wwPDB EM Validation Summary Report (i)

Sep 15, 2026 – 06:44 PM JST

PDB ID	:	9UH4 / pdb_00009uh4
EMDB ID	:	EMD-64154
Title	:	PSI-4 FCPI supercomplex from haptophyte Chrysotila roscoffensis
Authors	:	La Rocca, R.; Tsai, P.-C.; Kato, K.; Nakajima, Y.; Akita, F.; Shen, J.-R.
Deposited on	:	2025-04-14
Resolution	:	2.12 Å(reported)

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

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

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

The following versions of software and data (see references (1)) were used in the production of this report:

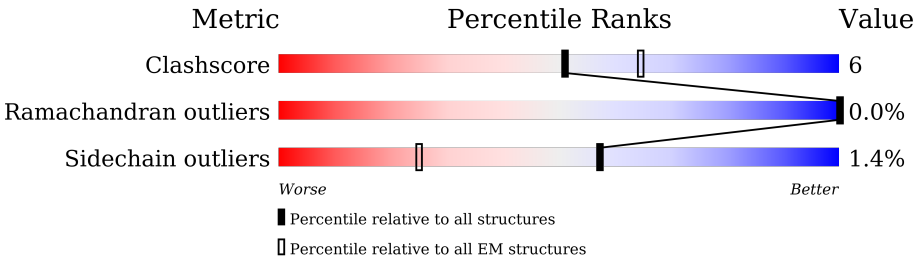
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using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

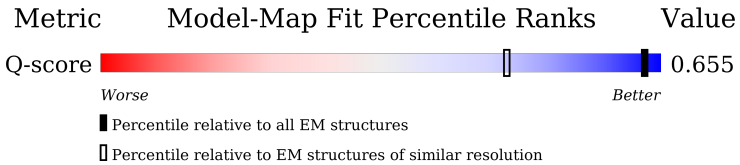
1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.12 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	2398 (1.64 - 2.62)

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

Mol	Chain	Length	Quality of chain
1	A	752	90% 8% •
2	B	734	92% 7%
3	C	81	95% • •
4	D	142	88% 9% •

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Mol	Chain	Length	Quality of chain
5	E	67	90% 6%
6	F	184	81% 6% 12%
7	I	35	83% 14%
8	J	39	74% 26%
9	L	141	87% 12%
10	M	29	97%
11	U	191	68% 6% 26%
12	G	209	57% 17% 24%
13	H	169	7% 72% 15% 12%
14	K	200	14% 40% 7% 52%
15	k	89	53% 8% 39%

2 Entry composition (i)

There are 28 unique types of molecules in this entry. The entry contains 31069 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	741	5813	3807	984	994	28	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	732	5805	3823	977	984	21	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	80	599	366	106	116	11	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	D	138	1092	697	188	204	3	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	E	64	494	314	86	93	1	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	F	161	1246	802	209	229	6	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	I	34	266	183	35	46	2	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	J	39	305	204	45	54	2	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	L	140	1056	693	168	194	1	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	M	29	216	144	34	37	1	0	0

- Molecule 11 is a protein called Fucoxanthin chlorophyll a/c binding protein I (FCPI-1).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	U	141	1082	692	183	198	9	0	0

- Molecule 12 is a protein called Fucoxanthin chlorophyll a/c binding protein VII (FCPI-7).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	G	158	1201	769	194	229	9	0	0

- Molecule 13 is a protein called Fucoxanthin chlorophyll a/c binding protein VIII (FCPI-8).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	H	149	1128	725	185	206	12	0	0

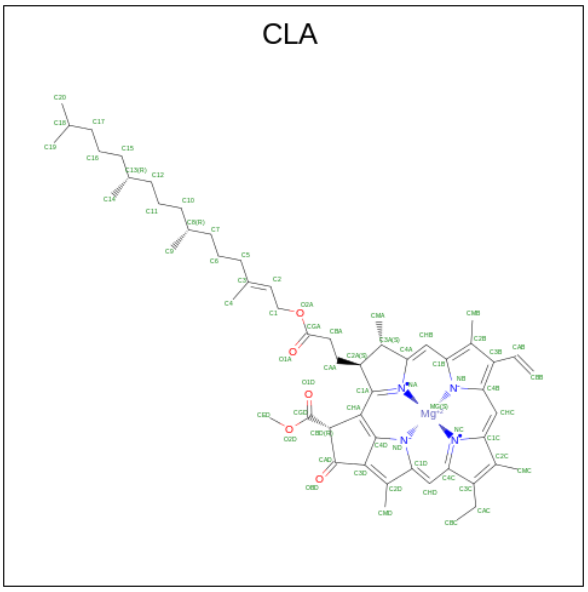
- Molecule 14 is a protein called Fucoxanthin chlorophyll a/c binding protein IX (FCPI-9).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	K	95	737	488	119	123	7	0	0

- Molecule 15 is a protein called Photosystem I reaction center subunit psaK.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
15	k	54	375	245	61	66	3	0	0

- Molecule 16 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	
16	A	1	65	55	1	4	5	0
16	A	1	55	45	1	4	5	0
16	A	1	65	55	1	4	5	0
16	A	1	65	55	1	4	5	0
16	A	1	49	39	1	4	5	0
16	A	1	65	55	1	4	5	0
16	A	1	55	45	1	4	5	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
16	A	1	56	46	1	4	5	0
			Total	C	Mg	N	O	
16	A	1	62	52	1	4	5	0
			Total	C	Mg	N	O	
16	A	1	54	44	1	4	5	0
			Total	C	Mg	N	O	
16	A	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
16	A	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
16	A	1	50	40	1	4	5	0
			Total	C	Mg	N	O	
16	A	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
16	A	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
16	A	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
16	A	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
16	A	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
16	A	1	43	35	1	4	3	0
			Total	C	Mg	N	O	
16	A	1	51	41	1	4	5	0
			Total	C	Mg	N	O	
16	A	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
16	A	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
16	A	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
16	A	1	62	52	1	4	5	0
			Total	C	Mg	N	O	
16	A	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
16	A	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
16	A	1	50	40	1	4	5	0
			Total	C	Mg	N	O	
16	A	1	65	55	1	4	5	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
16	A	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
16	A	1	50	40	1	4	5	0
			Total	C	Mg	N	O	
16	A	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
16	A	1	51	41	1	4	5	0
			Total	C	Mg	N	O	
16	A	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
16	A	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
16	A	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
16	A	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
16	A	1	52	42	1	4	5	0
			Total	C	Mg	N	O	
16	A	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
16	A	1	60	50	1	4	5	0
			Total	C	Mg	N	O	
16	A	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
16	A	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
16	A	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
16	A	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
16	B	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
16	B	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
16	B	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
16	B	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
16	B	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
16	B	1	65	55	1	4	5	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
16	B	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
16	B	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
16	B	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
16	B	1	54	44	1	4	5	0
			Total	C	Mg	N	O	
16	B	1	55	45	1	4	5	0
			Total	C	Mg	N	O	
16	B	1	54	44	1	4	5	0
			Total	C	Mg	N	O	
16	B	1	59	49	1	4	5	0
			Total	C	Mg	N	O	
16	B	1	55	45	1	4	5	0
			Total	C	Mg	N	O	
16	B	1	59	49	1	4	5	0
			Total	C	Mg	N	O	
16	B	1	60	50	1	4	5	0
			Total	C	Mg	N	O	
16	B	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
16	B	1	46	36	1	4	5	0
			Total	C	Mg	N	O	
16	B	1	53	43	1	4	5	0
			Total	C	Mg	N	O	
16	B	1	63	53	1	4	5	0
			Total	C	Mg	N	O	
16	B	1	55	45	1	4	5	0
			Total	C	Mg	N	O	
16	B	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
16	B	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
16	B	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
16	B	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
16	B	1	50	40	1	4	5	0
			Total	C	Mg	N	O	
16	B	1	49	39	1	4	5	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
16	B	1	58	48	1	4	5	0
			Total	C	Mg	N	O	
16	B	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
16	B	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
16	B	1	58	48	1	4	5	0
			Total	C	Mg	N	O	
16	B	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
16	B	1	47	37	1	4	5	0
			Total	C	Mg	N	O	
16	B	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
16	B	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
16	B	1	57	47	1	4	5	0
			Total	C	Mg	N	O	
16	B	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
16	B	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
16	B	1	52	42	1	4	5	0
			Total	C	Mg	N	O	
16	B	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
16	B	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
16	F	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
16	F	1	48	38	1	4	5	0
			Total	C	Mg	N	O	
16	F	1	46	36	1	4	5	0
			Total	C	Mg	N	O	
16	I	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
16	J	1	42	34	1	4	3	0
			Total	C	Mg	N	O	
16	L	1	49	39	1	4	5	0
			Total	C	Mg	N	O	
16	L	1	65	55	1	4	5	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
16	L	1	50	40	1	4	5	0
			Total	C	Mg	N	O	
16	U	1	61	51	1	4	5	0
			Total	C	Mg	N	O	
16	U	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
16	U	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
16	U	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
16	U	1	46	36	1	4	5	0
			Total	C	Mg	N	O	
16	U	1	42	34	1	4	3	0
			Total	C	Mg	N	O	
16	U	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
16	U	1	52	42	1	4	5	0
			Total	C	Mg	N	O	
16	G	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
16	G	1	41	33	1	4	3	0
			Total	C	Mg	N	O	
16	G	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
16	G	1	43	35	1	4	3	0
			Total	C	Mg	N	O	
16	G	1	61	51	1	4	5	0
			Total	C	Mg	N	O	
16	G	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
16	G	1	60	50	1	4	5	0
			Total	C	Mg	N	O	
16	G	1	55	45	1	4	5	0
			Total	C	Mg	N	O	
16	G	1	56	46	1	4	5	0
			Total	C	Mg	N	O	
16	G	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
16	G	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
16	H	1	40	32	1	4	3	0

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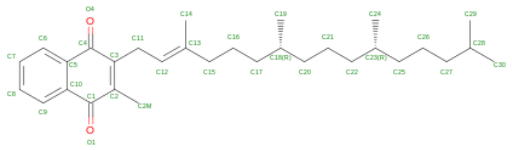
Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
16	H	1	60	50	1	4	5	0
			Total	C	Mg	N	O	
16	H	1	61	51	1	4	5	0
			Total	C	Mg	N	O	
16	H	1	44	35	1	4	4	0
			Total	C	Mg	N	O	
16	H	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
16	H	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
16	H	1	58	48	1	4	5	0
			Total	C	Mg	N	O	
16	H	1	41	33	1	4	3	0
			Total	C	Mg	N	O	
16	H	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
16	H	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
16	K	1	42	34	1	4	3	0
			Total	C	Mg	N	O	
16	K	1	55	45	1	4	5	0
			Total	C	Mg	N	O	
16	K	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
16	K	1	58	48	1	4	5	0
			Total	C	Mg	N	O	
16	K	1	40	32	1	4	3	0
			Total	C	Mg	N	O	
16	K	1	46	36	1	4	5	0
			Total	C	Mg	N	O	
16	k	1	42	34	1	4	3	0
			Total	C	Mg	N	O	
16	k	1	55	45	1	4	5	0

- Molecule 17 is PHYLLOQUINONE (CCD ID: PQN) (formula: $C_{31}H_{46}O_2$) (labeled as "Ligand of Interest" by depositor).

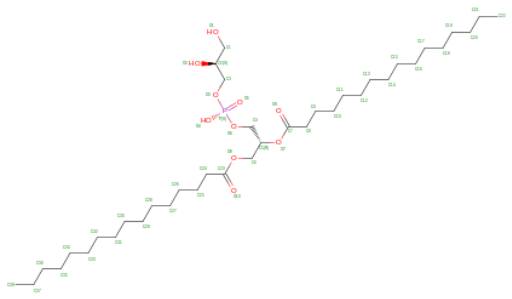
PQN



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

- Molecule 18 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: $C_{38}H_{75}O_{10}P$) (labeled as "Ligand of Interest" by depositor).

LHG



Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
18	A	1	48	37	10	1	0

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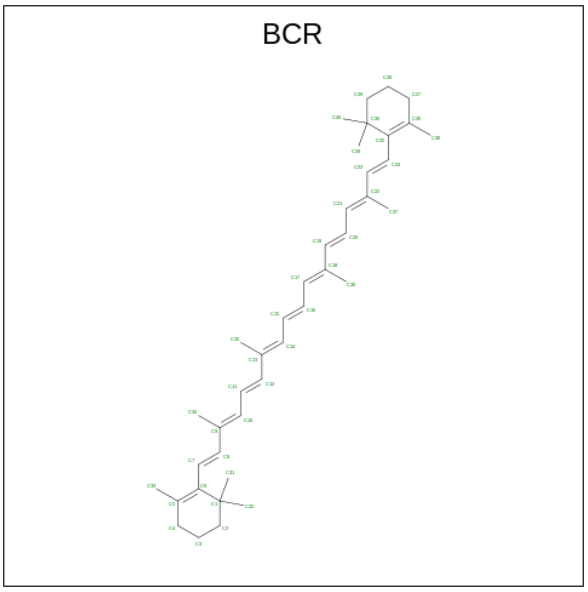
Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
18	A	1	27	16	10	1	0
18	G	1	27	16	10	1	0

- Molecule 19 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	
19	A	1	40	40	0
19	A	1	40	40	0
19	A	1	40	40	0
19	A	1	40	40	0
19	B	1	40	40	0
19	B	1	40	40	0
19	B	1	40	40	0
19	B	1	40	40	0
19	B	1	40	40	0

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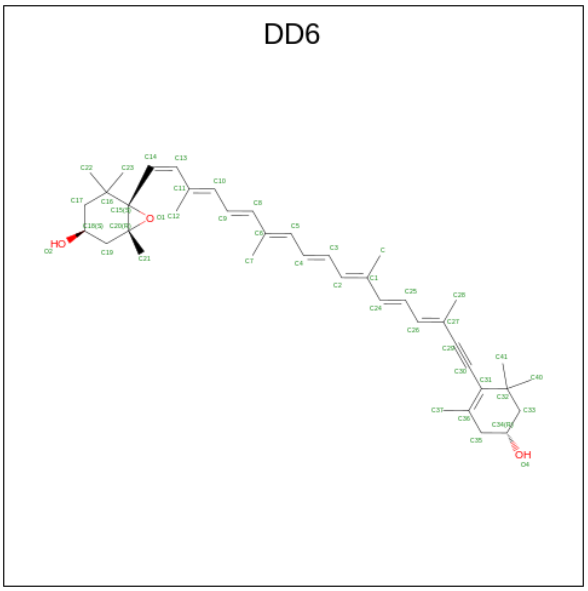
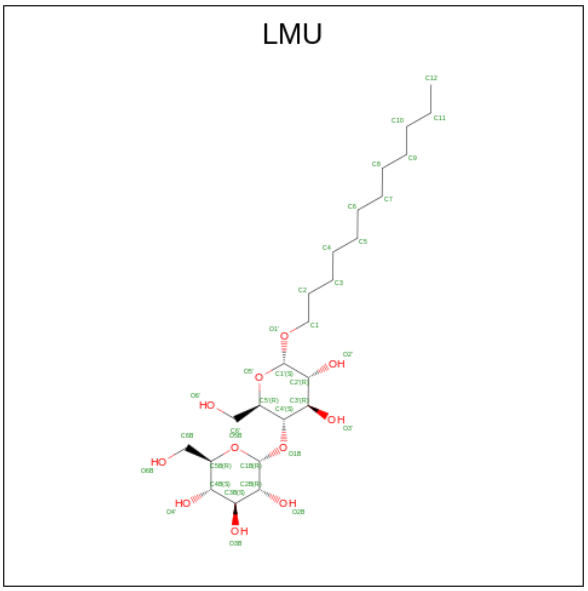
Mol	Chain	Residues	Atoms		AltConf
			Total	C	
19	B	1	39	39	0
			Total	C	
19	F	1	40	40	0
			Total	C	
19	F	1	40	40	0
			Total	C	
19	I	1	40	40	0
			Total	C	
19	I	1	40	40	0
			Total	C	
19	J	1	40	40	0
			Total	C	
19	L	1	40	40	0
			Total	C	
19	L	1	40	40	0
			Total	C	
19	M	1	40	40	0
			Total	C	
19	k	1	40	40	0

- Molecule 20 is (3S,3'R,5R,6S,7cis)-7',8'-didehydro-5,6-dihydro-5,6-epoxy-beta,beta-carotene-3,3'-diol (CCD ID: DD6) (formula: $C_{40}H_{54}O_3$) (labeled as "Ligand of Interest" by depositor).



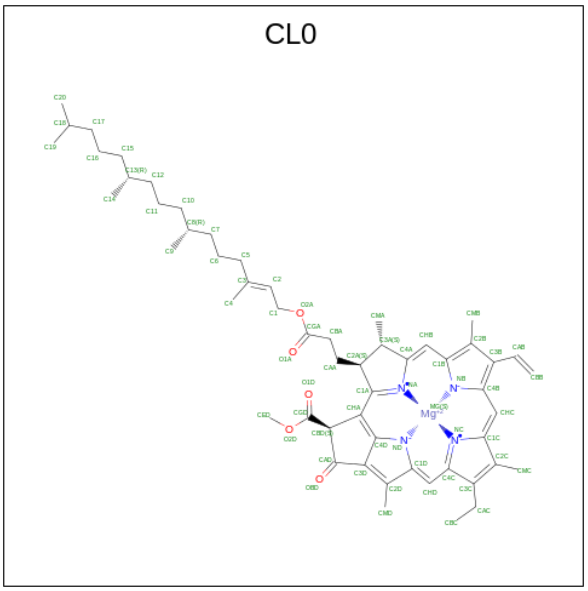
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
20	A	1	43	40	3	0
20	J	1	43	40	3	0
20	U	1	43	40	3	0
20	U	1	43	40	3	0
20	U	1	26	25	1	0
20	G	1	43	40	3	0
20	G	1	27	25	2	0
20	G	1	43	40	3	0
20	G	1	43	40	3	0
20	G	1	43	40	3	0
20	H	1	43	40	3	0
20	H	1	43	40	3	0
20	K	1	43	40	3	0

- Molecule 21 is DODECYL-ALPHA-D-MALTOSIDE (CCD ID: LMU) (formula: $C_{24}H_{46}O_{11}$) (labeled as "Ligand of Interest" by depositor).



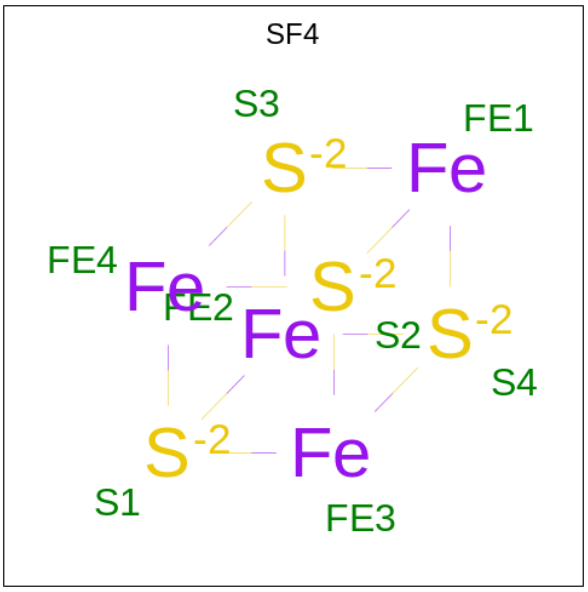
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
21	A	1	35	24	11	0
			Total	C	O	
21	A	1	35	24	11	0
			Total	C	O	
21	F	1	35	24	11	0
			Total	C	O	
21	J	1	35	24	11	0
			Total	C	O	
21	K	1	35	24	11	0

- Molecule 22 is CHLOROPHYLL A ISOMER (CCD ID: CL0) (formula: $C_{55}H_{72}MgN_4O_5$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 23 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	
23	A	1	8	4	4	0
23	C	1	8	4	4	0

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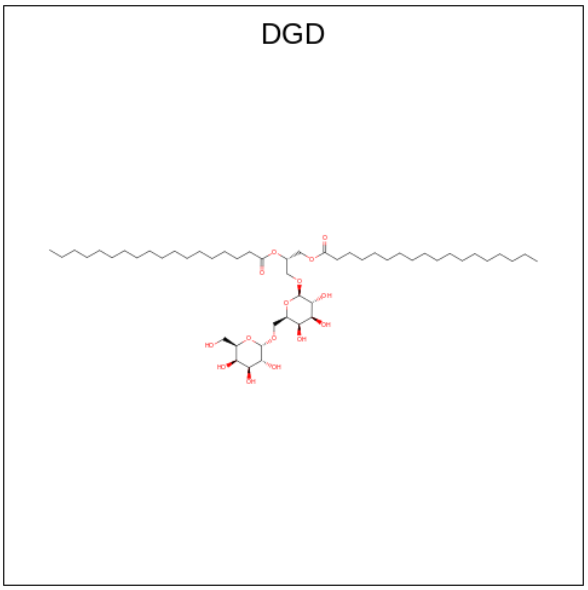
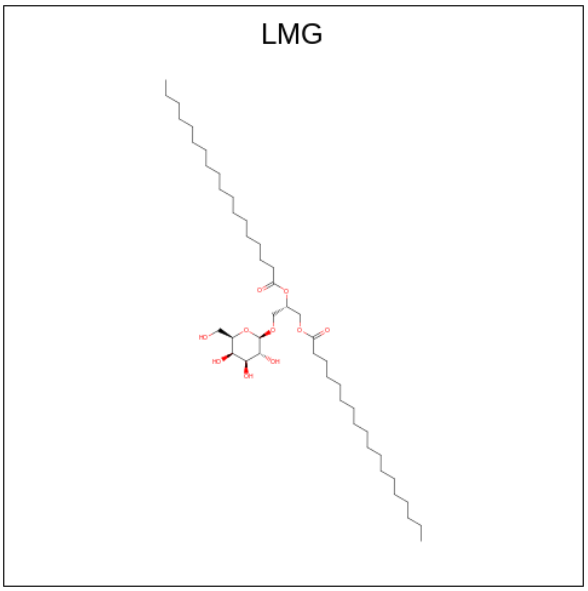
Mol	Chain	Residues	Atoms			AltConf
			Total	Fe	S	
23	C	1	8	4	4	0

- Molecule 24 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: $C_{51}H_{96}O_{15}$) (labeled as "Ligand of Interest" by depositor).



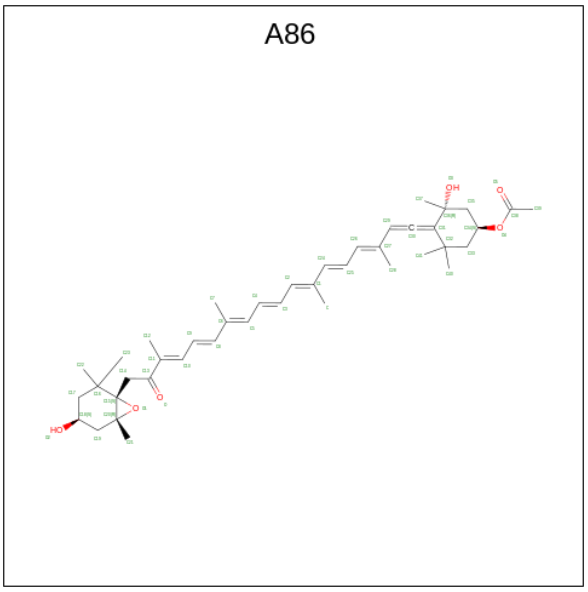
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
24	B	1	60	45	15	0

- Molecule 25 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$) (labeled as "Ligand of Interest" by depositor).



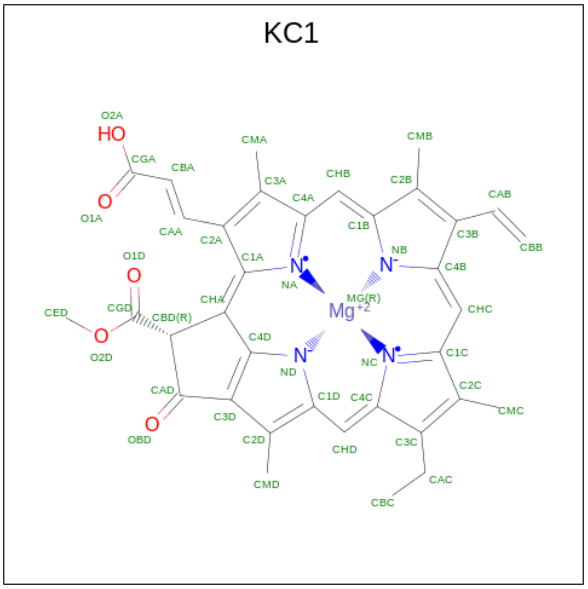
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
25	J	1	39	29	10	0
25	U	1	32	22	10	0

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



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

- Molecule 27 is Chlorophyll c1 (CCD ID: KC1) (formula: $C_{35}H_{30}MgN_4O_5$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
27	U	1	45	35	1	4	5	0

- Molecule 28 is water.

Mol	Chain	Residues	Atoms		AltConf
			Total	O	
28	A	132	132	132	0
28	B	146	146	146	0
28	C	32	32	32	0
28	D	19	19	19	0
28	E	8	8	8	0
28	F	24	24	24	0
28	J	1	1	1	0
28	L	14	14	14	0
28	M	1	1	1	0

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Mol	Chain	Residues	Atoms		AltConf
			Total	O	
28	U	3	3	3	0
			Total	O	
28	G	5	5	5	0
			Total	O	
28	H	1	1	1	0
			Total	O	
28	K	7	7	7	0
			Total	O	
28	k	2	2	2	0

3 Residue-property plots (i)

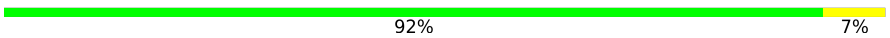
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

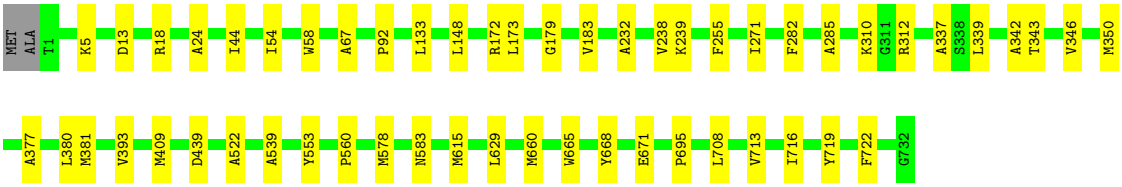
• Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1 (psaA)

Chain A:

• Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2 (psaB)

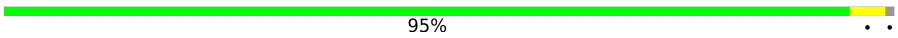
Chain B:





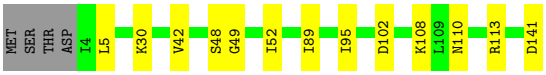
• Molecule 3: Photosystem I iron-sulfur center (psaC)

Chain C:



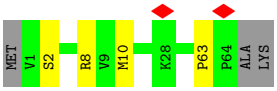
• Molecule 4: Photosystem I reaction center subunit II (psaD)

Chain D:



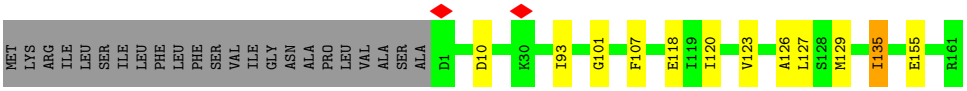
• Molecule 5: Photosystem I reaction center subunit IV (psaE)

Chain E: 90% 6%



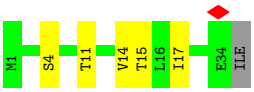
• Molecule 6: Photosystem I reaction center subunit III (psaF)

Chain F: 81% 6% 12%



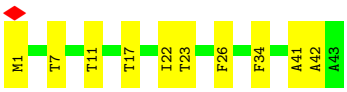
• Molecule 7: Photosystem I reaction center subunit VIII (psaI)

Chain I: 83% 14%



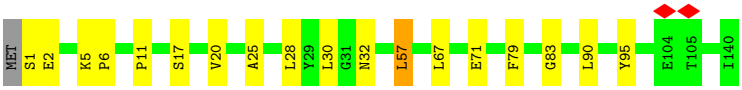
• Molecule 8: Photosystem I reaction center subunit IX (psaJ)

Chain J: 74% 26%



• Molecule 9: Photosystem I reaction center subunit XI (psaL)

Chain L: 87% 12%

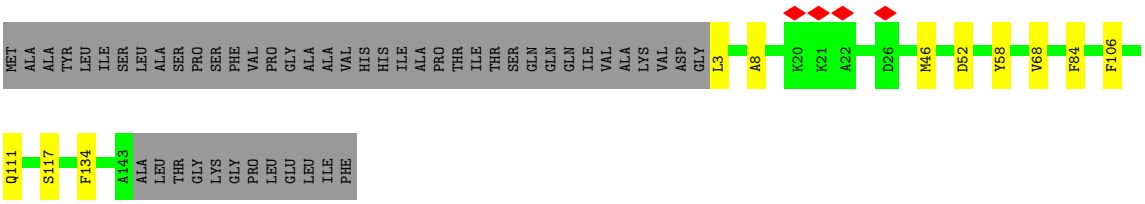


• Molecule 10: Photosystem I reaction center subunit XII (psaM)

Chain M: 97%

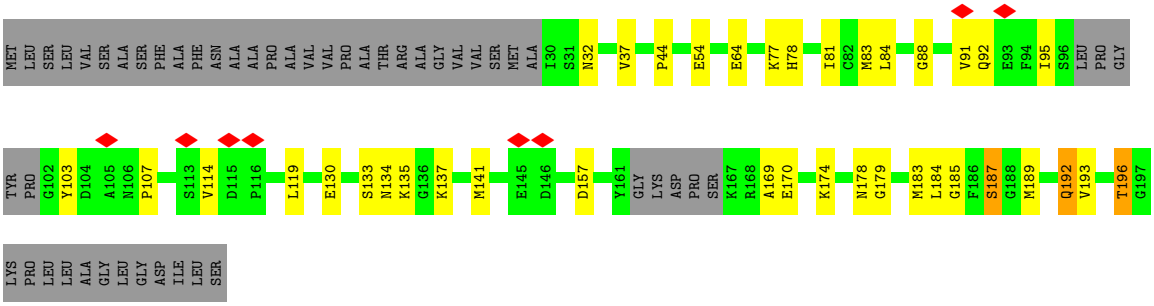
• Molecule 11: Fucoxanthin chlorophyll a/c binding protein I (FCPI-1)

Chain U: 68% 6% 26%



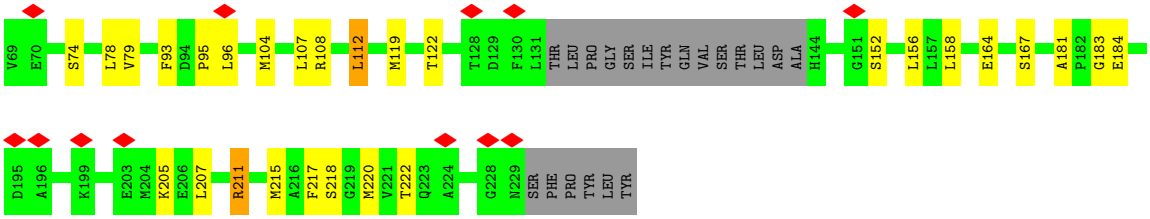
• Molecule 12: Fucoxanthin chlorophyll a/c binding protein VII (FCPI-7)

Chain G:



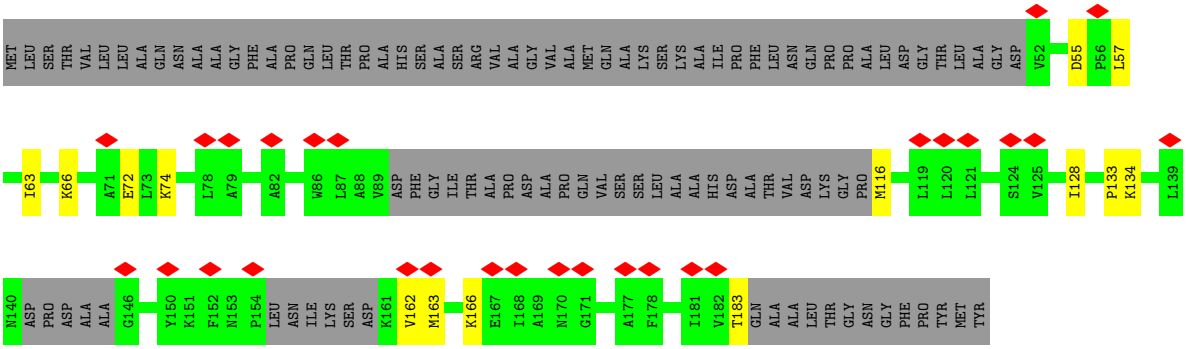
• Molecule 13: Fucoxanthin chlorophyll a/c binding protein VIII (FCPI-8)

Chain H:



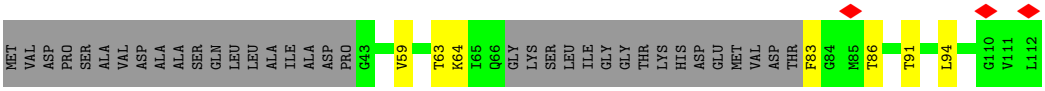
• Molecule 14: Fucoxanthin chlorophyll a/c binding protein IX (FCPI-9)

Chain K:



• Molecule 15: Photosystem I reaction center subunit psaK

Chain k:


MET
VAL
ASP
PRO
SER
ALA
VAL
ASP
ALA
ALA
SER
GLN
LEU
LEU
ALA
ILE
ALA
ASP
PRO
G43
V59
T63
K64
I65
Q66
GLY
LYS
SER
LEU
ILE
GLY
GLY
THR
LYS
HIS
ASP
GLU
MET
VAL
ASP
THR
F83
G84
M85
T86
T91
L94
G110
V111
L112

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	22619	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	165000	Depositor
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	0.576	Depositor
Minimum map value	-0.256	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.014	Depositor
Recommended contour level	0.065	Depositor
Map size (Å)	436.2, 436.2, 436.2	wwPDB
Map dimensions	600, 600, 600	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.727, 0.727, 0.727	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: LMU, DD6, LHG, A86, BCR, LMG, KC1, PQN, DGD, CLA, CL0, SF4

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
1	A	0.29	0/6007	0.48	1/8185 (0.0%)
2	B	0.30	0/6015	0.50	0/8205
3	C	0.18	0/609	0.41	0/826
4	D	0.30	0/1116	0.52	1/1503 (0.1%)
5	E	0.21	0/505	0.48	0/689
6	F	0.21	0/1275	0.44	0/1728
7	I	0.38	0/273	0.65	0/373
8	J	0.45	0/313	0.82	1/427 (0.2%)
9	L	0.21	0/1081	0.42	0/1470
10	M	0.24	0/218	0.52	0/295
11	U	0.28	0/1109	0.57	1/1499 (0.1%)
12	G	0.33	0/1226	0.70	1/1655 (0.1%)
13	H	0.32	0/1149	0.59	0/1546
14	K	0.33	0/752	0.63	0/1012
15	k	0.17	0/379	0.39	0/514
All	All	0.29	0/22027	0.52	5/29927 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
13	H	0	1

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	J	42	ALA	N-CA-C	-6.01	106.56	114.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	G	169	ALA	N-CA-C	-5.56	108.28	114.62
1	A	398	HIS	CA-CB-CG	-5.33	108.47	113.80
4	D	49	GLY	CA-C-O	-5.18	118.85	122.22
11	U	68	VAL	N-CA-C	-5.13	107.83	112.96

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
13	H	211	ARG	Sidechain

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5813	0	5695	47	0
2	B	5805	0	5634	45	0
3	C	599	0	577	2	0
4	D	1092	0	1093	6	0
5	E	494	0	488	2	0
6	F	1246	0	1256	11	0
7	I	266	0	278	3	0
8	J	305	0	310	10	0
9	L	1056	0	1068	17	0
10	M	216	0	234	0	0
11	U	1082	0	1055	8	0
12	G	1201	0	1185	24	0
13	H	1128	0	1131	20	0
14	K	737	0	764	7	0
15	k	375	0	403	5	0
16	A	2540	0	2556	68	0
16	B	2439	0	2456	68	0
16	F	159	0	141	3	0
16	G	561	0	486	16	0
16	H	524	0	475	22	0
16	I	65	0	72	2	0
16	J	42	0	31	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
16	K	286	0	229	8	0
16	L	164	0	150	4	0
16	U	441	0	417	12	0
16	k	97	0	80	3	0
17	A	33	0	46	3	0
17	B	33	0	46	1	0
18	A	75	0	93	2	0
18	G	27	0	24	2	0
19	A	160	0	224	6	0
19	B	239	0	333	16	0
19	F	80	0	112	0	0
19	I	80	0	112	3	0
19	J	40	0	56	2	0
19	L	80	0	112	3	0
19	M	40	0	56	3	0
19	k	40	0	56	3	0
20	A	43	0	0	0	0
20	G	199	0	0	1	0
20	H	86	0	0	0	0
20	J	43	0	0	0	0
20	K	43	0	0	0	0
20	U	112	0	0	0	0
21	A	70	0	92	2	0
21	F	35	0	46	0	0
21	J	35	0	46	3	0
21	K	35	0	46	0	0
22	A	65	0	72	2	0
23	A	8	0	0	0	0
23	C	16	0	0	0	0
24	B	60	0	81	2	0
25	J	39	0	48	2	0
25	U	32	0	34	2	0
26	U	48	0	0	1	0
27	U	45	0	0	0	0
28	A	132	0	0	2	0
28	B	146	0	0	0	0
28	C	32	0	0	0	0
28	D	19	0	0	0	0
28	E	8	0	0	0	0
28	F	24	0	0	0	0
28	G	5	0	0	0	0
28	H	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
28	J	1	0	0	0	0
28	K	7	0	0	0	0
28	L	14	0	0	0	0
28	M	1	0	0	0	0
28	U	3	0	0	1	0
28	k	2	0	0	0	0
All	All	31069	0	29999	335	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 6.

The worst 5 of 335 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)
13:H:122:THR:HA	13:H:220:MET:HE1	1.57	0.86
13:H:112:LEU:HD12	13:H:183:GLY:HA3	1.63	0.81
7:I:17:ILE:HD11	16:I:102:CLA:HAB	1.69	0.75
16:A:822:CLA:H91	19:A:844:BCR:H23C	1.70	0.74
16:A:803:CLA:H72	19:A:842:BCR:HC8	1.71	0.72

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	739/752 (98%)	723 (98%)	16 (2%)	0	100	100
2	B	730/734 (100%)	713 (98%)	17 (2%)	0	100	100
3	C	78/81 (96%)	77 (99%)	1 (1%)	0	100	100
4	D	136/142 (96%)	131 (96%)	4 (3%)	1 (1%)	18	15
5	E	62/67 (92%)	60 (97%)	2 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	F	159/184 (86%)	157 (99%)	2 (1%)	0	100	100
7	I	32/35 (91%)	30 (94%)	2 (6%)	0	100	100
8	J	37/39 (95%)	37 (100%)	0	0	100	100
9	L	138/141 (98%)	136 (99%)	2 (1%)	0	100	100
10	M	27/29 (93%)	27 (100%)	0	0	100	100
11	U	139/191 (73%)	135 (97%)	4 (3%)	0	100	100
12	G	152/209 (73%)	142 (93%)	10 (7%)	0	100	100
13	H	145/169 (86%)	143 (99%)	2 (1%)	0	100	100
14	K	87/200 (44%)	85 (98%)	2 (2%)	0	100	100
15	k	50/89 (56%)	50 (100%)	0	0	100	100
All	All	2711/3062 (88%)	2646 (98%)	64 (2%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	D	48	SER

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	603/612 (98%)	601 (100%)	2 (0%)	86	91
2	B	590/591 (100%)	589 (100%)	1 (0%)	87	92
3	C	68/69 (99%)	68 (100%)	0	100	100
4	D	118/122 (97%)	118 (100%)	0	100	100
5	E	53/55 (96%)	52 (98%)	1 (2%)	50	57
6	F	133/152 (88%)	131 (98%)	2 (2%)	57	65
7	I	31/32 (97%)	30 (97%)	1 (3%)	34	37
8	J	32/32 (100%)	32 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
9	L	111/112 (99%)	109 (98%)	2 (2%)	51	59
10	M	21/21 (100%)	20 (95%)	1 (5%)	23	22
11	U	110/148 (74%)	108 (98%)	2 (2%)	51	59
12	G	130/167 (78%)	125 (96%)	5 (4%)	29	30
13	H	119/137 (87%)	112 (94%)	7 (6%)	18	15
14	K	77/153 (50%)	70 (91%)	7 (9%)	9	6
15	k	38/65 (58%)	38 (100%)	0	100	100
All	All	2234/2468 (90%)	2203 (99%)	31 (1%)	57	67

5 of 31 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
12	G	187	SER
14	K	72	GLU
13	H	74	SER
14	K	134	LYS
14	K	57	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 20 such sidechains are listed below:

Mol	Chain	Res	Type
9	L	32	ASN
12	G	178	ASN
13	H	229	ASN
13	H	172	GLN
2	B	227	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)

180 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	$\#\|Z\| > 2$
16	CLA	A	851	1	69,73,73	1.21	7 (10%)	83,113,113	0.93	4 (4%)
16	CLA	A	801	-	69,73,73	1.17	8 (11%)	83,113,113	0.92	4 (4%)
16	CLA	B	816	2	64,68,73	1.25	7 (10%)	77,107,113	0.97	4 (5%)
16	CLA	A	812	1	49,53,73	1.44	7 (14%)	59,89,113	1.25	7 (11%)
16	CLA	A	827	1	54,58,73	1.41	7 (12%)	65,95,113	1.00	4 (6%)
16	CLA	G	306	12	69,73,73	1.26	7 (10%)	83,113,113	0.89	3 (3%)
16	CLA	A	854	1	69,73,73	1.18	7 (10%)	83,113,113	0.94	5 (6%)
16	CLA	I	102	-	69,73,73	1.17	7 (10%)	83,113,113	1.02	4 (4%)
16	CLA	L	203	9	69,73,73	1.15	7 (10%)	83,113,113	0.93	4 (4%)
16	CLA	H	308	13	45,49,73	1.42	6 (13%)	54,84,113	1.30	6 (11%)
16	CLA	B	808	2	69,73,73	1.25	7 (10%)	83,113,113	0.90	3 (3%)
16	CLA	A	803	1	69,73,73	1.16	7 (10%)	83,113,113	0.99	4 (4%)
16	CLA	B	845	2	69,73,73	1.23	7 (10%)	83,113,113	0.90	3 (3%)
20	DD6	H	311	-	39,45,45	1.59	7 (17%)	52,67,67	1.56	9 (17%)
16	CLA	K	202	14	46,50,73	1.42	8 (17%)	55,85,113	1.08	4 (7%)
16	CLA	H	309	13	49,53,73	1.42	7 (14%)	59,89,113	1.18	5 (8%)
16	CLA	A	806	1	69,73,73	1.17	7 (10%)	83,113,113	1.06	6 (7%)
16	CLA	B	804	2	49,53,73	1.46	8 (16%)	59,89,113	1.09	4 (6%)
20	DD6	G	313	-	39,45,45	1.62	8 (20%)	52,67,67	1.58	8 (15%)
16	CLA	H	304	13	48,52,73	1.39	8 (16%)	56,87,113	1.18	5 (8%)
16	CLA	B	817	28	69,73,73	1.20	7 (10%)	83,113,113	1.06	7 (8%)
16	CLA	B	803	-	69,73,73	1.18	7 (10%)	83,113,113	0.96	4 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
16	CLA	H	305	13	49,53,73	1.51	7 (14%)	59,89,113	0.98	3 (5%)
16	CLA	A	830	1	54,58,73	1.35	7 (12%)	65,95,113	1.01	3 (4%)
19	BCR	L	201	-	41,41,41	1.10	2 (4%)	56,56,56	1.18	4 (7%)
16	CLA	F	803	28	52,56,73	1.38	8 (15%)	62,92,113	1.18	5 (8%)
21	LMU	A	848	-	36,36,36	0.50	1 (2%)	47,47,47	0.98	2 (4%)
16	CLA	A	834	1	69,73,73	1.28	7 (10%)	83,113,113	0.95	4 (4%)
19	BCR	B	842	-	41,41,41	1.08	2 (4%)	56,56,56	1.16	4 (7%)
16	CLA	H	306	13	69,73,73	1.22	8 (11%)	83,113,113	1.15	7 (8%)
16	CLA	B	809	2	69,73,73	1.20	9 (13%)	83,113,113	0.94	4 (4%)
16	CLA	B	824	2	69,73,73	1.22	7 (10%)	83,113,113	1.01	5 (6%)
16	CLA	A	853	1	69,73,73	1.16	7 (10%)	83,113,113	0.95	4 (4%)
16	CLA	A	817	1	49,53,73	1.42	7 (14%)	59,89,113	1.21	6 (10%)
16	CLA	A	810	1	58,62,73	1.29	8 (13%)	69,99,113	1.07	5 (7%)
16	CLA	G	302	-	45,49,73	1.49	8 (17%)	54,84,113	1.05	4 (7%)
16	CLA	K	205	14	62,66,73	1.22	7 (11%)	74,104,113	1.30	7 (9%)
21	LMU	A	855	-	36,36,36	0.54	1 (2%)	47,47,47	0.96	1 (2%)
19	BCR	B	840	-	41,41,41	1.05	2 (4%)	56,56,56	1.23	6 (10%)
16	CLA	B	830	28	49,53,73	1.43	8 (16%)	59,89,113	1.19	5 (8%)
16	CLA	A	818	28	69,73,73	1.18	7 (10%)	83,113,113	0.92	4 (4%)
19	BCR	A	842	-	41,41,41	1.08	2 (4%)	56,56,56	1.15	4 (7%)
16	CLA	B	822	2	69,73,73	1.27	7 (10%)	83,113,113	0.98	5 (6%)
23	SF4	C	101	3	0,12,12	-	-	-		
16	CLA	B	814	2	59,63,73	1.35	7 (11%)	71,101,113	1.10	4 (5%)
16	CLA	G	305	12	65,69,73	1.19	6 (9%)	78,108,113	1.13	7 (8%)
16	CLA	K	206	28	43,48,73	1.52	8 (18%)	52,82,113	1.19	4 (7%)
19	BCR	L	205	-	41,41,41	1.05	2 (4%)	56,56,56	1.24	6 (10%)
21	LMU	K	201	-	36,36,36	1.18	2 (5%)	47,47,47	1.37	6 (12%)
16	CLA	A	816	1	69,73,73	1.18	7 (10%)	83,113,113	0.99	4 (4%)
16	CLA	A	811	1	69,73,73	1.21	7 (10%)	83,113,113	0.93	3 (3%)
23	SF4	A	852	1,2	0,12,12	-	-	-		
25	LMG	J	103	-	39,39,55	0.87	1 (2%)	47,47,63	1.27	3 (6%)
16	CLA	A	845	28	69,73,73	1.17	7 (10%)	83,113,113	0.94	3 (3%)
16	CLA	G	304	12	47,51,73	1.39	6 (12%)	56,86,113	1.20	4 (7%)
19	BCR	J	105	-	41,41,41	1.06	2 (4%)	56,56,56	1.21	4 (7%)
16	CLA	A	831	1	49,53,73	1.39	5 (10%)	59,89,113	1.21	5 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
19	BCR	F	801	-	41,41,41	1.05	2 (4%)	56,56,56	1.21	3 (5%)
16	CLA	B	805	2	69,73,73	1.17	7 (10%)	83,113,113	0.95	4 (4%)
16	CLA	H	307	-	62,66,73	1.22	8 (12%)	74,104,113	1.00	4 (5%)
16	CLA	A	824	1	66,70,73	1.22	7 (10%)	79,109,113	1.06	5 (6%)
16	CLA	B	835	2	69,73,73	1.25	8 (11%)	83,113,113	1.02	4 (4%)
16	CLA	A	805	1	53,57,73	1.40	7 (13%)	62,93,113	1.05	4 (6%)
16	CLA	B	807	2	69,73,73	1.20	7 (10%)	83,113,113	0.95	3 (3%)
16	CLA	B	833	2	51,55,73	1.41	7 (13%)	61,91,113	1.06	5 (8%)
17	PQN	A	837	-	34,34,34	0.39	0	42,45,45	0.41	0
16	CLA	U	206	11	49,53,73	1.40	7 (14%)	59,89,113	1.07	4 (6%)
16	CLA	A	828	1	69,73,73	1.24	7 (10%)	83,113,113	0.93	3 (3%)
20	DD6	K	208	-	39,45,45	1.60	7 (17%)	52,67,67	1.63	9 (17%)
20	DD6	G	311	-	39,45,45	1.55	8 (20%)	52,67,67	1.51	7 (13%)
19	BCR	A	843	-	41,41,41	1.09	2 (4%)	56,56,56	1.21	4 (7%)
16	CLA	H	303	13	65,69,73	1.22	5 (7%)	78,108,113	1.12	5 (6%)
20	DD6	U	212	-	39,45,45	1.61	6 (15%)	52,67,67	1.80	14 (26%)
16	CLA	G	301	12	49,53,73	1.40	6 (12%)	59,89,113	1.13	5 (8%)
20	DD6	G	312	-	24,28,45	1.78	6 (25%)	32,42,67	1.68	5 (15%)
18	LHG	A	840	16	26,26,48	0.83	0	29,32,54	1.33	3 (10%)
18	LHG	A	839	-	47,47,48	0.63	1 (2%)	50,53,54	1.25	6 (12%)
16	CLA	A	835	1	69,73,73	1.21	7 (10%)	83,113,113	0.98	4 (4%)
16	CLA	B	832	2	69,73,73	1.19	7 (10%)	83,113,113	0.94	3 (3%)
20	DD6	H	310	-	39,45,45	1.64	6 (15%)	52,67,67	1.67	10 (19%)
16	CLA	A	814	28	49,53,73	1.42	7 (14%)	59,89,113	1.14	5 (8%)
16	CLA	A	819	1	47,51,73	1.45	7 (14%)	56,86,113	1.11	4 (7%)
27	KC1	U	213	11	49,53,53	1.74	12 (24%)	63,89,89	1.02	4 (6%)
16	CLA	B	844	2	69,73,73	1.23	7 (10%)	83,113,113	0.92	3 (3%)
19	BCR	B	846	-	40,40,41	1.06	2 (5%)	54,54,56	1.31	8 (14%)
16	CLA	G	309	-	60,64,73	1.25	7 (11%)	72,102,113	1.09	6 (8%)
19	BCR	A	841	-	41,41,41	1.02	2 (4%)	56,56,56	1.23	3 (5%)
19	BCR	B	841	-	41,41,41	1.08	2 (4%)	56,56,56	1.27	5 (8%)
19	BCR	I	101	-	41,41,41	1.07	2 (4%)	56,56,56	1.25	4 (7%)
16	CLA	B	819	2	57,61,73	1.27	8 (14%)	68,98,113	1.04	5 (7%)
16	CLA	K	207	-	50,54,73	1.36	7 (14%)	60,90,113	1.10	4 (6%)
19	BCR	B	838	-	41,41,41	1.07	2 (4%)	56,56,56	1.17	6 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
16	CLA	A	820	1	55,59,73	1.38	8 (14%)	66,96,113	1.16	4 (6%)
24	DGD	B	843	-	61,61,67	0.92	2 (3%)	75,75,81	1.11	6 (8%)
16	CLA	L	202	9	53,57,73	1.37	8 (15%)	62,93,113	1.15	5 (8%)
16	CLA	B	823	2	69,73,73	1.24	8 (11%)	83,113,113	0.97	4 (4%)
16	CLA	U	210	11	69,73,73	1.16	5 (7%)	83,113,113	0.99	5 (6%)
16	CLA	K	203	14	59,63,73	1.26	7 (11%)	71,101,113	1.08	5 (7%)
16	CLA	B	820	28	67,71,73	1.22	8 (11%)	80,110,113	1.04	6 (7%)
16	CLA	B	801	28	69,73,73	1.19	7 (10%)	83,113,113	0.96	3 (3%)
20	DD6	U	214	-	24,26,45	1.84	5 (20%)	30,35,67	1.58	5 (16%)
26	A86	U	202	-	44,50,50	1.65	6 (13%)	51,76,76	1.52	8 (15%)
16	CLA	B	847	2	56,60,73	1.28	6 (10%)	67,97,113	1.07	4 (5%)
25	LMG	U	201	-	32,32,55	0.95	0	40,40,63	1.21	5 (12%)
16	CLA	U	205	11	69,73,73	1.20	7 (10%)	83,113,113	1.02	4 (4%)
16	CLA	A	826	1	69,73,73	1.30	8 (11%)	83,113,113	0.84	3 (3%)
16	CLA	F	804	6	50,54,73	1.39	7 (14%)	60,90,113	1.15	5 (8%)
16	CLA	A	802	1	59,63,73	1.26	7 (11%)	71,101,113	1.00	4 (5%)
16	CLA	B	825	2	69,73,73	1.26	7 (10%)	83,113,113	0.90	3 (3%)
21	LMU	F	806	-	36,36,36	1.20	2 (5%)	47,47,47	0.96	2 (4%)
16	CLA	H	301	-	43,48,73	1.48	6 (13%)	52,82,113	1.30	6 (11%)
19	BCR	F	805	-	41,41,41	1.03	2 (4%)	56,56,56	1.23	6 (10%)
16	CLA	A	823	1	69,73,73	1.27	8 (11%)	83,113,113	0.90	4 (4%)
16	CLA	U	207	-	69,73,73	1.14	6 (8%)	83,113,113	1.11	7 (8%)
16	CLA	L	204	28	54,58,73	1.36	8 (14%)	65,95,113	1.14	5 (7%)
16	CLA	U	209	-	46,50,73	1.40	6 (13%)	55,85,113	1.19	6 (10%)
16	CLA	H	302	13	64,68,73	1.26	8 (12%)	77,107,113	1.09	5 (6%)
16	CLA	F	802	28	69,73,73	1.20	7 (10%)	83,113,113	1.01	5 (6%)
16	CLA	B	811	2	59,63,73	1.27	6 (10%)	71,101,113	1.04	4 (5%)
20	DD6	A	846	-	39,45,45	1.55	8 (20%)	52,67,67	1.47	8 (15%)
16	CLA	A	809	1	66,70,73	1.25	7 (10%)	79,109,113	0.90	3 (3%)
16	CLA	B	848	2	69,73,73	1.28	8 (11%)	83,113,113	1.05	5 (6%)
20	DD6	U	203	-	39,45,45	1.63	6 (15%)	52,67,67	1.74	13 (25%)
16	CLA	A	836	28	69,73,73	1.17	7 (10%)	83,113,113	1.00	4 (4%)
16	CLA	A	815	1	69,73,73	1.22	7 (10%)	83,113,113	1.00	5 (6%)
16	CLA	k	202	28	59,63,73	1.32	8 (13%)	71,101,113	1.00	5 (7%)
16	CLA	A	813	1	54,58,73	1.39	7 (12%)	65,95,113	1.11	5 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
19	BCR	I	103	-	41,41,41	1.08	2 (4%)	56,56,56	1.21	4 (7%)
16	CLA	G	315	12	49,53,73	1.35	6 (12%)	59,89,113	1.33	7 (11%)
16	CLA	A	832	1	55,59,73	1.36	8 (14%)	66,96,113	1.07	4 (6%)
16	CLA	B	834	28	69,73,73	1.20	7 (10%)	83,113,113	1.02	6 (7%)
16	CLA	A	833	1	69,73,73	1.22	7 (10%)	83,113,113	0.98	5 (6%)
16	CLA	A	804	1	69,73,73	1.18	8 (11%)	83,113,113	0.95	4 (4%)
16	CLA	B	849	2	69,73,73	1.19	7 (10%)	83,113,113	1.03	6 (7%)
16	CLA	J	104	8	46,50,73	1.43	7 (15%)	55,85,113	1.11	4 (7%)
16	CLA	U	211	11	56,60,73	1.37	8 (14%)	67,97,113	1.09	6 (8%)
19	BCR	A	844	-	41,41,41	1.09	2 (4%)	56,56,56	1.23	5 (8%)
16	CLA	A	829	1	69,73,73	1.21	7 (10%)	83,113,113	0.93	3 (3%)
19	BCR	k	203	-	41,41,41	1.10	2 (4%)	56,56,56	1.34	9 (16%)
20	DD6	J	102	-	39,45,45	1.59	8 (20%)	52,67,67	1.67	9 (17%)
16	CLA	U	208	11	50,54,73	1.36	7 (14%)	60,90,113	1.20	6 (10%)
16	CLA	B	821	28	59,63,73	1.23	6 (10%)	71,101,113	1.00	4 (5%)
16	CLA	A	838	18	56,60,73	1.30	8 (14%)	67,97,113	1.13	5 (7%)
20	DD6	G	314	-	39,45,45	1.56	8 (20%)	52,67,67	1.57	9 (17%)
16	CLA	B	806	2	69,73,73	1.21	7 (10%)	83,113,113	0.94	4 (4%)
19	BCR	B	839	-	41,41,41	1.06	2 (4%)	56,56,56	1.23	5 (8%)
19	BCR	M	101	-	41,41,41	1.05	2 (4%)	56,56,56	1.26	5 (8%)
16	CLA	B	836	-	61,65,73	1.27	7 (11%)	73,103,113	1.09	6 (8%)
16	CLA	B	815	2	63,67,73	1.23	7 (11%)	75,105,113	0.99	4 (5%)
16	CLA	A	807	1	59,63,73	1.29	8 (13%)	71,101,113	1.11	6 (8%)
16	CLA	B	828	2	62,66,73	1.28	7 (11%)	74,104,113	1.04	6 (8%)
17	PQN	B	837	-	34,34,34	0.41	0	42,45,45	0.39	0
16	CLA	B	826	2	54,58,73	1.40	7 (12%)	65,95,113	1.01	4 (6%)
16	CLA	B	802	2	69,73,73	1.27	7 (10%)	83,113,113	0.82	4 (4%)
16	CLA	U	204	28	65,69,73	1.20	8 (12%)	78,108,113	1.01	5 (6%)
16	CLA	B	812	2	58,62,73	1.30	7 (12%)	69,99,113	1.03	4 (5%)
16	CLA	B	827	2	53,57,73	1.38	7 (13%)	62,93,113	1.02	3 (4%)
16	CLA	G	308	-	59,63,73	1.26	7 (11%)	71,101,113	1.11	6 (8%)
16	CLA	G	307	12	64,68,73	1.18	7 (10%)	77,107,113	1.03	4 (5%)
22	CL0	A	850	1	69,73,73	1.44	10 (14%)	83,113,113	1.05	5 (6%)
20	DD6	G	317	-	39,45,45	1.58	8 (20%)	52,67,67	1.54	10 (19%)
16	CLA	A	808	1	60,64,73	1.31	7 (11%)	72,102,113	0.97	3 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
16	CLA	A	847	1	64,68,73	1.32	8 (12%)	77,107,113	0.96	4 (5%)
23	SF4	C	102	3	0,12,12	-	-	-		
16	CLA	B	810	2	58,62,73	1.41	9 (15%)	73,100,113	1.01	4 (5%)
16	CLA	K	204	14	49,53,73	1.54	7 (14%)	59,89,113	1.01	3 (5%)
21	LMU	J	101	-	36,36,36	0.41	0	47,47,47	0.96	2 (4%)
16	CLA	H	312	-	69,73,73	1.11	5 (7%)	83,113,113	1.02	4 (4%)
16	CLA	A	825	1	69,73,73	1.24	7 (10%)	83,113,113	0.95	3 (3%)
16	CLA	G	303	-	49,53,73	1.43	8 (16%)	59,89,113	1.19	5 (8%)
16	CLA	B	818	2	50,54,73	1.40	7 (14%)	60,90,113	1.18	5 (8%)
16	CLA	B	813	2	63,67,73	1.27	8 (12%)	75,105,113	0.95	3 (4%)
18	LHG	G	316	-	26,26,48	0.35	0	29,32,54	0.43	0
16	CLA	A	849	1	69,73,73	1.20	6 (8%)	83,113,113	1.09	5 (6%)
16	CLA	G	310	12	49,53,73	1.44	7 (14%)	59,89,113	1.13	4 (6%)
16	CLA	B	829	28	69,73,73	1.17	7 (10%)	83,113,113	0.96	4 (4%)
16	CLA	A	821	28	69,73,73	1.21	9 (13%)	83,113,113	1.01	6 (7%)
16	CLA	k	201	15	46,50,73	1.45	5 (10%)	55,85,113	1.25	6 (10%)
16	CLA	A	822	28	69,73,73	1.14	7 (10%)	83,113,113	1.00	4 (4%)
16	CLA	B	831	2	62,66,73	1.33	8 (12%)	74,104,113	1.01	4 (5%)

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
16	CLA	A	851	1	-	6/39/115/115	-
16	CLA	A	801	-	-	1/39/115/115	-
16	CLA	B	816	2	-	0/33/109/115	-
16	CLA	A	812	1	-	2/15/91/115	-
16	CLA	A	827	1	-	3/21/97/115	-
16	CLA	G	306	12	-	10/39/115/115	-
16	CLA	A	854	1	-	6/39/115/115	-
16	CLA	I	102	-	-	4/39/115/115	-
16	CLA	L	203	9	-	1/39/115/115	-
16	CLA	H	308	13	-	2/10/86/115	-
16	CLA	B	808	2	-	5/39/115/115	-
16	CLA	A	803	1	-	5/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	CLA	B	845	2	-	3/39/115/115	-
20	DD6	H	311	-	-	11/26/80/80	0/3/3/3
16	CLA	K	202	14	-	0/12/88/115	-
16	CLA	H	309	13	-	4/15/91/115	-
16	CLA	A	806	1	-	8/39/115/115	-
16	CLA	B	804	2	-	4/15/91/115	-
20	DD6	G	313	-	-	6/26/80/80	0/3/3/3
16	CLA	H	304	13	-	1/13/90/115	-
16	CLA	B	817	28	-	5/39/115/115	-
16	CLA	B	803	-	-	3/39/115/115	-
16	CLA	H	305	13	-	2/15/91/115	-
16	CLA	A	830	1	-	0/21/97/115	-
19	BCR	L	201	-	-	10/29/63/63	0/2/2/2
16	CLA	F	803	28	-	3/19/95/115	-
21	LMU	A	848	-	-	10/21/61/61	0/2/2/2
16	CLA	A	834	1	-	9/39/115/115	-
19	BCR	B	842	-	-	7/29/63/63	0/2/2/2
16	CLA	H	306	13	-	6/39/115/115	-
16	CLA	B	809	2	-	6/39/115/115	-
16	CLA	B	824	2	-	3/39/115/115	-
16	CLA	A	853	1	-	11/39/115/115	-
16	CLA	A	817	1	-	3/15/91/115	-
16	CLA	A	810	1	-	4/26/102/115	-
16	CLA	G	302	-	-	1/10/86/115	-
16	CLA	K	205	14	-	5/31/107/115	-
21	LMU	A	855	-	-	8/21/61/61	0/2/2/2
19	BCR	B	840	-	-	6/29/63/63	0/2/2/2
16	CLA	B	830	28	-	0/15/91/115	-
16	CLA	A	818	28	-	3/39/115/115	-
19	BCR	A	842	-	-	10/29/63/63	0/2/2/2
16	CLA	B	822	2	-	2/39/115/115	-
23	SF4	C	101	3	-	-	0/6/5/5
16	CLA	B	814	2	-	8/27/103/115	-
16	CLA	G	305	12	-	13/35/111/115	-
16	CLA	K	206	28	-	1/10/82/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	BCR	L	205	-	-	8/29/63/63	0/2/2/2
21	LMU	K	201	-	-	12/21/61/61	0/2/2/2
16	CLA	A	816	1	-	2/39/115/115	-
16	CLA	A	811	1	-	3/39/115/115	-
23	SF4	A	852	1,2	-	-	0/6/5/5
25	LMG	J	103	-	-	22/34/54/70	0/1/1/1
16	CLA	A	845	28	-	7/39/115/115	-
16	CLA	G	304	12	-	3/13/89/115	-
19	BCR	J	105	-	-	10/29/63/63	0/2/2/2
16	CLA	A	831	1	-	4/15/91/115	-
19	BCR	F	801	-	-	10/29/63/63	0/2/2/2
16	CLA	B	805	2	-	7/39/115/115	-
16	CLA	H	307	-	-	7/31/107/115	-
16	CLA	A	824	1	-	5/36/112/115	-
16	CLA	B	835	2	-	8/39/115/115	-
16	CLA	A	805	1	-	3/20/96/115	-
16	CLA	B	807	2	-	5/39/115/115	-
16	CLA	B	833	2	-	2/18/94/115	-
17	PQN	A	837	-	-	3/23/43/43	0/2/2/2
16	CLA	U	206	11	-	2/15/91/115	-
16	CLA	A	828	1	-	3/39/115/115	-
20	DD6	K	208	-	-	11/26/80/80	0/3/3/3
20	DD6	G	311	-	-	7/26/80/80	0/3/3/3
19	BCR	A	843	-	-	4/29/63/63	0/2/2/2
16	CLA	H	303	13	-	4/35/111/115	-
20	DD6	U	212	-	-	14/26/80/80	0/3/3/3
16	CLA	G	301	12	-	3/15/91/115	-
20	DD6	G	312	-	-	6/19/50/80	0/2/2/3
18	LHG	A	840	16	-	6/31/31/53	-
18	LHG	A	839	-	-	19/52/52/53	-
16	CLA	A	835	1	-	1/39/115/115	-
16	CLA	B	832	2	-	3/39/115/115	-
20	DD6	H	310	-	-	15/26/80/80	0/3/3/3
16	CLA	A	814	28	-	3/15/91/115	-
16	CLA	A	819	1	-	1/13/89/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	KC1	U	213	11	-	0/15/71/71	-
16	CLA	B	844	2	-	5/39/115/115	-
19	BCR	B	846	-	-	17/27/61/63	0/2/2/2
16	CLA	G	309	-	-	8/29/105/115	-
19	BCR	A	841	-	-	7/29/63/63	0/2/2/2
19	BCR	B	841	-	-	6/29/63/63	0/2/2/2
19	BCR	I	101	-	-	9/29/63/63	0/2/2/2
16	CLA	B	819	2	-	5/25/101/115	-
16	CLA	K	207	-	-	4/17/93/115	-
19	BCR	B	838	-	-	9/29/63/63	0/2/2/2
16	CLA	A	820	1	-	3/23/99/115	-
24	DGD	B	843	-	-	25/49/89/95	0/2/2/2
16	CLA	L	202	9	-	6/20/96/115	-
16	CLA	B	823	2	-	5/39/115/115	-
16	CLA	U	210	11	-	3/39/115/115	-
16	CLA	K	203	14	-	3/27/103/115	-
16	CLA	B	820	28	-	5/37/113/115	-
16	CLA	B	801	28	-	2/39/115/115	-
20	DD6	U	214	-	-	3/14/37/80	0/1/1/3
26	A86	U	202	-	-	16/34/90/90	0/3/3/3
16	CLA	B	847	2	-	7/24/100/115	-
25	LMG	U	201	-	-	13/27/47/70	0/1/1/1
16	CLA	U	205	11	-	3/39/115/115	-
16	CLA	A	826	1	-	2/39/115/115	-
16	CLA	F	804	6	-	6/17/93/115	-
16	CLA	A	802	1	-	3/27/103/115	-
16	CLA	B	825	2	-	3/39/115/115	-
21	LMU	F	806	-	-	7/21/61/61	0/2/2/2
16	CLA	H	301	-	-	3/10/82/115	-
19	BCR	F	805	-	-	12/29/63/63	0/2/2/2
16	CLA	A	823	1	-	3/39/115/115	-
16	CLA	U	207	-	-	3/39/115/115	-
16	CLA	L	204	28	-	6/21/97/115	-
16	CLA	U	209	-	-	0/12/88/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	CLA	H	302	13	-	6/33/109/115	-
16	CLA	F	802	28	-	1/39/115/115	-
16	CLA	B	811	2	-	7/27/103/115	-
20	DD6	A	846	-	-	9/26/80/80	0/3/3/3
16	CLA	A	809	1	-	0/36/112/115	-
16	CLA	B	848	2	-	4/39/115/115	-
20	DD6	U	203	-	-	10/26/80/80	0/3/3/3
16	CLA	A	836	28	-	4/39/115/115	-
16	CLA	A	815	1	-	4/39/115/115	-
16	CLA	k	202	28	-	5/27/103/115	-
16	CLA	A	813	1	-	2/21/97/115	-
19	BCR	I	103	-	-	10/29/63/63	0/2/2/2
16	CLA	G	315	12	-	5/15/91/115	-
16	CLA	A	832	1	-	2/23/99/115	-
16	CLA	B	834	28	-	6/39/115/115	-
16	CLA	A	833	1	-	1/39/115/115	-
16	CLA	A	804	1	-	10/39/115/115	-
16	CLA	B	849	2	-	5/39/115/115	-
16	CLA	J	104	8	-	5/12/88/115	-
16	CLA	U	211	11	-	5/24/100/115	-
19	BCR	A	844	-	-	9/29/63/63	0/2/2/2
16	CLA	A	829	1	-	1/39/115/115	-
19	BCR	k	203	-	-	10/29/63/63	0/2/2/2
20	DD6	J	102	-	-	5/26/80/80	0/3/3/3
16	CLA	U	208	11	-	4/17/93/115	-
16	CLA	B	821	28	-	3/27/103/115	-
16	CLA	A	838	18	-	3/24/100/115	-
20	DD6	G	314	-	-	12/26/80/80	0/3/3/3
16	CLA	B	806	2	-	4/39/115/115	-
19	BCR	B	839	-	-	10/29/63/63	0/2/2/2
19	BCR	M	101	-	-	8/29/63/63	0/2/2/2
16	CLA	B	836	-	-	4/30/106/115	-
16	CLA	B	815	2	-	2/32/108/115	-
16	CLA	A	807	1	-	4/27/103/115	-
16	CLA	B	828	2	-	7/31/107/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	PQN	B	837	-	-	1/23/43/43	0/2/2/2
16	CLA	B	826	2	-	1/21/97/115	-
16	CLA	B	802	2	-	3/39/115/115	-
16	CLA	U	204	28	-	12/35/111/115	-
16	CLA	B	812	2	-	2/26/102/115	-
16	CLA	B	827	2	-	3/20/96/115	-
16	CLA	G	308	-	-	4/27/103/115	-
16	CLA	G	307	12	-	7/33/109/115	-
22	CL0	A	850	1	-	9/39/115/115	-
20	DD6	G	317	-	-	12/26/80/80	0/3/3/3
16	CLA	A	808	1	-	0/29/105/115	-
16	CLA	A	847	1	-	6/33/109/115	-
23	SF4	C	102	3	-	-	0/6/5/5
16	CLA	B	810	2	-	0/25/101/115	-
16	CLA	K	204	14	-	5/15/91/115	-
21	LMU	J	101	-	-	9/21/61/61	0/2/2/2
16	CLA	H	312	-	-	21/39/115/115	-
16	CLA	A	825	1	-	6/39/115/115	-
16	CLA	G	303	-	-	5/15/91/115	-
16	CLA	B	818	2	-	1/17/93/115	-
16	CLA	B	813	2	-	1/32/108/115	-
18	LHG	G	316	-	-	22/31/31/53	-
16	CLA	A	849	1	-	9/39/115/115	-
16	CLA	G	310	12	-	7/15/91/115	-
16	CLA	B	829	28	-	1/39/115/115	-
16	CLA	A	821	28	-	7/39/115/115	-
16	CLA	k	201	15	-	1/12/88/115	-
16	CLA	A	822	28	-	2/39/115/115	-
16	CLA	B	831	2	-	3/31/107/115	-

The worst 5 of 1087 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	U	202	A86	C13-C11	-6.10	1.37	1.49
16	K	204	CLA	MG-NA	5.17	2.18	2.06
16	B	848	CLA	MG-NA	5.05	2.18	2.06
16	A	826	CLA	MG-NA	5.04	2.18	2.06
16	H	305	CLA	MG-NA	5.03	2.18	2.06

The worst 5 of 846 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	U	212	DD6	C3-C4-C5	5.24	134.21	123.47
16	G	315	CLA	CHD-C1D-ND	-4.92	119.93	124.45
16	H	306	CLA	O2A-C1-C2	4.51	120.47	108.64
20	J	102	DD6	C12-C11-C10	-4.46	116.67	122.92
16	K	205	CLA	O2A-C1-C2	4.40	120.21	108.64

There are no chirality outliers.

5 of 1003 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
16	A	804	CLA	C1A-C2A-CAA-CBA
16	A	806	CLA	CBA-CGA-O2A-C1
16	A	806	CLA	O1A-CGA-O2A-C1
16	A	815	CLA	C3A-C2A-CAA-CBA
16	A	820	CLA	CBD-CGD-O2D-CED

There are no ring outliers.

138 monomers are involved in 235 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
16	A	851	CLA	5	0
16	A	801	CLA	2	0
16	B	816	CLA	1	0
16	A	812	CLA	2	0
16	G	306	CLA	2	0
16	A	854	CLA	5	0
16	I	102	CLA	2	0
16	L	203	CLA	1	0
16	H	308	CLA	3	0
16	B	808	CLA	2	0
16	A	803	CLA	2	0
16	B	845	CLA	1	0
16	K	202	CLA	1	0
16	H	309	CLA	2	0
16	A	806	CLA	1	0
16	H	304	CLA	1	0
16	B	817	CLA	2	0
16	B	803	CLA	2	0
16	H	305	CLA	3	0
16	A	830	CLA	1	0
19	L	201	BCR	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
21	A	848	LMU	1	0
19	B	842	BCR	3	0
16	H	306	CLA	7	0
16	B	809	CLA	1	0
16	B	824	CLA	2	0
16	A	853	CLA	2	0
16	A	817	CLA	2	0
16	A	810	CLA	1	0
16	G	302	CLA	1	0
16	K	205	CLA	3	0
21	A	855	LMU	1	0
19	B	840	BCR	1	0
16	B	830	CLA	1	0
16	A	818	CLA	1	0
19	A	842	BCR	1	0
16	B	822	CLA	2	0
16	B	814	CLA	1	0
16	K	206	CLA	2	0
19	L	205	BCR	2	0
16	A	816	CLA	4	0
16	A	811	CLA	2	0
25	J	103	LMG	2	0
16	A	845	CLA	3	0
16	G	304	CLA	1	0
19	J	105	BCR	2	0
16	A	831	CLA	3	0
16	B	805	CLA	2	0
16	A	824	CLA	4	0
16	B	835	CLA	4	0
16	B	807	CLA	5	0
17	A	837	PQN	3	0
16	U	206	CLA	1	0
16	A	828	CLA	4	0
20	G	311	DD6	1	0
19	A	843	BCR	2	0
16	H	303	CLA	1	0
16	G	301	CLA	1	0
18	A	839	LHG	2	0
16	A	835	CLA	3	0
16	B	832	CLA	1	0
16	A	814	CLA	2	0
16	A	819	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
16	B	844	CLA	2	0
19	B	846	BCR	3	0
16	G	309	CLA	4	0
19	B	841	BCR	3	0
19	I	101	BCR	2	0
16	B	819	CLA	3	0
19	B	838	BCR	2	0
16	A	820	CLA	2	0
24	B	843	DGD	2	0
16	L	202	CLA	2	0
16	B	823	CLA	1	0
16	U	210	CLA	1	0
16	K	203	CLA	2	0
16	B	820	CLA	1	0
16	B	801	CLA	2	0
26	U	202	A86	1	0
16	B	847	CLA	1	0
25	U	201	LMG	2	0
16	U	205	CLA	2	0
16	A	826	CLA	2	0
16	F	804	CLA	1	0
16	B	825	CLA	3	0
16	A	823	CLA	1	0
16	U	207	CLA	5	0
16	L	204	CLA	1	0
16	U	209	CLA	1	0
16	H	302	CLA	3	0
16	F	802	CLA	2	0
16	B	811	CLA	1	0
16	A	809	CLA	2	0
16	B	848	CLA	3	0
16	A	836	CLA	2	0
16	A	815	CLA	2	0
16	k	202	CLA	2	0
16	A	813	CLA	1	0
19	I	103	BCR	1	0
16	B	834	CLA	4	0
16	A	833	CLA	3	0
16	B	849	CLA	6	0
16	J	104	CLA	1	0
16	U	211	CLA	3	0
19	A	844	BCR	3	0

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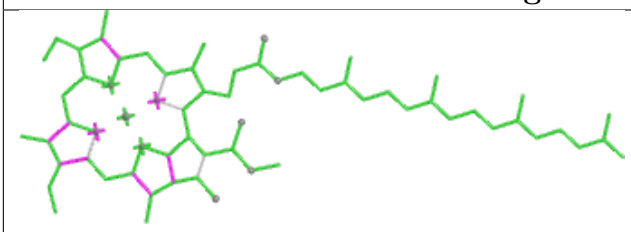
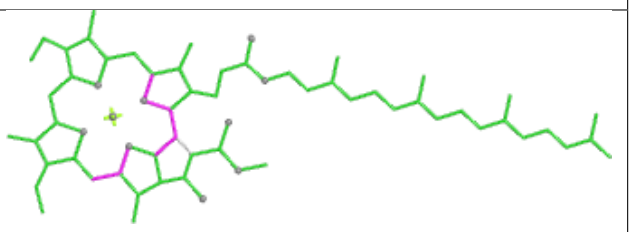
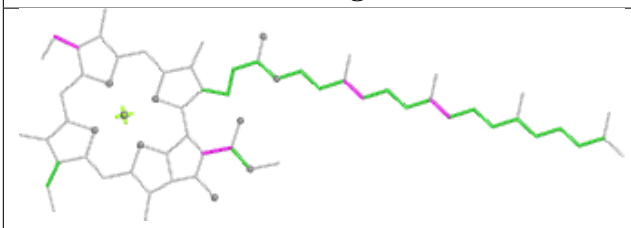
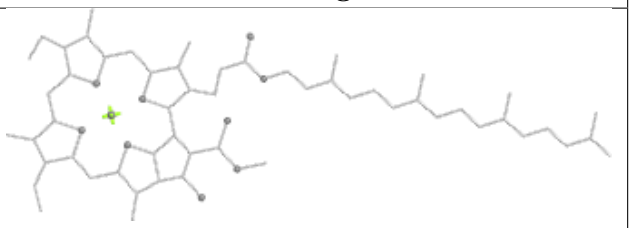
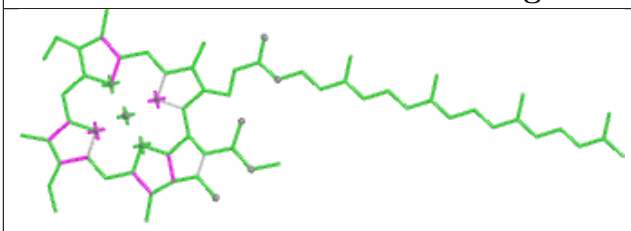
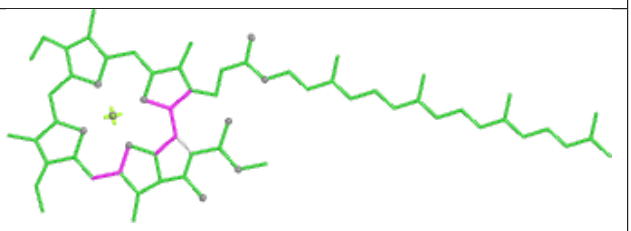
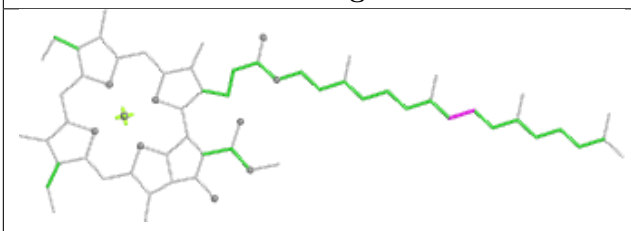
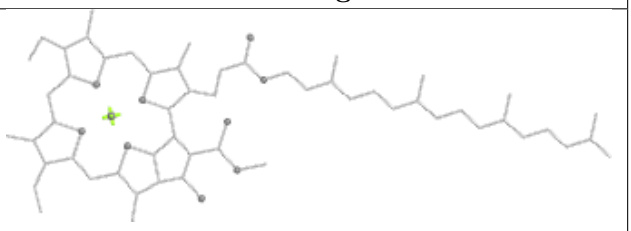
Mol	Chain	Res	Type	Clashes	Symm-Clashes
16	A	829	CLA	2	0
19	k	203	BCR	3	0
16	U	208	CLA	1	0
16	B	806	CLA	2	0
19	B	839	BCR	4	0
19	M	101	BCR	3	0
16	B	836	CLA	4	0
16	B	815	CLA	2	0
16	A	807	CLA	1	0
16	B	828	CLA	1	0
17	B	837	PQN	1	0
16	B	826	CLA	1	0
16	B	802	CLA	3	0
16	U	204	CLA	1	0
16	B	827	CLA	1	0
16	G	308	CLA	2	0
16	G	307	CLA	1	0
22	A	850	CL0	2	0
16	A	808	CLA	2	0
16	A	847	CLA	1	0
21	J	101	LMU	3	0
16	H	312	CLA	5	0
16	A	825	CLA	1	0
16	G	303	CLA	3	0
16	B	818	CLA	2	0
16	B	813	CLA	2	0
18	G	316	LHG	2	0
16	A	849	CLA	6	0
16	G	310	CLA	2	0
16	B	829	CLA	1	0
16	k	201	CLA	1	0
16	A	822	CLA	1	0
16	B	831	CLA	2	0

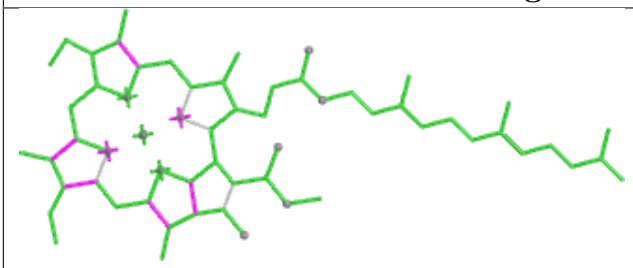
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

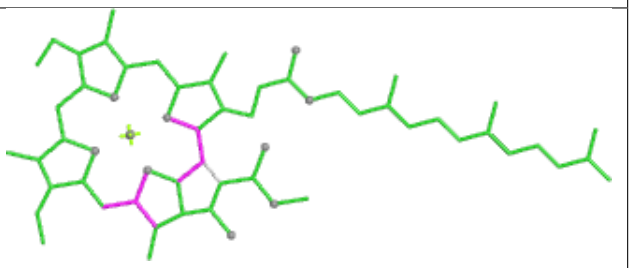
Ligand CLA A 851	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA A 801	
 Bond lengths	 Bond angles
 Torsions	 Rings

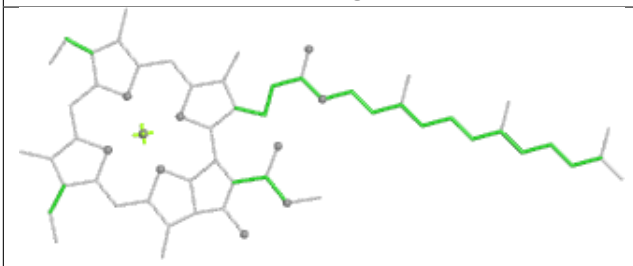
Ligand CLA B 816



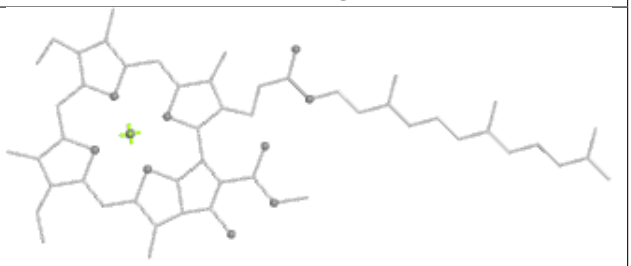
Bond lengths



Bond angles

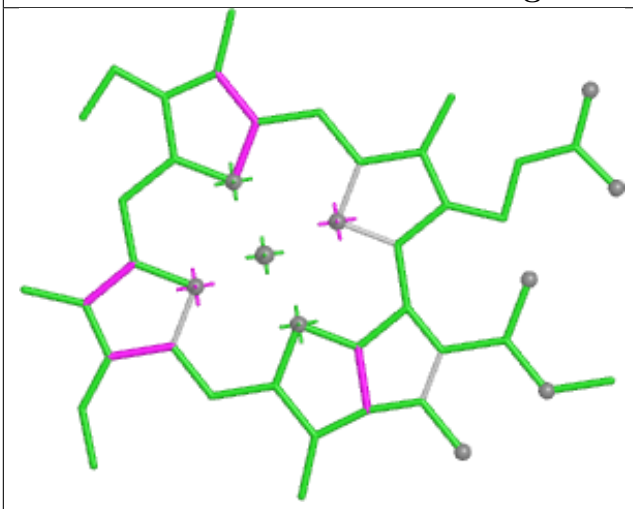


Torsions

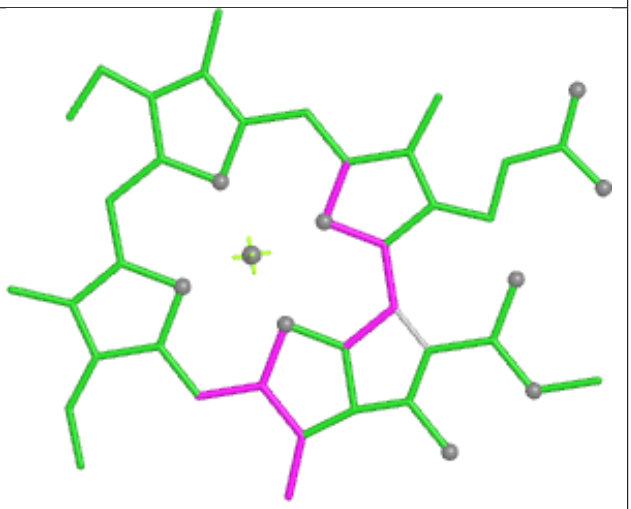


Rings

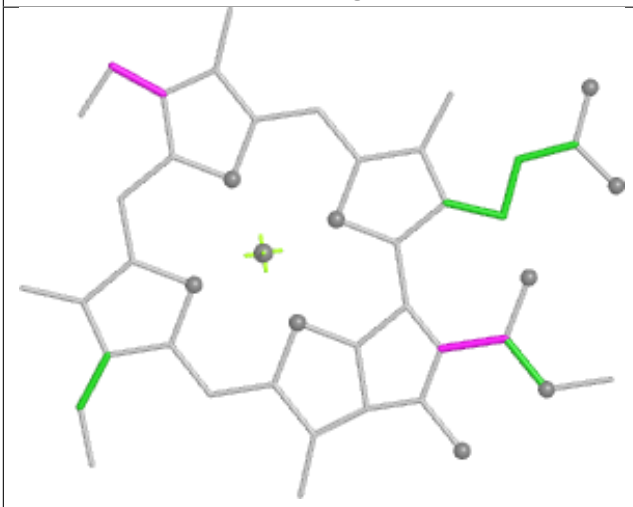
Ligand CLA A 812



Bond lengths



Bond angles



Torsions

Rings

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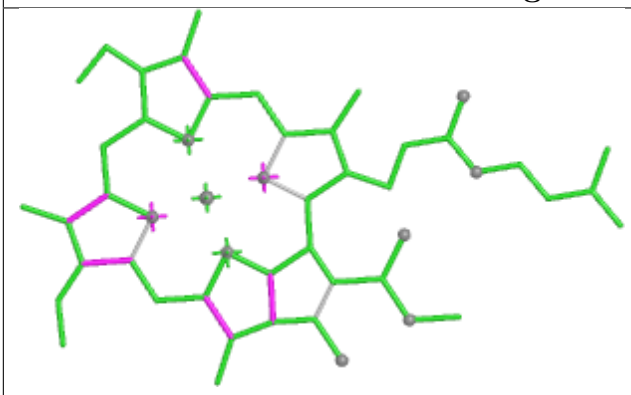
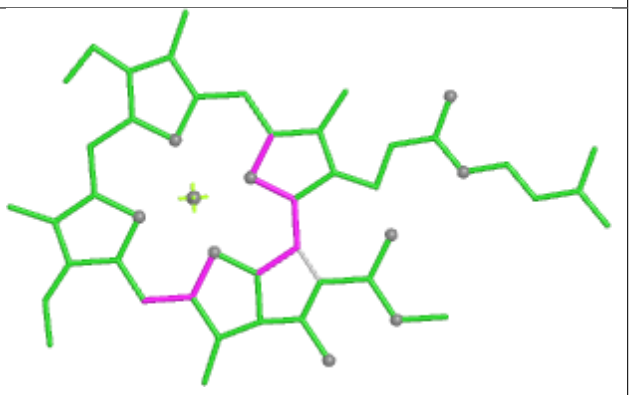
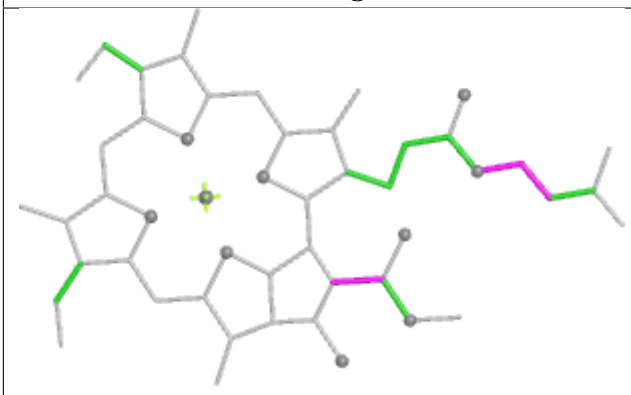
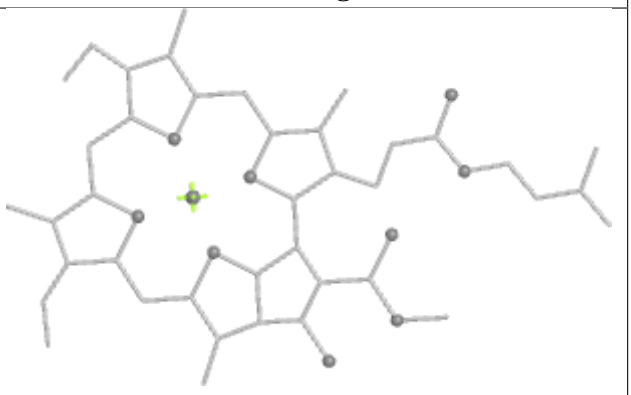
 Bond lengths	 Bond angles
 Torsions	 Rings

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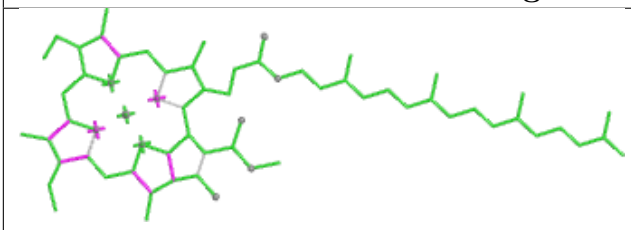
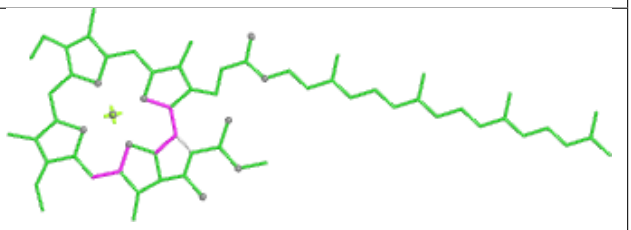
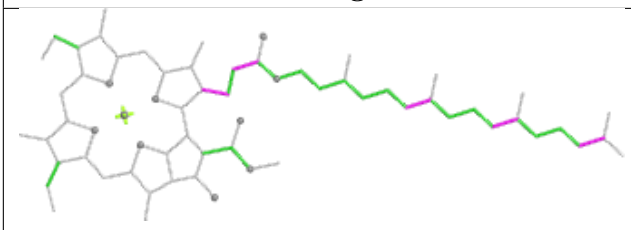
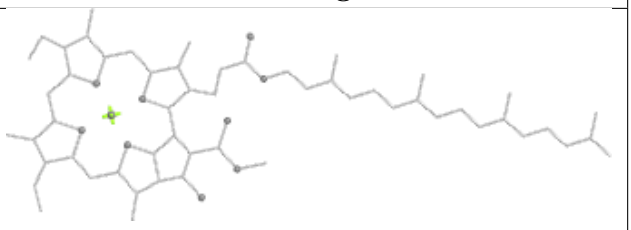
 Bond lengths	 Bond angles
 Torsions	 Rings

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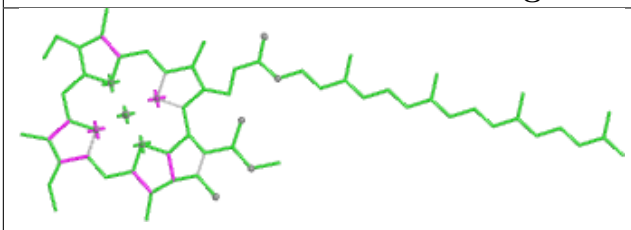
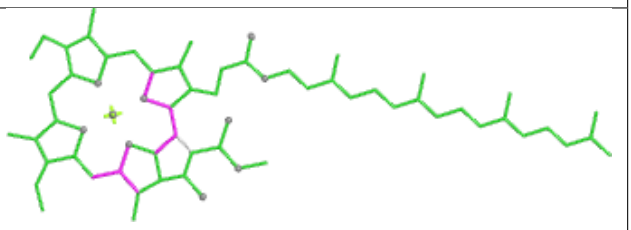
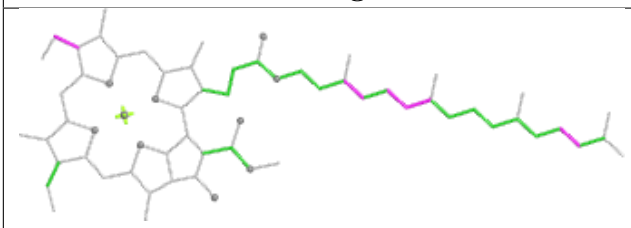
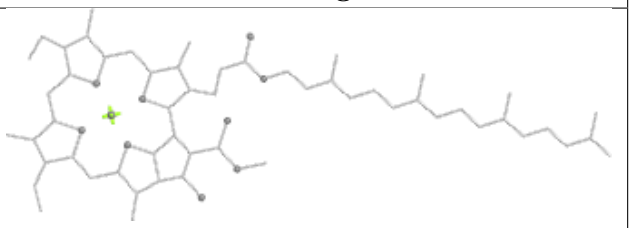
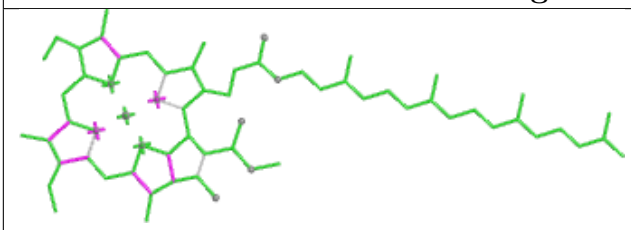
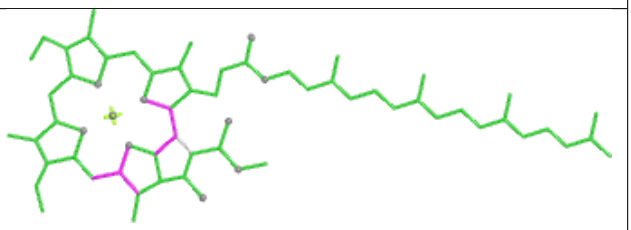
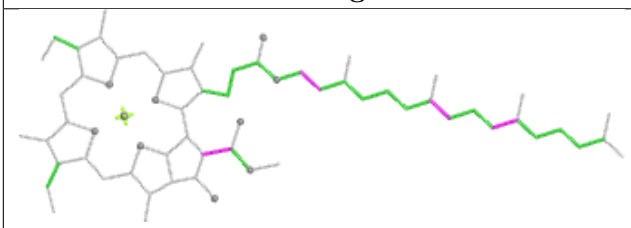
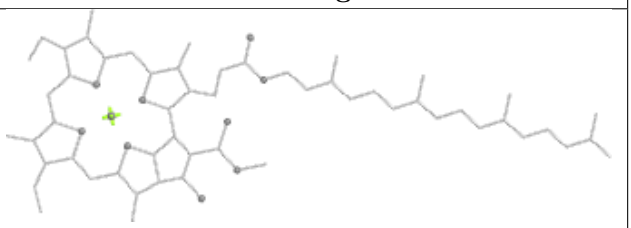
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA I 102	
 Bond lengths	 Bond angles
 Torsions	 Rings

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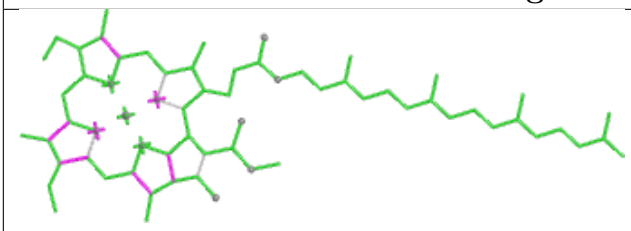
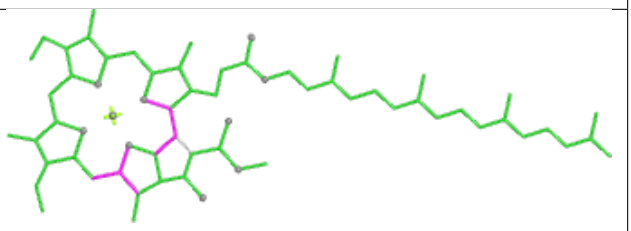
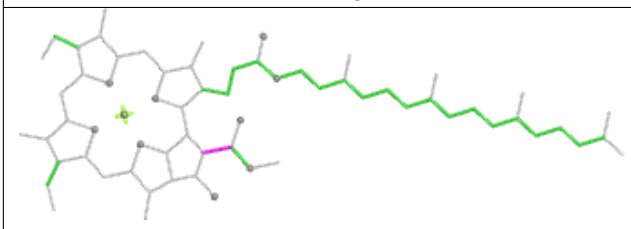
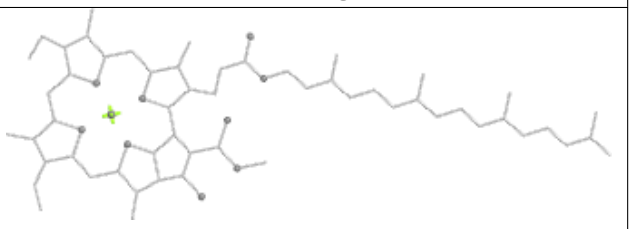
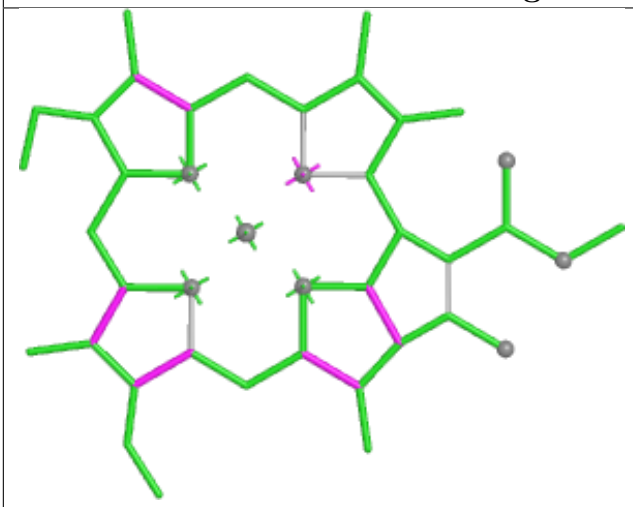
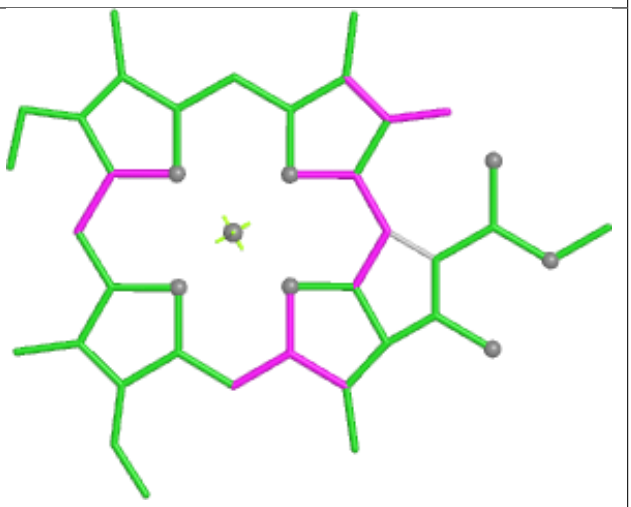
 Bond lengths	 Bond angles
 Torsions	 Rings

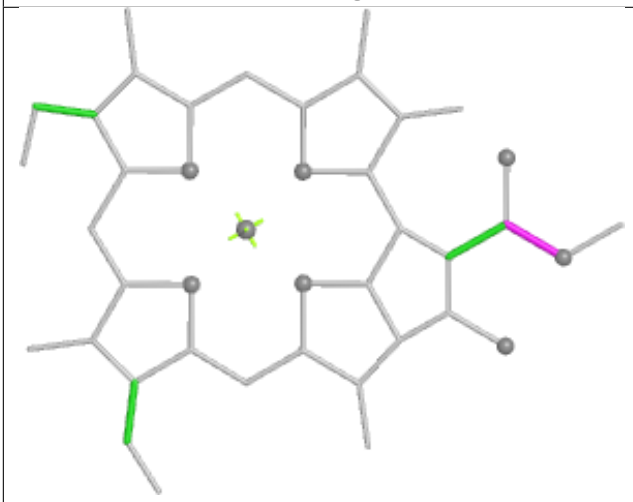
Ligand CLA H 308



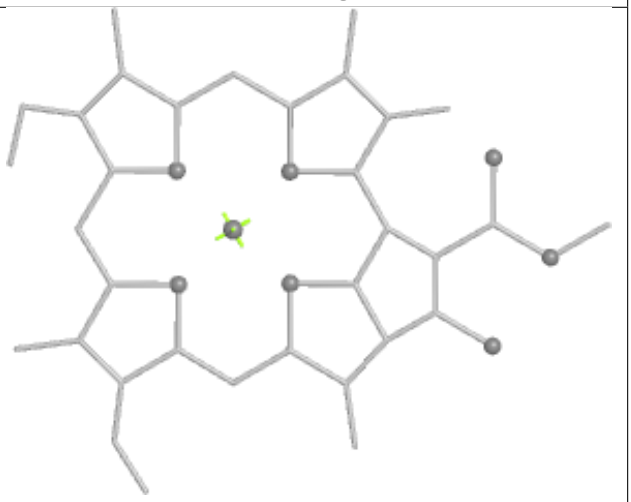
Bond lengths



Bond angles

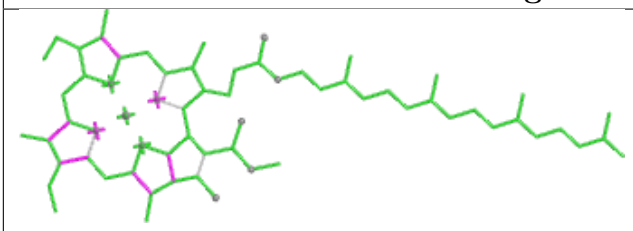


Torsions



Rings

Ligand CLA B 808



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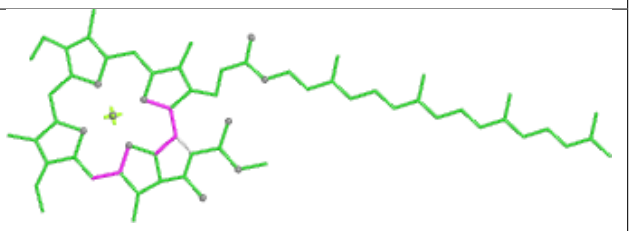
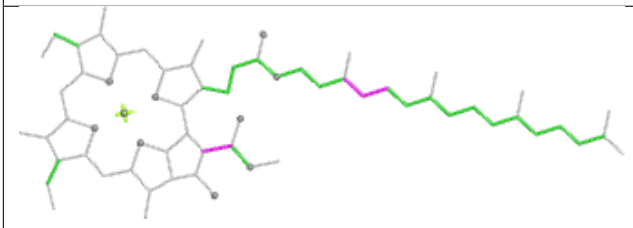
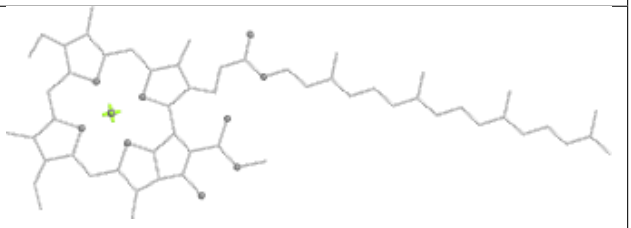


Bond angles

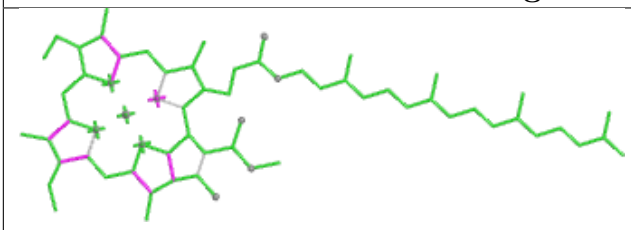


Torsions

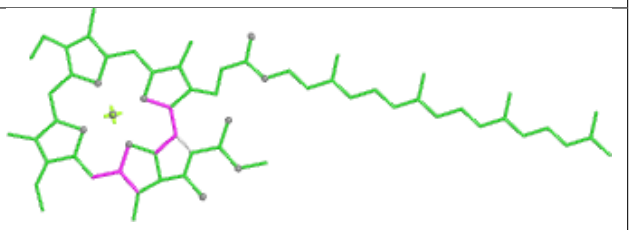


Rings

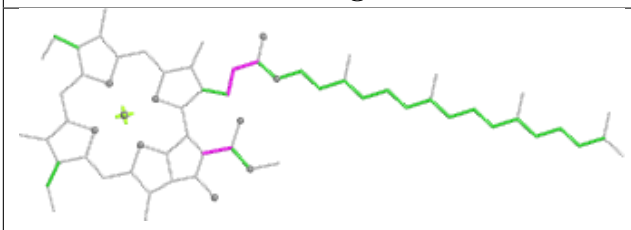
Ligand CLA A 803



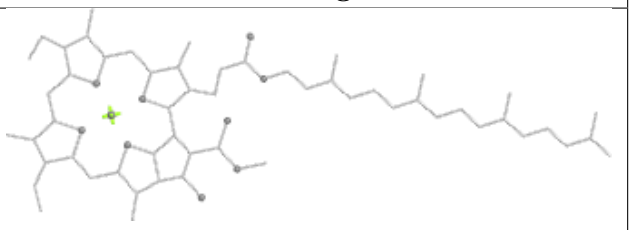
Bond lengths



Bond angles

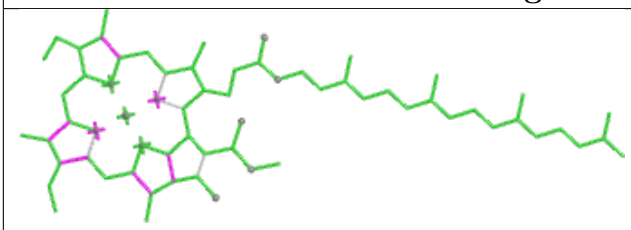


Torsions

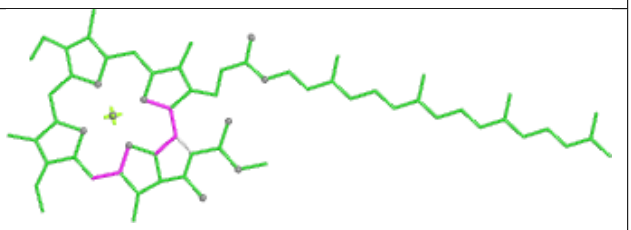


Rings

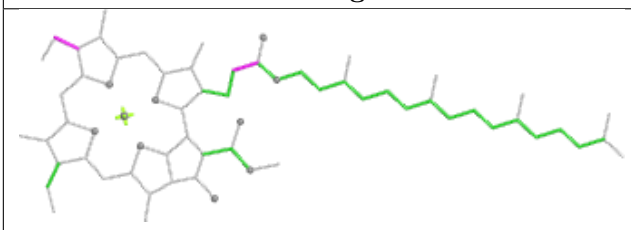
Ligand CLA B 845



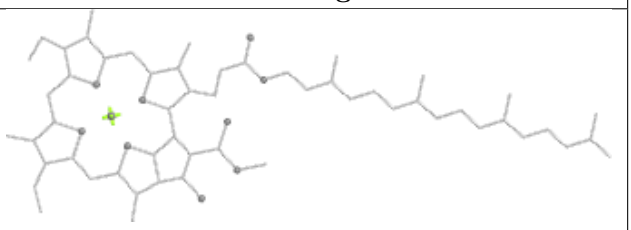
Bond lengths



Bond angles

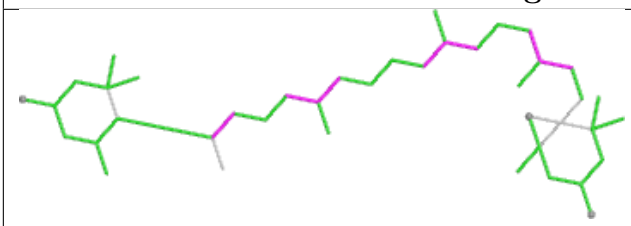


Torsions



Rings

Ligand DD6 H 311



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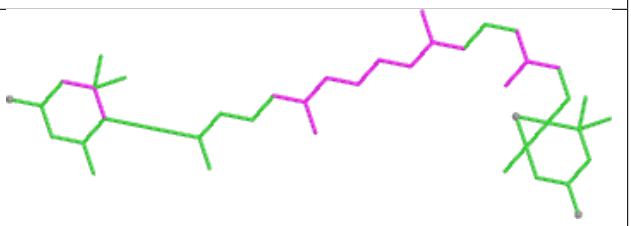
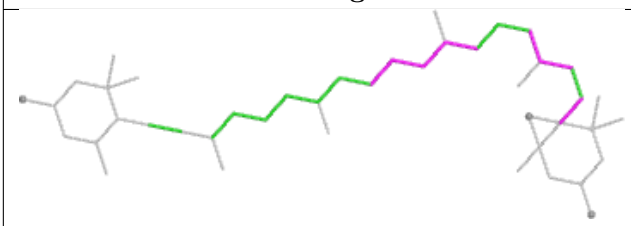


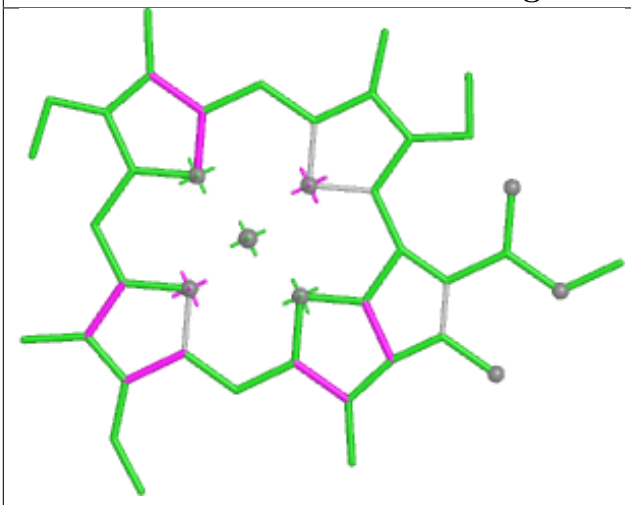
Bond angles



Torsions

Rings

Ligand CLA K 202



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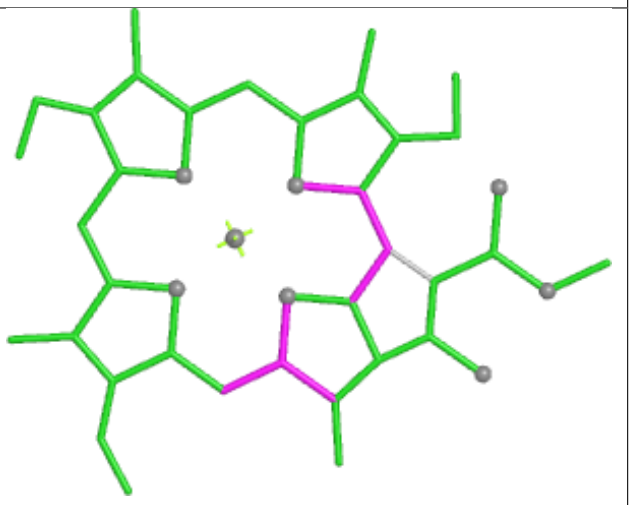
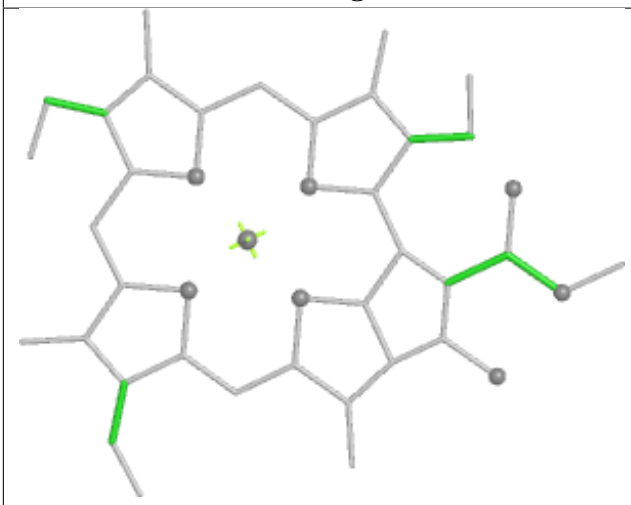


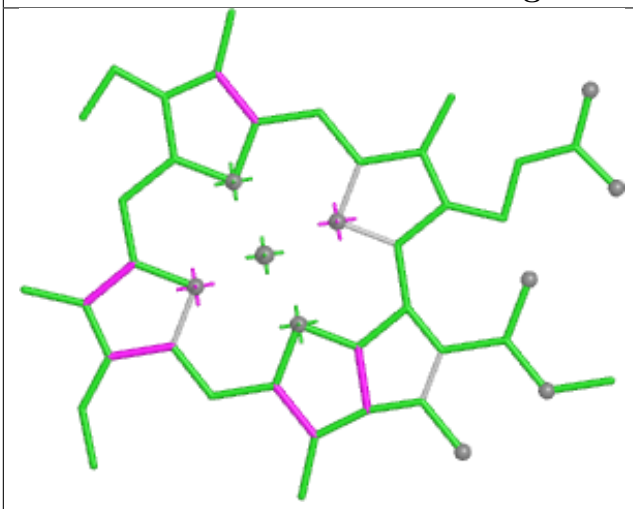
Bond angles



Torsions

Rings

Ligand CLA H 309



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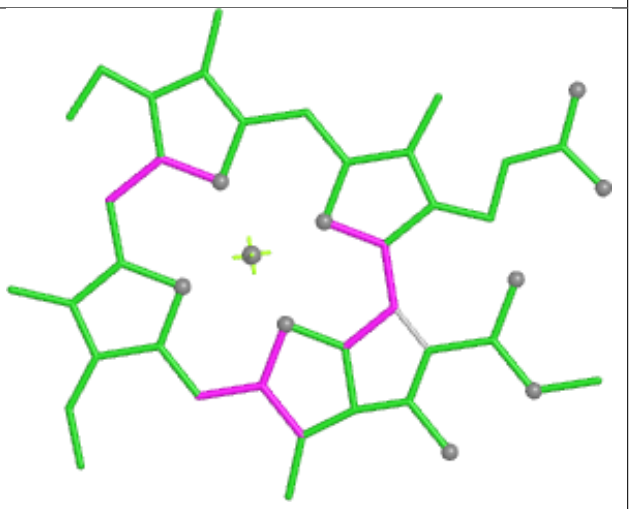

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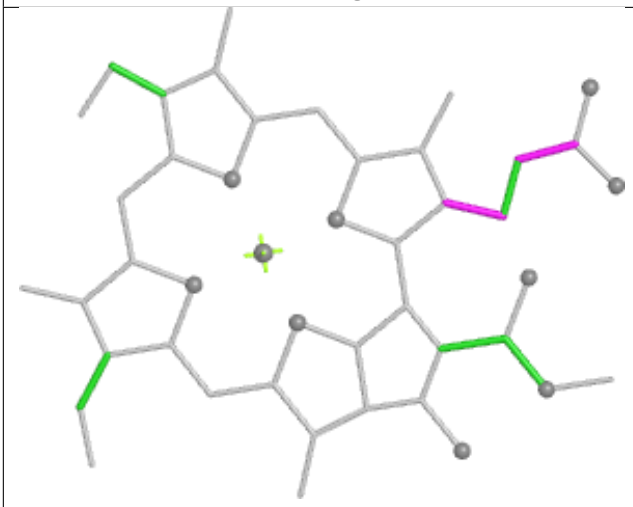
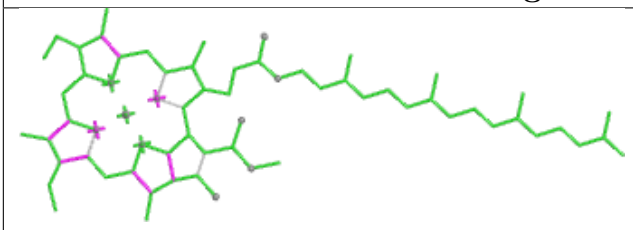


Torsions

Rings

Ligand CLA A 806



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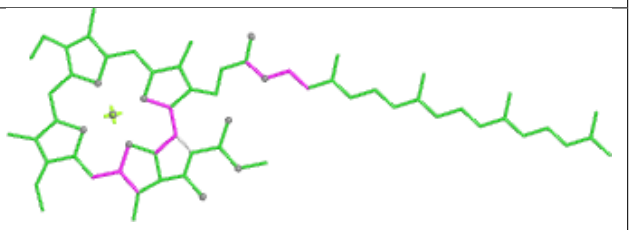

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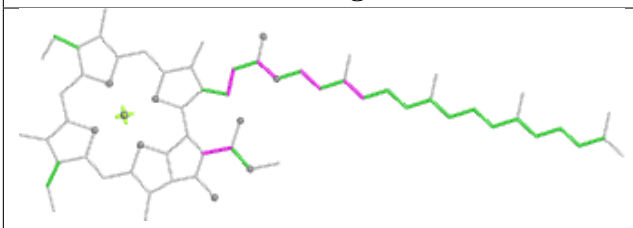

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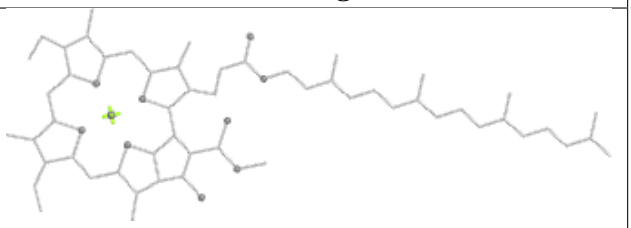
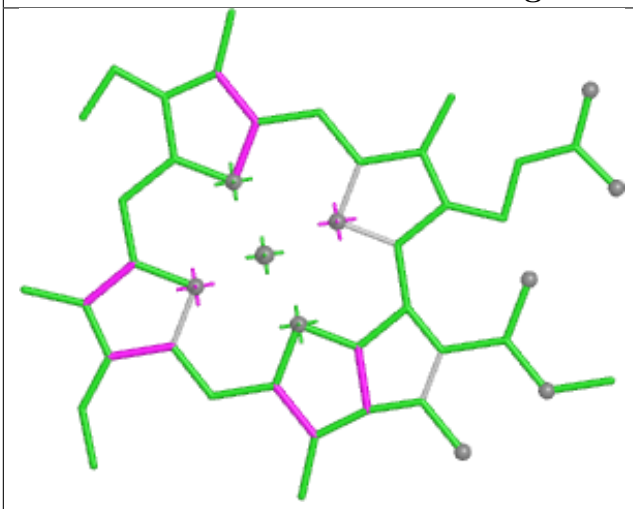
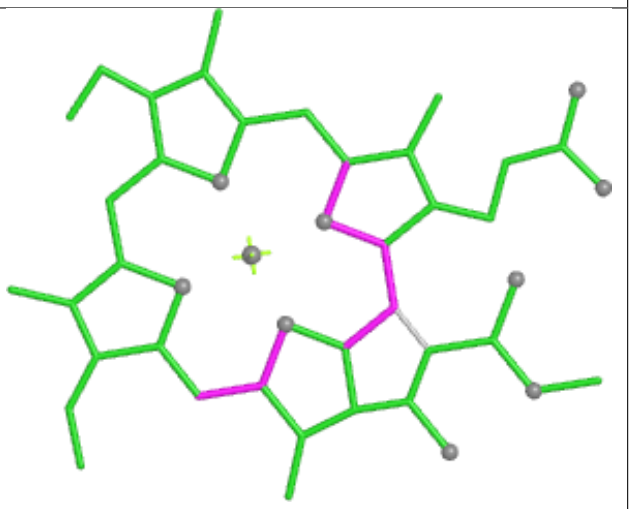


Rings

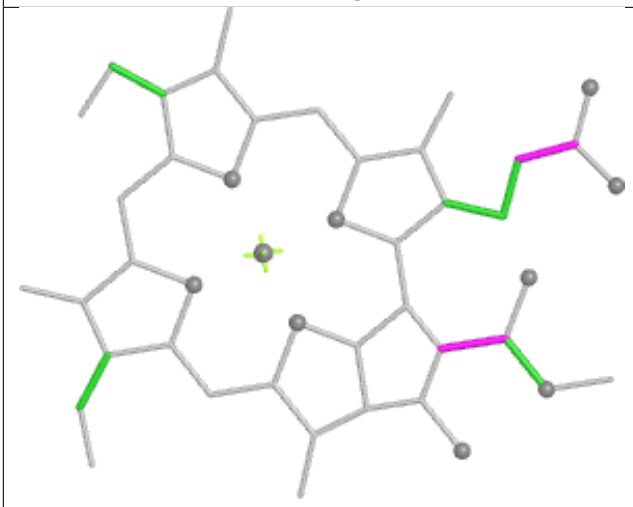
Ligand CLA B 804



Bond lengths



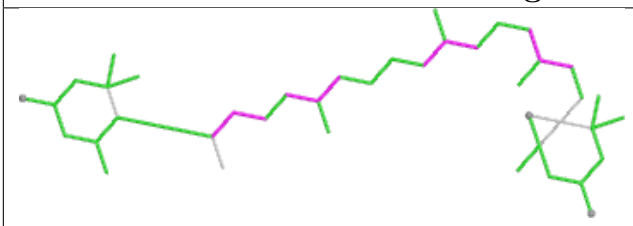
Bond angles



Torsions

Rings

Ligand DD6 G 313



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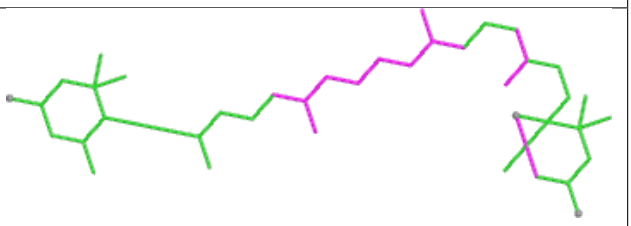
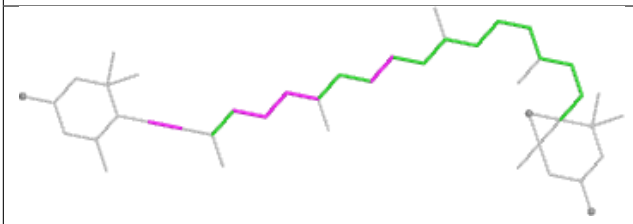
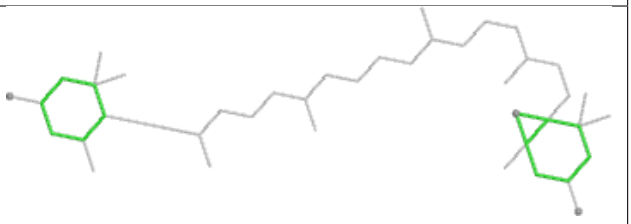


Bond angles

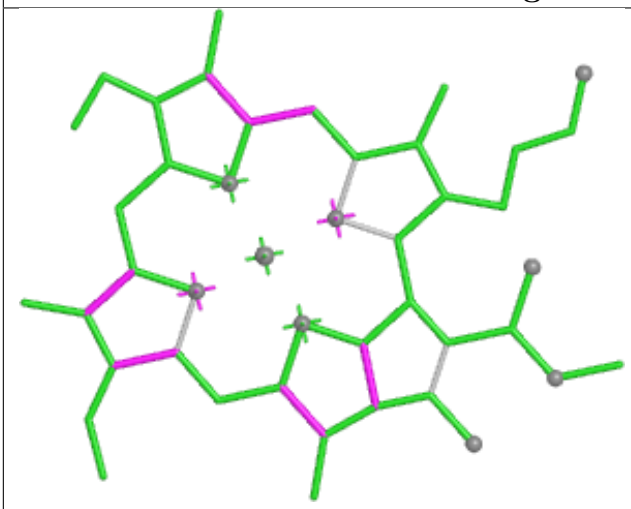


Torsions



Rings

Ligand CLA H 304



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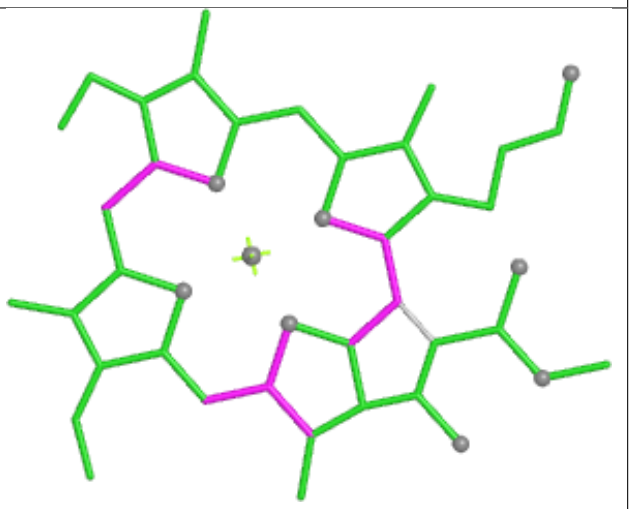
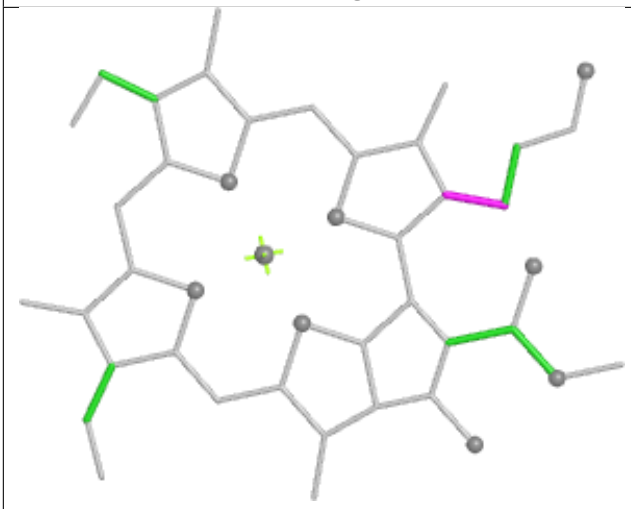


Bond angles



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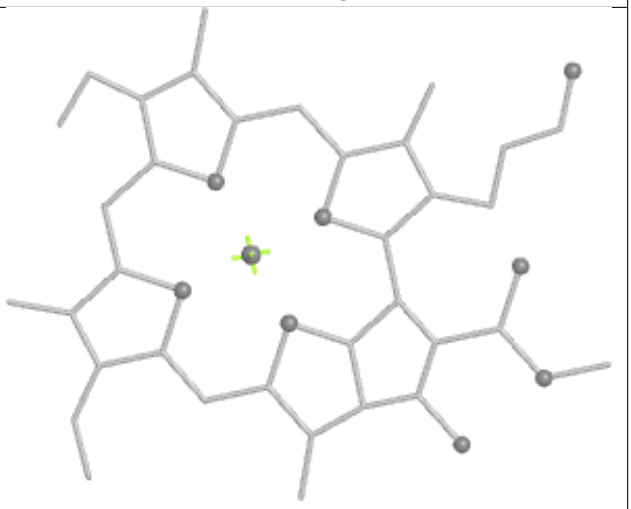
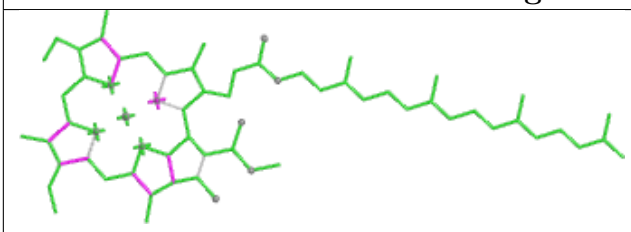


Rings

Ligand CLA B 817



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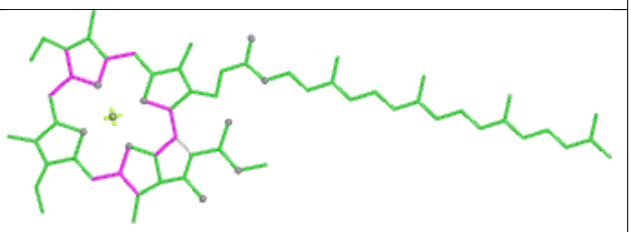
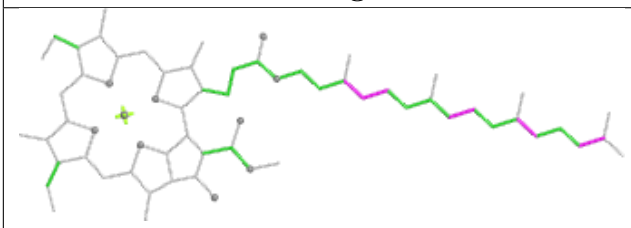


Bond angles



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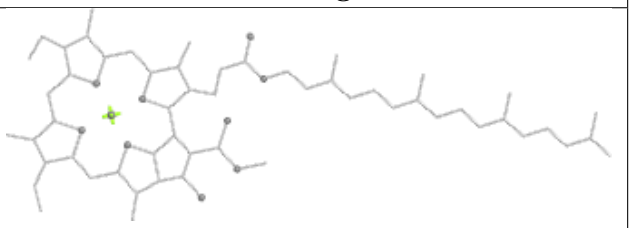
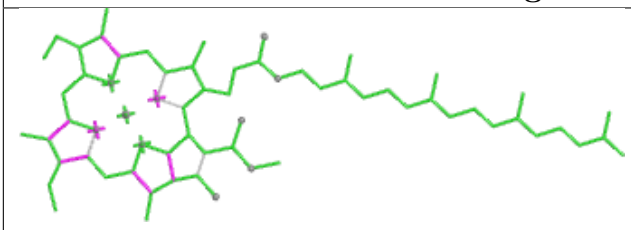
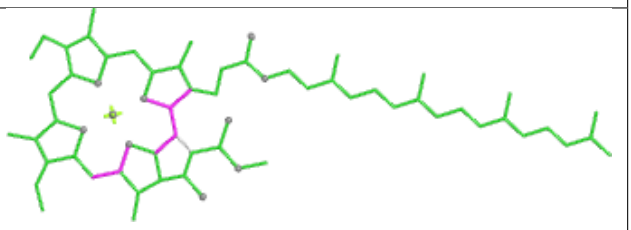


Rings

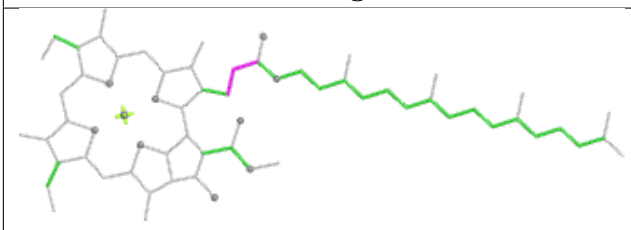
Ligand CLA B 803



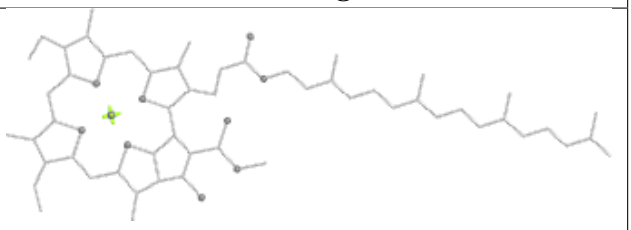
Bond lengths



Bond angles

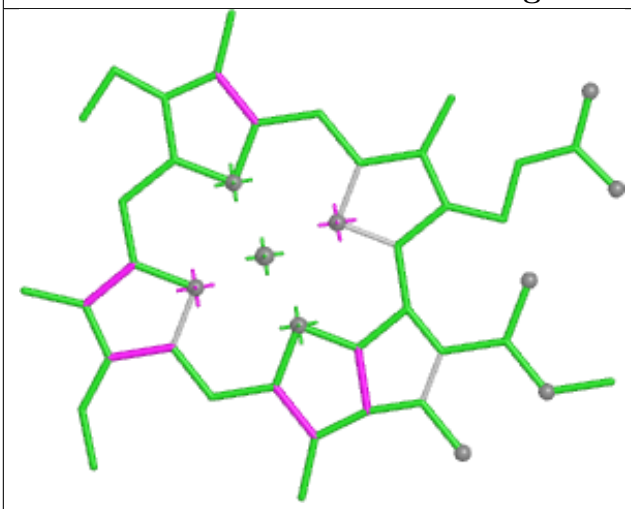


Torsions



Rings

Ligand CLA H 305



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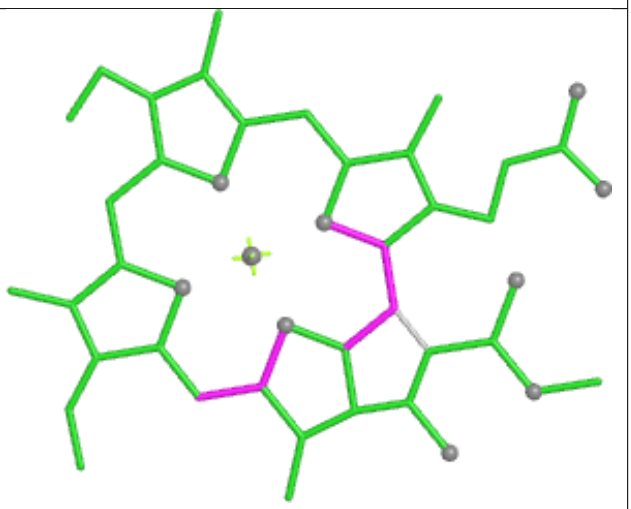
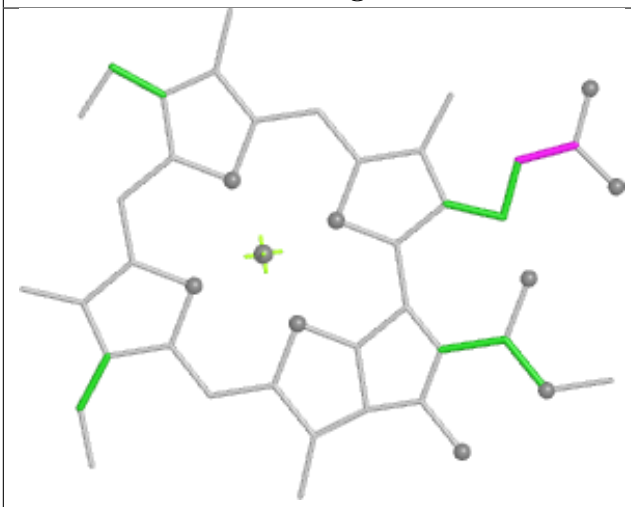
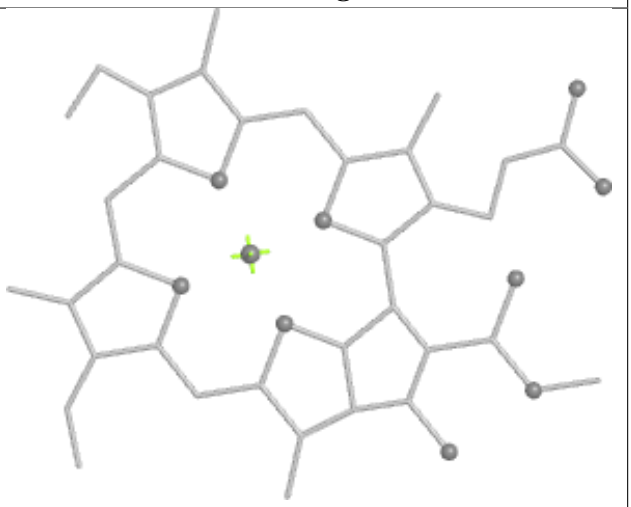


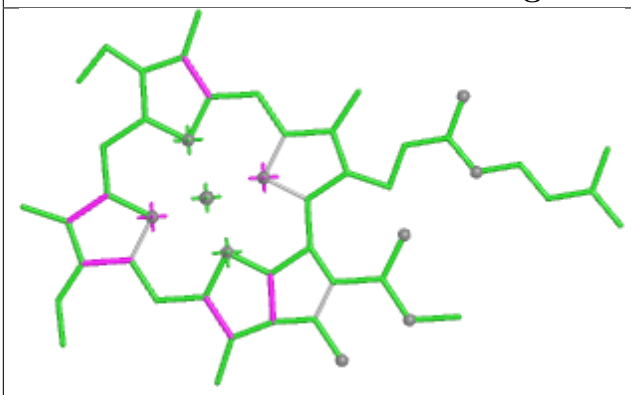
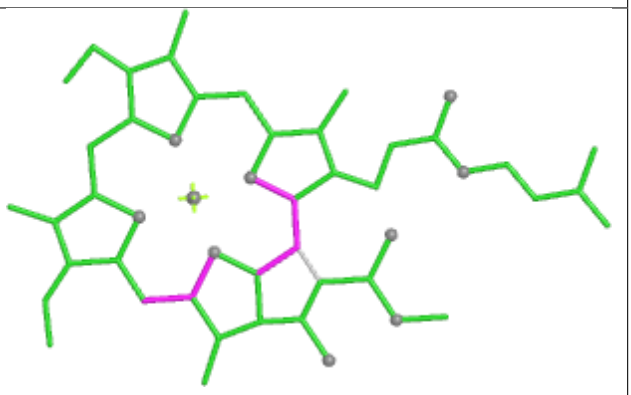
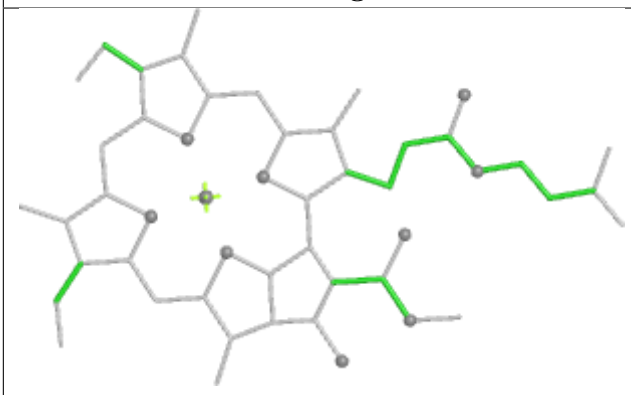
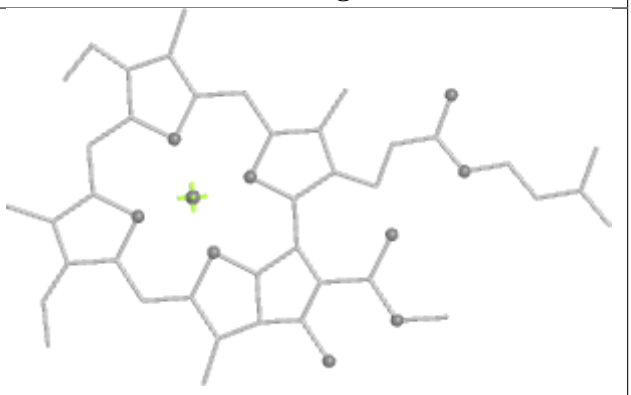
Bond angles

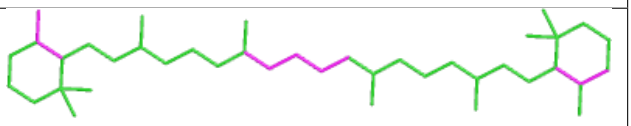
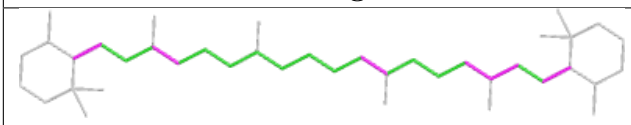
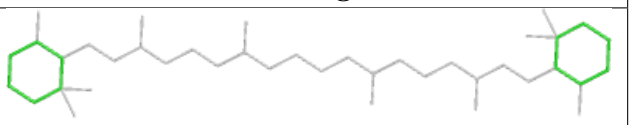


Torsions

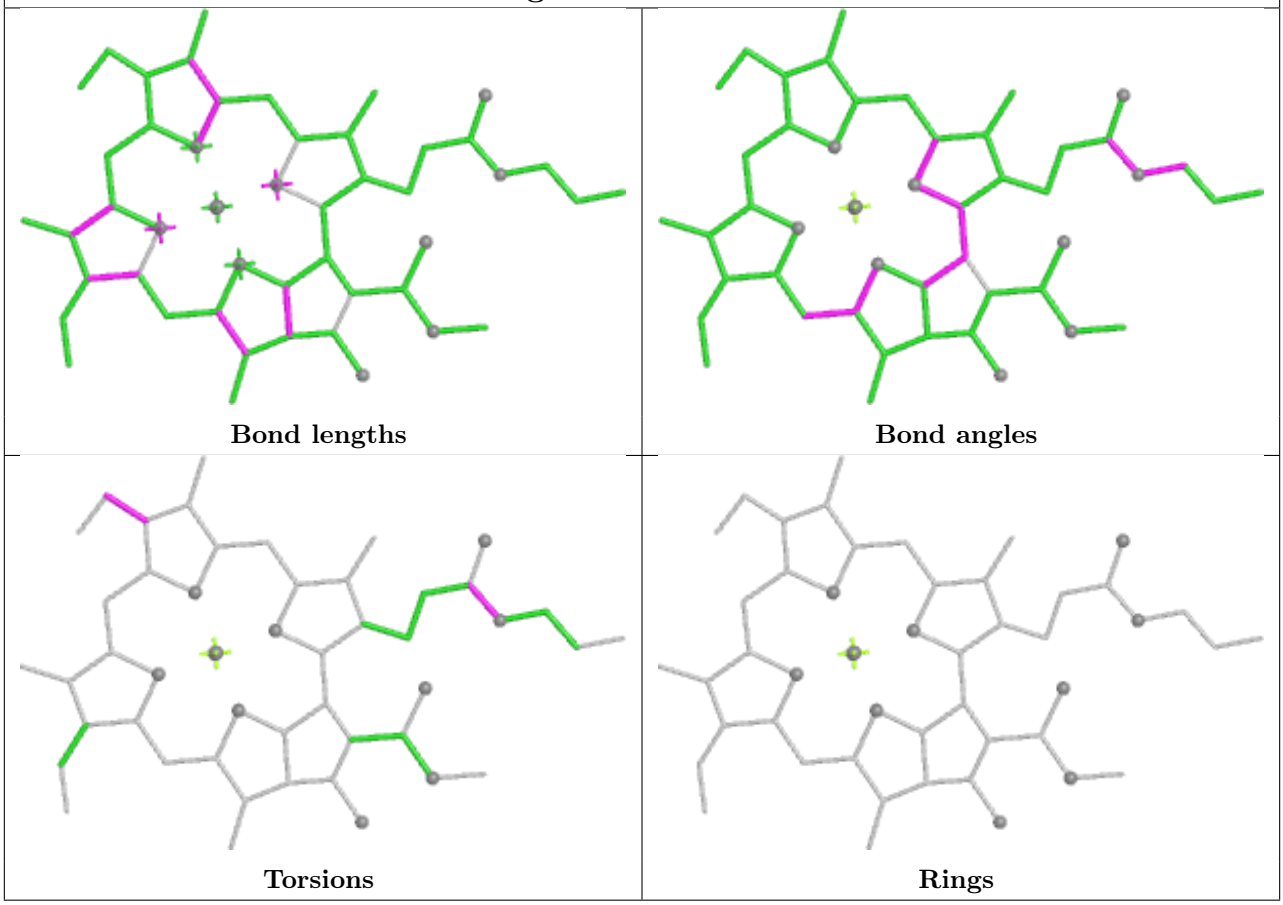


Rings

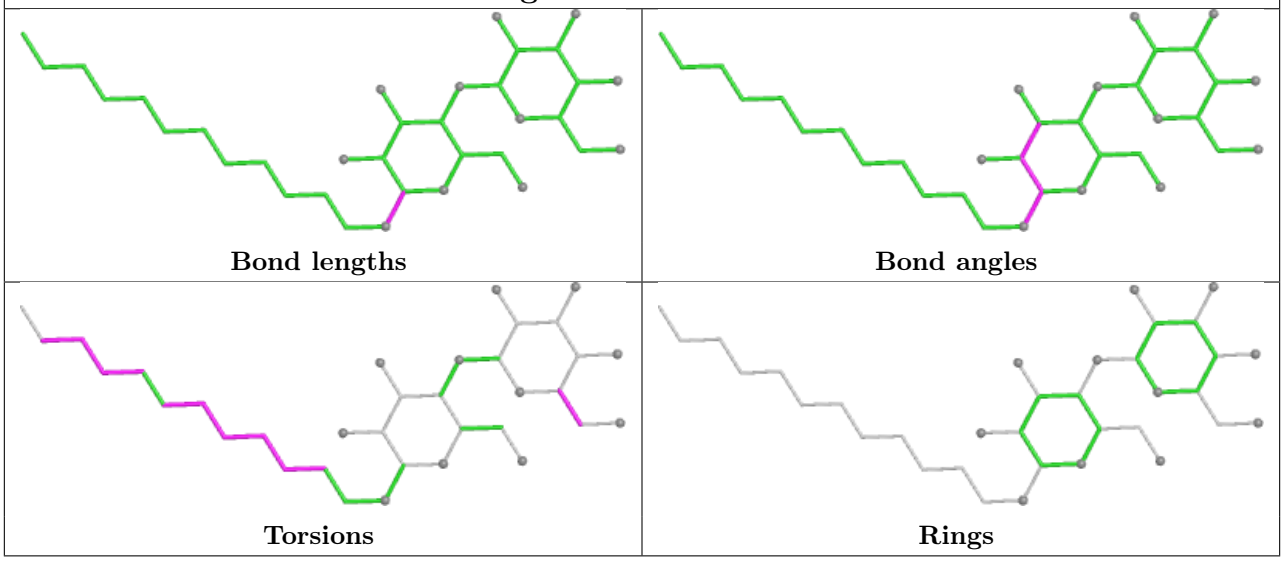
Ligand CLA A 830	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand BCR L 201	
Bond lengths	 Bond angles
 Torsions	 Rings

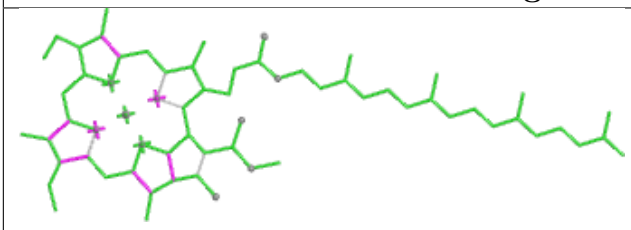
Ligand CLA F 803



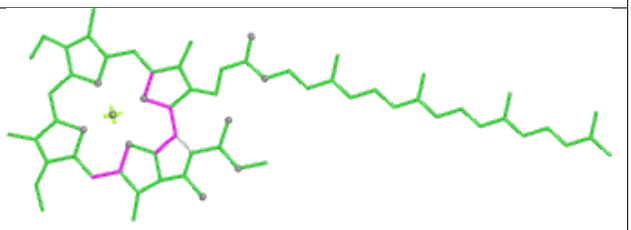
Ligand LMU A 848



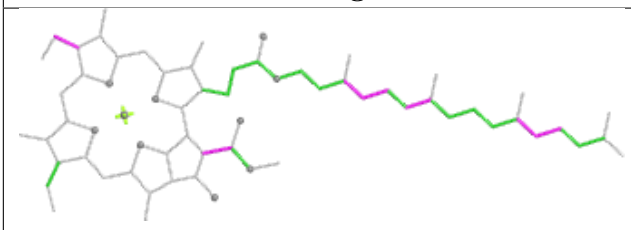
Ligand CLA A 834



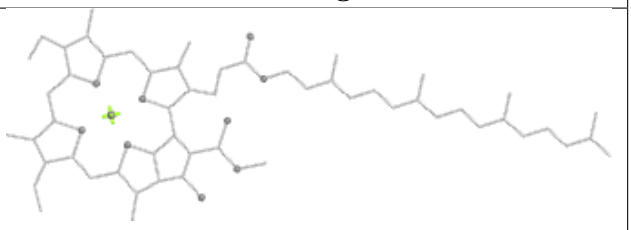
Bond lengths



Bond angles

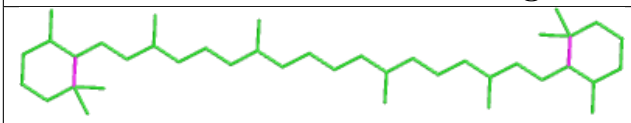


Torsions



Rings

Ligand BCR B 842



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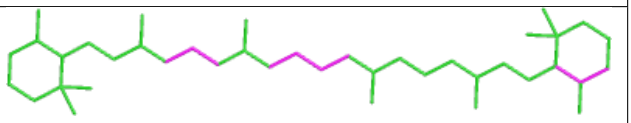
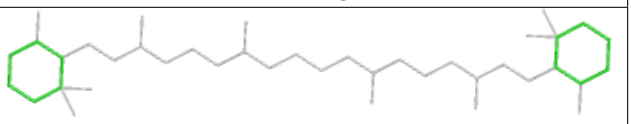


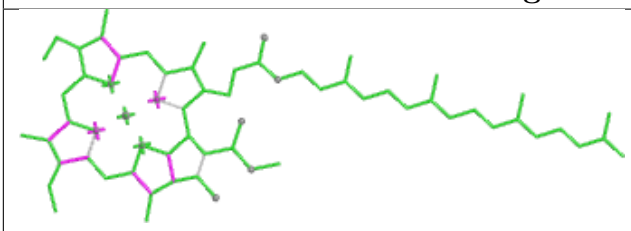
Bond angles

Torsions

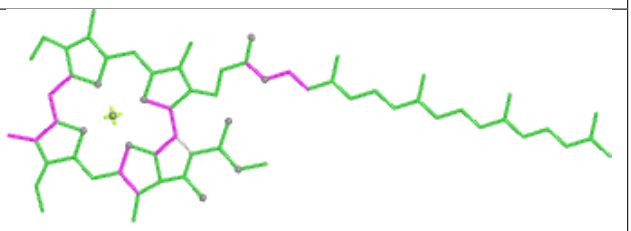


Rings

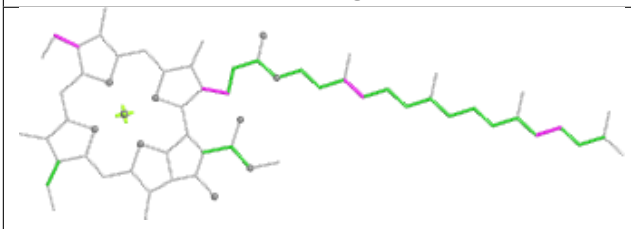
Ligand CLA H 306



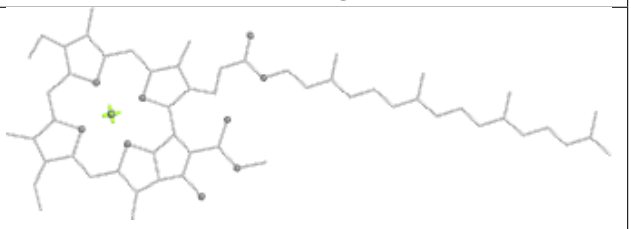
Bond lengths



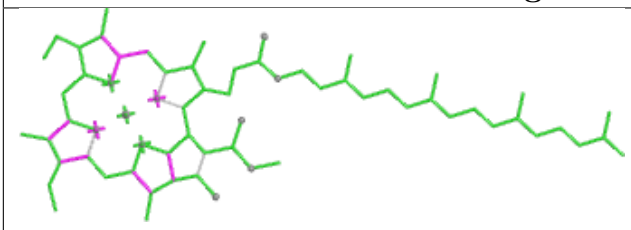
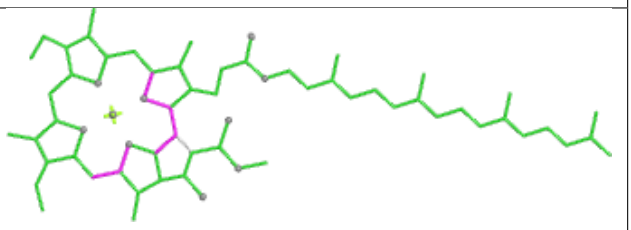
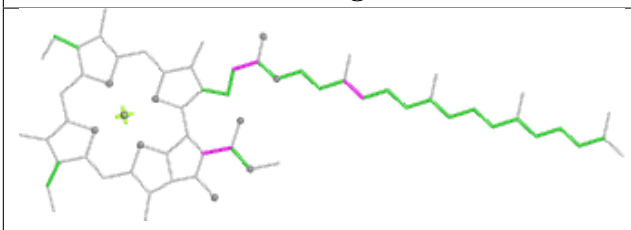
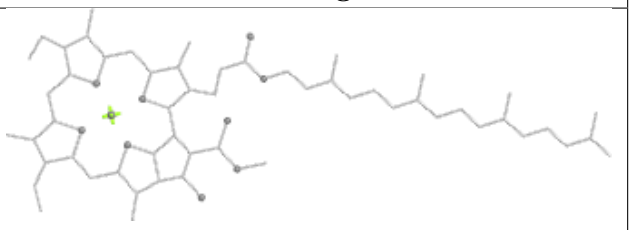
Bond angles

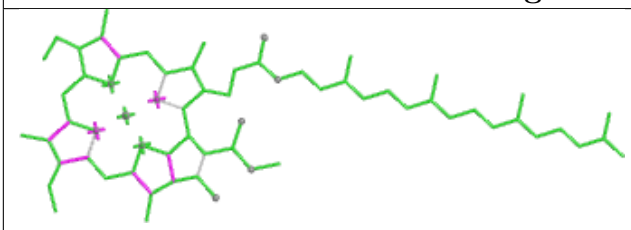
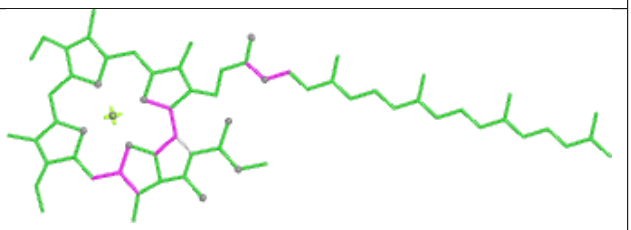
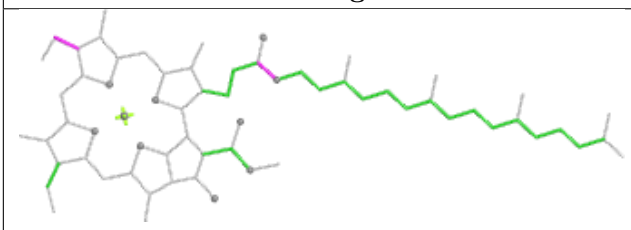
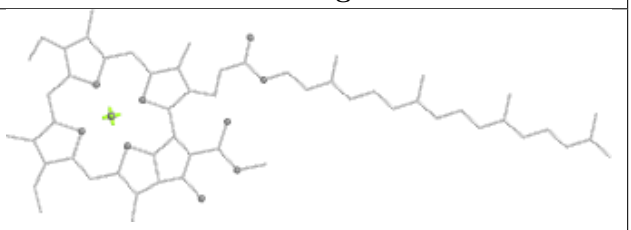


Torsions



Rings

Ligand CLA B 809	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA B 824	
 Bond lengths	 Bond angles
 Torsions	 Rings

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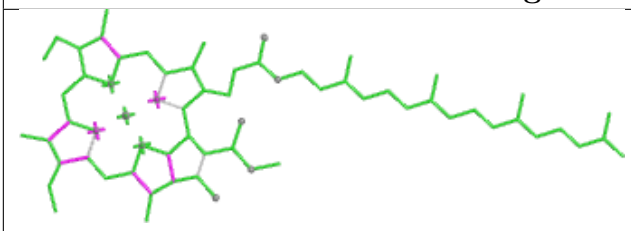
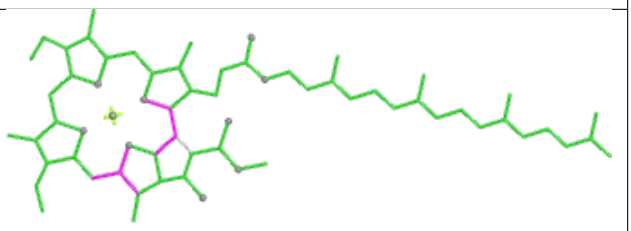
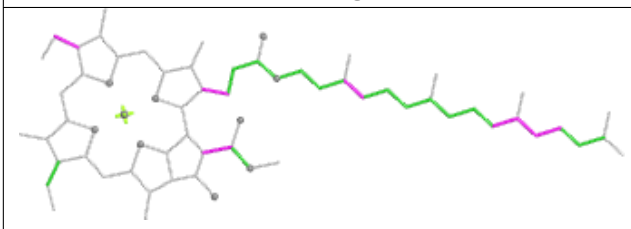
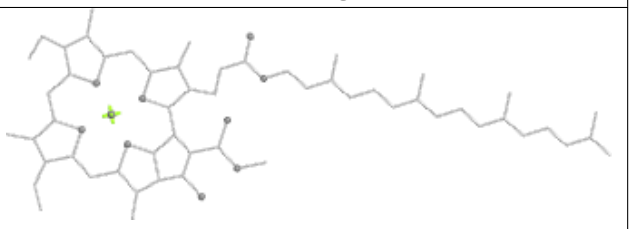
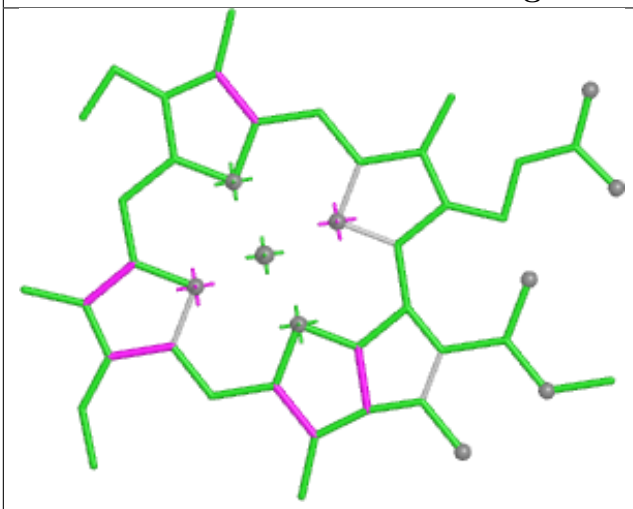
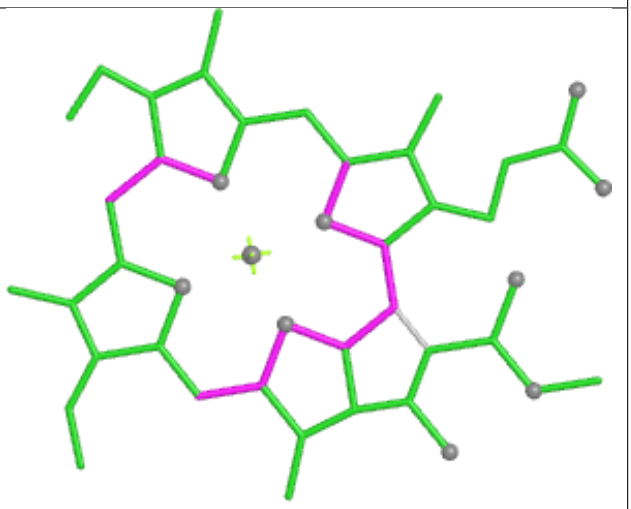
 Bond lengths	 Bond angles
 Torsions	 Rings

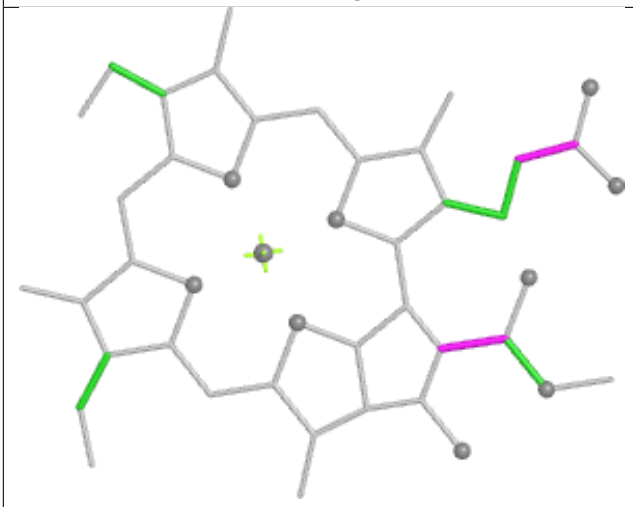
Ligand CLA A 817



Bond lengths

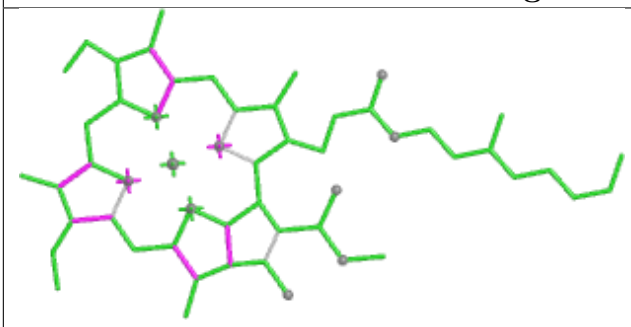
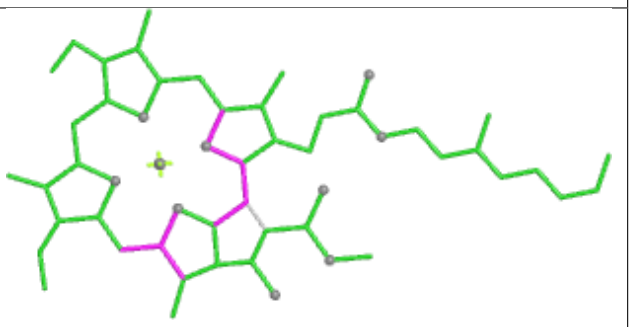
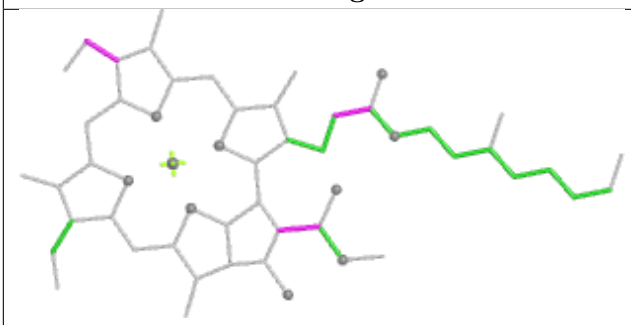
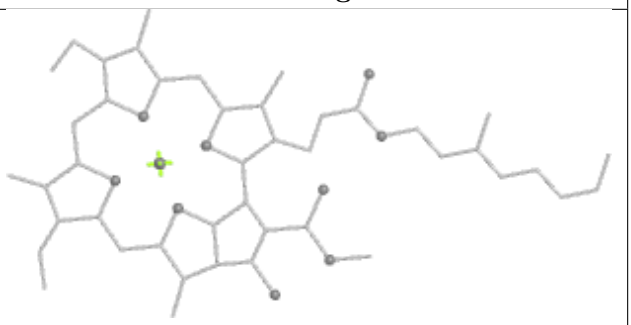


Bond angles

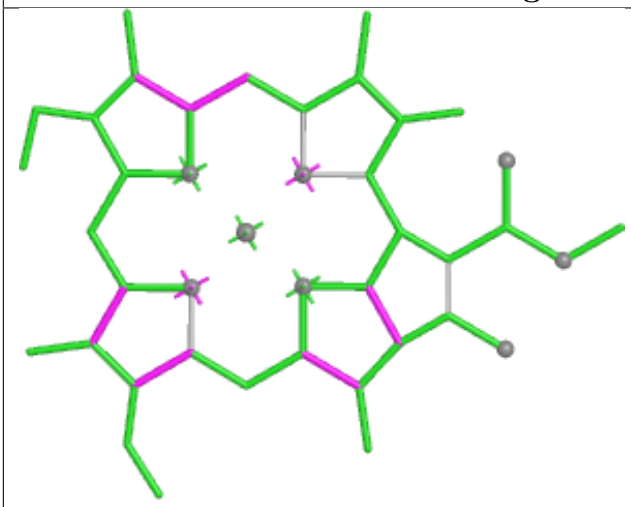


Torsions

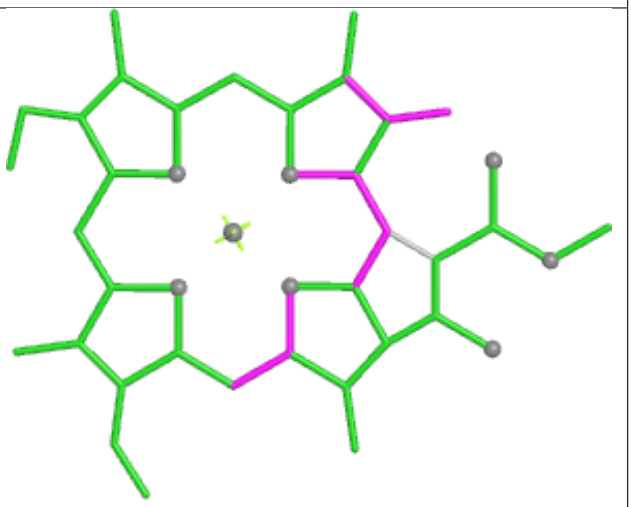
Rings

Ligand CLA A 810	
 Bond lengths	 Bond angles
 Torsions	 Rings

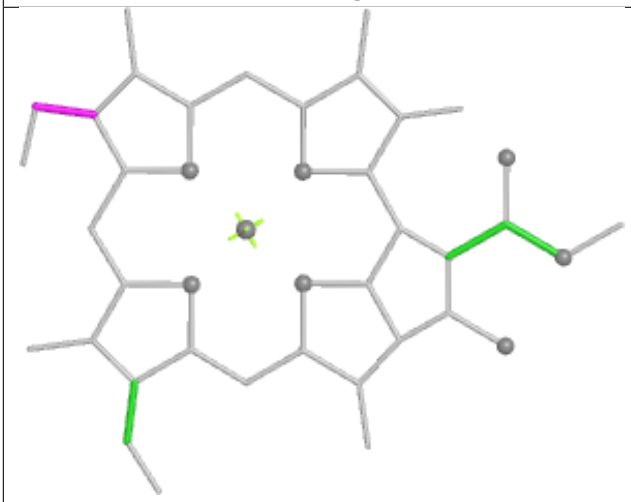
Ligand CLA G 302



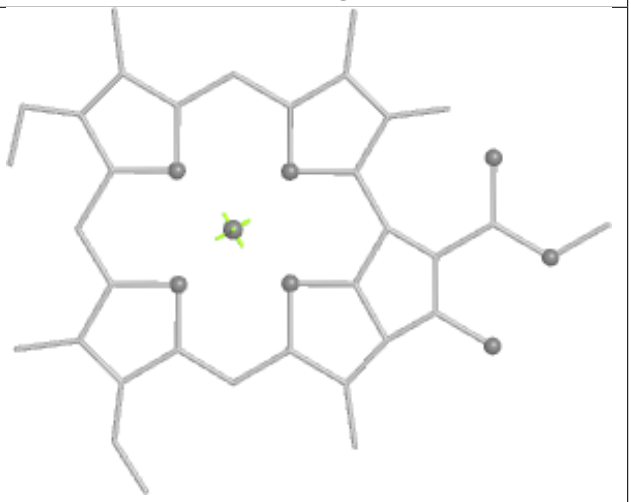
Bond lengths



Bond angles

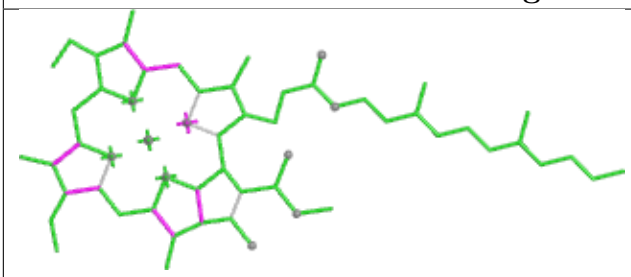


Torsions

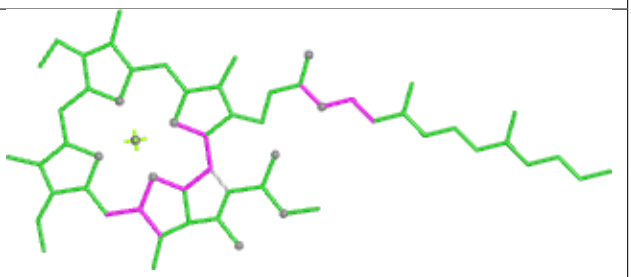


Rings

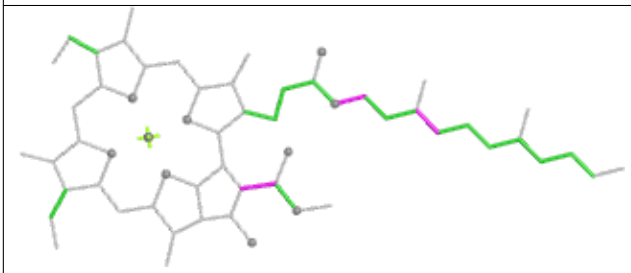
Ligand CLA K 205



Bond lengths



Bond angles



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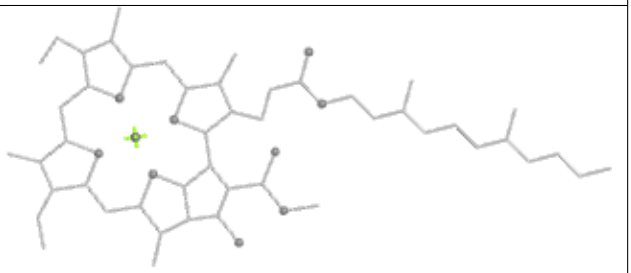
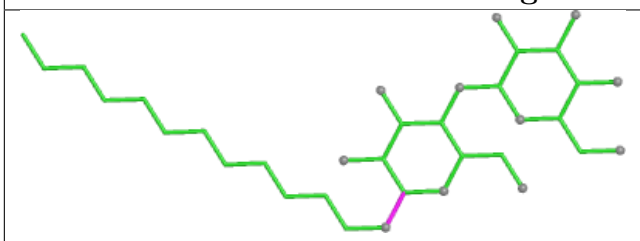
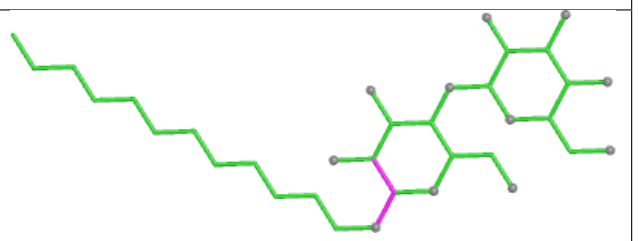
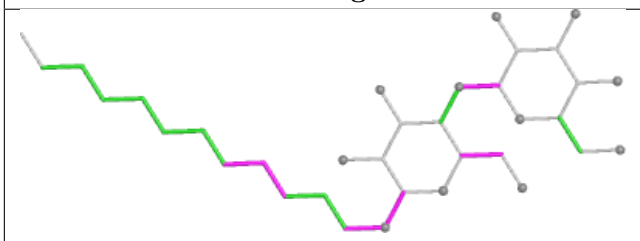
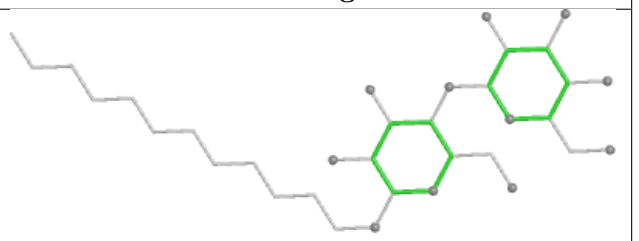
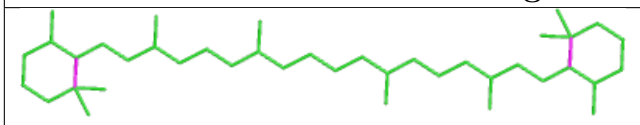
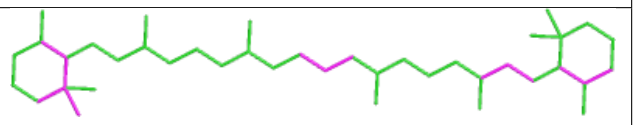
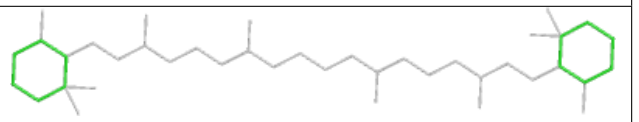
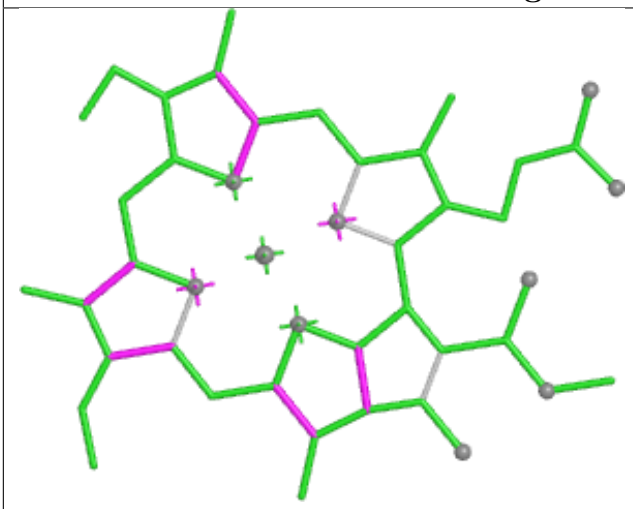


Rings

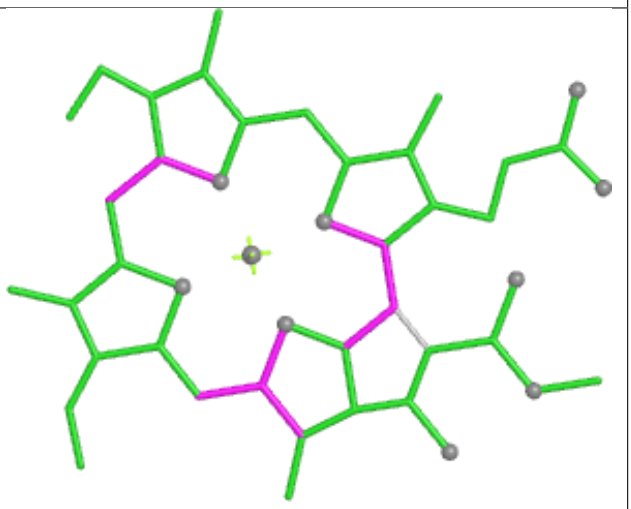
Ligand LMU A 855	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand BCR B 840	
 Bond lengths	 Bond angles
Torsions	 Rings

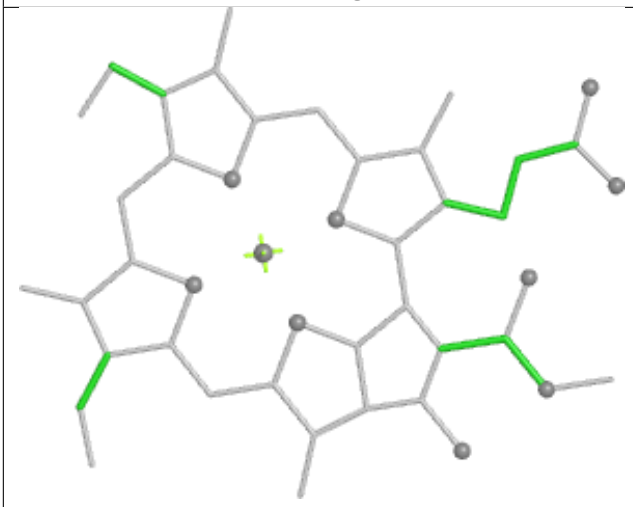
Ligand CLA B 830



Bond lengths



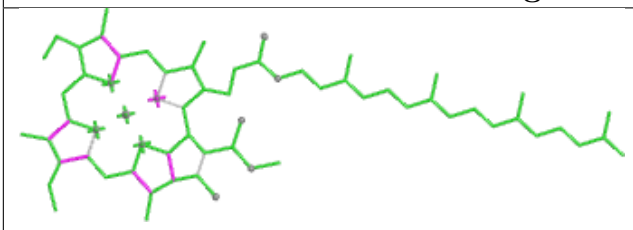
Bond angles



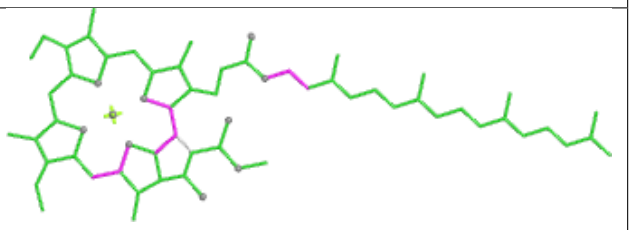
Torsions

Rings

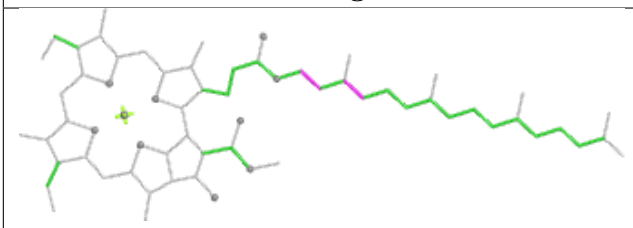
Ligand CLA A 818



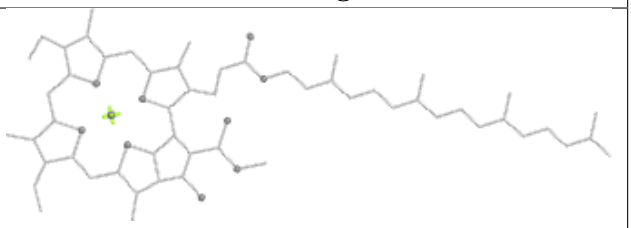
Bond lengths



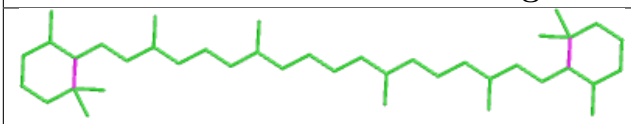
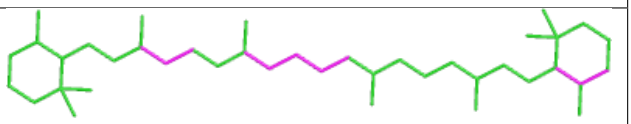
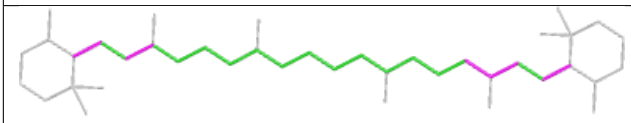
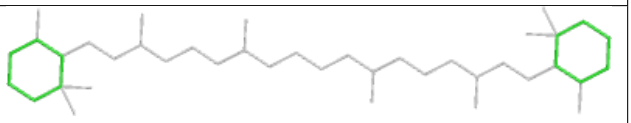
Bond angles

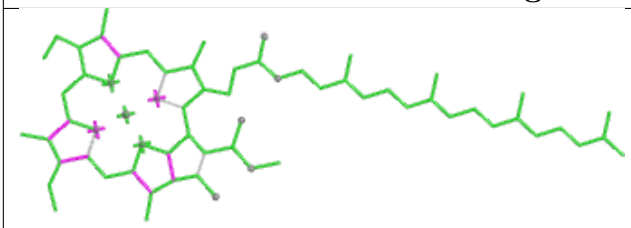
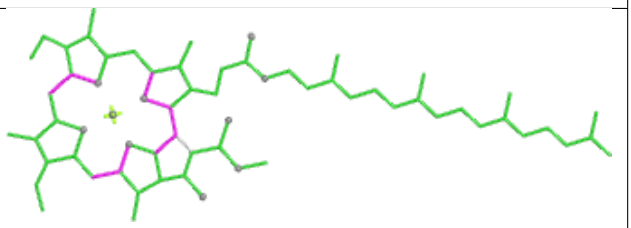
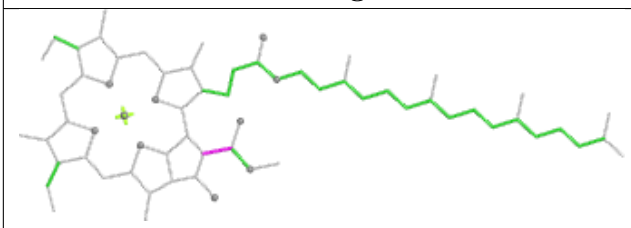
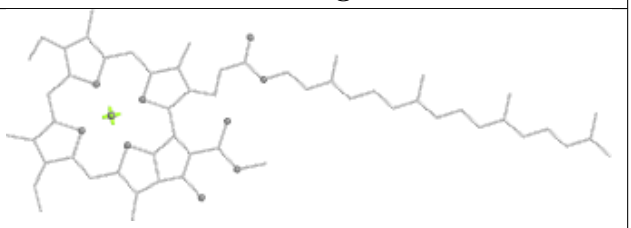


Torsions

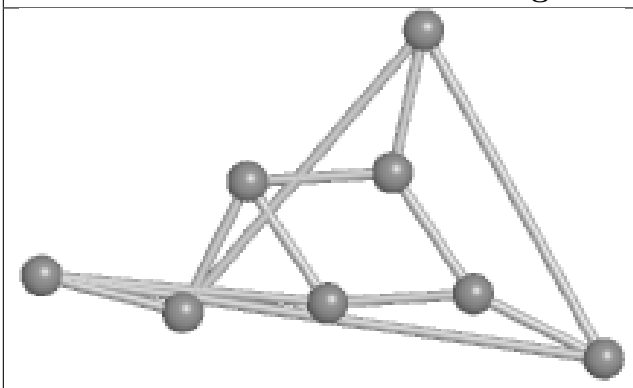


Rings

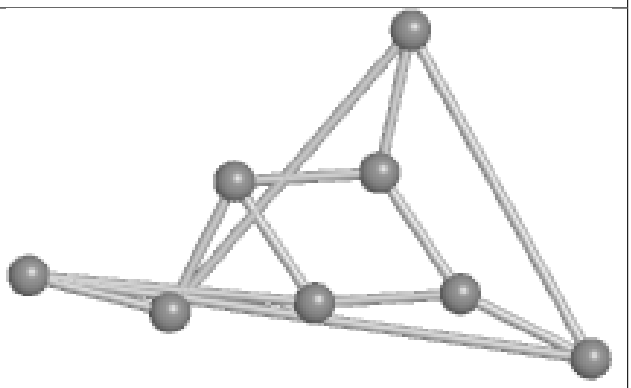
Ligand BCR A 842	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA B 822	
 Bond lengths	 Bond angles
 Torsions	 Rings

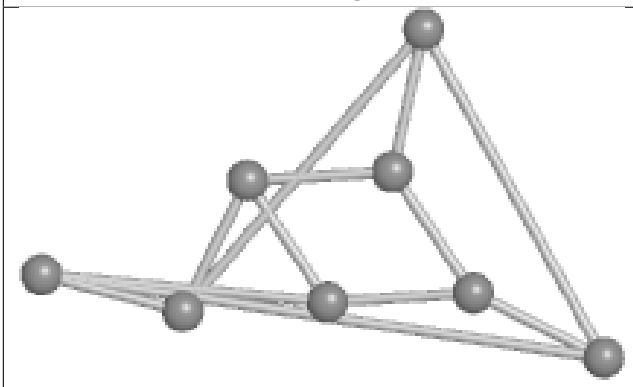
Ligand SF4 C 101



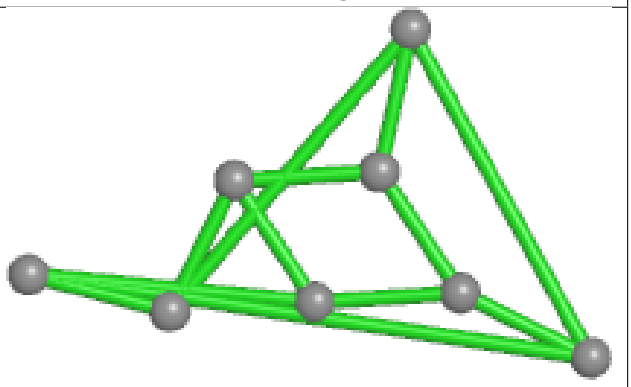
Bond lengths



Bond angles

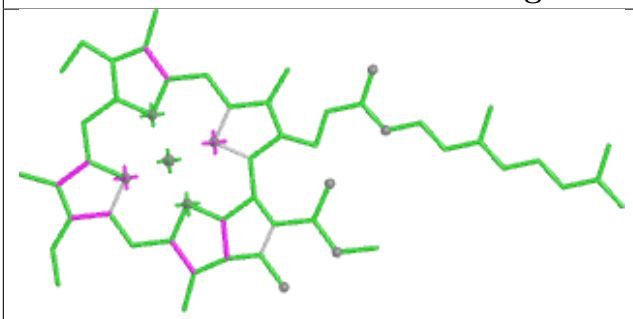


Torsions

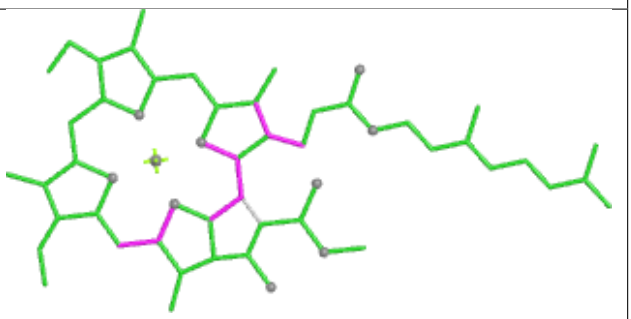


Rings

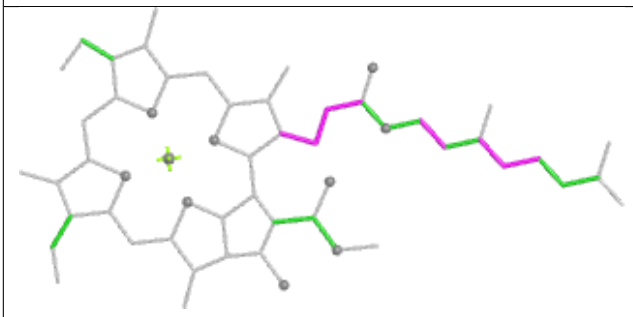
Ligand CLA B 814



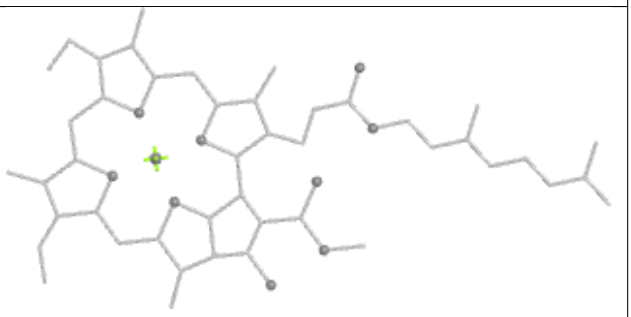
Bond lengths



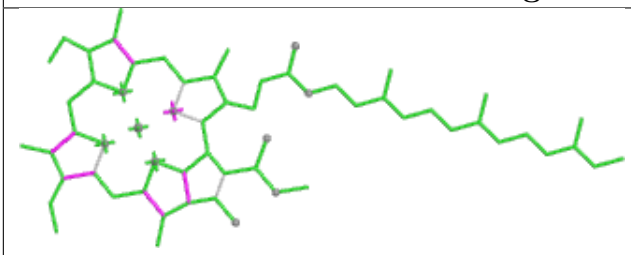
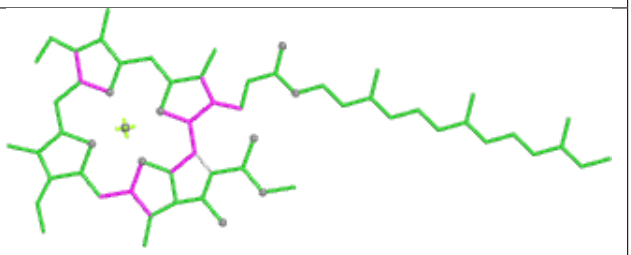
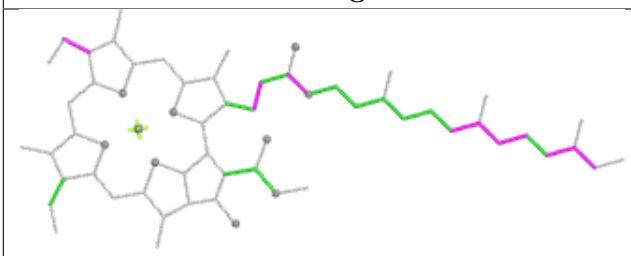
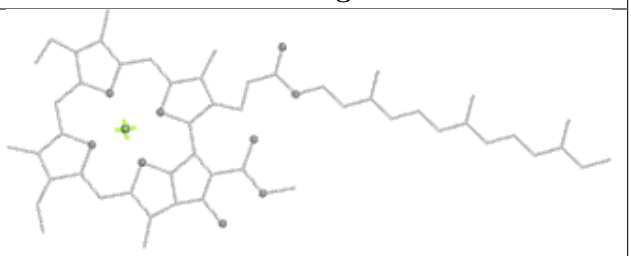
Bond angles

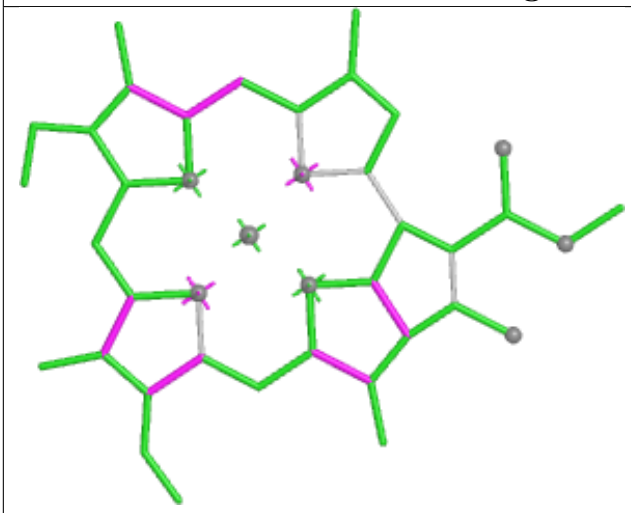
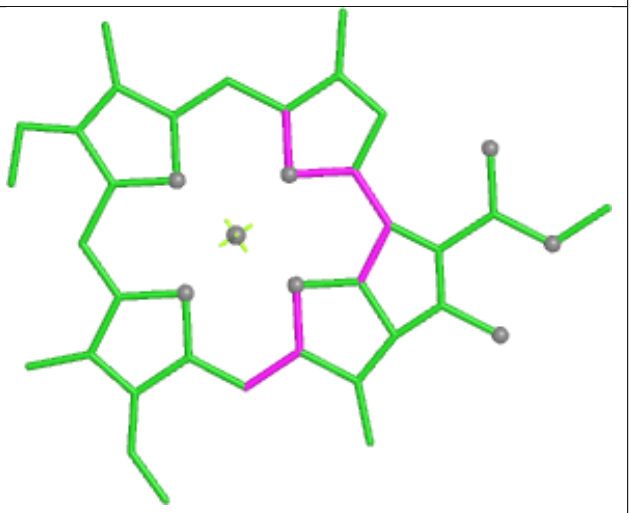
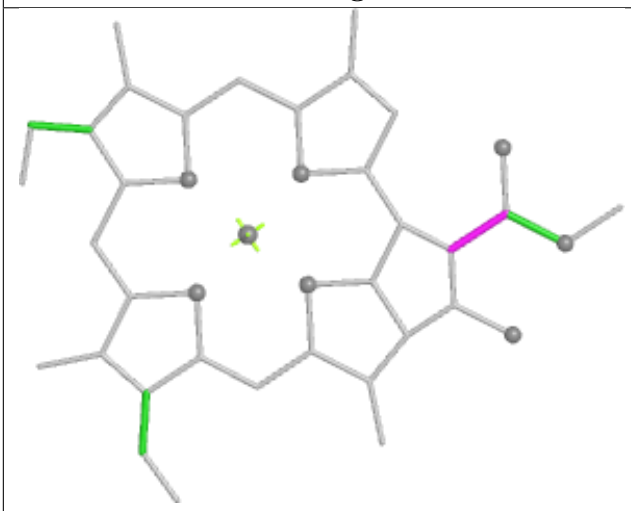
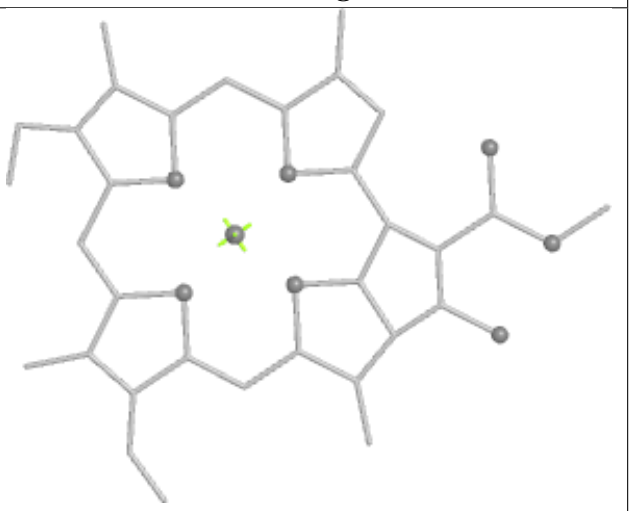


Torsions

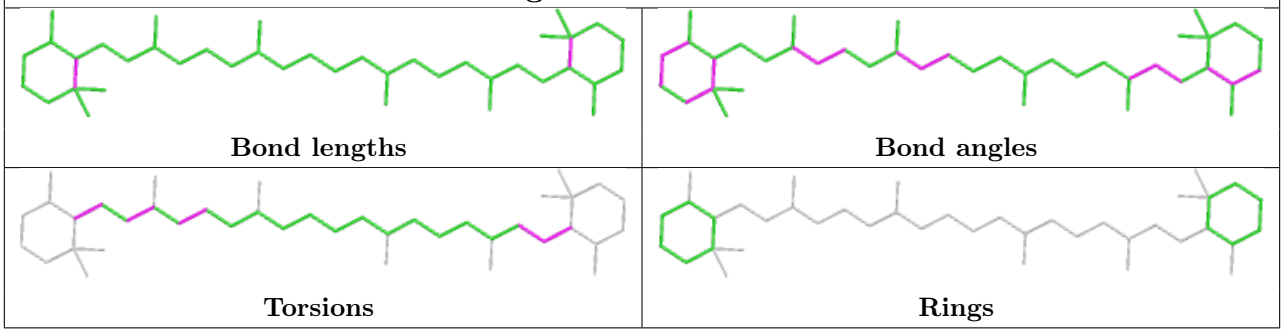


Rings

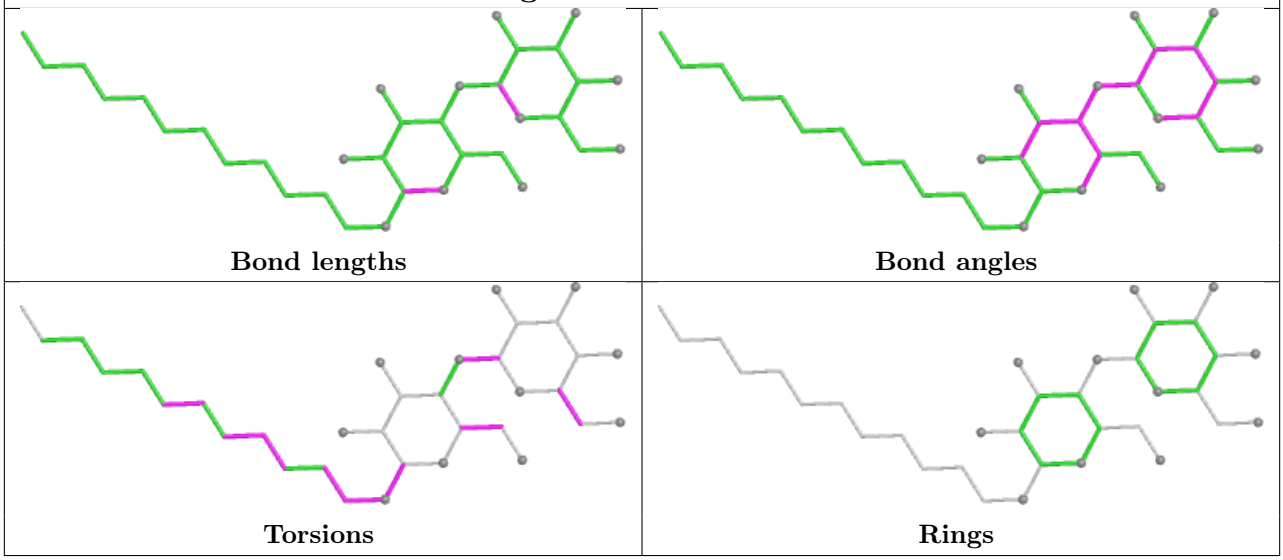
Ligand CLA G 305	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA K 206	
 Bond lengths	 Bond angles
 Torsions	 Rings

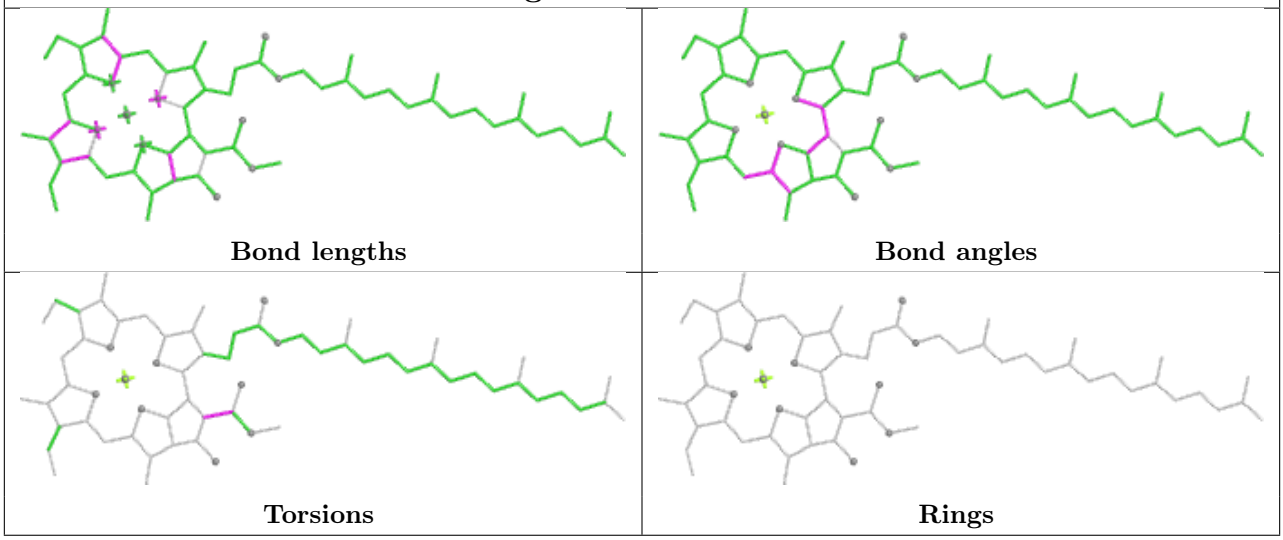
Ligand BCR L 205

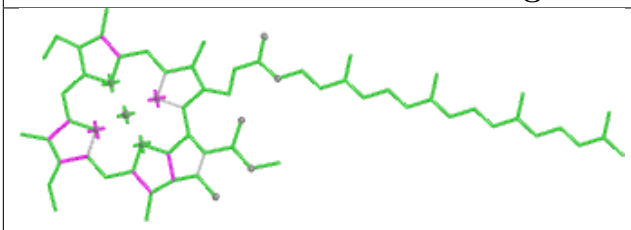
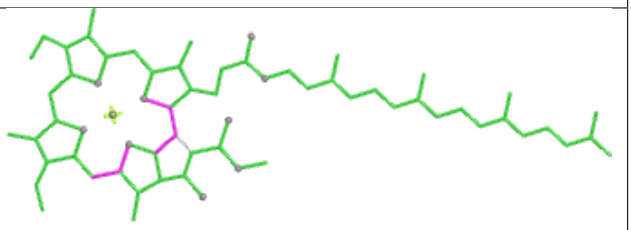
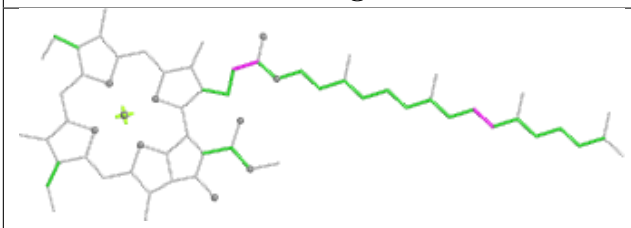
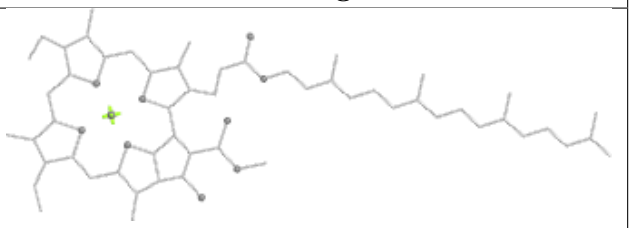


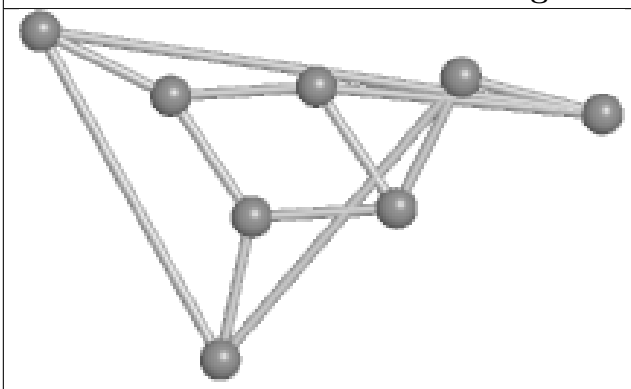
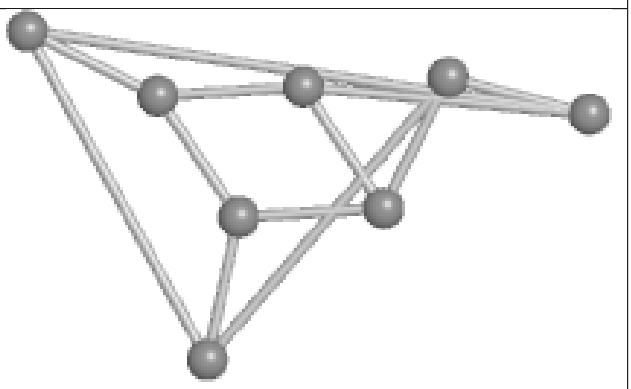
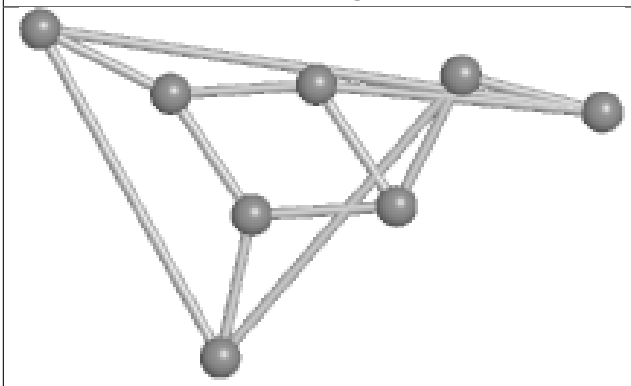
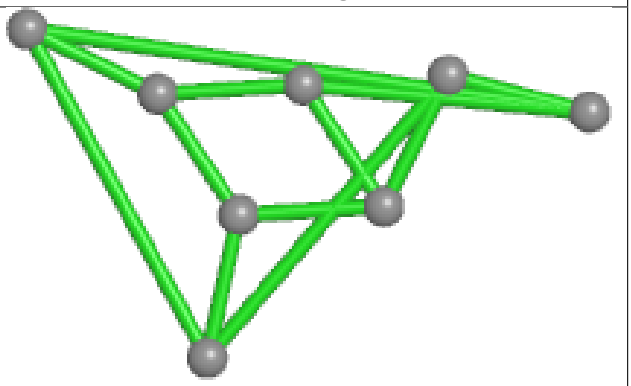
Ligand LMU K 201

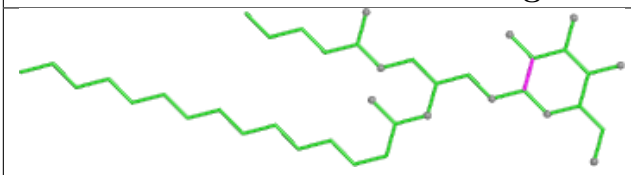
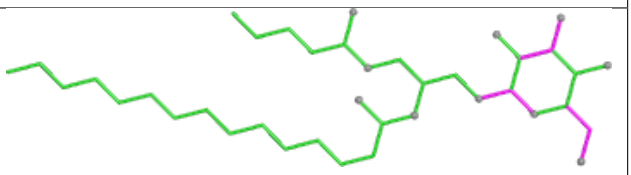
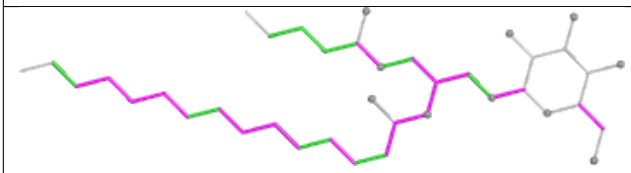
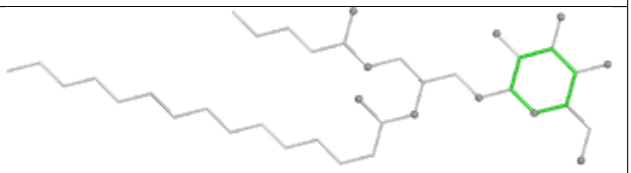


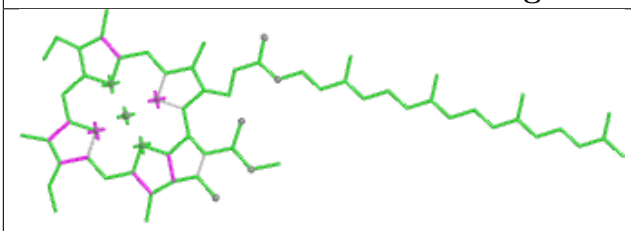
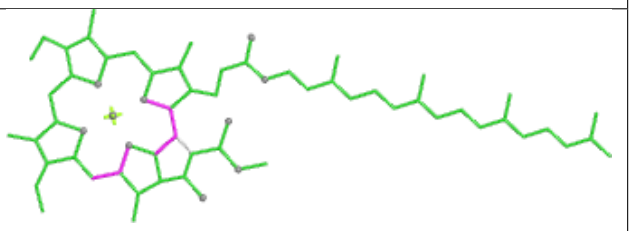
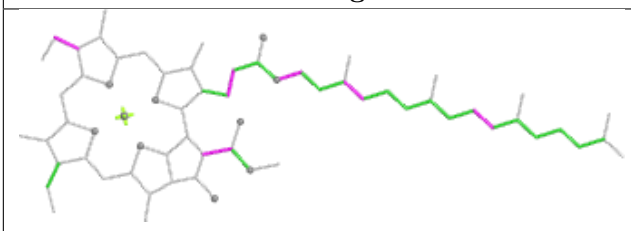
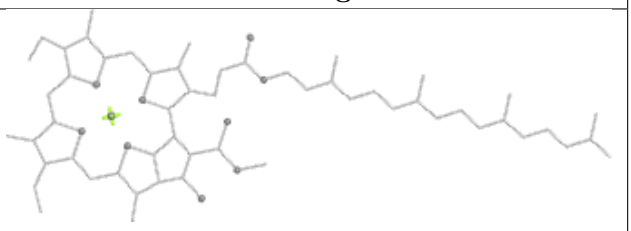
Ligand CLA A 816



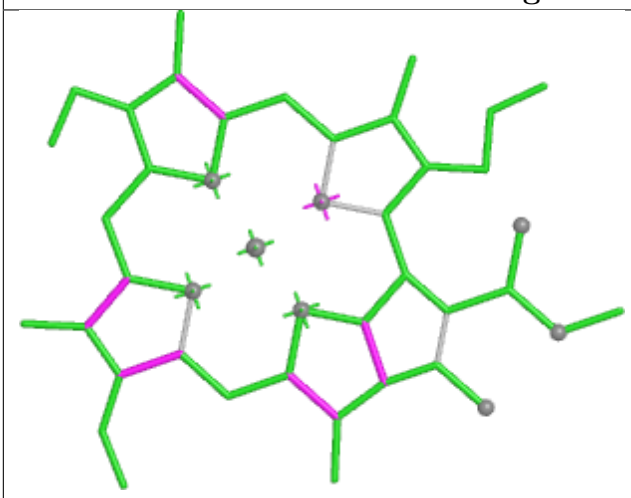
Ligand CLA A 811	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand SF4 A 852	
 Bond lengths	 Bond angles
 Torsions	 Rings

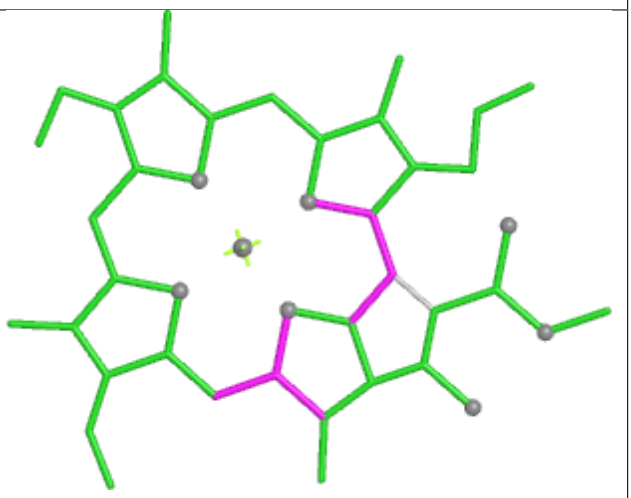
Ligand LMG J 103	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA A 845	
 Bond lengths	 Bond angles
 Torsions	 Rings

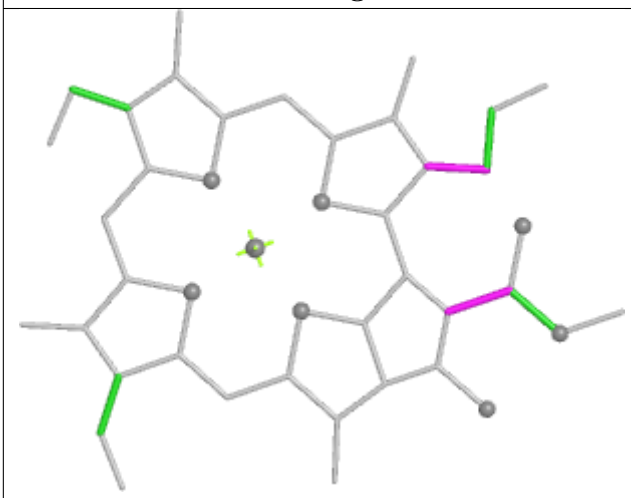
Ligand CLA G 304



Bond lengths



Bond angles



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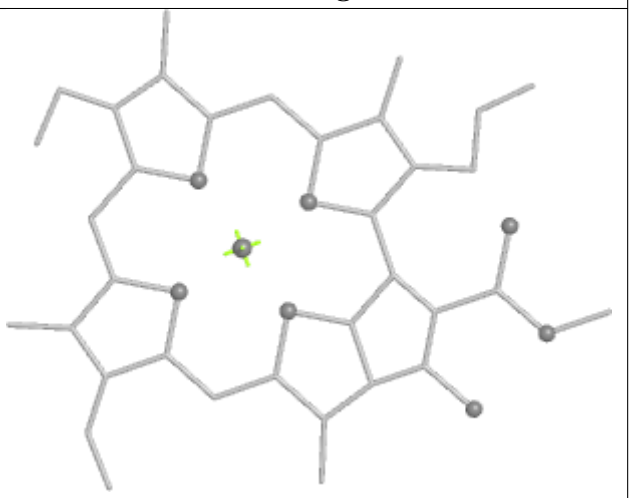
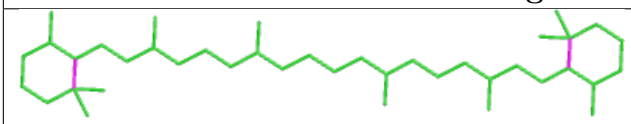


Rings

Ligand BCR J 105



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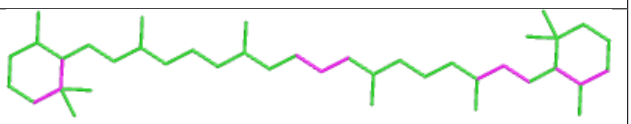
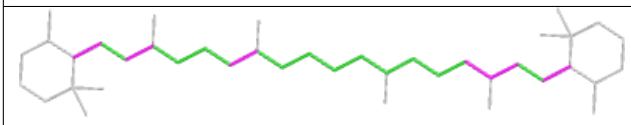


Bond angles



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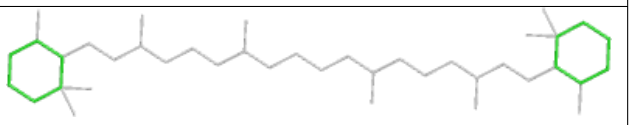
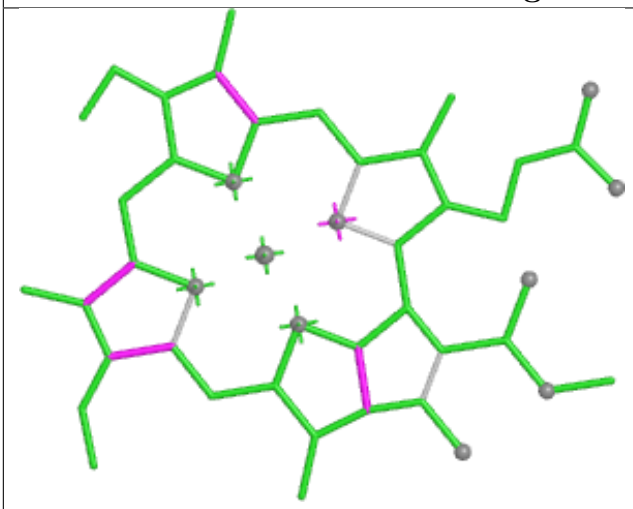
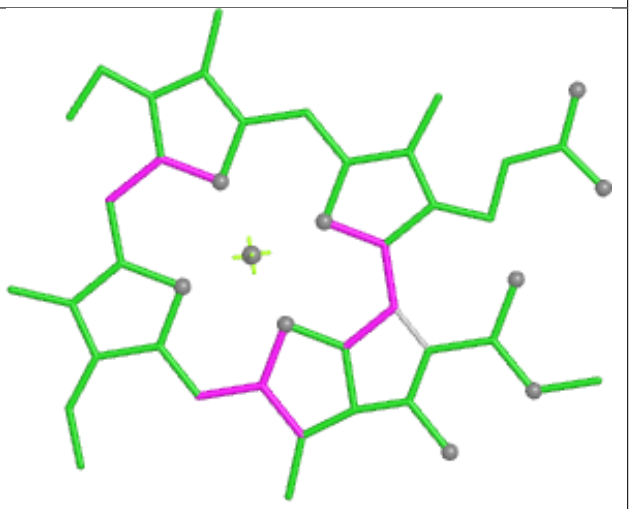


Rings

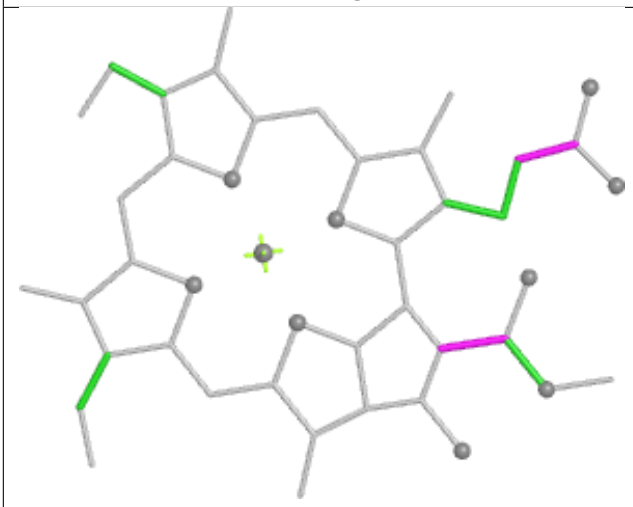
Ligand CLA A 831



Bond lengths



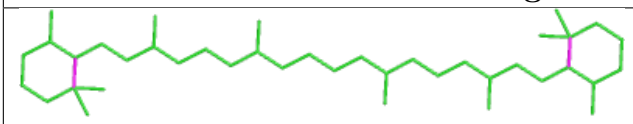
Bond angles



Torsions

Rings

Ligand BCR F 801



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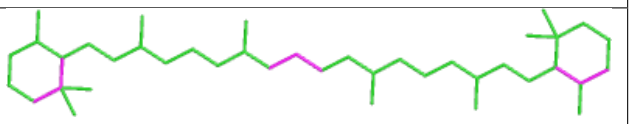
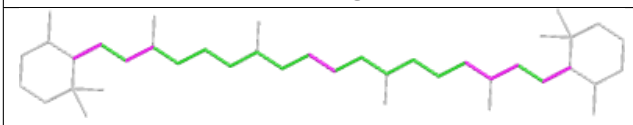
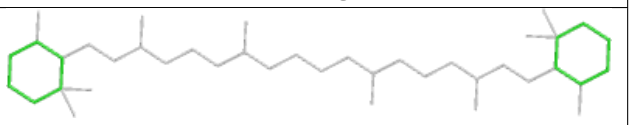


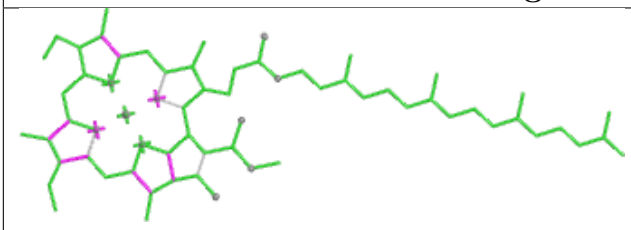
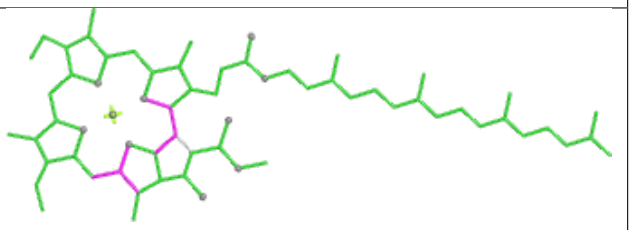
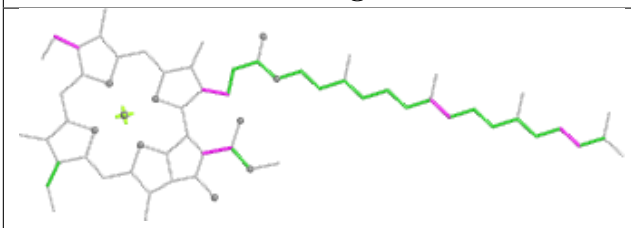
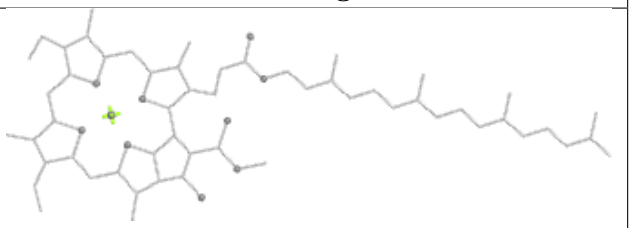
Bond angles

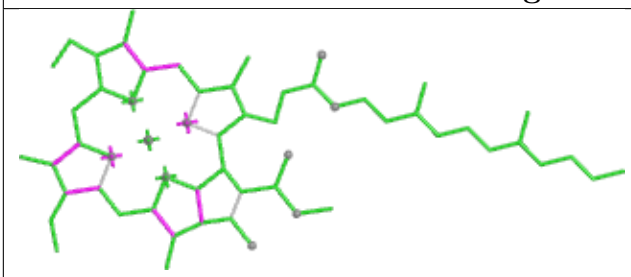
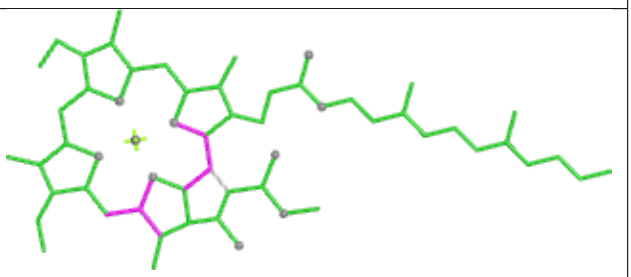
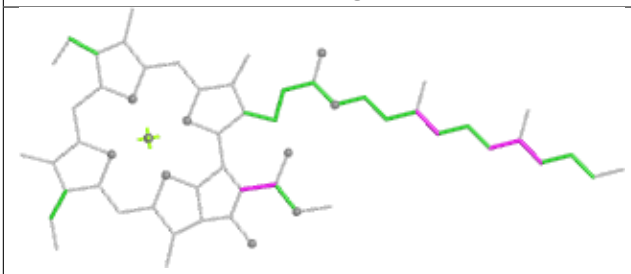
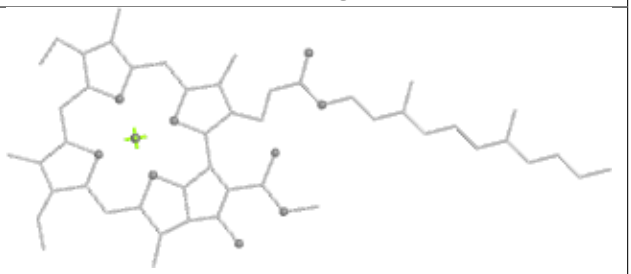


Torsions



Rings

Ligand CLA B 805	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA H 307	
 Bond lengths	 Bond angles
 Torsions	 Rings

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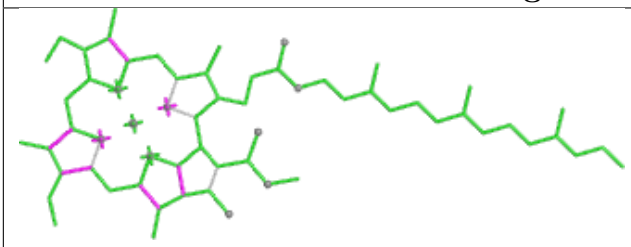
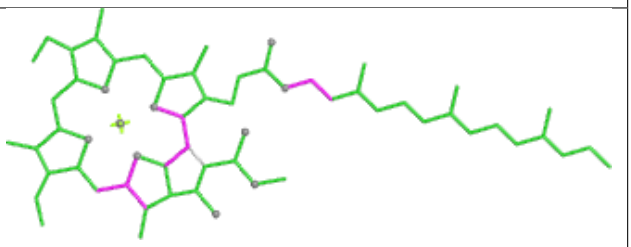
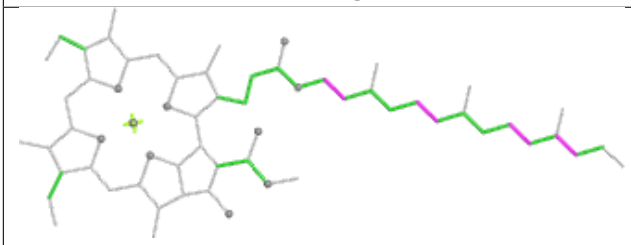
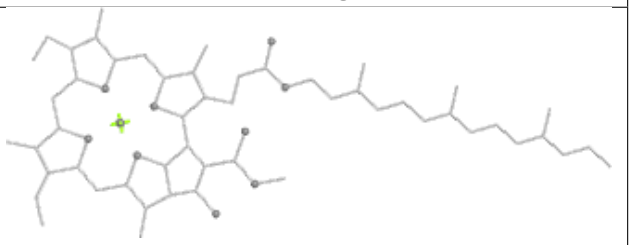
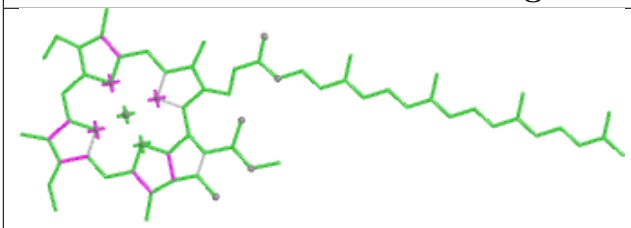
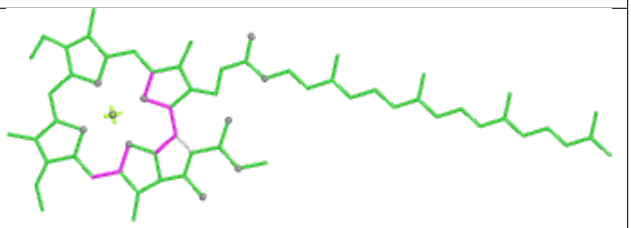
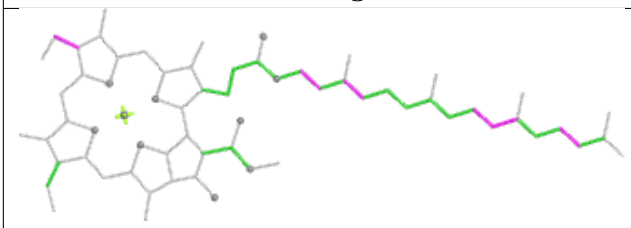
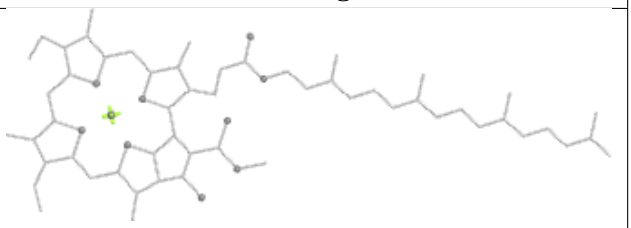
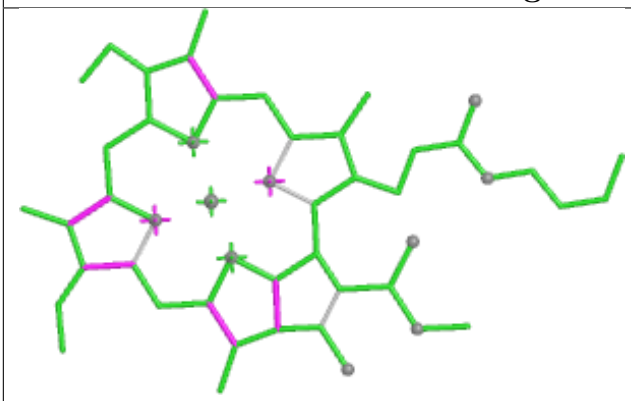
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA B 835	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA A 805



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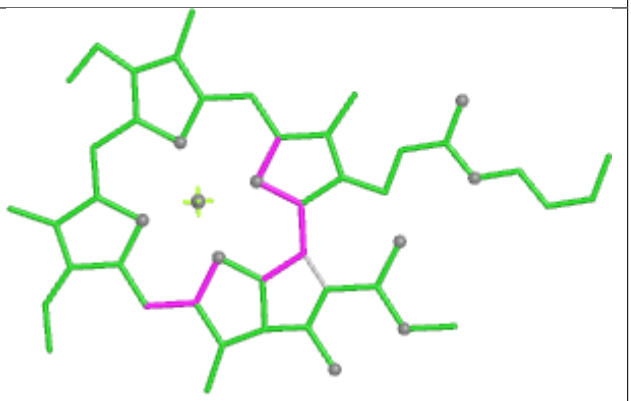
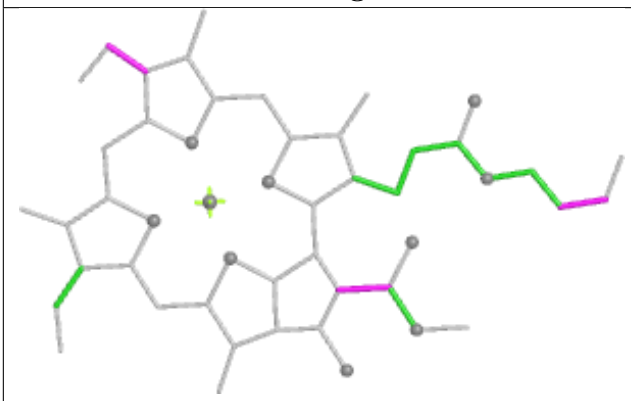


Bond angles



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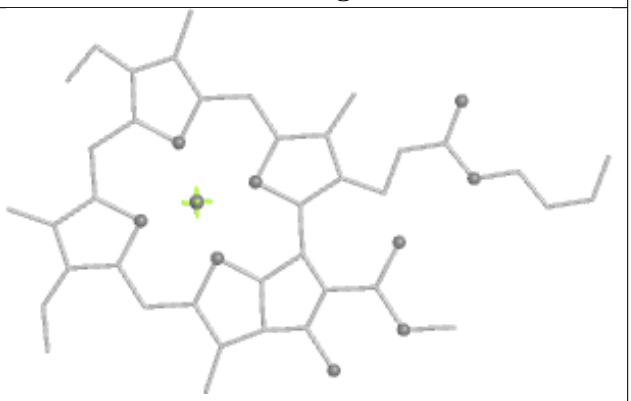
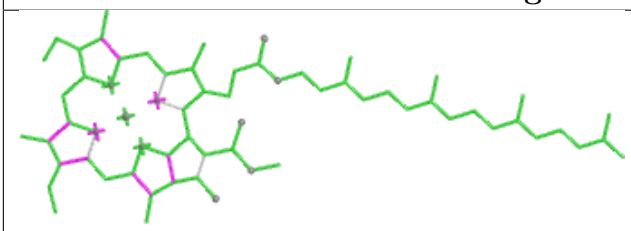


Rings

Ligand CLA B 807



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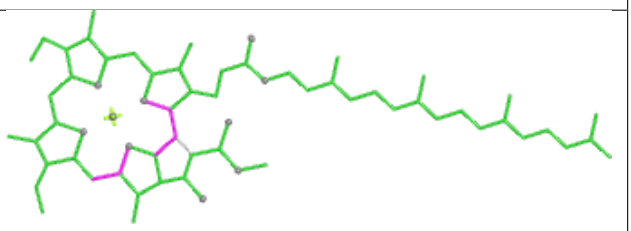
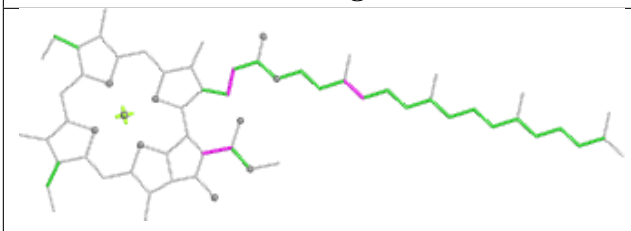
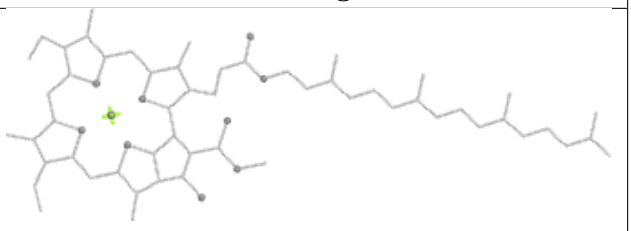


Bond angles

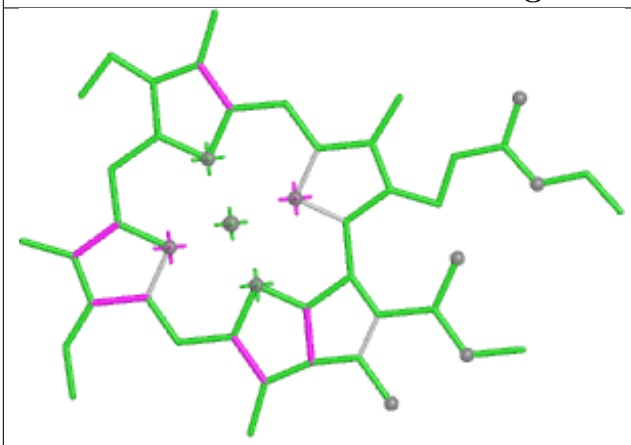


Torsions



Rings

Ligand CLA B 833



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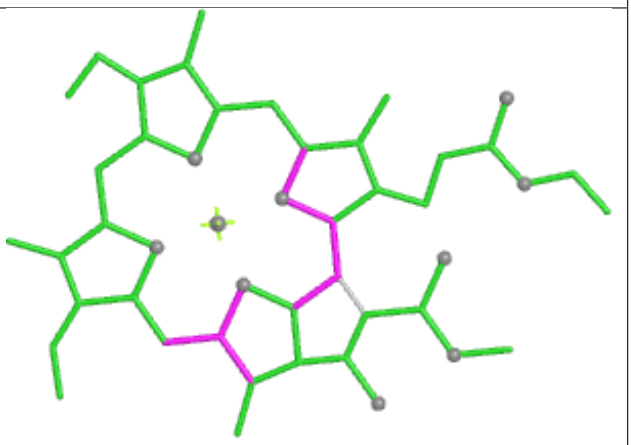
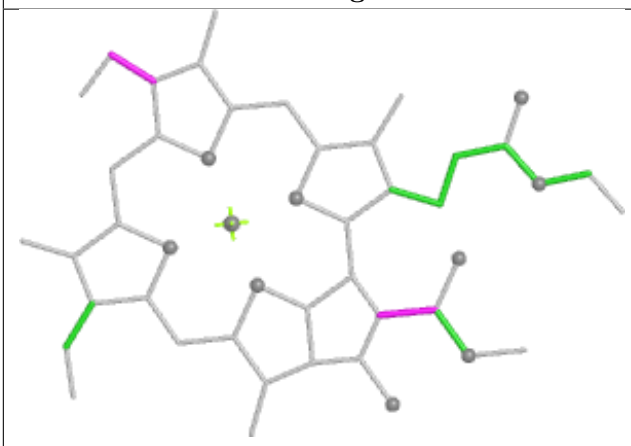


Bond angles



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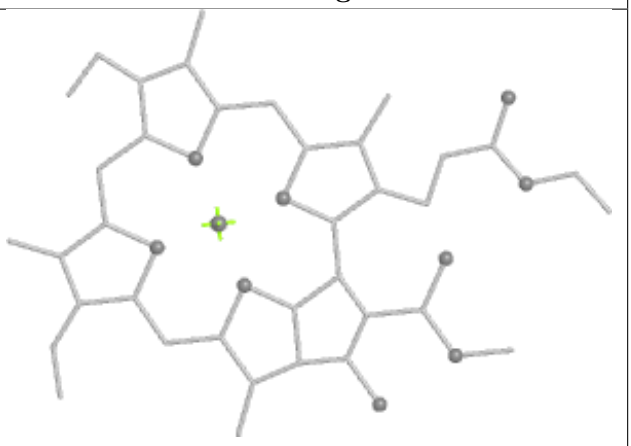
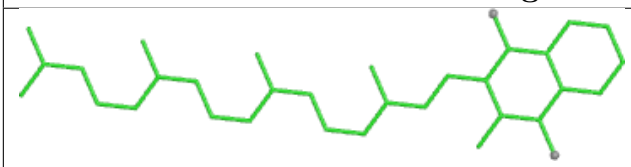


Rings

Ligand PQN A 837



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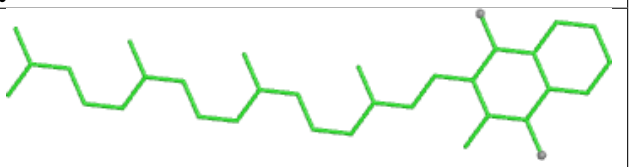

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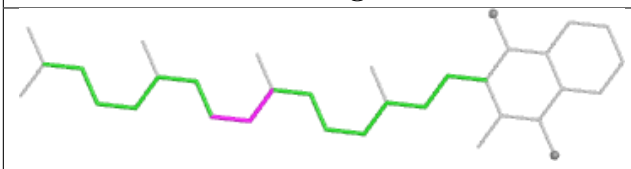

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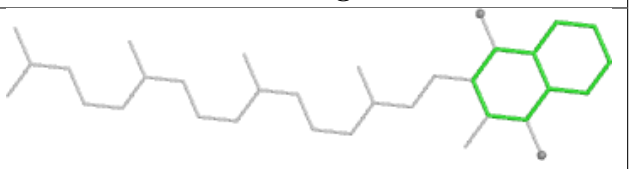
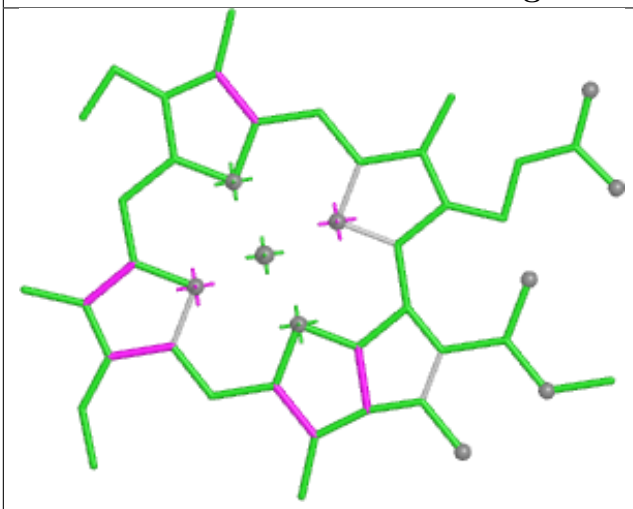
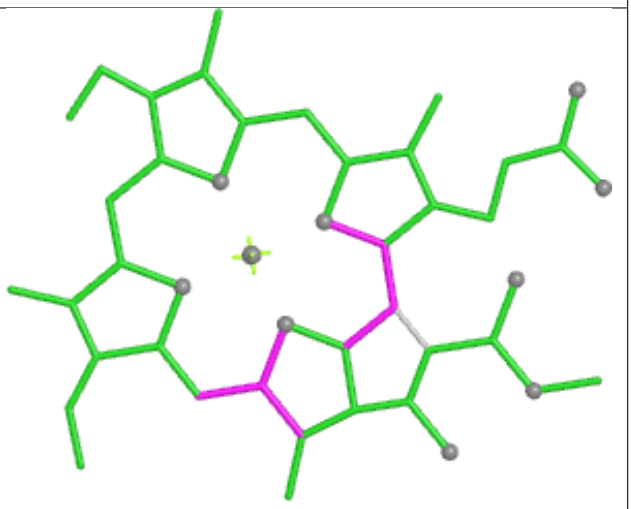


Rings

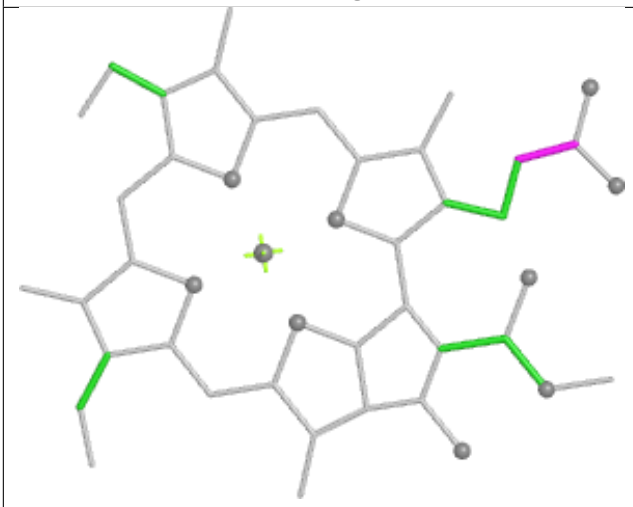
Ligand CLA U 206



Bond lengths



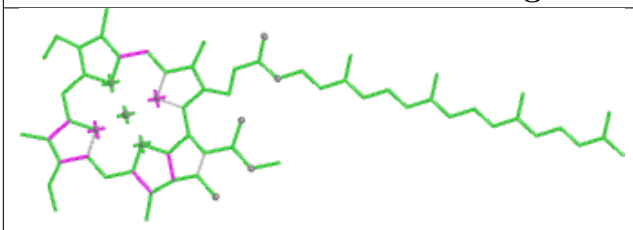
Bond angles



Torsions

Rings

Ligand CLA A 828



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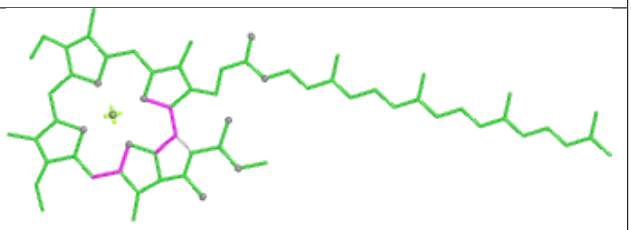
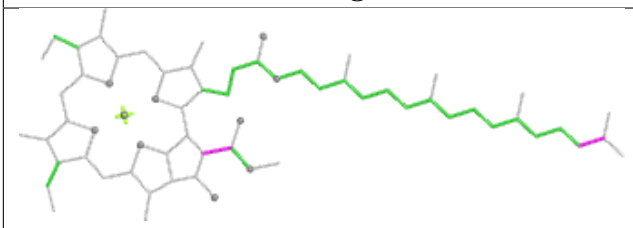
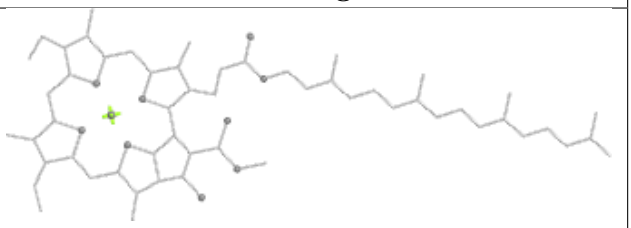


Bond angles

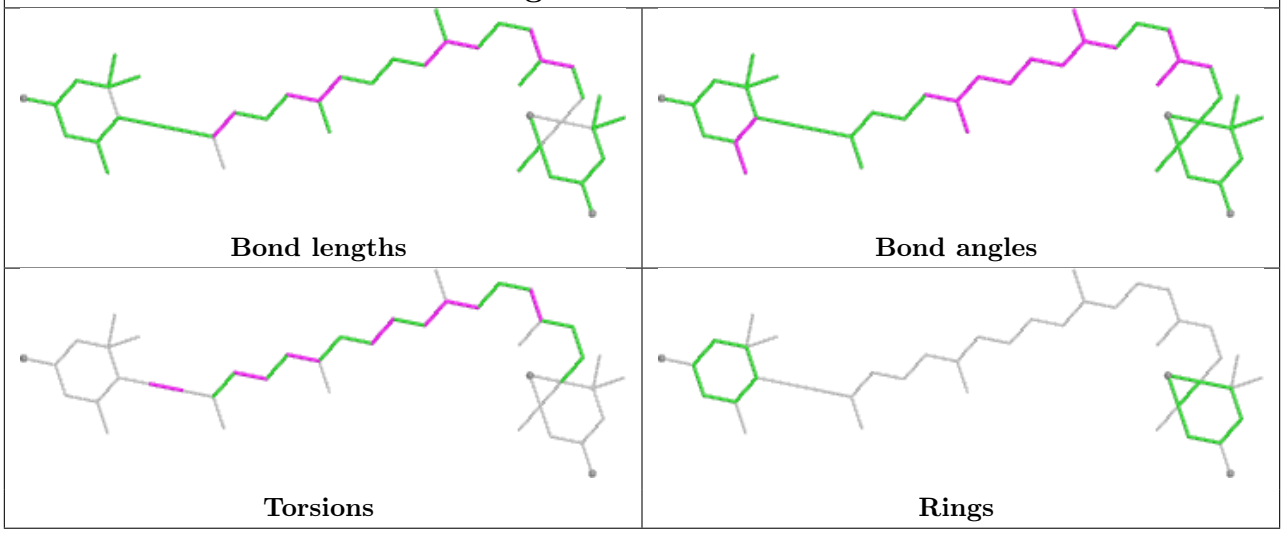


Torsions

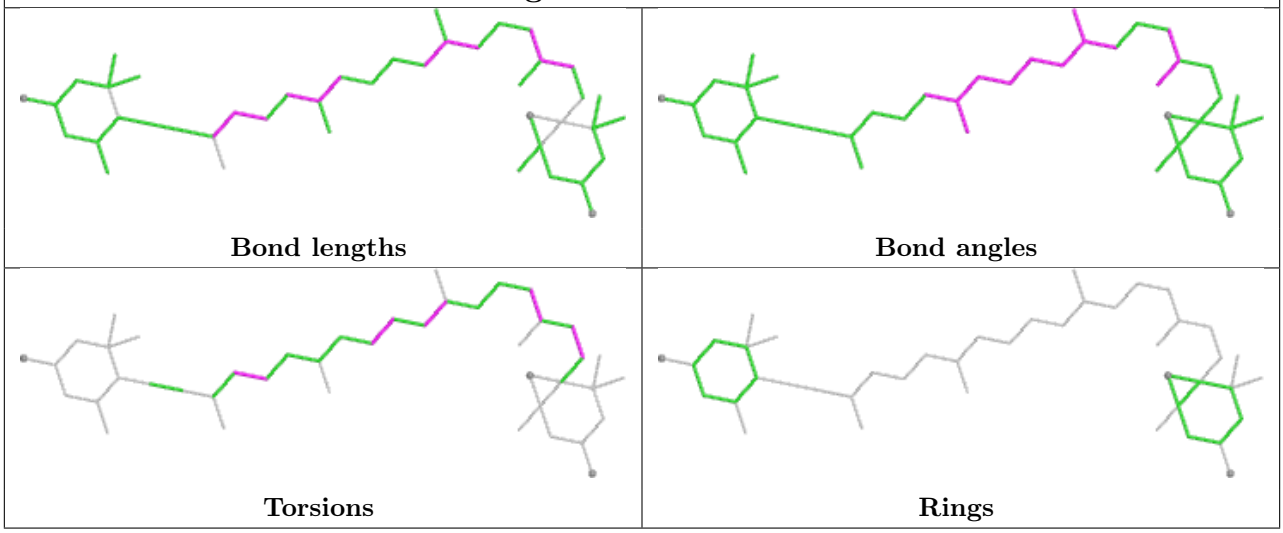


Rings

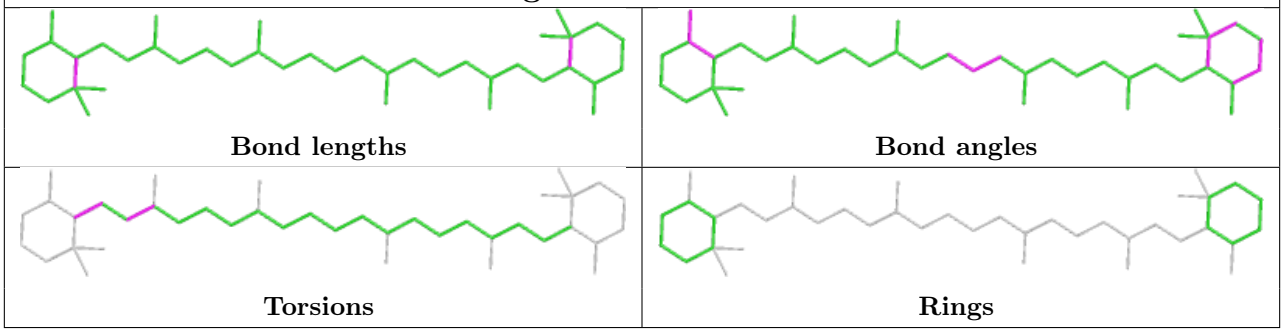
Ligand DD6 K 208

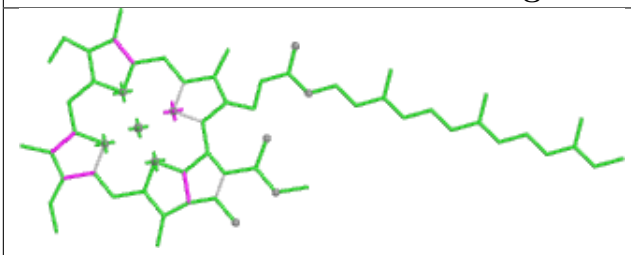
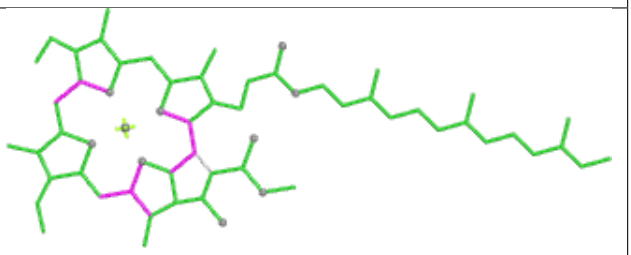
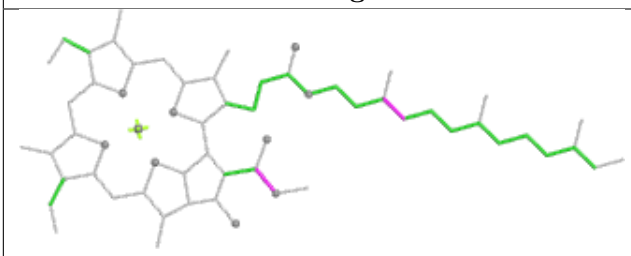
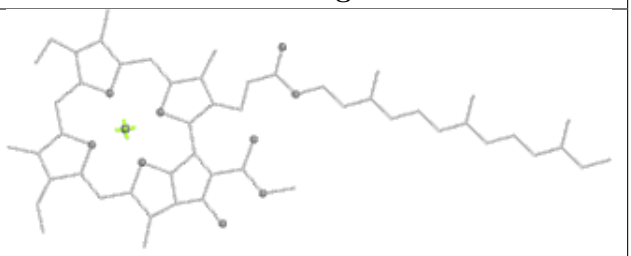


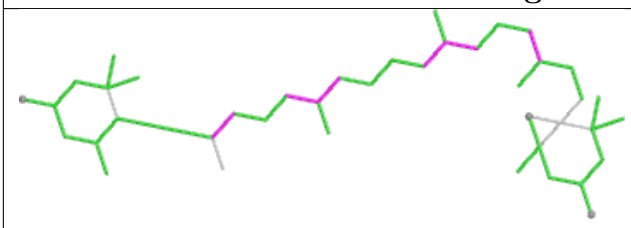
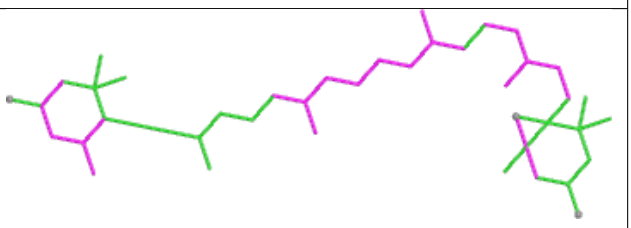
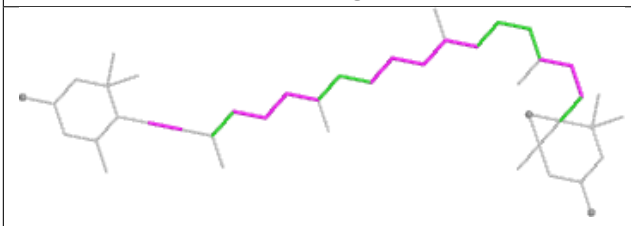
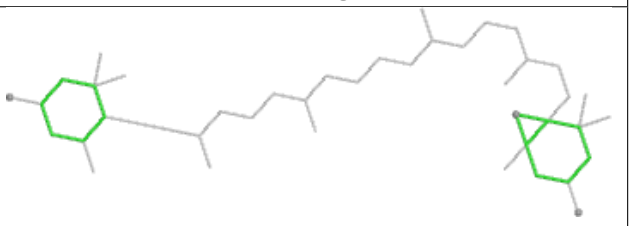
Ligand DD6 G 311



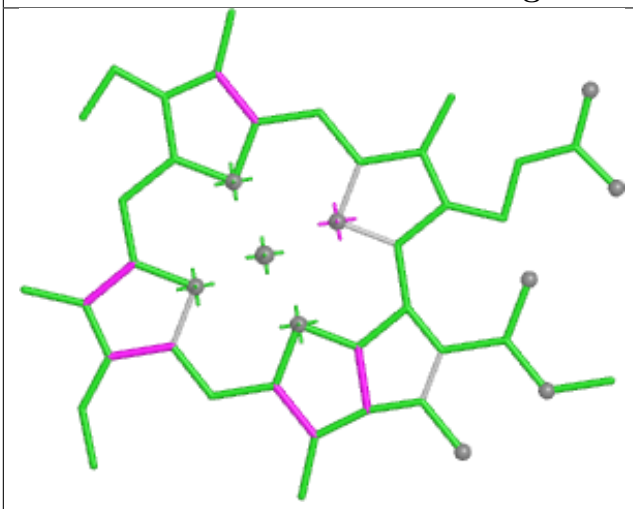
Ligand BCR A 843



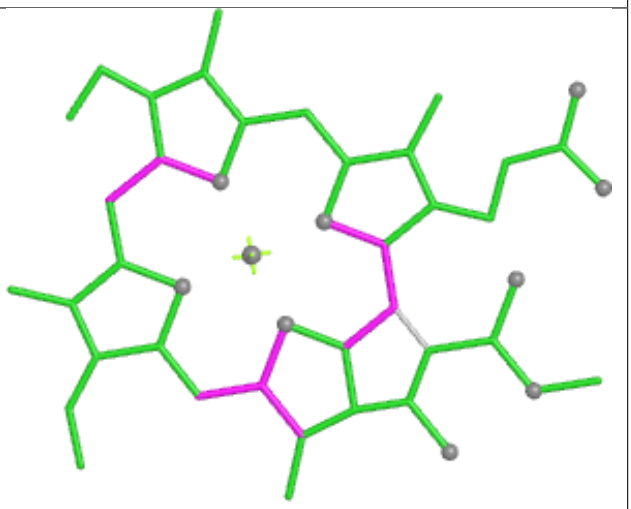
Ligand CLA H 303	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand DD6 U 212	
 Bond lengths	 Bond angles
 Torsions	 Rings

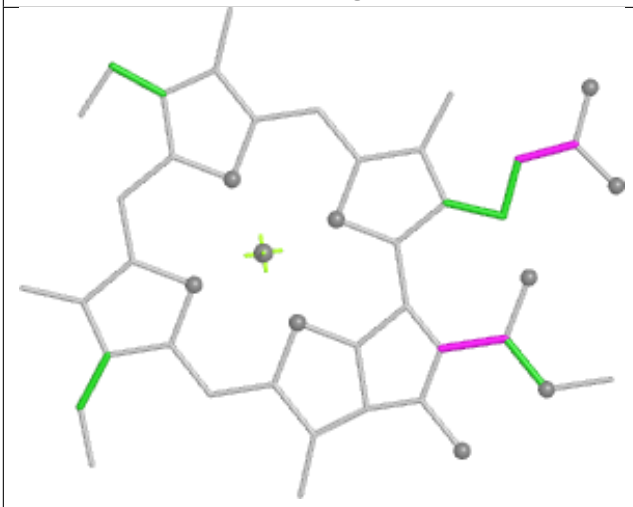
Ligand CLA G 301



Bond lengths

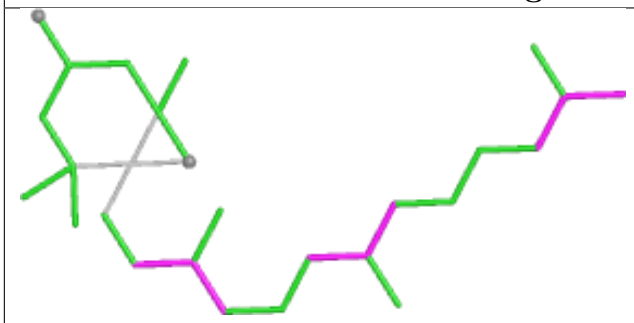
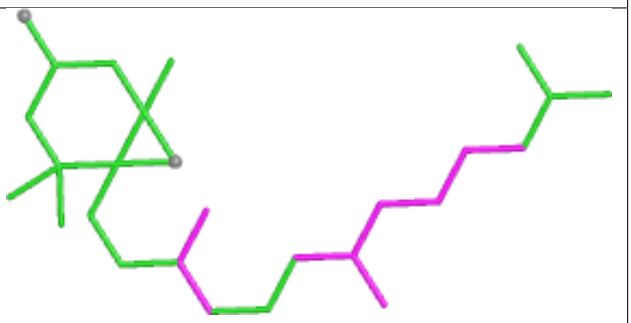
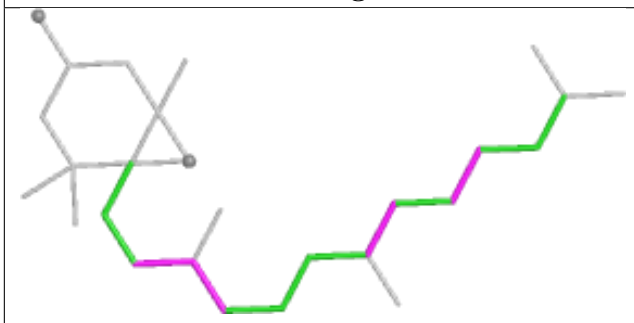
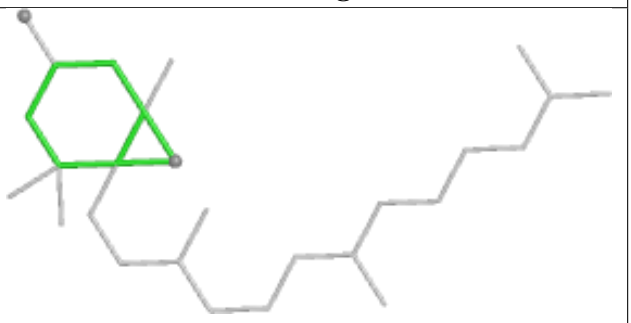


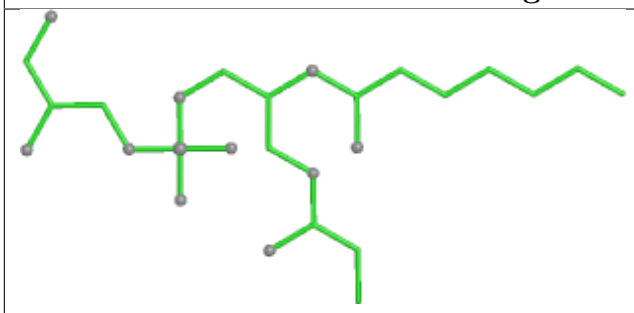
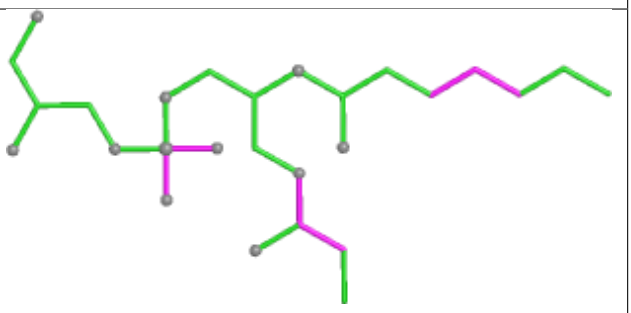
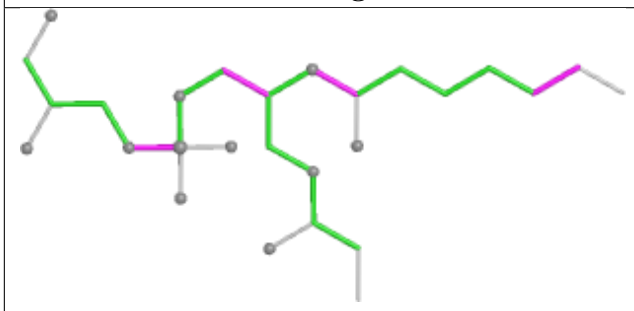
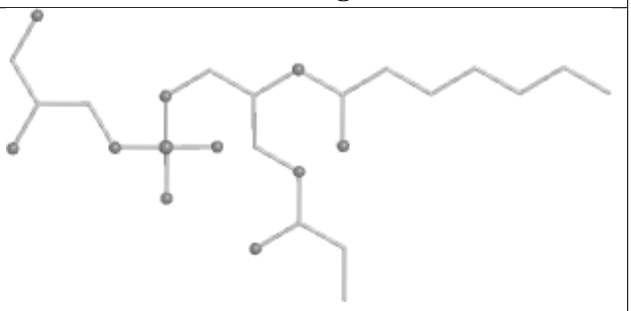
Bond angles



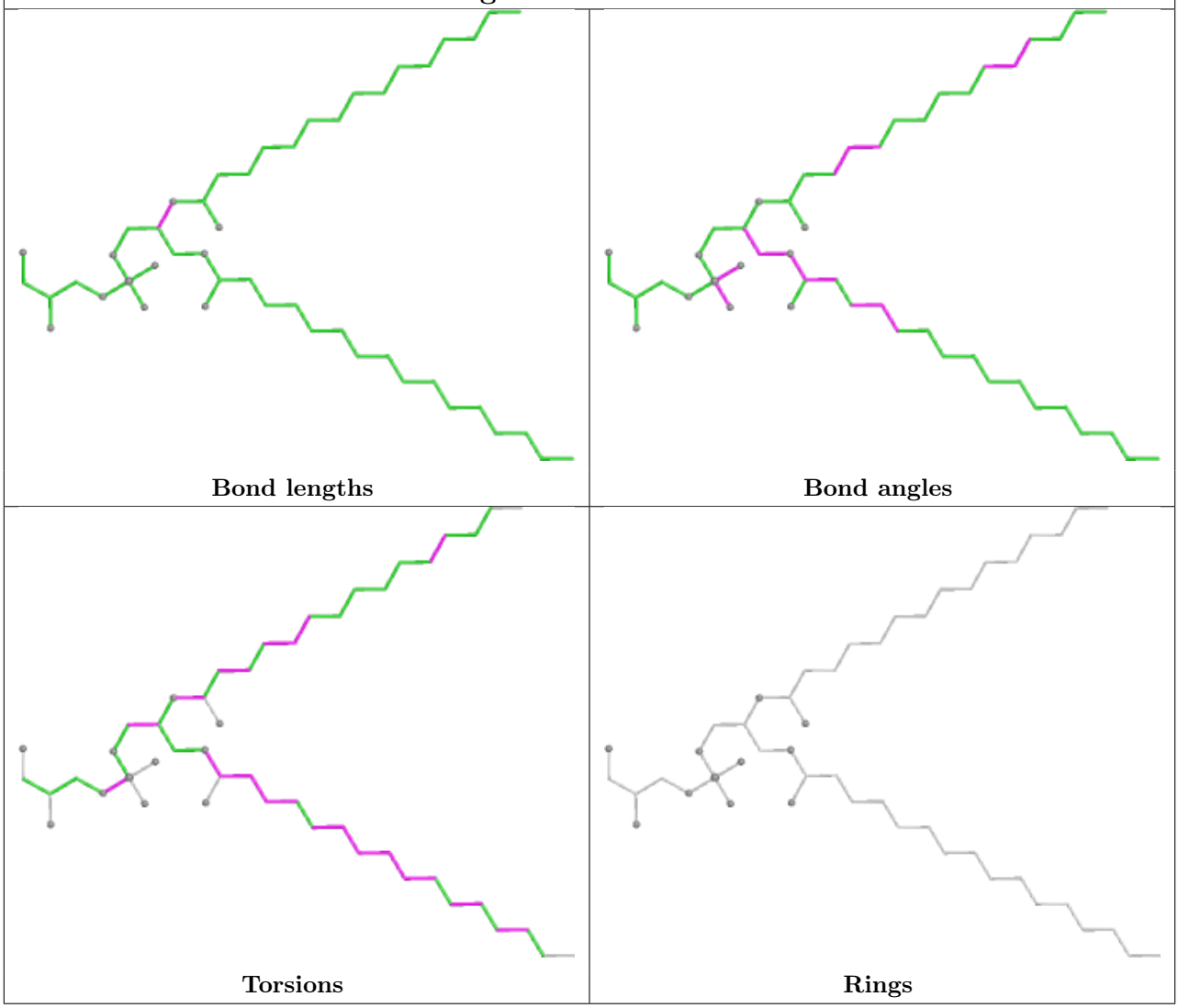
Torsions

Rings

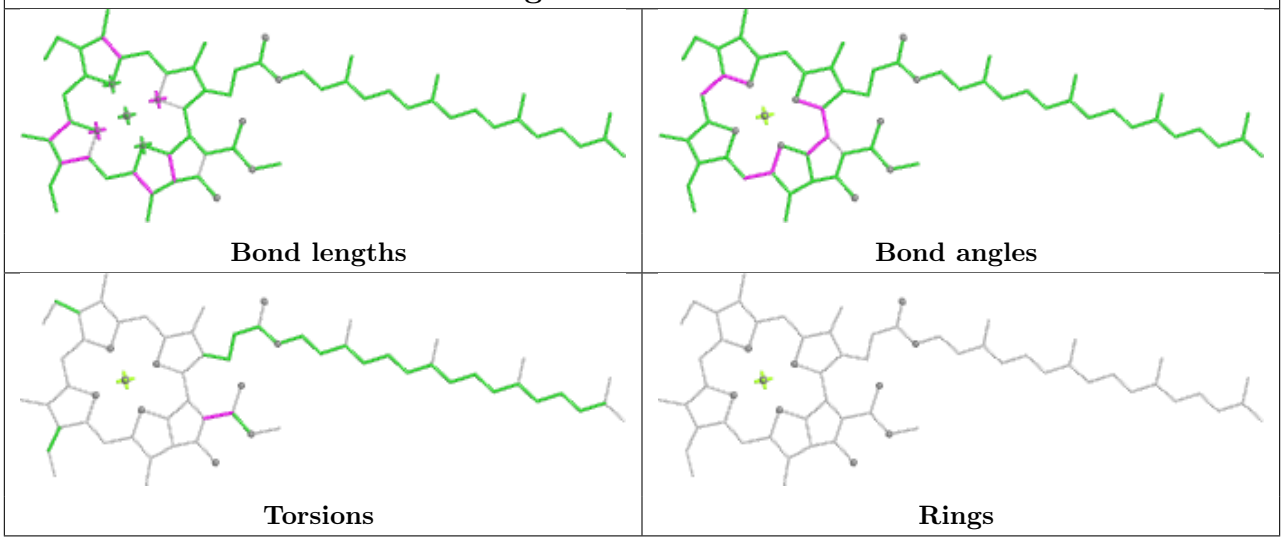
Ligand DD6 G 312	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand LHG A 840	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand LHG A 839



Ligand CLA A 835



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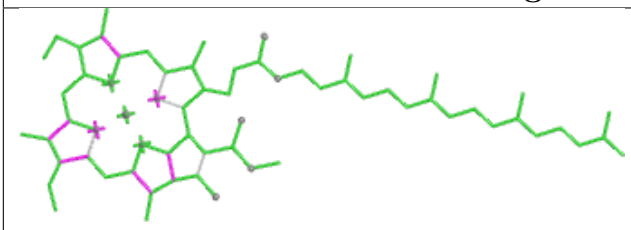
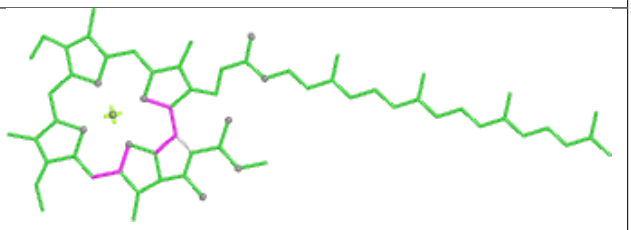
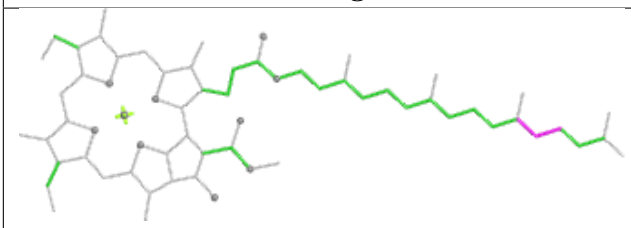
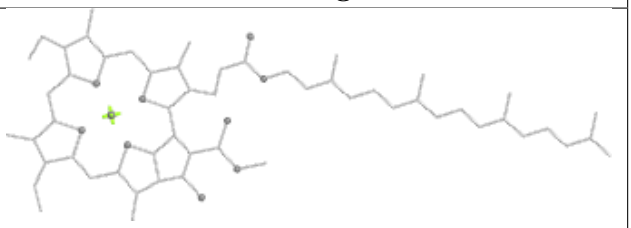
 Bond lengths	 Bond angles
 Torsions	 Rings

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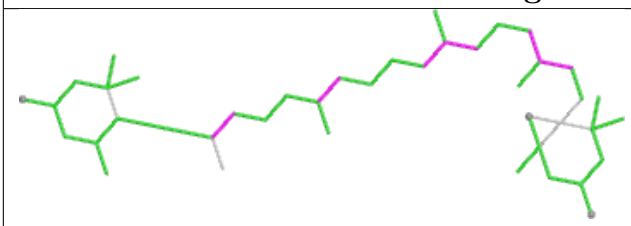
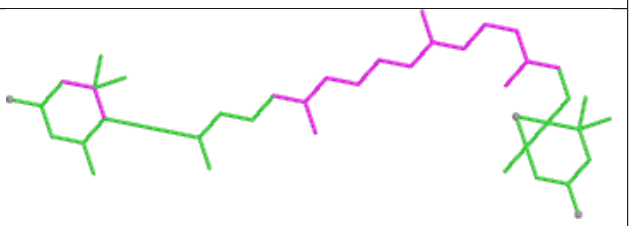
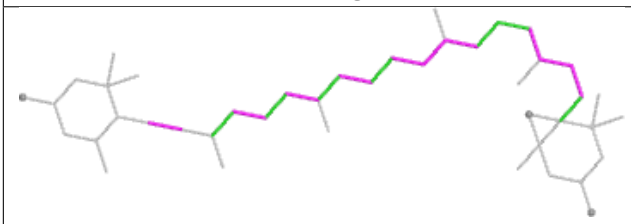
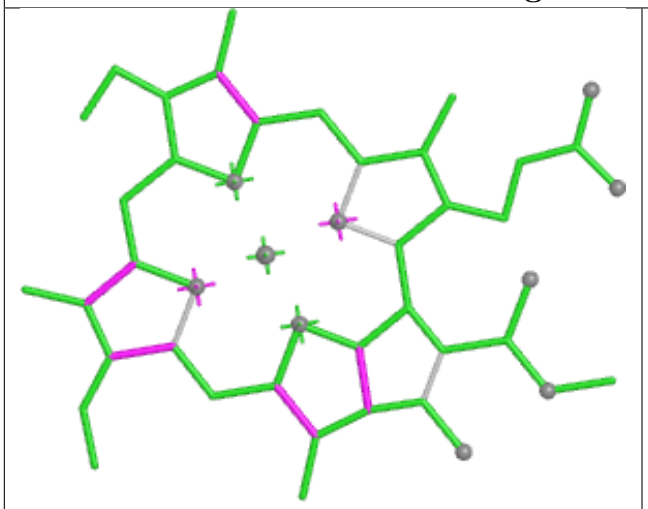
 Bond lengths	 Bond angles
 Torsions	Rings

Ligand CLA A 814



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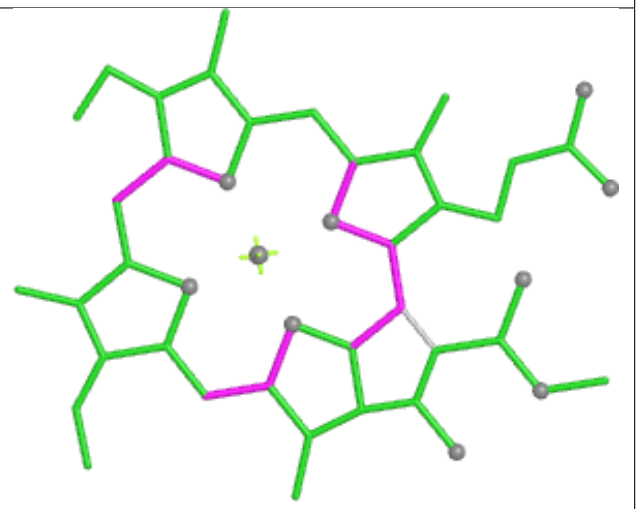
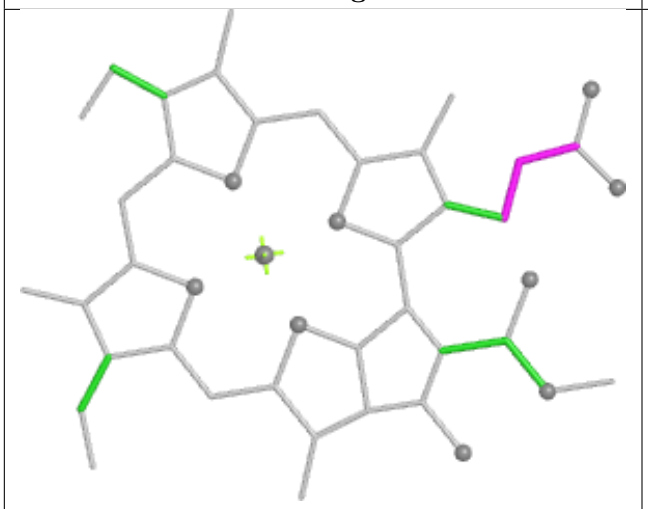


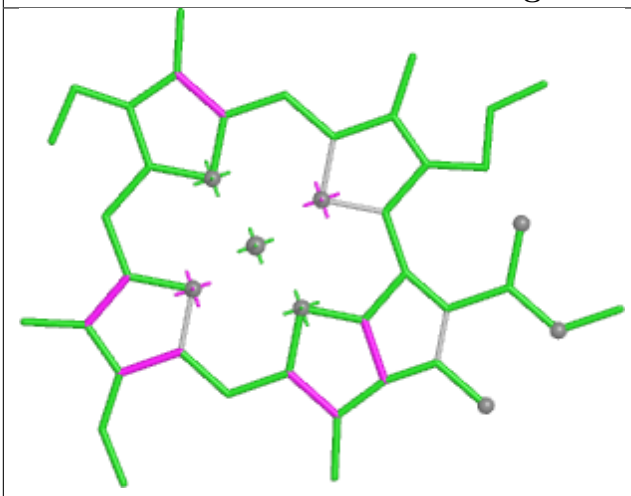
Bond angles



Torsions

Rings

Ligand CLA A 819



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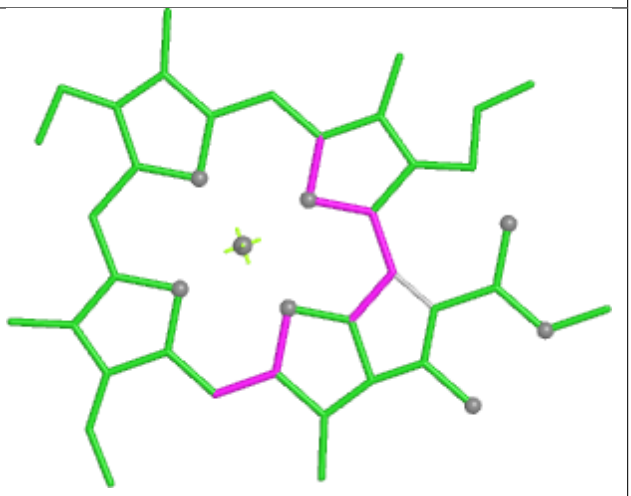
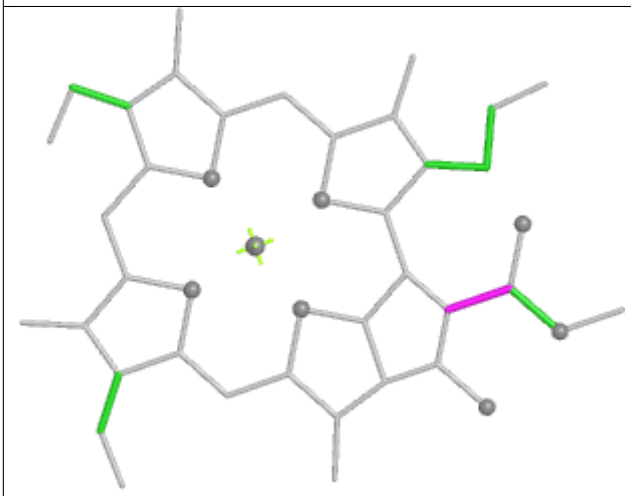


Bond angles



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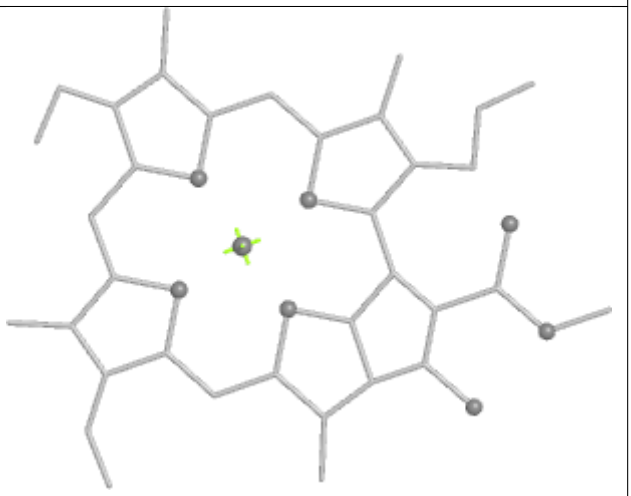
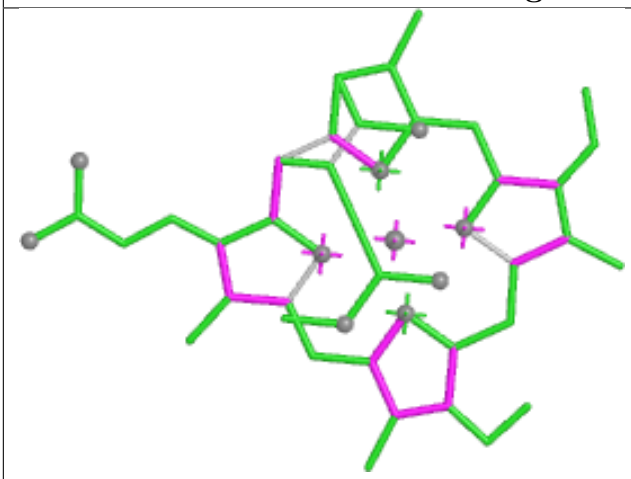


Rings

Ligand KC1 U 213



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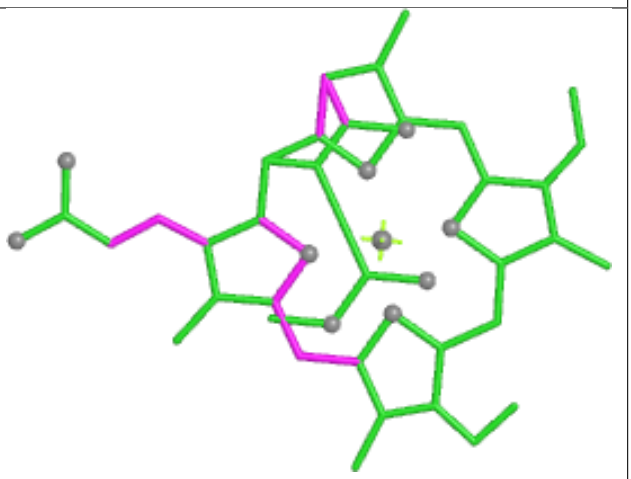

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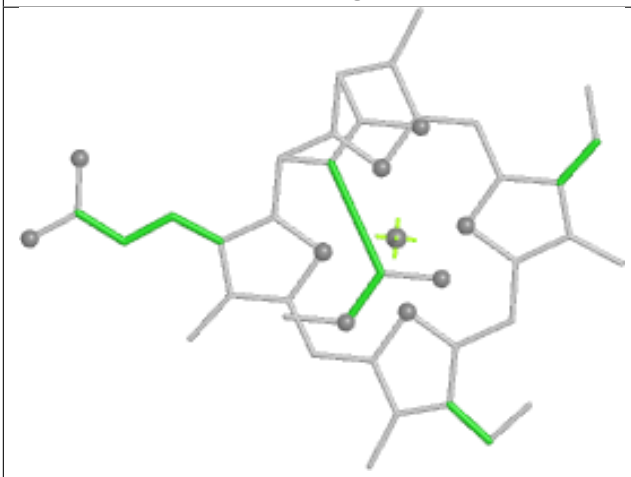

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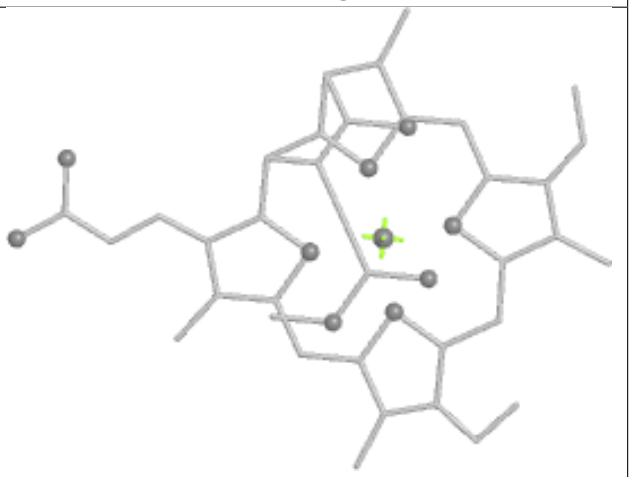
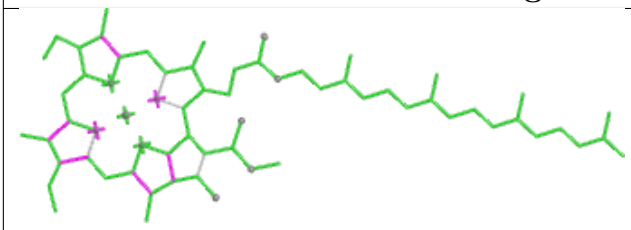


Rings

Ligand CLA B 844



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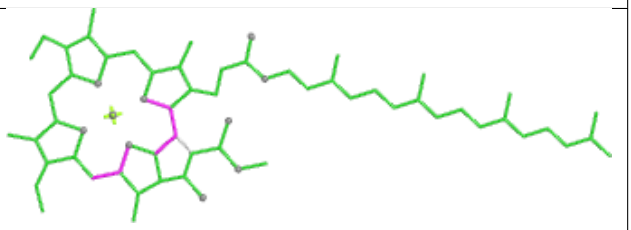

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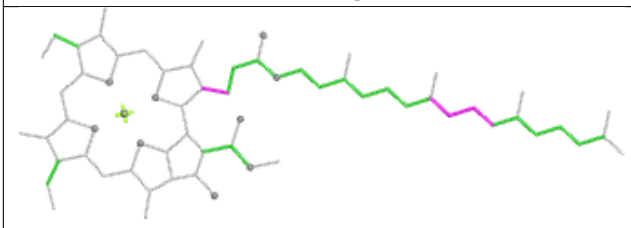

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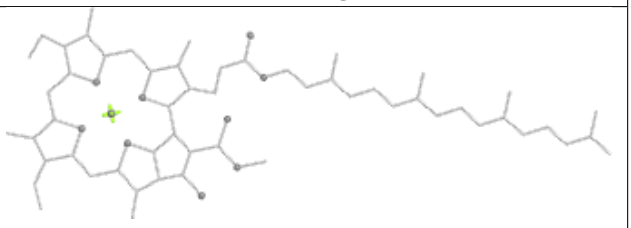
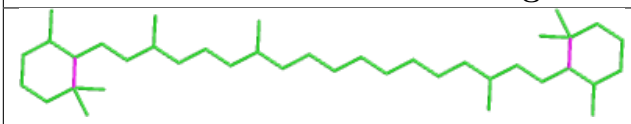


Rings

Ligand BCR B 846



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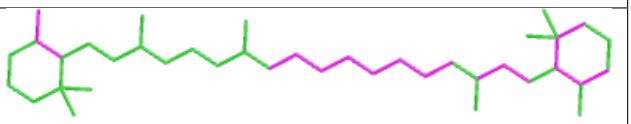

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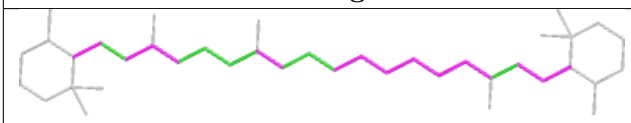

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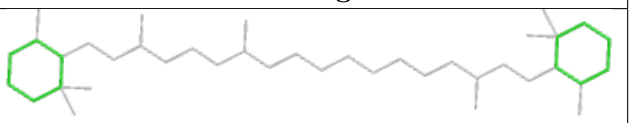
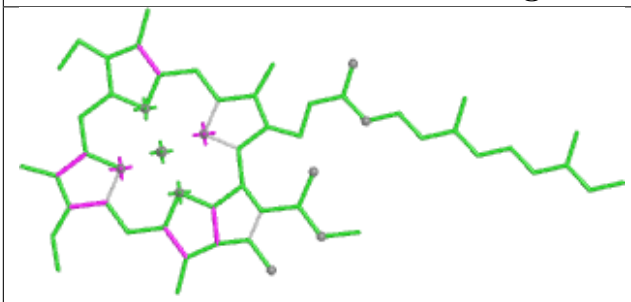


Rings

Ligand CLA G 309



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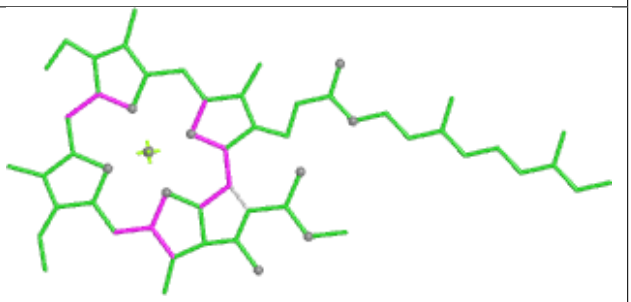

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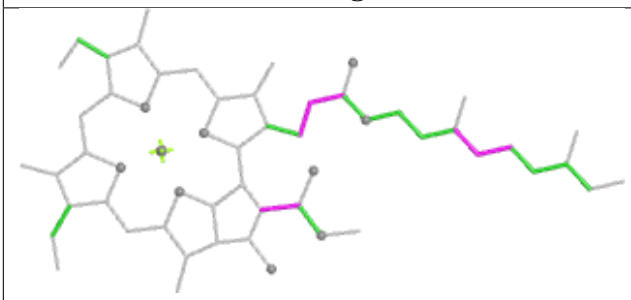

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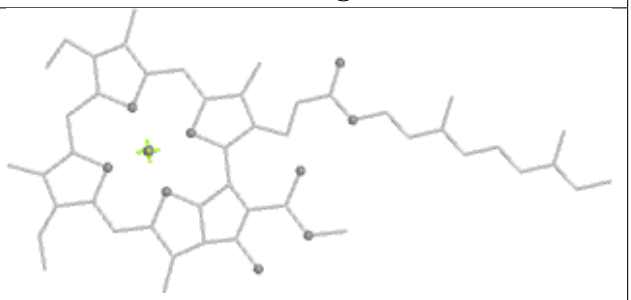
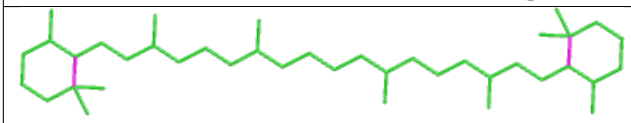


Rings

Ligand BCR A 841



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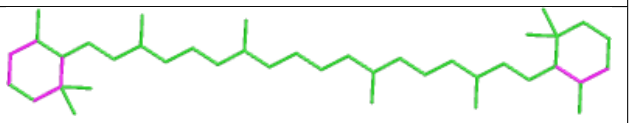
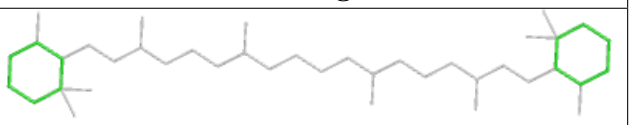


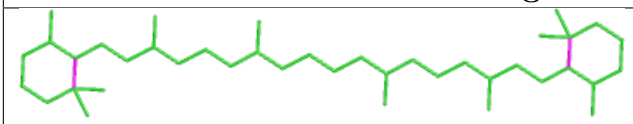
Bond angles

Torsions



Rings

Ligand BCR B 841



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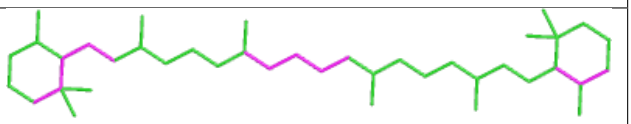

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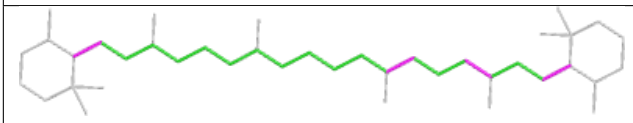

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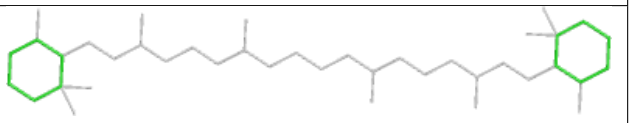
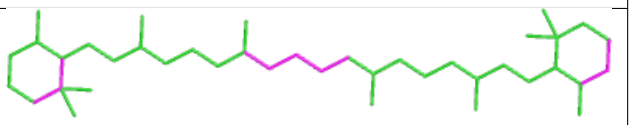


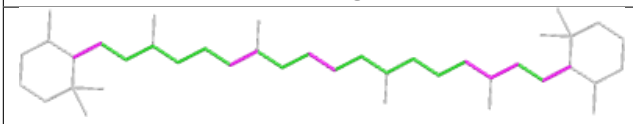
Rings

Ligand BCR I 101

Bond lengths



Bond angles



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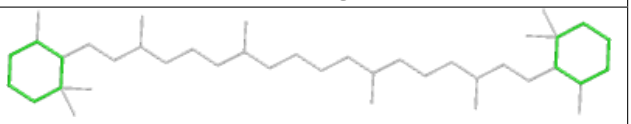
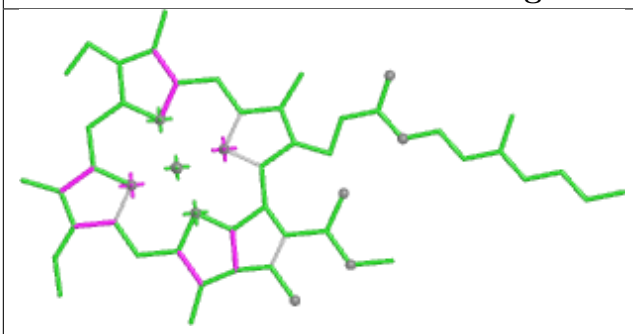


Rings

Ligand CLA B 819



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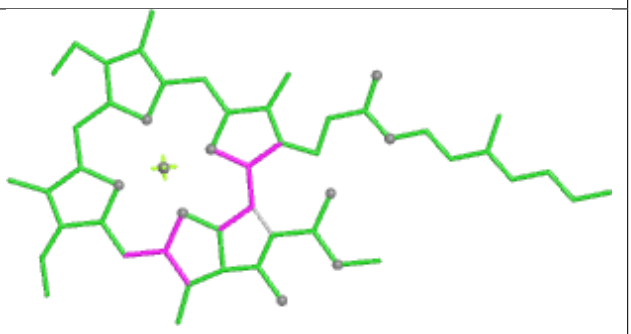
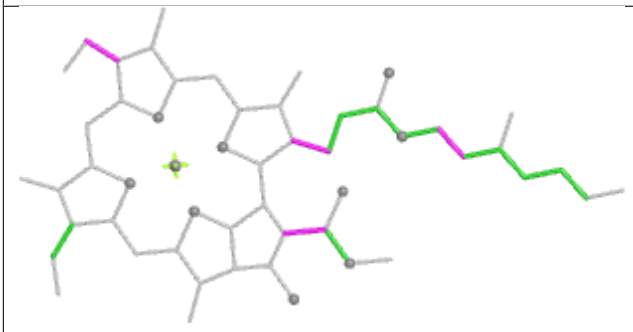
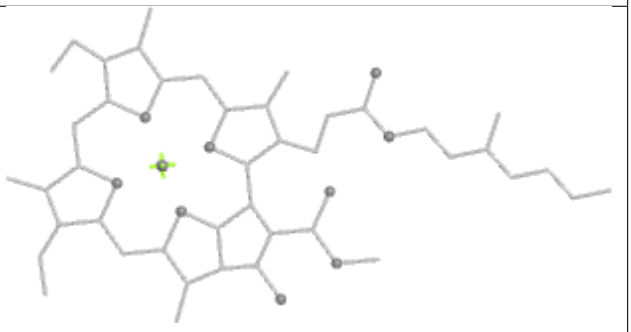


Bond angles

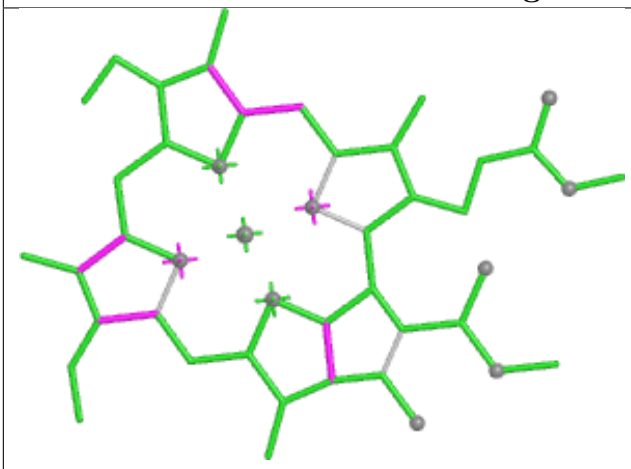


Torsions



Rings

Ligand CLA K 207



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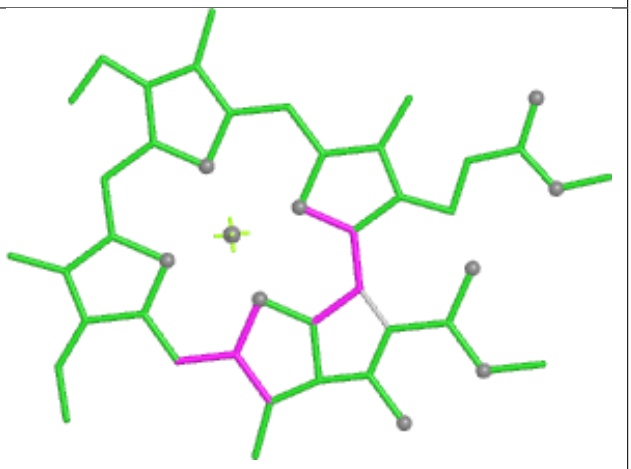
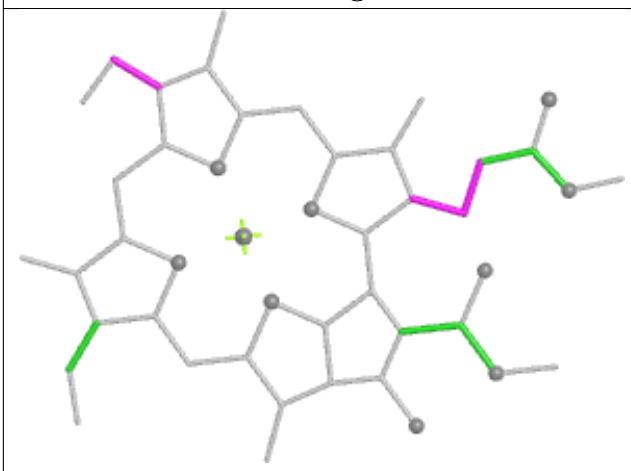
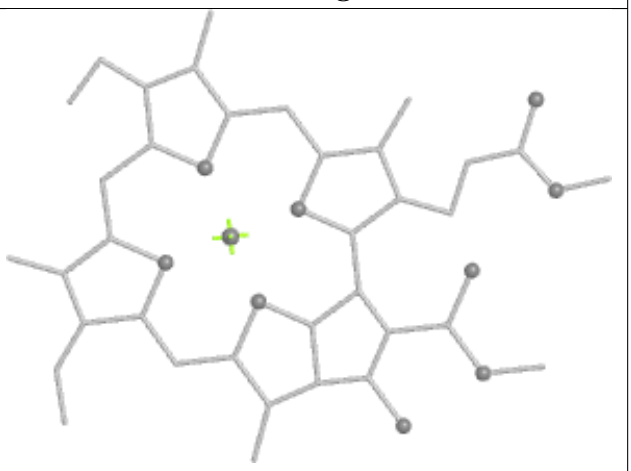


Bond angles



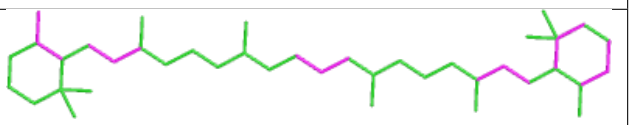
Torsions



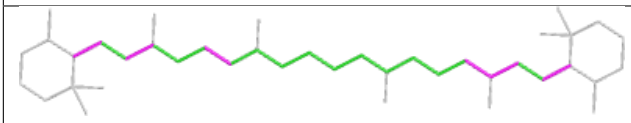
Rings

Ligand BCR B 838

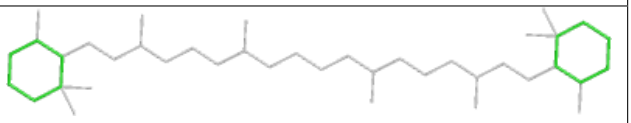
Bond lengths



Bond angles

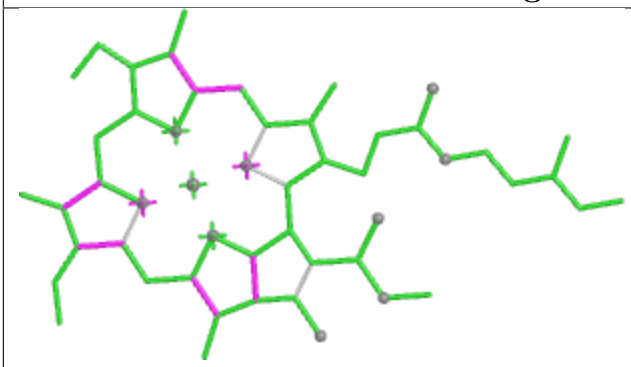


Torsions

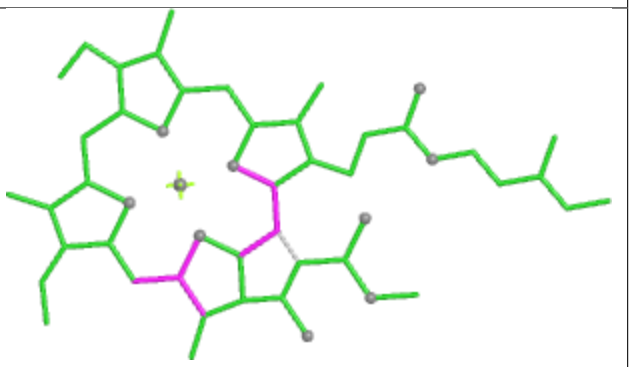


Rings

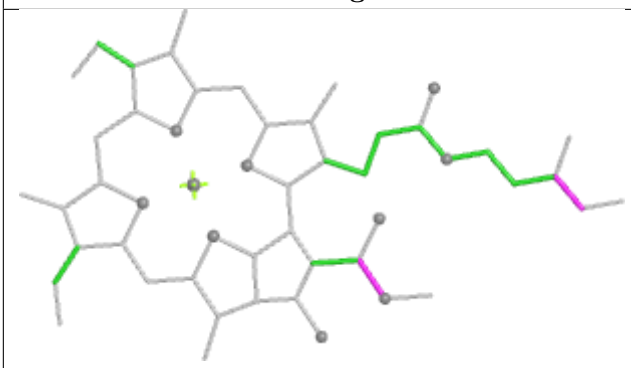
Ligand CLA A 820



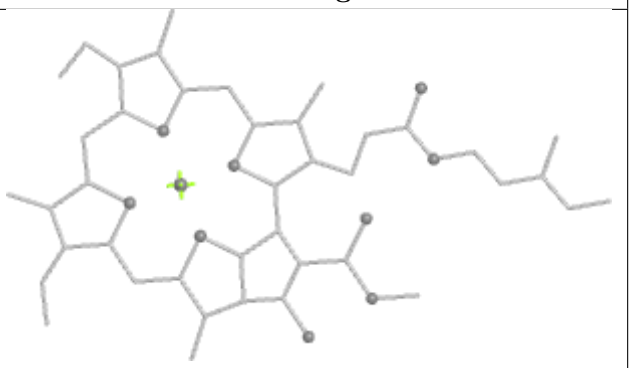
Bond lengths



Bond angles

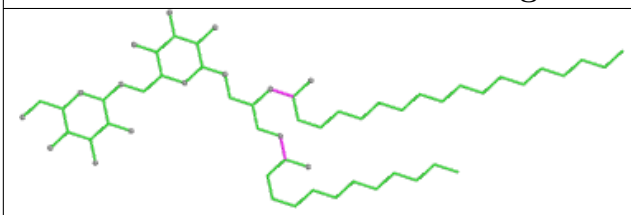


Torsions

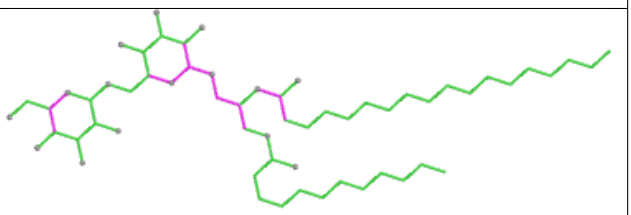


Rings

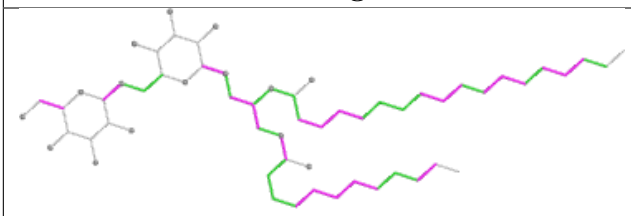
Ligand DGD B 843



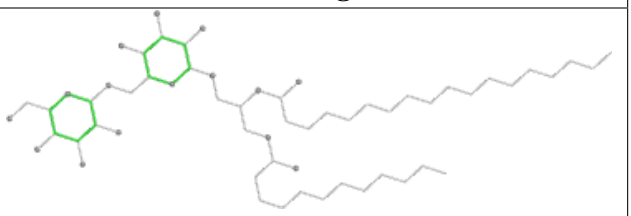
Bond lengths



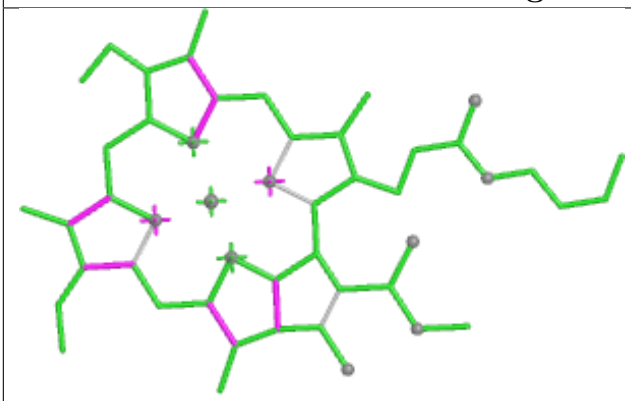
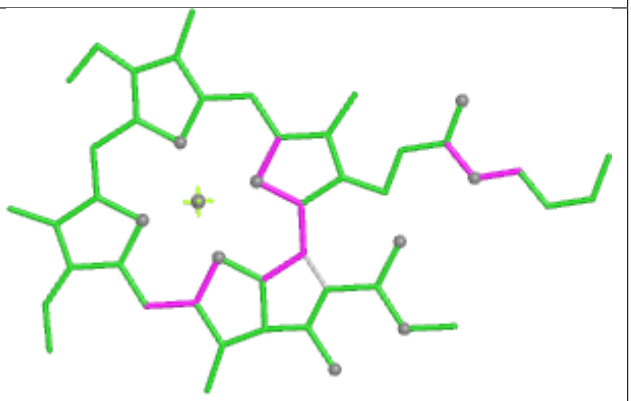
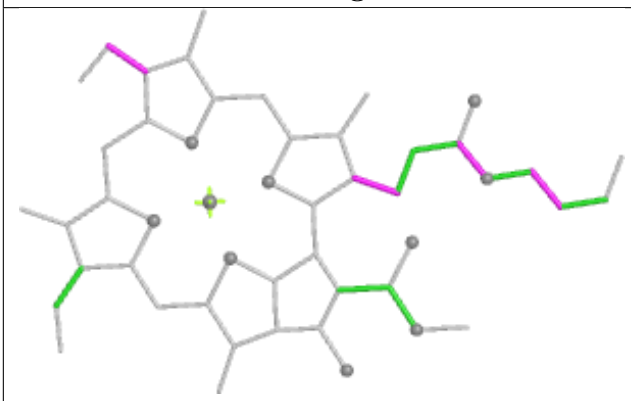
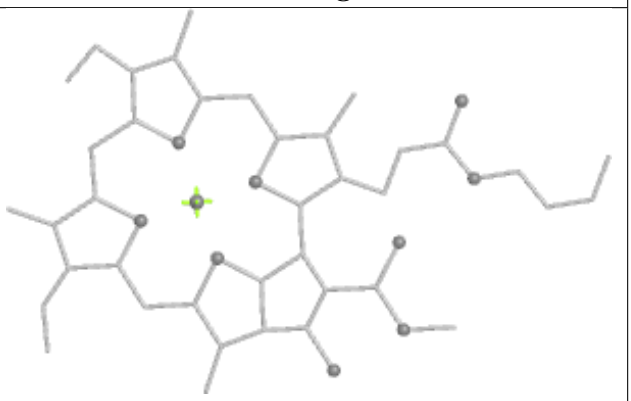
Bond angles

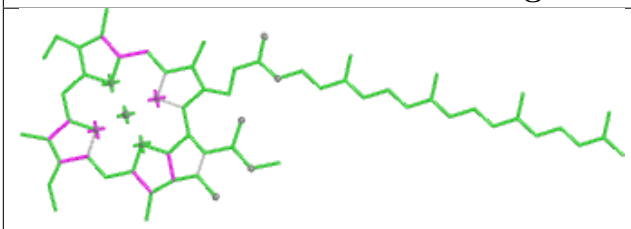
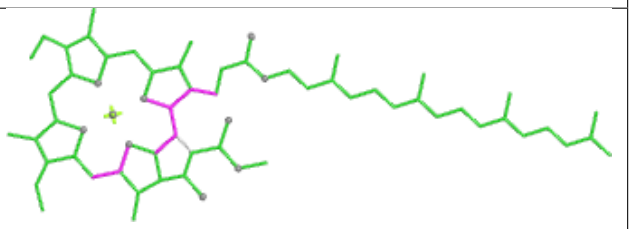
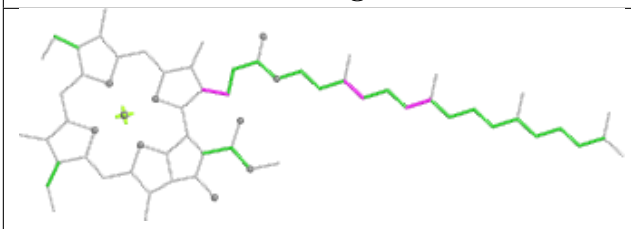
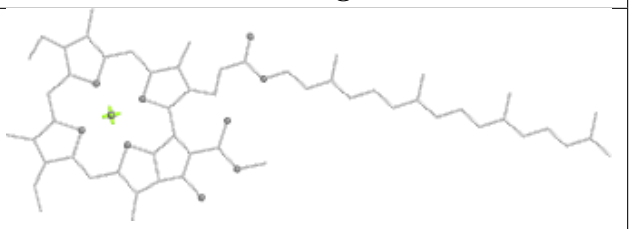


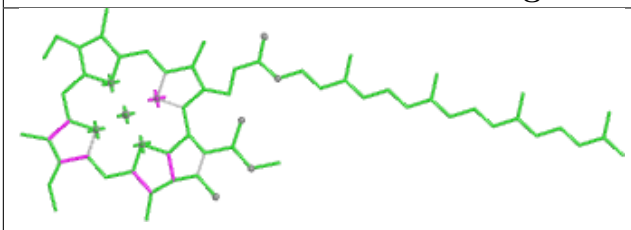
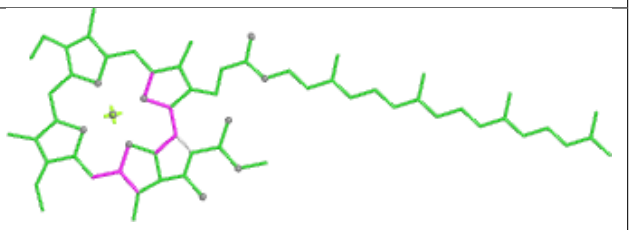
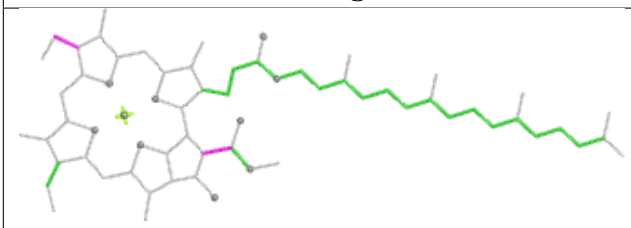
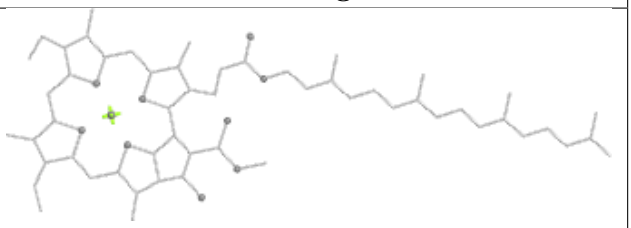
Torsions



Rings

Ligand CLA L 202	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA B 823	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA U 210	
 Bond lengths	 Bond angles
 Torsions	 Rings

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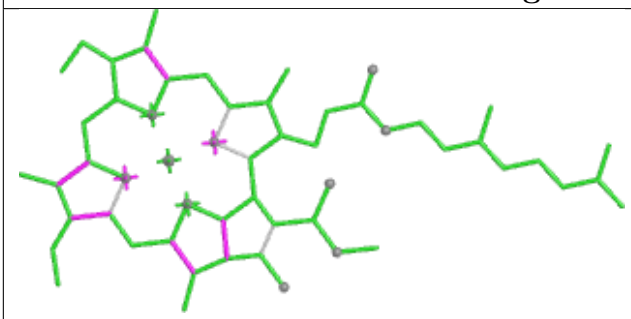
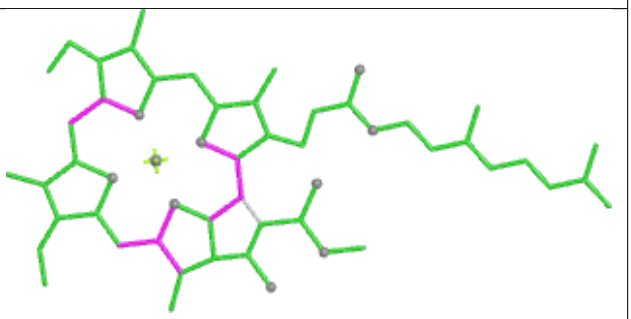
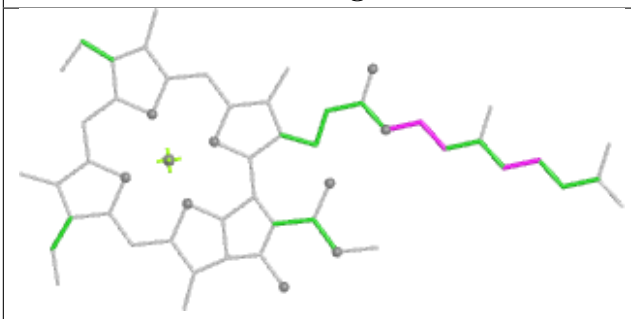
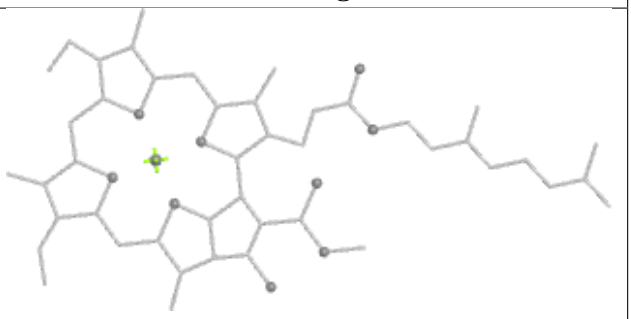
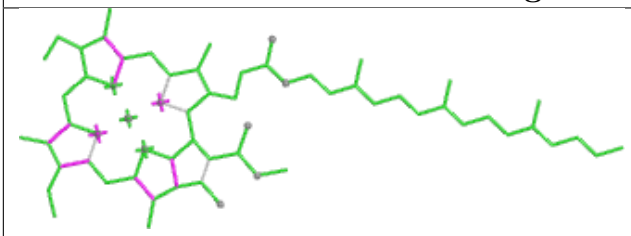
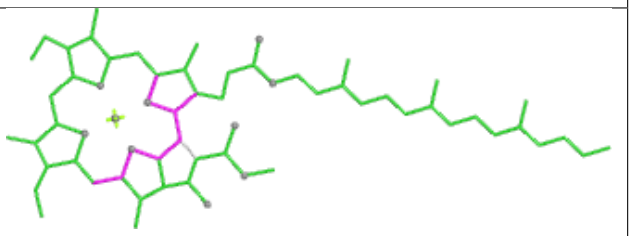
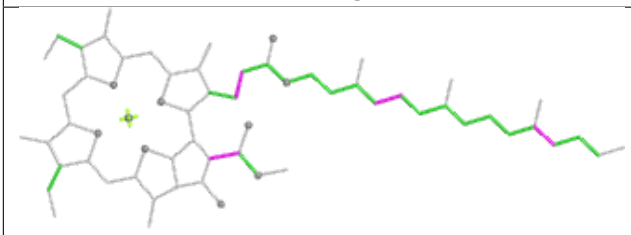
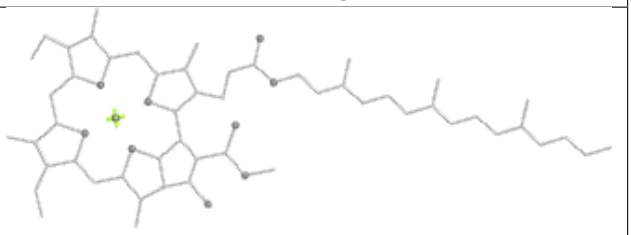
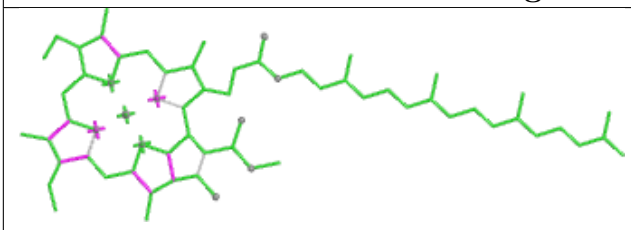
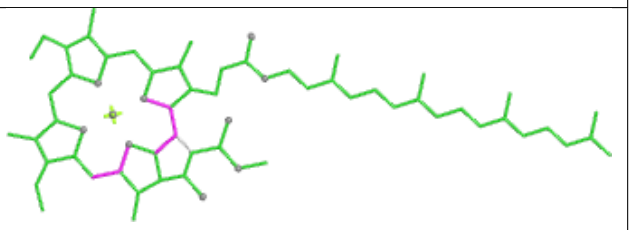
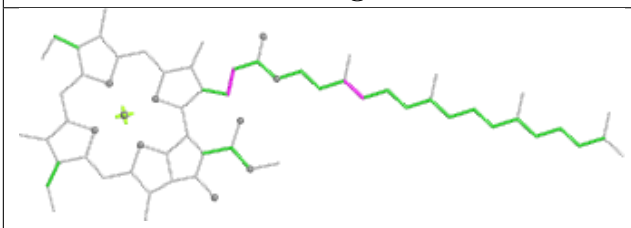
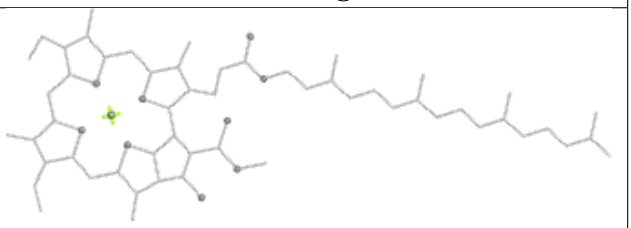
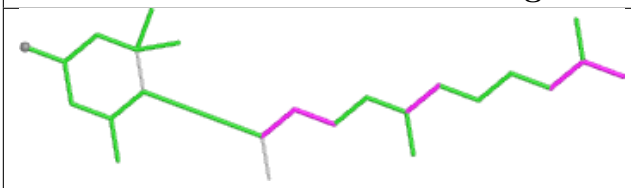
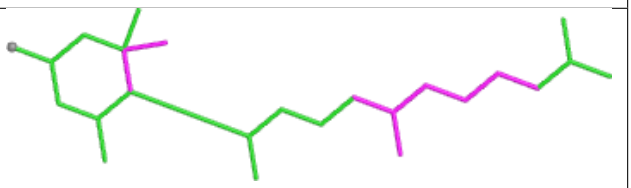
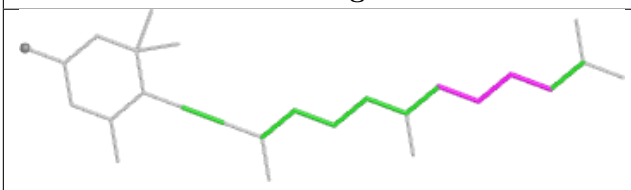
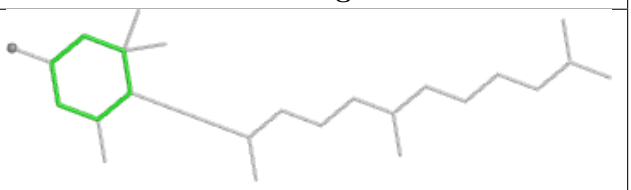
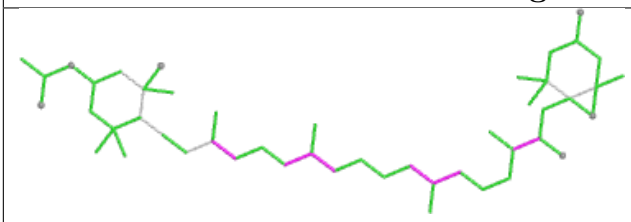
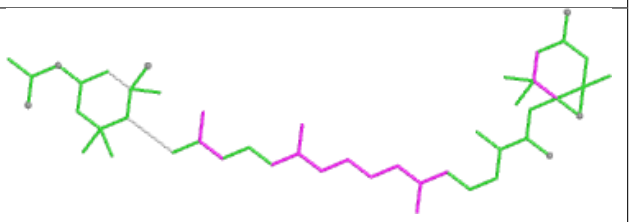
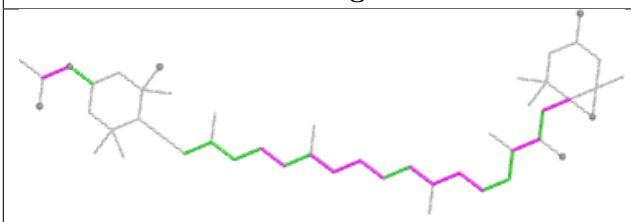
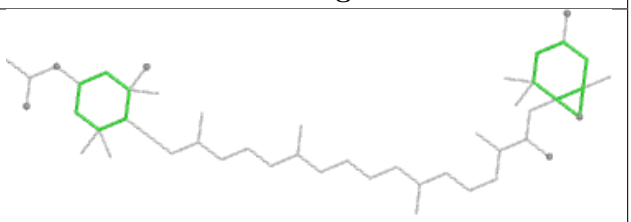
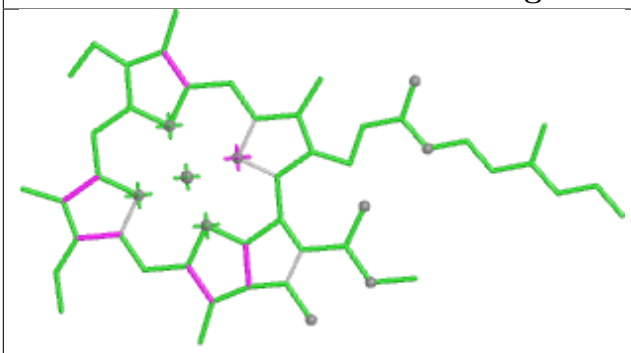
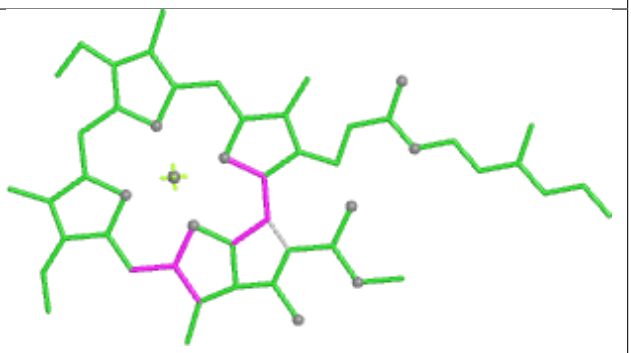
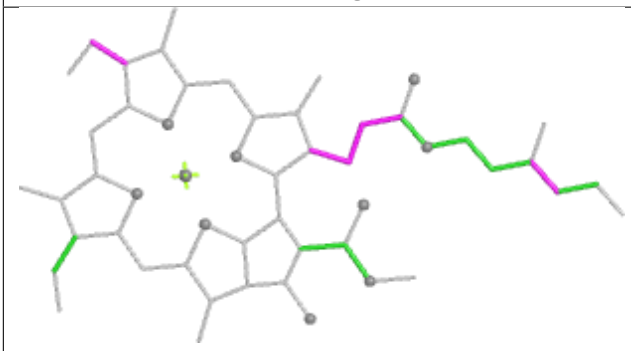
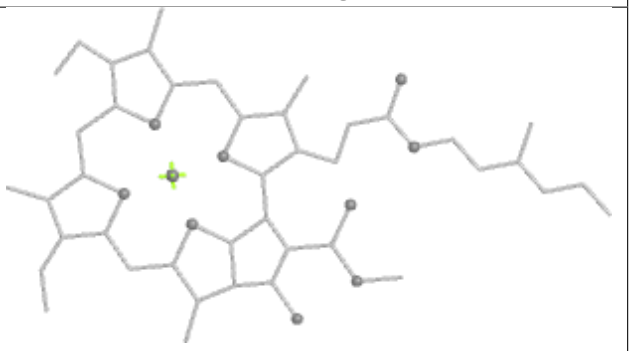
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA B 820	
 Bond lengths	 Bond angles
 Torsions	 Rings

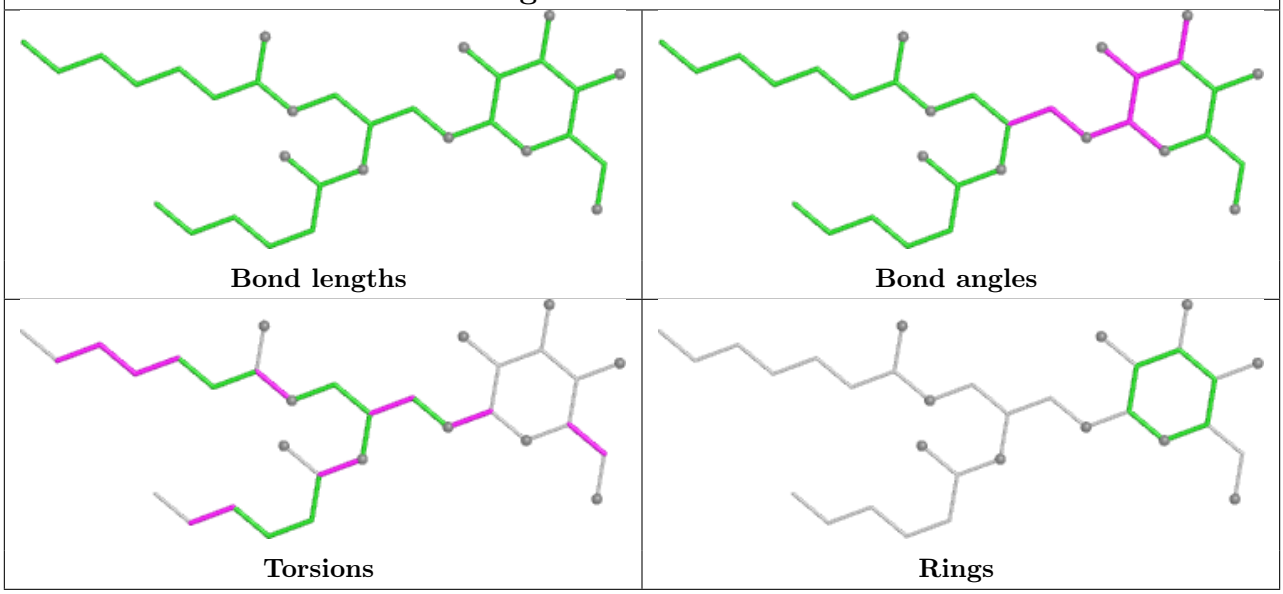
Ligand CLA B 801	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand DD6 U 214	
 Bond lengths	 Bond angles
 Torsions	 Rings

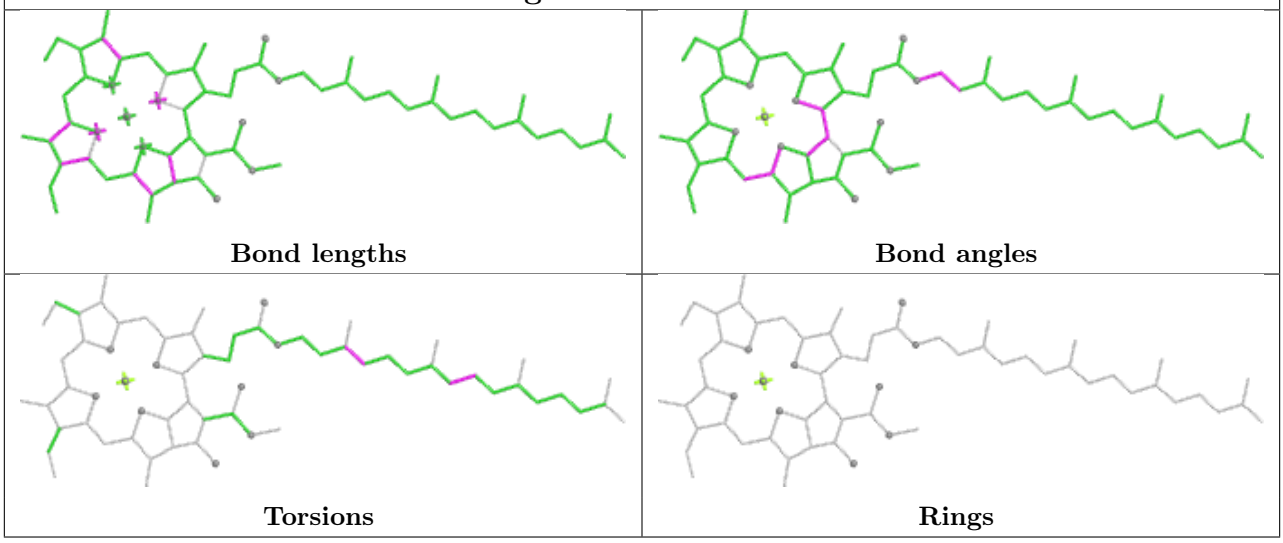
Ligand A86 U 202	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA B 847	
 Bond lengths	 Bond angles
 Torsions	 Rings

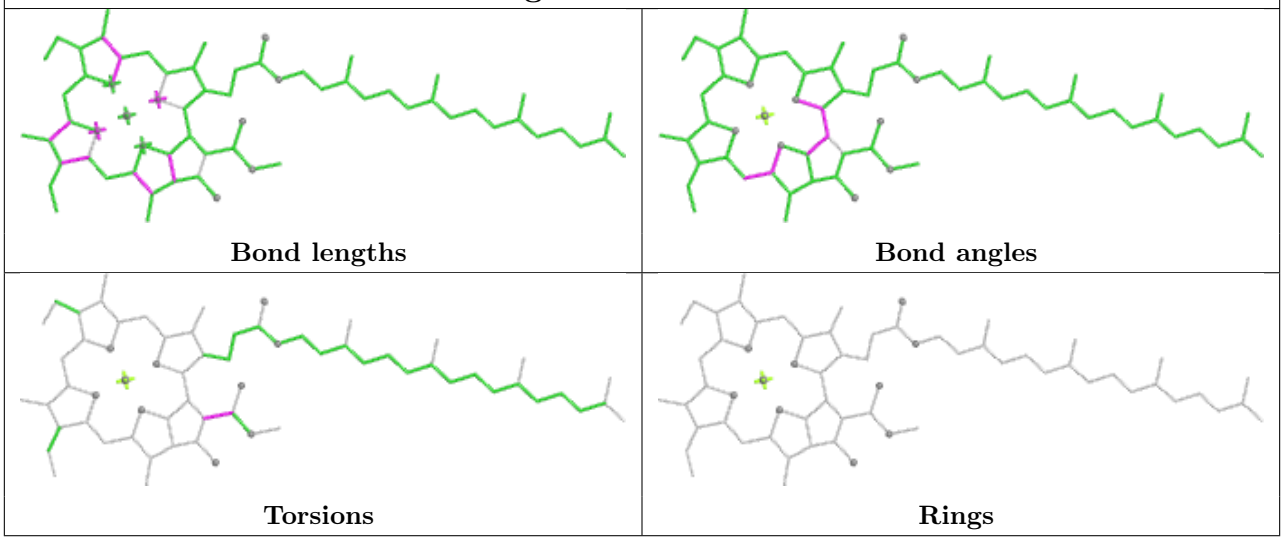
Ligand LMG U 201

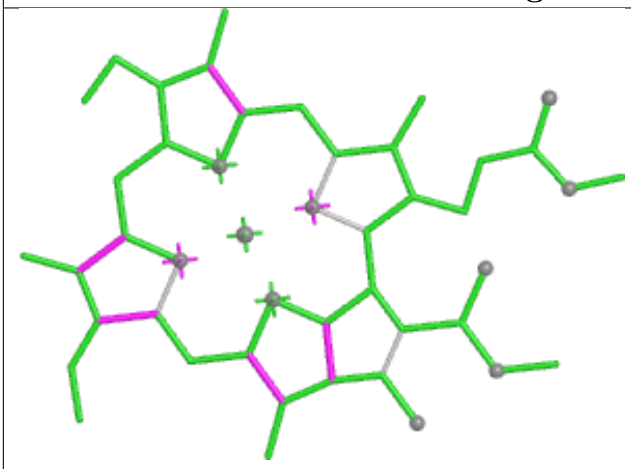
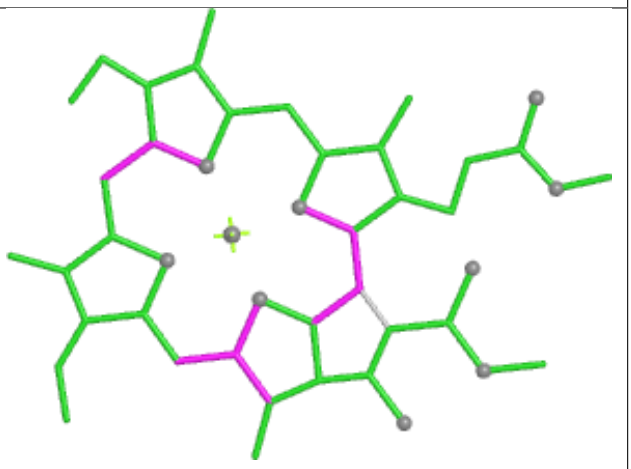
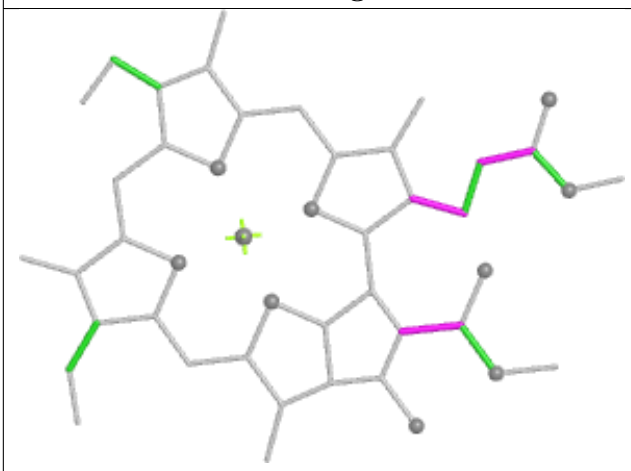
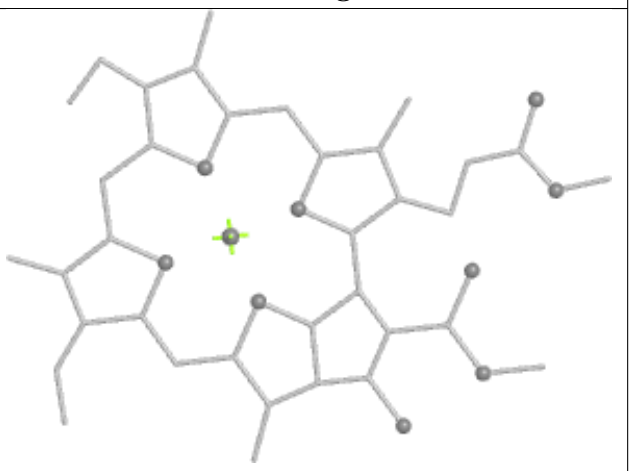


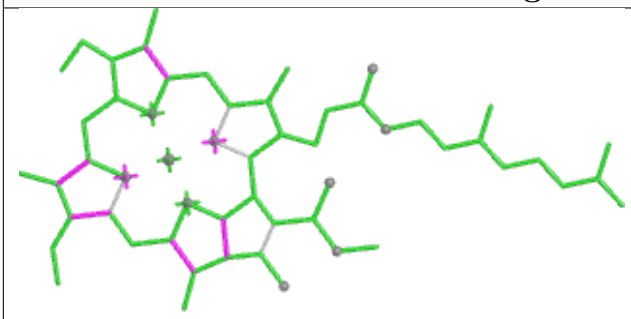
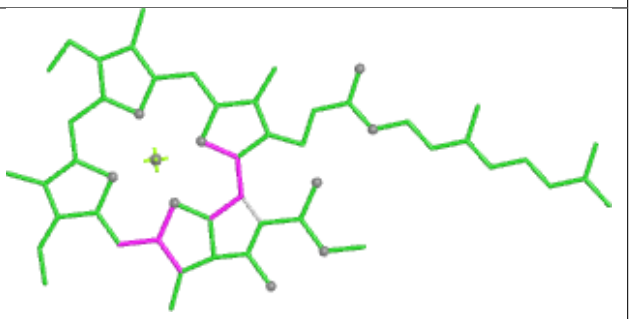
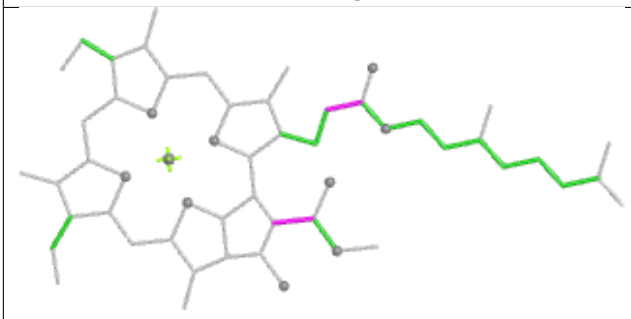
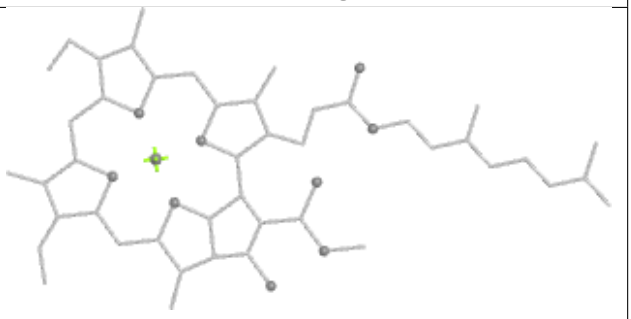
Ligand CLA U 205

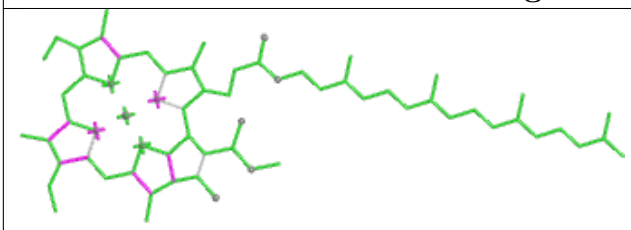
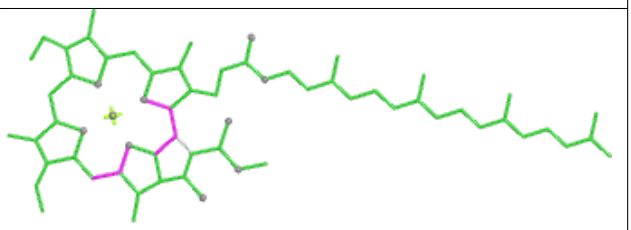
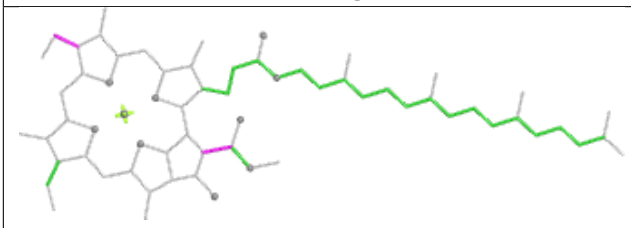
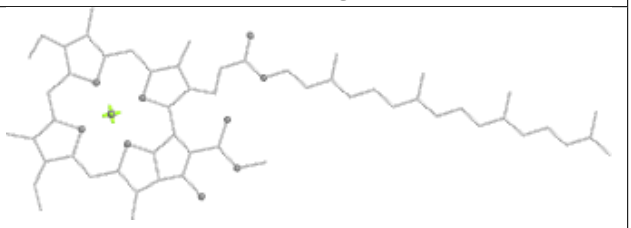


Ligand CLA A 826

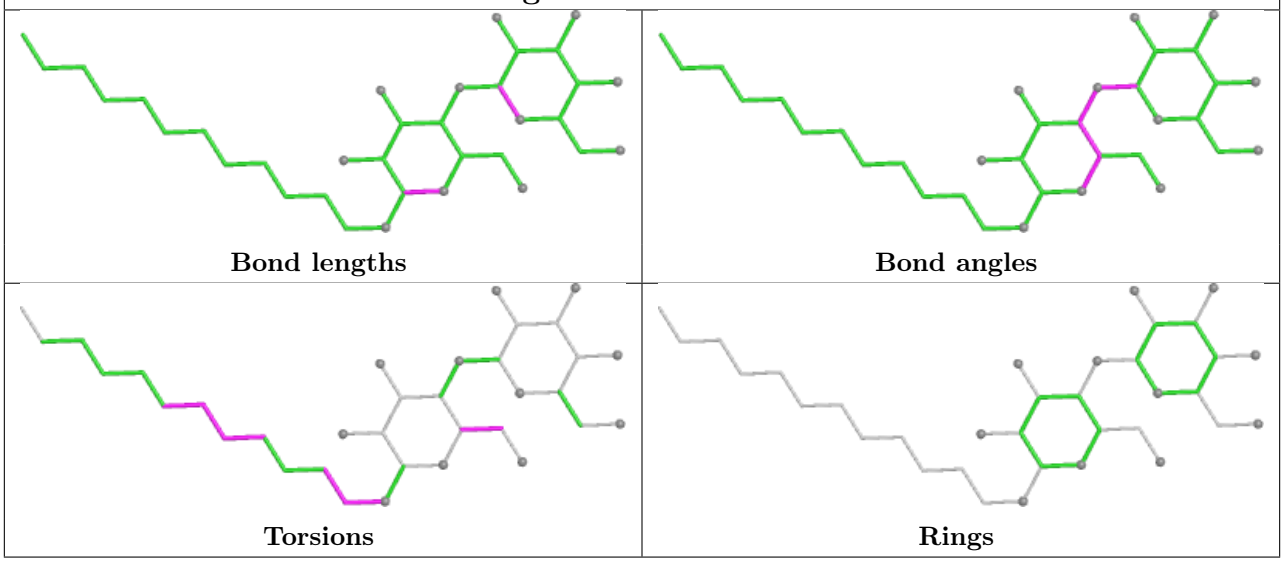


Ligand CLA F 804	
 Bond lengths	 Bond angles
 Torsions	 Rings

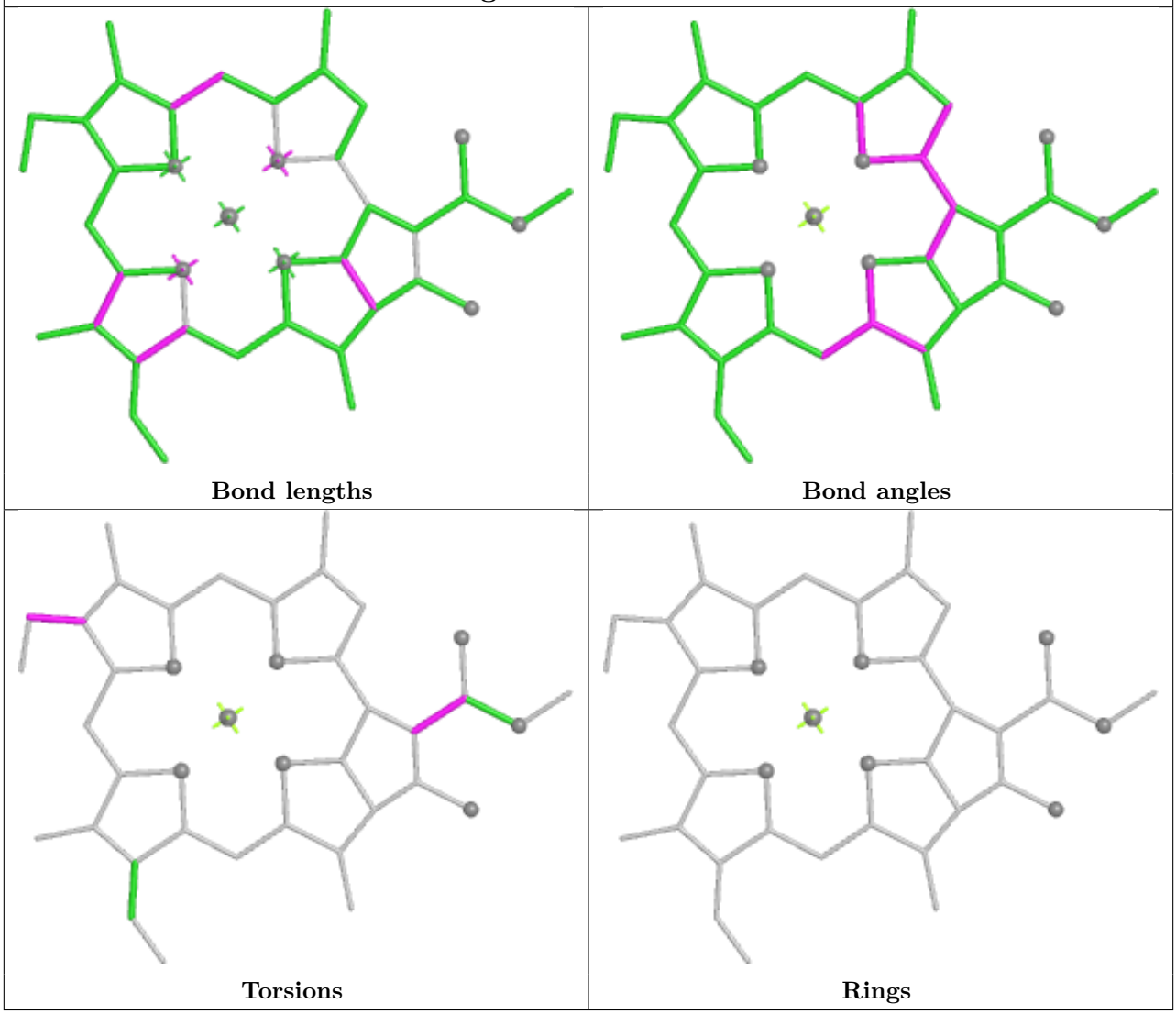
Ligand CLA A 802	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA B 825	
 Bond lengths	 Bond angles
 Torsions	 Rings

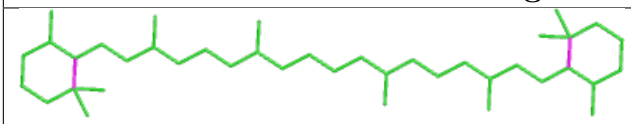
Ligand LMU F 806



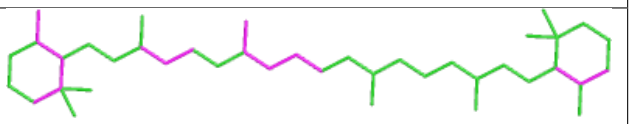
Ligand CLA H 301



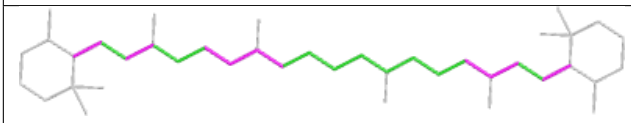
Ligand BCR F 805



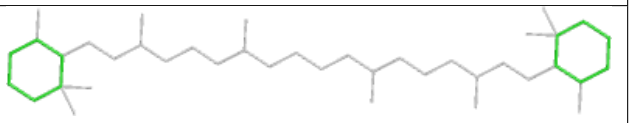
Bond lengths



Bond angles

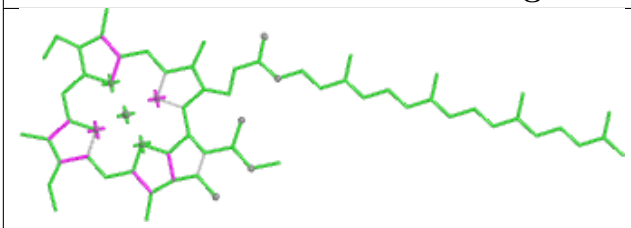


Torsions

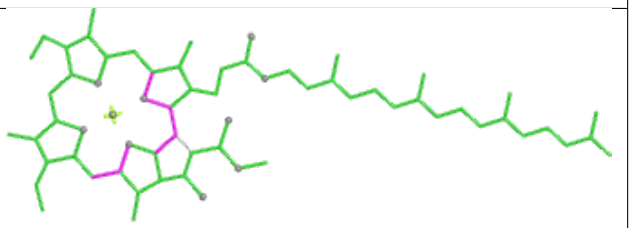


Rings

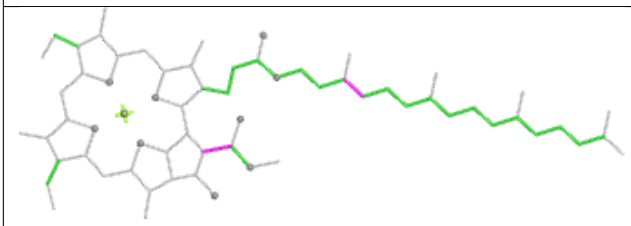
Ligand CLA A 823



Bond lengths



Bond angles



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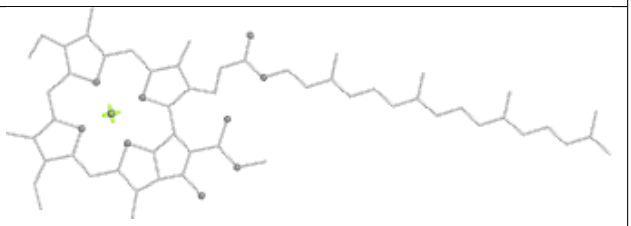
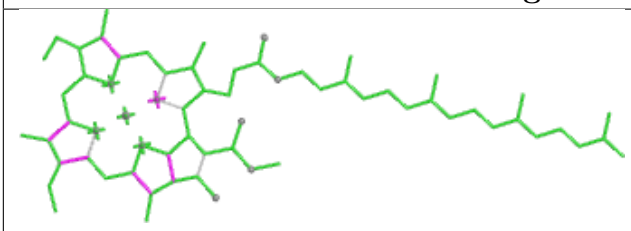
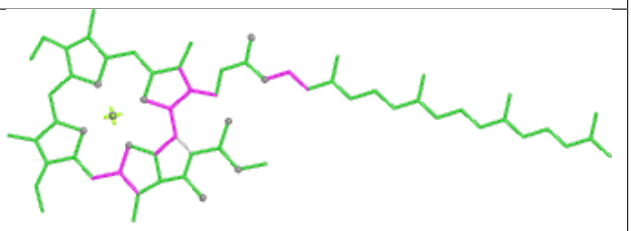


Rings

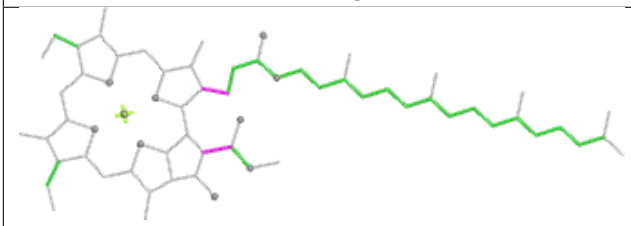
Ligand CLA U 207



Bond lengths



Bond angles



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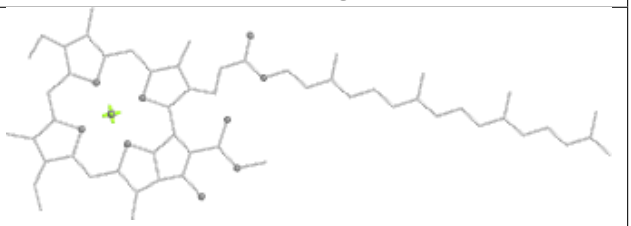
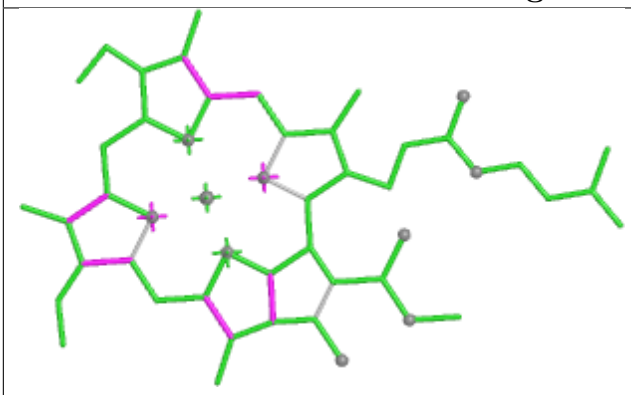
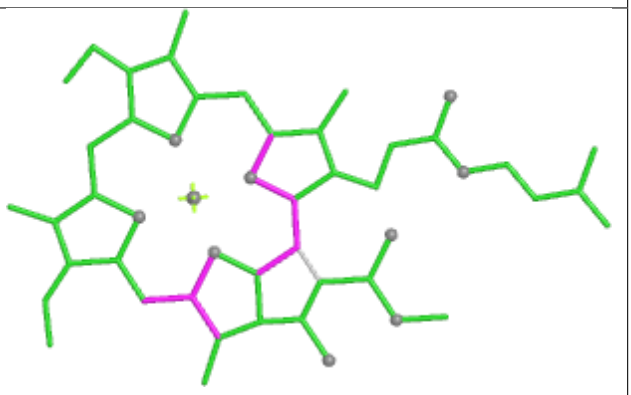
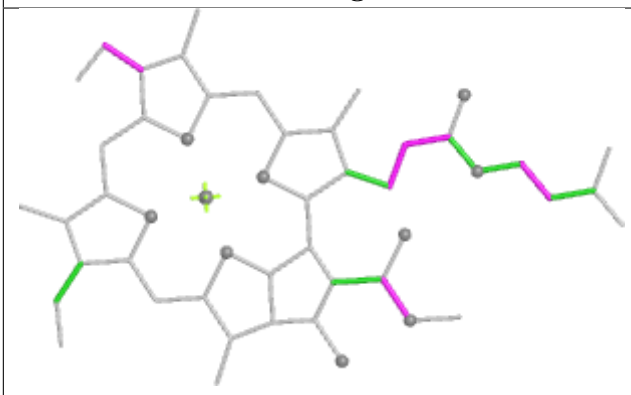
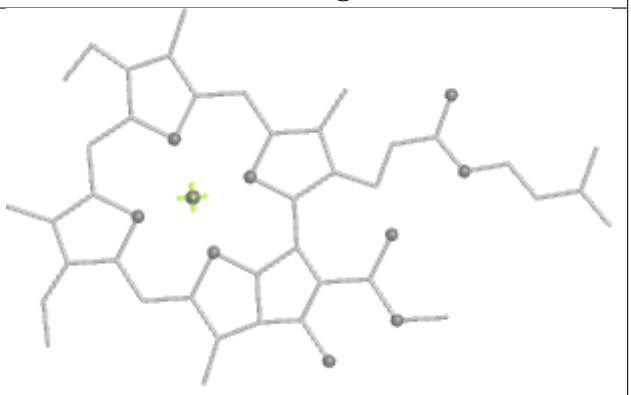
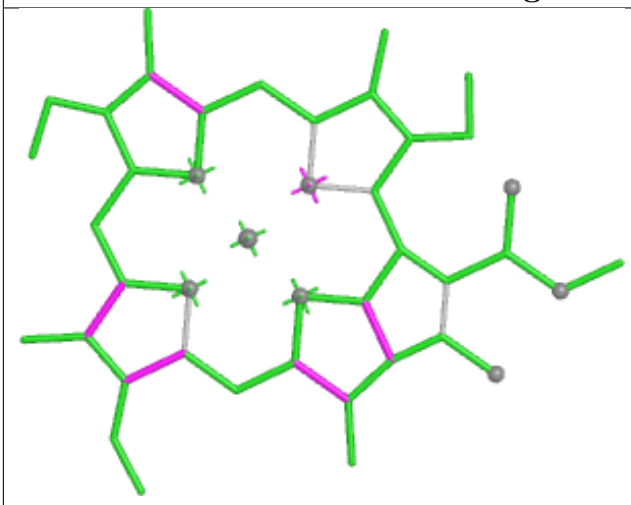


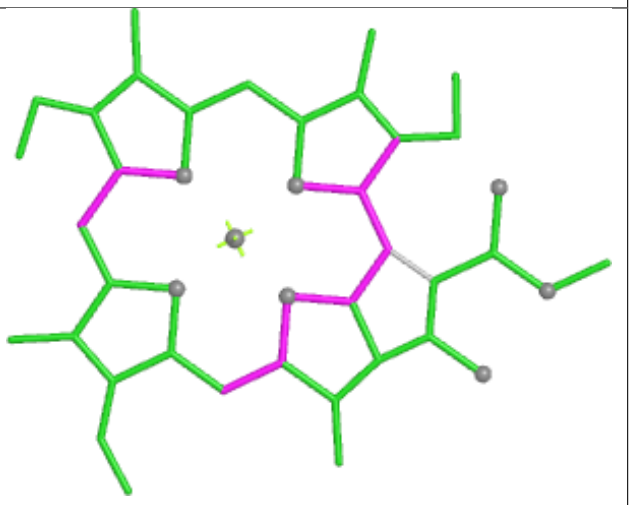
Rings

Ligand CLA L 204	
 Bond lengths	 Bond angles
 Torsions	 Rings

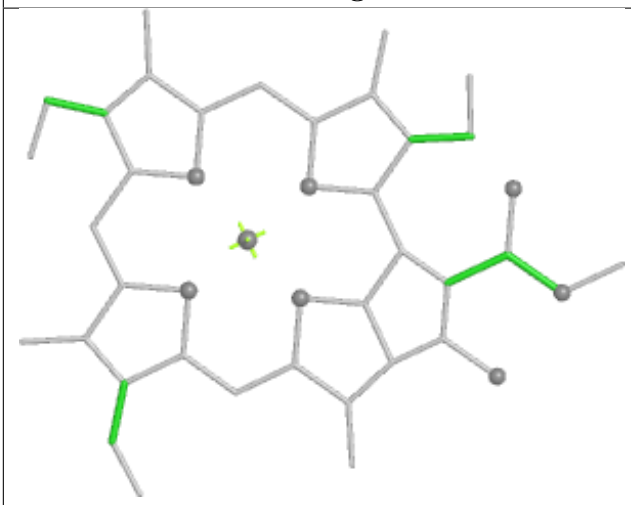
Ligand CLA U 209



Bond lengths



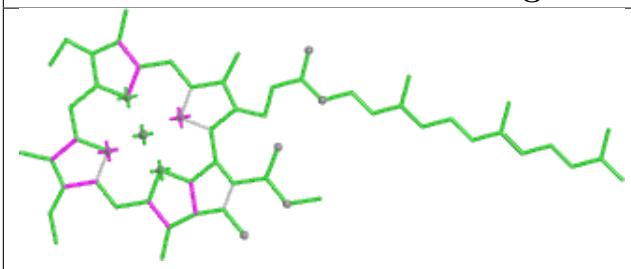
Bond angles



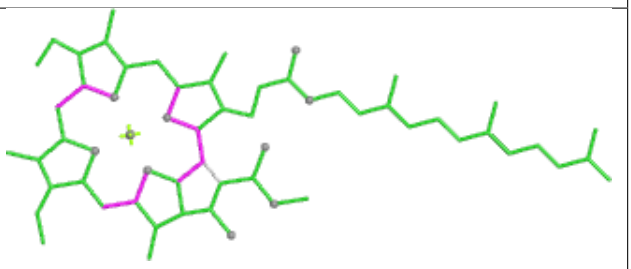
Torsions

Rings

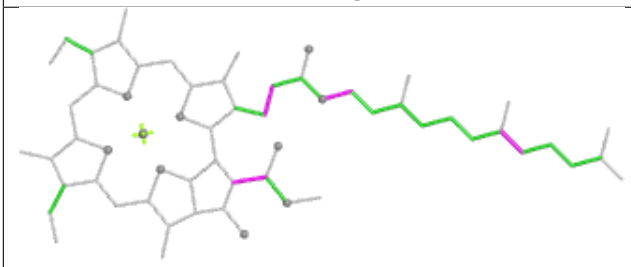
Ligand CLA H 302



Bond lengths



Bond angles



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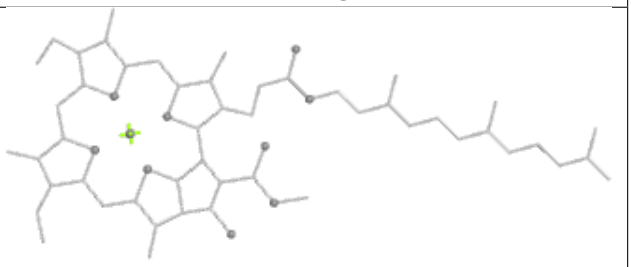
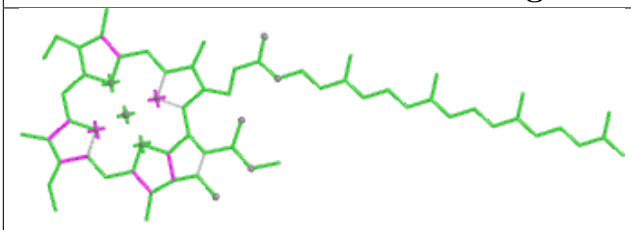
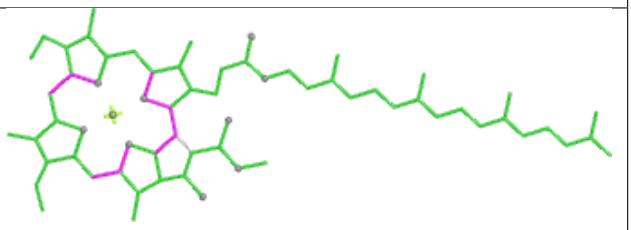
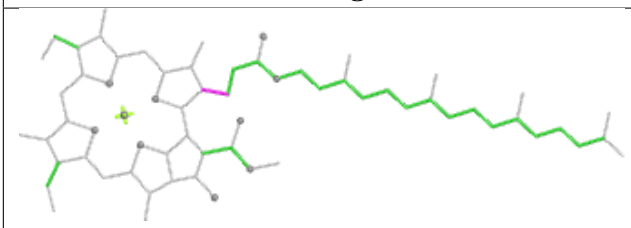
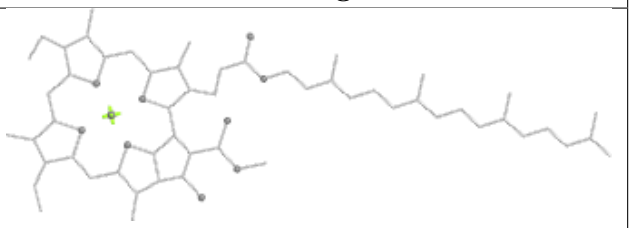
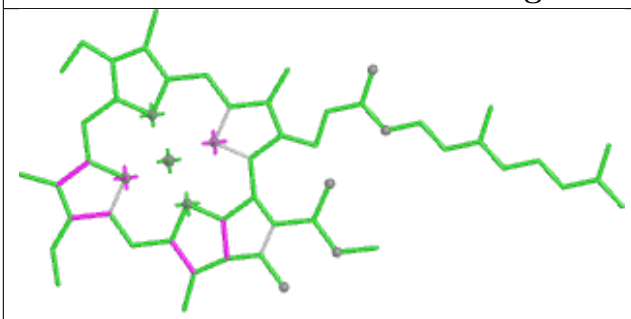
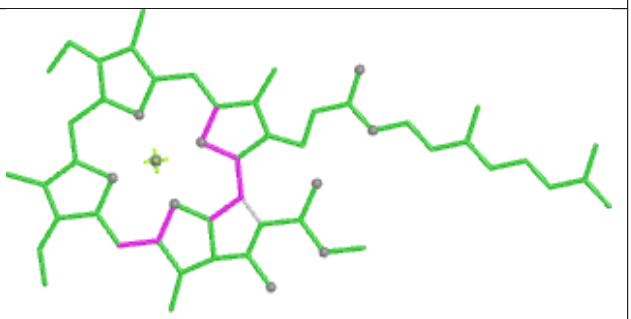
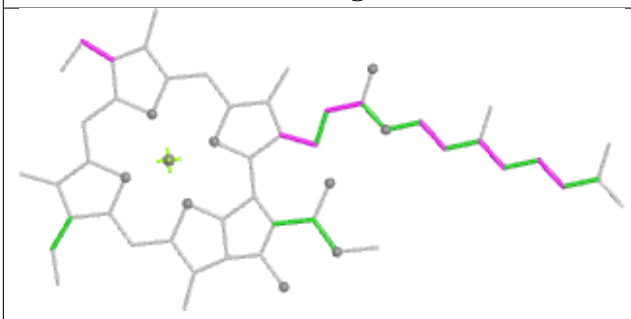
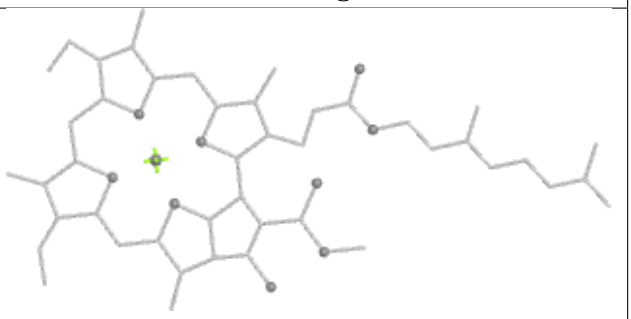
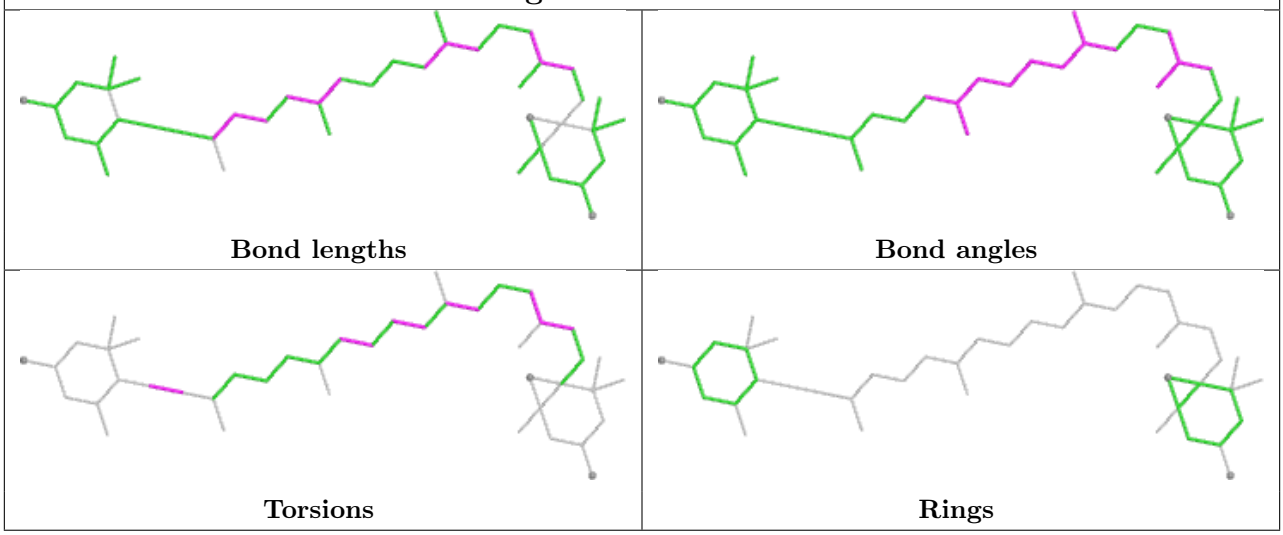


Rings

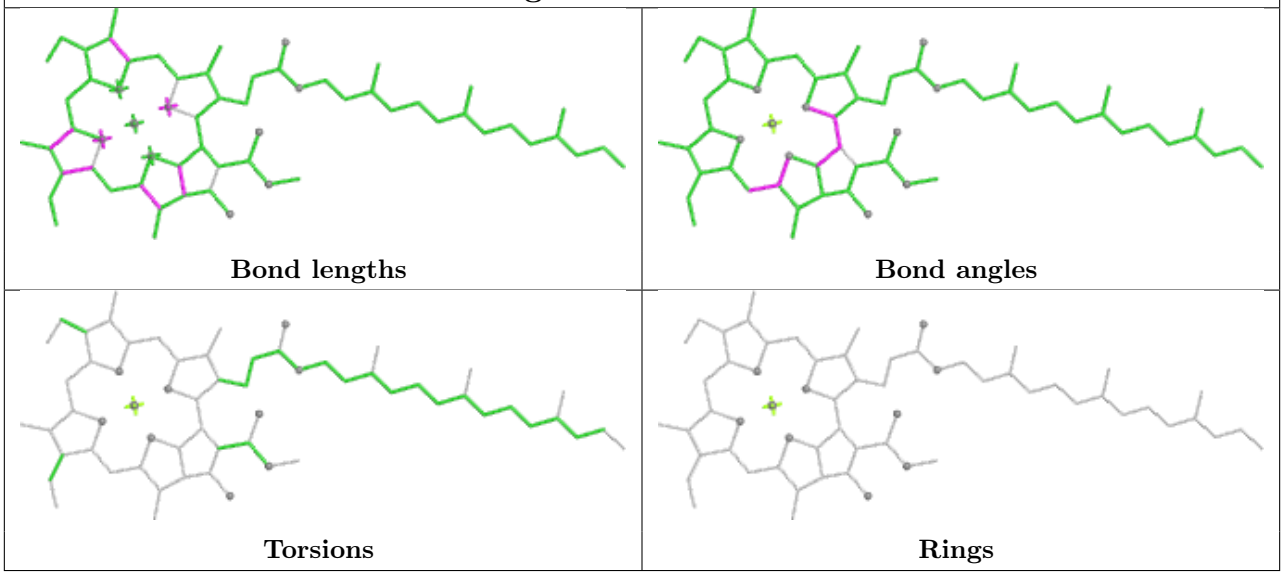
Ligand CLA F 802	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA B 811	
 Bond lengths	 Bond angles
 Torsions	 Rings

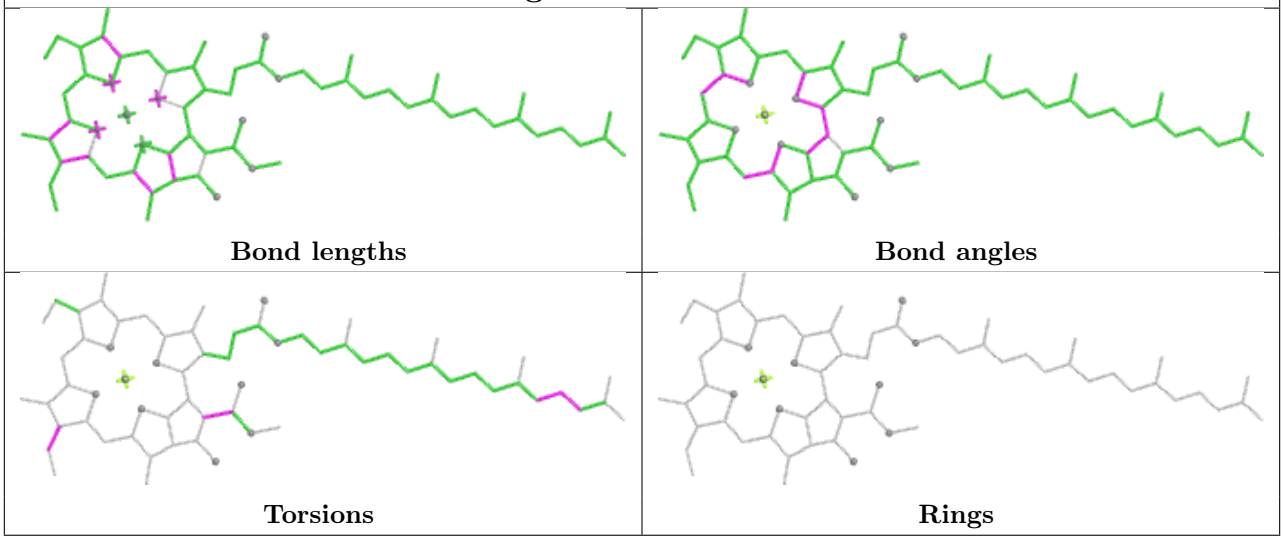
Ligand DD6 A 846



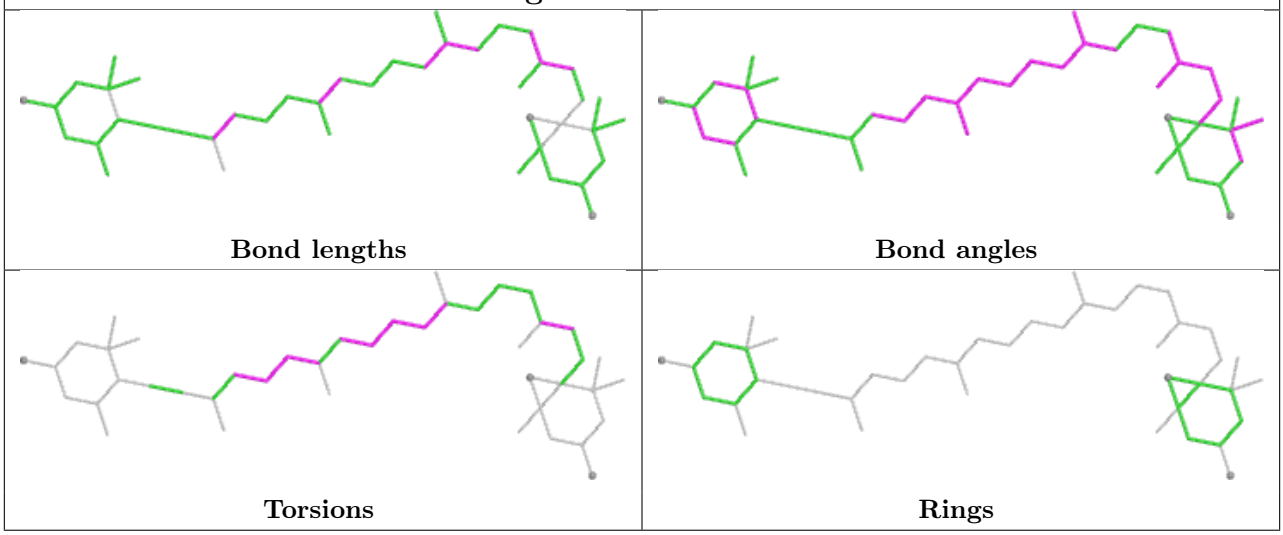
Ligand CLA A 809



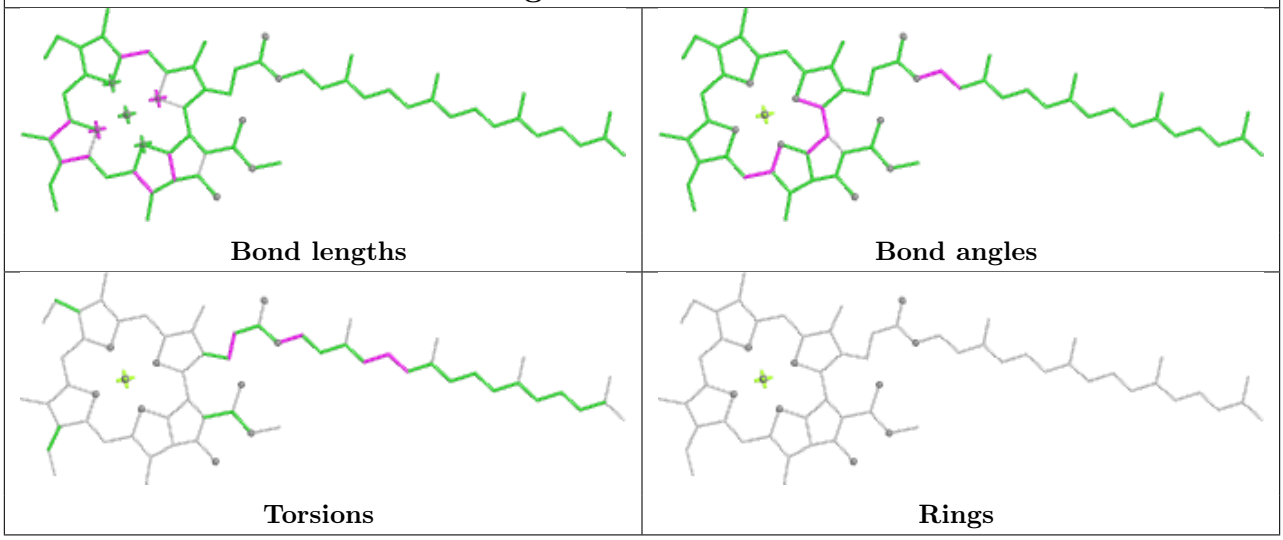
Ligand CLA B 848



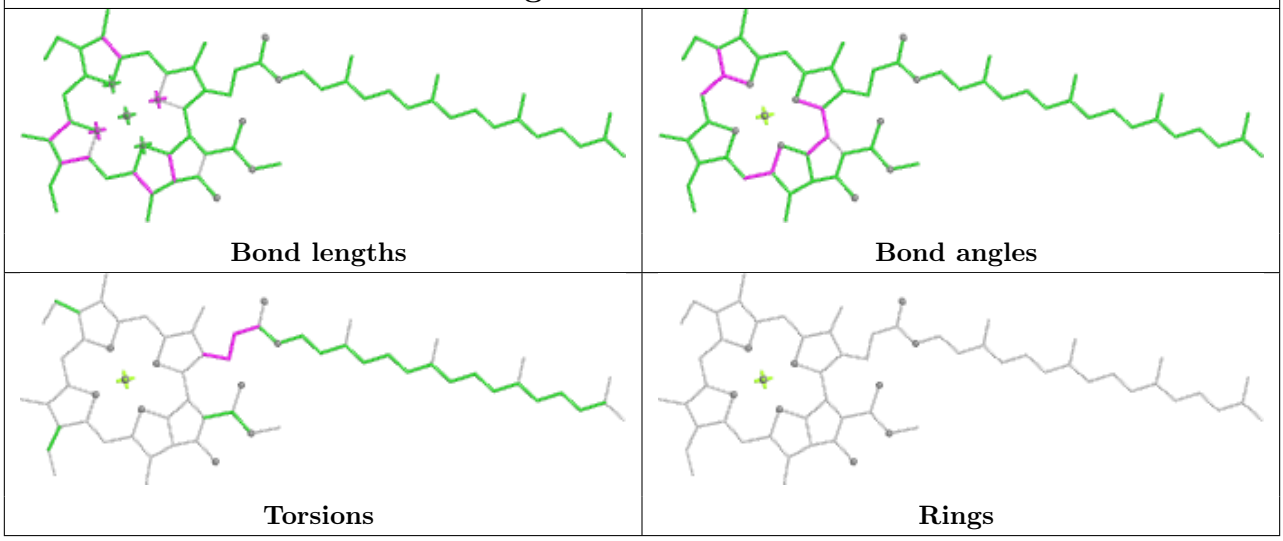
Ligand DD6 U 203

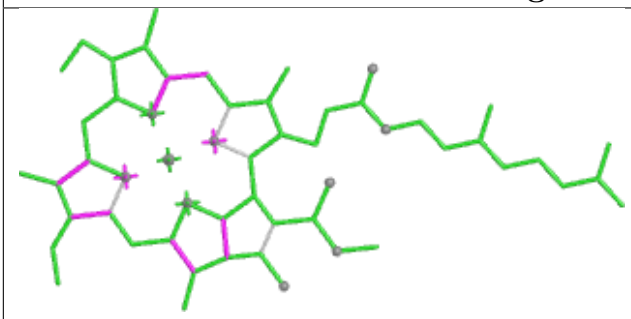
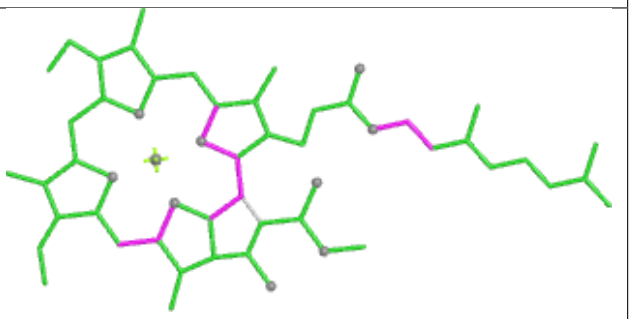
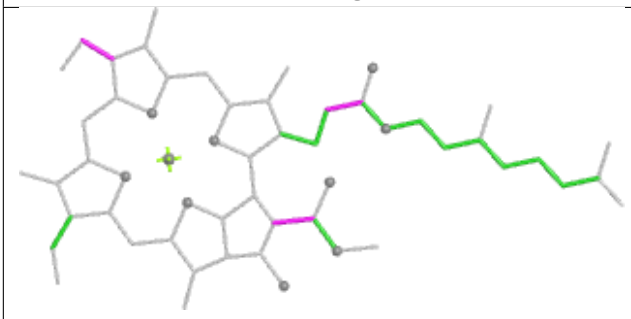
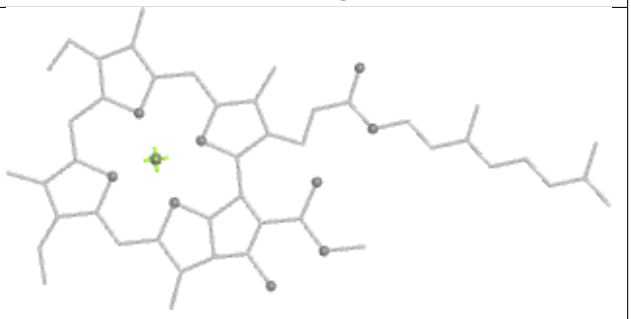


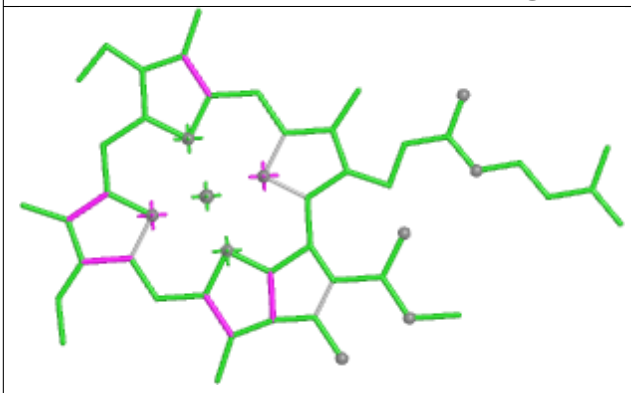
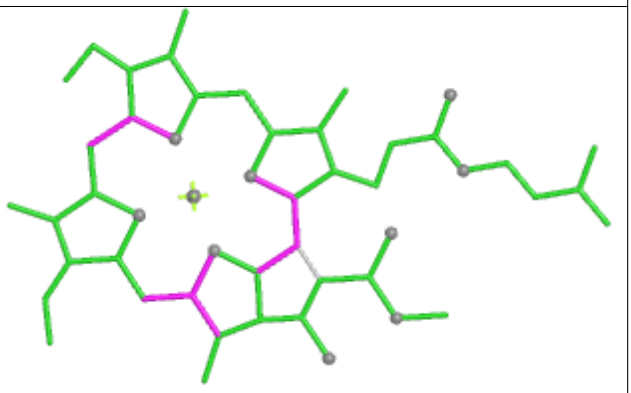
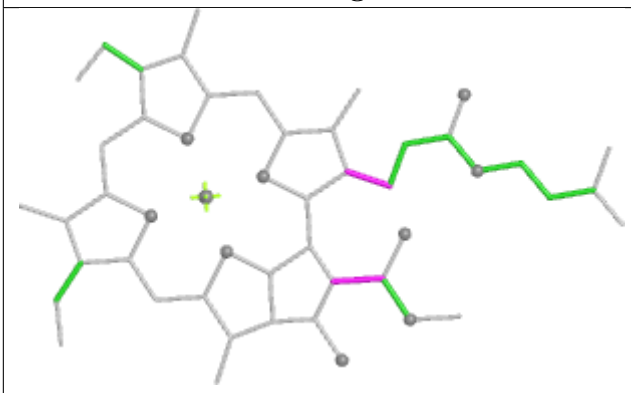
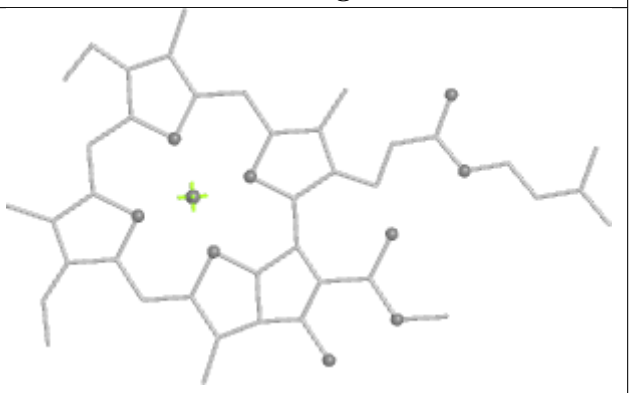
Ligand CLA A 836



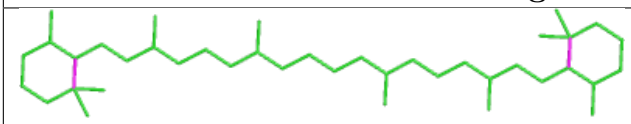
Ligand CLA A 815



Ligand CLA k 202	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA A 813	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand BCR I 103



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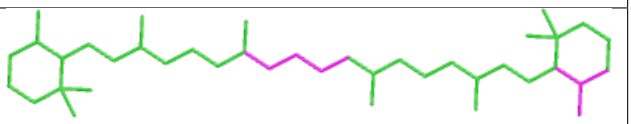
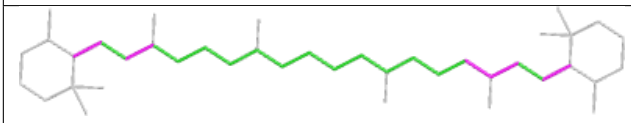


Bond angles



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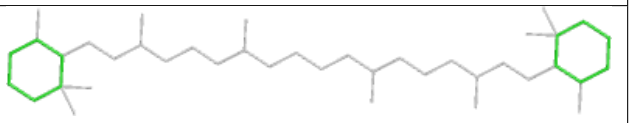
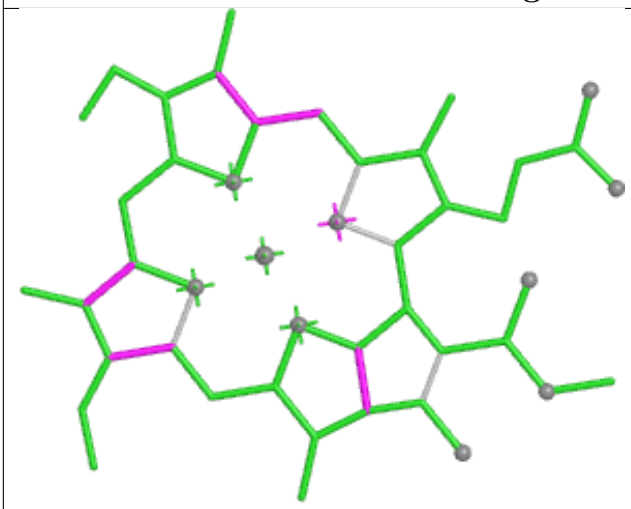


Rings

Ligand CLA G 315



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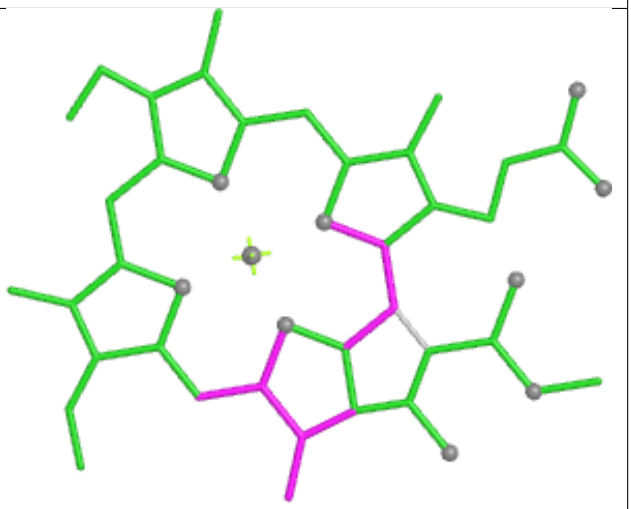

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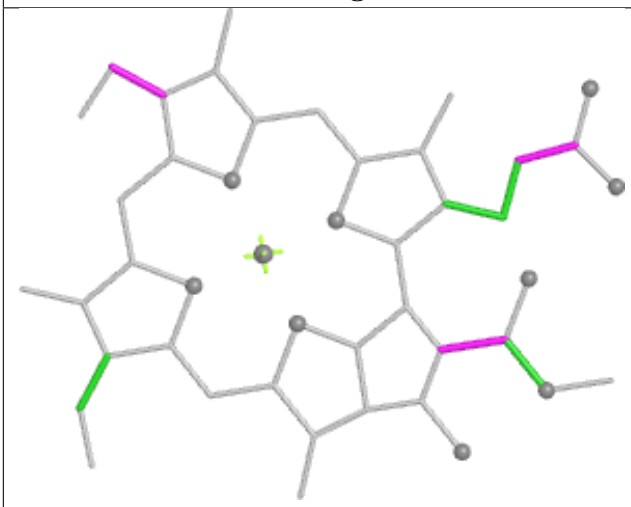

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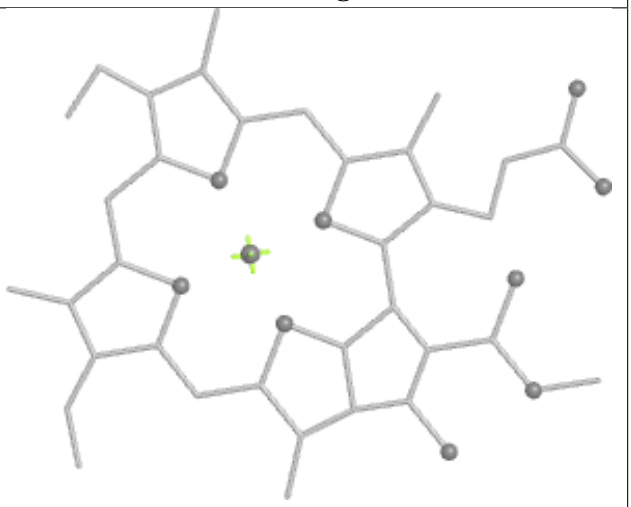
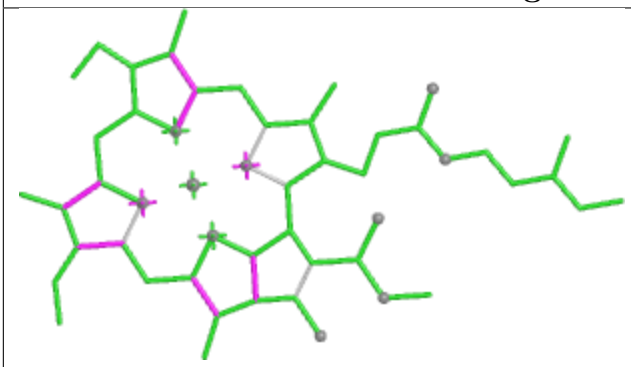
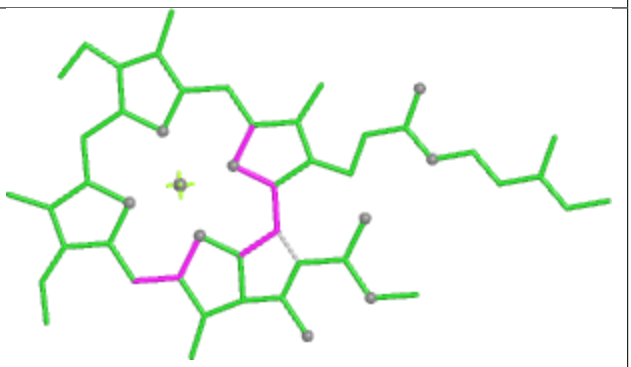
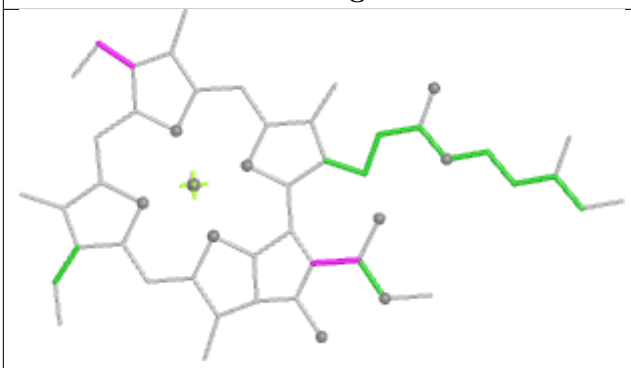
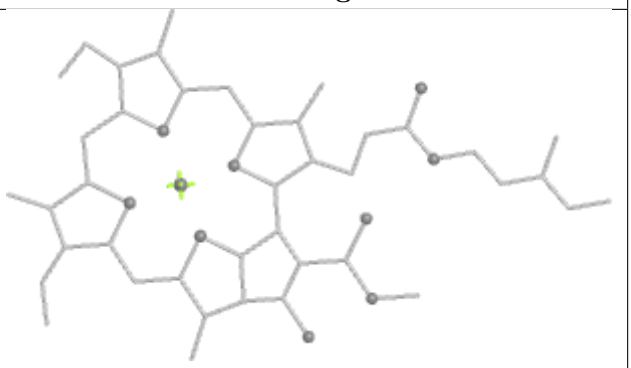
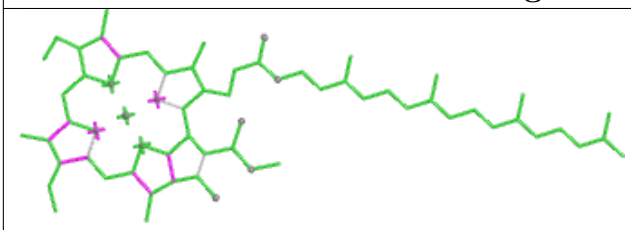
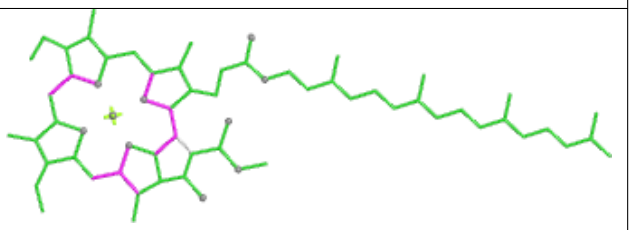
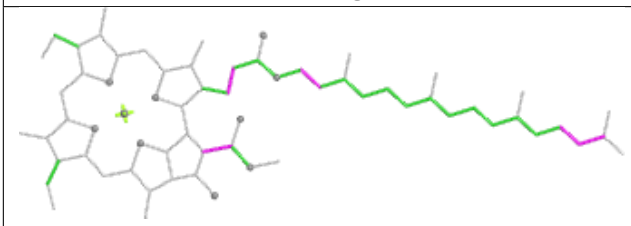
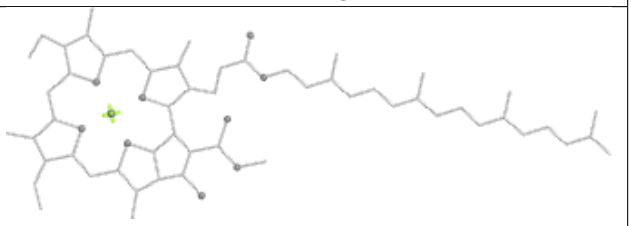
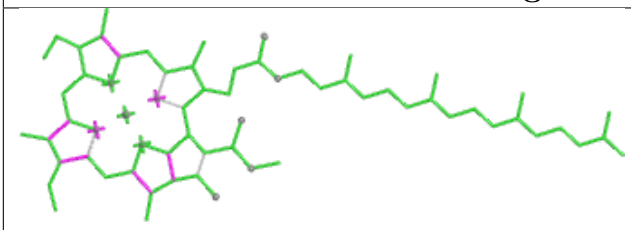


Rings

Ligand CLA A 832	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA B 834	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA A 833



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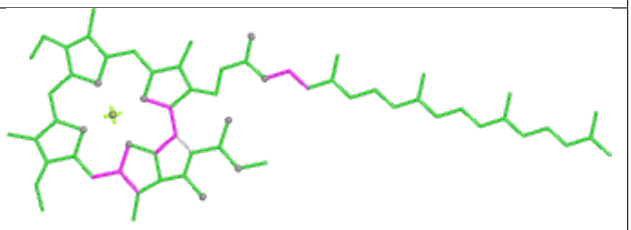
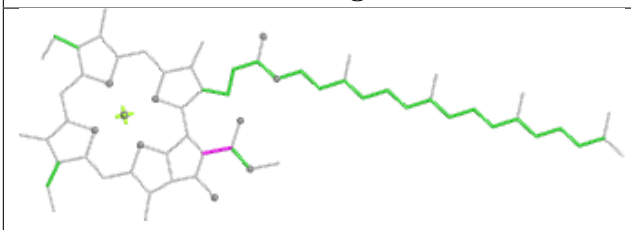


Bond angles



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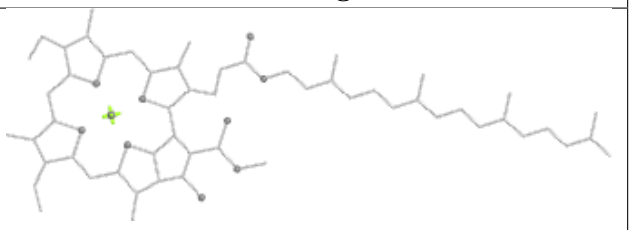
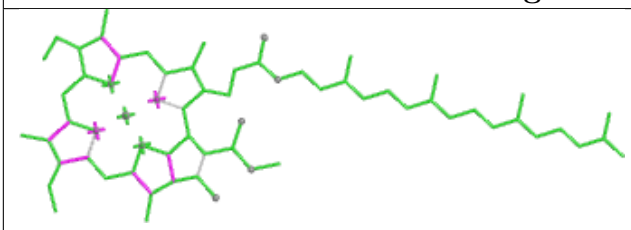


Rings

Ligand CLA A 804



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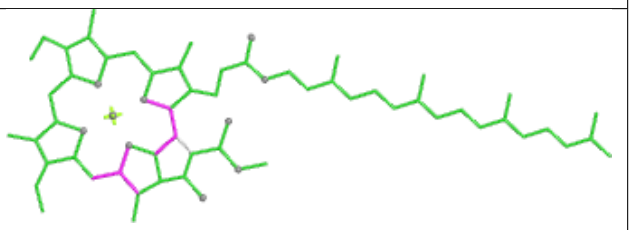

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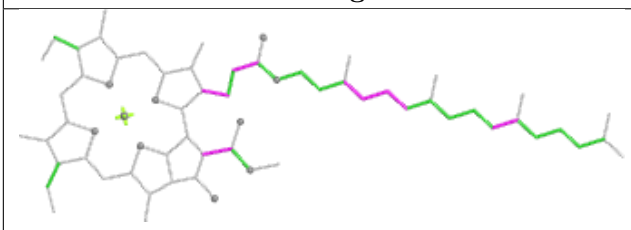

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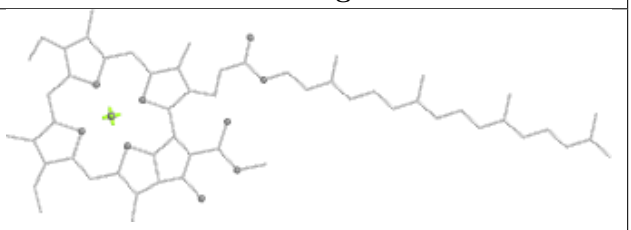
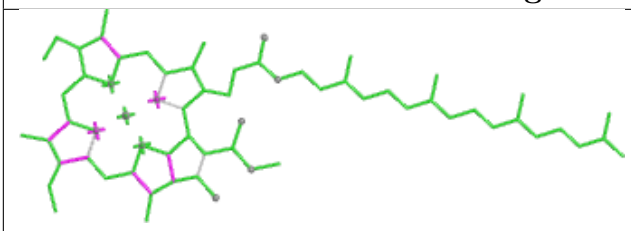


Rings

Ligand CLA B 849



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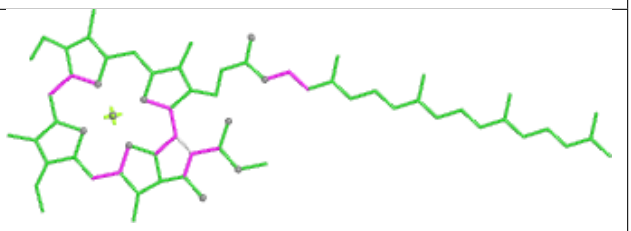

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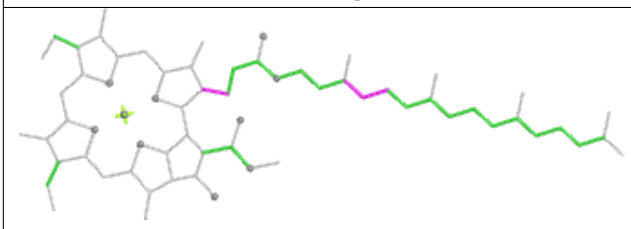

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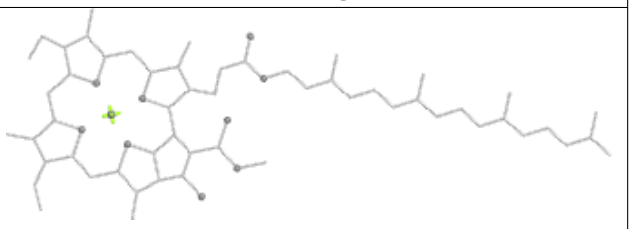
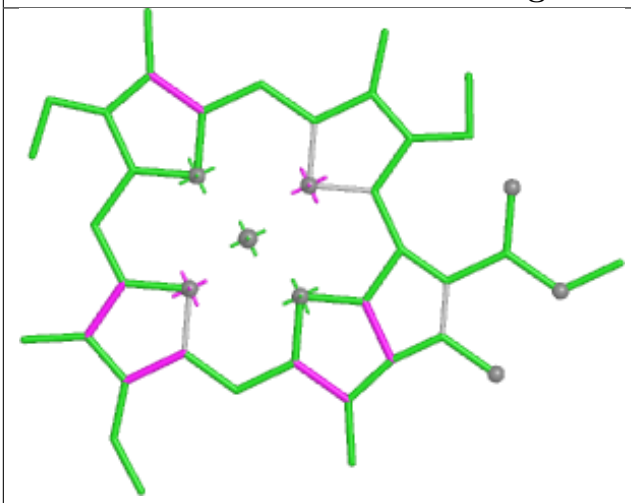


Rings

Ligand CLA J 104



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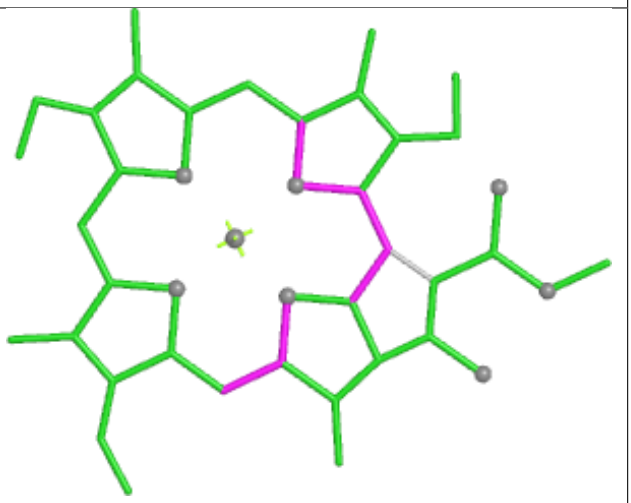

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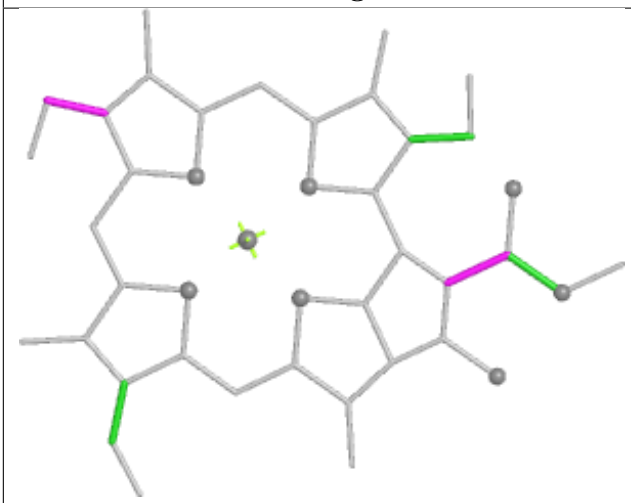
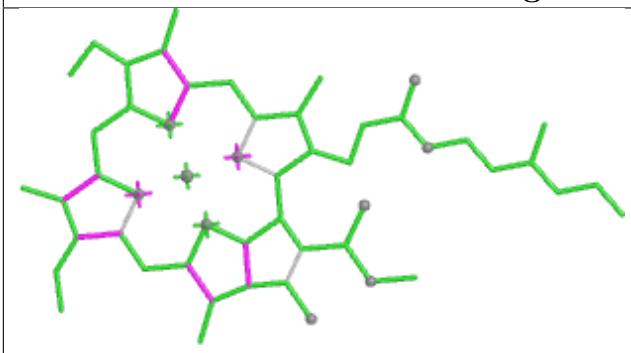


Torsions

Rings

Ligand CLA U 211



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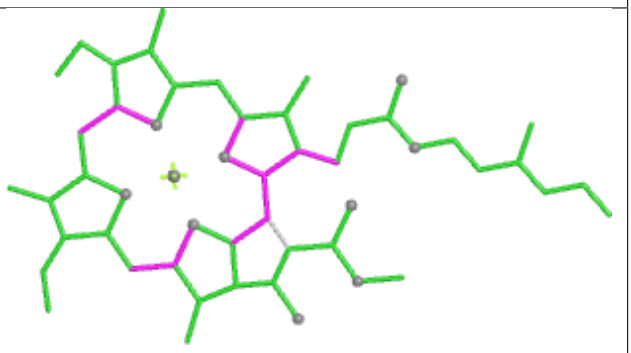

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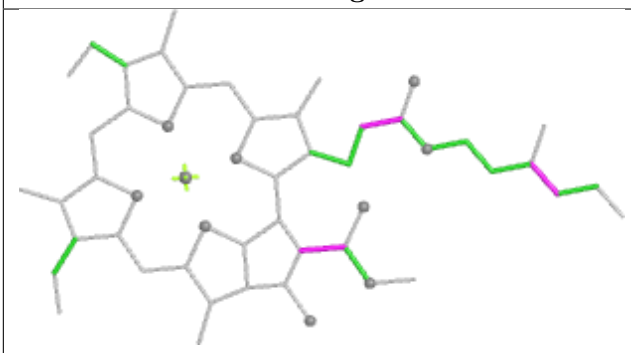

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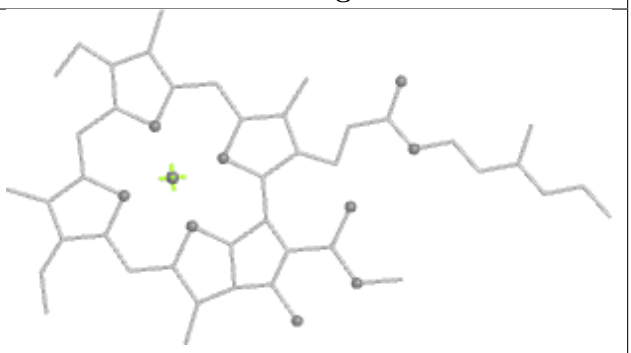
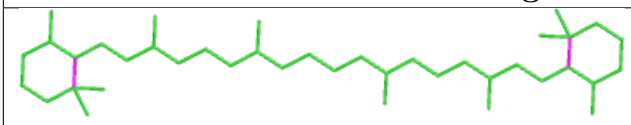


Rings

Ligand BCR A 844



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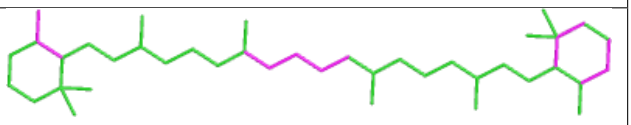
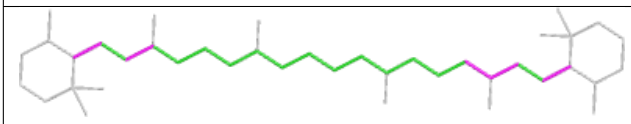


Bond angles



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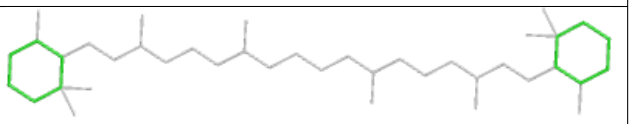
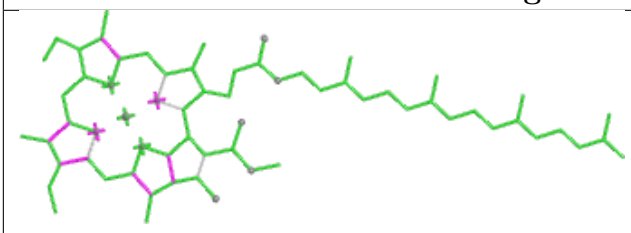


Rings

Ligand CLA A 829



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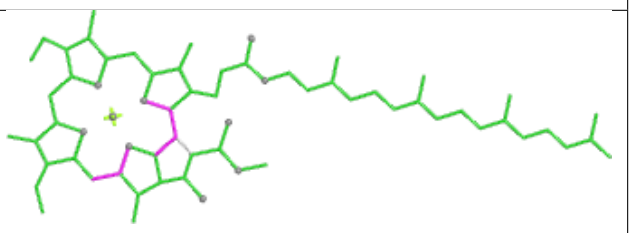
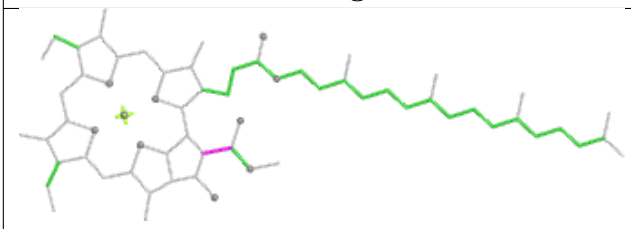


Bond angles



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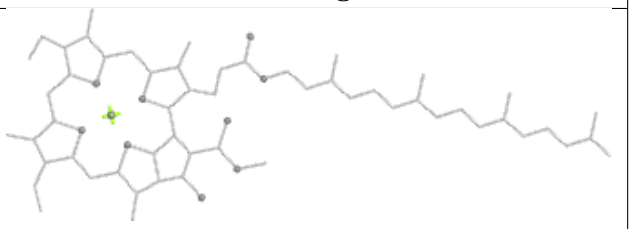
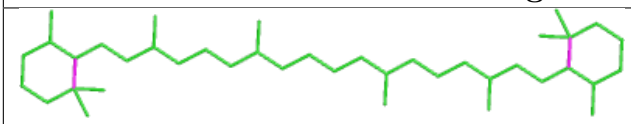
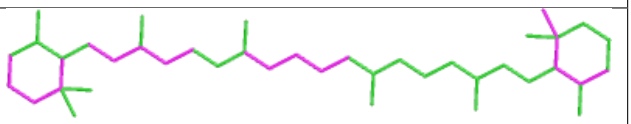
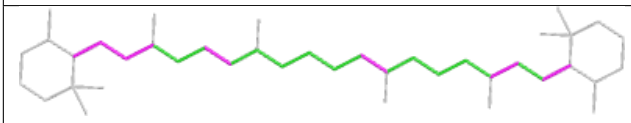
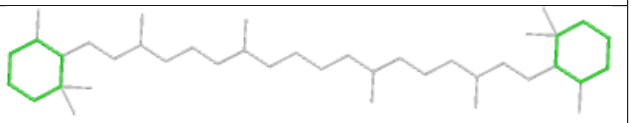
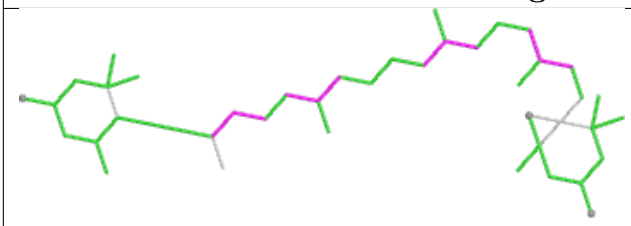
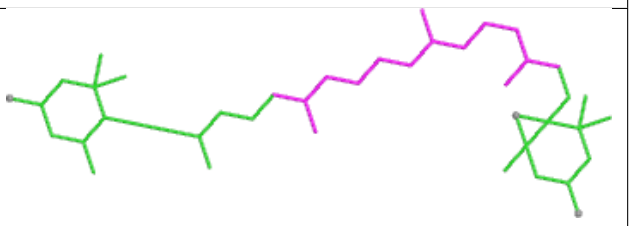
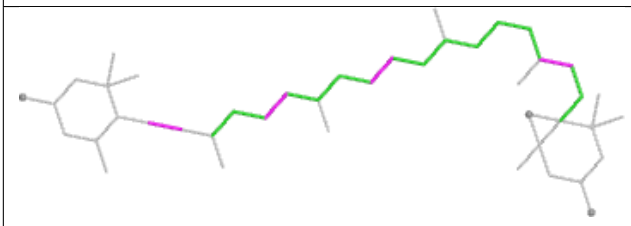
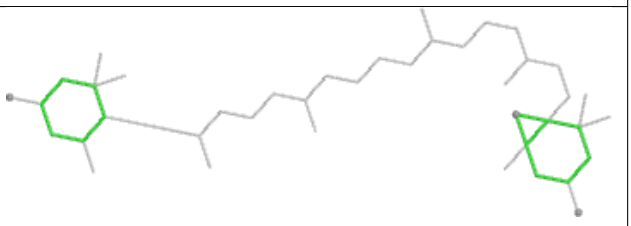
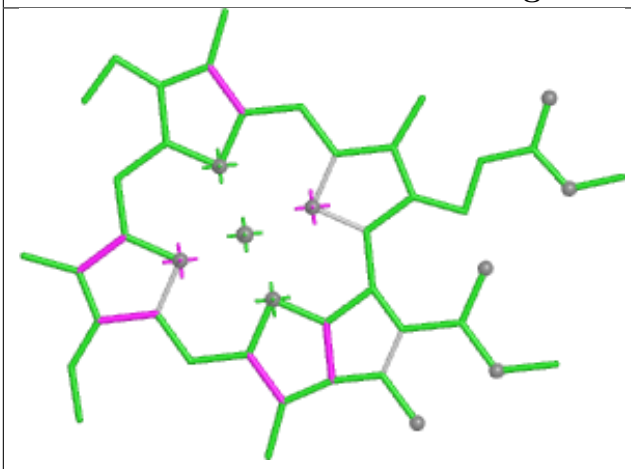
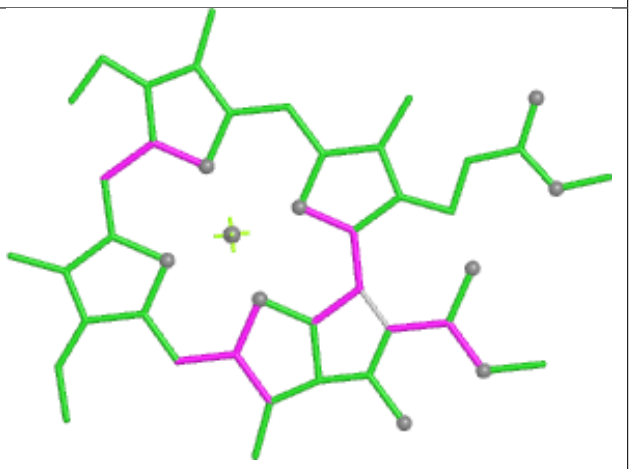
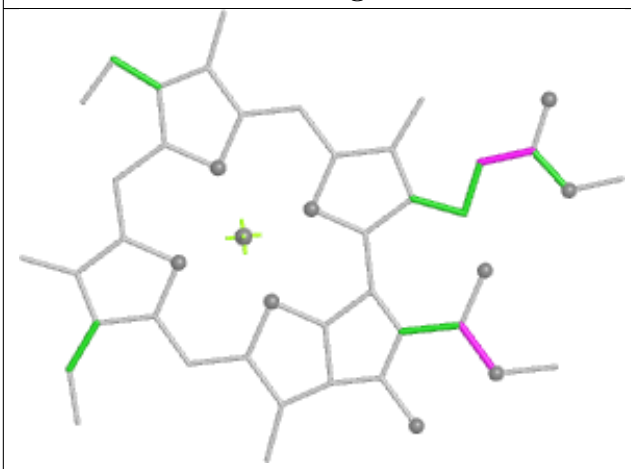
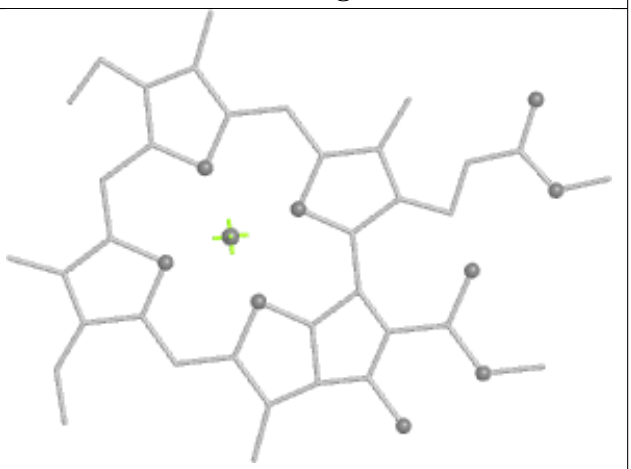
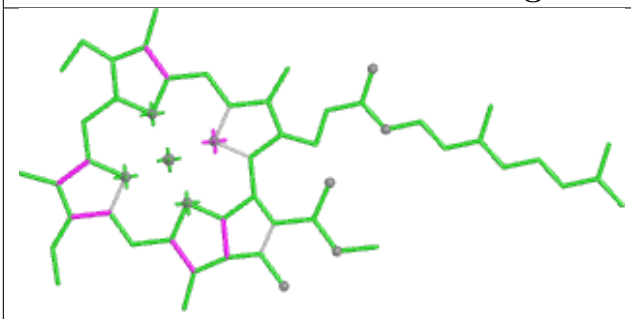
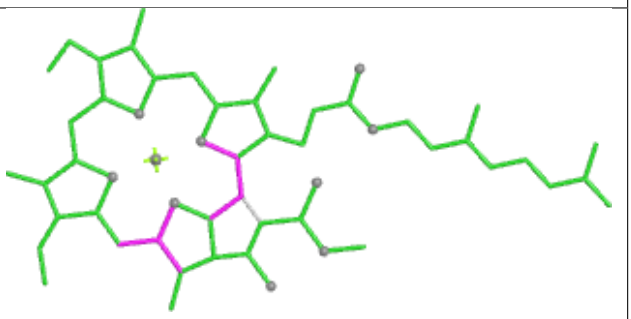
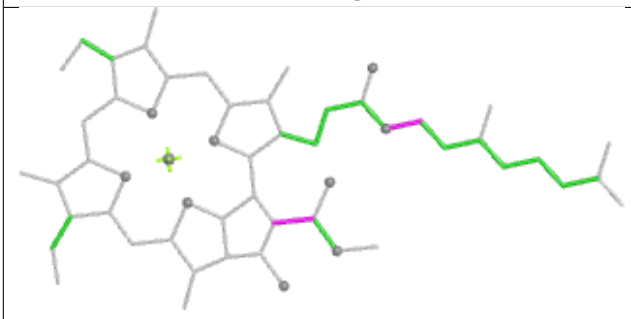
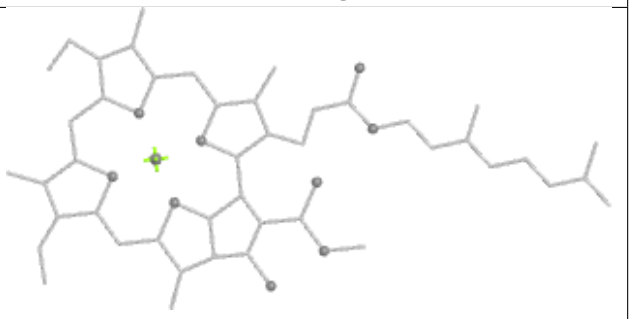


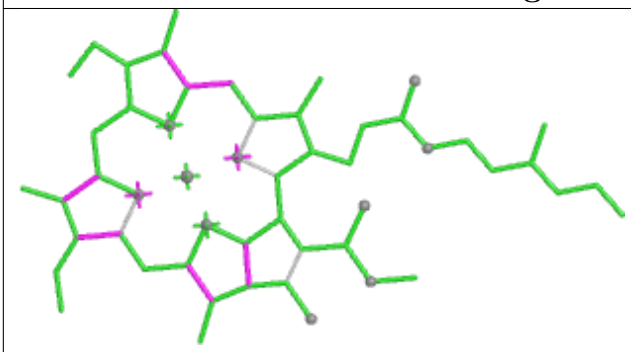
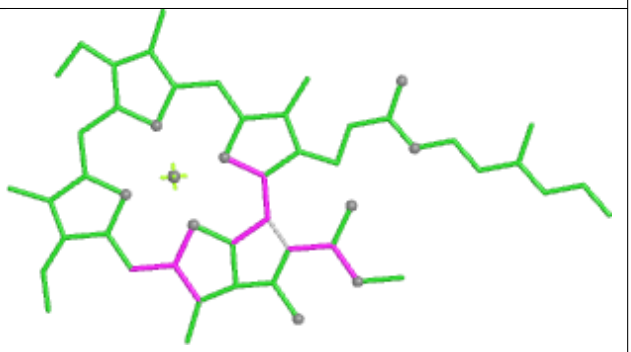
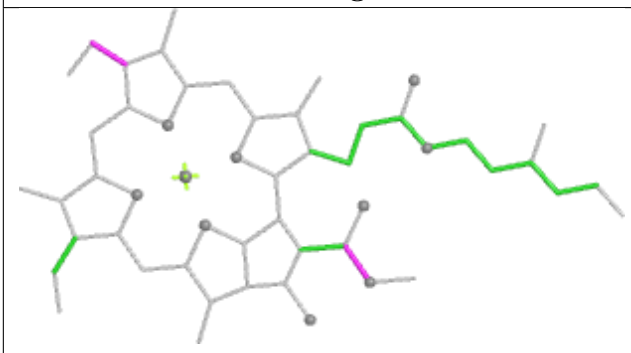
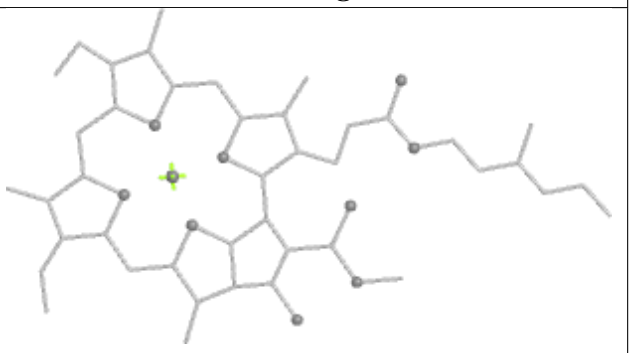
Rings

Ligand BCR k 203	
 Bond lengths	 Bond angles
 Torsions	 Rings

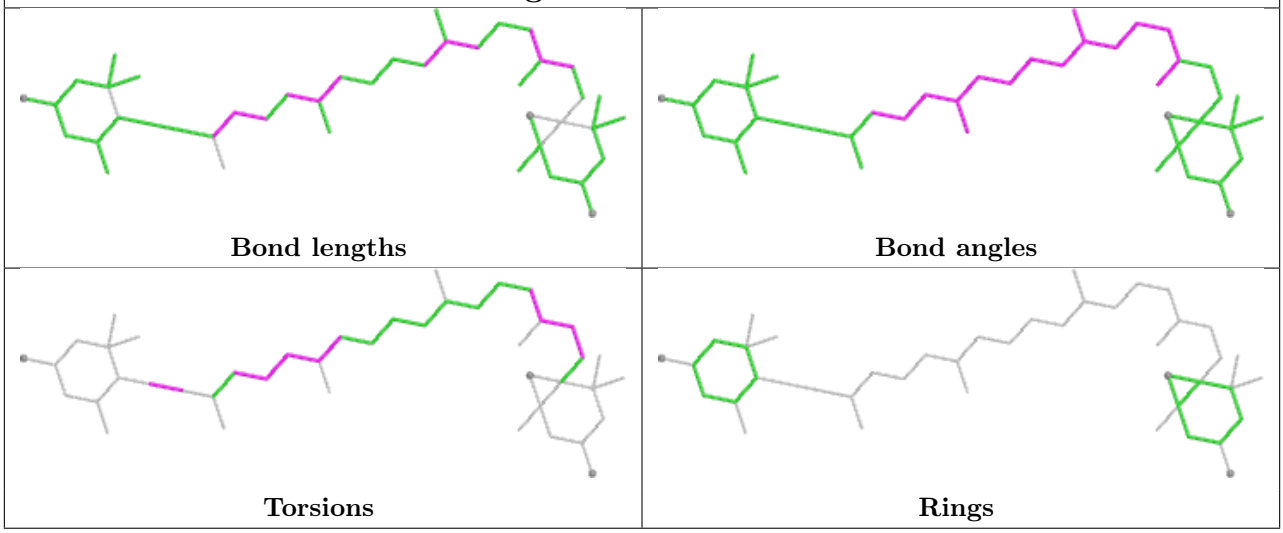
Ligand DD6 J 102	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA U 208	
 Bond lengths	 Bond angles
 Torsions	 Rings

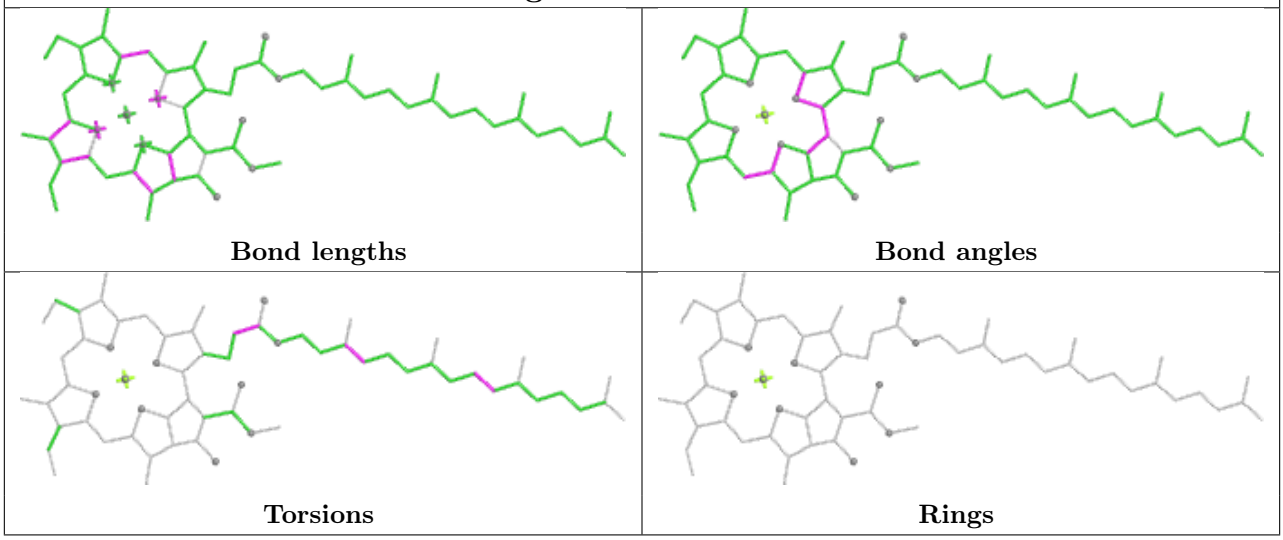
Ligand CLA B 821	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA A 838	
 Bond lengths	 Bond angles
 Torsions	 Rings

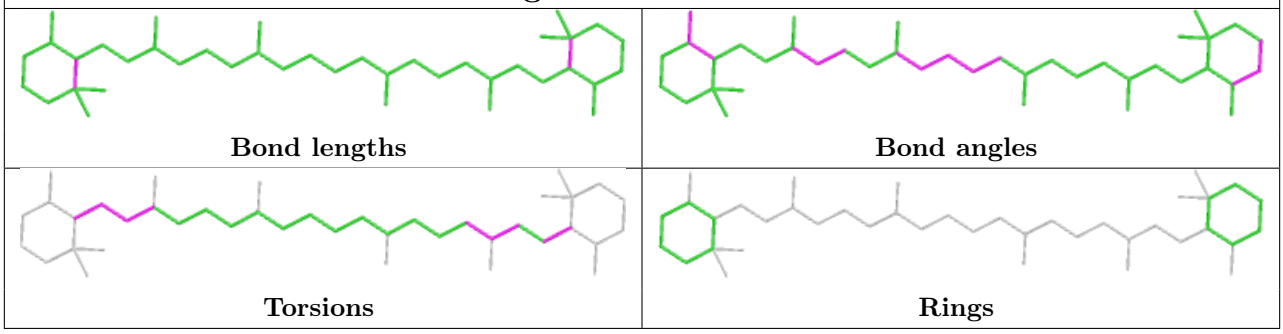
Ligand DD6 G 314



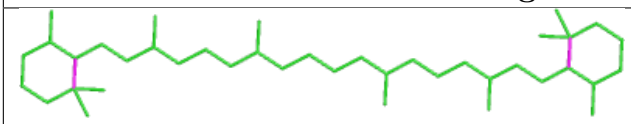
Ligand CLA B 806



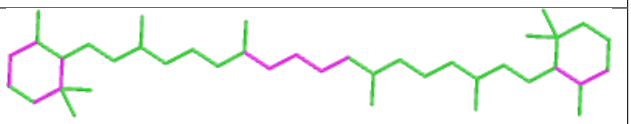
Ligand BCR B 839



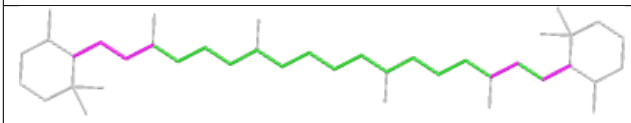
Ligand BCR M 101



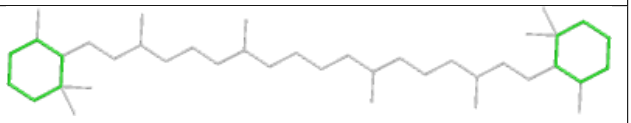
Bond lengths



Bond angles

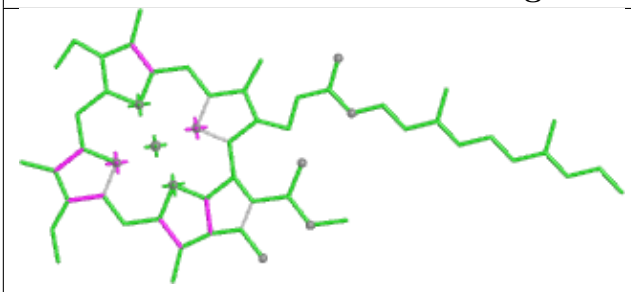


Torsions

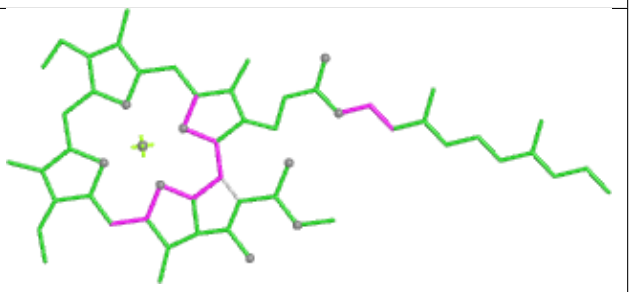


Rings

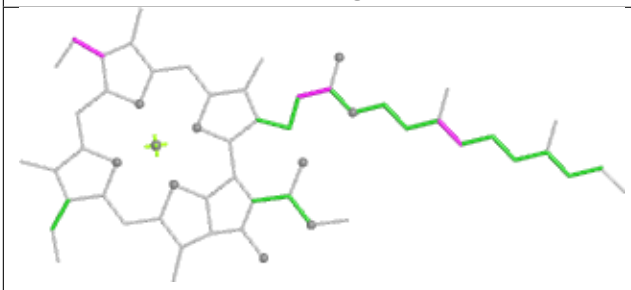
Ligand CLA B 836



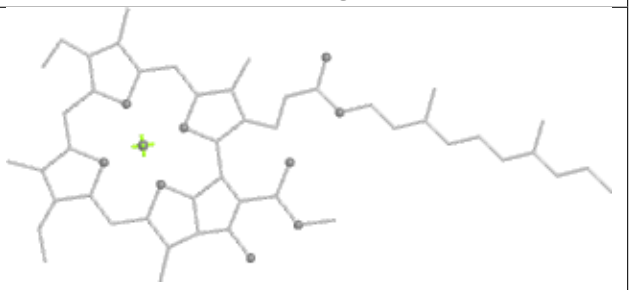
Bond lengths



Bond angles

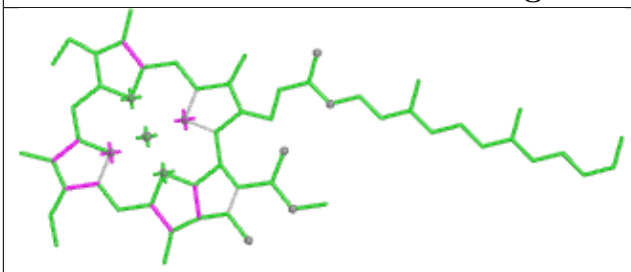


Torsions

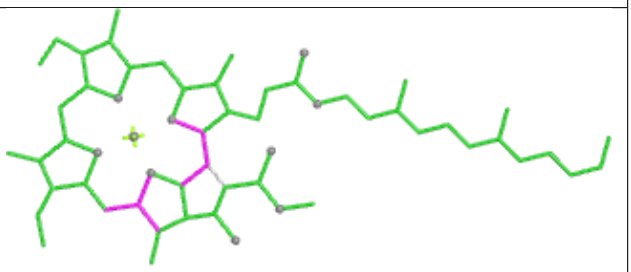


Rings

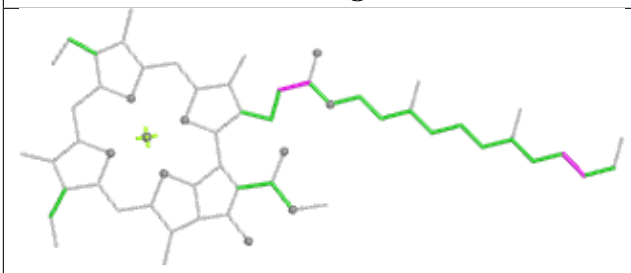
Ligand CLA B 815



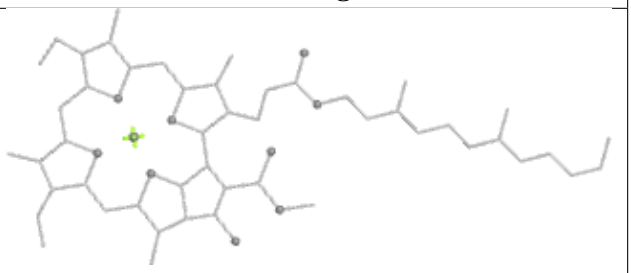
Bond lengths



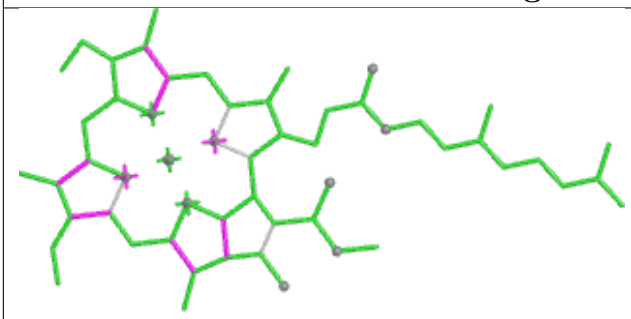
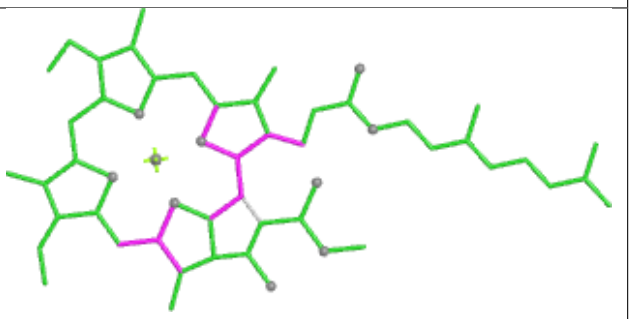
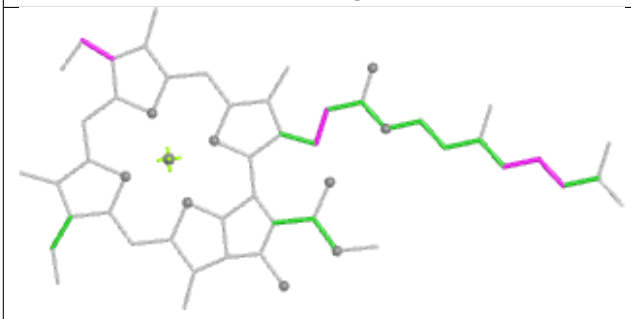
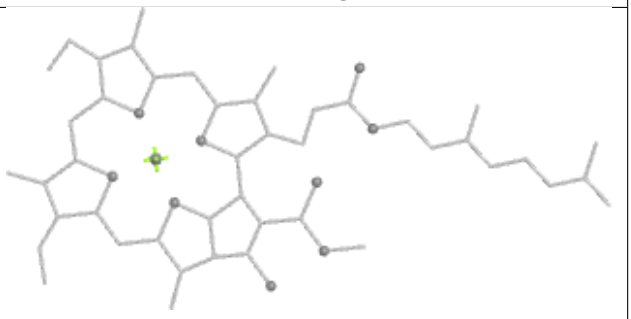
Bond angles

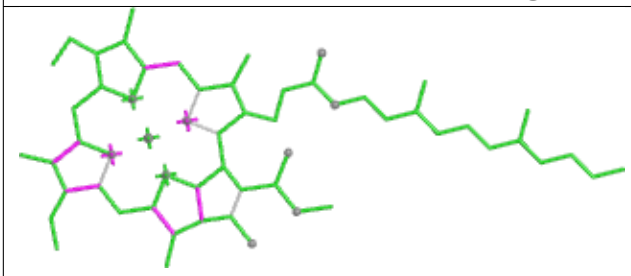
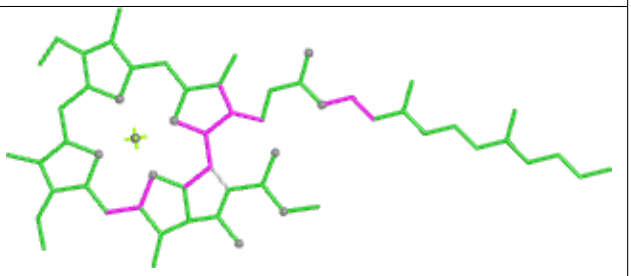
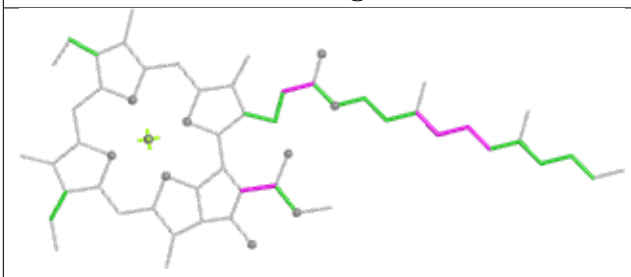
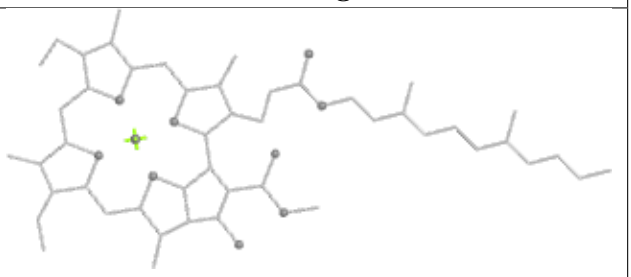


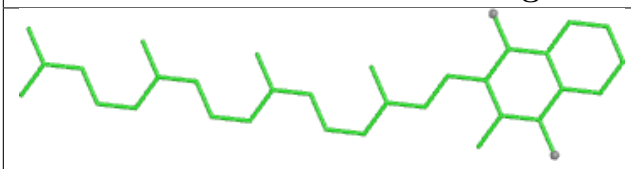
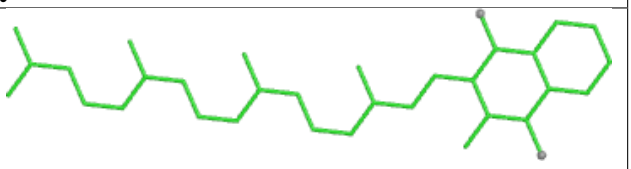
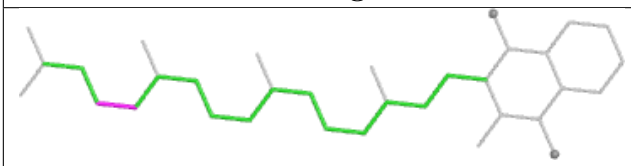
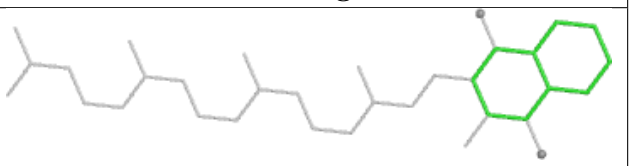
Torsions

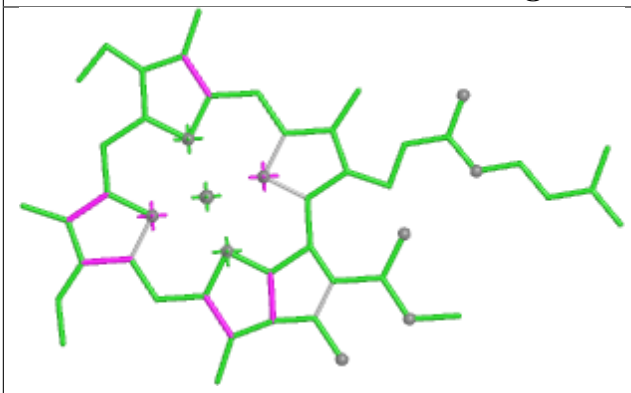
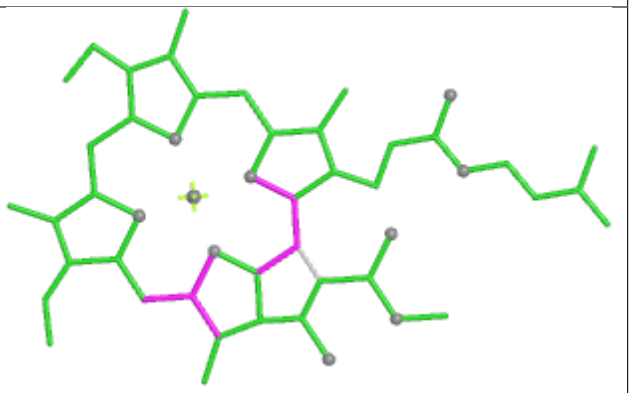
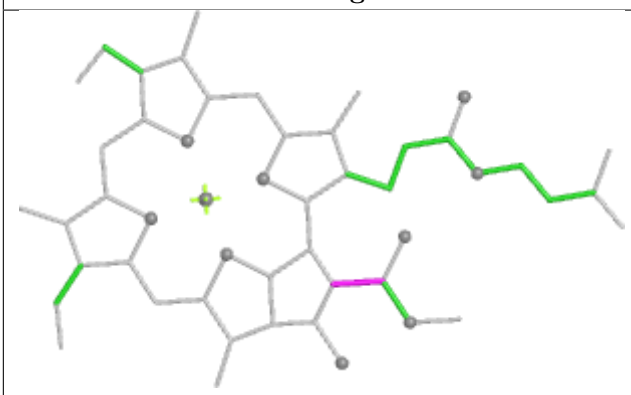
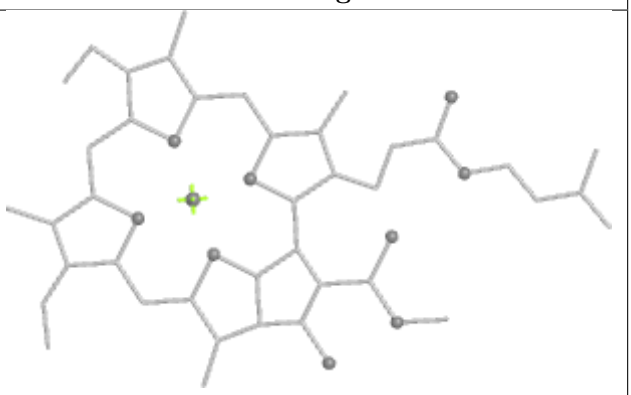


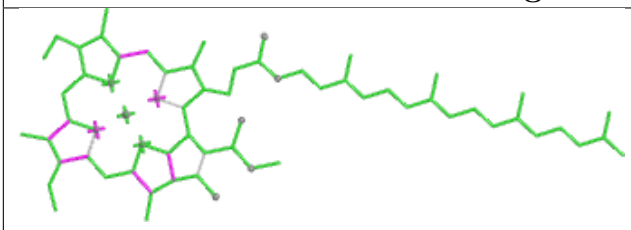
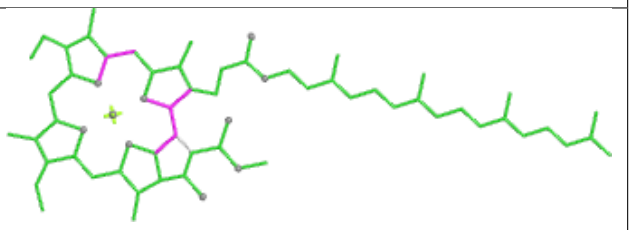
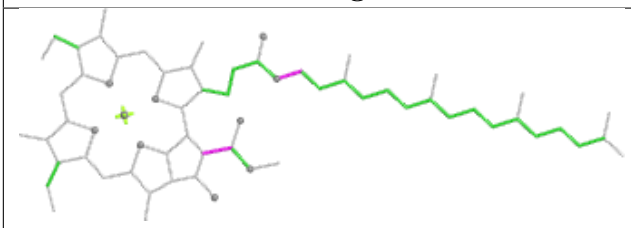
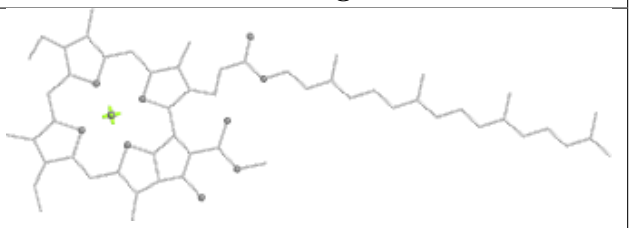
Rings

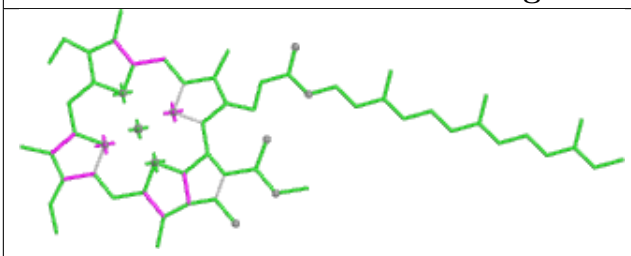
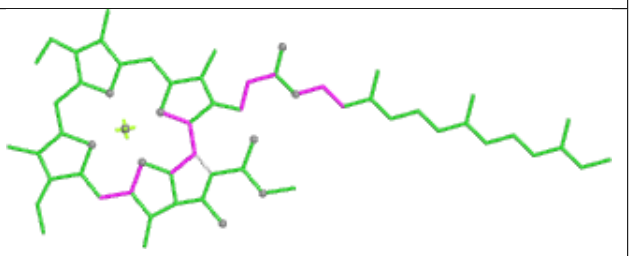
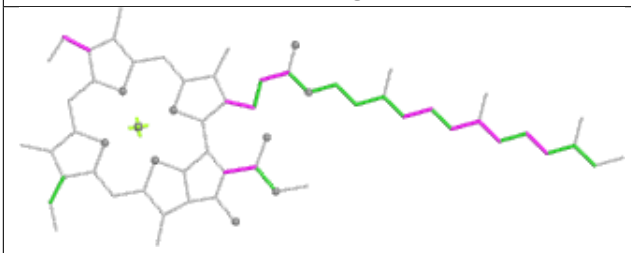
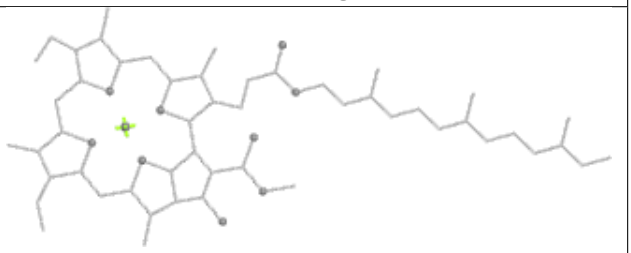
Ligand CLA A 807	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA B 828	
 Bond lengths	 Bond angles
 Torsions	 Rings

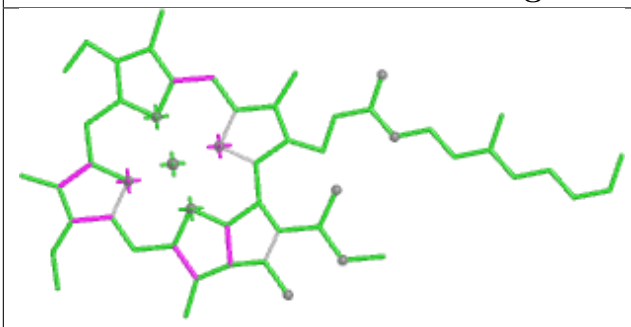
Ligand PQN B 837	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA B 826	
 Bond lengths	 Bond angles
 Torsions	 Rings

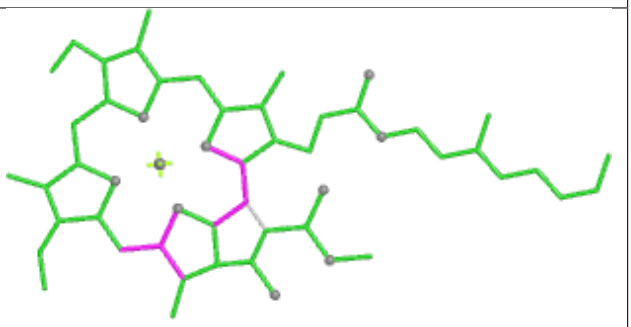
Ligand CLA B 802	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA U 204	
 Bond lengths	 Bond angles
 Torsions	 Rings

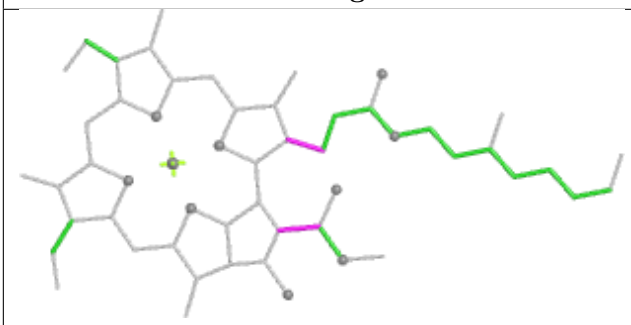
Ligand CLA B 812



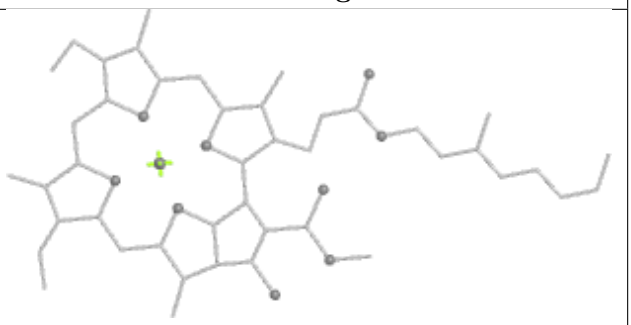
Bond lengths



Bond angles

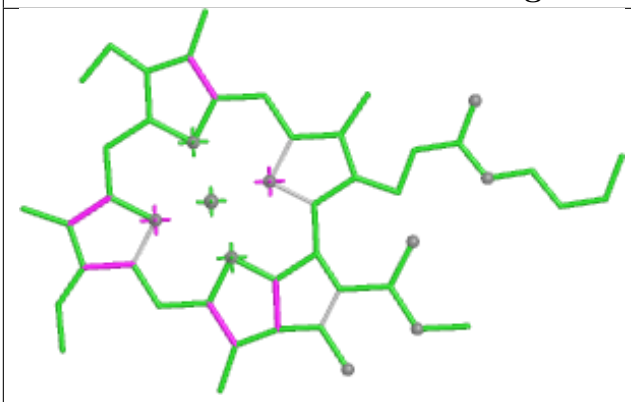


Torsions

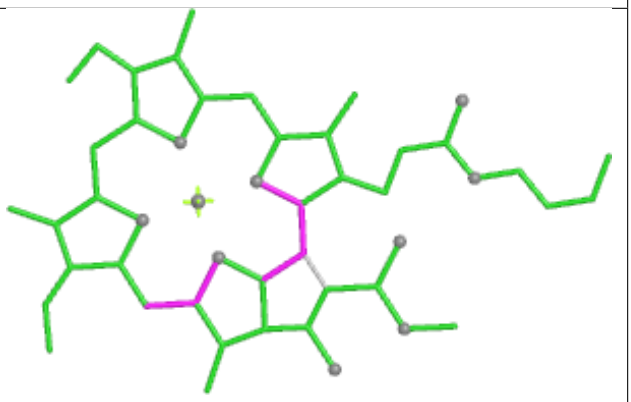


Rings

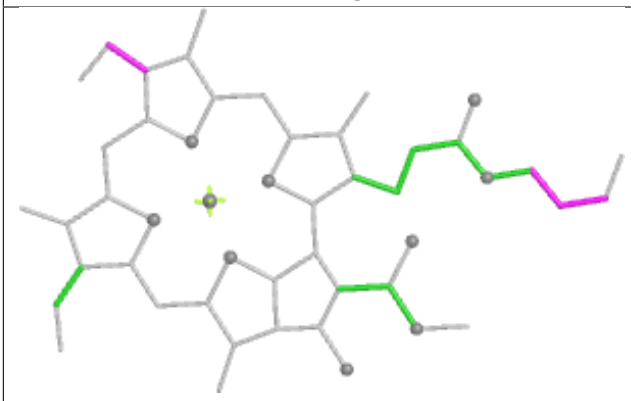
Ligand CLA B 827



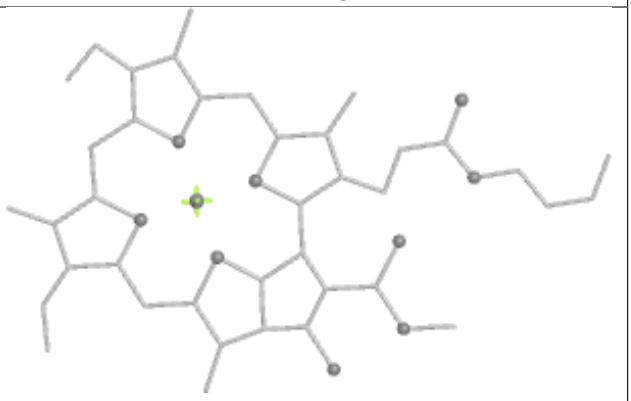
Bond lengths



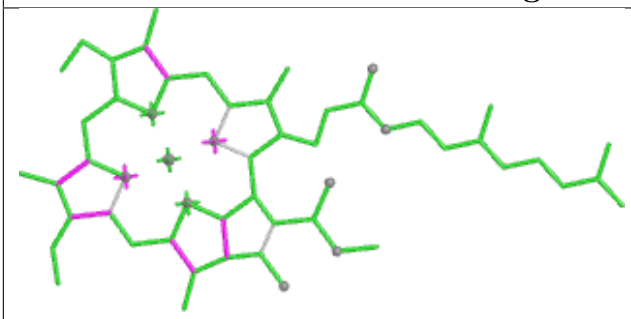
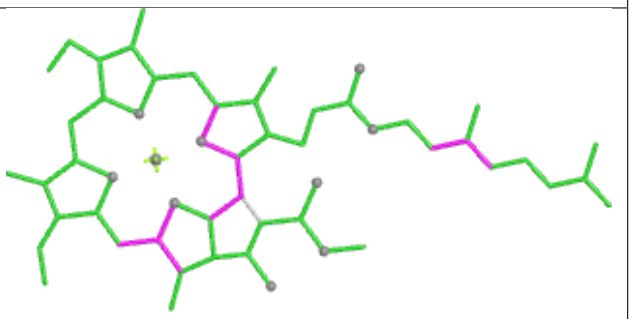
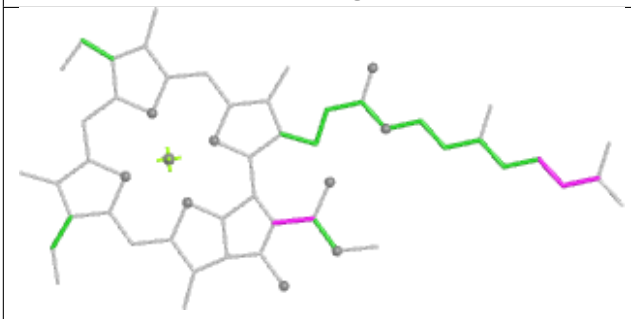
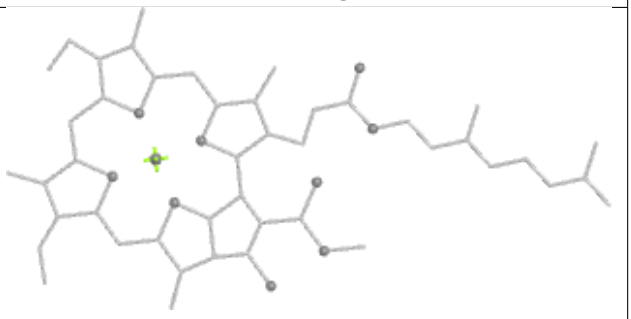
Bond angles

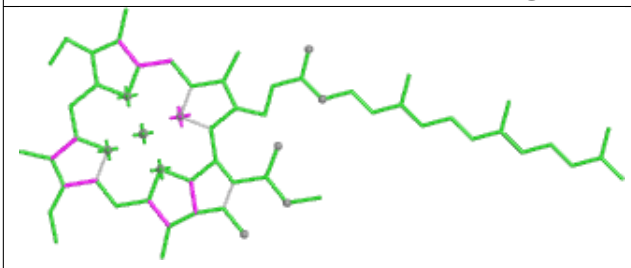
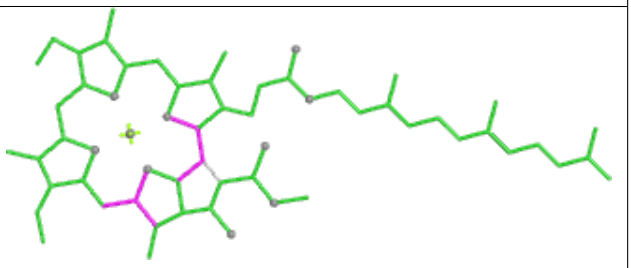
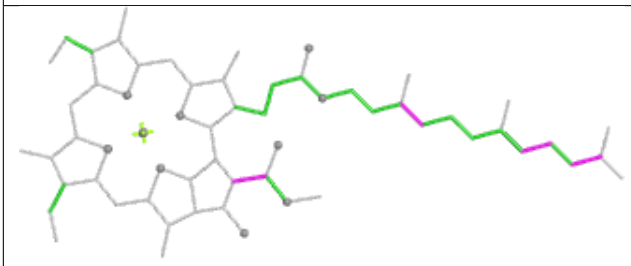
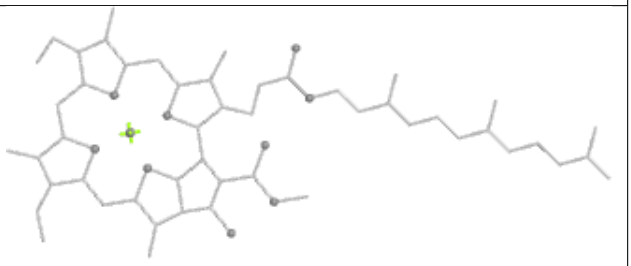


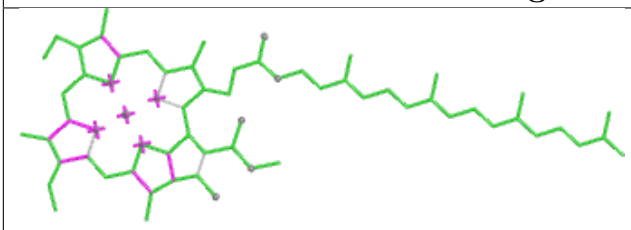
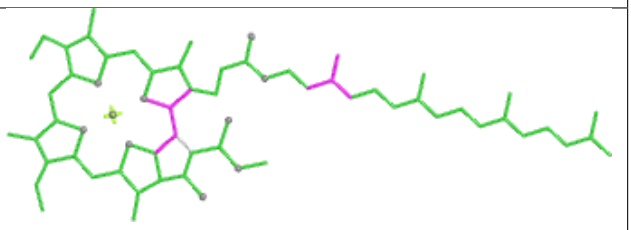
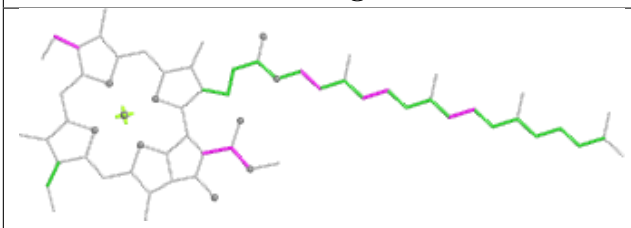
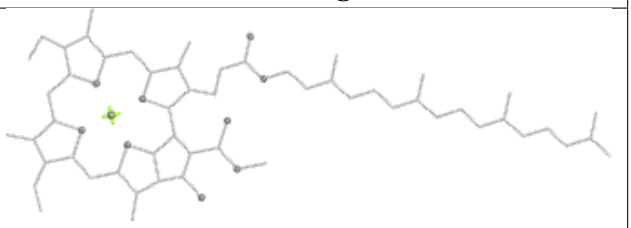
Torsions

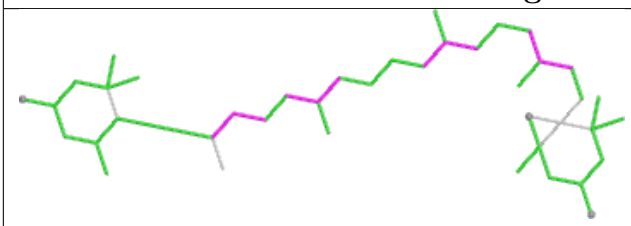
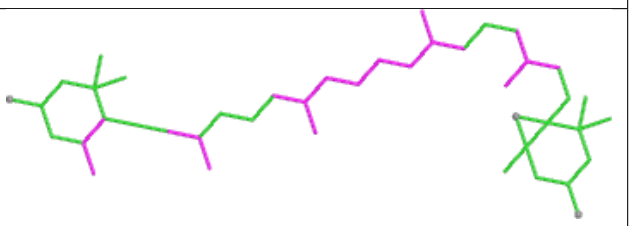
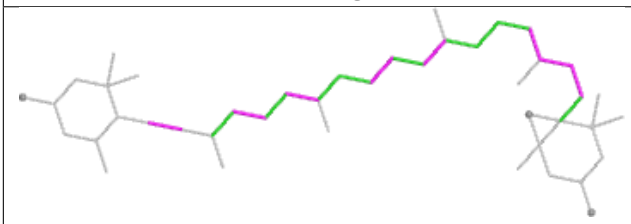


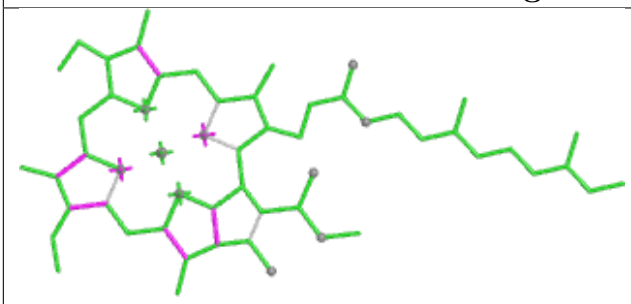
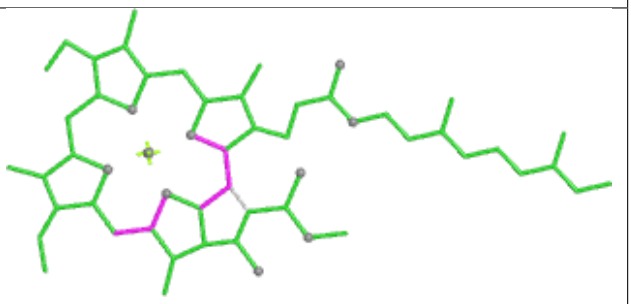
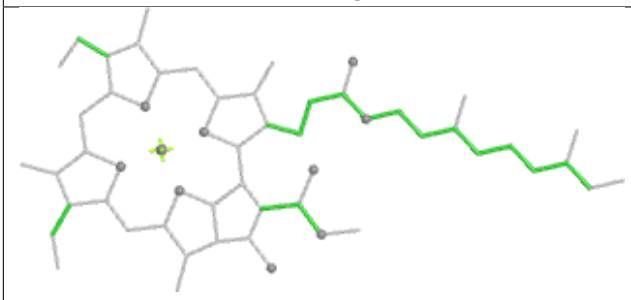
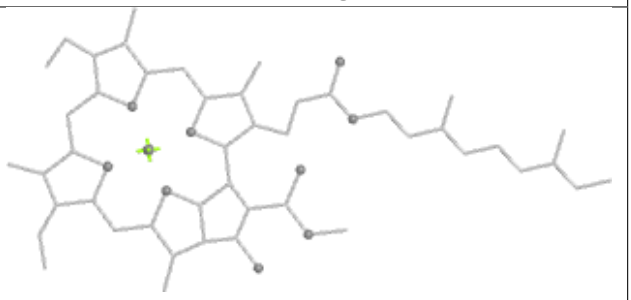
Rings

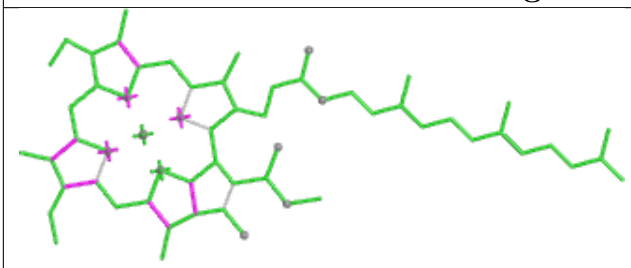
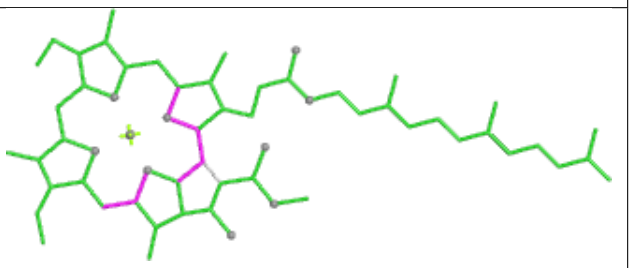
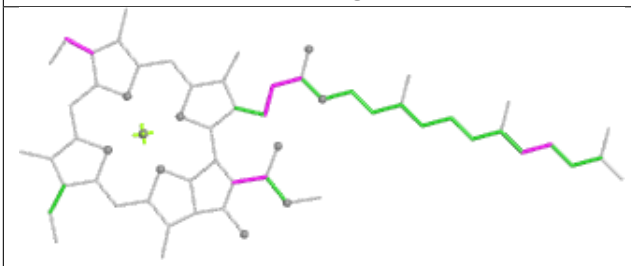
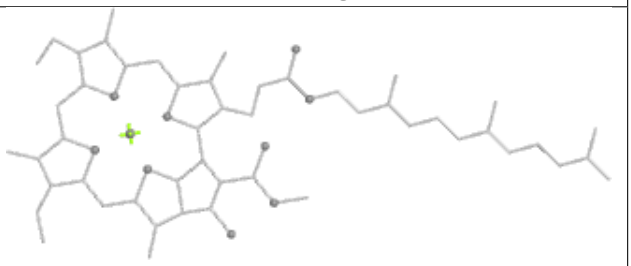
Ligand CLA G 308	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA G 307	
 Bond lengths	 Bond angles
 Torsions	 Rings

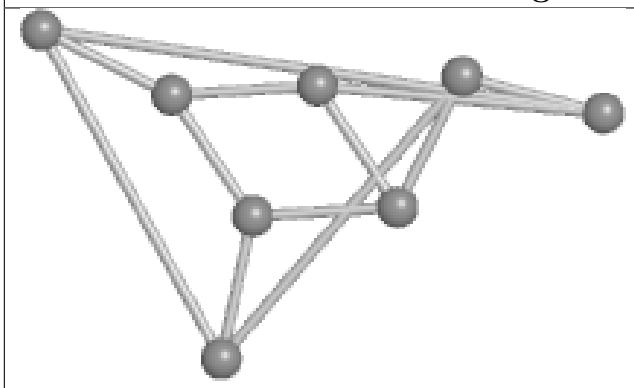
Ligand CL0 A 850	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand DD6 G 317	
 Bond lengths	 Bond angles
 Torsions	Rings

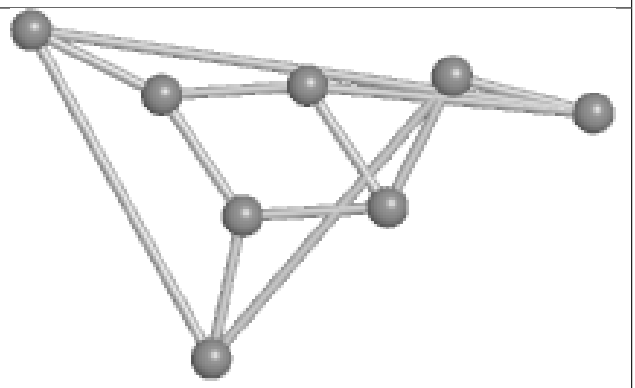
Ligand CLA A 808	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA A 847	
 Bond lengths	 Bond angles
 Torsions	 Rings

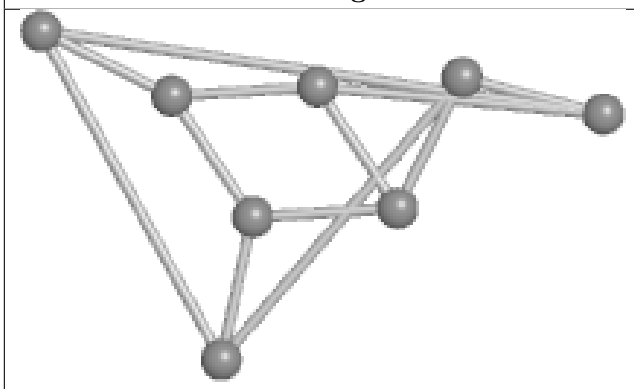
Ligand SF4 C 102



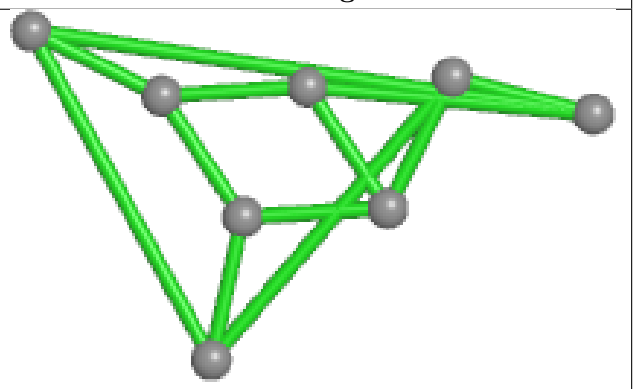
Bond lengths



Bond angles

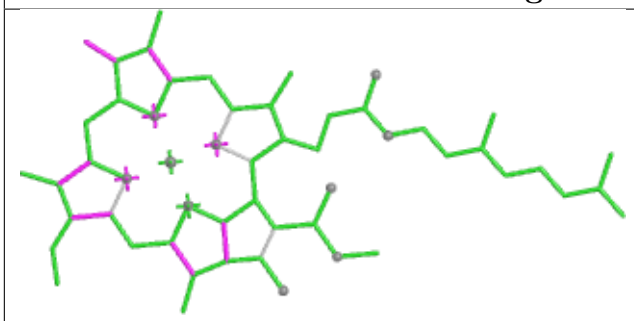


Torsions

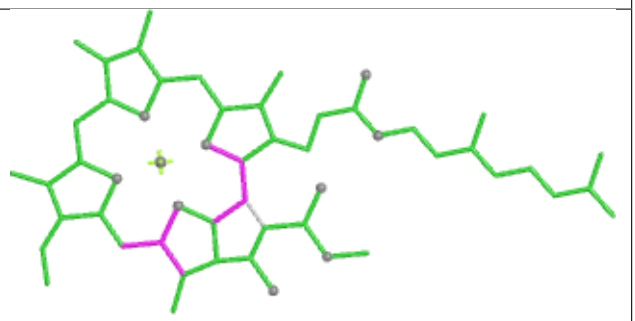


Rings

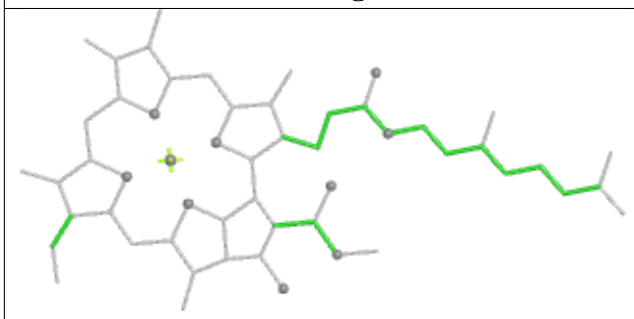
Ligand CLA B 810



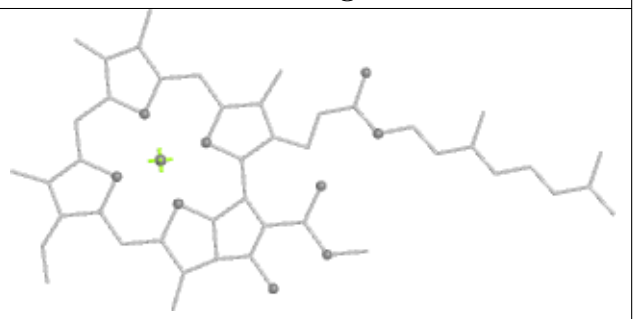
Bond lengths



Bond angles

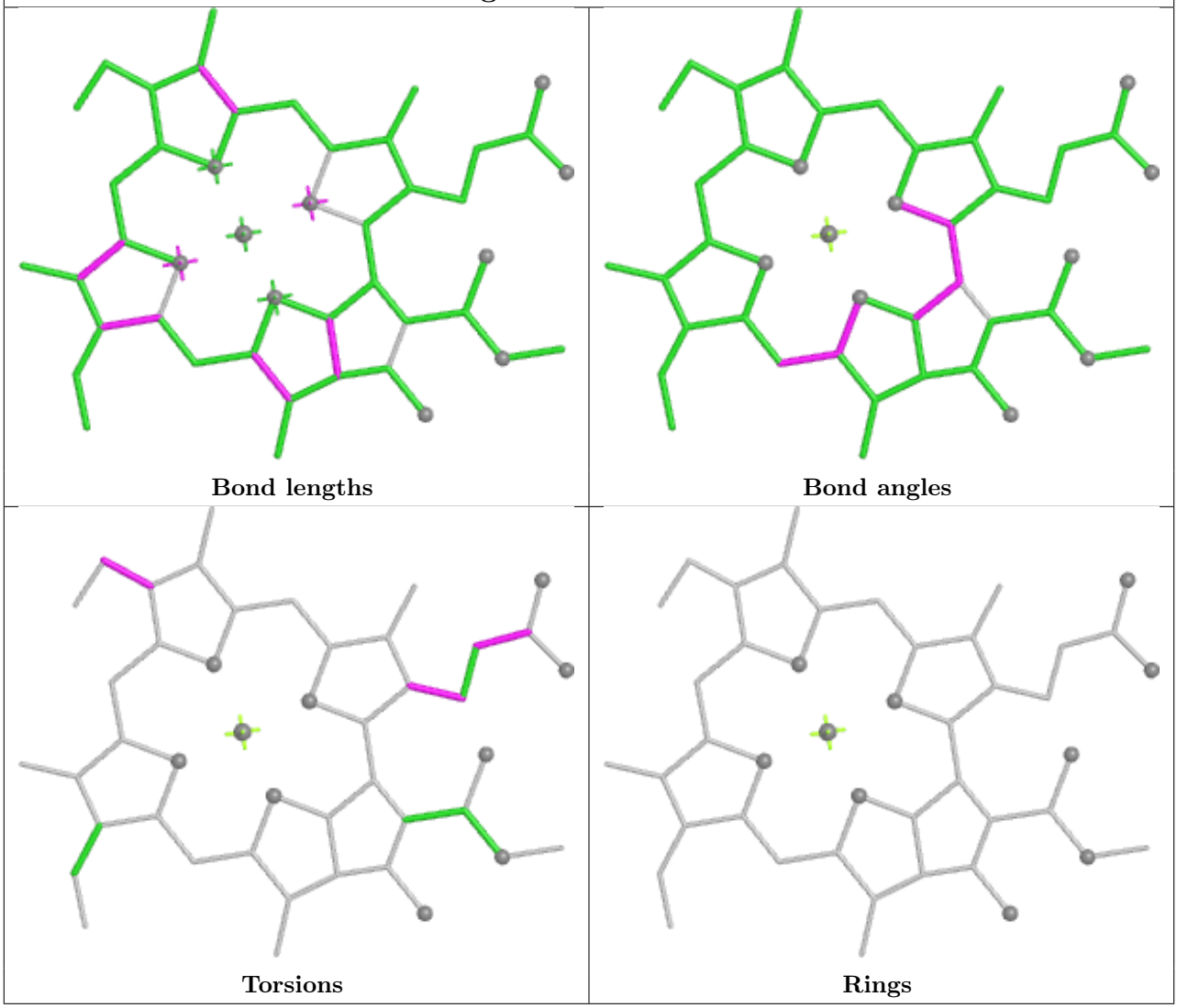


Torsions

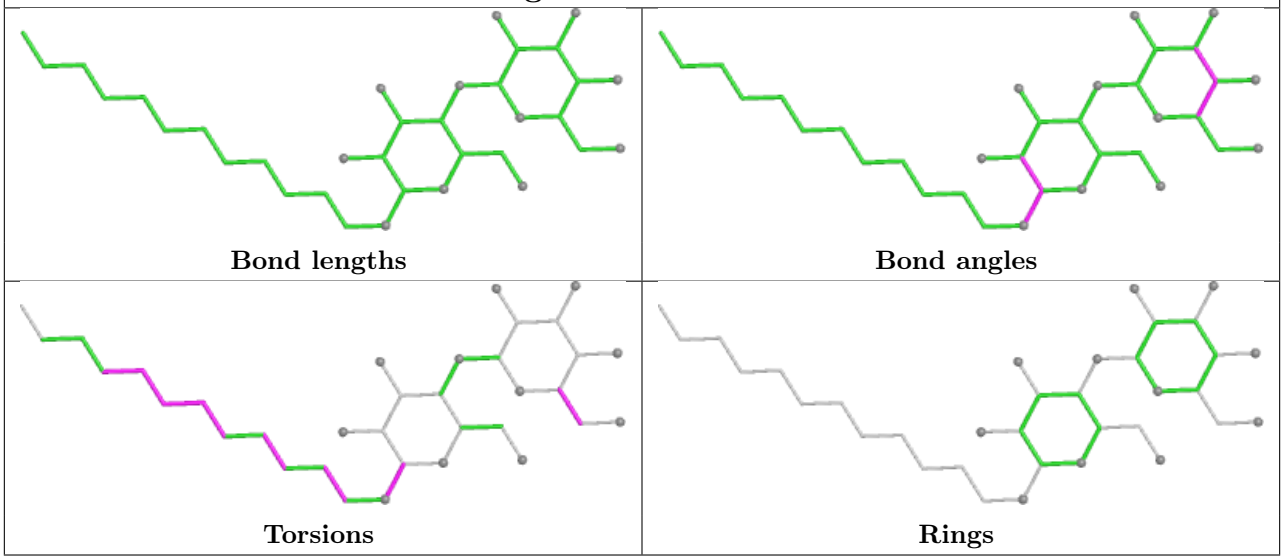


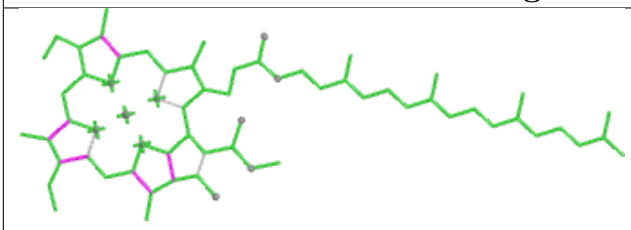
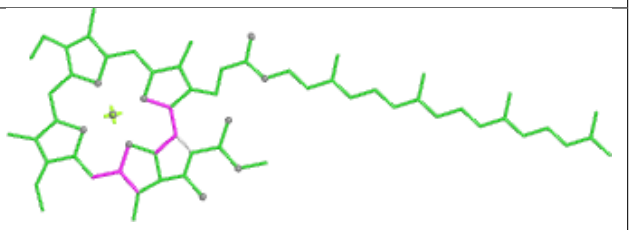
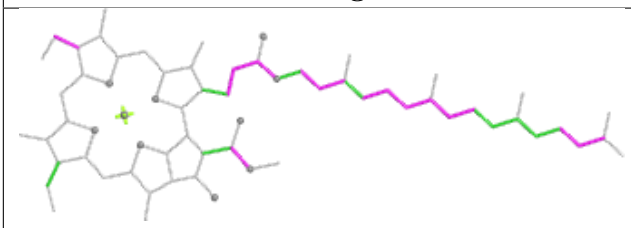
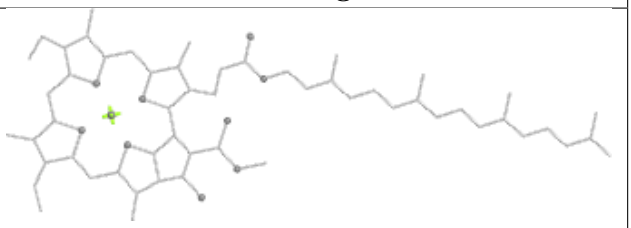
Rings

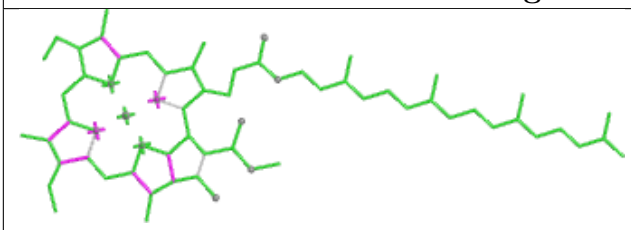
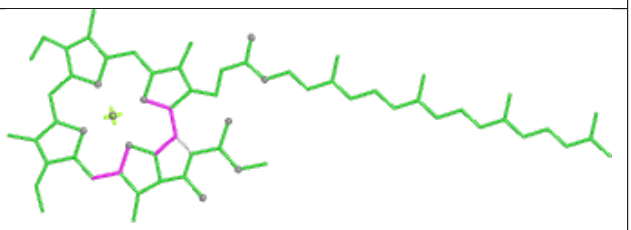
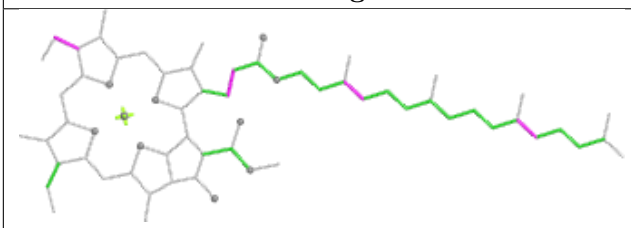
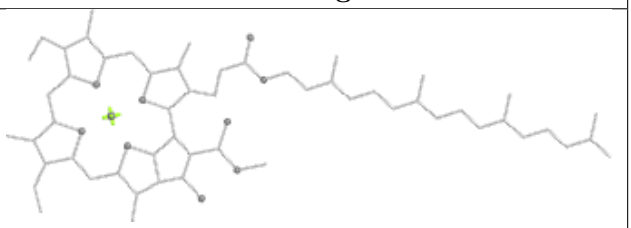
Ligand CLA K 204



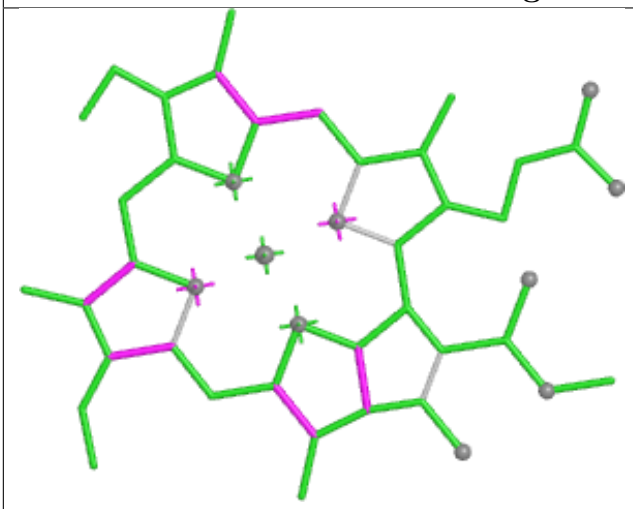
Ligand LMU J 101



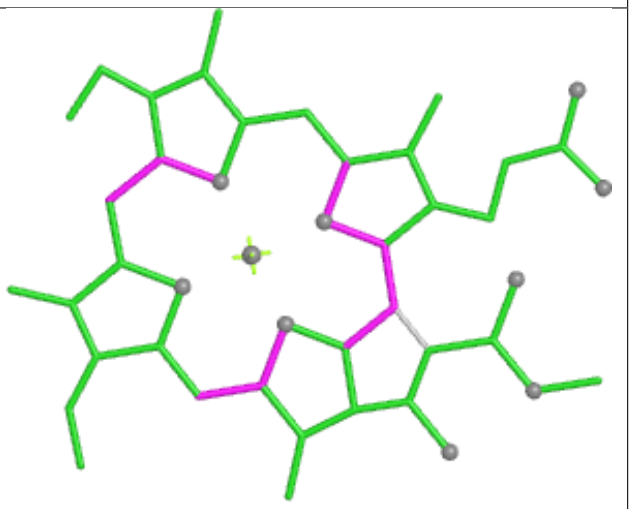
Ligand CLA H 312	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA A 825	
 Bond lengths	 Bond angles
 Torsions	 Rings

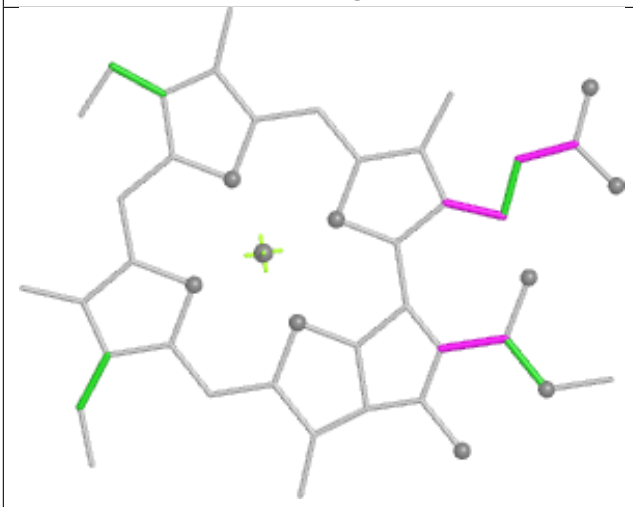
Ligand CLA G 303



Bond lengths



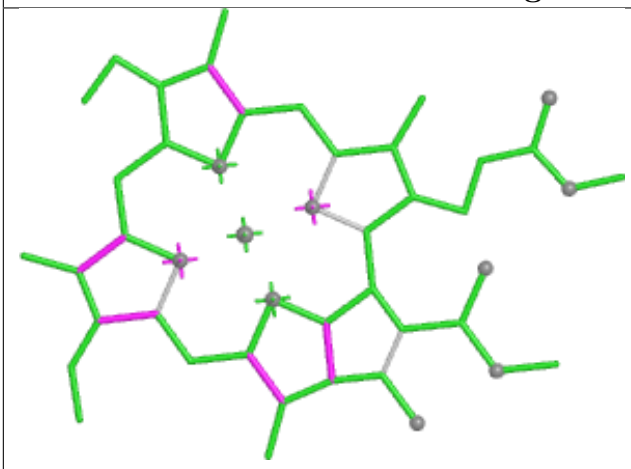
Bond angles



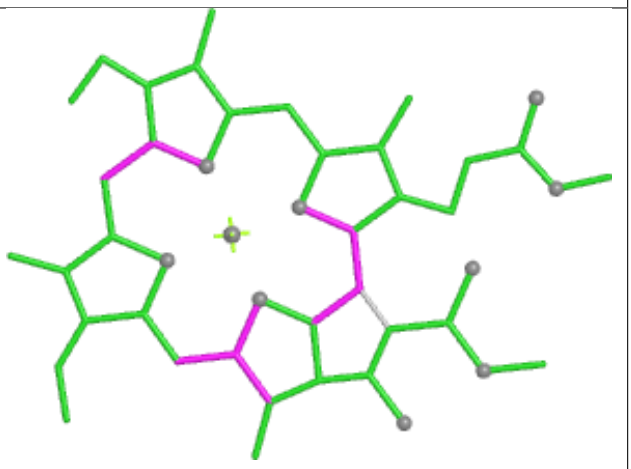
Torsions

Rings

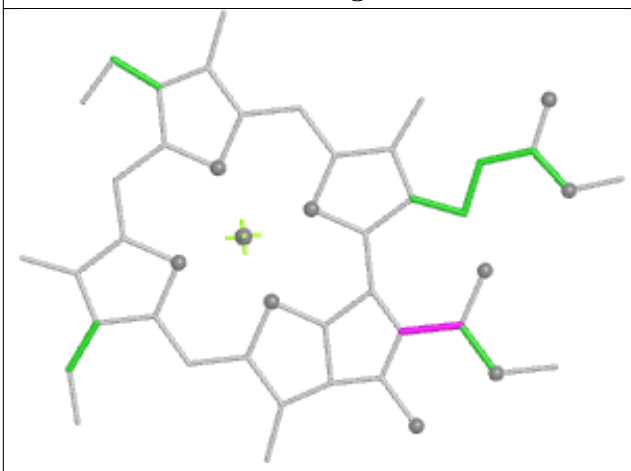
Ligand CLA B 818



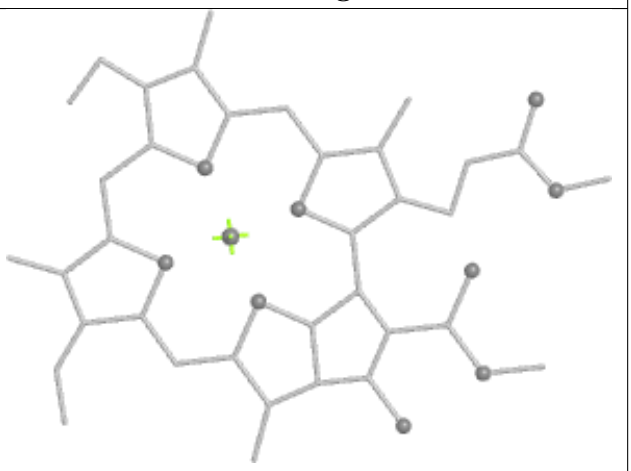
Bond lengths



Bond angles

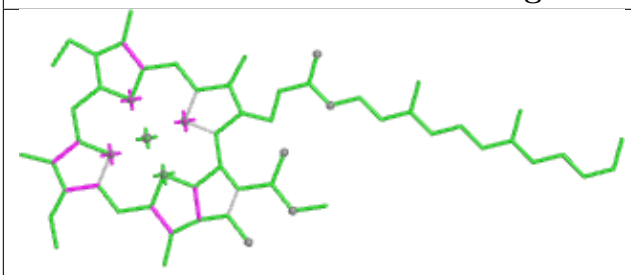


Torsions

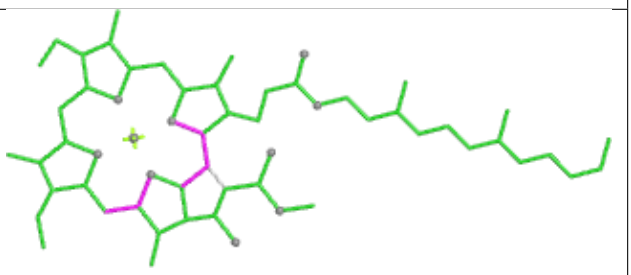


Rings

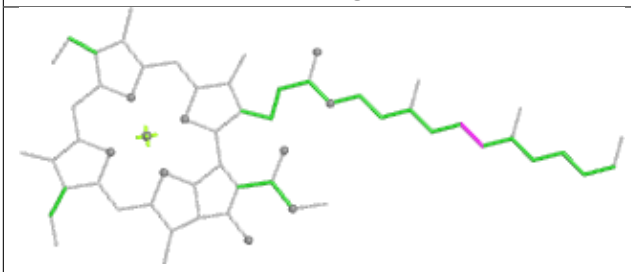
Ligand CLA B 813



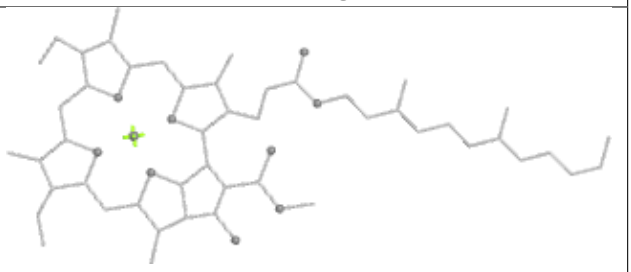
Bond lengths



Bond angles

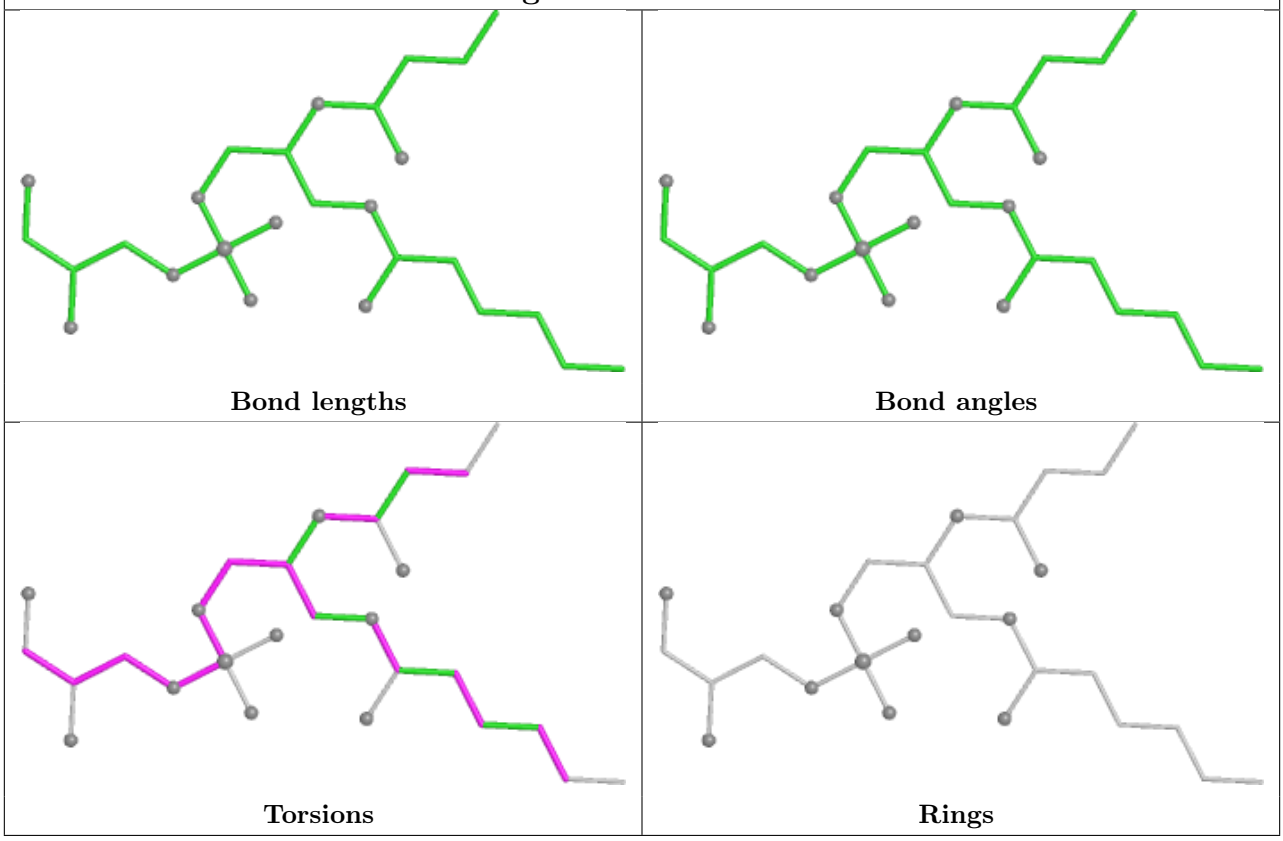


Torsions

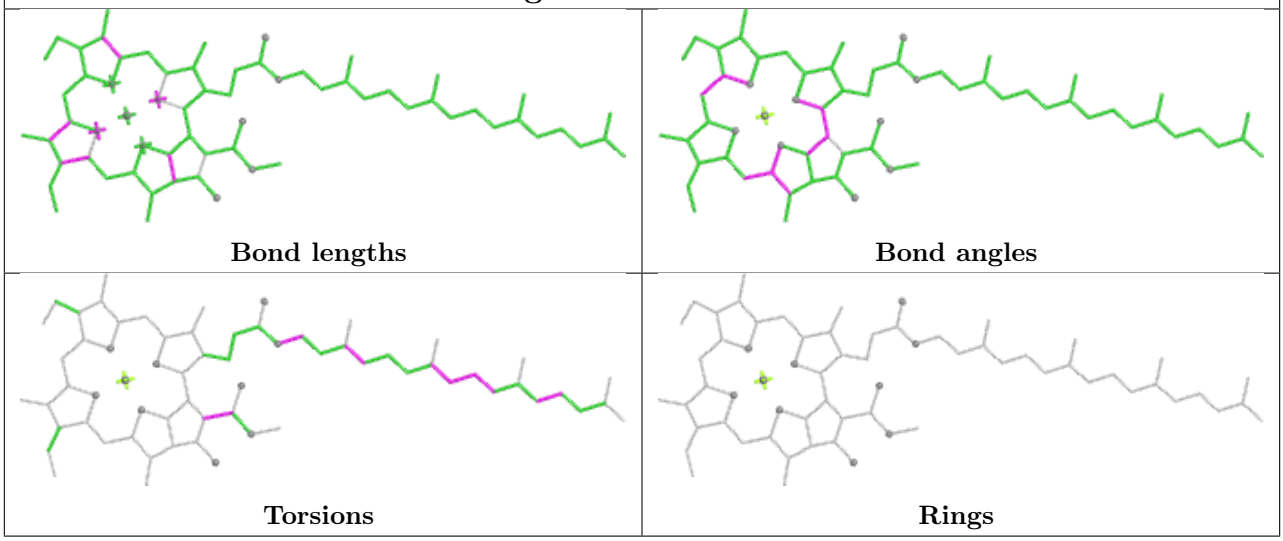


Rings

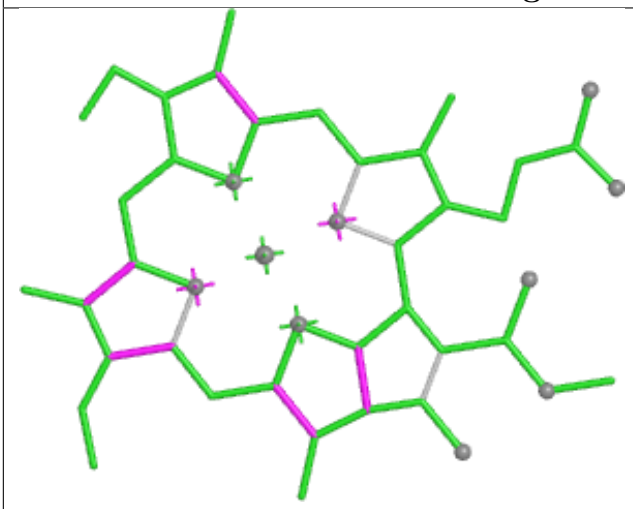
Ligand LHG G 316



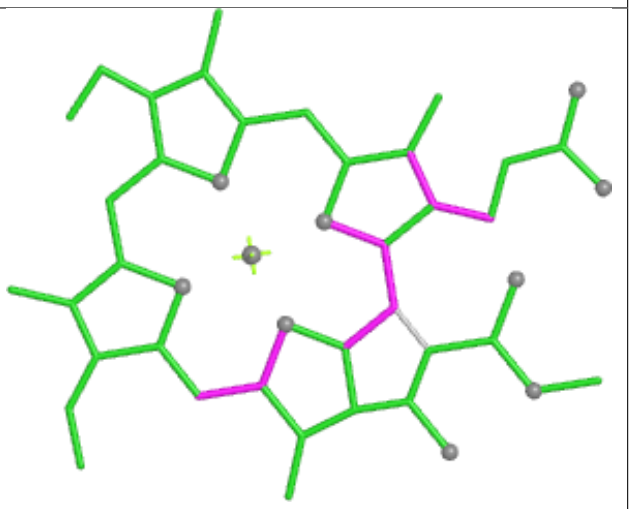
Ligand CLA A 849



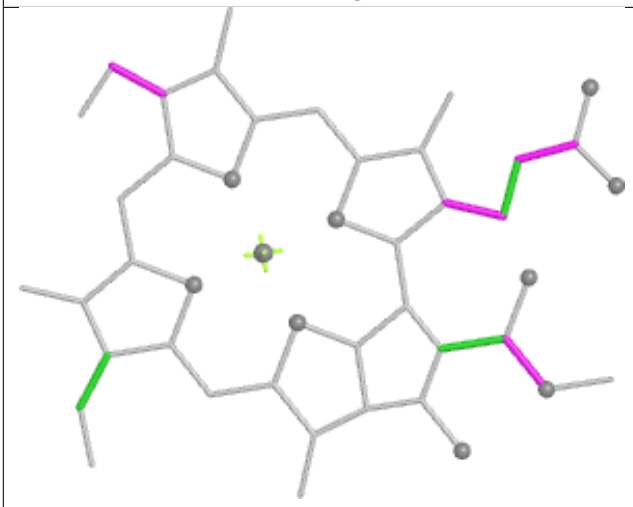
Ligand CLA G 310



Bond lengths



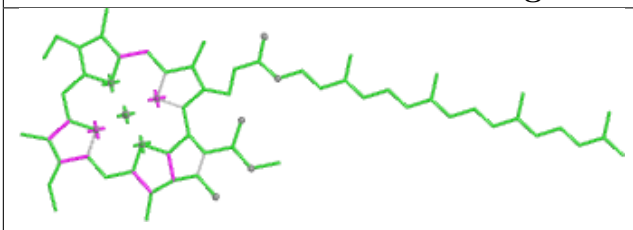
Bond angles



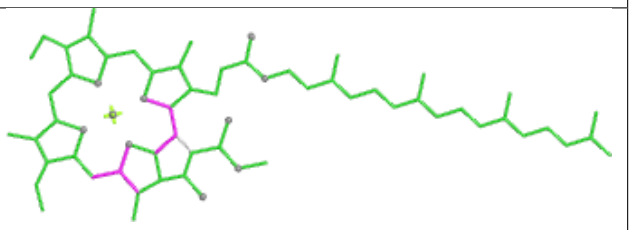
Torsions

Rings

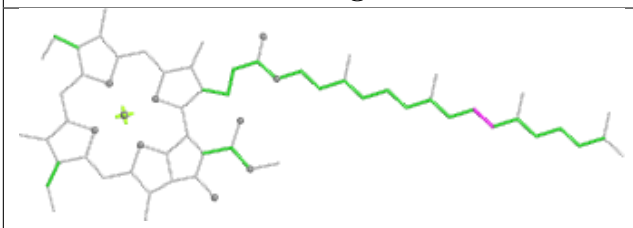
Ligand CLA B 829



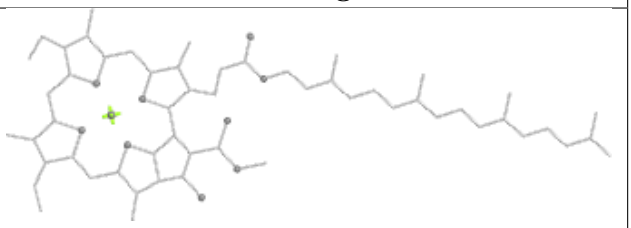
Bond lengths



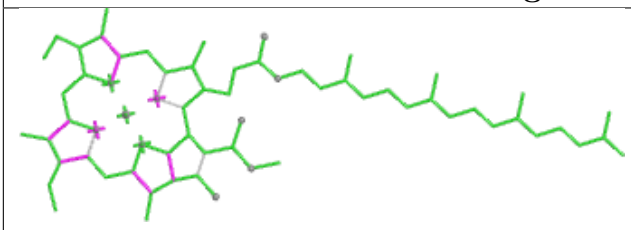
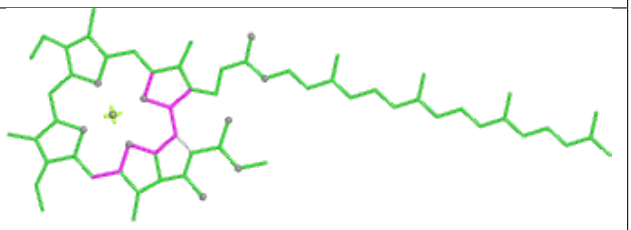
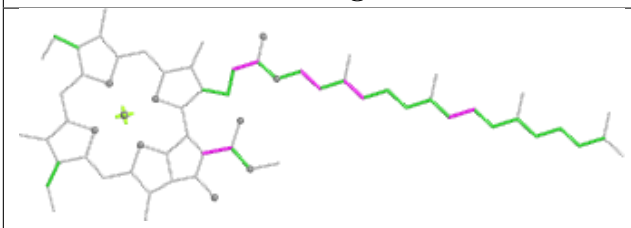
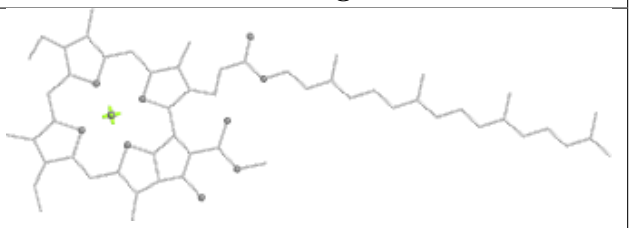
Bond angles

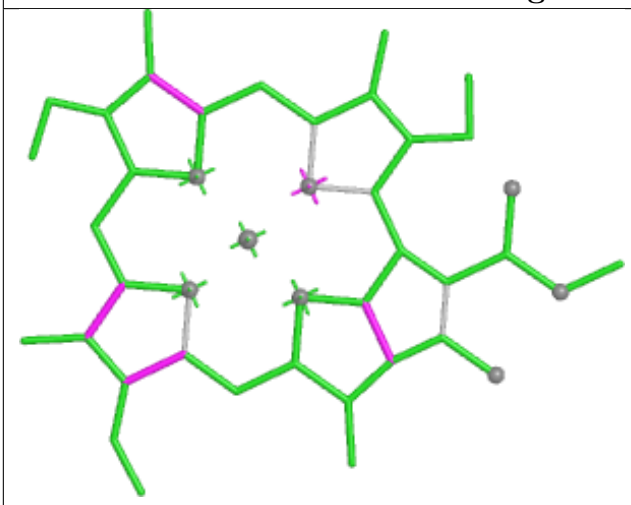
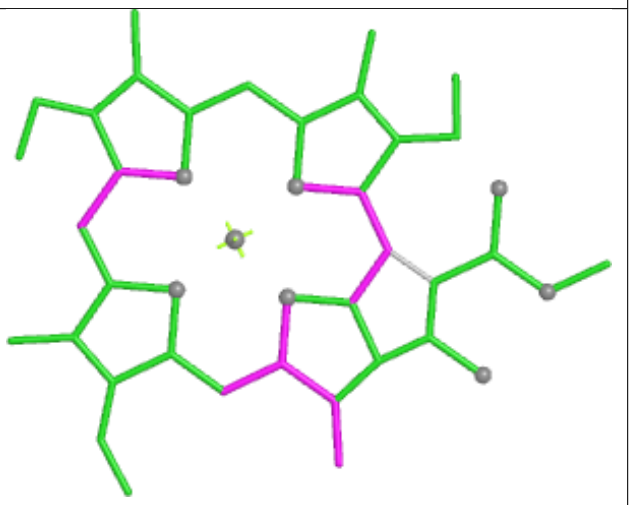
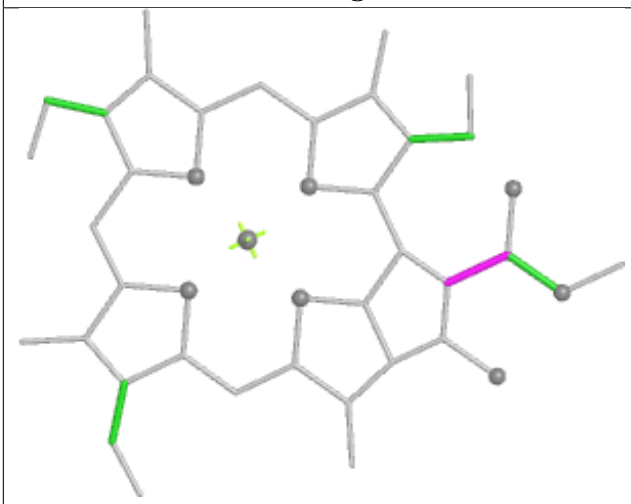
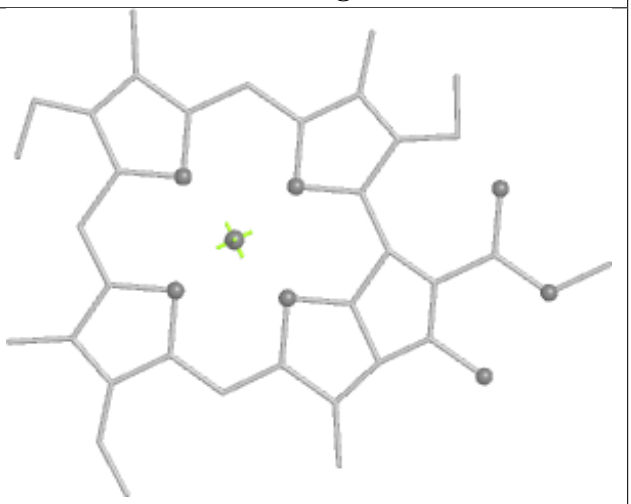


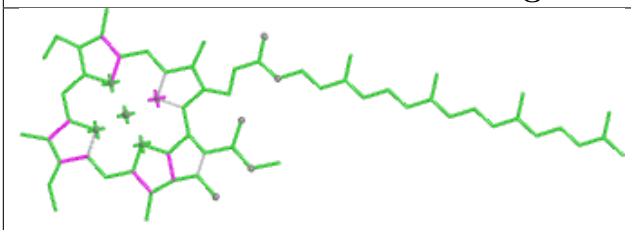
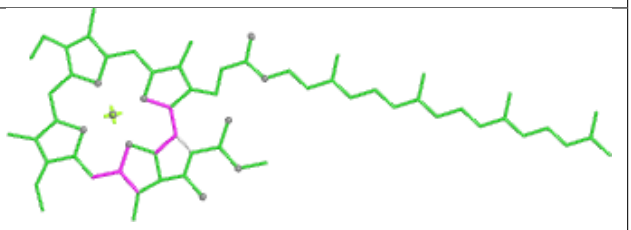
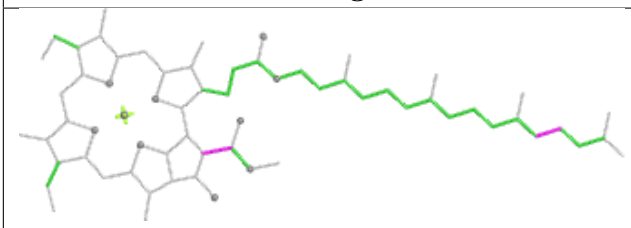
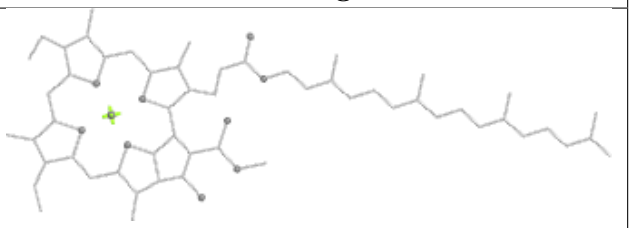
Torsions

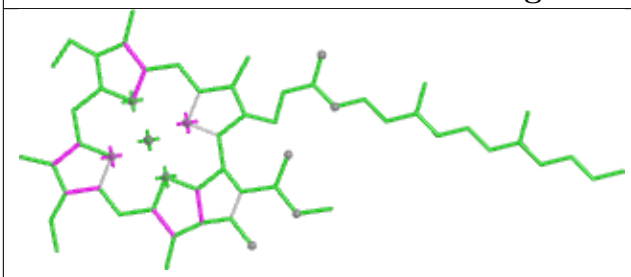
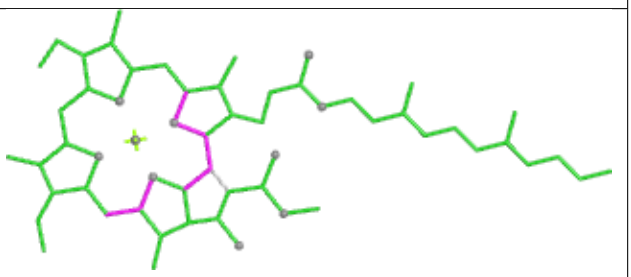
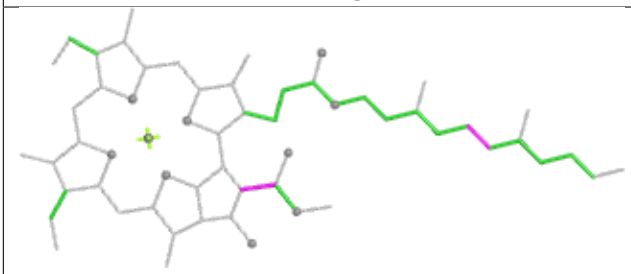
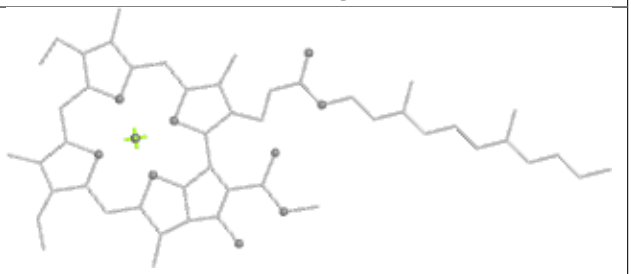


Rings

Ligand CLA A 821	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA k 201	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA A 822	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA B 831	
 Bond lengths	 Bond angles
 Torsions	 Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

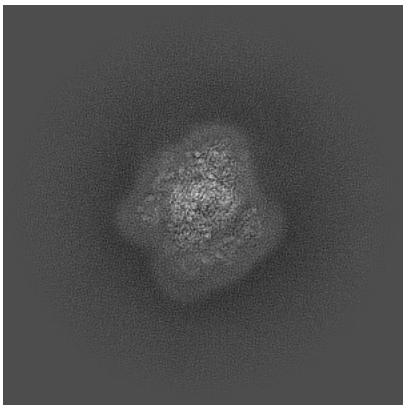
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-64154. These allow visual inspection of the internal detail of the map and identification of artifacts.

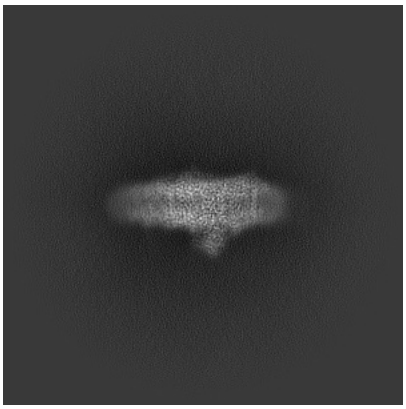
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections (i)

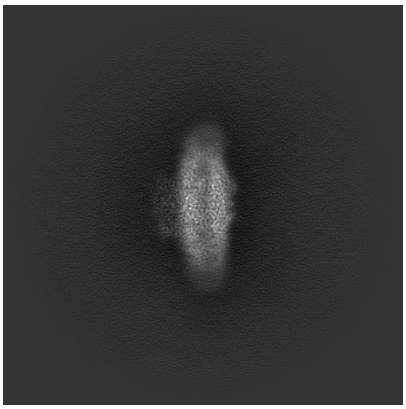
6.1.1 Primary map



X

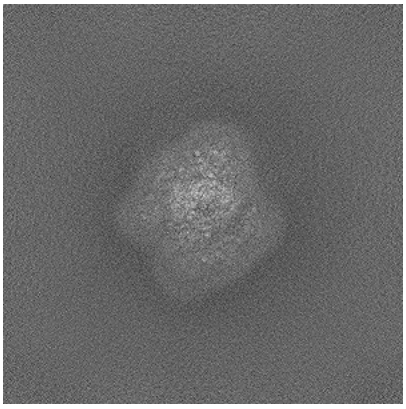


Y

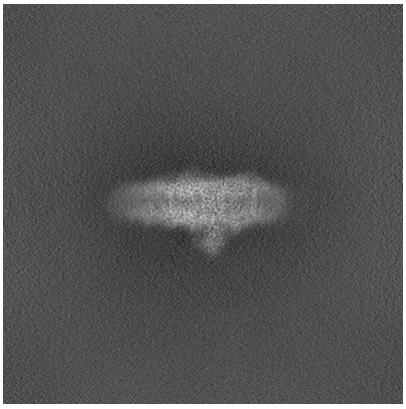


Z

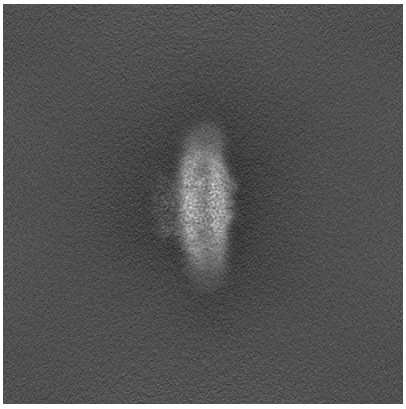
6.1.2 Raw map



X



Y

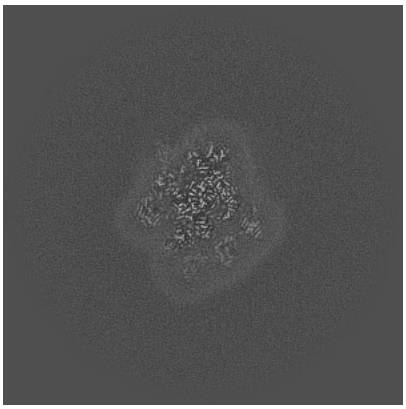


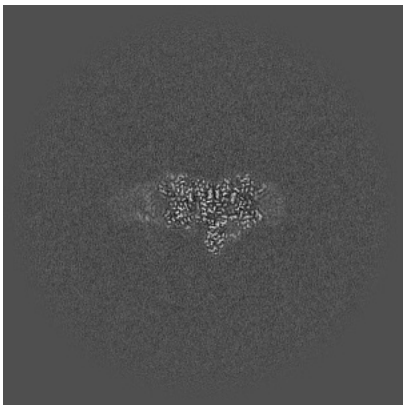
Z

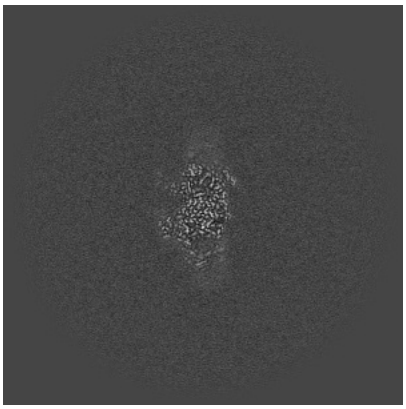
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

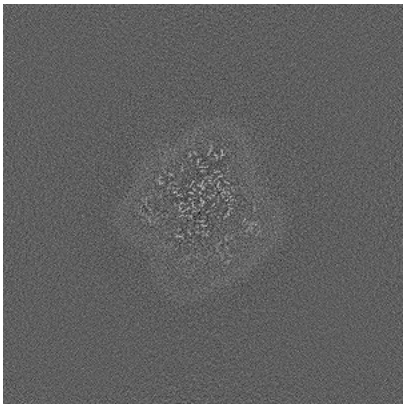
6.2.1 Primary map

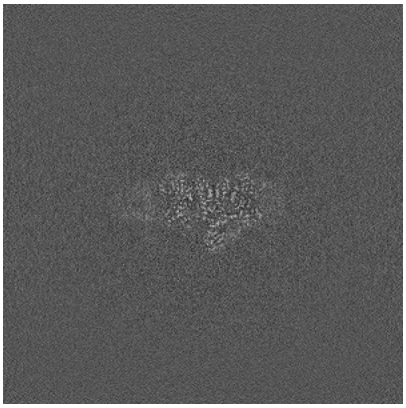

X Index: 300

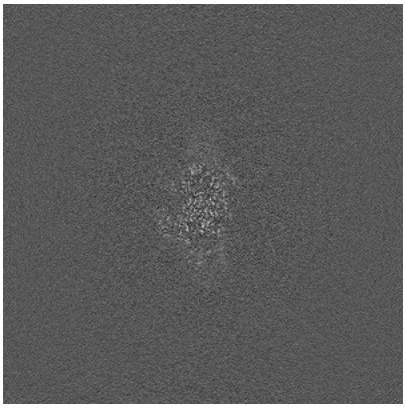

Y Index: 300


Z Index: 300

6.2.2 Raw map


X Index: 300

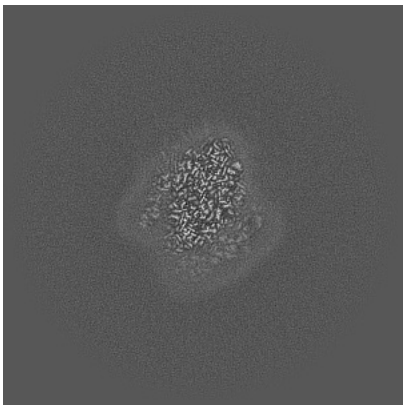

Y Index: 300

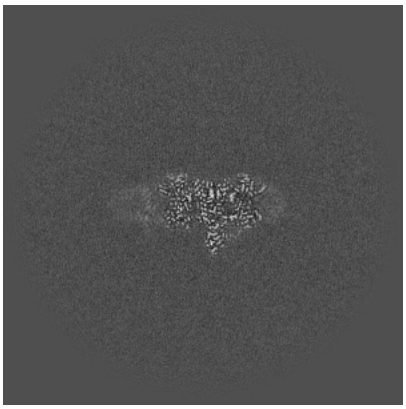

Z Index: 300

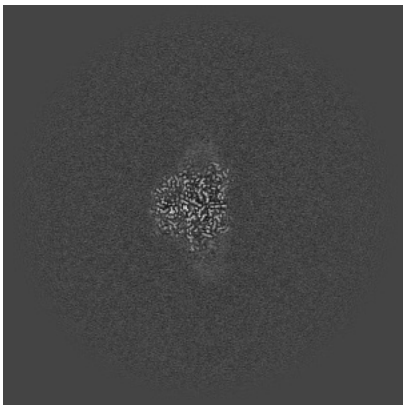
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

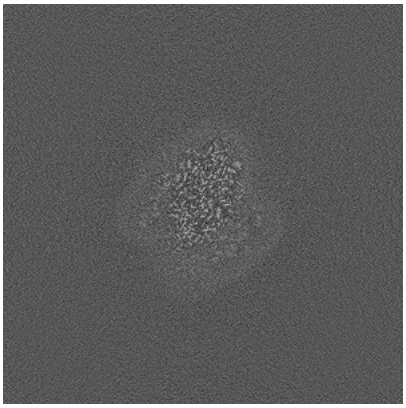
6.3.1 Primary map

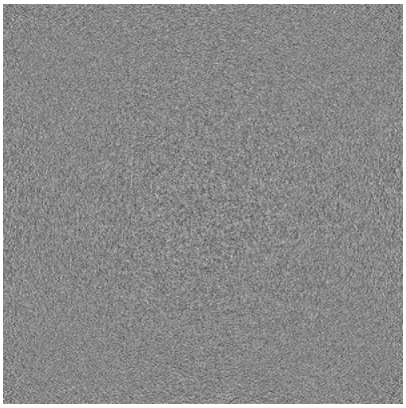

X Index: 316

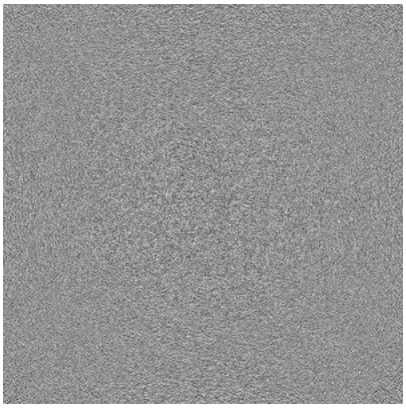

Y Index: 301


Z Index: 316

6.3.2 Raw map


X Index: 316

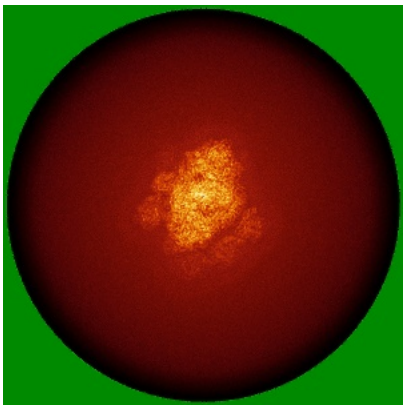

Y Index: 0

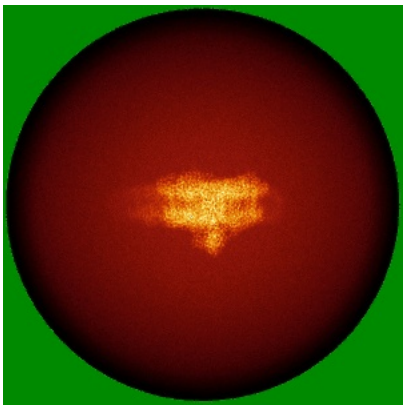

Z Index: 599

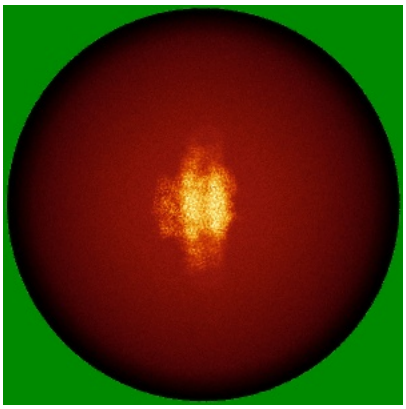
The images above show the largest variance slices of the map in three orthogonal directions.

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

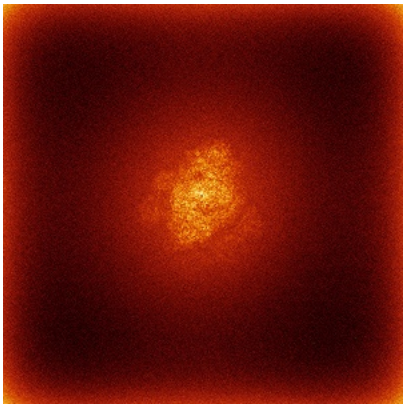
6.4.1 Primary map

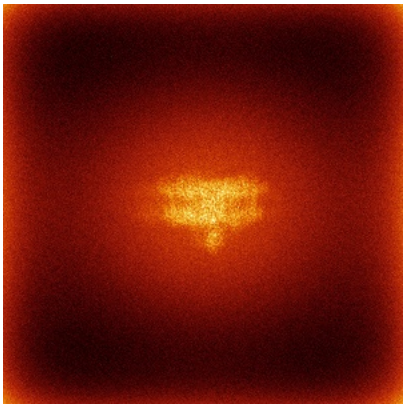

X

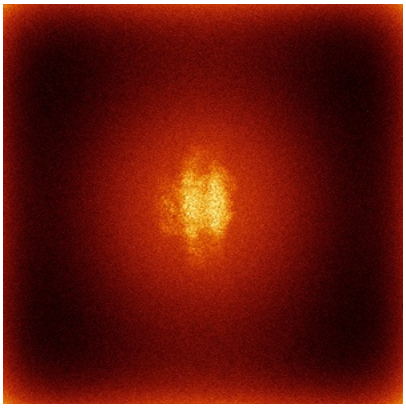

Y


Z

6.4.2 Raw map


X


Y


Z

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

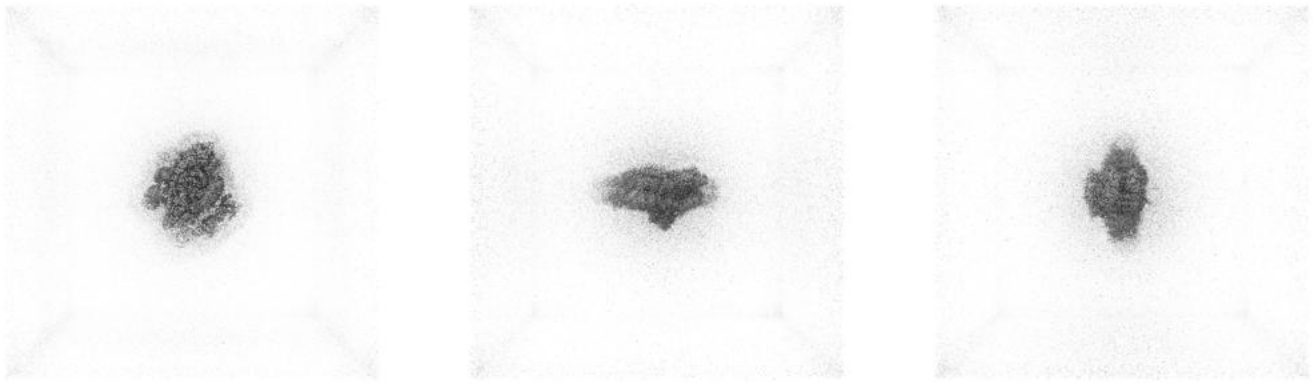
6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.065. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X Y Z

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

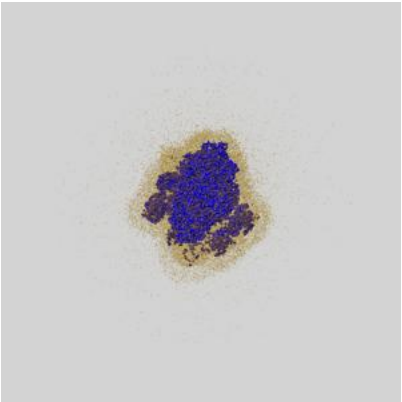
6.6 Mask visualisation (i)

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

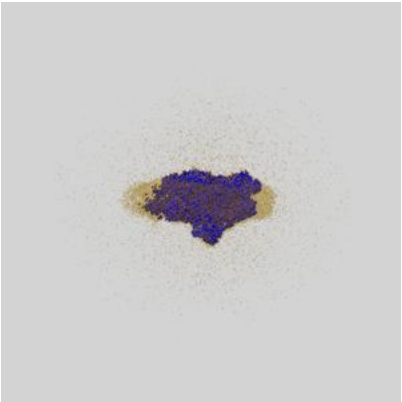
A mask typically either:

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

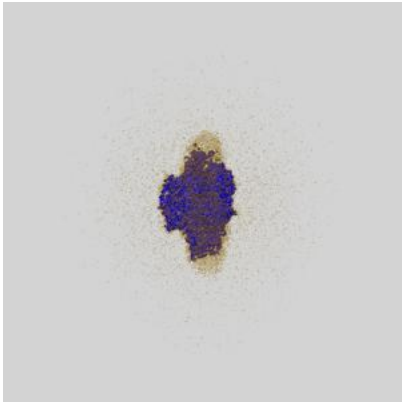
6.6.1 emd_64154_msk_1.map (i)



X



Y

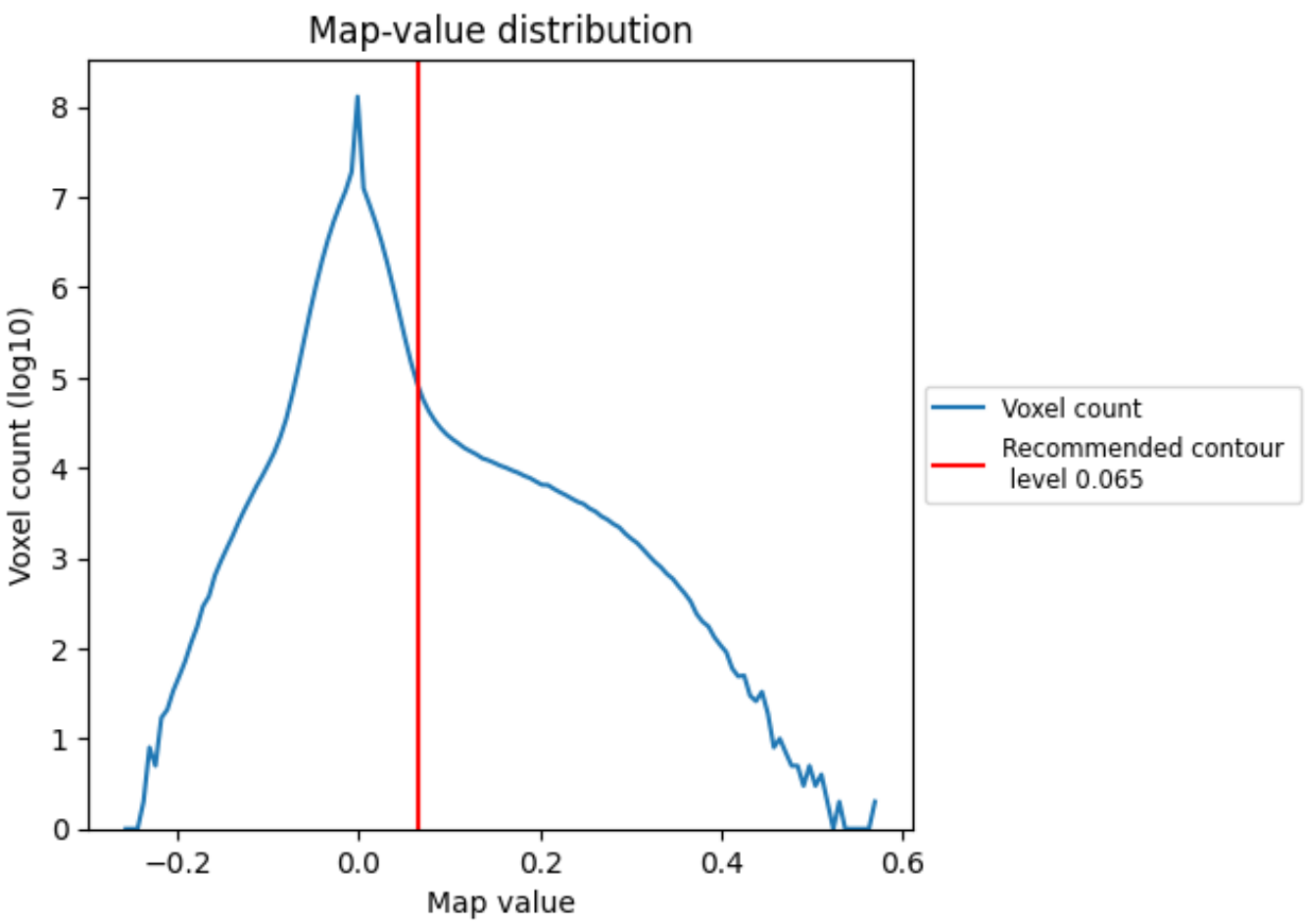


Z

7 Map analysis (i)

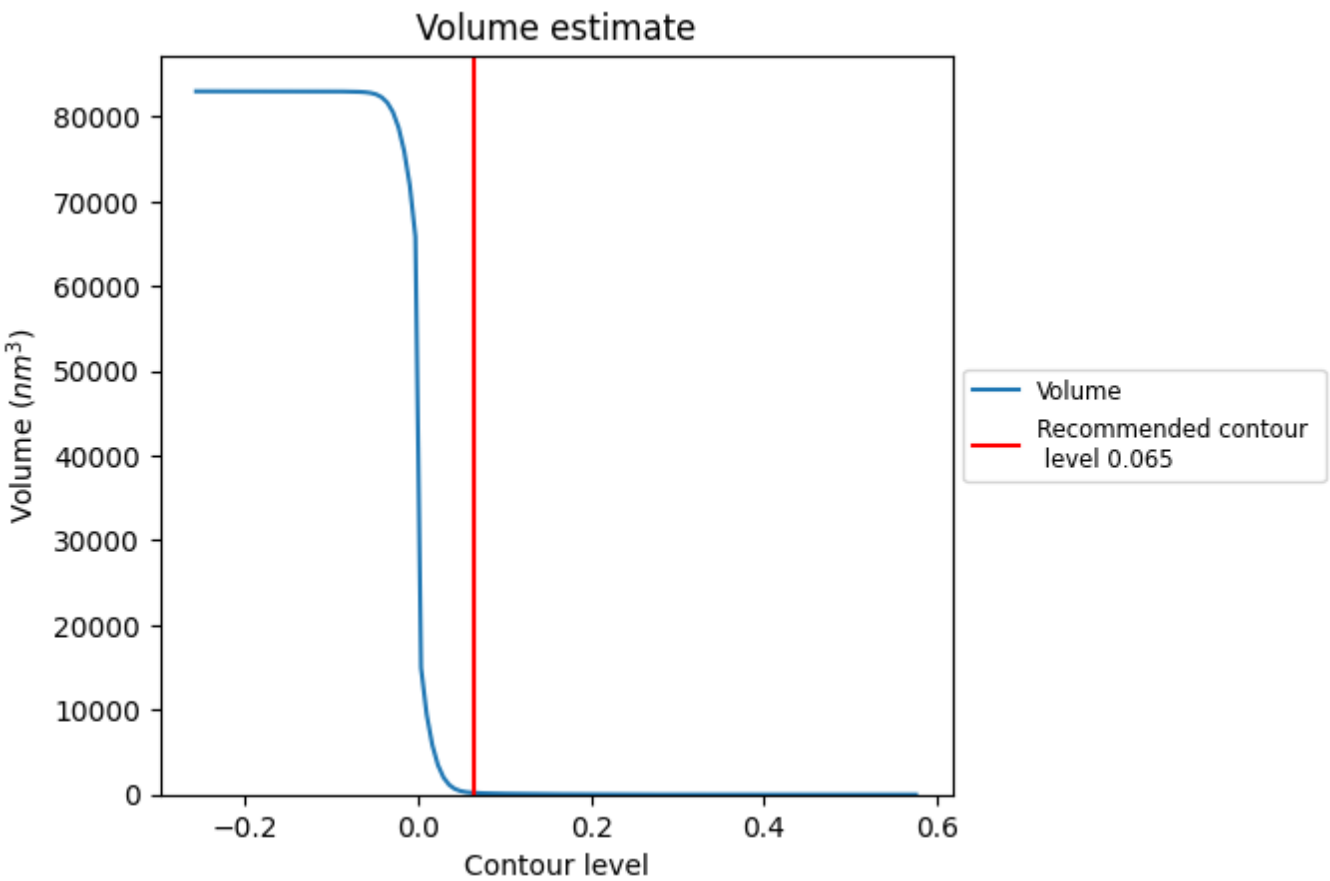
This section contains the results of statistical analysis of the map.

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.

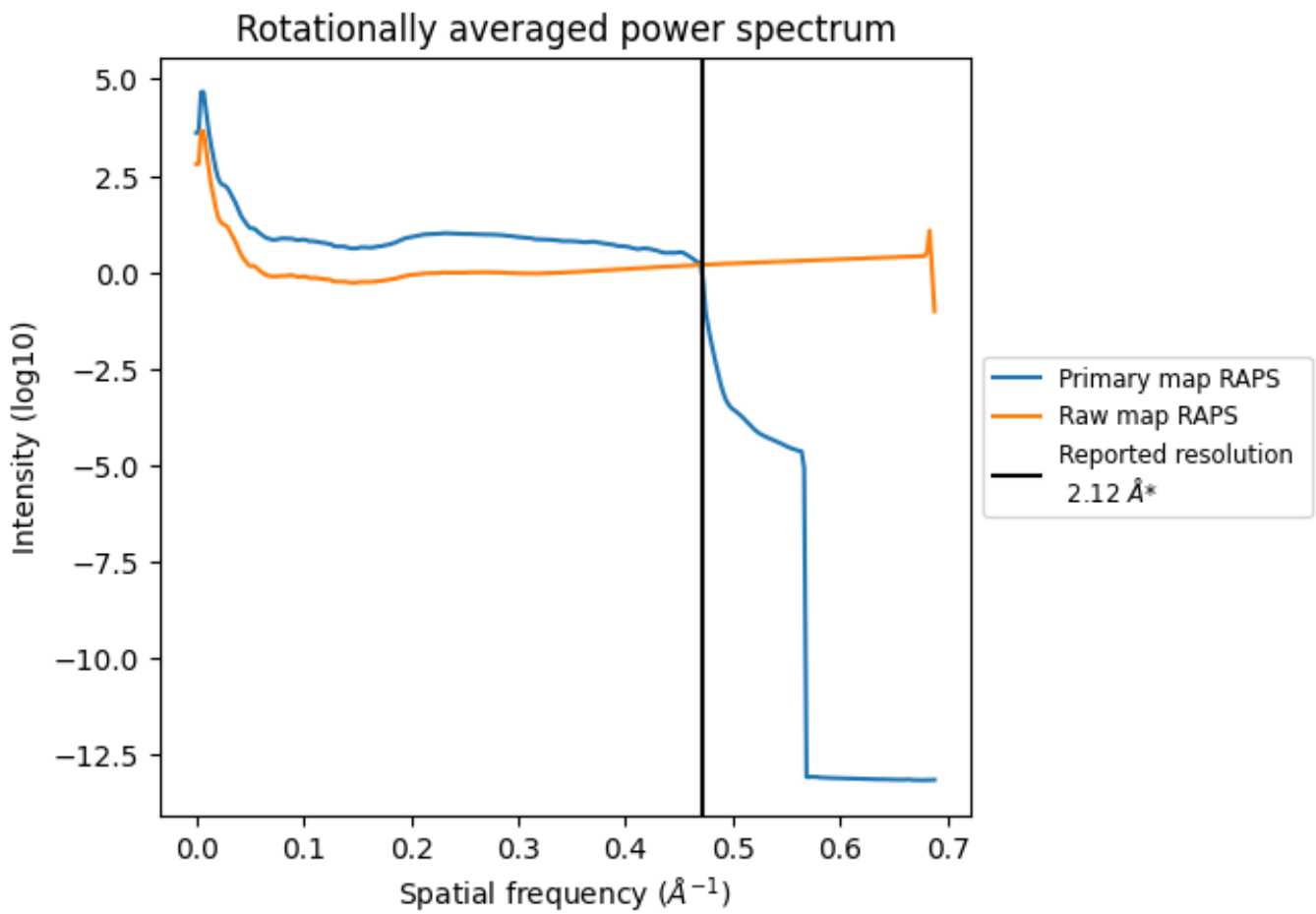
7.2 Volume estimate (i)



The volume at the recommended contour level is 203 nm^3; this corresponds to an approximate mass of 183 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)

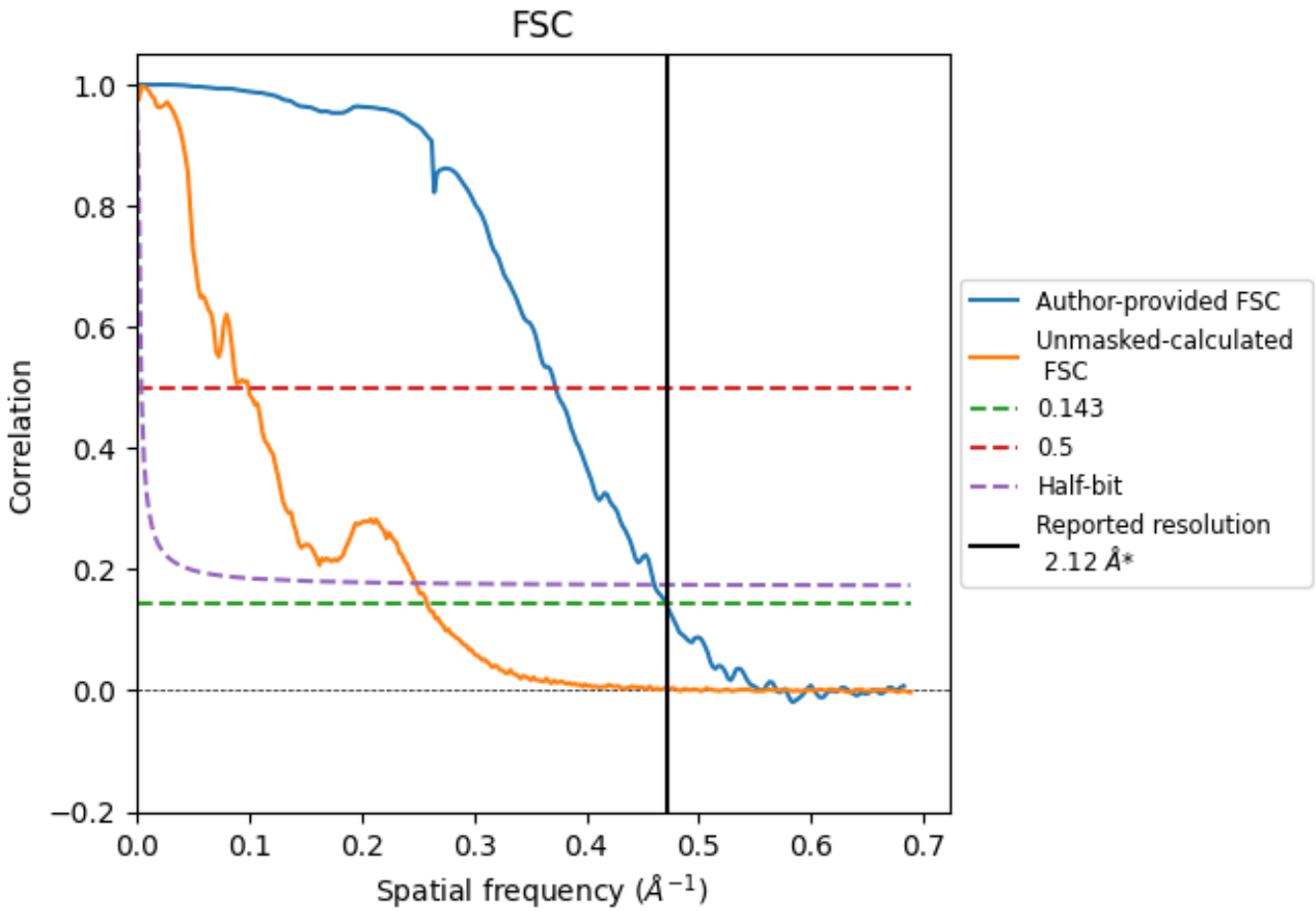


*Reported resolution corresponds to spatial frequency of 0.472 Å^{-1}

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 0.472 Å^{-1}

8.2 Resolution estimates (i)

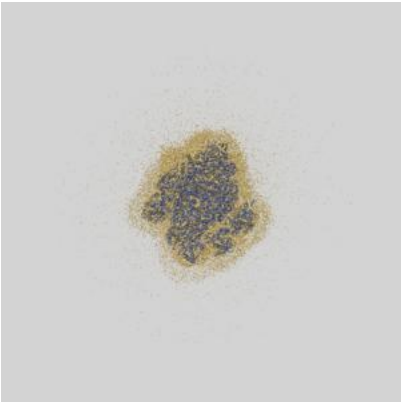
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.12	-	-
Author-provided FSC curve	2.12	2.68	2.17
Unmasked-calculated*	3.87	10.04	4.03

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.87 differs from the reported value 2.12 by more than 10 %

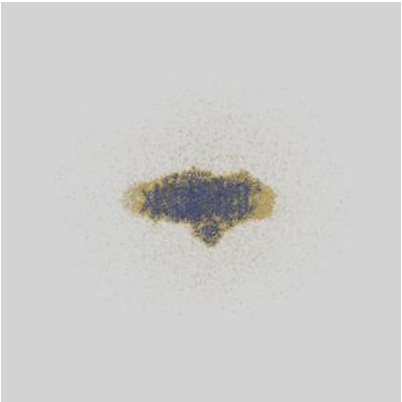
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-64154 and PDB model 9UH4. Per-residue inclusion information can be found in section 3 on page 23.

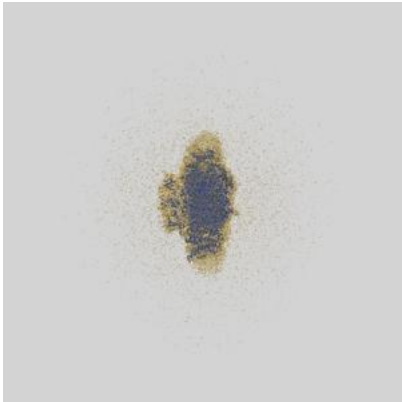
9.1 Map-model overlay (i)



X



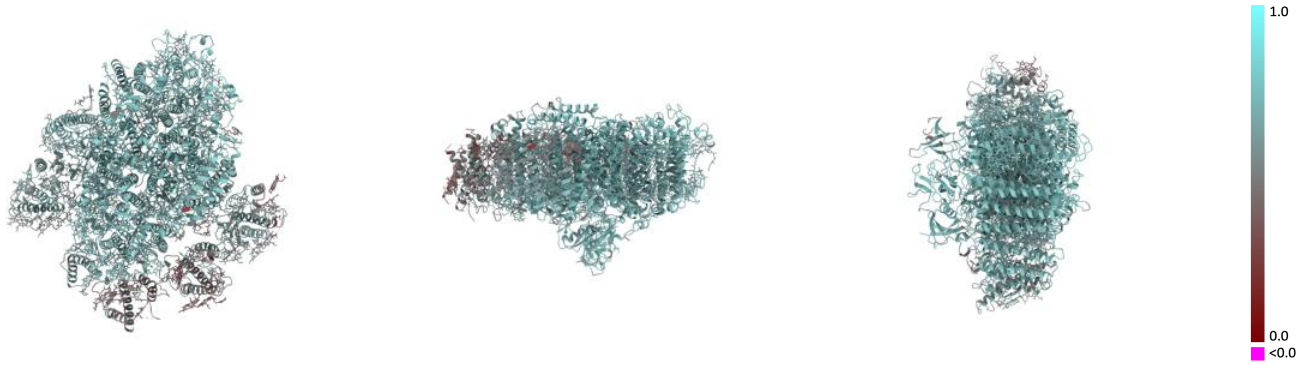
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.065 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.

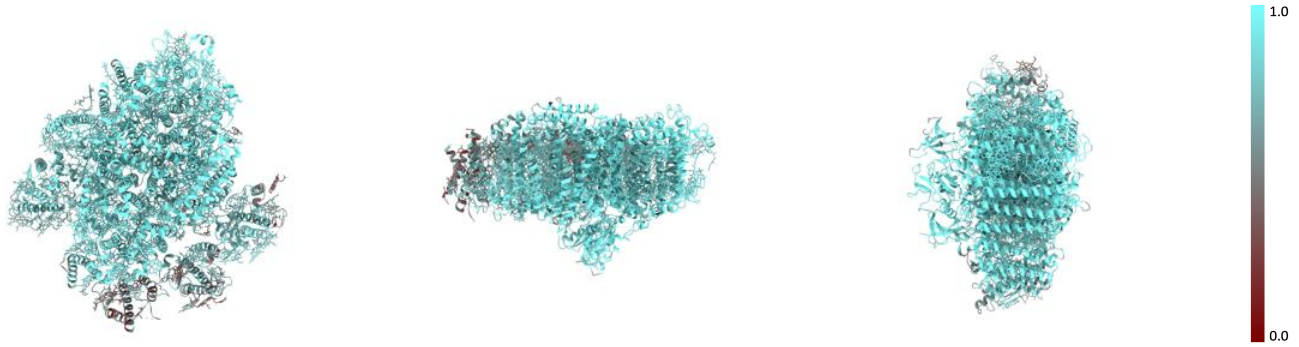
9.2 Q-score mapped to coordinate model (i)



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.

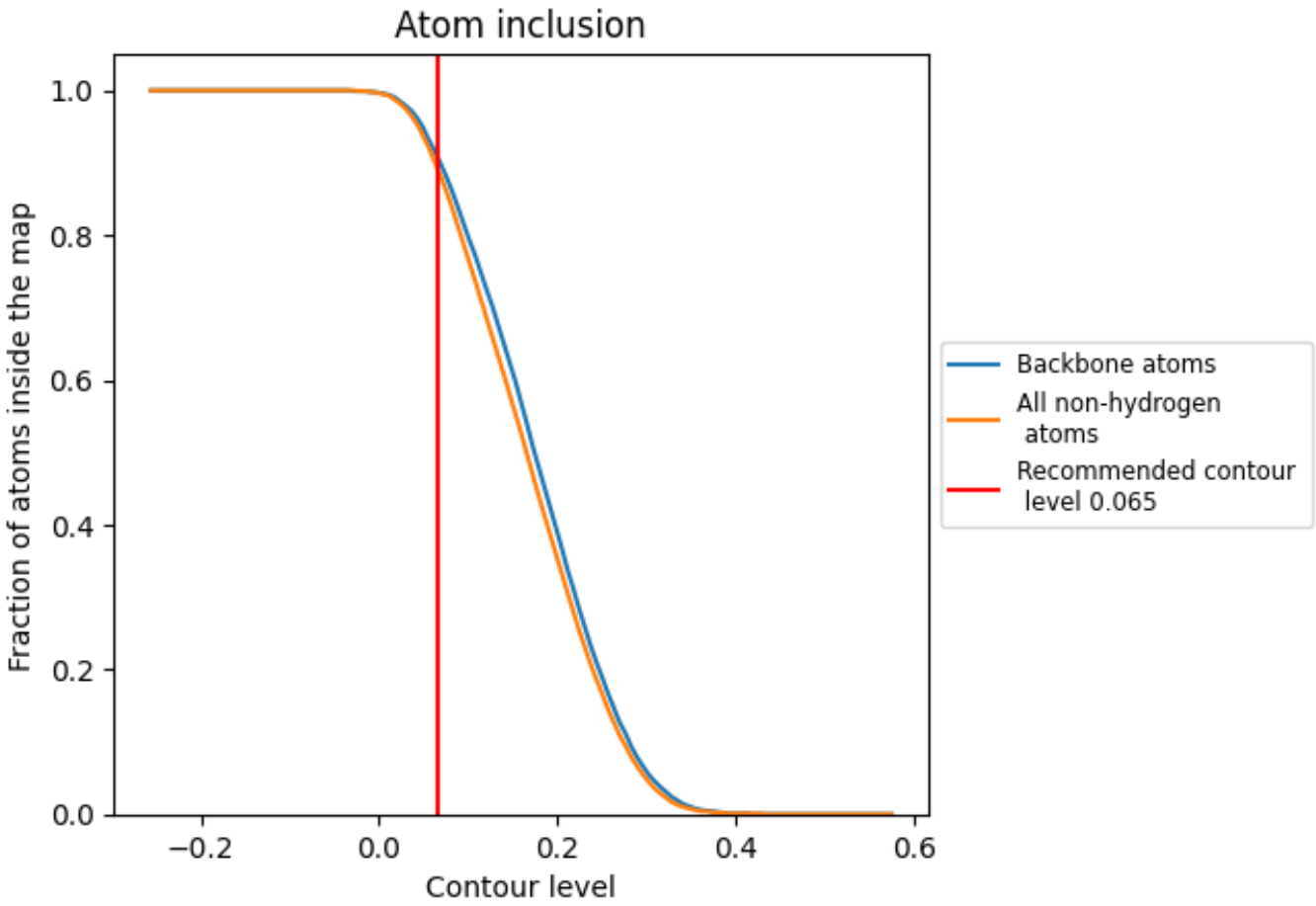
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.065).

9.4 Atom inclusion (i)



At the recommended contour level, 91% of all backbone atoms, 89% 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 (0.065) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8940	0.6550
A	0.9570	0.7000
B	0.9570	0.7010
C	0.9900	0.7210
D	0.9360	0.6750
E	0.9000	0.6590
F	0.9220	0.6710
G	0.7640	0.5610
H	0.6770	0.4970
I	0.8820	0.6410
J	0.9190	0.6580
K	0.4990	0.4400
L	0.9070	0.6540
M	0.9130	0.6530
U	0.7940	0.5820
k	0.7610	0.5750