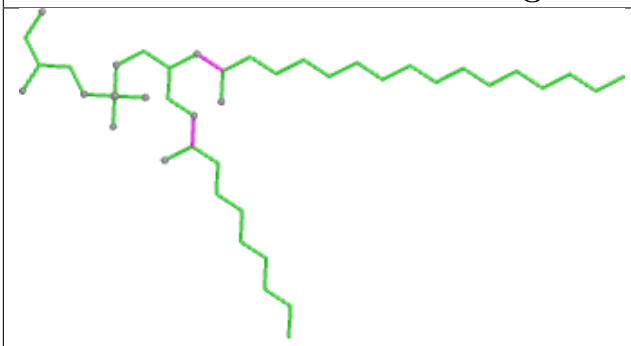
Ligand CLA a 823



Bond lengths | Bond angles

Torsions | Rings

Ligand LHG E 317



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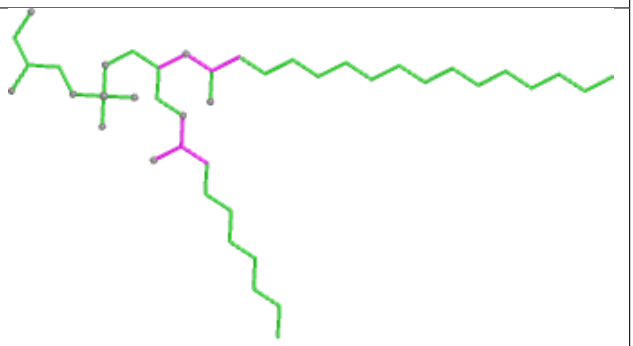
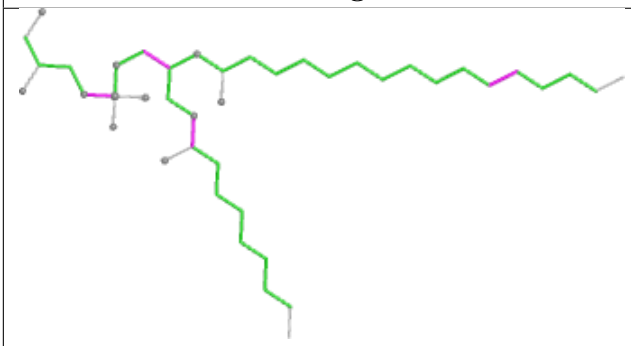


Bond angles



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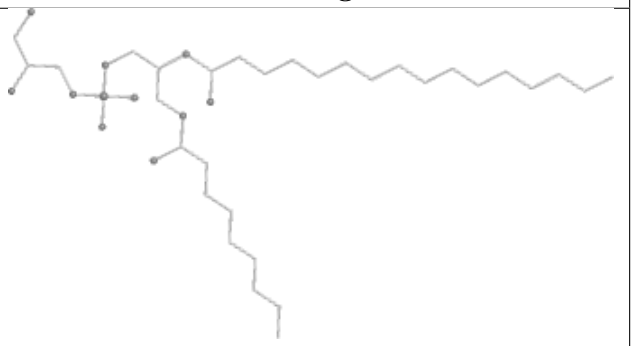
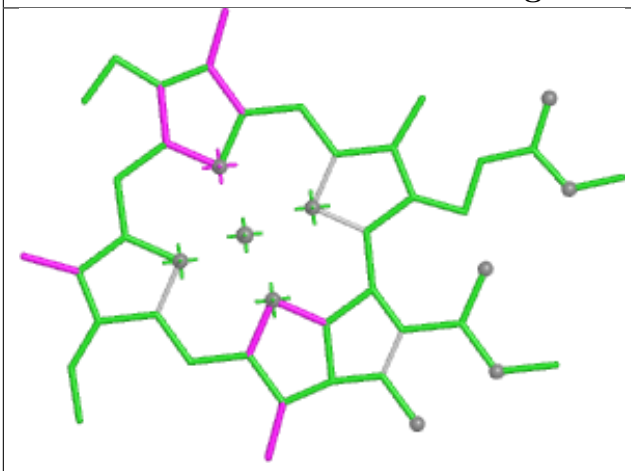
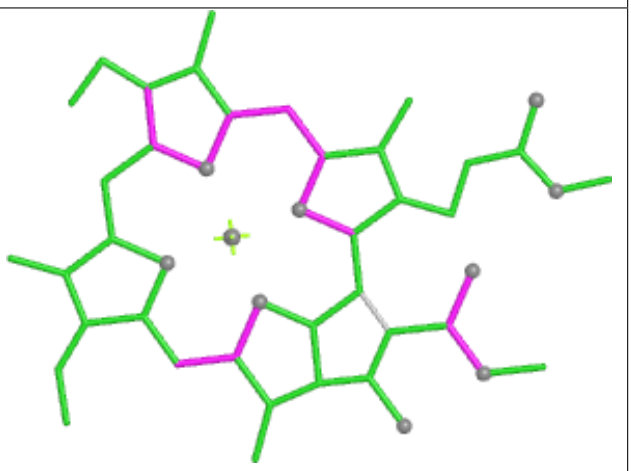
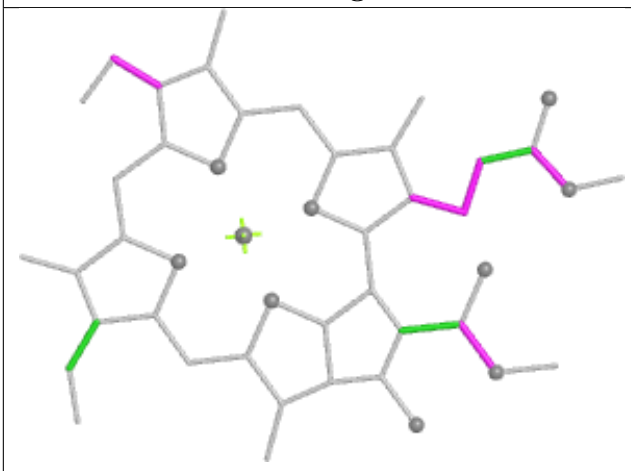
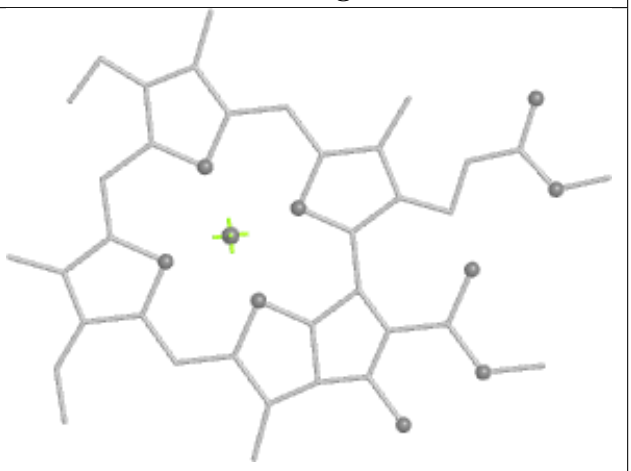
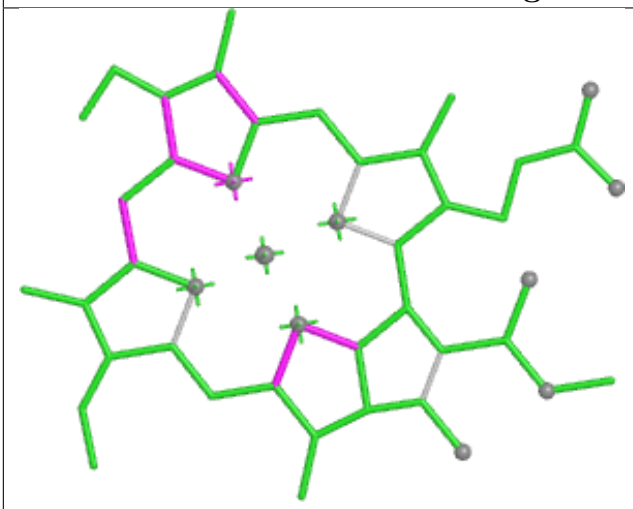


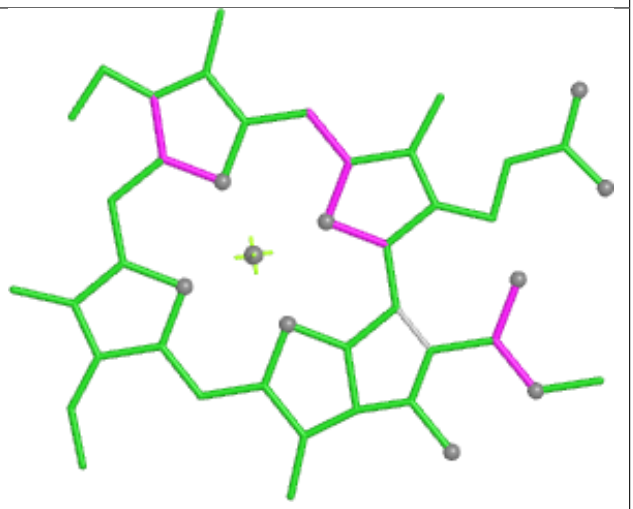
Rings

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

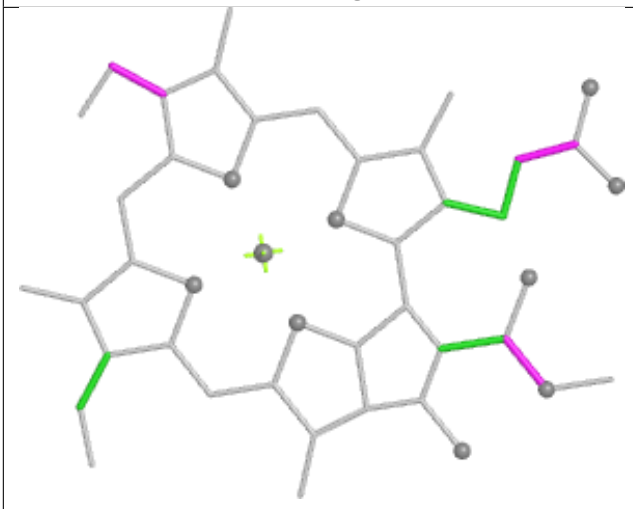
Ligand CLA H 315



Bond lengths



Bond angles

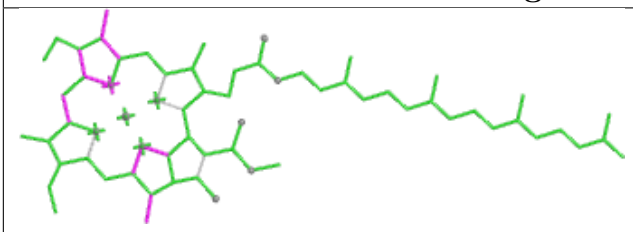


Torsions

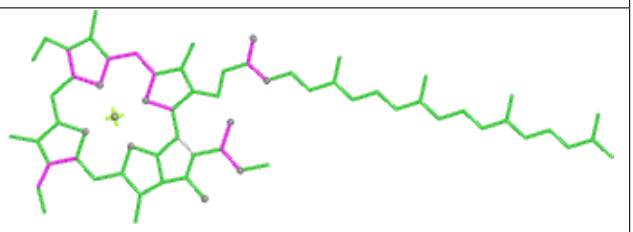


Rings

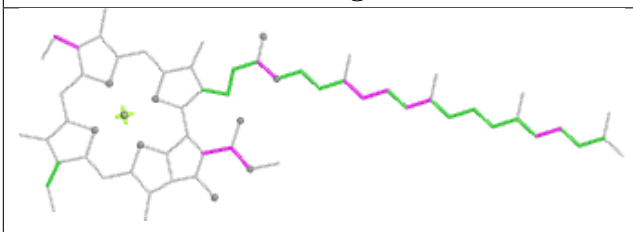
Ligand CLA B 311



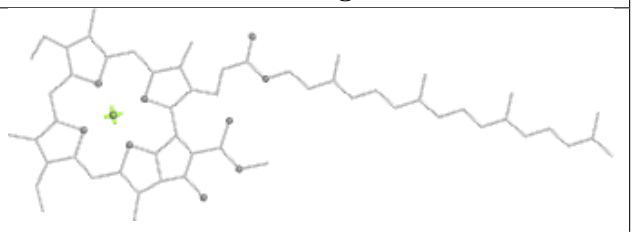
Bond lengths



Bond angles

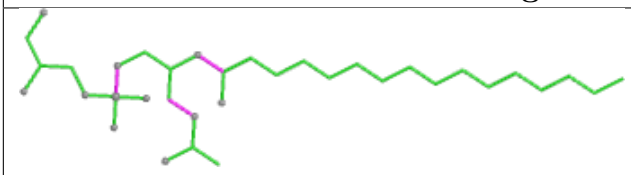


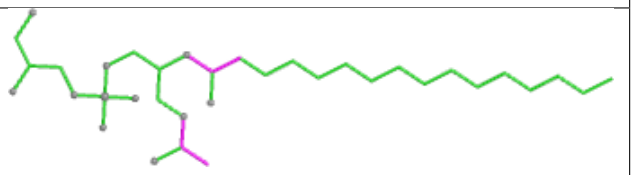
Torsions



Rings

Ligand LHG H 316


Bond lengths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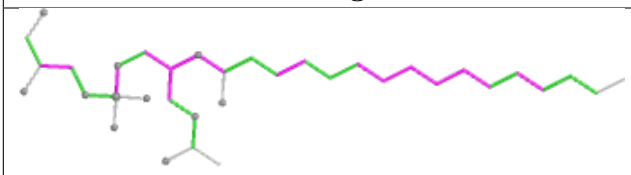
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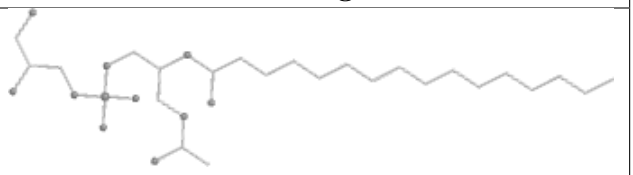
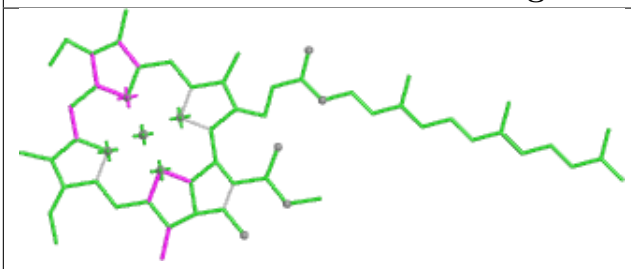

Rings

Ligand CLA b 826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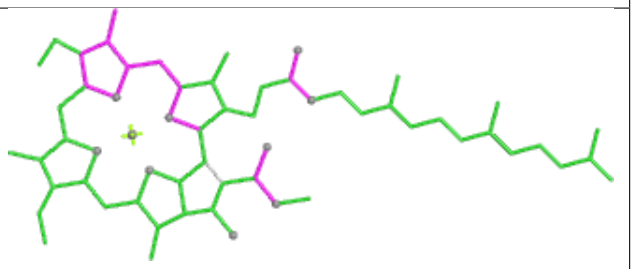
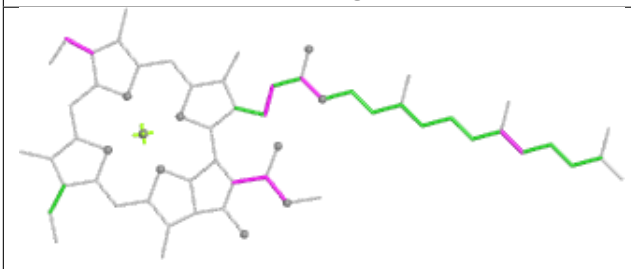

Bond angles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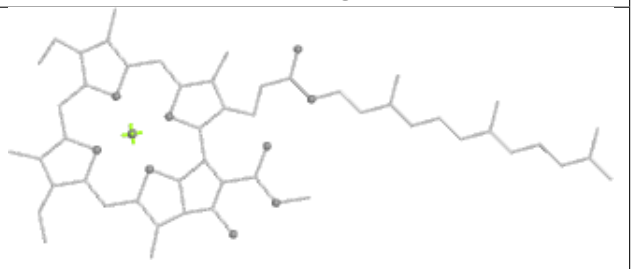
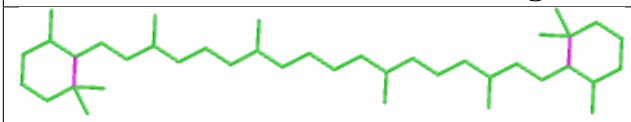

Rings

Ligand BCR a 845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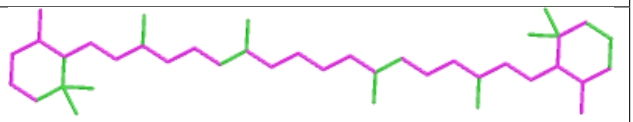
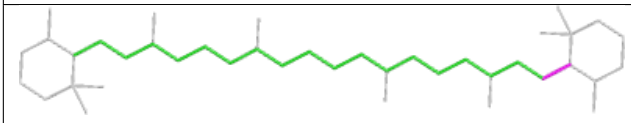

Bond angles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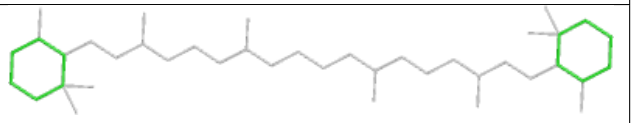
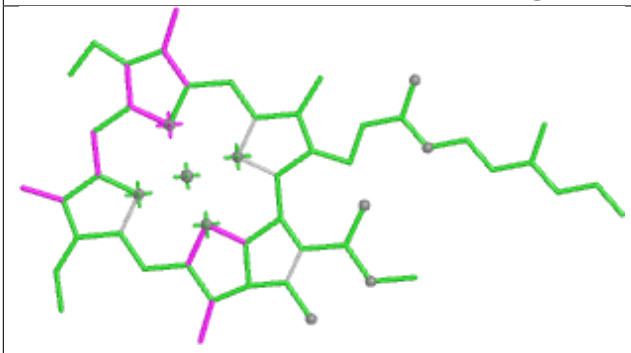
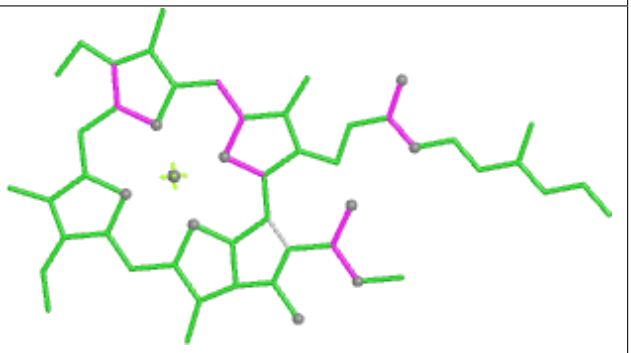
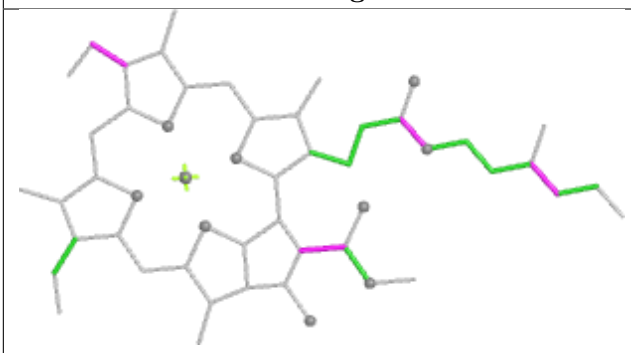
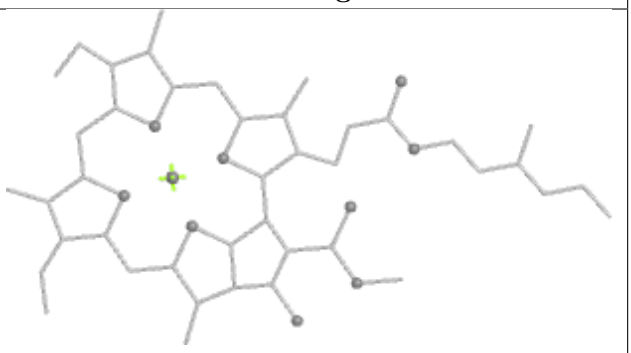
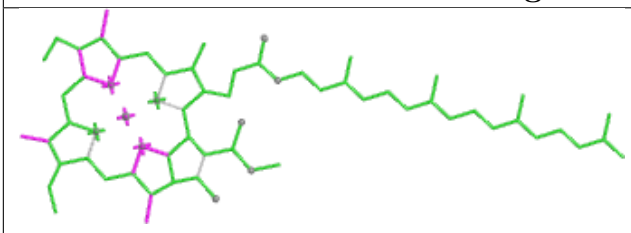
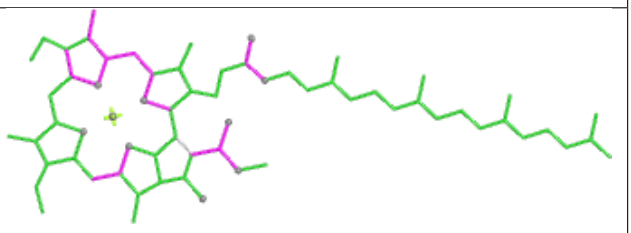
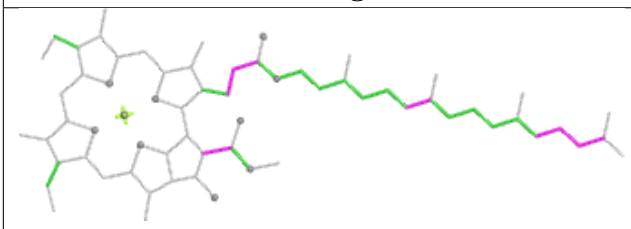
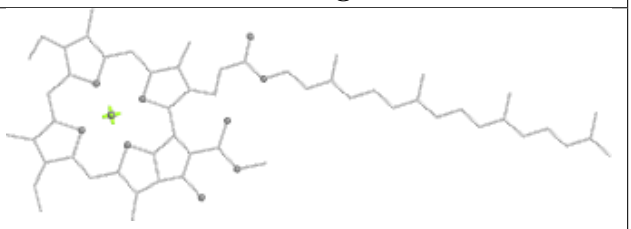
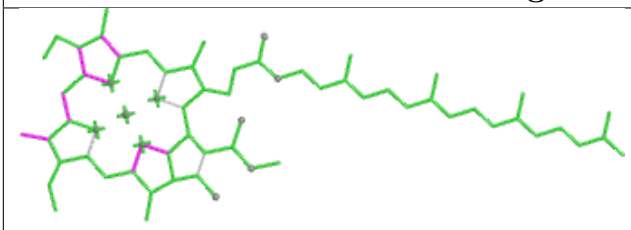

Rings

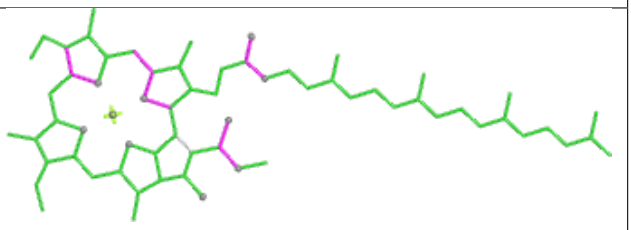
Ligand CLA a 830	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA C 307	
 Bond lengths	 Bond angles
 Torsions	 Rings

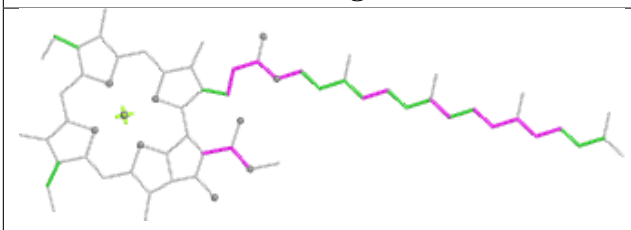
Ligand CLA b 806



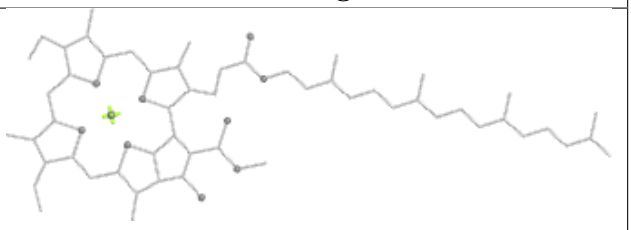
Bond lengths



Bond angles

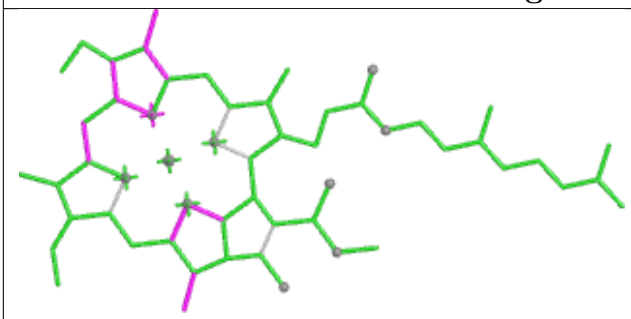


Torsions

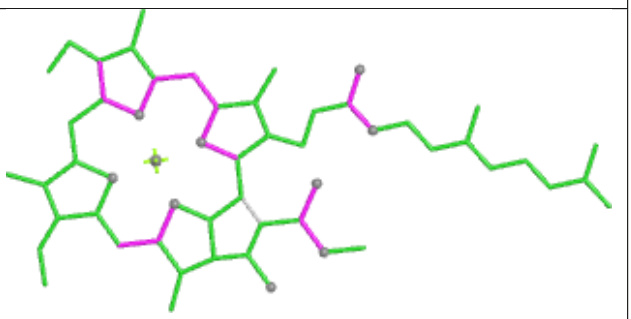


Rings

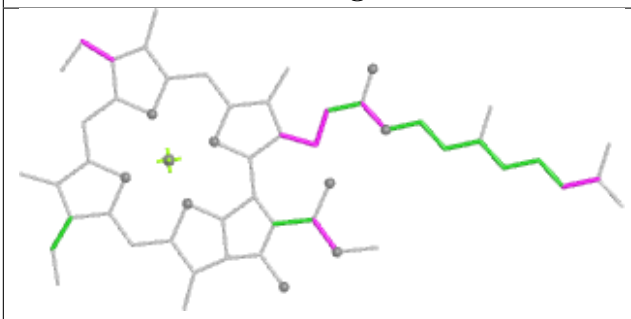
Ligand CLA E 313



Bond lengths



Bond angles



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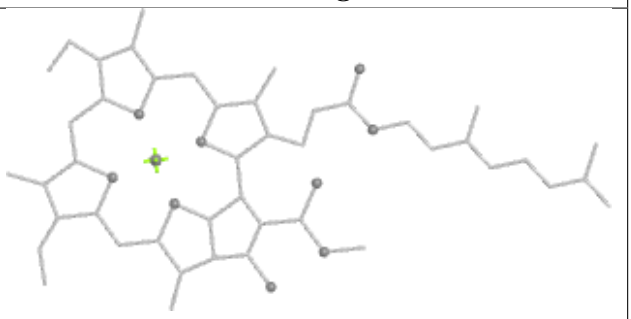
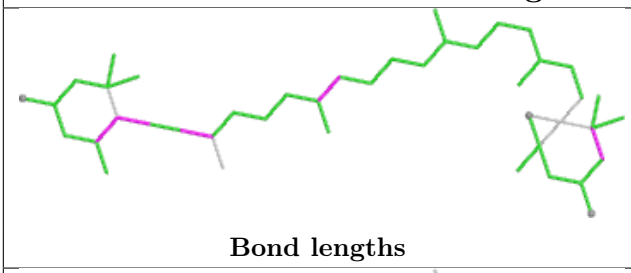


Rings

Ligand DD6 C 303



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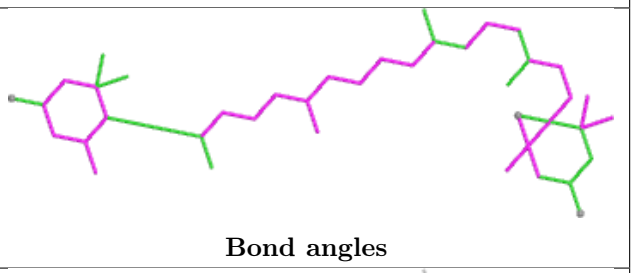

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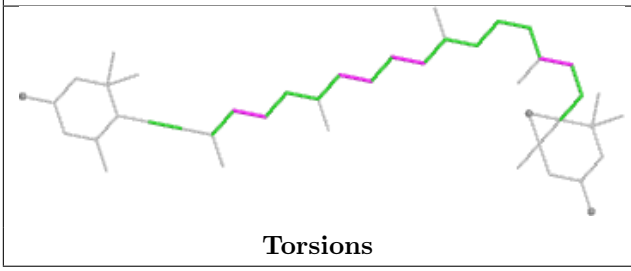

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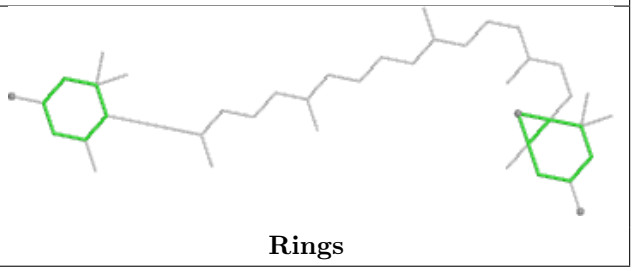
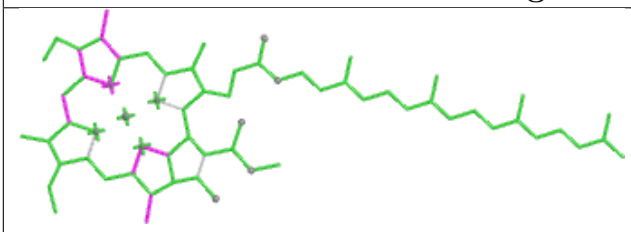


Rings

Ligand CLA b 814



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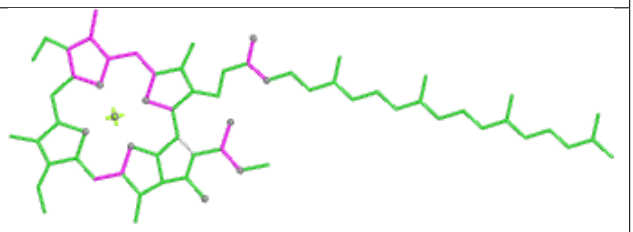

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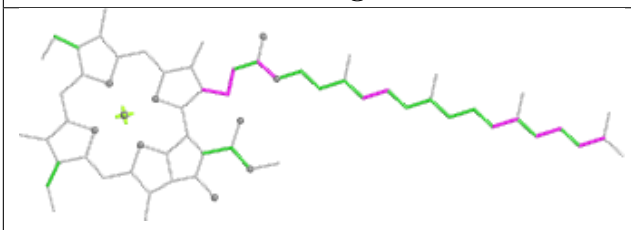

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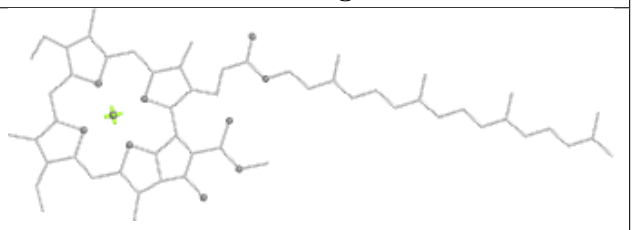
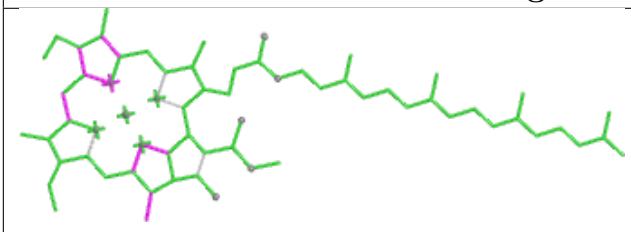


Rings

Ligand CLA b 830



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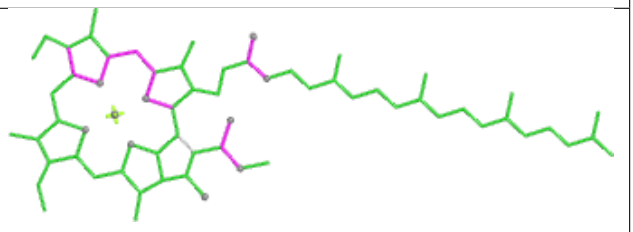

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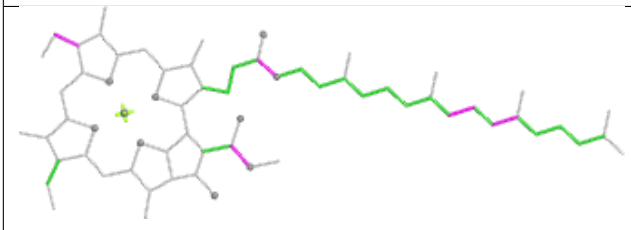

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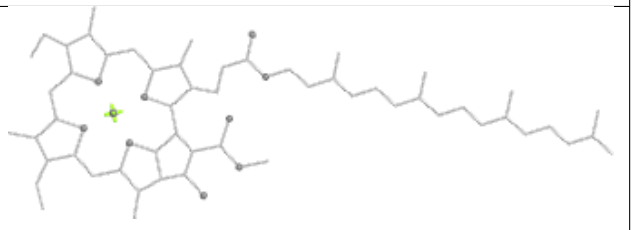
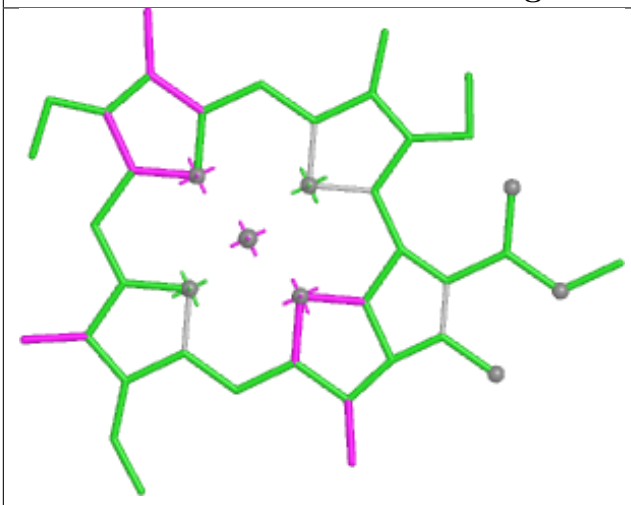


Rings

Ligand CLA C 318



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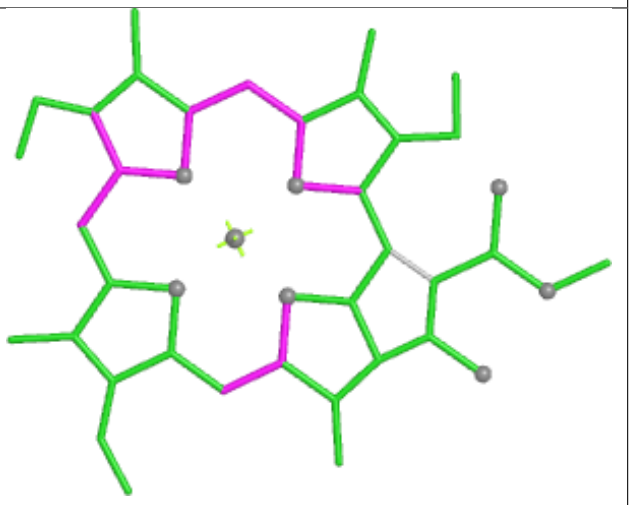

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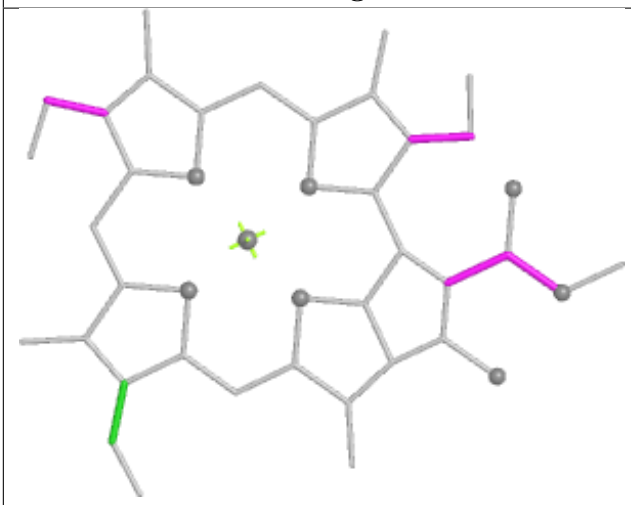


Torsions

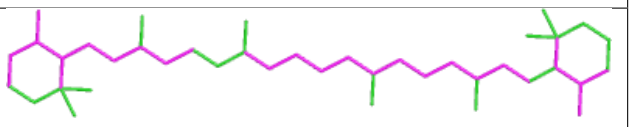


Rings

Ligand BCR i 102



Bond lengths



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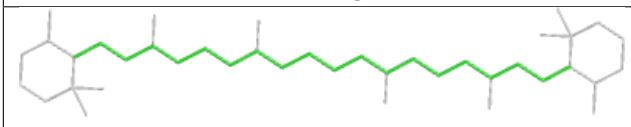

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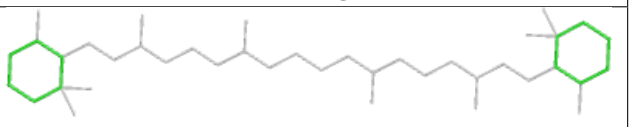
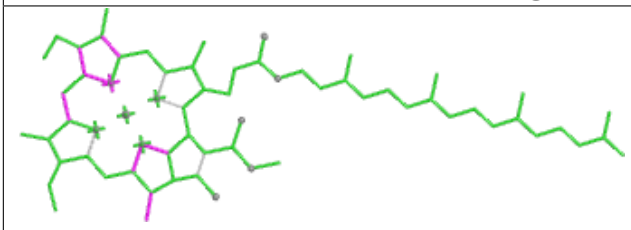
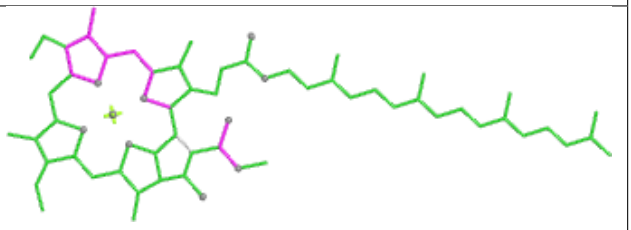
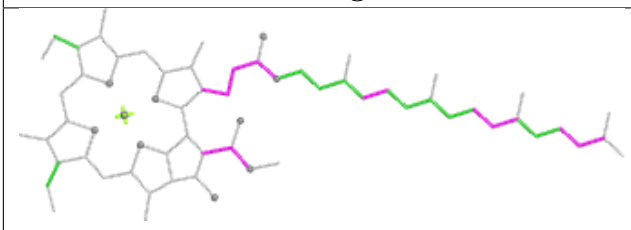
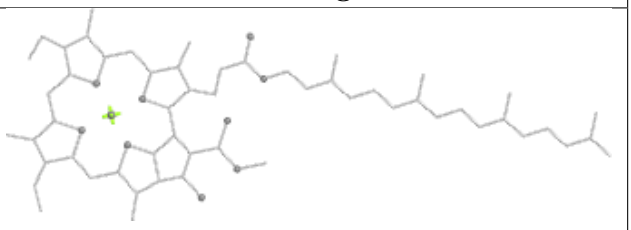
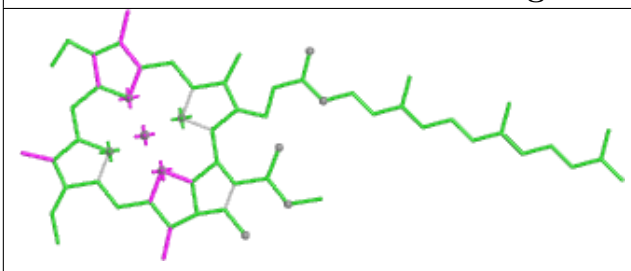
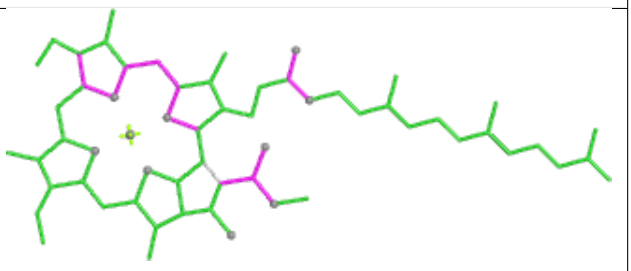
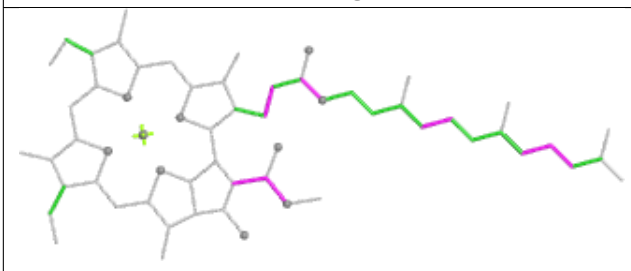
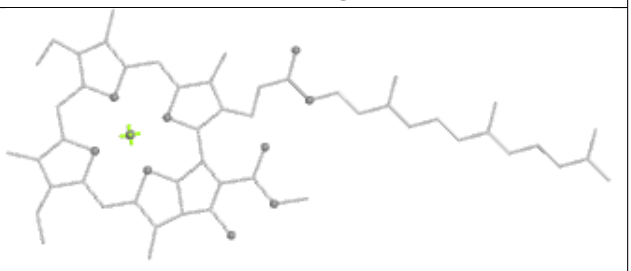
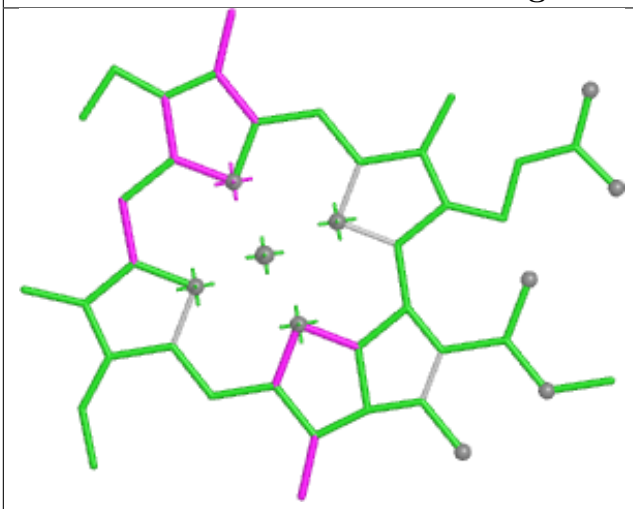


Rings

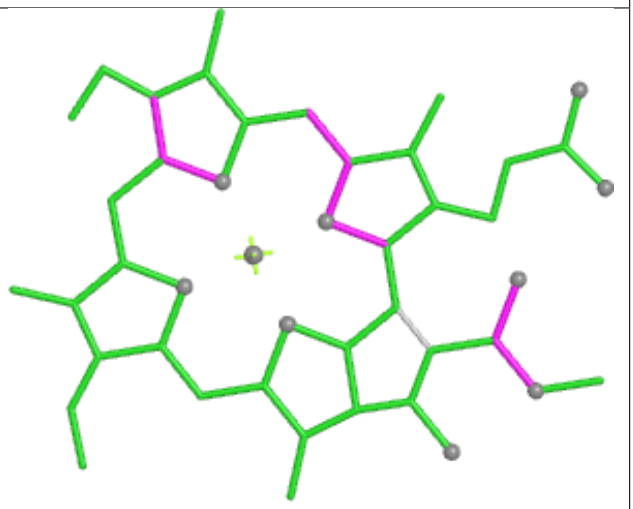
Ligand CLA b 822	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA b 811	
	
Bond lengths	Bond angles
	
Torsions	Rings

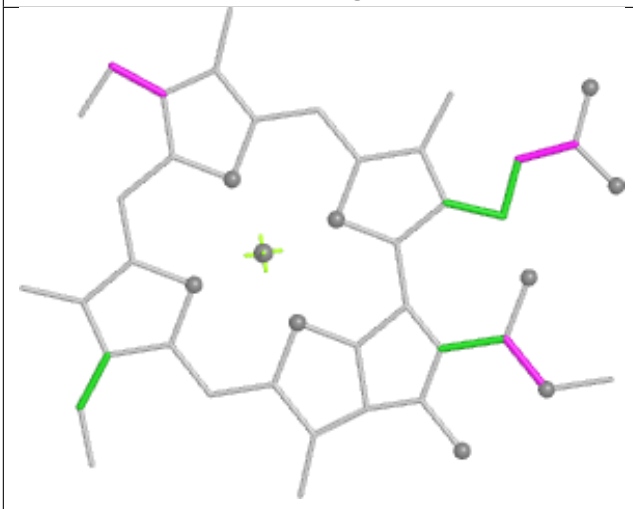
Ligand CLA a 812



Bond lengths



Bond angles

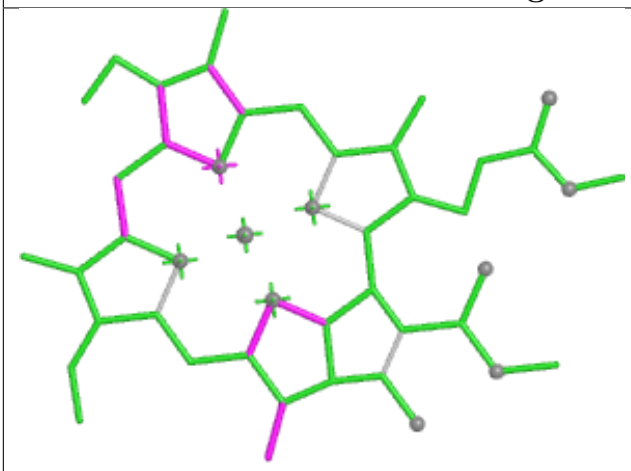


Torsions



Rings

Ligand CLA b 815



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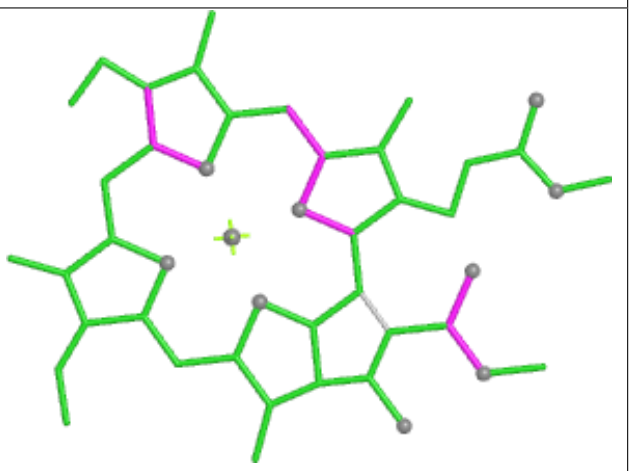
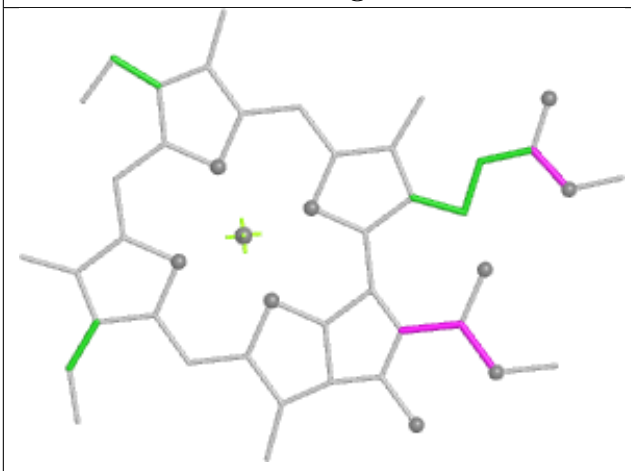


Bond angles



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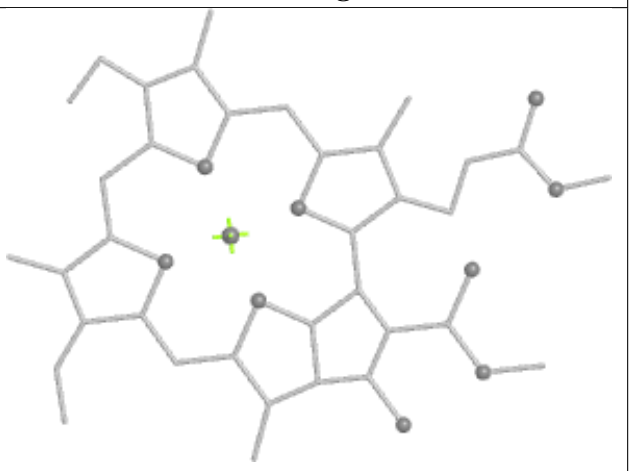
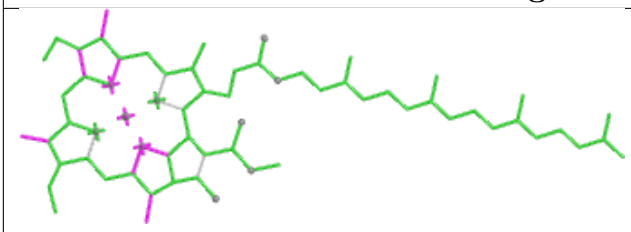


Rings

Ligand CLA a 854



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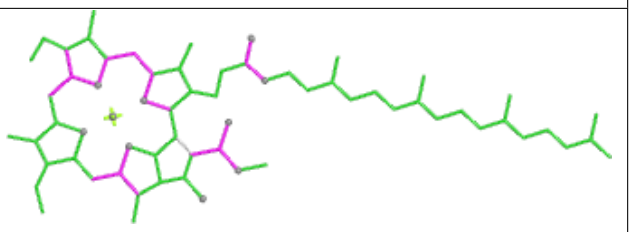
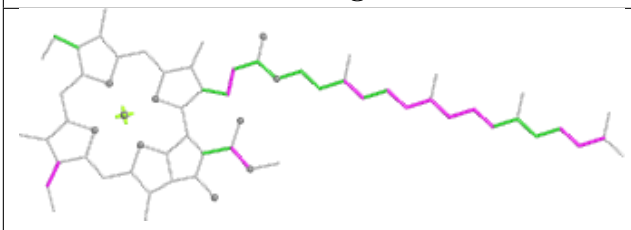


Bond angles



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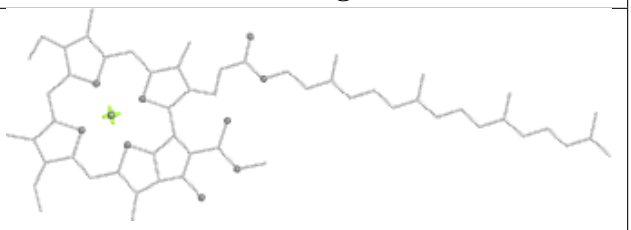
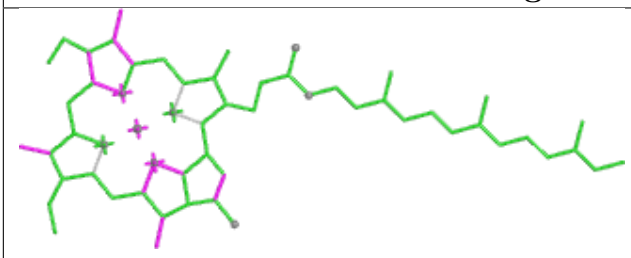


Rings

Ligand CLA B 306



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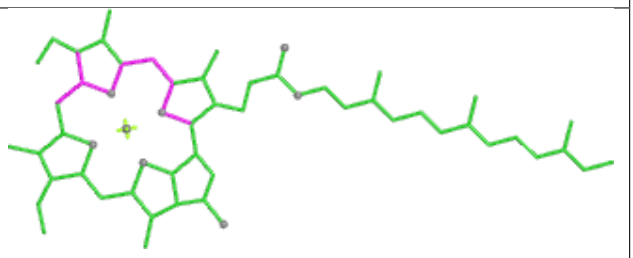
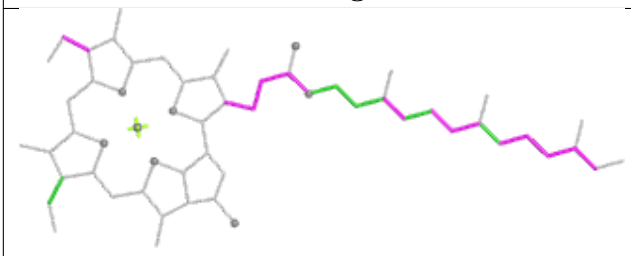


Bond angles



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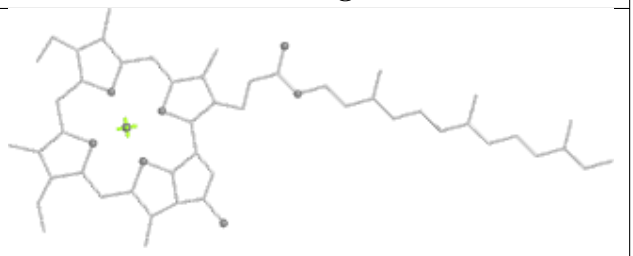
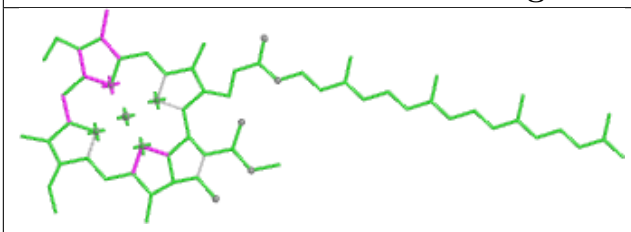


Rings

Ligand CLA b 842



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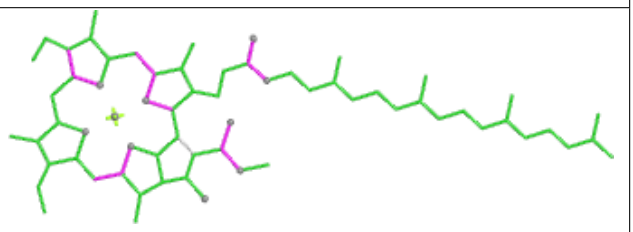
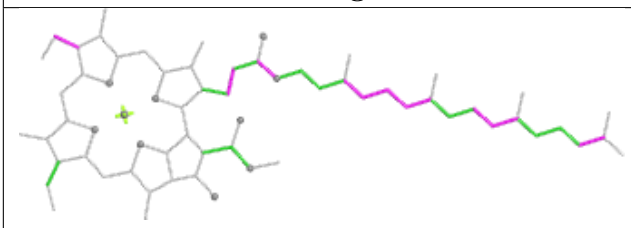


Bond angles



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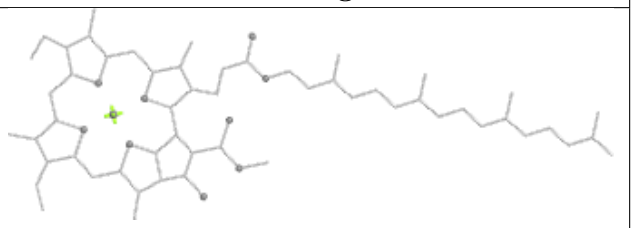
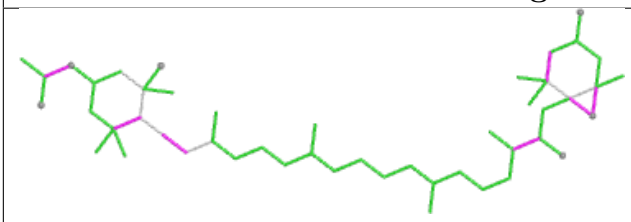


Rings

Ligand A86 C 305



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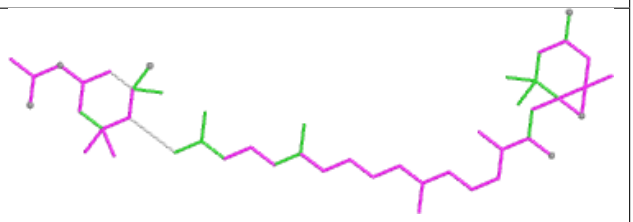
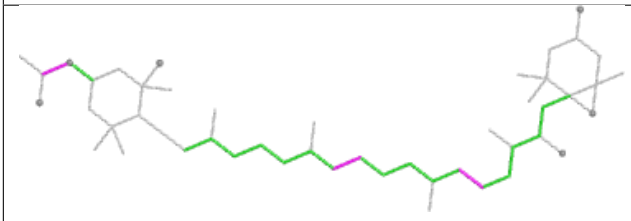


Bond angles



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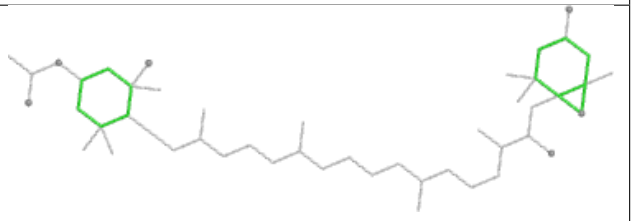
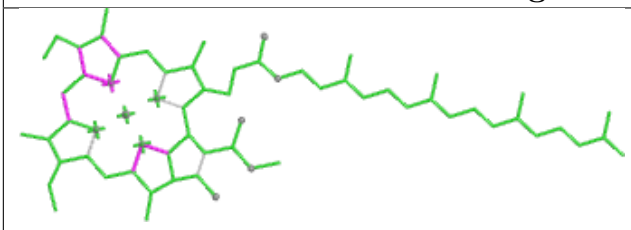
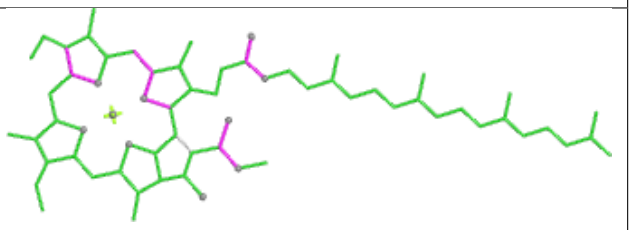


Rings

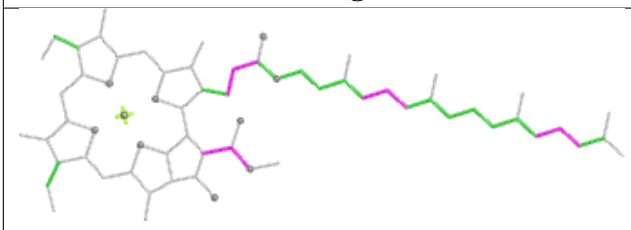
Ligand CLA a 827



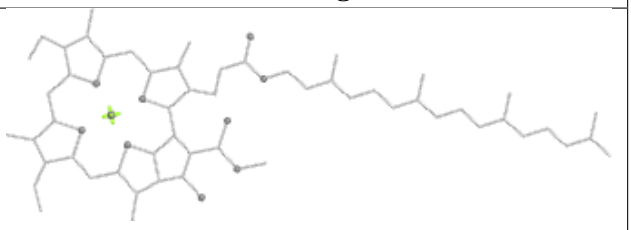
Bond lengths



Bond angles

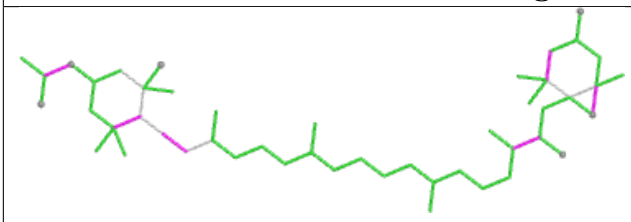


Torsions

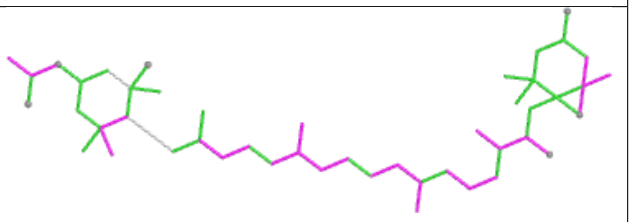


Rings

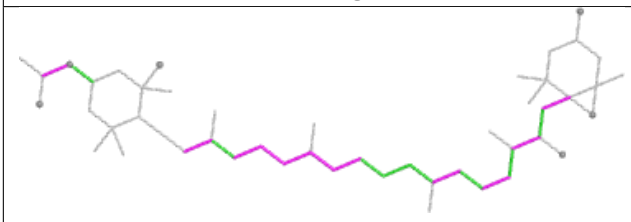
Ligand A86 b 847



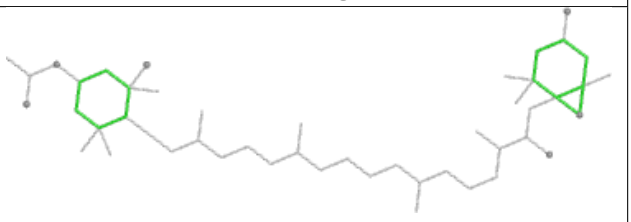
Bond lengths



Bond angles

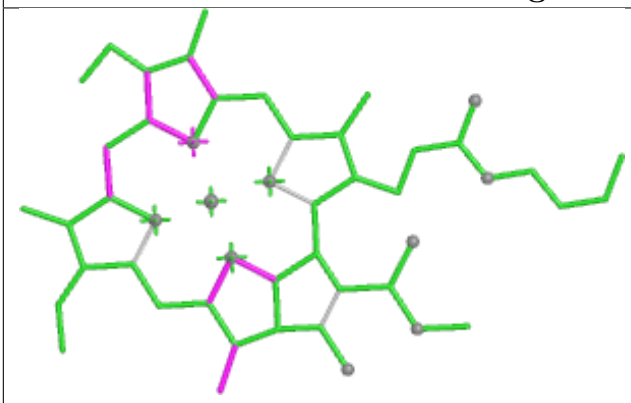


Torsions



Rings

Ligand CLA a 817



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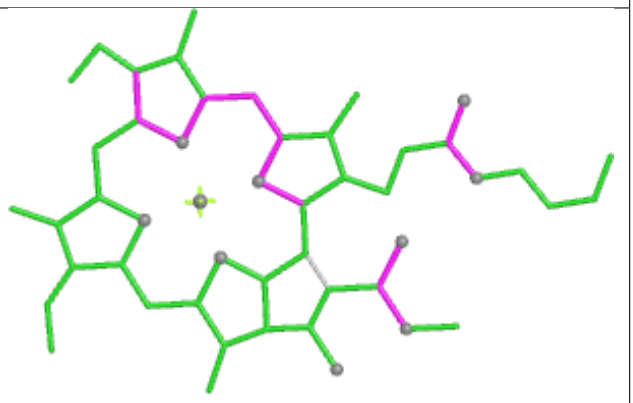

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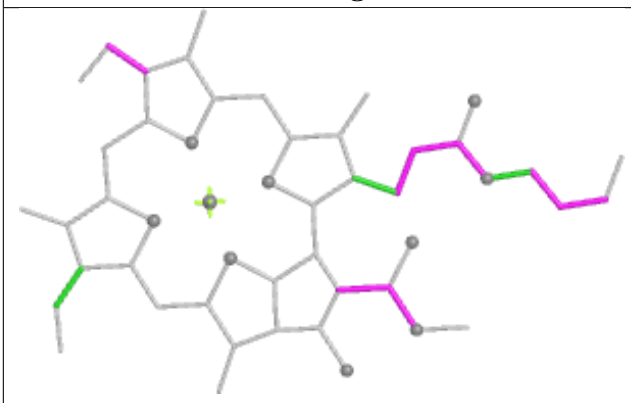

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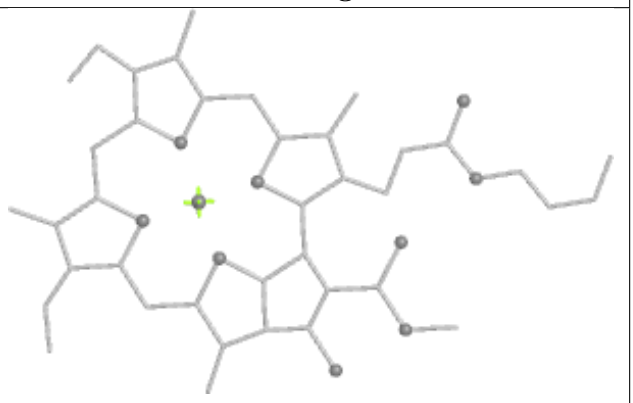
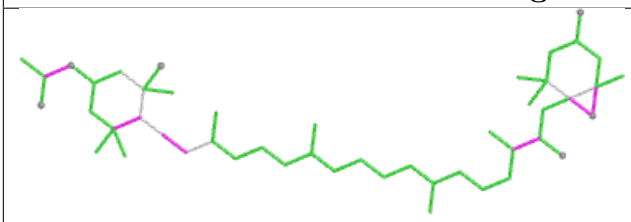


Rings

Ligand A86 C 302



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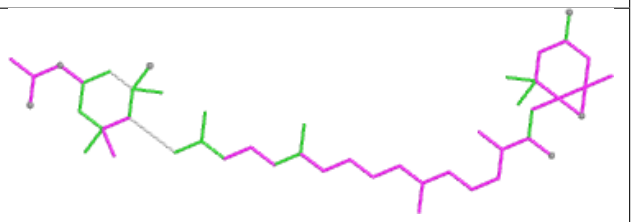

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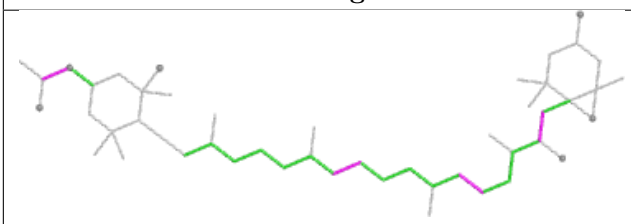

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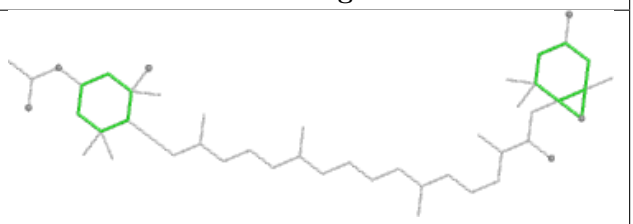
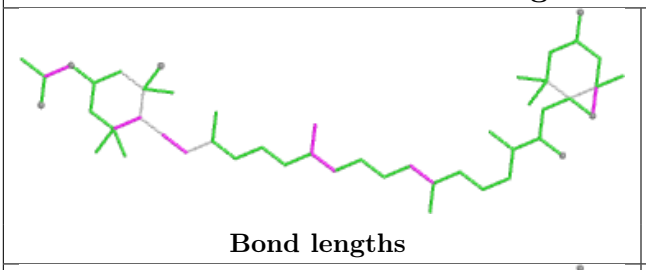


Rings

Ligand A86 B 304



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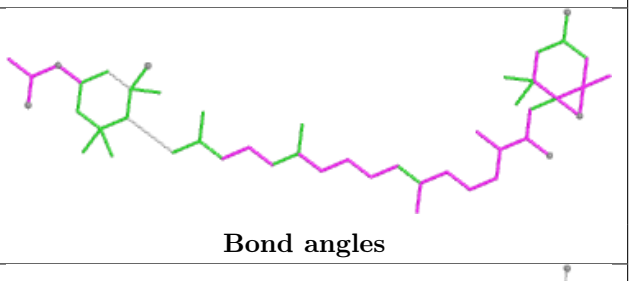
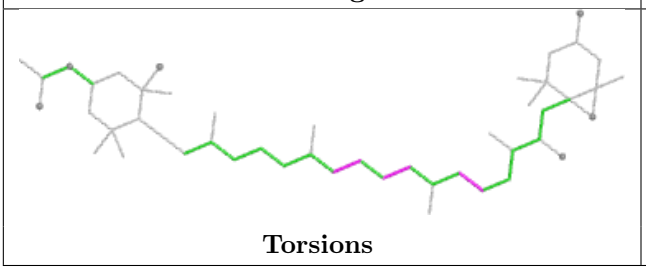


Bond angles



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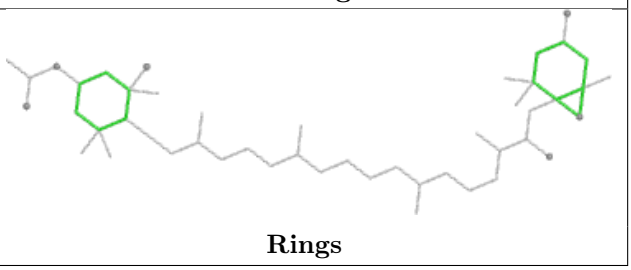
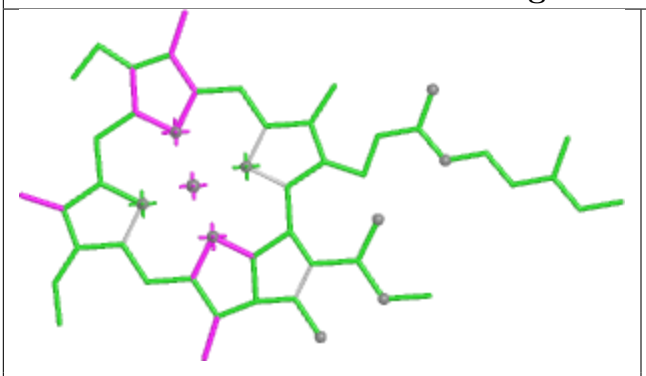


Rings

Ligand CLA a 818



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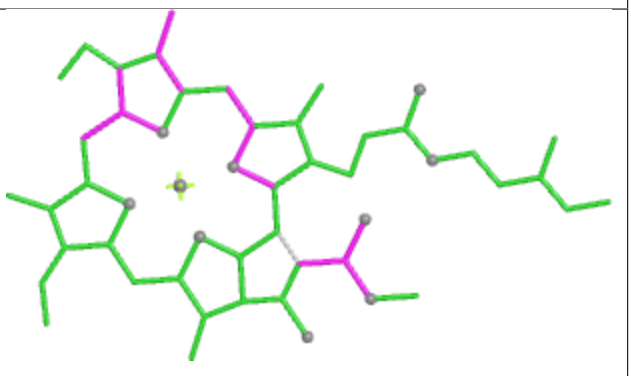

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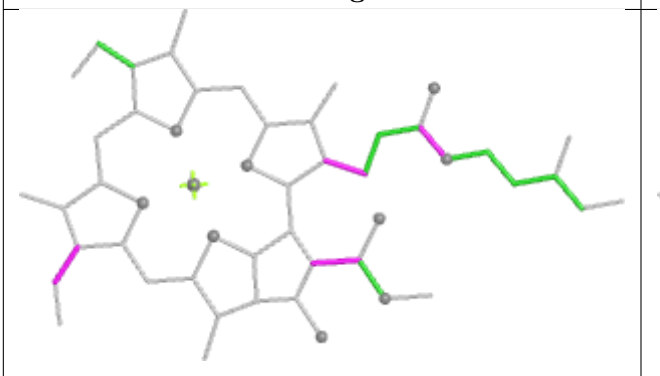

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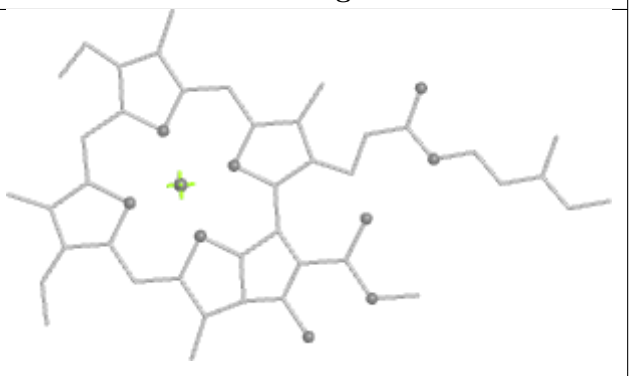
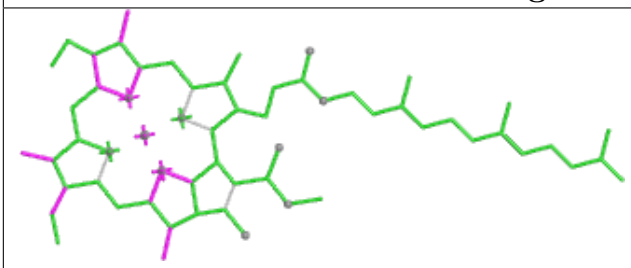
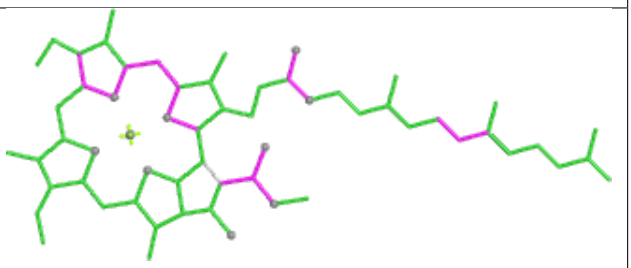
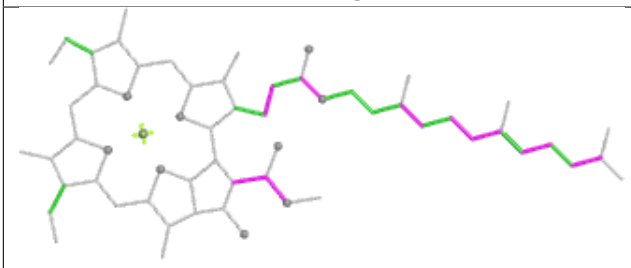
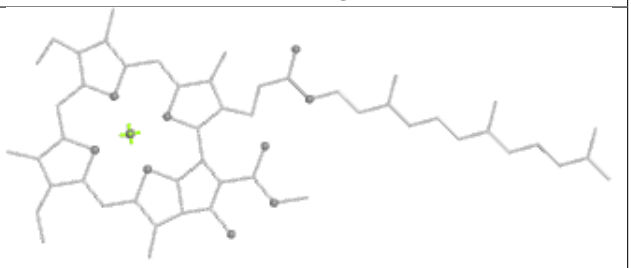


Rings

Ligand CLA a 825	
 Bond lengths	 Bond angles
 Torsions	 Rings

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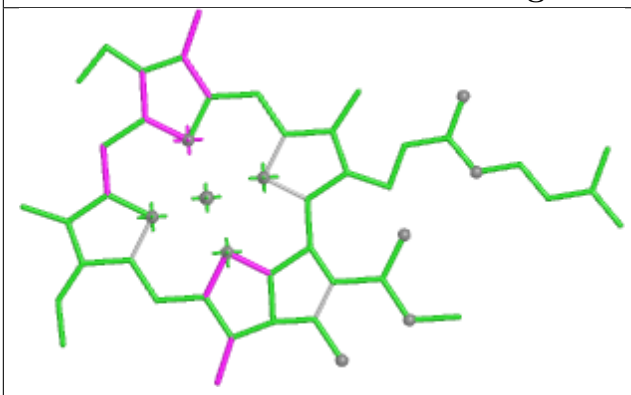
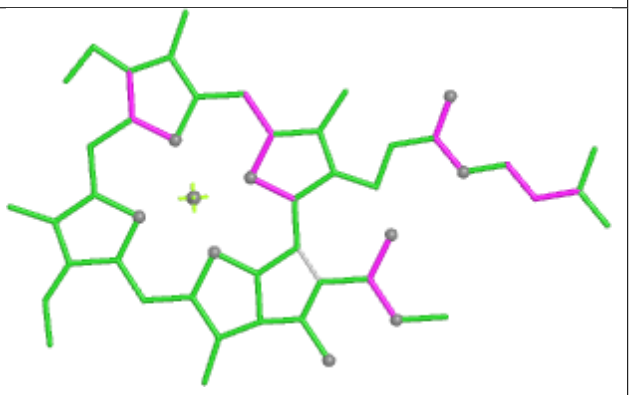
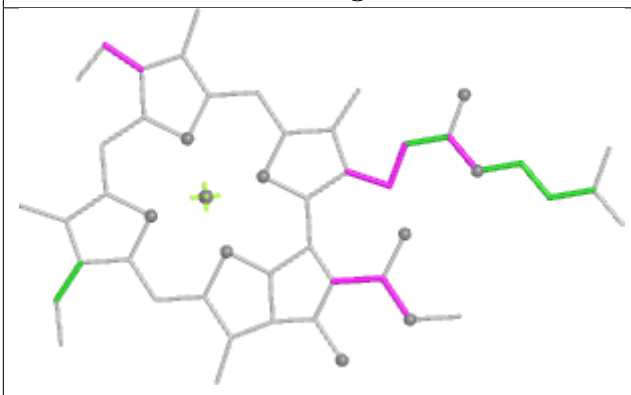
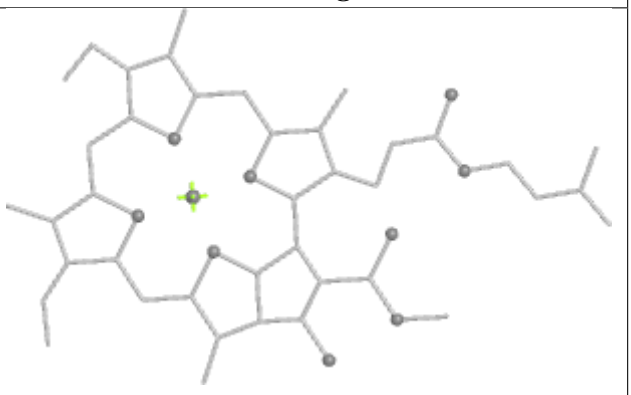
 Bond lengths	 Bond angles
 Torsions	 Rings

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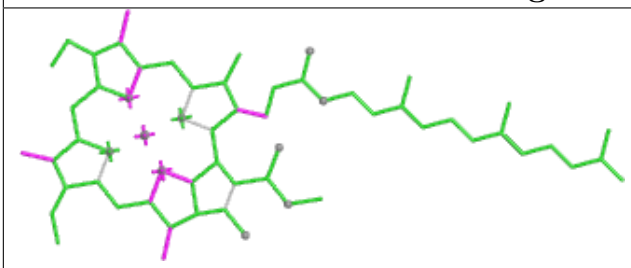
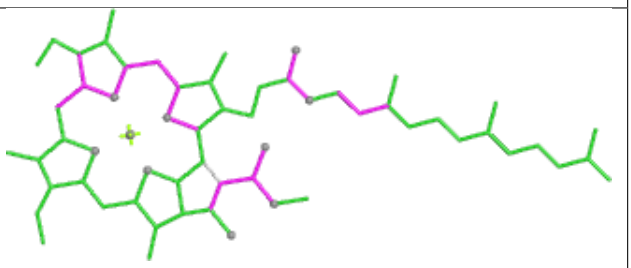
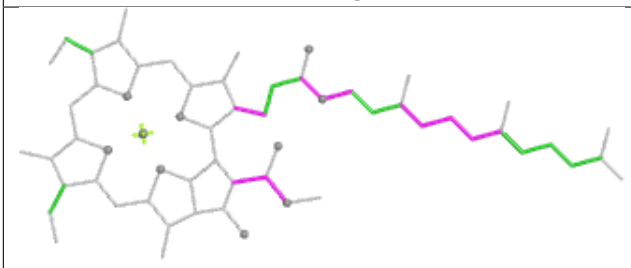
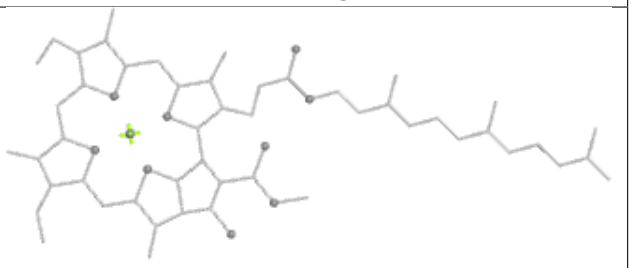
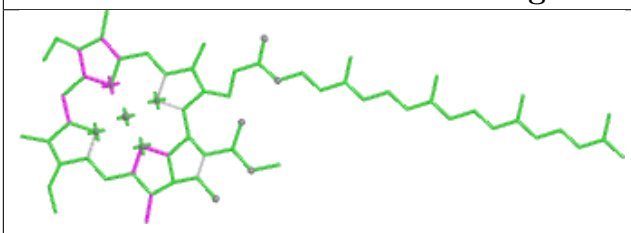
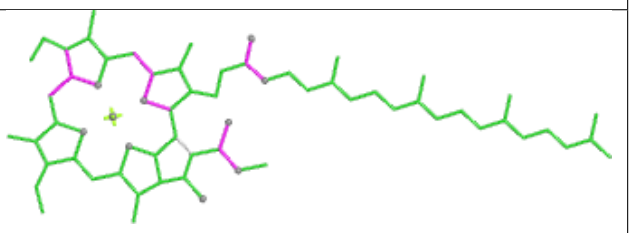
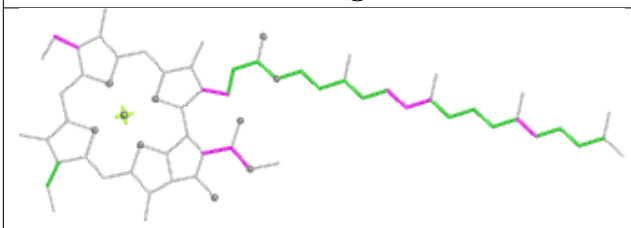
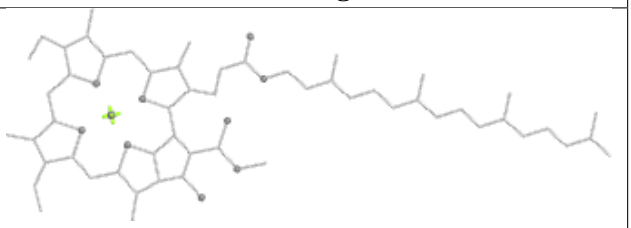
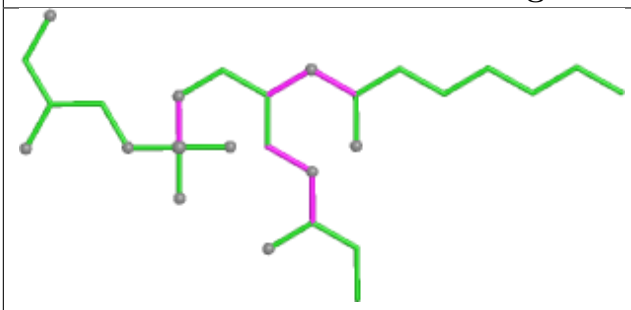
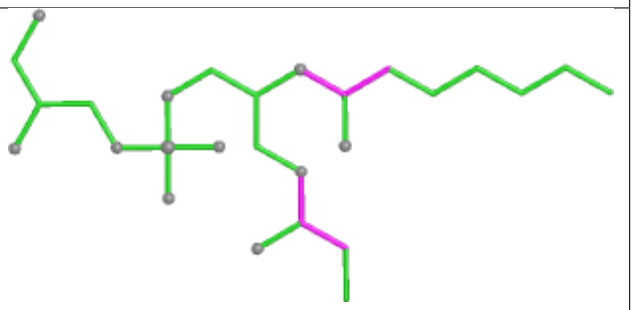
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

Ligand CLA a 828	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

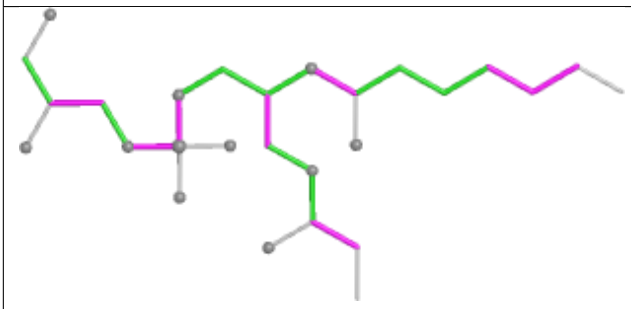
Ligand LHG a 832



Bond lengths



Bond angles



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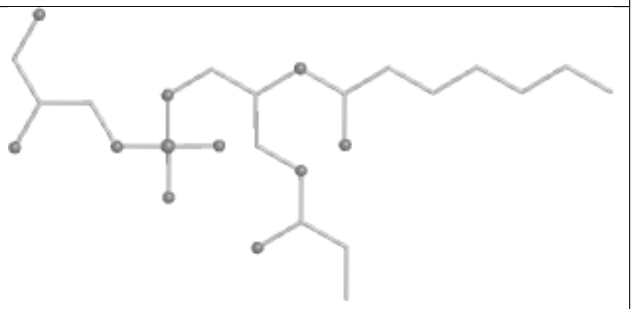
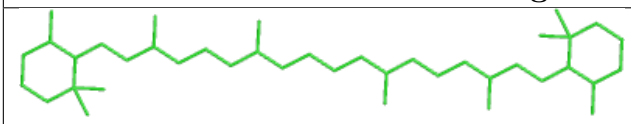


Rings

Ligand BCR i 103



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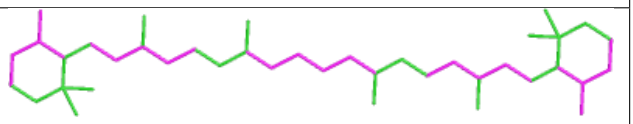
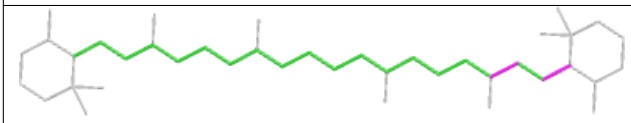


Bond angles



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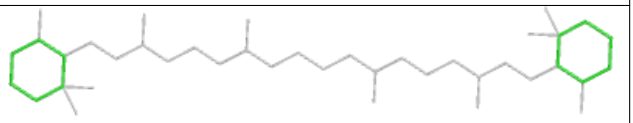
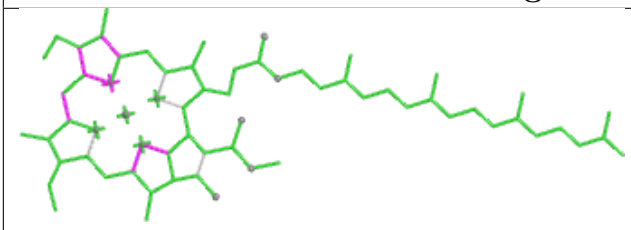


Rings

Ligand CLA B 312



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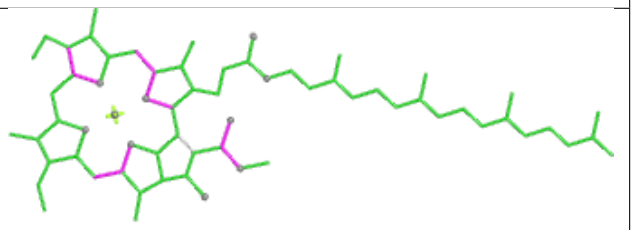

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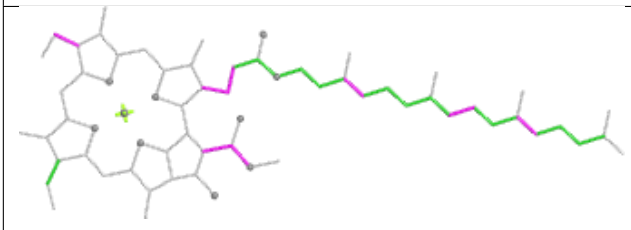

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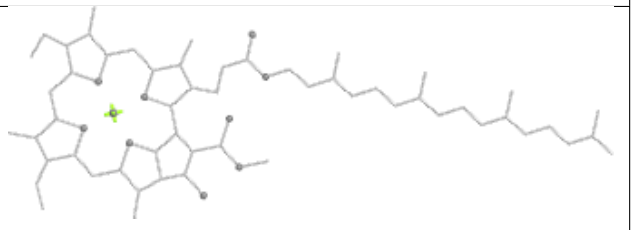
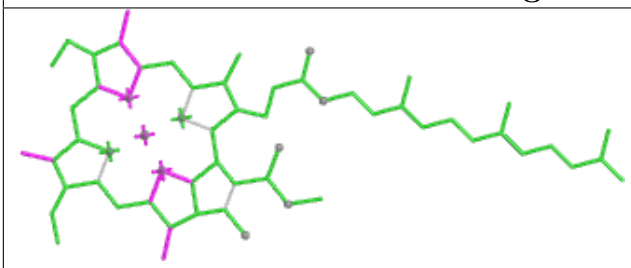
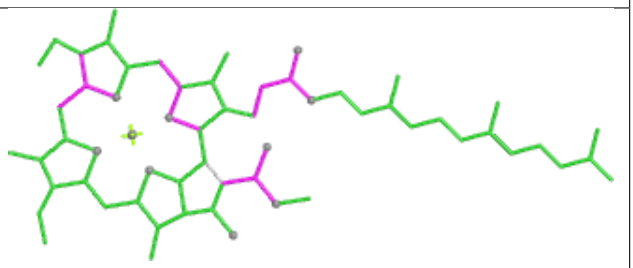


Rings

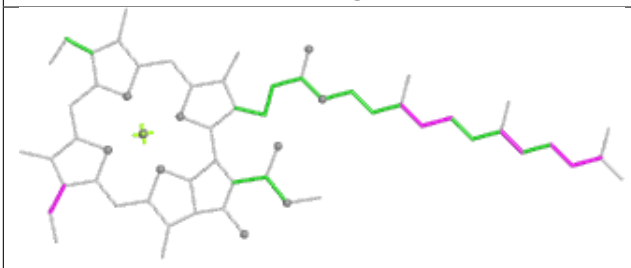
Ligand CLA H 310



Bond lengths



Bond angles



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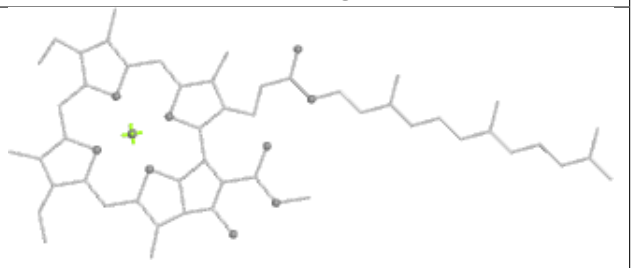
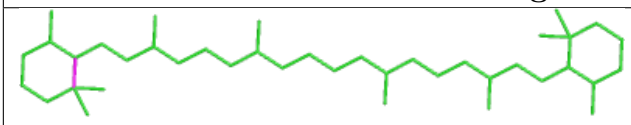
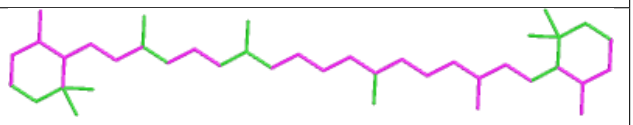


Rings

Ligand BCR f 201



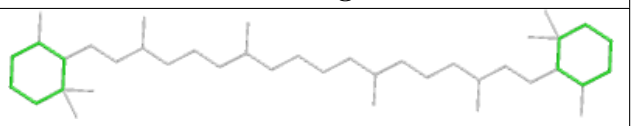
Bond lengths



Bond angles

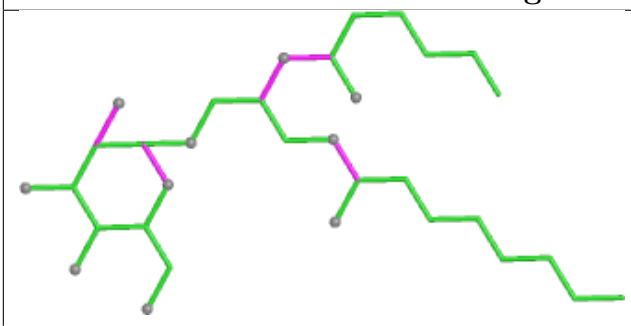


Torsions



Rings

Ligand LMG a 851



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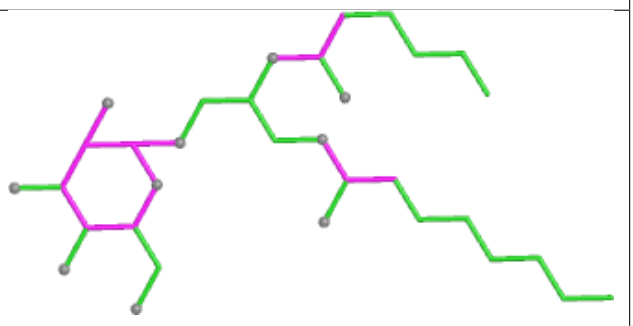
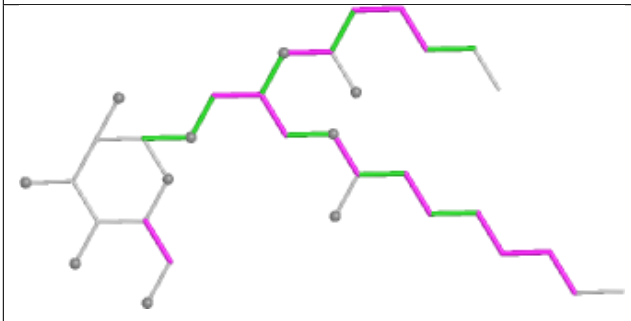


Bond angles



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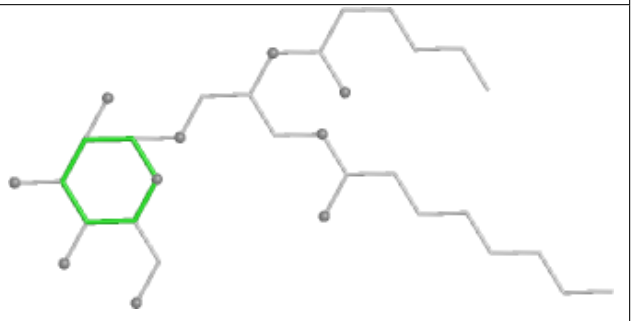
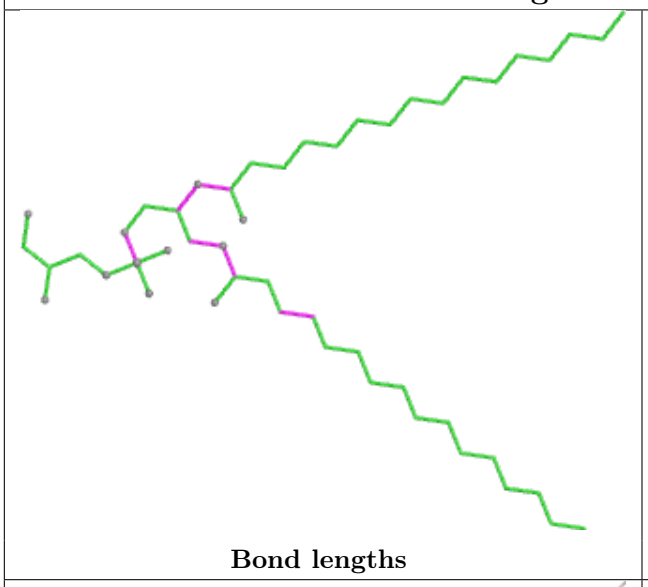


Rings

Ligand LHG j 102



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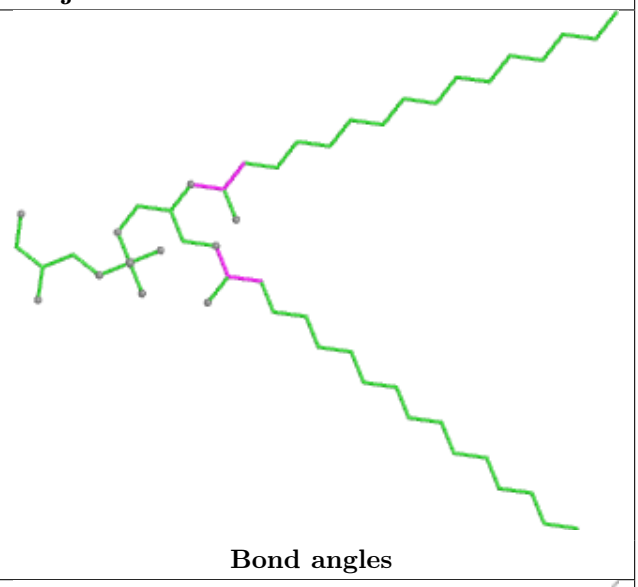
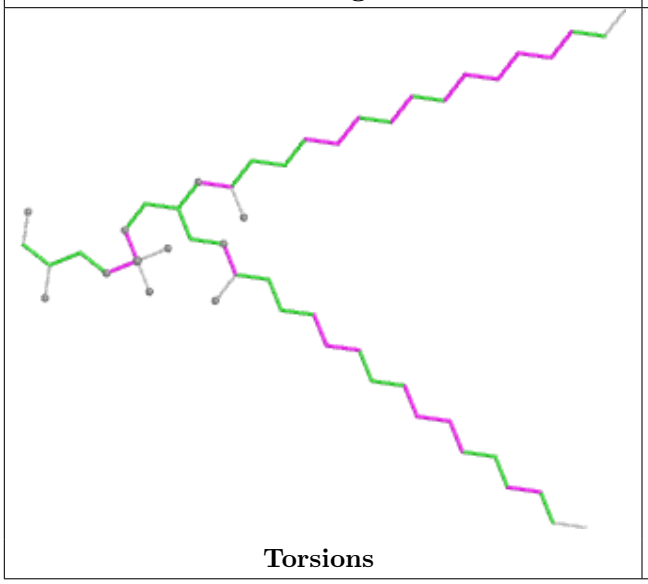
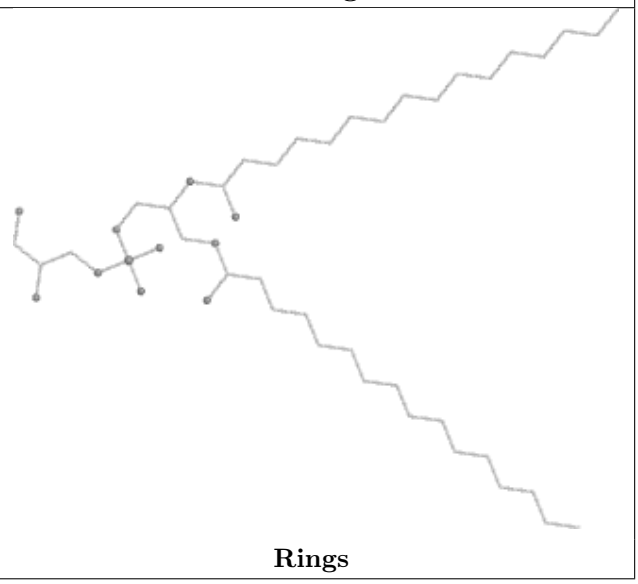


Bond angles

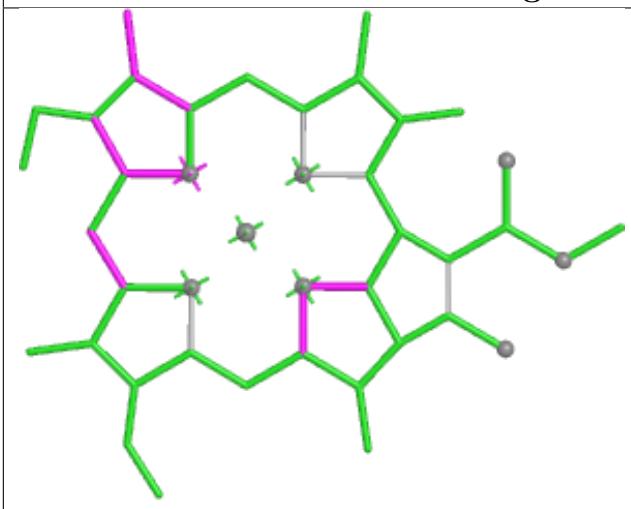


Torsions



Rings

Ligand CLA D 215



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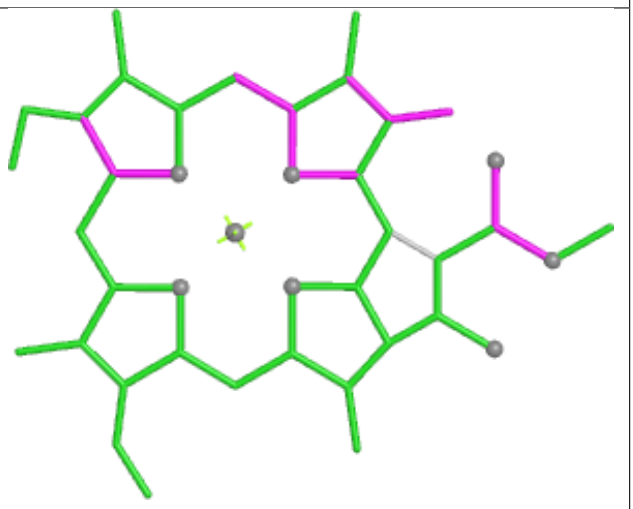

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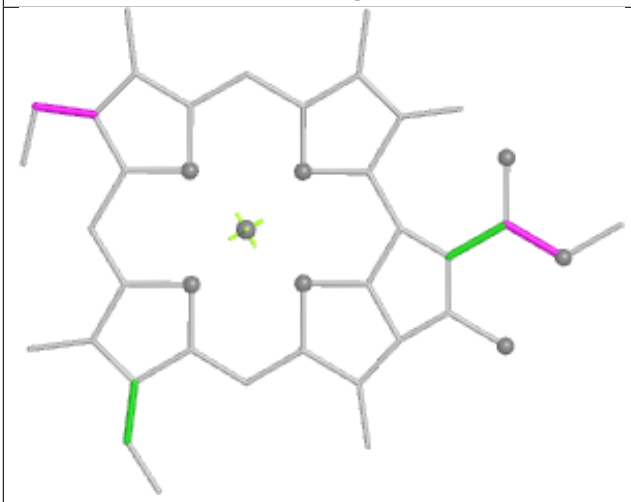

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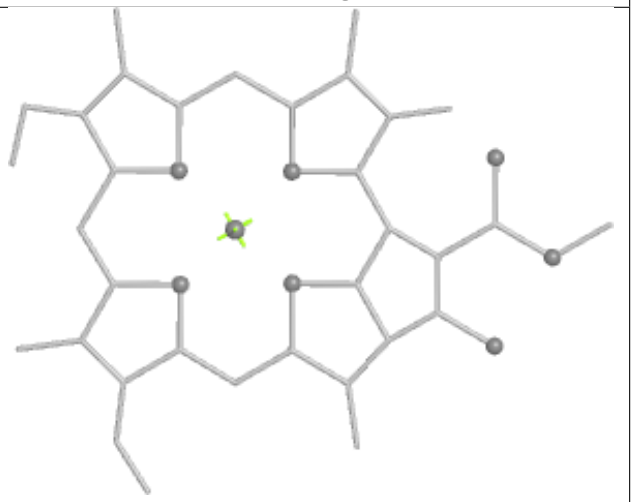
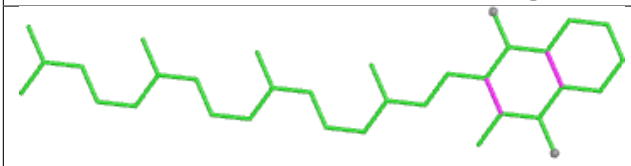


Rings

Ligand PQN b 831



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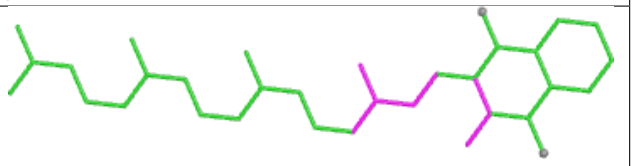

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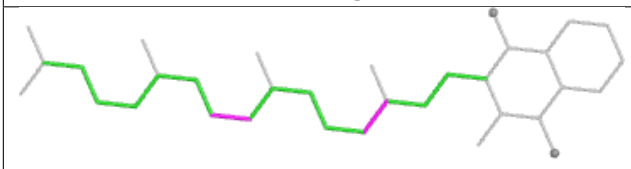

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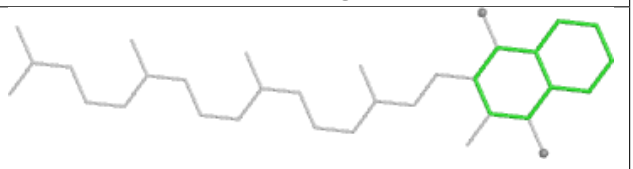
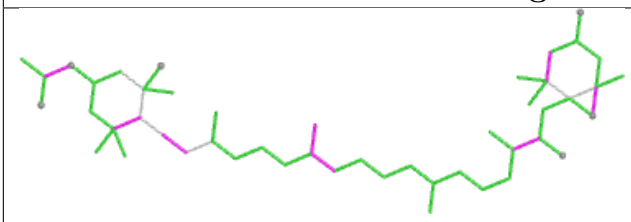


Rings

Ligand A86 D 204



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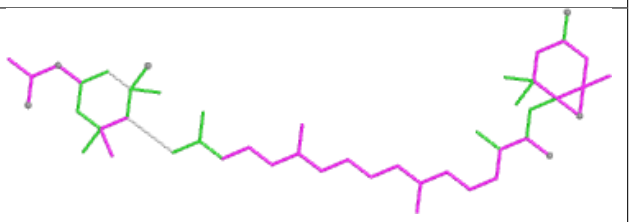

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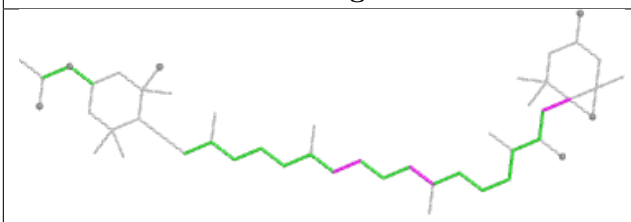

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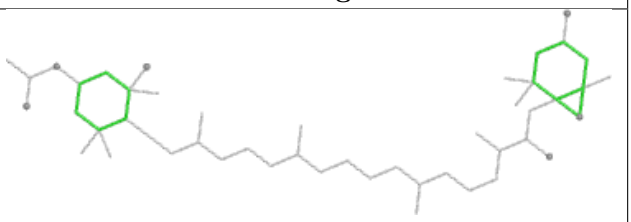
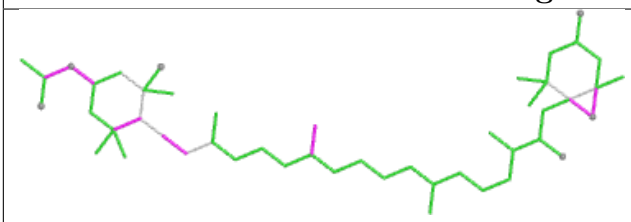


Rings

Ligand A86 r 203



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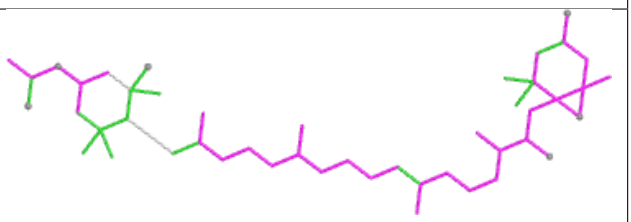

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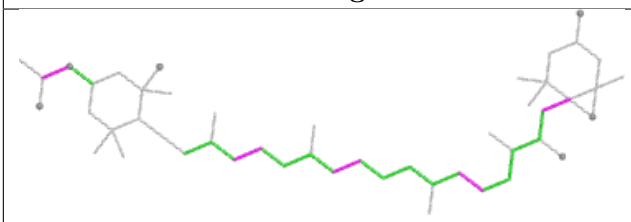

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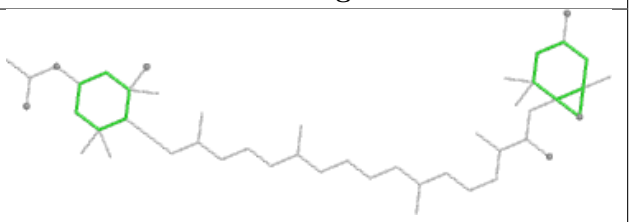
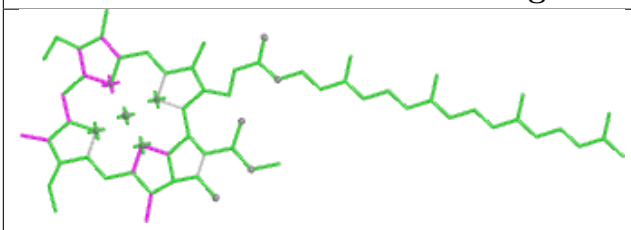


Rings

Ligand CLA a 847



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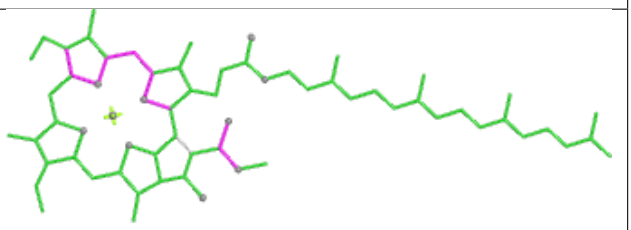
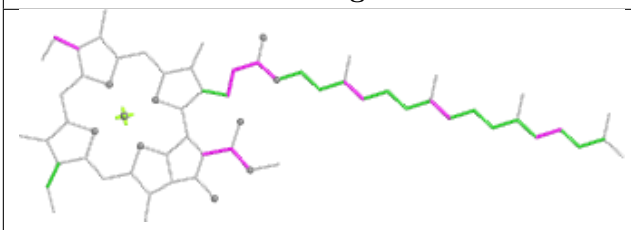


Bond angles



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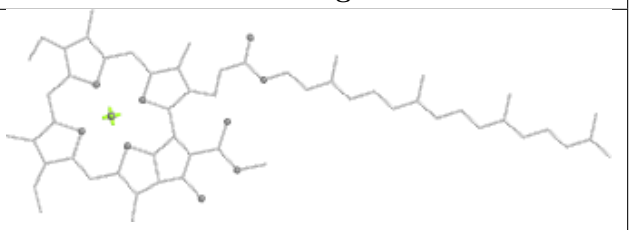
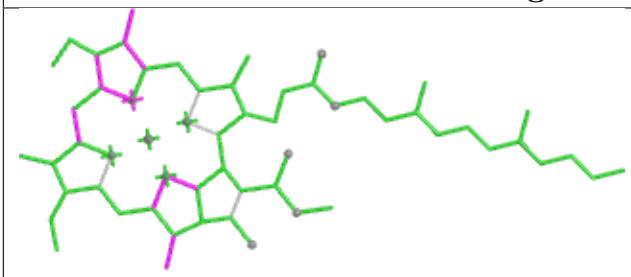


Rings

Ligand CLA b 823



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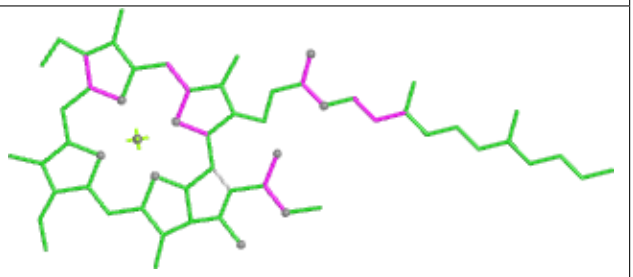
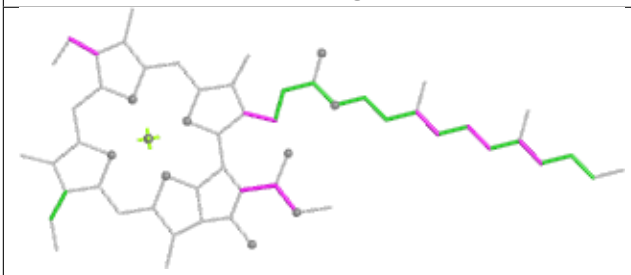


Bond angles



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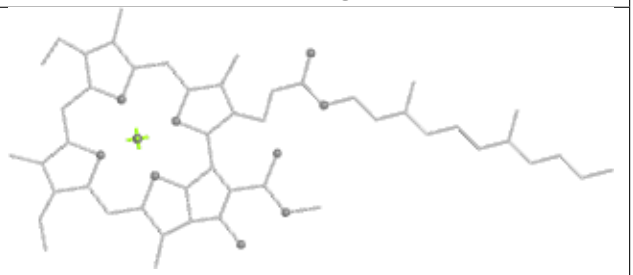
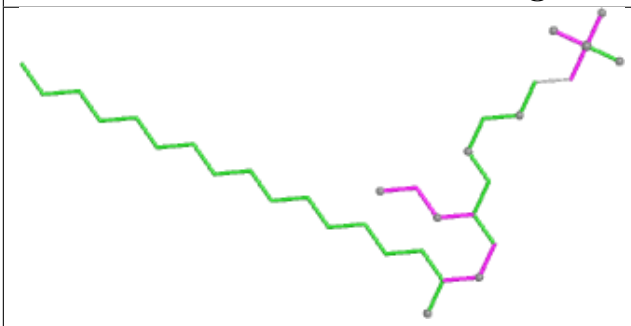


Rings

Ligand SQD a 849



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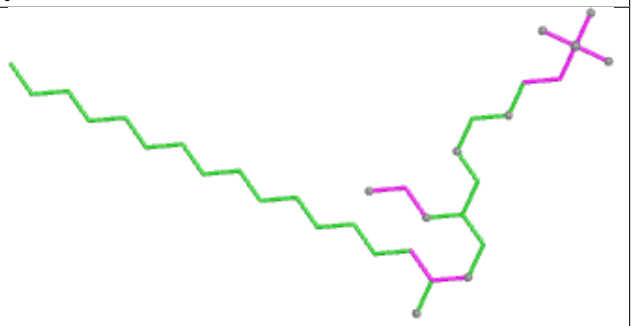
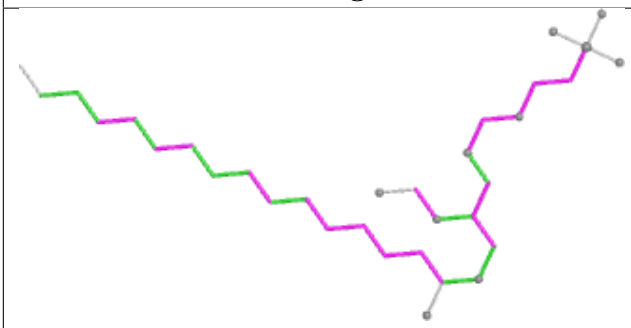


Bond angles



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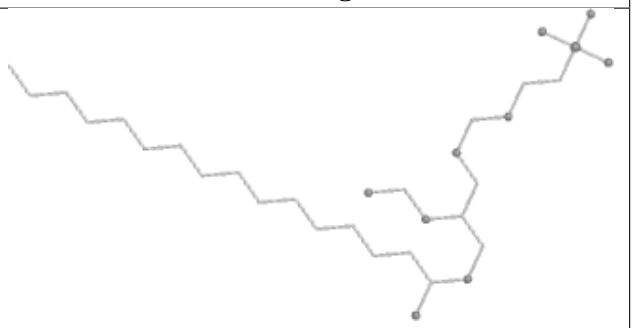
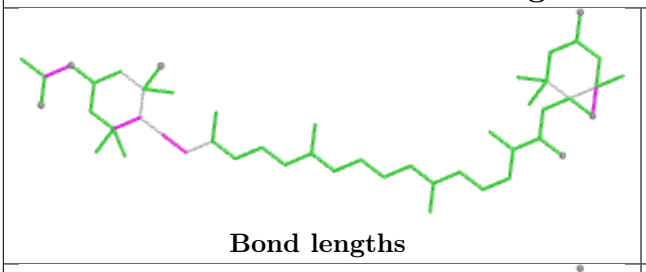


Rings

Ligand A86 m 102



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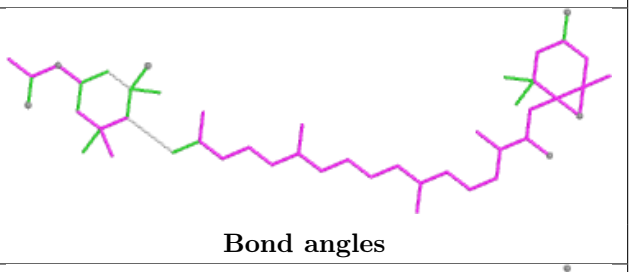
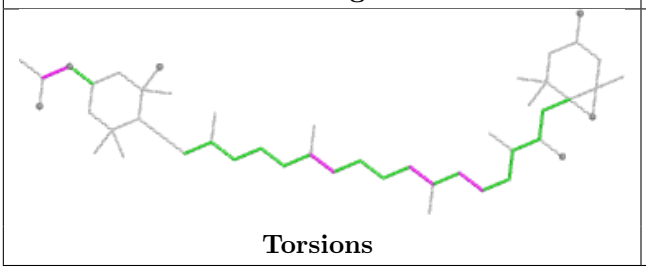


Bond angles



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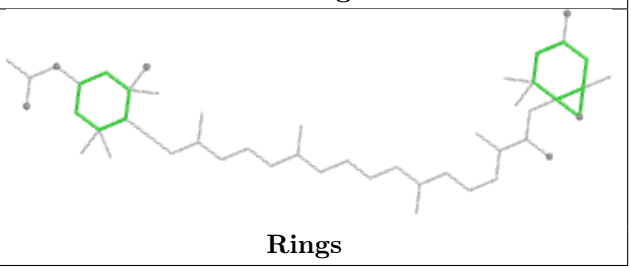
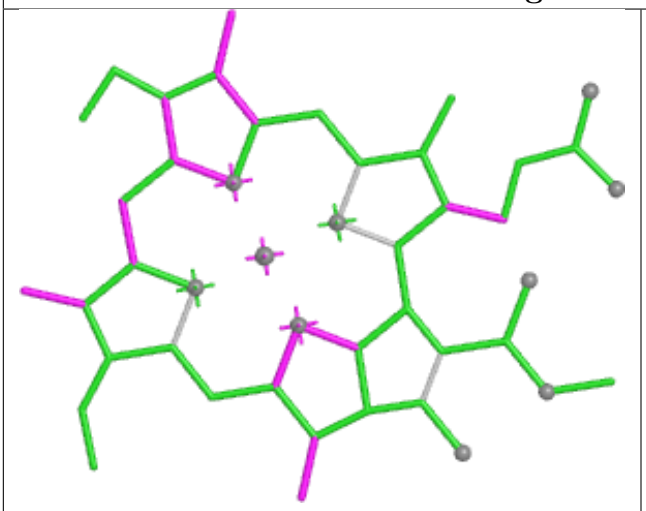


Rings

Ligand CLA E 314



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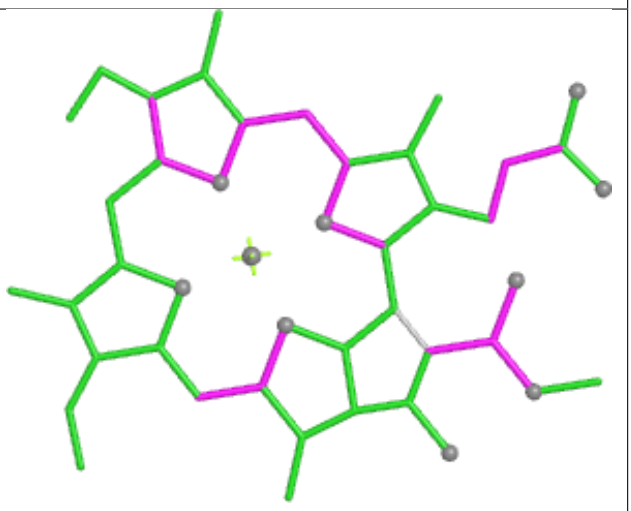

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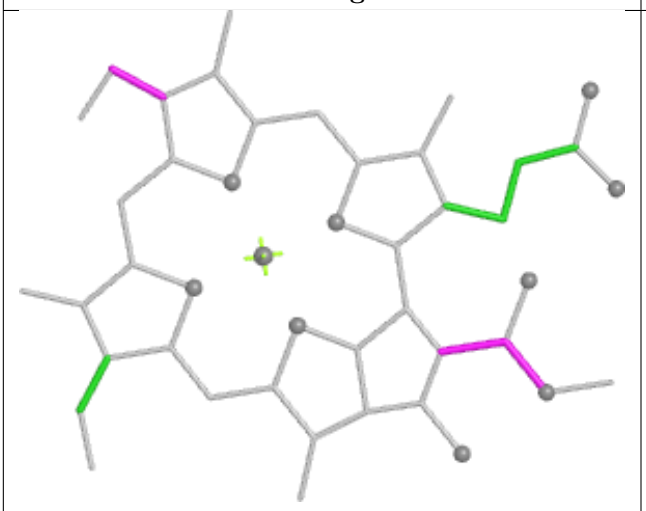

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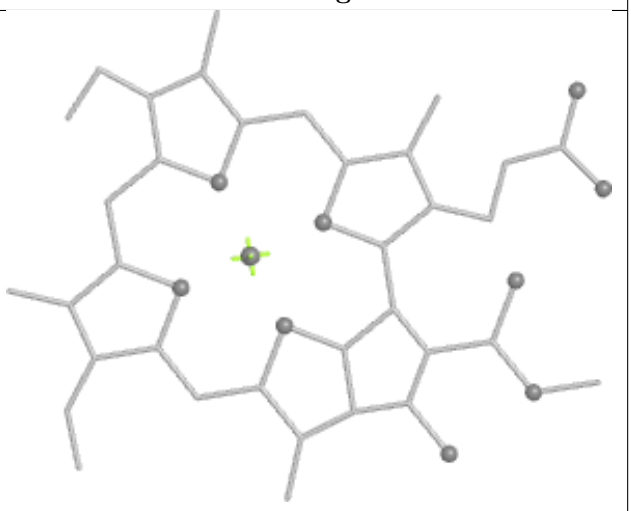
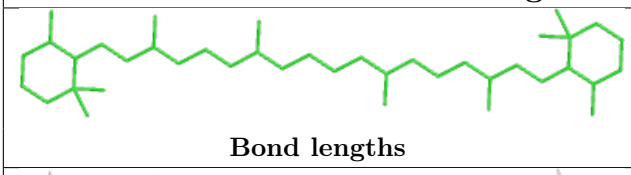


Rings

Ligand BCR b 833



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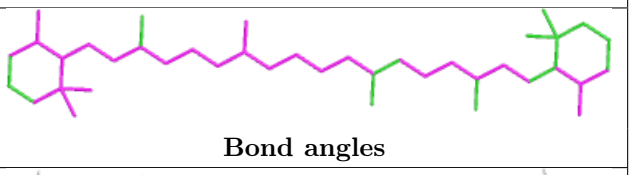
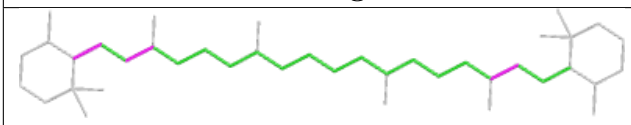


Bond angles



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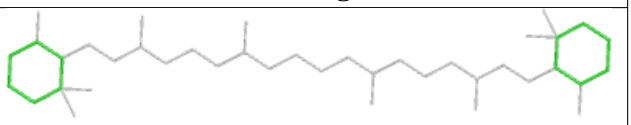
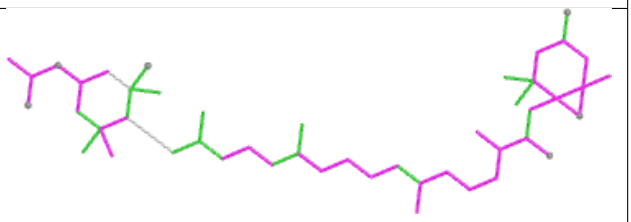


Rings

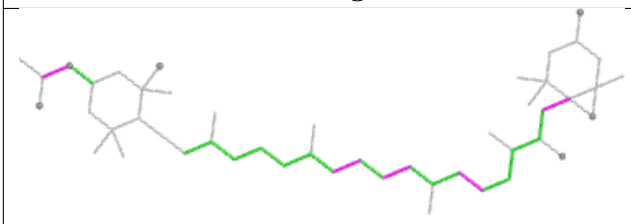
Ligand A86 D 206



Bond lengths



Bond angles



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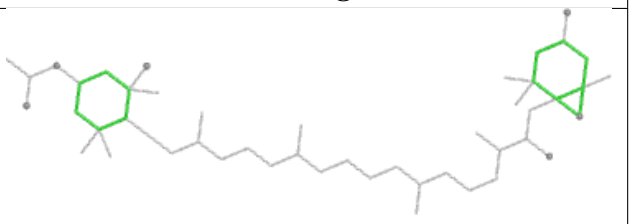
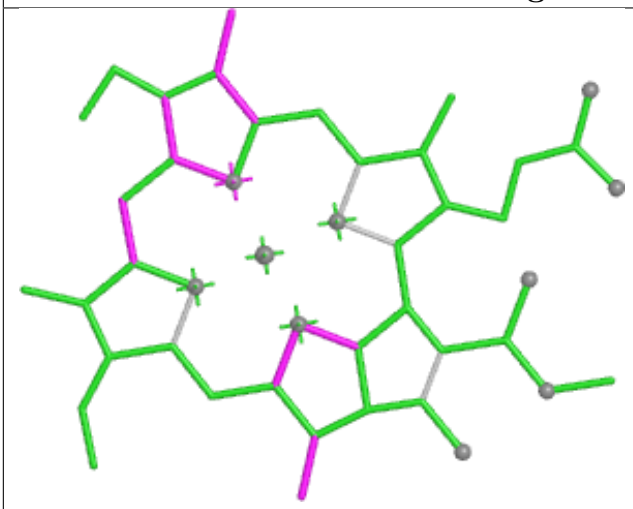


Rings

Ligand CLA b 825



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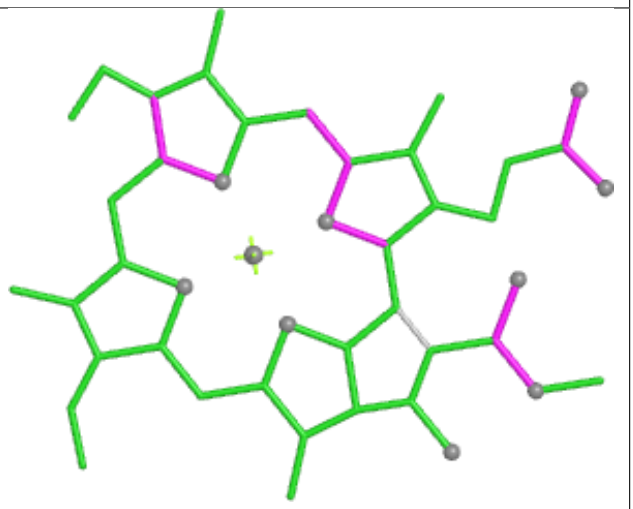
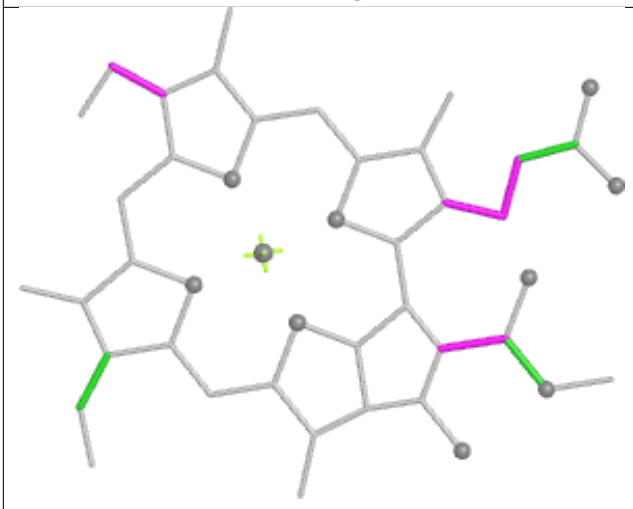


Bond angles

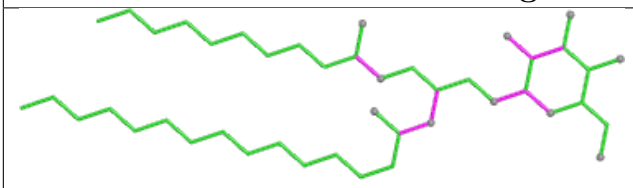


Torsions



Rings

Ligand LMG C 319



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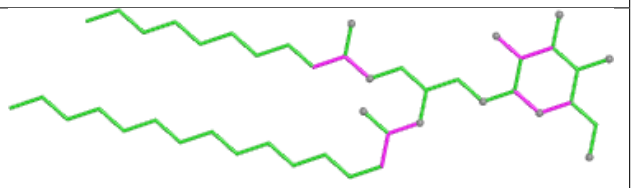
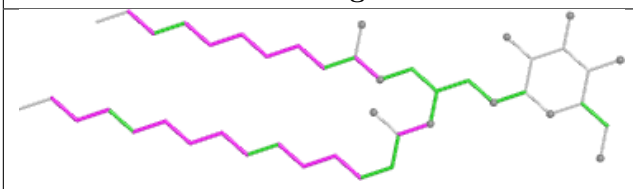
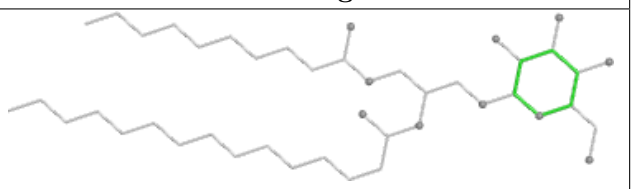


Bond angles

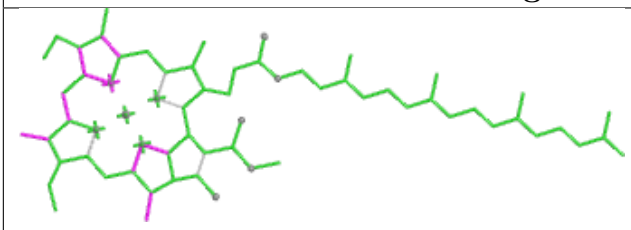


Torsions



Rings

Ligand CLA D 213



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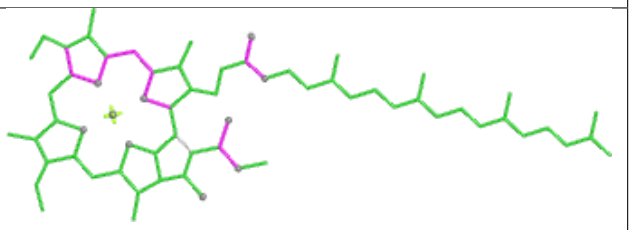
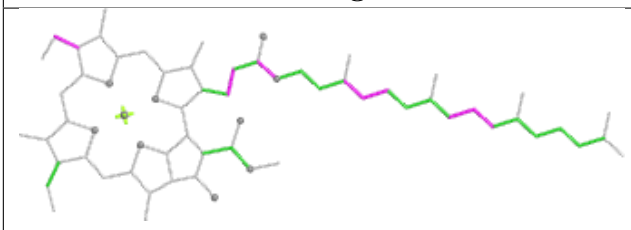


Bond angles



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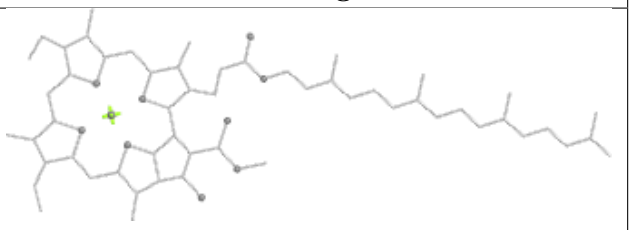
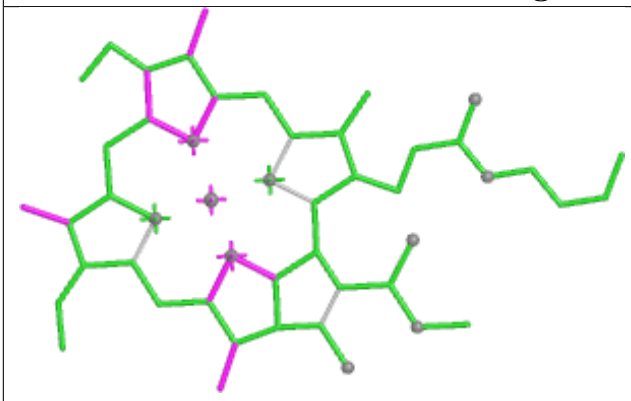
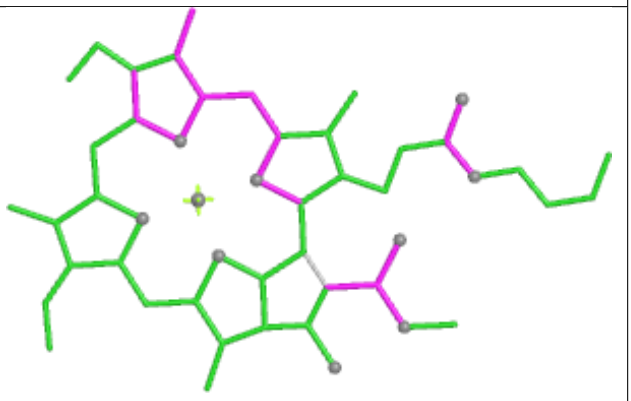


Rings

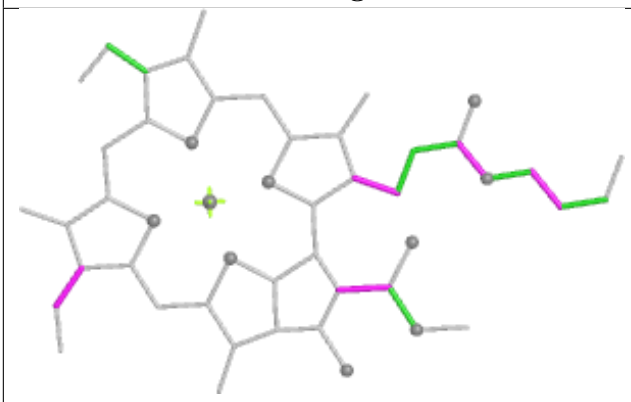
Ligand CLA l 202



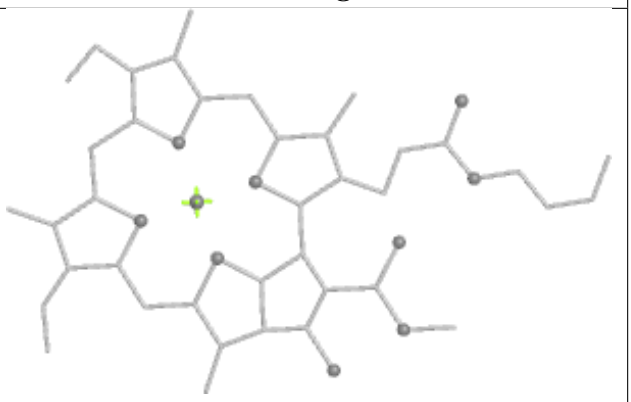
Bond lengths



Bond angles

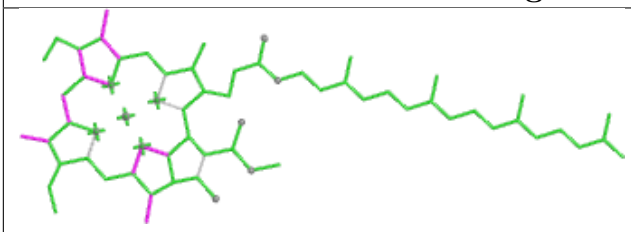


Torsions



Rings

Ligand CLA E 309



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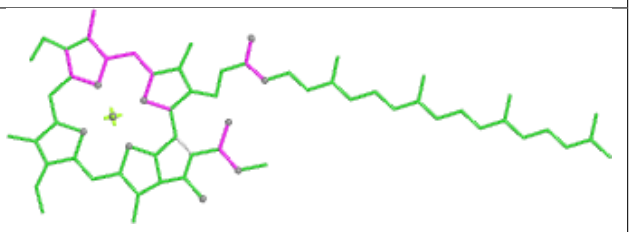

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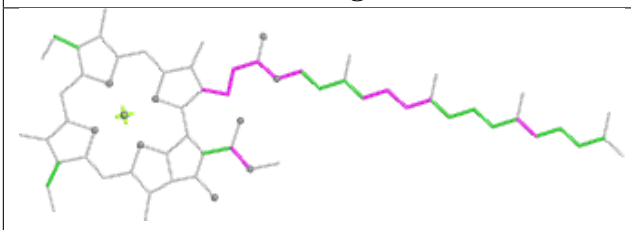

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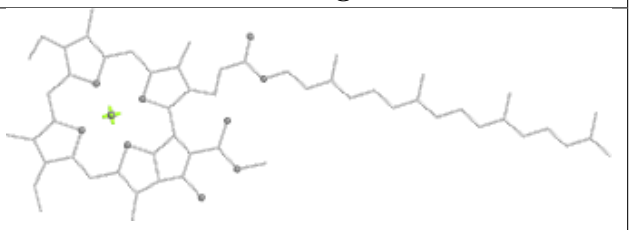
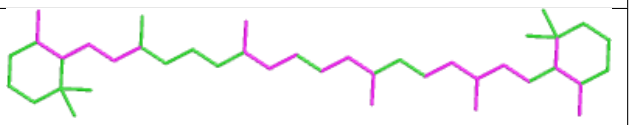


Rings

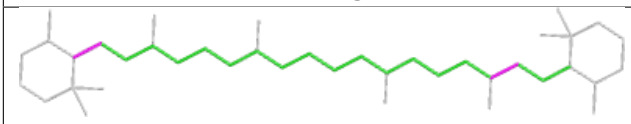
Ligand BCR a 850



Bond lengths



Bond angles



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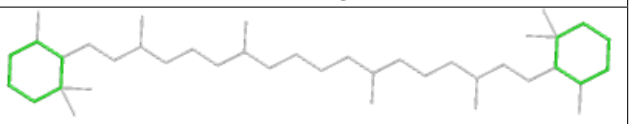
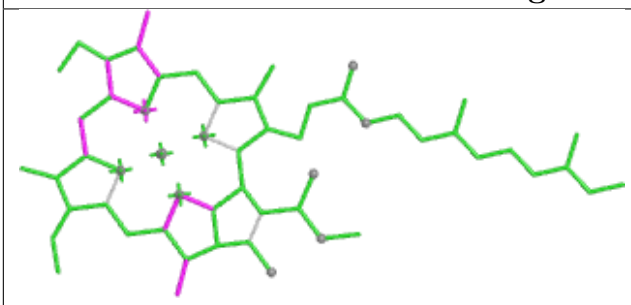


Rings

Ligand CLA a 848



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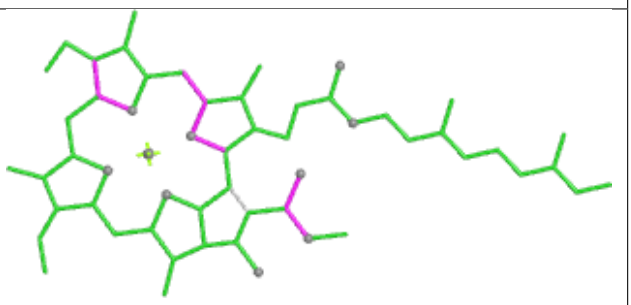
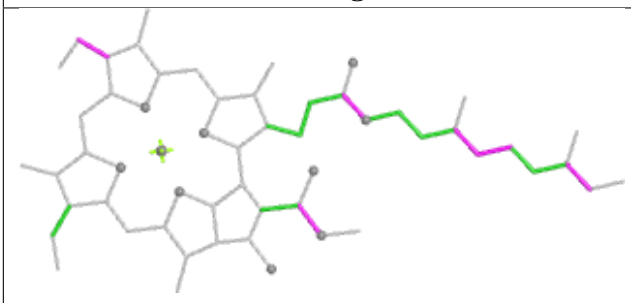


Bond angles



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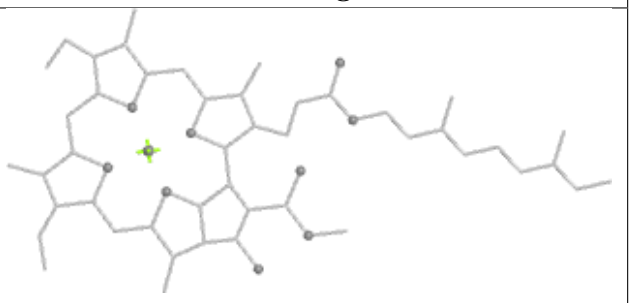
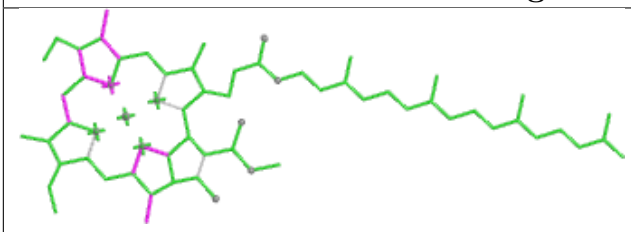


Rings

Ligand CLA b 808



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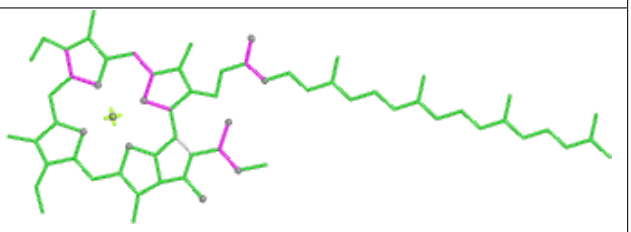
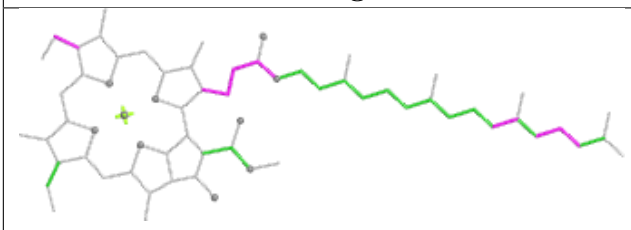


Bond angles



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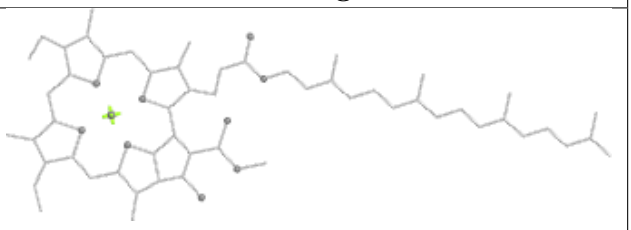
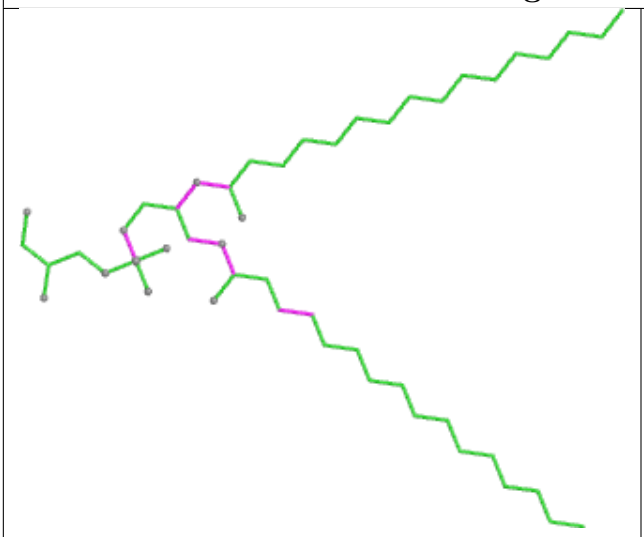


Rings

Ligand LHG E 301



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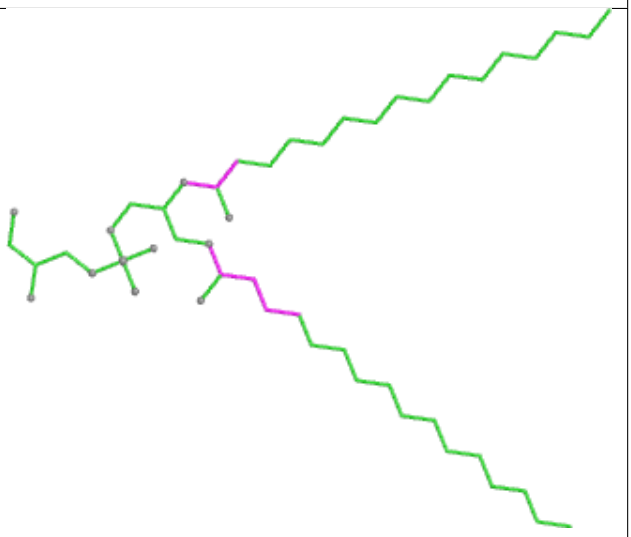

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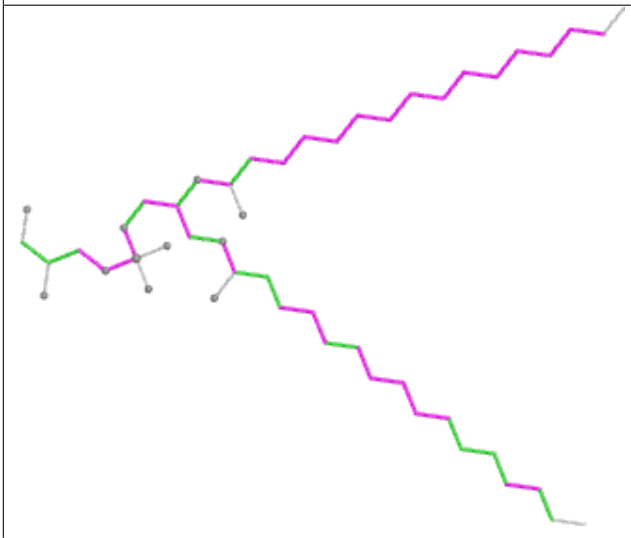

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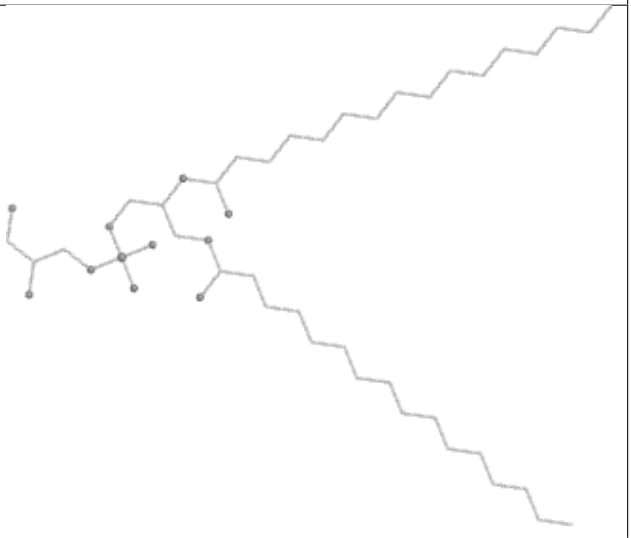
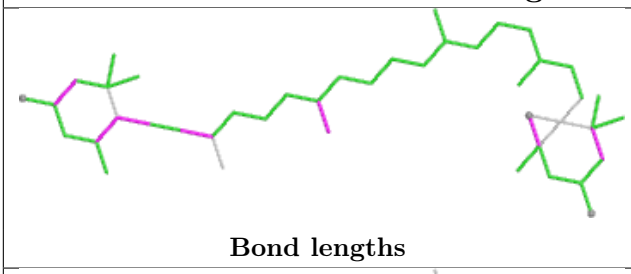


Rings

Ligand DD6 B 303



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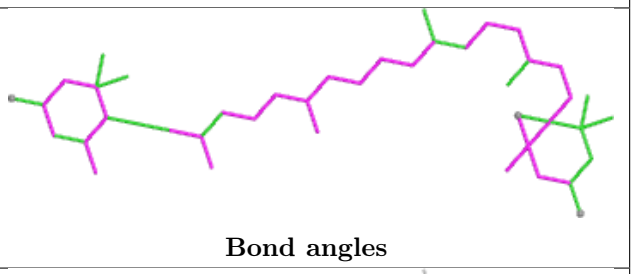
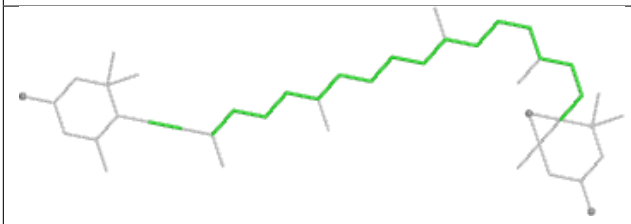


Bond angles



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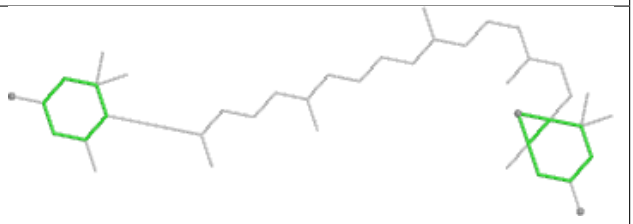
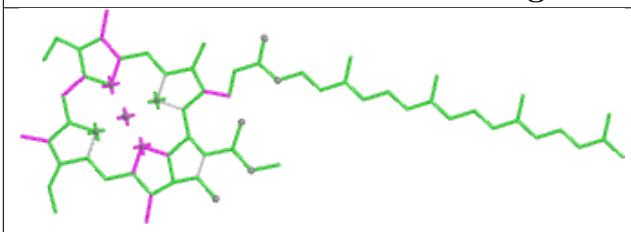


Rings

Ligand CLA b 803



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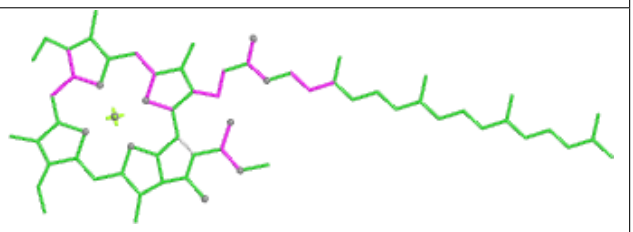
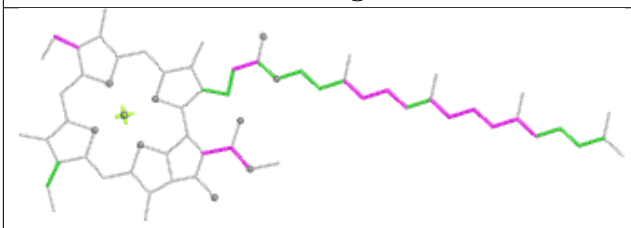


Bond angles



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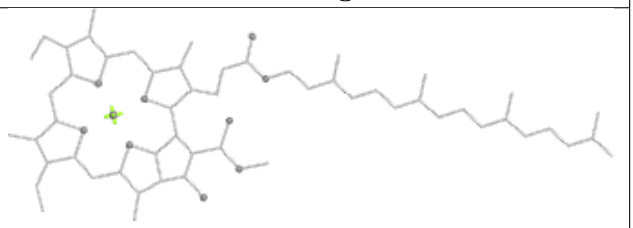
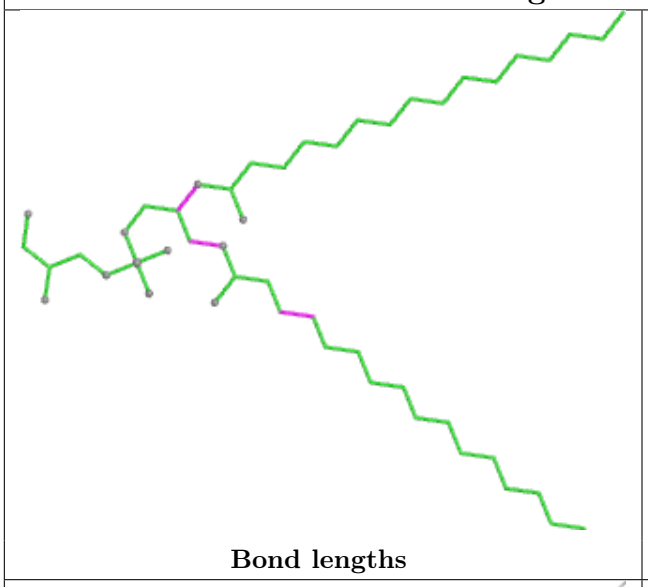


Rings

Ligand LHG a 831



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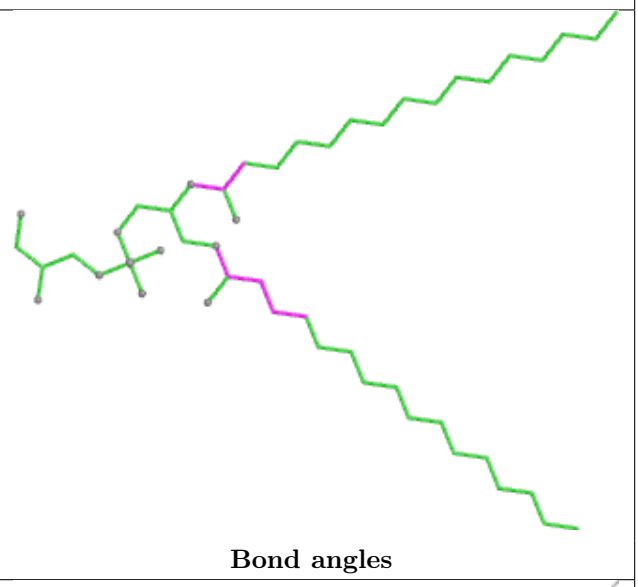

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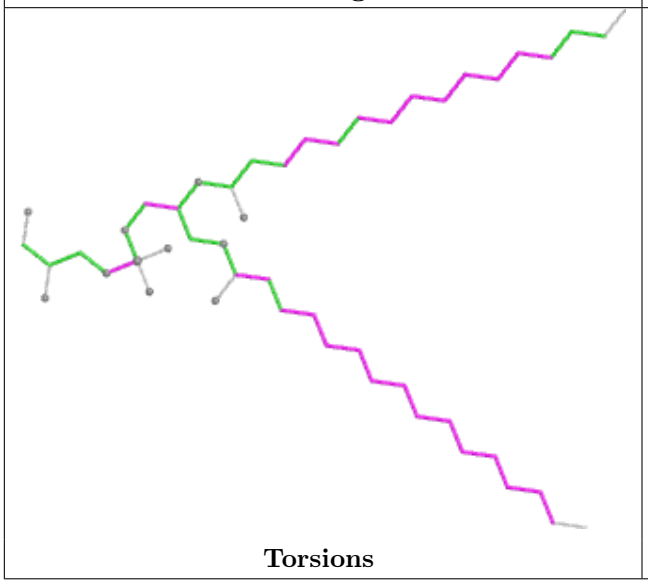

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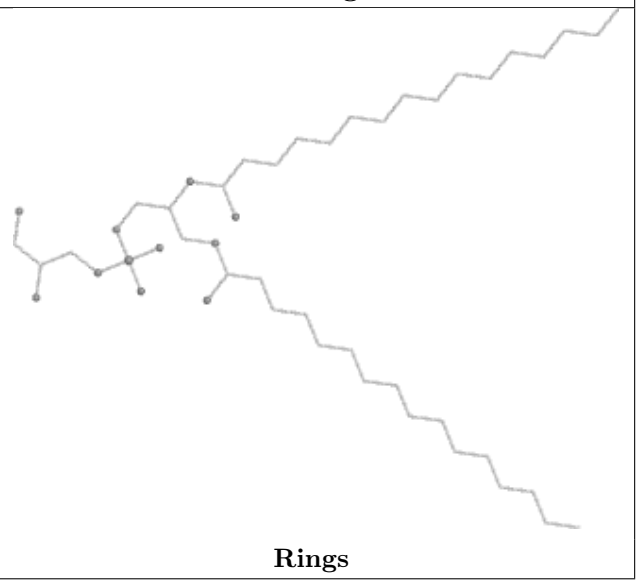
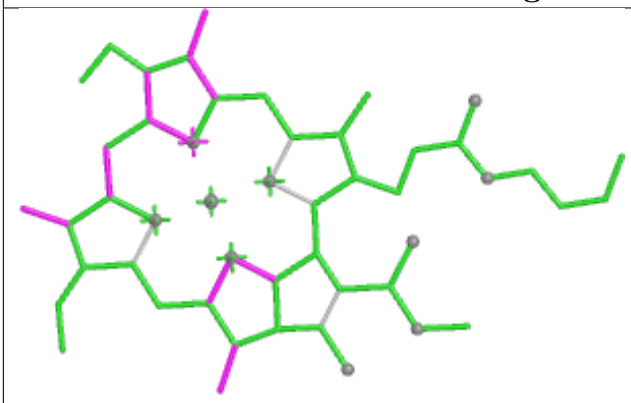


Rings

Ligand CLA D 209



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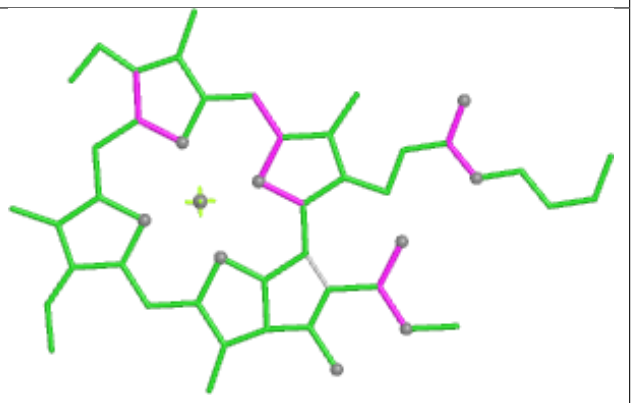
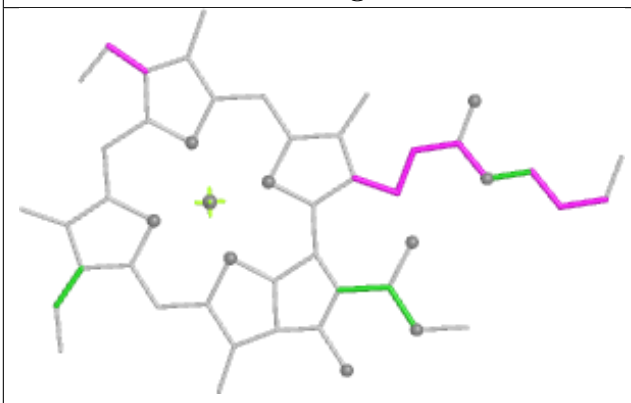


Bond angles



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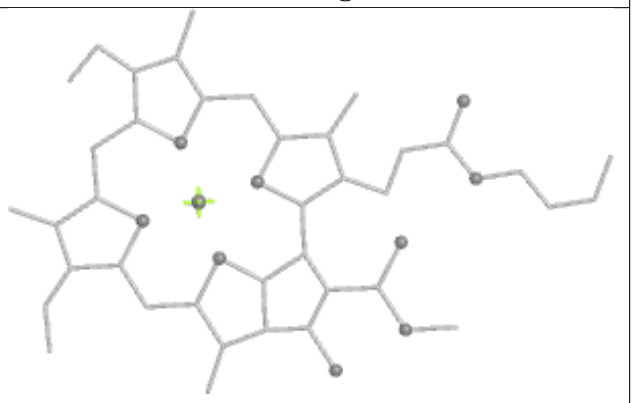
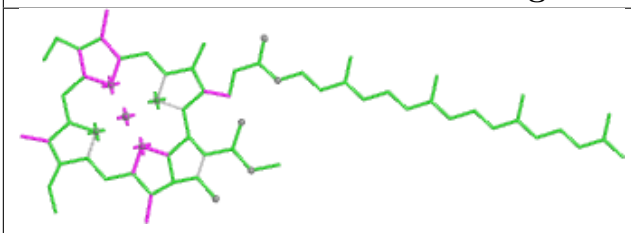


Rings

Ligand CLA a 803



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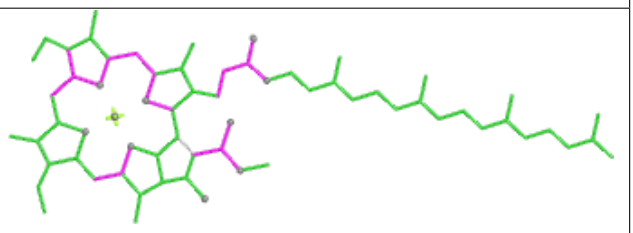
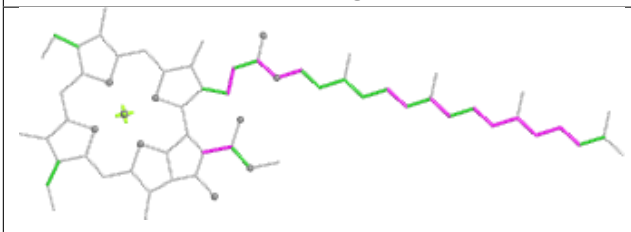


Bond angles



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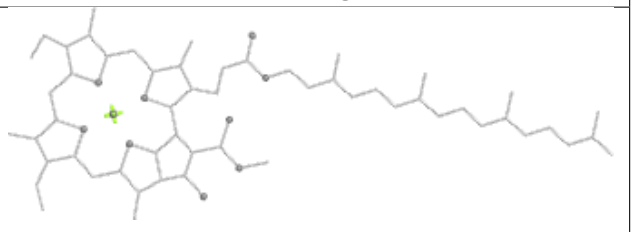
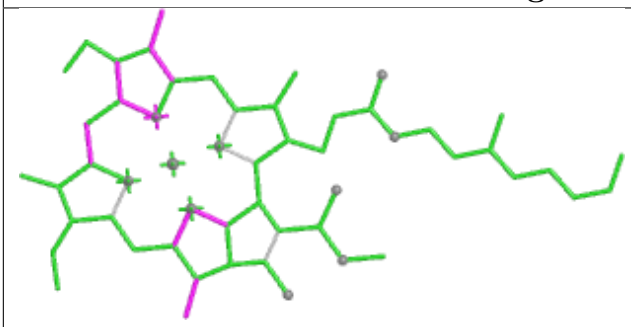
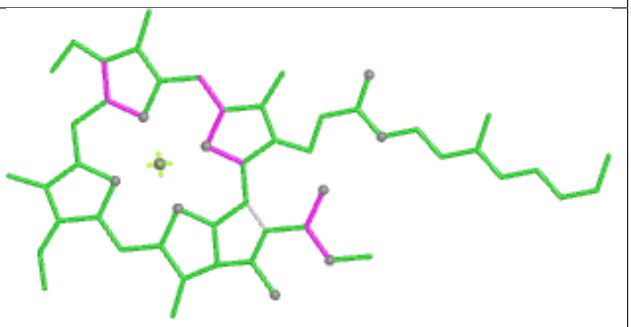
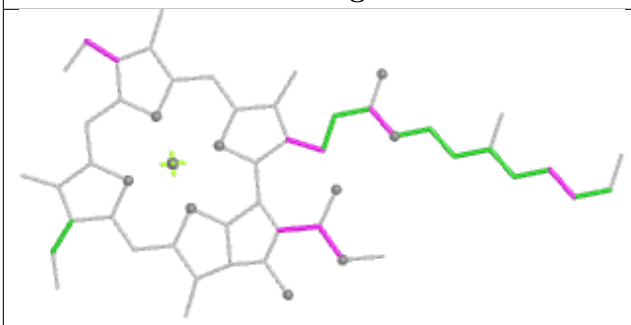
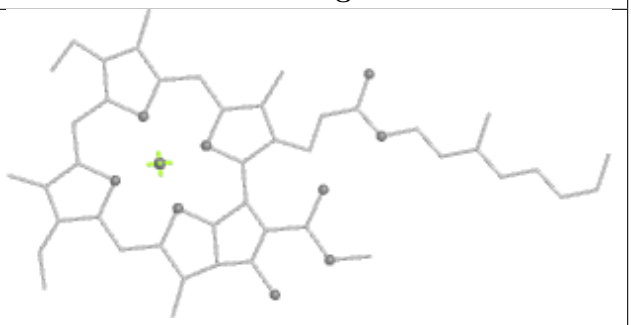
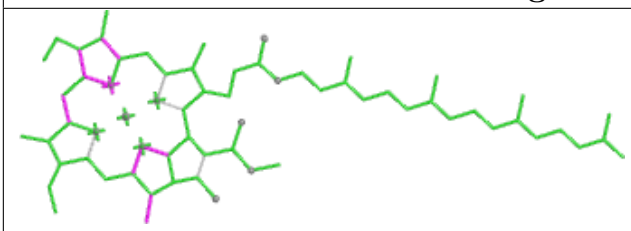
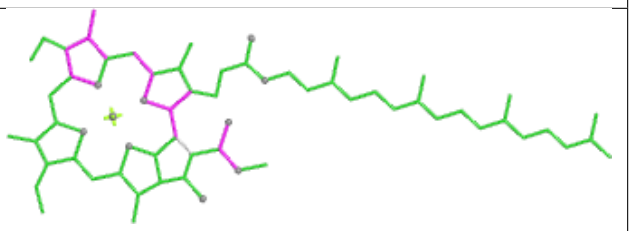
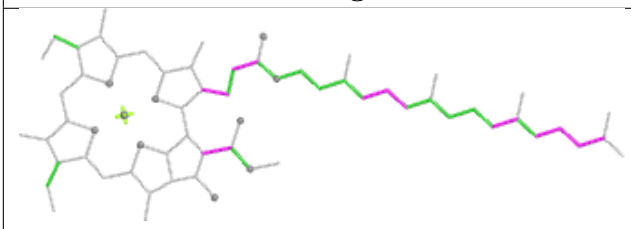
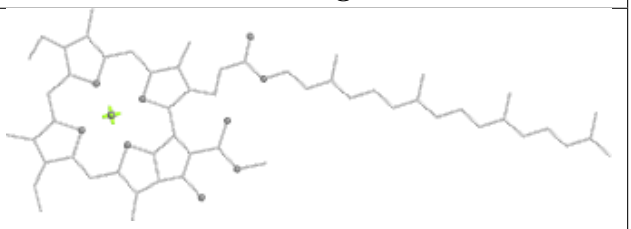
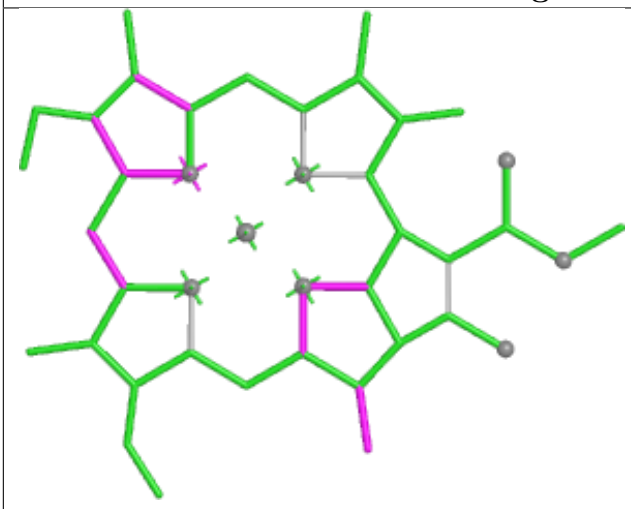


Rings

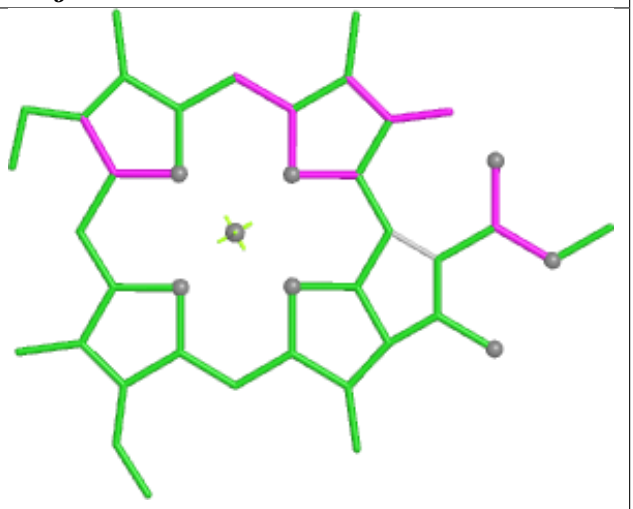
Ligand CLA b 848	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA a 843	
	
Bond lengths	Bond angles
	
Torsions	Rings

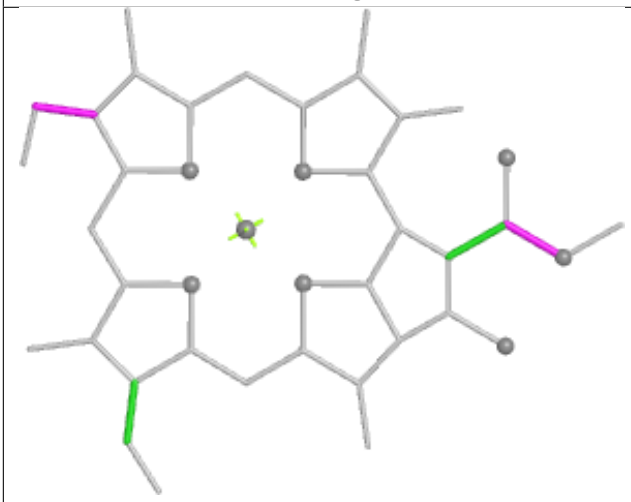
Ligand CLA j 104



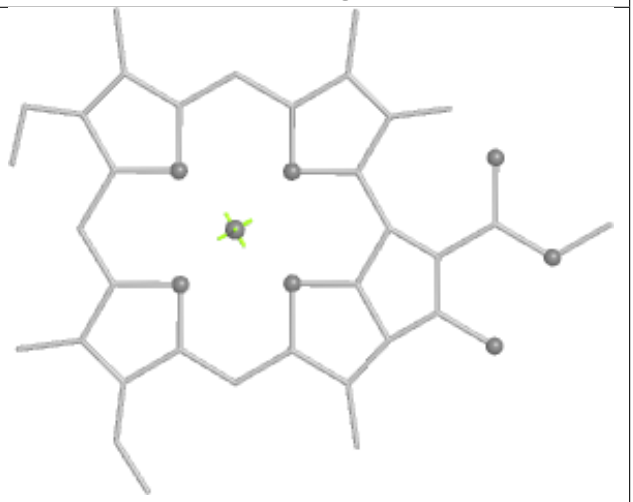
Bond lengths



Bond angles

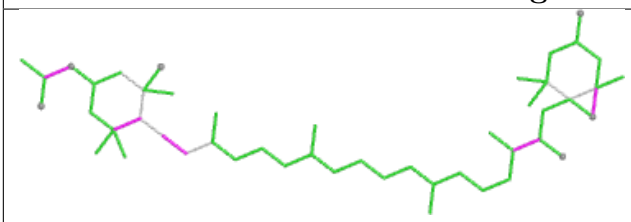


Torsions

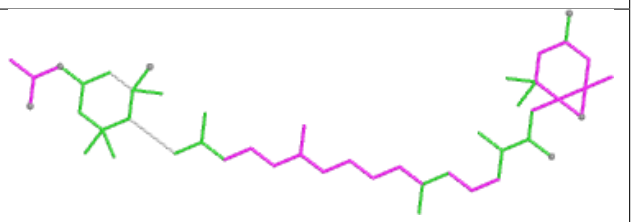


Rings

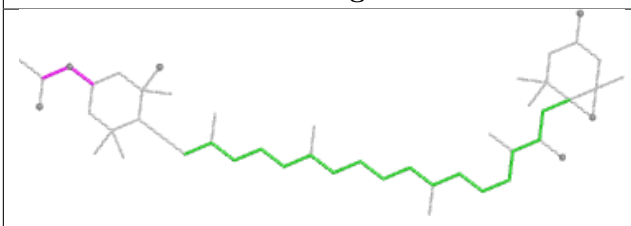
Ligand A86 C 304



Bond lengths



Bond angles



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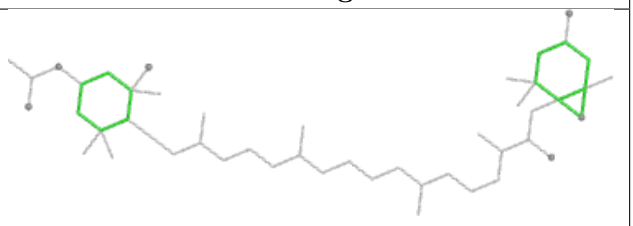
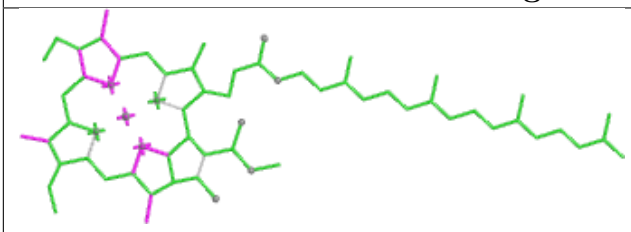
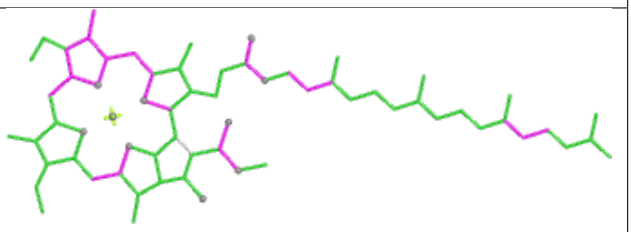


Rings

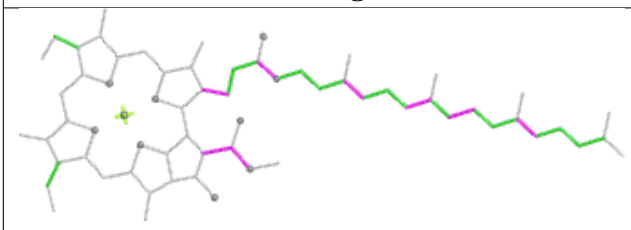
Ligand CLA H 314



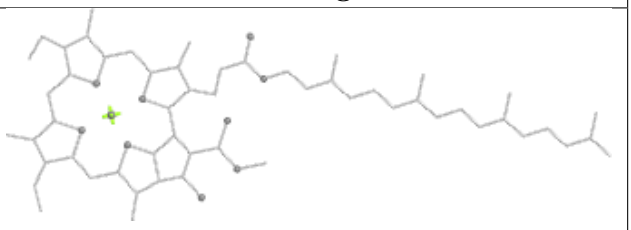
Bond lengths



Bond angles

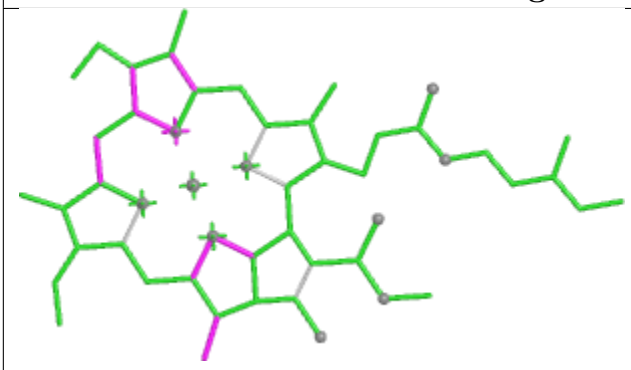


Torsions



Rings

Ligand CLA a 824



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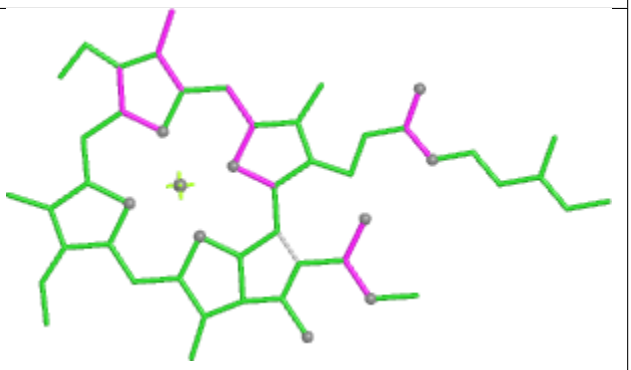

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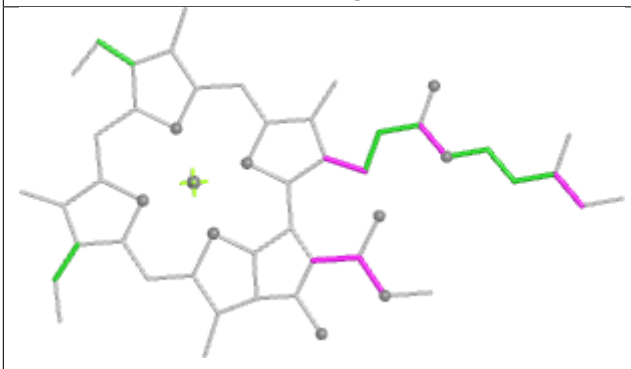

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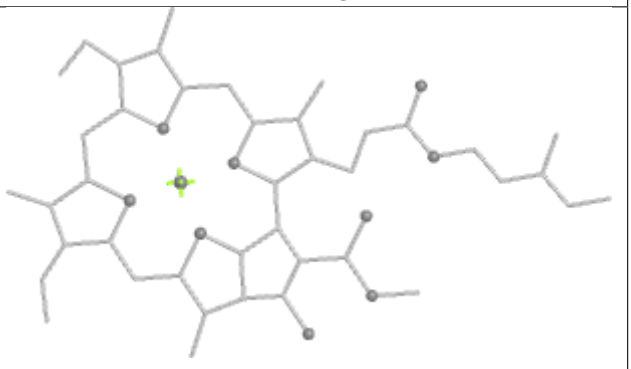
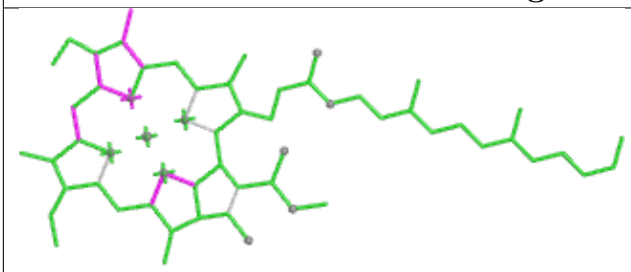


Rings

Ligand CLA b 812



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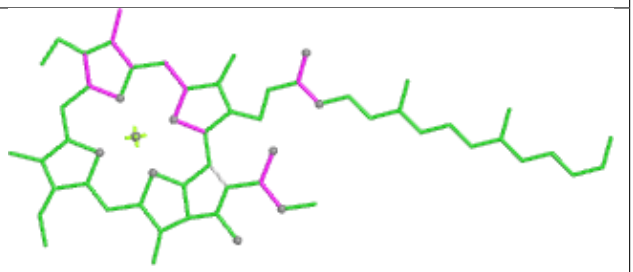
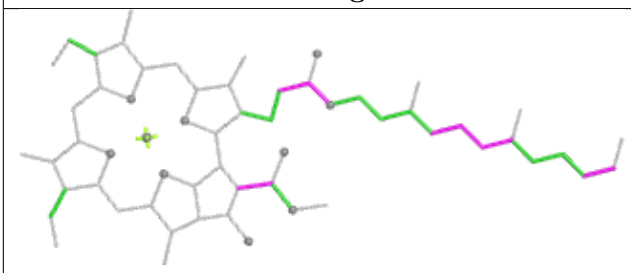


Bond angles



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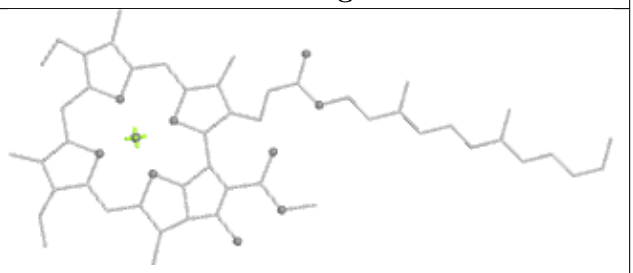
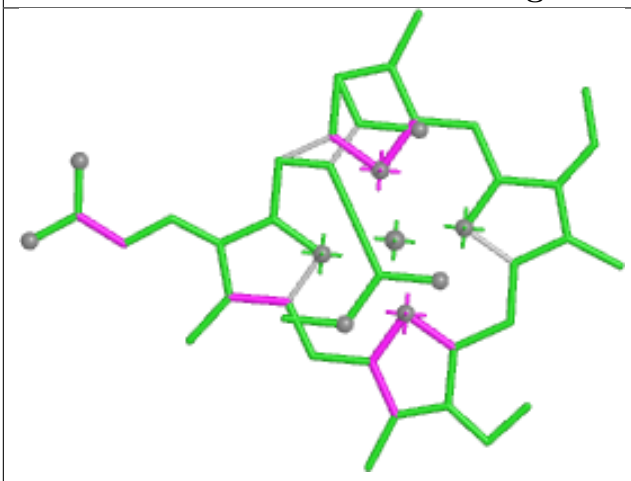


Rings

Ligand KC1 B 313



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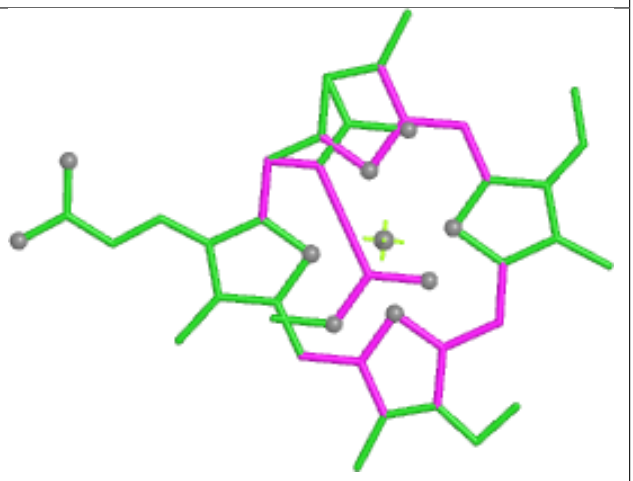
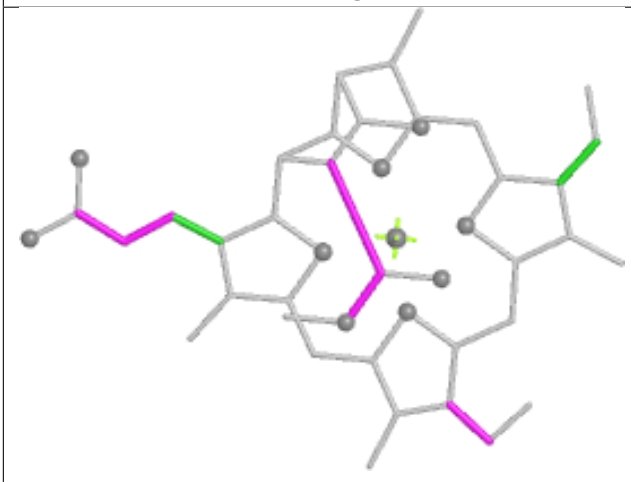


Bond angles



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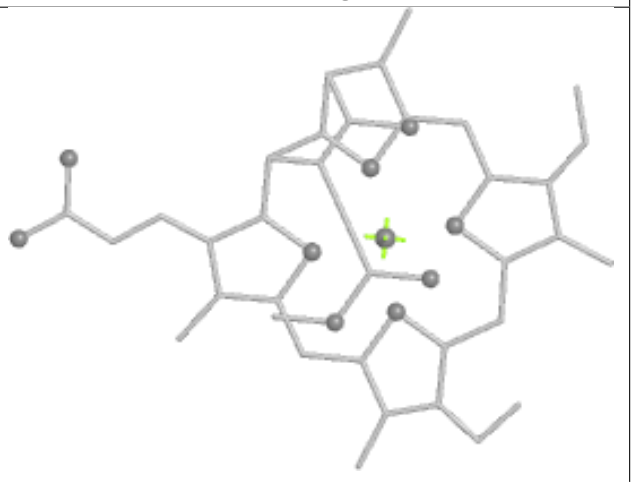
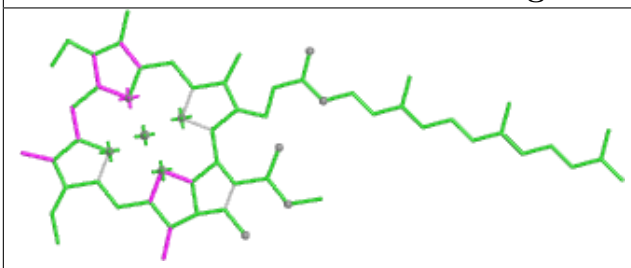
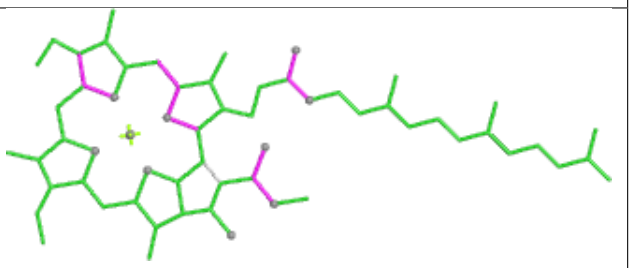
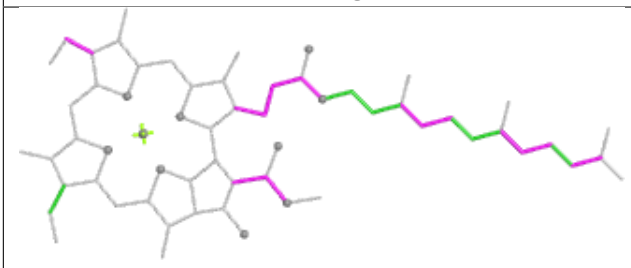
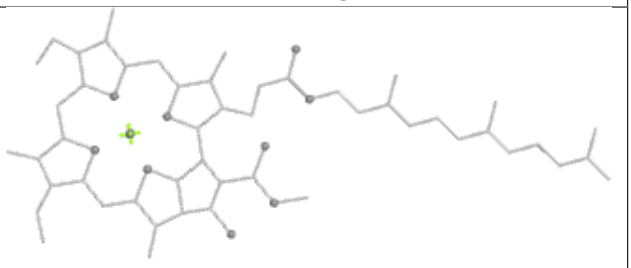
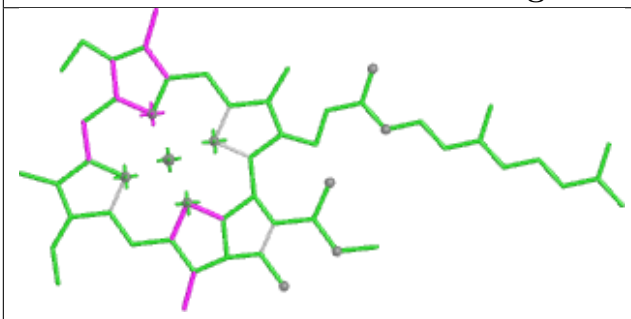
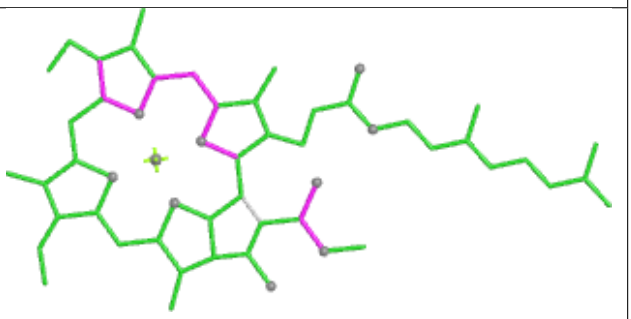
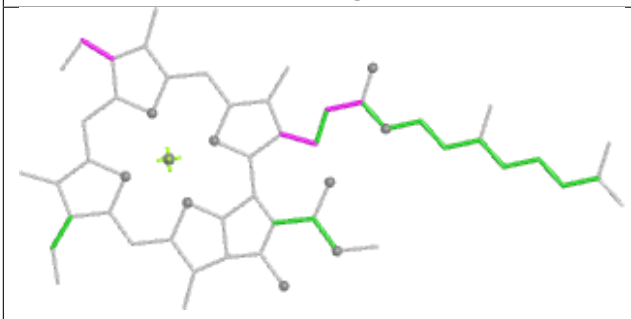
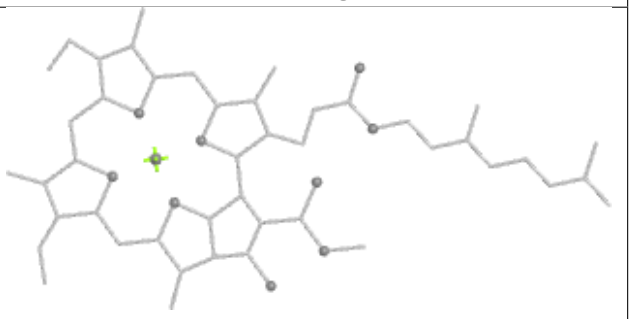


Rings

Ligand CLA b 817	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA b 809	
	
Bond lengths	Bond angles
	
Torsions	Rings

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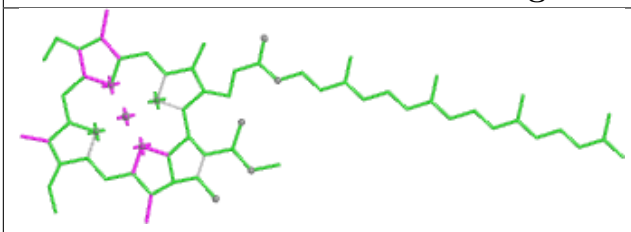
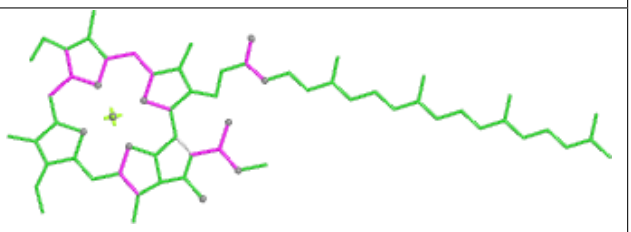
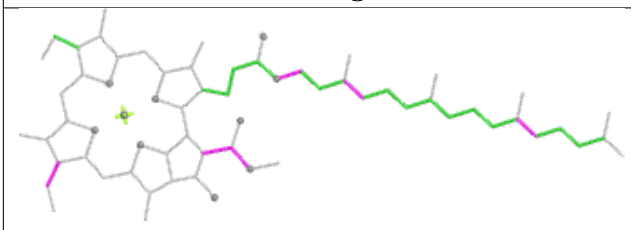
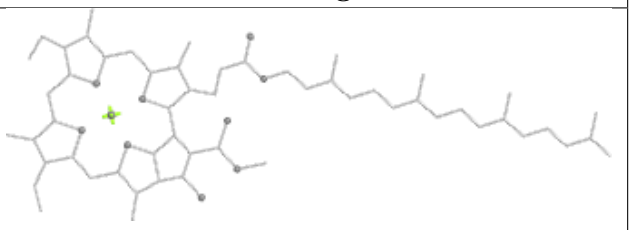
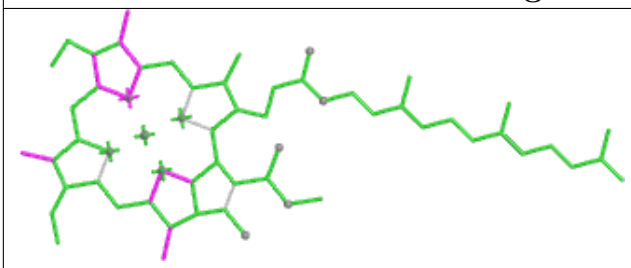
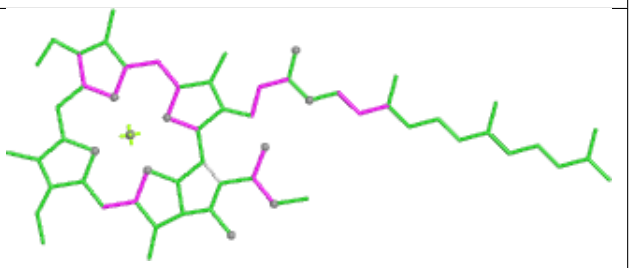
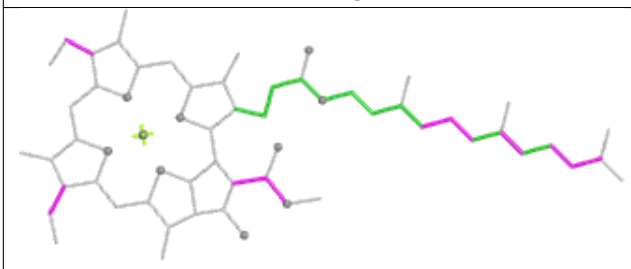
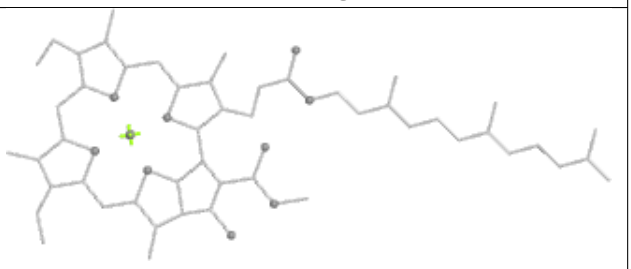
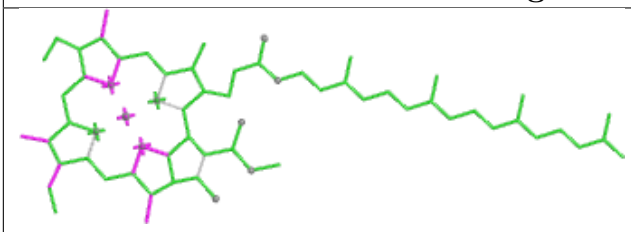
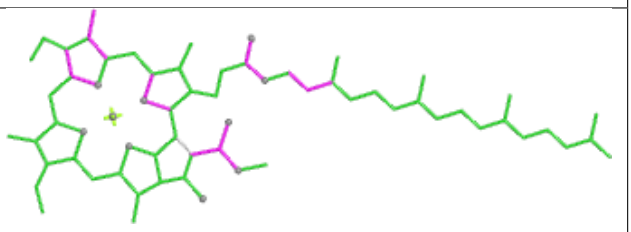
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA C 311	
 Bond lengths	 Bond angles
 Torsions	 Rings

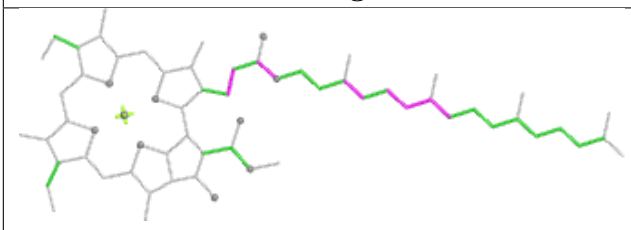
Ligand CLA b 801



Bond lengths



Bond angles



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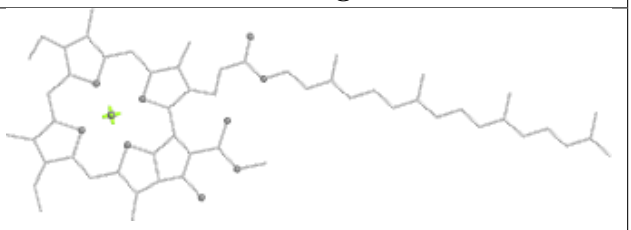
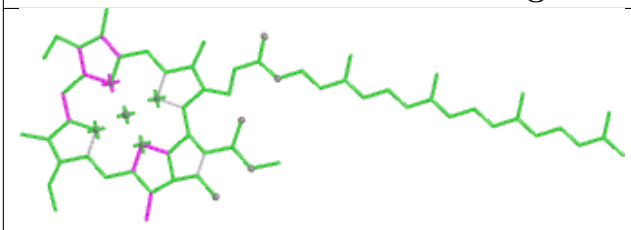


Rings

Ligand CLA b 807



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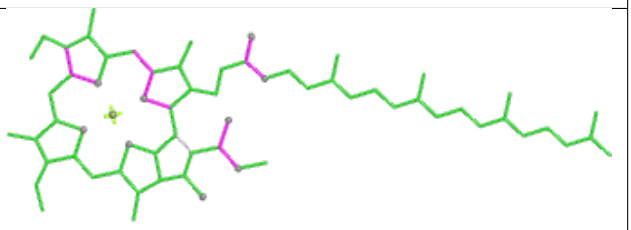
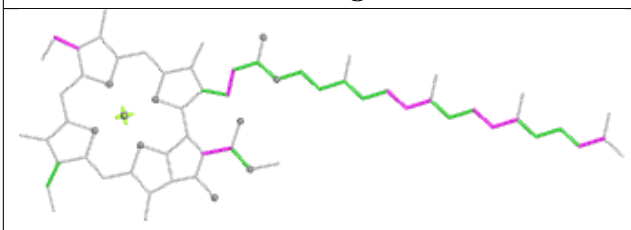


Bond angles



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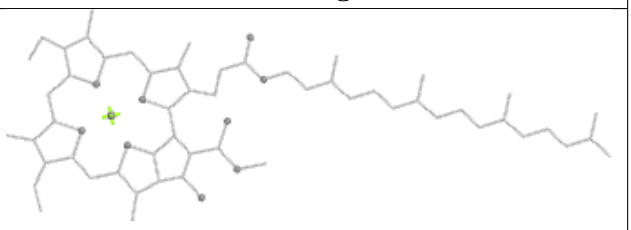
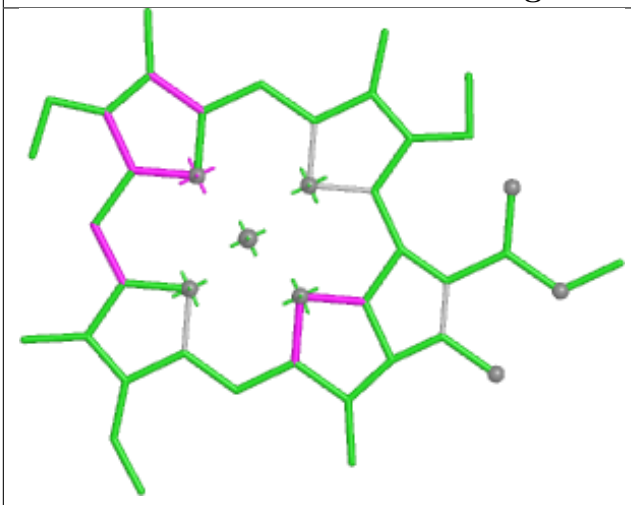


Rings

Ligand CLA C 315



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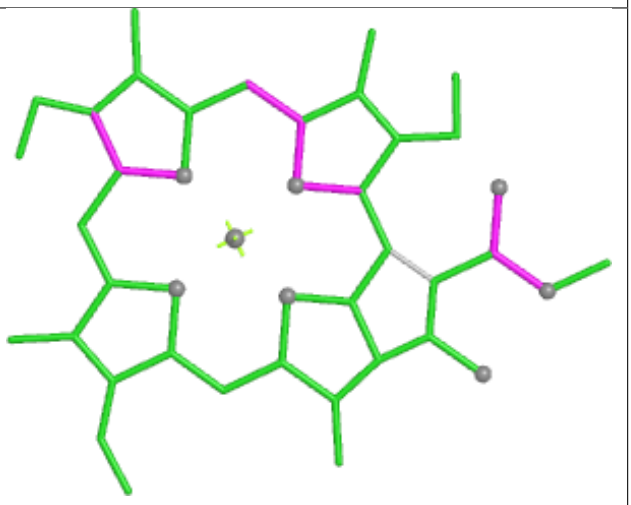

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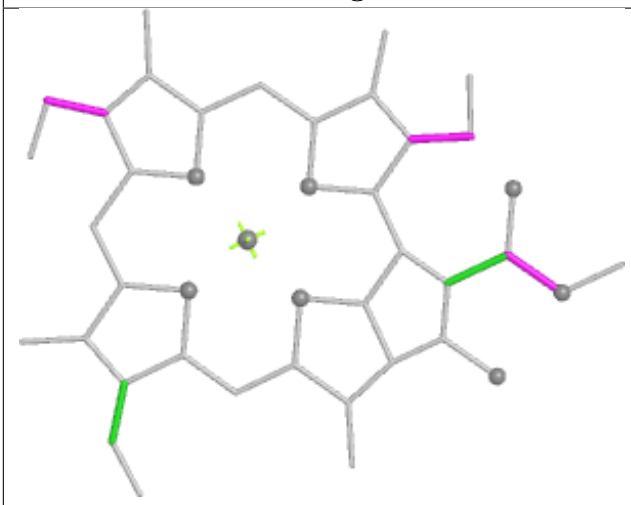
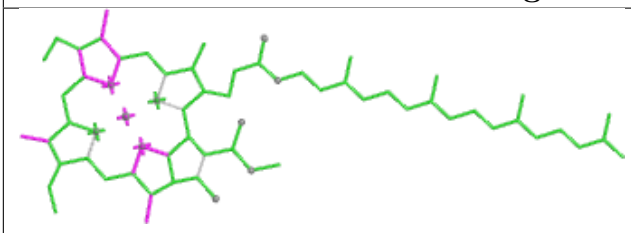


Torsions



Rings

Ligand CLA H 308



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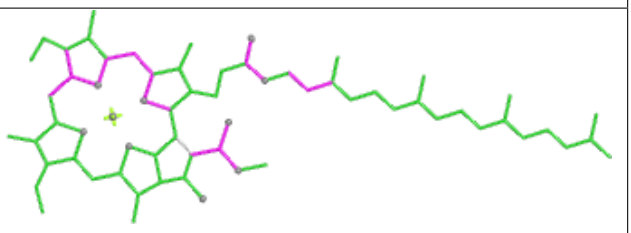
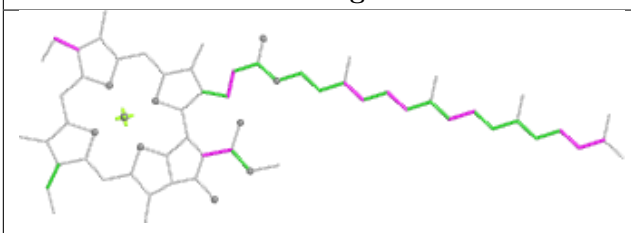


Bond angles



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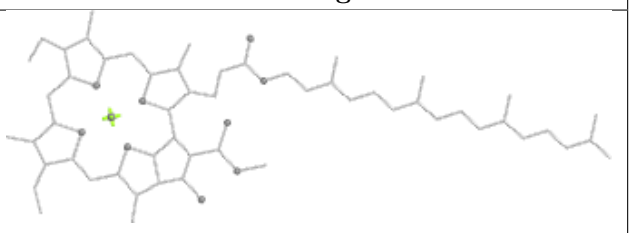
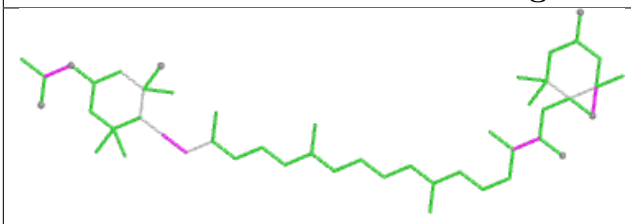


Rings

Ligand A86 D 203



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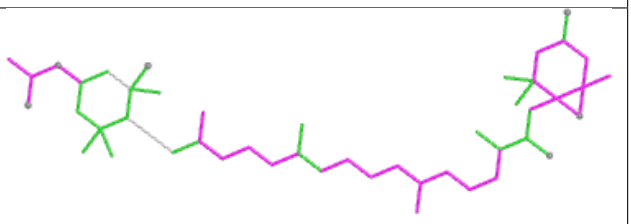
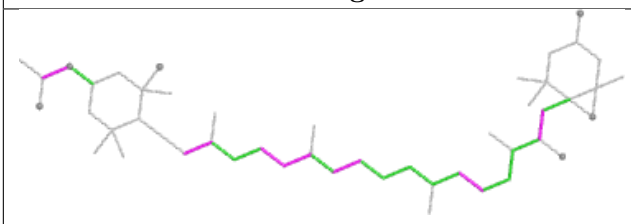


Bond angles



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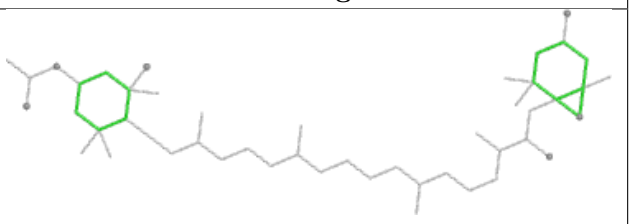
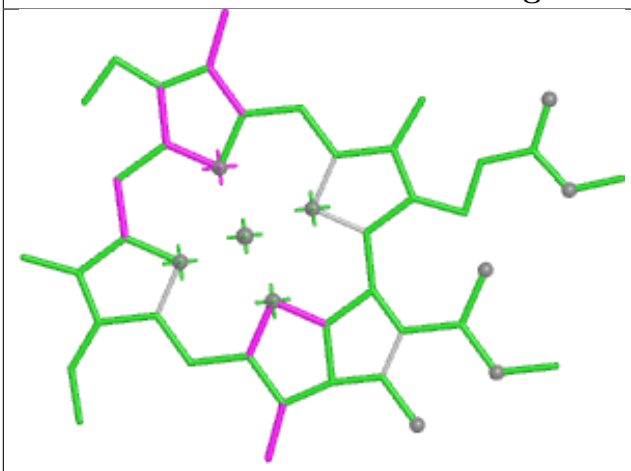


Rings

Ligand CLA H 309



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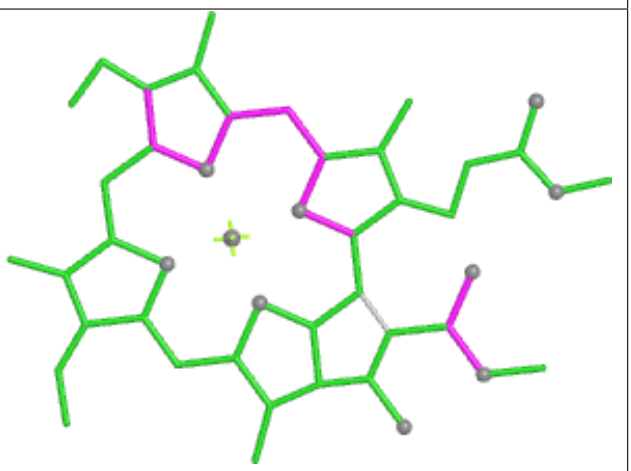
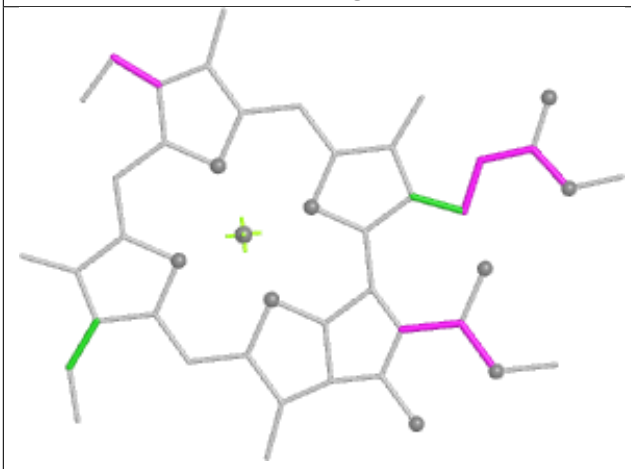


Bond angles



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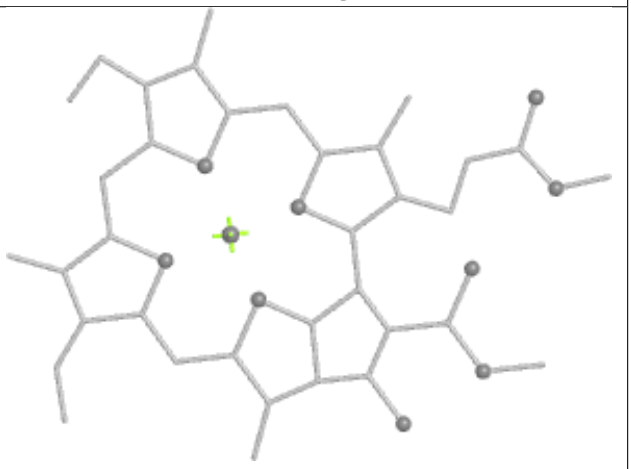
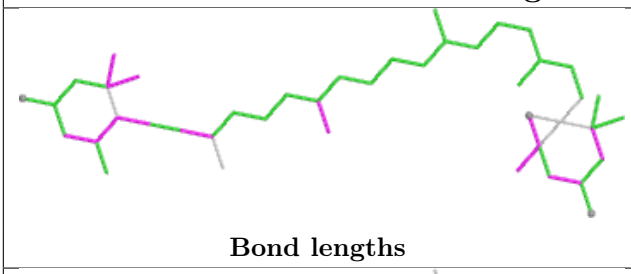


Rings

Ligand DD6 H 303



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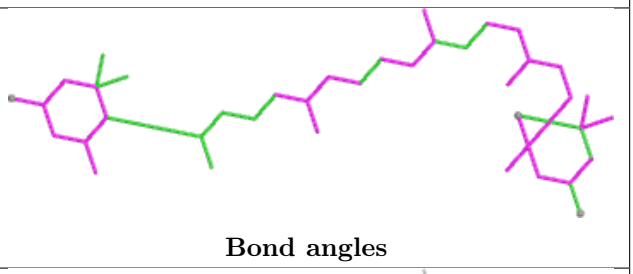
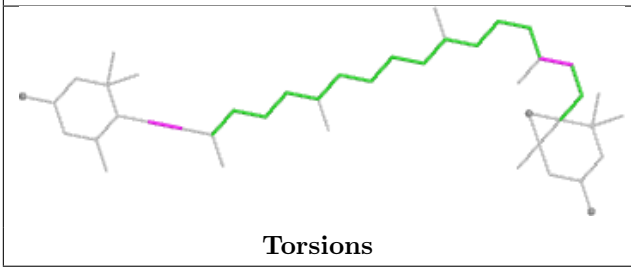


Bond angles



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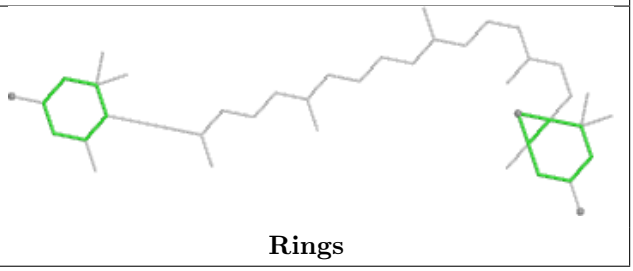
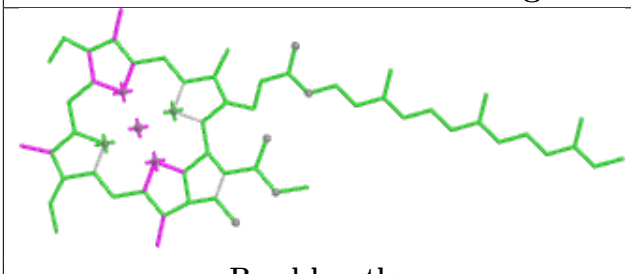
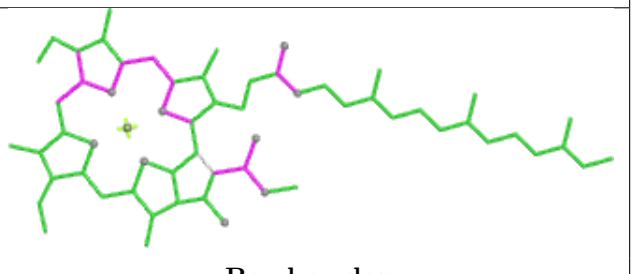


Rings

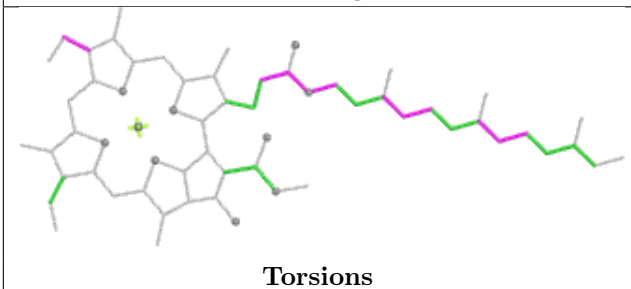
Ligand CLA D 207



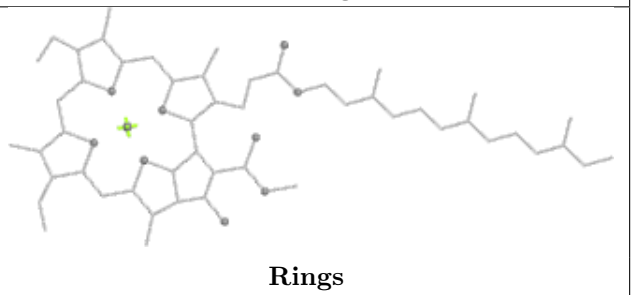
Bond lengths



Bond angles

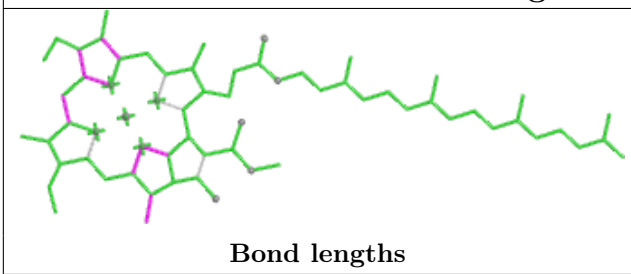


Torsions



Rings

Ligand CLA a 838



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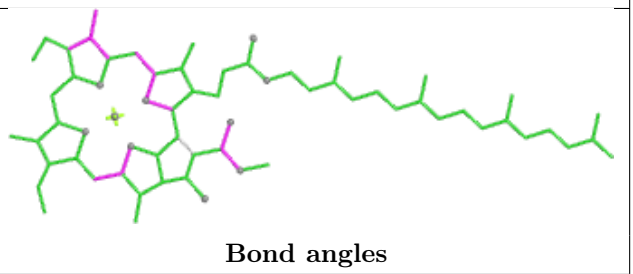

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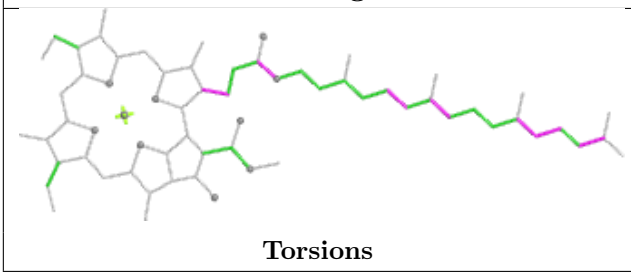

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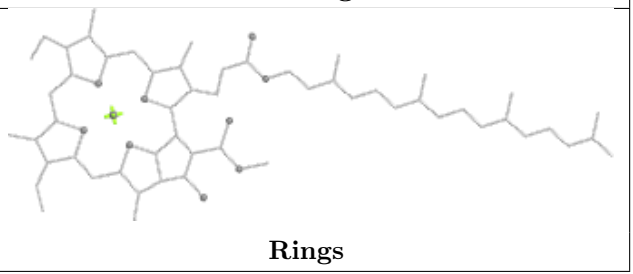
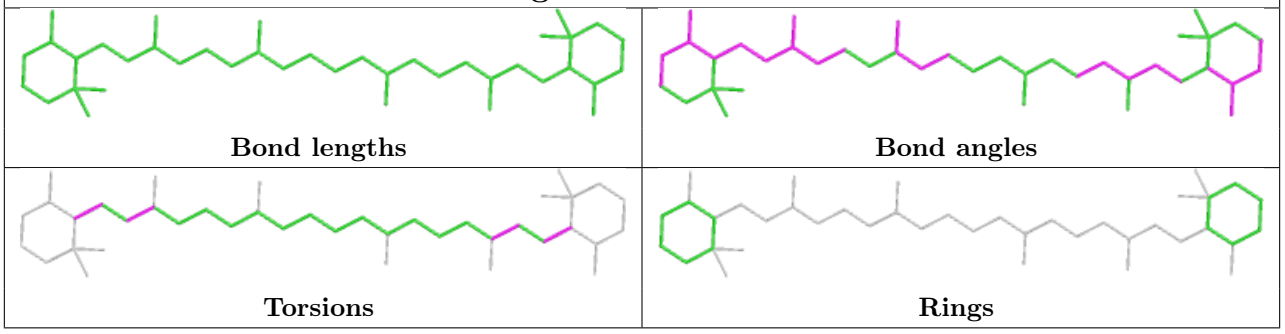
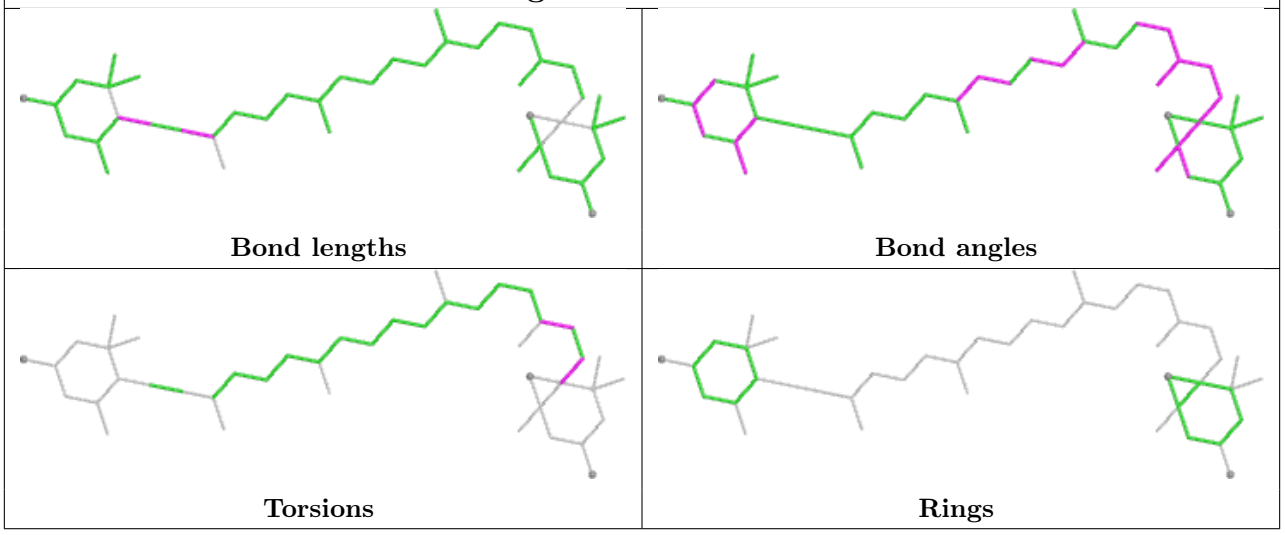


Rings

Ligand BCR l 204



Ligand DD6 E 303



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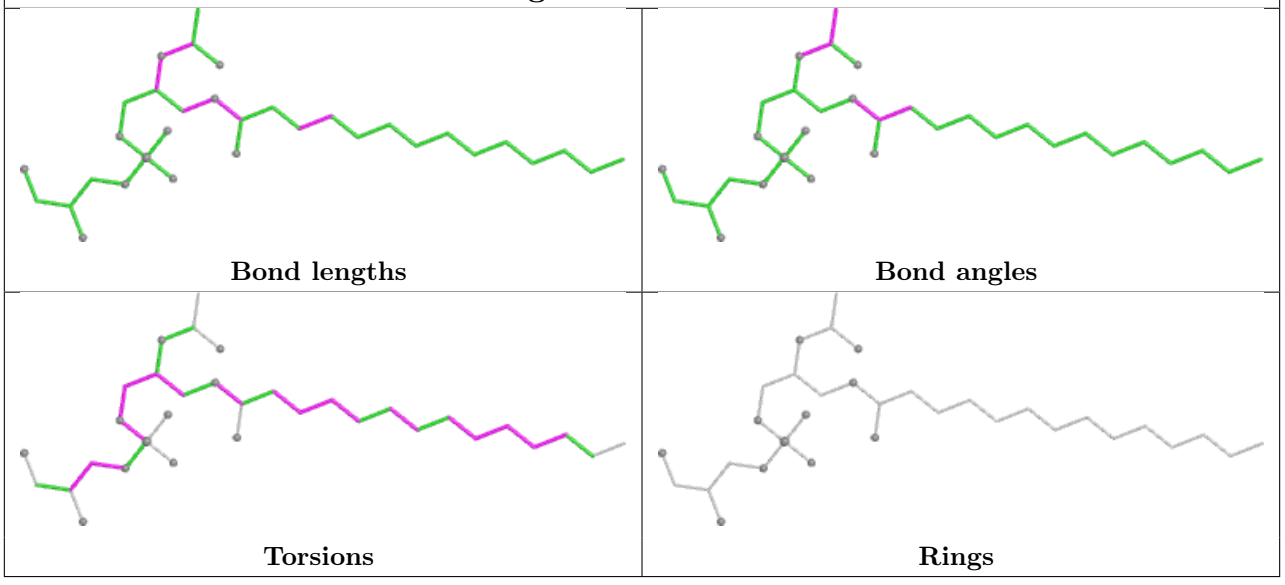
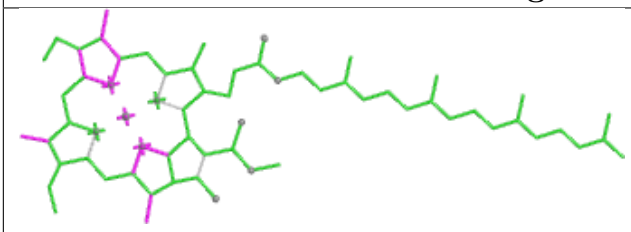
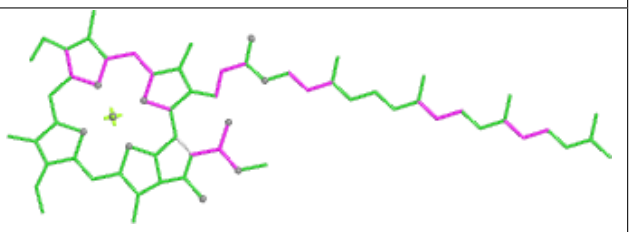


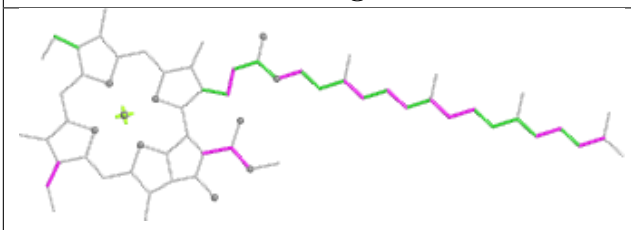
Ligand CLA b 829



Bond lengths



Bond angles



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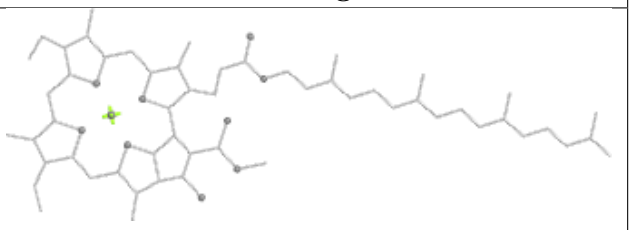
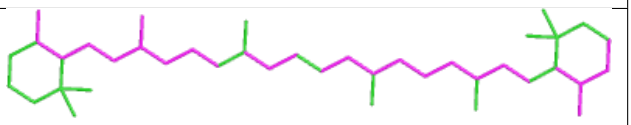


Rings

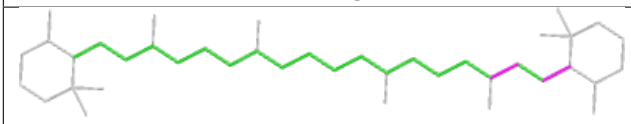
Ligand BCR a 834



Bond lengths



Bond angles



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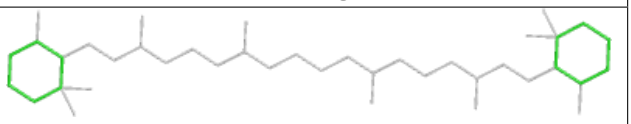
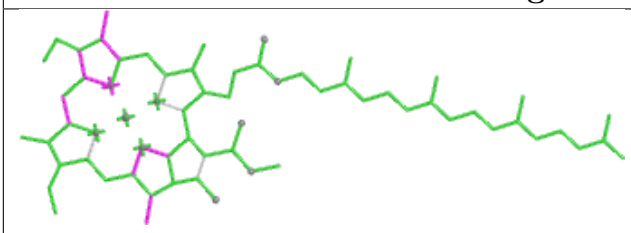


Rings

Ligand CLA b 828



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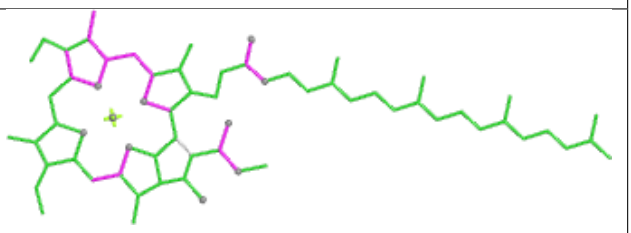

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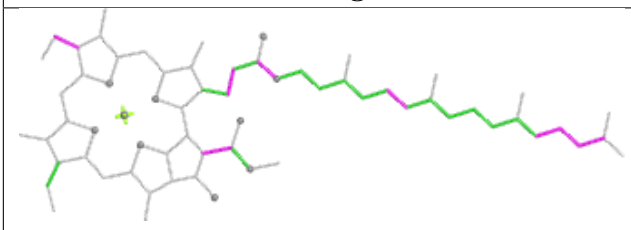

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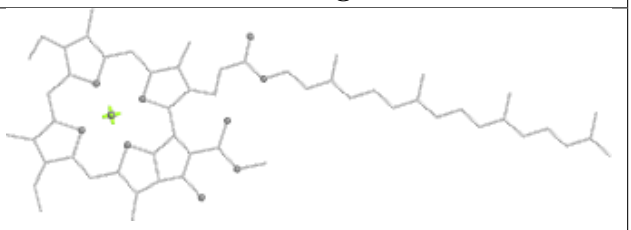
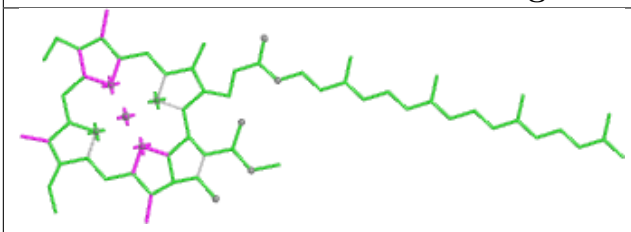


Rings

Ligand CLA a 840



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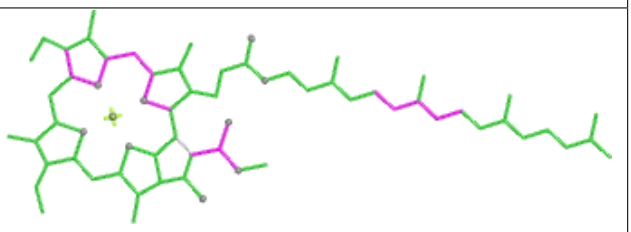

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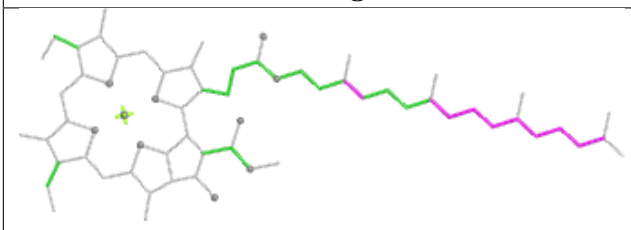

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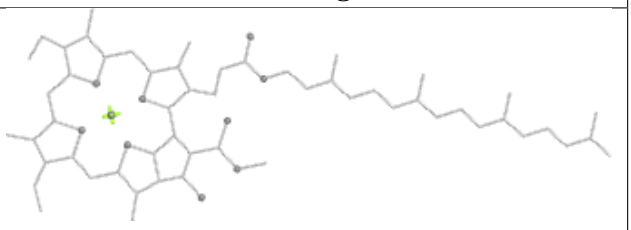
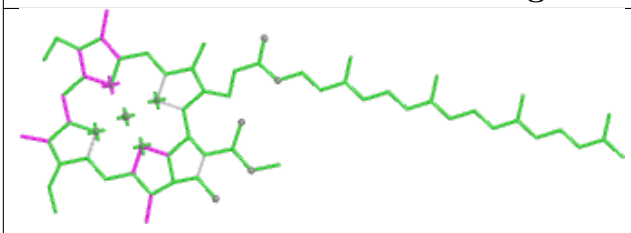


Rings

Ligand CLA b 810



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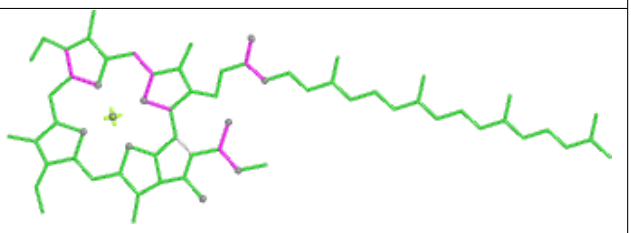
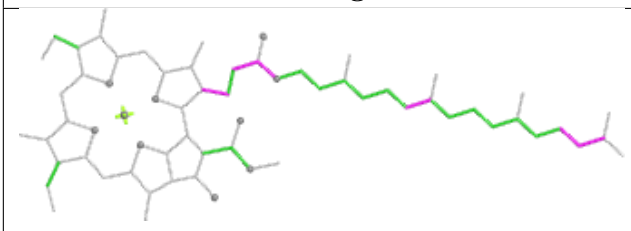


Bond angles



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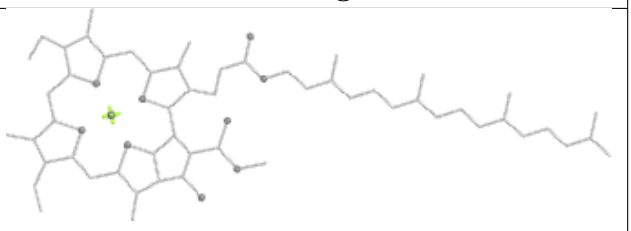
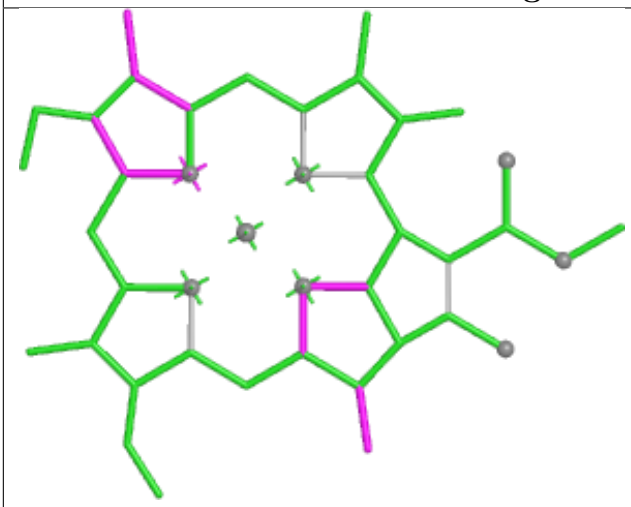


Rings

Ligand CLA D 217



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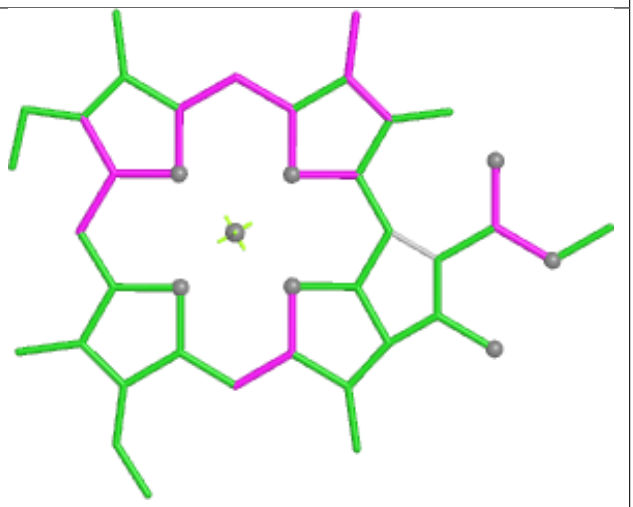
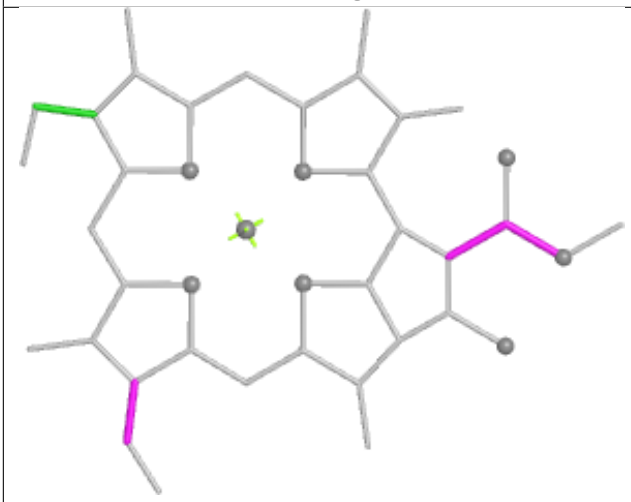


Bond angles



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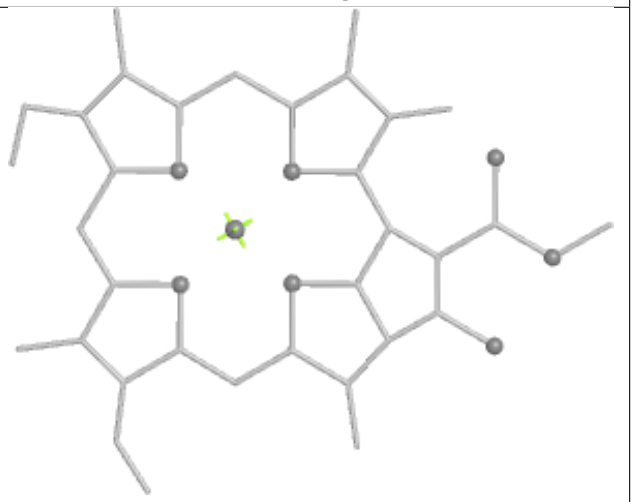
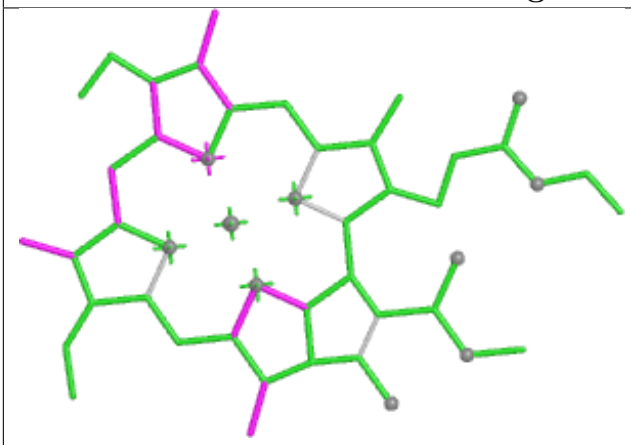


Rings

Ligand CLA b 827



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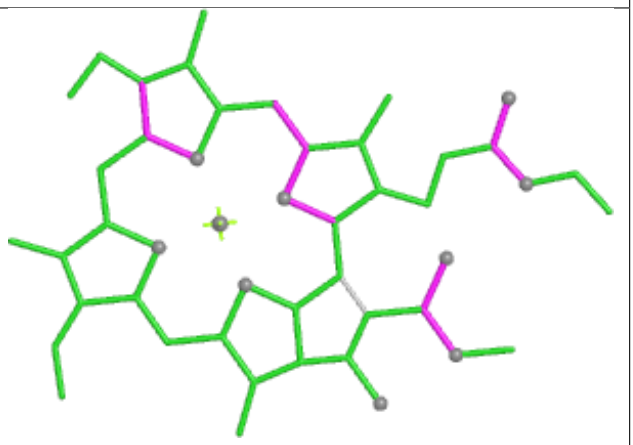
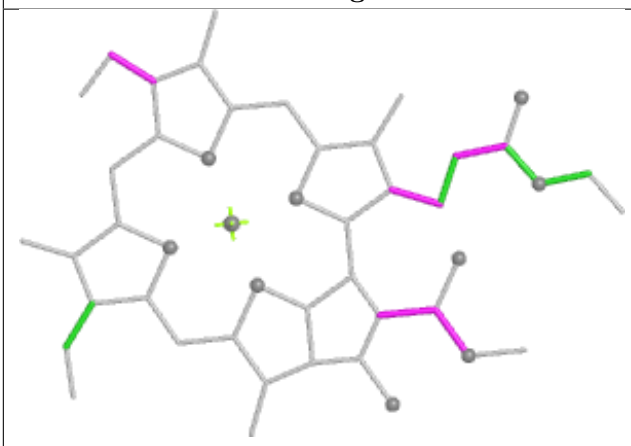


Bond angles



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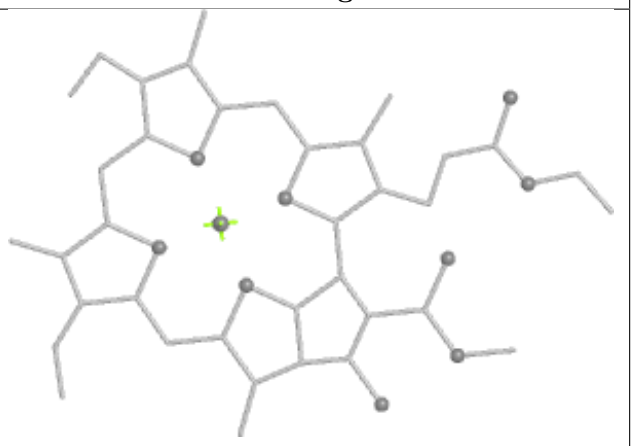
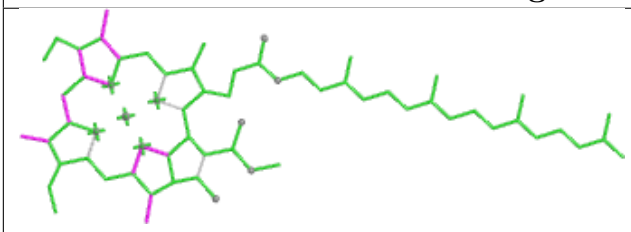


Rings

Ligand CLA a 819



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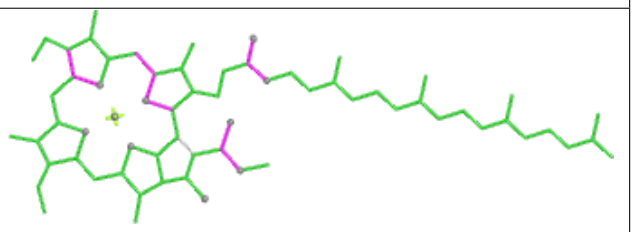

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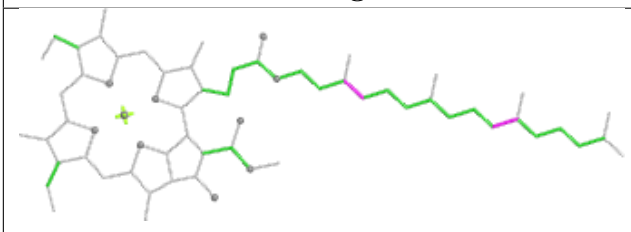

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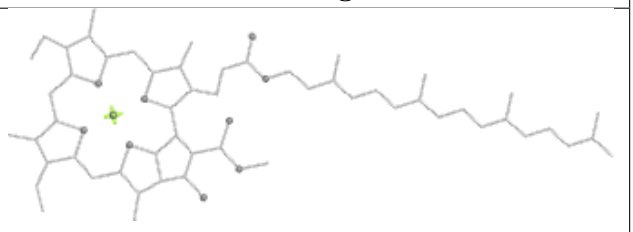
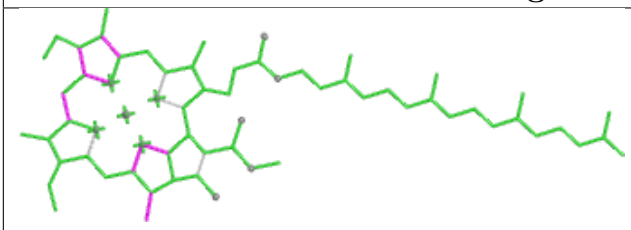
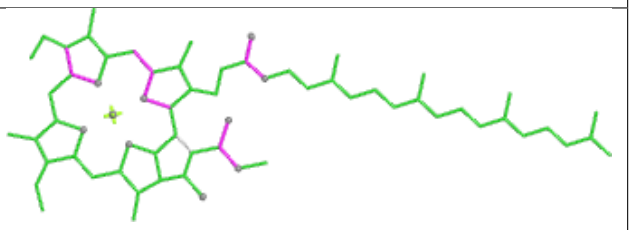
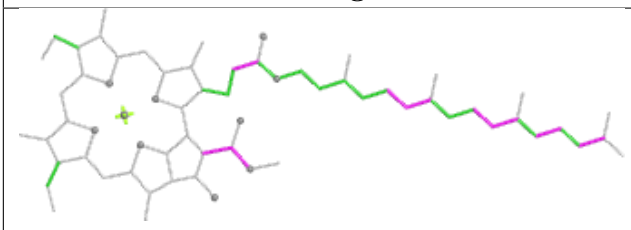
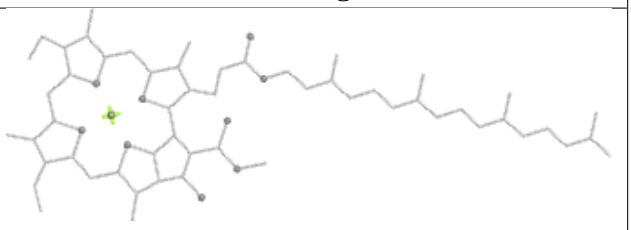


Rings

Ligand CLA b 850	
	
Bond lengths	Bond angles
	
Torsions	Rings

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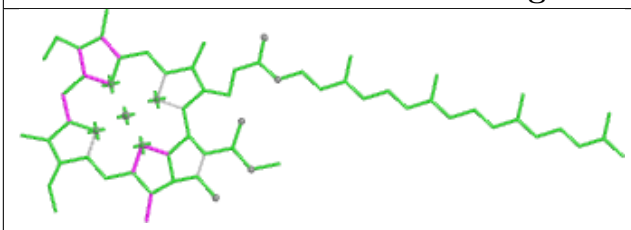
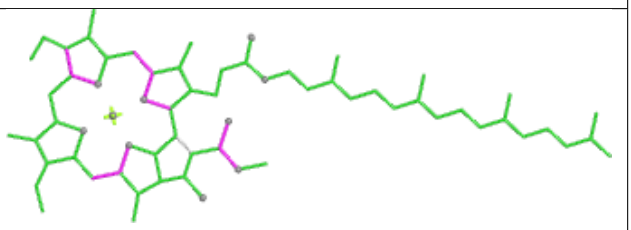
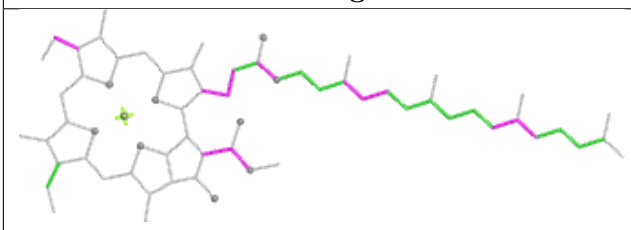
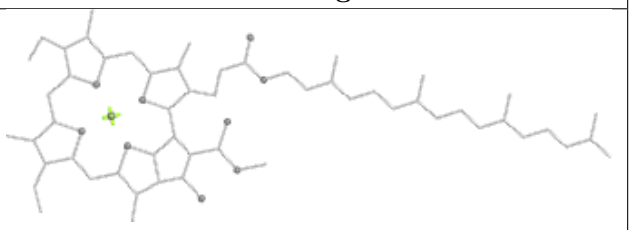
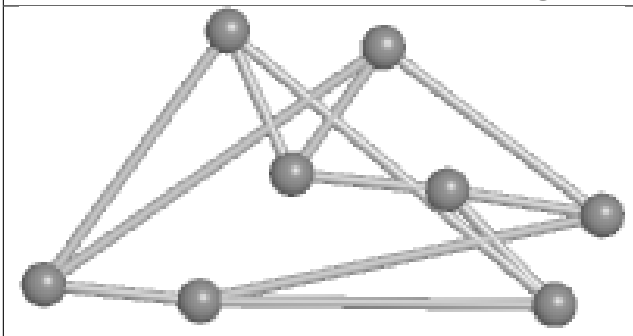
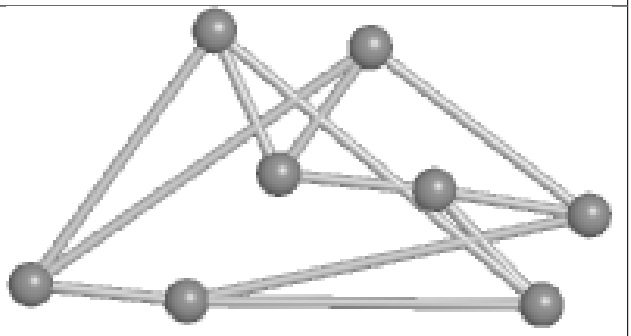
	
Bond lengths	Bond angles
	
Torsions	Rings

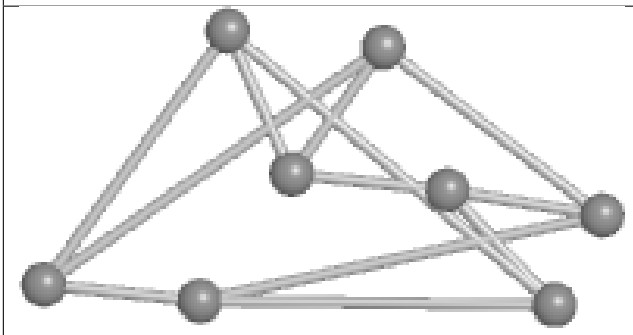
Ligand SF4 b 802



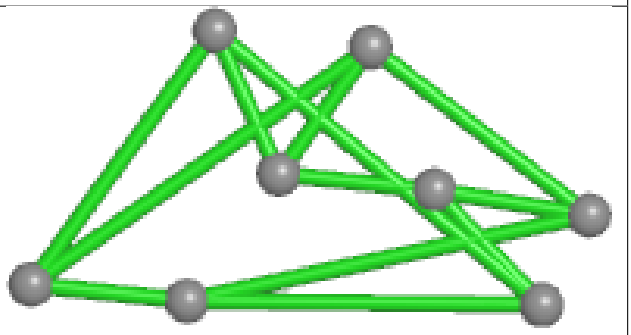
Bond lengths



Bond angles

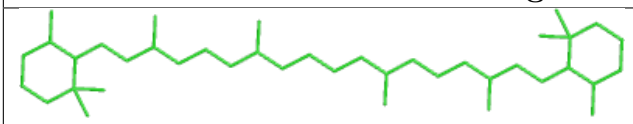


Torsions



Rings

Ligand BCR a 852



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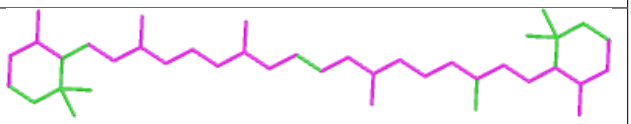
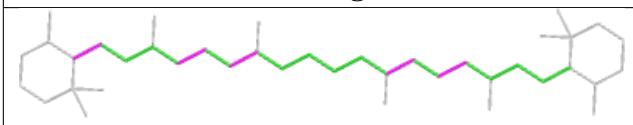


Bond angles



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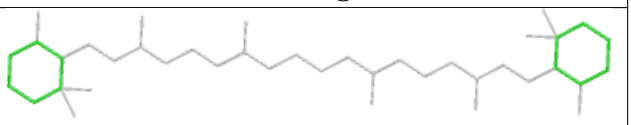
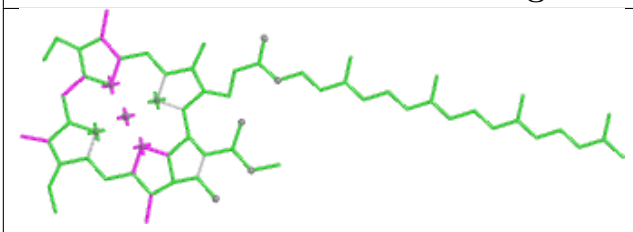
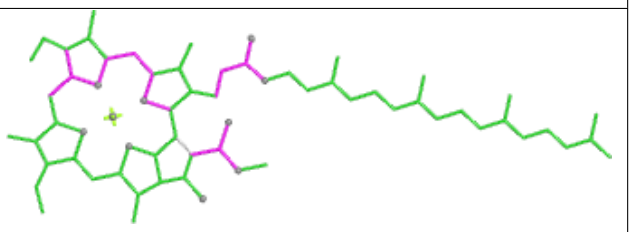


Rings

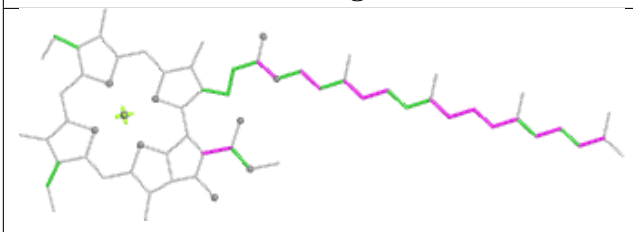
Ligand CLA b 820



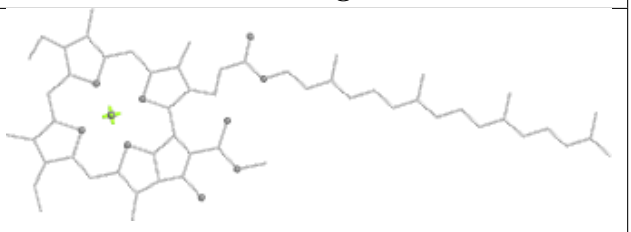
Bond lengths



Bond angles

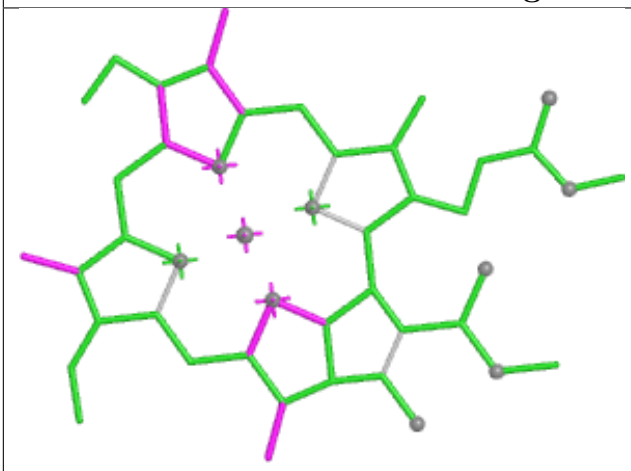


Torsions



Rings

Ligand CLA D 216



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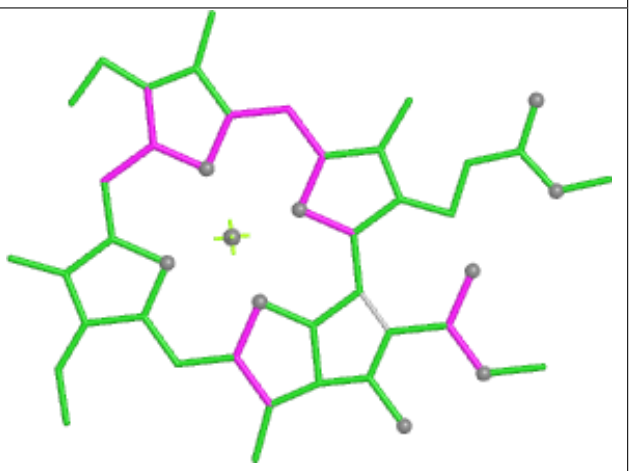

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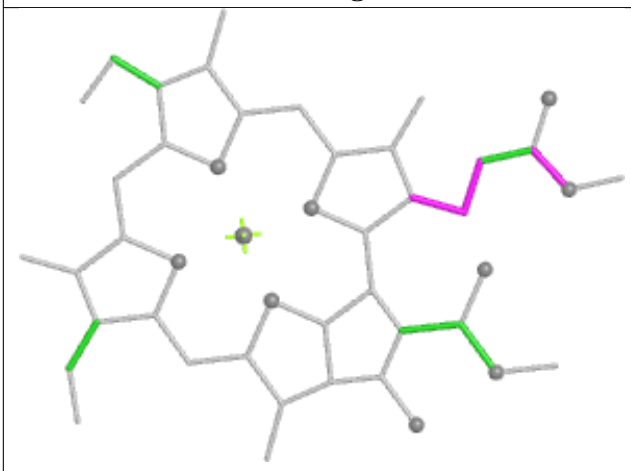

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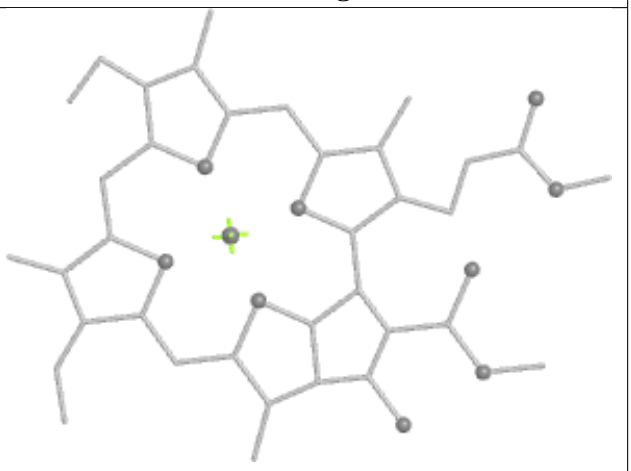
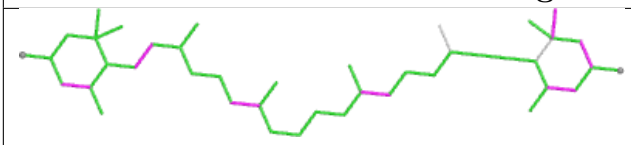


Rings

Ligand ET4 l 206



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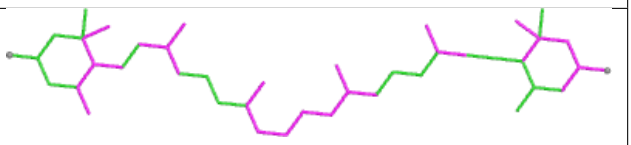

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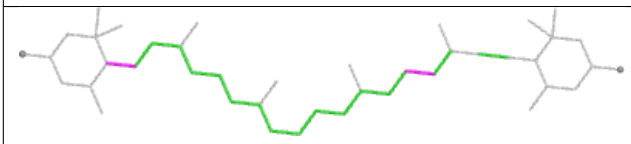

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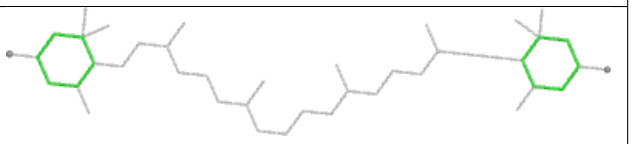
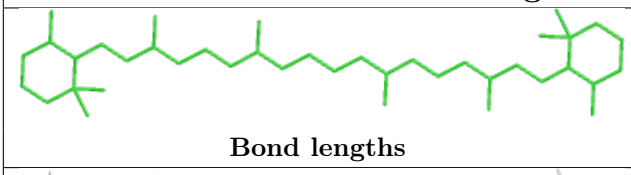


Rings

Ligand BCR E 306



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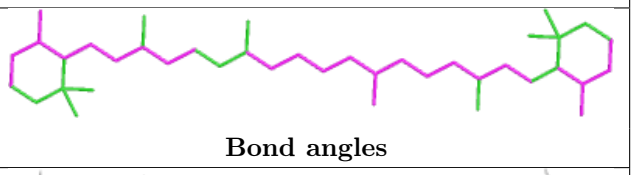
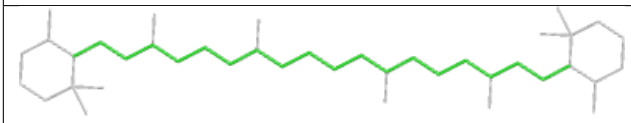


Bond angles



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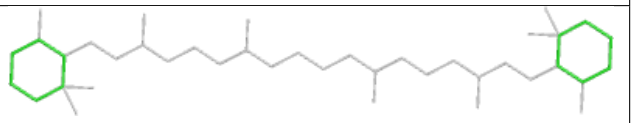


Rings

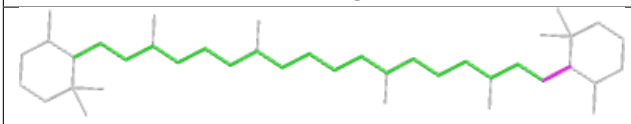
Ligand BCR E 305



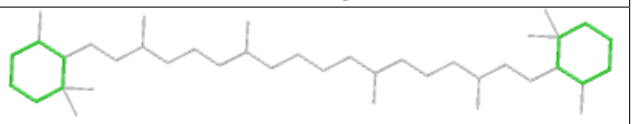
Bond lengths



Bond angles

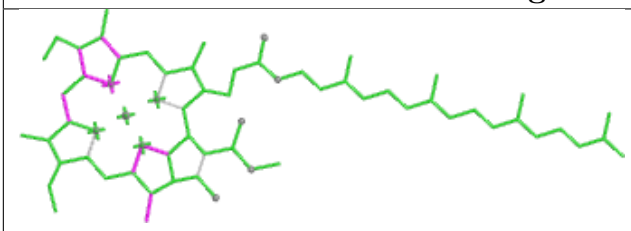


Torsions



Rings

Ligand CLA a 836



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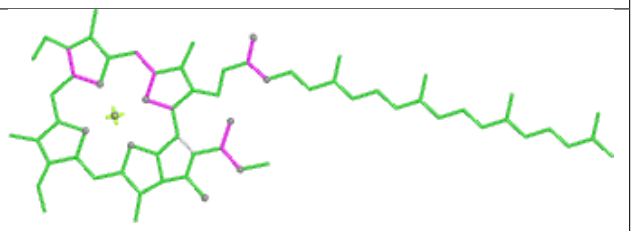
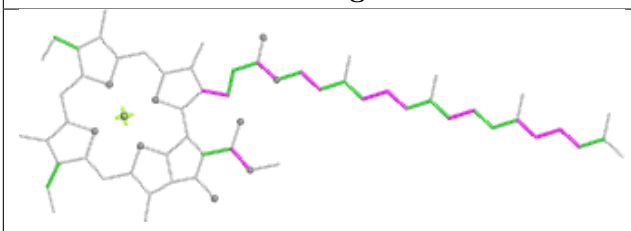


Bond angles



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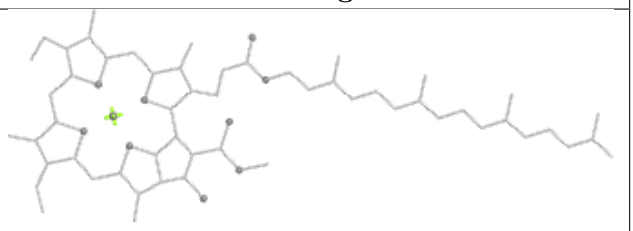
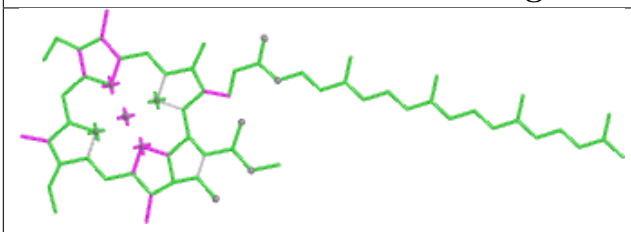


Rings

Ligand CLA E 312



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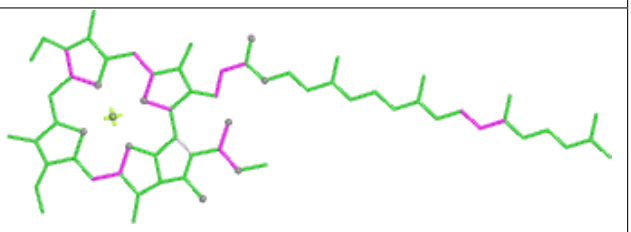
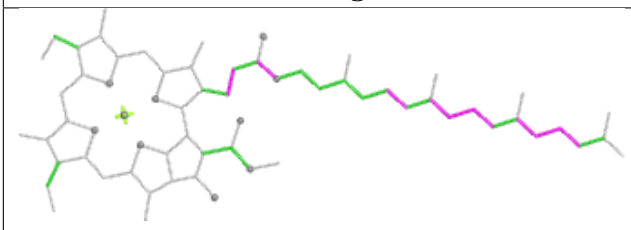


Bond angles



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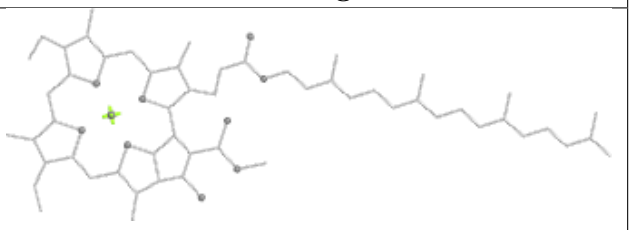
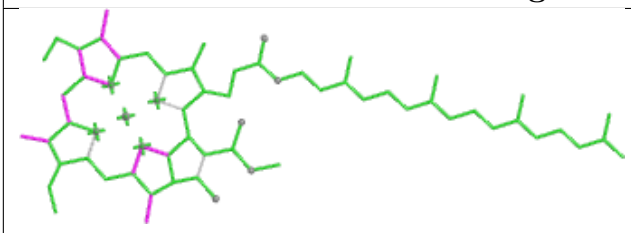


Rings

Ligand CLA a 805



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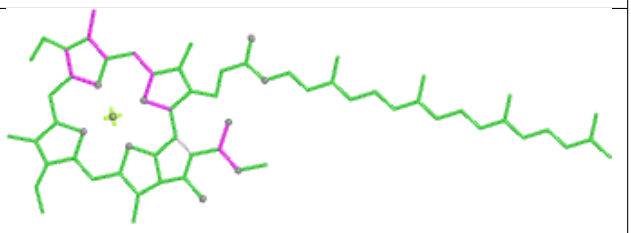
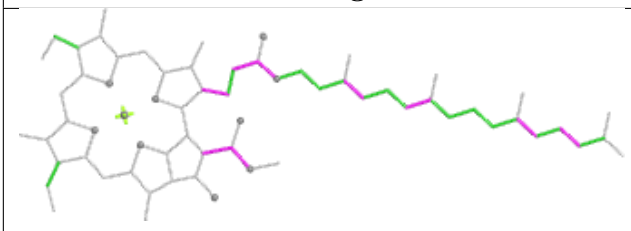


Bond angles



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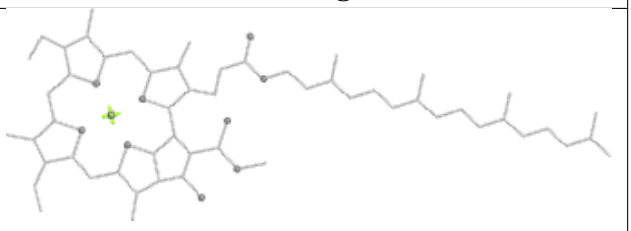
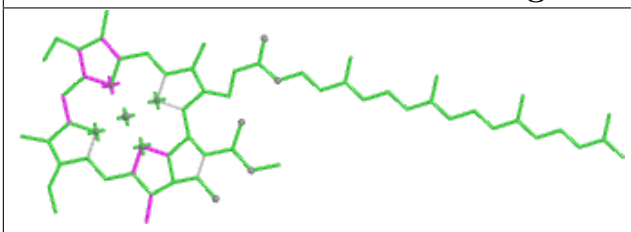


Rings

Ligand CLA b 841



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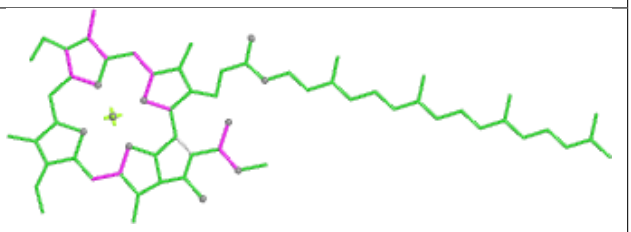
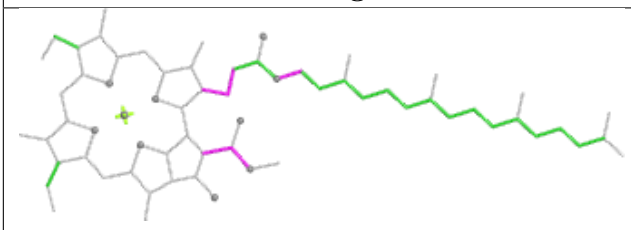


Bond angles



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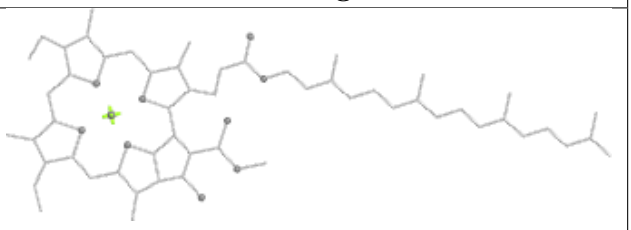
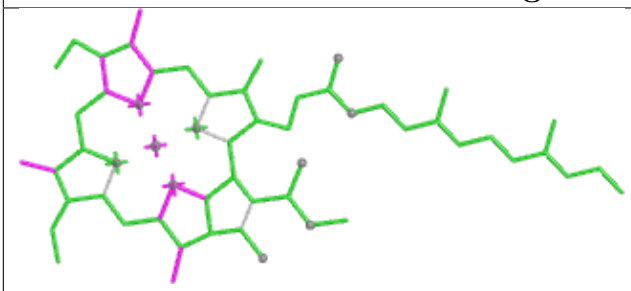


Rings

Ligand CLA H 311



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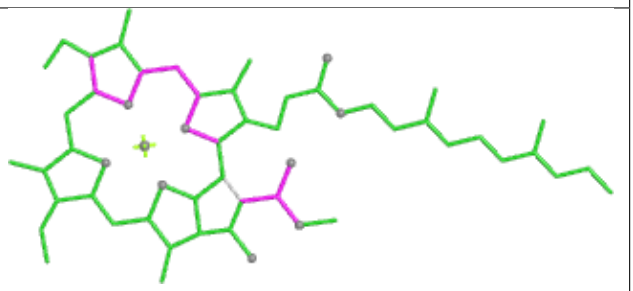
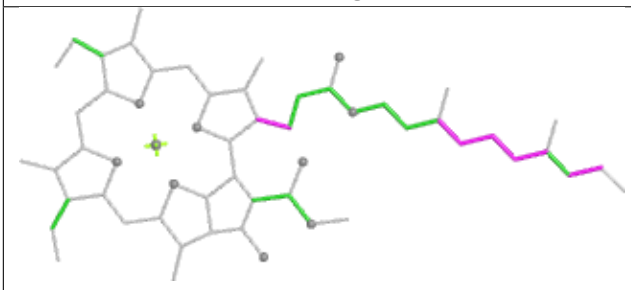


Bond angles



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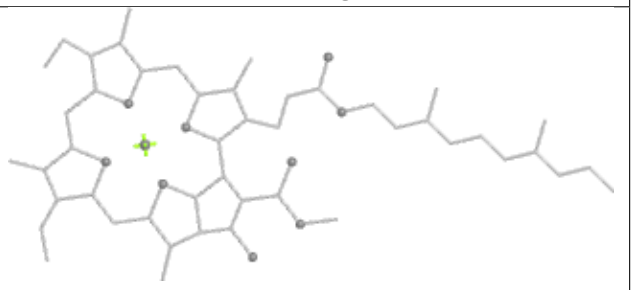
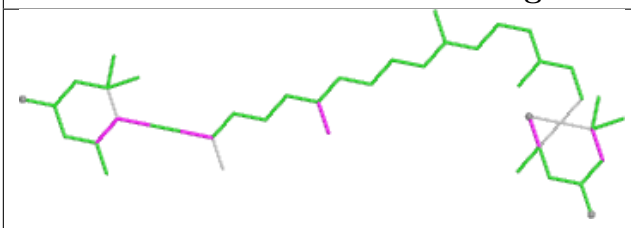


Rings

Ligand DD6 D 205



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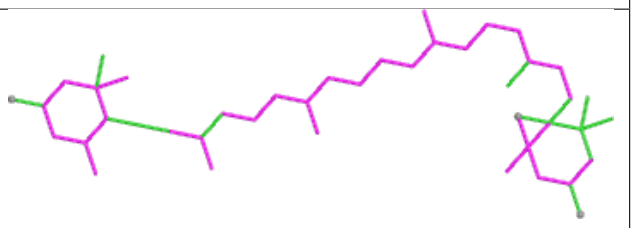
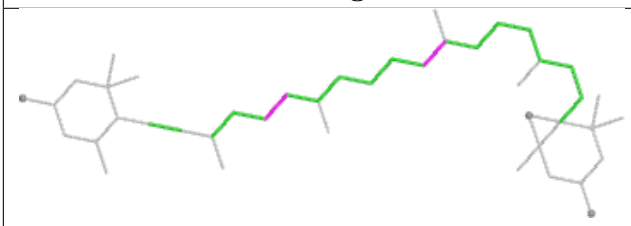


Bond angles



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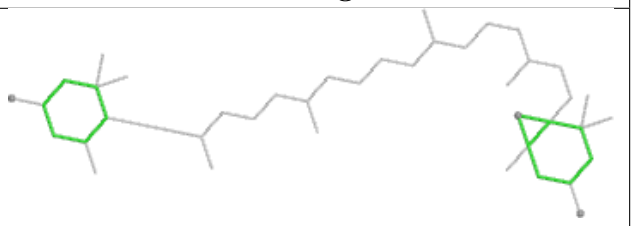
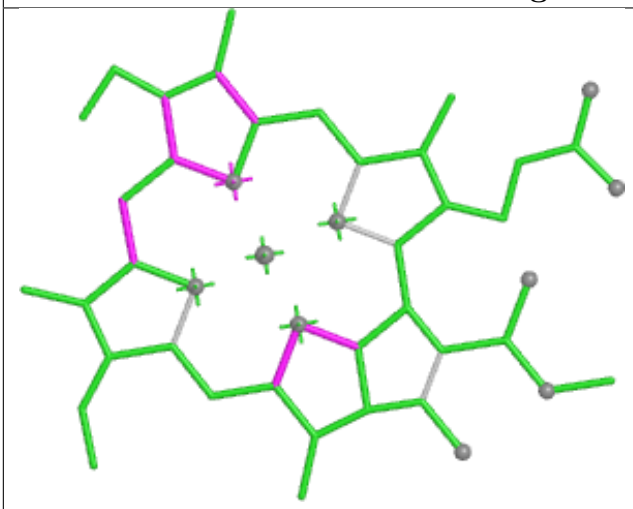


Rings

Ligand CLA r 202



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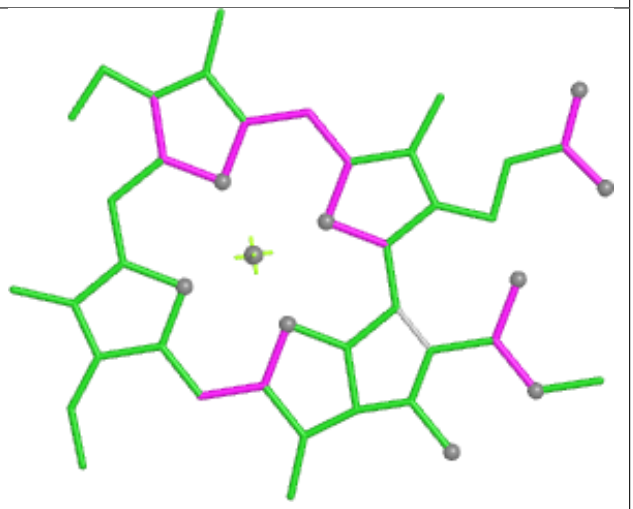
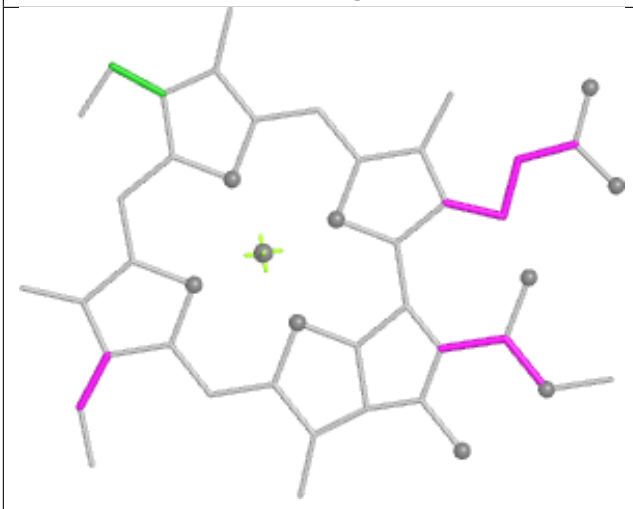


Bond angles

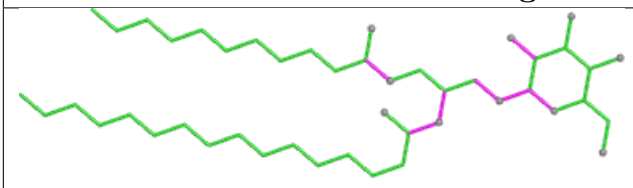


Torsions



Rings

Ligand LMG D 202



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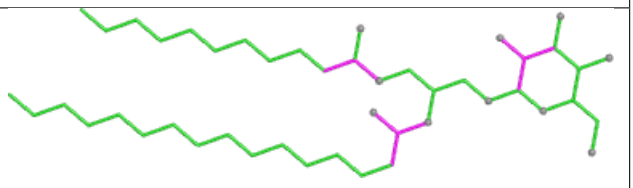
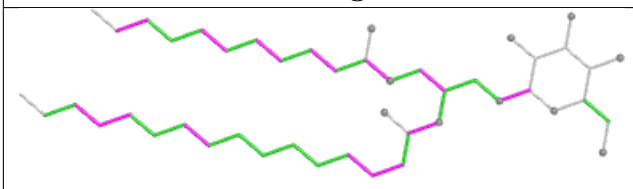


Bond angles



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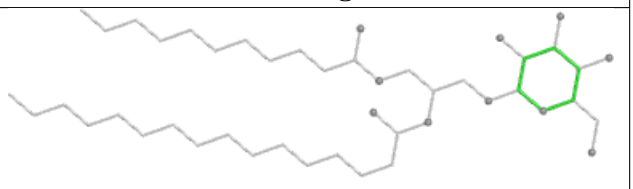
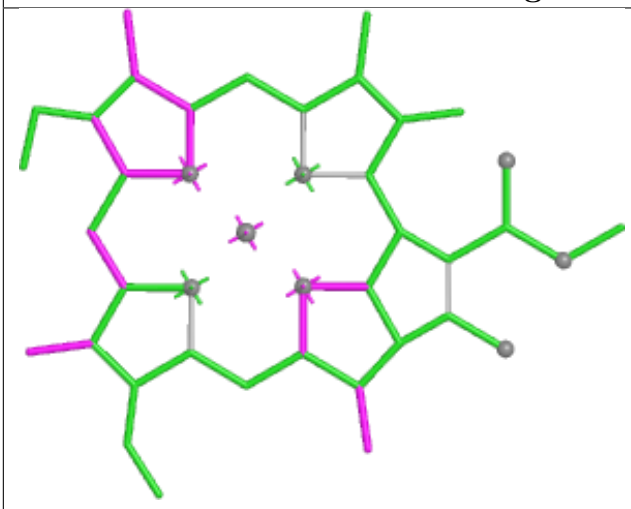


Rings

Ligand CLA C 314



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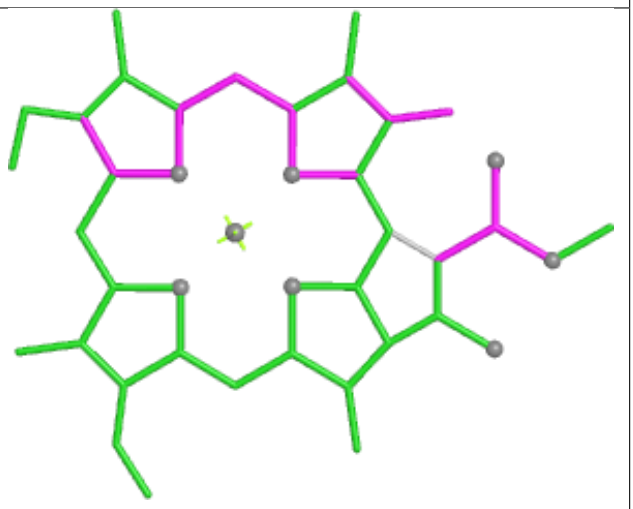
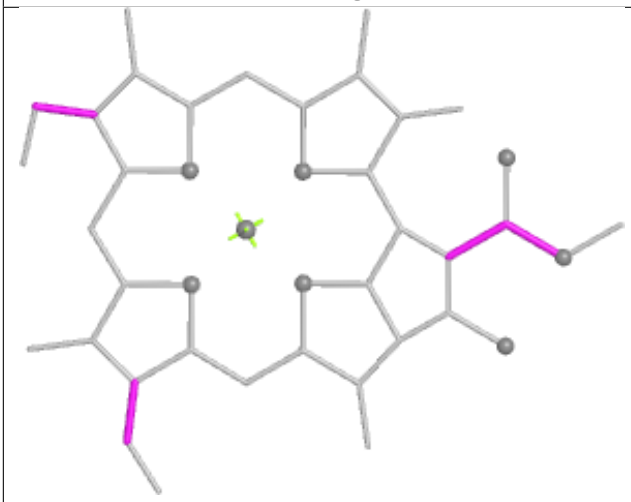


Bond angles



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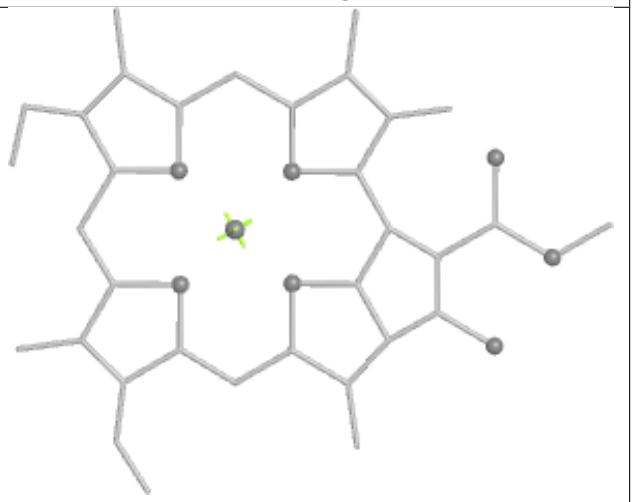
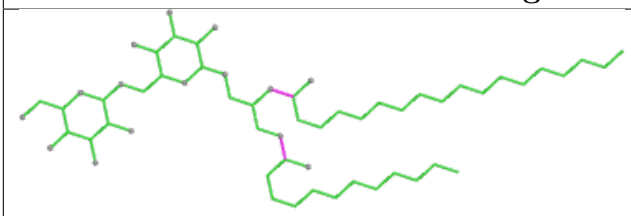


Rings

Ligand DGD b 834



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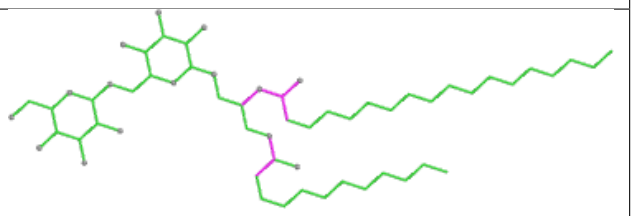
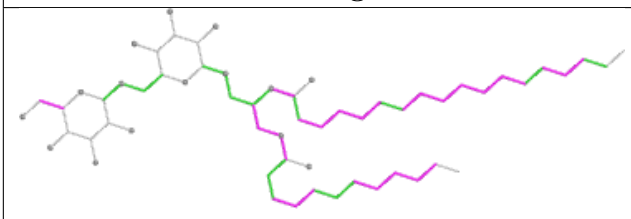


Bond angles



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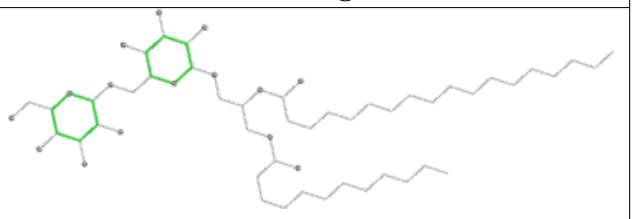
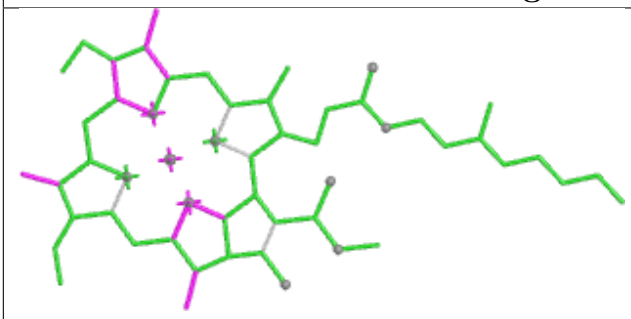
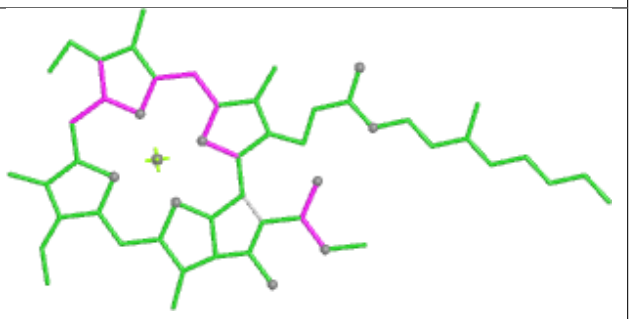


Rings

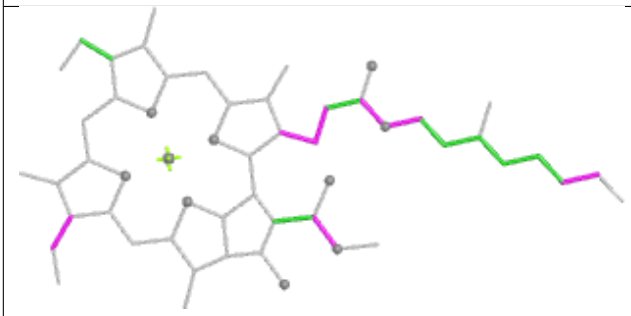
Ligand CLA H 305



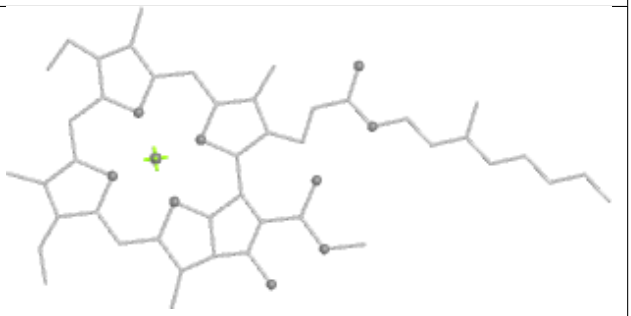
Bond lengths



Bond angles

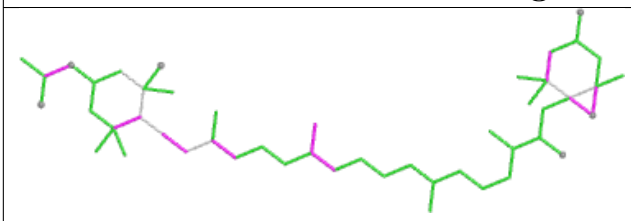


Torsions

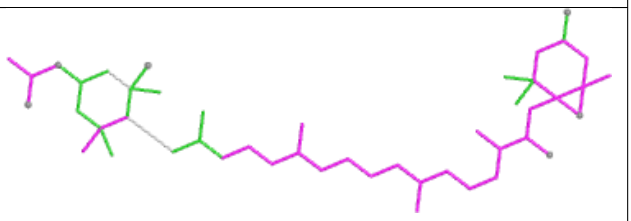


Rings

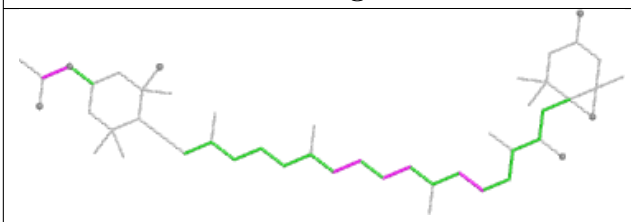
Ligand A86 B 302



Bond lengths



Bond angles



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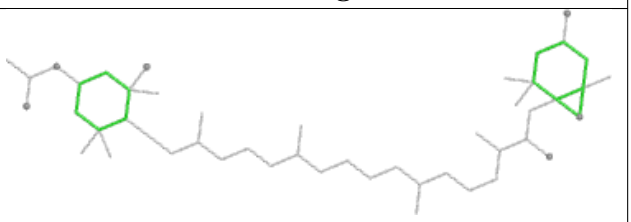
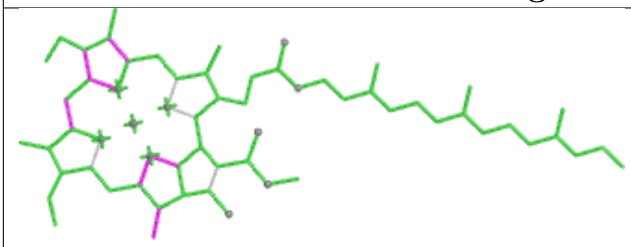


Rings

Ligand CLA a 809



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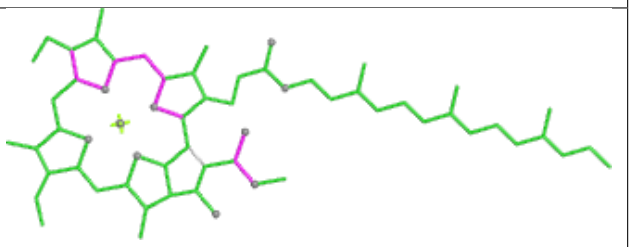

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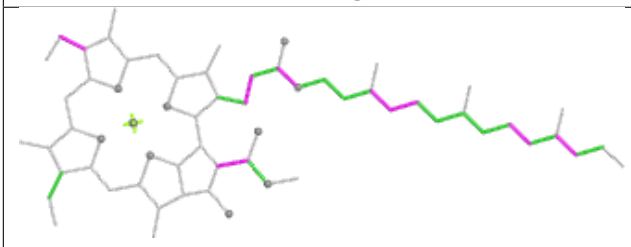

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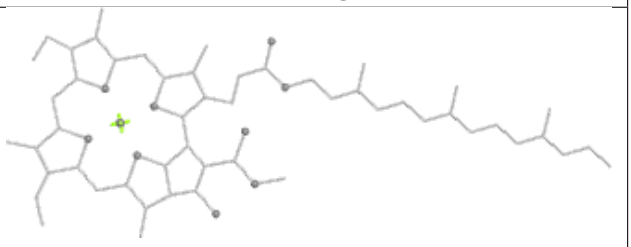
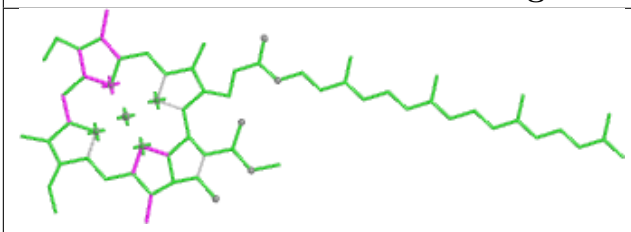


Rings

Ligand CLA b 819



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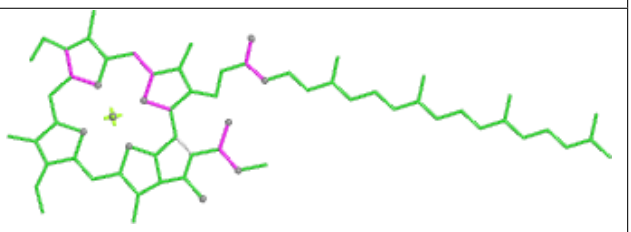
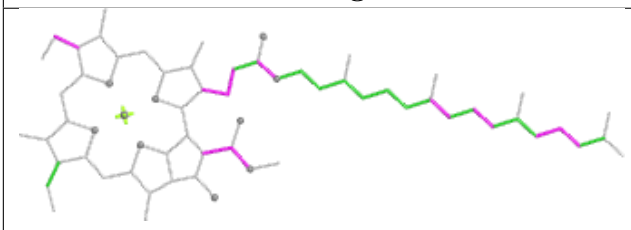


Bond angles



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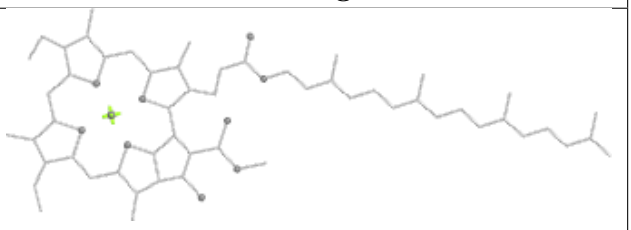
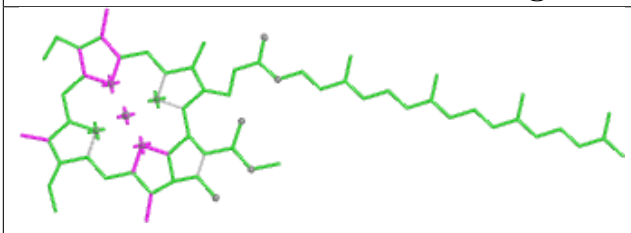
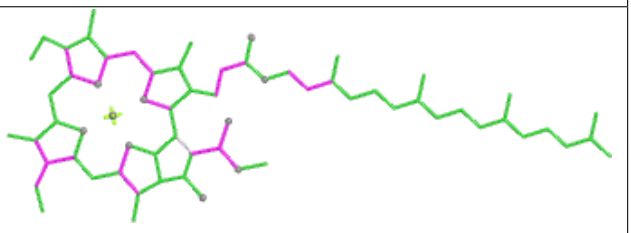


Rings

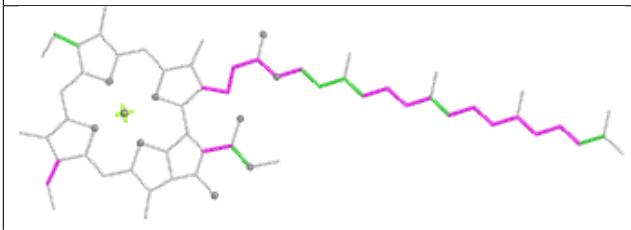
Ligand CLA a 813



Bond lengths



Bond angles



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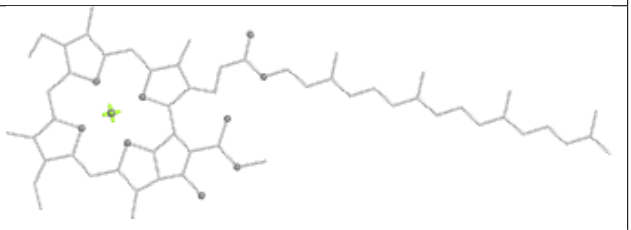
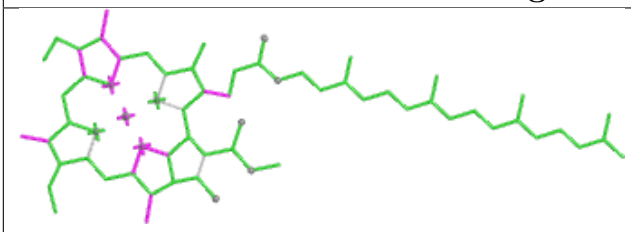
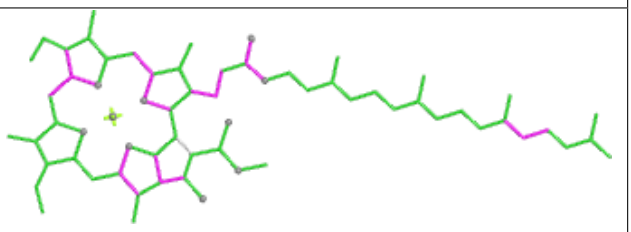
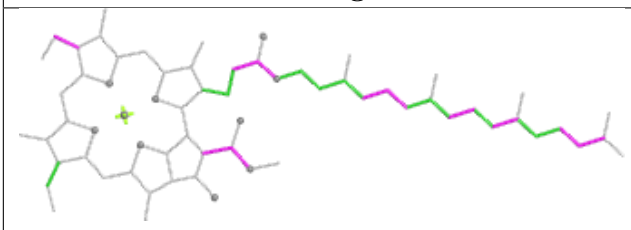
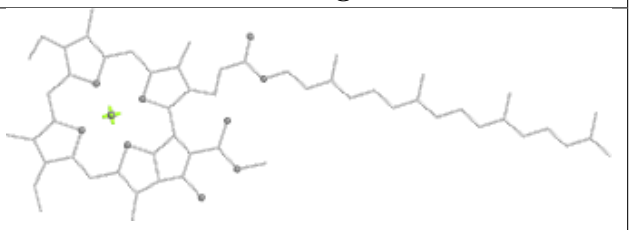
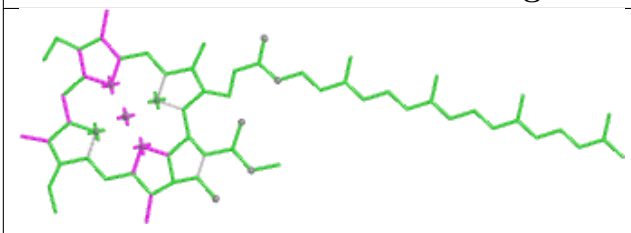
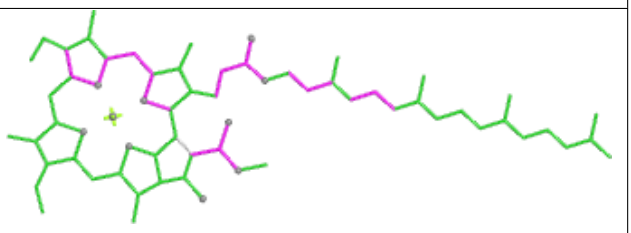
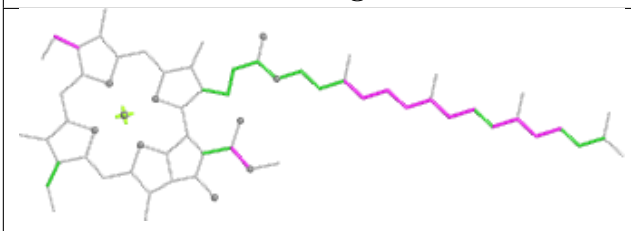
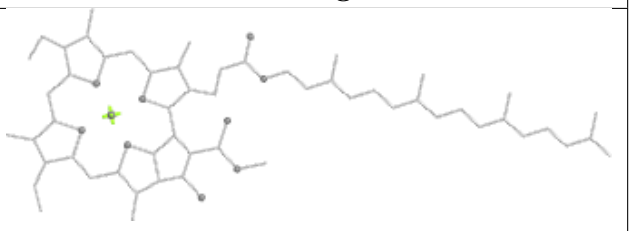
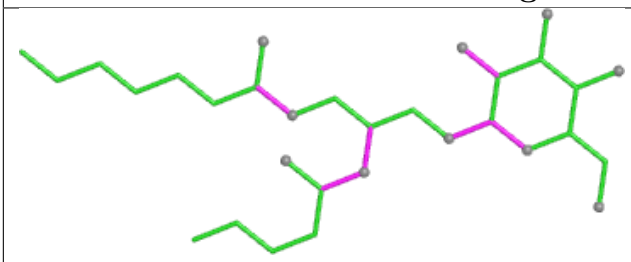


Rings

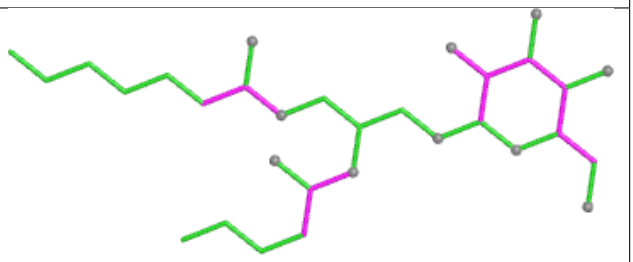
Ligand CLA a 801	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA D 208	
 Bond lengths	 Bond angles
 Torsions	 Rings

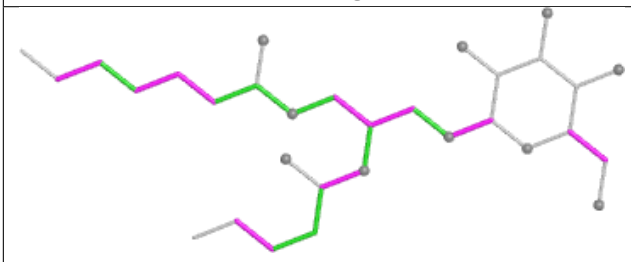
Ligand LMG C 301



Bond lengths



Bond angles



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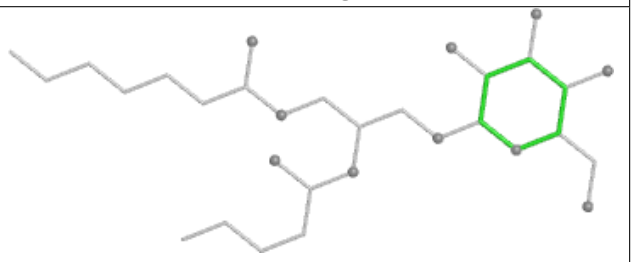
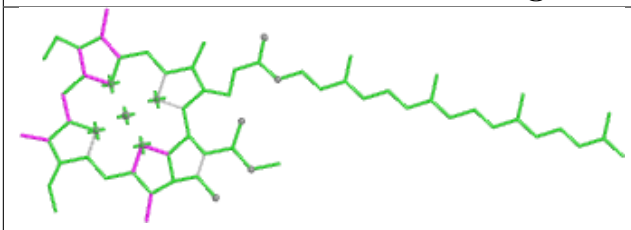


Rings

Ligand CLA b 846



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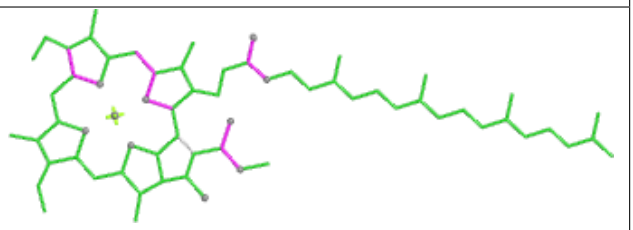
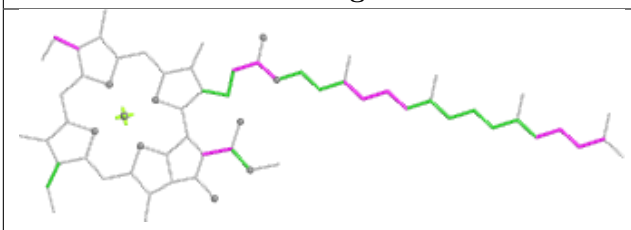


Bond angles



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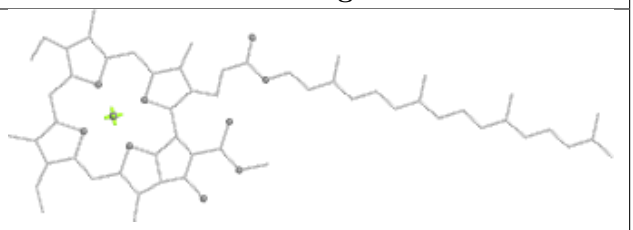
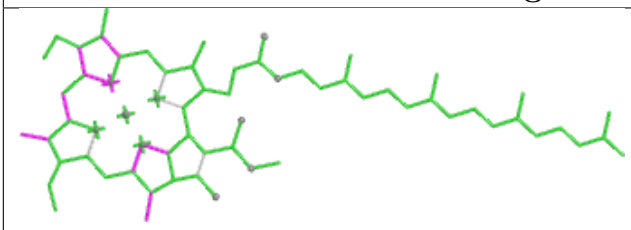
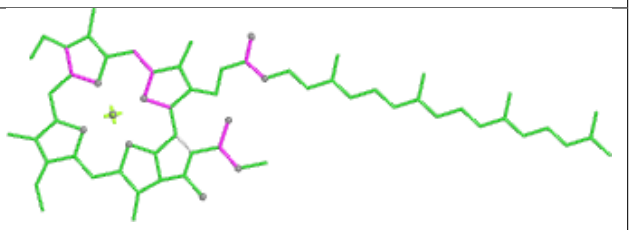


Rings

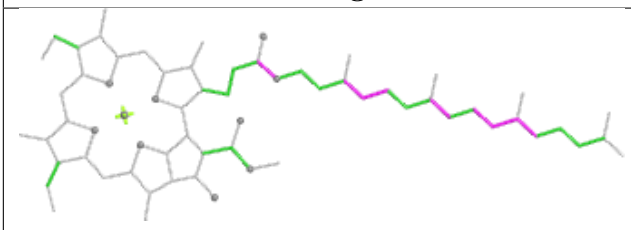
Ligand CLA B 308



Bond lengths



Bond angles



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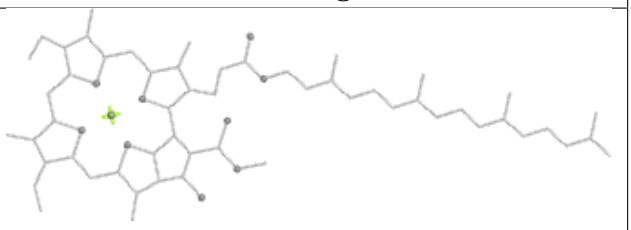
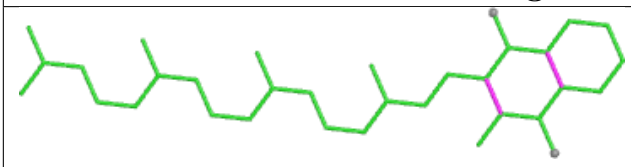


Rings

Ligand PQN a 829



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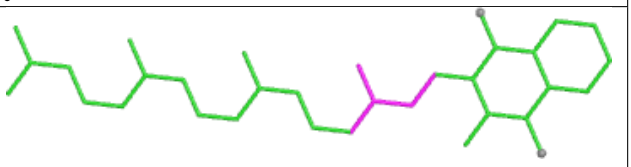
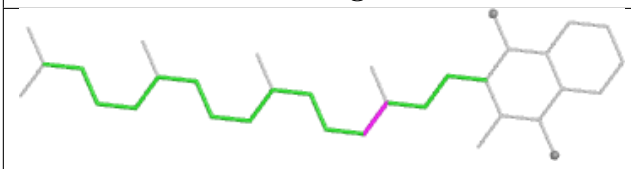


Bond angles



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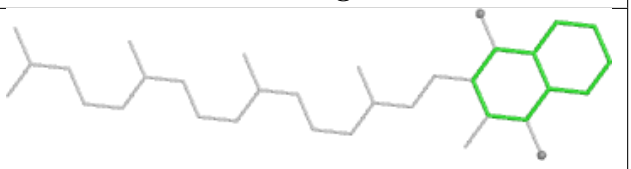
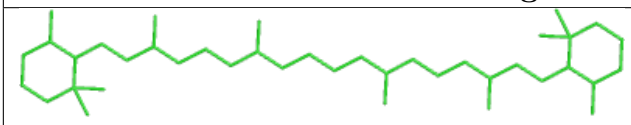


Rings

Ligand BCR m 101



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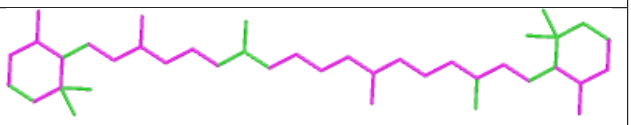
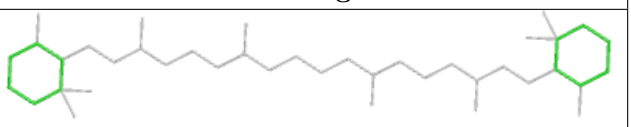


Bond angles

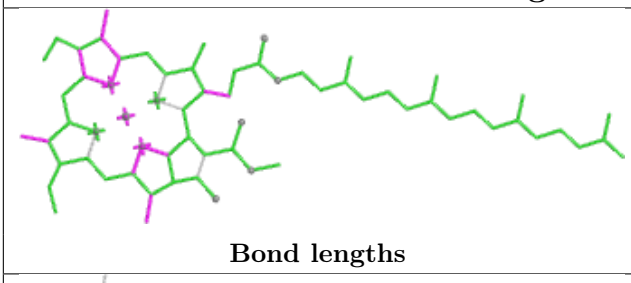


Torsions



Rings

Ligand CLA a 807



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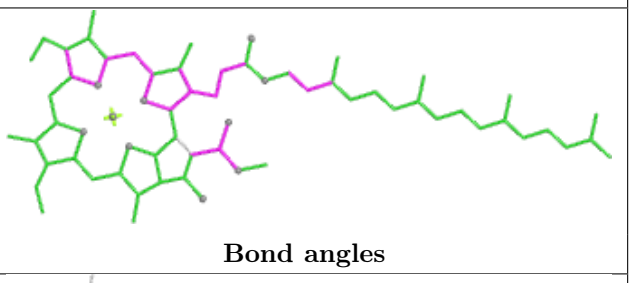
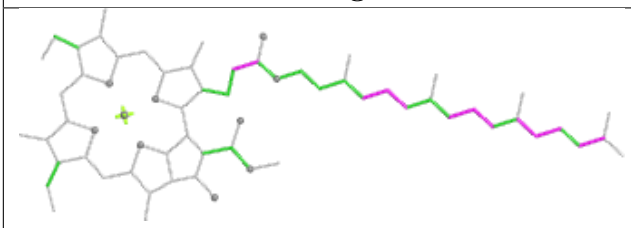


Bond angles



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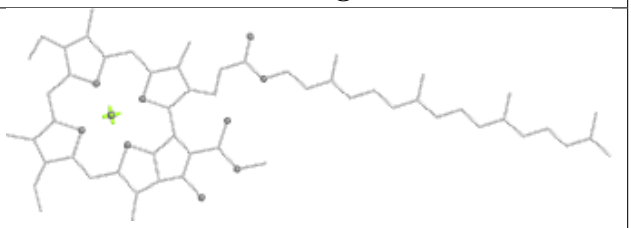
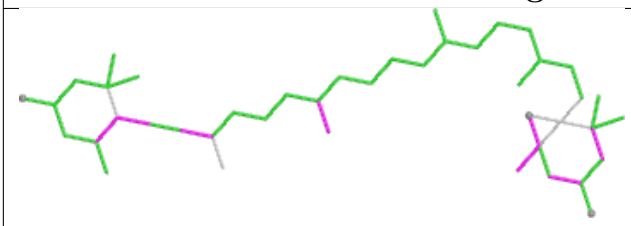


Rings

Ligand DD6 E 304



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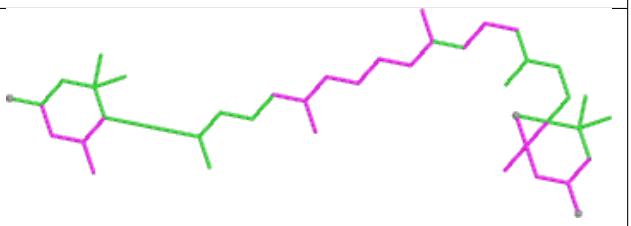
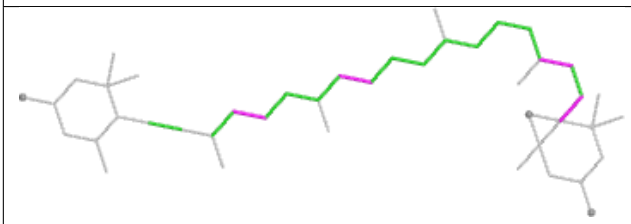


Bond angles



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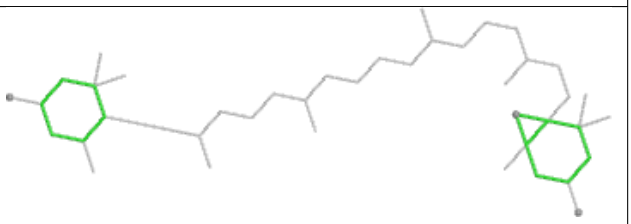
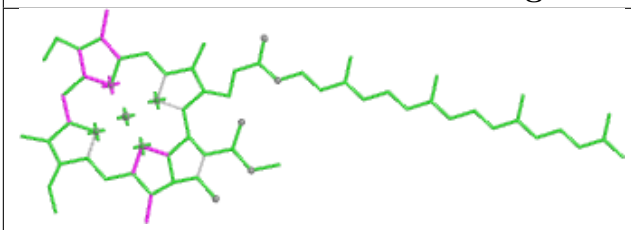


Rings

Ligand CLA E 315



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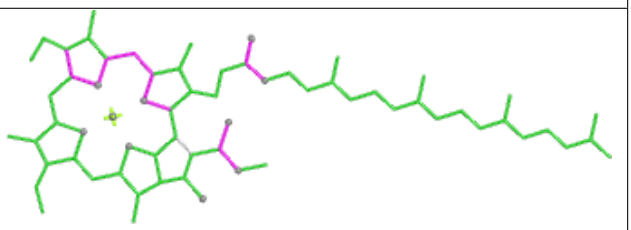
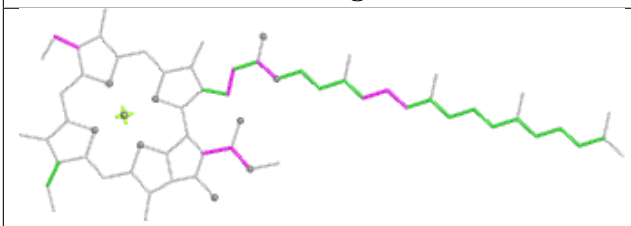


Bond angles



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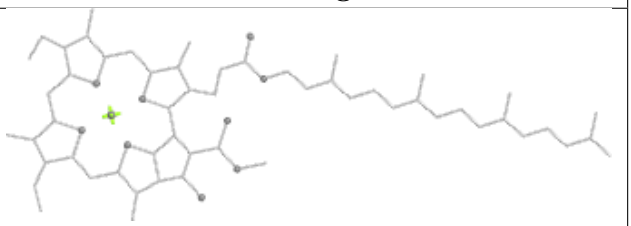
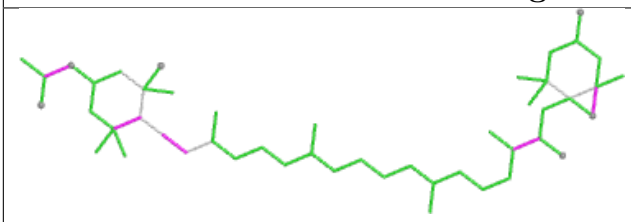
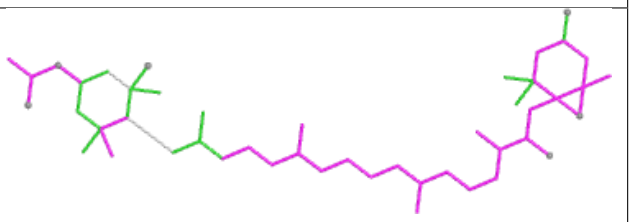


Rings

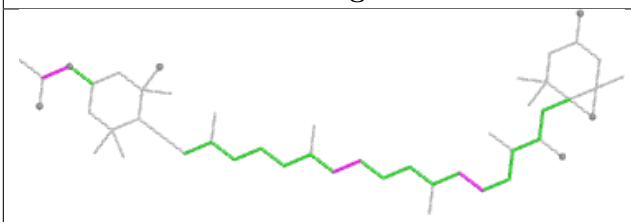
Ligand A86 H 304



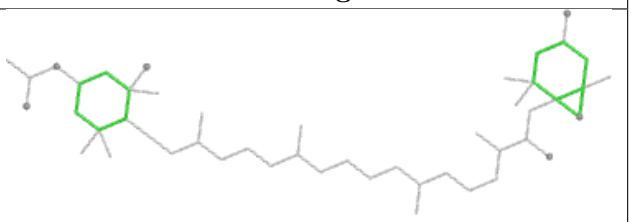
Bond lengths



Bond angles

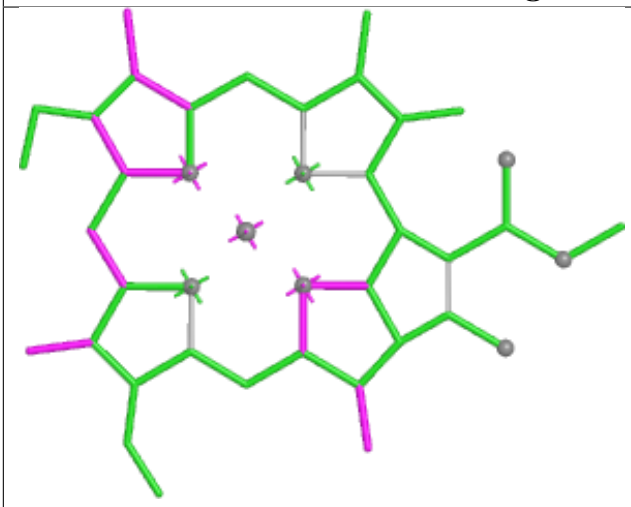


Torsions

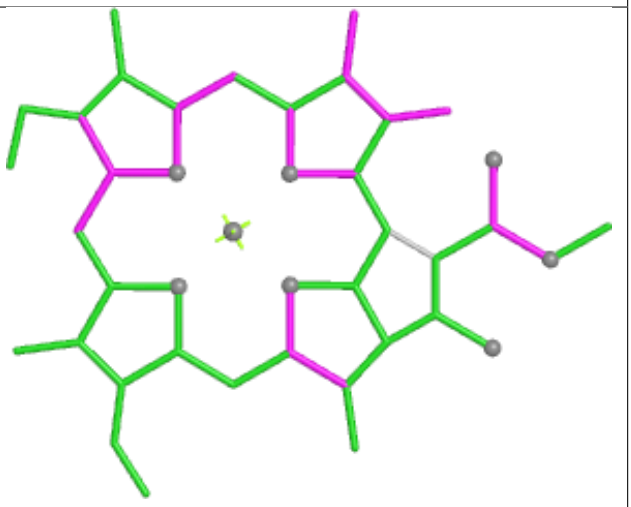


Rings

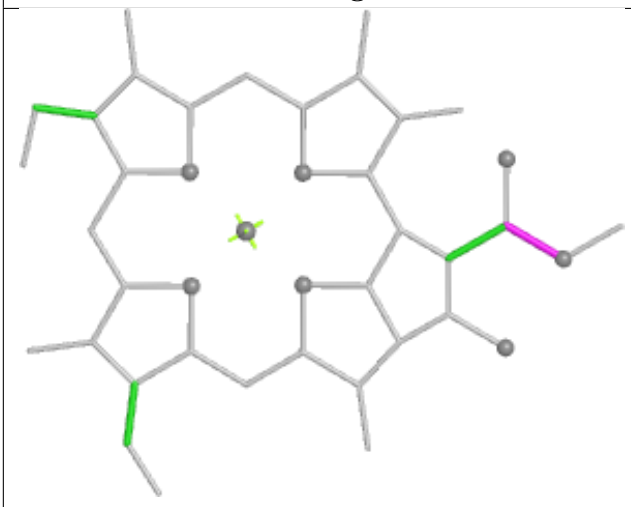
Ligand CLA B 314



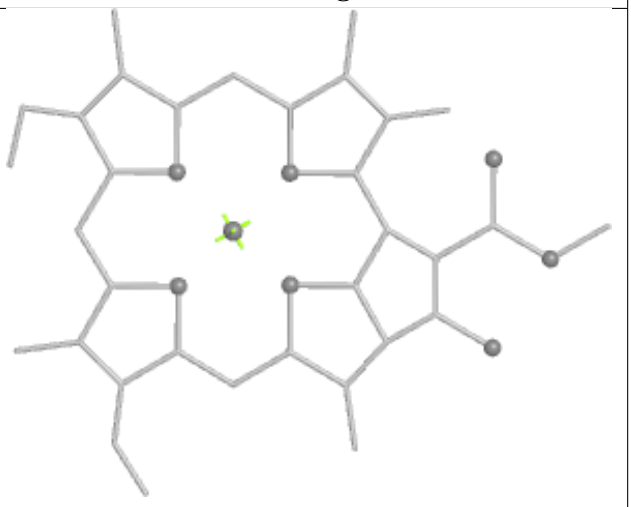
Bond lengths



Bond angles

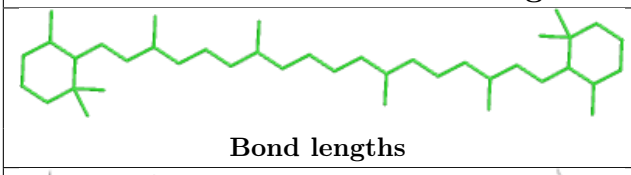


Torsions



Rings

Ligand BCR b 836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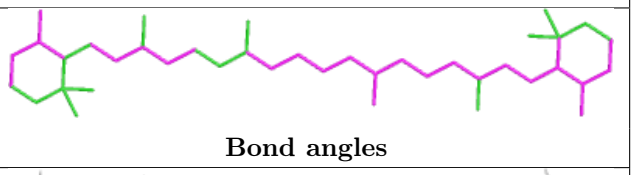
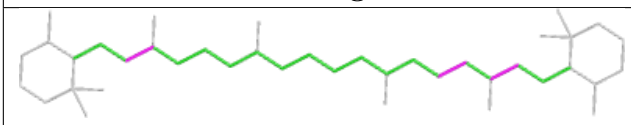
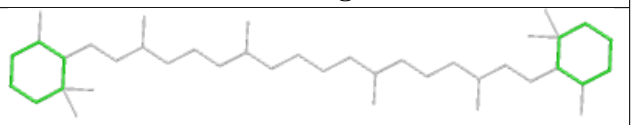
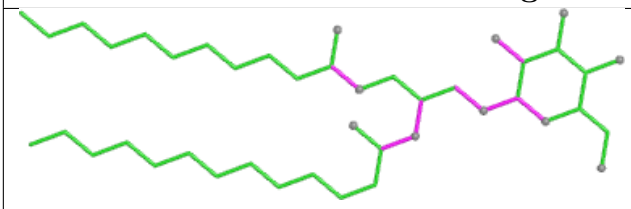
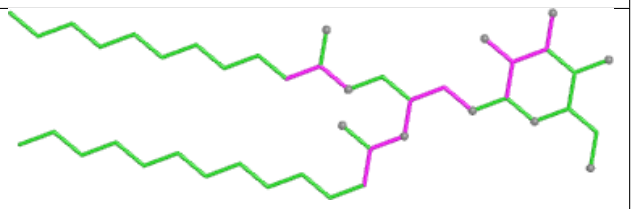

Bond angles

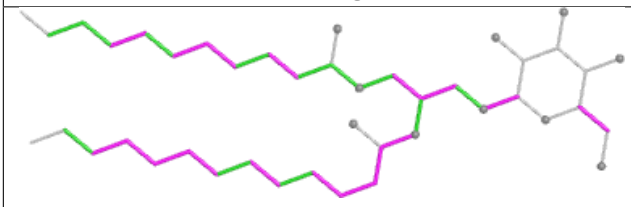

Torsions

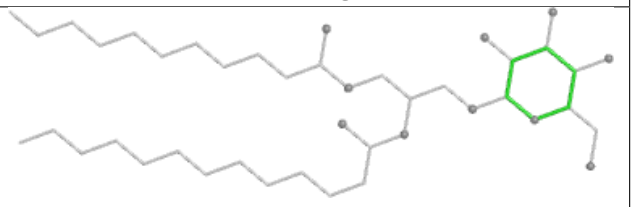

Rings

Ligand LMG E 318

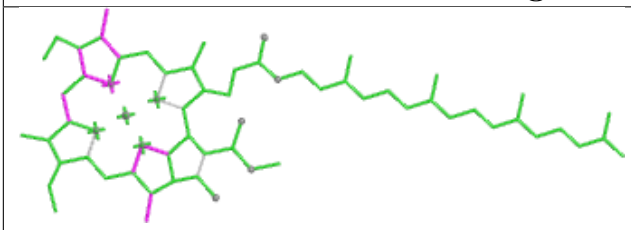

Bond lengths

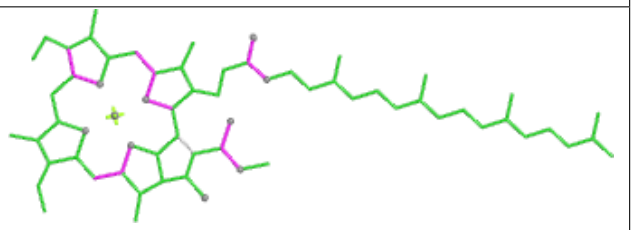

Bond angles

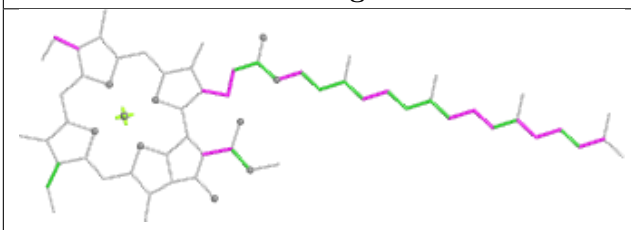

Torsions

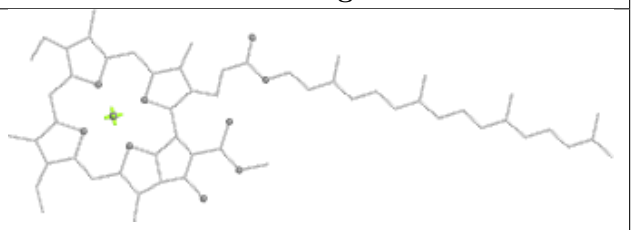

Rings

Ligand CLA b 845

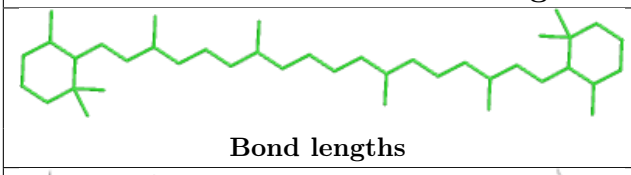

Bond lengths


Bond angles

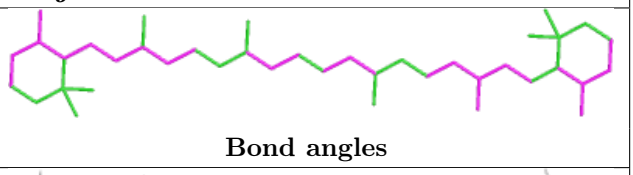

Torsions


Rings

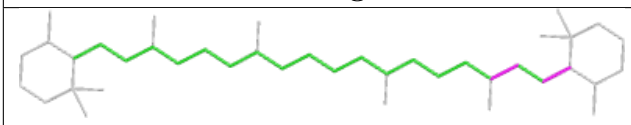
Ligand BCR j 101



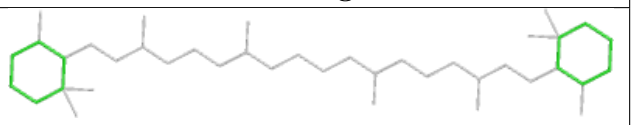
Bond lengths



Bond angles

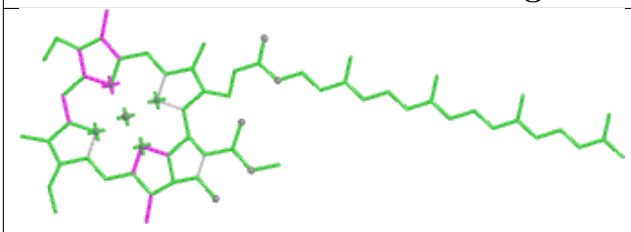


Torsions

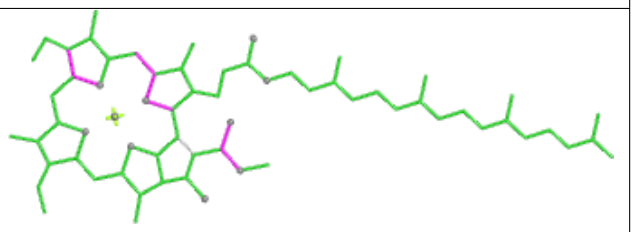


Rings

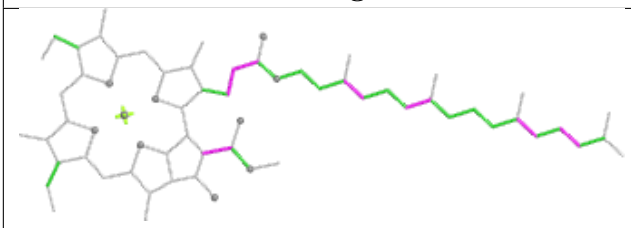
Ligand CLA B 309



Bond lengths



Bond angles



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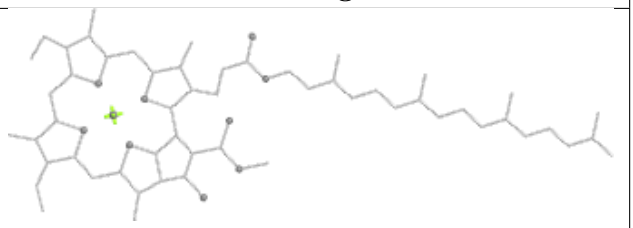
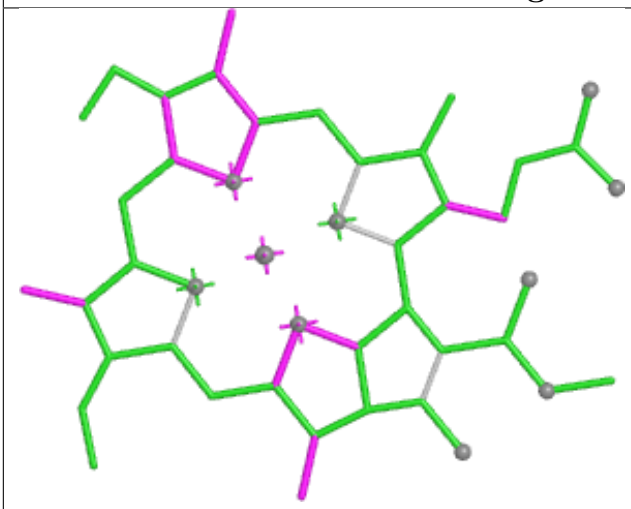
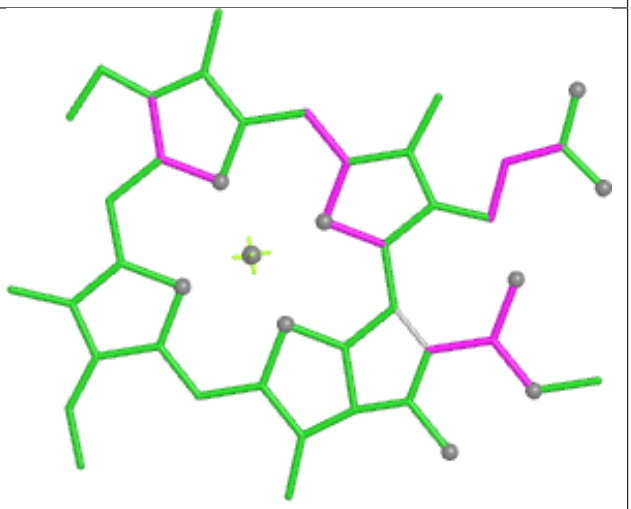


Rings

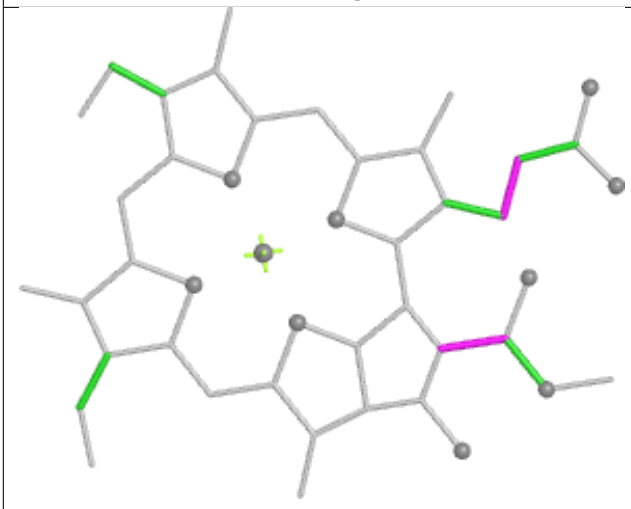
Ligand CLA b 804



Bond lengths



Bond angles

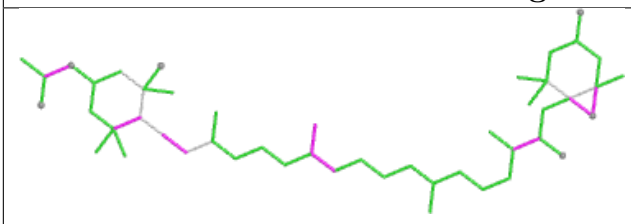


Torsions

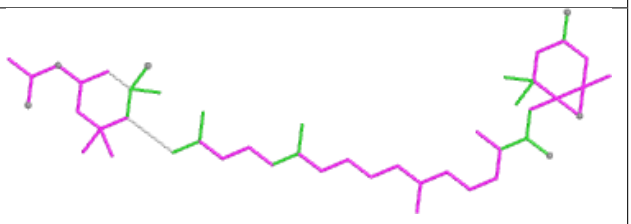


Rings

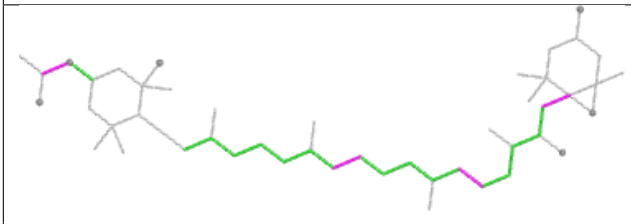
Ligand A86 H 301



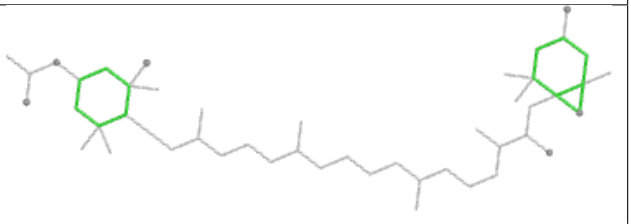
Bond lengths



Bond angles

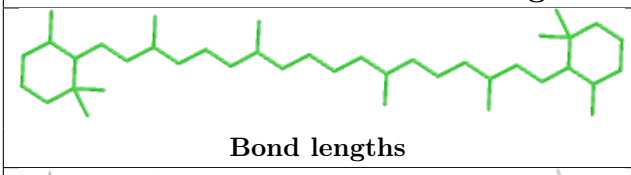


Torsions

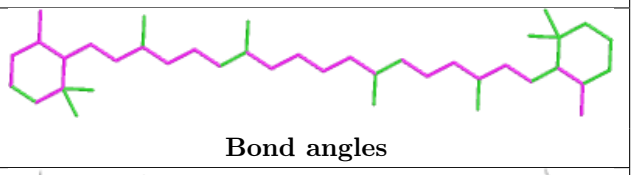


Rings

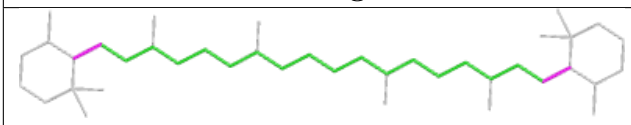
Ligand BCR r 201



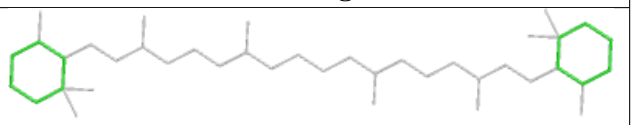
Bond lengths



Bond angles

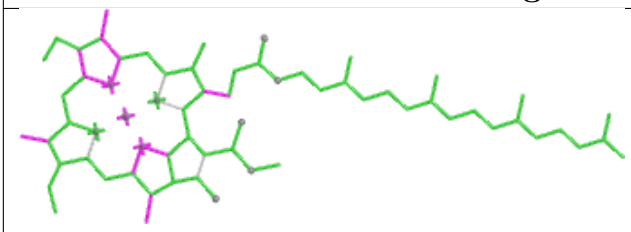


Torsions

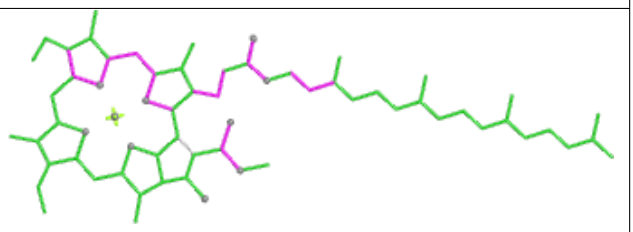


Rings

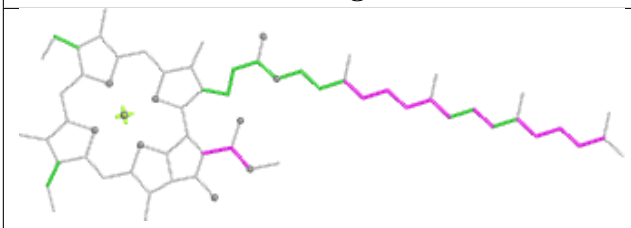
Ligand CLA H 313



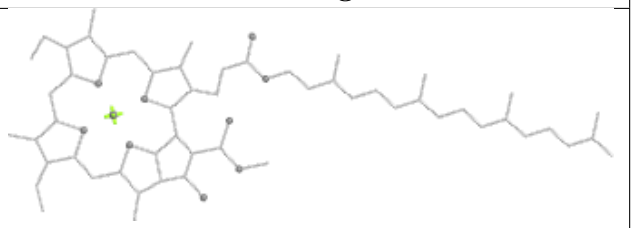
Bond lengths



Bond angles

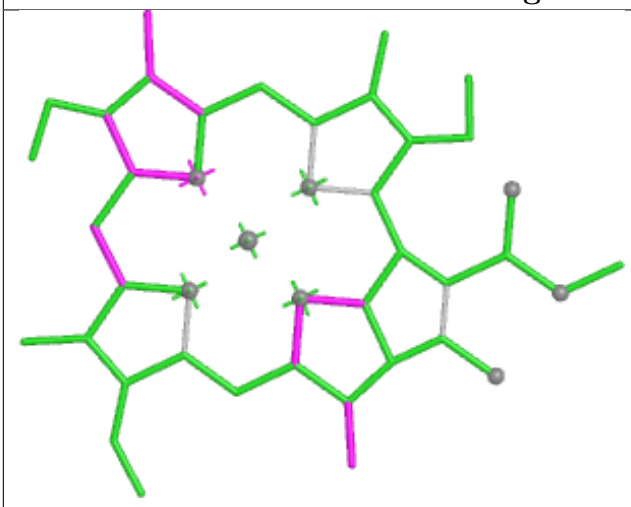


Torsions

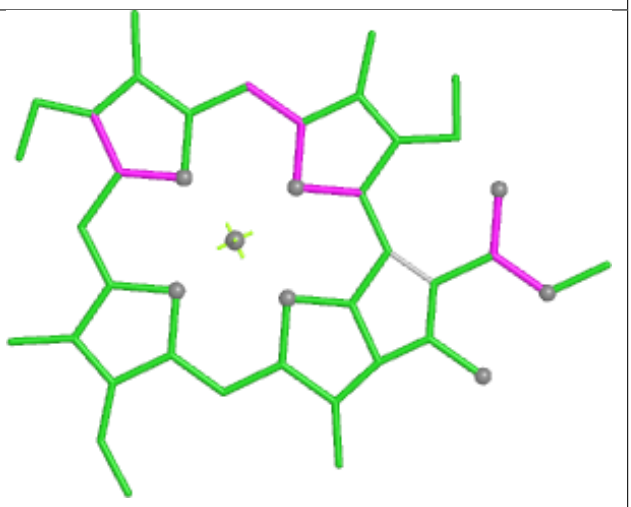


Rings

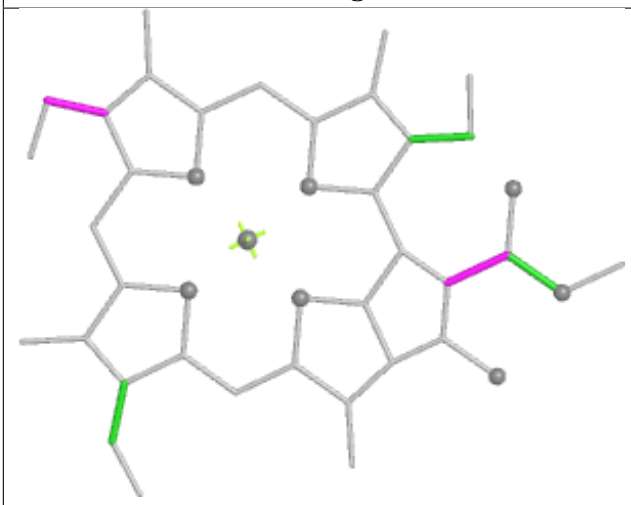
Ligand CLA D 212



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.

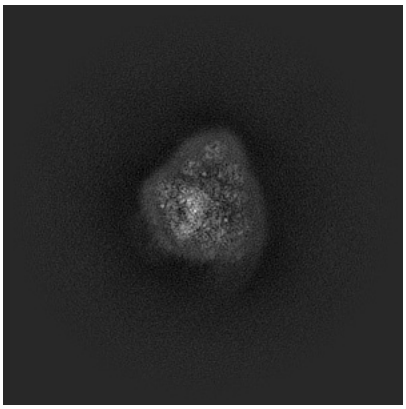
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-60044. These allow visual inspection of the internal detail of the map and identification of artifacts.

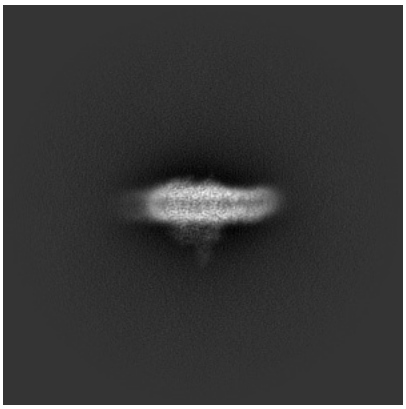
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

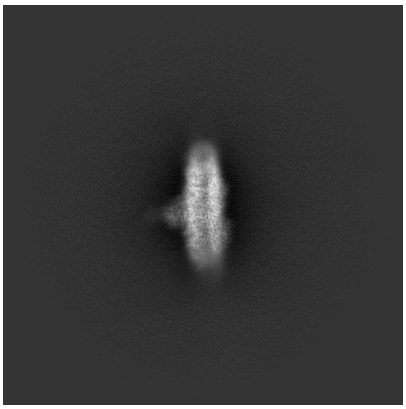
6.1.1 Primary map



X

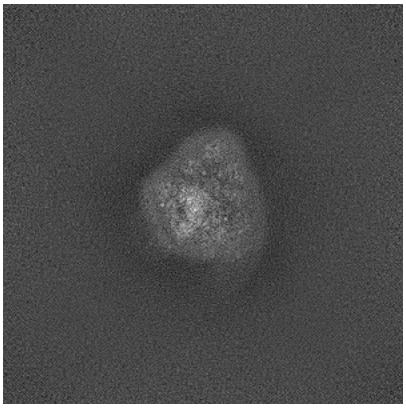


Y

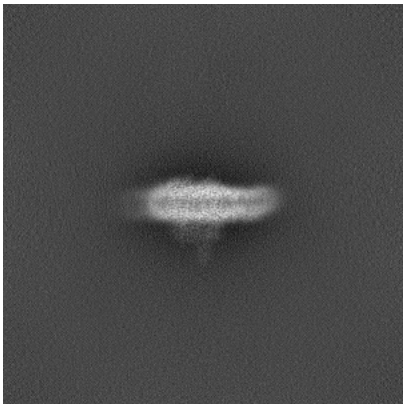


Z

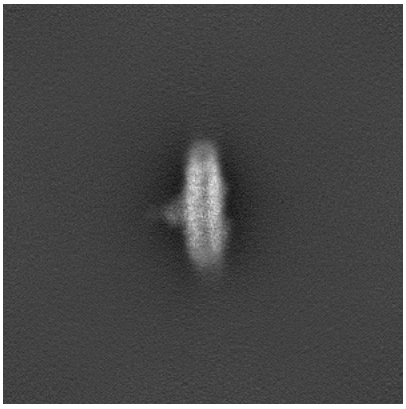
6.1.2 Raw map



X



Y

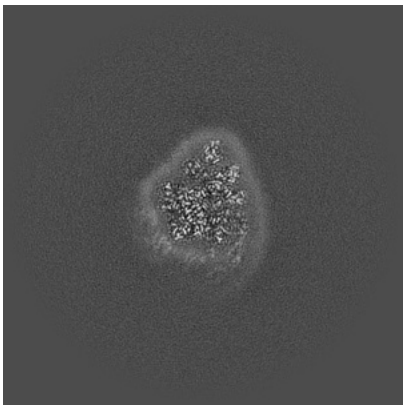


Z

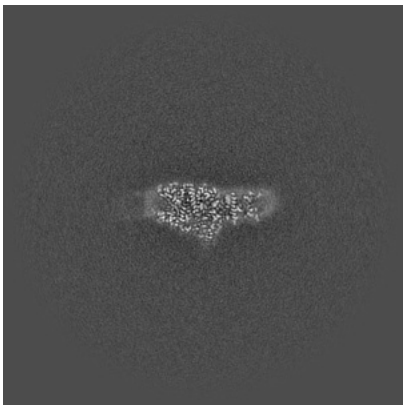
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

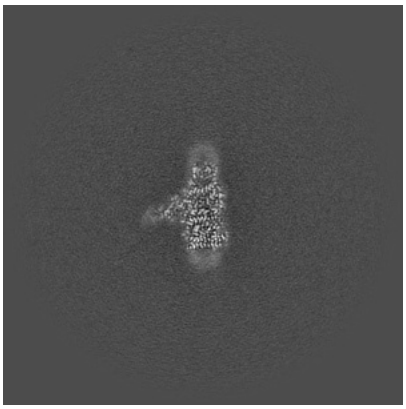
6.2.1 Primary map



X Index: 256

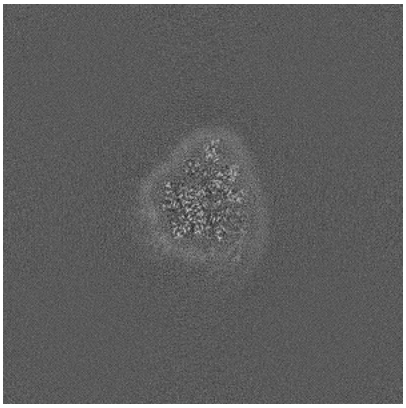


Y Index: 256

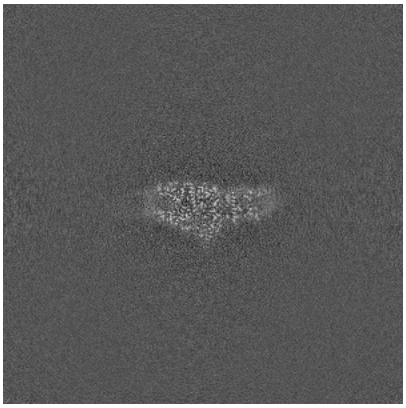


Z Index: 256

6.2.2 Raw map



X Index: 256



Y Index: 256

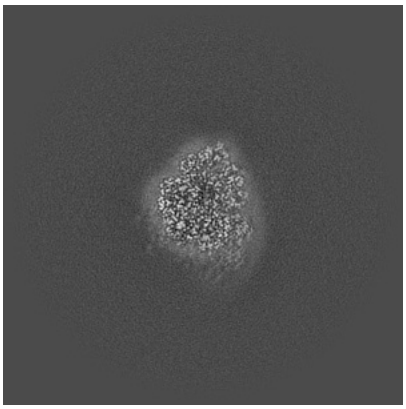


Z Index: 256

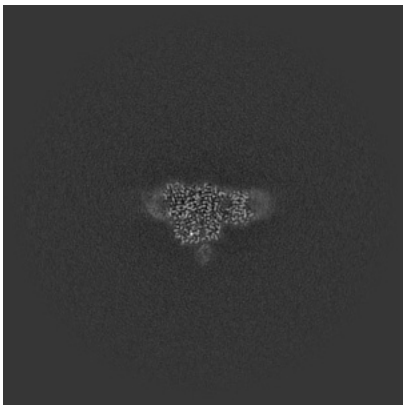
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

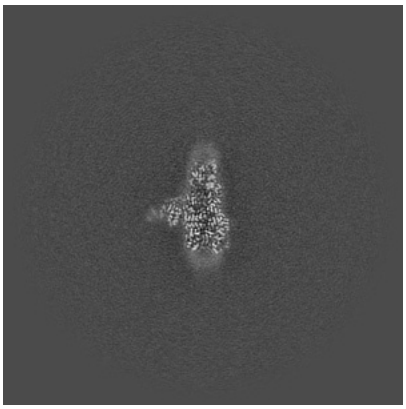
6.3.1 Primary map



X Index: 244

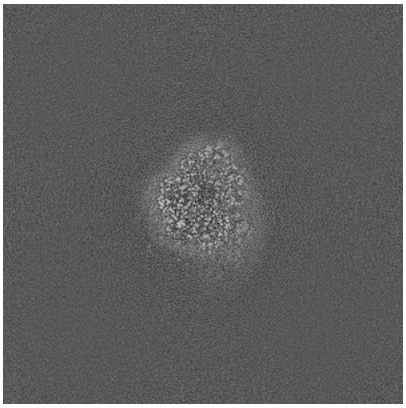


Y Index: 240

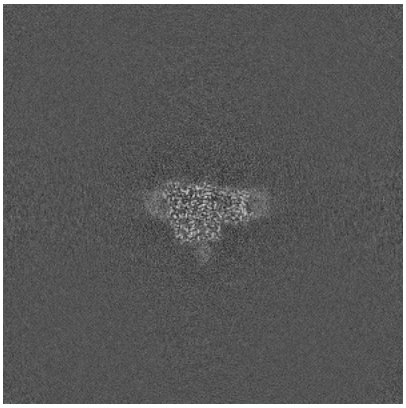


Z Index: 262

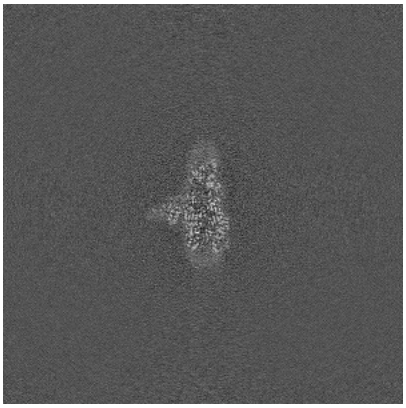
6.3.2 Raw map



X Index: 244



Y Index: 239

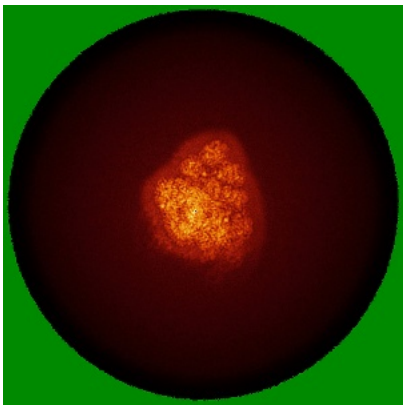


Z Index: 262

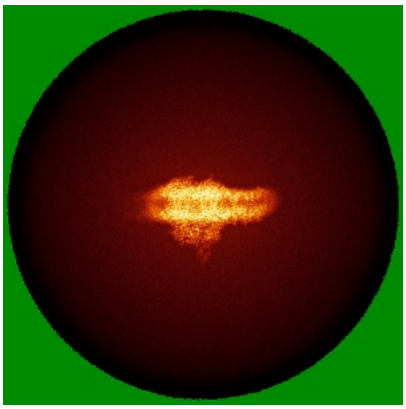
The images above show the largest variance slices of the map in three orthogonal directions.

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

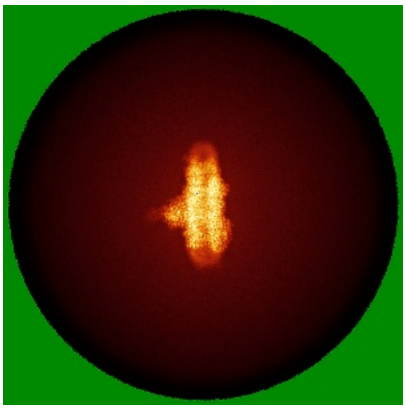
6.4.1 Primary map



X

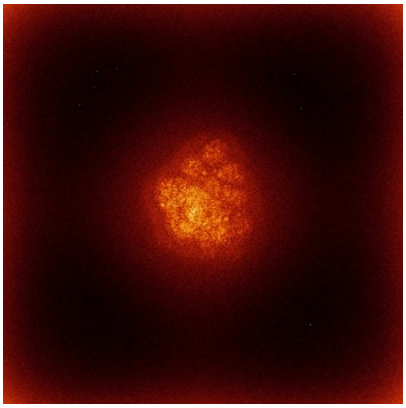


Y

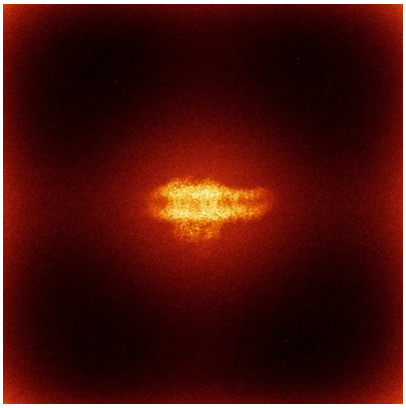


Z

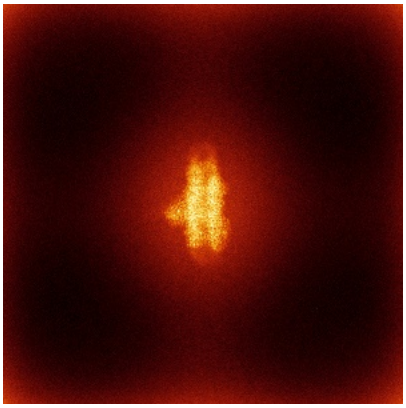
6.4.2 Raw map



X



Y



Z

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

6.5 Orthogonal surface views (i)

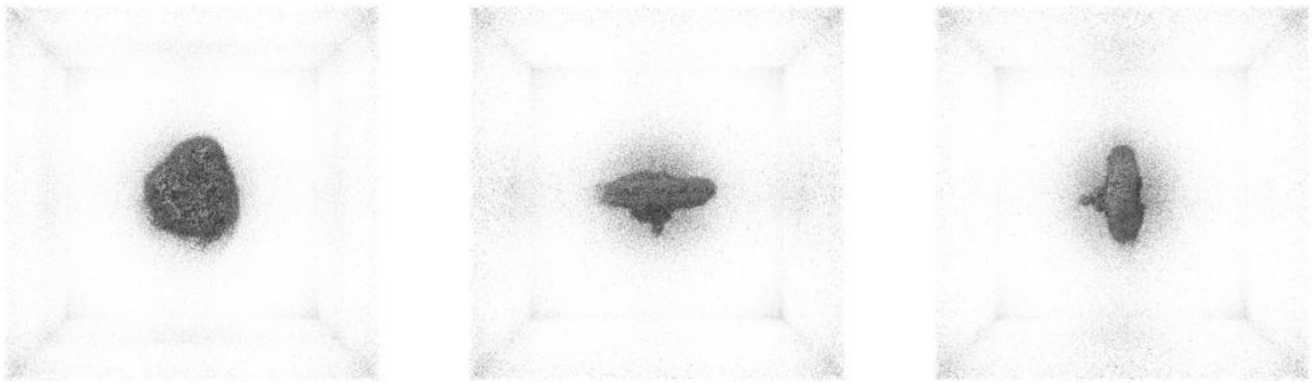
6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.08. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X Y Z

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

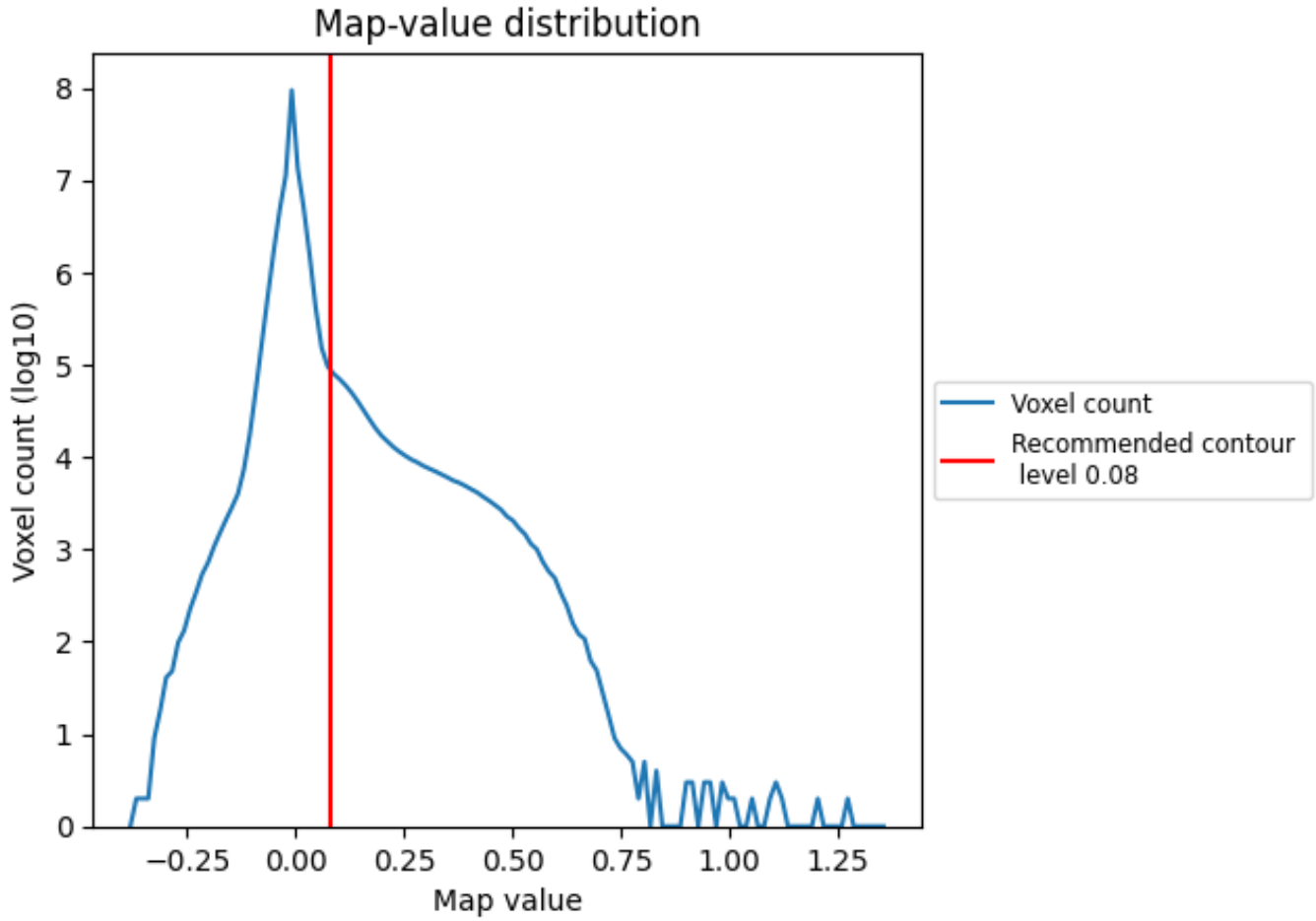
6.6 Mask visualisation (i)

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

7 Map analysis

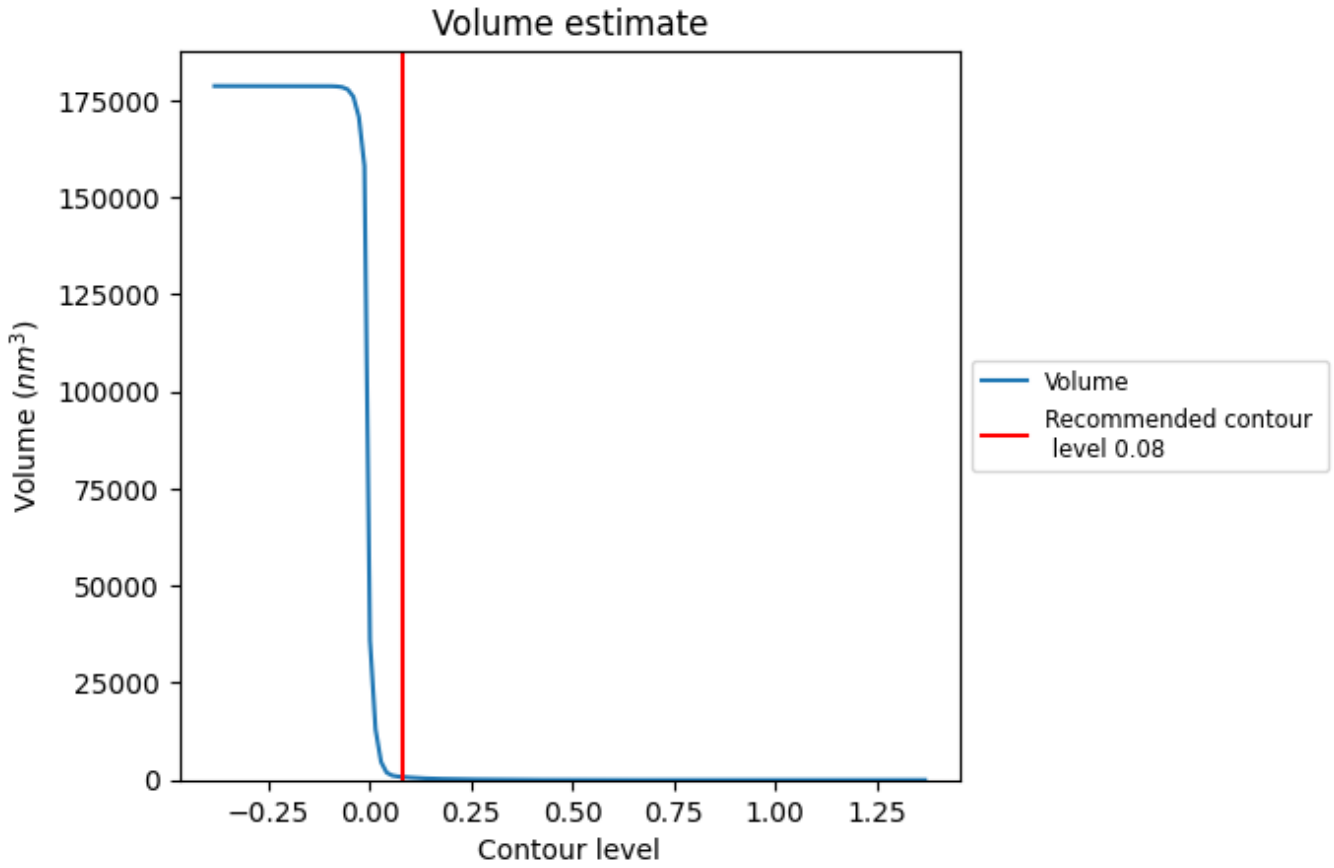
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

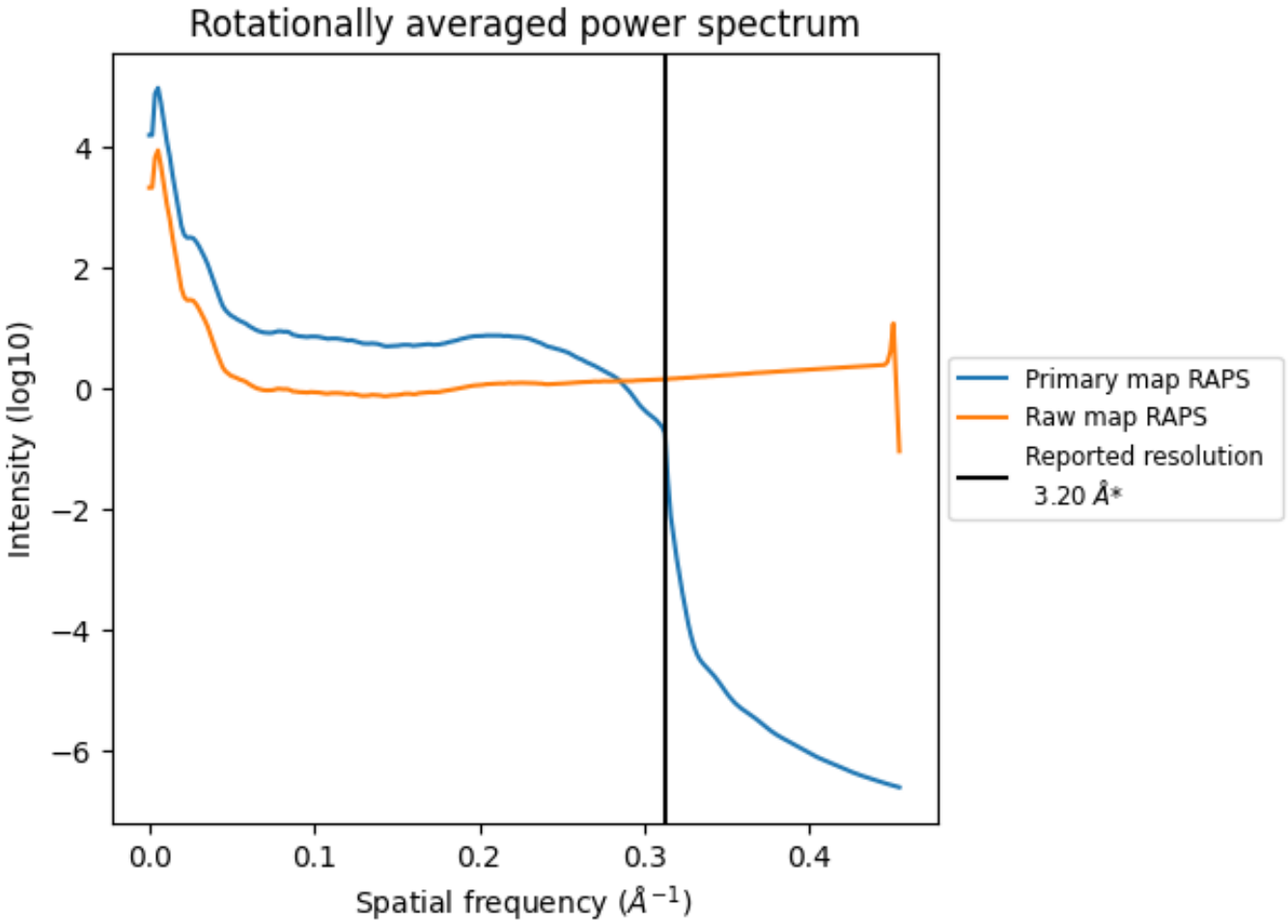
7.2 Volume estimate (i)



The volume at the recommended contour level is 799 nm^3; this corresponds to an approximate mass of 722 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)

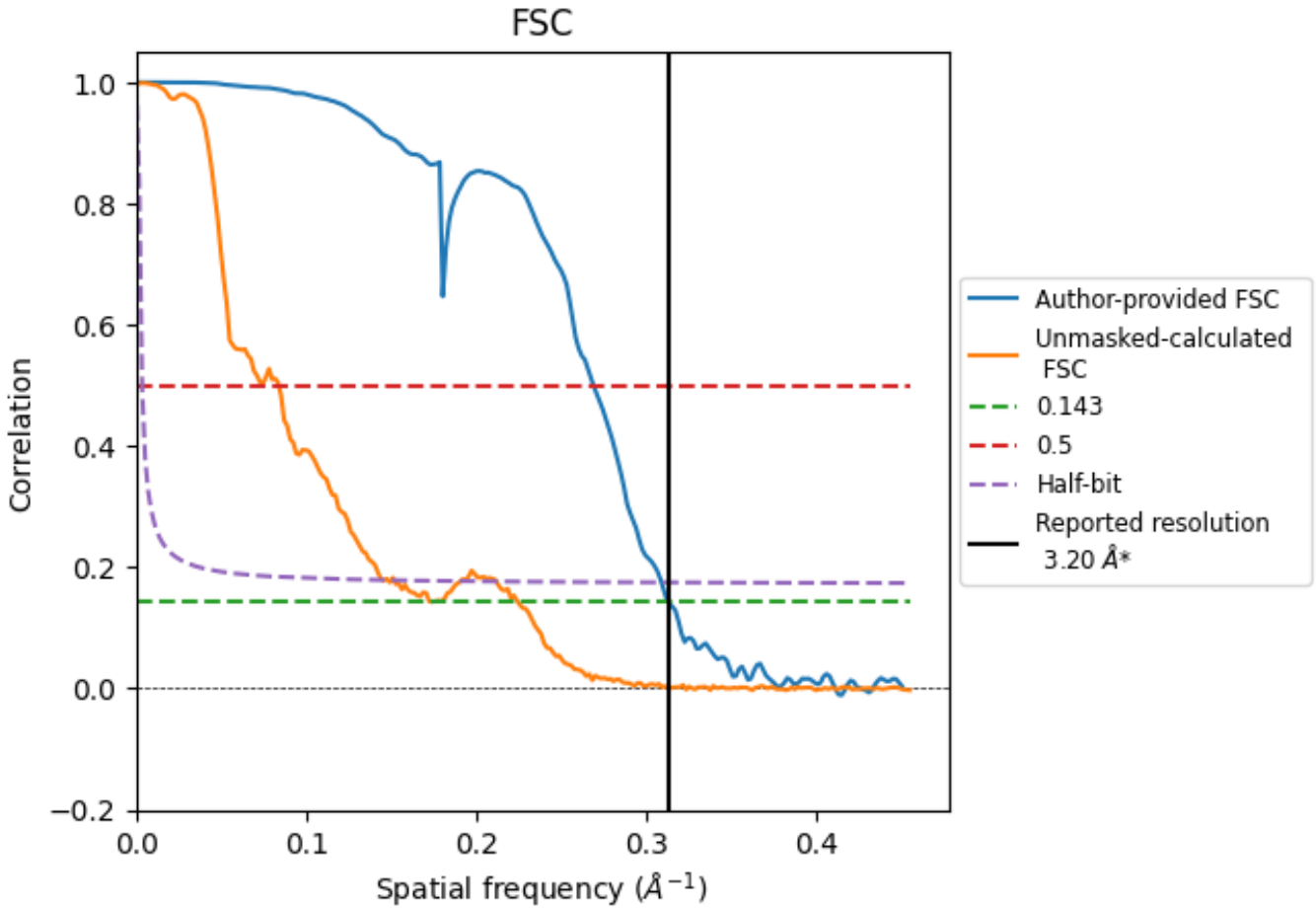


*Reported resolution corresponds to spatial frequency of 0.312 Å^{-1}

8 Fourier-Shell correlation

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

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.312 Å^{-1}

8.2 Resolution estimates (i)

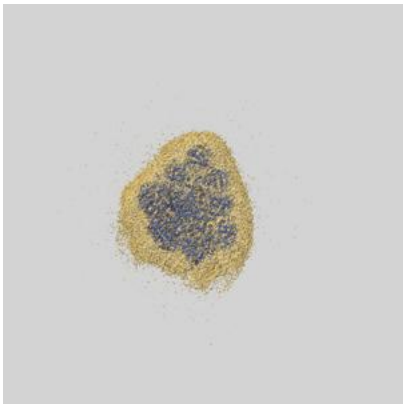
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.20	-	-
Author-provided FSC curve	3.20	3.72	3.24
Unmasked-calculated*	5.75	11.93	6.88

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 5.75 differs from the reported value 3.2 by more than 10 %

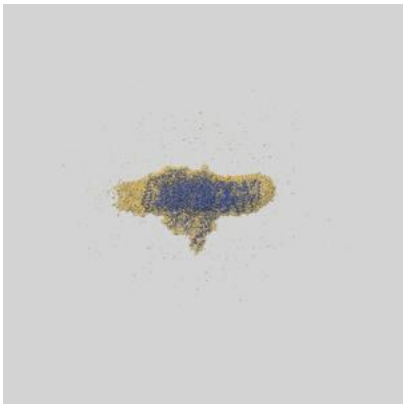
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-60044 and PDB model 8ZET. Per-residue inclusion information can be found in section 3 on page 23.

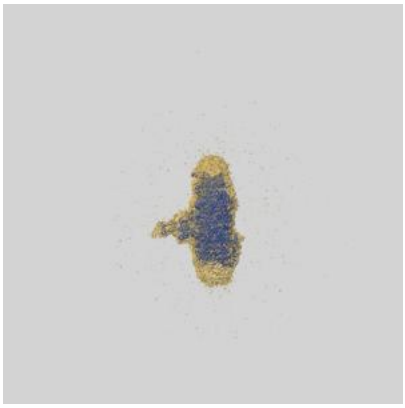
9.1 Map-model overlay



X



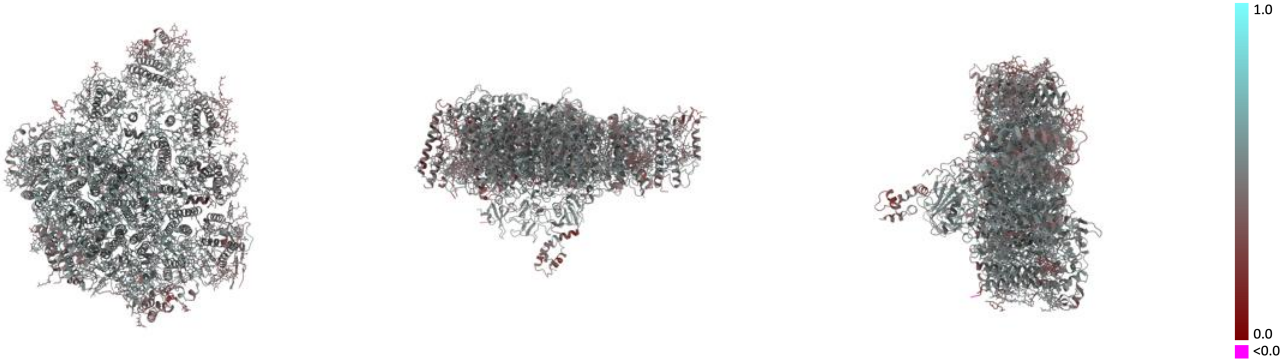
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.08 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

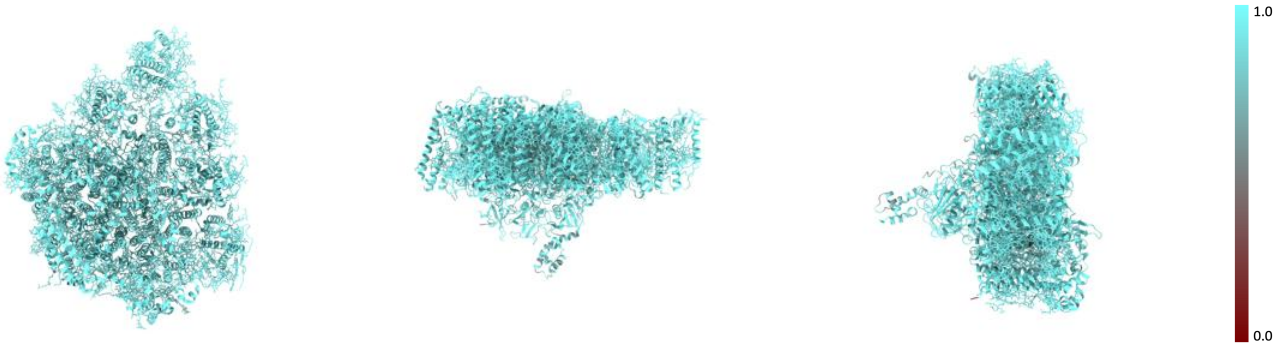
9.2 Q-score mapped to coordinate model



X Y Z

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

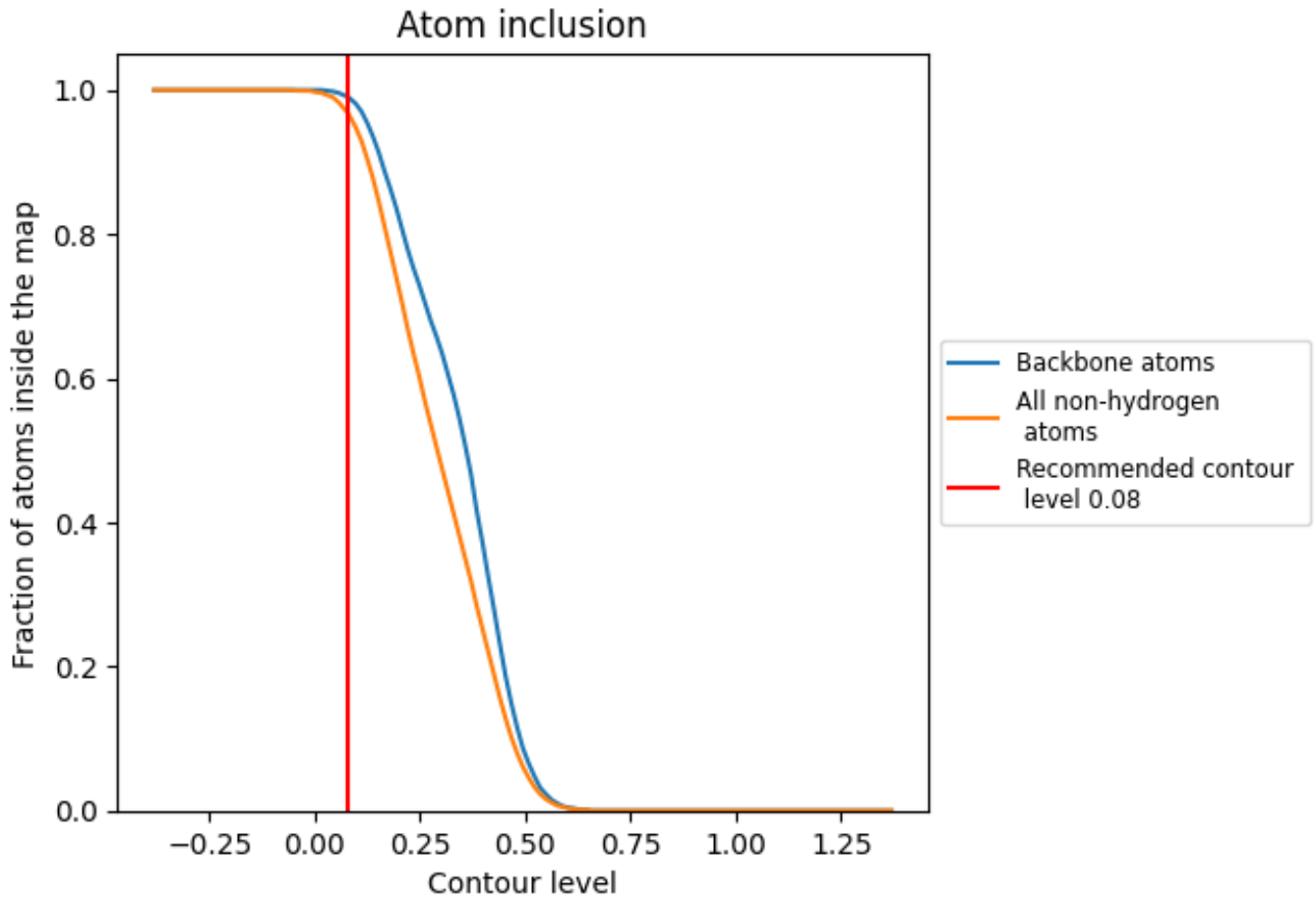
9.3 Atom inclusion mapped to coordinate model



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.08).

9.4 Atom inclusion (i)



At the recommended contour level, 99% of all backbone atoms, 97% 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 (0.08) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9670	0.4850
B	0.9740	0.4570
C	0.9780	0.4520
D	0.9670	0.4720
E	0.9700	0.4710
H	0.9600	0.4360
a	0.9740	0.5120
b	0.9690	0.5060
c	0.9880	0.5100
d	0.9790	0.5070
e	0.9510	0.4720
f	0.9650	0.4760
g	0.8680	0.4000
i	0.9640	0.5130
j	0.9490	0.4710
l	0.9770	0.5060
m	0.9440	0.4770
r	0.9330	0.3970

