wwPDB EM Validation Summary Report (i)

Sep 15, 2026 – 07:14 PM JST

PDB ID	:	9UOF / pdb_00009uof
EMDB ID	:	EMD-64378
Title	:	PSI-6 FCPI supercomplex from haptophyte Chrysotila roscoffensis
Authors	:	La Rocca, R.; Tsai, P.-C.; Kato, K.; Nakajima, Y.; Akita, F.; Shen, J.-R.
Deposited on	:	2025-04-25
Resolution	:	1.89 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:

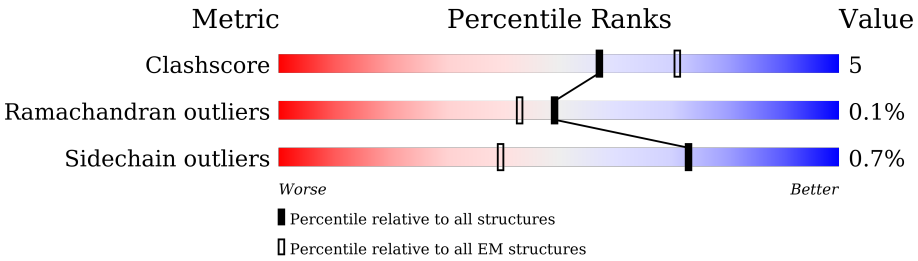
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using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

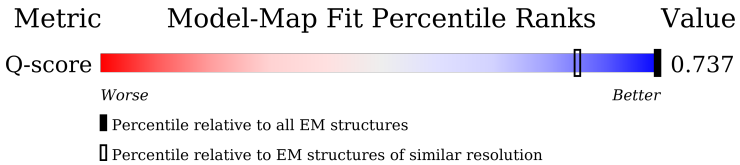
1 Overall quality at a glance (i)

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

The reported resolution of this entry is 1.89 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	1004 (1.39 - 2.38)

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	92% 6% •
2	B	734	94% 6%
3	C	81	96% • •
4	D	142	88% 9% •

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Mol	Chain	Length	Quality of chain
5	E	67	93%
6	F	184	82% 6% 12%
7	I	35	86% 11%
8	J	39	92% 8%
9	L	141	89% 11%
10	M	29	93% 7%
11	O	201	81% 6% 12%
12	P	231	78% 5% 16%
13	Q	197	75% 9% 15%
14	R	90	96%
15	S	215	68% 8% 23%
16	U	191	70% 26%
17	T	202	41% 8% 51%

2 Entry composition (i)

There are 30 unique types of molecules in this entry. The entry contains 36741 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 III (FCPI-3).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	O	176	1341	872	217	244	8	0	0

- Molecule 12 is a protein called Fucoxanthin chlorophyll a/c binding protein VI (FCPI-6), GLY-CYS-PRO.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	P	193	1441	927	239	264	11	0	0

- Molecule 13 is a protein called Fucoxanthin chlorophyll a/c binding protein IV (FCPI-4).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	Q	167	1257	809	202	234	12	0	0

- Molecule 14 is a protein called Photosystem I reaction center subunit psaR.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	R	88	664	434	106	123	1	0	0

- Molecule 15 is a protein called Fucoxanthin chlorophyll a/c binding protein II (FCPI-2).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
15	S	165	1238	802	204	226	6	0	0

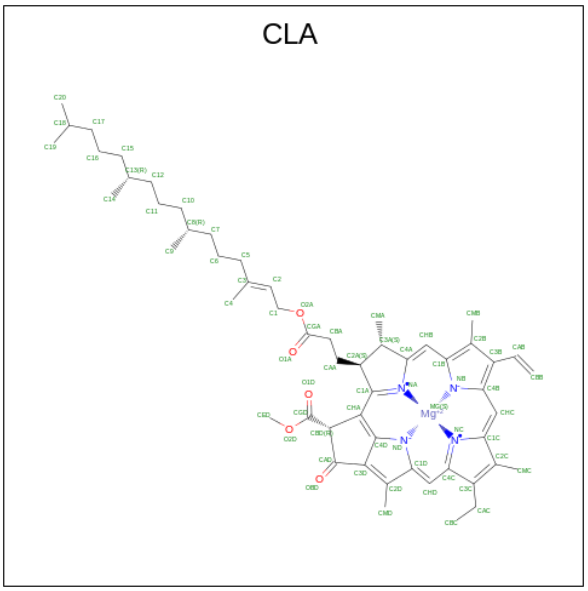
- Molecule 16 is a protein called Fucoxanthin chlorophyll a/c binding protein I (FCPI-1).

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

- Molecule 17 is a protein called Fucoxanthin chlorophyll a/c binding protein V (FCPI-5).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
17	T	99	731	471	122	130	8	0	0

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



Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
18	A	1	65	55	1	4	5	0
18	A	1	55	45	1	4	5	0
18	A	1	65	55	1	4	5	0
18	A	1	65	55	1	4	5	0
18	A	1	49	39	1	4	5	0
18	A	1	65	55	1	4	5	0
18	A	1	65	55	1	4	5	0
18	A	1	56	46	1	4	5	0
18	A	1	62	52	1	4	5	0
18	A	1	54	44	1	4	5	0
18	A	1	65	55	1	4	5	0
18	A	1	45	35	1	4	5	0
18	A	1	50	40	1	4	5	0
18	A	1	45	35	1	4	5	0
18	A	1	65	55	1	4	5	0
18	A	1	65	55	1	4	5	0
18	A	1	45	35	1	4	5	0
18	A	1	65	55	1	4	5	0
18	A	1	43	35	1	4	3	0
18	A	1	51	41	1	4	5	0
18	A	1	65	55	1	4	5	0
18	A	1	65	55	1	4	5	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
18	A	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
18	A	1	62	52	1	4	5	0
			Total	C	Mg	N	O	
18	A	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
18	A	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
18	A	1	50	40	1	4	5	0
			Total	C	Mg	N	O	
18	A	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
18	A	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
18	A	1	50	40	1	4	5	0
			Total	C	Mg	N	O	
18	A	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
18	A	1	51	41	1	4	5	0
			Total	C	Mg	N	O	
18	A	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
18	A	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
18	A	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
18	A	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
18	A	1	52	42	1	4	5	0
			Total	C	Mg	N	O	
18	A	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
18	A	1	60	50	1	4	5	0
			Total	C	Mg	N	O	
18	A	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
18	A	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
18	A	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
18	A	1	65	55	1	4	5	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
18	A	1	65	55	1	4	5	0
18	B	1	65	55	1	4	5	0
18	B	1	65	55	1	4	5	0
18	B	1	65	55	1	4	5	0
18	B	1	45	35	1	4	5	0
18	B	1	65	55	1	4	5	0
18	B	1	65	55	1	4	5	0
18	B	1	65	55	1	4	5	0
18	B	1	65	55	1	4	5	0
18	B	1	65	55	1	4	5	0
18	B	1	54	44	1	4	5	0
18	B	1	55	45	1	4	5	0
18	B	1	54	44	1	4	5	0
18	B	1	49	39	1	4	5	0
18	B	1	55	45	1	4	5	0
18	B	1	59	49	1	4	5	0
18	B	1	60	50	1	4	5	0
18	B	1	65	55	1	4	5	0
18	B	1	46	36	1	4	5	0
18	B	1	53	43	1	4	5	0
18	B	1	63	53	1	4	5	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
18	B	1	64	54	1	4	5	0
			Total	C	Mg	N	O	
18	B	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
18	B	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
18	B	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
18	B	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
18	B	1	50	40	1	4	5	0
			Total	C	Mg	N	O	
18	B	1	49	39	1	4	5	0
			Total	C	Mg	N	O	
18	B	1	58	48	1	4	5	0
			Total	C	Mg	N	O	
18	B	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
18	B	1	58	48	1	4	5	0
			Total	C	Mg	N	O	
18	B	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
18	B	1	47	37	1	4	5	0
			Total	C	Mg	N	O	
18	B	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
18	B	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
18	B	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
18	B	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
18	B	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
18	B	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
18	B	1	50	40	1	4	5	0
			Total	C	Mg	N	O	
18	F	1	48	38	1	4	5	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
18	F	1	46	36	1	4	5	0
			Total	C	Mg	N	O	
18	J	1	42	34	1	4	3	0
			Total	C	Mg	N	O	
18	L	1	49	39	1	4	5	0
			Total	C	Mg	N	O	
18	L	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
18	L	1	50	40	1	4	5	0
			Total	C	Mg	N	O	
18	O	1	43	35	1	4	3	0
			Total	C	Mg	N	O	
18	O	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
18	O	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
18	O	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
18	O	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
18	O	1	46	36	1	4	5	0
			Total	C	Mg	N	O	
18	O	1	60	50	1	4	5	0
			Total	C	Mg	N	O	
18	O	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
18	O	1	41	33	1	4	3	0
			Total	C	Mg	N	O	
18	P	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
18	P	1	56	46	1	4	5	0
			Total	C	Mg	N	O	
18	P	1	52	42	1	4	5	0
			Total	C	Mg	N	O	
18	P	1	47	37	1	4	5	0
			Total	C	Mg	N	O	
18	P	1	50	40	1	4	5	0
			Total	C	Mg	N	O	
18	P	1	41	33	1	4	3	0
			Total	C	Mg	N	O	
18	P	1	45	35	1	4	5	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
18	P	1	47	37	1	4	5	0
			Total	C	Mg	N	O	
18	Q	1	48	38	1	4	5	0
			Total	C	Mg	N	O	
18	Q	1	61	51	1	4	5	0
			Total	C	Mg	N	O	
18	Q	1	60	50	1	4	5	0
			Total	C	Mg	N	O	
18	Q	1	51	41	1	4	5	0
			Total	C	Mg	N	O	
18	Q	1	46	36	1	4	5	0
			Total	C	Mg	N	O	
18	Q	1	50	40	1	4	5	0
			Total	C	Mg	N	O	
18	Q	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
18	Q	1	41	33	1	4	3	0
			Total	C	Mg	N	O	
18	Q	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
18	Q	1	57	47	1	4	5	0
			Total	C	Mg	N	O	
18	Q	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
18	R	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
18	R	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
18	S	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
18	S	1	46	36	1	4	5	0
			Total	C	Mg	N	O	
18	S	1	46	36	1	4	5	0
			Total	C	Mg	N	O	
18	S	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
18	S	1	52	42	1	4	5	0
			Total	C	Mg	N	O	
18	S	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
18	S	1	65	55	1	4	5	0

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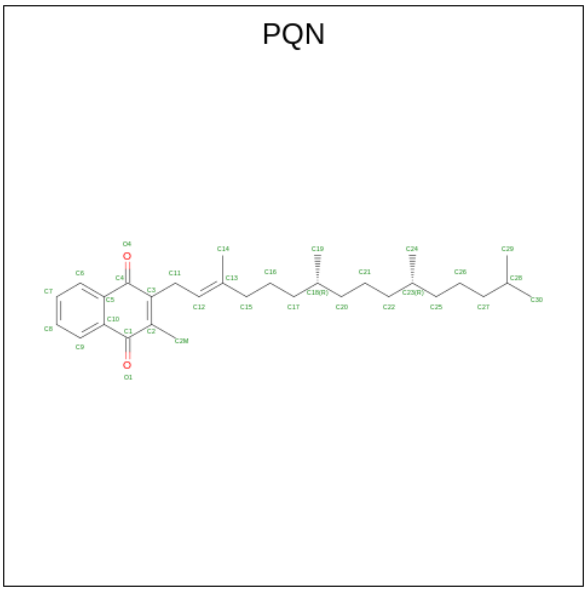
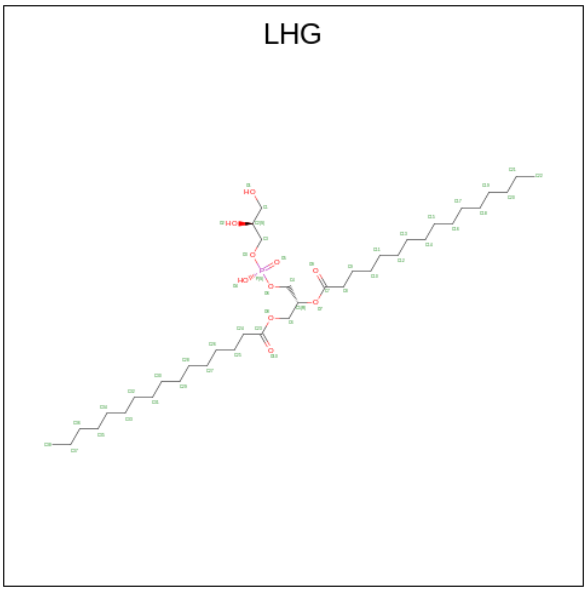
Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
18	U	1	61	51	1	4	5	0
18	U	1	65	55	1	4	5	0
18	U	1	45	35	1	4	5	0
18	U	1	65	55	1	4	5	0
18	U	1	46	36	1	4	5	0
18	U	1	42	34	1	4	3	0
18	U	1	65	55	1	4	5	0
18	U	1	52	42	1	4	5	0
18	T	1	42	34	1	4	3	0
18	T	1	41	33	1	4	3	0
18	T	1	46	36	1	4	5	0
18	T	1	57	47	1	4	5	0
18	T	1	46	36	1	4	5	0
18	T	1	42	34	1	4	3	0
18	T	1	65	55	1	4	5	0
18	T	1	41	33	1	4	3	0
18	T	1	46	36	1	4	5	0
18	T	1	47	37	1	4	5	0

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



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

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



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

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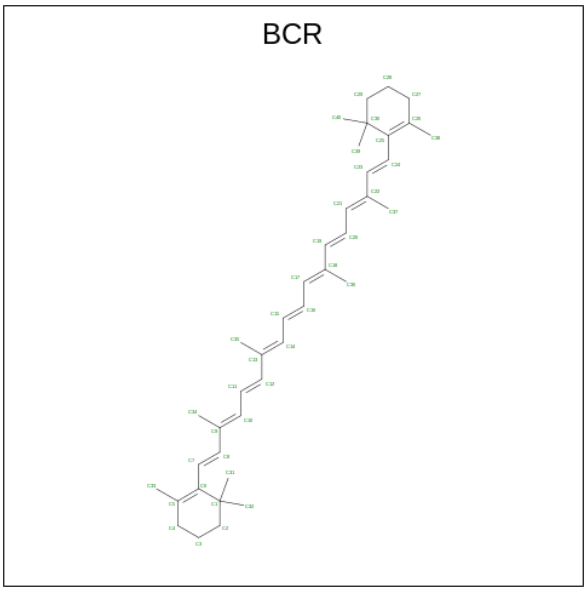
Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
20	A	1	27	16	10	1	0
			Total	C	O	P	
20	R	1	49	38	10	1	0

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



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

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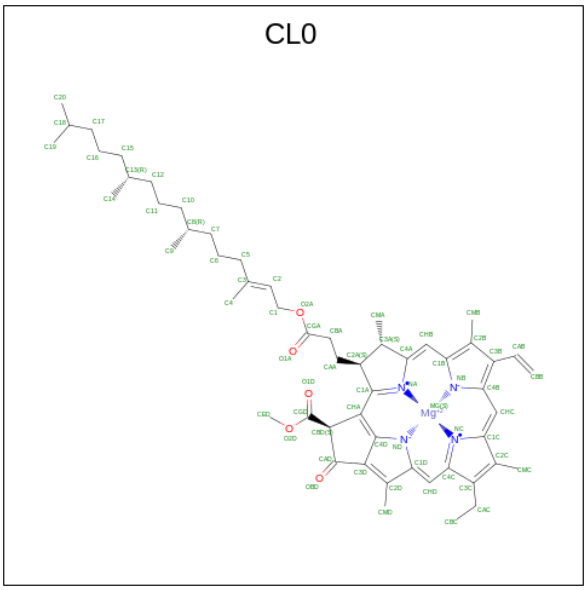
Mol	Chain	Residues	Atoms		AltConf
			Total	C	
21	F	1	40	40	0
			Total	C	
21	F	1	40	40	0
			Total	C	
21	I	1	40	40	0
			Total	C	
21	I	1	40	40	0
			Total	C	
21	J	1	40	40	0
			Total	C	
21	L	1	40	40	0
			Total	C	
21	L	1	40	40	0
			Total	C	
21	M	1	40	40	0
			Total	C	
21	R	1	39	39	0

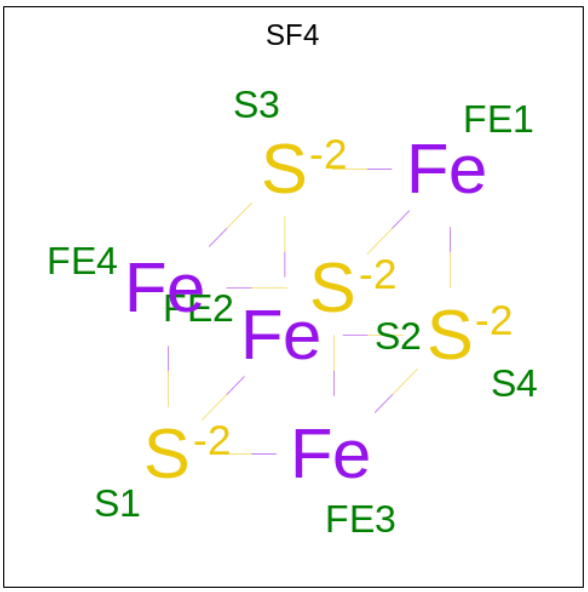
- Molecule 22 is CHLOROPHYLL A ISOMER (CCD ID: CL0) (formula: $C_{55}H_{72}MgN_4O_5$) (labeled as "Ligand of Interest" by depositor).



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

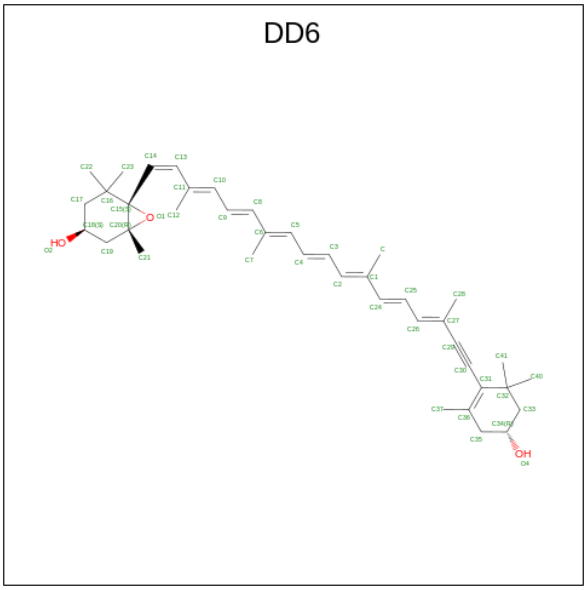
- Molecule 23 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4) (labeled as

"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
23	C	1	8	4	4	0

- Molecule 24 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	
24	A	1	43	40	3	0
24	J	1	43	40	3	0
24	O	1	43	40	3	0
24	O	1	43	40	3	0
24	O	1	43	40	3	0
24	O	1	43	40	3	0
24	O	1	43	40	3	0
24	P	1	43	40	3	0
24	P	1	43	40	3	0
24	P	1	43	40	3	0
24	P	1	23	21	2	0
24	Q	1	43	40	3	0
24	Q	1	43	40	3	0
24	S	1	43	40	3	0
24	S	1	43	40	3	0
24	S	1	43	40	3	0
24	S	1	43	40	3	0
24	S	1	43	40	3	0
24	U	1	43	40	3	0
24	U	1	43	40	3	0
24	U	1	26	25	1	0
24	T	1	43	40	3	0

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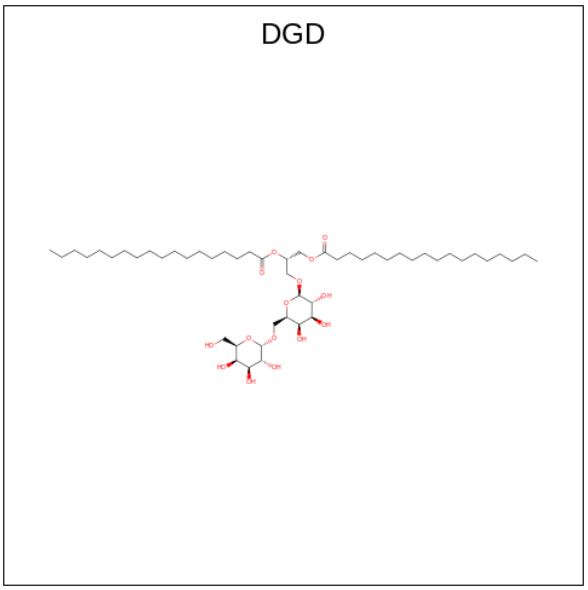
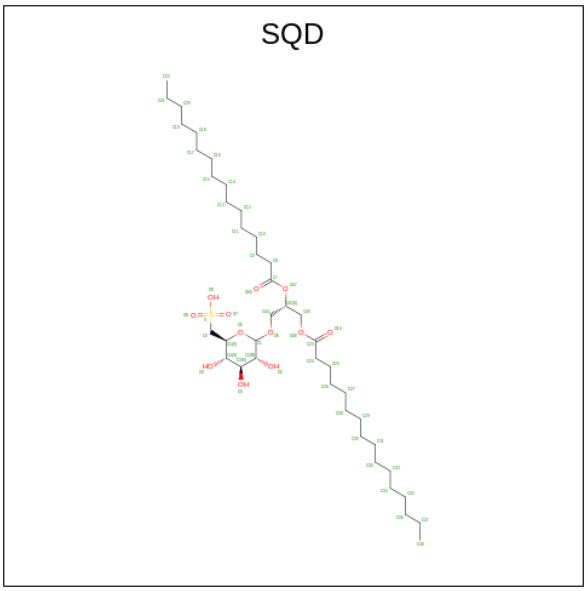
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
24	T	1	43	40	3	0

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



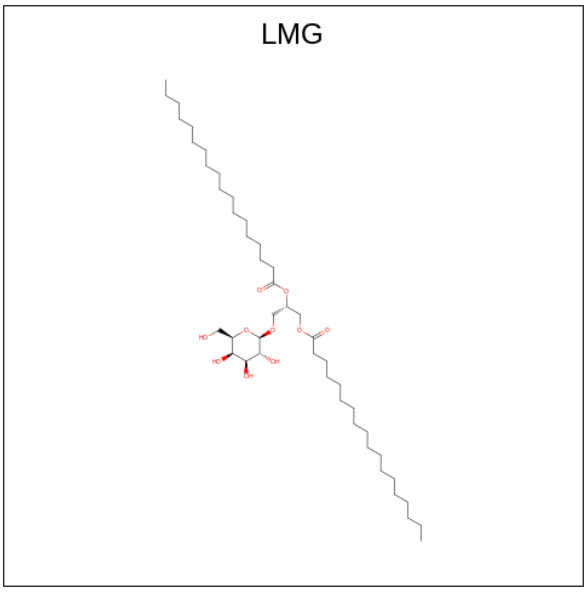
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
25	B	1	60	45	15	0

- Molecule 26 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (CCD ID: SQD) (formula: $C_{41}H_{78}O_{12}S$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
26	B	1	Total	C	O	S	0
			50	37	12	1	
26	M	1	Total	C	O	S	0
			46	33	12	1	

- Molecule 27 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
27	B	1	Total	C	O	0
			25	15	10	

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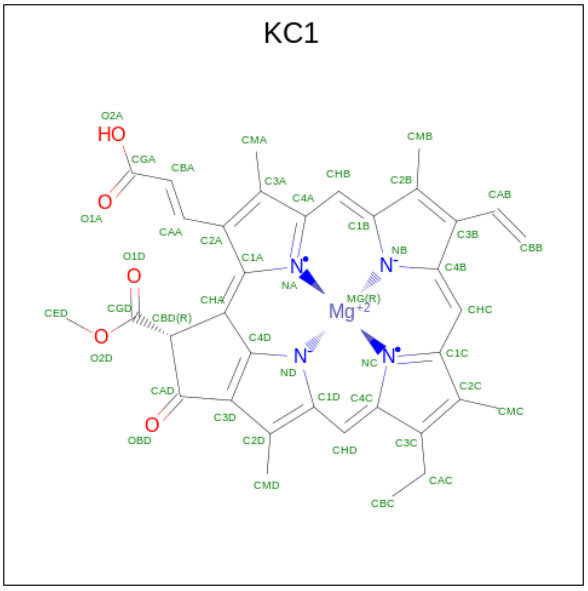
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
27	J	1	39	29	10	0
			Total	C	O	
27	P	1	34	24	10	0
			Total	C	O	
27	Q	1	55	45	10	0
			Total	C	O	
27	S	1	49	39	10	0
			Total	C	O	
27	U	1	32	22	10	0

- Molecule 28 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	
28	O	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
28	P	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
28	P	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
28	P	1	44	35	1	4	4	0
			Total	C	Mg	N	O	
28	Q	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
28	S	1	45	35	1	4	5	0

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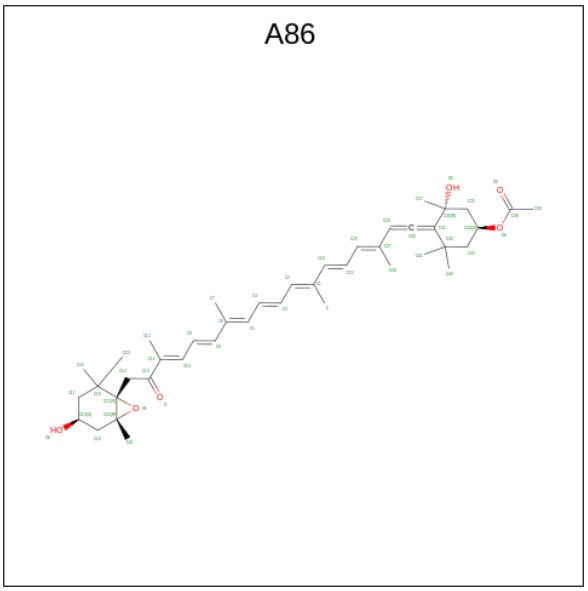
Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
28	S	1	45	35	1	4	5	0
28	U	1	45	35	1	4	5	0
28	T	1	45	35	1	4	5	0

- Molecule 29 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	
29	P	1	48	42	6	0
29	Q	1	48	42	6	0
29	Q	1	48	42	6	0
29	R	1	44	40	4	0
29	R	1	48	42	6	0
29	U	1	48	42	6	0
29	T	1	48	42	6	0

- Molecule 30 is water.

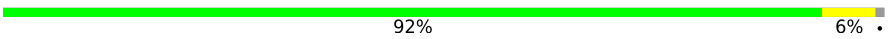
Mol	Chain	Residues	Atoms		AltConf
			Total	O	
30	A	189	189	189	0
			Total	O	
30	B	286	286	286	0
			Total	O	
30	C	59	59	59	0
			Total	O	
30	D	39	39	39	0
			Total	O	
30	E	13	13	13	0
			Total	O	
30	F	33	33	33	0
			Total	O	
30	I	2	2	2	0
			Total	O	
30	J	2	2	2	0
			Total	O	
30	L	23	23	23	0
			Total	O	
30	M	5	5	5	0
			Total	O	
30	O	22	22	22	0
			Total	O	
30	P	30	30	30	0
			Total	O	
30	Q	19	19	19	0
			Total	O	
30	R	27	27	27	0
			Total	O	
30	S	25	25	25	0
			Total	O	
30	U	9	9	9	0
			Total	O	
30	T	7	7	7	0

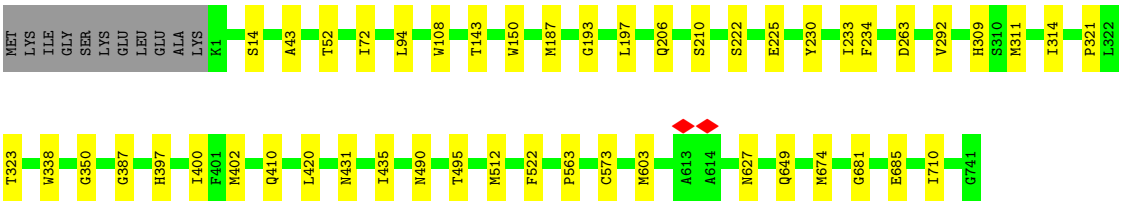
3 Residue-property plots (i)

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)

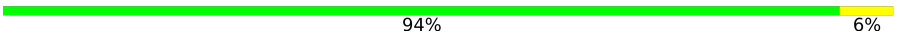
Chain A:

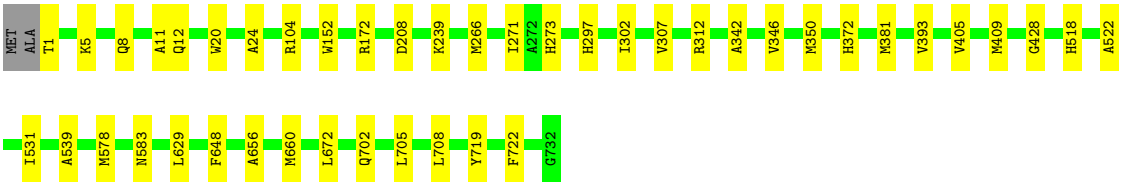




• Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2 (psaB)

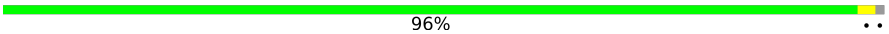
Chain B:





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

Chain C:

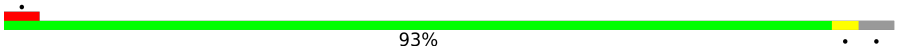


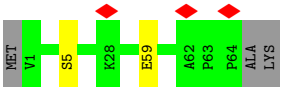
• Molecule 4: Photosystem I reaction center subunit II (psaD)

Chain D:

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

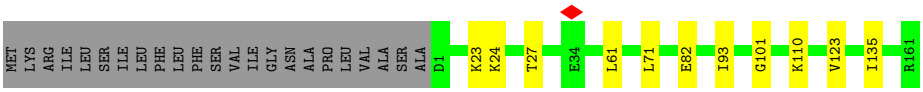
Chain E:





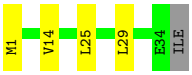
• Molecule 6: Photosystem I reaction center subunit III (psaF)

Chain F:



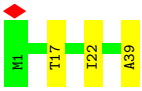
• Molecule 7: Photosystem I reaction center subunit VIII (psaI)

Chain I:



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

Chain J:

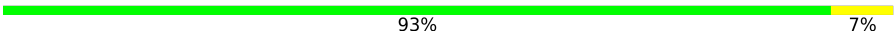


• Molecule 9: Photosystem I reaction center subunit XI (psaL)

Chain L:

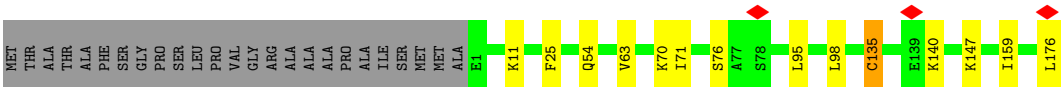
• Molecule 10: Photosystem I reaction center subunit XII (psaM)

Chain M:



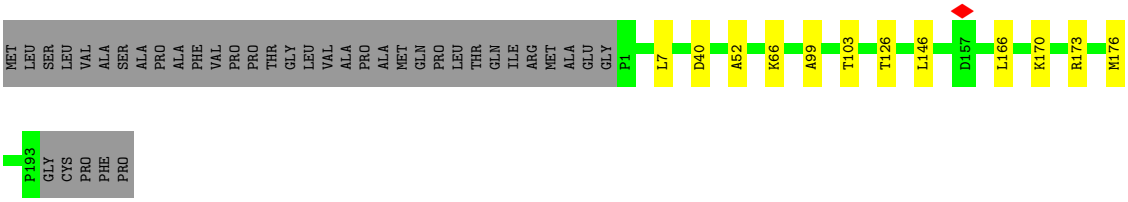
• Molecule 11: Fucoxanthin chlorophyll a/c binding protein III (FCPI-3)

Chain O:



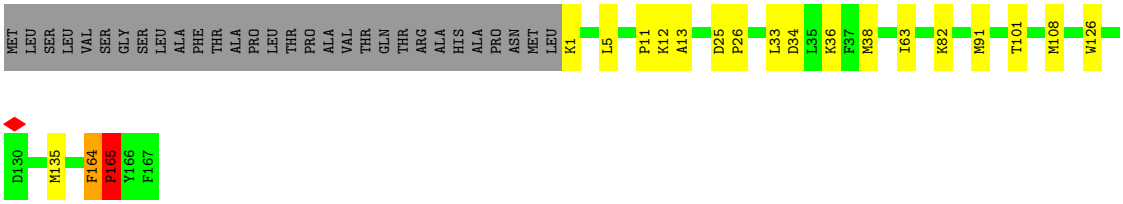
• Molecule 12: Fucoxanthin chlorophyll a/c binding protein VI (FCPI-6), GLY-CYS-PRO

Chain P:



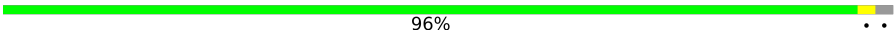
• Molecule 13: Fucoxanthin chlorophyll a/c binding protein IV (FCPI-4)

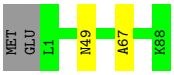
Chain Q:



• Molecule 14: Photosystem I reaction center subunit psaR

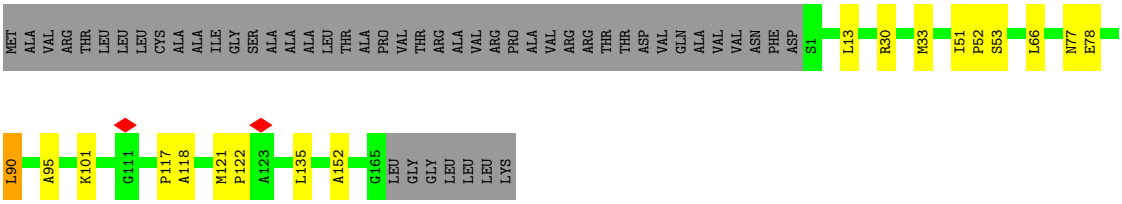
Chain R:





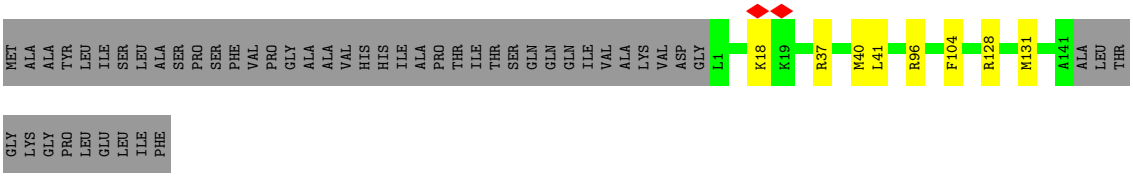
• Molecule 15: Fucoxanthin chlorophyll a/c binding protein II (FCPI-2)

Chain S:



• Molecule 16: Fucoxanthin chlorophyll a/c binding protein I (FCPI-1)

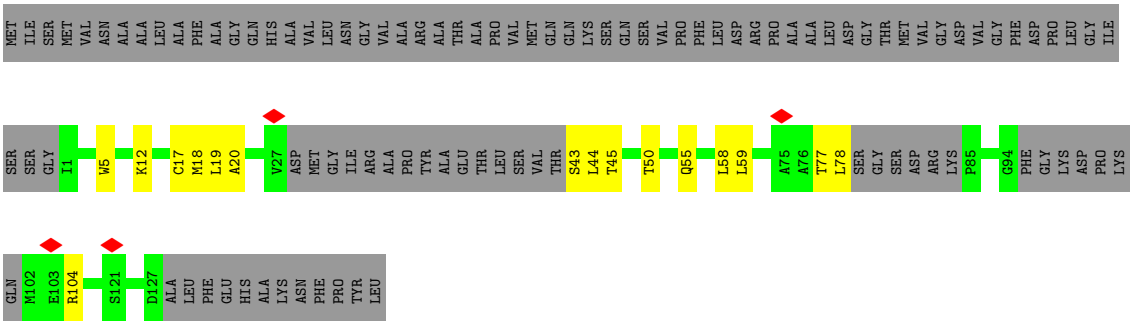
Chain U:



• Molecule 17: Fucoxanthin chlorophyll a/c binding protein V (FCPI-5)

Chain T:

41%
8%
51%


MET ILE SER MET VAL ASN ALA ALA LEU ALA PHE ALA GLY GLN HIS ALA VAL LEU ASN GLY VAL ALA ARG ALA THR ALA PRO VAL MET GLN GLN LYS SER GLN SER VAL PRO PHE LEU ASP ARG PRO ALA ALA LEU ASP GLY THR MET VAL GLY ASP VAL GLY PHE ASP PRO LEU GLY ILE
SER SER GLY I1 W5 K12 C17 M18 L19 A20 V27 ASP MET GLY ILE ARG ALA PRO TYR ALA GLU THR LEU SER VAL THR S43 L44 T45 T50 Q55 L58 L59 A75 A76 T77 L78 SER GLY SER ASP ARG LYS P85 G94 PHE GLY LYS ASP PRO LYS
GLN M102 E103 R104 S121 D127 ALA LEU PHE GLU HIS ALA LYS ASN PHE PRO TYR LEU

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	114380	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	1.114	Depositor
Minimum map value	-0.354	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.017	Depositor
Recommended contour level	0.08	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: CL0, PQN, KC1, DD6, CLA, LHG, BCR, SF4, DGD, SQD, LMG, A86

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	0.26	0/6007	0.48	0/8185
2	B	0.25	0/6015	0.47	0/8205
3	C	0.21	0/609	0.45	0/826
4	D	0.21	0/1116	0.50	0/1503
5	E	0.22	0/505	0.41	0/689
6	F	0.24	0/1275	0.47	0/1728
7	I	0.26	0/273	0.53	0/373
8	J	0.26	0/313	0.55	0/427
9	L	0.24	0/1081	0.52	0/1470
10	M	0.21	0/218	0.34	0/295
11	O	0.24	0/1376	0.51	0/1865
12	P	0.22	0/1480	0.49	0/2010
13	Q	0.30	0/1285	0.58	2/1736 (0.1%)
14	R	0.26	0/681	0.47	0/930
15	S	0.20	0/1272	0.41	0/1732
16	U	0.24	0/1109	0.49	0/1499
17	T	0.28	0/741	0.60	1/999 (0.1%)
All	All	0.25	0/25356	0.49	3/34472 (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	Q	0	1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	T	19	LEU	N-CA-C	-5.92	106.70	114.04
13	Q	91	MET	CB-CG-SD	5.04	127.83	112.70
13	Q	165	PRO	CA-N-CD	-5.00	105.00	112.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
13	Q	164	PHE	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5813	0	5698	32	0
2	B	5805	0	5634	36	0
3	C	599	0	577	1	0
4	D	1092	0	1096	7	0
5	E	494	0	488	1	0
6	F	1246	0	1256	8	0
7	I	266	0	278	4	0
8	J	305	0	310	3	0
9	L	1056	0	1068	14	0
10	M	216	0	234	3	0
11	O	1341	0	1347	10	0
12	P	1441	0	1421	8	0
13	Q	1257	0	1260	11	0
14	R	664	0	668	2	0
15	S	1238	0	1217	12	0
16	U	1082	0	1058	6	0
17	T	731	0	749	11	0
18	A	2615	0	2651	59	0
18	B	2399	0	2438	70	0
18	F	94	0	69	1	0
18	J	42	0	31	2	0
18	L	164	0	150	4	0
18	O	495	0	475	13	0
18	P	403	0	337	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
18	Q	609	0	566	13	0
18	R	110	0	105	4	0
18	S	384	0	358	13	0
18	T	473	0	379	13	0
18	U	441	0	417	13	0
19	A	33	0	46	2	0
19	B	33	0	46	1	0
20	A	75	0	93	2	0
20	R	49	0	74	2	0
21	A	160	0	224	5	0
21	B	200	0	280	7	0
21	F	80	0	112	4	0
21	I	80	0	112	4	0
21	J	40	0	56	1	0
21	L	80	0	112	6	0
21	M	40	0	56	4	0
21	R	39	0	53	3	0
22	A	65	0	72	3	0
23	A	8	0	0	0	0
23	C	16	0	0	0	0
24	A	43	0	0	0	0
24	J	43	0	0	0	0
24	O	215	0	0	0	0
24	P	152	0	0	1	0
24	Q	86	0	0	0	0
24	S	215	0	0	0	0
24	T	86	0	0	0	0
24	U	112	0	0	0	0
25	B	60	0	81	5	0
26	B	50	0	67	3	0
26	M	46	0	56	3	0
27	B	25	0	20	2	0
27	J	39	0	48	2	0
27	P	34	0	38	1	0
27	Q	55	0	86	6	0
27	S	49	0	68	6	0
27	U	32	0	34	2	0
28	O	45	0	0	1	0
28	P	134	0	0	0	0
28	Q	45	0	0	0	0
28	S	90	0	0	0	0
28	T	45	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
28	U	45	0	0	0	0
29	P	48	0	0	0	0
29	Q	96	0	0	0	0
29	R	92	0	0	2	0
29	T	48	0	0	0	0
29	U	48	0	0	1	0
30	A	189	0	0	1	0
30	B	286	0	0	1	0
30	C	59	0	0	0	0
30	D	39	0	0	1	0
30	E	13	0	0	0	0
30	F	33	0	0	1	0
30	I	2	0	0	0	0
30	J	2	0	0	0	0
30	L	23	0	0	0	0
30	M	5	0	0	0	0
30	O	22	0	0	0	0
30	P	30	0	0	0	0
30	Q	19	0	0	0	0
30	R	27	0	0	0	0
30	S	25	0	0	0	0
30	T	7	0	0	0	0
30	U	9	0	0	0	0
All	All	36741	0	34169	336	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 5.

The worst 5 of 336 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:193:GLY:O	1:A:197:LEU:HB2	1.87	0.75
27:U:201:LMG:H321	18:U:211:CLA:H42	1.74	0.69
1:A:522:PHE:HA	18:A:833:CLA:HED1	1.75	0.69
18:A:838:CLA:HED1	18:U:210:CLA:HAA2	1.76	0.68
18:Q:206:CLA:H42	27:Q:217:LMG:H182	1.76	0.67

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%)	722 (98%)	17 (2%)	0	100	100
2	B	730/734 (100%)	714 (98%)	16 (2%)	0	100	100
3	C	78/81 (96%)	78 (100%)	0	0	100	100
4	D	136/142 (96%)	132 (97%)	4 (3%)	0	100	100
5	E	62/67 (92%)	61 (98%)	1 (2%)	0	100	100
6	F	159/184 (86%)	157 (99%)	2 (1%)	0	100	100
7	I	32/35 (91%)	32 (100%)	0	0	100	100
8	J	37/39 (95%)	36 (97%)	1 (3%)	0	100	100
9	L	138/141 (98%)	137 (99%)	1 (1%)	0	100	100
10	M	27/29 (93%)	27 (100%)	0	0	100	100
11	O	174/201 (87%)	171 (98%)	3 (2%)	0	100	100
12	P	191/231 (83%)	190 (100%)	1 (0%)	0	100	100
13	Q	165/197 (84%)	157 (95%)	6 (4%)	2 (1%)	10	4
14	R	86/90 (96%)	86 (100%)	0	0	100	100
15	S	163/215 (76%)	161 (99%)	2 (1%)	0	100	100
16	U	139/191 (73%)	138 (99%)	1 (1%)	0	100	100
17	T	91/202 (45%)	90 (99%)	1 (1%)	0	100	100
All	All	3147/3531 (89%)	3089 (98%)	56 (2%)	2 (0%)	49	40

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
13	Q	165	PRO
13	Q	33	LEU

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%)	598 (99%)	5 (1%)	73	75
2	B	590/591 (100%)	587 (100%)	3 (0%)	81	84
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%)	53 (100%)	0	100	100
6	F	133/152 (88%)	132 (99%)	1 (1%)	73	75
7	I	31/32 (97%)	31 (100%)	0	100	100
8	J	32/32 (100%)	32 (100%)	0	100	100
9	L	111/112 (99%)	111 (100%)	0	100	100
10	M	21/21 (100%)	21 (100%)	0	100	100
11	O	145/161 (90%)	143 (99%)	2 (1%)	59	59
12	P	144/173 (83%)	144 (100%)	0	100	100
13	Q	133/157 (85%)	131 (98%)	2 (2%)	57	56
14	R	71/73 (97%)	71 (100%)	0	100	100
15	S	125/162 (77%)	122 (98%)	3 (2%)	43	38
16	U	110/148 (74%)	110 (100%)	0	100	100
17	T	73/153 (48%)	71 (97%)	2 (3%)	39	34
All	All	2561/2825 (91%)	2543 (99%)	18 (1%)	73	78

5 of 18 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
15	S	90	LEU
17	T	77	THR
17	T	43	SER
6	F	135	ILE
15	S	53	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 19

such sidechains are listed below:

Mol	Chain	Res	Type
14	R	49	ASN
15	S	72	ASN
16	U	120	GLN
15	S	46	GLN
6	F	15	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)

220 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	$\#\|Z\| > 2$
21	BCR	B	840	-	41,41,41	1.03	2 (4%)	56,56,56	1.25	7 (12%)
18	CLA	B	834	2	69,73,73	1.27	9 (13%)	83,113,113	1.02	4 (4%)
21	BCR	J	104	-	41,41,41	1.05	2 (4%)	56,56,56	1.12	4 (7%)
18	CLA	A	820	1	55,59,73	1.40	7 (12%)	66,96,113	1.20	6 (9%)
18	CLA	Q	212	13	69,73,73	1.25	8 (11%)	83,113,113	1.04	7 (8%)
18	CLA	T	202	-	46,50,73	1.46	7 (15%)	55,85,113	1.26	5 (9%)
18	CLA	Q	207	13	50,54,73	1.41	7 (14%)	60,90,113	1.23	5 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
18	CLA	A	826	1	69,73,73	1.32	8 (11%)	83,113,113	0.88	3 (3%)
23	SF4	A	850	2,1	0,12,12	-	-	-		
28	KC1	U	213	16	49,53,53	1.76	10 (20%)	63,89,89	1.02	4 (6%)
18	CLA	Q	204	-	65,69,73	1.21	6 (9%)	78,108,113	1.02	6 (7%)
18	CLA	A	846	1	64,68,73	1.40	9 (14%)	77,107,113	0.91	4 (5%)
18	CLA	B	843	2	69,73,73	1.30	8 (11%)	83,113,113	0.97	3 (3%)
24	DD6	S	203	-	39,45,45	1.65	8 (20%)	52,67,67	1.91	13 (25%)
18	CLA	Q	213	30	61,65,73	1.26	7 (11%)	73,103,113	1.04	5 (6%)
18	CLA	B	814	2	59,63,73	1.43	8 (13%)	71,101,113	1.03	4 (5%)
24	DD6	O	214	-	39,45,45	1.54	8 (20%)	52,67,67	1.57	12 (23%)
29	A86	R	204	-	40,46,50	1.75	4 (10%)	45,70,76	2.08	15 (33%)
18	CLA	B	848	2	54,58,73	1.37	8 (14%)	65,95,113	1.20	6 (9%)
18	CLA	A	845	30	69,73,73	1.18	8 (11%)	83,113,113	0.98	3 (3%)
24	DD6	P	317	-	20,24,45	1.80	6 (30%)	27,37,67	1.92	6 (22%)
18	CLA	B	819	2	57,61,73	1.31	7 (12%)	68,98,113	1.05	5 (7%)
18	CLA	A	829	1	69,73,73	1.23	8 (11%)	83,113,113	0.97	4 (4%)
18	CLA	L	202	9	53,57,73	1.39	8 (15%)	62,93,113	1.39	6 (9%)
18	CLA	U	209	16	46,50,73	1.48	7 (15%)	55,85,113	1.17	5 (9%)
26	SQD	M	102	-	45,46,54	0.99	4 (8%)	54,57,65	1.62	10 (18%)
18	CLA	B	810	2	58,62,73	1.44	9 (15%)	73,100,113	0.94	3 (4%)
18	CLA	A	806	1	69,73,73	1.16	7 (10%)	83,113,113	0.95	4 (4%)
18	CLA	Q	211	13	45,49,73	1.49	8 (17%)	54,84,113	1.24	6 (11%)
24	DD6	P	314	-	39,45,45	1.68	7 (17%)	52,67,67	1.99	10 (19%)
18	CLA	A	847	1	69,73,73	1.22	9 (13%)	83,113,113	1.10	6 (7%)
18	CLA	A	808	1	60,64,73	1.33	9 (15%)	72,102,113	1.29	7 (9%)
24	DD6	P	316	-	39,45,45	1.64	6 (15%)	52,67,67	1.81	12 (23%)
18	CLA	P	308	-	56,60,73	1.30	7 (12%)	67,97,113	1.08	5 (7%)
18	CLA	T	208	17	69,73,73	1.18	7 (10%)	83,113,113	1.16	7 (8%)
28	KC1	O	210	11	49,53,53	1.75	10 (20%)	63,89,89	1.17	5 (7%)
20	LHG	A	839	-	47,47,48	0.65	0	50,53,54	1.19	5 (10%)
18	CLA	A	821	-	69,73,73	1.24	8 (11%)	83,113,113	1.02	6 (7%)
18	CLA	L	204	-	54,58,73	1.36	8 (14%)	65,95,113	1.14	5 (7%)
18	CLA	P	310	12	54,58,73	1.33	7 (12%)	65,95,113	1.14	3 (4%)
18	CLA	B	835	30	69,73,73	1.23	7 (10%)	83,113,113	1.10	8 (9%)
18	CLA	B	831	2	69,73,73	1.23	8 (11%)	83,113,113	0.94	3 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
18	CLA	L	203	9	69,73,73	1.22	8 (11%)	83,113,113	0.97	4 (4%)
18	CLA	B	826	2	54,58,73	1.45	8 (14%)	65,95,113	1.08	4 (6%)
18	CLA	A	828	1	69,73,73	1.25	7 (10%)	83,113,113	0.95	4 (4%)
18	CLA	B	830	2	62,66,73	1.31	8 (12%)	74,104,113	1.04	5 (6%)
18	CLA	Q	206	13	54,59,73	1.40	7 (12%)	64,96,113	0.99	3 (4%)
18	CLA	Q	216	30	69,73,73	1.17	8 (11%)	83,113,113	0.99	4 (4%)
21	BCR	A	841	-	41,41,41	1.04	2 (4%)	56,56,56	1.23	5 (8%)
18	CLA	A	835	1	69,73,73	1.25	7 (10%)	83,113,113	0.99	4 (4%)
18	CLA	A	825	1	69,73,73	1.26	8 (11%)	83,113,113	0.90	3 (3%)
18	CLA	A	823	1	69,73,73	1.25	8 (11%)	83,113,113	0.89	4 (4%)
18	CLA	O	208	11	64,68,73	1.19	8 (12%)	77,107,113	1.07	5 (6%)
21	BCR	A	842	-	41,41,41	1.06	2 (4%)	56,56,56	1.12	4 (7%)
18	CLA	U	207	-	69,73,73	1.16	6 (8%)	83,113,113	1.18	8 (9%)
21	BCR	L	201	-	41,41,41	1.09	2 (4%)	56,56,56	1.17	4 (7%)
18	CLA	S	201	30	69,73,73	1.15	7 (10%)	83,113,113	1.13	7 (8%)
18	CLA	A	810	1	58,62,73	1.29	7 (12%)	69,99,113	1.09	6 (8%)
18	CLA	A	833	1	69,73,73	1.27	9 (13%)	83,113,113	1.12	6 (7%)
18	CLA	Q	208	13	54,58,73	1.33	9 (16%)	65,95,113	1.08	5 (7%)
28	KC1	P	305	12	49,53,53	2.06	11 (22%)	63,89,89	1.20	7 (11%)
18	CLA	B	820	-	67,71,73	1.23	8 (11%)	80,110,113	1.06	6 (7%)
21	BCR	I	101	-	41,41,41	1.10	2 (4%)	56,56,56	1.33	8 (14%)
24	DD6	U	214	-	24,26,45	1.63	6 (25%)	30,35,67	1.62	6 (20%)
18	CLA	P	313	12	49,53,73	1.44	6 (12%)	59,89,113	1.17	5 (8%)
25	DGD	B	842	-	61,61,67	0.98	1 (1%)	75,75,81	1.35	7 (9%)
18	CLA	Q	205	13	64,68,73	1.20	8 (12%)	77,107,113	1.04	4 (5%)
21	BCR	F	801	-	41,41,41	1.05	2 (4%)	56,56,56	1.29	6 (10%)
27	LMG	J	102	-	39,39,55	0.86	1 (2%)	47,47,63	1.21	2 (4%)
18	CLA	B	846	2	69,73,73	1.21	8 (11%)	83,113,113	1.25	7 (8%)
24	DD6	U	203	-	39,45,45	1.63	8 (20%)	52,67,67	1.91	13 (25%)
20	LHG	A	840	18	26,26,48	0.84	1 (3%)	29,32,54	1.33	3 (10%)
18	CLA	R	202	30	49,53,73	1.43	8 (16%)	59,89,113	1.20	6 (10%)
18	CLA	T	211	17	50,54,73	1.42	7 (14%)	60,90,113	1.27	7 (11%)
18	CLA	O	207	11	50,54,73	1.39	8 (16%)	60,90,113	1.15	4 (6%)
18	CLA	Q	209	13	69,73,73	1.15	6 (8%)	83,113,113	1.00	3 (3%)
18	CLA	S	205	15	50,54,73	1.47	8 (16%)	60,90,113	1.08	3 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
18	CLA	U	204	-	65,69,73	1.23	7 (10%)	78,108,113	0.95	5 (6%)
18	CLA	A	851	1	69,73,73	1.22	8 (11%)	83,113,113	0.95	3 (3%)
23	SF4	C	101	3	0,12,12	-	-	-		
18	CLA	A	815	1	69,73,73	1.24	7 (10%)	83,113,113	1.00	5 (6%)
24	DD6	S	213	-	39,45,45	1.65	8 (20%)	52,67,67	1.71	13 (25%)
27	LMG	S	211	-	49,49,55	0.73	1 (2%)	57,57,63	1.25	4 (7%)
18	CLA	S	204	15	50,54,73	1.38	7 (14%)	60,90,113	1.13	4 (6%)
18	CLA	T	210	17	45,49,73	1.42	5 (11%)	54,84,113	1.35	7 (12%)
18	CLA	A	807	1	69,73,73	1.22	8 (11%)	83,113,113	1.02	5 (6%)
18	CLA	B	818	2	50,54,73	1.42	8 (16%)	60,90,113	1.23	6 (10%)
18	CLA	B	811	2	59,63,73	1.28	7 (11%)	71,101,113	0.99	3 (4%)
18	CLA	B	816	2	64,68,73	1.28	8 (12%)	77,107,113	1.00	4 (5%)
18	CLA	B	813	2	53,57,73	1.43	9 (16%)	62,93,113	1.14	4 (6%)
18	CLA	B	845	2	69,73,73	1.29	9 (13%)	83,113,113	1.02	5 (6%)
18	CLA	P	307	12	60,64,73	1.29	8 (13%)	72,102,113	1.07	6 (8%)
18	CLA	B	802	2	69,73,73	1.29	7 (10%)	83,113,113	0.84	4 (4%)
18	CLA	P	312	12	45,49,73	1.45	7 (15%)	54,84,113	1.27	5 (9%)
21	BCR	B	841	-	41,41,41	1.07	2 (4%)	56,56,56	1.08	4 (7%)
18	CLA	A	803	1	69,73,73	1.21	8 (11%)	83,113,113	1.04	4 (4%)
18	CLA	B	815	2	63,67,73	1.24	7 (11%)	75,105,113	1.12	6 (8%)
18	CLA	B	823	2	69,73,73	1.26	7 (10%)	83,113,113	0.96	4 (4%)
18	CLA	B	825	2	69,73,73	1.29	8 (11%)	83,113,113	0.96	5 (6%)
24	DD6	U	212	-	39,45,45	1.53	7 (17%)	52,67,67	1.85	10 (19%)
24	DD6	O	201	-	39,45,45	1.62	8 (20%)	52,67,67	1.61	9 (17%)
18	CLA	B	808	2	69,73,73	1.26	8 (11%)	83,113,113	0.93	3 (3%)
27	LMG	Q	217	-	55,55,55	0.75	1 (1%)	63,63,63	1.33	8 (12%)
18	CLA	S	214	30	69,73,73	1.17	6 (8%)	83,113,113	1.03	5 (6%)
29	A86	Q	201	-	44,50,50	1.68	5 (11%)	51,76,76	1.76	10 (19%)
18	CLA	T	212	-	51,55,73	1.37	6 (11%)	61,91,113	1.20	6 (9%)
18	CLA	A	814	30	49,53,73	1.42	8 (16%)	59,89,113	1.15	5 (8%)
18	CLA	O	211	11	45,49,73	1.49	7 (15%)	54,84,113	1.23	6 (11%)
18	CLA	B	805	2	69,73,73	1.22	9 (13%)	83,113,113	0.98	4 (4%)
21	BCR	I	102	-	41,41,41	1.03	2 (4%)	56,56,56	1.17	4 (7%)
18	CLA	P	306	12	69,73,73	1.19	7 (10%)	83,113,113	1.05	5 (6%)
18	CLA	U	206	16	49,53,73	1.42	6 (12%)	59,89,113	1.14	5 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
24	DD6	O	215	-	39,45,45	1.54	8 (20%)	52,67,67	1.68	12 (23%)
18	CLA	B	821	-	68,72,73	1.17	8 (11%)	81,111,113	0.96	5 (6%)
21	BCR	R	203	-	40,40,41	1.16	2 (5%)	54,54,56	1.44	11 (20%)
18	CLA	A	853	30	69,73,73	1.20	7 (10%)	83,113,113	1.07	7 (8%)
18	CLA	P	309	30	51,55,73	1.35	8 (15%)	61,91,113	1.05	4 (6%)
18	CLA	A	838	20	56,60,73	1.30	8 (14%)	67,97,113	1.06	3 (4%)
24	DD6	S	202	-	39,45,45	1.53	8 (20%)	52,67,67	1.55	8 (15%)
18	CLA	A	827	1	54,58,73	1.45	8 (14%)	65,95,113	1.06	4 (6%)
23	SF4	C	102	3	0,12,12	-	-	-		
24	DD6	J	101	-	39,45,45	1.53	8 (20%)	52,67,67	1.66	9 (17%)
24	DD6	Q	215	-	39,45,45	1.55	7 (17%)	52,67,67	1.58	9 (17%)
21	BCR	F	804	-	41,41,41	1.02	2 (4%)	56,56,56	1.26	4 (7%)
18	CLA	A	849	1	69,73,73	1.25	6 (8%)	83,113,113	0.93	3 (3%)
28	KC1	T	209	17	49,53,53	1.80	11 (22%)	63,89,89	1.05	3 (4%)
18	CLA	B	817	-	69,73,73	1.24	7 (10%)	83,113,113	1.05	8 (9%)
18	CLA	S	207	15	56,60,73	1.28	7 (12%)	67,97,113	1.17	5 (7%)
18	CLA	B	803	-	69,73,73	1.18	7 (10%)	83,113,113	1.00	5 (6%)
21	BCR	M	101	-	41,41,41	1.04	2 (4%)	56,56,56	1.29	8 (14%)
18	CLA	A	817	1	49,53,73	1.44	8 (16%)	59,89,113	1.15	5 (8%)
18	CLA	O	209	11	69,73,73	1.20	7 (10%)	83,113,113	1.26	7 (8%)
18	CLA	O	202	11	47,51,73	1.44	7 (14%)	56,86,113	1.17	5 (8%)
24	DD6	P	304	-	39,45,45	1.49	8 (20%)	52,67,67	1.53	10 (19%)
28	KC1	S	208	15	49,53,53	1.74	10 (20%)	63,89,89	1.16	4 (6%)
18	CLA	S	206	15	49,53,73	1.35	6 (12%)	59,89,113	1.09	5 (8%)
24	DD6	T	214	-	39,45,45	1.55	7 (17%)	52,67,67	1.92	11 (21%)
18	CLA	U	205	16	69,73,73	1.19	7 (10%)	83,113,113	0.95	3 (3%)
18	CLA	A	804	1	69,73,73	1.18	8 (11%)	83,113,113	1.04	6 (7%)
24	DD6	Q	202	-	39,45,45	1.56	8 (20%)	52,67,67	1.69	10 (19%)
18	CLA	T	204	17	50,54,73	1.46	7 (14%)	60,90,113	0.99	3 (5%)
19	PQN	A	837	-	34,34,34	0.39	0	42,45,45	0.45	0
18	CLA	T	203	17	45,49,73	1.44	7 (15%)	54,84,113	1.19	4 (7%)
21	BCR	A	843	-	41,41,41	1.08	2 (4%)	56,56,56	1.21	3 (5%)
24	DD6	O	212	-	39,45,45	1.58	8 (20%)	52,67,67	1.73	9 (17%)
29	A86	T	201	-	44,50,50	1.64	6 (13%)	51,76,76	1.66	11 (21%)
21	BCR	B	839	-	41,41,41	1.04	2 (4%)	56,56,56	1.17	4 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
18	CLA	A	836	30	69,73,73	1.20	9 (13%)	83,113,113	1.06	6 (7%)
18	CLA	A	834	1	69,73,73	1.34	9 (13%)	83,113,113	0.96	4 (4%)
18	CLA	A	824	1	66,70,73	1.23	8 (12%)	79,109,113	1.13	6 (7%)
18	CLA	B	804	2	49,53,73	1.48	8 (16%)	59,89,113	1.06	3 (5%)
24	DD6	A	854	-	39,45,45	1.51	8 (20%)	52,67,67	1.59	10 (19%)
21	BCR	B	837	-	41,41,41	1.07	2 (4%)	56,56,56	1.13	4 (7%)
24	DD6	S	209	-	39,45,45	1.51	8 (20%)	52,67,67	1.50	9 (17%)
24	DD6	S	212	-	39,45,45	1.53	8 (20%)	52,67,67	1.53	10 (19%)
18	CLA	A	811	1	69,73,73	1.24	8 (11%)	83,113,113	0.98	4 (4%)
18	CLA	T	206	-	50,54,73	1.37	8 (16%)	60,90,113	1.19	6 (10%)
18	CLA	U	211	16	56,60,73	1.32	7 (12%)	67,97,113	1.06	5 (7%)
18	CLA	U	208	16	50,54,73	1.36	7 (14%)	60,90,113	1.18	5 (8%)
18	CLA	A	805	1	53,57,73	1.43	9 (16%)	62,93,113	1.12	4 (6%)
21	BCR	B	838	-	41,41,41	1.05	2 (4%)	56,56,56	1.19	7 (12%)
29	A86	Q	214	-	44,50,50	1.64	6 (13%)	51,76,76	1.49	10 (19%)
18	CLA	O	204	11	69,73,73	1.22	9 (13%)	83,113,113	0.95	5 (6%)
18	CLA	B	801	-	69,73,73	1.21	8 (11%)	83,113,113	0.98	5 (6%)
18	CLA	A	822	30	69,73,73	1.16	5 (7%)	83,113,113	1.01	4 (4%)
18	CLA	O	203	-	49,53,73	1.44	7 (14%)	59,89,113	1.14	5 (8%)
18	CLA	A	801	-	69,73,73	1.20	7 (10%)	83,113,113	0.96	4 (4%)
27	LMG	P	301	-	34,34,55	1.14	3 (8%)	42,42,63	1.30	2 (4%)
28	KC1	P	311	12	47,52,53	1.79	9 (19%)	57,87,89	1.41	8 (14%)
27	LMG	B	849	-	25,25,55	1.38	5 (20%)	33,33,63	1.24	5 (15%)
18	CLA	B	827	2	53,57,73	1.40	8 (15%)	62,93,113	1.12	5 (8%)
18	CLA	J	103	8	46,50,73	1.49	7 (15%)	55,85,113	1.15	4 (7%)
18	CLA	B	824	2	69,73,73	1.27	9 (13%)	83,113,113	1.71	11 (13%)
18	CLA	B	822	2	69,73,73	1.27	8 (11%)	83,113,113	1.00	5 (6%)
18	CLA	P	315	12	51,55,73	1.41	8 (15%)	61,91,113	1.18	5 (8%)
18	CLA	Q	203	13	52,56,73	1.35	6 (11%)	62,92,113	1.12	5 (8%)
18	CLA	B	806	2	69,73,73	1.27	8 (11%)	83,113,113	0.92	4 (4%)
26	SQD	B	847	-	49,50,54	1.01	6 (12%)	58,61,65	1.55	10 (17%)
28	KC1	S	210	15	49,53,53	1.71	10 (20%)	63,89,89	1.15	5 (7%)
18	CLA	O	206	-	69,73,73	1.17	8 (11%)	83,113,113	0.93	4 (4%)
21	BCR	A	844	-	41,41,41	1.08	2 (4%)	56,56,56	1.22	5 (8%)
29	A86	R	206	-	44,50,50	1.59	6 (13%)	51,76,76	1.57	10 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
18	CLA	T	205	-	61,65,73	1.23	7 (11%)	73,103,113	0.99	4 (5%)
18	CLA	A	831	1	49,53,73	1.38	7 (14%)	59,89,113	1.19	5 (8%)
18	CLA	B	828	2	62,66,73	1.32	8 (12%)	74,104,113	1.02	4 (5%)
18	CLA	B	807	2	69,73,73	1.22	8 (11%)	83,113,113	0.98	4 (4%)
18	CLA	A	819	1	47,51,73	1.45	8 (17%)	56,86,113	1.12	4 (7%)
18	CLA	A	852	1	69,73,73	1.19	8 (11%)	83,113,113	0.97	5 (6%)
18	CLA	F	802	30	52,56,73	1.42	7 (13%)	62,92,113	1.18	5 (8%)
18	CLA	B	844	2	69,73,73	1.28	8 (11%)	83,113,113	0.94	6 (7%)
18	CLA	B	832	2	51,55,73	1.44	8 (15%)	61,91,113	1.17	5 (8%)
18	CLA	B	809	2	69,73,73	1.21	8 (11%)	83,113,113	0.97	5 (6%)
21	BCR	L	205	-	41,41,41	1.05	2 (4%)	56,56,56	1.24	4 (7%)
18	CLA	A	832	1	55,59,73	1.41	8 (14%)	66,96,113	1.10	4 (6%)
18	CLA	A	809	1	66,70,73	1.25	8 (12%)	79,109,113	0.92	3 (3%)
28	KC1	Q	210	13	49,53,53	1.74	9 (18%)	63,89,89	1.30	8 (12%)
18	CLA	B	812	2	58,62,73	1.36	8 (13%)	69,99,113	1.06	4 (5%)
18	CLA	A	813	1	54,58,73	1.40	7 (12%)	65,95,113	1.17	7 (10%)
20	LHG	R	201	-	48,48,48	0.65	2 (4%)	51,54,54	1.25	5 (9%)
18	CLA	B	829	30	69,73,73	1.18	8 (11%)	83,113,113	1.05	6 (7%)
18	CLA	R	205	14	69,73,73	1.28	9 (13%)	83,113,113	0.98	4 (4%)
29	A86	P	303	-	44,50,50	1.65	6 (13%)	51,76,76	1.66	10 (19%)
18	CLA	A	802	1	59,63,73	1.34	8 (13%)	71,101,113	1.01	3 (4%)
27	LMG	U	201	-	32,32,55	1.01	0	40,40,63	1.15	4 (10%)
29	A86	U	202	-	44,50,50	1.60	6 (13%)	51,76,76	1.56	10 (19%)
18	CLA	U	210	16	69,73,73	1.17	8 (11%)	83,113,113	1.01	5 (6%)
18	CLA	T	207	17	46,50,73	1.44	6 (13%)	55,85,113	1.17	5 (9%)
24	DD6	T	213	-	39,45,45	1.62	7 (17%)	52,67,67	1.84	13 (25%)
22	CL0	A	848	1	69,73,73	1.44	6 (8%)	83,113,113	0.91	4 (4%)
24	DD6	O	213	-	39,45,45	1.49	7 (17%)	52,67,67	1.51	11 (21%)
18	CLA	S	215	15	69,73,73	1.18	7 (10%)	83,113,113	0.94	3 (3%)
18	CLA	A	830	1	54,58,73	1.34	8 (14%)	65,95,113	1.07	4 (6%)
18	CLA	F	803	6	50,54,73	1.40	7 (14%)	60,90,113	1.19	5 (8%)
18	CLA	O	205	11	69,73,73	1.21	7 (10%)	83,113,113	0.94	4 (4%)
18	CLA	A	818	30	69,73,73	1.20	7 (10%)	83,113,113	0.95	3 (3%)
18	CLA	B	833	-	69,73,73	1.21	8 (11%)	83,113,113	1.06	7 (8%)
19	PQN	B	836	-	34,34,34	0.41	0	42,45,45	0.35	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
18	CLA	A	812	1	49,53,73	1.48	8 (16%)	59,89,113	1.11	4 (6%)
28	KC1	P	302	12	49,53,53	1.80	11 (22%)	63,89,89	1.19	6 (9%)
18	CLA	A	816	1	69,73,73	1.24	8 (11%)	83,113,113	1.04	4 (4%)

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
21	BCR	B	840	-	-	5/29/63/63	0/2/2/2
18	CLA	B	834	2	-	7/39/115/115	-
21	BCR	J	104	-	-	13/29/63/63	0/2/2/2
18	CLA	A	820	1	-	3/23/99/115	-
18	CLA	Q	212	13	-	15/39/115/115	-
18	CLA	T	202	-	-	1/12/88/115	-
18	CLA	Q	207	13	-	4/17/93/115	-
18	CLA	A	826	1	-	3/39/115/115	-
28	KC1	U	213	16	-	3/15/71/71	-
23	SF4	A	850	2,1	-	-	0/6/5/5
18	CLA	Q	204	-	-	10/35/111/115	-
18	CLA	A	846	1	-	9/33/109/115	-
18	CLA	B	843	2	-	5/39/115/115	-
24	DD6	S	203	-	-	8/26/80/80	0/3/3/3
18	CLA	Q	213	30	-	6/30/106/115	-
18	CLA	B	814	2	-	4/27/103/115	-
24	DD6	O	214	-	-	8/26/80/80	0/3/3/3
29	A86	R	204	-	-	1/30/84/90	0/3/3/3
18	CLA	B	848	2	-	7/21/97/115	-
18	CLA	A	845	30	-	6/39/115/115	-
24	DD6	P	317	-	-	10/15/46/80	0/2/2/3
18	CLA	B	819	2	-	8/25/101/115	-
18	CLA	A	829	1	-	4/39/115/115	-
18	CLA	L	202	9	-	8/20/96/115	-
18	CLA	U	209	16	-	2/12/88/115	-
26	SQD	M	102	-	-	16/41/61/69	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	CLA	B	810	2	-	2/25/101/115	-
18	CLA	A	806	1	-	5/39/115/115	-
18	CLA	Q	211	13	-	4/10/86/115	-
24	DD6	P	314	-	-	13/26/80/80	0/3/3/3
18	CLA	A	847	1	-	9/39/115/115	-
18	CLA	A	808	1	-	5/29/105/115	-
24	DD6	P	316	-	-	14/26/80/80	0/3/3/3
18	CLA	P	308	-	-	7/24/100/115	-
18	CLA	T	208	17	-	12/39/115/115	-
28	KC1	O	210	11	-	0/15/71/71	-
20	LHG	A	839	-	-	20/52/52/53	-
18	CLA	A	821	-	-	10/39/115/115	-
18	CLA	L	204	-	-	8/21/97/115	-
18	CLA	P	310	12	-	4/21/97/115	-
18	CLA	B	835	30	-	1/39/115/115	-
18	CLA	B	831	2	-	4/39/115/115	-
18	CLA	L	203	9	-	1/39/115/115	-
18	CLA	B	826	2	-	0/21/97/115	-
18	CLA	A	828	1	-	6/39/115/115	-
18	CLA	B	830	2	-	3/31/107/115	-
18	CLA	Q	206	13	-	7/22/98/115	-
18	CLA	Q	216	30	-	14/39/115/115	-
21	BCR	A	841	-	-	7/29/63/63	0/2/2/2
18	CLA	A	835	1	-	5/39/115/115	-
18	CLA	A	825	1	-	5/39/115/115	-
18	CLA	A	823	1	-	9/39/115/115	-
18	CLA	O	208	11	-	3/33/109/115	-
21	BCR	A	842	-	-	10/29/63/63	0/2/2/2
18	CLA	U	207	-	-	8/39/115/115	-
21	BCR	L	201	-	-	11/29/63/63	0/2/2/2
18	CLA	S	201	30	-	9/39/115/115	-
18	CLA	A	810	1	-	1/26/102/115	-
18	CLA	A	833	1	-	6/39/115/115	-
18	CLA	Q	208	13	-	2/21/97/115	-
28	KC1	P	305	12	-	3/15/71/71	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	CLA	B	820	-	-	5/37/113/115	-
21	BCR	I	101	-	-	6/29/63/63	0/2/2/2
24	DD6	U	214	-	-	8/14/37/80	0/1/1/3
18	CLA	P	313	12	-	0/15/91/115	-
25	DGD	B	842	-	-	20/49/89/95	0/2/2/2
18	CLA	Q	205	13	-	7/33/109/115	-
21	BCR	F	801	-	-	8/29/63/63	0/2/2/2
27	LMG	J	102	-	-	24/34/54/70	0/1/1/1
18	CLA	B	846	2	-	7/39/115/115	-
24	DD6	U	203	-	-	15/26/80/80	0/3/3/3
20	LHG	A	840	18	-	8/31/31/53	-
18	CLA	R	202	30	-	0/15/91/115	-
18	CLA	T	211	17	-	5/17/93/115	-
18	CLA	O	207	11	-	2/17/93/115	-
18	CLA	Q	209	13	-	8/39/115/115	-
18	CLA	S	205	15	-	5/17/93/115	-
18	CLA	U	204	-	-	12/35/111/115	-
18	CLA	A	851	1	-	11/39/115/115	-
24	DD6	S	213	-	-	10/26/80/80	0/3/3/3
18	CLA	A	815	1	-	12/39/115/115	-
27	LMG	S	211	-	-	26/44/64/70	0/1/1/1
23	SF4	C	101	3	-	-	0/6/5/5
18	CLA	S	204	15	-	0/17/93/115	-
18	CLA	T	210	17	-	0/10/86/115	-
18	CLA	A	807	1	-	7/39/115/115	-
18	CLA	B	818	2	-	2/17/93/115	-
18	CLA	B	811	2	-	0/27/103/115	-
18	CLA	B	816	2	-	2/33/109/115	-
18	CLA	B	813	2	-	4/20/96/115	-
18	CLA	B	845	2	-	2/39/115/115	-
18	CLA	P	307	12	-	11/29/105/115	-
18	CLA	B	802	2	-	3/39/115/115	-
18	CLA	P	312	12	-	2/10/86/115	-
21	BCR	B	841	-	-	5/29/63/63	0/2/2/2
18	CLA	A	803	1	-	5/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	CLA	B	815	2	-	8/32/108/115	-
18	CLA	B	823	2	-	7/39/115/115	-
18	CLA	B	825	2	-	7/39/115/115	-
24	DD6	U	212	-	-	11/26/80/80	0/3/3/3
24	DD6	O	201	-	-	3/26/80/80	0/3/3/3
18	CLA	B	808	2	-	5/39/115/115	-
27	LMG	Q	217	-	-	23/50/70/70	0/1/1/1
18	CLA	S	214	30	-	1/39/115/115	-
29	A86	Q	201	-	-	24/34/90/90	0/3/3/3
18	CLA	T	212	-	-	4/18/94/115	-
18	CLA	A	814	30	-	4/15/91/115	-
18	CLA	O	211	11	-	0/10/86/115	-
18	CLA	B	805	2	-	9/39/115/115	-
21	BCR	I	102	-	-	9/29/63/63	0/2/2/2
18	CLA	P	306	12	-	9/39/115/115	-
18	CLA	U	206	16	-	4/15/91/115	-
24	DD6	O	215	-	-	12/26/80/80	0/3/3/3
18	CLA	B	821	-	-	4/38/114/115	-
21	BCR	R	203	-	-	10/27/61/63	0/2/2/2
18	CLA	A	853	30	-	2/39/115/115	-
18	CLA	P	309	30	-	2/18/94/115	-
18	CLA	A	838	20	-	5/24/100/115	-
24	DD6	S	202	-	-	8/26/80/80	0/3/3/3
18	CLA	A	827	1	-	2/21/97/115	-
24	DD6	J	101	-	-	6/26/80/80	0/3/3/3
23	SF4	C	102	3	-	-	0/6/5/5
24	DD6	Q	215	-	-	8/26/80/80	0/3/3/3
21	BCR	F	804	-	-	9/29/63/63	0/2/2/2
18	CLA	A	849	1	-	7/39/115/115	-
28	KC1	T	209	17	-	2/15/71/71	-
18	CLA	B	817	-	-	7/39/115/115	-
18	CLA	S	207	15	-	5/24/100/115	-
18	CLA	B	803	-	-	6/39/115/115	-
21	BCR	M	101	-	-	4/29/63/63	0/2/2/2
18	CLA	A	817	1	-	0/15/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	CLA	O	209	11	-	12/39/115/115	-
18	CLA	O	202	11	-	2/13/89/115	-
24	DD6	P	304	-	-	8/26/80/80	0/3/3/3
28	KC1	S	208	15	-	1/15/71/71	-
18	CLA	S	206	15	-	2/15/91/115	-
24	DD6	T	214	-	-	12/26/80/80	0/3/3/3
18	CLA	U	205	16	-	8/39/115/115	-
18	CLA	A	804	1	-	12/39/115/115	-
24	DD6	Q	202	-	-	6/26/80/80	0/3/3/3
18	CLA	T	204	17	-	4/17/93/115	-
19	PQN	A	837	-	-	7/23/43/43	0/2/2/2
18	CLA	T	203	17	-	2/10/86/115	-
21	BCR	A	843	-	-	4/29/63/63	0/2/2/2
24	DD6	O	212	-	-	11/26/80/80	0/3/3/3
29	A86	T	201	-	-	18/34/90/90	0/3/3/3
21	BCR	B	839	-	-	4/29/63/63	0/2/2/2
18	CLA	A	836	30	-	3/39/115/115	-
18	CLA	A	834	1	-	9/39/115/115	-
18	CLA	A	824	1	-	6/36/112/115	-
18	CLA	B	804	2	-	4/15/91/115	-
24	DD6	A	854	-	-	13/26/80/80	0/3/3/3
21	BCR	B	837	-	-	9/29/63/63	0/2/2/2
24	DD6	S	209	-	-	6/26/80/80	0/3/3/3
24	DD6	S	212	-	-	16/26/80/80	0/3/3/3
18	CLA	A	811	1	-	6/39/115/115	-
18	CLA	T	206	-	-	5/17/93/115	-
18	CLA	U	211	16	-	3/24/100/115	-
18	CLA	U	208	16	-	2/17/93/115	-
18	CLA	A	805	1	-	2/20/96/115	-
21	BCR	B	838	-	-	7/29/63/63	0/2/2/2
29	A86	Q	214	-	-	8/34/90/90	0/3/3/3
18	CLA	O	204	11	-	5/39/115/115	-
18	CLA	B	801	-	-	1/39/115/115	-
18	CLA	A	822	30	-	2/39/115/115	-
18	CLA	O	203	-	-	1/15/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	CLA	A	801	-	-	6/39/115/115	-
27	LMG	P	301	-	-	12/29/49/70	0/1/1/1
28	KC1	P	311	12	-	4/12/68/71	-
27	LMG	B	849	-	-	8/19/39/70	0/1/1/1
18	CLA	B	827	2	-	3/20/96/115	-
18	CLA	J	103	8	-	3/12/88/115	-
18	CLA	B	824	2	-	9/39/115/115	-
18	CLA	B	822	2	-	0/39/115/115	-
18	CLA	P	315	12	-	1/18/94/115	-
18	CLA	Q	203	13	-	5/19/95/115	-
18	CLA	B	806	2	-	8/39/115/115	-
26	SQD	B	847	-	-	23/45/65/69	0/1/1/1
28	KC1	S	210	15	-	4/15/71/71	-
18	CLA	O	206	-	-	1/39/115/115	-
21	BCR	A	844	-	-	9/29/63/63	0/2/2/2
29	A86	R	206	-	-	4/34/90/90	0/3/3/3
18	CLA	T	205	-	-	11/30/106/115	-
18	CLA	A	831	1	-	2/15/91/115	-
18	CLA	B	828	2	-	3/31/107/115	-
18	CLA	B	807	2	-	2/39/115/115	-
18	CLA	A	819	1	-	1/13/89/115	-
18	CLA	A	852	1	-	4/39/115/115	-
18	CLA	F	802	30	-	5/19/95/115	-
18	CLA	B	844	2	-	2/39/115/115	-
18	CLA	B	832	2	-	2/18/94/115	-
18	CLA	B	809	2	-	9/39/115/115	-
21	BCR	L	205	-	-	8/29/63/63	0/2/2/2
18	CLA	A	832	1	-	0/23/99/115	-
18	CLA	A	809	1	-	2/36/112/115	-
28	KC1	Q	210	13	-	2/15/71/71	-
18	CLA	B	812	2	-	2/26/102/115	-
18	CLA	A	813	1	-	2/21/97/115	-
20	LHG	R	201	-	-	31/53/53/53	-
18	CLA	B	829	30	-	1/39/115/115	-
18	CLA	R	205	14	-	11/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	A86	P	303	-	-	14/34/90/90	0/3/3/3
18	CLA	A	802	1	-	3/27/103/115	-
27	LMG	U	201	-	-	17/27/47/70	0/1/1/1
29	A86	U	202	-	-	14/34/90/90	0/3/3/3
18	CLA	U	210	16	-	8/39/115/115	-
18	CLA	T	207	17	-	1/12/88/115	-
24	DD6	T	213	-	-	12/26/80/80	0/3/3/3
22	CL0	A	848	1	-	1/39/115/115	-
24	DD6	O	213	-	-	5/26/80/80	0/3/3/3
18	CLA	S	215	15	-	4/39/115/115	-
18	CLA	A	830	1	-	0/21/97/115	-
18	CLA	F	803	6	-	4/17/93/115	-
18	CLA	O	205	11	-	6/39/115/115	-
18	CLA	A	818	30	-	3/39/115/115	-
18	CLA	B	833	-	-	5/39/115/115	-
19	PQN	B	836	-	-	1/23/43/43	0/2/2/2
18	CLA	A	812	1	-	1/15/91/115	-
28	KC1	P	302	12	-	1/15/71/71	-
18	CLA	A	816	1	-	2/39/115/115	-

The worst 5 of 1468 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	Q	214	A86	C13-C11	-6.67	1.36	1.49
29	T	201	A86	C13-C11	-6.53	1.37	1.49
29	U	202	A86	C13-C11	-6.42	1.37	1.49
29	R	206	A86	C13-C11	-6.40	1.37	1.49
29	P	303	A86	C13-C11	-6.37	1.37	1.49

The worst 5 of 1224 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	B	824	CLA	C1-O2A-CGA	7.98	137.38	116.44
24	U	212	DD6	C3-C4-C5	7.17	138.16	123.47
18	B	824	CLA	C5-C3-C2	6.10	133.46	121.12
24	P	317	DD6	C3-C4-C5	5.90	131.04	123.25
24	S	203	DD6	C3-C4-C5	5.84	135.44	123.47

There are no chirality outliers.

5 of 1386 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
18	A	804	CLA	C1A-C2A-CAA-CBA
18	A	804	CLA	C3A-C2A-CAA-CBA
18	A	806	CLA	CHA-CBD-CGD-O2D
18	A	808	CLA	CBA-CGA-O2A-C1
18	A	815	CLA	C1A-C2A-CAA-CBA

There are no ring outliers.

151 monomers are involved in 253 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
21	B	840	BCR	1	0
18	B	834	CLA	3	0
21	J	104	BCR	1	0
18	A	820	CLA	1	0
18	Q	212	CLA	1	0
18	T	202	CLA	2	0
18	Q	207	CLA	1	0
18	A	826	CLA	2	0
18	A	846	CLA	1	0
18	B	843	CLA	3	0
29	R	204	A86	1	0
18	B	848	CLA	3	0
18	A	845	CLA	3	0
18	B	819	CLA	5	0
18	L	202	CLA	2	0
18	U	209	CLA	1	0
26	M	102	SQD	3	0
18	B	810	CLA	1	0
18	A	847	CLA	3	0
18	A	808	CLA	1	0
18	T	208	CLA	3	0
28	O	210	KC1	1	0
20	A	839	LHG	1	0
18	A	821	CLA	1	0
18	B	835	CLA	8	0
18	B	831	CLA	3	0
18	L	203	CLA	2	0
18	A	828	CLA	2	0
18	B	830	CLA	2	0
18	Q	206	CLA	2	0
18	Q	216	CLA	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
21	A	841	BCR	1	0
18	A	835	CLA	3	0
18	A	825	CLA	1	0
18	A	823	CLA	3	0
18	O	208	CLA	2	0
21	A	842	BCR	1	0
18	U	207	CLA	3	0
21	L	201	BCR	2	0
18	S	201	CLA	4	0
18	A	810	CLA	1	0
18	A	833	CLA	5	0
18	Q	208	CLA	5	0
18	B	820	CLA	3	0
21	I	101	BCR	2	0
18	P	313	CLA	1	0
25	B	842	DGD	5	0
18	Q	205	CLA	1	0
21	F	801	BCR	1	0
27	J	102	LMG	2	0
18	B	846	CLA	7	0
20	A	840	LHG	1	0
18	R	202	CLA	1	0
18	T	211	CLA	2	0
18	O	207	CLA	2	0
18	Q	209	CLA	1	0
18	A	851	CLA	1	0
18	A	815	CLA	2	0
27	S	211	LMG	6	0
18	S	204	CLA	2	0
18	T	210	CLA	1	0
18	A	807	CLA	2	0
18	B	818	CLA	1	0
18	B	816	CLA	2	0
18	B	845	CLA	1	0
18	P	307	CLA	1	0
18	B	802	CLA	2	0
21	B	841	BCR	2	0
18	A	803	CLA	2	0
18	B	815	CLA	3	0
18	B	825	CLA	1	0
18	B	808	CLA	4	0
27	Q	217	LMG	6	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	S	214	CLA	4	0
18	T	212	CLA	1	0
18	A	814	CLA	2	0
21	I	102	BCR	2	0
18	P	306	CLA	1	0
18	U	206	CLA	2	0
18	B	821	CLA	4	0
21	R	203	BCR	3	0
18	A	853	CLA	2	0
18	A	838	CLA	1	0
21	F	804	BCR	3	0
18	A	849	CLA	1	0
28	T	209	KC1	2	0
18	B	817	CLA	2	0
18	S	207	CLA	2	0
18	B	803	CLA	3	0
21	M	101	BCR	4	0
18	A	817	CLA	1	0
18	O	209	CLA	2	0
18	O	202	CLA	2	0
24	P	304	DD6	1	0
18	S	206	CLA	2	0
18	U	205	CLA	1	0
18	A	804	CLA	1	0
19	A	837	PQN	2	0
21	A	843	BCR	2	0
21	B	839	BCR	1	0
18	A	836	CLA	2	0
18	A	834	CLA	3	0
18	A	824	CLA	3	0
21	B	837	BCR	2	0
18	A	811	CLA	2	0
18	U	211	CLA	3	0
18	U	208	CLA	1	0
21	B	838	BCR	1	0
18	O	204	CLA	1	0
18	B	801	CLA	1	0
18	A	822	CLA	1	0
18	O	203	CLA	1	0
18	A	801	CLA	4	0
27	P	301	LMG	1	0
27	B	849	LMG	2	0

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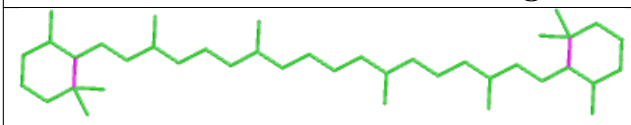
Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	B	827	CLA	4	0
18	J	103	CLA	2	0
18	B	824	CLA	3	0
18	B	822	CLA	1	0
18	P	315	CLA	1	0
18	Q	203	CLA	1	0
18	B	806	CLA	1	0
26	B	847	SQD	3	0
18	O	206	CLA	1	0
21	A	844	BCR	1	0
29	R	206	A86	1	0
18	T	205	CLA	2	0
18	A	831	CLA	2	0
18	B	828	CLA	1	0
18	B	807	CLA	4	0
18	A	852	CLA	4	0
18	B	844	CLA	2	0
21	L	205	BCR	4	0
18	B	812	CLA	1	0
18	A	813	CLA	1	0
20	R	201	LHG	2	0
18	B	829	CLA	2	0
18	R	205	CLA	3	0
27	U	201	LMG	2	0
29	U	202	A86	1	0
18	U	210	CLA	4	0
18	T	207	CLA	2	0
22	A	848	CL0	3	0
18	S	215	CLA	2	0
18	A	830	CLA	1	0
18	F	803	CLA	1	0
18	O	205	CLA	2	0
18	A	818	CLA	2	0
18	B	833	CLA	2	0
19	B	836	PQN	1	0
18	A	816	CLA	2	0

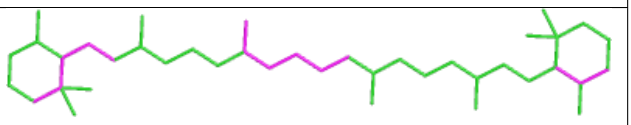
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

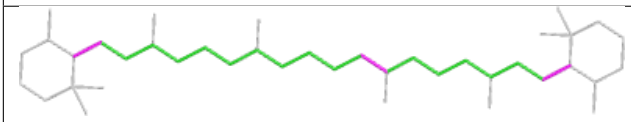
Ligand BCR B 840



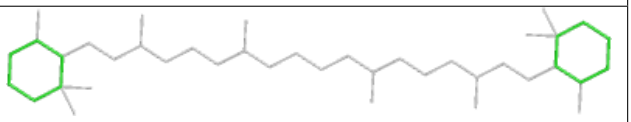
Bond lengths



Bond angles

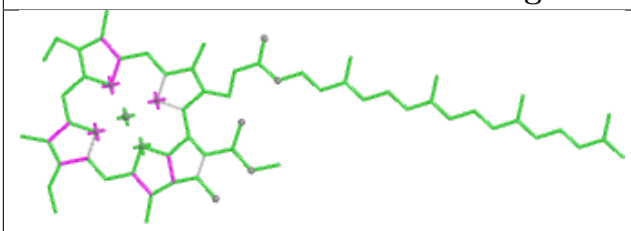


Torsions

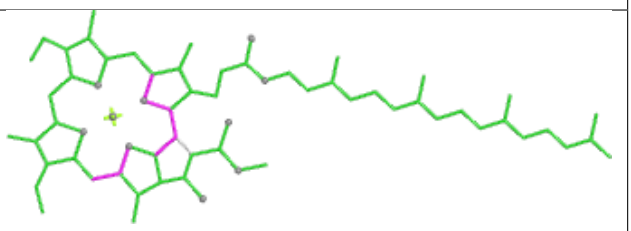


Rings

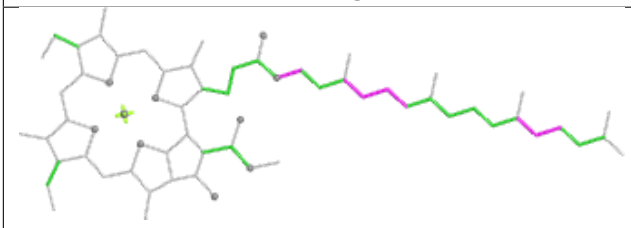
Ligand CLA B 834



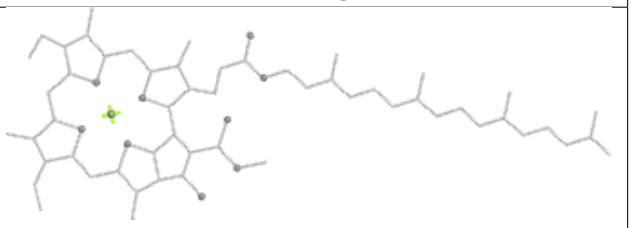
Bond lengths



Bond angles

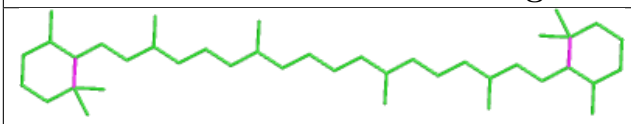


Torsions

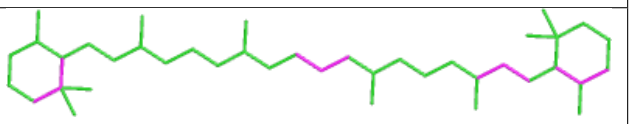


Rings

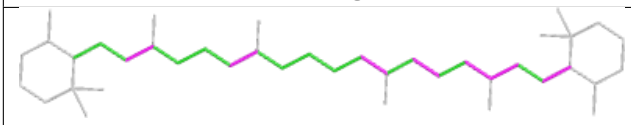
Ligand BCR J 104



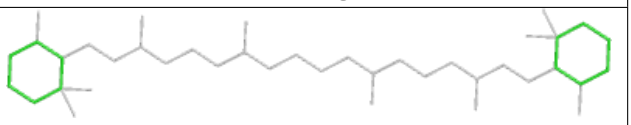
Bond lengths



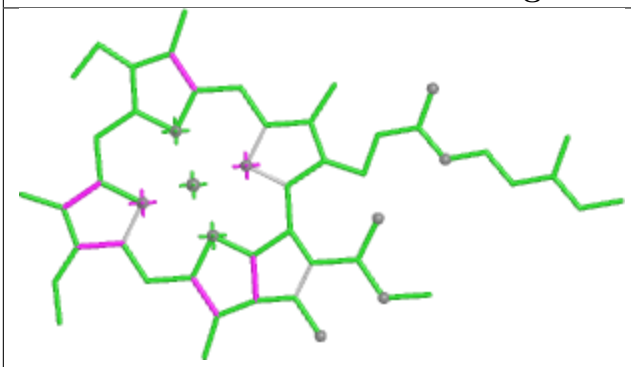
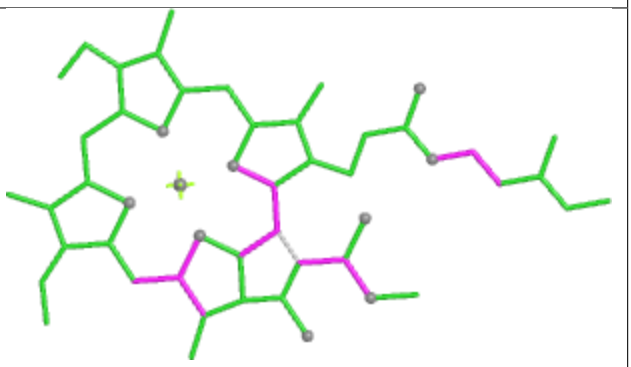
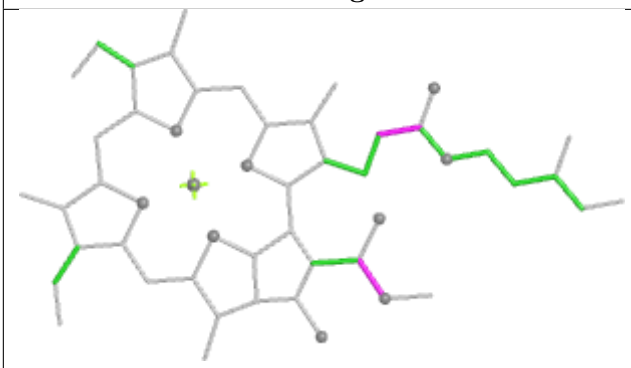
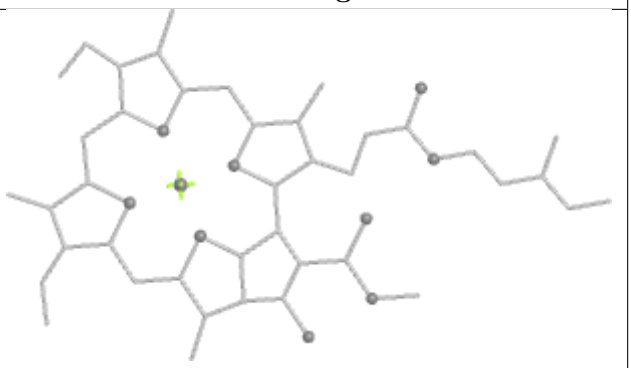
Bond angles

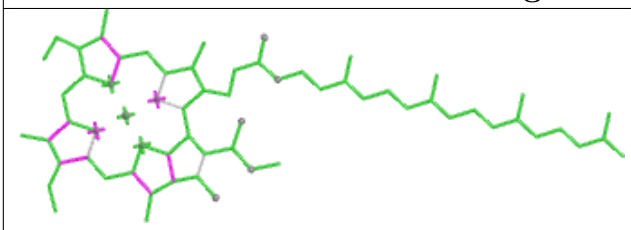
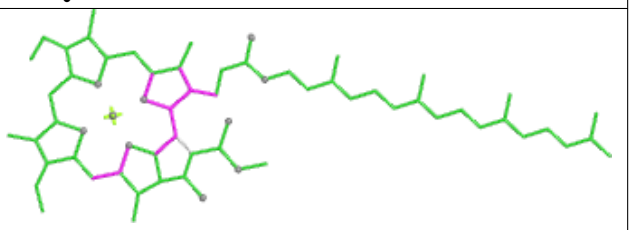
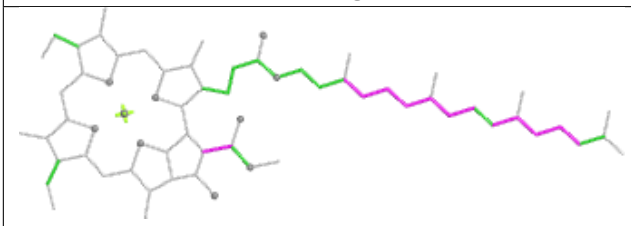
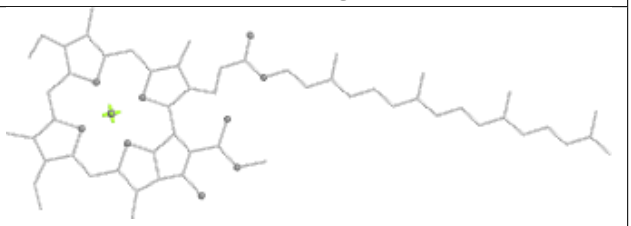


Torsions

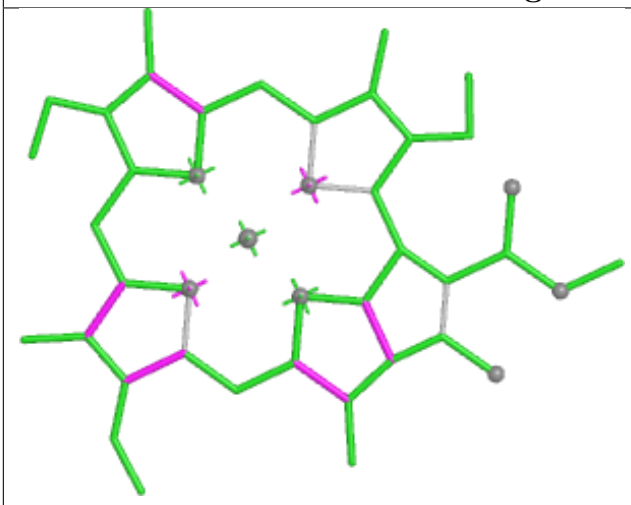


Rings

Ligand CLA A 820	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA Q 212	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA T 202



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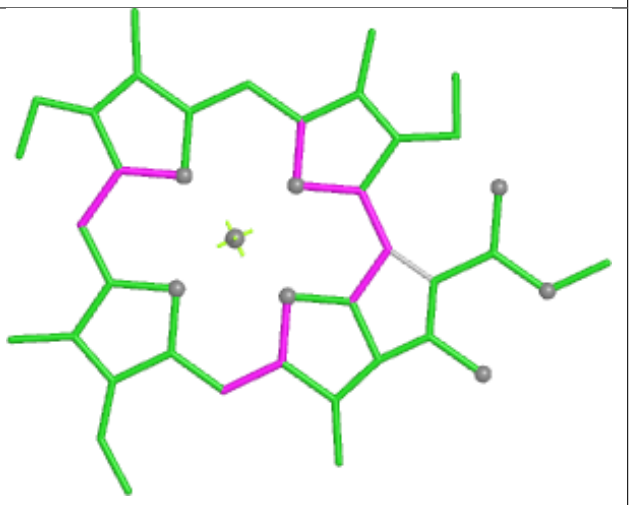
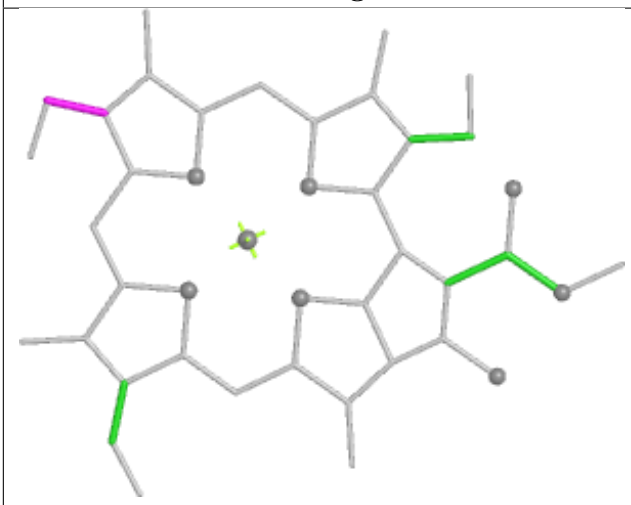


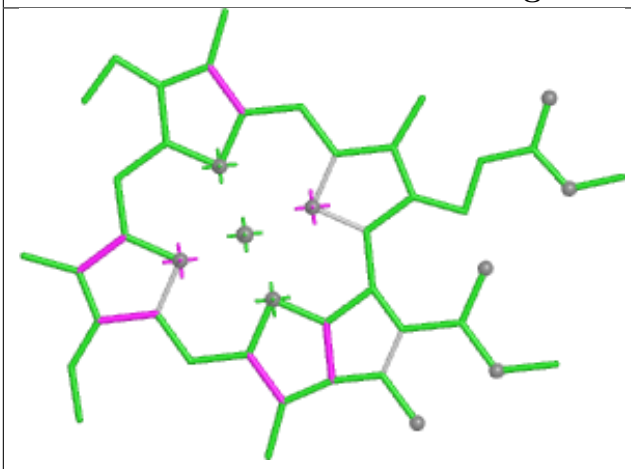
Bond angles



Torsions

Rings

Ligand CLA Q 207



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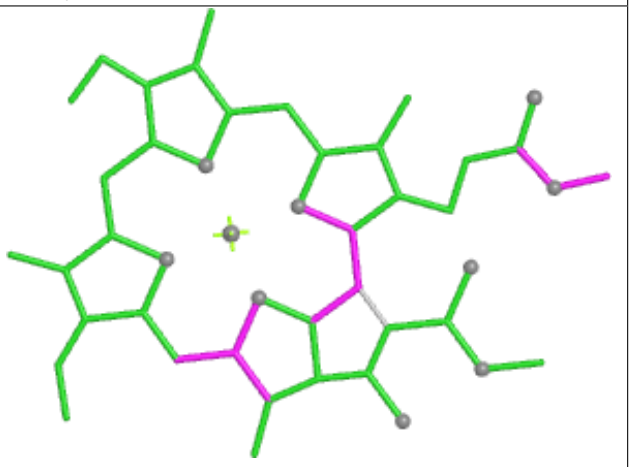

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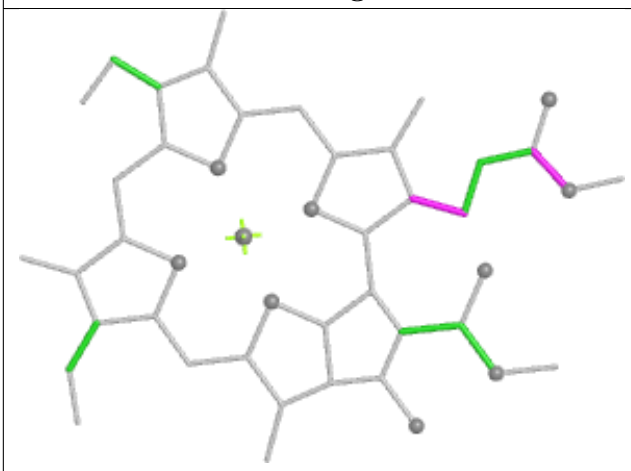

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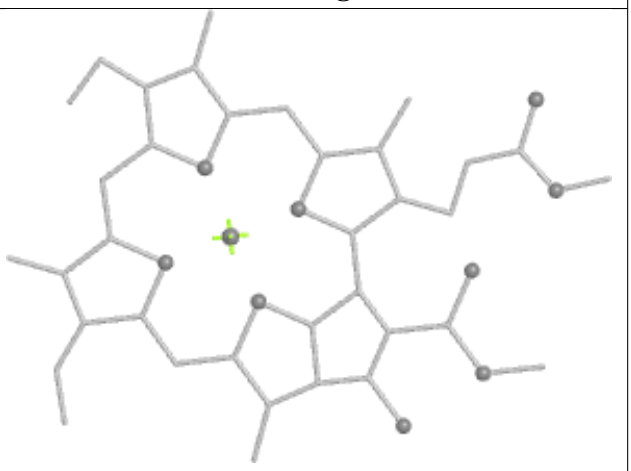
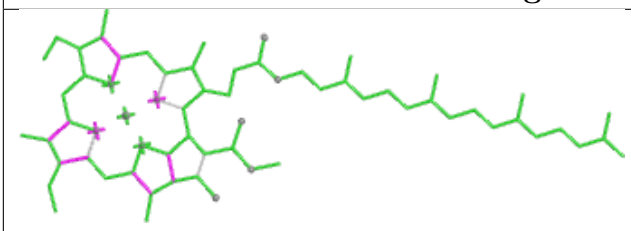


Rings

Ligand CLA A 826



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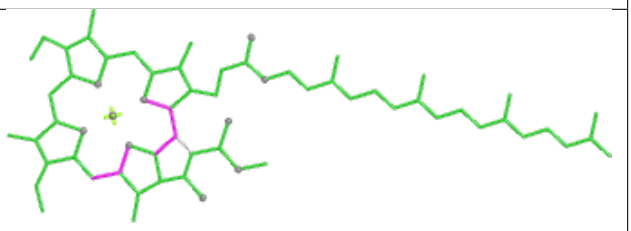

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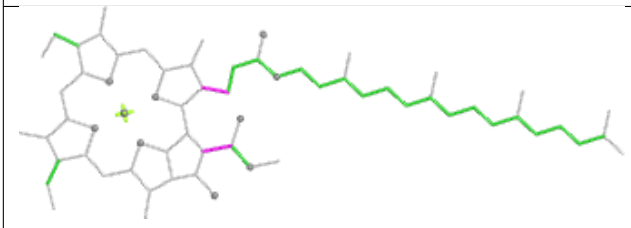

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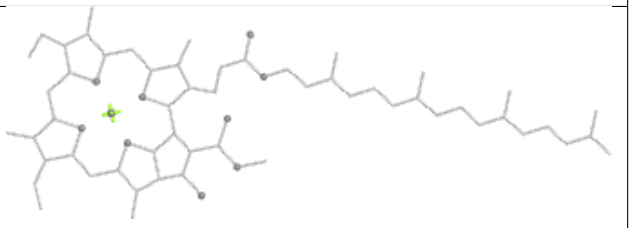
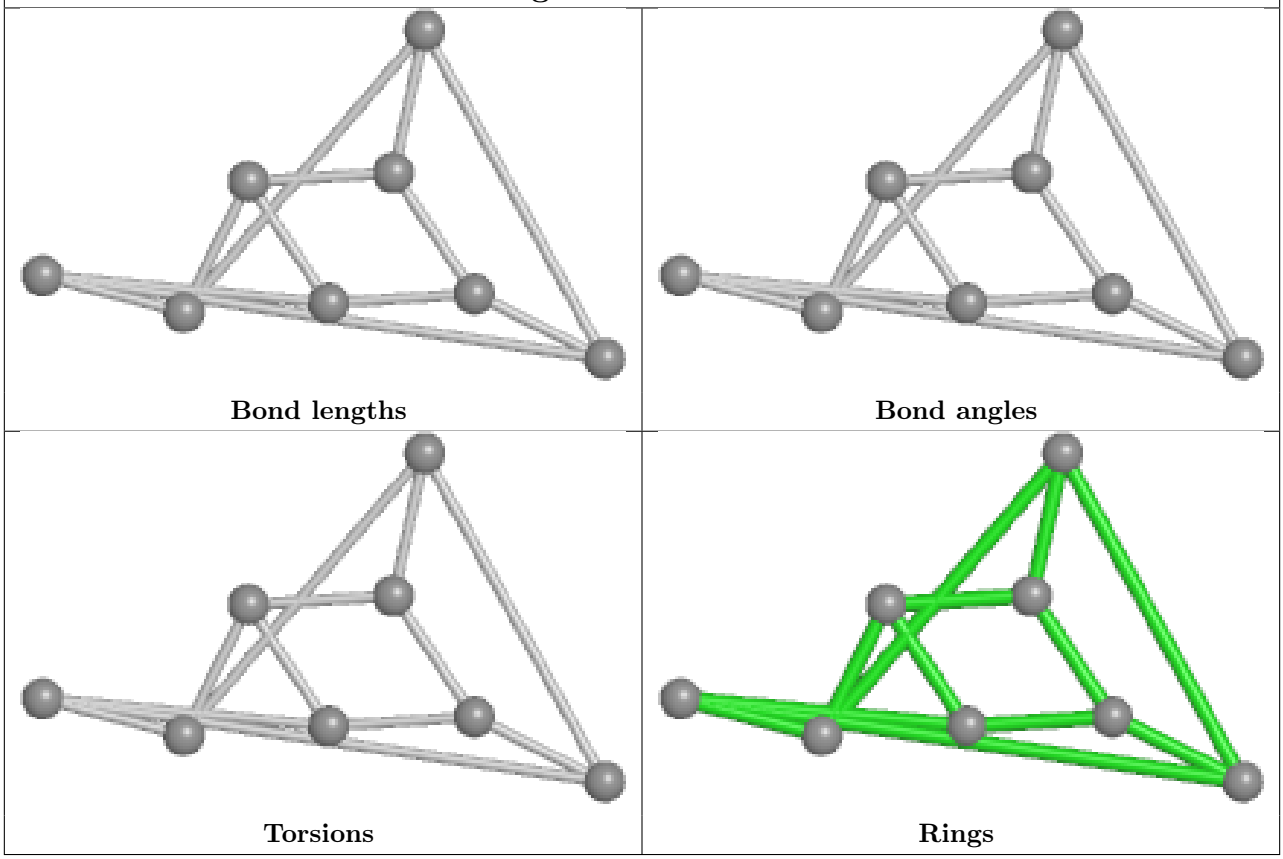
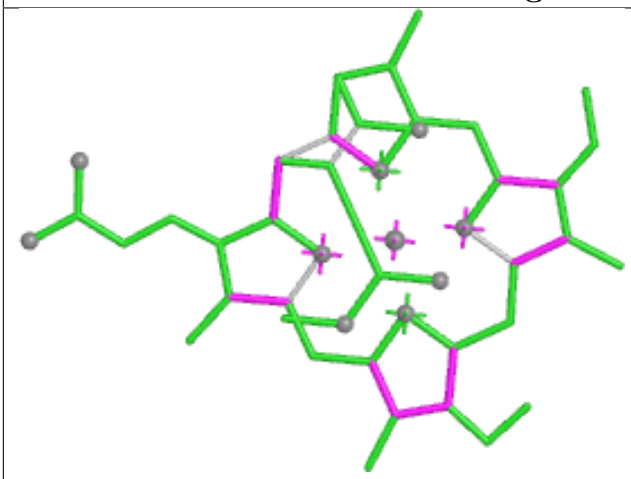


Rings

Ligand SF4 A 850



Ligand KC1 U 213



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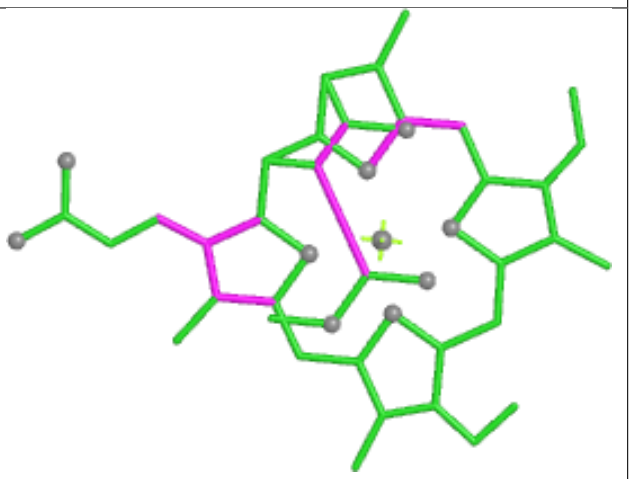
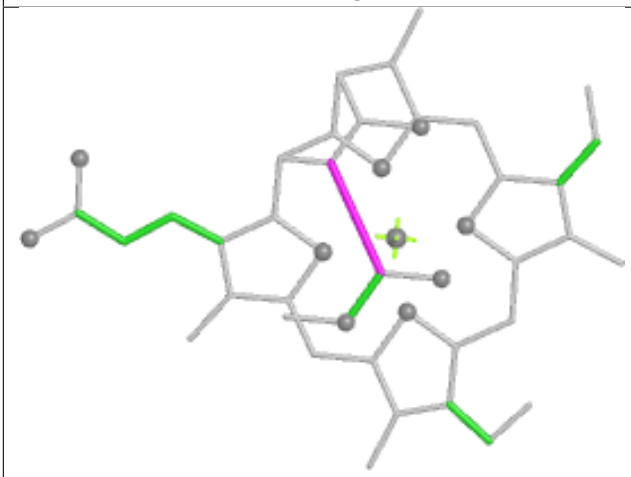


Bond angles



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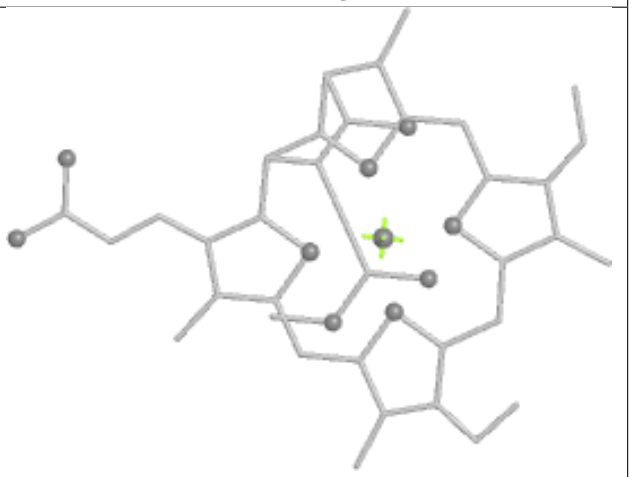
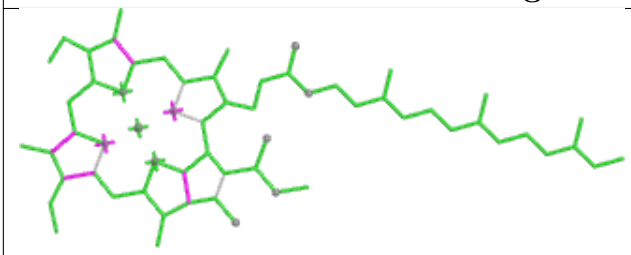


Rings

Ligand CLA Q 204



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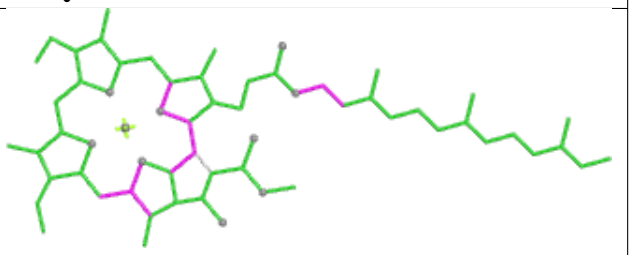
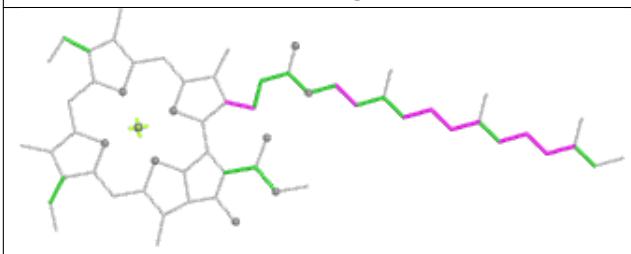


Bond angles



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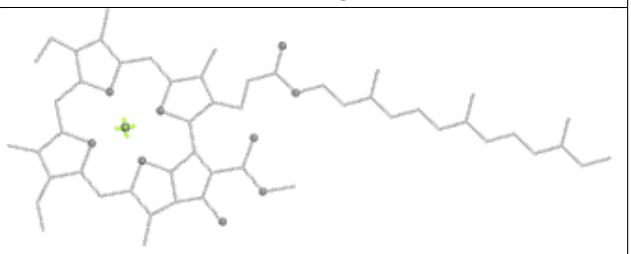
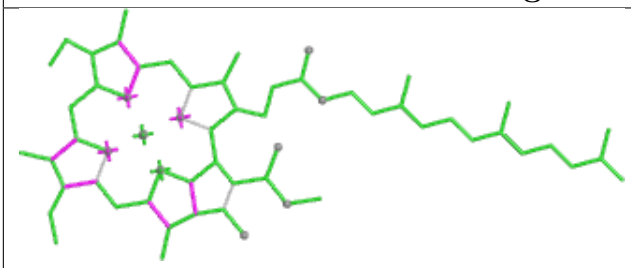
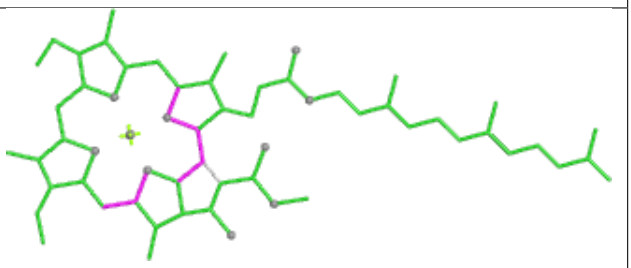
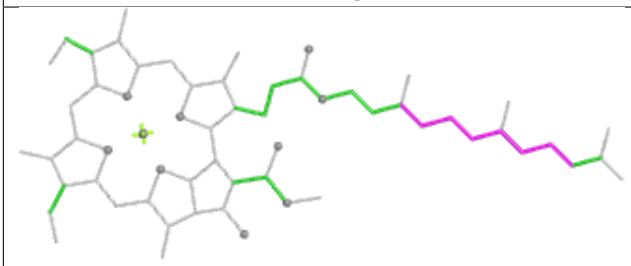
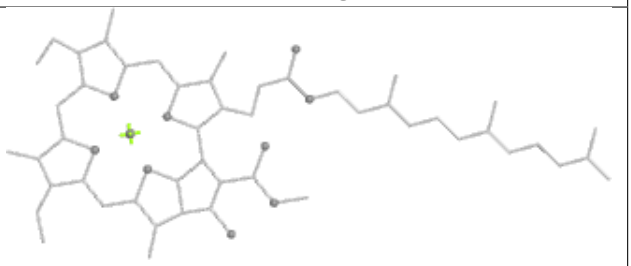
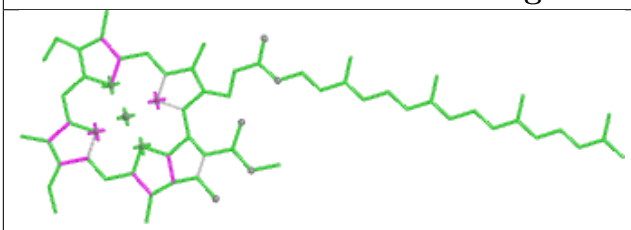
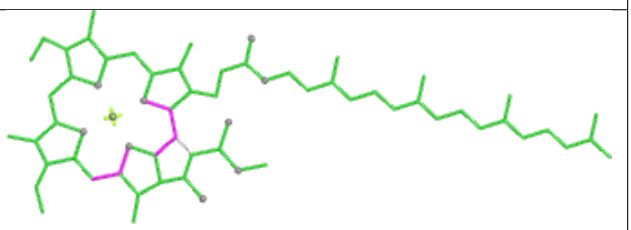
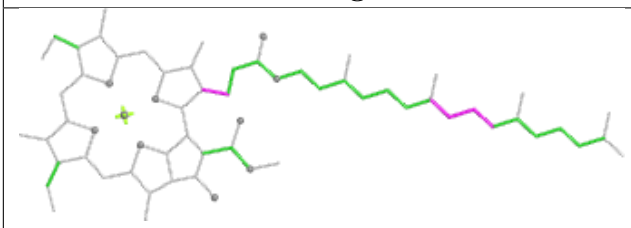
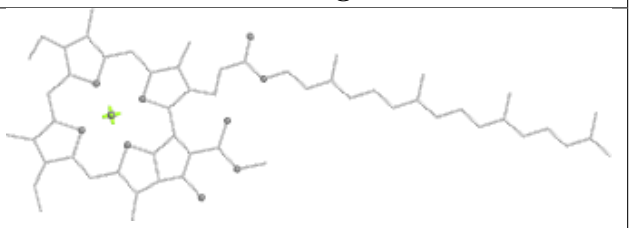
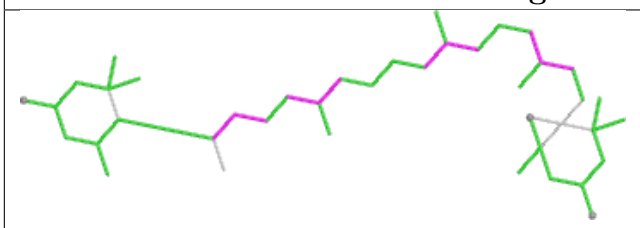
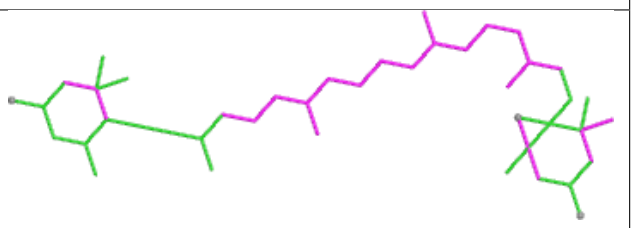
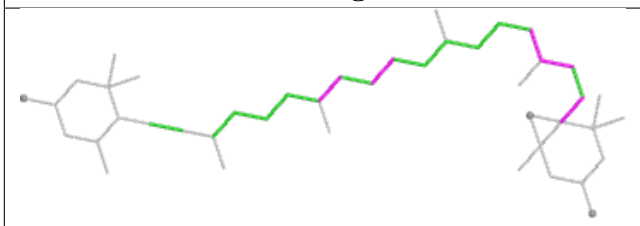
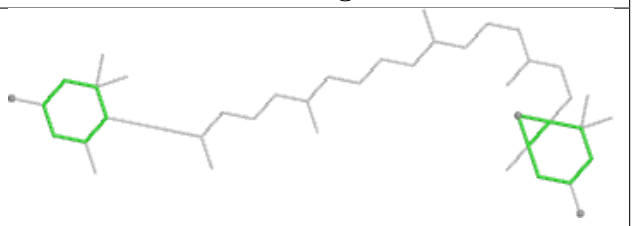


Rings

Ligand CLA A 846	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA B 843	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand DD6 S 203	
 Bond lengths	 Bond angles
 Torsions	 Rings

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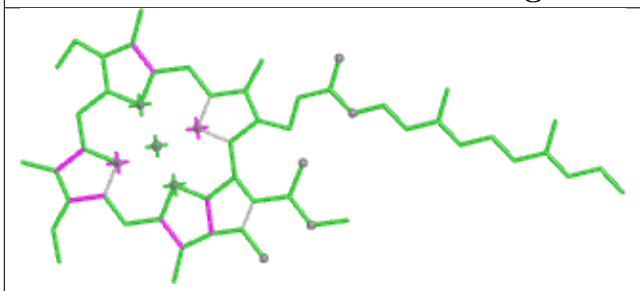
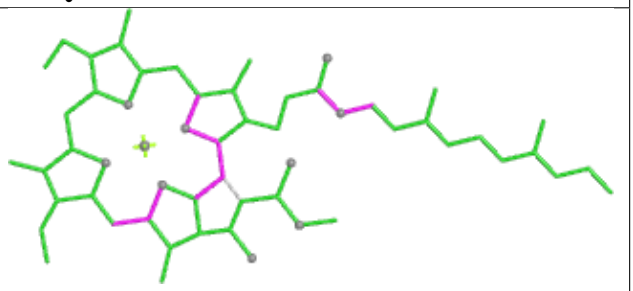
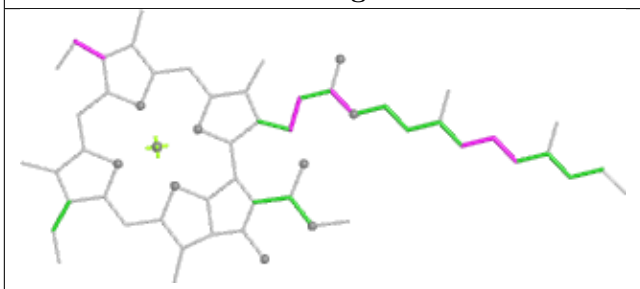
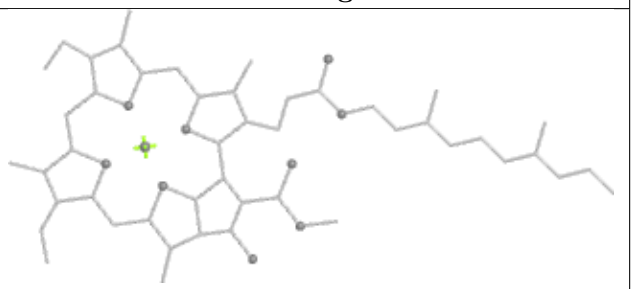
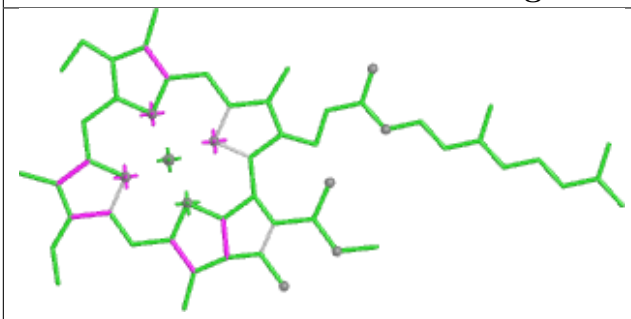
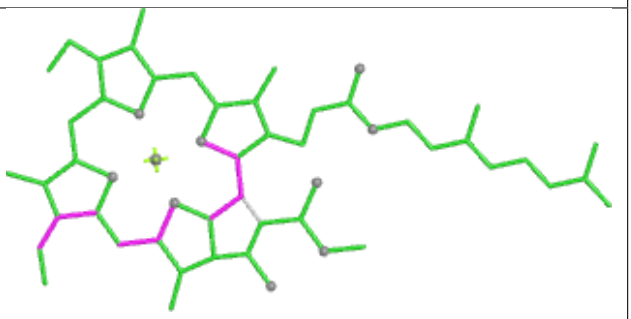
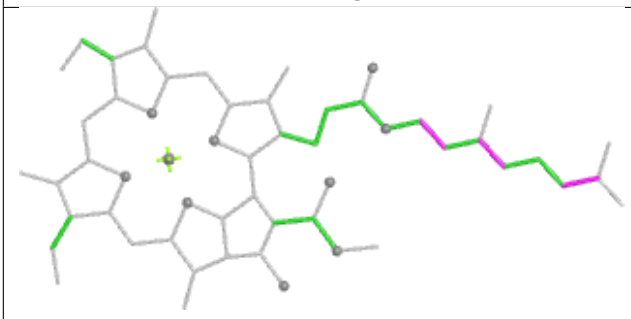
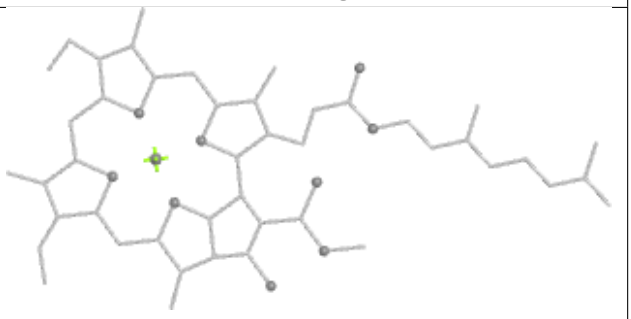
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA B 814	
 Bond lengths	 Bond angles
 Torsions	 Rings

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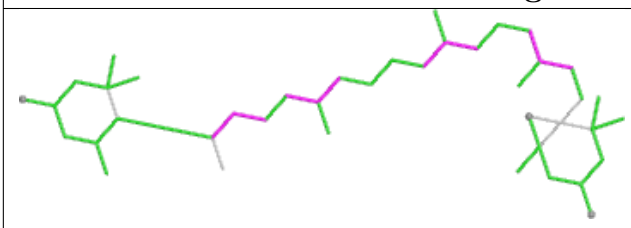
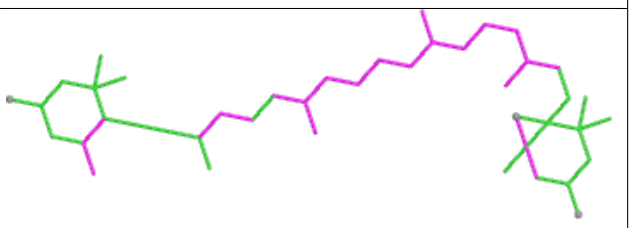
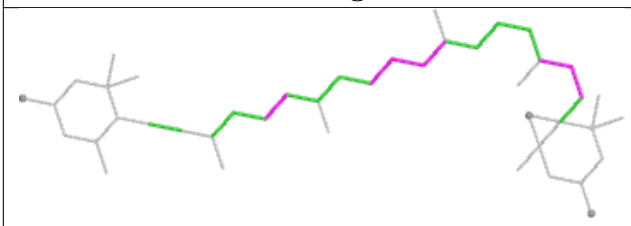
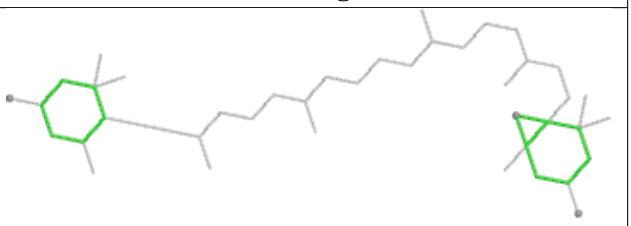
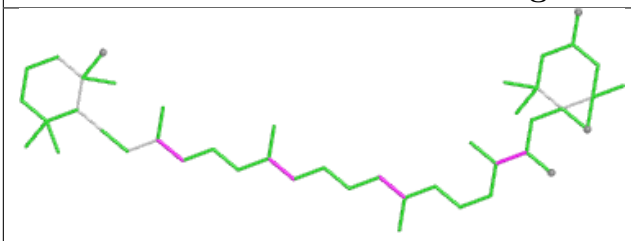
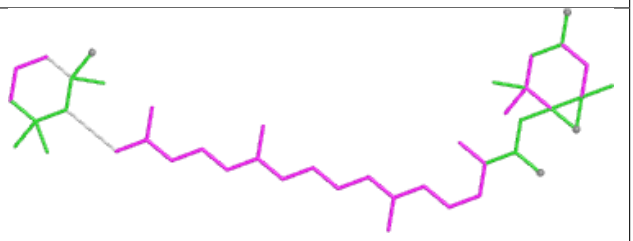
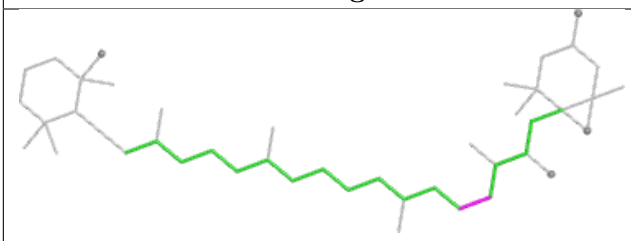
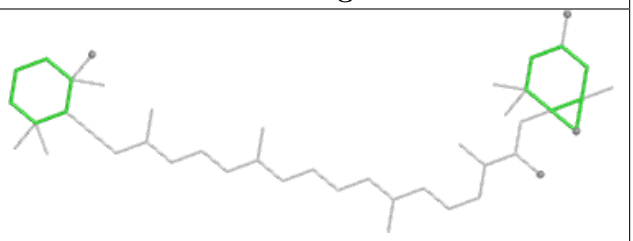
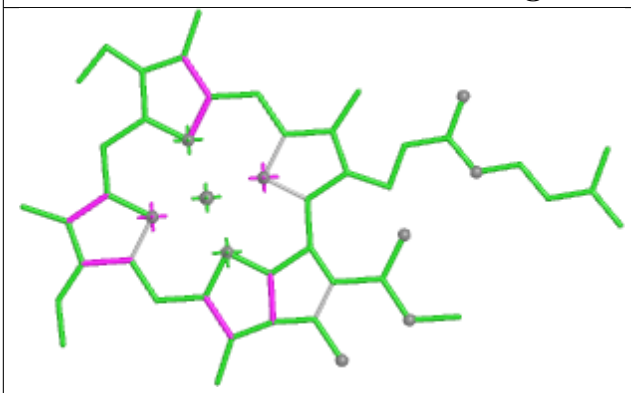
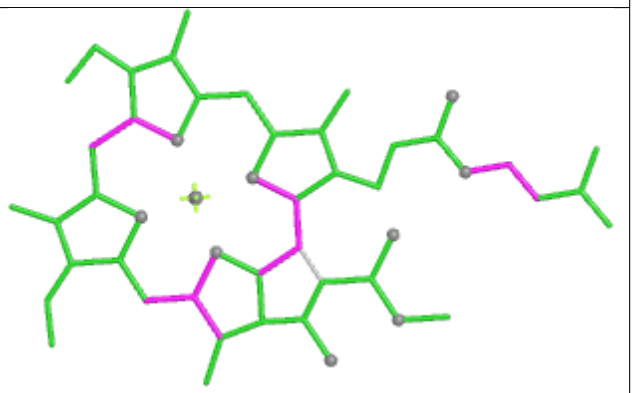
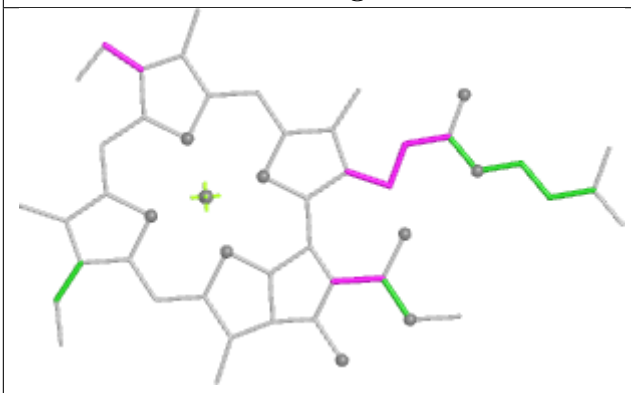
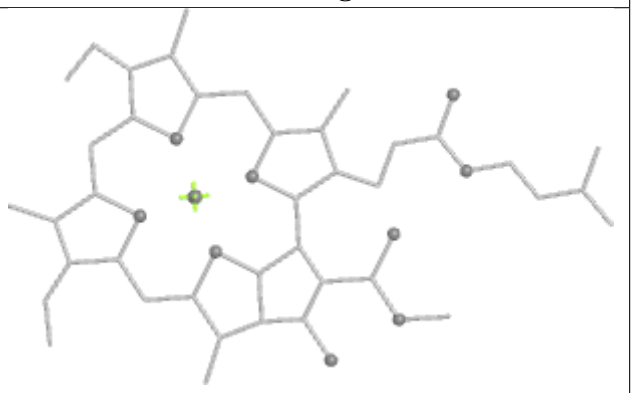
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand A86 R 204	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA B 848	
 Bond lengths	 Bond angles
 Torsions	 Rings

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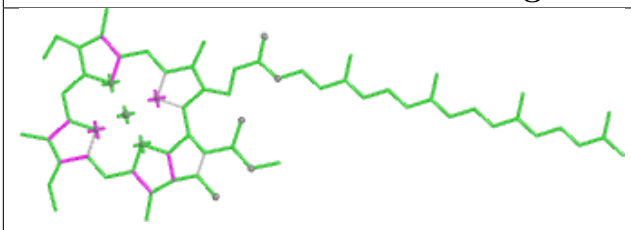
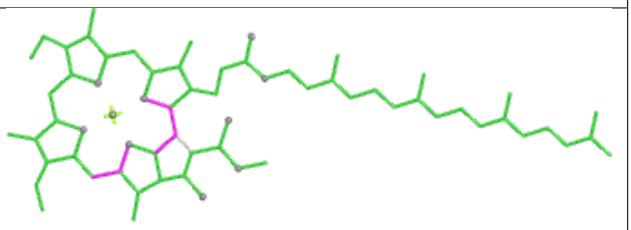
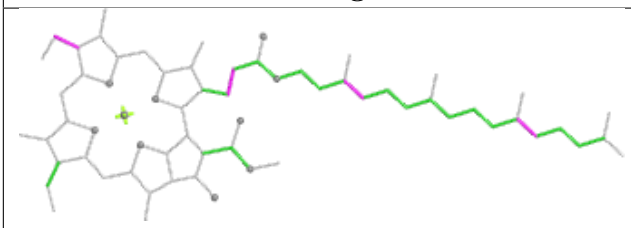
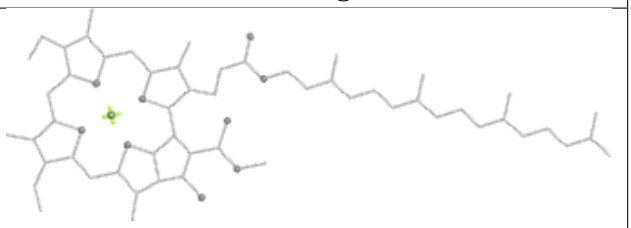
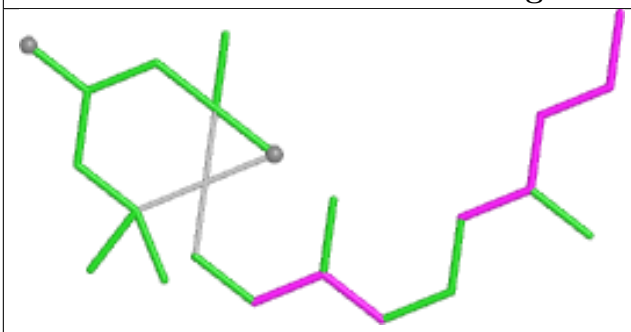
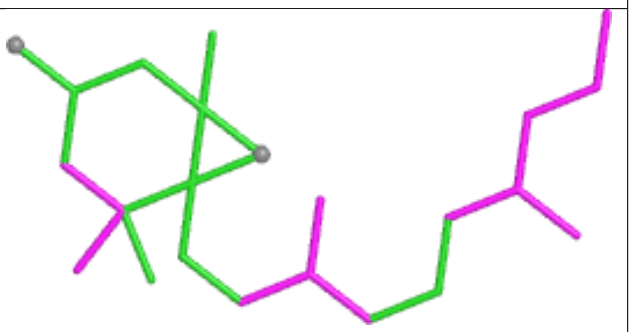
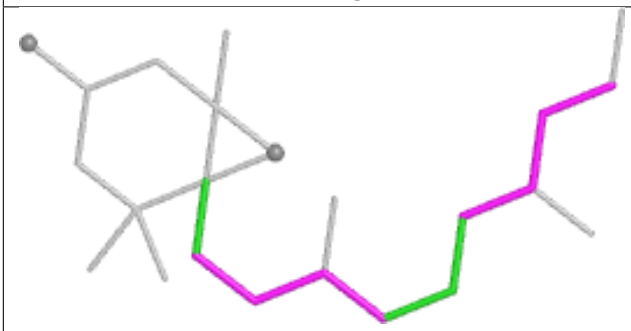
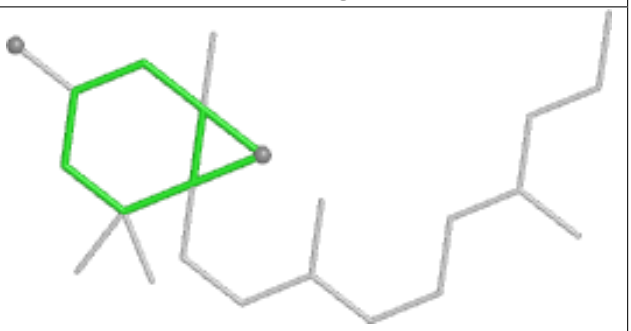
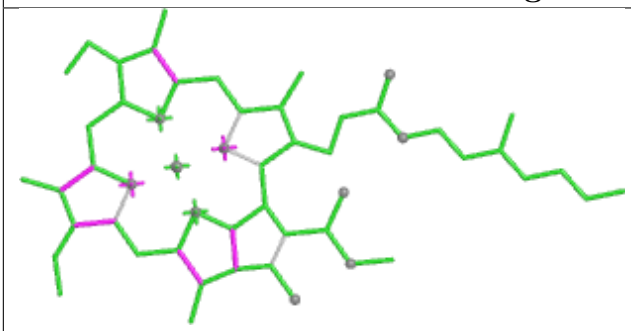
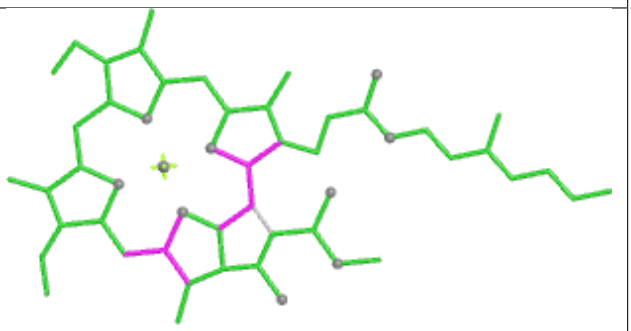
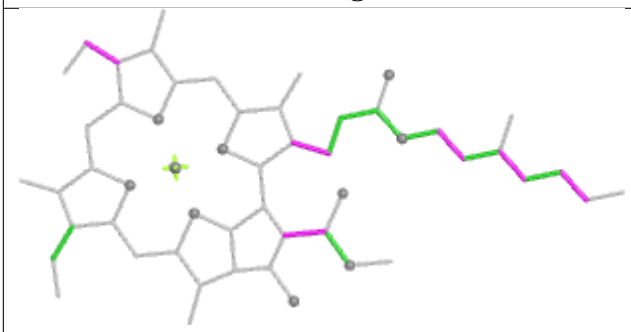
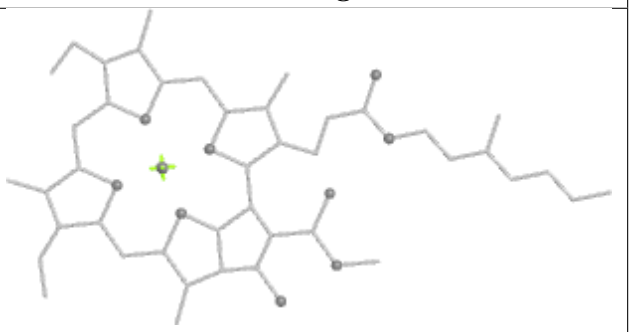
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand DD6 P 317	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA B 819	
 Bond lengths	 Bond angles
 Torsions	 Rings

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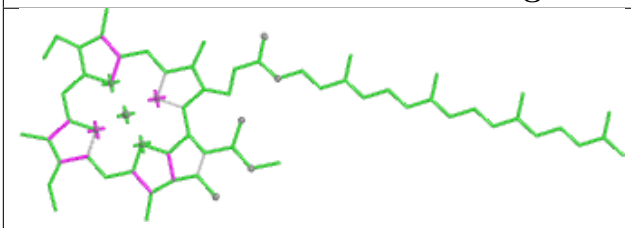
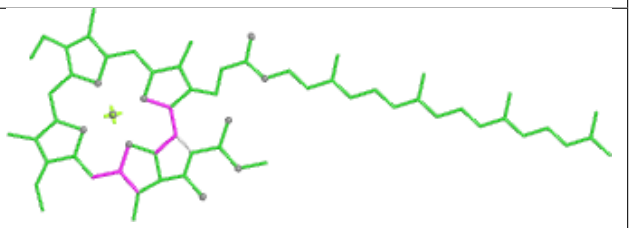
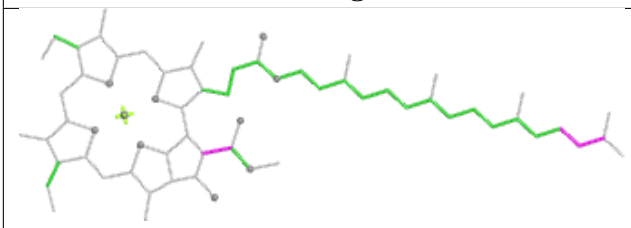
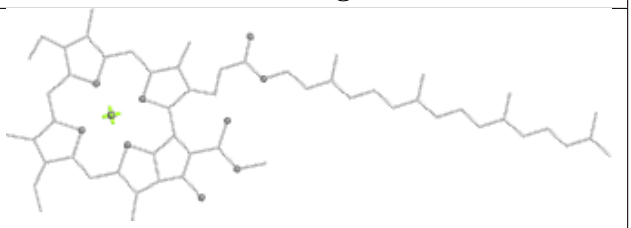
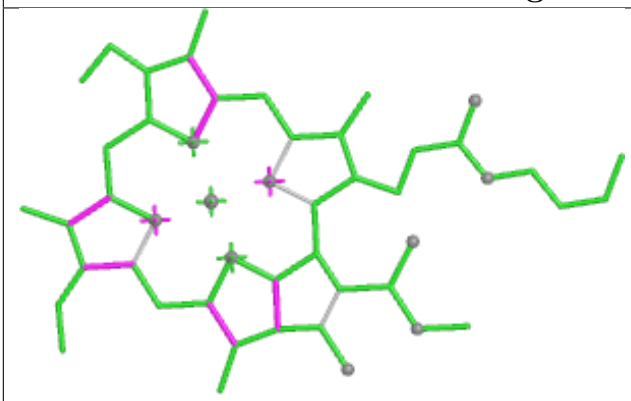
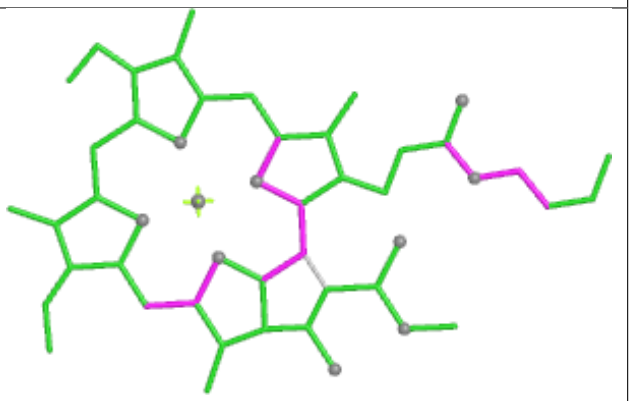
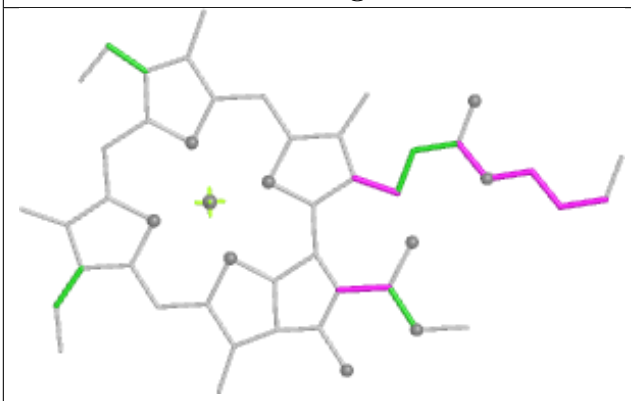
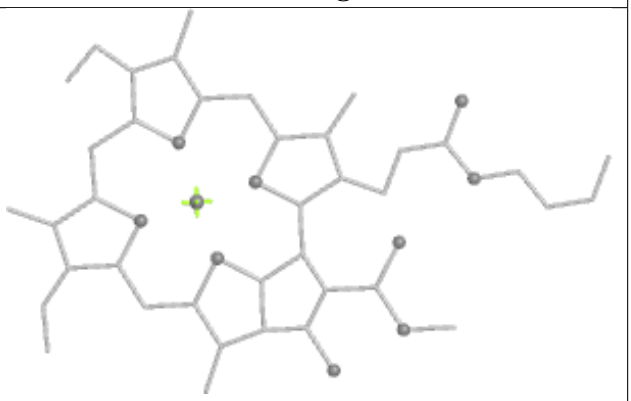
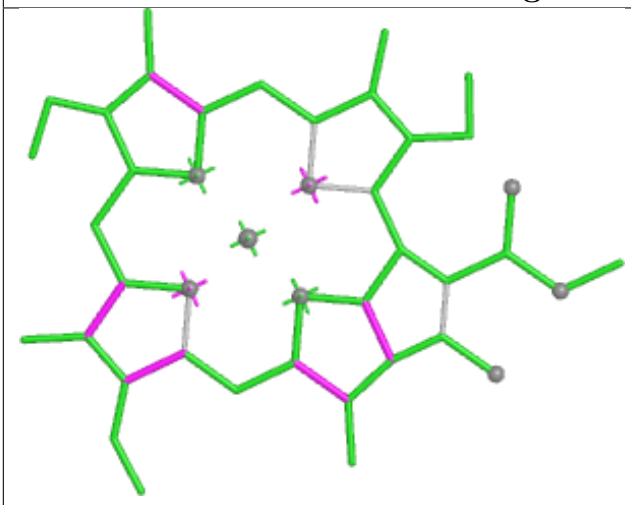
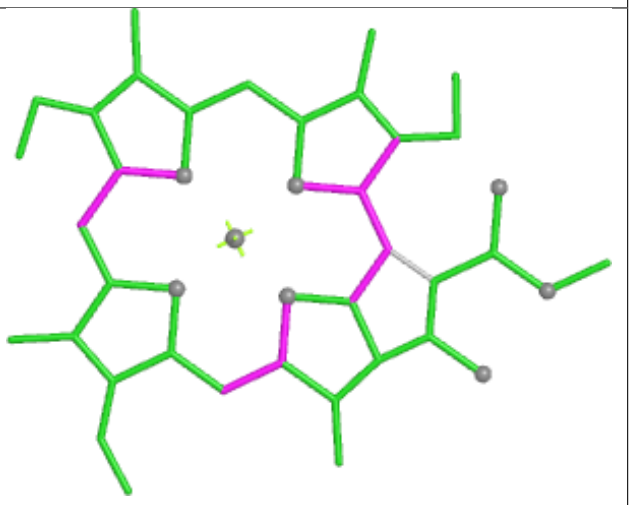
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA L 202	
 Bond lengths	 Bond angles
 Torsions	 Rings

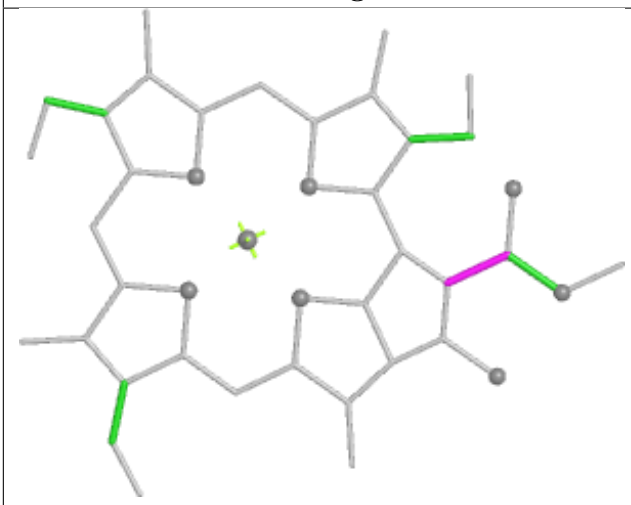
Ligand CLA U 209



Bond lengths



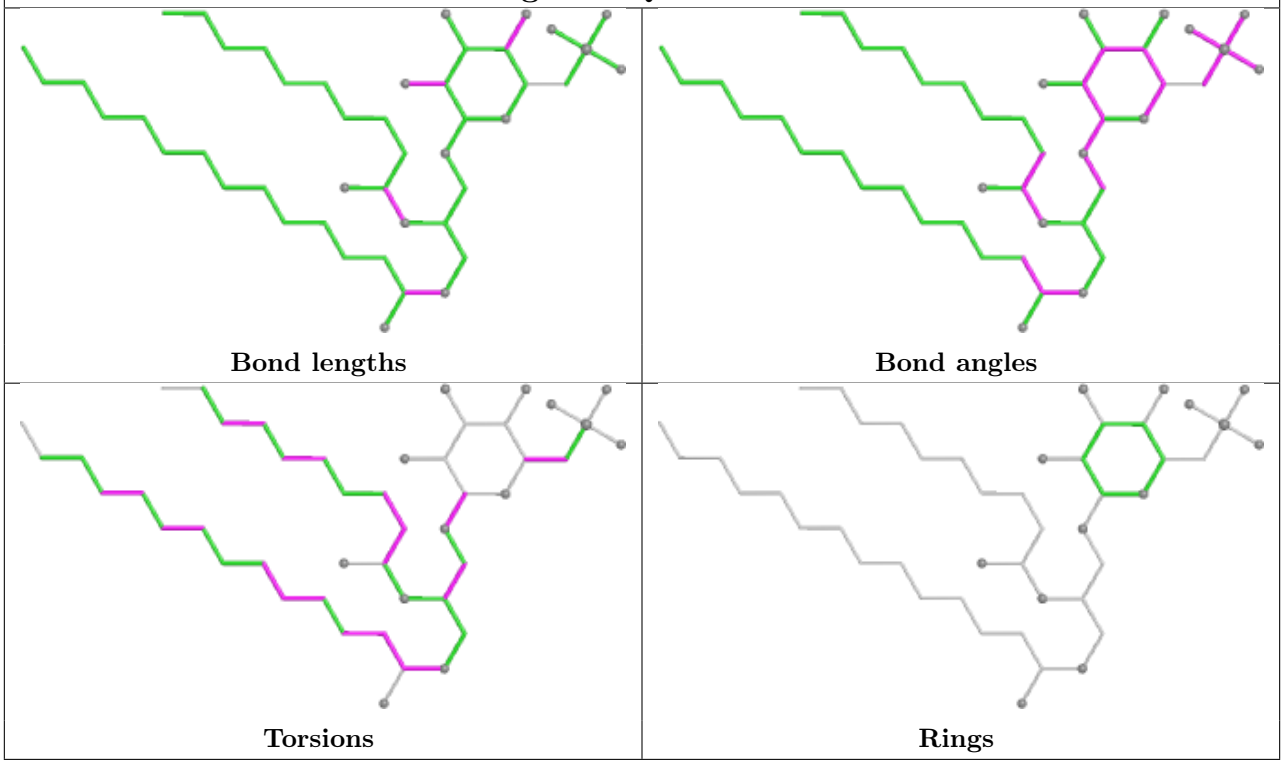
Bond angles



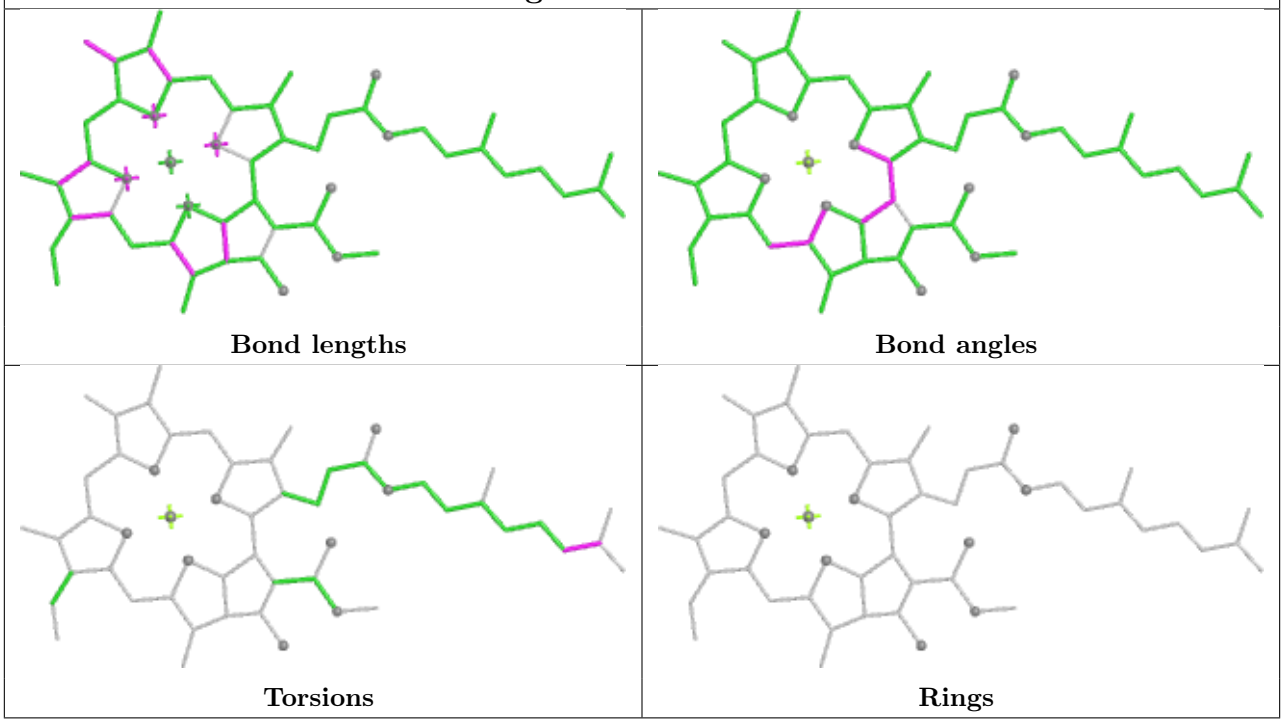
Torsions

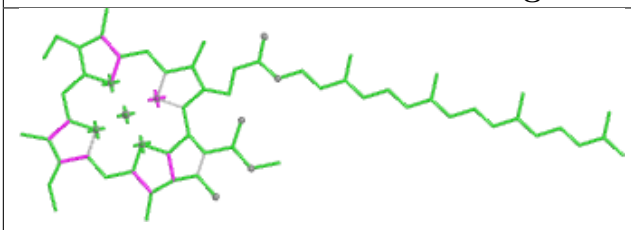
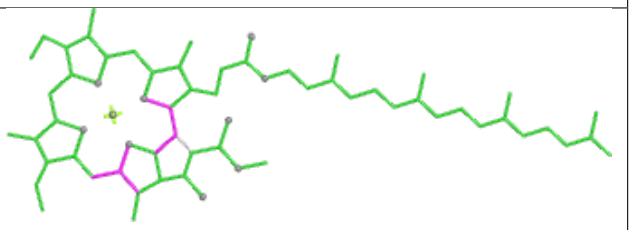
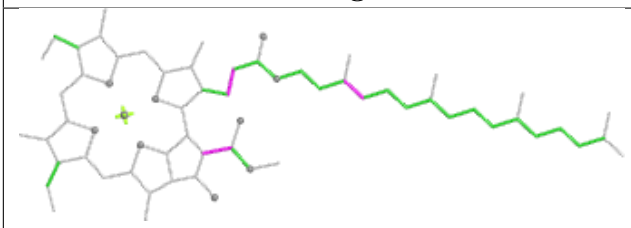
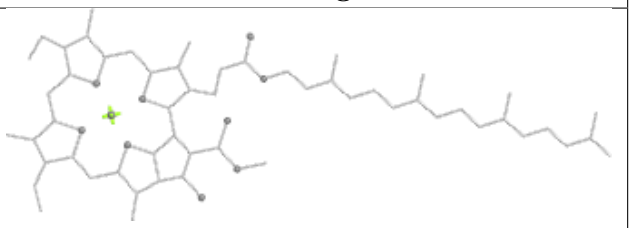
Rings

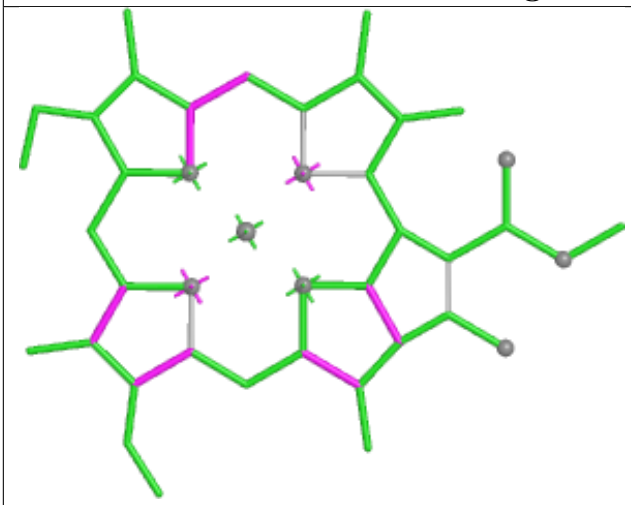
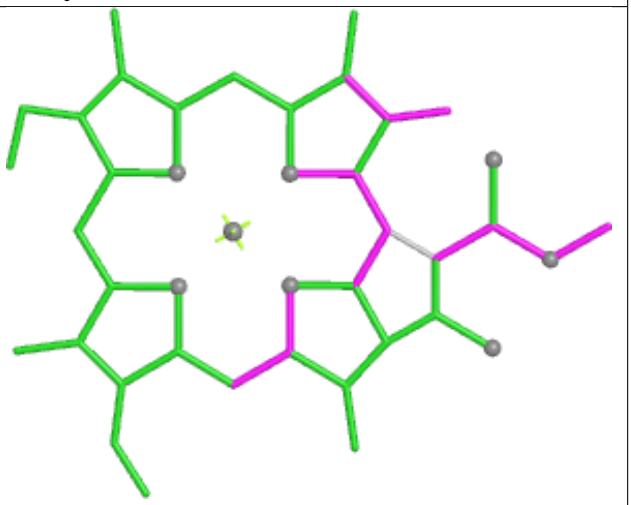
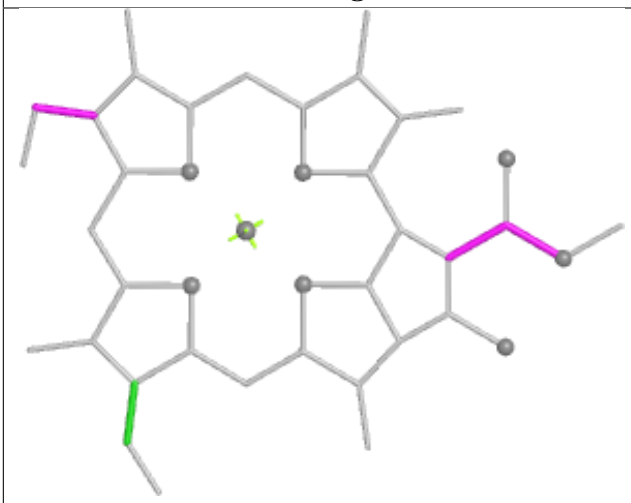
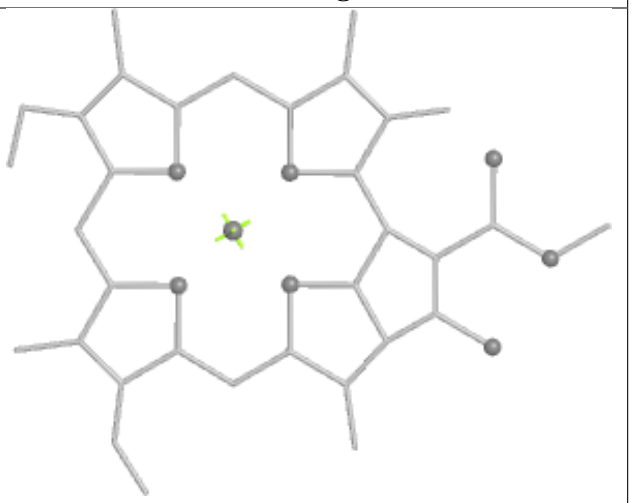
Ligand SQD M 102

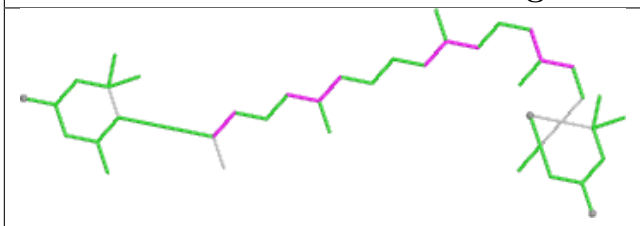
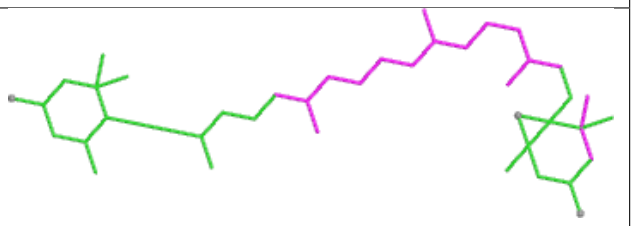
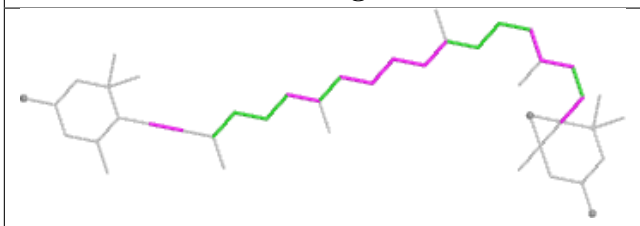
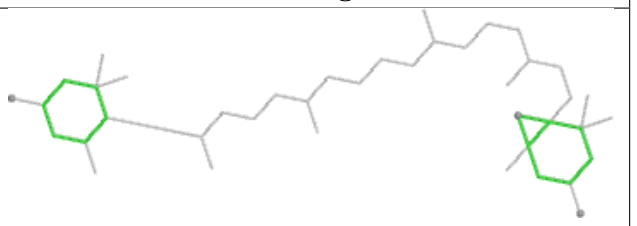


Ligand CLA B 810



Ligand CLA A 806	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA Q 211	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand DD6 P 314	
 Bond lengths	 Bond angles
 Torsions	 Rings

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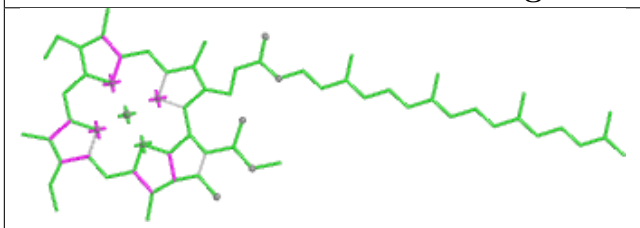
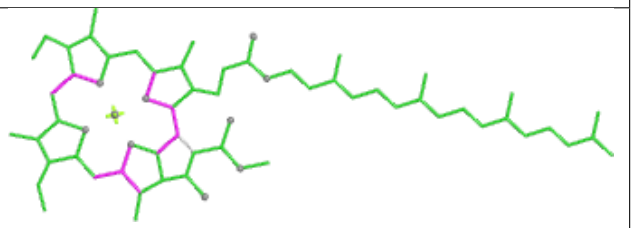
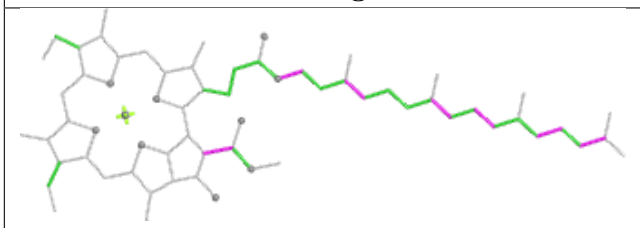
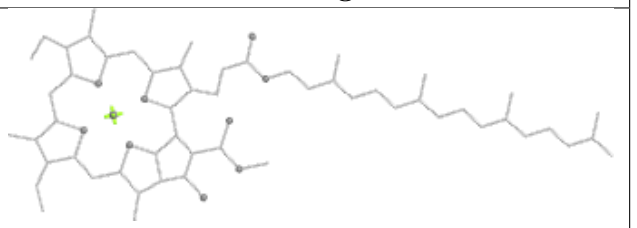
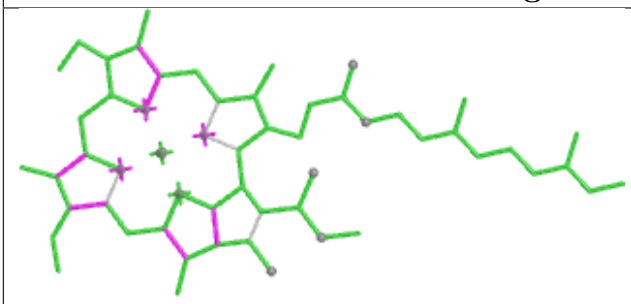
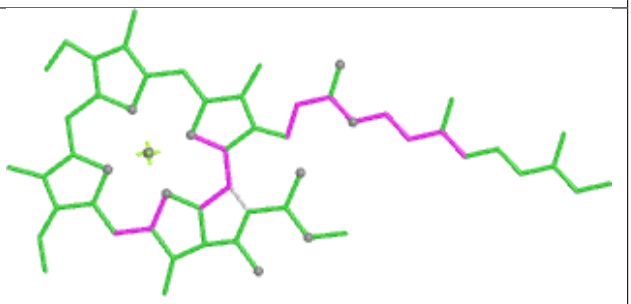
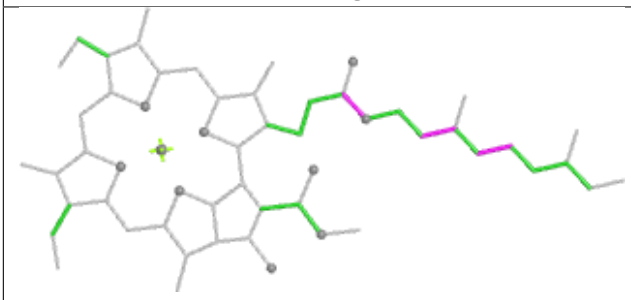
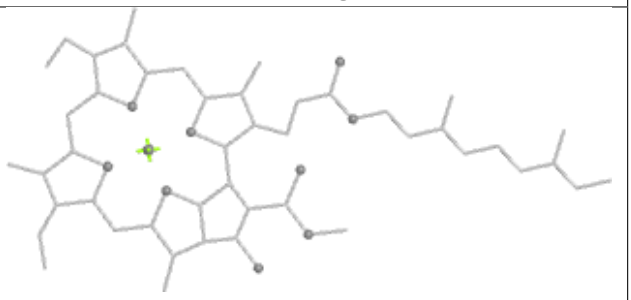
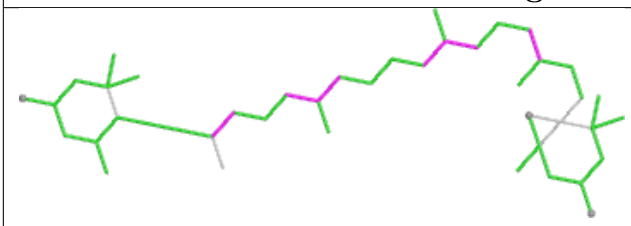
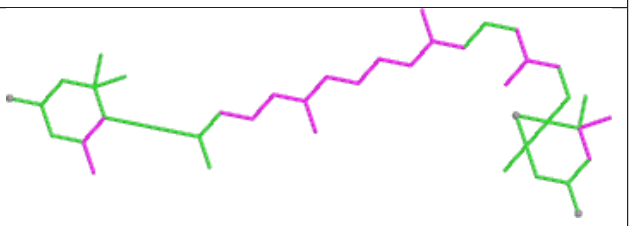
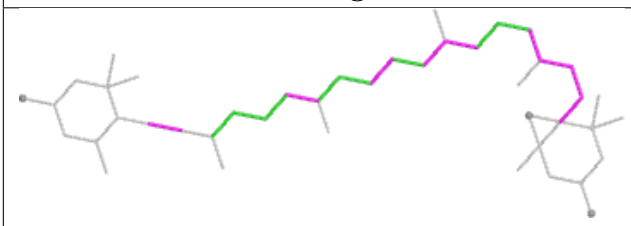
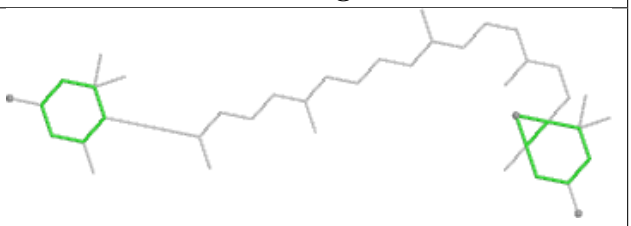
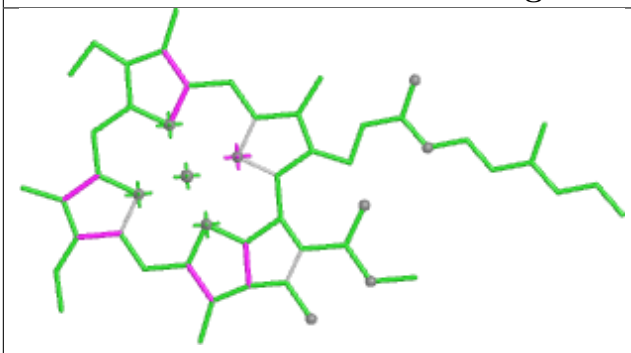
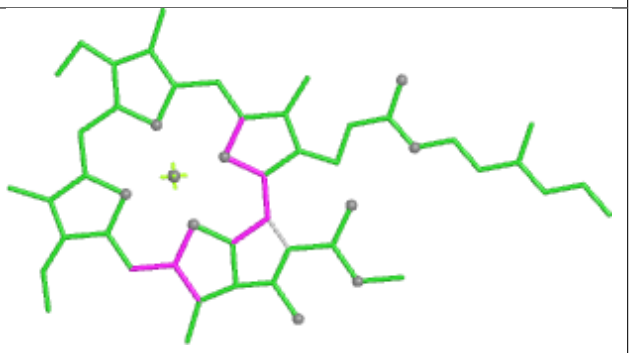
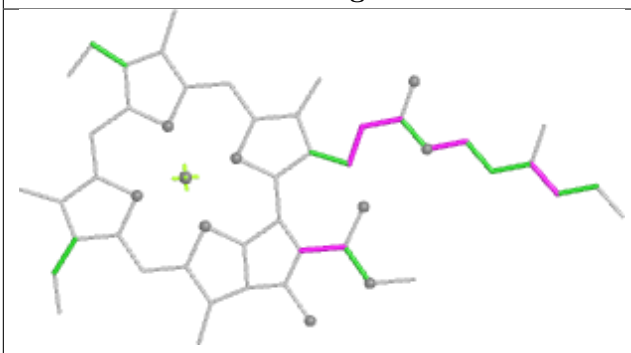
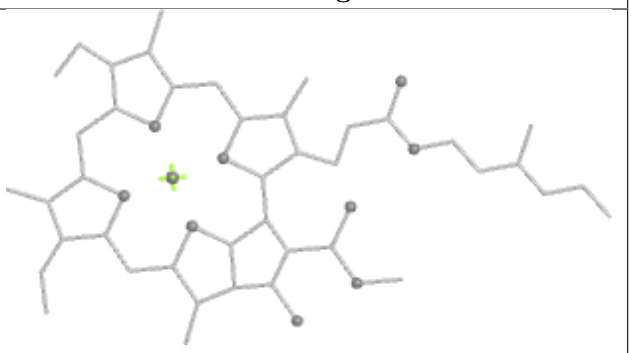
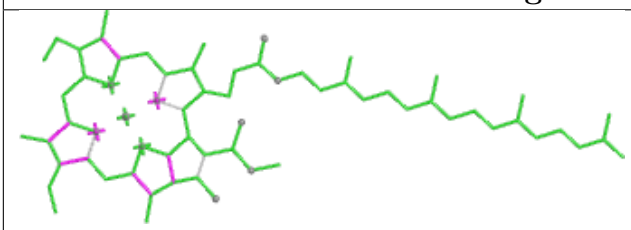
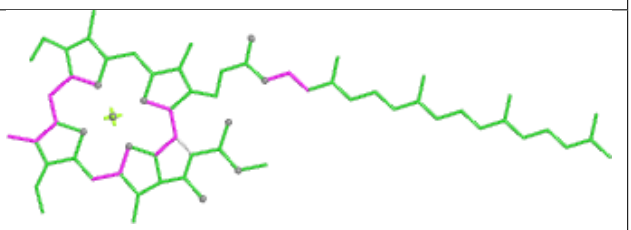
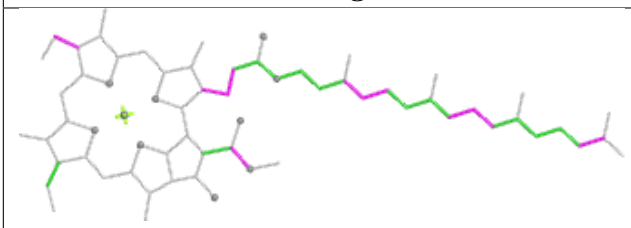
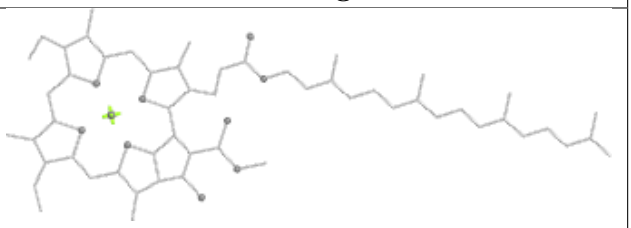
 Bond lengths	 Bond angles
 Torsions	 Rings

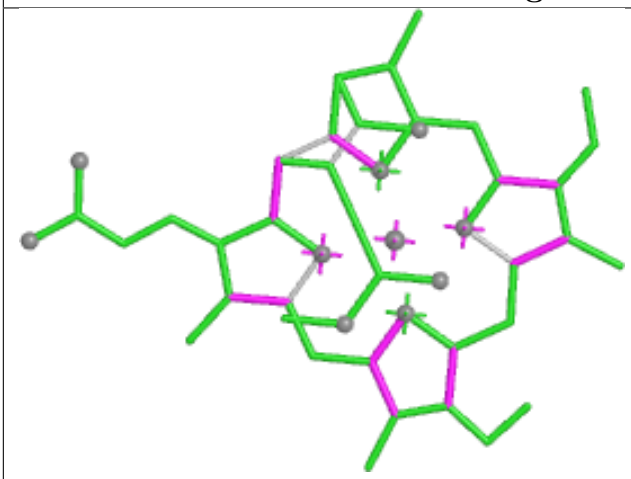
Ligand CLA A 808	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand DD6 P 316	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA P 308	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA T 208	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand KC1 O 210



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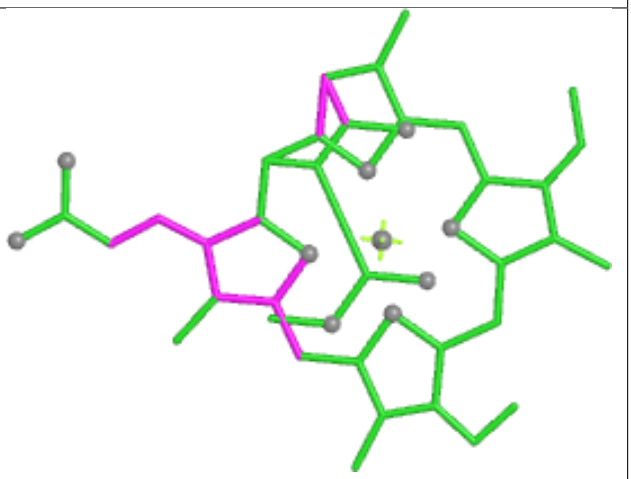
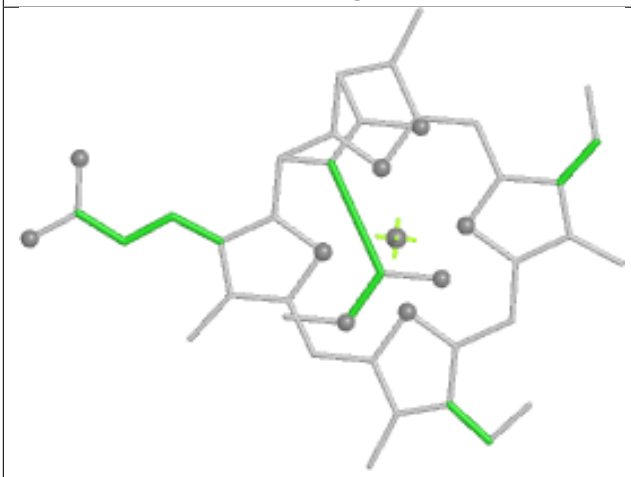


Bond angles



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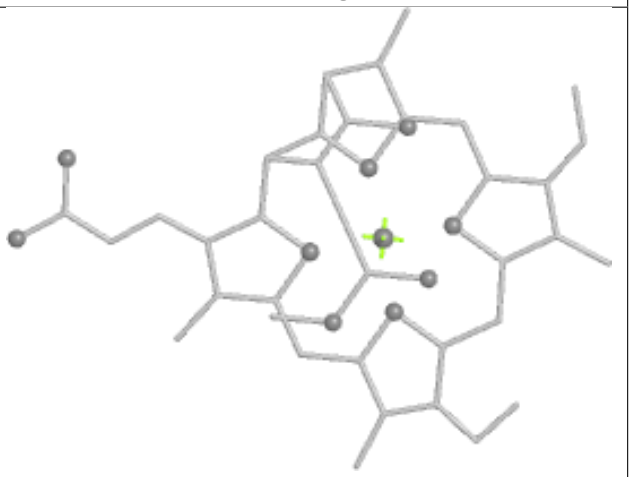
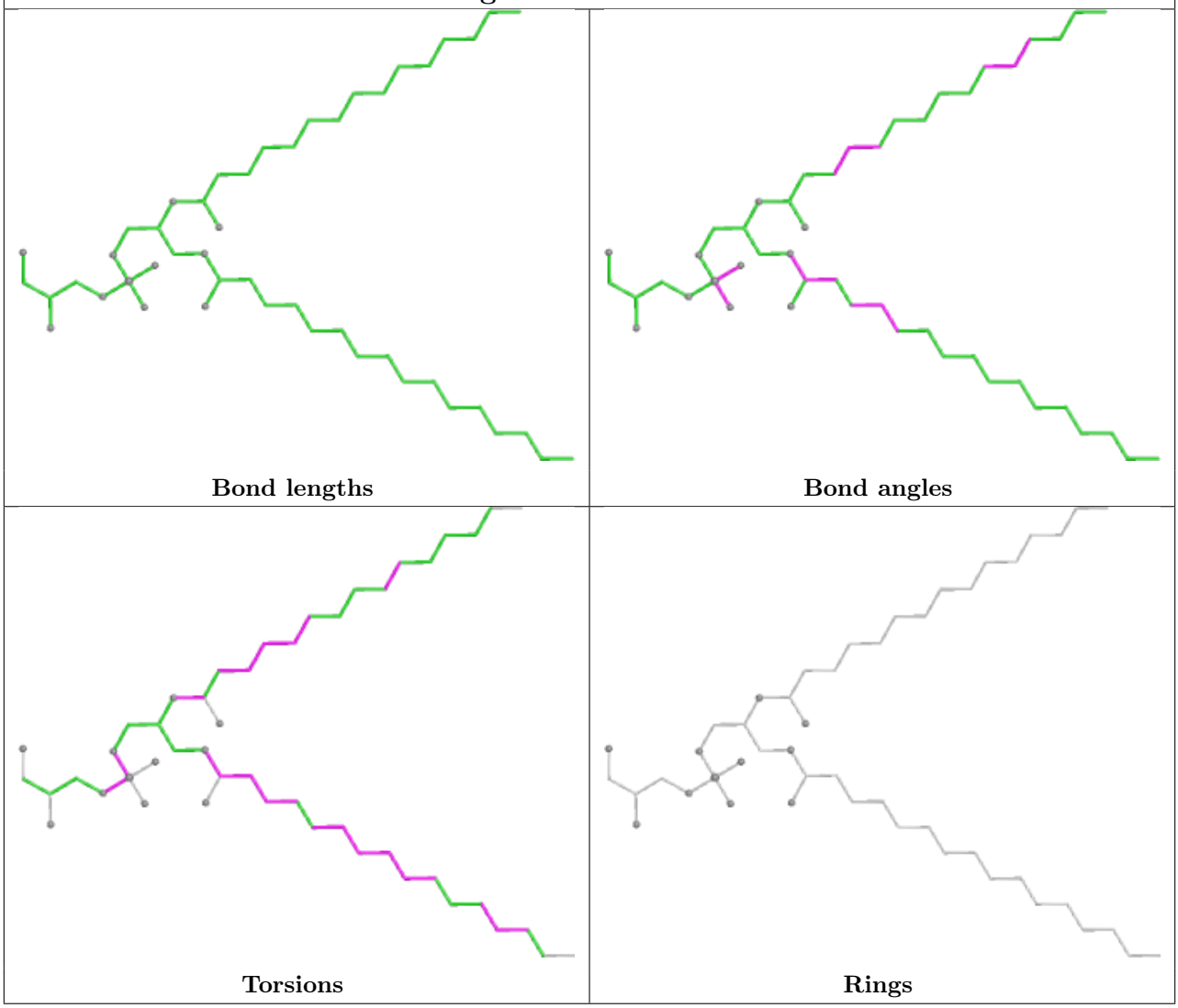
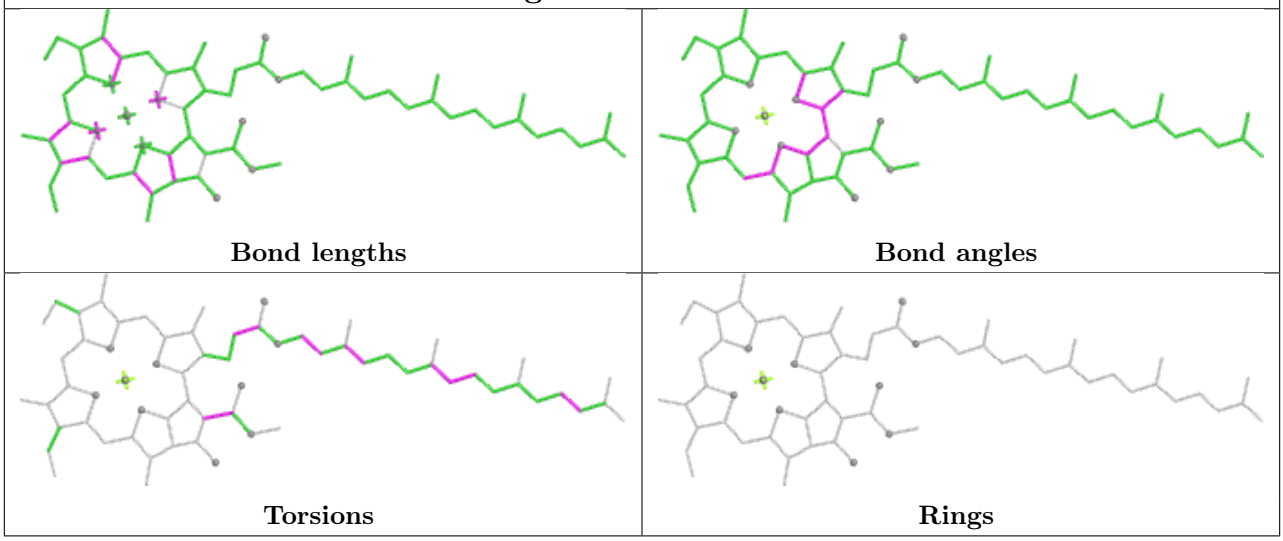


Rings

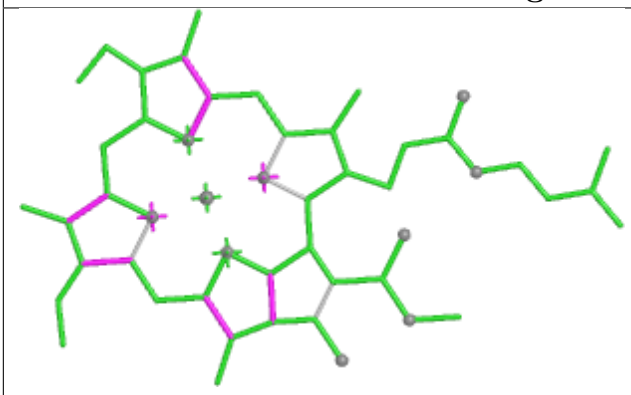
Ligand LHG A 839



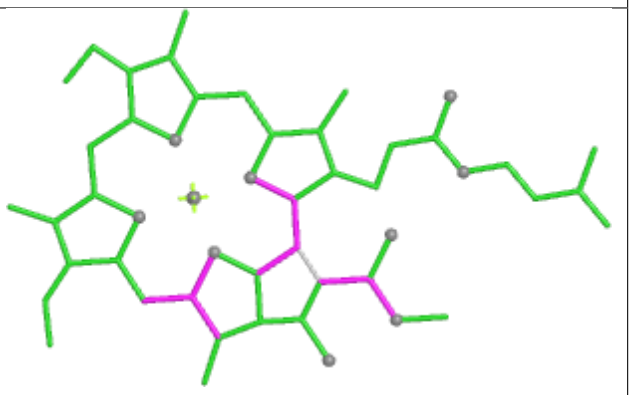
Ligand CLA A 821



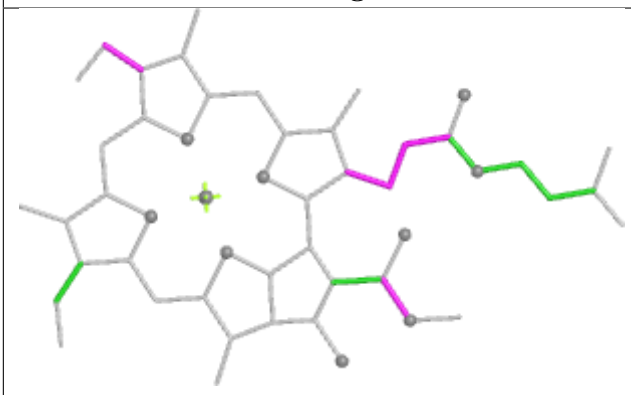
Ligand CLA L 204



Bond lengths



Bond angles



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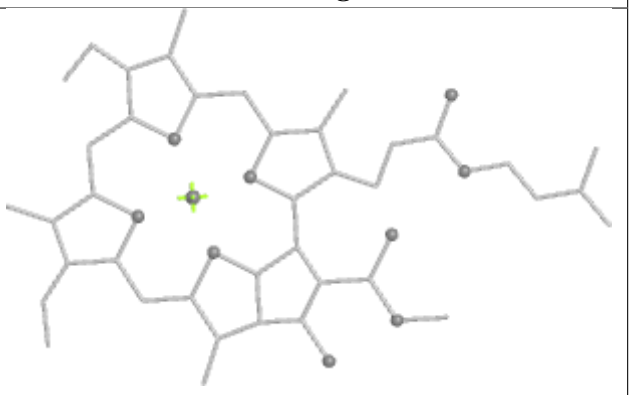
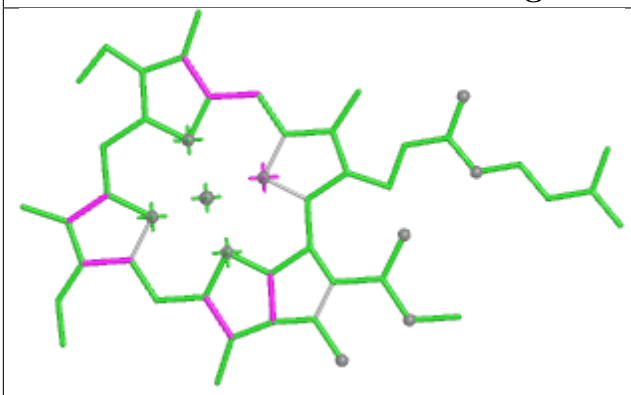
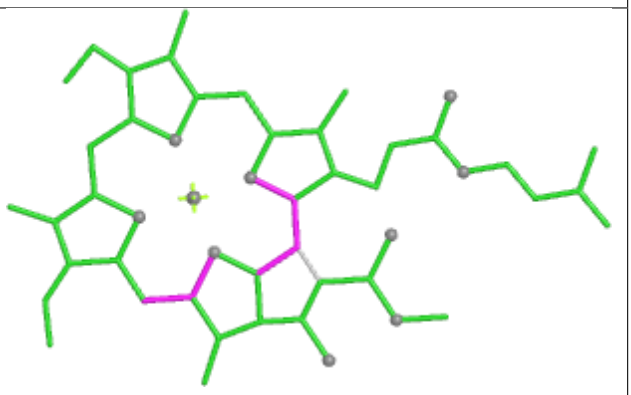
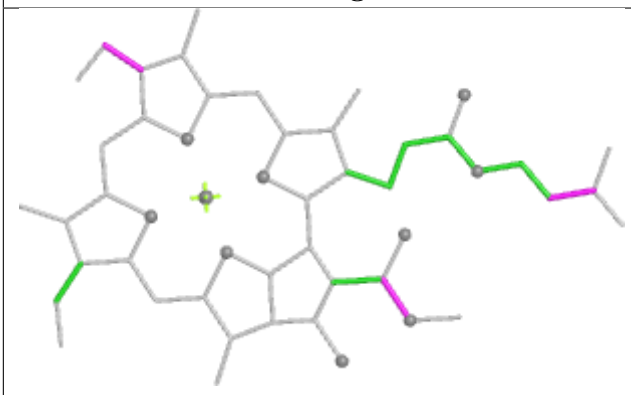
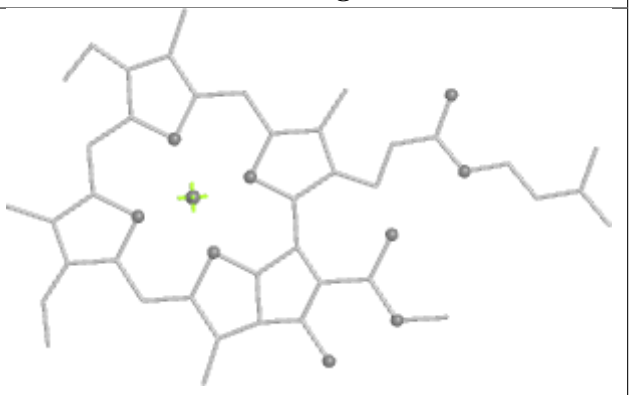
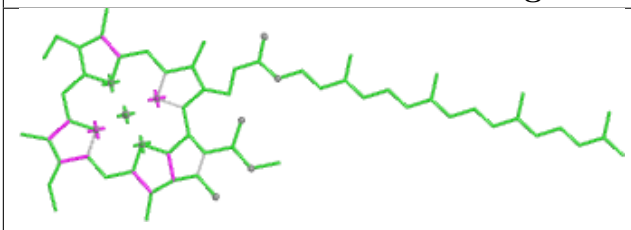
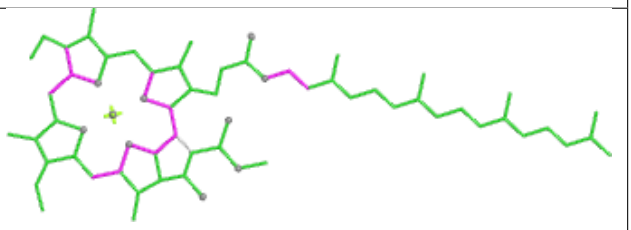
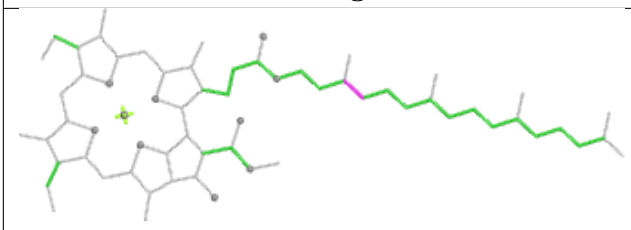
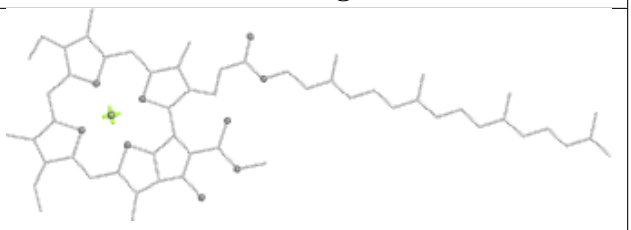


Rings

Ligand CLA P 310	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA B 835	
 Bond lengths	 Bond angles
 Torsions	 Rings

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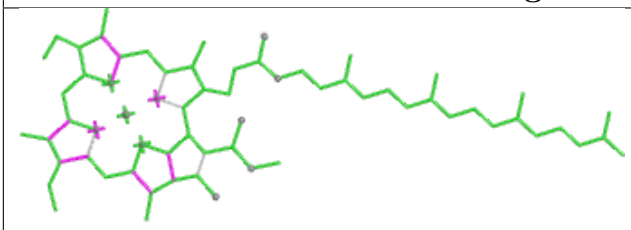
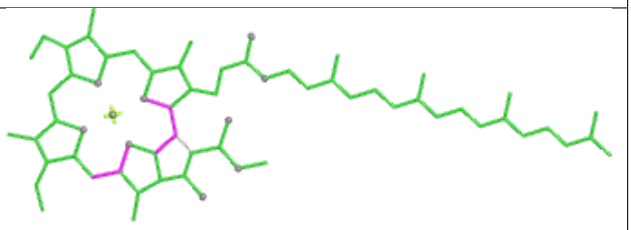
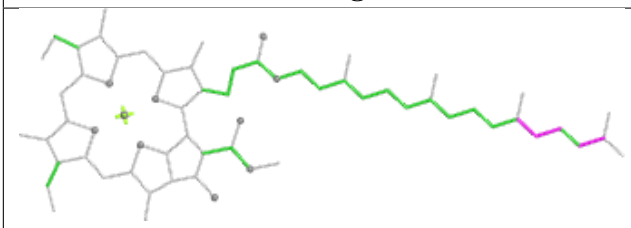
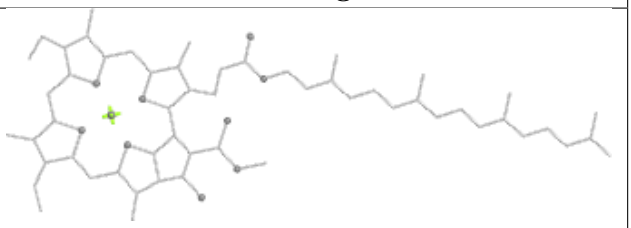
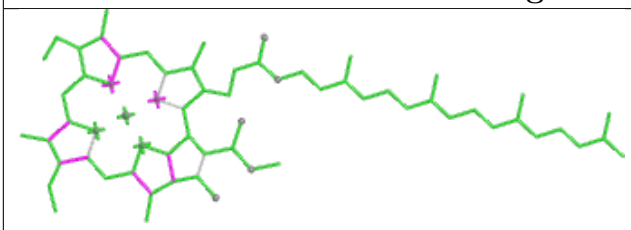
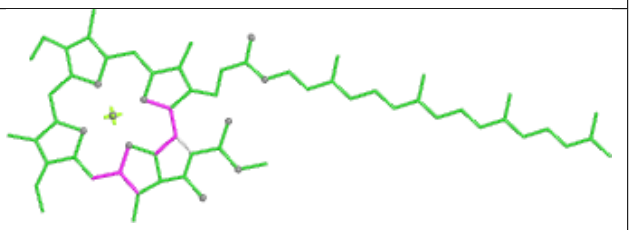
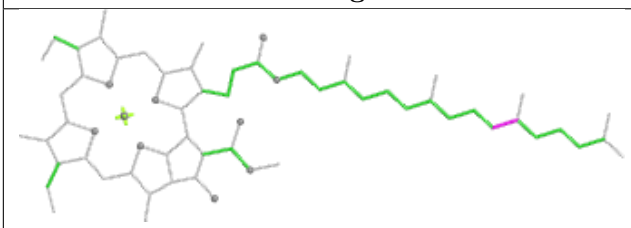
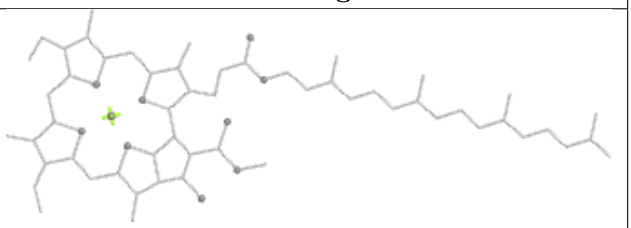
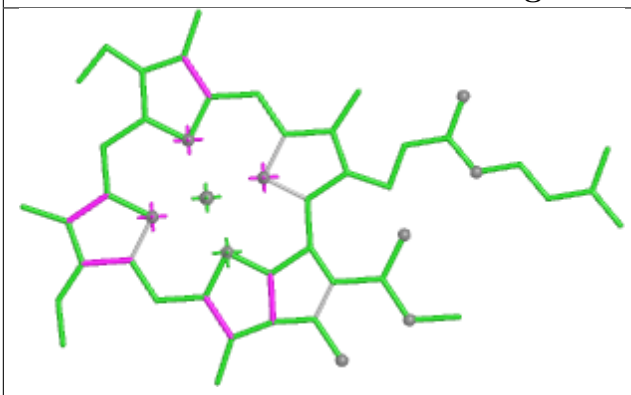
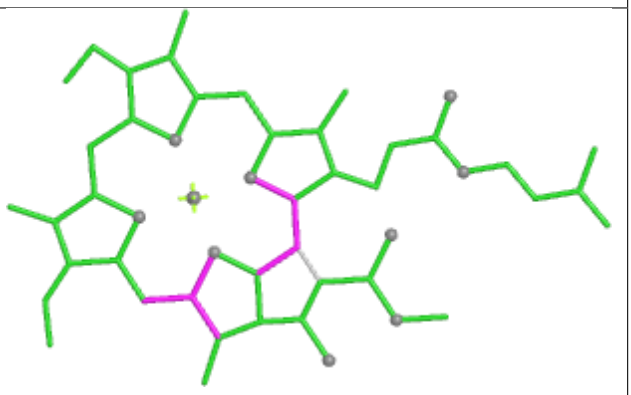
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA L 203	
 Bond lengths	 Bond angles
 Torsions	 Rings

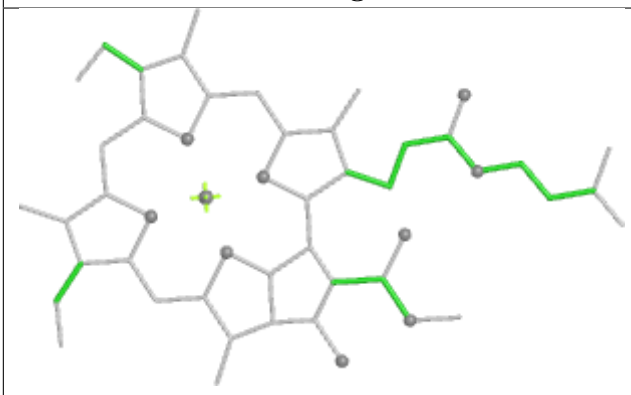
Ligand CLA B 826



Bond lengths



Bond angles



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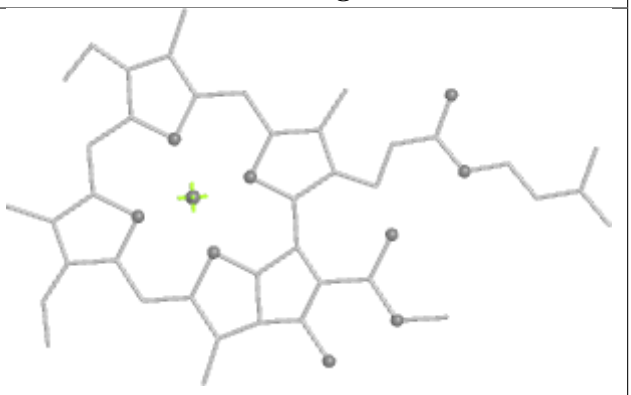
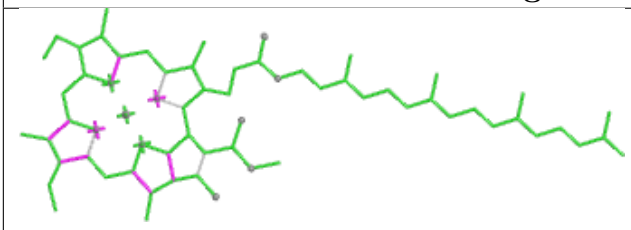


Rings

Ligand CLA A 828



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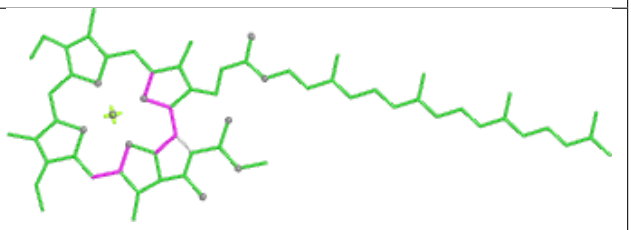
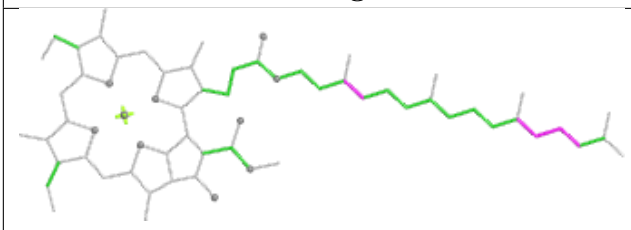


Bond angles



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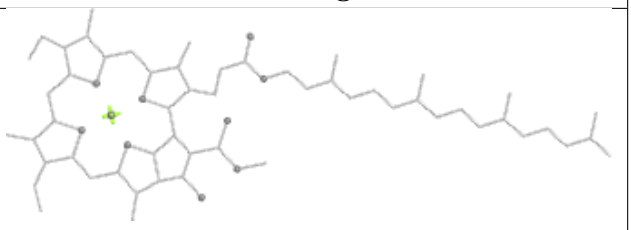
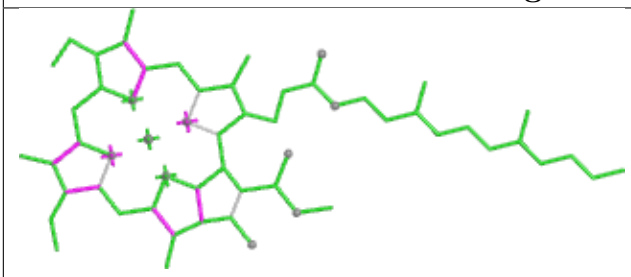
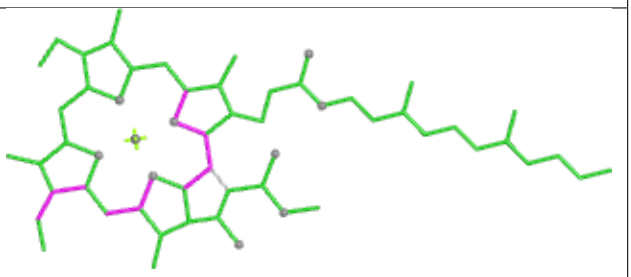
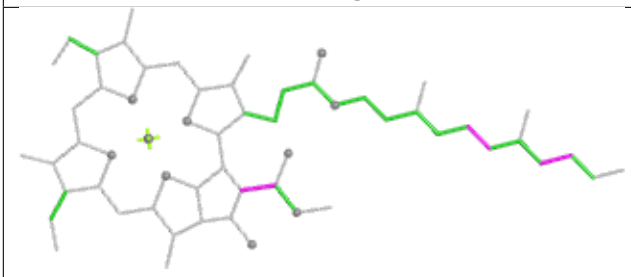
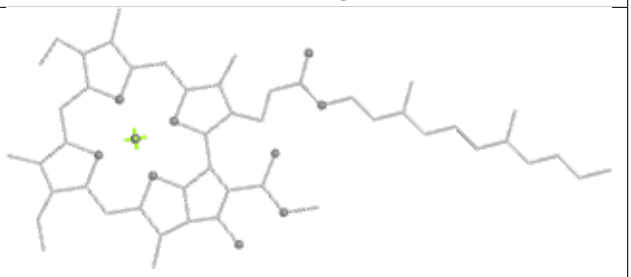
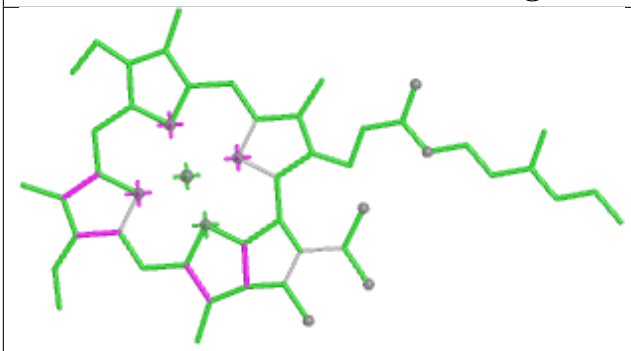
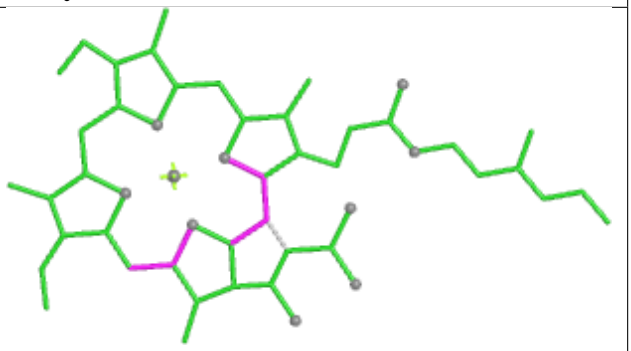
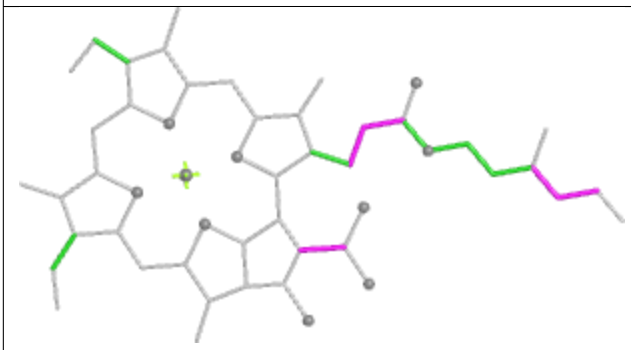
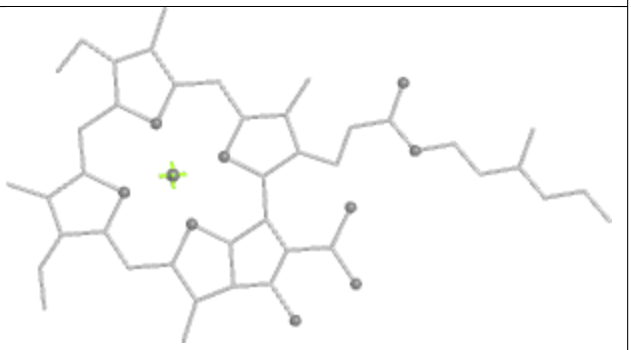
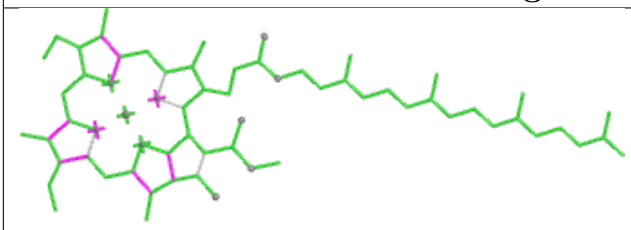


Rings

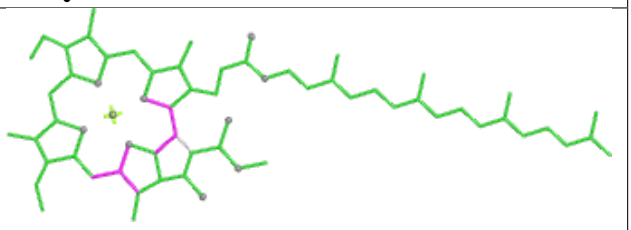
Ligand CLA B 830	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA Q 206	
 Bond lengths	 Bond angles
 Torsions	 Rings

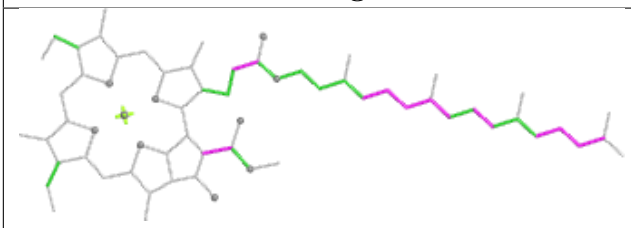
Ligand CLA Q 216



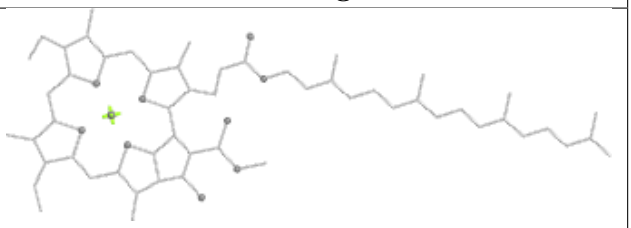
Bond lengths



Bond angles

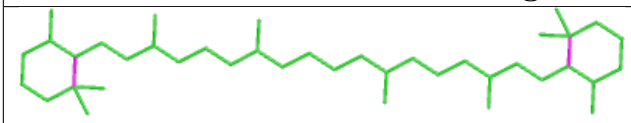


Torsions



Rings

Ligand BCR A 841



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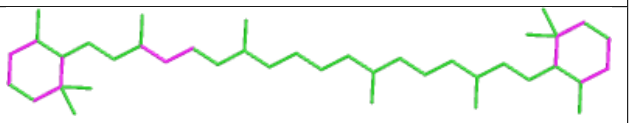
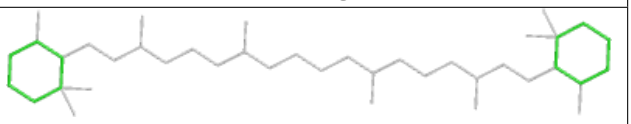


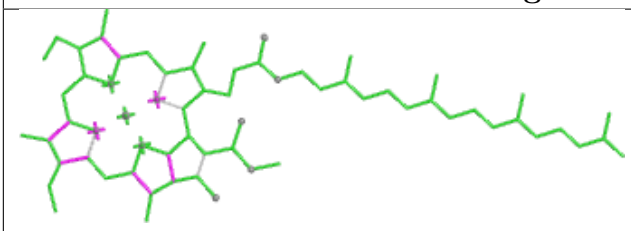
Bond angles

Torsions



Rings

Ligand CLA A 835



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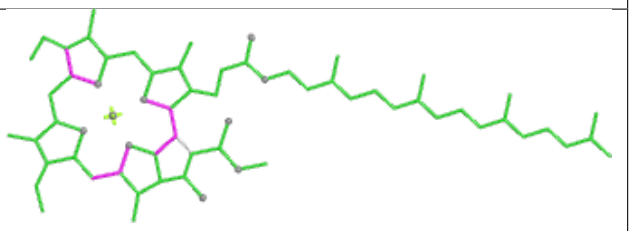

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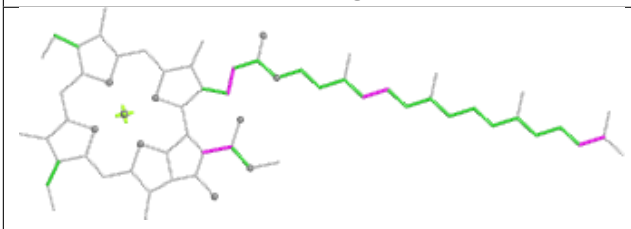

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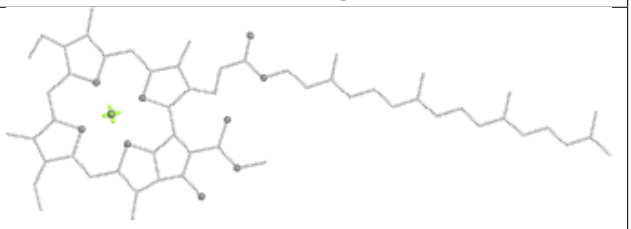
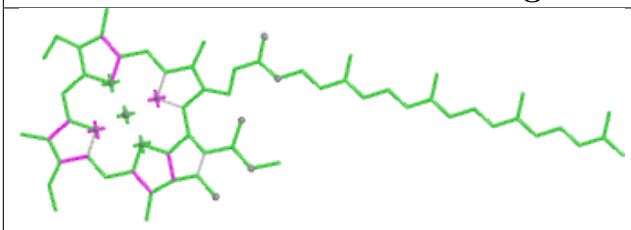
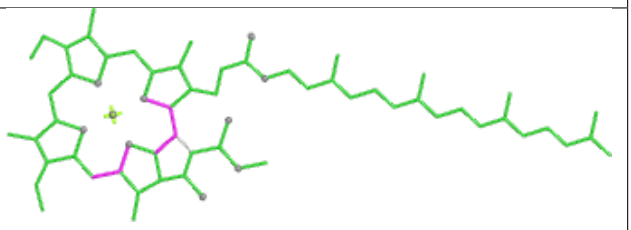
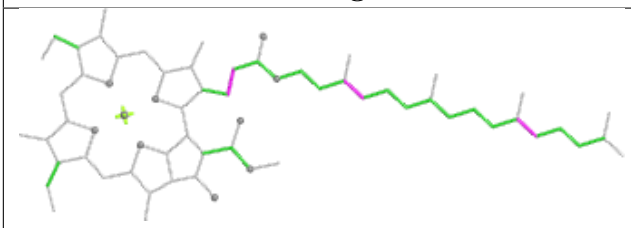
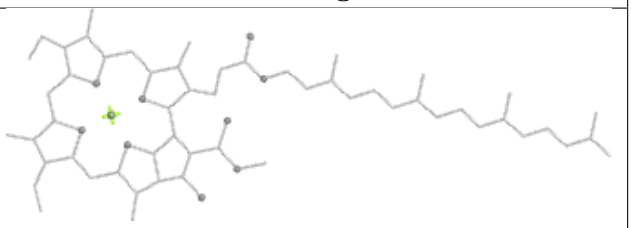
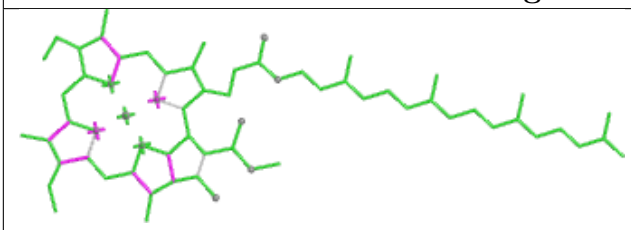
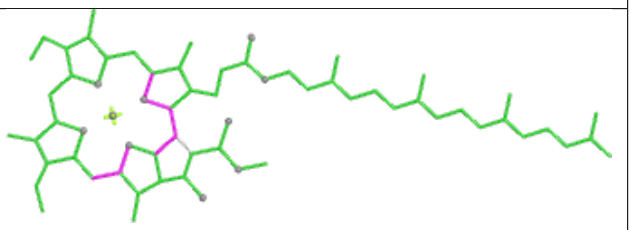
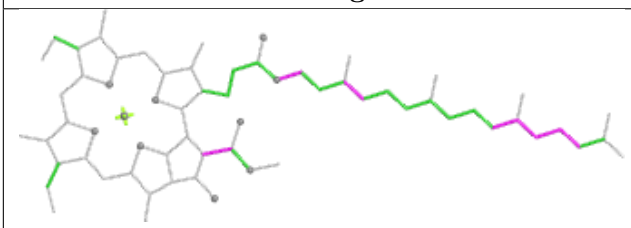
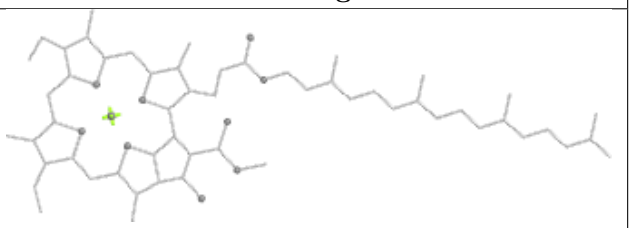
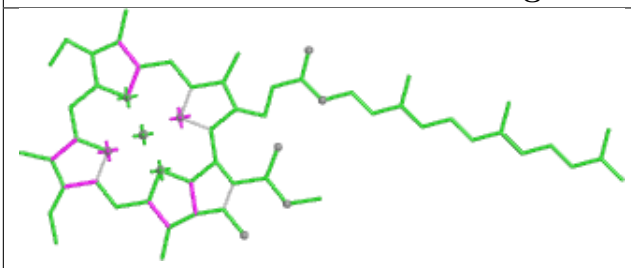


Rings

Ligand CLA A 825	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA A 823	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA O 208



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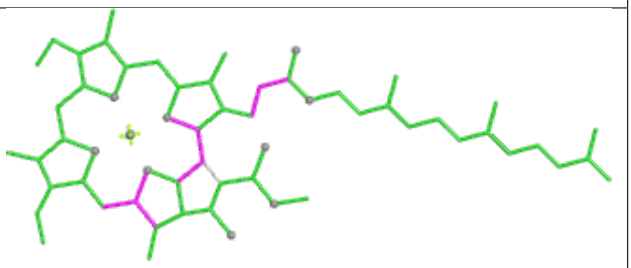
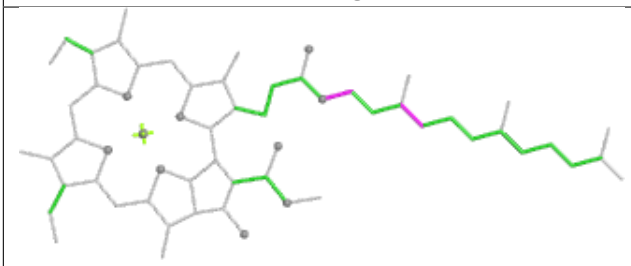


Bond angles



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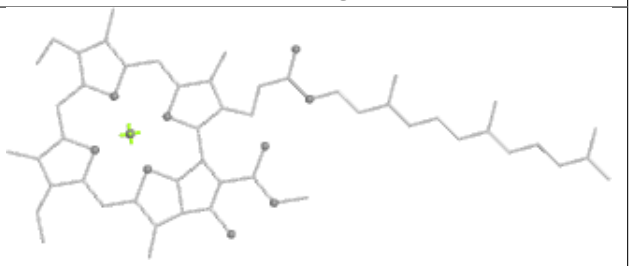
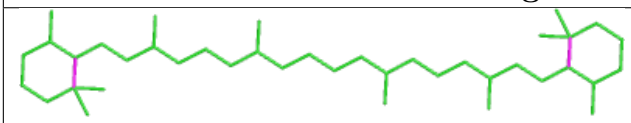


Rings

Ligand BCR A 842



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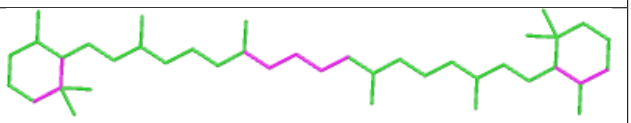
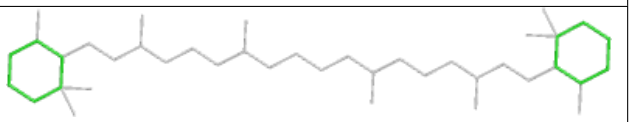


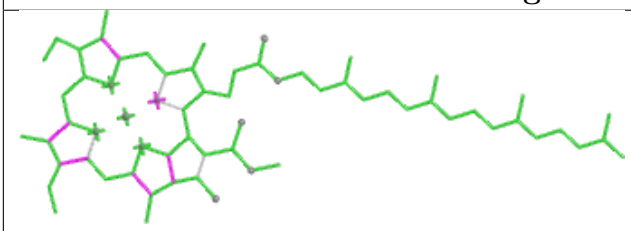
Bond angles

Torsions



Rings

Ligand CLA U 207



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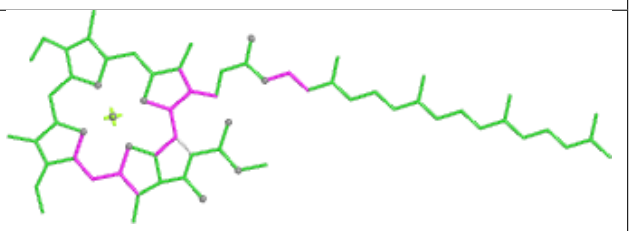

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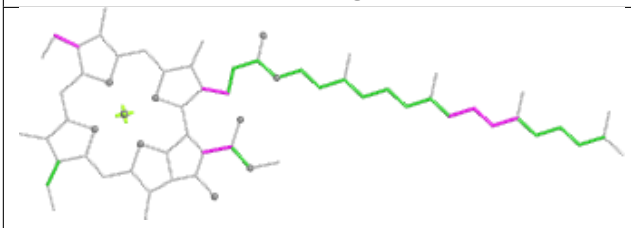

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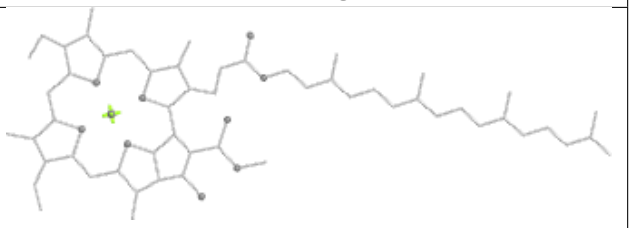
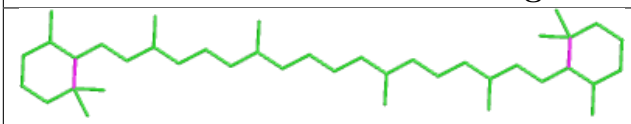


Rings

Ligand BCR L 201



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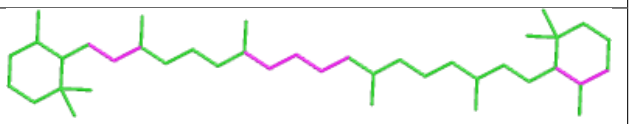

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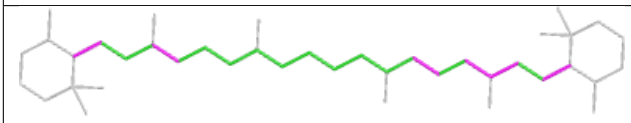

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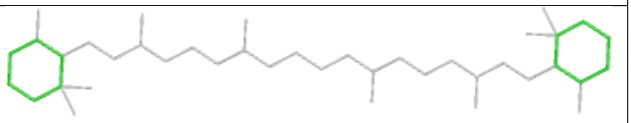
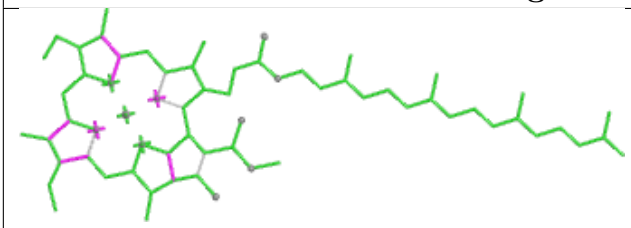


Rings

Ligand CLA S 201



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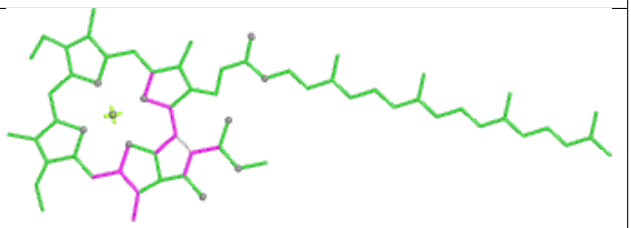
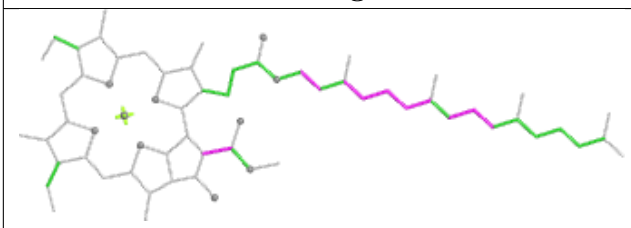


Bond angles



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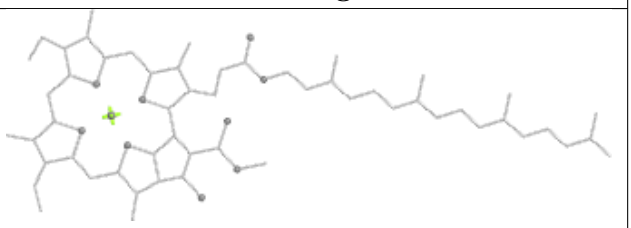
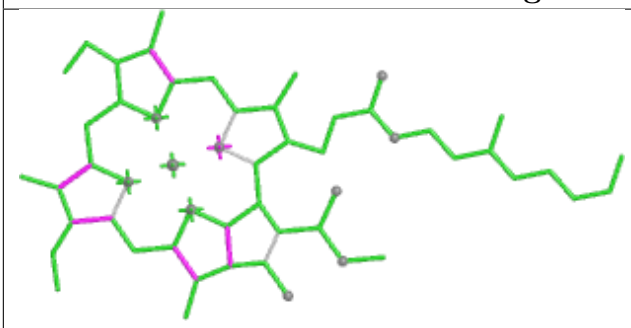


Rings

Ligand CLA A 810



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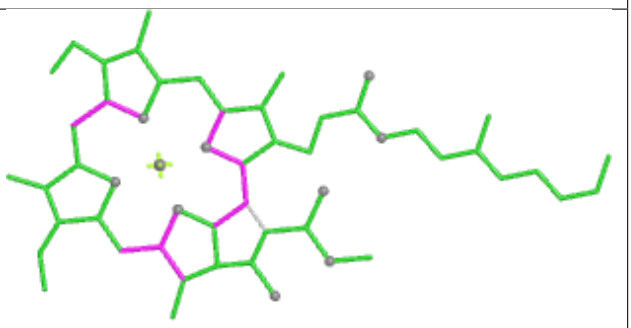
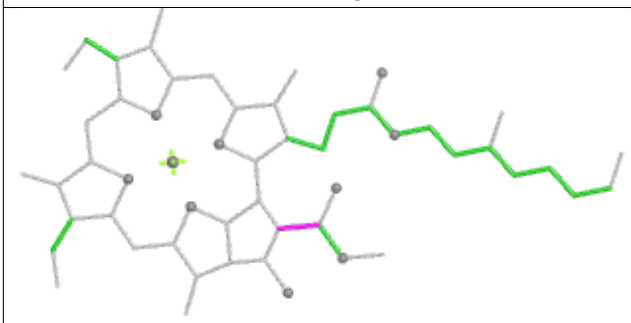


Bond angles



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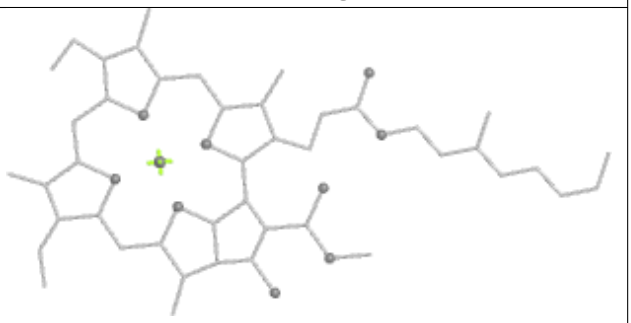
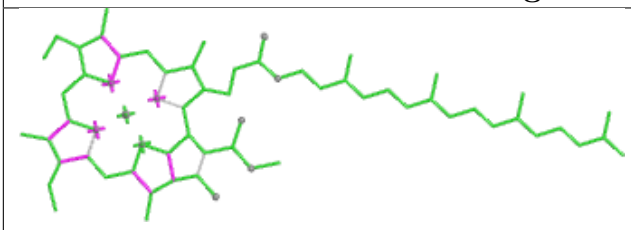
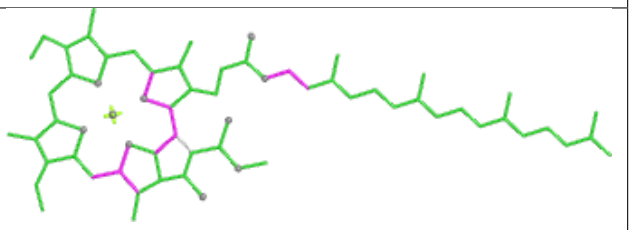
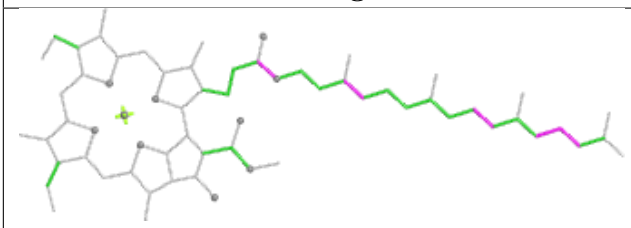
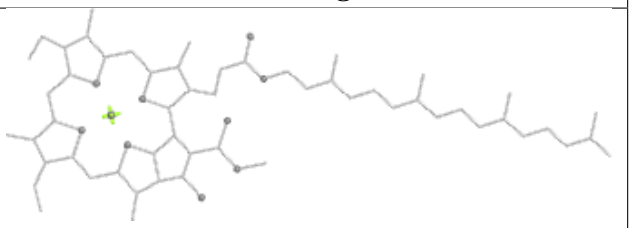
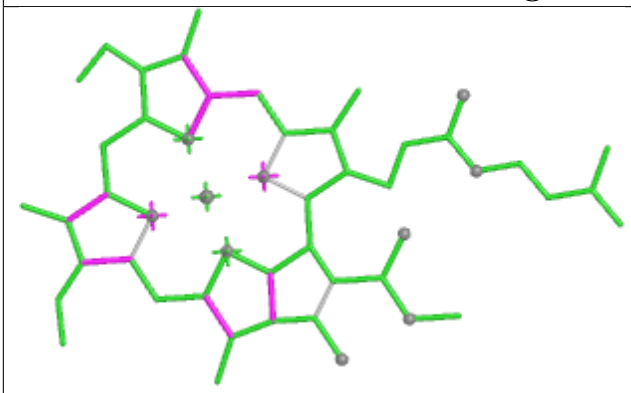
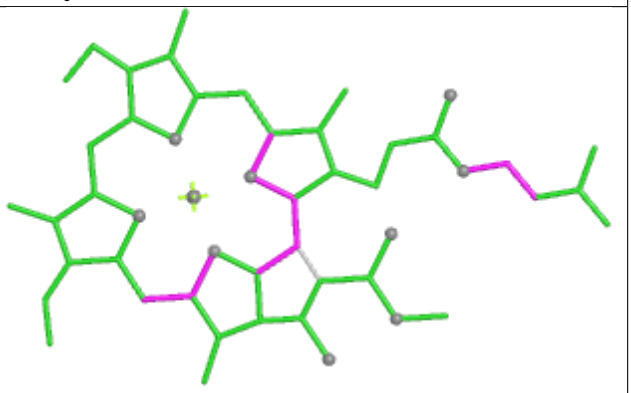
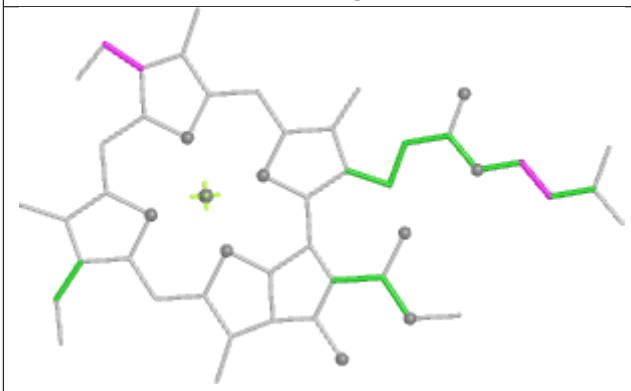
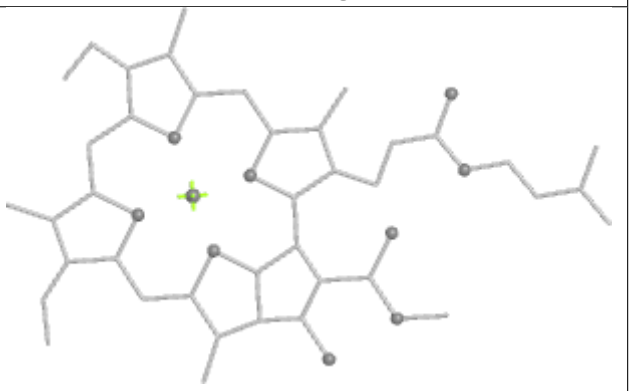
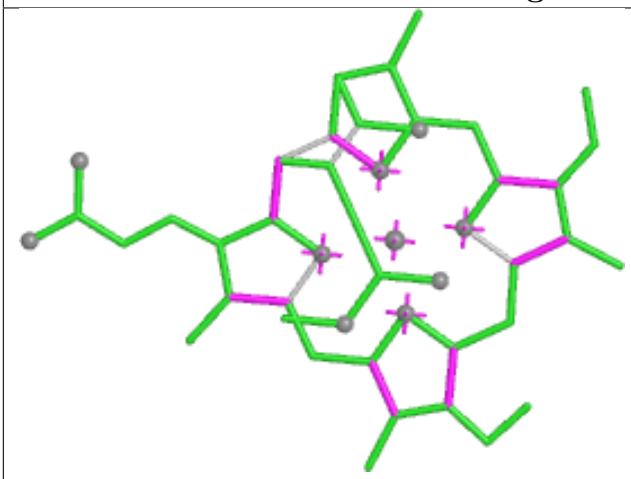


Rings

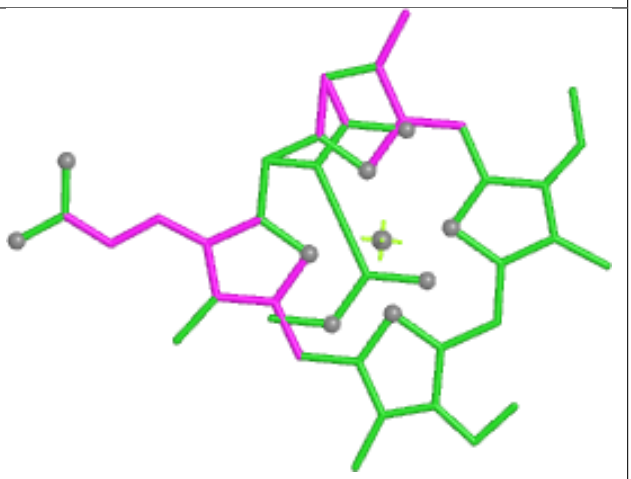
Ligand CLA A 833	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA Q 208	
 Bond lengths	 Bond angles
 Torsions	 Rings

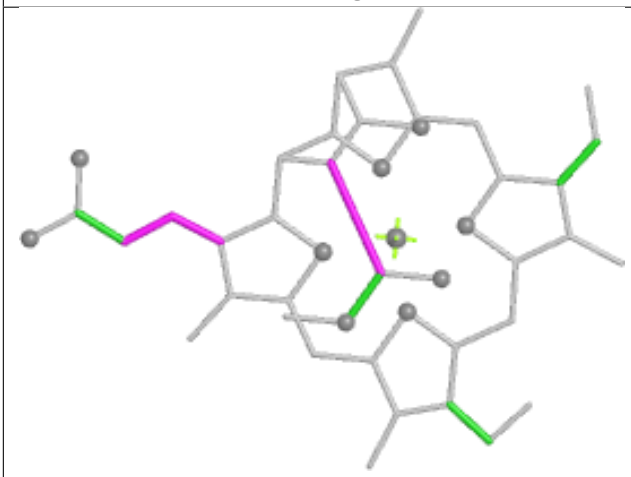
Ligand KC1 P 305



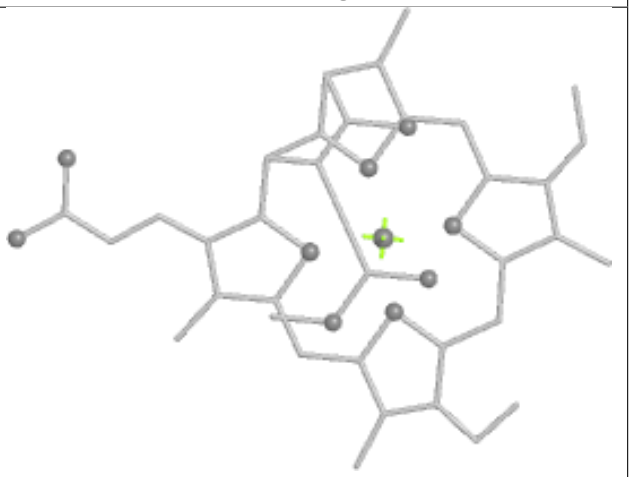
Bond lengths



Bond angles

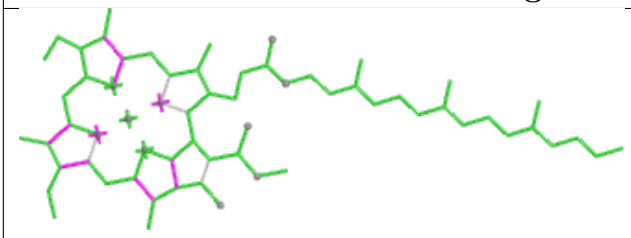


Torsions

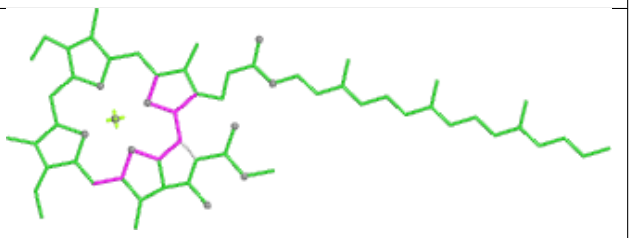


Rings

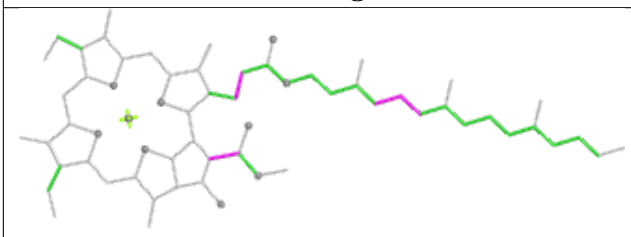
Ligand CLA B 820



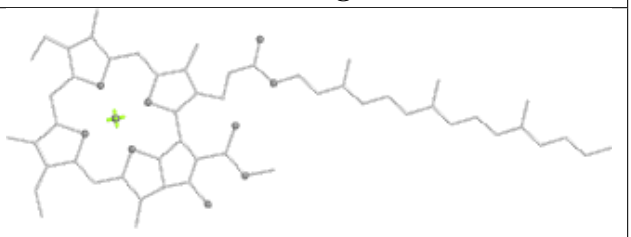
Bond lengths



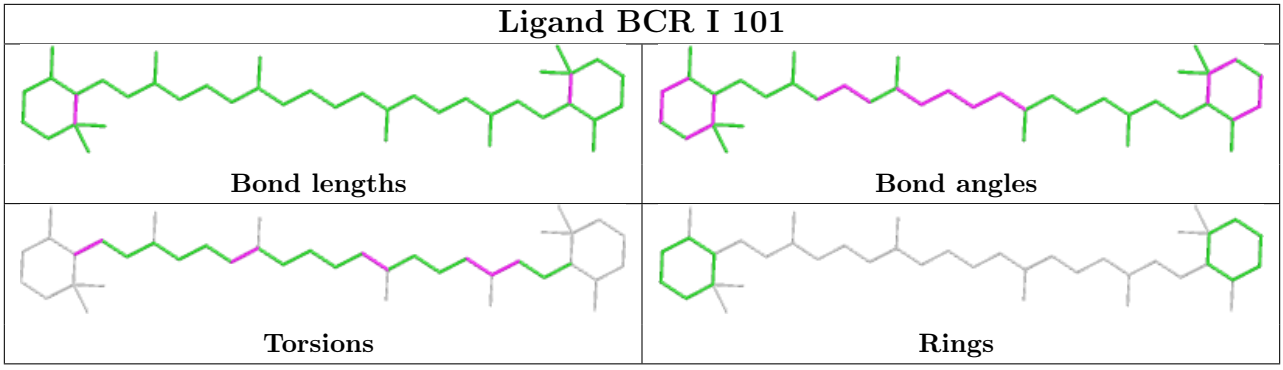
Bond angles

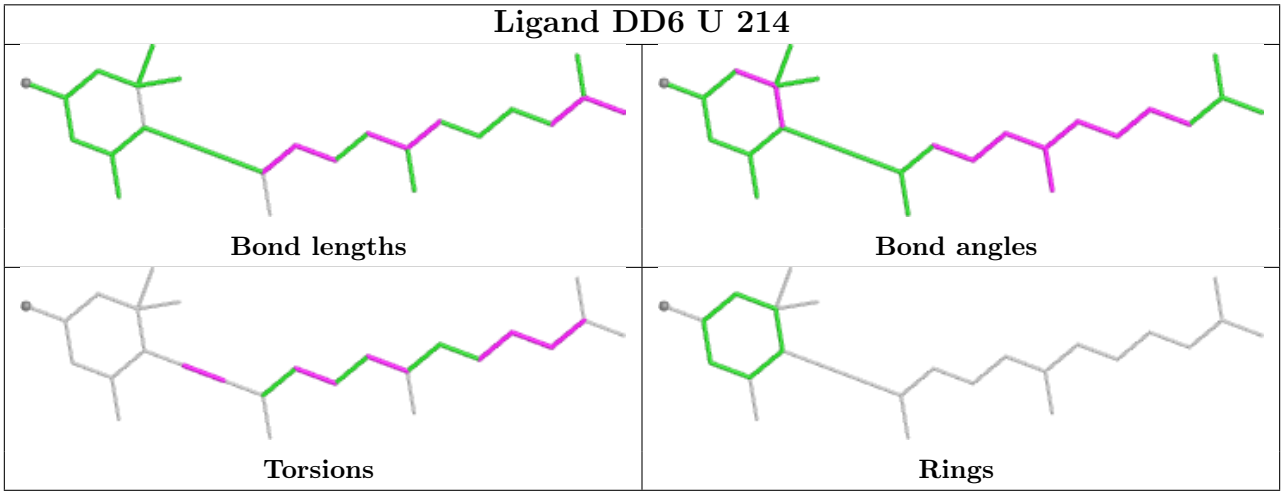


Torsions

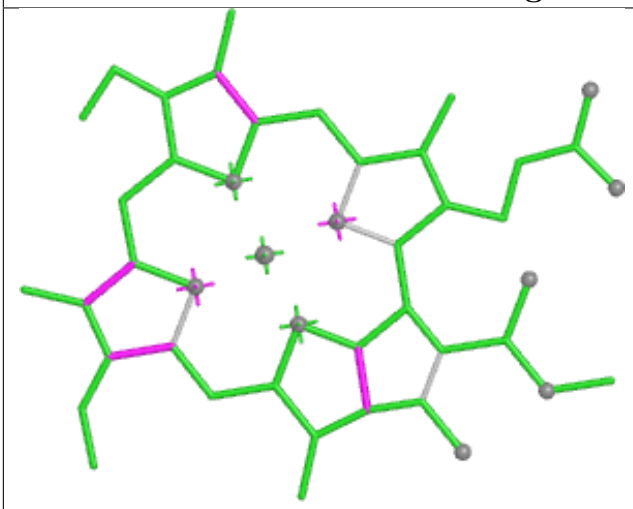


Rings


Ligand BCR I 101
Bond lengths
Bond angles
Torsions
Rings


Ligand DD6 U 214
Bond lengths
Bond angles
Torsions
Rings

Ligand CLA P 313



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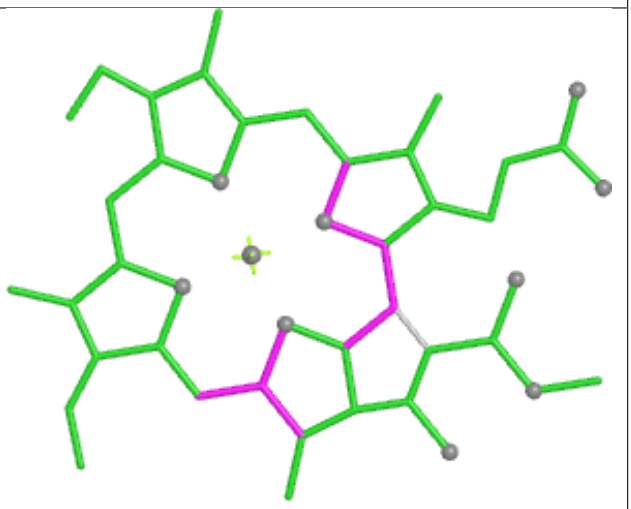
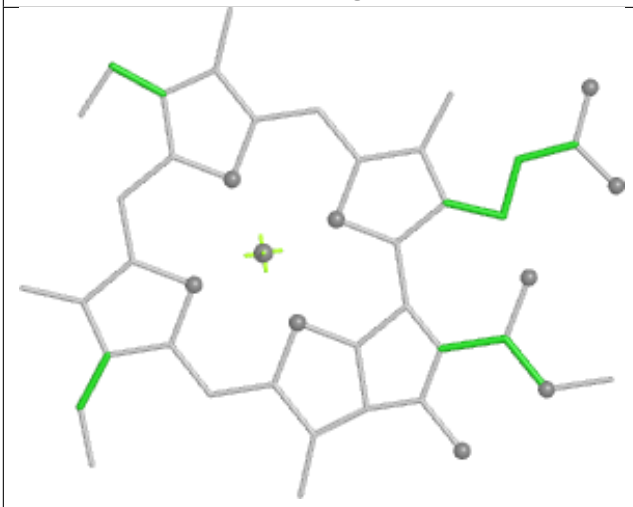


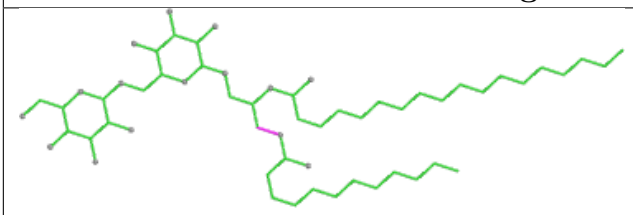
Bond angles



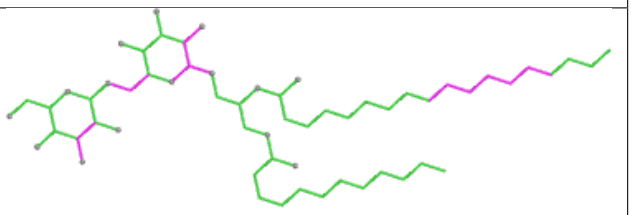
Torsions

Rings

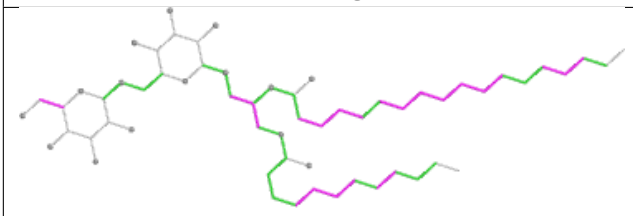
Ligand DGD B 842



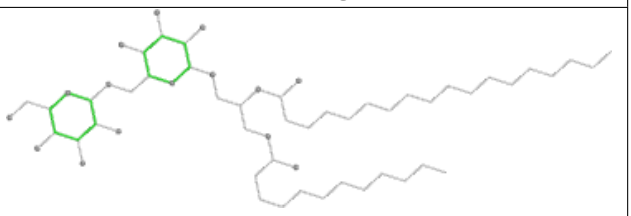
Bond lengths



Bond angles

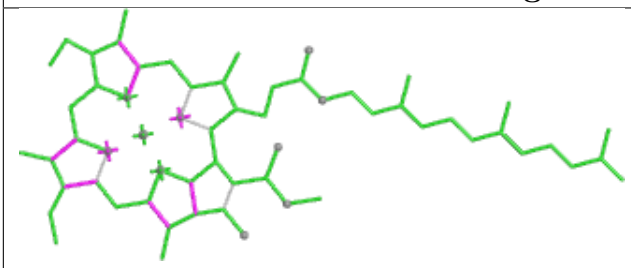


Torsions

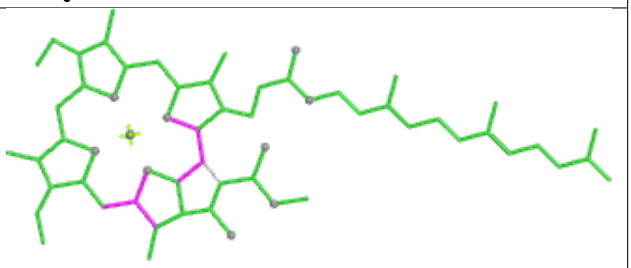


Rings

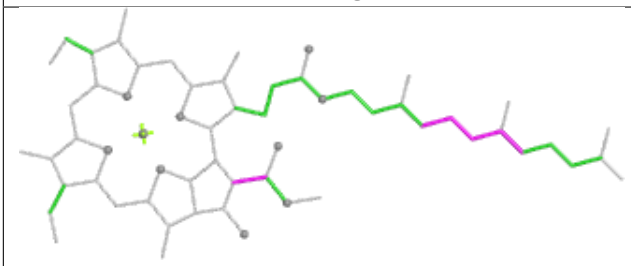
Ligand CLA Q 205



Bond lengths



Bond angles



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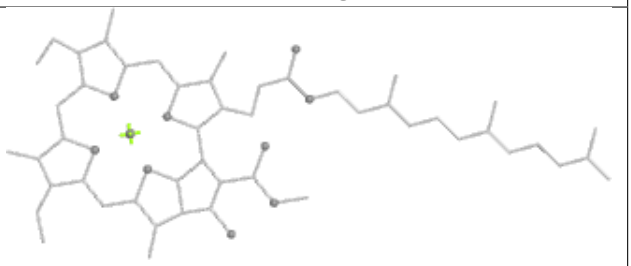
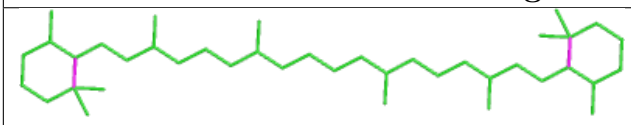


Rings

Ligand BCR F 801



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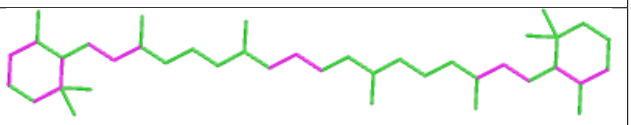
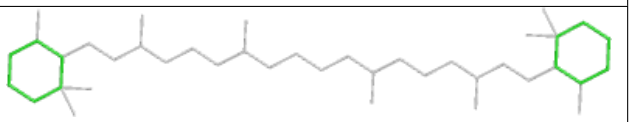


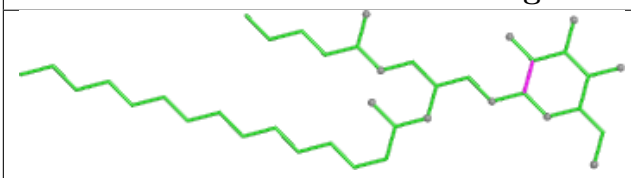
Bond angles

Torsions



Rings

Ligand LMG J 102



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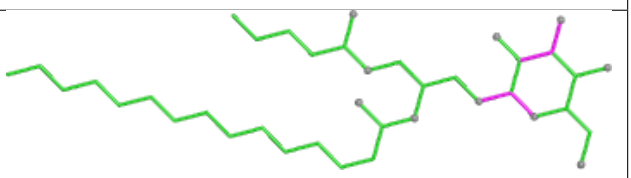
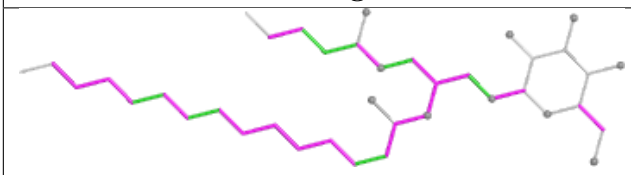
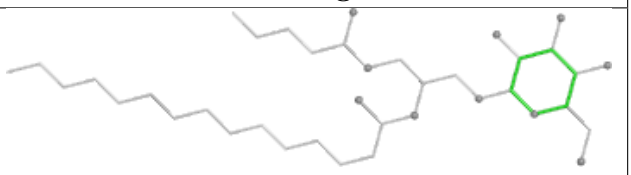


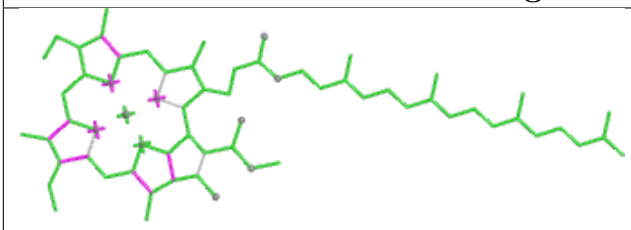
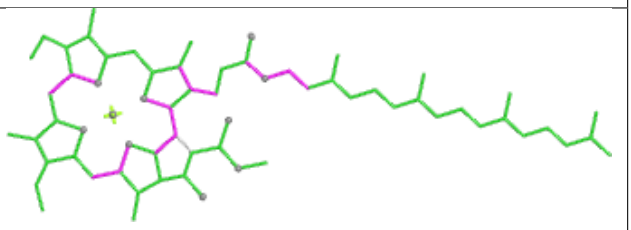
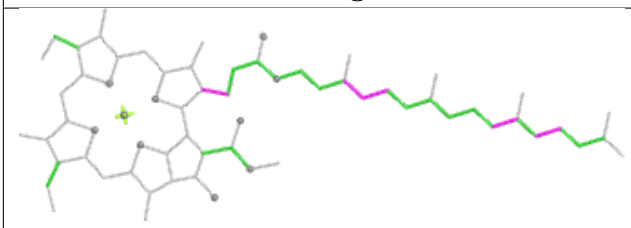
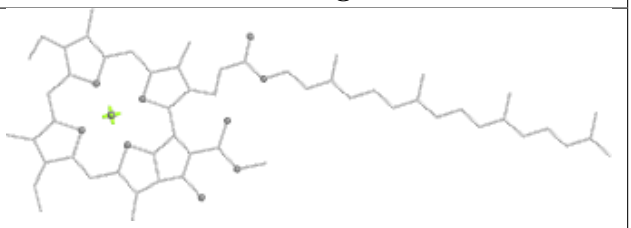
Bond angles



Torsions



Rings

Ligand CLA B 846	
 Bond lengths	 Bond angles
 Torsions	 Rings

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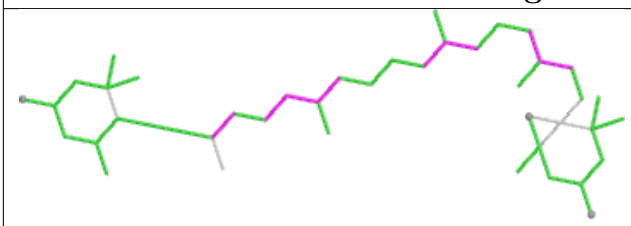
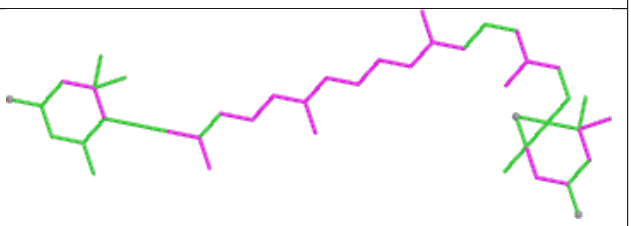
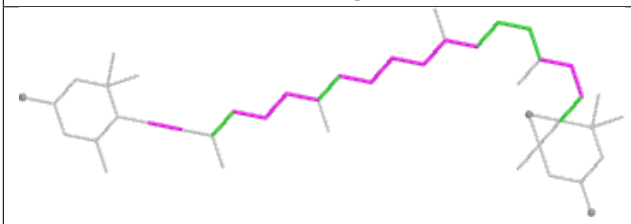
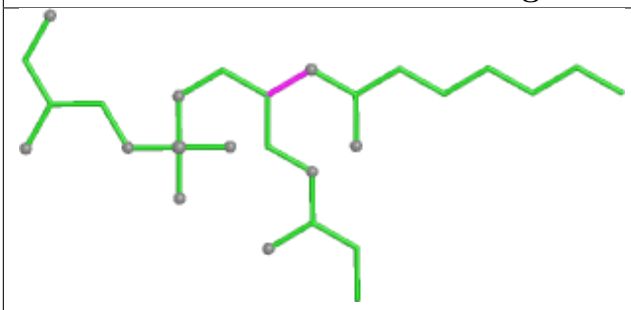
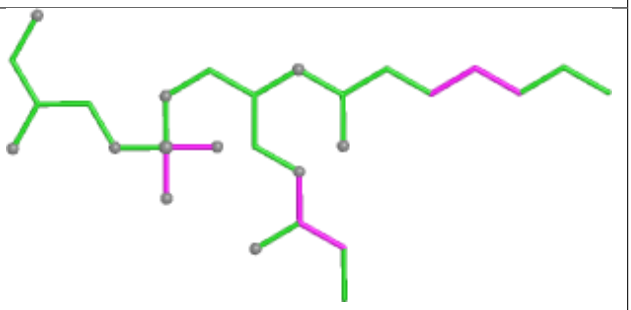
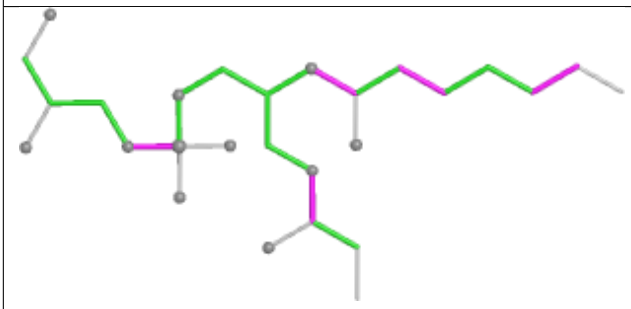
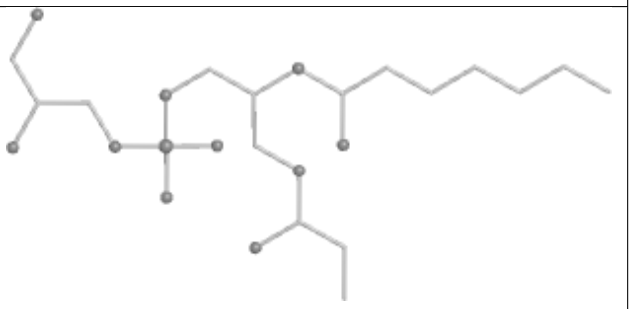
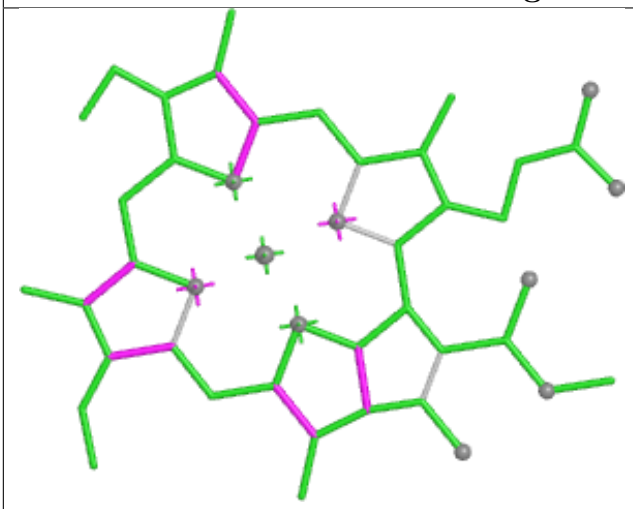
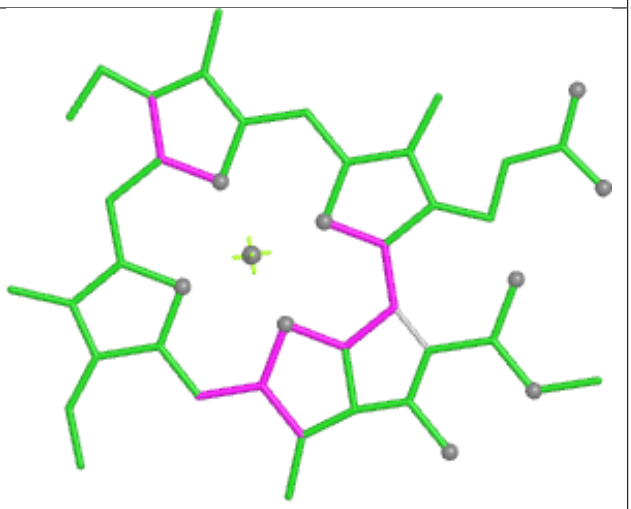
 Bond lengths	 Bond angles
 Torsions	Rings

Ligand LHG A 840	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

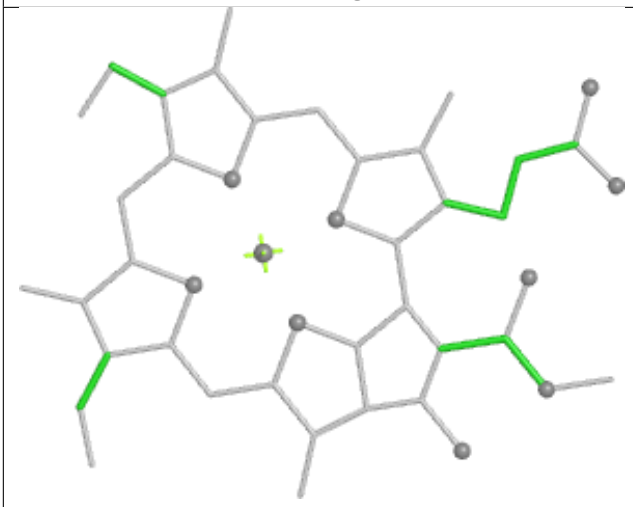
Ligand CLA R 202



Bond lengths



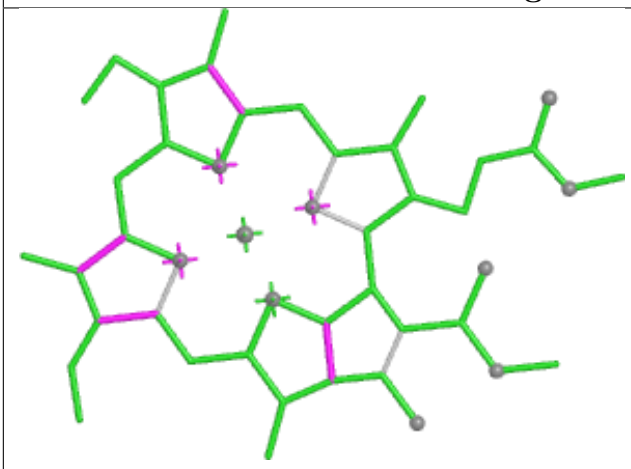
Bond angles



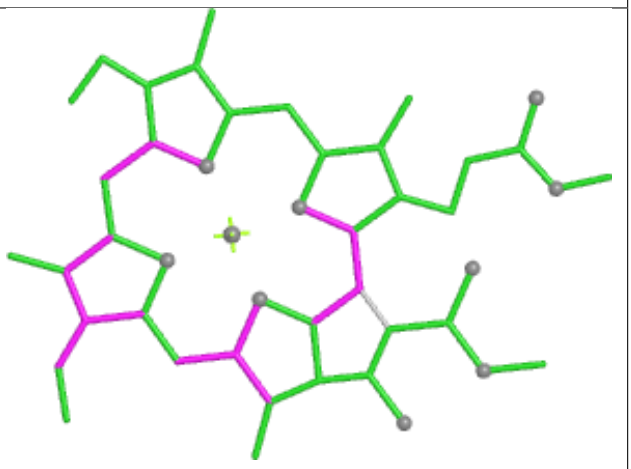
Torsions

Rings

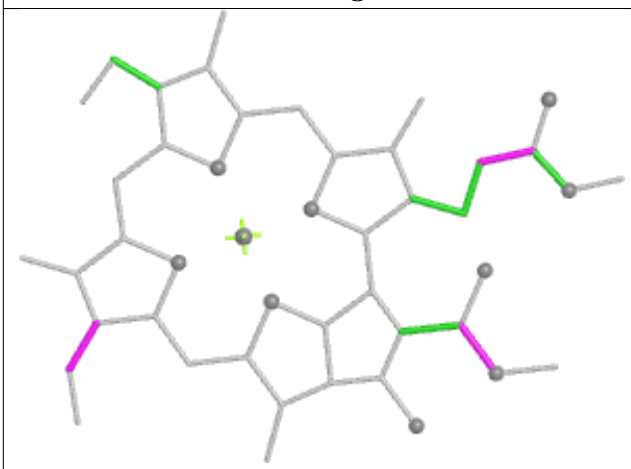
Ligand CLA T 211



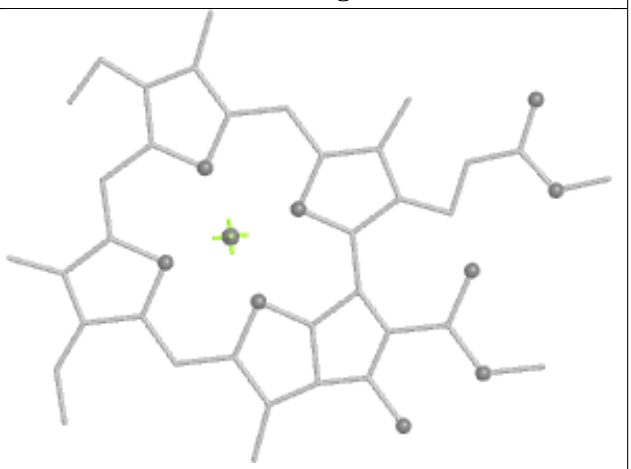
Bond lengths



Bond angles

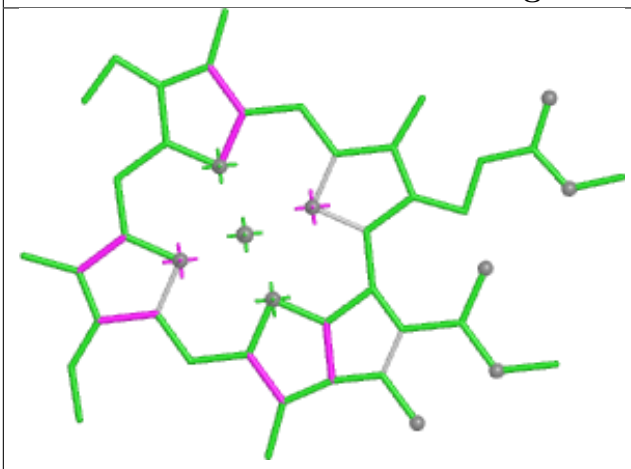


Torsions



Rings

Ligand CLA O 207



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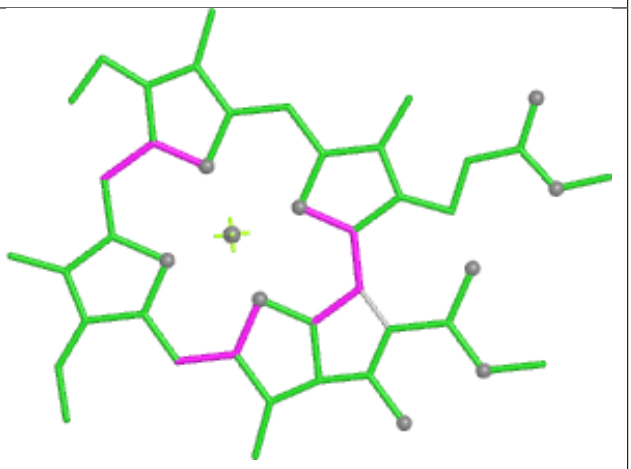
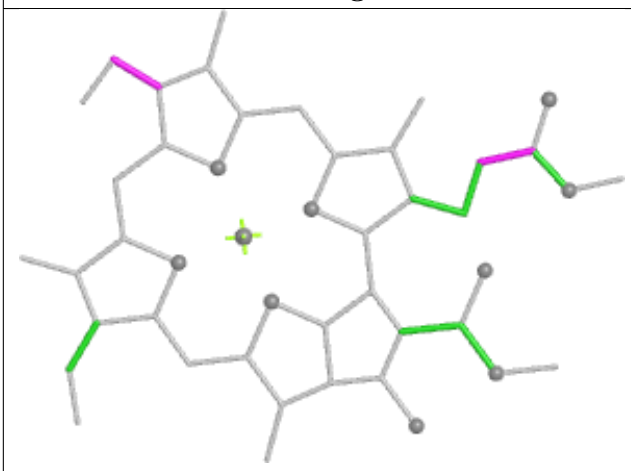
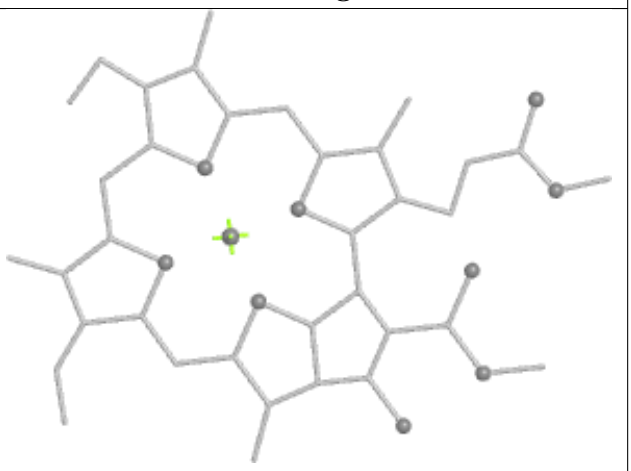


Bond angles

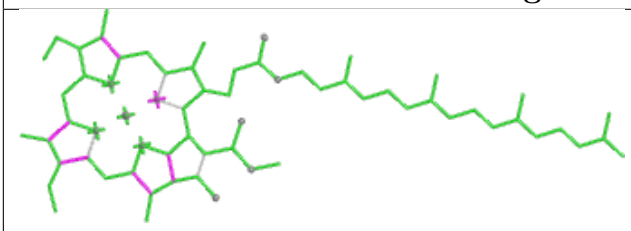


Torsions

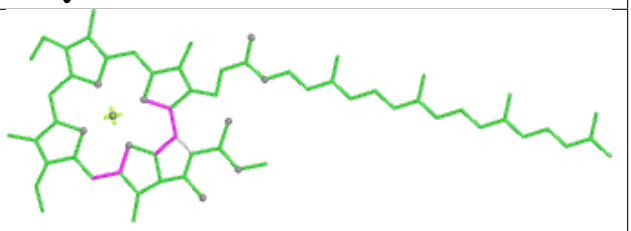


Rings

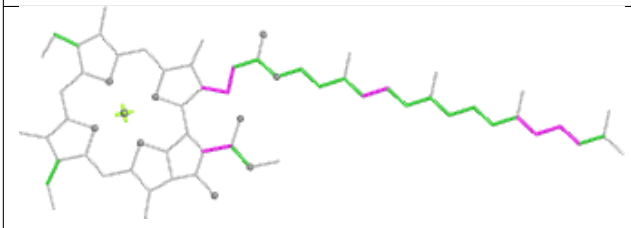
Ligand CLA Q 209



Bond lengths



Bond angles



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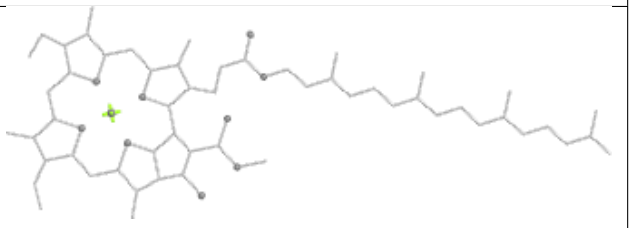
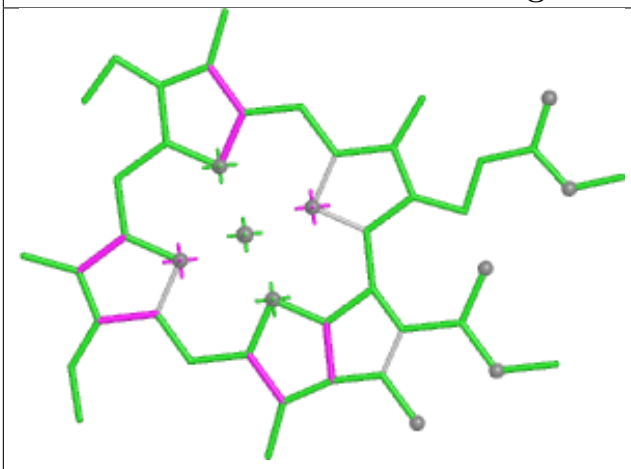
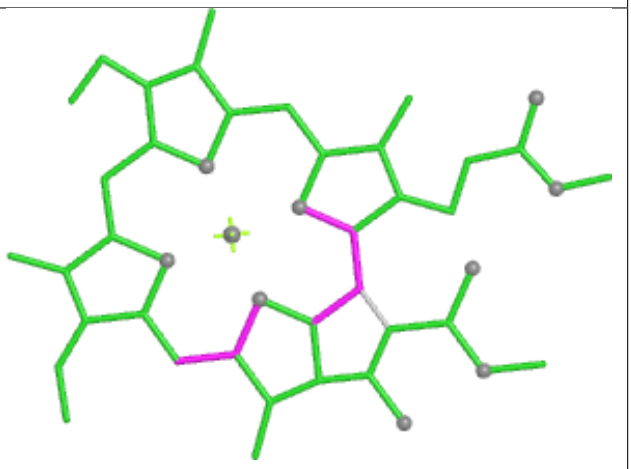


Rings

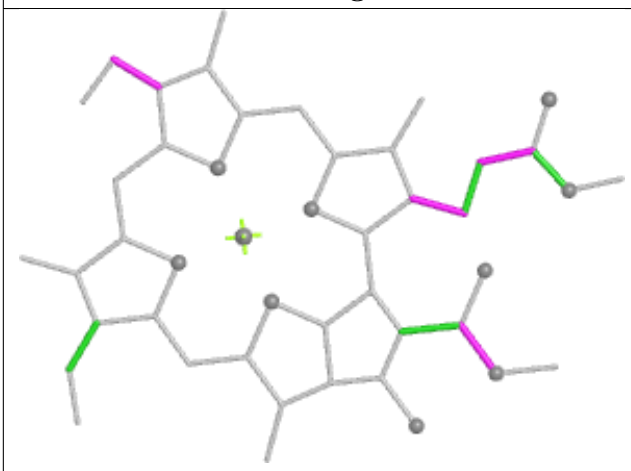
Ligand CLA S 205



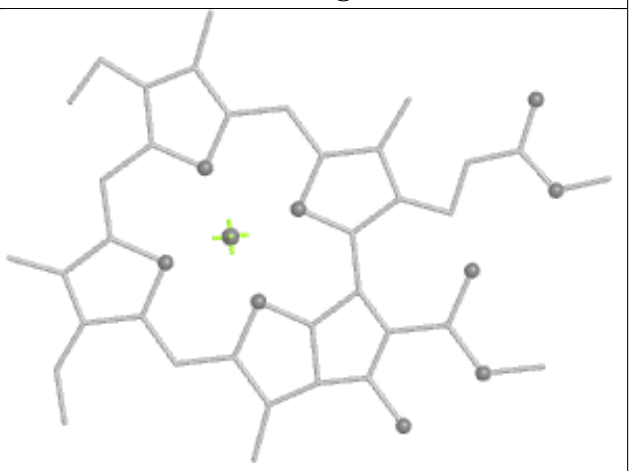
Bond lengths



Bond angles

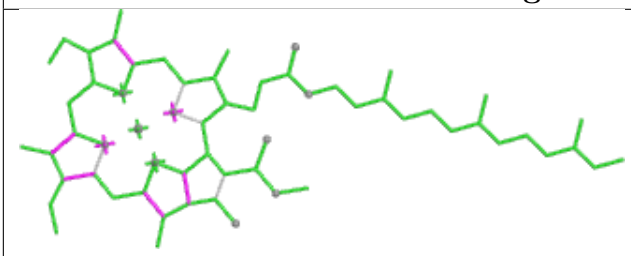


Torsions

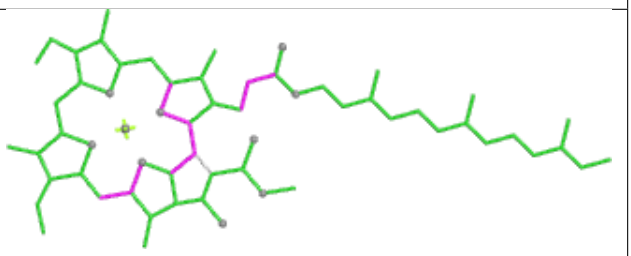


Rings

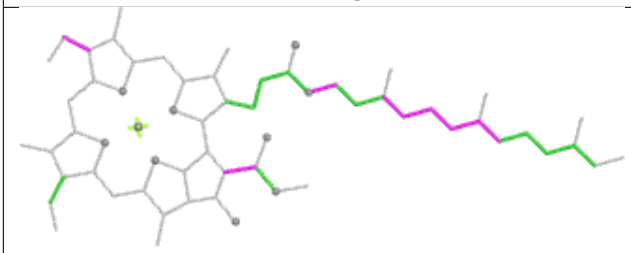
Ligand CLA U 204



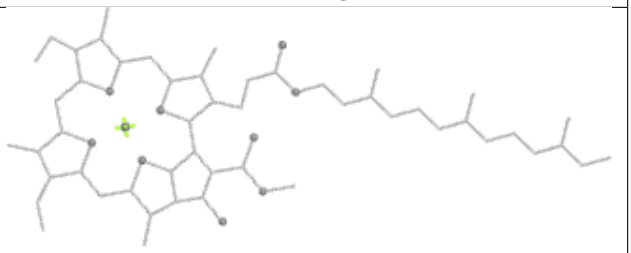
Bond lengths



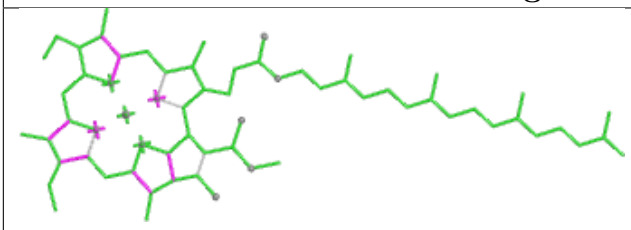
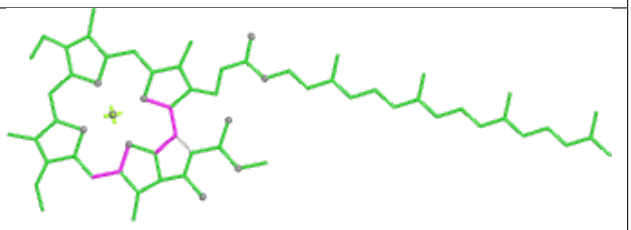
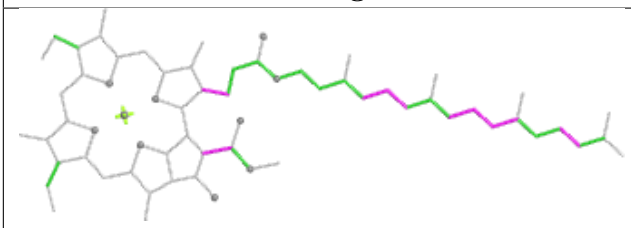
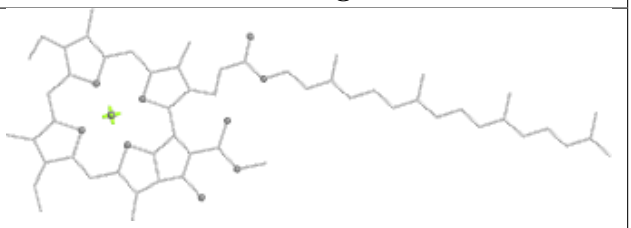
Bond angles

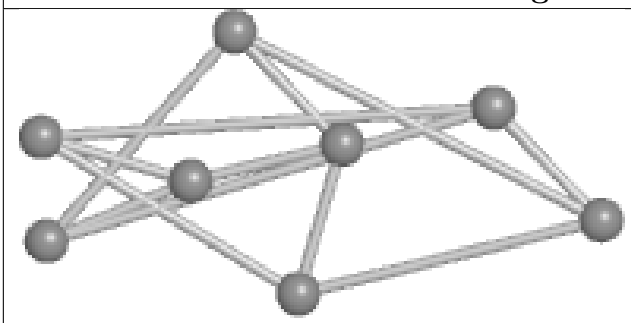
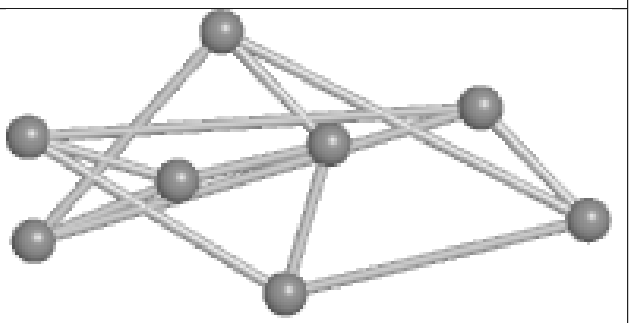
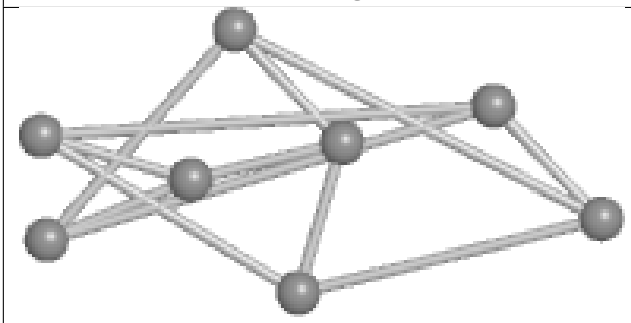
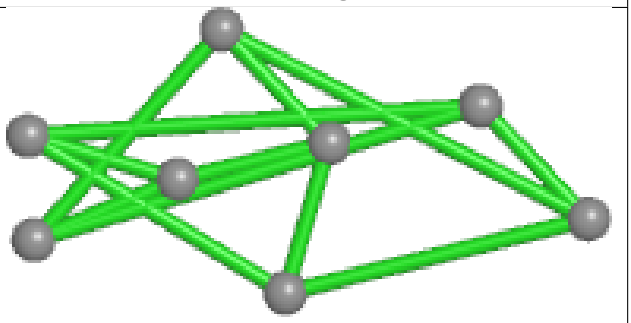


Torsions

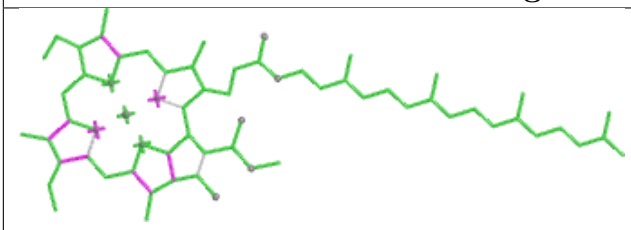


Rings

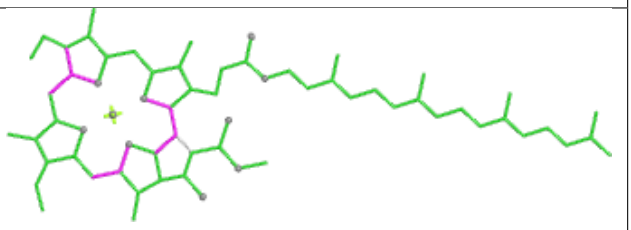
Ligand CLA A 851	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand SF4 C 101	
 Bond lengths	 Bond angles
 Torsions	 Rings

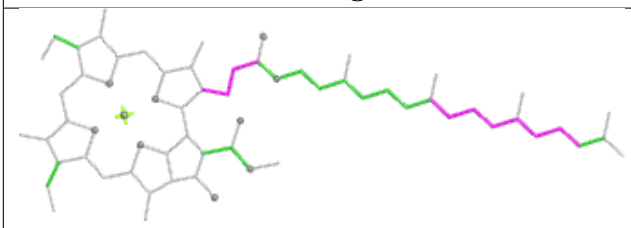
Ligand CLA A 815



Bond lengths



Bond angles



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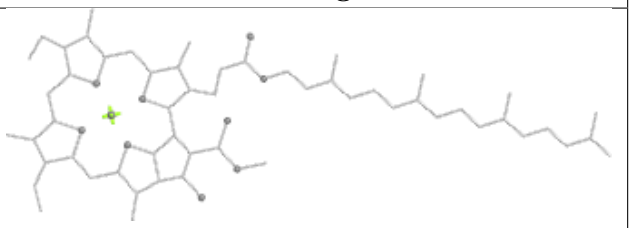
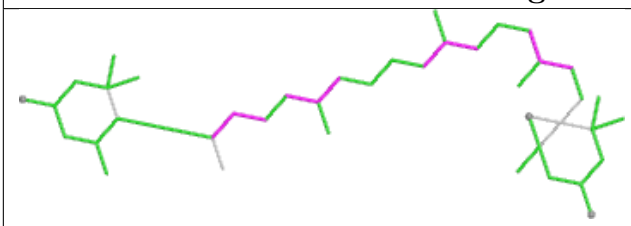
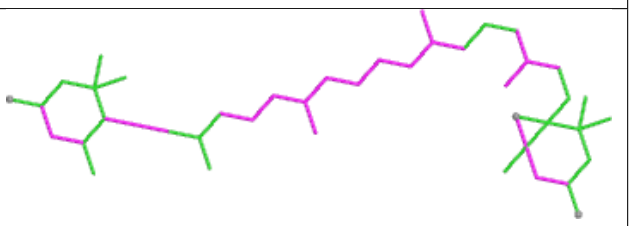


Rings

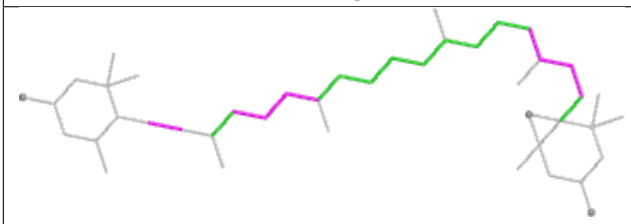
Ligand DD6 S 213



Bond lengths



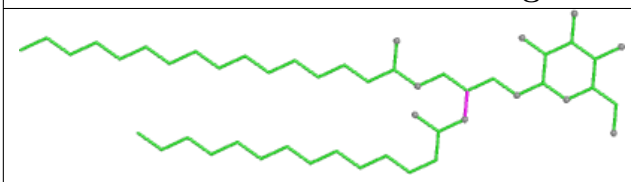
Bond angles



Torsions

Rings

Ligand LMG S 211



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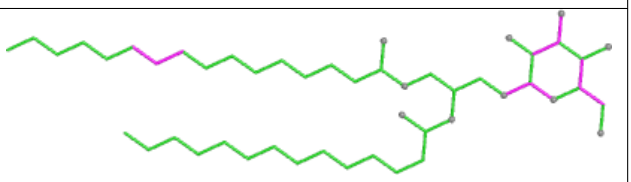

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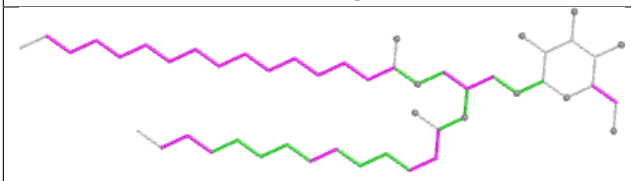

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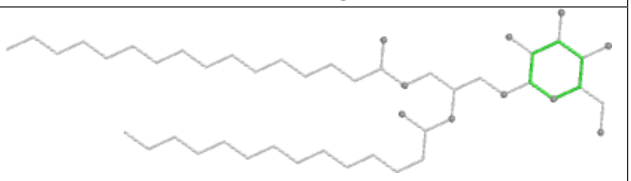
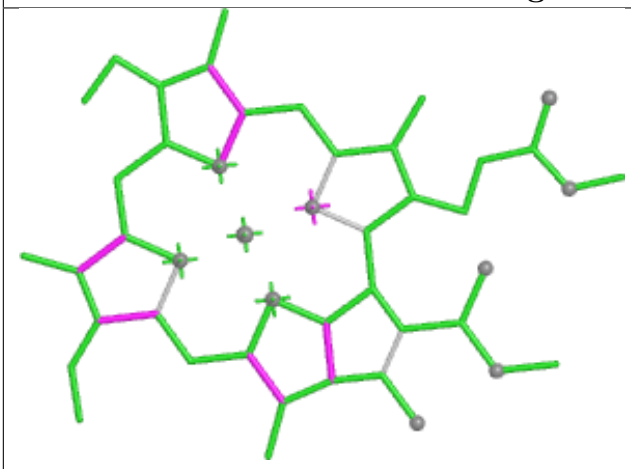


Rings

Ligand CLA S 204



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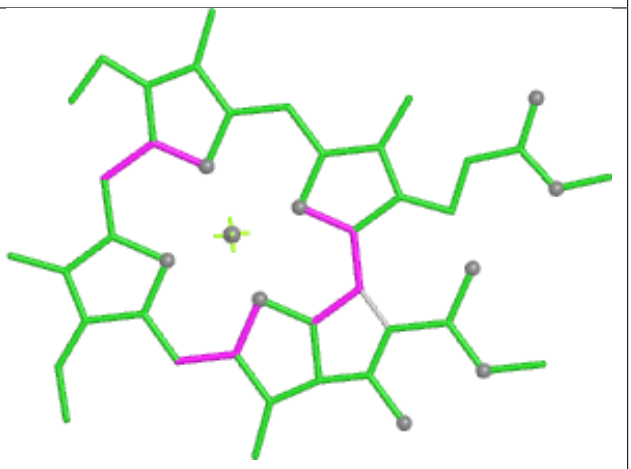
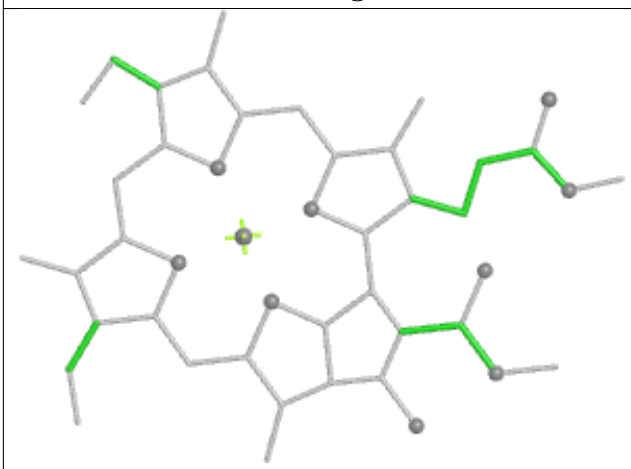


Bond angles



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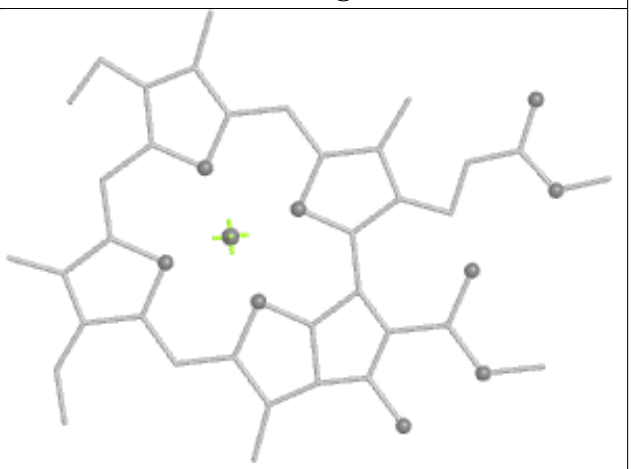
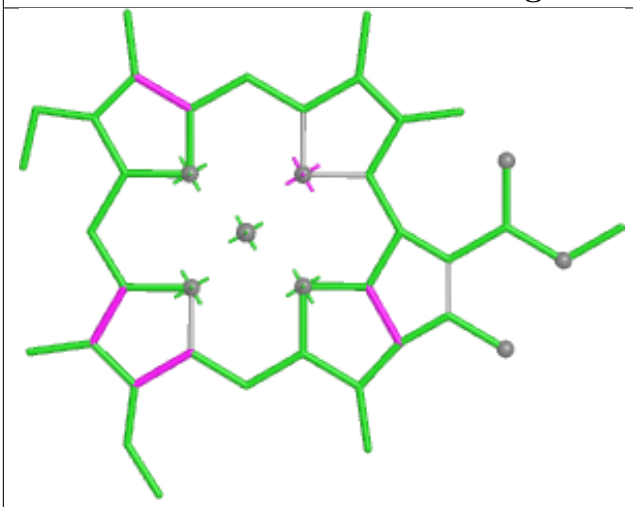


Rings

Ligand CLA T 210



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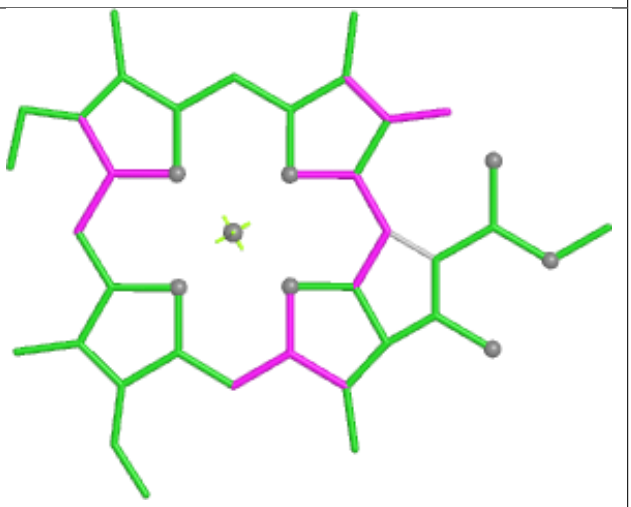

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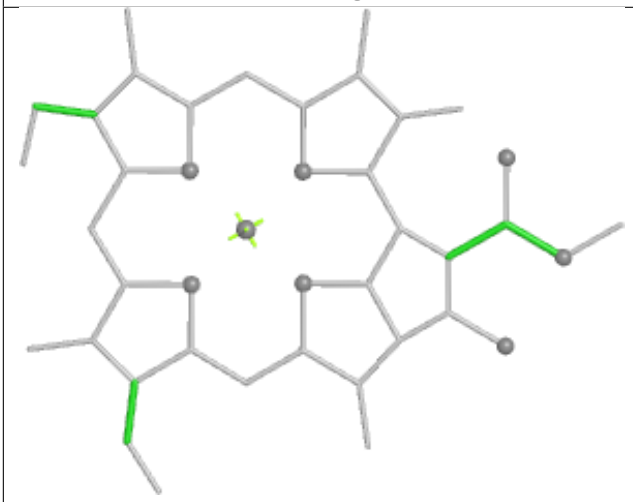

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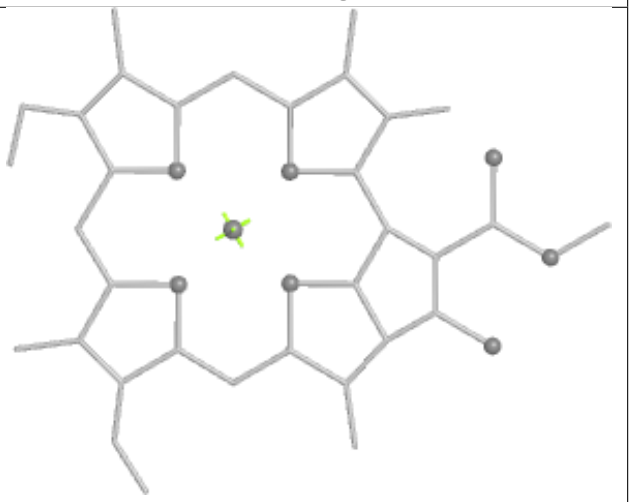
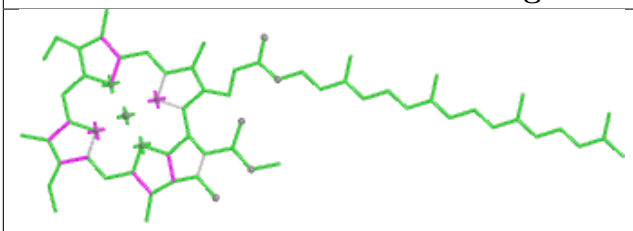


Rings

Ligand CLA A 807



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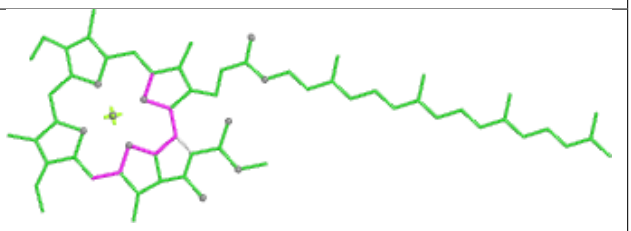
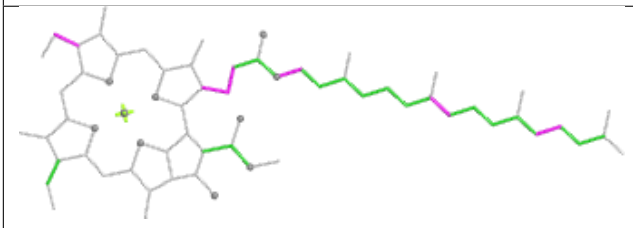
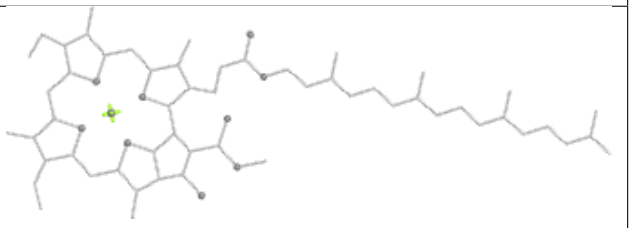


Bond angles

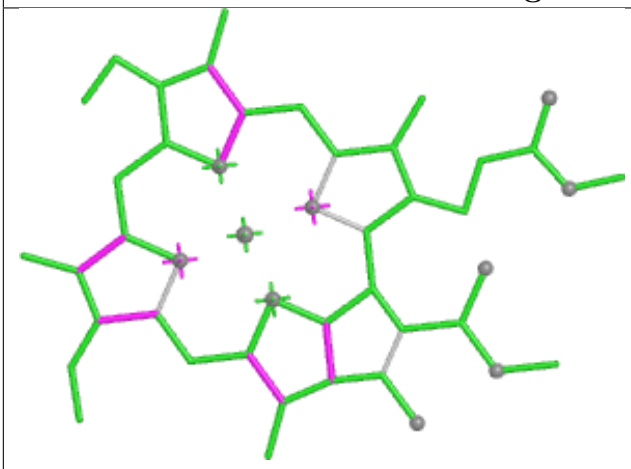


Torsions



Rings

Ligand CLA B 818



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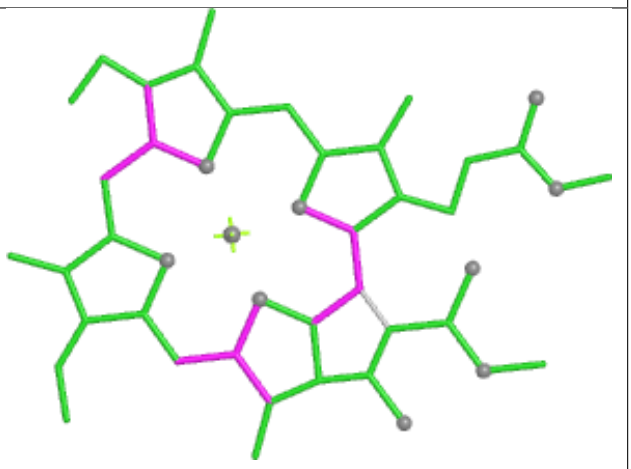
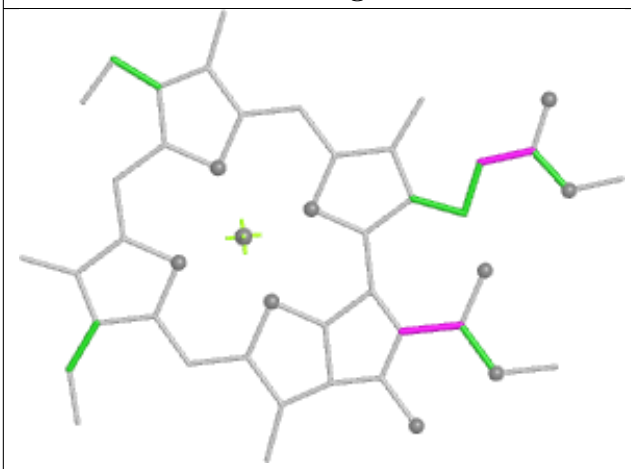


Bond angles



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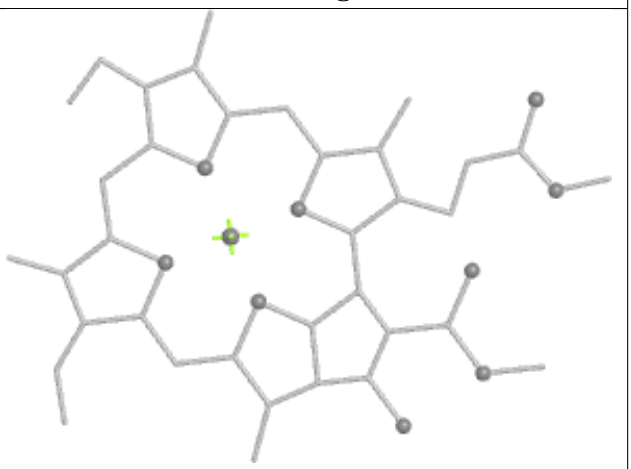
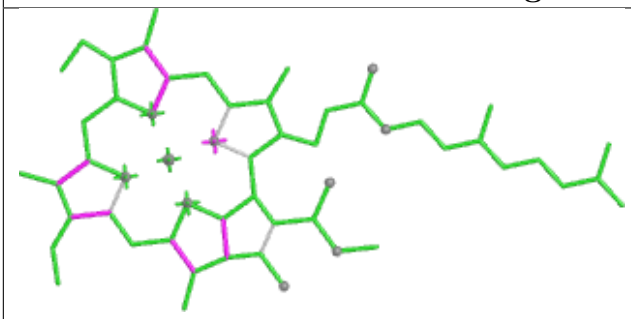
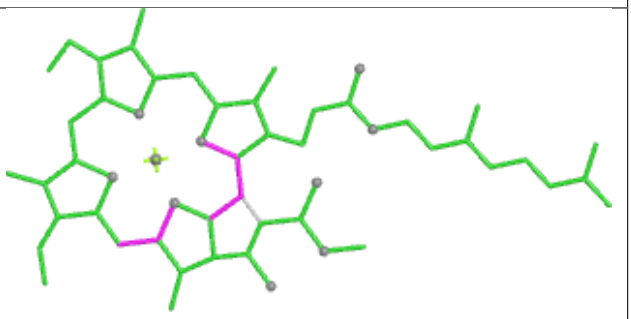
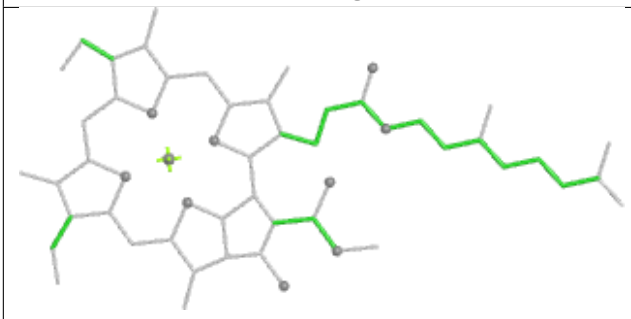
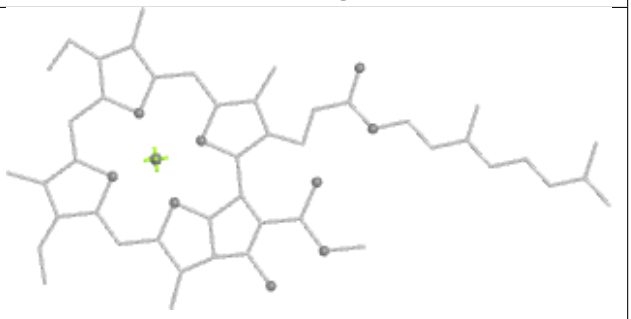


Rings

Ligand CLA B 811	
 Bond lengths	 Bond angles
 Torsions	 Rings

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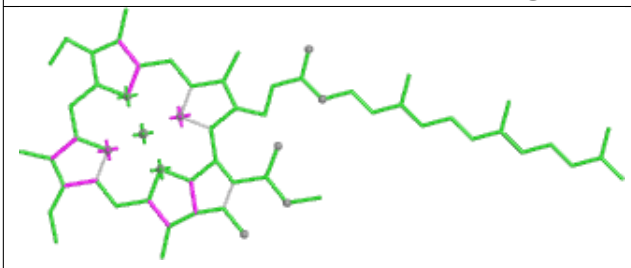
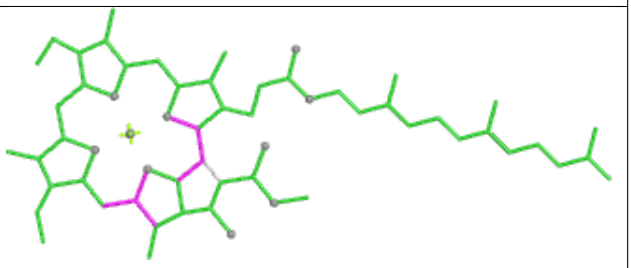
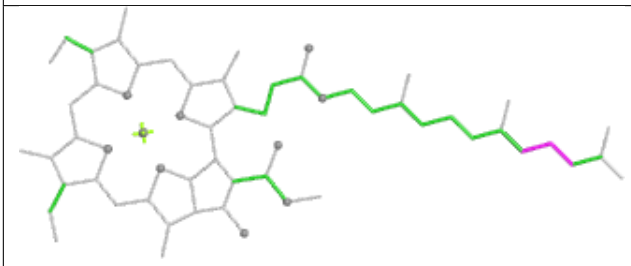
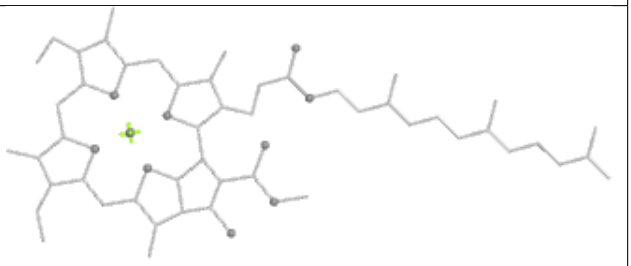
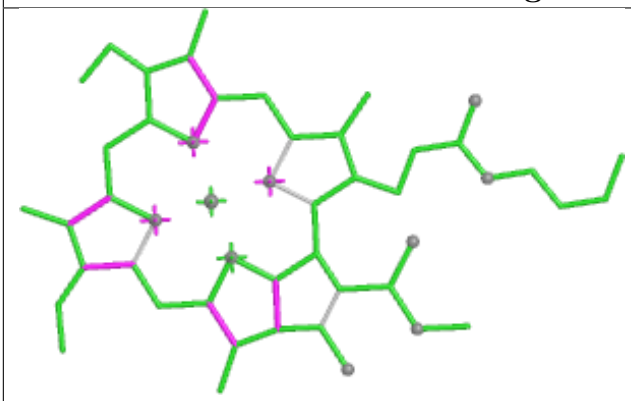
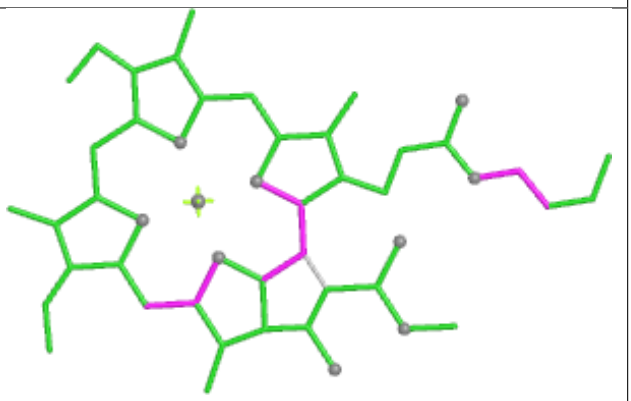
 Bond lengths	 Bond angles
 Torsions	 Rings

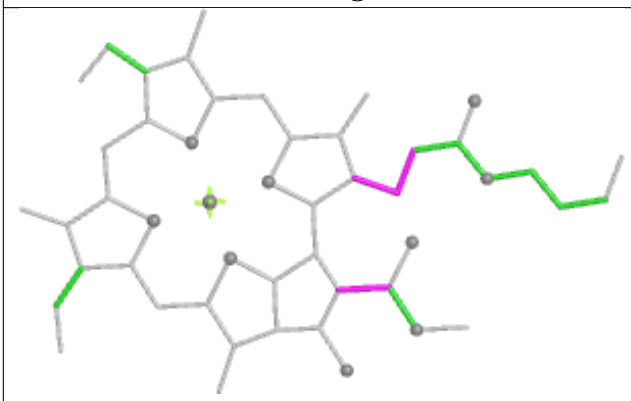
Ligand CLA B 813



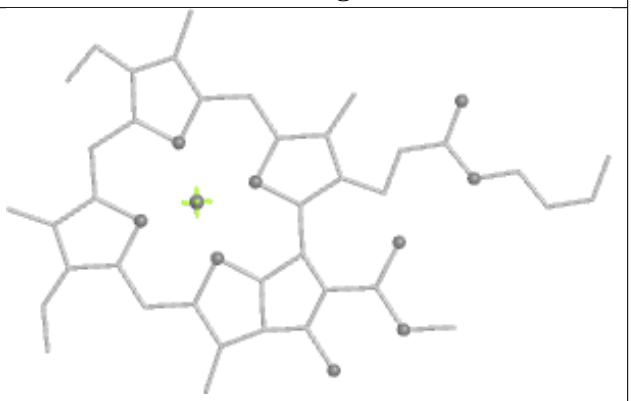
Bond lengths



Bond angles

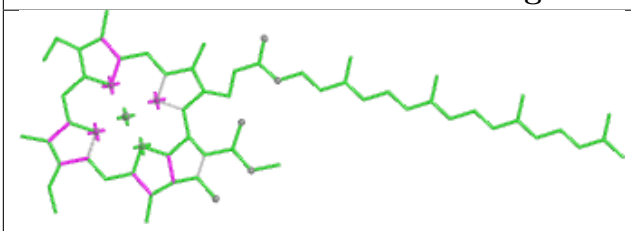


Torsions



Rings

Ligand CLA B 845



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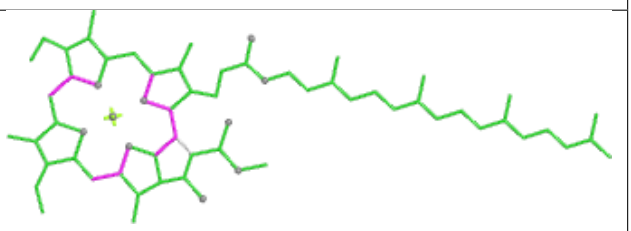
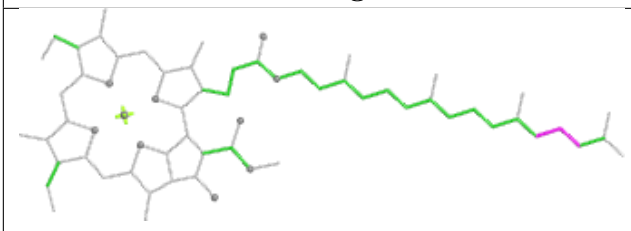
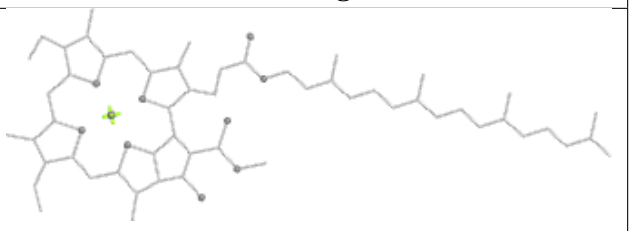


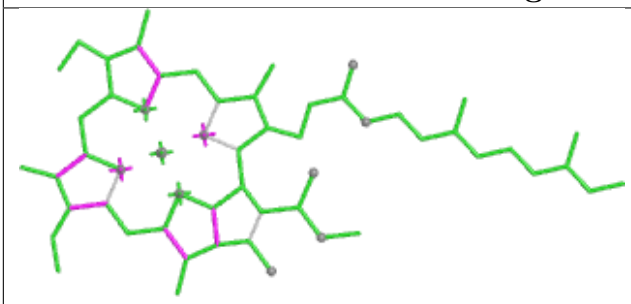
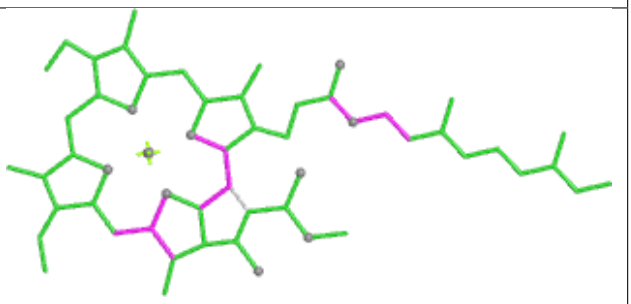
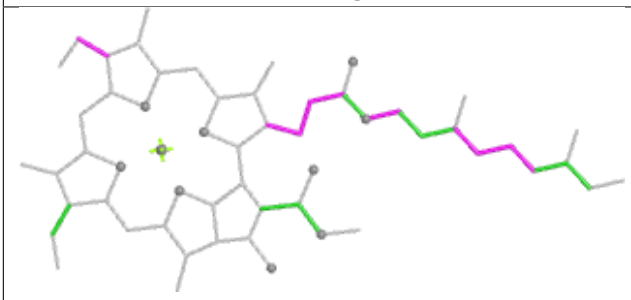
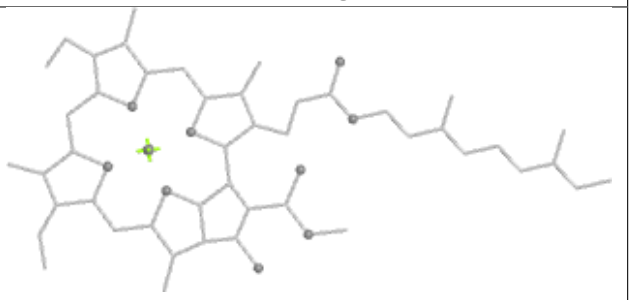
Bond angles

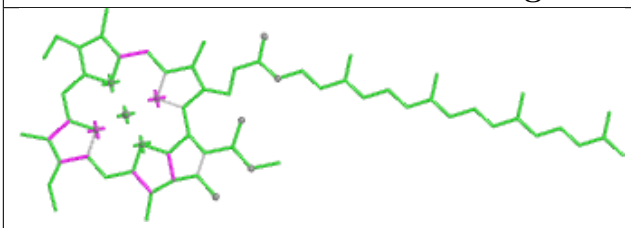
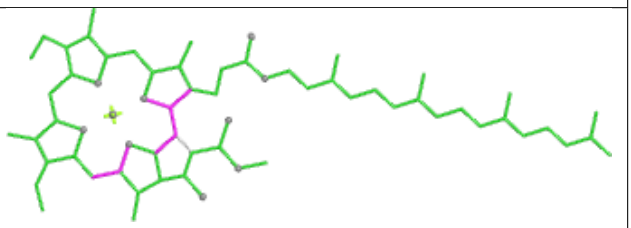
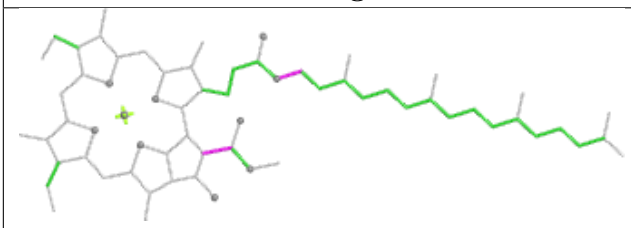
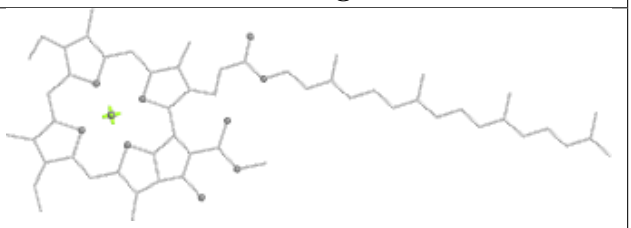


Torsions

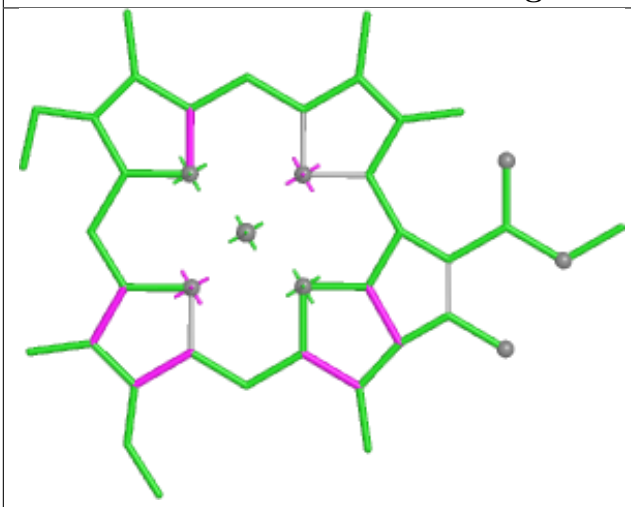


Rings

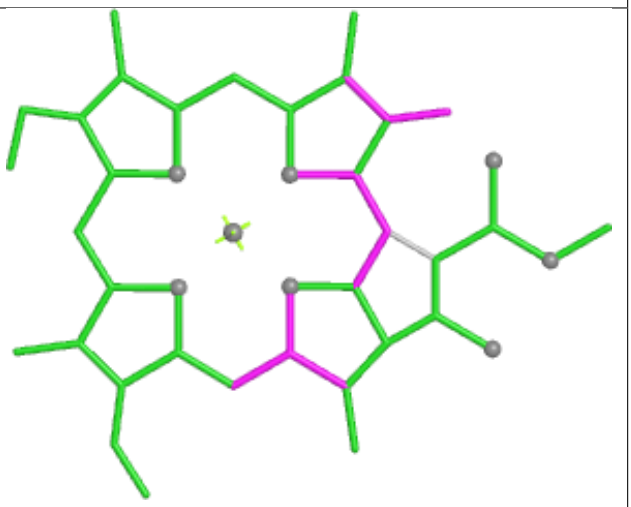
Ligand CLA P 307	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA B 802	
 Bond lengths	 Bond angles
 Torsions	 Rings

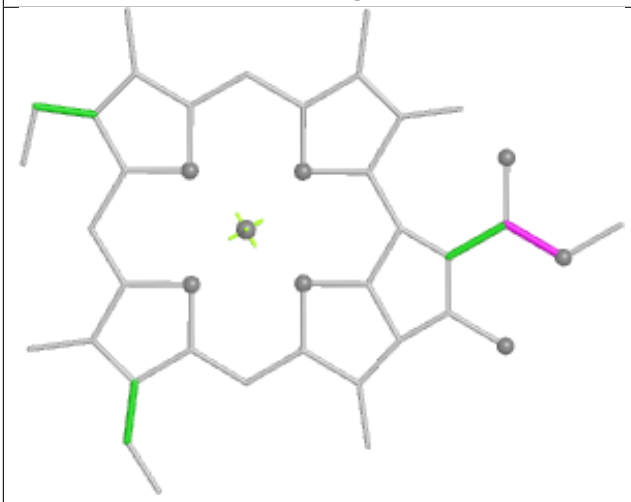
Ligand CLA P 312



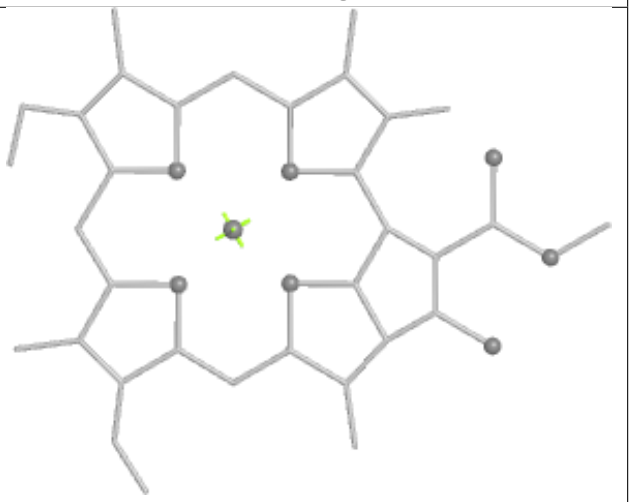
Bond lengths



Bond angles

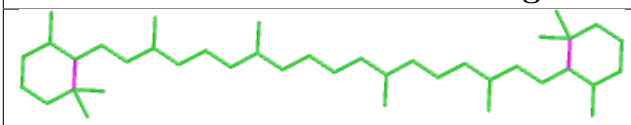


Torsions

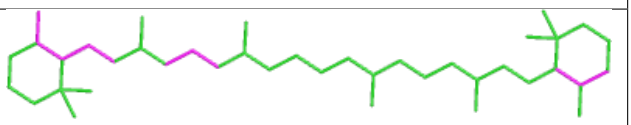


Rings

Ligand BCR B 841



Bond lengths



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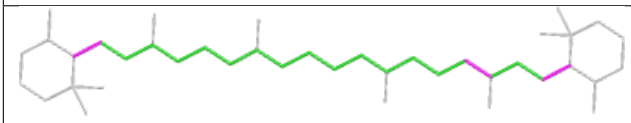
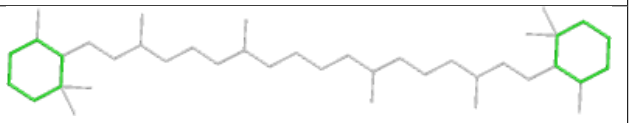
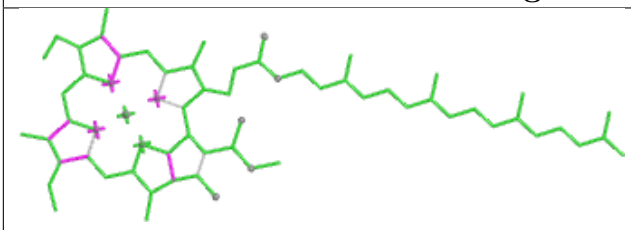
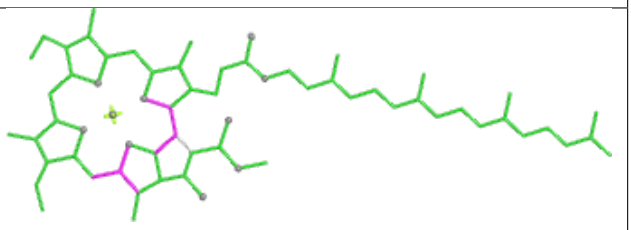
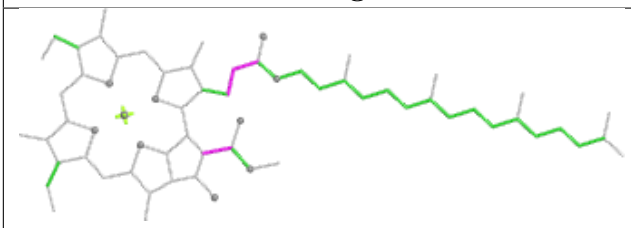
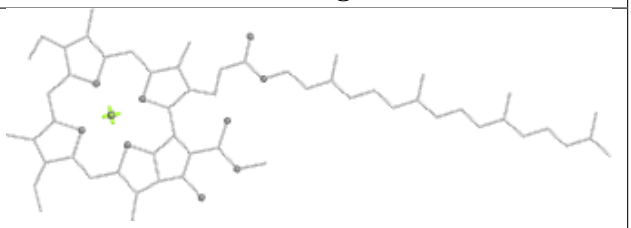
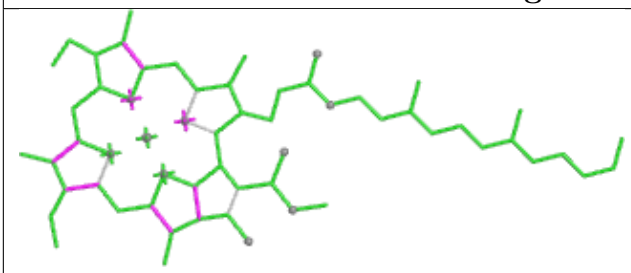
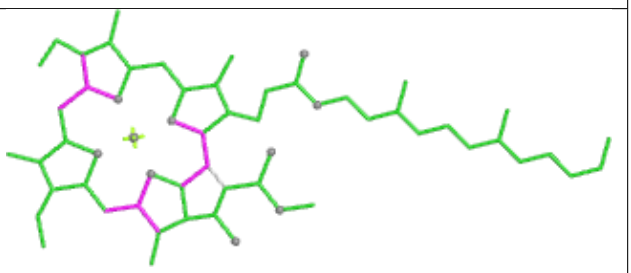
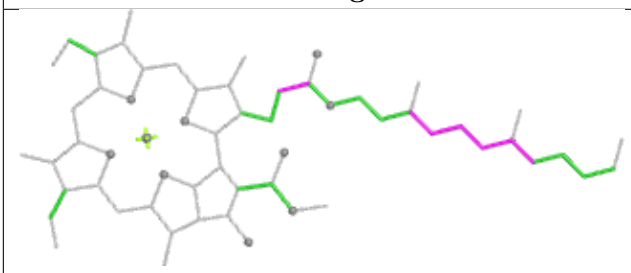
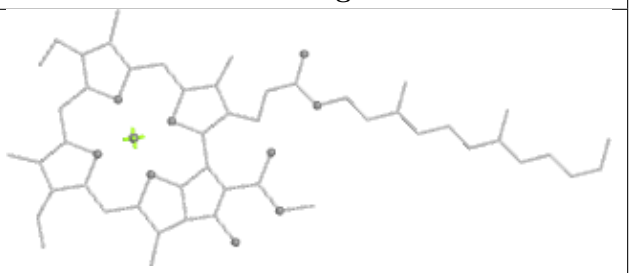


Torsions

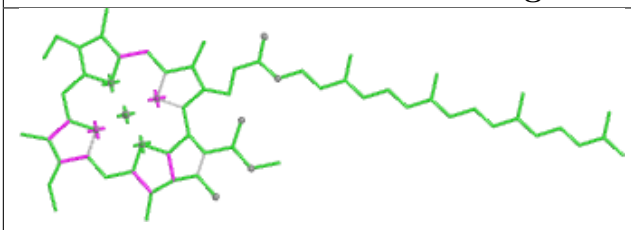


Rings

Ligand CLA A 803	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA B 815	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA B 823



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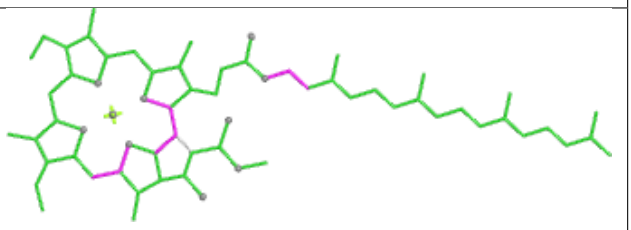
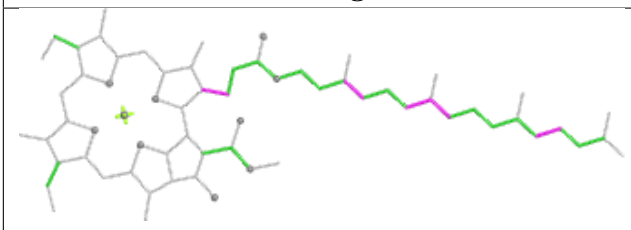
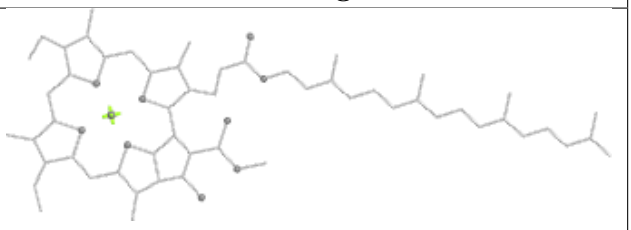


Bond angles

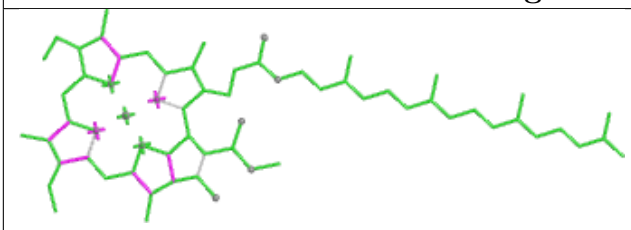


Torsions

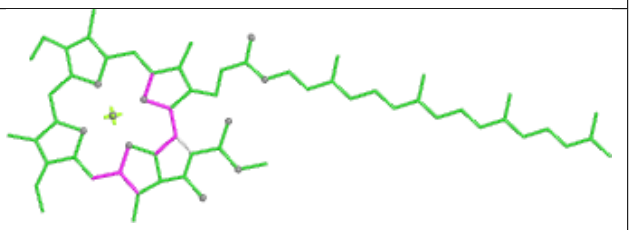


Rings

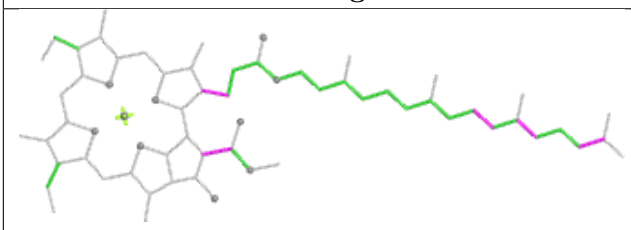
Ligand CLA B 825



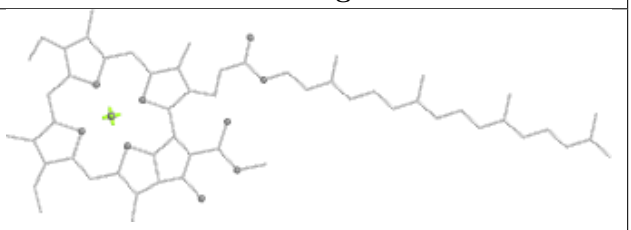
Bond lengths



Bond angles

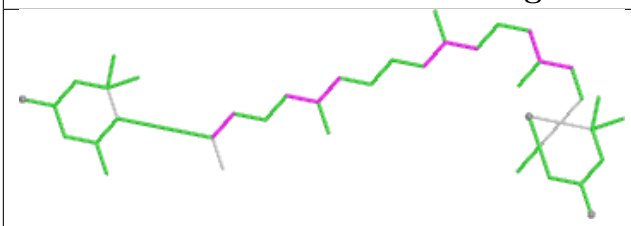


Torsions

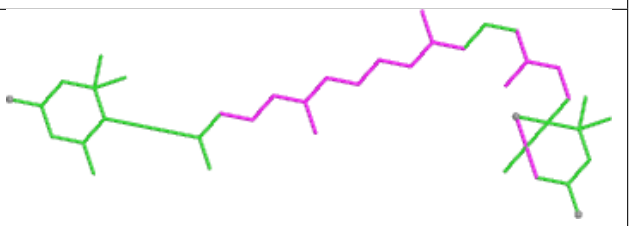


Rings

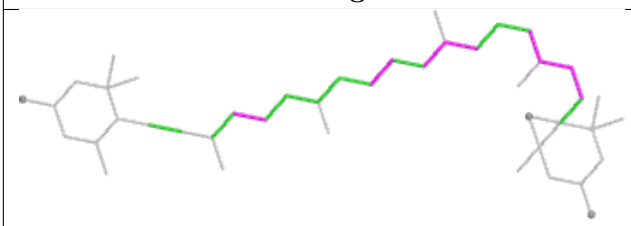
Ligand DD6 U 212



Bond lengths



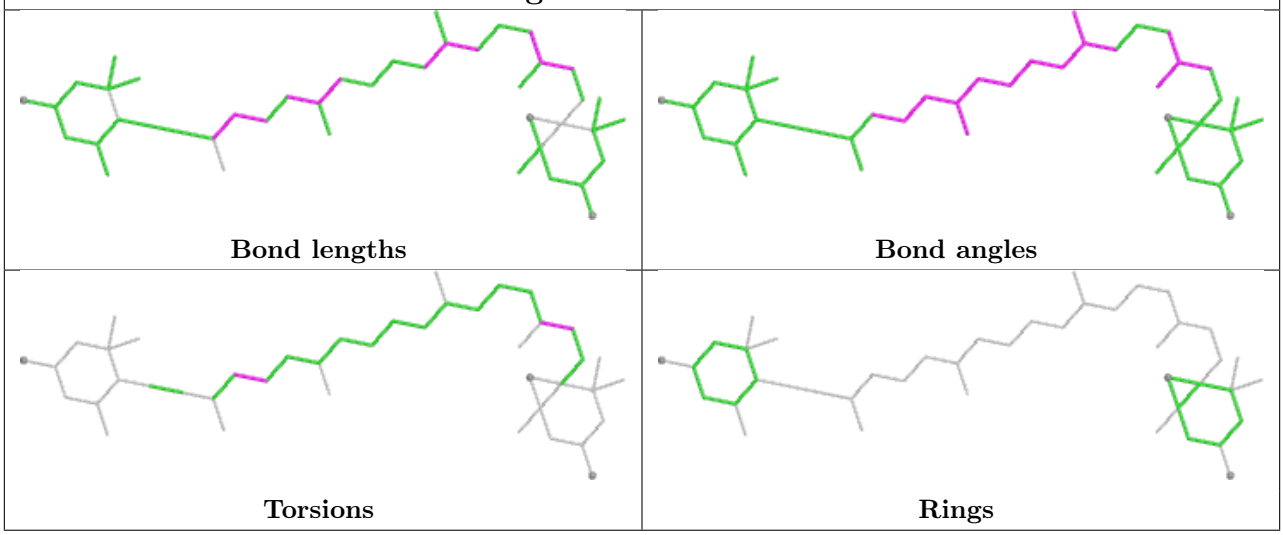
Bond angles



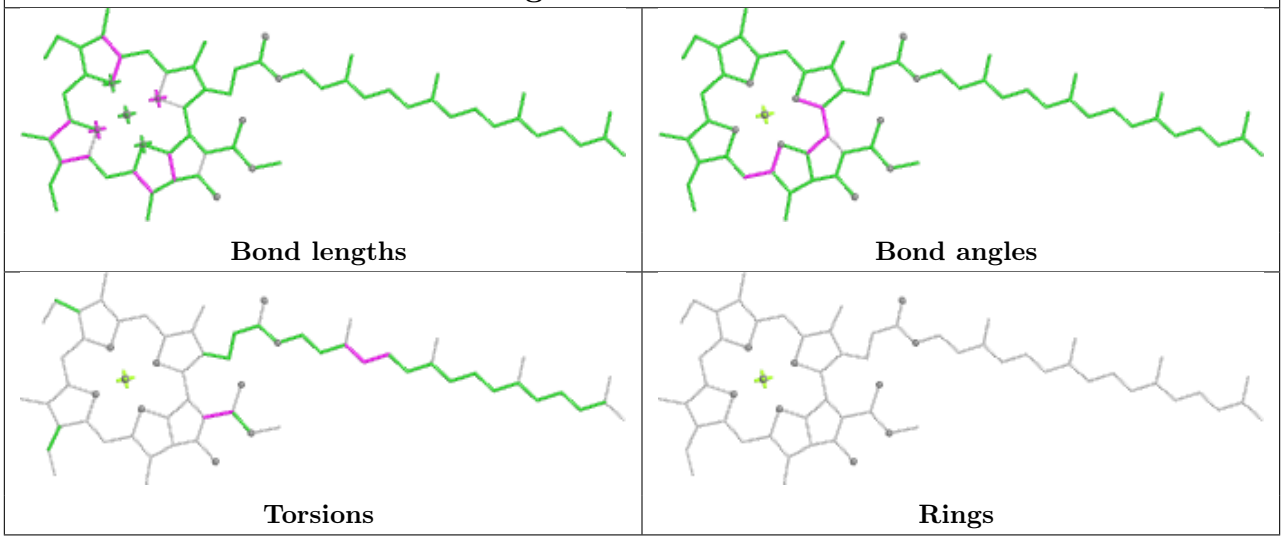
Torsions

Rings

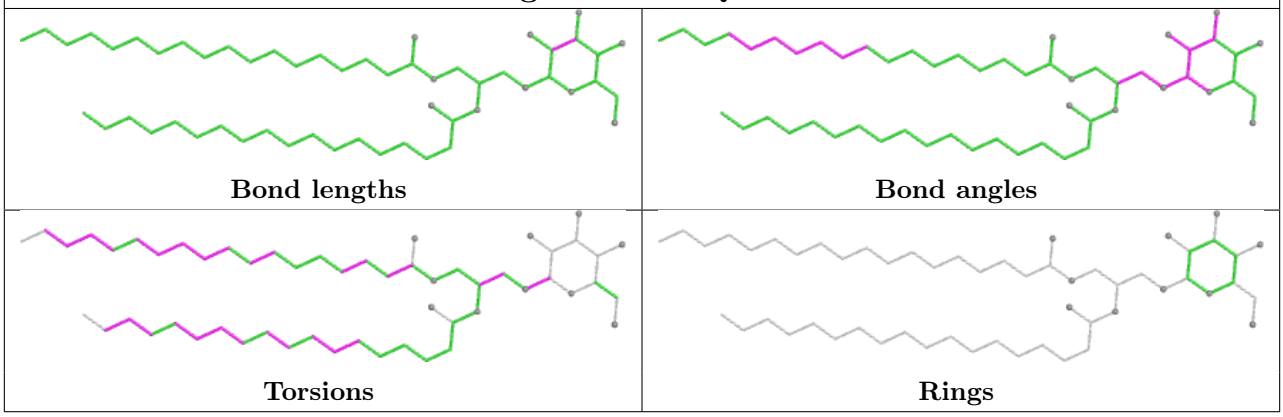
Ligand DD6 O 201

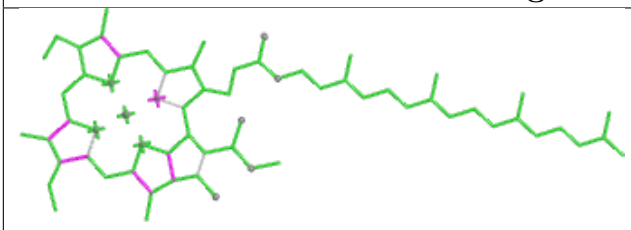
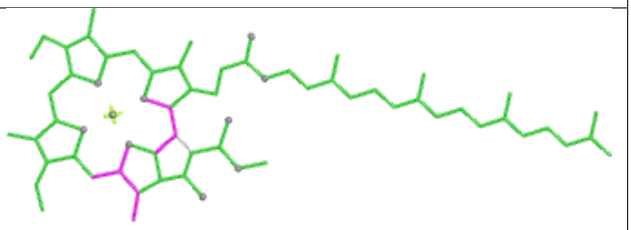
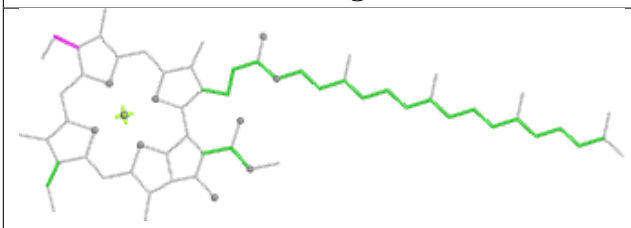
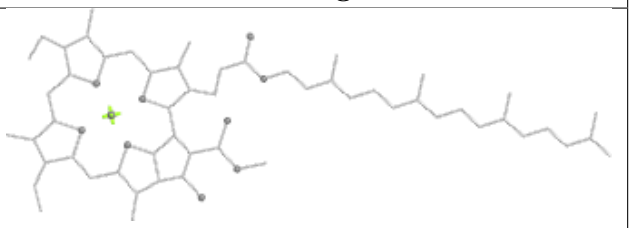


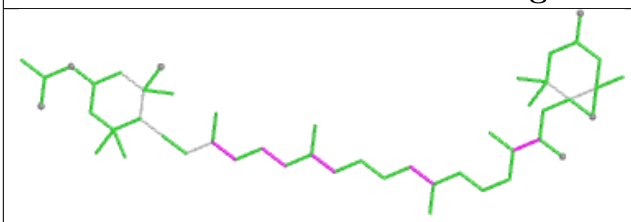
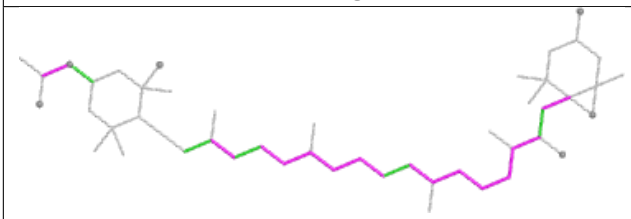
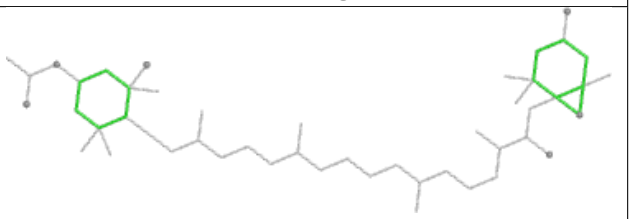
Ligand CLA B 808

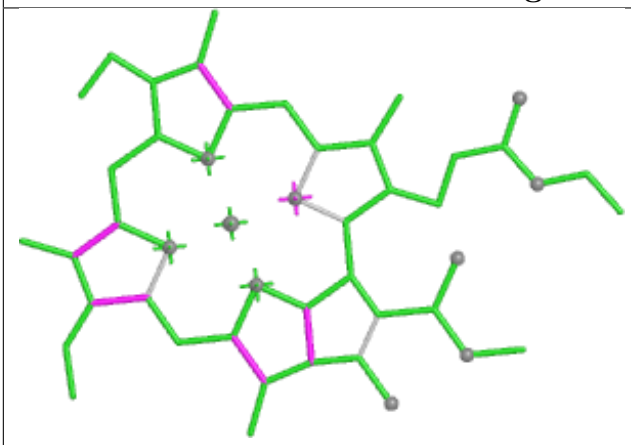
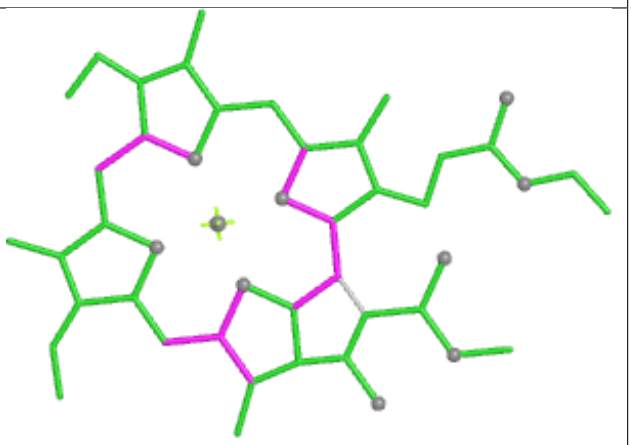
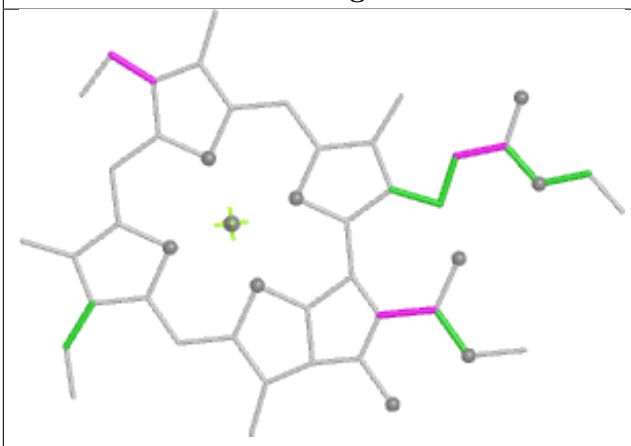
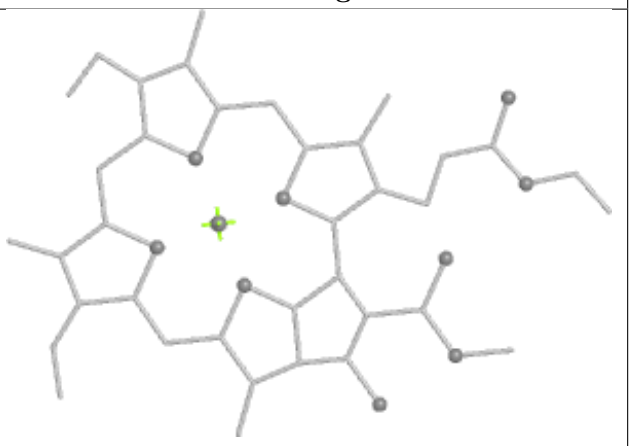


Ligand LMG Q 217

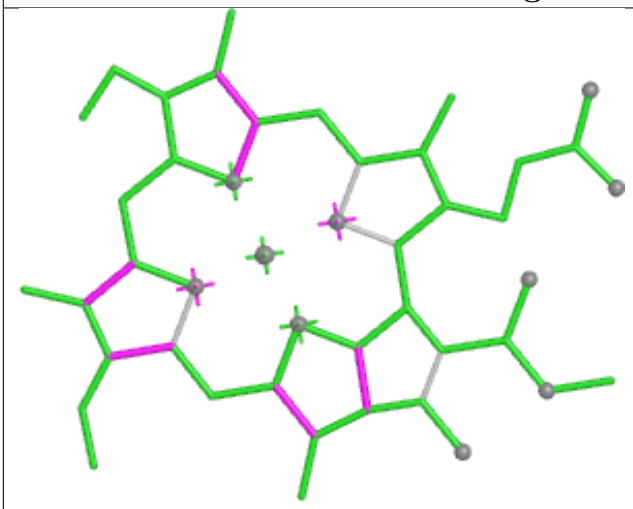


Ligand CLA S 214	
 Bond lengths	 Bond angles
 Torsions	 Rings

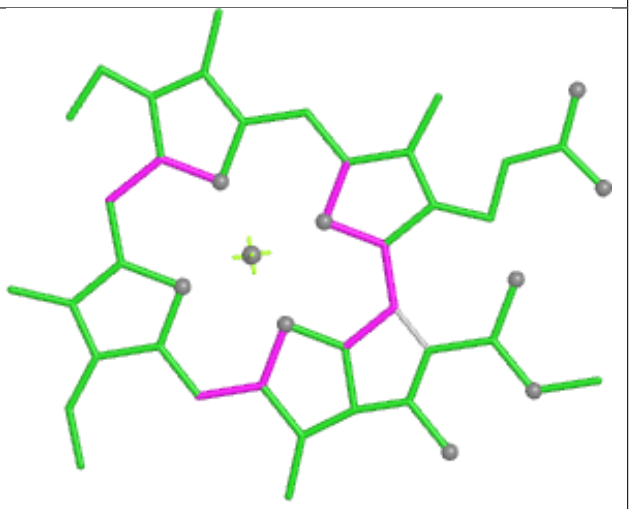
Ligand A86 Q 201	
 Bond lengths	Bond angles
 Torsions	 Rings

Ligand CLA T 212	
 Bond lengths	 Bond angles
 Torsions	 Rings

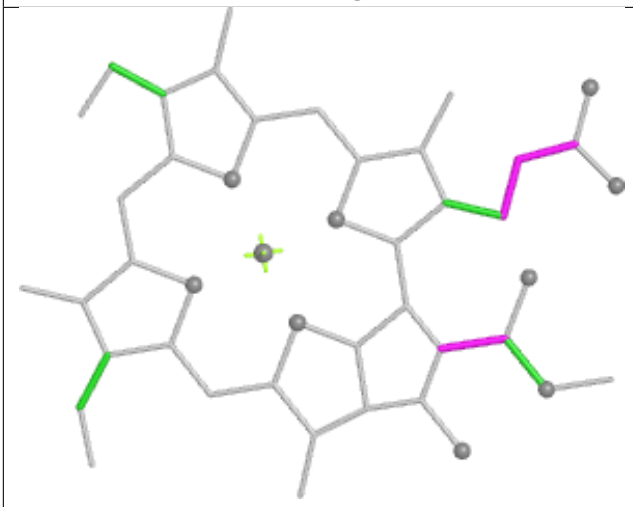
Ligand CLA A 814



Bond lengths



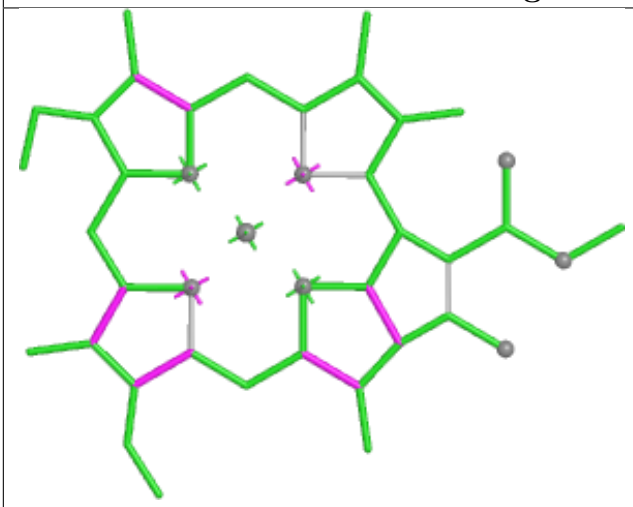
Bond angles



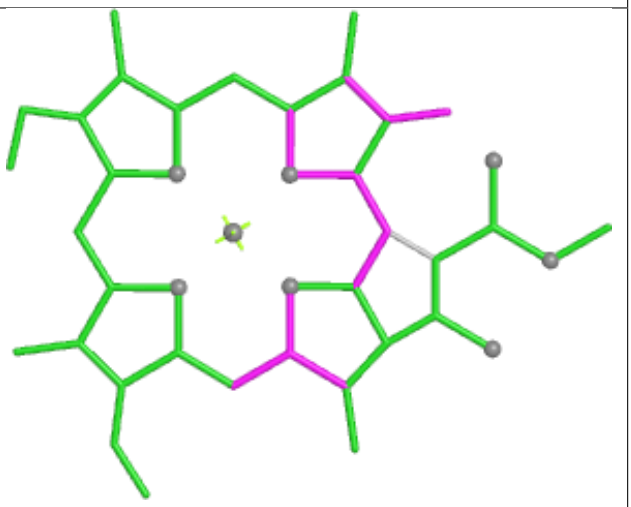
Torsions

Rings

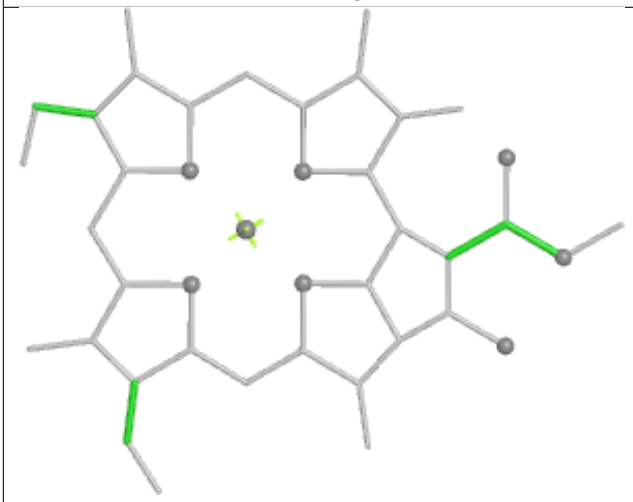
Ligand CLA O 211



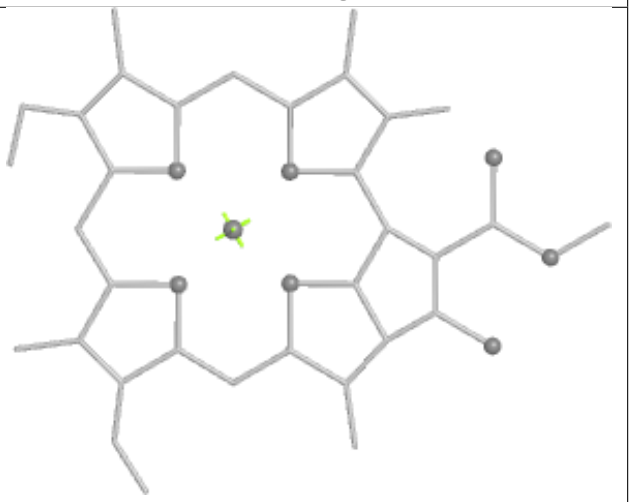
Bond lengths



Bond angles

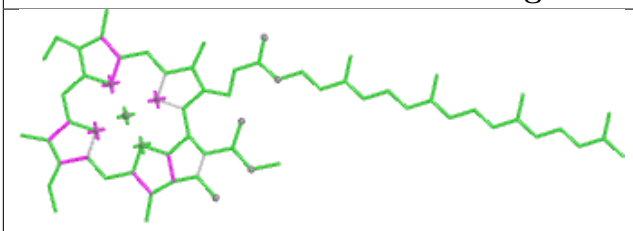


Torsions

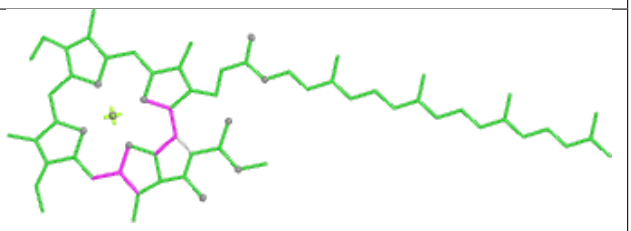


Rings

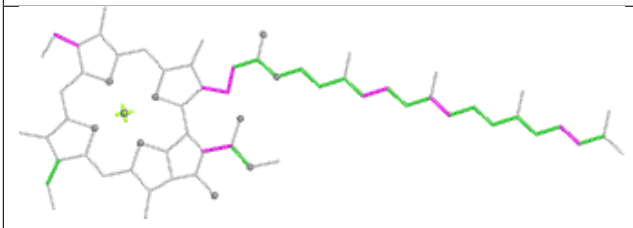
Ligand CLA B 805



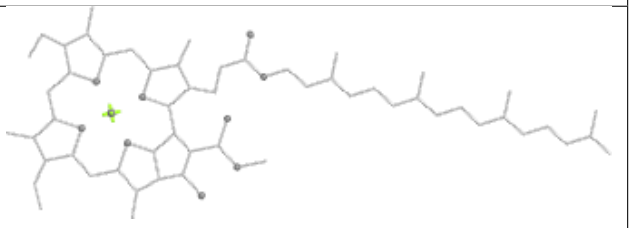
Bond lengths



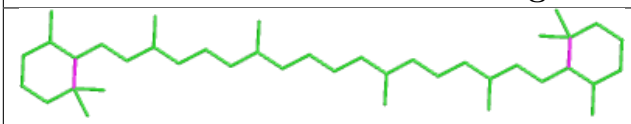
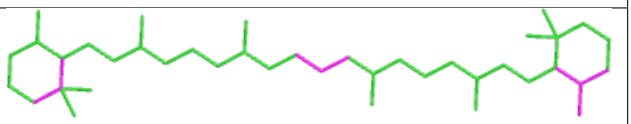
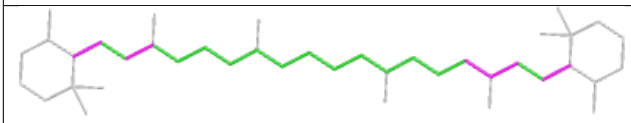
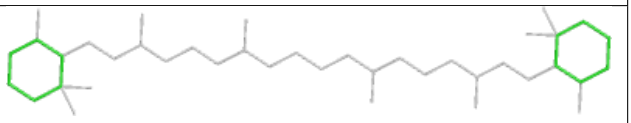
Bond angles

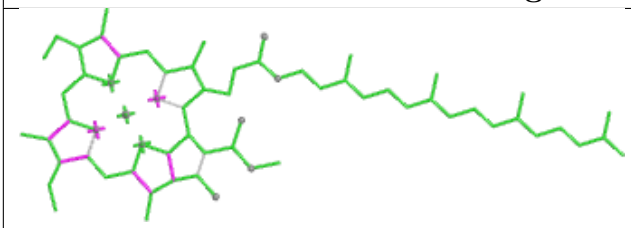
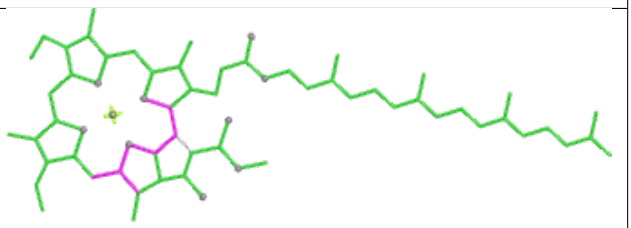
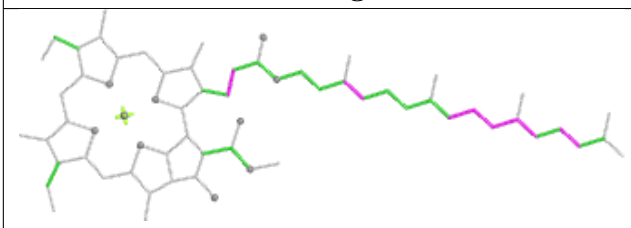
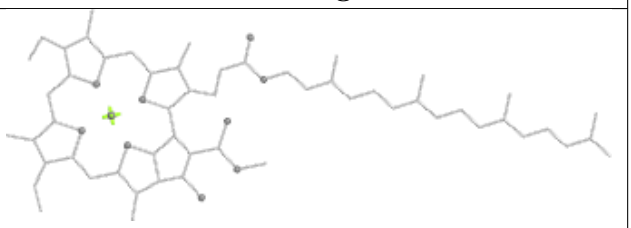


Torsions

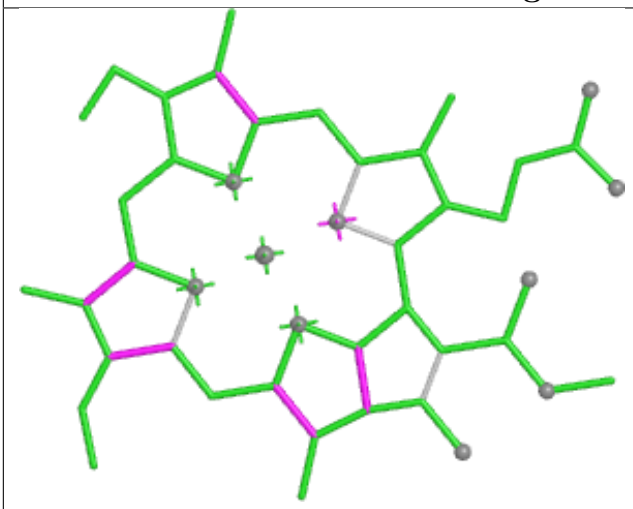


Rings

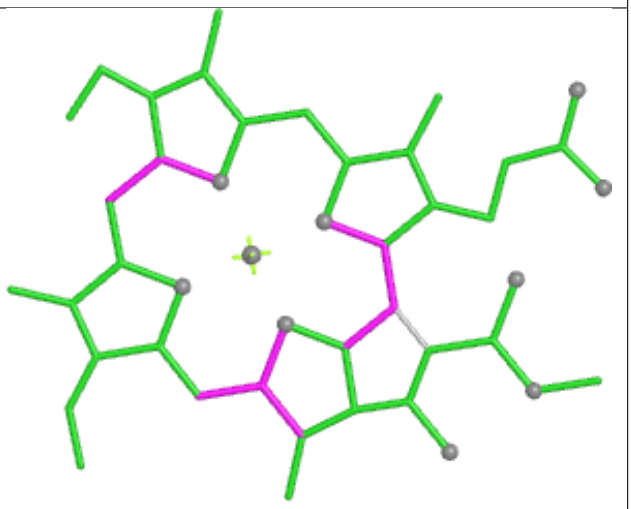
Ligand BCR I 102	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA P 306	
 Bond lengths	 Bond angles
 Torsions	 Rings

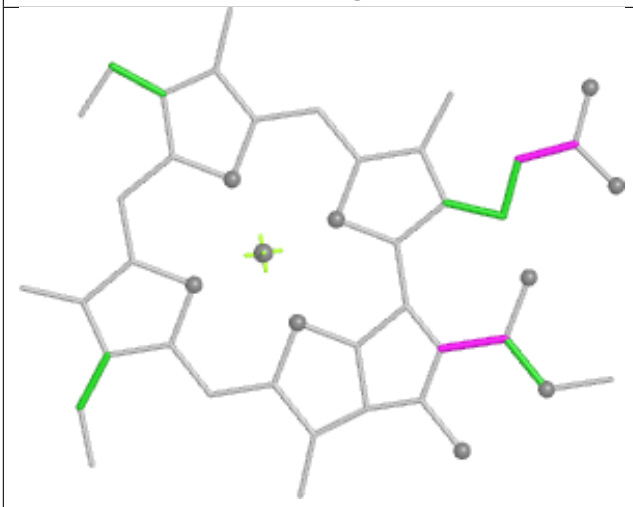
Ligand CLA U 206



Bond lengths



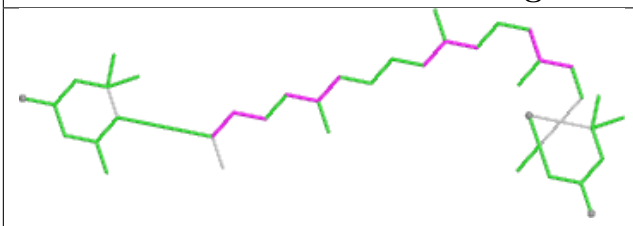
Bond angles



Torsions

Rings

Ligand DD6 O 215



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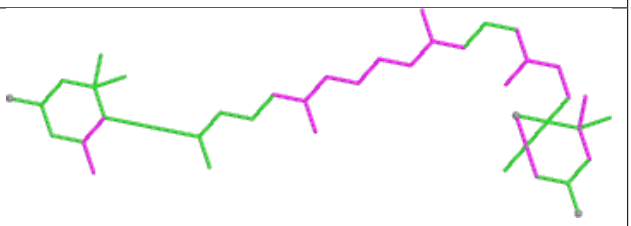
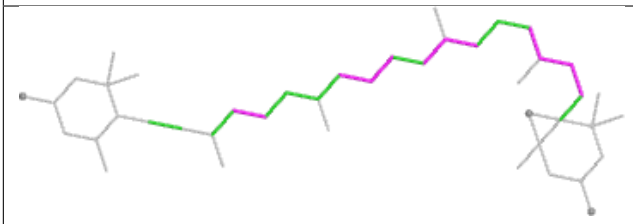
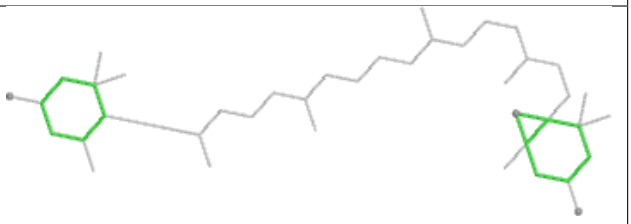


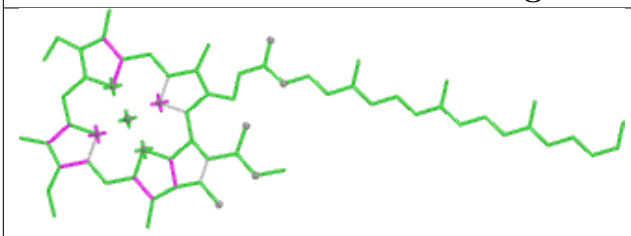
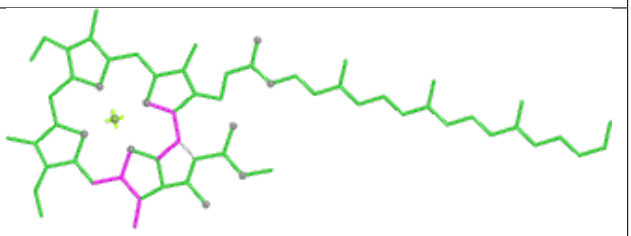
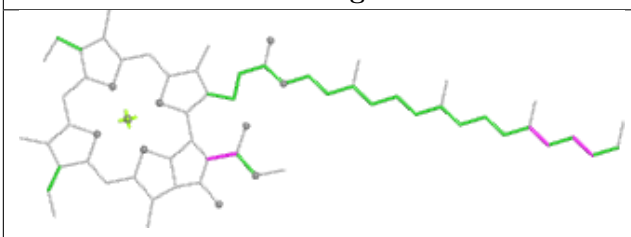
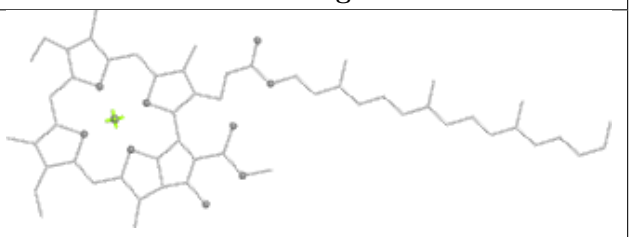
Bond angles

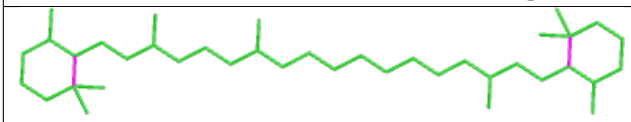
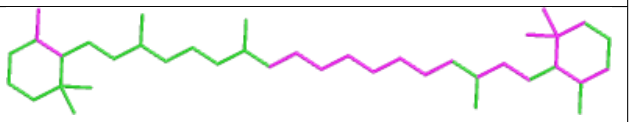
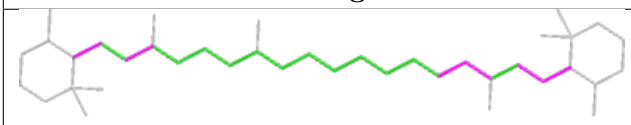
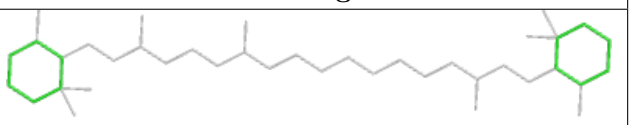


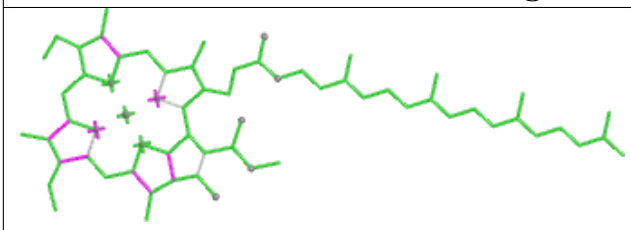
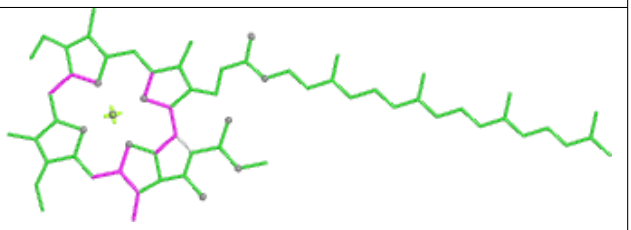
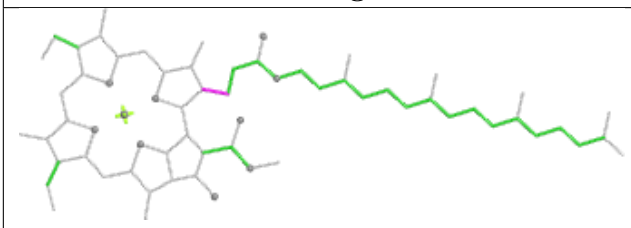
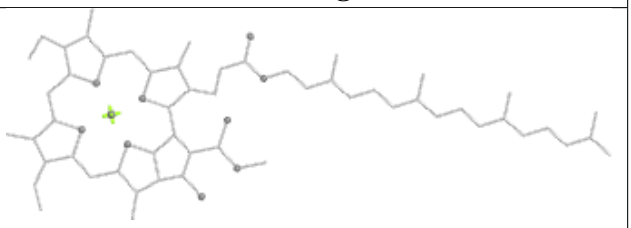
Torsions



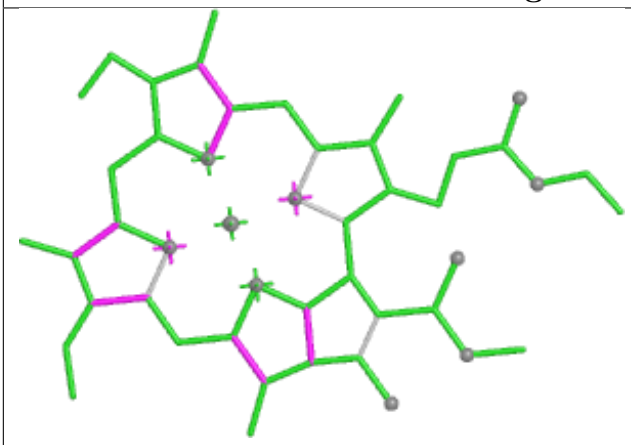
Rings

Ligand CLA B 821	
 Bond lengths	 Bond angles
 Torsions	 Rings

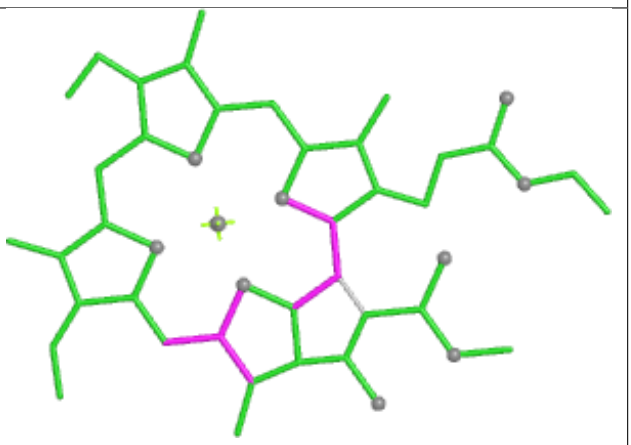
Ligand BCR R 203	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA A 853	
 Bond lengths	 Bond angles
 Torsions	 Rings

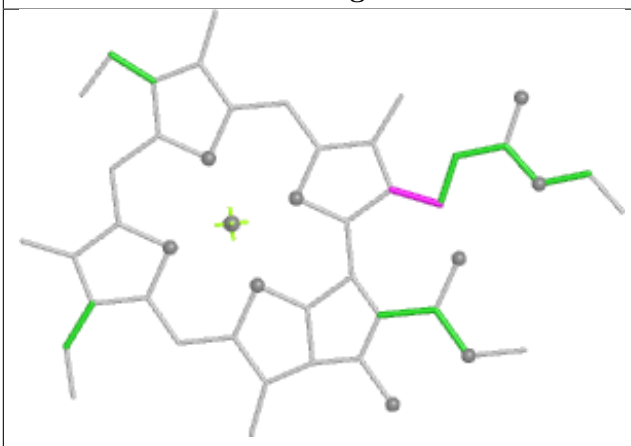
Ligand CLA P 309



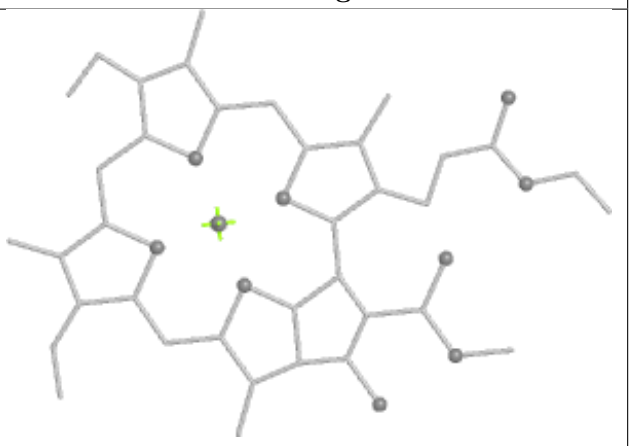
Bond lengths



Bond angles

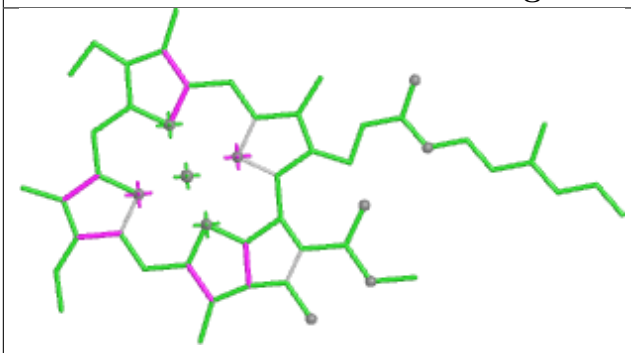


Torsions



Rings

Ligand CLA A 838



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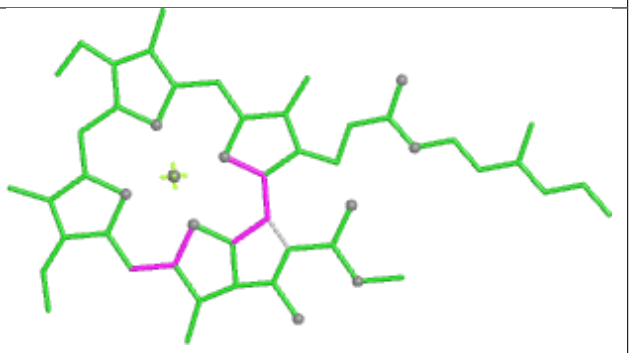
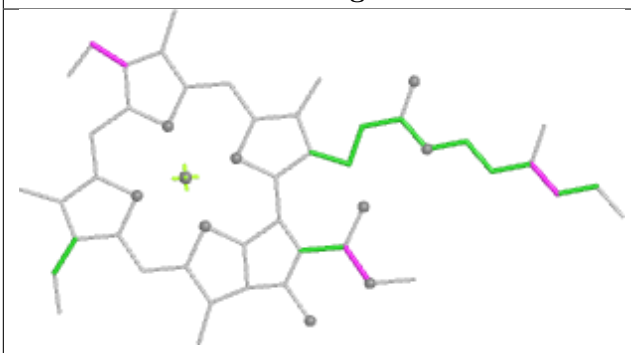


Bond angles



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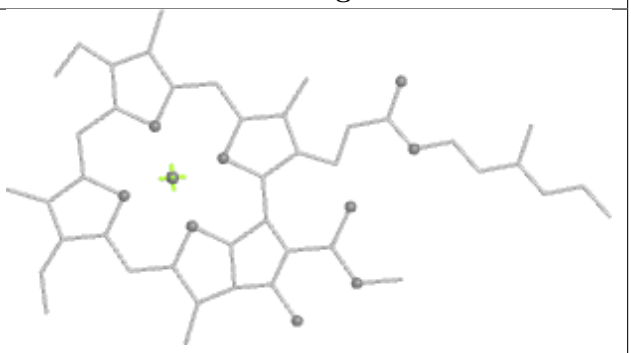
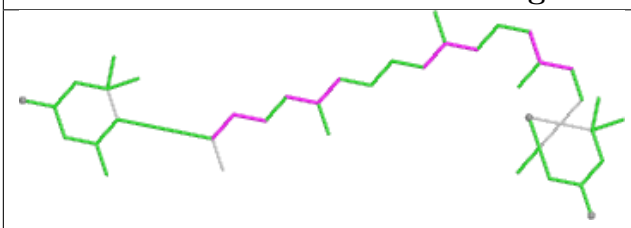


Rings

Ligand DD6 S 202



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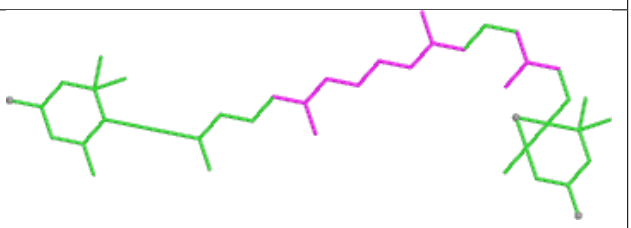
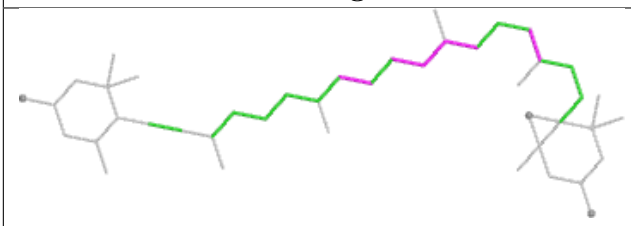


Bond angles



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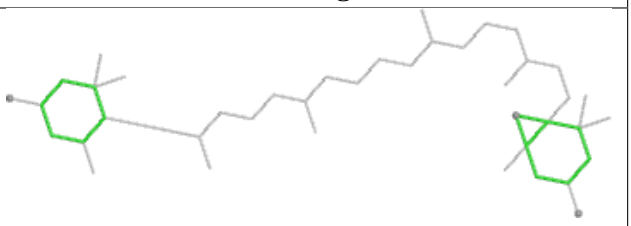
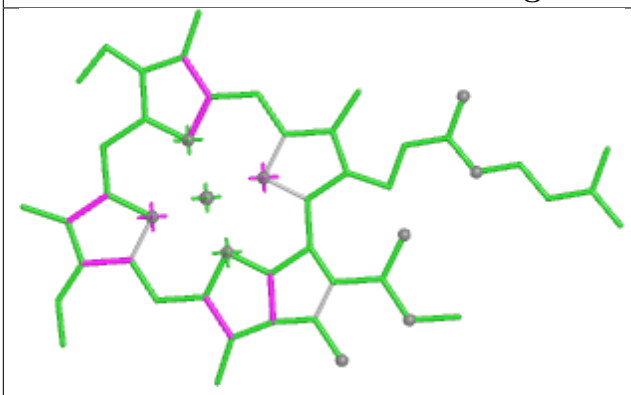


Rings

Ligand CLA A 827



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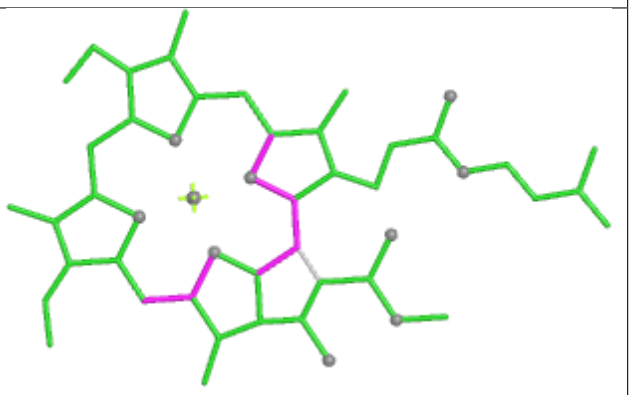
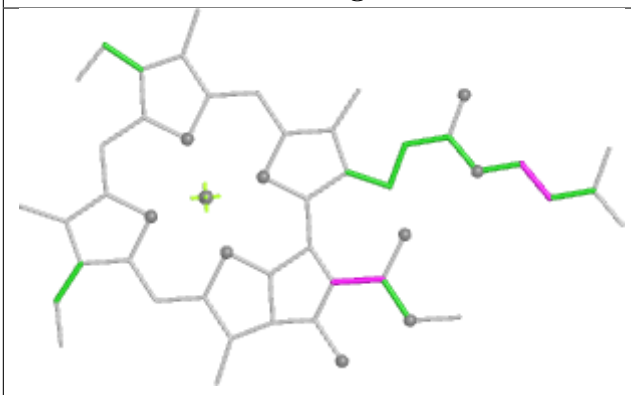


Bond angles



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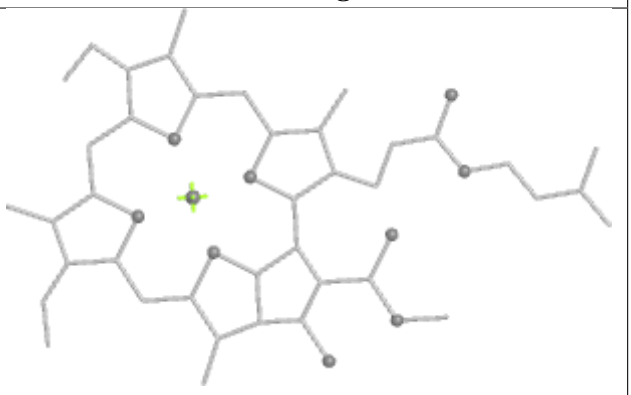
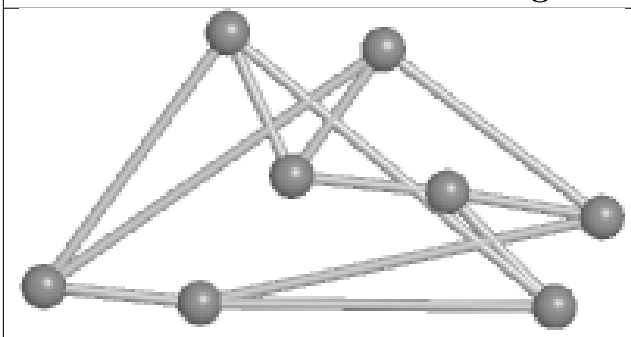
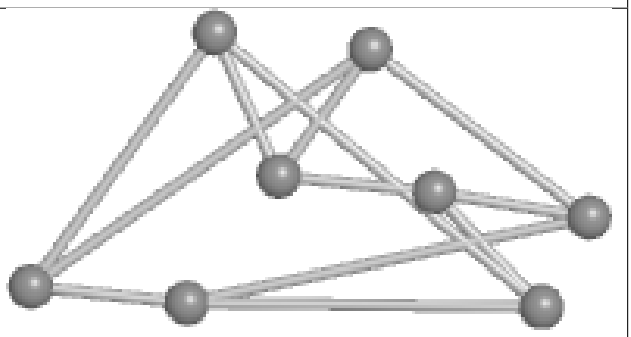


Rings

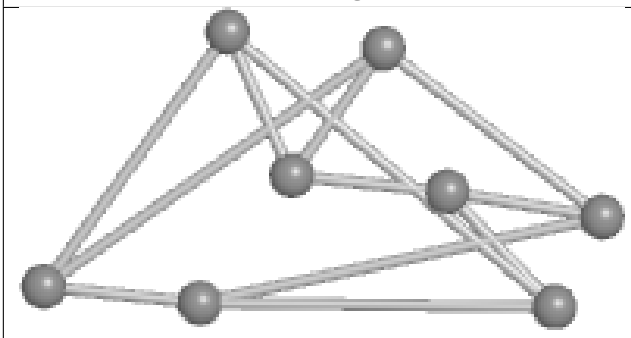
Ligand SF4 C 102



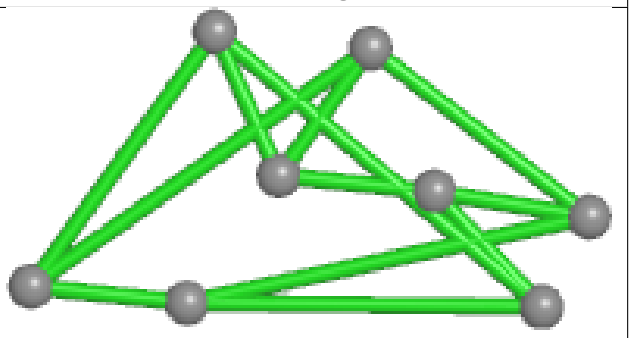
Bond lengths



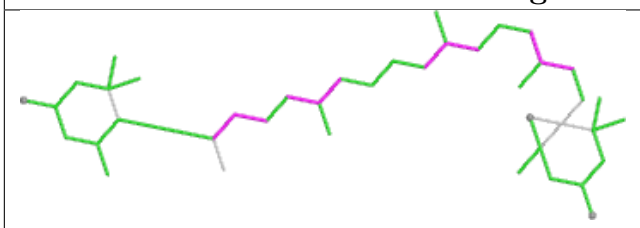
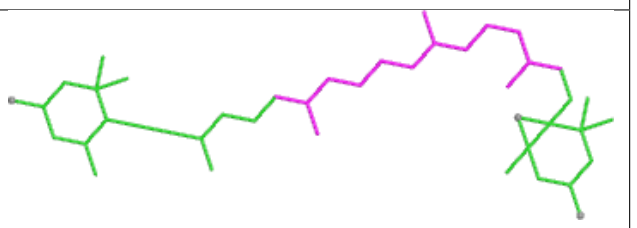
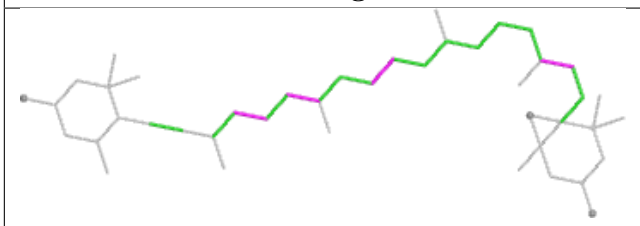
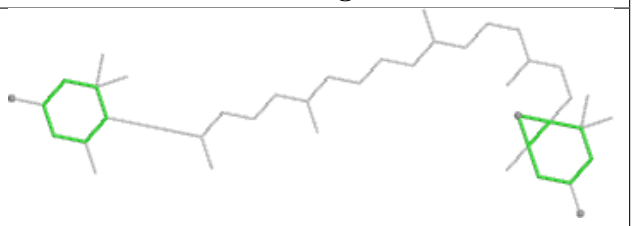
Bond angles

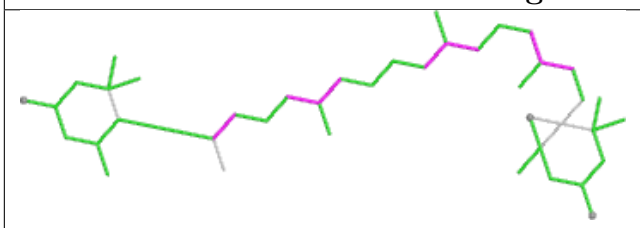
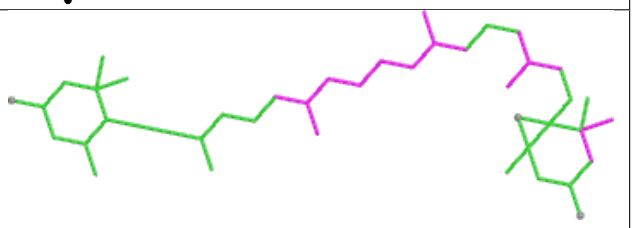
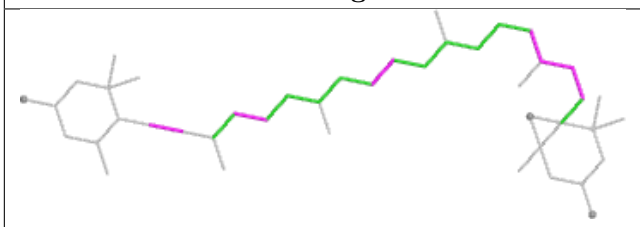
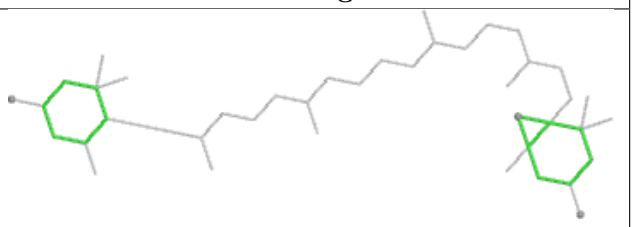


Torsions



Rings

Ligand DD6 J 101	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand DD6 Q 215	
 Bond lengths	 Bond angles
 Torsions	 Rings

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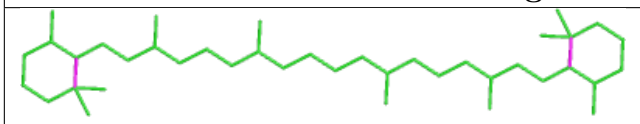
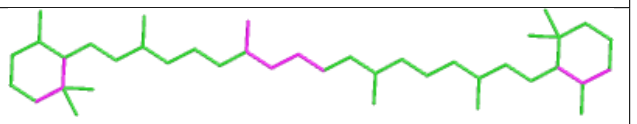
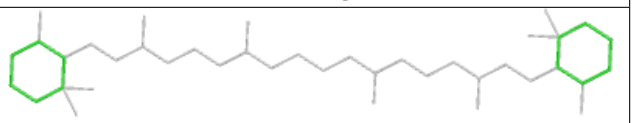
 Bond lengths	 Bond angles
Torsions	 Rings

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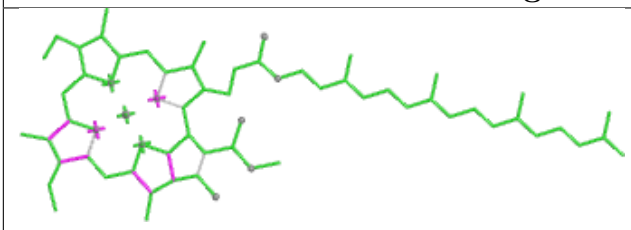
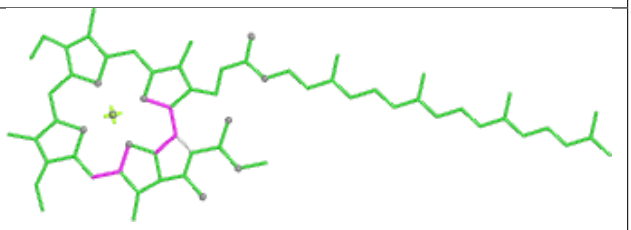
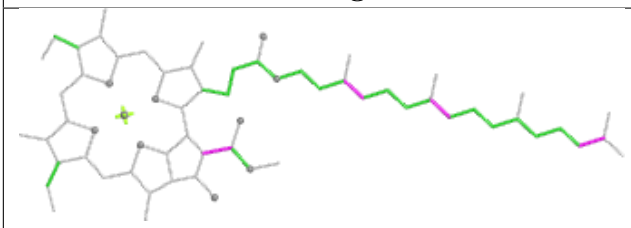
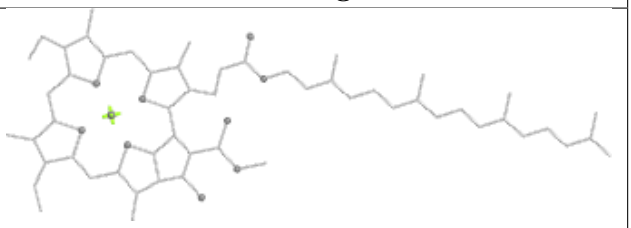
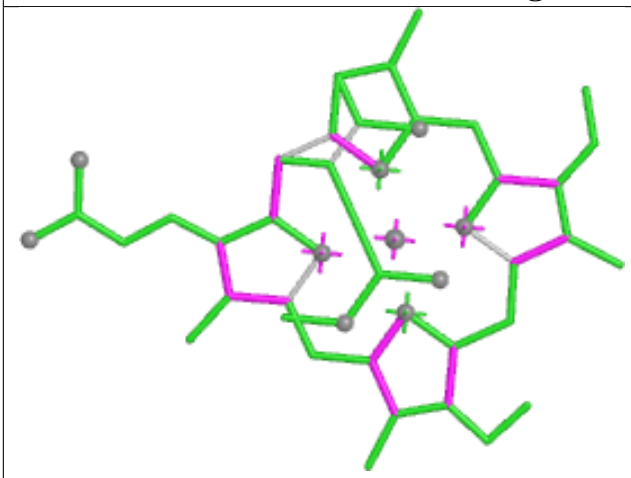
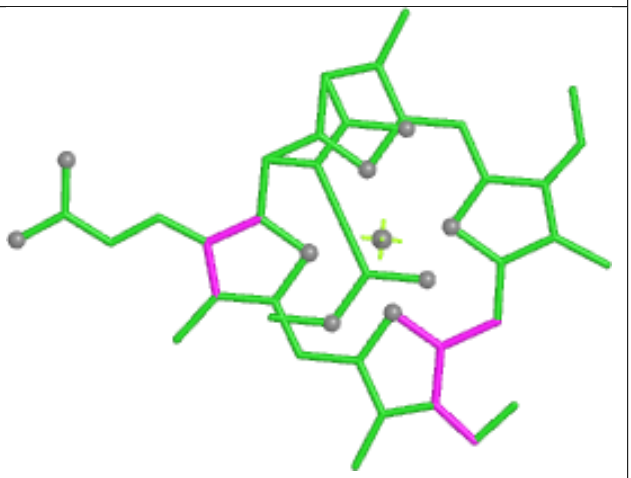
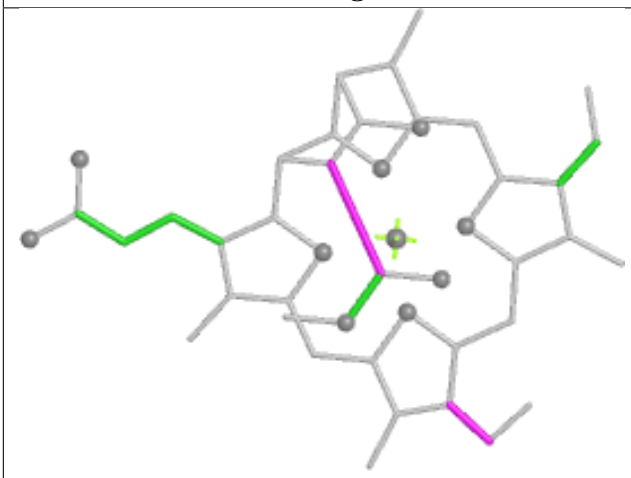
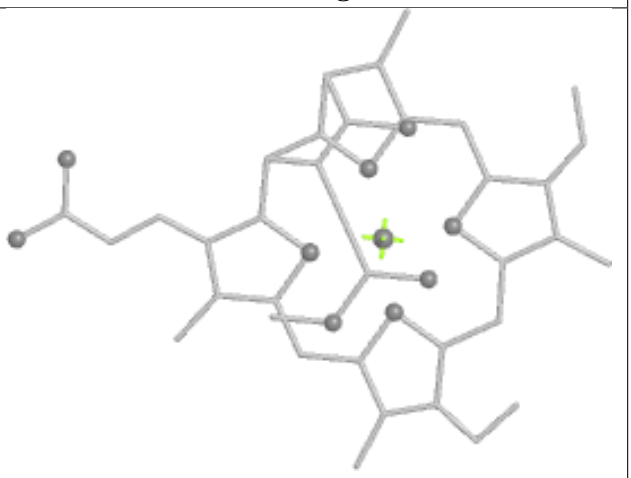
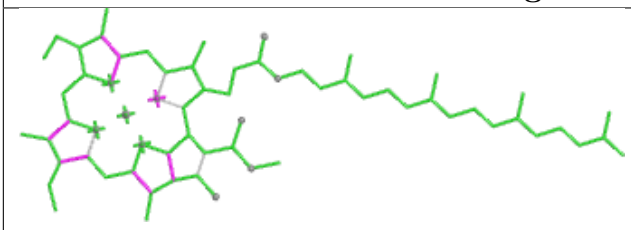
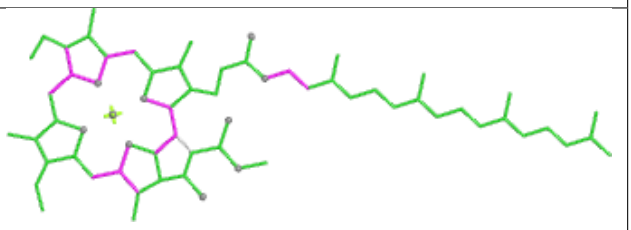
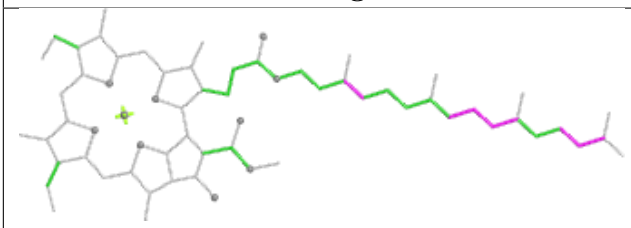
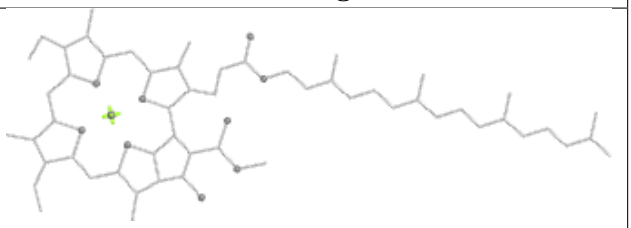
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand KC1 T 209	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA B 817	
 Bond lengths	 Bond angles
 Torsions	 Rings

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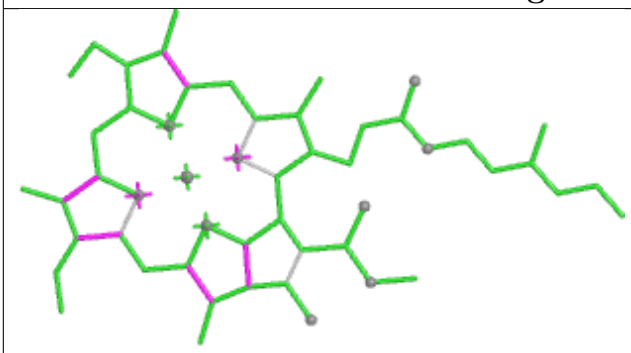
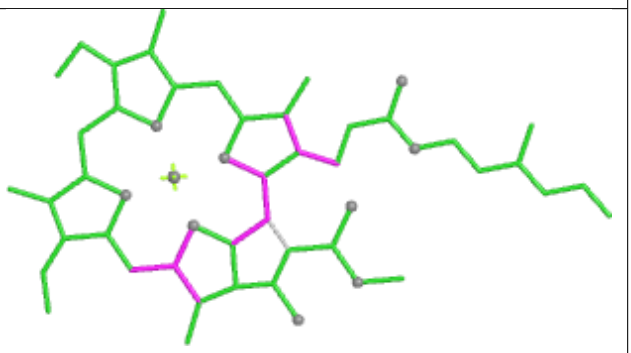
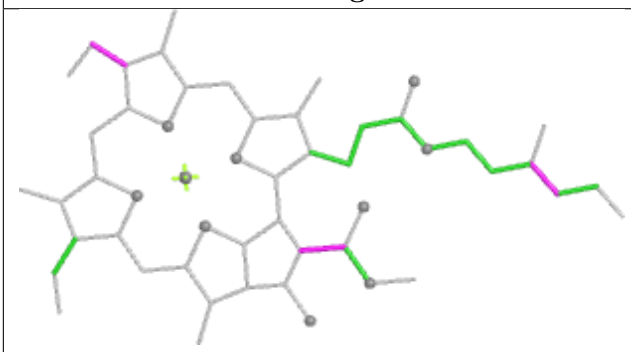
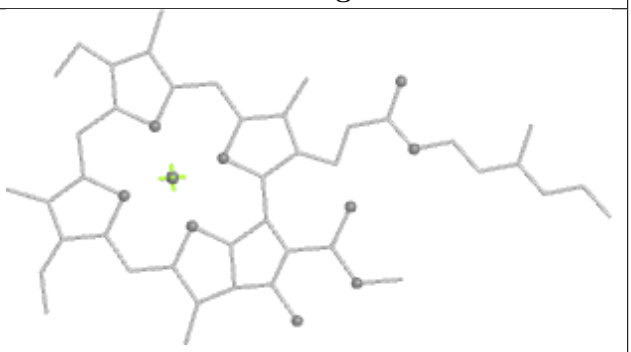
 Bond lengths	 Bond angles
 Torsions	 Rings

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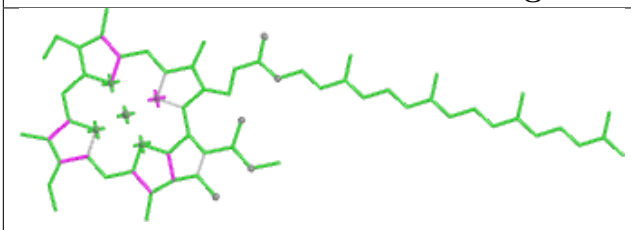
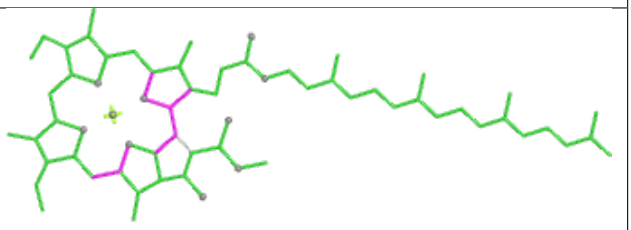
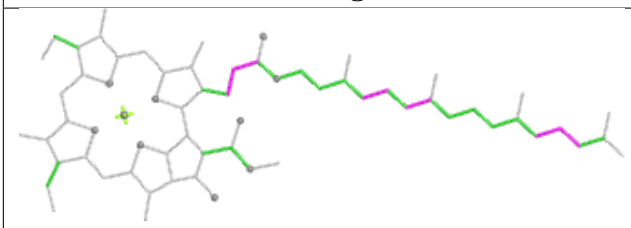
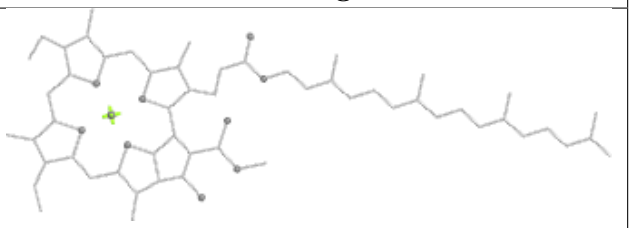
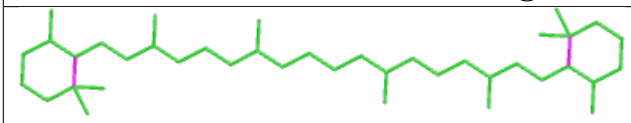
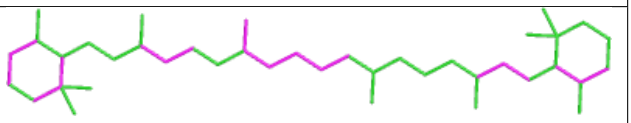
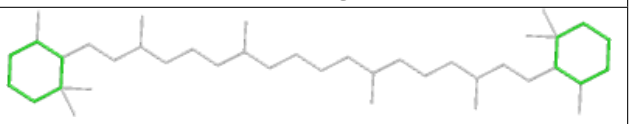
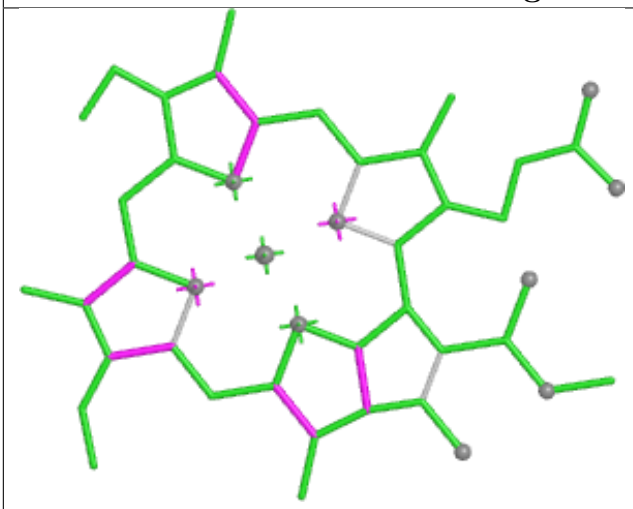
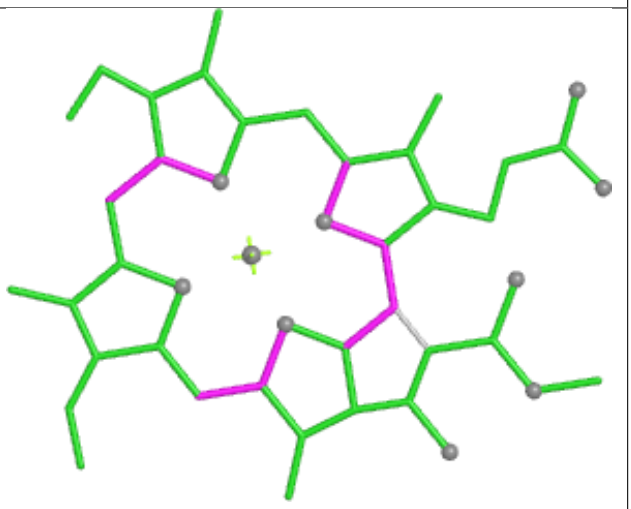
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand BCR M 101	
 Bond lengths	 Bond angles
Torsions	 Rings

Ligand CLA A 817



Bond lengths



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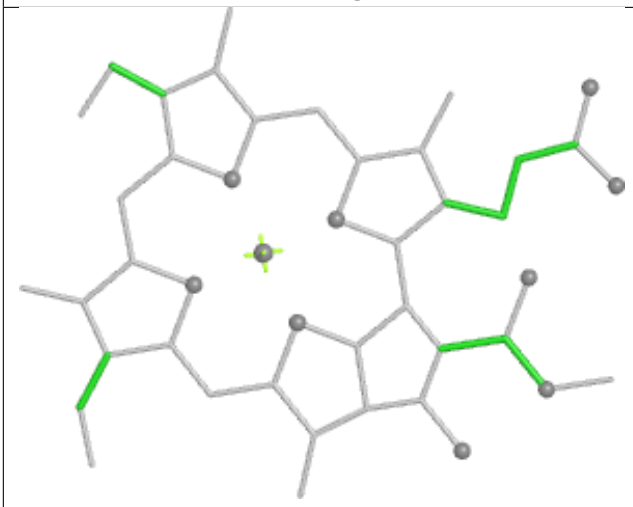
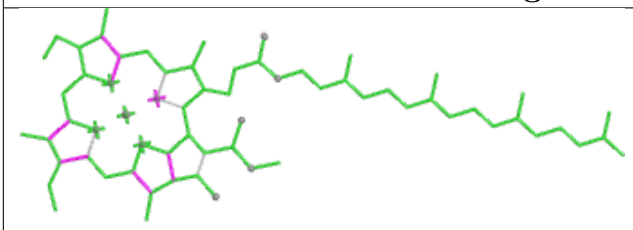


Torsions

Rings

Ligand CLA O 209



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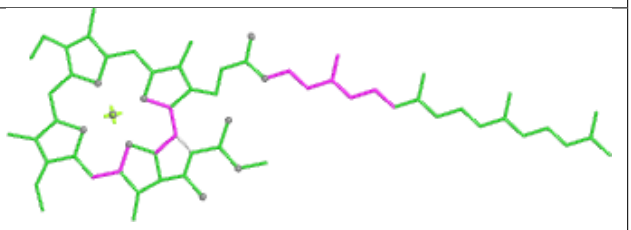
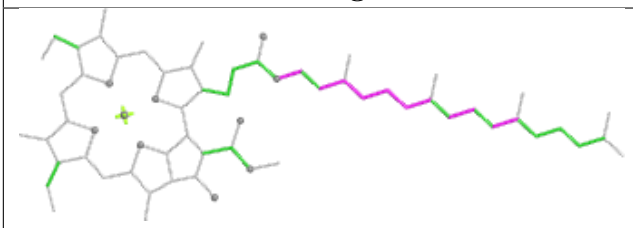
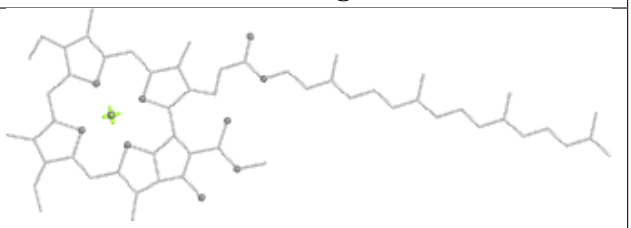


Bond angles

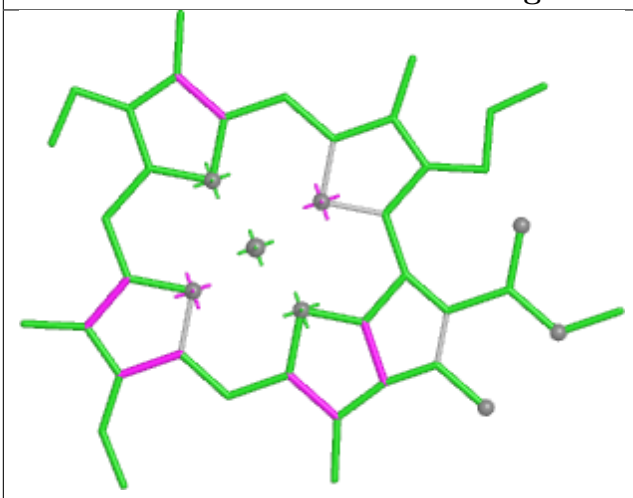


Torsions



Rings

Ligand CLA O 202



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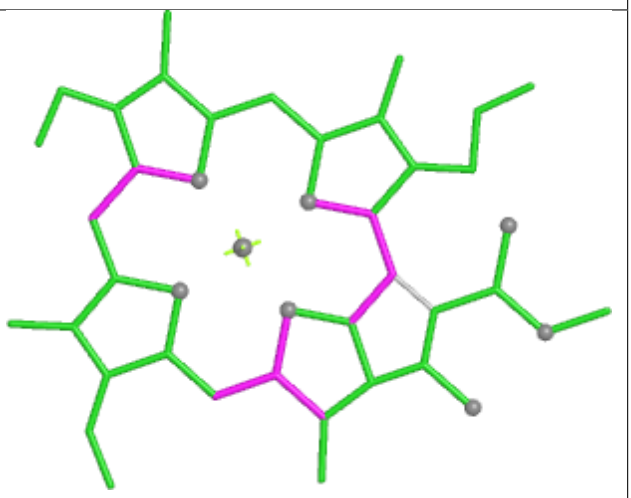
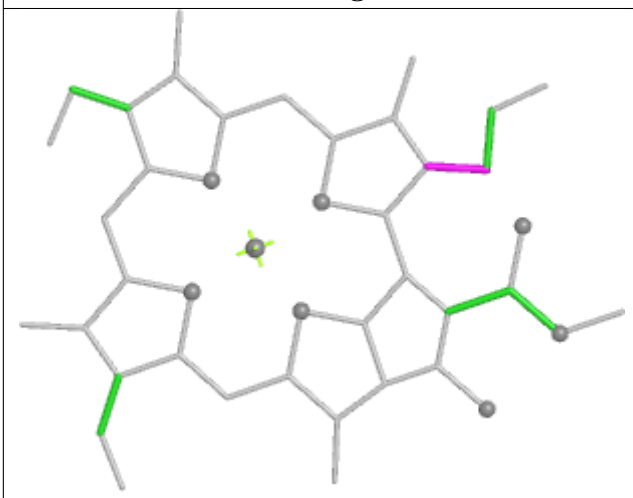


Bond angles



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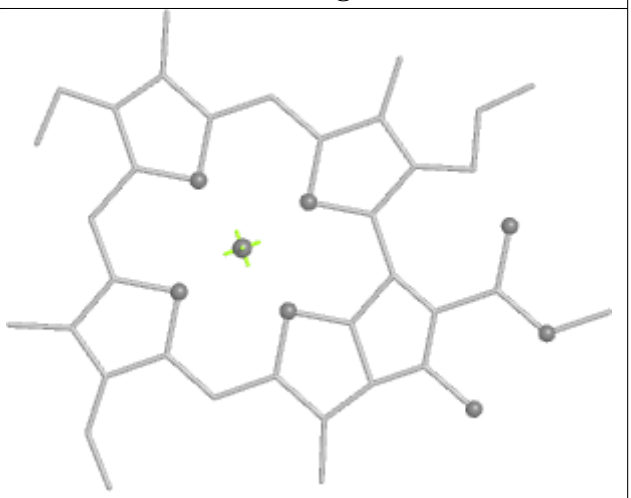
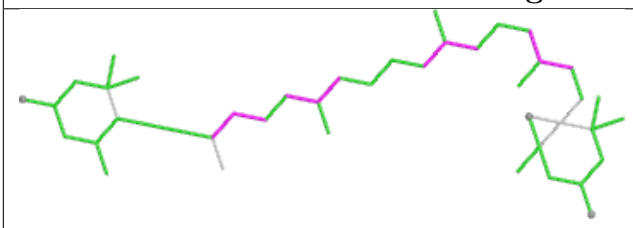


Rings

Ligand DD6 P 304



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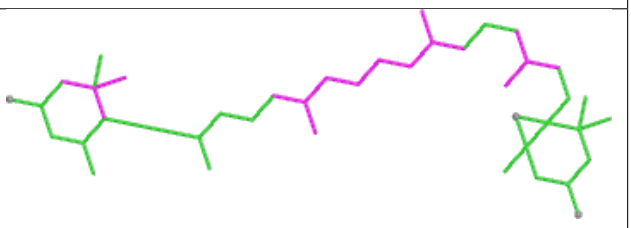
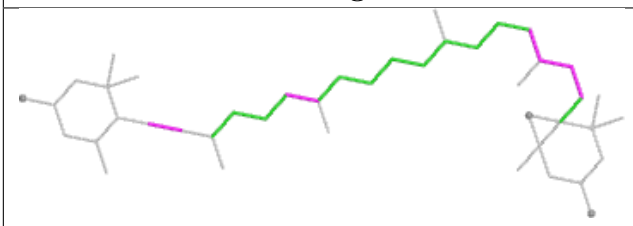


Bond angles



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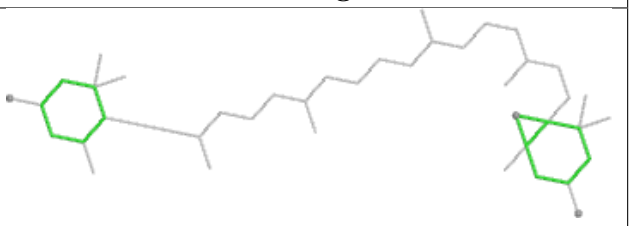
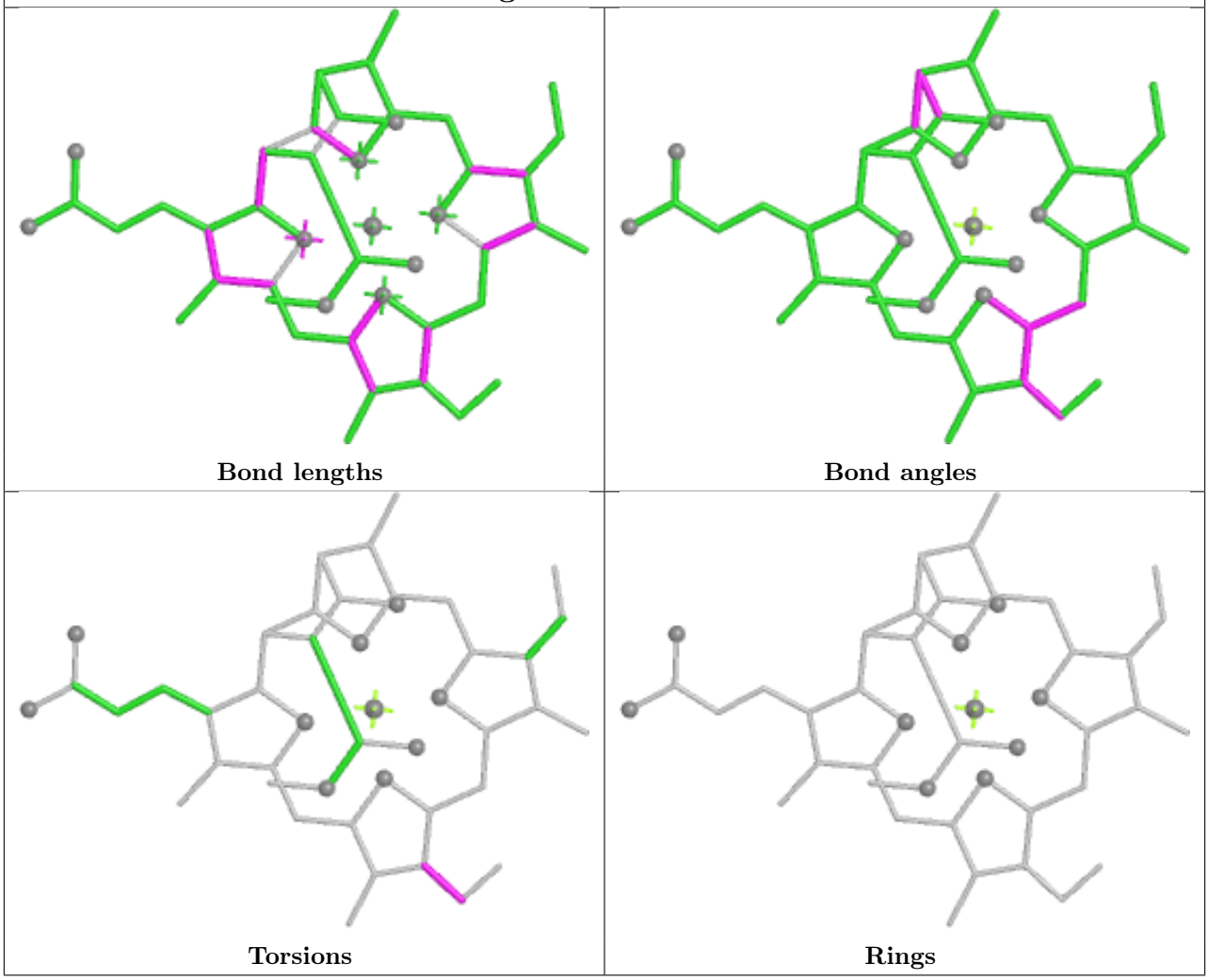
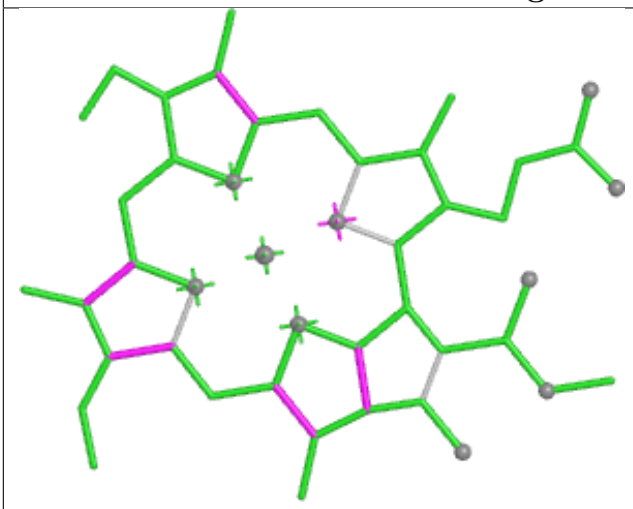


Rings

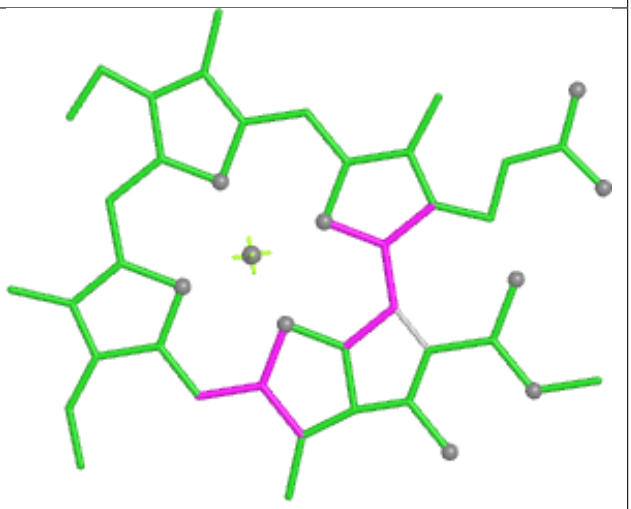
Ligand KC1 S 208



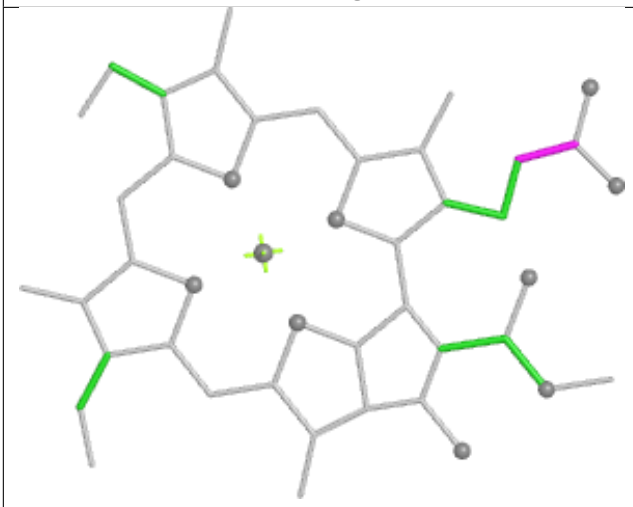
Ligand CLA S 206



Bond lengths



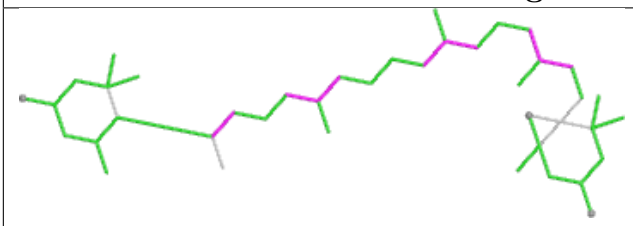
Bond angles



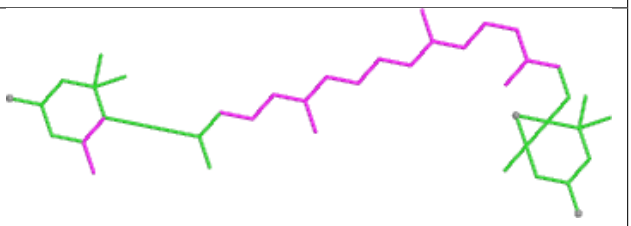
Torsions

Rings

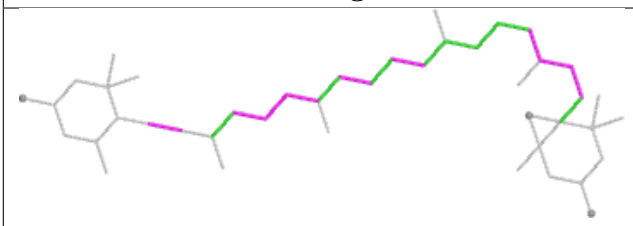
Ligand DD6 T 214



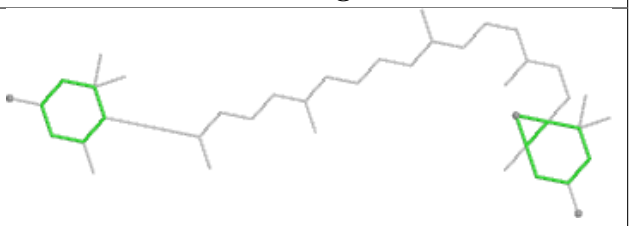
Bond lengths



Bond angles

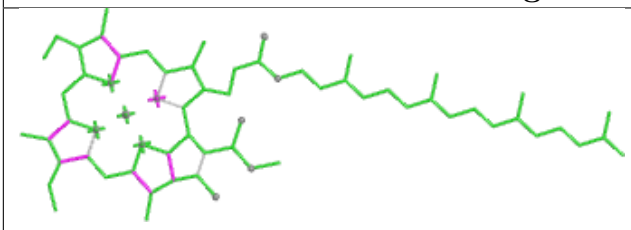


Torsions

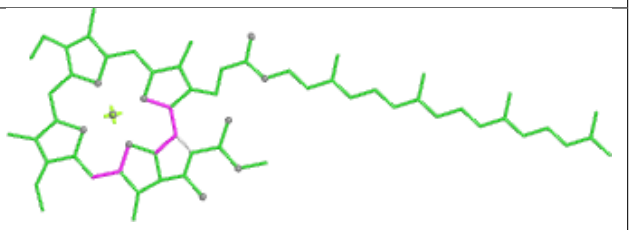


Rings

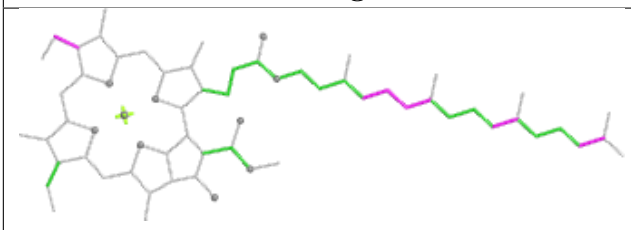
Ligand CLA U 205



Bond lengths



Bond angles



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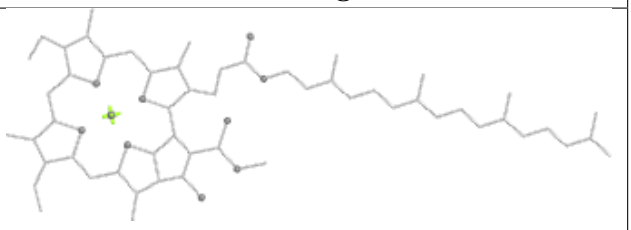
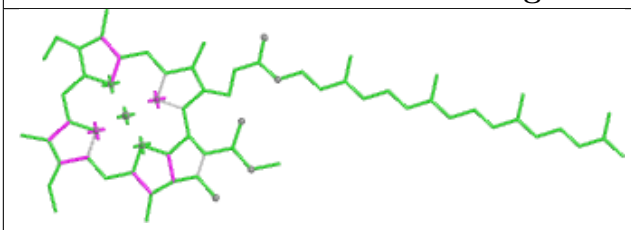


Rings

Ligand CLA A 804



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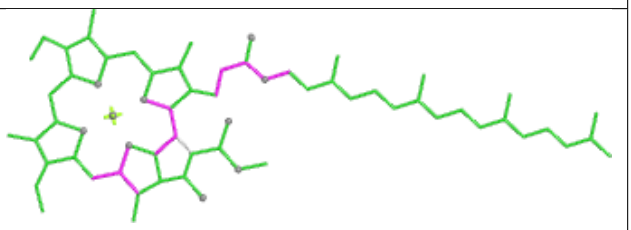
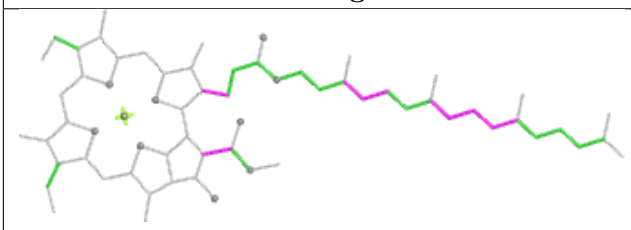


Bond angles



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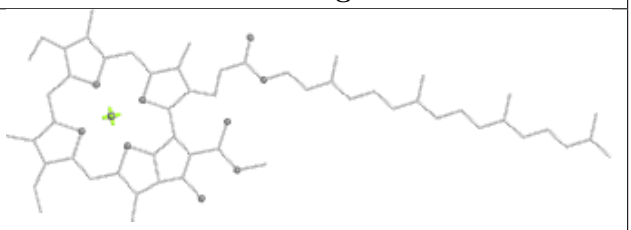
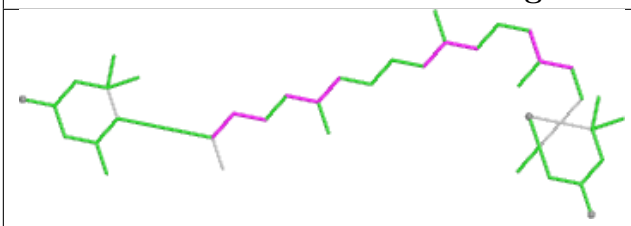


Rings

Ligand DD6 Q 202



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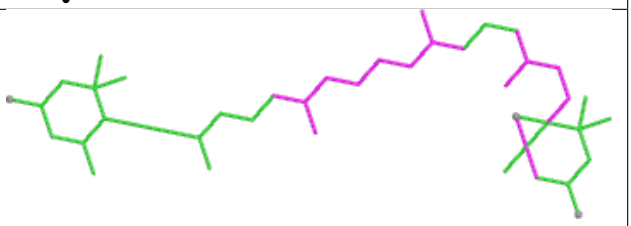
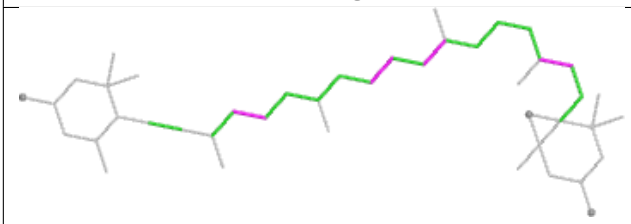


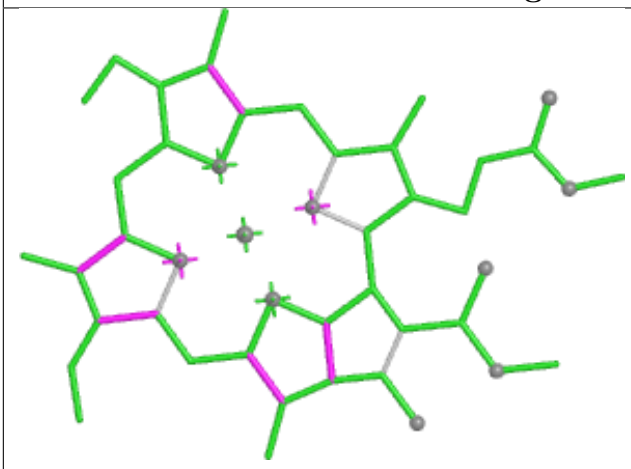
Bond angles



Torsions

Rings

Ligand CLA T 204



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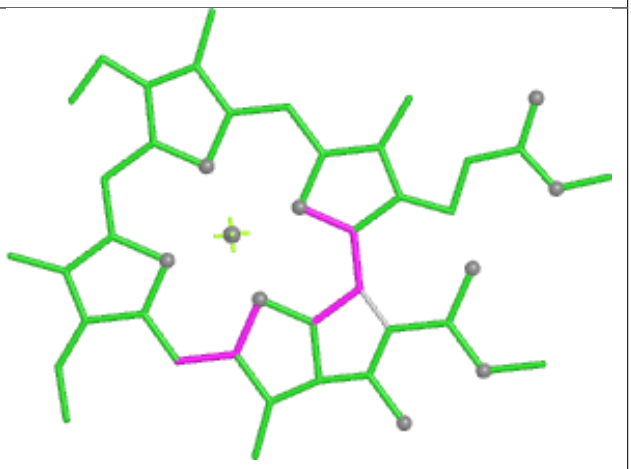
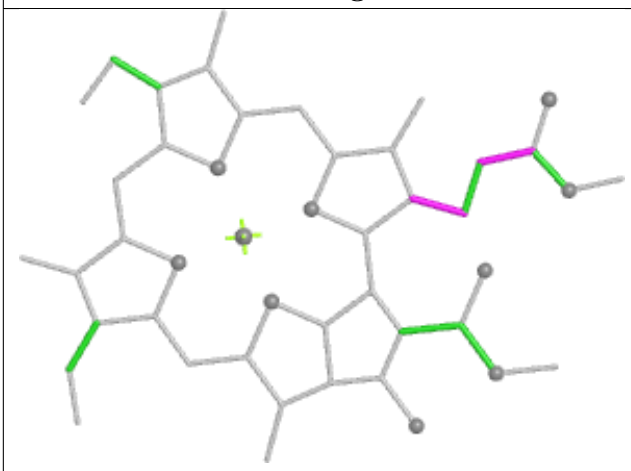


Bond angles



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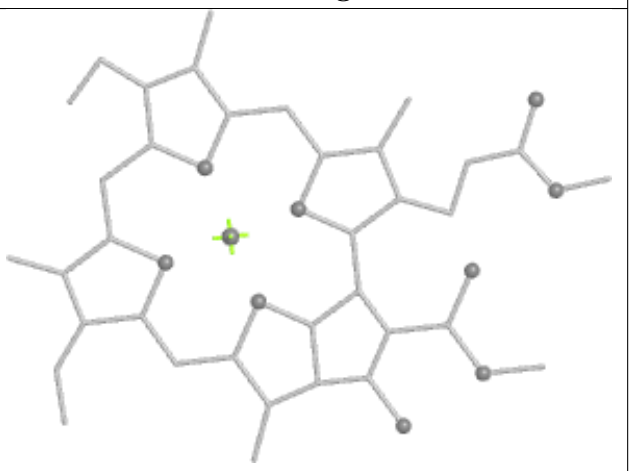
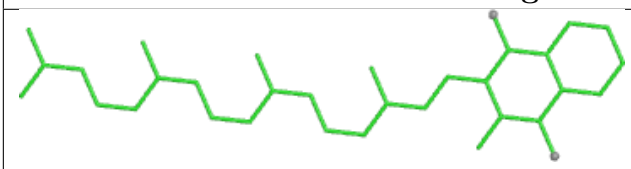


Rings

Ligand PQN A 837



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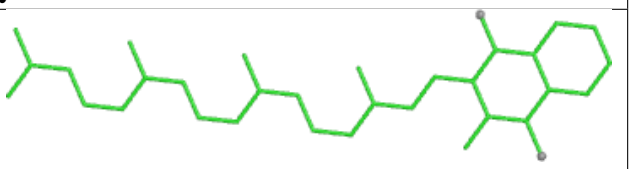
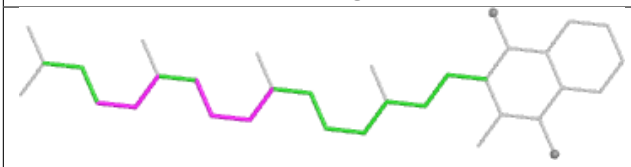


Bond angles



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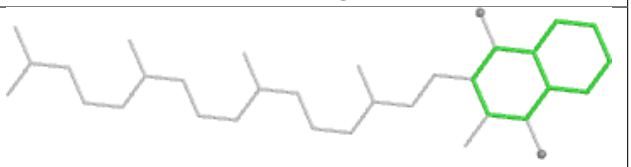
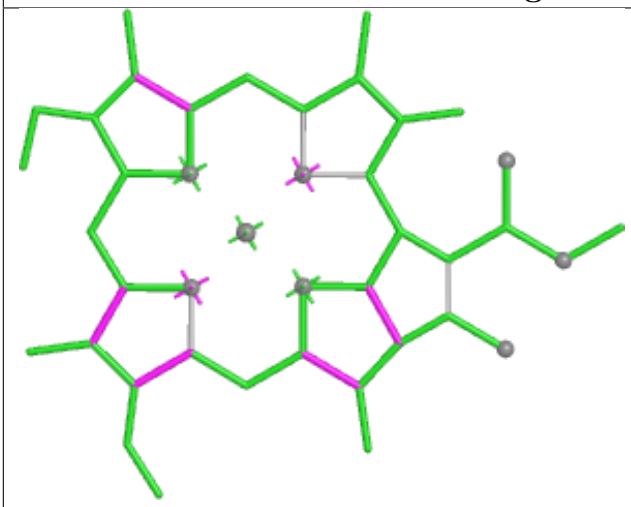
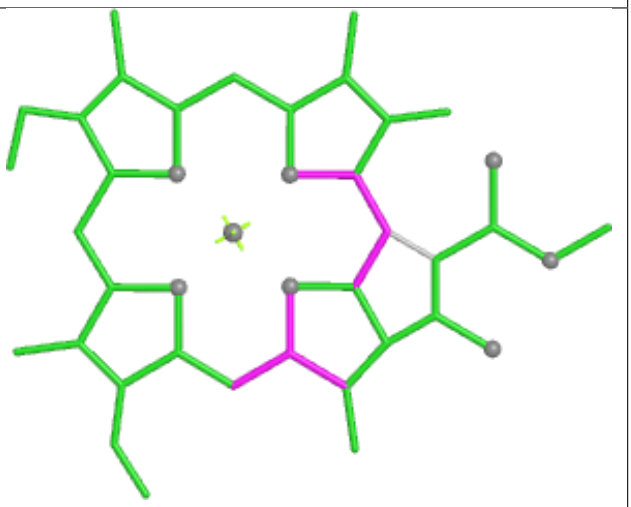


Rings

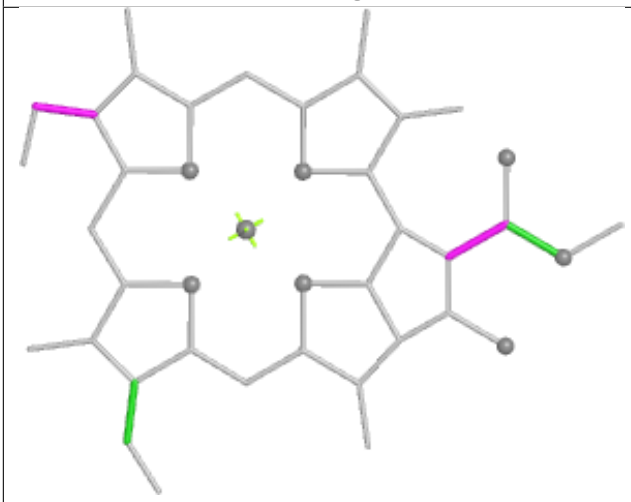
Ligand CLA T 203



Bond lengths



Bond angles



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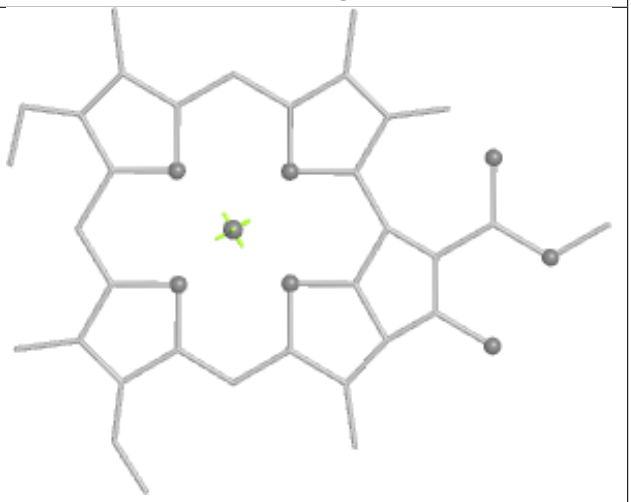
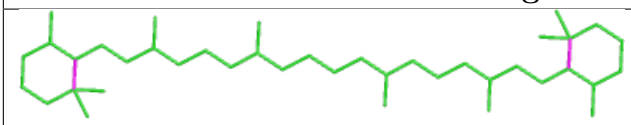


Rings

Ligand BCR A 843



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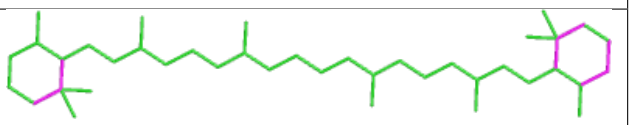
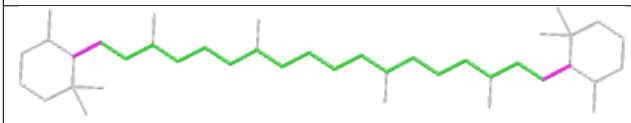
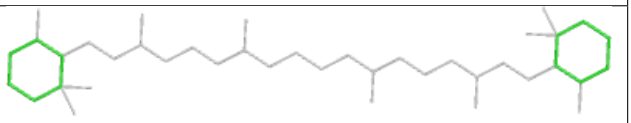


Bond angles

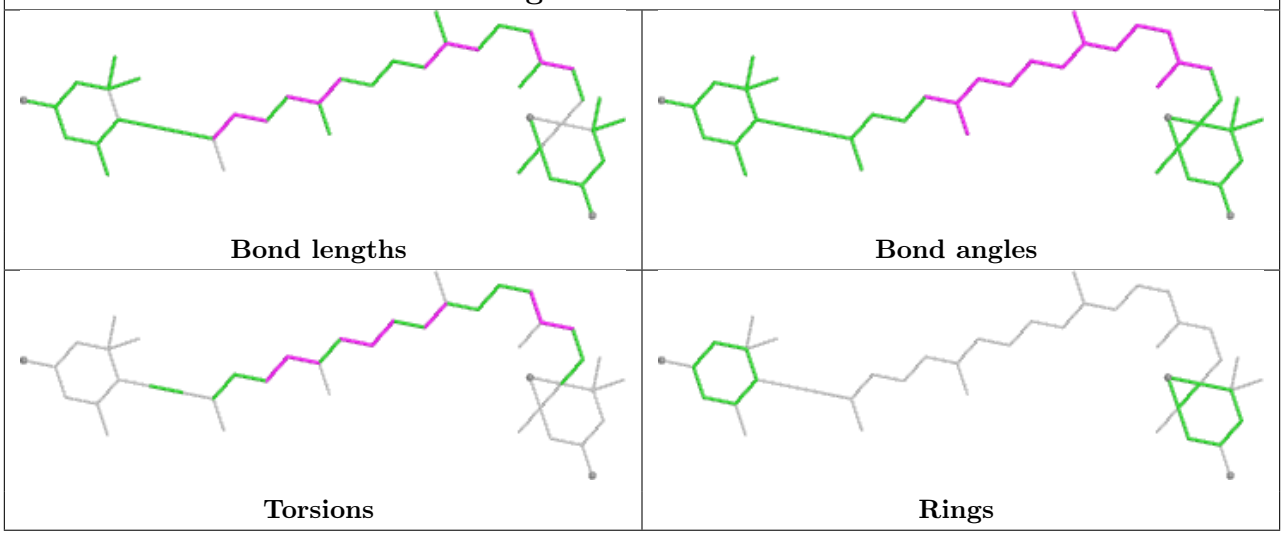


Torsions

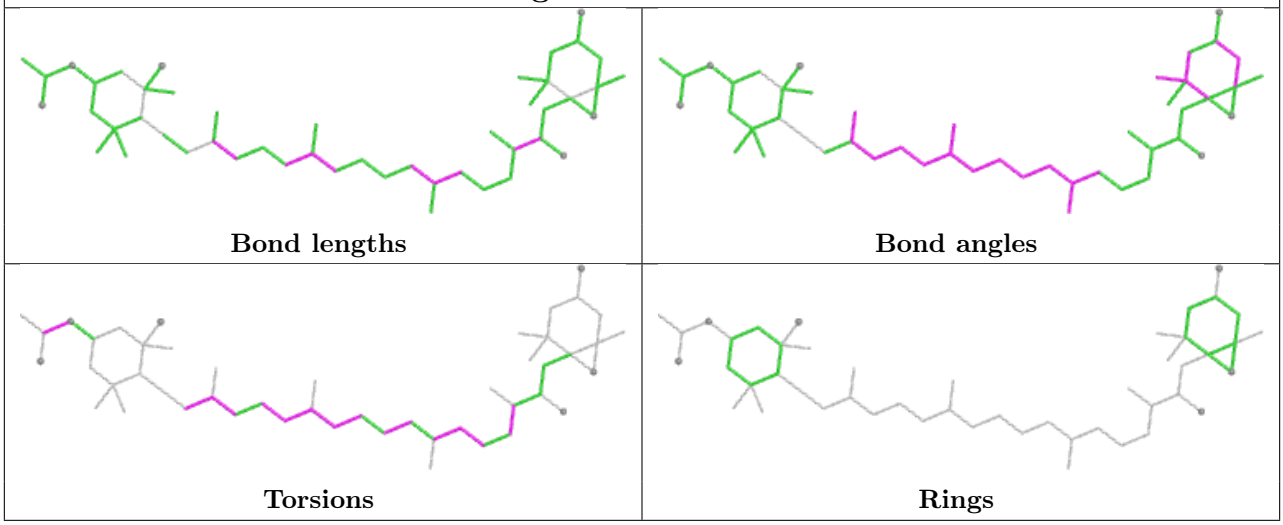


Rings

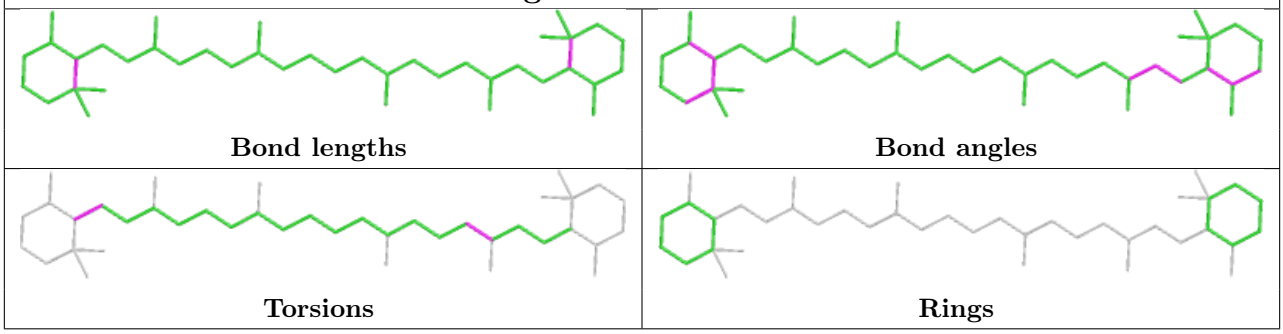
Ligand DD6 O 212



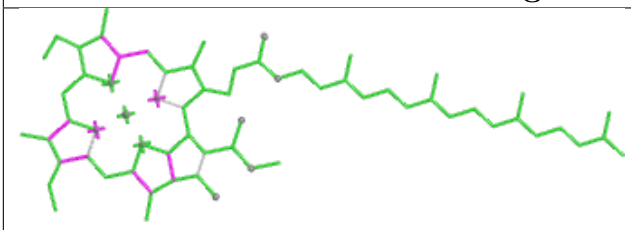
Ligand A86 T 201



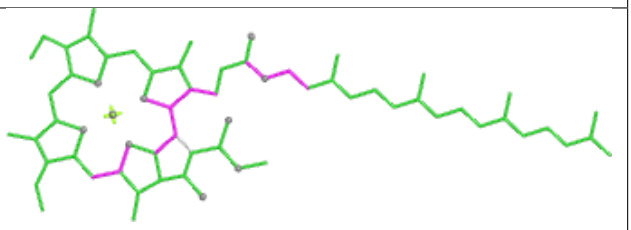
Ligand BCR B 839



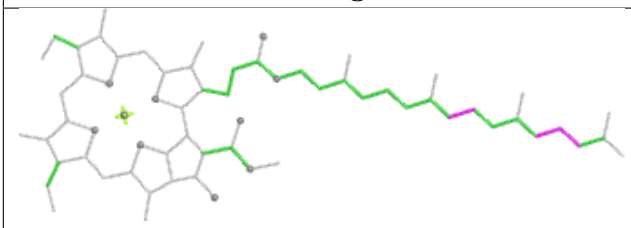
Ligand CLA A 836



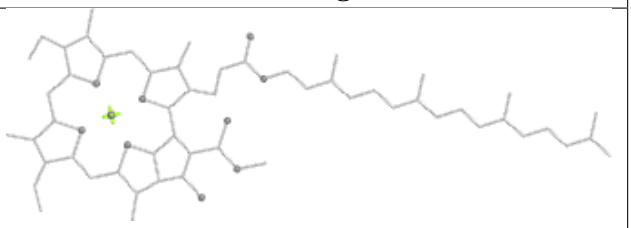
Bond lengths



Bond angles

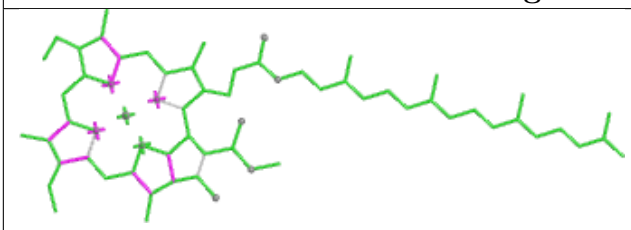


Torsions



Rings

Ligand CLA A 834



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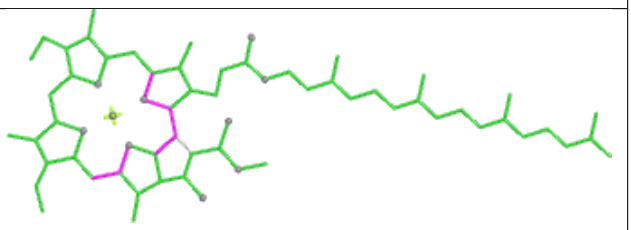
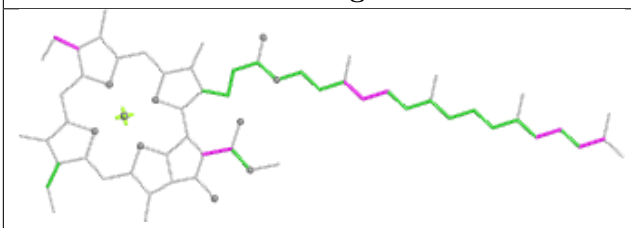


Bond angles



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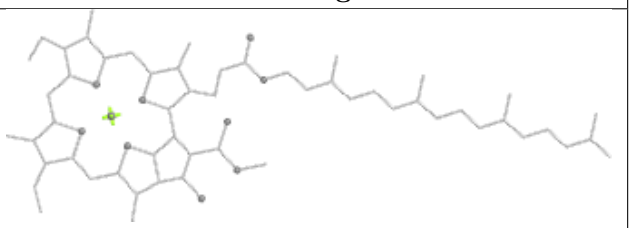
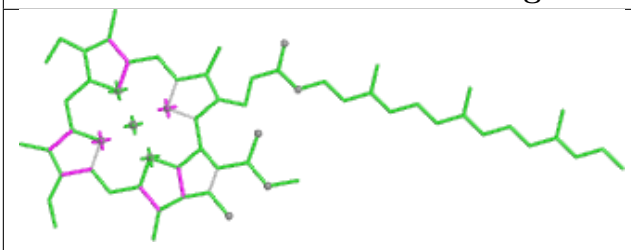


Rings

Ligand CLA A 824



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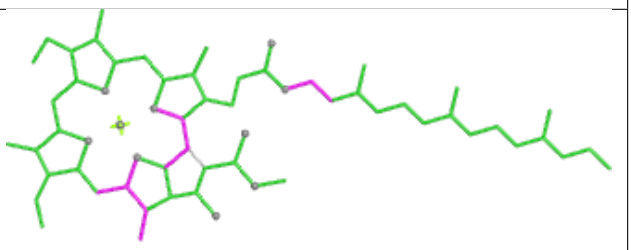
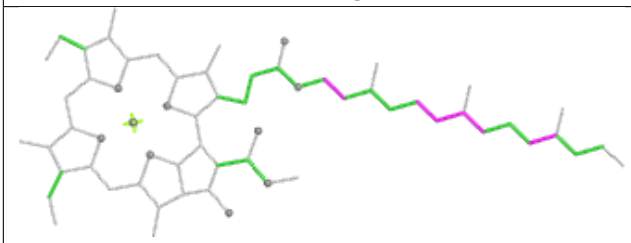


Bond angles



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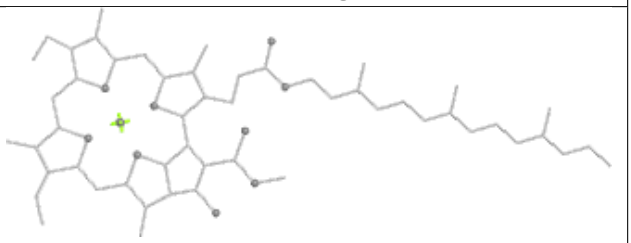
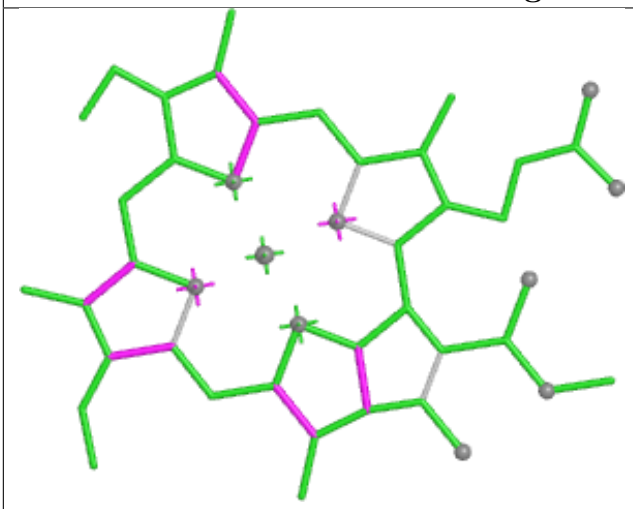
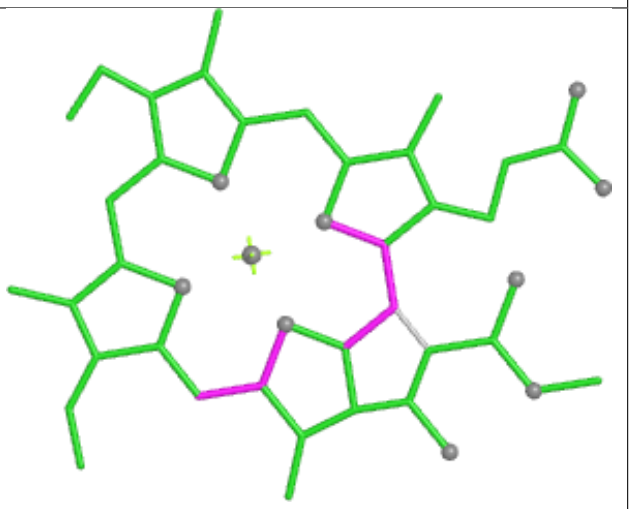


Rings

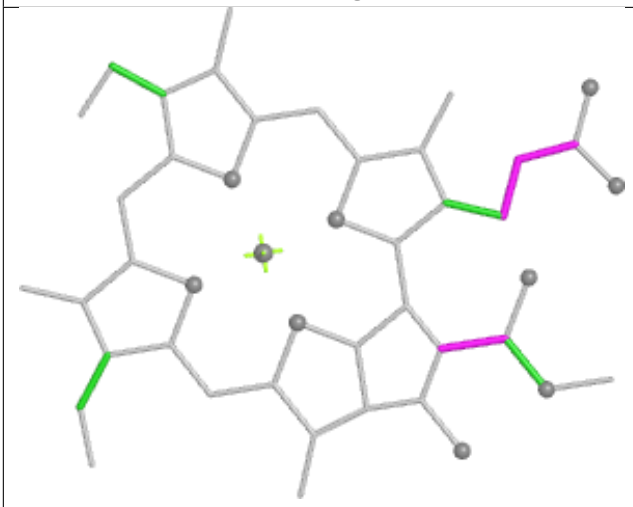
Ligand CLA B 804



Bond lengths



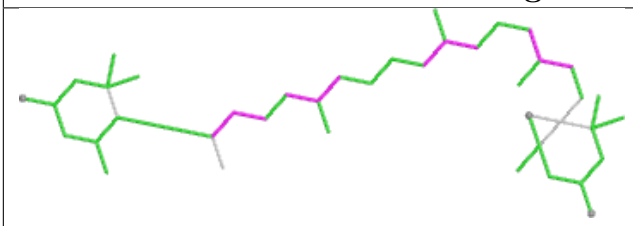
Bond angles



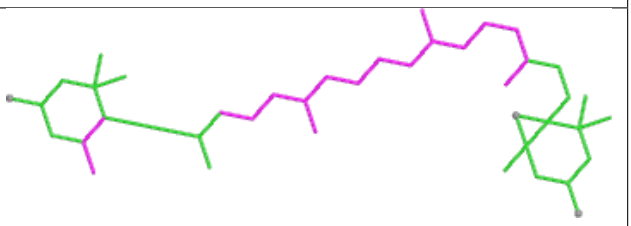
Torsions

Rings

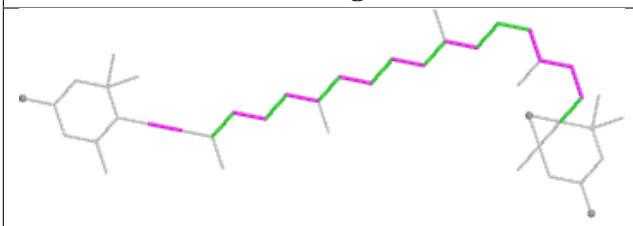
Ligand DD6 A 854



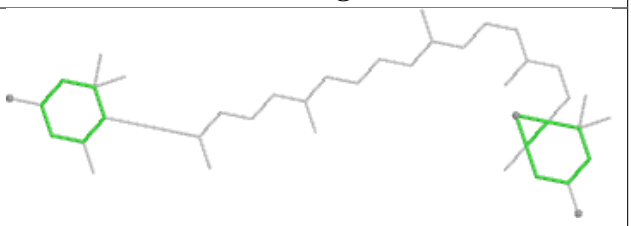
Bond lengths



Bond angles

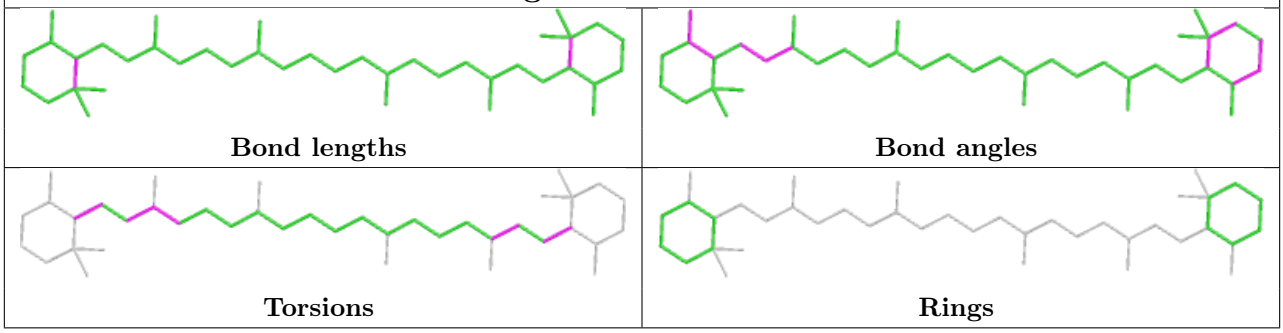


Torsions

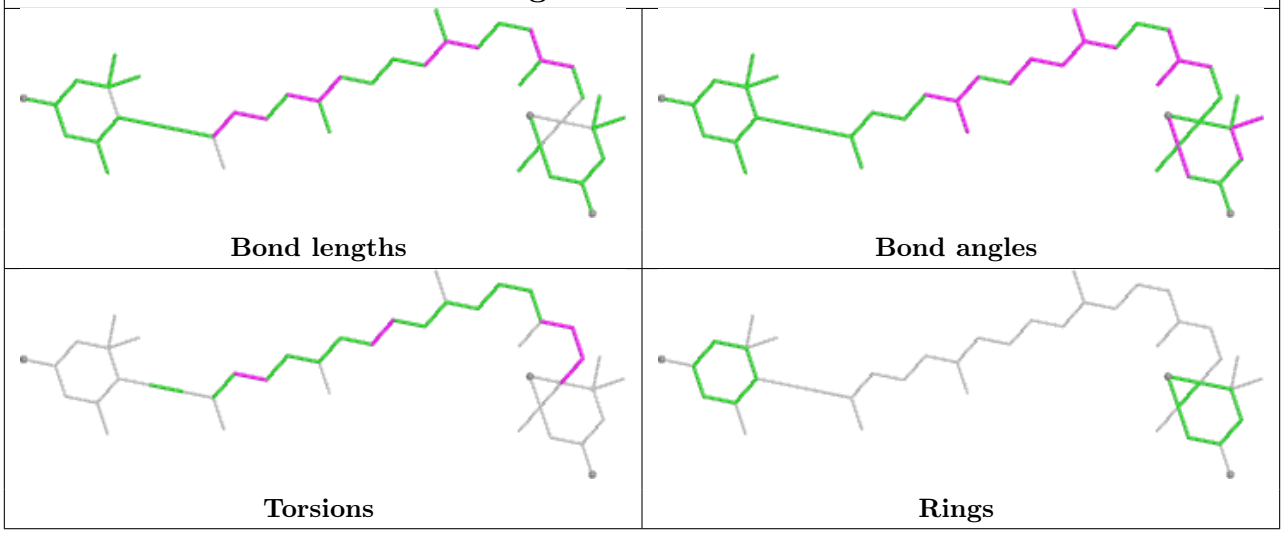


Rings

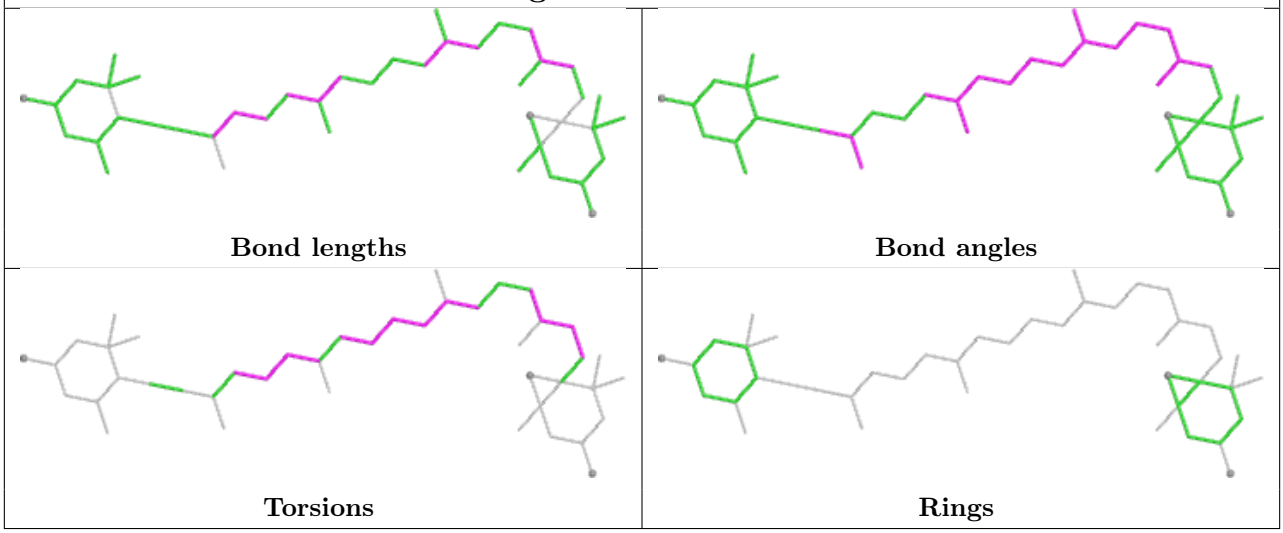
Ligand BCR B 837



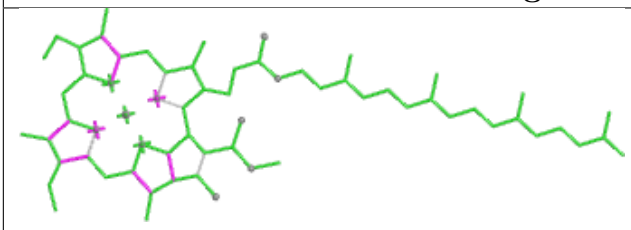
Ligand DD6 S 209



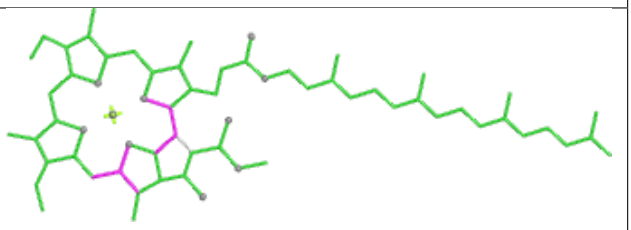
Ligand DD6 S 212



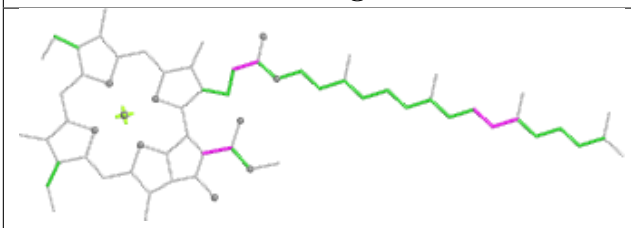
Ligand CLA A 811



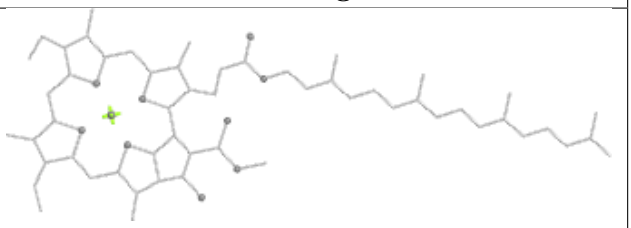
Bond lengths



Bond angles

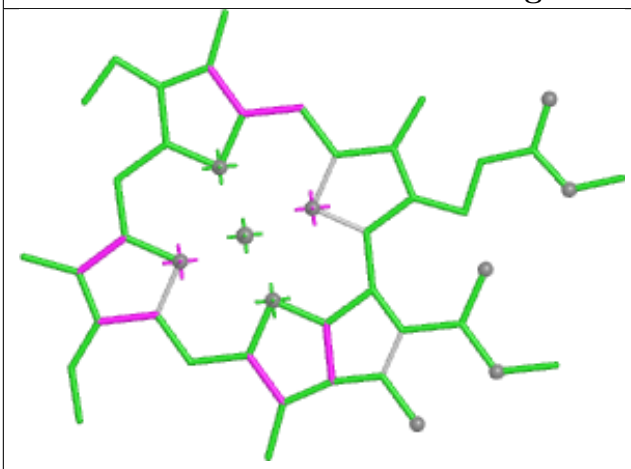


Torsions



Rings

Ligand CLA T 206



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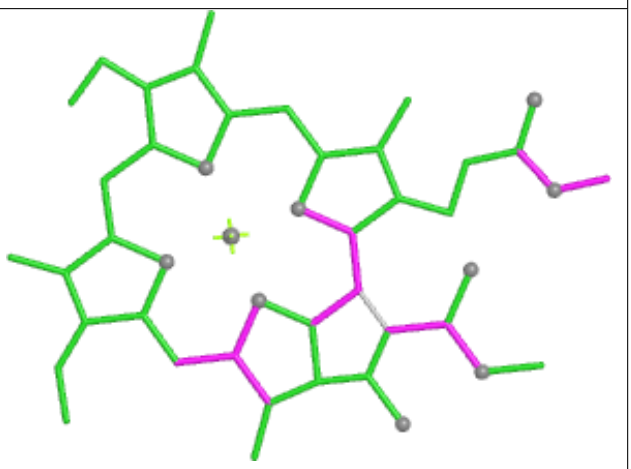

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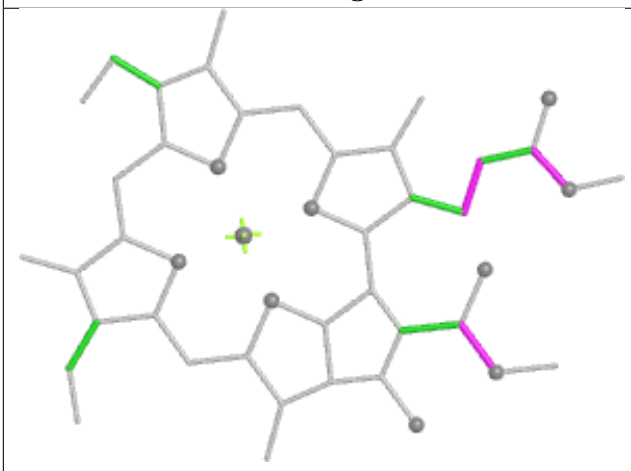
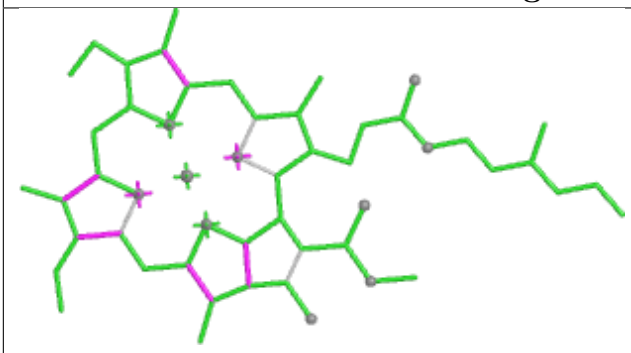
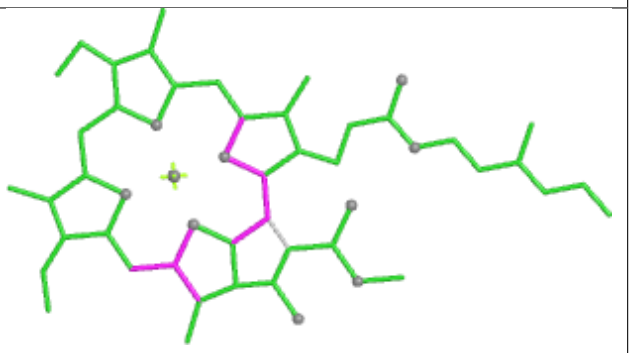
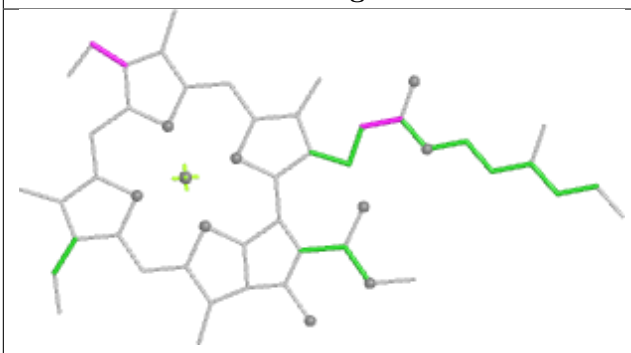
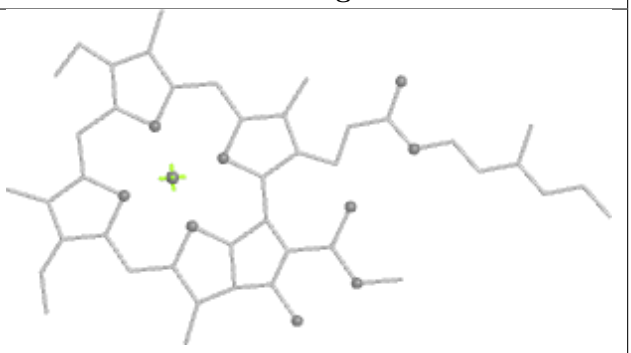
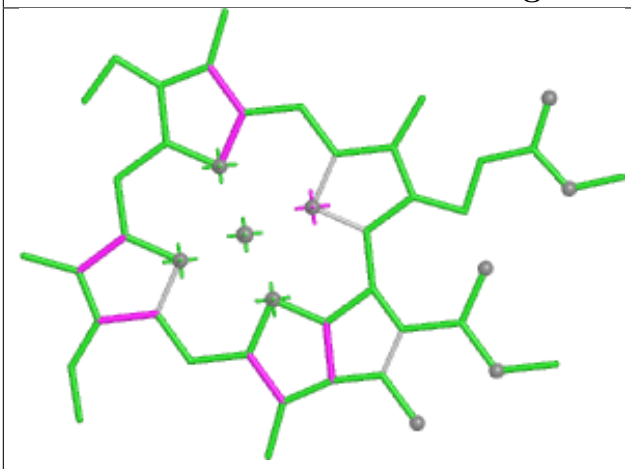


Torsions

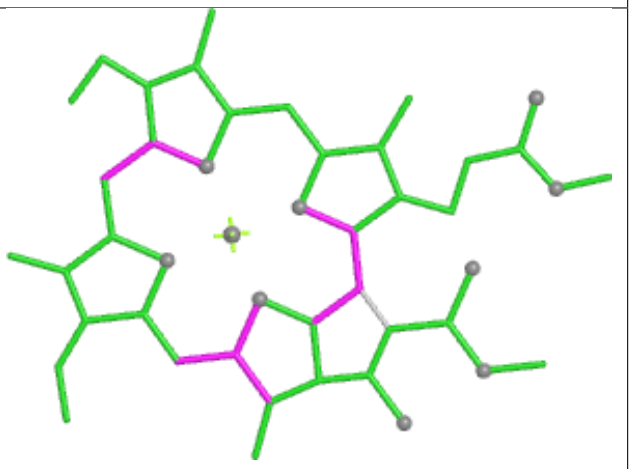
Rings

Ligand CLA U 211	
 Bond lengths	 Bond angles
 Torsions	 Rings

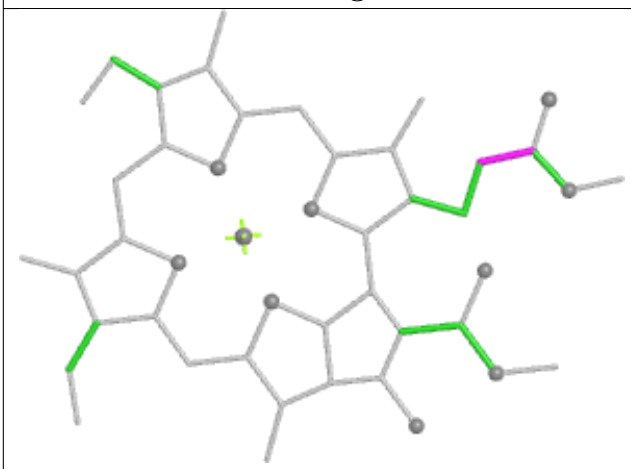
Ligand CLA U 208



Bond lengths



Bond angles



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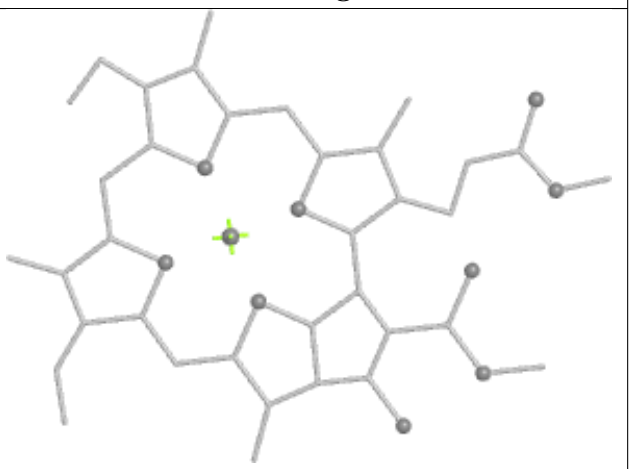
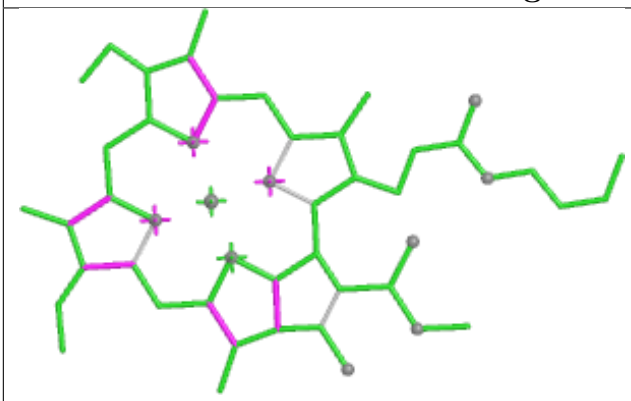


Rings

Ligand CLA A 805



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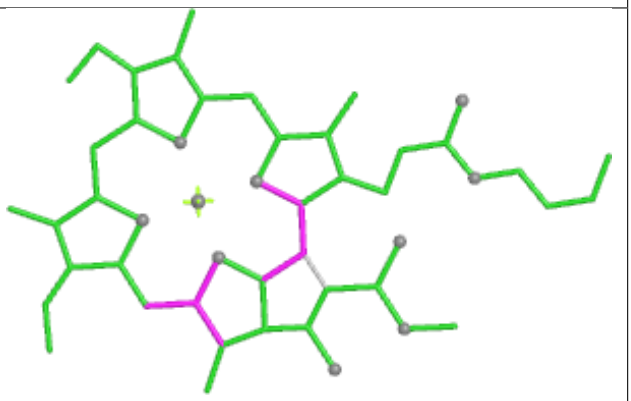
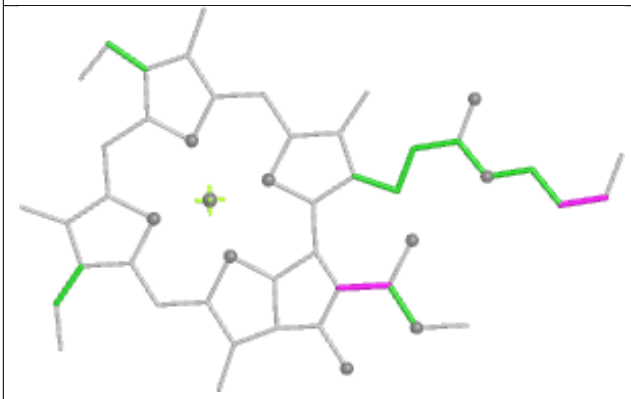


Bond angles



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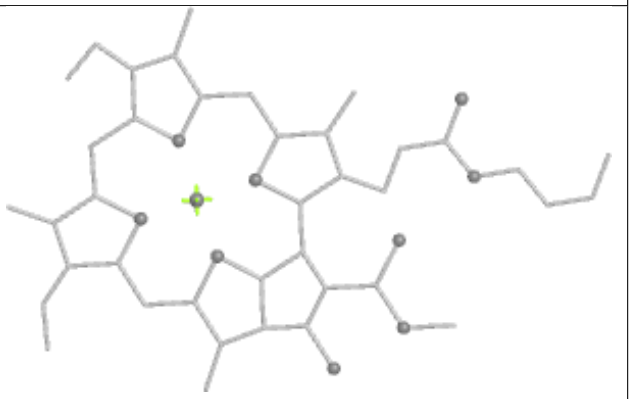
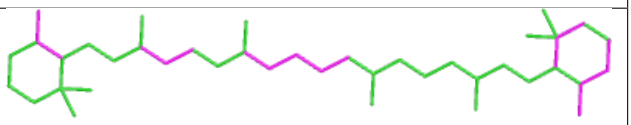


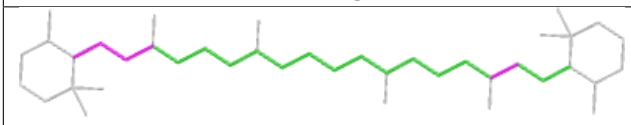
Rings

Ligand BCR B 838

Bond lengths



Bond angles



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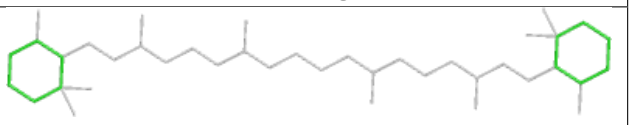
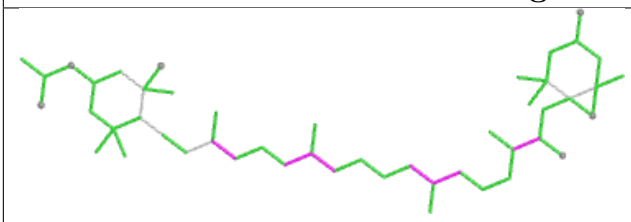


Rings

Ligand A86 Q 214



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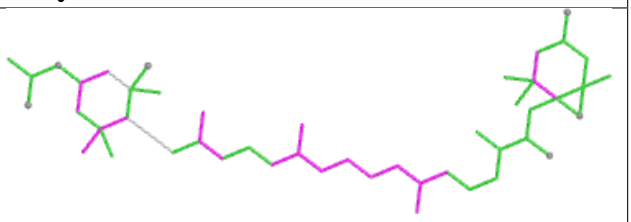
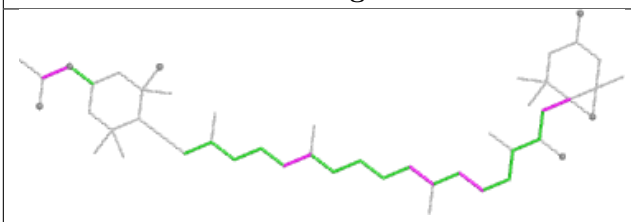


Bond angles



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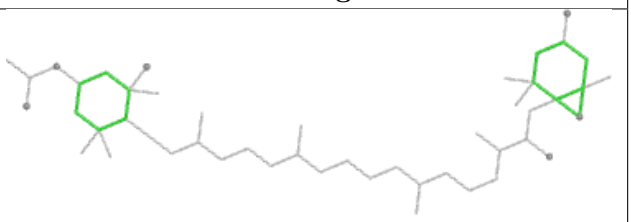
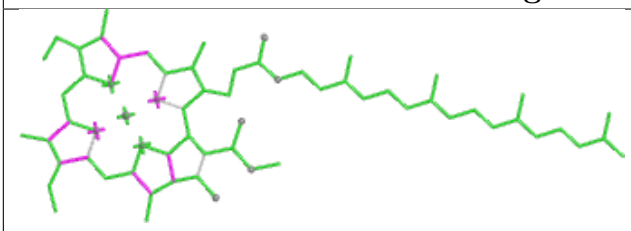


Rings

Ligand CLA O 204



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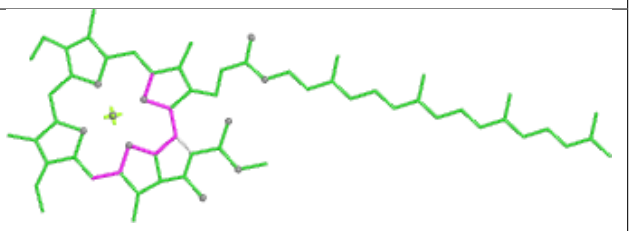
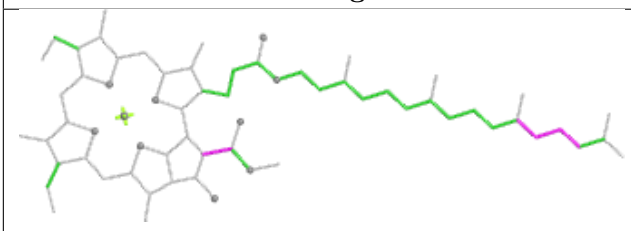


Bond angles



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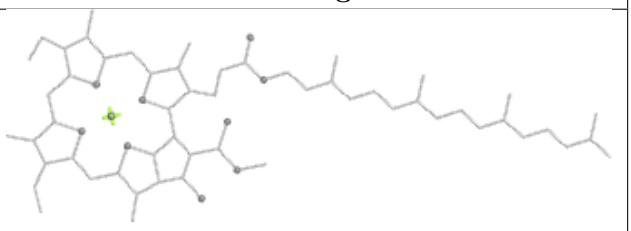
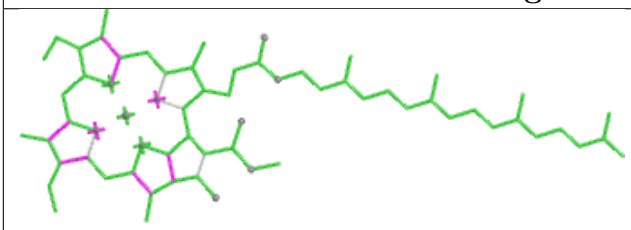


Rings

Ligand CLA B 801



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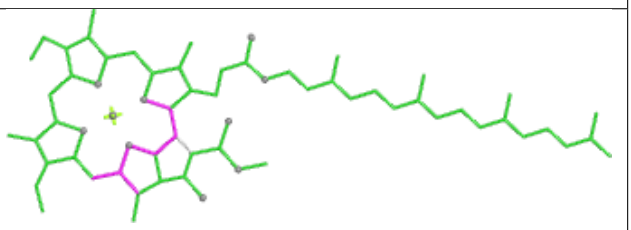
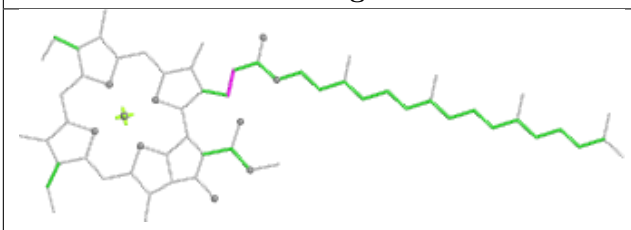


Bond angles



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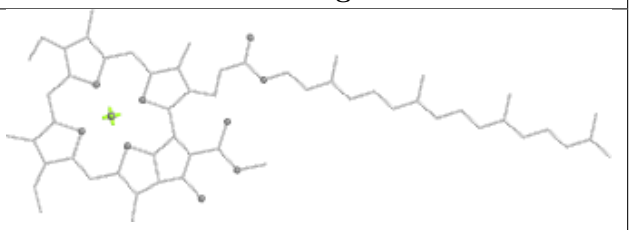
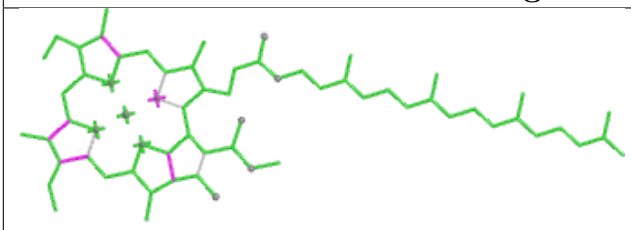


Rings

Ligand CLA A 822



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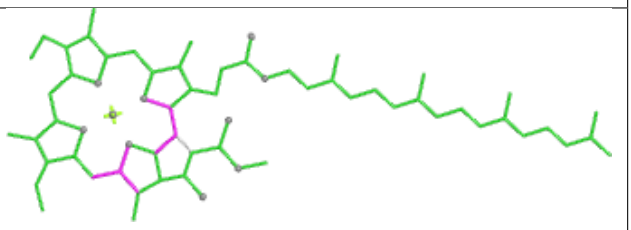
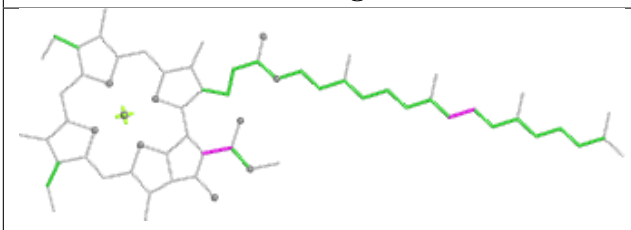


Bond angles



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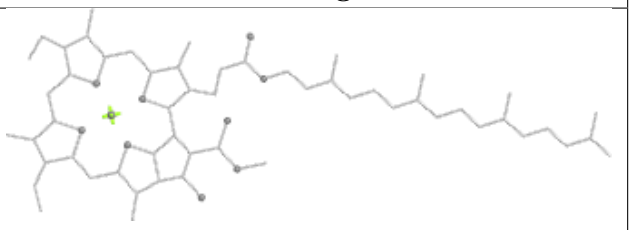
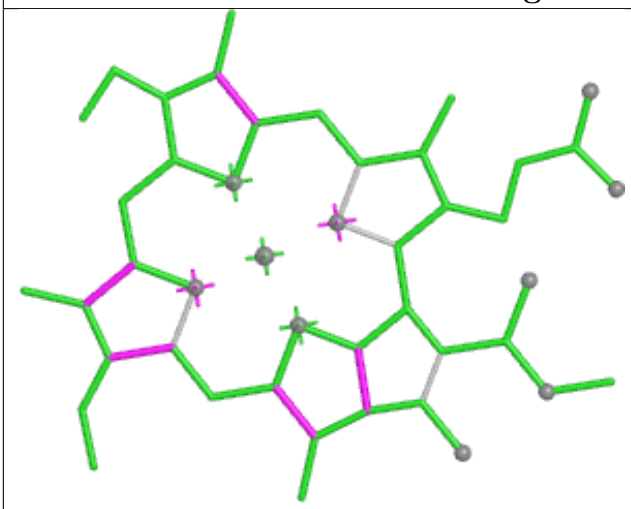


Rings

Ligand CLA O 203



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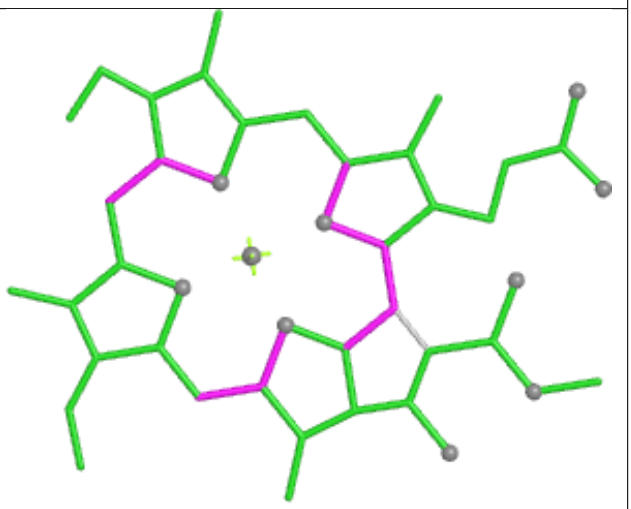
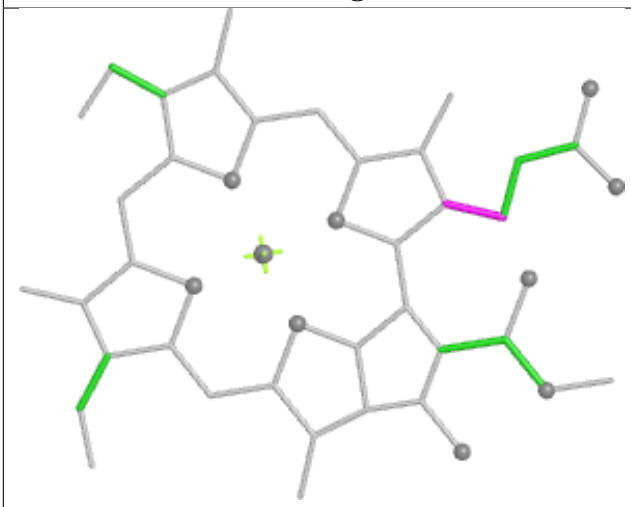


Bond angles



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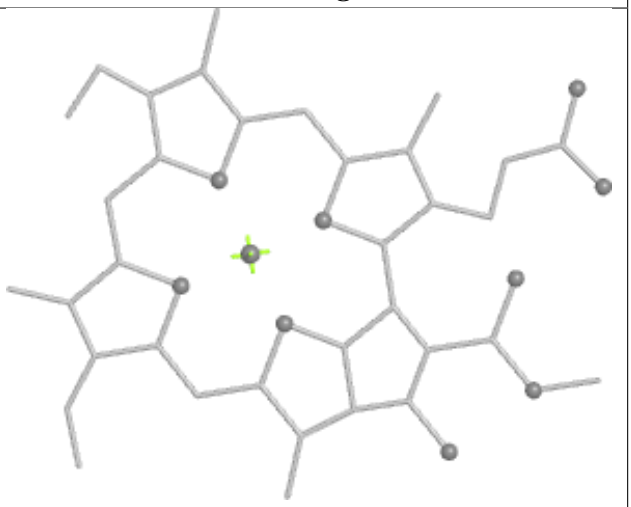
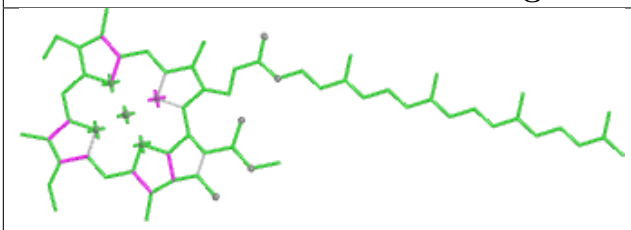
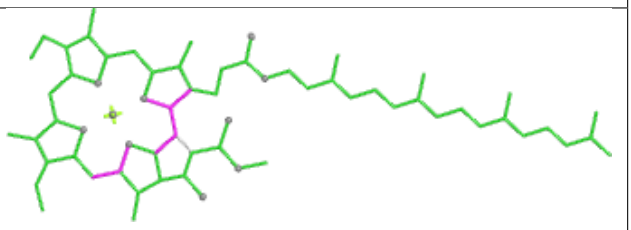
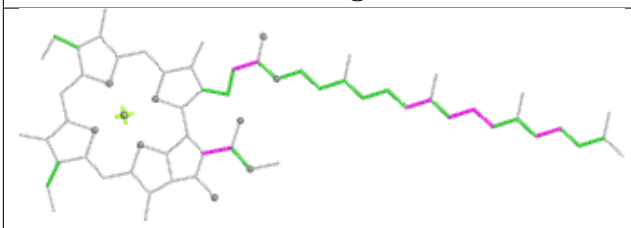
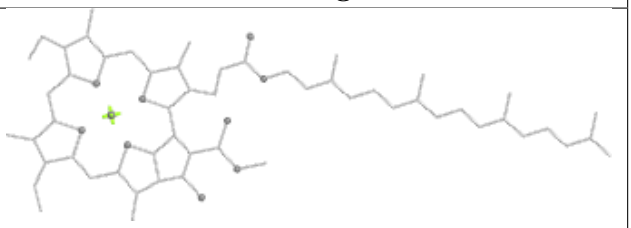
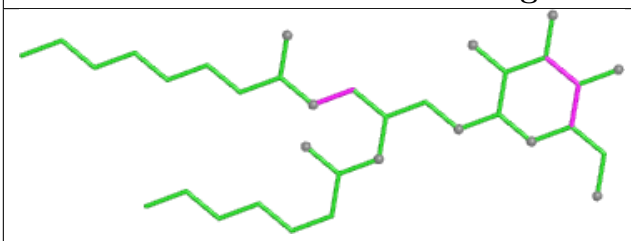
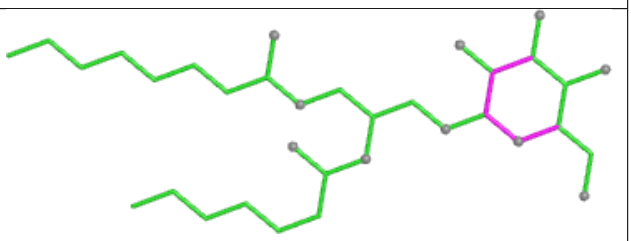
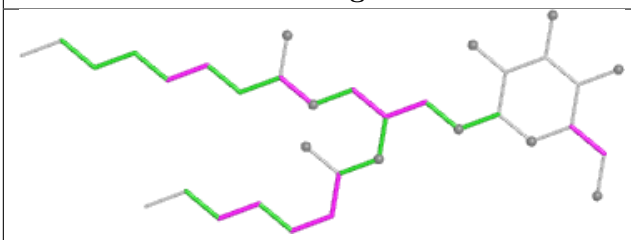
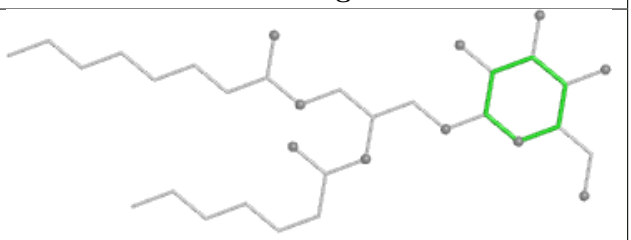
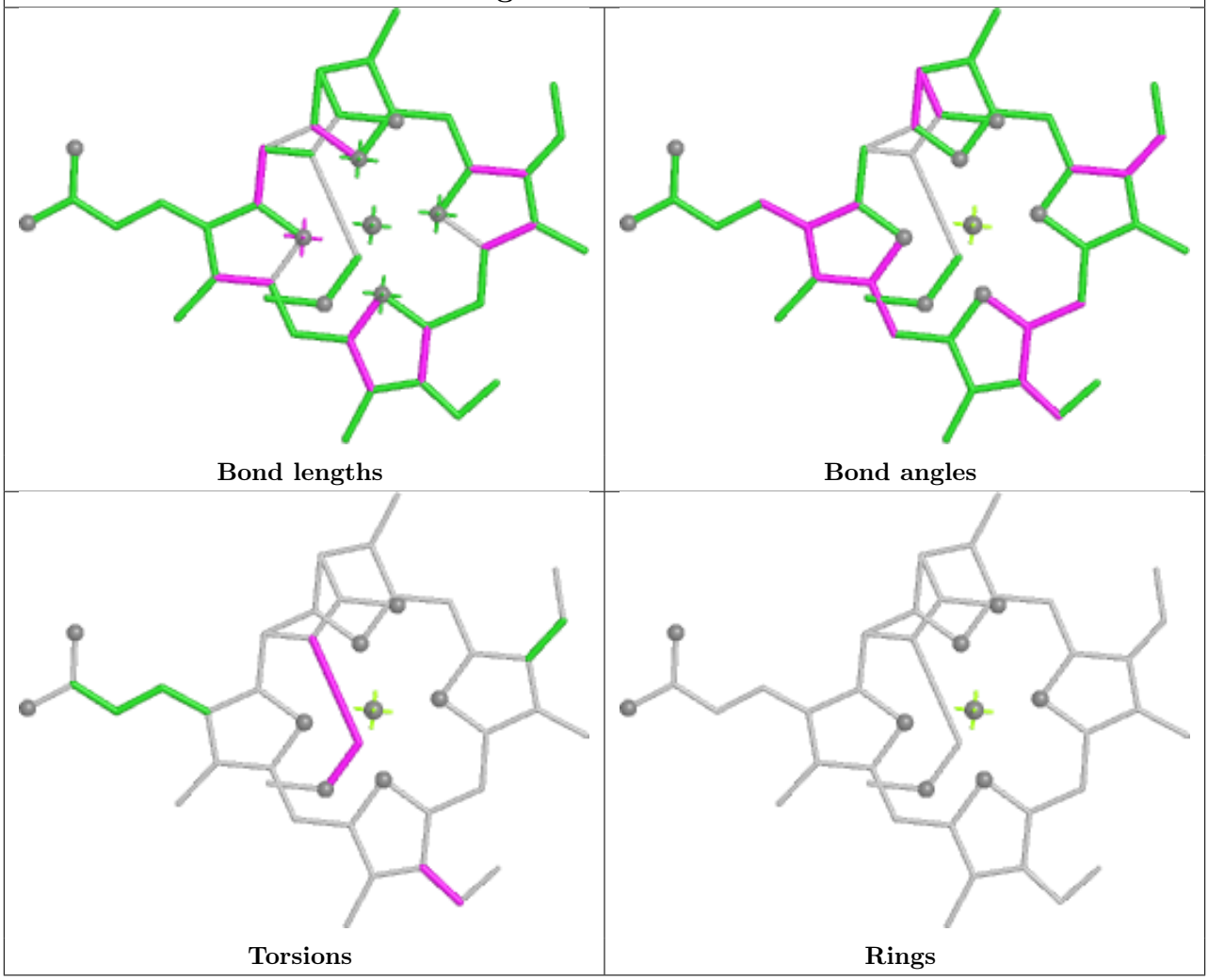


Rings

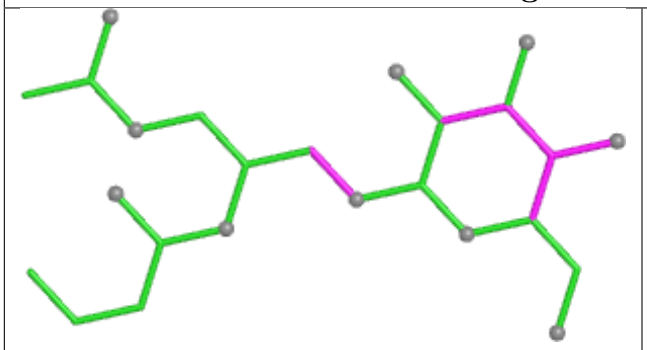
Ligand CLA A 801	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand LMG P 301	
 Bond lengths	 Bond angles
 Torsions	 Rings

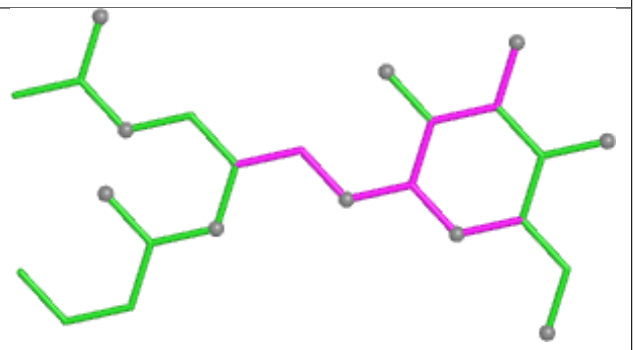
Ligand KC1 P 311



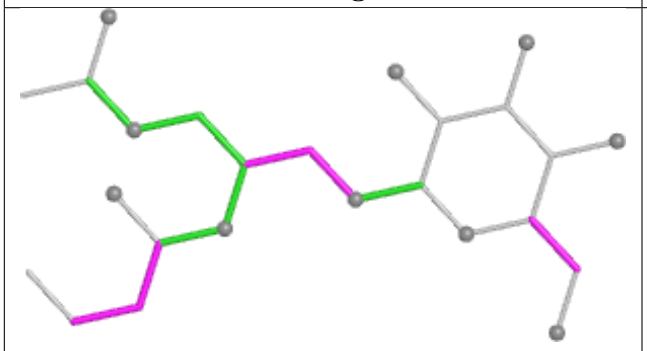
Ligand LMG B 849



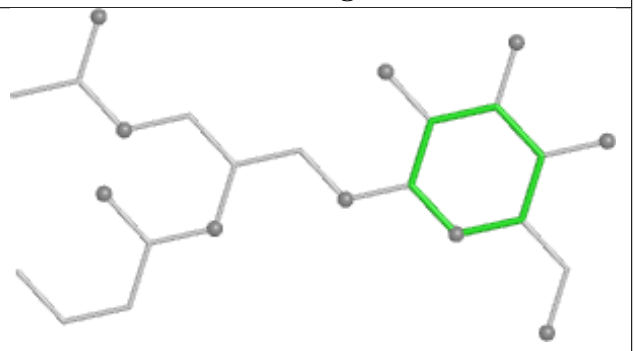
Bond lengths



Bond angles

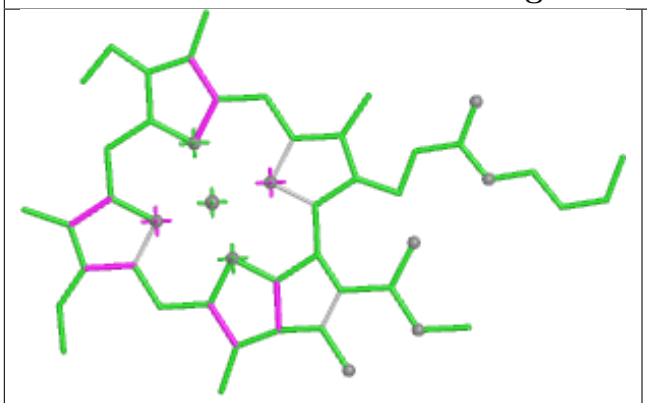


Torsions

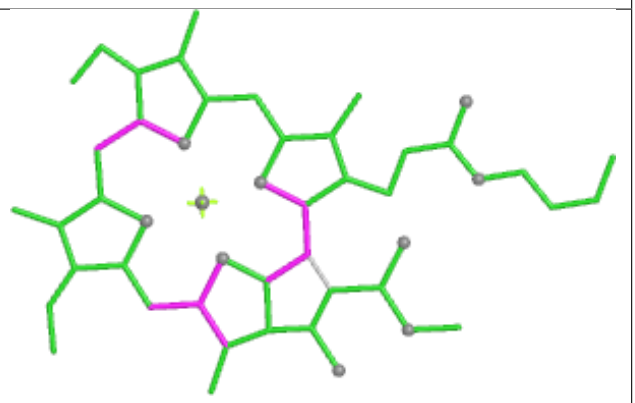


Rings

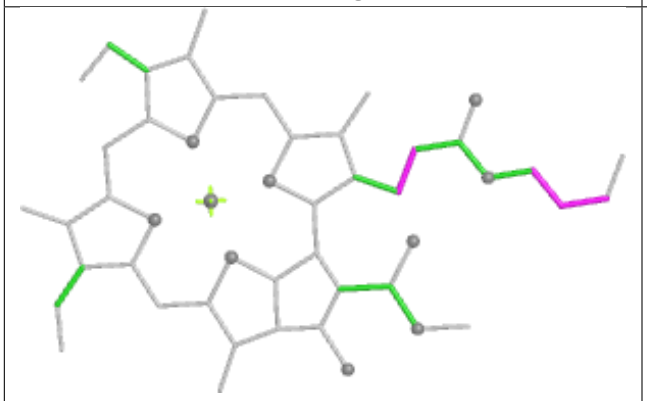
Ligand CLA B 827



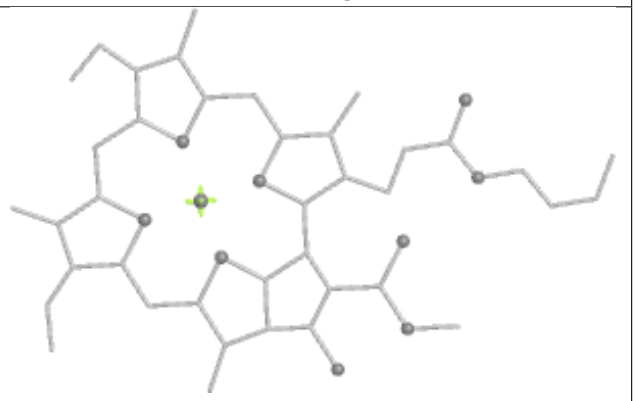
Bond lengths



Bond angles

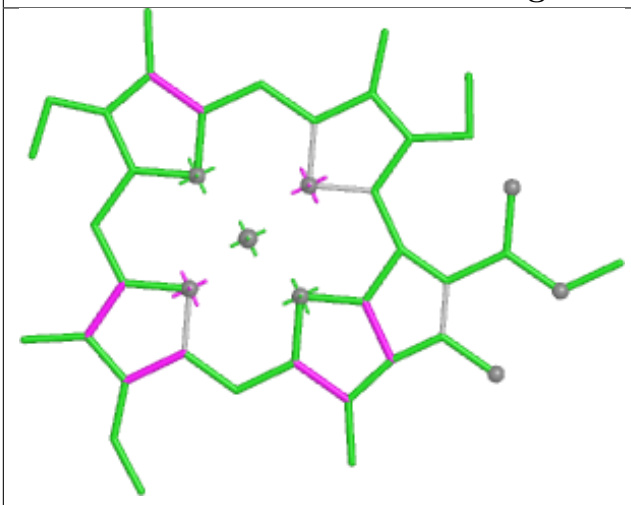


Torsions



Rings

Ligand CLA J 103



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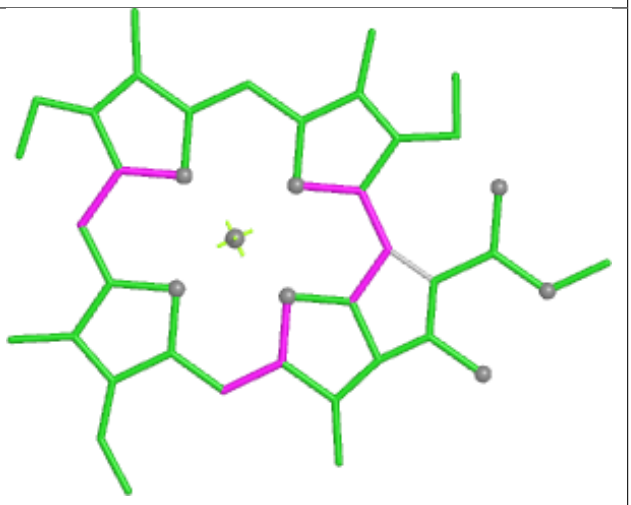
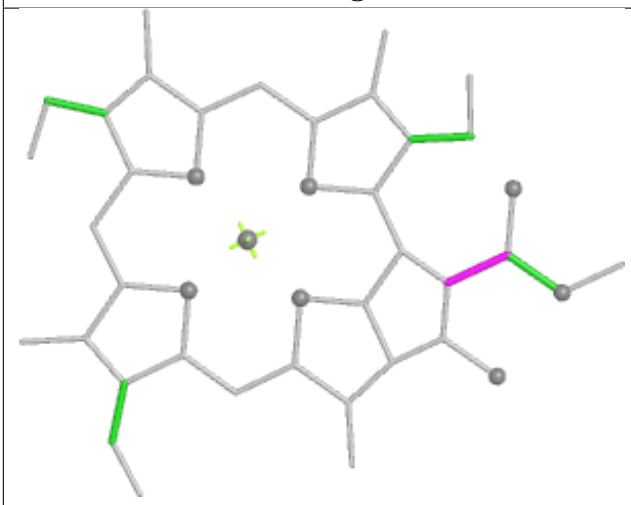


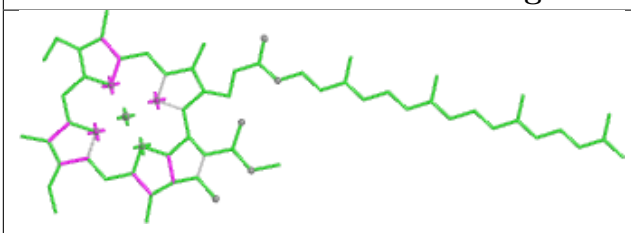
Bond angles



Torsions

Rings

Ligand CLA B 824



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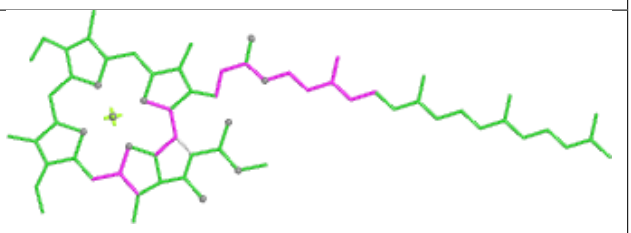
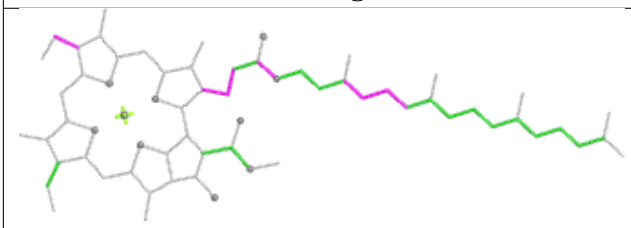
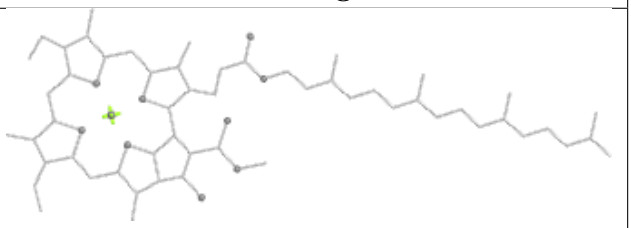


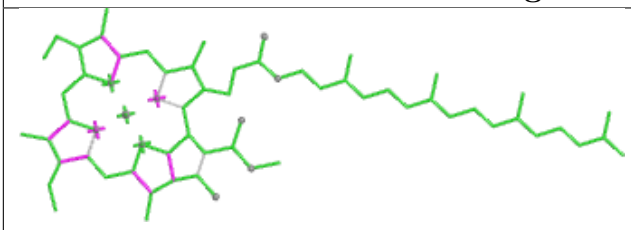
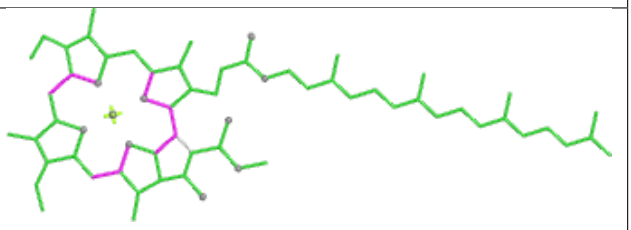
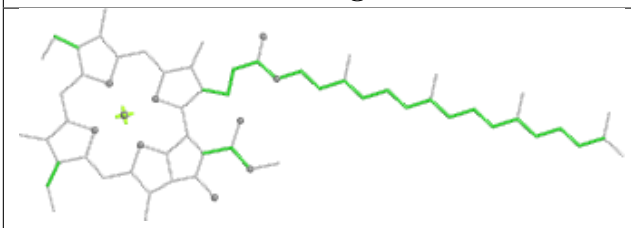
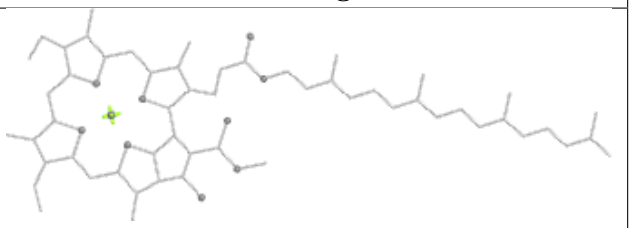
Bond angles

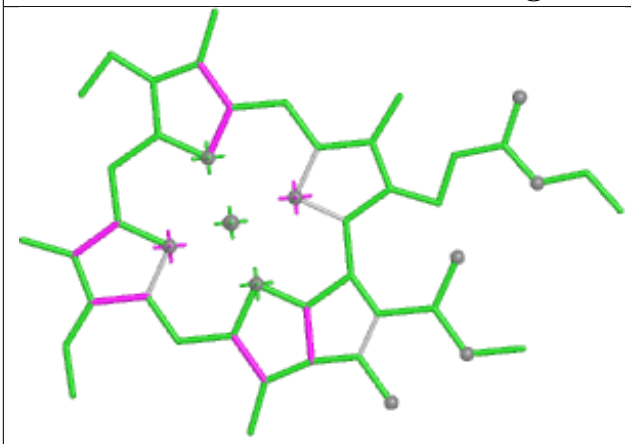
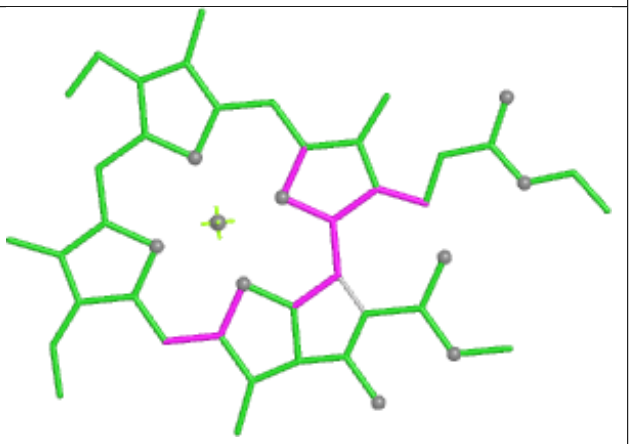
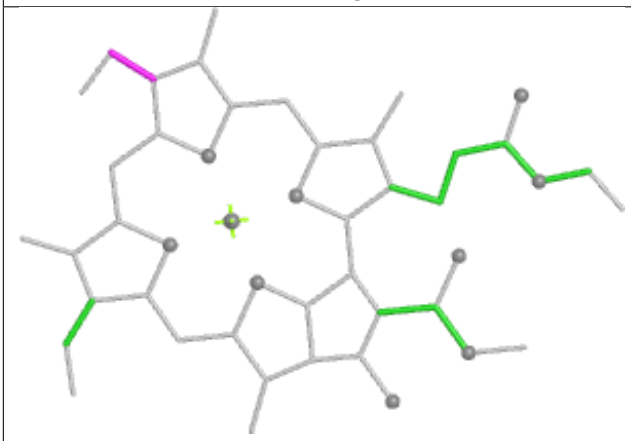
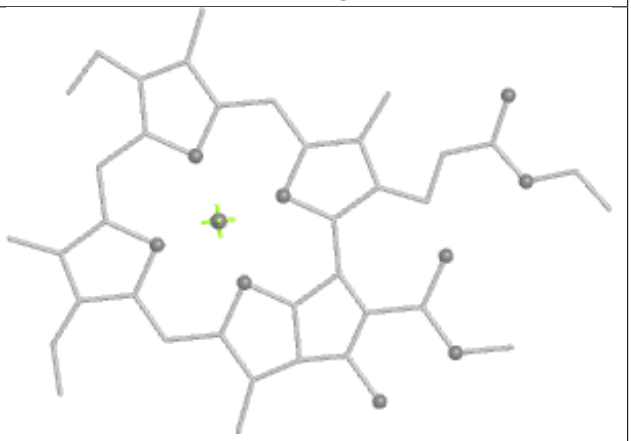


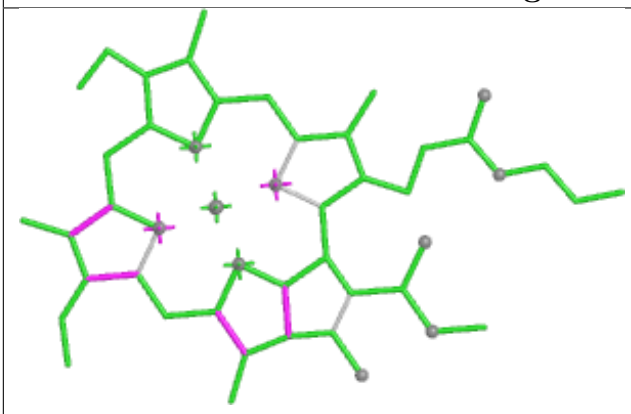
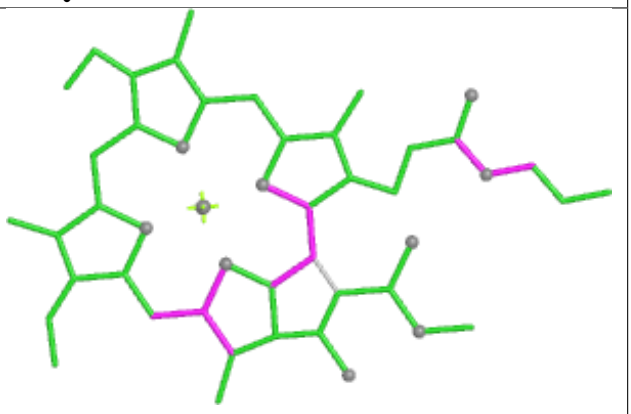
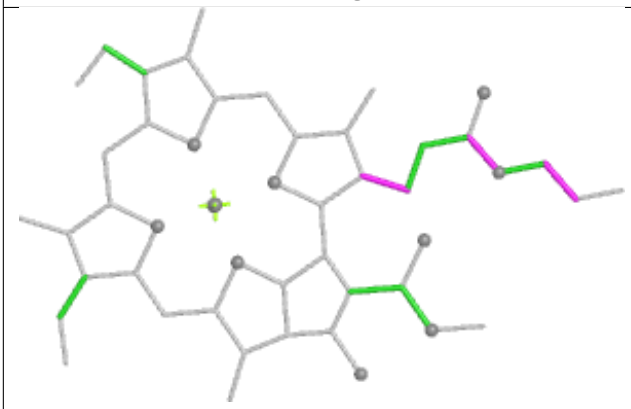
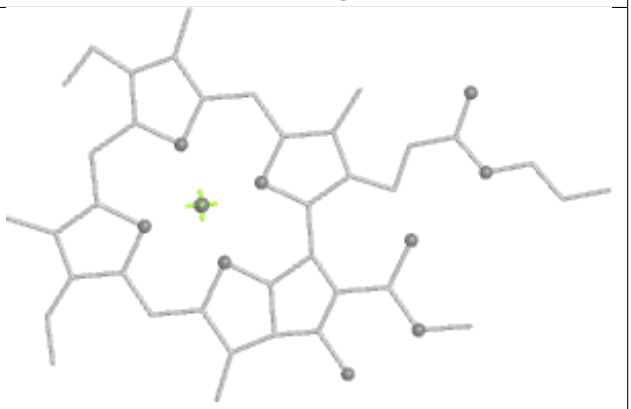
Torsions

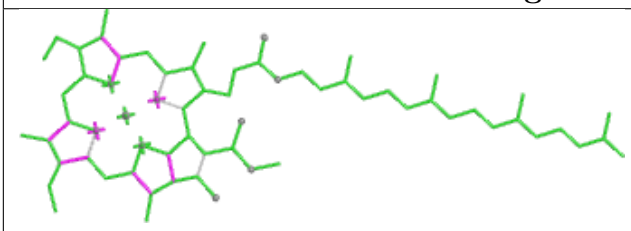
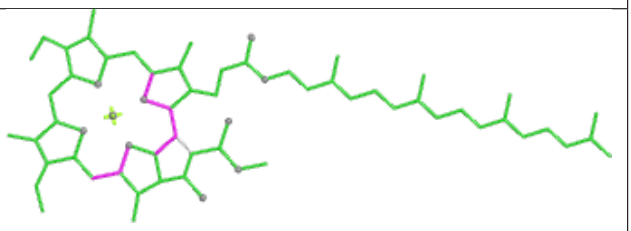
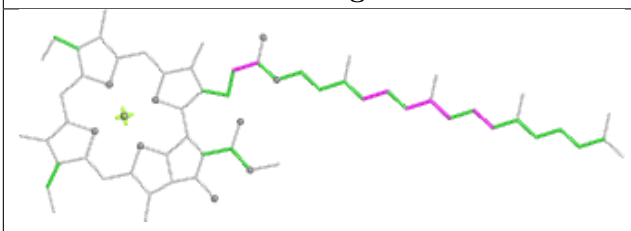
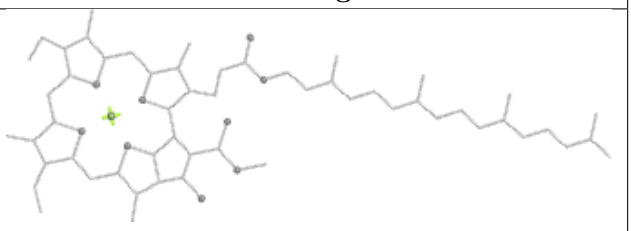


Rings

Ligand CLA B 822	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA P 315	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA Q 203	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA B 806	
 Bond lengths	 Bond angles
 Torsions	 Rings

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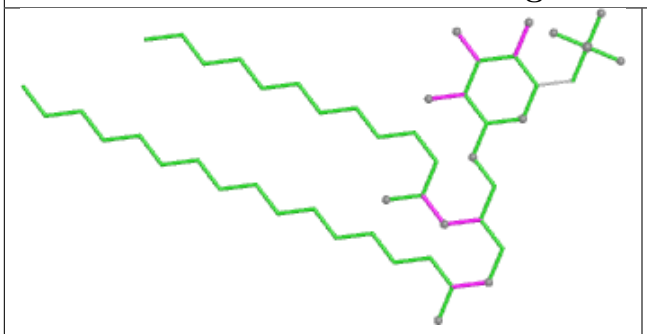
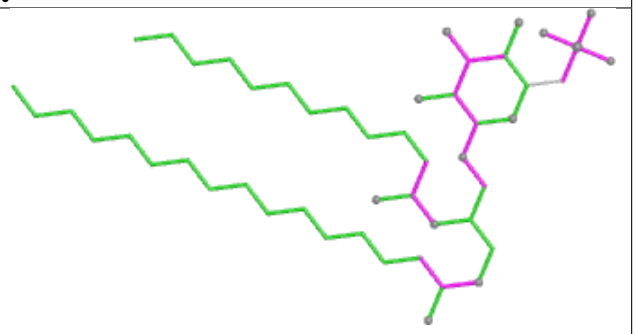
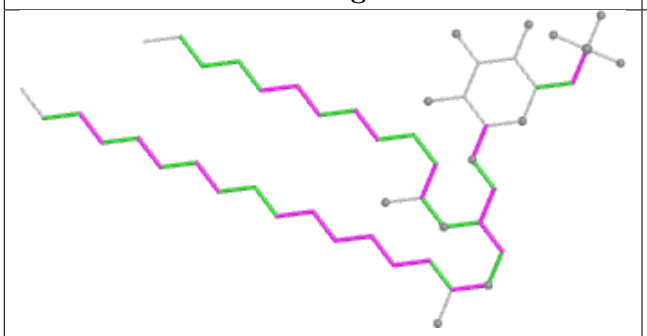
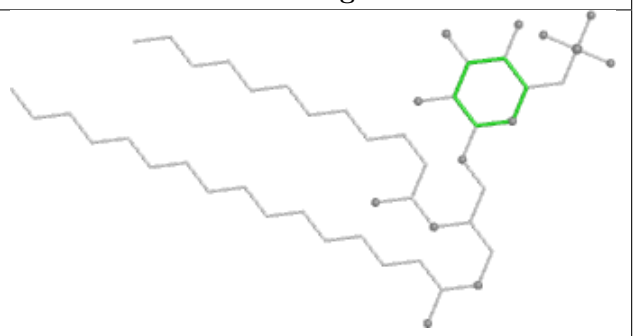
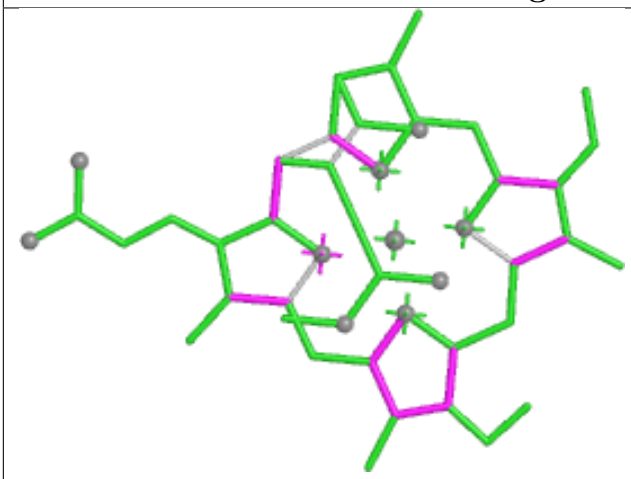
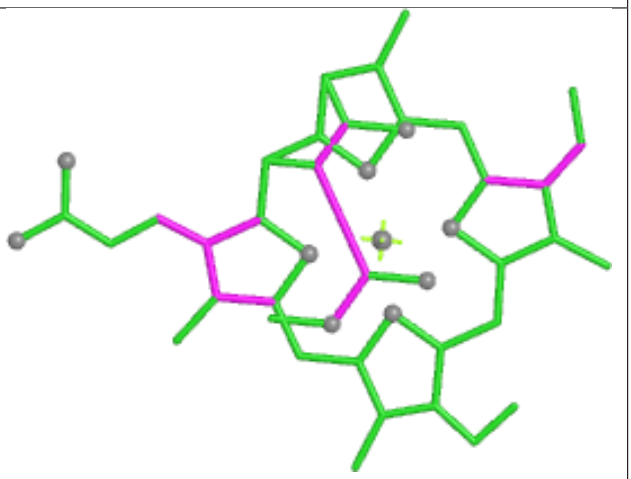
 Bond lengths	 Bond angles
 Torsions	 Rings

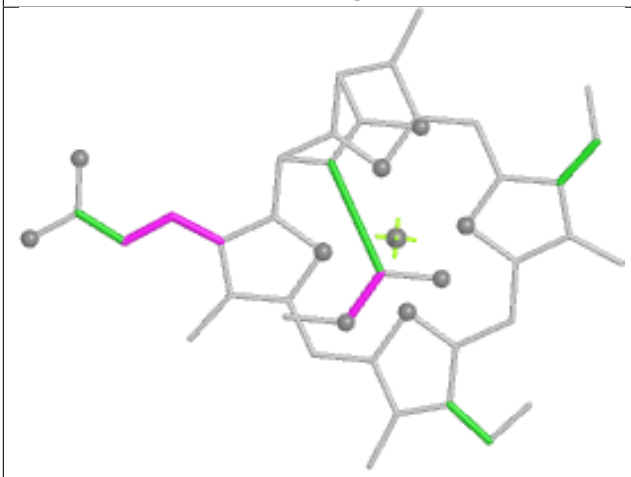
Ligand KC1 S 210



Bond lengths



Bond angles



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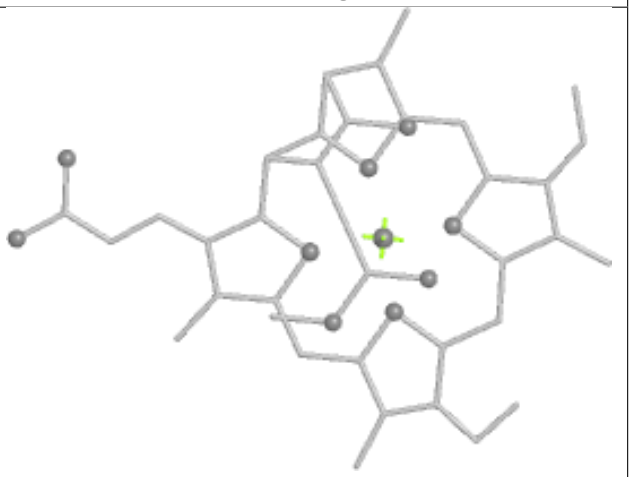
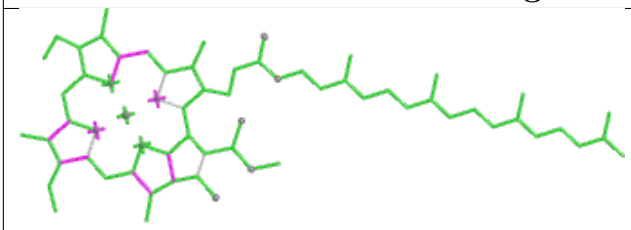
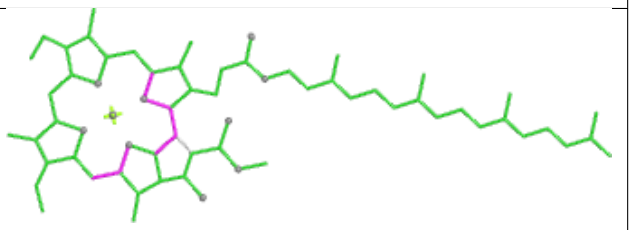


Rings

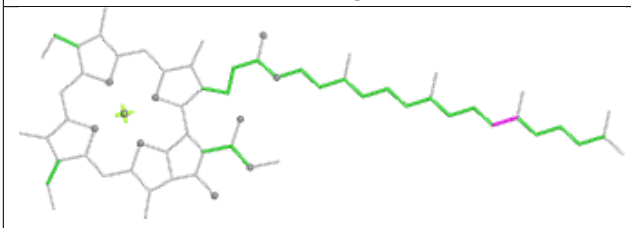
Ligand CLA O 206



Bond lengths



Bond angles



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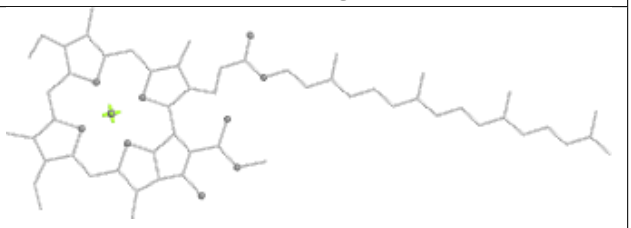
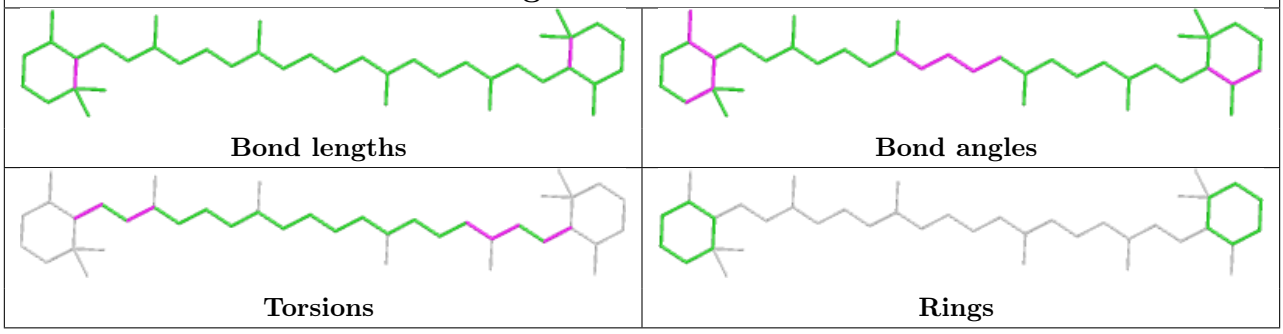
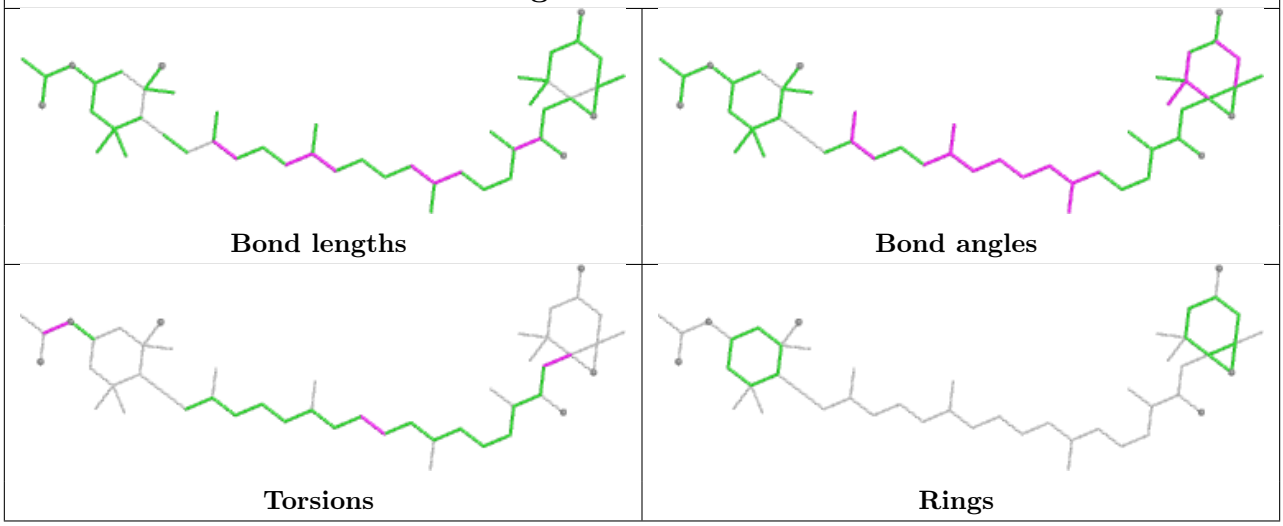


Rings

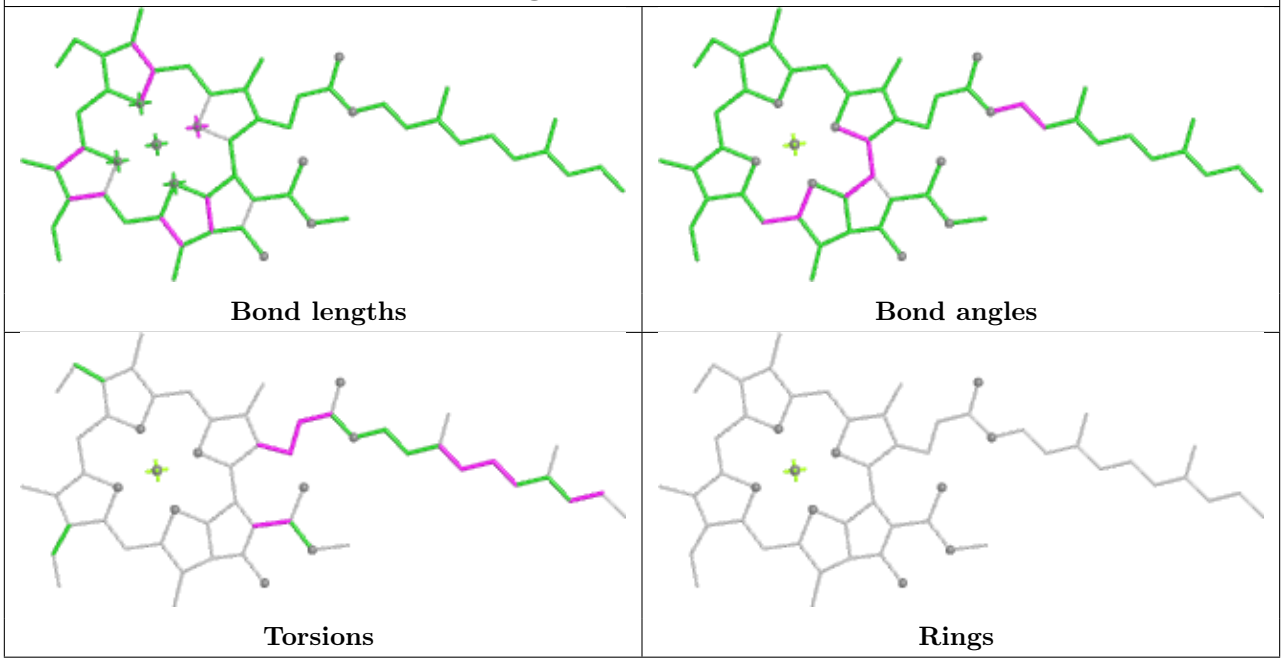
Ligand BCR A 844



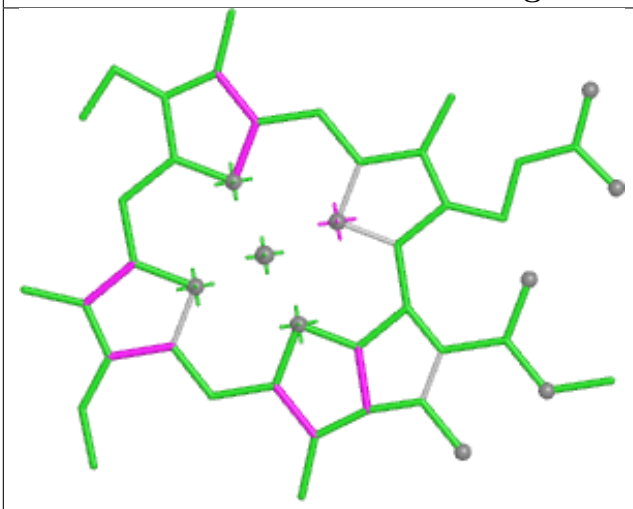
Ligand A86 R 206



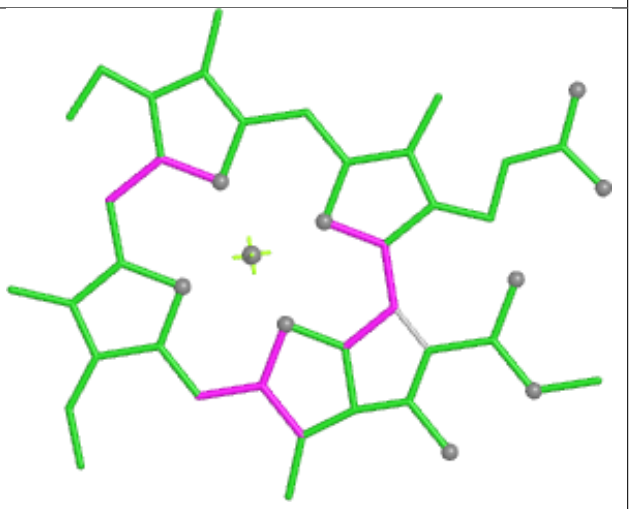
Ligand CLA T 205



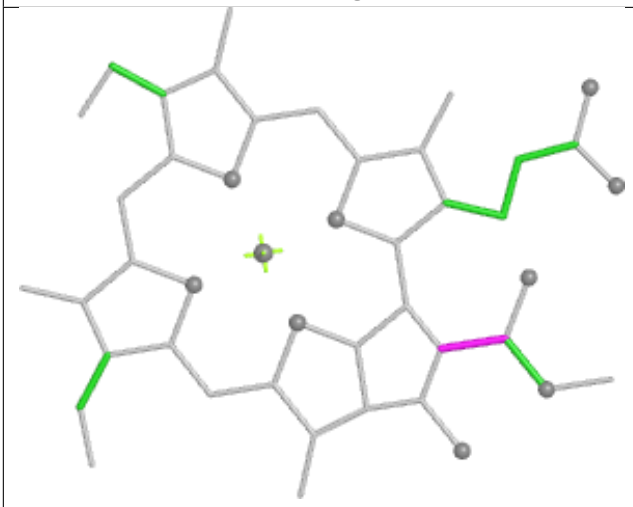
Ligand CLA A 831



Bond lengths



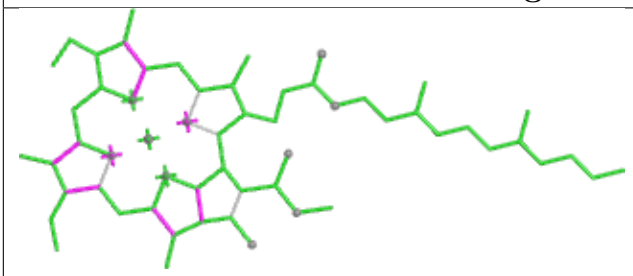
Bond angles



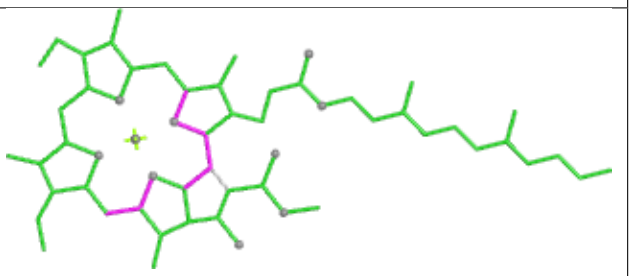
Torsions

Rings

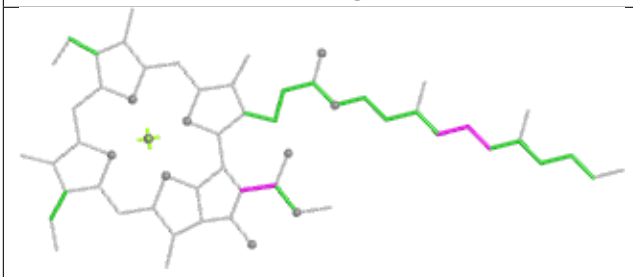
Ligand CLA B 828



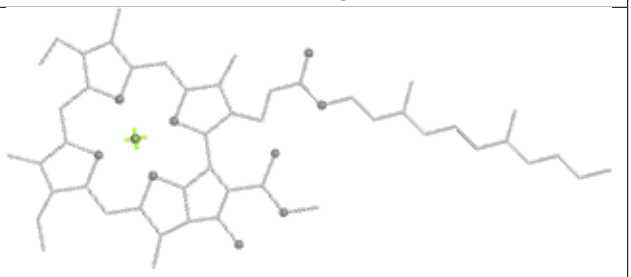
Bond lengths



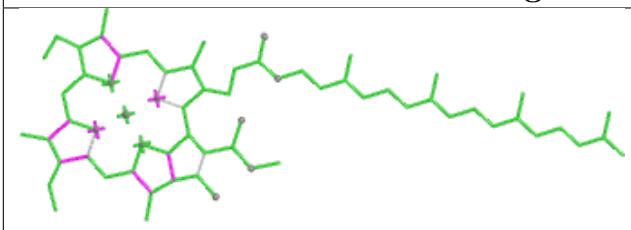
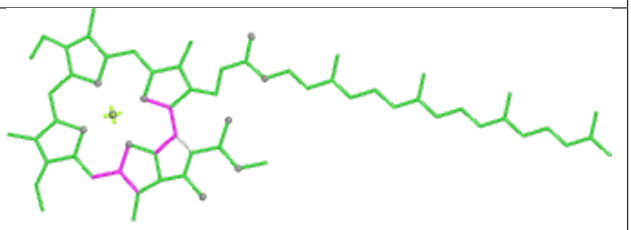
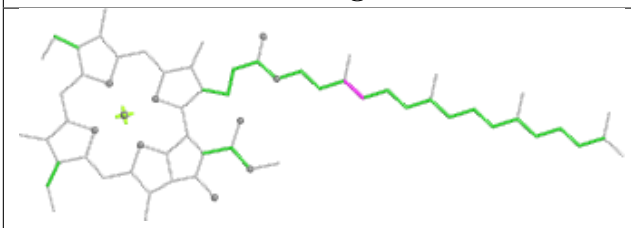
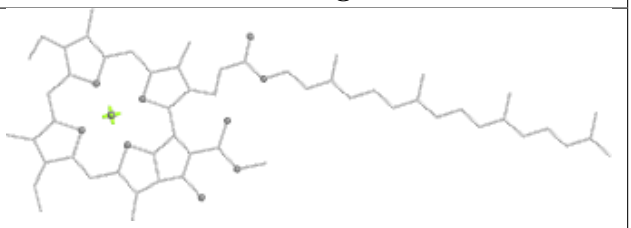
Bond angles

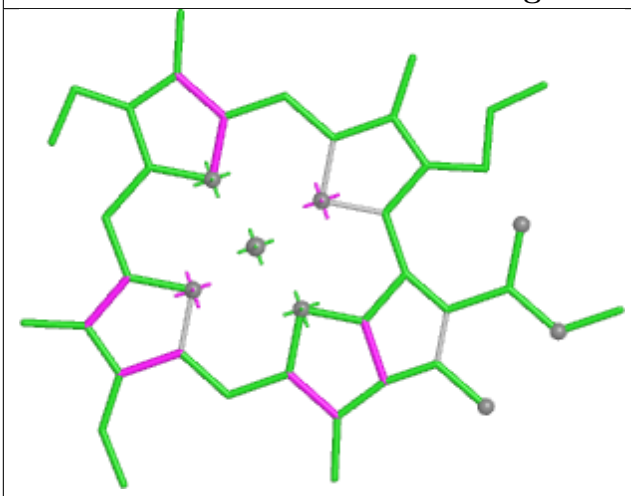
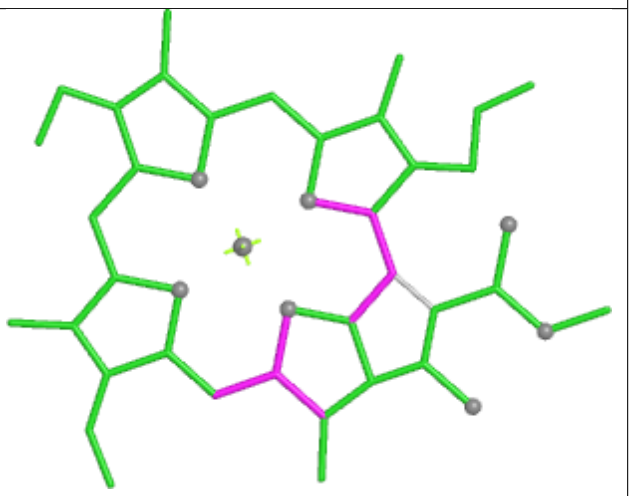
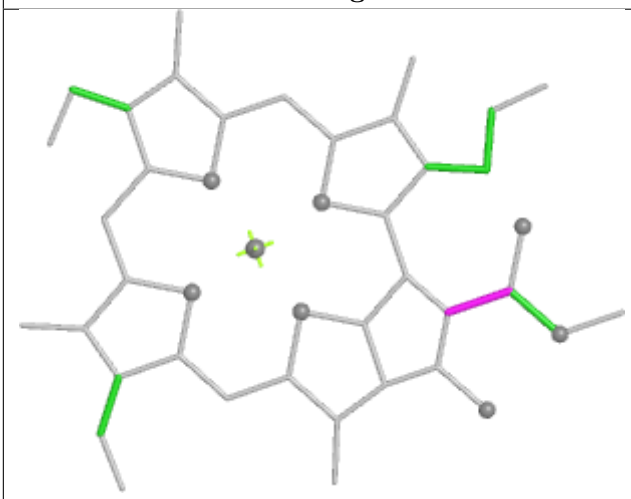
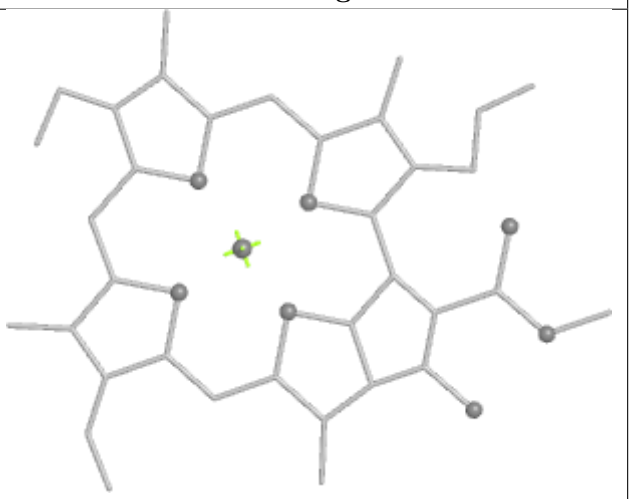


Torsions



Rings

Ligand CLA B 807	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA A 819	
 Bond lengths	 Bond angles
 Torsions	 Rings

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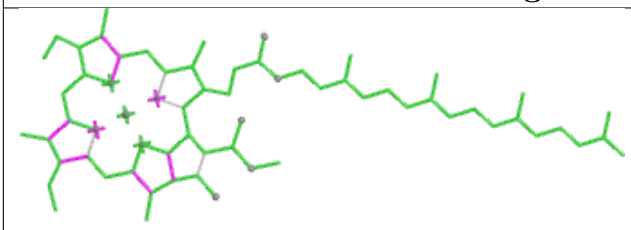
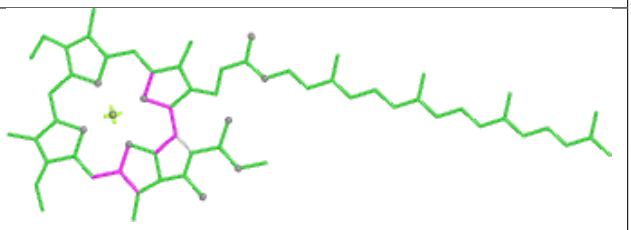
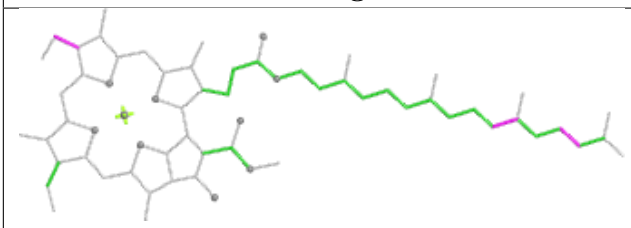
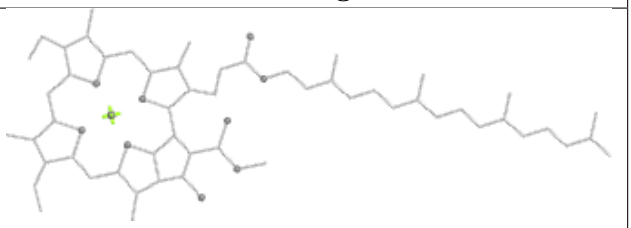
 Bond lengths	 Bond angles
 Torsions	 Rings

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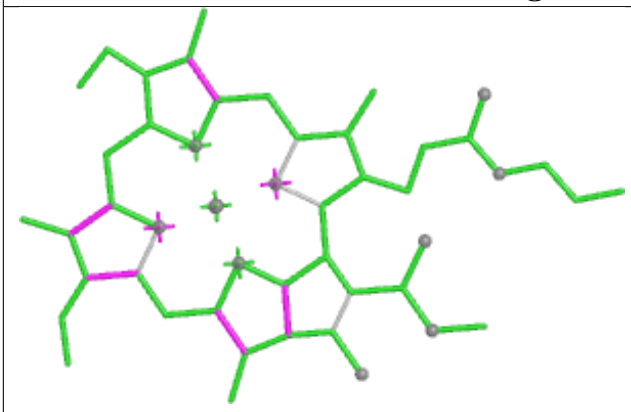
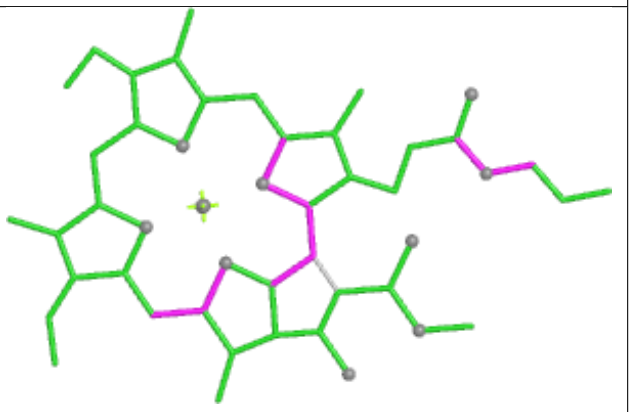
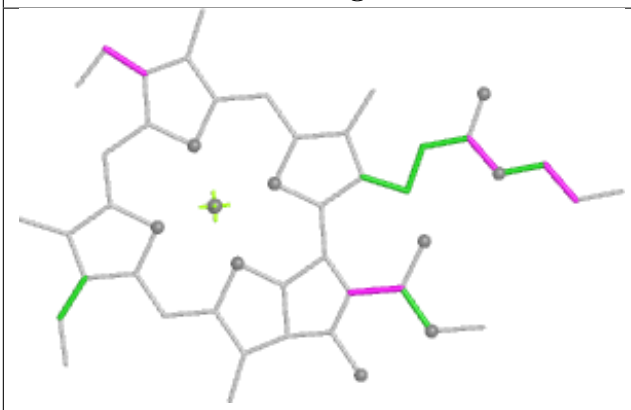
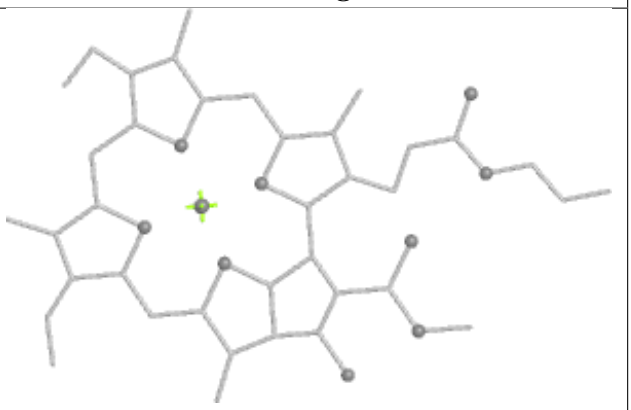
 Bond lengths	 Bond angles
 Torsions	 Rings

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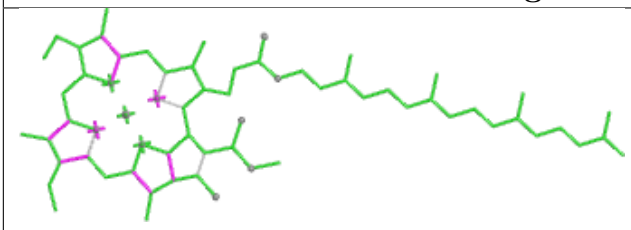
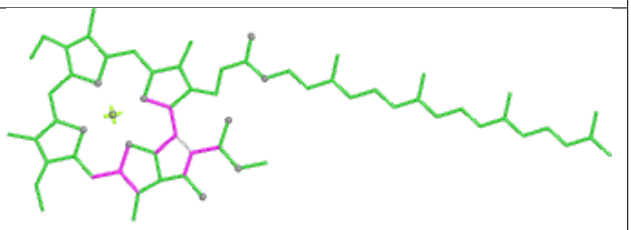
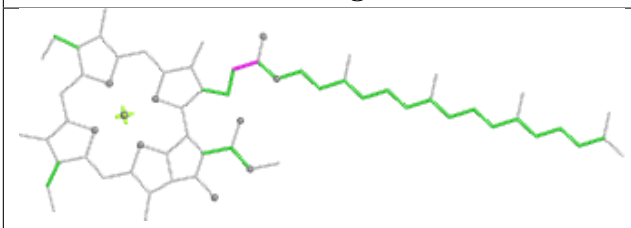
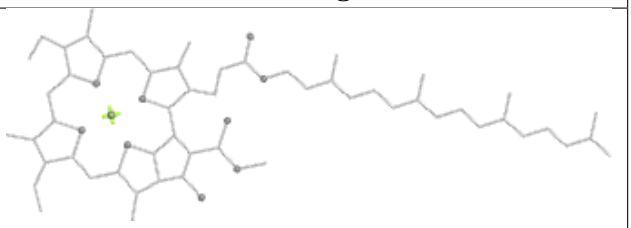
 Bond lengths	 Bond angles
 Torsions	 Rings

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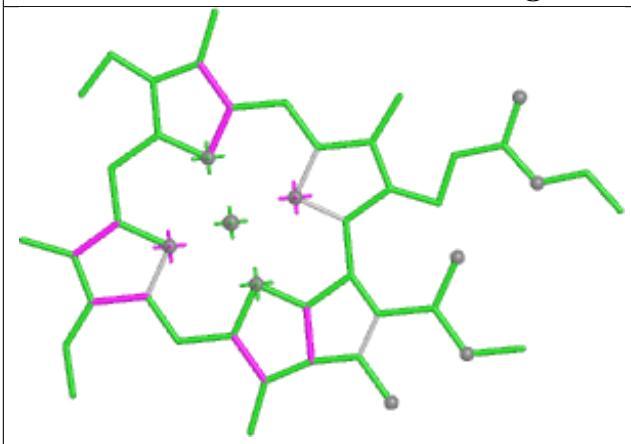
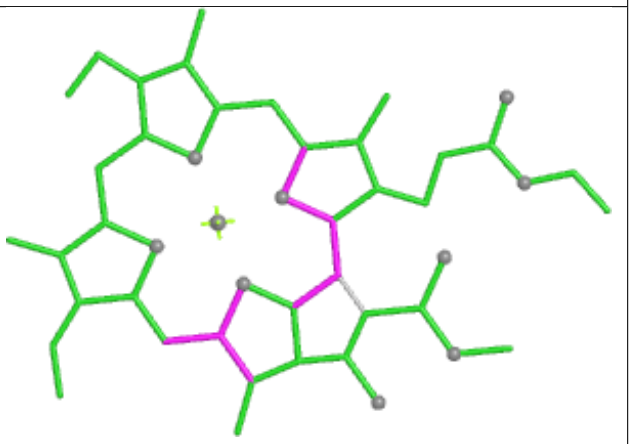
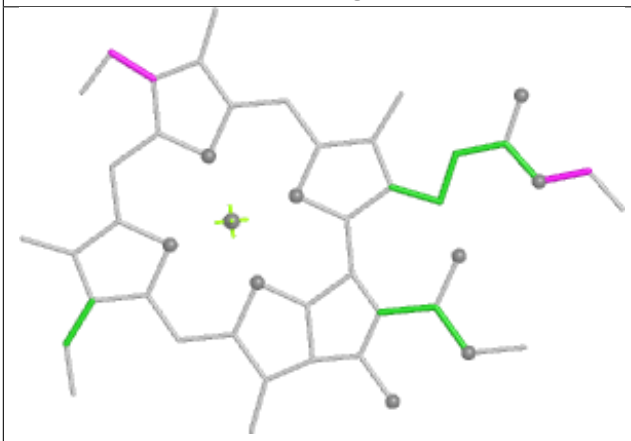
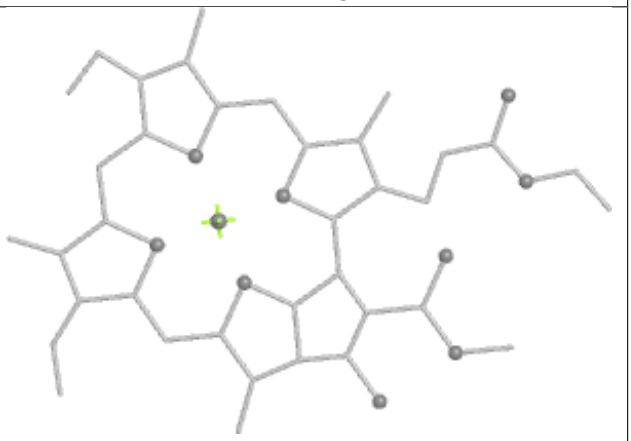
 Bond lengths	 Bond angles
 Torsions	 Rings

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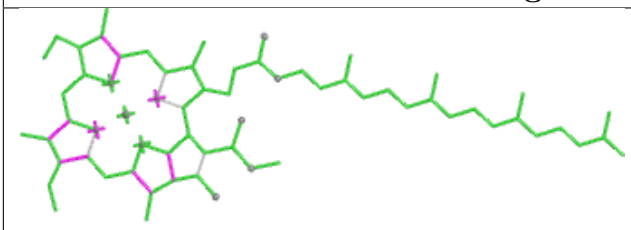
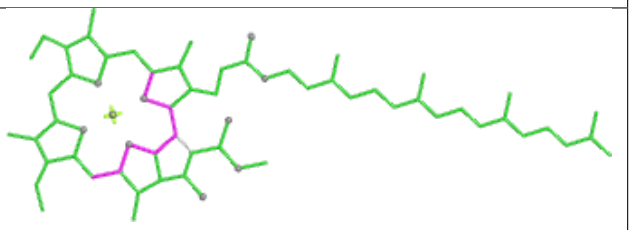
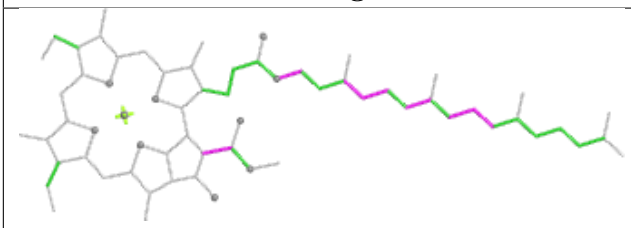
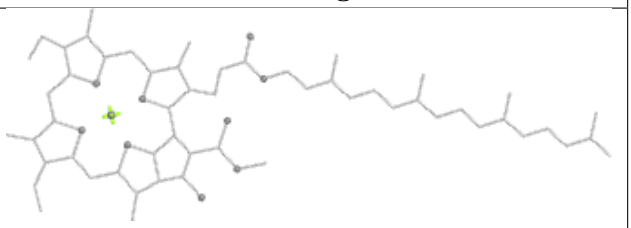
 Bond lengths	 Bond angles
 Torsions	 Rings

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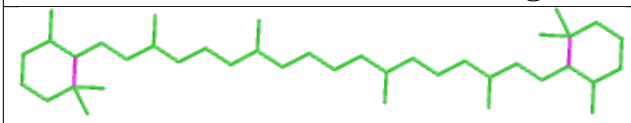
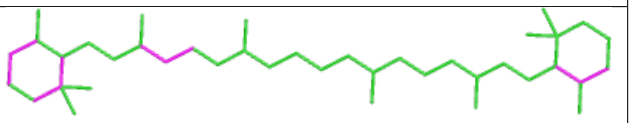
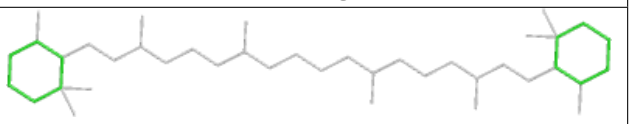
 Bond lengths	 Bond angles
Torsions	 Rings

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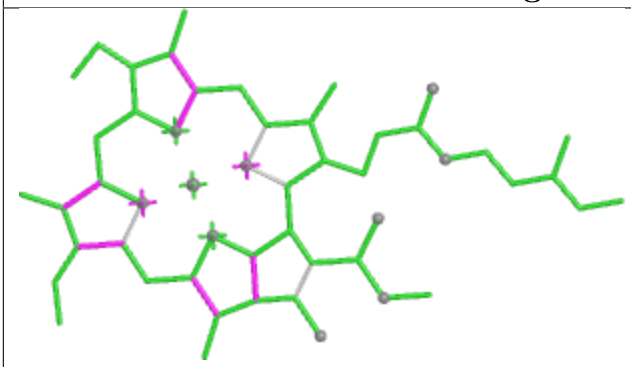
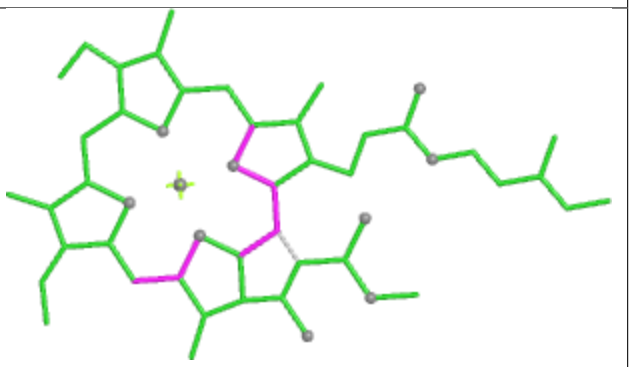
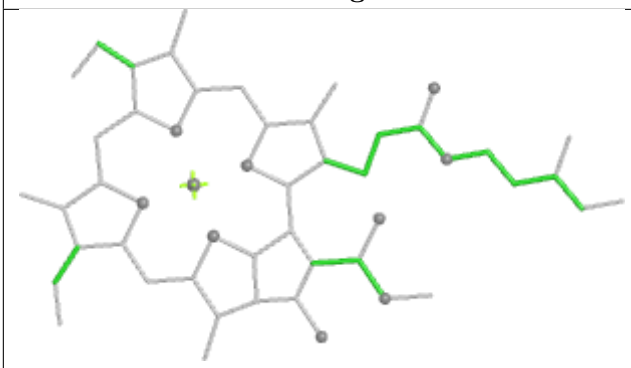
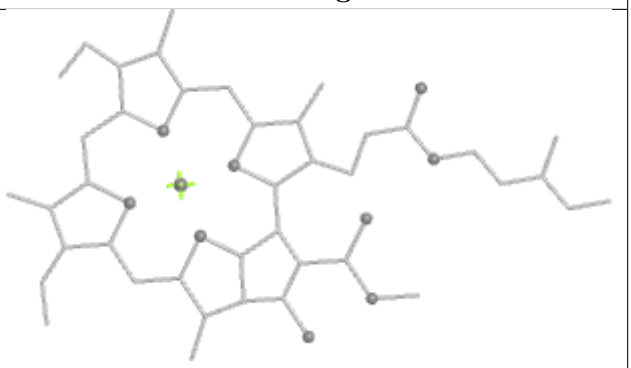
 Bond lengths	 Bond angles
 Torsions	 Rings

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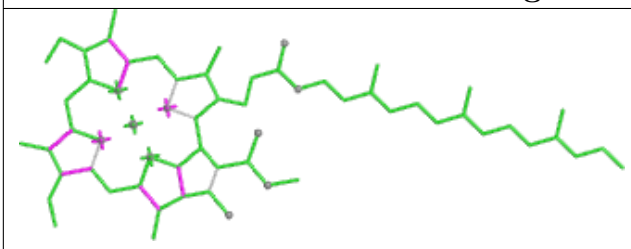
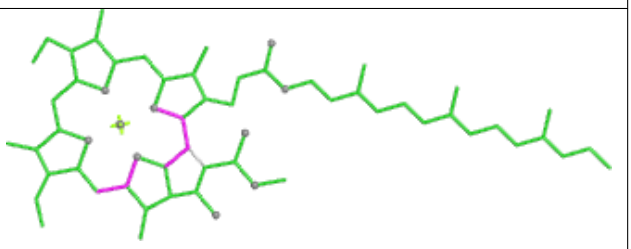
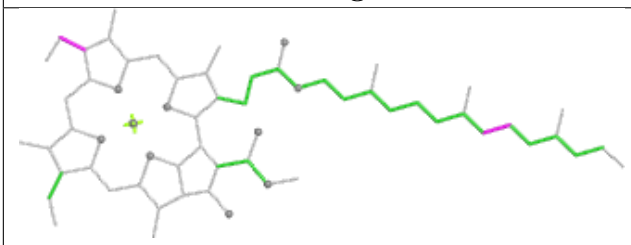
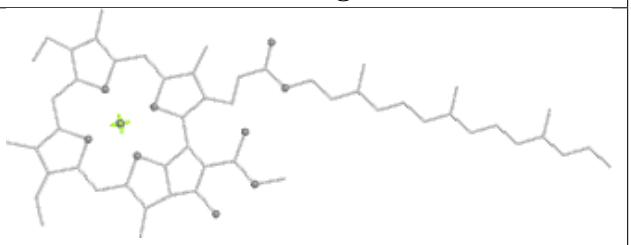
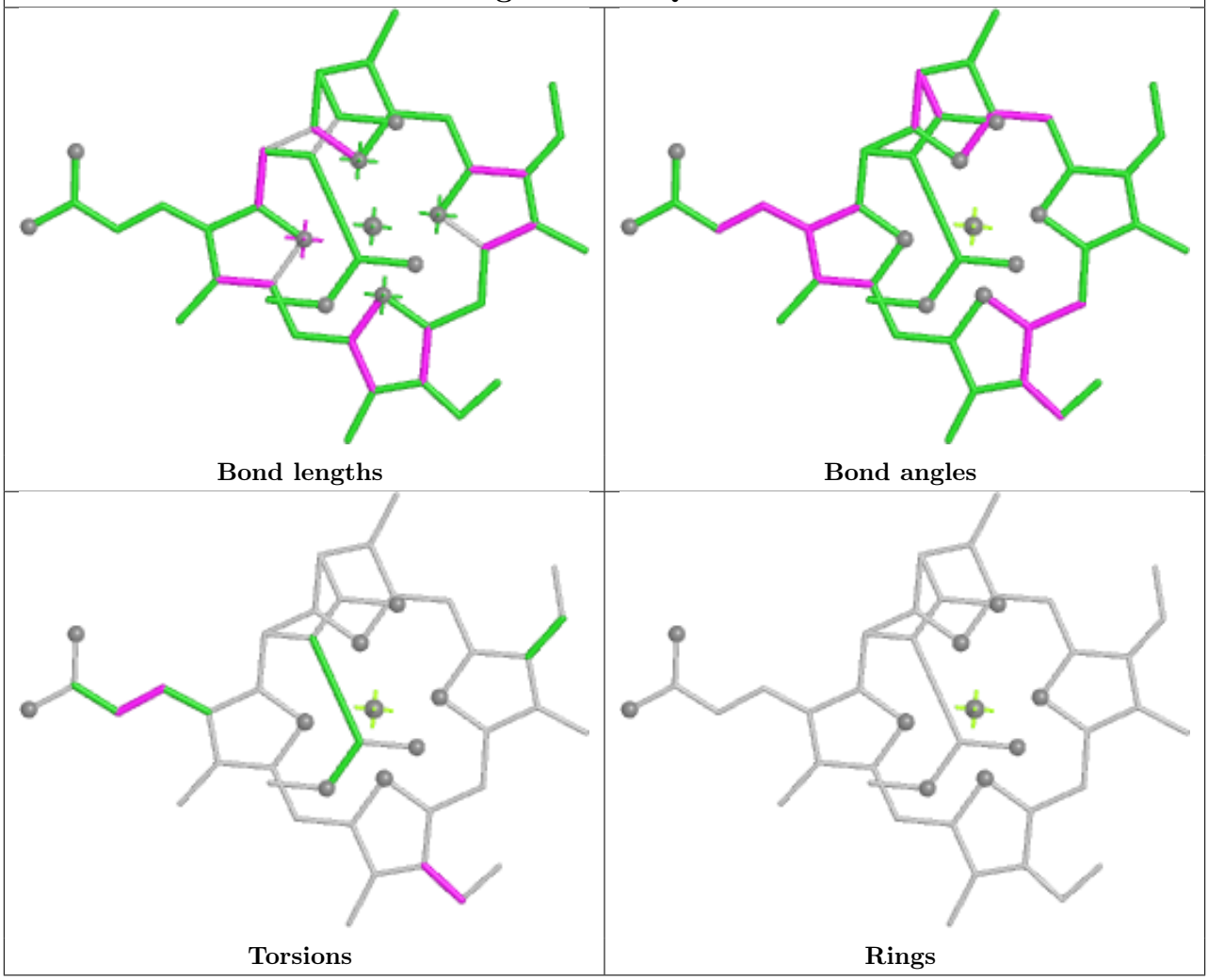
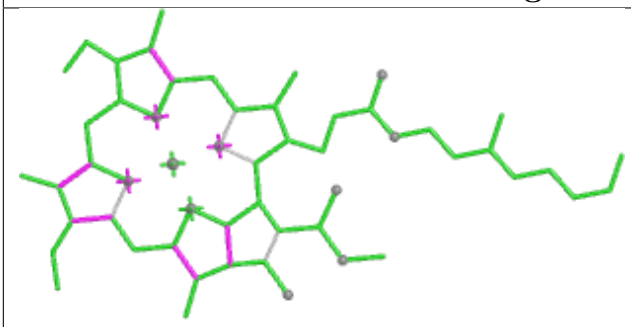
 Bond lengths	 Bond angles
 Torsions	 Rings

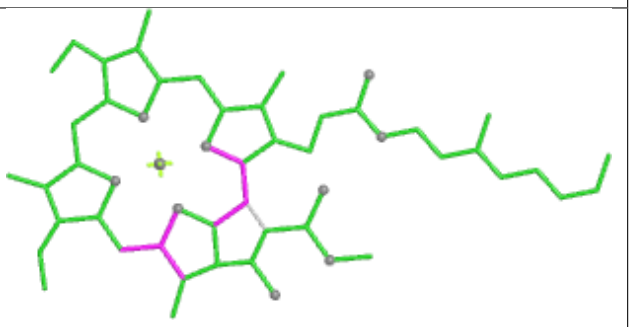
Ligand KC1 Q 210



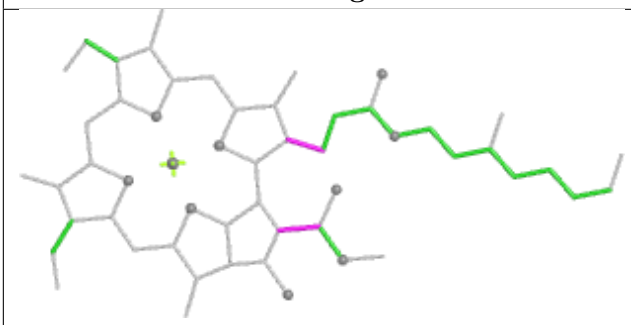
Ligand CLA B 812



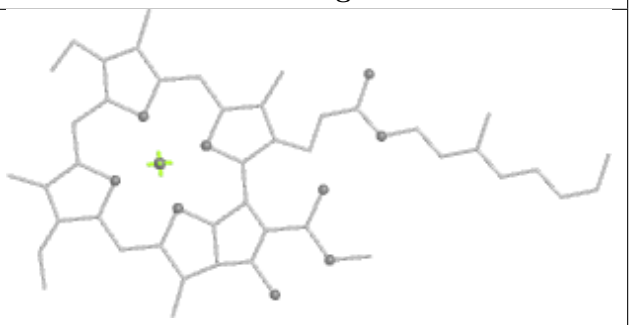
Bond lengths



Bond angles

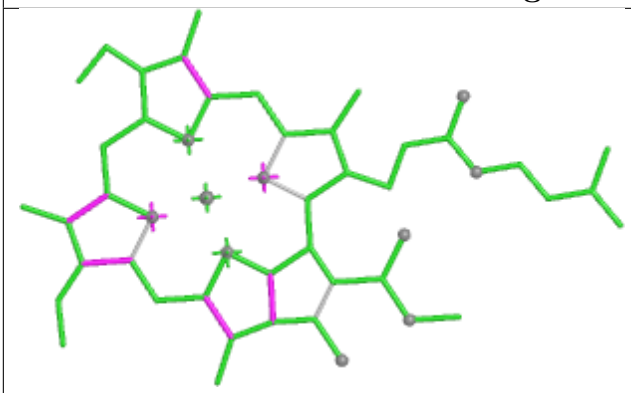


Torsions



Rings

Ligand CLA A 813



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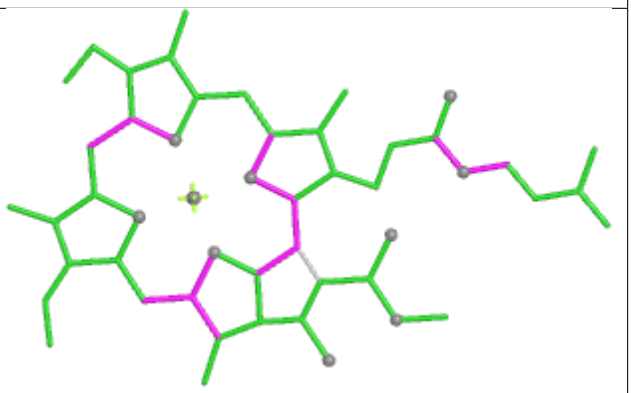
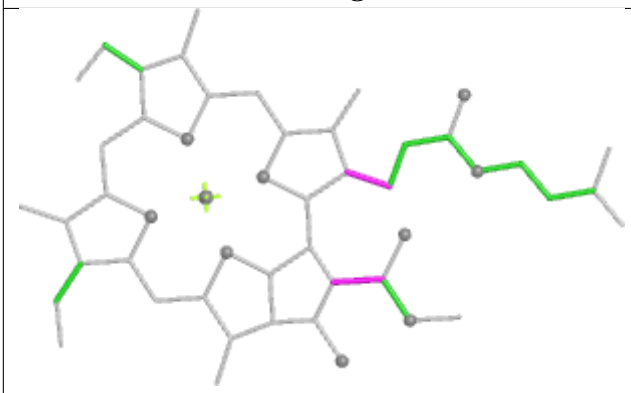


Bond angles



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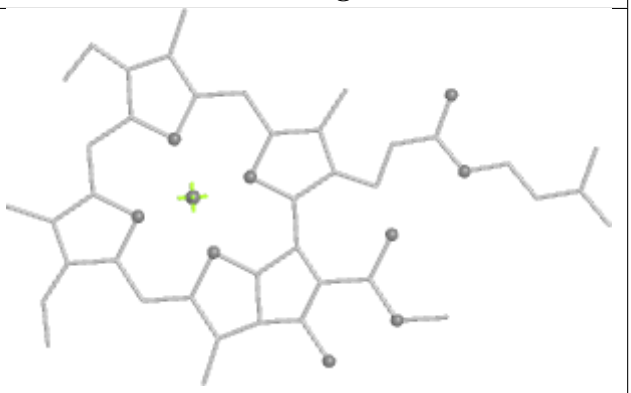
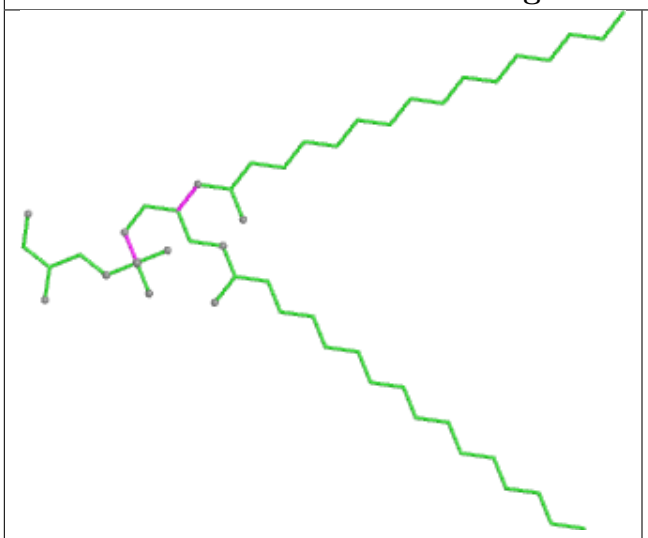


Rings

Ligand LHG R 201



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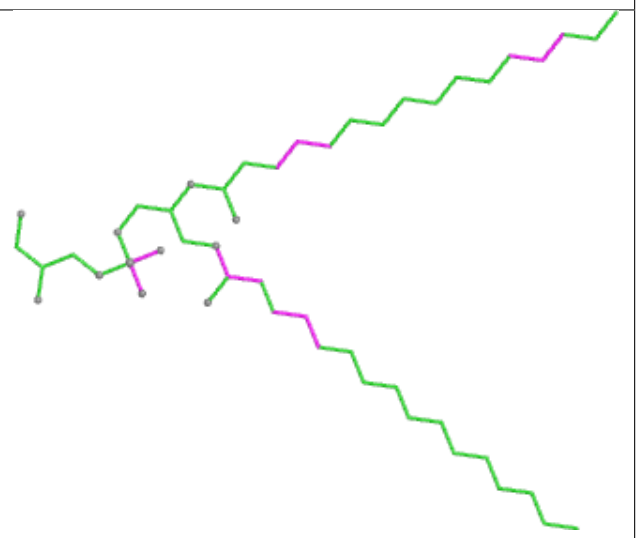
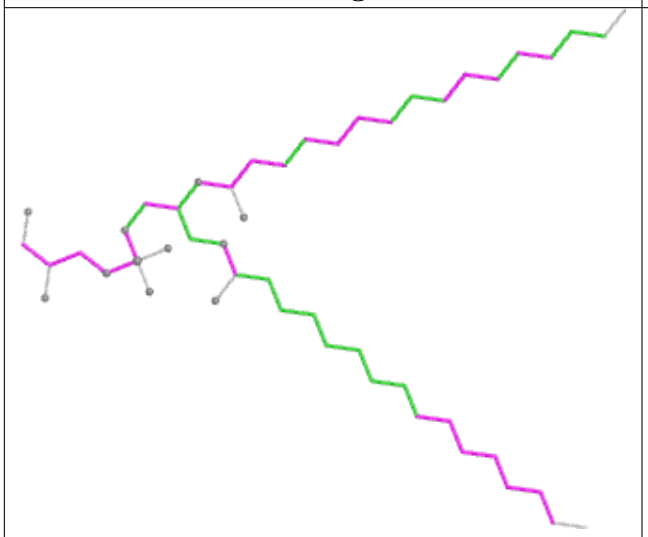


Bond angles



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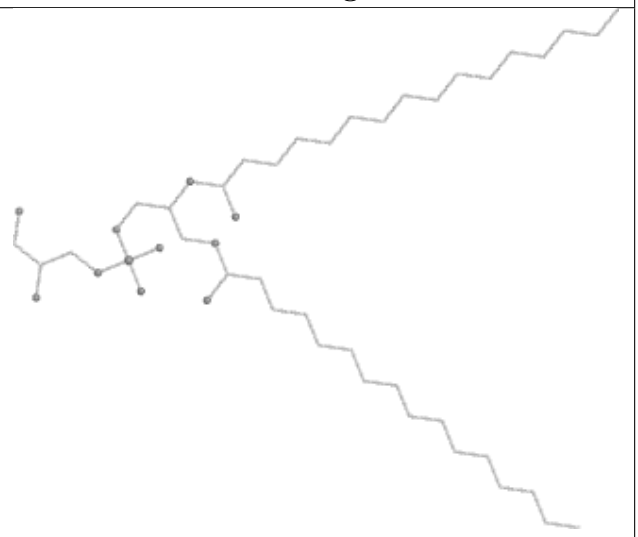
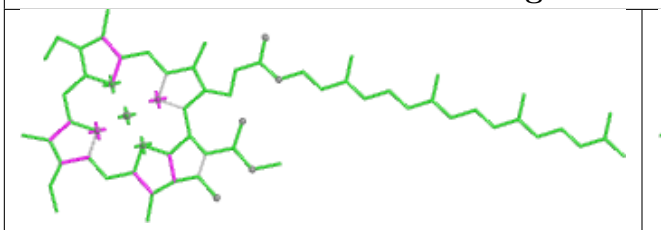
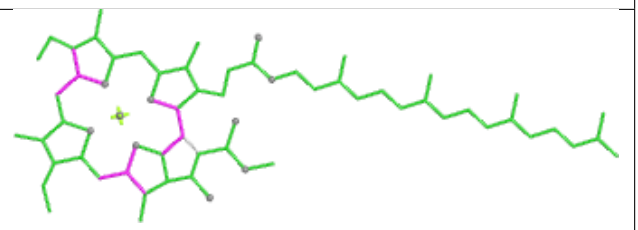


Rings

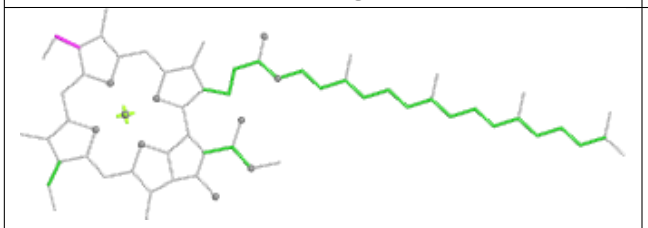
Ligand CLA B 829



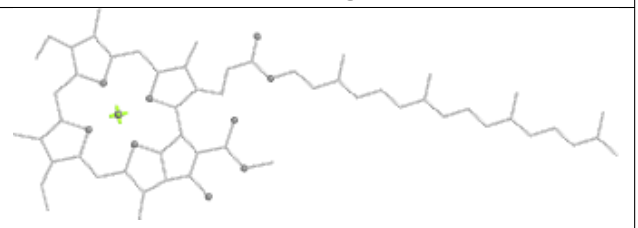
Bond lengths



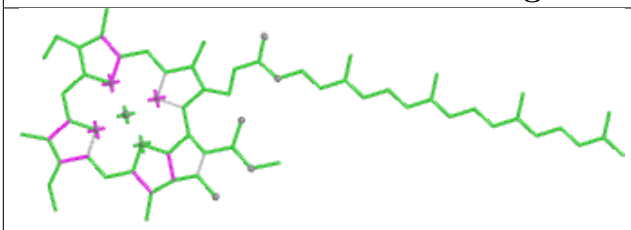
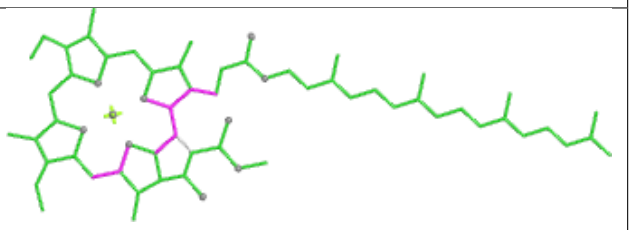
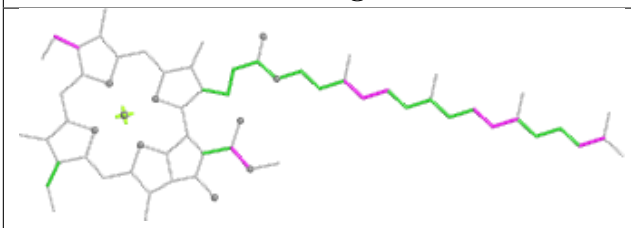
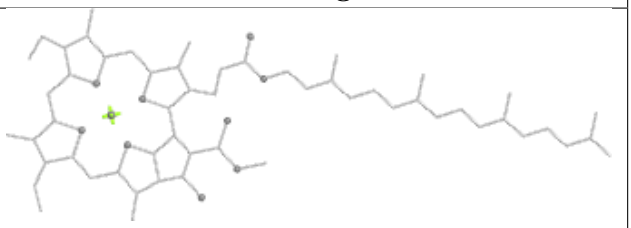
Bond angles

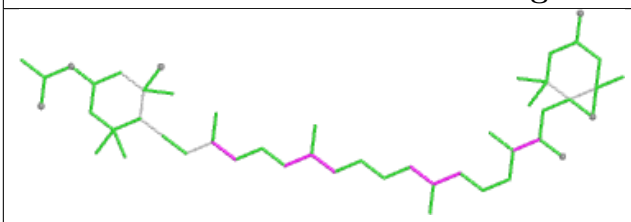
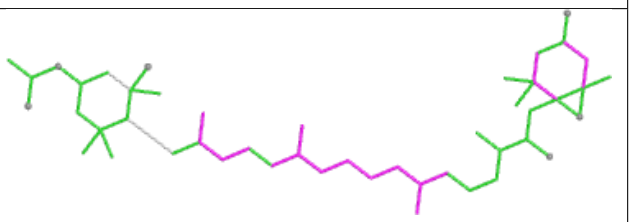
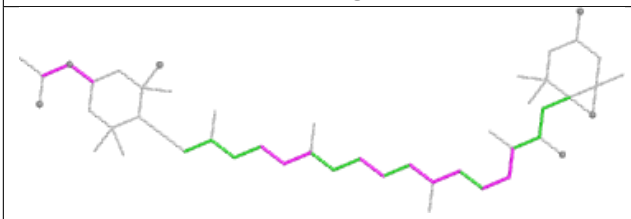
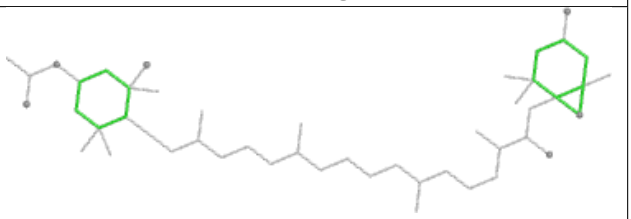


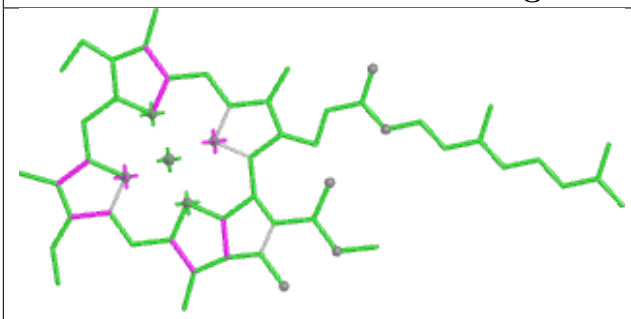
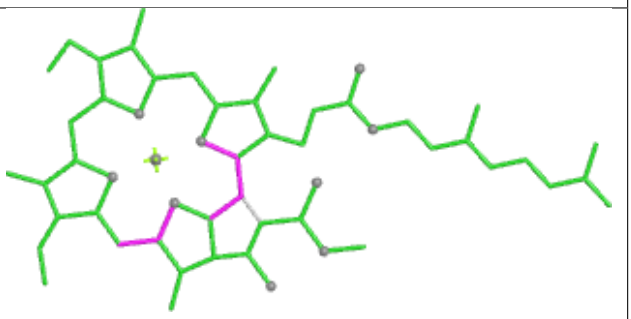
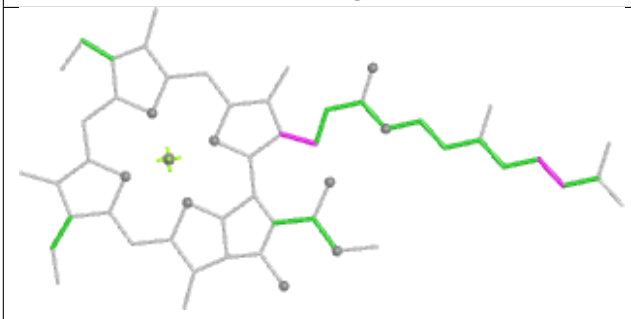
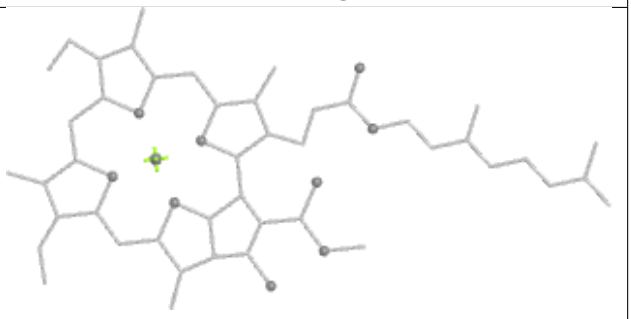
Torsions

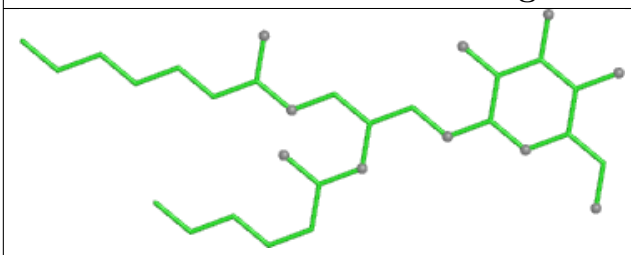
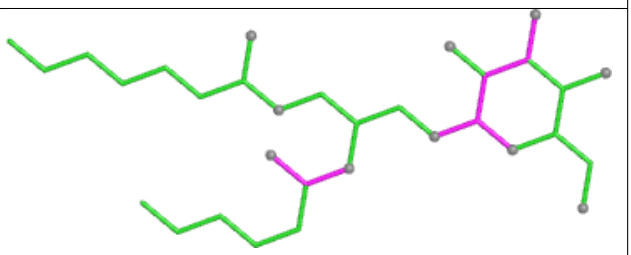
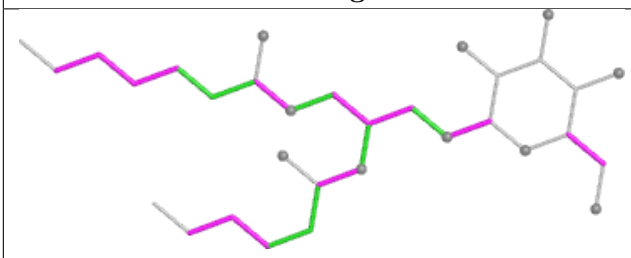
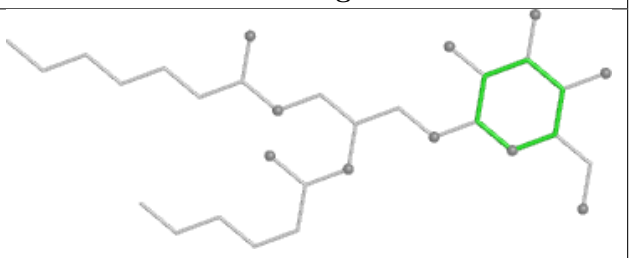


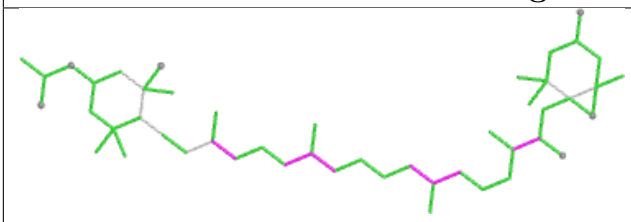
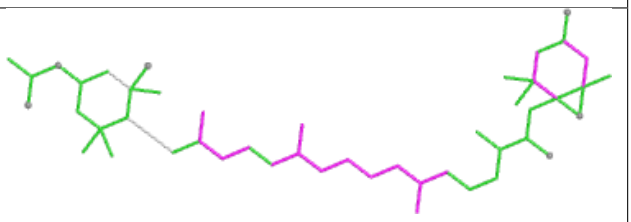
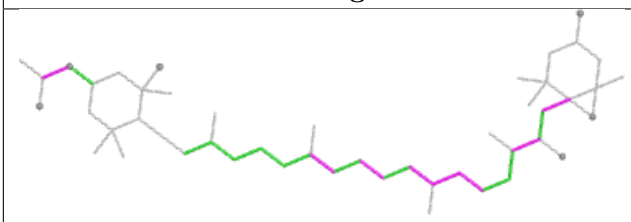
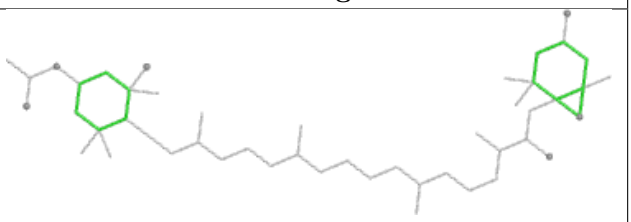
Rings

Ligand CLA R 205	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand A86 P 303	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA A 802	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand LMG U 201	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand A86 U 202	
 Bond lengths	 Bond angles
 Torsions	 Rings

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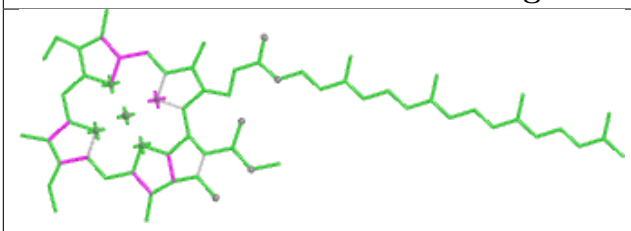
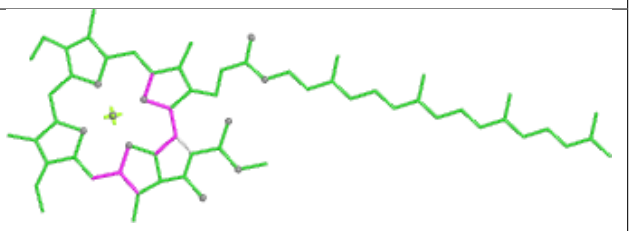
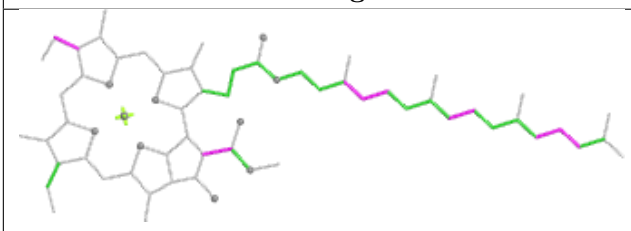
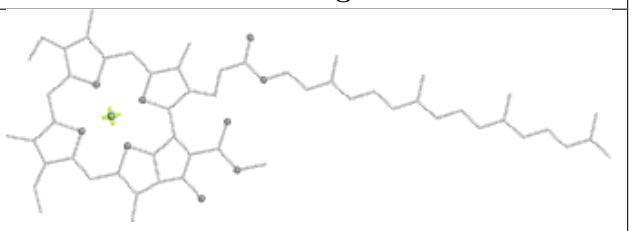
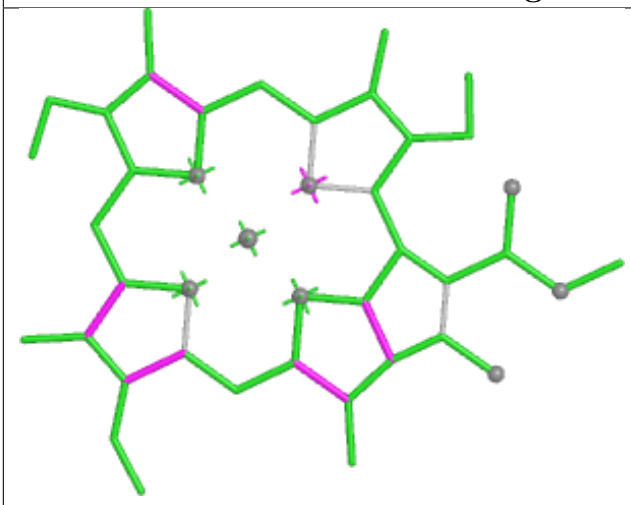
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA T 207



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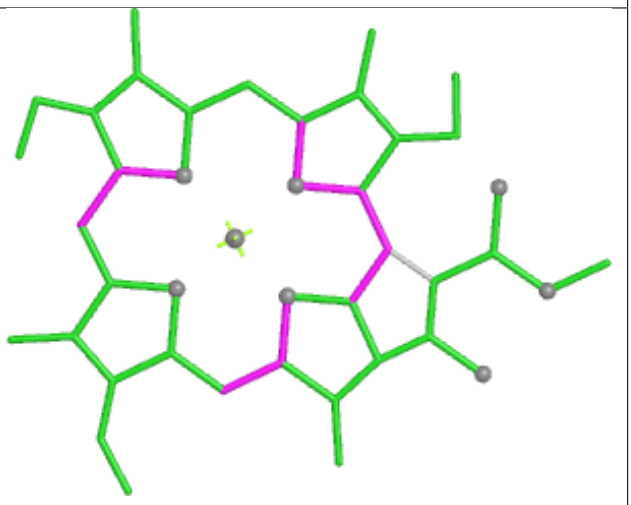
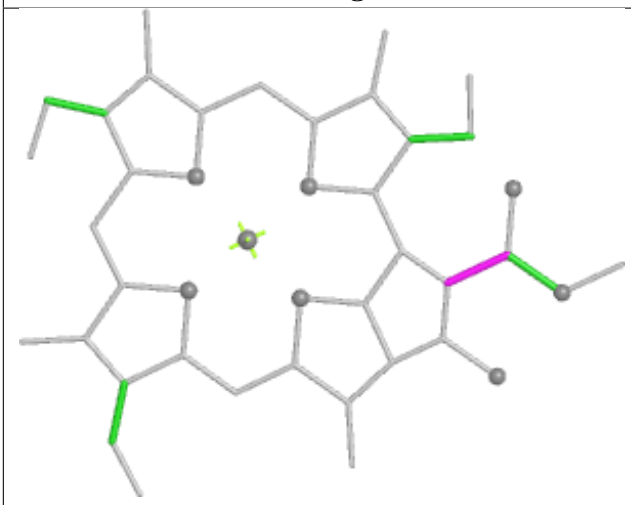


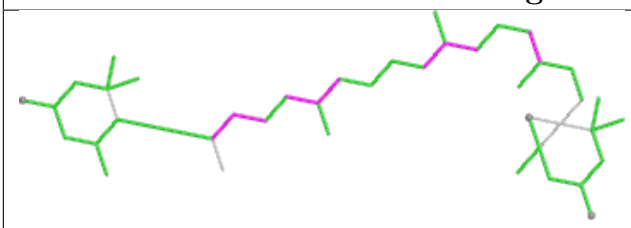
Bond angles



Torsions

Rings

Ligand DD6 T 213



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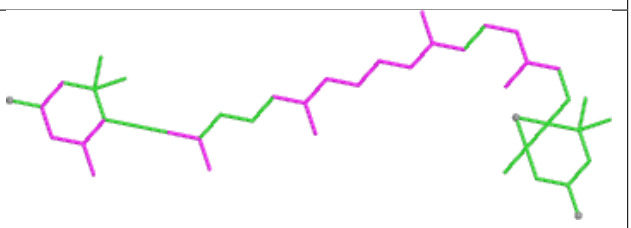

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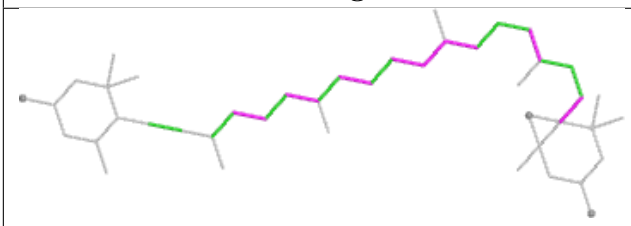

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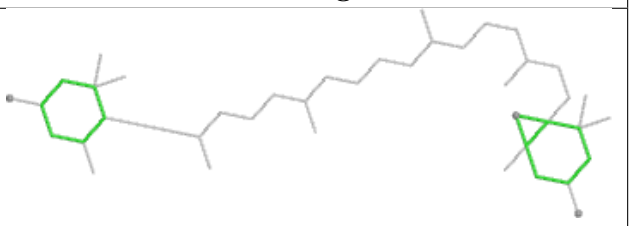
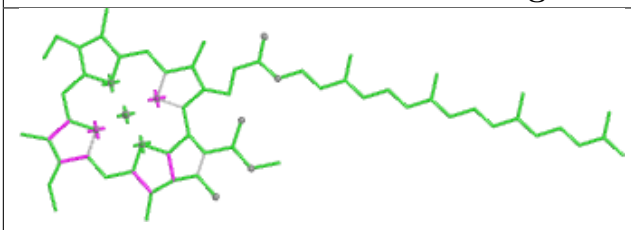


Rings

Ligand CL0 A 848



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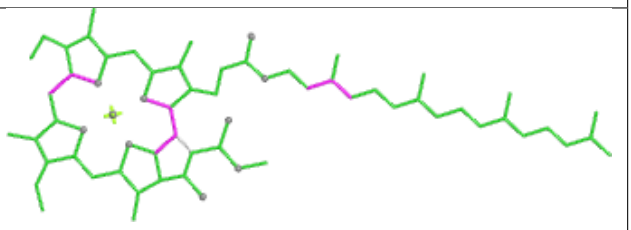

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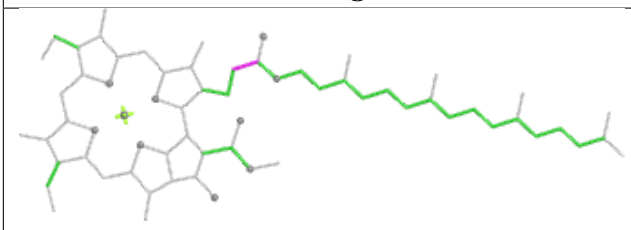

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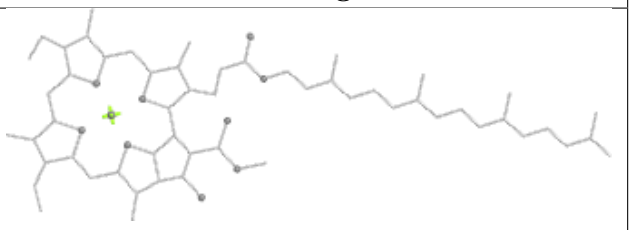
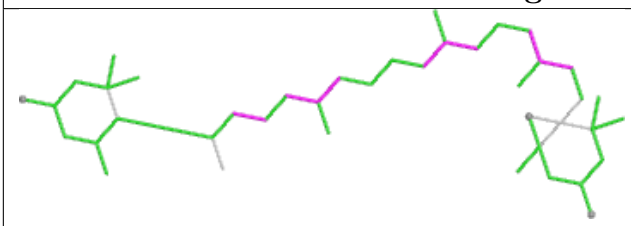


Rings

Ligand DD6 O 213



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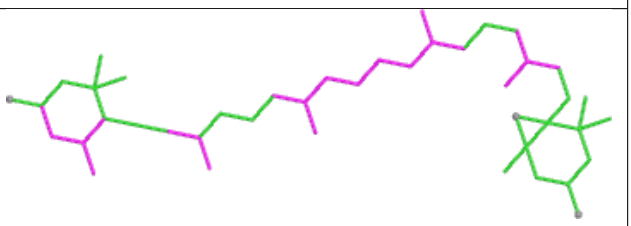

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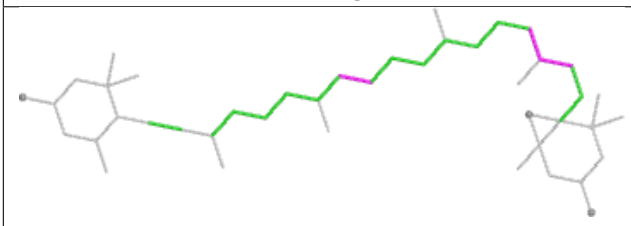

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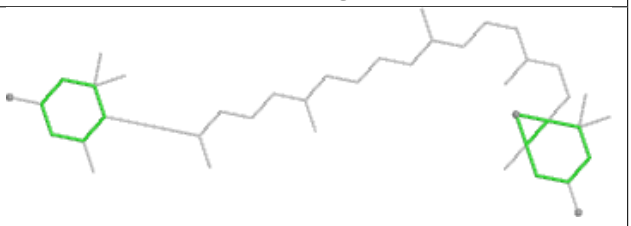
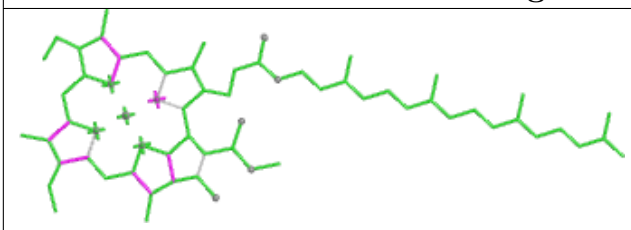


Rings

Ligand CLA S 215



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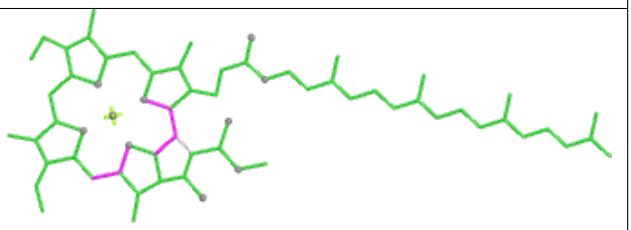

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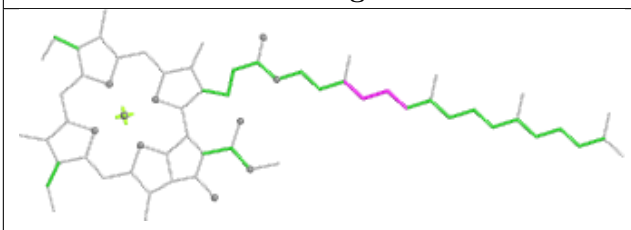

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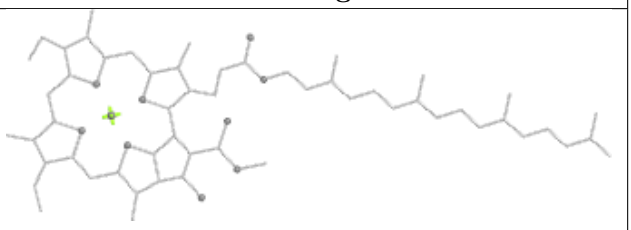
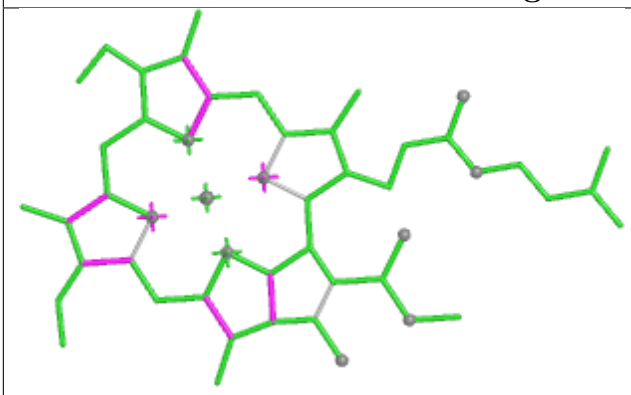
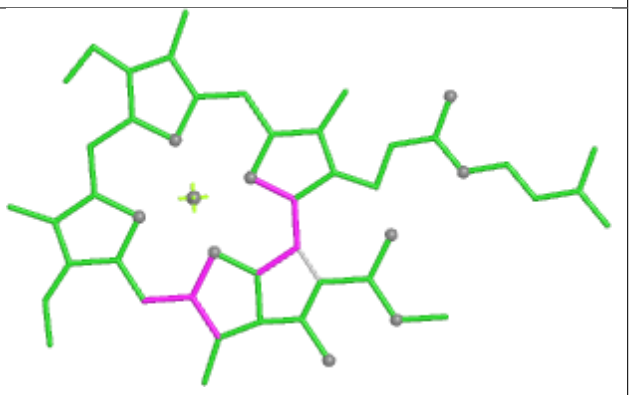
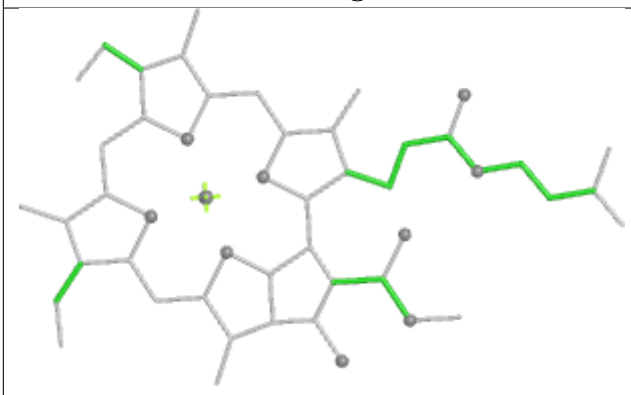
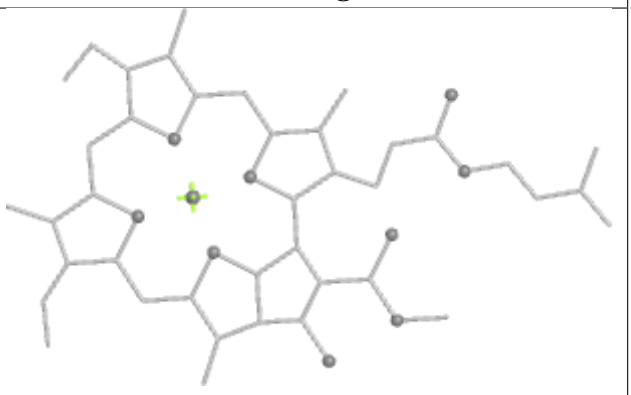
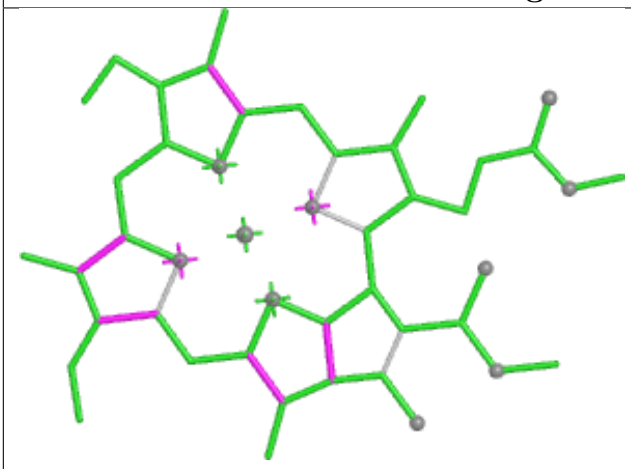


Rings

Ligand CLA A 830	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA F 803



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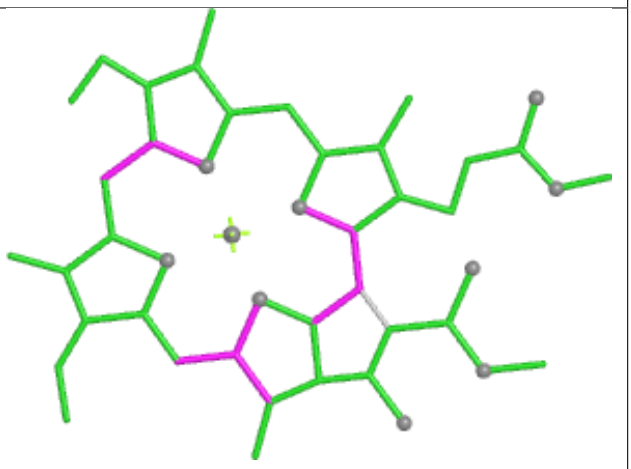
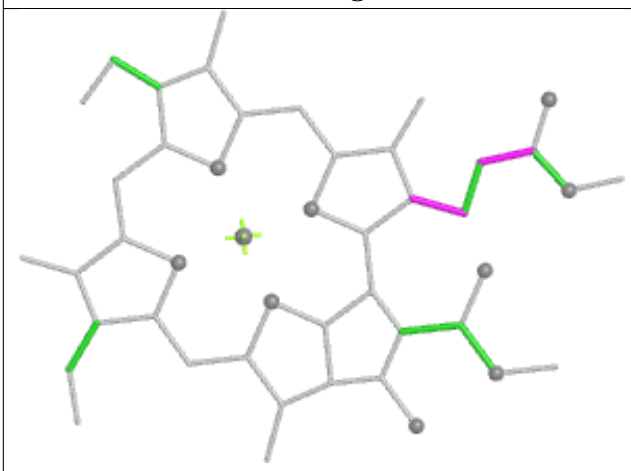
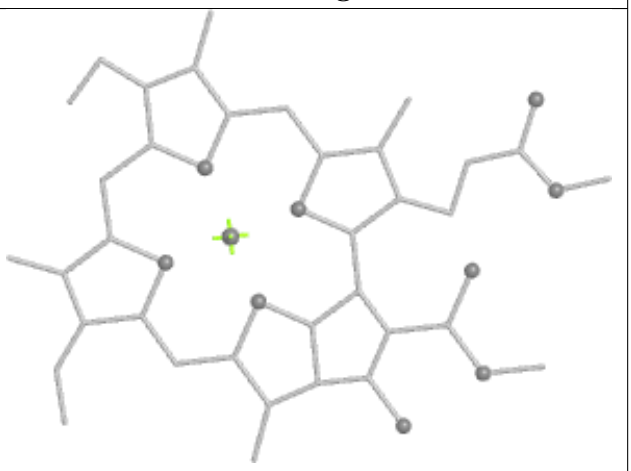


Bond angles

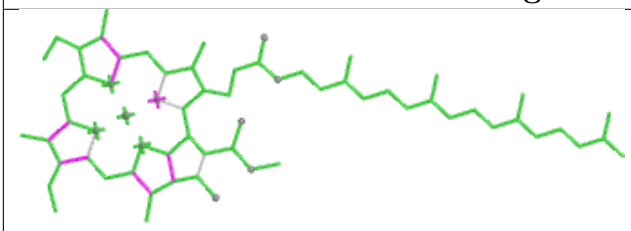


Torsions



Rings

Ligand CLA O 205



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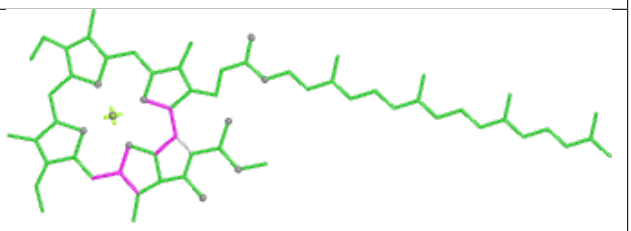

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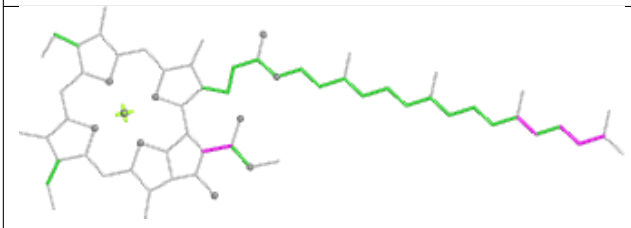
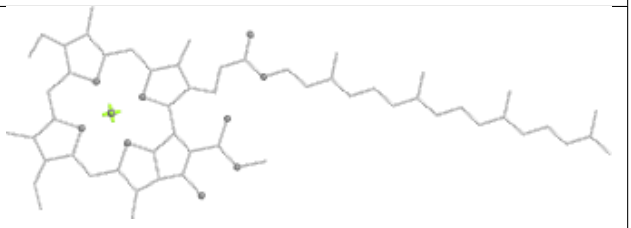
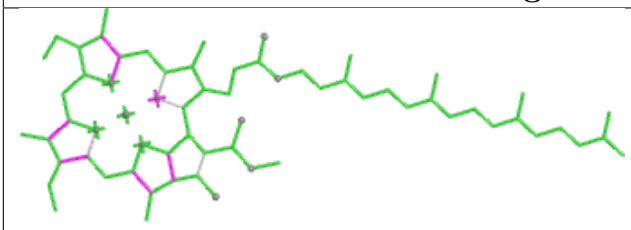


Torsions

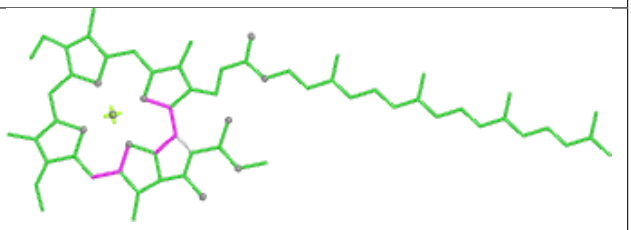


Rings

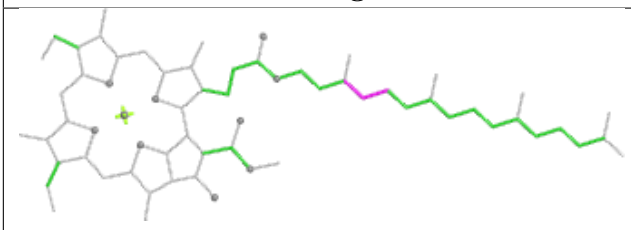
Ligand CLA A 818



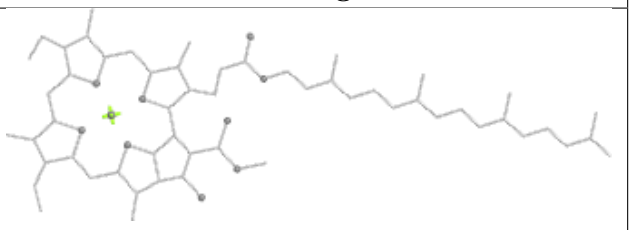
Bond lengths



Bond angles

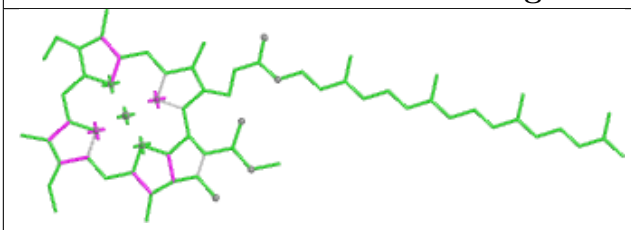


Torsions

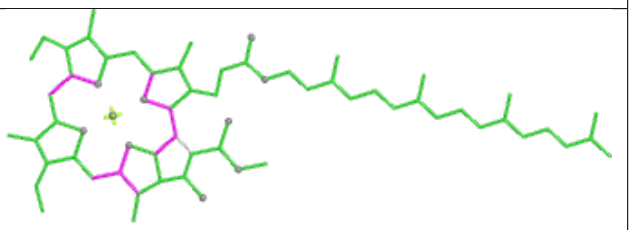


Rings

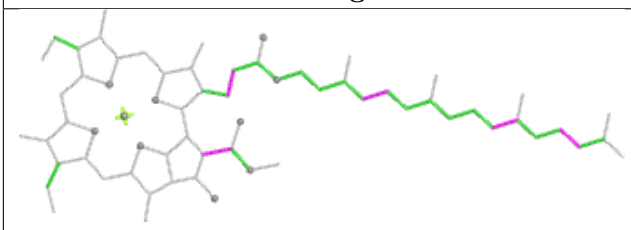
Ligand CLA B 833



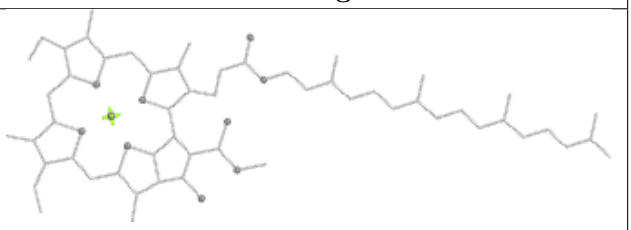
Bond lengths



Bond angles

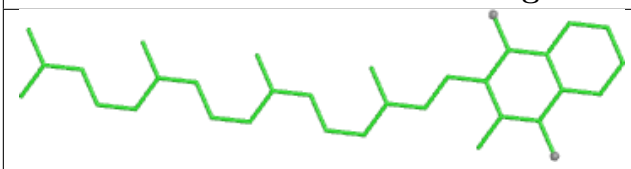


Torsions

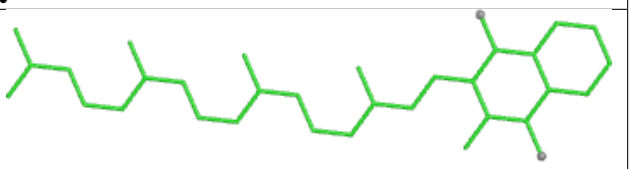


Rings

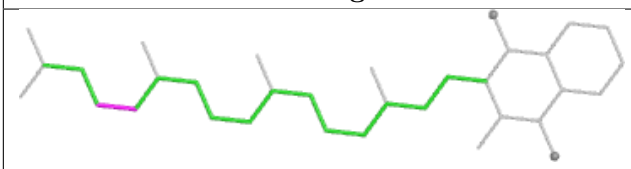
Ligand PQN B 836



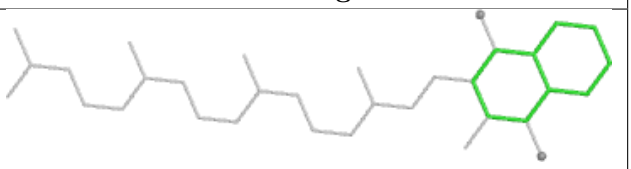
Bond lengths



Bond angles

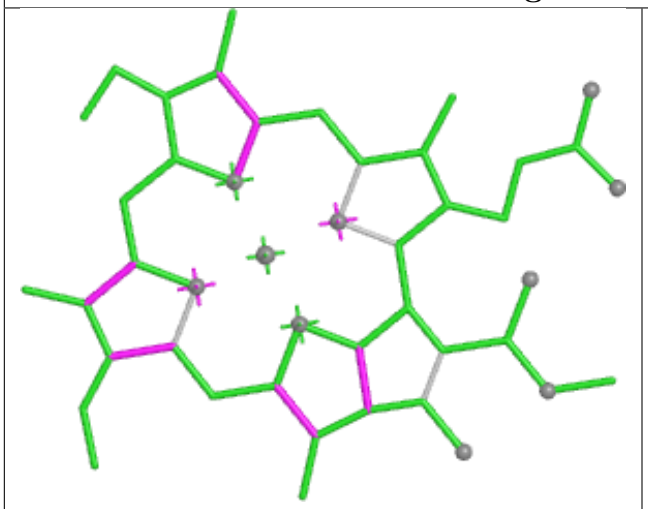


Torsions

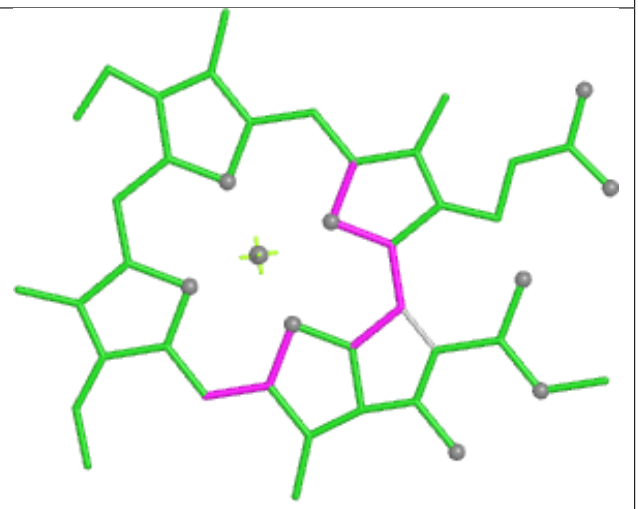


Rings

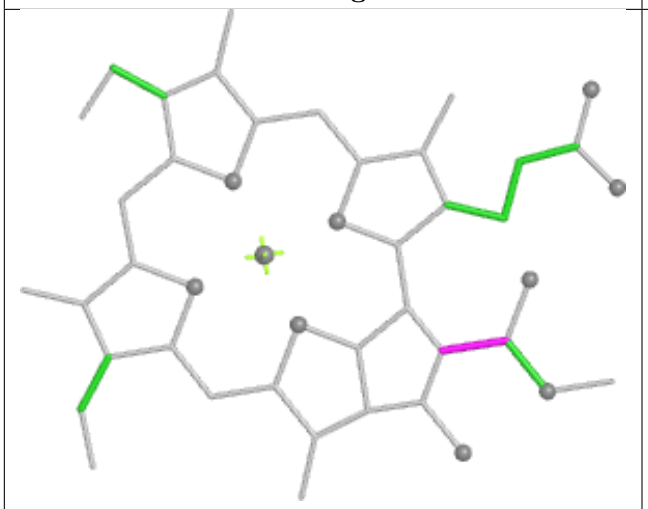
Ligand CLA A 812



Bond lengths



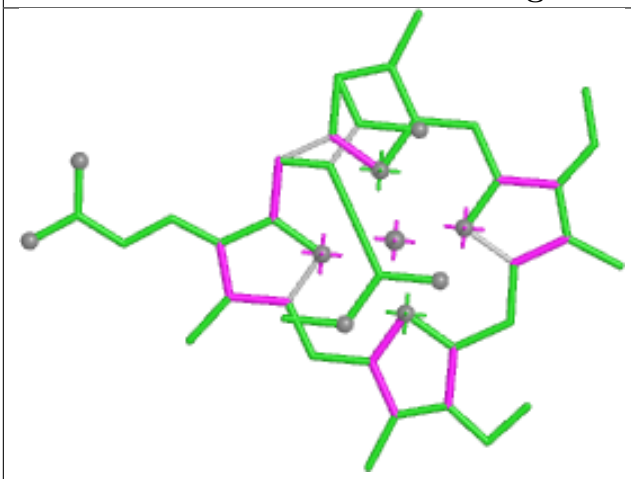
Bond angles



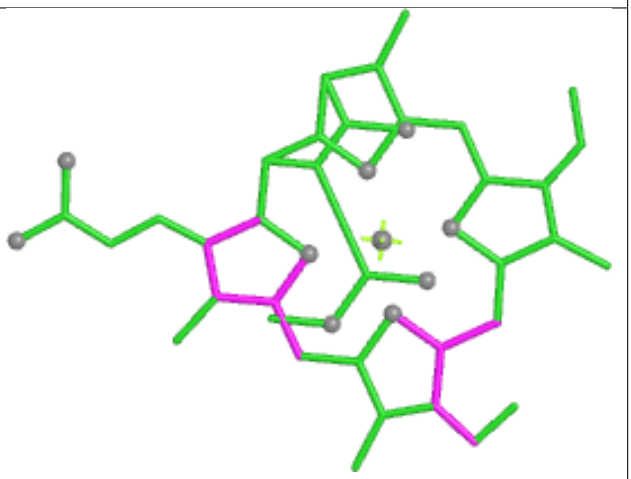
Torsions

Rings

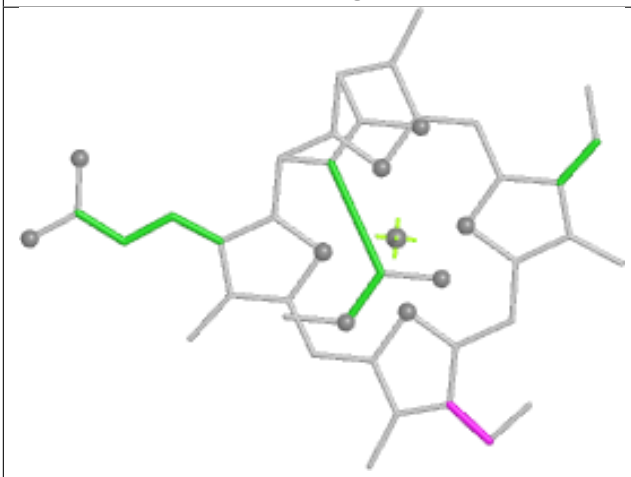
Ligand KC1 P 302



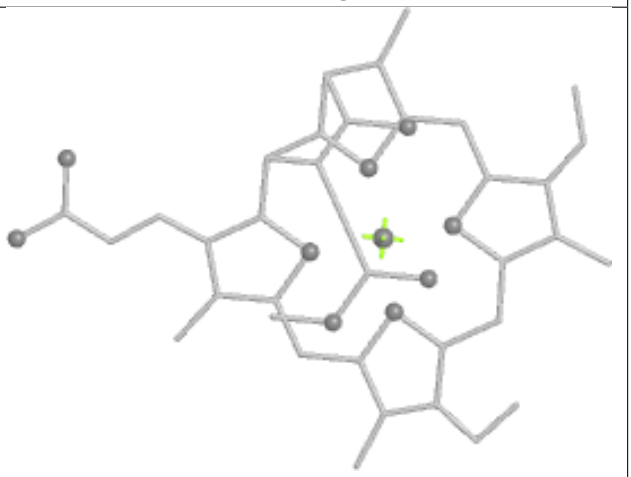
Bond lengths



Bond angles

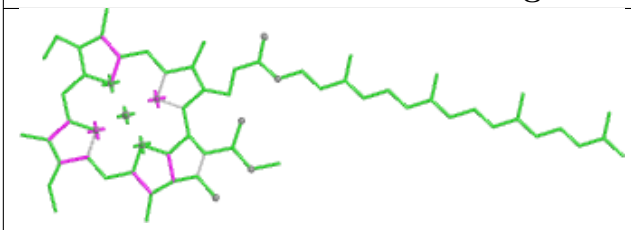


Torsions

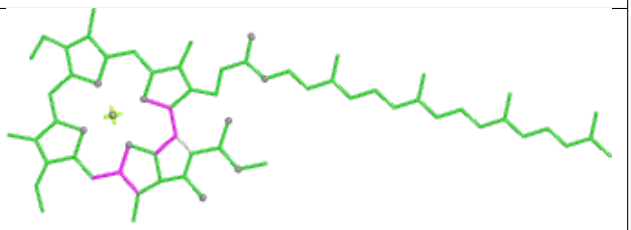


Rings

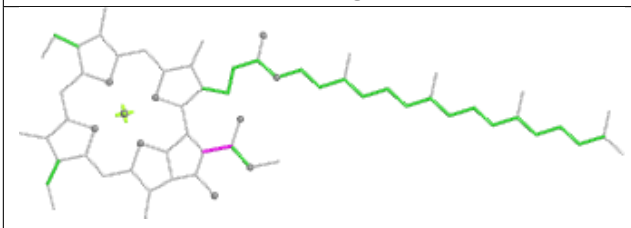
Ligand CLA A 816



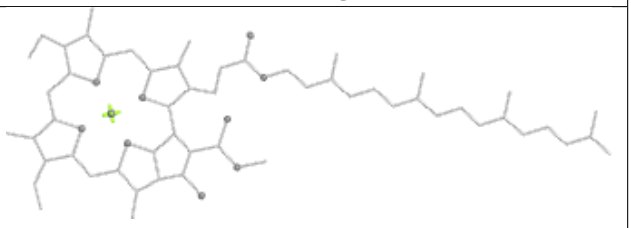
Bond lengths



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.

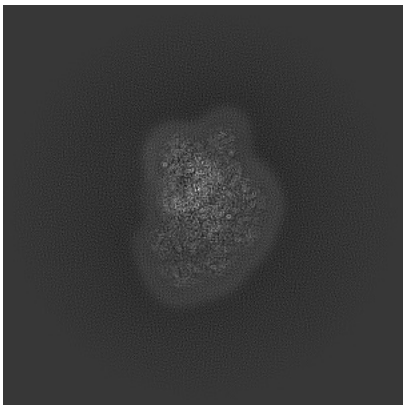
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-64378. These allow visual inspection of the internal detail of the map and identification of artifacts.

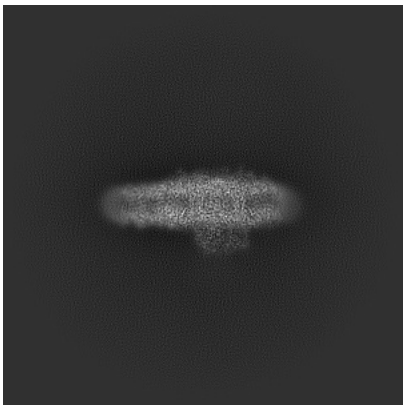
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections (i)

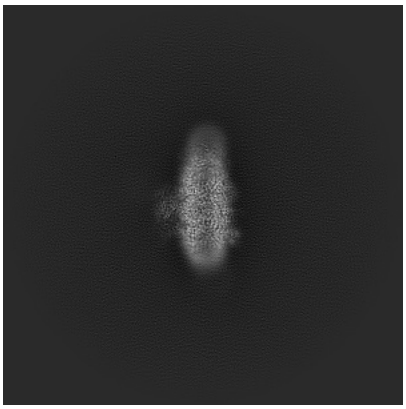
6.1.1 Primary map



X

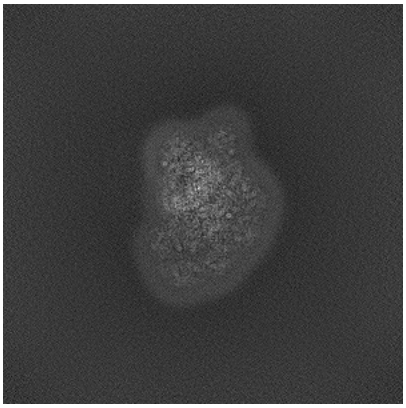


Y

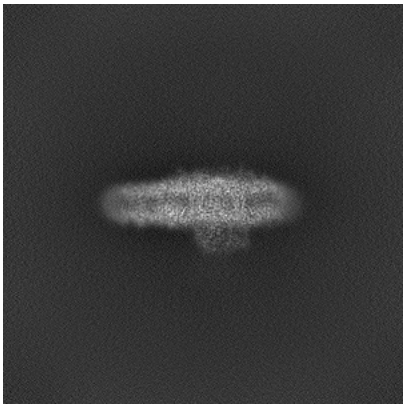


Z

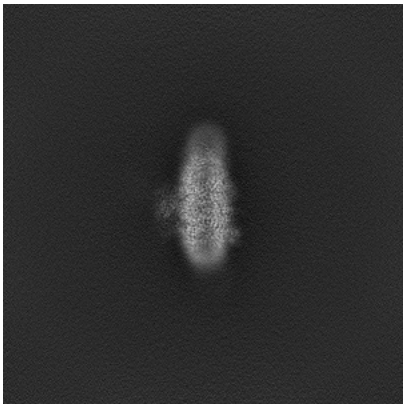
6.1.2 Raw map



X



Y

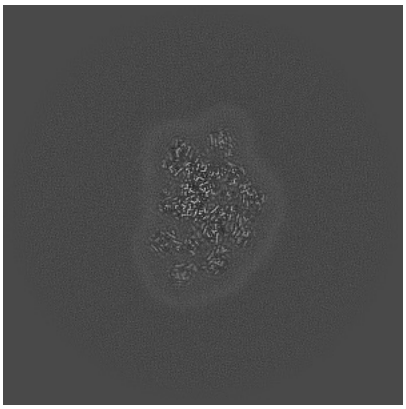


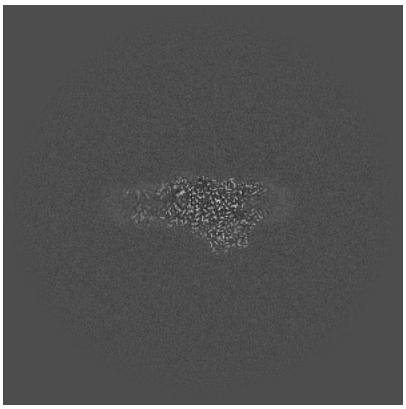
Z

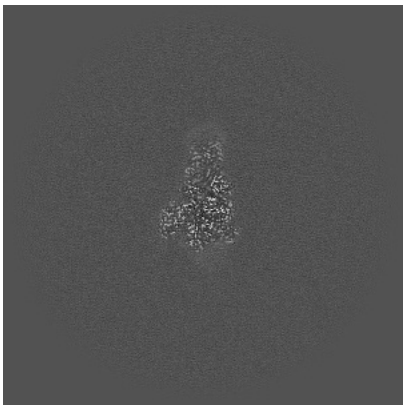
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

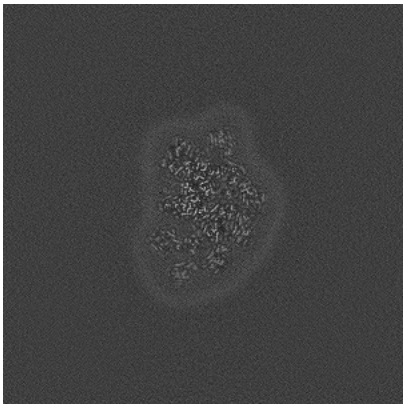
6.2.1 Primary map

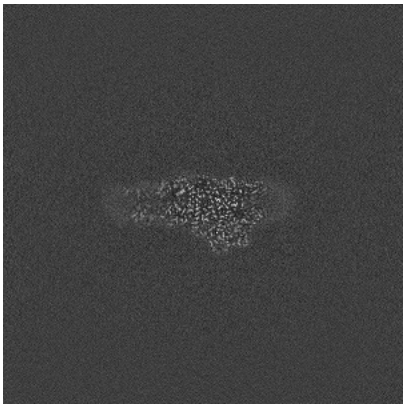

X Index: 300

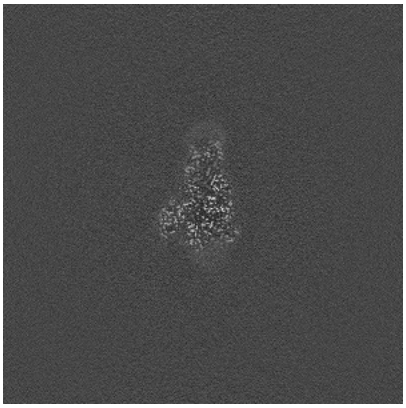

Y Index: 300


Z Index: 300

6.2.2 Raw map


X Index: 300

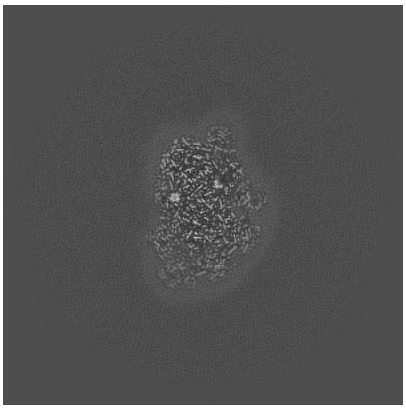

Y Index: 300


Z Index: 300

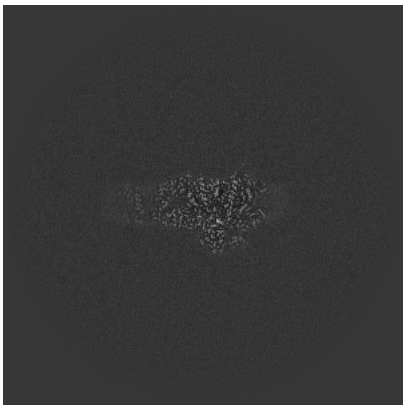
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

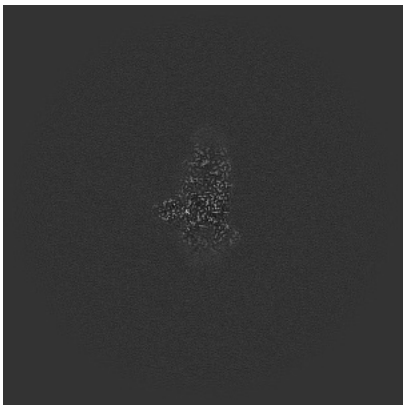
6.3.1 Primary map



X Index: 284

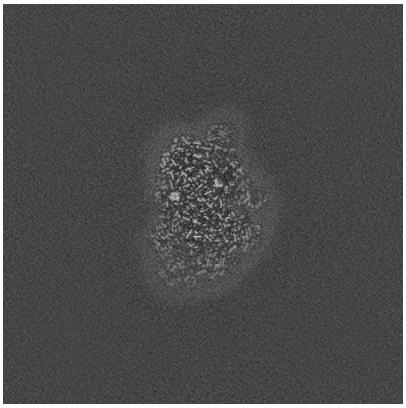


Y Index: 289

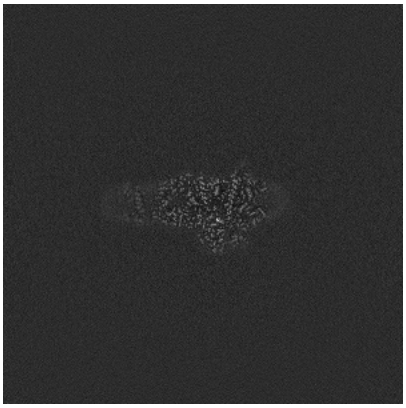


Z Index: 320

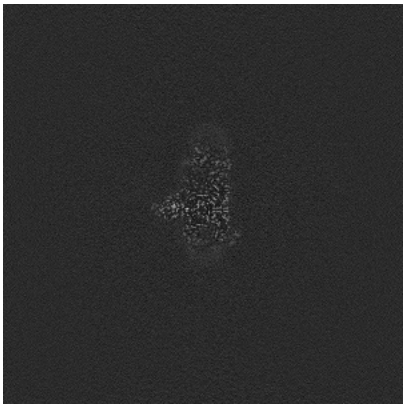
6.3.2 Raw map



X Index: 284



Y Index: 289

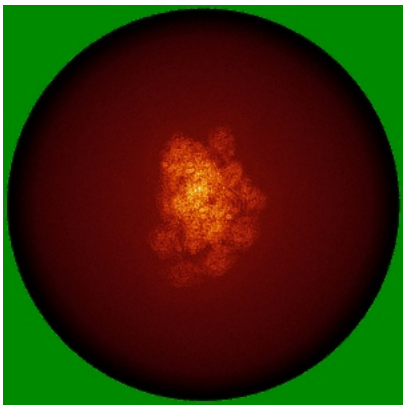


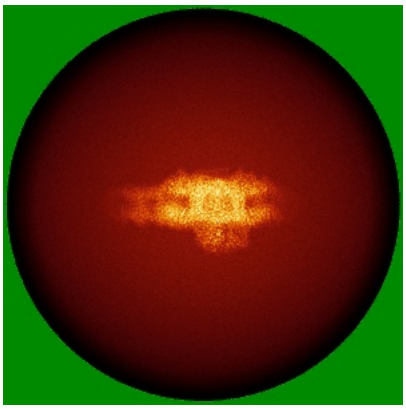
Z Index: 322

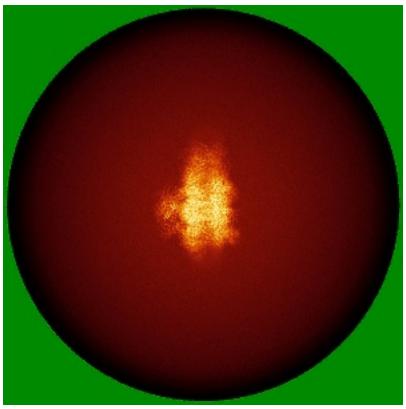
The images above show the largest variance slices of the map in three orthogonal directions.

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

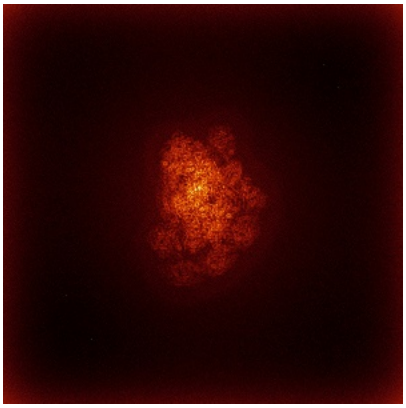
6.4.1 Primary map

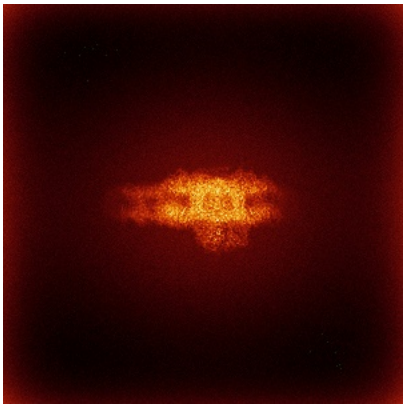

X

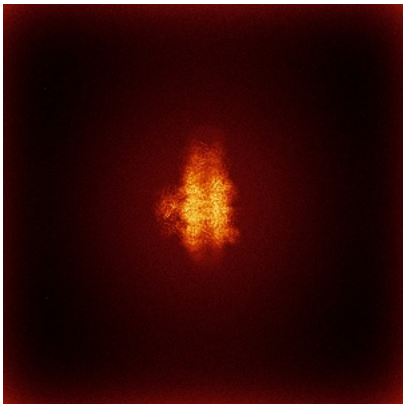

Y


Z

6.4.2 Raw map


X

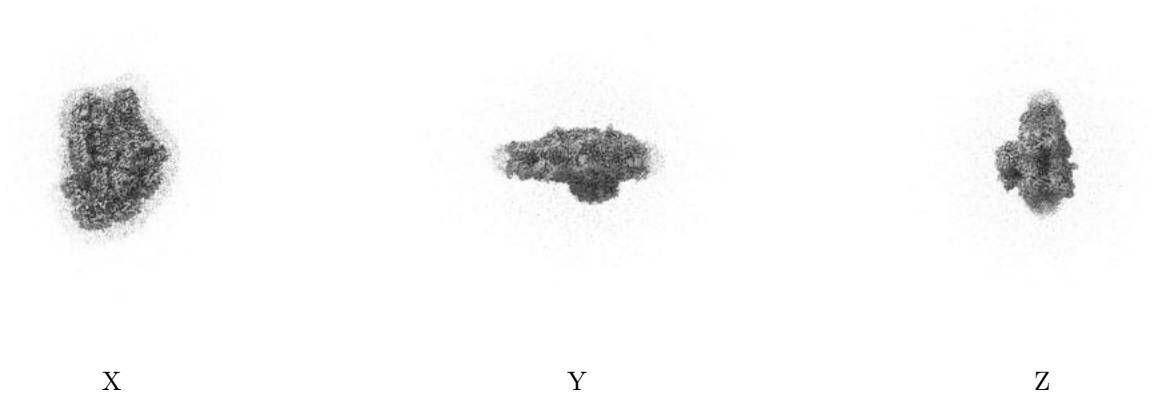

Y


Z

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

6.5 Orthogonal surface views (i)

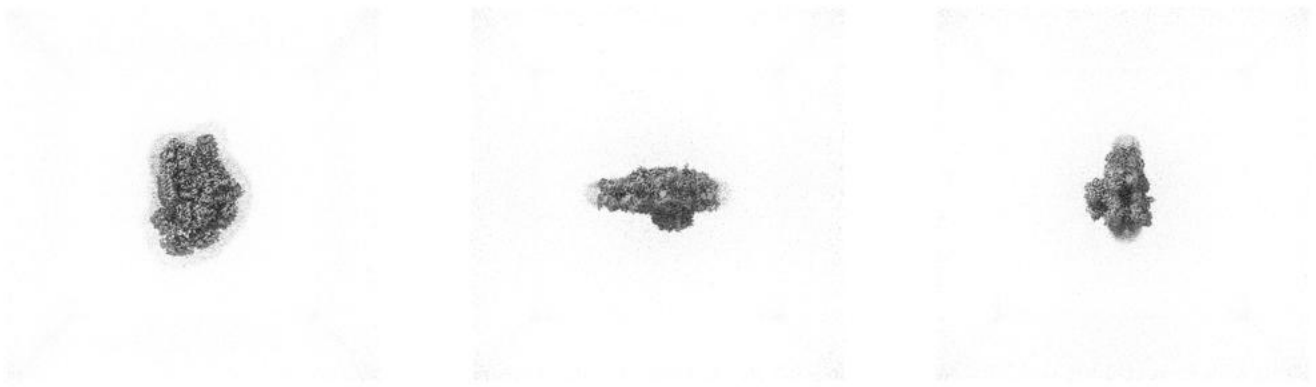
6.5.1 Primary map



X Y Z

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

6.5.2 Raw map



X Y Z

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

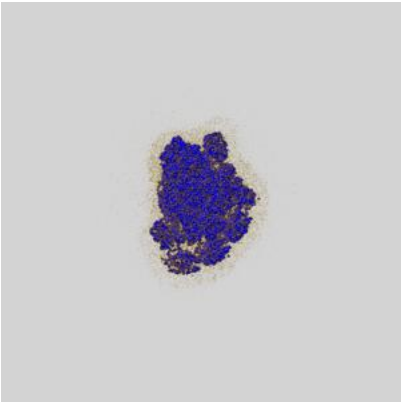
6.6 Mask visualisation (i)

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

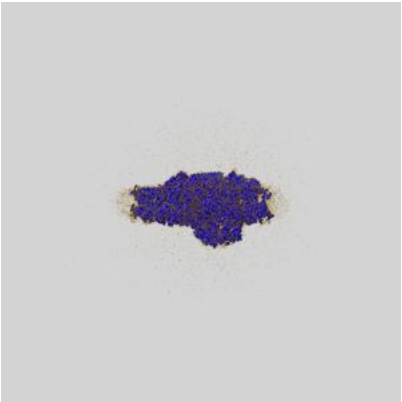
A mask typically either:

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

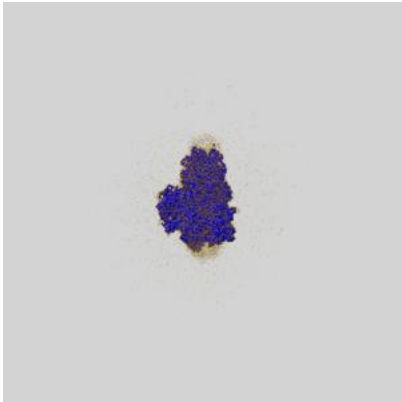
6.6.1 emd_64378_msk_1.map (i)



X



Y

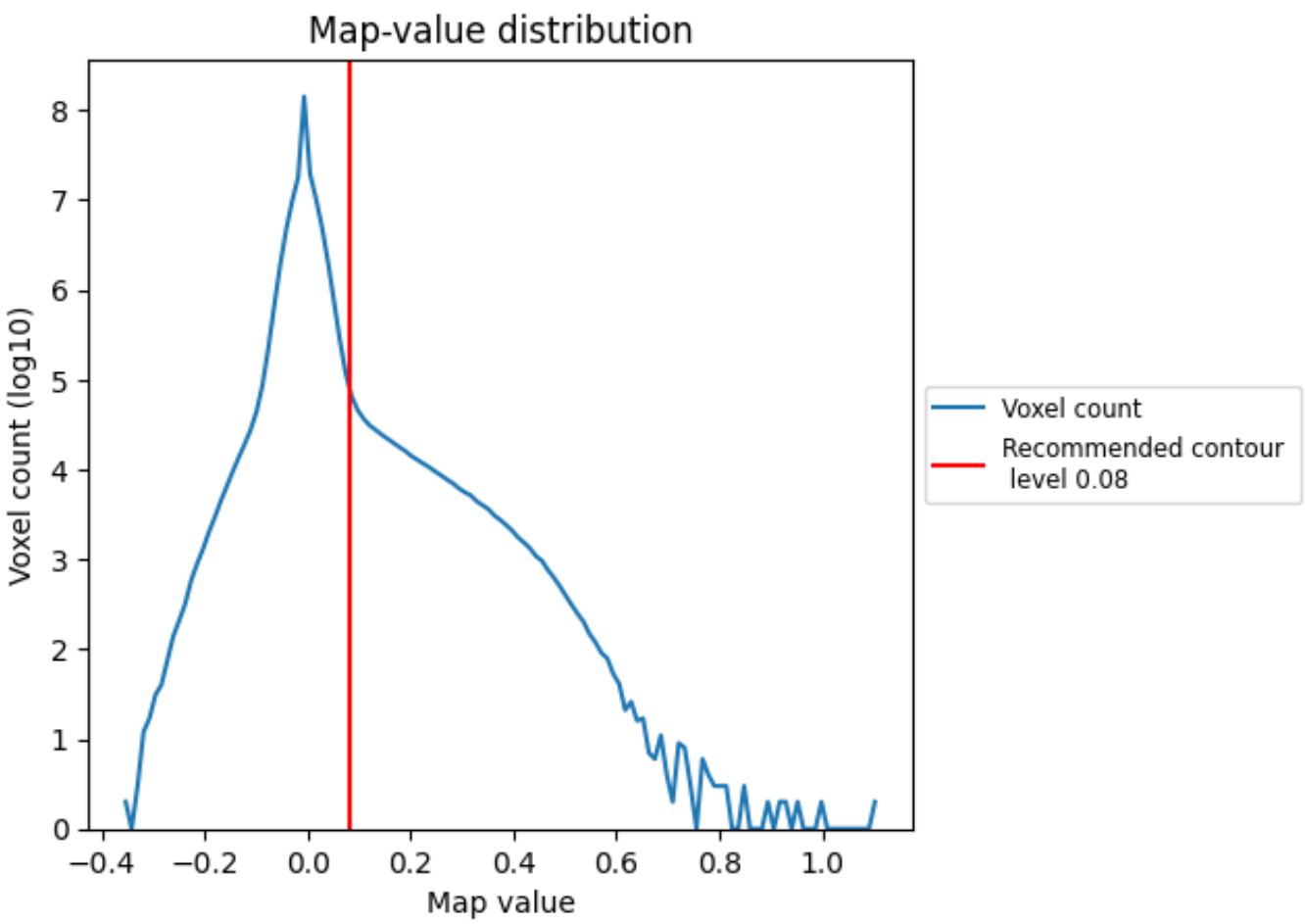


Z

7 Map analysis (i)

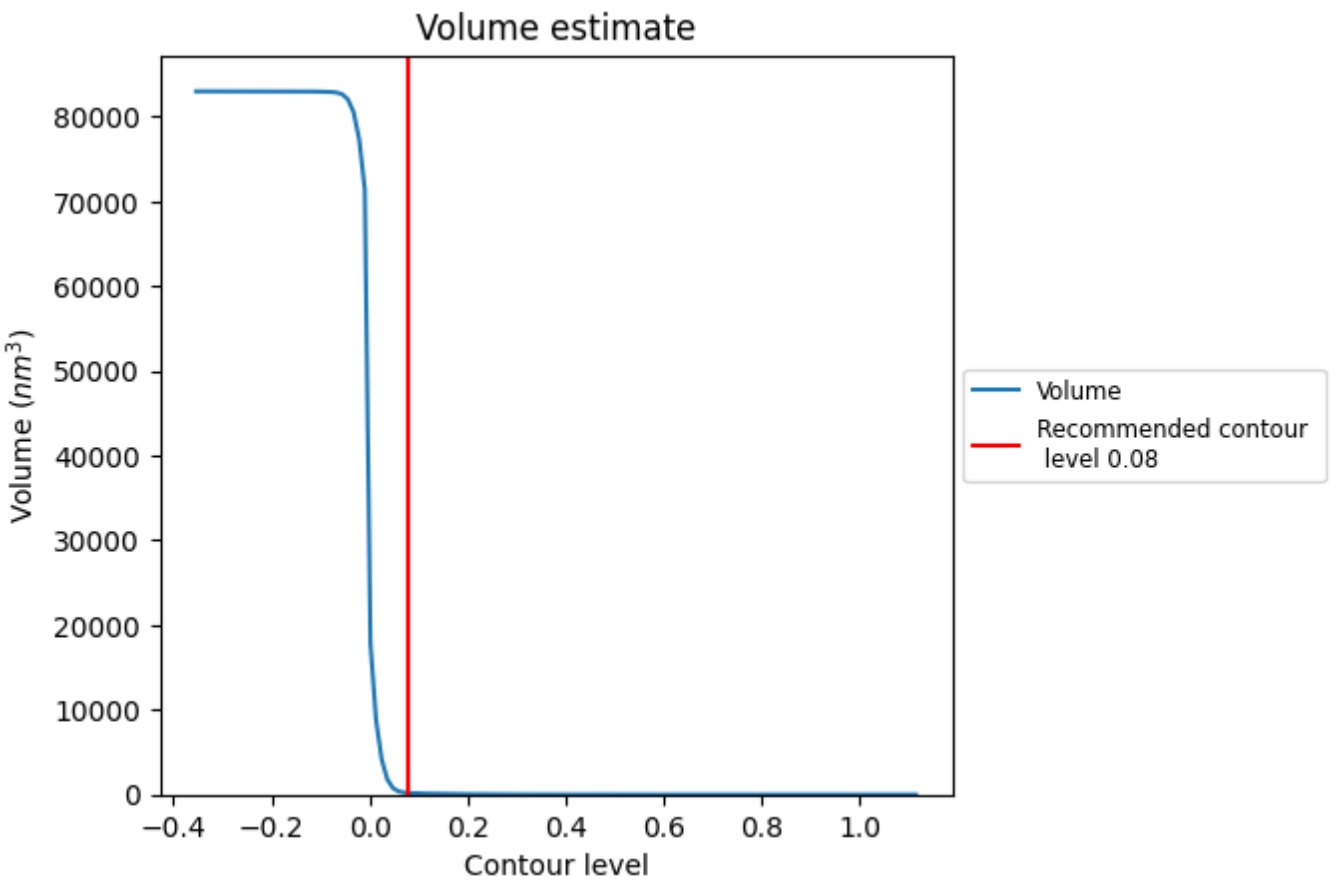
This section contains the results of statistical analysis of the map.

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.

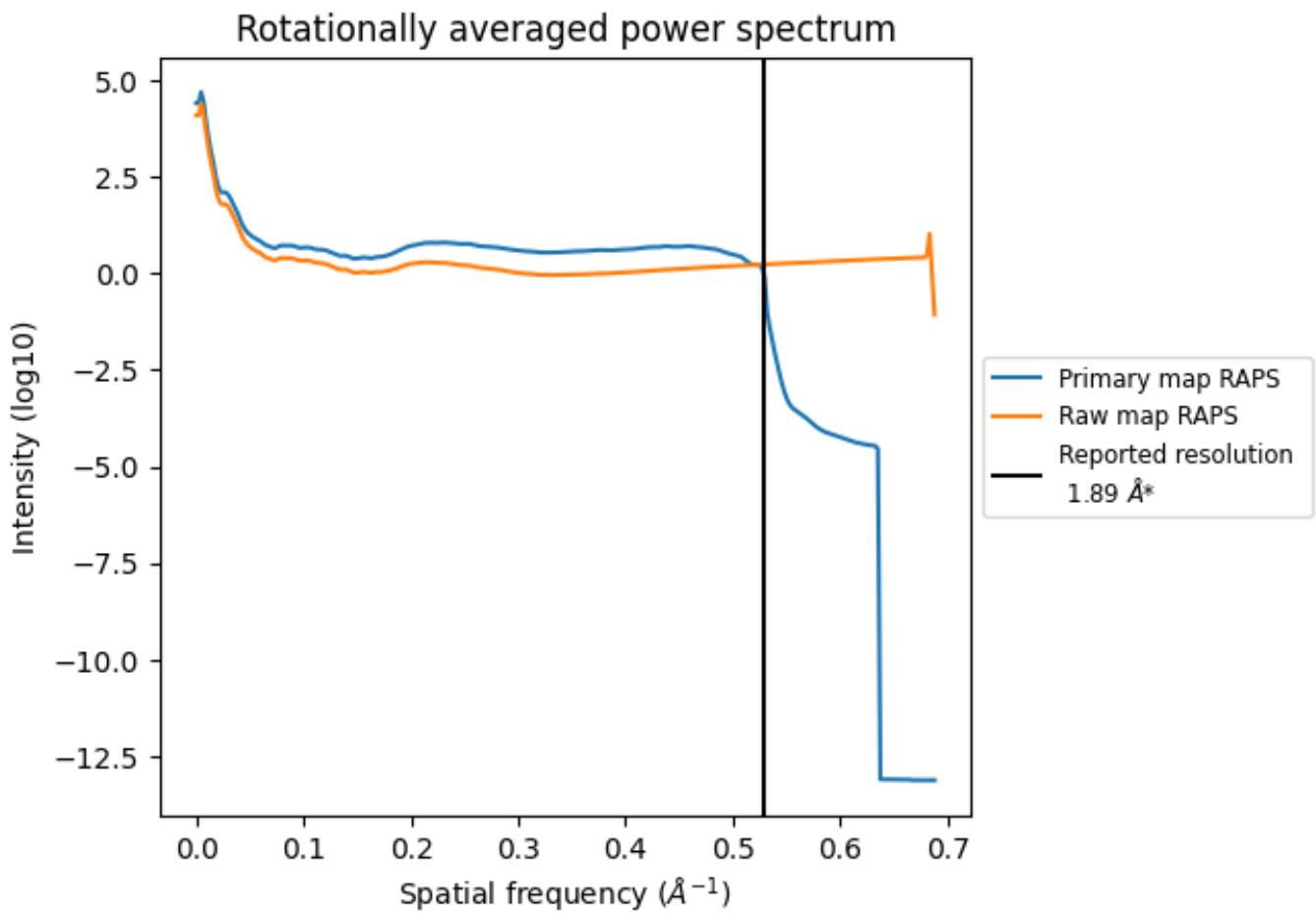
7.2 Volume estimate (i)



The volume at the recommended contour level is 189 nm^3; this corresponds to an approximate mass of 171 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)

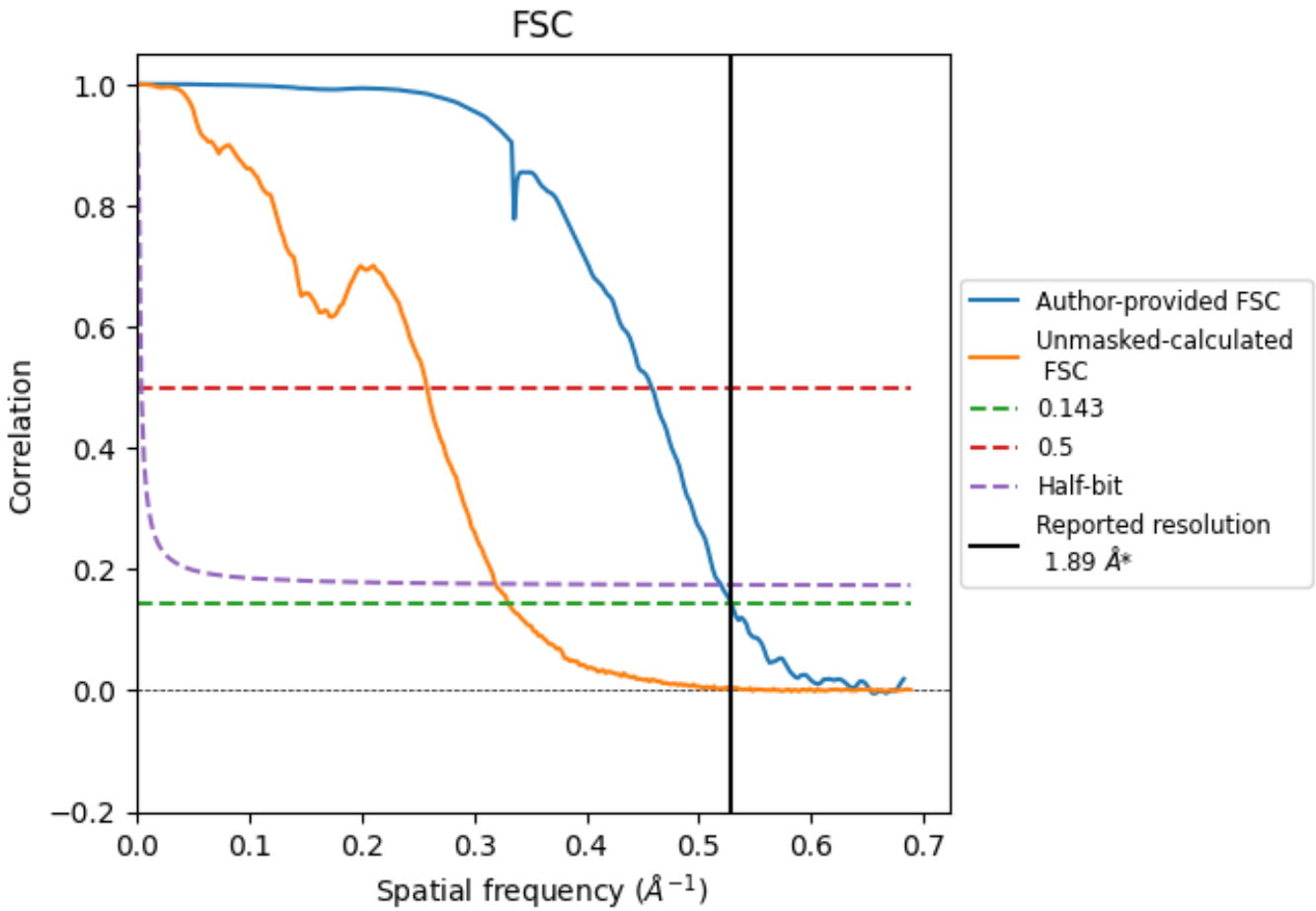


*Reported resolution corresponds to spatial frequency of 0.529 Å^{-1}

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 0.529 Å^{-1}

8.2 Resolution estimates (i)

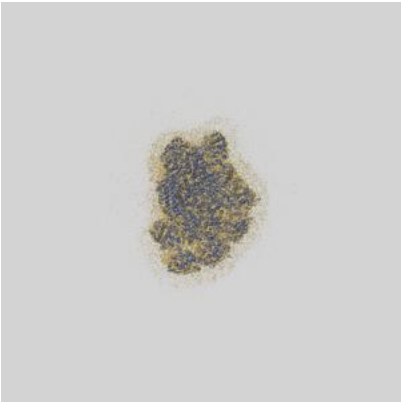
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	1.89	-	-
Author-provided FSC curve	1.89	2.18	1.92
Unmasked-calculated*	3.02	3.87	3.13

*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 3.02 differs from the reported value 1.89 by more than 10 %

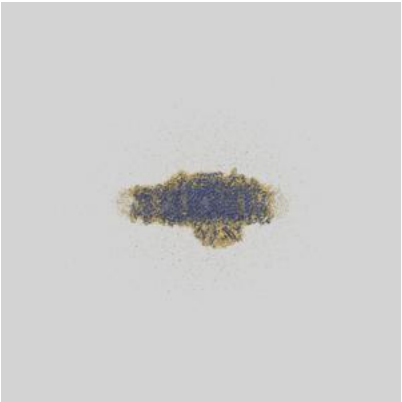
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-64378 and PDB model 9UOF. Per-residue inclusion information can be found in section 3 on page 24.

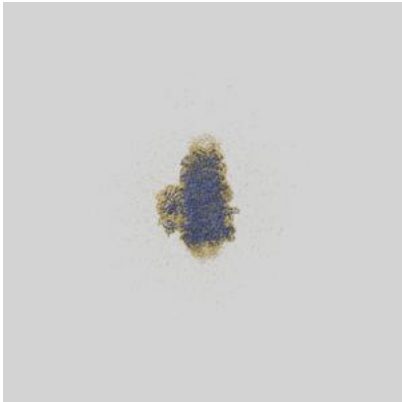
9.1 Map-model overlay (i)



X



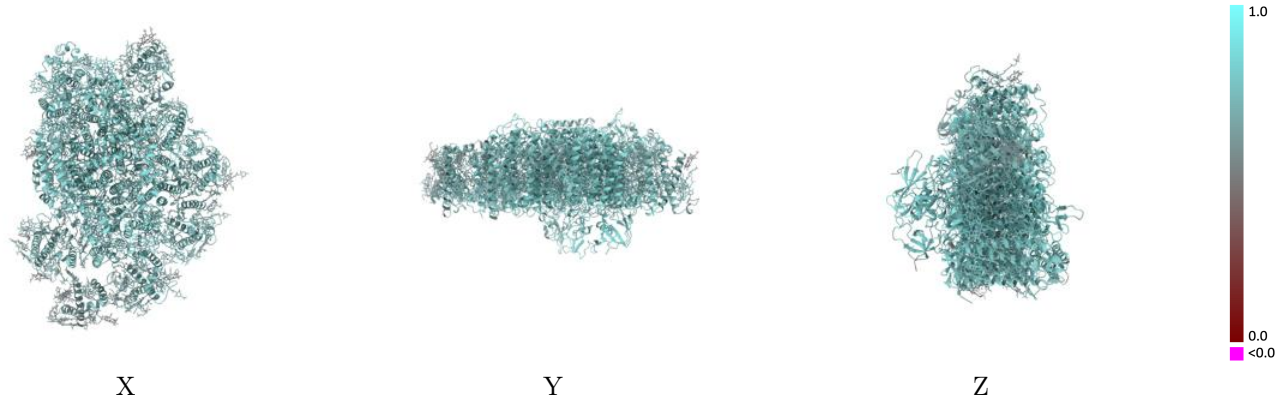
Y



Z

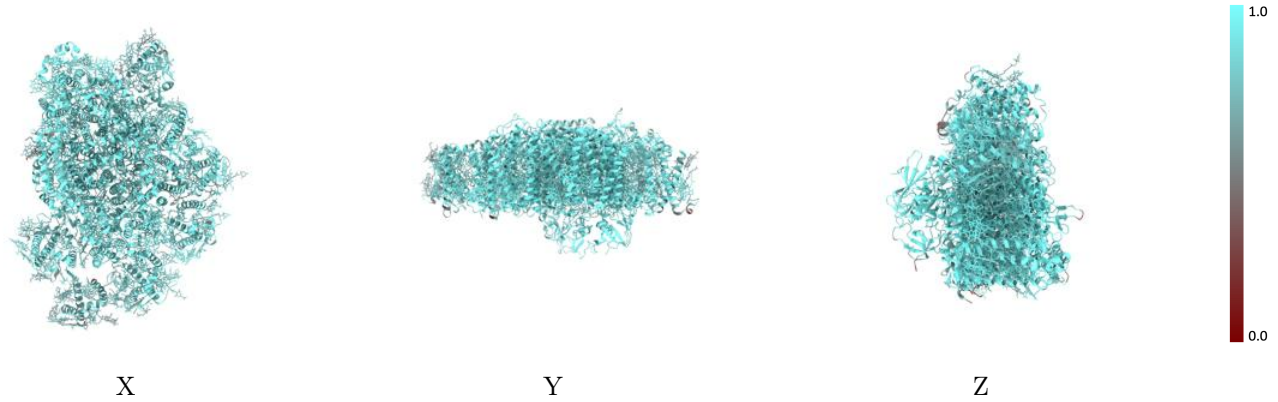
The images above show the 3D surface view of the map at the recommended contour level 0.08 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model (i)



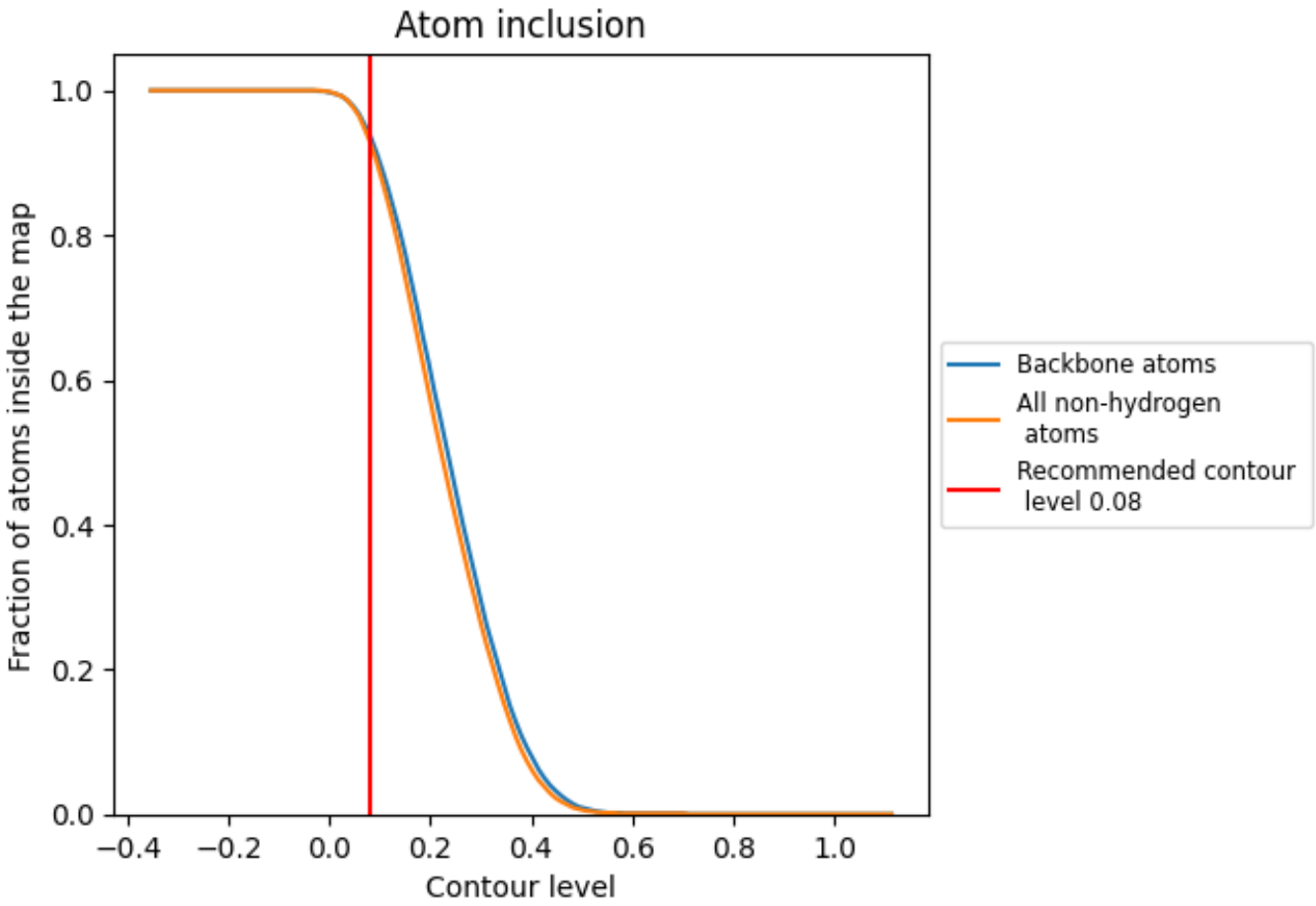
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

9.3 Atom inclusion mapped to coordinate model (i)



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

9.4 Atom inclusion (i)



At the recommended contour level, 94% of all backbone atoms, 93% 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 (0.08) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9300	0.7370
A	0.9580	0.7640
B	0.9770	0.7850
C	0.9920	0.8000
D	0.9440	0.7530
E	0.9060	0.7410
F	0.9400	0.7380
I	0.9740	0.7650
J	0.8270	0.6700
L	0.9540	0.7540
M	0.9530	0.7490
O	0.9110	0.7000
P	0.8790	0.6780
Q	0.8560	0.6690
R	0.9380	0.7320
S	0.9110	0.7100
T	0.7480	0.6010
U	0.8360	0.6690