wwPDB EM Validation Summary Report (i)

Oct 4, 2026 – 04:44 PM JST

PDB ID	:	8WMW / pdb_00008wmw
EMDB ID	:	EMD-37660
Title	:	The structure of PSI-11CAC at the stationary growth phase
Authors	:	Zhang, S.M.; Si, L.; Li, M.
Deposited on	:	2023-10-04
Resolution	:	3.30 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 (1)) were used in the production of this report:

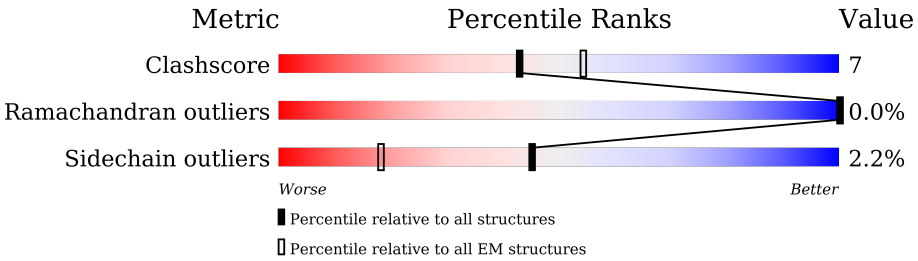
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.2
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using 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)	:	2.51

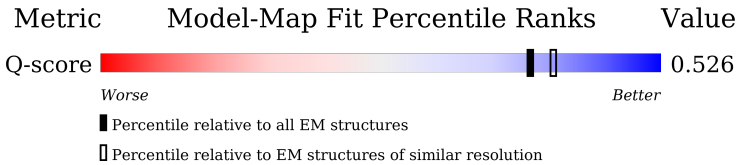
1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.30 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	15087 (2.80 - 3.80)

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	752	87% 11% •
2	B	734	88% 12%
3	C	81	86% 12% •
4	D	141	85% 13% •

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Mol	Chain	Length	Quality of chain
5	E	64	78% 14% 6%
6	F	188	78% 7% 14%
7	I	36	81% 14% 6%
8	J	42	88% 12%
9	L	153	90% 8%
10	M	30	87% 13%
11	O	146	5% 58% 13% 29%
12	K	87	66% 13% 21%
13	c	216	6% 64% 12% 21%
14	a	216	69% 11% 19%
15	b	223	11% 74% 12% 13%
16	h	225	61% 10% 28%
17	e	203	70% 13% 17%
18	k	241	61% 13% 25%
19	f	212	68% 13% 18%
19	j	212	67% 14% 19%
20	i	218	15% 72% 8% 20%
21	d	213	11% 47% 11% 41%
22	g	255	72% 13% 14%
23	R	129	64% 5% 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
29	SF4	A	854	-	-	X	-
29	SF4	C	101	-	-	X	-

2 Entry composition (i)

There are 36 unique types of molecules in this entry. The entry contains 51054 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	742	5825	3802	994	1001	28	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	5826	3844	982	985	15	1	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	592	361	103	116	12	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	139	1084	692	186	203	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		
5	E	60	485	309	84	92	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	161	1254	814	212	226	2	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	I	34	264	182	35	45	2	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	J	42	351	240	49	59	3	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	L	151	1146	753	182	208	3	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	M	30	232	155	38	38	1	0	0

- Molecule 11 is a protein called PsaO.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	O	104	773	515	117	138	3	0	0

- Molecule 12 is a protein called Photosystem I reaction center subunit PsaK.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	K	69	488	319	80	87	2	0	0

- Molecule 13 is a protein called CAC-c.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	c	170	1357	897	221	236	3	0	0

- Molecule 14 is a protein called CAC-a.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	a	175	1361	889	217	245	10	0	0

- Molecule 15 is a protein called CAC-b.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
15	b	194	1439	916	251	258	14	0	0

- Molecule 16 is a protein called CAC-h.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
16	h	162	1200	778	202	214	6	0	0

- Molecule 17 is a protein called CAC-e.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
17	e	169	1286	843	207	228	8	0	0

- Molecule 18 is a protein called CAC-k.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
18	k	180	1346	872	223	239	12	0	0

- Molecule 19 is a protein called CAC-f.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
19	f	174	1302	842	212	240	8	0	0
19	j	172	1293	834	212	239	8	0	0

- Molecule 20 is a protein called CAC-i.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
20	i	175	1324	849	227	237	11	0	0

- Molecule 21 is a protein called CAC-d.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
21	d	126	950	609	165	167	9	0	0

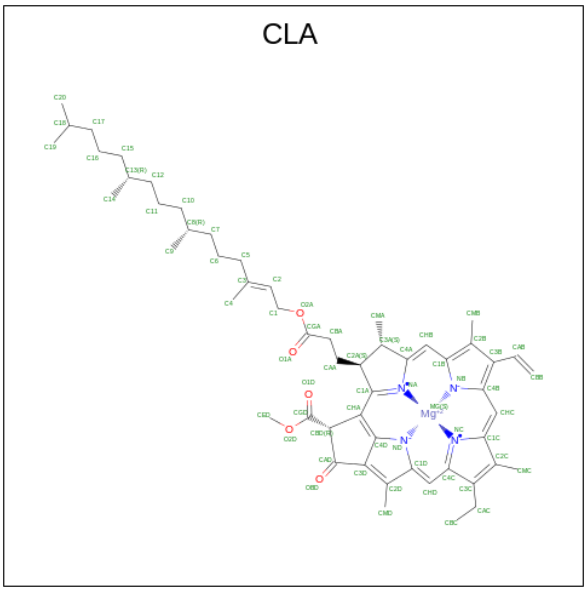
- Molecule 22 is a protein called CAC-g.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
22	g	219	1630	1060	267	292	11	0	0

- Molecule 23 is a protein called PsaR.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
23	R	90	664	434	105	124	1	0	0

- Molecule 24 is CHLOROPHYLL A (CCD ID: CLA) (formula: $C_{55}H_{72}MgN_4O_5$).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
24	A	1	65	55	1	4	5	0
24	A	1	65	55	1	4	5	0
24	A	1	55	45	1	4	5	0
24	A	1	65	55	1	4	5	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
24	A	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
24	A	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
24	A	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
24	A	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
24	A	1	56	46	1	4	5	0
			Total	C	Mg	N	O	
24	A	1	62	52	1	4	5	0
			Total	C	Mg	N	O	
24	A	1	54	44	1	4	5	0
			Total	C	Mg	N	O	
24	A	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
24	A	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
24	A	1	50	40	1	4	5	0
			Total	C	Mg	N	O	
24	A	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
24	A	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
24	A	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
24	A	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
24	A	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
24	A	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
24	A	1	49	39	1	4	5	0
			Total	C	Mg	N	O	
24	A	1	51	41	1	4	5	0
			Total	C	Mg	N	O	
24	A	1	55	45	1	4	5	0
			Total	C	Mg	N	O	
24	A	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
24	A	1	65	55	1	4	5	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
24	A	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
24	A	1	62	52	1	4	5	0
			Total	C	Mg	N	O	
24	A	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
24	A	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
24	A	1	50	40	1	4	5	0
			Total	C	Mg	N	O	
24	A	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
24	A	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
24	A	1	50	40	1	4	5	0
			Total	C	Mg	N	O	
24	A	1	51	41	1	4	5	0
			Total	C	Mg	N	O	
24	A	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
24	A	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
24	A	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
24	A	1	52	42	1	4	5	0
			Total	C	Mg	N	O	
24	A	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
24	A	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
24	A	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
24	A	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
24	A	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
24	A	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
24	A	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
24	A	1	41	33	1	4	3	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
24	B	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
24	B	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
24	B	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
24	B	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
24	B	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
24	B	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
24	B	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
24	B	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
24	B	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
24	B	1	54	44	1	4	5	0
			Total	C	Mg	N	O	
24	B	1	55	45	1	4	5	0
			Total	C	Mg	N	O	
24	B	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
24	B	1	60	50	1	4	5	0
			Total	C	Mg	N	O	
24	B	1	59	49	1	4	5	0
			Total	C	Mg	N	O	
24	B	1	55	45	1	4	5	0
			Total	C	Mg	N	O	
24	B	1	59	49	1	4	5	0
			Total	C	Mg	N	O	
24	B	1	57	47	1	4	5	0
			Total	C	Mg	N	O	
24	B	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
24	B	1	46	36	1	4	5	0
			Total	C	Mg	N	O	
24	B	1	55	45	1	4	5	0
			Total	C	Mg	N	O	
24	B	1	53	43	1	4	5	0
			Total	C	Mg	N	O	
24	B	1	65	55	1	4	5	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
24	B	1	64	54	1	4	5	0
			Total	C	Mg	N	O	
24	B	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
24	B	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
24	B	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
24	B	1	50	40	1	4	5	0
			Total	C	Mg	N	O	
24	B	1	49	39	1	4	5	0
			Total	C	Mg	N	O	
24	B	1	50	40	1	4	5	0
			Total	C	Mg	N	O	
24	B	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
24	B	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
24	B	1	58	48	1	4	5	0
			Total	C	Mg	N	O	
24	B	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
24	B	1	47	37	1	4	5	0
			Total	C	Mg	N	O	
24	B	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
24	B	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
24	B	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
24	B	1	57	47	1	4	5	0
			Total	C	Mg	N	O	
24	B	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
24	B	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
24	B	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
24	F	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
24	F	1	52	42	1	4	5	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
24	I	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
24	J	1	42	34	1	4	3	0
			Total	C	Mg	N	O	
24	J	1	51	41	1	4	5	0
			Total	C	Mg	N	O	
24	L	1	49	39	1	4	5	0
			Total	C	Mg	N	O	
24	L	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
24	L	1	50	40	1	4	5	0
			Total	C	Mg	N	O	
24	L	1	51	41	1	4	5	0
			Total	C	Mg	N	O	
24	O	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
24	O	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
24	K	1	51	41	1	4	5	0
			Total	C	Mg	N	O	
24	K	1	42	34	1	4	3	0
			Total	C	Mg	N	O	
24	c	1	51	41	1	4	5	0
			Total	C	Mg	N	O	
24	c	1	50	40	1	4	5	0
			Total	C	Mg	N	O	
24	c	1	51	41	1	4	5	0
			Total	C	Mg	N	O	
24	c	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
24	c	1	51	41	1	4	5	0
			Total	C	Mg	N	O	
24	c	1	52	42	1	4	5	0
			Total	C	Mg	N	O	
24	c	1	46	36	1	4	5	0
			Total	C	Mg	N	O	
24	c	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
24	c	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
24	c	1	45	35	1	4	5	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
24	c	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
24	a	1	52	42	1	4	5	0
			Total	C	Mg	N	O	
24	a	1	50	40	1	4	5	0
			Total	C	Mg	N	O	
24	a	1	51	41	1	4	5	0
			Total	C	Mg	N	O	
24	a	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
24	a	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
24	a	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
24	a	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
24	a	1	48	38	1	4	5	0
			Total	C	Mg	N	O	
24	a	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
24	a	1	47	37	1	4	5	0
			Total	C	Mg	N	O	
24	a	1	48	38	1	4	5	0
			Total	C	Mg	N	O	
24	b	1	51	41	1	4	5	0
			Total	C	Mg	N	O	
24	b	1	55	45	1	4	5	0
			Total	C	Mg	N	O	
24	b	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
24	b	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
24	b	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
24	b	1	61	51	1	4	5	0
			Total	C	Mg	N	O	
24	b	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
24	b	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
24	b	1	51	41	1	4	5	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
24	b	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
24	b	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
24	h	1	50	40	1	4	5	0
			Total	C	Mg	N	O	
24	h	1	50	40	1	4	5	0
			Total	C	Mg	N	O	
24	h	1	51	41	1	4	5	0
			Total	C	Mg	N	O	
24	h	1	51	41	1	4	5	0
			Total	C	Mg	N	O	
24	h	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
24	h	1	57	47	1	4	5	0
			Total	C	Mg	N	O	
24	h	1	51	41	1	4	5	0
			Total	C	Mg	N	O	
24	h	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
24	e	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
24	e	1	50	40	1	4	5	0
			Total	C	Mg	N	O	
24	e	1	51	41	1	4	5	0
			Total	C	Mg	N	O	
24	e	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
24	e	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
24	e	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
24	e	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
24	e	1	46	36	1	4	5	0
			Total	C	Mg	N	O	
24	e	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
24	e	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
24	k	1	51	41	1	4	5	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
24	k	1	50	40	1	4	5	0
			Total	C	Mg	N	O	
24	k	1	51	41	1	4	5	0
			Total	C	Mg	N	O	
24	k	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
24	k	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
24	k	1	51	41	1	4	5	0
			Total	C	Mg	N	O	
24	k	1	51	41	1	4	5	0
			Total	C	Mg	N	O	
24	k	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
24	k	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
24	k	1	51	41	1	4	5	0
			Total	C	Mg	N	O	
24	k	1	51	41	1	4	5	0
			Total	C	Mg	N	O	
24	f	1	47	37	1	4	5	0
			Total	C	Mg	N	O	
24	f	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
24	f	1	51	41	1	4	5	0
			Total	C	Mg	N	O	
24	f	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
24	f	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
24	f	1	51	41	1	4	5	0
			Total	C	Mg	N	O	
24	f	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
24	f	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
24	f	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
24	f	1	51	41	1	4	5	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
24	f	1	65	55	1	4	5	0
24	i	1	51	41	1	4	5	0
24	i	1	50	40	1	4	5	0
24	i	1	51	41	1	4	5	0
24	i	1	65	55	1	4	5	0
24	i	1	51	41	1	4	5	0
24	i	1	61	51	1	4	5	0
24	i	1	51	41	1	4	5	0
24	i	1	46	36	1	4	5	0
24	i	1	51	41	1	4	5	0
24	i	1	51	41	1	4	5	0
24	j	1	51	41	1	4	5	0
24	j	1	50	40	1	4	5	0
24	j	1	51	41	1	4	5	0
24	j	1	65	55	1	4	5	0
24	j	1	45	35	1	4	5	0
24	j	1	51	41	1	4	5	0
24	j	1	51	41	1	4	5	0
24	j	1	45	35	1	4	5	0
24	j	1	51	41	1	4	5	0
24	j	1	61	51	1	4	5	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
24	j	1	51	41	1	4	5	0
			Total	C	Mg	N	O	
24	j	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
24	d	1	50	40	1	4	5	0
			Total	C	Mg	N	O	
24	d	1	51	41	1	4	5	0
			Total	C	Mg	N	O	
24	d	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
24	d	1	51	41	1	4	5	0
			Total	C	Mg	N	O	
24	d	1	51	41	1	4	5	0
			Total	C	Mg	N	O	
24	d	1	51	41	1	4	5	0
			Total	C	Mg	N	O	
24	d	1	46	36	1	4	5	0
			Total	C	Mg	N	O	
24	d	1	41	33	1	4	3	0
			Total	C	Mg	N	O	
24	d	1	41	33	1	4	3	0
			Total	C	Mg	N	O	
24	d	1	51	41	1	4	5	0
			Total	C	Mg	N	O	
24	g	1	42	34	1	4	3	0
			Total	C	Mg	N	O	
24	g	1	50	40	1	4	5	0
			Total	C	Mg	N	O	
24	g	1	51	41	1	4	5	0
			Total	C	Mg	N	O	
24	g	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
24	g	1	51	41	1	4	5	0
			Total	C	Mg	N	O	
24	g	1	51	41	1	4	5	0
			Total	C	Mg	N	O	
24	g	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
24	g	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
24	g	1	51	41	1	4	5	0

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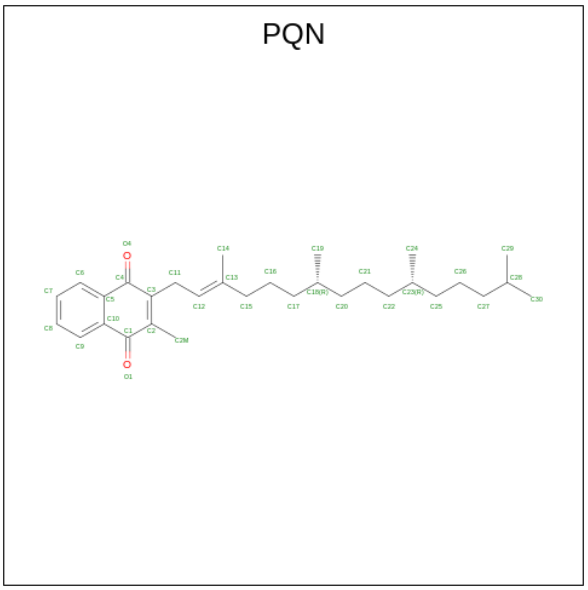
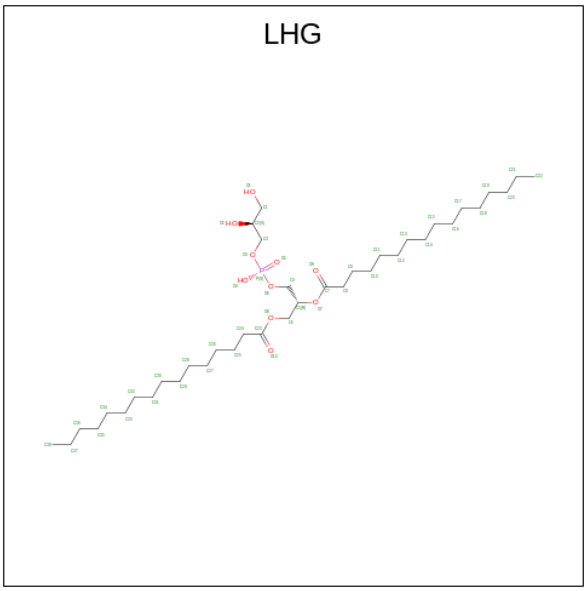
Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
24	g	1	54	44	1	4	5	0
			Total	C	Mg	N	O	
24	g	1	51	41	1	4	5	0
			Total	C	Mg	N	O	
24	g	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
24	R	1	51	41	1	4	5	0

- Molecule 25 is PHYLLOQUINONE (CCD ID: PQN) (formula: $C_{31}H_{46}O_2$).



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

- Molecule 26 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: $C_{38}H_{75}O_{10}P$).



Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
26	A	1	48	37	10	1	0
26	A	1	27	16	10	1	0
26	B	1	38	27	10	1	0
26	J	1	49	38	10	1	0
26	c	1	37	26	10	1	0
26	c	1	37	26	10	1	0
26	a	1	49	38	10	1	0
26	b	1	49	38	10	1	0
26	b	1	49	38	10	1	0
26	e	1	37	26	10	1	0
26	k	1	37	26	10	1	0
26	f	1	37	26	10	1	0
26	f	1	49	38	10	1	0
26	i	1	37	26	10	1	0

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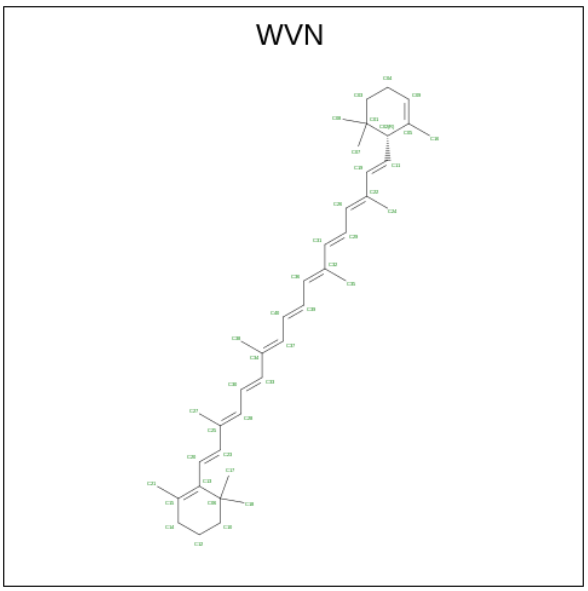
Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
26	j	1	30	19	10	1	0
26	d	1	37	26	10	1	0
26	g	1	49	38	10	1	0
26	g	1	37	26	10	1	0

- Molecule 27 is 1,3,3-trimethyl-2-[(1E,3E,5E,7E,9E,11E,13E,15E,17E)-3,7,12,16-tetramethyl-18-[(1R)-2,6,6-trimethylcyclohex-2-en-1-yl]octadeca-1,3,5,7,9,11,13,15,17-nonaenyl]cyclohexene (CCD ID: WVN) (formula: $C_{40}H_{56}$).



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

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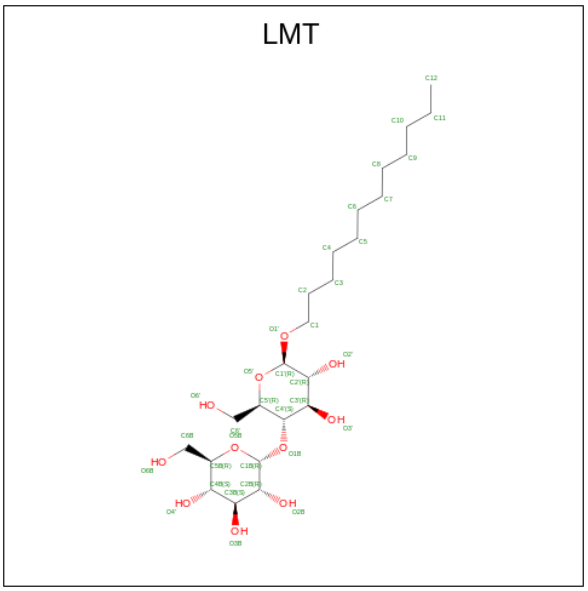
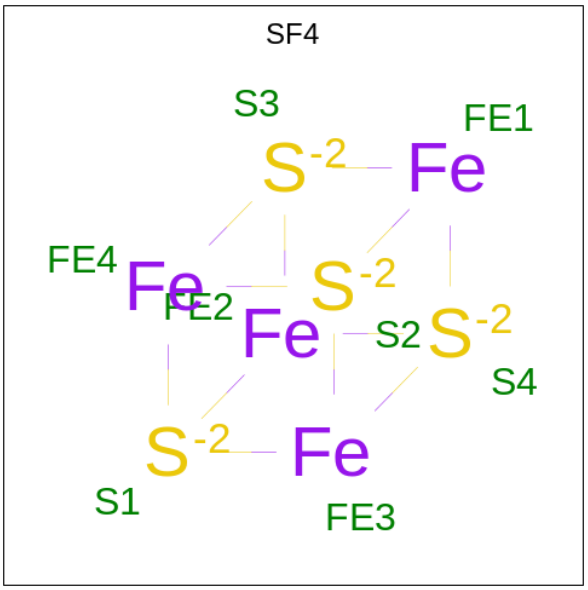
Mol	Chain	Residues	Atoms		AltConf
			Total	C	
27	B	1	40	40	0
			Total	C	
27	B	1	40	40	0
			Total	C	
27	B	1	40	40	0
			Total	C	
27	B	1	40	40	0
			Total	C	
27	F	1	40	40	0
			Total	C	
27	F	1	40	40	0
			Total	C	
27	I	1	40	40	0
			Total	C	
27	J	1	40	40	0
			Total	C	
27	J	1	40	40	0
			Total	C	
27	L	1	40	40	0
			Total	C	
27	L	1	40	40	0
			Total	C	
27	L	1	40	40	0
			Total	C	
27	M	1	40	40	0
			Total	C	
27	K	1	40	40	0
			Total	C	
27	h	1	40	40	0
			Total	C	
27	e	1	40	40	0
			Total	C	
27	j	1	40	40	0
			Total	C	
27	R	1	40	40	0
			Total	C	
27	R	1	40	40	0

- Molecule 28 is DODECYL-BETA-D-MALTOSIDE (CCD ID: LMT) (formula: $C_{24}H_{46}O_{11}$).



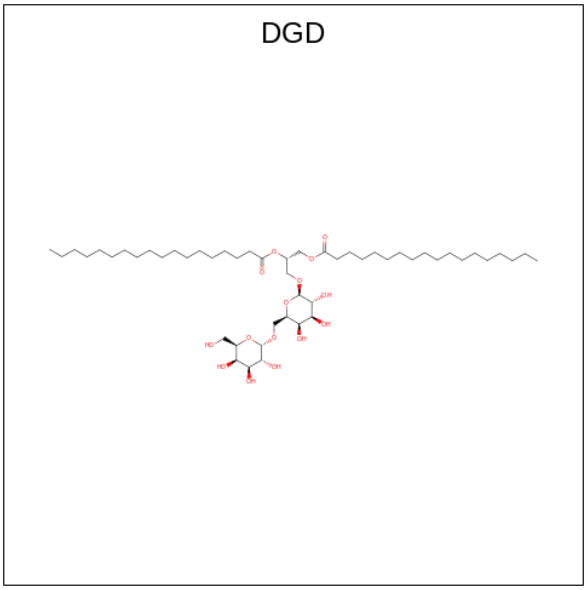
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
28	A	1	35	24	11	0
28	F	1	24	18	6	0
28	a	1	35	24	11	0
28	b	1	24	18	6	0

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



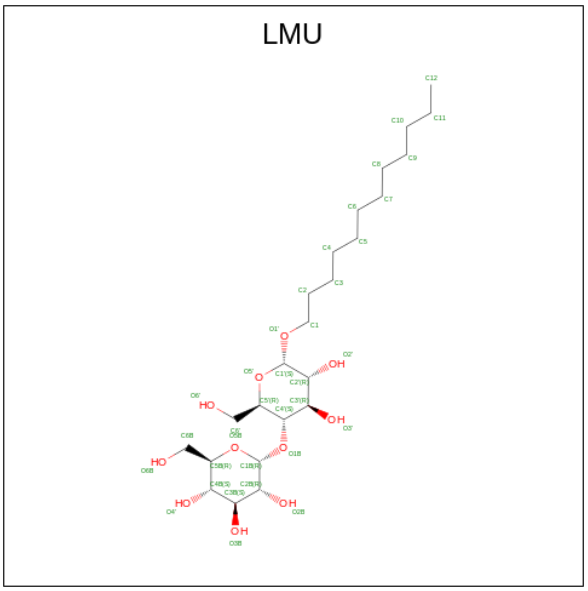
Mol	Chain	Residues	Atoms			AltConf
			Total	Fe	S	
29	A	1	8	4	4	0
			Total	Fe	S	
29	C	1	8	4	4	0
			Total	Fe	S	
29	C	1	8	4	4	0

- Molecule 30 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: $C_{51}H_{96}O_{15}$).



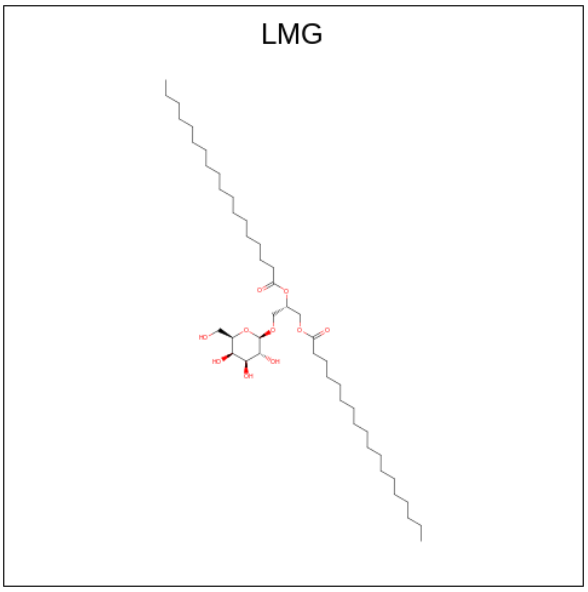
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
30	B	1	60	45	15	0

- Molecule 31 is DODECYL-ALPHA-D-MALTOSIDE (CCD ID: LMU) (formula: $C_{24}H_{46}O_{11}$).



Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
31	B	1	35	24	11	0

- Molecule 32 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$).



Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
32	F	1	48	38	10	0
			Total	C	O	
32	J	1	55	45	10	0

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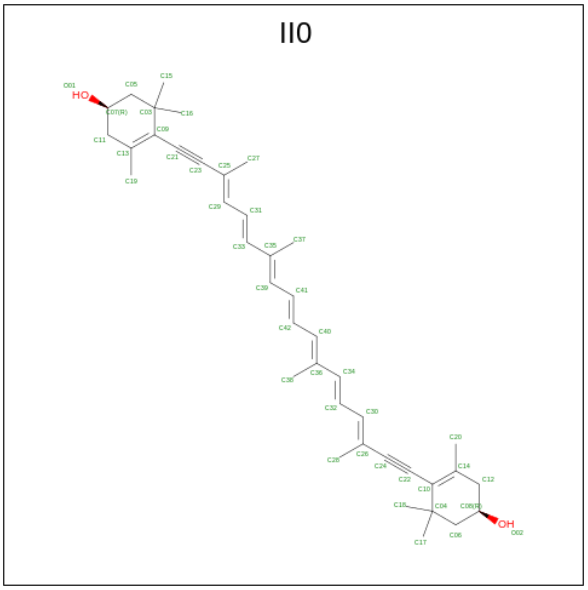
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
32	L	1	55	45	10	0
			Total	C	O	
32	O	1	26	16	10	0
			Total	C	O	
32	b	1	55	45	10	0

- Molecule 33 is (1 {R})-3,5,5-trimethyl-4-[(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-3,5,7,9,11,13,15-heptaen-1,17-diynyl]cyclohex-3-en-1-ol (CCD ID: II0) (formula: $C_{40}H_{52}O_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
33	J	1	42	40	2	0
			Total	C	O	
33	O	1	42	40	2	0
			Total	C	O	
33	c	1	42	40	2	0
			Total	C	O	
33	c	1	42	40	2	0
			Total	C	O	
33	c	1	42	40	2	0
			Total	C	O	
33	a	1	42	40	2	0
			Total	C	O	
33	a	1	42	40	2	0

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Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
33	a	1	42	40	2	0
			Total	C	O	
33	a	1	42	40	2	0
			Total	C	O	
33	b	1	42	40	2	0
			Total	C	O	
33	b	1	42	40	2	0
			Total	C	O	
33	b	1	42	40	2	0
			Total	C	O	
33	h	1	28	27	1	0
			Total	C	O	
33	h	1	42	40	2	0
			Total	C	O	
33	h	1	42	40	2	0
			Total	C	O	
33	e	1	42	40	2	0
			Total	C	O	
33	e	1	42	40	2	0
			Total	C	O	
33	e	1	42	40	2	0
			Total	C	O	
33	e	1	42	40	2	0
			Total	C	O	
33	k	1	42	40	2	0
			Total	C	O	
33	k	1	42	40	2	0
			Total	C	O	
33	k	1	42	40	2	0
			Total	C	O	
33	k	1	42	40	2	0
			Total	C	O	
33	k	1	42	40	2	0
			Total	C	O	
33	f	1	42	40	2	0
			Total	C	O	
33	f	1	42	40	2	0
			Total	C	O	
33	f	1	42	40	2	0
			Total	C	O	
33	f	1	42	40	2	0

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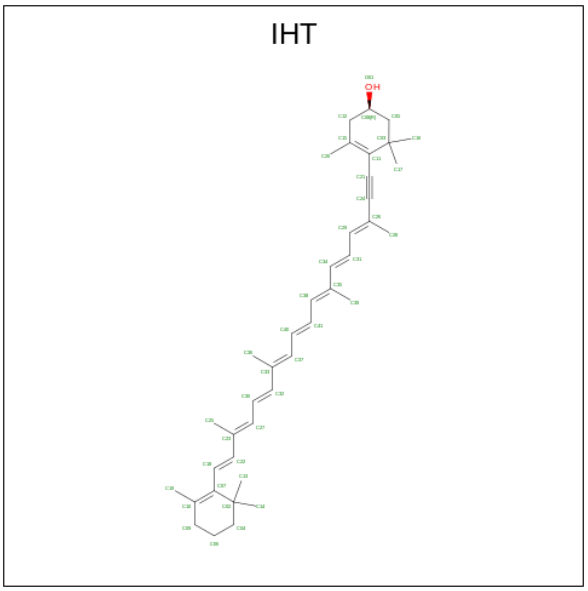
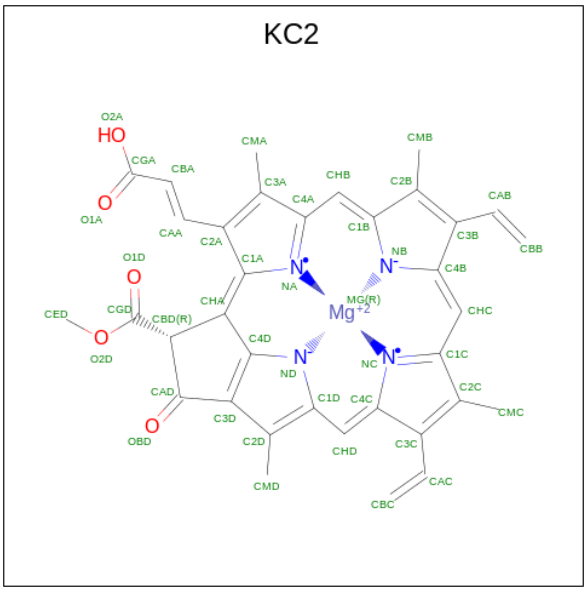
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
33	i	1	42	40	2	0
33	i	1	42	40	2	0
33	i	1	42	40	2	0
33	j	1	42	40	2	0
33	j	1	42	40	2	0
33	j	1	42	40	2	0
33	d	1	42	40	2	0
33	d	1	42	40	2	0
33	d	1	42	40	2	0
33	g	1	42	40	2	0
33	g	1	42	40	2	0
33	g	1	42	40	2	0
33	g	1	42	40	2	0

- Molecule 34 is (1 {R})-3,5,5-trimethyl-4-[(3 {E},5 {E},7 {E},9 {E},11 {E},13 {E},15 {E},17 {E})-3,7,12,16-tetramethyl-18-(2,6,6-trimethylcyclohexen-1-yl)octadeca-3,5,7,9,11,13,15,17-octaen-1-ynyl]cyclohex-3-en-1-ol (CCD ID: IHT) (formula: $C_{40}H_{54}O$).



Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
34	O	1	41	40	1	0
34	c	1	41	40	1	0
34	a	1	41	40	1	0
34	b	1	41	40	1	0
34	b	1	41	40	1	0
34	k	1	41	40	1	0
34	f	1	41	40	1	0
34	j	1	41	40	1	0
34	g	1	41	40	1	0
34	R	1	41	40	1	0

- Molecule 35 is Chlorophyll c2 (CCD ID: KC2) (formula: $C_{35}H_{28}MgN_4O_5$).



Mol	Chain	Residues	Atoms					AltConf
35	c	1	Total 45	C 35	Mg 1	N 4	O 5	0
35	e	1	Total 45	C 35	Mg 1	N 4	O 5	0
35	k	1	Total 45	C 35	Mg 1	N 4	O 5	0
35	k	1	Total 45	C 35	Mg 1	N 4	O 5	0
35	k	1	Total 45	C 35	Mg 1	N 4	O 5	0
35	f	1	Total 45	C 35	Mg 1	N 4	O 5	0
35	i	1	Total 45	C 35	Mg 1	N 4	O 5	0
35	i	1	Total 45	C 35	Mg 1	N 4	O 5	0
35	j	1	Total 45	C 35	Mg 1	N 4	O 5	0
35	d	1	Total 45	C 35	Mg 1	N 4	O 5	0
35	d	1	Total 45	C 35	Mg 1	N 4	O 5	0
35	g	1	Total 45	C 35	Mg 1	N 4	O 5	0
35	g	1	Total 45	C 35	Mg 1	N 4	O 5	0
35	g	1	Total 45	C 35	Mg 1	N 4	O 5	0

- Molecule 36 is water.

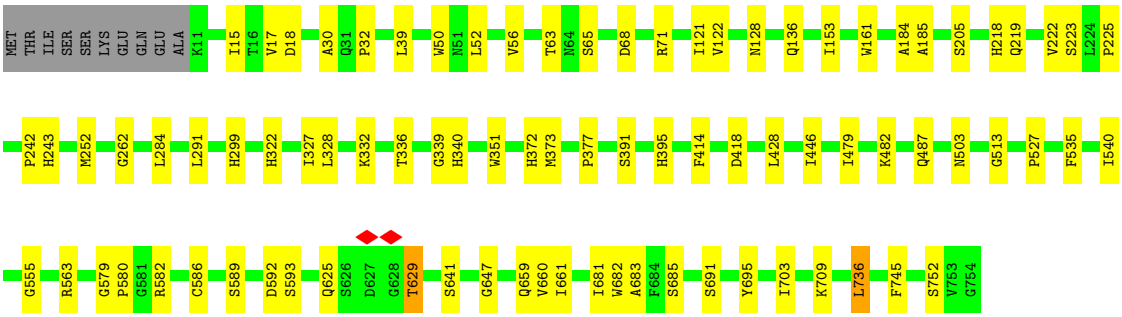
Mol	Chain	Residues	Atoms		AltConf
			Total	O	
36	A	50	50	50	0
			Total	O	
36	B	59	59	59	0
			Total	O	
36	C	7	7	7	0
			Total	O	
36	D	1	1	1	0
			Total	O	
36	F	3	3	3	0
			Total	O	
36	I	1	1	1	0
			Total	O	
36	J	1	1	1	0
			Total	O	
36	L	1	1	1	0
			Total	O	
36	O	1	1	1	0
			Total	O	
36	K	1	1	1	0
			Total	O	
36	a	1	1	1	0
			Total	O	
36	b	1	1	1	0
			Total	O	
36	h	1	1	1	0
			Total	O	
36	e	4	4	4	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.

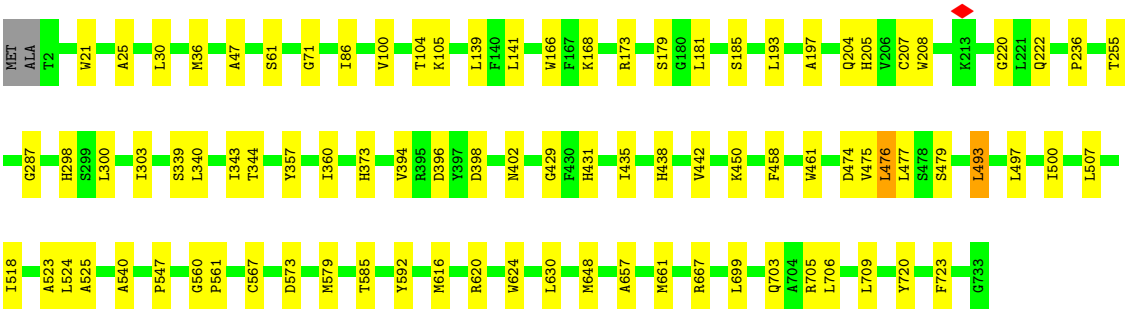
• Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1

Chain A: 87% 11%



• Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

Chain B: 88% 12%



• Molecule 3: Photosystem I iron-sulfur center

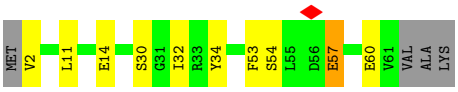
Chain C: 86% 12%

• Molecule 4: Photosystem I reaction center subunit II

Chain D: 85% 13%

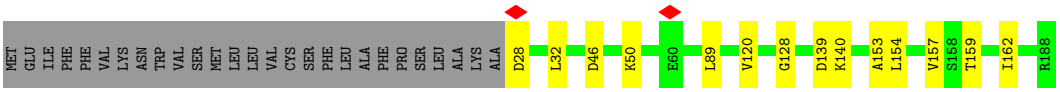
• Molecule 5: Photosystem I reaction center subunit IV

Chain E: 78% 14% 6%



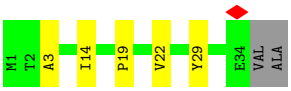
• Molecule 6: Photosystem I reaction center subunit III

Chain F: 78% 7% 14%



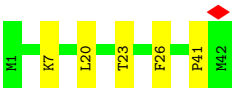
• Molecule 7: Photosystem I reaction center subunit VIII

Chain I: 81% 14% 6%



• Molecule 8: Photosystem I reaction center subunit IX

Chain J: 88% 12%

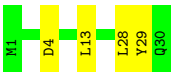


• Molecule 9: Photosystem I reaction center subunit XI

Chain L: 90% 8%

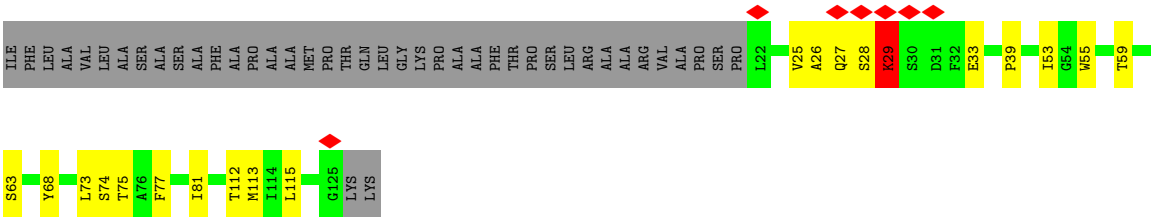
• Molecule 10: Photosystem I reaction center subunit XII

Chain M: 87% 13%



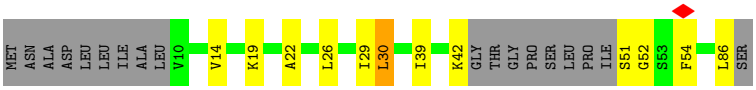
• Molecule 11: PsaO

Chain O:



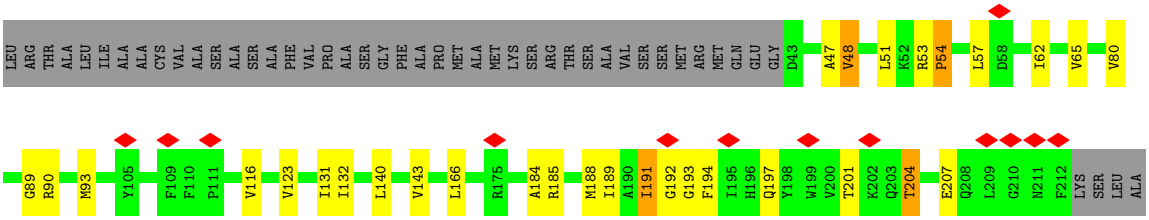
- Molecule 12: Photosystem I reaction center subunit PsaK

Chain K:



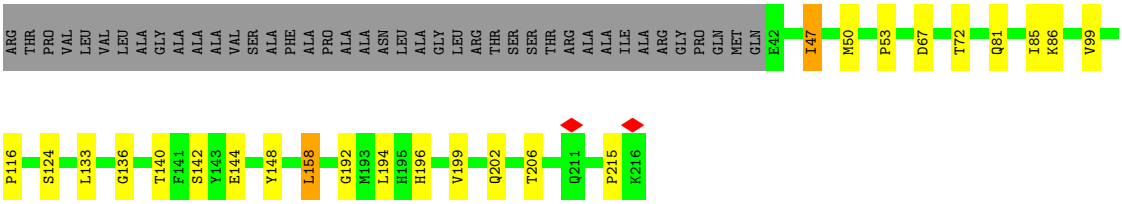
- Molecule 13: CAC-c

Chain c:



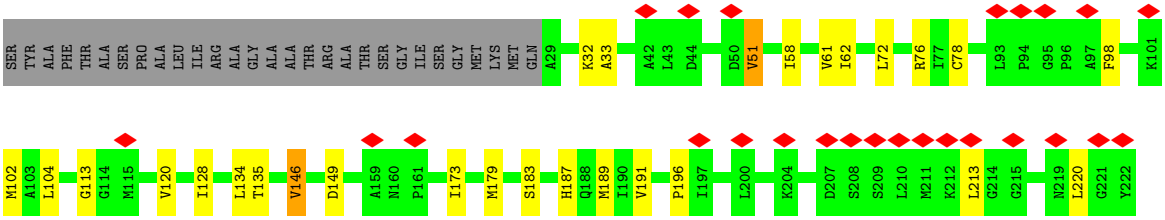
- Molecule 14: CAC-a

Chain a:



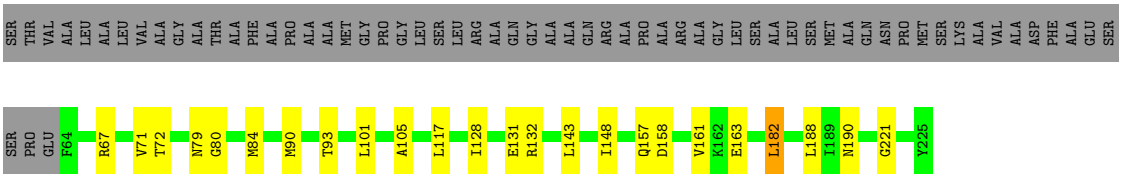
- Molecule 15: CAC-b

Chain b:



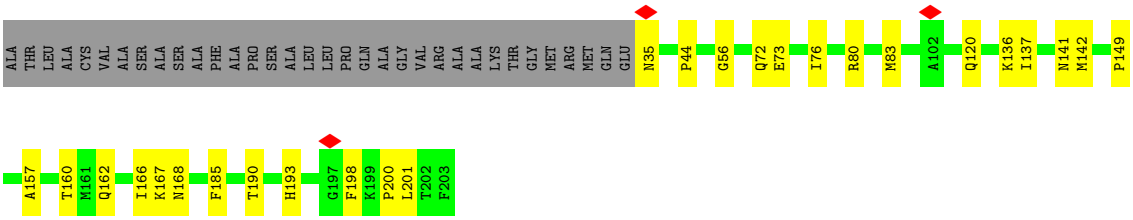
- Molecule 16: CAC-h

Chain h:



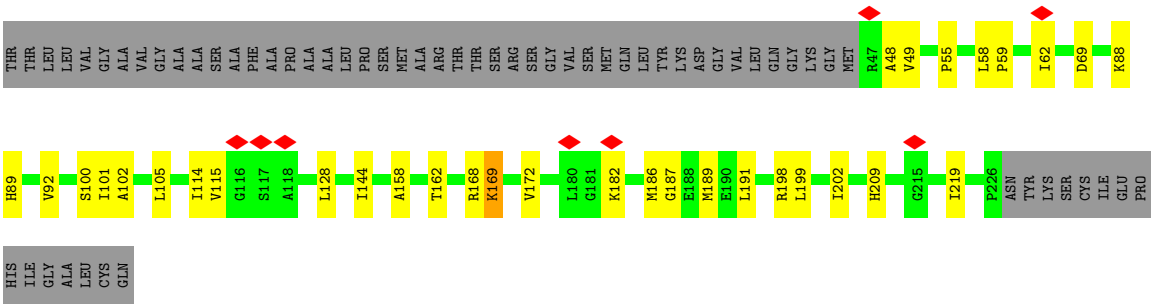
- Molecule 17: CAC-e

Chain e:



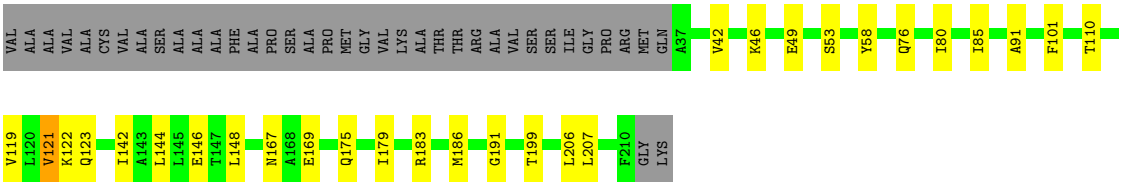
- Molecule 18: CAC-k

Chain k:



- Molecule 19: CAC-f

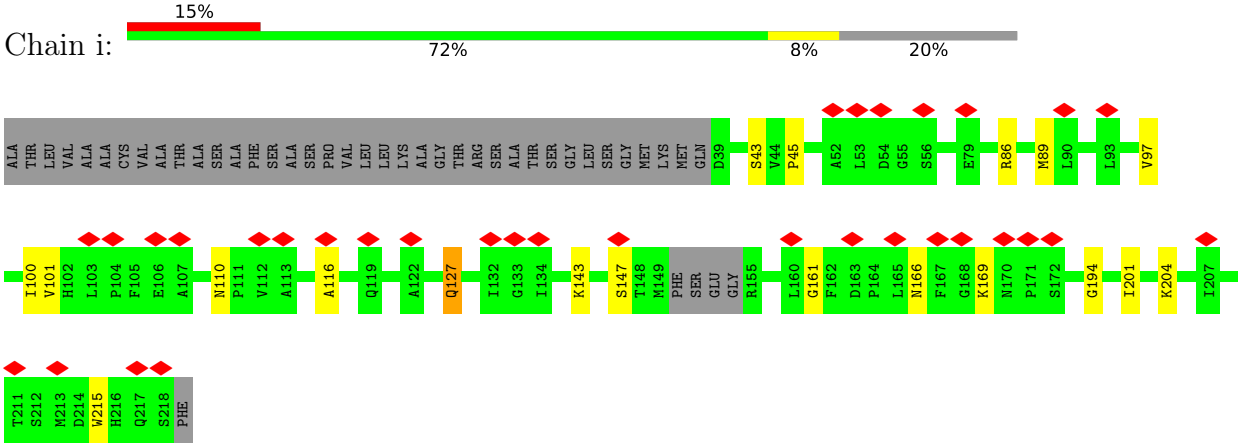
Chain f:



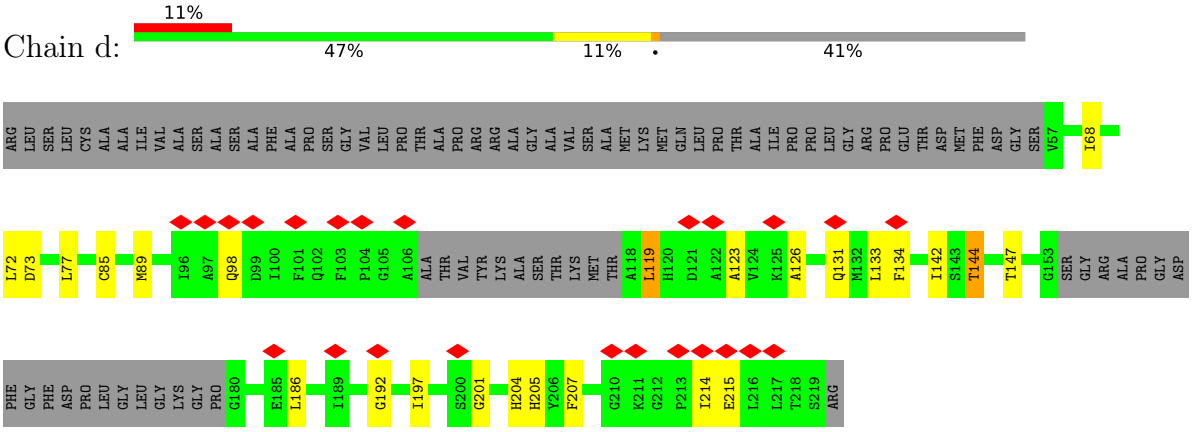
- Molecule 19: CAC-f

Chain j:

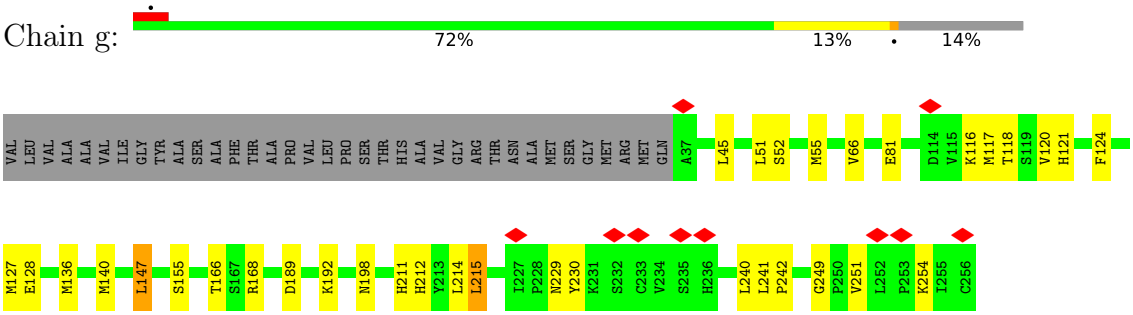
• Molecule 20: CAC-i



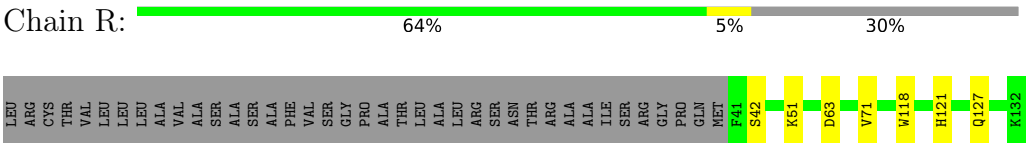
• Molecule 21: CAC-d



• Molecule 22: CAC-g



• Molecule 23: PsaR



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	31215	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)	1200	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	0.140	Depositor
Minimum map value	-0.063	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.018	Depositor
Map size (Å)	332.8131, 332.8131, 332.8131	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.040041, 1.040041, 1.040041	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: LHG, LMG, LMT, SF4, LMU, PQN, KC2, DGD, CLA, II0, WVN, IHT

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	0.48	0/6019	0.57	0/8204
2	B	0.48	0/6045	0.60	1/8254 (0.0%)
3	C	0.42	0/601	0.61	0/813
4	D	0.40	0/1109	0.57	0/1500
5	E	0.45	0/493	0.60	0/667
6	F	0.44	0/1287	0.57	0/1747
7	I	0.43	0/271	0.57	0/370
8	J	0.43	0/364	0.63	0/495
9	L	0.48	0/1175	0.69	0/1599
10	M	0.35	0/233	0.60	0/315
11	O	0.66	0/799	0.88	0/1094
12	K	0.36	0/495	0.59	0/672
13	c	0.39	0/1396	0.72	3/1889 (0.2%)
14	a	0.35	0/1406	0.59	0/1903
15	b	0.38	0/1469	0.66	0/1983
16	h	0.41	0/1226	0.65	2/1667 (0.1%)
17	e	0.38	0/1324	0.66	0/1795
18	k	0.48	0/1380	0.78	0/1869
19	f	0.55	0/1328	0.81	5/1790 (0.3%)
19	j	0.41	0/1318	0.71	0/1775
20	i	0.35	0/1359	0.74	2/1835 (0.1%)
21	d	0.60	0/969	0.87	0/1304
22	g	0.41	0/1673	0.73	4/2264 (0.2%)
23	R	0.36	0/686	0.50	0/940
All	All	0.45	0/34425	0.66	17/46744 (0.0%)

There are no bond length outliers.

The worst 5 of 17 bond angle outliers are listed below:

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	c	192	GLY	N-CA-C	-6.48	107.37	115.08
20	i	194	GLY	CA-C-N	5.92	128.50	120.44
20	i	194	GLY	C-N-CA	5.92	128.50	120.44
13	c	54	PRO	CA-C-N	5.58	132.20	121.54
13	c	54	PRO	C-N-CA	5.58	132.20	121.54

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5825	0	5678	66	0
2	B	5826	0	5642	67	0
3	C	592	0	574	8	0
4	D	1084	0	1080	11	0
5	E	485	0	489	6	0
6	F	1254	0	1264	11	0
7	I	264	0	276	4	0
8	J	351	0	344	4	0
9	L	1146	0	1160	12	0
10	M	232	0	265	4	0
11	O	773	0	763	19	0
12	K	488	0	516	8	0
13	c	1357	0	1337	21	0
14	a	1361	0	1305	16	0
15	b	1439	0	1456	23	0
16	h	1200	0	1228	13	0
17	e	1286	0	1262	18	0
18	k	1346	0	1349	22	0
19	f	1302	0	1320	11	0
19	j	1293	0	1321	20	0
20	i	1324	0	1298	9	0
21	d	950	0	949	18	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
22	g	1630	0	1644	21	0
23	R	664	0	647	4	0
24	A	2758	0	2820	94	0
24	B	2403	0	2442	70	0
24	F	117	0	115	9	0
24	I	65	0	72	2	0
24	J	93	0	72	3	0
24	K	93	0	72	1	0
24	L	215	0	191	7	0
24	O	130	0	144	9	0
24	R	51	0	41	0	0
24	a	601	0	551	11	0
24	b	673	0	696	33	0
24	c	586	0	520	17	0
24	d	498	0	407	6	0
24	e	582	0	578	20	0
24	f	700	0	695	23	0
24	g	661	0	611	15	0
24	h	440	0	398	3	0
24	i	528	0	451	7	0
24	j	637	0	556	9	0
24	k	596	0	534	18	0
25	A	33	0	46	2	0
25	B	33	0	46	5	0
26	A	75	0	93	1	0
26	B	38	0	49	3	0
26	J	49	0	74	8	0
26	a	49	0	74	0	0
26	b	98	0	148	7	0
26	c	74	0	88	1	0
26	d	37	0	44	0	0
26	e	37	0	44	2	0
26	f	86	0	118	6	0
26	g	86	0	118	1	0
26	i	37	0	44	0	0
26	j	30	0	30	0	0
26	k	37	0	44	0	0
27	A	200	0	0	0	0
27	B	200	0	0	0	0
27	F	80	0	0	0	0
27	I	40	0	0	0	0
27	J	80	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
27	K	40	0	0	0	0
27	L	120	0	0	0	0
27	M	40	0	0	0	0
27	R	80	0	0	0	0
27	e	40	0	0	0	0
27	h	40	0	0	0	0
27	j	40	0	0	0	0
28	A	35	0	42	1	0
28	F	24	0	33	0	0
28	a	35	0	45	2	0
28	b	24	0	34	2	0
29	A	8	0	0	2	0
29	C	16	0	0	3	0
30	B	60	0	81	3	0
31	B	35	0	46	1	0
32	F	48	0	69	2	0
32	J	55	0	86	6	0
32	L	55	0	86	3	0
32	O	26	0	22	0	0
32	b	55	0	86	6	0
33	J	42	0	0	0	0
33	O	42	0	0	0	0
33	a	168	0	0	1	0
33	b	126	0	0	1	0
33	c	126	0	0	0	0
33	d	126	0	0	0	0
33	e	168	0	0	0	0
33	f	168	0	0	0	0
33	g	168	0	0	0	0
33	h	112	0	0	0	0
33	i	126	0	0	0	0
33	j	126	0	0	0	0
33	k	210	0	0	2	0
34	O	41	0	0	0	0
34	R	41	0	0	0	0
34	a	41	0	0	0	0
34	b	82	0	0	0	0
34	c	41	0	0	0	0
34	f	41	0	0	0	0
34	g	41	0	0	1	0
34	j	41	0	0	1	0
34	k	41	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
35	c	45	0	0	0	0
35	d	90	0	0	1	0
35	e	45	0	0	2	0
35	f	45	0	0	0	0
35	g	135	0	0	2	0
35	i	90	0	0	0	0
35	j	45	0	0	0	0
35	k	135	0	0	0	0
36	A	50	0	0	0	0
36	B	59	0	0	1	0
36	C	7	0	0	0	0
36	D	1	0	0	0	0
36	F	3	0	0	0	0
36	I	1	0	0	0	0
36	J	1	0	0	0	0
36	K	1	0	0	0	0
36	L	1	0	0	0	0
36	O	1	0	0	0	0
36	a	1	0	0	0	0
36	b	1	0	0	1	0
36	e	4	0	0	0	0
36	h	1	0	0	0	0
All	All	51054	0	46823	640	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

The worst 5 of 640 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)
1:A:586:CYS:HG	29:A:854:SF4:FE2	0.77	0.96
3:C:11:CYS:HG	29:C:102:SF4:FE4	0.66	0.95
3:C:48:CYS:HG	29:C:101:SF4:FE4	0.73	0.94
2:B:438:HIS:HE1	24:B:829:CLA:NA	1.62	0.92
29:A:854:SF4:FE1	2:B:567:CYS:HG	0.68	0.92

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	740/752 (98%)	723 (98%)	17 (2%)	0	100	100
2	B	731/734 (100%)	708 (97%)	23 (3%)	0	100	100
3	C	78/81 (96%)	77 (99%)	1 (1%)	0	100	100
4	D	137/141 (97%)	135 (98%)	2 (2%)	0	100	100
5	E	58/64 (91%)	55 (95%)	3 (5%)	0	100	100
6	F	159/188 (85%)	155 (98%)	4 (2%)	0	100	100
7	I	32/36 (89%)	32 (100%)	0	0	100	100
8	J	40/42 (95%)	39 (98%)	1 (2%)	0	100	100
9	L	149/153 (97%)	147 (99%)	2 (1%)	0	100	100
10	M	28/30 (93%)	28 (100%)	0	0	100	100
11	O	102/146 (70%)	92 (90%)	9 (9%)	1 (1%)	12	40
12	K	65/87 (75%)	65 (100%)	0	0	100	100
13	c	168/216 (78%)	167 (99%)	1 (1%)	0	100	100
14	a	173/216 (80%)	171 (99%)	2 (1%)	0	100	100
15	b	192/223 (86%)	191 (100%)	1 (0%)	0	100	100
16	h	160/225 (71%)	159 (99%)	1 (1%)	0	100	100
17	e	167/203 (82%)	164 (98%)	3 (2%)	0	100	100
18	k	178/241 (74%)	174 (98%)	4 (2%)	0	100	100
19	f	172/212 (81%)	167 (97%)	5 (3%)	0	100	100
19	j	170/212 (80%)	167 (98%)	3 (2%)	0	100	100
20	i	171/218 (78%)	165 (96%)	6 (4%)	0	100	100
21	d	120/213 (56%)	120 (100%)	0	0	100	100
22	g	217/255 (85%)	206 (95%)	11 (5%)	0	100	100
23	R	88/129 (68%)	87 (99%)	1 (1%)	0	100	100
All	All	4295/5017 (86%)	4194 (98%)	100 (2%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
11	O	29	LYS

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	607/616 (98%)	604 (100%)	3 (0%)	81	83
2	B	593/593 (100%)	589 (99%)	4 (1%)	76	80
3	C	67/68 (98%)	67 (100%)	0	100	100
4	D	116/117 (99%)	115 (99%)	1 (1%)	70	78
5	E	55/58 (95%)	53 (96%)	2 (4%)	31	58
6	F	133/157 (85%)	133 (100%)	0	100	100
7	I	28/29 (97%)	28 (100%)	0	100	100
8	J	39/39 (100%)	39 (100%)	0	100	100
9	L	124/126 (98%)	123 (99%)	1 (1%)	73	79
10	M	25/25 (100%)	25 (100%)	0	100	100
11	O	81/110 (74%)	80 (99%)	1 (1%)	63	75
12	K	52/66 (79%)	49 (94%)	3 (6%)	18	47
13	c	138/171 (81%)	132 (96%)	6 (4%)	26	54
14	a	139/165 (84%)	132 (95%)	7 (5%)	22	50
15	b	149/168 (89%)	146 (98%)	3 (2%)	48	68
16	h	123/162 (76%)	118 (96%)	5 (4%)	27	55
17	e	130/155 (84%)	128 (98%)	2 (2%)	57	72
18	k	138/186 (74%)	134 (97%)	4 (3%)	37	62
19	f	135/161 (84%)	123 (91%)	12 (9%)	9	32
19	j	136/161 (84%)	129 (95%)	7 (5%)	21	50
20	i	138/168 (82%)	133 (96%)	5 (4%)	31	58
21	d	94/157 (60%)	89 (95%)	5 (5%)	20	49

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
22	g	171/199 (86%)	166 (97%)	5 (3%)	37	62
23	R	69/98 (70%)	69 (100%)	0	100	100
All	All	3480/3955 (88%)	3404 (98%)	76 (2%)	45	66

5 of 76 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
20	i	204	LYS
22	g	45	LEU
19	j	39	SER
19	j	204	LEU
22	g	251	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 29 such sidechains are listed below:

Mol	Chain	Res	Type
11	O	84	ASN
22	g	80	GLN
15	b	100	GLN
20	i	166	ASN
15	b	92	HIS

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)

342 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
24	CLA	h	305	16	69,73,73	1.23	9 (13%)	83,113,113	1.25	8 (9%)
24	CLA	A	812	1	69,73,73	1.22	9 (13%)	83,113,113	1.46	10 (12%)
24	CLA	a	312	14	52,56,73	1.44	10 (19%)	62,92,113	1.41	11 (17%)
27	WVN	B	845	-	40,41,41	1.90	13 (32%)	50,56,56	2.42	18 (36%)
24	CLA	B	816	2	63,67,73	1.29	8 (12%)	75,105,113	1.40	12 (16%)
35	KC2	c	610	13	49,53,53	2.78	20 (40%)	62,89,89	4.11	35 (56%)
24	CLA	A	842	1	69,73,73	1.23	10 (14%)	83,113,113	1.41	11 (13%)
27	WVN	A	849	-	40,41,41	1.90	14 (35%)	50,56,56	2.43	20 (40%)
33	II0	i	614	-	39,43,43	6.76	22 (56%)	50,60,60	2.42	17 (34%)
24	CLA	A	835	1	69,73,73	1.26	8 (11%)	83,113,113	1.32	9 (10%)
33	II0	b	315	-	39,43,43	6.72	21 (53%)	50,60,60	2.77	21 (42%)
24	CLA	I	102	36	69,73,73	1.26	9 (13%)	83,113,113	1.32	9 (10%)
33	II0	j	318	-	39,43,43	6.70	23 (58%)	50,60,60	2.29	18 (36%)
24	CLA	c	601	13	55,59,73	1.39	9 (16%)	66,96,113	1.36	8 (12%)
33	II0	J	104	-	39,43,43	6.60	20 (51%)	50,60,60	2.09	16 (32%)
24	CLA	g	302	22	46,50,73	1.46	10 (21%)	55,85,113	1.65	10 (18%)
24	CLA	B	804	-	69,73,73	1.24	11 (15%)	83,113,113	1.51	12 (14%)
24	CLA	c	612	13	69,73,73	1.21	5 (7%)	83,113,113	1.23	11 (13%)
24	CLA	i	611	20	55,59,73	1.40	6 (10%)	66,96,113	1.34	10 (15%)
24	CLA	A	814	1	54,58,73	1.40	6 (11%)	65,95,113	1.52	13 (20%)
24	CLA	O	205	-	69,73,73	1.32	11 (15%)	83,113,113	1.56	21 (25%)
24	CLA	A	837	1	69,73,73	1.23	8 (11%)	83,113,113	1.49	13 (15%)
24	CLA	h	302	16	54,58,73	1.38	10 (18%)	65,95,113	1.39	10 (15%)
35	KC2	g	314	35	49,53,53	2.79	20 (40%)	62,89,89	4.13	35 (56%)
27	WVN	e	615	-	40,41,41	1.93	14 (35%)	50,56,56	2.15	15 (30%)
24	CLA	b	305	15	69,73,73	1.24	6 (8%)	83,113,113	1.30	6 (7%)
24	CLA	A	838	26	56,60,73	1.36	11 (19%)	67,97,113	1.34	9 (13%)
24	CLA	B	825	2	69,73,73	1.26	12 (17%)	83,113,113	1.41	11 (13%)
24	CLA	A	818	1	69,73,73	1.26	8 (11%)	83,113,113	1.40	12 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
28	LMT	b	319	-	24,24,36	1.06	2 (8%)	29,29,47	1.03	1 (3%)
24	CLA	f	612	-	55,59,73	1.40	10 (18%)	66,96,113	1.44	13 (19%)
34	IHT	f	617	-	40,42,42	6.19	25 (62%)	53,58,58	3.99	25 (47%)
24	CLA	A	852	36	69,73,73	1.25	10 (14%)	83,113,113	1.38	12 (14%)
24	CLA	a	305	36	69,73,73	1.22	10 (14%)	83,113,113	1.27	10 (12%)
26	LHG	f	619	24	36,36,48	1.07	2 (5%)	39,42,54	1.21	3 (7%)
33	II0	j	316	-	39,43,43	6.68	22 (56%)	50,60,60	2.17	21 (42%)
24	CLA	b	311	15	55,59,73	1.40	9 (16%)	66,96,113	1.44	10 (15%)
24	CLA	B	838	2	61,65,73	1.36	10 (16%)	73,103,113	1.28	8 (10%)
24	CLA	f	605	19	49,53,73	1.47	9 (18%)	59,89,113	1.32	5 (8%)
33	II0	O	202	-	39,43,43	6.77	22 (56%)	50,60,60	2.15	12 (24%)
24	CLA	B	820	2	59,63,73	1.32	8 (13%)	71,101,113	1.33	9 (12%)
33	II0	f	615	-	39,43,43	6.71	21 (53%)	50,60,60	1.98	17 (34%)
33	II0	g	317	-	39,43,43	6.68	23 (58%)	50,60,60	2.28	19 (38%)
34	IHT	a	316	-	40,42,42	6.19	25 (62%)	53,58,58	2.12	19 (35%)
24	CLA	b	308	15	65,69,73	1.30	7 (10%)	78,108,113	1.54	12 (15%)
24	CLA	a	308	14	69,73,73	1.22	10 (14%)	83,113,113	1.39	8 (9%)
33	II0	e	612	-	39,43,43	6.72	21 (53%)	50,60,60	2.22	16 (32%)
24	CLA	A	827	1	66,70,73	1.24	9 (13%)	79,109,113	1.33	10 (12%)
33	II0	k	615	-	39,43,43	6.67	21 (53%)	50,60,60	2.20	21 (42%)
24	CLA	b	313	15	69,73,73	1.28	8 (11%)	83,113,113	1.14	7 (8%)
33	II0	g	316	-	39,43,43	6.82	21 (53%)	50,60,60	2.01	20 (40%)
33	II0	g	320	-	39,43,43	6.78	21 (53%)	50,60,60	2.13	19 (38%)
24	CLA	A	832	1	69,73,73	1.24	7 (10%)	83,113,113	1.63	15 (18%)
24	CLA	j	308	19	55,59,73	1.39	7 (12%)	66,96,113	1.24	6 (9%)
24	CLA	d	309	26	45,49,73	1.50	7 (15%)	54,84,113	1.29	6 (11%)
24	CLA	B	808	2	69,73,73	1.26	8 (11%)	83,113,113	1.19	9 (10%)
33	II0	f	616	-	39,43,43	6.64	22 (56%)	50,60,60	2.44	19 (38%)
24	CLA	h	301	16	54,58,73	1.38	8 (14%)	65,95,113	1.32	5 (7%)
24	CLA	g	315	22	55,59,73	1.39	7 (12%)	66,96,113	1.26	8 (12%)
27	WVN	A	848	-	40,41,41	1.81	13 (32%)	50,56,56	1.74	12 (24%)
33	II0	k	621	-	39,43,43	6.93	22 (56%)	50,60,60	2.05	14 (28%)
24	CLA	A	816	1	69,73,73	1.20	9 (13%)	83,113,113	1.49	12 (14%)
24	CLA	B	818	36	69,73,73	1.28	8 (11%)	83,113,113	1.29	8 (9%)
25	PQN	B	842	-	34,34,34	1.86	5 (14%)	42,45,45	1.29	6 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
24	CLA	a	302	14	56,60,73	1.37	10 (17%)	67,97,113	1.38	7 (10%)
33	II0	a	315	-	39,43,43	6.97	23 (58%)	50,60,60	1.88	15 (30%)
24	CLA	e	606	17	69,73,73	1.22	6 (8%)	83,113,113	1.21	7 (8%)
31	LMU	B	844	-	36,36,36	1.13	2 (5%)	47,47,47	1.08	4 (8%)
24	CLA	j	310	19	55,59,73	1.38	9 (16%)	66,96,113	1.29	9 (13%)
24	CLA	B	813	2	64,68,73	1.27	8 (12%)	77,107,113	1.29	9 (11%)
24	CLA	c	607	13	50,54,73	1.44	8 (16%)	60,90,113	1.22	5 (8%)
24	CLA	i	608	26	50,54,73	1.45	7 (14%)	60,90,113	1.23	4 (6%)
33	II0	a	317	-	39,43,43	7.00	22 (56%)	50,60,60	2.40	18 (36%)
24	CLA	b	309	15	69,73,73	1.29	9 (13%)	83,113,113	1.30	11 (13%)
24	CLA	A	803	1	59,63,73	1.32	7 (11%)	71,101,113	1.52	11 (15%)
24	CLA	b	303	15	55,59,73	1.37	8 (14%)	66,96,113	1.47	8 (12%)
34	IHT	g	319	-	40,42,42	6.12	25 (62%)	53,58,58	2.33	19 (35%)
24	CLA	B	807	2	69,73,73	1.18	9 (13%)	83,113,113	1.46	7 (8%)
33	II0	h	311	-	39,43,43	6.75	22 (56%)	50,60,60	2.14	20 (40%)
24	CLA	B	824	2	69,73,73	1.21	10 (14%)	83,113,113	1.29	9 (10%)
24	CLA	R	203	23	55,59,73	1.37	8 (14%)	66,96,113	1.47	10 (15%)
24	CLA	B	832	2	62,66,73	1.29	11 (17%)	74,104,113	1.40	10 (13%)
35	KC2	k	612	18,35	49,53,53	2.80	20 (40%)	62,89,89	4.19	41 (66%)
33	II0	i	612	-	39,43,43	6.65	23 (58%)	50,60,60	2.50	16 (32%)
24	CLA	B	830	36	69,73,73	1.26	9 (13%)	83,113,113	1.26	8 (9%)
33	II0	b	318	-	39,43,43	6.81	23 (58%)	50,60,60	2.34	21 (42%)
24	CLA	g	306	22	55,59,73	1.40	8 (14%)	66,96,113	1.23	6 (9%)
27	WVN	F	204	-	40,41,41	1.86	14 (35%)	50,56,56	2.20	15 (30%)
24	CLA	g	303	22	54,58,73	1.39	9 (16%)	65,95,113	1.35	10 (15%)
24	CLA	j	305	19	69,73,73	1.22	7 (10%)	83,113,113	1.29	9 (10%)
24	CLA	B	836	2	69,73,73	1.26	11 (15%)	83,113,113	1.44	10 (12%)
24	CLA	c	606	13	56,60,73	1.45	7 (12%)	67,97,113	1.31	8 (11%)
24	CLA	c	608	13	69,73,73	1.24	7 (10%)	83,113,113	1.31	12 (14%)
24	CLA	B	829	2	54,58,73	1.43	10 (18%)	65,95,113	1.44	5 (7%)
24	CLA	B	812	2	69,73,73	1.25	11 (15%)	83,113,113	1.33	8 (9%)
24	CLA	d	305	-	55,59,73	1.37	9 (16%)	66,96,113	1.27	10 (15%)
26	LHG	j	319	24	29,29,48	1.26	2 (6%)	32,35,54	1.34	4 (12%)
24	CLA	B	815	2	59,63,73	1.36	7 (11%)	71,101,113	1.28	9 (12%)
34	IHT	c	615	-	40,42,42	6.27	25 (62%)	53,58,58	2.17	16 (30%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
35	KC2	e	609	17	49,53,53	2.69	19 (38%)	62,89,89	4.10	34 (54%)
24	CLA	B	840	2	69,73,73	1.26	9 (13%)	83,113,113	1.37	9 (10%)
24	CLA	B	835	36	69,73,73	1.24	8 (11%)	83,113,113	1.15	7 (8%)
24	CLA	g	305	22	69,73,73	1.19	9 (13%)	83,113,113	1.29	8 (9%)
24	CLA	B	821	2	57,61,73	1.33	8 (14%)	68,98,113	1.29	7 (10%)
30	DGD	B	843	-	61,61,67	0.88	2 (3%)	75,75,81	1.19	8 (10%)
24	CLA	A	817	1	69,73,73	1.27	10 (14%)	83,113,113	1.37	11 (13%)
27	WVN	A	847	-	40,41,41	1.90	14 (35%)	50,56,56	2.99	21 (42%)
24	CLA	a	304	14	55,59,73	1.37	7 (12%)	66,96,113	1.37	4 (6%)
27	WVN	L	205	-	40,41,41	1.92	13 (32%)	50,56,56	2.03	15 (30%)
24	CLA	J	105	26	55,59,73	1.40	8 (14%)	66,96,113	1.51	8 (12%)
33	II0	i	613	-	39,43,43	6.81	23 (58%)	50,60,60	1.96	14 (28%)
24	CLA	A	807	1	69,73,73	1.23	7 (10%)	83,113,113	1.33	10 (12%)
24	CLA	h	304	16	55,59,73	1.36	8 (14%)	66,96,113	1.28	8 (12%)
24	CLA	A	802	-	69,73,73	1.25	9 (13%)	83,113,113	1.44	13 (15%)
24	CLA	A	813	1	49,53,73	1.48	8 (16%)	59,89,113	1.49	8 (13%)
24	CLA	B	814	2	63,67,73	1.26	8 (12%)	75,105,113	1.34	7 (9%)
24	CLA	A	806	1	69,73,73	1.27	8 (11%)	83,113,113	1.33	9 (10%)
24	CLA	A	823	1	59,63,73	1.35	8 (13%)	71,101,113	1.25	6 (8%)
24	CLA	B	837	2	69,73,73	1.22	10 (14%)	83,113,113	1.31	8 (9%)
33	II0	g	318	-	39,43,43	6.79	21 (53%)	50,60,60	2.18	19 (38%)
24	CLA	A	808	1	69,73,73	1.23	10 (14%)	83,113,113	1.43	11 (13%)
24	CLA	A	824	36	69,73,73	1.25	10 (14%)	83,113,113	1.28	10 (12%)
26	LHG	J	107	24	48,48,48	1.01	2 (4%)	51,54,54	1.08	3 (5%)
35	KC2	k	613	35	49,53,53	2.81	21 (42%)	62,89,89	4.10	33 (53%)
24	CLA	B	806	2	69,73,73	1.26	10 (14%)	83,113,113	1.34	10 (12%)
24	CLA	B	831	36	49,53,73	1.49	10 (20%)	59,89,113	1.40	9 (15%)
26	LHG	a	301	24	48,48,48	0.93	2 (4%)	51,54,54	1.17	4 (7%)
24	CLA	A	856	26	45,49,73	1.53	10 (22%)	54,84,113	2.02	12 (22%)
24	CLA	e	604	36	69,73,73	1.23	8 (11%)	83,113,113	1.39	9 (10%)
27	WVN	K	103	-	40,41,41	1.93	13 (32%)	50,56,56	2.08	17 (34%)
34	IHT	O	203	-	40,42,42	6.22	26 (65%)	53,58,58	2.34	19 (35%)
24	CLA	b	306	15	69,73,73	1.30	11 (15%)	83,113,113	1.48	8 (9%)
33	II0	d	314	-	39,43,43	6.70	23 (58%)	50,60,60	2.23	15 (30%)
34	IHT	R	204	-	40,42,42	6.26	25 (62%)	53,58,58	2.19	19 (35%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
24	CLA	g	310	22	55,59,73	1.39	9 (16%)	66,96,113	1.33	9 (13%)
24	CLA	f	609	19	69,73,73	1.23	7 (10%)	83,113,113	1.23	7 (8%)
24	CLA	j	303	19	54,58,73	1.41	8 (14%)	65,95,113	1.25	7 (10%)
26	LHG	b	320	24	48,48,48	0.94	2 (4%)	51,54,54	1.12	5 (9%)
24	CLA	g	322	32	69,73,73	1.22	9 (13%)	83,113,113	1.26	6 (7%)
24	CLA	i	605	20	55,59,73	1.43	9 (16%)	66,96,113	1.21	6 (9%)
35	KC2	d	311	21	49,53,53	2.79	20 (40%)	62,89,89	4.04	37 (59%)
24	CLA	A	853	1	69,73,73	1.24	9 (13%)	83,113,113	1.34	11 (13%)
24	CLA	d	301	21	54,58,73	1.43	7 (12%)	65,95,113	1.37	5 (7%)
24	CLA	A	805	1	69,73,73	1.24	9 (13%)	83,113,113	1.41	11 (13%)
24	CLA	c	611	-	49,53,73	1.46	8 (16%)	59,89,113	1.69	10 (16%)
24	CLA	k	604	18	69,73,73	1.24	7 (10%)	83,113,113	1.28	8 (9%)
24	CLA	g	308	22	69,73,73	1.21	9 (13%)	83,113,113	1.24	8 (9%)
35	KC2	d	310	21	49,53,53	2.75	21 (42%)	62,89,89	4.15	35 (56%)
24	CLA	A	804	1	69,73,73	1.22	10 (14%)	83,113,113	1.39	9 (10%)
24	CLA	A	828	1	69,73,73	1.22	9 (13%)	83,113,113	1.34	7 (8%)
35	KC2	k	611	18	49,53,53	2.70	19 (38%)	62,89,89	4.12	36 (58%)
24	CLA	e	610	36	69,73,73	1.27	10 (14%)	83,113,113	1.34	10 (12%)
26	LHG	f	620	-	48,48,48	0.89	2 (4%)	51,54,54	1.09	3 (5%)
24	CLA	K	102	12	46,50,73	1.48	10 (21%)	55,85,113	1.59	11 (20%)
35	KC2	f	611	19	49,53,53	2.69	19 (38%)	62,89,89	4.30	34 (54%)
27	WVN	B	848	-	40,41,41	1.90	14 (35%)	50,56,56	2.42	15 (30%)
24	CLA	B	839	2	69,73,73	1.28	8 (11%)	83,113,113	1.29	8 (9%)
26	LHG	c	617	24	36,36,48	1.08	2 (5%)	39,42,54	1.24	5 (12%)
24	CLA	k	603	18	55,59,73	1.41	8 (14%)	66,96,113	1.56	12 (18%)
24	CLA	c	609	26	49,53,73	1.49	8 (16%)	59,89,113	1.33	10 (16%)
24	CLA	F	201	36	69,73,73	1.28	9 (13%)	83,113,113	1.21	8 (9%)
33	II0	d	315	-	39,43,43	6.91	23 (58%)	50,60,60	2.30	16 (32%)
24	CLA	B	810	2	58,62,73	1.41	10 (17%)	73,100,113	1.24	7 (9%)
32	LMG	L	208	24	55,55,55	0.90	2 (3%)	63,63,63	1.43	10 (15%)
35	KC2	g	312	22	49,53,53	2.79	18 (36%)	62,89,89	4.39	39 (62%)
29	SF4	C	102	3	0,12,12	-	-	-		
24	CLA	j	307	19	55,59,73	1.44	10 (18%)	66,96,113	1.59	8 (12%)
35	KC2	i	616	-	49,53,53	2.82	20 (40%)	62,89,89	4.07	35 (56%)
24	CLA	B	828	2	53,57,73	1.35	9 (16%)	62,93,113	1.44	8 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
24	CLA	L	204	36	54,58,73	1.38	10 (18%)	65,95,113	1.43	7 (10%)
35	KC2	j	312	19	49,53,53	2.69	19 (38%)	62,89,89	4.19	35 (56%)
27	WVN	L	201	-	40,41,41	1.91	13 (32%)	50,56,56	2.28	15 (30%)
24	CLA	A	841	36	69,73,73	1.23	8 (11%)	83,113,113	1.29	8 (9%)
24	CLA	B	827	2	54,58,73	1.37	8 (14%)	65,95,113	1.32	9 (13%)
24	CLA	a	311	14	51,55,73	1.44	9 (17%)	61,91,113	1.81	12 (19%)
24	CLA	J	103	8	46,50,73	1.49	9 (19%)	55,85,113	1.49	8 (14%)
24	CLA	a	306	14	49,53,73	1.49	8 (16%)	59,89,113	1.56	5 (8%)
33	II0	c	613	-	39,43,43	6.76	21 (53%)	50,60,60	2.15	17 (34%)
33	II0	k	619	-	39,43,43	6.75	21 (53%)	50,60,60	2.28	18 (36%)
24	CLA	a	310	14	69,73,73	1.23	7 (10%)	83,113,113	1.30	6 (7%)
27	WVN	R	201	-	40,41,41	1.89	14 (35%)	50,56,56	1.84	12 (24%)
24	CLA	B	803	2	69,73,73	1.22	7 (10%)	83,113,113	1.32	9 (10%)
27	WVN	A	846	-	40,41,41	1.92	14 (35%)	50,56,56	2.27	14 (28%)
27	WVN	F	205	-	40,41,41	1.92	14 (35%)	50,56,56	3.08	18 (36%)
33	II0	f	618	-	39,43,43	6.71	20 (51%)	50,60,60	2.38	17 (34%)
24	CLA	j	309	19	49,53,73	1.47	9 (18%)	59,89,113	1.42	8 (13%)
24	CLA	B	801	36	69,73,73	1.25	10 (14%)	83,113,113	1.38	10 (12%)
24	CLA	g	309	22	69,73,73	1.25	7 (10%)	83,113,113	1.25	8 (9%)
24	CLA	a	307	14	69,73,73	1.25	7 (10%)	83,113,113	1.27	11 (13%)
24	CLA	e	602	17	54,58,73	1.37	9 (16%)	65,95,113	1.37	6 (9%)
24	CLA	f	604	19	69,73,73	1.20	7 (10%)	83,113,113	1.29	8 (9%)
24	CLA	g	304	22	55,59,73	1.40	11 (20%)	66,96,113	1.45	13 (19%)
29	SF4	C	101	3	0,12,12	-	-	-		
33	II0	c	614	-	39,43,43	6.93	21 (53%)	50,60,60	2.21	17 (34%)
27	WVN	B	846	-	40,41,41	1.86	13 (32%)	50,56,56	2.10	16 (32%)
24	CLA	B	811	2	59,63,73	1.38	8 (13%)	71,101,113	1.29	6 (8%)
24	CLA	j	302	19	55,59,73	1.42	8 (14%)	66,96,113	1.28	5 (7%)
33	II0	b	314	-	39,43,43	6.91	23 (58%)	50,60,60	2.20	13 (26%)
33	II0	j	315	-	39,43,43	6.61	20 (51%)	50,60,60	2.53	18 (36%)
24	CLA	k	614	18	55,59,73	1.41	6 (10%)	66,96,113	1.33	8 (12%)
24	CLA	B	823	36	68,72,73	1.26	13 (19%)	81,111,113	1.38	10 (12%)
24	CLA	a	309	26	52,56,73	1.43	8 (15%)	62,92,113	1.25	7 (11%)
27	WVN	J	101	-	40,41,41	1.88	14 (35%)	50,56,56	2.02	15 (30%)
24	CLA	K	101	36	55,59,73	1.38	10 (18%)	66,96,113	1.53	11 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
24	CLA	A	809	1	60,64,73	1.35	8 (13%)	72,102,113	1.28	8 (11%)
24	CLA	f	603	19	55,59,73	1.38	8 (14%)	66,96,113	1.45	10 (15%)
24	CLA	B	817	2	61,65,73	1.28	9 (14%)	73,103,113	1.44	10 (13%)
28	LMT	A	851	-	36,36,36	1.22	6 (16%)	47,47,47	1.36	5 (10%)
35	KC2	i	609	20	49,53,53	2.75	19 (38%)	62,89,89	4.21	37 (59%)
33	II0	h	310	-	39,43,43	6.55	20 (51%)	50,60,60	2.22	20 (40%)
26	LHG	b	302	24	48,48,48	0.93	2 (4%)	51,54,54	1.20	5 (9%)
24	CLA	d	303	21	69,73,73	1.28	9 (13%)	83,113,113	1.34	10 (12%)
33	II0	c	616	-	39,43,43	6.90	22 (56%)	50,60,60	2.05	16 (32%)
27	WVN	L	206	-	40,41,41	1.84	13 (32%)	50,56,56	2.33	20 (40%)
24	CLA	k	601	18	55,59,73	1.44	9 (16%)	66,96,113	1.50	6 (9%)
24	CLA	j	306	19	49,53,73	1.49	8 (16%)	59,89,113	1.62	10 (16%)
24	CLA	f	606	19	55,59,73	1.39	7 (12%)	66,96,113	1.45	7 (10%)
27	WVN	R	202	-	40,41,41	1.88	13 (32%)	50,56,56	2.49	17 (34%)
24	CLA	k	602	18	54,58,73	1.44	9 (16%)	65,95,113	1.40	8 (12%)
24	CLA	b	312	15	69,73,73	1.27	8 (11%)	83,113,113	1.25	9 (10%)
28	LMT	F	203	-	24,24,36	1.07	1 (4%)	29,29,47	0.98	2 (6%)
34	IHT	k	618	-	40,42,42	6.25	25 (62%)	53,58,58	1.79	15 (28%)
33	II0	k	617	-	39,43,43	6.87	22 (56%)	50,60,60	2.61	18 (36%)
24	CLA	A	822	1	55,59,73	1.40	8 (14%)	66,96,113	1.41	10 (15%)
33	II0	h	309	-	26,28,43	6.13	12 (46%)	31,37,60	2.13	12 (38%)
34	IHT	j	317	-	40,42,42	6.22	25 (62%)	53,58,58	2.34	18 (33%)
24	CLA	B	826	2	69,73,73	1.22	9 (13%)	83,113,113	1.24	9 (10%)
27	WVN	I	101	-	40,41,41	1.85	14 (35%)	50,56,56	1.78	15 (30%)
24	CLA	d	304	21	55,59,73	1.42	5 (9%)	66,96,113	1.39	8 (12%)
24	CLA	B	805	2	69,73,73	1.21	9 (13%)	83,113,113	1.35	8 (9%)
24	CLA	A	821	1	53,57,73	1.37	9 (16%)	62,93,113	1.50	8 (12%)
24	CLA	i	606	20	65,69,73	1.28	7 (10%)	78,108,113	1.12	4 (5%)
24	CLA	h	306	16	61,65,73	1.37	7 (11%)	73,103,113	1.16	6 (8%)
24	CLA	d	302	21	55,59,73	1.44	8 (14%)	66,96,113	1.36	12 (18%)
27	WVN	B	849	-	40,41,41	1.90	14 (35%)	50,56,56	1.67	10 (20%)
24	CLA	A	834	1	55,59,73	1.41	9 (16%)	66,96,113	1.61	14 (21%)
24	CLA	k	609	18	69,73,73	1.27	7 (10%)	83,113,113	1.33	11 (13%)
24	CLA	d	308	21	45,49,73	1.50	8 (17%)	54,84,113	1.33	5 (9%)
24	CLA	A	829	1	69,73,73	1.24	8 (11%)	83,113,113	1.26	9 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
24	CLA	j	304	19	55,59,73	1.37	6 (10%)	66,96,113	1.41	9 (13%)
24	CLA	L	203	9	69,73,73	1.24	9 (13%)	83,113,113	1.28	12 (14%)
24	CLA	c	604	13	69,73,73	1.25	9 (13%)	83,113,113	1.18	9 (10%)
24	CLA	B	822	36	69,73,73	1.27	10 (14%)	83,113,113	1.63	17 (20%)
33	II0	e	616	-	39,43,43	6.81	21 (53%)	50,60,60	2.02	18 (36%)
26	LHG	B	802	-	37,37,48	1.04	2 (5%)	40,43,54	1.14	4 (10%)
24	CLA	A	801	1	69,73,73	1.23	7 (10%)	83,113,113	1.23	8 (9%)
33	II0	f	614	-	39,43,43	6.70	21 (53%)	50,60,60	2.36	15 (30%)
24	CLA	j	314	19	69,73,73	1.22	6 (8%)	83,113,113	1.26	8 (9%)
24	CLA	A	810	1	66,70,73	1.24	8 (12%)	79,109,113	1.18	8 (10%)
26	LHG	g	321	24	36,36,48	1.08	2 (5%)	39,42,54	1.54	9 (23%)
26	LHG	k	620	24	36,36,48	1.14	2 (5%)	39,42,54	1.15	5 (12%)
24	CLA	c	602	13	54,58,73	1.41	9 (16%)	65,95,113	1.44	10 (15%)
24	CLA	b	304	15	59,63,73	1.32	9 (15%)	71,101,113	1.40	6 (8%)
24	CLA	c	603	13	55,59,73	1.39	10 (18%)	66,96,113	1.33	6 (9%)
24	CLA	c	605	13	55,59,73	1.39	7 (12%)	66,96,113	1.45	11 (16%)
24	CLA	i	603	20	55,59,73	1.40	9 (16%)	66,96,113	1.39	7 (10%)
24	CLA	h	307	16	55,59,73	1.41	9 (16%)	66,96,113	1.48	8 (12%)
24	CLA	f	602	19	69,73,73	1.24	8 (11%)	83,113,113	1.25	8 (9%)
32	LMG	F	206	-	48,48,55	0.96	2 (4%)	56,56,63	1.26	5 (8%)
24	CLA	d	312	21	55,59,73	1.39	6 (10%)	66,96,113	1.53	13 (19%)
24	CLA	A	826	1	69,73,73	1.25	9 (13%)	83,113,113	1.45	14 (16%)
34	IHT	b	316	-	40,42,42	6.23	25 (62%)	53,58,58	2.19	17 (32%)
26	LHG	c	618	24	36,36,48	1.11	2 (5%)	39,42,54	1.20	6 (15%)
24	CLA	a	303	14	54,58,73	1.38	8 (14%)	65,95,113	1.35	9 (13%)
33	II0	d	313	-	39,43,43	6.84	23 (58%)	50,60,60	2.23	18 (36%)
33	II0	e	613	-	39,43,43	6.70	23 (58%)	50,60,60	2.04	16 (32%)
32	LMG	O	204	-	26,26,55	1.26	2 (7%)	34,34,63	1.31	4 (11%)
24	CLA	B	841	26	69,73,73	1.24	9 (13%)	83,113,113	1.30	10 (12%)
24	CLA	i	604	20	69,73,73	1.27	6 (8%)	83,113,113	1.57	9 (10%)
24	CLA	L	202	9	53,57,73	1.45	9 (16%)	62,93,113	1.42	8 (12%)
24	CLA	b	310	26	69,73,73	1.29	6 (8%)	83,113,113	1.21	12 (14%)
24	CLA	k	607	18	55,59,73	1.43	8 (14%)	66,96,113	1.37	9 (13%)
26	LHG	A	844	-	47,47,48	0.91	2 (4%)	50,53,54	1.15	5 (10%)
24	CLA	A	820	36	69,73,73	1.27	10 (14%)	83,113,113	1.38	9 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
24	CLA	O	201	-	69,73,73	1.27	11 (15%)	83,113,113	1.30	8 (9%)
24	CLA	j	313	-	55,59,73	1.42	8 (14%)	66,96,113	1.32	6 (9%)
24	CLA	A	825	36	69,73,73	1.20	9 (13%)	83,113,113	1.27	9 (10%)
24	CLA	h	303	16	55,59,73	1.40	10 (18%)	66,96,113	1.42	11 (16%)
24	CLA	h	312	36	69,73,73	1.22	7 (10%)	83,113,113	1.30	7 (8%)
24	CLA	A	840	1	69,73,73	1.20	10 (14%)	83,113,113	1.25	8 (9%)
24	CLA	e	607	17	69,73,73	1.19	6 (8%)	83,113,113	1.24	8 (9%)
24	CLA	A	811	1	58,62,73	1.38	8 (13%)	69,99,113	1.40	10 (14%)
24	CLA	d	307	21	50,54,73	1.40	6 (12%)	60,90,113	1.36	5 (8%)
27	WVN	J	102	-	40,41,41	1.86	14 (35%)	50,56,56	2.17	16 (32%)
24	CLA	A	831	1	69,73,73	1.25	10 (14%)	83,113,113	1.31	7 (8%)
24	CLA	k	608	18	69,73,73	1.23	7 (10%)	83,113,113	1.13	5 (6%)
32	LMG	b	301	-	55,55,55	0.89	2 (3%)	63,63,63	1.13	5 (7%)
24	CLA	e	611	17	69,73,73	1.25	8 (11%)	83,113,113	1.33	11 (13%)
32	LMG	J	106	-	55,55,55	0.85	3 (5%)	63,63,63	0.96	4 (6%)
24	CLA	A	819	1	49,53,73	1.48	10 (20%)	59,89,113	1.66	14 (23%)
24	CLA	e	608	26	50,54,73	1.43	9 (18%)	60,90,113	1.60	6 (10%)
24	CLA	e	603	17	55,59,73	1.42	6 (10%)	66,96,113	1.44	12 (18%)
25	PQN	A	843	-	34,34,34	1.89	5 (14%)	42,45,45	1.23	5 (11%)
24	CLA	k	610	26	55,59,73	1.37	7 (12%)	66,96,113	1.32	6 (9%)
24	CLA	B	833	2	69,73,73	1.20	10 (14%)	83,113,113	1.38	11 (13%)
24	CLA	k	606	18	55,59,73	1.37	9 (16%)	66,96,113	1.34	7 (10%)
24	CLA	i	607	20	55,59,73	1.39	8 (14%)	66,96,113	1.32	10 (15%)
24	CLA	j	311	26	65,69,73	1.29	7 (10%)	78,108,113	1.12	4 (5%)
26	LHG	i	615	24	36,36,48	1.12	2 (5%)	39,42,54	1.19	3 (7%)
26	LHG	e	617	24	36,36,48	1.12	2 (5%)	39,42,54	1.16	4 (10%)
24	CLA	b	307	36	69,73,73	1.27	6 (8%)	83,113,113	1.36	11 (13%)
24	CLA	B	819	2	50,54,73	1.39	8 (16%)	60,90,113	1.42	9 (15%)
24	CLA	g	311	26	58,62,73	1.34	7 (12%)	69,99,113	1.20	4 (5%)
27	WVN	j	301	-	40,41,41	1.92	14 (35%)	50,56,56	2.11	18 (36%)
34	IHT	b	317	-	40,42,42	6.31	26 (65%)	53,58,58	2.85	17 (32%)
24	CLA	e	605	17	69,73,73	1.21	8 (11%)	83,113,113	1.23	7 (8%)
24	CLA	i	601	20	55,59,73	1.41	7 (12%)	66,96,113	1.38	3 (4%)
24	CLA	A	815	36	49,53,73	1.49	10 (20%)	59,89,113	1.59	8 (13%)
27	WVN	h	308	-	40,41,41	1.89	13 (32%)	50,56,56	2.29	19 (38%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
24	CLA	f	607	19	69,73,73	1.24	9 (13%)	83,113,113	1.18	7 (8%)
26	LHG	d	316	24	36,36,48	1.10	2 (5%)	39,42,54	1.23	5 (12%)
33	II0	k	616	-	39,43,43	6.84	22 (56%)	50,60,60	2.14	16 (32%)
27	WVN	A	850	-	40,41,41	1.89	14 (35%)	50,56,56	2.09	12 (24%)
24	CLA	i	610	-	55,59,73	1.42	9 (16%)	66,96,113	1.47	10 (15%)
24	CLA	A	830	1	54,58,73	1.41	11 (20%)	65,95,113	1.45	9 (13%)
24	CLA	g	307	22	55,59,73	1.37	8 (14%)	66,96,113	1.36	10 (15%)
28	LMT	a	318	-	36,36,36	1.21	5 (13%)	47,47,47	1.15	3 (6%)
24	CLA	d	306	21	55,59,73	1.39	9 (16%)	66,96,113	1.09	3 (4%)
24	CLA	f	613	19	69,73,73	1.26	8 (11%)	83,113,113	1.19	7 (8%)
26	LHG	g	301	-	48,48,48	0.94	2 (4%)	51,54,54	1.04	2 (3%)
24	CLA	B	809	2	69,73,73	1.26	10 (14%)	83,113,113	1.35	10 (12%)
24	CLA	f	608	19	69,73,73	1.21	7 (10%)	83,113,113	1.26	9 (10%)
24	CLA	F	202	6	56,60,73	1.36	8 (14%)	67,97,113	1.52	11 (16%)
29	SF4	A	854	2,1	0,12,12	-	-	-		
24	CLA	A	839	1	69,73,73	1.31	9 (13%)	83,113,113	1.35	9 (10%)
26	LHG	A	845	24	26,26,48	1.25	2 (7%)	29,32,54	1.53	5 (17%)
24	CLA	A	855	36	69,73,73	1.30	10 (14%)	83,113,113	1.43	11 (13%)
24	CLA	B	834	2	51,55,73	1.39	9 (17%)	61,91,113	1.55	7 (11%)
33	II0	a	313	-	39,43,43	6.70	22 (56%)	50,60,60	2.15	16 (32%)
33	II0	a	314	-	39,43,43	6.70	22 (56%)	50,60,60	2.13	20 (40%)
24	CLA	f	601	19	51,55,73	1.43	7 (13%)	61,91,113	1.34	4 (6%)
24	CLA	A	833	1	54,58,73	1.41	10 (18%)	65,95,113	1.35	6 (9%)
24	CLA	e	601	17	49,53,73	1.49	9 (18%)	59,89,113	1.48	6 (10%)
27	WVN	B	847	-	40,41,41	1.85	13 (32%)	50,56,56	2.34	17 (34%)
35	KC2	g	313	22,35	49,53,53	2.75	19 (38%)	62,89,89	4.09	35 (56%)
24	CLA	L	207	36	55,59,73	1.36	8 (14%)	66,96,113	1.36	8 (12%)
33	II0	e	614	-	39,43,43	6.91	20 (51%)	50,60,60	2.10	20 (40%)
24	CLA	f	610	26	69,73,73	1.24	7 (10%)	83,113,113	1.25	6 (7%)
24	CLA	i	602	20	54,58,73	1.39	8 (14%)	65,95,113	1.37	6 (9%)
27	WVN	M	101	-	40,41,41	1.87	14 (35%)	50,56,56	2.11	15 (30%)
24	CLA	k	605	18	49,53,73	1.44	8 (16%)	59,89,113	1.38	7 (11%)
24	CLA	A	836	1	69,73,73	1.23	8 (11%)	83,113,113	1.47	12 (14%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CLA	h	305	16	-	11/39/115/115	-
24	CLA	A	812	1	-	22/39/115/115	-
24	CLA	a	312	14	-	6/19/95/115	-
27	WVN	B	845	-	-	6/29/63/63	0/2/2/2
24	CLA	B	816	2	-	9/32/108/115	-
35	KC2	c	610	13	-	10/15/71/71	-
24	CLA	A	842	1	-	22/39/115/115	-
27	WVN	A	849	-	-	8/29/63/63	0/2/2/2
33	II0	i	614	-	-	4/21/67/67	0/2/2/2
24	CLA	A	835	1	-	13/39/115/115	-
33	II0	b	315	-	-	5/21/67/67	0/2/2/2
24	CLA	I	102	36	-	17/39/115/115	-
33	II0	j	318	-	-	5/21/67/67	0/2/2/2
24	CLA	c	601	13	-	12/23/99/115	-
33	II0	J	104	-	-	7/21/67/67	0/2/2/2
24	CLA	g	302	22	-	0/12/88/115	-
24	CLA	B	804	-	-	9/39/115/115	-
24	CLA	c	612	13	-	11/39/115/115	-
24	CLA	i	611	20	-	13/23/99/115	-
24	CLA	A	814	1	-	9/21/97/115	-
24	CLA	O	205	-	-	18/39/115/115	-
24	CLA	A	837	1	-	11/39/115/115	-
24	CLA	h	302	16	-	11/21/97/115	-
35	KC2	g	314	35	-	9/15/71/71	-
27	WVN	e	615	-	-	11/29/63/63	0/2/2/2
24	CLA	b	305	15	-	13/39/115/115	-
24	CLA	A	838	26	-	5/24/100/115	-
24	CLA	B	825	2	-	11/39/115/115	-
24	CLA	A	818	1	-	19/39/115/115	-
28	LMT	b	319	-	-	9/15/35/61	0/1/1/2
24	CLA	f	612	-	-	6/23/99/115	-
34	IHT	f	617	-	-	4/25/65/65	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CLA	A	852	36	-	3/39/115/115	-
24	CLA	a	305	36	-	9/39/115/115	-
26	LHG	f	619	24	-	22/41/41/53	-
33	II0	j	316	-	-	2/21/67/67	0/2/2/2
24	CLA	b	311	15	-	6/23/99/115	-
24	CLA	B	838	2	-	11/30/106/115	-
24	CLA	f	605	19	-	9/15/91/115	-
33	II0	O	202	-	-	3/21/67/67	0/2/2/2
24	CLA	B	820	2	-	10/27/103/115	-
33	II0	f	615	-	-	4/21/67/67	0/2/2/2
33	II0	g	317	-	-	5/21/67/67	0/2/2/2
34	IHT	a	316	-	-	9/25/65/65	0/2/2/2
24	CLA	b	308	15	-	14/35/111/115	-
24	CLA	a	308	14	-	14/39/115/115	-
33	II0	e	612	-	-	4/21/67/67	0/2/2/2
24	CLA	A	827	1	-	9/36/112/115	-
33	II0	k	615	-	-	5/21/67/67	0/2/2/2
24	CLA	b	313	15	-	25/39/115/115	-
33	II0	g	316	-	-	7/21/67/67	0/2/2/2
33	II0	g	320	-	-	4/21/67/67	0/2/2/2
24	CLA	A	832	1	-	14/39/115/115	-
24	CLA	j	308	19	-	10/23/99/115	-
24	CLA	d	309	26	-	2/10/86/115	-
24	CLA	B	808	2	-	13/39/115/115	-
33	II0	f	616	-	-	5/21/67/67	0/2/2/2
24	CLA	h	301	16	-	8/21/97/115	-
24	CLA	g	315	22	-	9/23/99/115	-
27	WVN	A	848	-	-	9/29/63/63	0/2/2/2
33	II0	k	621	-	-	4/21/67/67	0/2/2/2
24	CLA	A	816	1	-	16/39/115/115	-
24	CLA	B	818	36	-	7/39/115/115	-
25	PQN	B	842	-	-	13/23/43/43	0/2/2/2
24	CLA	a	302	14	-	11/24/100/115	-
33	II0	a	315	-	-	3/21/67/67	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CLA	e	606	17	-	11/39/115/115	-
31	LMU	B	844	-	-	8/21/61/61	0/2/2/2
24	CLA	j	310	19	-	5/23/99/115	-
24	CLA	B	813	2	-	14/33/109/115	-
24	CLA	c	607	13	-	3/17/93/115	-
24	CLA	i	608	26	-	7/17/93/115	-
33	II0	a	317	-	-	7/21/67/67	0/2/2/2
24	CLA	b	309	15	-	20/39/115/115	-
24	CLA	A	803	1	-	6/27/103/115	-
24	CLA	b	303	15	-	9/23/99/115	-
34	IHT	g	319	-	-	11/25/65/65	0/2/2/2
24	CLA	B	807	2	-	10/39/115/115	-
33	II0	h	311	-	-	7/21/67/67	0/2/2/2
24	CLA	B	824	2	-	3/39/115/115	-
24	CLA	R	203	23	-	9/23/99/115	-
24	CLA	B	832	2	-	8/31/107/115	-
35	KC2	k	612	18,35	-	8/15/71/71	-
33	II0	i	612	-	-	7/21/67/67	0/2/2/2
24	CLA	B	830	36	-	13/39/115/115	-
33	II0	b	318	-	-	4/21/67/67	0/2/2/2
24	CLA	g	306	22	-	9/23/99/115	-
27	WVN	F	204	-	-	10/29/63/63	0/2/2/2
24	CLA	g	303	22	-	8/21/97/115	-
24	CLA	j	305	19	-	11/39/115/115	-
24	CLA	B	836	2	-	25/39/115/115	-
24	CLA	c	606	13	-	8/24/100/115	-
24	CLA	c	608	13	-	17/39/115/115	-
24	CLA	B	829	2	-	7/21/97/115	-
24	CLA	B	812	2	-	14/39/115/115	-
24	CLA	d	305	-	-	7/23/99/115	-
26	LHG	j	319	24	-	5/34/34/53	-
24	CLA	B	815	2	-	7/27/103/115	-
34	IHT	c	615	-	-	10/25/65/65	0/2/2/2
35	KC2	e	609	17	-	5/15/71/71	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CLA	B	840	2	-	11/39/115/115	-
24	CLA	B	835	36	-	11/39/115/115	-
24	CLA	g	305	22	-	16/39/115/115	-
24	CLA	B	821	2	-	9/25/101/115	-
30	DGD	B	843	-	-	5/49/89/95	0/2/2/2
24	CLA	A	817	1	-	15/39/115/115	-
27	WVN	A	847	-	-	10/29/63/63	0/2/2/2
24	CLA	a	304	14	-	3/23/99/115	-
27	WVN	L	205	-	-	6/29/63/63	0/2/2/2
24	CLA	J	105	26	-	7/23/99/115	-
33	II0	i	613	-	-	4/21/67/67	0/2/2/2
24	CLA	A	807	1	-	9/39/115/115	-
24	CLA	h	304	16	-	6/23/99/115	-
24	CLA	A	802	-	-	16/39/115/115	-
24	CLA	A	813	1	-	7/15/91/115	-
24	CLA	B	814	2	-	13/32/108/115	-
24	CLA	A	806	1	-	10/39/115/115	-
24	CLA	A	823	1	-	8/27/103/115	-
24	CLA	B	837	2	-	15/39/115/115	-
33	II0	g	318	-	-	2/21/67/67	0/2/2/2
24	CLA	A	808	1	-	11/39/115/115	-
24	CLA	A	824	36	-	11/39/115/115	-
26	LHG	J	107	24	-	19/53/53/53	-
35	KC2	k	613	35	-	7/15/71/71	-
24	CLA	B	806	2	-	14/39/115/115	-
24	CLA	B	831	36	-	6/15/91/115	-
26	LHG	a	301	24	-	15/53/53/53	-
24	CLA	A	856	26	-	6/10/86/115	-
24	CLA	e	604	36	-	11/39/115/115	-
27	WVN	K	103	-	-	6/29/63/63	0/2/2/2
34	IHT	O	203	-	-	5/25/65/65	0/2/2/2
24	CLA	b	306	15	-	19/39/115/115	-
33	II0	d	314	-	-	5/21/67/67	0/2/2/2
34	IHT	R	204	-	-	4/25/65/65	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CLA	g	310	22	-	6/23/99/115	-
24	CLA	f	609	19	-	5/39/115/115	-
24	CLA	j	303	19	-	2/21/97/115	-
26	LHG	b	320	24	-	17/53/53/53	-
24	CLA	g	322	32	-	15/39/115/115	-
24	CLA	i	605	20	-	8/23/99/115	-
35	KC2	d	311	21	-	7/15/71/71	-
24	CLA	A	853	1	-	16/39/115/115	-
24	CLA	d	301	21	-	7/21/97/115	-
24	CLA	A	805	1	-	7/39/115/115	-
24	CLA	c	611	-	-	7/15/91/115	-
24	CLA	k	604	18	-	11/39/115/115	-
24	CLA	g	308	22	-	18/39/115/115	-
35	KC2	d	310	21	-	5/15/71/71	-
24	CLA	A	804	1	-	7/39/115/115	-
24	CLA	A	828	1	-	8/39/115/115	-
35	KC2	k	611	18	-	7/15/71/71	-
24	CLA	e	610	36	-	14/39/115/115	-
26	LHG	f	620	-	-	17/53/53/53	-
24	CLA	K	102	12	-	7/12/88/115	-
35	KC2	f	611	19	-	7/15/71/71	-
27	WVN	B	848	-	-	7/29/63/63	0/2/2/2
24	CLA	B	839	2	-	10/39/115/115	-
26	LHG	c	617	24	-	14/41/41/53	-
24	CLA	k	603	18	-	3/23/99/115	-
24	CLA	c	609	26	-	4/15/91/115	-
24	CLA	F	201	36	-	14/39/115/115	-
33	II0	d	315	-	-	8/21/67/67	0/2/2/2
24	CLA	B	810	2	-	5/25/101/115	-
32	LMG	L	208	24	-	19/50/70/70	0/1/1/1
35	KC2	g	312	22	-	9/15/71/71	-
29	SF4	C	102	3	-	-	0/6/5/5
24	CLA	j	307	19	-	11/23/99/115	-
35	KC2	i	616	-	-	10/15/71/71	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CLA	B	828	2	-	4/20/96/115	-
24	CLA	L	204	36	-	7/21/97/115	-
35	KC2	j	312	19	-	5/15/71/71	-
27	WVN	L	201	-	-	10/29/63/63	0/2/2/2
24	CLA	A	841	36	-	22/39/115/115	-
24	CLA	B	827	2	-	11/21/97/115	-
24	CLA	a	311	14	-	10/18/94/115	-
24	CLA	J	103	8	-	5/12/88/115	-
24	CLA	a	306	14	-	8/15/91/115	-
33	II0	c	613	-	-	3/21/67/67	0/2/2/2
33	II0	k	619	-	-	5/21/67/67	0/2/2/2
24	CLA	a	310	14	-	13/39/115/115	-
27	WVN	R	201	-	-	6/29/63/63	0/2/2/2
24	CLA	B	803	2	-	21/39/115/115	-
27	WVN	A	846	-	-	8/29/63/63	0/2/2/2
27	WVN	F	205	-	-	12/29/63/63	0/2/2/2
33	II0	f	618	-	-	7/21/67/67	0/2/2/2
24	CLA	j	309	19	-	6/15/91/115	-
24	CLA	B	801	36	-	13/39/115/115	-
24	CLA	g	309	22	-	6/39/115/115	-
24	CLA	a	307	14	-	16/39/115/115	-
24	CLA	e	602	17	-	6/21/97/115	-
24	CLA	f	604	19	-	8/39/115/115	-
24	CLA	g	304	22	-	4/23/99/115	-
29	SF4	C	101	3	-	-	0/6/5/5
33	II0	c	614	-	-	1/21/67/67	0/2/2/2
27	WVN	B	846	-	-	0/29/63/63	0/2/2/2
24	CLA	B	811	2	-	6/27/103/115	-
24	CLA	j	302	19	-	7/23/99/115	-
33	II0	b	314	-	-	7/21/67/67	0/2/2/2
33	II0	j	315	-	-	5/21/67/67	0/2/2/2
24	CLA	k	614	18	-	9/23/99/115	-
24	CLA	B	823	36	-	11/38/114/115	-
24	CLA	a	309	26	-	8/19/95/115	-
27	WVN	J	101	-	-	8/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CLA	K	101	36	-	3/23/99/115	-
24	CLA	A	809	1	-	9/29/105/115	-
24	CLA	f	603	19	-	5/23/99/115	-
24	CLA	B	817	2	-	7/30/106/115	-
28	LMT	A	851	-	-	9/21/61/61	0/2/2/2
35	KC2	i	609	20	-	9/15/71/71	-
33	II0	h	310	-	-	8/21/67/67	0/2/2/2
26	LHG	b	302	24	-	13/53/53/53	-
24	CLA	d	303	21	-	17/39/115/115	-
33	II0	c	616	-	-	3/21/67/67	0/2/2/2
27	WVN	L	206	-	-	3/29/63/63	0/2/2/2
24	CLA	k	601	18	-	12/23/99/115	-
24	CLA	j	306	19	-	7/15/91/115	-
24	CLA	f	606	19	-	4/23/99/115	-
27	WVN	R	202	-	-	10/29/63/63	0/2/2/2
24	CLA	k	602	18	-	6/21/97/115	-
24	CLA	b	312	15	-	22/39/115/115	-
28	LMT	F	203	-	-	4/15/35/61	0/1/1/2
34	IHT	k	618	-	-	7/25/65/65	0/2/2/2
33	II0	k	617	-	-	3/21/67/67	0/2/2/2
24	CLA	A	822	1	-	8/23/99/115	-
33	II0	h	309	-	-	3/17/40/67	0/1/1/2
34	IHT	j	317	-	-	7/25/65/65	0/2/2/2
24	CLA	B	826	2	-	9/39/115/115	-
27	WVN	I	101	-	-	9/29/63/63	0/2/2/2
24	CLA	d	304	21	-	11/23/99/115	-
24	CLA	B	805	2	-	17/39/115/115	-
24	CLA	A	821	1	-	7/20/96/115	-
24	CLA	i	606	20	-	11/35/111/115	-
24	CLA	h	306	16	-	9/30/106/115	-
24	CLA	d	302	21	-	3/23/99/115	-
27	WVN	B	849	-	-	13/29/63/63	0/2/2/2
24	CLA	A	834	1	-	4/23/99/115	-
24	CLA	k	609	18	-	13/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CLA	d	308	21	-	3/10/86/115	-
24	CLA	A	829	1	-	14/39/115/115	-
24	CLA	j	304	19	-	0/23/99/115	-
24	CLA	L	203	9	-	13/39/115/115	-
24	CLA	c	604	13	-	5/39/115/115	-
24	CLA	B	822	36	-	10/39/115/115	-
33	II0	e	616	-	-	5/21/67/67	0/2/2/2
26	LHG	B	802	-	-	16/42/42/53	-
24	CLA	A	801	1	-	10/39/115/115	-
33	II0	f	614	-	-	4/21/67/67	0/2/2/2
24	CLA	j	314	19	-	14/39/115/115	-
24	CLA	A	810	1	-	10/36/112/115	-
26	LHG	g	321	24	-	12/41/41/53	-
26	LHG	k	620	24	-	14/41/41/53	-
24	CLA	c	602	13	-	13/21/97/115	-
24	CLA	b	304	15	-	8/27/103/115	-
24	CLA	c	603	13	-	3/23/99/115	-
24	CLA	c	605	13	-	9/23/99/115	-
24	CLA	i	603	20	-	4/23/99/115	-
24	CLA	h	307	16	-	11/23/99/115	-
24	CLA	f	602	19	-	19/39/115/115	-
32	LMG	F	206	-	-	11/43/63/70	0/1/1/1
24	CLA	d	312	21	-	5/23/99/115	-
24	CLA	A	826	1	-	8/39/115/115	-
34	IHT	b	316	-	-	3/25/65/65	0/2/2/2
26	LHG	c	618	24	-	11/41/41/53	-
24	CLA	a	303	14	-	6/21/97/115	-
33	II0	d	313	-	-	6/21/67/67	0/2/2/2
33	II0	e	613	-	-	6/21/67/67	0/2/2/2
32	LMG	O	204	-	-	7/21/41/70	0/1/1/1
24	CLA	B	841	26	-	3/39/115/115	-
24	CLA	i	604	20	-	12/39/115/115	-
24	CLA	L	202	9	-	9/20/96/115	-
24	CLA	b	310	26	-	11/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CLA	k	607	18	-	9/23/99/115	-
26	LHG	A	844	-	-	7/52/52/53	-
24	CLA	A	820	36	-	5/39/115/115	-
24	CLA	O	201	-	-	16/39/115/115	-
24	CLA	j	313	-	-	6/23/99/115	-
24	CLA	A	825	36	-	10/39/115/115	-
24	CLA	h	303	16	-	5/23/99/115	-
24	CLA	h	312	36	-	9/39/115/115	-
24	CLA	A	840	1	-	16/39/115/115	-
24	CLA	e	607	17	-	10/39/115/115	-
24	CLA	A	811	1	-	7/26/102/115	-
24	CLA	d	307	21	-	6/17/93/115	-
27	WVN	J	102	-	-	8/29/63/63	0/2/2/2
24	CLA	A	831	1	-	11/39/115/115	-
24	CLA	k	608	18	-	14/39/115/115	-
32	LMG	b	301	-	-	17/50/70/70	0/1/1/1
24	CLA	e	611	17	-	16/39/115/115	-
32	LMG	J	106	-	-	13/50/70/70	0/1/1/1
24	CLA	A	819	1	-	6/15/91/115	-
24	CLA	e	608	26	-	12/17/93/115	-
24	CLA	e	603	17	-	5/23/99/115	-
25	PQN	A	843	-	-	6/23/43/43	0/2/2/2
24	CLA	k	610	26	-	13/23/99/115	-
24	CLA	B	833	2	-	9/39/115/115	-
24	CLA	k	606	18	-	8/23/99/115	-
24	CLA	i	607	20	-	1/23/99/115	-
24	CLA	j	311	26	-	15/35/111/115	-
26	LHG	i	615	24	-	12/41/41/53	-
26	LHG	e	617	24	-	11/41/41/53	-
24	CLA	b	307	36	-	10/39/115/115	-
24	CLA	B	819	2	-	3/17/93/115	-
24	CLA	g	311	26	-	12/26/102/115	-
27	WVN	j	301	-	-	9/29/63/63	0/2/2/2
34	IHT	b	317	-	-	7/25/65/65	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CLA	e	605	17	-	17/39/115/115	-
24	CLA	i	601	20	-	9/23/99/115	-
24	CLA	A	815	36	-	7/15/91/115	-
27	WVN	h	308	-	-	5/29/63/63	0/2/2/2
24	CLA	f	607	19	-	18/39/115/115	-
26	LHG	d	316	24	-	11/41/41/53	-
33	II0	k	616	-	-	6/21/67/67	0/2/2/2
27	WVN	A	850	-	-	14/29/63/63	0/2/2/2
24	CLA	i	610	-	-	7/23/99/115	-
24	CLA	A	830	1	-	5/21/97/115	-
24	CLA	g	307	22	-	9/23/99/115	-
28	LMT	a	318	-	-	3/21/61/61	0/2/2/2
24	CLA	d	306	21	-	12/23/99/115	-
24	CLA	f	613	19	-	22/39/115/115	-
26	LHG	g	301	-	-	14/53/53/53	-
24	CLA	B	809	2	-	11/39/115/115	-
24	CLA	f	608	19	-	9/39/115/115	-
24	CLA	F	202	6	-	13/24/100/115	-
29	SF4	A	854	2,1	-	-	0/6/5/5
24	CLA	A	839	1	-	15/39/115/115	-
26	LHG	A	845	24	-	6/31/31/53	-
24	CLA	A	855	36	-	16/39/115/115	-
24	CLA	B	834	2	-	4/18/94/115	-
33	II0	a	313	-	-	1/21/67/67	0/2/2/2
33	II0	a	314	-	-	7/21/67/67	0/2/2/2
24	CLA	f	601	19	-	12/18/94/115	-
24	CLA	A	833	1	-	6/21/97/115	-
24	CLA	e	601	17	-	9/15/91/115	-
27	WVN	B	847	-	-	12/29/63/63	0/2/2/2
35	KC2	g	313	22,35	-	2/15/71/71	-
24	CLA	L	207	36	-	5/23/99/115	-
33	II0	e	614	-	-	3/21/67/67	0/2/2/2
24	CLA	f	610	26	-	15/39/115/115	-
24	CLA	i	602	20	-	9/21/97/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	WVN	M	101	-	-	9/29/63/63	0/2/2/2
24	CLA	k	605	18	-	7/15/91/115	-
24	CLA	A	836	1	-	8/39/115/115	-

The worst 5 of 3669 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	b	317	IHT	C15-C11	25.48	1.63	1.34
34	R	204	IHT	C15-C11	25.36	1.63	1.34
34	c	615	IHT	C15-C11	25.20	1.63	1.34
34	k	618	IHT	C15-C11	25.15	1.63	1.34
34	j	317	IHT	C15-C11	25.06	1.62	1.34

The worst 5 of 3844 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
34	f	617	IHT	C40-C37-C33	-13.58	107.93	127.31
35	f	611	KC2	C1A-NA-C4A	-12.51	101.08	106.71
34	b	317	IHT	C40-C37-C33	-12.44	109.55	127.31
35	k	613	KC2	C1A-NA-C4A	-11.85	101.38	106.71
34	f	617	IHT	C30-C27-C23	-11.73	110.57	127.31

There are no chirality outliers.

5 of 3092 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
24	A	801	CLA	CBD-CGD-O2D-CED
24	A	802	CLA	C1A-C2A-CAA-CBA
24	A	802	CLA	CBA-CGA-O2A-C1
24	A	802	CLA	O1A-CGA-O2A-C1
24	A	802	CLA	C11-C10-C8-C9

There are no ring outliers.

200 monomers are involved in 400 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	h	305	CLA	1	0
24	A	812	CLA	1	0
24	B	816	CLA	2	0
24	A	842	CLA	6	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	A	835	CLA	2	0
33	b	315	II0	1	0
24	I	102	CLA	2	0
24	c	601	CLA	1	0
24	B	804	CLA	3	0
24	c	612	CLA	2	0
24	i	611	CLA	1	0
24	A	814	CLA	3	0
24	O	205	CLA	6	0
24	A	837	CLA	2	0
24	h	302	CLA	1	0
24	b	305	CLA	3	0
24	A	838	CLA	1	0
24	B	825	CLA	2	0
24	A	818	CLA	3	0
28	b	319	LMT	2	0
24	A	852	CLA	1	0
26	f	619	LHG	3	0
24	B	820	CLA	4	0
24	b	308	CLA	6	0
24	a	308	CLA	2	0
24	A	827	CLA	4	0
33	k	615	II0	1	0
24	b	313	CLA	6	0
24	j	308	CLA	1	0
24	B	808	CLA	1	0
25	B	842	PQN	5	0
24	a	302	CLA	1	0
24	e	606	CLA	4	0
31	B	844	LMU	1	0
24	c	607	CLA	2	0
24	b	309	CLA	2	0
24	A	803	CLA	3	0
24	b	303	CLA	1	0
34	g	319	IHT	1	0
24	B	807	CLA	2	0
24	B	824	CLA	1	0
24	B	832	CLA	2	0
24	B	830	CLA	2	0
24	g	303	CLA	2	0
24	B	836	CLA	4	0
24	c	606	CLA	5	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	c	608	CLA	2	0
24	B	829	CLA	2	0
24	B	812	CLA	3	0
24	d	305	CLA	1	0
24	B	815	CLA	1	0
35	e	609	KC2	2	0
24	B	840	CLA	1	0
24	B	835	CLA	3	0
24	B	821	CLA	1	0
30	B	843	DGD	3	0
24	A	817	CLA	4	0
24	J	105	CLA	3	0
24	A	807	CLA	1	0
24	A	802	CLA	6	0
24	A	813	CLA	2	0
24	B	814	CLA	1	0
24	A	806	CLA	5	0
24	A	823	CLA	2	0
24	B	837	CLA	4	0
24	A	824	CLA	1	0
26	J	107	LHG	8	0
24	B	806	CLA	2	0
24	B	831	CLA	1	0
24	A	856	CLA	5	0
24	e	604	CLA	1	0
24	b	306	CLA	2	0
24	g	310	CLA	1	0
24	f	609	CLA	2	0
26	b	320	LHG	5	0
24	g	322	CLA	2	0
24	i	605	CLA	1	0
35	d	311	KC2	1	0
24	A	853	CLA	4	0
24	d	301	CLA	1	0
24	A	805	CLA	1	0
24	c	611	CLA	1	0
24	k	604	CLA	1	0
24	g	308	CLA	5	0
24	A	804	CLA	3	0
24	A	828	CLA	2	0
24	e	610	CLA	3	0
26	f	620	LHG	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	B	839	CLA	2	0
24	k	603	CLA	3	0
24	F	201	CLA	7	0
24	B	810	CLA	2	0
32	L	208	LMG	3	0
35	g	312	KC2	1	0
29	C	102	SF4	1	0
24	B	828	CLA	3	0
24	A	841	CLA	3	0
24	B	827	CLA	3	0
24	a	311	CLA	4	0
24	a	310	CLA	2	0
24	B	803	CLA	2	0
24	j	309	CLA	2	0
24	B	801	CLA	6	0
24	g	309	CLA	4	0
24	a	307	CLA	3	0
24	e	602	CLA	1	0
24	f	604	CLA	1	0
24	g	304	CLA	1	0
29	C	101	SF4	2	0
24	B	811	CLA	1	0
24	j	302	CLA	1	0
24	k	614	CLA	1	0
24	B	823	CLA	5	0
24	K	101	CLA	1	0
24	A	809	CLA	2	0
24	f	603	CLA	1	0
24	B	817	CLA	2	0
28	A	851	LMT	1	0
26	b	302	LHG	2	0
24	d	303	CLA	2	0
24	k	601	CLA	3	0
24	j	306	CLA	2	0
24	f	606	CLA	2	0
24	k	602	CLA	3	0
24	b	312	CLA	6	0
34	k	618	IHT	2	0
24	A	822	CLA	2	0
34	j	317	IHT	1	0
24	B	826	CLA	1	0
24	d	304	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	B	805	CLA	1	0
24	A	821	CLA	1	0
24	i	606	CLA	1	0
24	k	609	CLA	2	0
24	A	829	CLA	3	0
24	L	203	CLA	4	0
24	B	822	CLA	4	0
26	B	802	LHG	3	0
24	A	801	CLA	2	0
24	c	602	CLA	2	0
24	b	304	CLA	2	0
24	c	603	CLA	1	0
24	c	605	CLA	1	0
24	h	307	CLA	1	0
24	f	602	CLA	4	0
32	F	206	LMG	2	0
26	c	618	LHG	1	0
24	a	303	CLA	1	0
24	B	841	CLA	4	0
24	L	202	CLA	2	0
24	b	310	CLA	3	0
24	k	607	CLA	2	0
26	A	844	LHG	1	0
24	A	820	CLA	3	0
24	O	201	CLA	3	0
24	j	313	CLA	1	0
24	A	840	CLA	5	0
24	e	607	CLA	3	0
24	A	811	CLA	2	0
24	A	831	CLA	1	0
24	k	608	CLA	3	0
32	b	301	LMG	6	0
24	e	611	CLA	3	0
32	J	106	LMG	6	0
24	A	819	CLA	1	0
24	e	608	CLA	1	0
25	A	843	PQN	2	0
24	k	610	CLA	2	0
24	B	833	CLA	3	0
24	i	607	CLA	1	0
24	j	311	CLA	2	0
26	e	617	LHG	2	0

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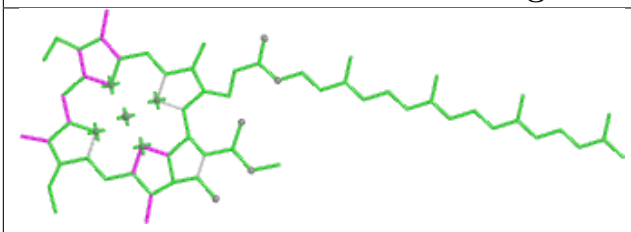
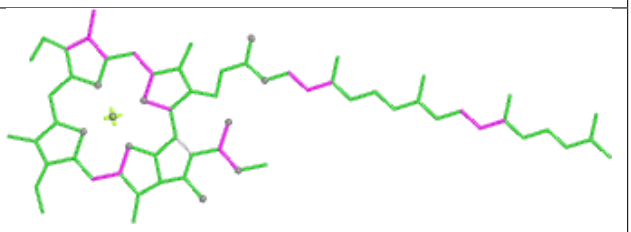
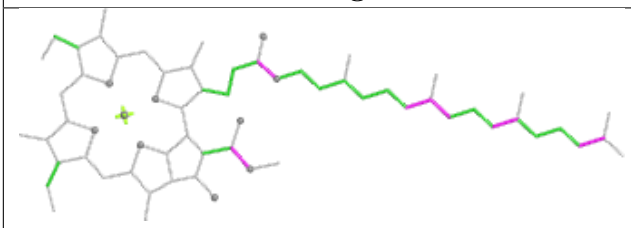
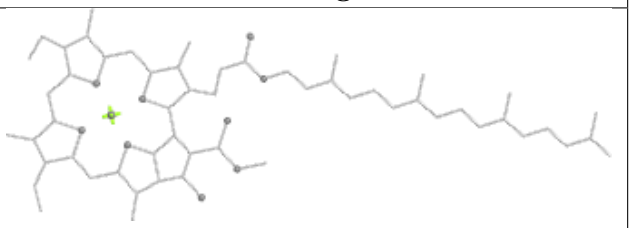
Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	b	307	CLA	3	0
24	B	819	CLA	1	0
24	e	605	CLA	3	0
24	i	601	CLA	1	0
24	A	815	CLA	2	0
24	f	607	CLA	3	0
33	k	616	II0	1	0
24	i	610	CLA	1	0
24	A	830	CLA	1	0
24	g	307	CLA	1	0
28	a	318	LMT	2	0
24	d	306	CLA	1	0
24	f	613	CLA	1	0
26	g	301	LHG	1	0
24	f	608	CLA	4	0
24	F	202	CLA	2	0
29	A	854	SF4	2	0
24	A	839	CLA	4	0
24	A	855	CLA	6	0
24	B	834	CLA	1	0
33	a	314	II0	1	0
24	f	601	CLA	2	0
24	e	601	CLA	1	0
35	g	313	KC2	1	0
24	L	207	CLA	1	0
24	f	610	CLA	4	0
24	i	602	CLA	1	0
24	A	836	CLA	3	0

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

Ligand CLA h 305	
 Bond lengths	 Bond angles
 Torsions	 Rings

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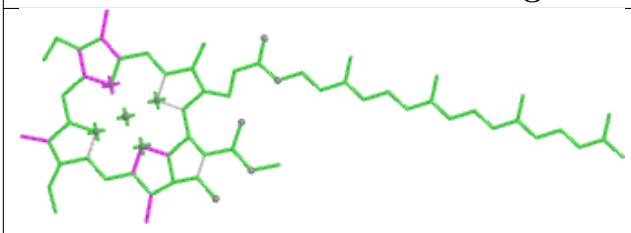
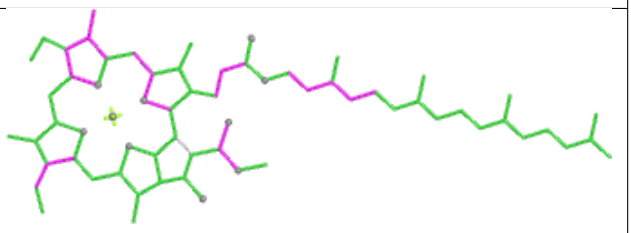
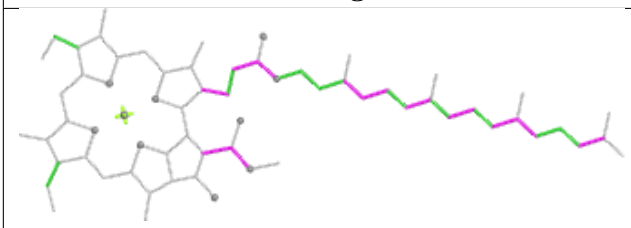
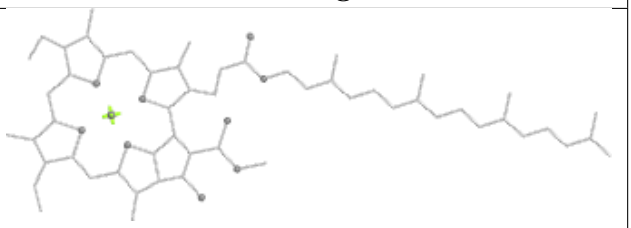
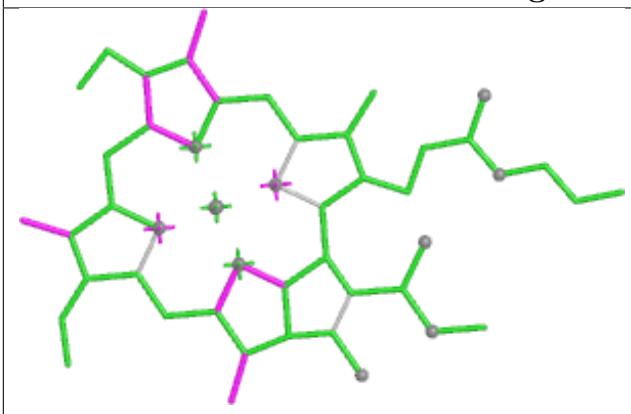
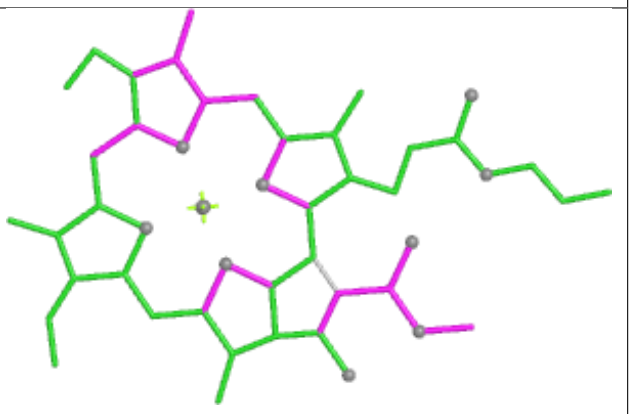
 Bond lengths	 Bond angles
 Torsions	 Rings

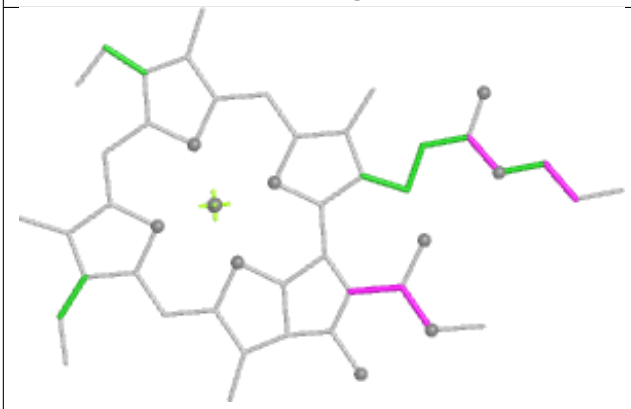
Ligand CLA a 312



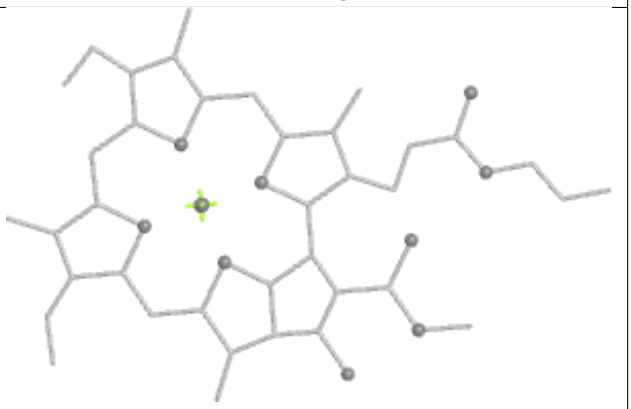
Bond lengths



Bond angles

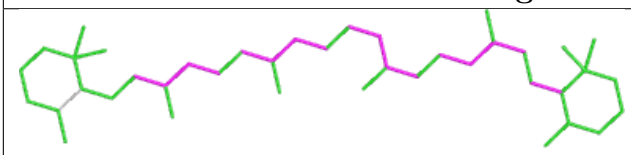


Torsions



Rings

Ligand WVN B 845



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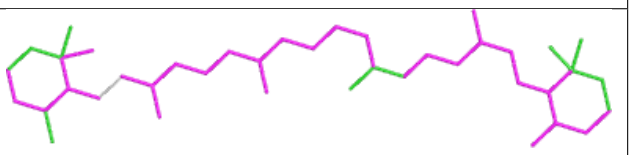

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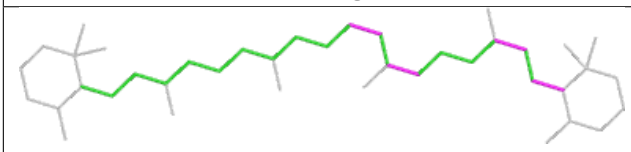

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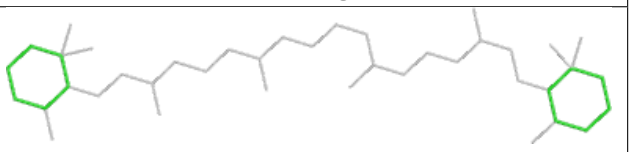
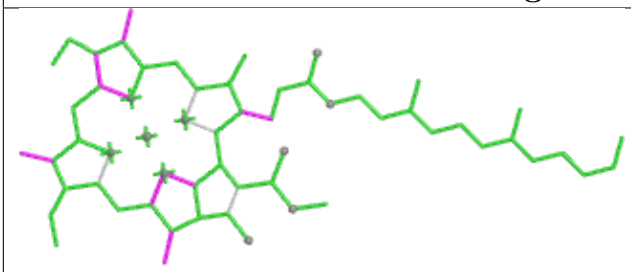
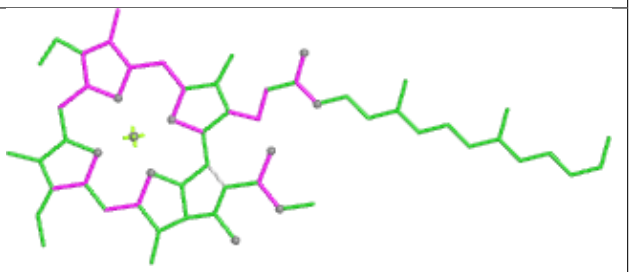


Rings

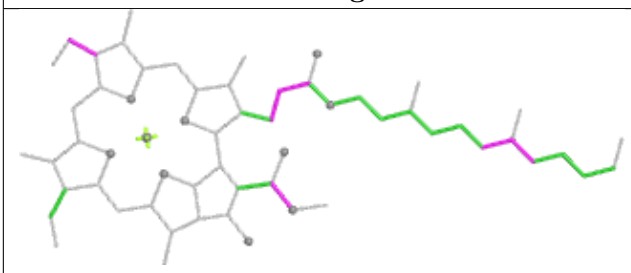
Ligand CLA B 816



Bond lengths



Bond angles



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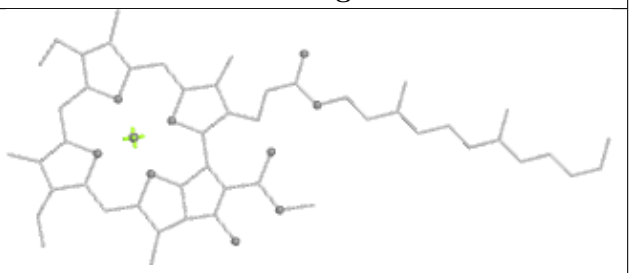
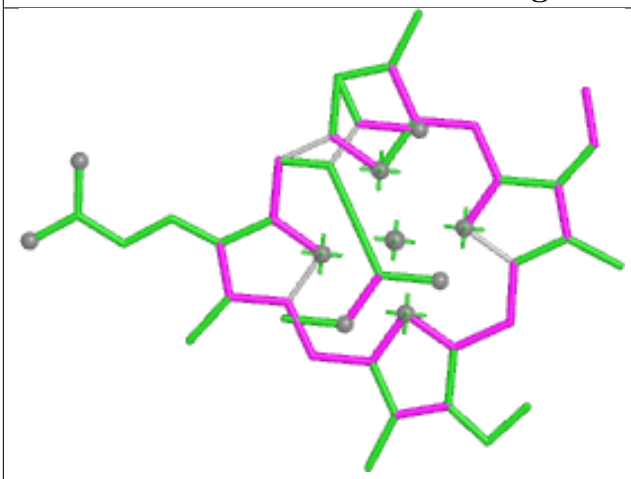


Rings

Ligand KC2 c 610



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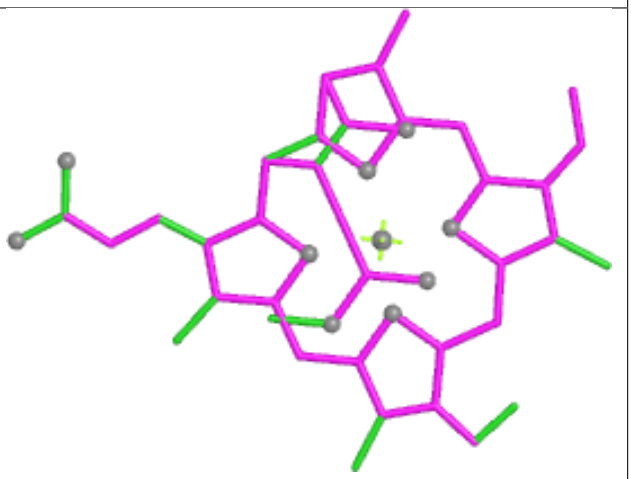

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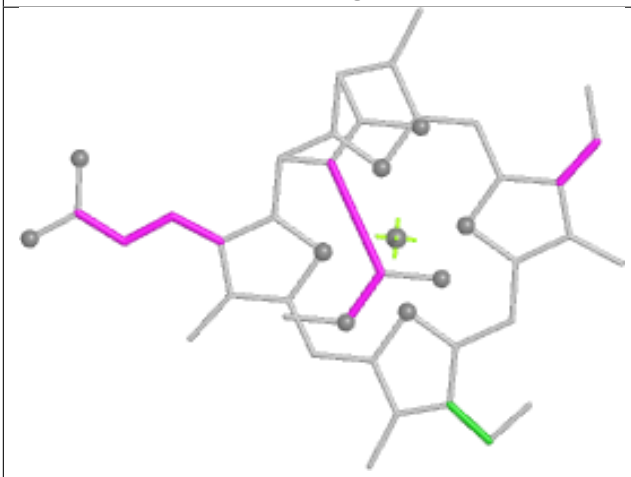
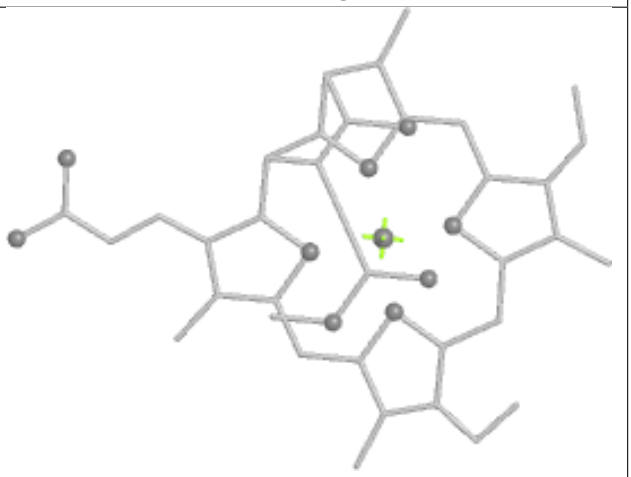
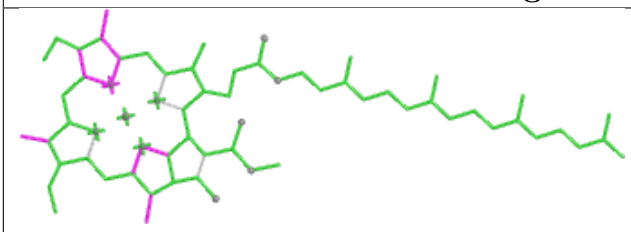


Torsions

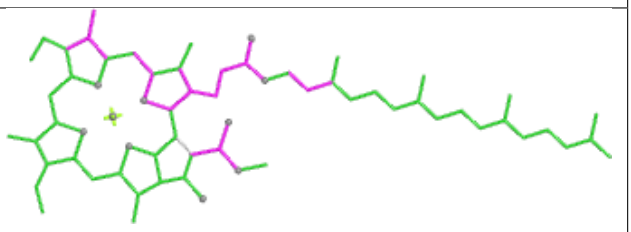


Rings

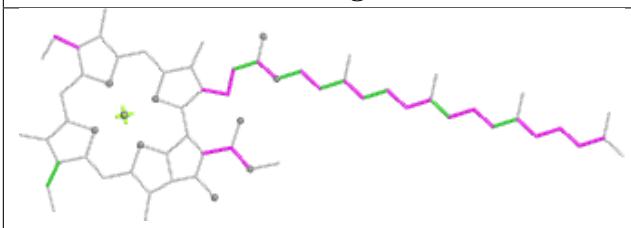
Ligand CLA A 842



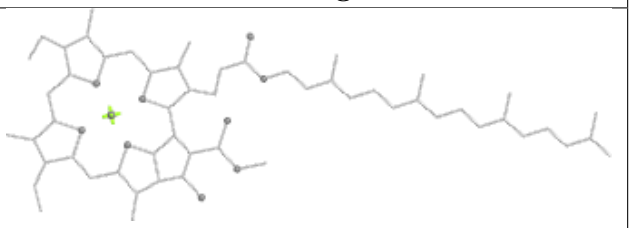
Bond lengths



Bond angles

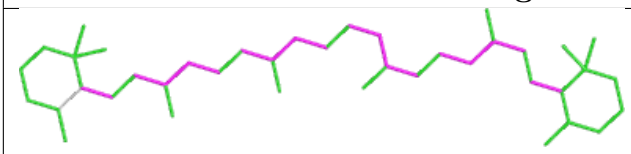


Torsions

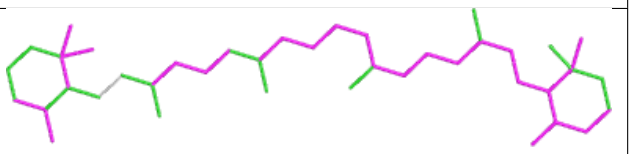


Rings

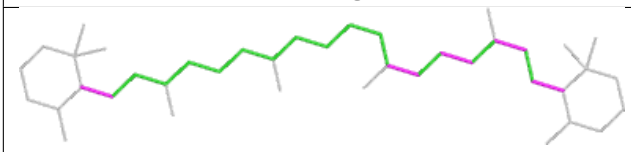
Ligand WVN A 849



Bond lengths



Bond angles



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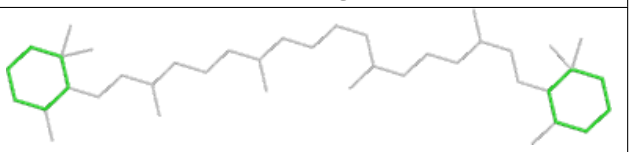
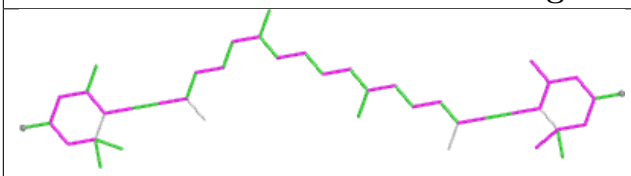


Rings

Ligand II0 i 614



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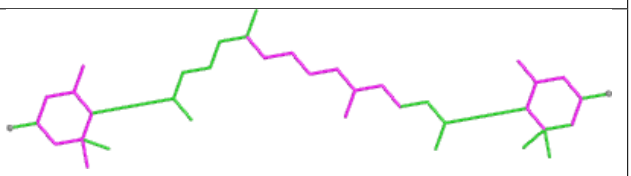
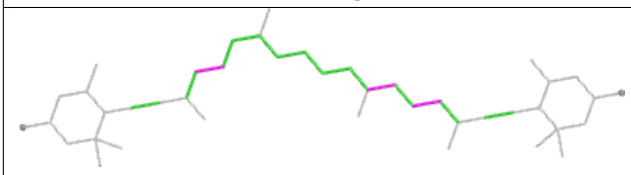


Bond angles



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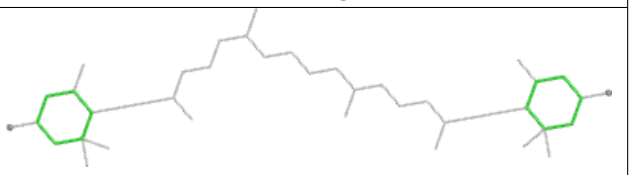
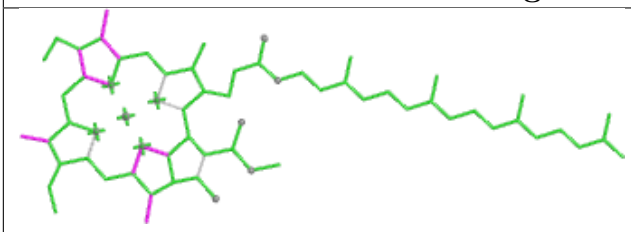


Rings

Ligand CLA A 835



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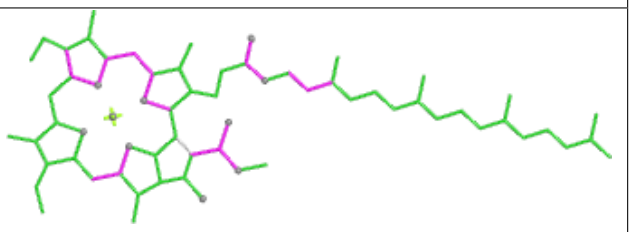
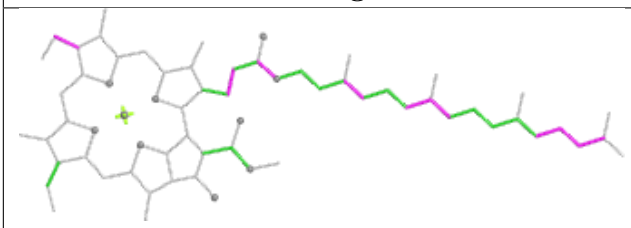


Bond angles



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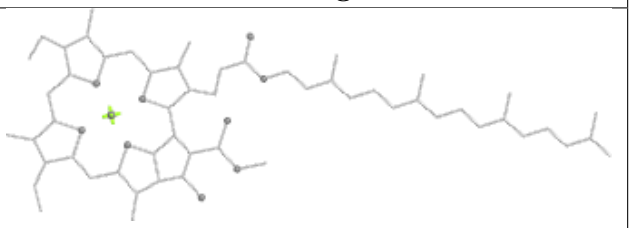
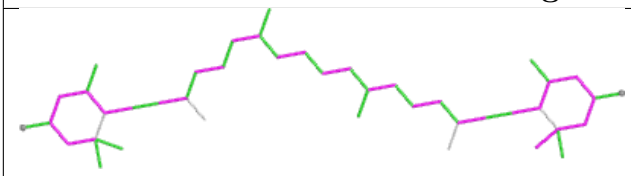


Rings

Ligand II0 b 315



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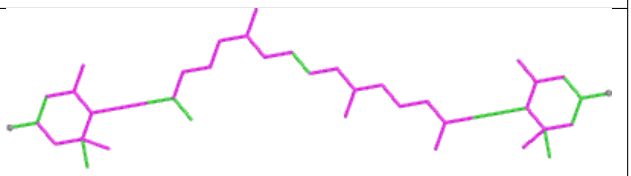
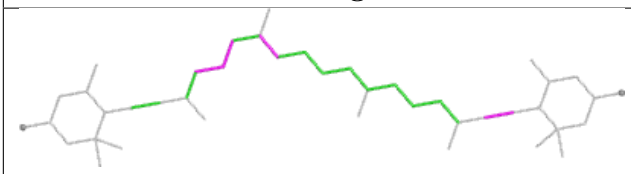


Bond angles



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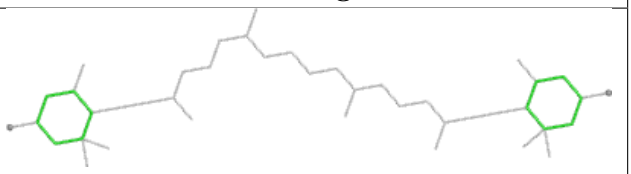
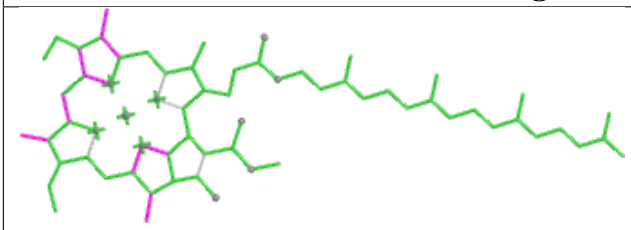


Rings

Ligand CLA I 102



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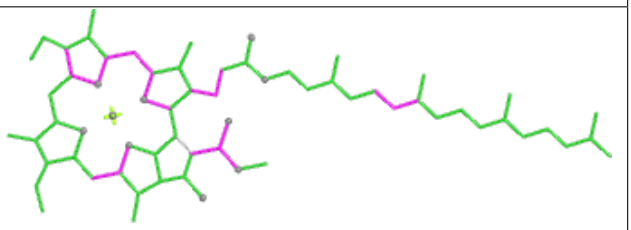

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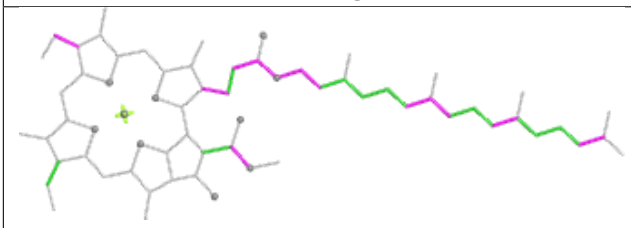

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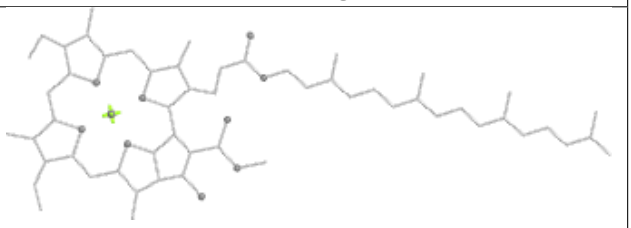
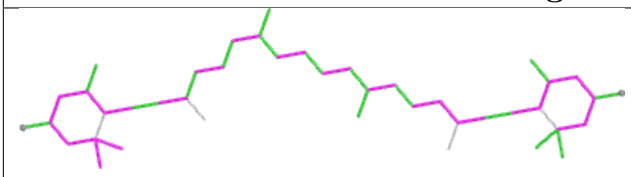


Rings

Ligand II0 j 318



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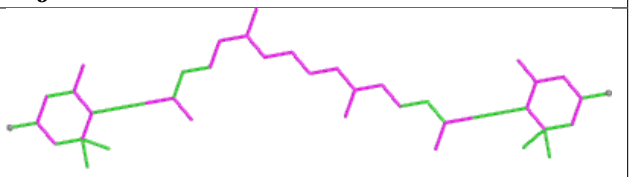
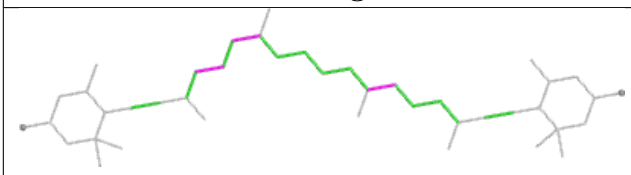


Bond angles



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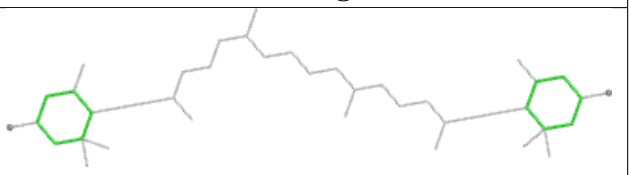
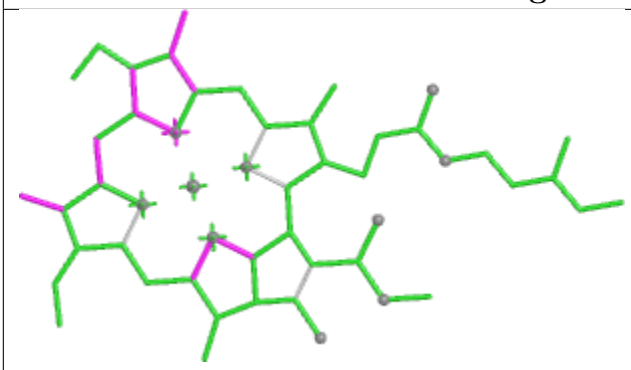


Rings

Ligand CLA c 601



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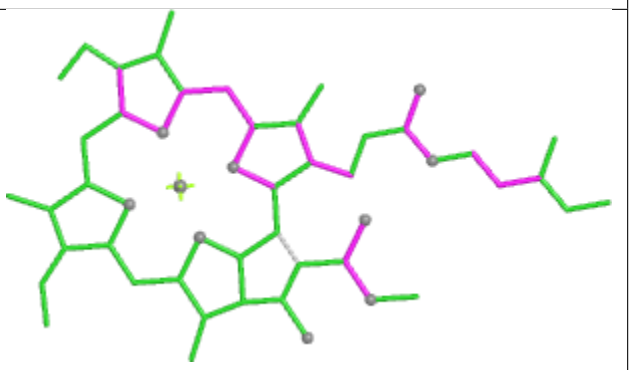

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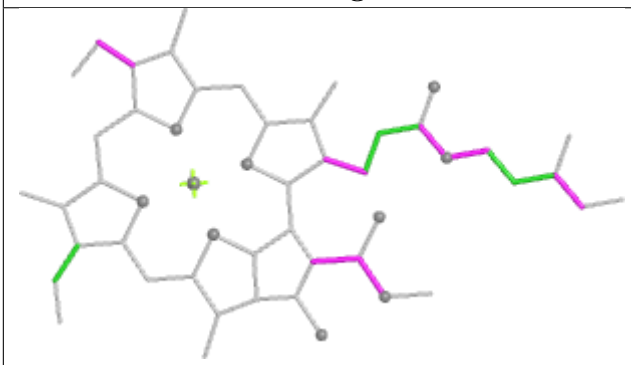

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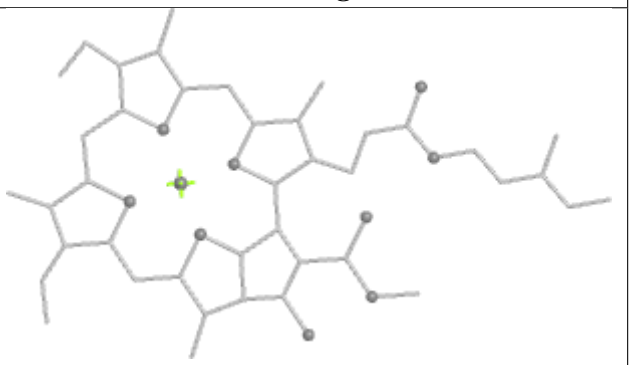
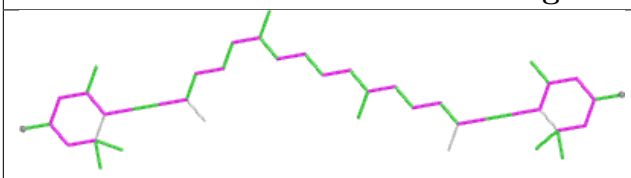


Rings

Ligand II0 J 104



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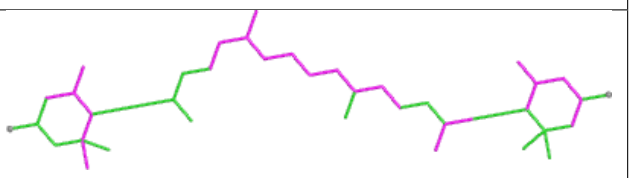
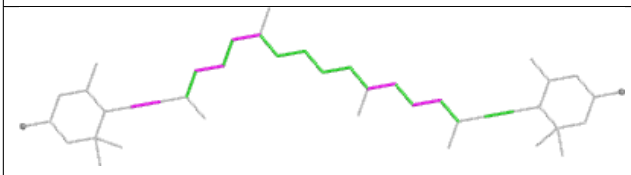


Bond angles



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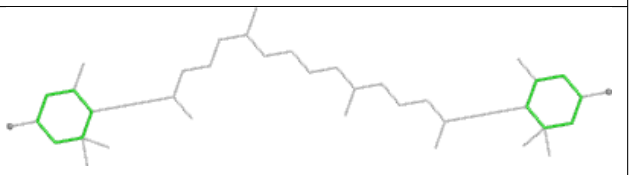
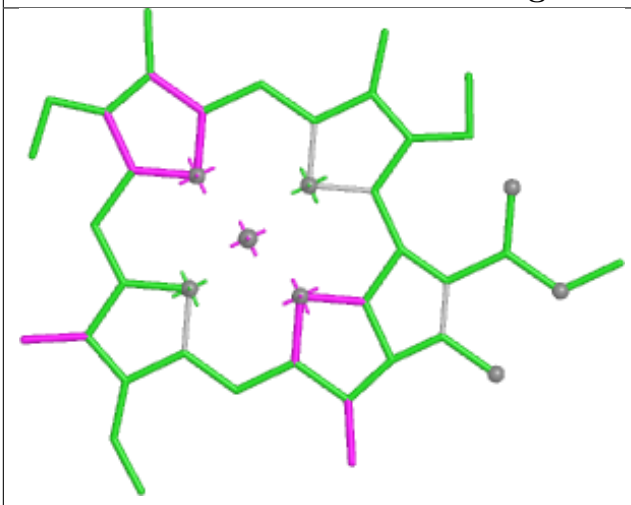


Rings

Ligand CLA g 302



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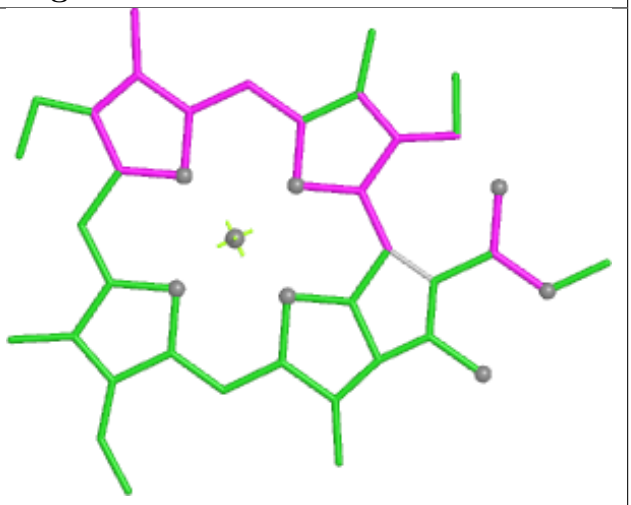

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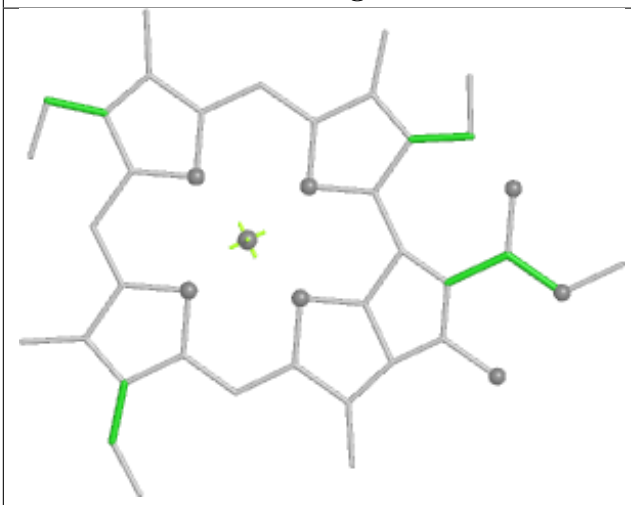
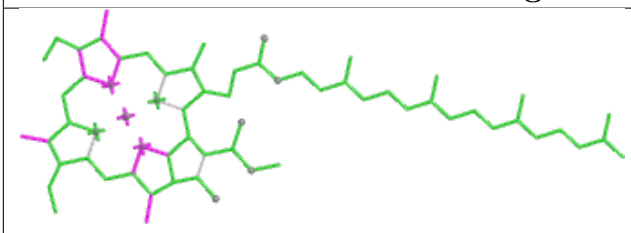


Torsions

Rings

Ligand CLA B 804



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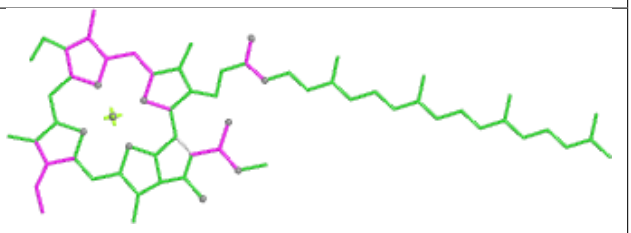
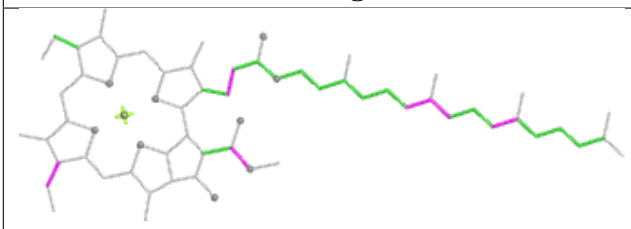


Bond angles



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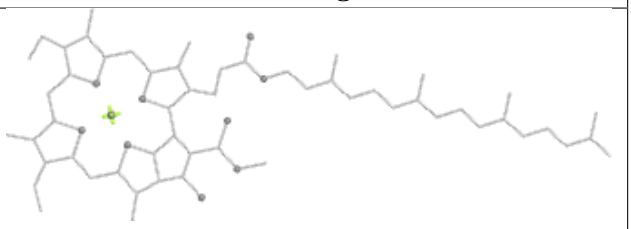
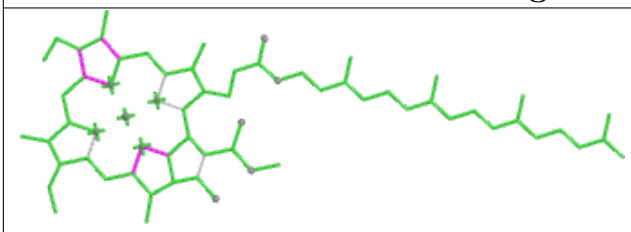
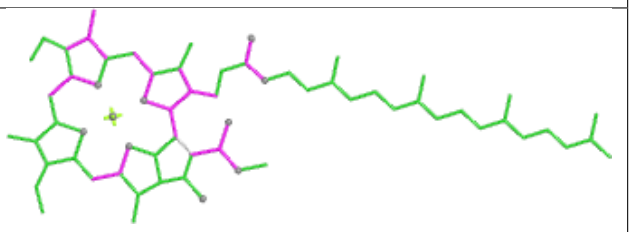
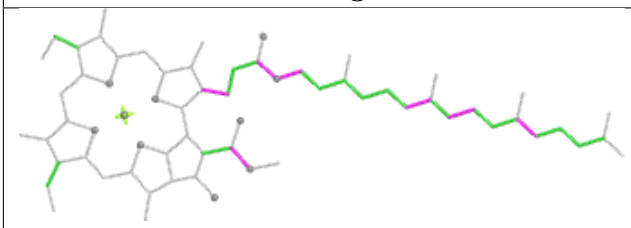
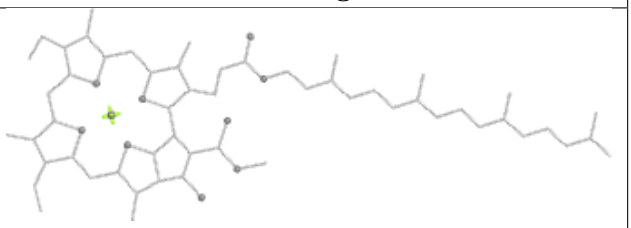
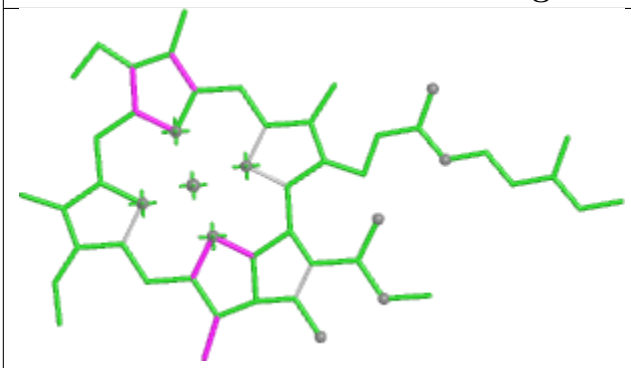
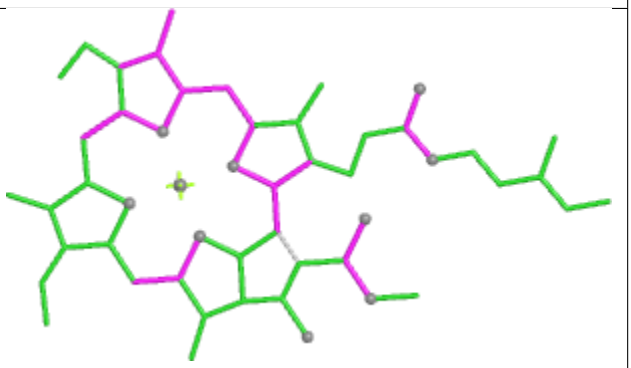
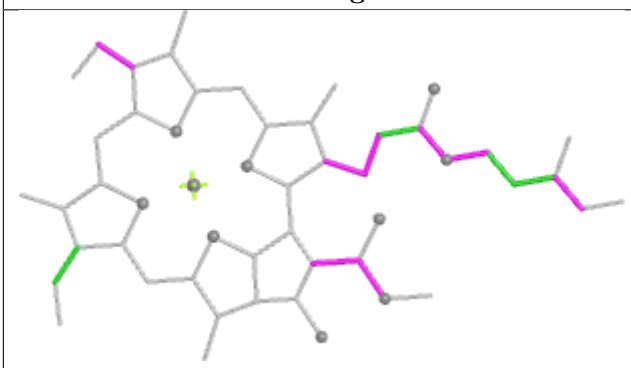
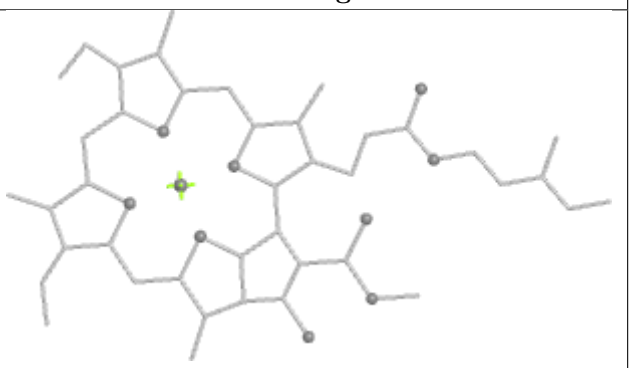
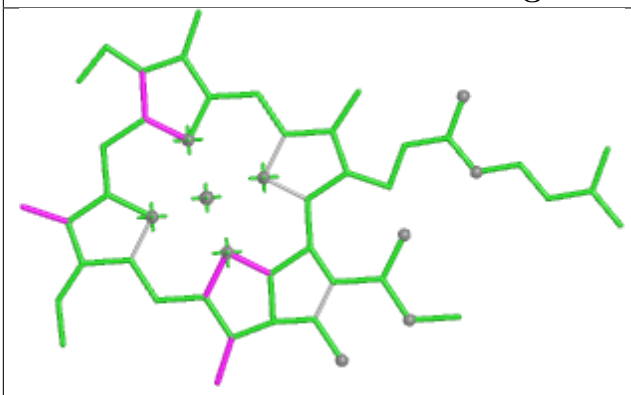
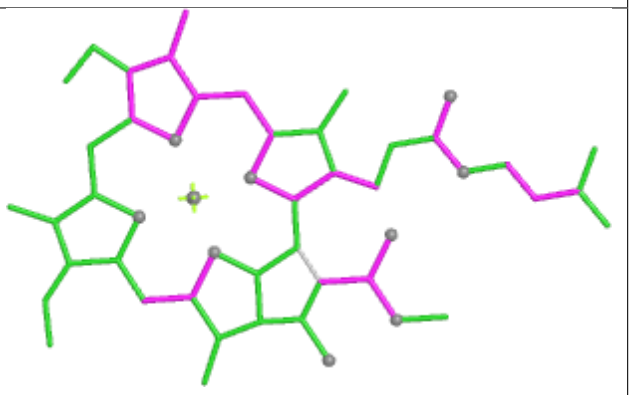
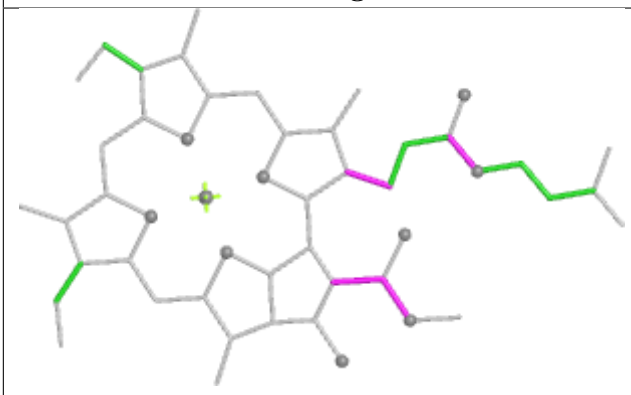
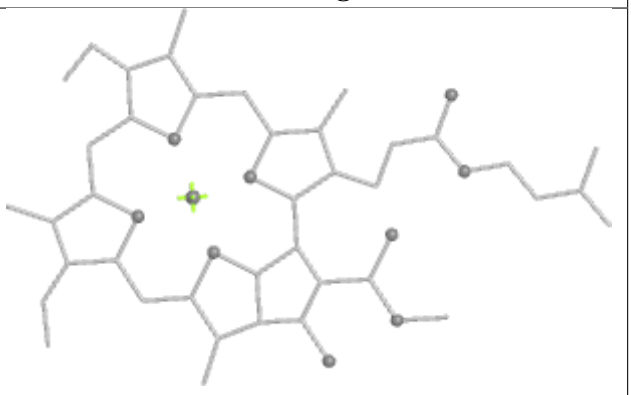
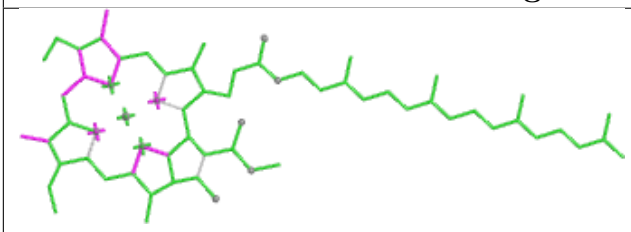
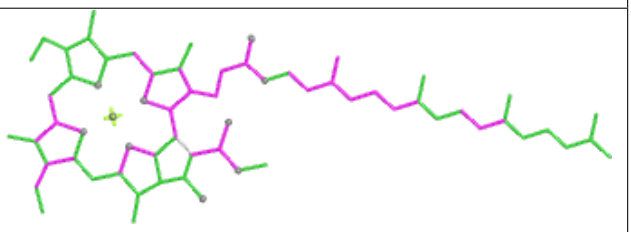
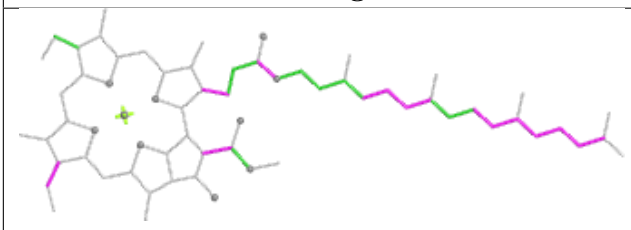
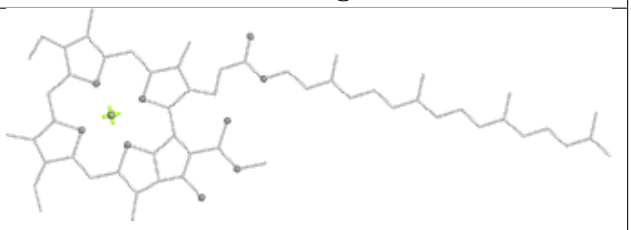


Rings

Ligand CLA c 612	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA i 611	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA A 814	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA O 205	
 Bond lengths	 Bond angles
 Torsions	 Rings

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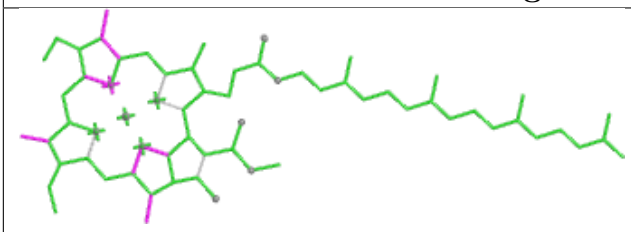
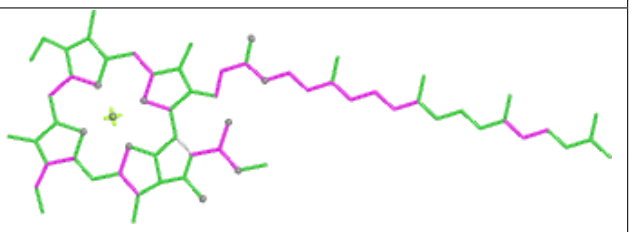
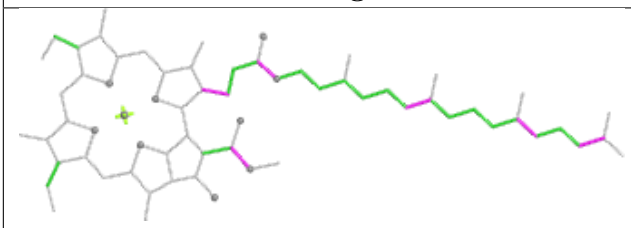
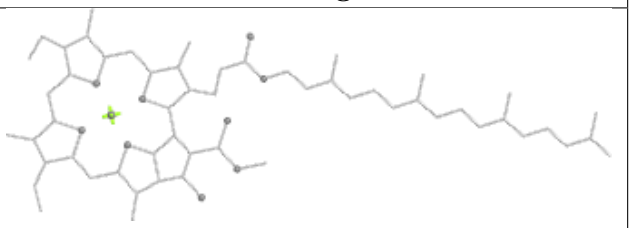
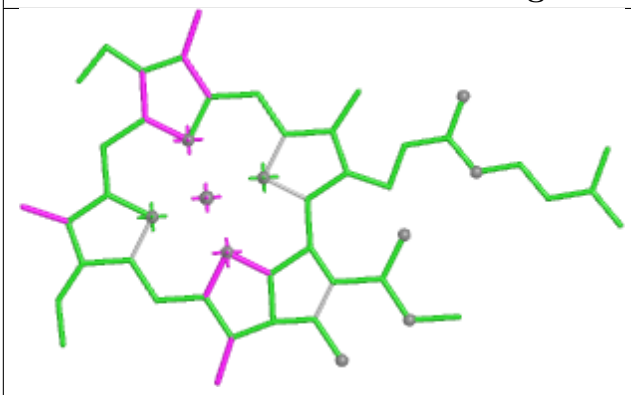
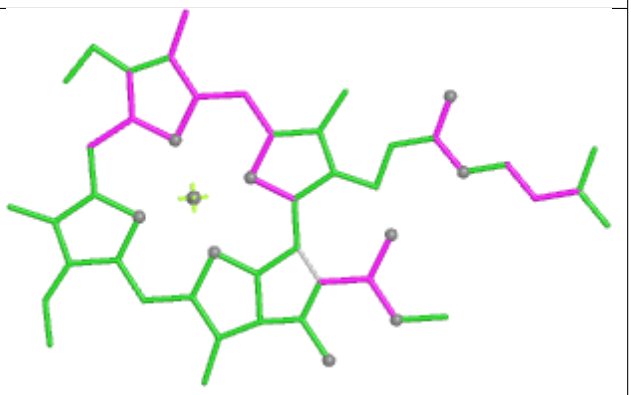
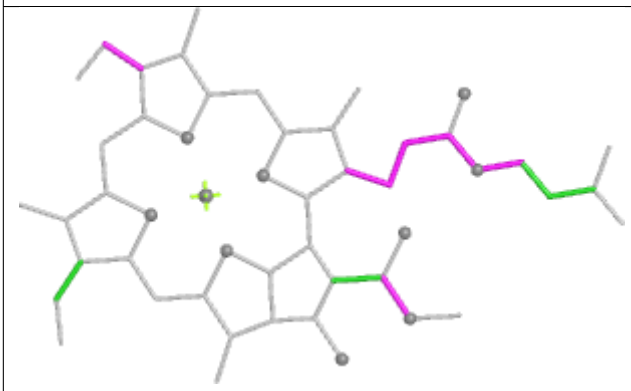
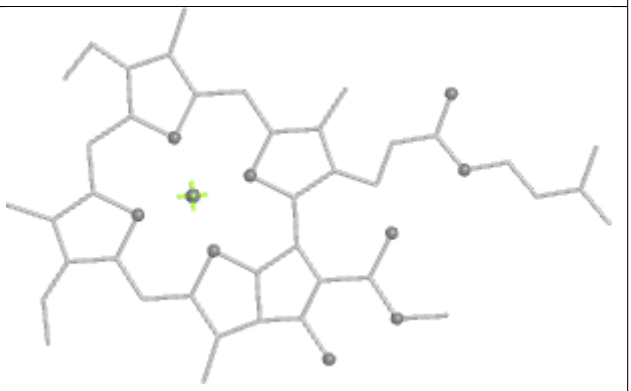
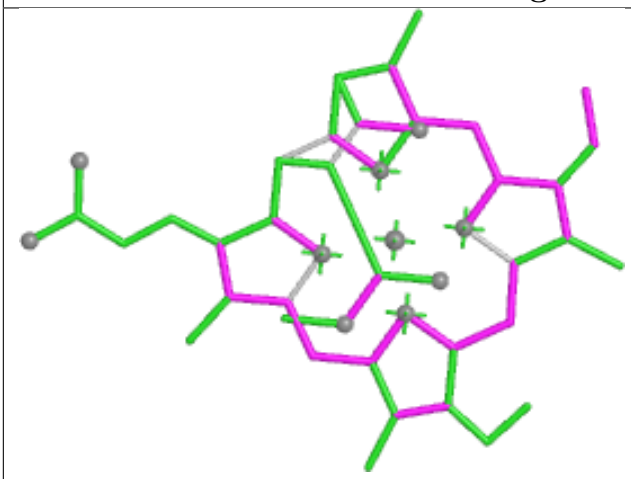
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA h 302	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand KC2 g 314



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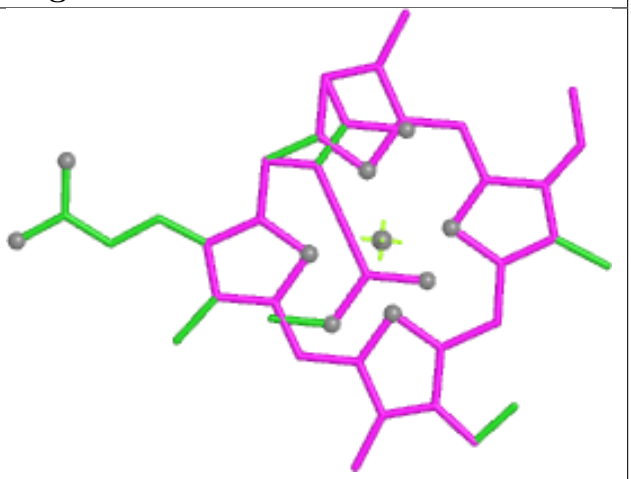

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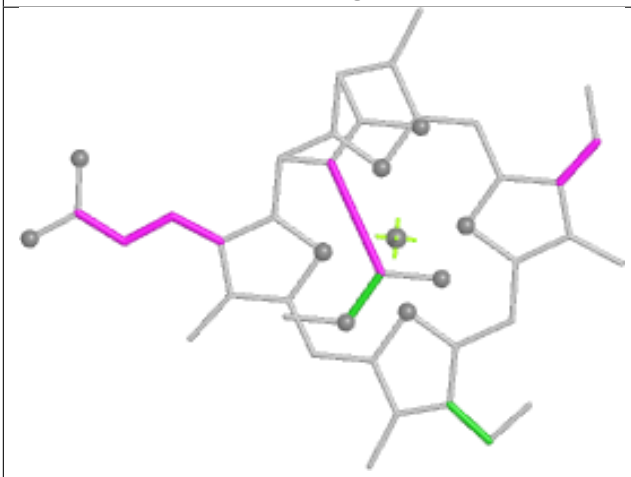

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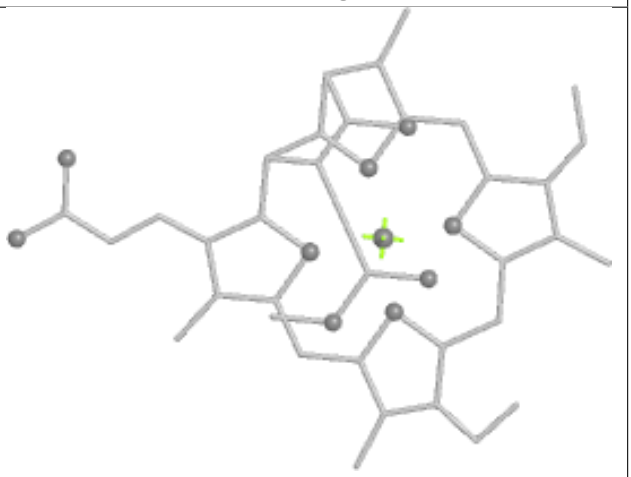
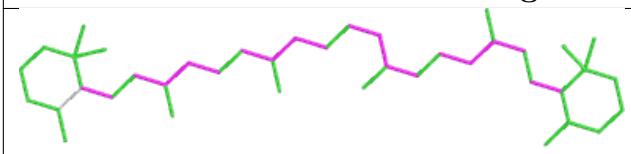


Rings

Ligand WVN e 615



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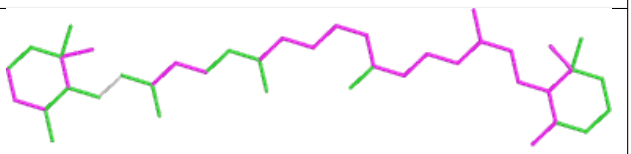

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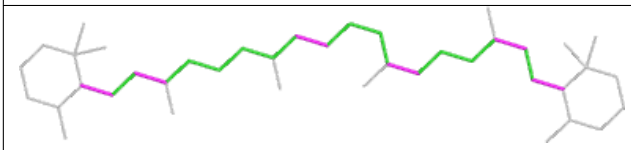

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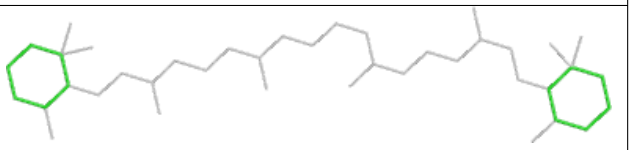
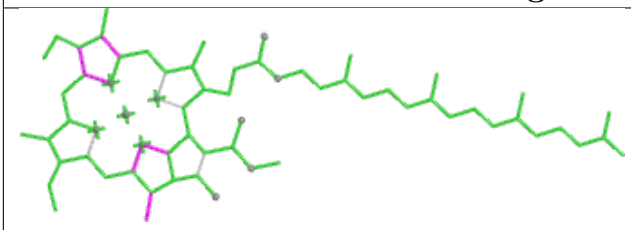
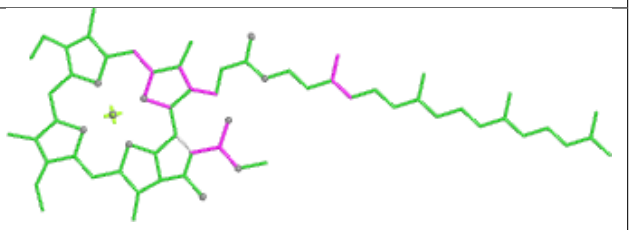
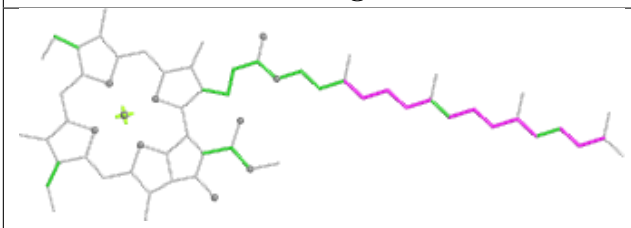
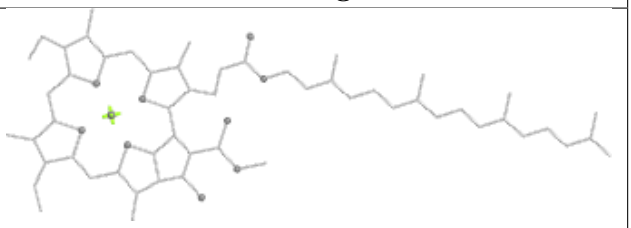


Rings

Ligand CLA b 305	
 Bond lengths	 Bond angles
 Torsions	 Rings

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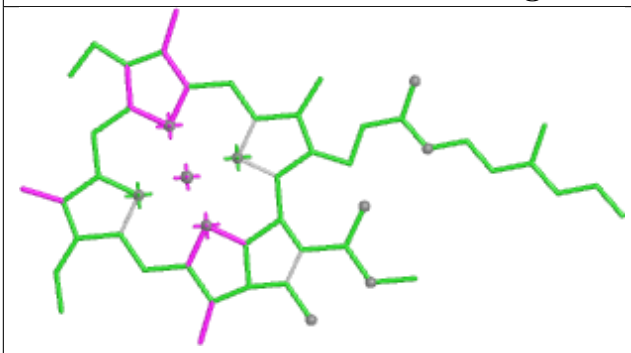
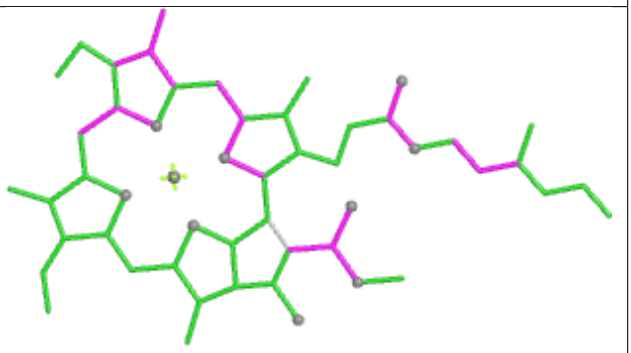
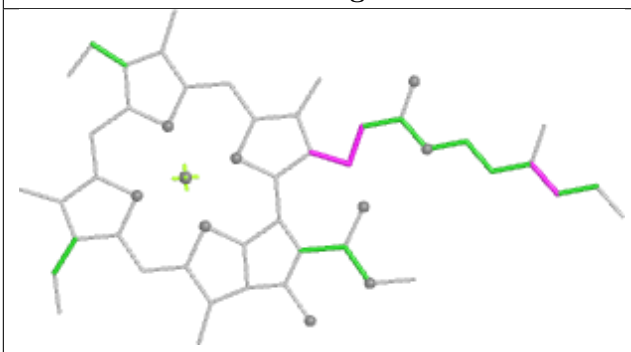
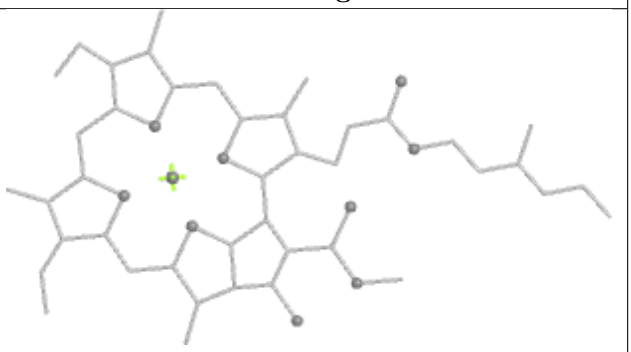
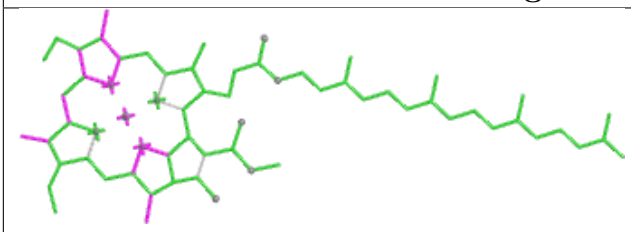
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA B 825



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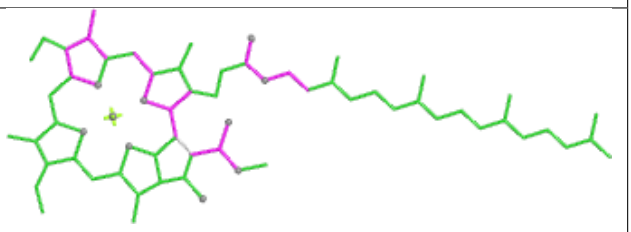
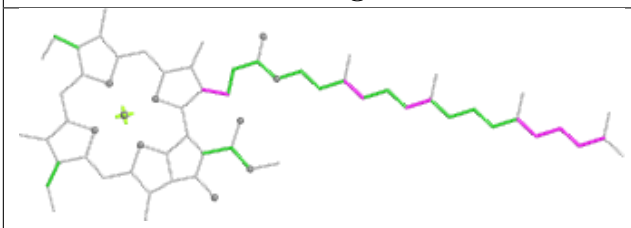


Bond angles



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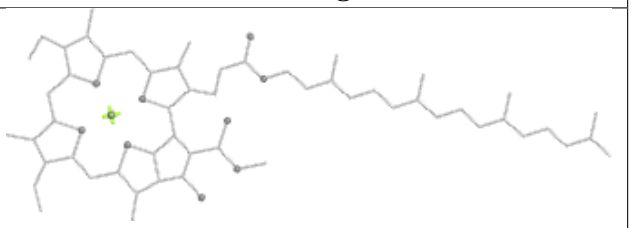
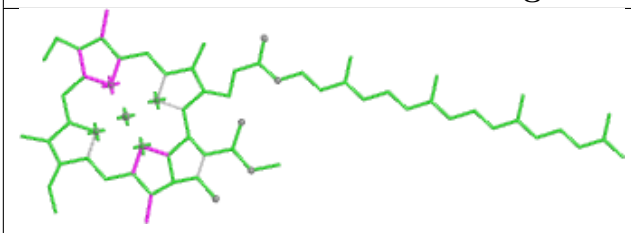


Rings

Ligand CLA A 818



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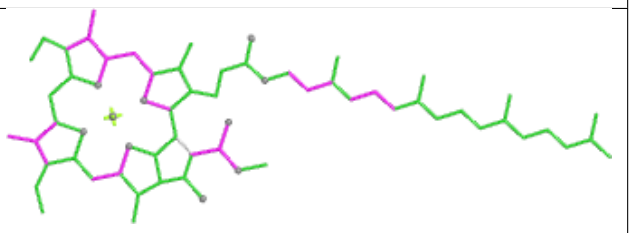

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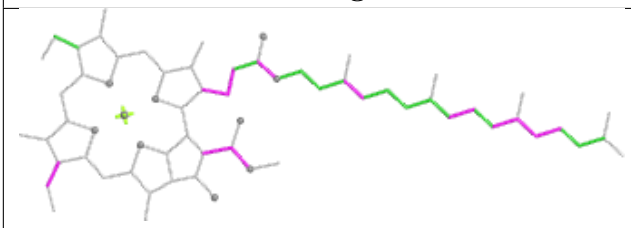

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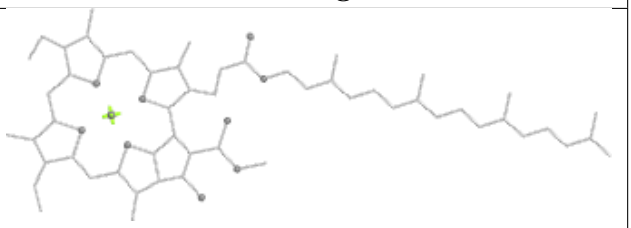
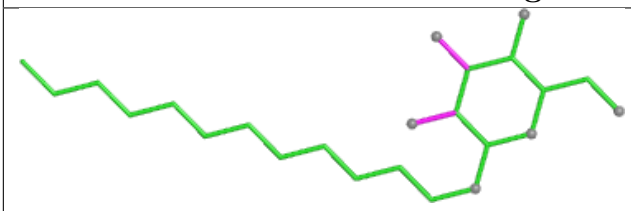


Rings

Ligand LMT b 319



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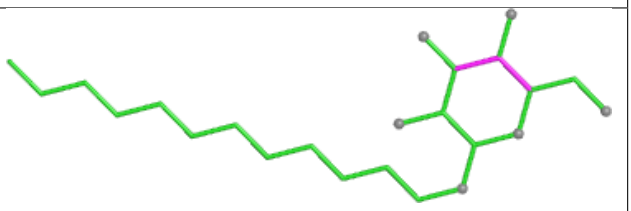

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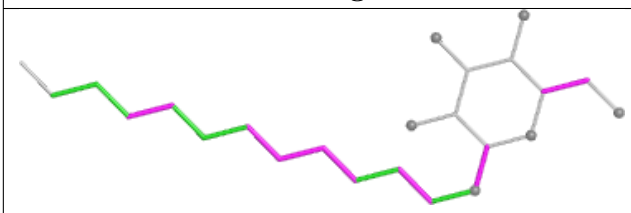

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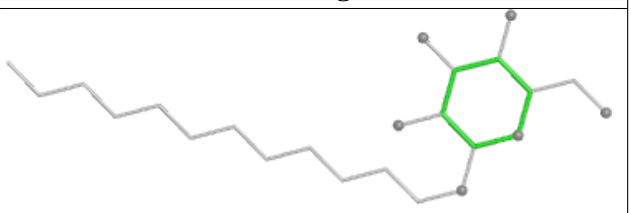
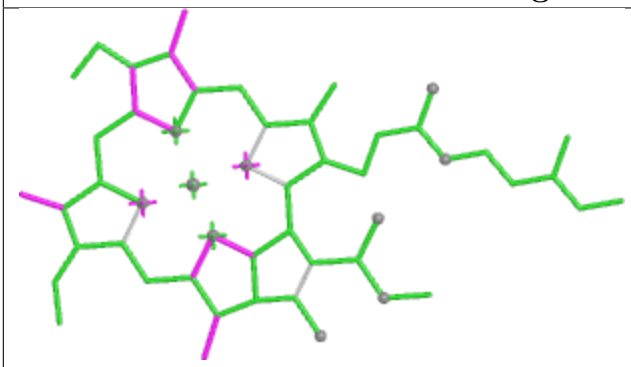
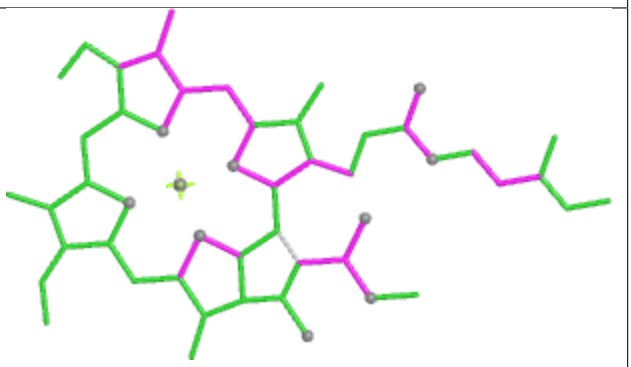
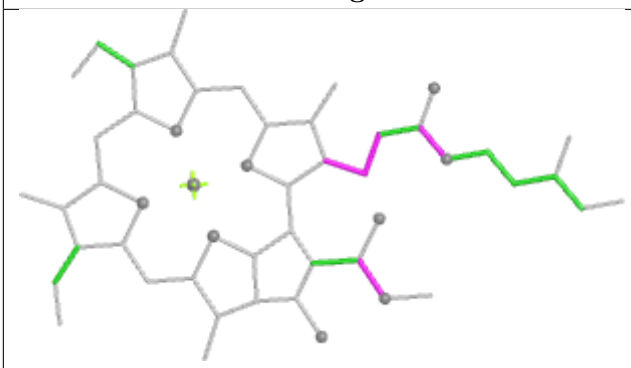
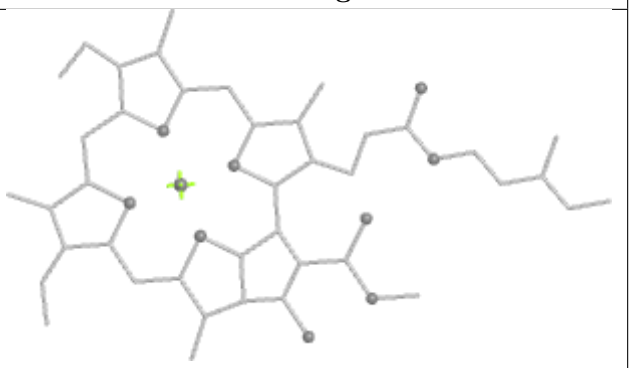


Rings

Ligand CLA f 612	
 Bond lengths	 Bond angles
 Torsions	 Rings

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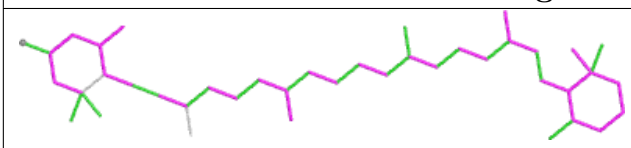
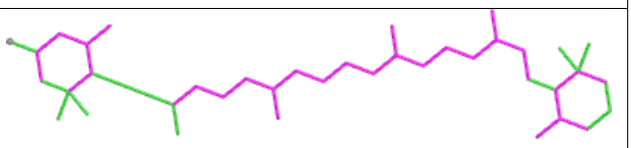
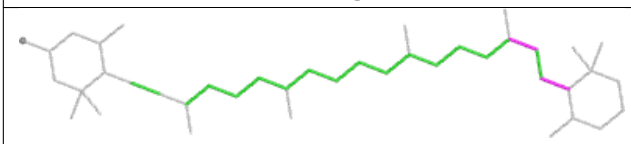
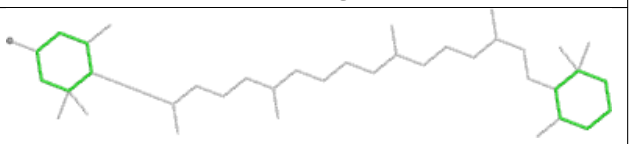
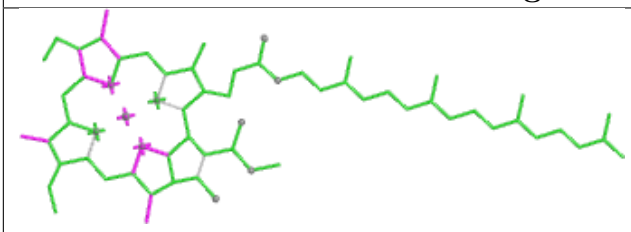
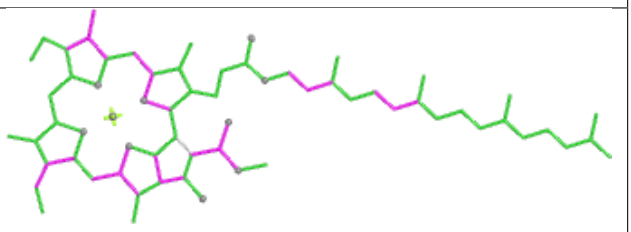
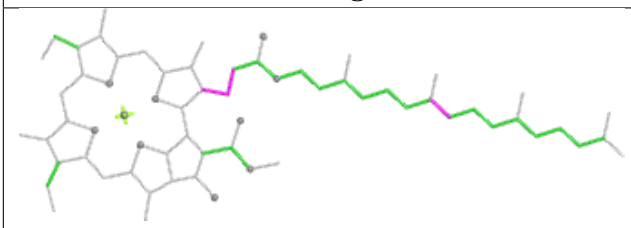
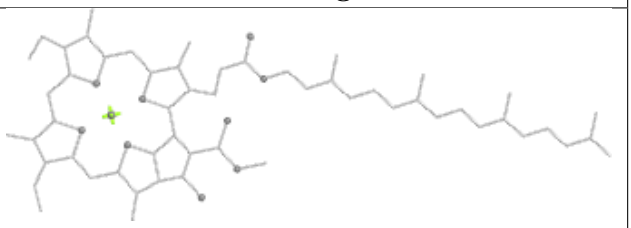
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA A 852	
 Bond lengths	 Bond angles
 Torsions	 Rings

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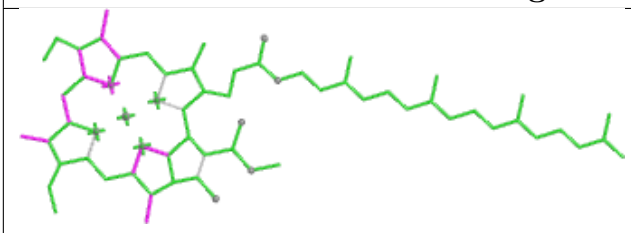
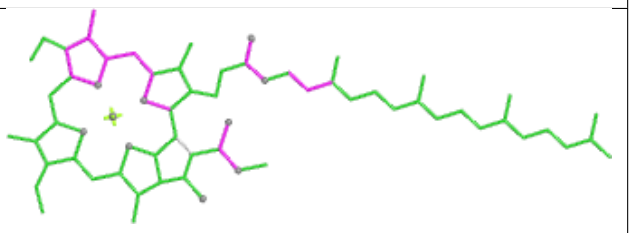
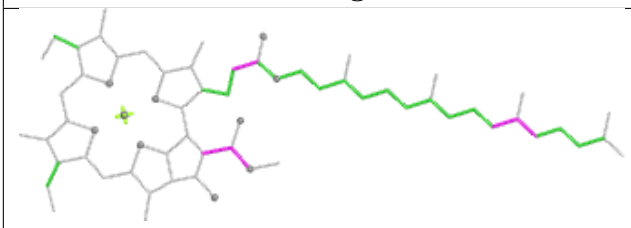
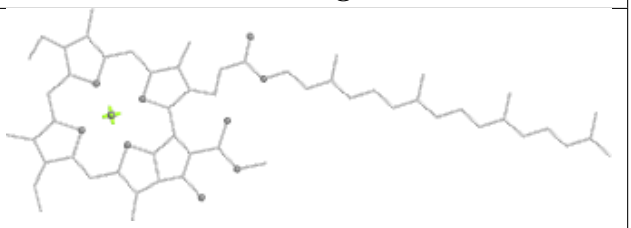
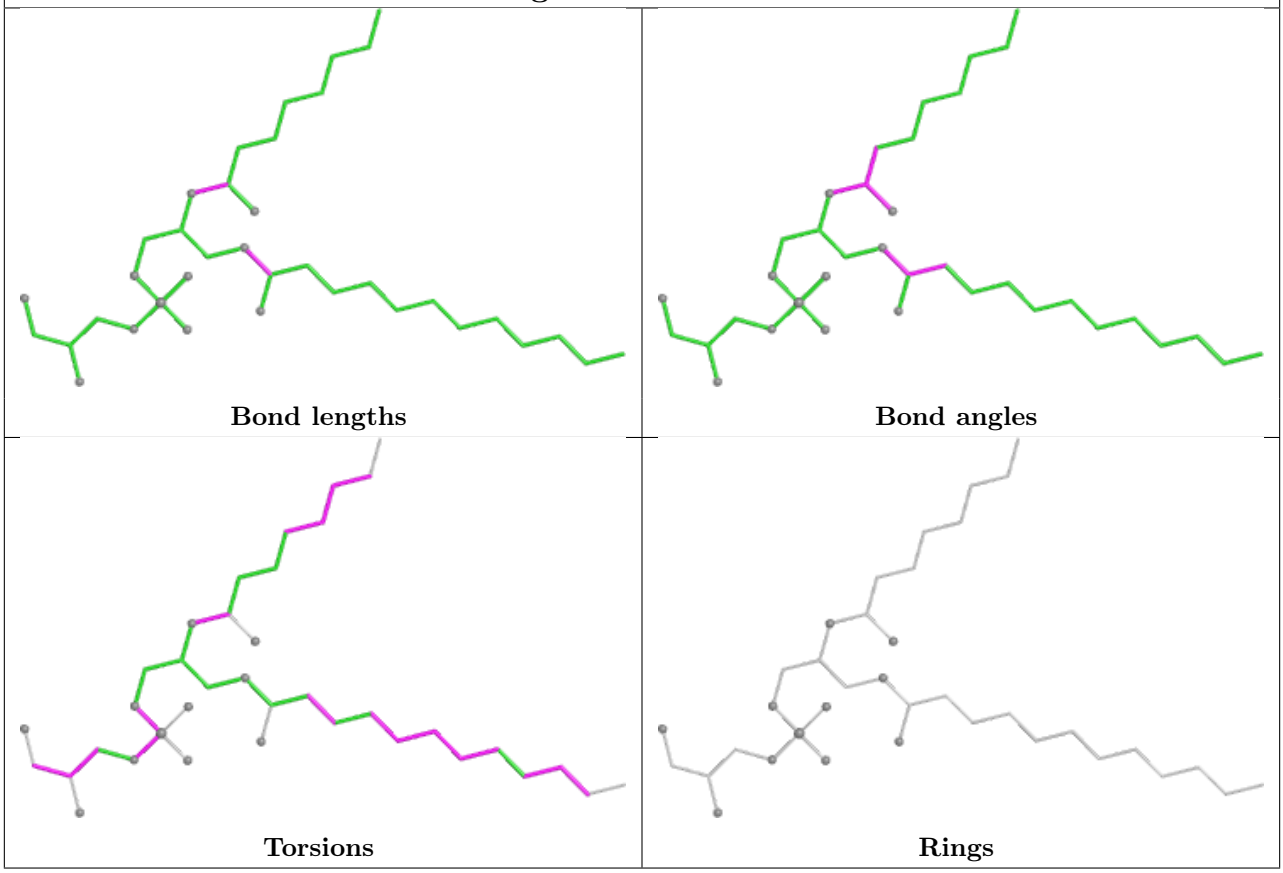
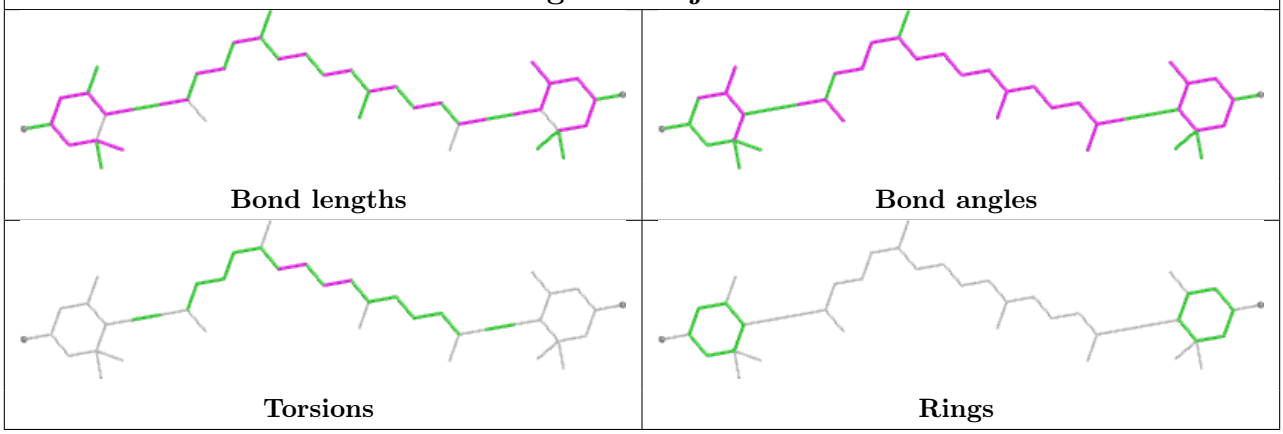
 Bond lengths	 Bond angles
 Torsions	 Rings

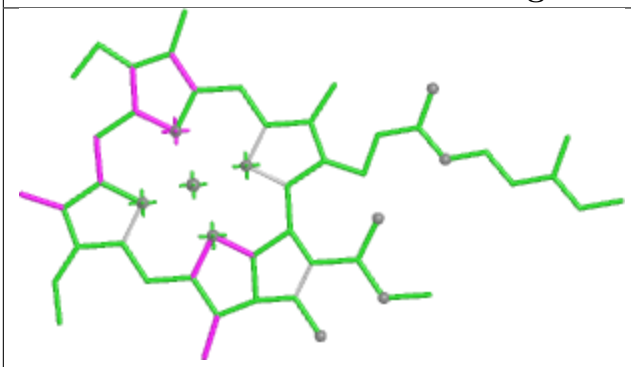
Ligand LHG f 619



Ligand II0 j 316



Ligand CLA b 311



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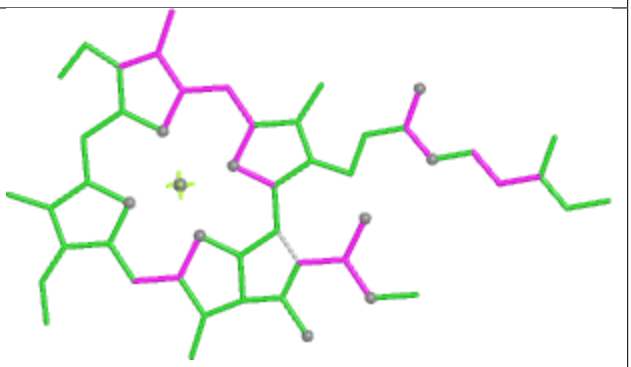

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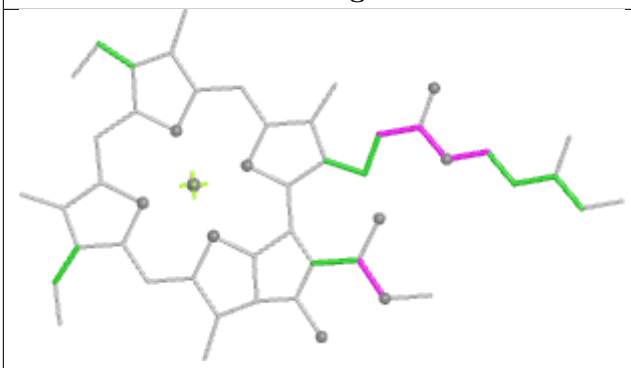

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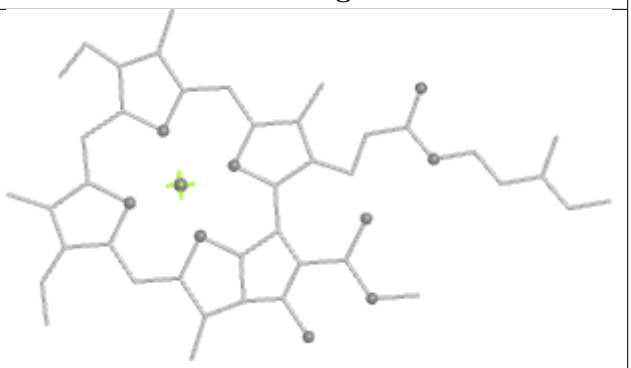
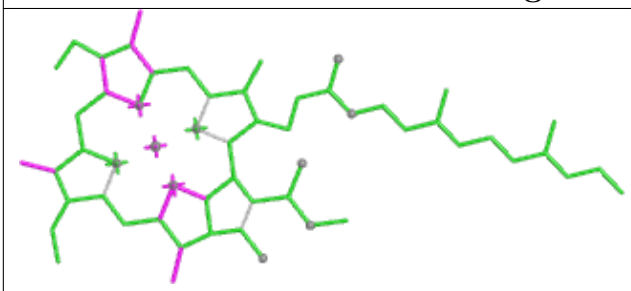


Rings

Ligand CLA B 838



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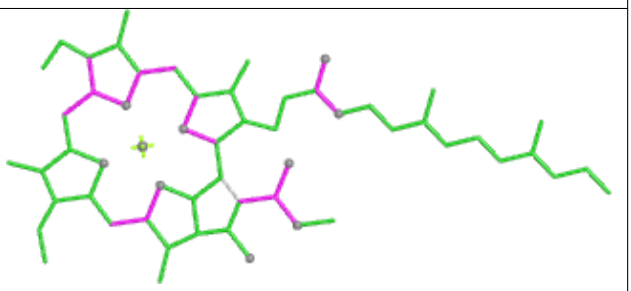

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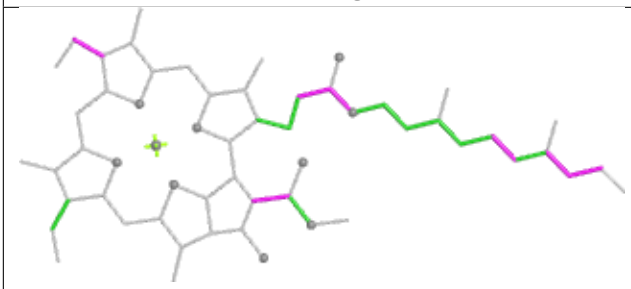

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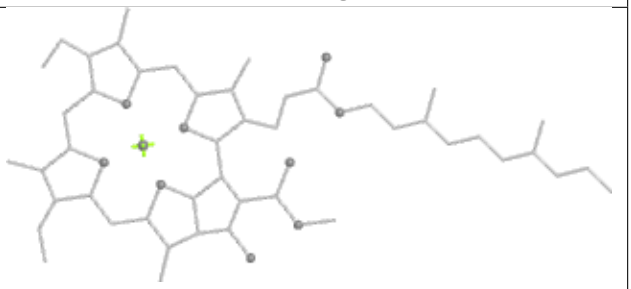
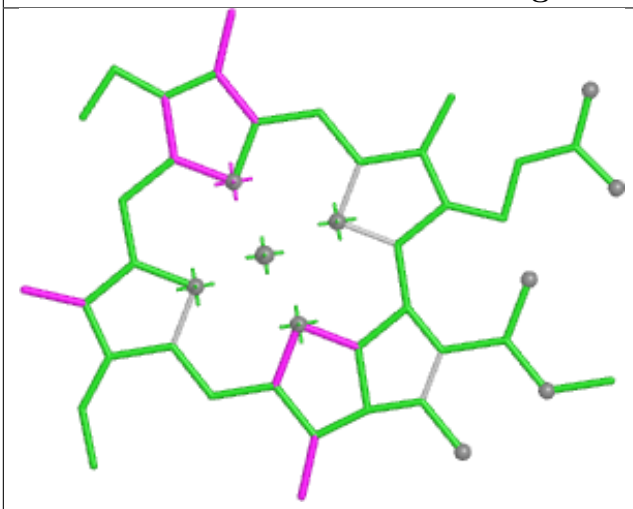


Rings

Ligand CLA f 605



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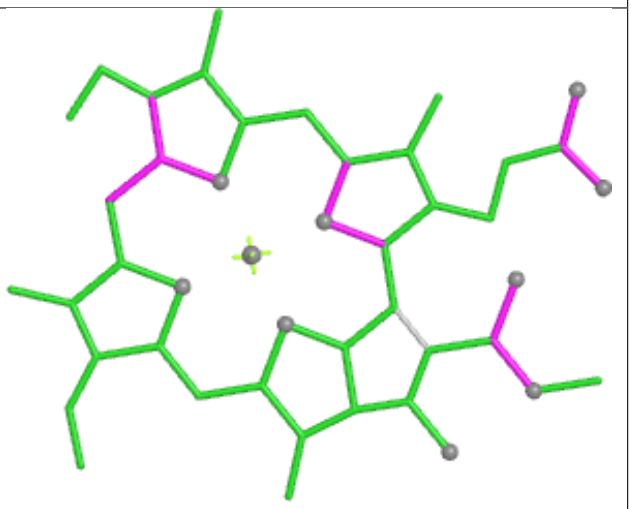

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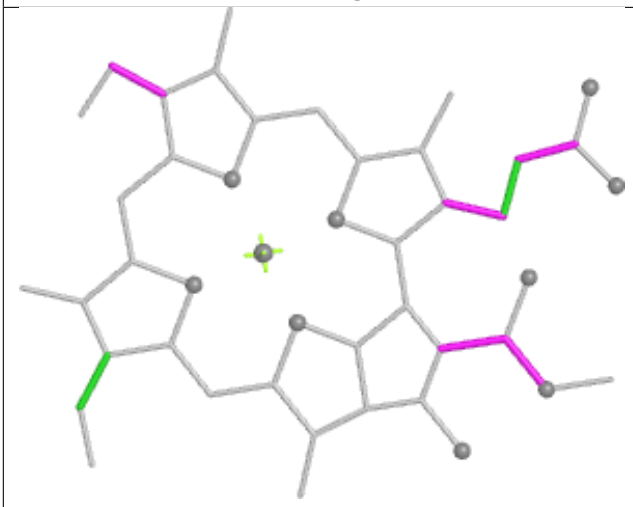
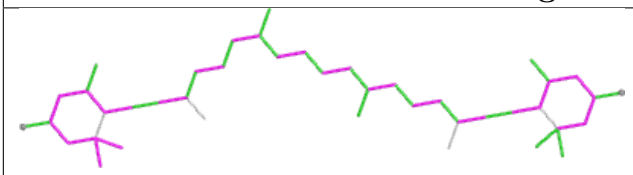


Torsions

Rings

Ligand II0 O 202



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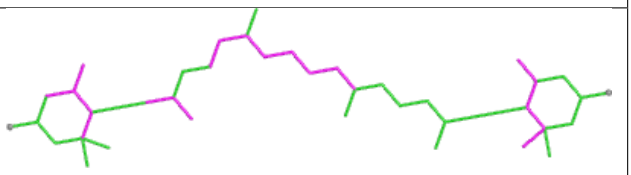

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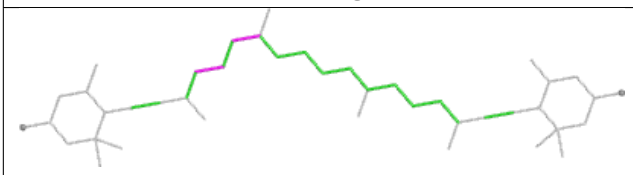

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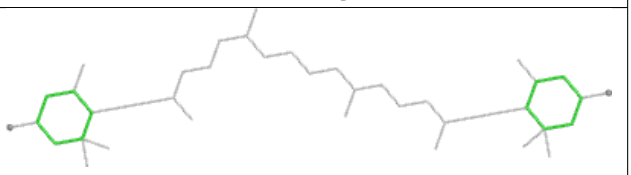
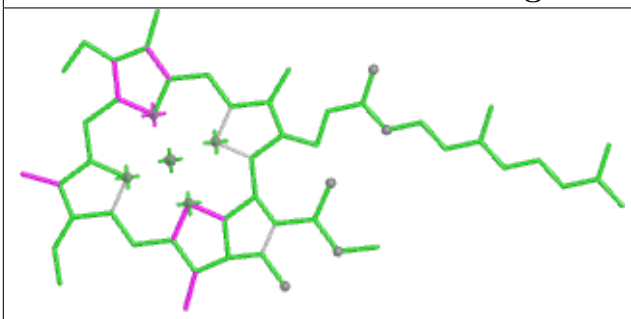


Rings

Ligand CLA B 820



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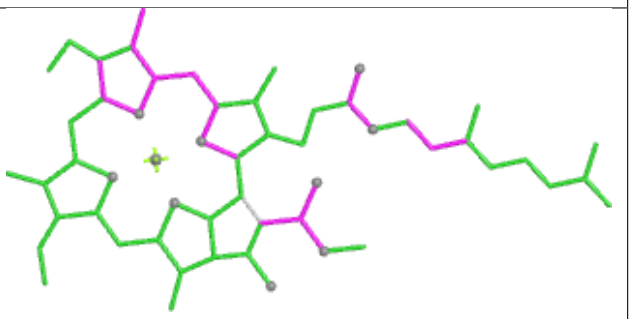

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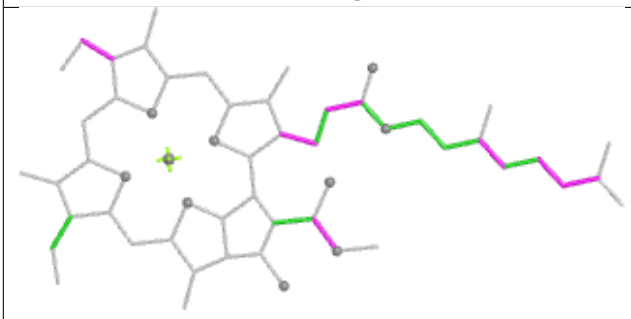

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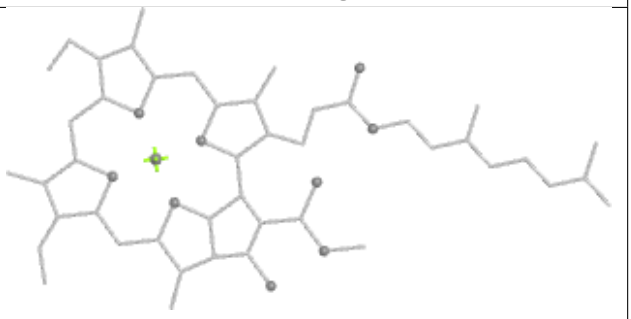
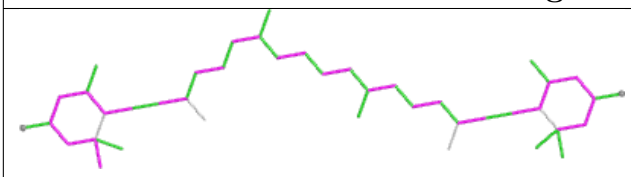


Rings

Ligand II0 f 615



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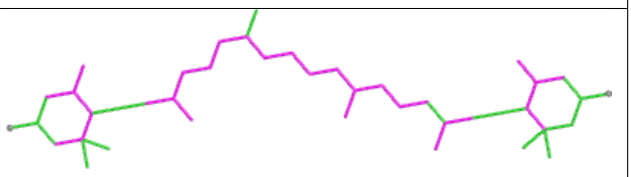

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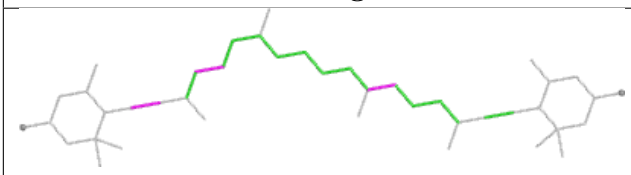

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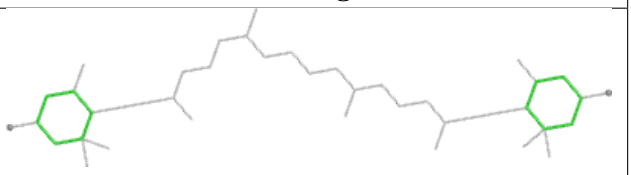
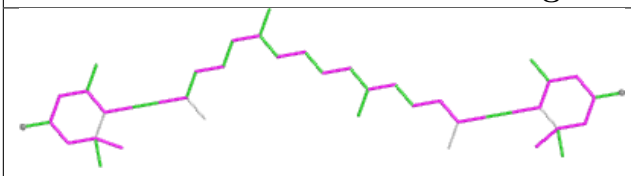


Rings

Ligand II0 g 317



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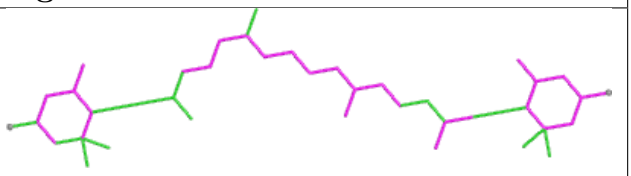

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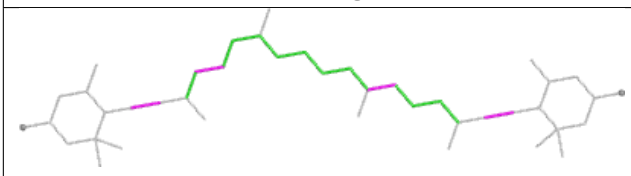

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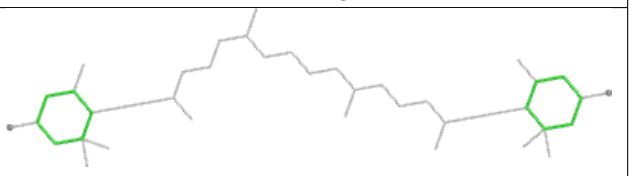

Rings

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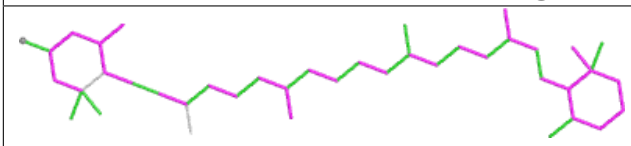
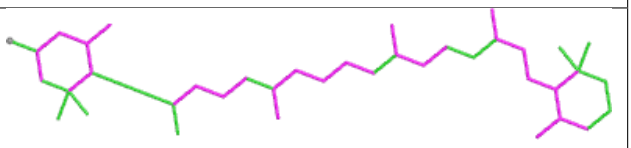
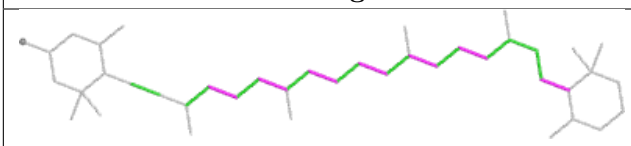
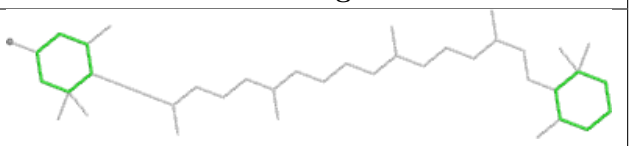
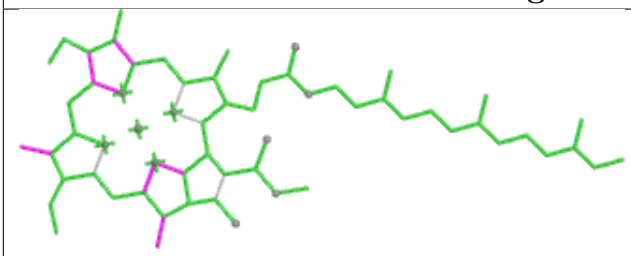
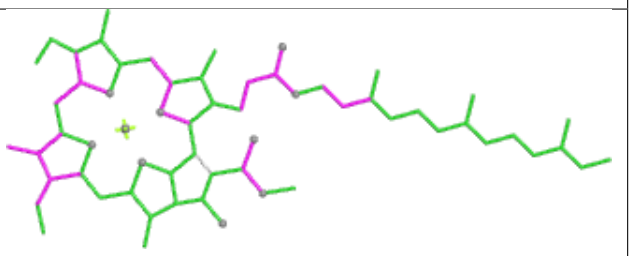
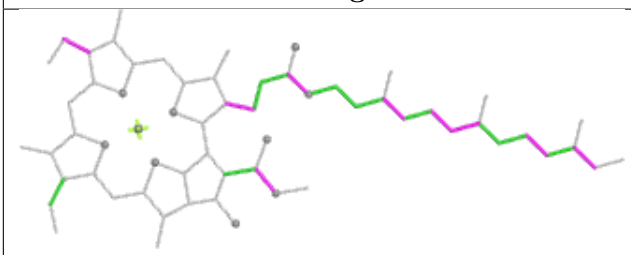
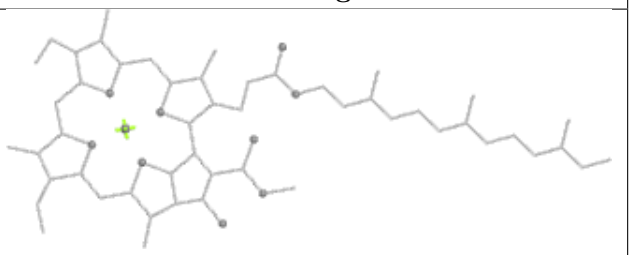
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA b 308	
 Bond lengths	 Bond angles
 Torsions	 Rings

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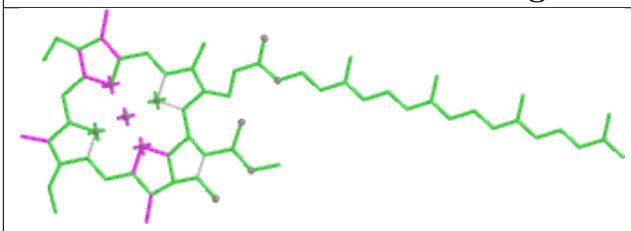
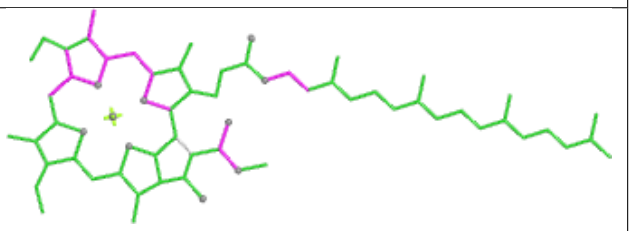
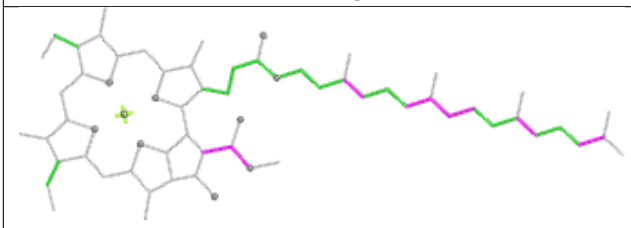
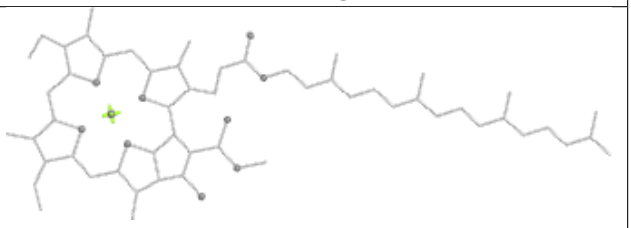
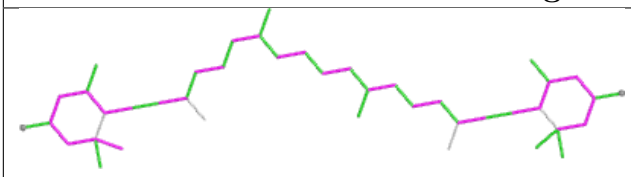
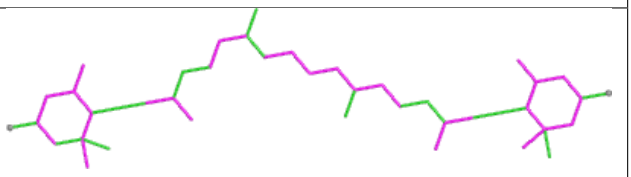
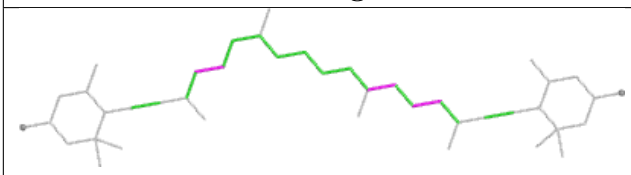
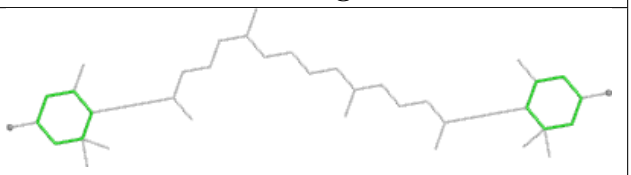
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand II0 e 612	
 Bond lengths	 Bond angles
 Torsions	 Rings

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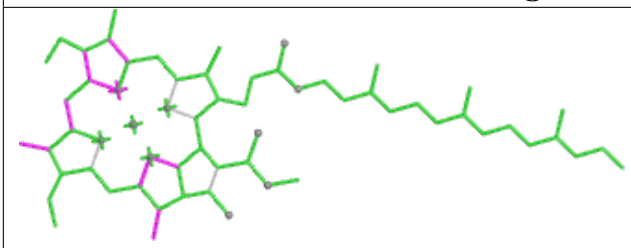
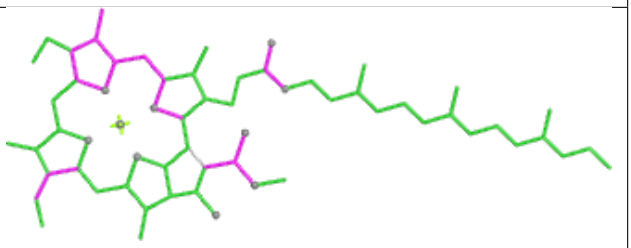
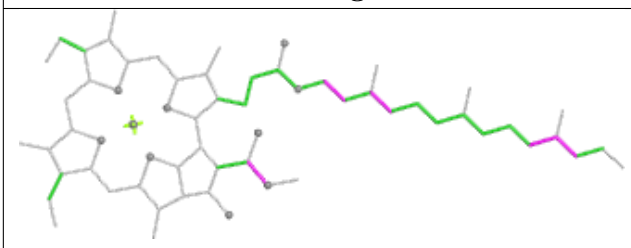
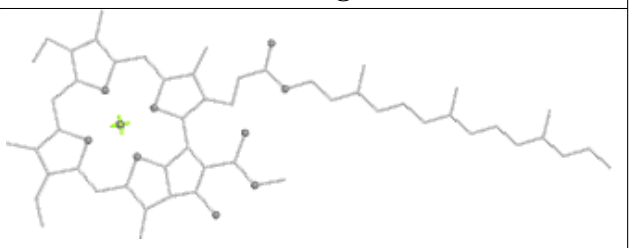
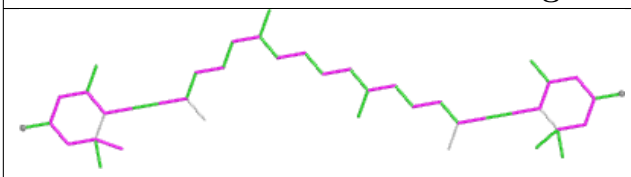
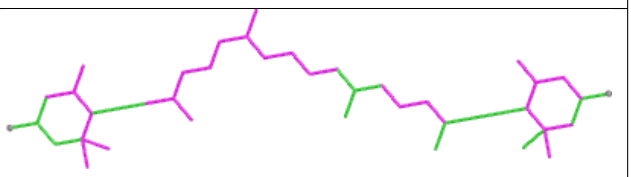
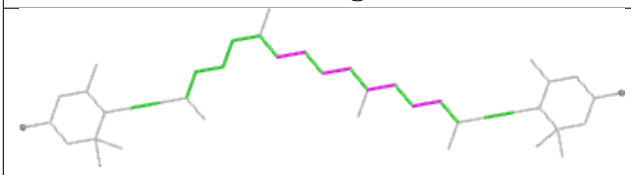
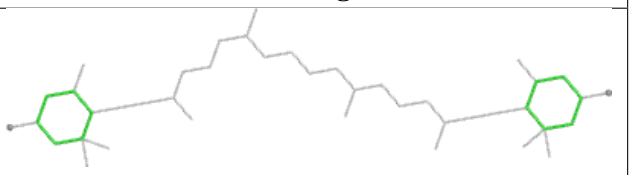
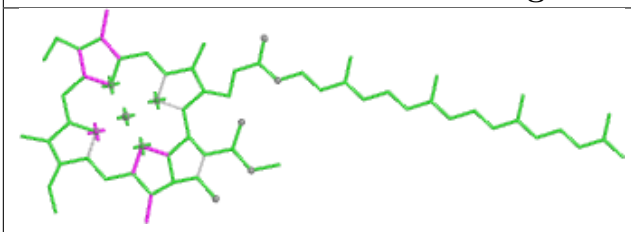
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand II0 k 615	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA b 313



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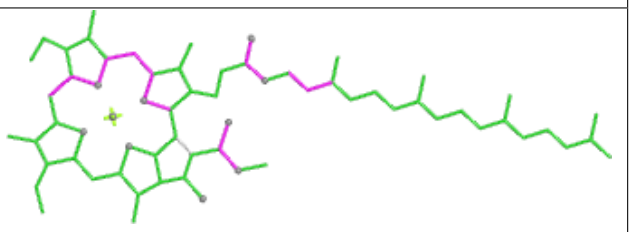
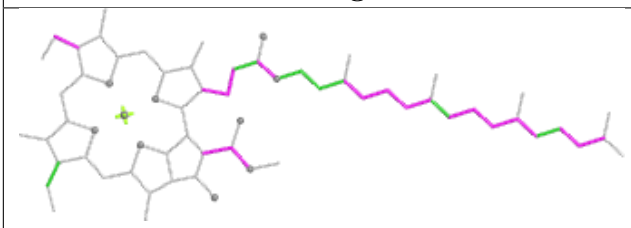
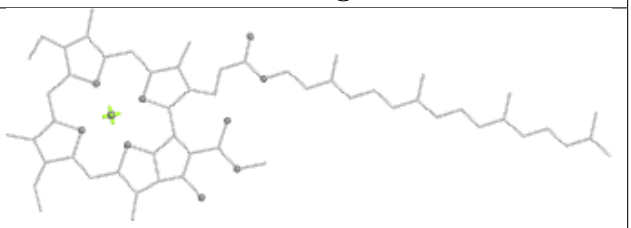


Bond angles

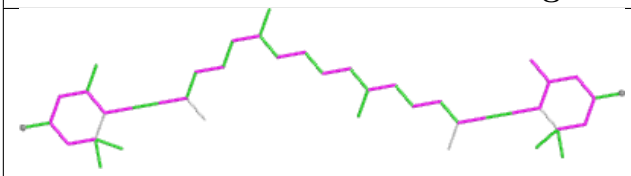


Torsions



Rings

Ligand II0 g 316



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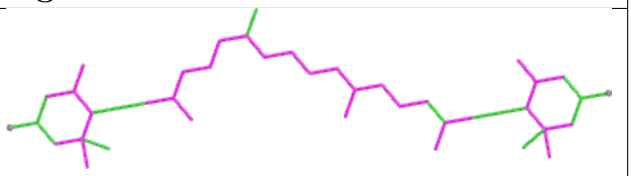
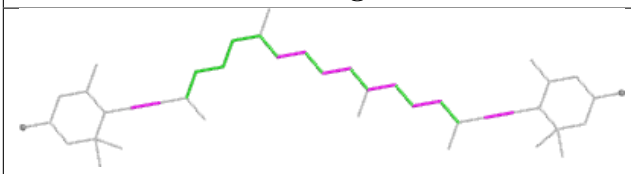


Bond angles



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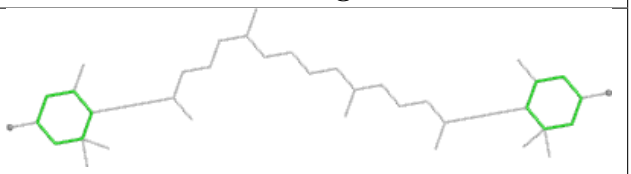
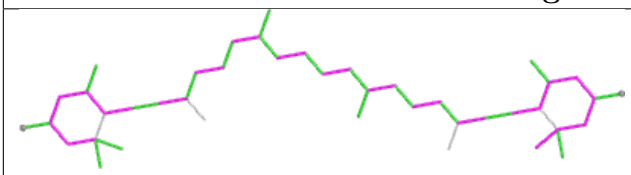


Rings

Ligand II0 g 320



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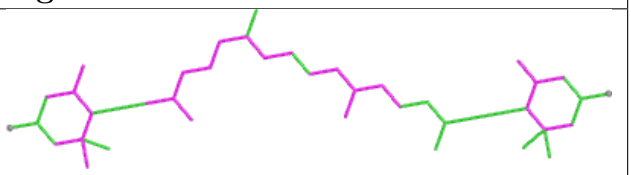
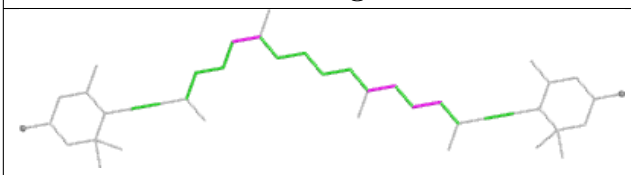
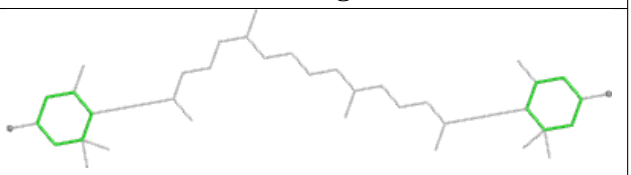


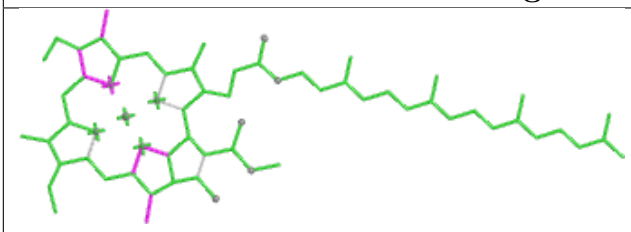
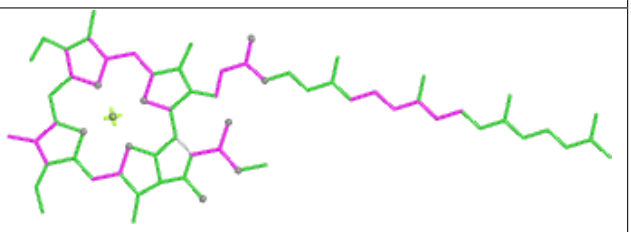
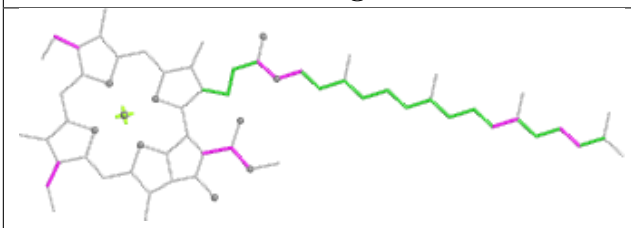
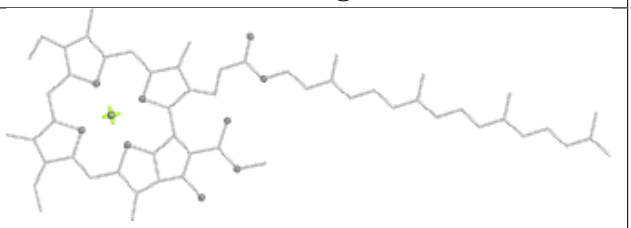
Bond angles

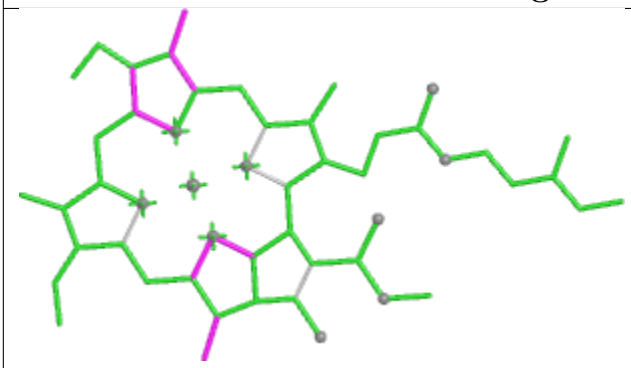
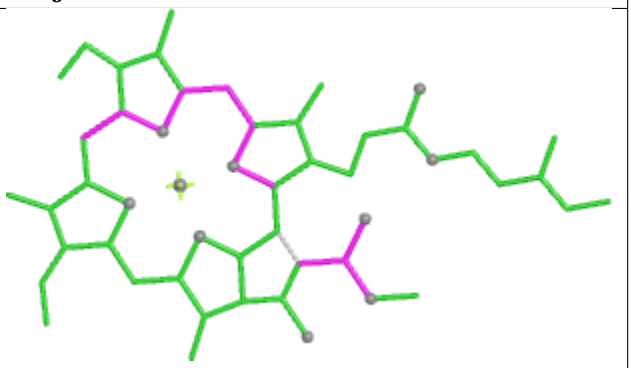
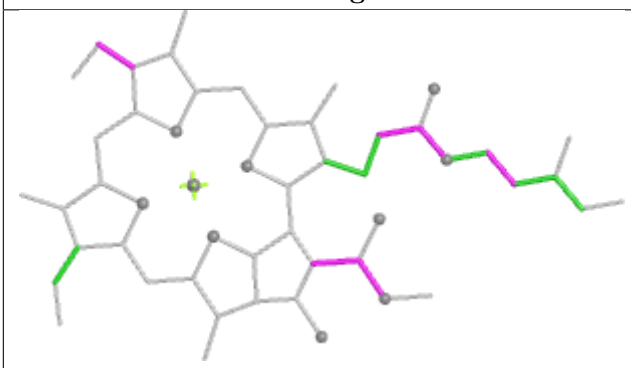
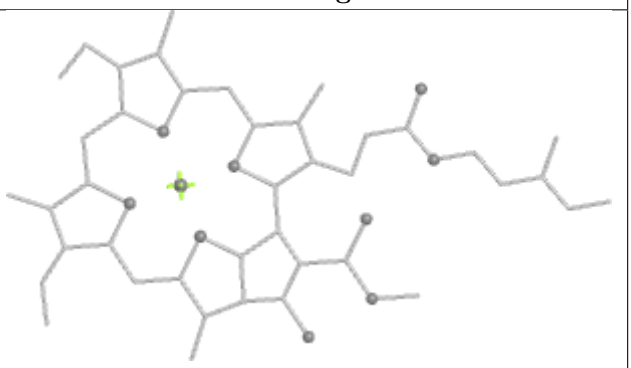


Torsions

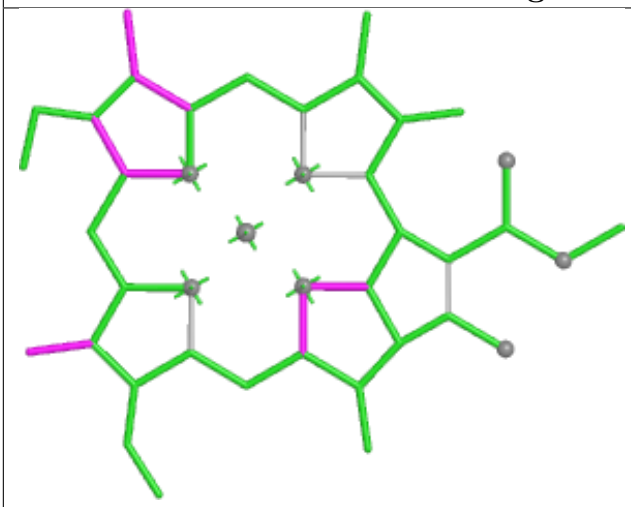


Rings

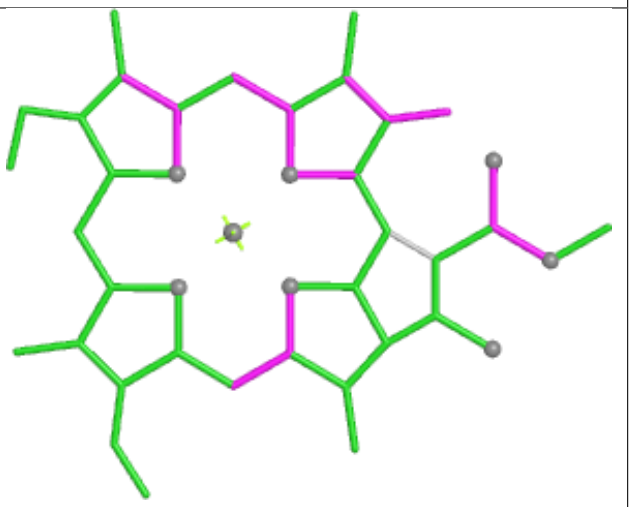
Ligand CLA A 832	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA j 308	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA d 309



Bond lengths



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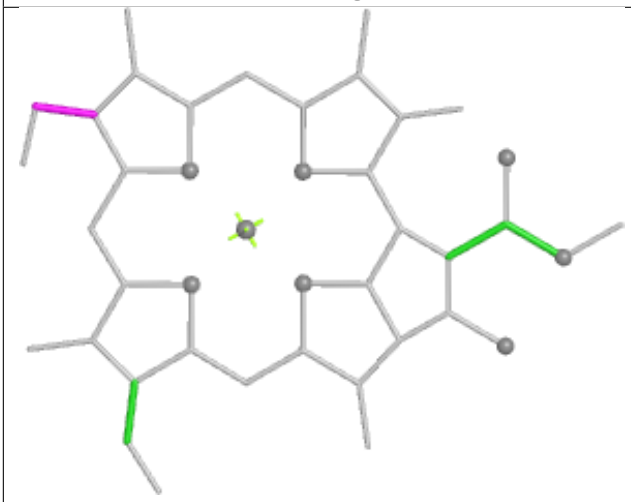

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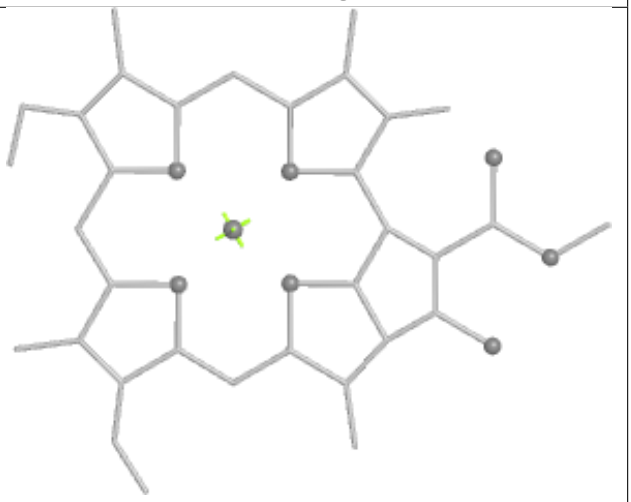
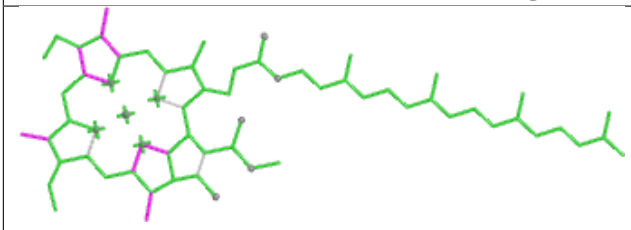


Rings

Ligand CLA B 808



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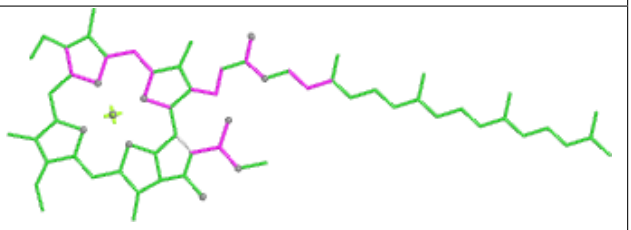
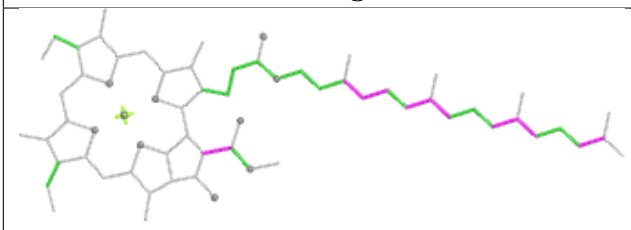


Bond angles



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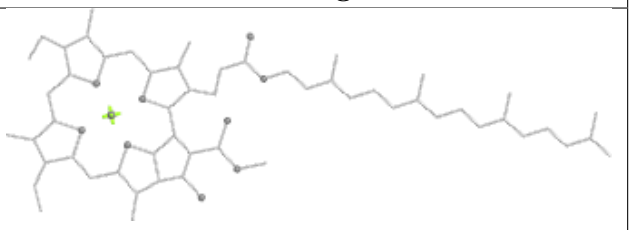
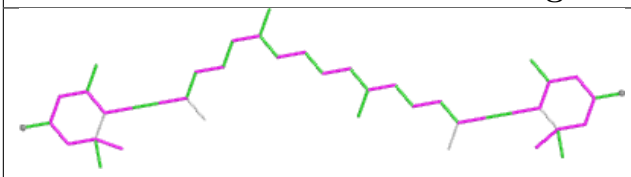
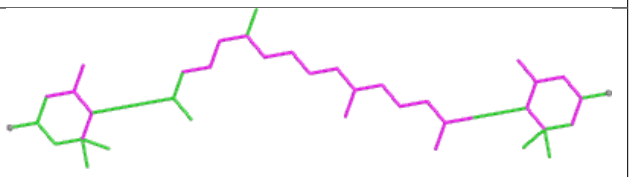
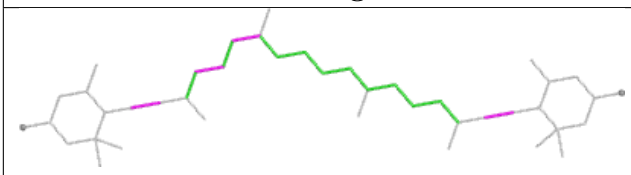
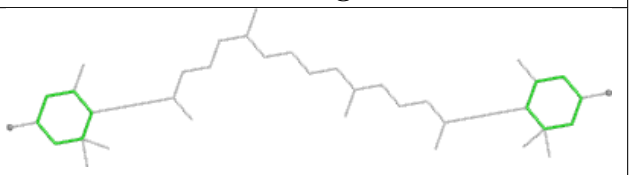
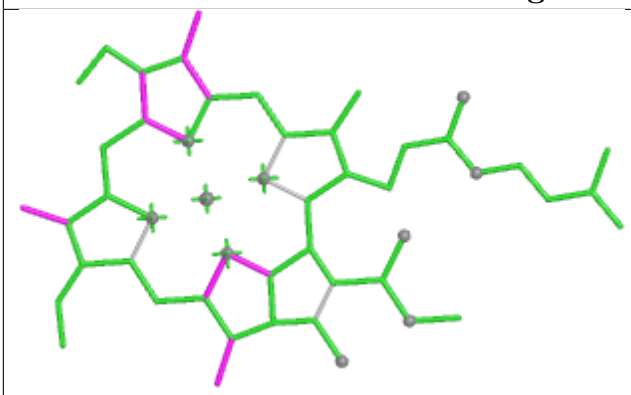
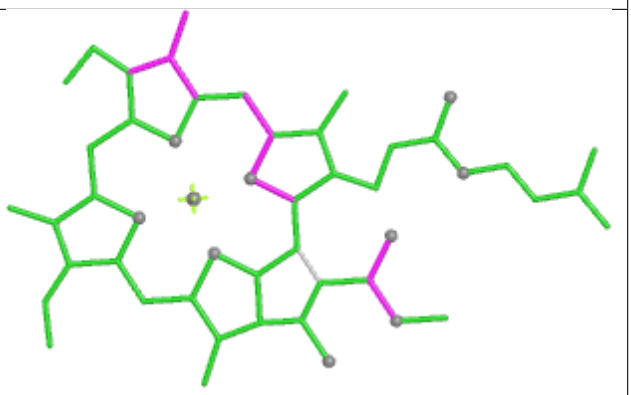
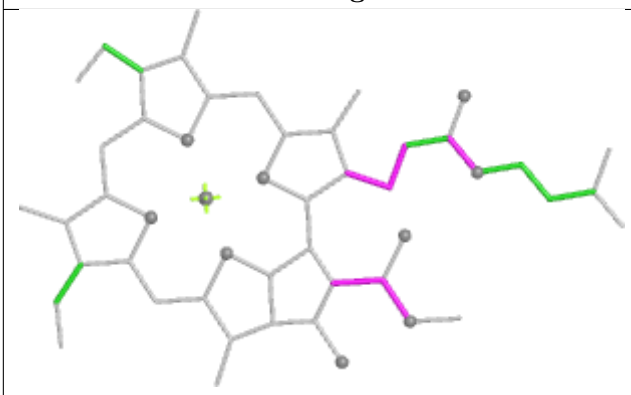
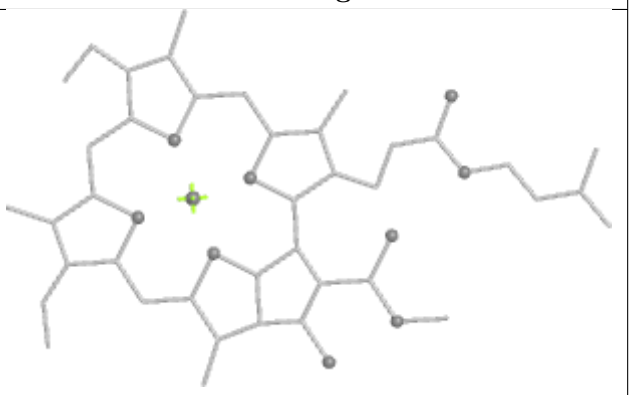
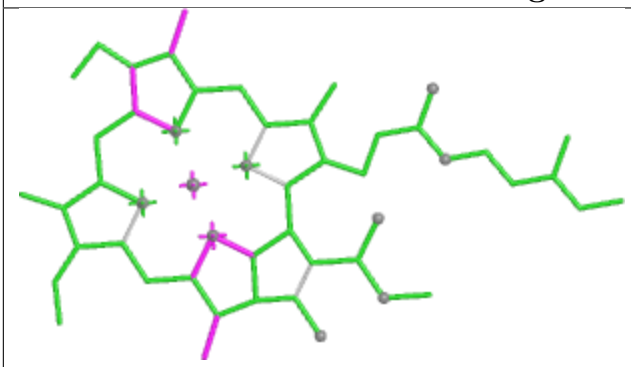


Rings

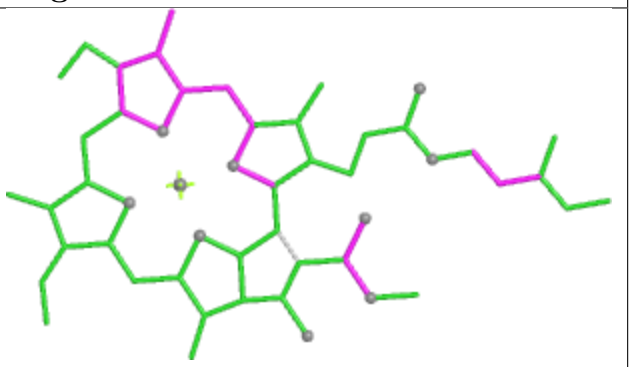
Ligand II0 f 616	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA h 301	
 Bond lengths	 Bond angles
 Torsions	 Rings

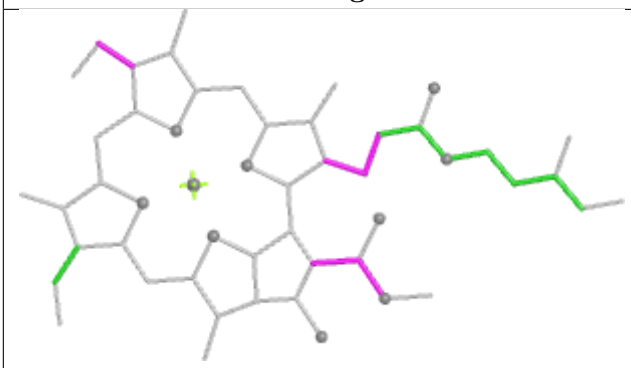
Ligand CLA g 315



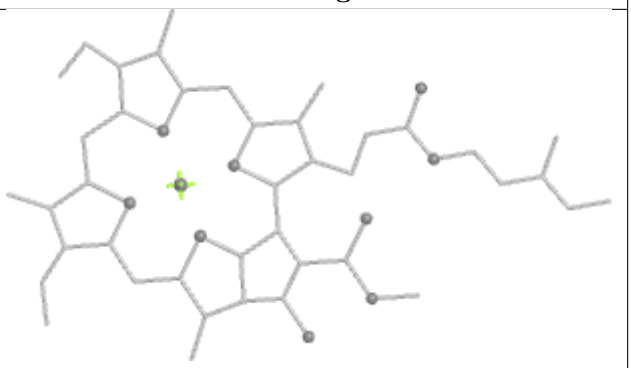
Bond lengths



Bond angles

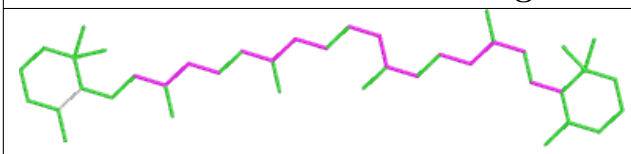


Torsions



Rings

Ligand WVN A 848



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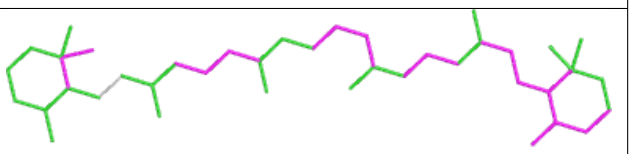
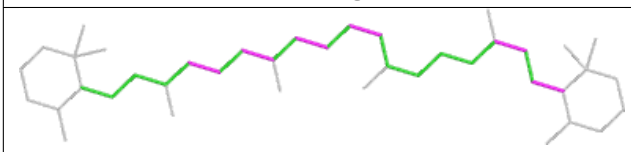
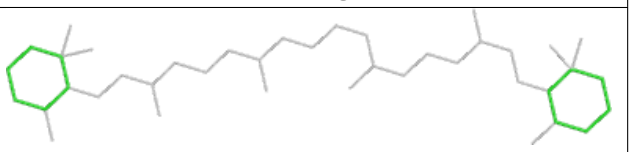


Bond angles

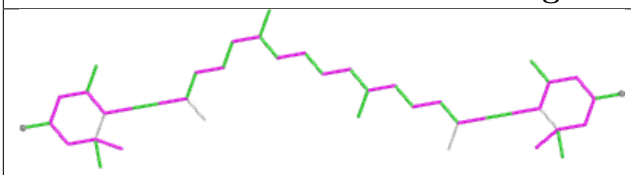


Torsions



Rings

Ligand II0 k 621



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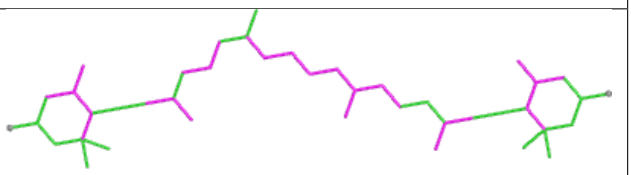
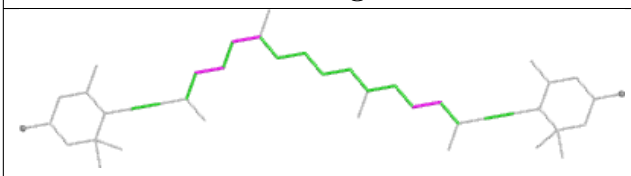
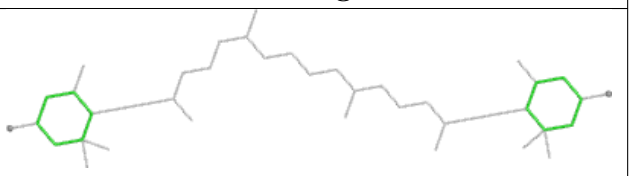


Bond angles

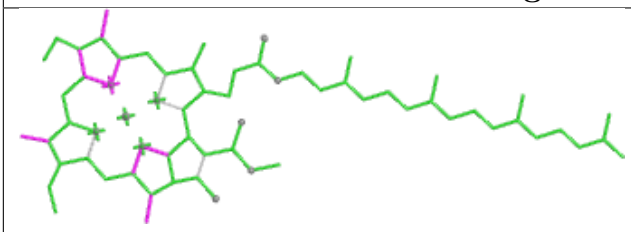


Torsions



Rings

Ligand CLA A 816



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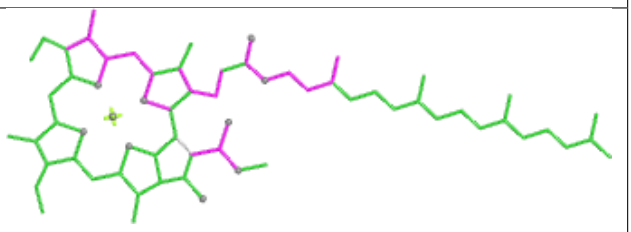
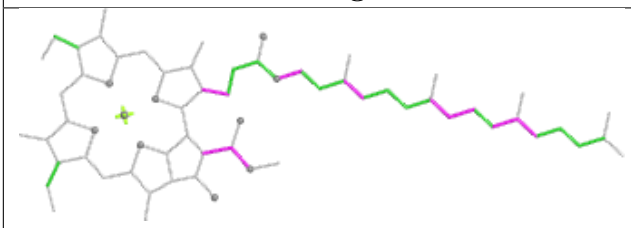
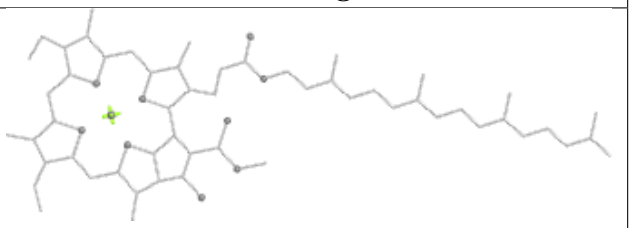


Bond angles

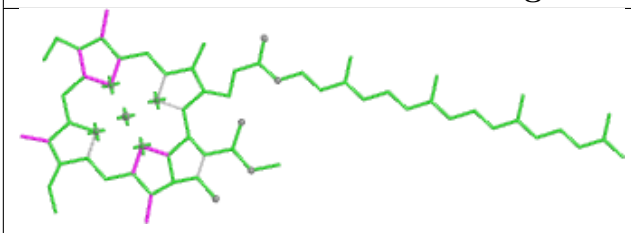


Torsions

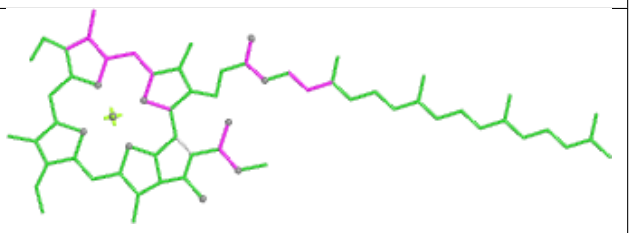


Rings

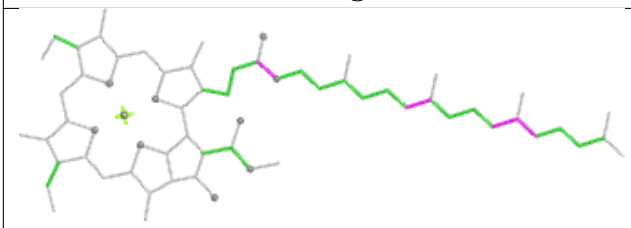
Ligand CLA B 818



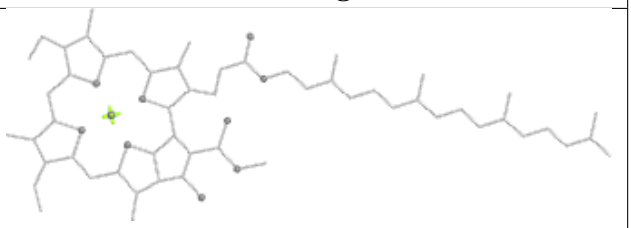
Bond lengths



Bond angles

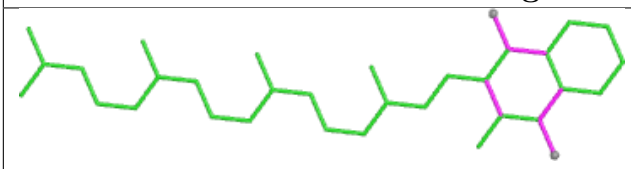


Torsions

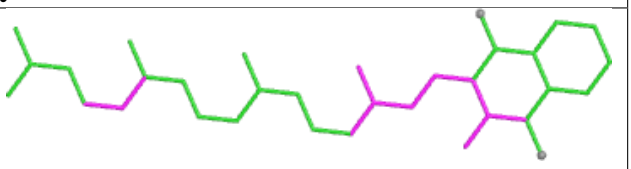


Rings

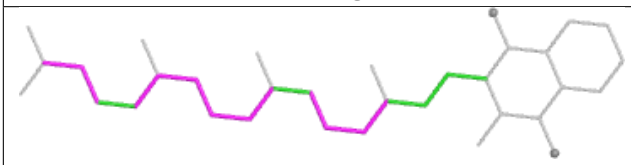
Ligand PQN B 842



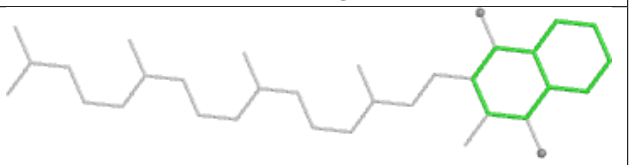
Bond lengths



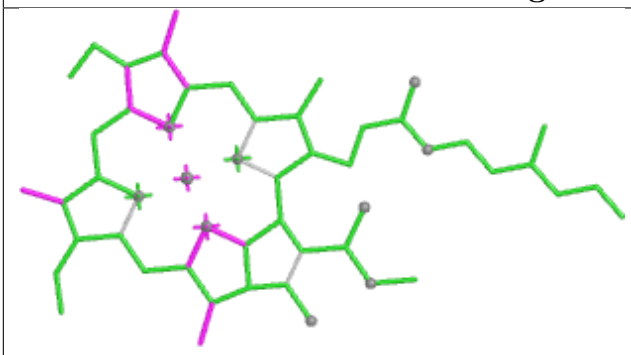
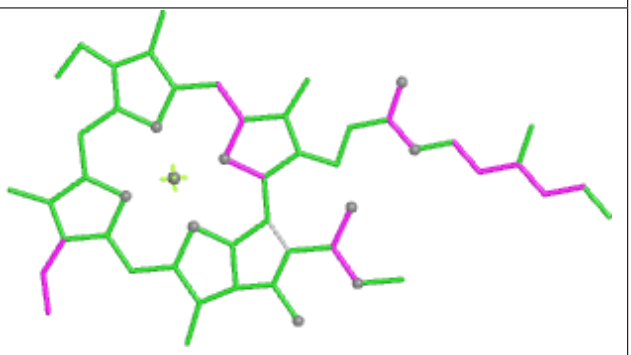
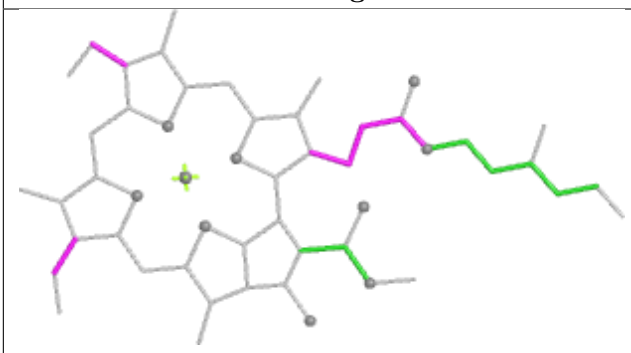
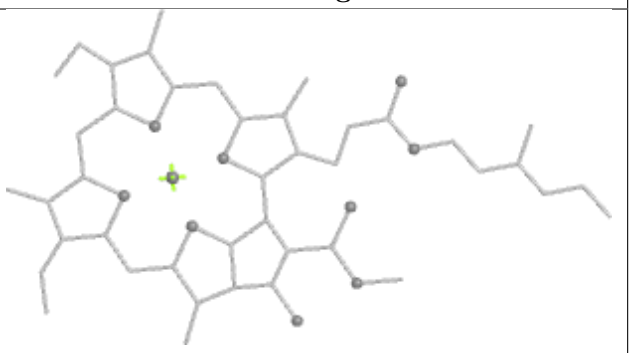
Bond angles

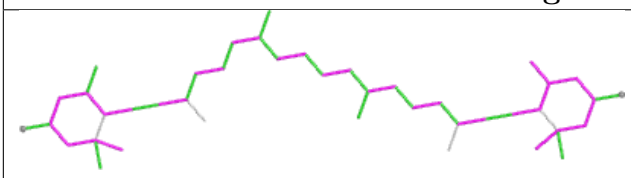
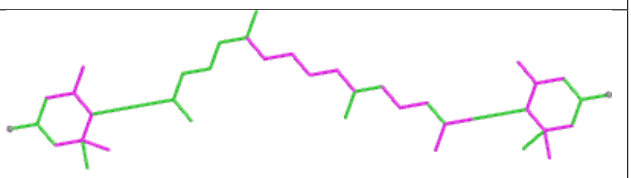
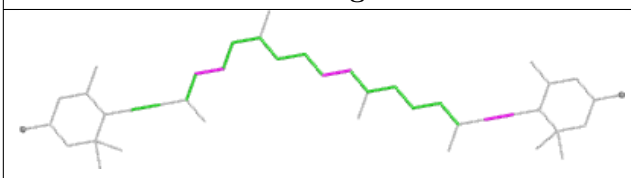
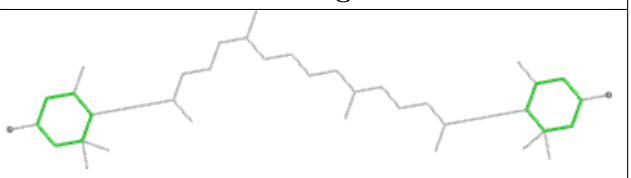


Torsions

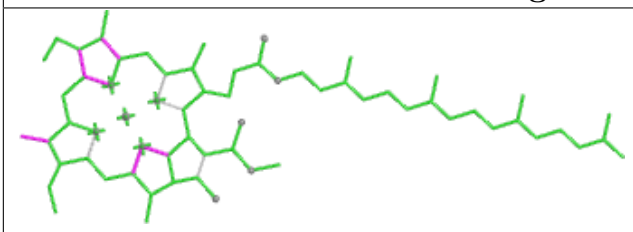


Rings

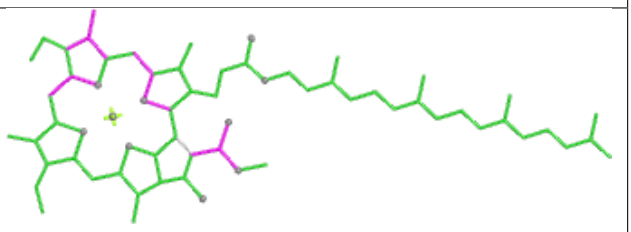
Ligand CLA a 302	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand II0 a 315	
 Bond lengths	 Bond angles
 Torsions	 Rings

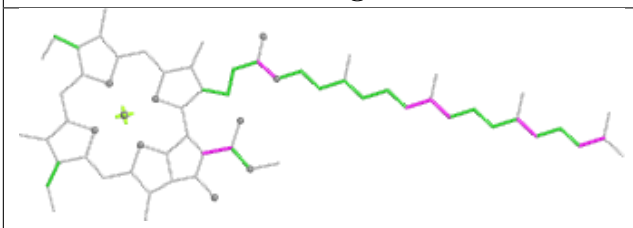
Ligand CLA e 606



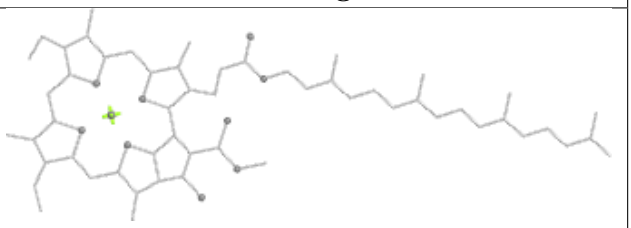
Bond lengths



Bond angles

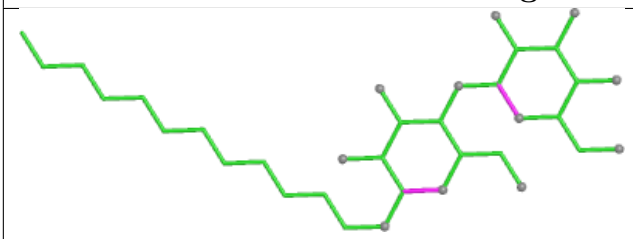


Torsions

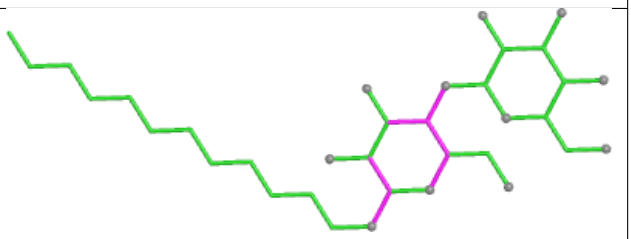


Rings

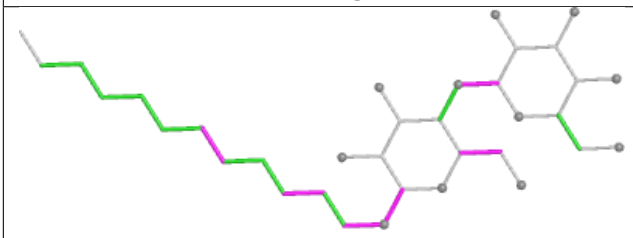
Ligand LMU B 844



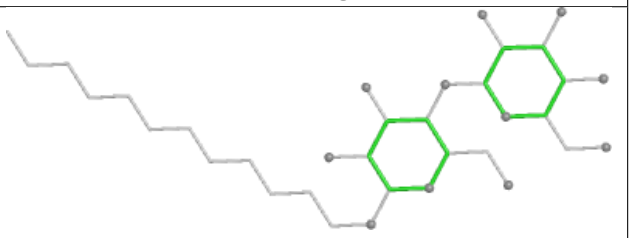
Bond lengths



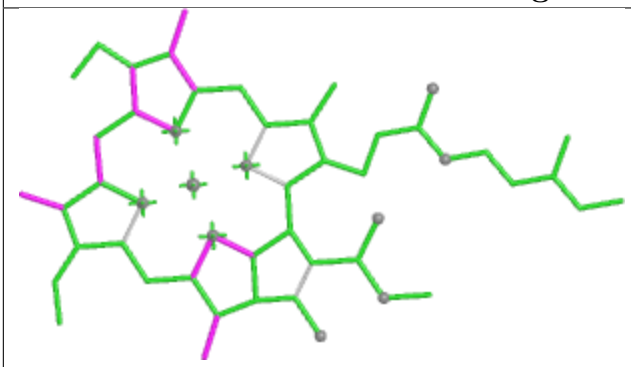
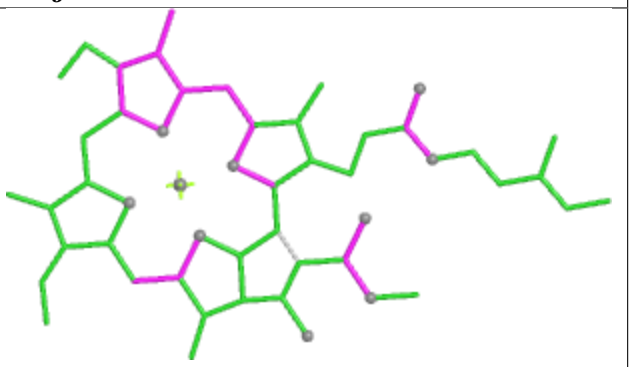
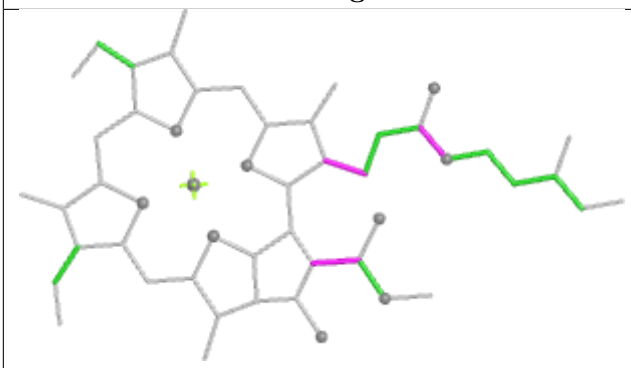
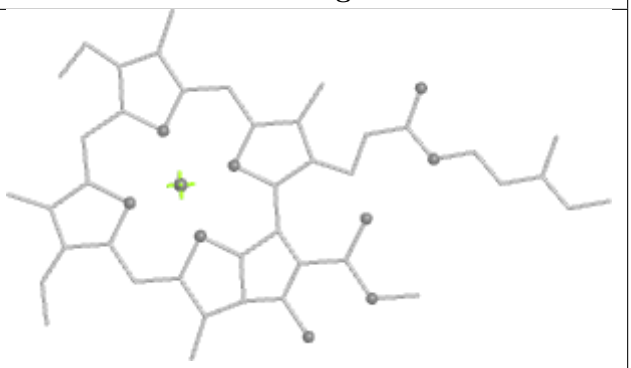
Bond angles

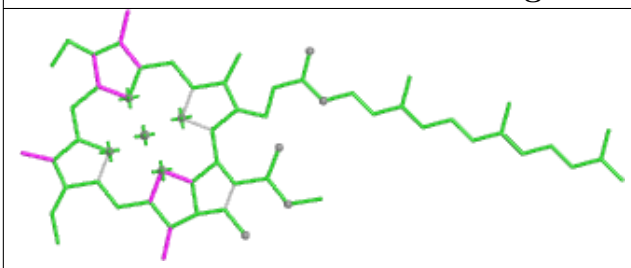
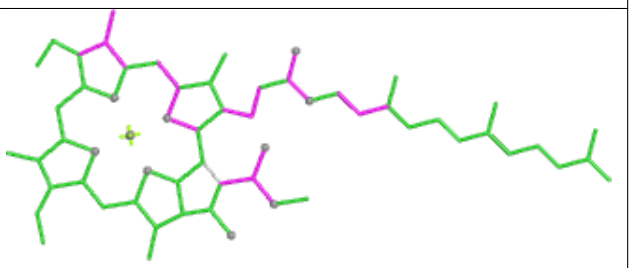
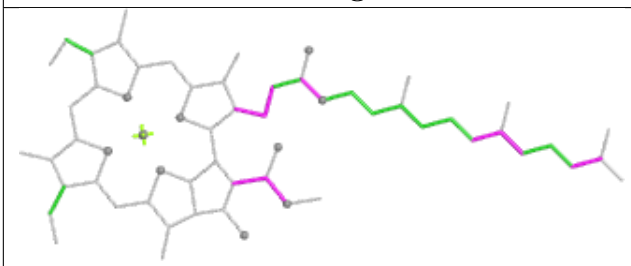
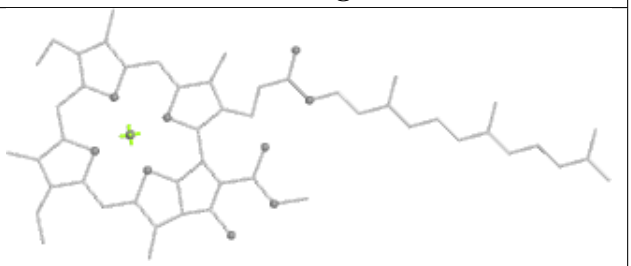


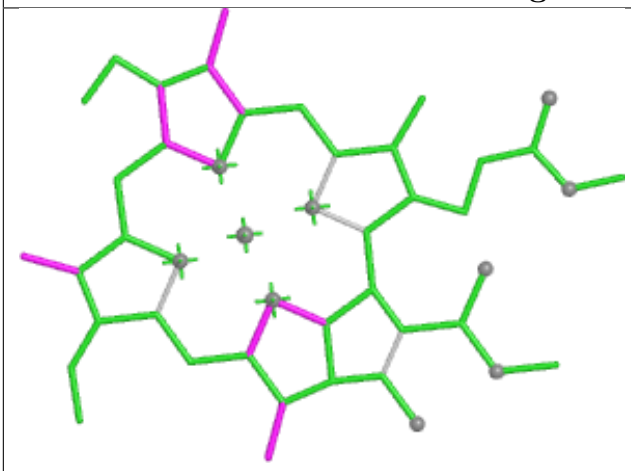
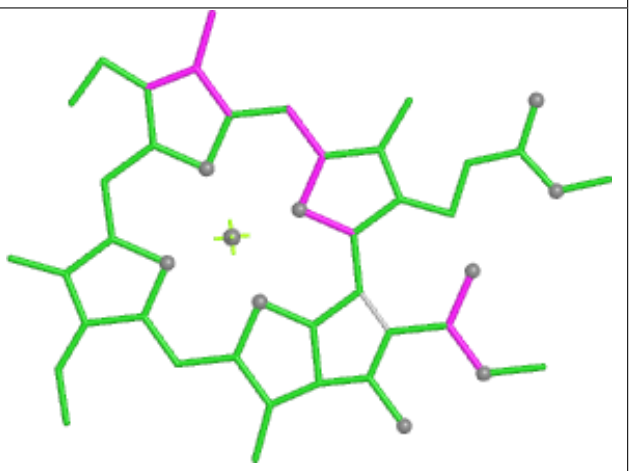
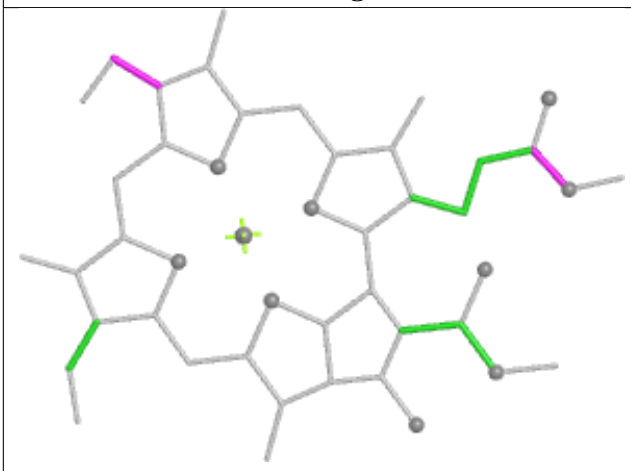
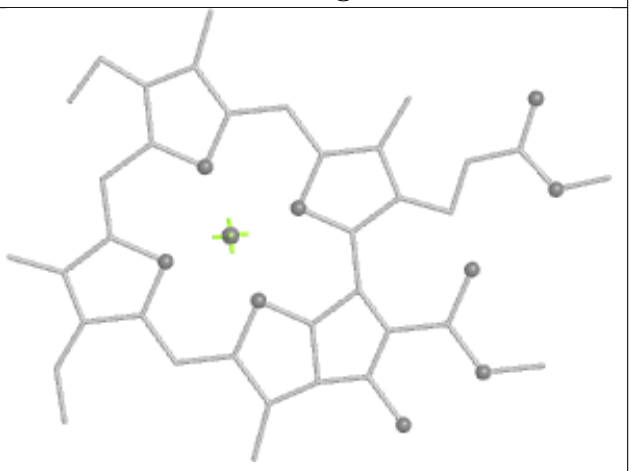
Torsions



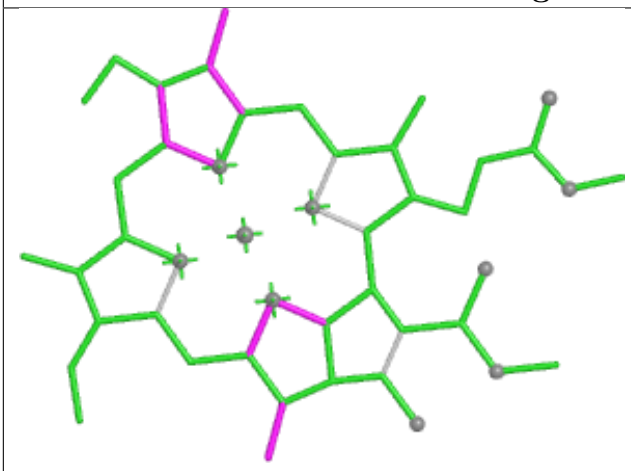
Rings

Ligand CLA j 310	
 Bond lengths	 Bond angles
 Torsions	 Rings

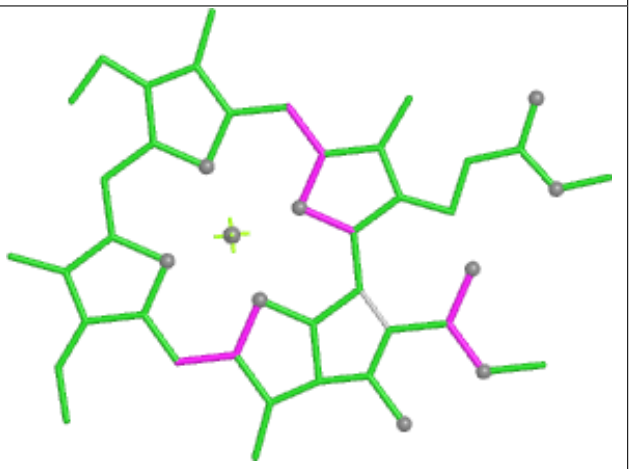
Ligand CLA B 813	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA c 607	
 Bond lengths	 Bond angles
 Torsions	 Rings

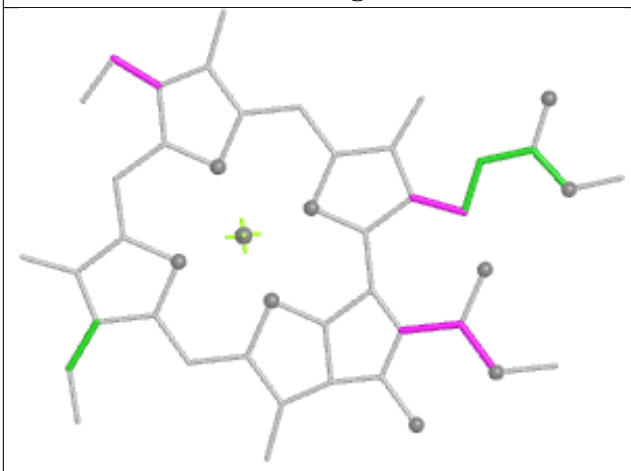
Ligand CLA i 608



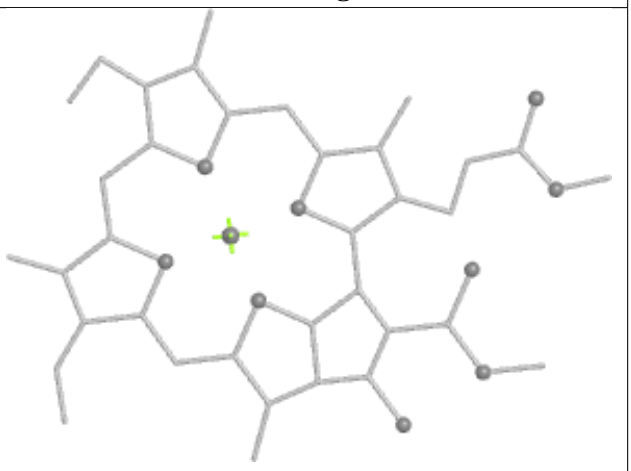
Bond lengths



Bond angles

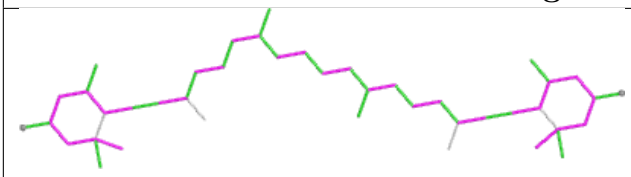


Torsions

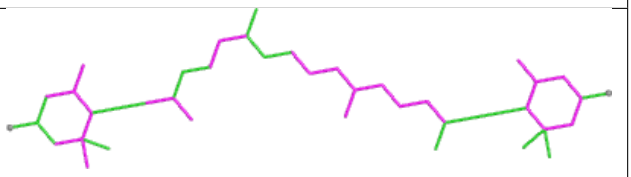


Rings

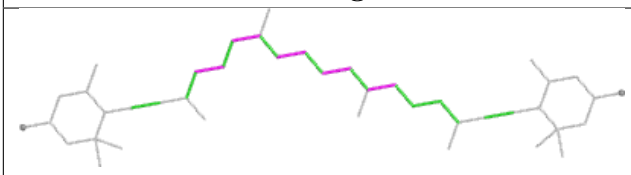
Ligand II0 a 317



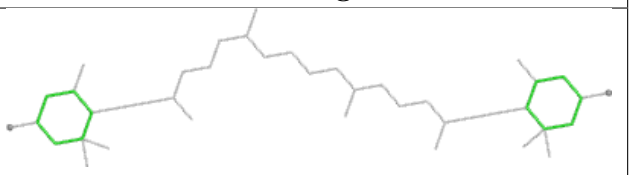
Bond lengths



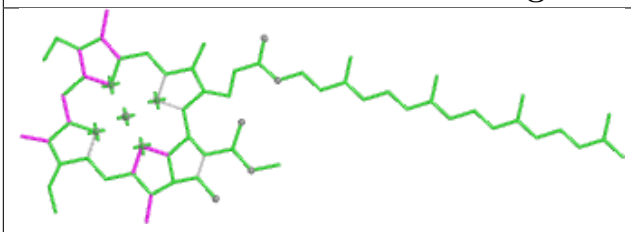
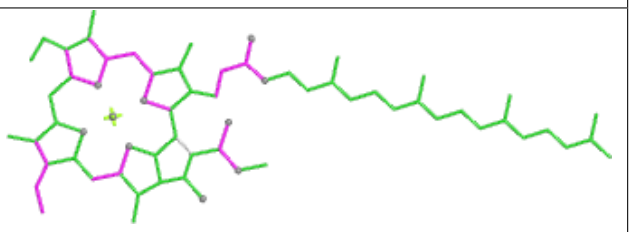
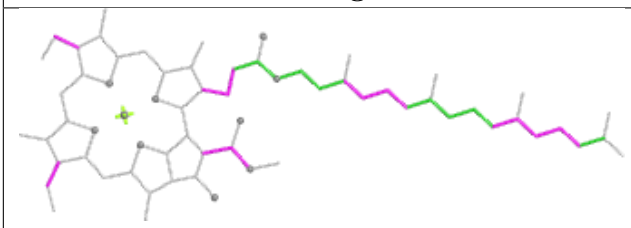
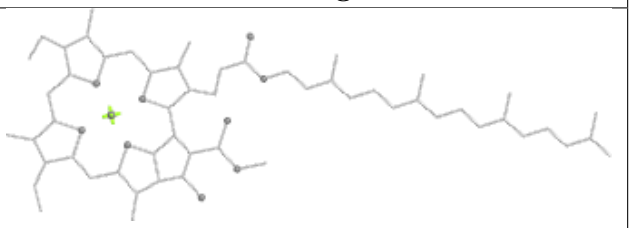
Bond angles

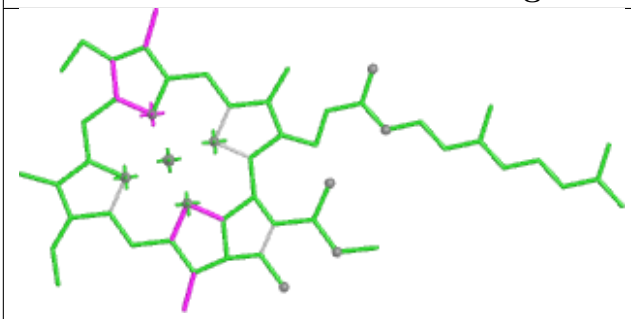
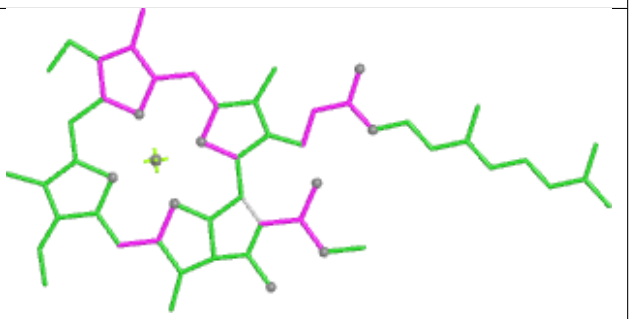
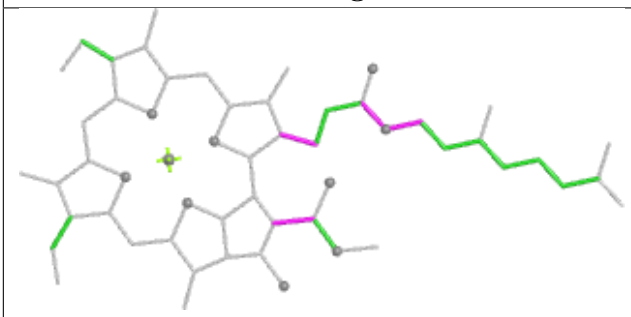
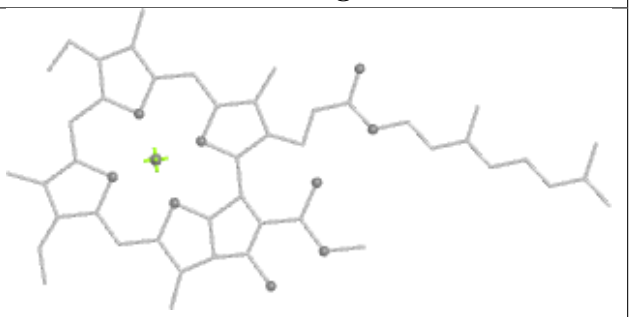


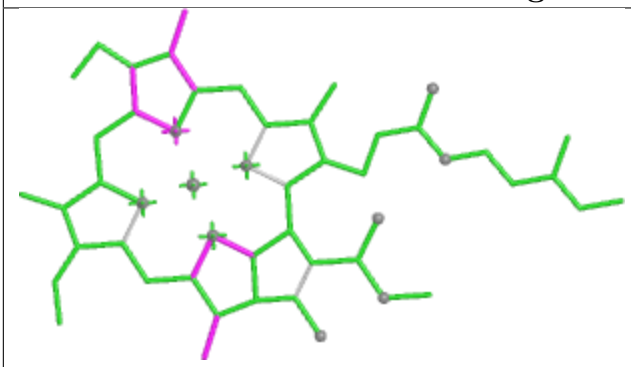
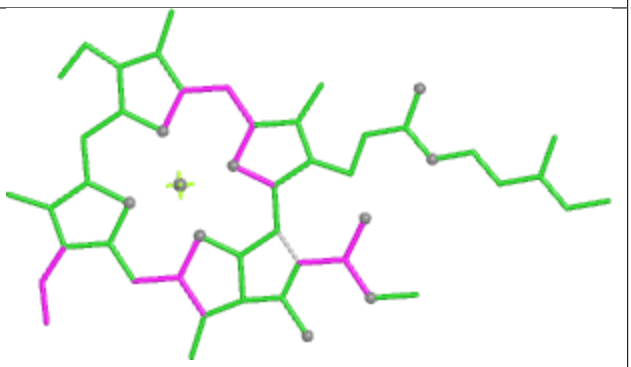
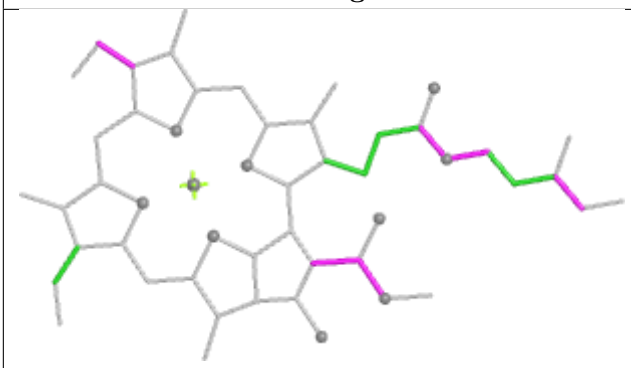
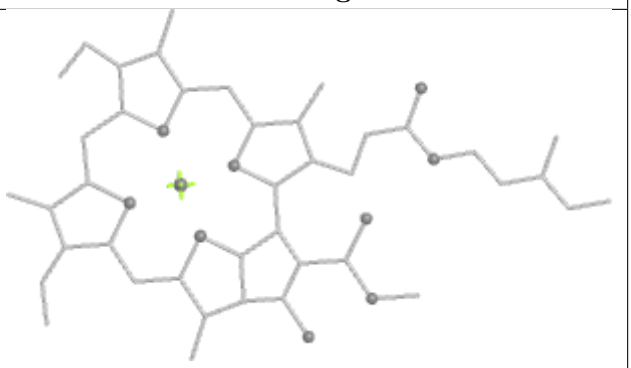
Torsions

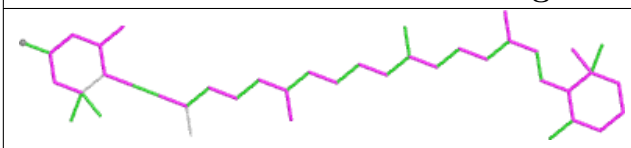
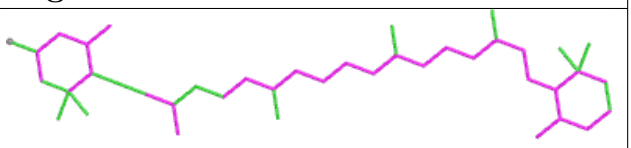
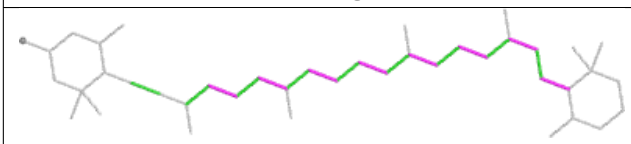
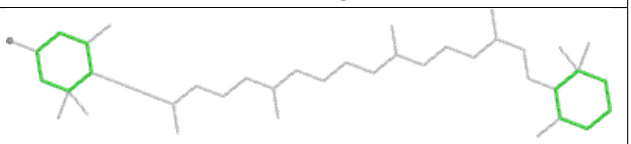


Rings

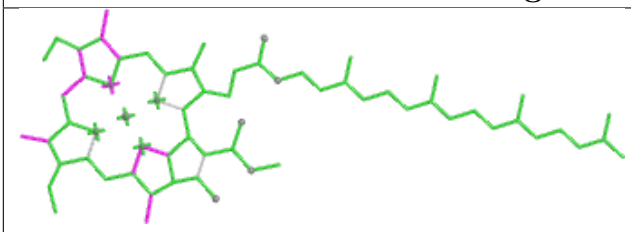
Ligand CLA b 309	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA A 803	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA b 303	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand IHT g 319	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA B 807



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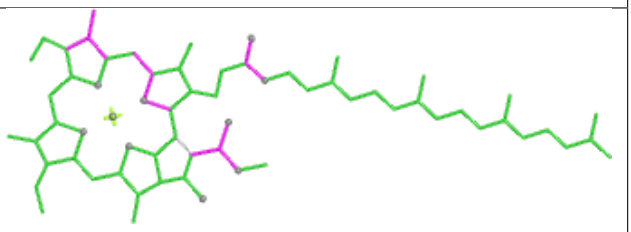

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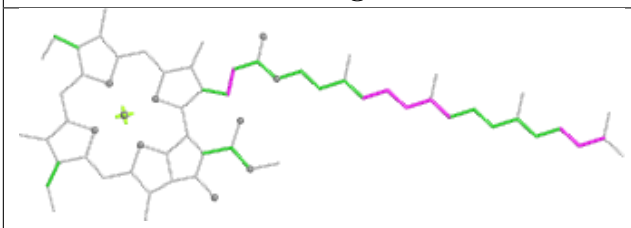

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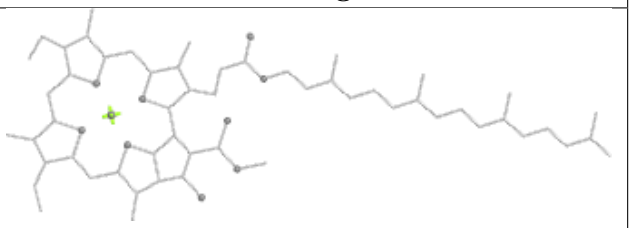
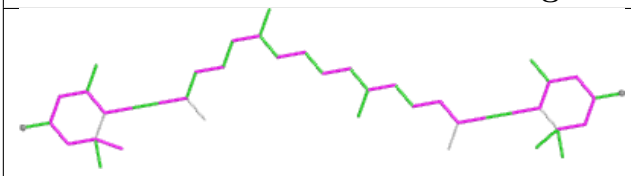


Rings

Ligand II0 h 311



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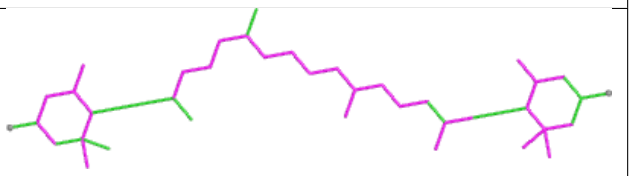

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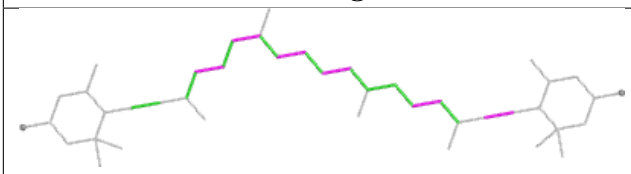

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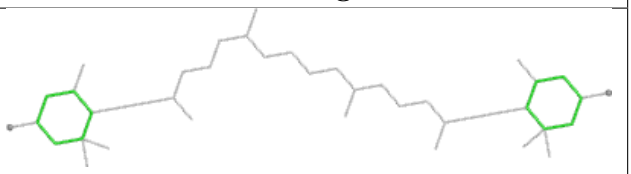
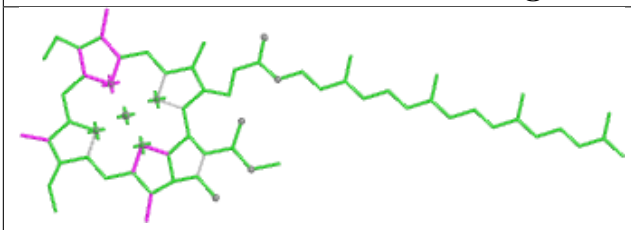


Rings

Ligand CLA B 824



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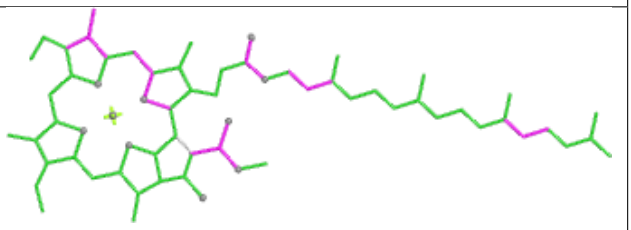
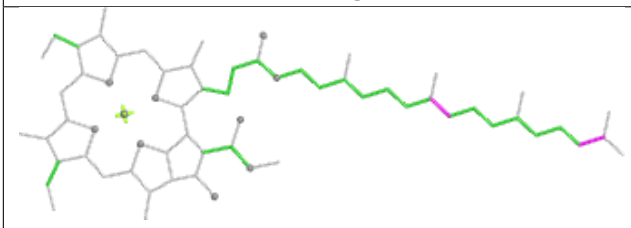


Bond angles



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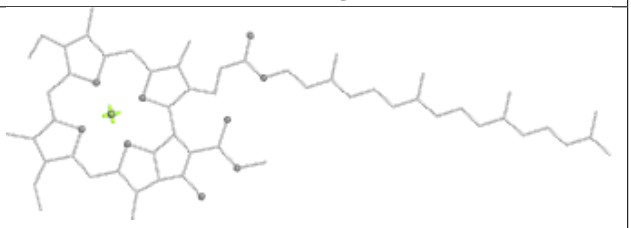
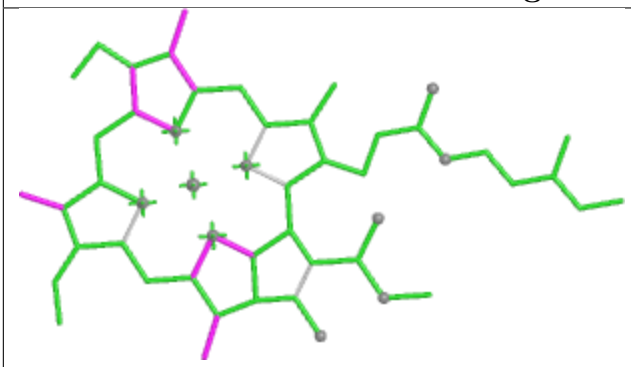
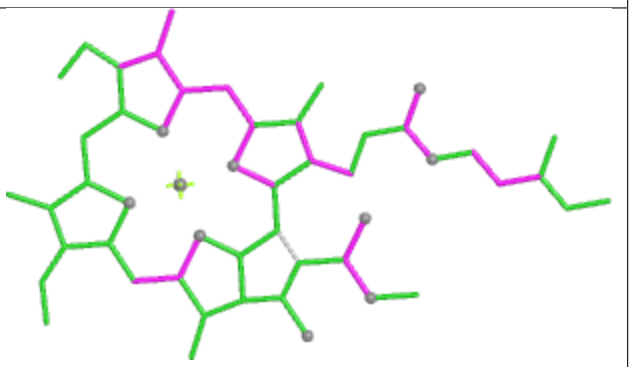
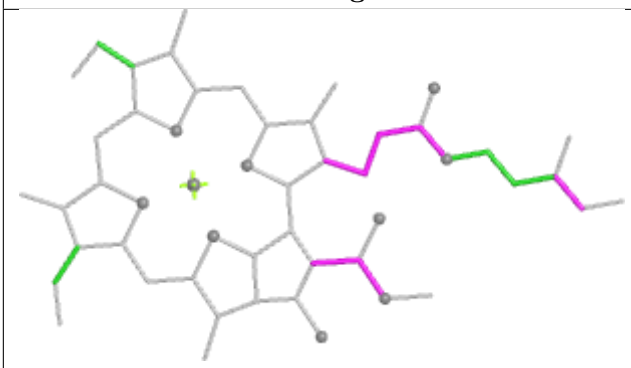
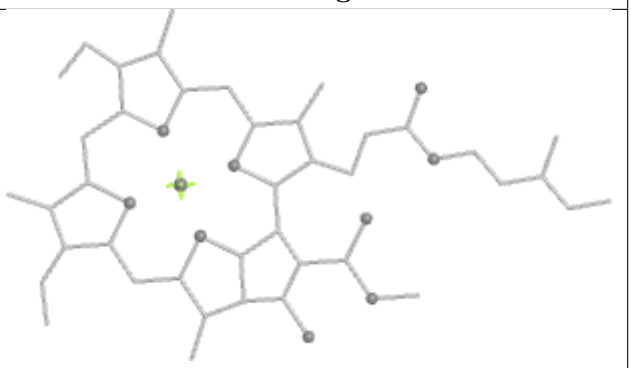


Rings

Ligand CLA R 203	
 Bond lengths	 Bond angles
 Torsions	 Rings

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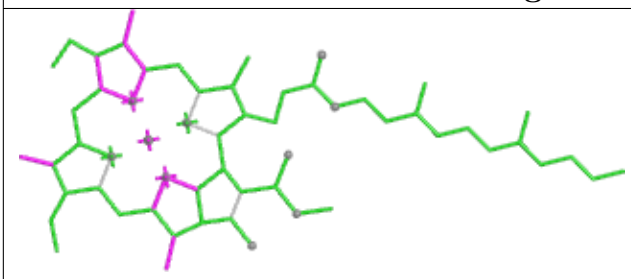
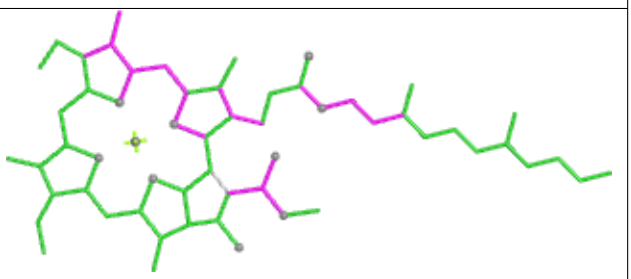
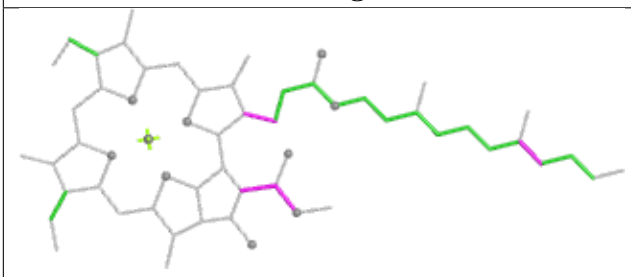
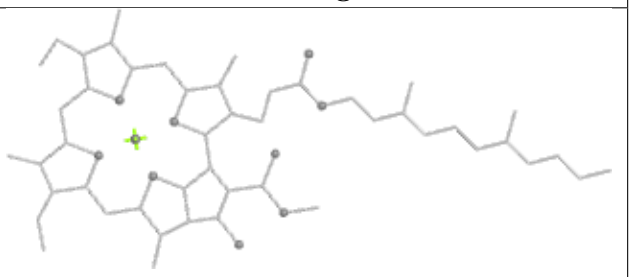
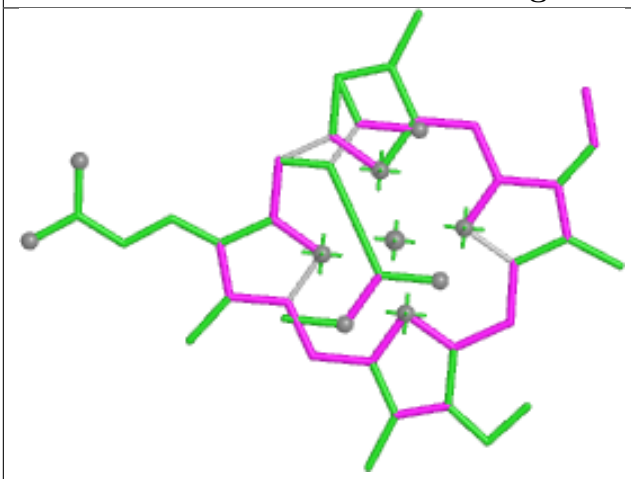
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand KC2 k 612



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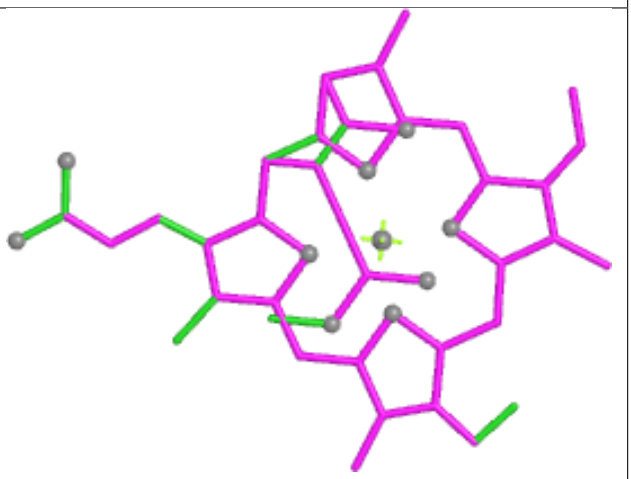
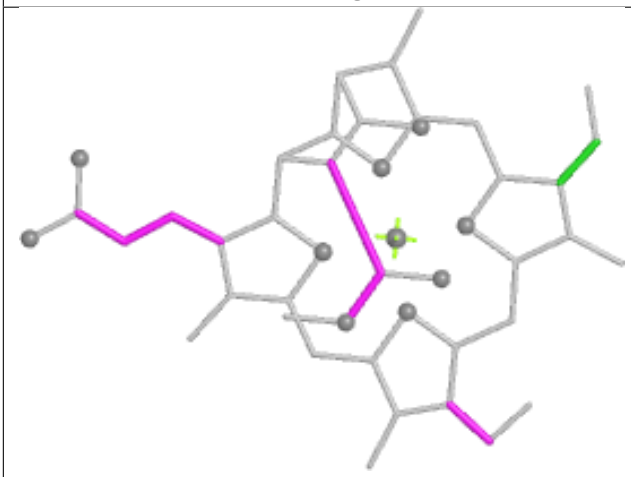


Bond angles



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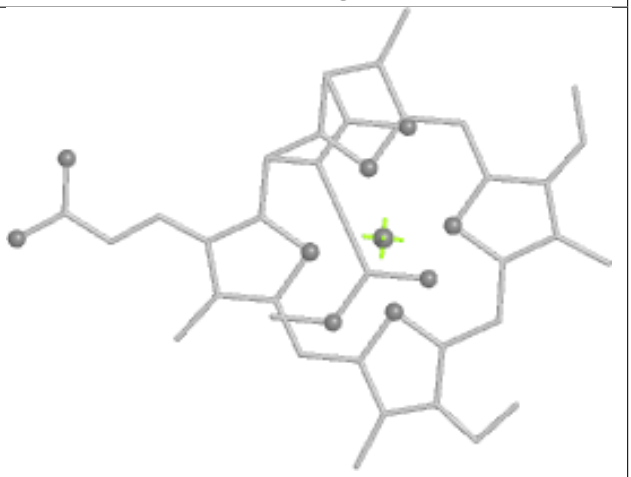
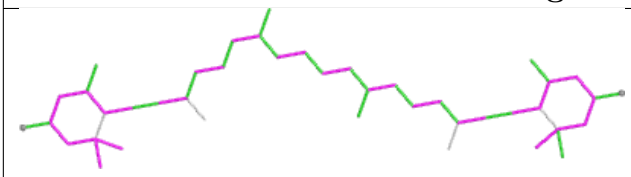


Rings

Ligand II0 i 612



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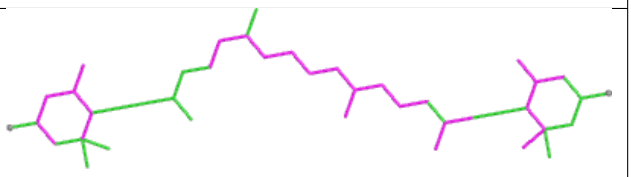

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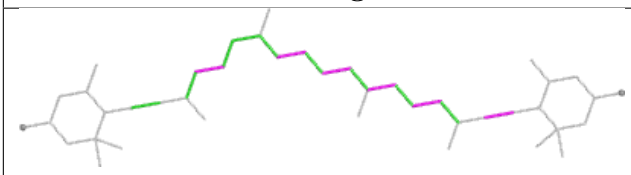

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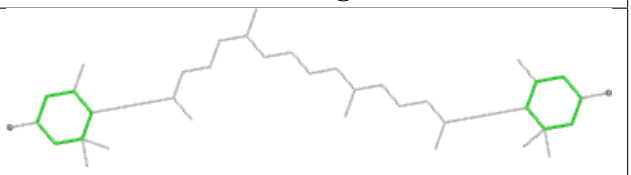
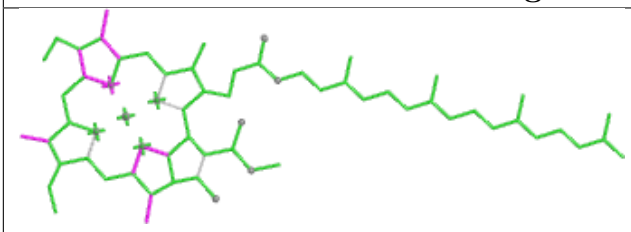
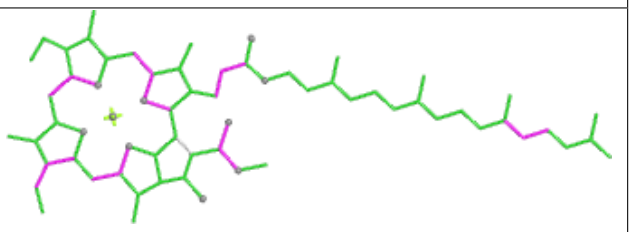
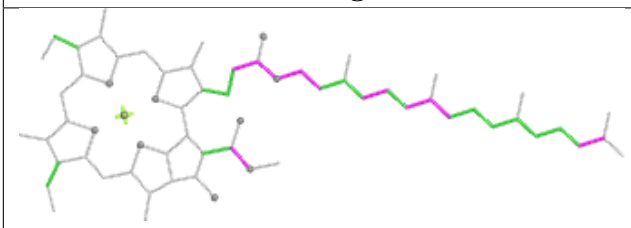
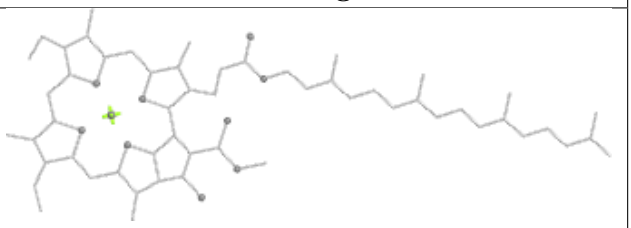
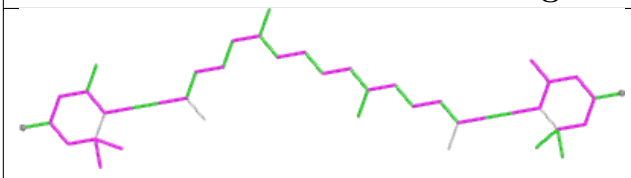
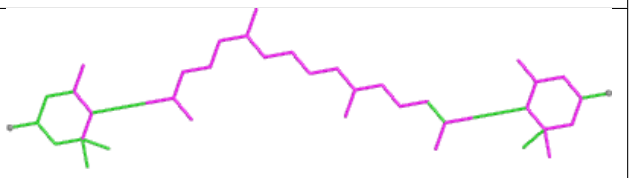
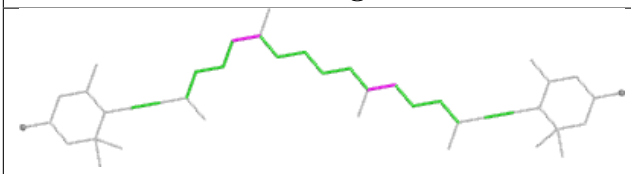
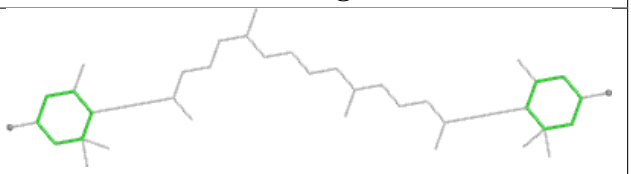
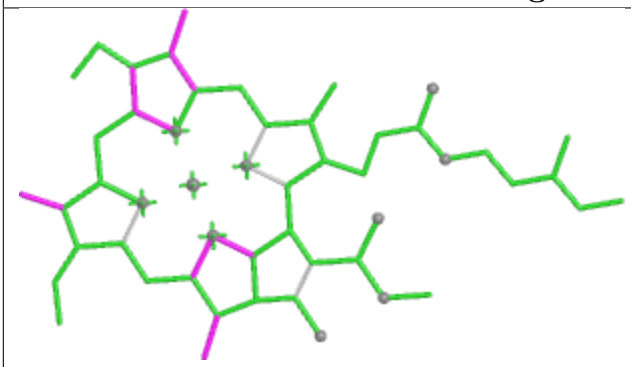
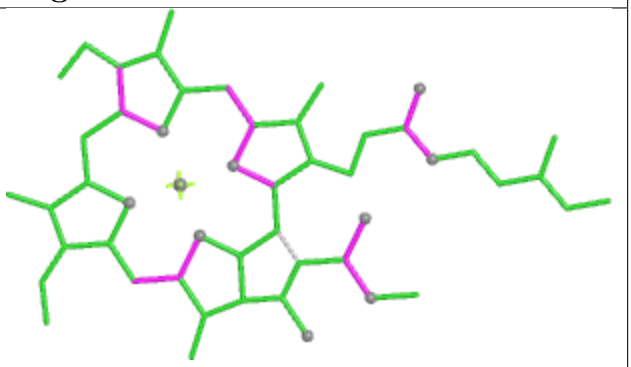
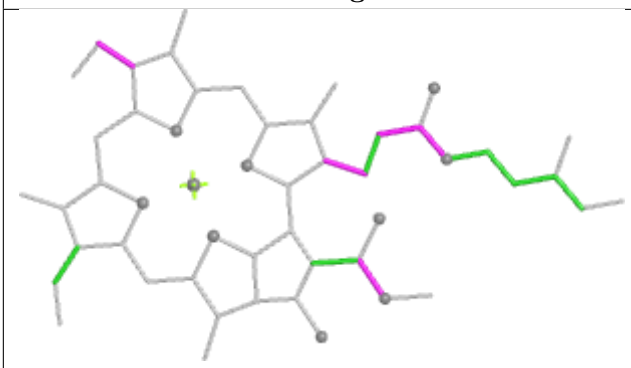
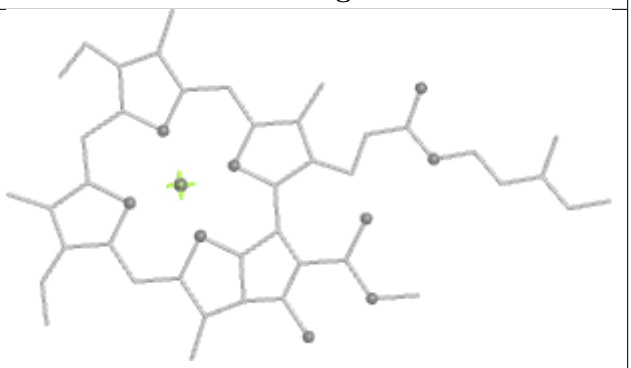
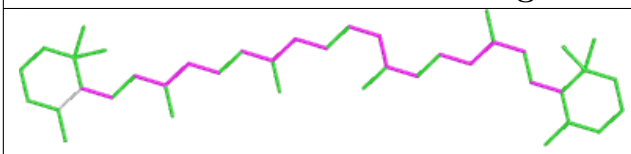
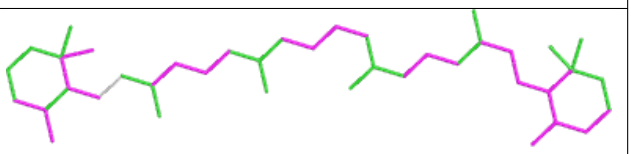
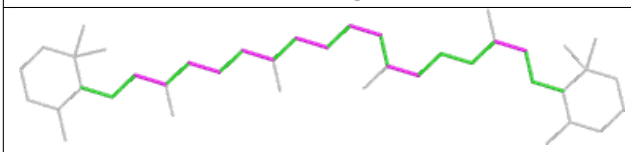
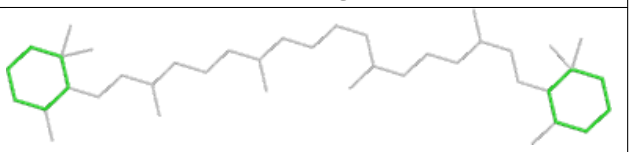


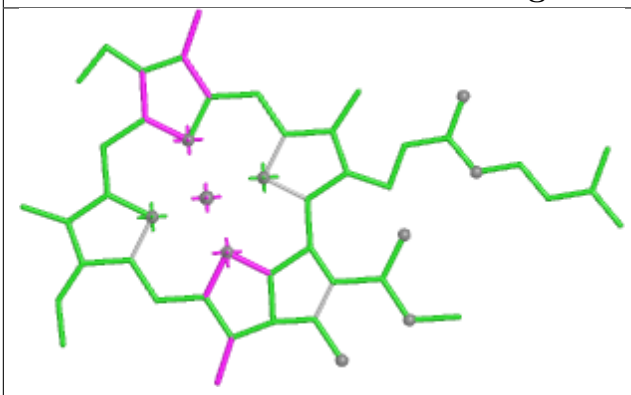
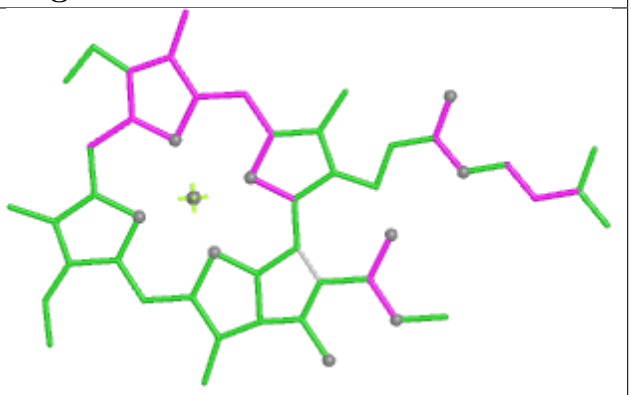
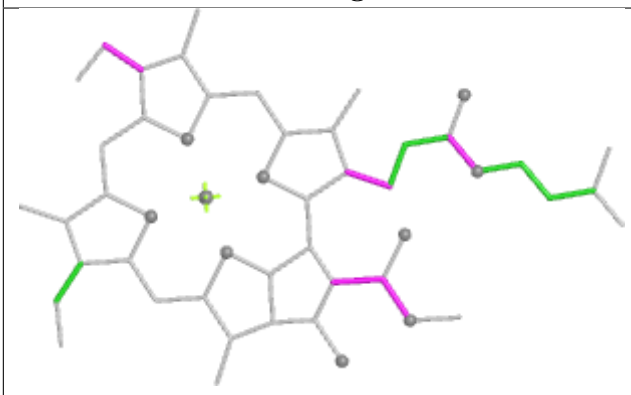
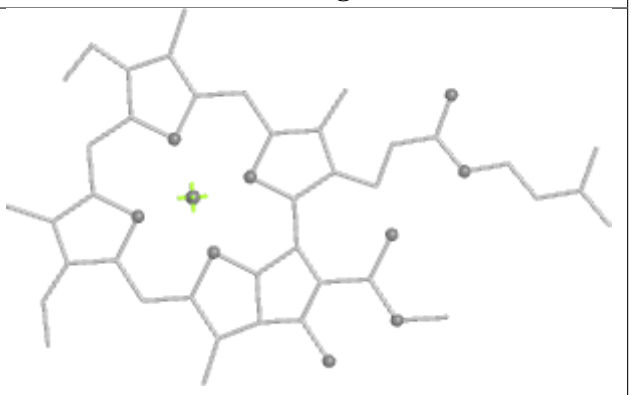
Rings

Ligand CLA B 830	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand II0 b 318	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA g 306	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand WVN F 204	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA g 303	
 Bond lengths	 Bond angles
 Torsions	 Rings

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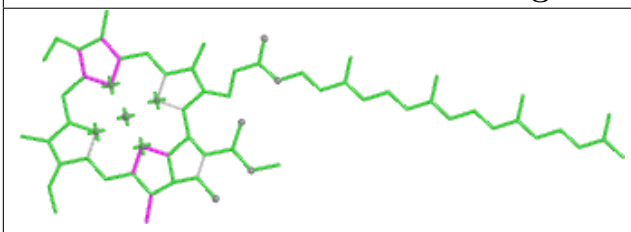
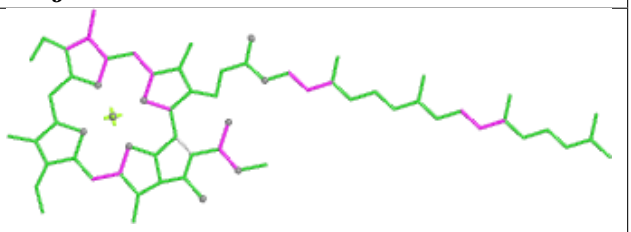
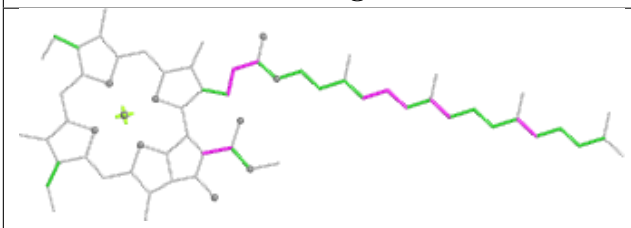
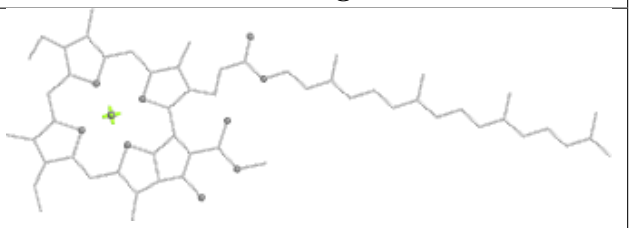
 Bond lengths	 Bond angles
 Torsions	 Rings

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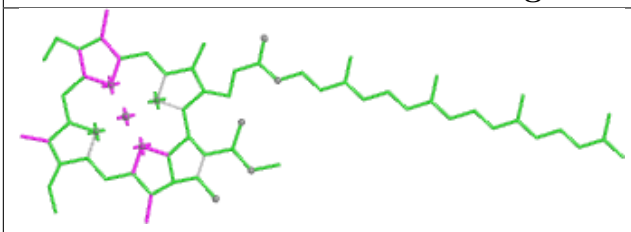
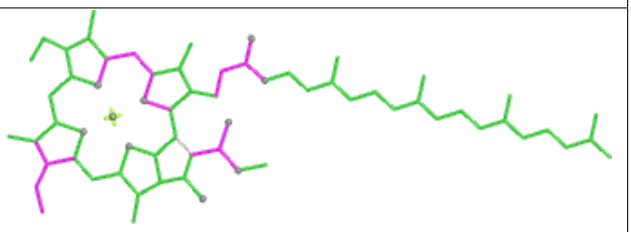
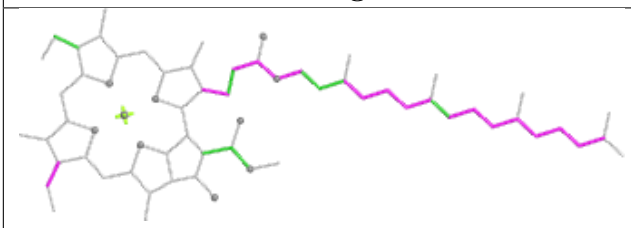
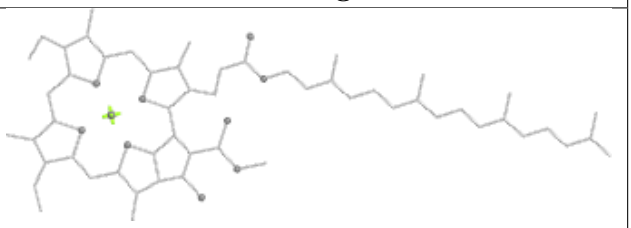
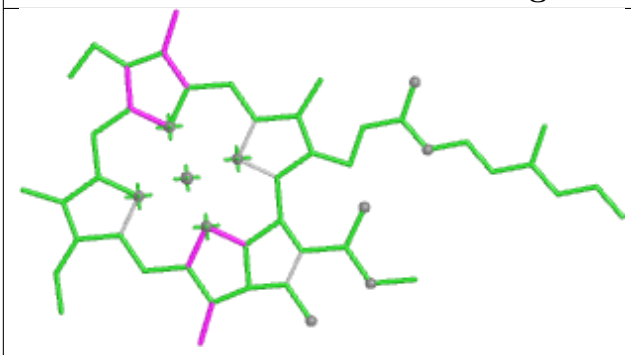
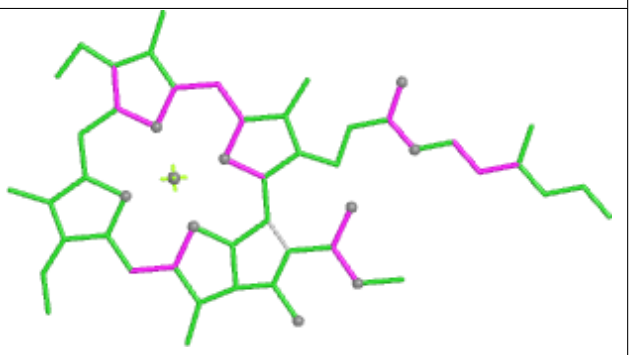
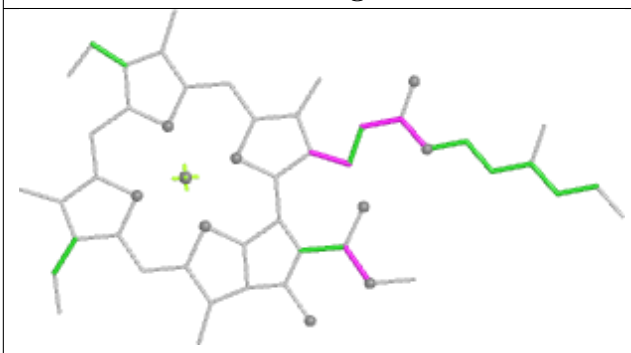
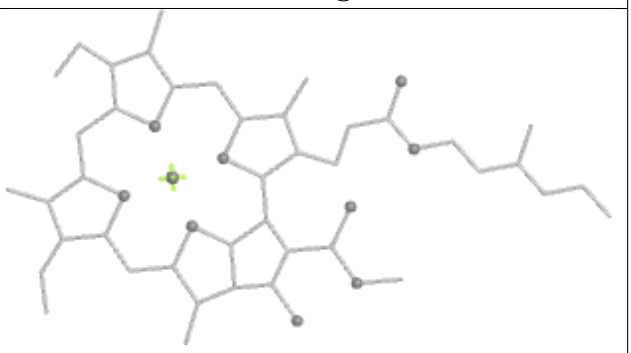
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA c 606	
 Bond lengths	 Bond angles
 Torsions	 Rings

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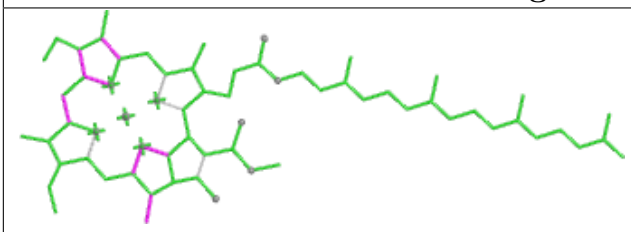
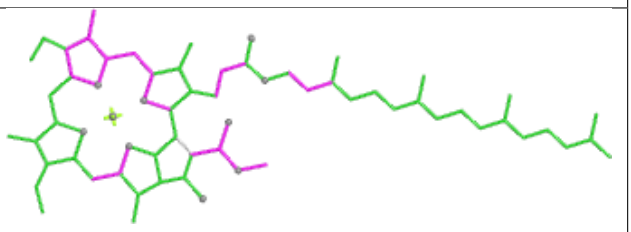
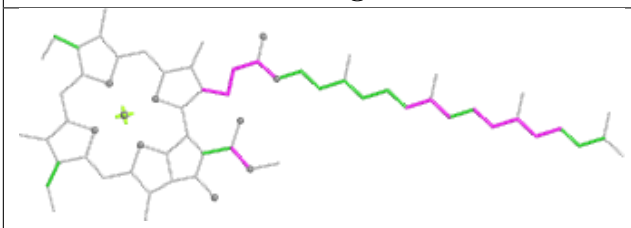
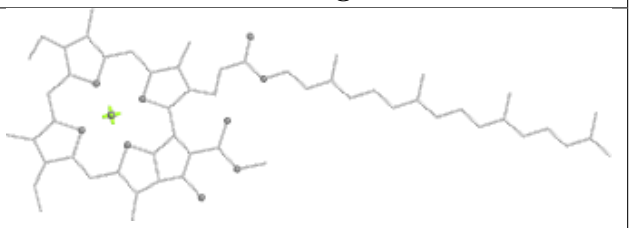
 Bond lengths	 Bond angles
 Torsions	 Rings

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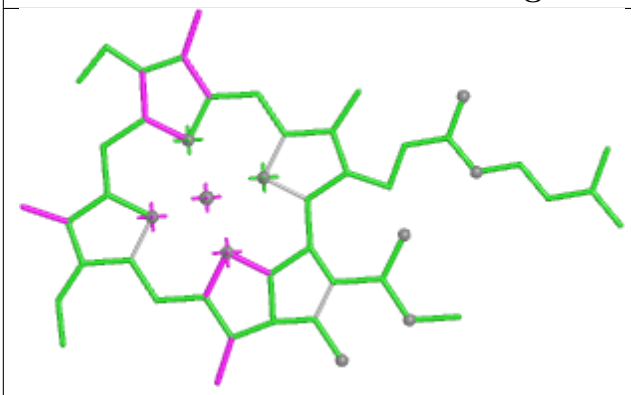
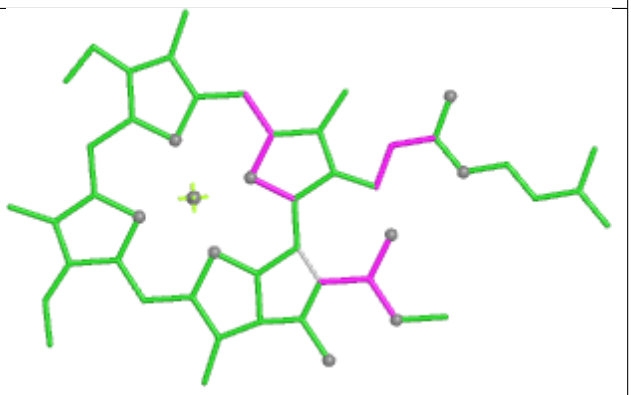
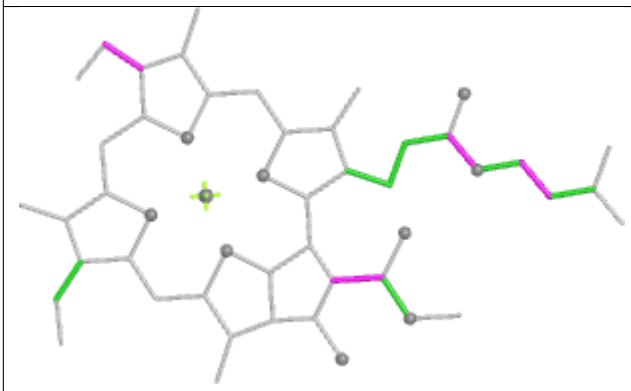
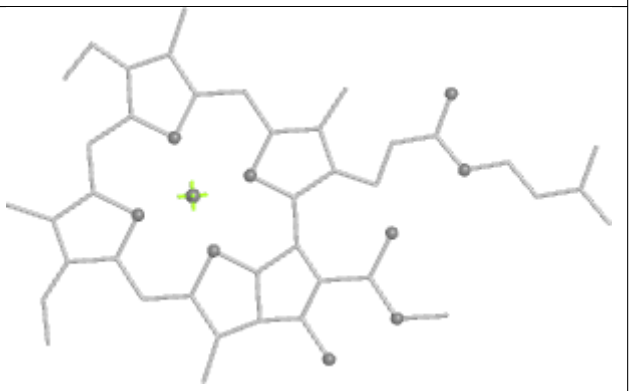
 Bond lengths	 Bond angles
 Torsions	 Rings

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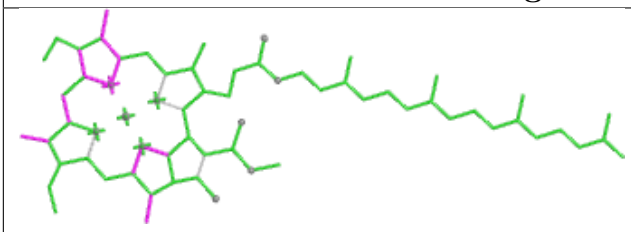
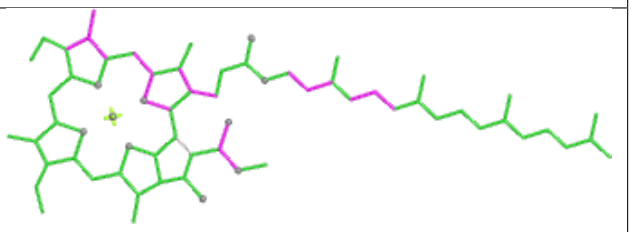
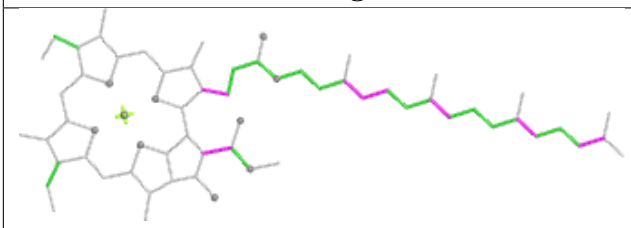
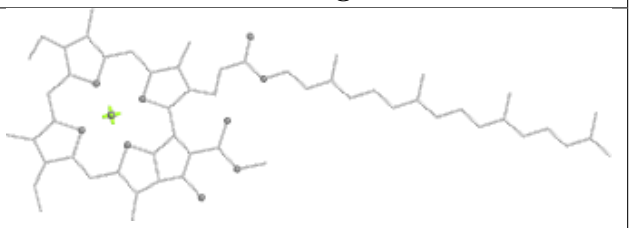
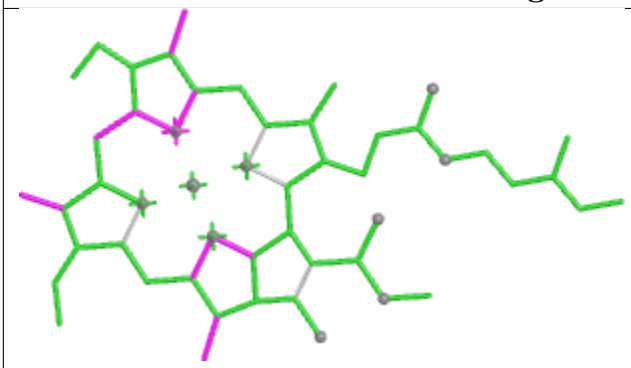
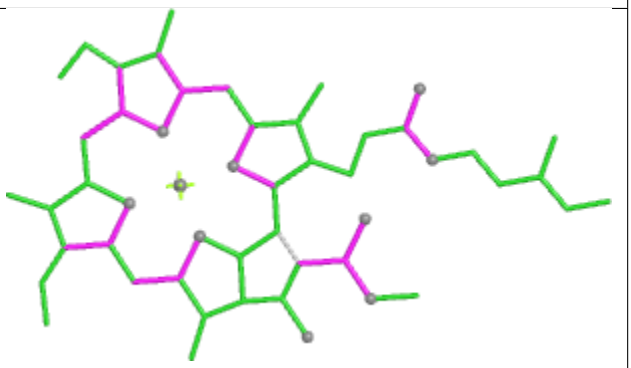
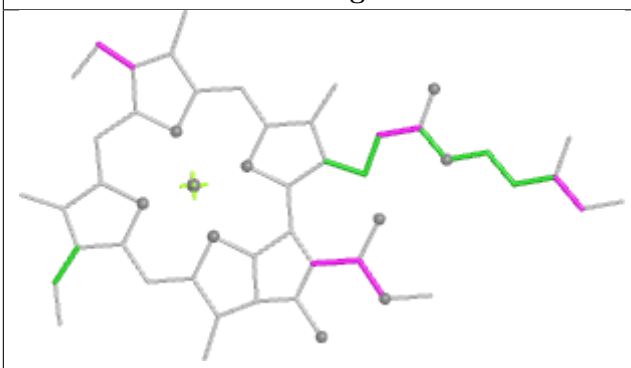
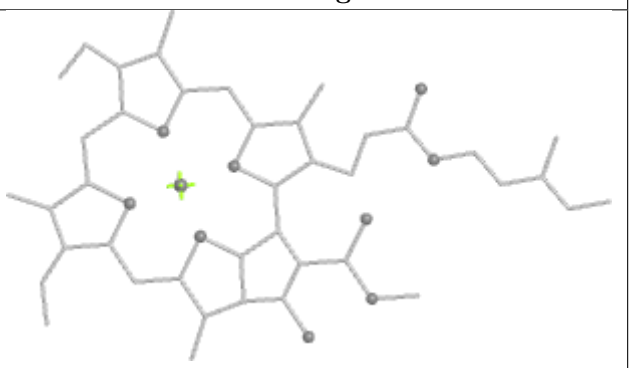
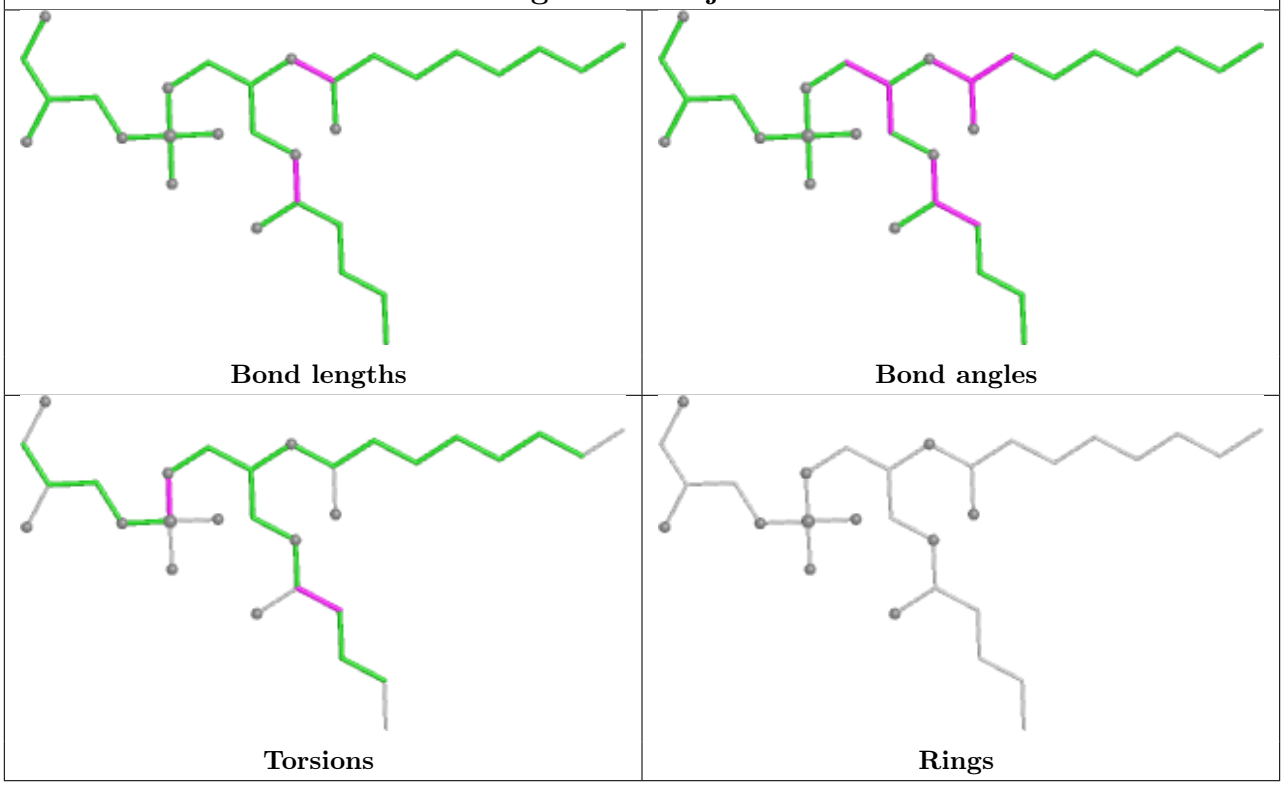
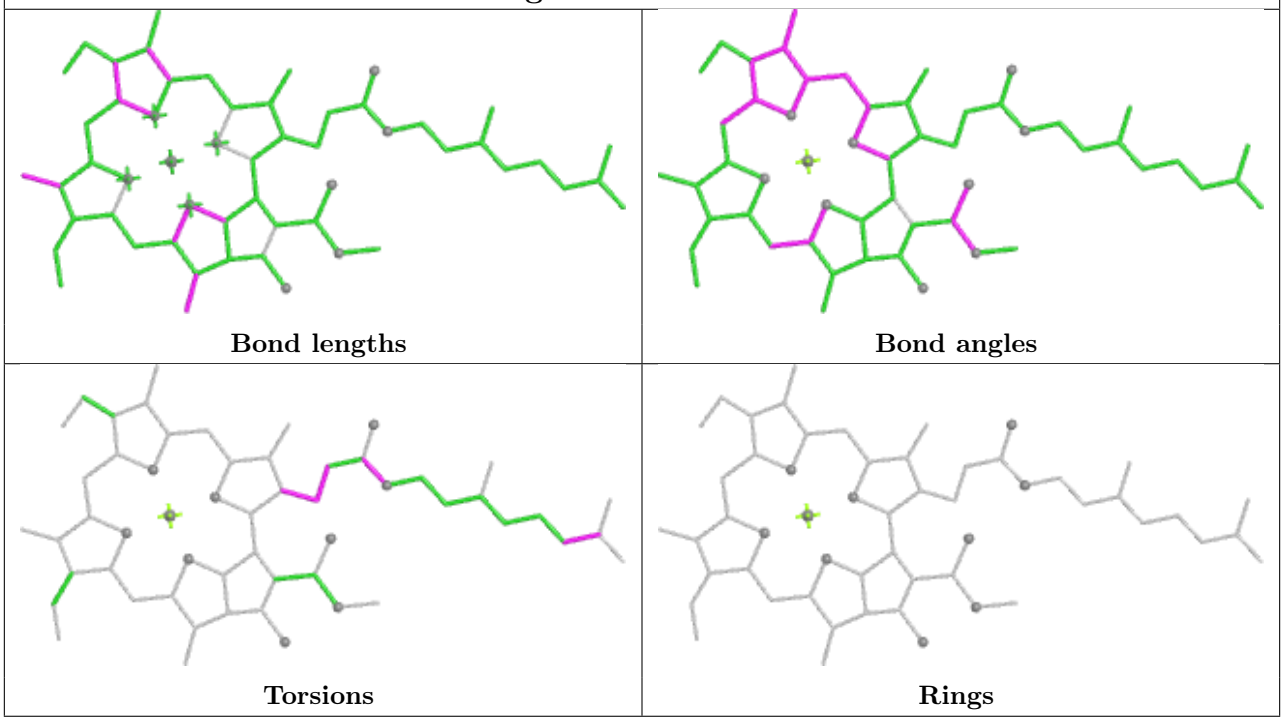
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA d 305	
 Bond lengths	 Bond angles
 Torsions	 Rings

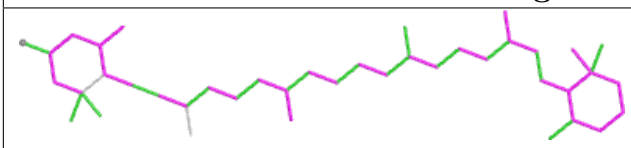
Ligand LHG j 319



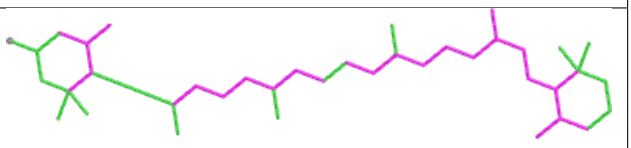
Ligand CLA B 815



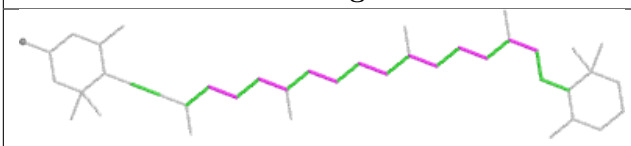
Ligand IHT c 615



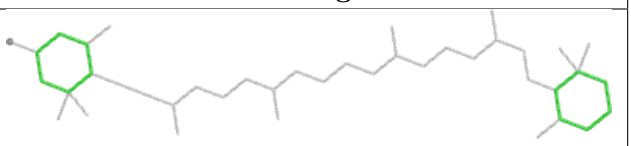
Bond lengths



Bond angles

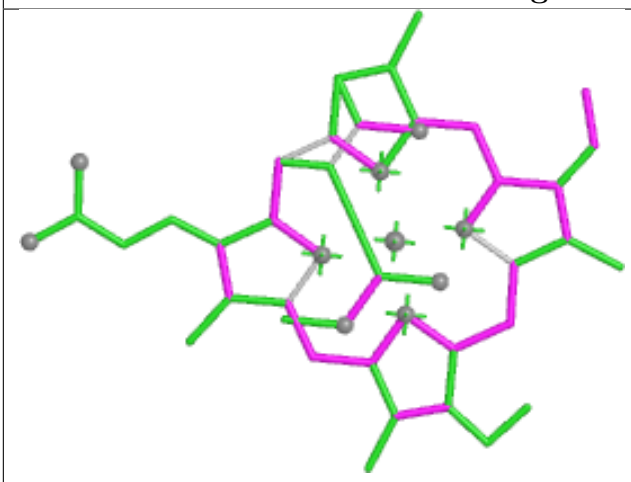


Torsions



Rings

Ligand KC2 e 609



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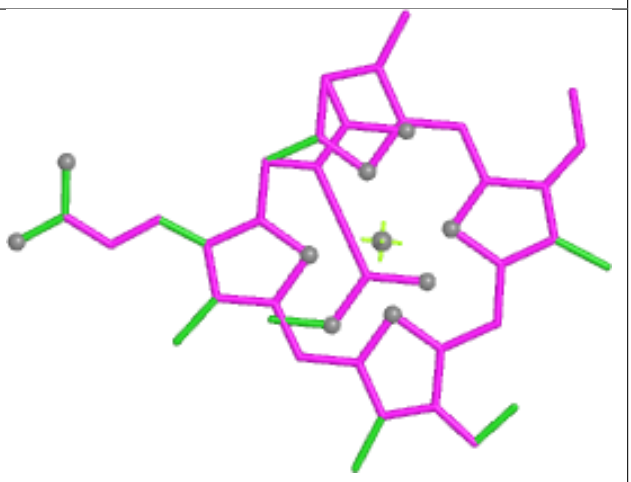

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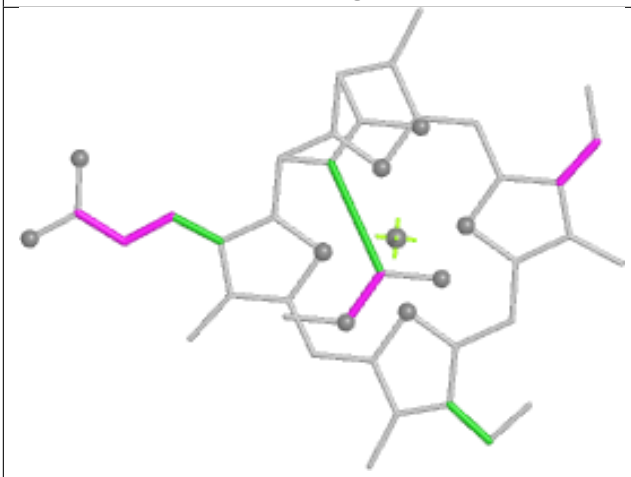

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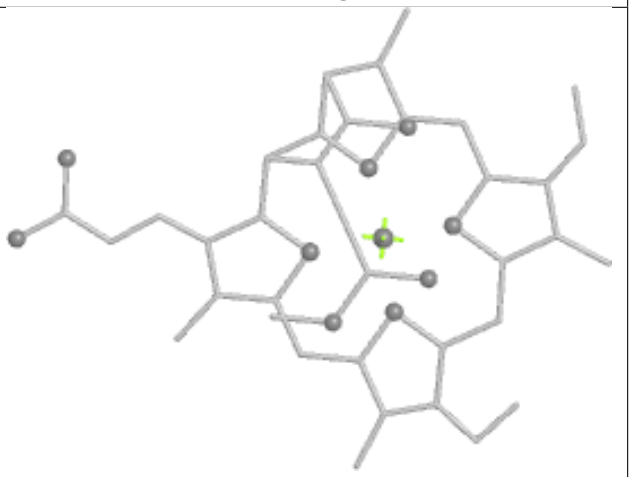
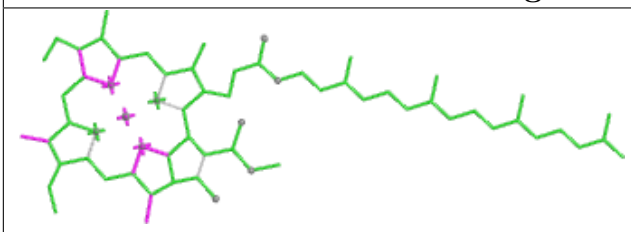


Rings

Ligand CLA B 840



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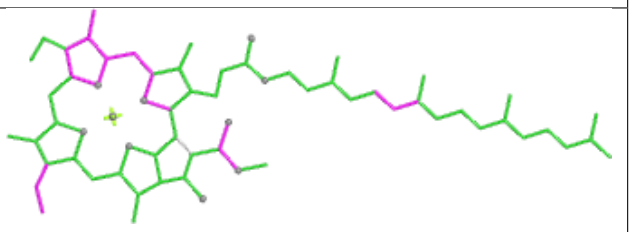
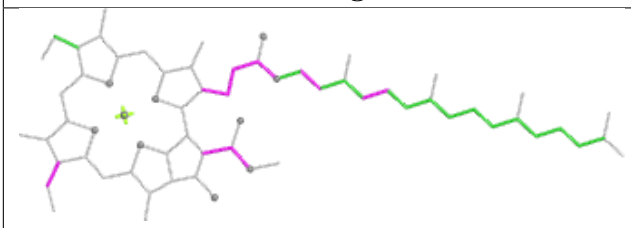


Bond angles



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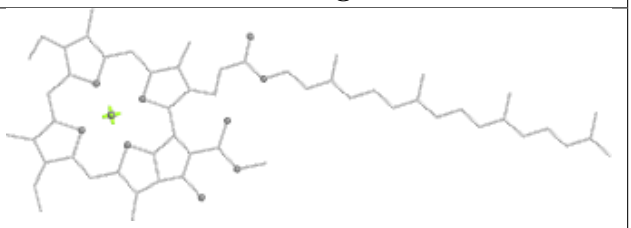
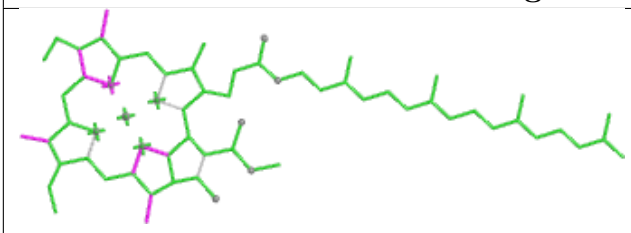


Rings

Ligand CLA B 835



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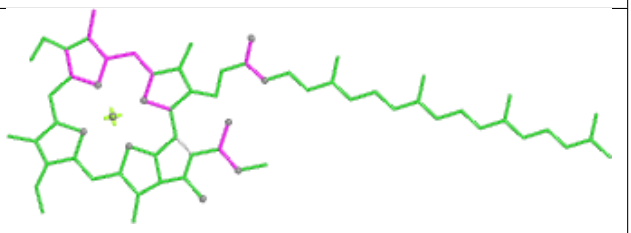

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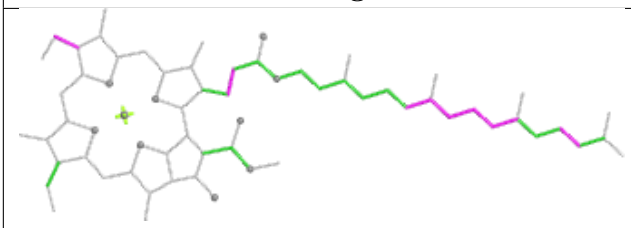

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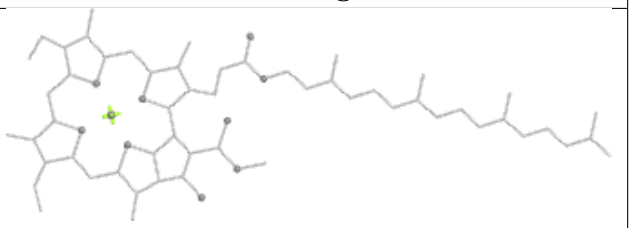
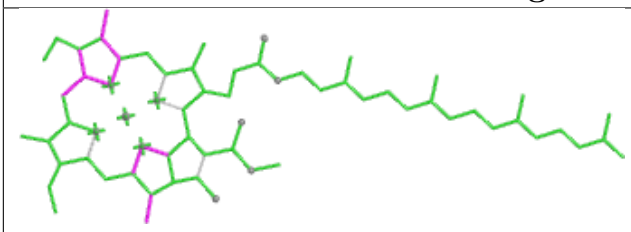


Rings

Ligand CLA g 305



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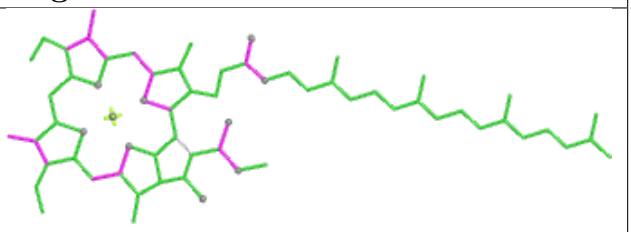

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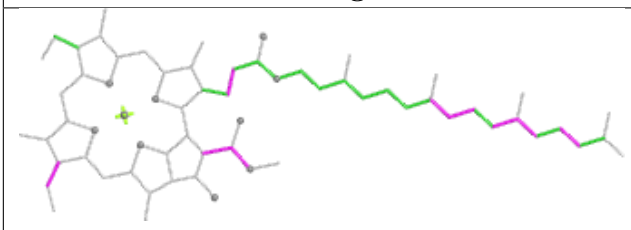

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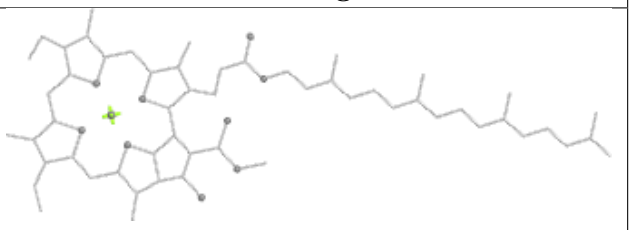
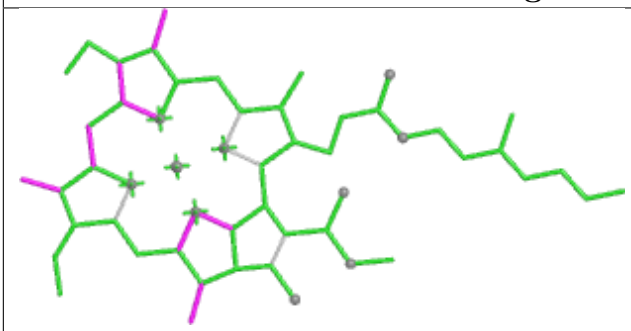
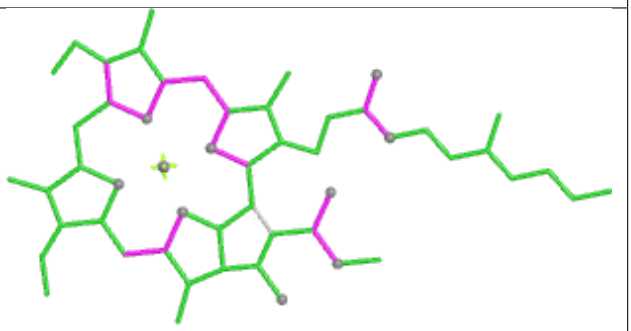


Rings

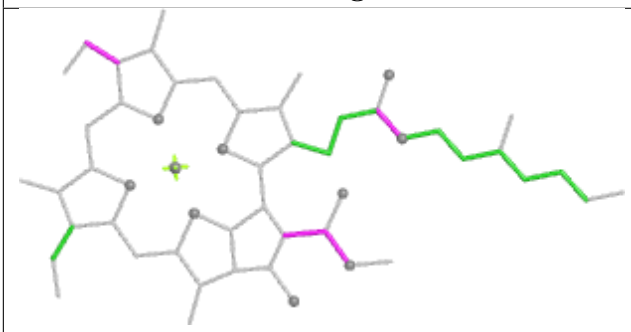
Ligand CLA B 821



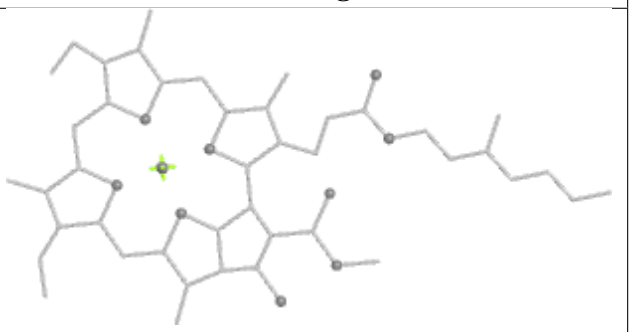
Bond lengths



Bond angles

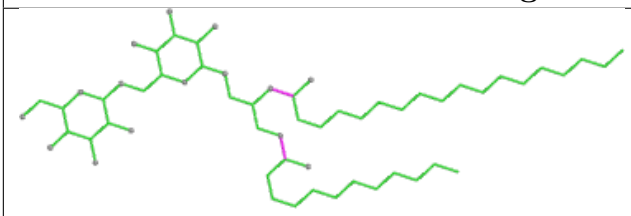


Torsions

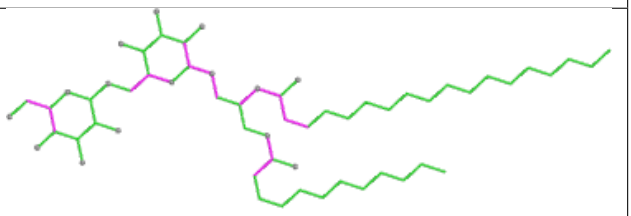


Rings

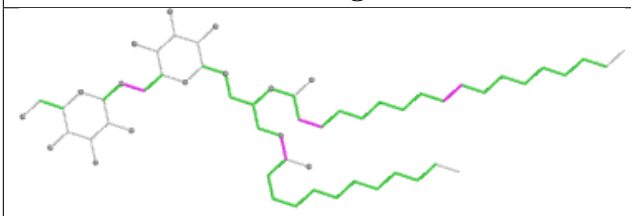
Ligand DGD B 843



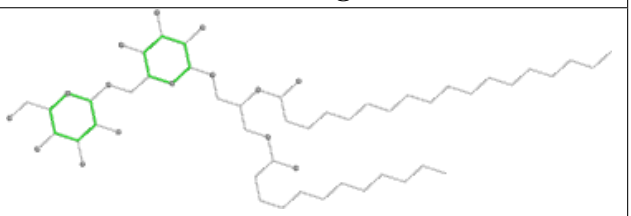
Bond lengths



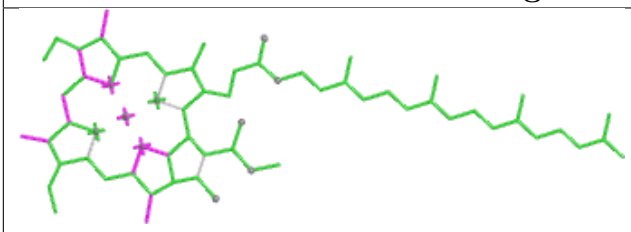
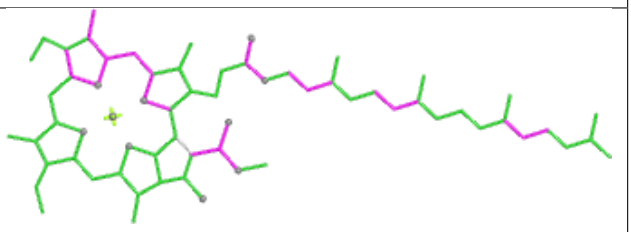
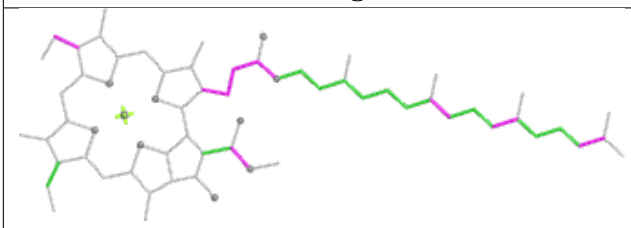
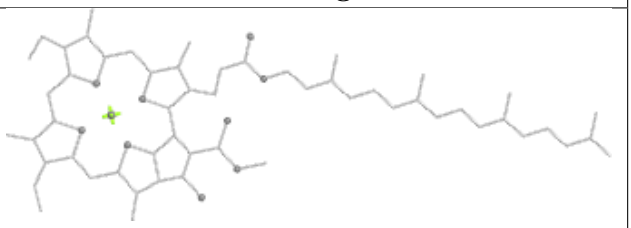
Bond angles

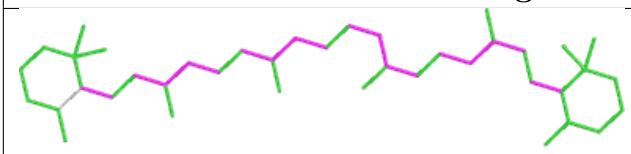
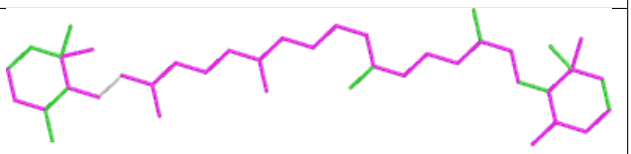
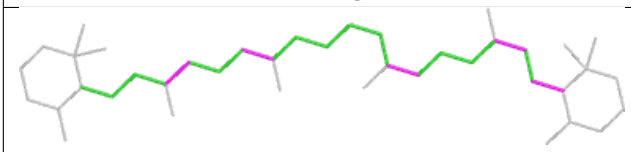
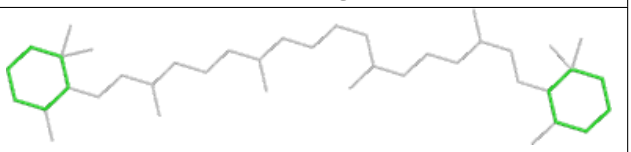


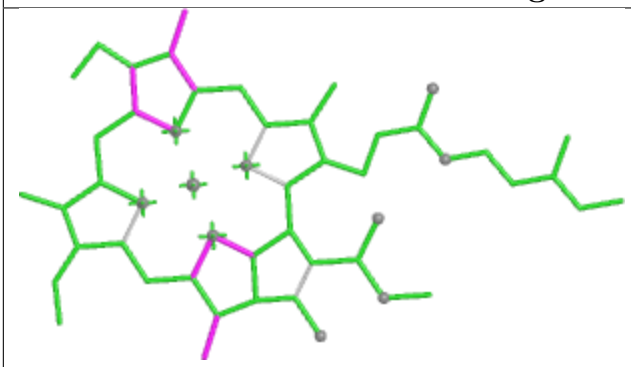
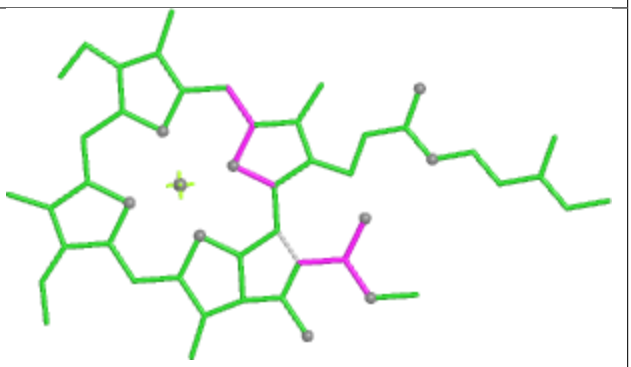
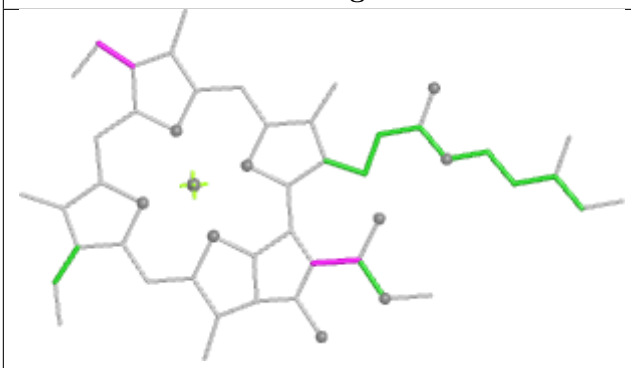
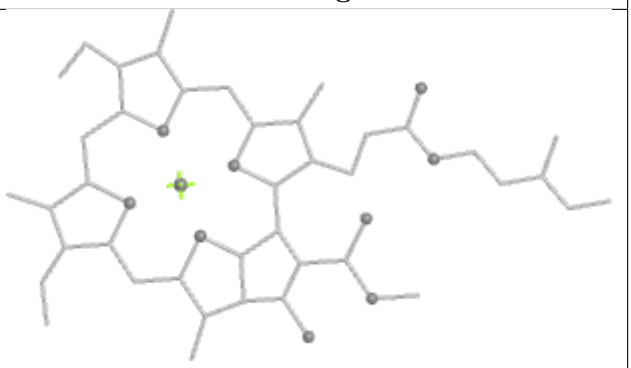
Torsions

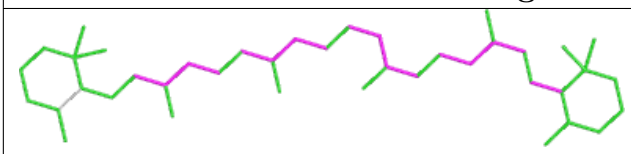
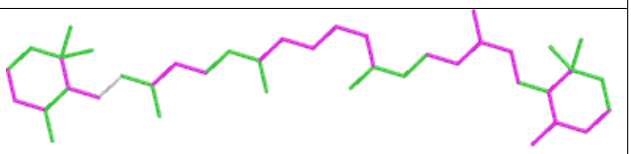
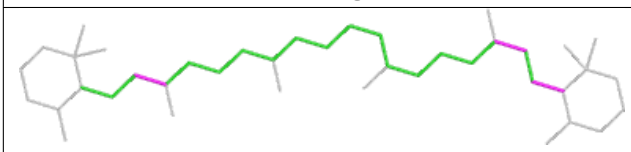
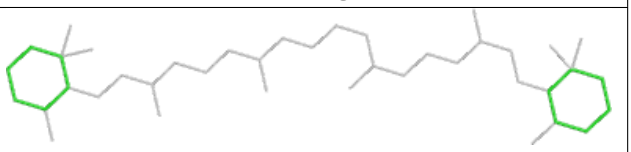


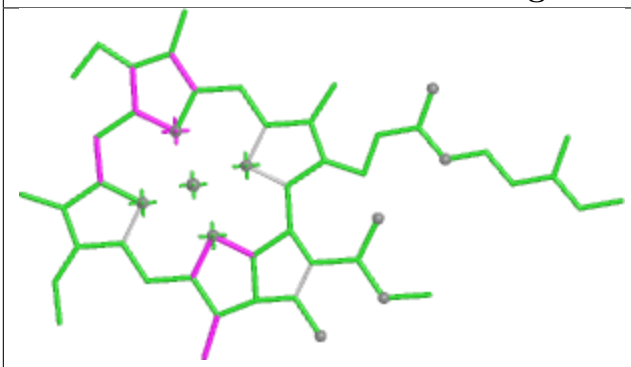
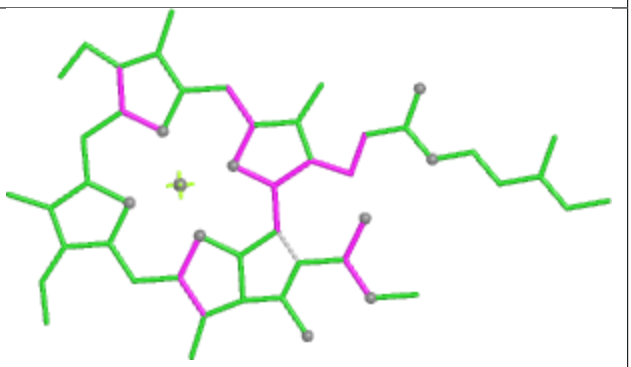
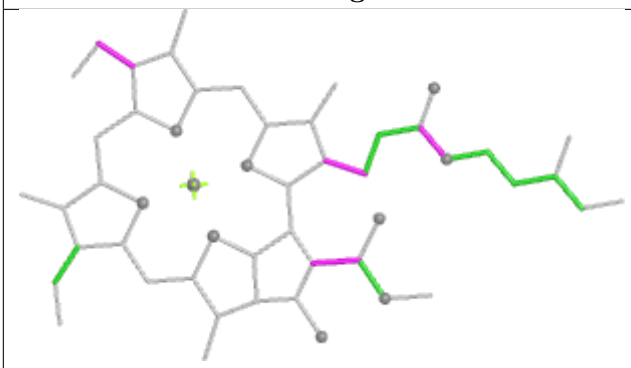
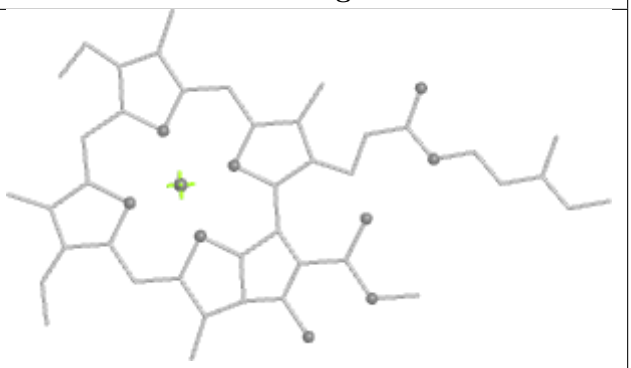
Rings

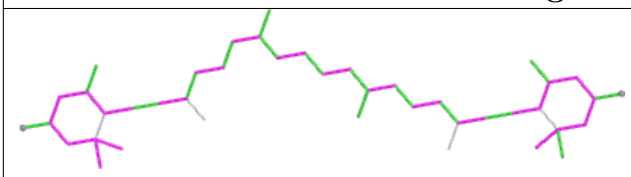
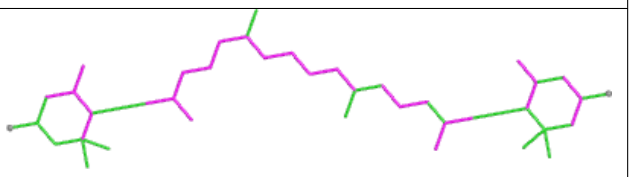
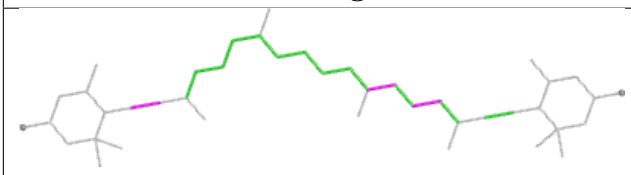
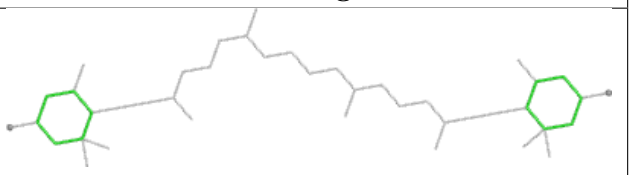
Ligand CLA A 817	
 Bond lengths	 Bond angles
 Torsions	 Rings

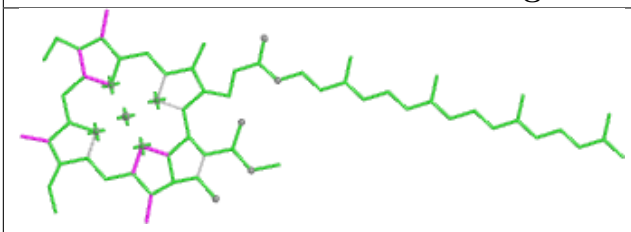
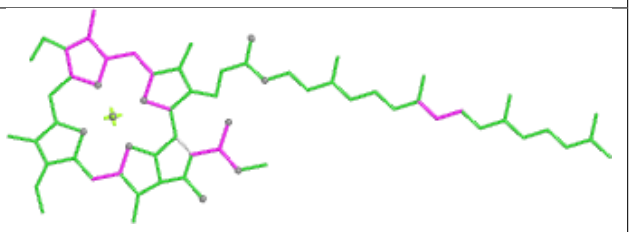
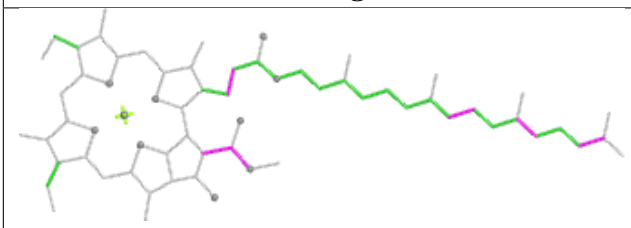
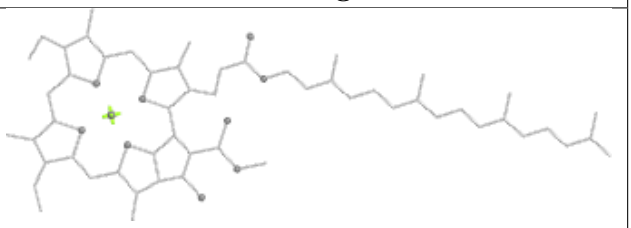
Ligand WVN A 847	
 Bond lengths	 Bond angles
 Torsions	 Rings

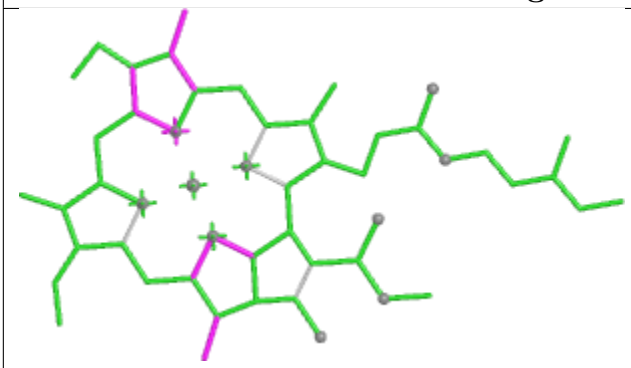
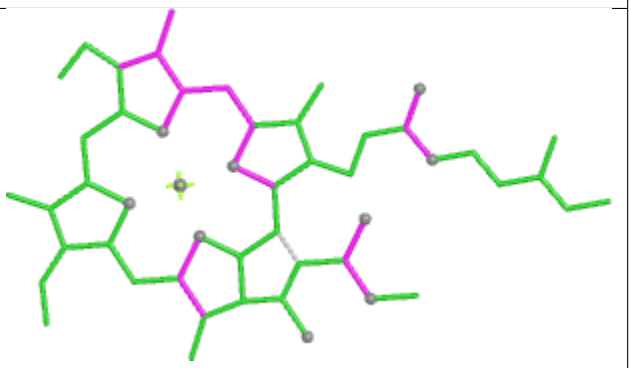
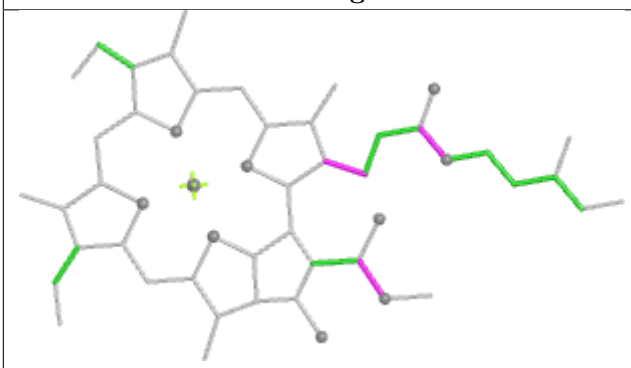
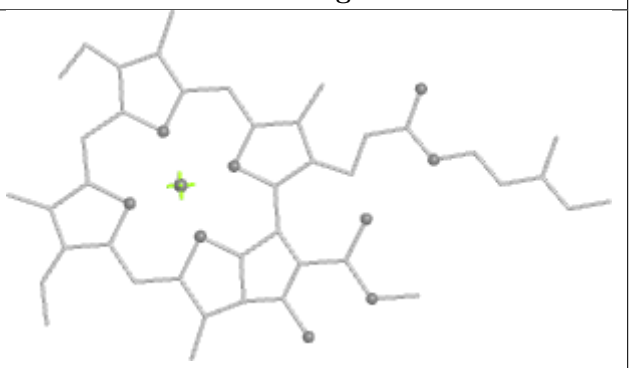
Ligand CLA a 304	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand WVN L 205	
 Bond lengths	 Bond angles
 Torsions	 Rings

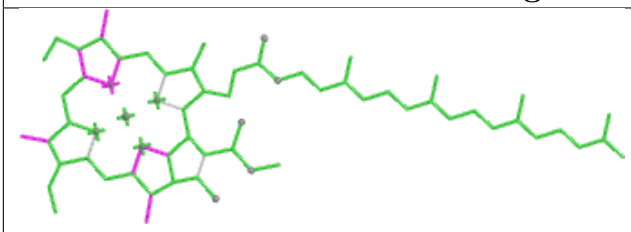
Ligand CLA J 105	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand II0 i 613	
 Bond lengths	 Bond angles
 Torsions	 Rings

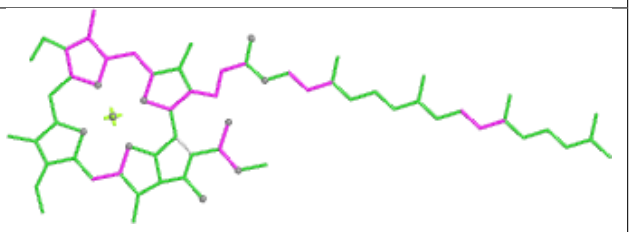
Ligand CLA A 807	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA h 304	
 Bond lengths	 Bond angles
 Torsions	 Rings

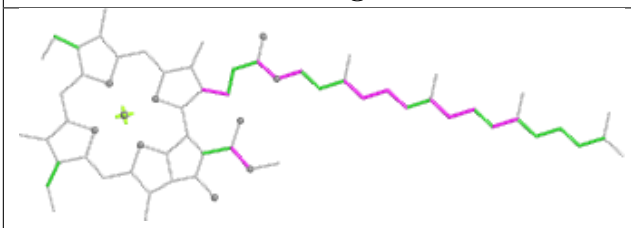
Ligand CLA A 802



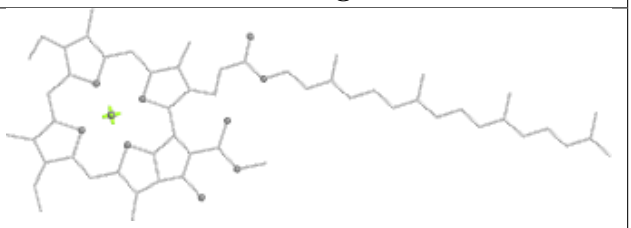
Bond lengths



Bond angles

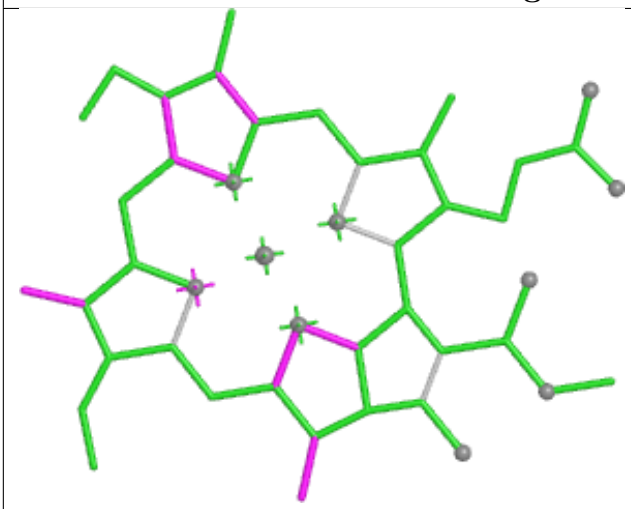


Torsions

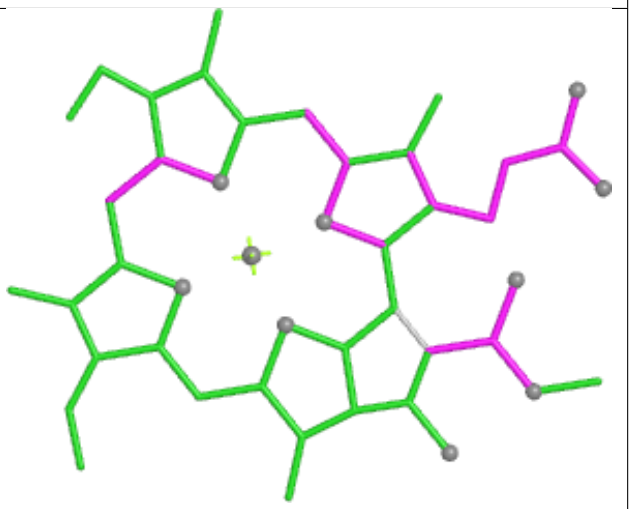


Rings

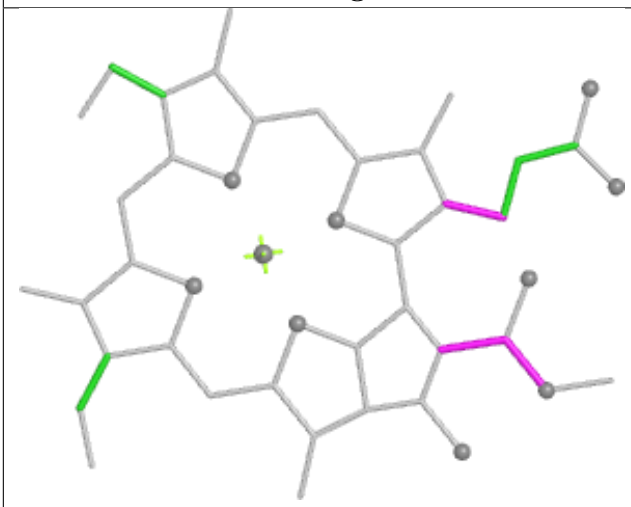
Ligand CLA A 813



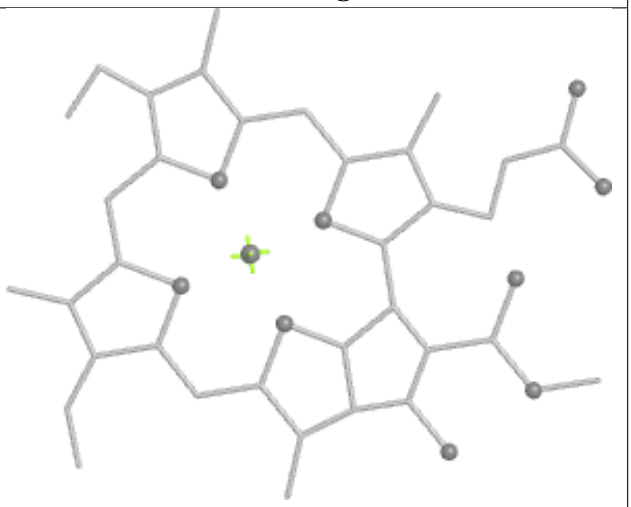
Bond lengths



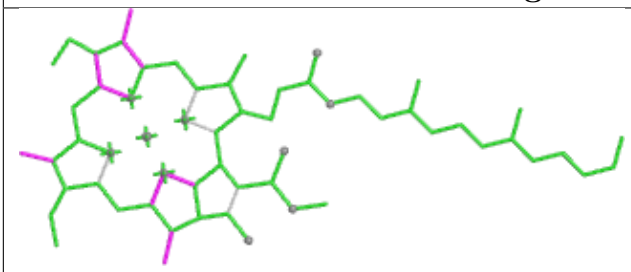
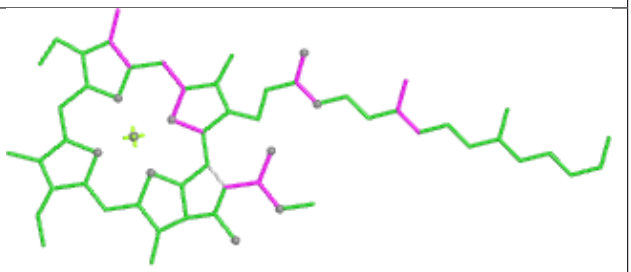
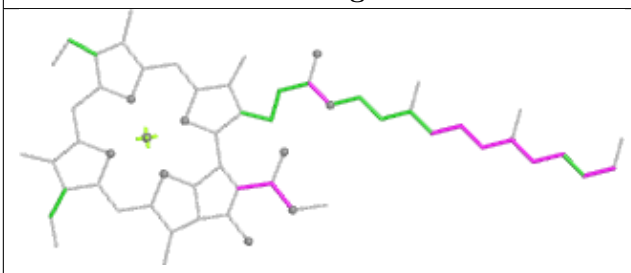
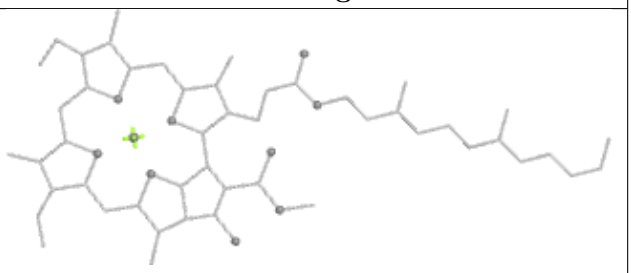
Bond angles

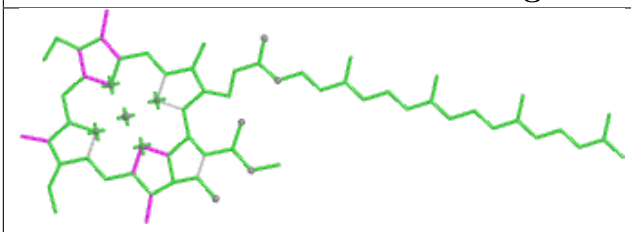
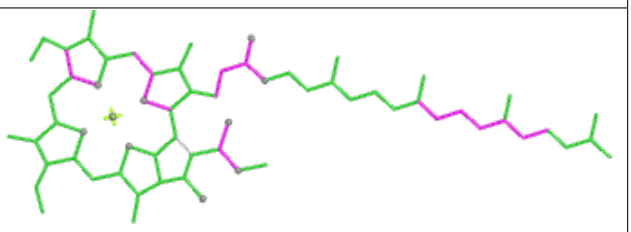
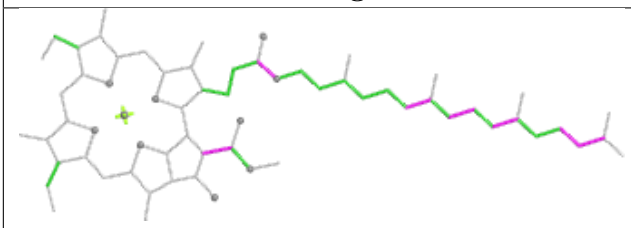
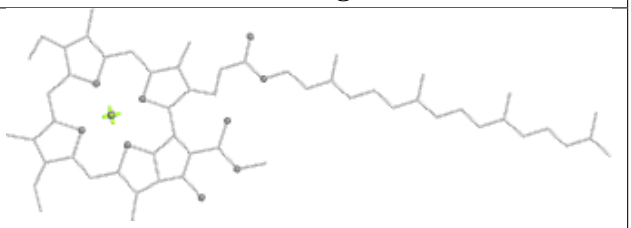


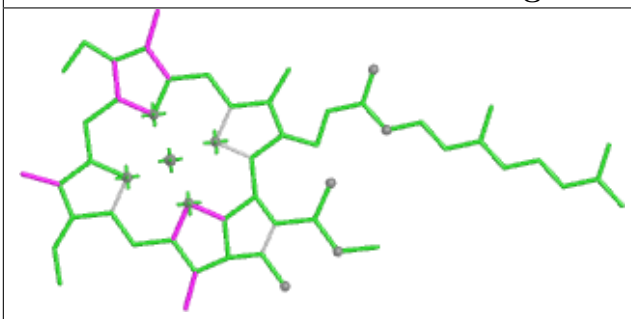
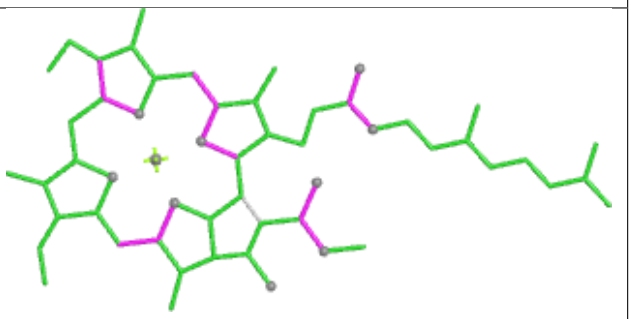
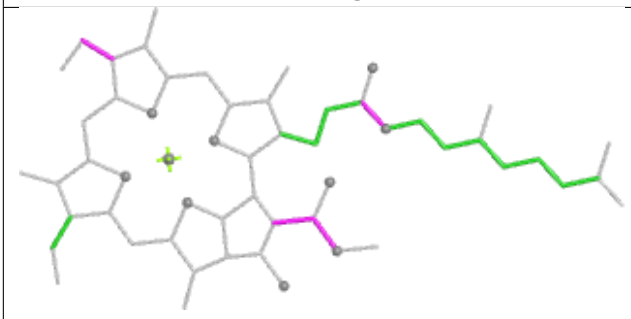
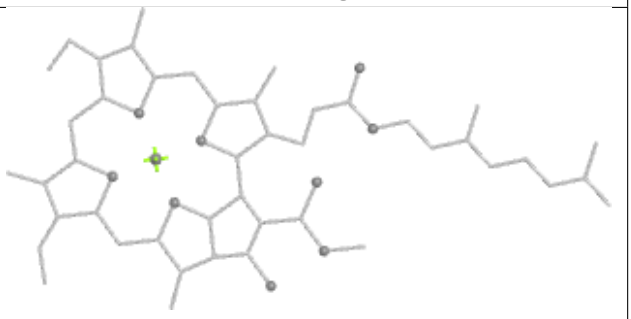
Torsions



Rings

Ligand CLA B 814	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA A 806	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA A 823	
 Bond lengths	 Bond angles
 Torsions	 Rings

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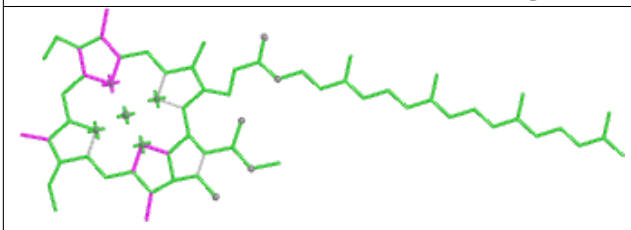
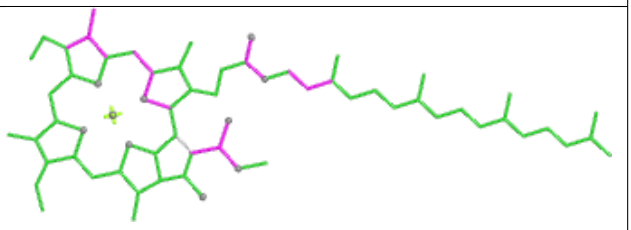
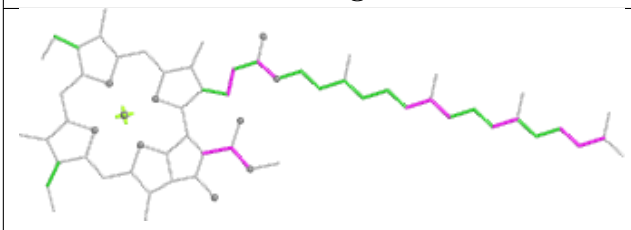
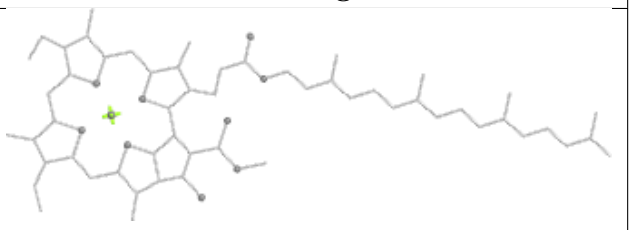
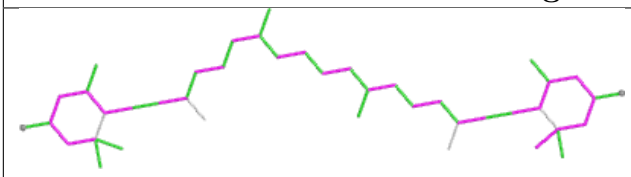
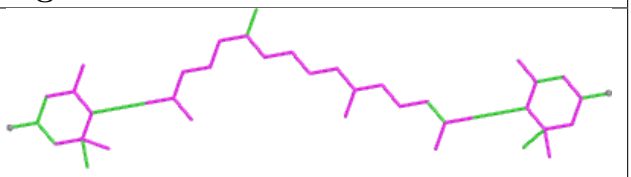
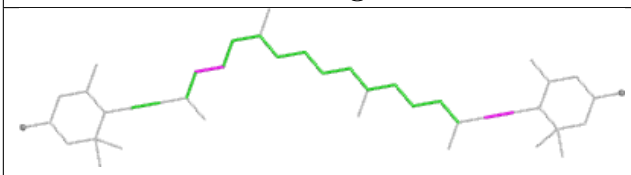
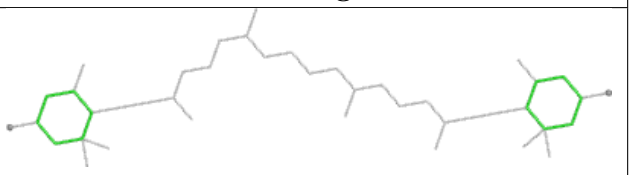
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand II0 g 318	
 Bond lengths	 Bond angles
 Torsions	 Rings

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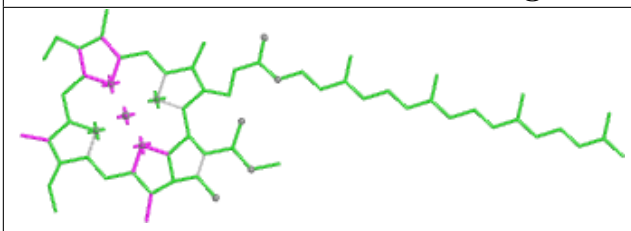
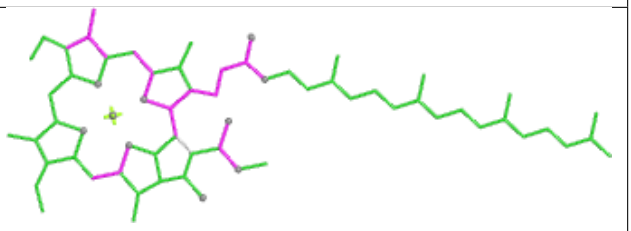
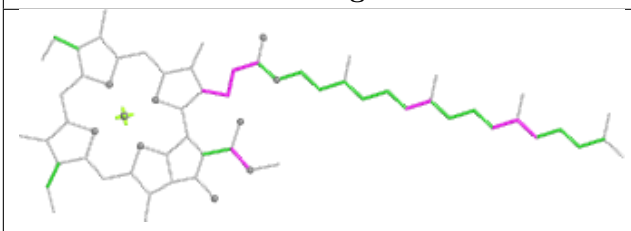
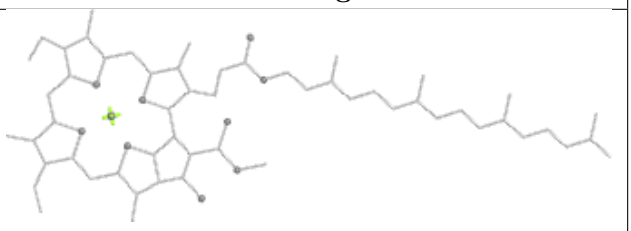
 Bond lengths	 Bond angles
 Torsions	 Rings

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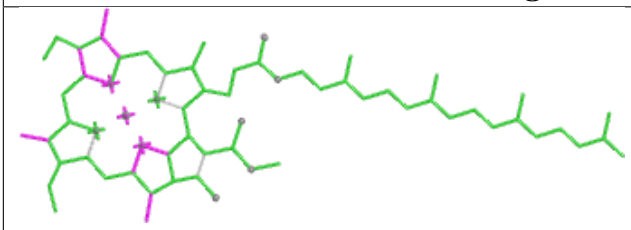
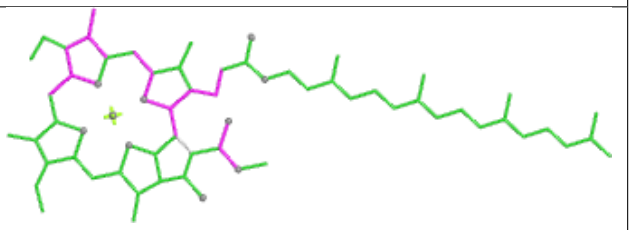
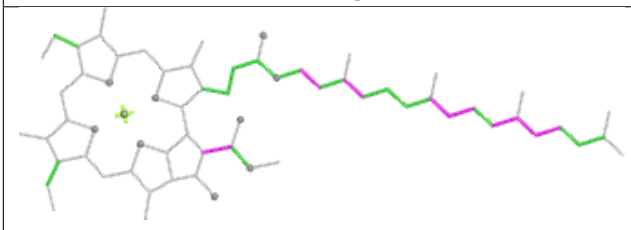
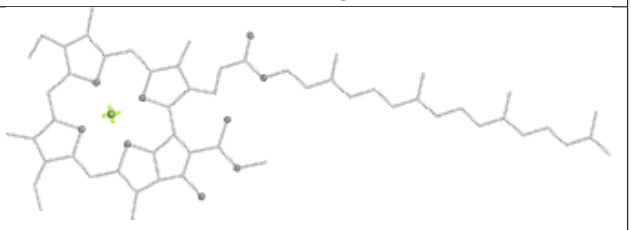
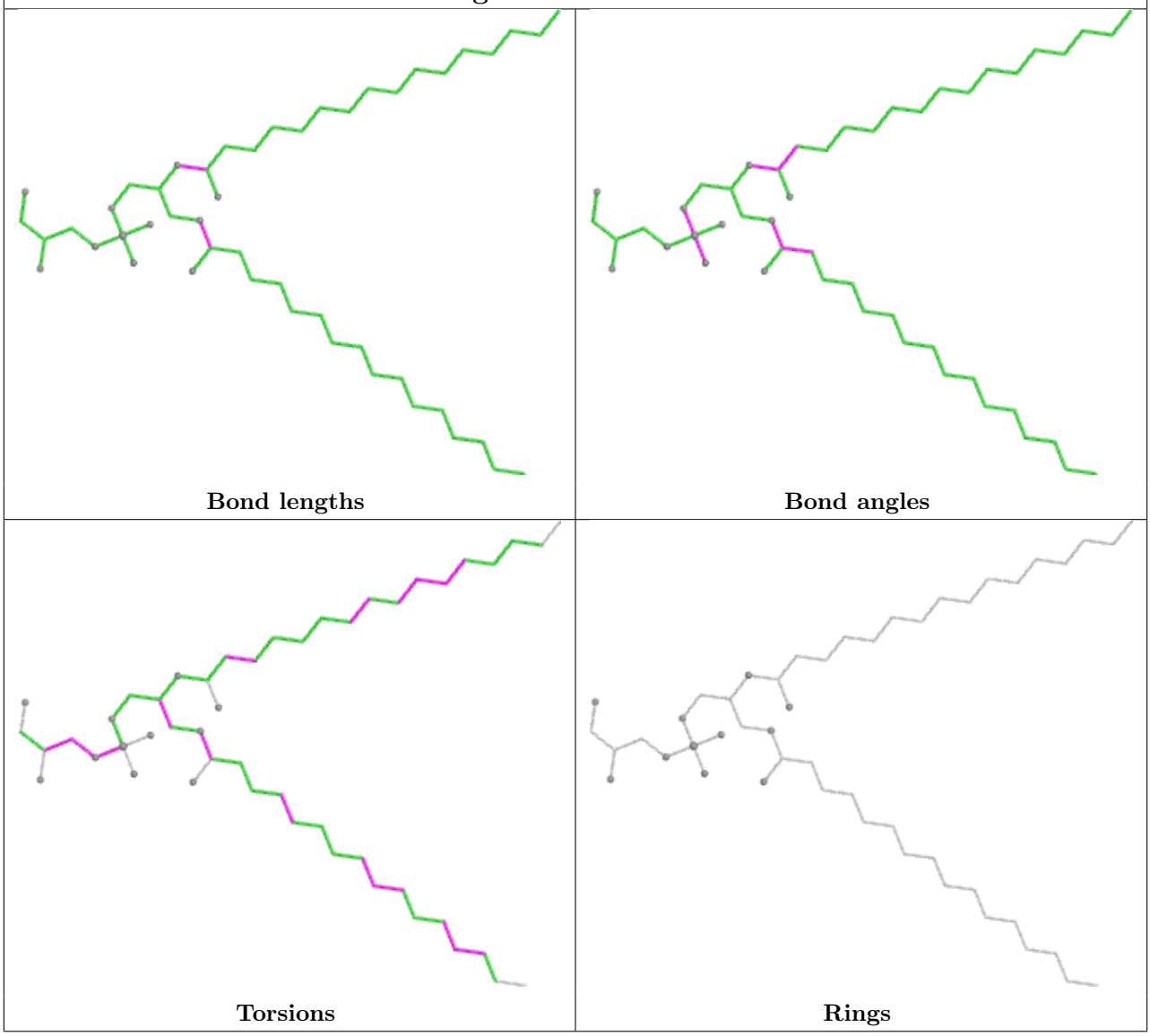
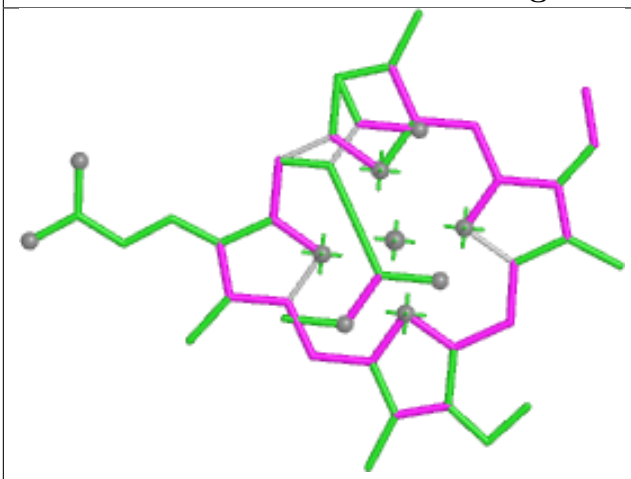
 Bond lengths	 Bond angles
 Torsions	 Rings

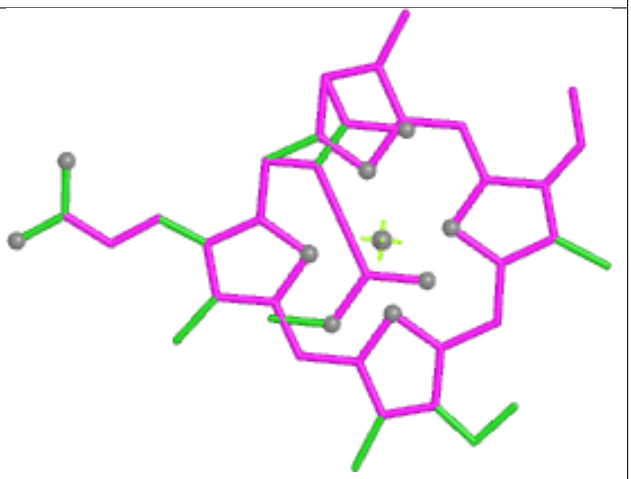
Ligand LHG J 107



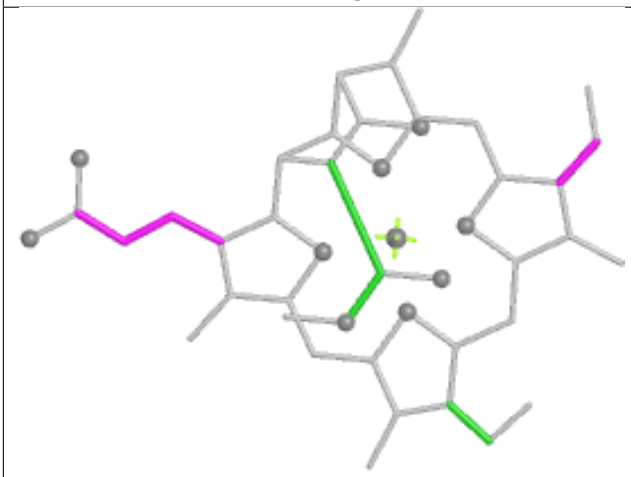
Ligand KC2 k 613



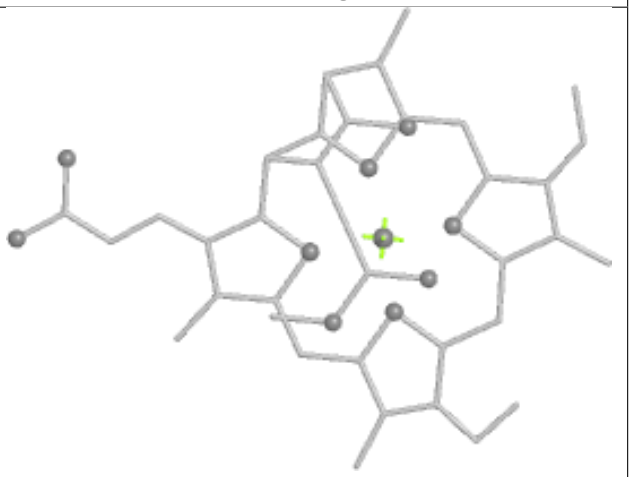
Bond lengths



Bond angles

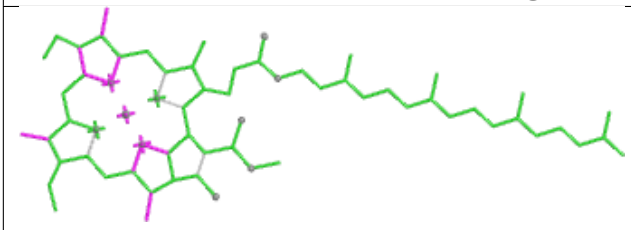


Torsions

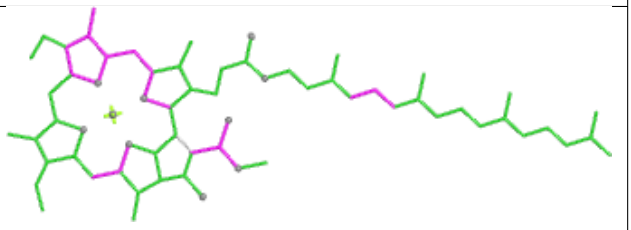


Rings

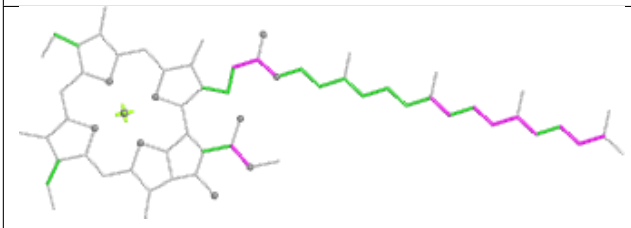
Ligand CLA B 806



Bond lengths



Bond angles



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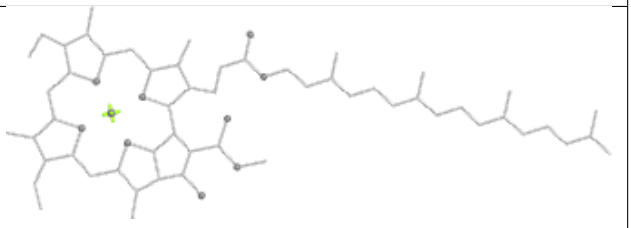
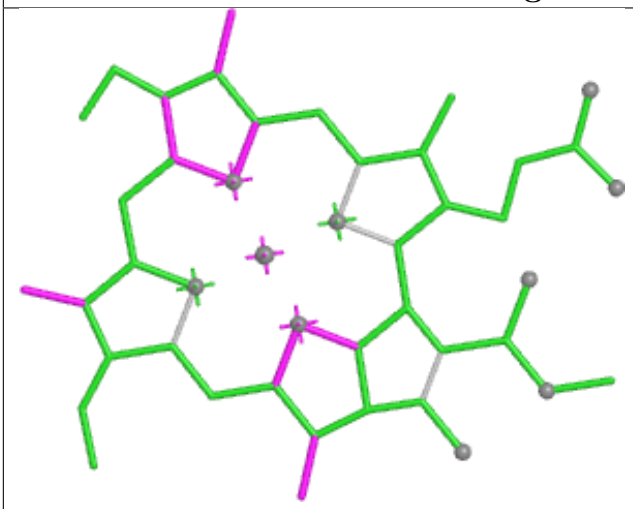


Rings

Ligand CLA B 831



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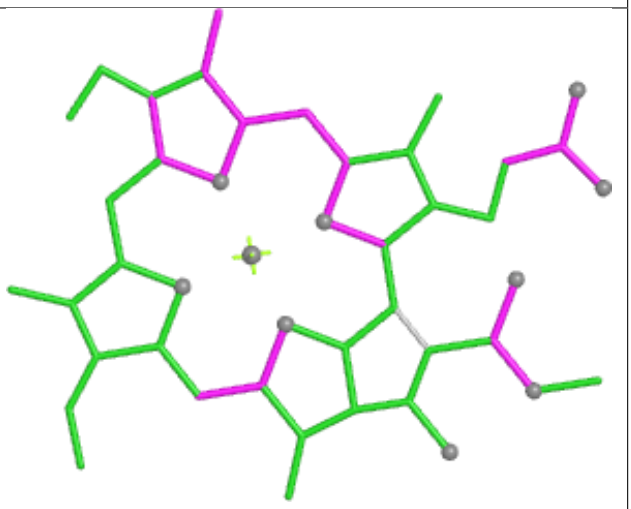
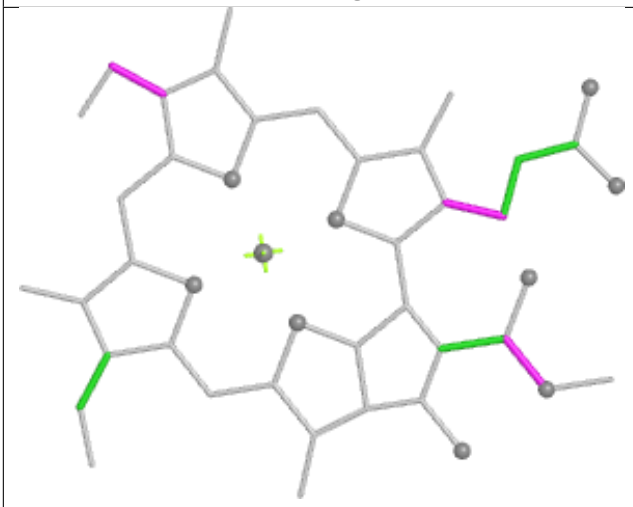


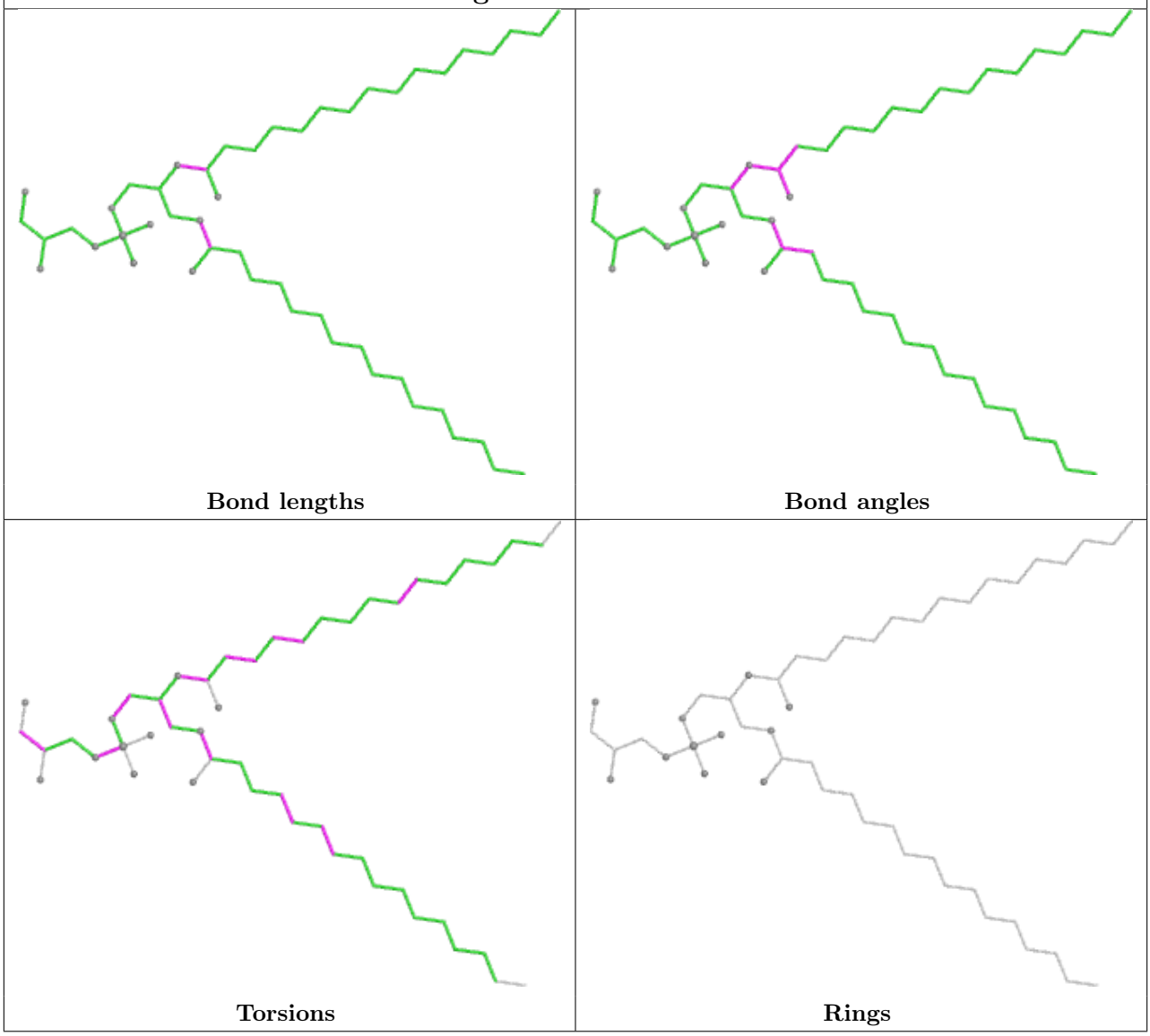
Bond angles



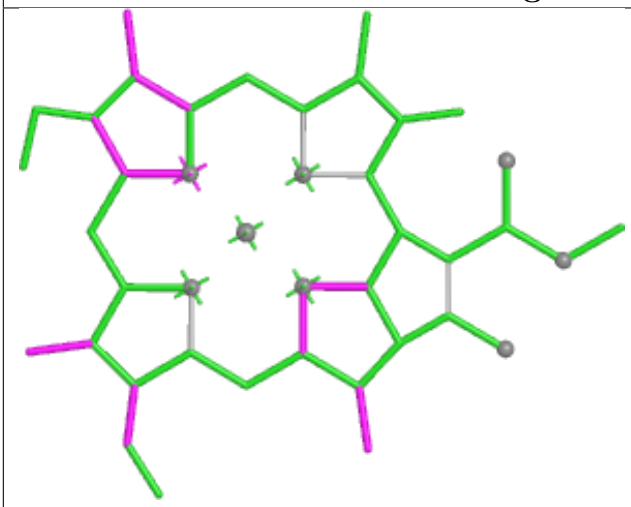
Torsions

Rings

Ligand LHG a 301



Ligand CLA A 856



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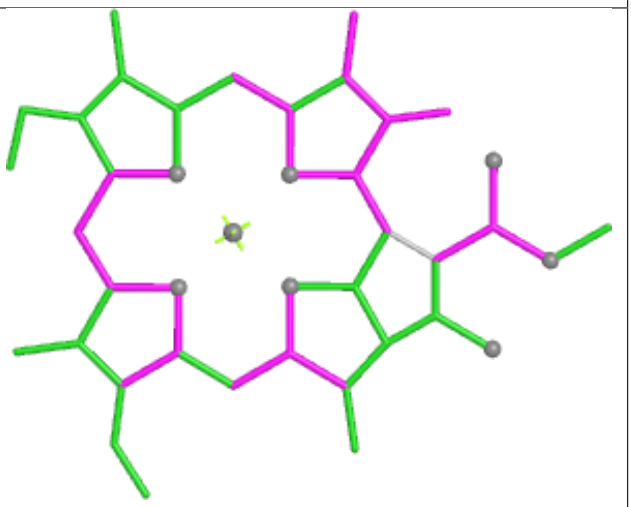
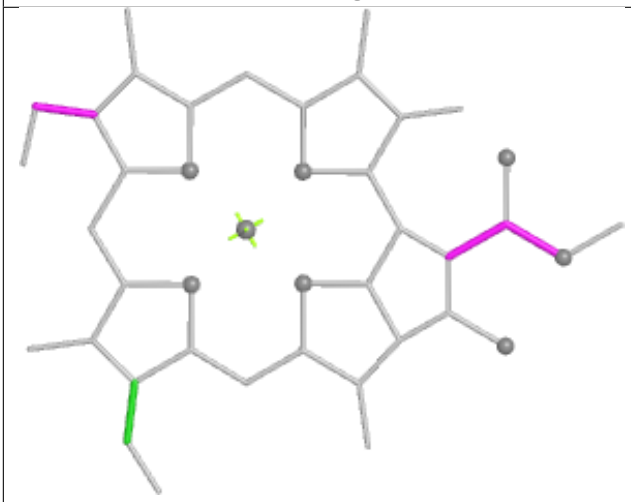


Bond angles



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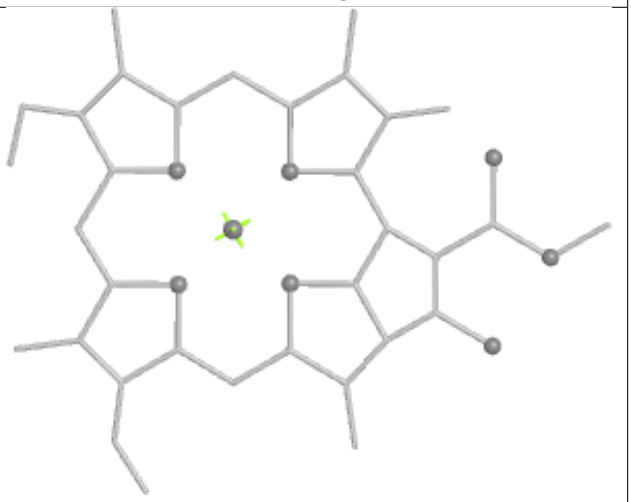
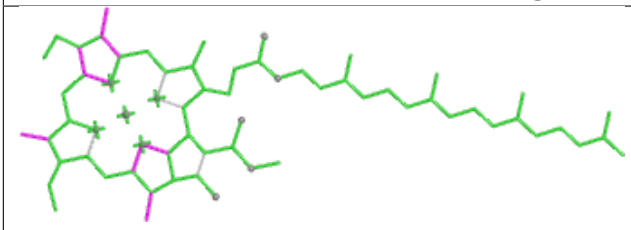


Rings

Ligand CLA e 604



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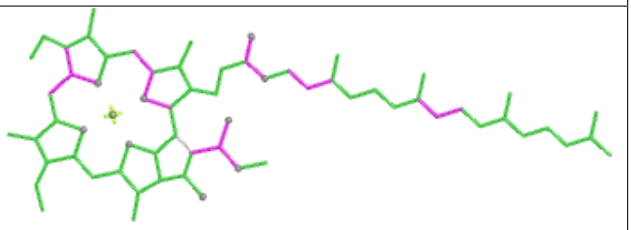
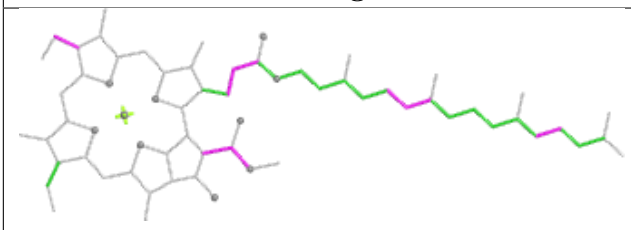


Bond angles



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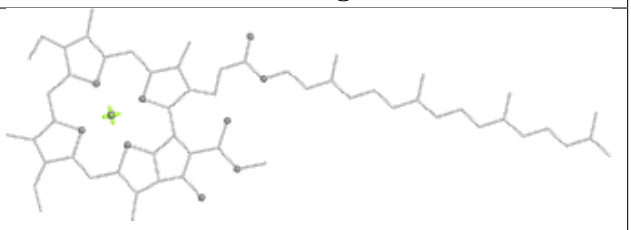
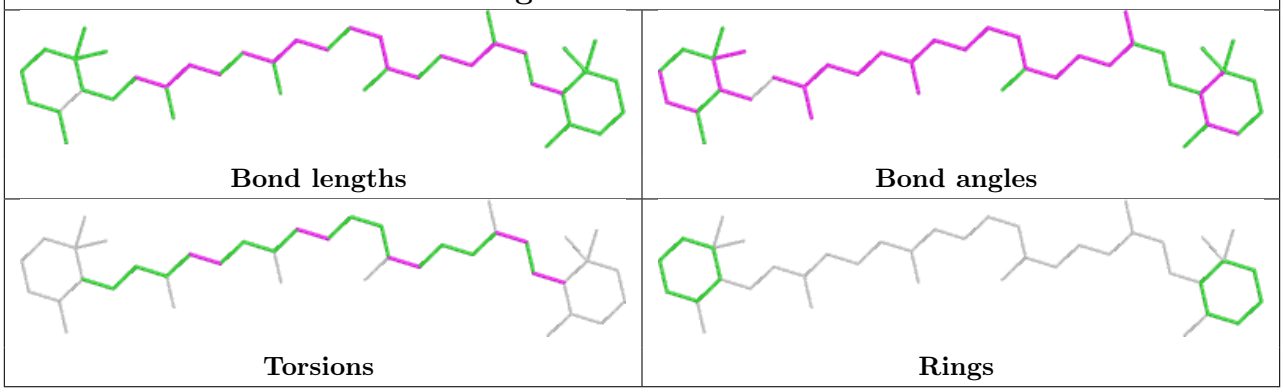
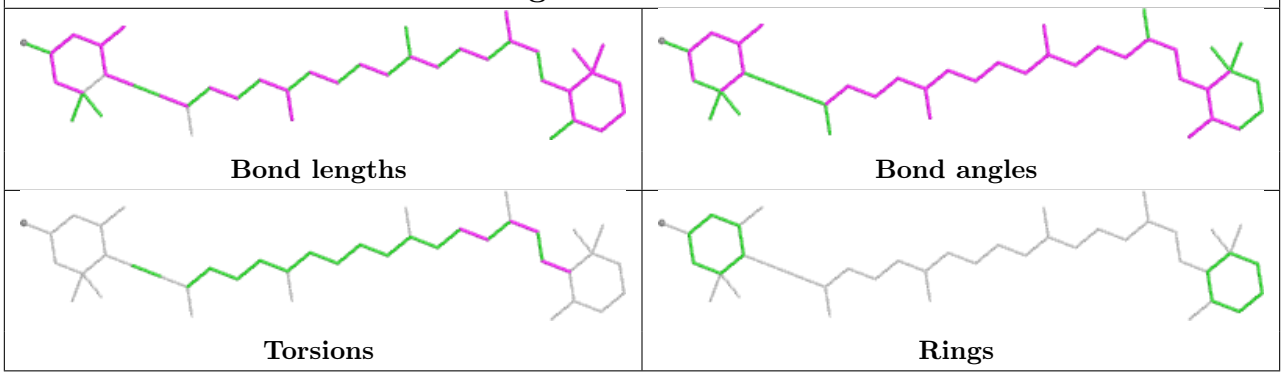


Rings

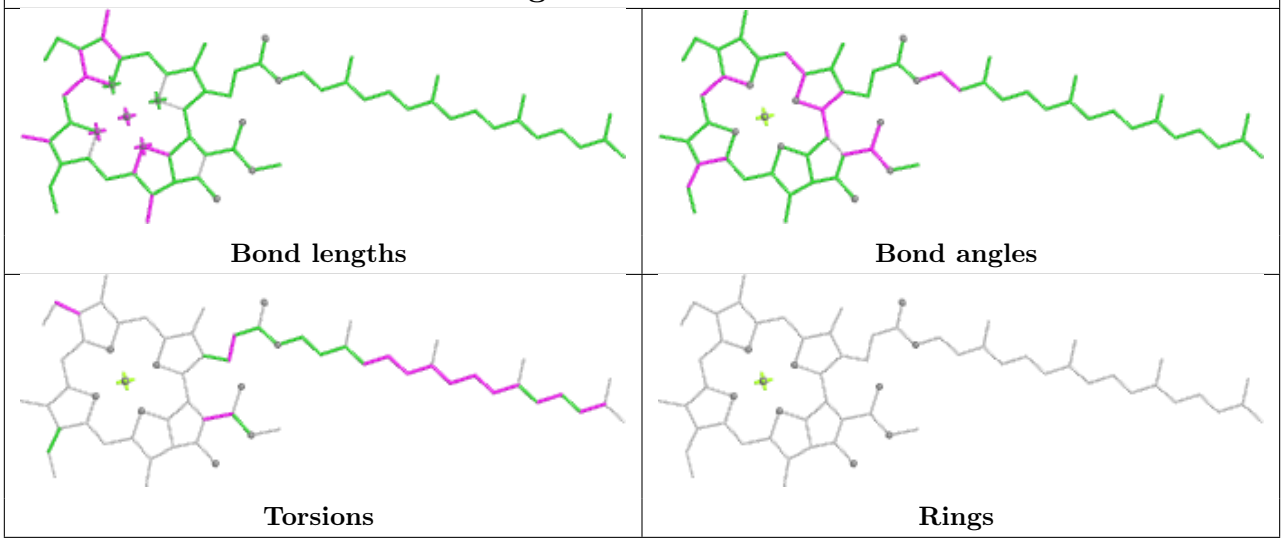
Ligand WVN K 103



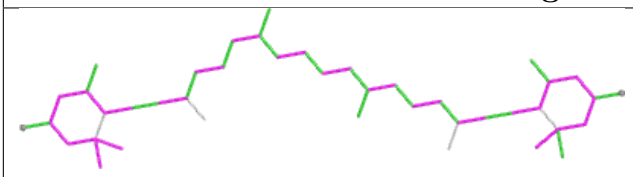
Ligand IHT O 203



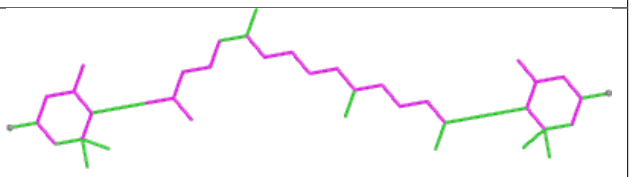
Ligand CLA b 306



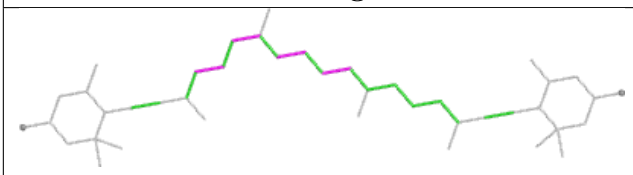
Ligand II0 d 314



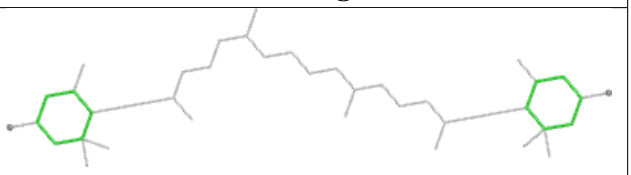
Bond lengths



Bond angles

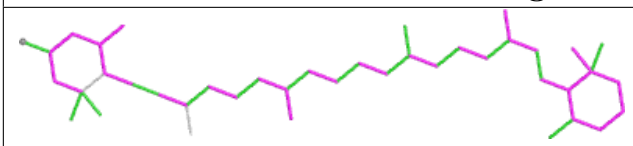


Torsions



Rings

Ligand IHT R 204



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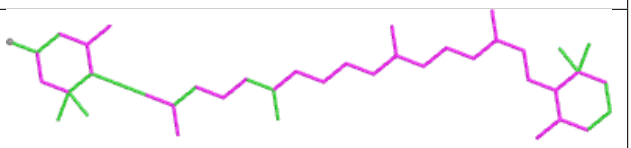
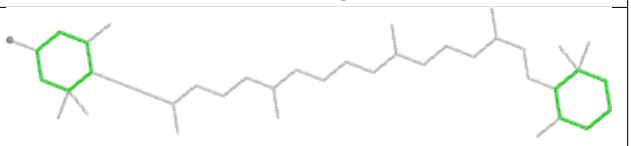


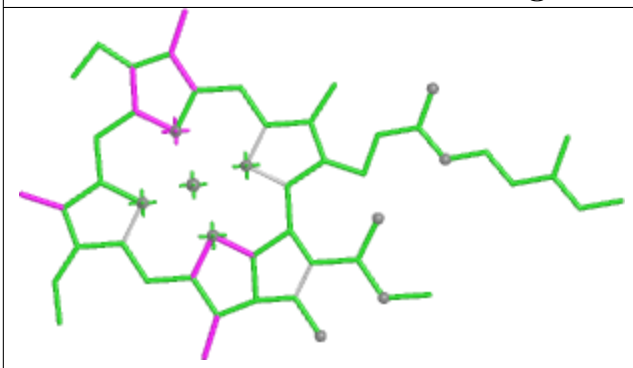
Bond angles

Torsions

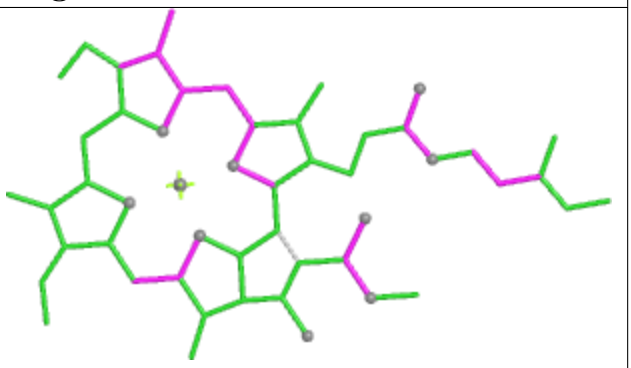


Rings

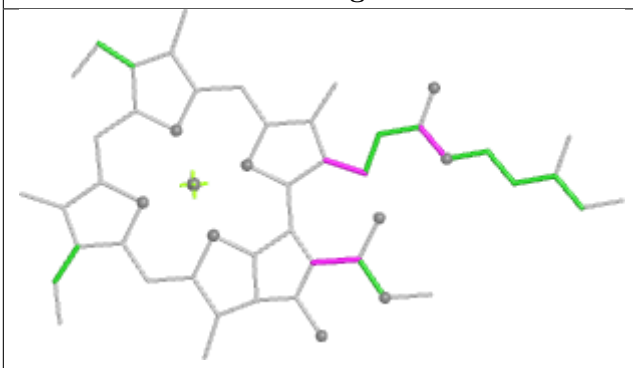
Ligand CLA g 310



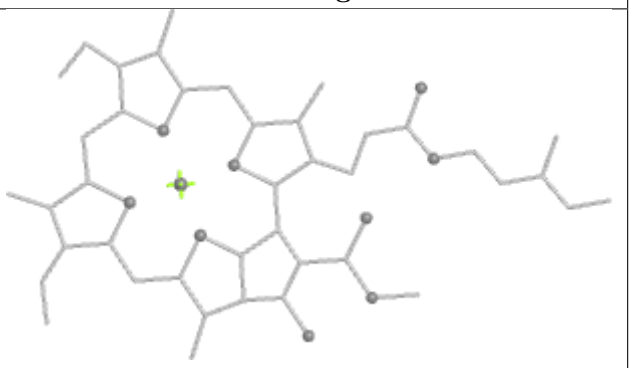
Bond lengths



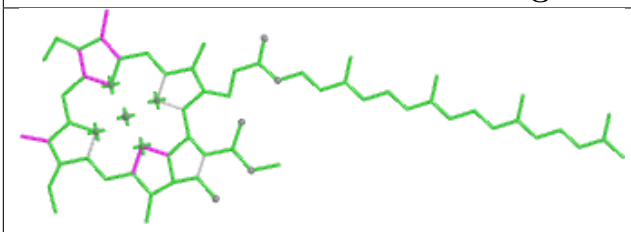
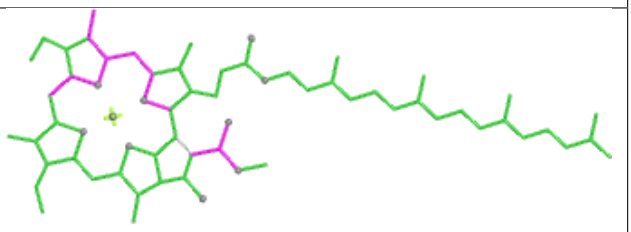
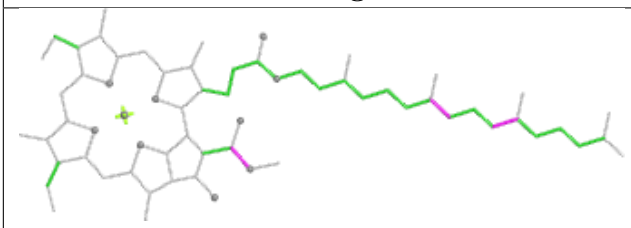
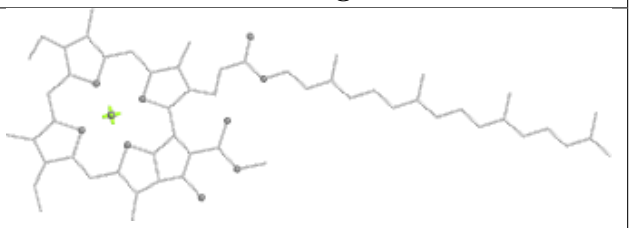
Bond angles

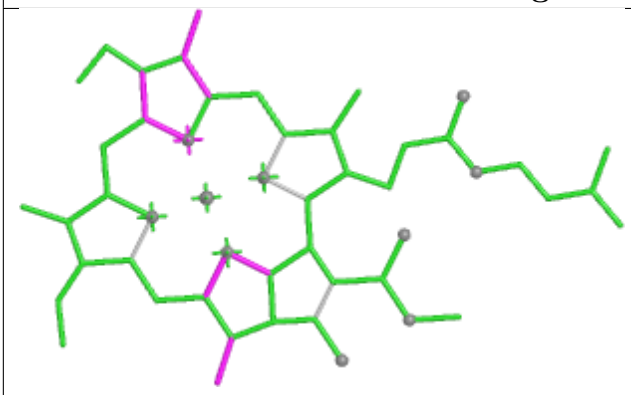
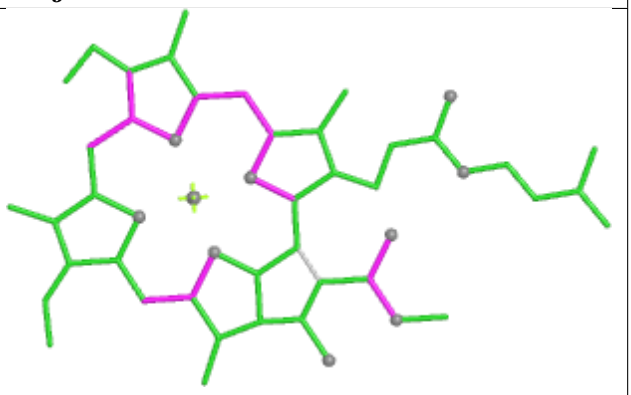
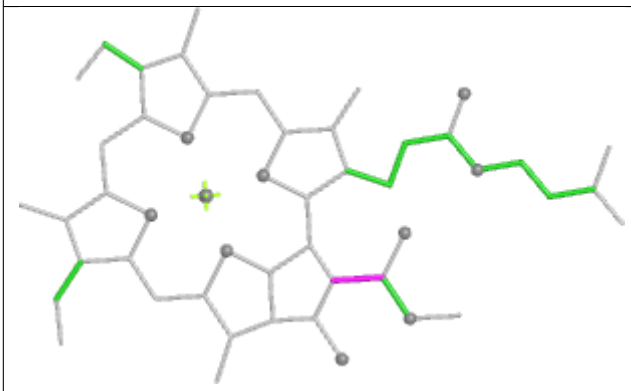
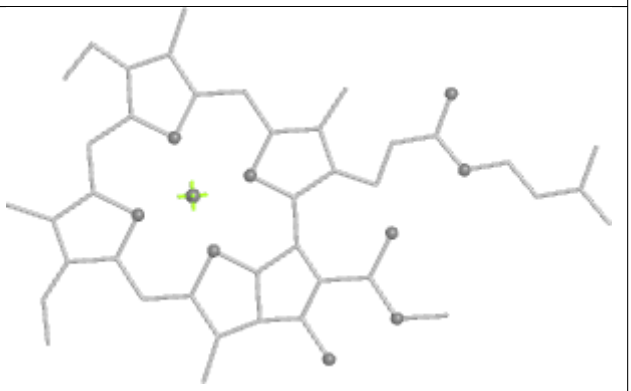


Torsions

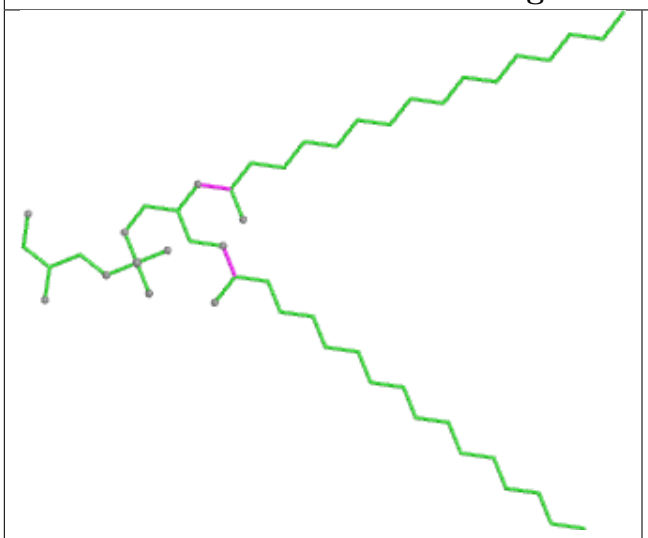


Rings

Ligand CLA f 609	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA j 303	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand LHG b 320



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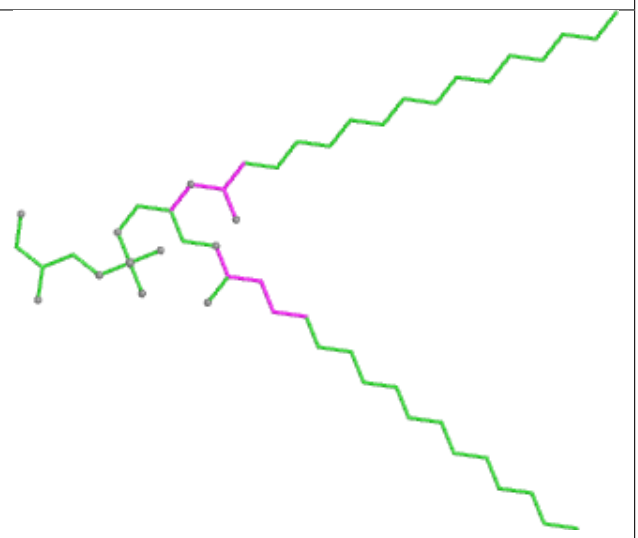
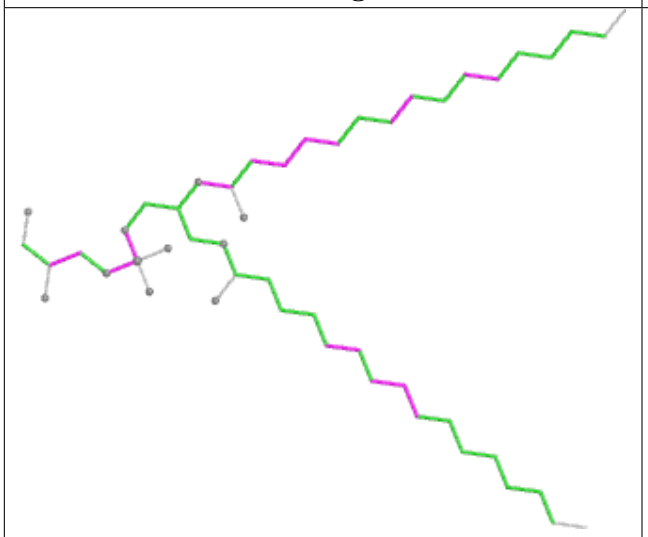
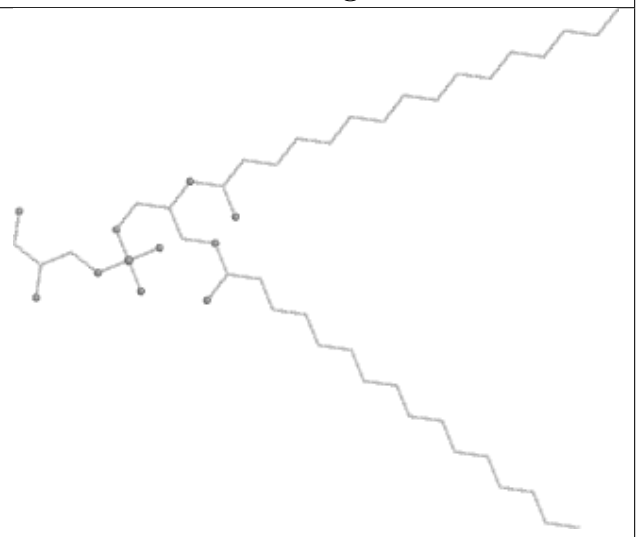


Bond angles

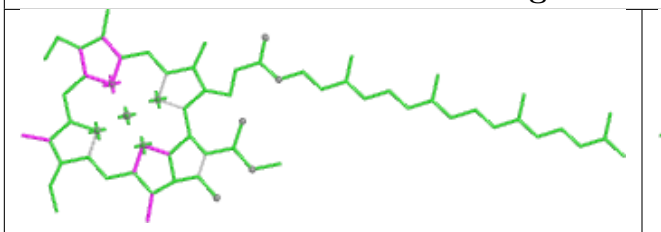


Torsions



Rings

Ligand CLA g 322



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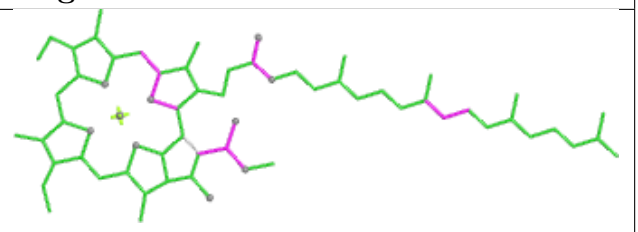
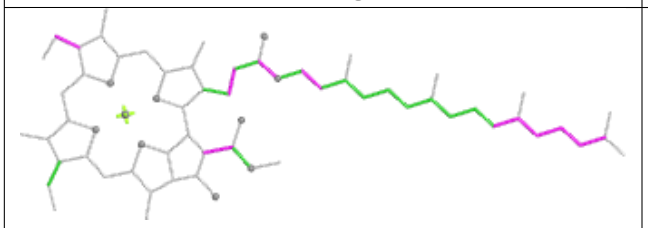


Bond angles



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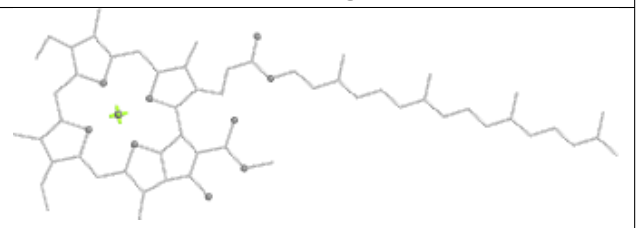
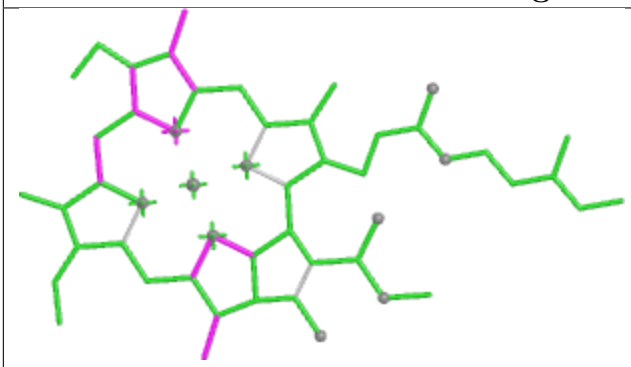
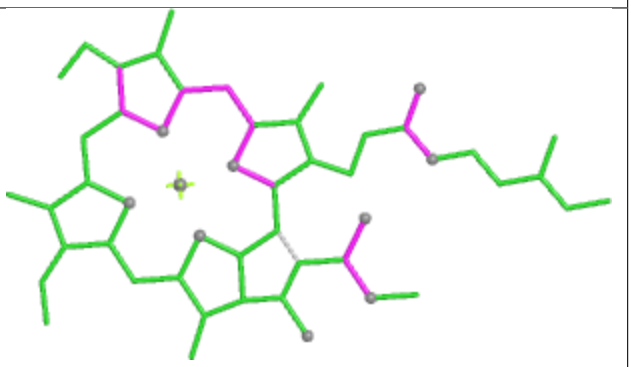
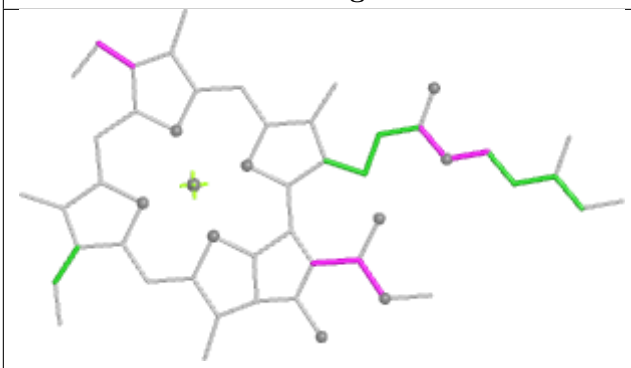
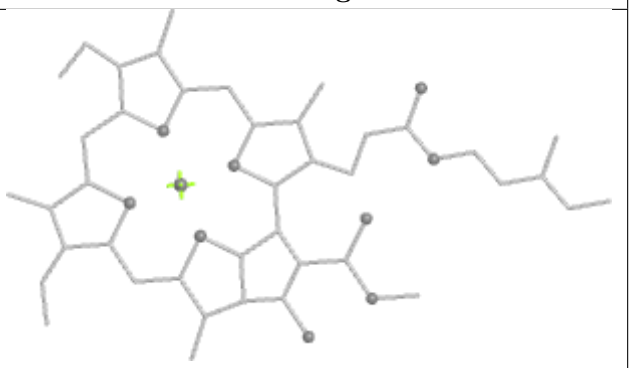
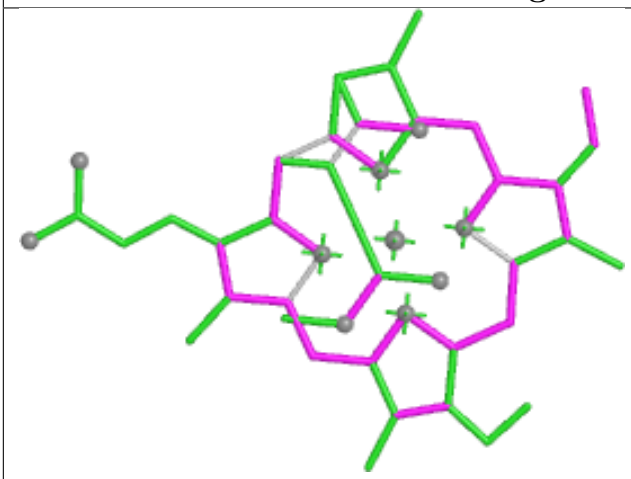


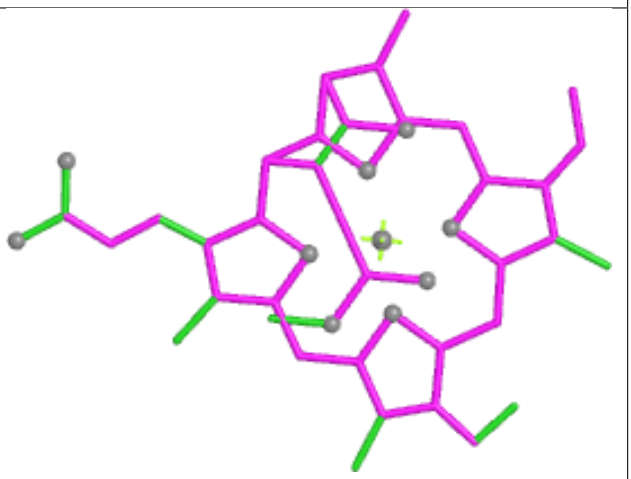
Rings

Ligand CLA i 605	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

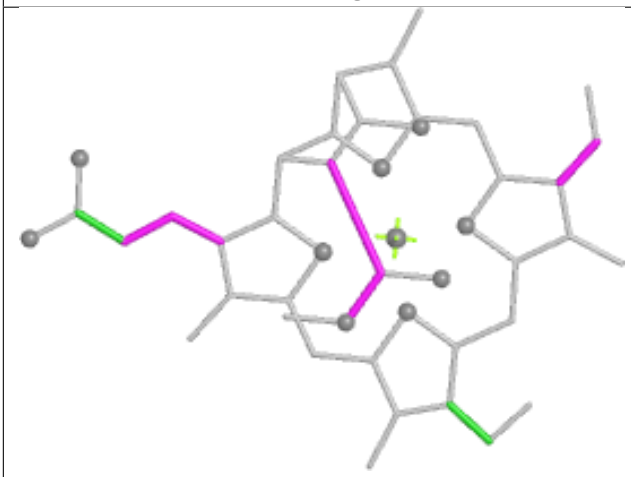
Ligand KC2 d 311



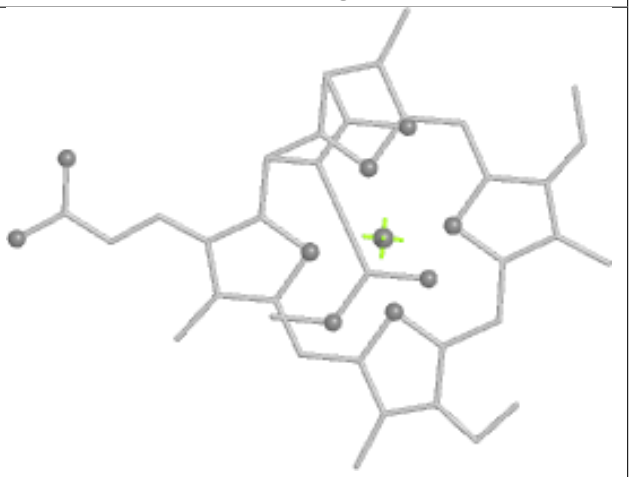
Bond lengths



Bond angles

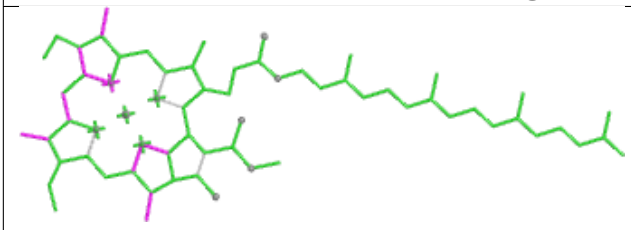


Torsions

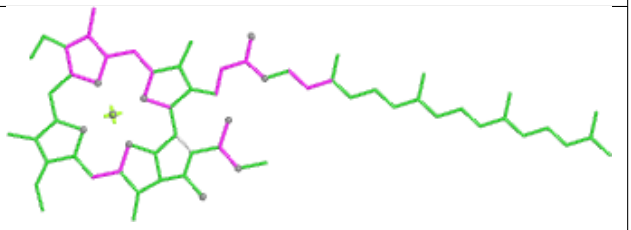


Rings

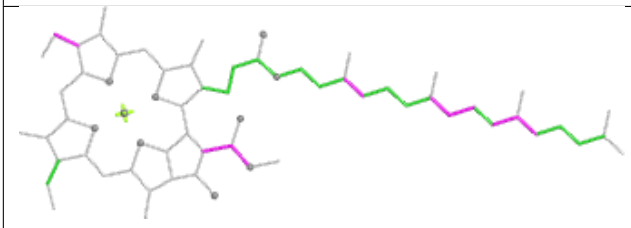
Ligand CLA A 853



Bond lengths



Bond angles



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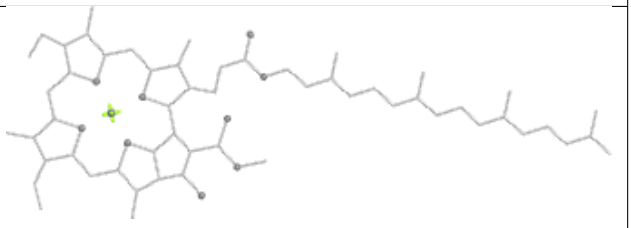
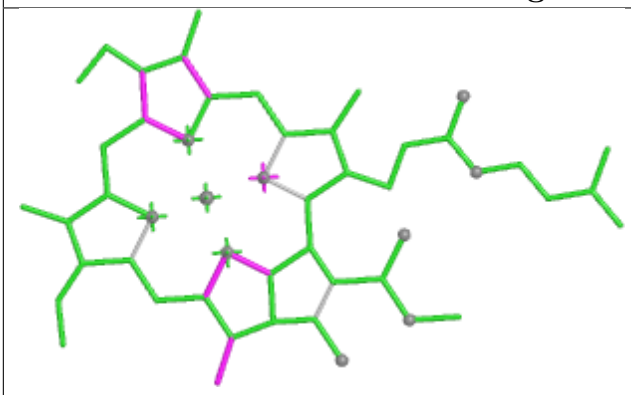
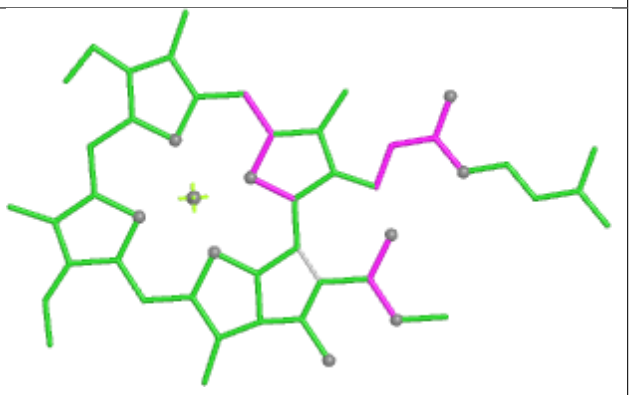
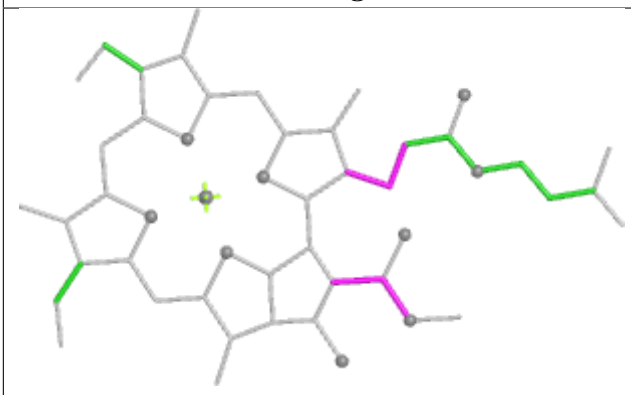
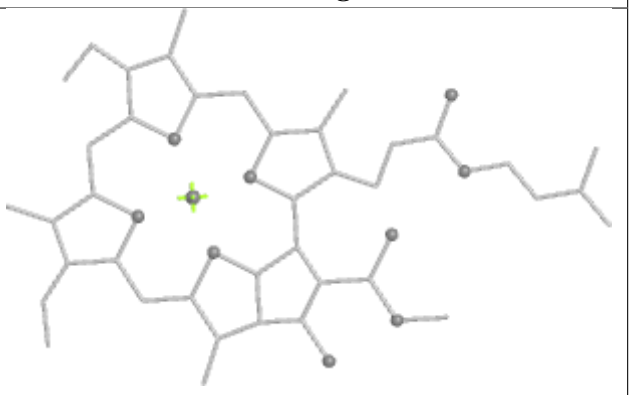
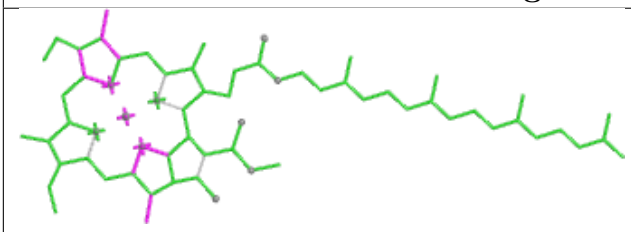
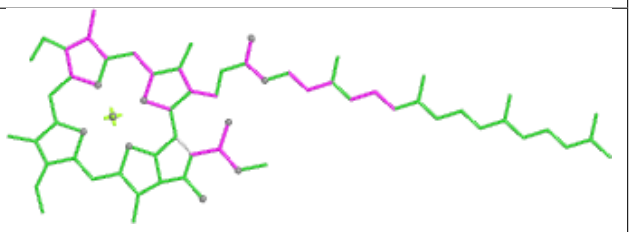
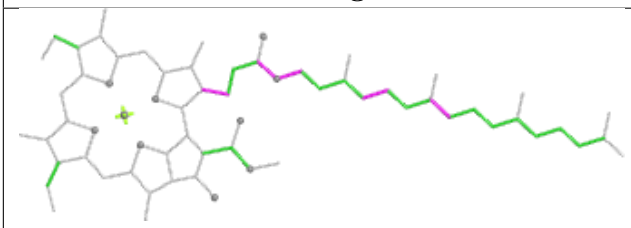
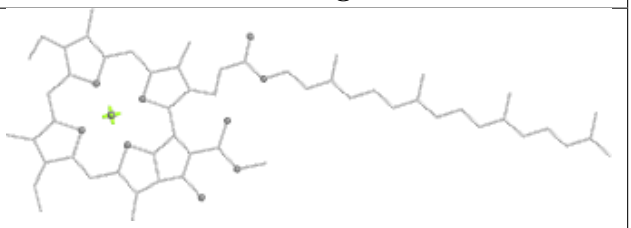
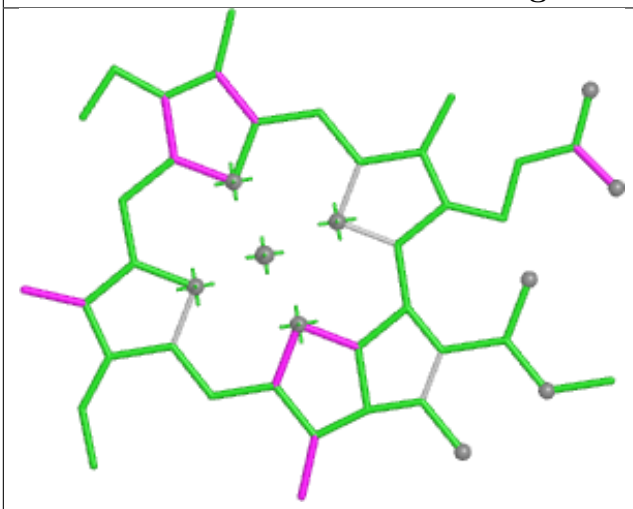


Rings

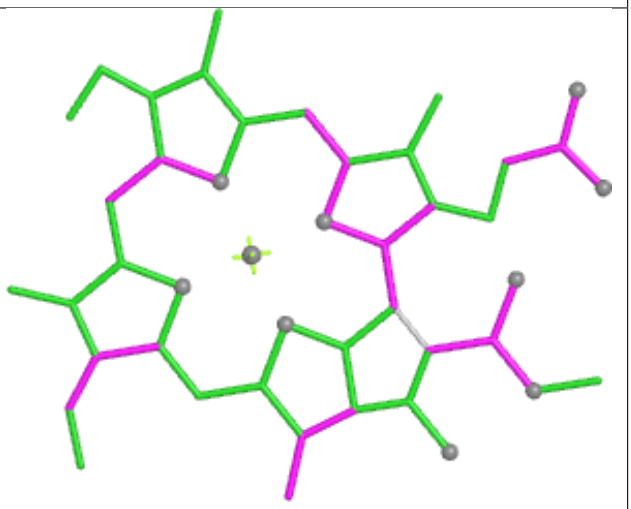
Ligand CLA d 301	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA A 805	
 Bond lengths	 Bond angles
 Torsions	 Rings

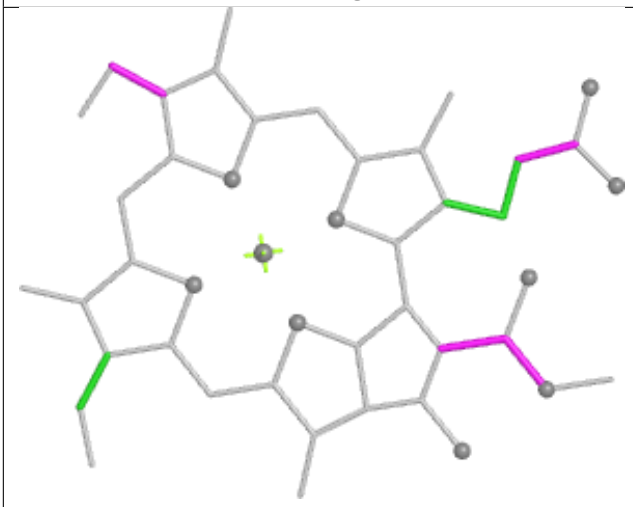
Ligand CLA c 611



Bond lengths



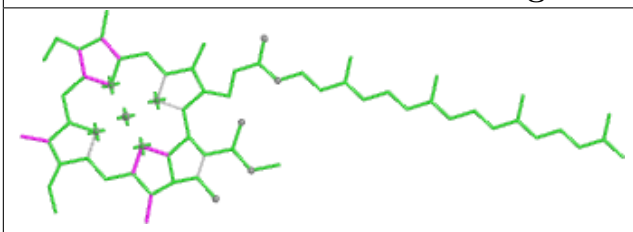
Bond angles



Torsions

Rings

Ligand CLA k 604



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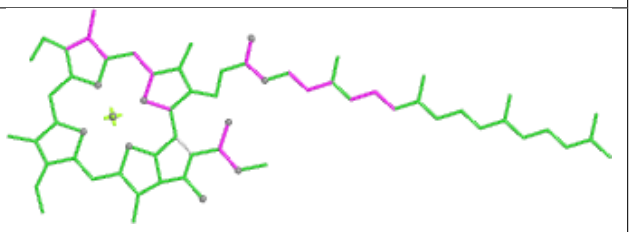
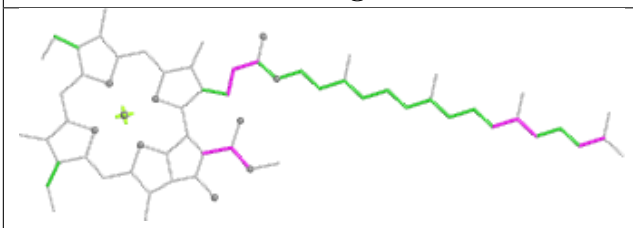
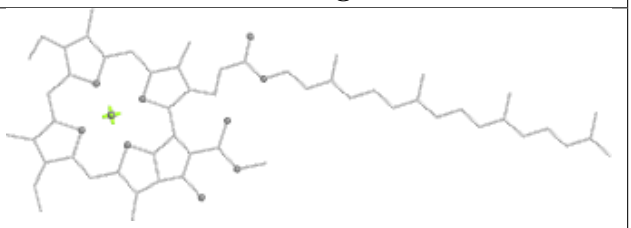


Bond angles

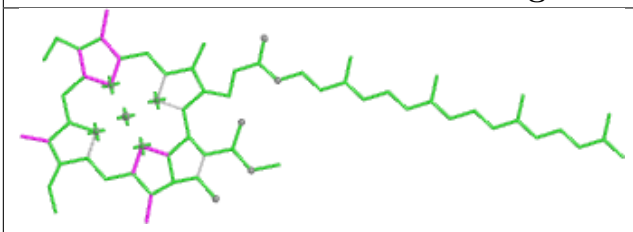


Torsions

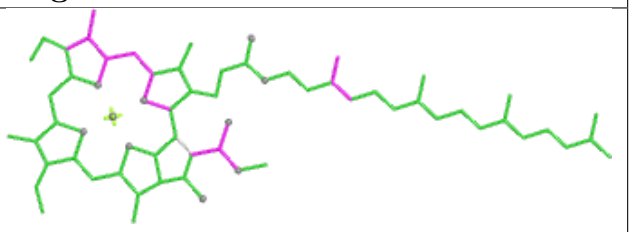


Rings

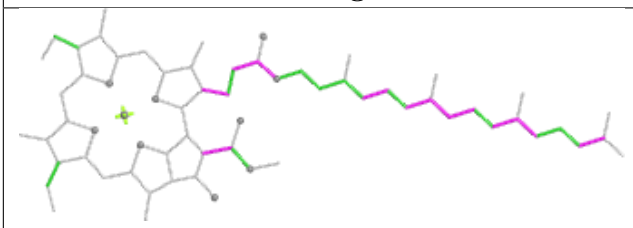
Ligand CLA g 308



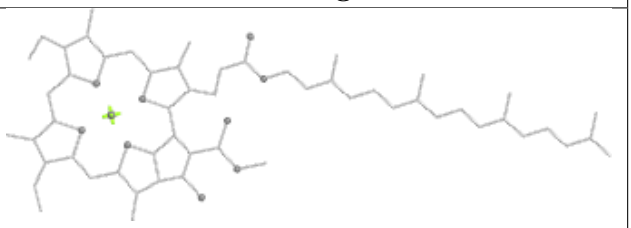
Bond lengths



Bond angles

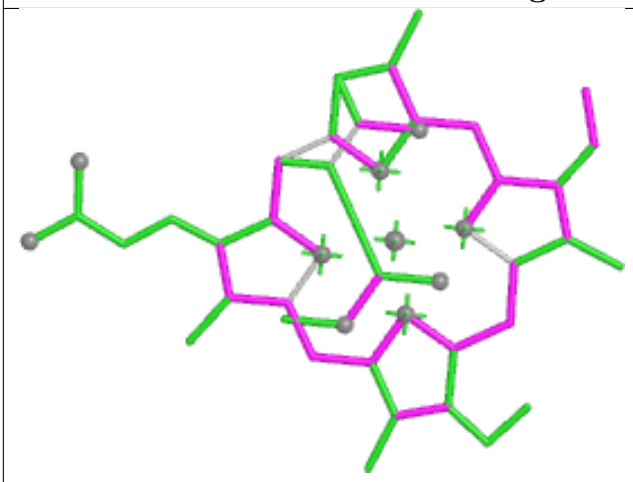


Torsions

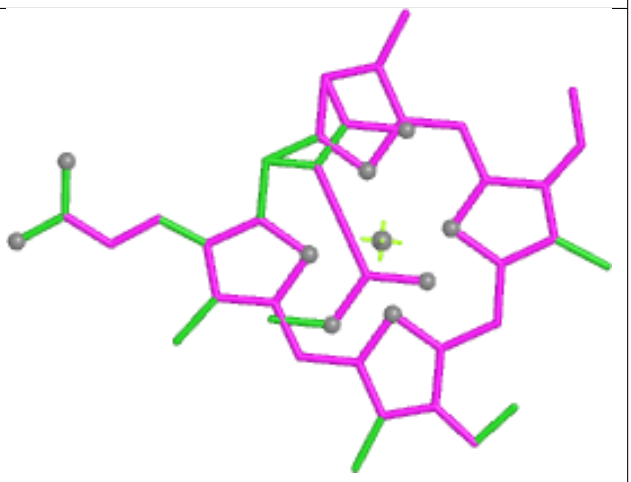


Rings

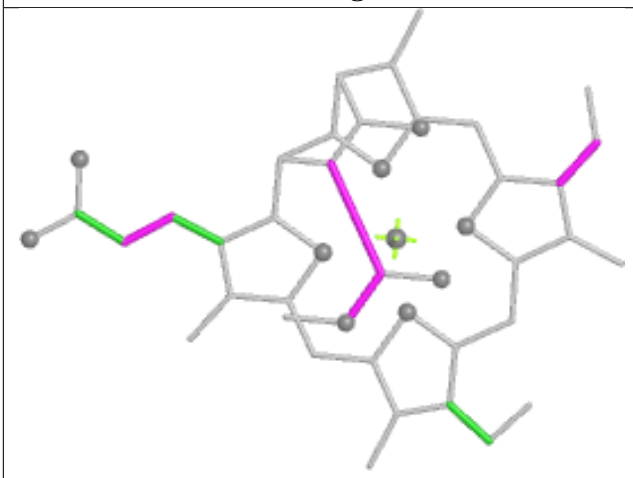
Ligand KC2 d 310



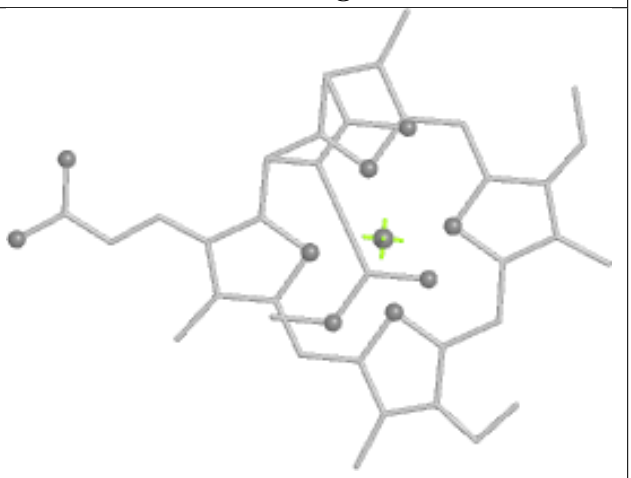
Bond lengths



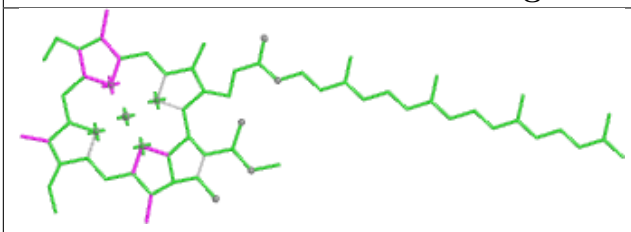
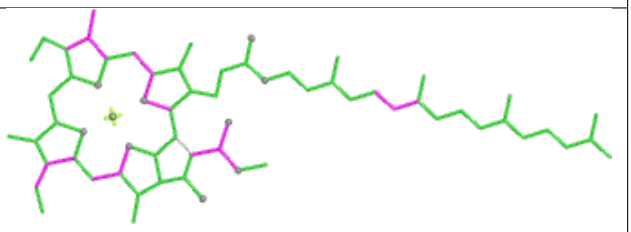
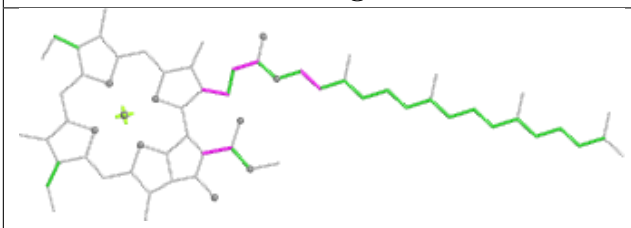
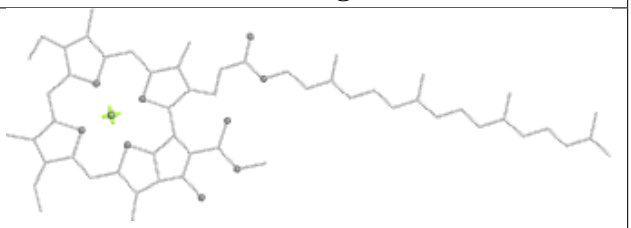
Bond angles

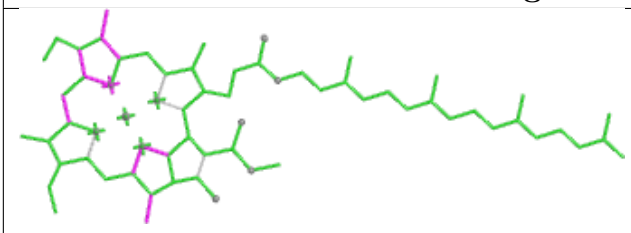
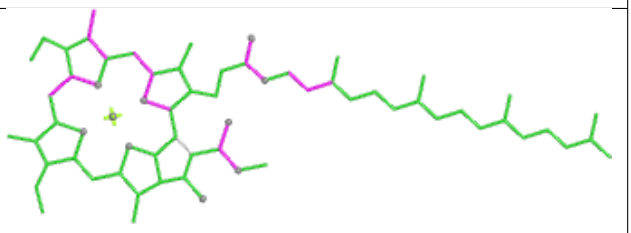
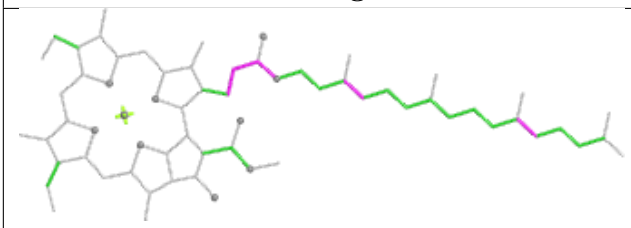
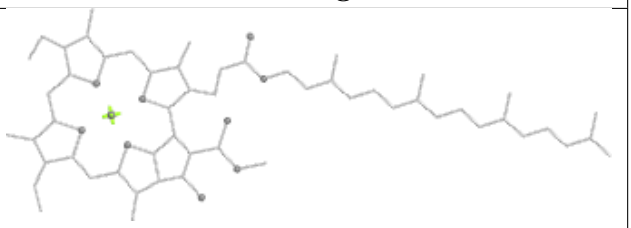


Torsions

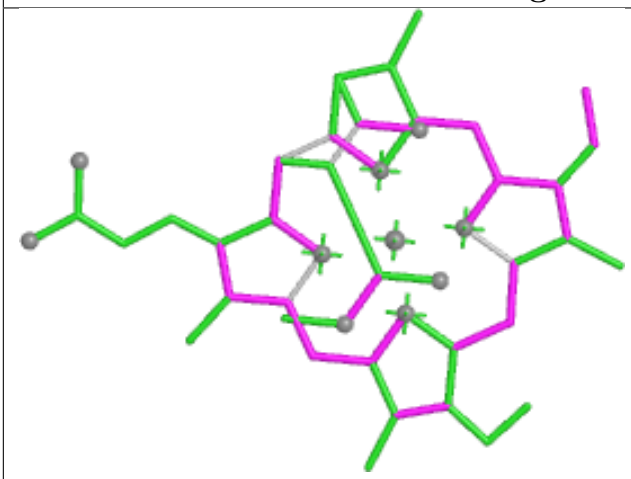


Rings

Ligand CLA A 804	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA A 828	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand KC2 k 611



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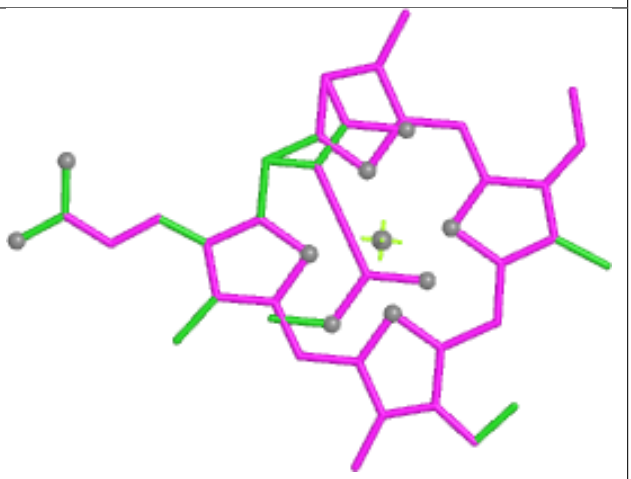

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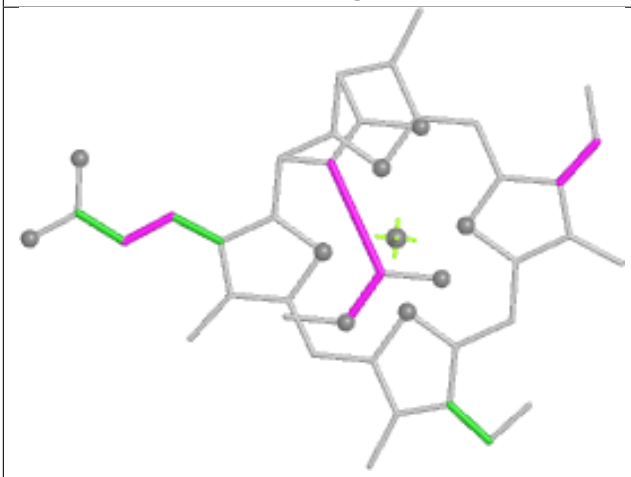

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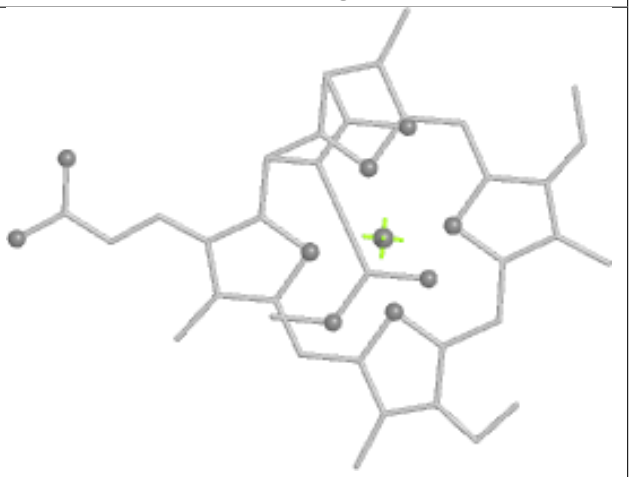
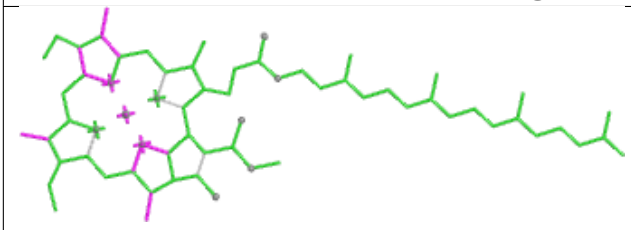


Rings

Ligand CLA e 610



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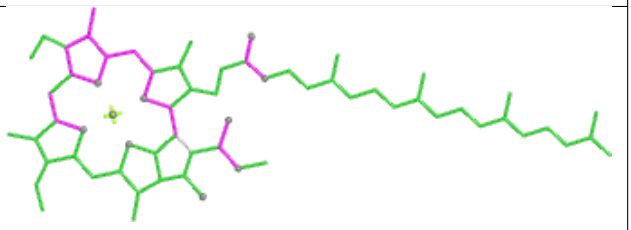
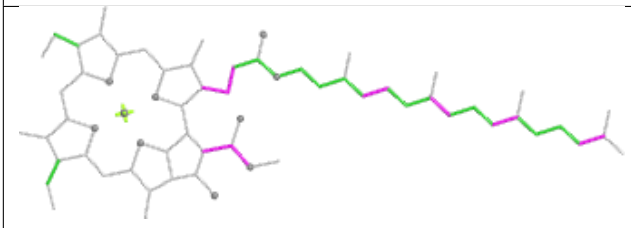


Bond angles



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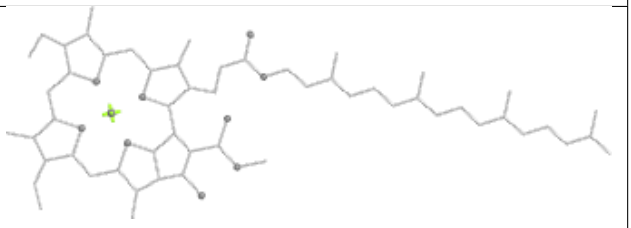
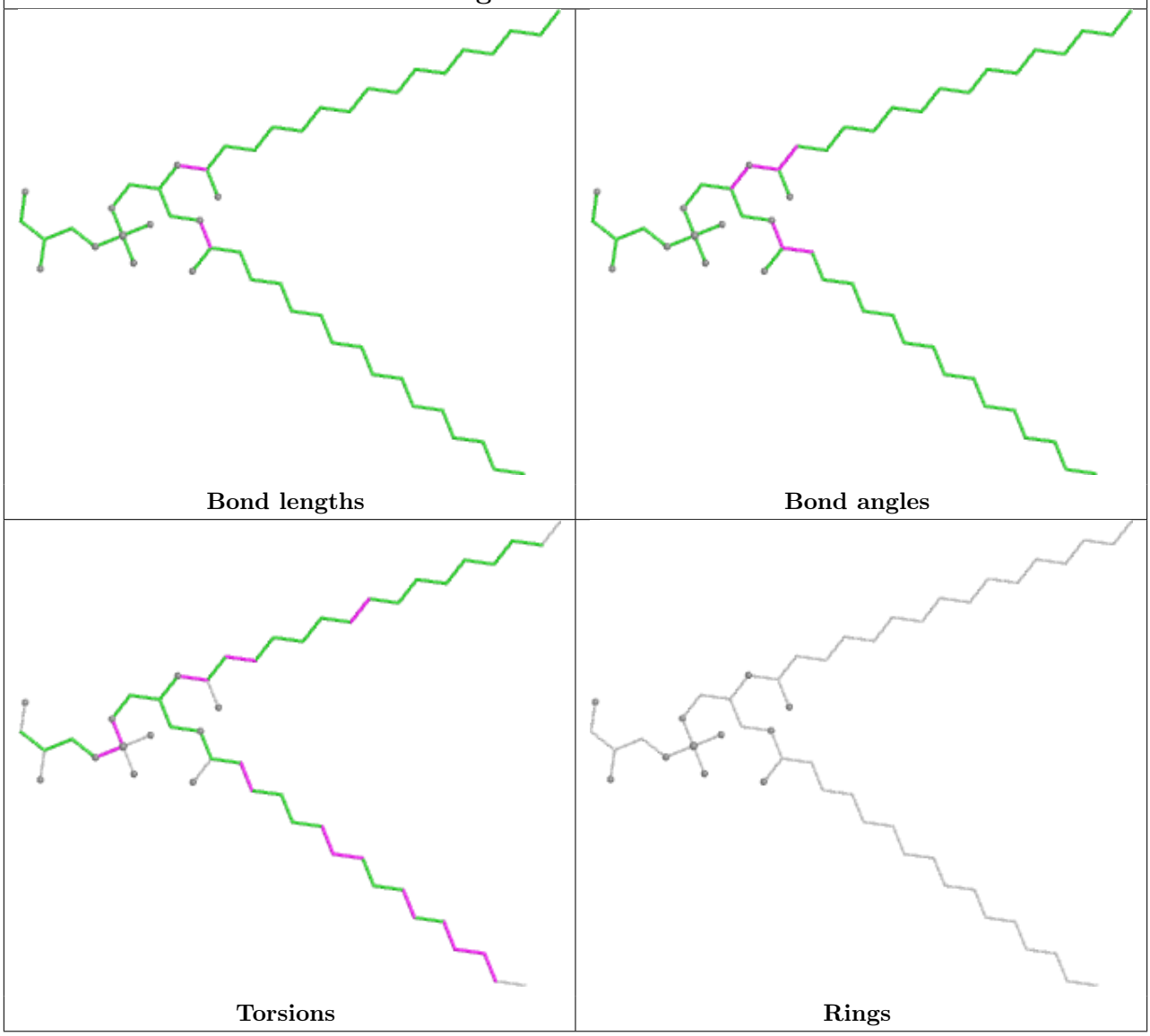
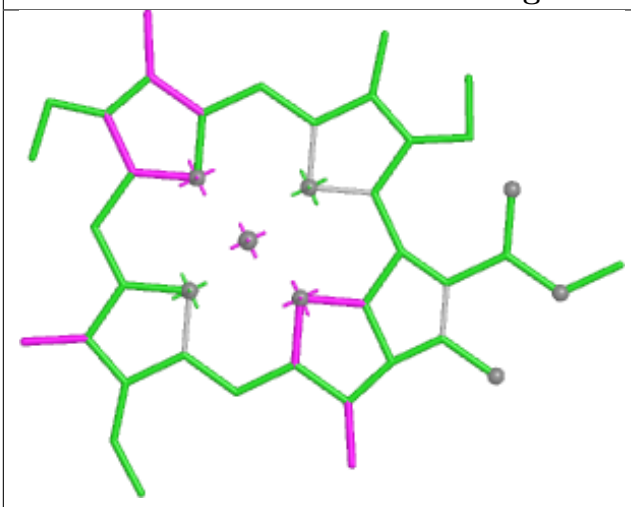


Rings

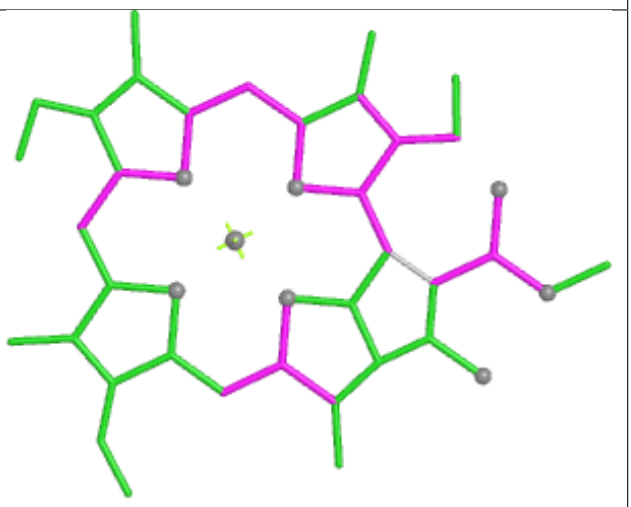
Ligand LHG f 620



Ligand CLA K 102



Bond lengths



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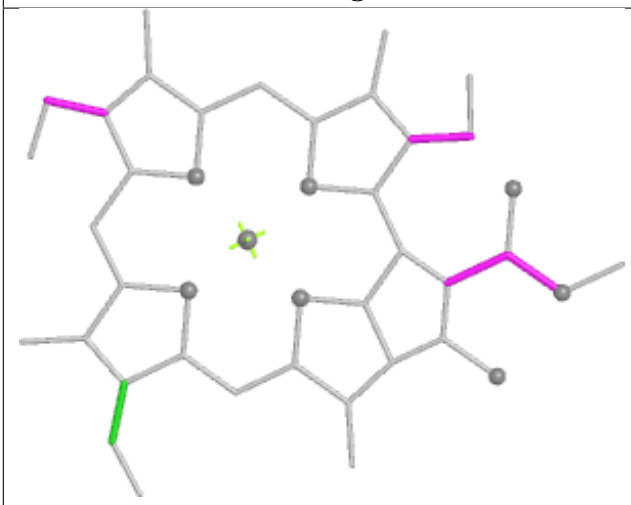
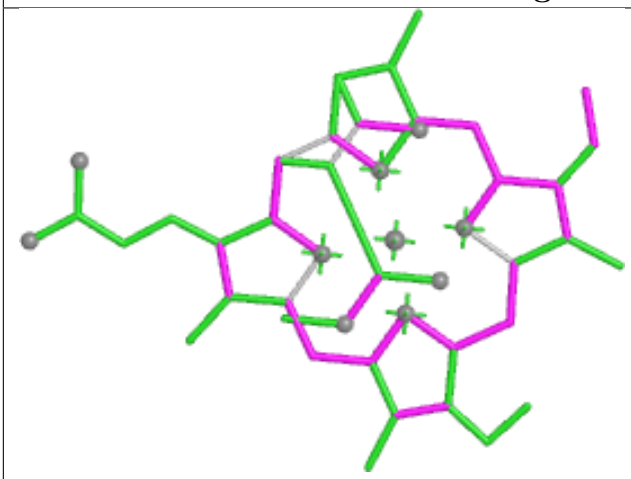


Torsions

Rings

Ligand KC2 f 611



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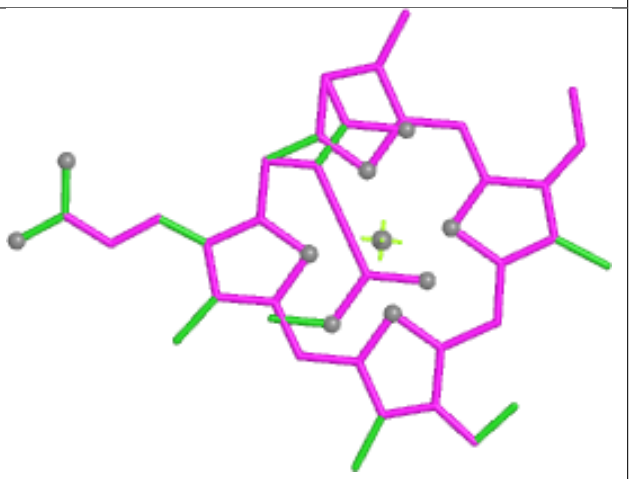

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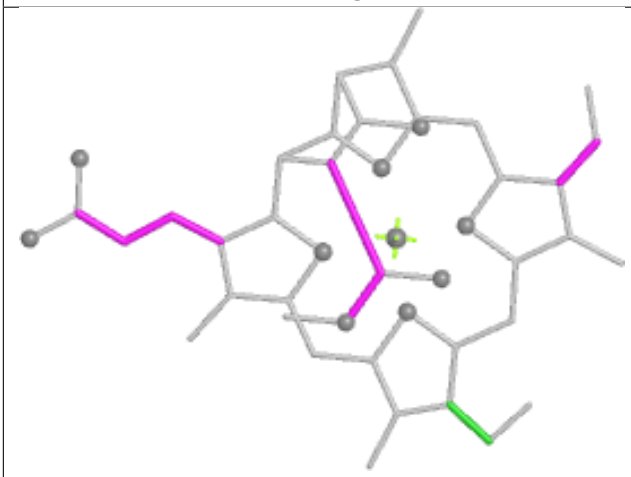

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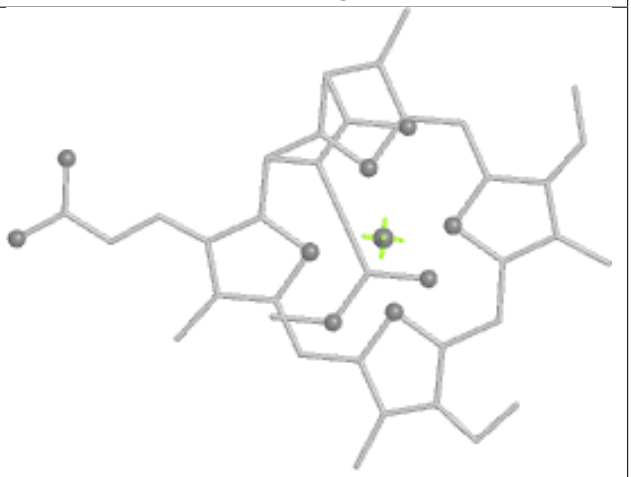
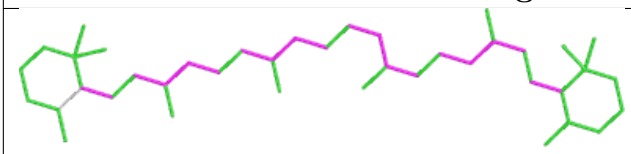


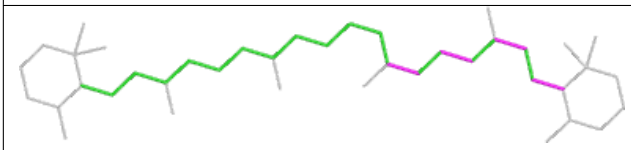
Rings

Ligand WVN B 848



Bond lengths

Bond angles



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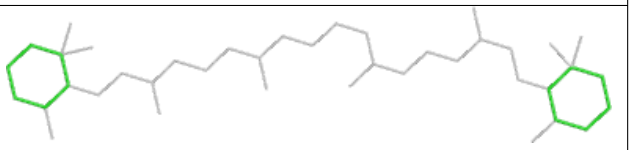
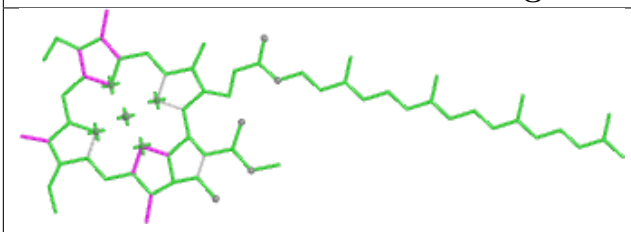


Rings

Ligand CLA B 839



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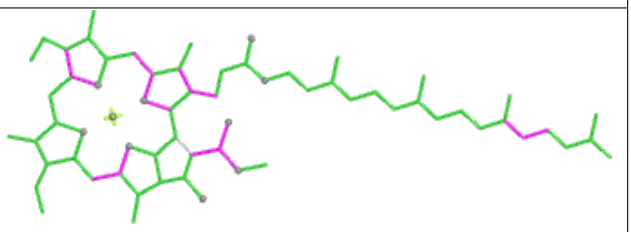
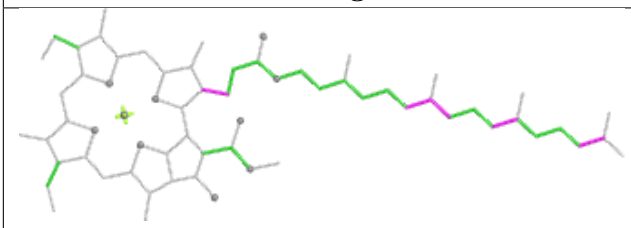


Bond angles



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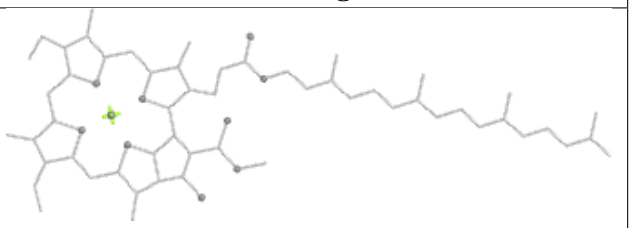
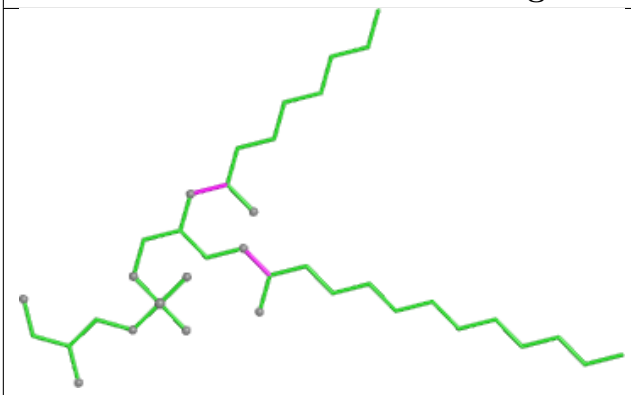


Rings

Ligand LHG c 617



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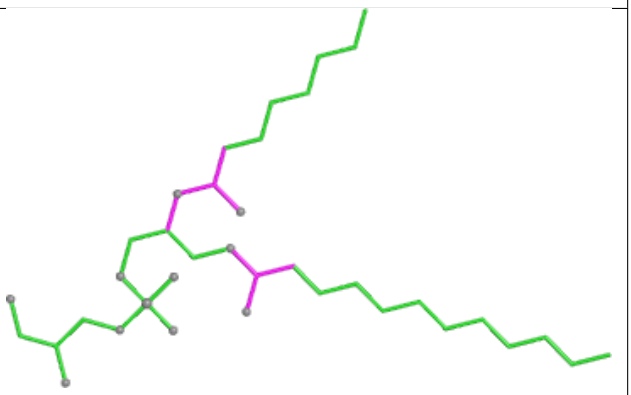
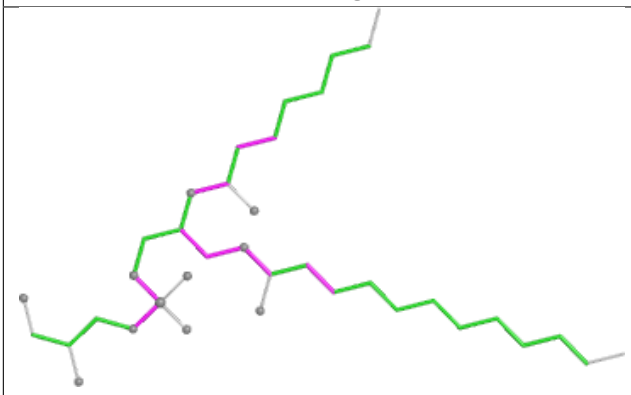


Bond angles



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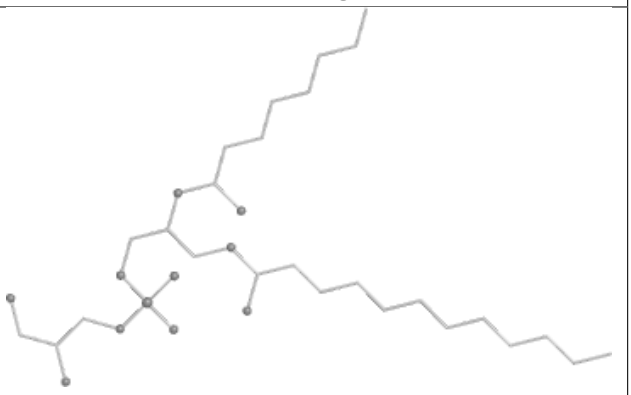
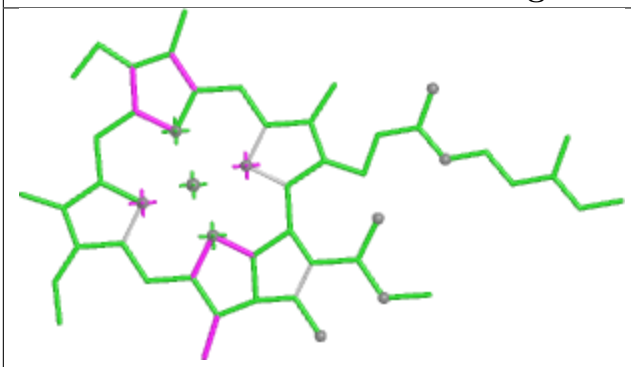
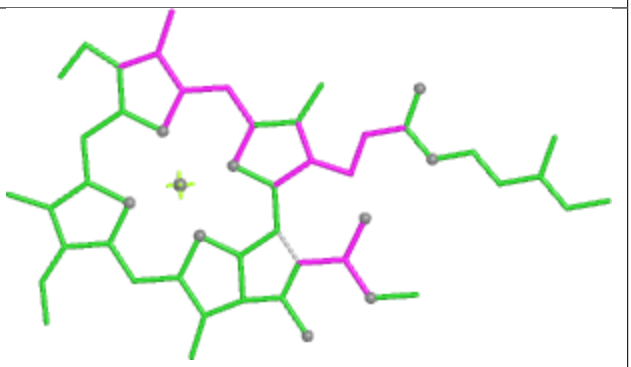


Rings

Ligand CLA k 603	
	
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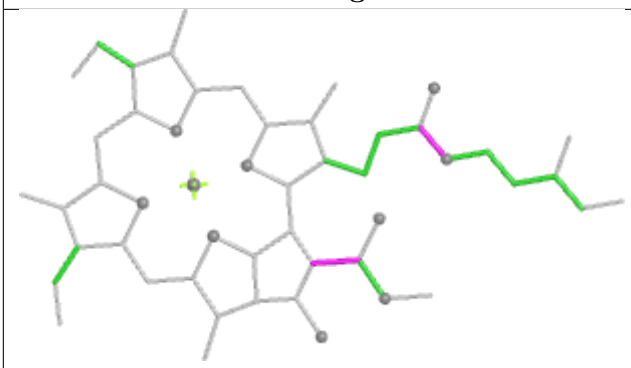
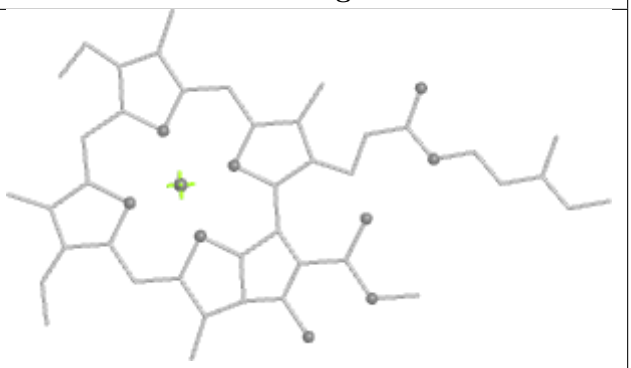
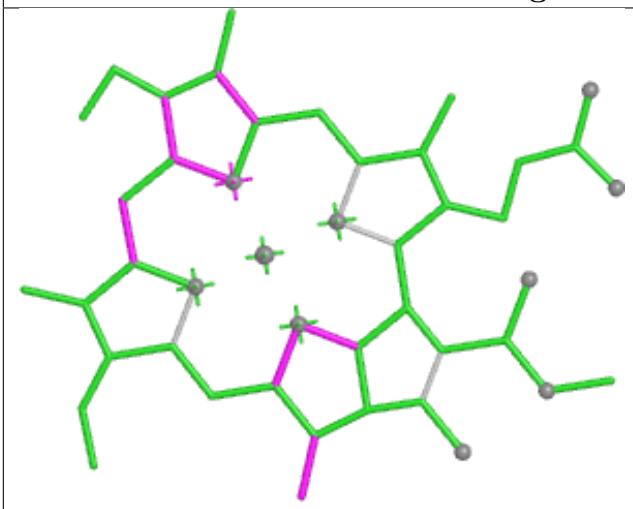
	
Torsions	**Rings**

Ligand CLA c 609



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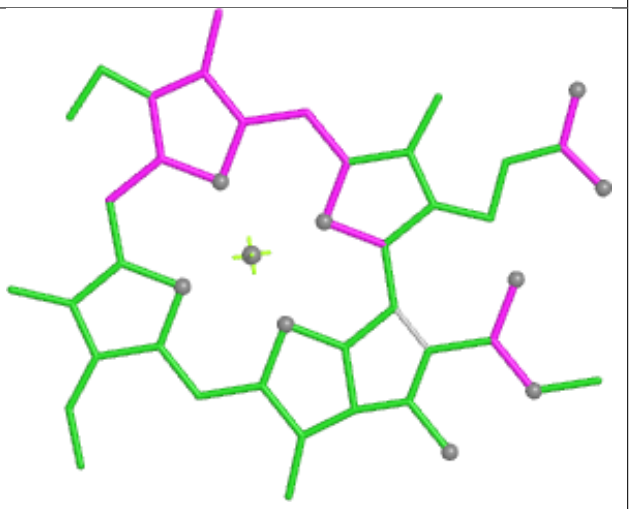
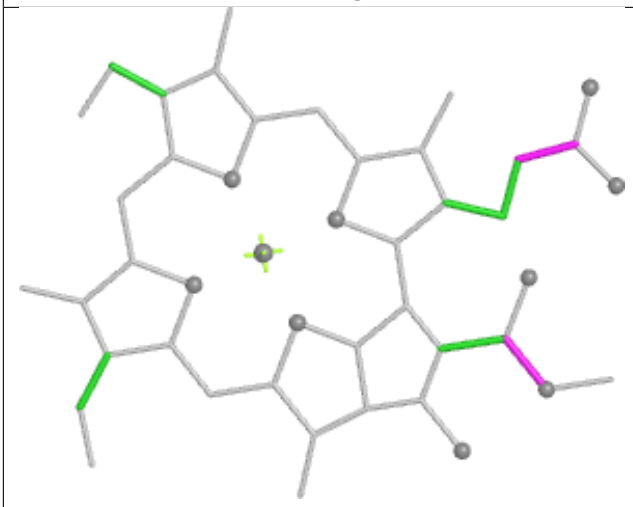


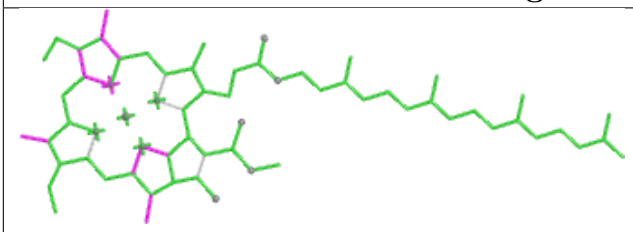
Bond angles



Torsions

Rings

Ligand CLA F 201



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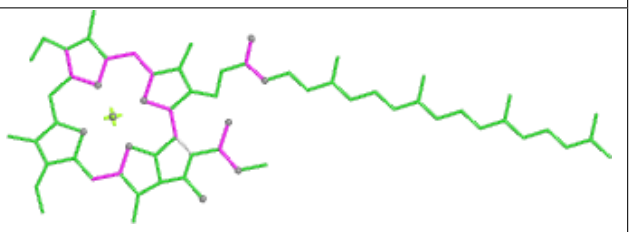
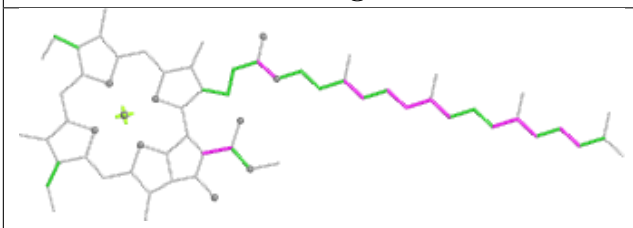
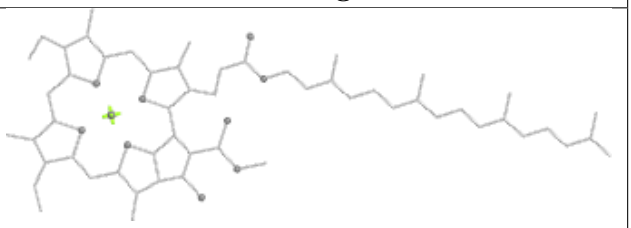


Bond angles

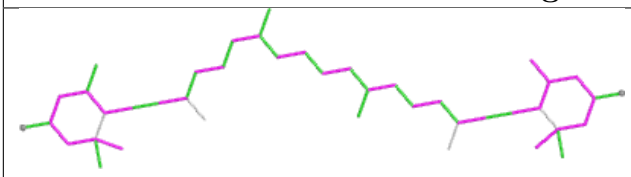


Torsions



Rings

Ligand II0 d 315



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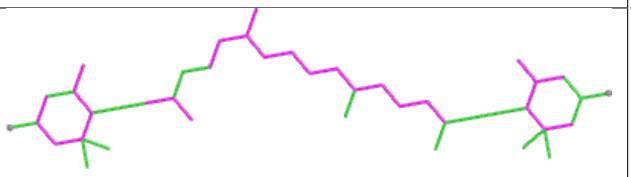
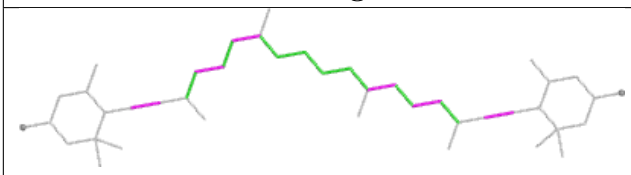


Bond angles



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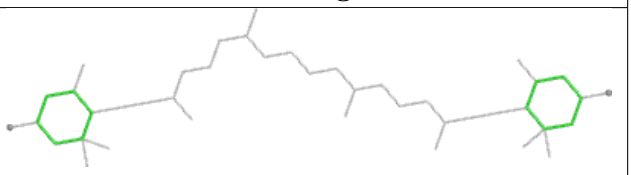
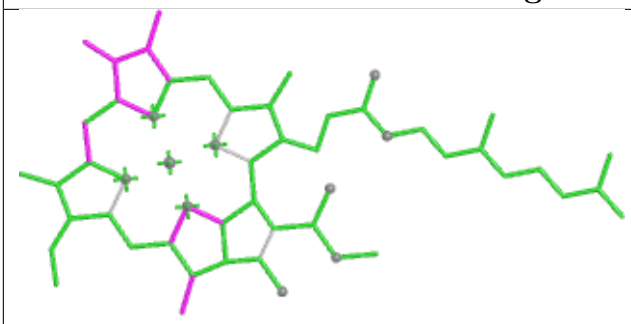
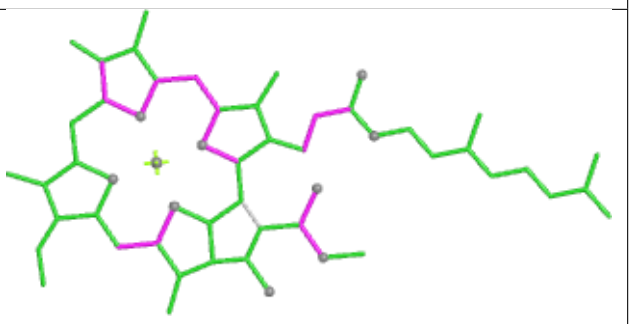


Rings

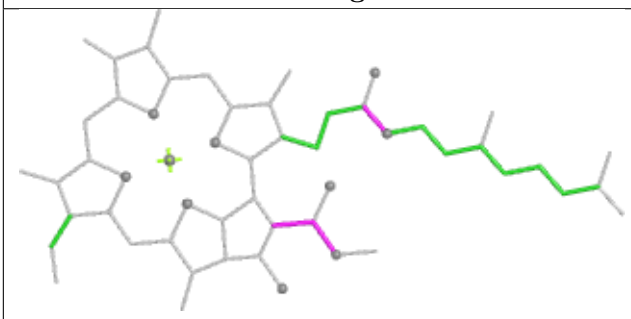
Ligand CLA B 810



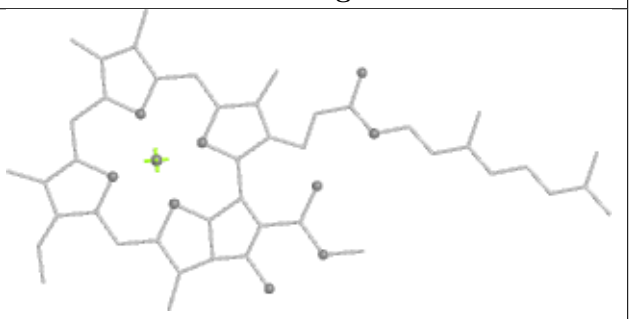
Bond lengths



Bond angles

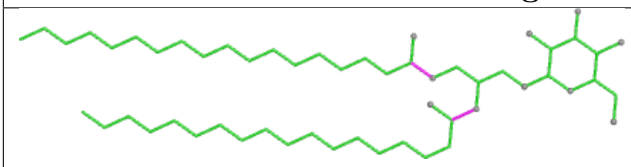


Torsions

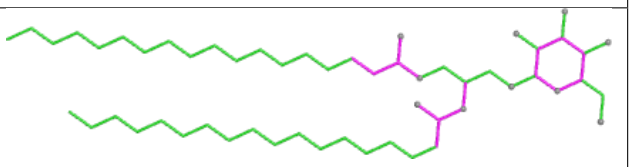


Rings

Ligand LMG L 208



Bond lengths

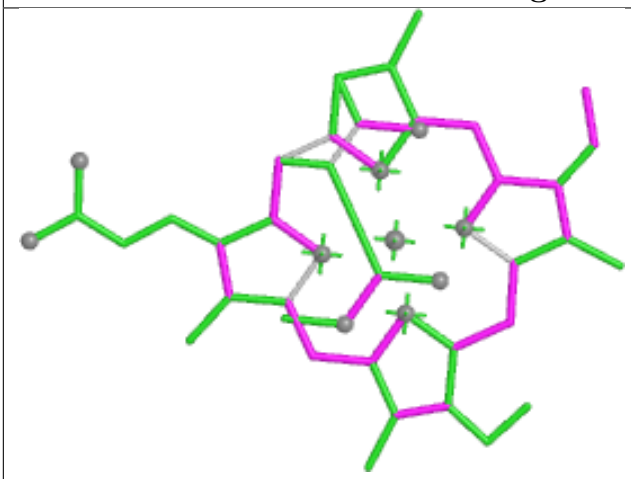


Bond angles

Torsions

Rings

Ligand KC2 g 312



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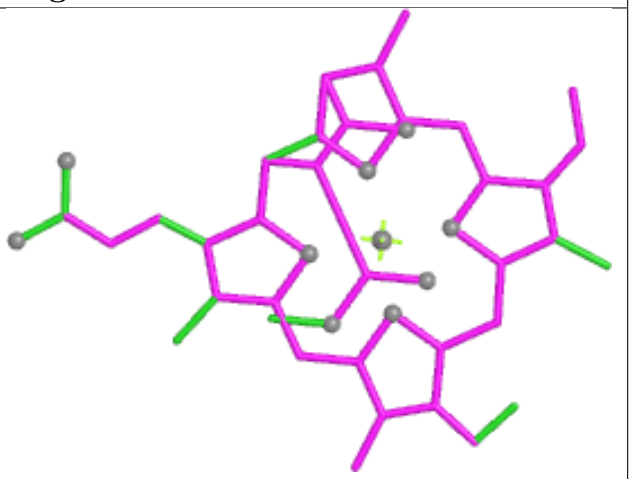
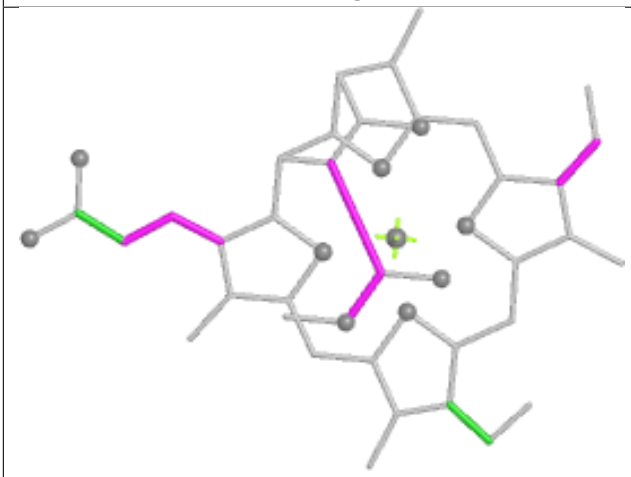
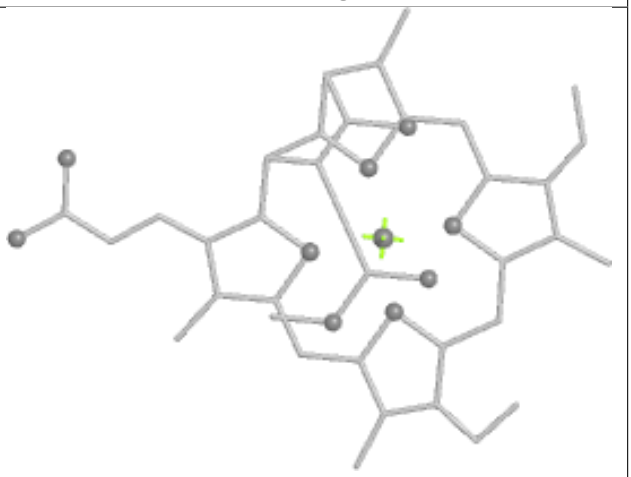


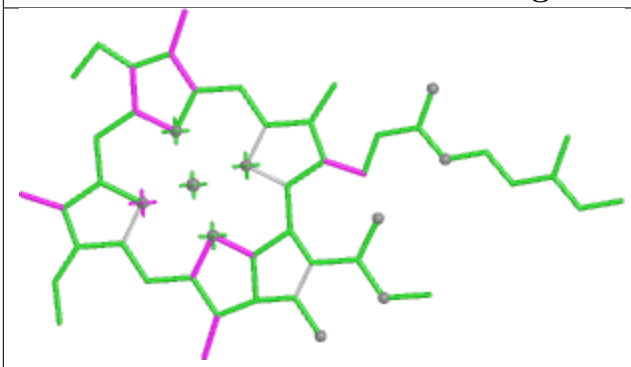
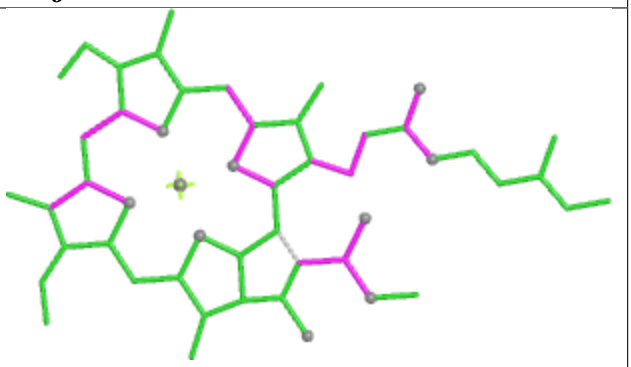
Bond angles



Torsions



Rings

Ligand CLA j 307	
	
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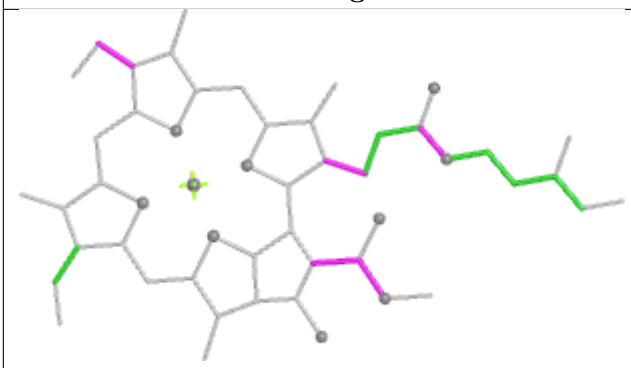
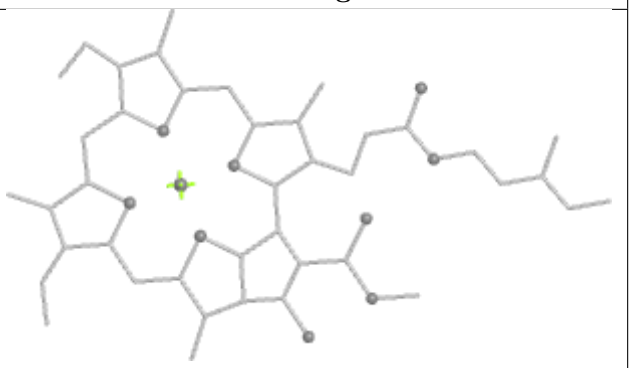
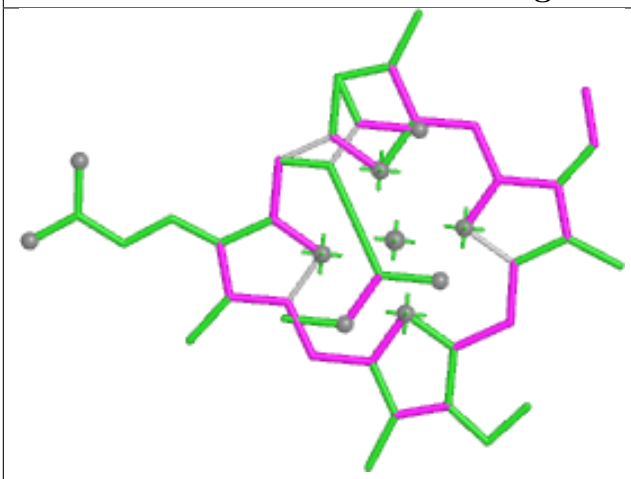
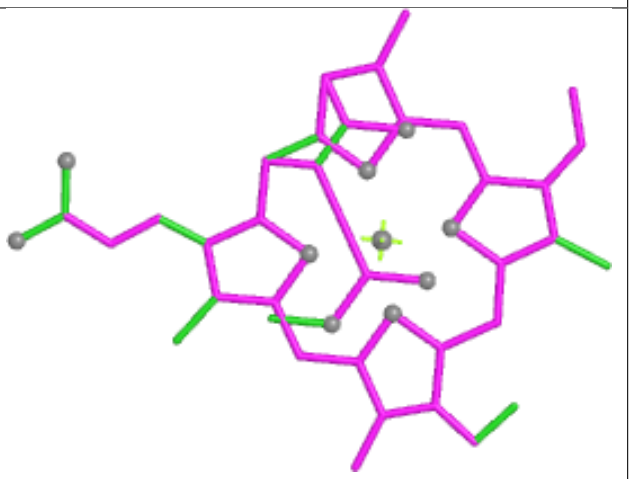
	
Torsions	**Rings**

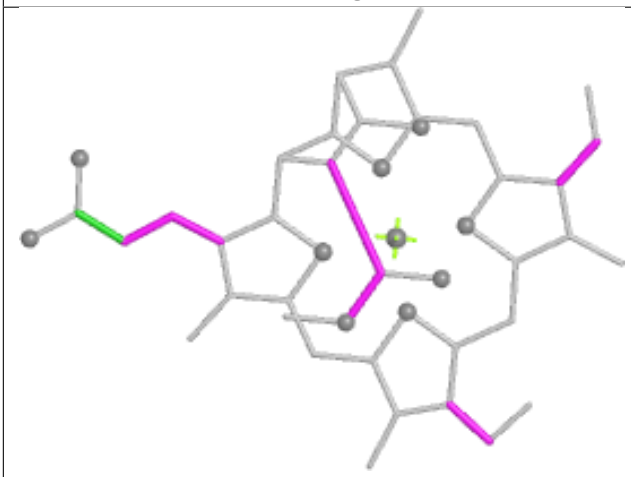
Ligand KC2 i 616



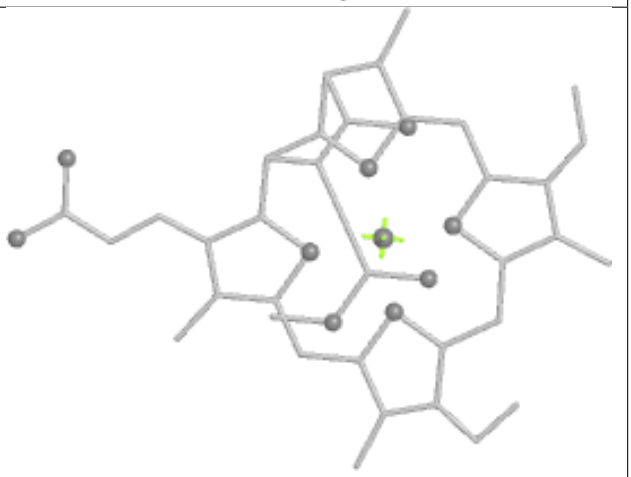
Bond lengths



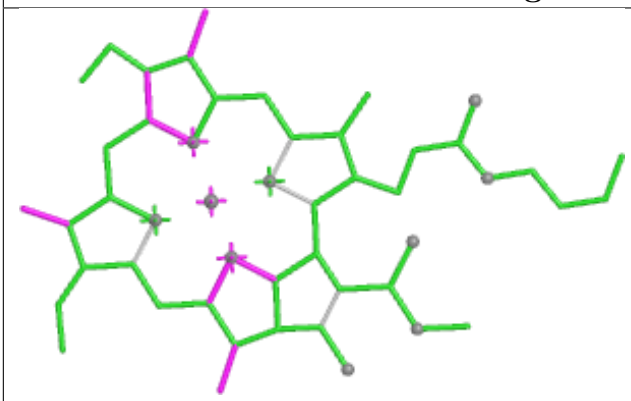
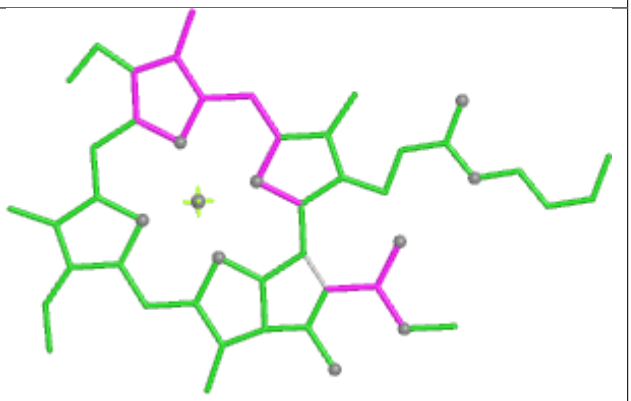
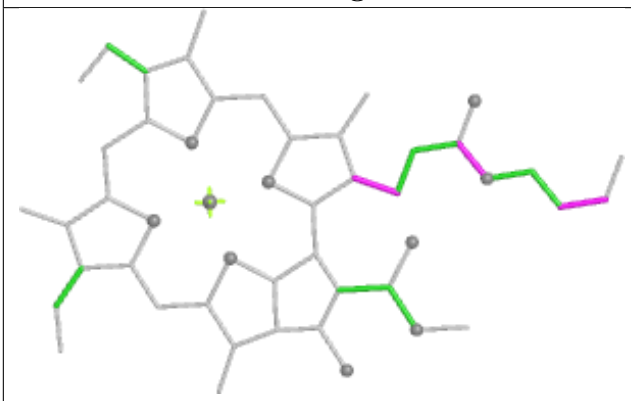
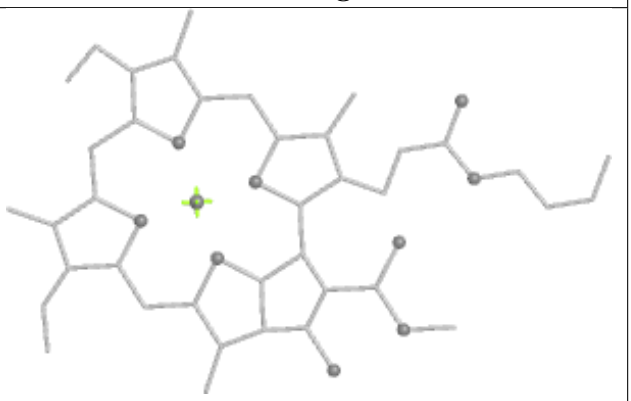
Bond angles

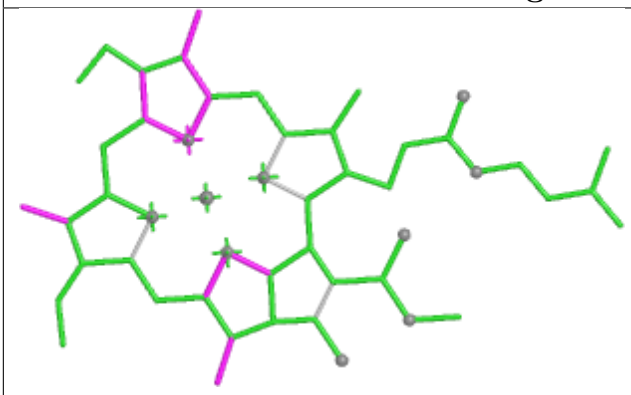
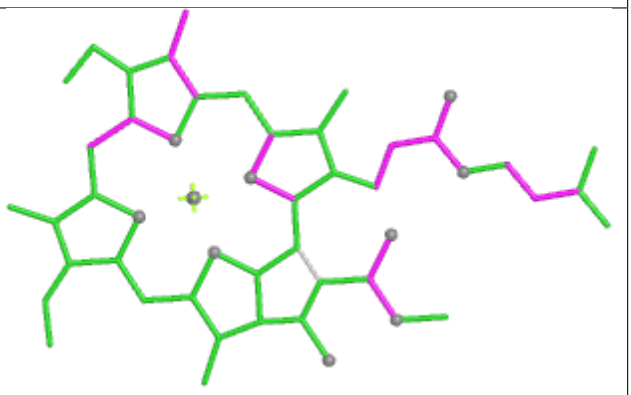
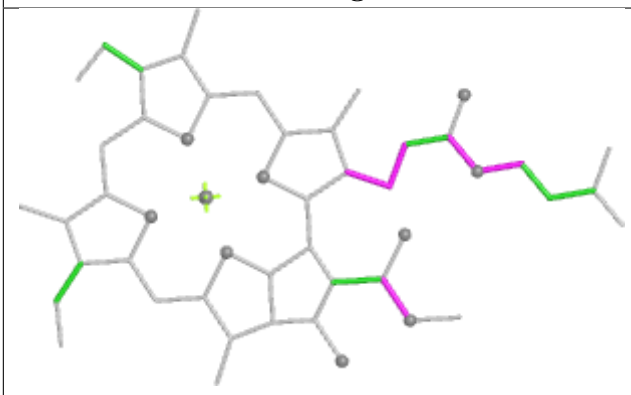
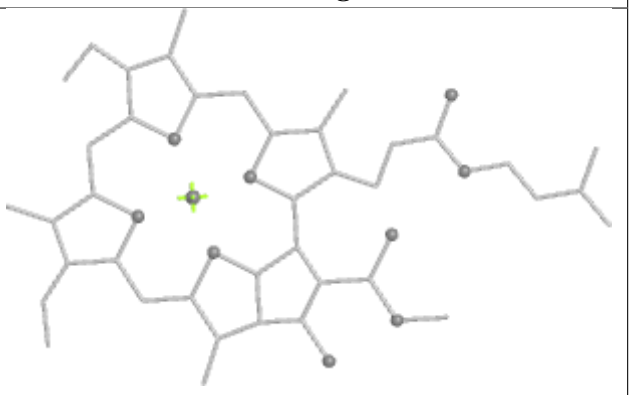


Torsions

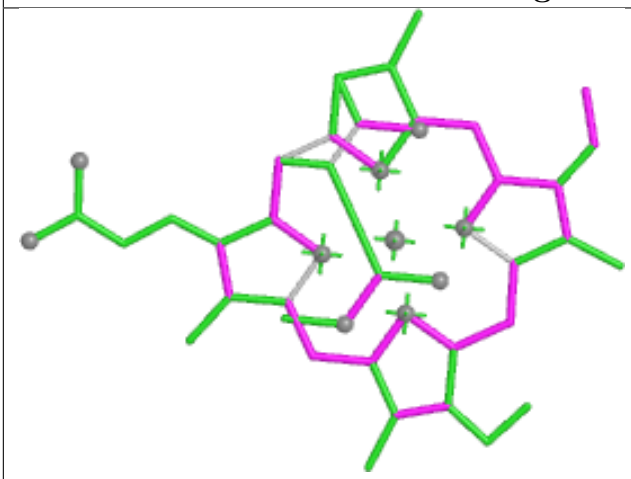


Rings

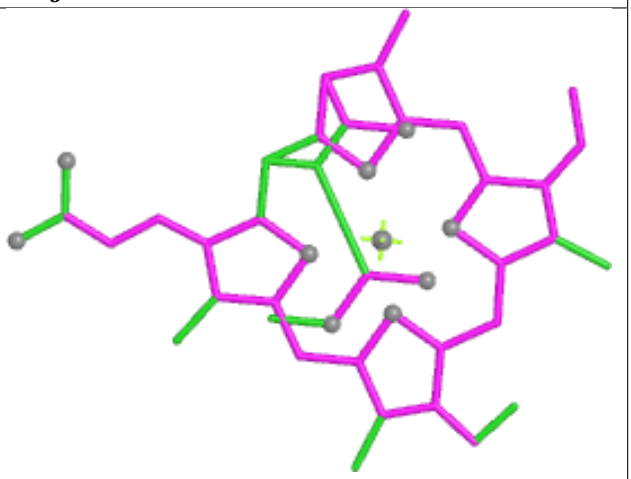
Ligand CLA B 828	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA L 204	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand KC2 j 312



Bond lengths



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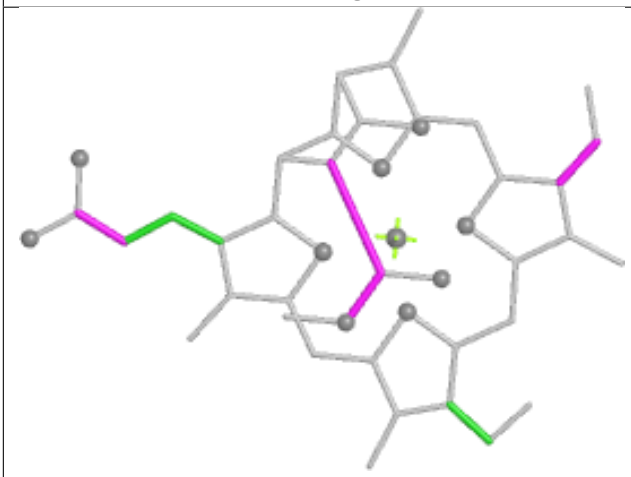

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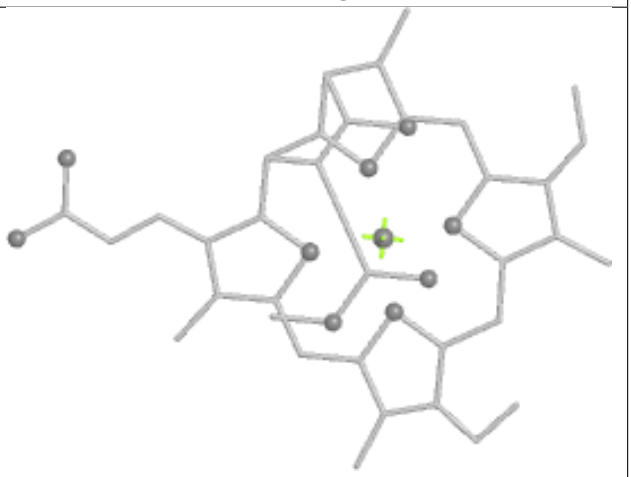
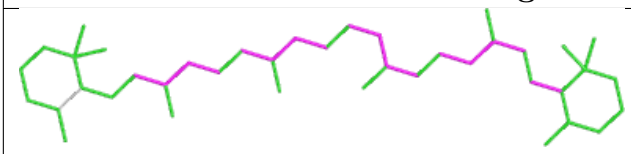
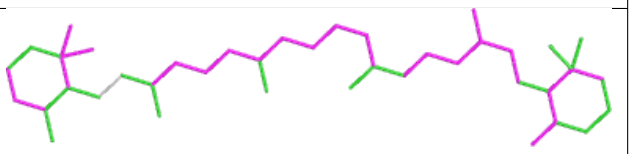


Rings

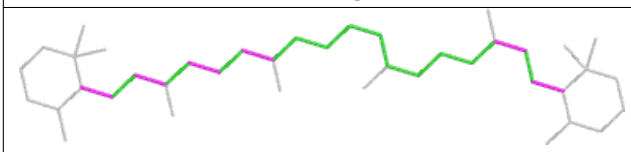
Ligand WVN L 201



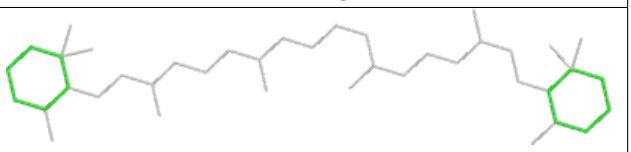
Bond lengths



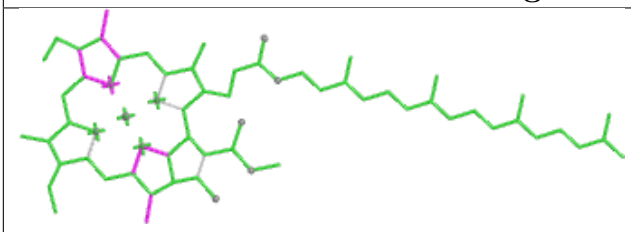
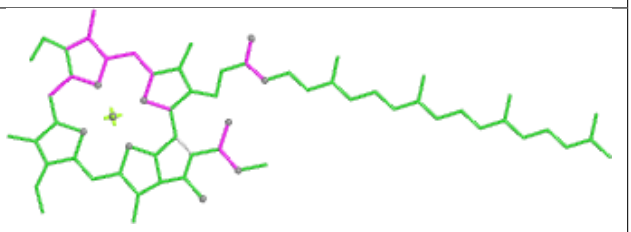
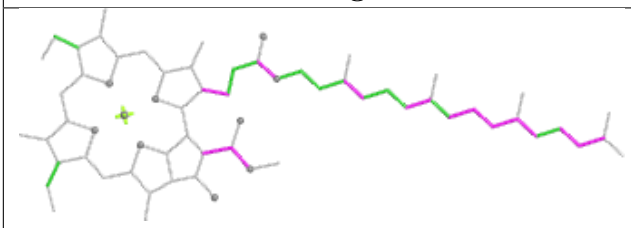
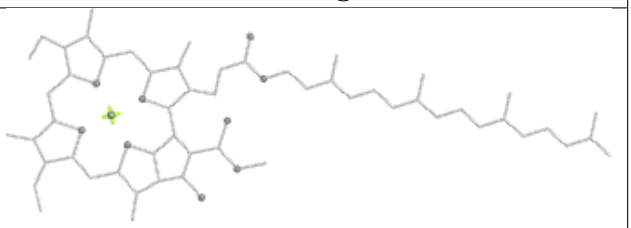
Bond angles

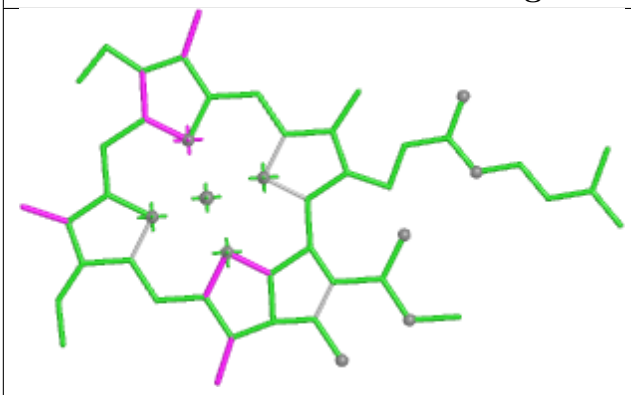
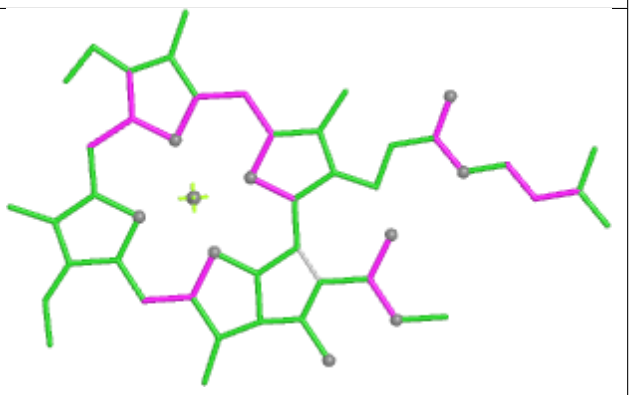
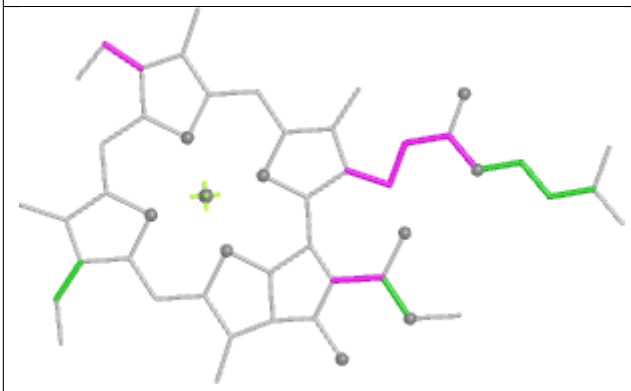
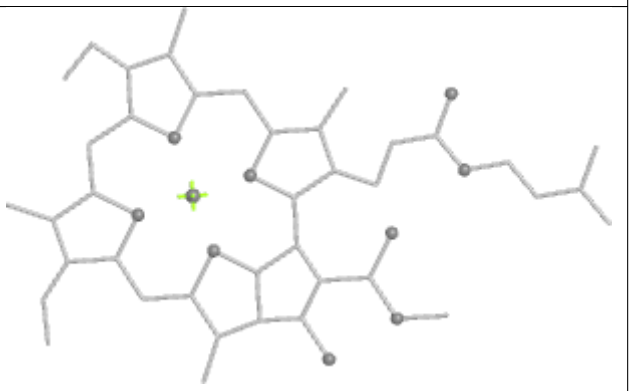


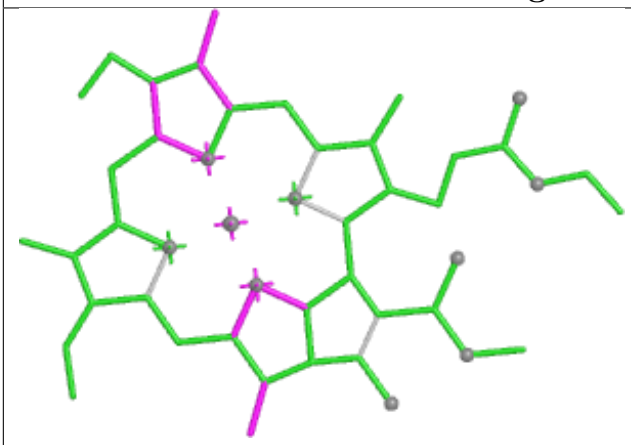
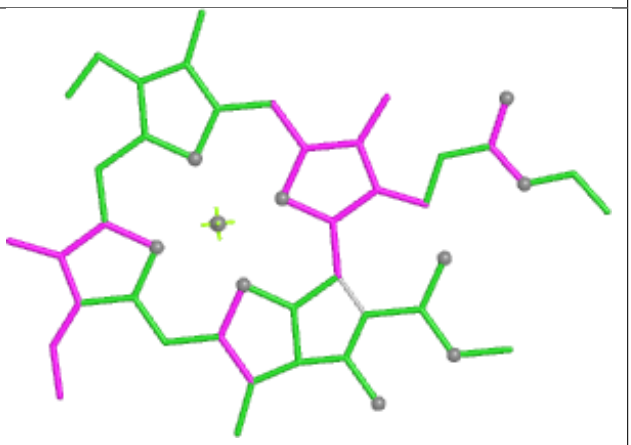
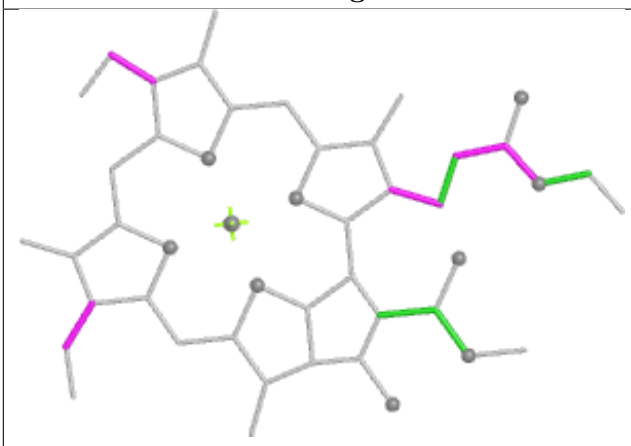
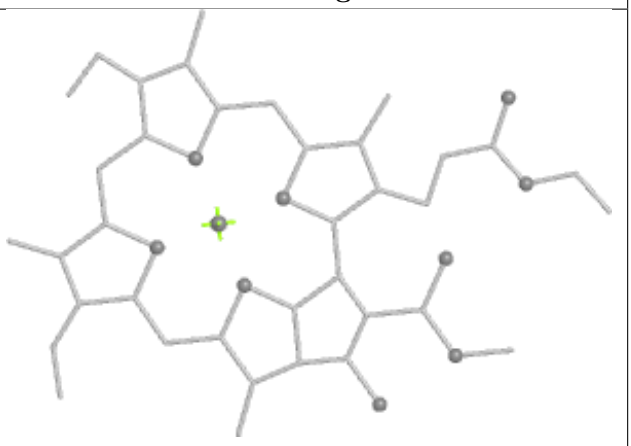
Torsions



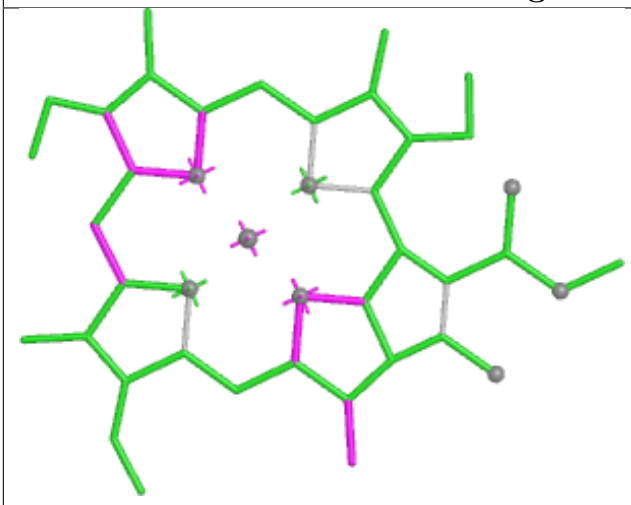
Rings

Ligand CLA A 841	
 Bond lengths	 Bond angles
 Torsions	 Rings

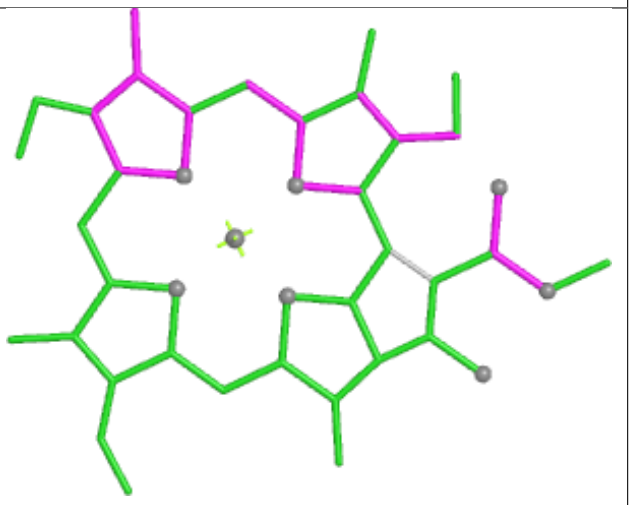
Ligand CLA B 827	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA a 311	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

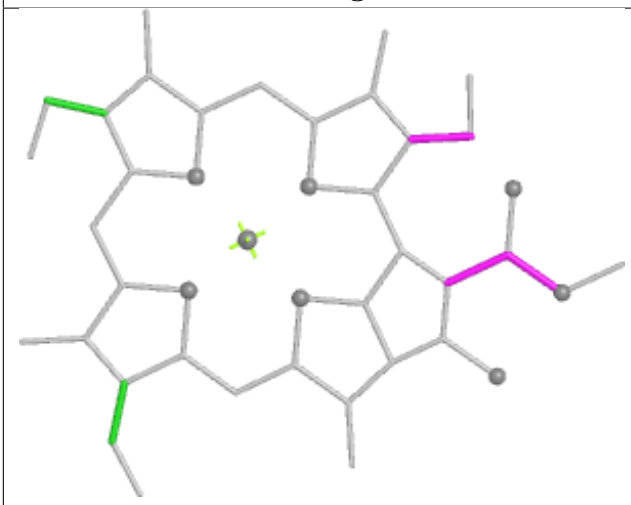
Ligand CLA J 103



Bond lengths



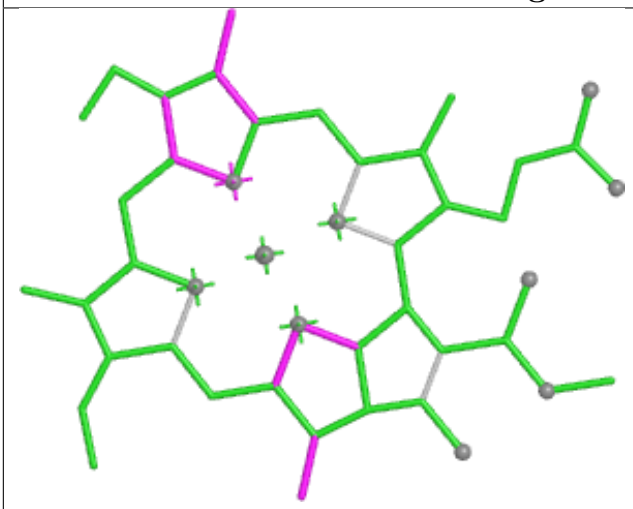
Bond angles



Torsions

Rings

Ligand CLA a 306



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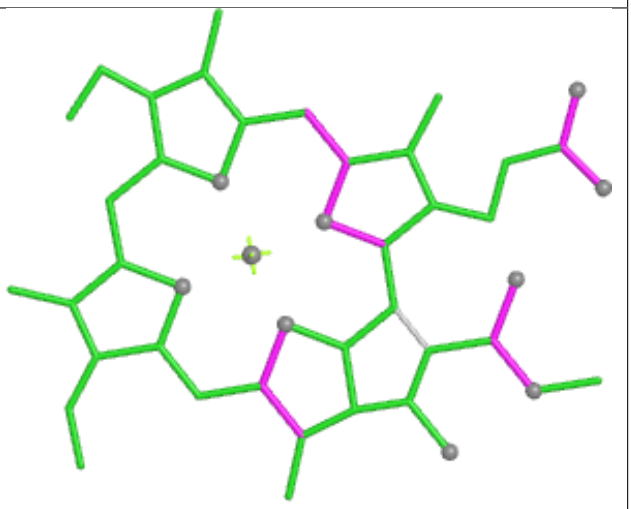
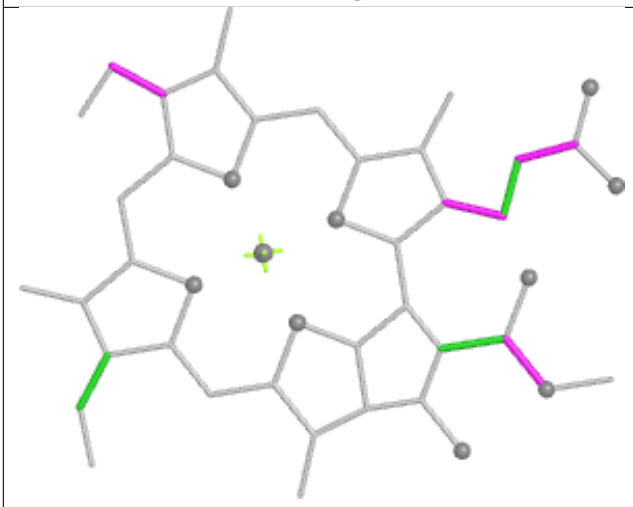


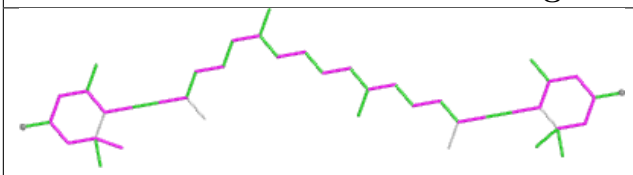
Bond angles



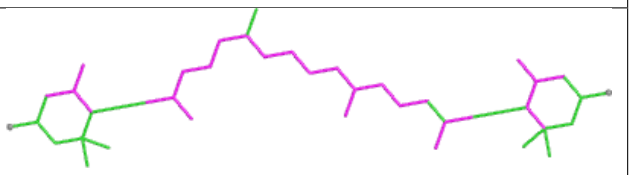
Torsions

Rings

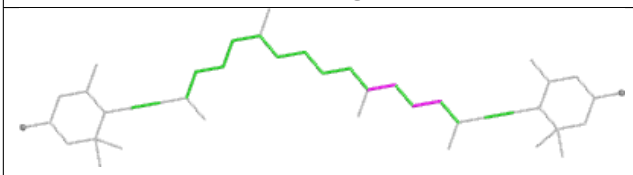
Ligand II0 c 613



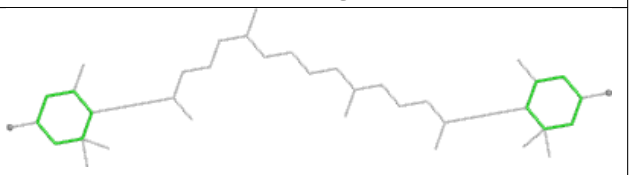
Bond lengths



Bond angles

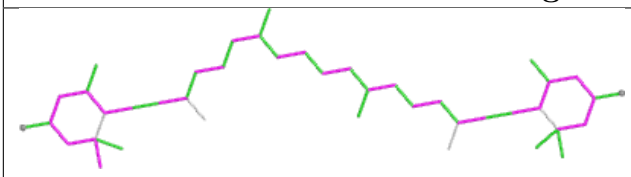


Torsions

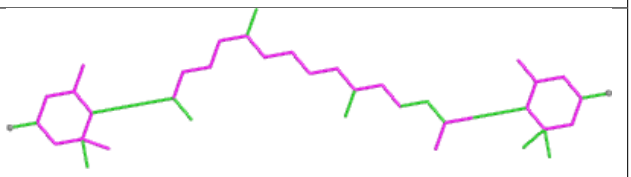


Rings

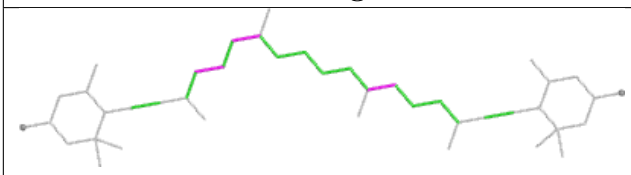
Ligand II0 k 619



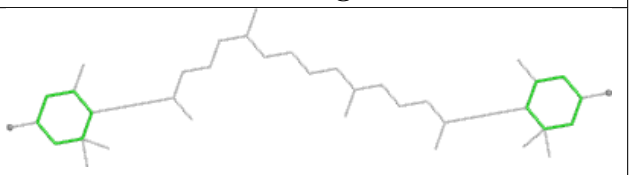
Bond lengths



Bond angles

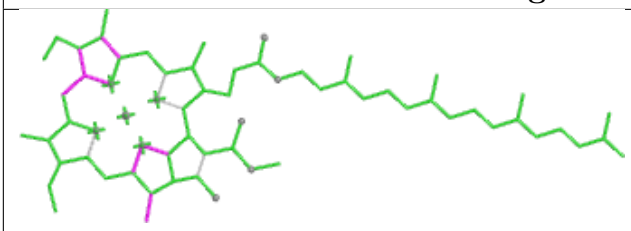


Torsions

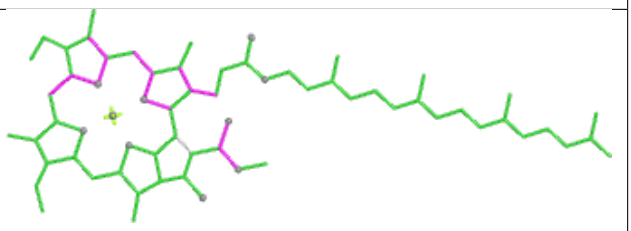


Rings

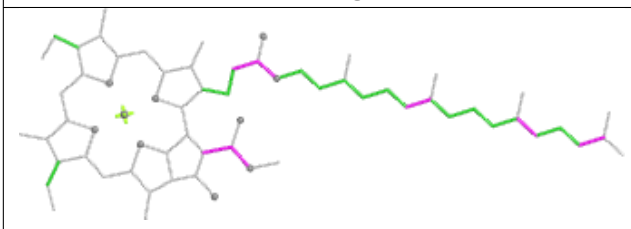
Ligand CLA a 310



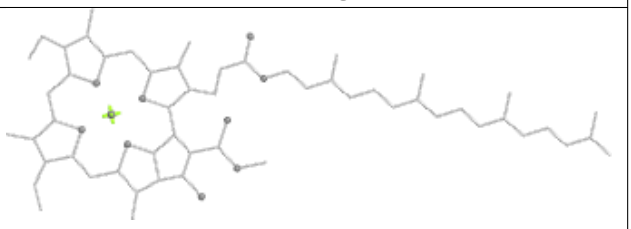
Bond lengths



Bond angles

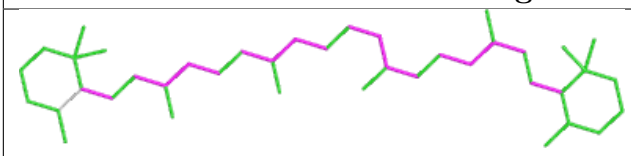


Torsions



Rings

Ligand WVN R 201



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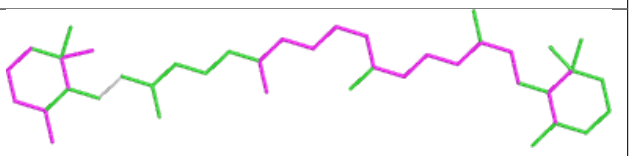
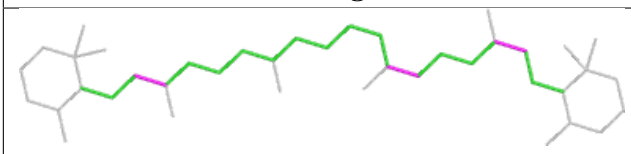
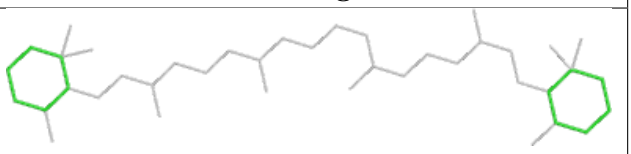


Bond angles

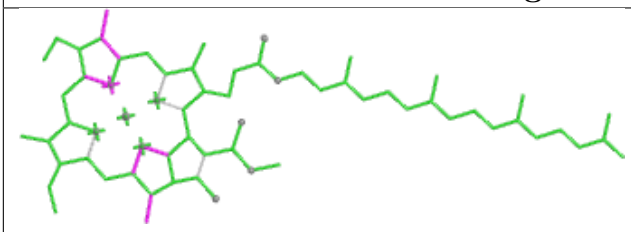


Torsions



Rings

Ligand CLA B 803



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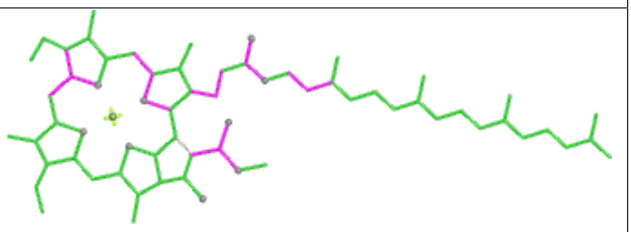
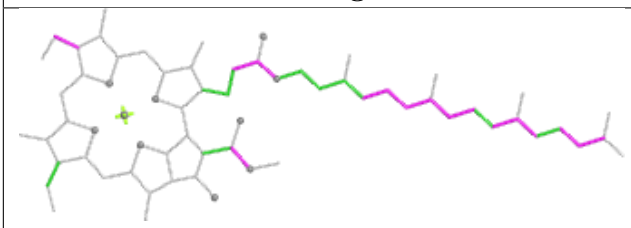
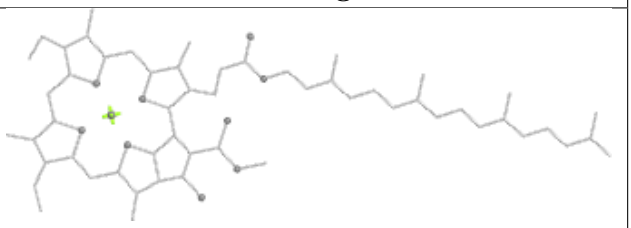


Bond angles

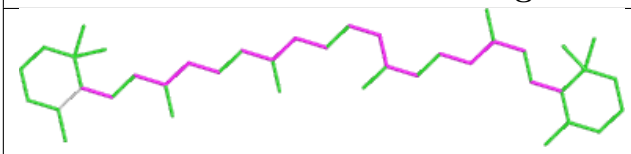


Torsions



Rings

Ligand WVN A 846



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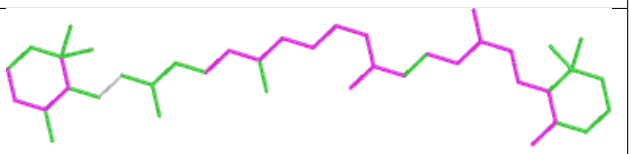
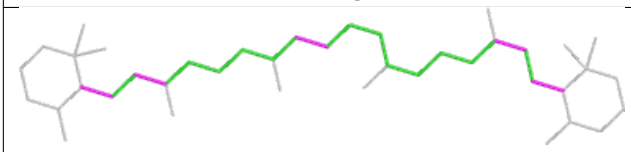


Bond angles



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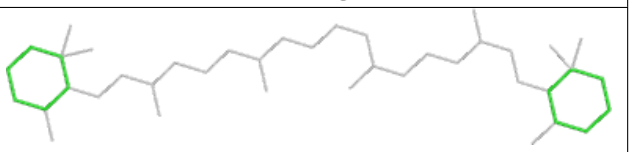
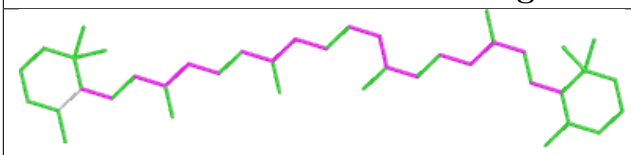
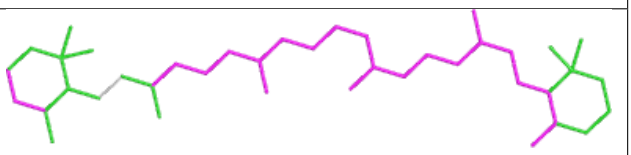


Rings

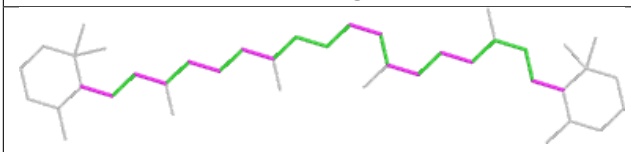
Ligand WVN F 205



Bond lengths



Bond angles



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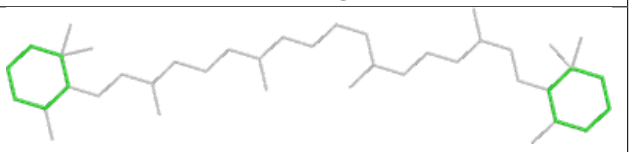
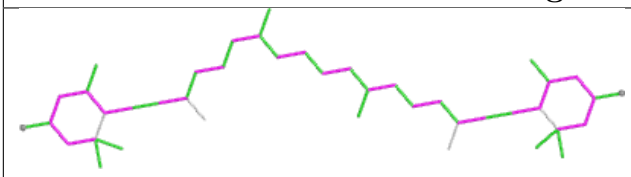
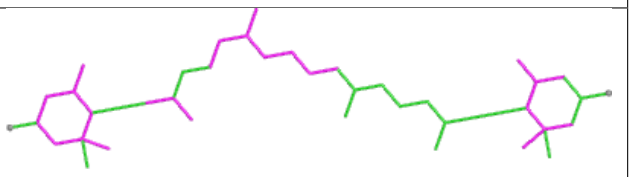
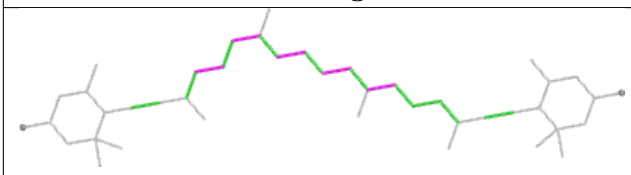
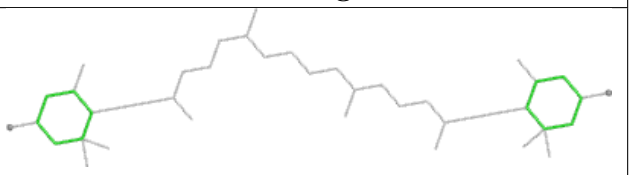
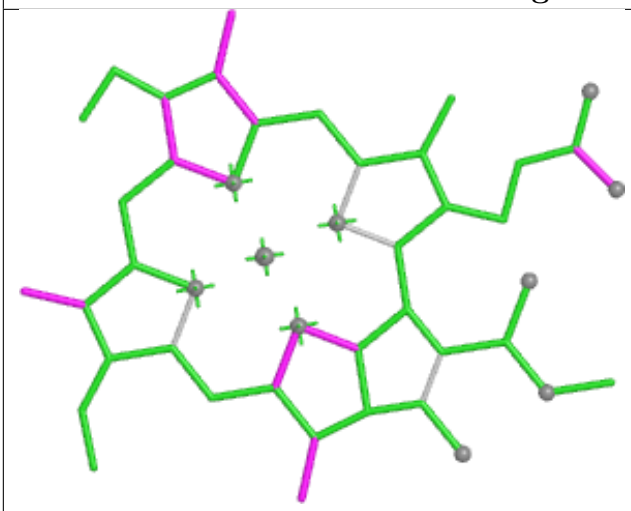
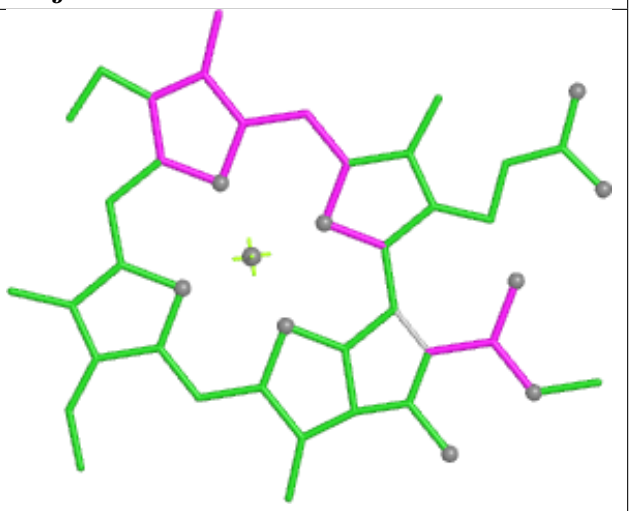
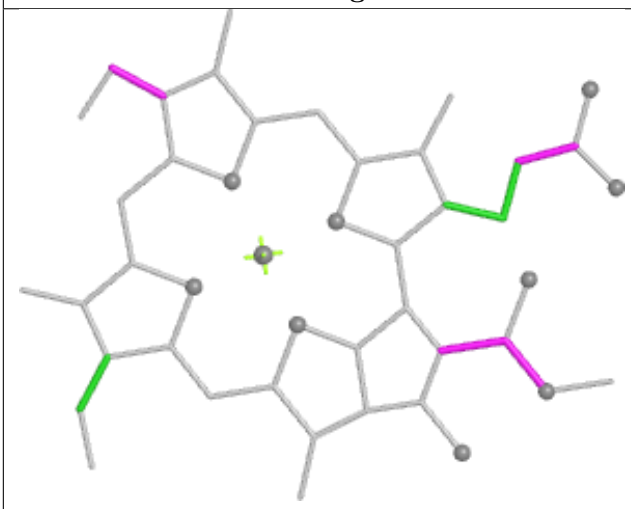
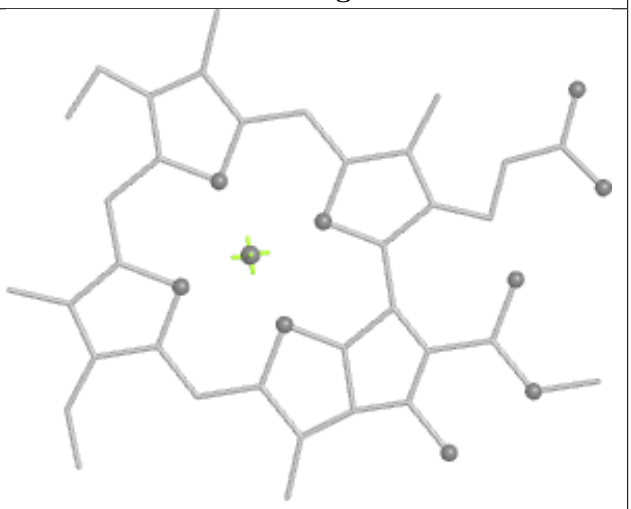
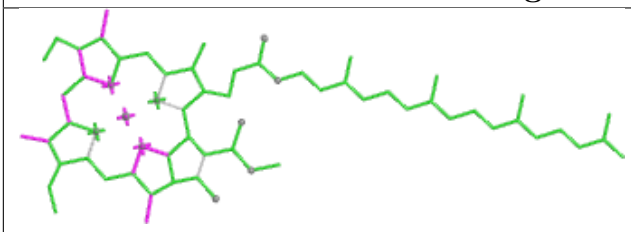
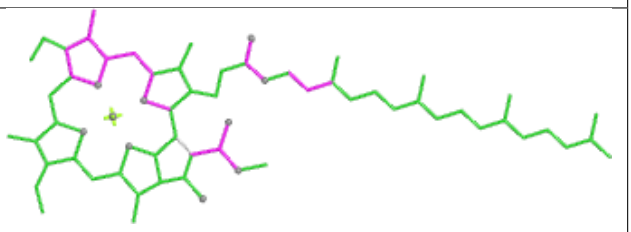
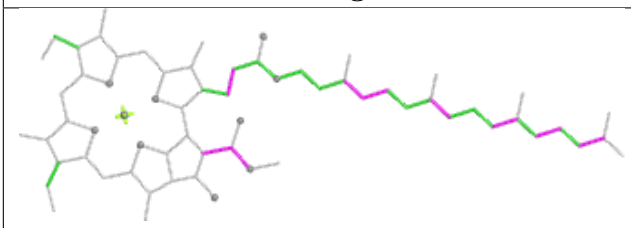
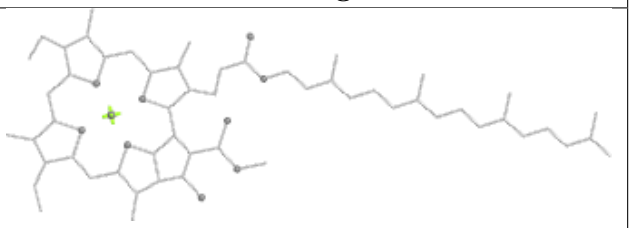
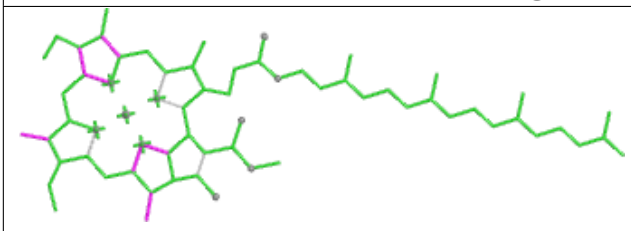
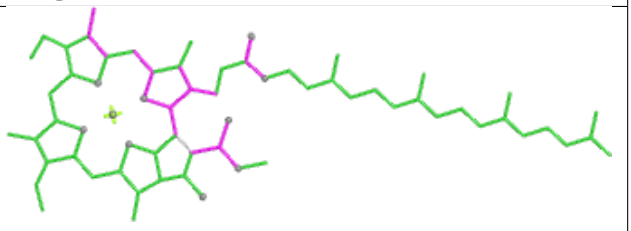
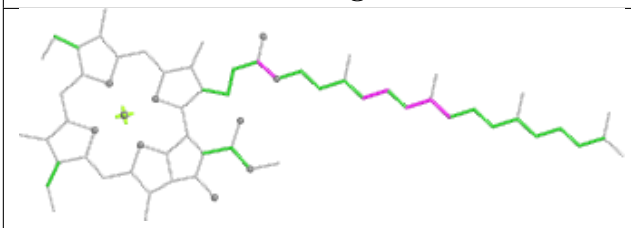
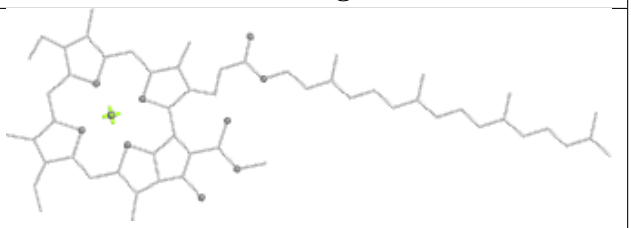


Rings

Ligand II0 f 618	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA j 309	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA B 801	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA g 309	
 Bond lengths	 Bond angles
 Torsions	 Rings

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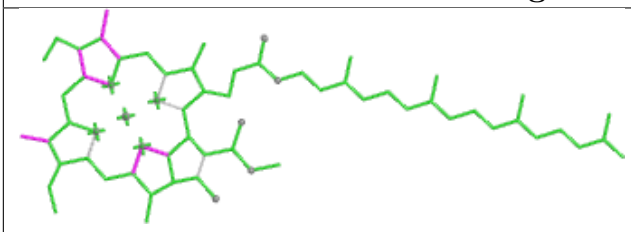
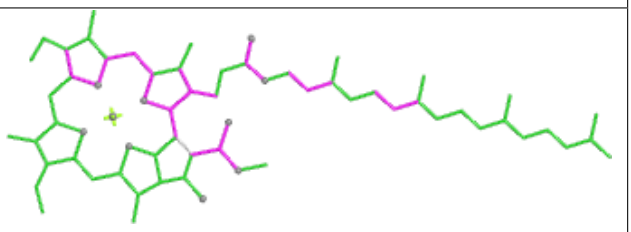
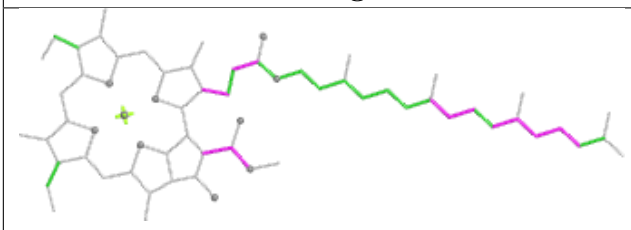
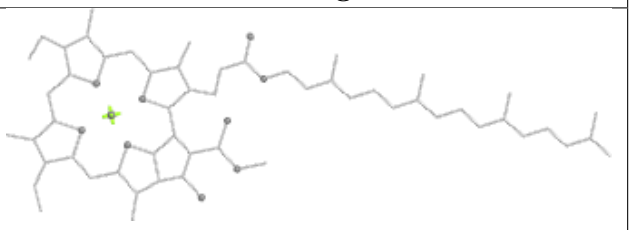
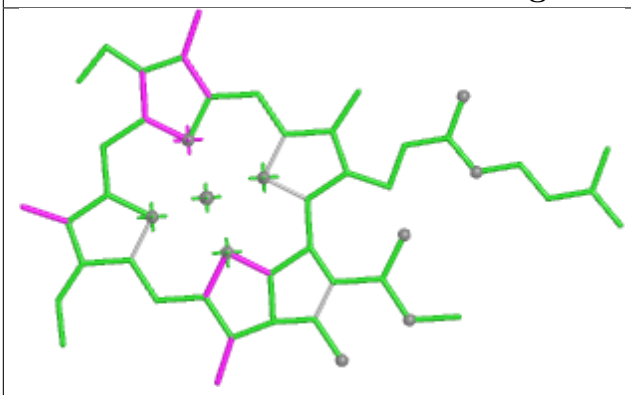
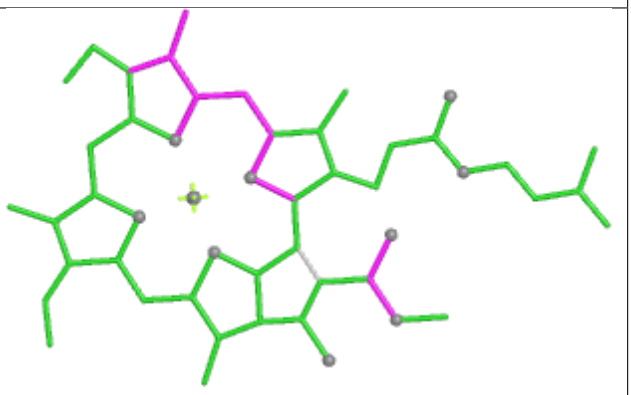
 Bond lengths	 Bond angles
 Torsions	 Rings

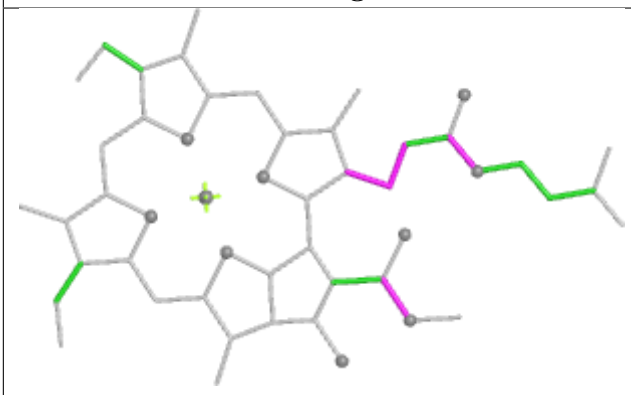
Ligand CLA e 602



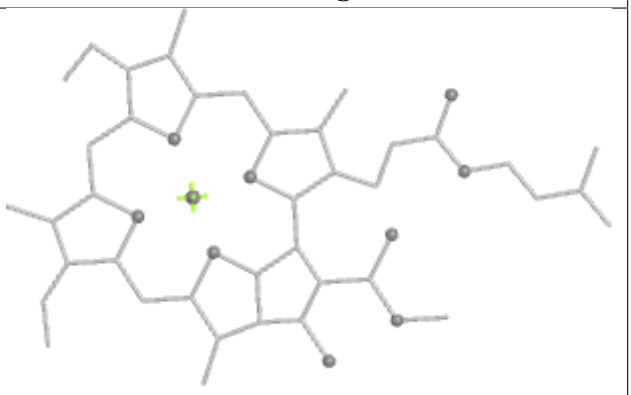
Bond lengths



Bond angles

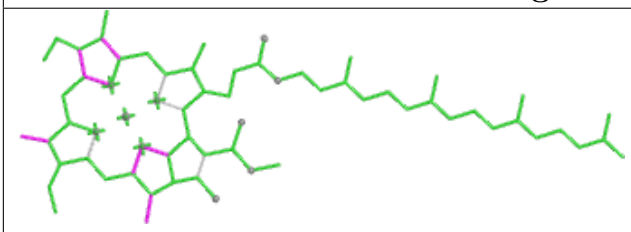


Torsions



Rings

Ligand CLA f 604



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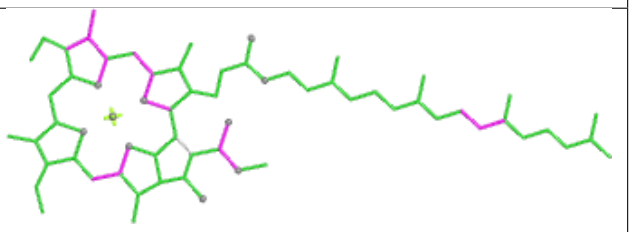
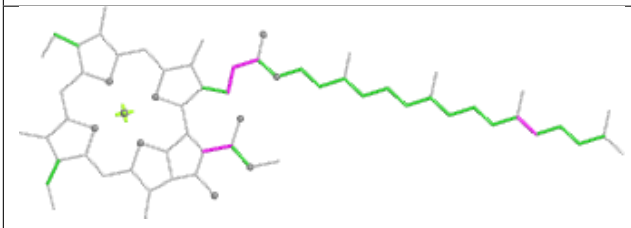


Bond angles



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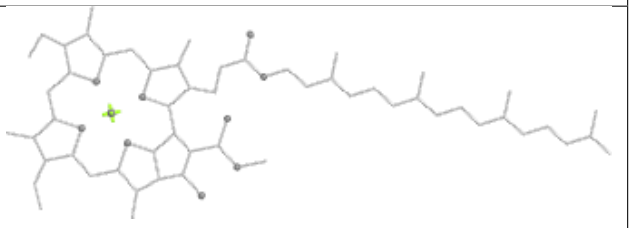
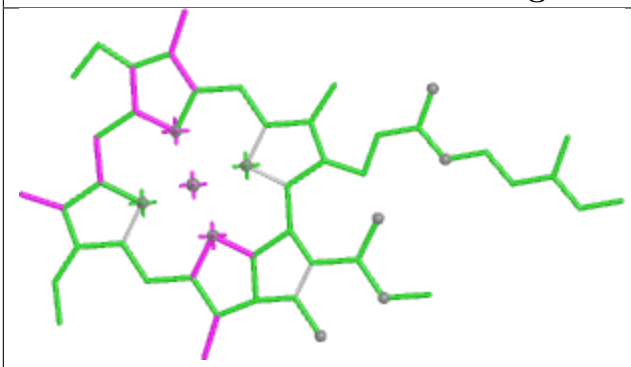
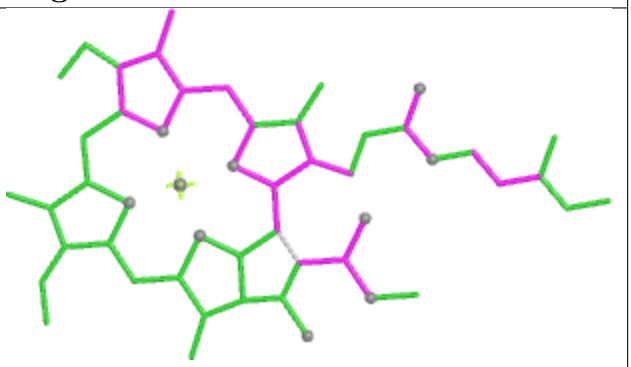


Rings

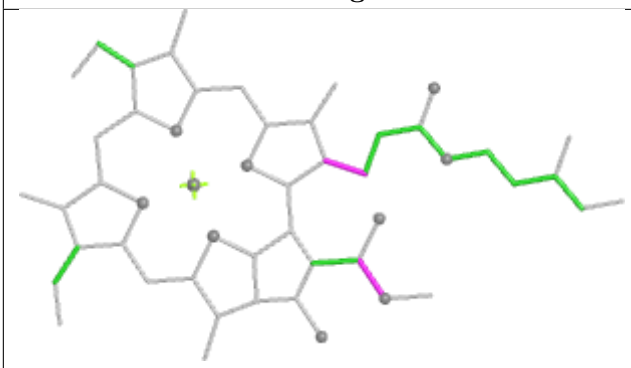
Ligand CLA g 304



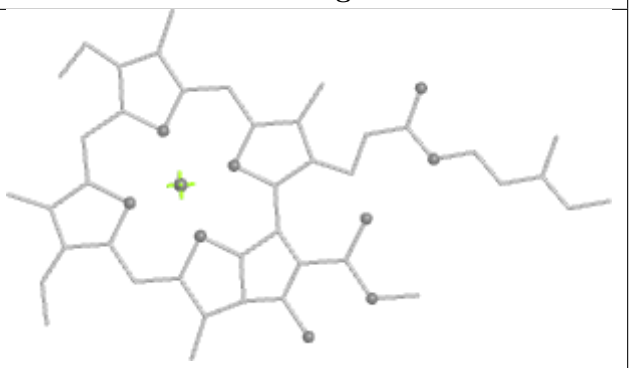
Bond lengths



Bond angles

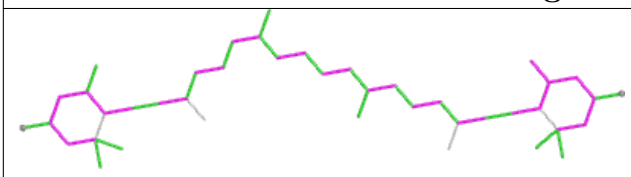


Torsions

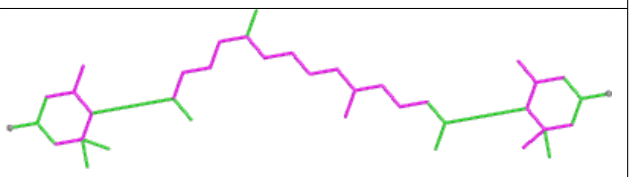


Rings

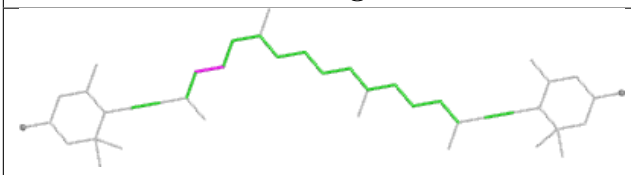
Ligand II0 c 614



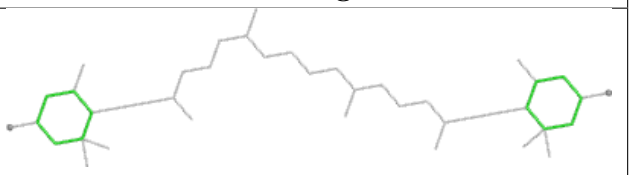
Bond lengths



Bond angles

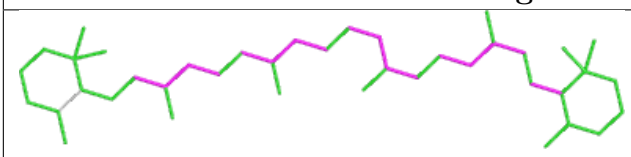


Torsions

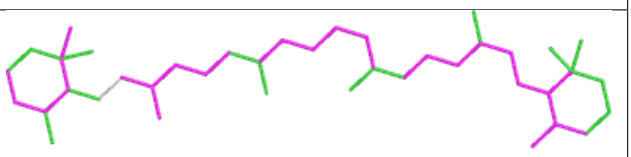


Rings

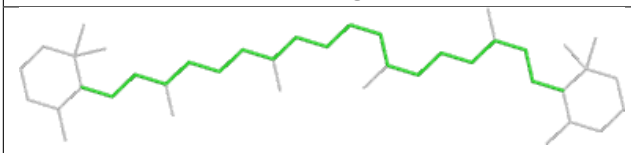
Ligand WVN B 846



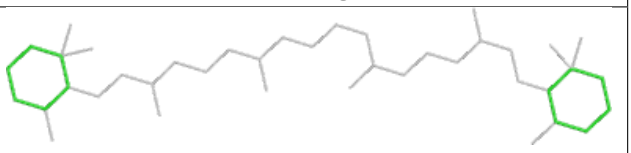
Bond lengths



Bond angles

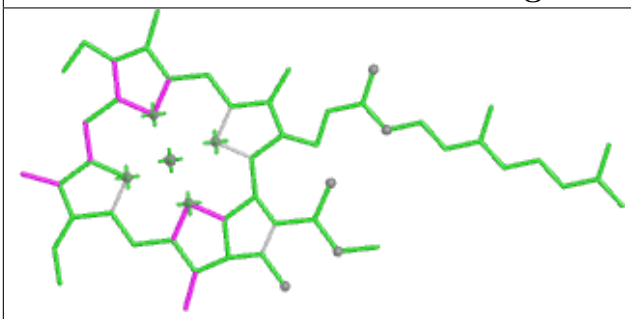


Torsions

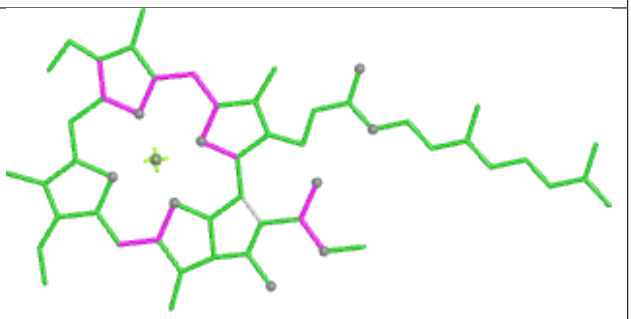


Rings

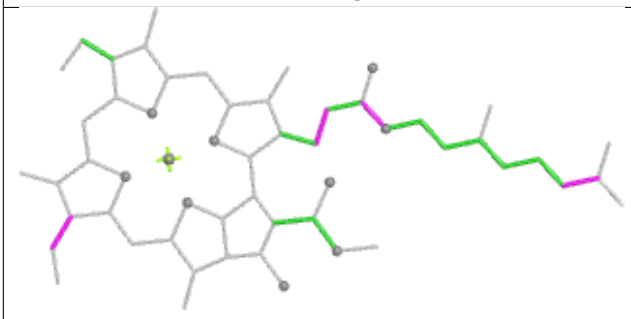
Ligand CLA B 811



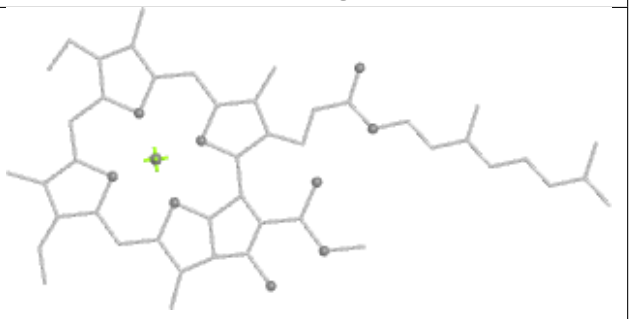
Bond lengths



Bond angles

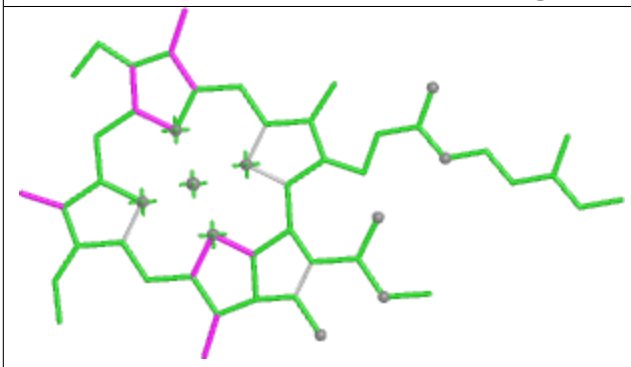


Torsions



Rings

Ligand CLA j 302



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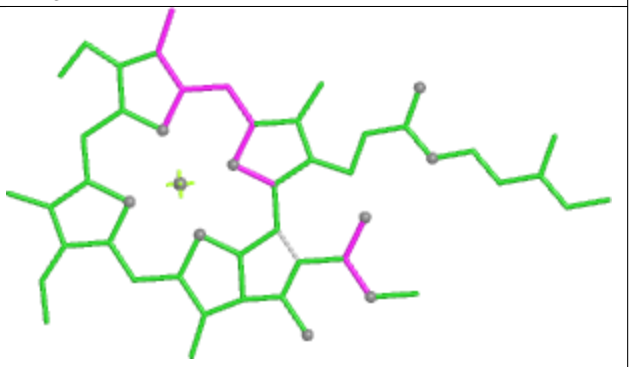
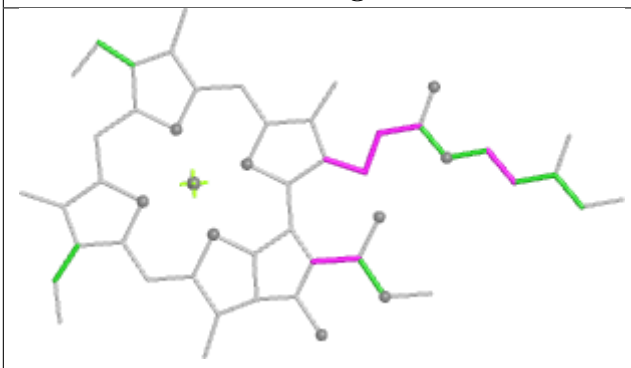


Bond angles



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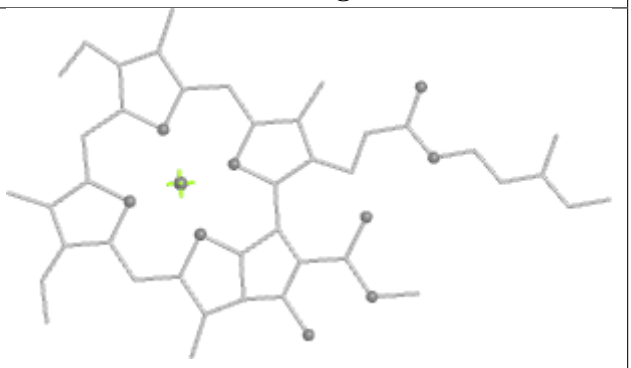
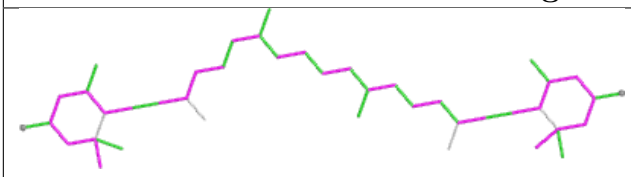


Rings

Ligand II0 b 314



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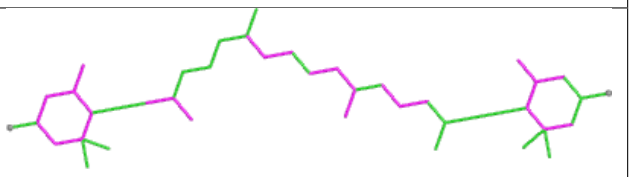
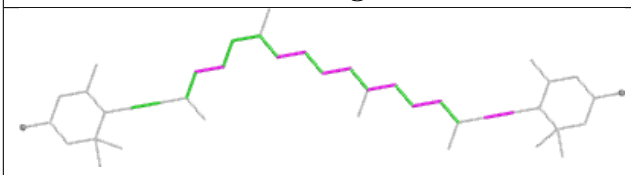


Bond angles



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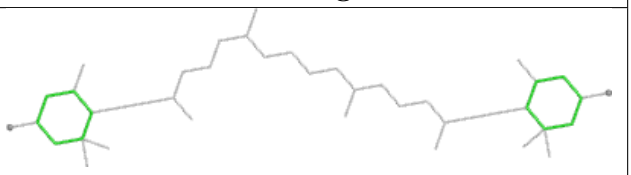
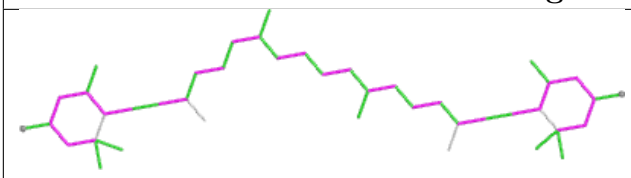
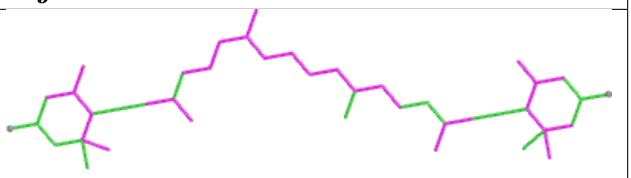


Rings

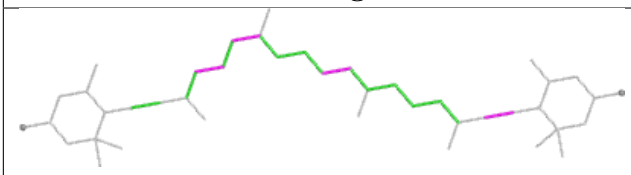
Ligand II0 j 315



Bond lengths



Bond angles



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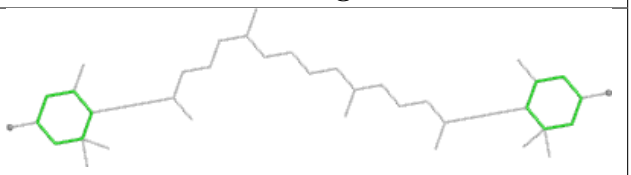
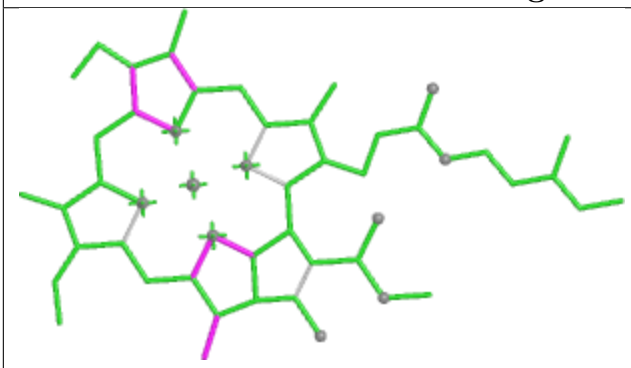
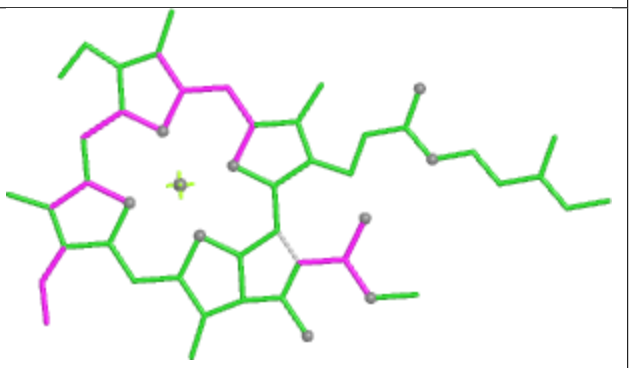


Rings

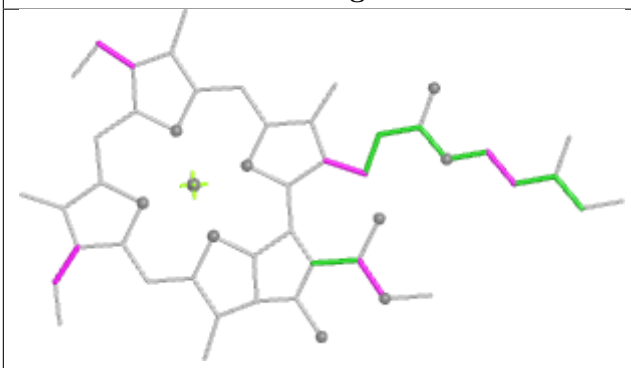
Ligand CLA k 614



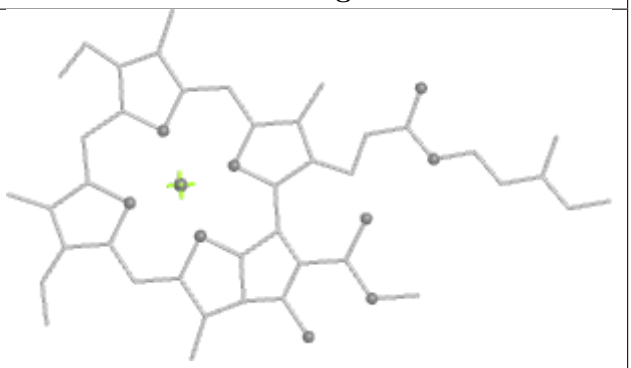
Bond lengths



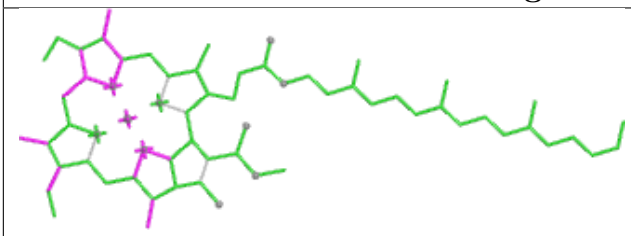
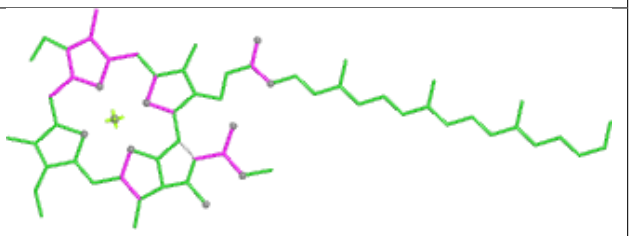
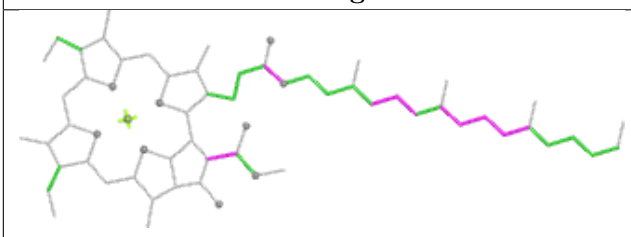
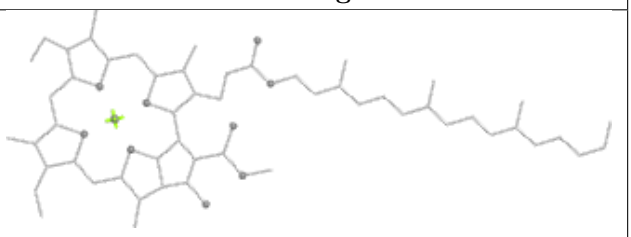
Bond angles

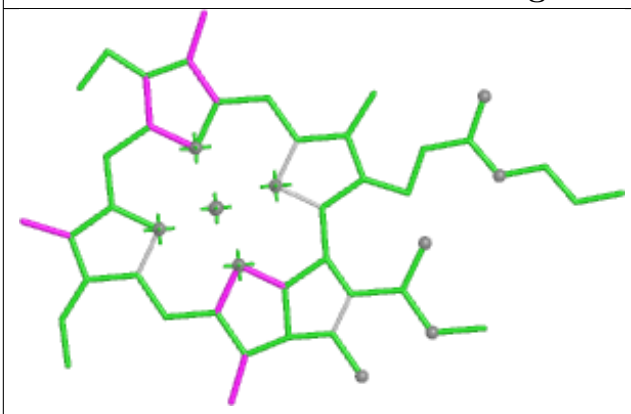
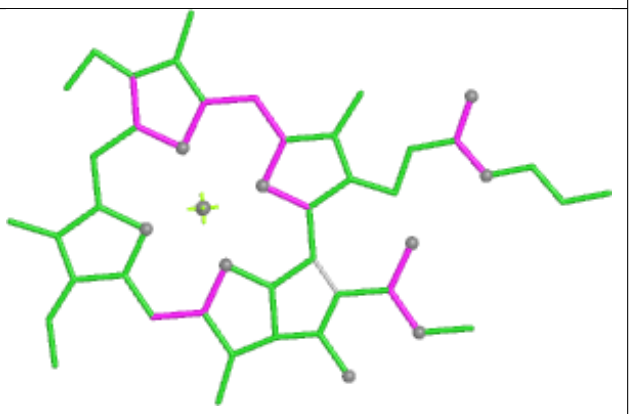
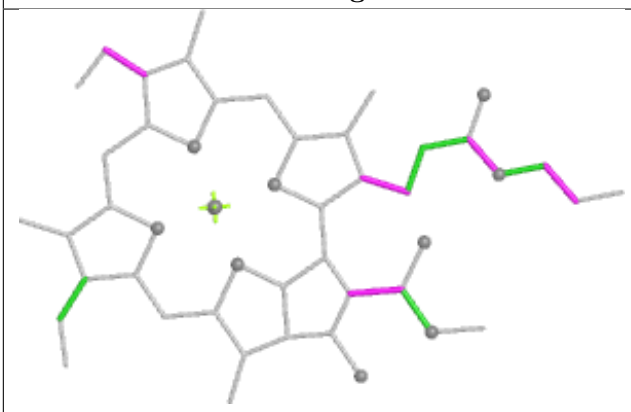
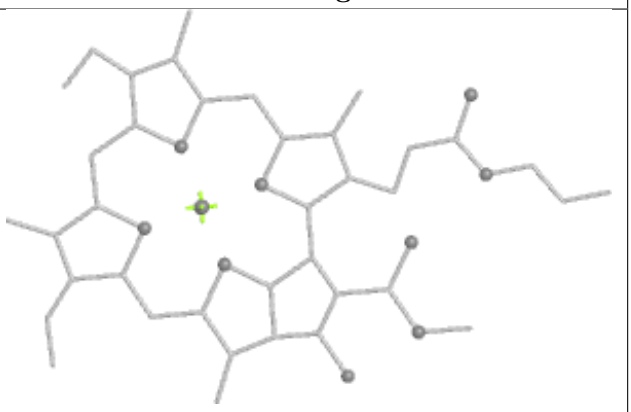


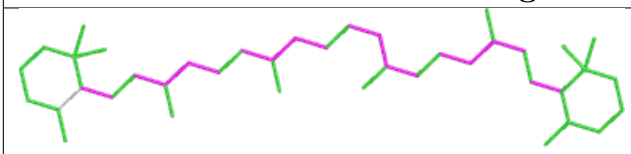
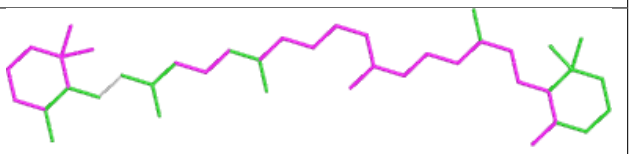
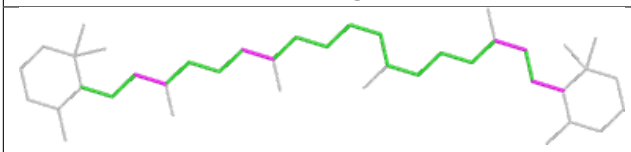
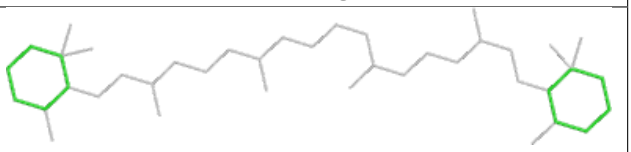
Torsions

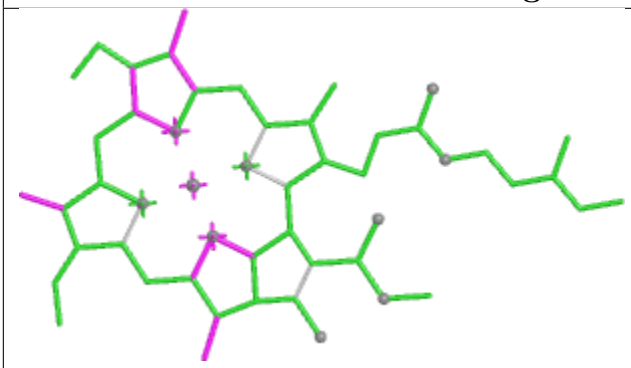
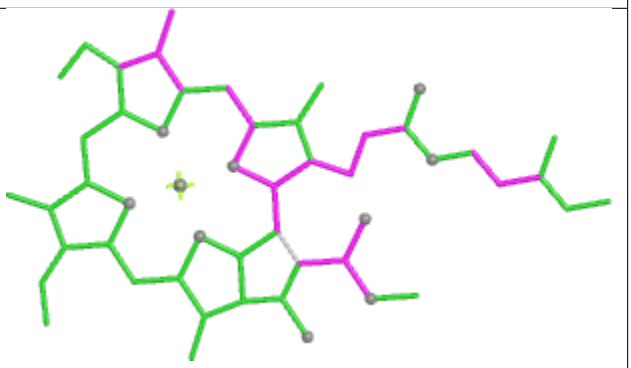
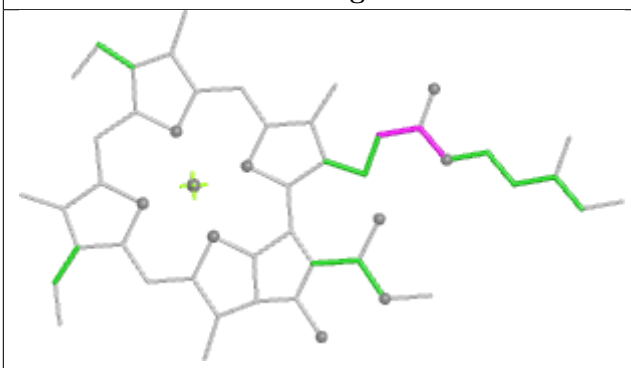
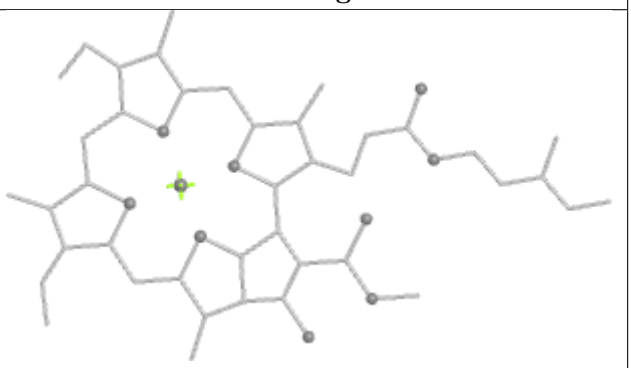


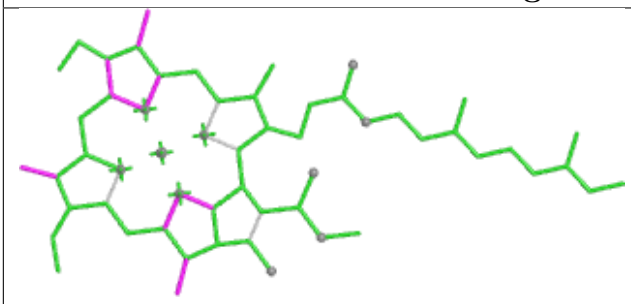
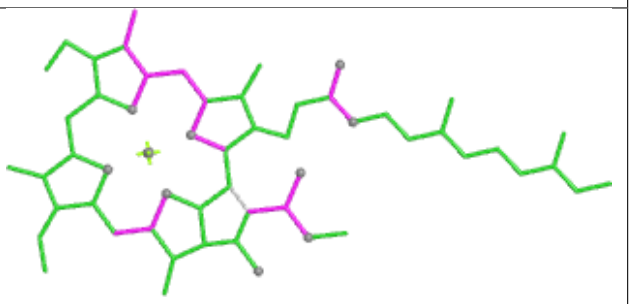
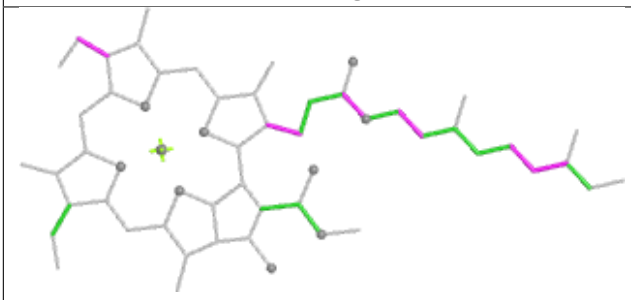
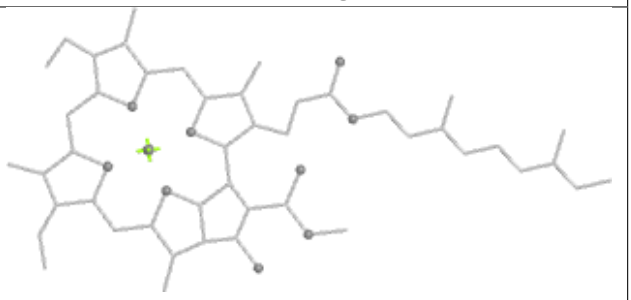
Rings

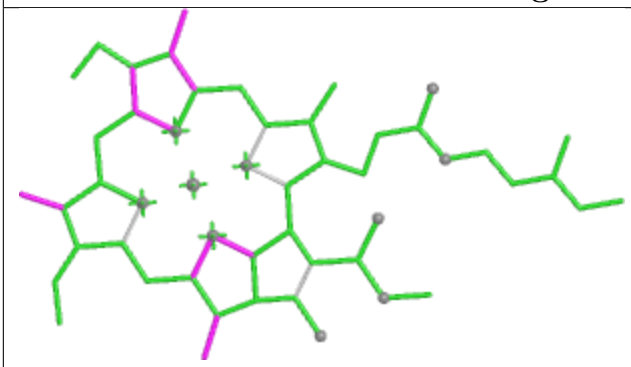
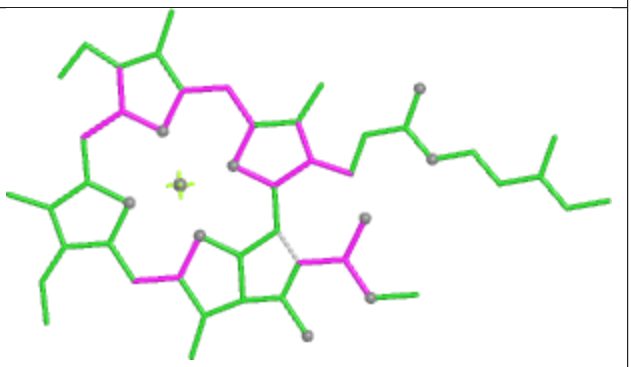
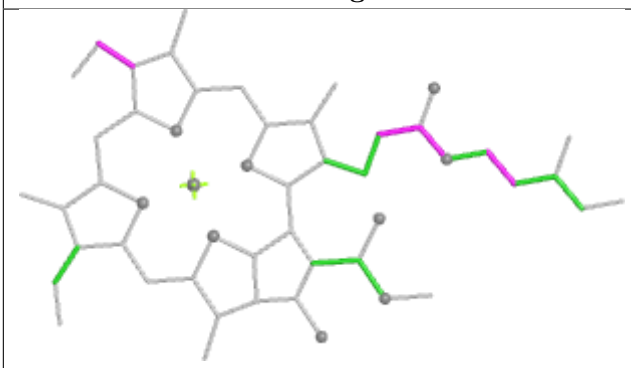
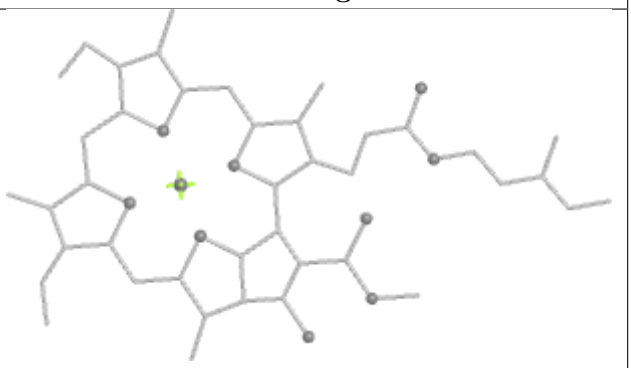
Ligand CLA B 823	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA a 309	
 Bond lengths	 Bond angles
 Torsions	 Rings

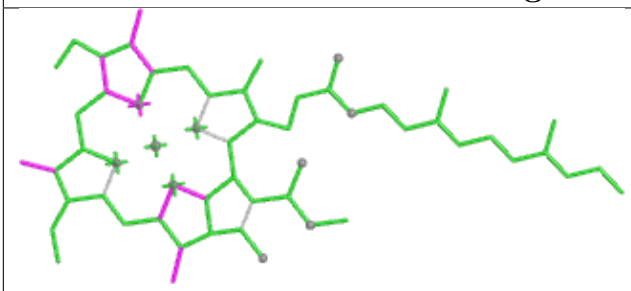
Ligand WVN J 101	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA K 101	
 Bond lengths	 Bond angles
 Torsions	 Rings

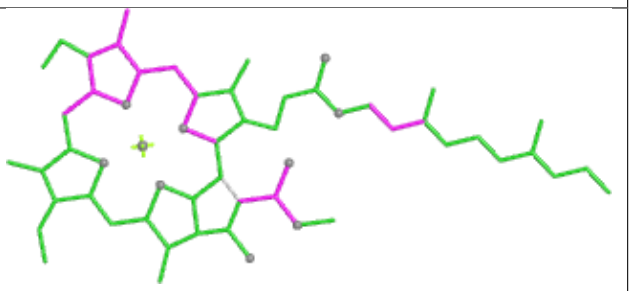
Ligand CLA A 809	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA f 603	
 Bond lengths	 Bond angles
 Torsions	 Rings

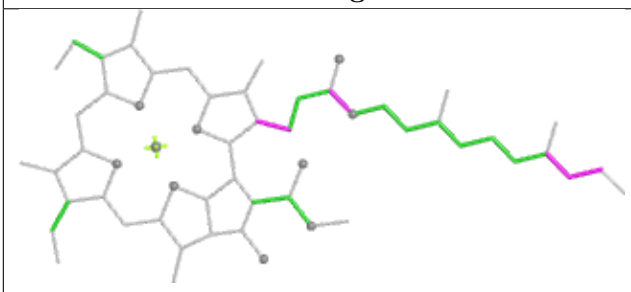
Ligand CLA B 817



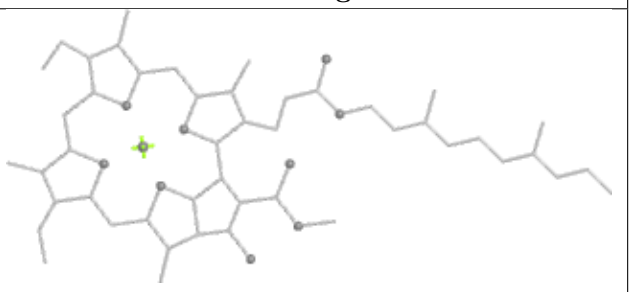
Bond lengths



Bond angles

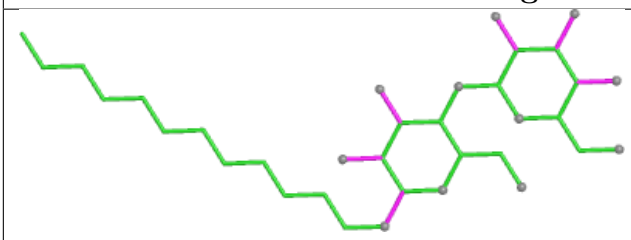


Torsions

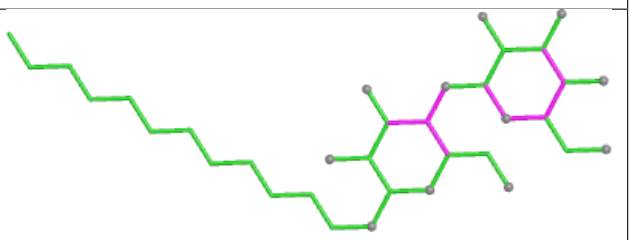


Rings

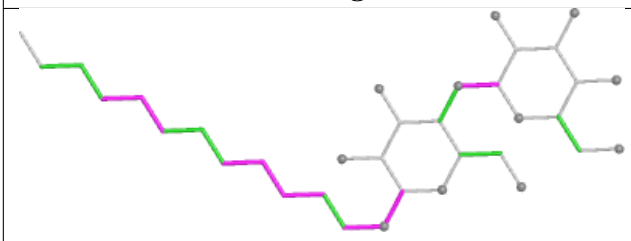
Ligand LMT A 851



Bond lengths



Bond angles



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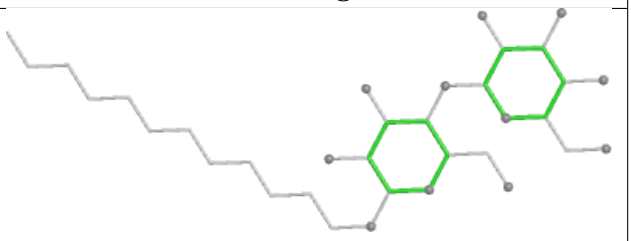
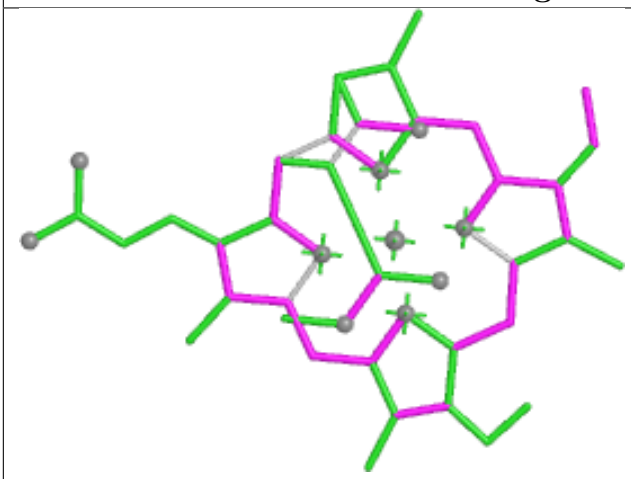


Rings

Ligand KC2 i 609



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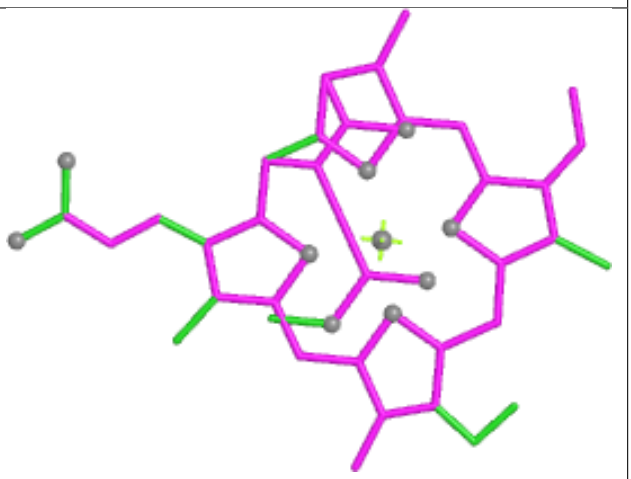
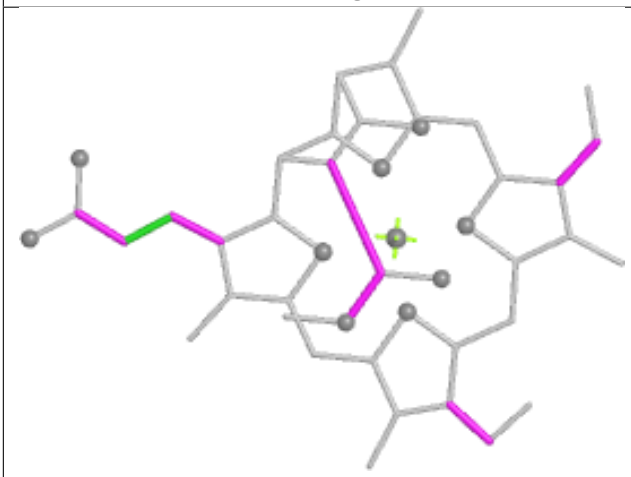


Bond angles



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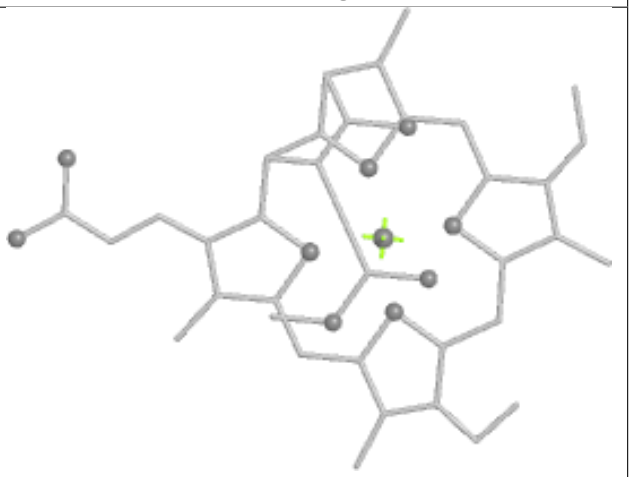
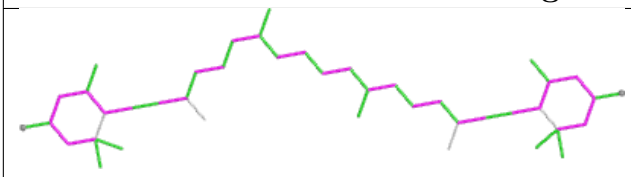


Rings

Ligand II0 h 310



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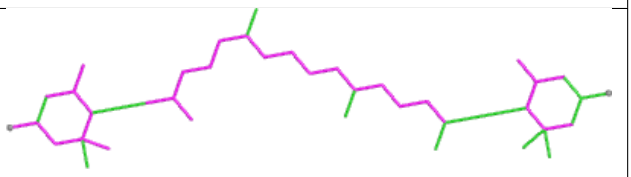
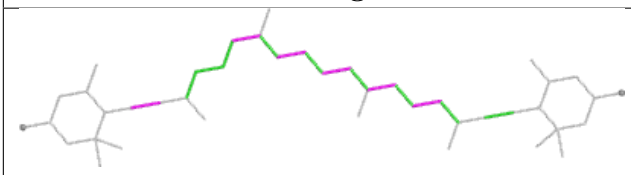


Bond angles



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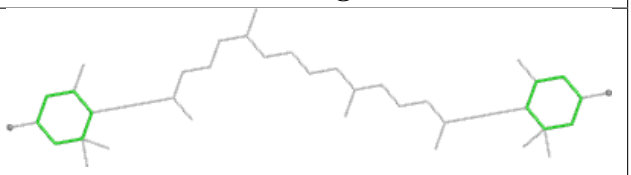
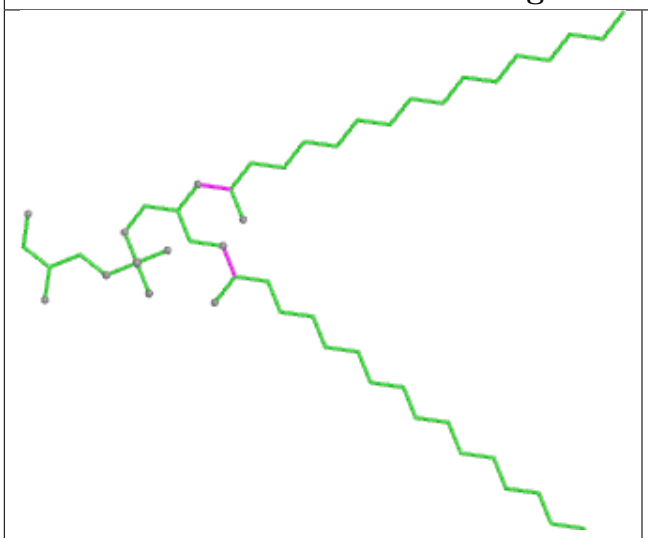


Rings

Ligand LHG b 302



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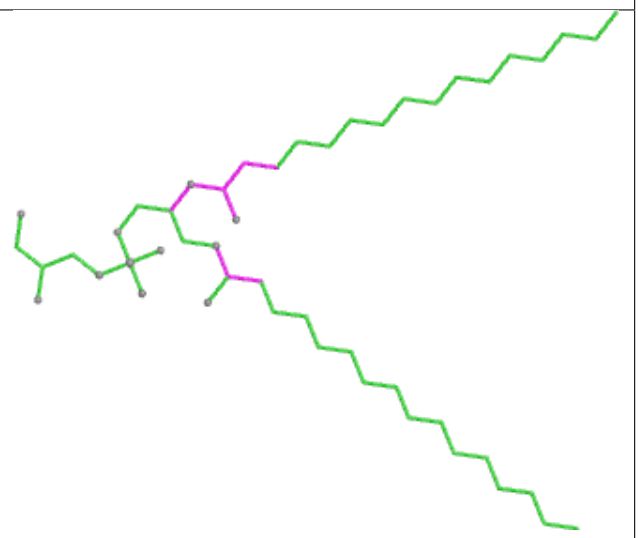
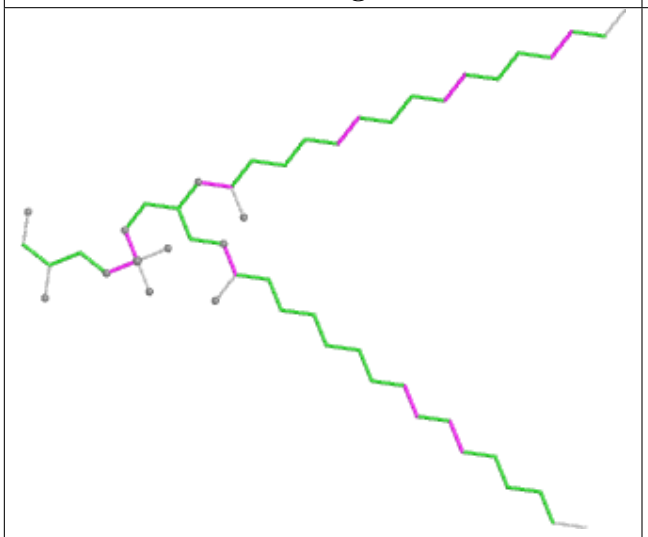


Bond angles



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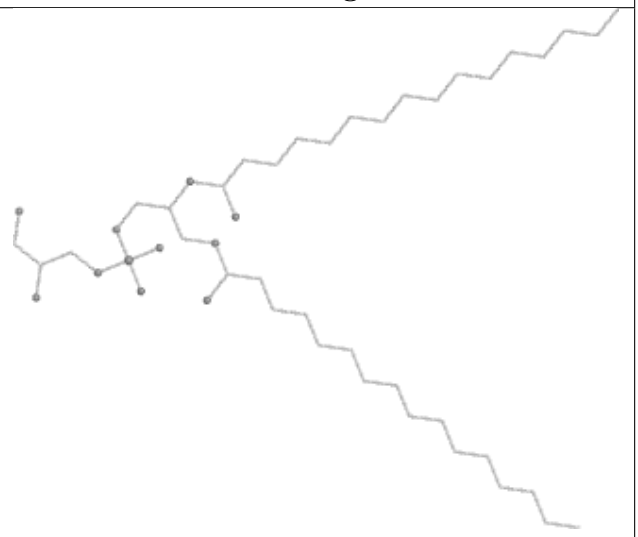
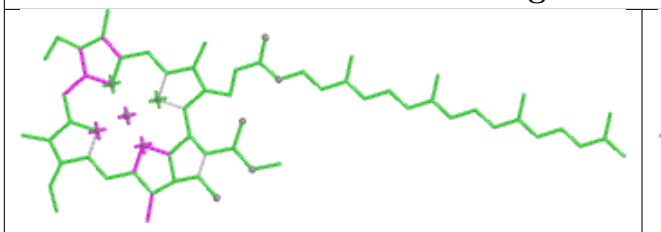


Rings

Ligand CLA d 303



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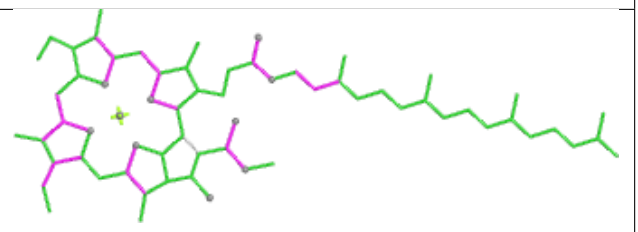
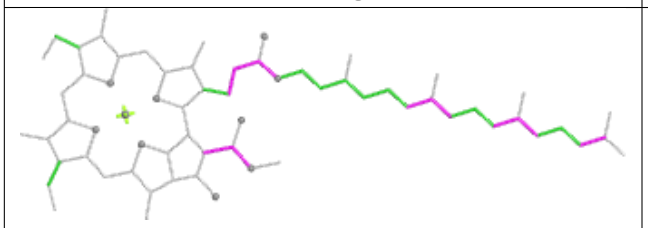


Bond angles



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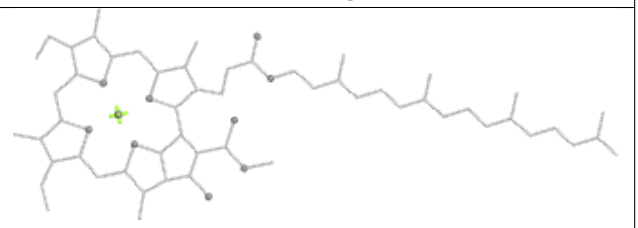
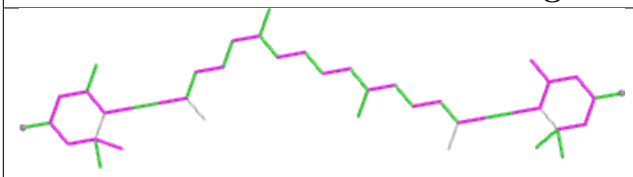


Rings

Ligand II0 c 616



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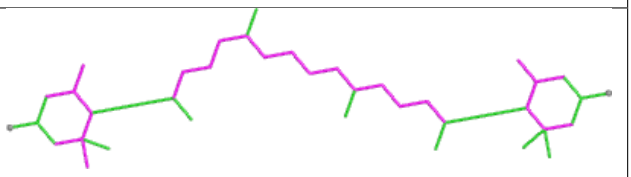
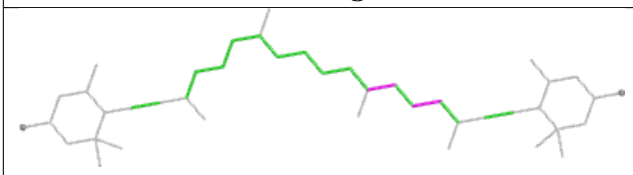


Bond angles



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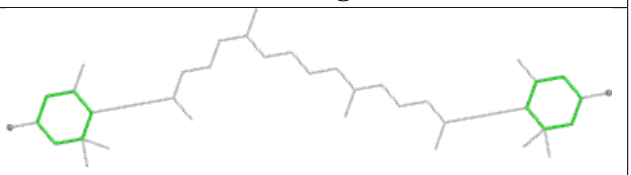
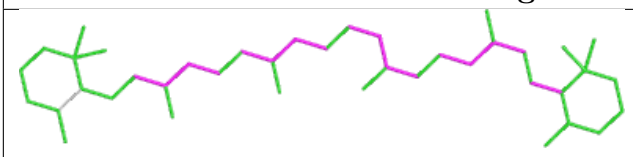


Rings

Ligand WVN L 206



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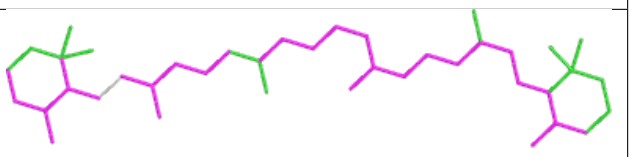
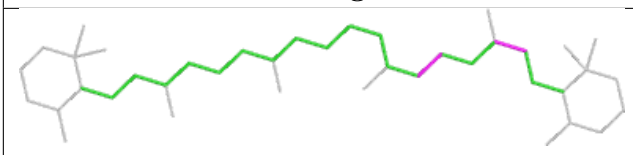


Bond angles



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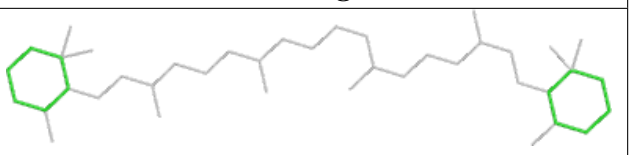
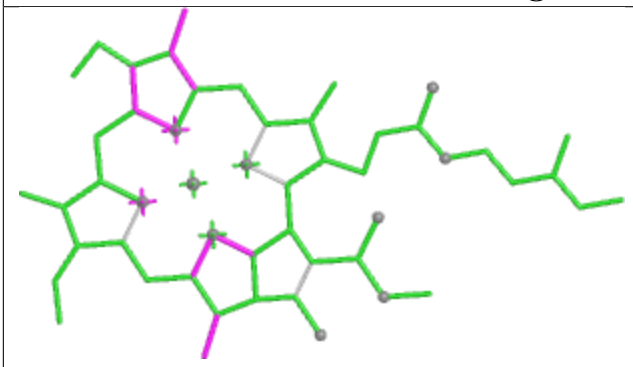


Rings

Ligand CLA k 601



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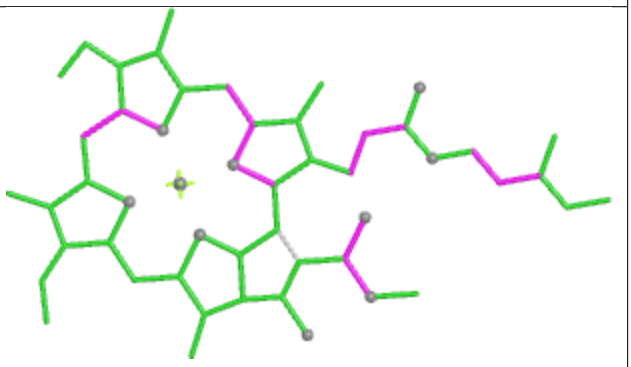
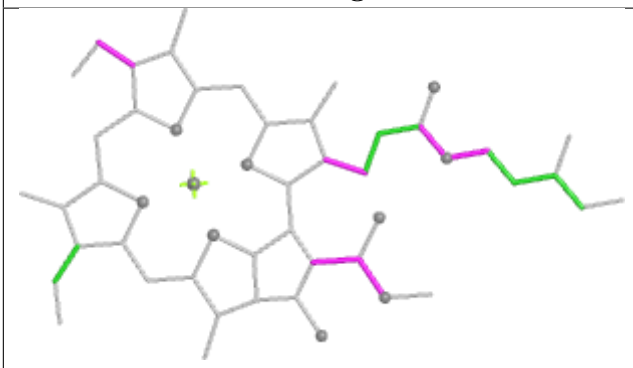


Bond angles



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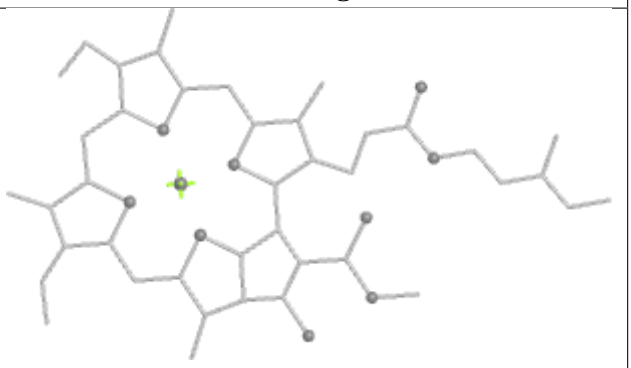
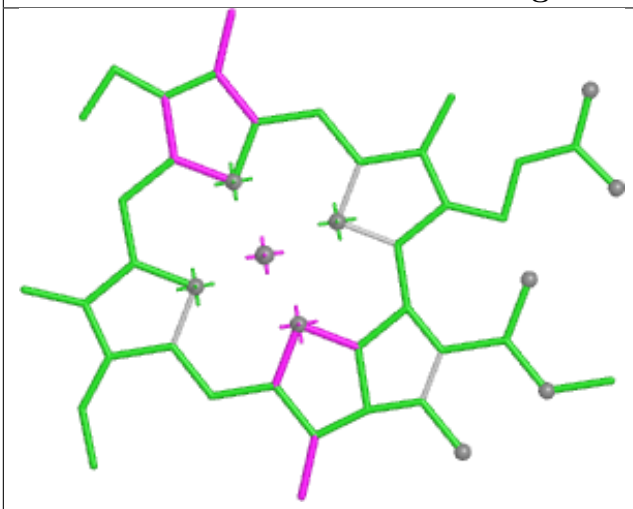


Rings

Ligand CLA j 306



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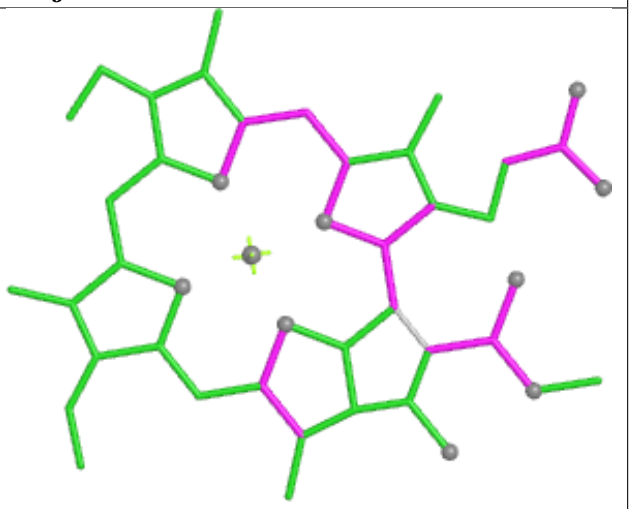
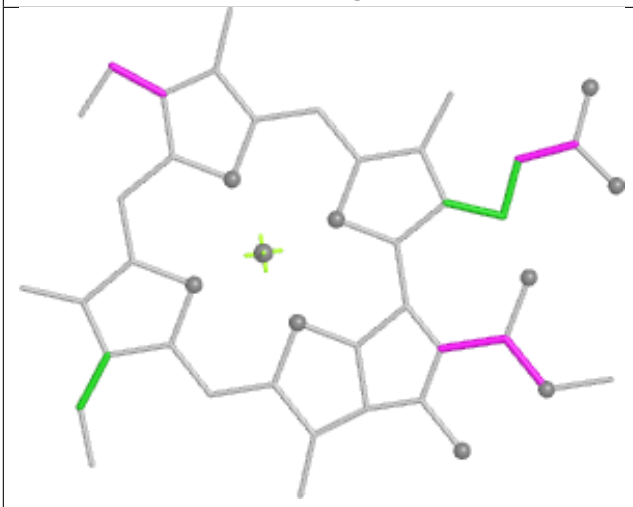
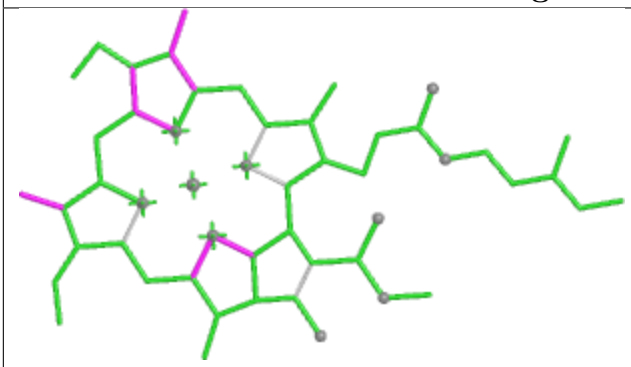
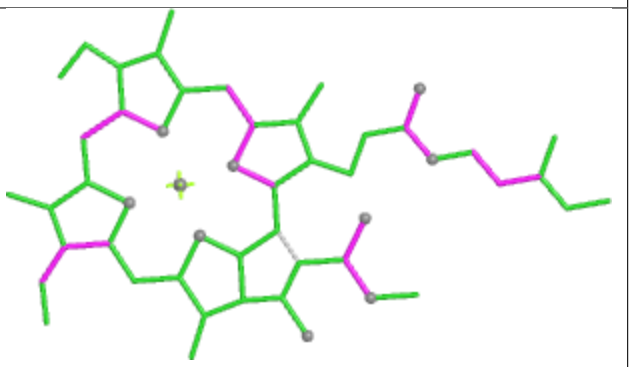
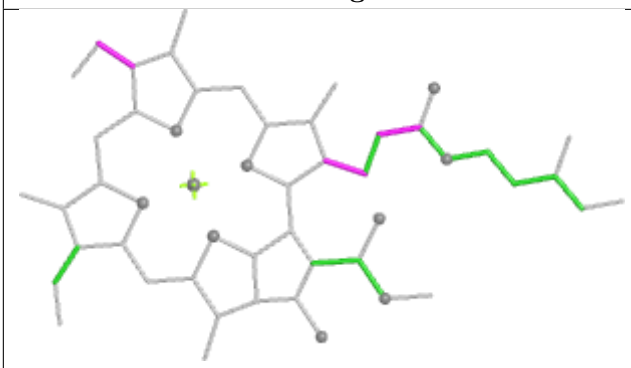
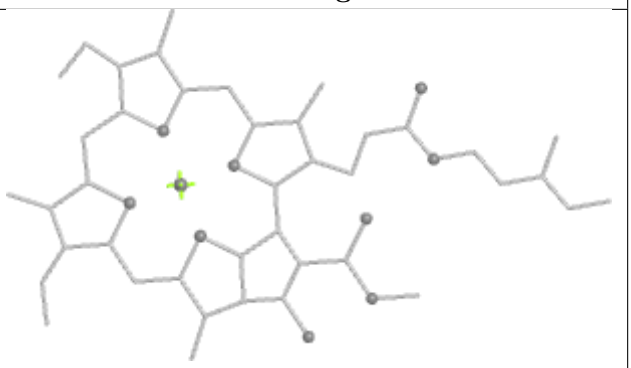


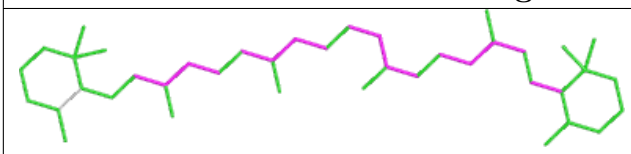
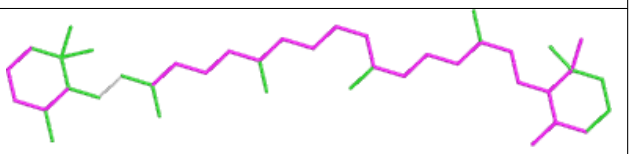
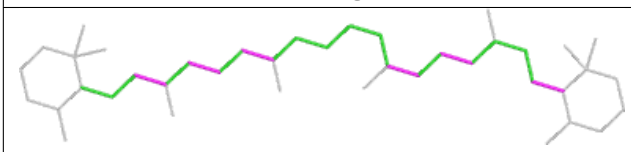
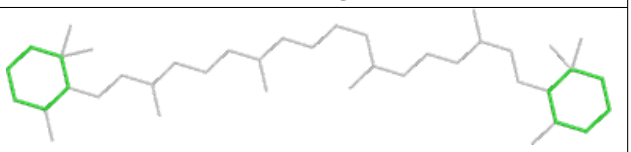
Bond angles

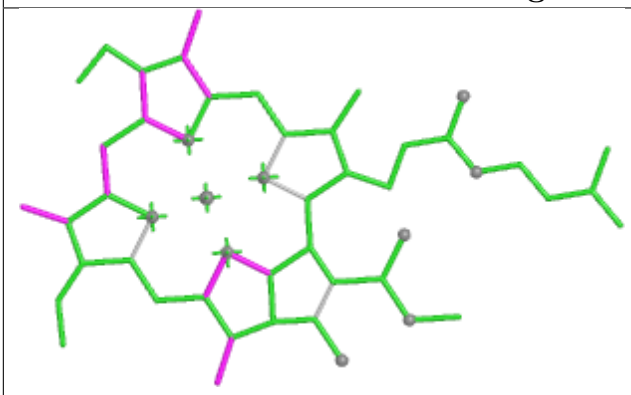
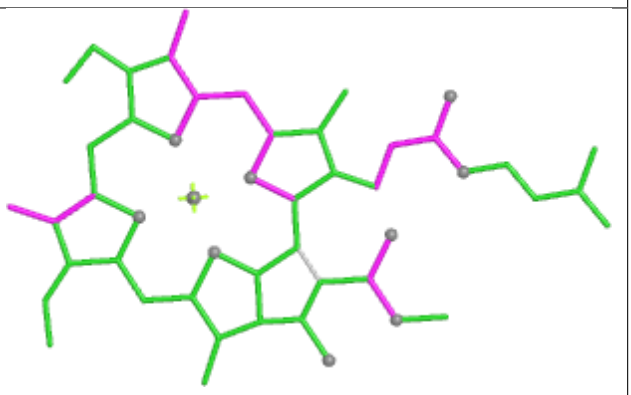
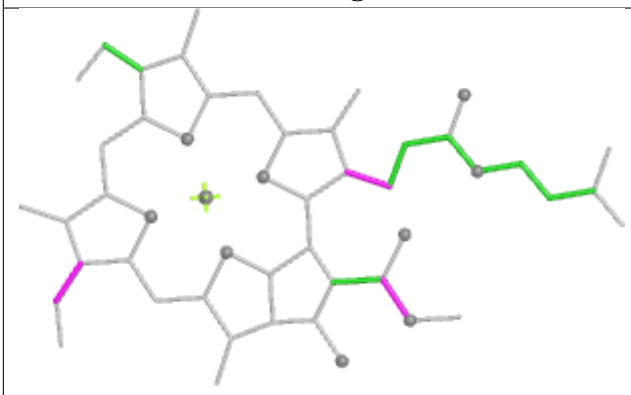
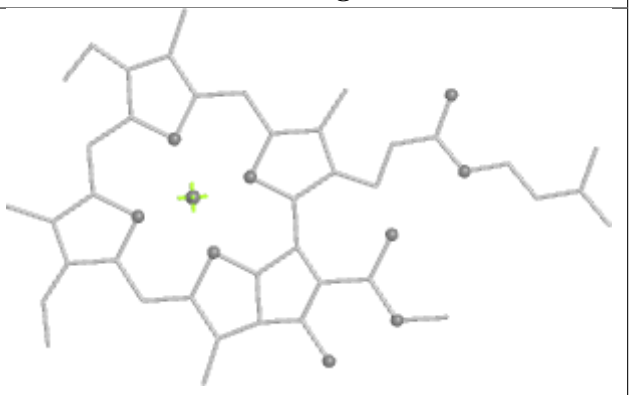


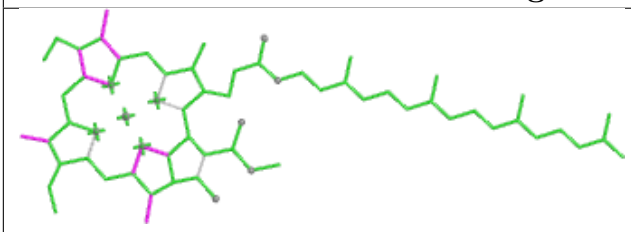
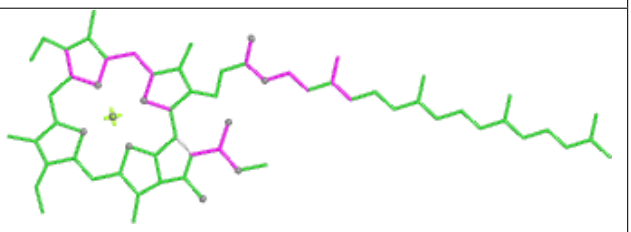
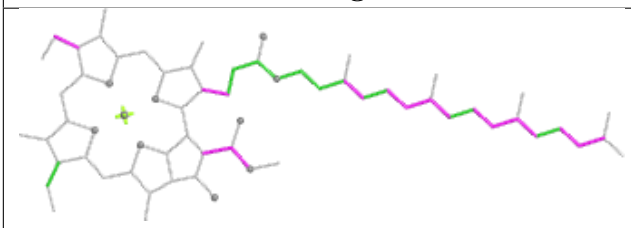
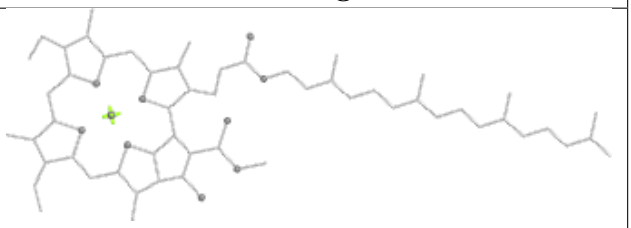
Torsions

Rings

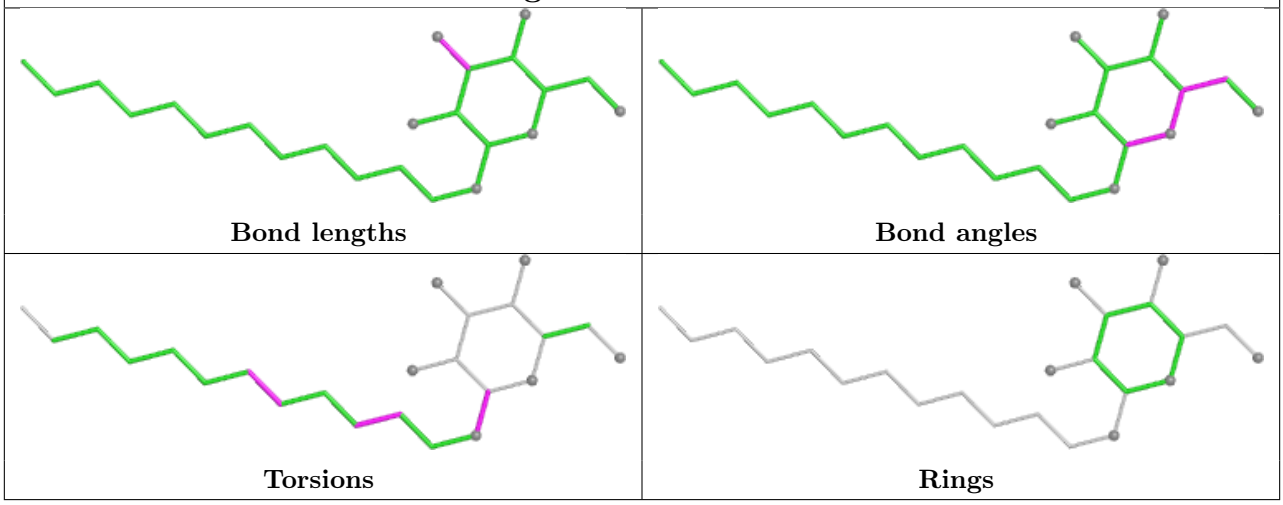
Ligand CLA f 606	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand WVN R 202	
 Bond lengths	 Bond angles
 Torsions	 Rings

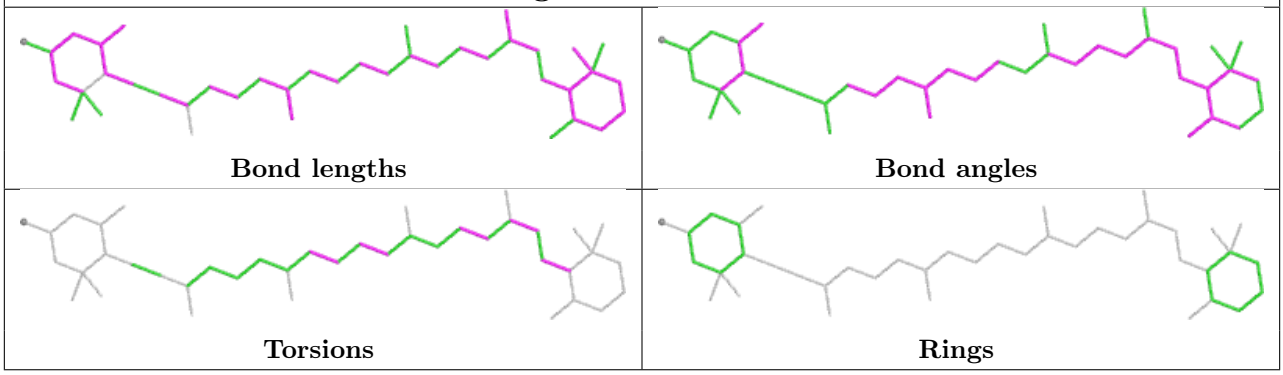
Ligand CLA k 602	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA b 312	
 Bond lengths	 Bond angles
 Torsions	 Rings

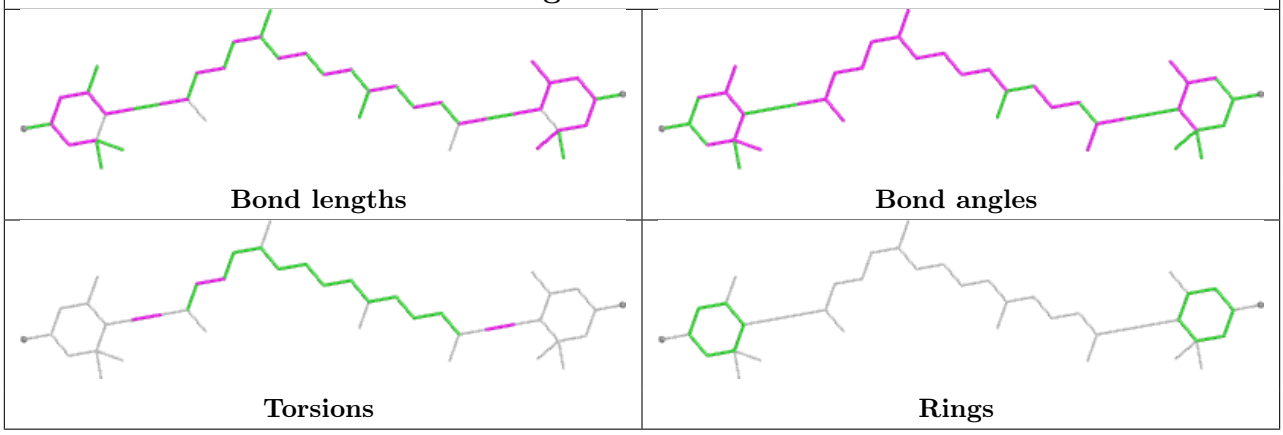
Ligand LMT F 203



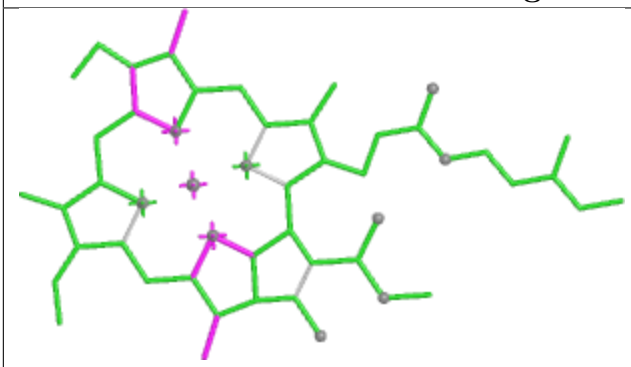
Ligand IHT k 618



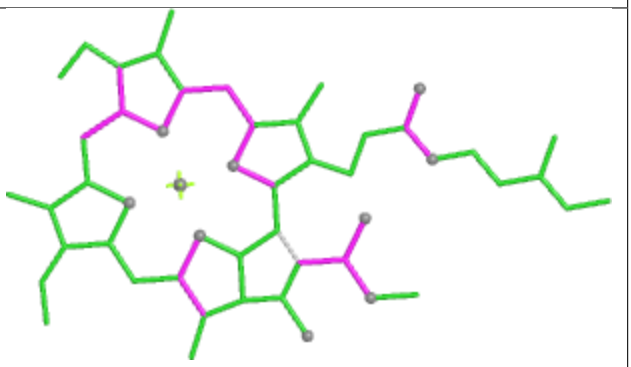
Ligand II0 k 617



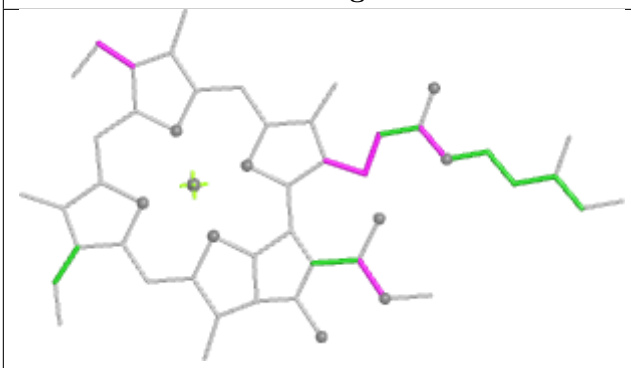
Ligand CLA A 822



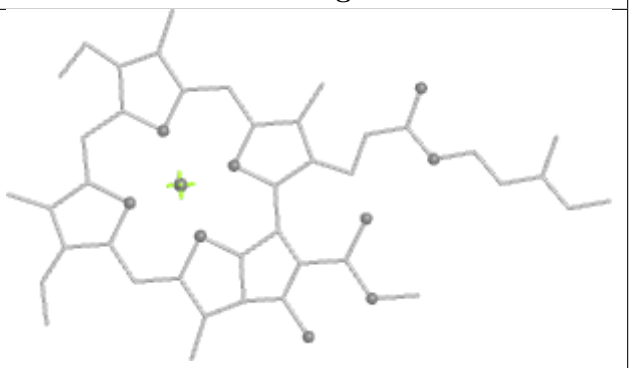
Bond lengths



Bond angles

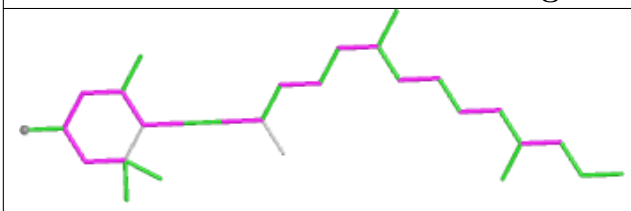


Torsions



Rings

Ligand II0 h 309



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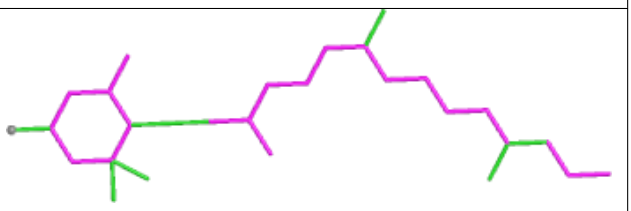
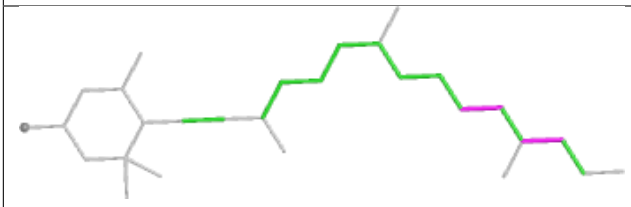
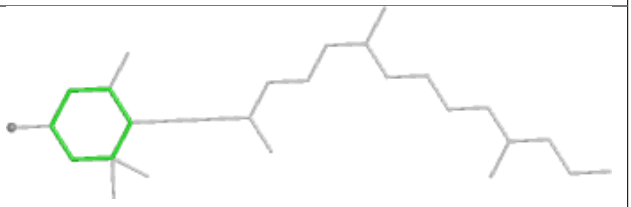


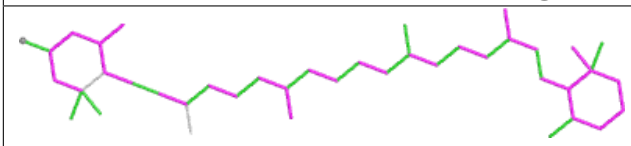
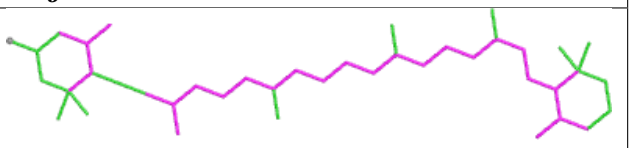
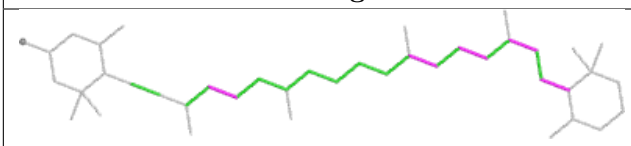
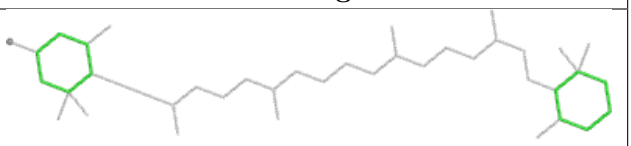
Bond angles

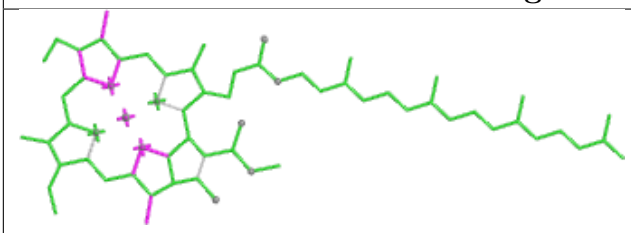
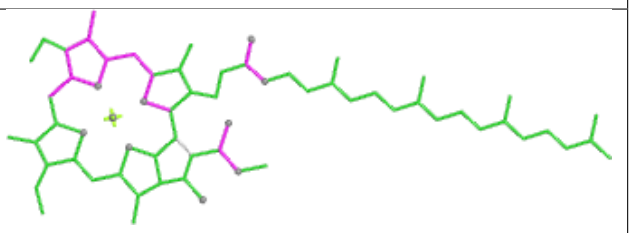
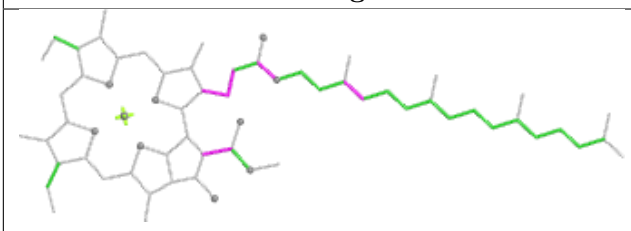
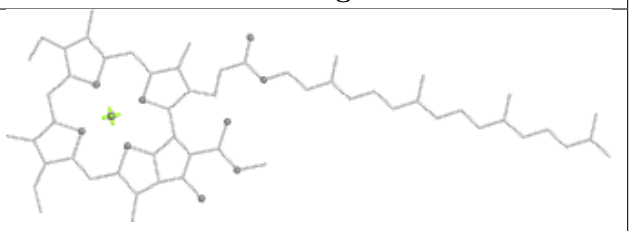


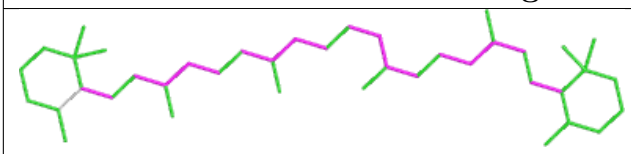
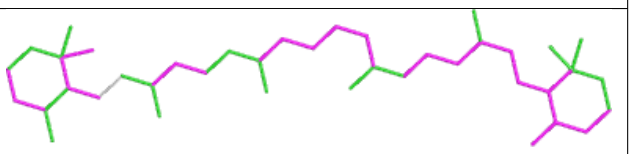
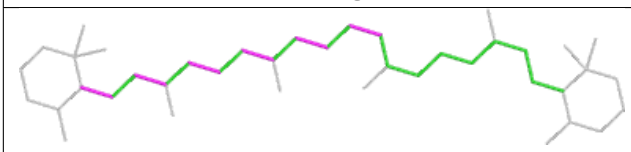
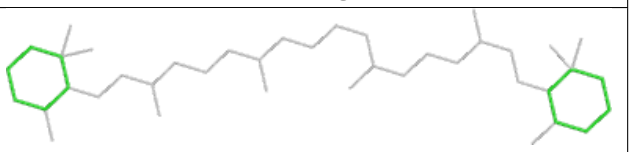
Torsions



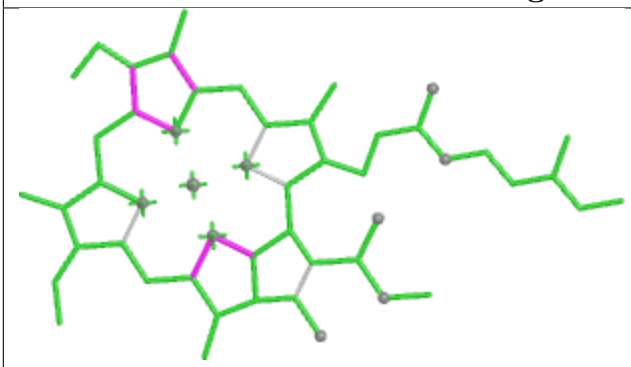
Rings

Ligand IHT j 317	
 Bond lengths	 Bond angles
 Torsions	 Rings

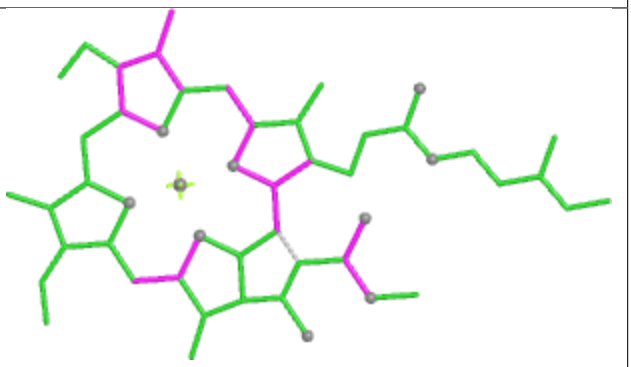
Ligand CLA B 826	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand WVN I 101	
 Bond lengths	 Bond angles
 Torsions	 Rings

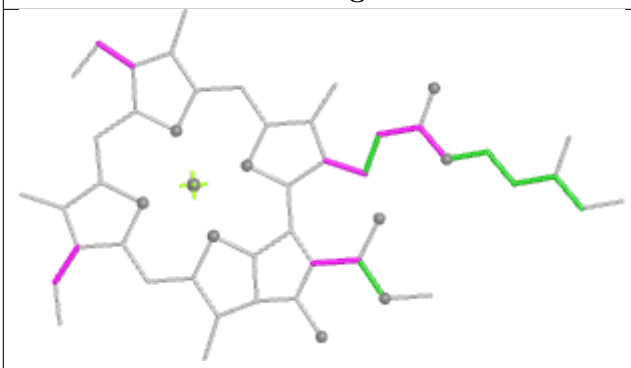
Ligand CLA d 304



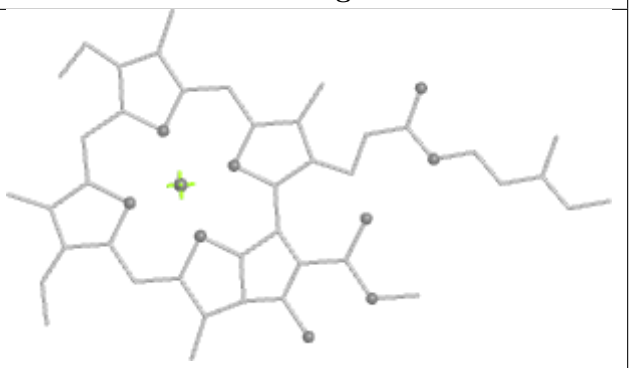
Bond lengths



Bond angles

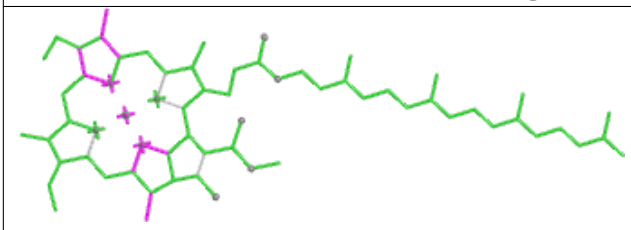


Torsions

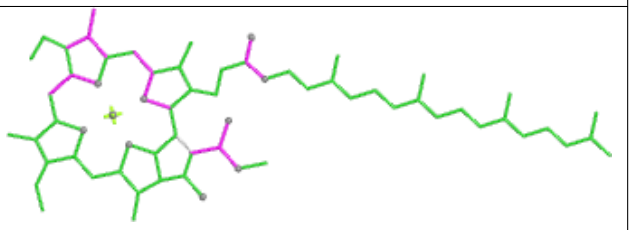


Rings

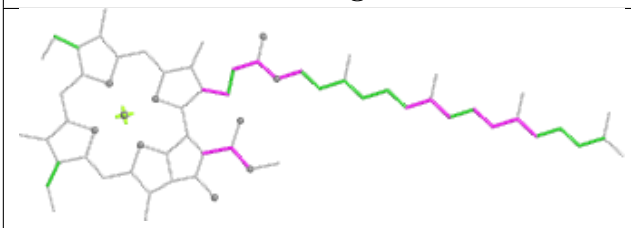
Ligand CLA B 805



Bond lengths



Bond angles



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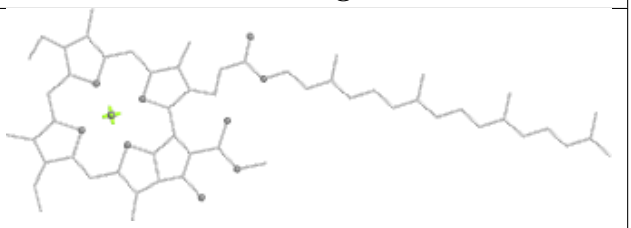
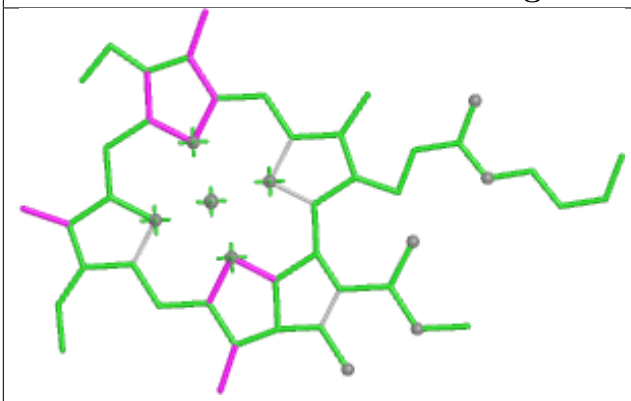
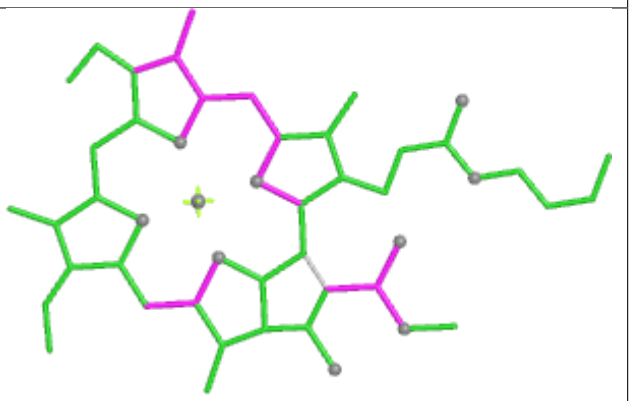


Rings

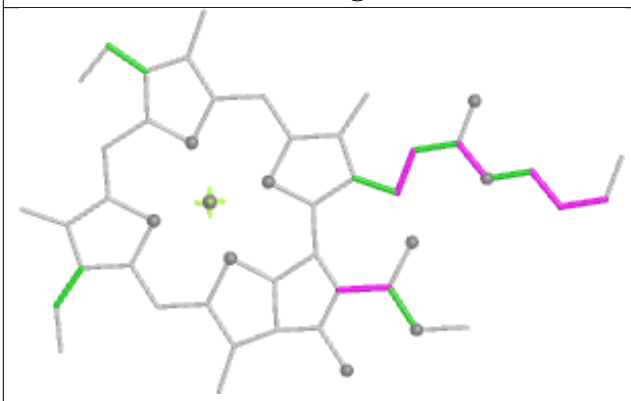
Ligand CLA A 821



Bond lengths



Bond angles



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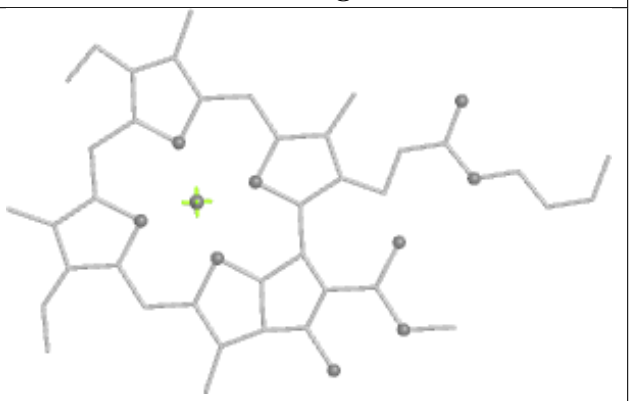
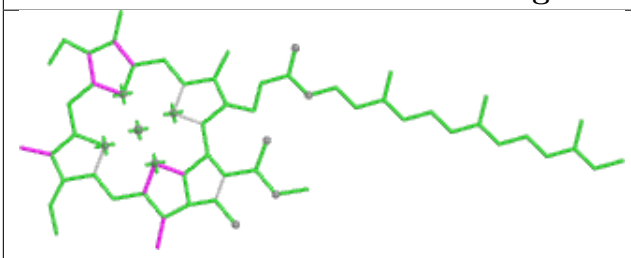
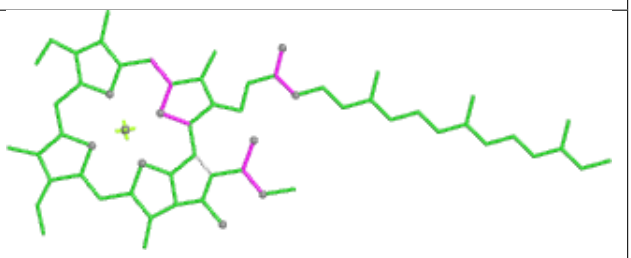


Rings

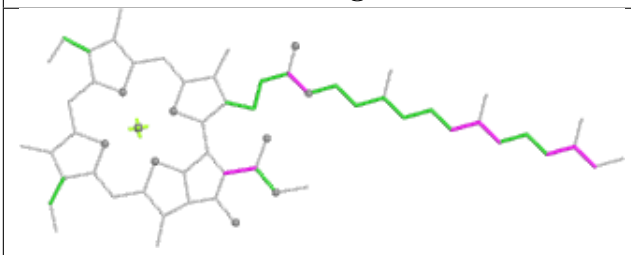
Ligand CLA i 606



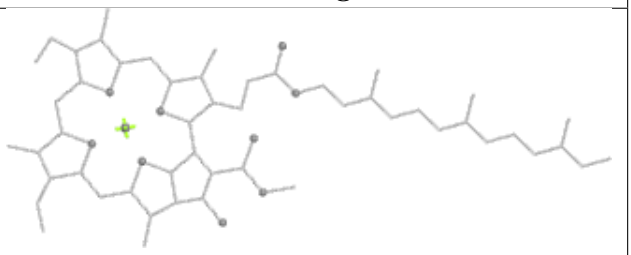
Bond lengths



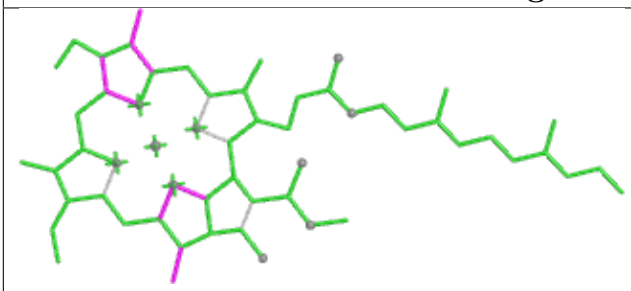
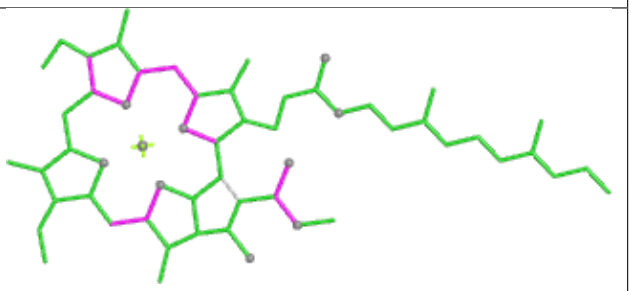
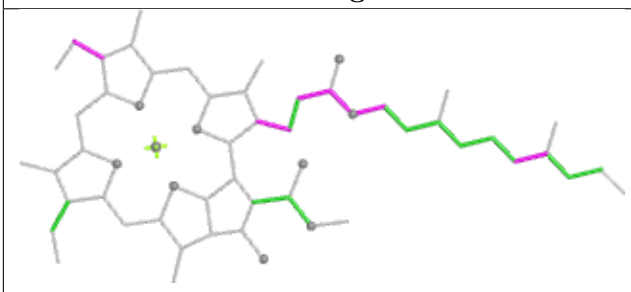
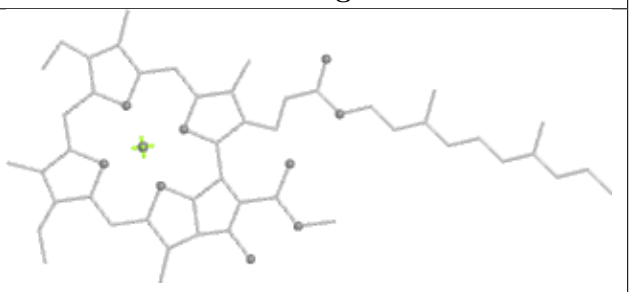
Bond angles

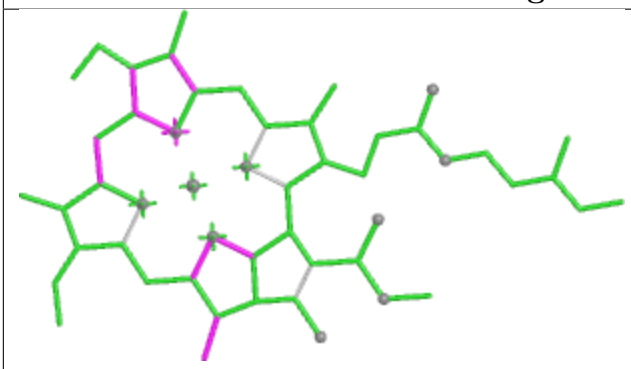
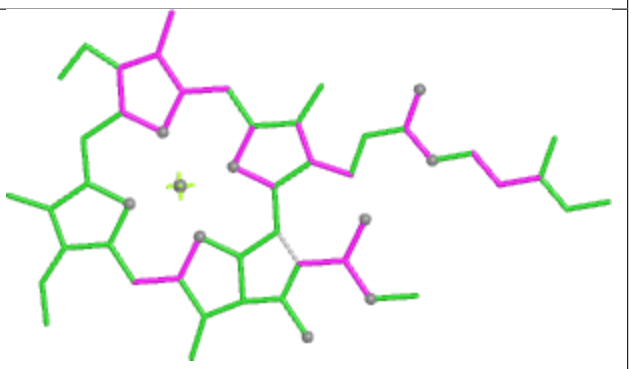
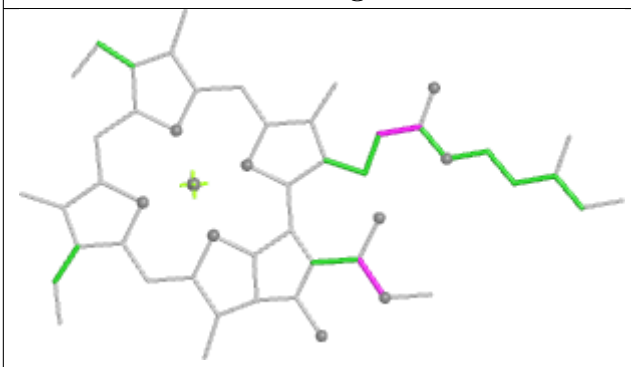
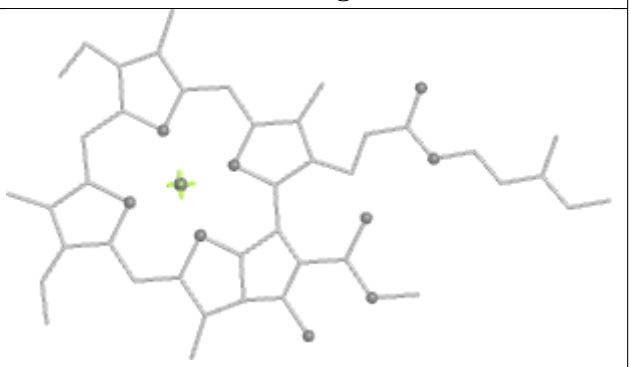


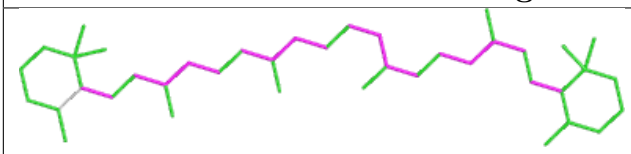
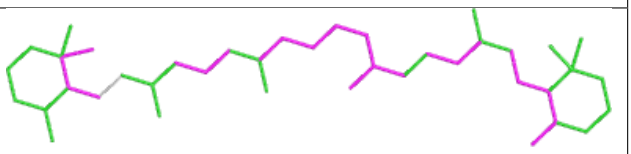
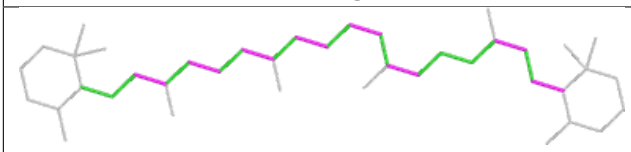
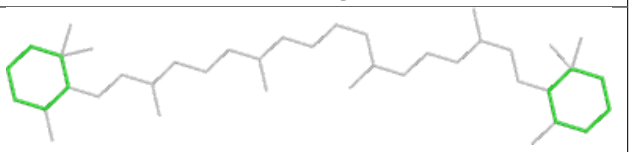
Torsions

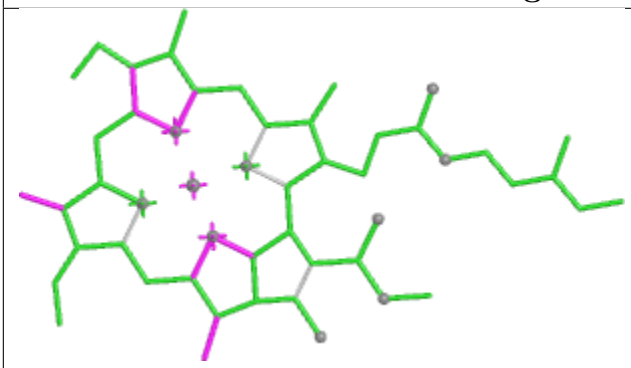
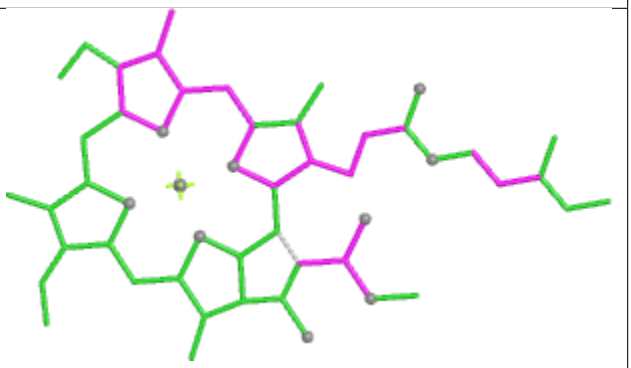
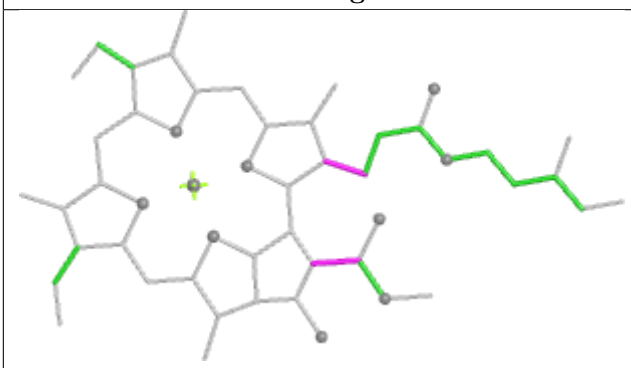
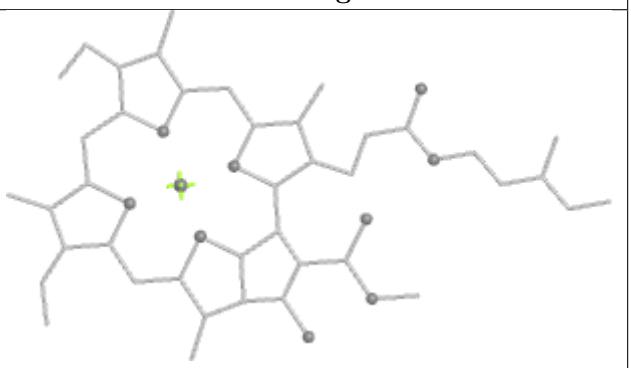


Rings

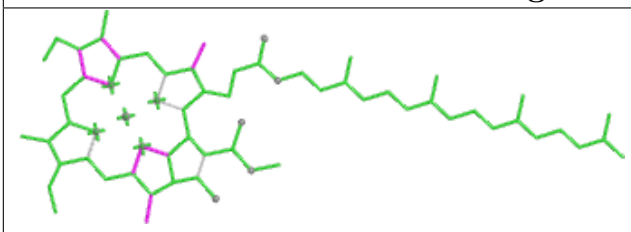
Ligand CLA h 306	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA d 302	
 Bond lengths	 Bond angles
 Torsions	 Rings

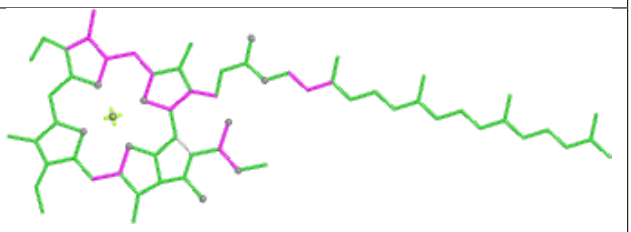
Ligand WVN B 849	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA A 834	
 Bond lengths	 Bond angles
 Torsions	 Rings

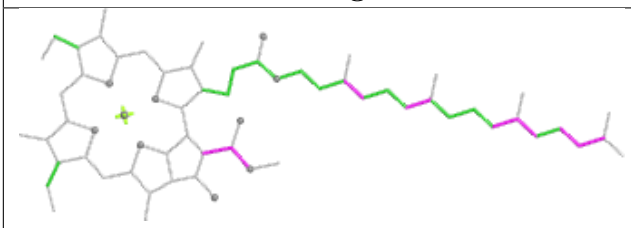
Ligand CLA k 609



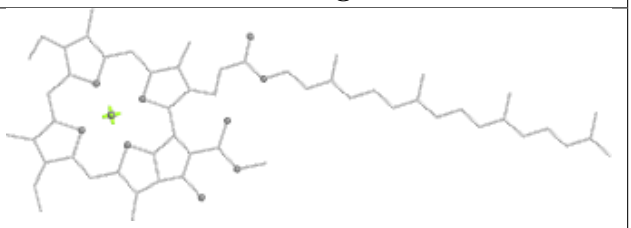
Bond lengths



Bond angles

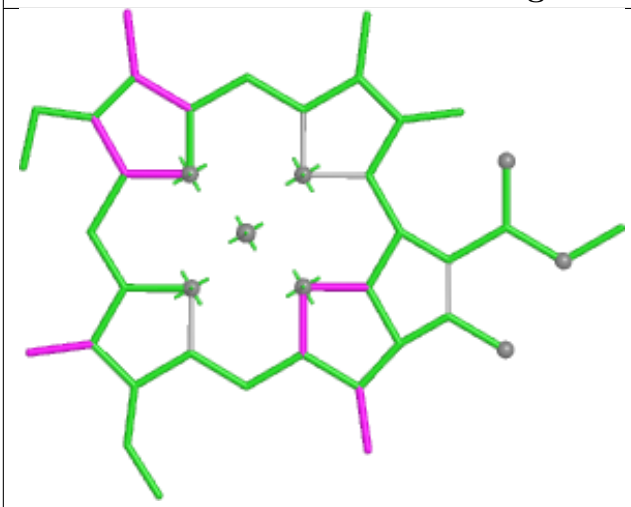


Torsions



Rings

Ligand CLA d 308



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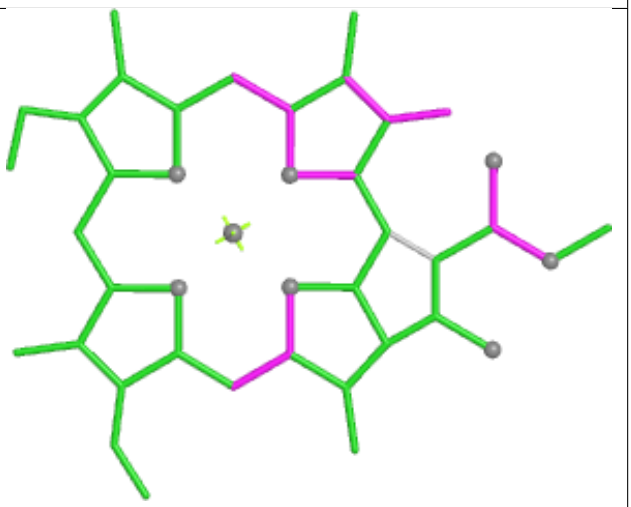

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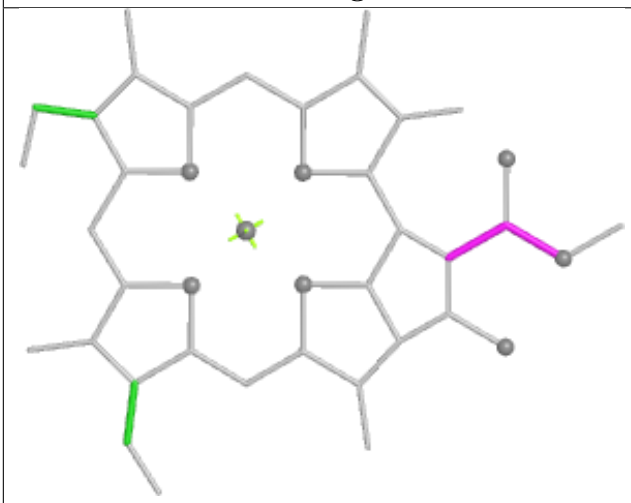

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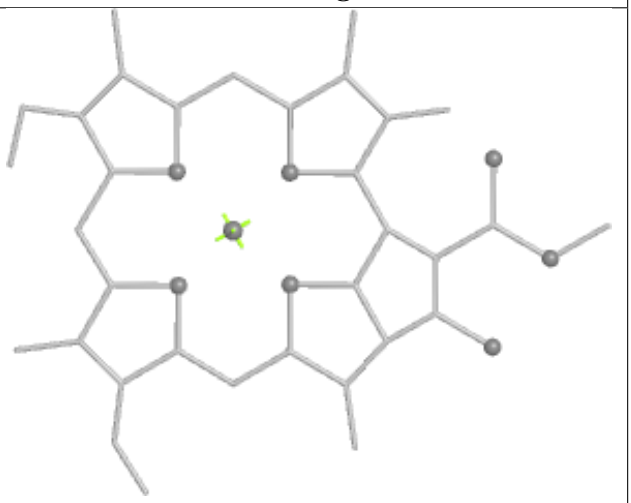
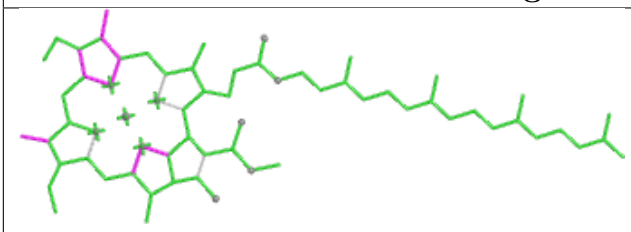


Rings

Ligand CLA A 829



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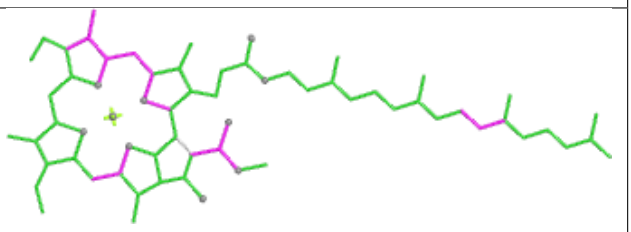
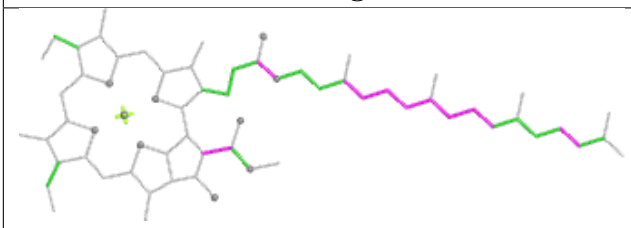


Bond angles



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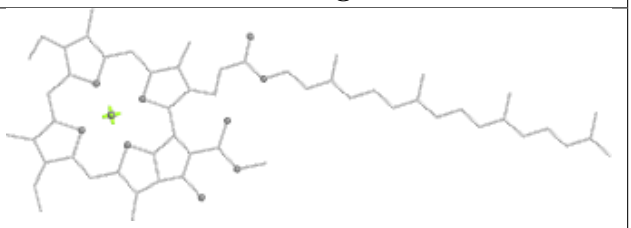
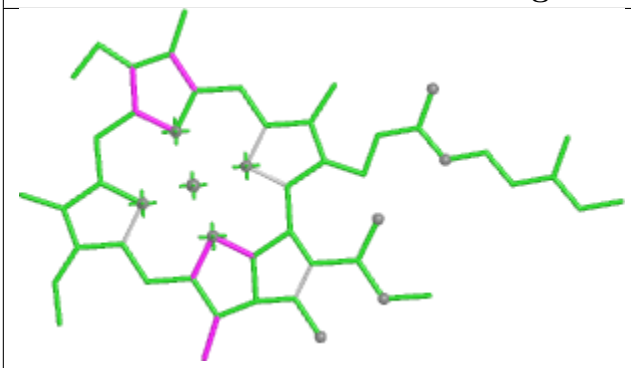


Rings

Ligand CLA j 304



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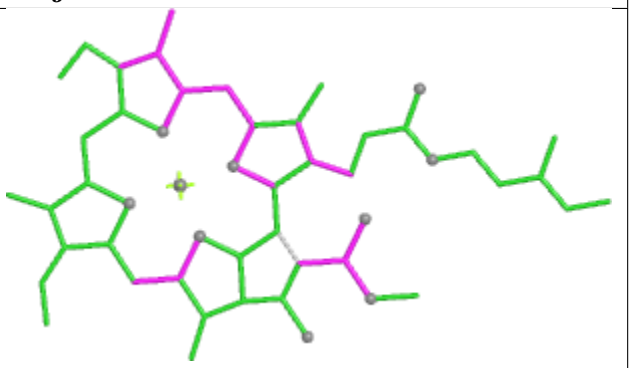
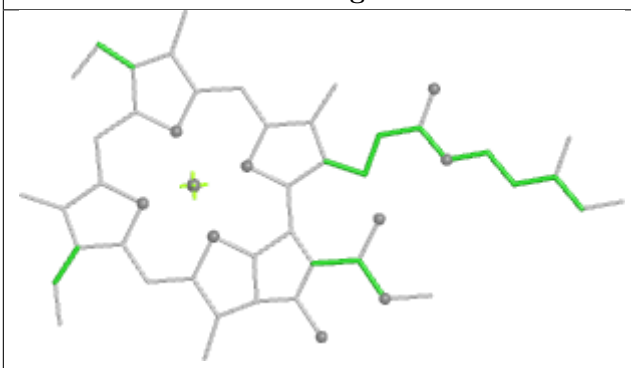


Bond angles



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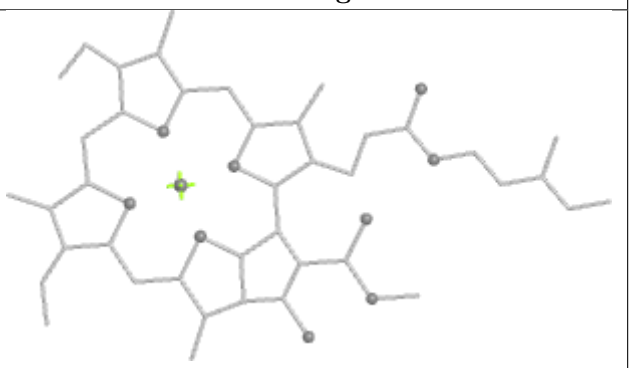
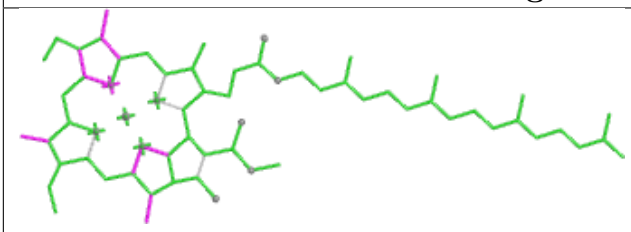


Rings

Ligand CLA L 203



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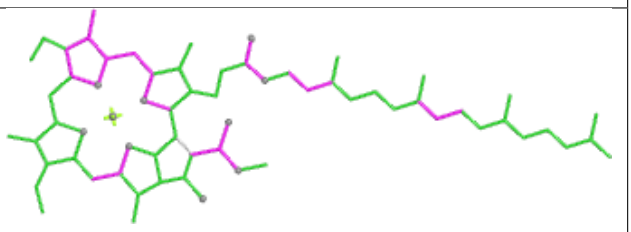
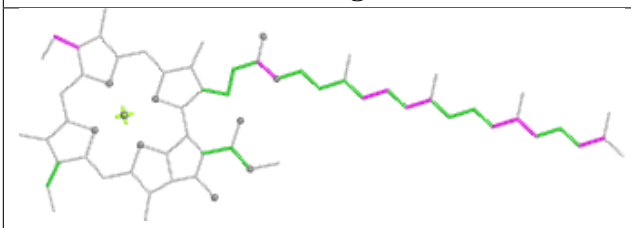


Bond angles



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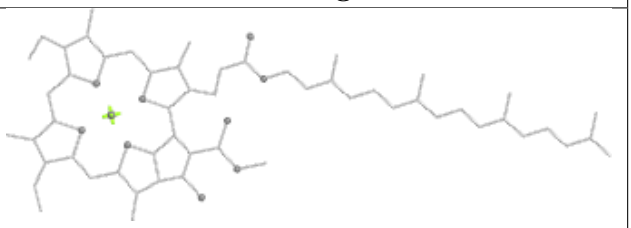
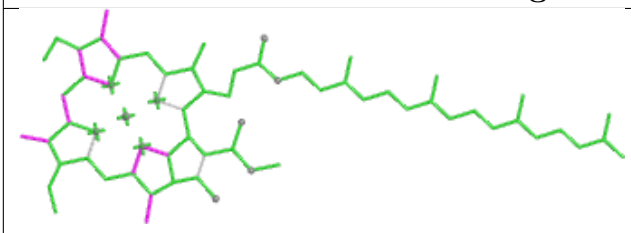


Rings

Ligand CLA c 604



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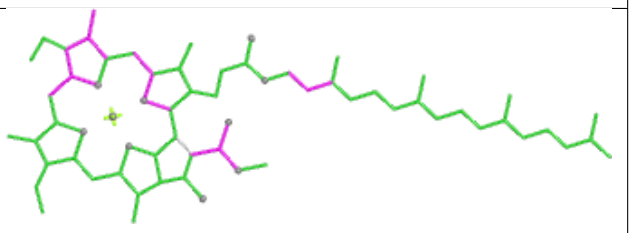
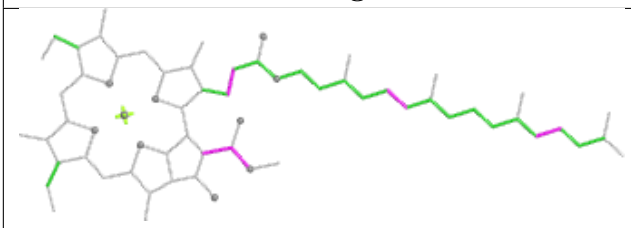


Bond angles



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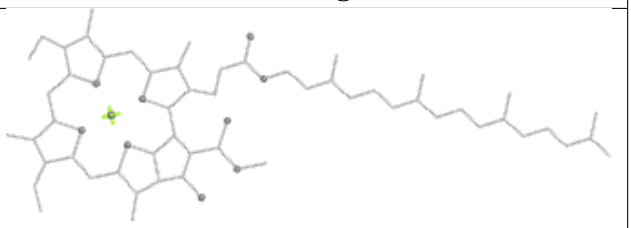
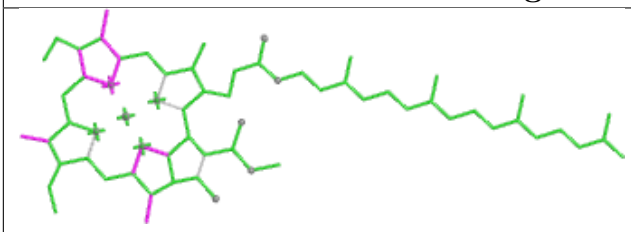


Rings

Ligand CLA B 822



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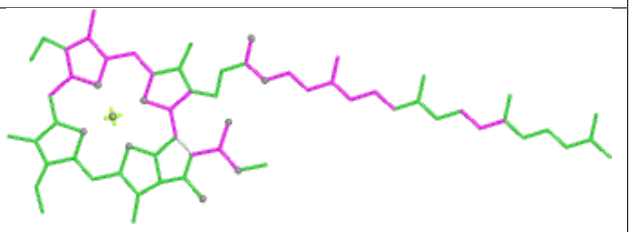
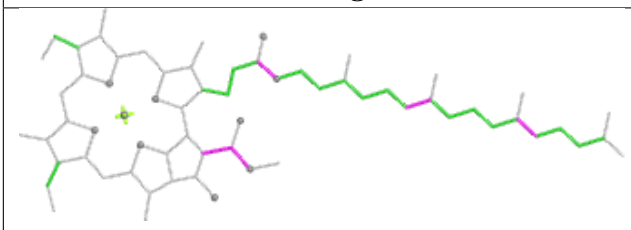


Bond angles



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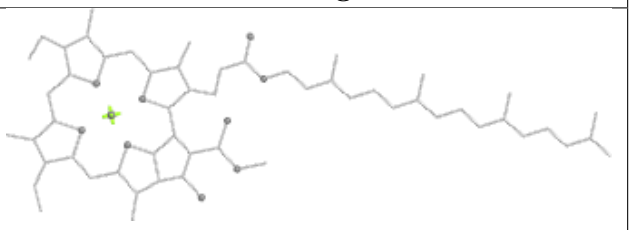
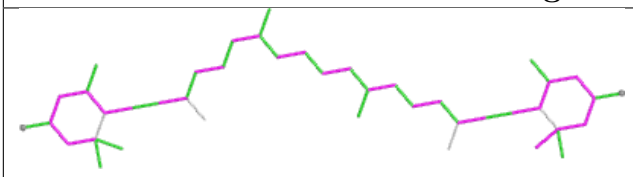


Rings

Ligand II0 e 616



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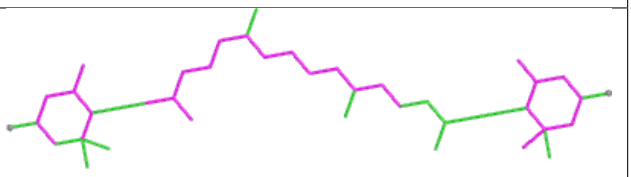
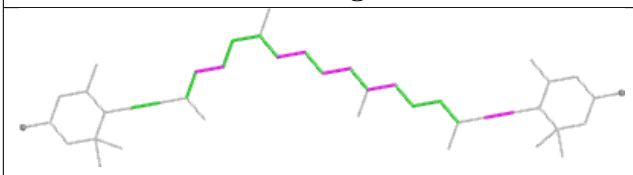


Bond angles



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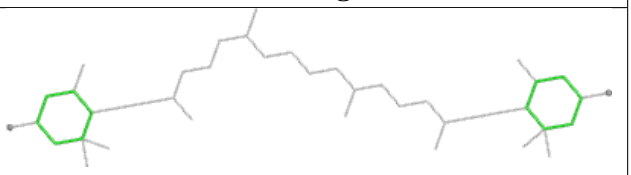
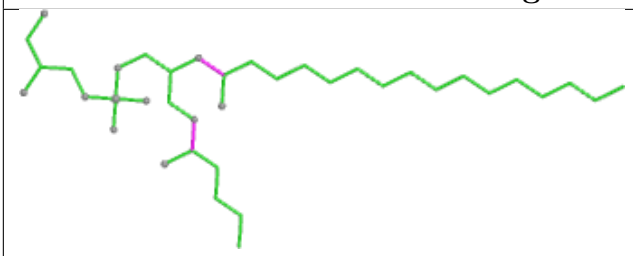


Rings

Ligand LHG B 802



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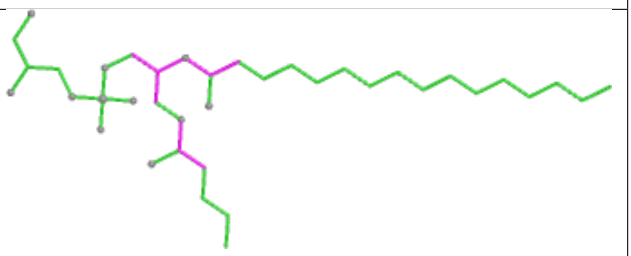
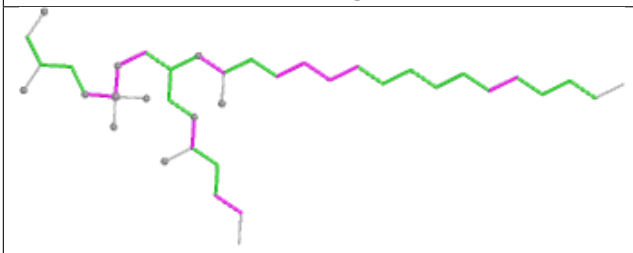


Bond angles



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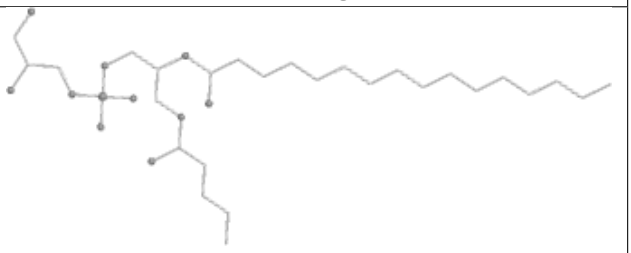
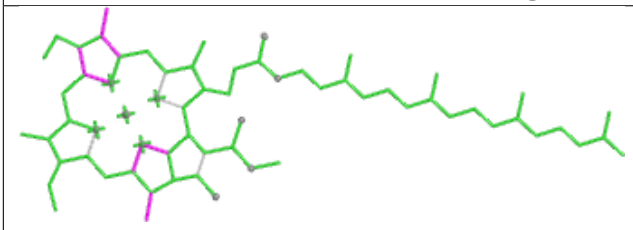


Rings

Ligand CLA A 801



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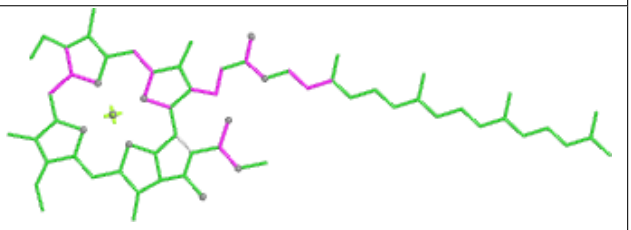

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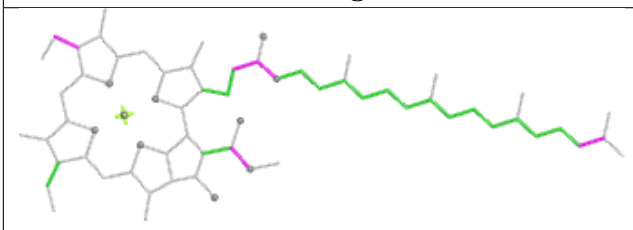

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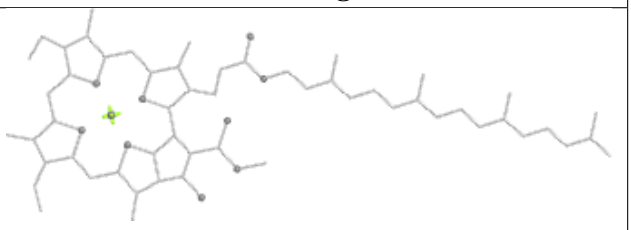
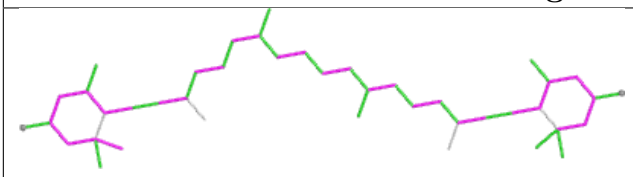


Rings

Ligand II0 f 614



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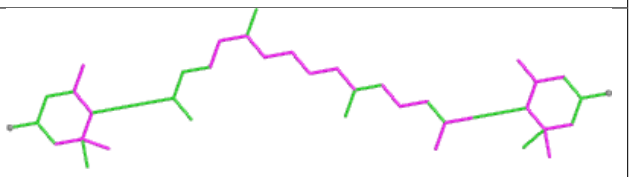

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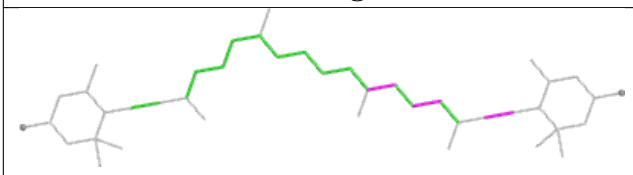

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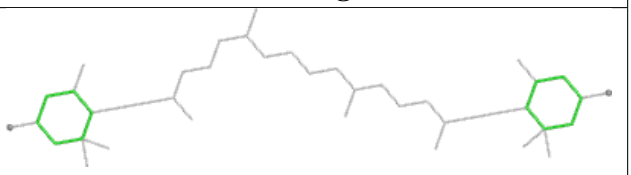
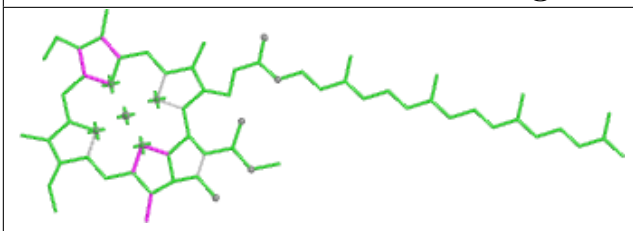


Rings

Ligand CLA j 314



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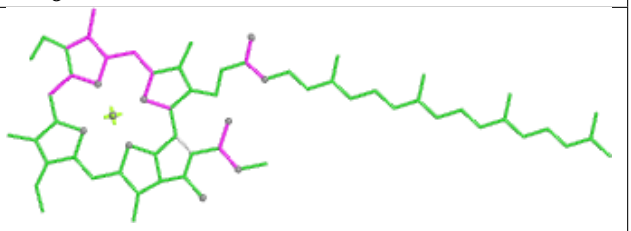
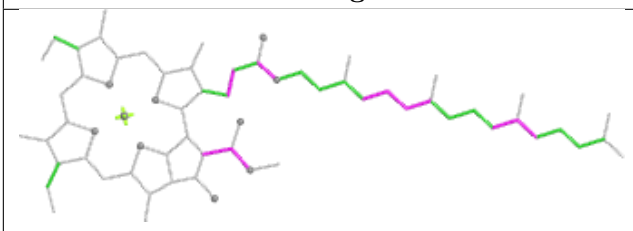


Bond angles



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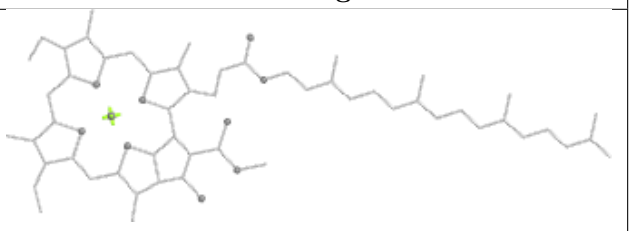
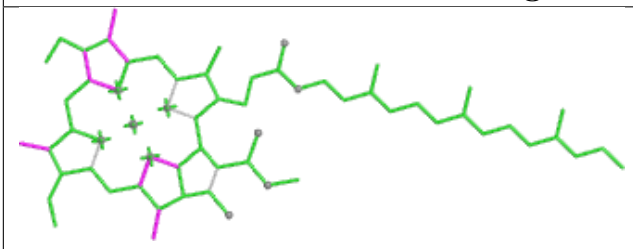


Rings

Ligand CLA A 810



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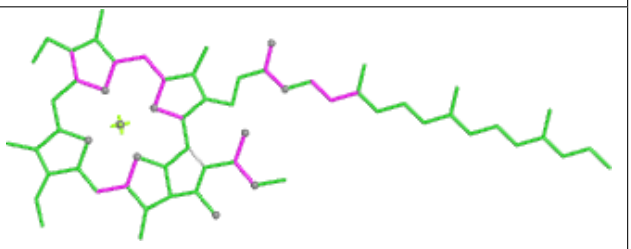
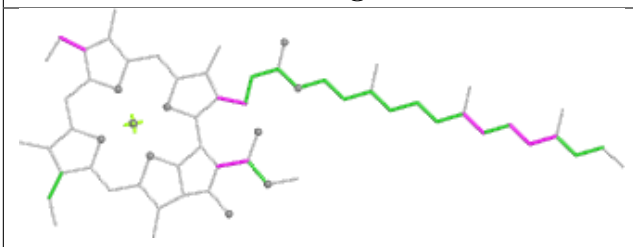


Bond angles



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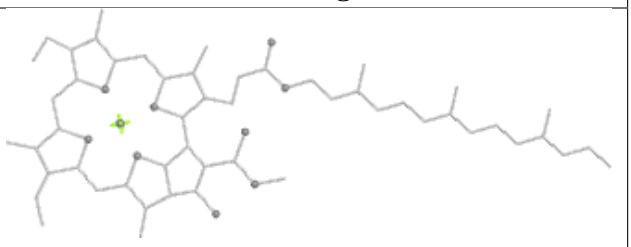
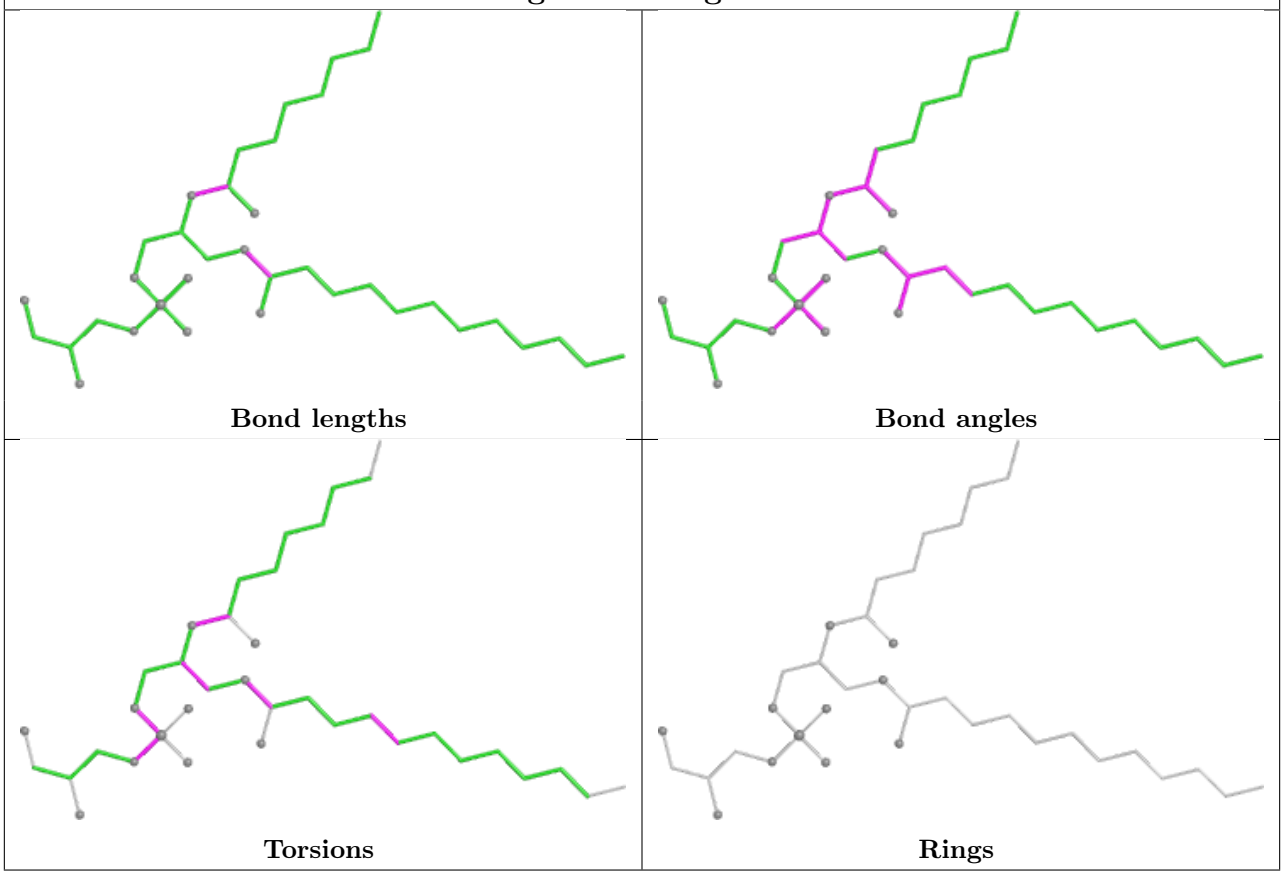
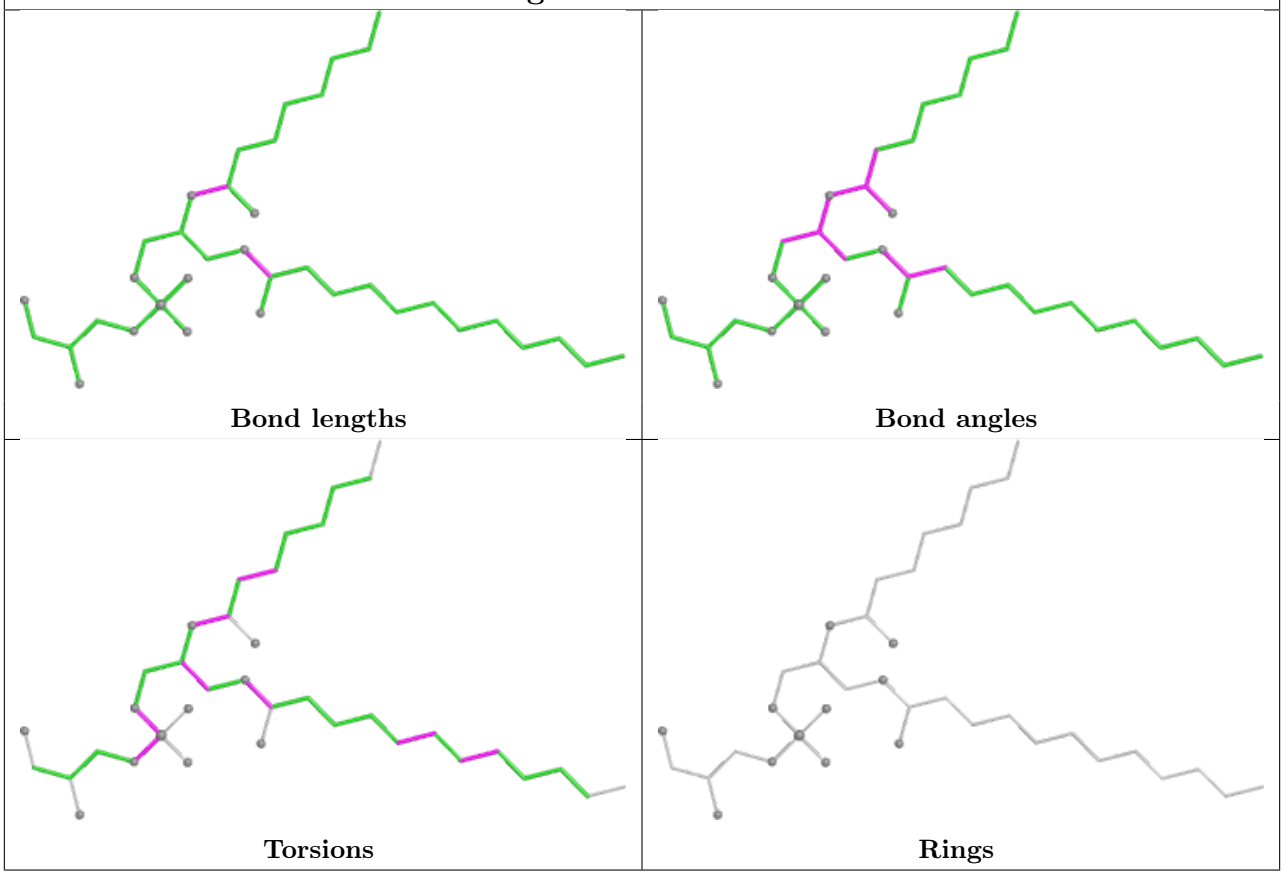


Rings

Ligand LHG g 321



Ligand LHG k 620



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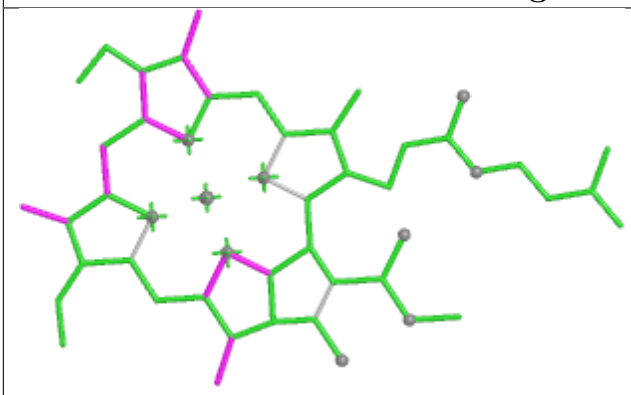
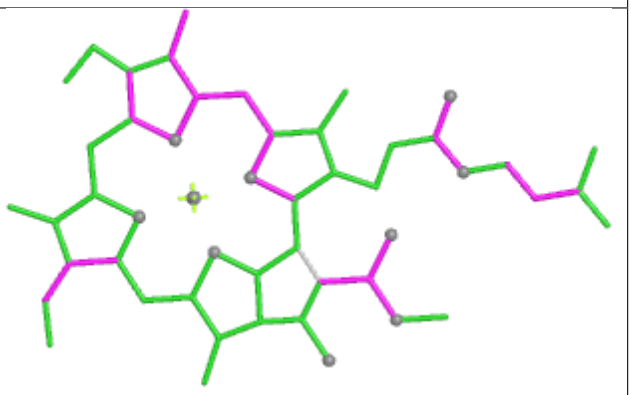
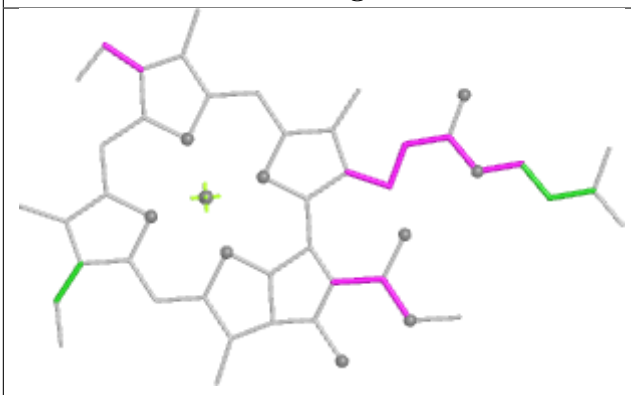
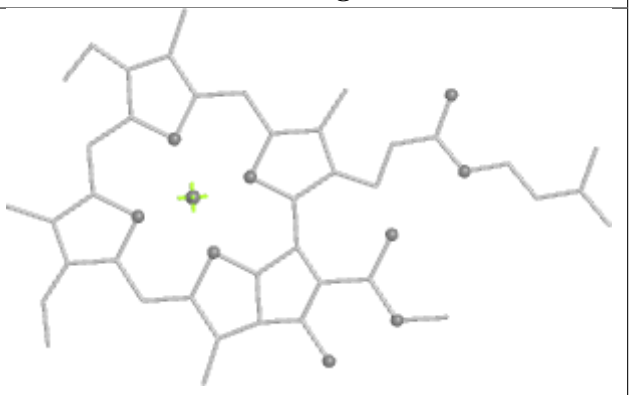
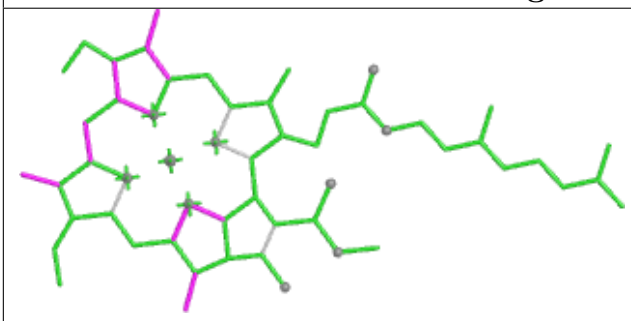
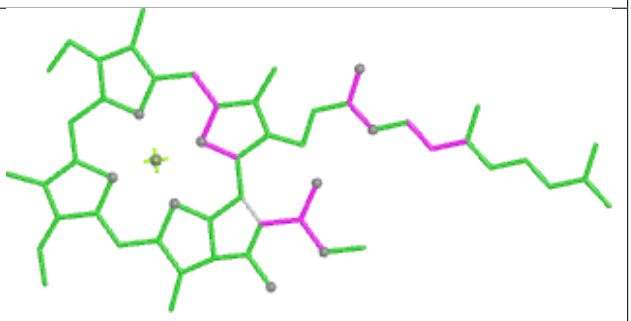
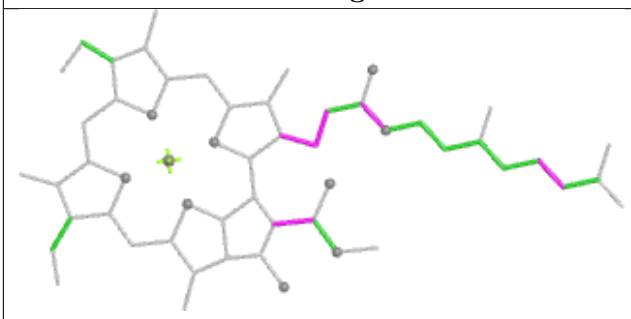
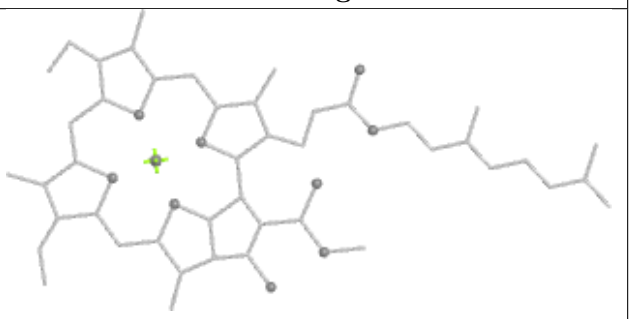
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA b 304	
 Bond lengths	 Bond angles
 Torsions	 Rings

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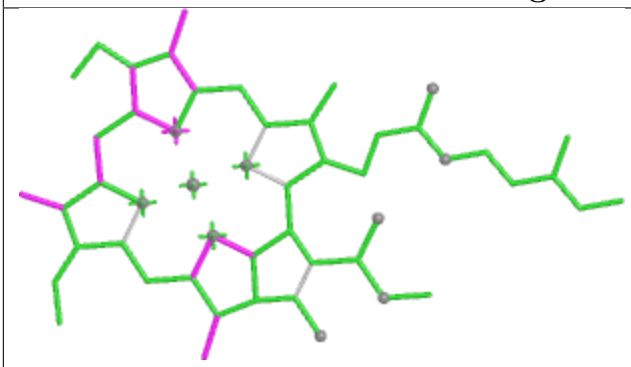
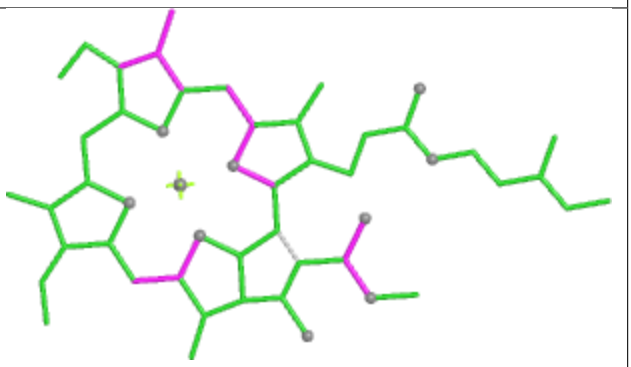
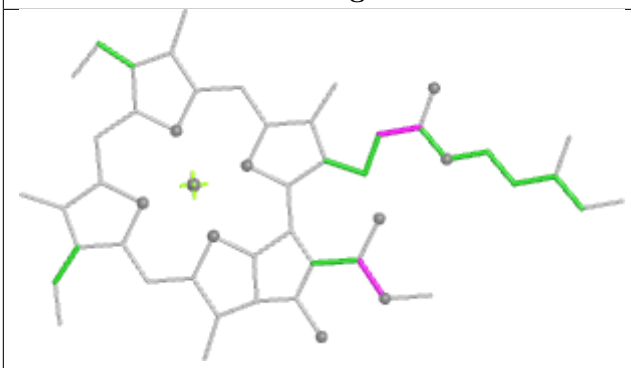
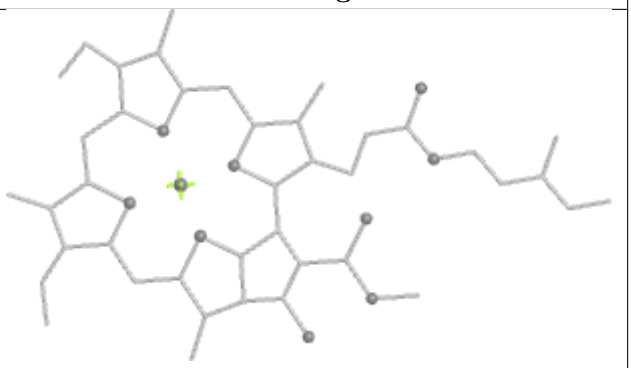
 Bond lengths	 Bond angles
 Torsions	 Rings

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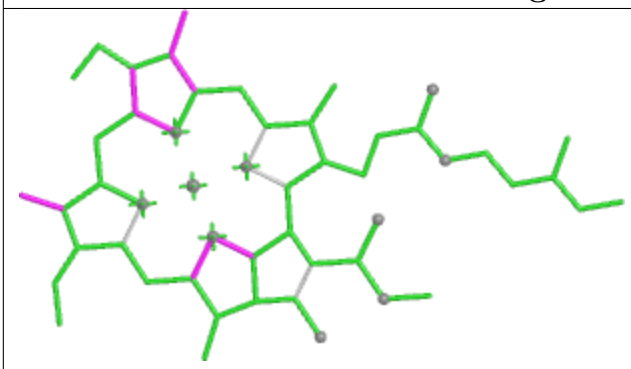
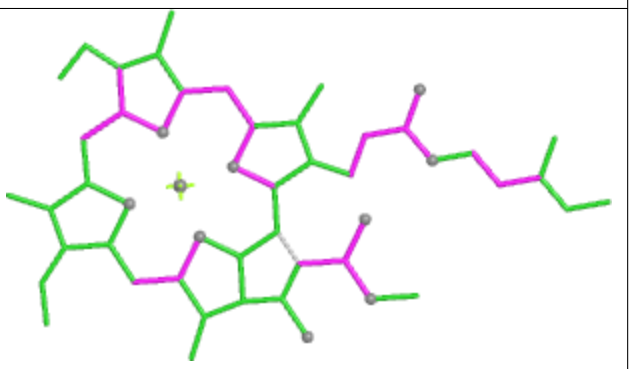
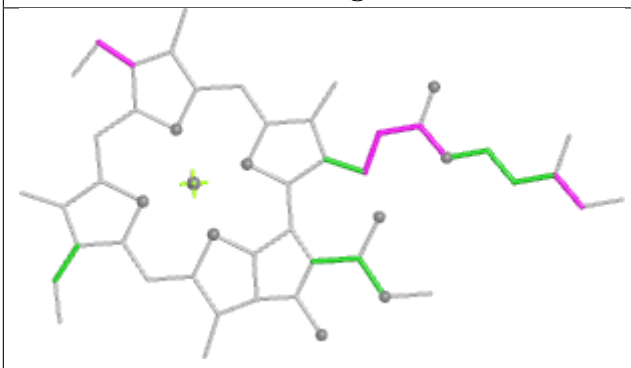
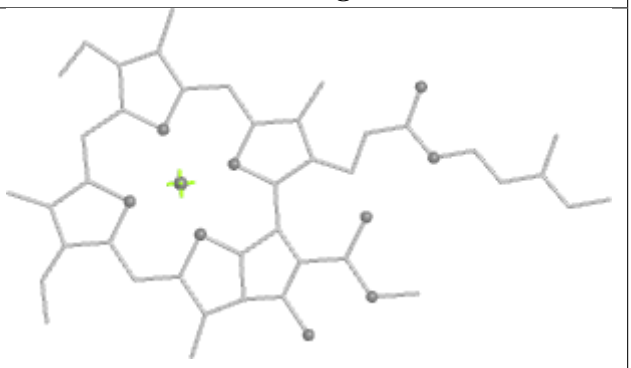
 Bond lengths	 Bond angles
 Torsions	 Rings

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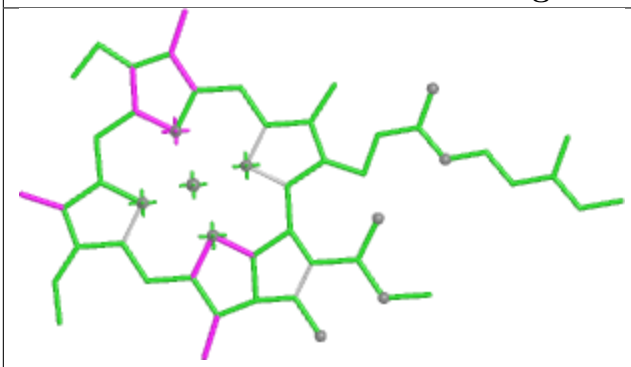
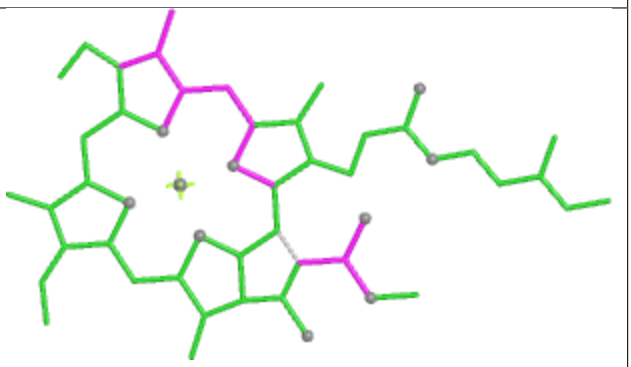
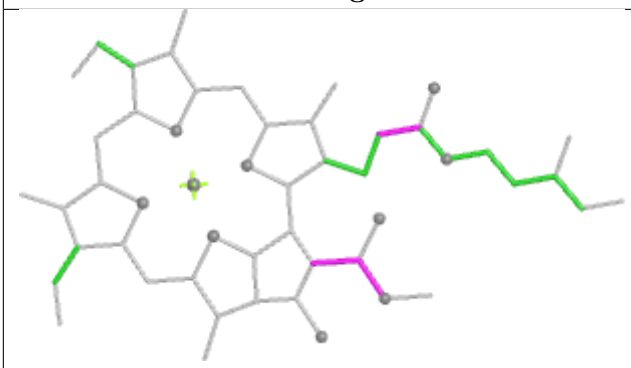
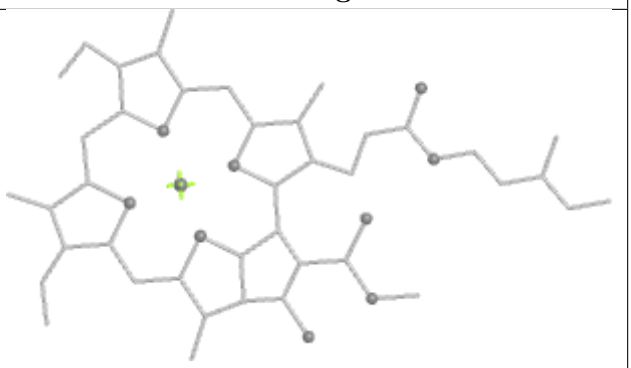
 Bond lengths	 Bond angles
 Torsions	 Rings

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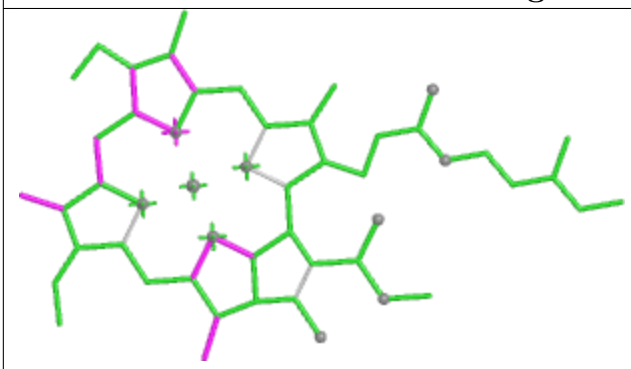
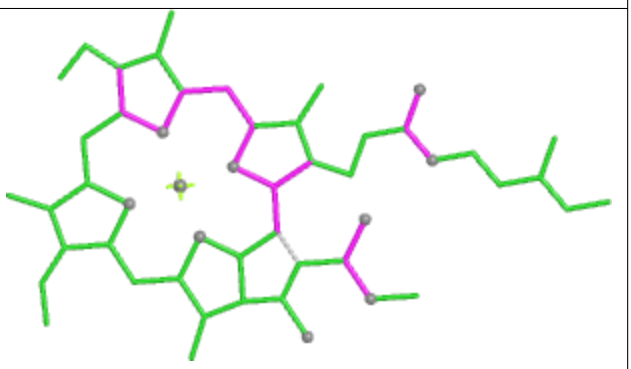
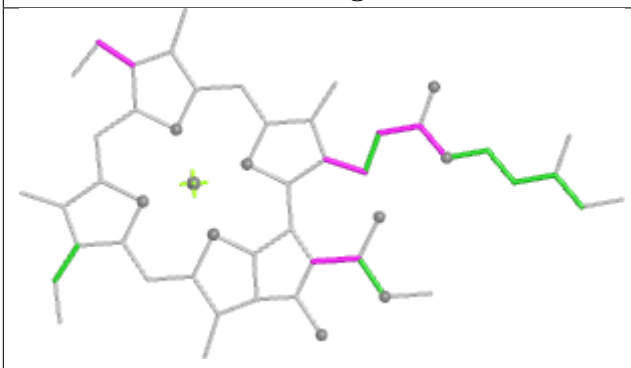
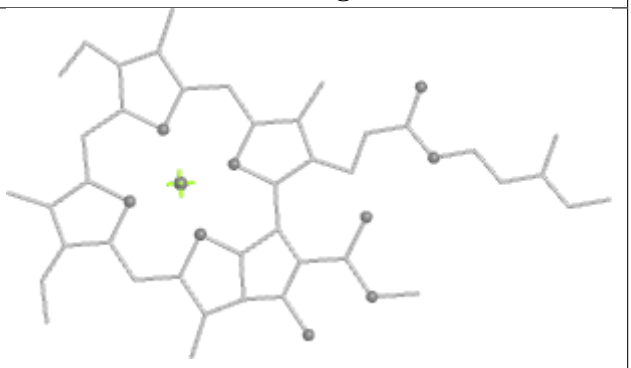
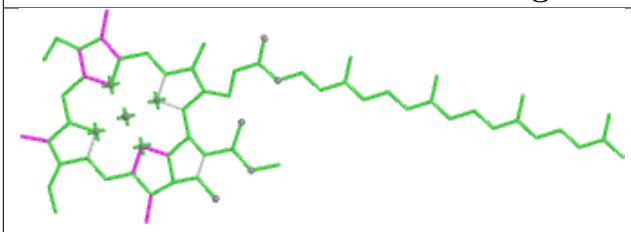
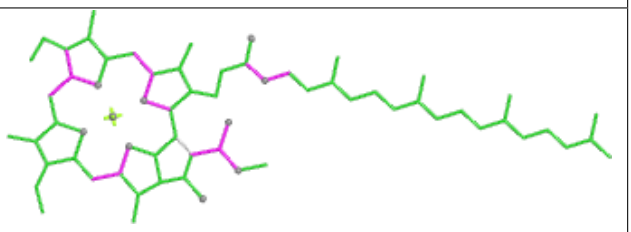
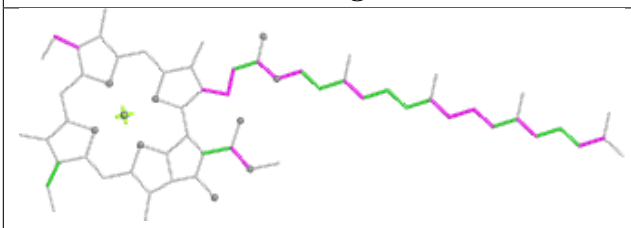
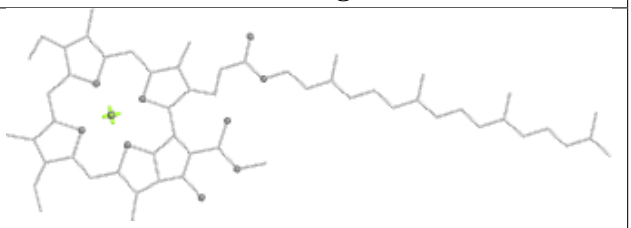
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA f 602	
 Bond lengths	 Bond angles
 Torsions	 Rings

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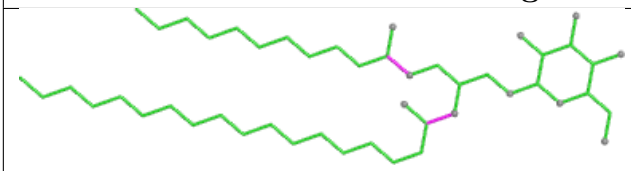
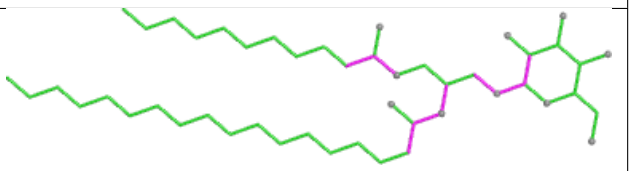
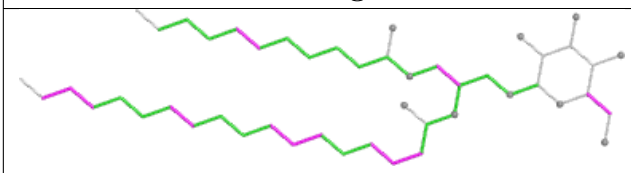
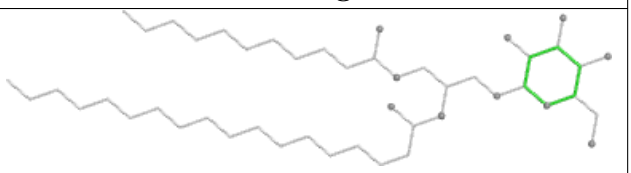
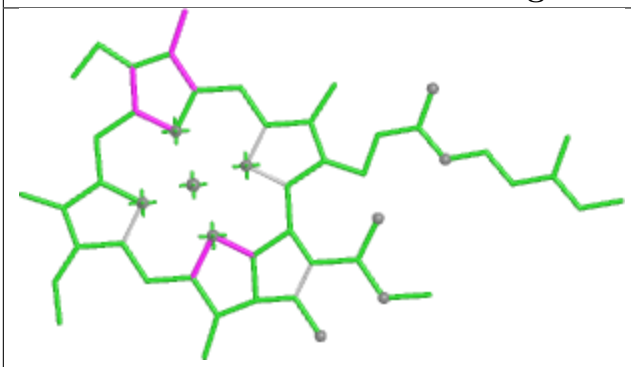
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA d 312



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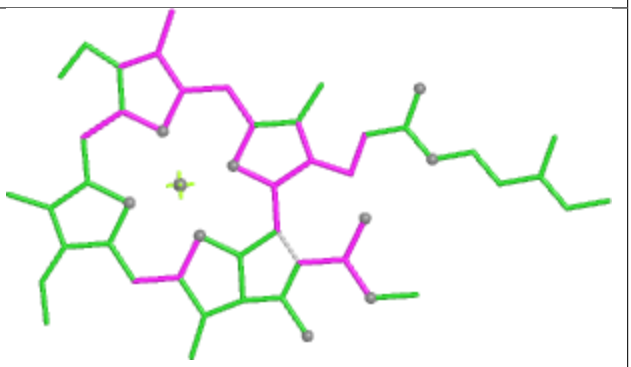
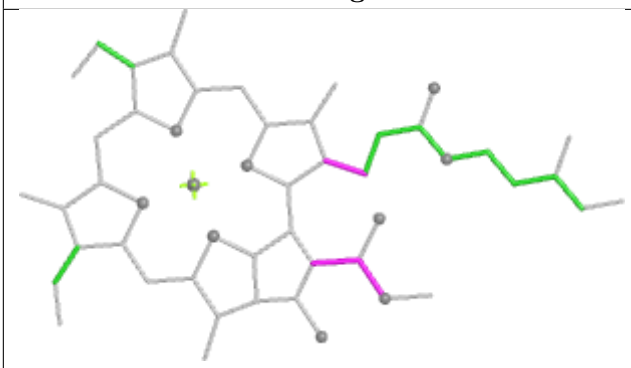


Bond angles



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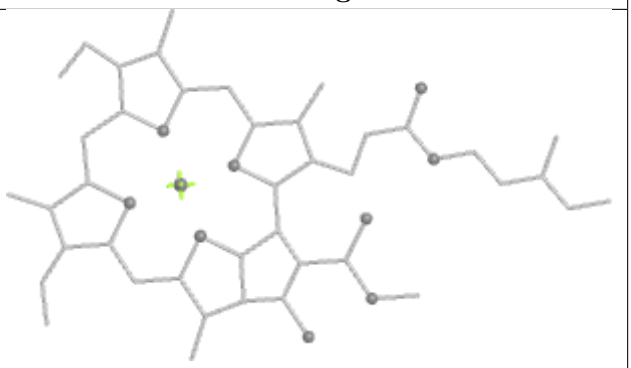
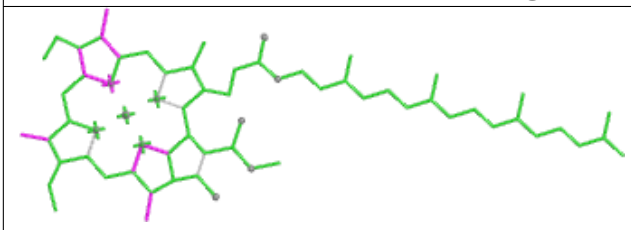


Rings

Ligand CLA A 826



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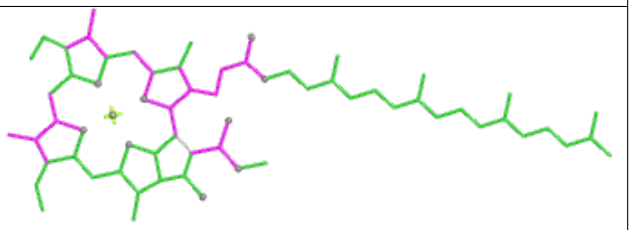
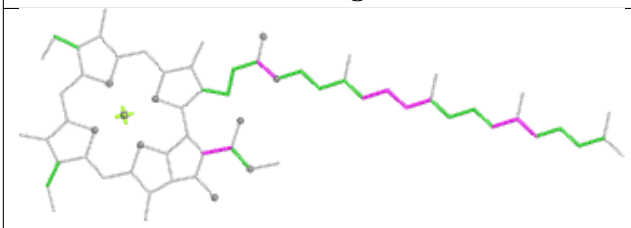


Bond angles



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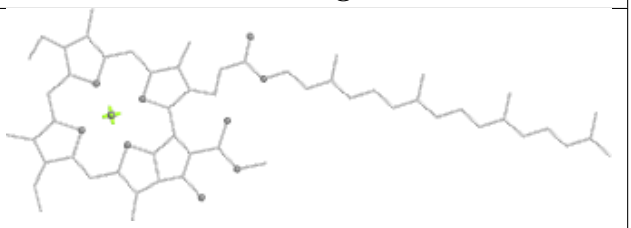
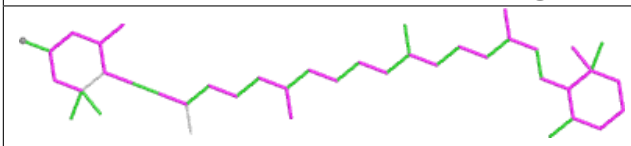
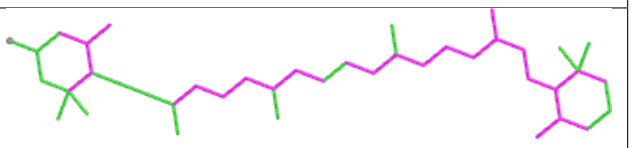
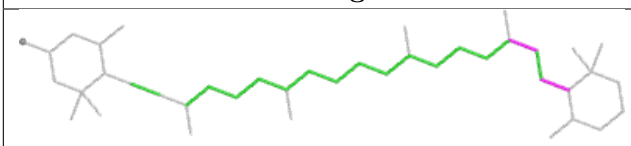
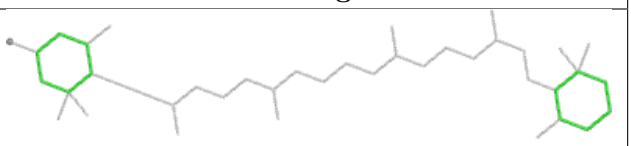
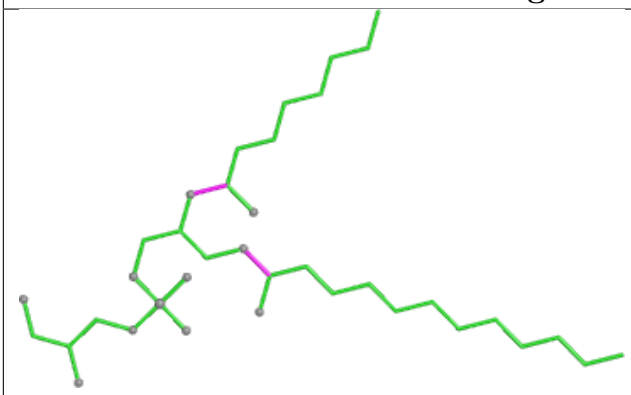
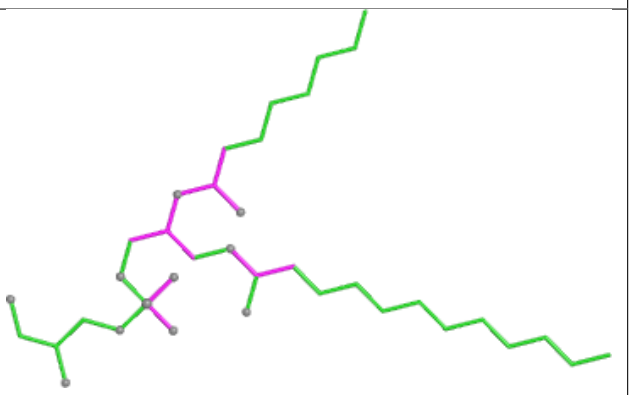
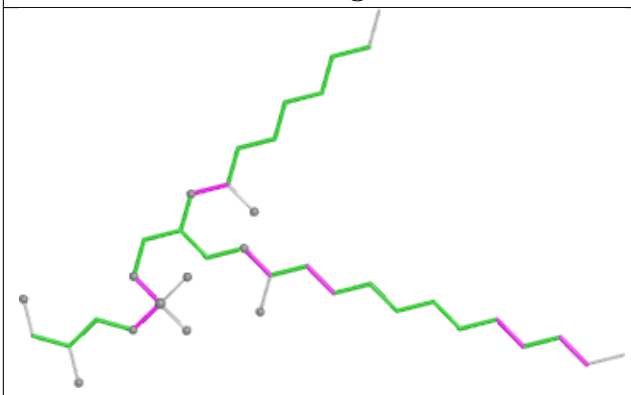
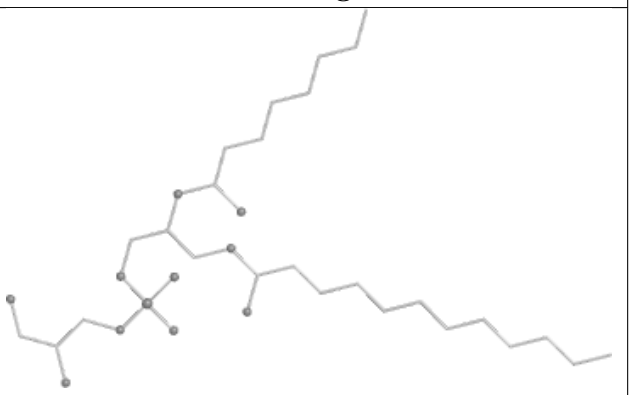
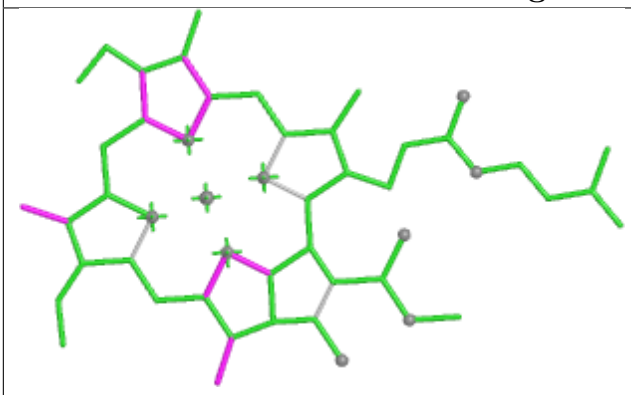


Rings

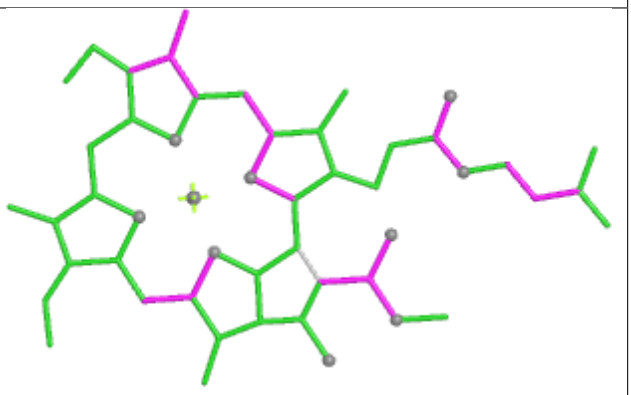
Ligand IHT b 316	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand LHG c 618	
 Bond lengths	 Bond angles
 Torsions	 Rings

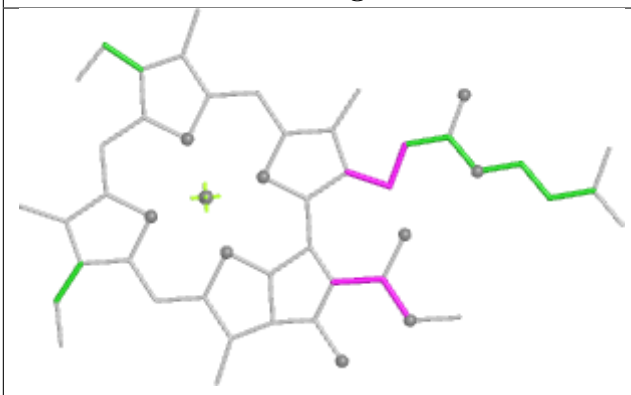
Ligand CLA a 303



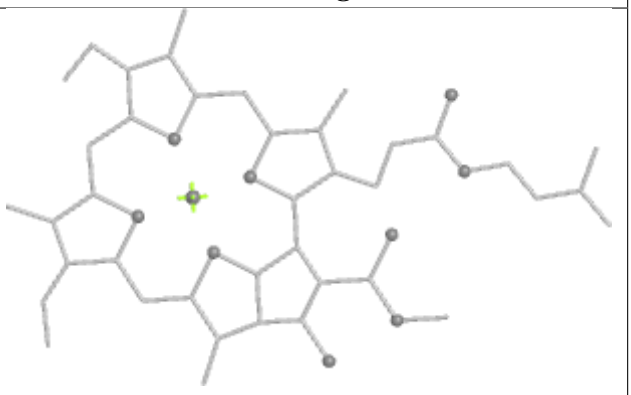
Bond lengths



Bond angles

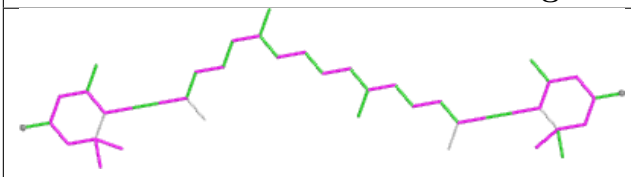


Torsions



Rings

Ligand II0 d 313



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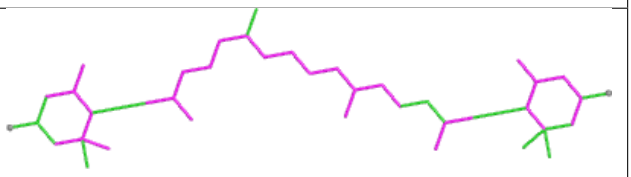

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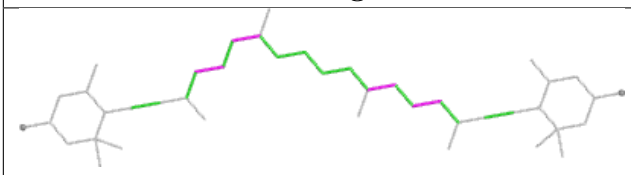
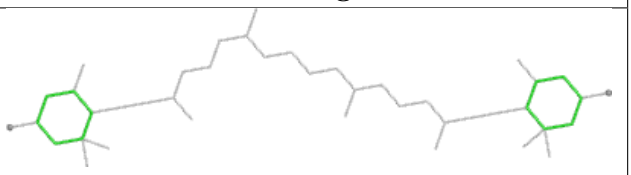
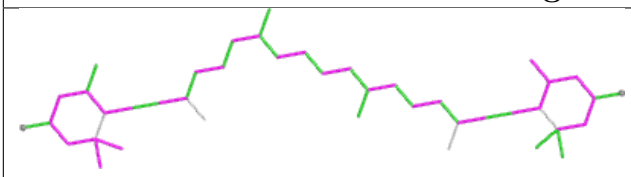


Torsions

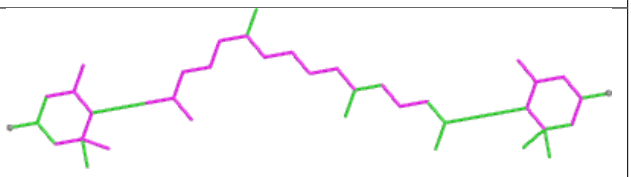


Rings

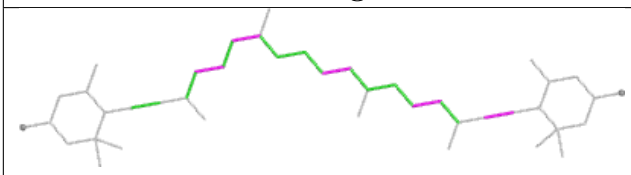
Ligand II0 e 613



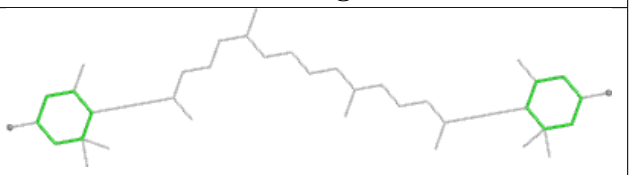
Bond lengths



Bond angles

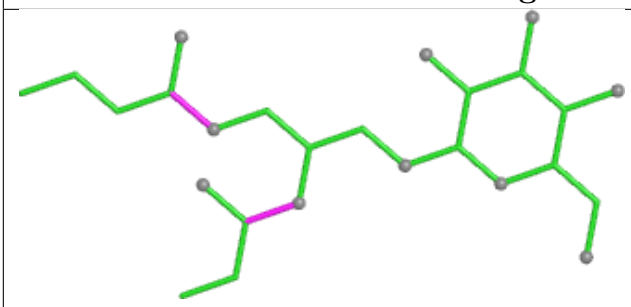


Torsions



Rings

Ligand LMG O 204



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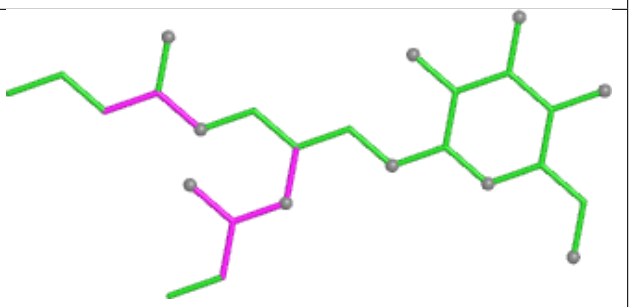
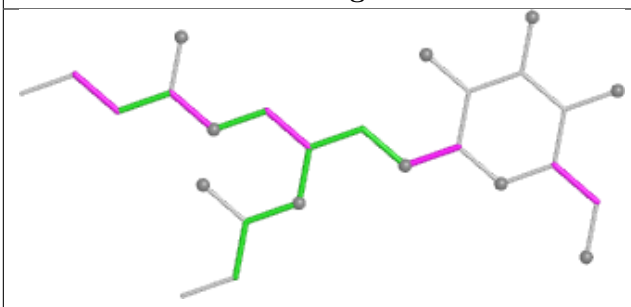


Bond angles



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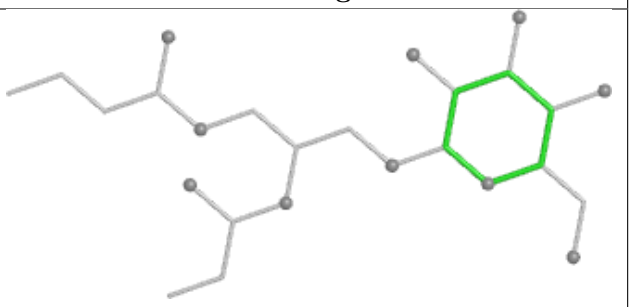
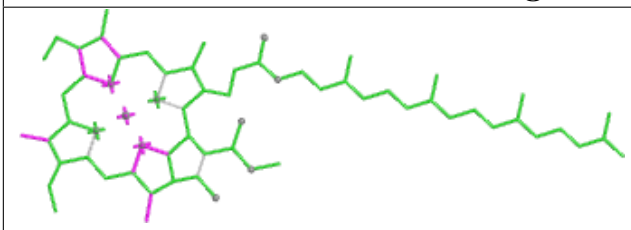


Rings

Ligand CLA B 841



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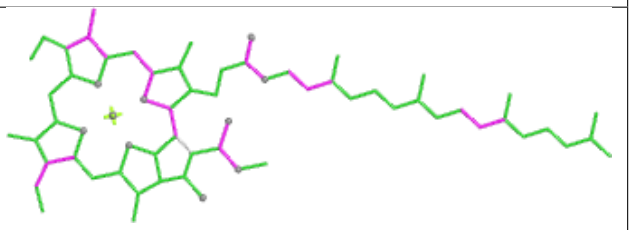

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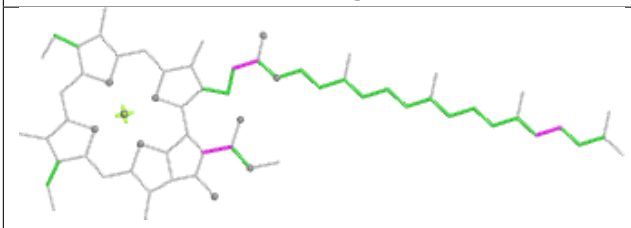

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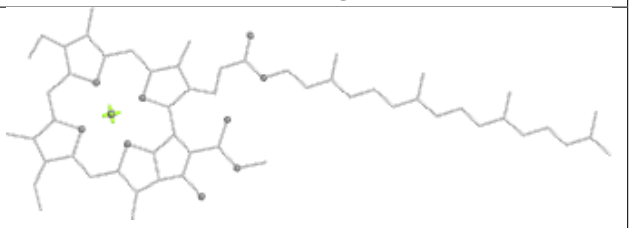
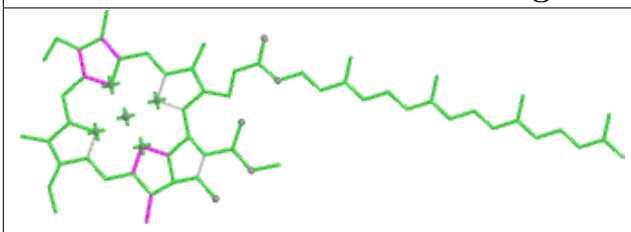
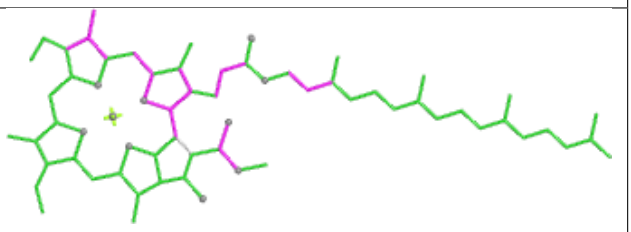
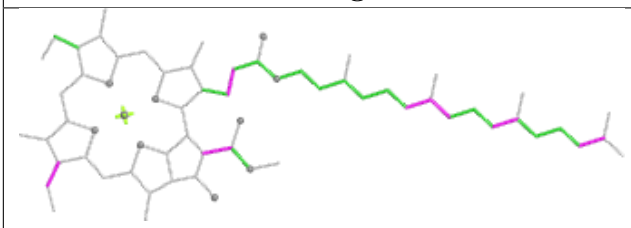
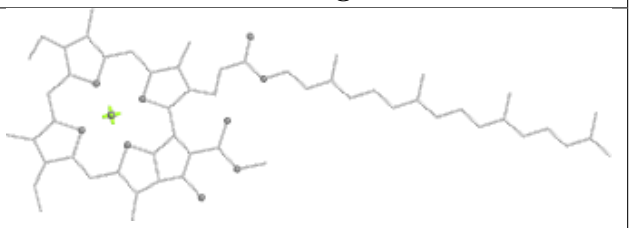
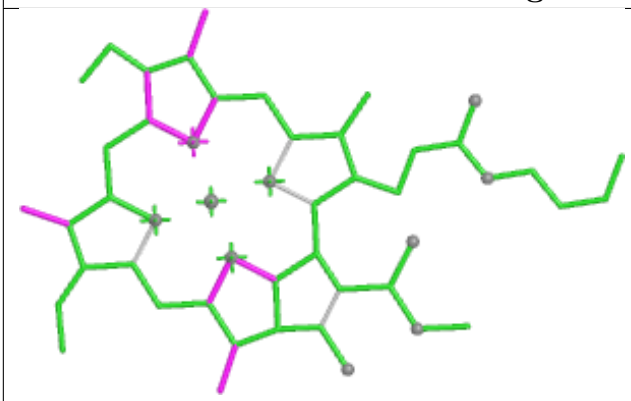
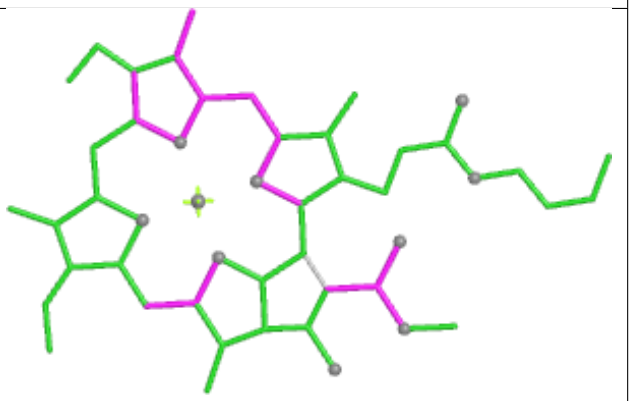
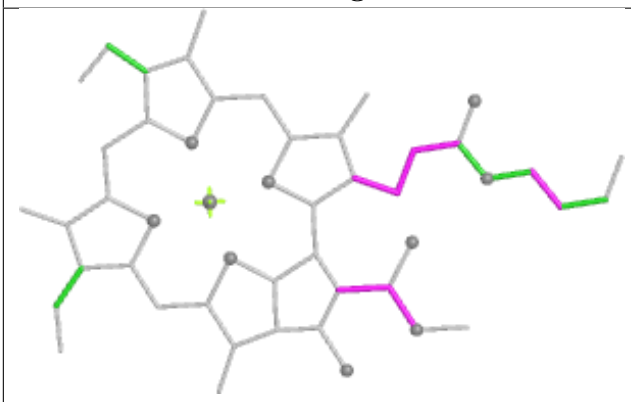
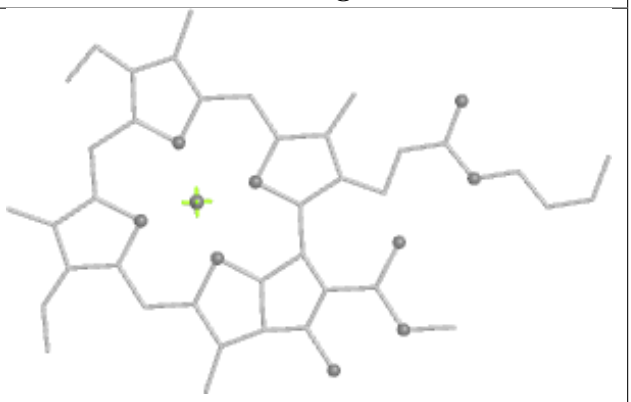
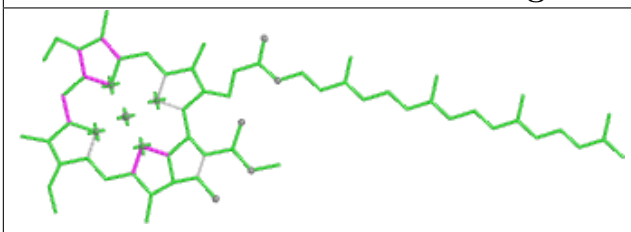
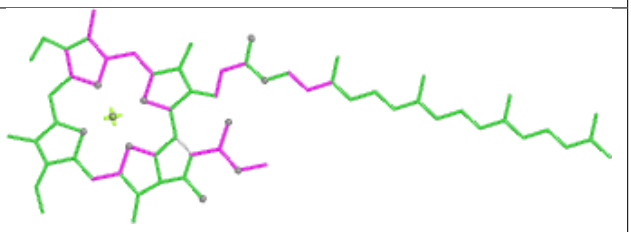
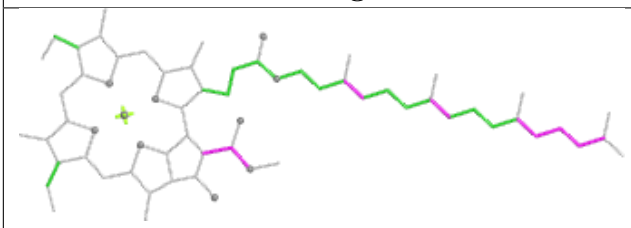
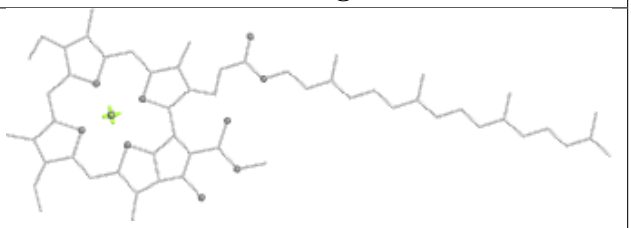


Rings

Ligand CLA i 604	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA L 202	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA b 310	
 Bond lengths	 Bond angles
 Torsions	 Rings

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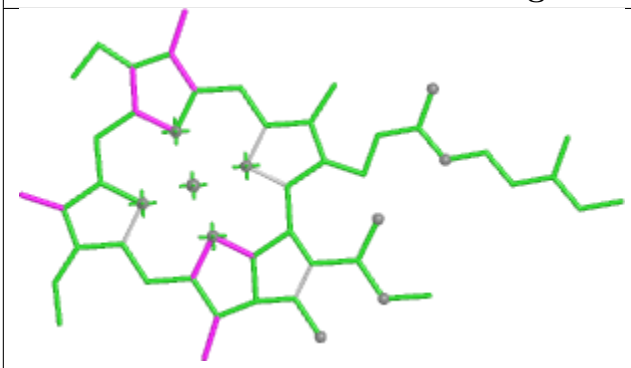
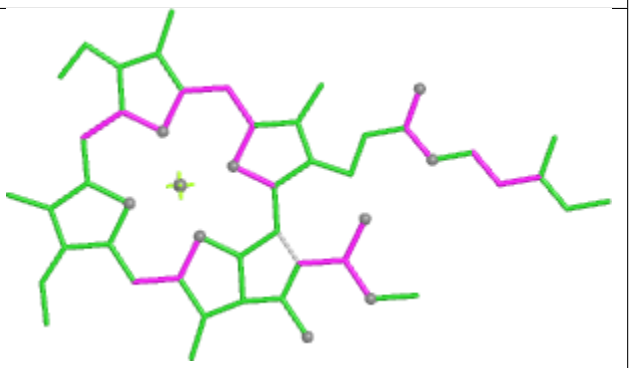
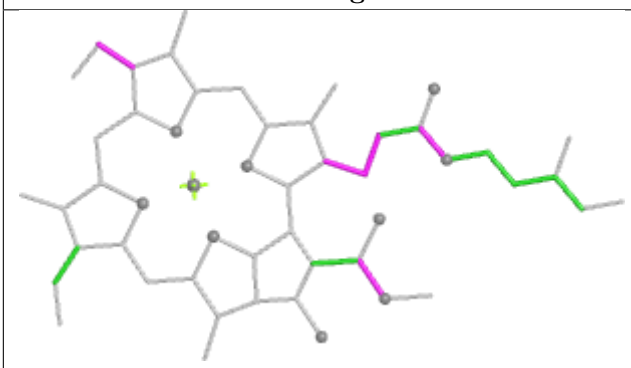
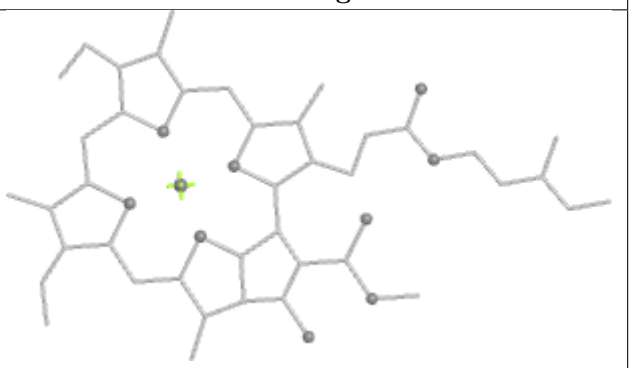
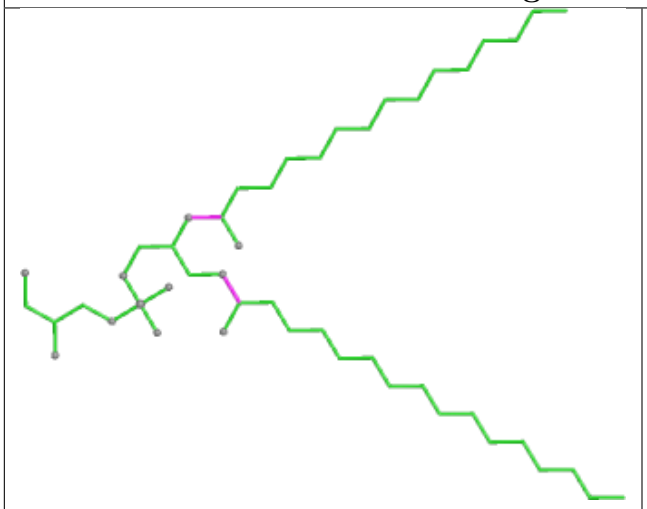
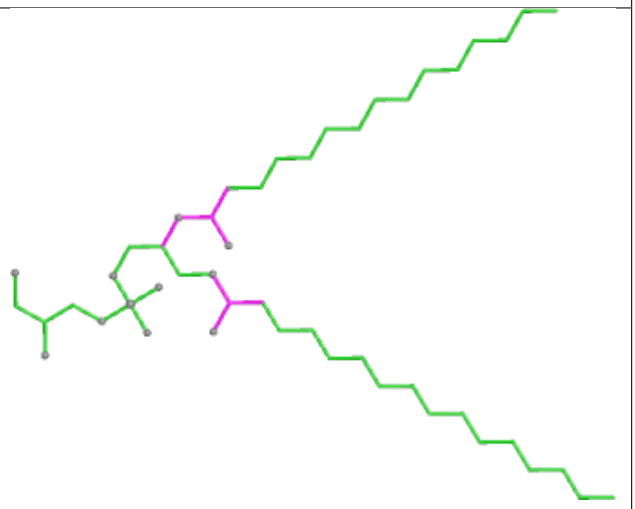
 Bond lengths	 Bond angles
 Torsions	 Rings

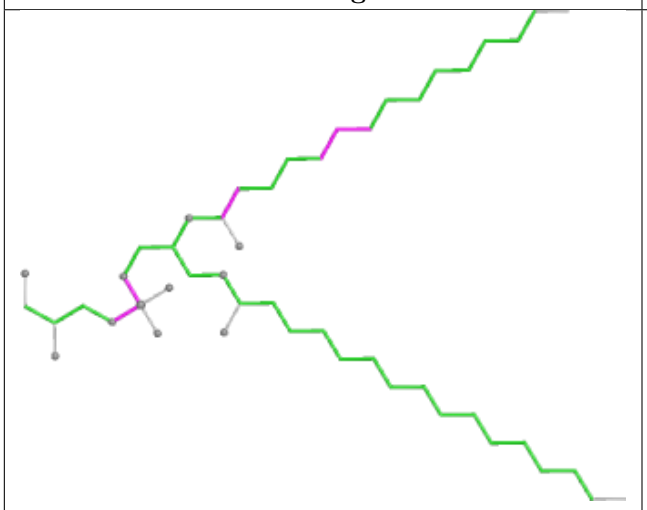
Ligand LHG A 844



Bond lengths



Bond angles



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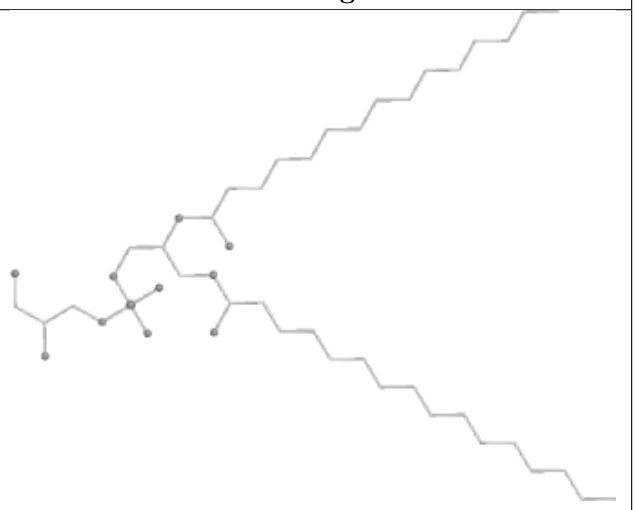
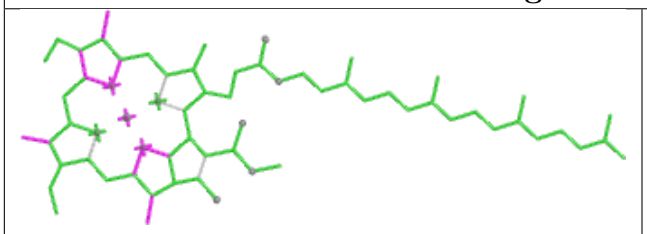
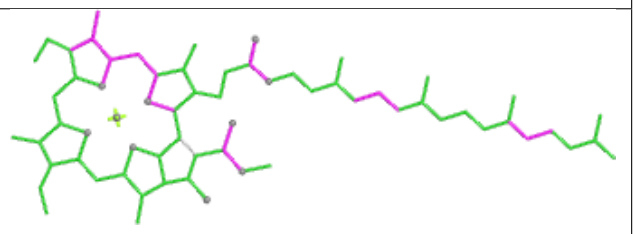


Rings

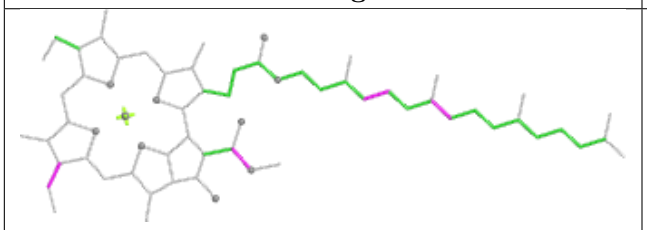
Ligand CLA A 820



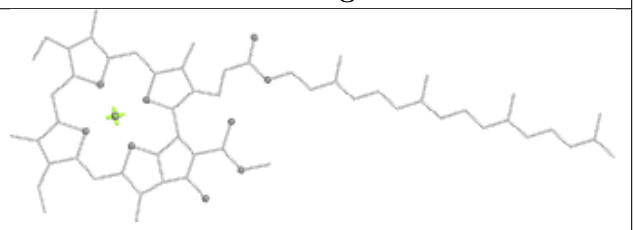
Bond lengths



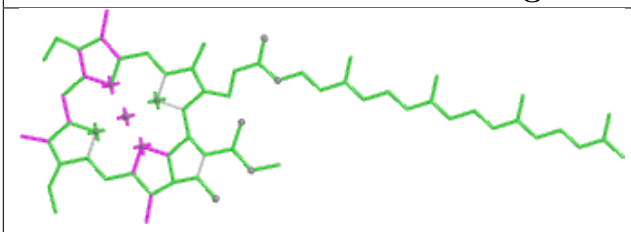
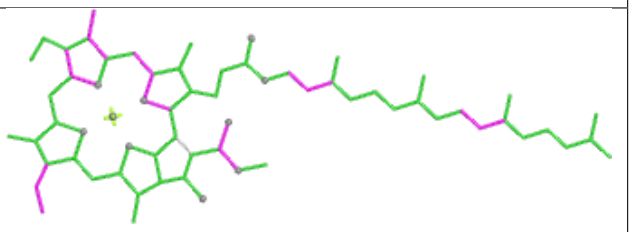
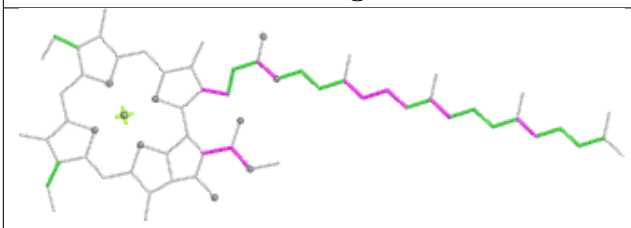
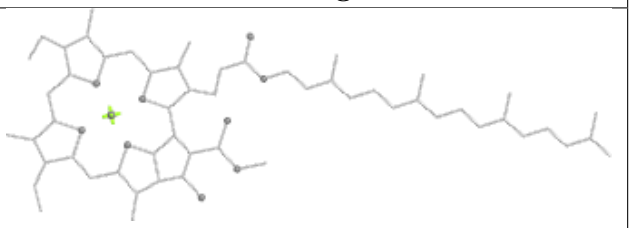
Bond angles

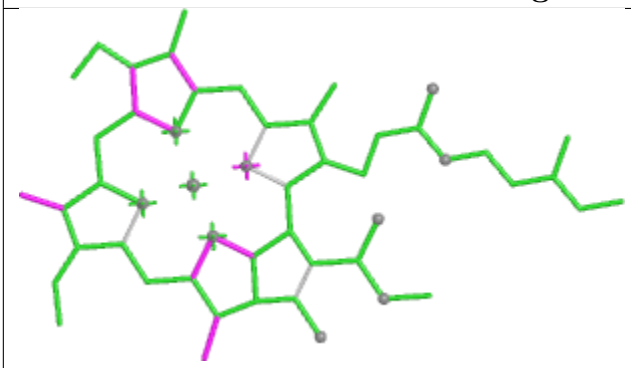
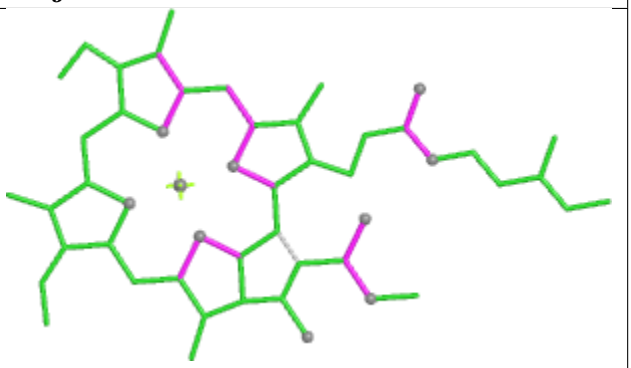
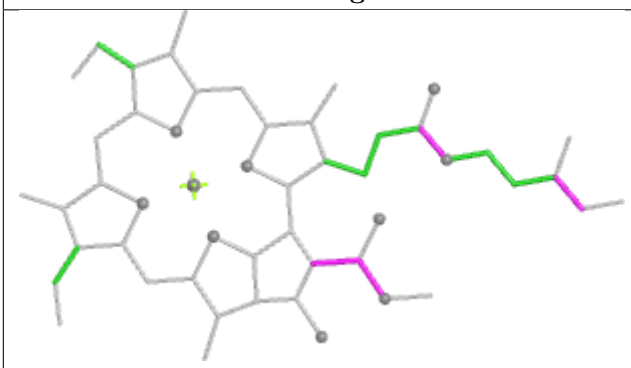
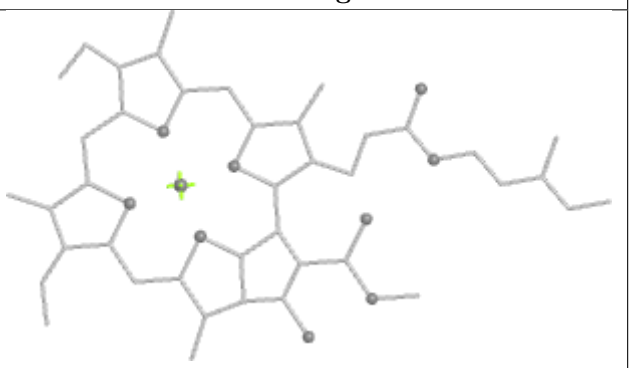


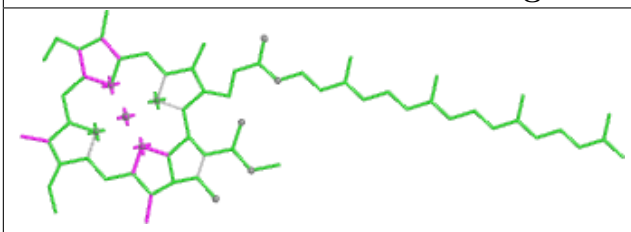
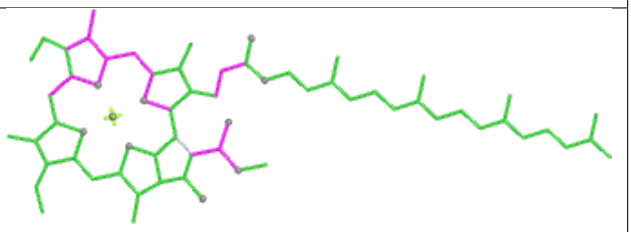
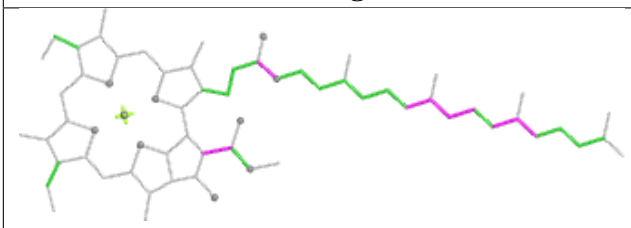
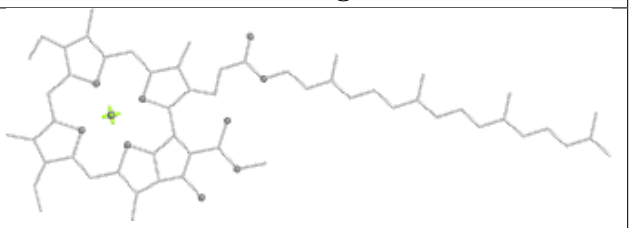
Torsions

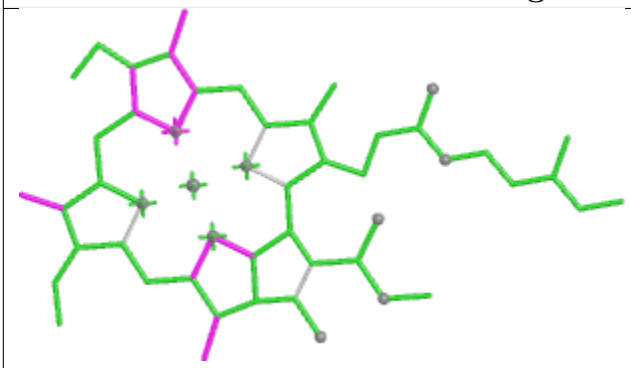
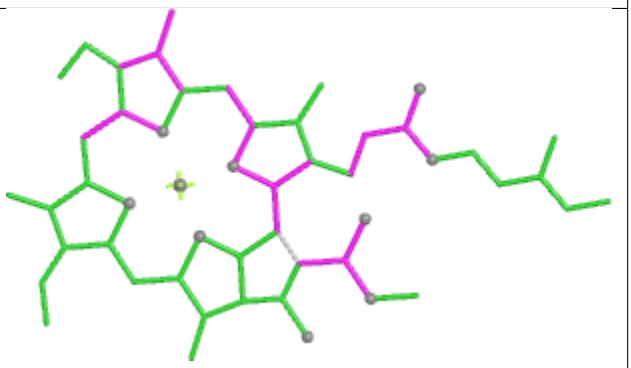
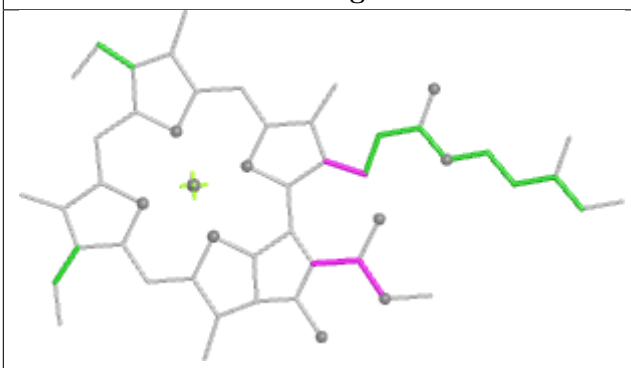
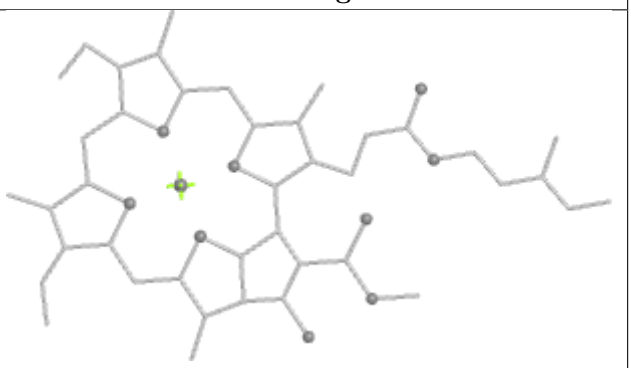


Rings

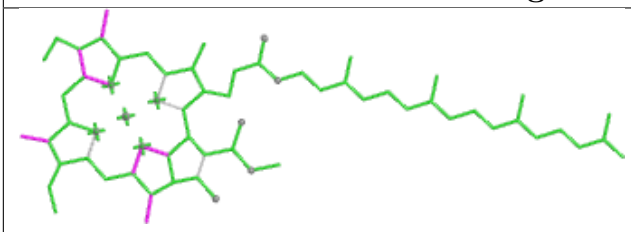
Ligand CLA O 201	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA j 313	
 Bond lengths	 Bond angles
 Torsions	 Rings

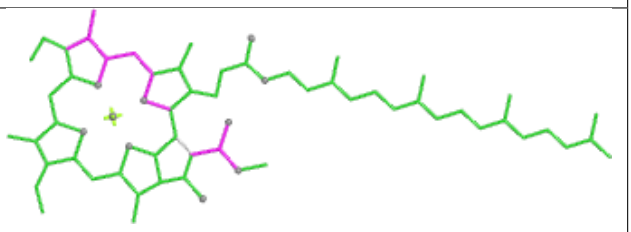
Ligand CLA A 825	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA h 303	
 Bond lengths	 Bond angles
 Torsions	 Rings

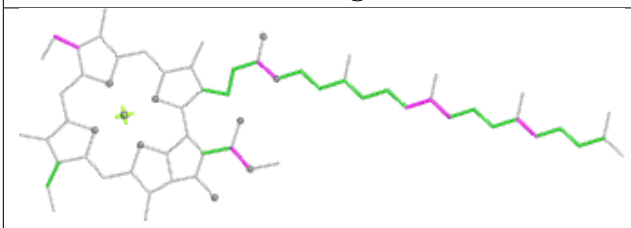
Ligand CLA h 312



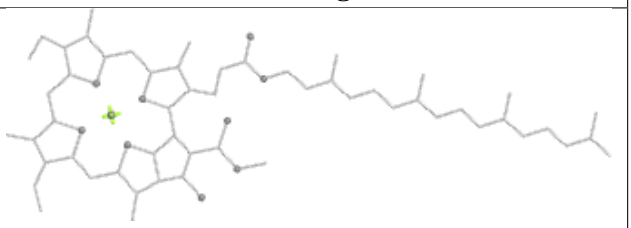
Bond lengths



Bond angles

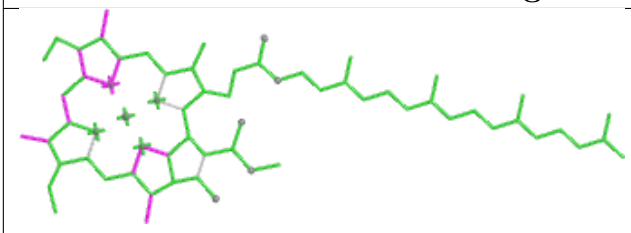


Torsions

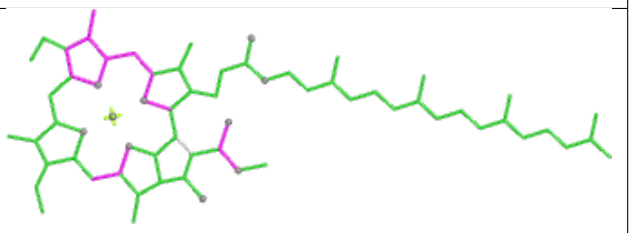


Rings

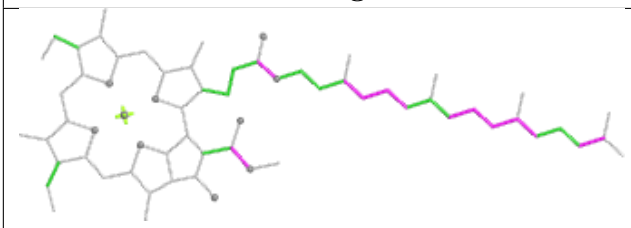
Ligand CLA A 840



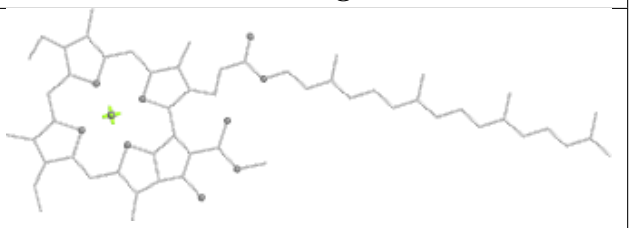
Bond lengths



Bond angles

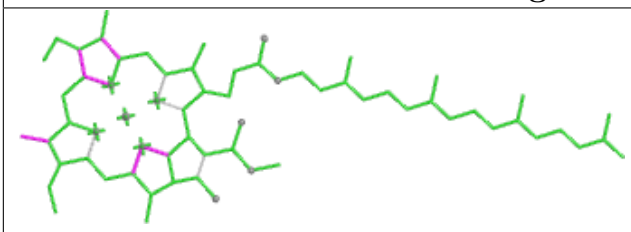


Torsions



Rings

Ligand CLA e 607



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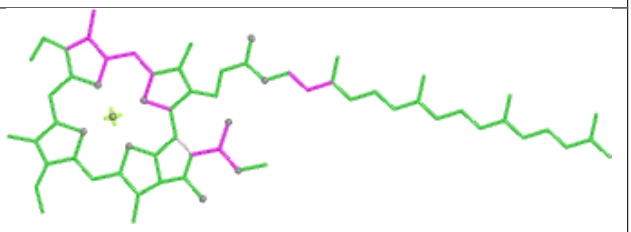
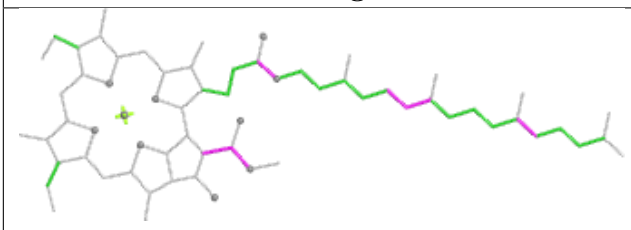
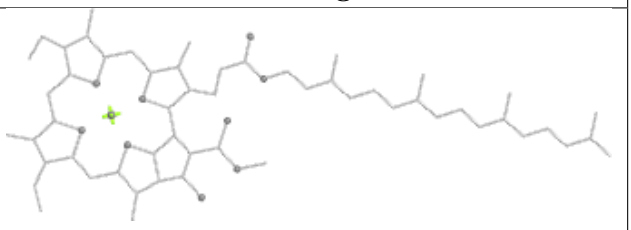


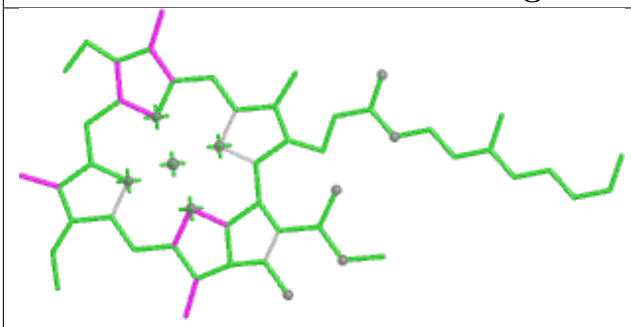
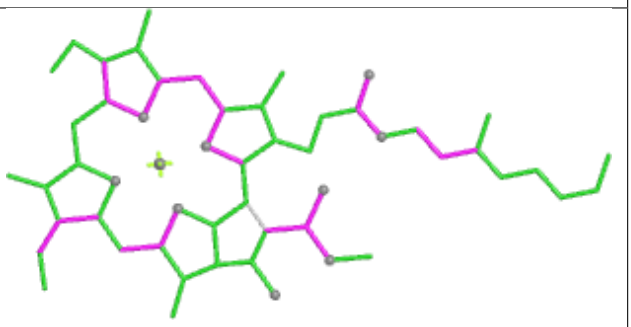
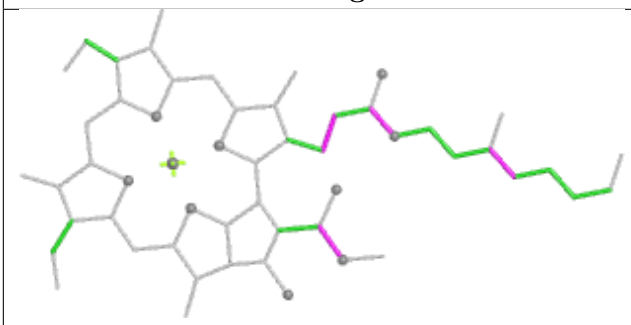
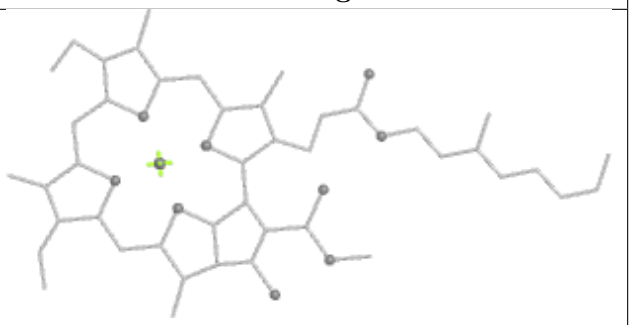
Bond angles



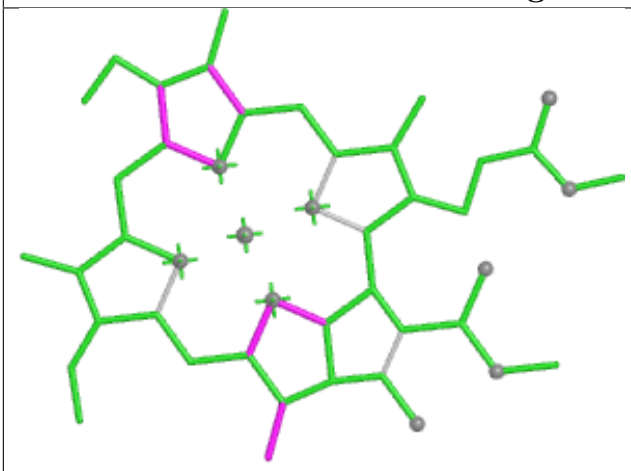
Torsions



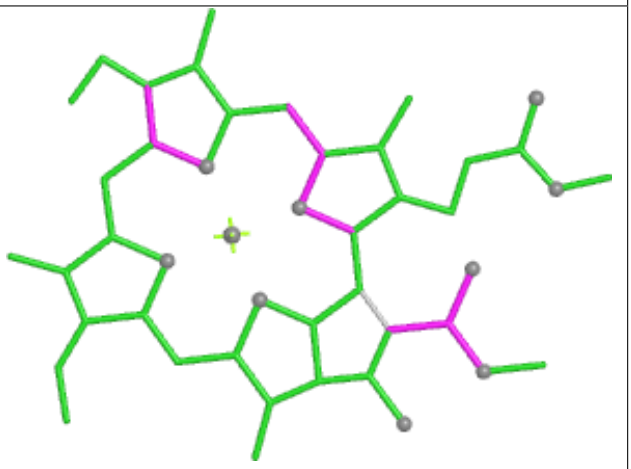
Rings

Ligand CLA A 811	
 Bond lengths	 Bond angles
 Torsions	 Rings

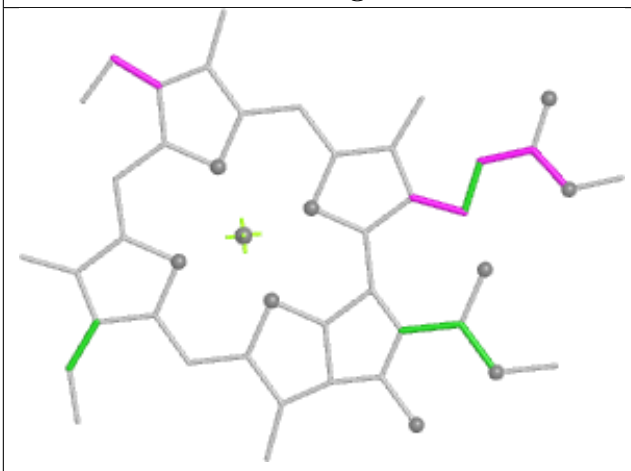
Ligand CLA d 307



Bond lengths



Bond angles



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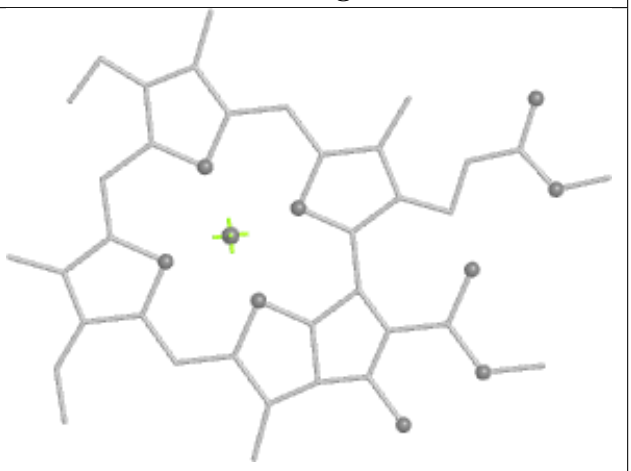
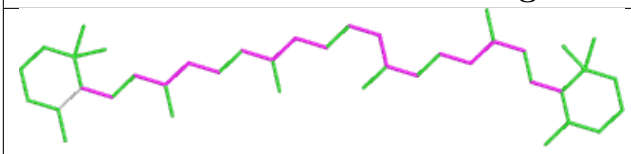


Rings

Ligand WVN J 102



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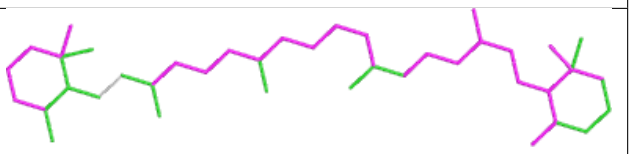
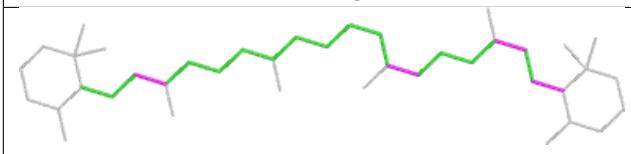


Bond angles



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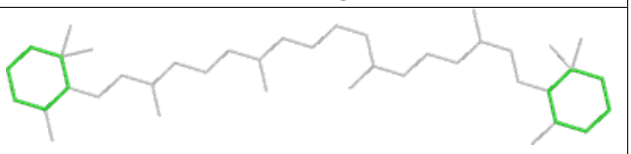
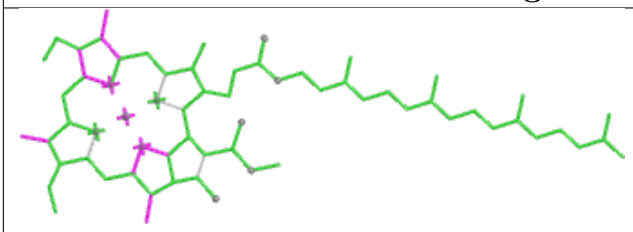
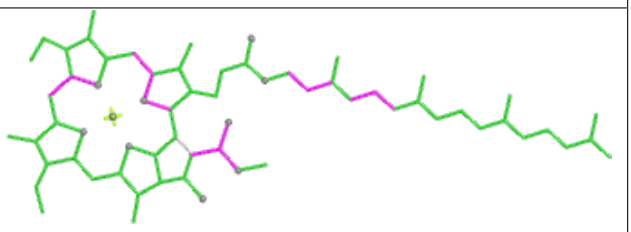


Rings

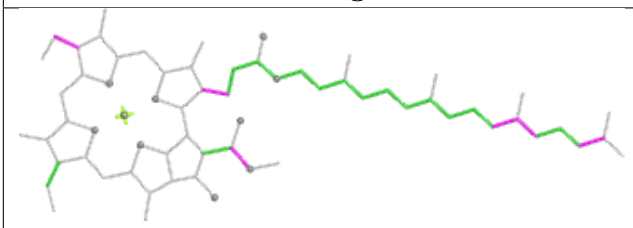
Ligand CLA A 831



Bond lengths



Bond angles



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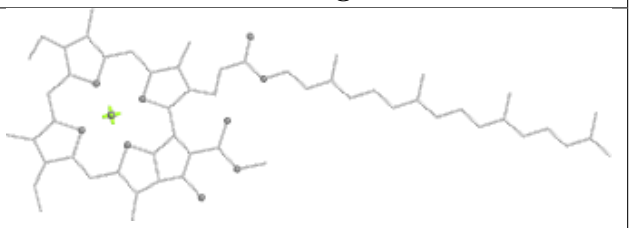
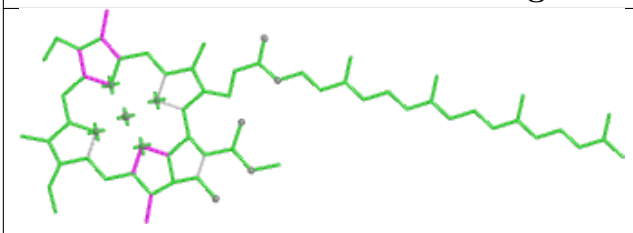


Rings

Ligand CLA k 608



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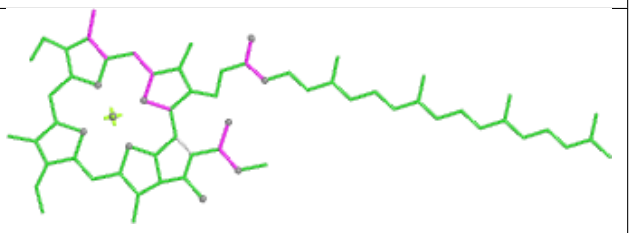
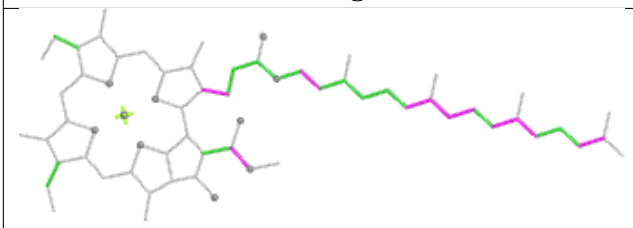


Bond angles



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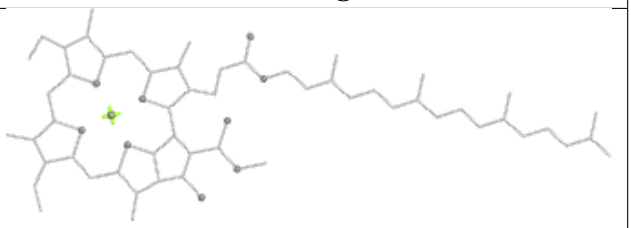
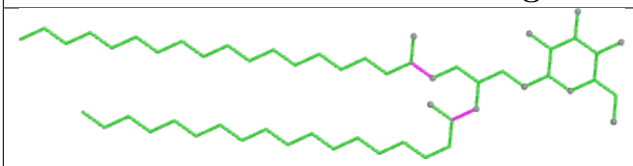
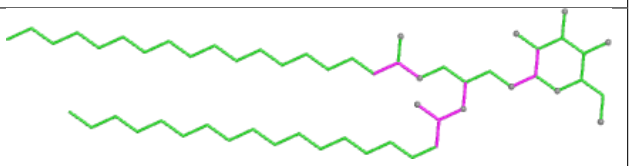


Rings

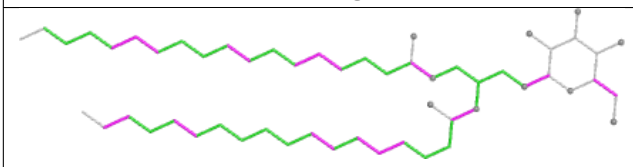
Ligand LMG b 301



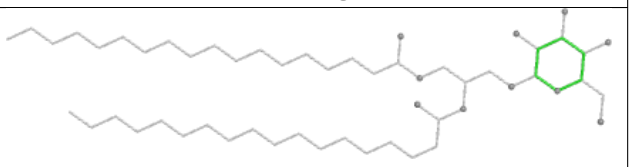
Bond lengths



Bond angles

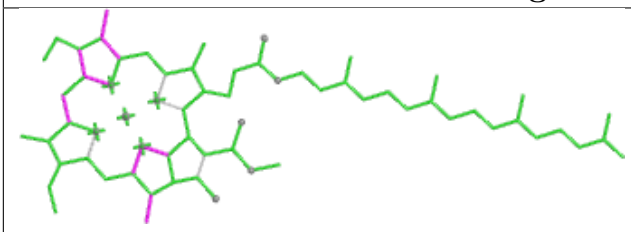


Torsions

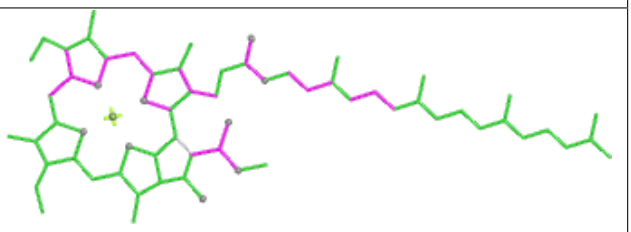


Rings

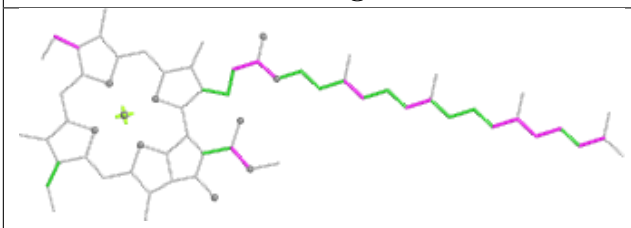
Ligand CLA e 611



Bond lengths



Bond angles



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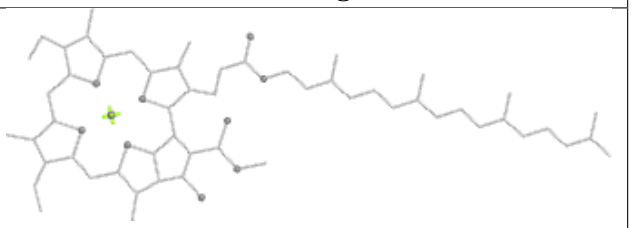
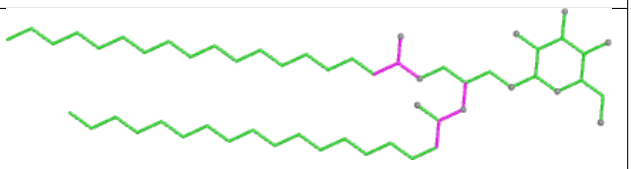


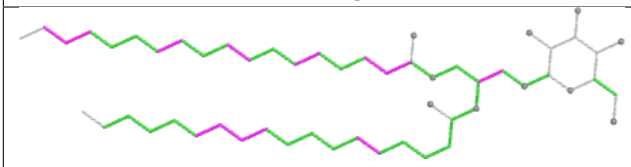
Rings

Ligand LMG J 106

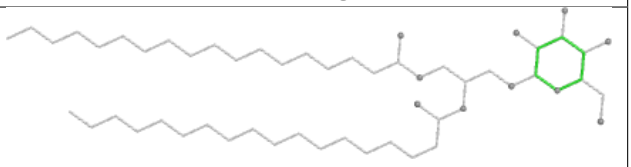
Bond lengths



Bond angles

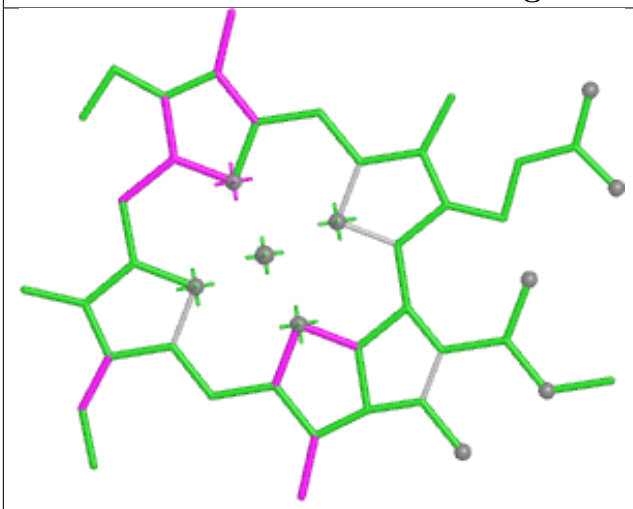


Torsions



Rings

Ligand CLA A 819



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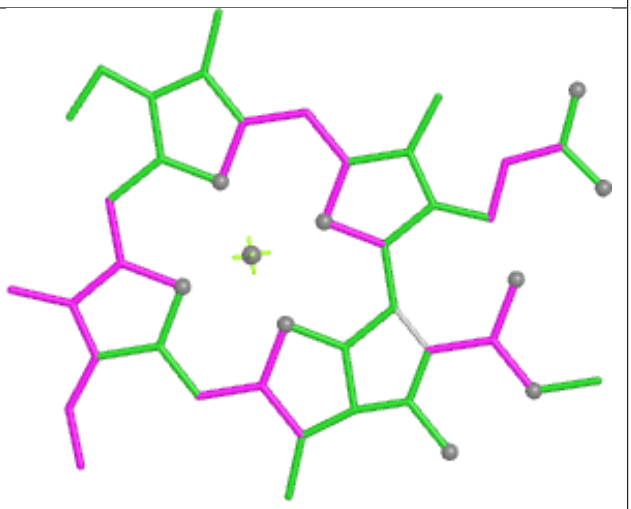
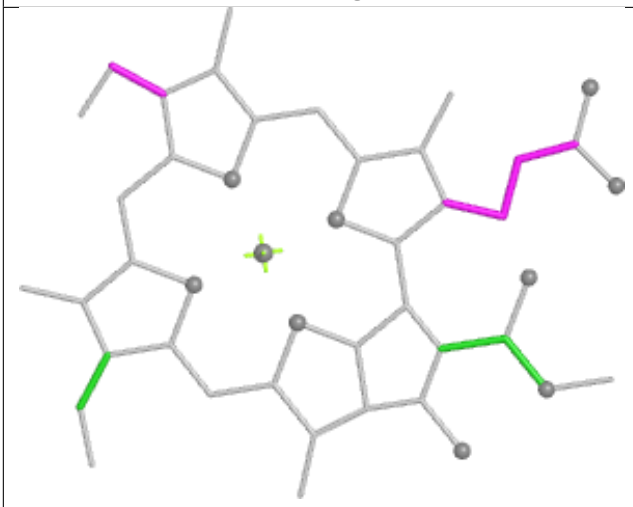


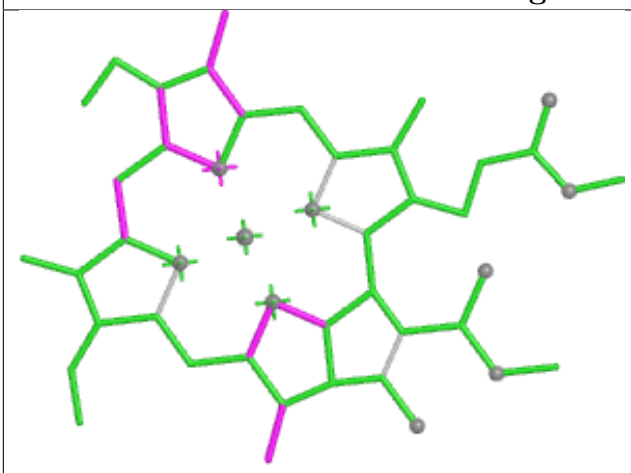
Bond angles



Torsions

Rings

Ligand CLA e 608



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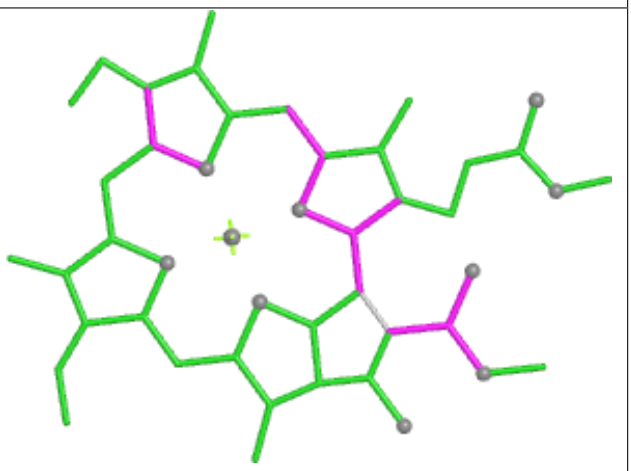
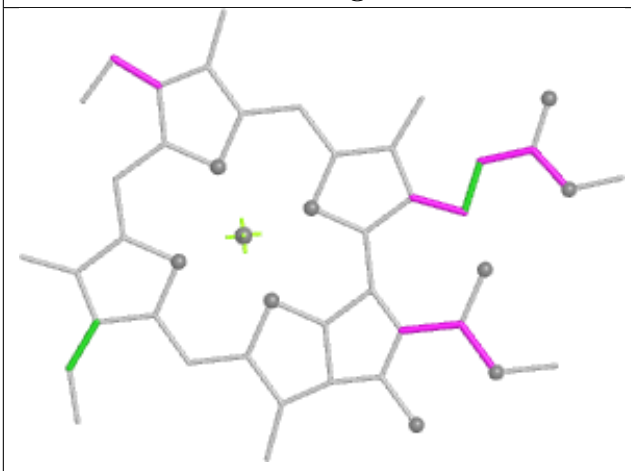
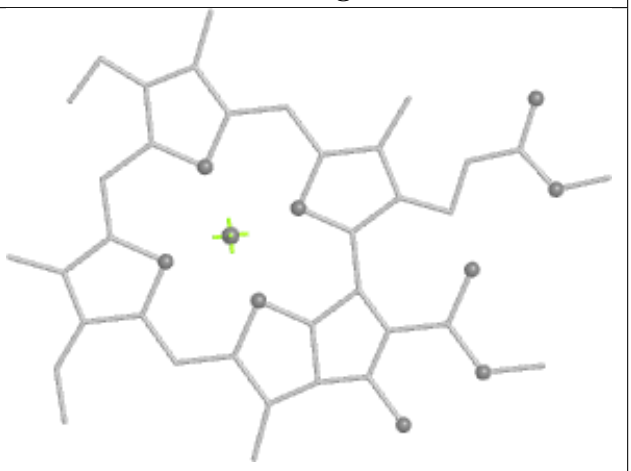


Bond angles

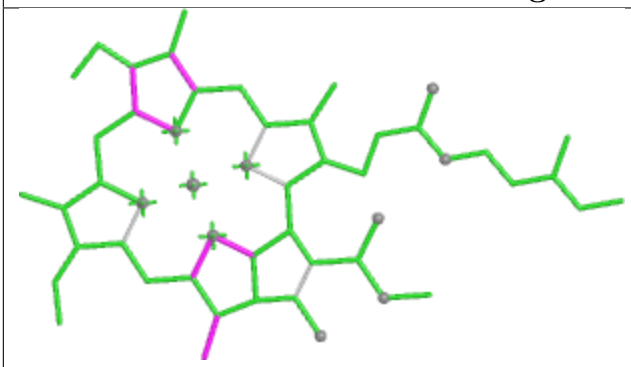


Torsions

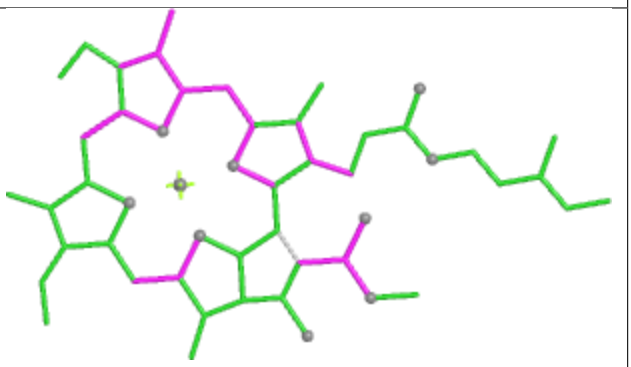


Rings

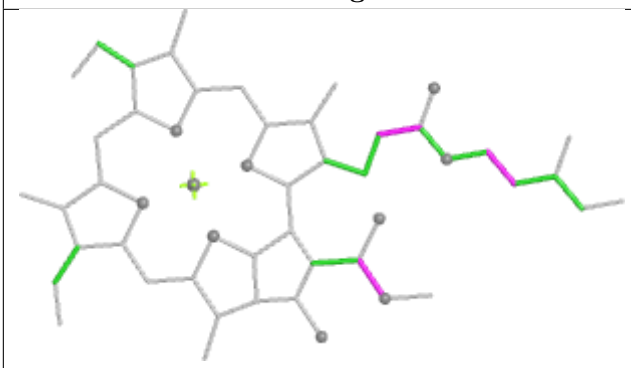
Ligand CLA e 603



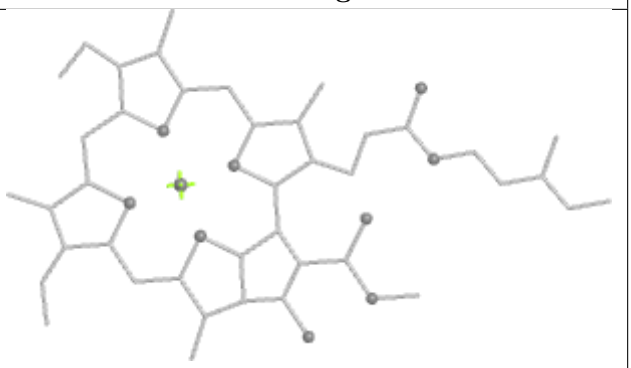
Bond lengths



Bond angles

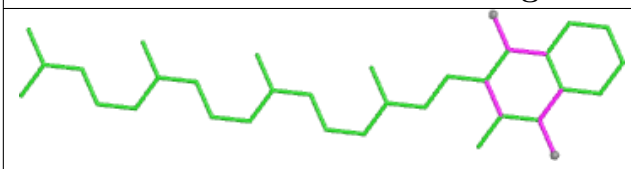


Torsions



Rings

Ligand PQN A 843



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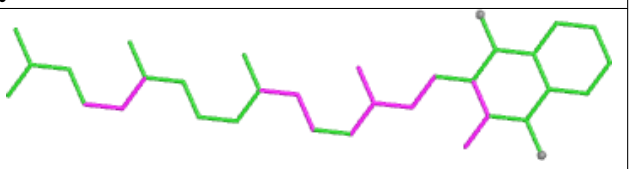
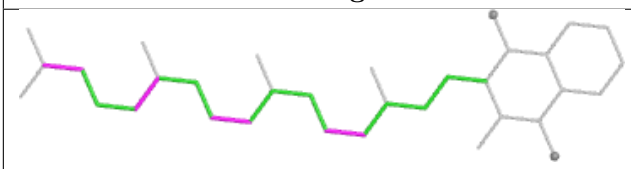
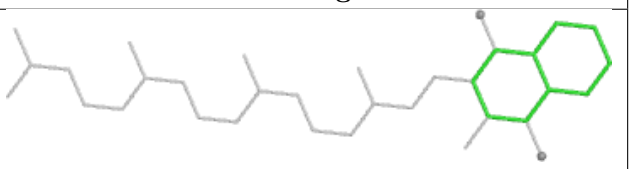


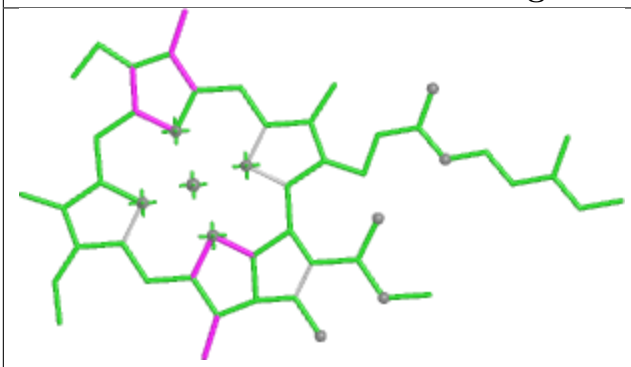
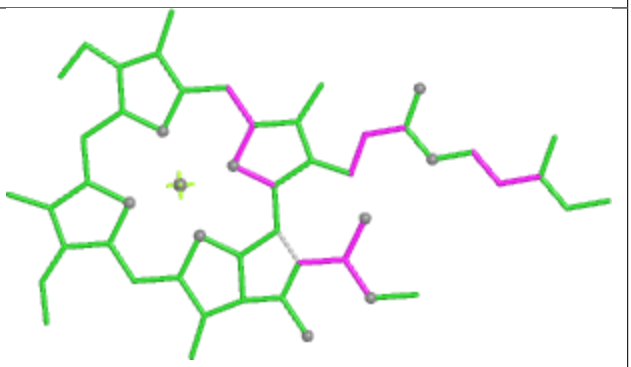
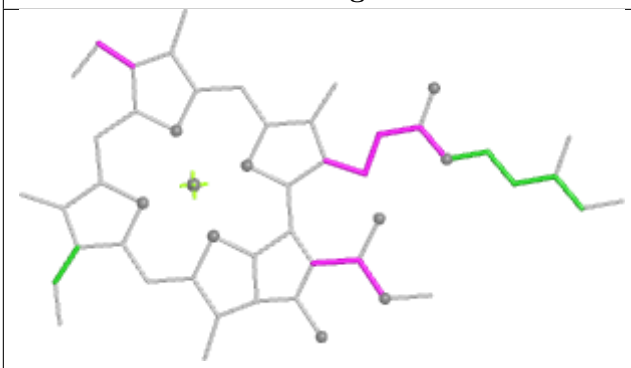
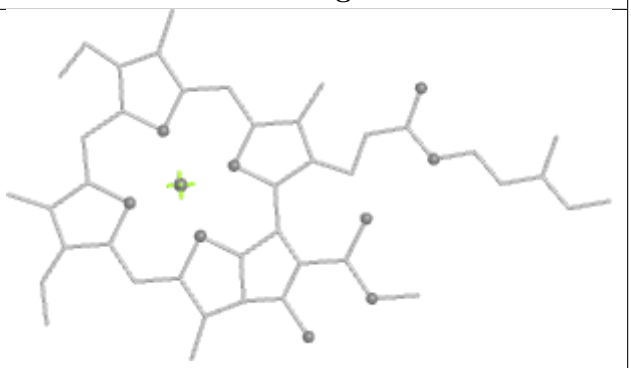
Bond angles

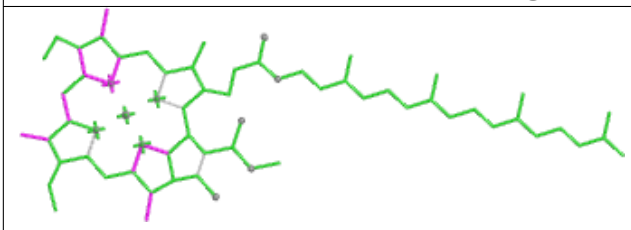
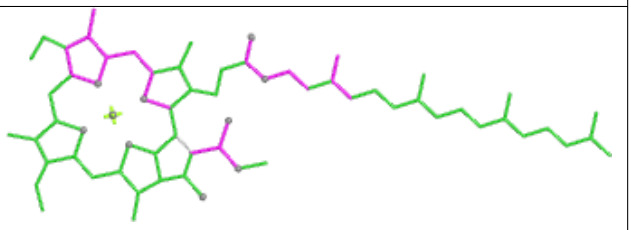
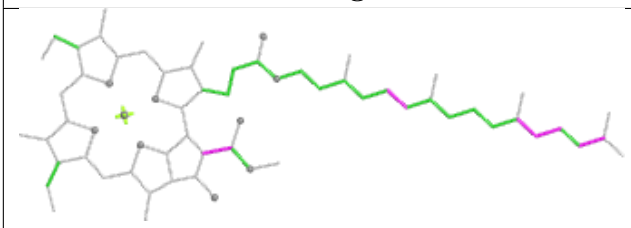
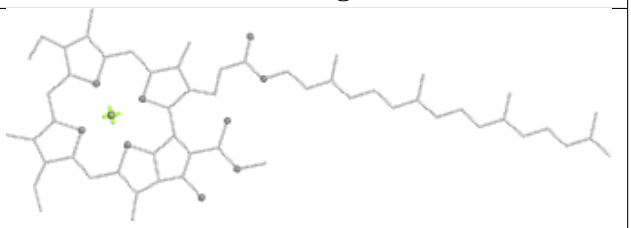


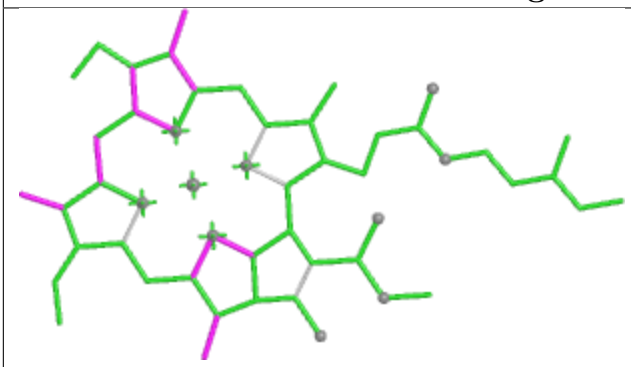
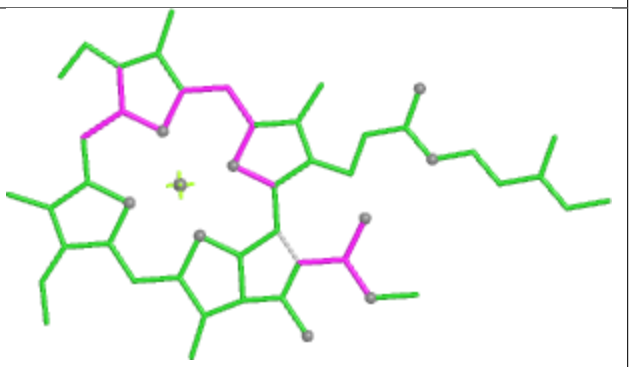
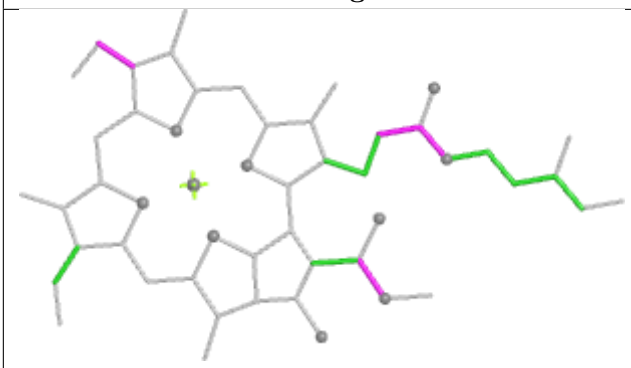
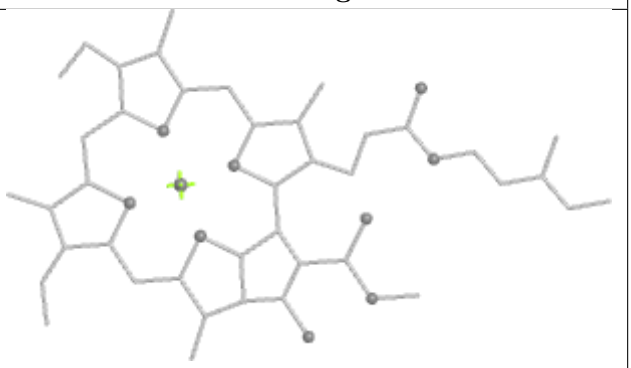
Torsions

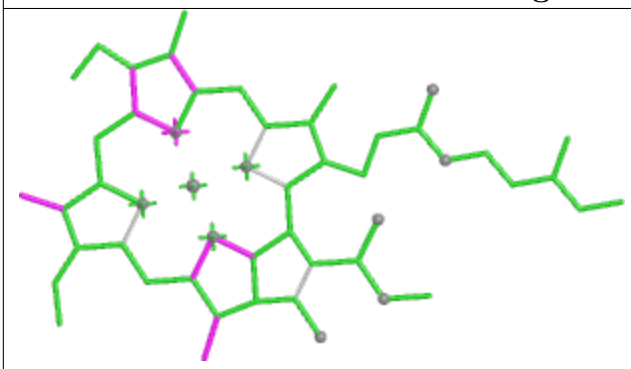
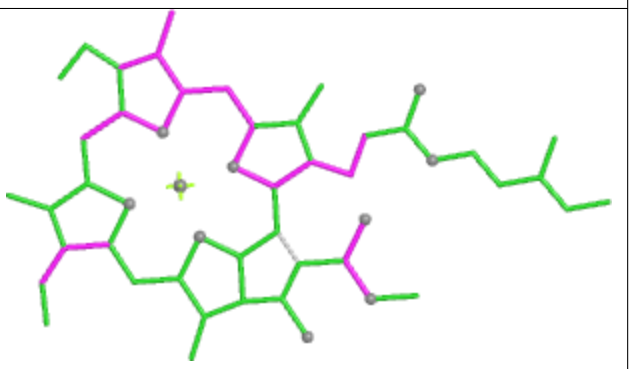
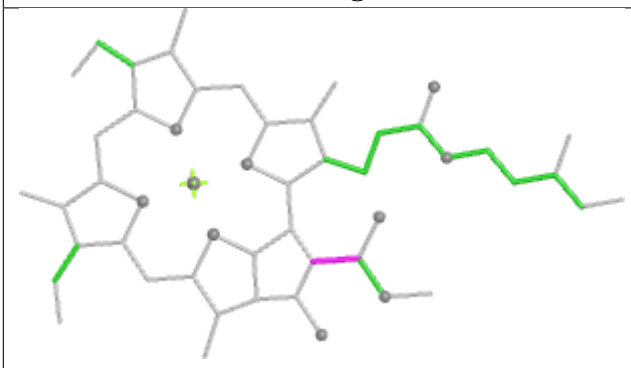
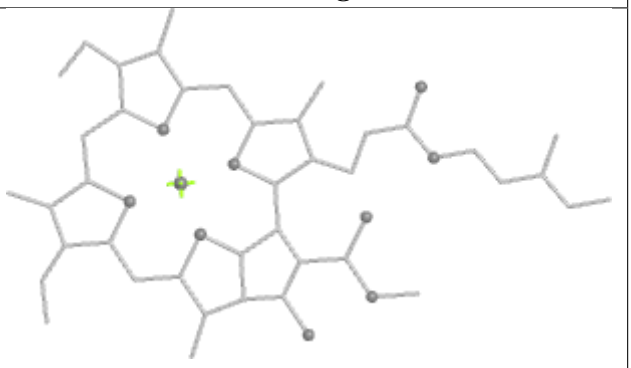


Rings

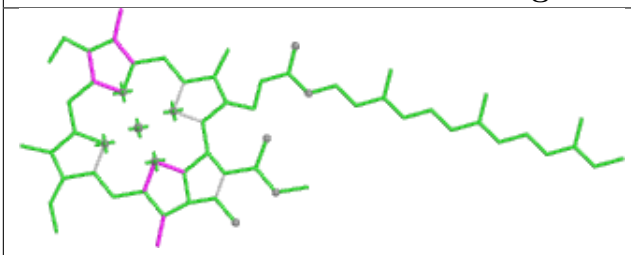
Ligand CLA k 610	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA B 833	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA k 606	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA i 607	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA j 311



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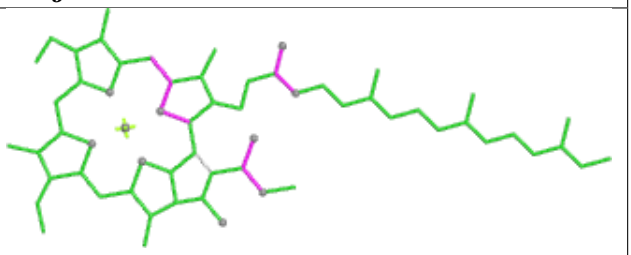
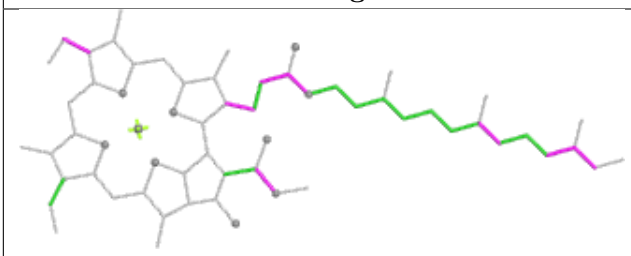


Bond angles



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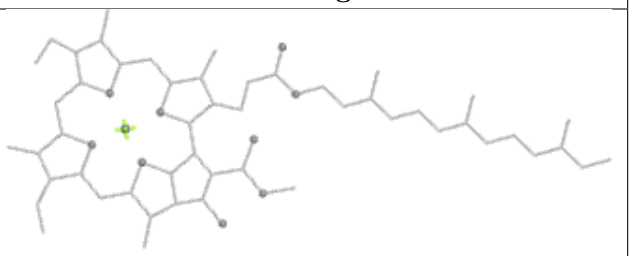
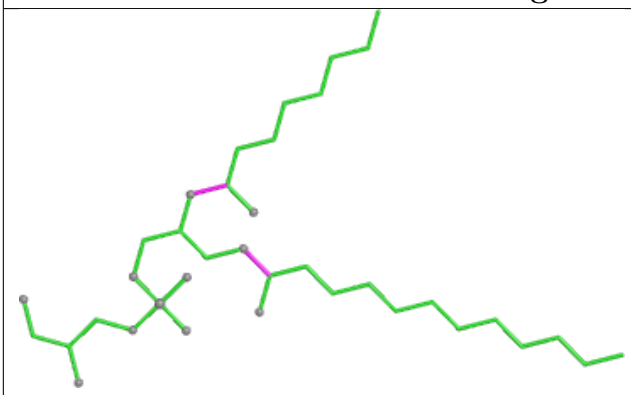


Rings

Ligand LHG i 615



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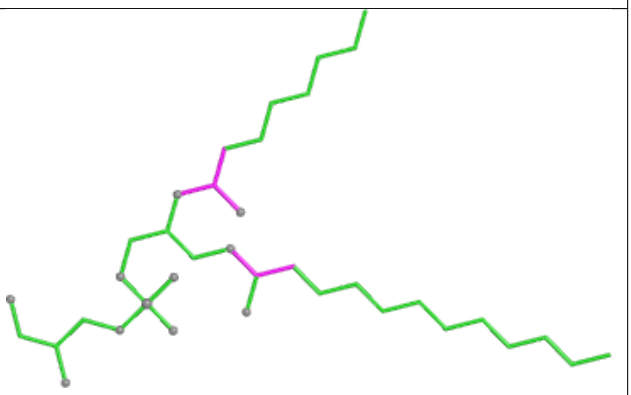

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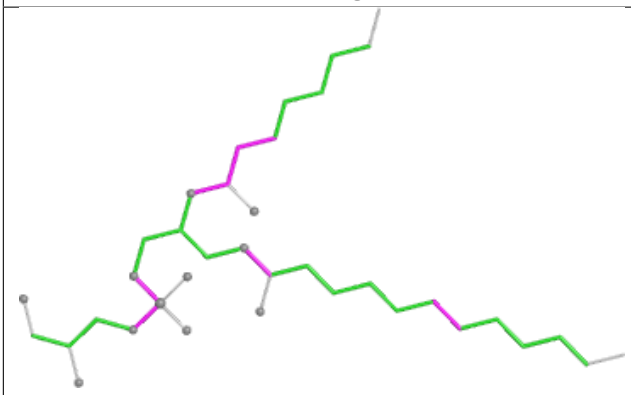

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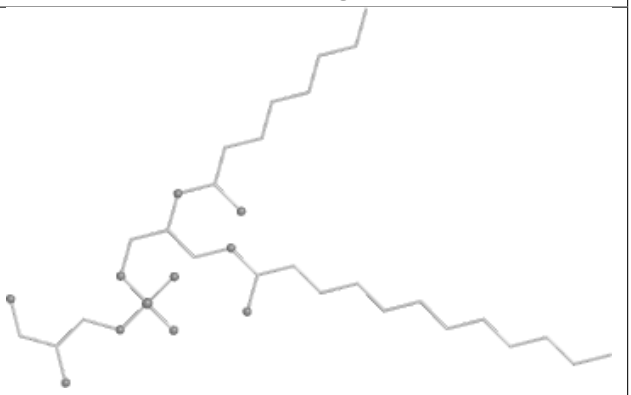
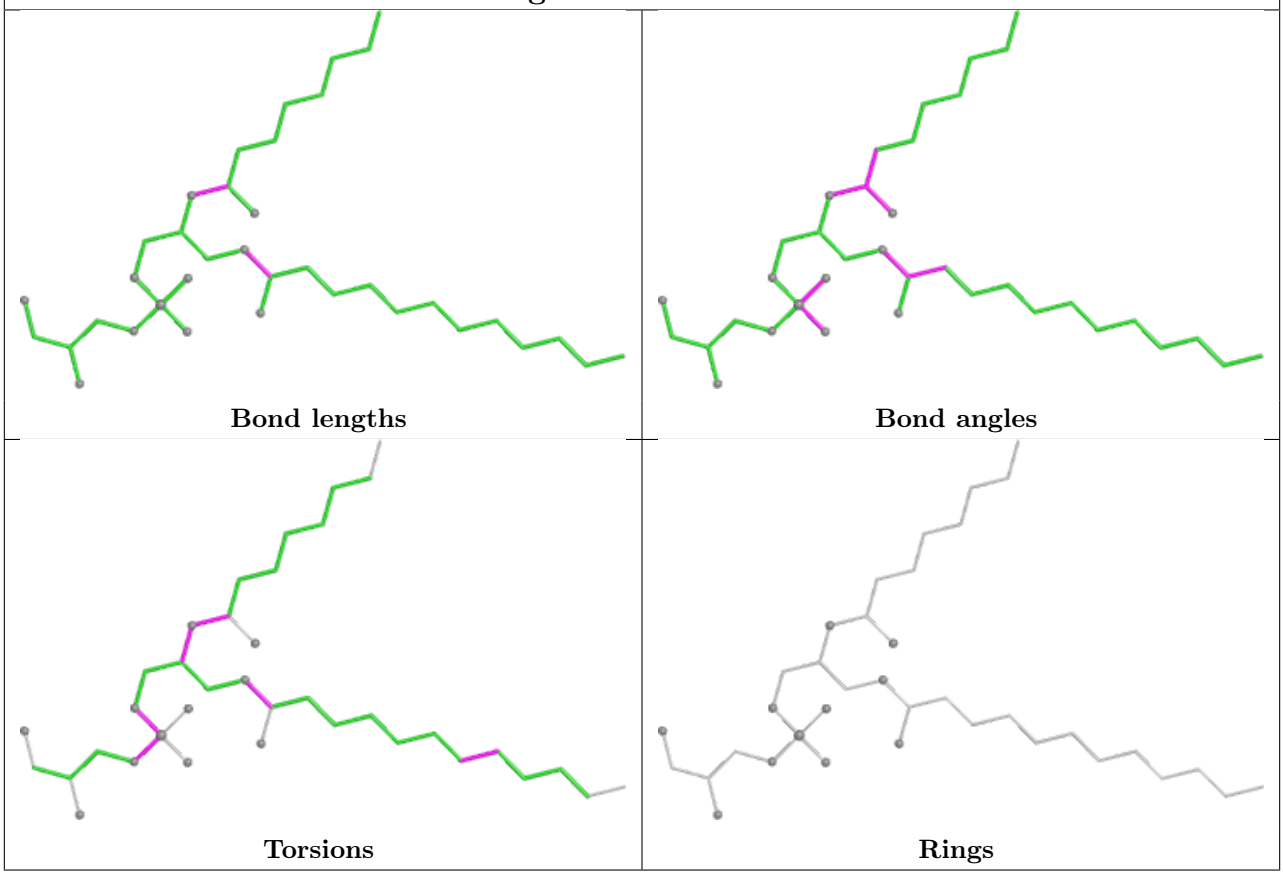
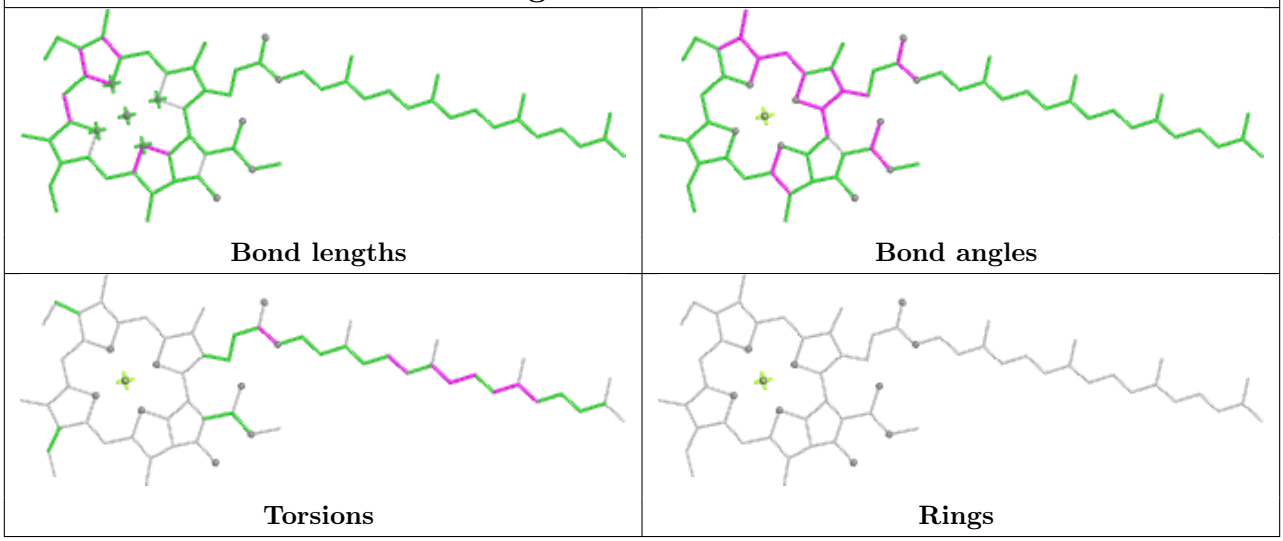


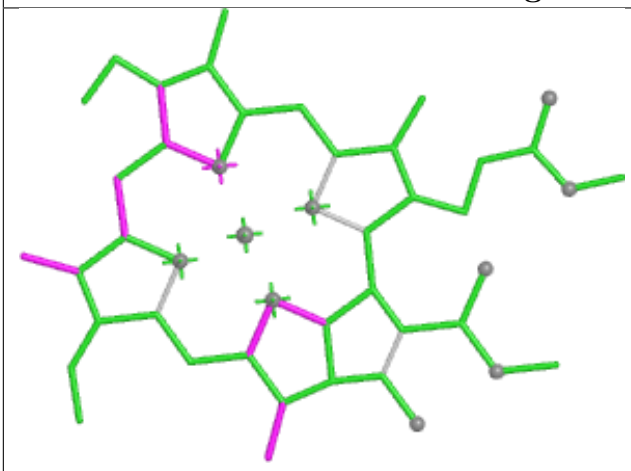
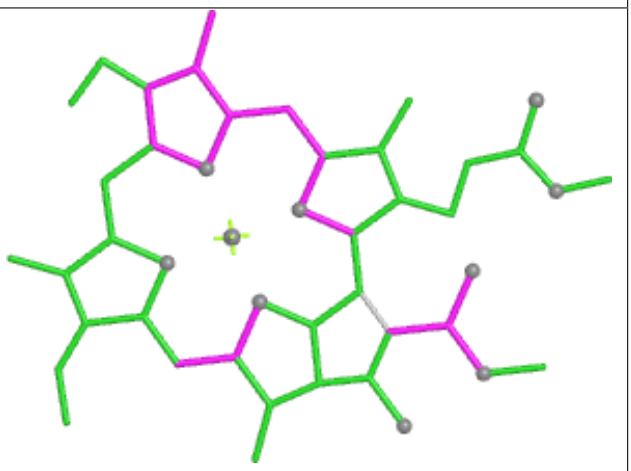
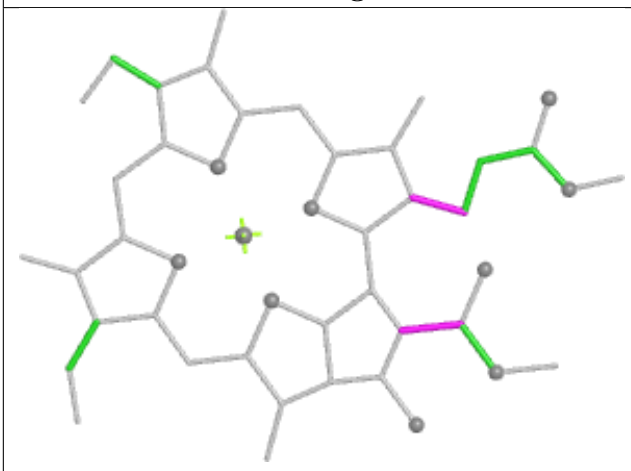
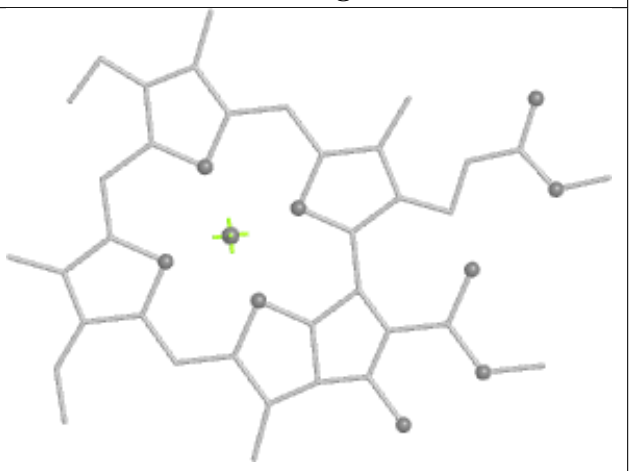
Rings

Ligand LHG e 617

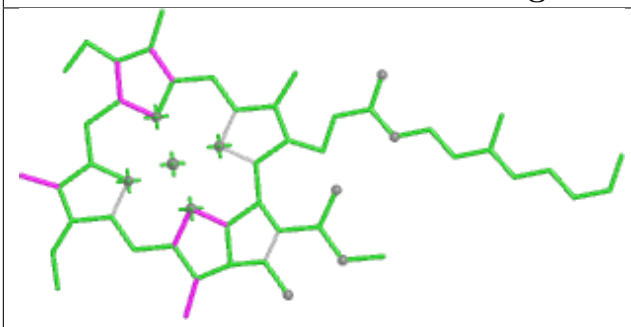


Ligand CLA b 307



Ligand CLA B 819	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA g 311



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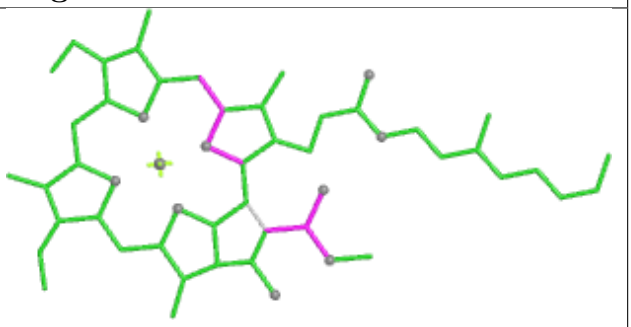
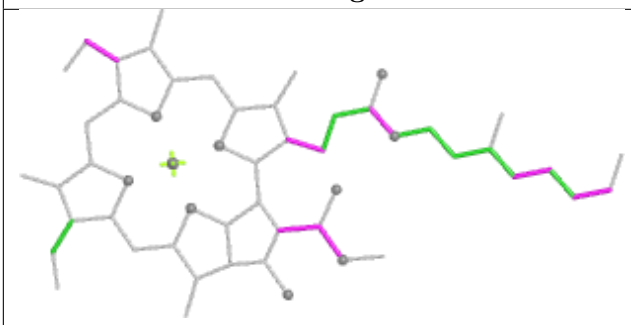


Bond angles



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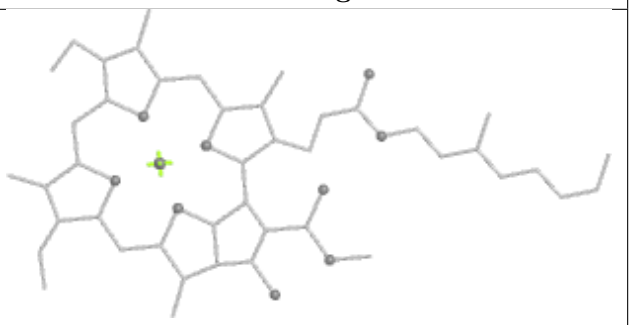
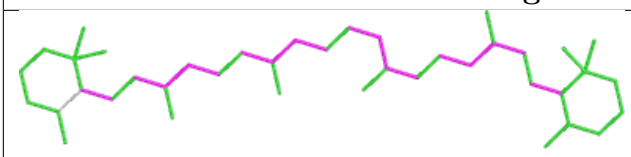


Rings

Ligand WVN j 301



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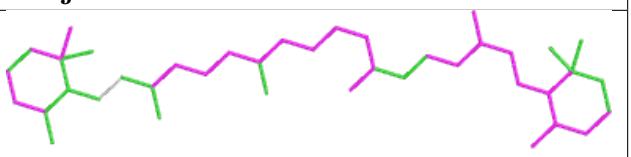

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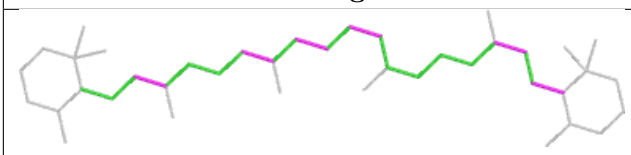

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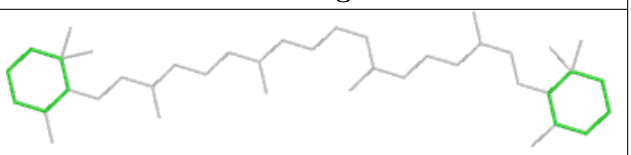
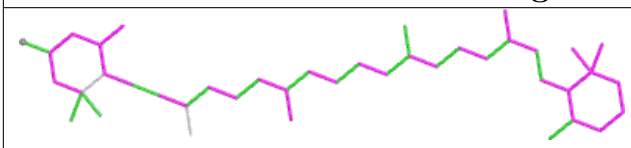


Rings

Ligand IHT b 317



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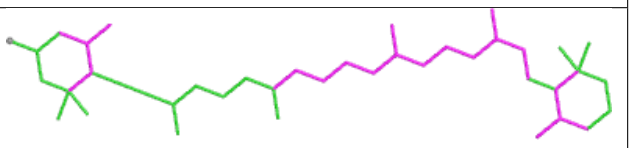
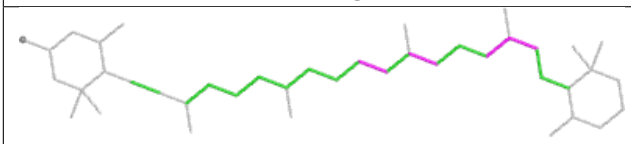


Bond angles



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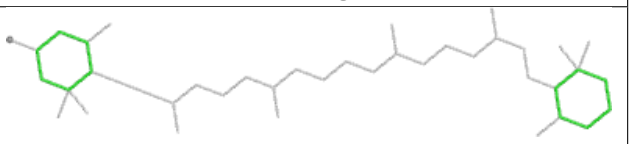
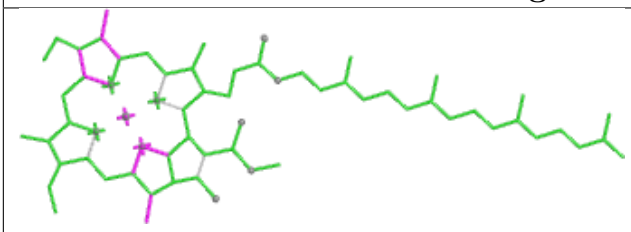
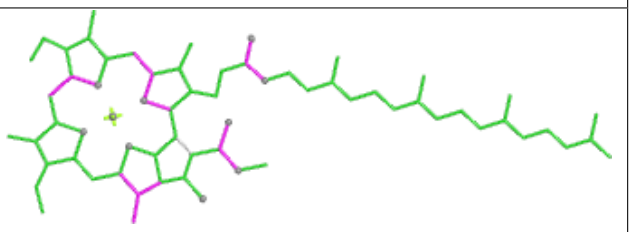
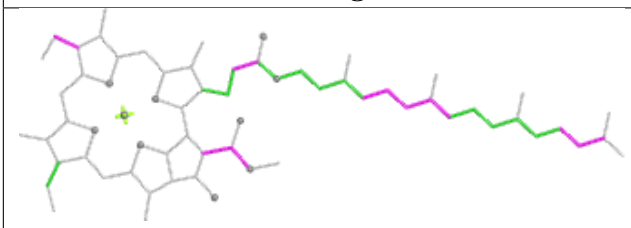
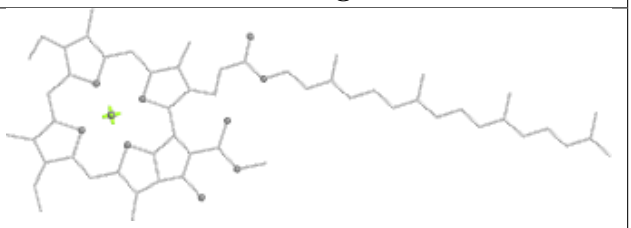
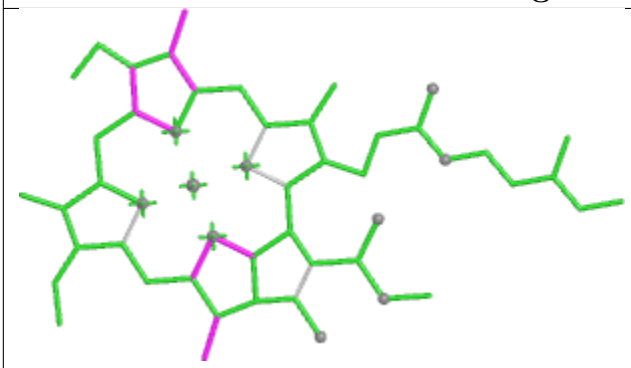
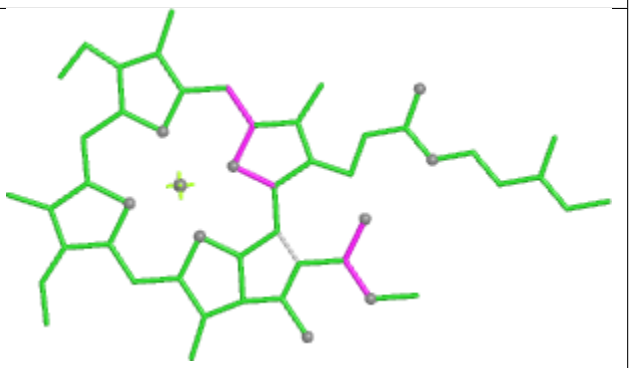
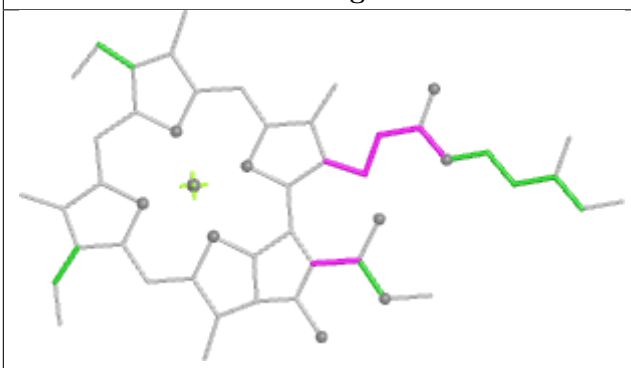
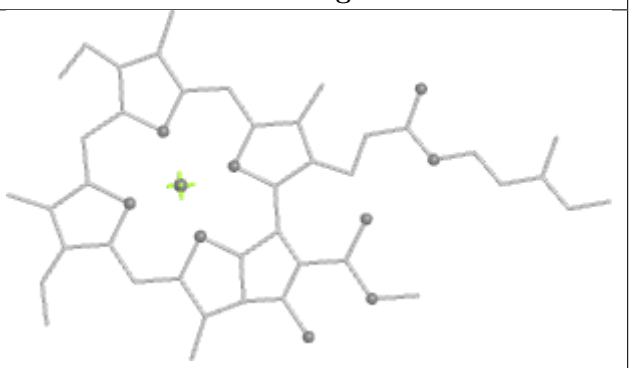
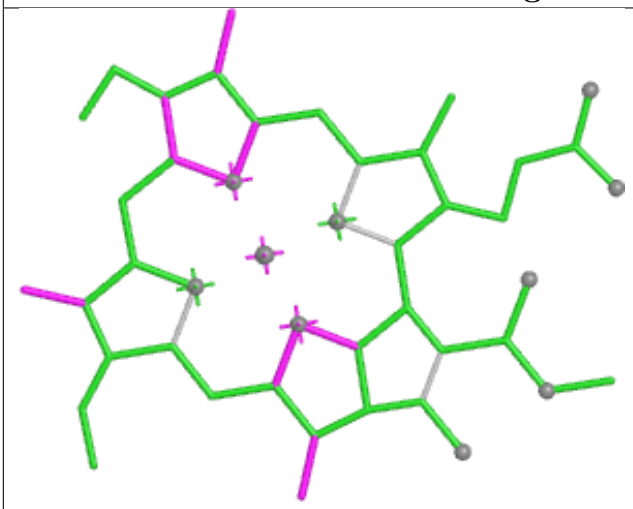


Rings

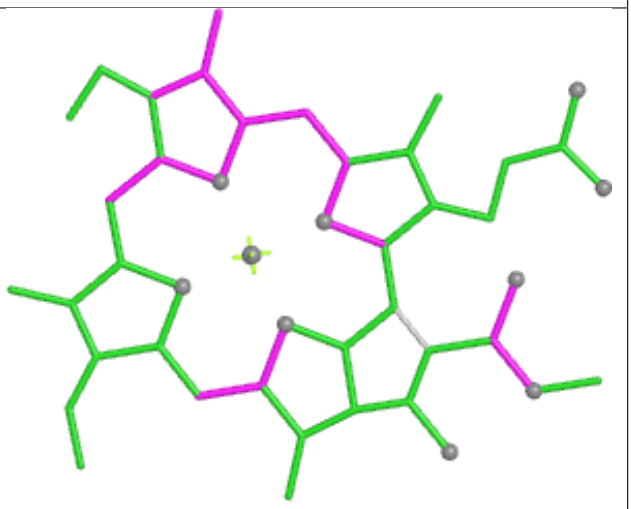
Ligand CLA e 605	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA i 601	
 Bond lengths	 Bond angles
 Torsions	 Rings

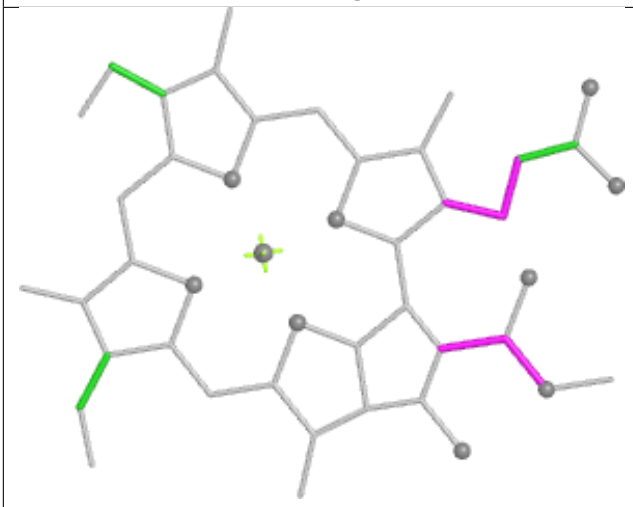
Ligand CLA A 815



Bond lengths



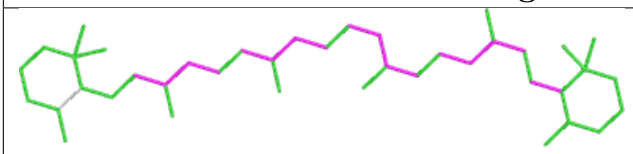
Bond angles



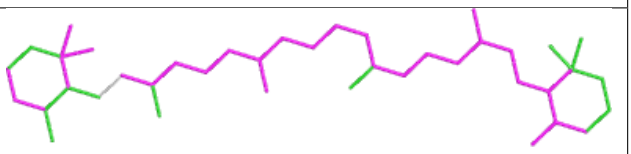
Torsions

Rings

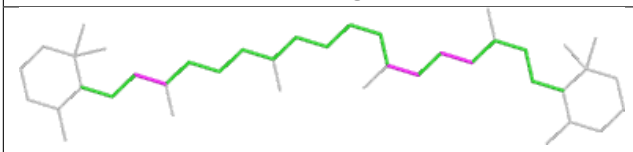
Ligand WVN h 308



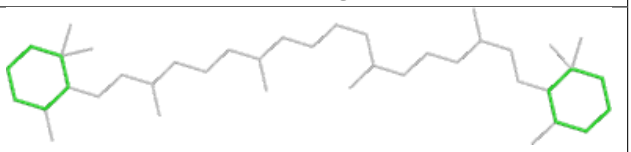
Bond lengths



Bond angles

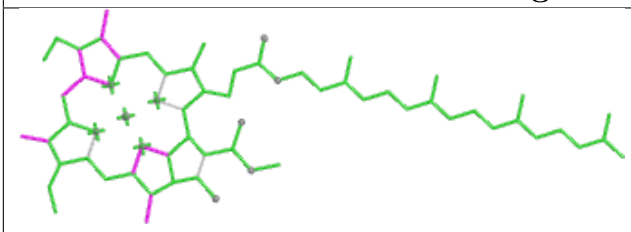


Torsions



Rings

Ligand CLA f 607



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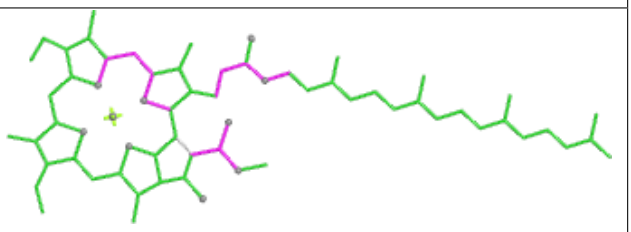

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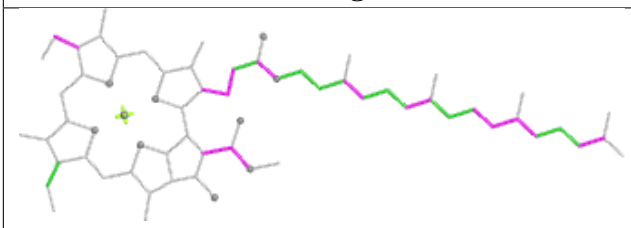

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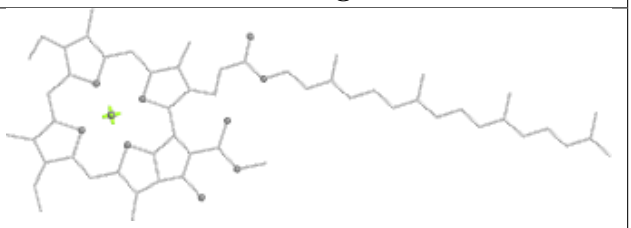
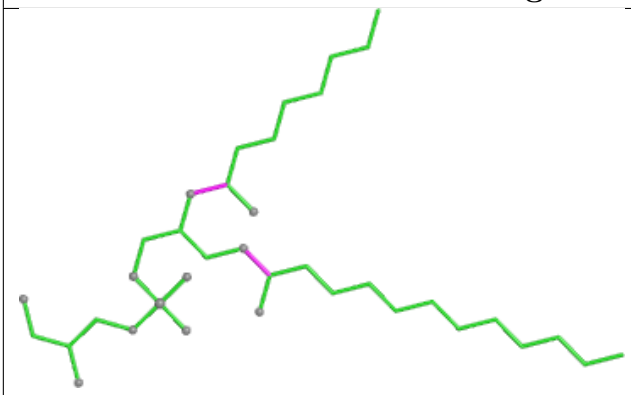


Rings

Ligand LHG d 316



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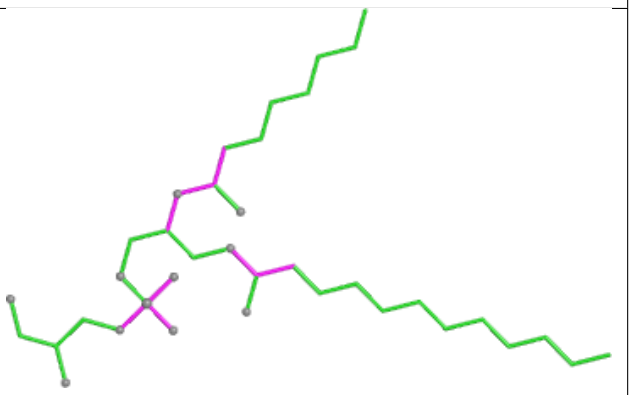

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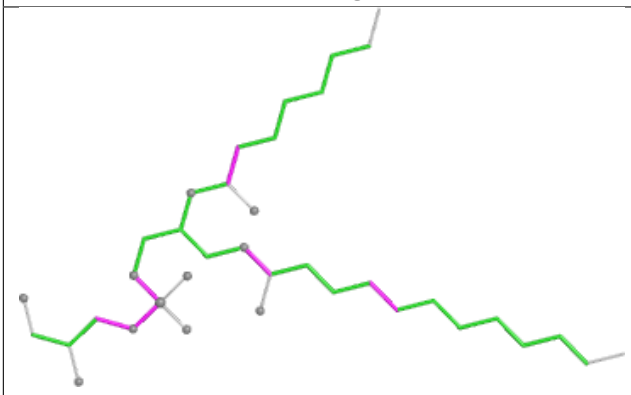

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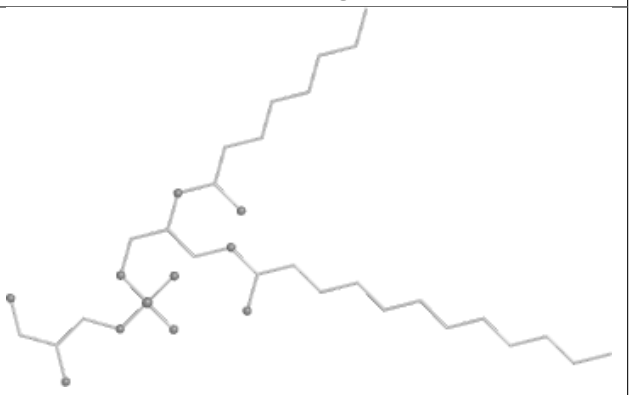
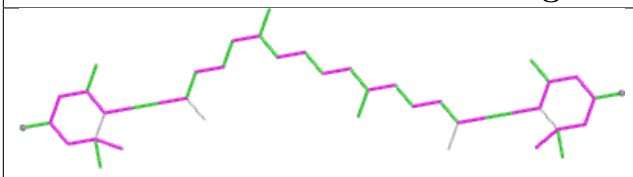


Rings

Ligand II0 k 616



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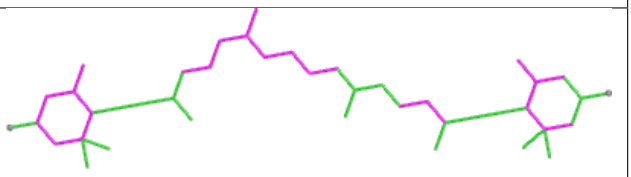

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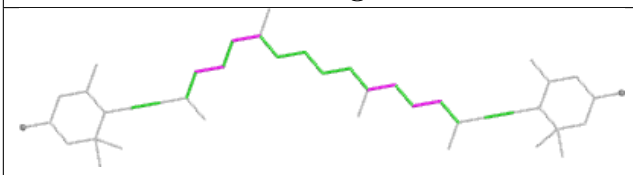

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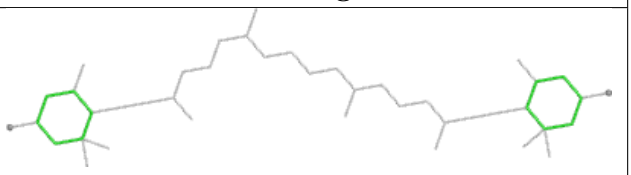
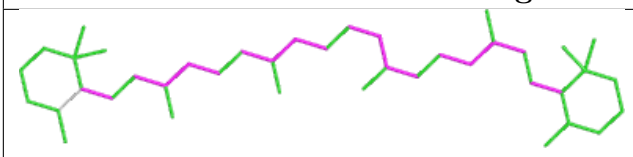


Rings

Ligand WVN A 850



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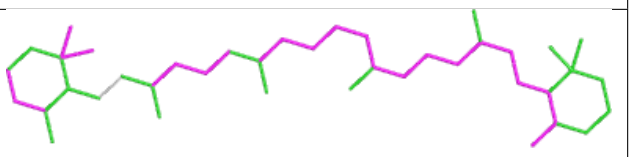

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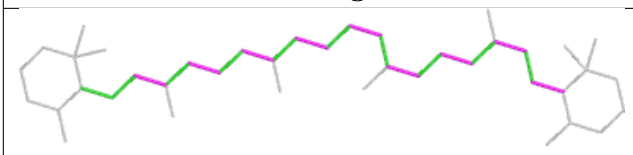

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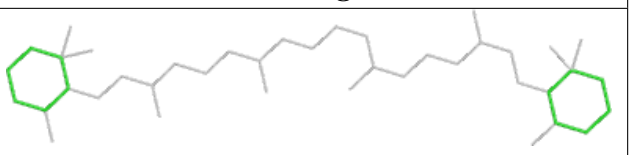
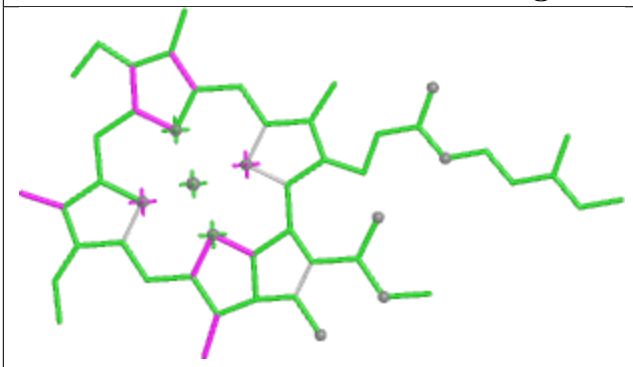


Rings

Ligand CLA i 610



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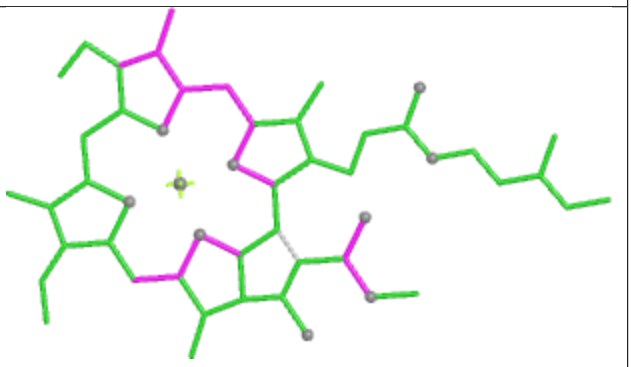

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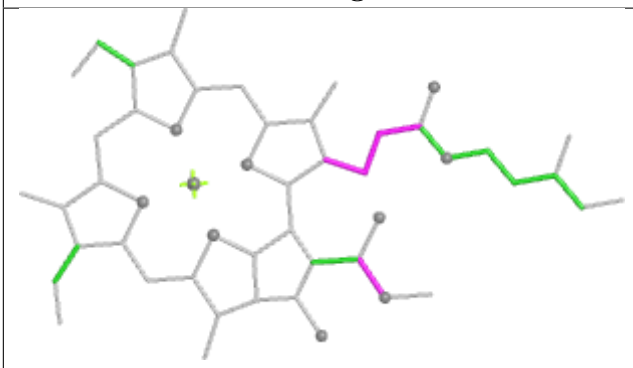

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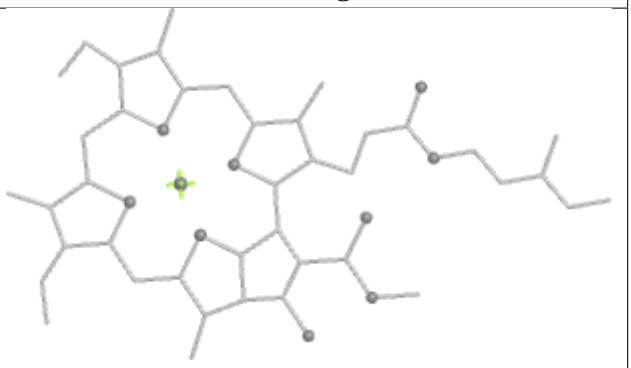
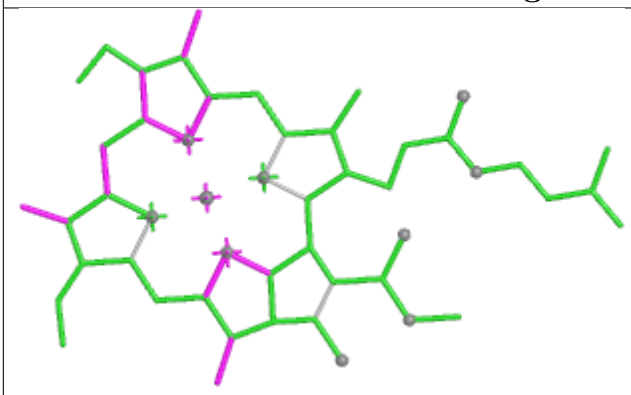


Rings

Ligand CLA A 830



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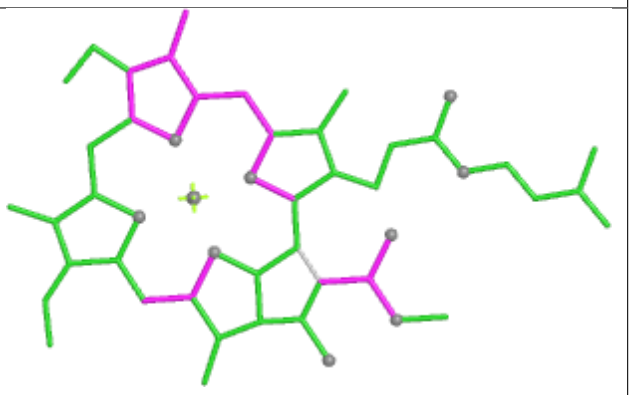

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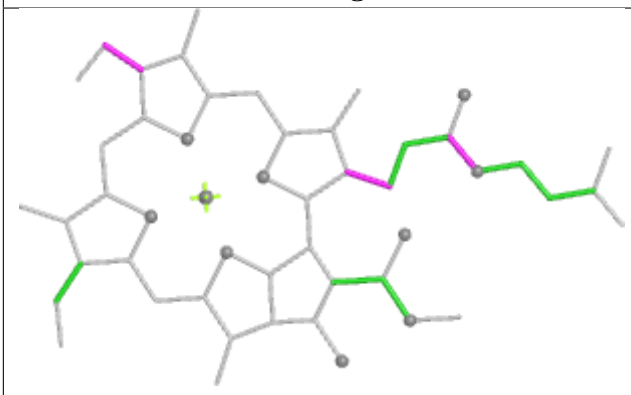

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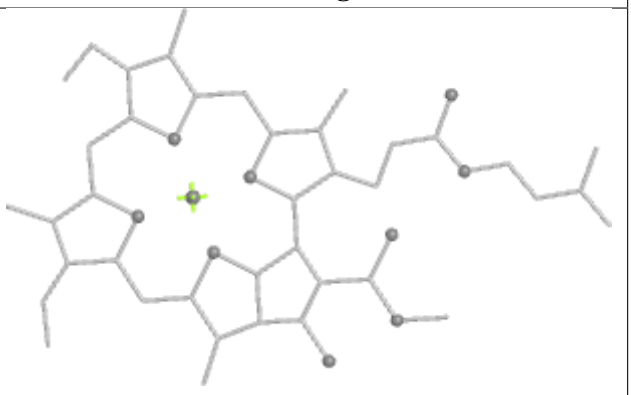
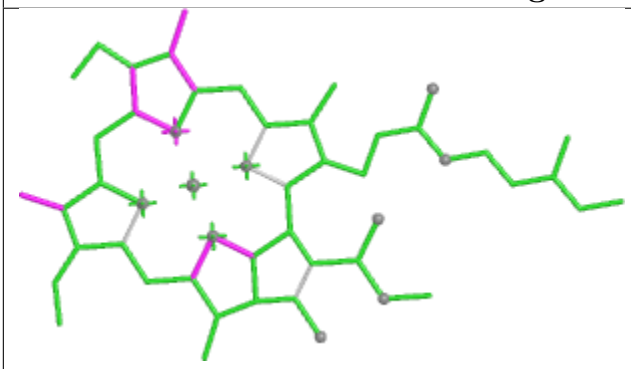


Rings

Ligand CLA g 307



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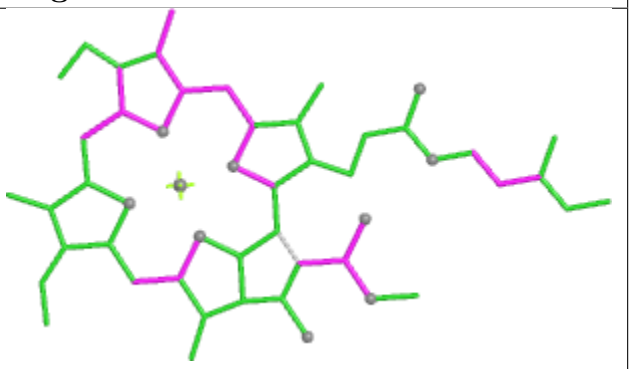

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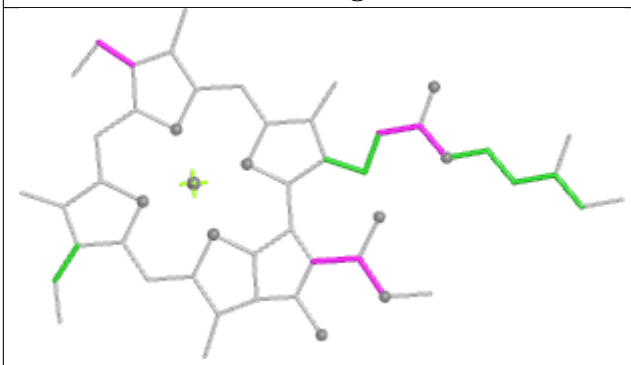

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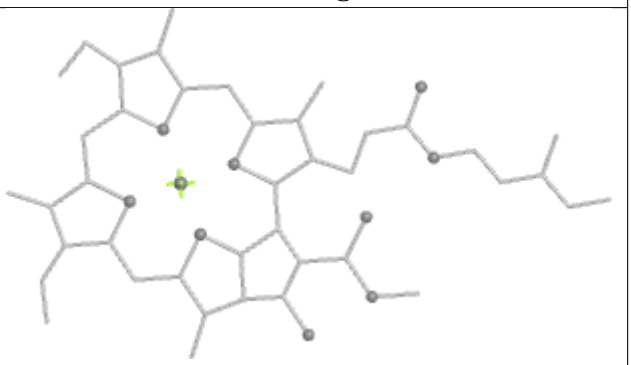
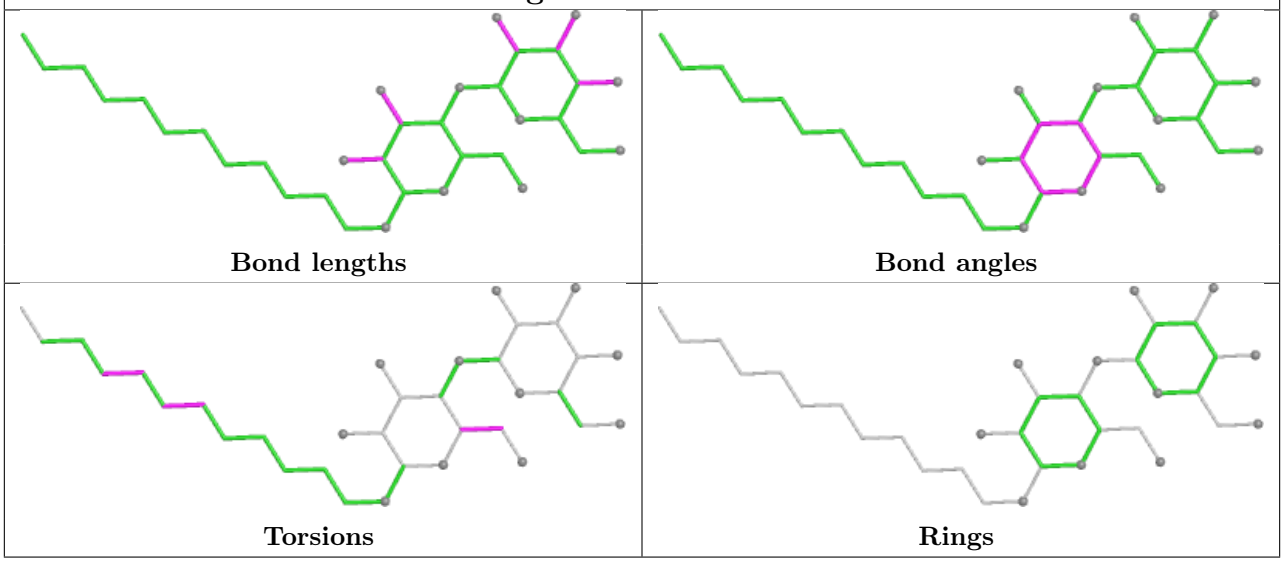
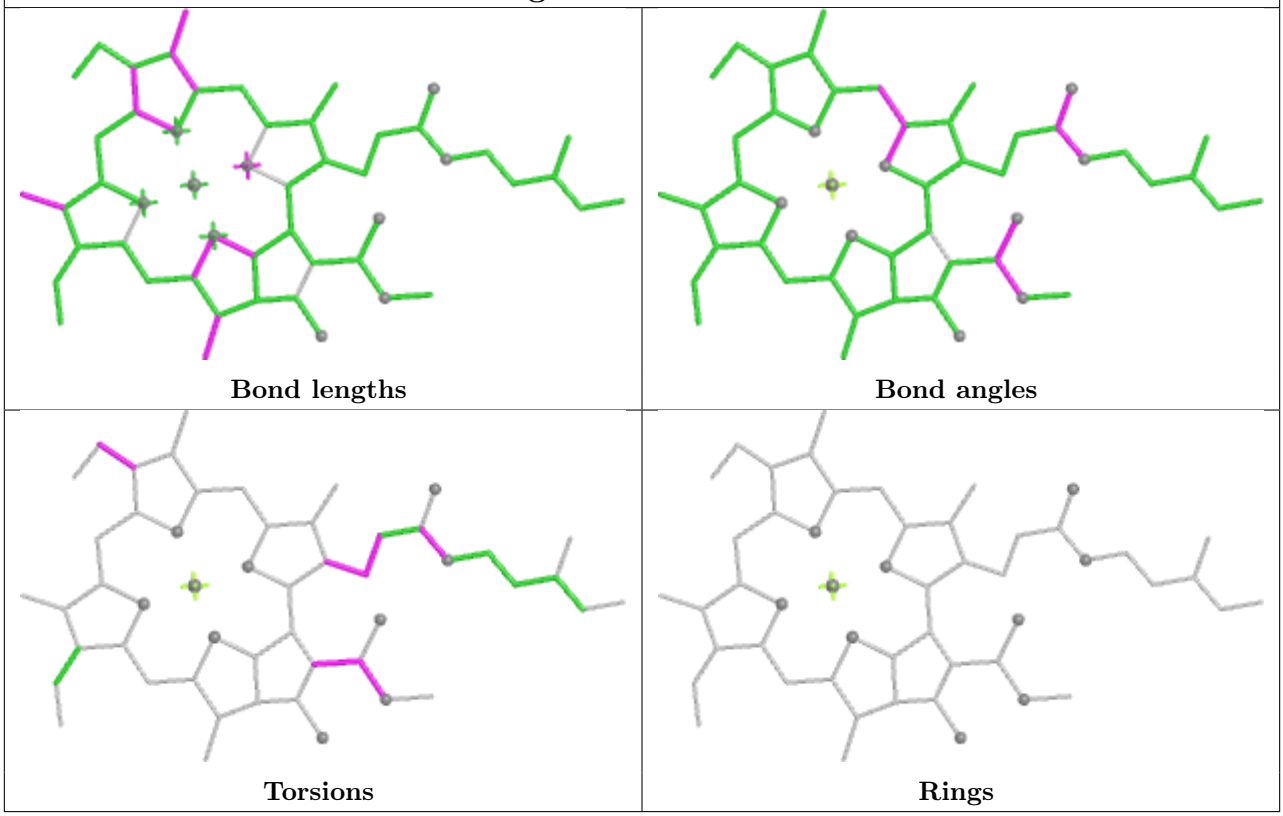


Rings

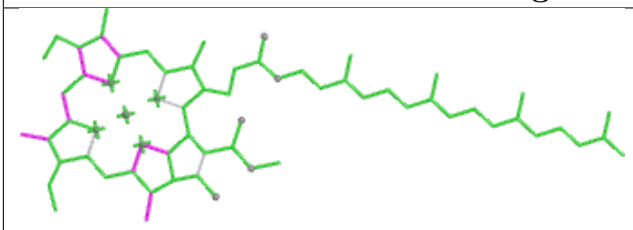
Ligand LMT a 318



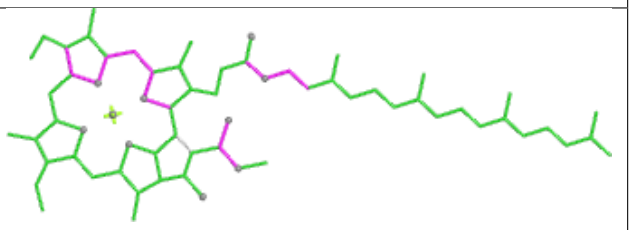
Ligand CLA d 306



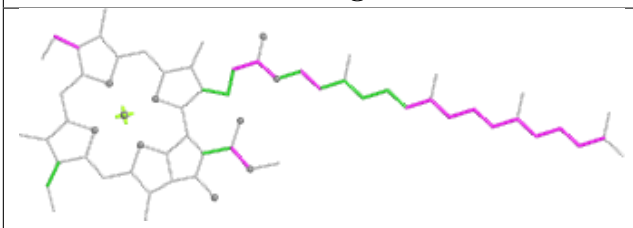
Ligand CLA f 613



Bond lengths



Bond angles



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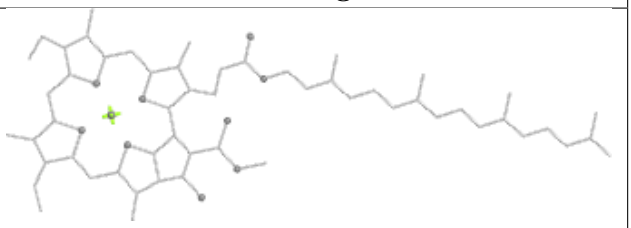
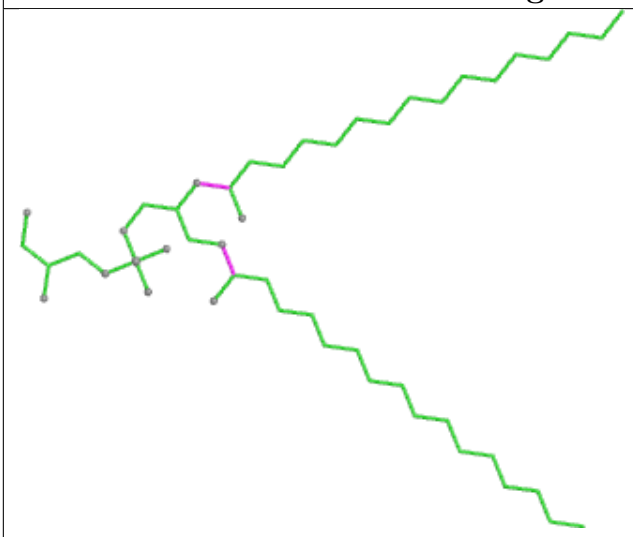


Rings

Ligand LHG g 301



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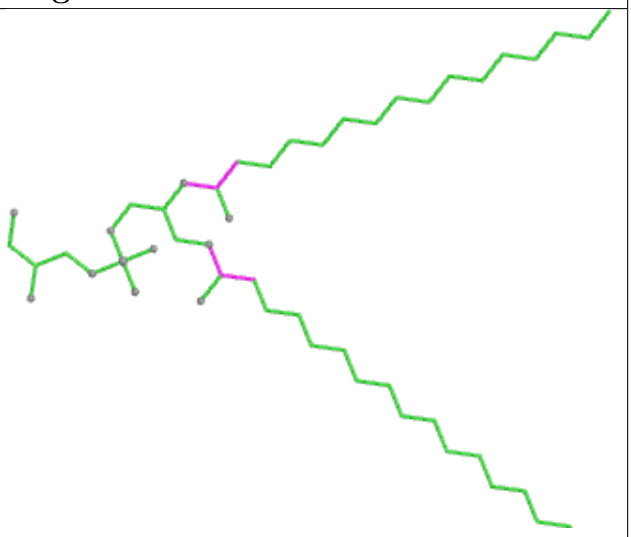
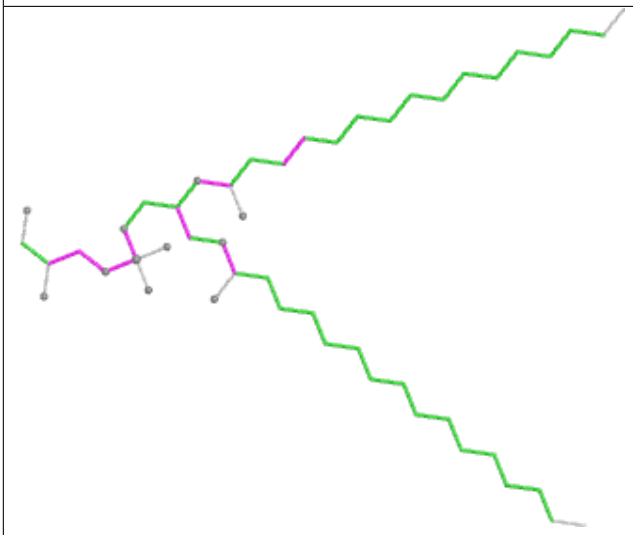


Bond angles



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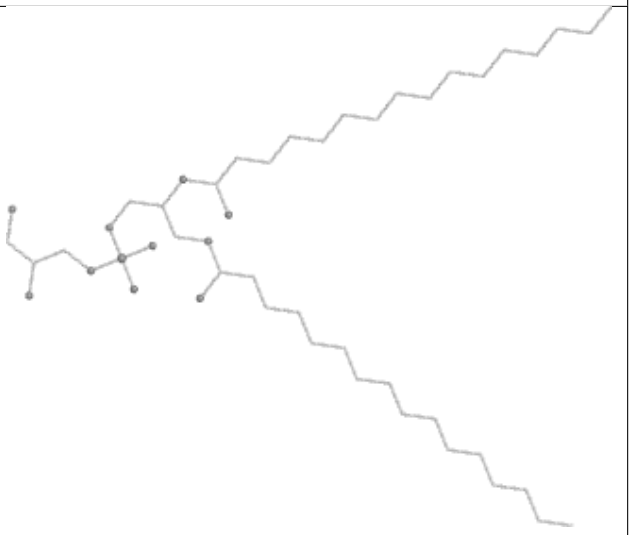
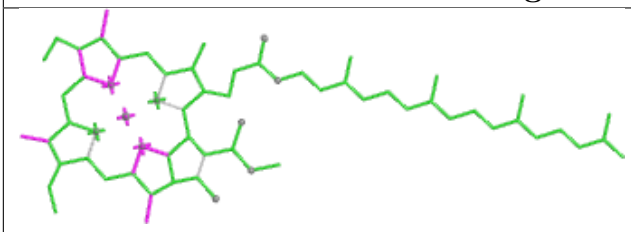
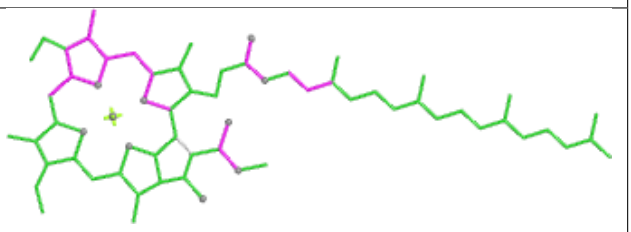
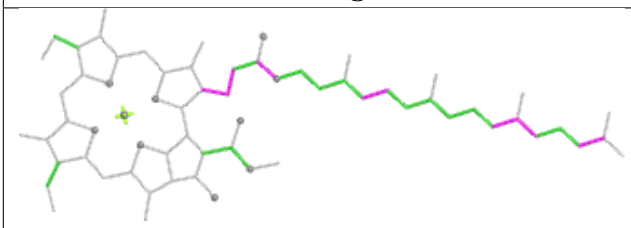
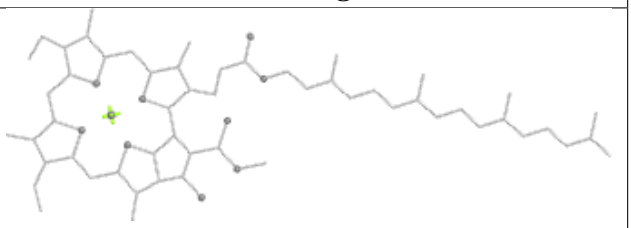


Rings

Ligand CLA B 809	
 Bond lengths	 Bond angles
 Torsions	 Rings

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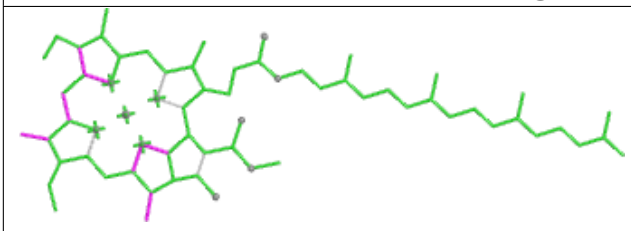
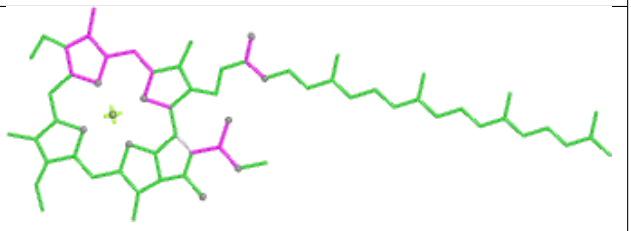
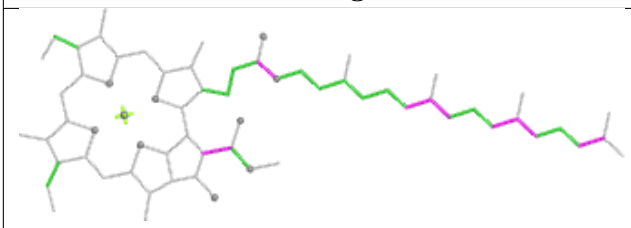
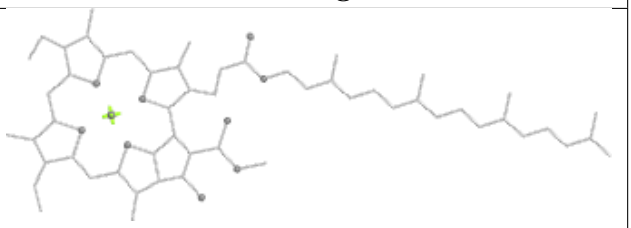
 Bond lengths	 Bond angles
 Torsions	 Rings

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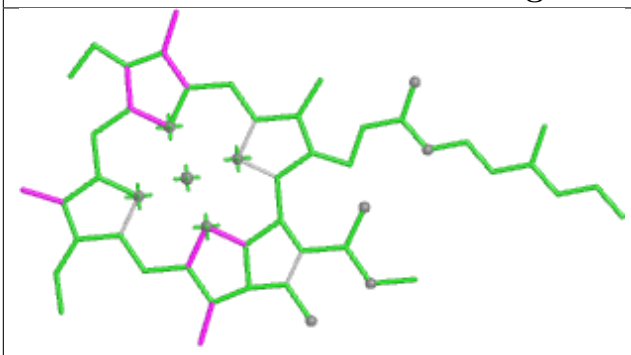
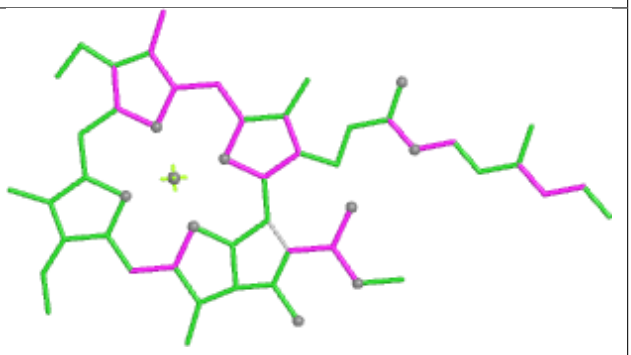
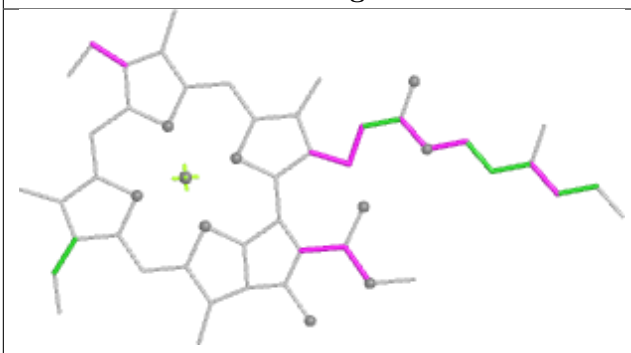
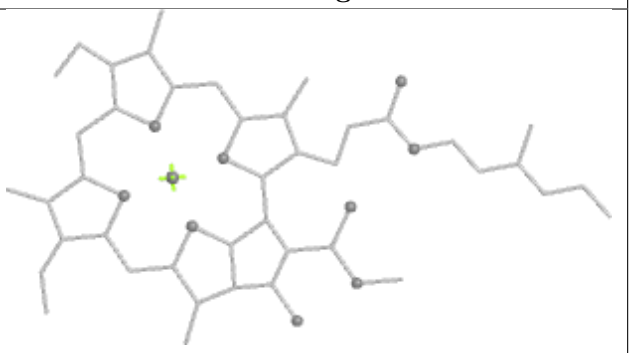
 Bond lengths	 Bond angles
 Torsions	 Rings

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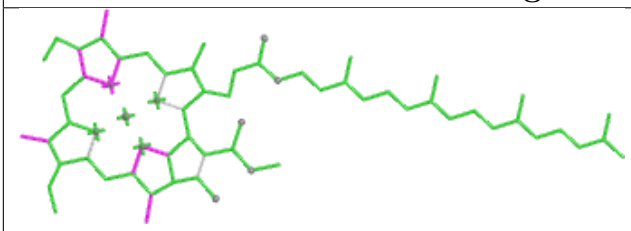
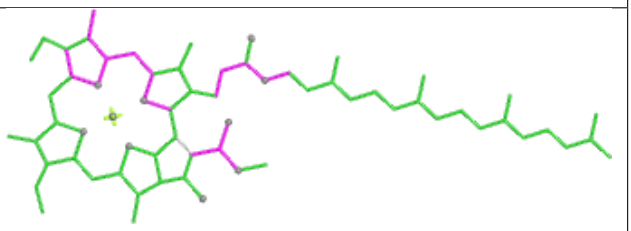
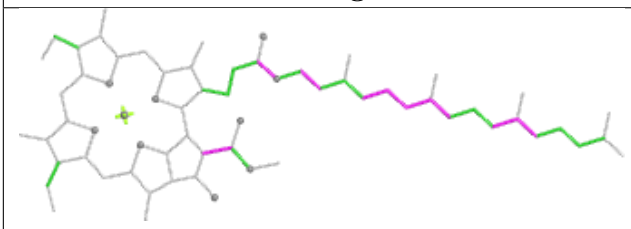
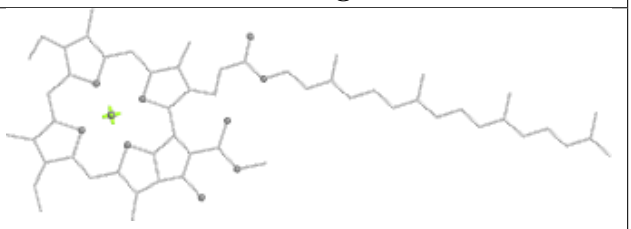
 Bond lengths	 Bond angles
 Torsions	 Rings

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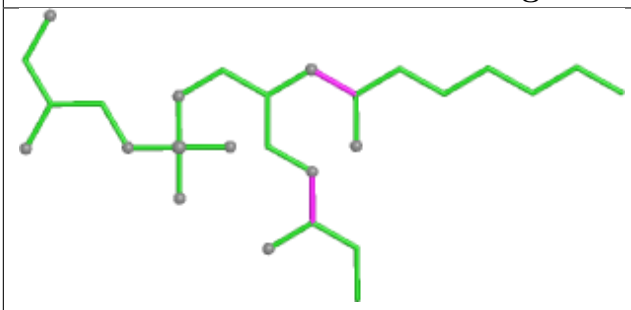
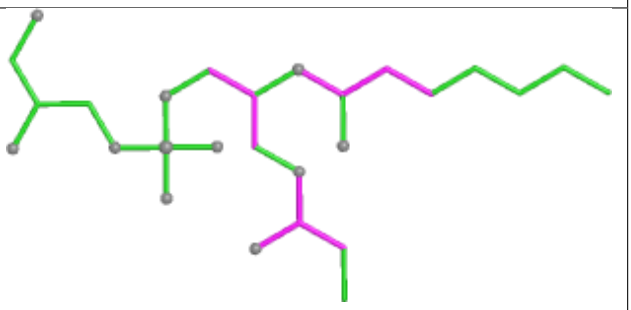
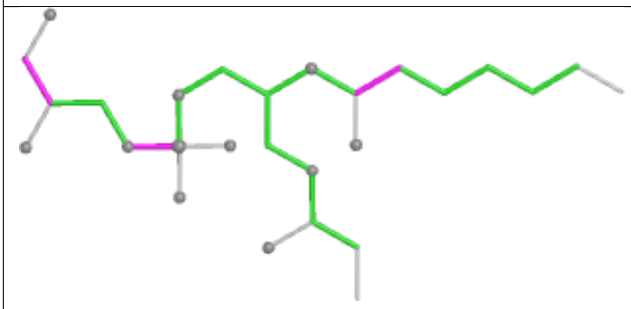
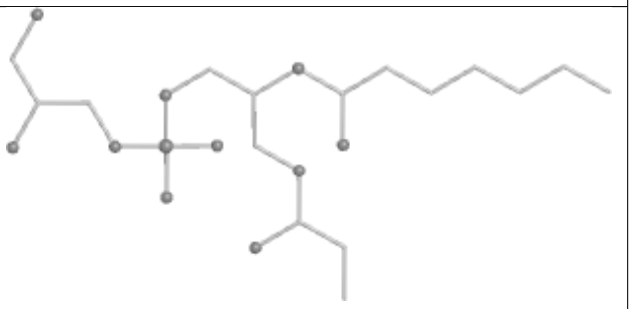
 Bond lengths	 Bond angles
 Torsions	 Rings

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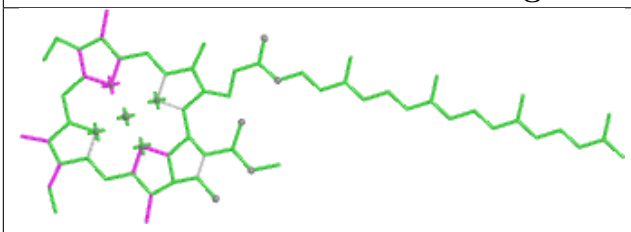
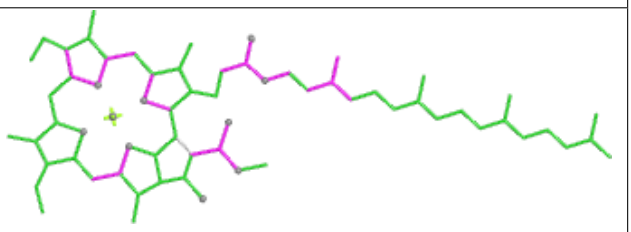
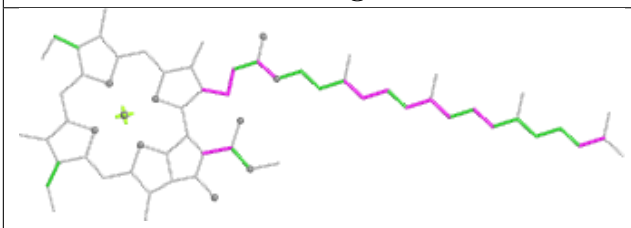
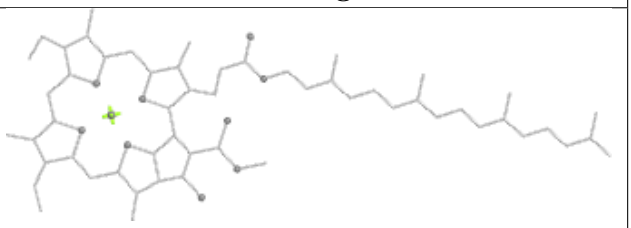
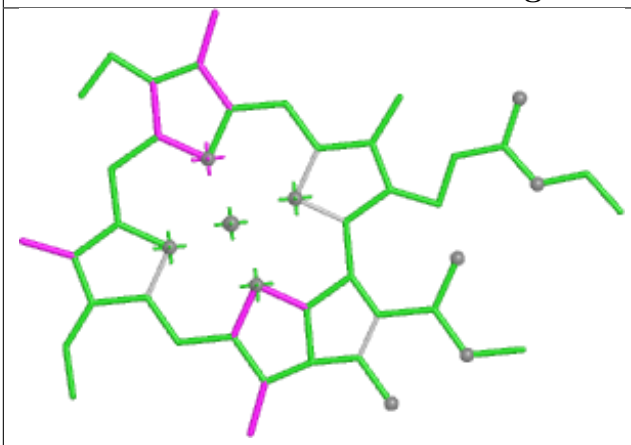
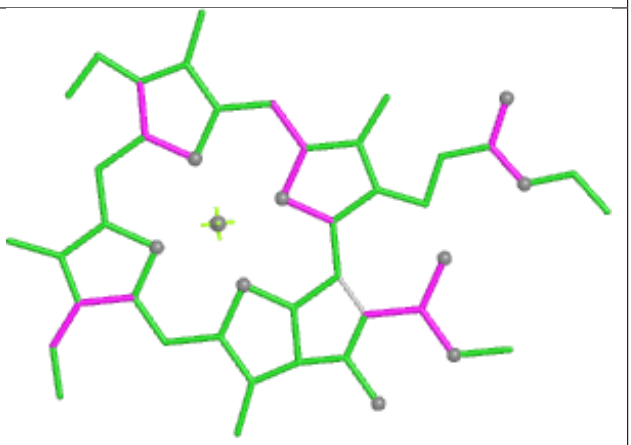
 Bond lengths	 Bond angles
 Torsions	 Rings

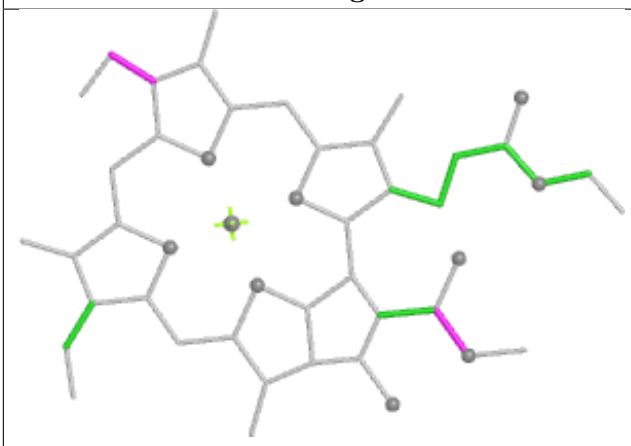
Ligand CLA B 834



Bond lengths



Bond angles



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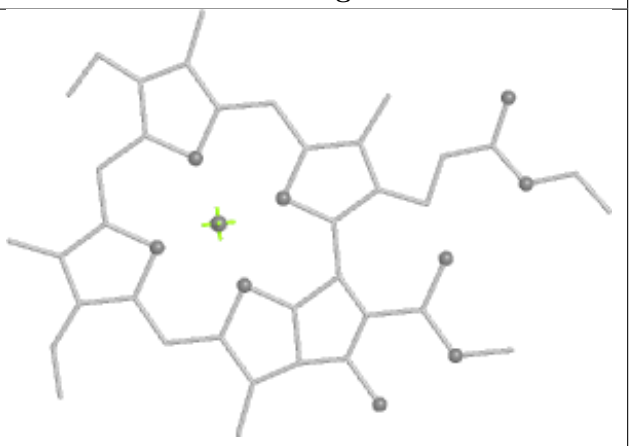
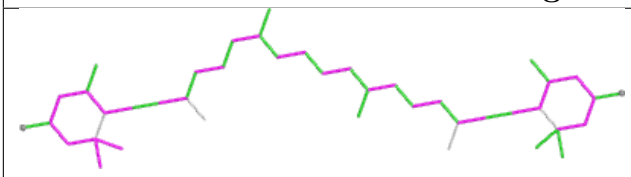


Rings

Ligand II0 a 313



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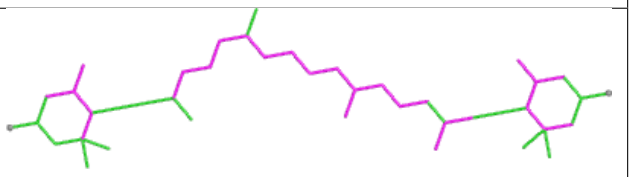

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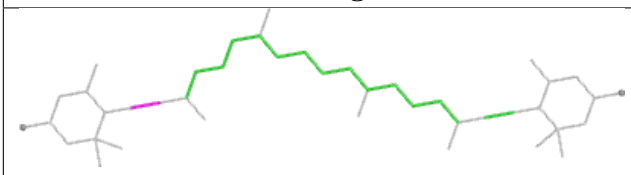

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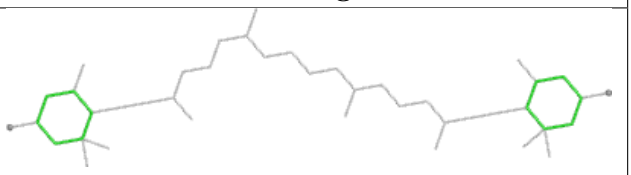
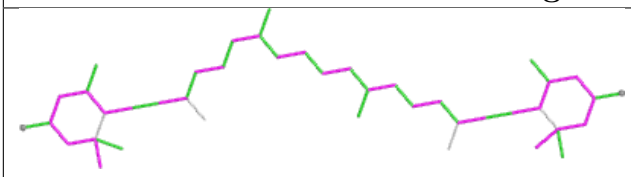
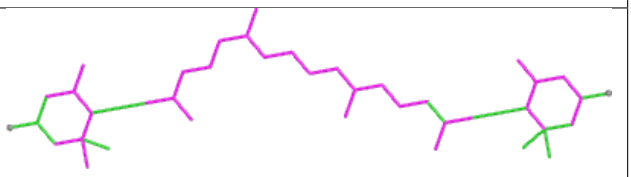
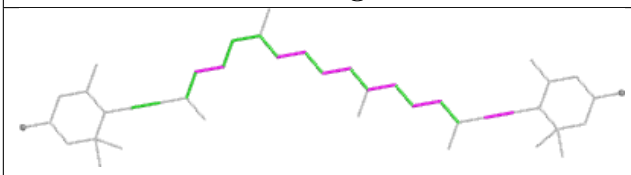
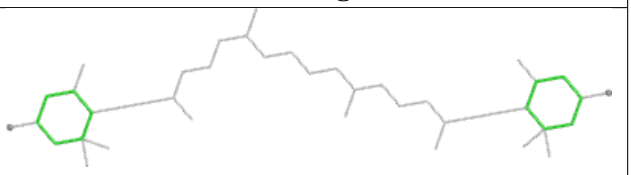
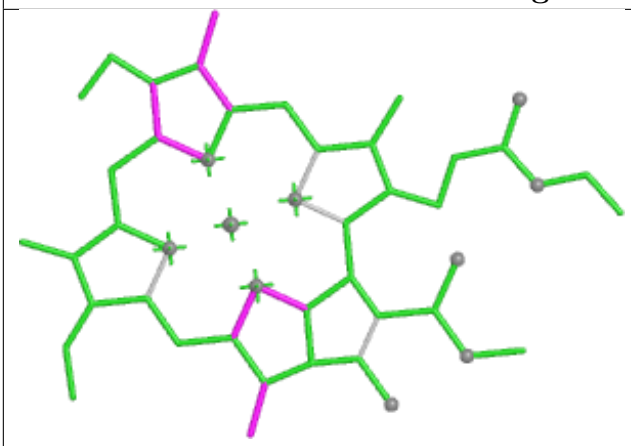
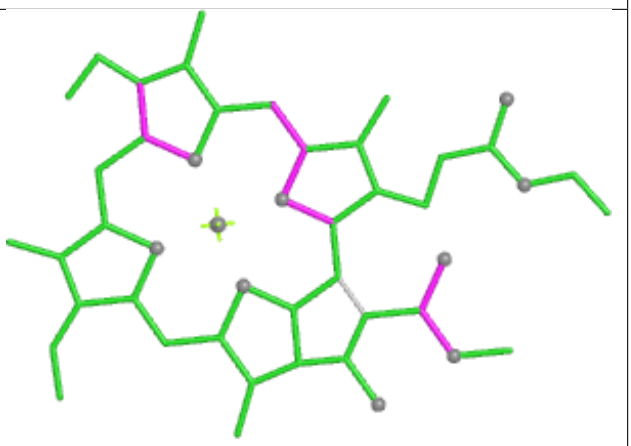
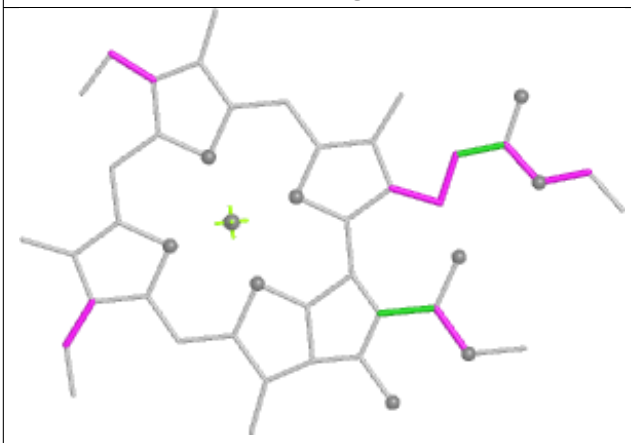
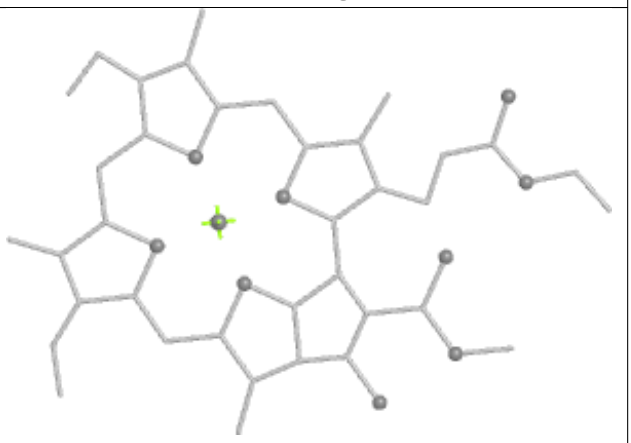
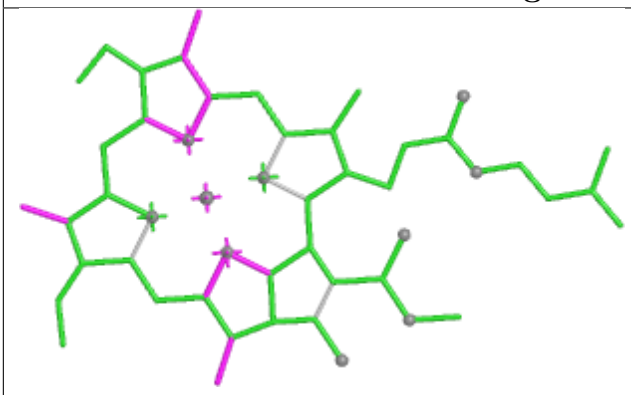
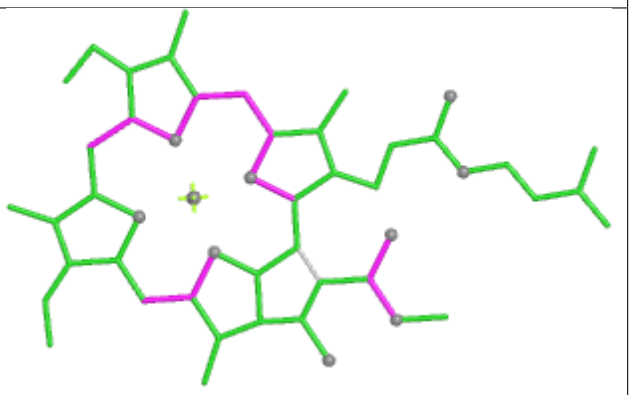
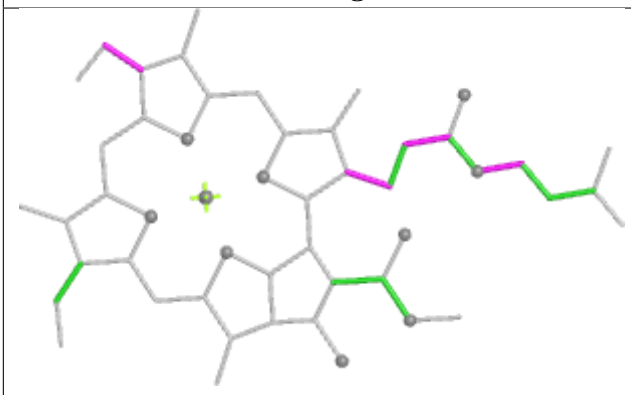
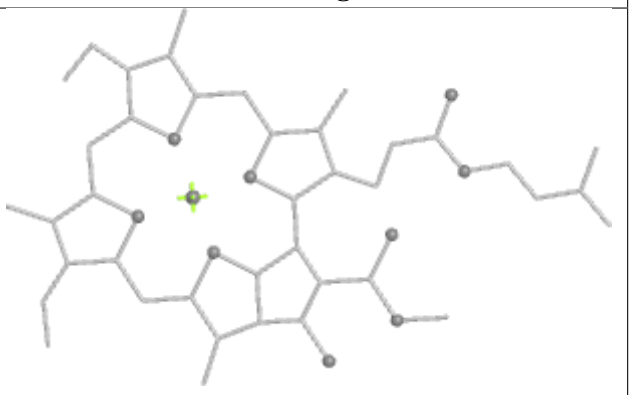


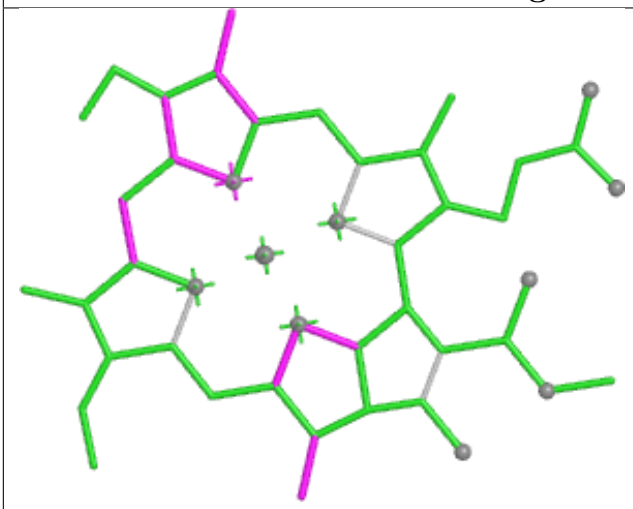
Rings

Ligand II0 a 314	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA f 601	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA A 833	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA e 601



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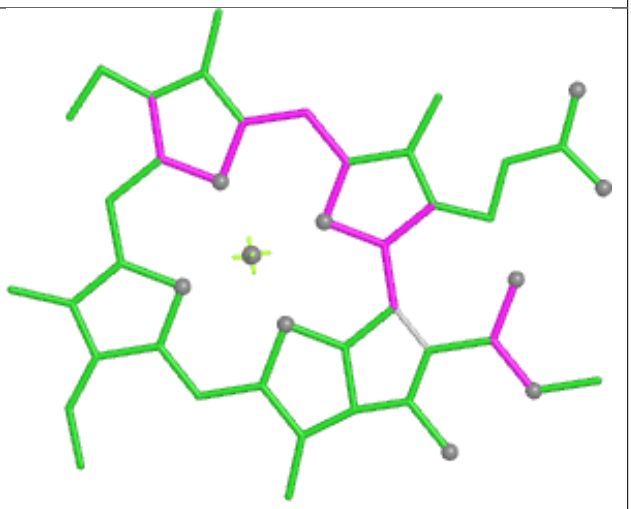

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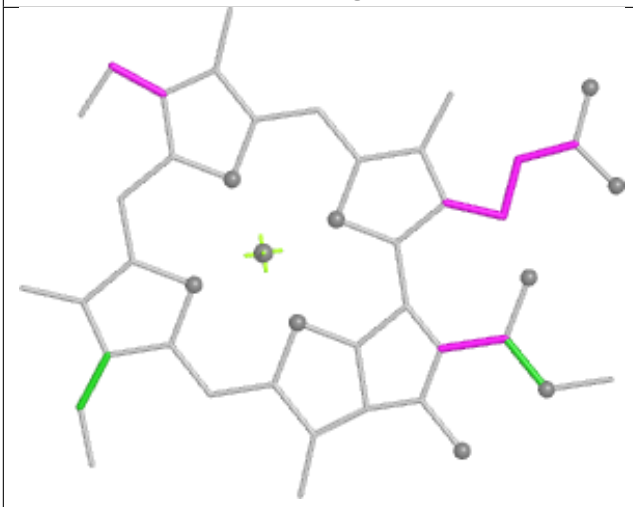
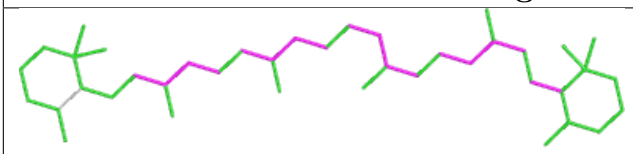


Torsions

Rings

Ligand WVN B 847



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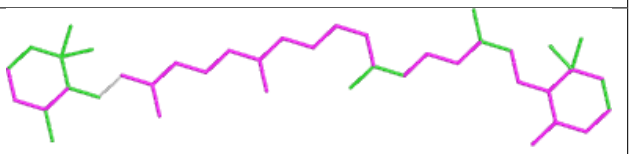

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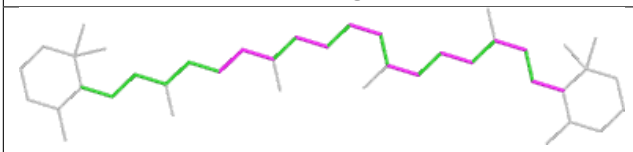

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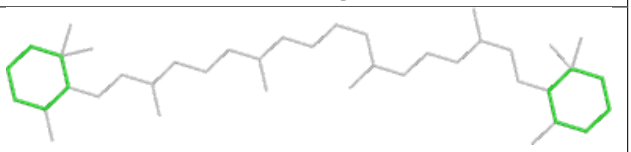
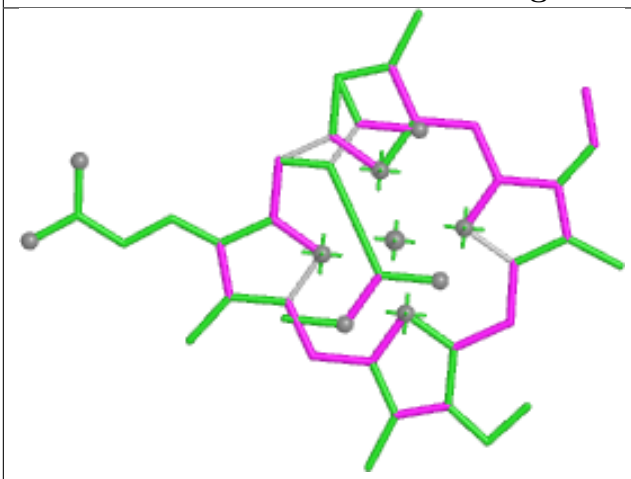


Rings

Ligand KC2 g 313



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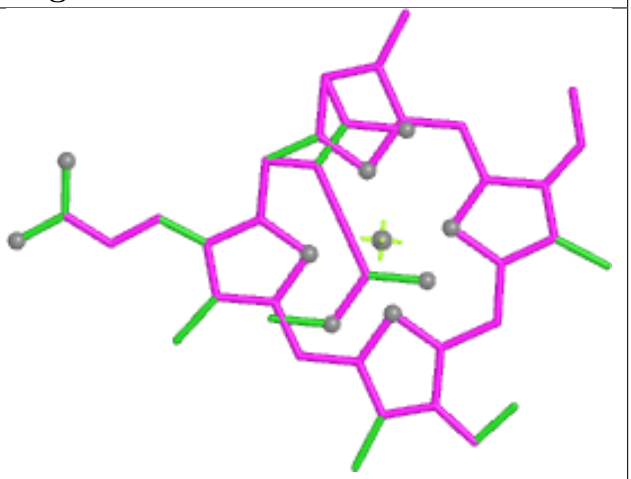

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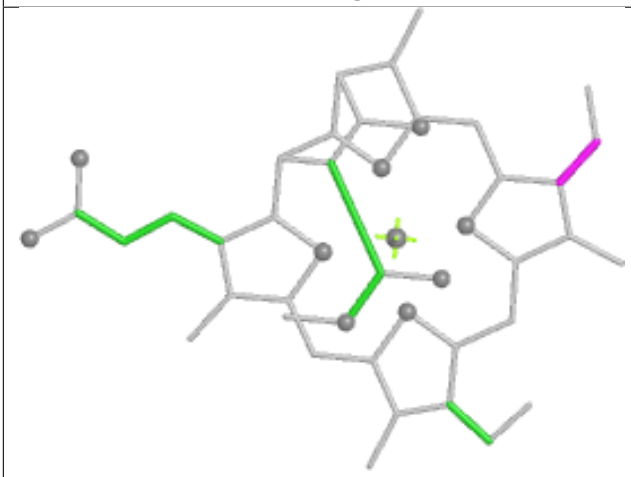

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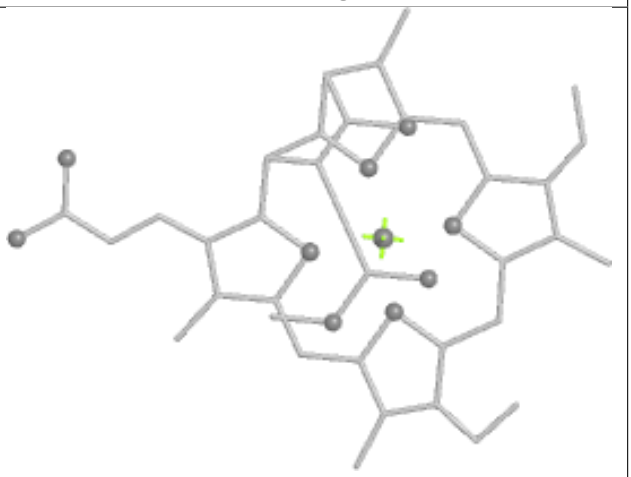
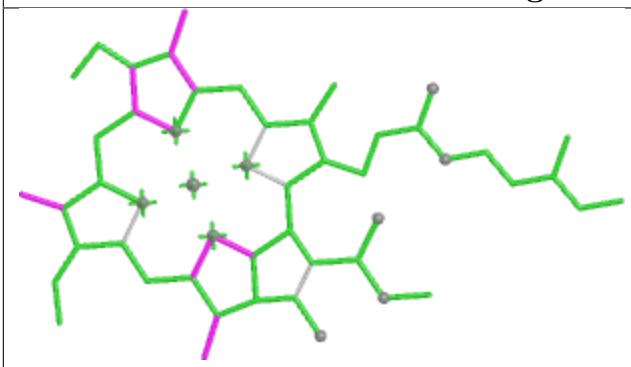


Rings

Ligand CLA L 207



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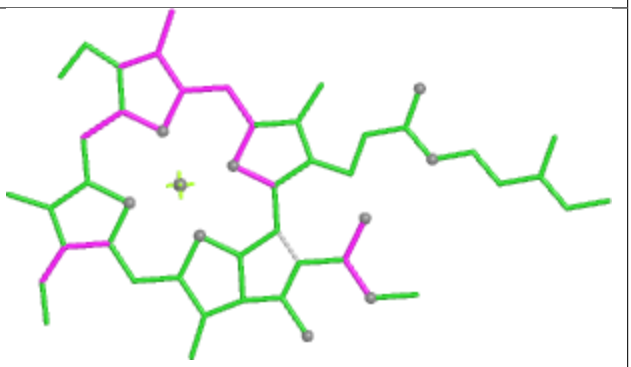

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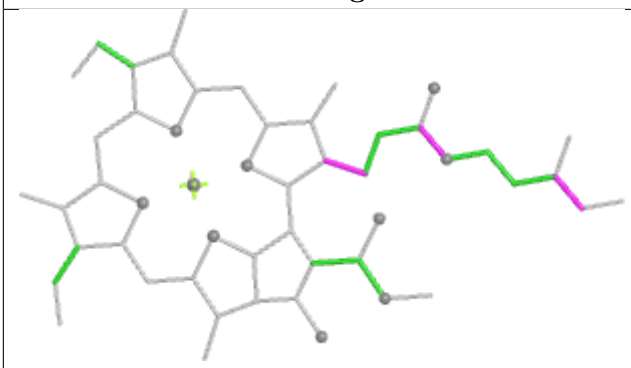

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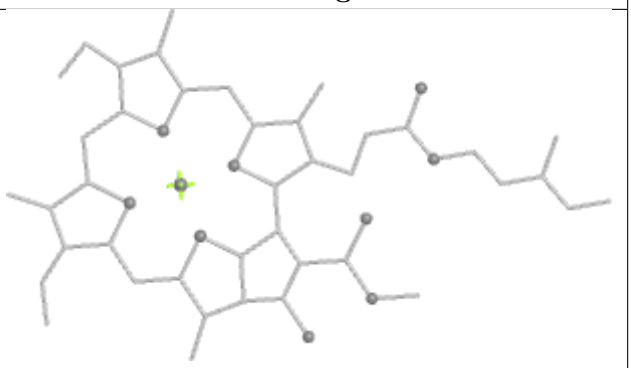
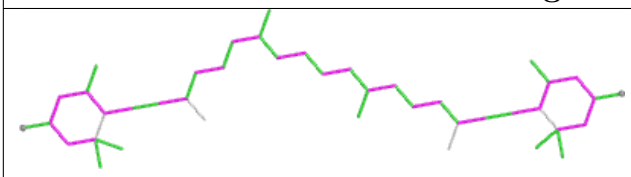


Rings

Ligand II0 e 614



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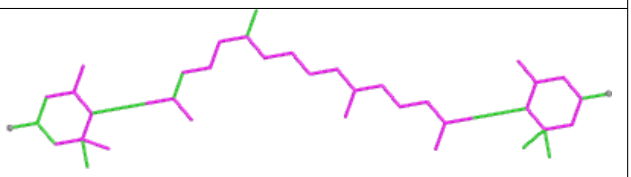
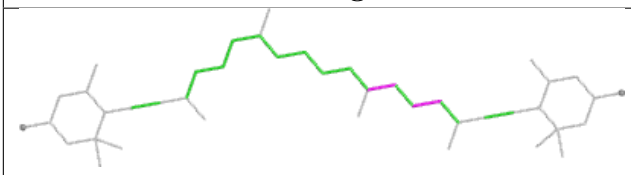


Bond angles



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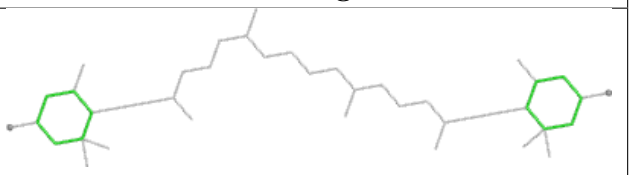
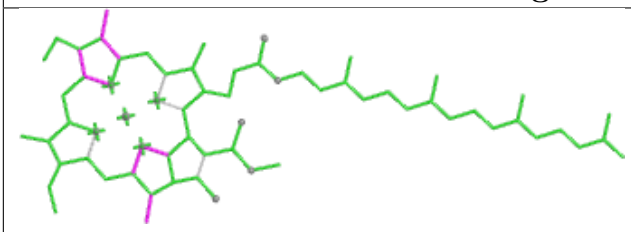
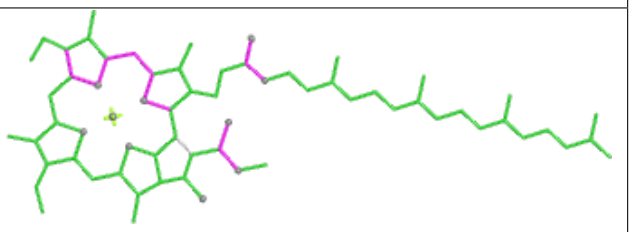
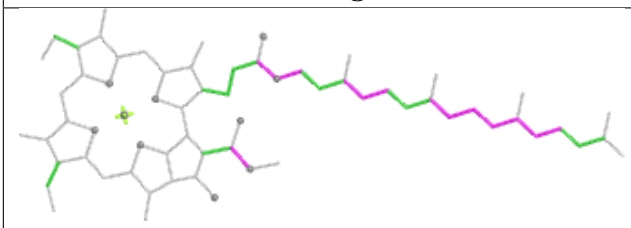
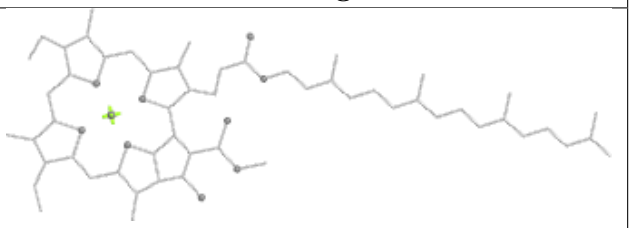
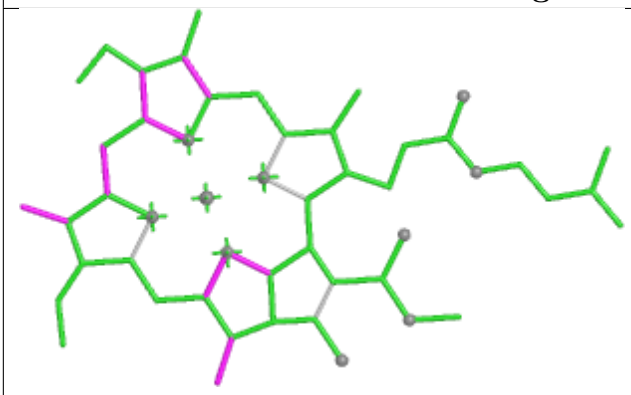
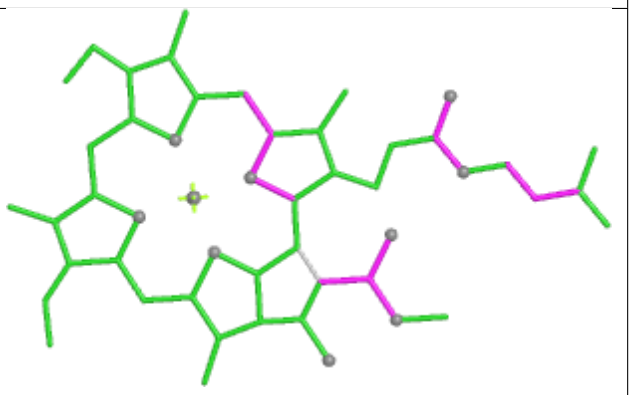
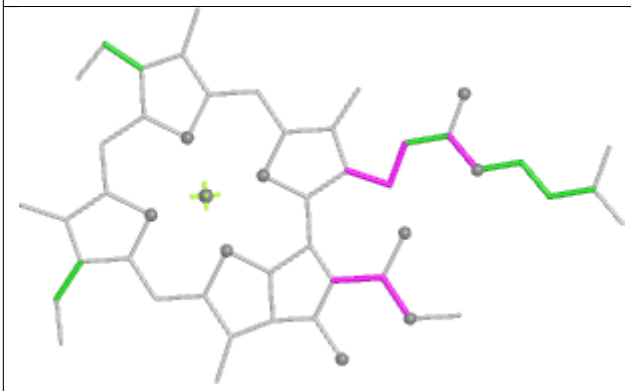
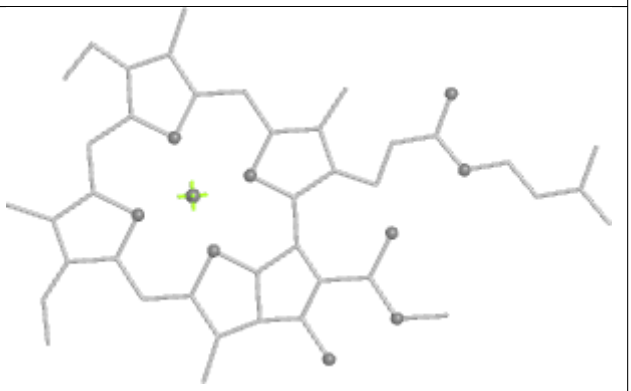
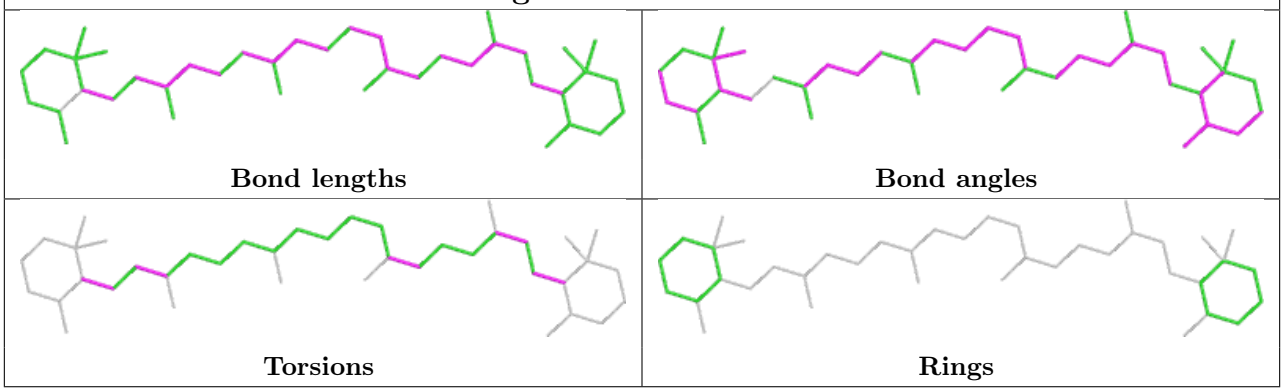


Rings

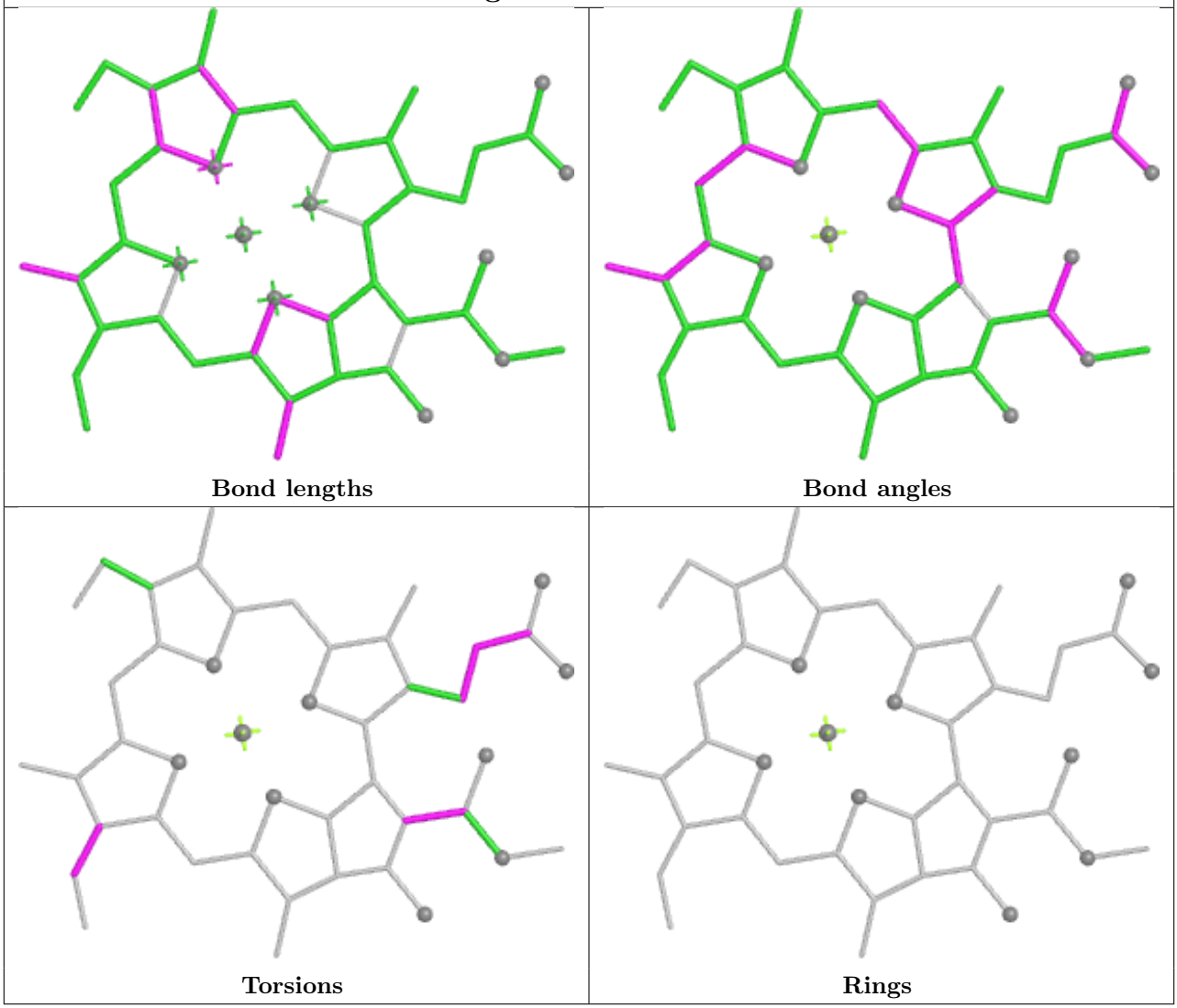
Ligand CLA f 610	
 Bond lengths	 Bond angles
 Torsions	 Rings

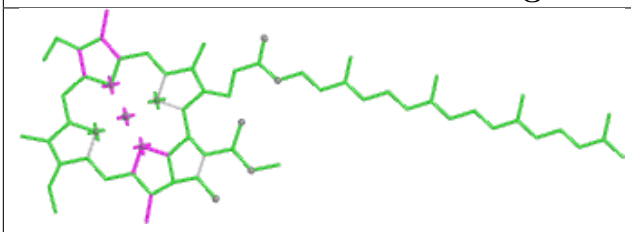
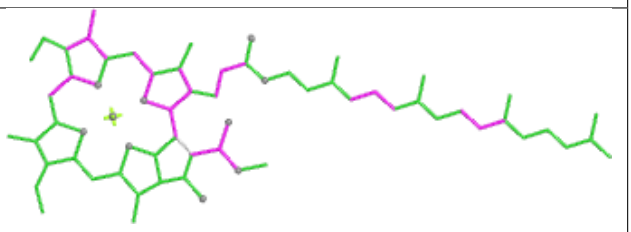
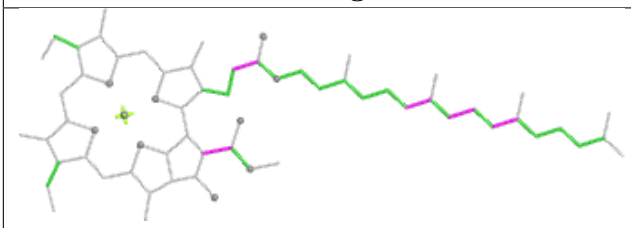
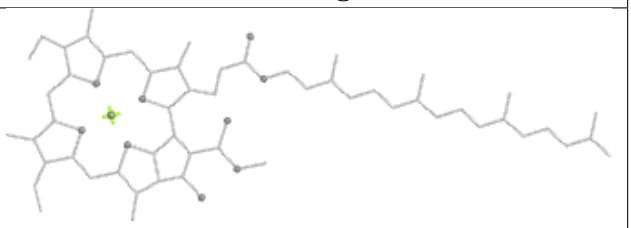
Ligand CLA i 602	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand WVN M 101



Ligand CLA k 605



Ligand CLA A 836	
 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.

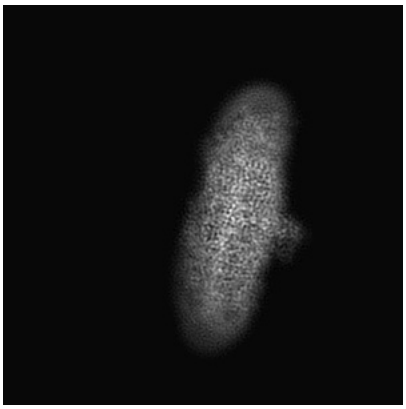
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-37660. These allow visual inspection of the internal detail of the map and identification of artifacts.

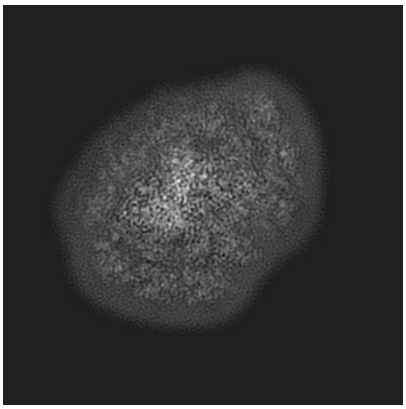
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections (i)

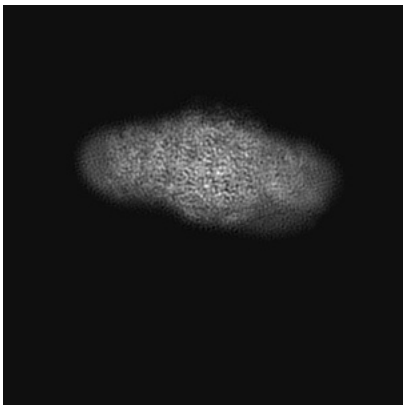
6.1.1 Primary map



X

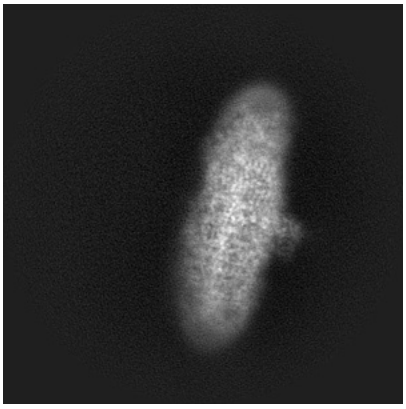


Y

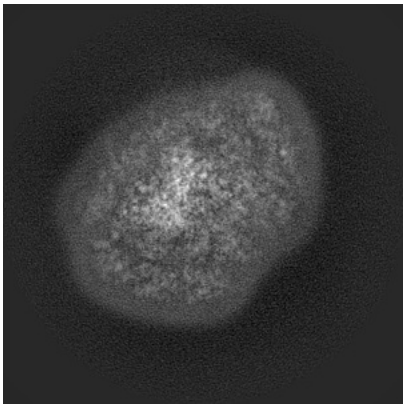


Z

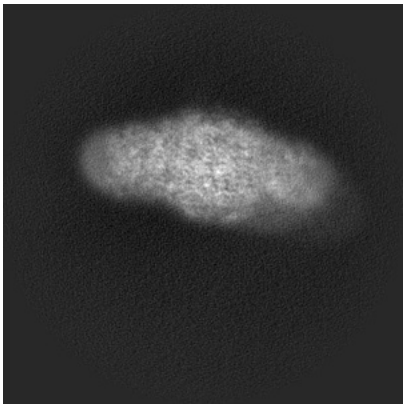
6.1.2 Raw map



X



Y



Z

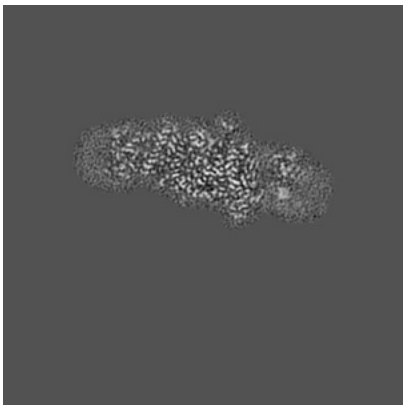
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

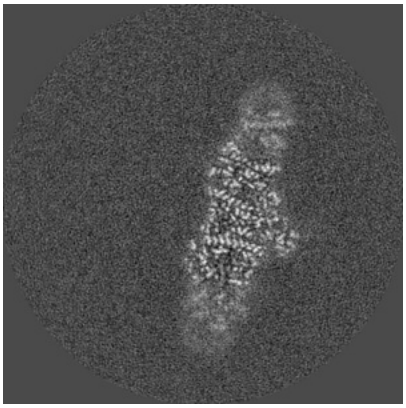
6.2.1 Primary map

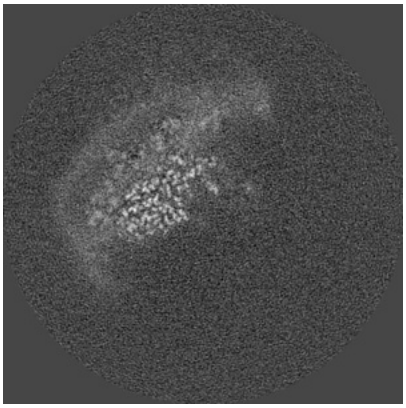
X Index: 160

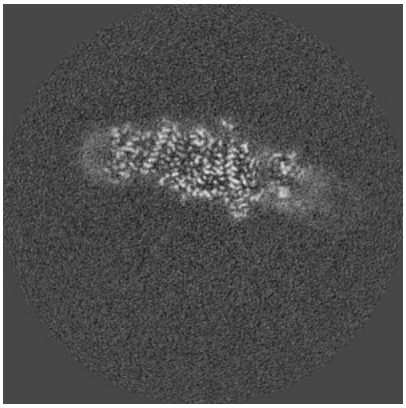
Y Index: 160


Z Index: 160

6.2.2 Raw map


X Index: 160

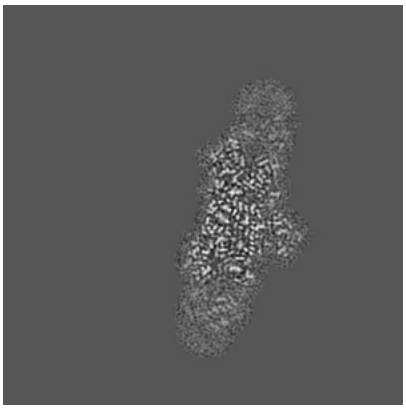

Y Index: 160


Z Index: 160

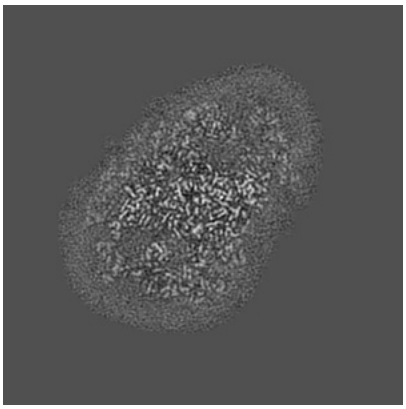
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

6.3.1 Primary map



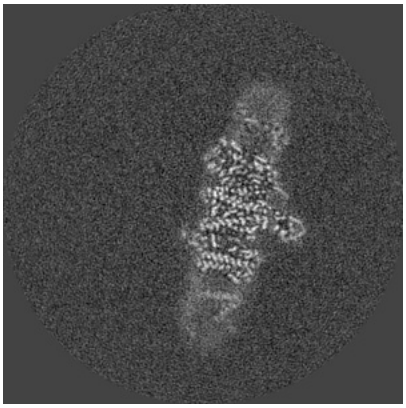
X Index: 164



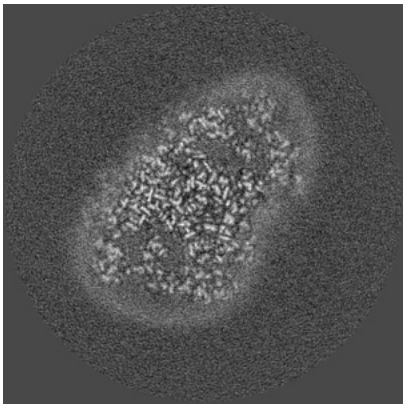
Y Index: 185

Z Index: 148

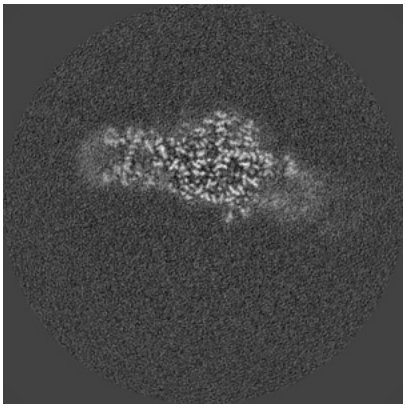
6.3.2 Raw map



X Index: 173



Y Index: 189

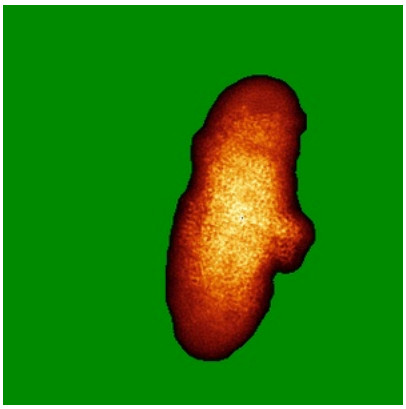


Z Index: 148

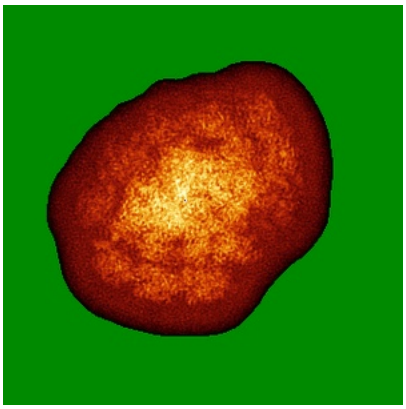
The images above show the largest variance slices of the map in three orthogonal directions.

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

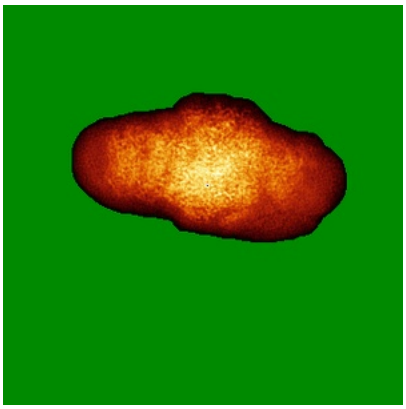
6.4.1 Primary map



X

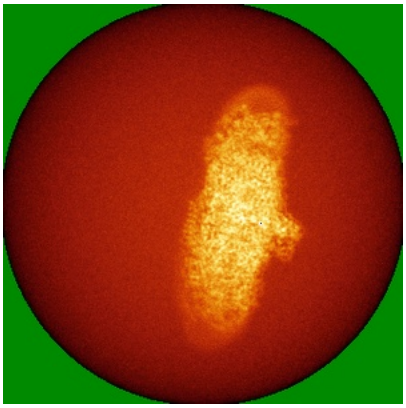


Y

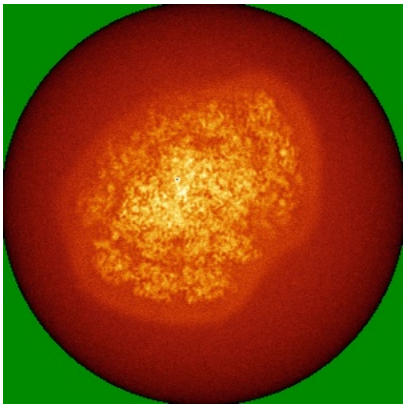


Z

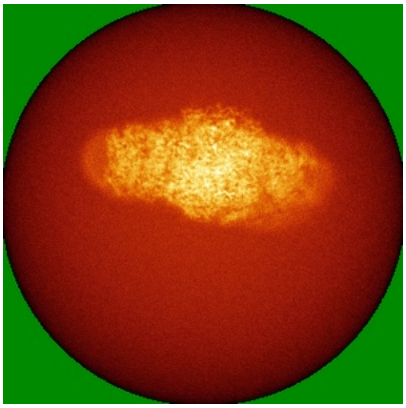
6.4.2 Raw map



X



Y

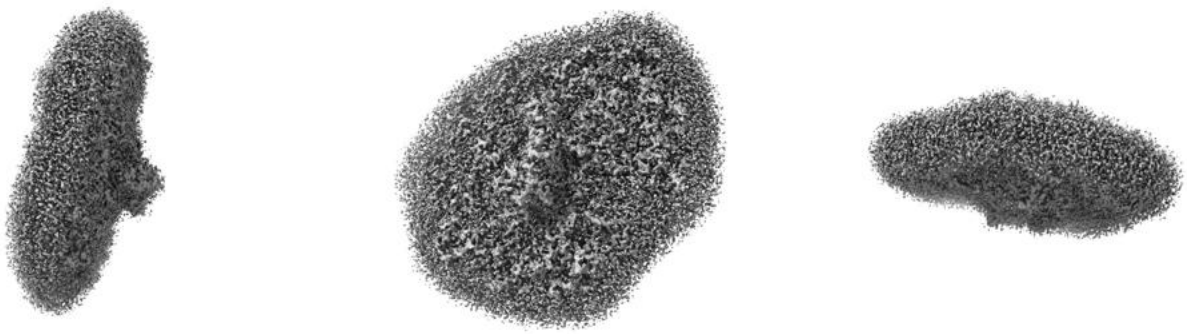


Z

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)

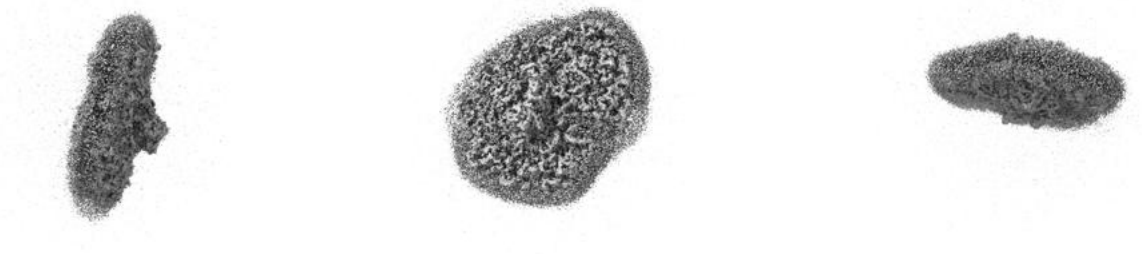
6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.018. 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.

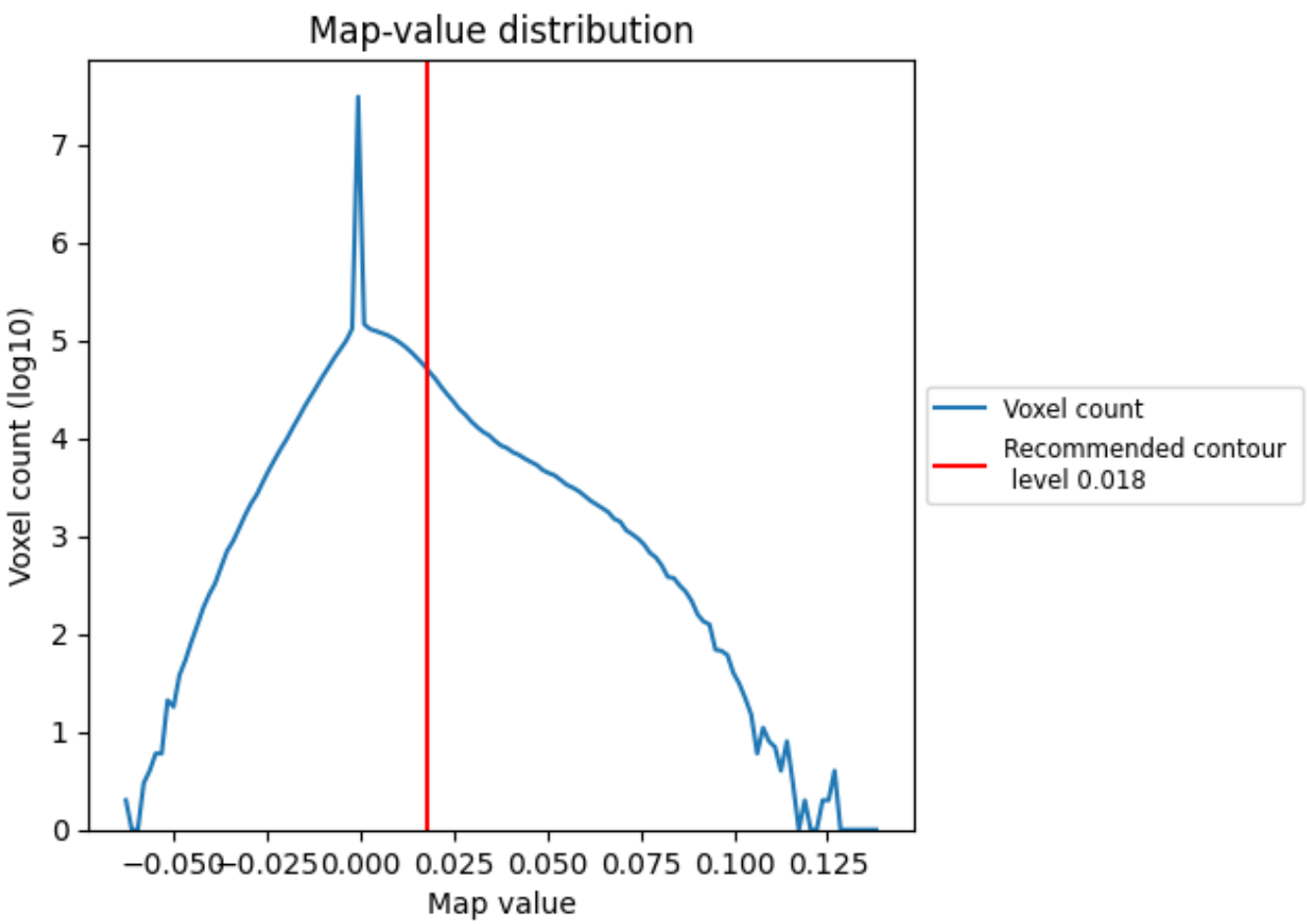
6.6 Mask visualisation (i)

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

7 Map analysis (i)

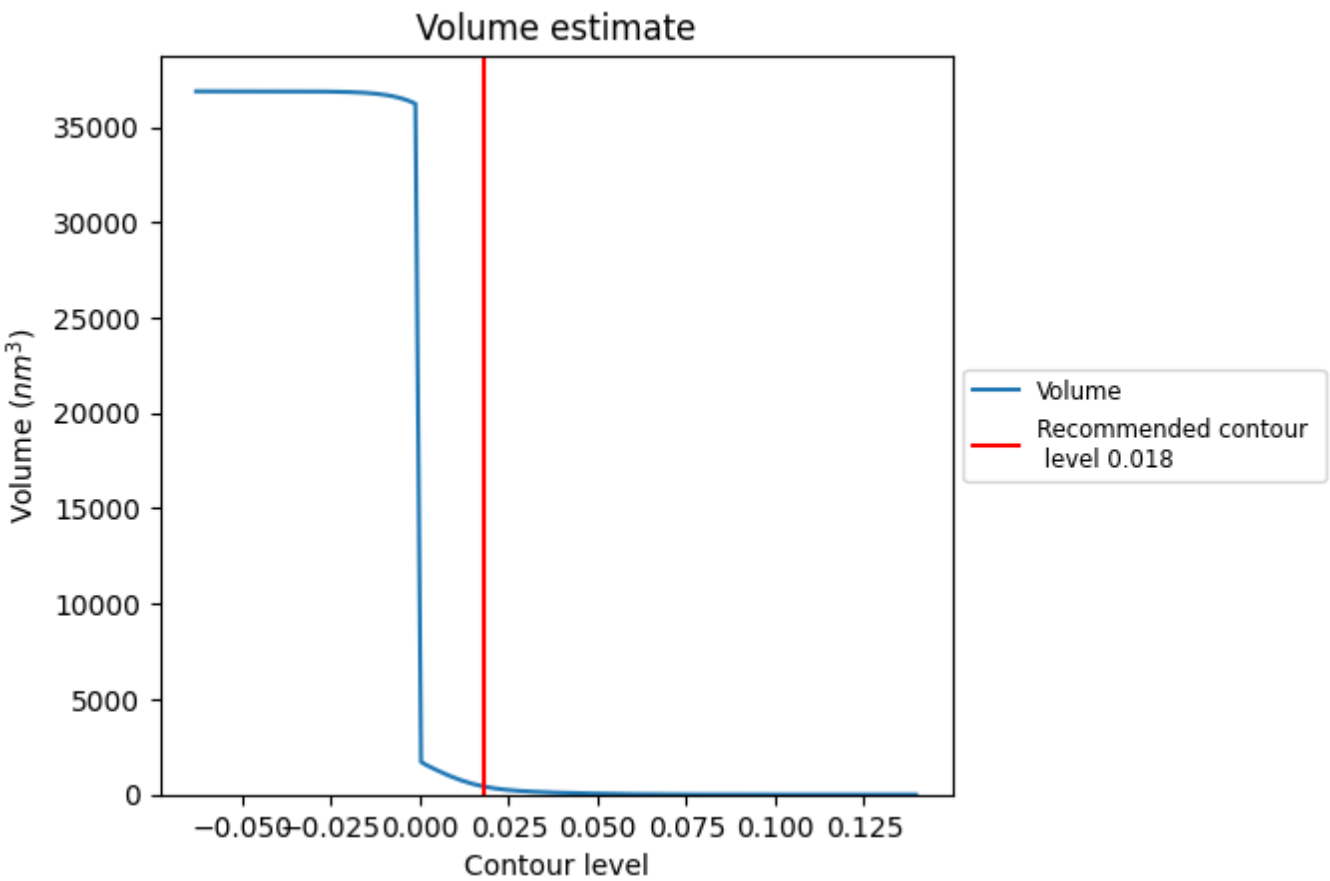
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)



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.

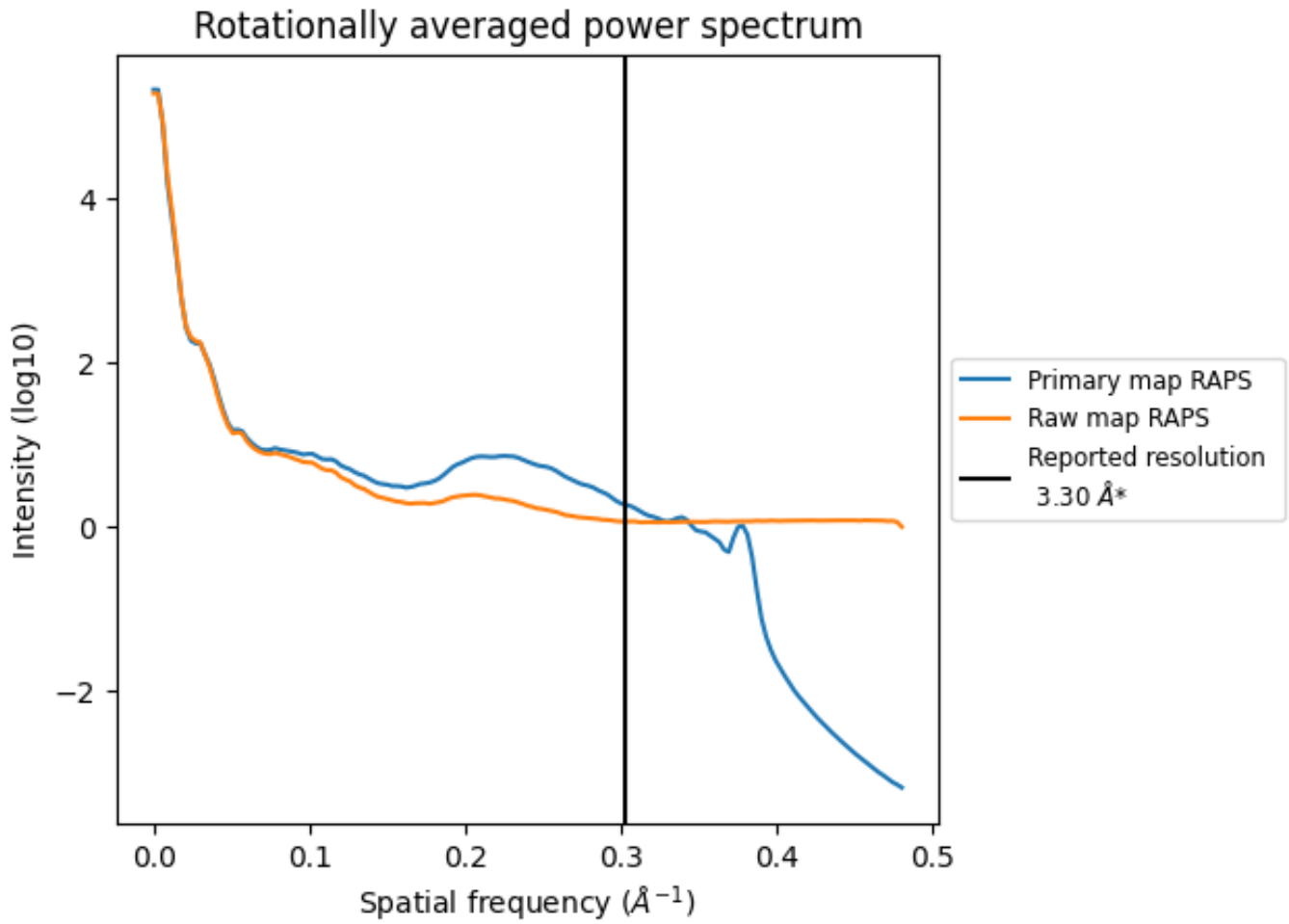
7.2 Volume estimate (i)



The volume at the recommended contour level is 425 nm^3; this corresponds to an approximate mass of 384 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)

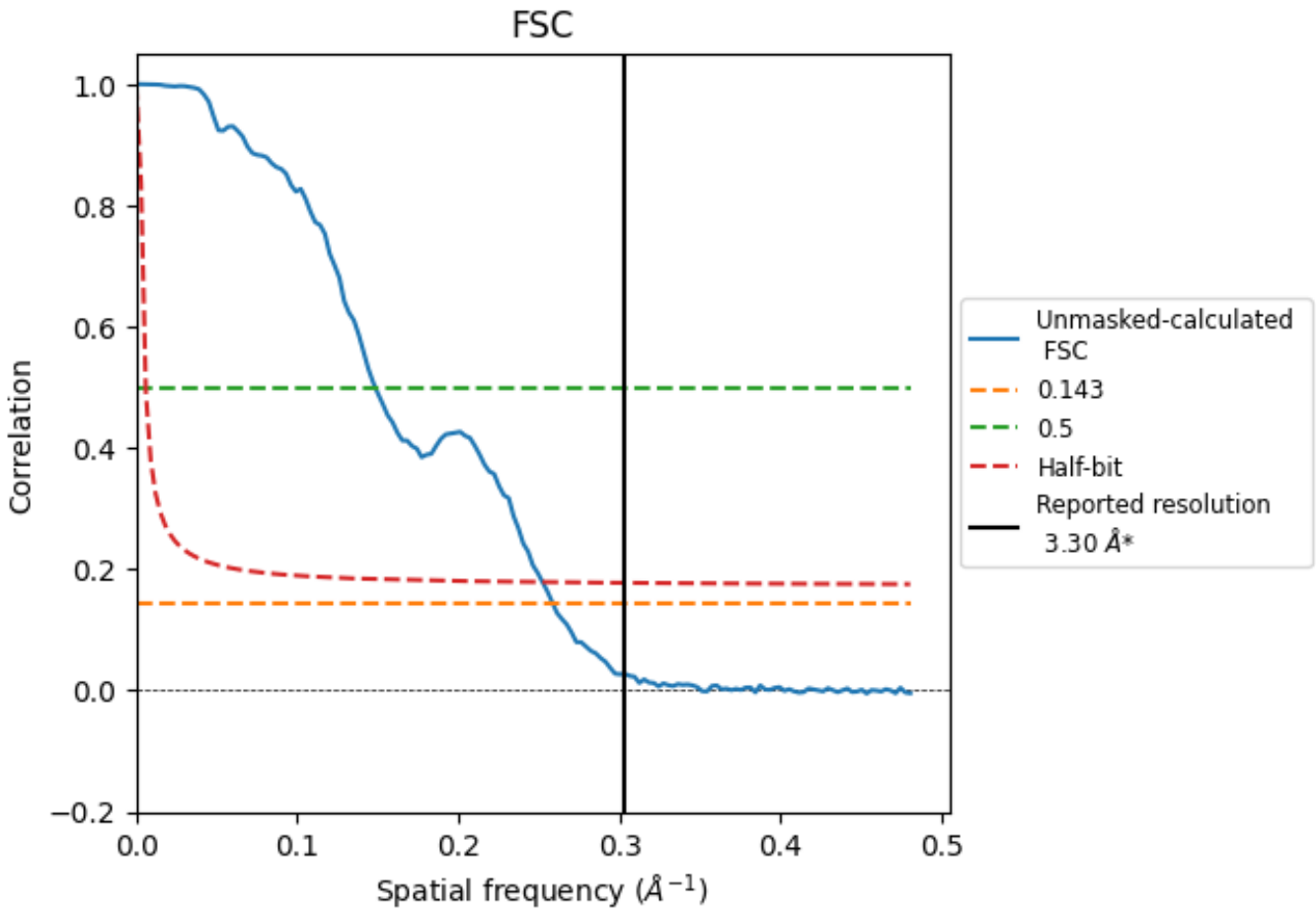


*Reported resolution corresponds to spatial frequency of 0.303 Å^{-1}

8 Fourier-Shell correlation (i)

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 (i)



*Reported resolution corresponds to spatial frequency of 0.303 Å^{-1}

8.2 Resolution estimates (i)

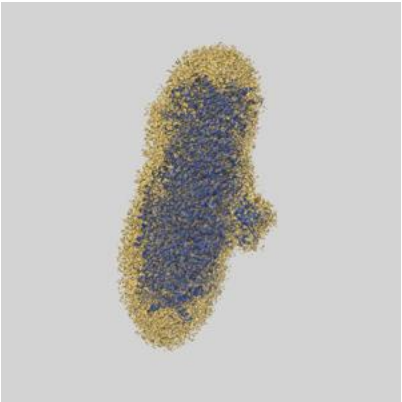
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.30	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.86	6.73	3.96

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.86 differs from the reported value 3.3 by more than 10 %

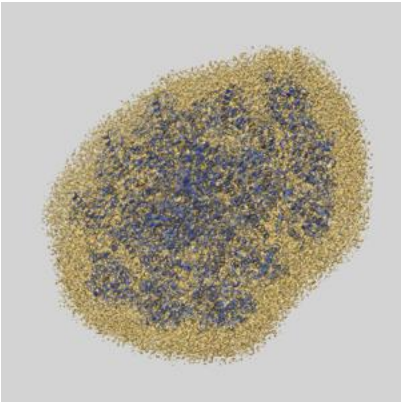
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-37660 and PDB model 8WMW. Per-residue inclusion information can be found in section 3 on page 31.

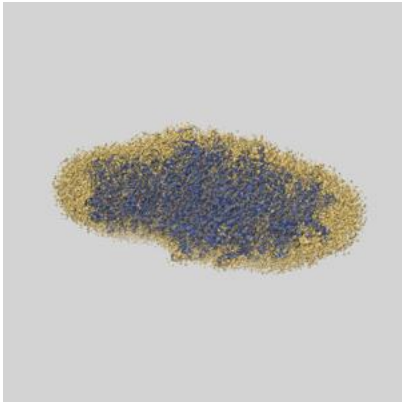
9.1 Map-model overlay (i)



X



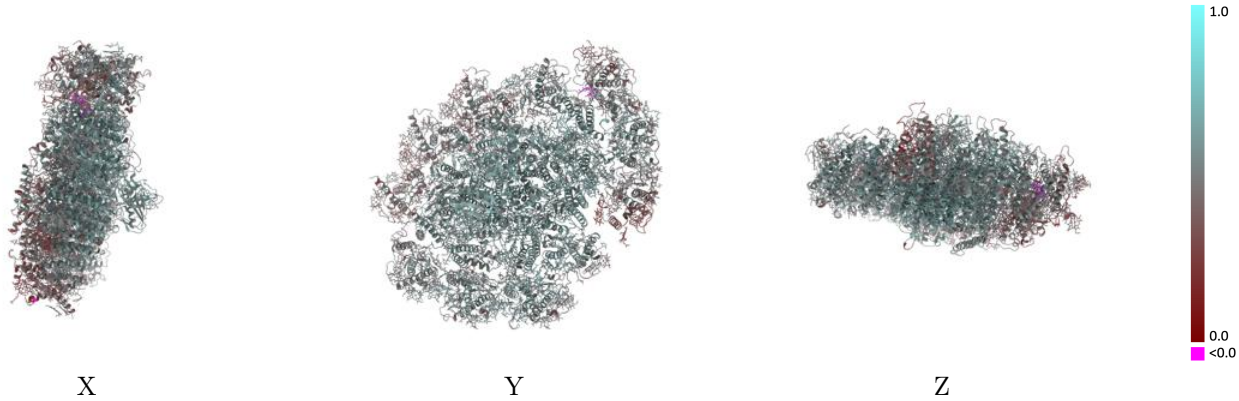
Y



Z

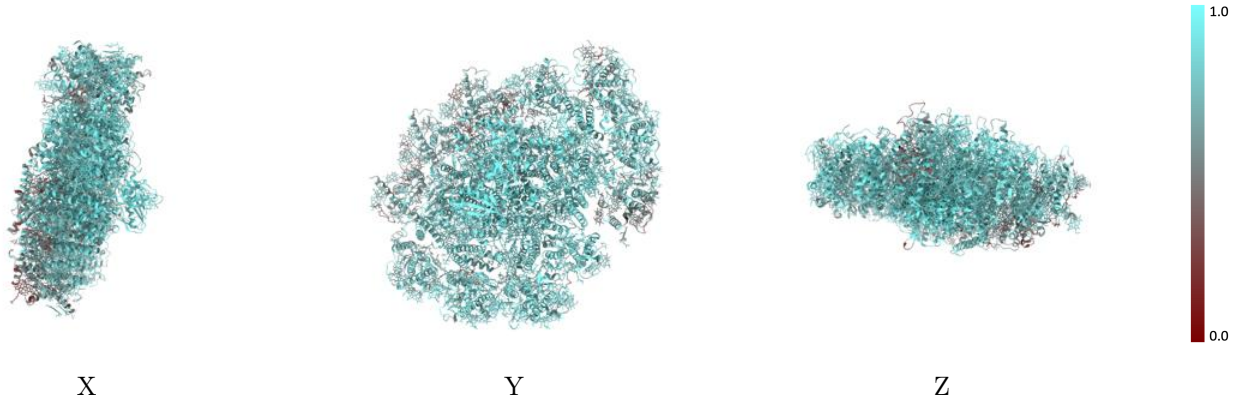
The images above show the 3D surface view of the map at the recommended contour level 0.018 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model (i)



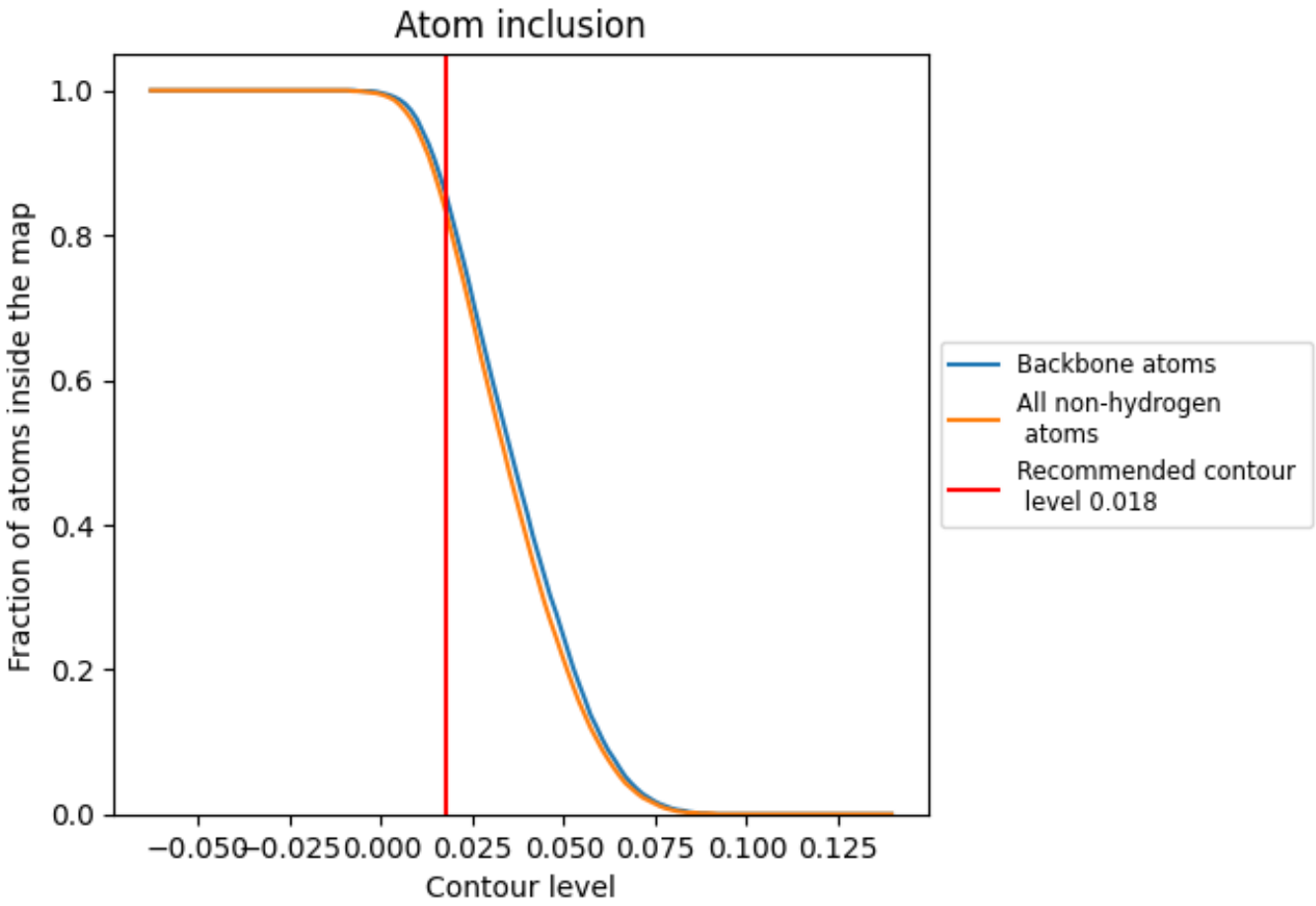
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

9.3 Atom inclusion mapped to coordinate model (i)



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 (0.018).

9.4 Atom inclusion (i)



At the recommended contour level, 85% of all backbone atoms, 83% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.018) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8280	0.5260
A	0.9240	0.5940
B	0.9400	0.6010
C	0.9580	0.5970
D	0.8850	0.5460
E	0.8530	0.5280
F	0.8620	0.5410
I	0.9090	0.5670
J	0.7980	0.5290
K	0.8520	0.5270
L	0.8780	0.5610
M	0.8990	0.5650
O	0.8330	0.5300
R	0.8860	0.5630
a	0.7950	0.4970
b	0.6090	0.4170
c	0.6560	0.4220
d	0.6030	0.3760
e	0.7660	0.4850
f	0.8260	0.5290
g	0.8100	0.5240
h	0.8530	0.5400
i	0.6260	0.3890
j	0.8120	0.5130
k	0.7100	0.4220