wwPDB EM Validation Summary Report (i)

Sep 29, 2026 – 01:16 PM JST

PDB ID	:	8ZOE / pdb_00008zoe
EMDB ID	:	EMD-60290
Title	:	Structure of the canthaxanthin mutant PSI-4VCPI supercomplex in Nannochloropsis oceanica
Authors	:	Shen, L.L.; Li, Z.H.; Shen, J.R.; Wang, W.D.
Deposited on	:	2024-05-28
Resolution	:	3.02 Å(reported)

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

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

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

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

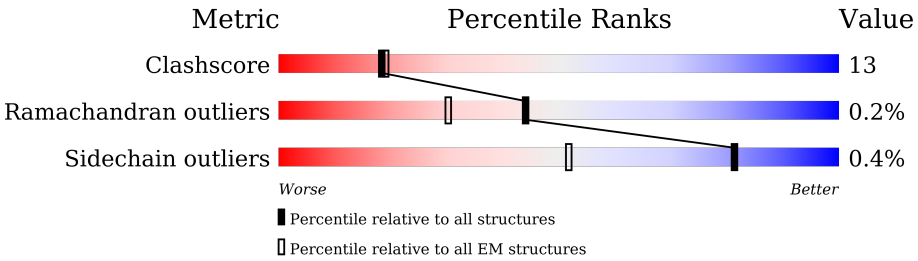
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.2
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using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

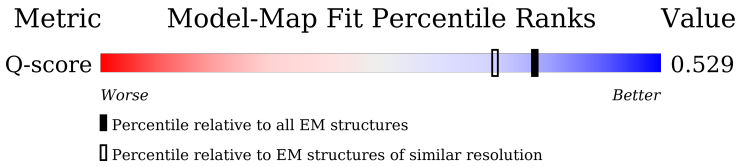
1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.02 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	13913 (2.52 - 3.52)

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	9	232	26% 65% 21% • 13%
2	8	200	29% 62% 19% • 18%
3	7	202	56% 59% 23% 18%
4	1	208	15% 51% 26% 22%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
5	a	745	74% 24%
6	b	737	75% 25%
7	d	136	18% 76% 19%
8	e	67	24% 84% 7% 9%
9	f	185	14% 75% 12% 14%
10	h	128	49% 51% 14% 34%
11	i	45	16% 53% 22% 24%
12	j	41	17% 63% 37%
13	l	172	22% 78% 21%
14	m	30	10% 90% 10%
15	g	55	65% 91% 9%
16	c	81	5% 72% 27%

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
27	SF4	c	102	-	-	X	-

2 Entry composition (i)

There are 28 unique types of molecules in this entry. The entry contains 33183 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 VCPI-9.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	9	201	1466	936	256	269	5	0	0

- Molecule 2 is a protein called VCPI-8.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	8	164	1258	822	203	227	6	0	0

- Molecule 3 is a protein called VCPI-7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	7	166	1220	791	202	222	5	0	0

- Molecule 4 is a protein called VCPI-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	1	162	1262	816	209	234	3	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	a	739	5827	3828	982	1000	17	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	b	735	5865	3874	985	989	17	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	d	130	1014	652	175	184	3	0	0

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

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
8	e	61	494	314	86	94	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	f	160	1266	815	213	235	3	0	0

- Molecule 10 is a protein called PsaR.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	h	85	646	427	100	117	2	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	i	34	271	189	36	45	1	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	j	41	339	233	48	57	1	0	0

- Molecule 13 is a protein called PSI subunit V.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
13	l	171	1283	848	203	232	0	0

- Molecule 14 is a protein called PsaM.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
14	m	30	210	137	35	38	0	0

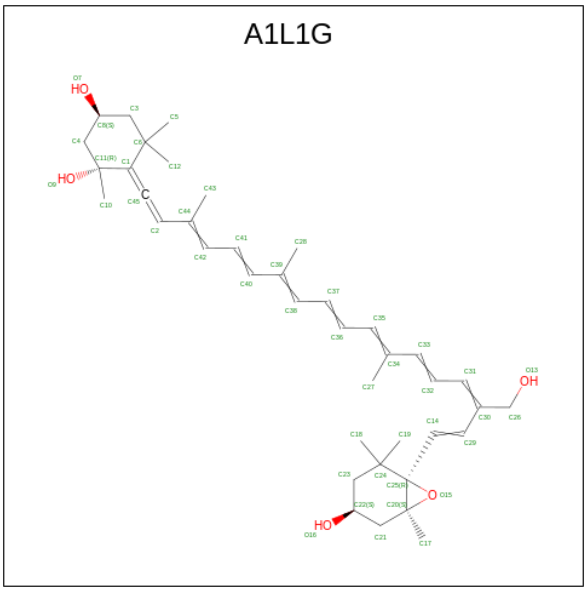
- Molecule 15 is a protein called PsaS.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
15	g	55	275	165	55	55	0	0

- Molecule 16 is a protein called Photosystem I iron-sulfur center.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
16	c	80	596	366	103	117	10	0	0

- Molecule 17 is (1 {R},3 {S})-6-[(3 {E},5 {E},7 {E},9 {E},11 {E},13 {E},15 {Z},17 {E})-16 -(hydroxymethyl)-3,7,12-trimethyl-18-[(1 {S},4 {S},6 {R})-2,2,6-trimethyl-4-oxidanyl-7-oxa bicyclo[4.1.0]heptan-1-yl]octadeca-1,3,5,7,9,11,13,15,17-nonaenylidene]-1,5,5-trimethyl-cyclo hexane-1,3-diol (CCD ID: A1L1G) (formula: $C_{40}H_{56}O_5$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
17	9	1	45	40	5	0
17	9	1	45	40	5	0

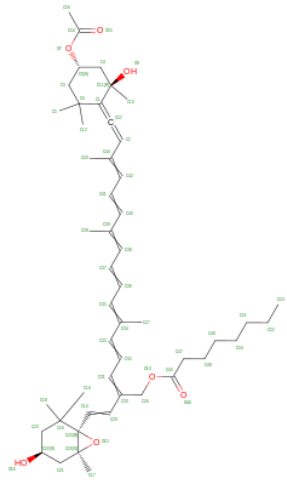
Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
17	7	1	45	40	5	0
17	1	1	45	40	5	0

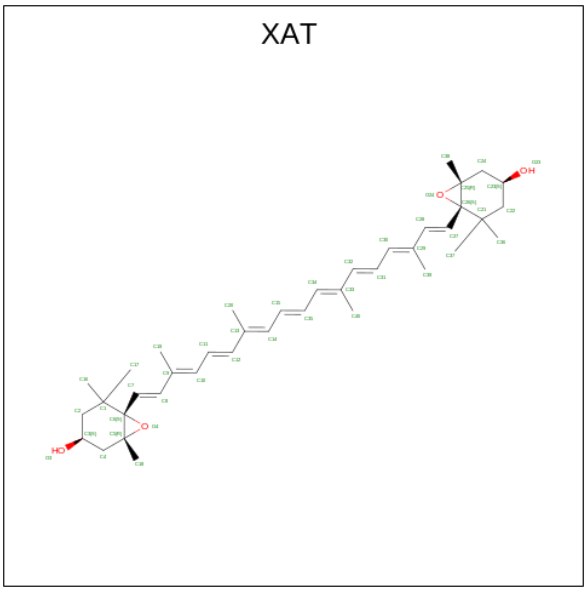
- Molecule 18 is [(2 {Z},4 {E},6 {E},8 {E},10 {E},12 {E},14 {E})-17-[(4 {S},6 {R})-4-acetyloxy-2,2,6-trimethyl-6-oxidanyl-cyclohexylidene]-6,11,15-trimethyl-2-[({E})-2-[(1 {S},4 {S},6 {R})-2,2,6-trimethyl-4-oxidanyl-7-oxabicyclo[4.1.0]heptan-1-yl]ethenyl]heptadeca-2,4,6,8,10,12,14,16-octaenyl] octanoate (CCD ID: A1L1F) (formula: $C_{50}H_{72}O_7$) (labeled as "Ligand of Interest" by depositor).

A1L1F



Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
18	9	1	57	50	7	0
18	8	1	57	50	7	0
18	1	1	57	50	7	0
18	h	1	57	50	7	0

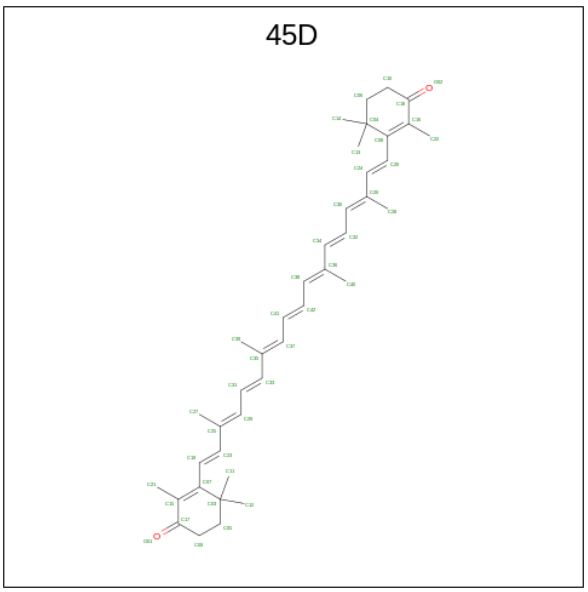
- Molecule 19 is (3S,5R,6S,3'S,5'R,6'S)-5,6,5',6'-DIEPOXY-5,6,5',6'- TETRAHYDRO-BETA,BETA-CAROTENE-3,3'-DIOL (CCD ID: XAT) (formula: $C_{40}H_{56}O_4$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
19	9	1	44	40	4	0
			Total	C	O	
19	9	1	44	40	4	0
			Total	C	O	
19	8	1	44	40	4	0
			Total	C	O	
19	8	1	44	40	4	0
			Total	C	O	
19	8	1	44	40	4	0
			Total	C	O	
19	7	1	44	40	4	0
			Total	C	O	
19	7	1	44	40	4	0
			Total	C	O	
19	7	1	44	40	4	0
			Total	C	O	
19	7	1	44	40	4	0
			Total	C	O	
19	1	1	44	40	4	0
			Total	C	O	
19	1	1	44	40	4	0
			Total	C	O	
19	a	1	44	40	4	0
			Total	C	O	
19	j	1	44	40	4	0

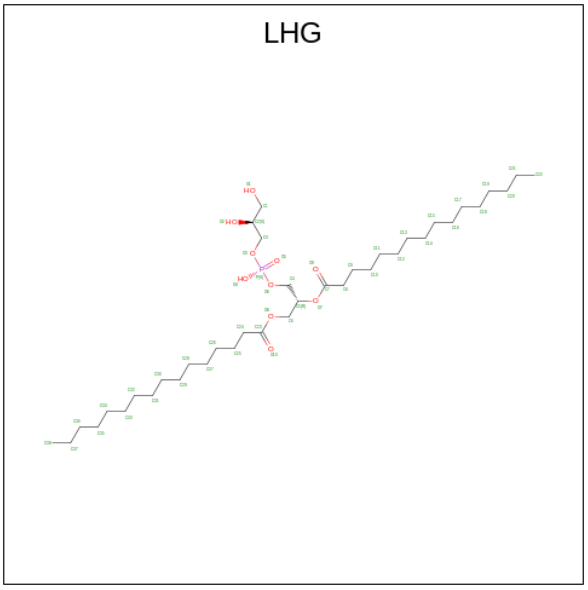
- Molecule 20 is beta,beta-carotene-4,4'-dione (CCD ID: 45D) (formula: $C_{40}H_{52}O_2$) (labeled

as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
20	9	1	42	40	2	0

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



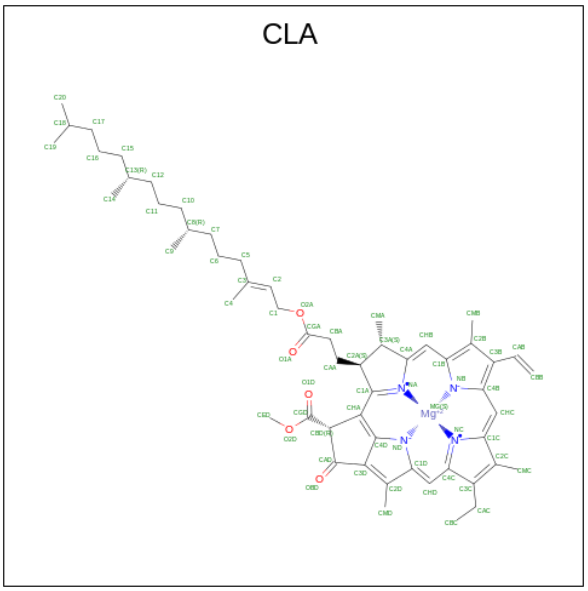
Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
21	9	1	36	25	10	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
21	9	1	46	35	10	1	0
			Total	C	O	P	
21	a	1	48	37	10	1	0
			Total	C	O	P	
21	a	1	27	16	10	1	0
			Total	C	O	P	
21	b	1	31	20	10	1	0

- Molecule 22 is CHLOROPHYLL A (CCD ID: CLA) (formula: $C_{55}H_{72}MgN_4O_5$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
22	9	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
22	9	1	46	36	1	4	5	0
			Total	C	Mg	N	O	
22	9	1	46	36	1	4	5	0
			Total	C	Mg	N	O	
22	9	1	46	36	1	4	5	0
			Total	C	Mg	N	O	
22	9	1	46	36	1	4	5	0
			Total	C	Mg	N	O	
22	9	1	46	36	1	4	5	0
			Total	C	Mg	N	O	
22	9	1	55	45	1	4	5	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
22	9	1	42	34	1	4	3	0
			Total	C	Mg	N	O	
22	9	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
22	9	1	62	52	1	4	5	0
			Total	C	Mg	N	O	
22	8	1	43	35	1	4	3	0
			Total	C	Mg	N	O	
22	8	1	46	36	1	4	5	0
			Total	C	Mg	N	O	
22	8	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
22	8	1	55	45	1	4	5	0
			Total	C	Mg	N	O	
22	8	1	57	47	1	4	5	0
			Total	C	Mg	N	O	
22	8	1	46	36	1	4	5	0
			Total	C	Mg	N	O	
22	8	1	56	46	1	4	5	0
			Total	C	Mg	N	O	
22	8	1	52	42	1	4	5	0
			Total	C	Mg	N	O	
22	8	1	46	36	1	4	5	0
			Total	C	Mg	N	O	
22	8	1	41	33	1	4	3	0
			Total	C	Mg	N	O	
22	7	1	48	38	1	4	5	0
			Total	C	Mg	N	O	
22	7	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
22	7	1	60	50	1	4	5	0
			Total	C	Mg	N	O	
22	7	1	47	37	1	4	5	0
			Total	C	Mg	N	O	
22	7	1	46	36	1	4	5	0
			Total	C	Mg	N	O	
22	7	1	46	36	1	4	5	0
			Total	C	Mg	N	O	
22	7	1	48	38	1	4	5	0
			Total	C	Mg	N	O	
22	7	1	54	44	1	4	5	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
22	7	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
22	7	1	41	33	1	4	3	0
			Total	C	Mg	N	O	
22	7	1	51	41	1	4	5	0
			Total	C	Mg	N	O	
22	7	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
22	1	1	61	51	1	4	5	0
			Total	C	Mg	N	O	
22	1	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
22	1	1	54	44	1	4	5	0
			Total	C	Mg	N	O	
22	1	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
22	1	1	46	36	1	4	5	0
			Total	C	Mg	N	O	
22	1	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
22	1	1	53	43	1	4	5	0
			Total	C	Mg	N	O	
22	1	1	52	42	1	4	5	0
			Total	C	Mg	N	O	
22	1	1	41	33	1	4	3	0
			Total	C	Mg	N	O	
22	1	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
22	a	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
22	a	1	58	48	1	4	5	0
			Total	C	Mg	N	O	
22	a	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
22	a	1	55	45	1	4	5	0
			Total	C	Mg	N	O	
22	a	1	55	45	1	4	5	0
			Total	C	Mg	N	O	
22	a	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
22	a	1	65	55	1	4	5	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
22	a	1	51	41	1	4	5	0
			Total	C	Mg	N	O	
22	a	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
22	a	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
22	a	1	56	46	1	4	5	0
			Total	C	Mg	N	O	
22	a	1	62	52	1	4	5	0
			Total	C	Mg	N	O	
22	a	1	54	44	1	4	5	0
			Total	C	Mg	N	O	
22	a	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
22	a	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
22	a	1	50	40	1	4	5	0
			Total	C	Mg	N	O	
22	a	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
22	a	1	56	46	1	4	5	0
			Total	C	Mg	N	O	
22	a	1	54	44	1	4	5	0
			Total	C	Mg	N	O	
22	a	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
22	a	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
22	a	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
22	a	1	49	39	1	4	5	0
			Total	C	Mg	N	O	
22	a	1	46	36	1	4	5	0
			Total	C	Mg	N	O	
22	a	1	55	45	1	4	5	0
			Total	C	Mg	N	O	
22	a	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
22	a	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
22	a	1	65	55	1	4	5	0

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
22	b	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
22	b	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
22	b	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
22	b	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
22	b	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
22	b	1	54	44	1	4	5	0
			Total	C	Mg	N	O	
22	b	1	53	43	1	4	5	0
			Total	C	Mg	N	O	
22	b	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
22	b	1	55	45	1	4	5	0
			Total	C	Mg	N	O	
22	b	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
22	b	1	55	45	1	4	5	0
			Total	C	Mg	N	O	
22	b	1	59	49	1	4	5	0
			Total	C	Mg	N	O	
22	b	1	60	50	1	4	5	0
			Total	C	Mg	N	O	
22	b	1	55	45	1	4	5	0
			Total	C	Mg	N	O	
22	b	1	50	40	1	4	5	0
			Total	C	Mg	N	O	
22	b	1	51	41	1	4	5	0
			Total	C	Mg	N	O	
22	b	1	60	50	1	4	5	0
			Total	C	Mg	N	O	
22	b	1	53	43	1	4	5	0
			Total	C	Mg	N	O	
22	b	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
22	b	1	64	54	1	4	5	0
			Total	C	Mg	N	O	
22	b	1	65	55	1	4	5	0

Continued on next page...

Continued from previous page...

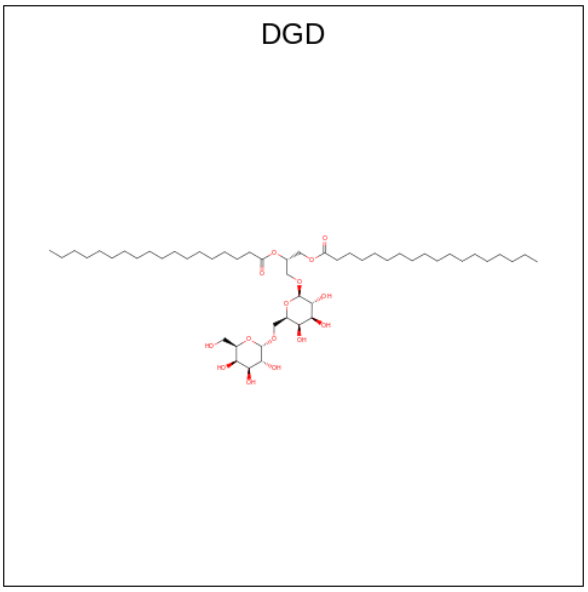
Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
22	b	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
22	b	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
22	b	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
22	b	1	41	33	1	4	3	0
			Total	C	Mg	N	O	
22	b	1	49	39	1	4	5	0
			Total	C	Mg	N	O	
22	b	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
22	b	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
22	b	1	53	43	1	4	5	0
			Total	C	Mg	N	O	
22	b	1	58	48	1	4	5	0
			Total	C	Mg	N	O	
22	b	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
22	b	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
22	b	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
22	b	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
22	b	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
22	f	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
22	f	1	52	42	1	4	5	0
			Total	C	Mg	N	O	
22	h	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
22	h	1	55	45	1	4	5	0
			Total	C	Mg	N	O	
22	j	1	58	48	1	4	5	0
			Total	C	Mg	N	O	
22	j	1	42	34	1	4	3	0
			Total	C	Mg	N	O	
22	l	1	42	34	1	4	3	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
22	l	1	60	50	1	4	5	0
22	l	1	46	36	1	4	5	0

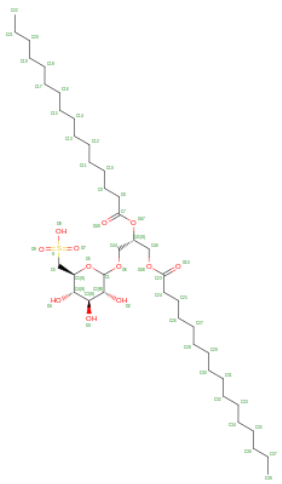
- Molecule 23 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: $C_{51}H_{96}O_{15}$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	O			
23	8	1	40	25	15			0
23	b	1	57	42	15			0

- Molecule 24 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (CCD ID: SQD) (formula: $C_{41}H_{78}O_{12}S$) (labeled as "Ligand of Interest" by depositor).

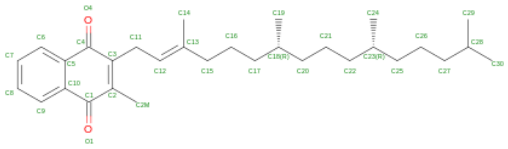
SQD



Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	S	
24	1	1	45	32	12	1	0

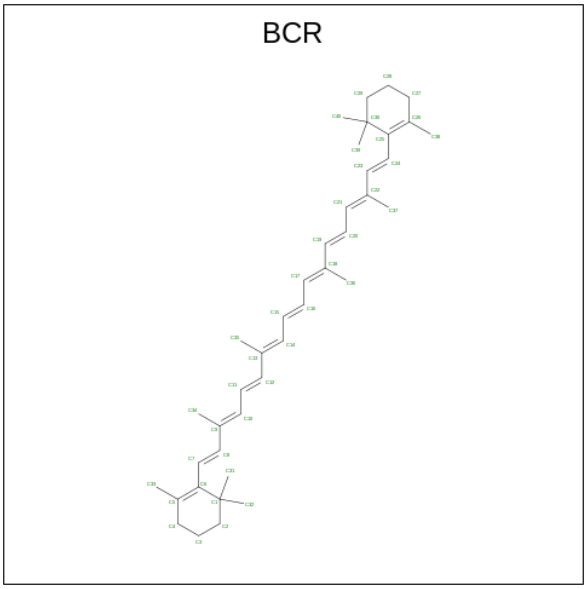
- Molecule 25 is PHYLLOQUINONE (CCD ID: PQN) (formula: $C_{31}H_{46}O_2$) (labeled as "Ligand of Interest" by depositor).

PQN



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

- Molecule 26 is BETA-CAROTENE (CCD ID: BCR) (formula: $C_{40}H_{56}$) (labeled as "Ligand of Interest" by depositor).



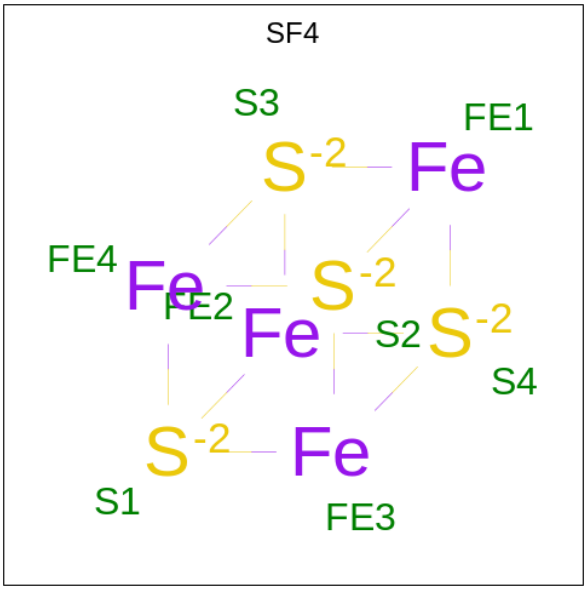
Mol	Chain	Residues	Atoms		AltConf
			Total	C	
26	a	1	40	40	0
			Total	C	
26	a	1	40	40	0
			Total	C	
26	a	1	40	40	0
			Total	C	
26	a	1	40	40	0
			Total	C	
26	b	1	40	40	0
			Total	C	
26	b	1	40	40	0
			Total	C	
26	b	1	40	40	0
			Total	C	
26	b	1	40	40	0
			Total	C	
26	b	1	40	40	0
			Total	C	
26	b	1	40	40	0
			Total	C	
26	f	1	40	40	0
			Total	C	
26	f	1	40	40	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		AltConf
			Total	C	
26	h	1	40	40	0
			Total	C	
26	h	1	40	40	0
			Total	C	
26	i	1	40	40	0
			Total	C	
26	j	1	40	40	0
			Total	C	
26	l	1	40	40	0
			Total	C	
26	l	1	40	40	0
			Total	C	
26	m	1	40	40	0

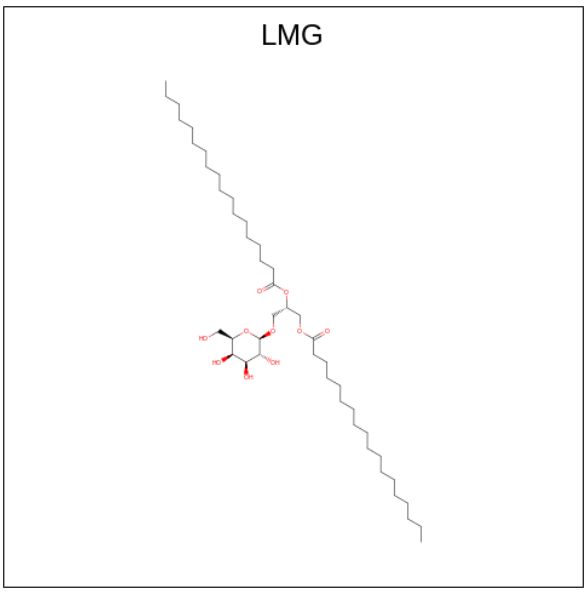
- Molecule 27 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
			Total	Fe	S	
27	a	1	8	4	4	0
			Total	Fe	S	
27	c	1	8	4	4	0
			Total	Fe	S	
27	c	1	8	4	4	0

- Molecule 28 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID:

LMG) (formula: $C_{45}H_{86}O_{10}$) (labeled as "Ligand of Interest" by depositor).



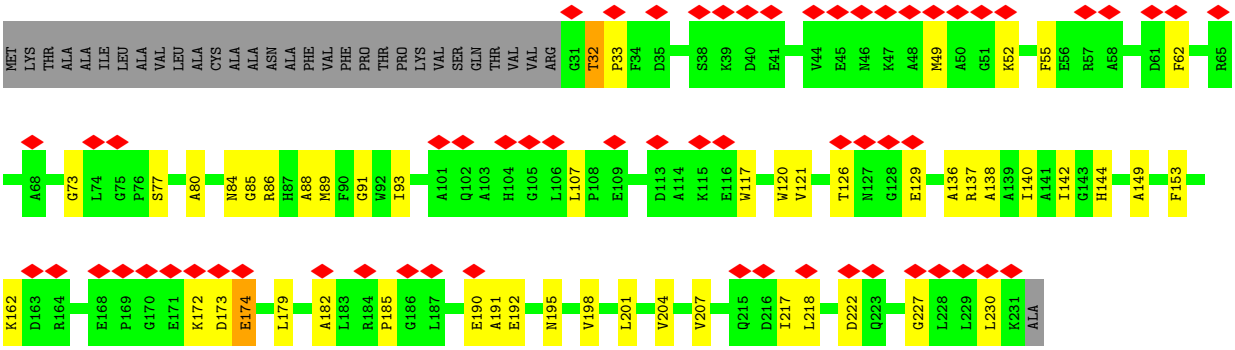
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
28	a	1	34	24	10	0
			Total	C	O	
28	j	1	32	22	10	0

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.

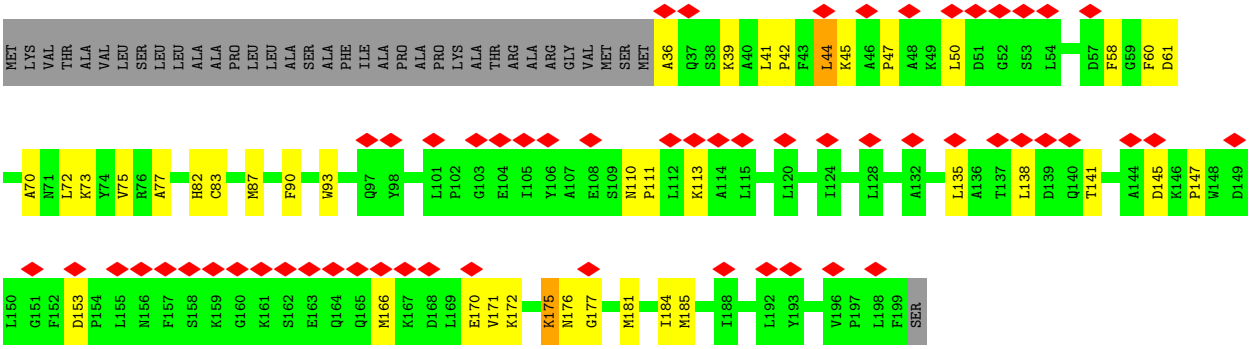
- Molecule 1: VCPI-9

Chain 9:



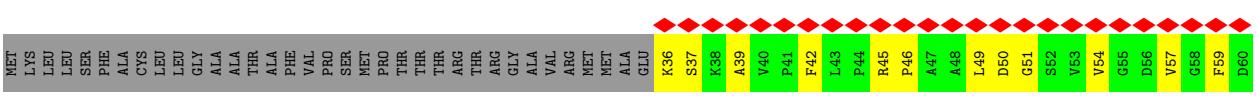
- Molecule 2: VCPI-8

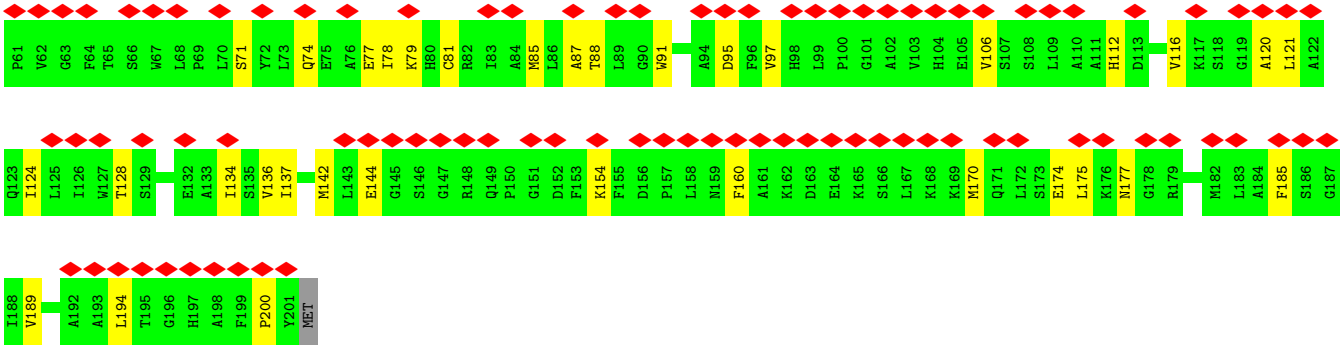
Chain 8:



- Molecule 3: VCPI-7

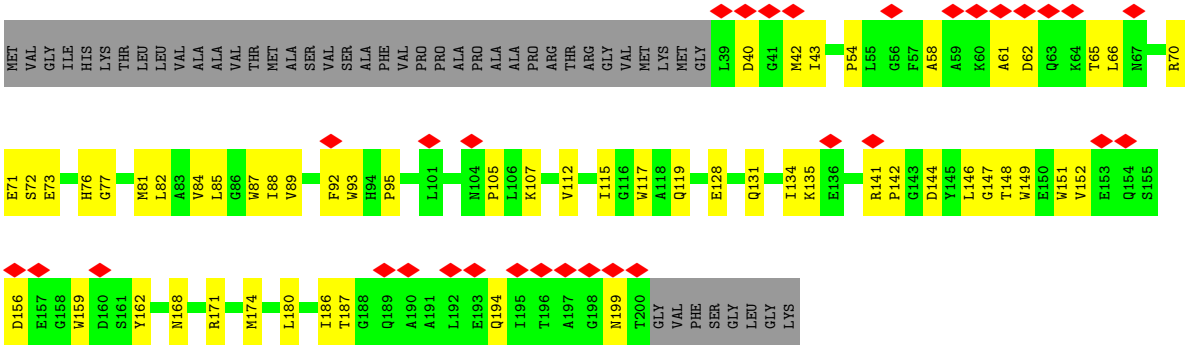
Chain 7:





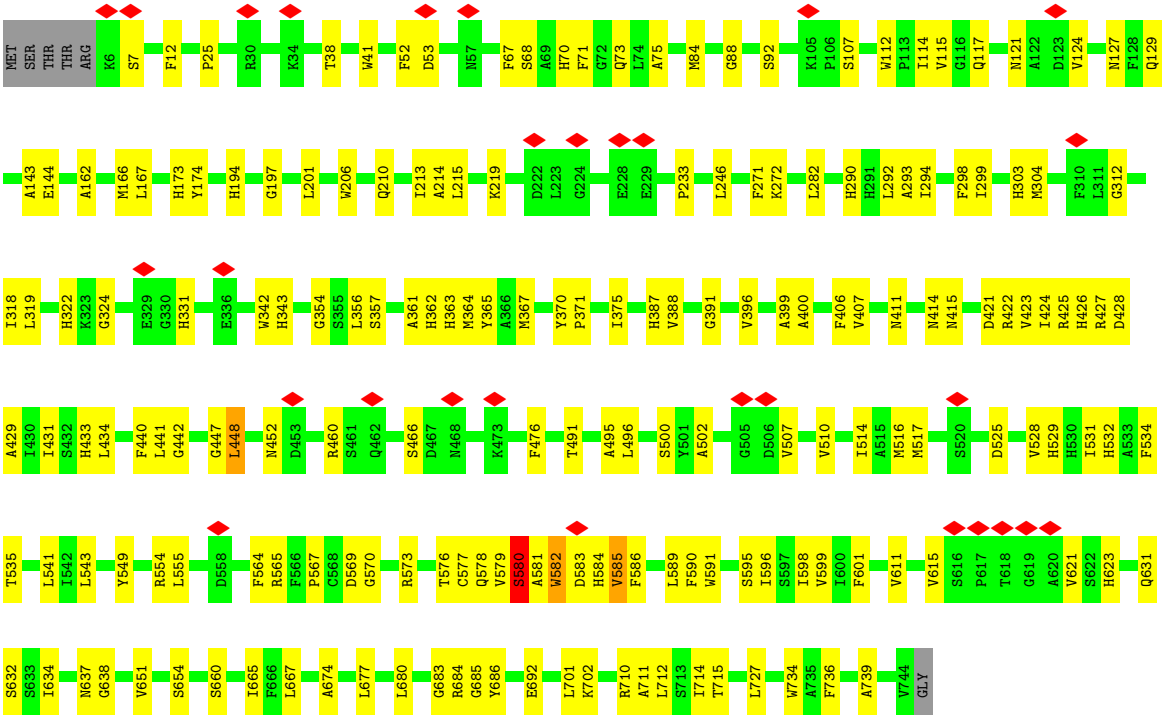
• Molecule 4: VCPI-1

Chain 1:



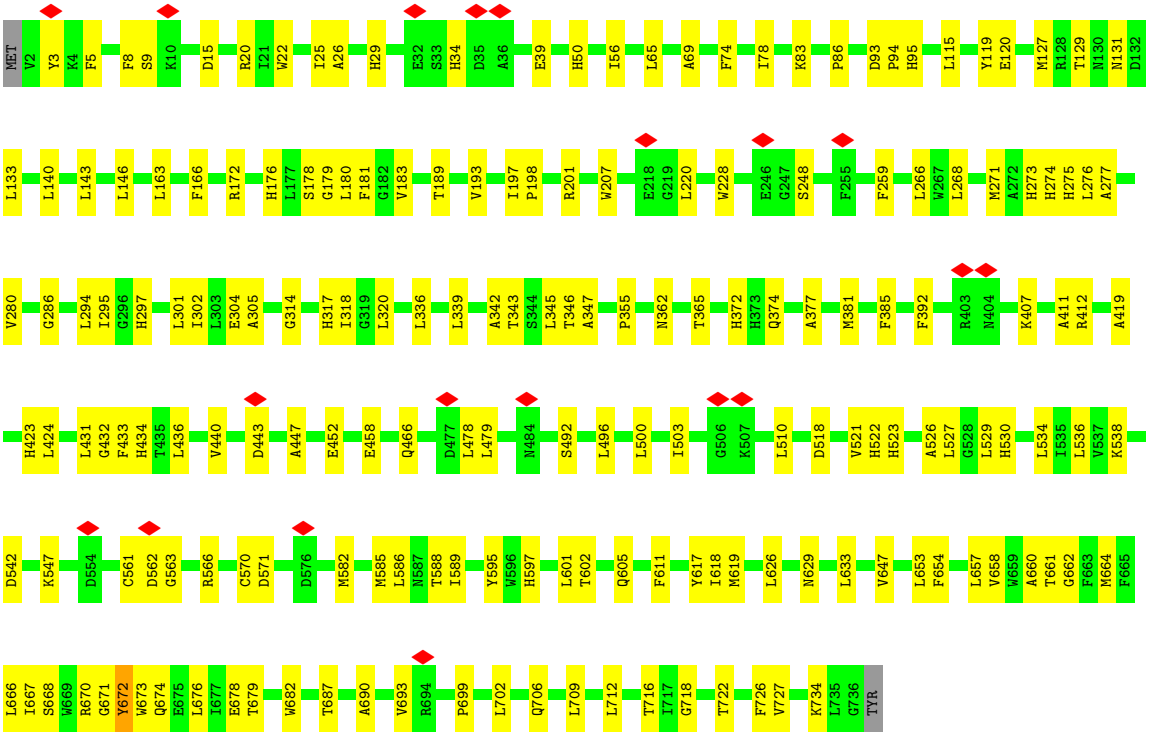
• Molecule 5: Photosystem I P700 chlorophyll a apoprotein A1

Chain a:



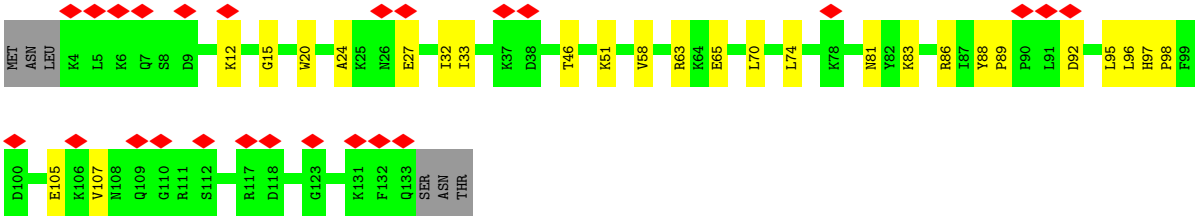
• Molecule 6: Photosystem I P700 chlorophyll a apoprotein A2

Chain b:



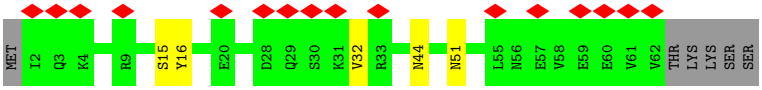
• Molecule 7: Photosystem I reaction center subunit II

Chain d:



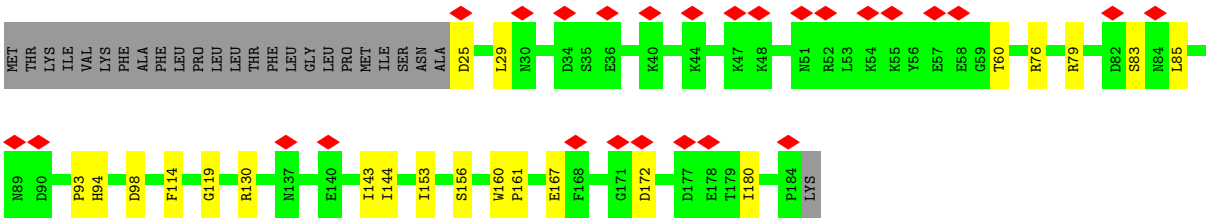
• Molecule 8: Photosystem I reaction center subunit IV

Chain e:



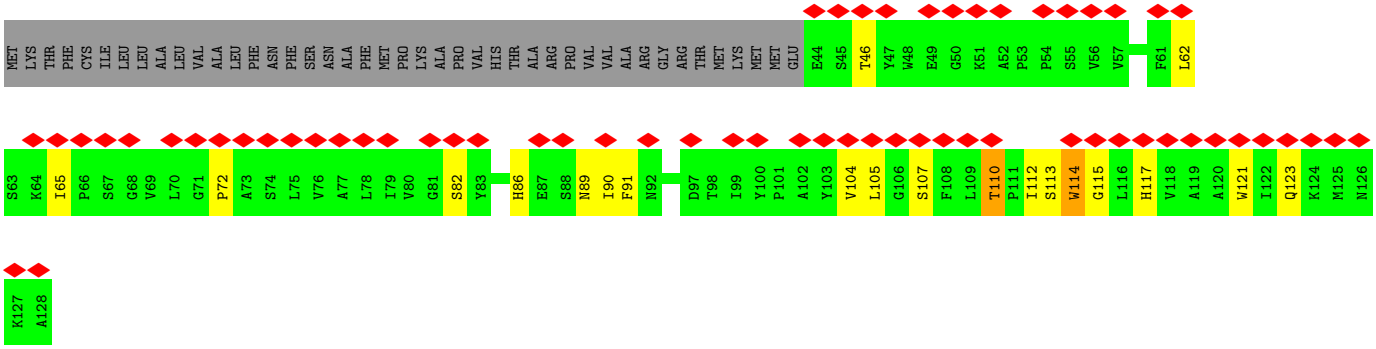
• Molecule 9: Photosystem I reaction center subunit III

Chain f:



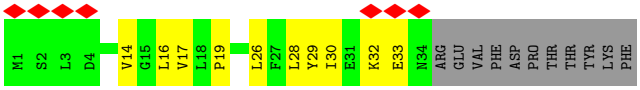
- Molecule 10: PsaR

Chain h:



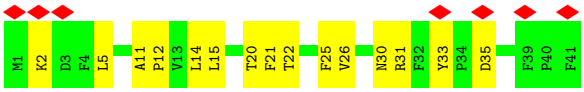
- Molecule 11: Photosystem I reaction center subunit VIII

Chain i:



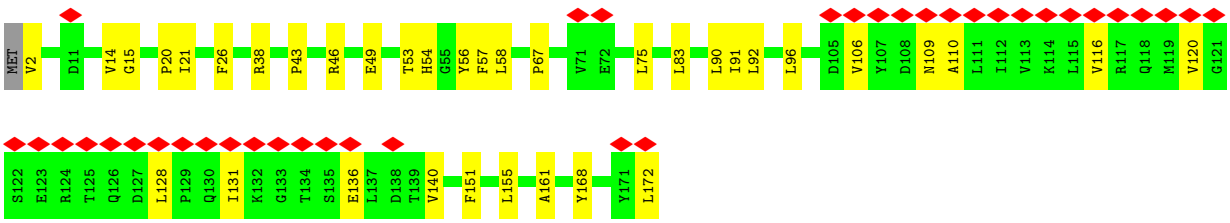
- Molecule 12: Photosystem I reaction center subunit IX

Chain j:



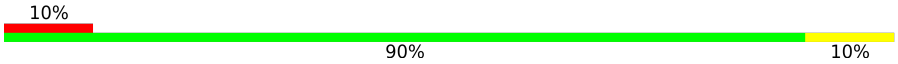
- Molecule 13: PSI subunit V

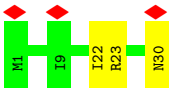
Chain l:



- Molecule 14: PsaM

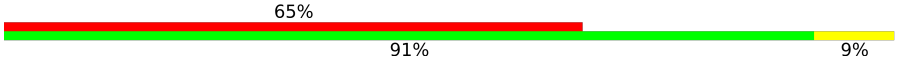
Chain m:

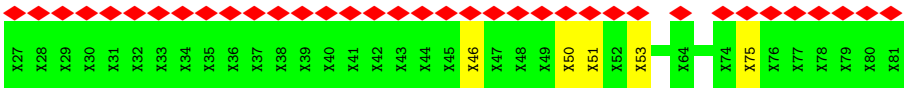




- Molecule 15: PsaS

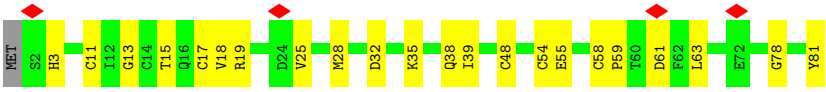
Chain g:





- Molecule 16: Photosystem I iron-sulfur center

Chain c:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	41262	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	60	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOCONTINUUM (6k x 4k)	Depositor
Maximum map value	1.615	Depositor
Minimum map value	-0.373	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.023	Depositor
Recommended contour level	0.343	Depositor
Map size (Å)	532.48, 532.48, 532.48	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.04, 1.04, 1.04	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: A1L1F, SF4, 45D, DGD, PQN, CLA, A1L1G, LHG, BCR, XAT, LMG, SQD

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	9	0.35	0/1496	0.33	0/2032
2	8	0.47	1/1286 (0.1%)	0.44	3/1743 (0.2%)
3	7	0.18	0/1248	0.37	0/1700
4	1	0.14	0/1293	0.33	0/1759
5	a	0.28	3/6024 (0.0%)	0.33	4/8219 (0.0%)
6	b	0.20	0/6080	0.32	1/8302 (0.0%)
7	d	0.12	0/1040	0.32	0/1402
8	e	0.09	0/502	0.20	0/681
9	f	0.14	0/1297	0.31	0/1762
10	h	0.51	1/667 (0.1%)	0.52	0/915
11	i	0.14	0/278	0.33	0/378
12	j	0.16	0/351	0.36	0/478
13	l	0.14	0/1315	0.31	0/1796
14	m	0.09	0/210	0.28	0/288
16	c	0.13	0/606	0.34	0/822
All	All	0.25	5/23693 (0.0%)	0.34	8/32277 (0.0%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	a	580	SER	CA-C	-7.05	1.43	1.52
2	8	44	LEU	C-O	-6.16	1.15	1.23
5	a	581	ALA	CA-C	-5.45	1.45	1.52
10	h	114	TRP	C-O	-5.25	1.18	1.24
5	a	582	TRP	CA-C	-5.03	1.45	1.52

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	a	581	ALA	N-CA-C	-8.63	102.50	113.72

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	a	448	LEU	N-CA-C	-6.10	104.18	111.69
2	8	39	LYS	N-CA-C	-6.09	105.68	113.23
5	a	584	HIS	N-CA-C	-5.82	106.52	113.97
6	b	672	TYR	N-CA-C	-5.58	106.31	113.23

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	9	1466	0	1470	49	0
2	8	1258	0	1280	33	0
3	7	1220	0	1209	44	0
4	1	1262	0	1237	39	0
5	a	5827	0	5697	140	0
6	b	5865	0	5710	149	0
7	d	1014	0	1015	20	0
8	e	494	0	495	5	0
9	f	1266	0	1262	20	0
10	h	646	0	649	18	0
11	i	271	0	292	12	0
12	j	339	0	342	21	0
13	l	1283	0	1278	29	0
14	m	210	0	226	3	0
15	g	275	0	62	3	0
16	c	596	0	583	19	0
17	1	45	0	0	1	0
17	7	45	0	0	2	0
17	9	90	0	0	3	0
18	1	57	0	0	2	0
18	8	57	0	0	2	0
18	9	57	0	0	2	0
18	h	57	0	0	4	0
19	1	88	0	112	6	0
19	7	176	0	224	28	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	8	132	0	168	17	0
19	9	88	0	112	14	0
19	a	44	0	56	6	0
19	j	44	0	56	6	0
20	9	42	0	52	8	0
21	9	82	0	110	5	0
21	a	75	0	93	7	0
21	b	31	0	32	0	0
22	1	547	0	508	14	0
22	7	576	0	444	25	0
22	8	507	0	429	24	0
22	9	519	0	452	35	0
22	a	2579	0	2562	140	0
22	b	2410	0	2464	129	0
22	f	117	0	115	1	0
22	h	120	0	121	6	0
22	j	100	0	86	9	0
22	l	148	0	123	3	0
23	8	40	0	38	2	0
23	b	57	0	72	6	0
24	1	45	0	54	3	0
25	a	33	0	46	3	0
25	b	33	0	46	2	0
26	a	160	0	224	13	0
26	b	240	0	336	25	0
26	f	80	0	112	15	0
26	h	80	0	112	5	0
26	i	40	0	56	2	0
26	j	40	0	56	9	0
26	l	80	0	112	12	0
26	m	40	0	56	1	0
27	a	8	0	0	0	0
27	c	16	0	0	2	0
28	a	34	0	38	10	0
28	j	32	0	34	7	0
All	All	33183	0	32518	863	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 13.

The worst 5 of 863 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)
22:a:806:CLA:O1A	22:a:814:CLA:HBA1	1.81	0.81
5:a:531:ILE:HD12	22:a:801:CLA:H172	1.63	0.80
19:8:303:XAT:H12	22:8:312:CLA:HAB	1.67	0.77
22:b:825:CLA:HMA1	26:b:845:BCR:H17C	1.66	0.77
22:1:312:CLA:HHC	22:1:312:CLA:HBB1	1.69	0.73

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	9	199/232 (86%)	182 (92%)	16 (8%)	1 (0%)	24 59
2	8	162/200 (81%)	157 (97%)	5 (3%)	0	100 100
3	7	164/202 (81%)	144 (88%)	20 (12%)	0	100 100
4	1	160/208 (77%)	149 (93%)	11 (7%)	0	100 100
5	a	737/745 (99%)	713 (97%)	23 (3%)	1 (0%)	48 79
6	b	733/737 (100%)	702 (96%)	31 (4%)	0	100 100
7	d	128/136 (94%)	113 (88%)	15 (12%)	0	100 100
8	e	59/67 (88%)	54 (92%)	5 (8%)	0	100 100
9	f	158/185 (85%)	151 (96%)	7 (4%)	0	100 100
10	h	83/128 (65%)	76 (92%)	6 (7%)	1 (1%)	10 38
11	i	32/45 (71%)	30 (94%)	2 (6%)	0	100 100
12	j	39/41 (95%)	39 (100%)	0	0	100 100
13	l	169/172 (98%)	154 (91%)	13 (8%)	2 (1%)	10 38
14	m	28/30 (93%)	27 (96%)	1 (4%)	0	100 100
16	c	78/81 (96%)	74 (95%)	4 (5%)	0	100 100
All	All	2929/3209 (91%)	2765 (94%)	159 (5%)	5 (0%)	44 75

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	9	32	THR
13	l	120	VAL
5	a	580	SER
13	l	131	ILE
10	h	90	ILE

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	9	141/167 (84%)	139 (99%)	2 (1%)	59	79
2	8	132/160 (82%)	131 (99%)	1 (1%)	73	85
3	7	122/159 (77%)	121 (99%)	1 (1%)	73	85
4	1	128/165 (78%)	128 (100%)	0	100	100
5	a	607/613 (99%)	603 (99%)	4 (1%)	76	85
6	b	599/602 (100%)	599 (100%)	0	100	100
7	d	107/113 (95%)	107 (100%)	0	100	100
8	e	56/62 (90%)	56 (100%)	0	100	100
9	f	138/162 (85%)	138 (100%)	0	100	100
10	h	71/107 (66%)	70 (99%)	1 (1%)	59	79
11	i	32/43 (74%)	32 (100%)	0	100	100
12	j	36/36 (100%)	36 (100%)	0	100	100
13	l	130/141 (92%)	130 (100%)	0	100	100
14	m	21/24 (88%)	21 (100%)	0	100	100
16	c	67/68 (98%)	67 (100%)	0	100	100
All	All	2387/2622 (91%)	2378 (100%)	9 (0%)	81	89

5 of 9 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	a	580	SER
10	h	110	THR
3	7	95	ASP
5	a	428	ASP
5	a	448	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 19 such sidechains are listed below:

Mol	Chain	Res	Type
6	b	605	GLN
9	f	166	GLN
13	l	144	GLN
7	d	7	GLN
5	a	239	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

191 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	$\#\|Z\| > 2$
18	A1L1F	9	302	-	50,59,59	1.37	5 (10%)	62,85,85	2.71	19 (30%)
22	CLA	a	833	5	59,63,73	1.34	7 (11%)	71,101,113	1.41	8 (11%)
22	CLA	8	307	2	69,73,73	1.26	7 (10%)	83,113,113	1.27	6 (7%)
22	CLA	b	803	6	69,73,73	1.24	8 (11%)	83,113,113	1.25	5 (6%)
18	A1L1F	h	204	-	50,59,59	1.38	5 (10%)	62,85,85	2.61	22 (35%)
22	CLA	b	833	-	69,73,73	1.26	8 (11%)	83,113,113	1.26	5 (6%)
22	CLA	1	309	4	50,54,73	1.47	9 (18%)	60,90,113	1.36	5 (8%)
22	CLA	8	308	2	59,63,73	1.36	7 (11%)	71,101,113	1.36	9 (12%)
27	SF4	c	102	-	0,12,12	-	-	-		
22	CLA	8	313	-	50,54,73	1.47	9 (18%)	60,90,113	1.41	5 (8%)
17	A1L1G	7	302	-	38,47,47	1.44	6 (15%)	49,71,71	1.50	9 (18%)
22	CLA	a	831	5	69,73,73	1.26	8 (11%)	83,113,113	1.35	7 (8%)
22	CLA	9	314	-	59,63,73	1.35	8 (13%)	71,101,113	1.35	7 (9%)
22	CLA	b	832	6	69,73,73	1.26	8 (11%)	83,113,113	1.28	6 (7%)
22	CLA	1	307	4	58,62,73	1.37	7 (12%)	69,99,113	1.37	8 (11%)
22	CLA	l	204	-	50,54,73	1.46	8 (16%)	60,90,113	1.42	5 (8%)
22	CLA	b	826	-	69,73,73	1.26	8 (11%)	83,113,113	1.25	4 (4%)
17	A1L1G	9	306	-	38,47,47	1.41	6 (15%)	49,71,71	1.54	8 (16%)
22	CLA	b	821	6	55,59,73	1.40	7 (12%)	66,96,113	1.42	7 (10%)
19	XAT	7	305	-	39,47,47	0.86	0	54,74,74	2.65	19 (35%)
22	CLA	b	808	6	69,73,73	1.24	8 (11%)	83,113,113	1.25	7 (8%)
22	CLA	f	803	9	56,60,73	1.39	6 (10%)	67,97,113	1.39	7 (10%)
17	A1L1G	1	301	-	38,47,47	1.45	6 (15%)	49,71,71	1.57	11 (22%)
22	CLA	a	801	5	69,73,73	1.26	10 (14%)	83,113,113	1.30	5 (6%)
22	CLA	a	808	-	55,59,73	1.43	9 (16%)	66,96,113	1.39	7 (10%)
26	BCR	b	845	-	41,41,41	0.77	0	56,56,56	2.19	22 (39%)
22	CLA	b	829	6	69,73,73	1.27	8 (11%)	83,113,113	1.33	9 (10%)
22	CLA	a	823	-	53,57,73	1.41	8 (15%)	62,93,113	1.44	6 (9%)
22	CLA	b	820	6	54,58,73	1.41	8 (14%)	65,95,113	1.45	8 (12%)
22	CLA	7	306	3	52,56,73	1.45	7 (13%)	62,92,113	1.40	5 (8%)
22	CLA	b	840	21	69,73,73	1.28	7 (10%)	83,113,113	1.28	7 (8%)
22	CLA	a	813	5	58,62,73	1.37	8 (13%)	69,99,113	1.33	6 (8%)
22	CLA	b	811	6	58,62,73	1.42	9 (15%)	73,100,113	1.39	7 (9%)
22	CLA	a	809	5	69,73,73	1.23	7 (10%)	83,113,113	1.31	7 (8%)
22	CLA	b	824	-	69,73,73	1.27	7 (10%)	83,113,113	1.30	5 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
22	CLA	b	835	6	62,66,73	1.34	7 (11%)	74,104,113	1.39	8 (10%)
22	CLA	a	825	5	59,63,73	1.35	7 (11%)	71,101,113	1.35	7 (9%)
22	CLA	b	828	-	69,73,73	1.27	9 (13%)	83,113,113	1.22	5 (6%)
22	CLA	a	844	21	69,73,73	1.25	7 (10%)	83,113,113	1.28	8 (9%)
22	CLA	b	801	-	69,73,73	1.26	9 (13%)	83,113,113	1.28	6 (7%)
22	CLA	a	815	-	49,53,73	1.49	7 (14%)	59,89,113	1.44	6 (10%)
22	CLA	1	308	4	69,73,73	1.25	7 (10%)	83,113,113	1.30	6 (7%)
22	CLA	b	827	6	69,73,73	1.25	7 (10%)	83,113,113	1.27	5 (6%)
22	CLA	1	313	4	45,49,73	1.52	8 (17%)	54,84,113	1.50	5 (9%)
22	CLA	b	837	6	69,73,73	1.26	8 (11%)	83,113,113	1.24	6 (7%)
22	CLA	1	306	-	69,73,73	1.25	7 (10%)	83,113,113	1.31	8 (9%)
22	CLA	9	312	-	50,54,73	1.47	8 (16%)	60,90,113	1.51	6 (10%)
22	CLA	1	312	4	56,60,73	1.42	7 (12%)	67,97,113	1.37	7 (10%)
22	CLA	a	854	-	69,73,73	1.26	8 (11%)	83,113,113	1.27	7 (8%)
22	CLA	1	311	-	57,61,73	1.38	7 (12%)	68,98,113	1.38	7 (10%)
19	XAT	8	302	-	39,47,47	0.93	1 (2%)	54,74,74	2.66	20 (37%)
22	CLA	9	316	6	69,73,73	1.25	7 (10%)	83,113,113	1.32	7 (8%)
22	CLA	7	313	-	58,62,73	1.40	8 (13%)	69,99,113	1.37	8 (11%)
22	CLA	a	804	5	59,63,73	1.36	8 (13%)	71,101,113	1.41	9 (12%)
28	LMG	j	105	-	32,32,55	1.12	2 (6%)	40,40,63	1.14	3 (7%)
26	BCR	b	843	-	41,41,41	0.71	0	56,56,56	1.92	16 (28%)
22	CLA	8	305	2	47,51,73	1.49	7 (14%)	56,86,113	1.46	6 (10%)
19	XAT	8	303	-	39,47,47	0.87	1 (2%)	54,74,74	2.64	18 (33%)
22	CLA	a	819	5	58,62,73	1.36	7 (12%)	69,99,113	1.35	5 (7%)
22	CLA	b	813	-	69,73,73	1.26	8 (11%)	83,113,113	1.27	7 (8%)
22	CLA	7	315	3	45,49,73	1.53	8 (17%)	54,84,113	1.51	5 (9%)
22	CLA	a	821	5	49,53,73	1.49	8 (16%)	59,89,113	1.49	4 (6%)
22	CLA	8	312	2	56,60,73	1.38	7 (12%)	67,97,113	1.39	7 (10%)
26	BCR	a	848	-	41,41,41	0.75	0	56,56,56	1.94	18 (32%)
26	BCR	b	846	-	41,41,41	0.75	0	56,56,56	1.78	15 (26%)
22	CLA	9	310	1	50,54,73	1.47	7 (14%)	60,90,113	1.50	4 (6%)
19	XAT	1	303	-	39,47,47	0.91	0	54,74,74	2.53	18 (33%)
22	CLA	a	816	5	54,58,73	1.42	8 (14%)	65,95,113	1.43	8 (12%)
21	LHG	a	845	-	47,47,48	1.12	6 (12%)	50,53,54	0.97	2 (4%)
22	CLA	a	829	5	66,70,73	1.29	7 (10%)	79,109,113	1.25	8 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
21	LHG	a	846	22	26,26,48	1.28	5 (19%)	29,32,54	1.20	2 (6%)
19	XAT	1	302	-	39,47,47	0.91	1 (2%)	54,74,74	2.59	16 (29%)
22	CLA	b	805	6	69,73,73	1.25	6 (8%)	83,113,113	1.29	6 (7%)
22	CLA	7	308	-	64,68,73	1.29	8 (12%)	77,107,113	1.31	6 (7%)
22	CLA	h	203	-	69,73,73	1.26	6 (8%)	83,113,113	1.34	5 (6%)
22	CLA	a	814	5	69,73,73	1.27	7 (10%)	83,113,113	1.29	6 (7%)
22	CLA	l	202	-	46,50,73	1.52	9 (19%)	55,85,113	1.47	5 (9%)
22	CLA	9	311	1	50,54,73	1.45	6 (12%)	60,90,113	1.48	6 (10%)
22	CLA	b	814	-	59,63,73	1.36	7 (11%)	71,101,113	1.42	7 (9%)
22	CLA	h	205	10	59,63,73	1.38	8 (13%)	71,101,113	1.36	8 (11%)
26	BCR	a	847	-	41,41,41	0.70	0	56,56,56	1.94	16 (28%)
22	CLA	a	835	-	69,73,73	1.24	7 (10%)	83,113,113	1.32	7 (8%)
22	CLA	1	305	-	65,69,73	1.29	7 (10%)	78,108,113	1.30	5 (6%)
22	CLA	a	828	5	69,73,73	1.25	8 (11%)	83,113,113	1.29	5 (6%)
22	CLA	a	827	-	69,73,73	1.26	7 (10%)	83,113,113	1.34	7 (8%)
22	CLA	b	834	-	57,61,73	1.40	9 (15%)	68,98,113	1.39	8 (11%)
25	PQN	a	843	-	34,34,34	1.59	2 (5%)	42,45,45	1.10	3 (7%)
26	BCR	a	850	-	41,41,41	0.74	0	56,56,56	2.16	14 (25%)
22	CLA	a	830	5	69,73,73	1.26	9 (13%)	83,113,113	1.27	6 (7%)
22	CLA	a	822	-	69,73,73	1.27	8 (11%)	83,113,113	1.29	7 (8%)
22	CLA	a	837	5	49,53,73	1.49	9 (18%)	59,89,113	1.44	6 (10%)
22	CLA	b	810	-	69,73,73	1.25	8 (11%)	83,113,113	1.30	7 (8%)
18	A1L1F	8	304	-	50,59,59	1.31	4 (8%)	62,85,85	2.79	23 (37%)
28	LMG	a	853	-	34,34,55	1.14	2 (5%)	42,42,63	1.16	3 (7%)
22	CLA	a	826	-	69,73,73	1.25	8 (11%)	83,113,113	1.32	6 (7%)
22	CLA	j	103	12	46,50,73	1.50	7 (15%)	55,85,113	1.51	4 (7%)
22	CLA	a	834	-	69,73,73	1.26	7 (10%)	83,113,113	1.27	7 (8%)
26	BCR	l	201	-	41,41,41	0.71	0	56,56,56	1.96	18 (32%)
22	CLA	1	314	4	49,53,73	1.49	6 (12%)	59,89,113	1.43	4 (6%)
22	CLA	b	822	6	64,68,73	1.29	8 (12%)	77,107,113	1.27	6 (7%)
25	PQN	b	841	-	34,34,34	1.55	2 (5%)	42,45,45	1.20	4 (9%)
22	CLA	a	802	-	62,66,73	1.30	8 (12%)	74,104,113	1.36	8 (10%)
22	CLA	8	306	23	50,54,73	1.46	7 (14%)	60,90,113	1.41	4 (6%)
22	CLA	7	310	-	50,54,73	1.48	8 (16%)	60,90,113	1.42	5 (8%)
22	CLA	a	818	5	60,64,73	1.36	7 (11%)	72,102,113	1.33	7 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
22	CLA	l	203	-	64,68,73	1.31	9 (14%)	77,107,113	1.36	6 (7%)
22	CLA	a	840	5	69,73,73	1.28	8 (11%)	83,113,113	1.27	7 (8%)
22	CLA	b	836	-	69,73,73	1.25	7 (10%)	83,113,113	1.31	7 (8%)
22	CLA	b	802	-	69,73,73	1.25	7 (10%)	83,113,113	1.20	4 (4%)
23	DGD	b	848	-	58,58,67	1.15	6 (10%)	72,72,81	1.53	10 (13%)
22	CLA	9	315	1	46,50,73	1.50	7 (15%)	55,85,113	1.44	5 (9%)
22	CLA	b	806	6	69,73,73	1.25	6 (8%)	83,113,113	1.31	5 (6%)
19	XAT	9	304	-	39,47,47	0.94	1 (2%)	54,74,74	2.42	19 (35%)
22	CLA	7	311	-	50,54,73	1.48	9 (18%)	60,90,113	1.42	7 (11%)
18	A1L1F	1	304	-	50,59,59	1.30	5 (10%)	62,85,85	2.30	18 (29%)
22	CLA	j	102	6	62,66,73	1.34	7 (11%)	74,104,113	1.31	7 (9%)
27	SF4	a	851	-	0,12,12	-	-	-		
26	BCR	h	202	-	41,41,41	0.73	0	56,56,56	1.88	17 (30%)
22	CLA	b	817	6	63,67,73	1.33	9 (14%)	75,105,113	1.39	10 (13%)
26	BCR	b	842	-	41,41,41	0.71	0	56,56,56	2.29	21 (37%)
21	LHG	9	317	-	45,45,48	1.14	6 (13%)	48,51,54	0.95	2 (4%)
26	BCR	a	849	-	41,41,41	0.73	0	56,56,56	2.17	20 (35%)
26	BCR	l	205	-	41,41,41	0.70	0	56,56,56	2.03	13 (23%)
26	BCR	j	104	-	41,41,41	0.73	0	56,56,56	2.08	18 (32%)
19	XAT	9	303	-	39,47,47	0.95	1 (2%)	54,74,74	2.61	19 (35%)
22	CLA	8	311	-	60,64,73	1.34	7 (11%)	72,102,113	1.37	7 (9%)
22	CLA	b	819	-	59,63,73	1.36	9 (15%)	71,101,113	1.34	7 (9%)
22	CLA	7	316	3	55,59,73	1.40	8 (14%)	66,96,113	1.45	7 (10%)
22	CLA	b	838	-	69,73,73	1.27	9 (13%)	83,113,113	1.29	7 (8%)
22	CLA	9	308	1	69,73,73	1.26	9 (13%)	83,113,113	1.32	8 (9%)
22	CLA	a	836	5	54,58,73	1.41	8 (14%)	65,95,113	1.40	7 (10%)
22	CLA	7	309	3	50,55,73	1.46	7 (14%)	59,91,113	1.40	6 (10%)
22	CLA	a	803	-	69,73,73	1.25	9 (13%)	83,113,113	1.23	6 (7%)
22	CLA	b	807	6	69,73,73	1.26	8 (11%)	83,113,113	1.29	7 (8%)
26	BCR	b	844	-	41,41,41	0.69	0	56,56,56	2.10	16 (28%)
22	CLA	a	806	5	69,73,73	1.32	11 (15%)	83,113,113	1.57	13 (15%)
20	45D	9	305	-	43,43,43	1.10	4 (9%)	54,60,60	2.16	18 (33%)
19	XAT	7	304	-	39,47,47	0.92	1 (2%)	54,74,74	2.68	21 (38%)
22	CLA	a	824	5	50,54,73	1.47	9 (18%)	60,90,113	1.38	5 (8%)
22	CLA	9	309	1	50,54,73	1.46	9 (18%)	60,90,113	1.38	7 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
22	CLA	7	312	-	52,56,73	1.43	8 (15%)	62,92,113	1.42	6 (9%)
22	CLA	b	839	6	69,73,73	1.26	6 (8%)	83,113,113	1.33	6 (7%)
22	CLA	a	832	5	54,58,73	1.42	9 (16%)	65,95,113	1.42	7 (10%)
19	XAT	7	301	-	39,47,47	0.92	1 (2%)	54,74,74	2.62	20 (37%)
22	CLA	b	812	6	57,61,73	1.39	7 (12%)	68,98,113	1.39	7 (10%)
22	CLA	b	815	6	49,53,73	1.48	7 (14%)	59,89,113	1.44	6 (10%)
23	DGD	8	315	22	41,41,67	1.05	2 (4%)	55,55,81	1.11	5 (9%)
22	CLA	a	841	5	69,73,73	1.25	7 (10%)	83,113,113	1.32	7 (8%)
26	BCR	f	801	-	41,41,41	0.68	0	56,56,56	2.14	16 (28%)
22	CLA	a	807	-	69,73,73	1.25	7 (10%)	83,113,113	1.29	6 (7%)
26	BCR	f	804	-	41,41,41	0.72	0	56,56,56	2.04	17 (30%)
22	CLA	9	313	1	50,54,73	1.47	6 (12%)	60,90,113	1.49	5 (8%)
22	CLA	8	310	-	50,54,73	1.48	9 (18%)	60,90,113	1.41	6 (10%)
22	CLA	b	823	-	57,61,73	1.38	8 (14%)	68,98,113	1.36	6 (8%)
19	XAT	j	101	-	39,47,47	0.88	0	54,74,74	2.72	18 (33%)
22	CLA	7	307	-	49,53,73	1.49	7 (14%)	59,89,113	1.43	5 (8%)
17	A1L1G	9	301	-	38,47,47	1.46	6 (15%)	49,71,71	1.57	10 (20%)
22	CLA	7	314	-	49,53,73	1.50	9 (18%)	59,89,113	1.52	5 (8%)
22	CLA	a	820	5	69,73,73	1.26	8 (11%)	83,113,113	1.33	9 (10%)
26	BCR	m	101	-	41,41,41	1.18	2 (4%)	56,56,56	1.22	6 (10%)
22	CLA	a	842	5	69,73,73	1.28	8 (11%)	83,113,113	1.28	5 (6%)
22	CLA	b	830	6	45,49,73	1.52	9 (20%)	54,84,113	1.51	7 (12%)
22	CLA	a	839	5	69,73,73	1.25	8 (11%)	83,113,113	1.32	8 (9%)
22	CLA	8	314	-	45,49,73	1.54	7 (15%)	54,84,113	1.50	6 (11%)
22	CLA	a	811	5	60,64,73	1.35	8 (13%)	72,102,113	1.36	6 (8%)
22	CLA	f	802	-	69,73,73	1.26	7 (10%)	83,113,113	1.28	7 (8%)
22	CLA	a	810	5	69,73,73	1.27	9 (13%)	83,113,113	1.34	6 (7%)
22	CLA	b	809	6	69,73,73	1.24	9 (13%)	83,113,113	1.34	6 (7%)
21	LHG	9	307	-	35,35,48	1.22	6 (17%)	38,41,54	0.96	2 (5%)
22	CLA	a	812	22,5	66,70,73	1.27	7 (10%)	79,109,113	1.33	6 (7%)
22	CLA	9	318	-	66,70,73	1.30	8 (12%)	79,109,113	1.29	7 (8%)
21	LHG	b	847	22	30,30,48	1.33	6 (20%)	33,36,54	1.15	2 (6%)
22	CLA	b	825	-	68,72,73	1.26	8 (11%)	81,111,113	1.32	8 (9%)
27	SF4	c	101	-	0,12,12	-	-	-		
19	XAT	a	852	-	39,47,47	0.95	2 (5%)	54,74,74	2.69	20 (37%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
26	BCR	h	201	-	41,41,41	0.71	0	56,56,56	1.98	21 (37%)
22	CLA	a	805	22,5	59,63,73	1.35	6 (10%)	71,101,113	1.37	7 (9%)
22	CLA	b	818	6	64,68,73	1.30	8 (12%)	77,107,113	1.29	5 (6%)
19	XAT	7	303	-	39,47,47	0.98	1 (2%)	54,74,74	2.59	19 (35%)
22	CLA	1	310	4	69,73,73	1.27	7 (10%)	83,113,113	1.24	7 (8%)
19	XAT	8	301	-	39,47,47	0.91	1 (2%)	54,74,74	2.53	18 (33%)
26	BCR	i	101	-	41,41,41	0.75	0	56,56,56	2.13	14 (25%)
24	SQD	1	315	-	44,45,54	1.29	4 (9%)	53,56,65	1.16	5 (9%)
22	CLA	8	309	-	61,65,73	1.34	7 (11%)	73,103,113	1.35	8 (10%)
22	CLA	b	804	-	69,73,73	1.22	8 (11%)	83,113,113	1.45	10 (12%)
22	CLA	b	831	6	53,57,73	1.42	7 (13%)	62,93,113	1.42	7 (11%)
22	CLA	a	838	5	55,59,73	1.40	7 (12%)	66,96,113	1.42	6 (9%)
22	CLA	b	816	-	59,63,73	1.36	7 (11%)	71,101,113	1.34	7 (9%)
22	CLA	a	817	-	49,53,73	1.49	8 (16%)	59,89,113	1.45	5 (8%)
26	BCR	b	849	-	41,41,41	0.73	0	56,56,56	2.05	15 (26%)
22	CLA	7	317	-	49,53,73	1.49	6 (12%)	59,89,113	1.46	5 (8%)

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
18	A1L1F	9	302	-	-	13/43/99/99	0/3/3/3
22	CLA	a	833	5	-	2/27/103/115	-
22	CLA	8	307	2	-	13/39/115/115	-
22	CLA	b	803	6	-	19/39/115/115	-
18	A1L1F	h	204	-	-	11/43/99/99	1/3/3/3
22	CLA	b	833	-	-	14/39/115/115	-
22	CLA	1	309	4	-	8/17/93/115	-
22	CLA	8	308	2	-	7/27/103/115	-
27	SF4	c	102	-	-	-	0/6/5/5
22	CLA	8	313	-	-	5/17/93/115	-
17	A1L1G	7	302	-	-	15/29/85/85	0/3/3/3
22	CLA	a	831	5	-	11/39/115/115	-
22	CLA	9	314	-	-	9/27/103/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	b	832	6	-	13/39/115/115	-
22	CLA	1	307	4	-	6/26/102/115	-
22	CLA	l	204	-	-	4/17/93/115	-
22	CLA	b	826	-	-	5/39/115/115	-
17	A1L1G	9	306	-	-	18/29/85/85	0/3/3/3
22	CLA	b	821	6	-	2/23/99/115	-
19	XAT	7	305	-	-	2/31/93/93	0/4/4/4
22	CLA	b	808	6	-	12/39/115/115	-
22	CLA	f	803	9	-	4/24/100/115	-
17	A1L1G	1	301	-	-	11/29/85/85	0/3/3/3
22	CLA	a	801	5	-	24/39/115/115	-
22	CLA	a	808	-	-	5/23/99/115	-
26	BCR	b	845	-	-	1/29/63/63	0/2/2/2
22	CLA	b	829	6	-	11/39/115/115	-
22	CLA	a	823	-	-	7/20/96/115	-
22	CLA	b	820	6	-	7/21/97/115	-
22	CLA	7	306	3	-	10/19/95/115	-
22	CLA	b	840	21	-	11/39/115/115	-
22	CLA	a	813	5	-	11/26/102/115	-
22	CLA	b	811	6	-	5/25/101/115	-
22	CLA	a	809	5	-	15/39/115/115	-
22	CLA	b	824	-	-	14/39/115/115	-
22	CLA	b	835	6	-	11/31/107/115	-
22	CLA	a	825	5	-	10/27/103/115	-
22	CLA	b	828	-	-	13/39/115/115	-
22	CLA	a	844	21	-	16/39/115/115	-
22	CLA	b	801	-	-	22/39/115/115	-
22	CLA	a	815	-	-	2/15/91/115	-
22	CLA	1	308	4	-	13/39/115/115	-
22	CLA	b	827	6	-	14/39/115/115	-
22	CLA	1	313	4	-	5/10/86/115	-
22	CLA	b	837	6	-	10/39/115/115	-
22	CLA	1	306	-	-	15/39/115/115	-
22	CLA	9	312	-	-	9/17/93/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	1	312	4	-	3/24/100/115	-
22	CLA	a	854	-	-	15/39/115/115	-
22	CLA	1	311	-	-	6/25/101/115	-
19	XAT	8	302	-	-	4/31/93/93	0/4/4/4
22	CLA	9	316	6	-	17/39/115/115	-
22	CLA	7	313	-	-	7/26/102/115	-
22	CLA	a	804	5	-	10/27/103/115	-
28	LMG	j	105	-	-	11/27/47/70	0/1/1/1
26	BCR	b	843	-	-	2/29/63/63	0/2/2/2
22	CLA	8	305	2	-	2/13/89/115	-
19	XAT	8	303	-	-	0/31/93/93	0/4/4/4
22	CLA	a	819	5	-	6/26/102/115	-
22	CLA	b	813	-	-	14/39/115/115	-
22	CLA	7	315	3	-	6/10/86/115	-
22	CLA	a	821	5	-	2/15/91/115	-
22	CLA	8	312	2	-	2/24/100/115	-
26	BCR	a	848	-	-	0/29/63/63	0/2/2/2
26	BCR	b	846	-	-	2/29/63/63	0/2/2/2
22	CLA	9	310	1	-	6/17/93/115	-
19	XAT	1	303	-	-	0/31/93/93	0/4/4/4
22	CLA	a	816	5	-	5/21/97/115	-
21	LHG	a	845	-	-	27/52/52/53	-
22	CLA	a	829	5	-	15/36/112/115	-
21	LHG	a	846	22	-	16/31/31/53	-
19	XAT	1	302	-	-	0/31/93/93	0/4/4/4
22	CLA	b	805	6	-	12/39/115/115	-
22	CLA	7	308	-	-	14/33/109/115	-
22	CLA	h	203	-	-	9/39/115/115	-
22	CLA	a	814	5	-	20/39/115/115	-
22	CLA	l	202	-	-	2/12/88/115	-
22	CLA	9	311	1	-	8/17/93/115	-
22	CLA	b	814	-	-	13/27/103/115	-
22	CLA	h	205	10	-	9/27/103/115	-
26	BCR	a	847	-	-	0/29/63/63	0/2/2/2
22	CLA	a	835	-	-	12/39/115/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	1	305	-	-	12/35/111/115	-
22	CLA	a	828	5	-	9/39/115/115	-
22	CLA	a	827	-	-	8/39/115/115	-
22	CLA	b	834	-	-	10/25/101/115	-
25	PQN	a	843	-	-	5/23/43/43	0/2/2/2
26	BCR	a	850	-	-	4/29/63/63	0/2/2/2
22	CLA	a	830	5	-	15/39/115/115	-
22	CLA	a	822	-	-	5/39/115/115	-
22	CLA	a	837	5	-	6/15/91/115	-
22	CLA	b	810	-	-	16/39/115/115	-
18	A1L1F	8	304	-	-	12/43/99/99	0/3/3/3
28	LMG	a	853	-	-	13/29/49/70	0/1/1/1
22	CLA	a	826	-	-	10/39/115/115	-
22	CLA	j	103	12	-	7/12/88/115	-
22	CLA	a	834	-	-	9/39/115/115	-
26	BCR	l	201	-	-	4/29/63/63	0/2/2/2
22	CLA	1	314	4	-	7/15/91/115	-
22	CLA	b	822	6	-	7/33/109/115	-
25	PQN	b	841	-	-	1/23/43/43	0/2/2/2
22	CLA	a	802	-	-	7/31/107/115	-
22	CLA	8	306	23	-	4/17/93/115	-
22	CLA	7	310	-	-	6/17/93/115	-
22	CLA	a	818	5	-	11/29/105/115	-
22	CLA	l	203	-	-	6/33/109/115	-
22	CLA	a	840	5	-	9/39/115/115	-
22	CLA	b	836	-	-	8/39/115/115	-
22	CLA	b	802	-	-	17/39/115/115	-
23	DGD	b	848	-	-	20/46/86/95	0/2/2/2
22	CLA	9	315	1	-	6/12/88/115	-
22	CLA	b	806	6	-	16/39/115/115	-
19	XAT	9	304	-	-	1/31/93/93	0/4/4/4
22	CLA	7	311	-	-	5/17/93/115	-
18	A1L1F	1	304	-	-	12/43/99/99	0/3/3/3
22	CLA	j	102	6	-	18/31/107/115	-
27	SF4	a	851	-	-	-	0/6/5/5

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	BCR	h	202	-	-	2/29/63/63	0/2/2/2
22	CLA	b	817	6	-	12/32/108/115	-
26	BCR	b	842	-	-	2/29/63/63	0/2/2/2
21	LHG	9	317	-	-	28/50/50/53	-
26	BCR	a	849	-	-	0/29/63/63	0/2/2/2
26	BCR	l	205	-	-	8/29/63/63	0/2/2/2
26	BCR	j	104	-	-	4/29/63/63	0/2/2/2
19	XAT	9	303	-	-	4/31/93/93	0/4/4/4
22	CLA	8	311	-	-	8/29/105/115	-
22	CLA	b	819	-	-	5/27/103/115	-
22	CLA	7	316	3	-	11/23/99/115	-
22	CLA	b	838	-	-	15/39/115/115	-
22	CLA	9	308	1	-	15/39/115/115	-
22	CLA	a	836	5	-	8/21/97/115	-
22	CLA	7	309	3	-	5/17/93/115	-
22	CLA	a	803	-	-	3/39/115/115	-
22	CLA	b	807	6	-	19/39/115/115	-
26	BCR	b	844	-	-	6/29/63/63	0/2/2/2
22	CLA	a	806	5	-	12/39/115/115	-
20	45D	9	305	-	-	9/29/69/69	0/2/2/2
19	XAT	7	304	-	-	6/31/93/93	0/4/4/4
22	CLA	a	824	5	-	6/17/93/115	-
22	CLA	9	309	1	-	5/17/93/115	-
22	CLA	7	312	-	-	3/19/95/115	-
22	CLA	b	839	6	-	17/39/115/115	-
22	CLA	a	832	5	-	7/21/97/115	-
19	XAT	7	301	-	-	6/31/93/93	0/4/4/4
22	CLA	b	812	6	-	6/25/101/115	-
22	CLA	b	815	6	-	3/15/91/115	-
23	DGD	8	315	22	-	11/29/69/95	0/2/2/2
22	CLA	a	841	5	-	17/39/115/115	-
26	BCR	f	801	-	-	3/29/63/63	0/2/2/2
22	CLA	a	807	-	-	20/39/115/115	-
26	BCR	f	804	-	-	4/29/63/63	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	9	313	1	-	11/17/93/115	-
22	CLA	8	310	-	-	7/17/93/115	-
22	CLA	b	823	-	-	10/25/101/115	-
19	XAT	j	101	-	-	5/31/93/93	0/4/4/4
22	CLA	7	307	-	-	7/15/91/115	-
17	A1L1G	9	301	-	-	16/29/85/85	0/3/3/3
22	CLA	7	314	-	-	6/15/91/115	-
22	CLA	a	820	5	-	15/39/115/115	-
26	BCR	m	101	-	-	9/29/63/63	0/2/2/2
22	CLA	a	842	5	-	9/39/115/115	-
22	CLA	b	830	6	-	3/10/86/115	-
22	CLA	a	839	5	-	15/39/115/115	-
22	CLA	8	314	-	-	7/10/86/115	-
22	CLA	a	811	5	-	8/29/105/115	-
22	CLA	f	802	-	-	13/39/115/115	-
22	CLA	a	810	5	-	15/39/115/115	-
22	CLA	b	809	6	-	13/39/115/115	-
21	LHG	9	307	-	-	21/40/40/53	-
22	CLA	a	812	22,5	-	9/36/112/115	-
22	CLA	9	318	-	-	11/36/112/115	-
21	LHG	b	847	22	-	20/35/35/53	-
22	CLA	b	825	-	-	6/38/114/115	-
27	SF4	c	101	-	-	-	0/6/5/5
19	XAT	a	852	-	-	7/31/93/93	0/4/4/4
26	BCR	h	201	-	-	0/29/63/63	0/2/2/2
22	CLA	a	805	22,5	-	6/27/103/115	-
22	CLA	b	818	6	-	16/33/109/115	-
19	XAT	7	303	-	-	8/31/93/93	0/4/4/4
22	CLA	1	310	4	-	18/39/115/115	-
19	XAT	8	301	-	-	3/31/93/93	0/4/4/4
26	BCR	i	101	-	-	3/29/63/63	0/2/2/2
24	SQD	1	315	-	-	19/40/60/69	0/1/1/1
22	CLA	8	309	-	-	8/30/106/115	-
22	CLA	b	804	-	-	10/39/115/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	b	831	6	-	6/20/96/115	-
22	CLA	a	838	5	-	6/23/99/115	-
22	CLA	b	816	-	-	4/27/103/115	-
22	CLA	a	817	-	-	8/15/91/115	-
26	BCR	b	849	-	-	5/29/63/63	0/2/2/2
22	CLA	7	317	-	-	7/15/91/115	-

The worst 5 of 1147 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	a	843	PQN	C3-C2	7.58	1.49	1.35
25	b	841	PQN	C3-C2	7.33	1.48	1.35
25	a	843	PQN	C10-C5	4.88	1.48	1.40
25	b	841	PQN	C10-C5	4.83	1.48	1.40
18	9	302	A1L1F	O7-C54	4.62	1.45	1.35

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	9	302	A1L1F	O15-C20-C21	13.20	123.30	113.38
18	8	304	A1L1F	O15-C20-C21	8.53	119.79	113.38
18	9	302	A1L1F	C17-C20-C25	-8.46	108.08	122.26
18	h	204	A1L1F	O15-C20-C21	8.43	119.72	113.38
18	h	204	A1L1F	C17-C20-C25	-8.37	108.23	122.26

There are no chirality outliers.

5 of 1708 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
17	9	301	A1L1G	O13-C26-C30-C29
17	9	301	A1L1G	C26-C30-C31-C32
17	9	301	A1L1G	C31-C32-C33-C34
17	9	301	A1L1G	C28-C39-C40-C41
17	9	301	A1L1G	C38-C39-C40-C41

All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
18	h	204	A1L1F	C1-C11-C3-C4-C6-C8

170 monomers are involved in 528 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	9	302	A1L1F	2	0
22	a	833	CLA	2	0
22	8	307	CLA	6	0
22	b	803	CLA	3	0
18	h	204	A1L1F	4	0
22	b	833	CLA	3	0
22	8	308	CLA	1	0
27	c	102	SF4	2	0
22	8	313	CLA	3	0
17	7	302	A1L1G	2	0
22	a	831	CLA	4	0
22	9	314	CLA	7	0
22	b	832	CLA	3	0
22	b	826	CLA	3	0
17	9	306	A1L1G	1	0
22	b	821	CLA	2	0
19	7	305	XAT	2	0
22	b	808	CLA	2	0
17	1	301	A1L1G	1	0
22	a	801	CLA	7	0
22	a	808	CLA	1	0
26	b	845	BCR	5	0
22	b	829	CLA	4	0
22	a	823	CLA	3	0
22	b	820	CLA	2	0
22	7	306	CLA	2	0
22	b	840	CLA	6	0
22	b	811	CLA	3	0
22	a	809	CLA	3	0
22	b	824	CLA	8	0
22	b	835	CLA	4	0
22	a	825	CLA	4	0
22	b	828	CLA	3	0
22	a	844	CLA	6	0
22	b	801	CLA	5	0
22	1	308	CLA	3	0
22	b	827	CLA	3	0
22	b	837	CLA	6	0
22	1	306	CLA	5	0
22	9	312	CLA	3	0
22	1	312	CLA	2	0
22	a	854	CLA	3	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	1	311	CLA	2	0
19	8	302	XAT	8	0
22	9	316	CLA	6	0
22	7	313	CLA	4	0
22	a	804	CLA	4	0
28	j	105	LMG	7	0
26	b	843	BCR	2	0
22	8	305	CLA	5	0
19	8	303	XAT	7	0
22	a	819	CLA	5	0
22	b	813	CLA	7	0
22	7	315	CLA	2	0
22	8	312	CLA	3	0
26	a	848	BCR	5	0
26	b	846	BCR	3	0
22	9	310	CLA	2	0
19	1	303	XAT	3	0
22	a	816	CLA	2	0
21	a	845	LHG	4	0
22	a	829	CLA	6	0
21	a	846	LHG	3	0
19	1	302	XAT	3	0
22	b	805	CLA	4	0
22	7	308	CLA	7	0
22	h	203	CLA	4	0
22	a	814	CLA	3	0
22	l	202	CLA	1	0
22	9	311	CLA	2	0
22	b	814	CLA	3	0
22	h	205	CLA	2	0
26	a	847	BCR	4	0
22	a	835	CLA	5	0
22	a	828	CLA	4	0
22	a	827	CLA	3	0
25	a	843	PQN	3	0
26	a	850	BCR	2	0
22	a	830	CLA	7	0
22	a	822	CLA	5	0
22	a	837	CLA	1	0
22	b	810	CLA	1	0
18	8	304	A1L1F	2	0
28	a	853	LMG	10	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	a	826	CLA	6	0
22	j	103	CLA	2	0
22	a	834	CLA	5	0
26	l	201	BCR	3	0
22	b	822	CLA	6	0
25	b	841	PQN	2	0
22	a	802	CLA	5	0
22	8	306	CLA	1	0
22	7	310	CLA	1	0
22	a	818	CLA	11	0
22	l	203	CLA	2	0
22	a	840	CLA	6	0
22	b	836	CLA	5	0
22	b	802	CLA	4	0
23	b	848	DGD	6	0
22	9	315	CLA	1	0
22	b	806	CLA	2	0
19	9	304	XAT	6	0
22	7	311	CLA	3	0
18	1	304	A1L1F	2	0
22	j	102	CLA	7	0
26	h	202	BCR	4	0
22	b	817	CLA	8	0
26	b	842	BCR	4	0
21	9	317	LHG	3	0
26	a	849	BCR	3	0
26	l	205	BCR	9	0
26	j	104	BCR	9	0
19	9	303	XAT	8	0
22	8	311	CLA	3	0
22	b	819	CLA	1	0
22	7	316	CLA	2	0
22	b	838	CLA	4	0
22	9	308	CLA	6	0
22	a	836	CLA	1	0
22	a	803	CLA	5	0
22	b	807	CLA	7	0
26	b	844	BCR	5	0
22	a	806	CLA	9	0
20	9	305	45D	8	0
19	7	304	XAT	12	0
22	a	824	CLA	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	9	309	CLA	1	0
22	7	312	CLA	1	0
22	b	839	CLA	5	0
22	a	832	CLA	2	0
19	7	301	XAT	3	0
22	b	812	CLA	4	0
23	8	315	DGD	2	0
22	a	841	CLA	7	0
26	f	801	BCR	9	0
22	a	807	CLA	4	0
26	f	804	BCR	6	0
22	9	313	CLA	2	0
22	b	823	CLA	6	0
19	j	101	XAT	6	0
22	7	307	CLA	2	0
17	9	301	A1L1G	2	0
22	7	314	CLA	3	0
22	a	820	CLA	6	0
26	m	101	BCR	1	0
22	a	842	CLA	3	0
22	b	830	CLA	5	0
22	a	839	CLA	6	0
22	8	314	CLA	1	0
22	f	802	CLA	1	0
22	a	810	CLA	4	0
22	b	809	CLA	3	0
21	9	307	LHG	2	0
22	9	318	CLA	6	0
22	b	825	CLA	2	0
19	a	852	XAT	6	0
26	h	201	BCR	1	0
22	a	805	CLA	1	0
22	b	818	CLA	3	0
19	7	303	XAT	11	0
22	1	310	CLA	2	0
19	8	301	XAT	2	0
26	i	101	BCR	2	0
24	1	315	SQD	3	0
22	8	309	CLA	1	0
22	b	804	CLA	4	0
22	b	831	CLA	2	0
22	a	838	CLA	1	0

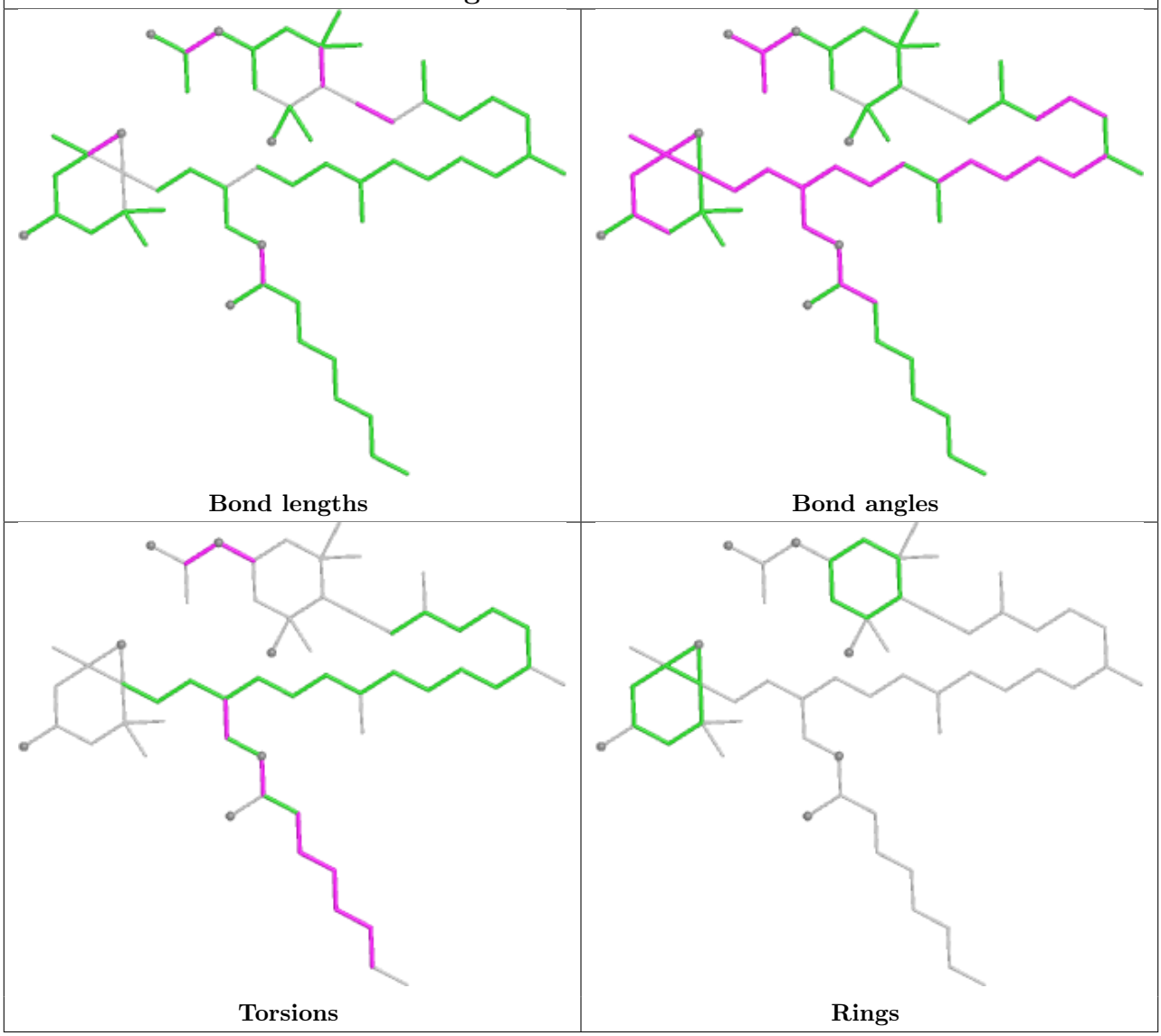
Continued on next page...

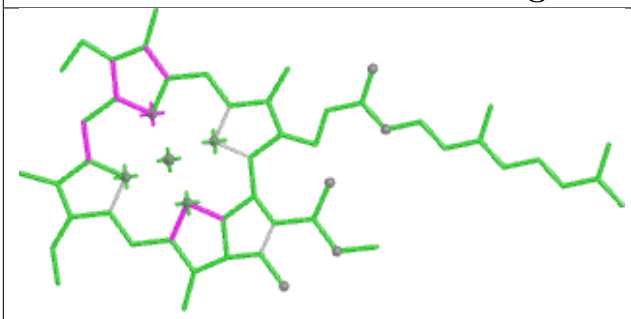
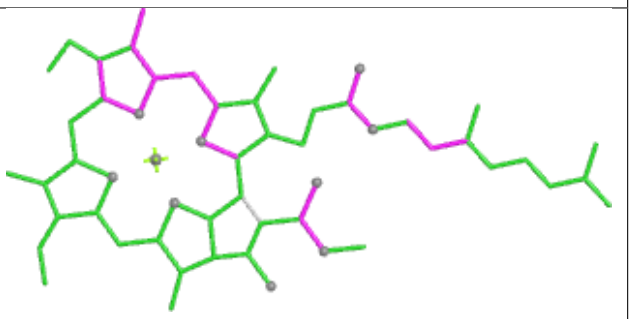
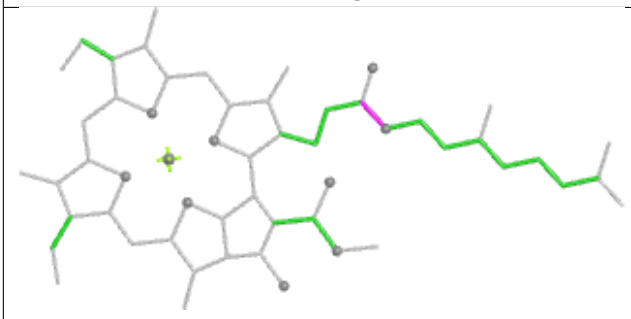
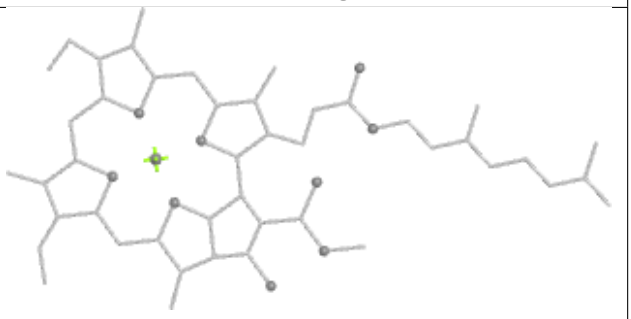
Continued from previous page...

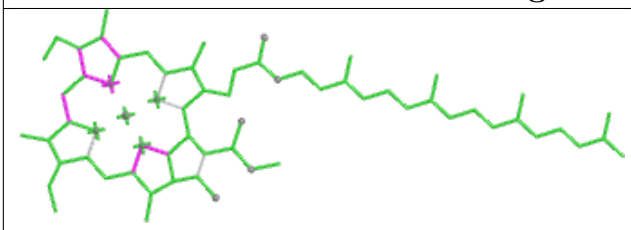
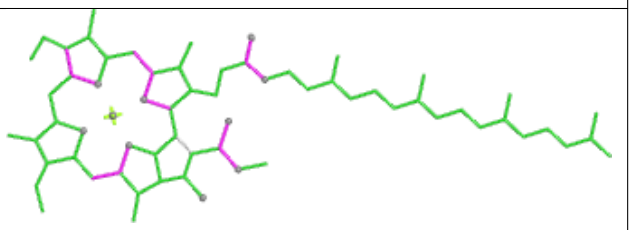
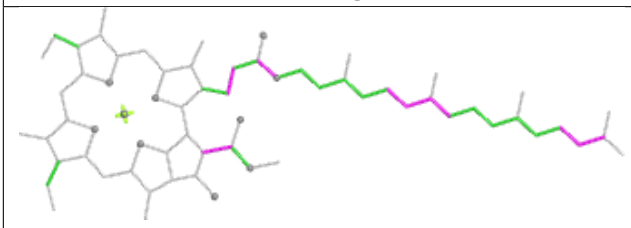
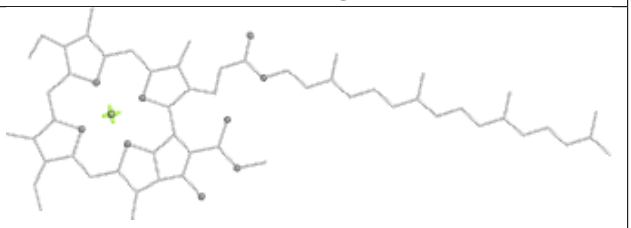
Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	b	816	CLA	6	0
26	b	849	BCR	6	0

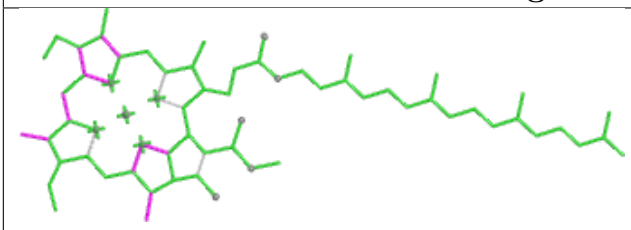
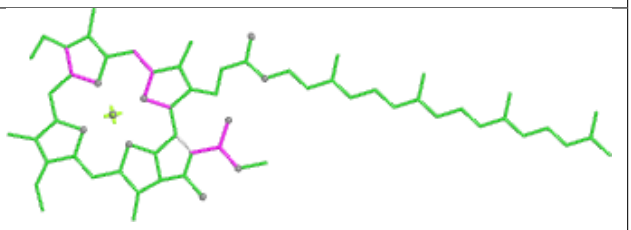
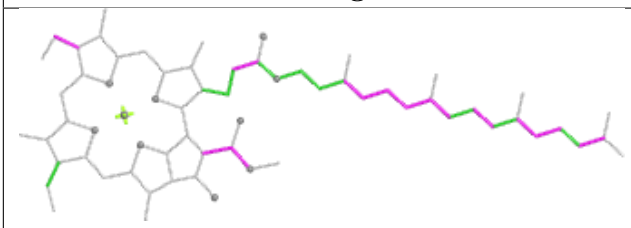
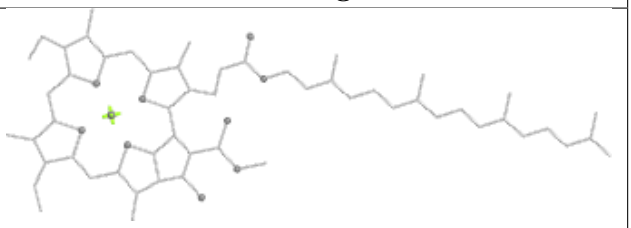
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

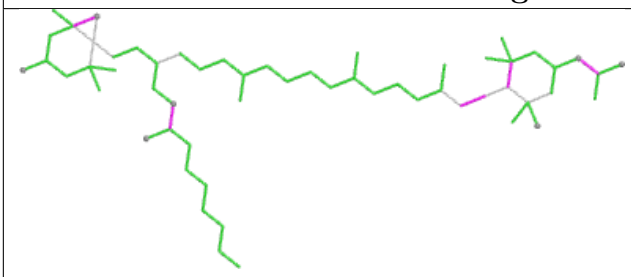
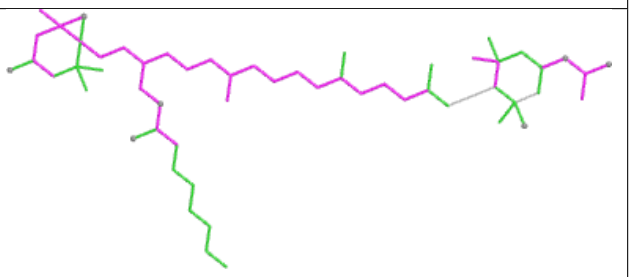
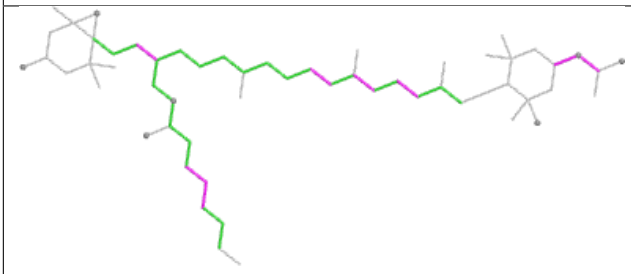
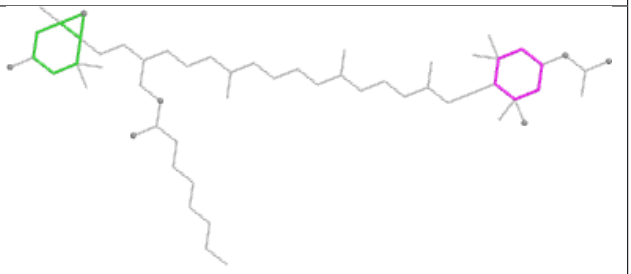
Ligand A1L1F 9 302

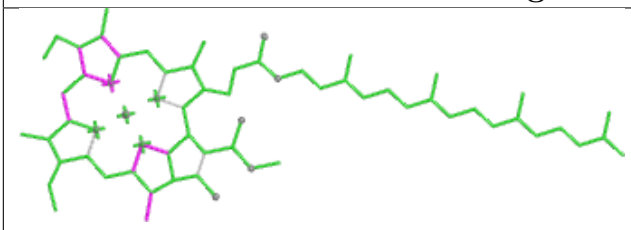
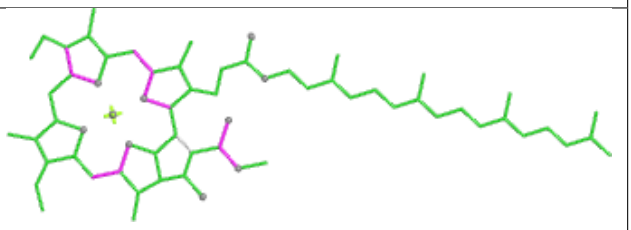
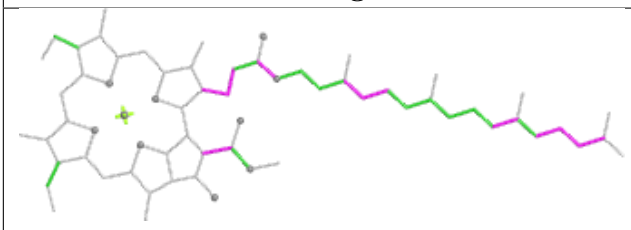
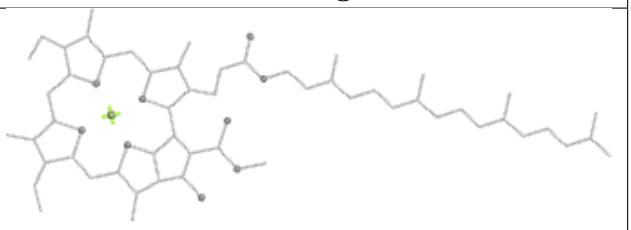


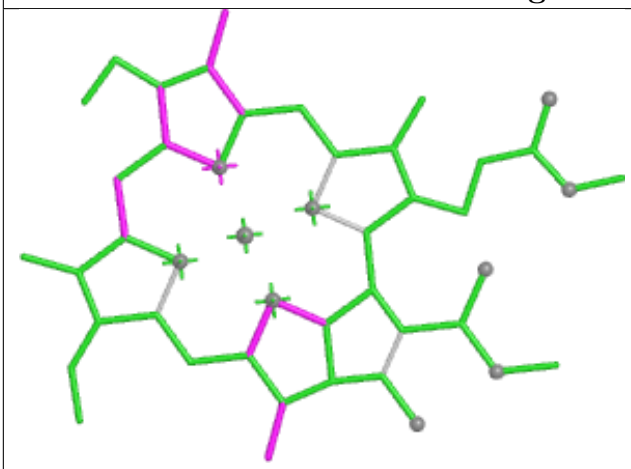
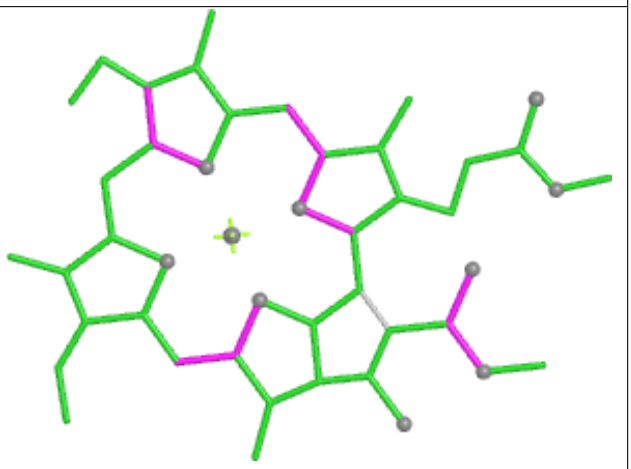
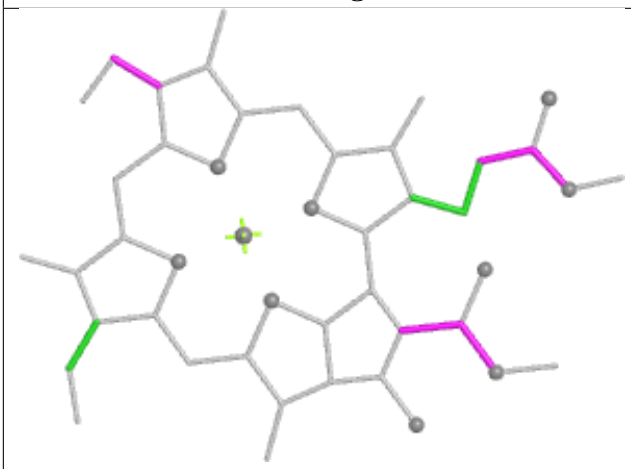
Ligand CLA a 833	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA 8 307	
 Bond lengths	 Bond angles
 Torsions	 Rings

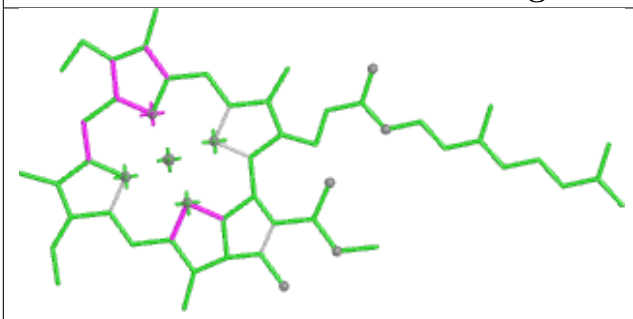
Ligand CLA b 803	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand A1L1F h 204	
 Bond lengths	 Bond angles
 Torsions	 Rings

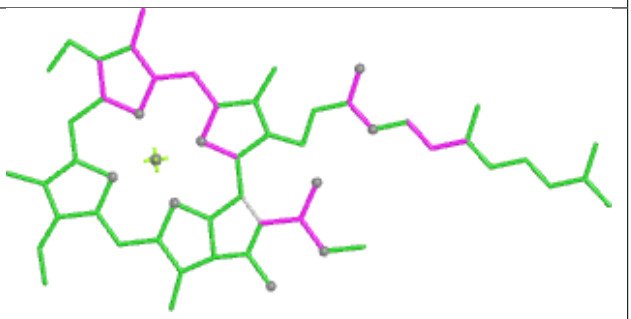
Ligand CLA b 833	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA 1 309	
 Bond lengths	 Bond angles
 Torsions	Rings

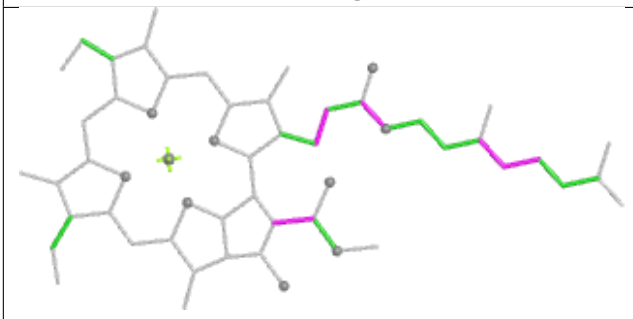
Ligand CLA 8 308



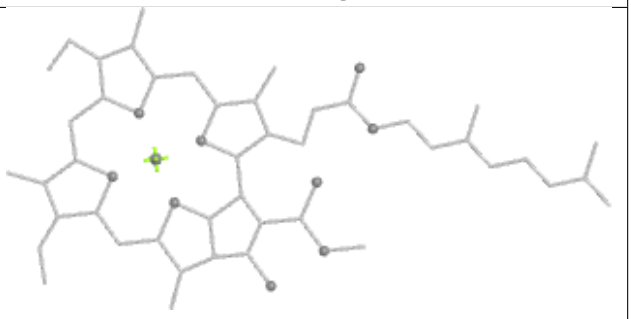
Bond lengths



Bond angles

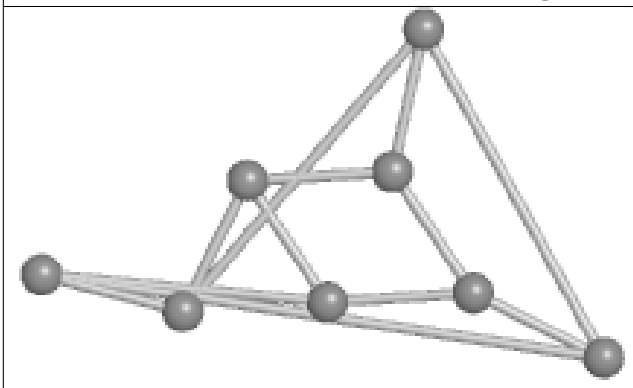


Torsions

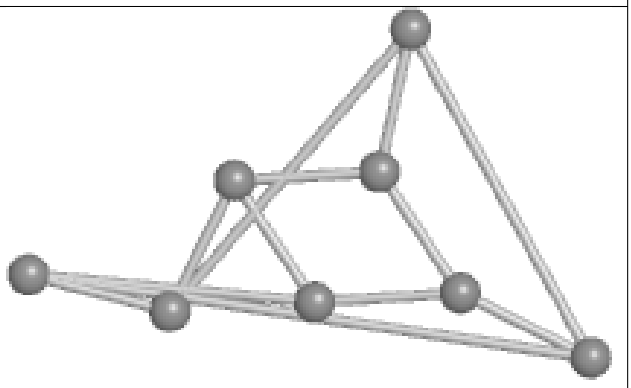


Rings

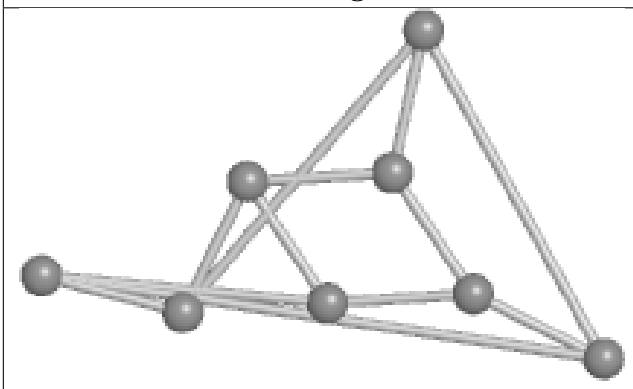
Ligand SF4 c 102



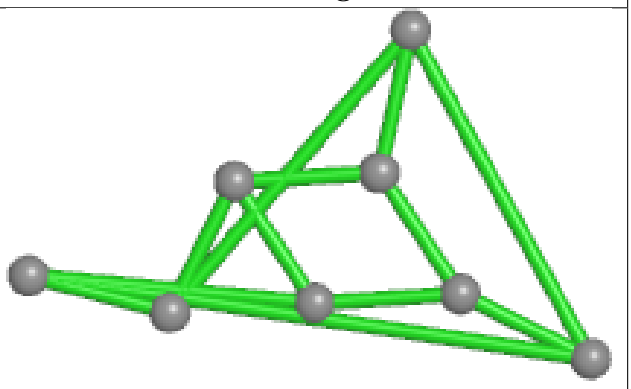
Bond lengths



Bond angles

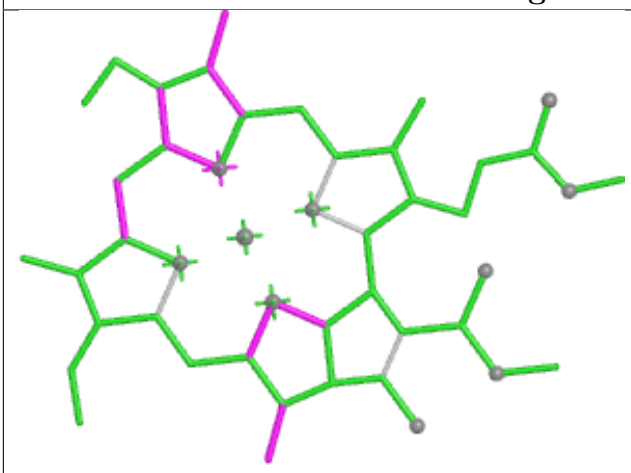


Torsions

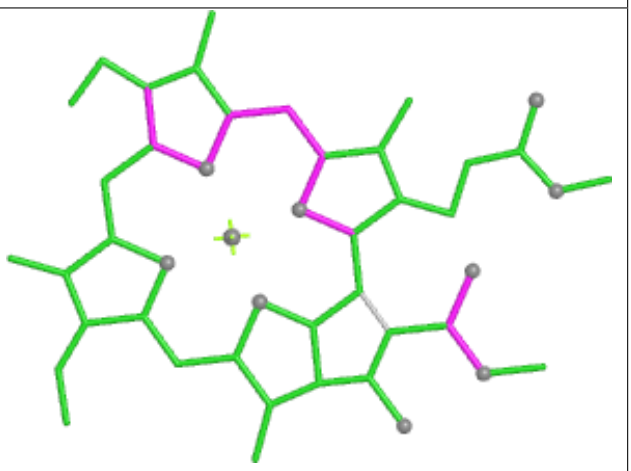


Rings

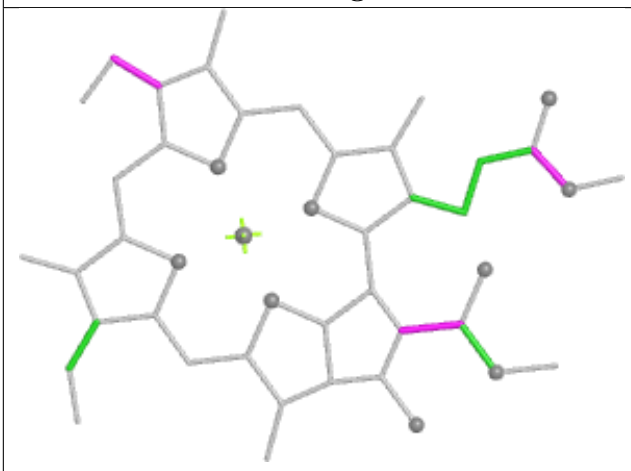
Ligand CLA 8 313



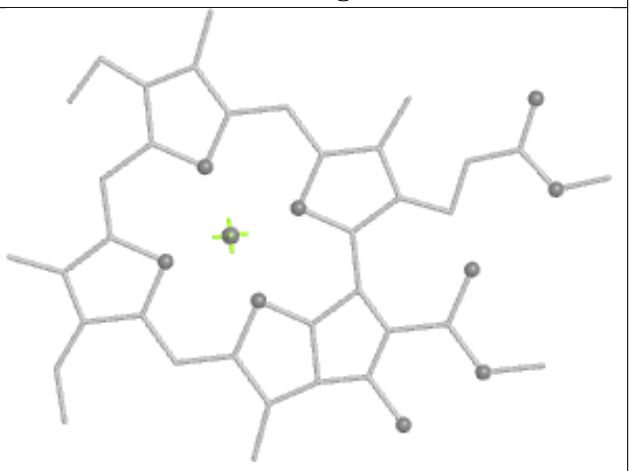
Bond lengths



Bond angles

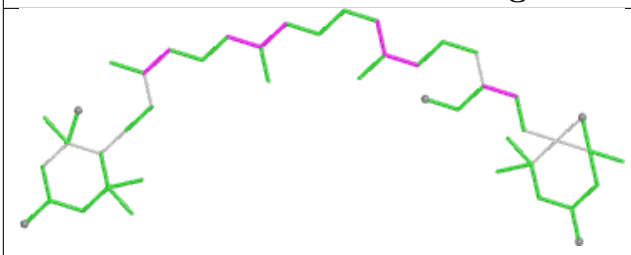


Torsions

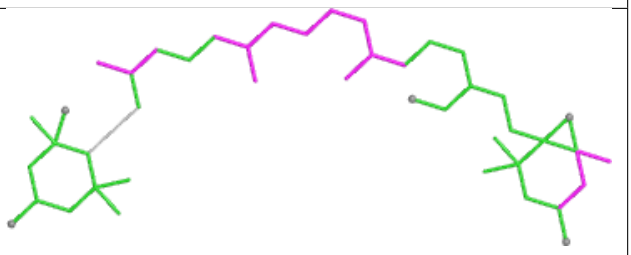


Rings

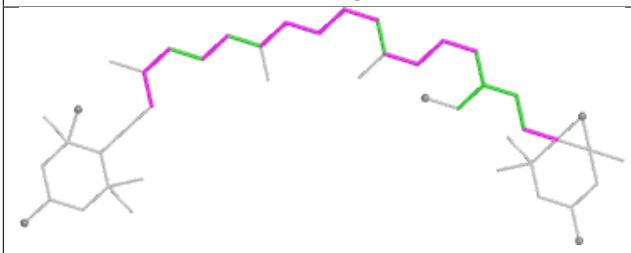
Ligand A1L1G 7 302



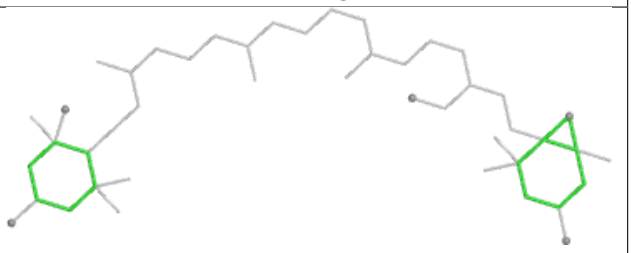
Bond lengths



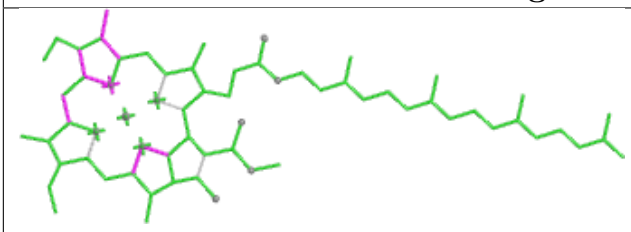
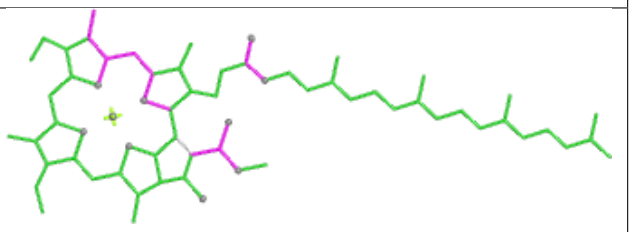
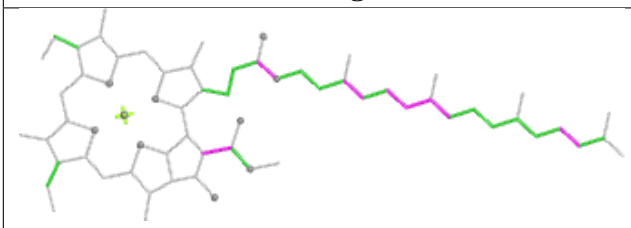
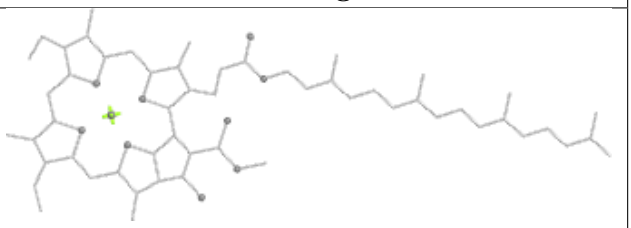
Bond angles

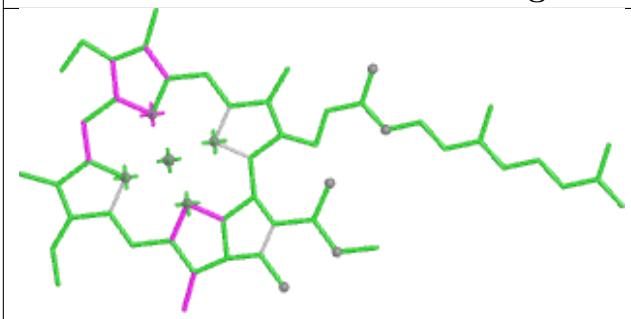
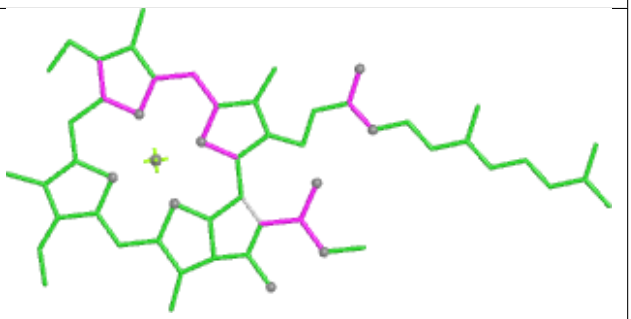
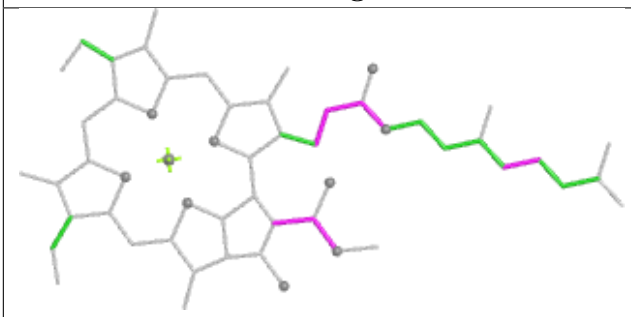
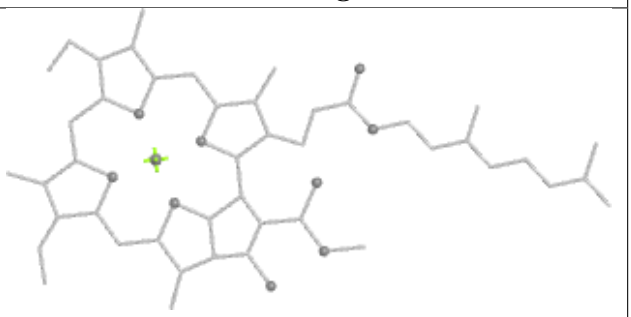


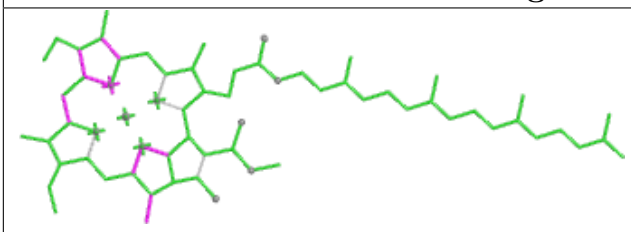
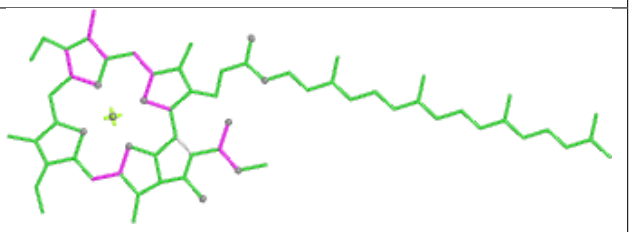
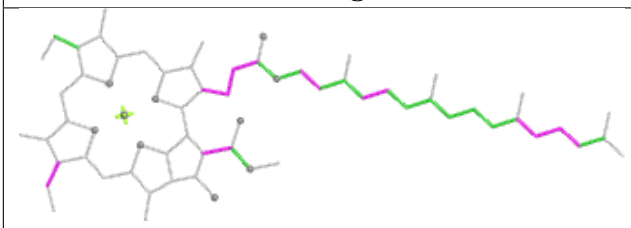
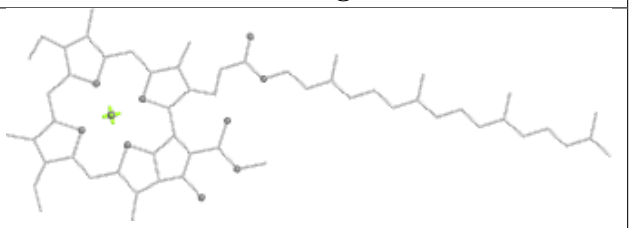
Torsions

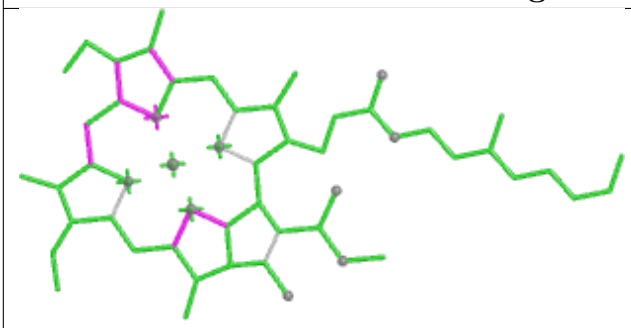
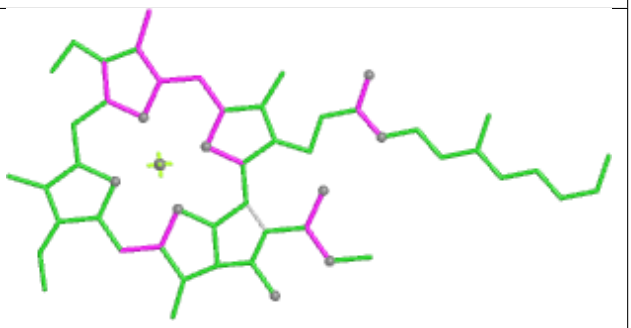
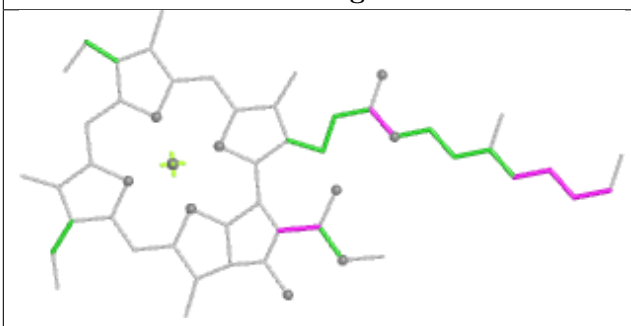
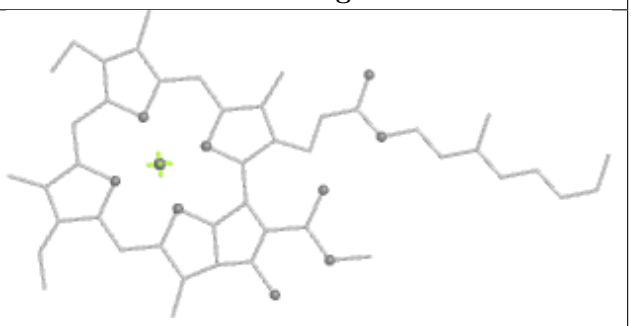


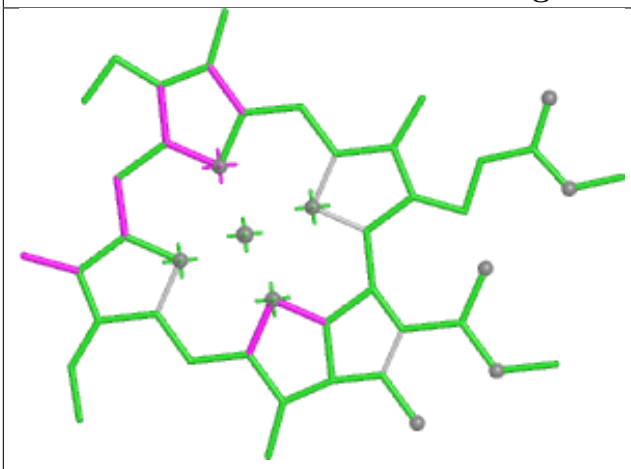
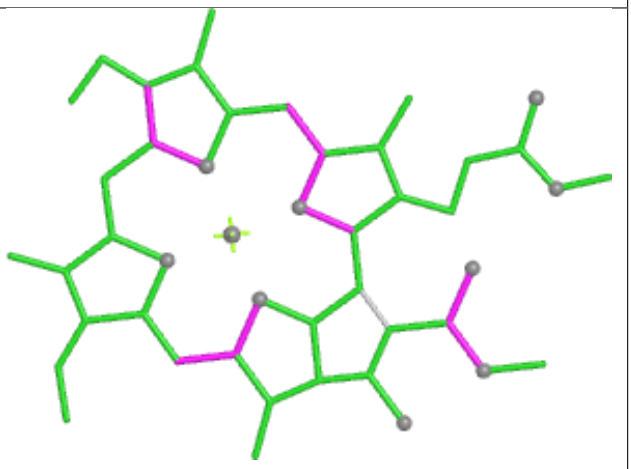
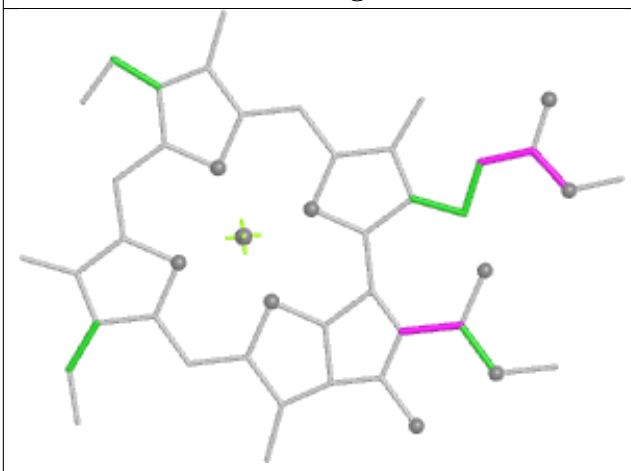
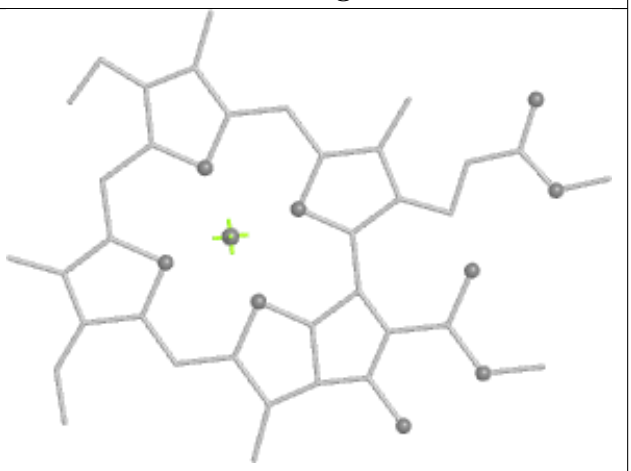
Rings

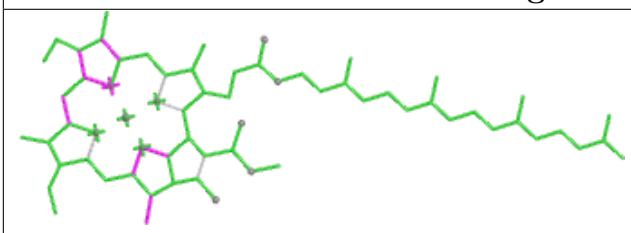
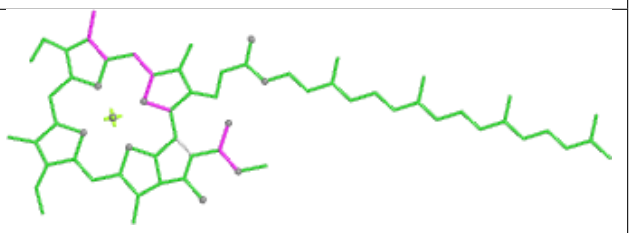
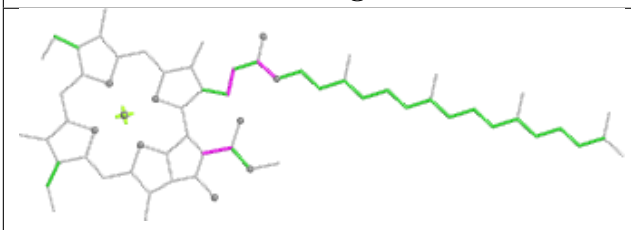
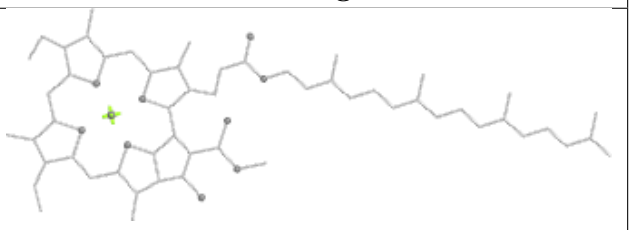
Ligand CLA a 831	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA 9 314	
 Bond lengths	 Bond angles
 Torsions	 Rings

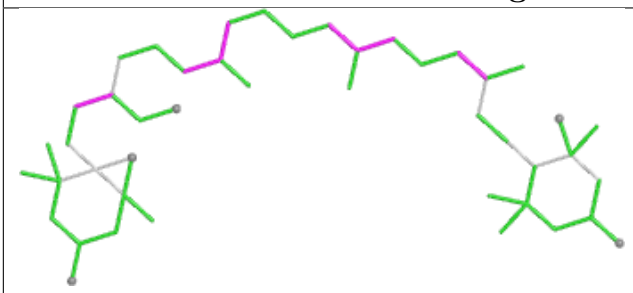
Ligand CLA b 832	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA 1 307	
 Bond lengths	 Bond angles
 Torsions	 Rings

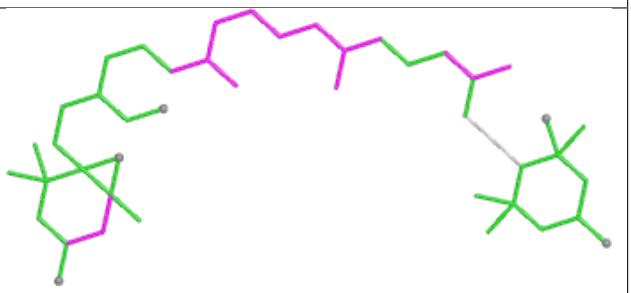
Ligand CLA l 204	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA b 826	
 Bond lengths	 Bond angles
 Torsions	 Rings

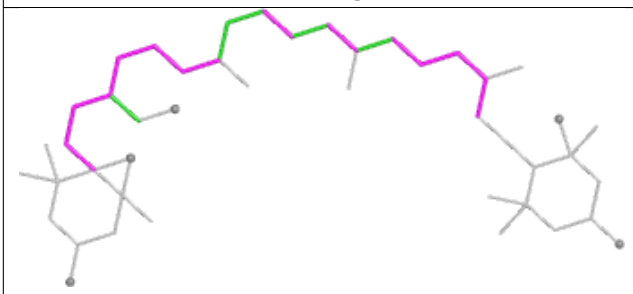
Ligand A1L1G 9 306



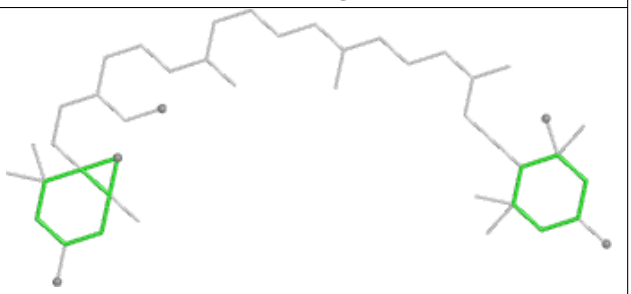
Bond lengths



Bond angles

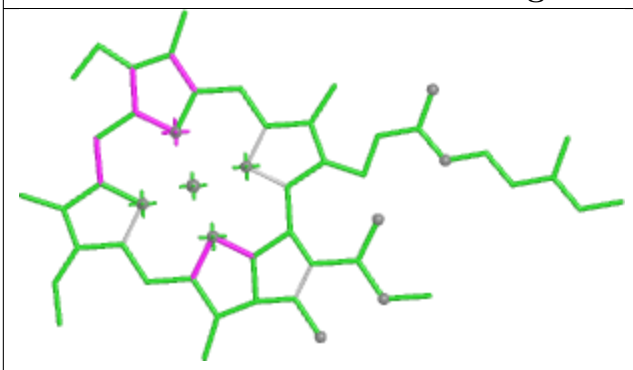


Torsions

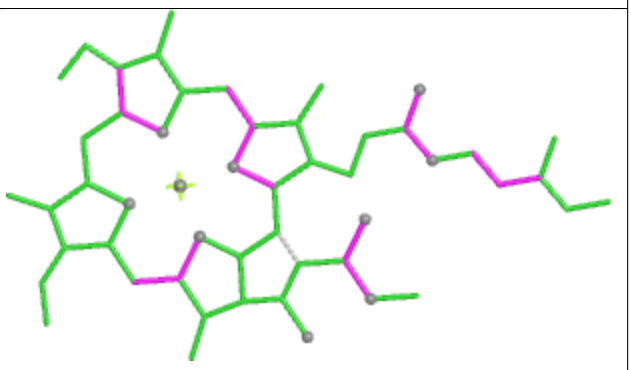


Rings

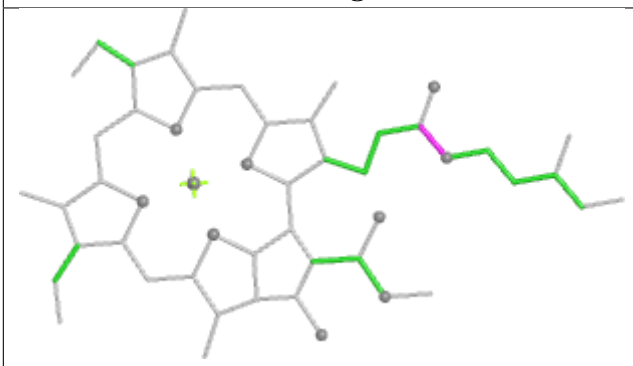
Ligand CLA b 821



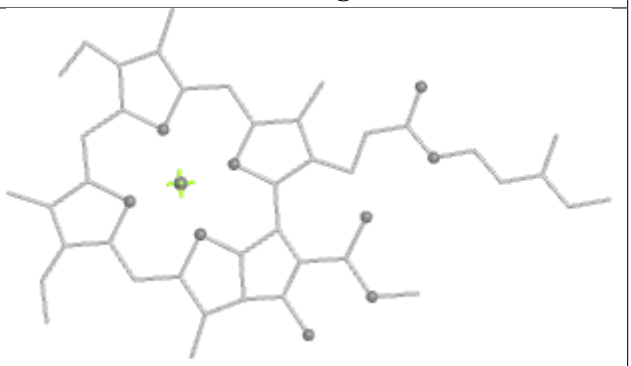
Bond lengths



Bond angles

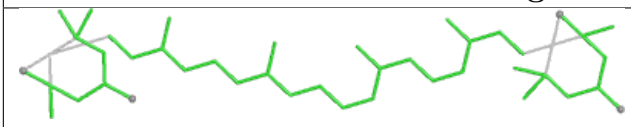


Torsions

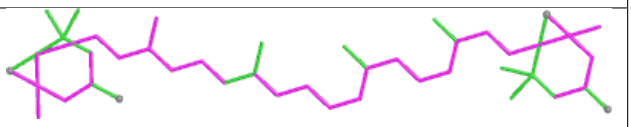


Rings

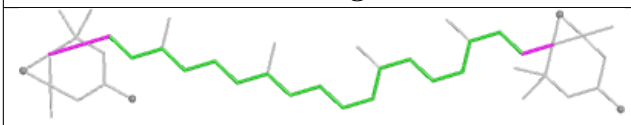
Ligand XAT 7 305



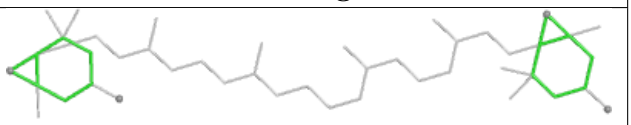
Bond lengths



Bond angles

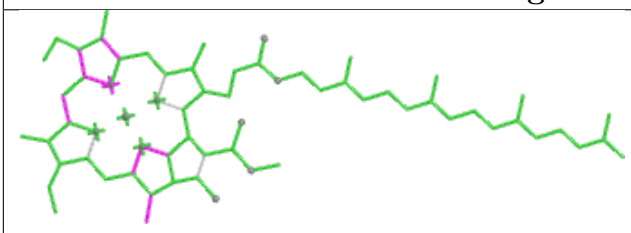


Torsions

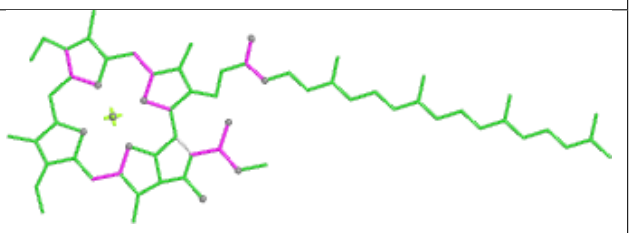


Rings

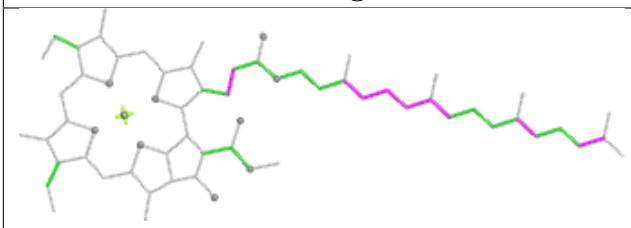
Ligand CLA b 808



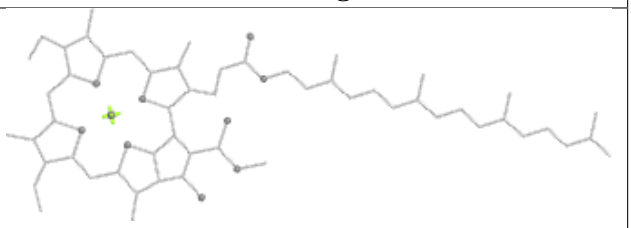
Bond lengths



Bond angles

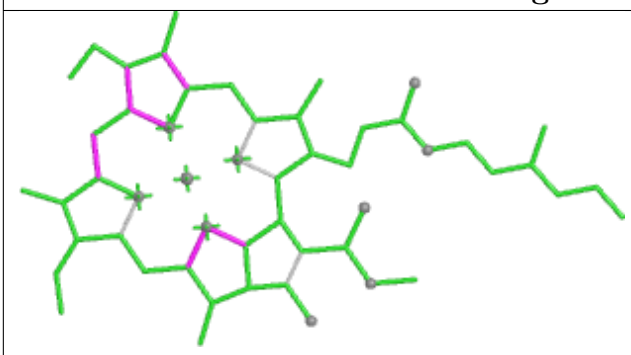


Torsions

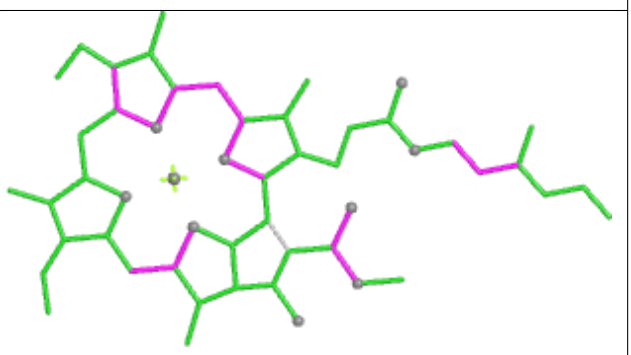


Rings

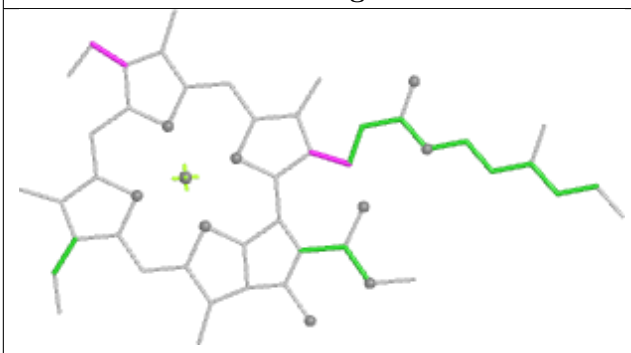
Ligand CLA f 803



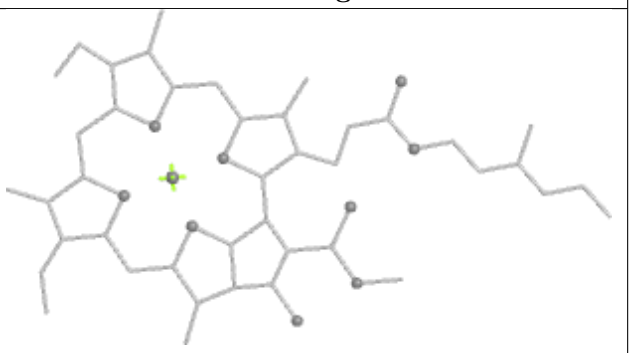
Bond lengths



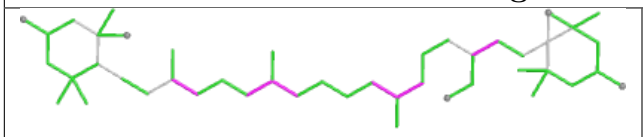
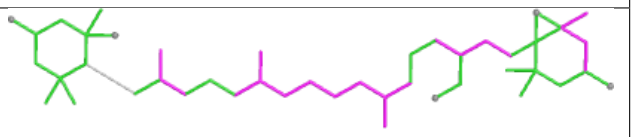
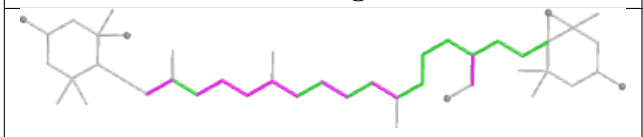
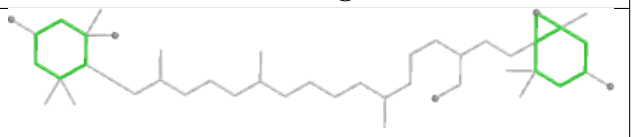
Bond angles

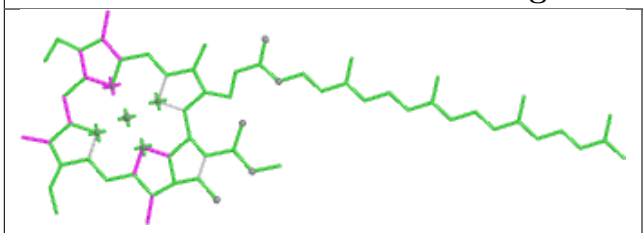
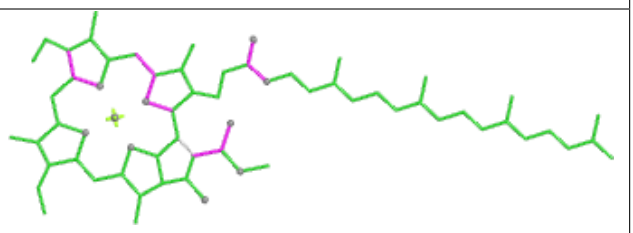
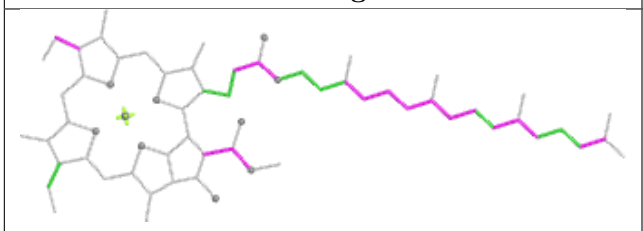
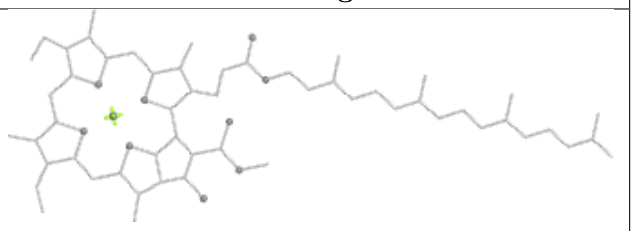


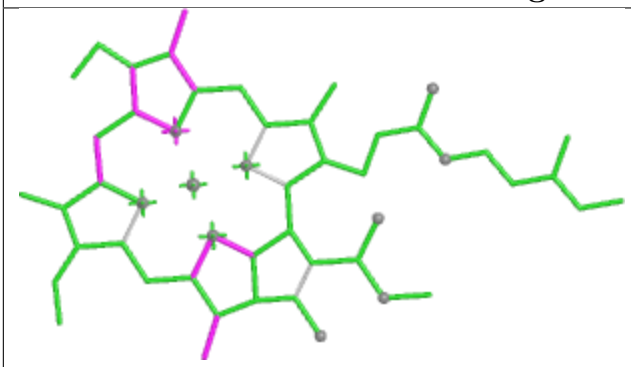
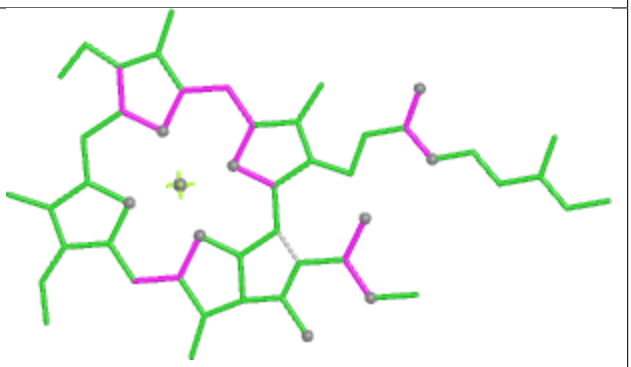
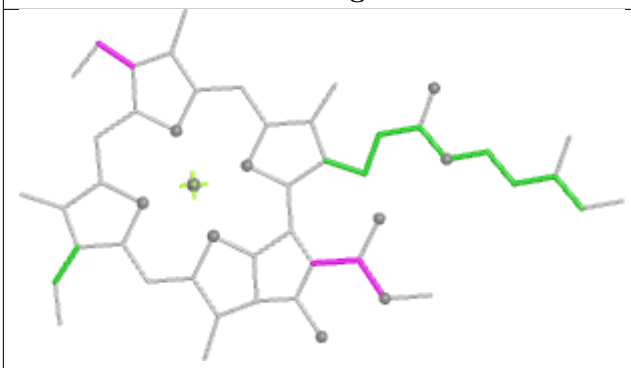
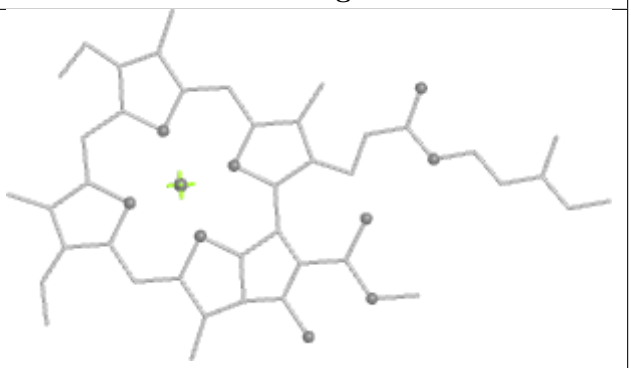
Torsions

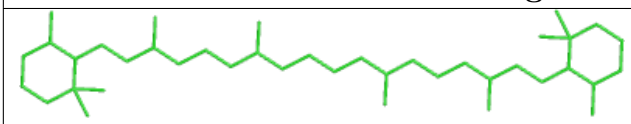
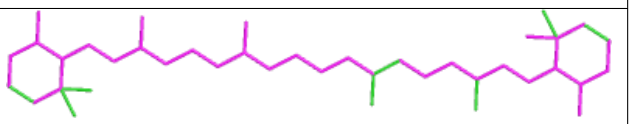
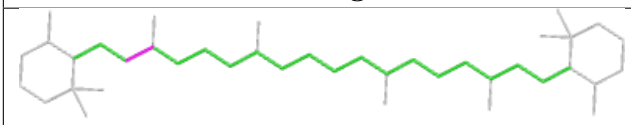
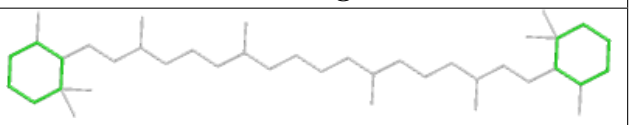


Rings

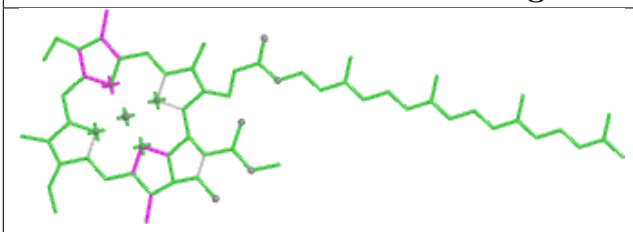
Ligand A1L1G 1 301	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA a 801	
 Bond lengths	 Bond angles
 Torsions	 Rings

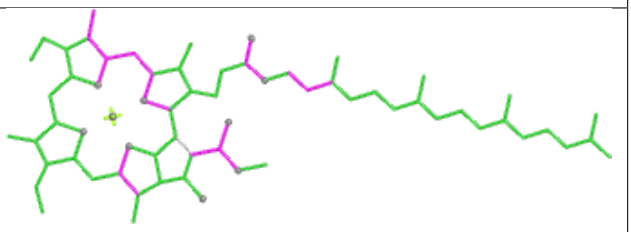
Ligand CLA a 808	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand BCR b 845	
 Bond lengths	 Bond angles
 Torsions	 Rings

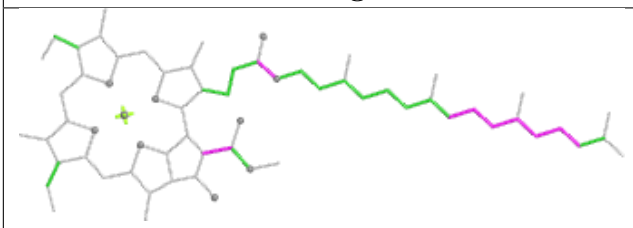
Ligand CLA b 829



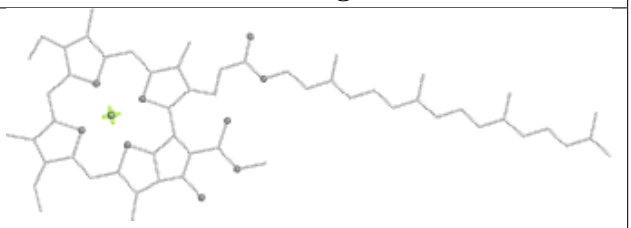
Bond lengths



Bond angles

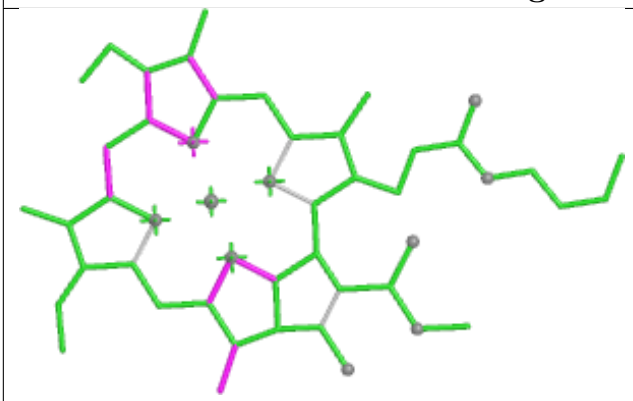


Torsions

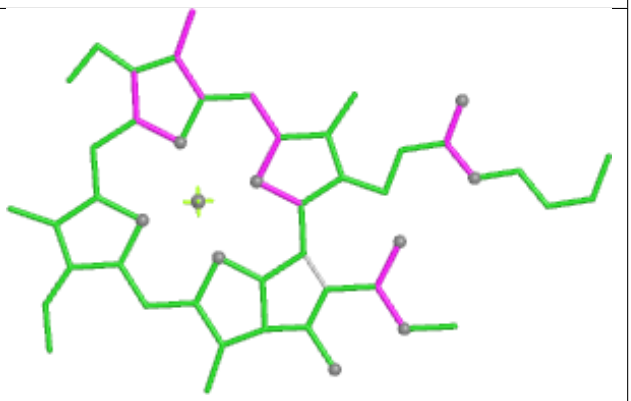


Rings

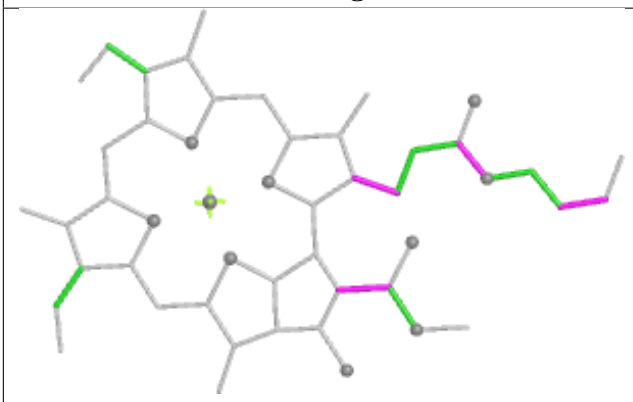
Ligand CLA a 823



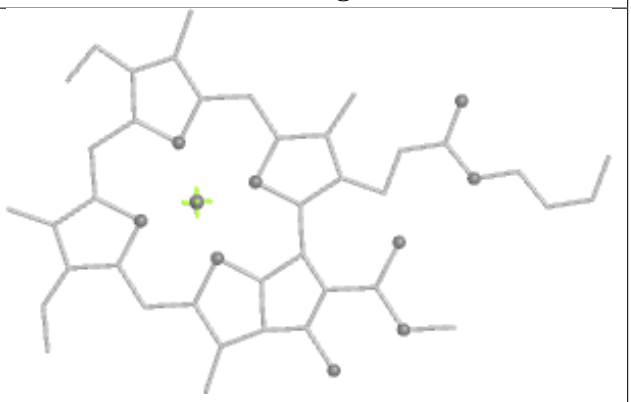
Bond lengths



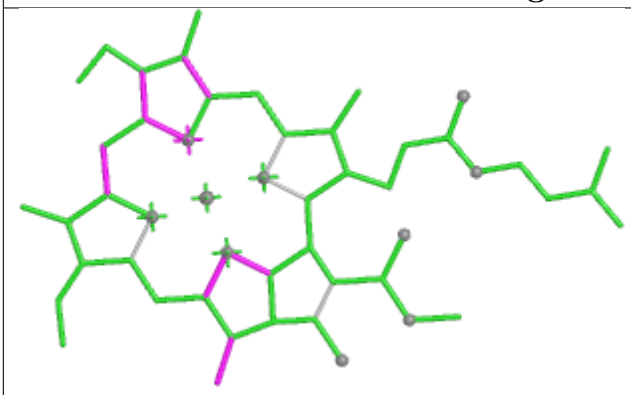
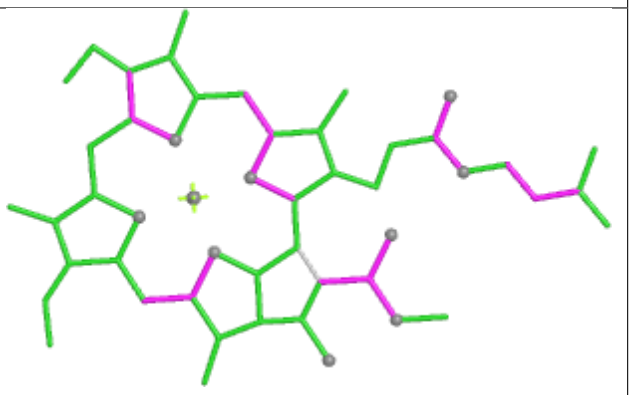
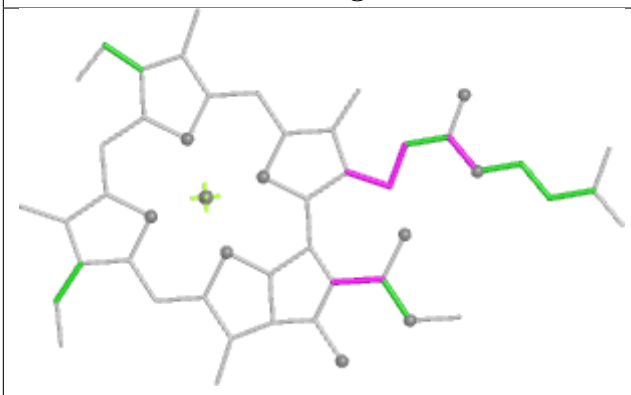
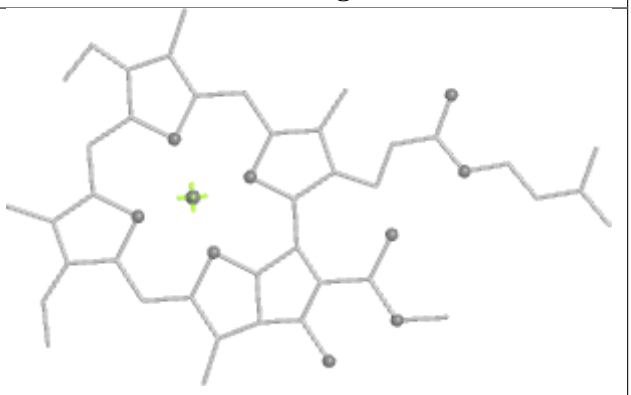
Bond angles

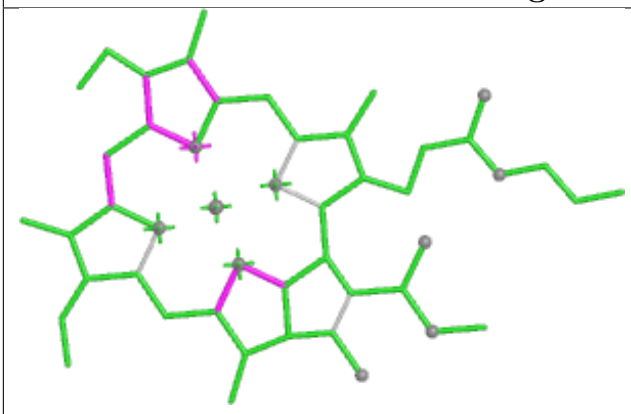
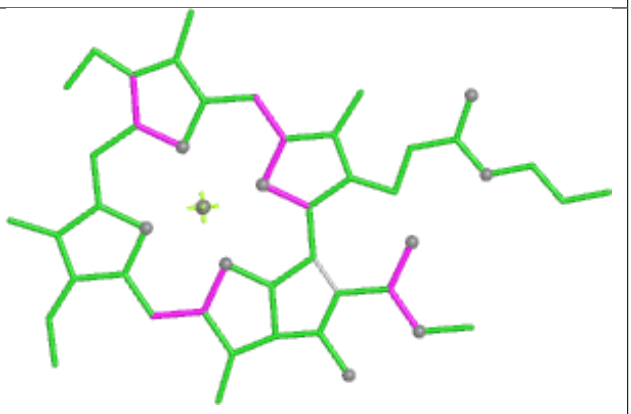
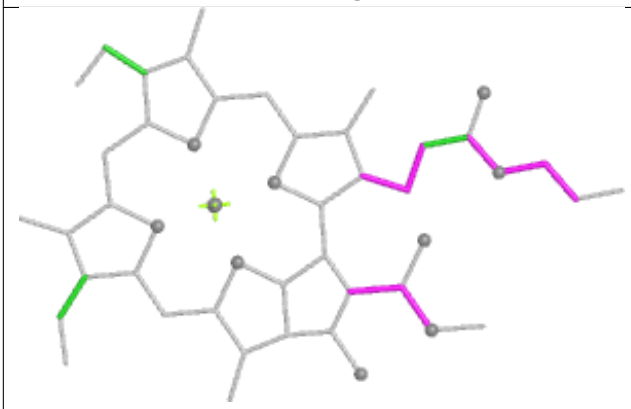
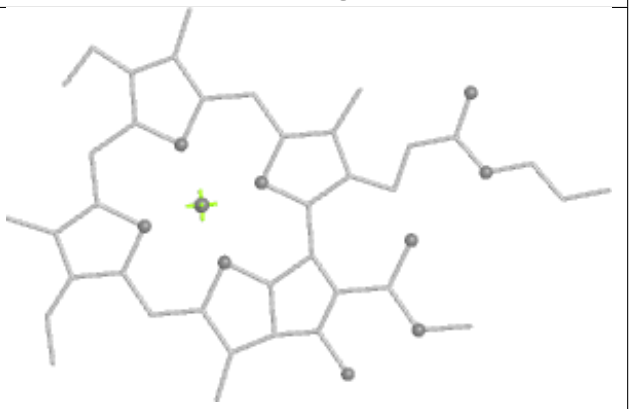


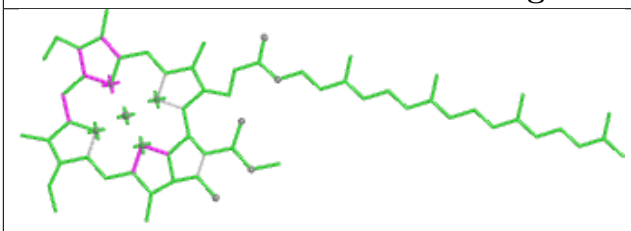
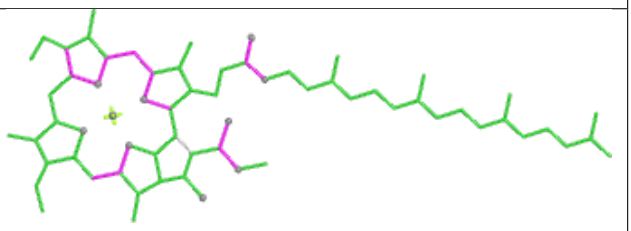
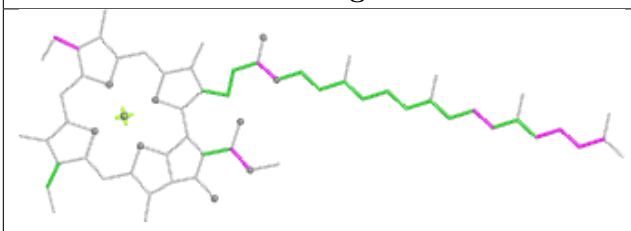
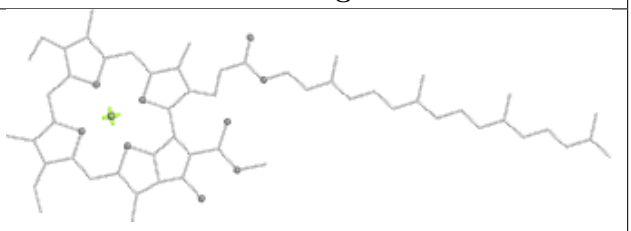
Torsions

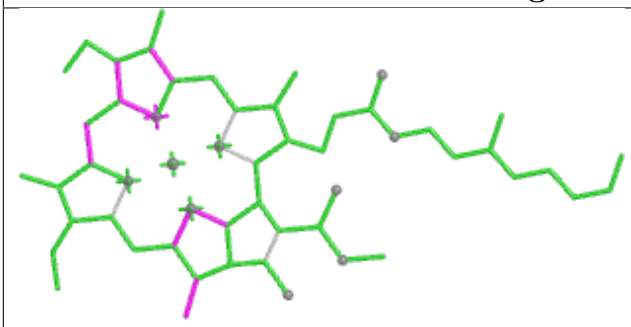
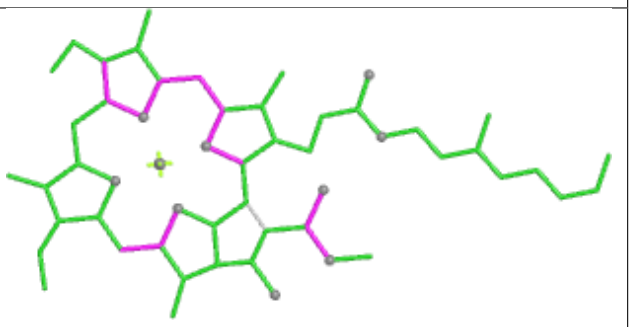
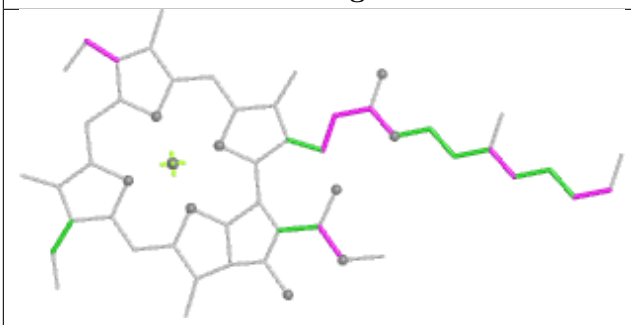
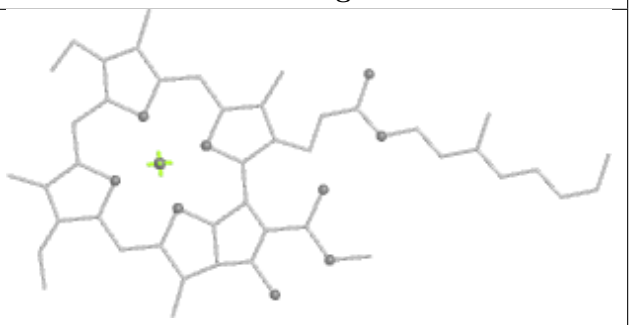


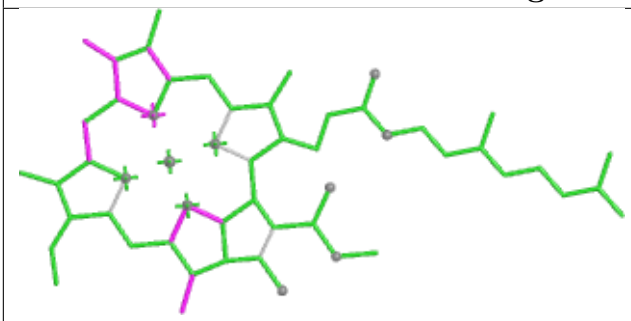
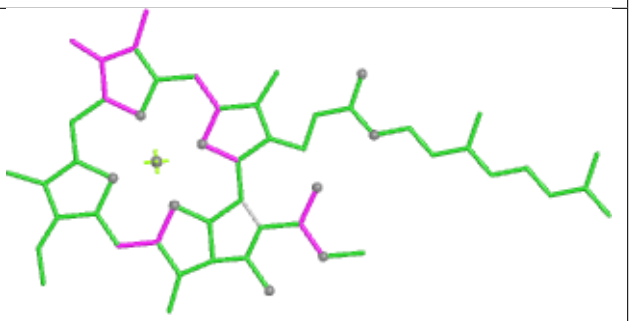
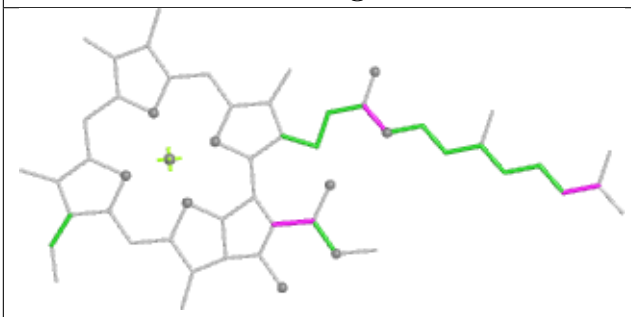
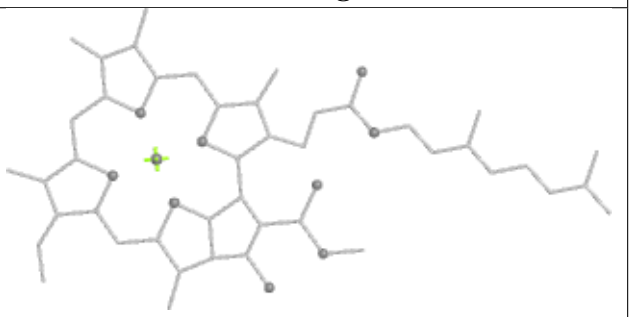
Rings

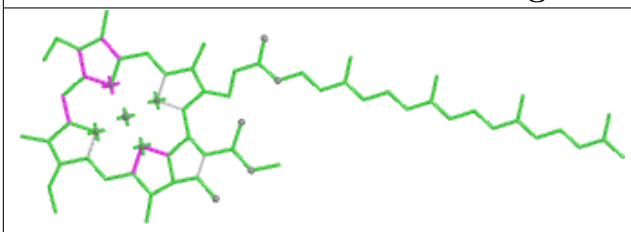
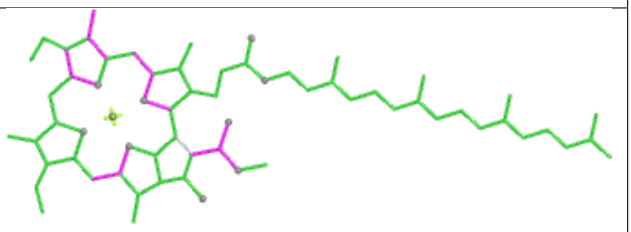
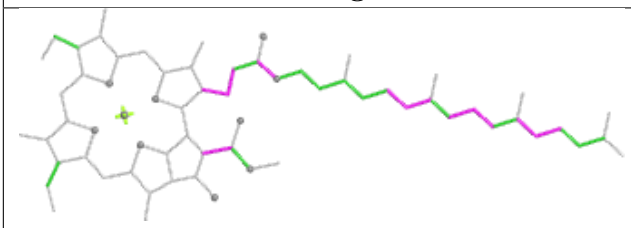
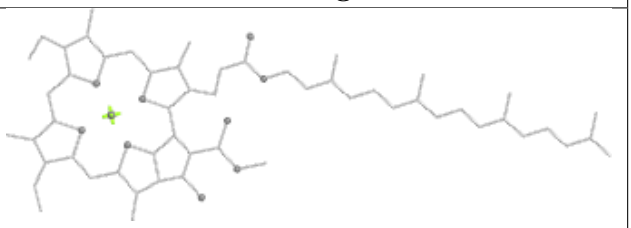
Ligand CLA b 820	
 Bond lengths	 Bond angles
 Torsions	 Rings

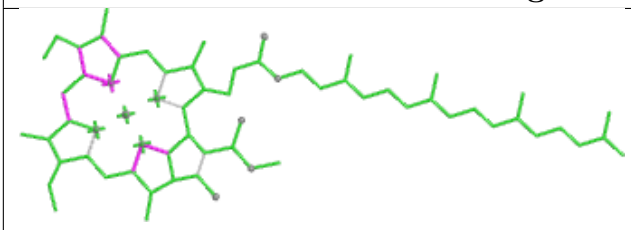
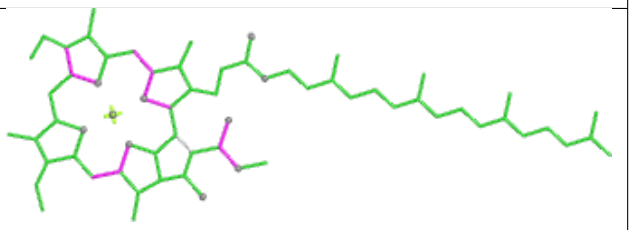
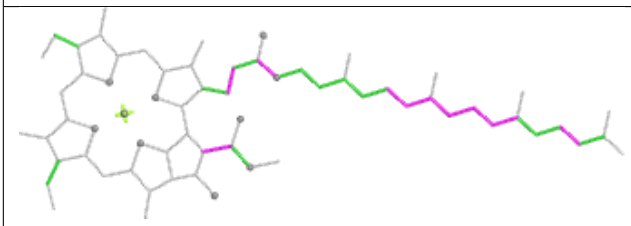
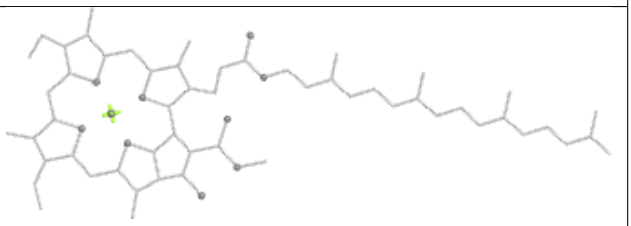
Ligand CLA 7 306	
 Bond lengths	 Bond angles
 Torsions	 Rings

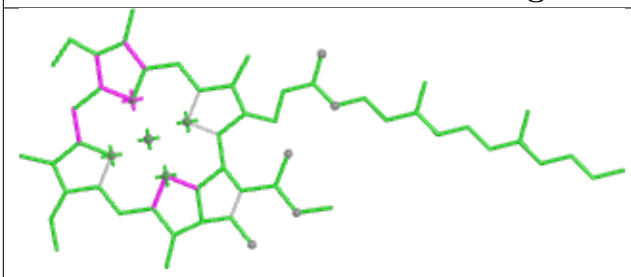
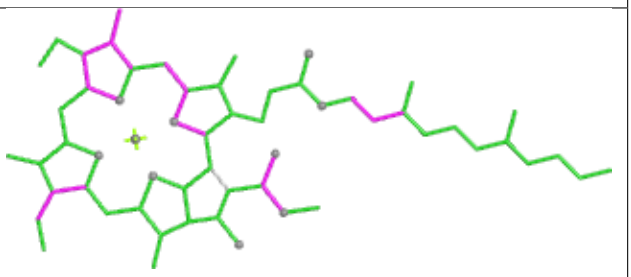
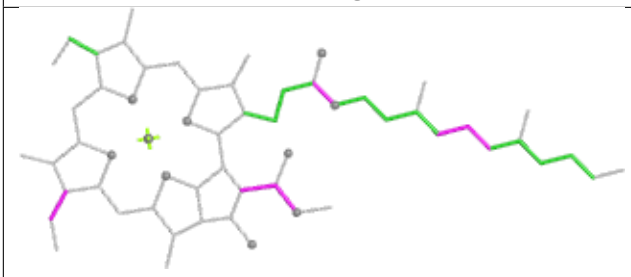
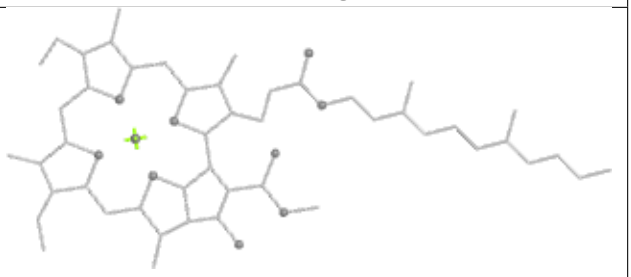
Ligand CLA b 840	
 Bond lengths	 Bond angles
 Torsions	 Rings

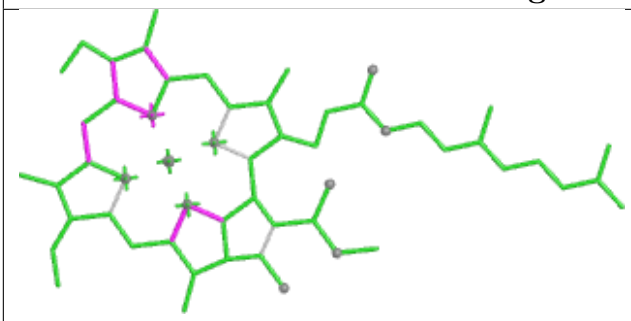
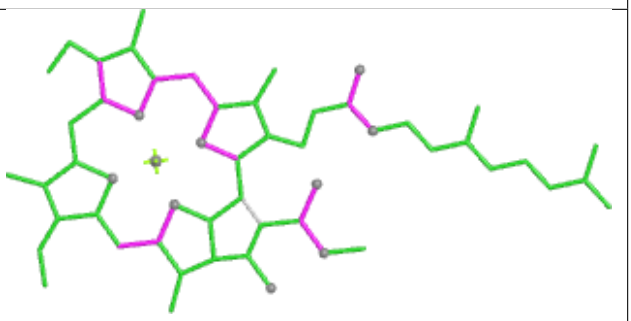
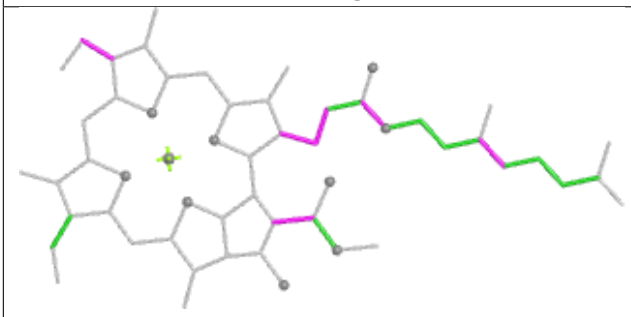
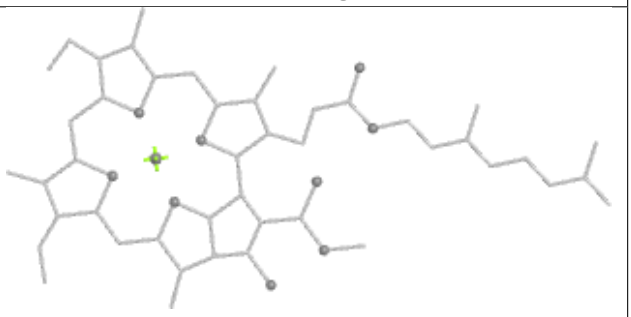
Ligand CLA a 813	
 Bond lengths	 Bond angles
 Torsions	 Rings

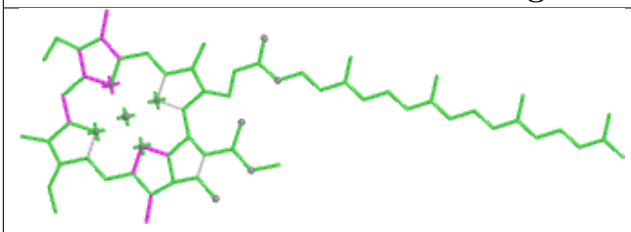
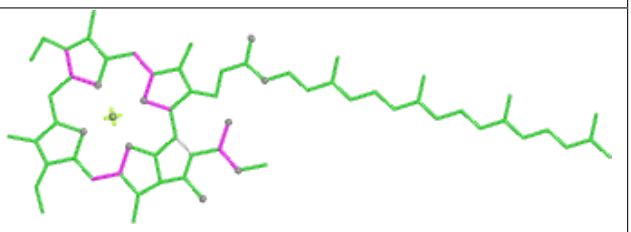
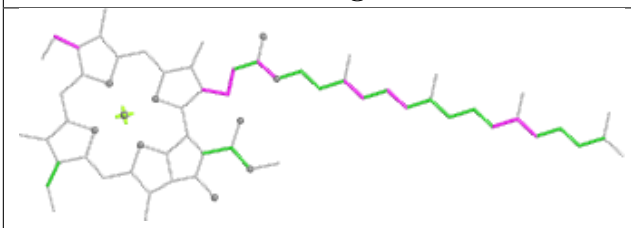
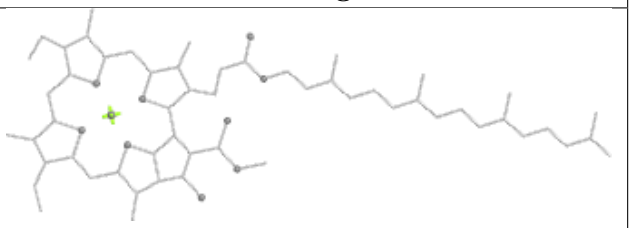
Ligand CLA b 811	
 Bond lengths	 Bond angles
 Torsions	 Rings

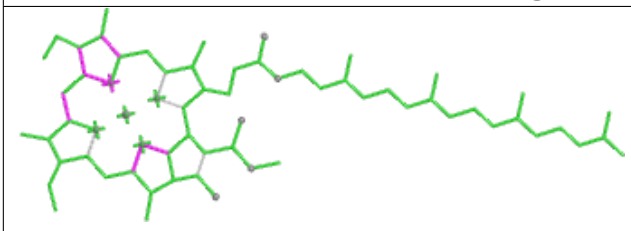
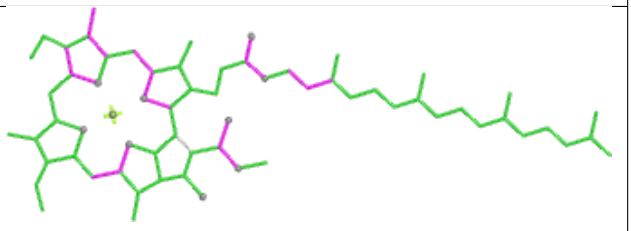
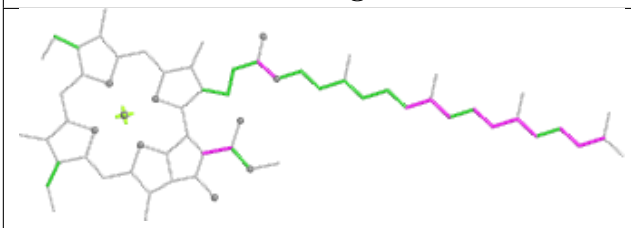
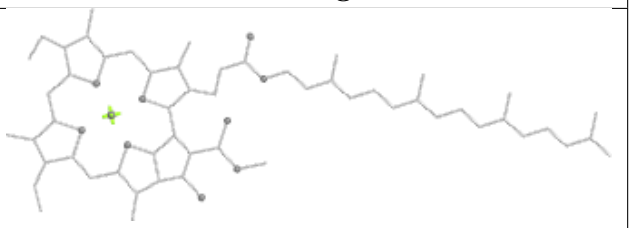
Ligand CLA a 809	
 Bond lengths	 Bond angles
 Torsions	 Rings

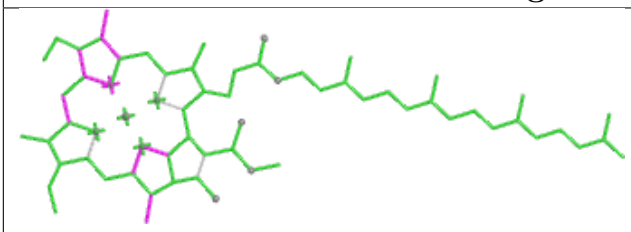
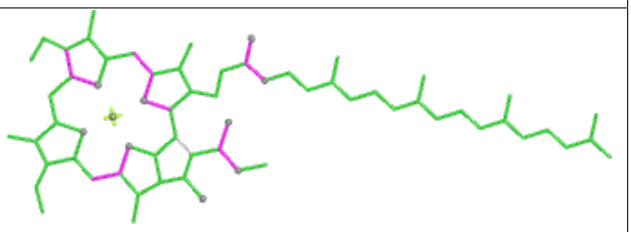
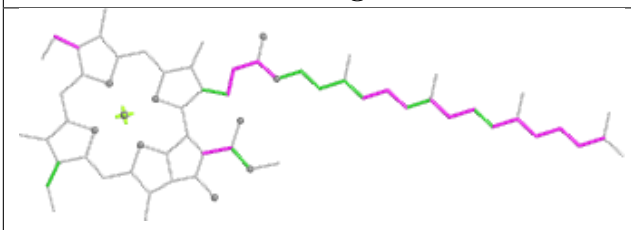
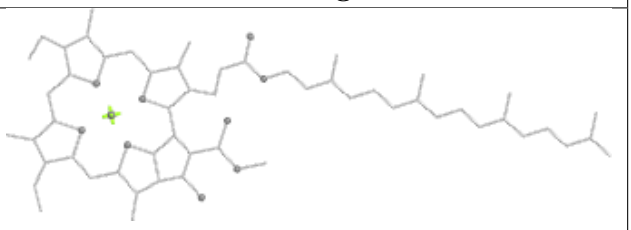
Ligand CLA b 824	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA b 835	
 Bond lengths	 Bond angles
 Torsions	 Rings

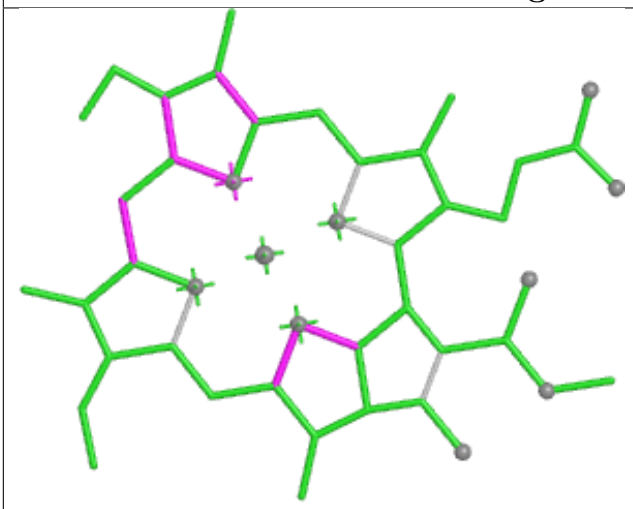
Ligand CLA a 825	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA b 828	
 Bond lengths	 Bond angles
 Torsions	 Rings

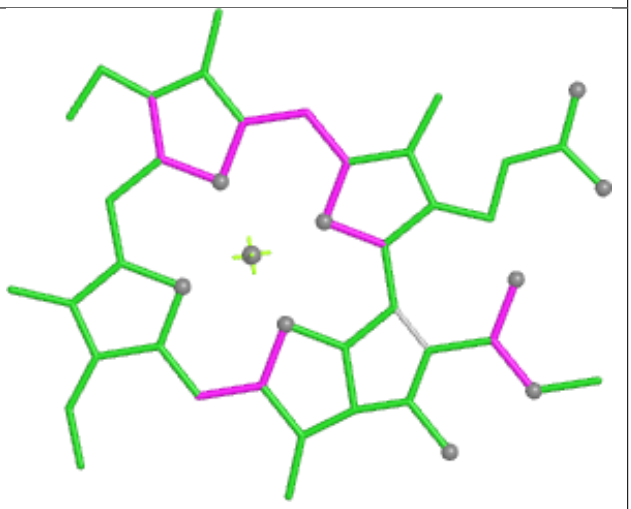
Ligand CLA a 844	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA b 801	
 Bond lengths	 Bond angles
 Torsions	 Rings

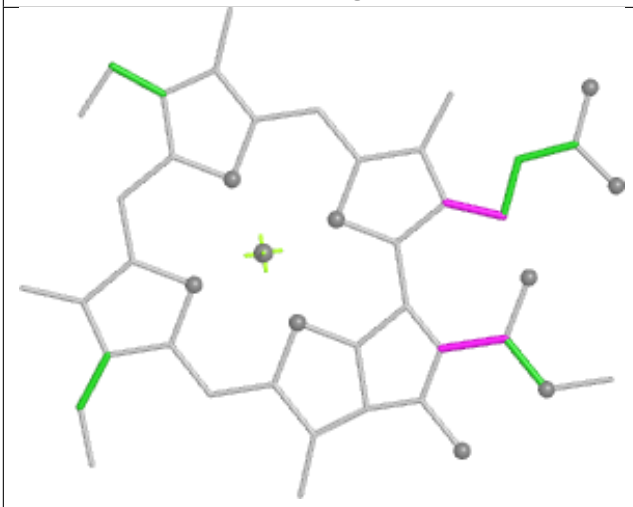
Ligand CLA a 815



Bond lengths



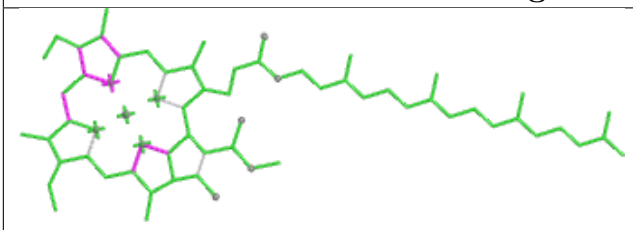
Bond angles



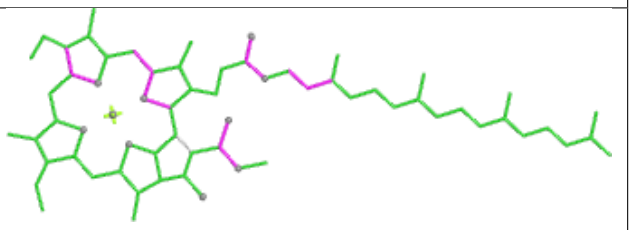
Torsions

Rings

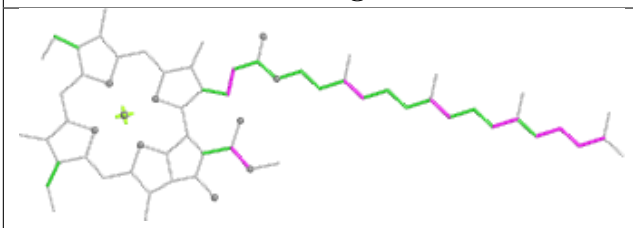
Ligand CLA 1 308



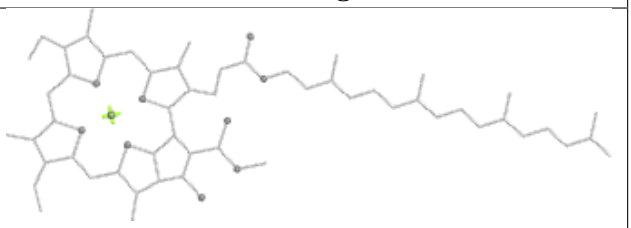
Bond lengths



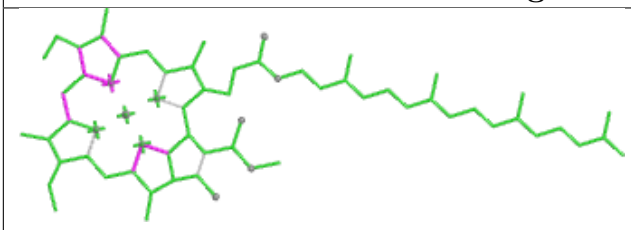
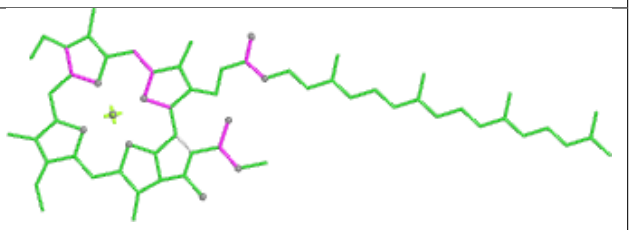
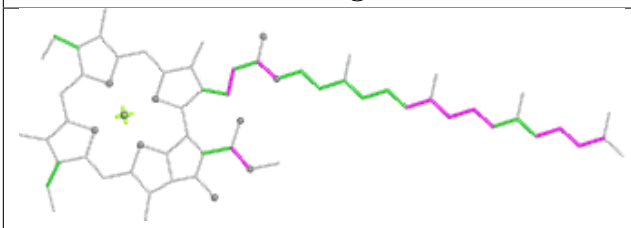
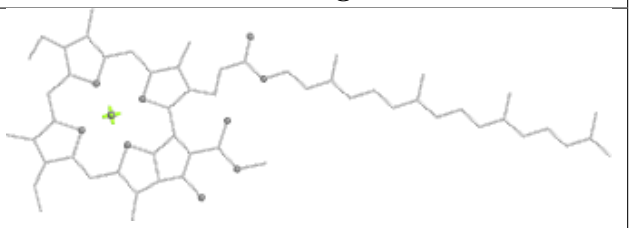
Bond angles

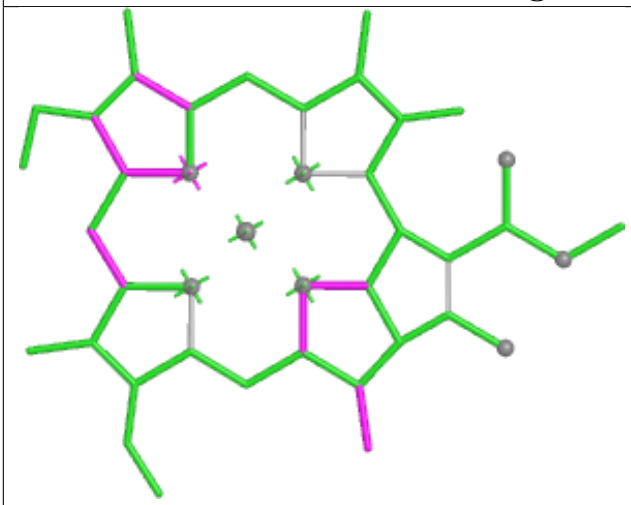
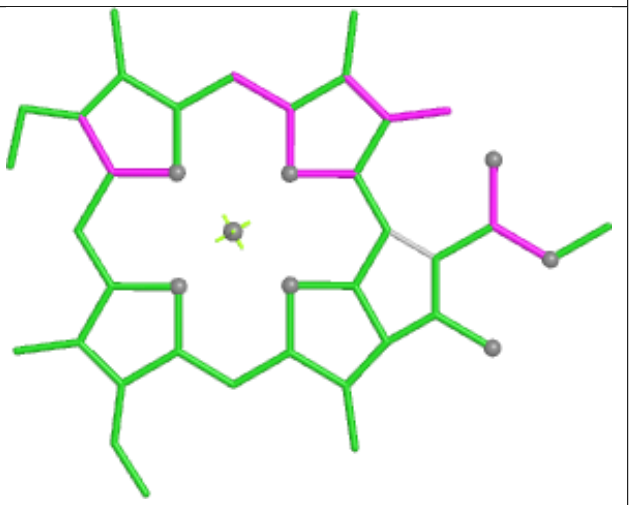
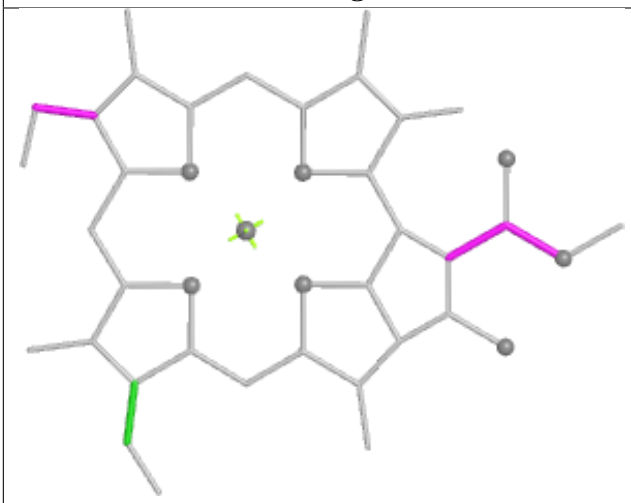
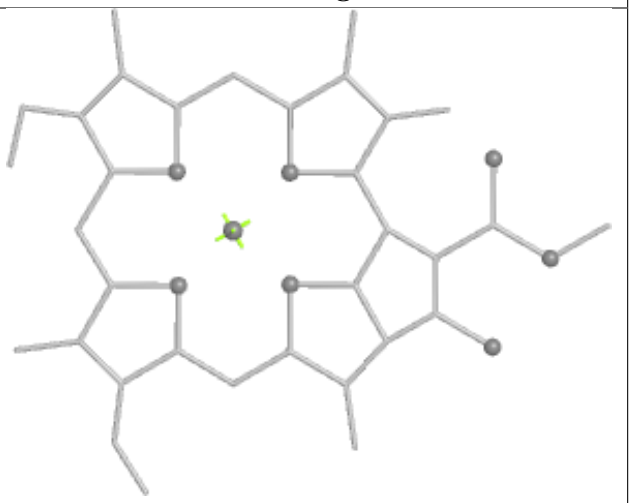


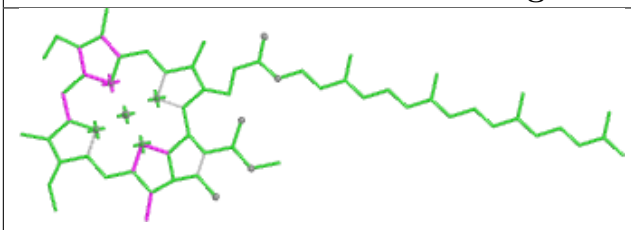
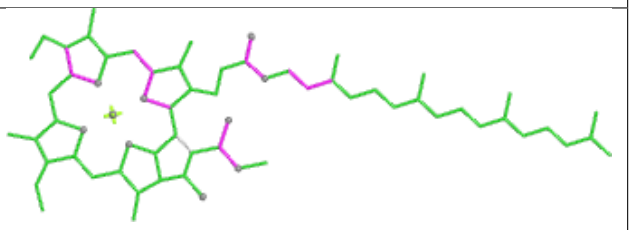
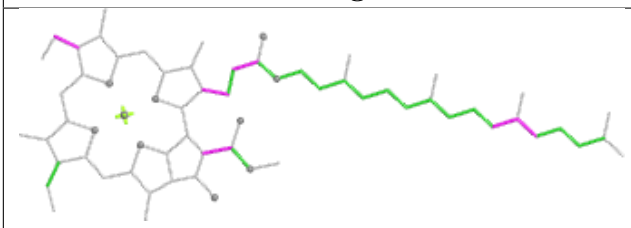
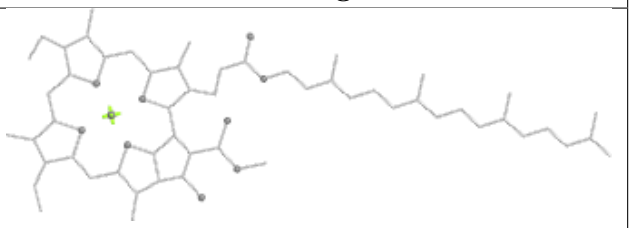
Torsions

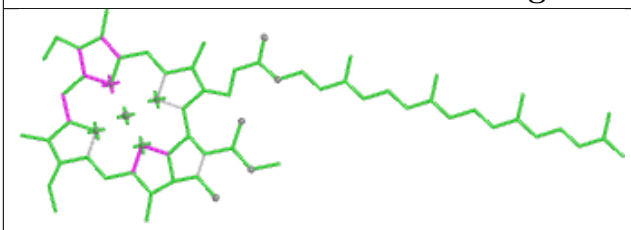
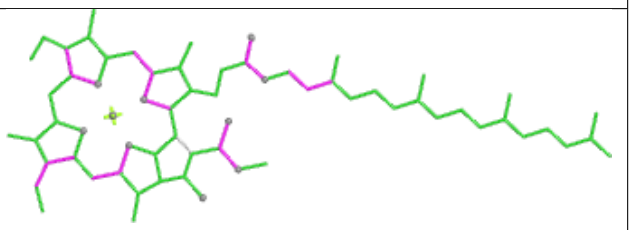
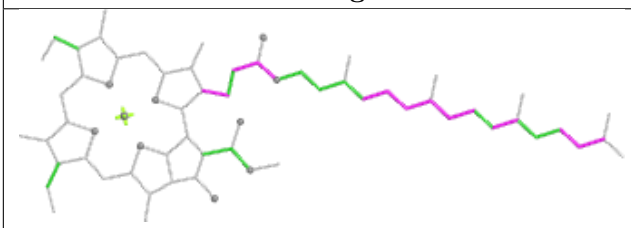
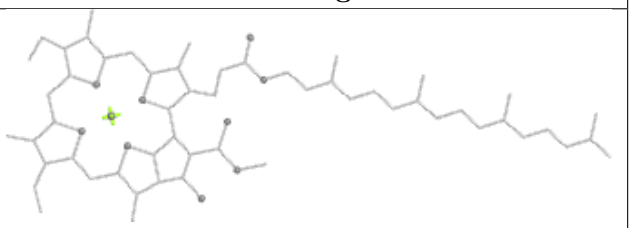


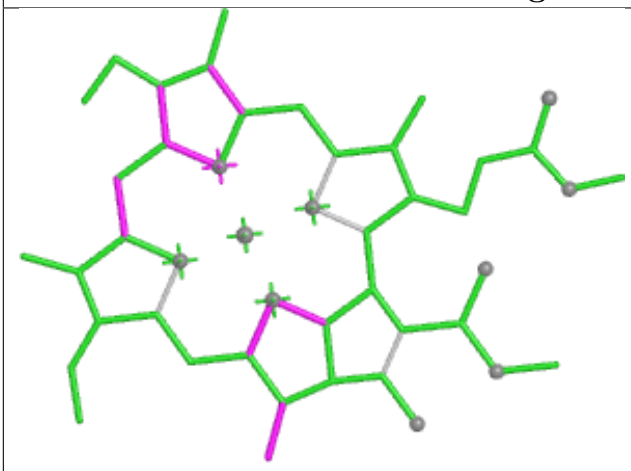
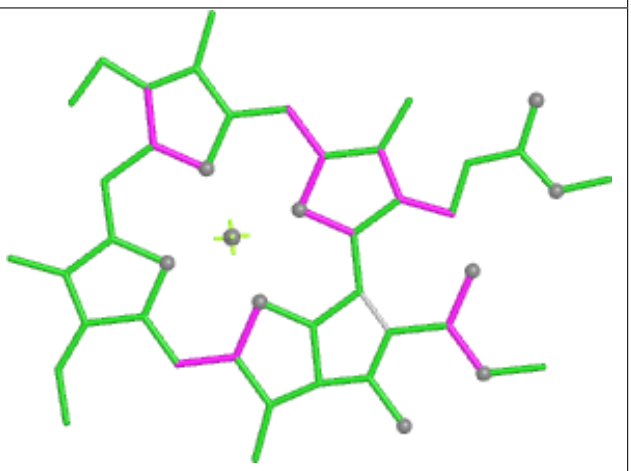
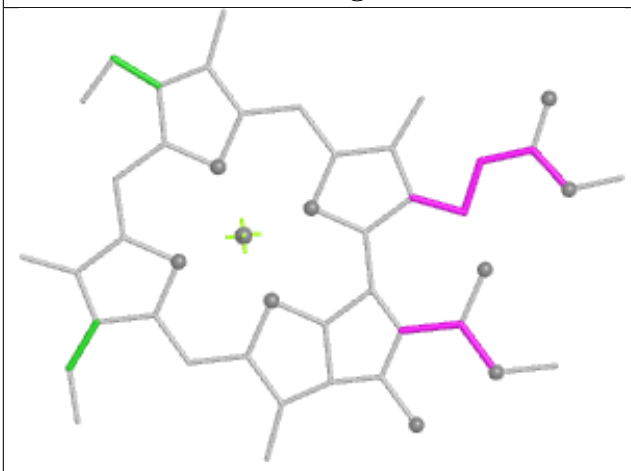
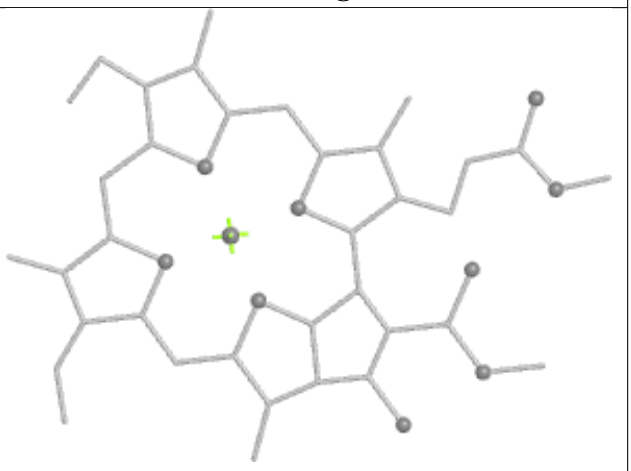
Rings

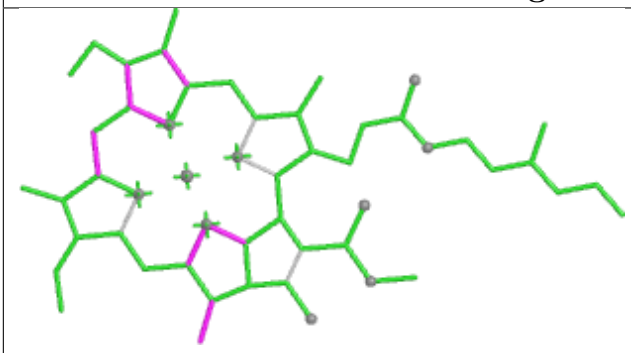
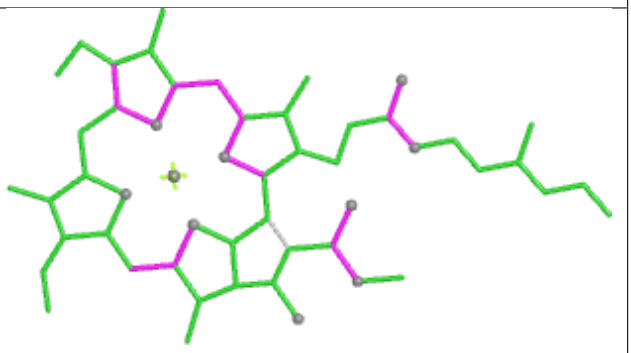
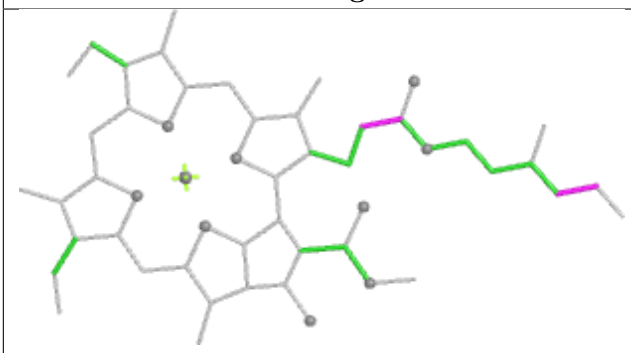
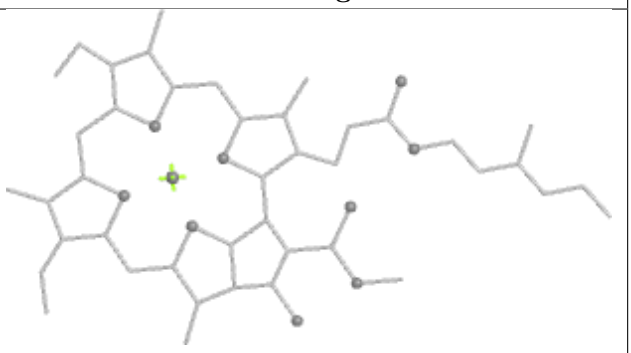
Ligand CLA b 827	
 Bond lengths	 Bond angles
 Torsions	 Rings

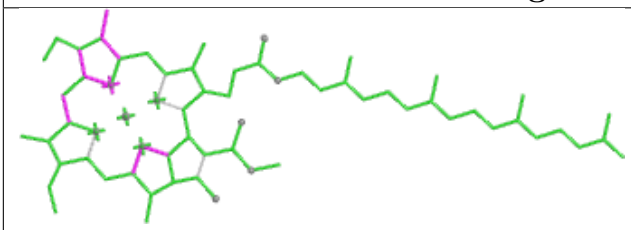
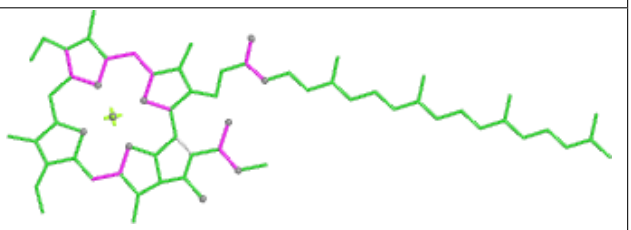
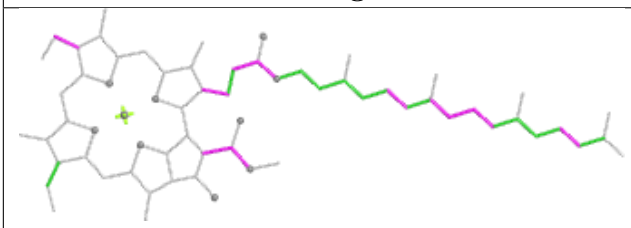
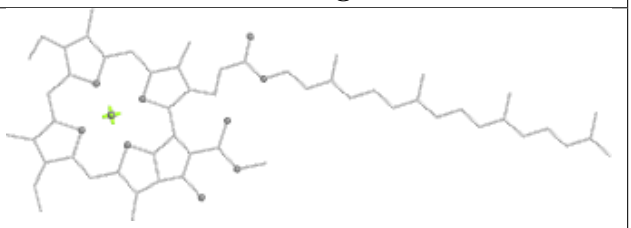
Ligand CLA 1 313	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA b 837	
 Bond lengths	 Bond angles
 Torsions	 Rings

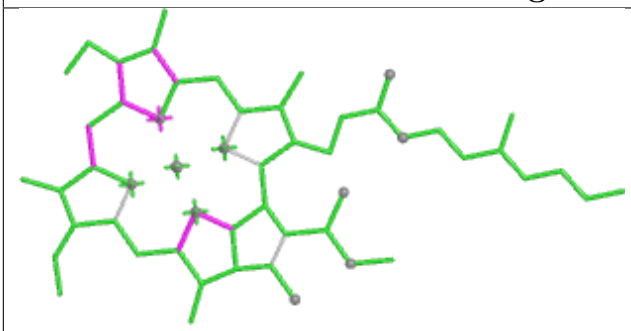
Ligand CLA 1 306	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA 9 312	
 Bond lengths	 Bond angles
 Torsions	 Rings

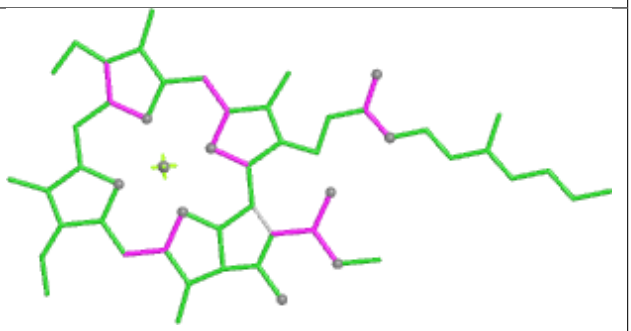
Ligand CLA 1 312	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA a 854	
 Bond lengths	 Bond angles
 Torsions	 Rings

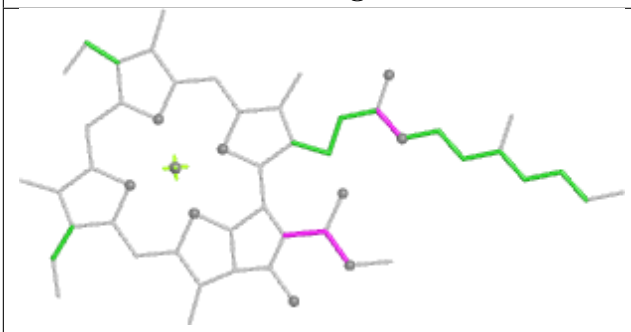
Ligand CLA 1 311



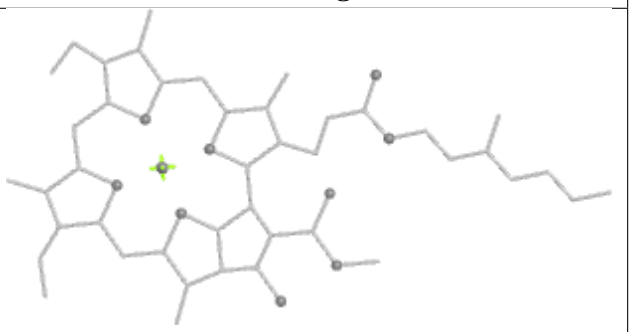
Bond lengths



Bond angles

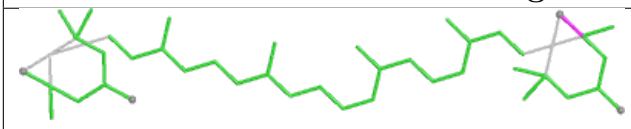


Torsions

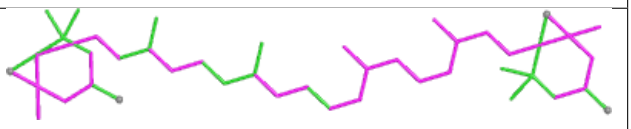


Rings

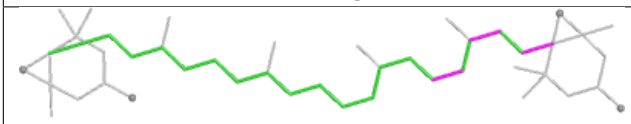
Ligand XAT 8 302



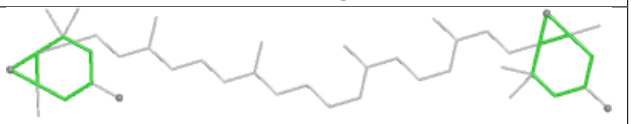
Bond lengths



Bond angles

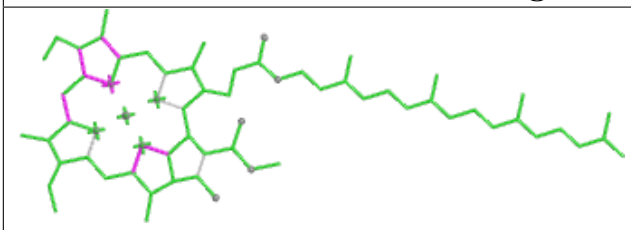


Torsions

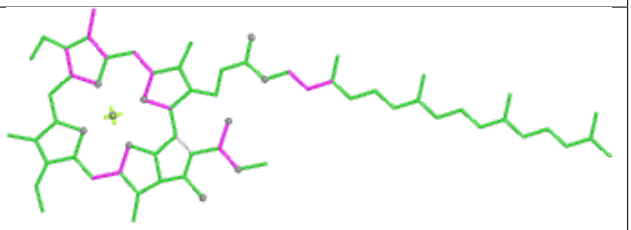


Rings

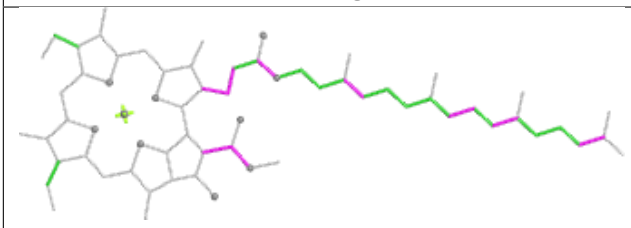
Ligand CLA 9 316



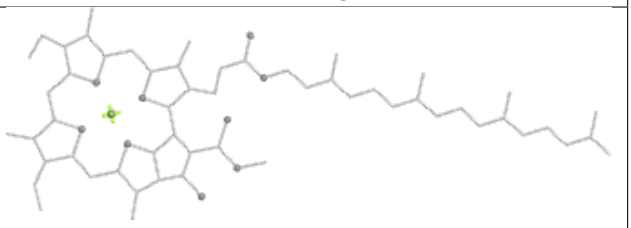
Bond lengths



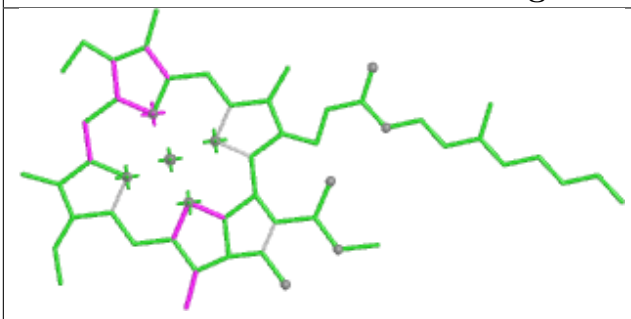
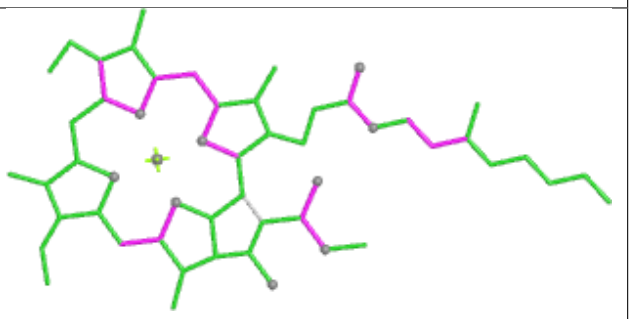
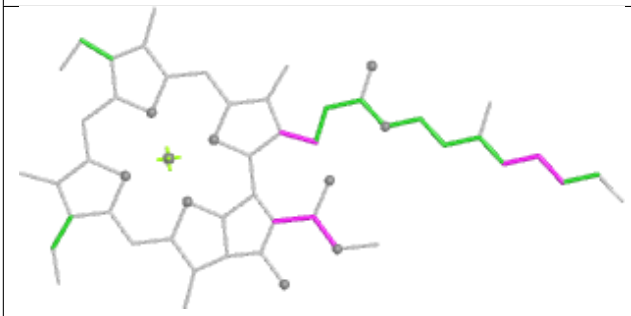
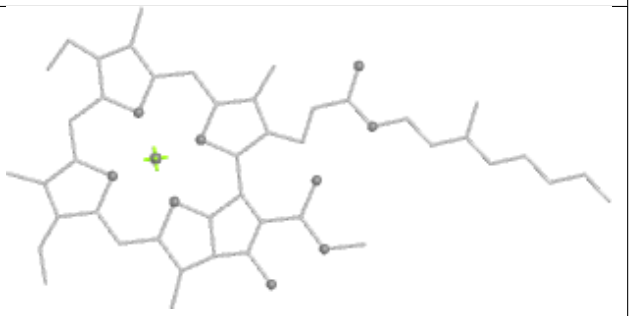
Bond angles

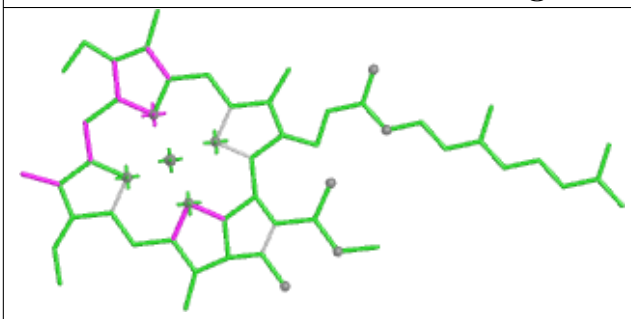
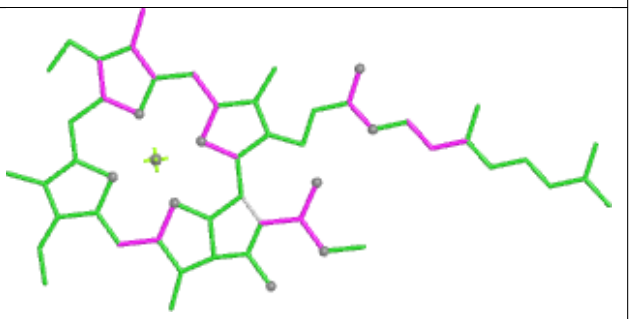
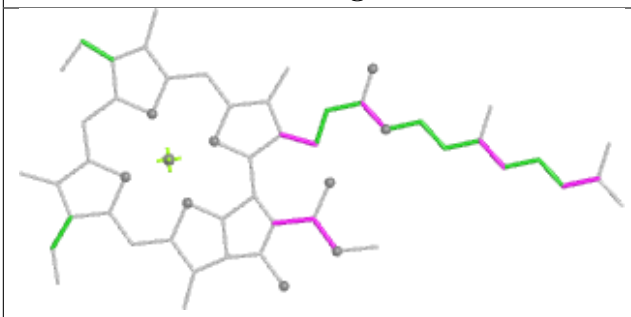
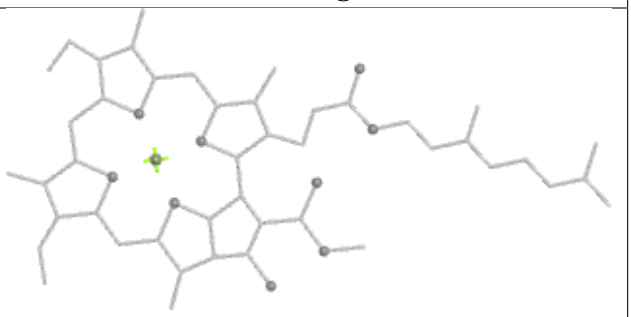


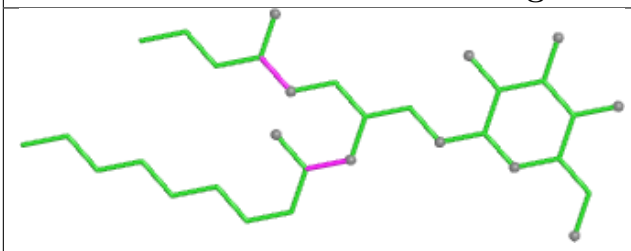
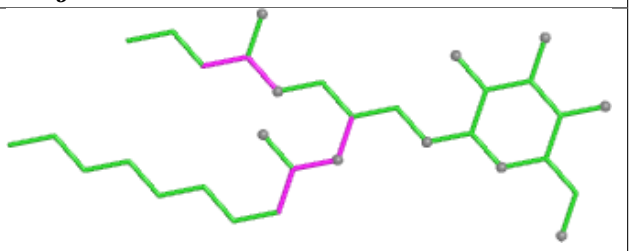
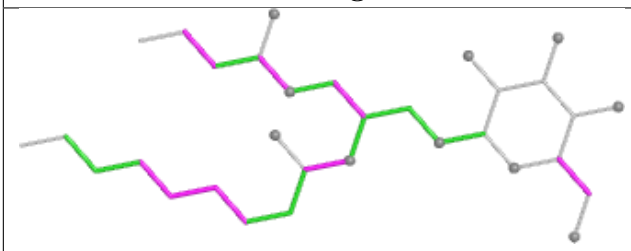
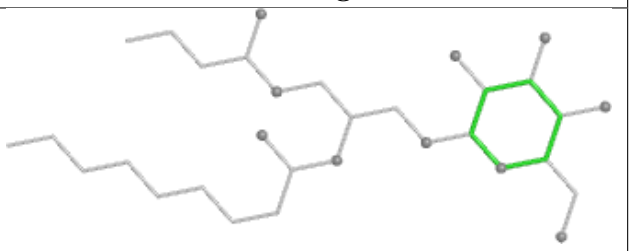
Torsions

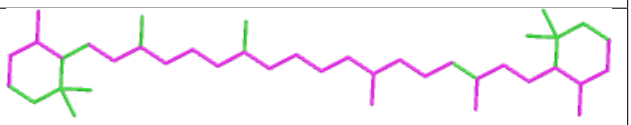
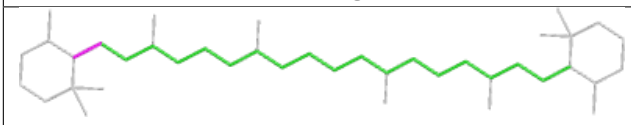
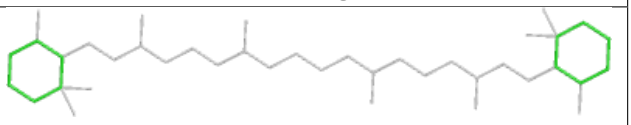


Rings

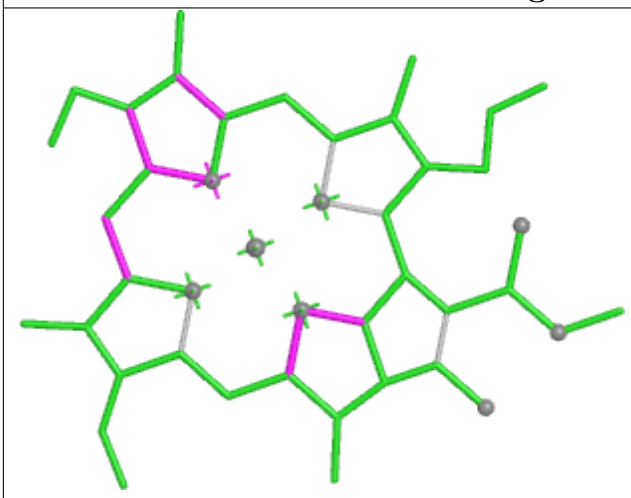
Ligand CLA 7 313	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA a 804	
 Bond lengths	 Bond angles
 Torsions	 Rings

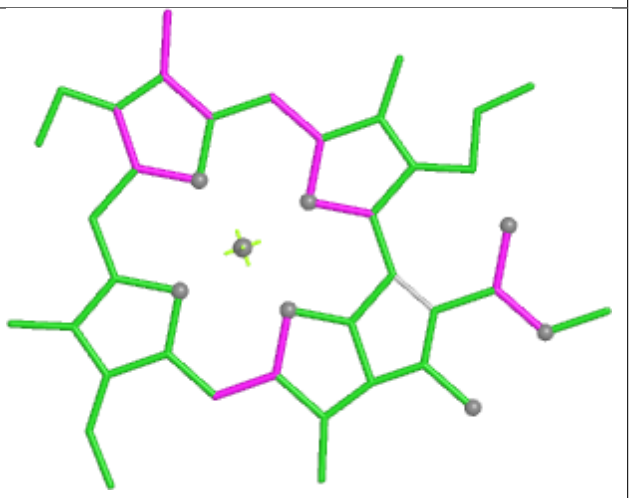
Ligand LMG j 105	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand BCR b 843	
Bond lengths	 Bond angles
 Torsions	 Rings

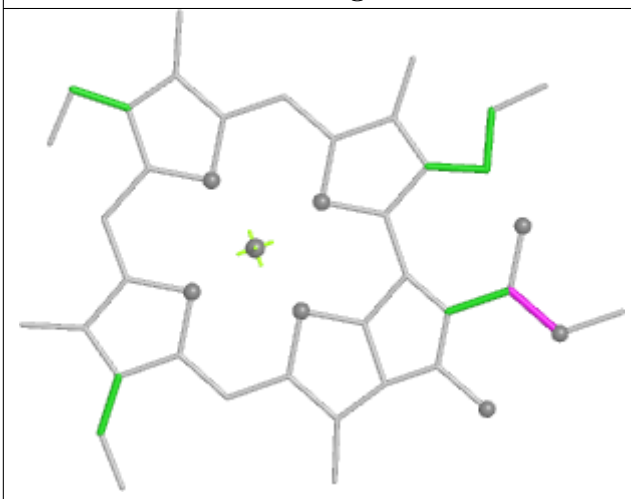
Ligand CLA 8 305



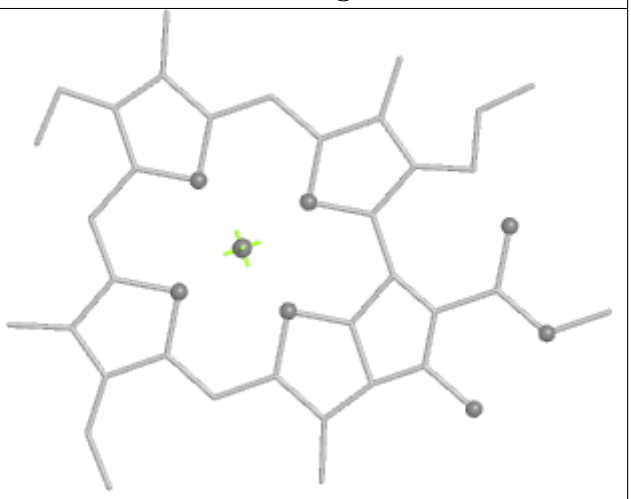
Bond lengths



Bond angles

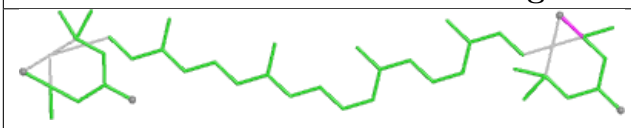


Torsions

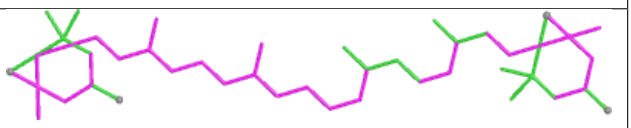


Rings

Ligand XAT 8 303

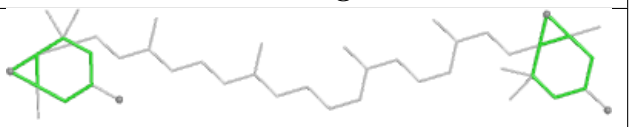


Bond lengths

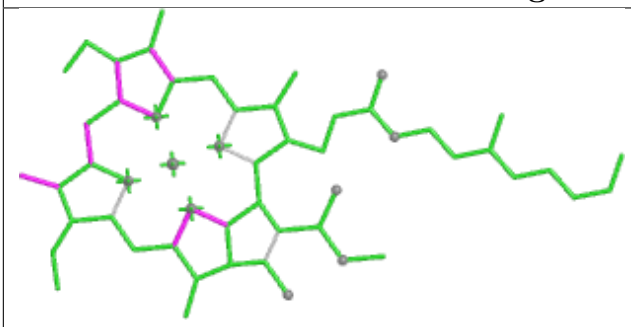
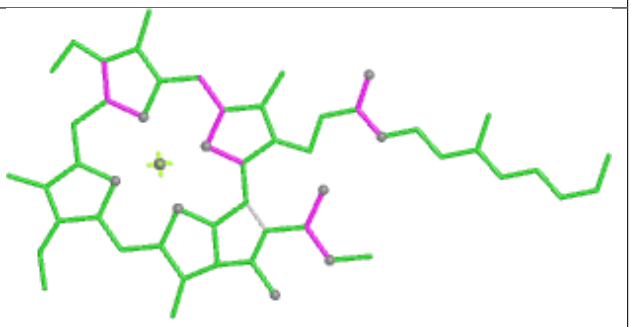
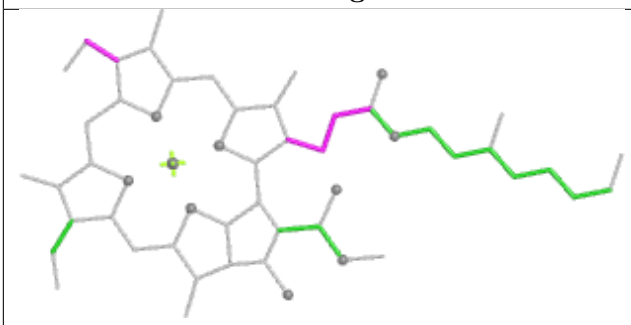
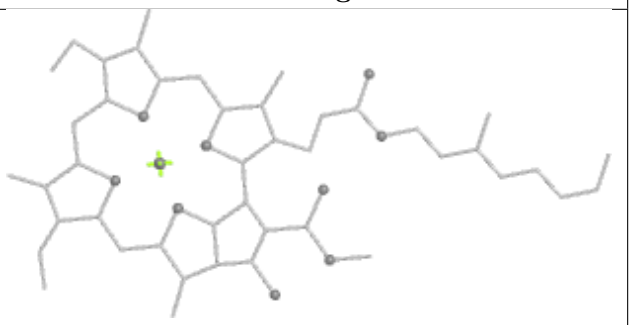


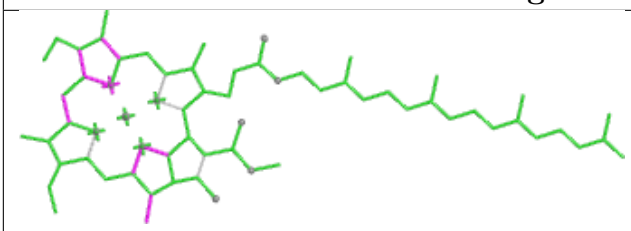
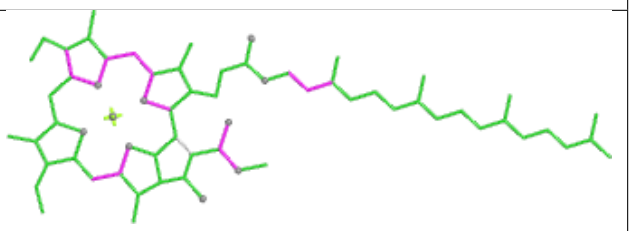
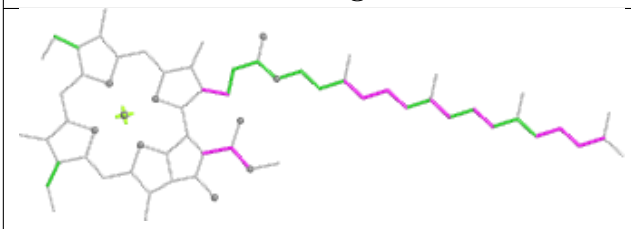
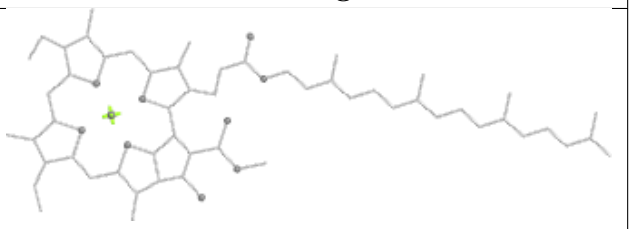
Bond angles

Torsions

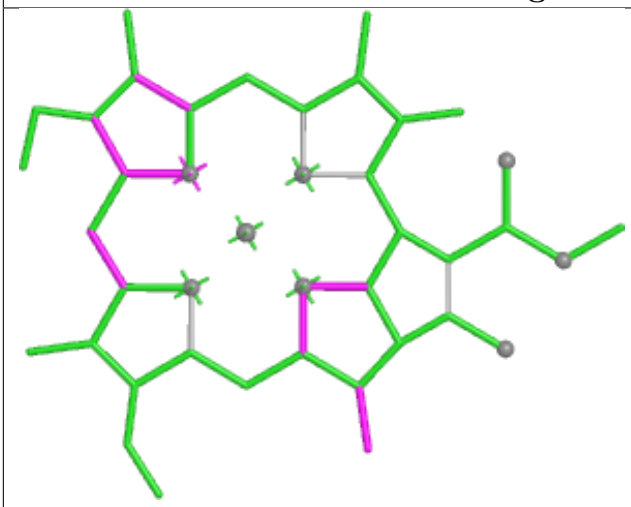


Rings

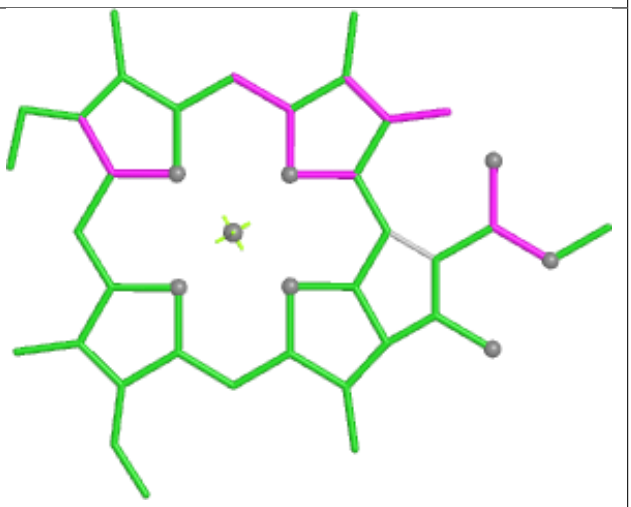
Ligand CLA a 819	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA b 813	
 Bond lengths	 Bond angles
 Torsions	 Rings

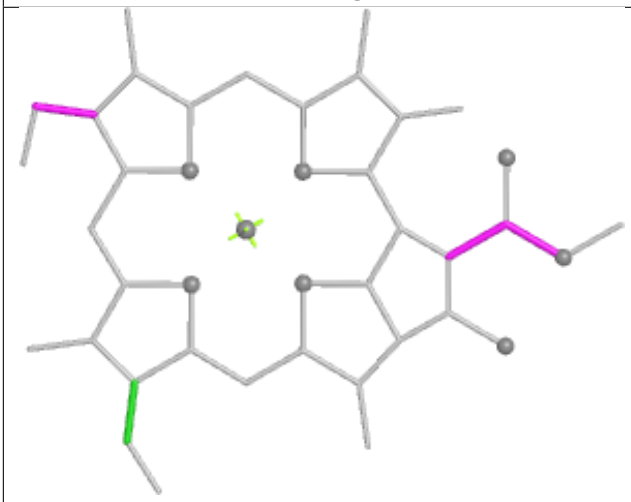
Ligand CLA 7 315



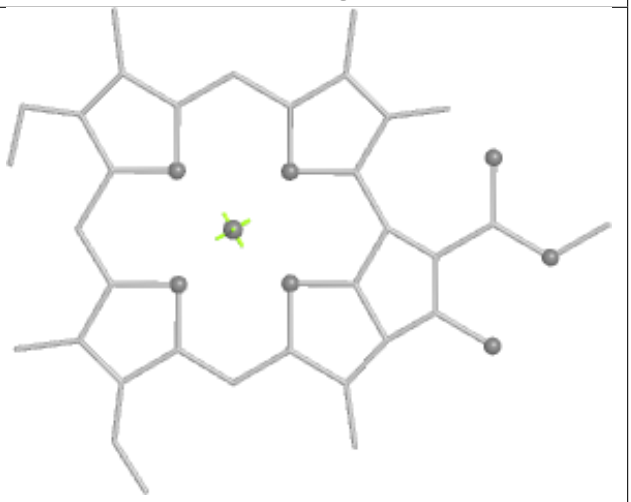
Bond lengths



Bond angles

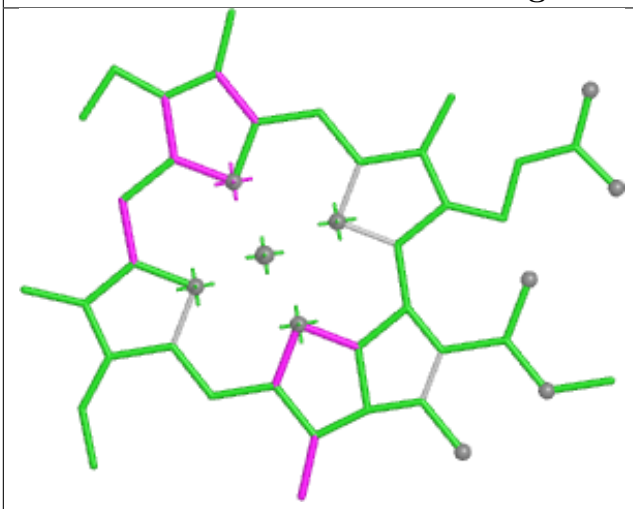


Torsions

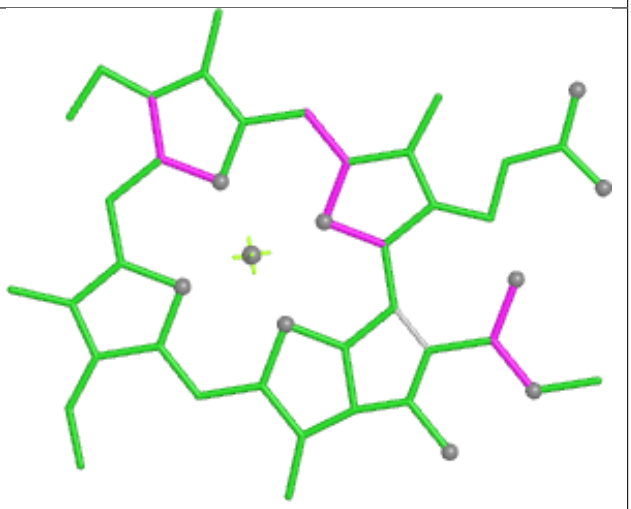


Rings

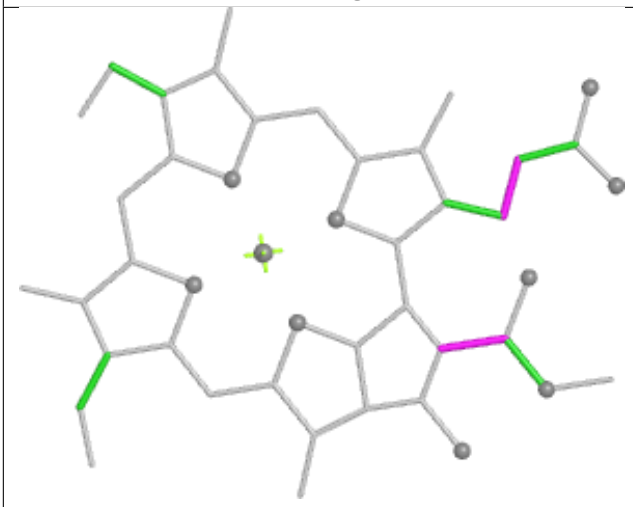
Ligand CLA a 821



Bond lengths



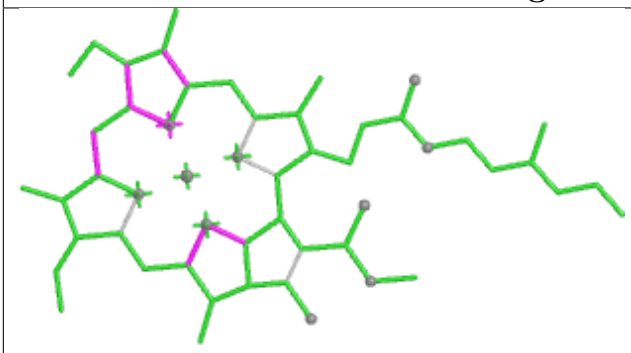
Bond angles



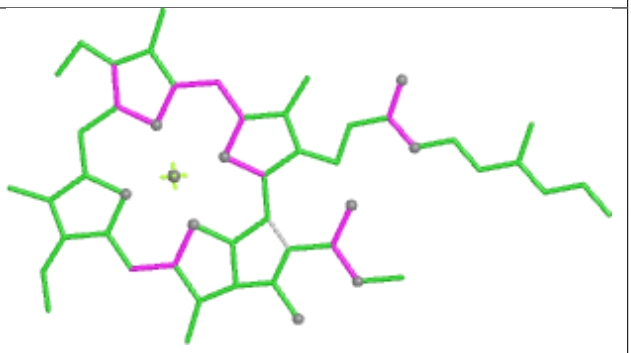
Torsions

Rings

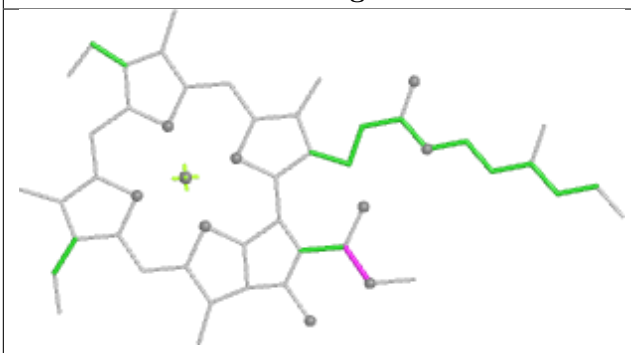
Ligand CLA 8 312



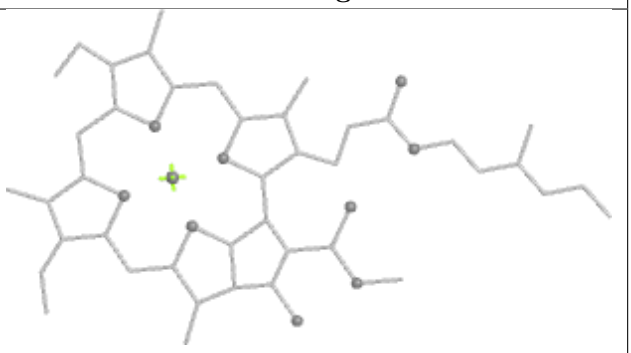
Bond lengths



Bond angles

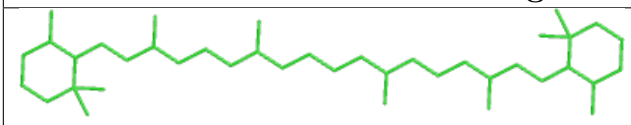


Torsions

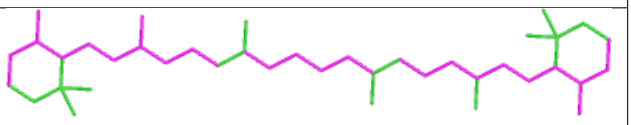


Rings

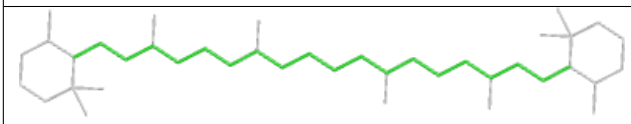
Ligand BCR a 848



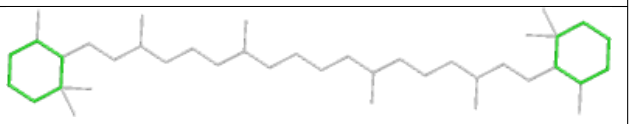
Bond lengths



Bond angles



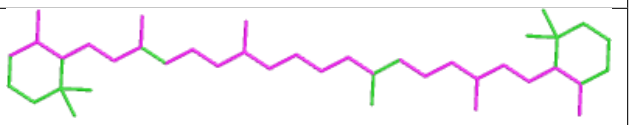
Torsions



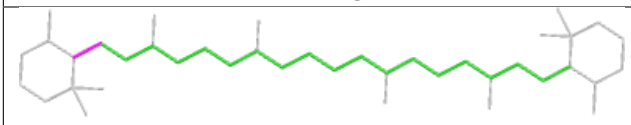
Rings

Ligand BCR b 846

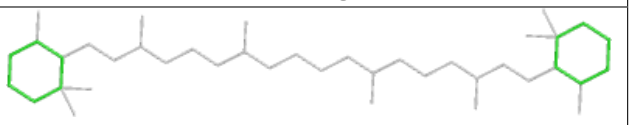
Bond lengths



Bond angles

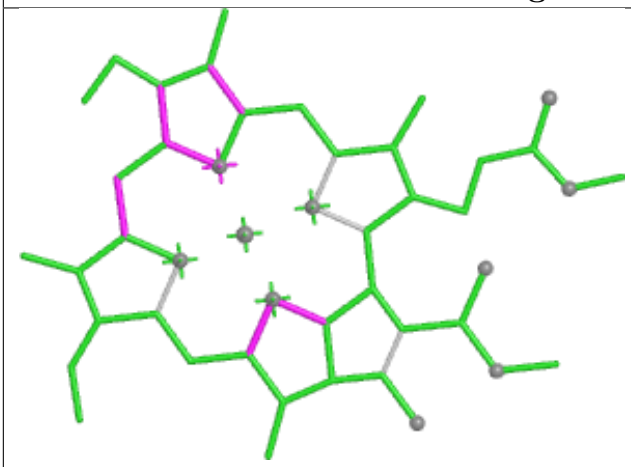


Torsions

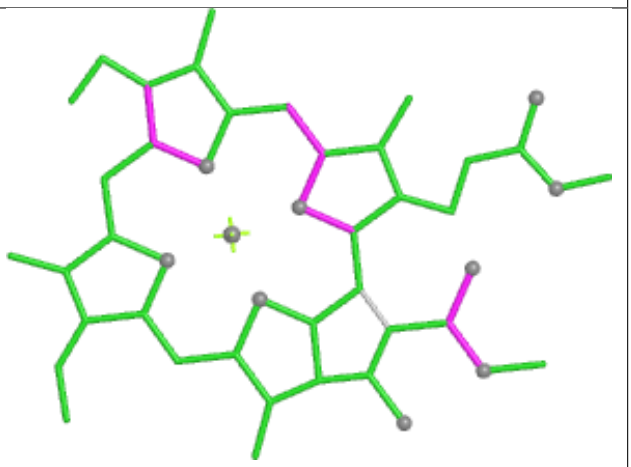


Rings

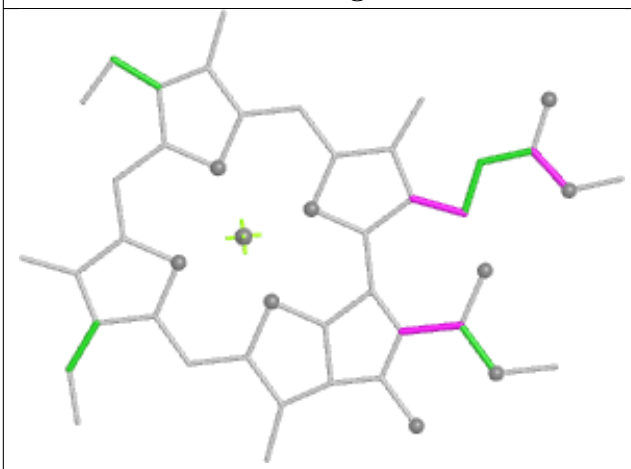
Ligand CLA 9 310



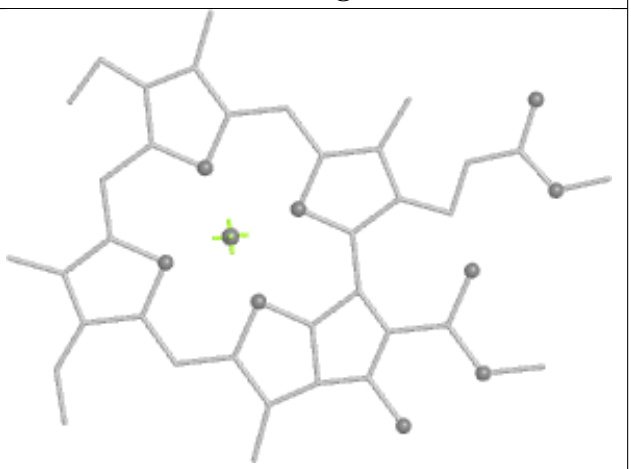
Bond lengths



Bond angles



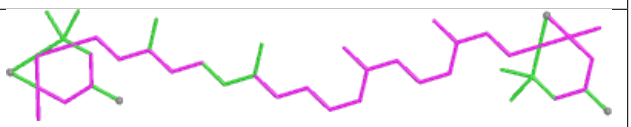
Torsions



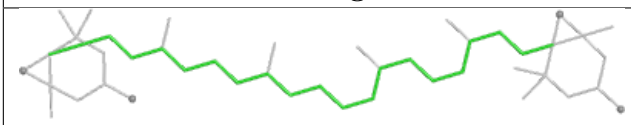
Rings

Ligand XAT 1 303

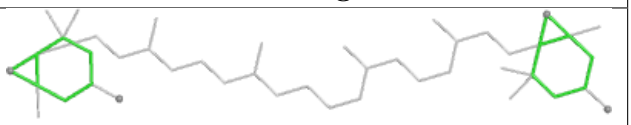
Bond lengths



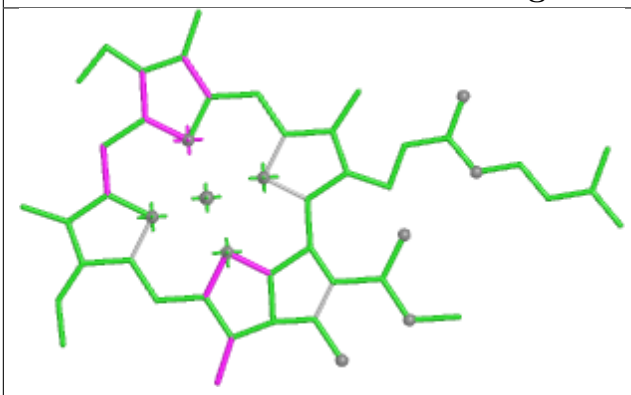
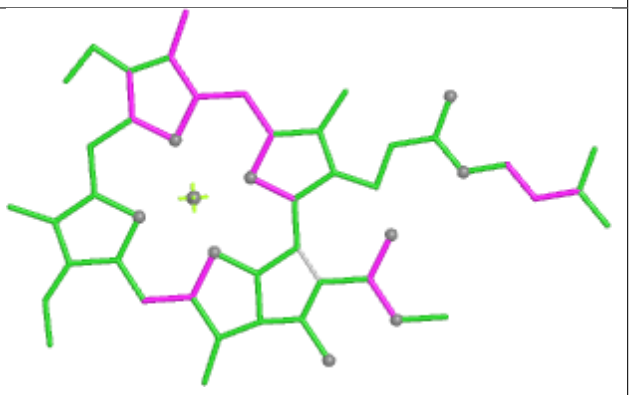
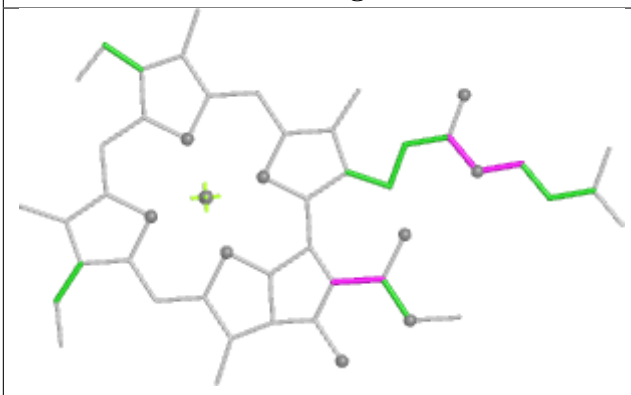
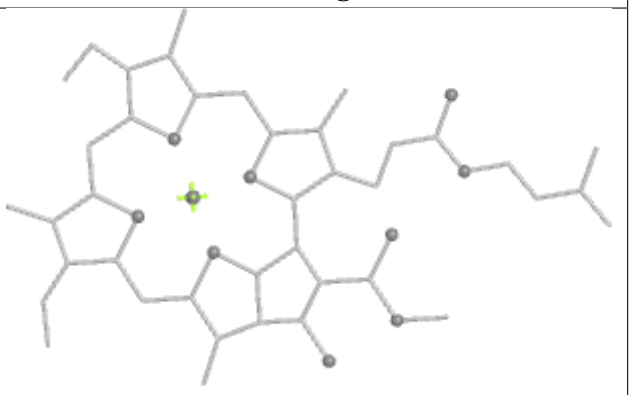
Bond angles



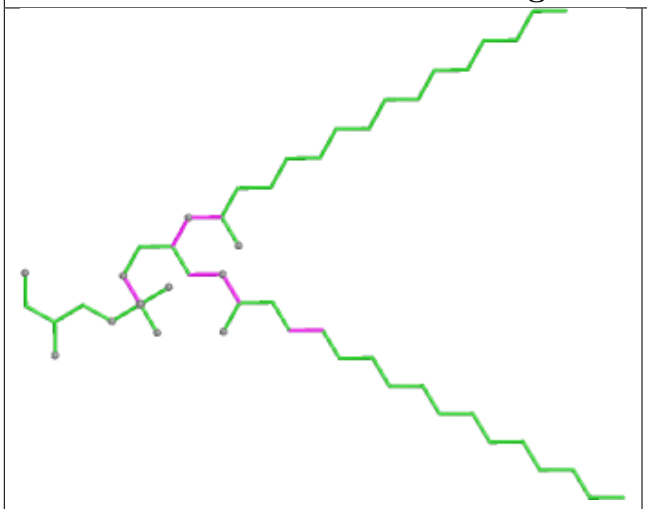
Torsions



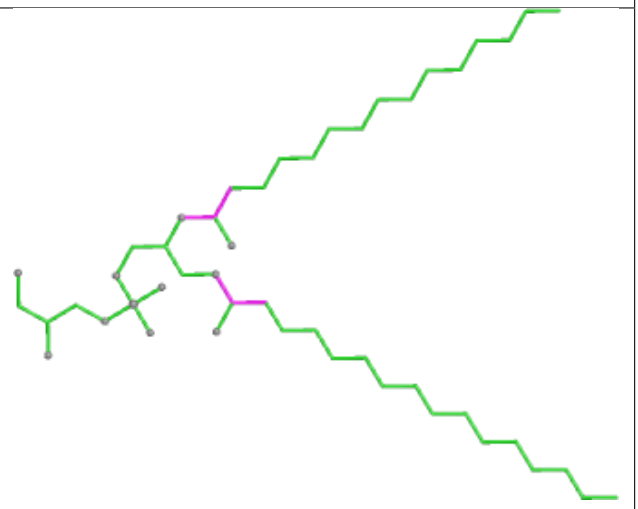
Rings

Ligand CLA a 816	
 Bond lengths	 Bond angles
 Torsions	 Rings

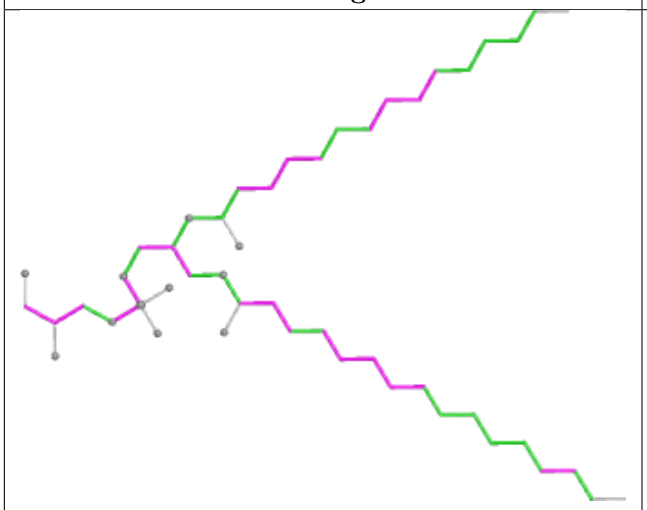
Ligand LHG a 845



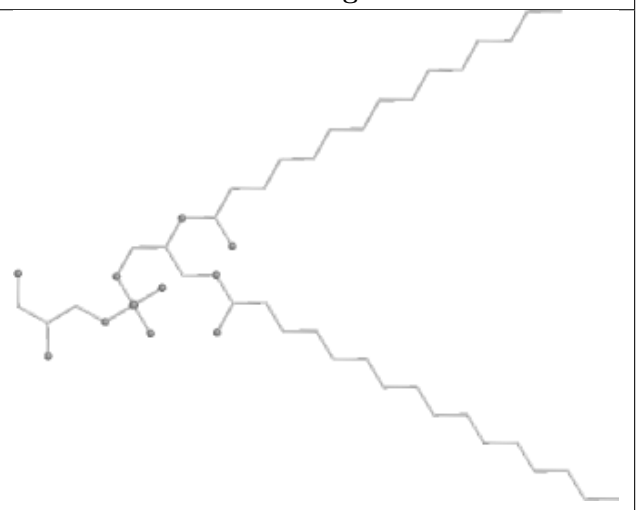
Bond lengths



Bond angles

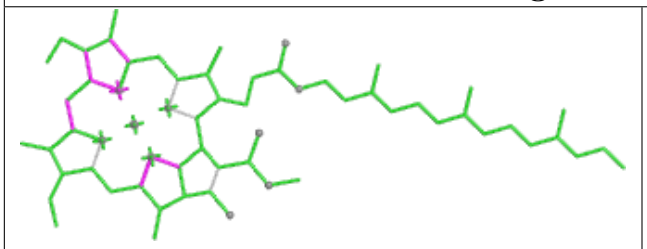


Torsions

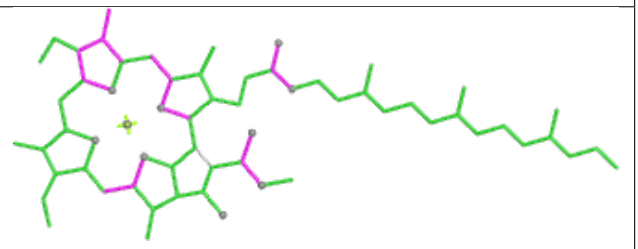


Rings

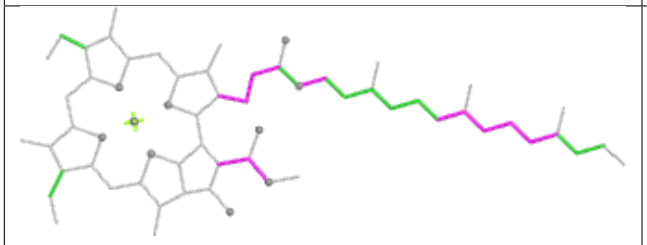
Ligand CLA a 829



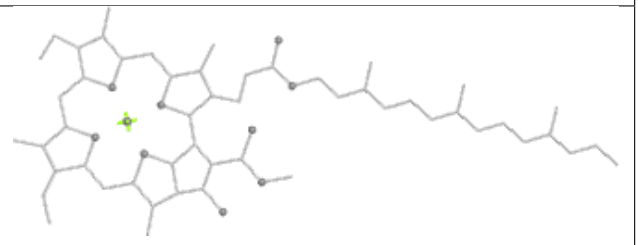
Bond lengths



Bond angles

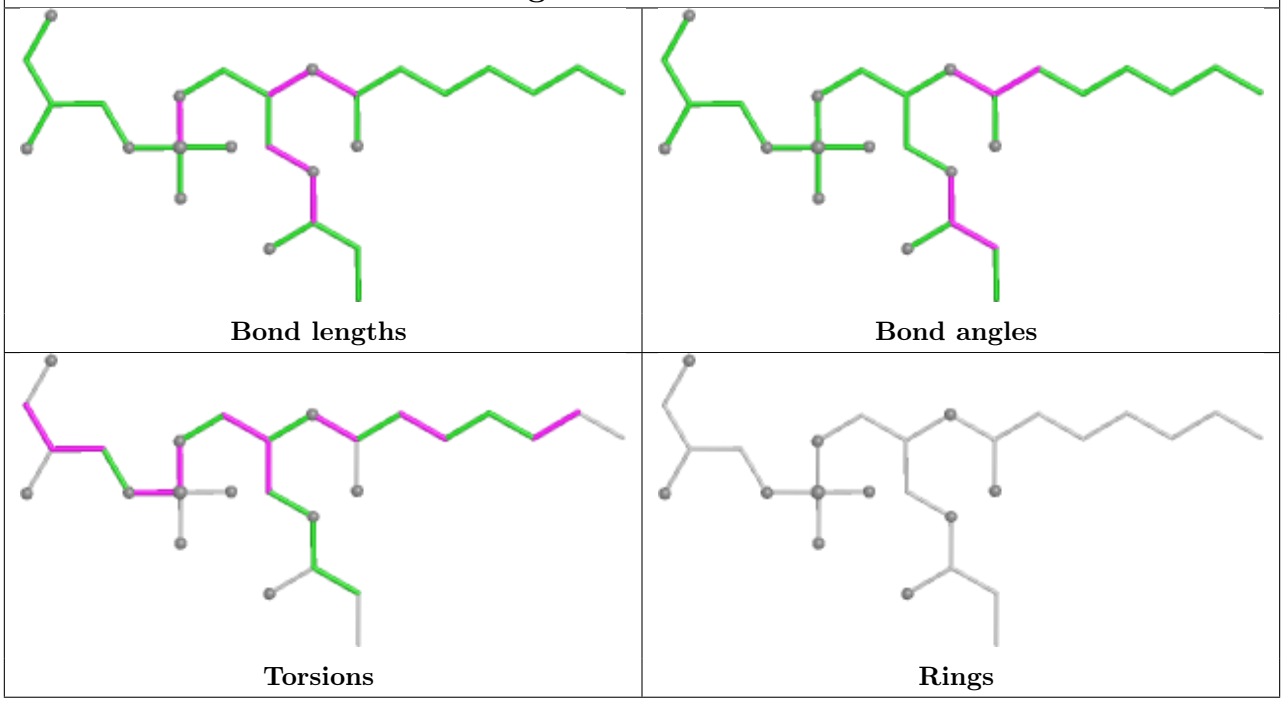


Torsions

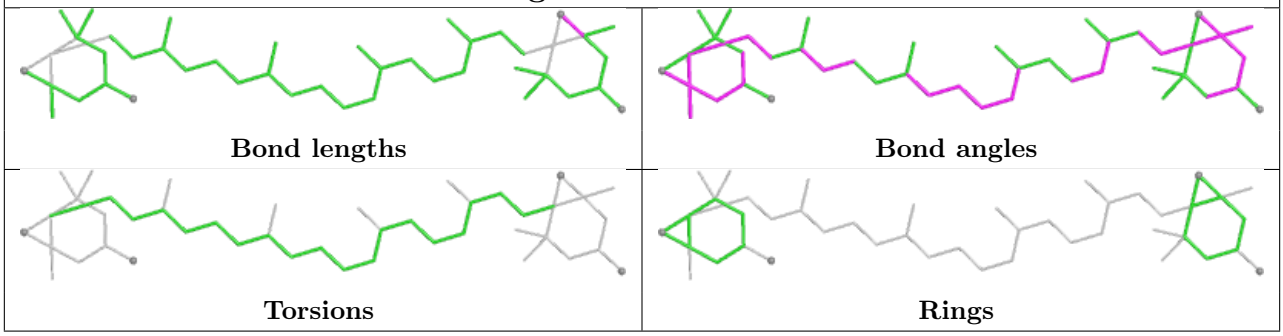


Rings

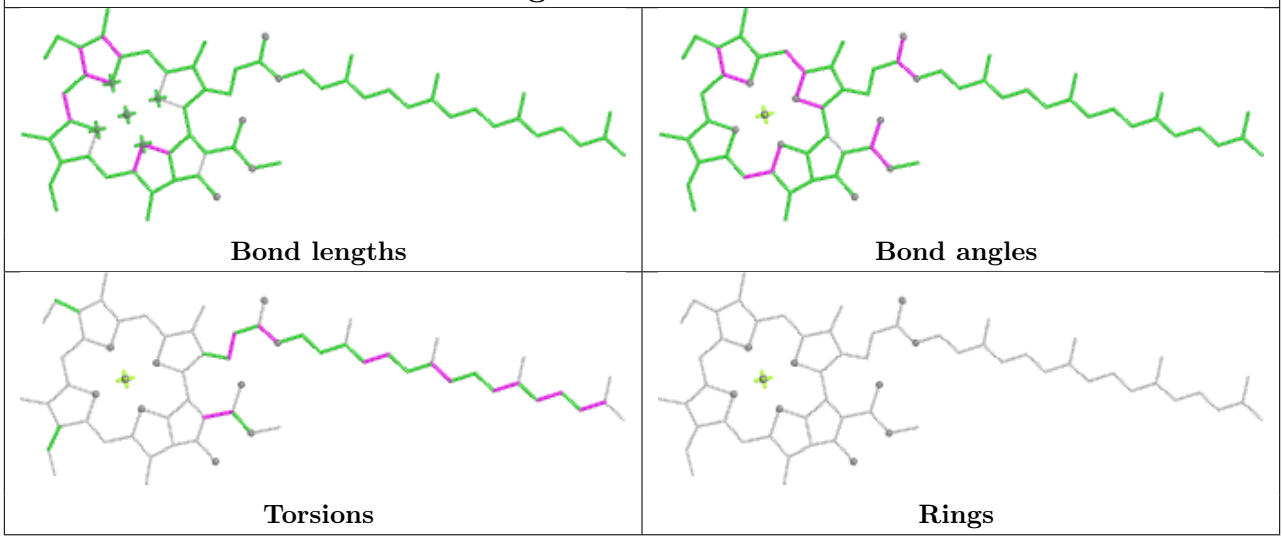
Ligand LHG a 846

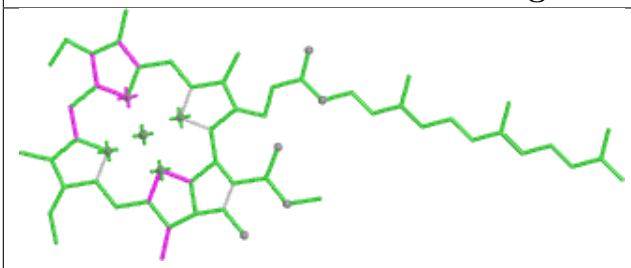
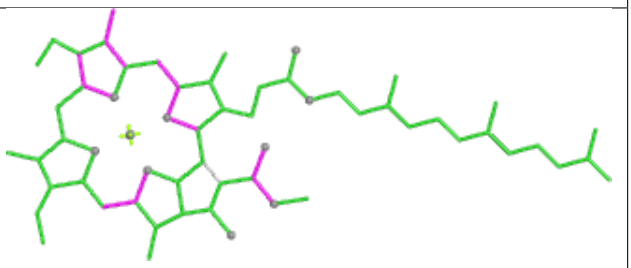
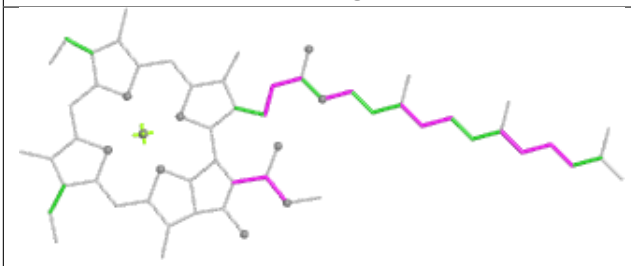
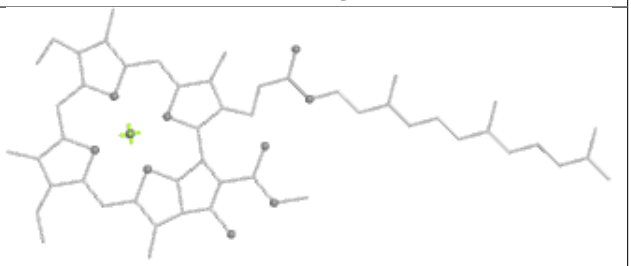


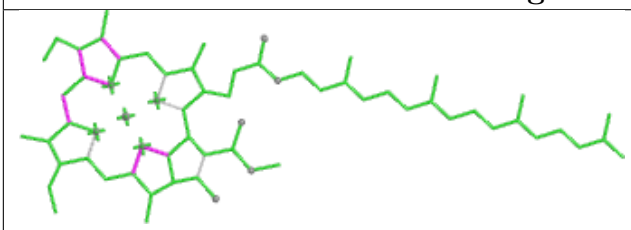
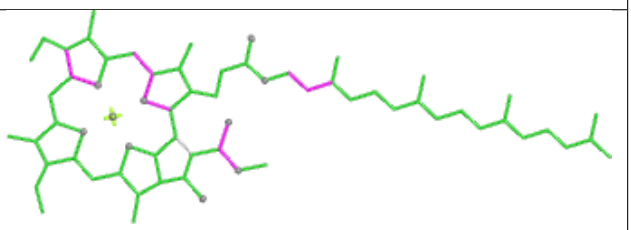
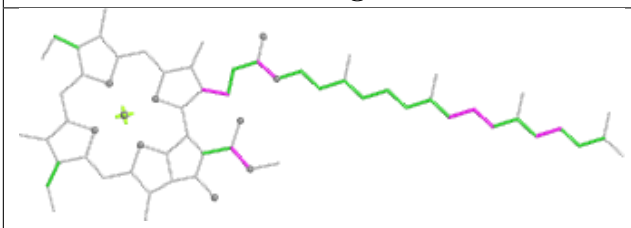
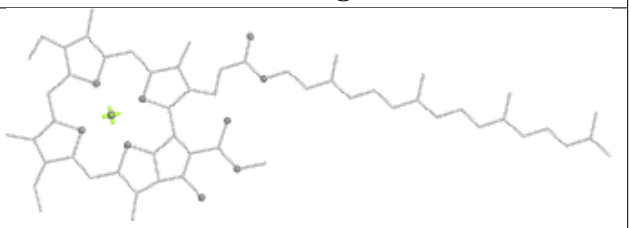
Ligand XAT 1 302

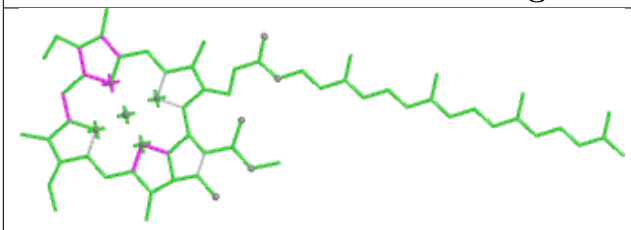
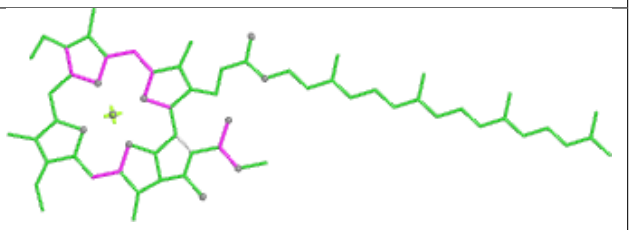
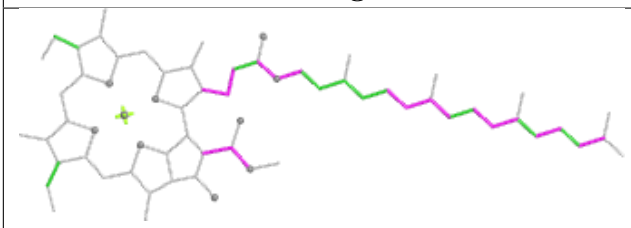
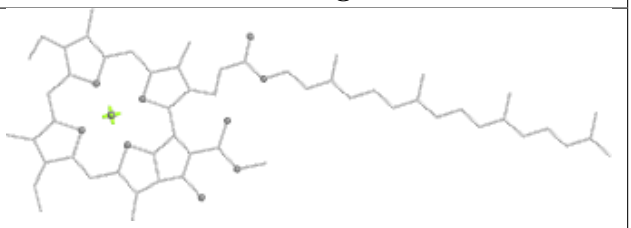


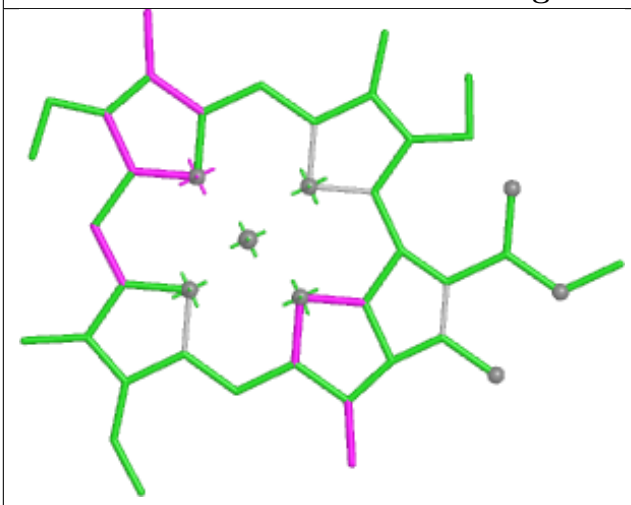
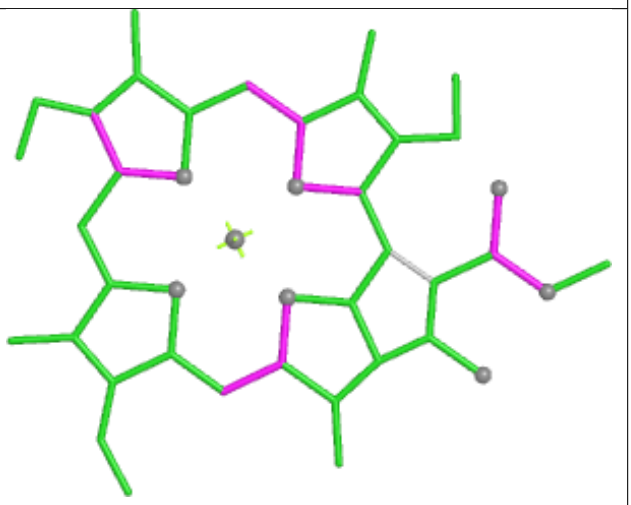
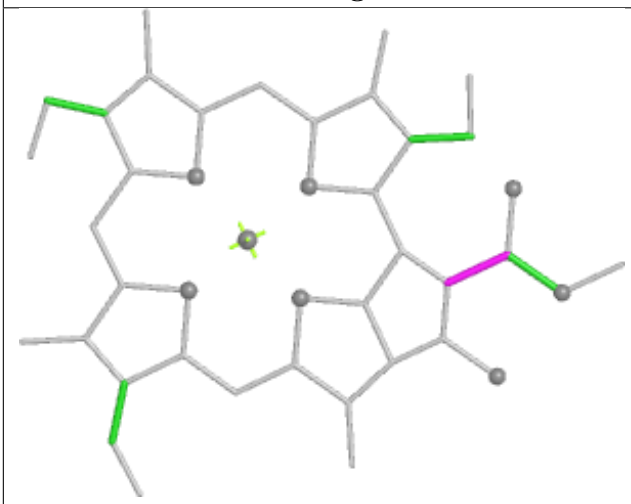
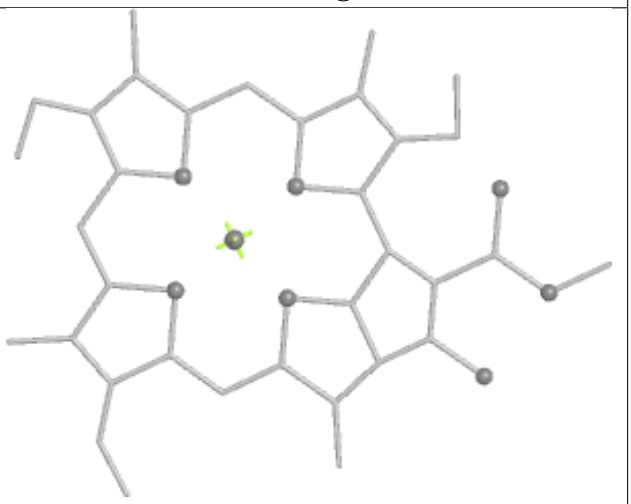
Ligand CLA b 805

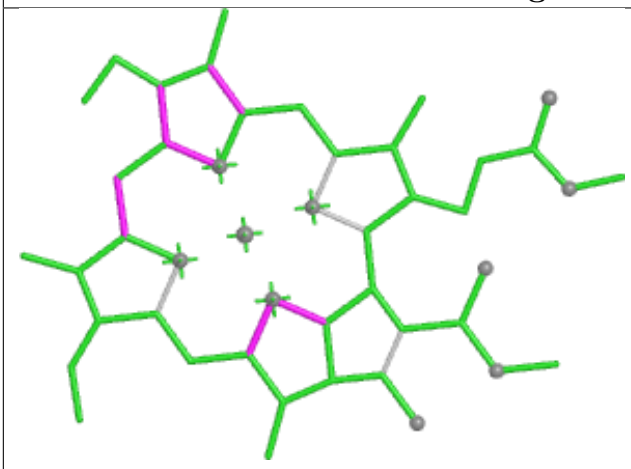
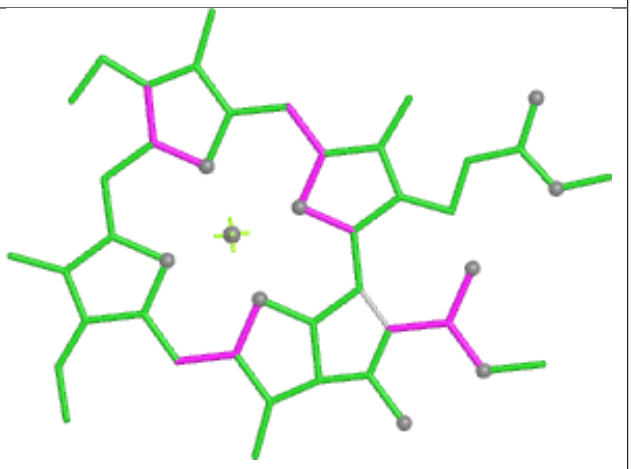
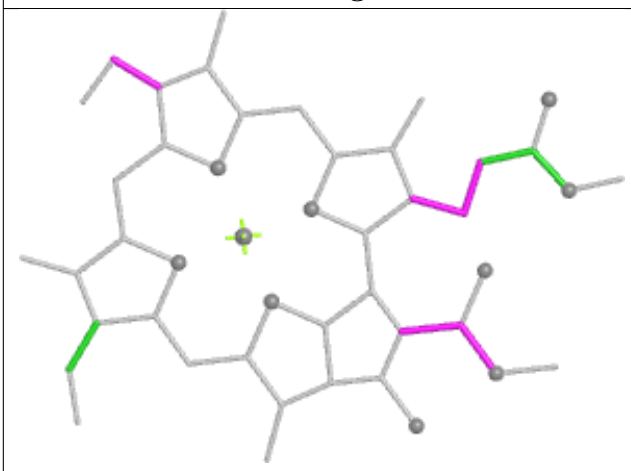
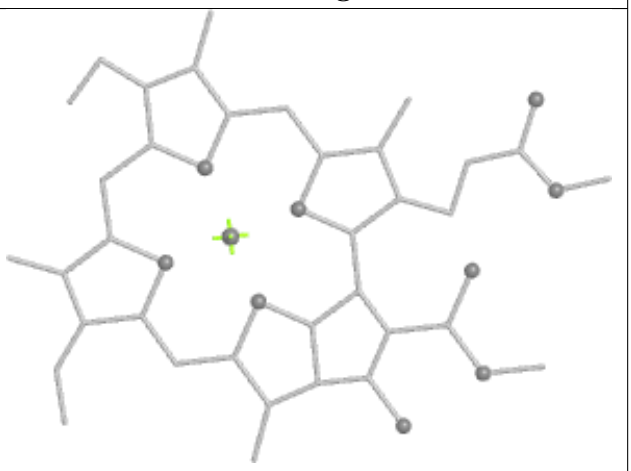


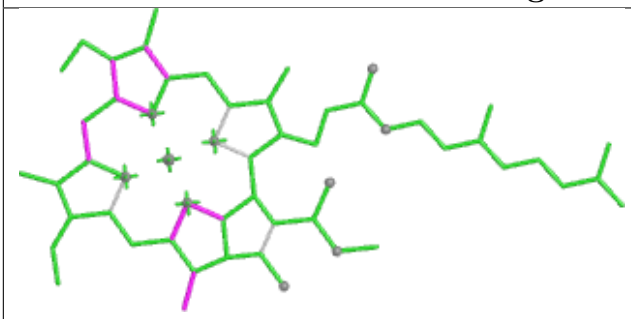
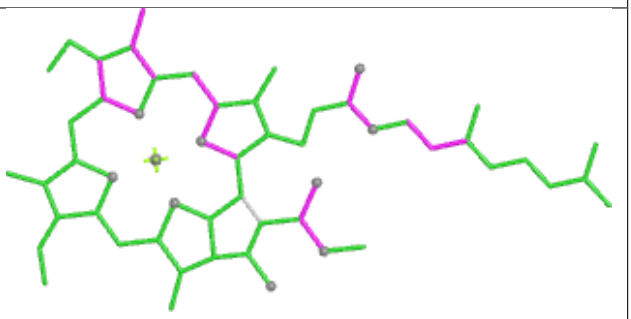
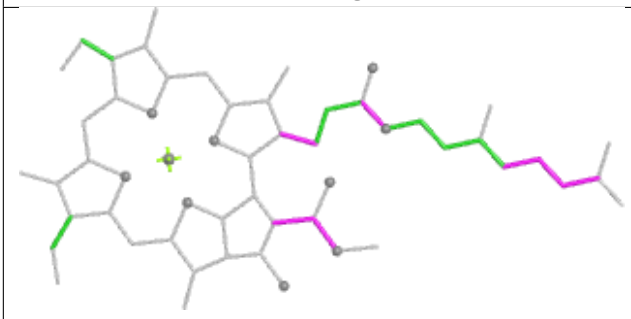
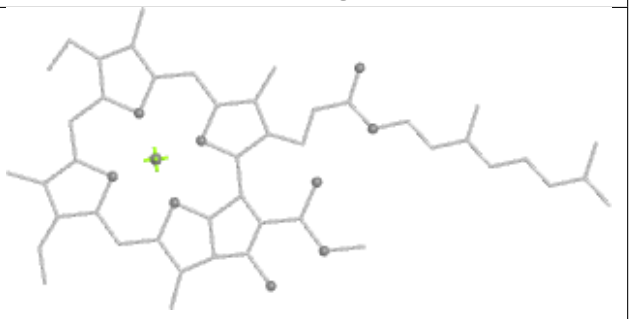
Ligand CLA 7 308	
 Bond lengths	 Bond angles
 Torsions	 Rings

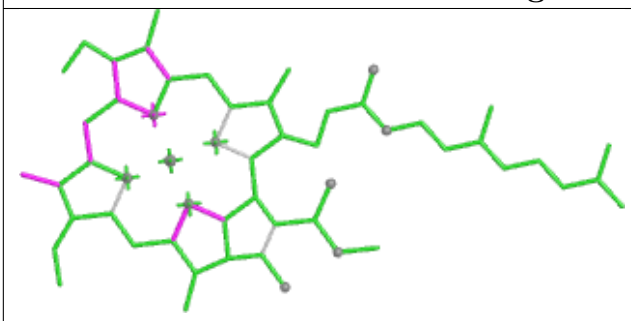
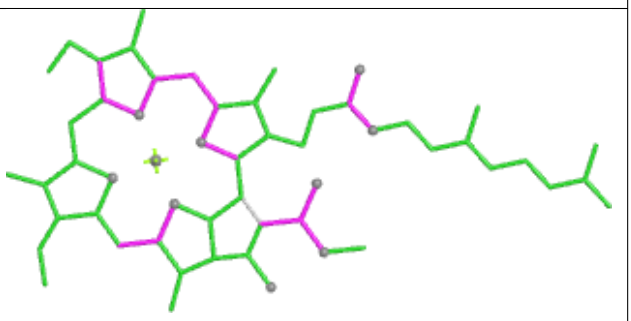
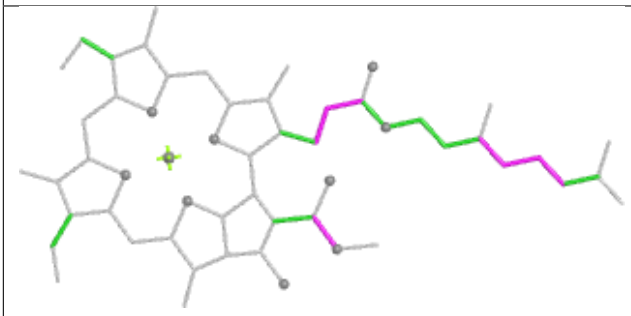
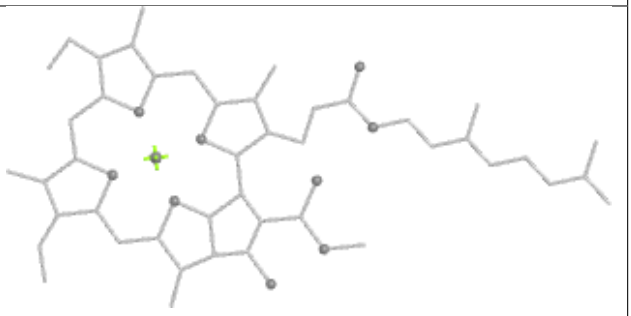
Ligand CLA h 203	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA a 814	
 Bond lengths	 Bond angles
 Torsions	 Rings

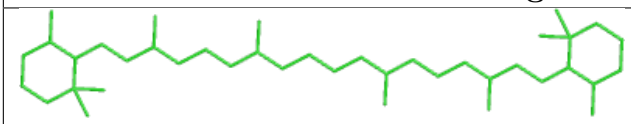
Ligand CLA l 202	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA 9 311	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

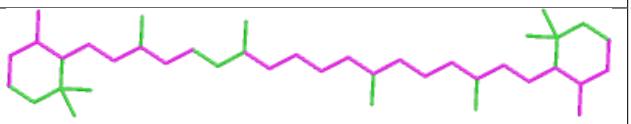
Ligand CLA b 814	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA h 205	
 Bond lengths	 Bond angles
 Torsions	 Rings

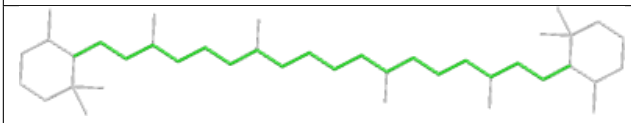
Ligand BCR a 847



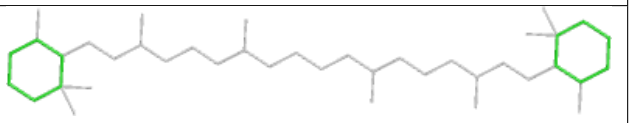
Bond lengths



Bond angles

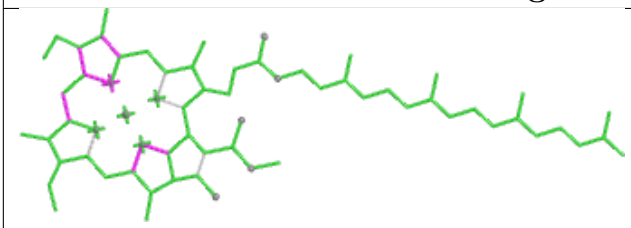


Torsions

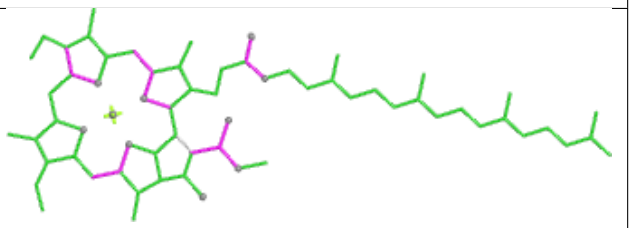


Rings

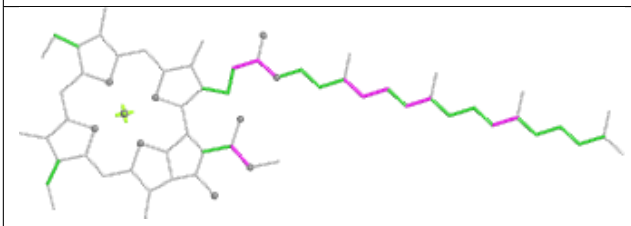
Ligand CLA a 835



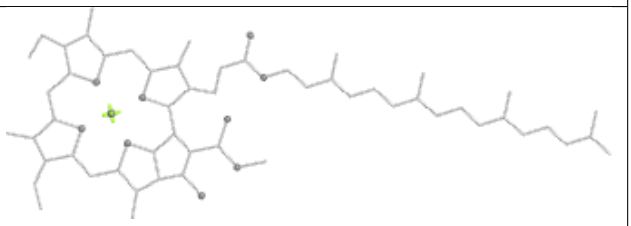
Bond lengths



Bond angles

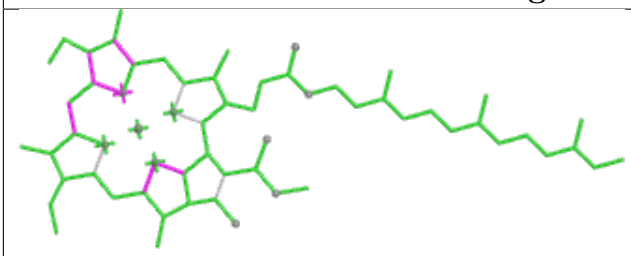


Torsions

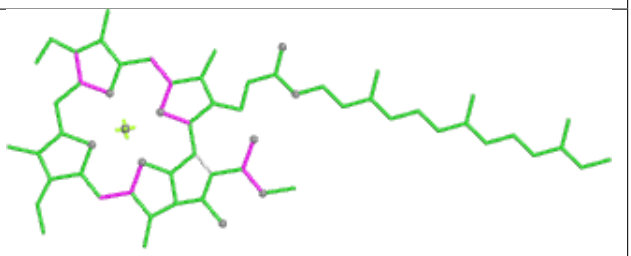


Rings

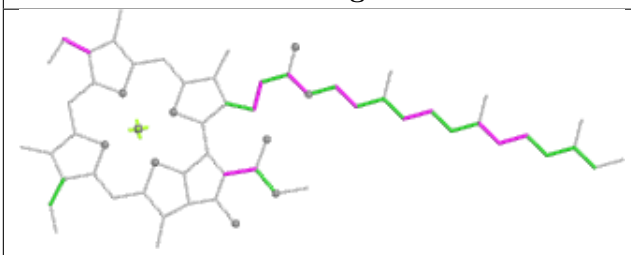
Ligand CLA 1 305



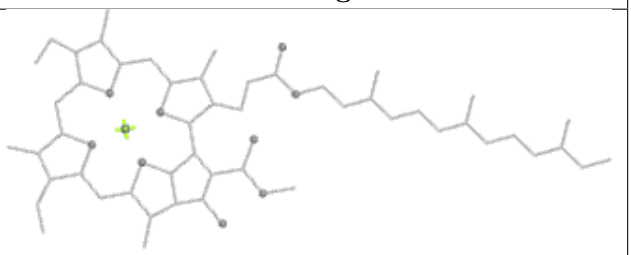
Bond lengths



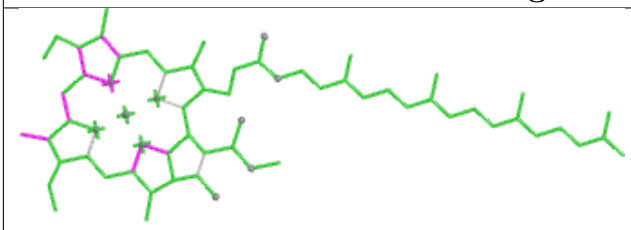
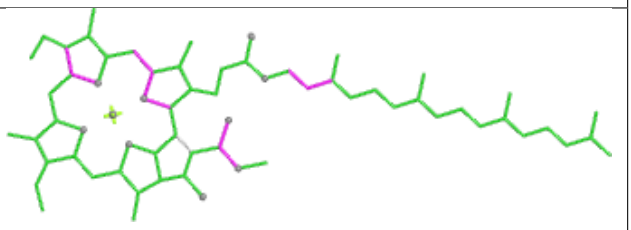
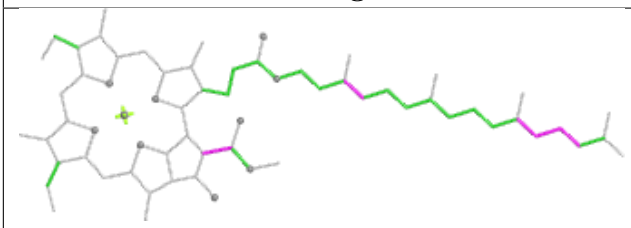
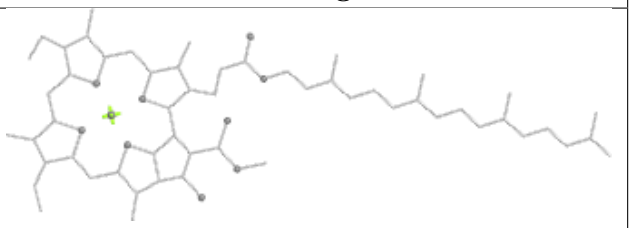
Bond angles

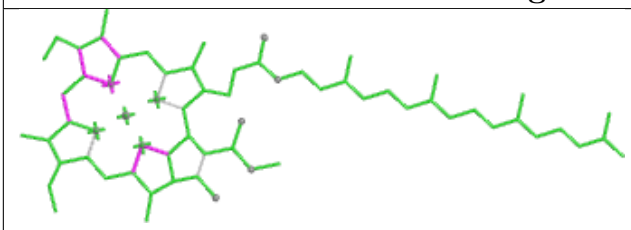
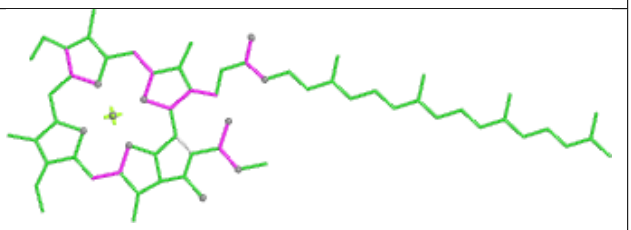
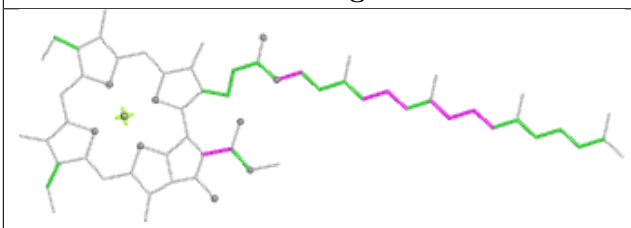
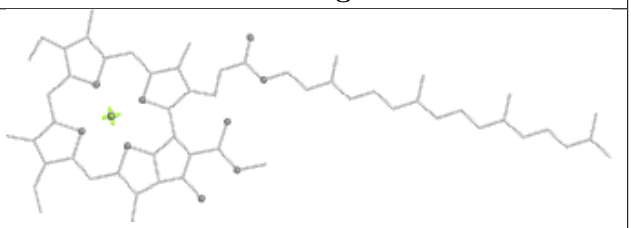


Torsions

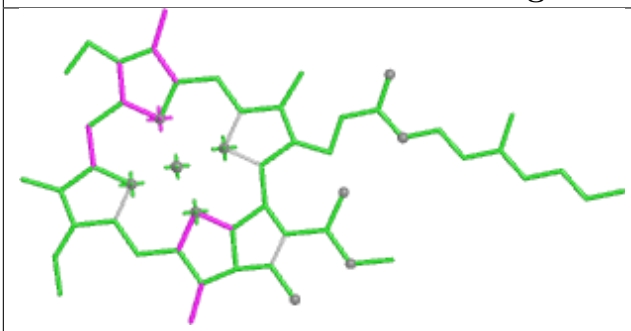


Rings

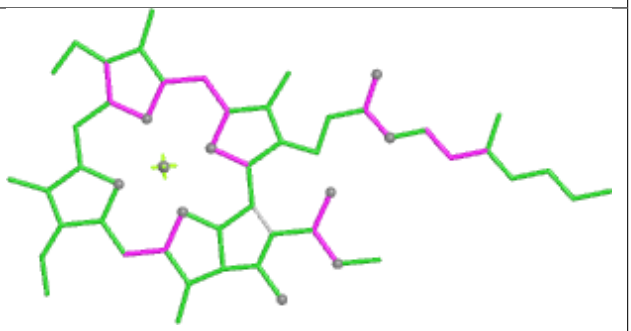
Ligand CLA a 828	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA a 827	
 Bond lengths	 Bond angles
 Torsions	 Rings

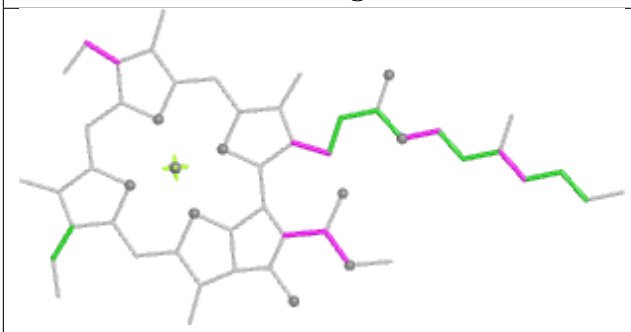
Ligand CLA b 834



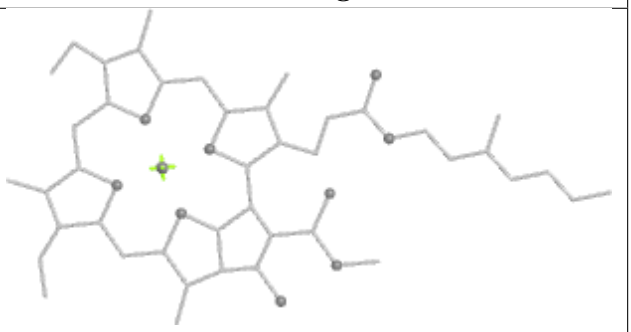
Bond lengths



Bond angles

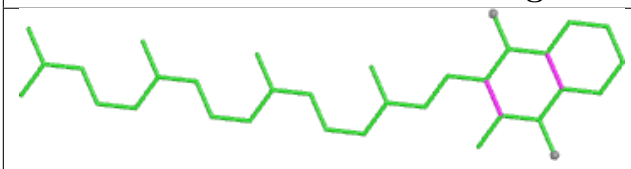


Torsions

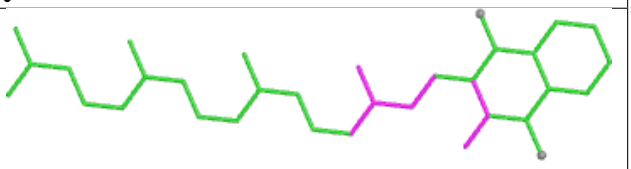


Rings

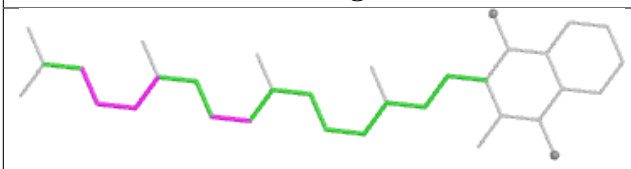
Ligand PQN a 843



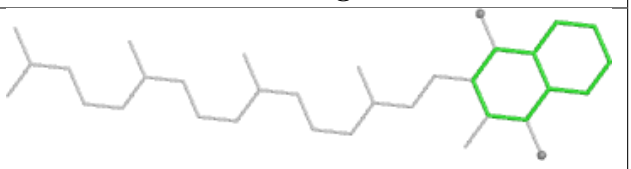
Bond lengths



Bond angles



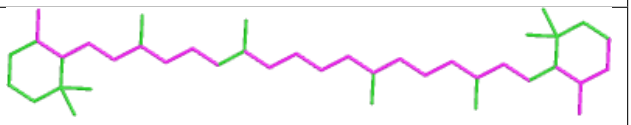
Torsions



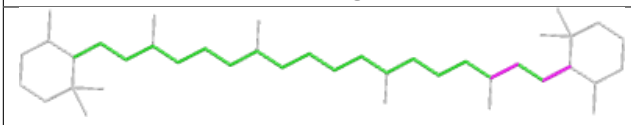
Rings

Ligand BCR a 850

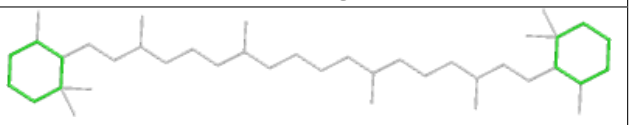
Bond lengths



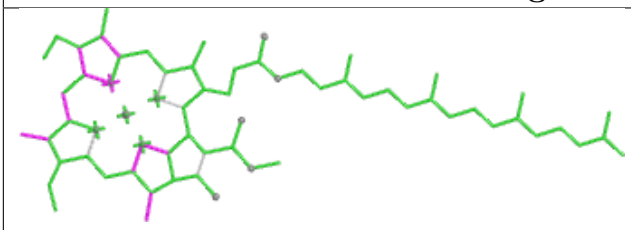
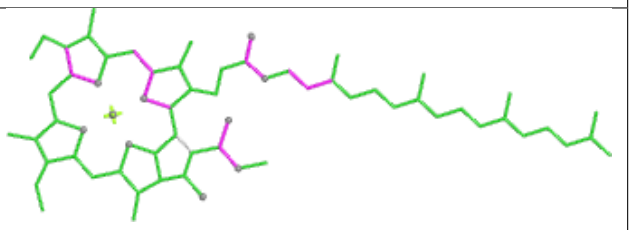
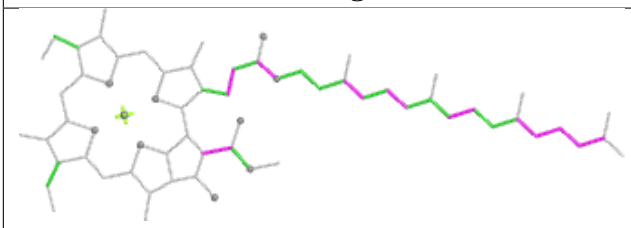
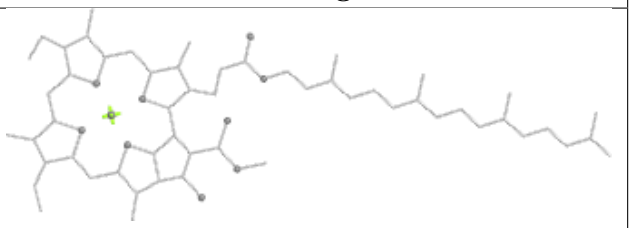
Bond angles

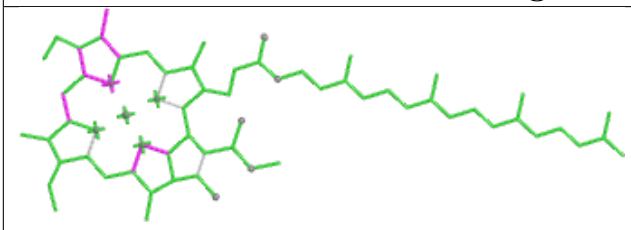
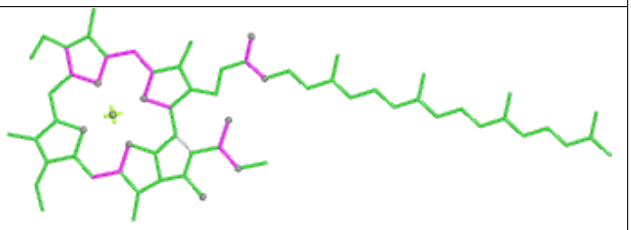
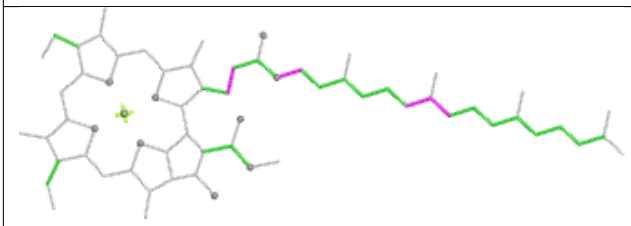
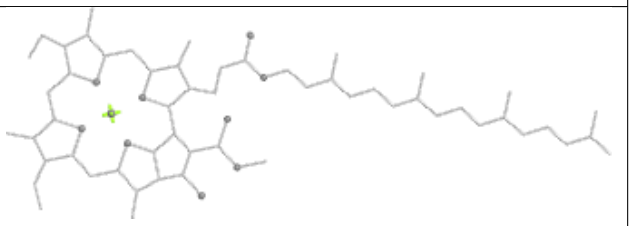


Torsions

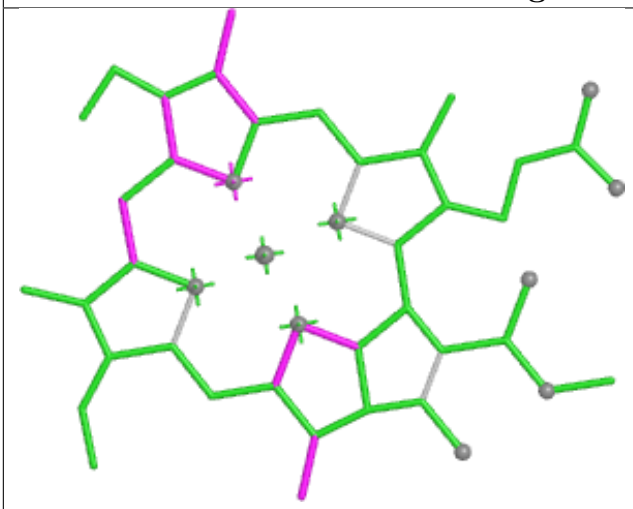


Rings

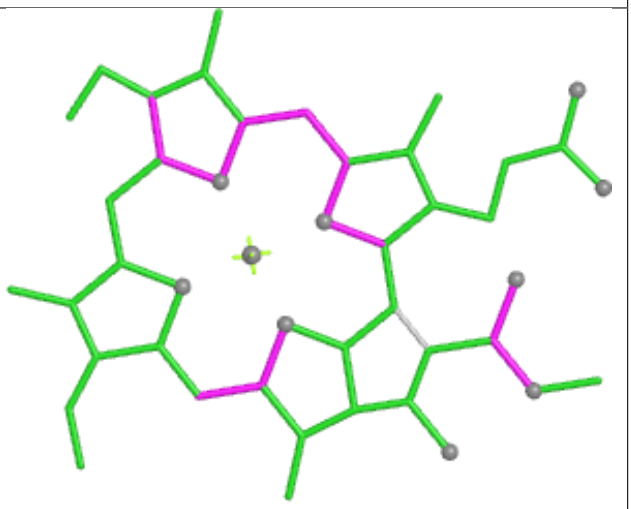
Ligand CLA a 830	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA a 822	
 Bond lengths	 Bond angles
 Torsions	 Rings

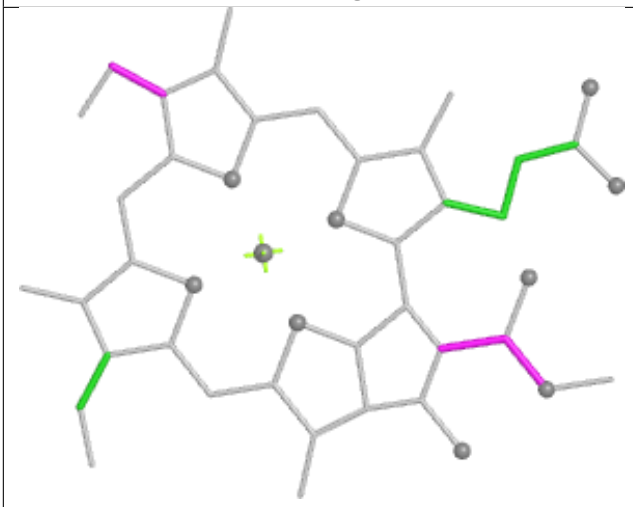
Ligand CLA a 837



Bond lengths



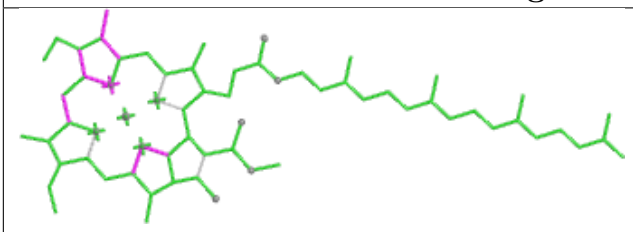
Bond angles



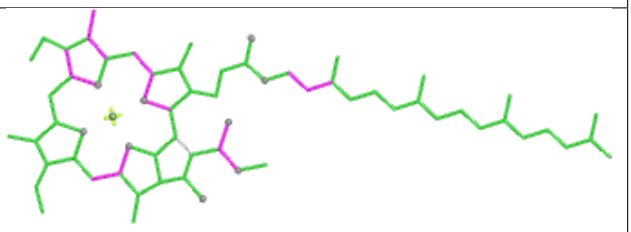
Torsions

Rings

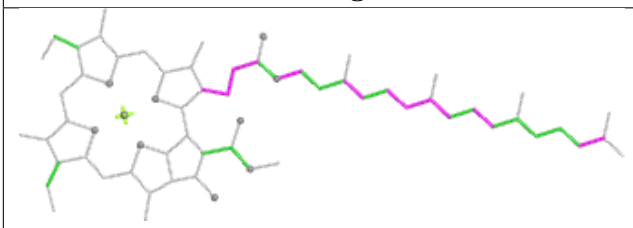
Ligand CLA b 810



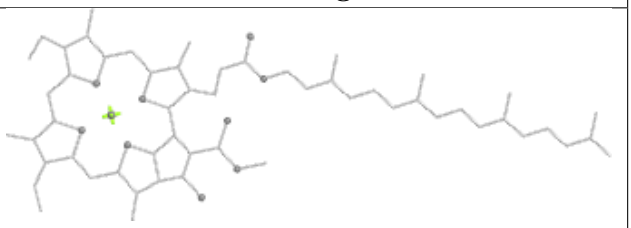
Bond lengths



Bond angles

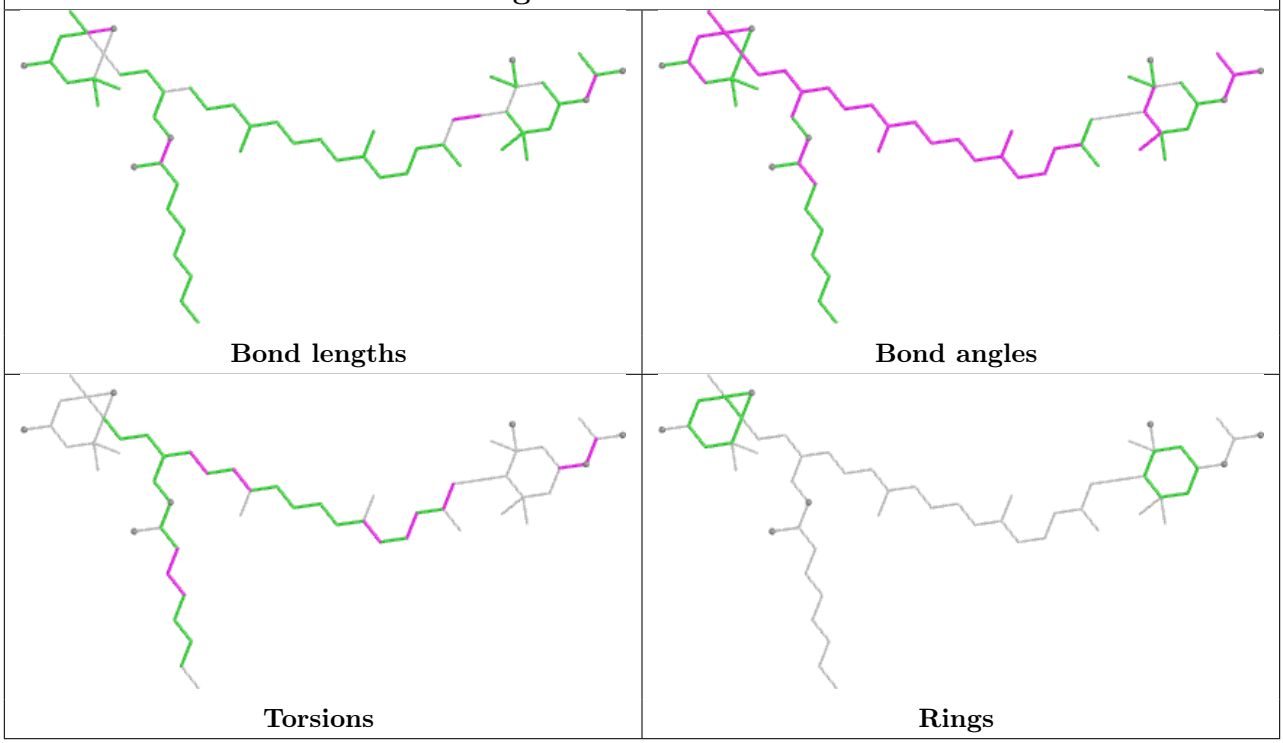


Torsions

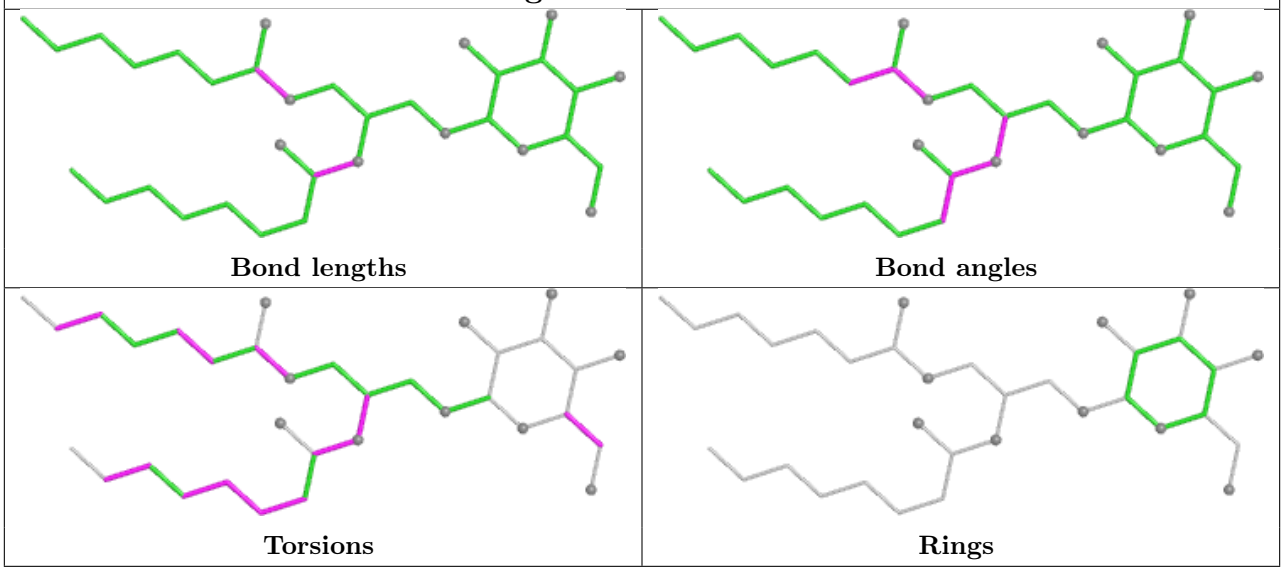


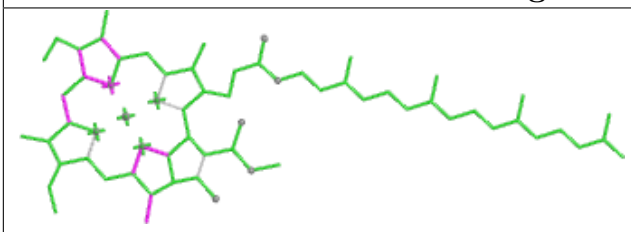
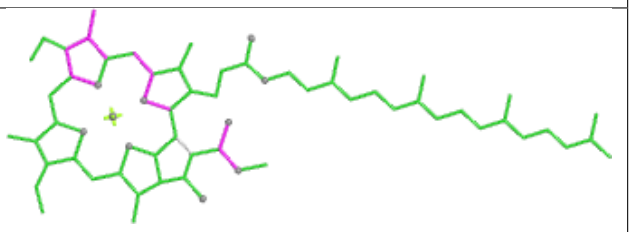
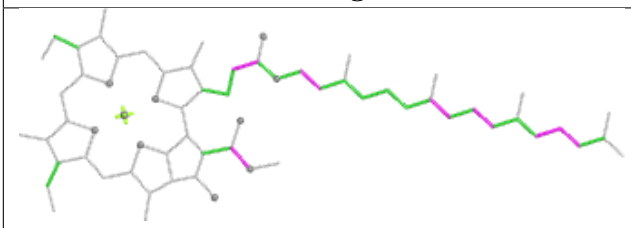
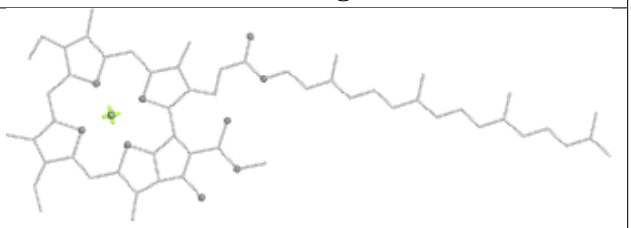
Rings

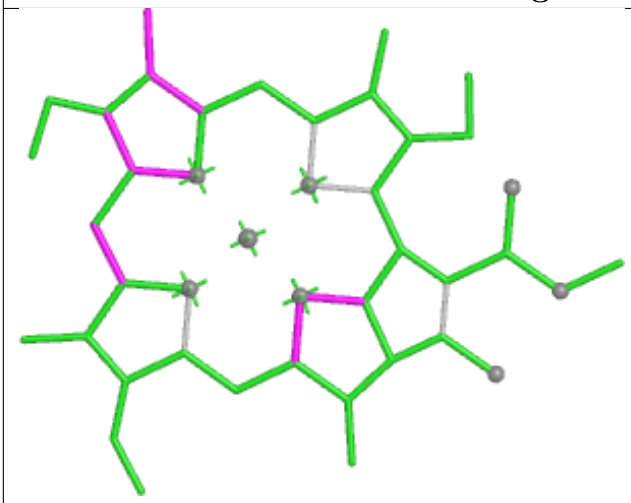
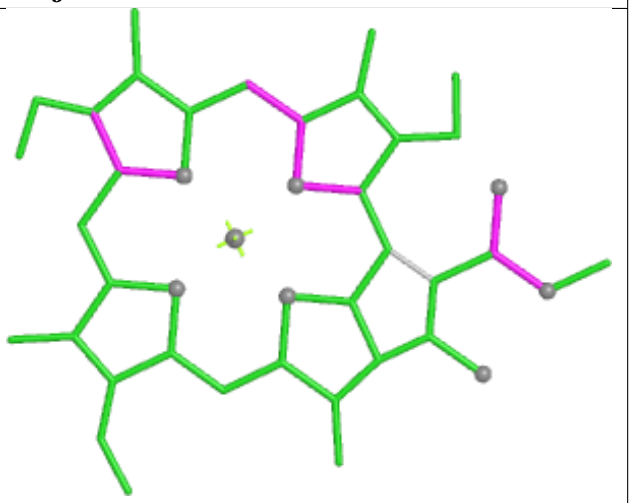
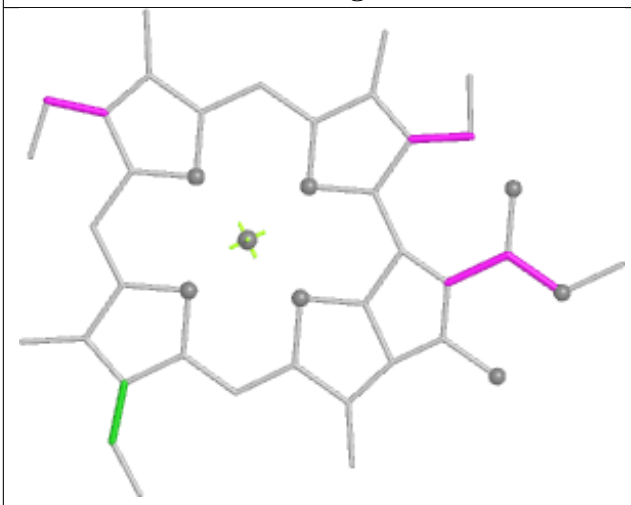
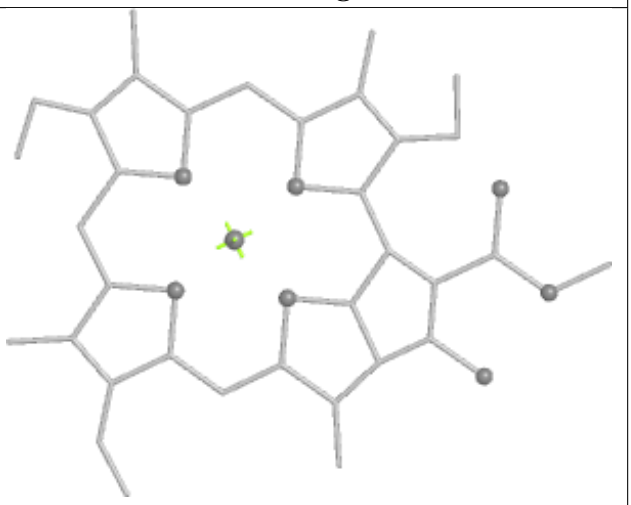
Ligand A1L1F 8 304

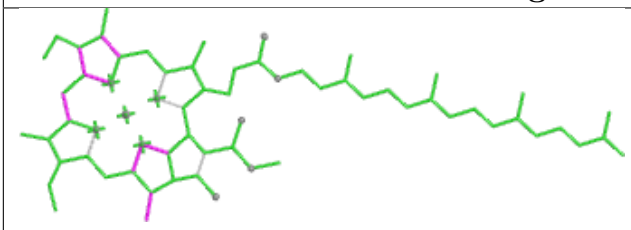
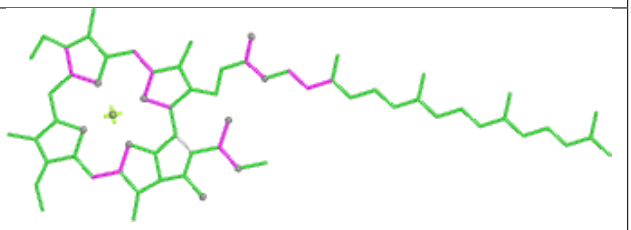
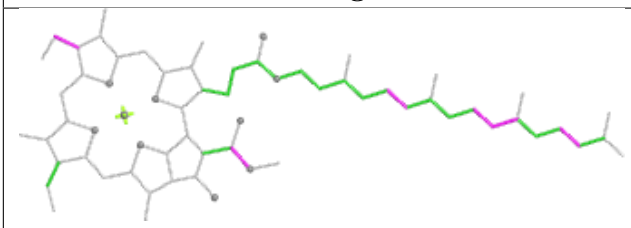
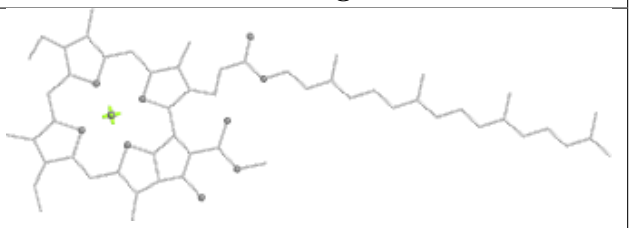


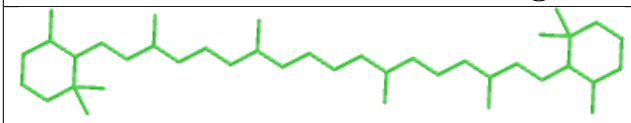
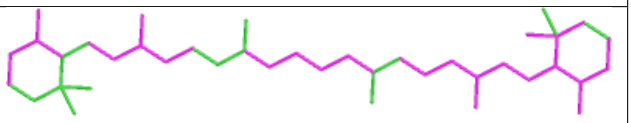
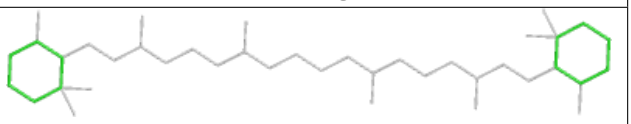
Ligand LMG a 853



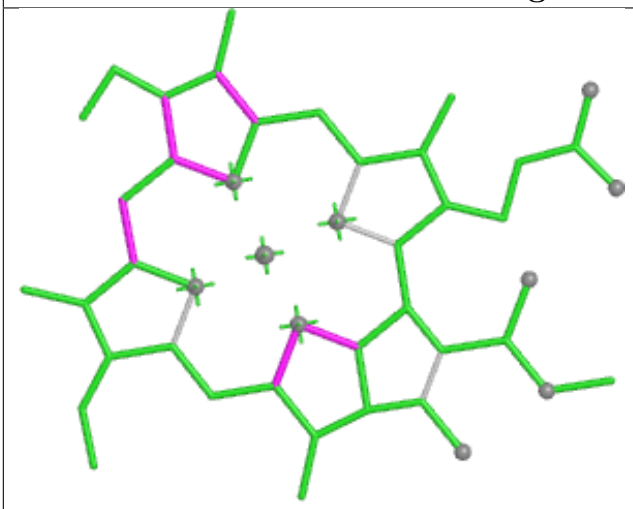
Ligand CLA a 826	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA j 103	
 Bond lengths	 Bond angles
 Torsions	 Rings

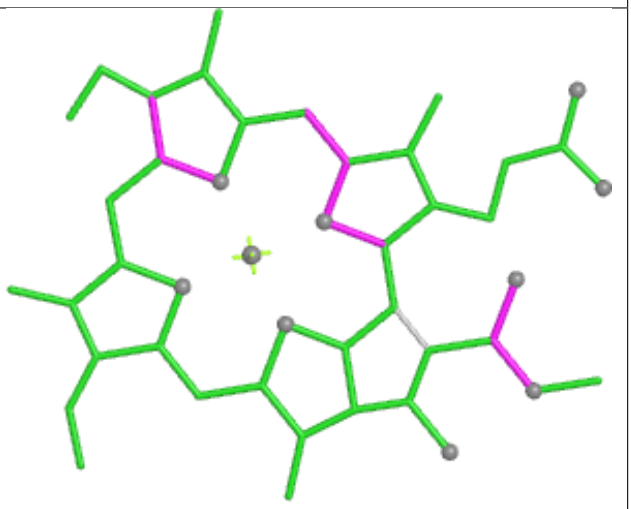
Ligand CLA a 834	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand BCR l 201	
 Bond lengths	 Bond angles
Torsions	 Rings

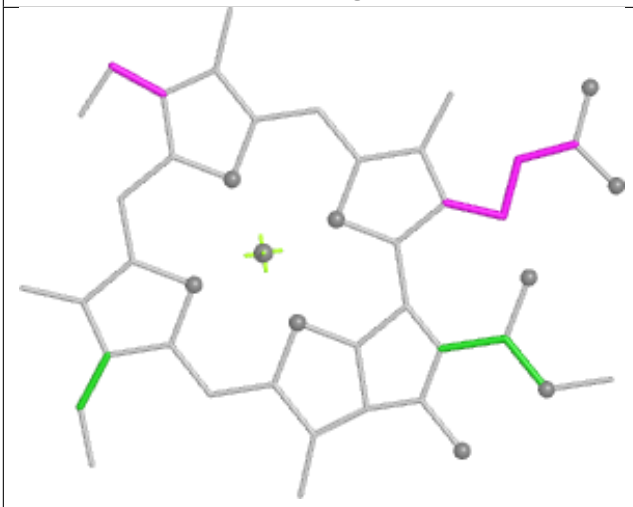
Ligand CLA 1 314



Bond lengths



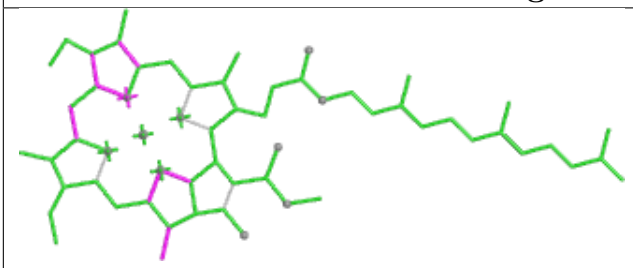
Bond angles



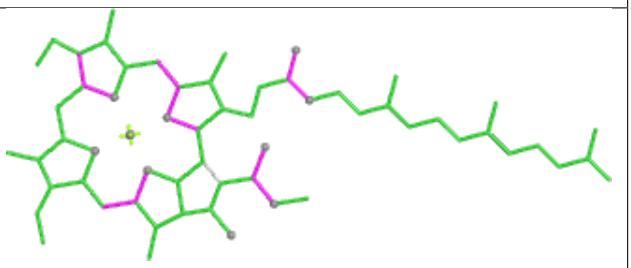
Torsions

Rings

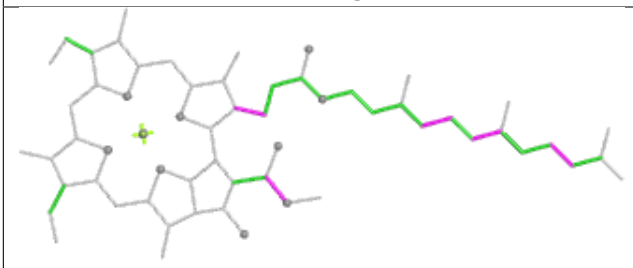
Ligand CLA b 822



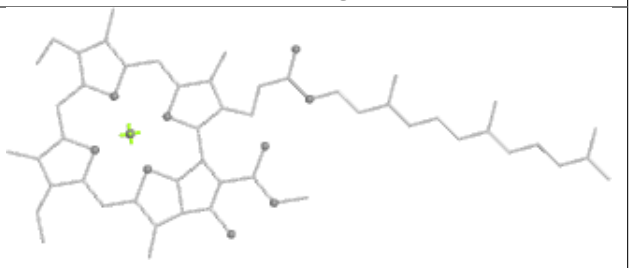
Bond lengths



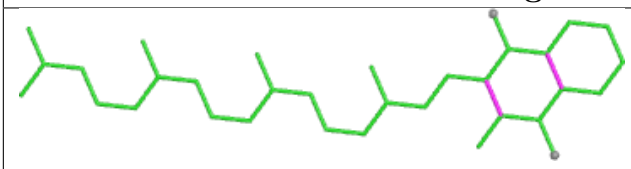
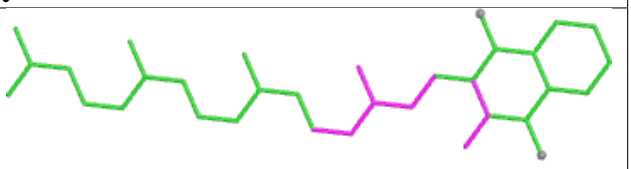
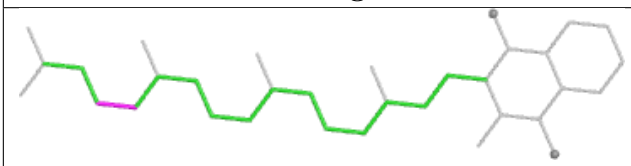
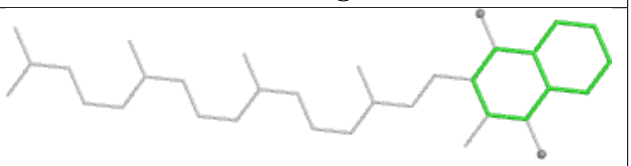
Bond angles

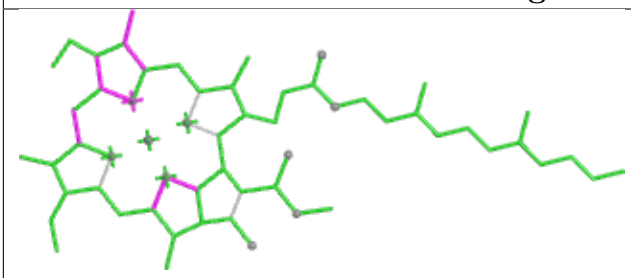
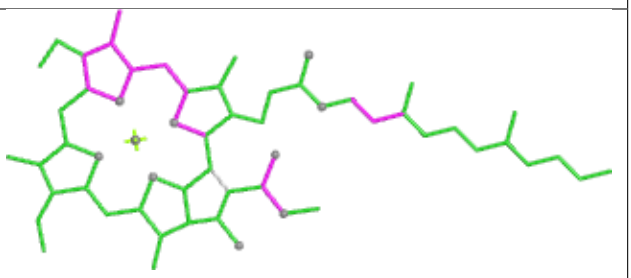
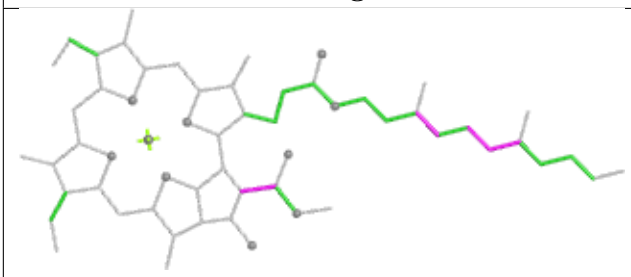
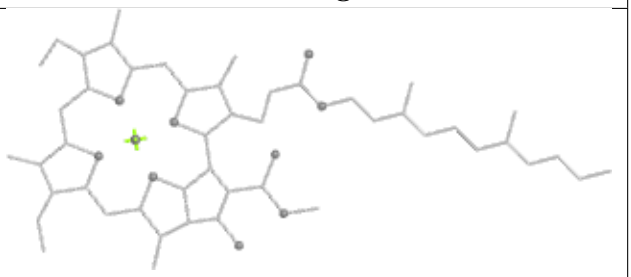


Torsions

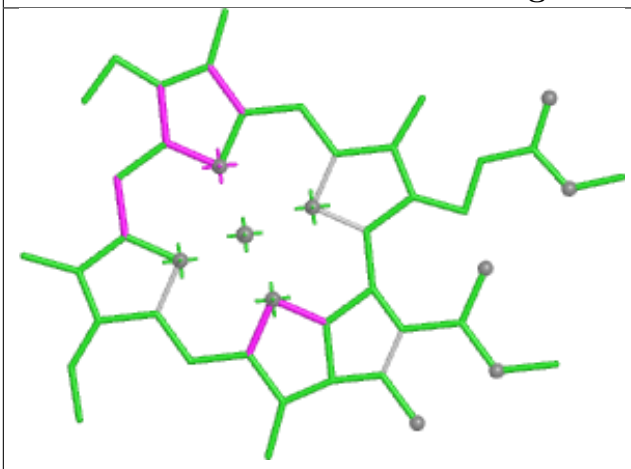


Rings

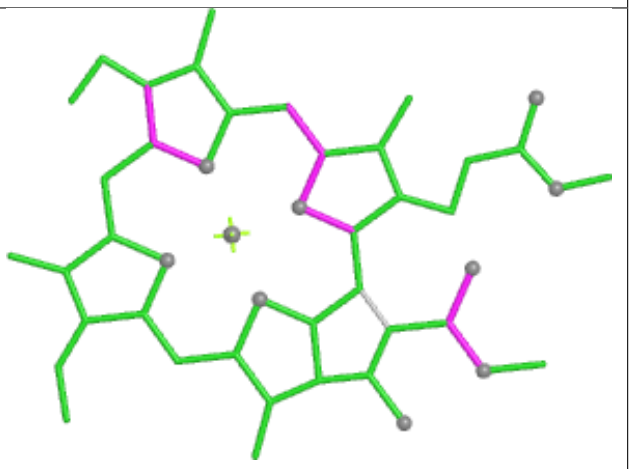
Ligand PQN b 841	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA a 802	
 Bond lengths	 Bond angles
 Torsions	 Rings

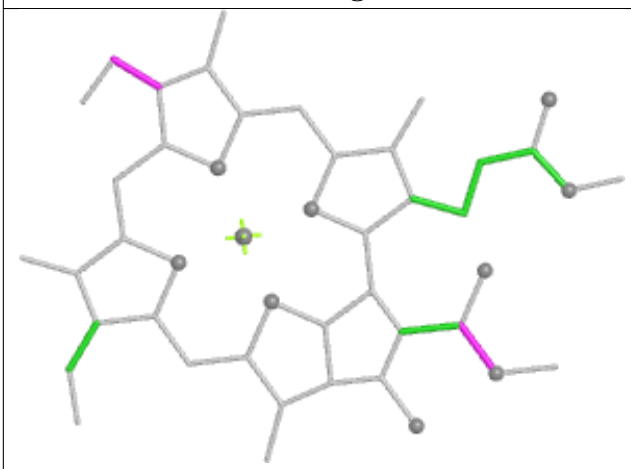
Ligand CLA 8 306



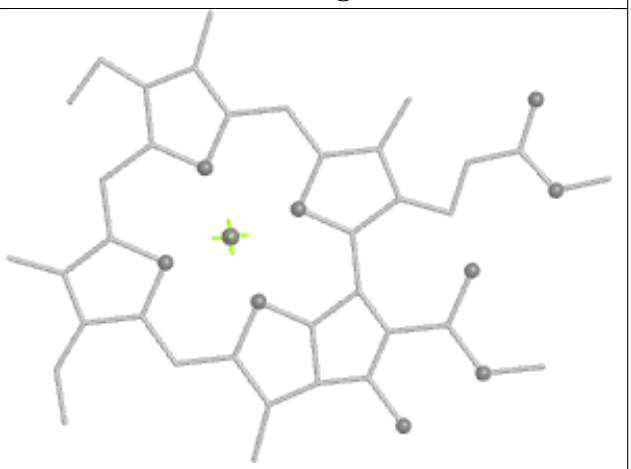
Bond lengths



Bond angles

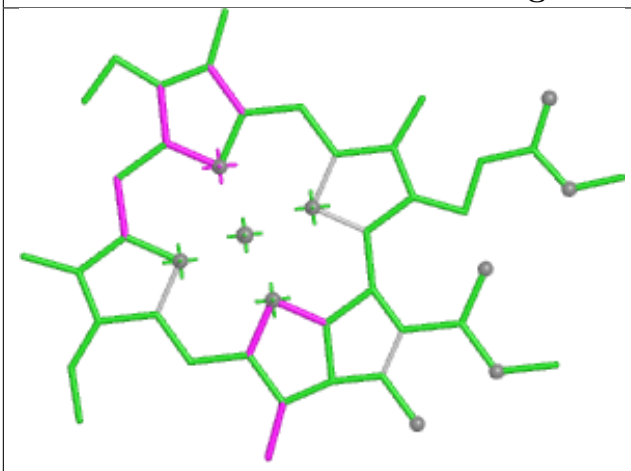


Torsions

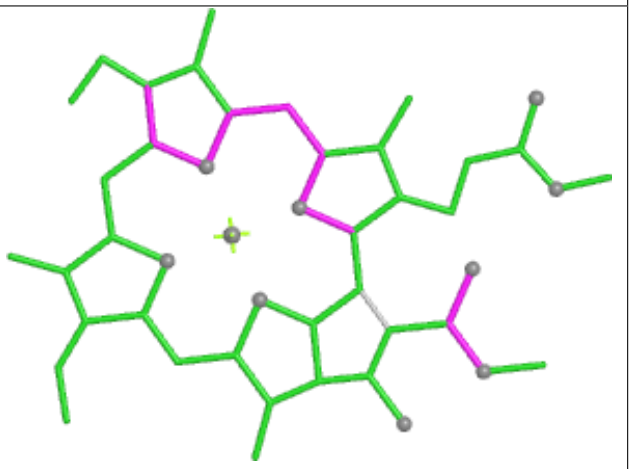


Rings

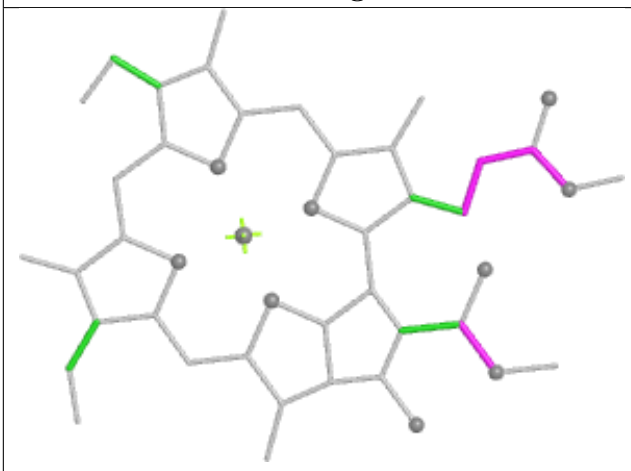
Ligand CLA 7 310



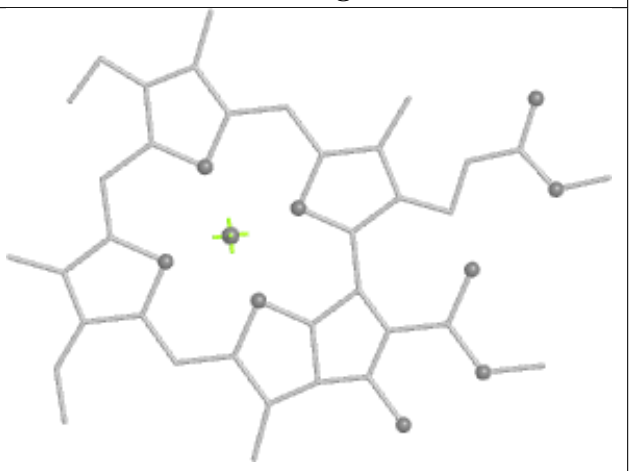
Bond lengths



Bond angles

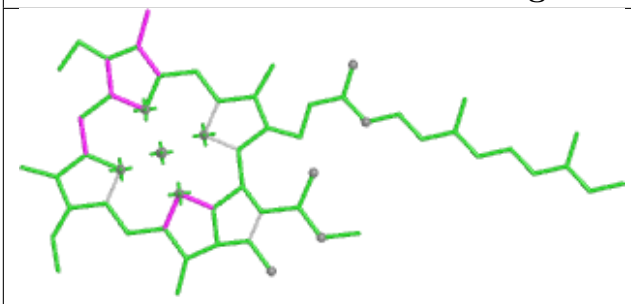


Torsions

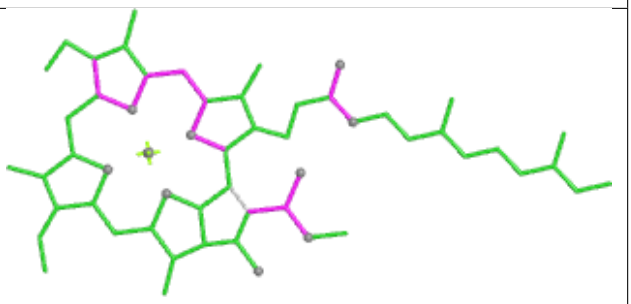


Rings

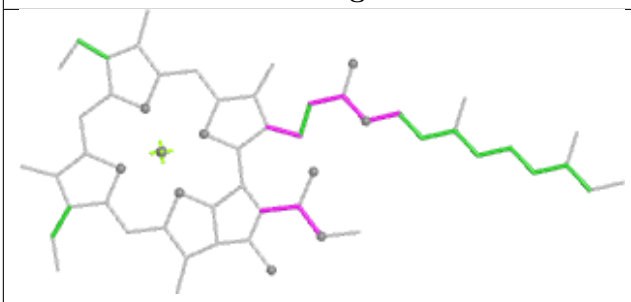
Ligand CLA a 818



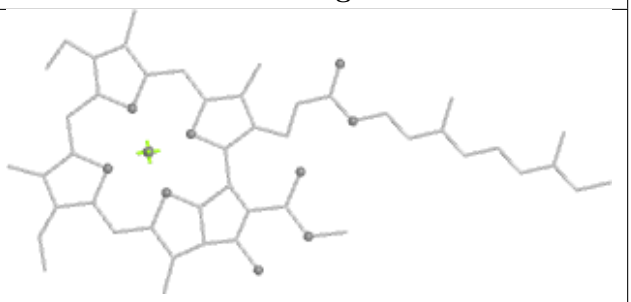
Bond lengths



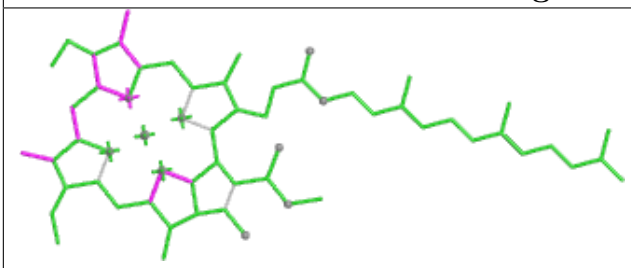
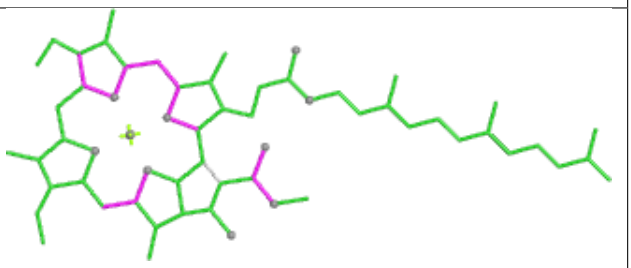
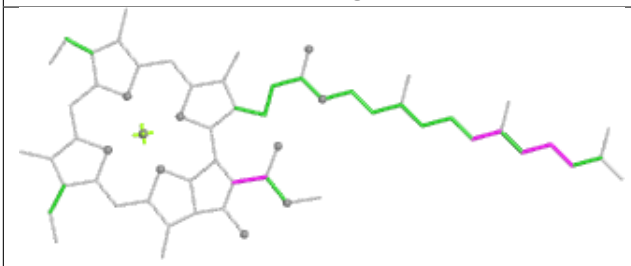
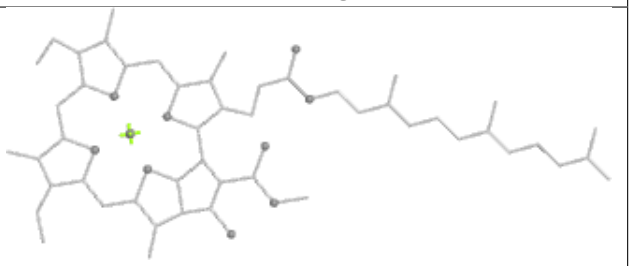
Bond angles

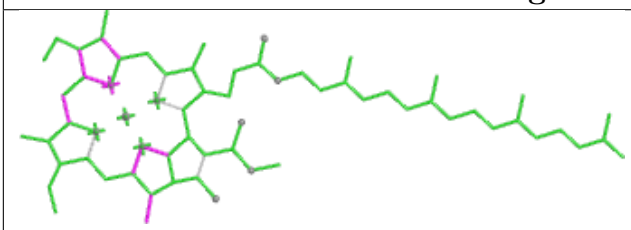
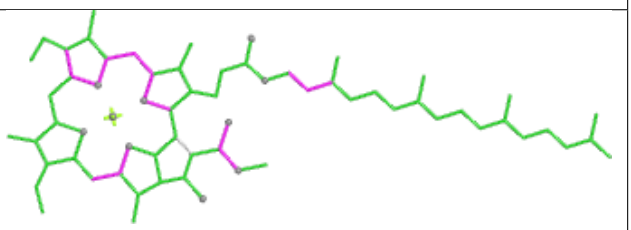
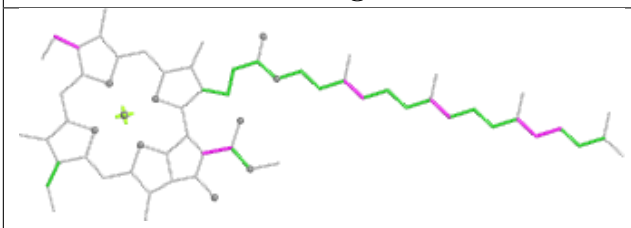
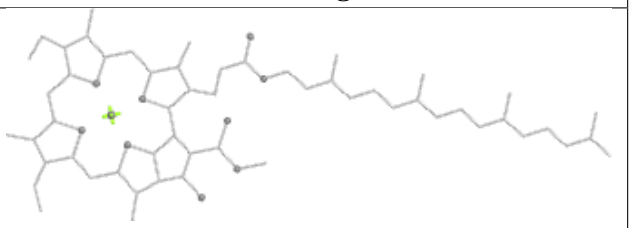


Torsions

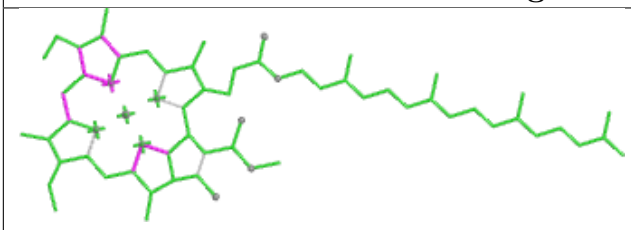


Rings

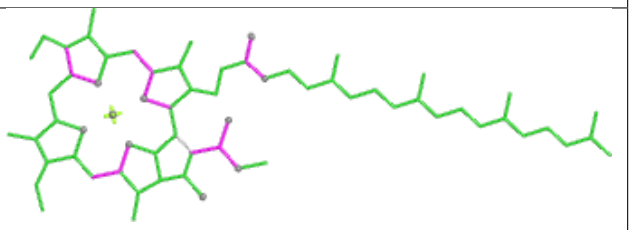
Ligand CLA l 203	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA a 840	
 Bond lengths	 Bond angles
 Torsions	 Rings

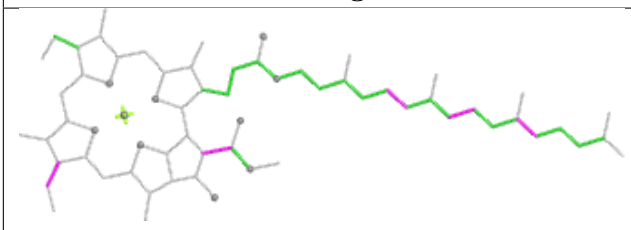
Ligand CLA b 836



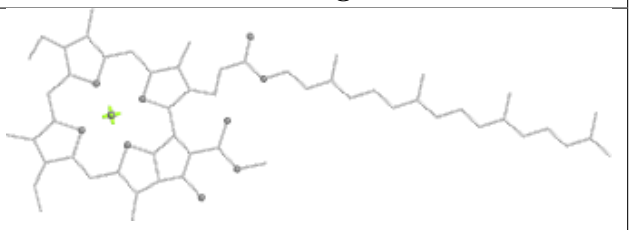
Bond lengths



Bond angles

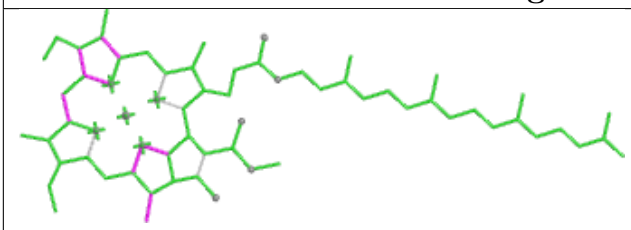


Torsions

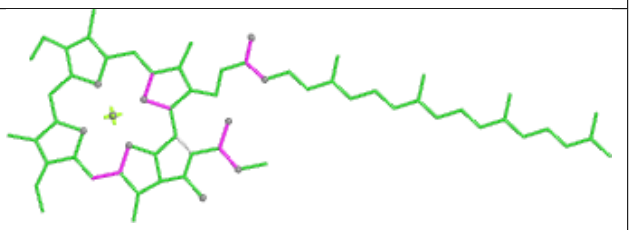


Rings

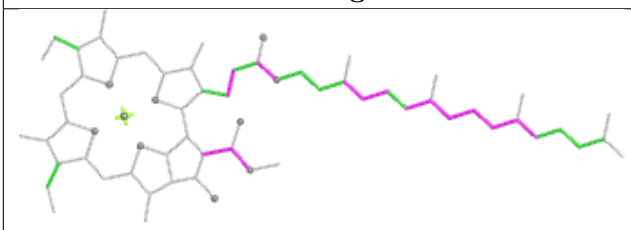
Ligand CLA b 802



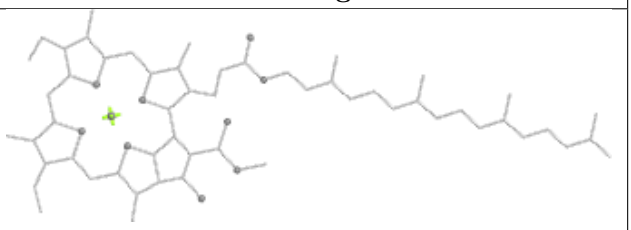
Bond lengths



Bond angles

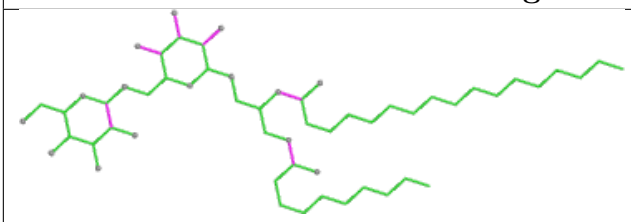


Torsions

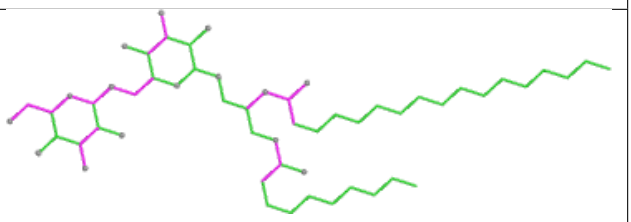


Rings

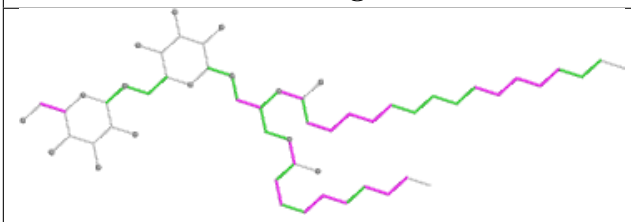
Ligand DGD b 848



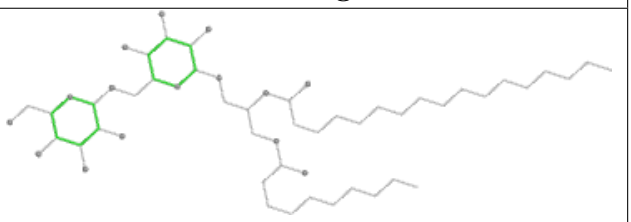
Bond lengths



Bond angles

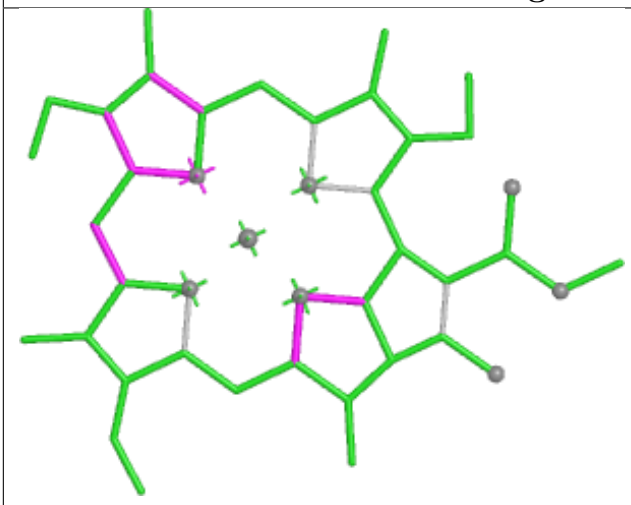


Torsions

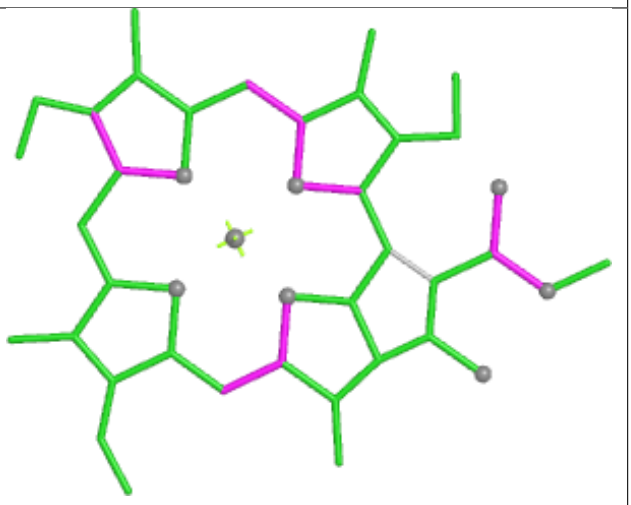


Rings

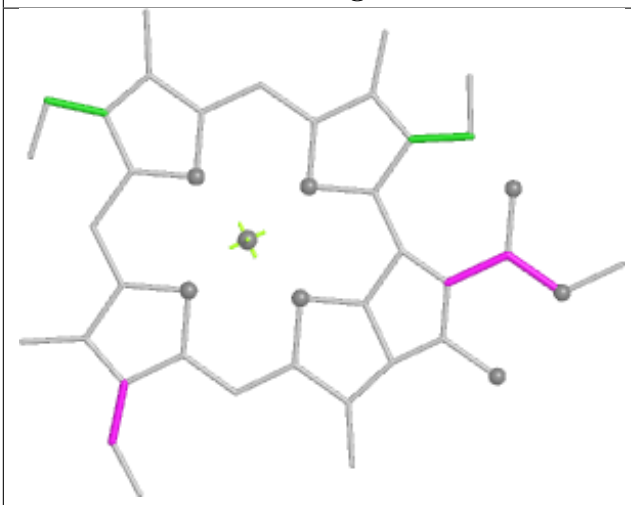
Ligand CLA 9 315



Bond lengths



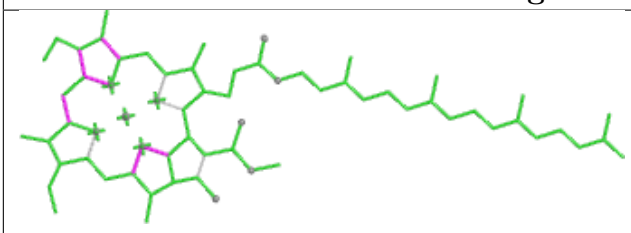
Bond angles



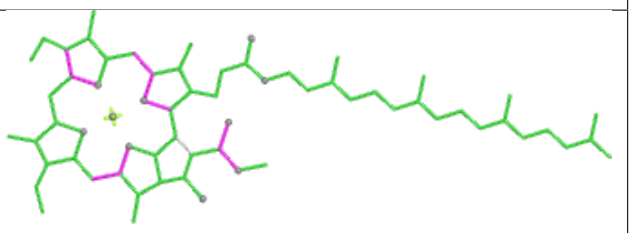
Torsions

Rings

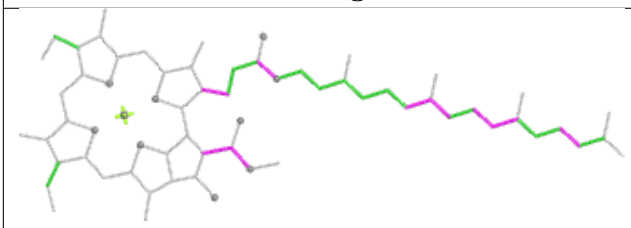
Ligand CLA b 806



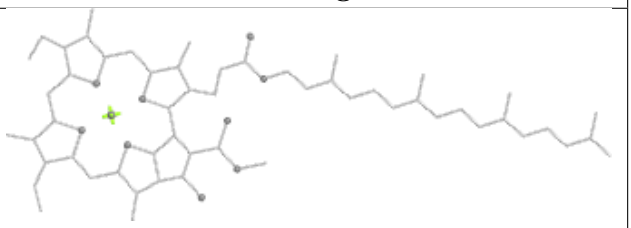
Bond lengths



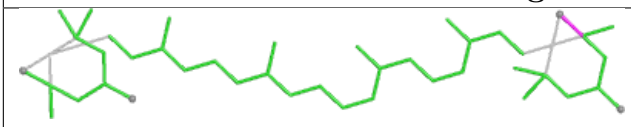
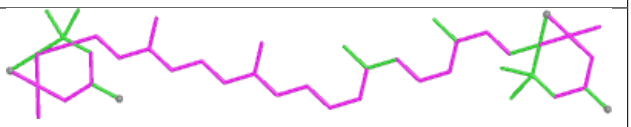
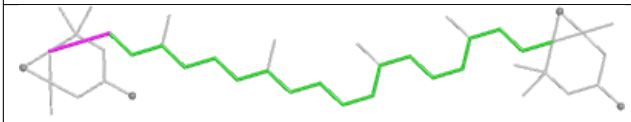
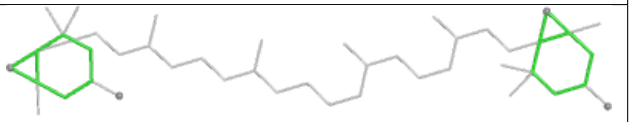
Bond angles

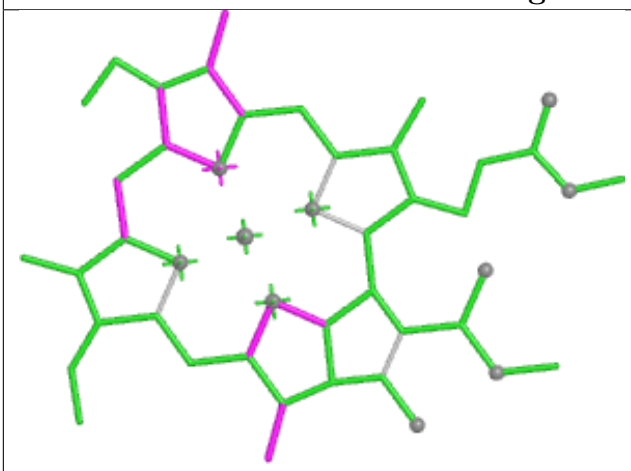
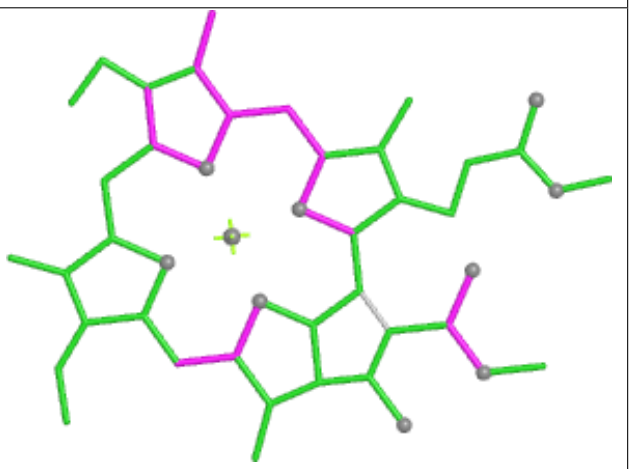
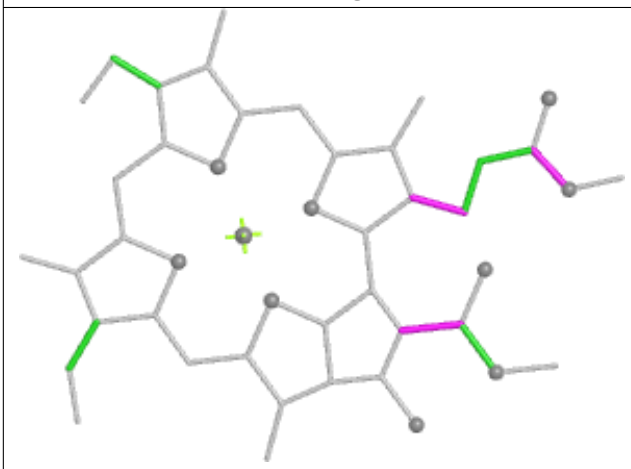
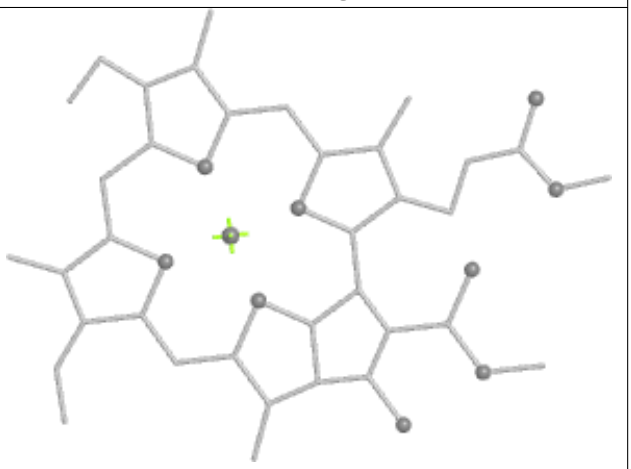


Torsions

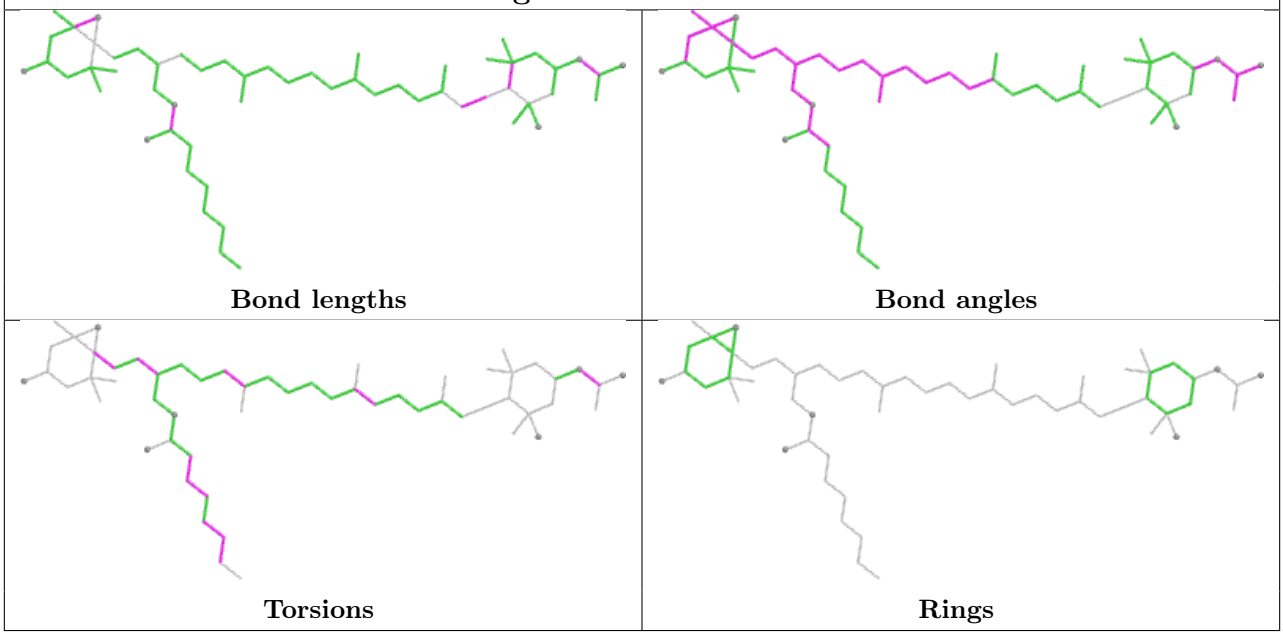


Rings

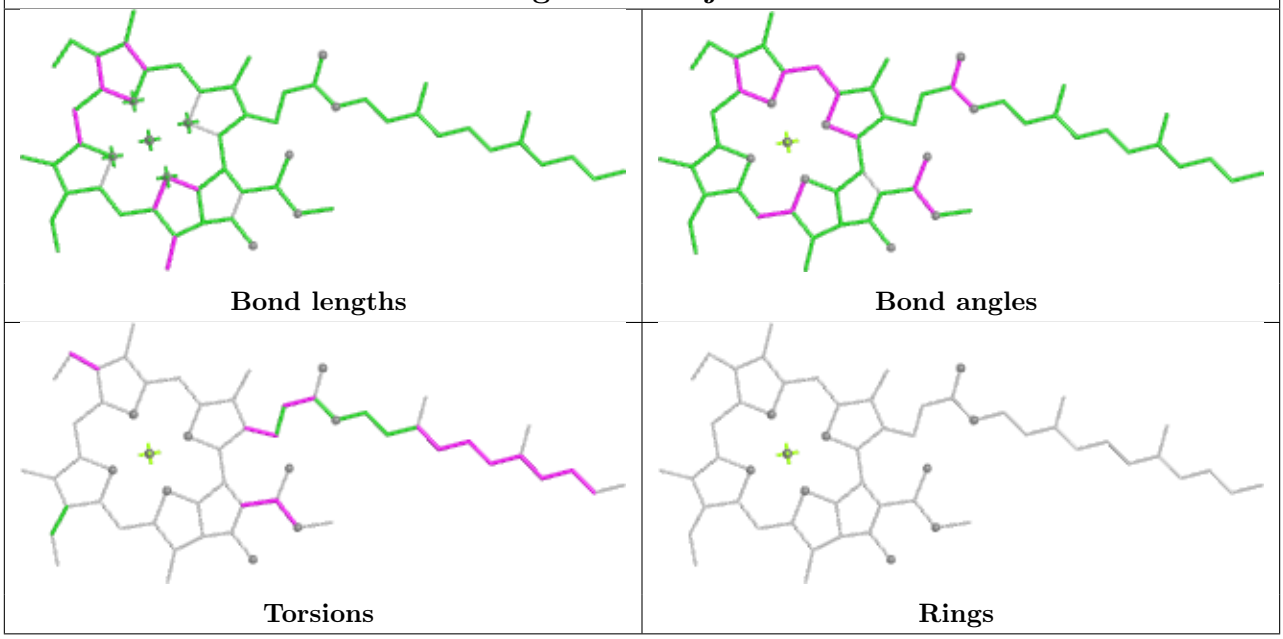
Ligand XAT 9 304	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA 7 311	
 Bond lengths	 Bond angles
 Torsions	 Rings

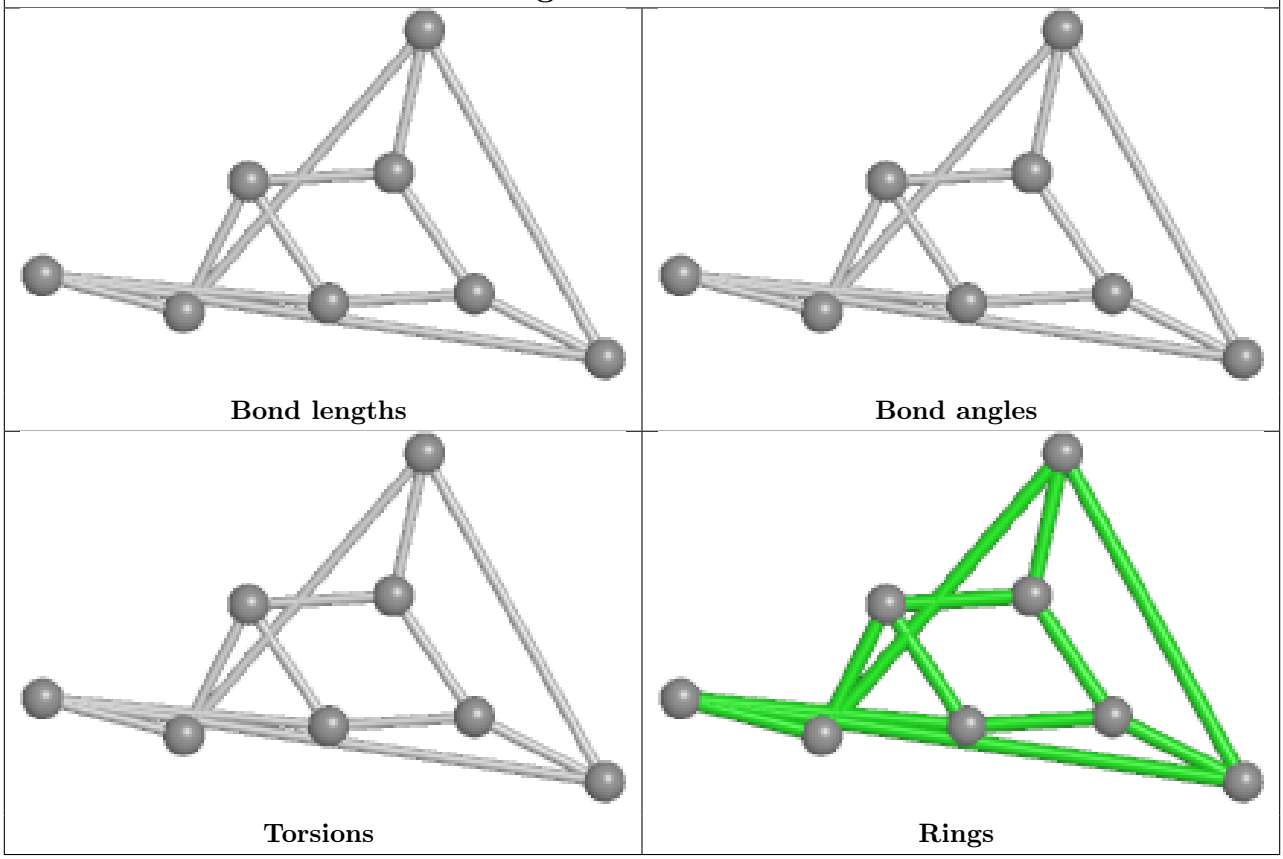
Ligand A1L1F 1 304



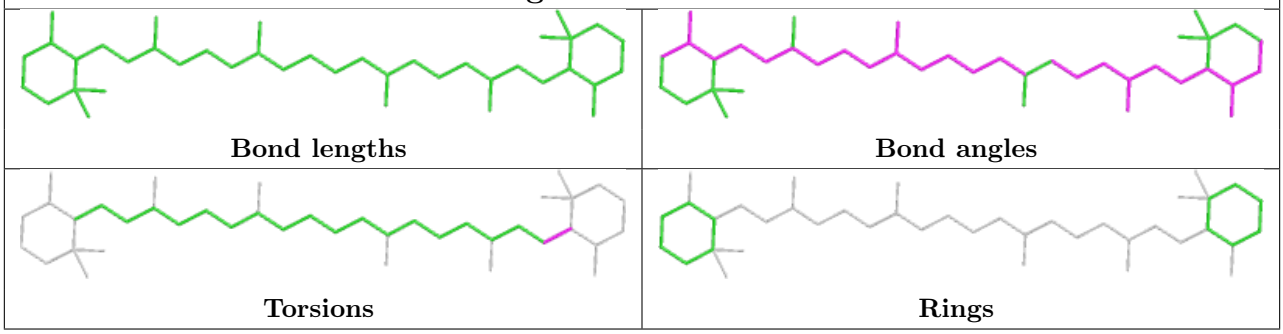
Ligand CLA j 102

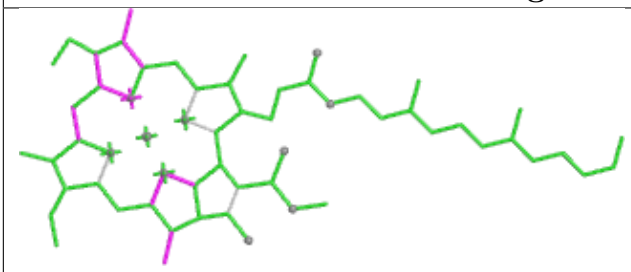
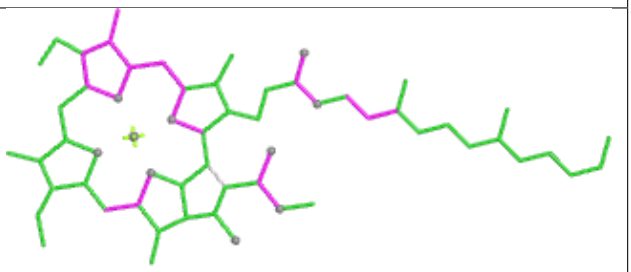
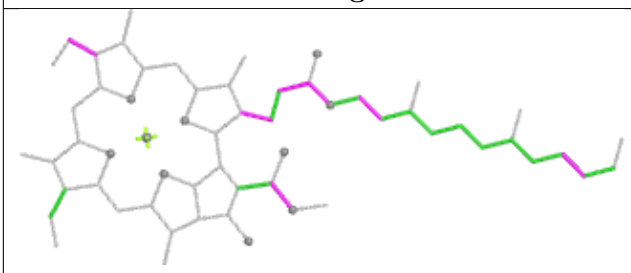
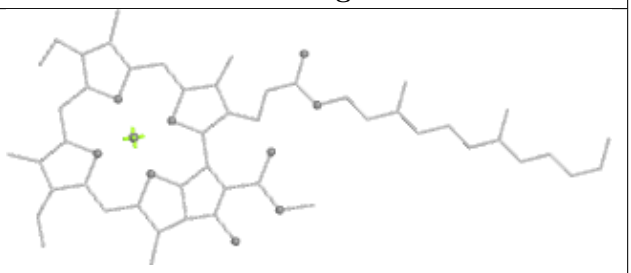


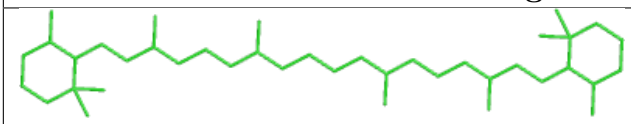
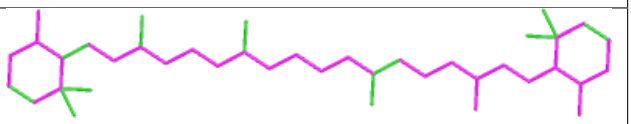
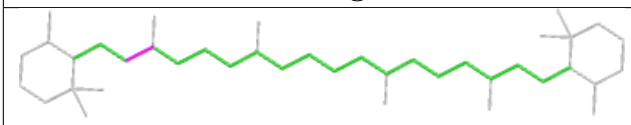
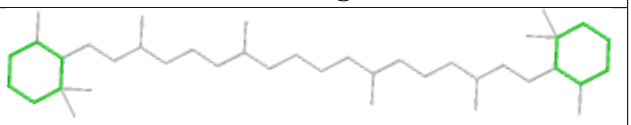
Ligand SF4 a 851



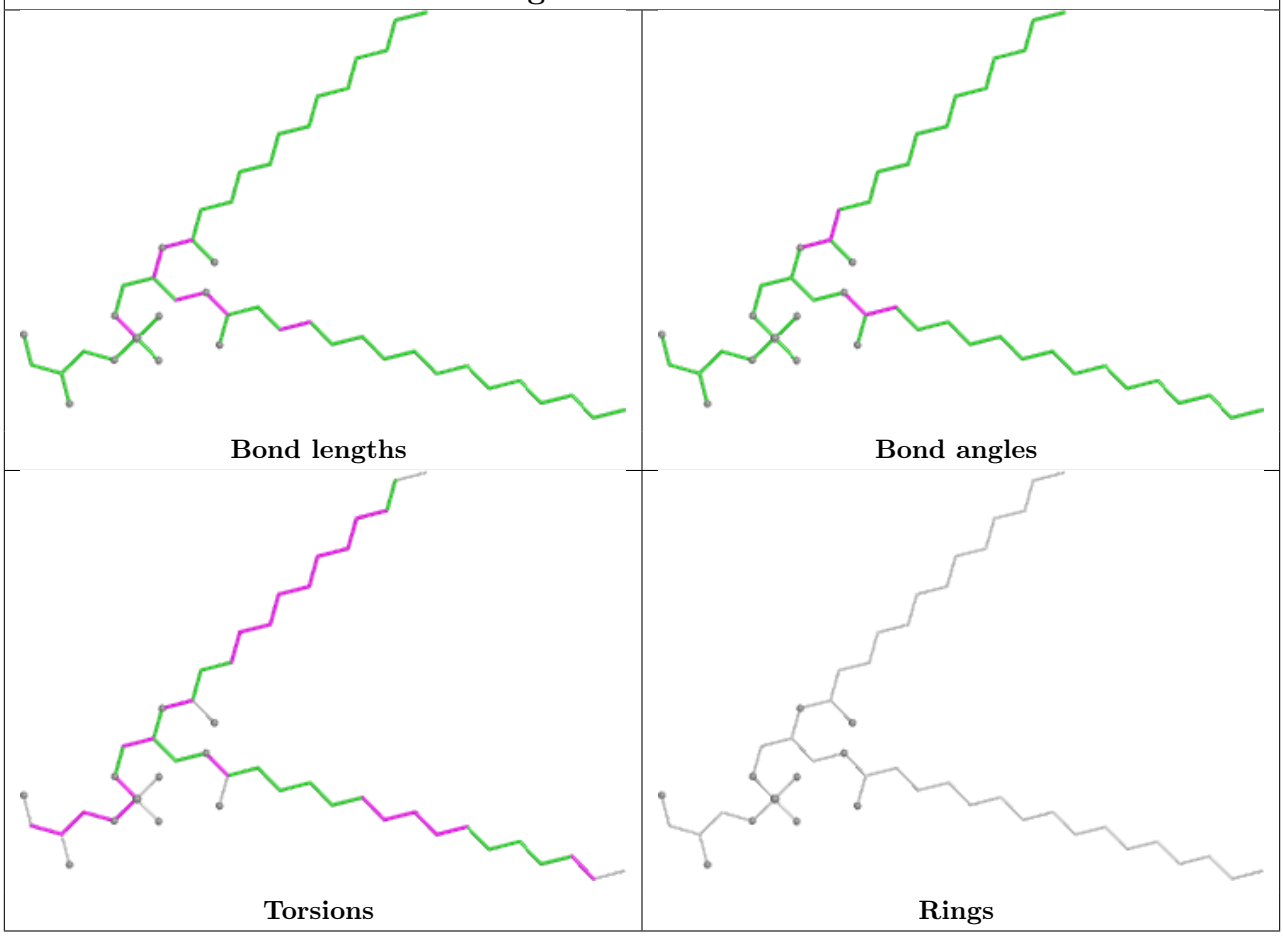
Ligand BCR h 202



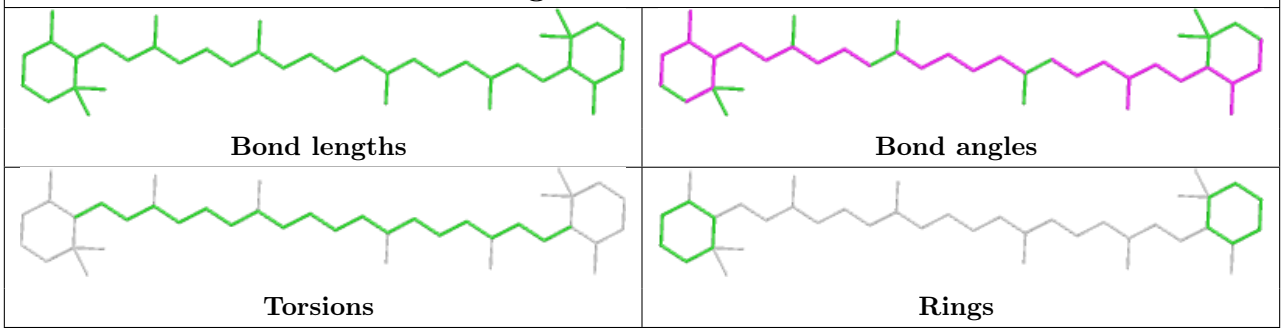
Ligand CLA b 817	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand BCR b 842	
 Bond lengths	 Bond angles
 Torsions	 Rings

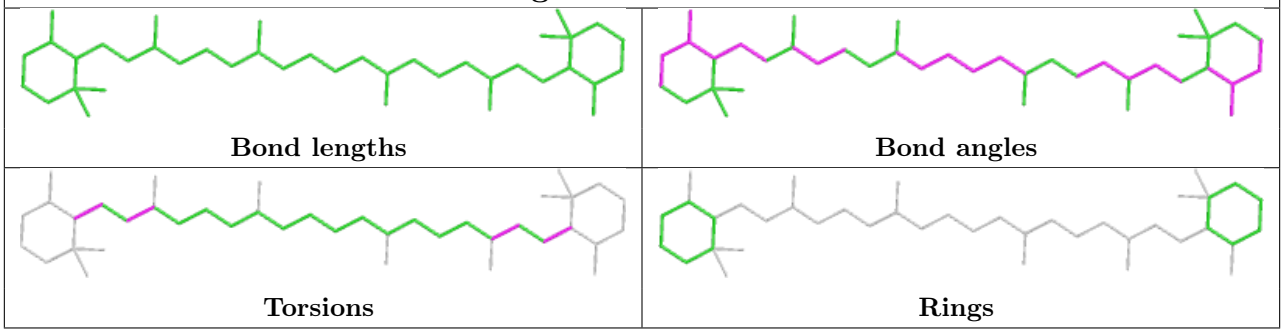
Ligand LHG 9 317



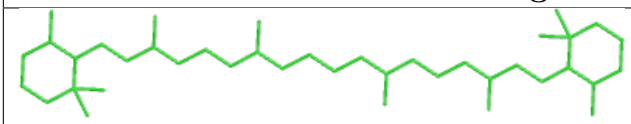
Ligand BCR a 849



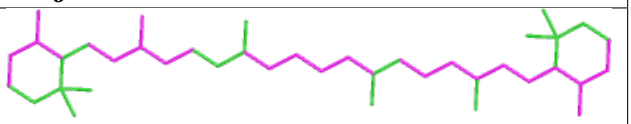
Ligand BCR l 205



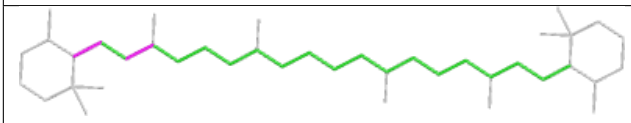
Ligand BCR j 104



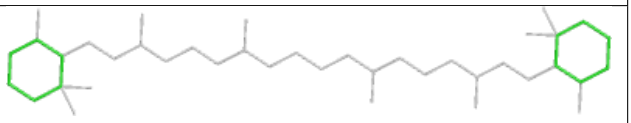
Bond lengths



Bond angles



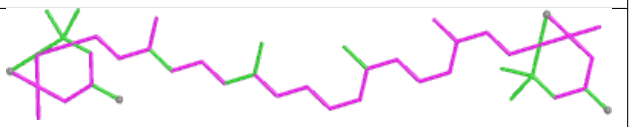
Torsions



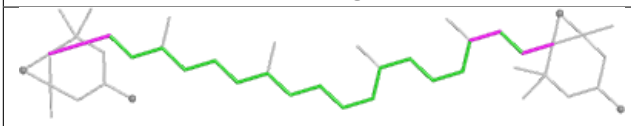
Rings

Ligand XAT 9 303

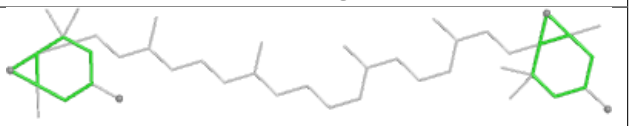
Bond lengths



Bond angles

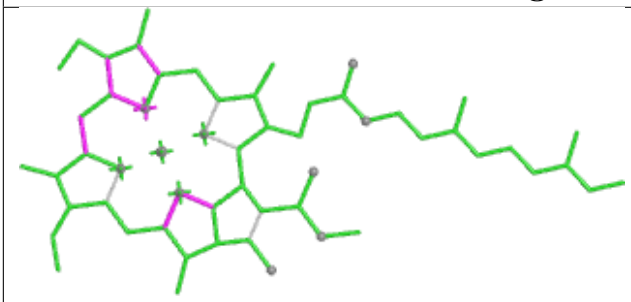


Torsions

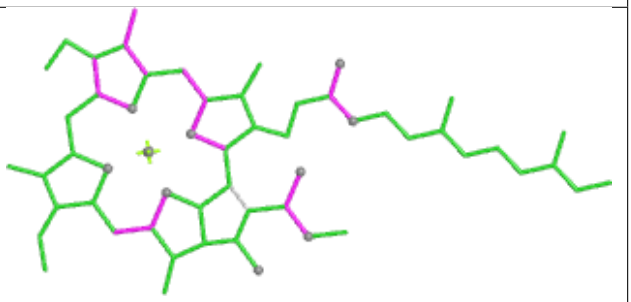


Rings

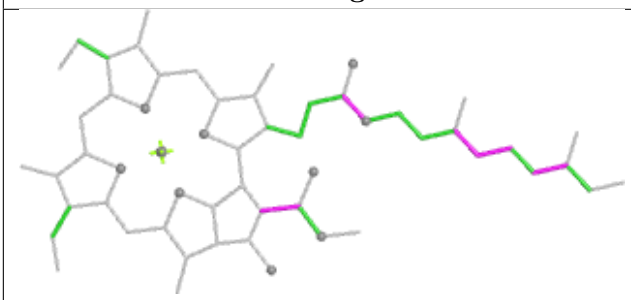
Ligand CLA 8 311



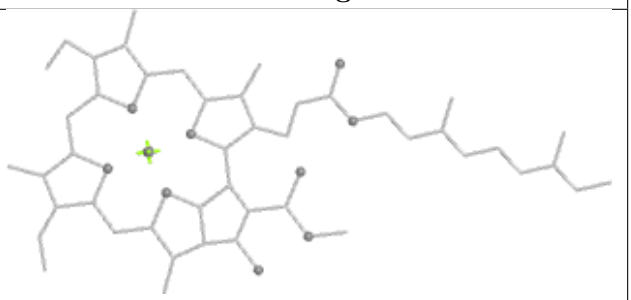
Bond lengths



Bond angles

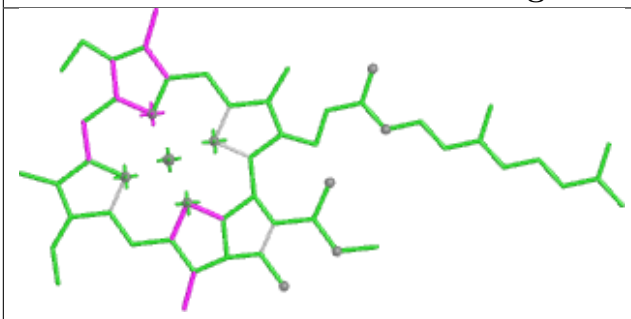


Torsions

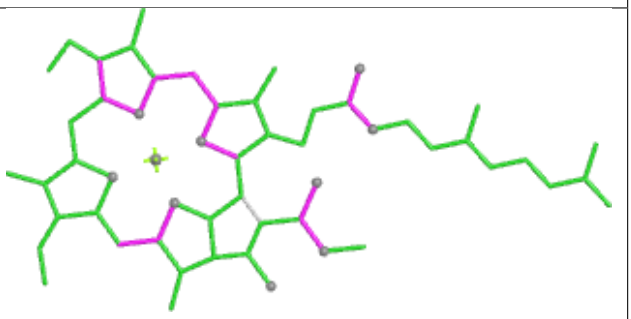


Rings

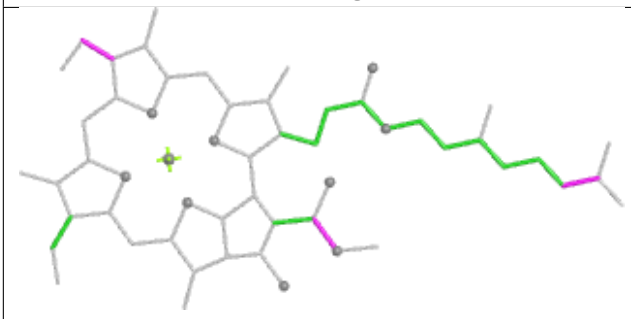
Ligand CLA b 819



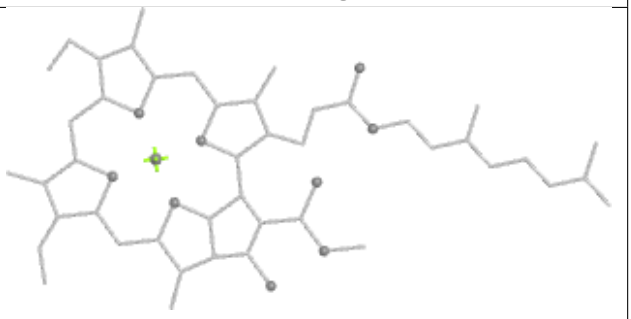
Bond lengths



Bond angles

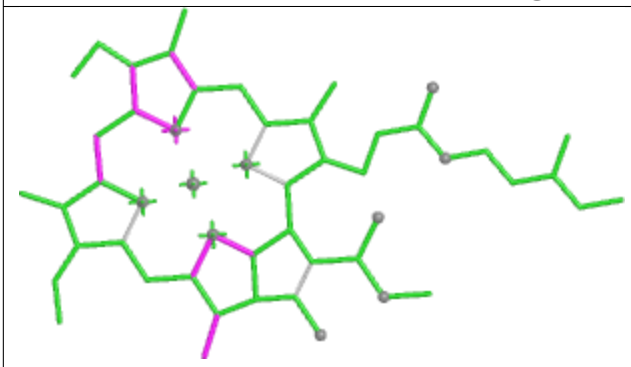


Torsions

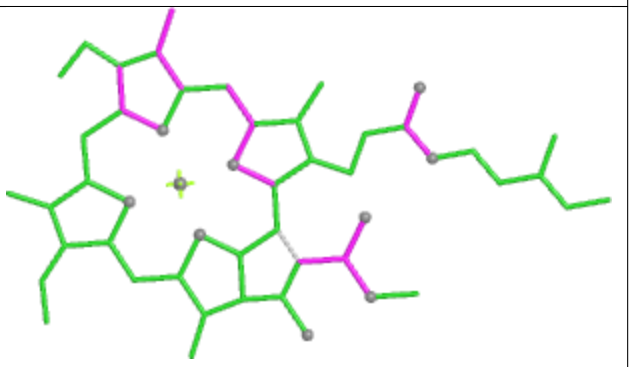


Rings

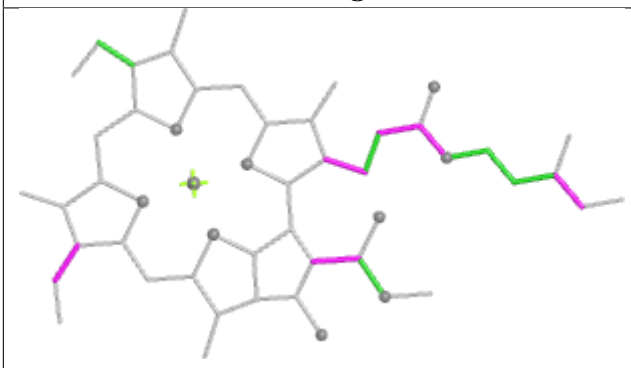
Ligand CLA 7 316



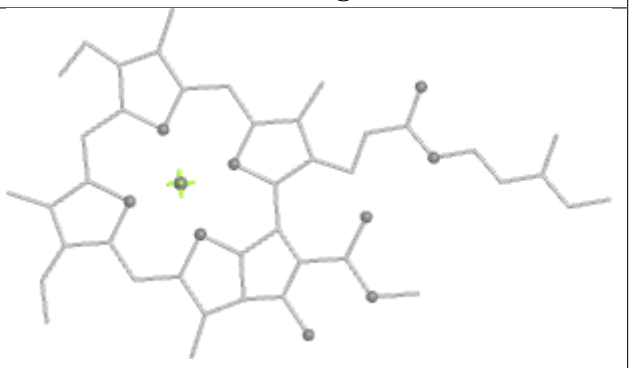
Bond lengths



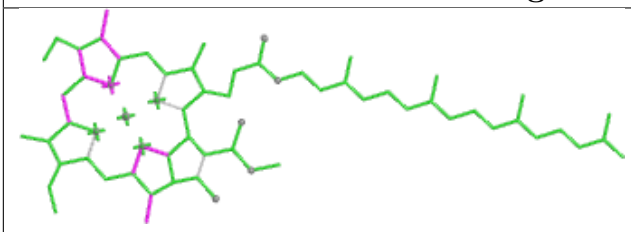
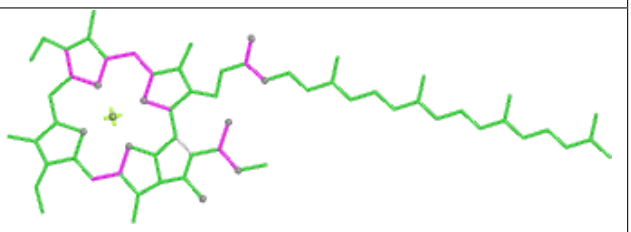
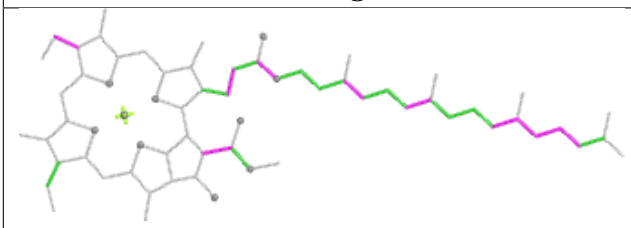
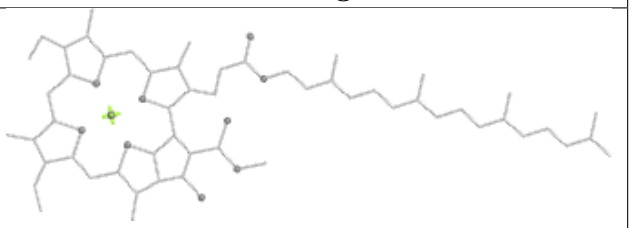
Bond angles

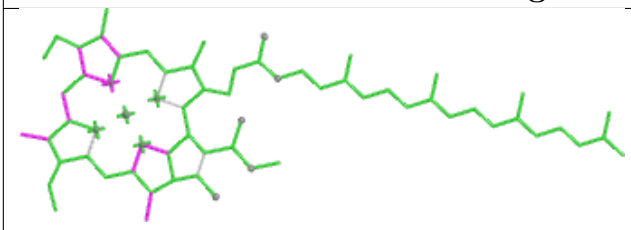
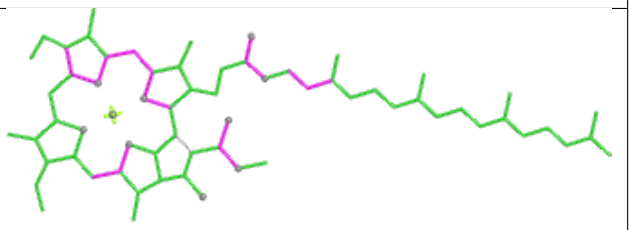
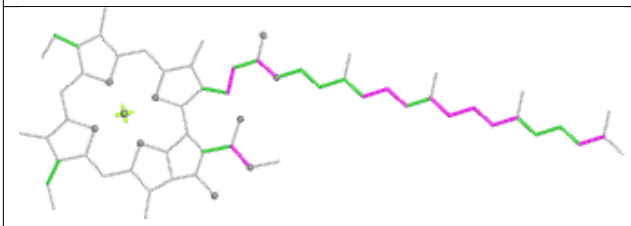
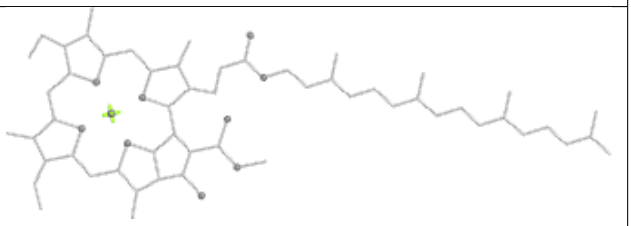


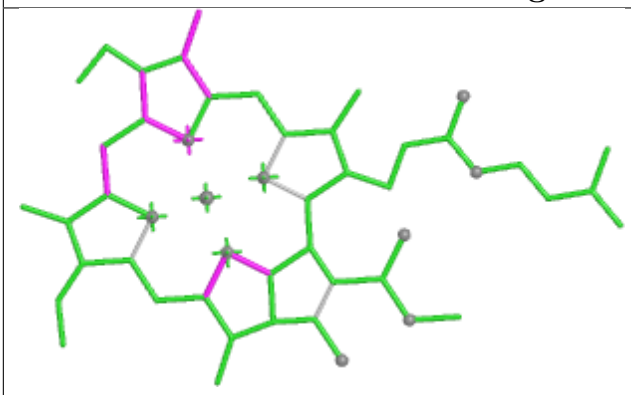
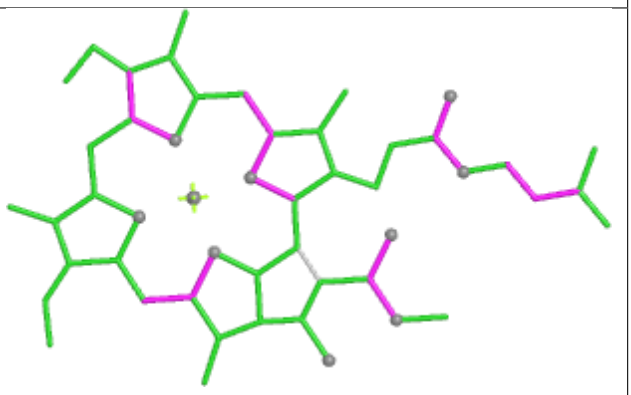
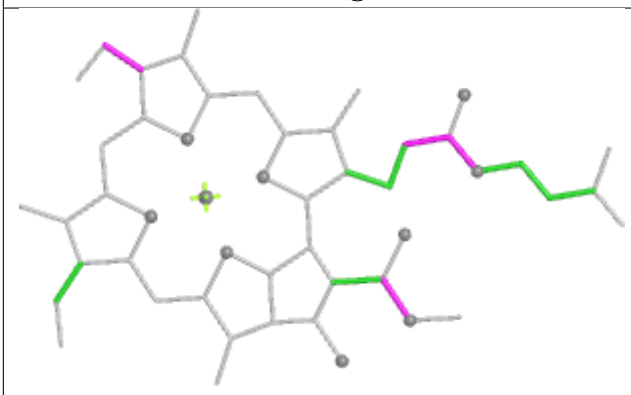
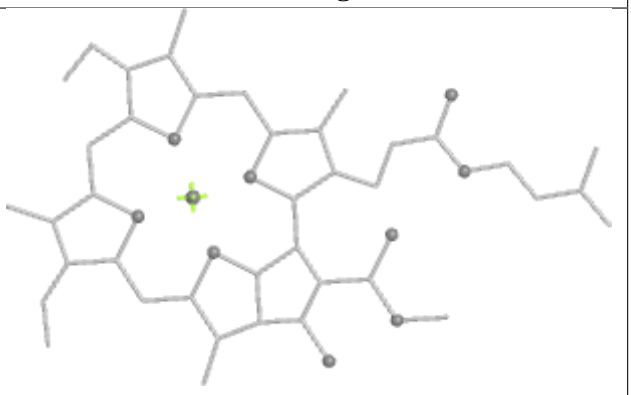
Torsions

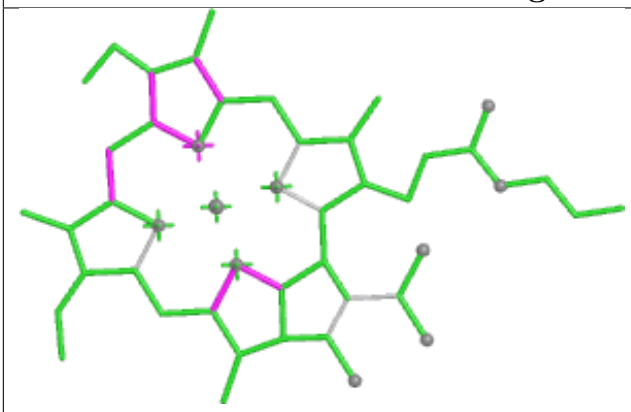
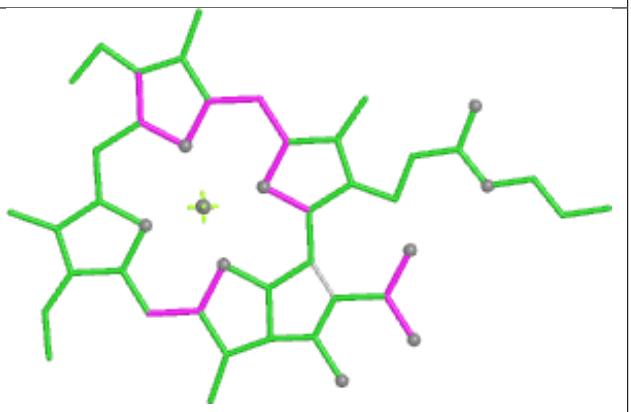
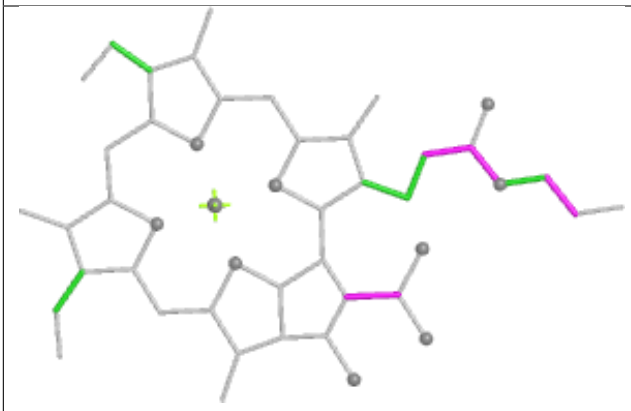
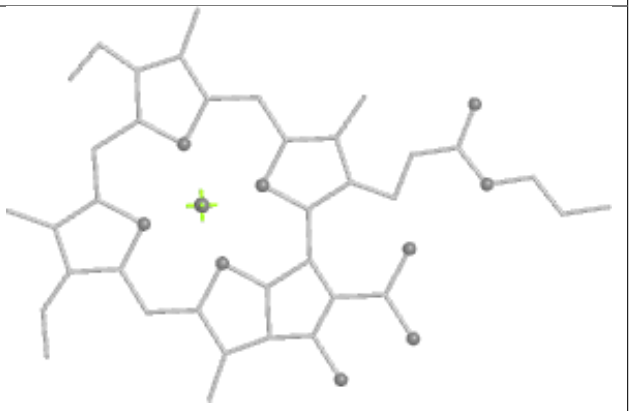


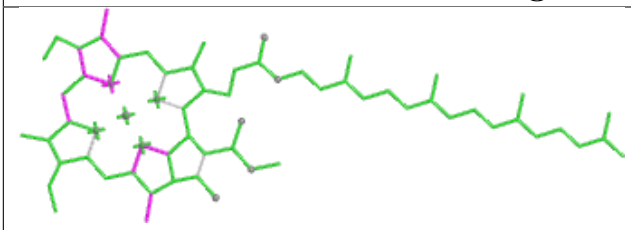
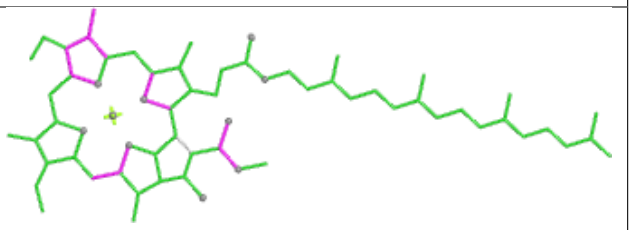
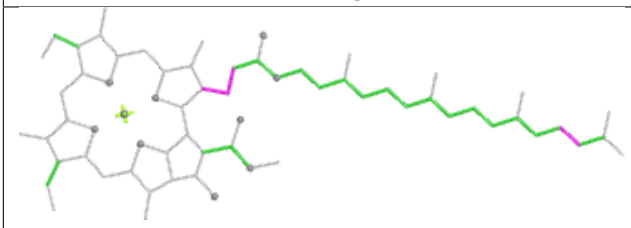
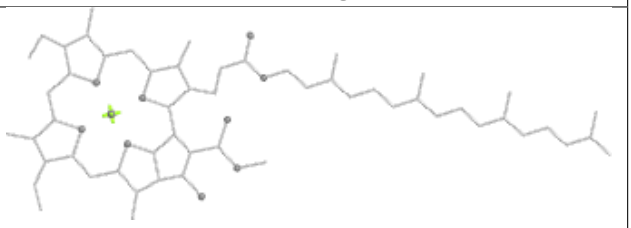
Rings

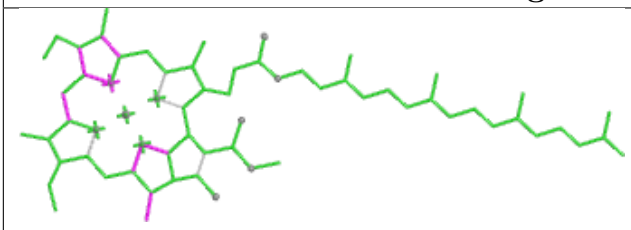
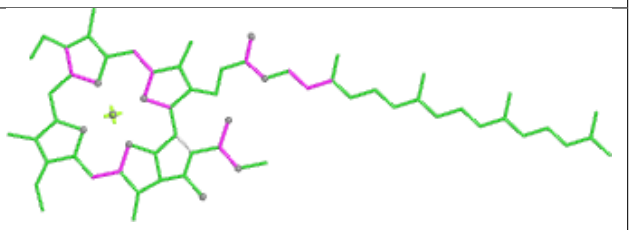
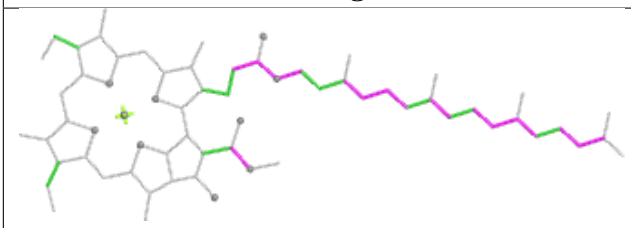
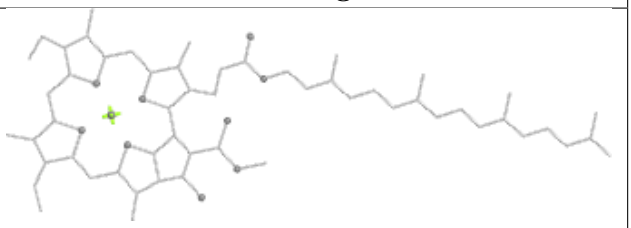
Ligand CLA b 838	
 Bond lengths	 Bond angles
 Torsions	 Rings

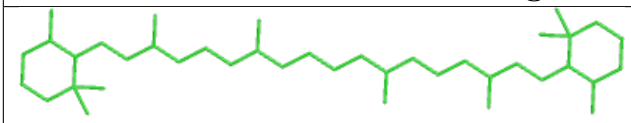
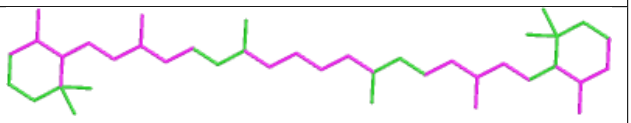
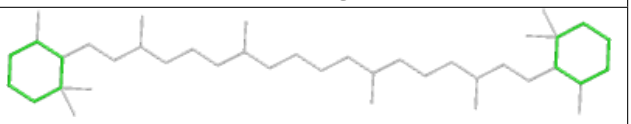
Ligand CLA 9 308	
 Bond lengths	 Bond angles
 Torsions	 Rings

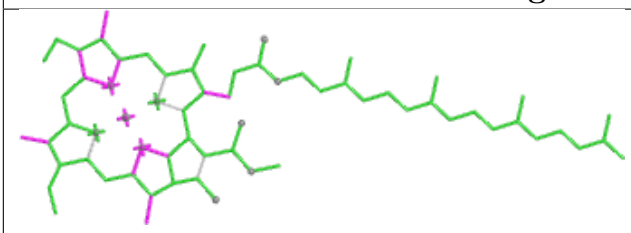
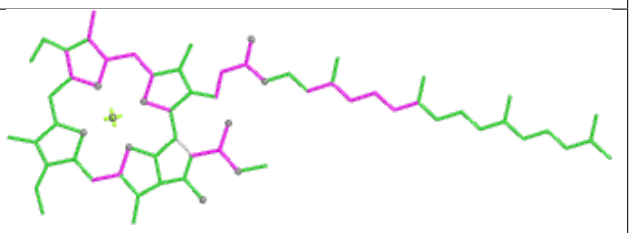
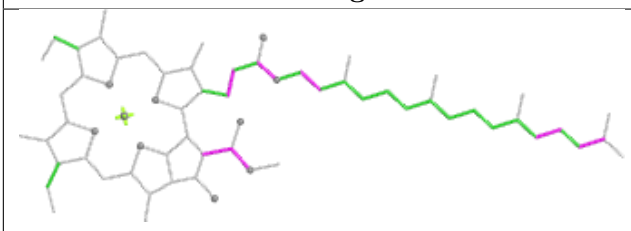
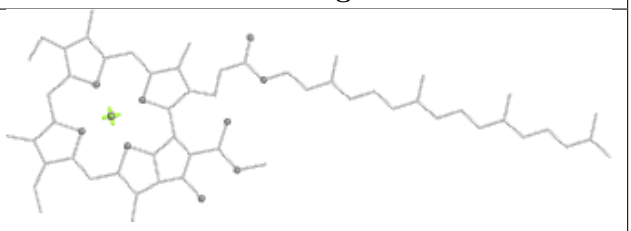
Ligand CLA a 836	
 Bond lengths	 Bond angles
 Torsions	 Rings

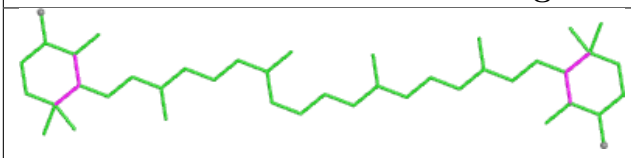
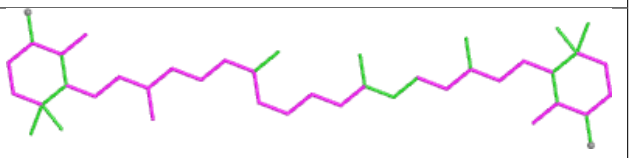
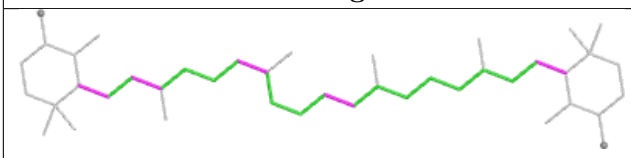
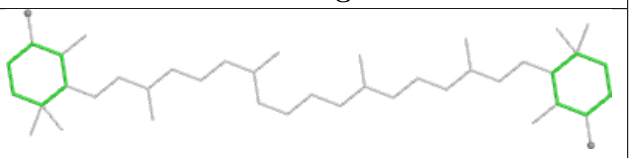
Ligand CLA 7 309	
 Bond lengths	 Bond angles
 Torsions	 Rings

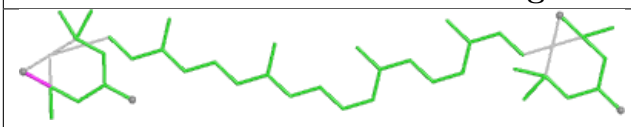
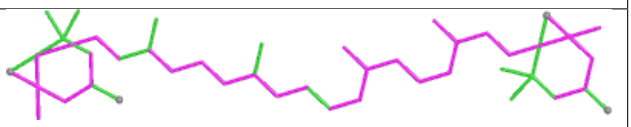
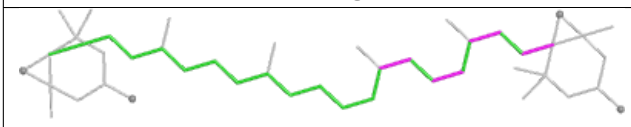
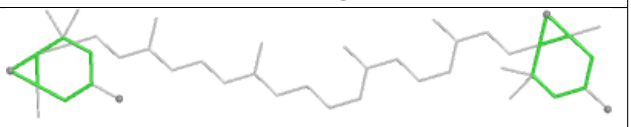
Ligand CLA a 803	
 Bond lengths	 Bond angles
 Torsions	 Rings

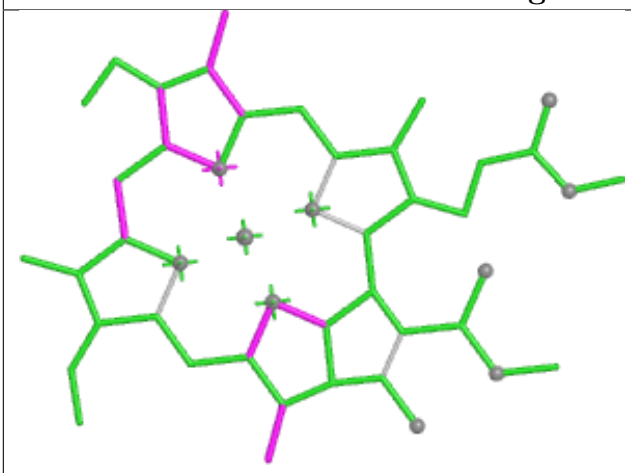
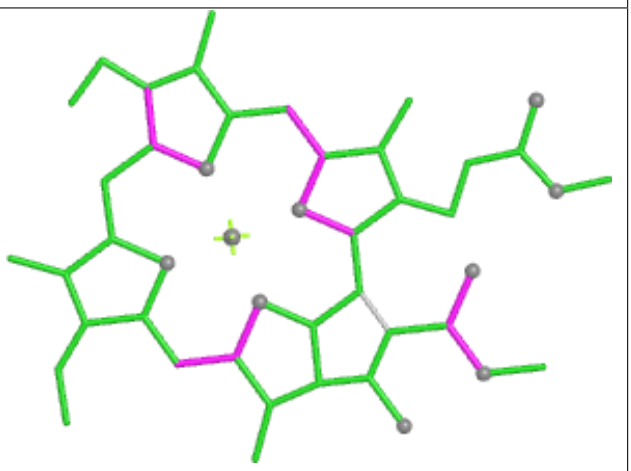
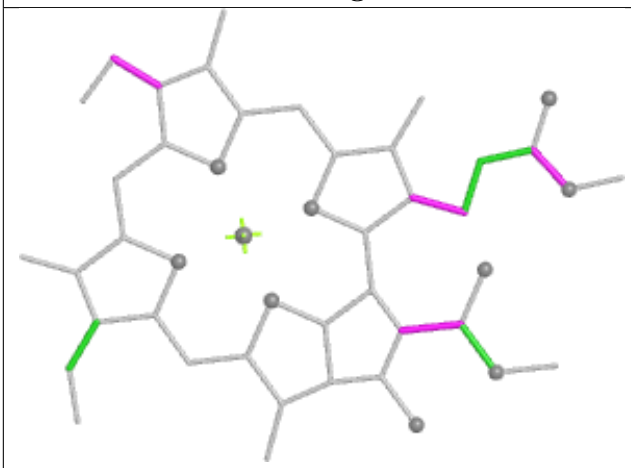
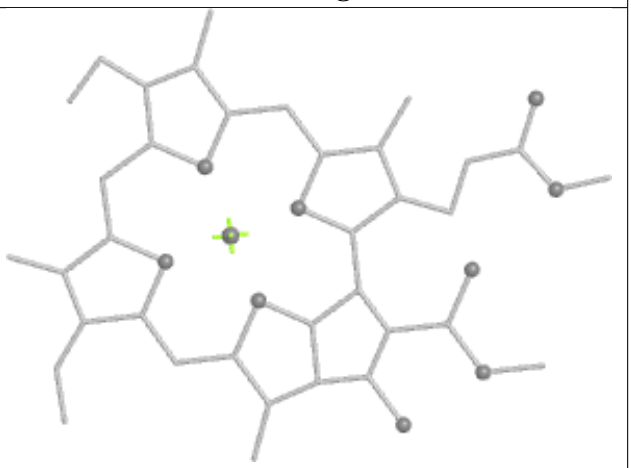
Ligand CLA b 807	
 Bond lengths	 Bond angles
 Torsions	 Rings

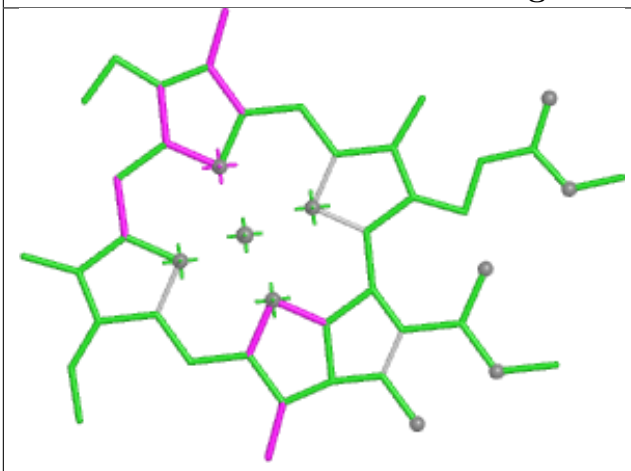
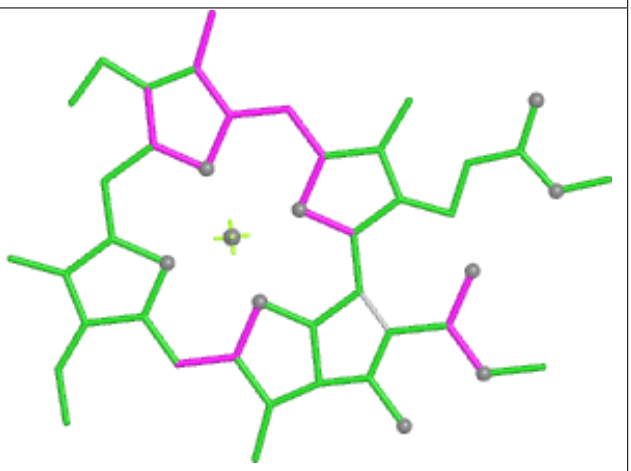
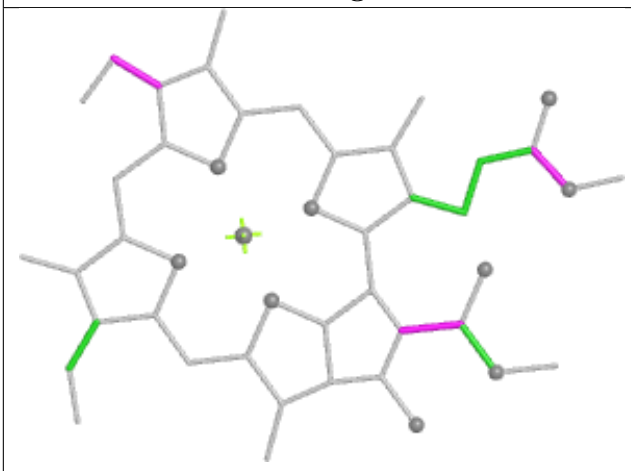
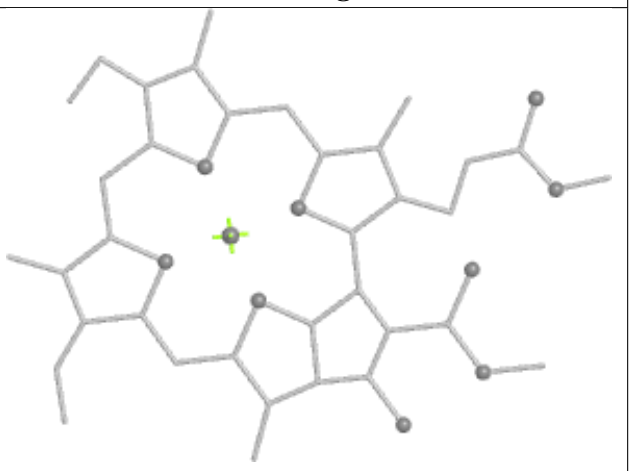
Ligand BCR b 844	
 Bond lengths	 Bond angles
Torsions	 Rings

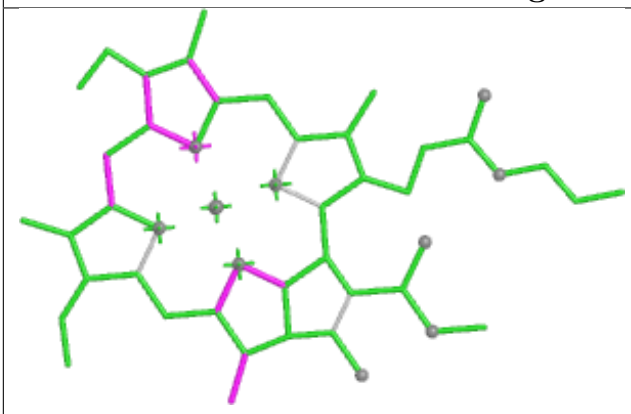
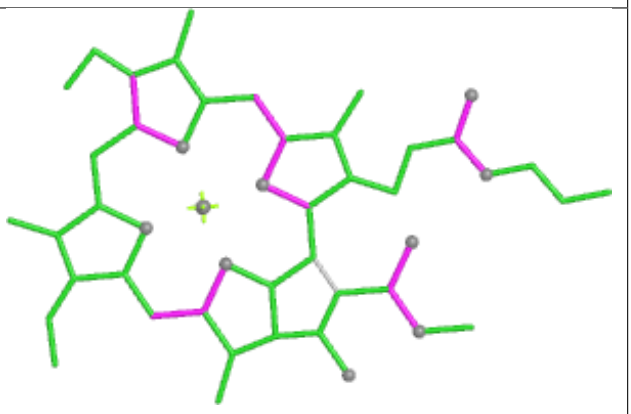
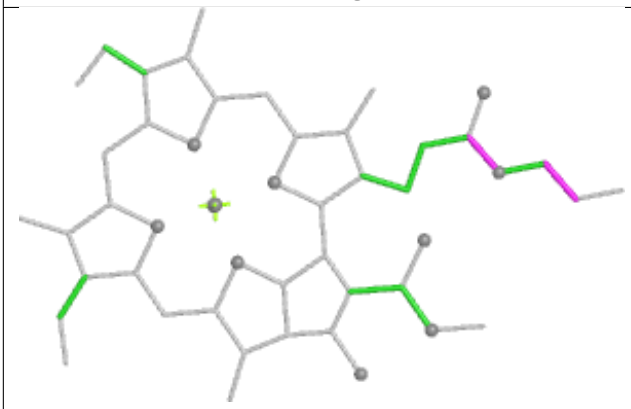
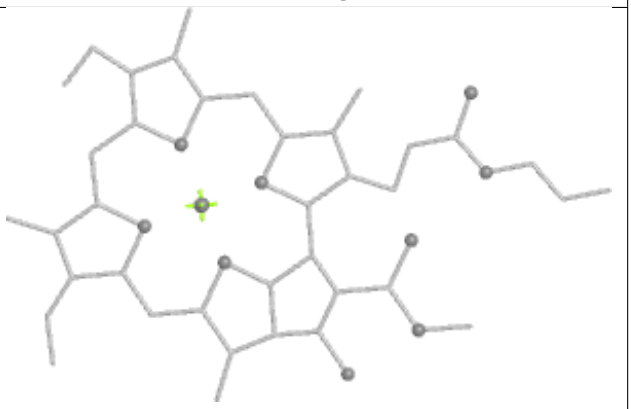
Ligand CLA a 806	
 Bond lengths	 Bond angles
 Torsions	 Rings

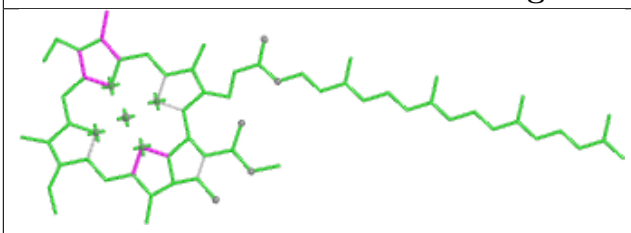
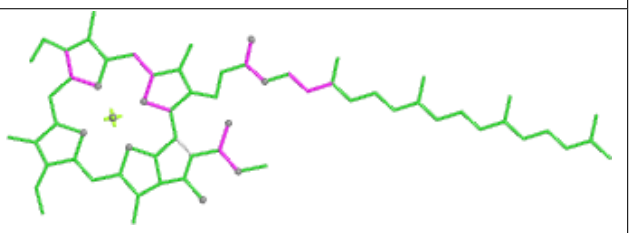
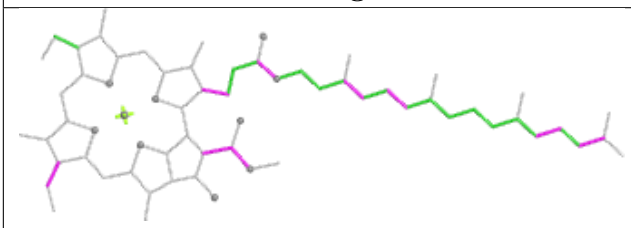
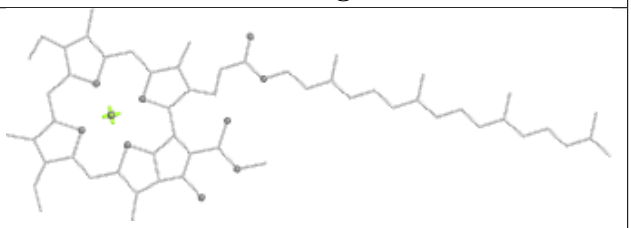
Ligand 45D 9 305	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand XAT 7 304	
 Bond lengths	 Bond angles
 Torsions	 Rings

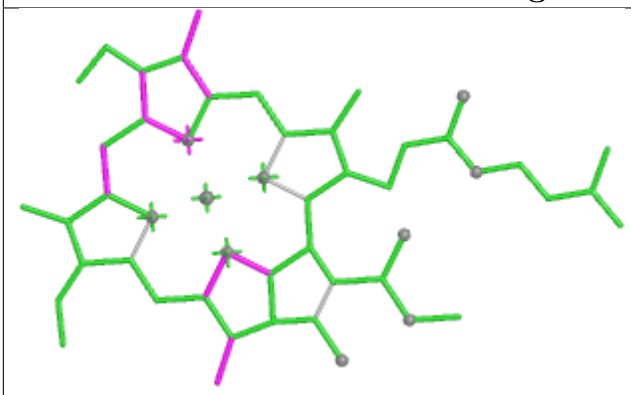
Ligand CLA a 824	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA 9 309	
 Bond lengths	 Bond angles
 Torsions	 Rings

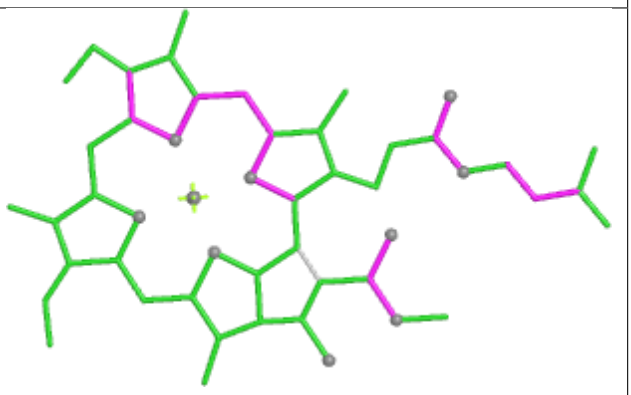
Ligand CLA 7 312	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA b 839	
 Bond lengths	 Bond angles
 Torsions	 Rings

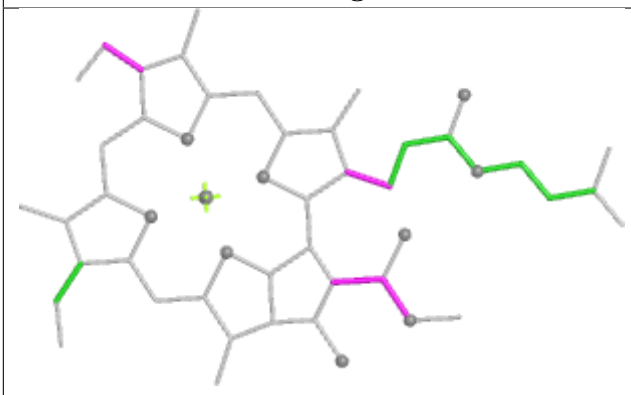
Ligand CLA a 832



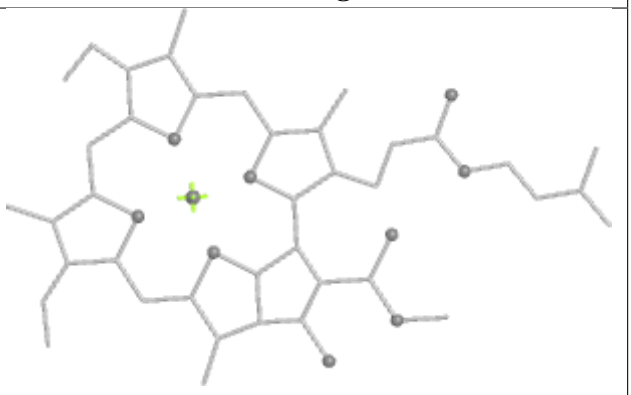
Bond lengths



Bond angles

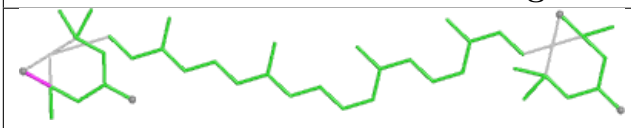


Torsions

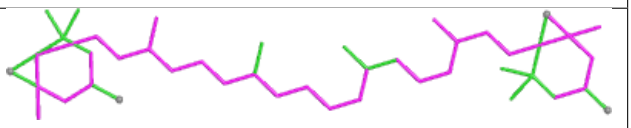


Rings

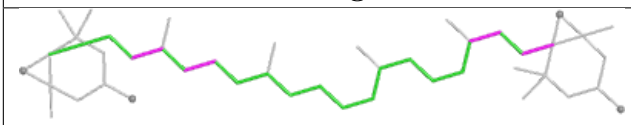
Ligand XAT 7 301



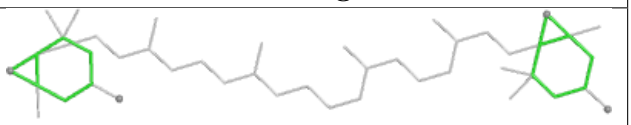
Bond lengths



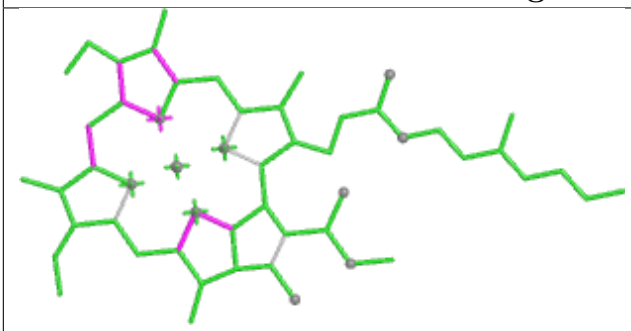
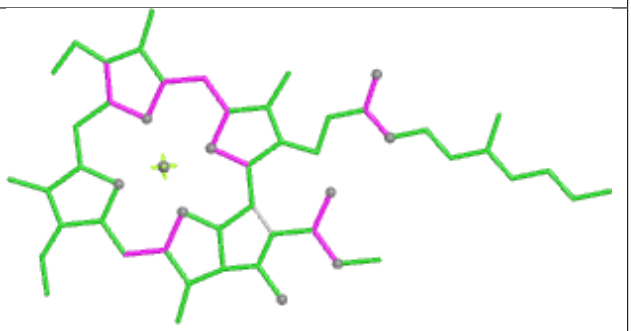
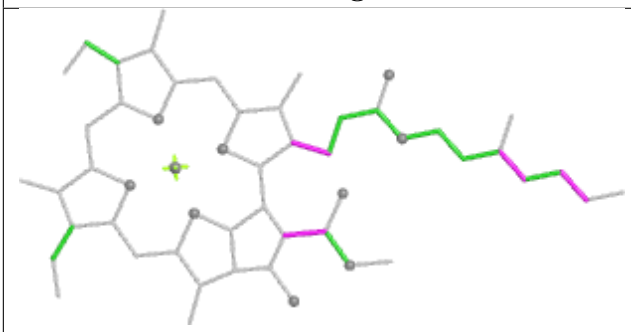
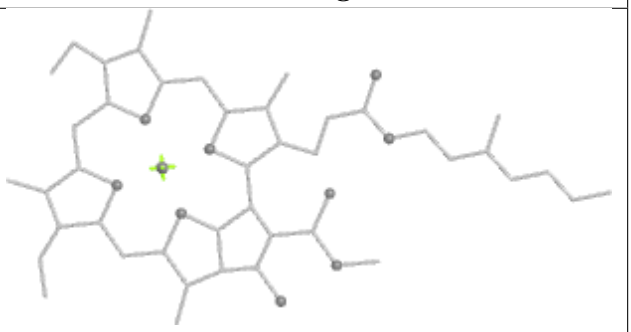
Bond angles



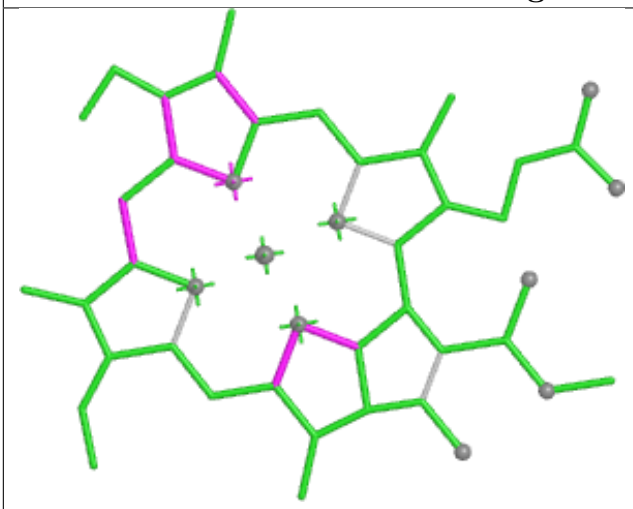
Torsions



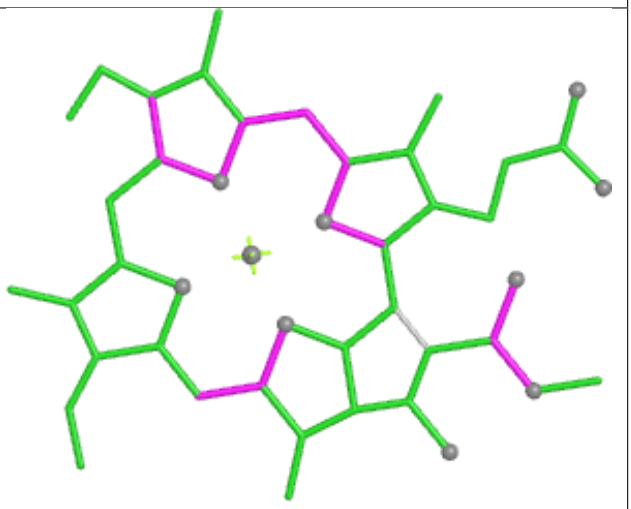
Rings

Ligand CLA b 812	
 Bond lengths	 Bond angles
 Torsions	 Rings

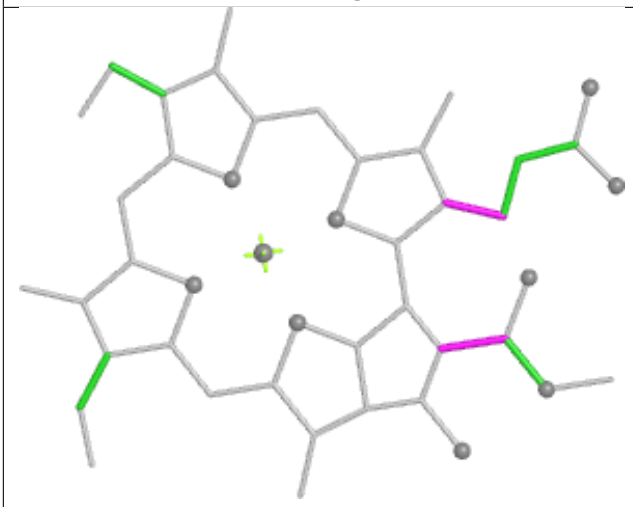
Ligand CLA b 815



Bond lengths



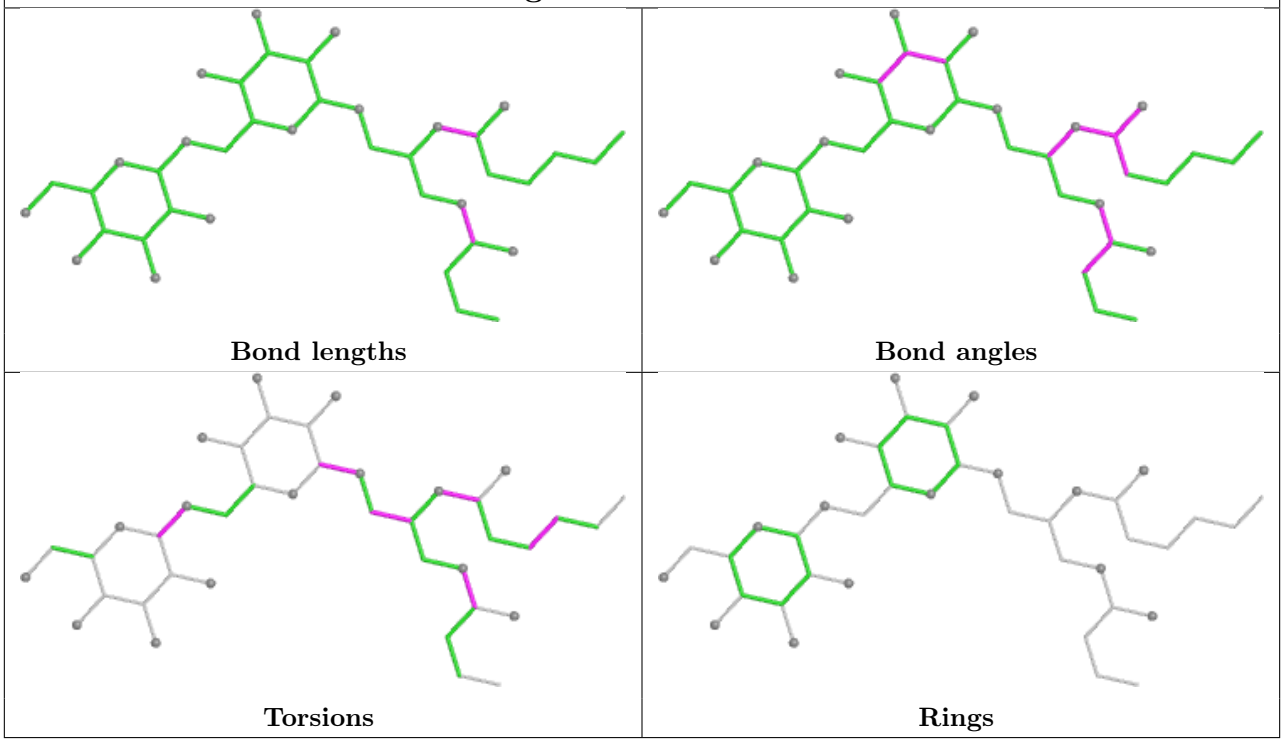
Bond angles



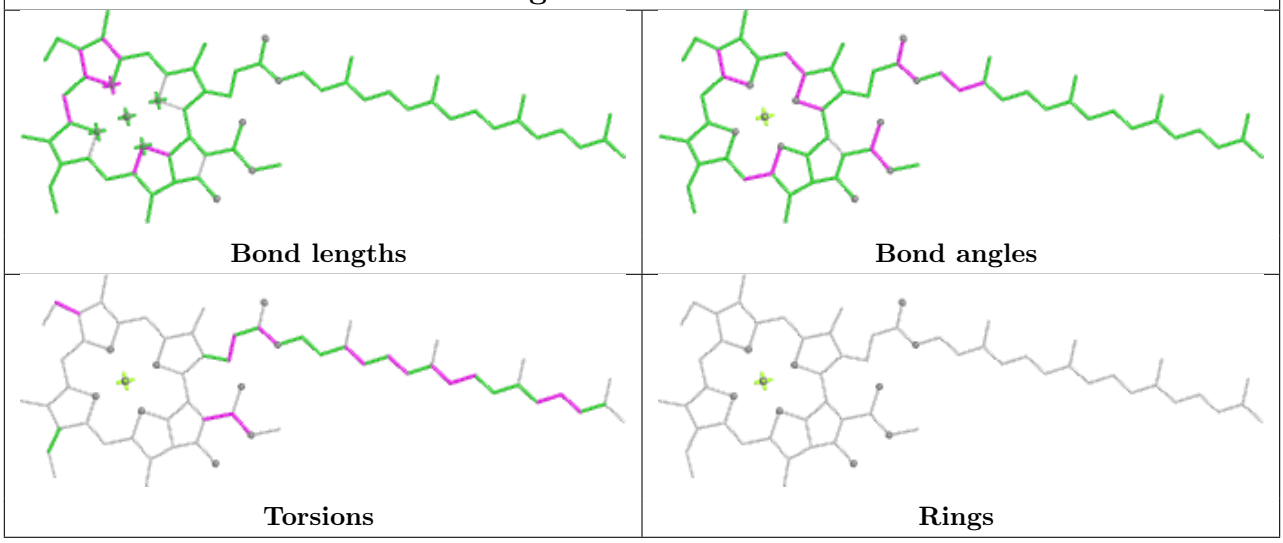
Torsions

Rings

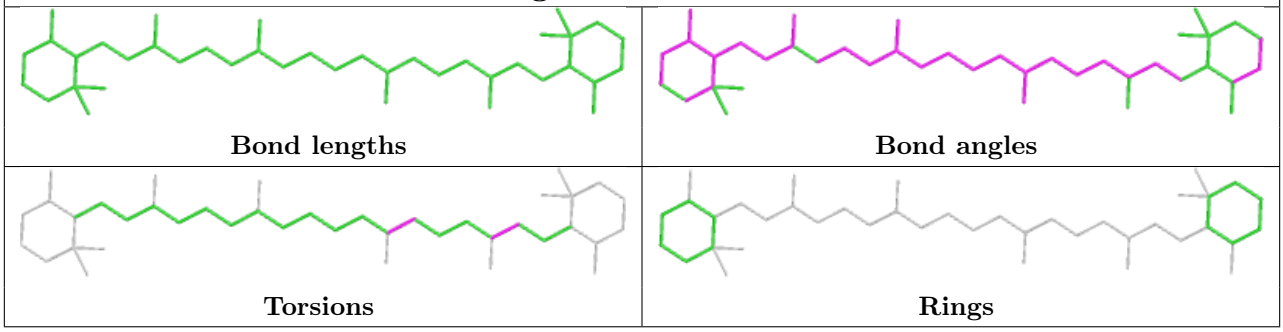
Ligand DGD 8 315

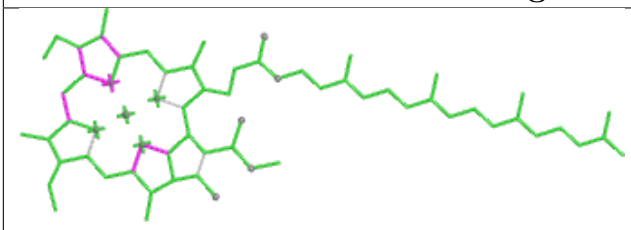
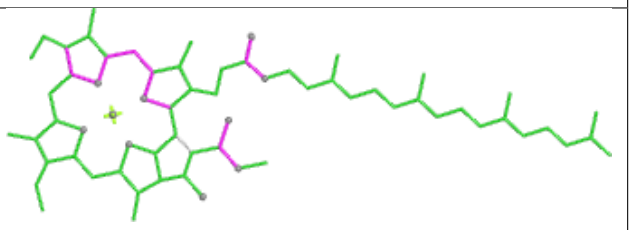
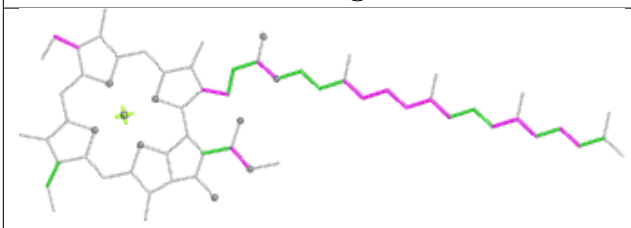
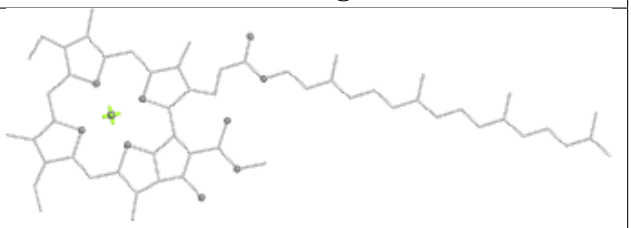


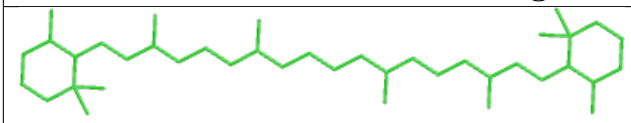
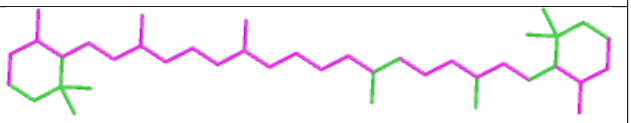
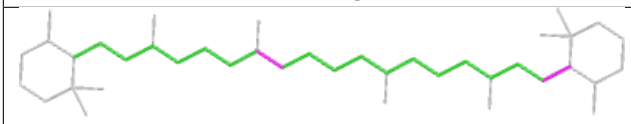
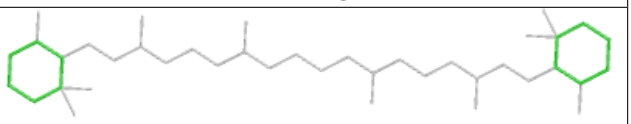
Ligand CLA a 841

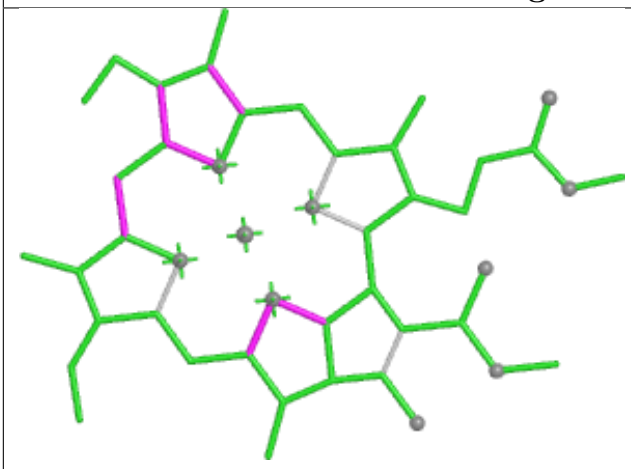
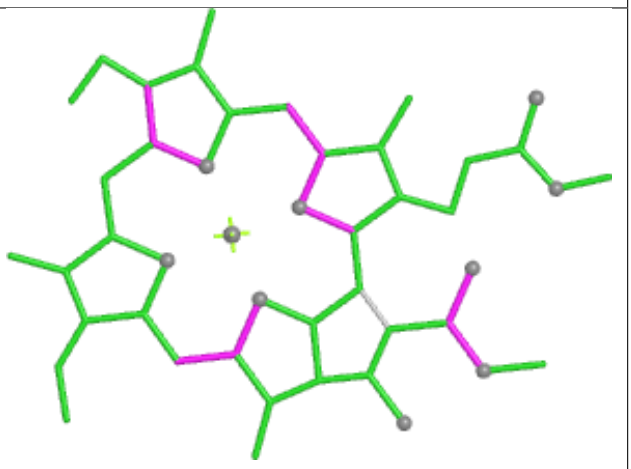
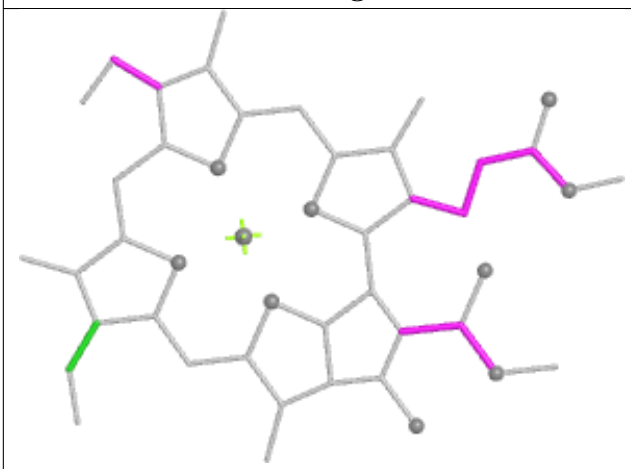
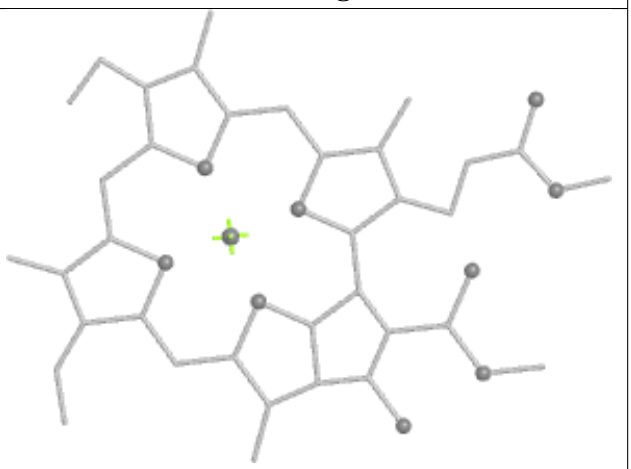


Ligand BCR f 801

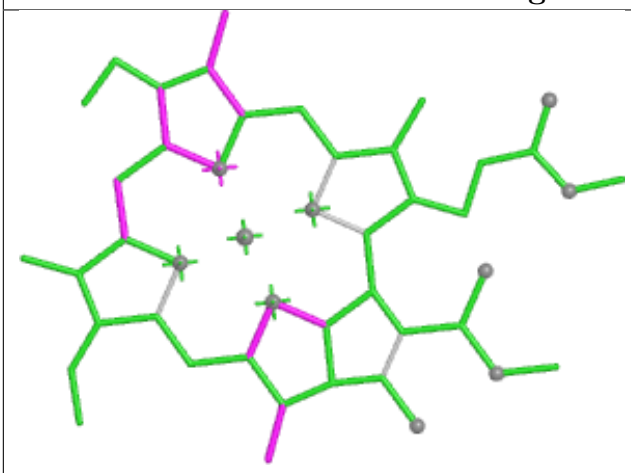


Ligand CLA a 807	
 Bond lengths	 Bond angles
 Torsions	 Rings

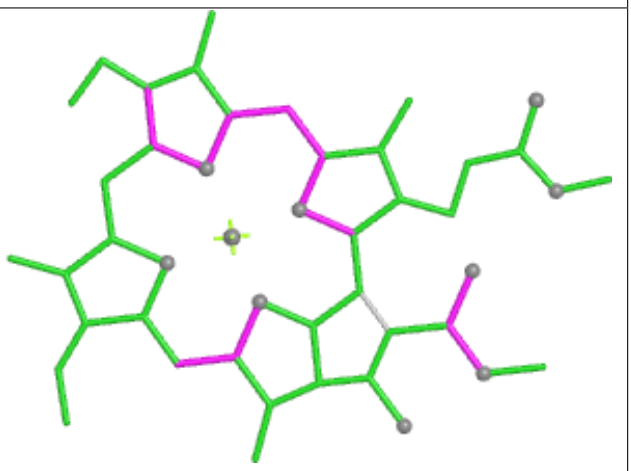
Ligand BCR f 804	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA 9 313	
 Bond lengths	 Bond angles
 Torsions	 Rings

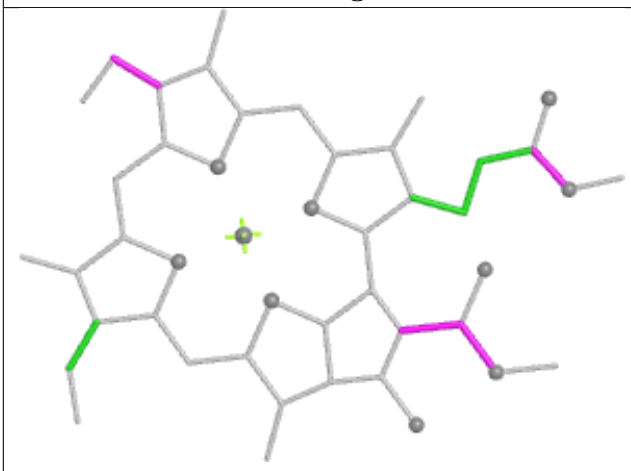
Ligand CLA 8 310



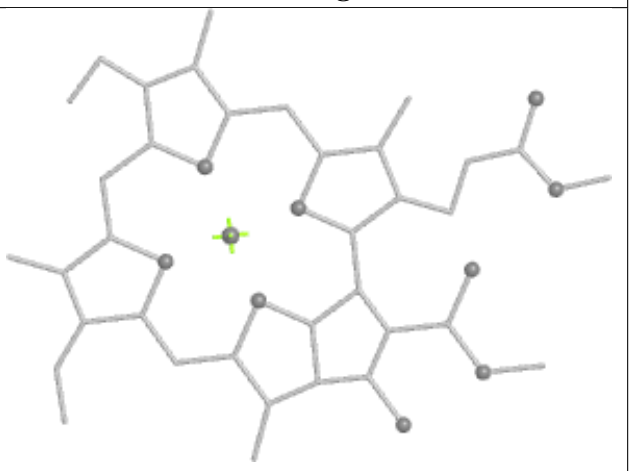
Bond lengths



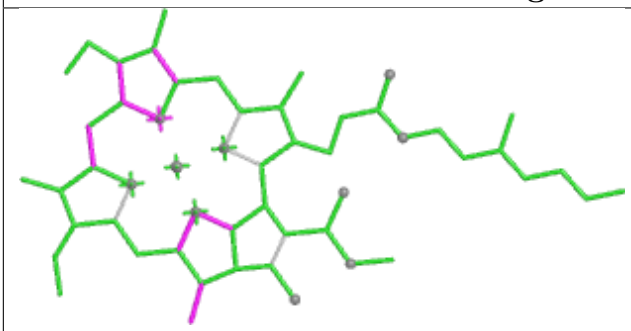
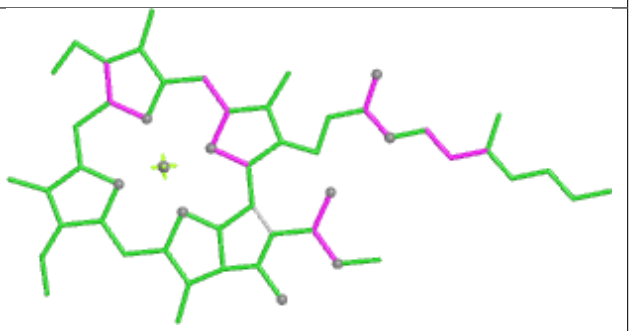
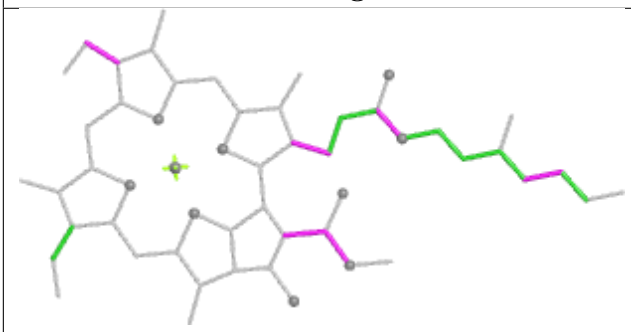
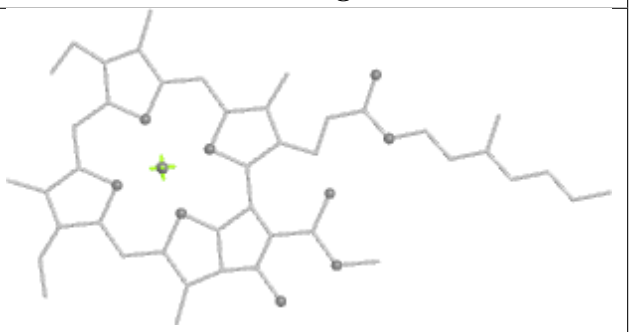
Bond angles

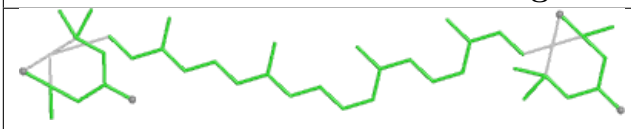
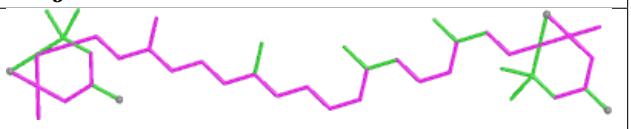
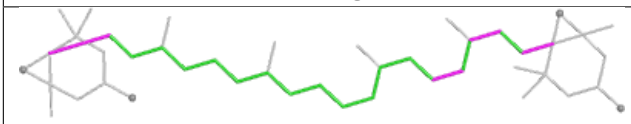
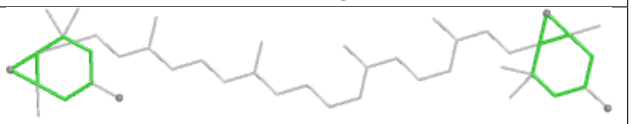


Torsions

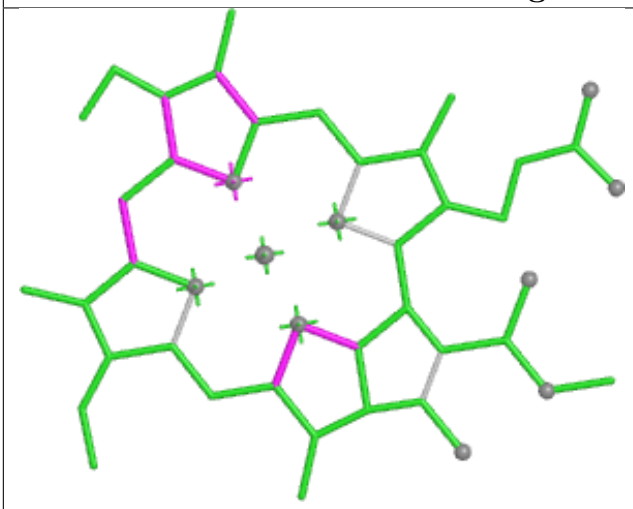


Rings

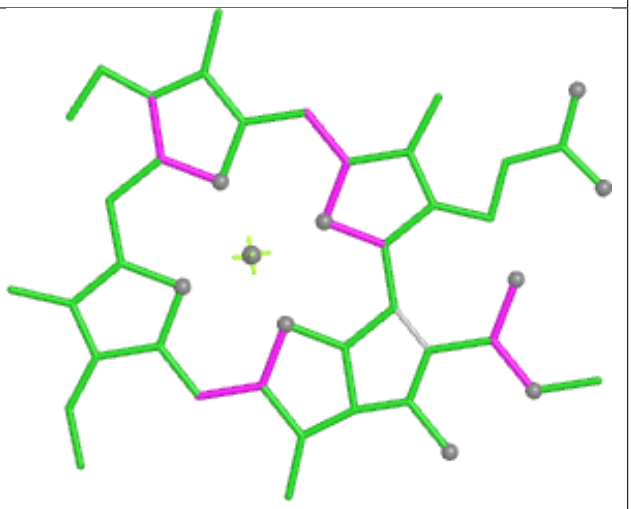
Ligand CLA b 823	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand XAT j 101	
 Bond lengths	 Bond angles
 Torsions	 Rings

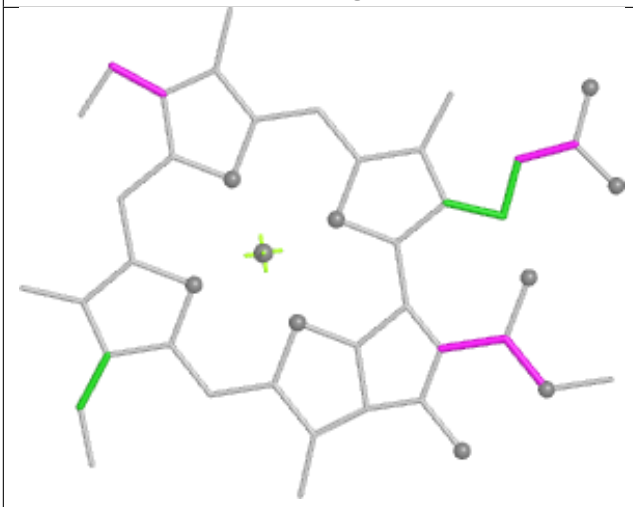
Ligand CLA 7 307



Bond lengths



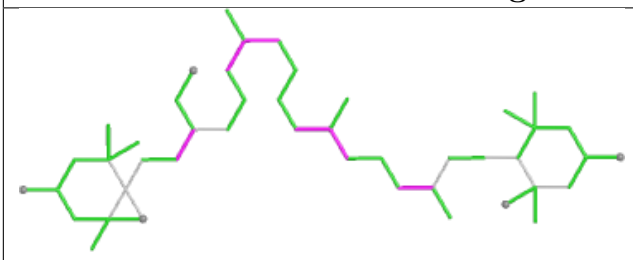
Bond angles



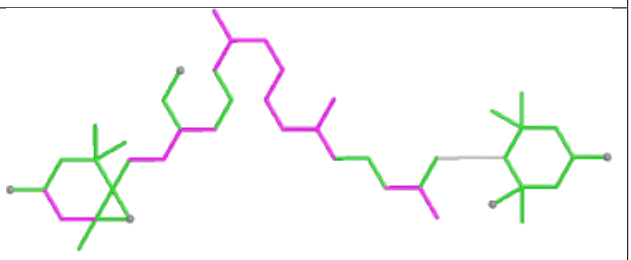
Torsions

Rings

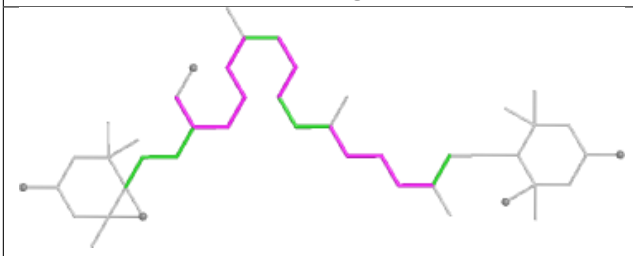
Ligand A1L1G 9 301



Bond lengths



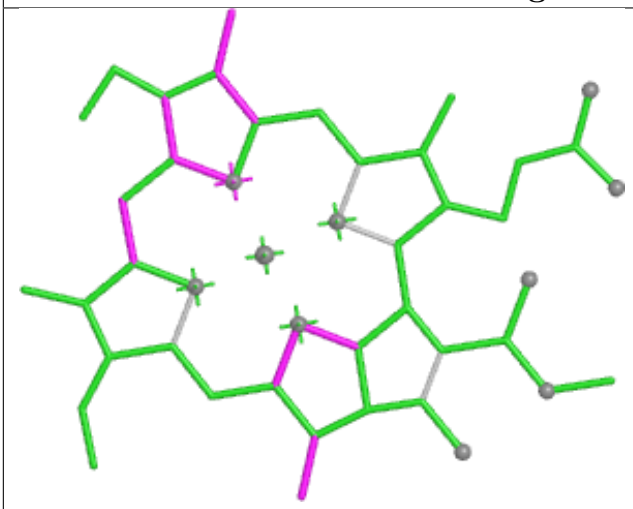
Bond angles



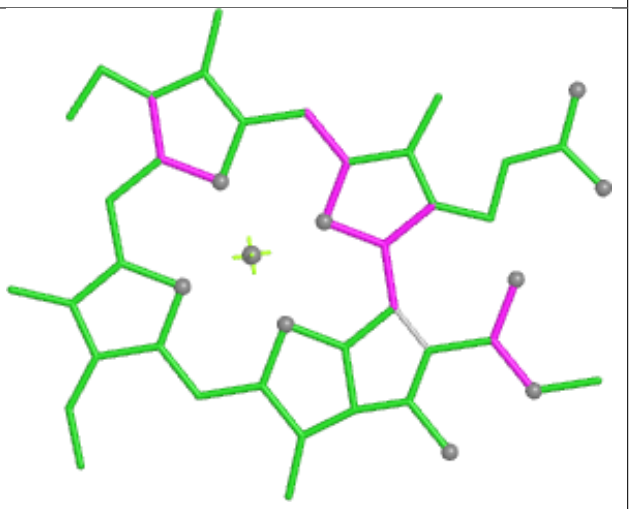
Torsions

Rings

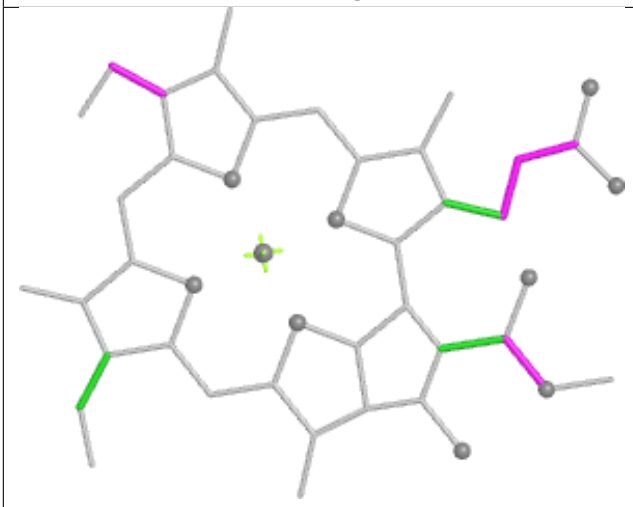
Ligand CLA 7 314



Bond lengths



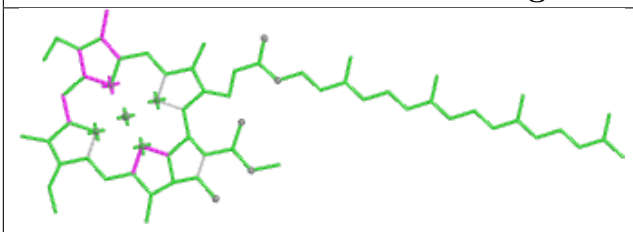
Bond angles



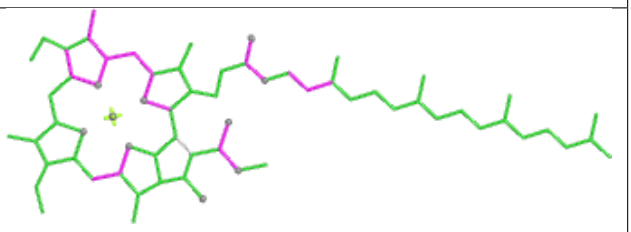
Torsions

Rings

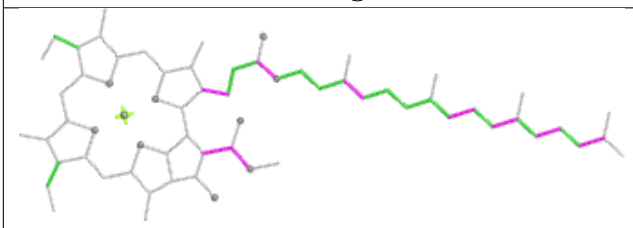
Ligand CLA a 820



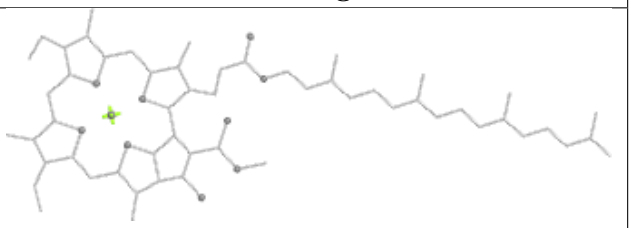
Bond lengths



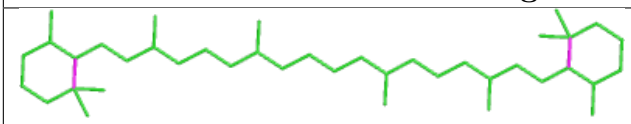
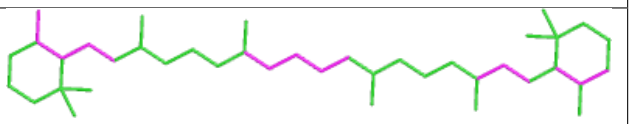
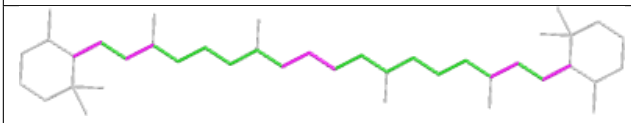
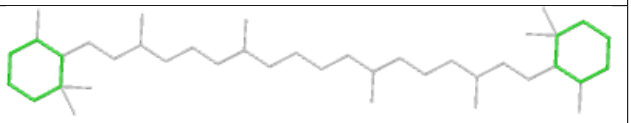
Bond angles

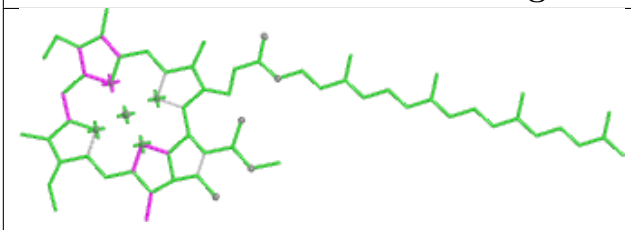
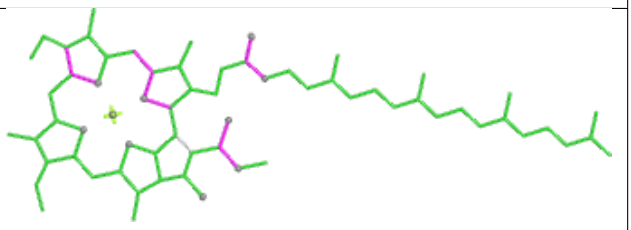
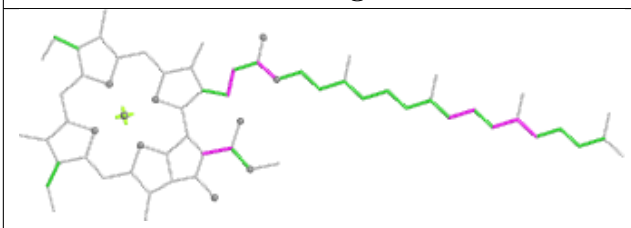
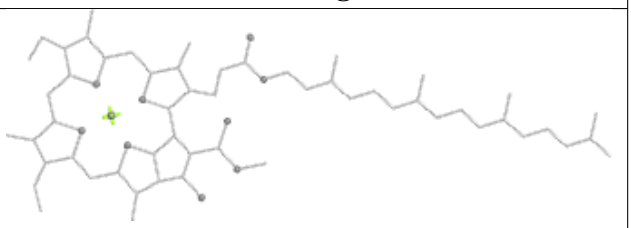


Torsions

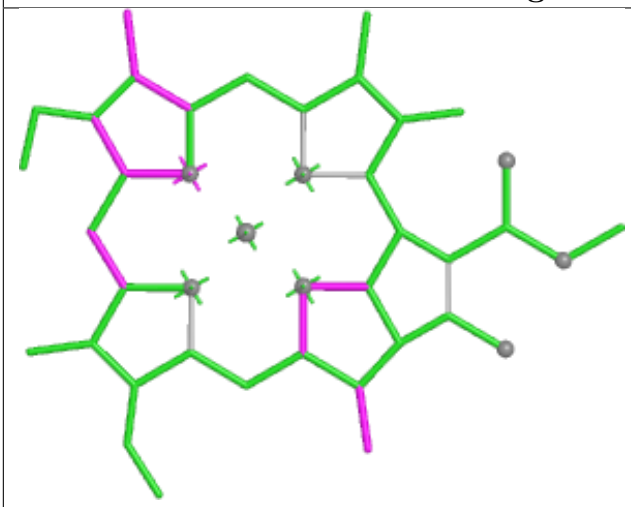


Rings

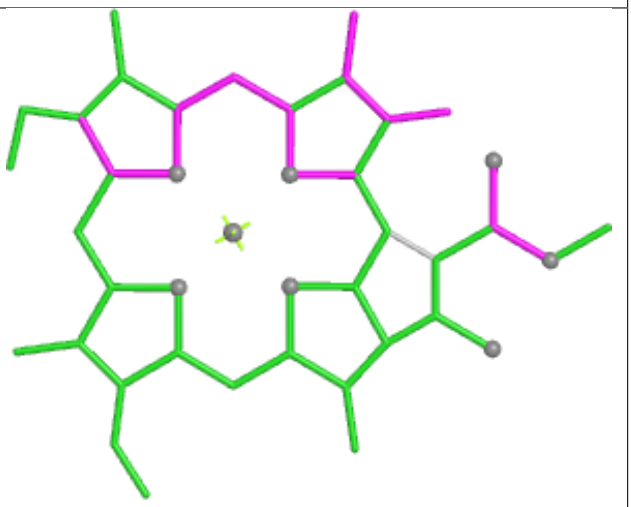
Ligand BCR m 101	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA a 842	
 Bond lengths	 Bond angles
 Torsions	 Rings

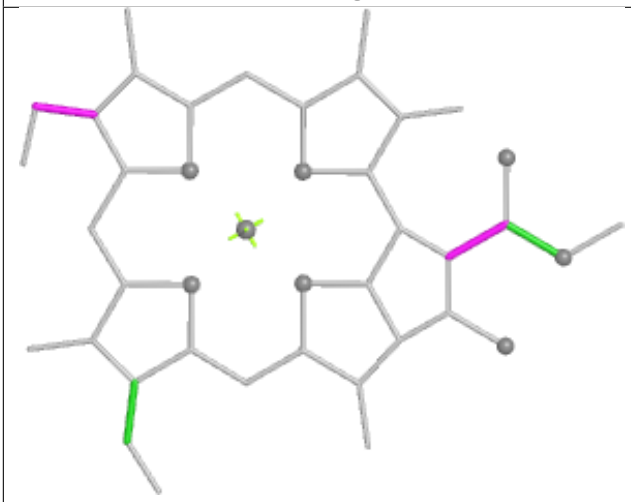
Ligand CLA b 830



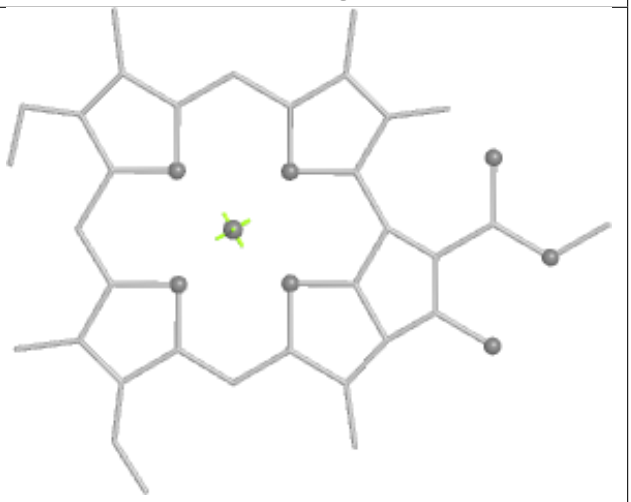
Bond lengths



Bond angles

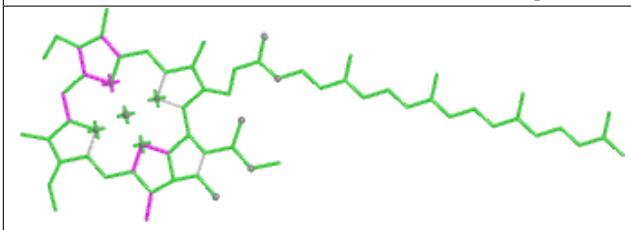


Torsions

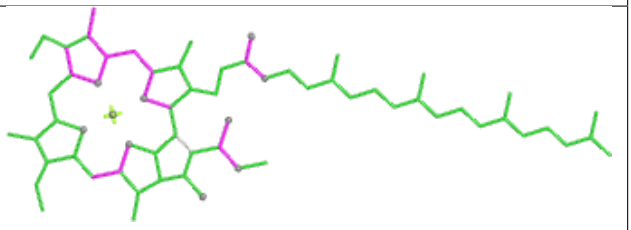


Rings

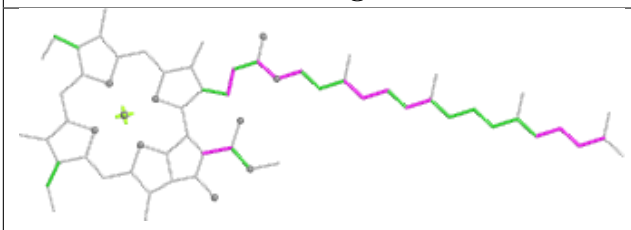
Ligand CLA a 839



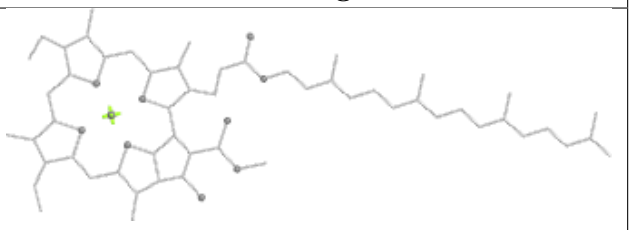
Bond lengths



Bond angles

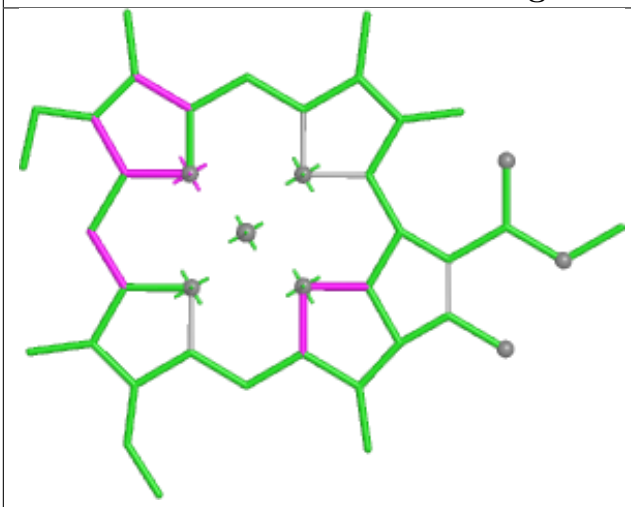


Torsions

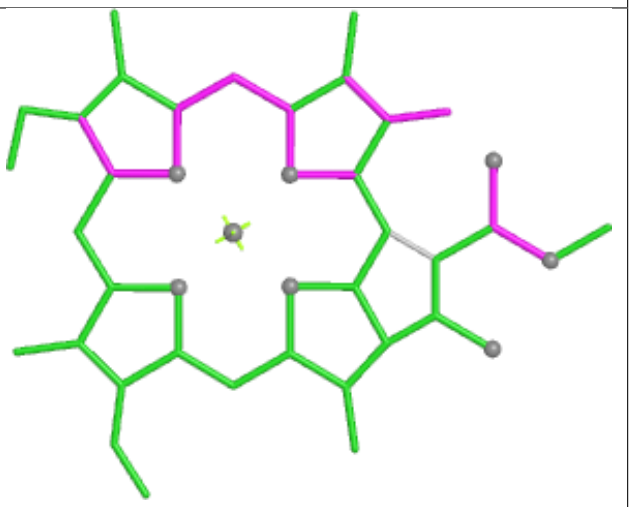


Rings

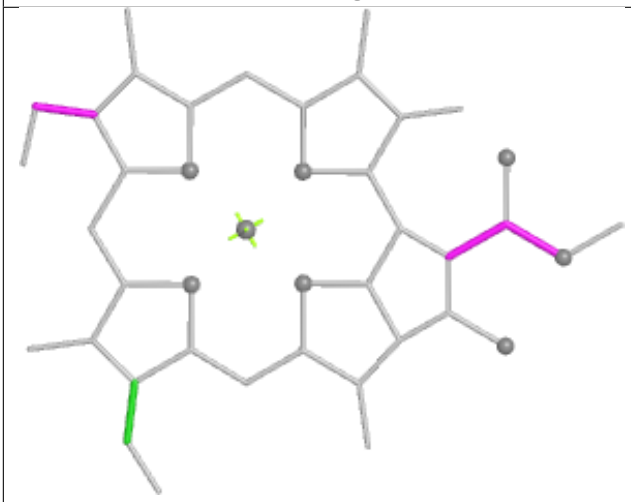
Ligand CLA 8 314



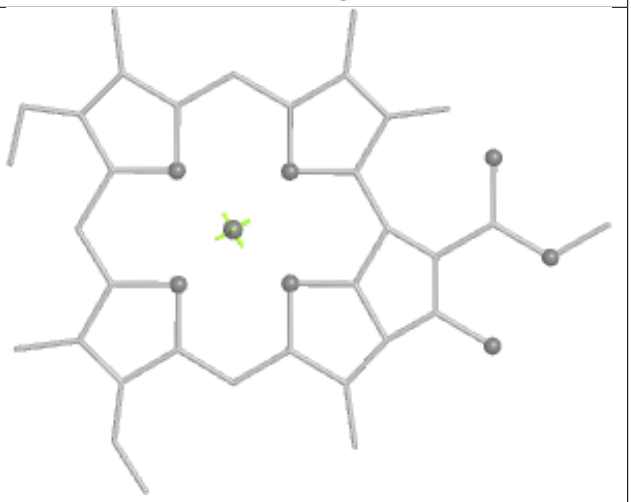
Bond lengths



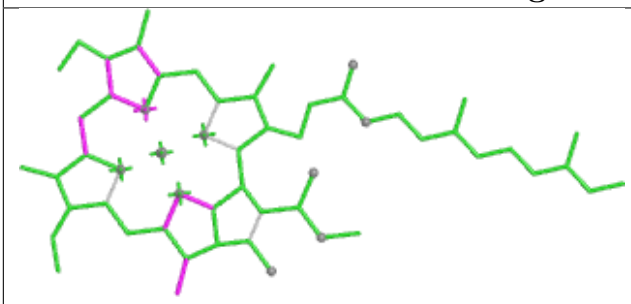
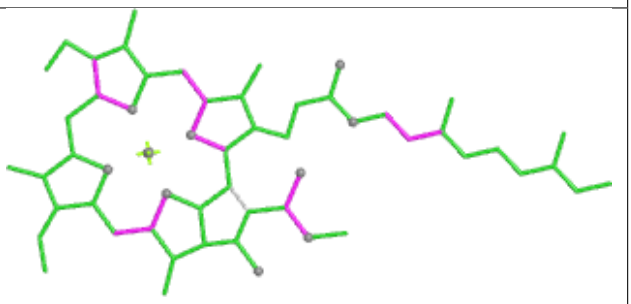
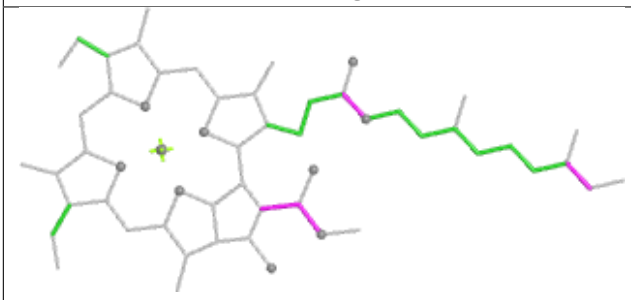
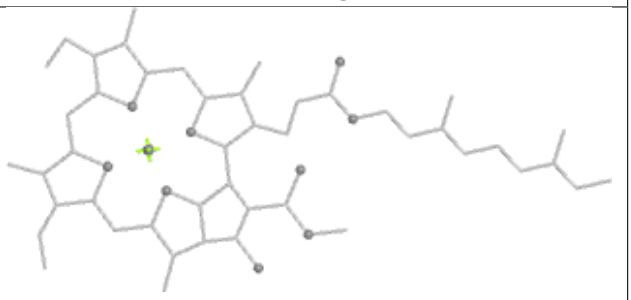
Bond angles

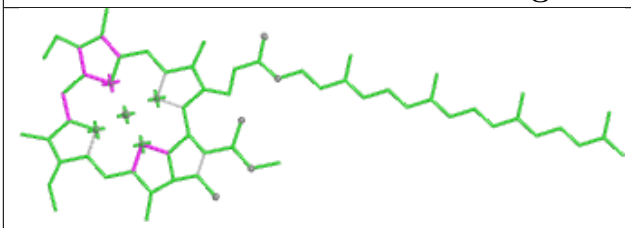
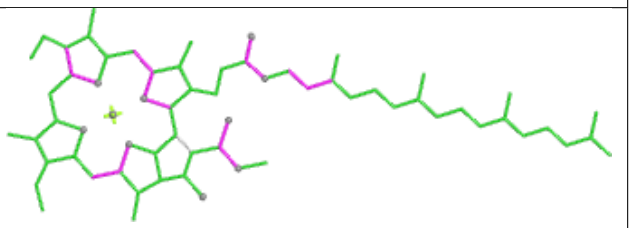
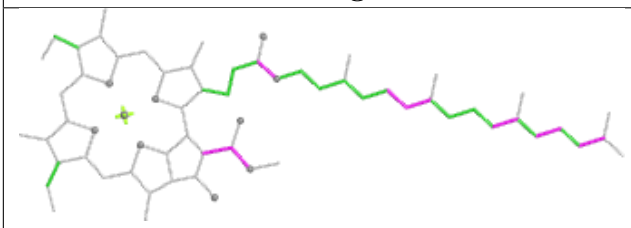
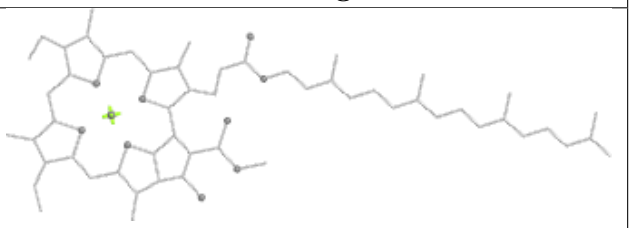


Torsions

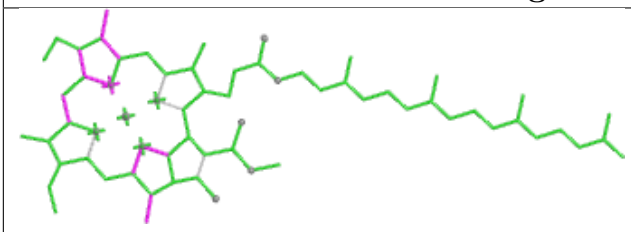


Rings

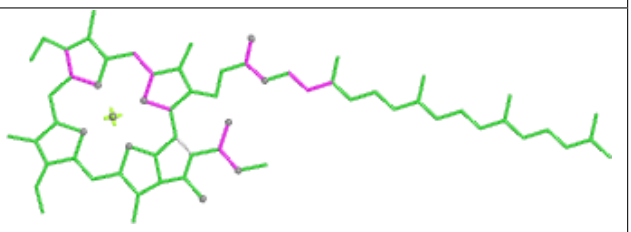
Ligand CLA a 811	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA f 802	
 Bond lengths	 Bond angles
 Torsions	 Rings

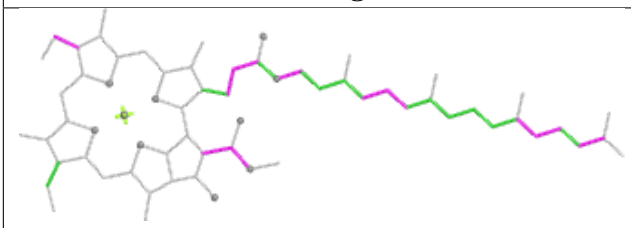
Ligand CLA a 810



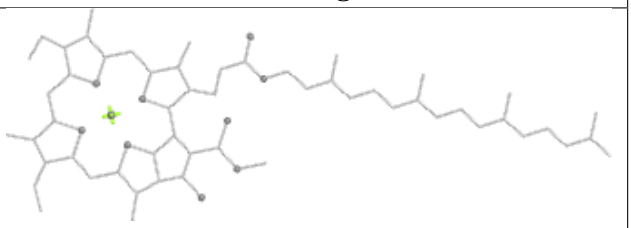
Bond lengths



Bond angles

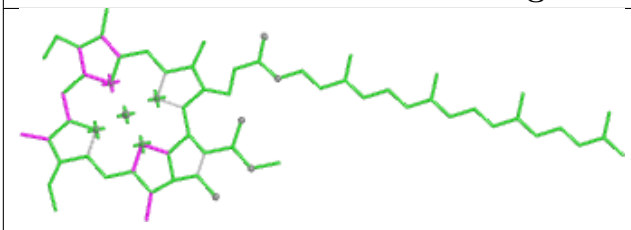


Torsions

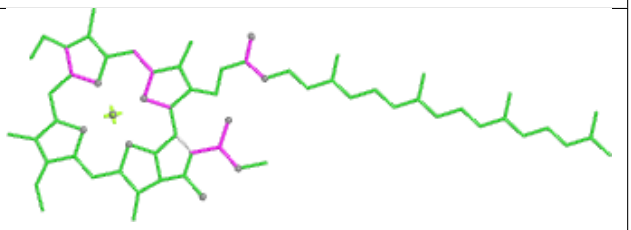


Rings

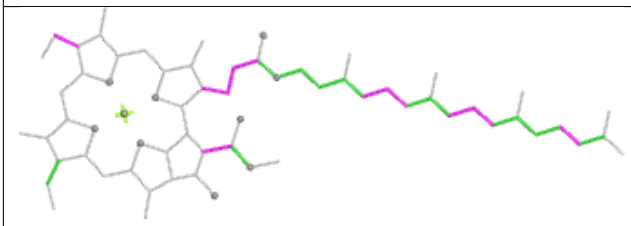
Ligand CLA b 809



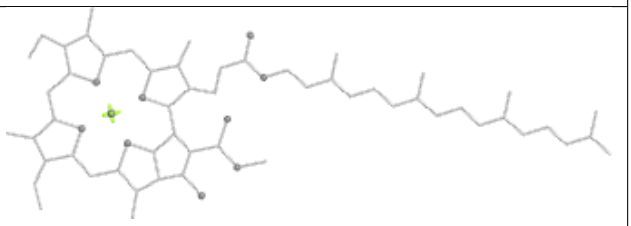
Bond lengths



Bond angles

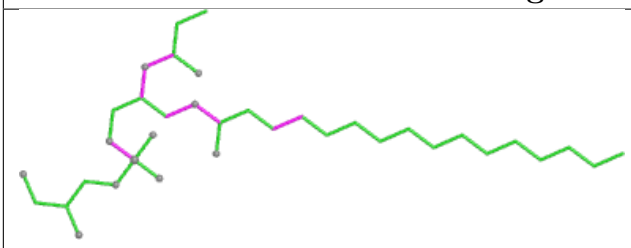


Torsions

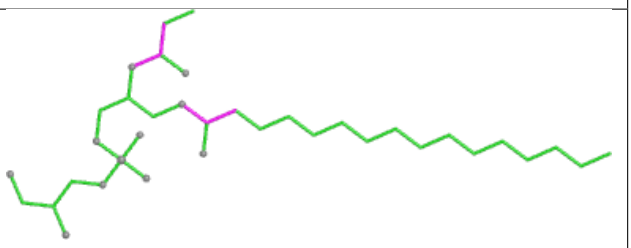


Rings

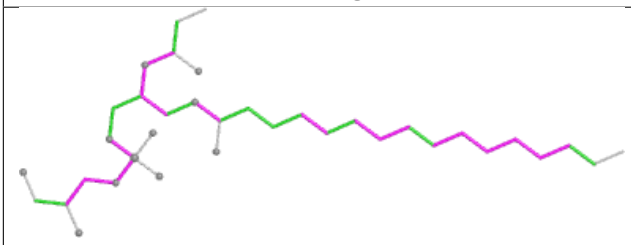
Ligand LHG 9 307



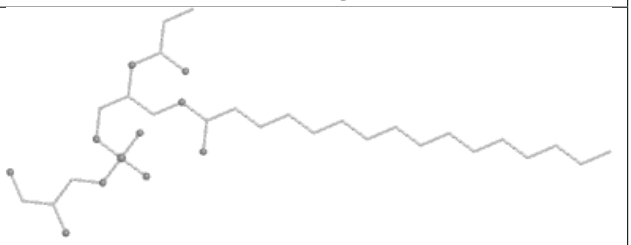
Bond lengths



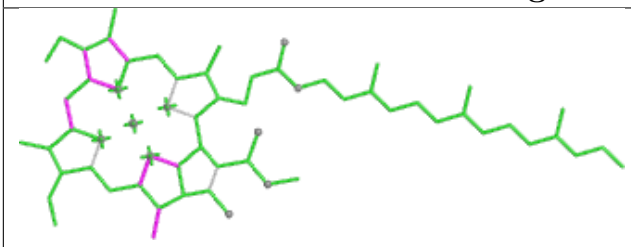
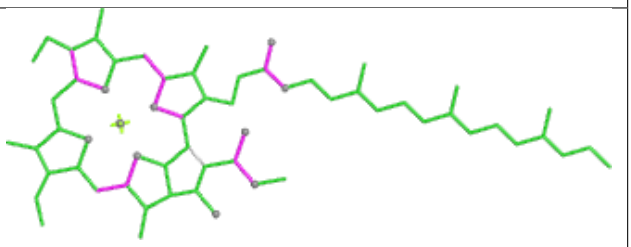
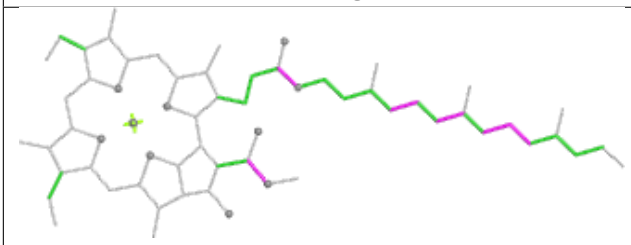
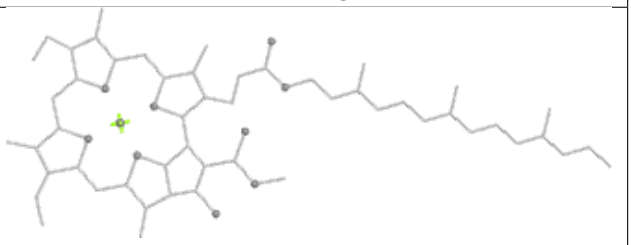
Bond angles

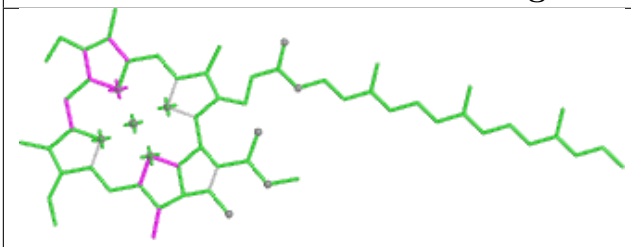
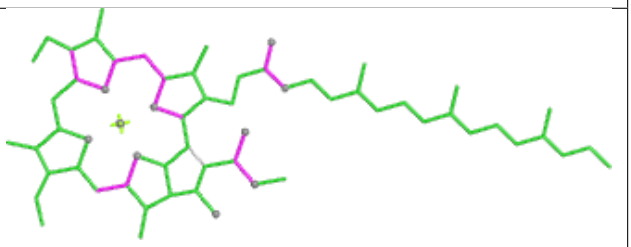
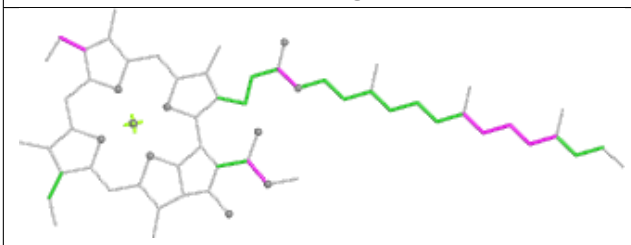
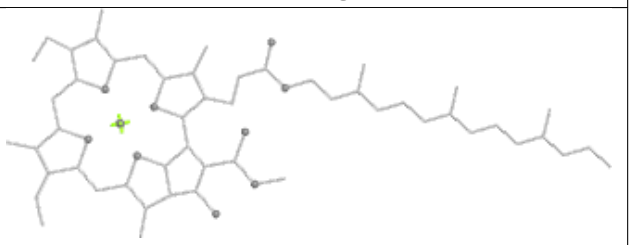


Torsions

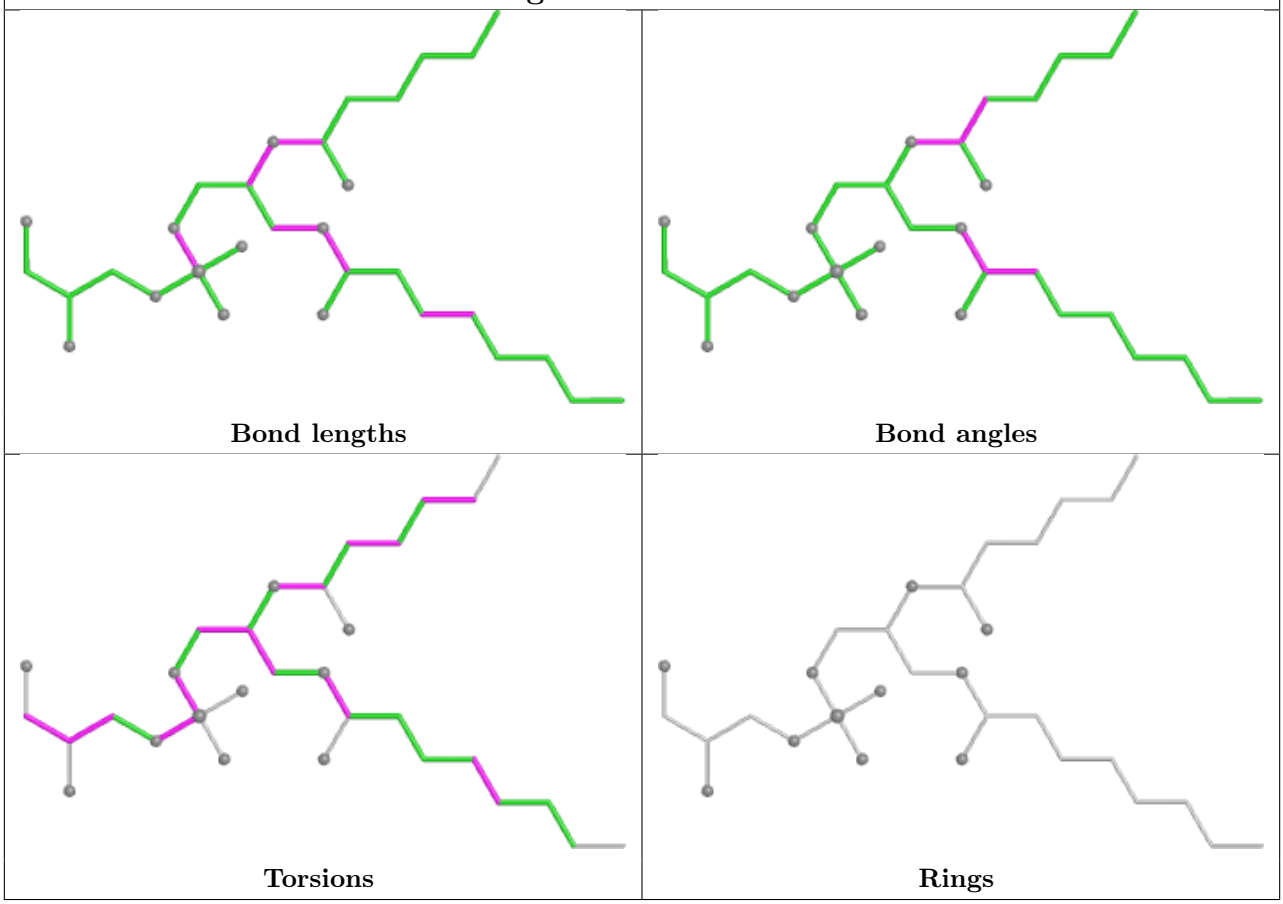


Rings

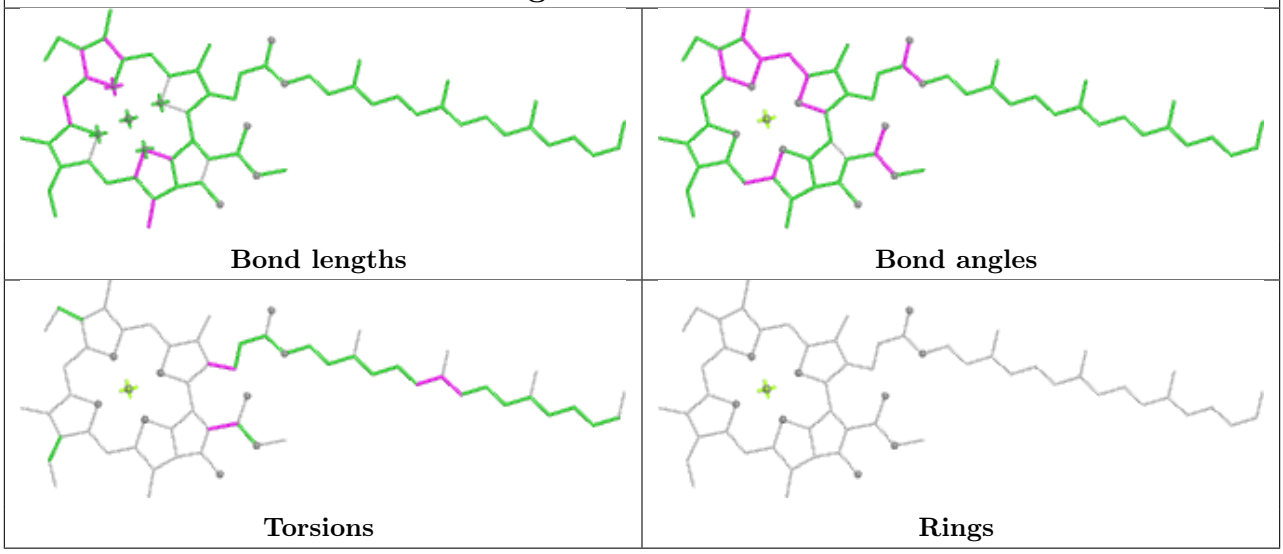
Ligand CLA a 812	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA 9 318	
 Bond lengths	 Bond angles
 Torsions	 Rings

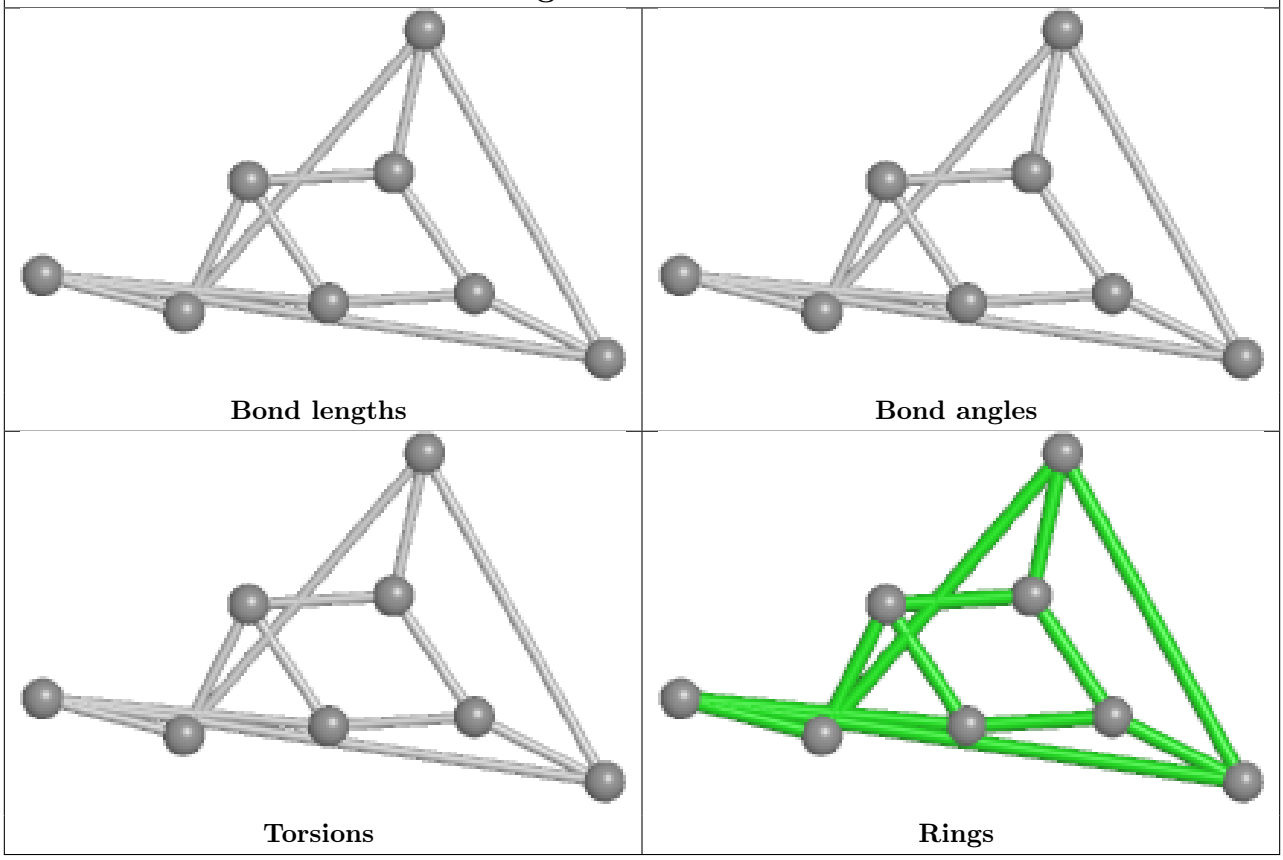
Ligand LHG b 847



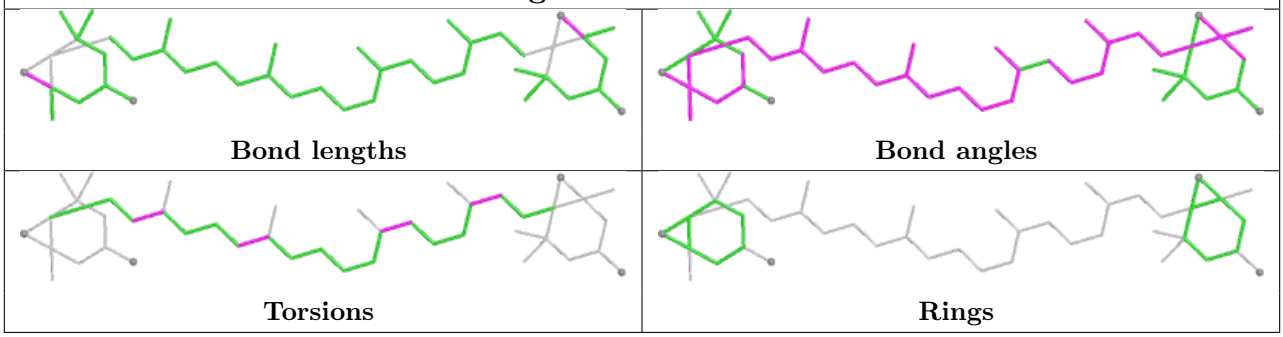
Ligand CLA b 825



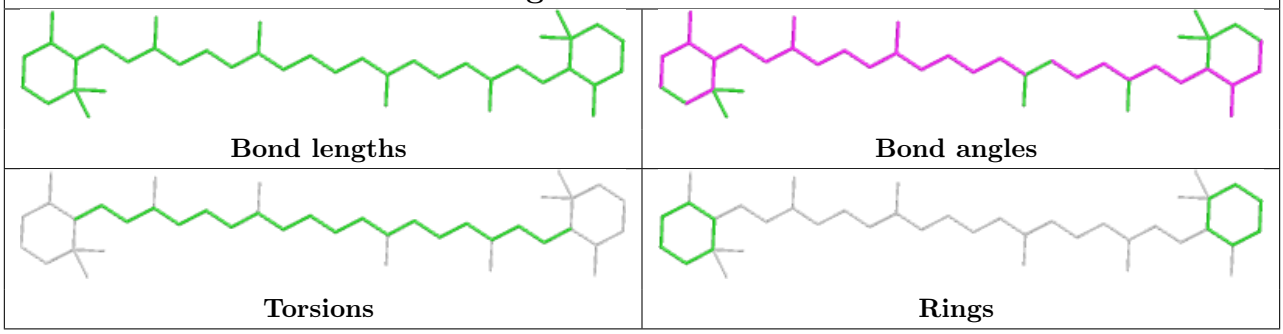
Ligand SF4 c 101



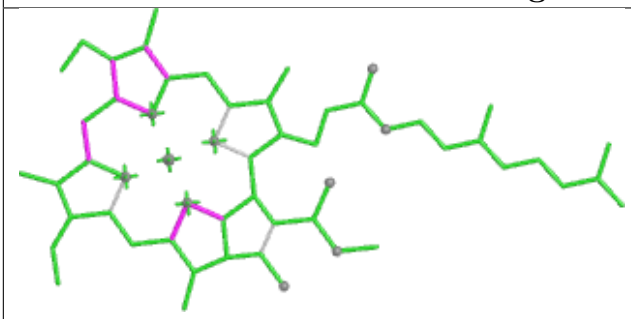
Ligand XAT a 852



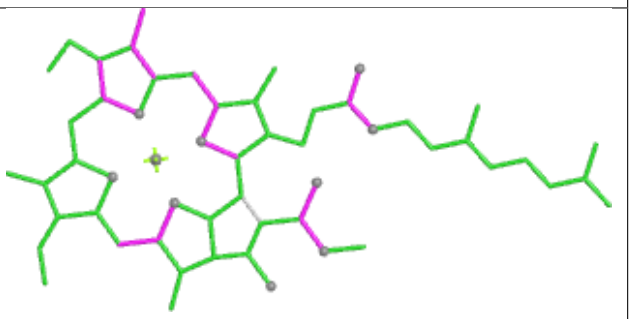
Ligand BCR h 201



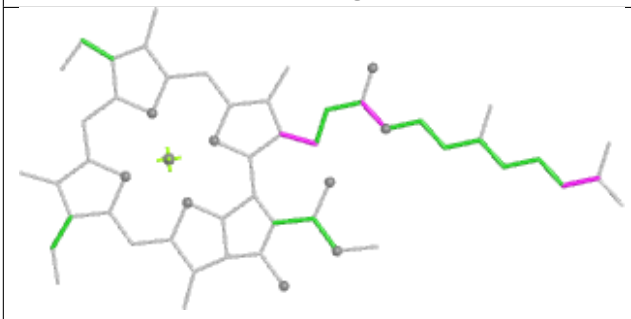
Ligand CLA a 805



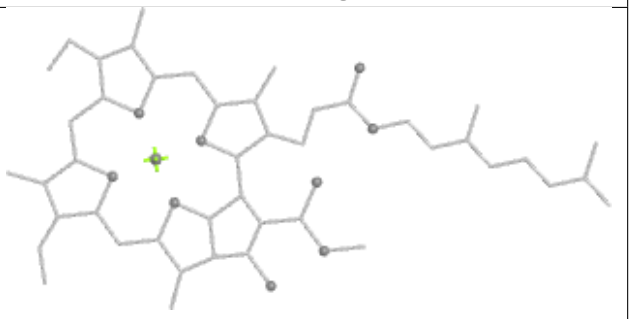
Bond lengths



Bond angles

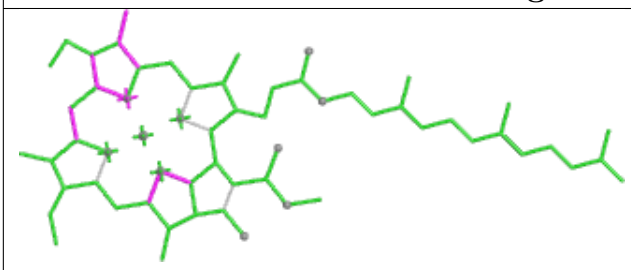


Torsions

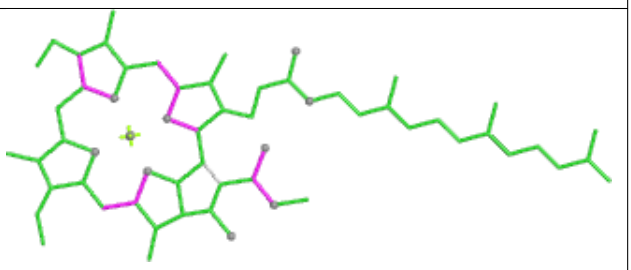


Rings

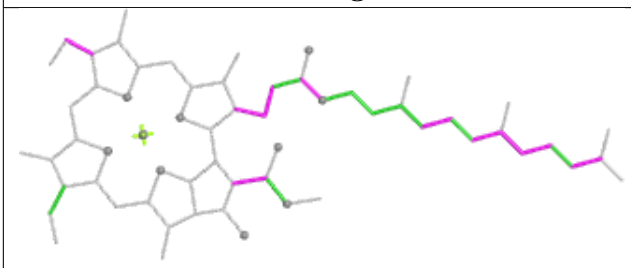
Ligand CLA b 818



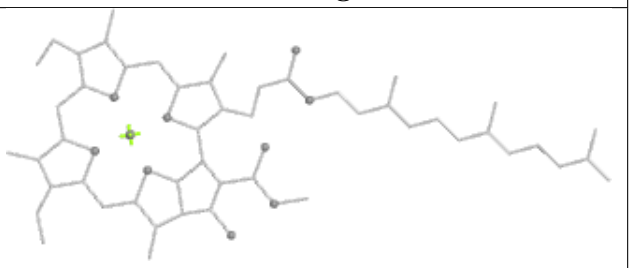
Bond lengths



Bond angles



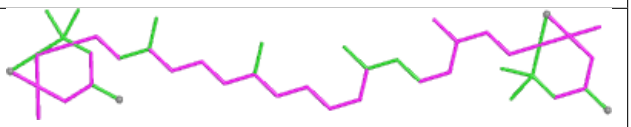
Torsions



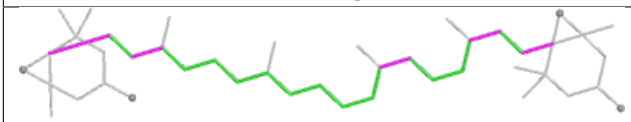
Rings

Ligand XAT 7 303

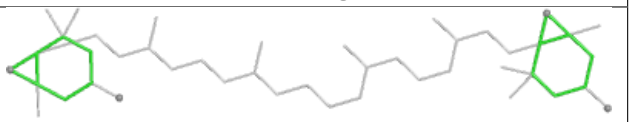
Bond lengths



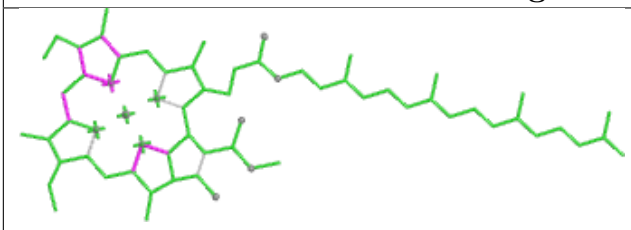
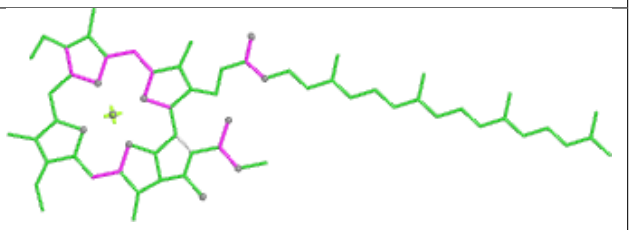
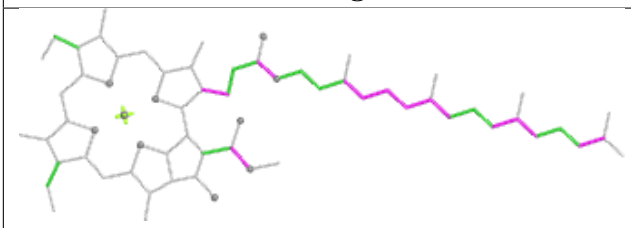
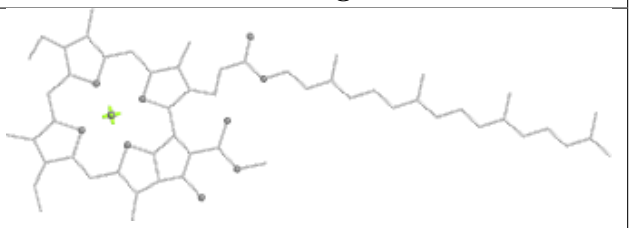
Bond angles

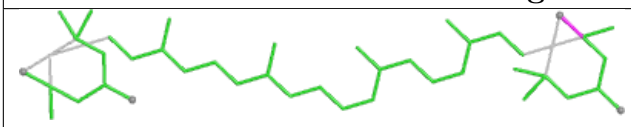
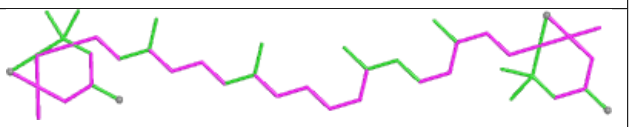
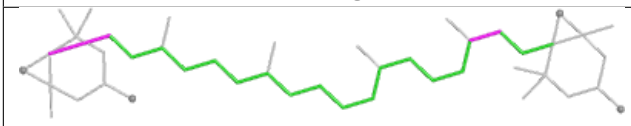
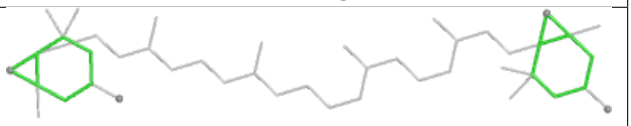


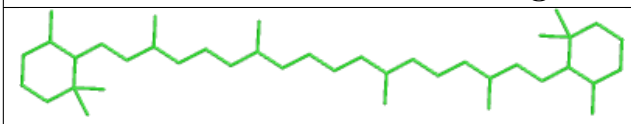
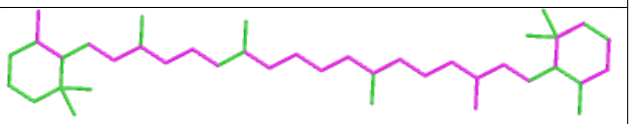
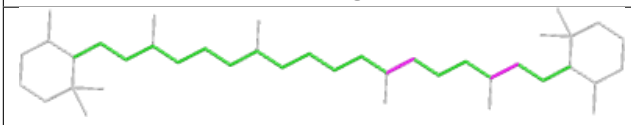
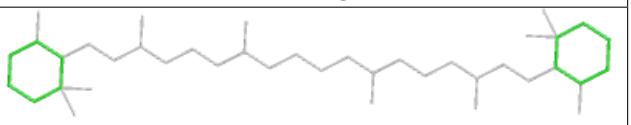
Torsions



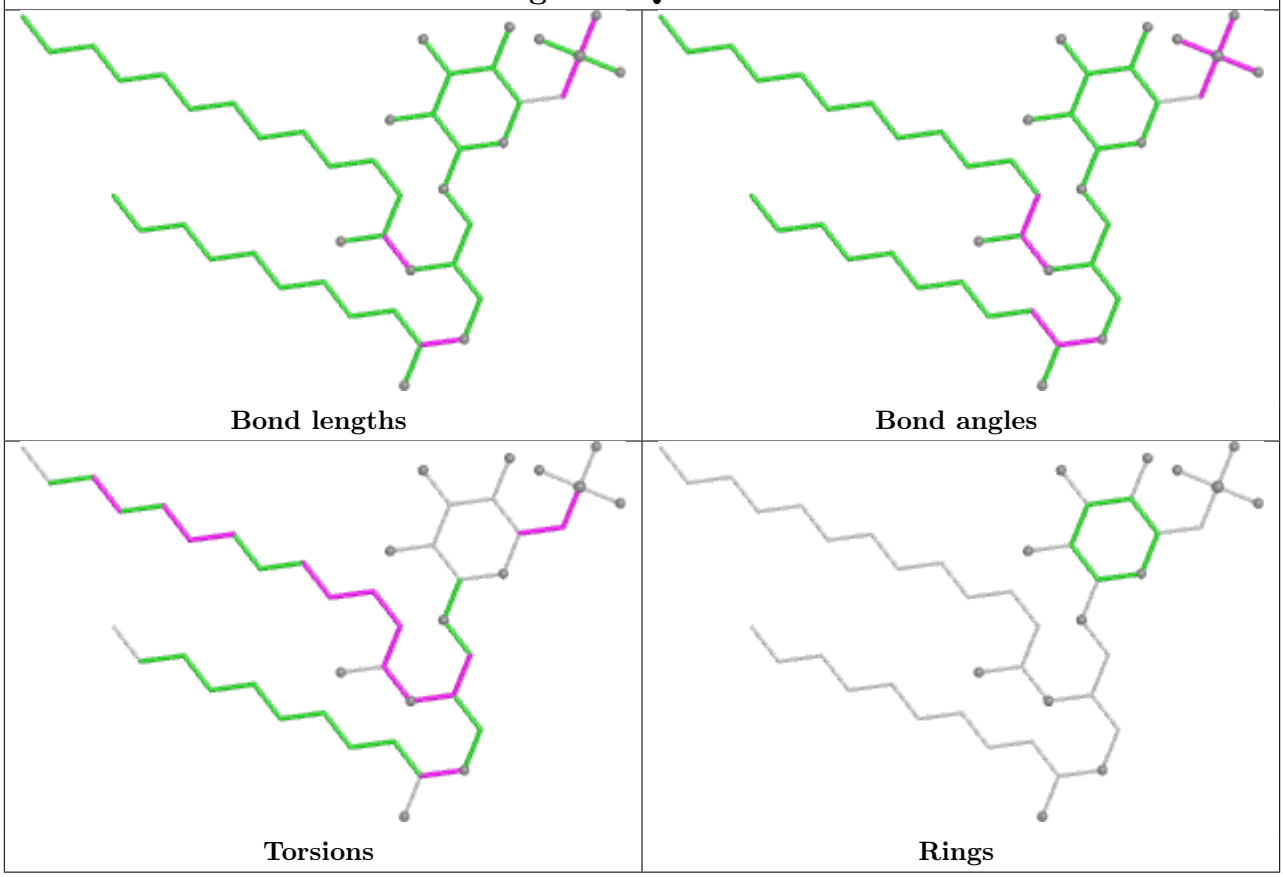
Rings

Ligand CLA 1 310	
 Bond lengths	 Bond angles
 Torsions	 Rings

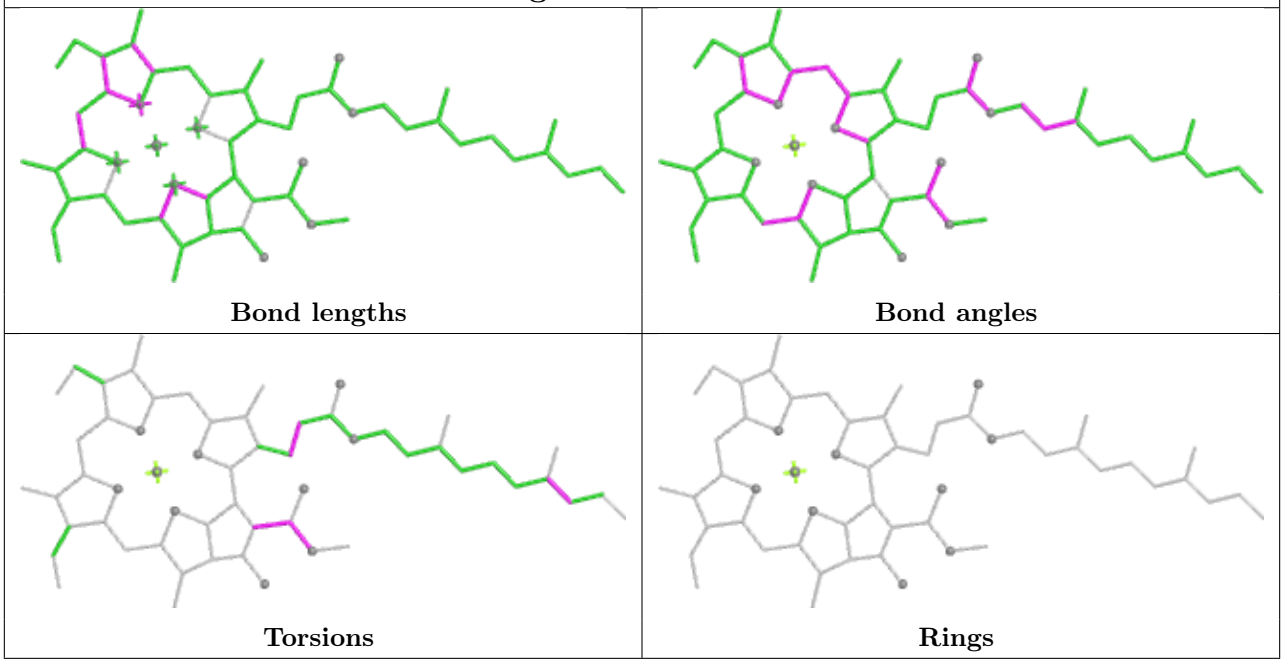
Ligand XAT 8 301	
 Bond lengths	 Bond angles
 Torsions	 Rings

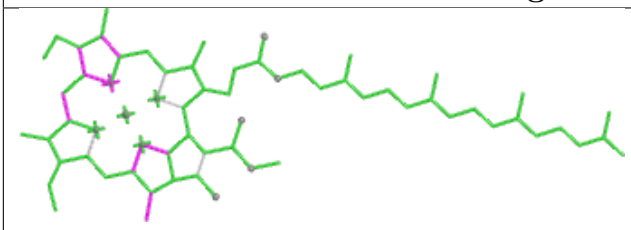
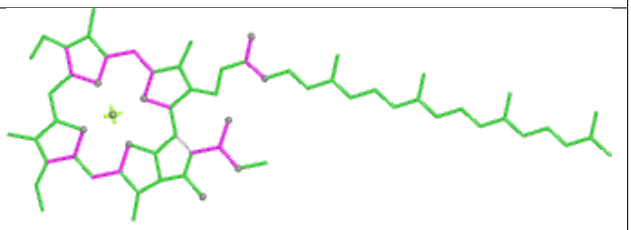
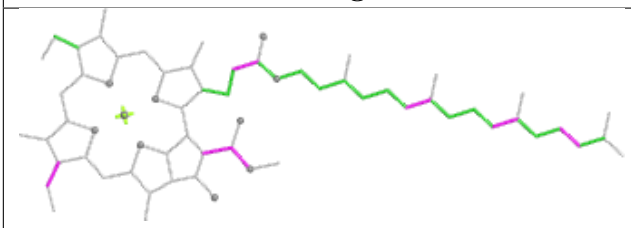
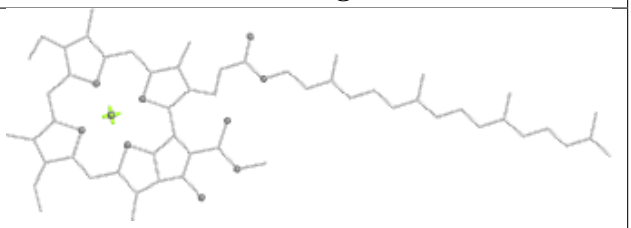
Ligand BCR i 101	
 Bond lengths	 Bond angles
 Torsions	 Rings

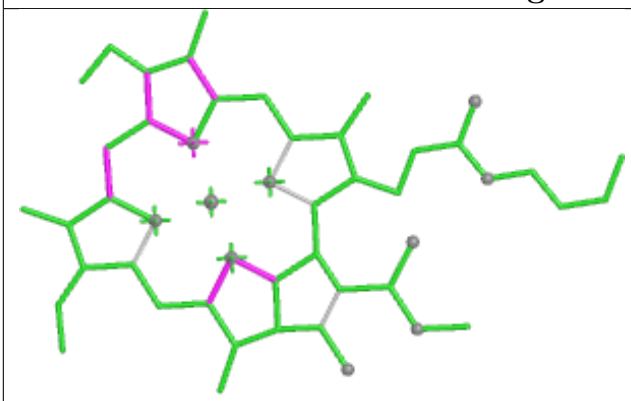
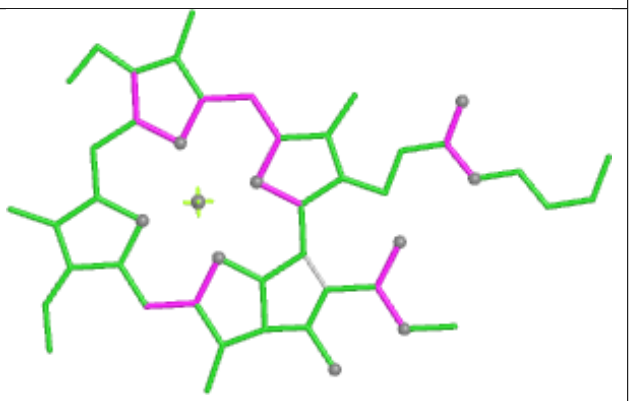
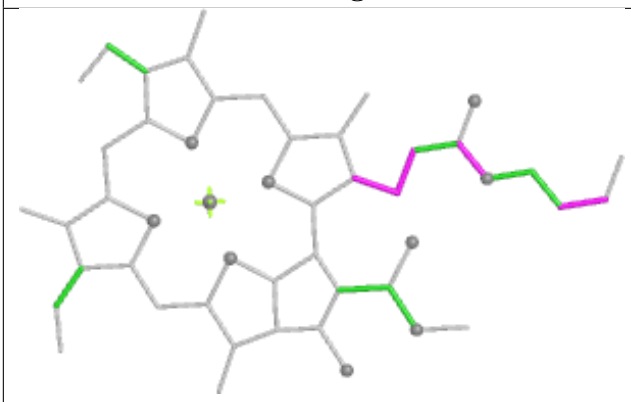
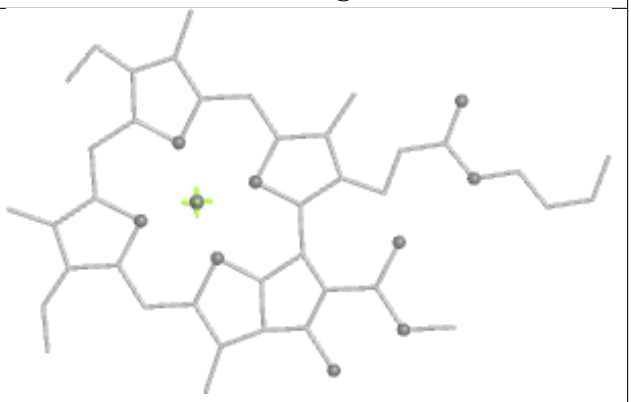
Ligand SQD 1 315

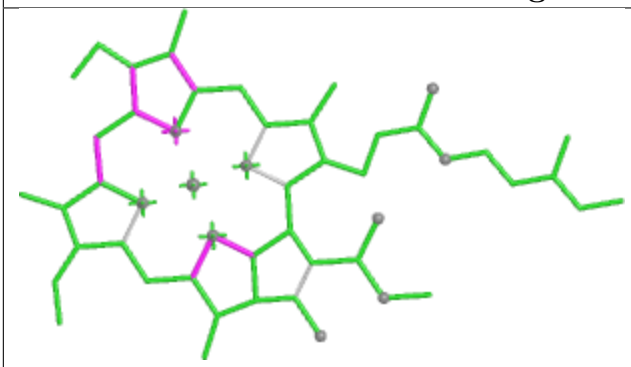
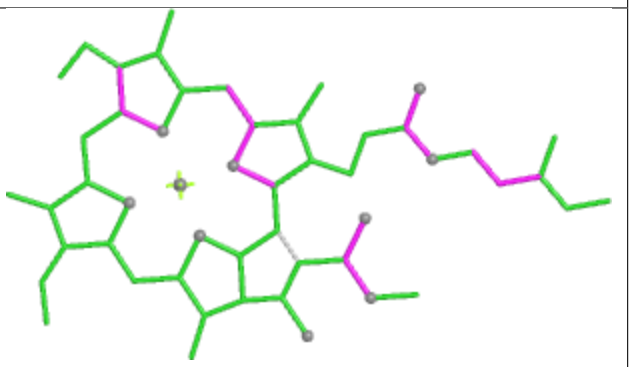
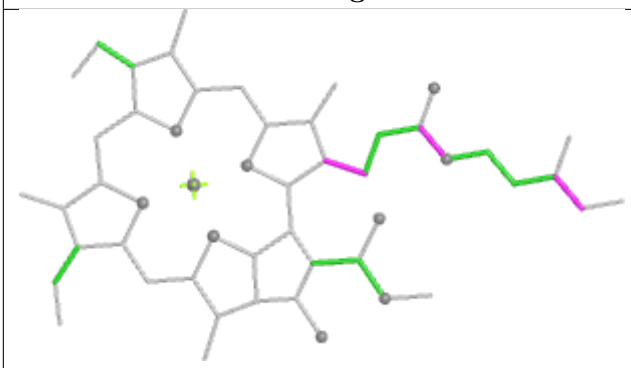
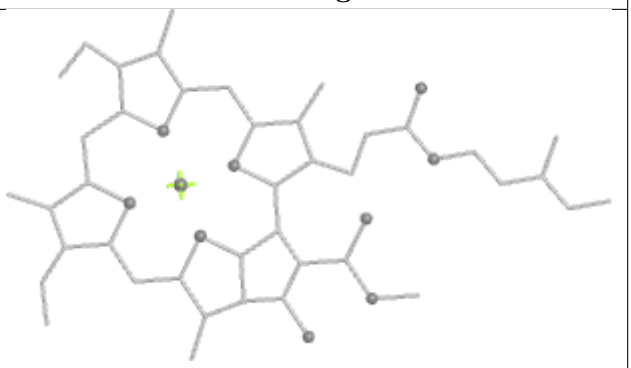


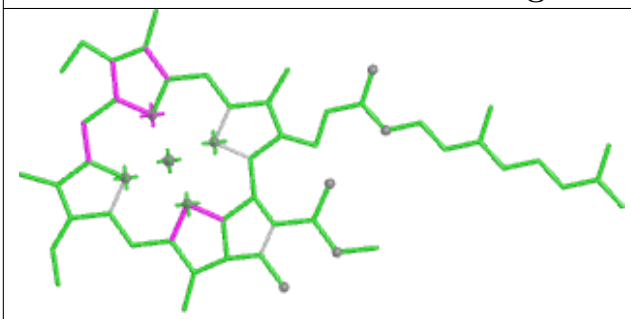
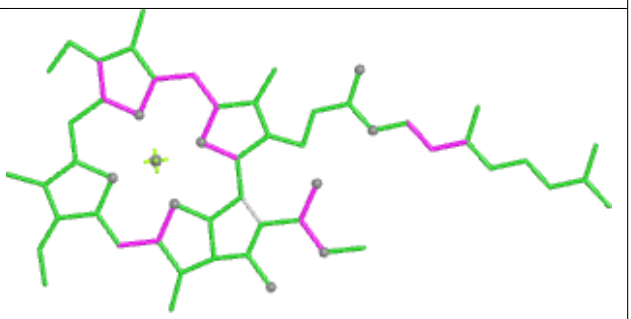
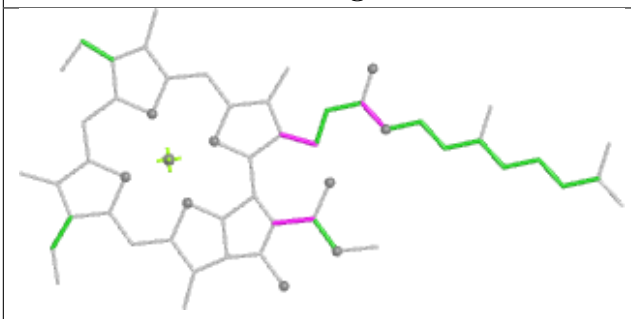
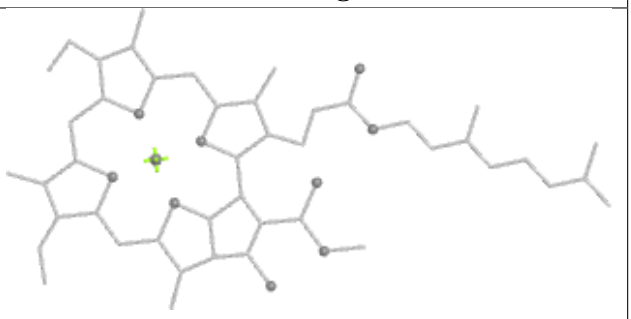
Ligand CLA 8 309



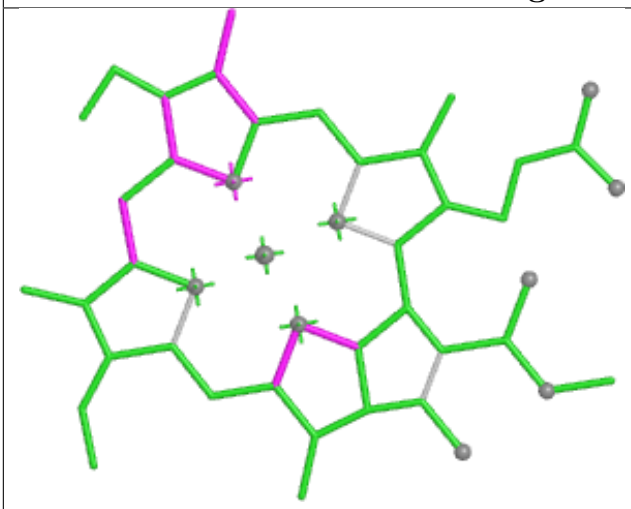
Ligand CLA b 804	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA b 831	
 Bond lengths	 Bond angles
 Torsions	 Rings

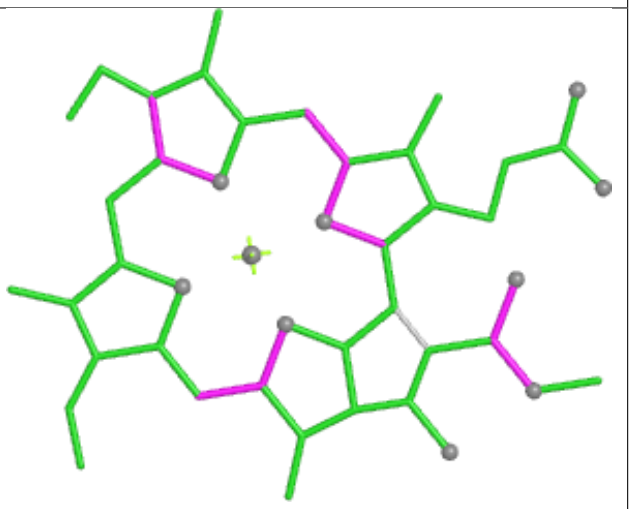
Ligand CLA a 838	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA b 816	
 Bond lengths	 Bond angles
 Torsions	 Rings

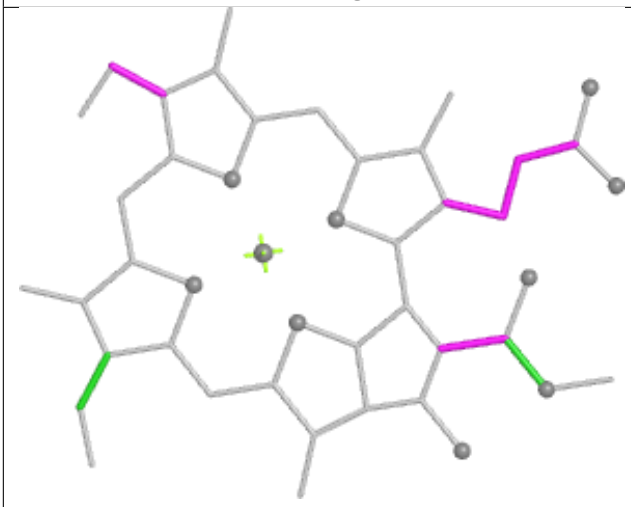
Ligand CLA a 817



Bond lengths



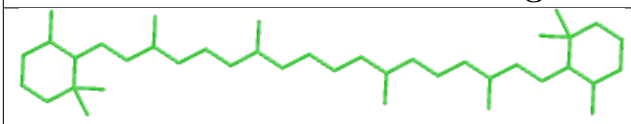
Bond angles



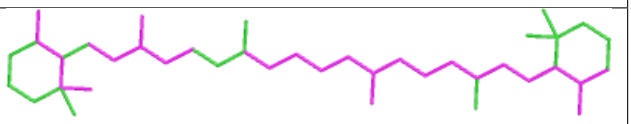
Torsions

Rings

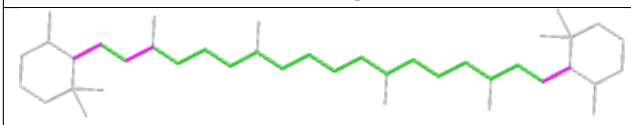
Ligand BCR b 849



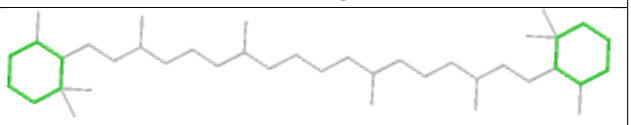
Bond lengths



Bond angles

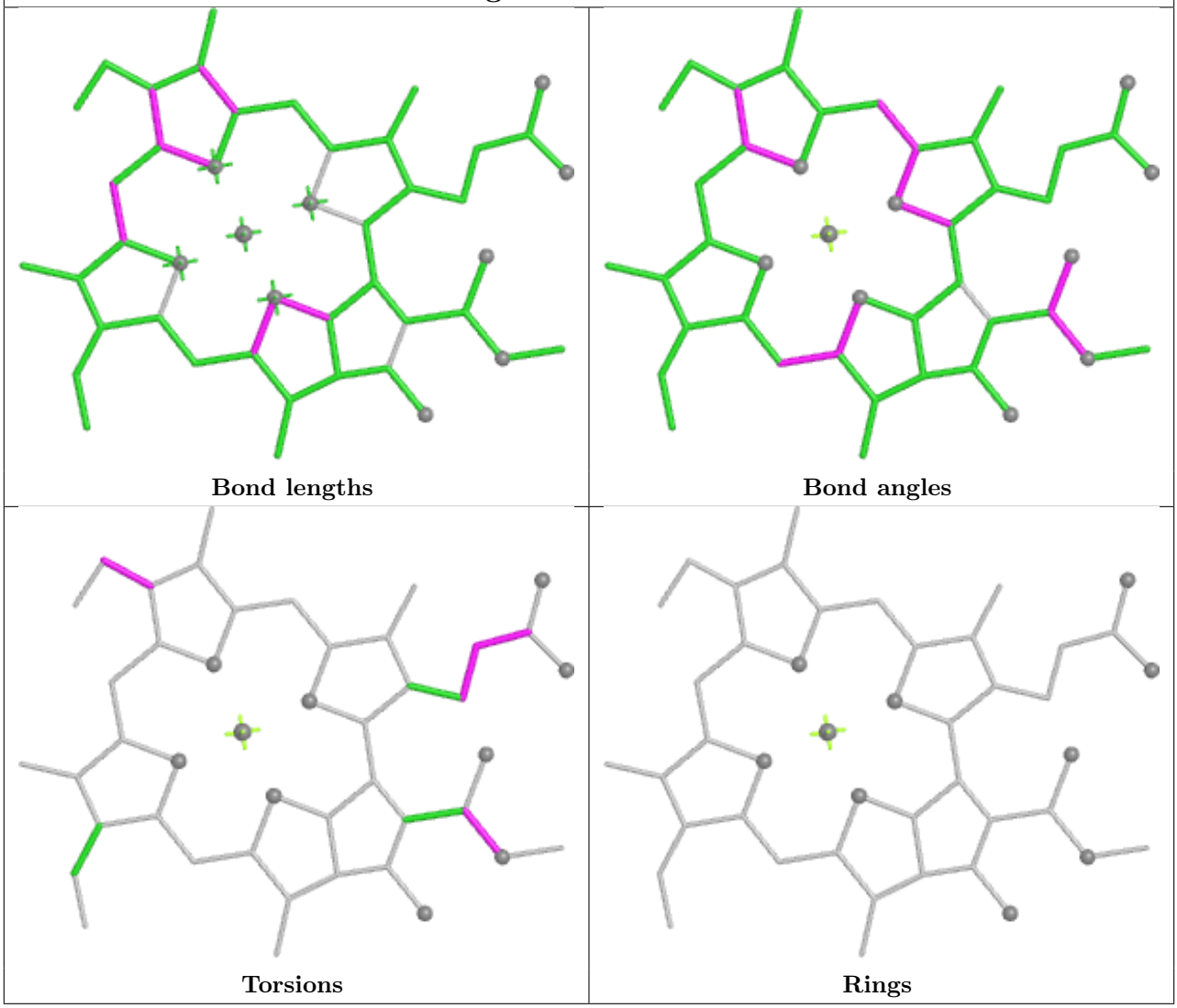


Torsions



Rings

Ligand CLA 7 317



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.

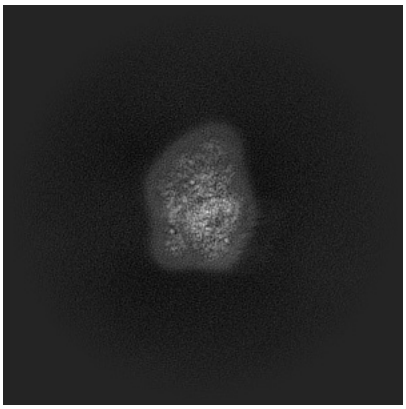
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-60290. These allow visual inspection of the internal detail of the map and identification of artifacts.

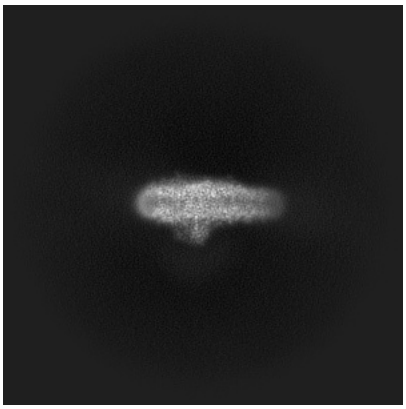
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections (i)

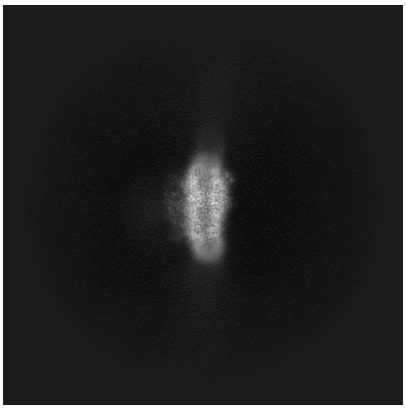
6.1.1 Primary map



X

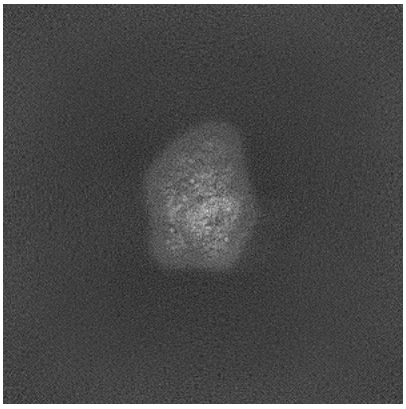


Y

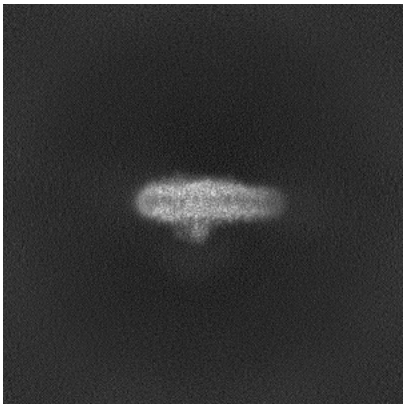


Z

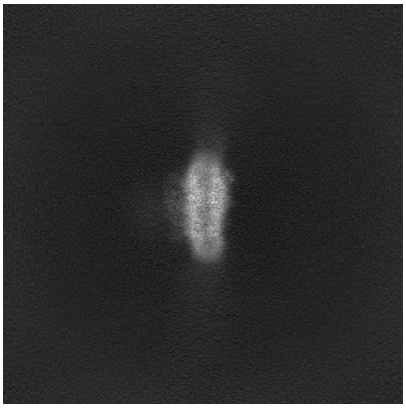
6.1.2 Raw map



X



Y

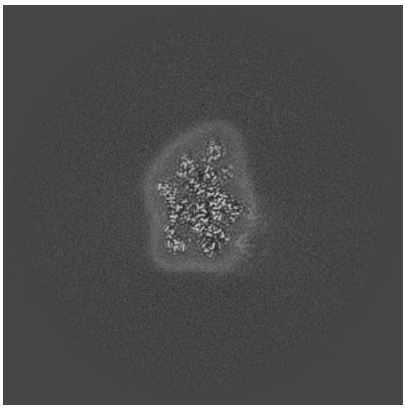


Z

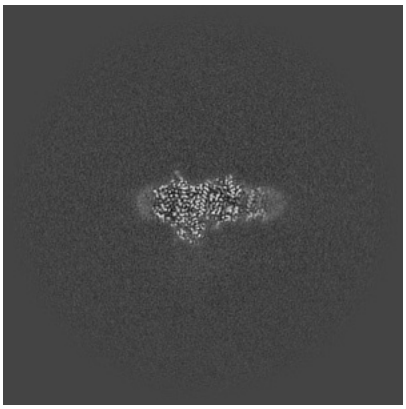
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

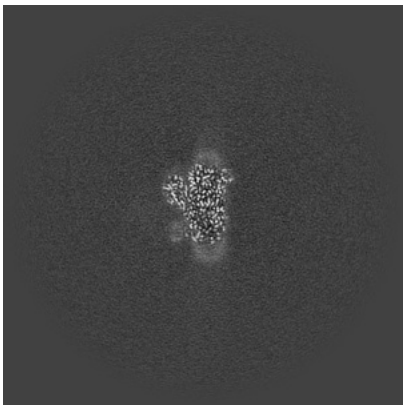
6.2.1 Primary map



X Index: 256

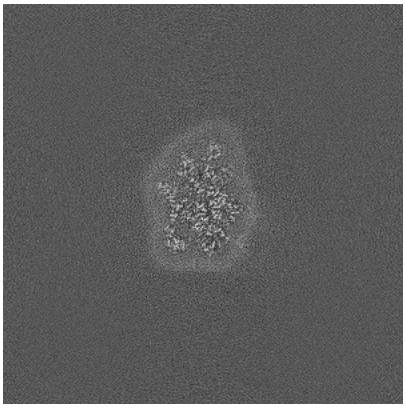


Y Index: 256

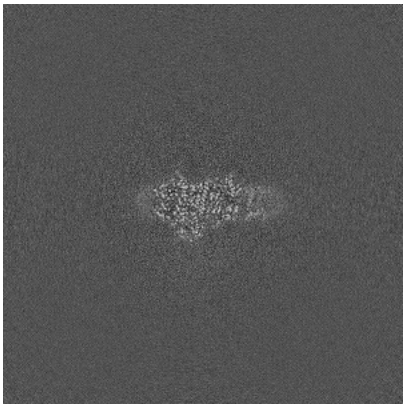


Z Index: 256

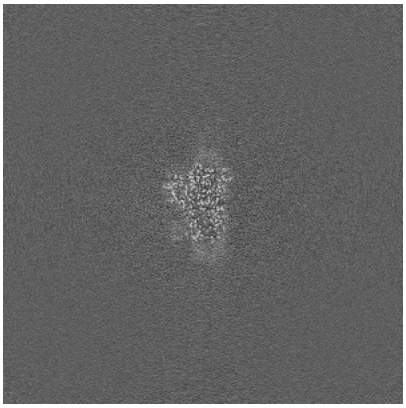
6.2.2 Raw map



X Index: 256



Y Index: 256

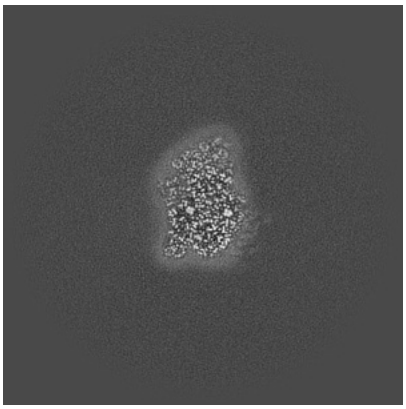


Z Index: 256

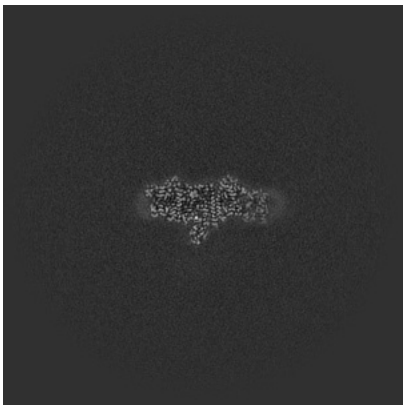
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

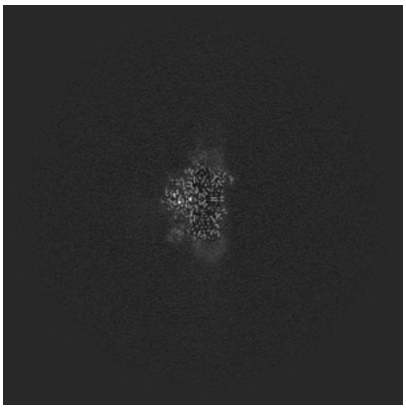
6.3.1 Primary map



X Index: 245

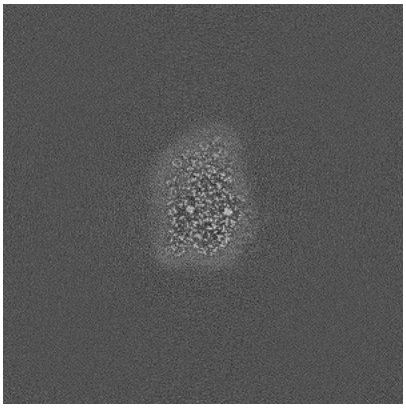


Y Index: 264

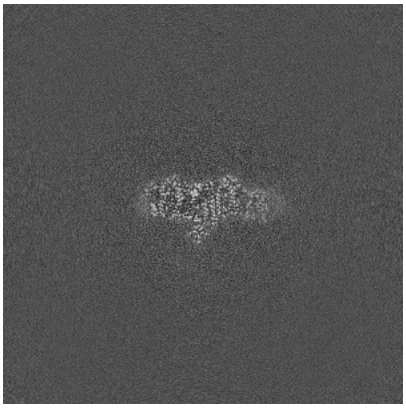


Z Index: 247

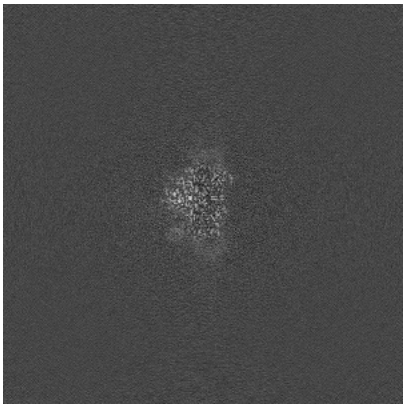
6.3.2 Raw map



X Index: 245



Y Index: 265

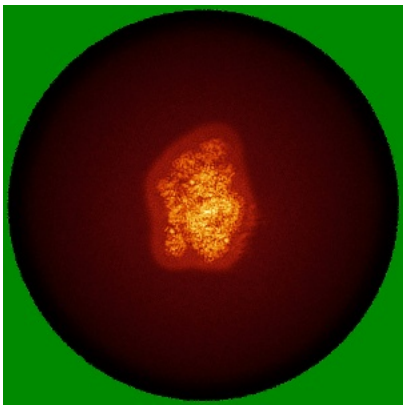


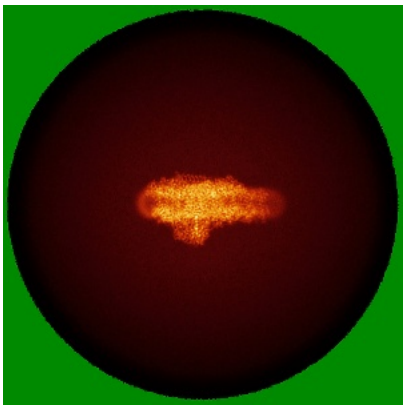
Z Index: 247

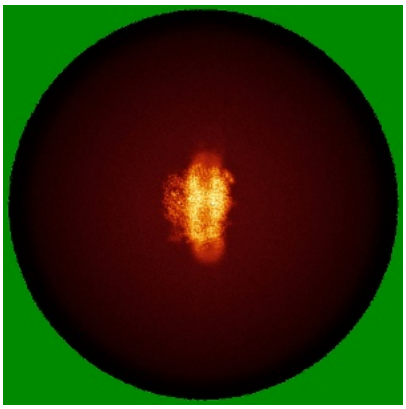
The images above show the largest variance slices of the map in three orthogonal directions.

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

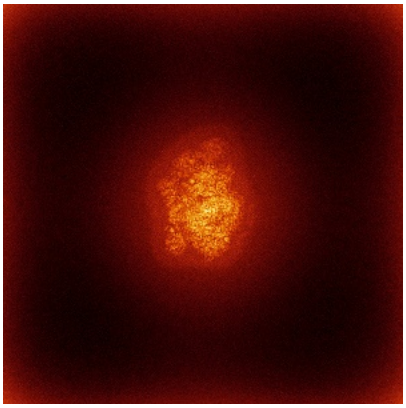
6.4.1 Primary map

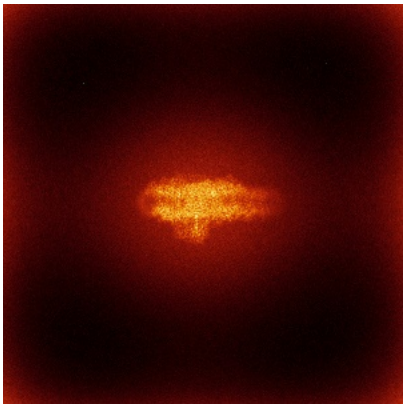

X

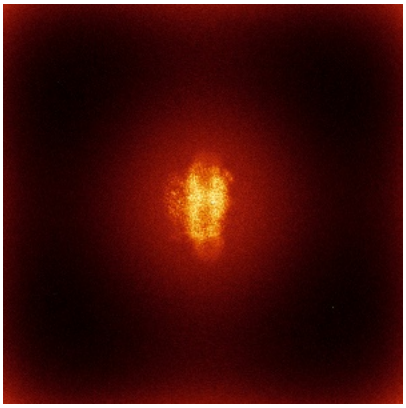

Y


Z

6.4.2 Raw map


X

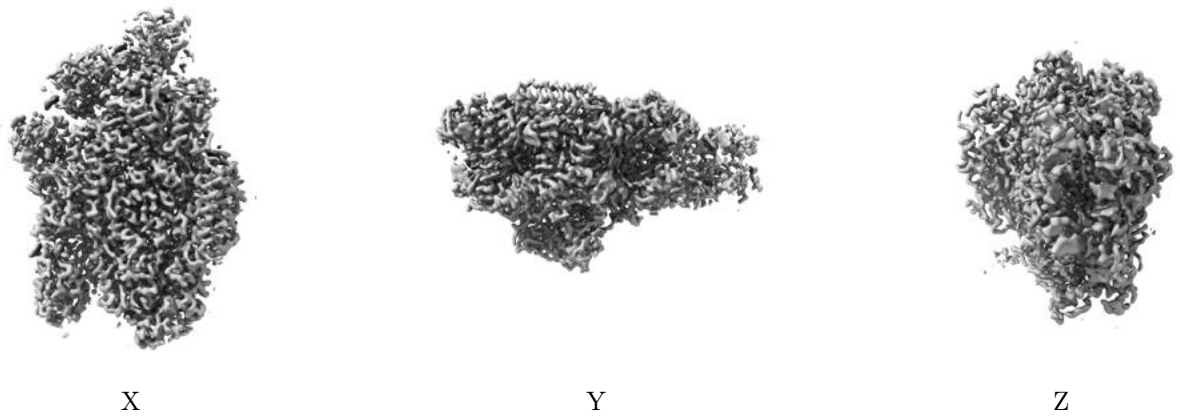

Y


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.

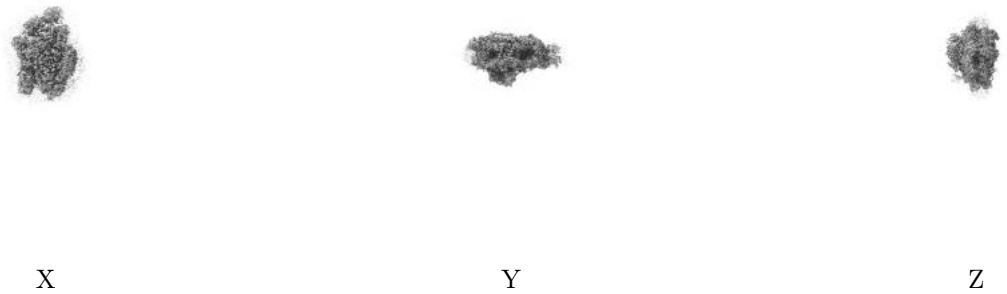
6.5 Orthogonal surface views (i)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.343. 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



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.

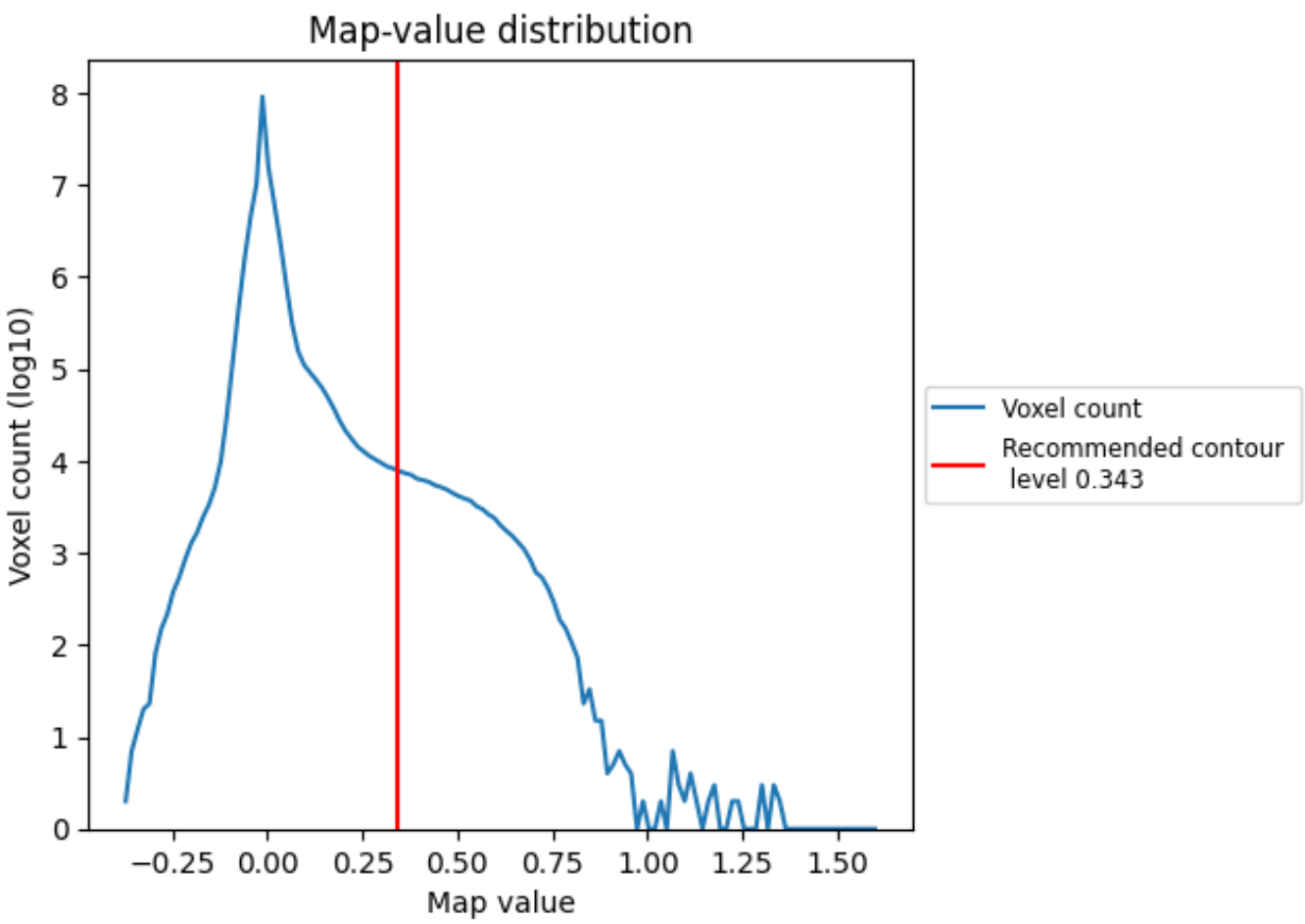
6.6 Mask visualisation (i)

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

7 Map analysis (i)

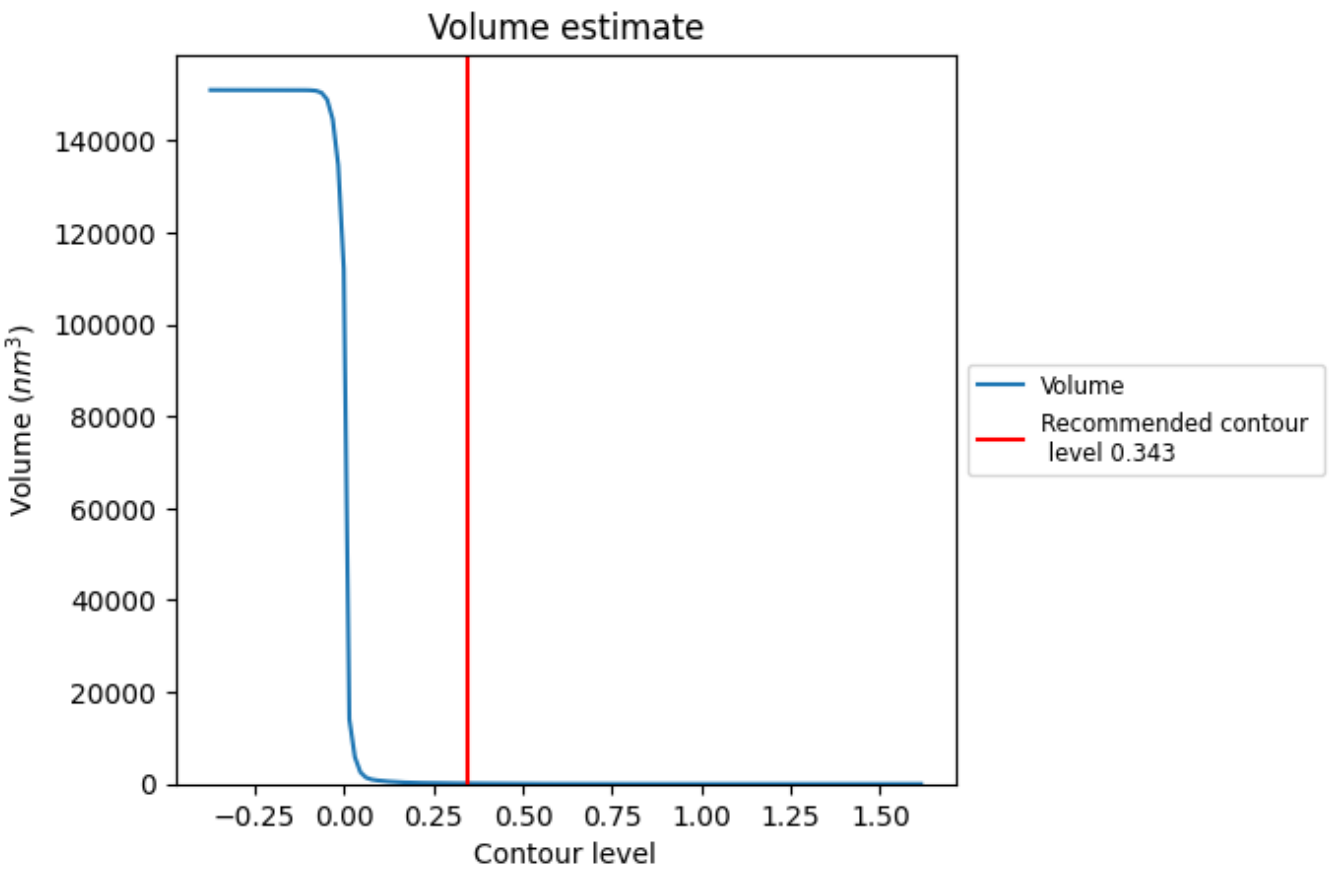
This section contains the results of statistical analysis of the map.

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.

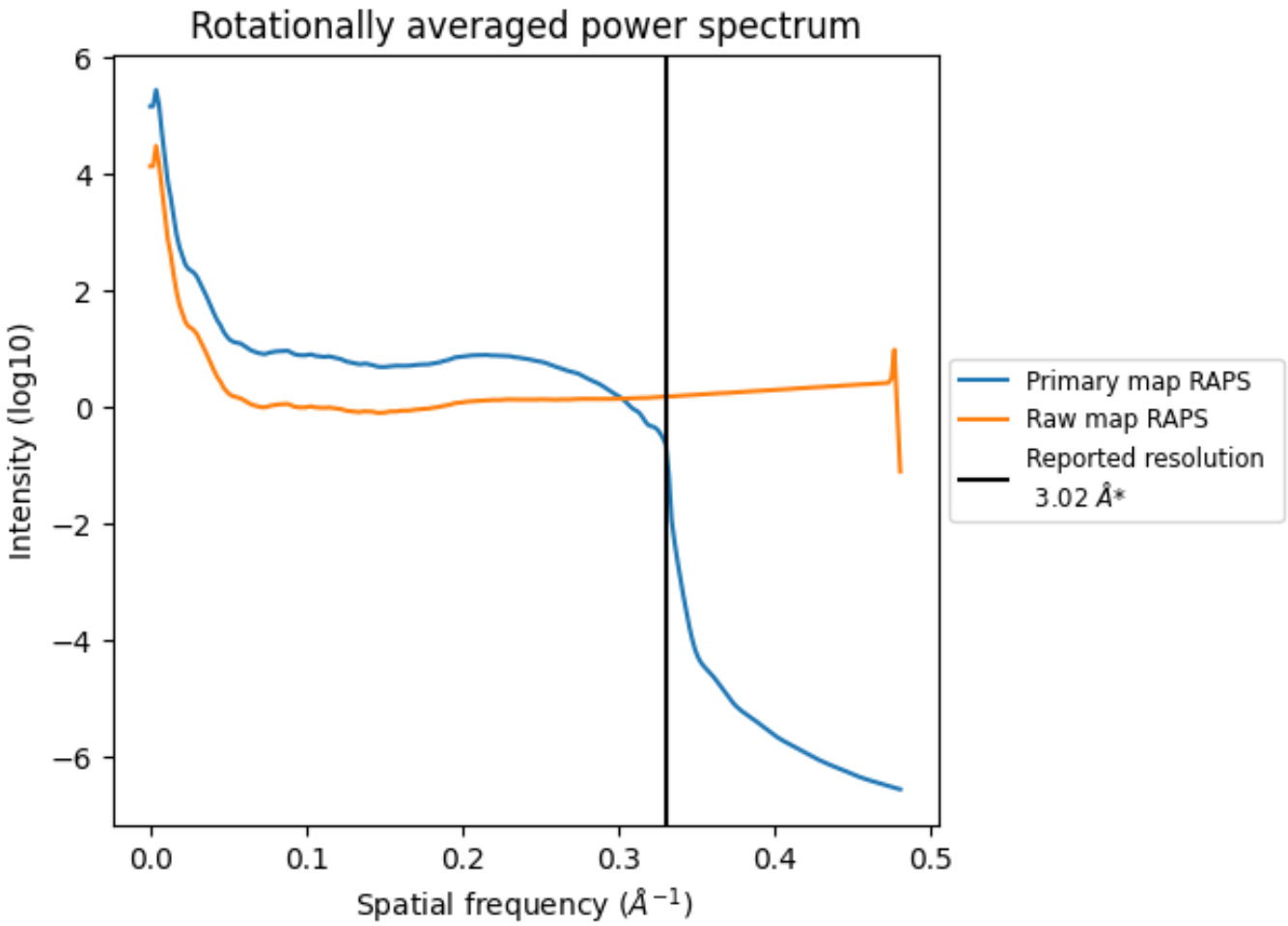
7.2 Volume estimate (i)



The volume at the recommended contour level is 109 nm^3; this corresponds to an approximate mass of 98 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)

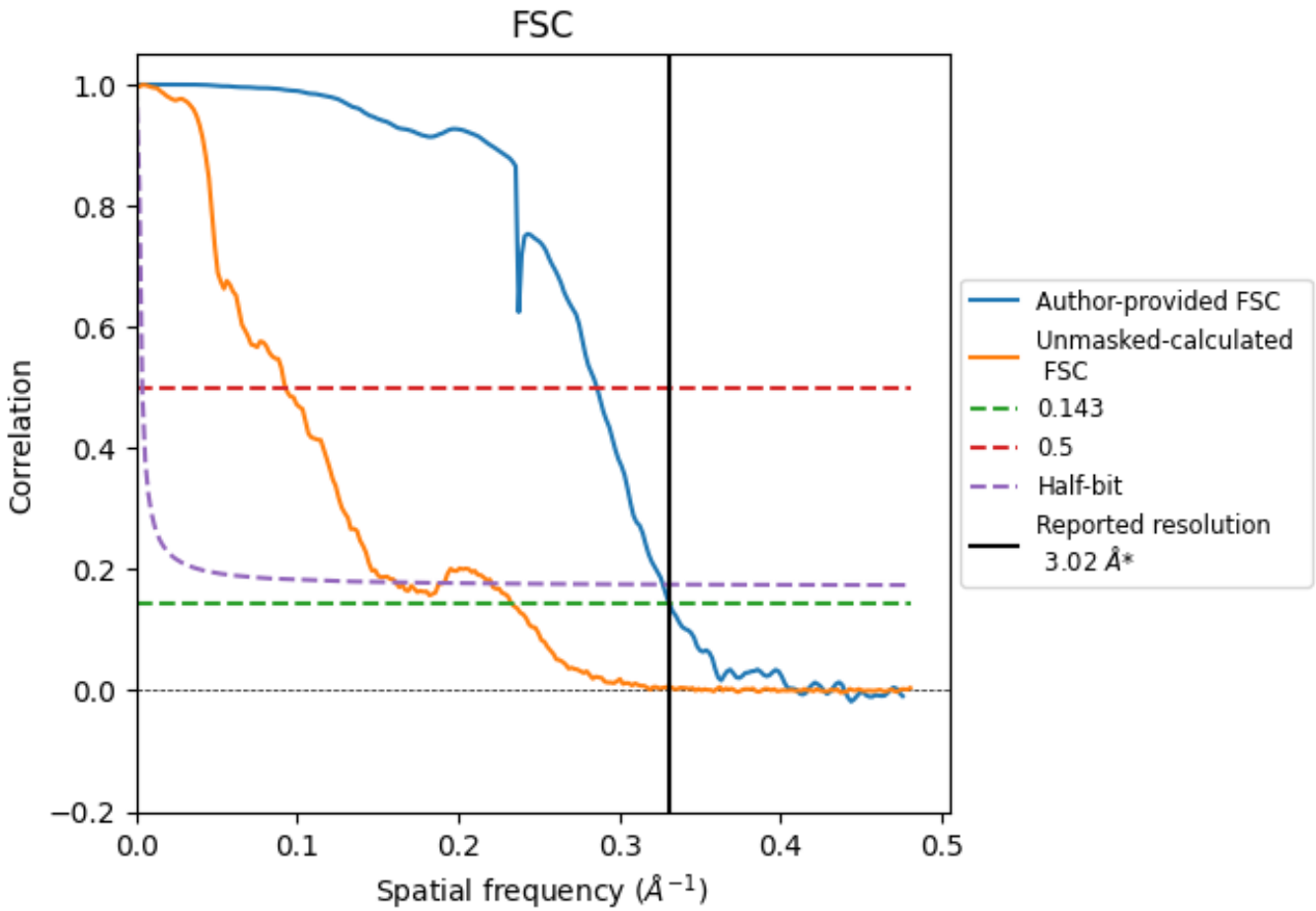


*Reported resolution corresponds to spatial frequency of 0.331 Å^{-1}

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 0.331 Å^{-1}

8.2 Resolution estimates (i)

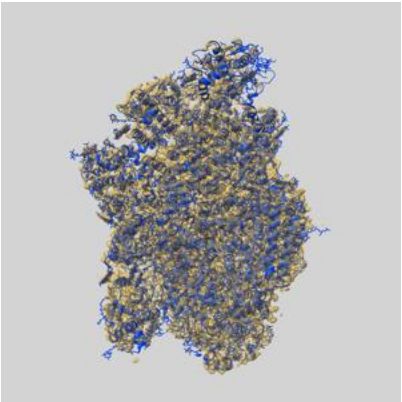
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.02	-	-
Author-provided FSC curve	3.02	3.49	3.06
Unmasked-calculated*	4.29	10.78	6.20

*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 4.29 differs from the reported value 3.02 by more than 10 %

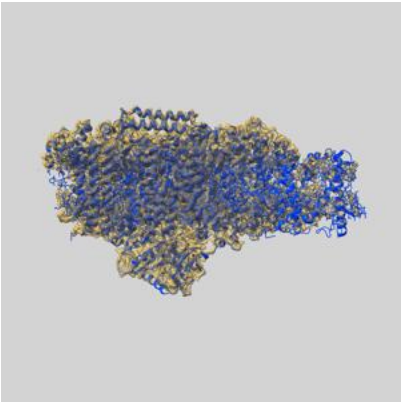
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-60290 and PDB model 8ZOE. Per-residue inclusion information can be found in section 3 on page 22.

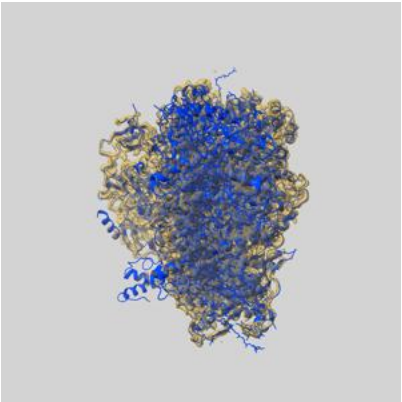
9.1 Map-model overlay (i)



X



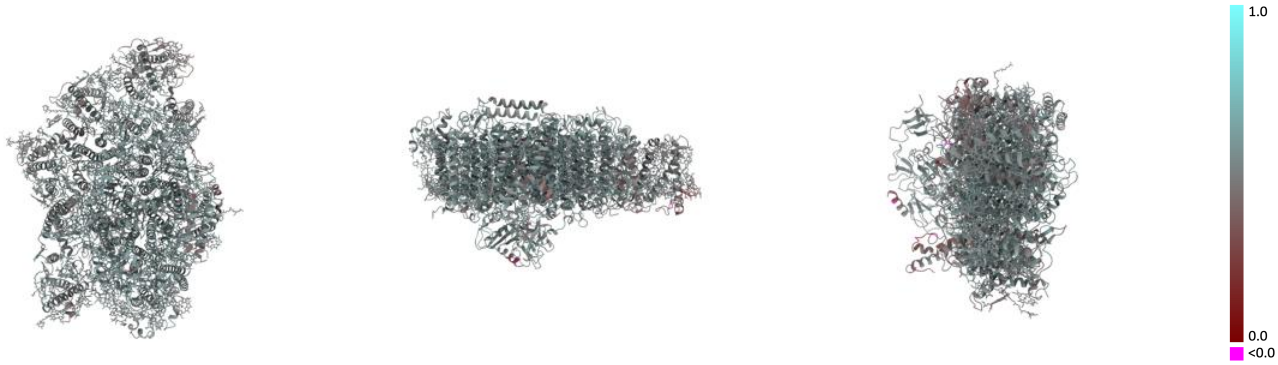
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.343 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

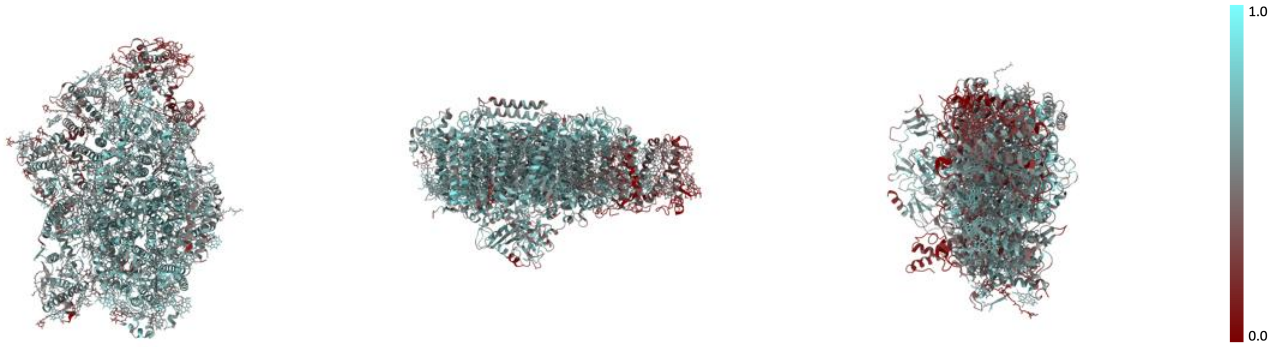
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

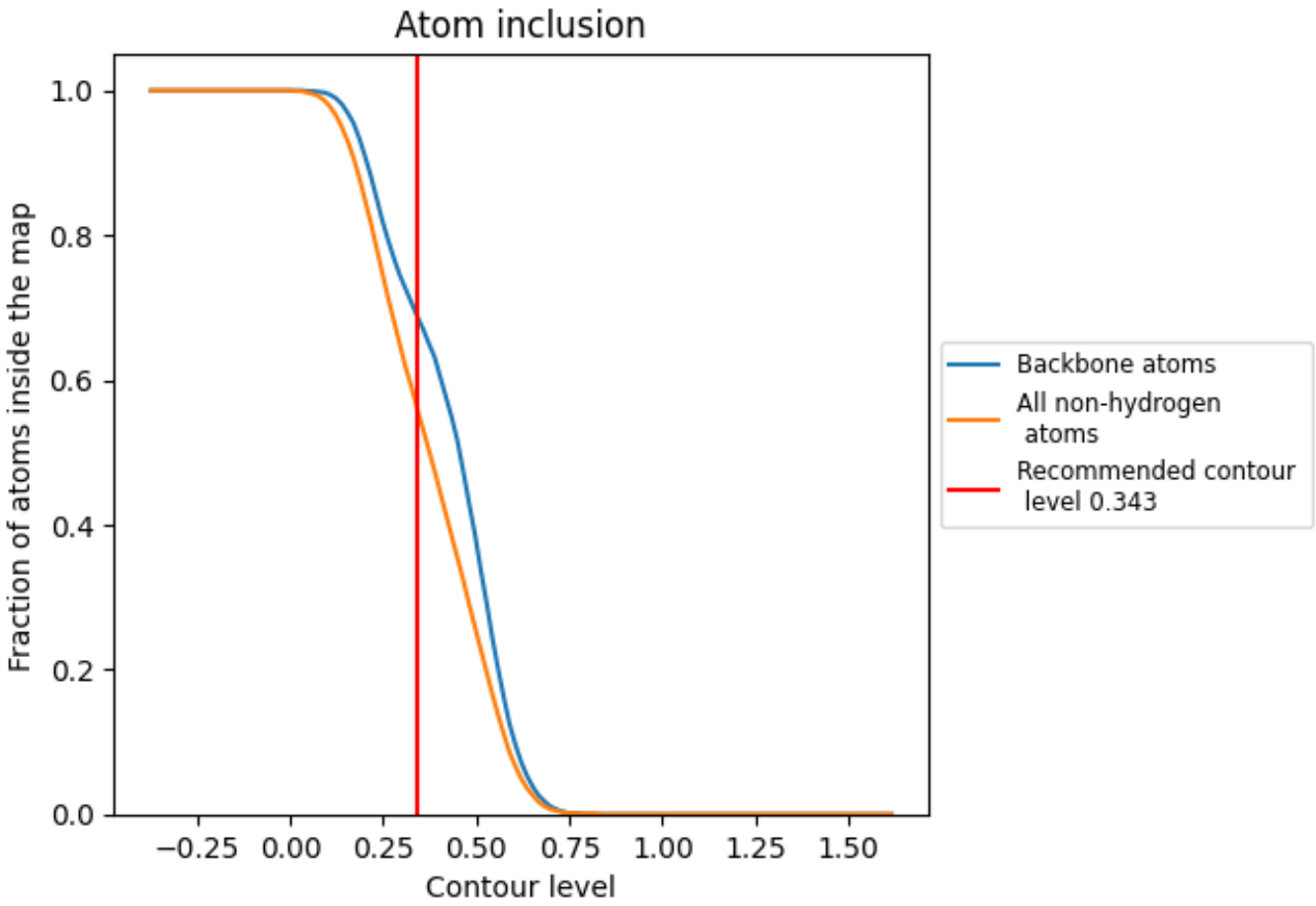
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.343).

9.4 Atom inclusion (i)



At the recommended contour level, 69% of all backbone atoms, 56% 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 (0.343) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5570	0.5290
1	0.5270	0.5130
7	0.2950	0.4690
8	0.4750	0.5070
9	0.4600	0.5090
a	0.6330	0.5490
b	0.6330	0.5530
c	0.6690	0.5330
d	0.5610	0.5350
e	0.5360	0.5270
f	0.5450	0.5040
g	0.3020	0.4240
h	0.2560	0.4810
i	0.5160	0.5240
j	0.5020	0.5350
l	0.5560	0.5060
m	0.5790	0.5080