wwPDB EM Validation Summary Report

Sep 11, 2026 – 03:54 am BST

PDB ID	:	7ZQD / pdb_00007zqd
EMDB ID	:	EMD-14871
Title	:	Dimeric PSI of Chlamydomonas reinhardtii at 2.97 A resolution
Authors	:	Naschberger, A.; Amunts, A.
Deposited on	:	2022-04-29
Resolution	:	2.97 Å(reported)

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

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

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

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

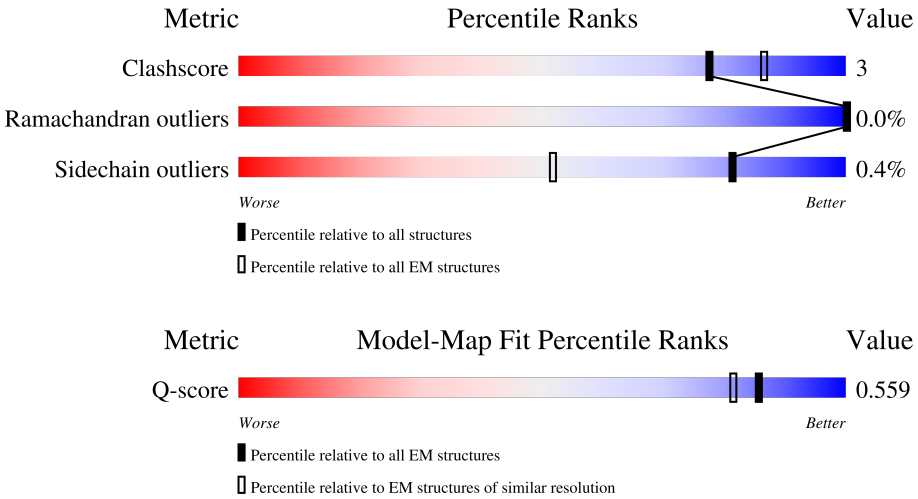
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data 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

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

The reported resolution of this entry is 2.97 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	13205 (2.47 - 3.47)

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	751	93% 5%
1	A2	751	94% 5%
2	B	735	94% 5%
2	B2	735	93% 6%

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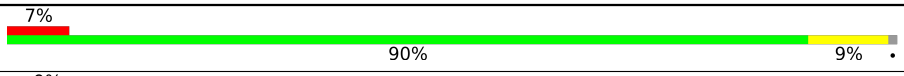
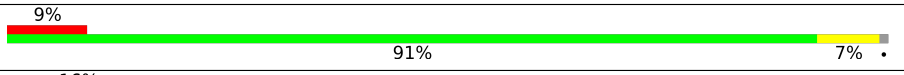
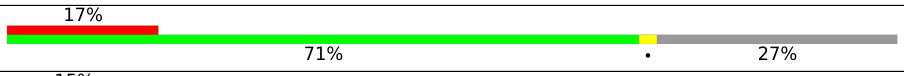
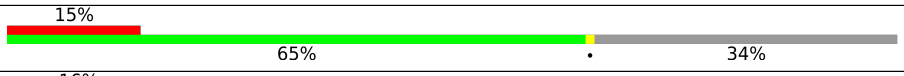
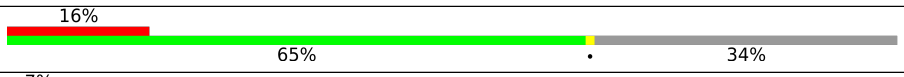
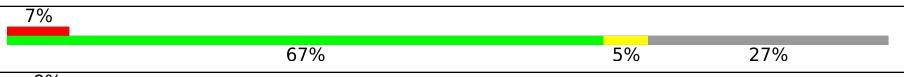
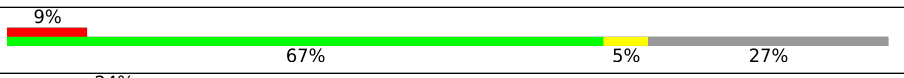
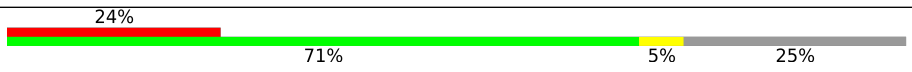
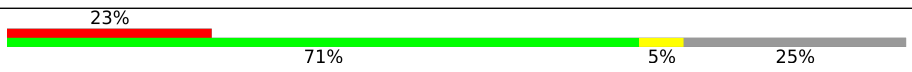
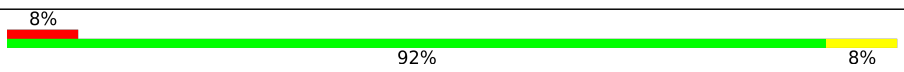
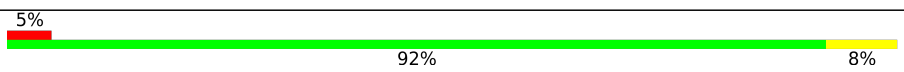
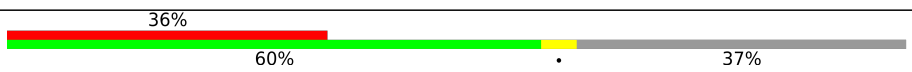
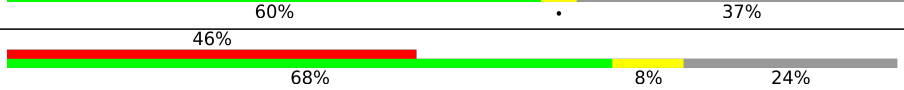
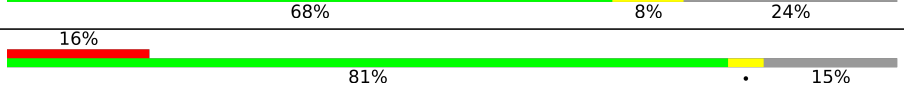
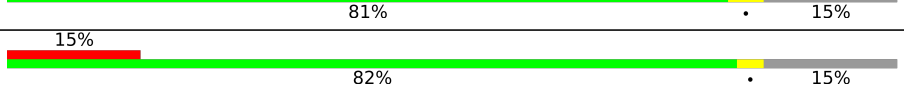
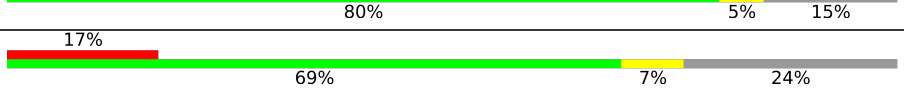
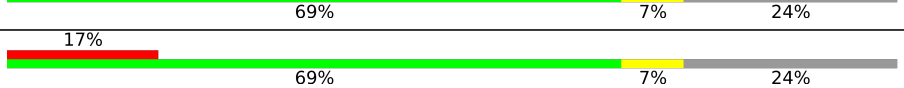
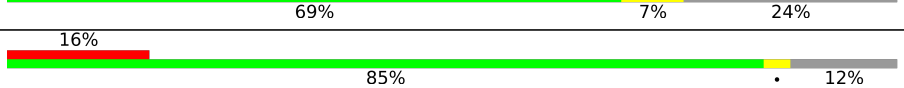
Mol	Chain	Length	Quality of chain
3	C	81	
3	C2	81	
4	D	196	
4	D2	196	
5	E	97	
5	E2	97	
6	F	227	
6	F2	227	
7	G	126	
7	G2	126	
8	I	106	
8	I2	106	
9	J	40	
9	J2	40	
10	L	196	
10	L2	196	
11	K	113	
11	K2	113	
12	1	228	
12	12	228	
12	Z	228	
12	Z2	228	
13	3	298	
13	32	298	
14	7	241	

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Mol	Chain	Length	Quality of chain
14	72	241	17% 85% 12%
15	8	243	13% 86% 11%
15	82	243	12% 87% 11%
16	4	264	69% 77% 20%
16	42	264	69% 77% 20%
17	5	257	68% 83% 5% 12%
17	52	257	70% 83% 5% 12%
18	6	257	77% 86% 11%
18	62	257	75% 86% 11%
19	9	213	23% 83% 5% 13%
19	92	213	23% 83% 5% 13%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
31	XAT	5	624	X	-	-	-
31	XAT	52	624	X	-	-	-

2 Entry composition (i)

There are 33 unique types of molecules in this entry. The entry contains 202818 atoms, of which 101988 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	742	Total	C	H	N	O	S	0	0
			11500	3808	5675	994	1001	22		
1	A2	742	Total	C	H	N	O	S	0	0
			11500	3808	5675	994	1001	22		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
2	B	733	Total	C	H	N	O	S	0	0
			11400	3824	5576	977	1005	18		
2	B2	733	Total	C	H	N	O	S	0	0
			11400	3824	5576	977	1005	18		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
3	C	80	Total	C	H	N	O	S	0	0
			1183	369	582	103	117	12		
3	C2	80	Total	C	H	N	O	S	0	0
			1183	369	582	103	117	12		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
4	D	144	Total	C	H	N	O	S	0	0
			2284	725	1151	200	201	7		
4	D2	144	Total	C	H	N	O	S	0	0
			2284	725	1151	200	201	7		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	64	Total	C	H	N	O	0	0
			1011	322	505	89	95		
5	E2	64	Total	C	H	N	O	0	0
			1011	322	505	89	95		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
6	F	165	Total	C	H	N	O	S	0	0
			2568	817	1302	213	233	3		
6	F2	165	Total	C	H	N	O	S	0	0
			2568	817	1302	213	233	3		

- Molecule 7 is a protein called Photosystem I reaction center subunit V, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	95	Total	C	H	N	O	0	0
			1393	452	687	119	135		
7	G2	95	Total	C	H	N	O	0	0
			1393	452	687	119	135		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
8	I	37	Total	C	H	N	O	S	0	0
			573	195	292	39	46	1		
8	I2	37	Total	C	H	N	O	S	0	0
			573	195	292	39	46	1		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
9	J	40	Total	C	H	N	O	S	0	0
			657	224	328	46	58	1		
9	J2	40	Total	C	H	N	O	S	0	0
			657	224	328	46	58	1		

- Molecule 10 is a protein called PSI subunit V.

Mol	Chain	Residues	Atoms						AltConf	Trace
10	L	124	Total	C	H	N	O	S	0	0
			1806	586	907	146	164	3		

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Mol	Chain	Residues	Atoms						AltConf	Trace
10	L2	124	Total	C	H	N	O	S	0	0
			1806	586	907	146	164	3		

- Molecule 11 is a protein called Photosystem I reaction center subunit psaK, chloroplastic.

Mol	Chain	Residues	Atoms						AltConf	Trace
11	K	86	Total	C	H	N	O	S	0	0
			1203	370	620	100	111	2		
11	K2	86	Total	C	H	N	O	S	0	0
			1203	370	620	100	111	2		

- Molecule 12 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms						AltConf	Trace
12	1	194	Total	C	H	N	O	S	0	0
			2842	941	1397	240	261	3		
12	Z	194	Total	C	H	N	O	S	0	0
			2842	941	1397	240	261	3		
12	12	194	Total	C	H	N	O	S	0	0
			2842	941	1397	240	261	3		
12	Z2	194	Total	C	H	N	O	S	0	0
			2842	941	1397	240	261	3		

- Molecule 13 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms						AltConf	Trace
13	3	227	Total	C	H	N	O	S	0	0
			3431	1128	1695	283	317	8		
13	32	227	Total	C	H	N	O	S	0	0
			3431	1128	1695	283	317	8		

- Molecule 14 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms						AltConf	Trace
14	7	213	Total	C	H	N	O	S	0	0
			3240	1072	1590	274	298	6		
14	72	213	Total	C	H	N	O	S	0	0
			3240	1072	1590	274	298	6		

- Molecule 15 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms						AltConf	Trace
15	8	217	Total	C	H	N	O	S	0	0
			3280	1073	1630	280	293	4		
15	82	217	Total	C	H	N	O	S	0	0
			3280	1073	1630	280	293	4		

- Molecule 16 is a protein called Chlorophyll a-b binding protein, chloroplastic (Lhca4).

Mol	Chain	Residues	Atoms						AltConf	Trace
16	4	212	Total	C	H	N	O	S	0	0
			3251	1080	1603	268	295	5		
16	42	212	Total	C	H	N	O	S	0	0
			3251	1080	1603	268	295	5		

- Molecule 17 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms						AltConf	Trace
17	5	227	Total	C	H	N	O	S	0	0
			3522	1154	1747	297	316	8		
17	52	227	Total	C	H	N	O	S	0	0
			3522	1154	1747	297	316	8		

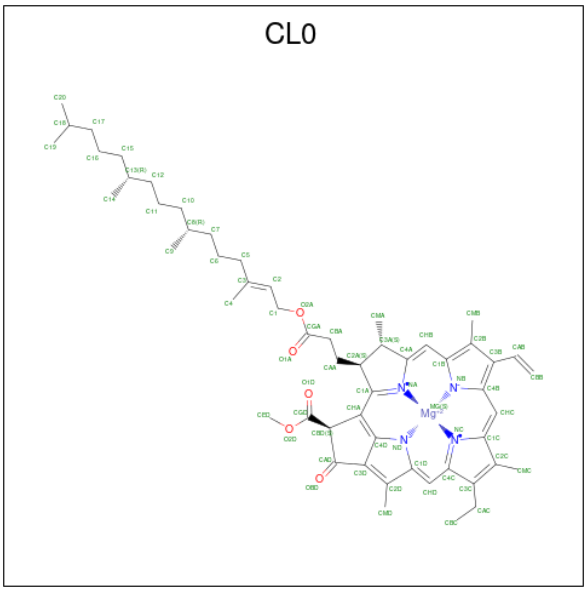
- Molecule 18 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms						AltConf	Trace
18	6	230	Total	C	H	N	O	S	0	0
			3542	1167	1770	293	306	6		
18	62	230	Total	C	H	N	O	S	0	0
			3542	1167	1770	293	306	6		

- Molecule 19 is a protein called Chlorophyll a-b binding protein, chloroplastic.

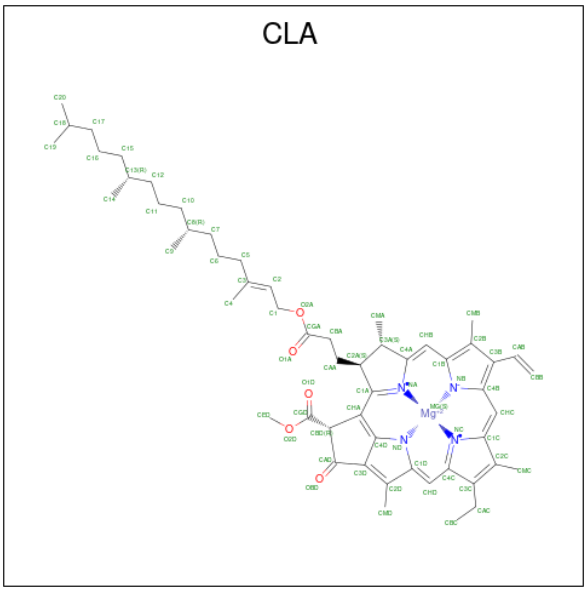
Mol	Chain	Residues	Atoms						AltConf	Trace
19	9	186	Total	C	H	N	O	S	0	0
			2820	918	1400	238	257	7		
19	92	186	Total	C	H	N	O	S	0	0
			2820	918	1400	238	257	7		

- Molecule 20 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
20	A	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
20	A2	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	

- Molecule 21 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
21	A	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	

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Mol	Chain	Residues	Atoms						AltConf
21	A	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
21	A	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
21	A	1	Total	C	H	Mg	N	O	0
			104	45	49	1	4	5	
21	A	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
21	A	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
21	A	1	Total	C	H	Mg	N	O	0
			89	40	39	1	4	5	
21	A	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
21	A	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
21	A	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
21	A	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
21	A	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
21	A	1	Total	C	H	Mg	N	O	0
			104	45	49	1	4	5	
21	A	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
21	A	1	Total	C	H	Mg	N	O	0
			104	45	49	1	4	5	
21	A	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
21	A	1	Total	C	H	Mg	N	O	0
			119	50	59	1	4	5	
21	A	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
21	A	1	Total	C	H	Mg	N	O	0
			104	45	49	1	4	5	
21	A	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
21	A	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	

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Mol	Chain	Residues	Atoms						AltConf
21	A	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	
21	A	1	Total	C	H	Mg	N	O	0
			104	45	49	1	4	5	
21	A	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
21	A	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
21	A	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
21	A	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
21	A	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
21	A	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
21	A	1	Total	C	H	Mg	N	O	0
			104	45	49	1	4	5	
21	A	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
21	A	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
21	A	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
21	A	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
21	A	1	Total	C	H	Mg	N	O	0
			110	47	53	1	4	5	
21	A	1	Total	C	H	Mg	N	O	0
			92	41	41	1	4	5	
21	A	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
21	A	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
21	A	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
21	A	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
21	A	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	

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Mol	Chain	Residues	Atoms						AltConf
21	A	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
21	B	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
21	B	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
21	B	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	
21	B	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
21	B	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
21	B	1	Total	C	H	Mg	N	O	0
			104	45	49	1	4	5	
21	B	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
21	B	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
21	B	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
21	B	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
21	B	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
21	B	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
21	B	1	Total	C	H	Mg	N	O	0
			119	50	59	1	4	5	
21	B	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
21	B	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
21	B	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
21	B	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
21	B	1	Total	C	H	Mg	N	O	0
			119	50	59	1	4	5	
21	B	1	Total	C	H	Mg	N	O	0
			107	46	51	1	4	5	
21	B	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	

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Mol	Chain	Residues	Atoms						AltConf
21	B	1	Total	C	H	Mg	N	O	0
			117	49	58	1	4	5	
21	B	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
21	B	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
21	B	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
21	B	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
21	B	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
21	B	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
21	B	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
21	B	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	
21	B	1	Total	C	H	Mg	N	O	0
			104	45	49	1	4	5	
21	B	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
21	B	1	Total	C	H	Mg	N	O	0
			113	48	55	1	4	5	
21	B	1	Total	C	H	Mg	N	O	0
			119	50	59	1	4	5	
21	B	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	
21	B	1	Total	C	H	Mg	N	O	0
			119	50	59	1	4	5	
21	B	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
21	B	1	Total	C	H	Mg	N	O	0
			89	40	39	1	4	5	
21	B	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
21	B	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
21	B	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
21	F	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	

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Mol	Chain	Residues	Atoms						AltConf
21	F	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	
21	F	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
21	G	1	Total	C	H	Mg	N	O	0
			119	50	59	1	4	5	
21	G	1	Total	C	H	Mg	N	O	0
			79	36	33	1	4	5	
21	J	1	Total	C	H	Mg	N	O	0
			104	45	49	1	4	5	
21	L	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
21	L	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	
21	K	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	
21	K	1	Total	C	H	Mg	N	O	0
			119	50	59	1	4	5	
21	K	1	Total	C	H	Mg	N	O	0
			79	36	33	1	4	5	
21	K	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	
21	1	1	Total	C	H	Mg	N	O	0
			119	50	59	1	4	5	
21	1	1	Total	C	H	Mg	N	O	0
			110	47	53	1	4	5	
21	1	1	Total	C	H	Mg	N	O	0
			89	40	39	1	4	5	
21	1	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
21	1	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
21	1	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
21	1	1	Total	C	H	Mg	N	O	0
			122	51	61	1	4	5	
21	1	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	
21	1	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
21	1	1	Total	C	H	Mg	N	O	0
			119	50	59	1	4	5	

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Mol	Chain	Residues	Atoms						AltConf
21	1	1	Total	C	H	Mg	N	O	0
			79	36	33	1	4	5	
21	3	1	Total	C	H	Mg	N	O	0
			119	50	59	1	4	5	
21	3	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
21	3	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
21	3	1	Total	C	H	Mg	N	O	0
			73	34	31	1	4	3	
21	3	1	Total	C	H	Mg	N	O	0
			104	45	49	1	4	5	
21	3	1	Total	C	H	Mg	N	O	0
			122	51	61	1	4	5	
21	3	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
21	3	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
21	3	1	Total	C	H	Mg	N	O	0
			79	36	33	1	4	5	
21	3	1	Total	C	H	Mg	N	O	0
			119	50	59	1	4	5	
21	3	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	
21	3	1	Total	C	H	Mg	N	O	0
			79	36	33	1	4	5	
21	3	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
21	7	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
21	7	1	Total	C	H	Mg	N	O	0
			95	42	43	1	4	5	
21	7	1	Total	C	H	Mg	N	O	0
			92	41	41	1	4	5	
21	7	1	Total	C	H	Mg	N	O	0
			89	40	39	1	4	5	
21	7	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	
21	7	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
21	7	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	

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Mol	Chain	Residues	Atoms						AltConf
21	7	1	Total	C	H	Mg	N	O	0
			95	42	43	1	4	5	
21	7	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
21	7	1	Total	C	H	Mg	N	O	0
			76	35	33	1	4	3	
21	7	1	Total	C	H	Mg	N	O	0
			79	36	33	1	4	5	
21	7	1	Total	C	H	Mg	N	O	0
			98	43	45	1	4	5	
21	8	1	Total	C	H	Mg	N	O	0
			125	52	63	1	4	5	
21	8	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
21	8	1	Total	C	H	Mg	N	O	0
			119	50	59	1	4	5	
21	8	1	Total	C	H	Mg	N	O	0
			89	40	39	1	4	5	
21	8	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	
21	8	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
21	8	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	
21	8	1	Total	C	H	Mg	N	O	0
			104	45	49	1	4	5	
21	8	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
21	8	1	Total	C	H	Mg	N	O	0
			110	47	53	1	4	5	
21	8	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	
21	Z	1	Total	C	H	Mg	N	O	0
			119	50	59	1	4	5	
21	Z	1	Total	C	H	Mg	N	O	0
			104	45	49	1	4	5	
21	Z	1	Total	C	H	Mg	N	O	0
			110	47	53	1	4	5	
21	Z	1	Total	C	H	Mg	N	O	0
			89	40	39	1	4	5	
21	Z	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	

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Mol	Chain	Residues	Atoms						AltConf
21	Z	1	Total	C	H	Mg	N	O	0
			119	50	59	1	4	5	
21	Z	1	Total	C	H	Mg	N	O	0
			119	50	59	1	4	5	
21	Z	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	
21	Z	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
21	Z	1	Total	C	H	Mg	N	O	0
			89	40	39	1	4	5	
21	Z	1	Total	C	H	Mg	N	O	0
			119	50	59	1	4	5	
21	4	1	Total	C	H	Mg	N	O	0
			119	50	59	1	4	5	
21	4	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
21	4	1	Total	C	H	Mg	N	O	0
			89	40	39	1	4	5	
21	4	1	Total	C	H	Mg	N	O	0
			119	50	59	1	4	5	
21	4	1	Total	C	H	Mg	N	O	0
			119	50	59	1	4	5	
21	4	1	Total	C	H	Mg	N	O	0
			119	50	59	1	4	5	
21	4	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	
21	4	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
21	4	1	Total	C	H	Mg	N	O	0
			104	45	49	1	4	5	
21	4	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	
21	5	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
21	5	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
21	5	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
21	5	1	Total	C	H	Mg	N	O	0
			104	45	49	1	4	5	
21	5	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	

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Mol	Chain	Residues	Atoms						AltConf
21	5	1	Total	C	H	Mg	N	O	0
			119	50	59	1	4	5	
21	5	1	Total	C	H	Mg	N	O	0
			104	45	49	1	4	5	
21	5	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	
21	5	1	Total	C	H	Mg	N	O	0
			107	46	51	1	4	5	
21	5	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	
21	5	1	Total	C	H	Mg	N	O	0
			98	43	45	1	4	5	
21	5	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
21	5	1	Total	C	H	Mg	N	O	0
			79	36	33	1	4	5	
21	6	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
21	6	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
21	6	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
21	6	1	Total	C	H	Mg	N	O	0
			104	45	49	1	4	5	
21	6	1	Total	C	H	Mg	N	O	0
			119	50	59	1	4	5	
21	6	1	Total	C	H	Mg	N	O	0
			113	48	55	1	4	5	
21	6	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	
21	6	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
21	6	1	Total	C	H	Mg	N	O	0
			89	40	39	1	4	5	
21	6	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	
21	6	1	Total	C	H	Mg	N	O	0
			104	45	49	1	4	5	
21	9	1	Total	C	H	Mg	N	O	0
			79	36	33	1	4	5	
21	9	1	Total	C	H	Mg	N	O	0
			119	50	59	1	4	5	

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Mol	Chain	Residues	Atoms						AltConf
21	9	1	Total	C	H	Mg	N	O	0
			104	45	49	1	4	5	
21	9	1	Total	C	H	Mg	N	O	0
			98	43	45	1	4	5	
21	9	1	Total	C	H	Mg	N	O	0
			92	41	41	1	4	5	
21	9	1	Total	C	H	Mg	N	O	0
			119	50	59	1	4	5	
21	9	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
21	9	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
21	9	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
21	9	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	
21	A2	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
21	A2	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
21	A2	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
21	A2	1	Total	C	H	Mg	N	O	0
			104	45	49	1	4	5	
21	A2	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
21	A2	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
21	A2	1	Total	C	H	Mg	N	O	0
			89	40	39	1	4	5	
21	A2	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
21	A2	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
21	A2	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
21	A2	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
21	A2	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	

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Mol	Chain	Residues	Atoms						AltConf
21	A2	1	Total	C	H	Mg	N	O	0
			104	45	49	1	4	5	
21	A2	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
21	A2	1	Total	C	H	Mg	N	O	0
			104	45	49	1	4	5	
21	A2	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
21	A2	1	Total	C	H	Mg	N	O	0
			119	50	59	1	4	5	
21	A2	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
21	A2	1	Total	C	H	Mg	N	O	0
			104	45	49	1	4	5	
21	A2	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
21	A2	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
21	A2	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	
21	A2	1	Total	C	H	Mg	N	O	0
			104	45	49	1	4	5	
21	A2	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
21	A2	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
21	A2	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
21	A2	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
21	A2	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
21	A2	1	Total	C	H	Mg	N	O	0
			104	45	49	1	4	5	
21	A2	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
21	A2	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
21	A2	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	

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Mol	Chain	Residues	Atoms						AltConf
21	A2	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
21	A2	1	Total	C	H	Mg	N	O	0
			110	47	53	1	4	5	
21	A2	1	Total	C	H	Mg	N	O	0
			92	41	41	1	4	5	
21	A2	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
21	A2	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
21	A2	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
21	A2	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
21	A2	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
21	A2	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	
21	A2	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
21	B2	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
21	B2	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
21	B2	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	
21	B2	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
21	B2	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
21	B2	1	Total	C	H	Mg	N	O	0
			104	45	49	1	4	5	
21	B2	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
21	B2	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
21	B2	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
21	B2	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
21	B2	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	

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Mol	Chain	Residues	Atoms						AltConf
21	B2	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
21	B2	1	Total	C	H	Mg	N	O	0
			119	50	59	1	4	5	
21	B2	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
21	B2	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
21	B2	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
21	B2	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
21	B2	1	Total	C	H	Mg	N	O	0
			119	50	59	1	4	5	
21	B2	1	Total	C	H	Mg	N	O	0
			107	46	51	1	4	5	
21	B2	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
21	B2	1	Total	C	H	Mg	N	O	0
			117	49	58	1	4	5	
21	B2	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
21	B2	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
21	B2	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
21	B2	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
21	B2	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
21	B2	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
21	B2	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	
21	B2	1	Total	C	H	Mg	N	O	0
			104	45	49	1	4	5	
21	B2	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
21	B2	1	Total	C	H	Mg	N	O	0
			113	48	55	1	4	5	

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Mol	Chain	Residues	Atoms						AltConf
21	B2	1	Total	C	H	Mg	N	O	0
			119	50	59	1	4	5	
21	B2	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	
21	B2	1	Total	C	H	Mg	N	O	0
			119	50	59	1	4	5	
21	B2	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
21	B2	1	Total	C	H	Mg	N	O	0
			89	40	39	1	4	5	
21	B2	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
21	B2	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
21	B2	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
21	F2	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
21	F2	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	
21	F2	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
21	G2	1	Total	C	H	Mg	N	O	0
			119	50	59	1	4	5	
21	G2	1	Total	C	H	Mg	N	O	0
			79	36	33	1	4	5	
21	J2	1	Total	C	H	Mg	N	O	0
			104	45	49	1	4	5	
21	L2	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
21	L2	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	
21	K2	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	
21	K2	1	Total	C	H	Mg	N	O	0
			119	50	59	1	4	5	
21	K2	1	Total	C	H	Mg	N	O	0
			79	36	33	1	4	5	
21	K2	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	
21	12	1	Total	C	H	Mg	N	O	0
			119	50	59	1	4	5	

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Mol	Chain	Residues	Atoms						AltConf
21	12	1	Total	C	H	Mg	N	O	0
			110	47	53	1	4	5	
21	12	1	Total	C	H	Mg	N	O	0
			89	40	39	1	4	5	
21	12	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
21	12	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
21	12	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
21	12	1	Total	C	H	Mg	N	O	0
			122	51	61	1	4	5	
21	12	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	
21	12	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
21	12	1	Total	C	H	Mg	N	O	0
			119	50	59	1	4	5	
21	12	1	Total	C	H	Mg	N	O	0
			79	36	33	1	4	5	
21	32	1	Total	C	H	Mg	N	O	0
			119	50	59	1	4	5	
21	32	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
21	32	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
21	32	1	Total	C	H	Mg	N	O	0
			73	34	31	1	4	3	
21	32	1	Total	C	H	Mg	N	O	0
			104	45	49	1	4	5	
21	32	1	Total	C	H	Mg	N	O	0
			122	51	61	1	4	5	
21	32	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
21	32	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
21	32	1	Total	C	H	Mg	N	O	0
			79	36	33	1	4	5	
21	32	1	Total	C	H	Mg	N	O	0
			119	50	59	1	4	5	
21	32	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	

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Mol	Chain	Residues	Atoms						AltConf
21	32	1	Total	C	H	Mg	N	O	0
			79	36	33	1	4	5	
21	32	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
21	72	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
21	72	1	Total	C	H	Mg	N	O	0
			95	42	43	1	4	5	
21	72	1	Total	C	H	Mg	N	O	0
			92	41	41	1	4	5	
21	72	1	Total	C	H	Mg	N	O	0
			89	40	39	1	4	5	
21	72	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	
21	72	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
21	72	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
21	72	1	Total	C	H	Mg	N	O	0
			95	42	43	1	4	5	
21	72	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
21	72	1	Total	C	H	Mg	N	O	0
			76	35	33	1	4	3	
21	72	1	Total	C	H	Mg	N	O	0
			79	36	33	1	4	5	
21	72	1	Total	C	H	Mg	N	O	0
			98	43	45	1	4	5	
21	82	1	Total	C	H	Mg	N	O	0
			125	52	63	1	4	5	
21	82	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
21	82	1	Total	C	H	Mg	N	O	0
			119	50	59	1	4	5	
21	82	1	Total	C	H	Mg	N	O	0
			89	40	39	1	4	5	
21	82	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	
21	82	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
21	82	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	

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Mol	Chain	Residues	Atoms						AltConf
21	82	1	Total	C	H	Mg	N	O	0
			104	45	49	1	4	5	
21	82	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
21	82	1	Total	C	H	Mg	N	O	0
			110	47	53	1	4	5	
21	82	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	
21	Z2	1	Total	C	H	Mg	N	O	0
			119	50	59	1	4	5	
21	Z2	1	Total	C	H	Mg	N	O	0
			104	45	49	1	4	5	
21	Z2	1	Total	C	H	Mg	N	O	0
			110	47	53	1	4	5	
21	Z2	1	Total	C	H	Mg	N	O	0
			89	40	39	1	4	5	
21	Z2	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
21	Z2	1	Total	C	H	Mg	N	O	0
			119	50	59	1	4	5	
21	Z2	1	Total	C	H	Mg	N	O	0
			119	50	59	1	4	5	
21	Z2	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	
21	Z2	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
21	Z2	1	Total	C	H	Mg	N	O	0
			89	40	39	1	4	5	
21	Z2	1	Total	C	H	Mg	N	O	0
			119	50	59	1	4	5	
21	42	1	Total	C	H	Mg	N	O	0
			119	50	59	1	4	5	
21	42	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
21	42	1	Total	C	H	Mg	N	O	0
			89	40	39	1	4	5	
21	42	1	Total	C	H	Mg	N	O	0
			119	50	59	1	4	5	
21	42	1	Total	C	H	Mg	N	O	0
			119	50	59	1	4	5	
21	42	1	Total	C	H	Mg	N	O	0
			119	50	59	1	4	5	

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Mol	Chain	Residues	Atoms						AltConf
21	42	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	
21	42	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
21	42	1	Total	C	H	Mg	N	O	0
			104	45	49	1	4	5	
21	42	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	
21	52	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
21	52	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
21	52	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
21	52	1	Total	C	H	Mg	N	O	0
			104	45	49	1	4	5	
21	52	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
21	52	1	Total	C	H	Mg	N	O	0
			119	50	59	1	4	5	
21	52	1	Total	C	H	Mg	N	O	0
			104	45	49	1	4	5	
21	52	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	
21	52	1	Total	C	H	Mg	N	O	0
			107	46	51	1	4	5	
21	52	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	
21	52	1	Total	C	H	Mg	N	O	0
			98	43	45	1	4	5	
21	52	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
21	52	1	Total	C	H	Mg	N	O	0
			79	36	33	1	4	5	
21	62	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
21	62	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
21	62	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
21	62	1	Total	C	H	Mg	N	O	0
			104	45	49	1	4	5	

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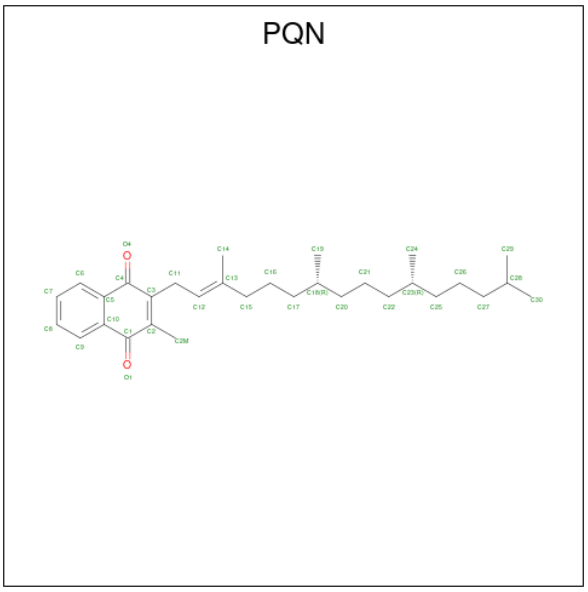
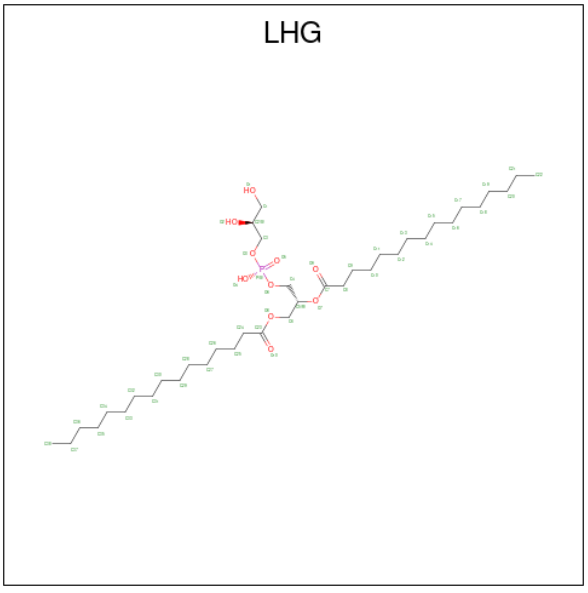
Mol	Chain	Residues	Atoms						AltConf
21	62	1	Total	C	H	Mg	N	O	0
			119	50	59	1	4	5	
21	62	1	Total	C	H	Mg	N	O	0
			113	48	55	1	4	5	
21	62	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	
21	62	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
21	62	1	Total	C	H	Mg	N	O	0
			89	40	39	1	4	5	
21	62	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	
21	62	1	Total	C	H	Mg	N	O	0
			104	45	49	1	4	5	
21	92	1	Total	C	H	Mg	N	O	0
			79	36	33	1	4	5	
21	92	1	Total	C	H	Mg	N	O	0
			119	50	59	1	4	5	
21	92	1	Total	C	H	Mg	N	O	0
			104	45	49	1	4	5	
21	92	1	Total	C	H	Mg	N	O	0
			98	43	45	1	4	5	
21	92	1	Total	C	H	Mg	N	O	0
			92	41	41	1	4	5	
21	92	1	Total	C	H	Mg	N	O	0
			119	50	59	1	4	5	
21	92	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
21	92	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
21	92	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
21	92	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	

- Molecule 22 is PHYLLOQUINONE (CCD ID: PQN) (formula: $C_{31}H_{46}O_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
22	A	1	Total	C	H	O	0
			79	31	46	2	
22	B	1	Total	C	H	O	0
			79	31	46	2	
22	A2	1	Total	C	H	O	0
			79	31	46	2	
22	B2	1	Total	C	H	O	0
			79	31	46	2	

- Molecule 23 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
23	A	1	Total	C	H	O	P	0
			123	38	74	10	1	
23	A	1	Total	C	H	O	P	0
			87	27	49	10	1	
23	B	1	Total	C	H	O	P	0
			108	34	63	10	1	
23	1	1	Total	C	H	O	P	0
			87	28	48	10	1	
23	3	1	Total	C	H	O	P	0
			63	20	32	10	1	
23	3	1	Total	C	H	O	P	0
			114	36	67	10	1	
23	7	1	Total	C	H	O	P	0
			123	38	74	10	1	
23	8	1	Total	C	H	O	P	0
			105	33	61	10	1	
23	Z	1	Total	C	H	O	P	0
			87	28	48	10	1	
23	4	1	Total	C	H	O	P	0
			123	38	74	10	1	
23	4	1	Total	C	H	O	P	0
			87	27	49	10	1	
23	5	1	Total	C	H	O	P	0
			81	26	44	10	1	
23	6	1	Total	C	H	O	P	0
			123	38	74	10	1	
23	6	1	Total	C	H	O	P	0
			78	25	42	10	1	
23	9	1	Total	C	H	O	P	0
			96	30	55	10	1	
23	A2	1	Total	C	H	O	P	0
			123	38	74	10	1	
23	A2	1	Total	C	H	O	P	0
			87	27	49	10	1	
23	B2	1	Total	C	H	O	P	0
			108	34	63	10	1	
23	12	1	Total	C	H	O	P	0
			87	28	48	10	1	
23	32	1	Total	C	H	O	P	0
			63	20	32	10	1	
23	32	1	Total	C	H	O	P	0
			114	36	67	10	1	
23	72	1	Total	C	H	O	P	0
			123	38	74	10	1	

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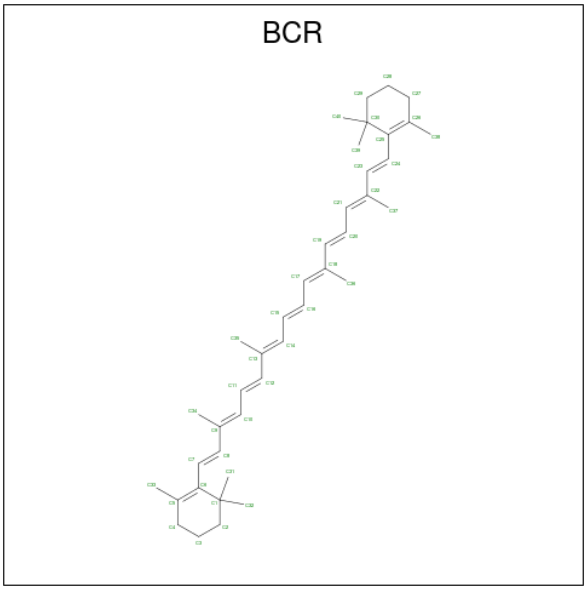
Mol	Chain	Residues	Atoms					AltConf
23	82	1	Total	C	H	O	P	0
			105	33	61	10	1	
23	Z2	1	Total	C	H	O	P	0
			87	28	48	10	1	
23	42	1	Total	C	H	O	P	0
			123	38	74	10	1	
23	42	1	Total	C	H	O	P	0
			87	27	49	10	1	
23	52	1	Total	C	H	O	P	0
			81	26	44	10	1	
23	62	1	Total	C	H	O	P	0
			123	38	74	10	1	
23	62	1	Total	C	H	O	P	0
			78	25	42	10	1	
23	92	1	Total	C	H	O	P	0
			96	30	55	10	1	

- Molecule 24 is BETA-CAROTENE (CCD ID: BCR) (formula: $C_{40}H_{56}$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
24	A	1	Total	C	H	0
			96	40	56	
24	A	1	Total	C	H	0
			96	40	56	
24	A	1	Total	C	H	0
			96	40	56	

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Mol	Chain	Residues	Atoms	AltConf
24	A	1	Total C H 96 40 56	0
24	A	1	Total C H 96 40 56	0
24	B	1	Total C H 96 40 56	0
24	B	1	Total C H 96 40 56	0
24	B	1	Total C H 96 40 56	0
24	B	1	Total C H 96 40 56	0
24	B	1	Total C H 96 40 56	0
24	B	1	Total C H 96 40 56	0
24	B	1	Total C H 96 40 56	0
24	G	1	Total C H 96 40 56	0
24	I	1	Total C H 96 40 56	0
24	J	1	Total C H 96 40 56	0
24	L	1	Total C H 96 40 56	0
24	L	1	Total C H 96 40 56	0
24	K	1	Total C H 96 40 56	0
24	K	1	Total C H 96 40 56	0
24	3	1	Total C H 96 40 56	0
24	3	1	Total C H 96 40 56	0
24	3	1	Total C H 96 40 56	0
24	7	1	Total C H 96 40 56	0
24	8	1	Total C H 96 40 56	0

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Mol	Chain	Residues	Atoms	AltConf
24	4	1	Total C H 96 40 56	0
24	5	1	Total C H 96 40 56	0
24	6	1	Total C H 96 40 56	0
24	9	1	Total C H 96 40 56	0
24	A2	1	Total C H 96 40 56	0
24	A2	1	Total C H 96 40 56	0
24	A2	1	Total C H 96 40 56	0
24	A2	1	Total C H 96 40 56	0
24	A2	1	Total C H 96 40 56	0
24	B2	1	Total C H 96 40 56	0
24	B2	1	Total C H 96 40 56	0
24	B2	1	Total C H 96 40 56	0
24	B2	1	Total C H 96 40 56	0
24	B2	1	Total C H 96 40 56	0
24	B2	1	Total C H 96 40 56	0
24	B2	1	Total C H 96 40 56	0
24	G2	1	Total C H 96 40 56	0
24	I2	1	Total C H 96 40 56	0
24	J2	1	Total C H 96 40 56	0
24	L2	1	Total C H 96 40 56	0
24	L2	1	Total C H 96 40 56	0

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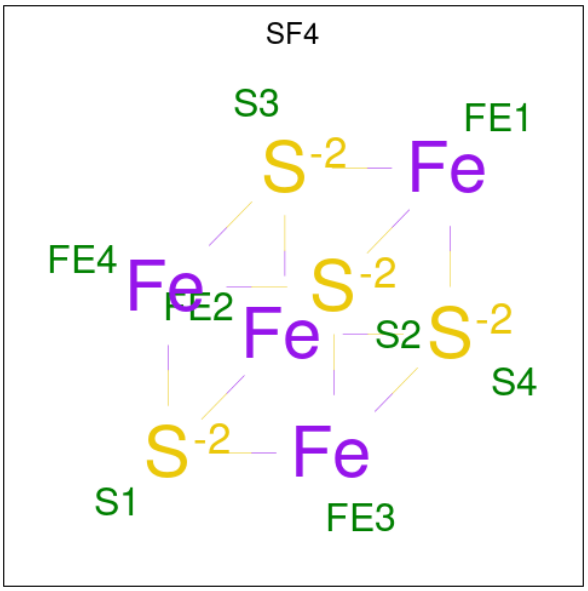
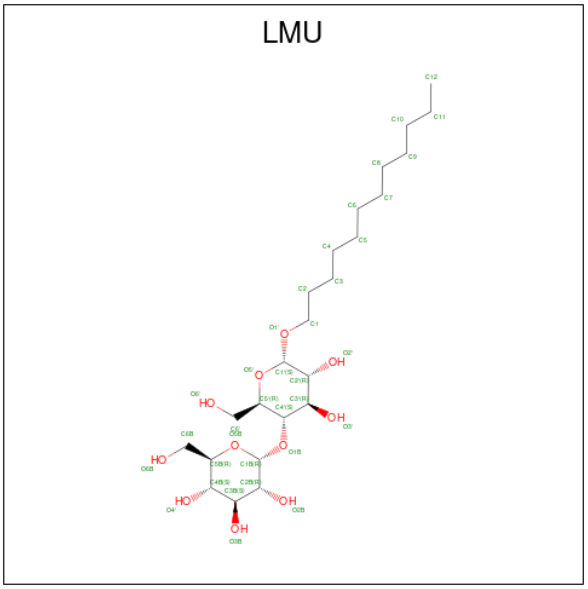
Mol	Chain	Residues	Atoms	AltConf
24	K2	1	Total C H 96 40 56	0
24	K2	1	Total C H 96 40 56	0
24	32	1	Total C H 96 40 56	0
24	32	1	Total C H 96 40 56	0
24	32	1	Total C H 96 40 56	0
24	72	1	Total C H 96 40 56	0
24	82	1	Total C H 96 40 56	0
24	42	1	Total C H 96 40 56	0
24	52	1	Total C H 96 40 56	0
24	62	1	Total C H 96 40 56	0
24	92	1	Total C H 96 40 56	0

- Molecule 25 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	AltConf
25	A	1	Total Fe S 8 4 4	0
25	C	1	Total Fe S 8 4 4	0
25	C	1	Total Fe S 8 4 4	0
25	A2	1	Total Fe S 8 4 4	0
25	C2	1	Total Fe S 8 4 4	0
25	C2	1	Total Fe S 8 4 4	0

- Molecule 26 is DODECYL-ALPHA-D-MALTOSIDE (CCD ID: LMU) (formula: $C_{24}H_{46}O_{11}$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	AltConf
26	A	1	Total C H O 75 23 41 11	0
26	A	1	Total C H O 81 24 46 11	0
26	A	1	Total C H O 44 14 24 6	0
26	A	1	Total C H O 59 18 35 6	0
26	A	1	Total C H O 81 24 46 11	0

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Mol	Chain	Residues	Atoms				AltConf
26	A	1	Total	C	H	O	0
			59	18	35	6	
26	A	1	Total	C	H	O	0
			59	18	35	6	
26	B	1	Total	C	H	O	0
			81	24	46	11	
26	G	1	Total	C	H	O	0
			59	18	35	6	
26	K	1	Total	C	H	O	0
			59	18	35	6	
26	1	1	Total	C	H	O	0
			81	24	46	11	
26	1	1	Total	C	H	O	0
			41	13	22	6	
26	1	1	Total	C	H	O	0
			59	18	35	6	
26	1	1	Total	C	H	O	0
			50	16	28	6	
26	1	1	Total	C	H	O	0
			59	18	35	6	
26	1	1	Total	C	H	O	0
			59	18	35	6	
26	7	1	Total	C	H	O	0
			69	21	37	11	
26	7	1	Total	C	H	O	0
			50	16	28	6	
26	7	1	Total	C	H	O	0
			54	16	27	11	
26	8	1	Total	C	H	O	0
			59	18	35	6	
26	8	1	Total	C	H	O	0
			59	18	35	6	
26	8	1	Total	C	H	O	0
			81	24	46	11	
26	8	1	Total	C	H	O	0
			59	18	35	6	
26	Z	1	Total	C	H	O	0
			66	20	35	11	
26	Z	1	Total	C	H	O	0
			50	16	28	6	
26	4	1	Total	C	H	O	0
			72	22	39	11	

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Mol	Chain	Residues	Atoms				AltConf
26	4	1	Total	C	H	O	0
			44	14	24	6	
26	5	1	Total	C	H	O	0
			59	18	35	6	
26	6	1	Total	C	H	O	0
			44	14	24	6	
26	6	1	Total	C	H	O	0
			59	18	35	6	
26	6	1	Total	C	H	O	0
			59	18	35	6	
26	6	1	Total	C	H	O	0
			59	18	35	6	
26	9	1	Total	C	H	O	0
			59	18	35	6	
26	A2	1	Total	C	H	O	0
			75	23	41	11	
26	A2	1	Total	C	H	O	0
			81	24	46	11	
26	A2	1	Total	C	H	O	0
			44	14	24	6	
26	A2	1	Total	C	H	O	0
			59	18	35	6	
26	A2	1	Total	C	H	O	0
			81	24	46	11	
26	A2	1	Total	C	H	O	0
			59	18	35	6	
26	A2	1	Total	C	H	O	0
			59	18	35	6	
26	B2	1	Total	C	H	O	0
			81	24	46	11	
26	G2	1	Total	C	H	O	0
			59	18	35	6	
26	K2	1	Total	C	H	O	0
			59	18	35	6	
26	12	1	Total	C	H	O	0
			81	24	46	11	
26	12	1	Total	C	H	O	0
			41	13	22	6	
26	12	1	Total	C	H	O	0
			59	18	35	6	
26	12	1	Total	C	H	O	0
			50	16	28	6	

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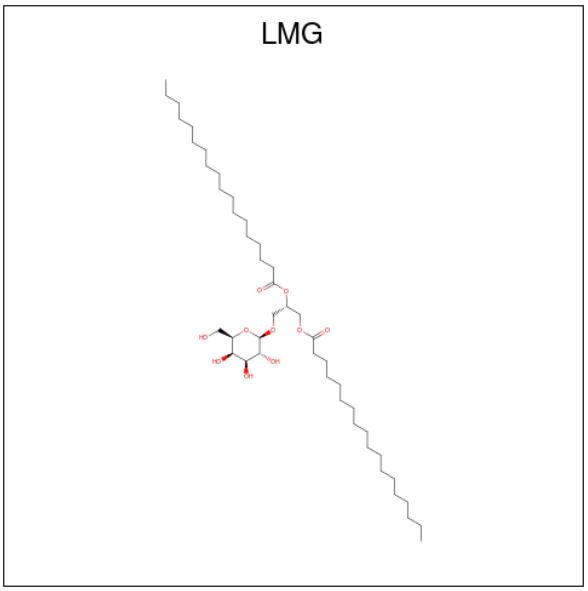
Mol	Chain	Residues	Atoms				AltConf
26	12	1	Total	C	H	O	0
			59	18	35	6	
26	12	1	Total	C	H	O	0
			59	18	35	6	
26	72	1	Total	C	H	O	0
			69	21	37	11	
26	72	1	Total	C	H	O	0
			50	16	28	6	
26	72	1	Total	C	H	O	0
			54	16	27	11	
26	82	1	Total	C	H	O	0
			59	18	35	6	
26	82	1	Total	C	H	O	0
			59	18	35	6	
26	82	1	Total	C	H	O	0
			81	24	46	11	
26	82	1	Total	C	H	O	0
			59	18	35	6	
26	Z2	1	Total	C	H	O	0
			66	20	35	11	
26	Z2	1	Total	C	H	O	0
			50	16	28	6	
26	42	1	Total	C	H	O	0
			72	22	39	11	
26	42	1	Total	C	H	O	0
			44	14	24	6	
26	52	1	Total	C	H	O	0
			59	18	35	6	
26	62	1	Total	C	H	O	0
			44	14	24	6	
26	62	1	Total	C	H	O	0
			59	18	35	6	
26	62	1	Total	C	H	O	0
			59	18	35	6	
26	62	1	Total	C	H	O	0
			59	18	35	6	
26	92	1	Total	C	H	O	0
			59	18	35	6	

- 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	A	1	Total 117	C 38	H 69	O 10	0
27	A	1	Total 78	C 26	H 42	O 10	0
27	B	1	Total 99	C 33	H 56	O 10	0
27	B	1	Total 78	C 26	H 42	O 10	0
27	J	1	Total 99	C 32	H 57	O 10	0
27	J	1	Total 75	C 25	H 40	O 10	0
27	1	1	Total 78	C 26	H 42	O 10	0
27	1	1	Total 96	C 32	H 54	O 10	0
27	3	1	Total 120	C 40	H 75	O 5	0
27	7	1	Total 81	C 27	H 44	O 10	0
27	8	1	Total 66	C 22	H 34	O 10	0
27	8	1	Total 99	C 32	H 57	O 10	0
27	4	1	Total 96	C 31	H 55	O 10	0
27	6	1	Total 55	C 18	H 35	O 2	0

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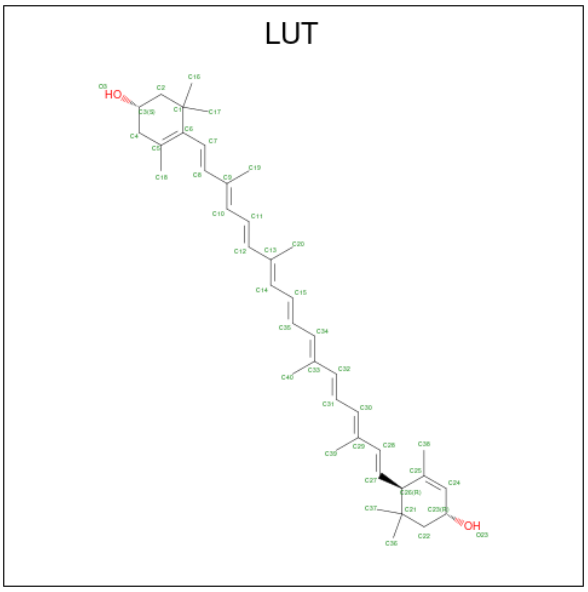
Mol	Chain	Residues	Atoms				AltConf
27	9	1	Total	C	H	O	0
			105	34	61	10	
27	A2	1	Total	C	H	O	0
			117	38	69	10	
27	A2	1	Total	C	H	O	0
			78	26	42	10	
27	B2	1	Total	C	H	O	0
			99	33	56	10	
27	B2	1	Total	C	H	O	0
			78	26	42	10	
27	J2	1	Total	C	H	O	0
			99	32	57	10	
27	J2	1	Total	C	H	O	0
			75	25	40	10	
27	12	1	Total	C	H	O	0
			78	26	42	10	
27	12	1	Total	C	H	O	0
			96	32	54	10	
27	32	1	Total	C	H	O	0
			120	40	75	5	
27	72	1	Total	C	H	O	0
			81	27	44	10	
27	82	1	Total	C	H	O	0
			66	22	34	10	
27	82	1	Total	C	H	O	0
			99	32	57	10	
27	42	1	Total	C	H	O	0
			96	31	55	10	
27	62	1	Total	C	H	O	0
			55	18	35	2	
27	92	1	Total	C	H	O	0
			105	34	61	10	

- Molecule 28 is (3R,3'R,6S)-4,5-DIDEHYDRO-5,6-DIHYDRO-BETA,BETA-CAROTENE-3,3'-DIOL (CCD ID: LUT) (formula: $C_{40}H_{56}O_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
28	A	1	Total	C	H	O	0
			98	40	56	2	
28	F	1	Total	C	H	O	0
			98	40	56	2	
28	1	1	Total	C	H	O	0
			98	40	56	2	
28	1	1	Total	C	H	O	0
			98	40	56	2	
28	3	1	Total	C	H	O	0
			98	40	56	2	
28	3	1	Total	C	H	O	0
			98	40	56	2	
28	3	1	Total	C	H	O	0
			98	40	56	2	
28	7	1	Total	C	H	O	0
			98	40	56	2	
28	7	1	Total	C	H	O	0
			98	40	56	2	
28	8	1	Total	C	H	O	0
			98	40	56	2	
28	Z	1	Total	C	H	O	0
			98	40	56	2	
28	Z	1	Total	C	H	O	0
			59	25	33	1	
28	4	1	Total	C	H	O	0
			98	40	56	2	
28	5	1	Total	C	H	O	0
			98	40	56	2	

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Mol	Chain	Residues	Atoms				AltConf
28	5	1	Total	C	H	O	0
			98	40	56	2	
28	6	1	Total	C	H	O	0
			98	40	56	2	
28	9	1	Total	C	H	O	0
			98	40	56	2	
28	9	1	Total	C	H	O	0
			98	40	56	2	
28	A2	1	Total	C	H	O	0
			98	40	56	2	
28	F2	1	Total	C	H	O	0
			98	40	56	2	
28	12	1	Total	C	H	O	0
			98	40	56	2	
28	12	1	Total	C	H	O	0
			98	40	56	2	
28	32	1	Total	C	H	O	0
			98	40	56	2	
28	32	1	Total	C	H	O	0
			98	40	56	2	
28	32	1	Total	C	H	O	0
			98	40	56	2	
28	72	1	Total	C	H	O	0
			98	40	56	2	
28	72	1	Total	C	H	O	0
			98	40	56	2	
28	82	1	Total	C	H	O	0
			98	40	56	2	
28	Z2	1	Total	C	H	O	0
			98	40	56	2	
28	Z2	1	Total	C	H	O	0
			59	25	33	1	
28	42	1	Total	C	H	O	0
			98	40	56	2	
28	52	1	Total	C	H	O	0
			98	40	56	2	
28	52	1	Total	C	H	O	0
			98	40	56	2	
28	62	1	Total	C	H	O	0
			98	40	56	2	
28	92	1	Total	C	H	O	0
			98	40	56	2	

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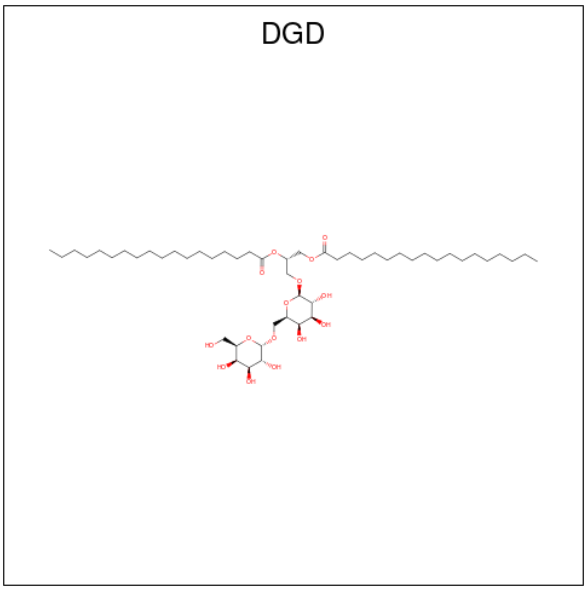
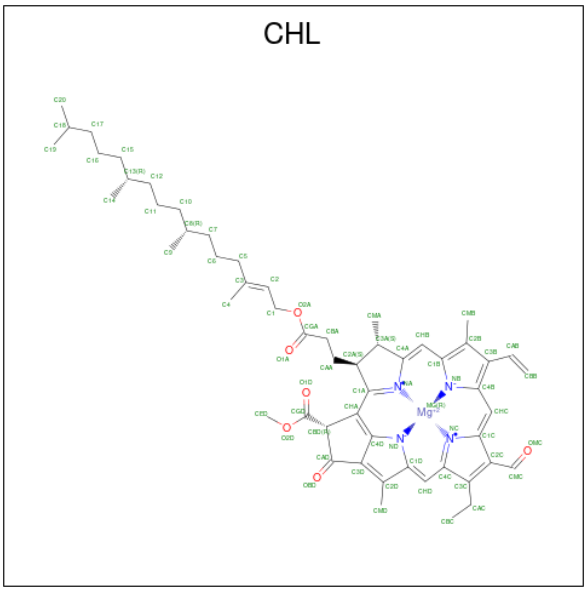
Mol	Chain	Residues	Atoms				AltConf
28	92	1	Total	C	H	O	0
			98	40	56	2	

- Molecule 29 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
29	B	1	Total	C	H	O	0
			138	44	79	15	
29	B2	1	Total	C	H	O	0
			138	44	79	15	

- Molecule 30 is CHLOROPHYLL B (CCD ID: CHL) (formula: $C_{55}H_{70}MgN_4O_6$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						AltConf
30	1	1	Total	C	H	Mg	N	O	0
			136	55	70	1	4	6	
30	1	1	Total	C	H	Mg	N	O	0
			77	35	31	1	4	6	
30	1	1	Total	C	H	Mg	N	O	0
			77	35	31	1	4	6	
30	3	1	Total	C	H	Mg	N	O	0
			136	55	70	1	4	6	
30	7	1	Total	C	H	Mg	N	O	0
			136	55	70	1	4	6	
30	7	1	Total	C	H	Mg	N	O	0
			77	35	31	1	4	6	
30	7	1	Total	C	H	Mg	N	O	0
			77	35	31	1	4	6	
30	8	1	Total	C	H	Mg	N	O	0
			136	55	70	1	4	6	
30	8	1	Total	C	H	Mg	N	O	0
			136	55	70	1	4	6	
30	8	1	Total	C	H	Mg	N	O	0
			136	55	70	1	4	6	
30	Z	1	Total	C	H	Mg	N	O	0
			136	55	70	1	4	6	
30	Z	1	Total	C	H	Mg	N	O	0
			77	35	31	1	4	6	
30	Z	1	Total	C	H	Mg	N	O	0
			136	55	70	1	4	6	
30	4	1	Total	C	H	Mg	N	O	0
			136	55	70	1	4	6	

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Mol	Chain	Residues	Atoms						AltConf
30	4	1	Total	C	H	Mg	N	O	0
			103	45	47	1	4	6	
30	4	1	Total	C	H	Mg	N	O	0
			136	55	70	1	4	6	
30	4	1	Total	C	H	Mg	N	O	0
			136	55	70	1	4	6	
30	4	1	Total	C	H	Mg	N	O	0
			77	35	31	1	4	6	
30	5	1	Total	C	H	Mg	N	O	0
			77	35	31	1	4	6	
30	5	1	Total	C	H	Mg	N	O	0
			136	55	70	1	4	6	
30	5	1	Total	C	H	Mg	N	O	0
			88	40	37	1	4	6	
30	5	1	Total	C	H	Mg	N	O	0
			72	34	29	1	4	4	
30	6	1	Total	C	H	Mg	N	O	0
			136	55	70	1	4	6	
30	6	1	Total	C	H	Mg	N	O	0
			109	47	51	1	4	6	
30	6	1	Total	C	H	Mg	N	O	0
			136	55	70	1	4	6	
30	6	1	Total	C	H	Mg	N	O	0
			88	40	37	1	4	6	
30	6	1	Total	C	H	Mg	N	O	0
			136	55	70	1	4	6	
30	6	1	Total	C	H	Mg	N	O	0
			72	34	29	1	4	4	
30	9	1	Total	C	H	Mg	N	O	0
			69	33	27	1	4	4	
30	9	1	Total	C	H	Mg	N	O	0
			88	40	37	1	4	6	
30	12	1	Total	C	H	Mg	N	O	0
			136	55	70	1	4	6	
30	12	1	Total	C	H	Mg	N	O	0
			77	35	31	1	4	6	
30	12	1	Total	C	H	Mg	N	O	0
			77	35	31	1	4	6	
30	32	1	Total	C	H	Mg	N	O	0
			136	55	70	1	4	6	
30	72	1	Total	C	H	Mg	N	O	0
			136	55	70	1	4	6	

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Mol	Chain	Residues	Atoms						AltConf
30	72	1	Total	C	H	Mg	N	O	0
			77	35	31	1	4	6	
30	72	1	Total	C	H	Mg	N	O	0
			77	35	31	1	4	6	
30	82	1	Total	C	H	Mg	N	O	0
			136	55	70	1	4	6	
30	82	1	Total	C	H	Mg	N	O	0
			136	55	70	1	4	6	
30	82	1	Total	C	H	Mg	N	O	0
			136	55	70	1	4	6	
30	Z2	1	Total	C	H	Mg	N	O	0
			136	55	70	1	4	6	
30	Z2	1	Total	C	H	Mg	N	O	0
			77	35	31	1	4	6	
30	Z2	1	Total	C	H	Mg	N	O	0
			136	55	70	1	4	6	
30	42	1	Total	C	H	Mg	N	O	0
			136	55	70	1	4	6	
30	42	1	Total	C	H	Mg	N	O	0
			103	45	47	1	4	6	
30	42	1	Total	C	H	Mg	N	O	0
			136	55	70	1	4	6	
30	42	1	Total	C	H	Mg	N	O	0
			136	55	70	1	4	6	
30	42	1	Total	C	H	Mg	N	O	0
			77	35	31	1	4	6	
30	52	1	Total	C	H	Mg	N	O	0
			77	35	31	1	4	6	
30	52	1	Total	C	H	Mg	N	O	0
			136	55	70	1	4	6	
30	52	1	Total	C	H	Mg	N	O	0
			88	40	37	1	4	6	
30	52	1	Total	C	H	Mg	N	O	0
			72	34	29	1	4	4	
30	62	1	Total	C	H	Mg	N	O	0
			136	55	70	1	4	6	
30	62	1	Total	C	H	Mg	N	O	0
			109	47	51	1	4	6	
30	62	1	Total	C	H	Mg	N	O	0
			136	55	70	1	4	6	
30	62	1	Total	C	H	Mg	N	O	0
			88	40	37	1	4	6	

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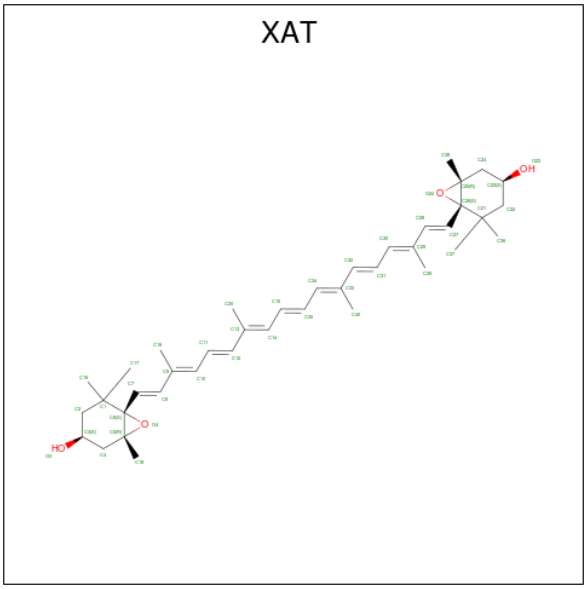
Mol	Chain	Residues	Atoms						AltConf
30	62	1	Total	C	H	Mg	N	O	0
			136	55	70	1	4	6	
30	62	1	Total	C	H	Mg	N	O	0
			72	34	29	1	4	4	
30	92	1	Total	C	H	Mg	N	O	0
			69	33	27	1	4	4	
30	92	1	Total	C	H	Mg	N	O	0
			88	40	37	1	4	6	

- Molecule 31 is (3S,5R,6S,3'S,5'R,6'S)-5,6,5',6'-DIEPOXY-5,6,5',6'- TETRAHYDRO-BETA ,BETA-CAROTENE-3,3'-DIOL (CCD ID: XAT) (formula: $C_{40}H_{56}O_4$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
31	1	1	Total	C	H	O	0
			100	40	56	4	
31	7	1	Total	C	H	O	0
			100	40	56	4	
31	8	1	Total	C	H	O	0
			100	40	56	4	
31	Z	1	Total	C	H	O	0
			100	40	56	4	
31	4	1	Total	C	H	O	0
			100	40	56	4	
31	5	1	Total	C	H	O	0
			100	40	56	4	

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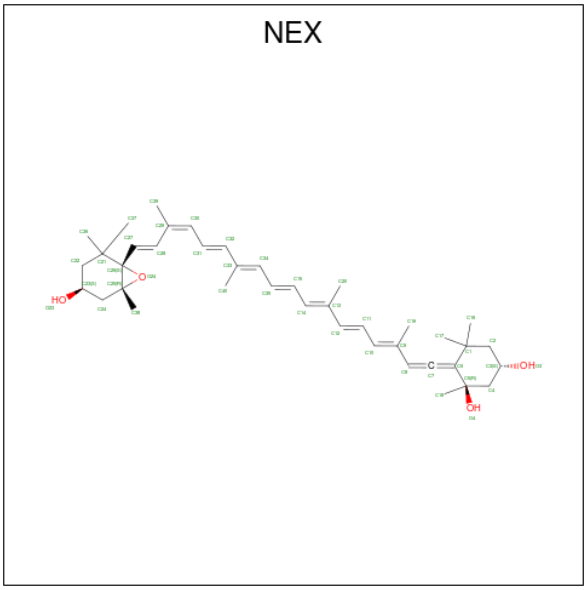
Mol	Chain	Residues	Atoms				AltConf
31	6	1	Total	C	H	O	0
			100	40	56	4	
31	12	1	Total	C	H	O	0
			100	40	56	4	
31	72	1	Total	C	H	O	0
			100	40	56	4	
31	82	1	Total	C	H	O	0
			100	40	56	4	
31	Z2	1	Total	C	H	O	0
			100	40	56	4	
31	42	1	Total	C	H	O	0
			100	40	56	4	
31	52	1	Total	C	H	O	0
			100	40	56	4	
31	62	1	Total	C	H	O	0
			100	40	56	4	

- Molecule 32 is (1R,3R)-6-{(3E,5E,7E,9E,11E,13E,15E,17E)-18-[(1S,4R,6R)-4-HYDROXY-2,2,6-TRIMETHYL-7-OXABICYCLO[4.1.0]HEPT-1-YL]-3,7,12,16-TETRAMETHYLOCTADECA-1,3,5,7,9,11,13,15,17-NONAENYLIDENE}-1,5,5-TRIMETHYLCYCLOHEXANE-1,3-DIOL (CCD ID: NEX) (formula: $C_{40}H_{56}O_4$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
32	5	1	Total	C	H	O	0
			100	40	56	4	

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Mol	Chain	Residues	Atoms				AltConf
32	6	1	Total	C	H	O	0
			100	40	56	4	
32	52	1	Total	C	H	O	0
			100	40	56	4	
32	62	1	Total	C	H	O	0
			100	40	56	4	

- Molecule 33 is water.

Mol	Chain	Residues	Atoms		AltConf
33	H	10	Total	O	0
			10	10	
33	H	19	Total	O	0
			19	19	
33	H	1	Total	O	0
			1	1	
33	H	1	Total	O	0
			1	1	
33	H	4	Total	O	0
			4	4	
33	H	1	Total	O	0
			1	1	
33	H	1	Total	O	0
			1	1	
33	H	7	Total	O	0
			7	7	
33	H	6	Total	O	0
			6	6	
33	H	6	Total	O	0
			6	6	
33	H	6	Total	O	0
			6	6	
33	H	5	Total	O	0
			5	5	
33	H	3	Total	O	0
			3	3	
33	H	5	Total	O	0
			5	5	
33	H	5	Total	O	0
			5	5	
33	H	1	Total	O	0
			1	1	

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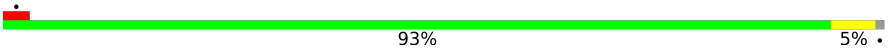
Mol	Chain	Residues	Atoms	AltConf
33	H	11	Total O 11 11	0
33	H	18	Total O 18 18	0
33	H	1	Total O 1 1	0
33	H	1	Total O 1 1	0
33	H	4	Total O 4 4	0
33	H	1	Total O 1 1	0
33	H	1	Total O 1 1	0
33	H	7	Total O 7 7	0
33	H	5	Total O 5 5	0
33	H	6	Total O 6 6	0
33	H	5	Total O 5 5	0
33	H	5	Total O 5 5	0
33	H	3	Total O 3 3	0
33	H	5	Total O 5 5	0
33	H	5	Total O 5 5	0
33	H	1	Total O 1 1	0

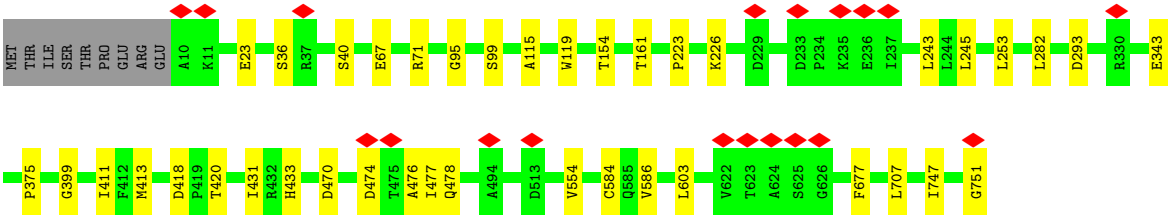
3 Residue-property plots (i)

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

• Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1

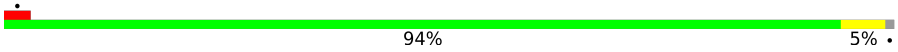
Chain A:

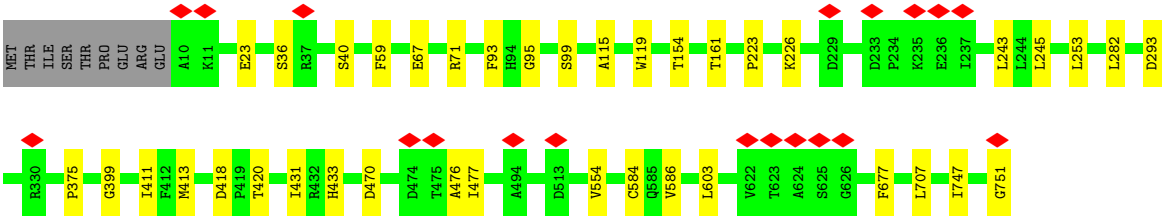




• Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1

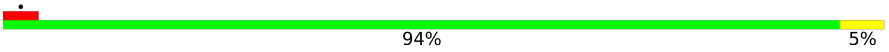
Chain A2:

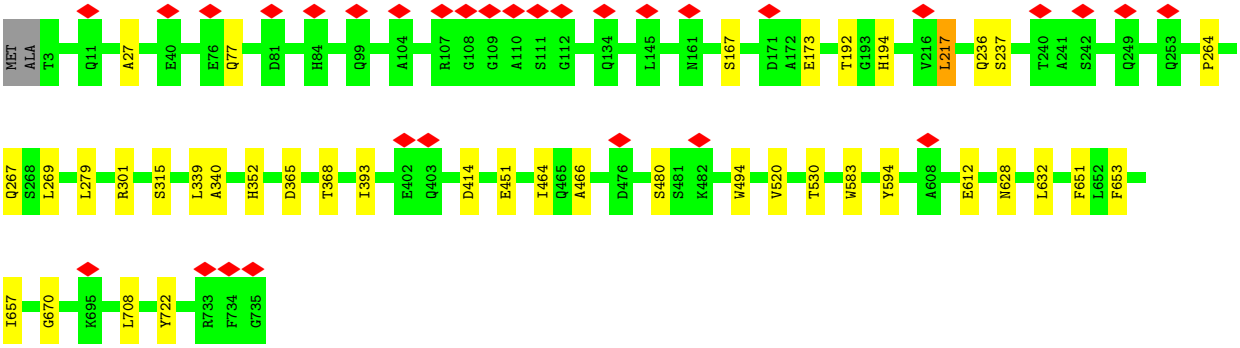




• Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

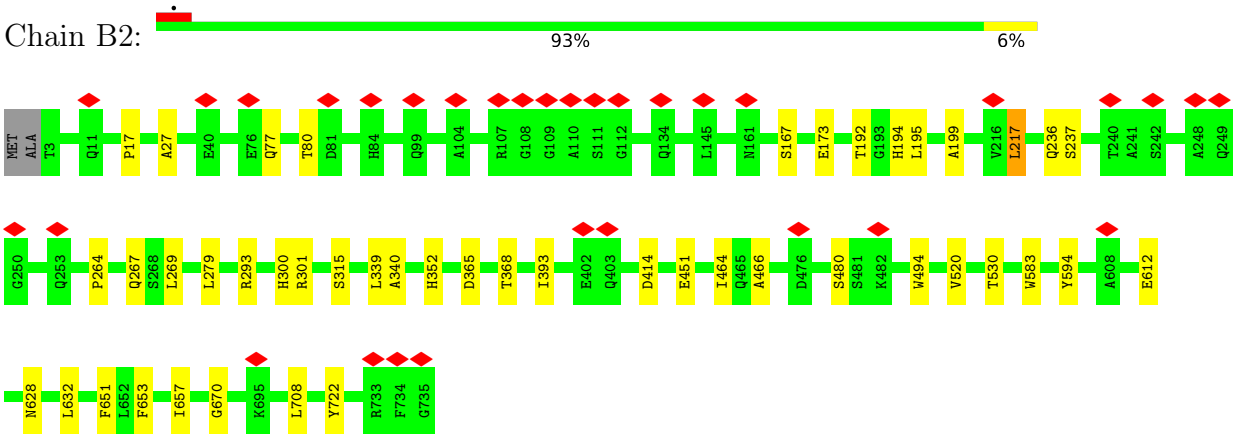
Chain B:





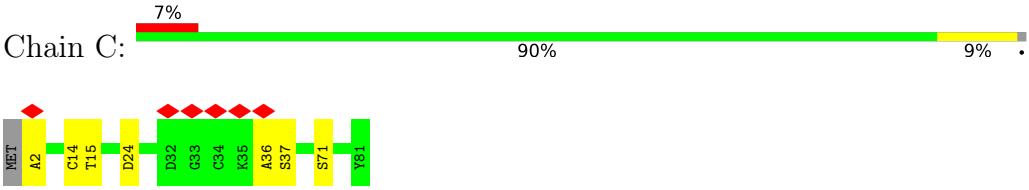
• Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

Chain B2:



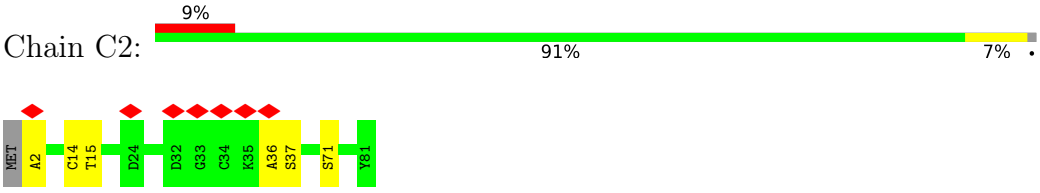
• Molecule 3: Photosystem I iron-sulfur center

Chain C:



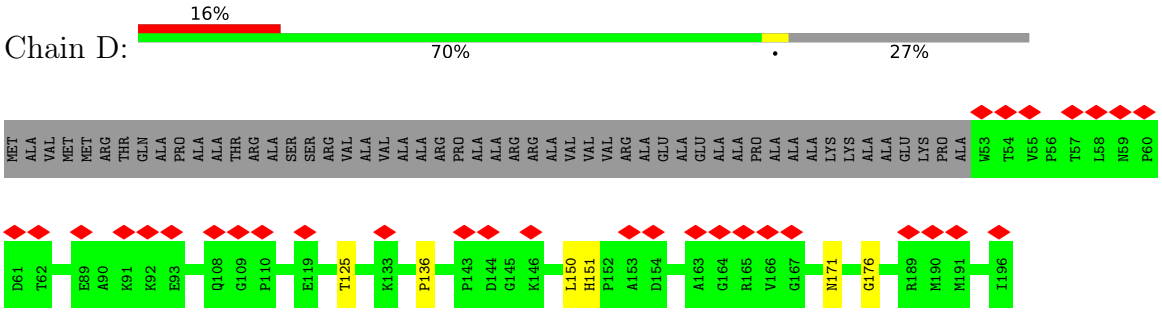
• Molecule 3: Photosystem I iron-sulfur center

Chain C2:



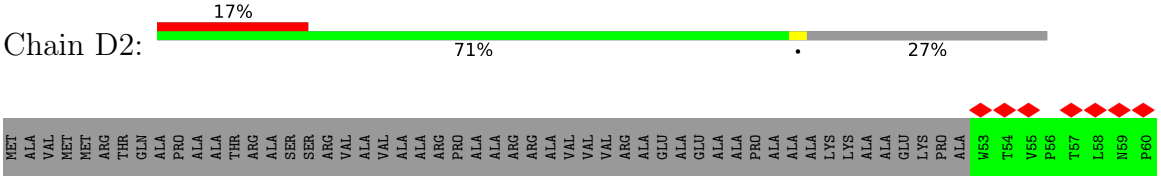
• Molecule 4: Photosystem I reaction center subunit II, chloroplastic

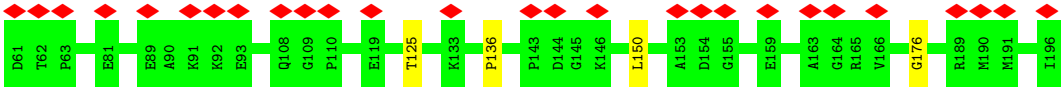
Chain D:



• Molecule 4: Photosystem I reaction center subunit II, chloroplastic

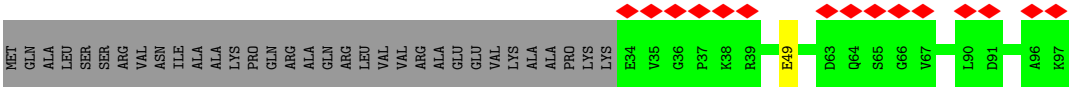
Chain D2:





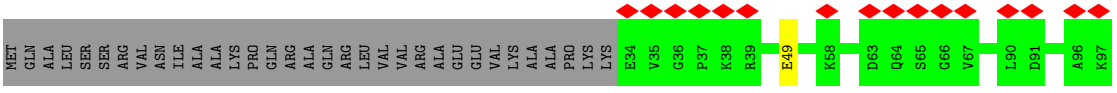
• Molecule 5: Photosystem I reaction center subunit IV, chloroplastic





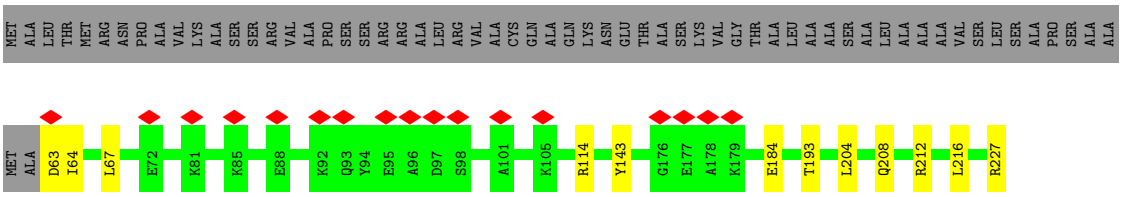
• Molecule 5: Photosystem I reaction center subunit IV, chloroplastic





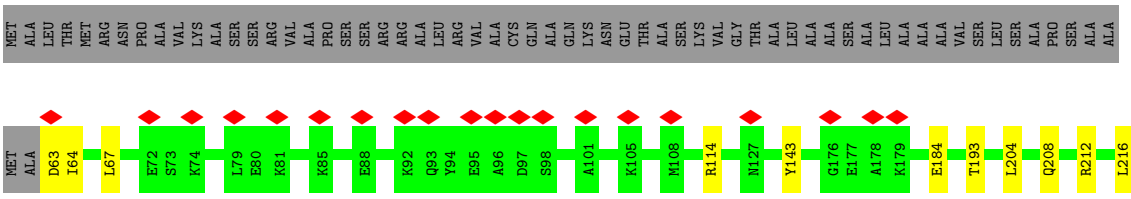
• Molecule 6: Photosystem I reaction center subunit III, chloroplastic





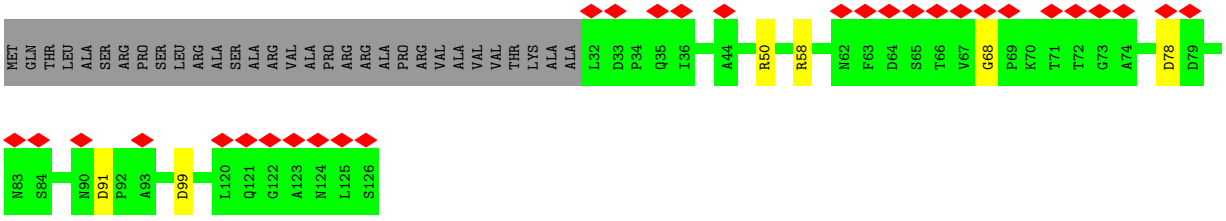
• Molecule 6: Photosystem I reaction center subunit III, chloroplastic





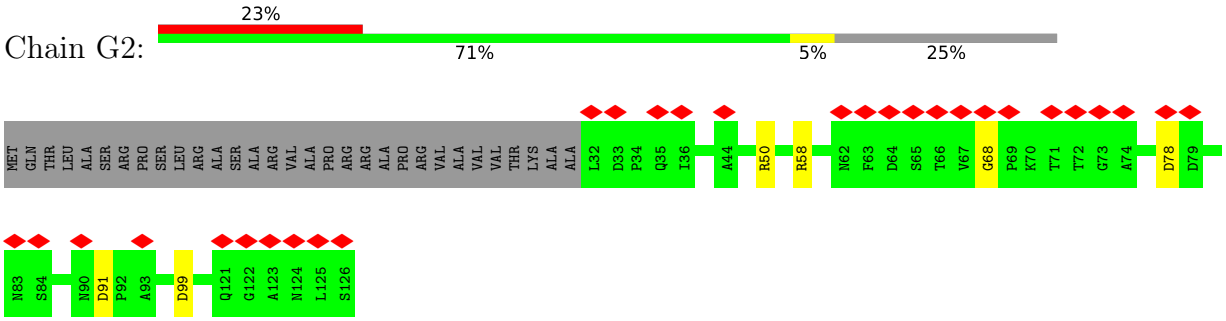
• Molecule 7: Photosystem I reaction center subunit V, chloroplastic





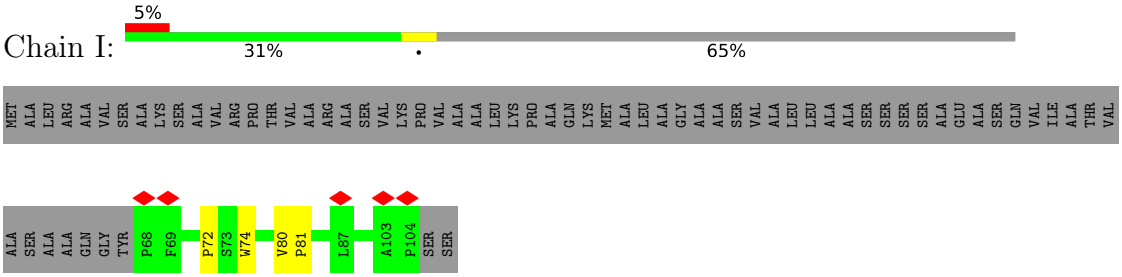
• Molecule 7: Photosystem I reaction center subunit V, chloroplastic

Chain G2:



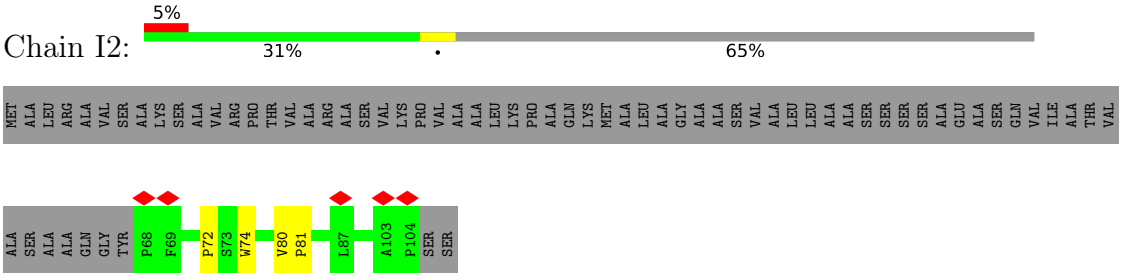
• Molecule 8: Photosystem I reaction center subunit VIII

Chain I:



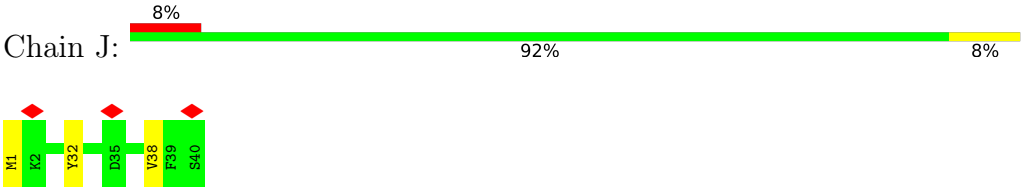
• Molecule 8: Photosystem I reaction center subunit VIII

Chain I2:



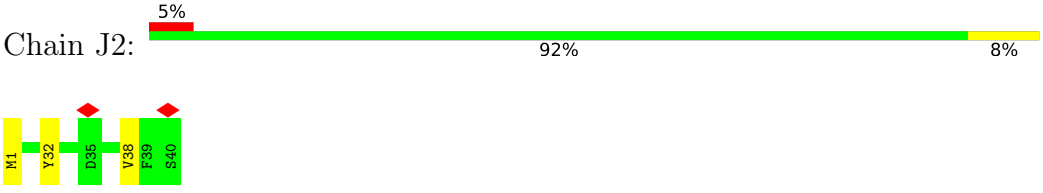
• Molecule 9: Photosystem I reaction center subunit IX

Chain J:



• Molecule 9: Photosystem I reaction center subunit IX

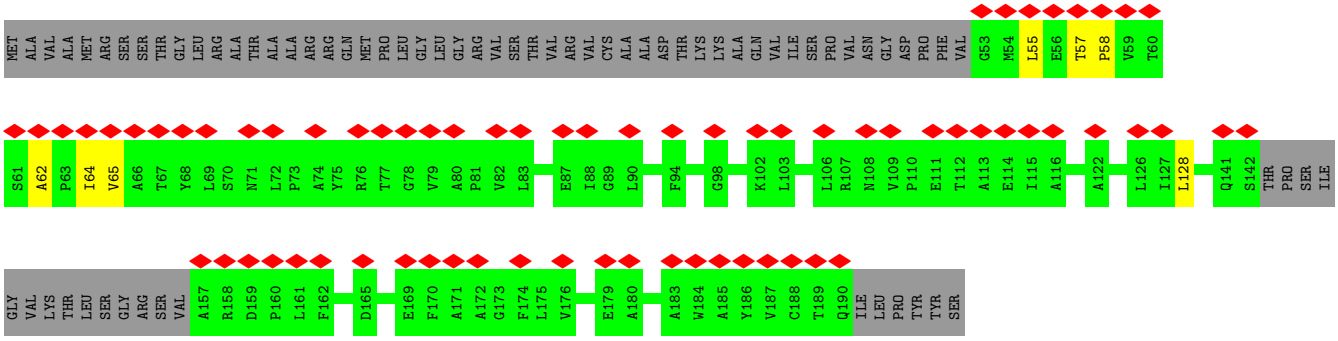
Chain J2:



• Molecule 10: PSI subunit V

Chain L:

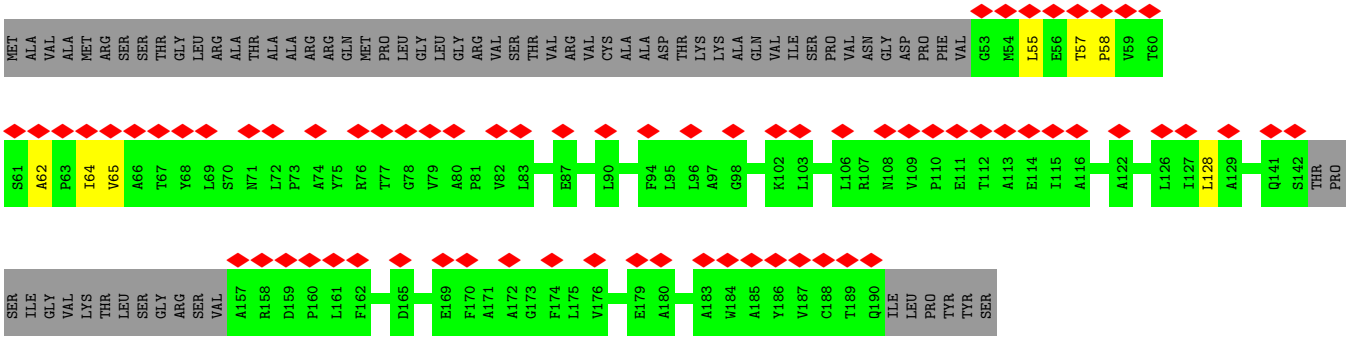




• Molecule 10: PSI subunit V

Chain L2:

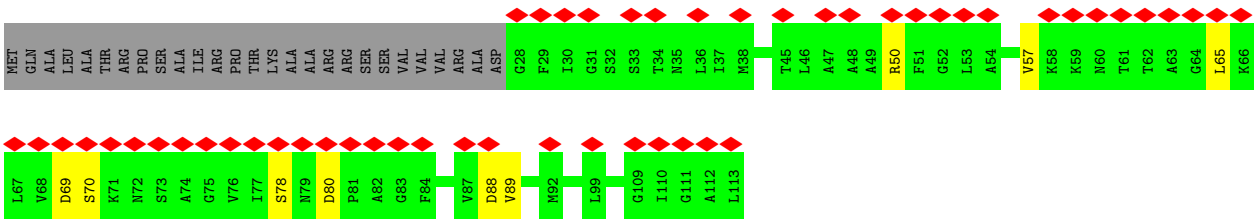




• Molecule 11: Photosystem I reaction center subunit psaK, chloroplastic

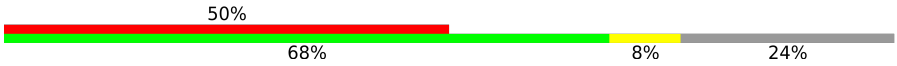
Chain K:

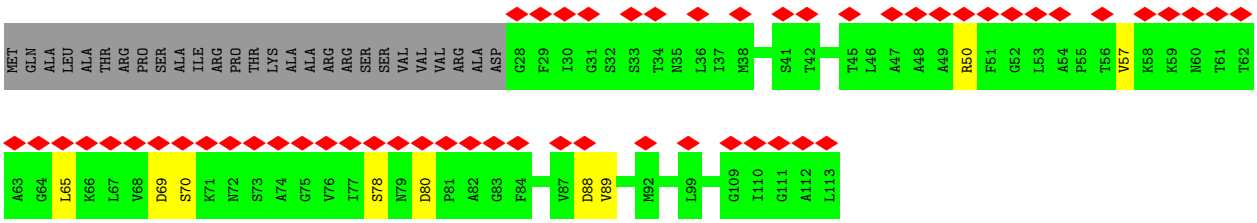




• Molecule 11: Photosystem I reaction center subunit psaK, chloroplastic

Chain K2:

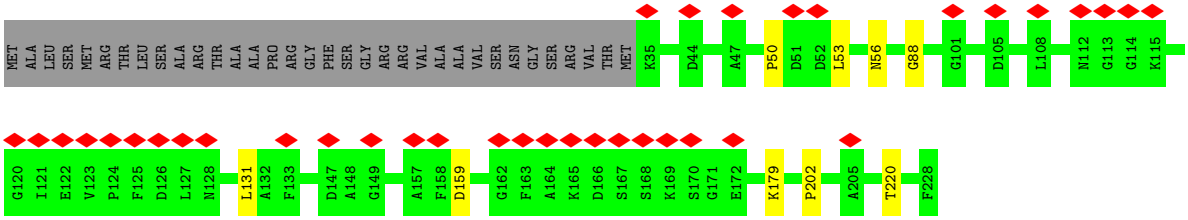




• Molecule 12: Chlorophyll a-b binding protein, chloroplastic

Chain 1:

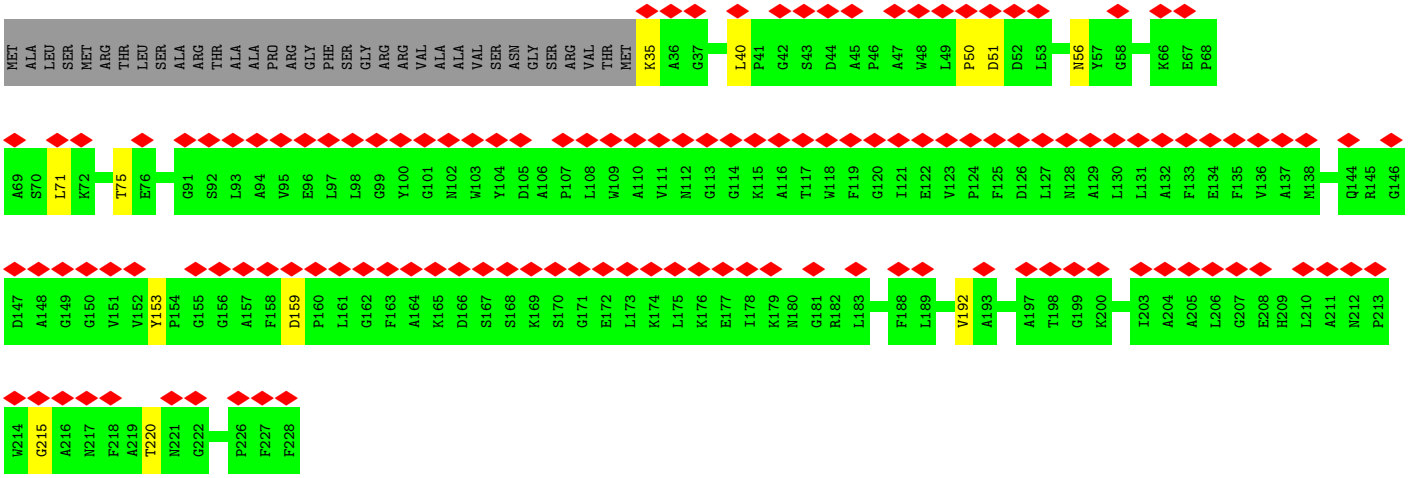




• Molecule 12: Chlorophyll a-b binding protein, chloroplastic

Chain Z:

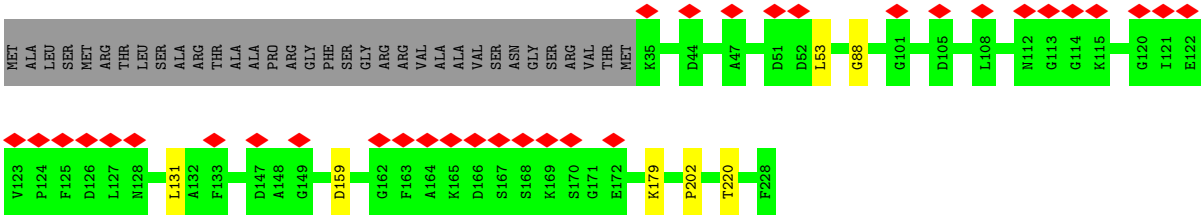




• Molecule 12: Chlorophyll a-b binding protein, chloroplastic

Chain 12:

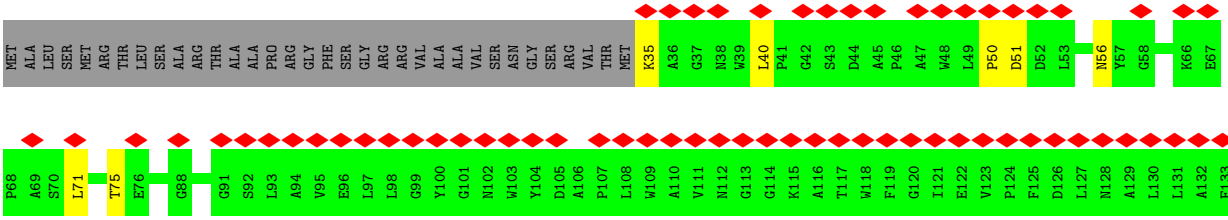




• Molecule 12: Chlorophyll a-b binding protein, chloroplastic

Chain Z2:

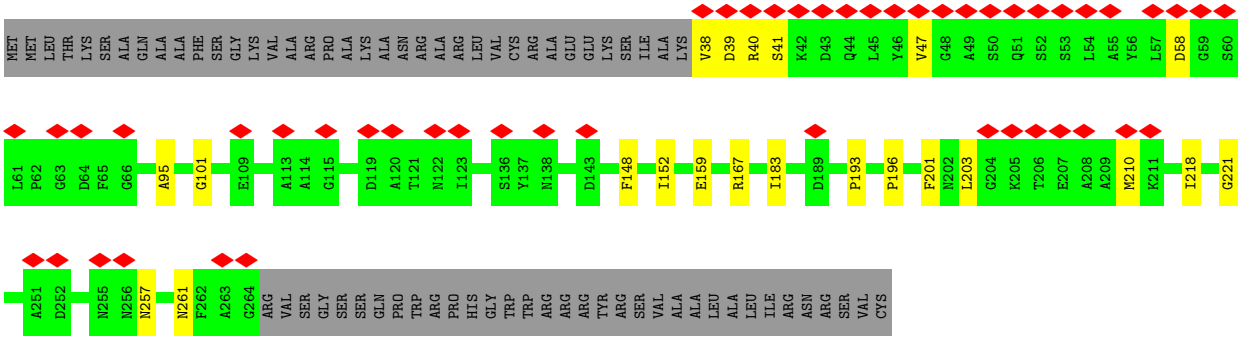






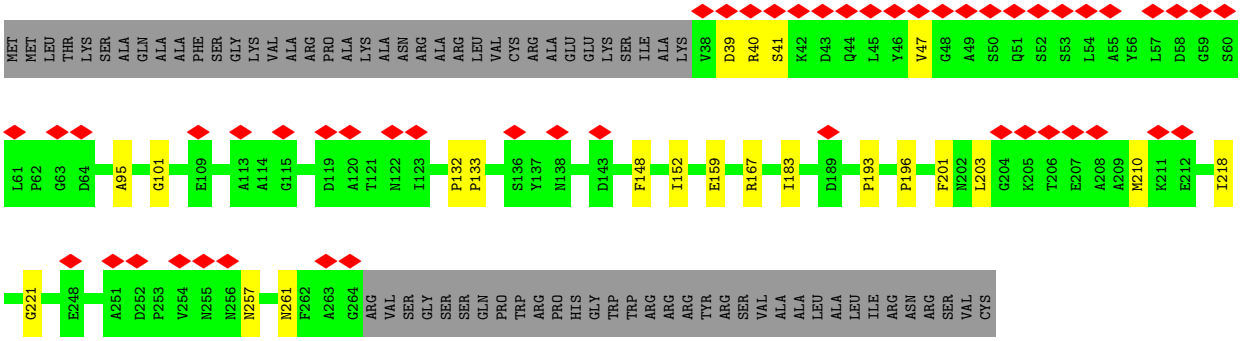
• Molecule 13: Chlorophyll a-b binding protein, chloroplastic



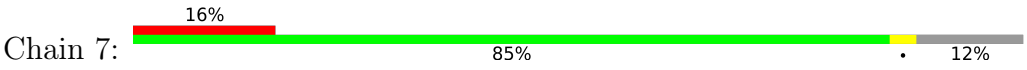


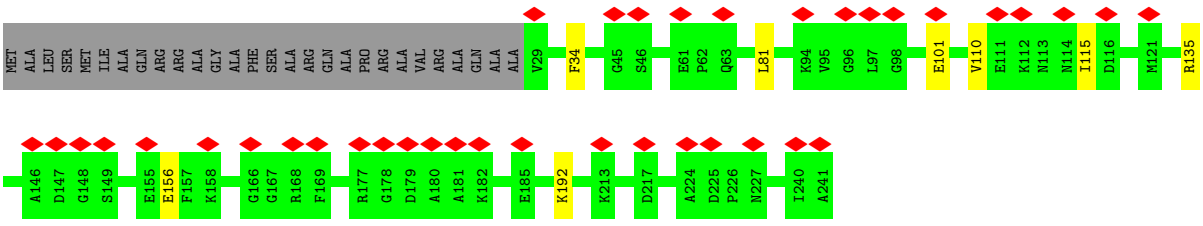
• Molecule 13: Chlorophyll a-b binding protein, chloroplastic





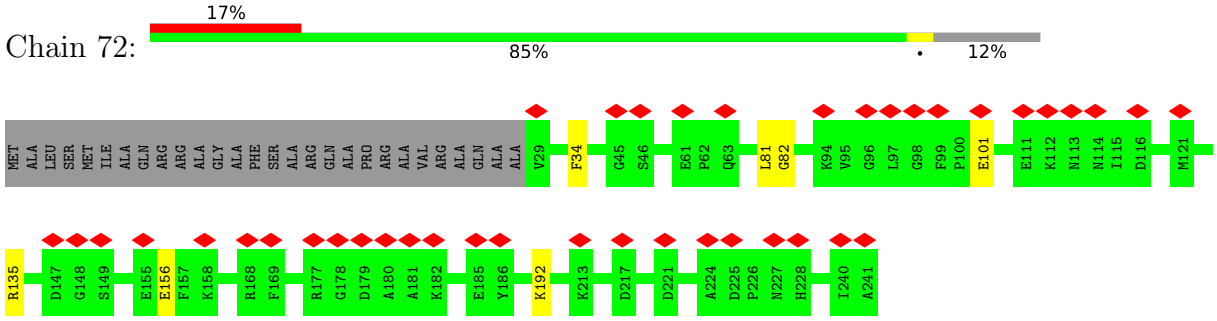
• Molecule 14: Chlorophyll a-b binding protein, chloroplastic





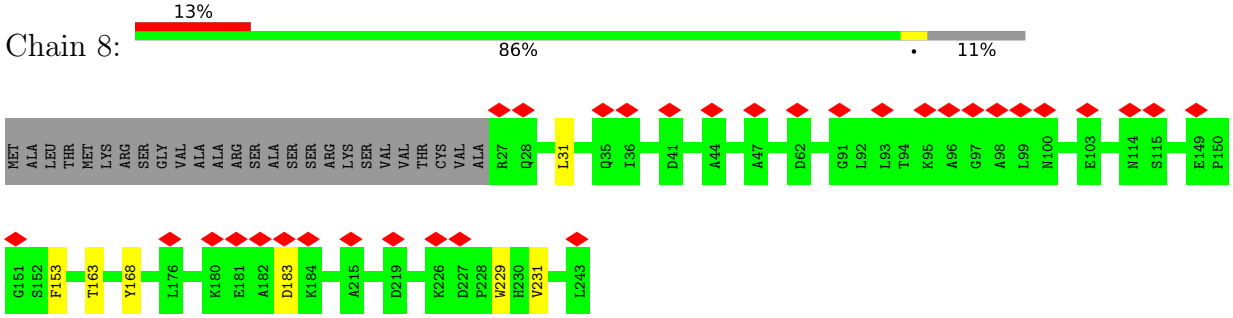
• Molecule 14: Chlorophyll a-b binding protein, chloroplastic

Chain 72:



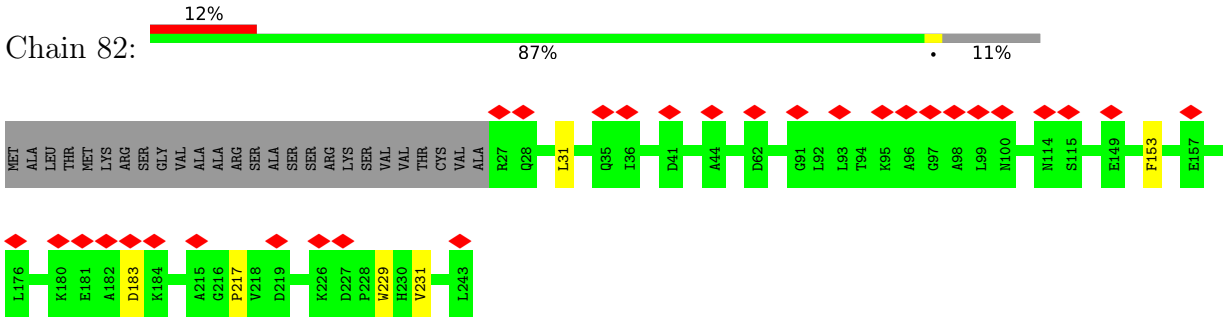
• Molecule 15: Chlorophyll a-b binding protein, chloroplastic

Chain 8:



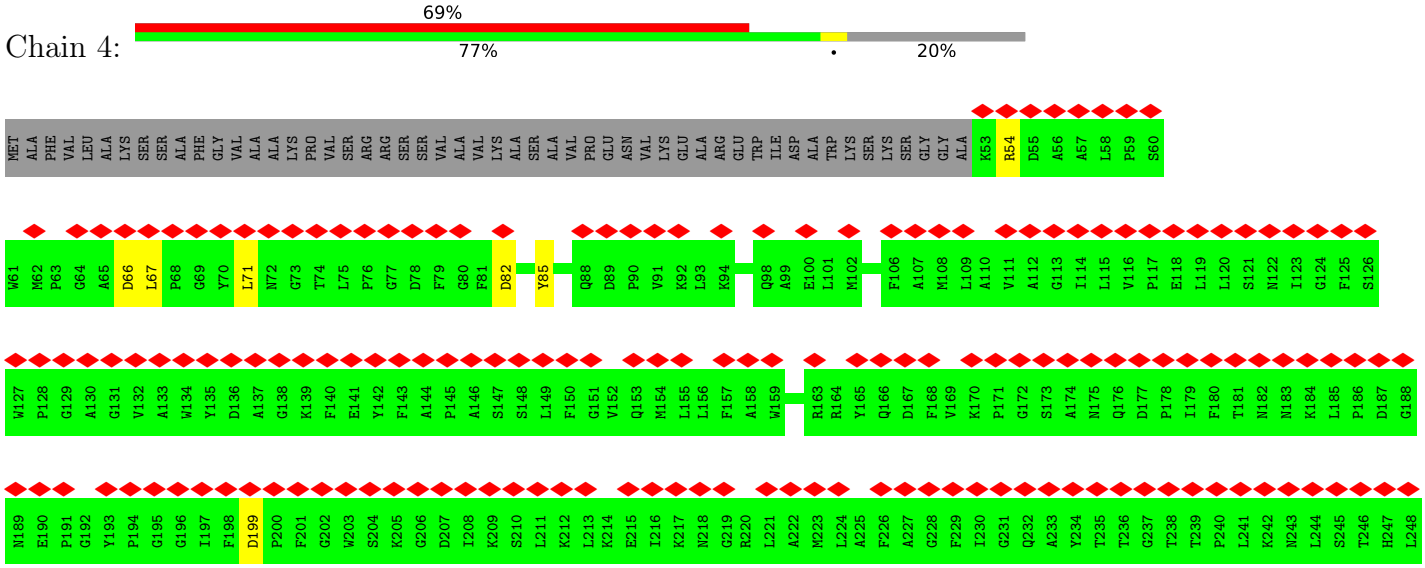
• Molecule 15: Chlorophyll a-b binding protein, chloroplastic

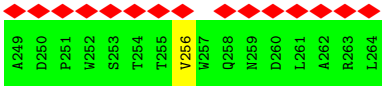
Chain 82:



• Molecule 16: Chlorophyll a-b binding protein, chloroplastic (Lhca4)

Chain 4:

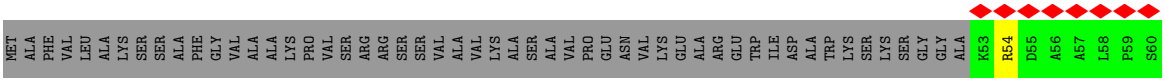


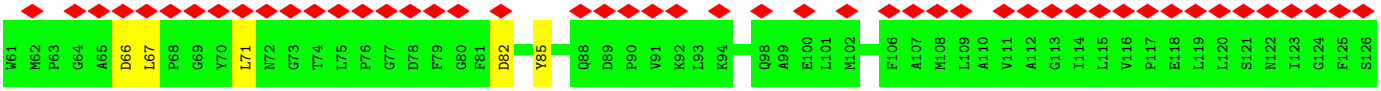


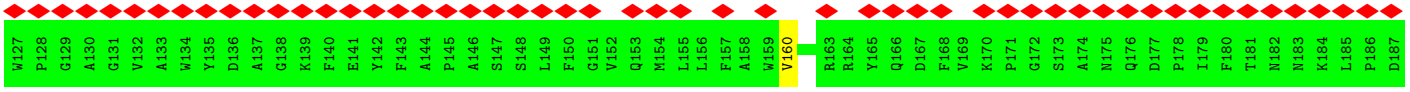
• Molecule 16: Chlorophyll a-b binding protein, chloroplastic (Lhca4)

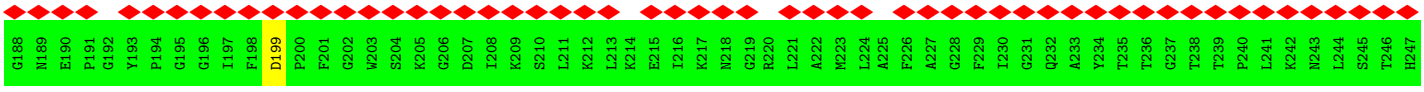
Chain 42:

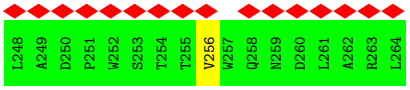








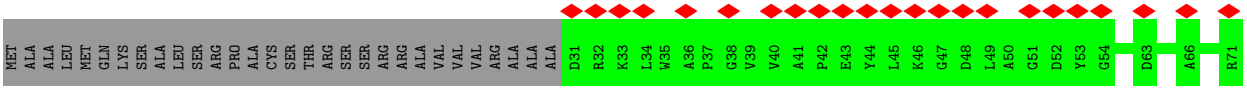


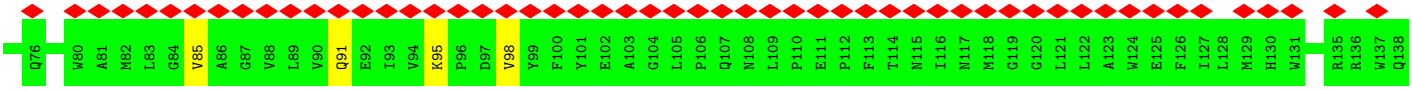


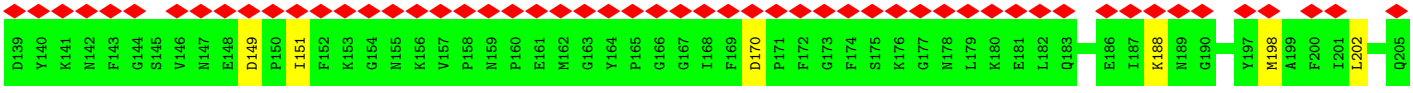
• Molecule 17: Chlorophyll a-b binding protein, chloroplastic

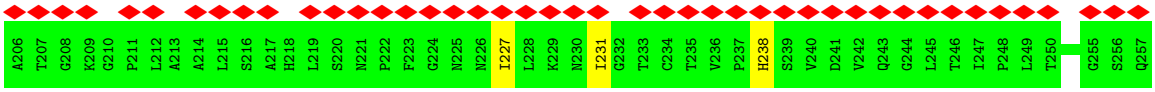
Chain 5:







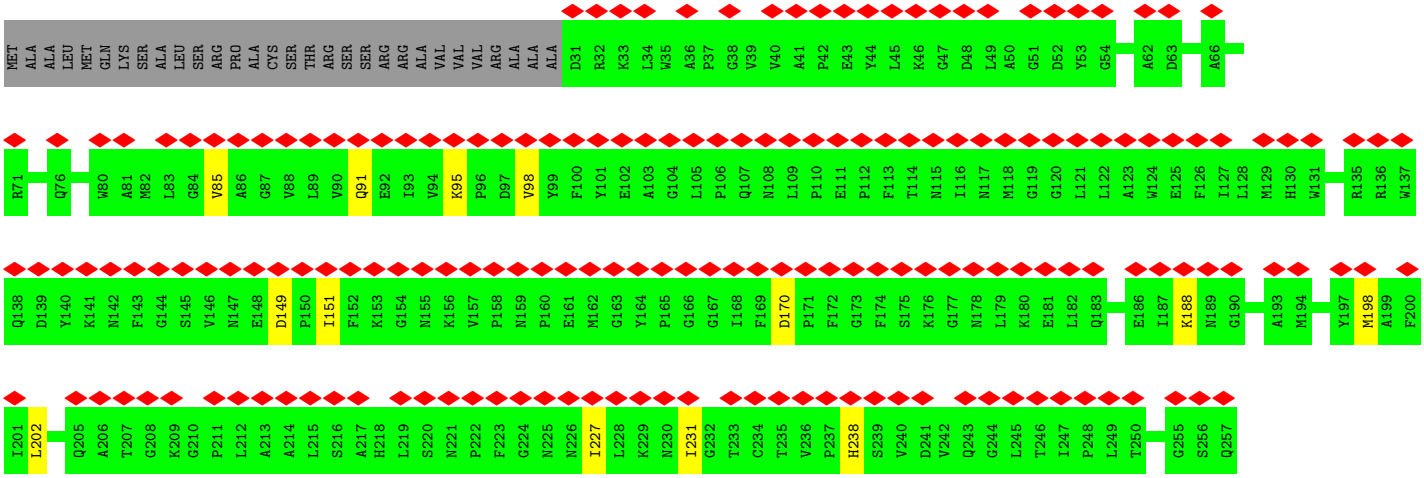




• Molecule 17: Chlorophyll a-b binding protein, chloroplastic

Chain 52:

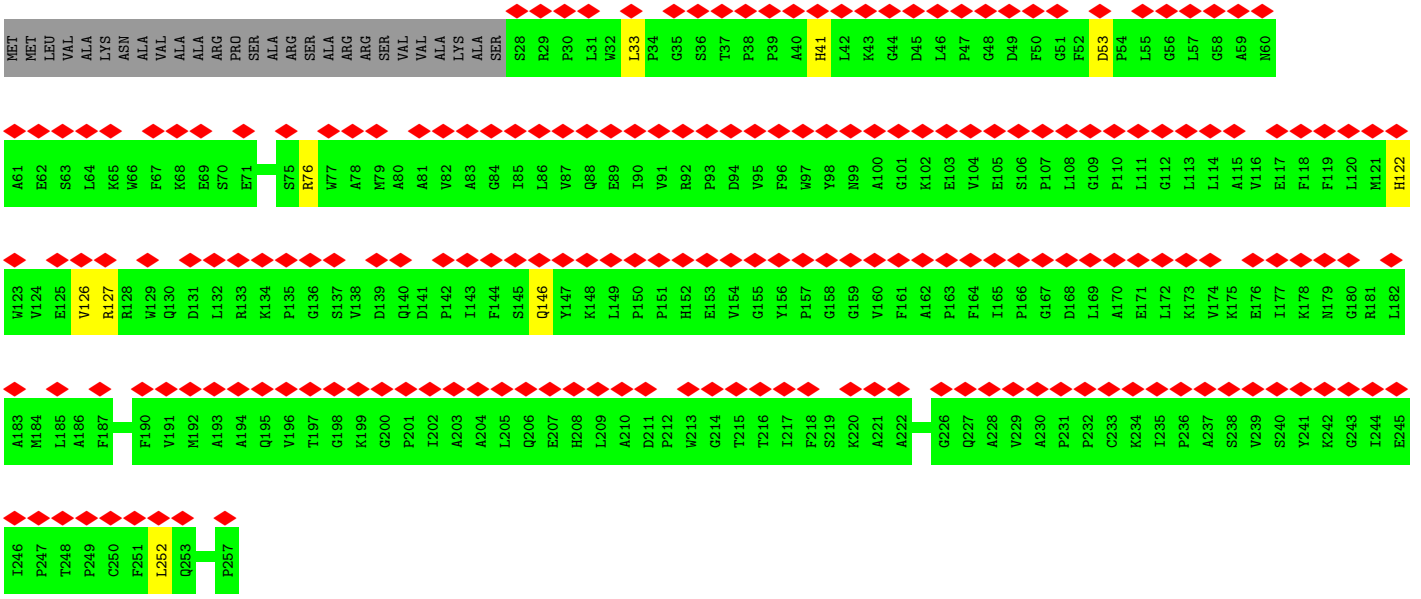




• Molecule 18: Chlorophyll a-b binding protein, chloroplastic

Chain 6:

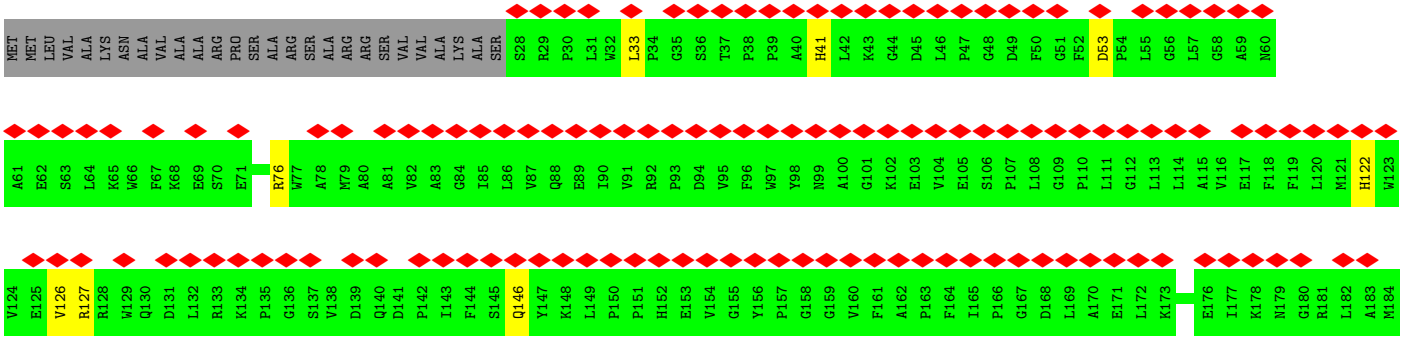




• Molecule 18: Chlorophyll a-b binding protein, chloroplastic

Chain 62:



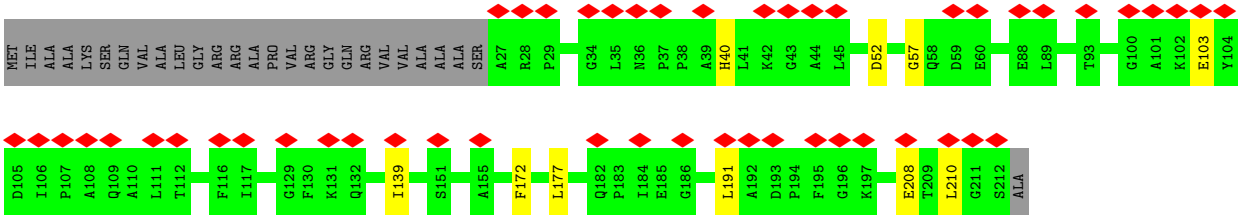




• Molecule 19: Chlorophyll a-b binding protein, chloroplastic

Chain 9:

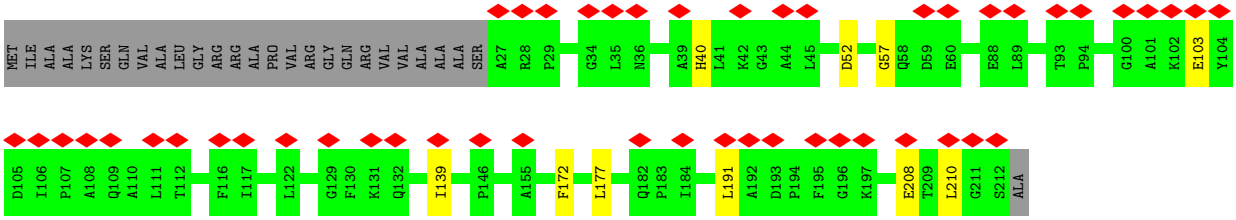




• Molecule 19: Chlorophyll a-b binding protein, chloroplastic

Chain 92:





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	17439	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	45.8	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	5000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.183	Depositor
Minimum map value	-0.090	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.036	Depositor
Map size (Å)	588.0, 588.0, 588.0	wwPDB
Map dimensions	700, 700, 700	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.84, 0.84, 0.84	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: NEX, DGD, CL0, CHL, LMG, LHG, LUT, XAT, PQN, SF4, AME, BCR, LMU, CLA

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.14	0/6021	0.22	0/8208
1	A2	0.15	0/6021	0.23	0/8208
2	B	0.15	0/6036	0.23	0/8240
2	B2	0.15	0/6036	0.22	0/8240
3	C	0.14	0/611	0.28	0/826
3	C2	0.14	0/611	0.27	0/826
4	D	0.13	0/1161	0.24	0/1567
4	D2	0.13	0/1161	0.24	0/1567
5	E	0.13	0/516	0.18	0/700
5	E2	0.13	0/516	0.18	0/700
6	F	0.13	0/1292	0.21	0/1747
6	F2	0.13	0/1292	0.21	0/1747
7	G	0.12	0/721	0.19	0/980
7	G2	0.12	0/721	0.19	0/980
8	I	0.13	0/293	0.26	0/406
8	I2	0.13	0/293	0.26	0/406
9	J	0.14	0/329	0.22	0/452
9	J2	0.14	0/329	0.22	0/452
10	L	0.12	0/920	0.19	0/1257
10	L2	0.12	0/920	0.19	0/1257
11	K	0.13	0/588	0.17	0/795
11	K2	0.13	0/588	0.17	0/795
12	1	0.12	0/1491	0.20	0/2028
12	12	0.12	0/1491	0.20	0/2028
12	Z	0.09	0/1491	0.18	0/2028
12	Z2	0.10	0/1491	0.18	0/2028
13	3	0.12	0/1784	0.23	0/2420
13	32	0.12	0/1784	0.23	0/2420
14	7	0.12	0/1702	0.20	0/2310
14	72	0.12	0/1702	0.20	0/2310
15	8	0.12	0/1701	0.21	0/2315
15	82	0.12	0/1701	0.20	0/2315

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
16	4	0.09	0/1703	0.19	0/2321
16	42	0.09	0/1703	0.19	0/2321
17	5	0.09	0/1830	0.21	0/2492
17	52	0.09	0/1830	0.21	0/2492
18	6	0.09	0/1834	0.20	0/2505
18	62	0.09	0/1834	0.20	0/2505
19	9	0.12	0/1461	0.20	0/1987
19	92	0.12	0/1461	0.21	0/1987
All	All	0.13	0/66970	0.21	0/91168

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5825	5675	5675	27	0
1	A2	5825	5675	5675	25	0
2	B	5824	5576	5577	35	0
2	B2	5824	5576	5577	38	0
3	C	601	582	581	4	0
3	C2	601	582	581	3	0
4	D	1133	1151	1150	4	0
4	D2	1133	1151	1150	2	0
5	E	506	505	504	1	0
5	E2	506	505	504	1	0
6	F	1266	1302	1301	10	0
6	F2	1266	1302	1301	9	0
7	G	706	687	686	4	0
7	G2	706	687	686	4	0
8	I	281	292	292	3	0
8	I2	281	292	292	3	0
9	J	329	328	328	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	J2	329	328	328	1	0
10	L	899	907	905	7	0
10	L2	899	907	905	8	0
11	K	583	620	620	6	0
11	K2	583	620	620	6	0
12	1	1445	1397	1396	8	0
12	12	1445	1397	1396	7	0
12	Z	1445	1397	1396	9	0
12	Z2	1445	1397	1396	9	0
13	3	1736	1695	1694	15	0
13	32	1736	1695	1694	15	0
14	7	1650	1590	1589	8	0
14	72	1650	1590	1589	8	0
15	8	1650	1630	1629	6	0
15	82	1650	1630	1629	6	0
16	4	1648	1603	1602	6	0
16	42	1648	1603	1602	7	0
17	5	1775	1747	1746	11	0
17	52	1775	1747	1746	11	0
18	6	1772	1770	1770	9	0
18	62	1772	1770	1770	9	0
19	9	1420	1400	1399	9	0
19	92	1420	1400	1399	9	0
20	A	65	72	72	0	0
20	A2	65	72	72	0	0
21	1	639	625	625	5	0
21	12	639	625	625	5	0
21	3	740	718	718	12	0
21	32	740	718	718	14	0
21	4	565	534	534	3	0
21	42	565	534	534	4	0
21	5	740	712	712	9	0
21	52	740	712	712	9	0
21	6	628	605	605	2	0
21	62	628	605	605	2	0
21	7	652	598	598	5	0
21	72	652	598	598	5	0
21	8	614	578	578	4	0
21	82	614	578	578	3	0
21	9	565	535	535	1	0
21	92	565	535	535	1	0
21	A	2718	2856	2856	26	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
21	A2	2718	2856	2856	26	0
21	B	2463	2580	2580	28	0
21	B2	2463	2580	2580	29	0
21	F	175	177	177	1	0
21	F2	175	177	177	1	0
21	G	106	92	92	0	0
21	G2	106	92	92	0	0
21	J	55	49	49	1	0
21	J2	55	49	49	1	0
21	K	196	158	158	2	0
21	K2	196	158	158	2	0
21	L	110	105	105	1	0
21	L2	110	105	105	0	0
21	Z	627	593	593	7	0
21	Z2	627	593	593	9	0
22	A	33	46	46	0	0
22	A2	33	46	46	0	0
22	B	33	46	46	0	0
22	B2	33	46	46	0	0
23	1	39	48	48	1	0
23	12	39	48	48	1	0
23	3	78	99	99	1	0
23	32	78	99	99	1	0
23	4	87	123	123	1	0
23	42	87	123	123	1	0
23	5	37	44	44	1	0
23	52	37	44	44	1	0
23	6	85	116	116	0	0
23	62	85	116	116	0	0
23	7	49	74	74	1	0
23	72	49	74	74	1	0
23	8	44	61	61	0	0
23	82	44	61	61	0	0
23	9	41	55	55	0	0
23	92	41	55	55	0	0
23	A	87	123	123	0	0
23	A2	87	123	123	0	0
23	B	45	63	63	0	0
23	B2	45	63	63	0	0
23	Z	39	48	48	0	0
23	Z2	39	48	48	1	0
24	3	120	168	168	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
24	32	120	168	168	4	0
24	4	40	56	56	0	0
24	42	40	56	56	1	0
24	5	40	56	56	0	0
24	52	40	56	56	0	0
24	6	40	56	56	2	0
24	62	40	56	56	1	0
24	7	40	56	56	0	0
24	72	40	56	56	0	0
24	8	40	56	56	2	0
24	82	40	56	56	2	0
24	9	40	56	56	1	0
24	92	40	56	56	2	0
24	A	200	280	280	12	0
24	A2	200	280	280	9	0
24	B	280	392	392	11	0
24	B2	280	392	392	11	0
24	G	40	56	56	0	0
24	G2	40	56	56	2	0
24	I	40	56	56	1	0
24	I2	40	56	56	1	0
24	J	40	56	56	1	0
24	J2	40	56	56	1	0
24	K	80	112	112	5	0
24	K2	80	112	112	6	0
24	L	80	112	112	5	0
24	L2	80	112	112	5	0
25	A	8	0	0	0	0
25	A2	8	0	0	0	0
25	C	16	0	0	0	0
25	C2	16	0	0	0	0
26	1	148	201	201	0	0
26	12	148	201	201	0	0
26	4	53	63	63	1	0
26	42	53	63	63	1	0
26	5	24	35	35	0	0
26	52	24	35	35	0	0
26	6	92	129	129	0	0
26	62	92	129	129	0	0
26	7	81	92	92	1	0
26	72	81	92	92	1	0
26	8	107	151	151	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
26	82	107	151	151	0	0
26	9	24	35	35	1	0
26	92	24	35	35	1	0
26	A	196	262	262	5	0
26	A2	196	262	262	2	0
26	B	35	46	46	3	0
26	B2	35	46	46	2	0
26	G	24	35	35	0	0
26	G2	24	35	35	0	0
26	K	24	35	35	0	0
26	K2	24	35	35	0	0
26	Z	53	63	63	1	0
26	Z2	53	63	63	1	0
27	1	78	96	96	0	0
27	12	78	96	96	0	0
27	3	45	75	75	1	0
27	32	45	75	75	1	0
27	4	41	55	55	0	0
27	42	41	55	55	0	0
27	6	20	35	35	0	0
27	62	20	35	35	0	0
27	7	37	44	44	0	0
27	72	37	44	44	0	0
27	8	74	91	91	1	0
27	82	74	91	91	0	0
27	9	44	61	61	1	0
27	92	44	61	61	1	0
27	A	84	111	111	1	0
27	A2	84	111	111	1	0
27	B	79	98	98	1	0
27	B2	79	98	98	1	0
27	J	77	97	97	2	0
27	J2	77	97	97	2	0
28	1	84	112	112	2	0
28	12	84	112	112	2	0
28	3	126	168	168	2	0
28	32	126	168	168	2	0
28	4	42	56	56	1	0
28	42	42	56	56	1	0
28	5	84	112	112	3	0
28	52	84	112	112	3	0
28	6	42	56	56	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
28	62	42	56	56	1	0
28	7	84	112	112	4	0
28	72	84	112	112	4	0
28	8	42	56	56	0	0
28	82	42	56	56	1	0
28	9	84	112	112	3	0
28	92	84	112	112	3	0
28	A	42	56	56	1	0
28	A2	42	56	56	2	0
28	F	42	56	56	3	0
28	F2	42	56	56	2	0
28	Z	68	89	89	2	0
28	Z2	68	89	89	2	0
29	B	59	79	79	1	0
29	B2	59	79	79	1	0
30	1	158	132	132	1	0
30	12	158	132	132	0	0
30	3	66	70	70	2	0
30	32	66	70	70	3	0
30	4	300	288	288	4	0
30	42	300	288	288	2	0
30	5	206	167	167	1	0
30	52	206	167	167	1	0
30	6	350	327	327	7	0
30	62	350	327	327	7	0
30	7	158	132	132	3	0
30	72	158	132	132	2	0
30	8	198	210	210	2	0
30	82	198	210	210	2	0
30	9	93	64	64	0	0
30	92	93	64	64	0	0
30	Z	178	171	171	1	0
30	Z2	178	171	171	1	0
31	1	44	56	56	1	0
31	12	44	56	56	1	0
31	4	44	56	56	0	0
31	42	44	56	56	0	0
31	5	44	56	56	0	0
31	52	44	56	56	0	0
31	6	44	56	56	1	0
31	62	44	56	56	1	0
31	7	44	56	56	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
31	72	44	56	56	1	0
31	8	44	56	56	0	0
31	82	44	56	56	0	0
31	Z	44	56	56	0	0
31	Z2	44	56	56	0	0
32	5	44	56	56	0	0
32	52	44	56	56	0	0
32	6	44	56	56	1	0
32	62	44	56	56	1	0
33	H	160	0	0	17	0
All	All	100830	101988	101960	579	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 3.

The worst 5 of 579 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)
28:7:624:LUT:H381	28:7:624:LUT:H28	1.51	0.93
28:72:624:LUT:H381	28:72:624:LUT:H28	1.51	0.91
1:A2:95:GLY:O	1:A2:99:SER:OG	1.95	0.83
17:5:170:ASP:OD1	28:5:620:LUT:O23	1.96	0.82
1:A:95:GLY:O	1:A:99:SER:OG	1.96	0.82

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	740/751 (98%)	727 (98%)	13 (2%)	0	100	100
1	A2	740/751 (98%)	727 (98%)	13 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	731/735 (100%)	718 (98%)	13 (2%)	0	100	100
2	B2	731/735 (100%)	718 (98%)	13 (2%)	0	100	100
3	C	78/81 (96%)	76 (97%)	2 (3%)	0	100	100
3	C2	78/81 (96%)	76 (97%)	2 (3%)	0	100	100
4	D	142/196 (72%)	139 (98%)	3 (2%)	0	100	100
4	D2	142/196 (72%)	139 (98%)	3 (2%)	0	100	100
5	E	62/97 (64%)	62 (100%)	0	0	100	100
5	E2	62/97 (64%)	62 (100%)	0	0	100	100
6	F	163/227 (72%)	163 (100%)	0	0	100	100
6	F2	163/227 (72%)	162 (99%)	1 (1%)	0	100	100
7	G	93/126 (74%)	92 (99%)	1 (1%)	0	100	100
7	G2	93/126 (74%)	92 (99%)	1 (1%)	0	100	100
8	I	35/106 (33%)	35 (100%)	0	0	100	100
8	I2	35/106 (33%)	35 (100%)	0	0	100	100
9	J	38/40 (95%)	37 (97%)	1 (3%)	0	100	100
9	J2	38/40 (95%)	37 (97%)	1 (3%)	0	100	100
10	L	120/196 (61%)	118 (98%)	2 (2%)	0	100	100
10	L2	120/196 (61%)	118 (98%)	2 (2%)	0	100	100
11	K	84/113 (74%)	82 (98%)	2 (2%)	0	100	100
11	K2	84/113 (74%)	82 (98%)	2 (2%)	0	100	100
12	1	192/228 (84%)	192 (100%)	0	0	100	100
12	12	192/228 (84%)	192 (100%)	0	0	100	100
12	Z	192/228 (84%)	190 (99%)	2 (1%)	0	100	100
12	Z2	192/228 (84%)	190 (99%)	2 (1%)	0	100	100
13	3	225/298 (76%)	218 (97%)	7 (3%)	0	100	100
13	32	225/298 (76%)	218 (97%)	7 (3%)	0	100	100
14	7	211/241 (88%)	210 (100%)	1 (0%)	0	100	100
14	72	211/241 (88%)	210 (100%)	1 (0%)	0	100	100
15	8	215/243 (88%)	212 (99%)	3 (1%)	0	100	100
15	82	215/243 (88%)	212 (99%)	3 (1%)	0	100	100
16	4	210/264 (80%)	207 (99%)	3 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
16	42	210/264 (80%)	207 (99%)	3 (1%)	0	100	100
17	5	225/257 (88%)	220 (98%)	5 (2%)	0	100	100
17	52	225/257 (88%)	220 (98%)	5 (2%)	0	100	100
18	6	228/257 (89%)	225 (99%)	3 (1%)	0	100	100
18	62	228/257 (89%)	225 (99%)	3 (1%)	0	100	100
19	9	184/213 (86%)	179 (97%)	4 (2%)	1 (0%)	24	58
19	92	184/213 (86%)	179 (97%)	4 (2%)	1 (0%)	24	58
All	All	8336/9794 (85%)	8203 (98%)	131 (2%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
19	9	139	ILE
19	92	139	ILE

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	601/610 (98%)	599 (100%)	2 (0%)	86	91
1	A2	601/610 (98%)	598 (100%)	3 (0%)	81	89
2	B	596/597 (100%)	594 (100%)	2 (0%)	86	91
2	B2	596/597 (100%)	593 (100%)	3 (0%)	81	89
3	C	69/70 (99%)	69 (100%)	0	100	100
3	C2	69/70 (99%)	69 (100%)	0	100	100
4	D	121/152 (80%)	120 (99%)	1 (1%)	73	86
4	D2	121/152 (80%)	120 (99%)	1 (1%)	73	86
5	E	55/81 (68%)	55 (100%)	0	100	100
5	E2	55/81 (68%)	55 (100%)	0	100	100
6	F	127/169 (75%)	127 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	F2	127/169 (75%)	127 (100%)	0	100	100
7	G	71/94 (76%)	71 (100%)	0	100	100
7	G2	71/94 (76%)	71 (100%)	0	100	100
8	I	31/76 (41%)	31 (100%)	0	100	100
8	I2	31/76 (41%)	31 (100%)	0	100	100
9	J	35/35 (100%)	34 (97%)	1 (3%)	37	68
9	J2	35/35 (100%)	34 (97%)	1 (3%)	37	68
10	L	90/148 (61%)	89 (99%)	1 (1%)	65	82
10	L2	90/148 (61%)	89 (99%)	1 (1%)	65	82
11	K	59/80 (74%)	59 (100%)	0	100	100
11	K2	59/80 (74%)	59 (100%)	0	100	100
12	1	137/162 (85%)	137 (100%)	0	100	100
12	12	137/162 (85%)	137 (100%)	0	100	100
12	Z	137/162 (85%)	137 (100%)	0	100	100
12	Z2	137/162 (85%)	137 (100%)	0	100	100
13	3	174/230 (76%)	172 (99%)	2 (1%)	65	82
13	32	174/230 (76%)	173 (99%)	1 (1%)	78	88
14	7	164/181 (91%)	164 (100%)	0	100	100
14	72	164/181 (91%)	164 (100%)	0	100	100
15	8	163/183 (89%)	162 (99%)	1 (1%)	78	88
15	82	163/183 (89%)	162 (99%)	1 (1%)	78	88
16	4	166/205 (81%)	166 (100%)	0	100	100
16	42	166/205 (81%)	166 (100%)	0	100	100
17	5	184/206 (89%)	181 (98%)	3 (2%)	55	78
17	52	184/206 (89%)	181 (98%)	3 (2%)	55	78
18	6	184/203 (91%)	184 (100%)	0	100	100
18	62	184/203 (91%)	184 (100%)	0	100	100
19	9	142/159 (89%)	142 (100%)	0	100	100
19	92	142/159 (89%)	142 (100%)	0	100	100
All	All	6612/7606 (87%)	6585 (100%)	27 (0%)	81	90

5 of 27 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A2	154	THR
2	B2	217	LEU
17	52	91	GLN
2	B2	17	PRO
2	B2	612	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 35 such sidechains are listed below:

Mol	Chain	Res	Type
12	12	195	HIS
15	82	220	ASN
17	52	72	GLN
16	4	166	GLN
12	Z	194	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues 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	$\#\|Z\| > 2$
9	AME	J	1	9	9,10,11	0.50	0	9,11,13	0.89	1 (11%)
9	AME	J2	1	9	9,10,11	0.51	0	9,11,13	0.89	1 (11%)

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
9	AME	J	1	9	-	2/9/10/12	-
9	AME	J2	1	9	-	2/9/10/12	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	J2	1	AME	O-C-CA	-2.52	118.17	124.78
9	J	1	AME	O-C-CA	-2.51	118.20	124.78

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	J	1	AME	C-CA-CB-CG
9	J	1	AME	N-CA-CB-CG
9	J2	1	AME	C-CA-CB-CG
9	J2	1	AME	N-CA-CB-CG

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

706 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	$\#\|Z\| > 2$
31	XAT	4	620	-	39,47,47	0.10	0	54,74,74	0.65	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
23	LHG	Z	620	21	38,38,48	0.25	0	41,44,54	0.28	0
26	LMU	7	628	-	22,22,36	0.15	0	27,27,47	0.33	0
21	CLA	42	602	16	64,68,73	1.24	4 (6%)	77,107,113	0.92	3 (3%)
26	LMU	A	862	-	20,20,36	0.14	0	25,25,47	0.28	0
21	CLA	A2	854	33	69,73,73	1.25	4 (5%)	83,113,113	0.87	3 (3%)
21	CLA	B2	818	2	69,73,73	1.19	5 (7%)	83,113,113	0.89	3 (3%)
21	CLA	42	611	23	64,68,73	1.23	4 (6%)	77,107,113	0.92	4 (5%)
23	LHG	8	620	21	43,43,48	0.25	0	46,49,54	0.26	0
23	LHG	42	623	-	37,37,48	0.25	0	40,43,54	0.29	0
30	CHL	62	601	18	70,74,74	1.76	8 (11%)	80,114,114	1.08	7 (8%)
24	BCR	K2	207	-	41,41,41	0.14	0	56,56,56	0.28	0
21	CLA	72	602	14	69,73,73	1.20	4 (5%)	83,113,113	0.89	3 (3%)
26	LMU	72	628	-	22,22,36	0.15	0	27,27,47	0.33	0
21	CLA	72	612	14	56,60,73	1.30	4 (7%)	67,97,113	0.95	3 (4%)
24	BCR	8	619	-	41,41,41	0.14	0	56,56,56	0.31	0
27	LMG	B	854	-	36,36,55	0.19	0	44,44,63	0.17	0
21	CLA	72	611	23	69,73,73	1.18	4 (5%)	83,113,113	0.88	3 (3%)
30	CHL	6	616	18	70,74,74	1.73	9 (12%)	80,114,114	1.07	8 (10%)
32	NEX	62	625	-	38,46,46	0.28	0	50,70,70	0.85	2 (4%)
26	LMU	Z	622	-	32,32,36	0.11	0	43,43,47	0.17	0
26	LMU	K2	208	-	24,24,36	0.11	0	29,29,47	0.31	0
21	CLA	A2	827	33	69,73,73	1.18	5 (7%)	83,113,113	0.89	3 (3%)
21	CLA	4	613	16	69,73,73	1.19	4 (5%)	83,113,113	0.91	3 (3%)
21	CLA	A2	818	1	69,73,73	1.16	4 (5%)	83,113,113	0.88	3 (3%)
21	CLA	A	804	1	69,73,73	1.18	5 (7%)	83,113,113	0.88	3 (3%)
21	CLA	Z2	603	12	59,63,73	1.30	4 (6%)	71,101,113	0.94	3 (4%)
21	CLA	6	613	33	69,73,73	1.18	4 (5%)	83,113,113	0.91	3 (3%)
24	BCR	32	620	-	41,41,41	0.19	0	56,56,56	0.36	0
30	CHL	7	601	14	70,74,74	1.74	9 (12%)	80,114,114	1.04	6 (7%)
21	CLA	72	608	33	54,58,73	1.35	4 (7%)	65,95,113	0.98	3 (4%)
21	CLA	42	604	33	54,58,73	1.34	4 (7%)	65,95,113	1.02	4 (6%)
26	LMU	K	208	-	24,24,36	0.12	0	29,29,47	0.30	0
21	CLA	B2	806	2	69,73,73	1.21	4 (5%)	83,113,113	0.83	3 (3%)
26	LMU	A	857	-	35,35,36	0.10	0	46,46,47	0.18	0
30	CHL	12	601	12	70,74,74	1.72	8 (11%)	80,114,114	1.02	6 (7%)
26	LMU	82	628	-	24,24,36	0.16	0	29,29,47	0.31	0
26	LMU	82	625	-	24,24,36	0.12	0	29,29,47	0.28	0
30	CHL	5	607	33	70,74,74	1.76	8 (11%)	80,114,114	1.08	8 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
21	CLA	L	204	-	49,53,73	1.42	4 (8%)	59,89,113	1.06	4 (6%)
23	LHG	6	619	21	48,48,48	0.23	0	51,54,54	0.24	0
26	LMU	62	632	-	20,20,36	0.16	0	25,25,47	0.26	0
26	LMU	12	621	-	36,36,36	0.10	0	47,47,47	0.28	0
30	CHL	42	618	16	50,54,74	2.05	8 (16%)	56,90,114	1.23	6 (10%)
26	LMU	12	625	-	24,24,36	0.12	0	29,29,47	0.31	0
21	CLA	Z	608	33	54,58,73	1.36	4 (7%)	65,95,113	1.02	3 (4%)
21	CLA	L2	203	10	69,73,73	1.19	4 (5%)	83,113,113	0.87	3 (3%)
21	CLA	A	814	1	69,73,73	1.17	4 (5%)	83,113,113	0.86	3 (3%)
21	CLA	A	826	33	69,73,73	1.21	4 (5%)	83,113,113	0.87	3 (3%)
30	CHL	82	607	33	70,74,74	1.74	8 (11%)	80,114,114	1.08	7 (8%)
21	CLA	B	819	33	64,68,73	1.25	4 (6%)	77,107,113	0.91	3 (3%)
21	CLA	Z	614	12	54,58,73	1.33	4 (7%)	65,95,113	1.01	4 (6%)
21	CLA	B2	816	2	69,73,73	1.17	4 (5%)	83,113,113	0.91	3 (3%)
26	LMU	Z2	621	-	22,22,36	0.15	0	27,27,47	0.27	0
27	LMG	6	633	-	19,19,55	0.31	0	19,19,63	0.29	0
21	CLA	B2	826	2	69,73,73	1.17	4 (5%)	83,113,113	0.87	3 (3%)
21	CLA	3	609	13	65,69,73	1.24	4 (6%)	78,108,113	0.91	3 (3%)
21	CLA	A2	810	1	69,73,73	1.21	4 (5%)	83,113,113	0.91	4 (4%)
21	CLA	62	611	23	62,66,73	1.26	4 (6%)	74,104,113	0.94	3 (4%)
22	PQN	A	844	-	34,34,34	0.31	0	42,45,45	0.36	0
24	BCR	3	620	-	41,41,41	0.19	0	56,56,56	0.36	0
26	LMU	A	858	-	36,36,36	0.08	0	47,47,47	0.19	0
21	CLA	A2	809	1	69,73,73	1.18	5 (7%)	83,113,113	0.95	4 (4%)
27	LMG	3	722	-	44,44,55	0.21	0	46,46,63	0.25	0
21	CLA	82	614	15	61,65,73	1.28	4 (6%)	73,103,113	0.93	3 (4%)
21	CLA	A	829	1	69,73,73	1.24	4 (5%)	83,113,113	0.89	5 (6%)
23	LHG	72	625	21	48,48,48	0.23	0	51,54,54	0.23	0
21	CLA	B2	803	-	69,73,73	1.21	4 (5%)	83,113,113	0.85	2 (2%)
24	BCR	A	848	-	41,41,41	0.14	0	56,56,56	0.30	0
21	CLA	K	203	33	64,68,73	1.25	4 (6%)	77,107,113	0.92	3 (3%)
25	SF4	C2	101	3	0,12,12	-	-	-		
21	CLA	62	604	-	69,73,73	1.18	4 (5%)	83,113,113	0.88	3 (3%)
30	CHL	5	606	33	50,54,74	2.05	8 (16%)	56,90,114	1.24	6 (10%)
21	CLA	A	845	23	49,53,73	1.41	4 (8%)	59,89,113	1.03	3 (5%)
30	CHL	52	606	33	50,54,74	2.05	8 (16%)	56,90,114	1.24	6 (10%)
21	CLA	A	811	1	69,73,73	1.17	5 (7%)	83,113,113	0.89	3 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
20	CL0	A2	801	1	69,73,73	1.60	10 (14%)	83,113,113	1.17	8 (9%)
28	LUT	7	621	-	42,43,43	0.25	0	51,60,60	0.38	0
21	CLA	5	617	17	69,73,73	1.17	4 (5%)	83,113,113	0.88	3 (3%)
25	SF4	A2	853	2,1	0,12,12	-	-	-		
26	LMU	12	626	-	24,24,36	0.12	0	29,29,47	0.27	0
21	CLA	8	612	15	59,63,73	1.25	4 (6%)	71,101,113	0.95	3 (4%)
27	LMG	8	629	-	42,42,55	0.19	0	50,50,63	0.16	0
21	CLA	A	833	1	69,73,73	1.20	5 (7%)	83,113,113	0.89	3 (3%)
21	CLA	42	603	16	69,73,73	1.18	5 (7%)	83,113,113	0.87	3 (3%)
21	CLA	A2	804	1	69,73,73	1.18	5 (7%)	83,113,113	0.87	3 (3%)
21	CLA	B	824	33	69,73,73	1.22	4 (5%)	83,113,113	0.89	3 (3%)
21	CLA	72	603	14	56,60,73	1.31	4 (7%)	67,97,113	0.99	3 (4%)
21	CLA	52	609	17	69,73,73	1.17	4 (5%)	83,113,113	0.89	4 (4%)
26	LMU	A2	864	-	24,24,36	0.12	0	29,29,47	0.29	0
21	CLA	B2	837	2	69,73,73	1.19	5 (7%)	83,113,113	0.90	3 (3%)
23	LHG	1	620	21	38,38,48	0.26	0	41,44,54	0.29	0
24	BCR	5	622	-	41,41,41	0.17	0	56,56,56	0.32	0
27	LMG	J2	103	-	42,42,55	0.18	0	50,50,63	0.39	0
28	LUT	32	622	-	42,43,43	0.32	0	51,60,60	0.35	0
21	CLA	6	604	-	69,73,73	1.19	4 (5%)	83,113,113	0.88	3 (3%)
21	CLA	Z2	614	12	54,58,73	1.33	4 (7%)	65,95,113	1.01	4 (6%)
31	XAT	52	624	-	39,47,47	0.10	0	54,74,74	0.58	0
27	LMG	A	860	-	36,36,55	0.20	0	44,44,63	0.26	0
21	CLA	B	803	-	69,73,73	1.21	4 (5%)	83,113,113	0.85	2 (2%)
21	CLA	A2	842	1	69,73,73	1.16	5 (7%)	83,113,113	0.91	4 (4%)
26	LMU	1	622	-	19,19,36	0.14	0	24,24,47	0.31	0
28	LUT	3	720	-	42,43,43	0.23	0	51,60,60	0.34	0
30	CHL	92	607	33	55,59,74	1.98	8 (14%)	62,96,114	1.22	8 (12%)
23	LHG	B2	851	21	44,44,48	0.25	0	47,50,54	0.31	0
24	BCR	3	719	-	41,41,41	0.12	0	56,56,56	0.40	0
21	CLA	A	809	1	69,73,73	1.17	5 (7%)	83,113,113	0.96	5 (6%)
28	LUT	52	620	-	42,43,43	0.24	0	51,60,60	0.44	0
21	CLA	62	613	33	69,73,73	1.18	4 (5%)	83,113,113	0.90	3 (3%)
21	CLA	G2	203	7	64,68,73	1.23	4 (6%)	77,107,113	0.88	3 (3%)
21	CLA	62	610	18	64,68,73	1.23	4 (6%)	77,107,113	0.92	3 (3%)
21	CLA	B	826	2	69,73,73	1.17	4 (5%)	83,113,113	0.87	3 (3%)
26	LMU	62	628	-	24,24,36	0.13	0	29,29,47	0.30	0
30	CHL	9	607	33	55,59,74	1.96	9 (16%)	62,96,114	1.19	7 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
21	CLA	52	611	23	59,63,73	1.28	4 (6%)	71,101,113	0.96	3 (4%)
21	CLA	Z2	604	33	61,65,73	1.26	4 (6%)	73,103,113	0.95	3 (4%)
21	CLA	Z	616	12	64,68,73	1.24	4 (6%)	77,107,113	0.93	3 (3%)
21	CLA	62	603	18	69,73,73	1.19	4 (5%)	83,113,113	0.86	3 (3%)
21	CLA	A	813	1	69,73,73	1.19	4 (5%)	83,113,113	0.93	3 (3%)
26	LMU	82	624	-	24,24,36	0.15	0	29,29,47	0.26	0
28	LUT	F	305	-	42,43,43	0.39	0	51,60,60	0.78	1 (1%)
21	CLA	B	828	2	69,73,73	1.17	4 (5%)	83,113,113	0.87	3 (3%)
21	CLA	B2	827	2	69,73,73	1.21	4 (5%)	83,113,113	0.90	3 (3%)
21	CLA	A2	803	33	69,73,73	1.24	5 (7%)	83,113,113	0.90	4 (4%)
21	CLA	A2	841	1	69,73,73	1.18	5 (7%)	83,113,113	0.91	3 (3%)
21	CLA	A2	836	1	69,73,73	1.21	5 (7%)	83,113,113	0.89	3 (3%)
24	BCR	I2	172	-	41,41,41	0.19	0	56,56,56	0.37	0
27	LMG	4	624	-	41,41,55	0.19	0	49,49,63	0.26	0
27	LMG	82	626	-	32,32,55	0.20	0	40,40,63	0.19	0
21	CLA	B	839	33	69,73,73	1.20	4 (5%)	83,113,113	0.92	3 (3%)
23	LHG	6	629	-	35,35,48	0.26	0	38,41,54	0.28	0
21	CLA	A	815	1	59,63,73	1.29	4 (6%)	71,101,113	0.94	3 (4%)
21	CLA	62	622	33	59,63,73	1.31	4 (6%)	71,101,113	0.95	4 (5%)
21	CLA	12	612	12	49,53,73	1.40	4 (8%)	59,89,113	1.04	3 (5%)
22	PQN	B2	842	-	34,34,34	0.30	0	42,45,45	0.37	0
30	CHL	42	607	33	70,74,74	1.73	9 (12%)	80,114,114	1.04	7 (8%)
26	LMU	A	864	-	24,24,36	0.12	0	29,29,47	0.28	0
30	CHL	9	606	-	46,50,74	2.19	10 (21%)	51,85,114	1.28	6 (11%)
21	CLA	L2	204	-	49,53,73	1.42	4 (8%)	59,89,113	1.06	4 (6%)
23	LHG	B	851	21	44,44,48	0.25	0	47,50,54	0.31	0
21	CLA	8	616	15	49,53,73	1.40	4 (8%)	59,89,113	1.08	4 (6%)
21	CLA	B	811	2	69,73,73	1.19	5 (7%)	83,113,113	0.91	3 (3%)
21	CLA	7	608	33	54,58,73	1.35	4 (7%)	65,95,113	0.99	3 (4%)
24	BCR	72	623	-	41,41,41	0.15	0	56,56,56	0.38	0
24	BCR	A	850	-	41,41,41	0.15	0	56,56,56	0.24	0
21	CLA	A2	814	1	69,73,73	1.18	4 (5%)	83,113,113	0.86	3 (3%)
27	LMG	32	722	-	44,44,55	0.21	0	46,46,63	0.26	0
21	CLA	B2	817	2	69,73,73	1.20	5 (7%)	83,113,113	0.89	3 (3%)
26	LMU	G	206	-	24,24,36	0.14	0	29,29,47	0.25	0
31	XAT	5	624	-	39,47,47	0.11	0	54,74,74	0.59	0
21	CLA	12	604	33	54,58,73	1.34	4 (7%)	65,95,113	1.03	3 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
30	CHL	4	607	33	70,74,74	1.72	9 (12%)	80,114,114	1.04	7 (8%)
21	CLA	42	614	16	59,63,73	1.30	4 (6%)	71,101,113	0.96	3 (4%)
21	CLA	9	611	23	69,73,73	1.20	4 (5%)	83,113,113	0.89	3 (3%)
27	LMG	B	852	-	43,43,55	0.18	0	51,51,63	0.24	0
21	CLA	G	203	7	64,68,73	1.24	4 (6%)	77,107,113	0.88	3 (3%)
21	CLA	32	607	13	59,63,73	1.29	4 (6%)	71,101,113	0.96	4 (5%)
21	CLA	72	614	14	47,51,73	1.45	4 (8%)	56,86,113	1.09	3 (5%)
30	CHL	6	618	18	47,51,74	2.10	9 (19%)	52,86,114	1.31	8 (15%)
21	CLA	A2	805	1	59,63,73	1.29	5 (8%)	71,101,113	0.93	3 (4%)
26	LMU	6	632	-	20,20,36	0.15	0	25,25,47	0.26	0
21	CLA	B2	821	2	69,73,73	1.22	5 (7%)	83,113,113	0.91	4 (4%)
21	CLA	Z	602	12	64,68,73	1.25	4 (6%)	77,107,113	0.94	3 (3%)
21	CLA	A2	824	1	49,53,73	1.40	5 (10%)	59,89,113	1.07	3 (5%)
21	CLA	Z	611	23	64,68,73	1.22	4 (6%)	77,107,113	0.93	3 (3%)
26	LMU	Z2	622	-	32,32,36	0.10	0	43,43,47	0.17	0
21	CLA	B	829	2	69,73,73	1.18	5 (7%)	83,113,113	0.92	4 (4%)
21	CLA	1	609	12	69,73,73	1.20	4 (5%)	83,113,113	0.91	4 (4%)
30	CHL	4	618	16	50,54,74	2.06	8 (16%)	56,90,114	1.23	6 (10%)
21	CLA	7	612	14	56,60,73	1.30	4 (7%)	67,97,113	0.96	3 (4%)
30	CHL	4	606	33	60,64,74	1.87	9 (15%)	68,102,114	1.19	7 (10%)
21	CLA	Z2	616	12	64,68,73	1.24	4 (6%)	77,107,113	0.93	3 (3%)
27	LMG	72	626	-	37,37,55	0.19	0	45,45,63	0.27	0
21	CLA	A	834	1	69,73,73	1.21	5 (7%)	83,113,113	0.91	4 (4%)
21	CLA	A2	843	33	69,73,73	1.18	5 (7%)	83,113,113	0.91	3 (3%)
21	CLA	F	303	33	49,53,73	1.40	4 (8%)	59,89,113	1.05	3 (5%)
21	CLA	A	832	1	59,63,73	1.27	5 (8%)	71,101,113	0.97	3 (4%)
21	CLA	B	812	2	69,73,73	1.20	5 (7%)	83,113,113	0.90	3 (3%)
24	BCR	B	844	-	41,41,41	0.13	0	56,56,56	0.45	0
23	LHG	A	847	21	37,37,48	0.26	0	40,43,54	0.30	0
30	CHL	42	606	33	60,64,74	1.87	8 (13%)	68,102,114	1.20	7 (10%)
21	CLA	Z	610	12	64,68,73	1.22	4 (6%)	77,107,113	0.91	3 (3%)
21	CLA	A	836	1	69,73,73	1.21	5 (7%)	83,113,113	0.89	3 (3%)
21	CLA	8	608	33	54,58,73	1.36	4 (7%)	65,95,113	0.99	3 (4%)
28	LUT	62	621	-	42,43,43	0.23	0	51,60,60	0.39	0
21	CLA	B	806	2	69,73,73	1.20	4 (5%)	83,113,113	0.82	3 (3%)
21	CLA	F	304	6	69,73,73	1.19	4 (5%)	83,113,113	0.97	4 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
27	LMG	42	624	-	41,41,55	0.19	0	49,49,63	0.26	0
31	XAT	62	624	-	39,47,47	0.12	0	54,74,74	0.59	0
21	CLA	82	610	15	69,73,73	1.18	4 (5%)	83,113,113	0.87	3 (3%)
21	CLA	4	614	16	59,63,73	1.30	4 (6%)	71,101,113	0.96	3 (4%)
21	CLA	A	821	1	59,63,73	1.28	4 (6%)	71,101,113	0.93	3 (4%)
32	NEX	6	625	-	38,46,46	0.19	0	50,70,70	0.83	2 (4%)
26	LMU	42	625	-	34,34,36	0.11	0	45,45,47	0.20	0
21	CLA	3	614	13	49,53,73	1.42	4 (8%)	59,89,113	1.06	3 (5%)
21	CLA	B	814	2	64,68,73	1.22	4 (6%)	77,107,113	0.93	4 (5%)
23	LHG	A2	847	21	37,37,48	0.26	0	40,43,54	0.29	0
27	LMG	A2	860	-	36,36,55	0.20	0	44,44,63	0.26	0
28	LUT	9	617	-	42,43,43	0.21	0	51,60,60	0.38	0
21	CLA	B	832	2	69,73,73	1.15	5 (7%)	83,113,113	0.89	3 (3%)
21	CLA	5	609	17	69,73,73	1.16	4 (5%)	83,113,113	0.89	4 (4%)
28	LUT	5	620	-	42,43,43	0.25	0	51,60,60	0.44	0
21	CLA	4	612	16	49,53,73	1.41	4 (8%)	59,89,113	1.03	3 (5%)
26	LMU	8	628	-	24,24,36	0.16	0	29,29,47	0.32	0
21	CLA	A	805	1	59,63,73	1.29	5 (8%)	71,101,113	0.93	3 (4%)
28	LUT	6	621	-	42,43,43	0.24	0	51,60,60	0.39	0
24	BCR	K2	202	-	41,41,41	0.15	0	56,56,56	0.36	0
21	CLA	82	608	33	54,58,73	1.37	4 (7%)	65,95,113	1.01	3 (4%)
30	CHL	92	606	-	46,50,74	2.19	10 (21%)	51,85,114	1.29	6 (11%)
30	CHL	5	618	17	47,51,74	2.11	8 (17%)	52,86,114	1.29	6 (11%)
28	LUT	Z	619	-	26,26,43	0.36	0	34,35,60	0.37	0
21	CLA	B2	802	2	69,73,73	1.19	4 (5%)	83,113,113	0.91	5 (6%)
26	LMU	G2	206	-	24,24,36	0.14	0	29,29,47	0.25	0
21	CLA	6	609	18	59,63,73	1.27	4 (6%)	71,101,113	1.01	5 (7%)
26	LMU	6	628	-	24,24,36	0.13	0	29,29,47	0.29	0
21	CLA	3	604	33	69,73,73	1.19	4 (5%)	83,113,113	0.89	3 (3%)
24	BCR	B	801	-	41,41,41	0.17	0	56,56,56	0.38	0
21	CLA	Z2	610	12	64,68,73	1.22	4 (6%)	77,107,113	0.91	3 (3%)
21	CLA	3	615	33	69,73,73	1.21	4 (5%)	83,113,113	0.91	3 (3%)
27	LMG	82	629	-	42,42,55	0.19	0	50,50,63	0.16	0
21	CLA	42	616	16	49,53,73	1.41	4 (8%)	59,89,113	1.05	3 (5%)
21	CLA	72	616	14	50,54,73	1.39	4 (8%)	60,90,113	1.03	3 (5%)
21	CLA	82	602	15	66,70,73	1.24	5 (7%)	79,109,113	0.92	3 (3%)
21	CLA	Z	603	12	59,63,73	1.31	4 (6%)	71,101,113	0.94	3 (4%)
27	LMG	B2	854	-	36,36,55	0.20	0	44,44,63	0.17	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
21	CLA	8	613	15	69,73,73	1.18	4 (5%)	83,113,113	0.90	3 (3%)
27	LMG	A2	859	-	48,48,55	0.18	0	56,56,63	0.17	0
21	CLA	B	838	2	54,58,73	1.37	4 (7%)	65,95,113	0.98	2 (3%)
21	CLA	92	613	19	69,73,73	1.18	4 (5%)	83,113,113	0.93	3 (3%)
21	CLA	A2	838	1	55,59,73	1.31	4 (7%)	66,96,113	0.99	3 (4%)
21	CLA	9	613	19	69,73,73	1.18	4 (5%)	83,113,113	0.93	3 (3%)
21	CLA	A2	806	1	69,73,73	1.17	5 (7%)	83,113,113	0.91	4 (4%)
21	CLA	72	604	33	55,59,73	1.32	4 (7%)	66,96,113	0.99	3 (4%)
21	CLA	1	611	23	65,69,73	1.22	4 (6%)	78,108,113	0.90	3 (3%)
26	LMU	9	624	-	24,24,36	0.15	0	29,29,47	0.38	0
21	CLA	B2	804	2	49,53,73	1.41	4 (8%)	59,89,113	1.02	3 (5%)
24	BCR	62	623	-	41,41,41	0.16	0	56,56,56	0.35	0
21	CLA	A2	812	1	69,73,73	1.16	5 (7%)	83,113,113	0.88	3 (3%)
21	CLA	52	617	17	69,73,73	1.18	4 (5%)	83,113,113	0.88	3 (3%)
30	CHL	6	608	33	55,59,74	1.96	9 (16%)	62,96,114	1.19	7 (11%)
21	CLA	12	610	12	69,73,73	1.19	5 (7%)	83,113,113	0.88	3 (3%)
23	LHG	32	721	-	30,30,48	0.27	0	33,36,54	0.35	0
26	LMU	12	622	-	19,19,36	0.14	0	24,24,47	0.31	0
21	CLA	B	830	2	49,53,73	1.36	5 (10%)	59,89,113	1.07	4 (6%)
21	CLA	72	620	33	57,61,73	1.31	4 (7%)	68,98,113	0.96	3 (4%)
21	CLA	3	617	13	50,54,73	1.39	4 (8%)	60,90,113	1.04	3 (5%)
26	LMU	6	631	-	24,24,36	0.15	0	29,29,47	0.28	0
21	CLA	8	609	15	49,53,73	1.42	4 (8%)	59,89,113	1.03	4 (6%)
21	CLA	A2	826	33	69,73,73	1.21	4 (5%)	83,113,113	0.87	3 (3%)
30	CHL	6	607	33	70,74,74	1.76	8 (11%)	80,114,114	1.09	7 (8%)
21	CLA	4	616	16	49,53,73	1.41	4 (8%)	59,89,113	1.05	3 (5%)
21	CLA	A2	839	1	69,73,73	1.19	5 (7%)	83,113,113	0.91	3 (3%)
30	CHL	7	606	33	50,54,74	2.04	9 (18%)	56,90,114	1.22	7 (12%)
23	LHG	7	625	21	48,48,48	0.24	0	51,54,54	0.23	0
28	LUT	9	616	-	42,43,43	0.26	0	51,60,60	0.37	0
21	CLA	7	602	14	69,73,73	1.19	4 (5%)	83,113,113	0.89	3 (3%)
21	CLA	J2	101	9	59,63,73	1.30	4 (6%)	71,101,113	0.95	3 (4%)
30	CHL	Z	606	33	50,54,74	2.05	9 (18%)	56,90,114	1.23	6 (10%)
31	XAT	Z	618	-	39,47,47	0.13	0	54,74,74	0.56	0
21	CLA	7	611	23	69,73,73	1.18	4 (5%)	83,113,113	0.88	3 (3%)
30	CHL	8	607	33	70,74,74	1.74	8 (11%)	80,114,114	1.08	7 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
30	CHL	3	608	33	70,74,74	1.74	9 (12%)	80,114,114	1.06	6 (7%)
21	CLA	3	606	33	46,50,73	1.49	4 (8%)	55,85,113	1.09	3 (5%)
21	CLA	9	609	19	55,59,73	1.33	4 (7%)	66,96,113	0.99	3 (4%)
21	CLA	5	603	17	69,73,73	1.19	4 (5%)	83,113,113	0.90	3 (3%)
26	LMU	72	627	-	33,33,36	0.11	0	44,44,47	0.16	0
21	CLA	A2	834	1	69,73,73	1.21	4 (5%)	83,113,113	0.90	4 (4%)
22	PQN	A2	844	-	34,34,34	0.31	0	42,45,45	0.36	0
24	BCR	K	202	-	41,41,41	0.15	0	56,56,56	0.36	0
21	CLA	A2	832	1	59,63,73	1.27	4 (6%)	71,101,113	0.98	3 (4%)
26	LMU	A2	858	-	36,36,36	0.08	0	47,47,47	0.19	0
30	CHL	Z2	607	33	70,74,74	1.73	8 (11%)	80,114,114	1.06	6 (7%)
21	CLA	A	820	1	69,73,73	1.17	5 (7%)	83,113,113	0.89	3 (3%)
24	BCR	A	851	-	41,41,41	0.14	0	56,56,56	0.33	0
21	CLA	32	614	13	49,53,73	1.41	4 (8%)	59,89,113	1.06	3 (5%)
21	CLA	A	838	1	55,59,73	1.31	4 (7%)	66,96,113	0.99	3 (4%)
21	CLA	42	612	16	49,53,73	1.40	4 (8%)	59,89,113	1.02	3 (5%)
21	CLA	B2	829	2	69,73,73	1.17	5 (7%)	83,113,113	0.91	4 (4%)
28	LUT	1	619	-	42,43,43	0.21	0	51,60,60	0.40	0
23	LHG	Z2	620	21	38,38,48	0.26	0	41,44,54	0.28	0
21	CLA	A2	811	1	69,73,73	1.16	5 (7%)	83,113,113	0.89	3 (3%)
21	CLA	B2	824	33	69,73,73	1.22	4 (5%)	83,113,113	0.90	3 (3%)
21	CLA	6	611	23	62,66,73	1.26	4 (6%)	74,104,113	0.94	3 (4%)
21	CLA	8	610	15	69,73,73	1.18	4 (5%)	83,113,113	0.88	3 (3%)
21	CLA	A	830	1	69,73,73	1.18	4 (5%)	83,113,113	0.87	2 (2%)
21	CLA	A	831	1	69,73,73	1.17	4 (5%)	83,113,113	0.89	3 (3%)
28	LUT	F2	305	-	42,43,43	0.38	0	51,60,60	0.78	1 (1%)
28	LUT	52	626	-	42,43,43	0.23	0	51,60,60	0.36	0
25	SF4	A	853	2,1	0,12,12	-	-	-		
21	CLA	B2	841	23	69,73,73	1.20	4 (5%)	83,113,113	0.91	3 (3%)
21	CLA	82	609	15	49,53,73	1.42	4 (8%)	59,89,113	1.03	4 (6%)
21	CLA	4	611	23	64,68,73	1.23	4 (6%)	77,107,113	0.92	4 (5%)
21	CLA	8	603	15	69,73,73	1.21	4 (5%)	83,113,113	0.87	3 (3%)
21	CLA	1	603	12	61,65,73	1.27	4 (6%)	73,103,113	0.94	3 (4%)
26	LMU	12	627	-	22,22,36	0.14	0	27,27,47	0.30	0
26	LMU	1	621	-	36,36,36	0.10	0	47,47,47	0.28	0
21	CLA	A2	819	1	64,68,73	1.26	4 (6%)	77,107,113	0.94	3 (3%)
21	CLA	4	610	16	64,68,73	1.23	4 (6%)	77,107,113	0.90	3 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
30	CHL	8	601	15	70,74,74	1.73	9 (12%)	80,114,114	1.01	6 (7%)
23	LHG	12	620	21	38,38,48	0.26	0	41,44,54	0.29	0
21	CLA	1	616	12	50,54,73	1.41	4 (8%)	60,90,113	1.05	3 (5%)
21	CLA	42	613	16	69,73,73	1.19	4 (5%)	83,113,113	0.89	3 (3%)
24	BCR	L	201	-	41,41,41	0.17	0	56,56,56	0.36	0
26	LMU	A2	865	-	24,24,36	0.13	0	29,29,47	0.46	0
21	CLA	F	301	33	69,73,73	1.16	4 (5%)	83,113,113	0.88	3 (3%)
30	CHL	Z2	601	12	70,74,74	1.73	8 (11%)	80,114,114	1.05	6 (7%)
28	LUT	32	720	-	42,43,43	0.22	0	51,60,60	0.33	0
21	CLA	A	818	1	69,73,73	1.18	4 (5%)	83,113,113	0.89	3 (3%)
21	CLA	72	610	14	69,73,73	1.22	4 (5%)	83,113,113	0.94	2 (2%)
30	CHL	1	607	33	50,54,74	2.06	8 (16%)	56,90,114	1.27	9 (16%)
21	CLA	Z	604	33	61,65,73	1.25	4 (6%)	73,103,113	0.94	3 (4%)
24	BCR	G2	205	-	41,41,41	0.14	0	56,56,56	0.32	0
21	CLA	B	823	2	69,73,73	1.19	5 (7%)	83,113,113	0.91	3 (3%)
21	CLA	F2	303	33	49,53,73	1.40	4 (8%)	59,89,113	1.05	3 (5%)
21	CLA	B	833	2	62,66,73	1.22	5 (8%)	74,104,113	0.96	3 (4%)
27	LMG	J	103	-	42,42,55	0.18	0	50,50,63	0.39	0
28	LUT	3	621	-	42,43,43	0.29	0	51,60,60	0.37	0
32	NEX	52	625	-	38,46,46	0.46	1 (2%)	50,70,70	0.80	2 (4%)
21	CLA	B	841	23	69,73,73	1.19	4 (5%)	83,113,113	0.91	3 (3%)
21	CLA	5	602	17	69,73,73	1.20	4 (5%)	83,113,113	0.88	3 (3%)
24	BCR	A2	851	-	41,41,41	0.13	0	56,56,56	0.33	0
24	BCR	92	623	-	41,41,41	0.15	0	56,56,56	0.34	0
21	CLA	5	614	17	49,53,73	1.42	4 (8%)	59,89,113	1.05	3 (5%)
28	LUT	7	624	-	42,43,43	0.21	0	51,60,60	0.41	0
26	LMU	A	861	-	24,24,36	0.13	0	29,29,47	0.30	0
30	CHL	8	606	33	70,74,74	1.72	9 (12%)	80,114,114	1.03	7 (8%)
21	CLA	9	603	27,19	59,63,73	1.28	5 (8%)	71,101,113	0.97	3 (4%)
21	CLA	F2	301	33	69,73,73	1.17	4 (5%)	83,113,113	0.87	3 (3%)
21	CLA	K2	201	11	49,53,73	1.43	4 (8%)	59,89,113	1.03	3 (5%)
31	XAT	1	618	-	39,47,47	0.13	0	54,74,74	0.68	2 (3%)
21	CLA	B	804	2	49,53,73	1.42	4 (8%)	59,89,113	1.02	3 (5%)
21	CLA	F2	304	6	69,73,73	1.18	4 (5%)	83,113,113	0.97	4 (4%)
21	CLA	A2	831	1	69,73,73	1.17	5 (7%)	83,113,113	0.89	3 (3%)
21	CLA	A2	815	1	59,63,73	1.30	4 (6%)	71,101,113	0.93	3 (4%)
21	CLA	5	612	17	49,53,73	1.40	4 (8%)	59,89,113	1.03	3 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
21	CLA	52	610	17	64,68,73	1.23	4 (6%)	77,107,113	0.90	3 (3%)
27	LMG	8	626	-	32,32,55	0.20	0	40,40,63	0.19	0
24	BCR	A2	852	-	41,41,41	0.14	0	56,56,56	0.38	0
21	CLA	82	604	33	64,68,73	1.24	5 (7%)	77,107,113	0.93	3 (3%)
21	CLA	3	610	13	69,73,73	1.19	4 (5%)	83,113,113	0.89	3 (3%)
21	CLA	9	602	19	64,68,73	1.25	5 (7%)	77,107,113	0.93	3 (3%)
21	CLA	92	614	19	49,53,73	1.44	4 (8%)	59,89,113	1.05	4 (6%)
31	XAT	8	618	-	39,47,47	0.16	0	54,74,74	0.57	0
21	CLA	32	615	33	69,73,73	1.21	4 (5%)	83,113,113	0.90	3 (3%)
21	CLA	Z2	609	12	69,73,73	1.22	4 (5%)	83,113,113	0.89	3 (3%)
30	CHL	62	616	18	70,74,74	1.73	9 (12%)	80,114,114	1.07	8 (10%)
21	CLA	B	831	2	59,63,73	1.27	5 (8%)	71,101,113	0.95	4 (5%)
27	LMG	B2	852	-	43,43,55	0.18	0	51,51,63	0.24	0
21	CLA	62	602	18	69,73,73	1.19	4 (5%)	83,113,113	0.89	3 (3%)
28	LUT	42	619	-	42,43,43	0.25	0	51,60,60	0.43	0
24	BCR	B	843	-	41,41,41	0.16	0	56,56,56	0.31	0
21	CLA	4	603	16	69,73,73	1.19	5 (7%)	83,113,113	0.87	3 (3%)
20	CL0	A	801	1	69,73,73	1.60	10 (14%)	83,113,113	1.16	8 (9%)
21	CLA	A2	825	1	59,63,73	1.29	4 (6%)	71,101,113	0.96	3 (4%)
21	CLA	3	603	13	69,73,73	1.20	4 (5%)	83,113,113	0.87	3 (3%)
24	BCR	G	205	-	41,41,41	0.14	0	56,56,56	0.32	0
21	CLA	62	617	18	49,53,73	1.42	4 (8%)	59,89,113	1.04	3 (5%)
21	CLA	92	612	19	69,73,73	1.17	4 (5%)	83,113,113	0.87	3 (3%)
23	LHG	62	619	21	48,48,48	0.23	0	51,54,54	0.24	0
21	CLA	92	601	19	50,54,73	1.42	4 (8%)	60,90,113	1.05	3 (5%)
24	BCR	B2	844	-	41,41,41	0.14	0	56,56,56	0.45	0
25	SF4	C	102	3	0,12,12	-	-	-		
29	DGD	B	850	-	60,60,67	0.18	0	74,74,81	0.52	0
21	CLA	B2	809	2	69,73,73	1.21	4 (5%)	83,113,113	0.87	4 (4%)
21	CLA	4	602	16	64,68,73	1.25	4 (6%)	77,107,113	0.92	3 (3%)
21	CLA	32	602	13	64,68,73	1.23	4 (6%)	77,107,113	0.92	3 (3%)
21	CLA	32	609	13	65,69,73	1.23	4 (6%)	78,108,113	0.91	3 (3%)
28	LUT	A2	856	-	42,43,43	0.27	0	51,60,60	0.35	0
23	LHG	52	623	21	36,36,48	0.26	0	39,42,54	0.27	0
24	BCR	9	623	-	41,41,41	0.14	0	56,56,56	0.34	0
21	CLA	A2	830	1	69,73,73	1.18	4 (5%)	83,113,113	0.87	4 (4%)
21	CLA	B2	835	33	49,53,73	1.42	4 (8%)	59,89,113	1.05	3 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
21	CLA	A	837	1	61,65,73	1.32	5 (8%)	73,103,113	0.97	4 (5%)
28	LUT	Z	617	-	42,43,43	0.26	0	51,60,60	0.40	0
21	CLA	7	620	33	57,61,73	1.30	4 (7%)	68,98,113	0.96	3 (4%)
21	CLA	B	815	2	69,73,73	1.18	4 (5%)	83,113,113	0.89	3 (3%)
21	CLA	3	612	13	50,54,73	1.38	4 (8%)	60,90,113	1.02	3 (5%)
21	CLA	A2	837	1	61,65,73	1.32	4 (6%)	73,103,113	0.98	3 (4%)
23	LHG	A2	846	-	48,48,48	0.24	0	51,54,54	0.29	0
23	LHG	3	623	-	46,46,48	0.23	0	49,52,54	0.26	0
24	BCR	L	205	-	41,41,41	0.15	0	56,56,56	0.37	0
28	LUT	4	619	-	42,43,43	0.25	0	51,60,60	0.43	0
21	CLA	32	610	13	69,73,73	1.19	5 (7%)	83,113,113	0.90	3 (3%)
21	CLA	9	614	19	49,53,73	1.44	4 (8%)	59,89,113	1.06	3 (5%)
26	LMU	82	627	-	36,36,36	0.10	0	47,47,47	0.37	0
21	CLA	5	616	17	57,61,73	1.31	4 (7%)	68,98,113	0.98	3 (4%)
26	LMU	1	626	-	24,24,36	0.12	0	29,29,47	0.27	0
21	CLA	B2	832	2	69,73,73	1.16	5 (7%)	83,113,113	0.89	3 (3%)
26	LMU	1	625	-	24,24,36	0.11	0	29,29,47	0.30	0
26	LMU	52	627	-	24,24,36	0.13	0	29,29,47	0.26	0
21	CLA	7	614	14	47,51,73	1.46	4 (8%)	56,86,113	1.09	3 (5%)
21	CLA	K2	203	33	64,68,73	1.25	4 (6%)	77,107,113	0.92	3 (3%)
21	CLA	A2	822	33	69,73,73	1.19	5 (7%)	83,113,113	0.90	4 (4%)
21	CLA	7	613	14	69,73,73	1.19	4 (5%)	83,113,113	0.90	3 (3%)
21	CLA	B	825	33	69,73,73	1.17	5 (7%)	83,113,113	0.86	3 (3%)
21	CLA	5	604	33	59,63,73	1.29	4 (6%)	71,101,113	0.95	3 (4%)
21	CLA	9	612	19	69,73,73	1.17	4 (5%)	83,113,113	0.87	3 (3%)
24	BCR	B	847	-	41,41,41	0.19	0	56,56,56	0.41	0
26	LMU	62	631	-	24,24,36	0.15	0	29,29,47	0.28	0
21	CLA	5	621	33	50,54,73	1.43	4 (8%)	60,90,113	1.12	6 (10%)
21	CLA	52	604	33	59,63,73	1.29	4 (6%)	71,101,113	0.95	3 (4%)
24	BCR	B2	843	-	41,41,41	0.16	0	56,56,56	0.30	0
21	CLA	A	803	33	69,73,73	1.24	5 (7%)	83,113,113	0.90	4 (4%)
21	CLA	82	613	15	69,73,73	1.18	4 (5%)	83,113,113	0.90	3 (3%)
21	CLA	B	817	2	69,73,73	1.19	4 (5%)	83,113,113	0.89	3 (3%)
21	CLA	J	101	9	59,63,73	1.30	4 (6%)	71,101,113	0.94	3 (4%)
21	CLA	B	835	33	49,53,73	1.42	4 (8%)	59,89,113	1.06	3 (5%)
25	SF4	C2	102	3	0,12,12	-	-	-		
24	BCR	B2	801	-	41,41,41	0.17	0	56,56,56	0.38	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
21	CLA	Z	612	12	49,53,73	1.38	4 (8%)	59,89,113	1.01	3 (5%)
21	CLA	52	612	17	49,53,73	1.39	4 (8%)	59,89,113	1.03	3 (5%)
21	CLA	A	827	33	69,73,73	1.18	5 (7%)	83,113,113	0.89	3 (3%)
21	CLA	B	834	2	64,68,73	1.23	4 (6%)	77,107,113	0.93	3 (3%)
21	CLA	12	602	12	64,68,73	1.24	5 (7%)	77,107,113	0.93	3 (3%)
21	CLA	Z2	608	33	54,58,73	1.36	4 (7%)	65,95,113	1.02	3 (4%)
21	CLA	8	614	15	61,65,73	1.27	4 (6%)	73,103,113	0.93	3 (4%)
21	CLA	52	613	17	60,64,73	1.26	4 (6%)	72,102,113	0.95	3 (4%)
26	LMU	7	627	-	33,33,36	0.11	0	44,44,47	0.16	0
21	CLA	62	609	18	59,63,73	1.27	4 (6%)	71,101,113	1.01	5 (7%)
21	CLA	42	609	16	64,68,73	1.27	4 (6%)	77,107,113	0.94	3 (3%)
21	CLA	Z	609	12	69,73,73	1.21	4 (5%)	83,113,113	0.89	3 (3%)
24	BCR	B2	845	-	41,41,41	0.13	0	56,56,56	0.37	0
21	CLA	A2	828	1	69,73,73	1.19	4 (5%)	83,113,113	0.84	3 (3%)
28	LUT	72	621	-	42,43,43	0.25	0	51,60,60	0.38	0
29	DGD	B2	850	-	60,60,67	0.17	0	74,74,81	0.34	0
24	BCR	42	621	-	41,41,41	0.14	0	56,56,56	0.35	0
28	LUT	32	621	-	42,43,43	0.29	0	51,60,60	0.37	0
26	LMU	5	627	-	24,24,36	0.13	0	29,29,47	0.26	0
21	CLA	B	808	2	69,73,73	1.17	4 (5%)	83,113,113	0.90	4 (4%)
30	CHL	52	618	17	47,51,74	2.11	8 (17%)	52,86,114	1.29	6 (11%)
21	CLA	72	609	14	49,53,73	1.44	4 (8%)	59,89,113	1.04	3 (5%)
21	CLA	32	603	13	69,73,73	1.21	4 (5%)	83,113,113	0.87	3 (3%)
21	CLA	92	611	23	69,73,73	1.19	4 (5%)	83,113,113	0.89	3 (3%)
21	CLA	B2	828	2	69,73,73	1.17	4 (5%)	83,113,113	0.87	3 (3%)
31	XAT	7	622	-	39,47,47	0.13	0	54,74,74	0.57	0
21	CLA	B2	830	2	49,53,73	1.38	5 (10%)	59,89,113	1.08	4 (6%)
28	LUT	5	626	-	42,43,43	0.24	0	51,60,60	0.36	0
21	CLA	A	822	33	69,73,73	1.19	5 (7%)	83,113,113	0.90	4 (4%)
21	CLA	A	808	1	54,58,73	1.35	5 (9%)	65,95,113	0.98	3 (4%)
21	CLA	B2	822	2	63,67,73	1.23	4 (6%)	75,105,113	0.94	3 (4%)
21	CLA	K	201	11	49,53,73	1.43	4 (8%)	59,89,113	1.03	3 (5%)
21	CLA	A2	802	-	69,73,73	1.17	5 (7%)	83,113,113	0.84	2 (2%)
21	CLA	92	602	19	64,68,73	1.25	4 (6%)	77,107,113	0.93	3 (3%)
21	CLA	B2	807	2	59,63,73	1.31	4 (6%)	71,101,113	0.96	3 (4%)
26	LMU	4	625	-	34,34,36	0.11	0	45,45,47	0.20	0
28	LUT	1	617	-	42,43,43	0.26	0	51,60,60	0.40	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
30	CHL	82	606	33	70,74,74	1.72	8 (11%)	80,114,114	1.03	7 (8%)
24	BCR	B	845	-	41,41,41	0.14	0	56,56,56	0.37	0
21	CLA	12	614	12	64,68,73	1.24	4 (6%)	77,107,113	0.96	3 (3%)
21	CLA	K2	206	11	49,53,73	1.42	4 (8%)	59,89,113	1.06	3 (5%)
21	CLA	6	622	33	59,63,73	1.31	4 (6%)	71,101,113	0.95	4 (5%)
32	NEX	5	625	-	38,46,46	0.54	1 (2%)	50,70,70	0.80	2 (4%)
21	CLA	32	612	13	50,54,73	1.38	4 (8%)	60,90,113	1.01	3 (5%)
21	CLA	7	616	14	50,54,73	1.38	5 (10%)	60,90,113	1.03	3 (5%)
21	CLA	52	602	17	69,73,73	1.20	4 (5%)	83,113,113	0.89	3 (3%)
26	LMU	1	623	-	24,24,36	0.13	0	29,29,47	0.27	0
23	LHG	32	623	-	46,46,48	0.23	0	49,52,54	0.26	0
24	BCR	J	102	-	41,41,41	0.14	0	56,56,56	0.31	0
26	LMU	1	627	-	22,22,36	0.13	0	27,27,47	0.29	0
27	LMG	J	104	-	35,35,55	0.20	0	43,43,63	0.20	0
26	LMU	B	853	-	36,36,36	0.13	0	47,47,47	0.67	2 (4%)
30	CHL	Z	607	33	70,74,74	1.72	8 (11%)	80,114,114	1.06	7 (8%)
21	CLA	A	828	1	69,73,73	1.20	4 (5%)	83,113,113	0.84	3 (3%)
24	BCR	32	719	-	41,41,41	0.11	0	56,56,56	0.40	0
26	LMU	8	624	-	24,24,36	0.14	0	29,29,47	0.26	0
21	CLA	3	611	-	69,73,73	1.20	4 (5%)	83,113,113	0.89	3 (3%)
21	CLA	A2	817	33	59,63,73	1.32	4 (6%)	71,101,113	0.96	3 (4%)
26	LMU	92	624	-	24,24,36	0.15	0	29,29,47	0.37	0
28	LUT	92	617	-	42,43,43	0.21	0	51,60,60	0.38	0
21	CLA	5	610	17	64,68,73	1.23	4 (6%)	77,107,113	0.91	3 (3%)
21	CLA	6	617	18	49,53,73	1.43	4 (8%)	59,89,113	1.05	4 (6%)
21	CLA	B	822	2	63,67,73	1.23	4 (6%)	75,105,113	0.95	3 (4%)
21	CLA	8	602	15	66,70,73	1.24	5 (7%)	79,109,113	0.91	3 (3%)
21	CLA	B2	812	2	69,73,73	1.20	5 (7%)	83,113,113	0.90	3 (3%)
30	CHL	52	608	33	55,59,74	1.96	9 (16%)	62,96,114	1.21	7 (11%)
30	CHL	82	601	15	70,74,74	1.73	9 (12%)	80,114,114	1.01	6 (7%)
21	CLA	1	612	12	49,53,73	1.40	4 (8%)	59,89,113	1.04	3 (5%)
21	CLA	A	819	1	64,68,73	1.27	4 (6%)	77,107,113	0.95	3 (3%)
24	BCR	3	718	-	41,41,41	0.15	0	56,56,56	0.34	0
21	CLA	K	204	11	50,54,73	1.40	4 (8%)	60,90,113	1.07	4 (6%)
30	CHL	5	608	33	55,59,74	1.96	9 (16%)	62,96,114	1.20	7 (11%)
21	CLA	4	604	33	54,58,73	1.34	4 (7%)	65,95,113	1.01	4 (6%)
30	CHL	52	607	33	70,74,74	1.76	8 (11%)	80,114,114	1.07	7 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
21	CLA	B2	814	2	64,68,73	1.22	4 (6%)	77,107,113	0.93	4 (5%)
21	CLA	B2	811	2	69,73,73	1.18	4 (5%)	83,113,113	0.90	3 (3%)
26	LMU	A2	857	-	35,35,36	0.10	0	46,46,47	0.17	0
24	BCR	A2	849	-	41,41,41	0.17	0	56,56,56	0.31	0
21	CLA	B2	819	33	64,68,73	1.25	5 (7%)	77,107,113	0.91	3 (3%)
31	XAT	42	620	-	39,47,47	0.11	0	54,74,74	0.65	0
24	BCR	A2	848	-	41,41,41	0.13	0	56,56,56	0.30	0
26	LMU	7	629	-	28,28,36	0.10	0	39,39,47	0.27	0
21	CLA	A2	808	1	54,58,73	1.34	4 (7%)	65,95,113	0.98	3 (4%)
21	CLA	72	613	14	69,73,73	1.19	4 (5%)	83,113,113	0.91	3 (3%)
21	CLA	92	610	19	64,68,73	1.23	5 (7%)	77,107,113	0.95	3 (3%)
21	CLA	9	610	19	64,68,73	1.23	5 (7%)	77,107,113	0.95	3 (3%)
21	CLA	32	613	13	64,68,73	1.24	4 (6%)	77,107,113	0.92	3 (3%)
21	CLA	A	806	1	69,73,73	1.16	5 (7%)	83,113,113	0.90	4 (4%)
24	BCR	K	207	-	41,41,41	0.14	0	56,56,56	0.27	0
26	LMU	6	630	-	24,24,36	0.15	0	29,29,47	0.29	0
31	XAT	12	618	-	39,47,47	0.13	0	54,74,74	0.69	2 (3%)
21	CLA	A	841	1	69,73,73	1.18	5 (7%)	83,113,113	0.90	3 (3%)
21	CLA	7	610	14	69,73,73	1.22	4 (5%)	83,113,113	0.94	2 (2%)
24	BCR	B2	848	-	41,41,41	0.13	0	56,56,56	0.46	0
21	CLA	A	812	1	69,73,73	1.16	5 (7%)	83,113,113	0.88	3 (3%)
21	CLA	1	608	33	69,73,73	1.20	4 (5%)	83,113,113	0.90	3 (3%)
21	CLA	92	603	27,19	59,63,73	1.28	4 (6%)	71,101,113	0.98	3 (4%)
24	BCR	A	849	-	41,41,41	0.17	0	56,56,56	0.31	0
28	LUT	12	617	-	42,43,43	0.26	0	51,60,60	0.40	0
21	CLA	A2	820	1	69,73,73	1.18	5 (7%)	83,113,113	0.89	2 (2%)
23	LHG	5	623	21	36,36,48	0.26	0	39,42,54	0.27	0
27	LMG	62	633	-	19,19,55	0.31	0	19,19,63	0.30	0
21	CLA	9	601	19	50,54,73	1.41	4 (8%)	60,90,113	1.05	3 (5%)
21	CLA	7	609	14	49,53,73	1.44	4 (8%)	59,89,113	1.03	3 (5%)
21	CLA	12	611	23	65,69,73	1.23	4 (6%)	78,108,113	0.90	3 (3%)
24	BCR	I	172	-	41,41,41	0.20	0	56,56,56	0.37	0
21	CLA	7	603	14	56,60,73	1.32	4 (7%)	67,97,113	1.00	3 (4%)
21	CLA	12	616	12	50,54,73	1.40	4 (8%)	60,90,113	1.04	3 (5%)
30	CHL	Z2	606	33	50,54,74	2.05	9 (18%)	56,90,114	1.23	6 (10%)
24	BCR	A	852	-	41,41,41	0.14	0	56,56,56	0.39	0
21	CLA	G2	204	7	50,54,73	1.40	4 (8%)	60,90,113	1.02	3 (5%)
26	LMU	A	865	-	24,24,36	0.13	0	29,29,47	0.47	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
21	CLA	A2	816	1	69,73,73	1.17	4 (5%)	83,113,113	0.89	3 (3%)
21	CLA	B2	820	2	60,64,73	1.30	4 (6%)	72,102,113	0.94	3 (4%)
21	CLA	6	612	18	49,53,73	1.39	4 (8%)	59,89,113	1.04	3 (5%)
21	CLA	B2	833	2	62,66,73	1.22	5 (8%)	74,104,113	0.97	4 (5%)
21	CLA	52	601	17	69,73,73	1.18	4 (5%)	83,113,113	0.88	2 (2%)
21	CLA	1	602	12	64,68,73	1.24	5 (7%)	77,107,113	0.93	3 (3%)
21	CLA	B2	838	2	54,58,73	1.37	4 (7%)	65,95,113	0.98	2 (3%)
23	LHG	42	622	21	48,48,48	0.24	0	51,54,54	0.27	0
26	LMU	42	626	-	20,20,36	0.15	0	25,25,47	0.28	0
21	CLA	Z2	612	12	49,53,73	1.38	4 (8%)	59,89,113	1.01	3 (5%)
24	BCR	B	848	-	41,41,41	0.13	0	56,56,56	0.46	0
21	CLA	B2	831	2	59,63,73	1.27	5 (8%)	71,101,113	0.95	4 (5%)
21	CLA	A2	829	1	69,73,73	1.24	4 (5%)	83,113,113	0.89	3 (3%)
21	CLA	52	614	17	49,53,73	1.42	4 (8%)	59,89,113	1.05	3 (5%)
26	LMU	A2	863	-	36,36,36	0.10	0	47,47,47	0.27	0
21	CLA	32	611	-	69,73,73	1.19	4 (5%)	83,113,113	0.89	3 (3%)
21	CLA	B	818	2	69,73,73	1.19	4 (5%)	83,113,113	0.88	3 (3%)
28	LUT	92	616	-	42,43,43	0.26	0	51,60,60	0.37	0
24	BCR	6	623	-	41,41,41	0.16	0	56,56,56	0.35	0
26	LMU	A2	861	-	24,24,36	0.13	0	29,29,47	0.30	0
21	CLA	32	617	13	50,54,73	1.39	4 (8%)	60,90,113	1.04	3 (5%)
24	BCR	B2	846	-	41,41,41	0.13	0	56,56,56	0.34	0
30	CHL	42	601	16	70,74,74	1.74	9 (12%)	80,114,114	1.05	6 (7%)
27	LMG	J2	104	-	35,35,55	0.20	0	43,43,63	0.20	0
23	LHG	82	620	21	43,43,48	0.25	0	46,49,54	0.26	0
21	CLA	B	820	2	60,64,73	1.29	4 (6%)	72,102,113	0.93	3 (4%)
21	CLA	A	824	1	49,53,73	1.40	4 (8%)	59,89,113	1.07	3 (5%)
30	CHL	Z	601	12	70,74,74	1.74	9 (12%)	80,114,114	1.05	6 (7%)
30	CHL	6	606	33	62,66,74	1.85	8 (12%)	70,104,114	1.12	6 (8%)
23	LHG	A	846	-	48,48,48	0.24	0	51,54,54	0.29	0
21	CLA	L	203	10	69,73,73	1.19	4 (5%)	83,113,113	0.87	3 (3%)
21	CLA	A	823	1	69,73,73	1.20	4 (5%)	83,113,113	0.88	4 (4%)
21	CLA	6	614	18	54,58,73	1.34	4 (7%)	65,95,113	1.02	3 (4%)
21	CLA	B2	813	2	69,73,73	1.18	4 (5%)	83,113,113	0.88	3 (3%)
23	LHG	92	622	21	40,40,48	0.25	0	43,46,54	0.28	0
30	CHL	32	608	33	70,74,74	1.74	9 (12%)	80,114,114	1.06	6 (7%)
24	BCR	32	718	-	41,41,41	0.16	0	56,56,56	0.34	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
21	CLA	12	613	33	69,73,73	1.18	5 (7%)	83,113,113	0.90	3 (3%)
21	CLA	32	606	33	46,50,73	1.48	4 (8%)	55,85,113	1.09	3 (5%)
30	CHL	62	608	33	55,59,74	1.97	9 (16%)	62,96,114	1.20	7 (11%)
21	CLA	A	816	1	69,73,73	1.17	4 (5%)	83,113,113	0.90	3 (3%)
21	CLA	32	604	33	69,73,73	1.19	4 (5%)	83,113,113	0.89	3 (3%)
21	CLA	42	610	16	64,68,73	1.24	4 (6%)	77,107,113	0.90	3 (3%)
28	LUT	8	617	-	42,43,43	0.29	0	51,60,60	0.42	0
21	CLA	A2	813	1	69,73,73	1.19	4 (5%)	83,113,113	0.93	3 (3%)
21	CLA	B2	815	2	69,73,73	1.18	4 (5%)	83,113,113	0.89	3 (3%)
26	LMU	4	626	-	20,20,36	0.15	0	25,25,47	0.28	0
28	LUT	82	617	-	42,43,43	0.29	0	51,60,60	0.42	0
30	CHL	62	618	18	47,51,74	2.11	9 (19%)	52,86,114	1.31	8 (15%)
24	BCR	4	621	-	41,41,41	0.13	0	56,56,56	0.36	0
30	CHL	62	606	33	62,66,74	1.84	8 (12%)	70,104,114	1.12	6 (8%)
30	CHL	4	608	-	70,74,74	1.74	9 (12%)	80,114,114	1.03	6 (7%)
23	LHG	9	622	21	40,40,48	0.25	0	43,46,54	0.28	0
26	LMU	A	863	-	36,36,36	0.10	0	47,47,47	0.27	0
21	CLA	12	603	12	61,65,73	1.27	4 (6%)	73,103,113	0.94	3 (4%)
31	XAT	6	624	-	39,47,47	0.12	0	54,74,74	0.60	0
21	CLA	G	204	7	50,54,73	1.40	4 (8%)	60,90,113	1.02	3 (5%)
21	CLA	B	816	2	69,73,73	1.17	4 (5%)	83,113,113	0.92	3 (3%)
21	CLA	A	810	1	69,73,73	1.22	4 (5%)	83,113,113	0.91	4 (4%)
21	CLA	K	206	11	49,53,73	1.41	4 (8%)	59,89,113	1.05	3 (5%)
23	LHG	3	721	-	30,30,48	0.27	0	33,36,54	0.35	0
26	LMU	8	627	-	36,36,36	0.10	0	47,47,47	0.37	0
24	BCR	B	846	-	41,41,41	0.13	0	56,56,56	0.33	0
27	LMG	1	624	-	36,36,55	0.20	0	44,44,63	0.19	0
21	CLA	Z	613	33	69,73,73	1.17	4 (5%)	83,113,113	0.91	4 (4%)
26	LMU	12	623	-	24,24,36	0.14	0	29,29,47	0.27	0
21	CLA	B2	825	33	69,73,73	1.18	5 (7%)	83,113,113	0.86	3 (3%)
21	CLA	B2	810	2	69,73,73	1.18	4 (5%)	83,113,113	0.90	3 (3%)
27	LMG	92	620	21	44,44,55	0.18	0	52,52,63	0.36	0
21	CLA	8	604	33	64,68,73	1.24	4 (6%)	77,107,113	0.93	3 (3%)
27	LMG	9	620	21	44,44,55	0.18	0	52,52,63	0.35	0
30	CHL	72	606	33	50,54,74	2.04	9 (18%)	56,90,114	1.23	7 (12%)
21	CLA	A	843	33	69,73,73	1.19	5 (7%)	83,113,113	0.91	3 (3%)
21	CLA	B2	839	33	69,73,73	1.20	4 (5%)	83,113,113	0.92	3 (3%)
31	XAT	72	622	-	39,47,47	0.12	0	54,74,74	0.57	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
21	CLA	A	840	1	69,73,73	1.19	4 (5%)	83,113,113	0.88	3 (3%)
21	CLA	82	612	15	59,63,73	1.26	4 (6%)	71,101,113	0.95	3 (4%)
21	CLA	82	611	23	49,53,73	1.41	4 (8%)	59,89,113	1.08	4 (6%)
23	LHG	4	622	21	48,48,48	0.24	0	51,54,54	0.27	0
21	CLA	A	817	33	59,63,73	1.31	4 (6%)	71,101,113	0.96	3 (4%)
21	CLA	82	616	15	49,53,73	1.40	4 (8%)	59,89,113	1.08	4 (6%)
22	PQN	B	842	-	34,34,34	0.31	0	42,45,45	0.37	0
30	CHL	72	607	33	50,54,74	2.03	7 (14%)	56,90,114	1.24	6 (10%)
21	CLA	A2	835	1	69,73,73	1.19	4 (5%)	83,113,113	0.90	4 (4%)
21	CLA	B2	836	2	64,68,73	1.22	4 (6%)	77,107,113	0.93	3 (3%)
21	CLA	6	602	18	69,73,73	1.19	4 (5%)	83,113,113	0.90	3 (3%)
21	CLA	52	616	17	57,61,73	1.31	4 (7%)	68,98,113	0.99	3 (4%)
24	BCR	7	623	-	41,41,41	0.15	0	56,56,56	0.38	0
21	CLA	B	813	2	69,73,73	1.18	4 (5%)	83,113,113	0.88	3 (3%)
30	CHL	1	606	33	50,54,74	2.05	9 (18%)	56,90,114	1.24	6 (10%)
23	LHG	4	623	-	37,37,48	0.25	0	40,43,54	0.28	0
31	XAT	Z2	618	-	39,47,47	0.14	0	54,74,74	0.56	0
21	CLA	B	837	2	69,73,73	1.19	5 (7%)	83,113,113	0.89	3 (3%)
24	BCR	52	622	-	41,41,41	0.17	0	56,56,56	0.32	0
21	CLA	1	614	12	64,68,73	1.24	4 (6%)	77,107,113	0.95	3 (3%)
21	CLA	A2	840	1	69,73,73	1.19	4 (5%)	83,113,113	0.88	3 (3%)
30	CHL	42	608	-	70,74,74	1.74	9 (12%)	80,114,114	1.03	6 (7%)
24	BCR	J2	102	-	41,41,41	0.16	0	56,56,56	0.30	0
21	CLA	A	842	1	69,73,73	1.16	5 (7%)	83,113,113	0.90	4 (4%)
27	LMG	A	859	-	48,48,55	0.18	0	56,56,63	0.17	0
21	CLA	A	825	1	59,63,73	1.30	5 (8%)	71,101,113	0.96	3 (4%)
21	CLA	B2	808	2	69,73,73	1.16	4 (5%)	83,113,113	0.89	4 (4%)
21	CLA	B	809	2	69,73,73	1.20	4 (5%)	83,113,113	0.88	4 (4%)
21	CLA	6	610	18	64,68,73	1.24	4 (6%)	77,107,113	0.92	3 (3%)
21	CLA	Z2	602	12	64,68,73	1.25	4 (6%)	77,107,113	0.94	3 (3%)
21	CLA	A	839	1	69,73,73	1.18	5 (7%)	83,113,113	0.90	3 (3%)
28	LUT	Z2	617	-	42,43,43	0.27	0	51,60,60	0.40	0
21	CLA	Z2	611	23	64,68,73	1.22	4 (6%)	77,107,113	0.93	3 (3%)
24	BCR	A2	850	-	41,41,41	0.15	0	56,56,56	0.24	0
21	CLA	Z2	613	33	69,73,73	1.17	4 (5%)	83,113,113	0.90	4 (4%)
21	CLA	B2	840	2	69,73,73	1.17	5 (7%)	83,113,113	0.90	3 (3%)
21	CLA	B	827	2	69,73,73	1.21	4 (5%)	83,113,113	0.90	3 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
26	LMU	8	625	-	24,24,36	0.12	0	29,29,47	0.28	0
21	CLA	B2	805	2	69,73,73	1.16	4 (5%)	83,113,113	0.91	3 (3%)
21	CLA	B	836	2	64,68,73	1.22	4 (6%)	77,107,113	0.94	3 (3%)
21	CLA	B	810	2	69,73,73	1.19	4 (5%)	83,113,113	0.90	3 (3%)
21	CLA	1	604	33	54,58,73	1.34	4 (7%)	65,95,113	1.02	3 (4%)
28	LUT	12	619	-	42,43,43	0.21	0	51,60,60	0.40	0
21	CLA	A	854	33	69,73,73	1.25	5 (7%)	83,113,113	0.86	3 (3%)
27	LMG	7	626	-	37,37,55	0.20	0	45,45,63	0.27	0
21	CLA	5	611	23	59,63,73	1.29	4 (6%)	71,101,113	0.96	3 (4%)
30	CHL	72	601	14	70,74,74	1.74	9 (12%)	80,114,114	1.04	6 (7%)
21	CLA	A	835	1	69,73,73	1.18	4 (5%)	83,113,113	0.90	3 (3%)
21	CLA	A2	823	1	69,73,73	1.20	5 (7%)	83,113,113	0.89	3 (3%)
21	CLA	B2	834	2	64,68,73	1.24	4 (6%)	77,107,113	0.94	3 (3%)
26	LMU	B2	853	-	36,36,36	0.13	0	47,47,47	0.67	2 (4%)
21	CLA	A2	833	1	69,73,73	1.20	5 (7%)	83,113,113	0.89	3 (3%)
21	CLA	A2	845	23	49,53,73	1.42	4 (8%)	59,89,113	1.03	3 (5%)
21	CLA	1	613	33	69,73,73	1.18	5 (7%)	83,113,113	0.90	3 (3%)
21	CLA	B2	823	2	69,73,73	1.19	5 (7%)	83,113,113	0.92	3 (3%)
24	BCR	L2	201	-	41,41,41	0.17	0	56,56,56	0.35	0
21	CLA	B	840	2	69,73,73	1.17	5 (7%)	83,113,113	0.90	3 (3%)
30	CHL	12	607	33	50,54,74	2.05	8 (16%)	56,90,114	1.27	9 (16%)
21	CLA	3	613	13	64,68,73	1.24	4 (6%)	77,107,113	0.93	3 (3%)
21	CLA	3	607	13	59,63,73	1.29	4 (6%)	71,101,113	0.95	4 (5%)
27	LMG	12	624	-	36,36,55	0.20	0	44,44,63	0.18	0
21	CLA	8	611	23	49,53,73	1.42	4 (8%)	59,89,113	1.08	4 (6%)
21	CLA	4	609	16	64,68,73	1.27	4 (6%)	77,107,113	0.93	3 (3%)
30	CHL	6	601	18	70,74,74	1.76	9 (12%)	80,114,114	1.07	7 (8%)
21	CLA	52	603	17	69,73,73	1.19	4 (5%)	83,113,113	0.89	4 (4%)
27	LMG	12	628	-	42,42,55	0.19	0	50,50,63	0.28	0
21	CLA	52	621	33	50,54,73	1.43	4 (8%)	60,90,113	1.12	6 (10%)
30	CHL	4	601	16	70,74,74	1.73	8 (11%)	80,114,114	1.05	6 (7%)
21	CLA	82	603	15	69,73,73	1.22	5 (7%)	83,113,113	0.87	3 (3%)
21	CLA	92	604	19	57,61,73	1.28	5 (8%)	68,98,113	0.97	4 (5%)
21	CLA	1	610	12	69,73,73	1.18	4 (5%)	83,113,113	0.89	3 (3%)
21	CLA	9	604	19	57,61,73	1.29	5 (8%)	68,98,113	0.98	4 (5%)
21	CLA	7	604	33	55,59,73	1.31	4 (7%)	66,96,113	0.99	3 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
21	CLA	5	613	17	60,64,73	1.26	4 (6%)	72,102,113	0.96	3 (4%)
23	LHG	62	629	-	35,35,48	0.27	0	38,41,54	0.28	0
31	XAT	82	618	-	39,47,47	0.15	0	54,74,74	0.57	0
26	LMU	A2	862	-	20,20,36	0.13	0	25,25,47	0.28	0
21	CLA	B	821	2	69,73,73	1.21	5 (7%)	83,113,113	0.90	4 (4%)
30	CHL	12	606	33	50,54,74	2.05	9 (18%)	56,90,114	1.24	6 (10%)
21	CLA	B	805	2	69,73,73	1.15	5 (7%)	83,113,113	0.90	3 (3%)
21	CLA	B	807	2	59,63,73	1.31	4 (6%)	71,101,113	0.96	3 (4%)
24	BCR	B2	847	-	41,41,41	0.19	0	56,56,56	0.41	0
27	LMG	1	628	-	42,42,55	0.19	0	50,50,63	0.28	0
28	LUT	A	856	-	42,43,43	0.28	0	51,60,60	0.35	0
28	LUT	72	624	-	42,43,43	0.21	0	51,60,60	0.41	0
30	CHL	62	607	33	70,74,74	1.75	8 (11%)	80,114,114	1.08	7 (8%)
26	LMU	62	630	-	24,24,36	0.15	0	29,29,47	0.28	0
25	SF4	C	101	3	0,12,12	-	-	-		
30	CHL	7	607	33	50,54,74	2.03	8 (16%)	56,90,114	1.25	6 (10%)
21	CLA	62	614	18	54,58,73	1.34	4 (7%)	65,95,113	1.02	3 (4%)
21	CLA	A	802	-	69,73,73	1.17	5 (7%)	83,113,113	0.84	2 (2%)
21	CLA	3	602	13	64,68,73	1.24	5 (7%)	77,107,113	0.92	3 (3%)
21	CLA	K2	204	11	50,54,73	1.38	4 (8%)	60,90,113	1.06	3 (5%)
21	CLA	12	609	12	69,73,73	1.20	4 (5%)	83,113,113	0.90	4 (4%)
21	CLA	5	601	17	69,73,73	1.18	4 (5%)	83,113,113	0.88	2 (2%)
28	LUT	Z2	619	-	26,26,43	0.36	0	34,35,60	0.37	0
21	CLA	A	807	1	69,73,73	1.20	5 (7%)	83,113,113	0.84	3 (3%)
26	LMU	72	629	-	28,28,36	0.10	0	39,39,47	0.27	0
21	CLA	12	608	33	69,73,73	1.20	4 (5%)	83,113,113	0.90	3 (3%)
21	CLA	A2	821	1	59,63,73	1.28	4 (6%)	71,101,113	0.93	3 (4%)
24	BCR	L2	205	-	41,41,41	0.15	0	56,56,56	0.37	0
21	CLA	B	802	2	69,73,73	1.18	4 (5%)	83,113,113	0.91	5 (6%)
21	CLA	6	603	18	69,73,73	1.19	4 (5%)	83,113,113	0.86	3 (3%)
21	CLA	62	612	18	49,53,73	1.39	4 (8%)	59,89,113	1.04	3 (5%)
21	CLA	A2	807	1	69,73,73	1.19	5 (7%)	83,113,113	0.84	3 (3%)
21	CLA	92	609	19	55,59,73	1.33	4 (7%)	66,96,113	1.00	4 (6%)
30	CHL	1	601	12	70,74,74	1.72	8 (11%)	80,114,114	1.03	6 (7%)
24	BCR	82	619	-	41,41,41	0.14	0	56,56,56	0.32	0
28	LUT	3	622	-	42,43,43	0.31	0	51,60,60	0.34	0
26	LMU	Z	621	-	22,22,36	0.15	0	27,27,47	0.26	0

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
31	XAT	4	620	-	-	0/31/93/93	0/4/4/4
23	LHG	Z	620	21	-	7/43/43/53	-
26	LMU	7	628	-	-	3/13/33/61	0/1/1/2
21	CLA	42	602	16	-	2/33/109/115	-
26	LMU	A	862	-	-	2/11/31/61	0/1/1/2
21	CLA	A2	854	33	-	1/39/115/115	-
21	CLA	B2	818	2	-	4/39/115/115	-
21	CLA	42	611	23	-	6/33/109/115	-
23	LHG	8	620	21	-	16/48/48/53	-
23	LHG	42	623	-	-	15/42/42/53	-
30	CHL	62	601	18	-	8/41/117/117	-
24	BCR	K2	207	-	-	4/29/63/63	0/2/2/2
21	CLA	72	602	14	-	2/39/115/115	-
26	LMU	72	628	-	-	3/13/33/61	0/1/1/2
21	CLA	72	612	14	-	3/24/100/115	-
24	BCR	8	619	-	-	4/29/63/63	0/2/2/2
27	LMG	B	854	-	-	2/31/51/70	0/1/1/1
21	CLA	72	611	23	-	7/39/115/115	-
30	CHL	6	616	18	-	5/41/117/117	-
32	NEX	62	625	-	-	5/27/83/83	0/3/3/3
26	LMU	Z	622	-	-	3/17/57/61	0/2/2/2
26	LMU	K2	208	-	-	3/15/35/61	0/1/1/2
21	CLA	A2	827	33	-	3/39/115/115	-
21	CLA	4	613	16	-	7/39/115/115	-
21	CLA	A2	818	1	-	2/39/115/115	-
21	CLA	A	804	1	-	5/39/115/115	-
21	CLA	Z2	603	12	-	6/27/103/115	-
21	CLA	6	613	33	-	4/39/115/115	-
24	BCR	32	620	-	-	4/29/63/63	0/2/2/2
30	CHL	7	601	14	-	5/41/117/117	-
21	CLA	72	608	33	-	0/21/97/115	-
21	CLA	42	604	33	-	2/21/97/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	LMU	K	208	-	-	3/15/35/61	0/1/1/2
21	CLA	B2	806	2	-	3/39/115/115	-
26	LMU	A	857	-	-	3/20/60/61	0/2/2/2
30	CHL	12	601	12	-	10/41/117/117	-
26	LMU	82	628	-	-	4/15/35/61	0/1/1/2
26	LMU	82	625	-	-	2/15/35/61	0/1/1/2
30	CHL	5	607	33	-	8/41/117/117	-
21	CLA	L	204	-	-	2/15/91/115	-
23	LHG	6	619	21	-	5/53/53/53	-
26	LMU	62	632	-	-	3/11/31/61	0/1/1/2
26	LMU	12	621	-	-	6/21/61/61	0/2/2/2
30	CHL	42	618	16	-	4/17/93/117	-
26	LMU	12	625	-	-	5/15/35/61	0/1/1/2
21	CLA	Z	608	33	-	2/21/97/115	-
21	CLA	L2	203	10	-	8/39/115/115	-
21	CLA	A	814	1	-	5/39/115/115	-
21	CLA	A	826	33	-	9/39/115/115	-
30	CHL	82	607	33	-	8/41/117/117	-
21	CLA	B	819	33	-	5/33/109/115	-
21	CLA	Z	614	12	-	0/21/97/115	-
21	CLA	B2	816	2	-	1/39/115/115	-
26	LMU	Z2	621	-	-	2/13/33/61	0/1/1/2
27	LMG	6	633	-	-	1/17/17/70	-
21	CLA	B2	826	2	-	5/39/115/115	-
21	CLA	3	609	13	-	3/35/111/115	-
21	CLA	A2	810	1	-	8/39/115/115	-
21	CLA	62	611	23	-	4/31/107/115	-
22	PQN	A	844	-	-	3/23/43/43	0/2/2/2
24	BCR	3	620	-	-	4/29/63/63	0/2/2/2
26	LMU	A	858	-	-	6/21/61/61	0/2/2/2
21	CLA	A2	809	1	-	7/39/115/115	-
27	LMG	3	722	-	-	6/46/46/70	-
21	CLA	82	614	15	-	9/30/106/115	-
21	CLA	A	829	1	-	7/39/115/115	-
23	LHG	72	625	21	-	15/53/53/53	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	CLA	B2	803	-	-	2/39/115/115	-
24	BCR	A	848	-	-	2/29/63/63	0/2/2/2
21	CLA	K	203	33	-	4/33/109/115	-
25	SF4	C2	101	3	-	-	0/6/5/5
21	CLA	62	604	-	-	4/39/115/115	-
30	CHL	5	606	33	-	2/17/93/117	-
21	CLA	A	845	23	-	4/15/91/115	-
30	CHL	52	606	33	-	2/17/93/117	-
21	CLA	A	811	1	-	5/39/115/115	-
20	CL0	A2	801	1	-	3/39/115/115	-
28	LUT	7	621	-	-	2/29/67/67	0/2/2/2
21	CLA	5	617	17	-	8/39/115/115	-
25	SF4	A2	853	2,1	-	-	0/6/5/5
26	LMU	12	626	-	-	0/15/35/61	0/1/1/2
21	CLA	8	612	15	-	6/27/103/115	-
27	LMG	8	629	-	-	8/37/57/70	0/1/1/1
21	CLA	A	833	1	-	1/39/115/115	-
21	CLA	42	603	16	-	7/39/115/115	-
21	CLA	A2	804	1	-	5/39/115/115	-
21	CLA	B	824	33	-	3/39/115/115	-
21	CLA	72	603	14	-	5/24/100/115	-
21	CLA	52	609	17	-	2/39/115/115	-
26	LMU	A2	864	-	-	2/15/35/61	0/1/1/2
21	CLA	B2	837	2	-	2/39/115/115	-
23	LHG	1	620	21	-	9/43/43/53	-
24	BCR	5	622	-	-	3/29/63/63	0/2/2/2
27	LMG	J2	103	-	-	2/37/57/70	0/1/1/1
28	LUT	32	622	-	-	2/29/67/67	0/2/2/2
21	CLA	6	604	-	-	4/39/115/115	-
21	CLA	Z2	614	12	-	0/21/97/115	-
31	XAT	52	624	-	1/1/26/26	0/31/93/93	0/4/4/4
27	LMG	A	860	-	-	6/31/51/70	0/1/1/1
21	CLA	B	803	-	-	2/39/115/115	-
21	CLA	A2	842	1	-	3/39/115/115	-
26	LMU	1	622	-	-	4/10/30/61	0/1/1/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	LUT	3	720	-	-	0/29/67/67	0/2/2/2
30	CHL	92	607	33	-	9/23/99/117	-
23	LHG	B2	851	21	-	13/49/49/53	-
24	BCR	3	719	-	-	2/29/63/63	0/2/2/2
21	CLA	A	809	1	-	7/39/115/115	-
28	LUT	52	620	-	-	2/29/67/67	0/2/2/2
21	CLA	62	613	33	-	5/39/115/115	-
21	CLA	G2	203	7	-	3/33/109/115	-
21	CLA	62	610	18	-	2/33/109/115	-
21	CLA	B	826	2	-	5/39/115/115	-
26	LMU	62	628	-	-	2/15/35/61	0/1/1/2
30	CHL	9	607	33	-	10/23/99/117	-
21	CLA	52	611	23	-	4/27/103/115	-
21	CLA	Z2	604	33	-	3/30/106/115	-
21	CLA	Z	616	12	-	4/33/109/115	-
21	CLA	62	603	18	-	7/39/115/115	-
21	CLA	A	813	1	-	5/39/115/115	-
26	LMU	82	624	-	-	1/15/35/61	0/1/1/2
28	LUT	F	305	-	-	5/29/67/67	0/2/2/2
21	CLA	B	828	2	-	6/39/115/115	-
21	CLA	B2	827	2	-	5/39/115/115	-
21	CLA	A2	803	33	-	2/39/115/115	-
21	CLA	A2	841	1	-	9/39/115/115	-
21	CLA	A2	836	1	-	6/39/115/115	-
24	BCR	I2	172	-	-	0/29/63/63	0/2/2/2
27	LMG	4	624	-	-	5/36/56/70	0/1/1/1
27	LMG	82	626	-	-	6/27/47/70	0/1/1/1
21	CLA	B	839	33	-	6/39/115/115	-
23	LHG	6	629	-	-	10/40/40/53	-
21	CLA	A	815	1	-	3/27/103/115	-
21	CLA	62	622	33	-	3/27/103/115	-
21	CLA	12	612	12	-	5/15/91/115	-
22	PQN	B2	842	-	-	1/23/43/43	0/2/2/2
30	CHL	42	607	33	-	2/41/117/117	-
26	LMU	A	864	-	-	2/15/35/61	0/1/1/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
30	CHL	9	606	-	-	0/12/88/117	-
21	CLA	L2	204	-	-	2/15/91/115	-
23	LHG	B	851	21	-	13/49/49/53	-
21	CLA	8	616	15	-	0/15/91/115	-
21	CLA	B	811	2	-	8/39/115/115	-
21	CLA	7	608	33	-	0/21/97/115	-
24	BCR	72	623	-	-	2/29/63/63	0/2/2/2
24	BCR	A	850	-	-	1/29/63/63	0/2/2/2
21	CLA	A2	814	1	-	6/39/115/115	-
27	LMG	32	722	-	-	5/46/46/70	-
21	CLA	B2	817	2	-	8/39/115/115	-
31	XAT	5	624	-	1/1/26/26	0/31/93/93	0/4/4/4
26	LMU	G	206	-	-	4/15/35/61	0/1/1/2
21	CLA	12	604	33	-	1/21/97/115	-
30	CHL	4	607	33	-	2/41/117/117	-
21	CLA	42	614	16	-	4/27/103/115	-
21	CLA	9	611	23	-	6/39/115/115	-
27	LMG	B	852	-	-	7/38/58/70	0/1/1/1
21	CLA	G	203	7	-	3/33/109/115	-
21	CLA	32	607	13	-	5/27/103/115	-
21	CLA	72	614	14	-	6/13/89/115	-
30	CHL	6	618	18	-	4/14/90/117	-
21	CLA	A2	805	1	-	1/27/103/115	-
26	LMU	6	632	-	-	3/11/31/61	0/1/1/2
21	CLA	B2	821	2	-	4/39/115/115	-
21	CLA	Z	602	12	-	1/33/109/115	-
21	CLA	A2	824	1	-	4/15/91/115	-
21	CLA	Z	611	23	-	6/33/109/115	-
26	LMU	Z2	622	-	-	3/17/57/61	0/2/2/2
21	CLA	B	829	2	-	3/39/115/115	-
21	CLA	1	609	12	-	5/39/115/115	-
30	CHL	4	618	16	-	4/17/93/117	-
21	CLA	7	612	14	-	3/24/100/115	-
30	CHL	4	606	33	-	1/29/105/117	-
21	CLA	Z2	616	12	-	4/33/109/115	-
27	LMG	72	626	-	-	7/32/52/70	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	CLA	A	834	1	-	7/39/115/115	-
21	CLA	A2	843	33	-	6/39/115/115	-
21	CLA	F	303	33	-	2/15/91/115	-
21	CLA	A	832	1	-	1/27/103/115	-
21	CLA	B	812	2	-	2/39/115/115	-
24	BCR	B	844	-	-	0/29/63/63	0/2/2/2
23	LHG	A	847	21	-	6/42/42/53	-
30	CHL	42	606	33	-	1/29/105/117	-
21	CLA	Z	610	12	-	0/33/109/115	-
21	CLA	A	836	1	-	6/39/115/115	-
21	CLA	8	608	33	-	2/21/97/115	-
28	LUT	62	621	-	-	2/29/67/67	0/2/2/2
21	CLA	B	806	2	-	3/39/115/115	-
21	CLA	F	304	6	-	9/39/115/115	-
27	LMG	42	624	-	-	5/36/56/70	0/1/1/1
31	XAT	62	624	-	-	0/31/93/93	0/4/4/4
21	CLA	82	610	15	-	2/39/115/115	-
21	CLA	4	614	16	-	4/27/103/115	-
21	CLA	A	821	1	-	4/27/103/115	-
32	NEX	6	625	-	-	4/27/83/83	0/3/3/3
26	LMU	42	625	-	-	3/19/59/61	0/2/2/2
21	CLA	3	614	13	-	2/15/91/115	-
21	CLA	B	814	2	-	3/33/109/115	-
23	LHG	A2	847	21	-	6/42/42/53	-
27	LMG	A2	860	-	-	7/31/51/70	0/1/1/1
28	LUT	9	617	-	-	0/29/67/67	0/2/2/2
21	CLA	B	832	2	-	5/39/115/115	-
21	CLA	5	609	17	-	2/39/115/115	-
28	LUT	5	620	-	-	2/29/67/67	0/2/2/2
21	CLA	4	612	16	-	4/15/91/115	-
26	LMU	8	628	-	-	4/15/35/61	0/1/1/2
21	CLA	A	805	1	-	1/27/103/115	-
28	LUT	6	621	-	-	2/29/67/67	0/2/2/2
24	BCR	K2	202	-	-	2/29/63/63	0/2/2/2
21	CLA	82	608	33	-	2/21/97/115	-
30	CHL	92	606	-	-	0/12/88/117	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
30	CHL	5	618	17	-	4/14/90/117	-
28	LUT	Z	619	-	-	2/18/37/67	0/1/1/2
21	CLA	B2	802	2	-	6/39/115/115	-
26	LMU	G2	206	-	-	4/15/35/61	0/1/1/2
21	CLA	6	609	18	-	4/27/103/115	-
26	LMU	6	628	-	-	2/15/35/61	0/1/1/2
21	CLA	3	604	33	-	1/39/115/115	-
24	BCR	B	801	-	-	0/29/63/63	0/2/2/2
21	CLA	Z2	610	12	-	0/33/109/115	-
21	CLA	3	615	33	-	6/39/115/115	-
27	LMG	82	629	-	-	8/37/57/70	0/1/1/1
21	CLA	42	616	16	-	0/15/91/115	-
21	CLA	72	616	14	-	4/17/93/115	-
21	CLA	82	602	15	-	2/36/112/115	-
21	CLA	Z	603	12	-	6/27/103/115	-
27	LMG	B2	854	-	-	2/31/51/70	0/1/1/1
21	CLA	8	613	15	-	7/39/115/115	-
27	LMG	A2	859	-	-	8/43/63/70	0/1/1/1
21	CLA	B	838	2	-	1/21/97/115	-
21	CLA	92	613	19	-	6/39/115/115	-
21	CLA	A2	838	1	-	1/23/99/115	-
21	CLA	9	613	19	-	6/39/115/115	-
21	CLA	A2	806	1	-	12/39/115/115	-
21	CLA	72	604	33	-	1/23/99/115	-
21	CLA	1	611	23	-	5/35/111/115	-
26	LMU	9	624	-	-	4/15/35/61	0/1/1/2
21	CLA	B2	804	2	-	5/15/91/115	-
24	BCR	62	623	-	-	2/29/63/63	0/2/2/2
21	CLA	A2	812	1	-	8/39/115/115	-
21	CLA	52	617	17	-	8/39/115/115	-
30	CHL	6	608	33	-	0/23/99/117	-
21	CLA	12	610	12	-	2/39/115/115	-
23	LHG	32	721	-	-	12/35/35/53	-
26	LMU	12	622	-	-	4/10/30/61	0/1/1/2
21	CLA	B	830	2	-	0/15/91/115	-
21	CLA	72	620	33	-	7/25/101/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	CLA	3	617	13	-	2/17/93/115	-
26	LMU	6	631	-	-	4/15/35/61	0/1/1/2
21	CLA	8	609	15	-	0/15/91/115	-
21	CLA	A2	826	33	-	9/39/115/115	-
30	CHL	6	607	33	-	7/41/117/117	-
21	CLA	4	616	16	-	0/15/91/115	-
21	CLA	A2	839	1	-	2/39/115/115	-
30	CHL	7	606	33	-	3/17/93/117	-
23	LHG	7	625	21	-	16/53/53/53	-
28	LUT	9	616	-	-	2/29/67/67	0/2/2/2
21	CLA	7	602	14	-	2/39/115/115	-
21	CLA	J2	101	9	-	5/27/103/115	-
30	CHL	Z	606	33	-	5/17/93/117	-
31	XAT	Z	618	-	-	0/31/93/93	0/4/4/4
21	CLA	7	611	23	-	7/39/115/115	-
30	CHL	8	607	33	-	8/41/117/117	-
30	CHL	3	608	33	-	3/41/117/117	-
21	CLA	3	606	33	-	0/12/88/115	-
21	CLA	9	609	19	-	4/23/99/115	-
21	CLA	5	603	17	-	16/39/115/115	-
26	LMU	72	627	-	-	2/18/58/61	0/2/2/2
21	CLA	A2	834	1	-	7/39/115/115	-
22	PQN	A2	844	-	-	3/23/43/43	0/2/2/2
24	BCR	K	202	-	-	2/29/63/63	0/2/2/2
21	CLA	A2	832	1	-	1/27/103/115	-
26	LMU	A2	858	-	-	6/21/61/61	0/2/2/2
30	CHL	Z2	607	33	-	4/41/117/117	-
21	CLA	A	820	1	-	8/39/115/115	-
24	BCR	A	851	-	-	2/29/63/63	0/2/2/2
21	CLA	32	614	13	-	2/15/91/115	-
21	CLA	A	838	1	-	1/23/99/115	-
21	CLA	42	612	16	-	4/15/91/115	-
21	CLA	B2	829	2	-	4/39/115/115	-
28	LUT	1	619	-	-	2/29/67/67	0/2/2/2
23	LHG	Z2	620	21	-	6/43/43/53	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	CLA	A2	811	1	-	5/39/115/115	-
21	CLA	B2	824	33	-	3/39/115/115	-
21	CLA	6	611	23	-	4/31/107/115	-
21	CLA	8	610	15	-	2/39/115/115	-
21	CLA	A	830	1	-	4/39/115/115	-
21	CLA	A	831	1	-	2/39/115/115	-
28	LUT	F2	305	-	-	5/29/67/67	0/2/2/2
28	LUT	52	626	-	-	4/29/67/67	0/2/2/2
25	SF4	A	853	2,1	-	-	0/6/5/5
21	CLA	B2	841	23	-	7/39/115/115	-
21	CLA	82	609	15	-	0/15/91/115	-
21	CLA	4	611	23	-	6/33/109/115	-
21	CLA	8	603	15	-	5/39/115/115	-
21	CLA	1	603	12	-	4/30/106/115	-
26	LMU	12	627	-	-	3/13/33/61	0/1/1/2
26	LMU	1	621	-	-	6/21/61/61	0/2/2/2
21	CLA	A2	819	1	-	3/33/109/115	-
21	CLA	4	610	16	-	3/33/109/115	-
30	CHL	8	601	15	-	12/41/117/117	-
23	LHG	12	620	21	-	9/43/43/53	-
21	CLA	1	616	12	-	4/17/93/115	-
21	CLA	42	613	16	-	7/39/115/115	-
24	BCR	L	201	-	-	4/29/63/63	0/2/2/2
26	LMU	A2	865	-	-	3/15/35/61	0/1/1/2
21	CLA	F	301	33	-	3/39/115/115	-
30	CHL	Z2	601	12	-	9/41/117/117	-
28	LUT	32	720	-	-	0/29/67/67	0/2/2/2
21	CLA	A	818	1	-	2/39/115/115	-
21	CLA	72	610	14	-	6/39/115/115	-
30	CHL	1	607	33	-	3/17/93/117	-
21	CLA	Z	604	33	-	3/30/106/115	-
24	BCR	G2	205	-	-	2/29/63/63	0/2/2/2
21	CLA	B	823	2	-	7/39/115/115	-
21	CLA	F2	303	33	-	2/15/91/115	-
21	CLA	B	833	2	-	4/31/107/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	LMG	J	103	-	-	2/37/57/70	0/1/1/1
28	LUT	3	621	-	-	2/29/67/67	0/2/2/2
32	NEX	52	625	-	-	2/27/83/83	1/3/3/3
21	CLA	B	841	23	-	7/39/115/115	-
21	CLA	5	602	17	-	0/39/115/115	-
24	BCR	A2	851	-	-	2/29/63/63	0/2/2/2
24	BCR	92	623	-	-	2/29/63/63	0/2/2/2
21	CLA	5	614	17	-	4/15/91/115	-
28	LUT	7	624	-	-	4/29/67/67	0/2/2/2
26	LMU	A	861	-	-	3/15/35/61	0/1/1/2
30	CHL	8	606	33	-	3/41/117/117	-
21	CLA	9	603	27,19	-	6/27/103/115	-
21	CLA	F2	301	33	-	3/39/115/115	-
21	CLA	K2	201	11	-	3/15/91/115	-
31	XAT	1	618	-	-	0/31/93/93	0/4/4/4
21	CLA	B	804	2	-	5/15/91/115	-
21	CLA	F2	304	6	-	9/39/115/115	-
21	CLA	A2	831	1	-	2/39/115/115	-
21	CLA	A2	815	1	-	3/27/103/115	-
21	CLA	5	612	17	-	5/15/91/115	-
21	CLA	52	610	17	-	2/33/109/115	-
27	LMG	8	626	-	-	6/27/47/70	0/1/1/1
24	BCR	A2	852	-	-	4/29/63/63	0/2/2/2
21	CLA	82	604	33	-	2/33/109/115	-
21	CLA	3	610	13	-	0/39/115/115	-
21	CLA	9	602	19	-	2/33/109/115	-
21	CLA	92	614	19	-	5/15/91/115	-
31	XAT	8	618	-	-	0/31/93/93	0/4/4/4
21	CLA	32	615	33	-	6/39/115/115	-
21	CLA	Z2	609	12	-	9/39/115/115	-
30	CHL	62	616	18	-	5/41/117/117	-
21	CLA	B	831	2	-	1/27/103/115	-
27	LMG	B2	852	-	-	7/38/58/70	0/1/1/1
21	CLA	62	602	18	-	2/39/115/115	-
28	LUT	42	619	-	-	2/29/67/67	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	BCR	B	843	-	-	0/29/63/63	0/2/2/2
21	CLA	4	603	16	-	7/39/115/115	-
20	CL0	A	801	1	-	3/39/115/115	-
21	CLA	A2	825	1	-	8/27/103/115	-
21	CLA	3	603	13	-	5/39/115/115	-
24	BCR	G	205	-	-	2/29/63/63	0/2/2/2
21	CLA	62	617	18	-	4/15/91/115	-
21	CLA	92	612	19	-	6/39/115/115	-
23	LHG	62	619	21	-	5/53/53/53	-
21	CLA	92	601	19	-	2/17/93/115	-
24	BCR	B2	844	-	-	0/29/63/63	0/2/2/2
25	SF4	C	102	3	-	-	0/6/5/5
29	DGD	B	850	-	-	15/48/88/95	0/2/2/2
21	CLA	B2	809	2	-	6/39/115/115	-
21	CLA	4	602	16	-	2/33/109/115	-
21	CLA	32	602	13	-	1/33/109/115	-
21	CLA	32	609	13	-	3/35/111/115	-
28	LUT	A2	856	-	-	4/29/67/67	0/2/2/2
23	LHG	52	623	21	-	12/41/41/53	-
24	BCR	9	623	-	-	2/29/63/63	0/2/2/2
21	CLA	A2	830	1	-	4/39/115/115	-
21	CLA	B2	835	33	-	1/15/91/115	-
21	CLA	A	837	1	-	3/30/106/115	-
28	LUT	Z	617	-	-	2/29/67/67	0/2/2/2
21	CLA	7	620	33	-	7/25/101/115	-
21	CLA	B	815	2	-	4/39/115/115	-
21	CLA	3	612	13	-	3/17/93/115	-
21	CLA	A2	837	1	-	3/30/106/115	-
23	LHG	A2	846	-	-	10/53/53/53	-
23	LHG	3	623	-	-	13/51/51/53	-
24	BCR	L	205	-	-	2/29/63/63	0/2/2/2
28	LUT	4	619	-	-	2/29/67/67	0/2/2/2
21	CLA	32	610	13	-	0/39/115/115	-
21	CLA	9	614	19	-	5/15/91/115	-
26	LMU	82	627	-	-	9/21/61/61	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	CLA	5	616	17	-	6/25/101/115	-
26	LMU	1	626	-	-	0/15/35/61	0/1/1/2
21	CLA	B2	832	2	-	5/39/115/115	-
26	LMU	1	625	-	-	5/15/35/61	0/1/1/2
26	LMU	52	627	-	-	1/15/35/61	0/1/1/2
21	CLA	7	614	14	-	6/13/89/115	-
21	CLA	K2	203	33	-	4/33/109/115	-
21	CLA	A2	822	33	-	0/39/115/115	-
21	CLA	7	613	14	-	1/39/115/115	-
21	CLA	B	825	33	-	2/39/115/115	-
21	CLA	5	604	33	-	4/27/103/115	-
21	CLA	9	612	19	-	5/39/115/115	-
24	BCR	B	847	-	-	2/29/63/63	0/2/2/2
26	LMU	62	631	-	-	4/15/35/61	0/1/1/2
21	CLA	5	621	33	-	10/17/93/115	-
21	CLA	52	604	33	-	4/27/103/115	-
24	BCR	B2	843	-	-	0/29/63/63	0/2/2/2
21	CLA	A	803	33	-	2/39/115/115	-
21	CLA	82	613	15	-	7/39/115/115	-
21	CLA	B	817	2	-	8/39/115/115	-
21	CLA	J	101	9	-	5/27/103/115	-
21	CLA	B	835	33	-	0/15/91/115	-
25	SF4	C2	102	3	-	-	0/6/5/5
24	BCR	B2	801	-	-	0/29/63/63	0/2/2/2
21	CLA	Z	612	12	-	4/15/91/115	-
21	CLA	52	612	17	-	5/15/91/115	-
21	CLA	A	827	33	-	3/39/115/115	-
21	CLA	B	834	2	-	8/33/109/115	-
21	CLA	12	602	12	-	2/33/109/115	-
21	CLA	Z2	608	33	-	2/21/97/115	-
21	CLA	8	614	15	-	9/30/106/115	-
21	CLA	52	613	17	-	6/29/105/115	-
26	LMU	7	627	-	-	2/18/58/61	0/2/2/2
21	CLA	62	609	18	-	4/27/103/115	-
21	CLA	42	609	16	-	7/33/109/115	-
21	CLA	Z	609	12	-	9/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	BCR	B2	845	-	-	4/29/63/63	0/2/2/2
21	CLA	A2	828	1	-	6/39/115/115	-
28	LUT	72	621	-	-	2/29/67/67	0/2/2/2
29	DGD	B2	850	-	-	10/48/88/95	0/2/2/2
24	BCR	42	621	-	-	2/29/63/63	0/2/2/2
28	LUT	32	621	-	-	2/29/67/67	0/2/2/2
26	LMU	5	627	-	-	1/15/35/61	0/1/1/2
21	CLA	B	808	2	-	9/39/115/115	-
30	CHL	52	618	17	-	4/14/90/117	-
21	CLA	72	609	14	-	2/15/91/115	-
21	CLA	32	603	13	-	5/39/115/115	-
21	CLA	92	611	23	-	6/39/115/115	-
21	CLA	B2	828	2	-	6/39/115/115	-
31	XAT	7	622	-	-	0/31/93/93	0/4/4/4
21	CLA	B2	830	2	-	0/15/91/115	-
28	LUT	5	626	-	-	4/29/67/67	0/2/2/2
21	CLA	A	822	33	-	0/39/115/115	-
21	CLA	A	808	1	-	1/21/97/115	-
21	CLA	B2	822	2	-	5/32/108/115	-
21	CLA	K	201	11	-	3/15/91/115	-
21	CLA	A2	802	-	-	0/39/115/115	-
21	CLA	92	602	19	-	2/33/109/115	-
21	CLA	B2	807	2	-	4/27/103/115	-
26	LMU	4	625	-	-	3/19/59/61	0/2/2/2
28	LUT	1	617	-	-	2/29/67/67	0/2/2/2
30	CHL	82	606	33	-	3/41/117/117	-
24	BCR	B	845	-	-	4/29/63/63	0/2/2/2
21	CLA	12	614	12	-	7/33/109/115	-
21	CLA	K2	206	11	-	4/15/91/115	-
21	CLA	6	622	33	-	3/27/103/115	-
32	NEX	5	625	-	-	2/27/83/83	1/3/3/3
21	CLA	32	612	13	-	3/17/93/115	-
21	CLA	7	616	14	-	4/17/93/115	-
21	CLA	52	602	17	-	0/39/115/115	-
26	LMU	1	623	-	-	1/15/35/61	0/1/1/2
23	LHG	32	623	-	-	13/51/51/53	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	BCR	J	102	-	-	2/29/63/63	0/2/2/2
26	LMU	1	627	-	-	3/13/33/61	0/1/1/2
27	LMG	J	104	-	-	8/30/50/70	0/1/1/1
26	LMU	B	853	-	-	7/21/61/61	0/2/2/2
30	CHL	Z	607	33	-	4/41/117/117	-
21	CLA	A	828	1	-	6/39/115/115	-
24	BCR	32	719	-	-	2/29/63/63	0/2/2/2
26	LMU	8	624	-	-	1/15/35/61	0/1/1/2
21	CLA	3	611	-	-	5/39/115/115	-
21	CLA	A2	817	33	-	4/27/103/115	-
26	LMU	92	624	-	-	4/15/35/61	0/1/1/2
28	LUT	92	617	-	-	0/29/67/67	0/2/2/2
21	CLA	5	610	17	-	2/33/109/115	-
21	CLA	6	617	18	-	3/15/91/115	-
21	CLA	B	822	2	-	5/32/108/115	-
21	CLA	8	602	15	-	1/36/112/115	-
21	CLA	B2	812	2	-	3/39/115/115	-
30	CHL	52	608	33	-	0/23/99/117	-
30	CHL	82	601	15	-	12/41/117/117	-
21	CLA	1	612	12	-	5/15/91/115	-
21	CLA	A	819	1	-	3/33/109/115	-
24	BCR	3	718	-	-	2/29/63/63	0/2/2/2
21	CLA	K	204	11	-	3/17/93/115	-
30	CHL	5	608	33	-	0/23/99/117	-
21	CLA	4	604	33	-	2/21/97/115	-
30	CHL	52	607	33	-	8/41/117/117	-
21	CLA	B2	814	2	-	3/33/109/115	-
21	CLA	B2	811	2	-	8/39/115/115	-
26	LMU	A2	857	-	-	3/20/60/61	0/2/2/2
24	BCR	A2	849	-	-	0/29/63/63	0/2/2/2
21	CLA	B2	819	33	-	5/33/109/115	-
31	XAT	42	620	-	-	0/31/93/93	0/4/4/4
24	BCR	A2	848	-	-	2/29/63/63	0/2/2/2
26	LMU	7	629	-	-	4/13/53/61	0/2/2/2
21	CLA	A2	808	1	-	1/21/97/115	-
21	CLA	72	613	14	-	1/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	CLA	92	610	19	-	0/33/109/115	-
21	CLA	9	610	19	-	0/33/109/115	-
21	CLA	32	613	13	-	5/33/109/115	-
21	CLA	A	806	1	-	12/39/115/115	-
24	BCR	K	207	-	-	4/29/63/63	0/2/2/2
26	LMU	6	630	-	-	1/15/35/61	0/1/1/2
31	XAT	12	618	-	-	0/31/93/93	0/4/4/4
21	CLA	A	841	1	-	9/39/115/115	-
21	CLA	7	610	14	-	6/39/115/115	-
24	BCR	B2	848	-	-	2/29/63/63	0/2/2/2
21	CLA	A	812	1	-	8/39/115/115	-
21	CLA	1	608	33	-	2/39/115/115	-
21	CLA	92	603	27,19	-	6/27/103/115	-
24	BCR	A	849	-	-	0/29/63/63	0/2/2/2
28	LUT	12	617	-	-	2/29/67/67	0/2/2/2
21	CLA	A2	820	1	-	8/39/115/115	-
23	LHG	5	623	21	-	12/41/41/53	-
27	LMG	62	633	-	-	1/17/17/70	-
21	CLA	9	601	19	-	2/17/93/115	-
21	CLA	7	609	14	-	2/15/91/115	-
21	CLA	12	611	23	-	5/35/111/115	-
24	BCR	I	172	-	-	0/29/63/63	0/2/2/2
21	CLA	7	603	14	-	4/24/100/115	-
21	CLA	12	616	12	-	4/17/93/115	-
30	CHL	Z2	606	33	-	5/17/93/117	-
24	BCR	A	852	-	-	4/29/63/63	0/2/2/2
21	CLA	G2	204	7	-	4/17/93/115	-
26	LMU	A	865	-	-	3/15/35/61	0/1/1/2
21	CLA	A2	816	1	-	6/39/115/115	-
21	CLA	B2	820	2	-	6/29/105/115	-
21	CLA	6	612	18	-	2/15/91/115	-
21	CLA	B2	833	2	-	4/31/107/115	-
21	CLA	52	601	17	-	5/39/115/115	-
21	CLA	1	602	12	-	2/33/109/115	-
21	CLA	B2	838	2	-	1/21/97/115	-
23	LHG	42	622	21	-	13/53/53/53	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	LMU	42	626	-	-	0/11/31/61	0/1/1/2
21	CLA	Z2	612	12	-	4/15/91/115	-
24	BCR	B	848	-	-	2/29/63/63	0/2/2/2
21	CLA	B2	831	2	-	1/27/103/115	-
21	CLA	A2	829	1	-	7/39/115/115	-
21	CLA	52	614	17	-	4/15/91/115	-
26	LMU	A2	863	-	-	7/21/61/61	0/2/2/2
21	CLA	32	611	-	-	5/39/115/115	-
21	CLA	B	818	2	-	4/39/115/115	-
28	LUT	92	616	-	-	2/29/67/67	0/2/2/2
24	BCR	6	623	-	-	2/29/63/63	0/2/2/2
26	LMU	A2	861	-	-	3/15/35/61	0/1/1/2
21	CLA	32	617	13	-	2/17/93/115	-
24	BCR	B2	846	-	-	2/29/63/63	0/2/2/2
30	CHL	42	601	16	-	6/41/117/117	-
27	LMG	J2	104	-	-	8/30/50/70	0/1/1/1
23	LHG	82	620	21	-	16/48/48/53	-
21	CLA	B	820	2	-	7/29/105/115	-
21	CLA	A	824	1	-	4/15/91/115	-
30	CHL	Z	601	12	-	9/41/117/117	-
30	CHL	6	606	33	-	0/32/108/117	-
23	LHG	A	846	-	-	10/53/53/53	-
21	CLA	L	203	10	-	8/39/115/115	-
21	CLA	A	823	1	-	8/39/115/115	-
21	CLA	6	614	18	-	2/21/97/115	-
21	CLA	B2	813	2	-	4/39/115/115	-
23	LHG	92	622	21	-	13/45/45/53	-
30	CHL	32	608	33	-	3/41/117/117	-
24	BCR	32	718	-	-	2/29/63/63	0/2/2/2
21	CLA	12	613	33	-	6/39/115/115	-
21	CLA	32	606	33	-	0/12/88/115	-
30	CHL	62	608	33	-	0/23/99/117	-
21	CLA	A	816	1	-	6/39/115/115	-
21	CLA	32	604	33	-	1/39/115/115	-
21	CLA	42	610	16	-	3/33/109/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	LUT	8	617	-	-	2/29/67/67	0/2/2/2
21	CLA	A2	813	1	-	5/39/115/115	-
21	CLA	B2	815	2	-	4/39/115/115	-
26	LMU	4	626	-	-	0/11/31/61	0/1/1/2
28	LUT	82	617	-	-	2/29/67/67	0/2/2/2
30	CHL	62	618	18	-	4/14/90/117	-
24	BCR	4	621	-	-	2/29/63/63	0/2/2/2
30	CHL	62	606	33	-	0/32/108/117	-
30	CHL	4	608	-	-	3/41/117/117	-
23	LHG	9	622	21	-	13/45/45/53	-
26	LMU	A	863	-	-	7/21/61/61	0/2/2/2
21	CLA	12	603	12	-	4/30/106/115	-
31	XAT	6	624	-	-	0/31/93/93	0/4/4/4
21	CLA	G	204	7	-	4/17/93/115	-
21	CLA	B	816	2	-	1/39/115/115	-
21	CLA	A	810	1	-	8/39/115/115	-
21	CLA	K	206	11	-	4/15/91/115	-
23	LHG	3	721	-	-	12/35/35/53	-
26	LMU	8	627	-	-	9/21/61/61	0/2/2/2
24	BCR	B	846	-	-	2/29/63/63	0/2/2/2
27	LMG	1	624	-	-	4/31/51/70	0/1/1/1
21	CLA	Z	613	33	-	4/39/115/115	-
26	LMU	12	623	-	-	1/15/35/61	0/1/1/2
21	CLA	B2	825	33	-	3/39/115/115	-
21	CLA	B2	810	2	-	3/39/115/115	-
27	LMG	92	620	21	-	6/39/59/70	0/1/1/1
21	CLA	8	604	33	-	2/33/109/115	-
27	LMG	9	620	21	-	6/39/59/70	0/1/1/1
30	CHL	72	606	33	-	3/17/93/117	-
21	CLA	A	843	33	-	6/39/115/115	-
21	CLA	B2	839	33	-	6/39/115/115	-
31	XAT	72	622	-	-	0/31/93/93	0/4/4/4
21	CLA	A	840	1	-	9/39/115/115	-
21	CLA	82	612	15	-	6/27/103/115	-
21	CLA	82	611	23	-	2/15/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	LHG	4	622	21	-	13/53/53/53	-
21	CLA	A	817	33	-	4/27/103/115	-
21	CLA	82	616	15	-	0/15/91/115	-
22	PQN	B	842	-	-	1/23/43/43	0/2/2/2
30	CHL	72	607	33	-	3/17/93/117	-
21	CLA	A2	835	1	-	6/39/115/115	-
21	CLA	B2	836	2	-	5/33/109/115	-
21	CLA	6	602	18	-	2/39/115/115	-
21	CLA	52	616	17	-	6/25/101/115	-
24	BCR	7	623	-	-	2/29/63/63	0/2/2/2
21	CLA	B	813	2	-	4/39/115/115	-
30	CHL	1	606	33	-	0/17/93/117	-
23	LHG	4	623	-	-	15/42/42/53	-
31	XAT	Z2	618	-	-	0/31/93/93	0/4/4/4
21	CLA	B	837	2	-	2/39/115/115	-
24	BCR	52	622	-	-	3/29/63/63	0/2/2/2
21	CLA	1	614	12	-	6/33/109/115	-
21	CLA	A2	840	1	-	9/39/115/115	-
30	CHL	42	608	-	-	3/41/117/117	-
24	BCR	J2	102	-	-	2/29/63/63	0/2/2/2
21	CLA	A	842	1	-	3/39/115/115	-
27	LMG	A	859	-	-	8/43/63/70	0/1/1/1
21	CLA	A	825	1	-	8/27/103/115	-
21	CLA	B2	808	2	-	9/39/115/115	-
21	CLA	B	809	2	-	6/39/115/115	-
21	CLA	6	610	18	-	3/33/109/115	-
21	CLA	Z2	602	12	-	1/33/109/115	-
21	CLA	A	839	1	-	2/39/115/115	-
28	LUT	Z2	617	-	-	2/29/67/67	0/2/2/2
21	CLA	Z2	611	23	-	6/33/109/115	-
24	BCR	A2	850	-	-	1/29/63/63	0/2/2/2
21	CLA	Z2	613	33	-	4/39/115/115	-
21	CLA	B2	840	2	-	7/39/115/115	-
21	CLA	B	827	2	-	5/39/115/115	-
26	LMU	8	625	-	-	2/15/35/61	0/1/1/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	CLA	B2	805	2	-	9/39/115/115	-
21	CLA	B	836	2	-	5/33/109/115	-
21	CLA	B	810	2	-	3/39/115/115	-
21	CLA	1	604	33	-	1/21/97/115	-
28	LUT	12	619	-	-	2/29/67/67	0/2/2/2
21	CLA	A	854	33	-	1/39/115/115	-
27	LMG	7	626	-	-	7/32/52/70	0/1/1/1
21	CLA	5	611	23	-	4/27/103/115	-
30	CHL	72	601	14	-	5/41/117/117	-
21	CLA	A	835	1	-	6/39/115/115	-
21	CLA	A2	823	1	-	8/39/115/115	-
21	CLA	B2	834	2	-	8/33/109/115	-
26	LMU	B2	853	-	-	7/21/61/61	0/2/2/2
21	CLA	A2	833	1	-	1/39/115/115	-
21	CLA	A2	845	23	-	4/15/91/115	-
21	CLA	1	613	33	-	6/39/115/115	-
21	CLA	B2	823	2	-	7/39/115/115	-
24	BCR	L2	201	-	-	4/29/63/63	0/2/2/2
21	CLA	B	840	2	-	7/39/115/115	-
30	CHL	12	607	33	-	3/17/93/117	-
21	CLA	3	613	13	-	5/33/109/115	-
21	CLA	3	607	13	-	4/27/103/115	-
27	LMG	12	624	-	-	4/31/51/70	0/1/1/1
21	CLA	8	611	23	-	2/15/91/115	-
21	CLA	4	609	16	-	7/33/109/115	-
30	CHL	6	601	18	-	8/41/117/117	-
21	CLA	52	603	17	-	16/39/115/115	-
27	LMG	12	628	-	-	6/37/57/70	0/1/1/1
21	CLA	52	621	33	-	10/17/93/115	-
30	CHL	4	601	16	-	6/41/117/117	-
21	CLA	82	603	15	-	5/39/115/115	-
21	CLA	92	604	19	-	1/25/101/115	-
21	CLA	1	610	12	-	2/39/115/115	-
21	CLA	9	604	19	-	1/25/101/115	-
21	CLA	7	604	33	-	1/23/99/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	CLA	5	613	17	-	6/29/105/115	-
23	LHG	62	629	-	-	10/40/40/53	-
31	XAT	82	618	-	-	0/31/93/93	0/4/4/4
26	LMU	A2	862	-	-	2/11/31/61	0/1/1/2
21	CLA	B	821	2	-	5/39/115/115	-
30	CHL	12	606	33	-	0/17/93/117	-
21	CLA	B	805	2	-	9/39/115/115	-
21	CLA	B	807	2	-	4/27/103/115	-
24	BCR	B2	847	-	-	2/29/63/63	0/2/2/2
27	LMG	1	628	-	-	6/37/57/70	0/1/1/1
28	LUT	A	856	-	-	4/29/67/67	0/2/2/2
28	LUT	72	624	-	-	4/29/67/67	0/2/2/2
30	CHL	62	607	33	-	7/41/117/117	-
26	LMU	62	630	-	-	1/15/35/61	0/1/1/2
25	SF4	C	101	3	-	-	0/6/5/5
30	CHL	7	607	33	-	3/17/93/117	-
21	CLA	62	614	18	-	2/21/97/115	-
21	CLA	A	802	-	-	0/39/115/115	-
21	CLA	3	602	13	-	1/33/109/115	-
21	CLA	K2	204	11	-	3/17/93/115	-
21	CLA	12	609	12	-	5/39/115/115	-
21	CLA	5	601	17	-	5/39/115/115	-
28	LUT	Z2	619	-	-	2/18/37/67	0/1/1/2
21	CLA	A	807	1	-	4/39/115/115	-
26	LMU	72	629	-	-	4/13/53/61	0/2/2/2
21	CLA	12	608	33	-	2/39/115/115	-
21	CLA	A2	821	1	-	4/27/103/115	-
24	BCR	L2	205	-	-	2/29/63/63	0/2/2/2
21	CLA	B	802	2	-	6/39/115/115	-
21	CLA	6	603	18	-	7/39/115/115	-
21	CLA	62	612	18	-	2/15/91/115	-
21	CLA	A2	807	1	-	4/39/115/115	-
21	CLA	92	609	19	-	4/23/99/115	-
30	CHL	1	601	12	-	10/41/117/117	-
24	BCR	82	619	-	-	4/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	LUT	3	622	-	-	2/29/67/67	0/2/2/2
26	LMU	Z	621	-	-	2/13/33/61	0/1/1/2

The worst 5 of 2211 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	62	601	CHL	MG-NB	-7.46	1.91	2.05
30	6	601	CHL	MG-NB	-7.43	1.91	2.05
30	Z	601	CHL	MG-NB	-7.41	1.91	2.05
30	Z2	601	CHL	MG-NB	-7.41	1.91	2.05
30	9	607	CHL	MG-NB	-7.33	1.91	2.05

The worst 5 of 1692 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	92	610	CLA	C1D-ND-C4D	-4.52	103.12	106.33
21	9	610	CLA	C1D-ND-C4D	-4.50	103.14	106.33
21	Z	613	CLA	C1D-ND-C4D	-4.41	103.20	106.33
21	9	604	CLA	C1D-ND-C4D	-4.38	103.22	106.33
30	3	608	CHL	CHD-C1D-ND	-4.36	120.44	124.45

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
31	5	624	XAT	C26
31	52	624	XAT	C26

5 of 2876 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
21	A	806	CLA	CHA-CBD-CGD-O1D
21	A	806	CLA	CHA-CBD-CGD-O2D
21	A	806	CLA	CAD-CBD-CGD-O1D
21	A	806	CLA	CAD-CBD-CGD-O2D
21	A	806	CLA	C4-C3-C5-C6

All (2) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
32	52	625	NEX	C1-C2-C3-C4-C5-C6
32	5	625	NEX	C1-C2-C3-C4-C5-C6

300 monomers are involved in 403 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
26	7	628	LMU	1	0
26	A	862	LMU	2	0
21	A2	854	CLA	3	0
23	42	623	LHG	1	0
30	62	601	CHL	3	0
24	K2	207	BCR	2	0
26	72	628	LMU	1	0
24	8	619	BCR	2	0
27	B	854	LMG	1	0
32	62	625	NEX	1	0
26	Z	622	LMU	1	0
21	4	613	CLA	2	0
21	A2	818	CLA	1	0
21	A	804	CLA	1	0
21	Z2	603	CLA	3	0
30	7	601	CHL	3	0
21	72	608	CLA	1	0
21	B2	806	CLA	1	0
26	A	857	LMU	1	0
21	Z	608	CLA	1	0
21	B2	816	CLA	2	0
21	B2	826	CLA	1	0
21	3	609	CLA	1	0
21	A2	810	CLA	1	0
24	3	620	BCR	1	0
26	A	858	LMU	2	0
21	A2	809	CLA	2	0
27	3	722	LMG	1	0
21	A	829	CLA	3	0
23	72	625	LHG	1	0
24	A	848	BCR	3	0
21	A	811	CLA	3	0
21	8	612	CLA	1	0
21	A	833	CLA	3	0
21	A2	804	CLA	1	0
21	B2	837	CLA	1	0
23	1	620	LHG	1	0
27	J2	103	LMG	1	0
28	32	622	LUT	2	0
27	A	860	LMG	1	0
24	3	719	BCR	5	0
21	A	809	CLA	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
28	52	620	LUT	3	0
21	B	826	CLA	1	0
21	Z	616	CLA	2	0
21	62	603	CLA	1	0
21	A	813	CLA	3	0
28	F	305	LUT	3	0
21	B2	827	CLA	1	0
21	A2	803	CLA	1	0
24	I2	172	BCR	1	0
21	B	839	CLA	1	0
30	42	607	CHL	1	0
21	7	608	CLA	1	0
24	A	850	BCR	1	0
27	32	722	LMG	1	0
21	B2	817	CLA	1	0
30	4	607	CHL	1	0
21	42	614	CLA	1	0
21	32	607	CLA	1	0
21	B2	821	CLA	1	0
26	Z2	622	LMU	1	0
21	B	829	CLA	6	0
30	4	606	CHL	2	0
21	Z2	616	CLA	2	0
21	A2	843	CLA	1	0
24	B	844	BCR	3	0
21	Z	610	CLA	1	0
28	62	621	LUT	1	0
21	B	806	CLA	1	0
21	F	304	CLA	1	0
31	62	624	XAT	1	0
21	4	614	CLA	1	0
32	6	625	NEX	1	0
26	42	625	LMU	1	0
21	B	814	CLA	1	0
27	A2	860	LMG	1	0
28	9	617	LUT	2	0
28	5	620	LUT	3	0
28	6	621	LUT	1	0
24	K2	202	BCR	4	0
21	B2	802	CLA	3	0
24	B	801	BCR	1	0
21	Z2	610	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
21	3	615	CLA	5	0
21	Z	603	CLA	2	0
27	B2	854	LMG	1	0
21	8	613	CLA	1	0
21	A2	806	CLA	1	0
26	9	624	LMU	1	0
24	62	623	BCR	1	0
21	A2	812	CLA	1	0
21	52	617	CLA	1	0
30	6	608	CHL	2	0
21	72	620	CLA	1	0
30	6	607	CHL	1	0
23	7	625	LHG	1	0
28	9	616	LUT	1	0
21	J2	101	CLA	1	0
30	3	608	CHL	2	0
21	5	603	CLA	3	0
24	K	202	BCR	3	0
21	A2	832	CLA	1	0
26	A2	858	LMU	1	0
24	A	851	BCR	3	0
21	B2	829	CLA	6	0
23	Z2	620	LHG	1	0
21	A2	811	CLA	2	0
21	A	831	CLA	2	0
28	F2	305	LUT	2	0
21	B2	841	CLA	2	0
21	8	603	CLA	1	0
21	1	603	CLA	3	0
30	8	601	CHL	1	0
23	12	620	LHG	1	0
21	42	613	CLA	3	0
24	L	201	BCR	1	0
30	Z2	601	CHL	1	0
21	A	818	CLA	1	0
21	72	610	CLA	3	0
24	G2	205	BCR	2	0
21	B	823	CLA	1	0
21	B	833	CLA	1	0
27	J	103	LMG	1	0
21	B	841	CLA	2	0
21	5	602	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	A2	851	BCR	1	0
24	92	623	BCR	2	0
28	7	624	LUT	4	0
30	8	606	CHL	1	0
21	K2	201	CLA	2	0
31	1	618	XAT	1	0
21	F2	304	CLA	1	0
21	A2	831	CLA	1	0
21	52	610	CLA	1	0
27	8	626	LMG	1	0
24	A2	852	BCR	2	0
21	82	604	CLA	1	0
21	3	610	CLA	2	0
21	92	614	CLA	1	0
21	32	615	CLA	6	0
21	62	602	CLA	1	0
28	42	619	LUT	1	0
24	B	843	BCR	2	0
21	3	603	CLA	2	0
24	B2	844	BCR	2	0
29	B	850	DGD	1	0
21	32	602	CLA	1	0
21	32	609	CLA	1	0
28	A2	856	LUT	2	0
23	52	623	LHG	1	0
24	9	623	BCR	1	0
21	A2	830	CLA	1	0
21	B2	835	CLA	1	0
28	Z	617	LUT	2	0
21	7	620	CLA	1	0
23	3	623	LHG	1	0
24	L	205	BCR	4	0
28	4	619	LUT	1	0
21	32	610	CLA	3	0
21	9	614	CLA	1	0
21	5	616	CLA	3	0
21	B2	832	CLA	1	0
21	A2	822	CLA	1	0
24	B	847	BCR	1	0
21	5	621	CLA	3	0
24	B2	843	BCR	2	0
21	A	803	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
21	82	613	CLA	1	0
21	B	817	CLA	1	0
21	J	101	CLA	1	0
21	B	835	CLA	1	0
24	B2	801	BCR	3	0
21	B	834	CLA	1	0
21	12	602	CLA	1	0
21	Z2	608	CLA	1	0
24	B2	845	BCR	2	0
29	B2	850	DGD	1	0
24	42	621	BCR	1	0
21	B	808	CLA	1	0
21	72	609	CLA	1	0
21	32	603	CLA	2	0
21	A	822	CLA	1	0
21	B2	822	CLA	1	0
21	K	201	CLA	2	0
21	A2	802	CLA	2	0
26	4	625	LMU	1	0
28	1	617	LUT	2	0
30	82	606	CHL	1	0
24	B	845	BCR	3	0
21	52	602	CLA	1	0
23	32	623	LHG	1	0
24	J	102	BCR	1	0
27	J	104	LMG	1	0
26	B	853	LMU	3	0
24	32	719	BCR	4	0
21	3	611	CLA	1	0
21	A2	817	CLA	1	0
26	92	624	LMU	1	0
28	92	617	LUT	2	0
21	B	822	CLA	1	0
30	52	608	CHL	1	0
30	82	601	CHL	1	0
24	3	718	BCR	1	0
30	5	608	CHL	1	0
21	B2	814	CLA	1	0
26	A2	857	LMU	1	0
24	A2	849	BCR	2	0
24	A2	848	BCR	2	0
24	K	207	BCR	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
31	12	618	XAT	1	0
21	7	610	CLA	3	0
24	B2	848	BCR	1	0
21	A	812	CLA	1	0
24	A	849	BCR	2	0
28	12	617	LUT	2	0
21	A2	820	CLA	1	0
23	5	623	LHG	1	0
21	7	609	CLA	1	0
24	I	172	BCR	1	0
24	A	852	BCR	4	0
21	1	602	CLA	1	0
24	B	848	BCR	1	0
21	A2	829	CLA	2	0
21	32	611	CLA	1	0
28	92	616	LUT	1	0
24	6	623	BCR	2	0
30	42	601	CHL	1	0
27	J2	104	LMG	1	0
30	Z	601	CHL	1	0
30	6	606	CHL	1	0
21	L	203	CLA	1	0
30	32	608	CHL	3	0
21	12	613	CLA	1	0
30	62	608	CHL	2	0
21	42	610	CLA	1	0
21	A2	813	CLA	2	0
28	82	617	LUT	1	0
30	62	606	CHL	1	0
26	A	863	LMU	2	0
21	12	603	CLA	3	0
31	6	624	XAT	1	0
21	B	816	CLA	2	0
21	A	810	CLA	2	0
26	8	627	LMU	1	0
21	Z	613	CLA	1	0
27	92	620	LMG	1	0
21	8	604	CLA	1	0
27	9	620	LMG	1	0
21	A	843	CLA	1	0
21	B2	839	CLA	1	0
31	72	622	XAT	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
21	A	840	CLA	1	0
21	A	817	CLA	1	0
21	A2	835	CLA	1	0
21	B2	836	CLA	1	0
21	6	602	CLA	1	0
21	52	616	CLA	2	0
23	4	623	LHG	1	0
21	B	837	CLA	2	0
21	A2	840	CLA	1	0
24	J2	102	BCR	1	0
21	B2	808	CLA	1	0
28	Z2	617	LUT	2	0
21	Z2	611	CLA	1	0
24	A2	850	BCR	3	0
21	Z2	613	CLA	1	0
21	B2	840	CLA	3	0
21	B	827	CLA	1	0
21	B	836	CLA	1	0
21	A	854	CLA	2	0
30	72	601	CHL	2	0
21	A	835	CLA	1	0
21	B2	834	CLA	1	0
26	B2	853	LMU	2	0
21	A2	833	CLA	3	0
21	1	613	CLA	1	0
21	B2	823	CLA	1	0
24	L2	201	BCR	1	0
21	B	840	CLA	2	0
21	3	607	CLA	1	0
21	4	609	CLA	1	0
30	6	601	CHL	3	0
21	52	603	CLA	3	0
21	52	621	CLA	2	0
30	4	601	CHL	1	0
21	82	603	CLA	1	0
21	B	821	CLA	1	0
24	B2	847	BCR	1	0
28	A	856	LUT	1	0
28	72	624	LUT	4	0
30	62	607	CHL	1	0
21	A	802	CLA	2	0
21	3	602	CLA	1	0

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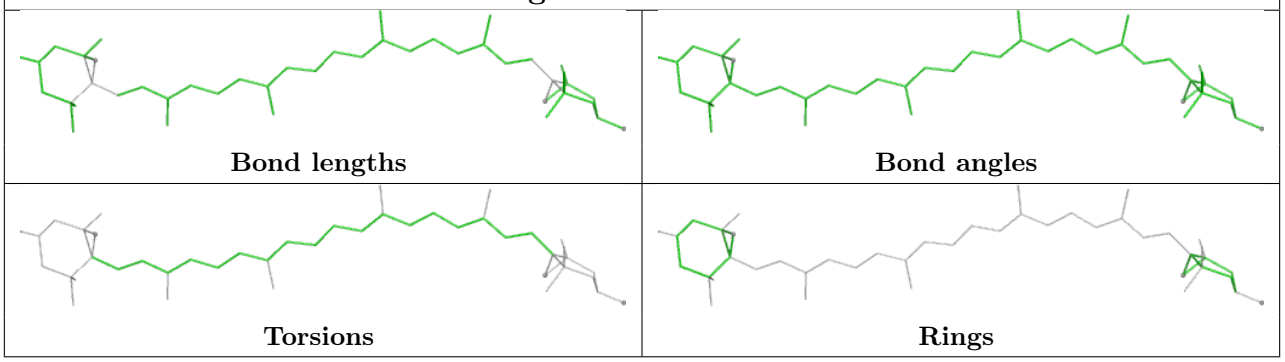
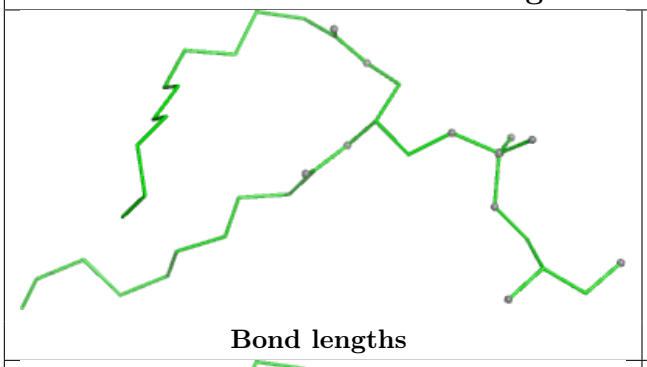
Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	L2	205	BCR	4	0
21	B	802	CLA	2	0
21	6	603	CLA	1	0
30	1	601	CHL	1	0
24	82	619	BCR	2	0
28	3	622	LUT	2	0

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.

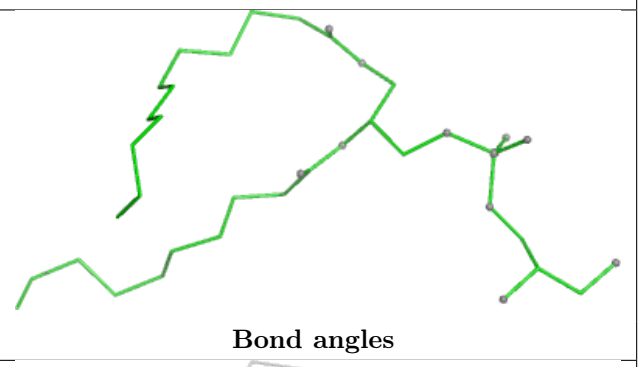
Ligand XAT 4 620



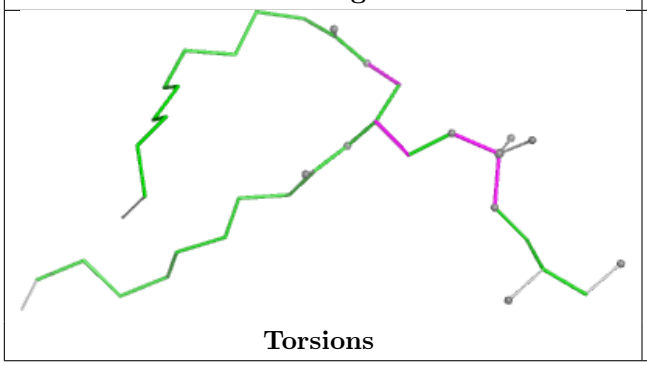
Ligand LHG Z 620



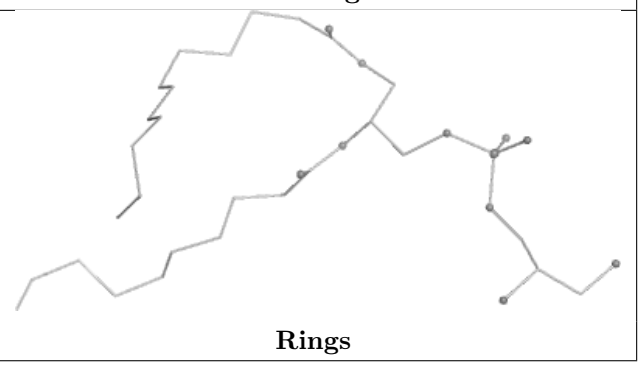
Bond lengths



Bond angles

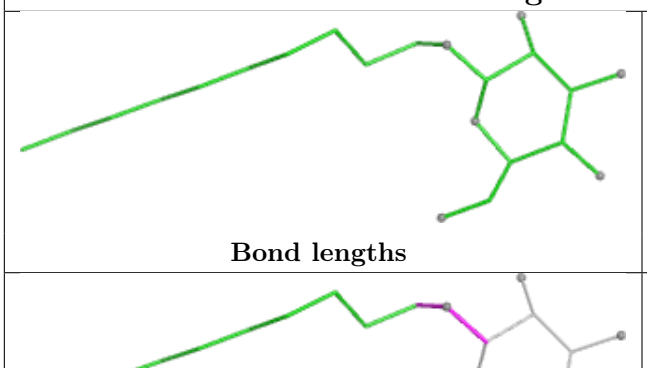


Torsions



Rings

Ligand LMU 7 628



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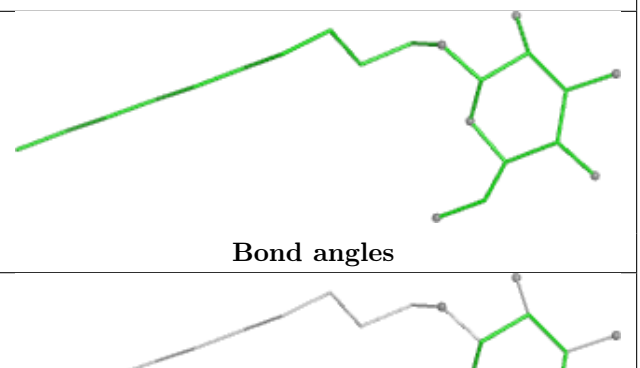

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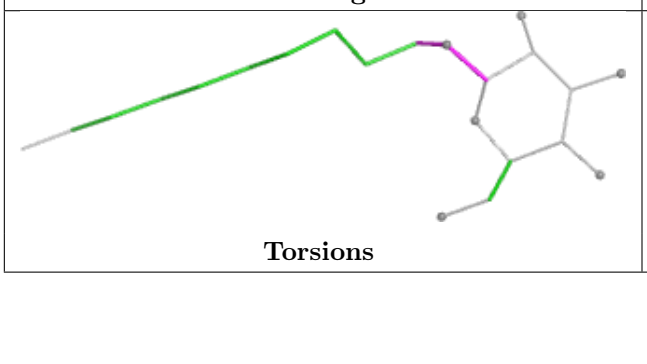

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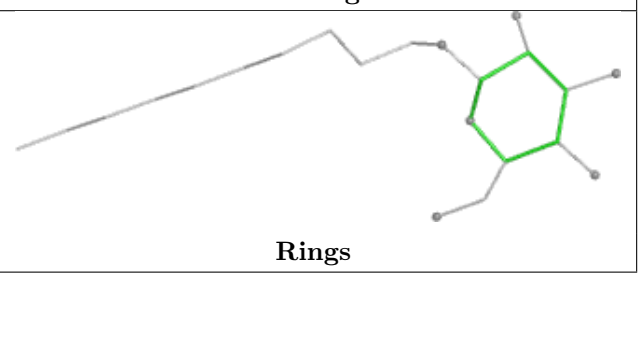
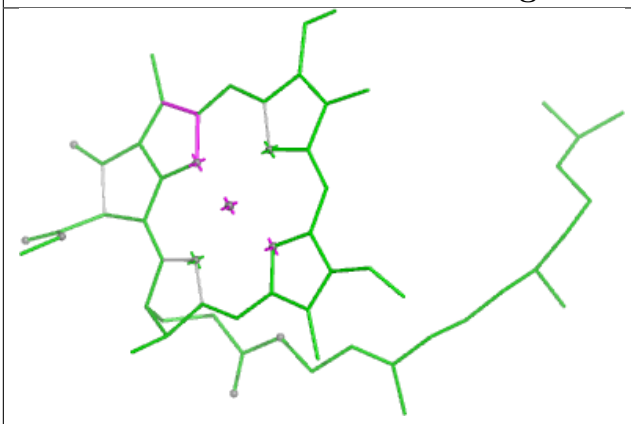


Rings

Ligand CLA 42 602



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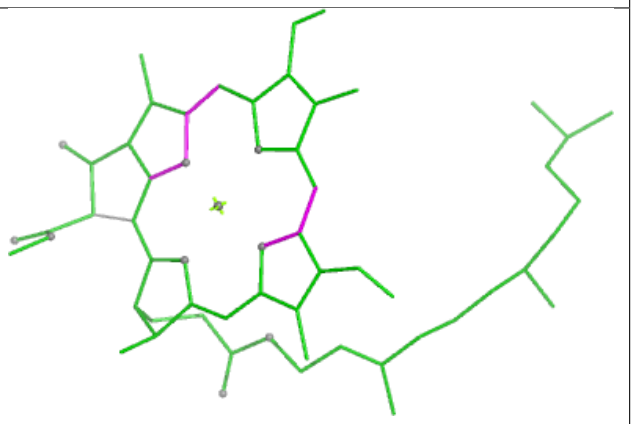
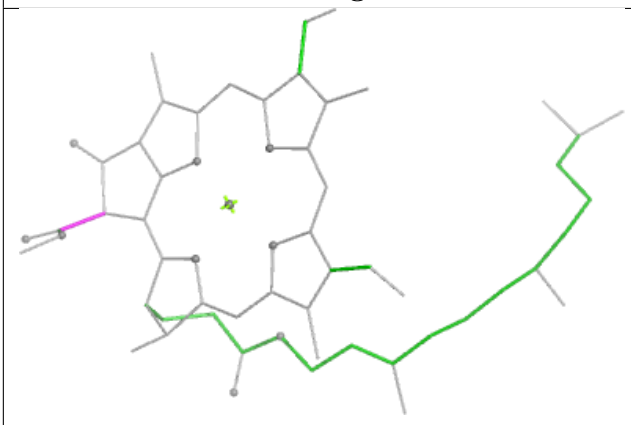
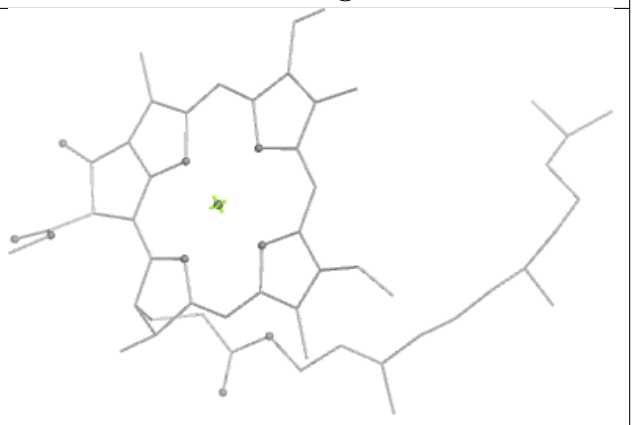


Bond angles

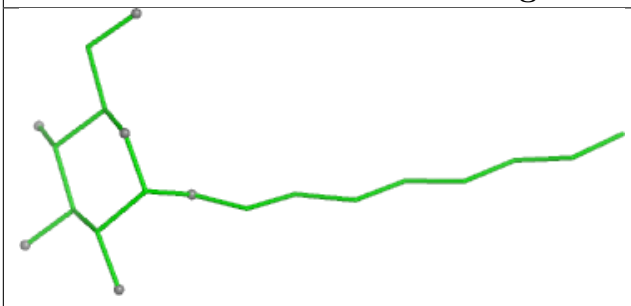


Torsions



Rings

Ligand LMU A 862



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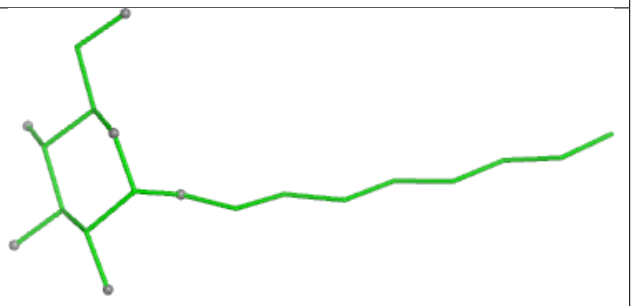
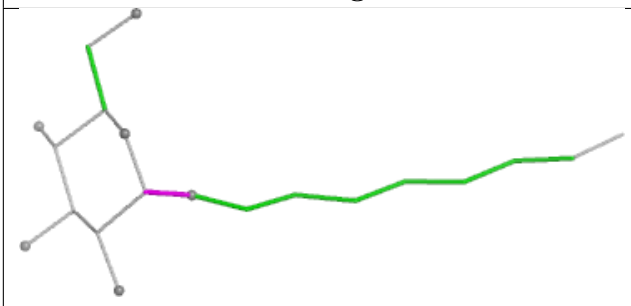


Bond angles



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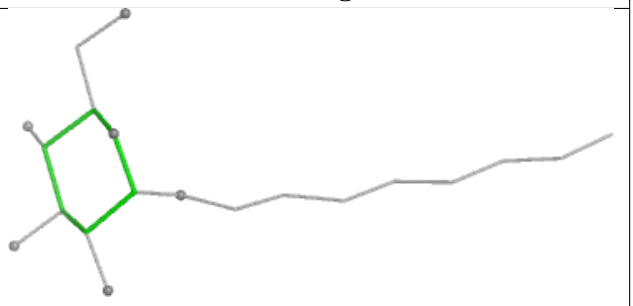
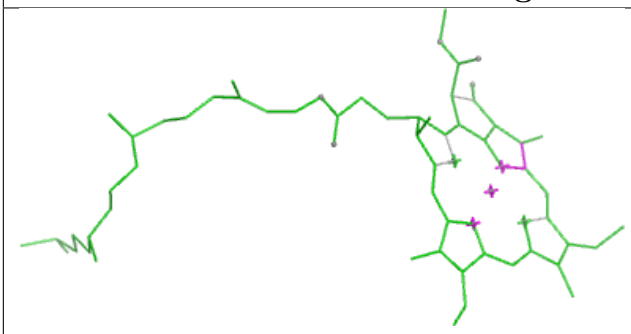


Rings

Ligand CLA A2 854



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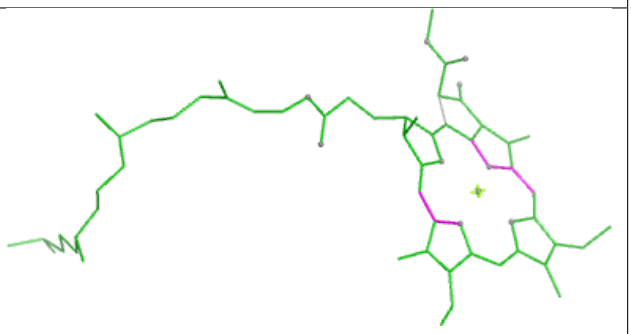

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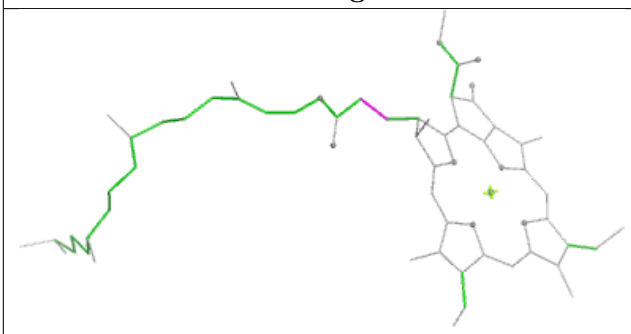

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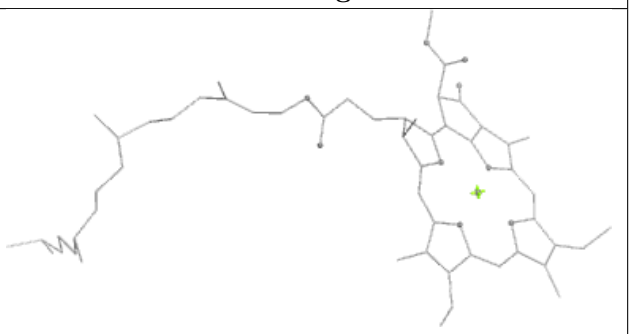
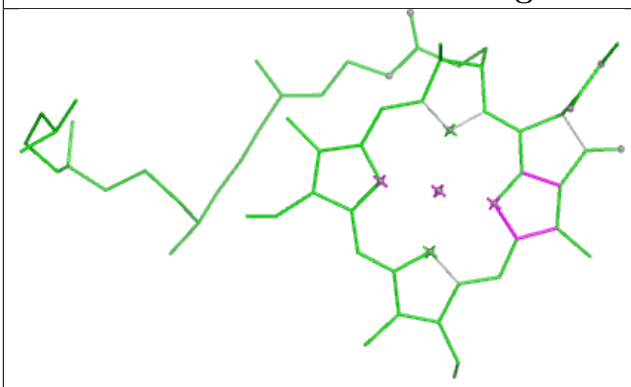


Rings

Ligand CLA B2 818



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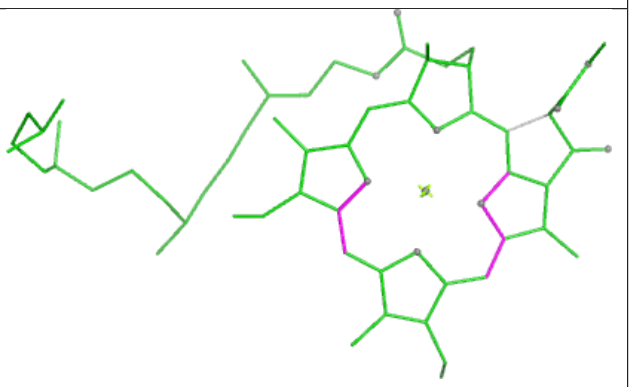

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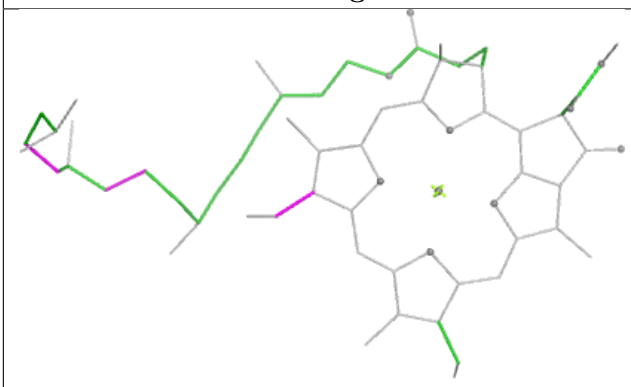

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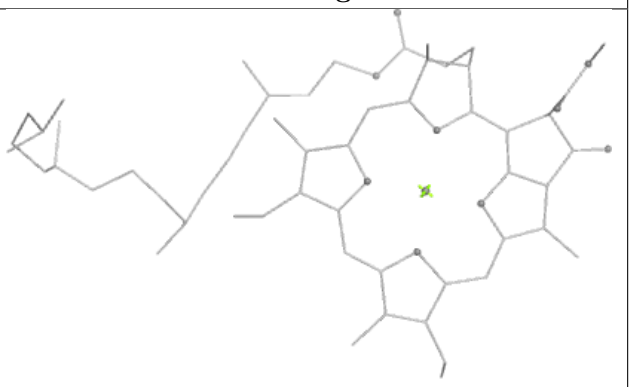
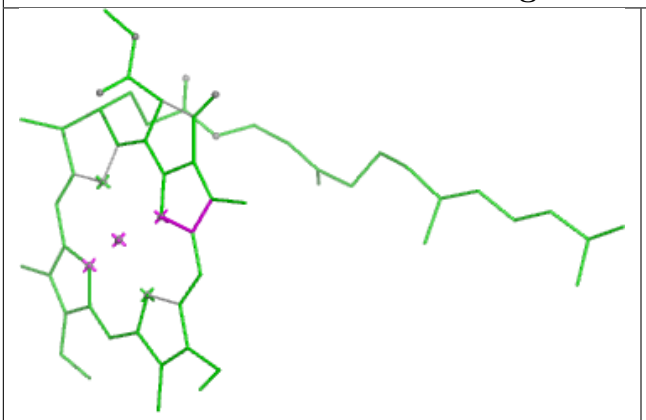


Rings

Ligand CLA 42 611



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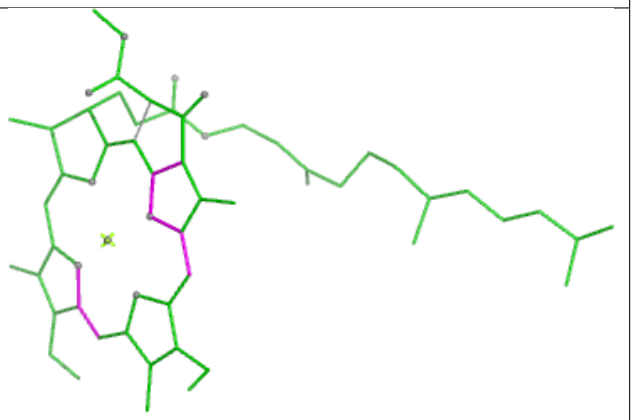

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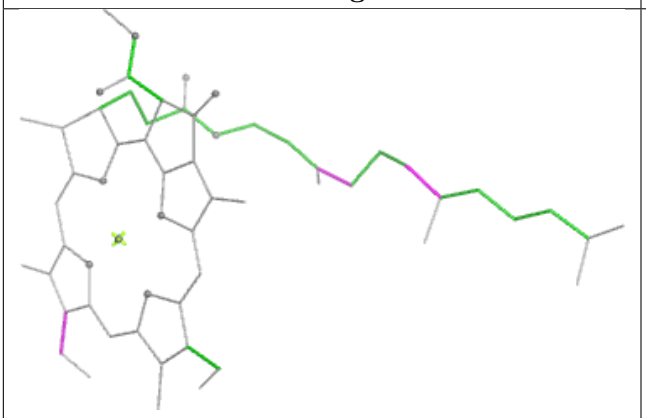

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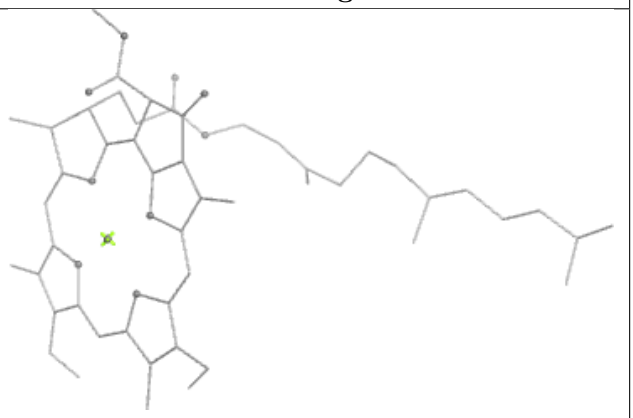
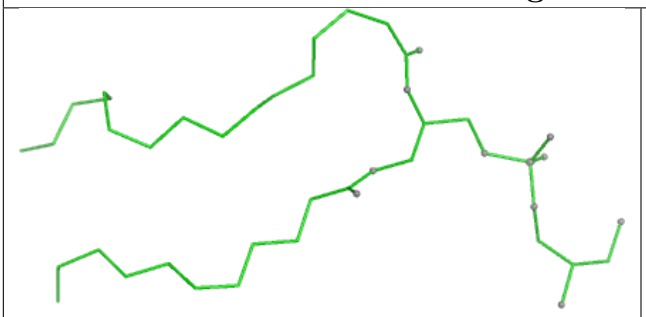


Rings

Ligand LHG 8 620



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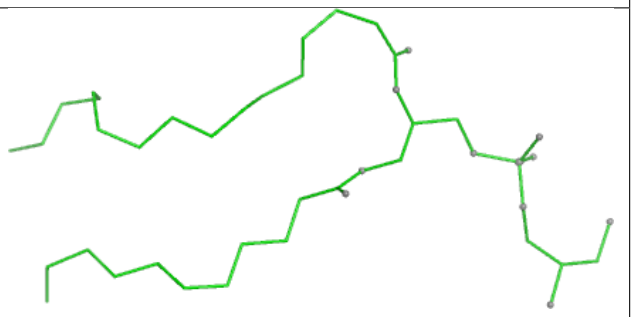

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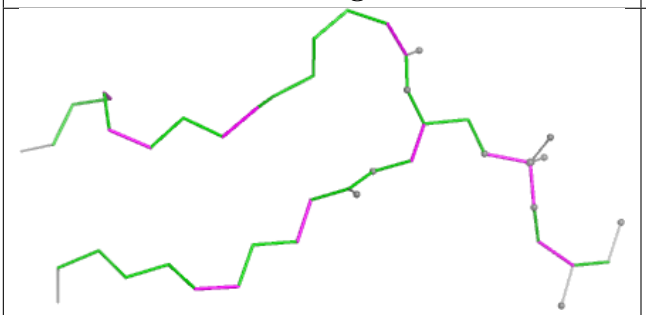

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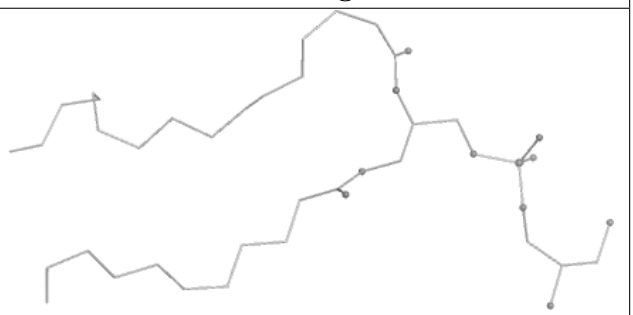
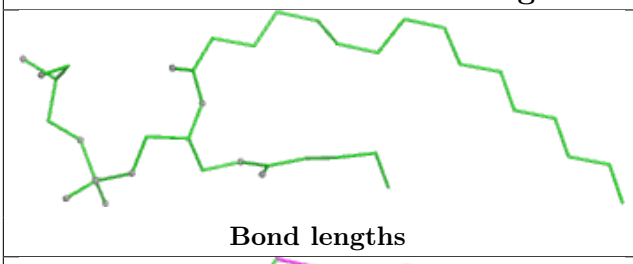


Rings

Ligand LHG 42 623



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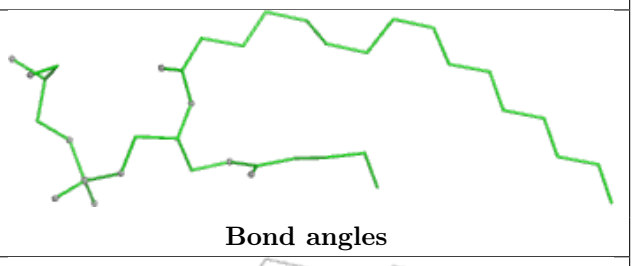

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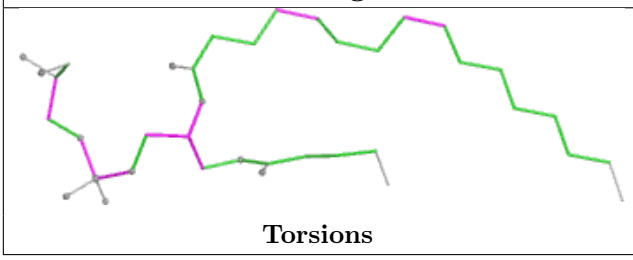

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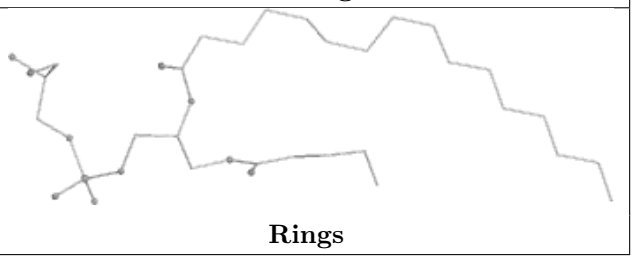


Rings

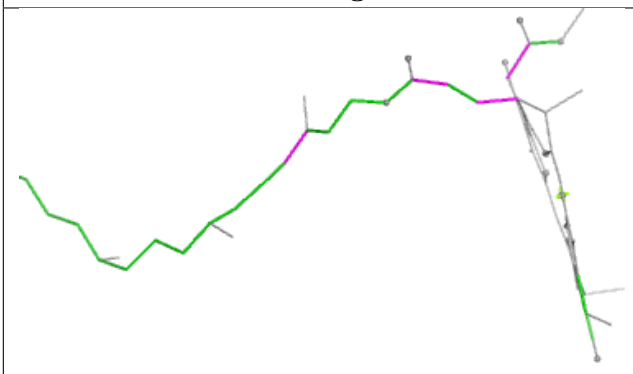
Ligand CHL 62 601



Bond lengths



Bond angles



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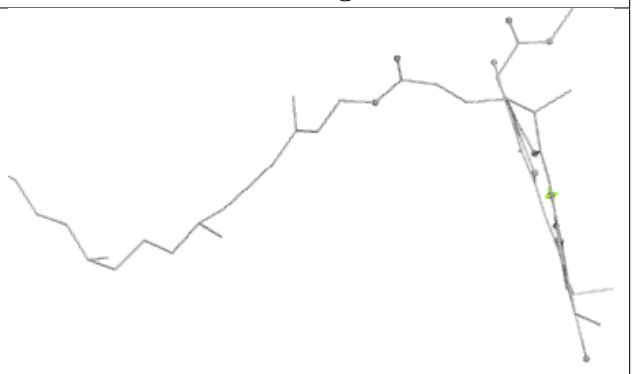
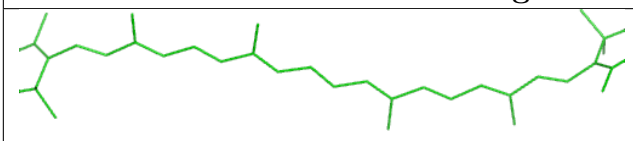


Rings

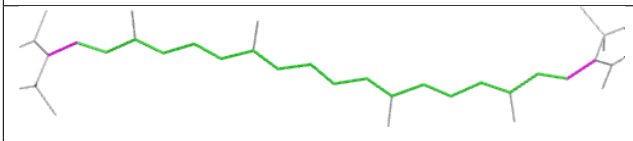
Ligand BCR K2 207



Bond lengths



Bond angles



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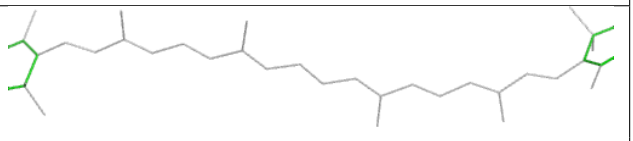
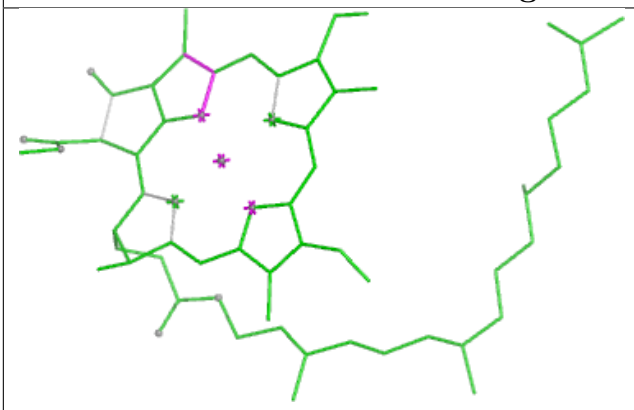


Rings

Ligand CLA 72 602



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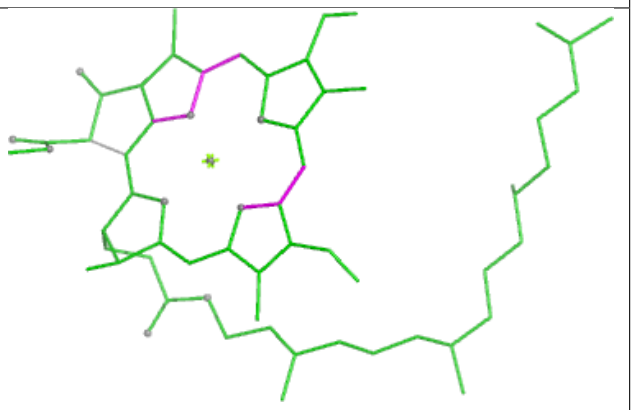
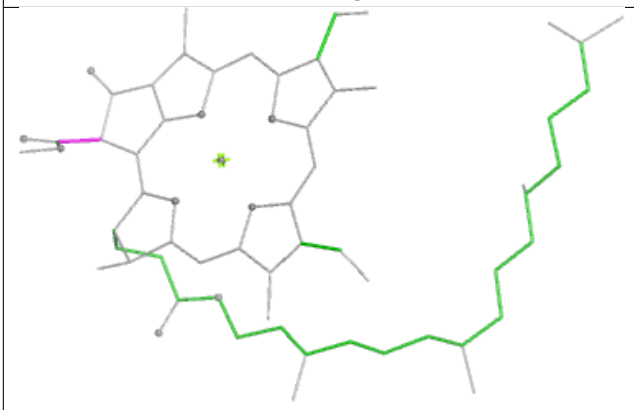


Bond angles



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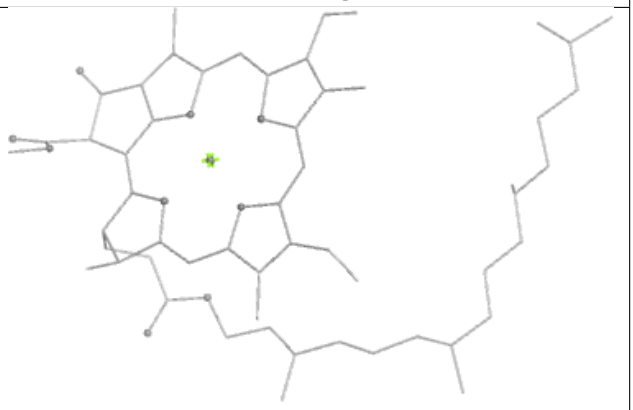


Rings

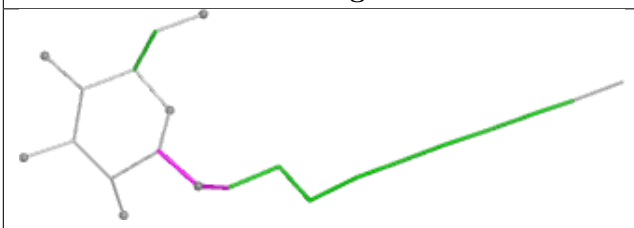
Ligand LMU 72 628



Bond lengths



Bond angles



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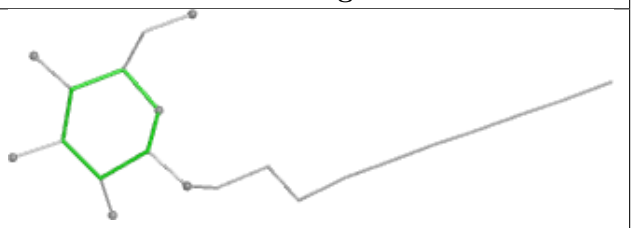
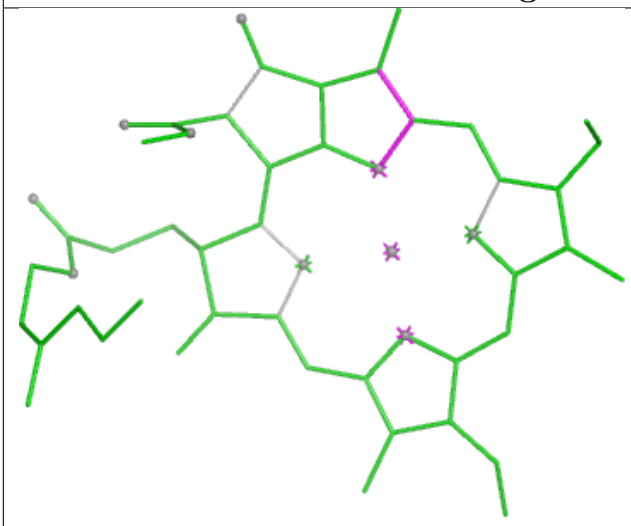
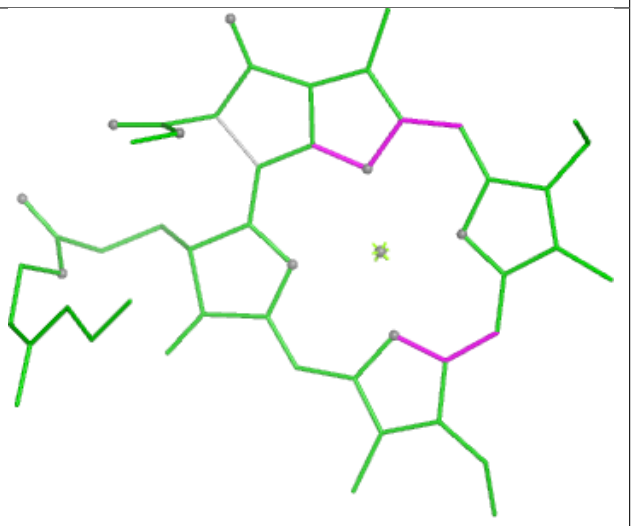


Rings

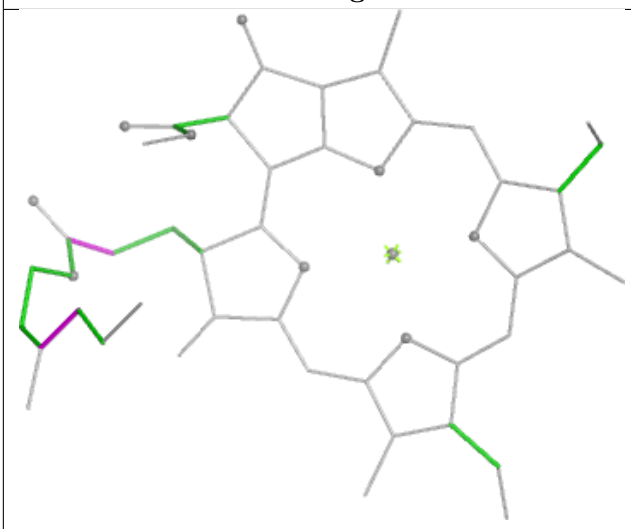
Ligand CLA 72 612



Bond lengths



Bond angles

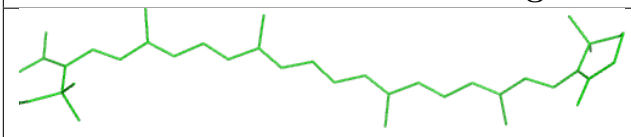


Torsions



Rings

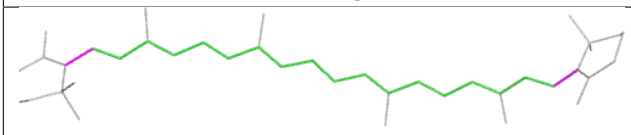
Ligand BCR 8 619



Bond lengths



Bond angles



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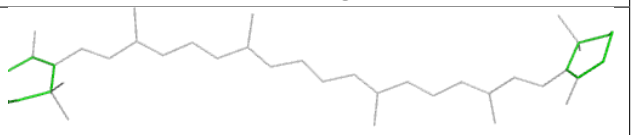
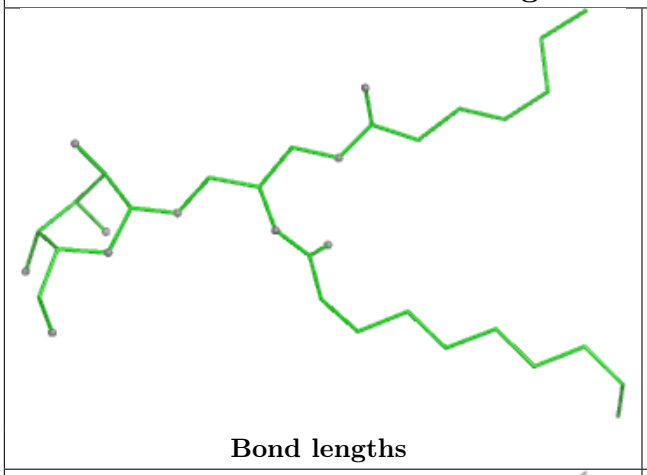


Rings

Ligand LMG B 854



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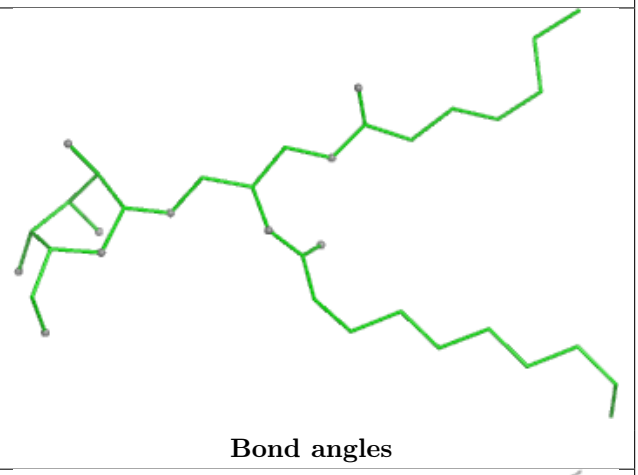
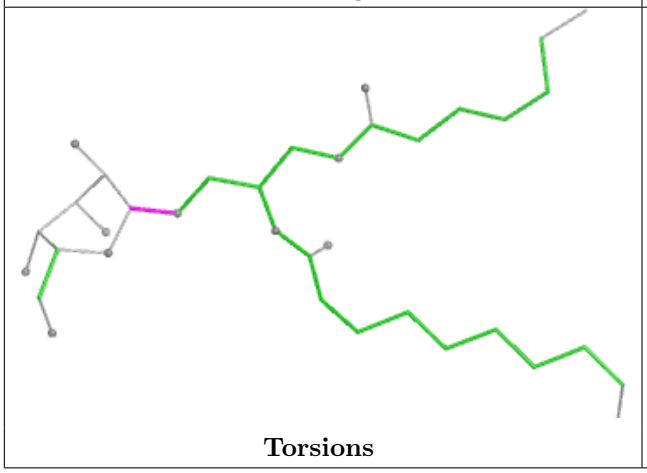
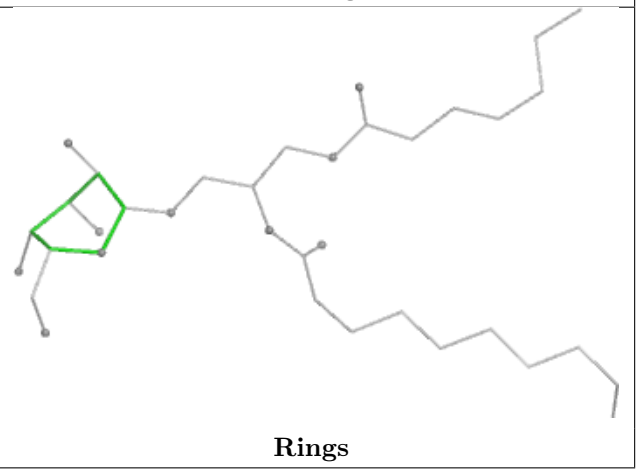


Bond angles

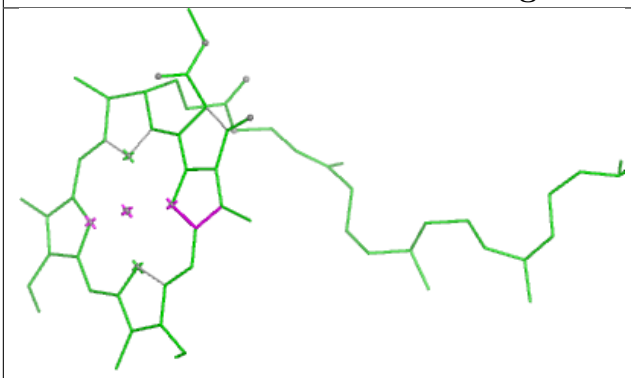


Torsions



Rings

Ligand CLA 72 611



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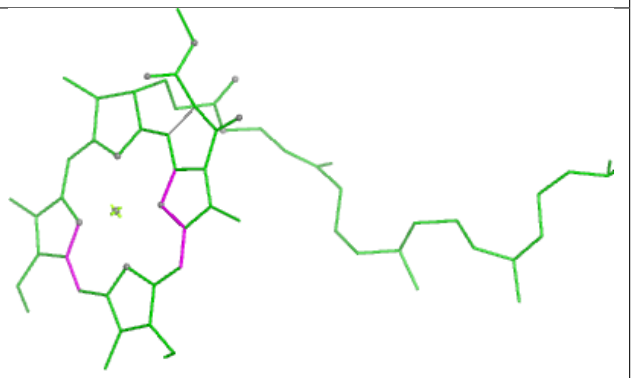
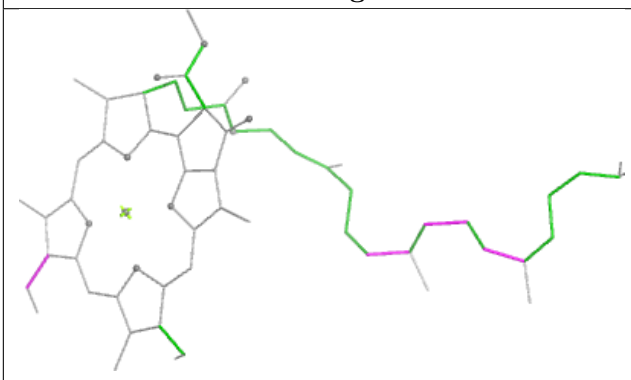


Bond angles



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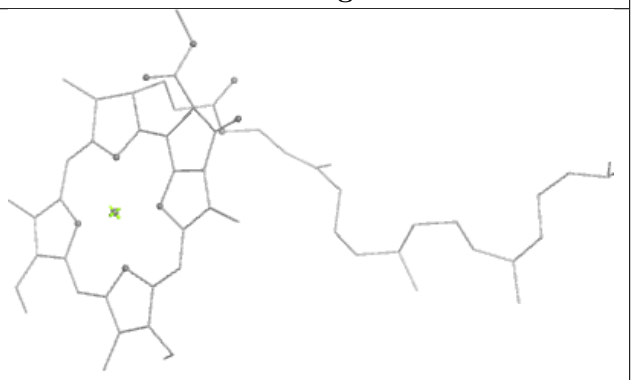
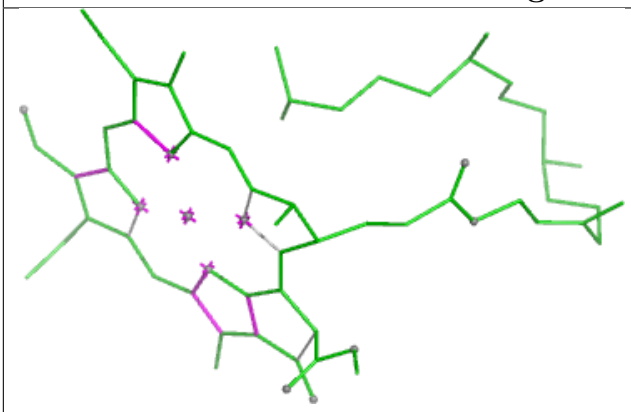


Rings

Ligand CHL 6 616



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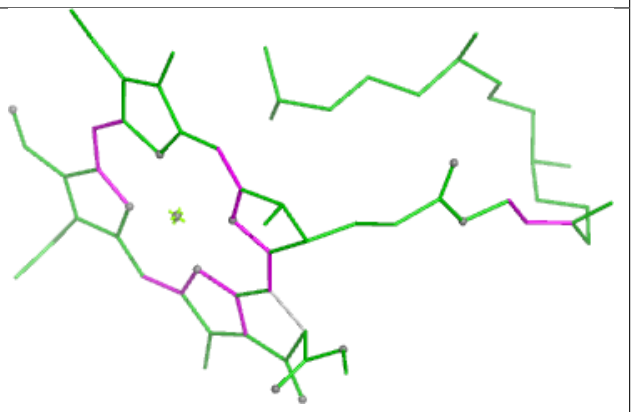

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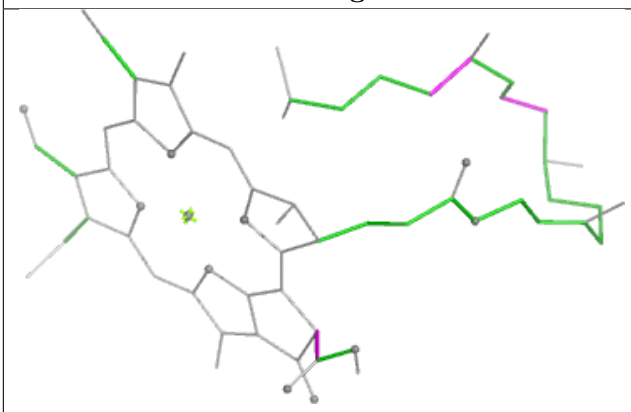

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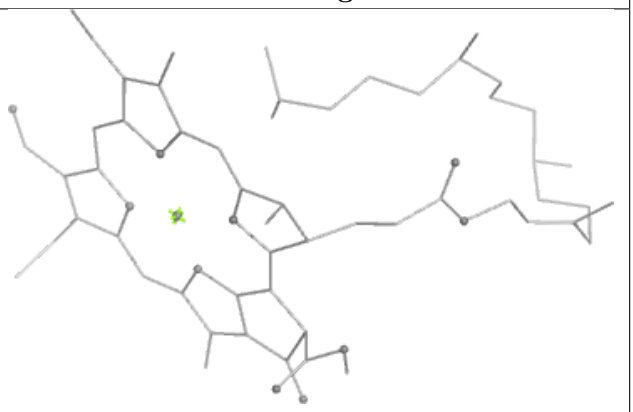
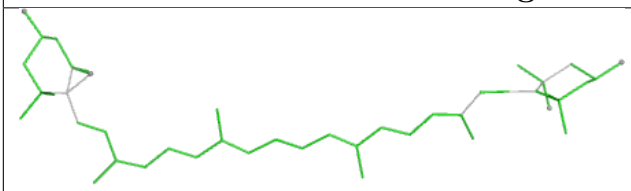


Rings

Ligand NEX 62 625



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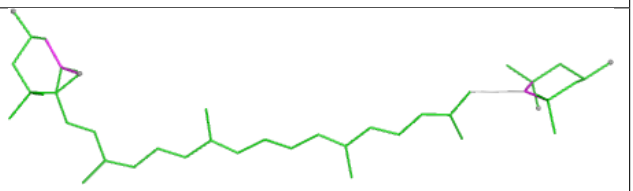
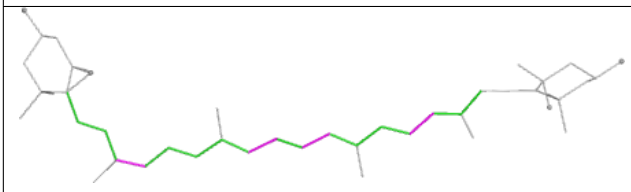


Bond angles



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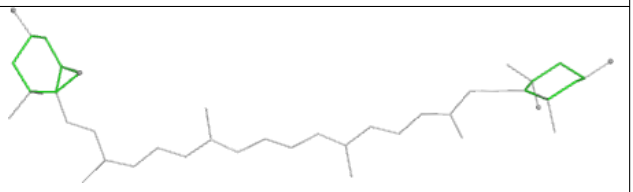
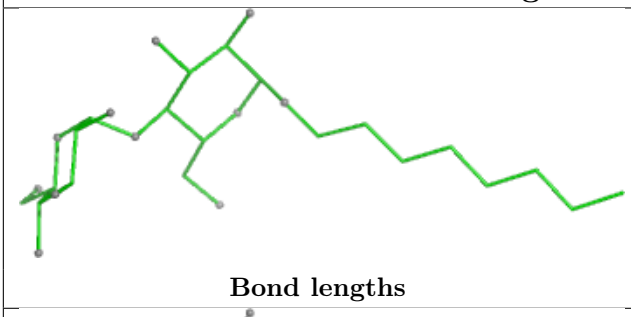


Rings

Ligand LMU Z 622



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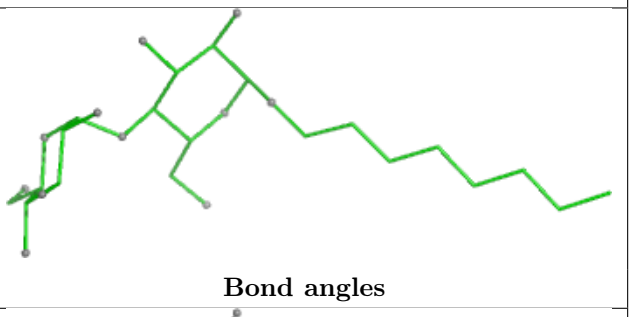

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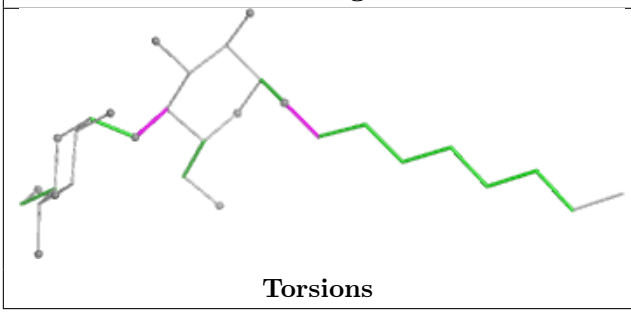

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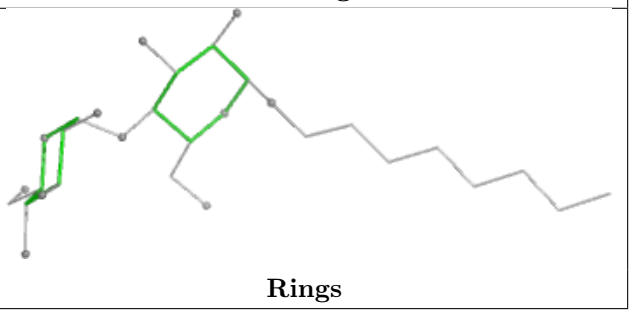
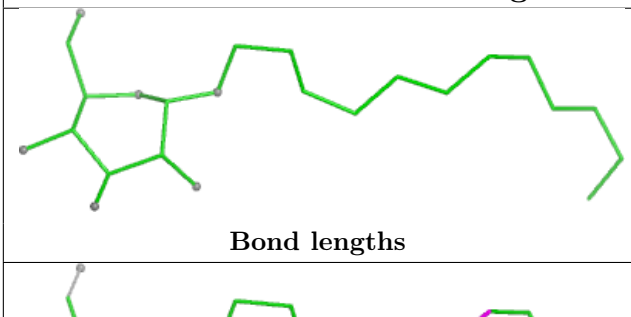


Rings

Ligand LMU K2 208



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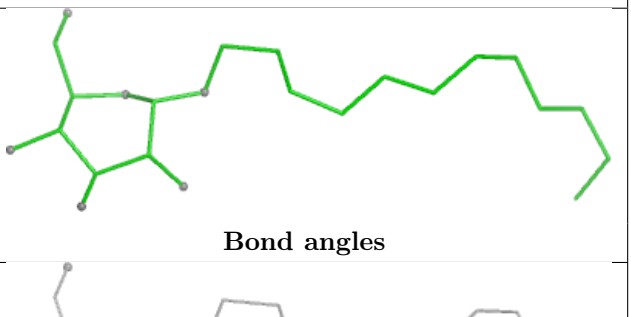

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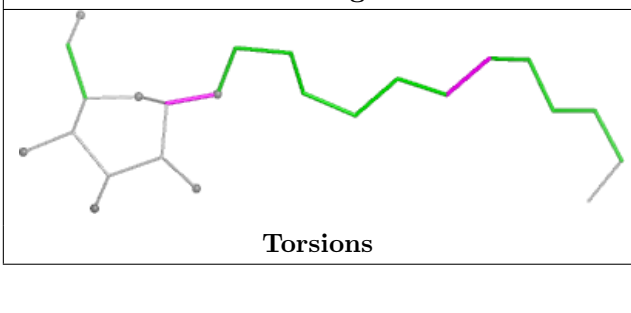

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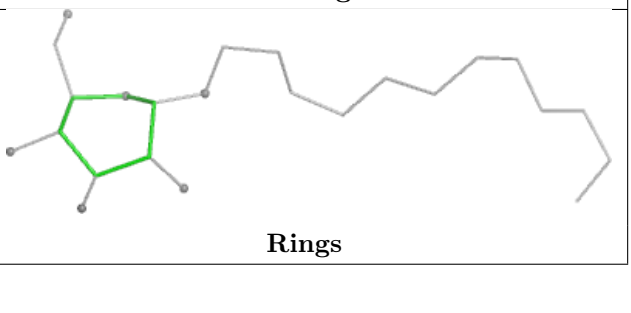
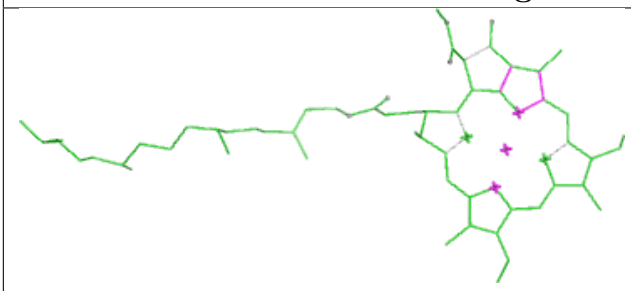


Rings

Ligand CLA A2 827



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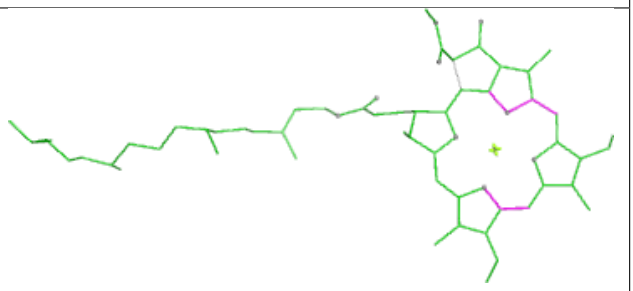
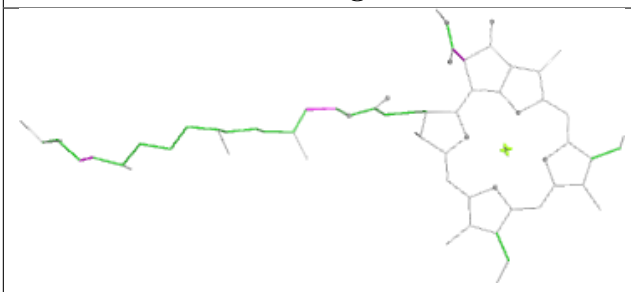


Bond angles

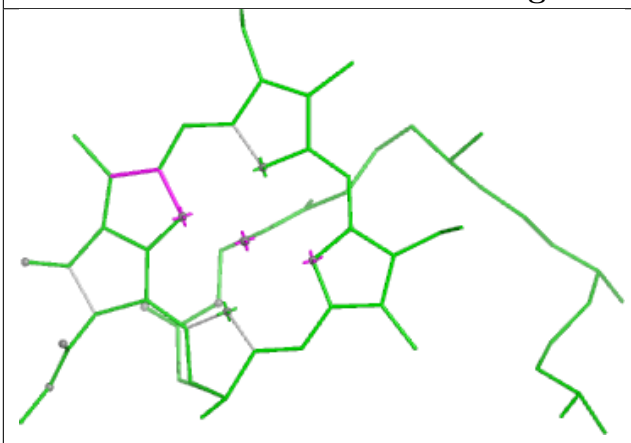


Torsions



Rings

Ligand CLA 4 613



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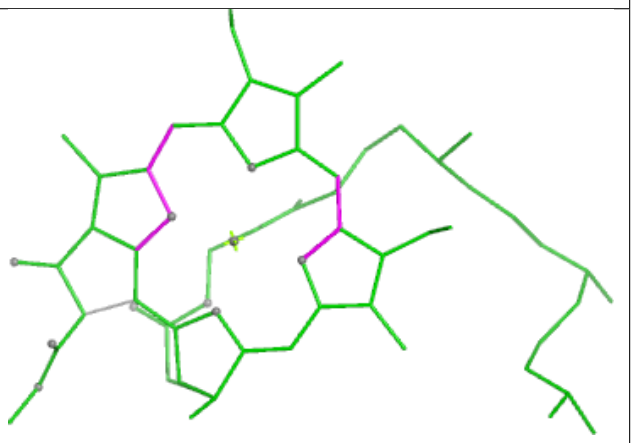
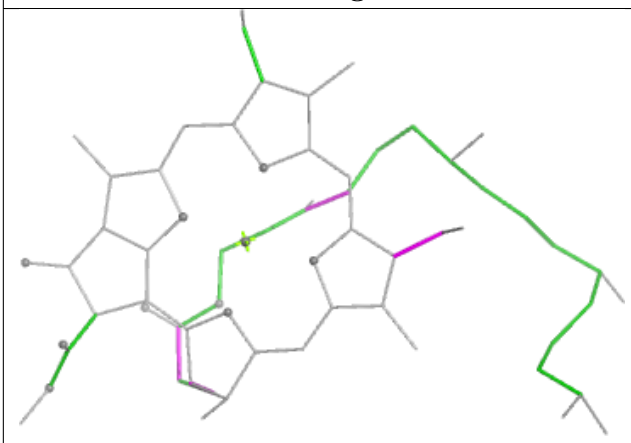


Bond angles



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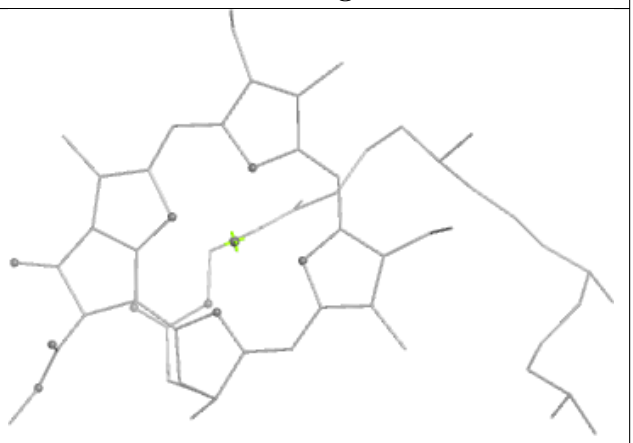
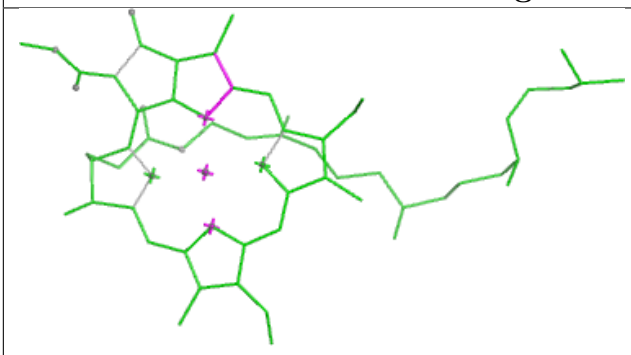


Rings

Ligand CLA A2 818



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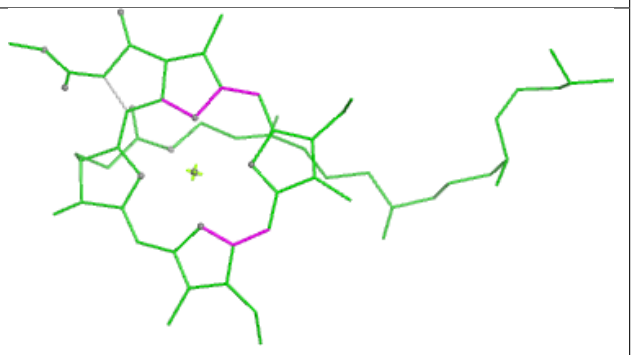

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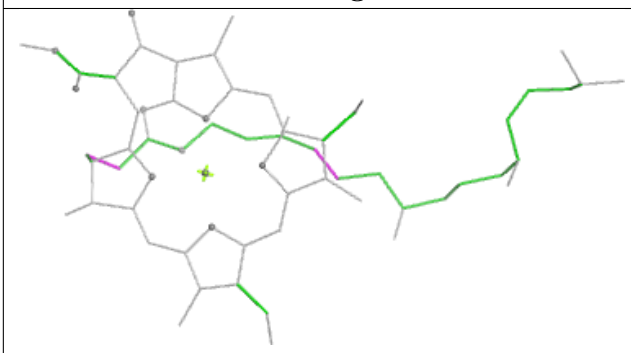

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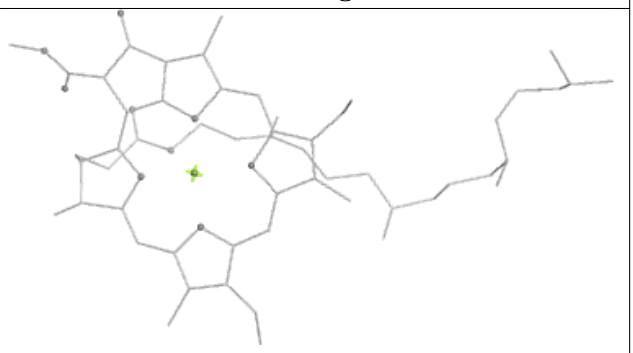
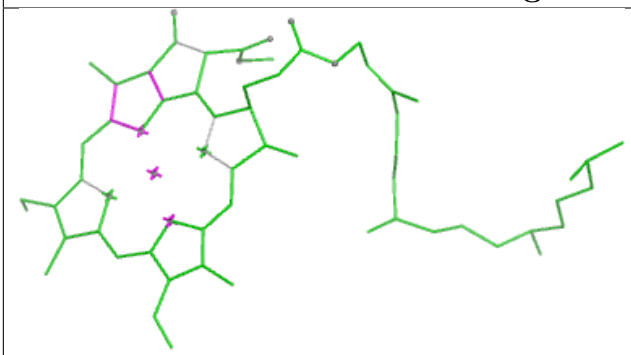


Rings

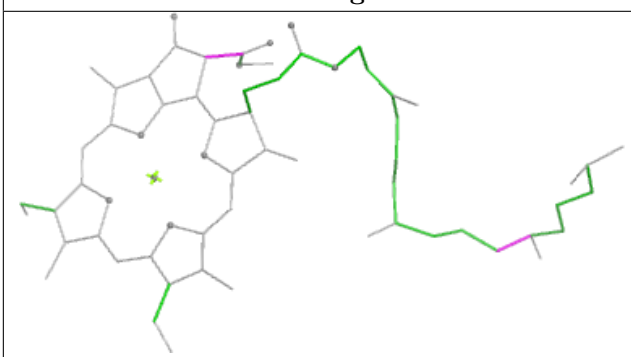
Ligand CLA A 804



Bond lengths



Bond angles



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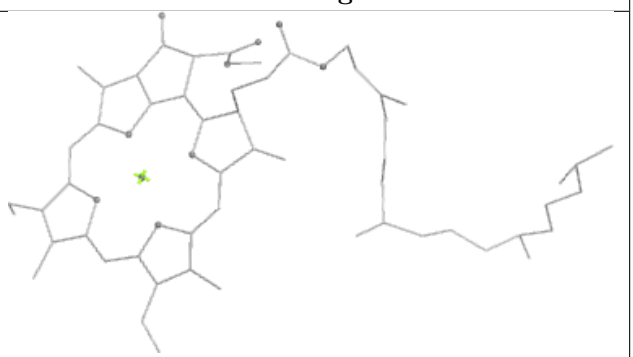
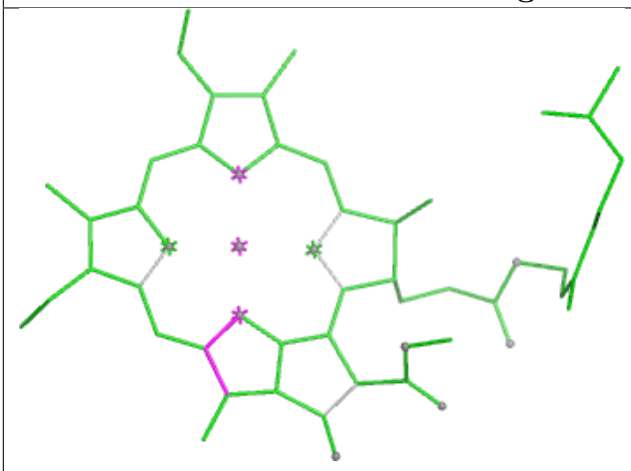


Rings

Ligand CLA Z2 603



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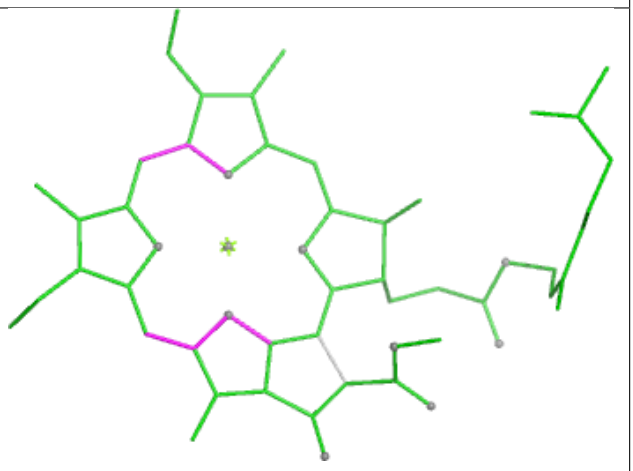

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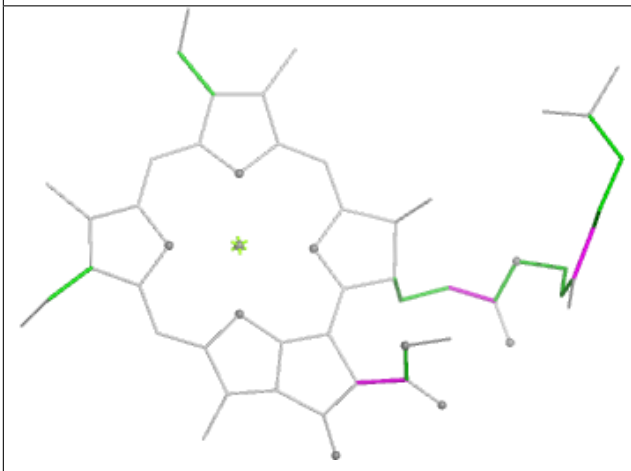

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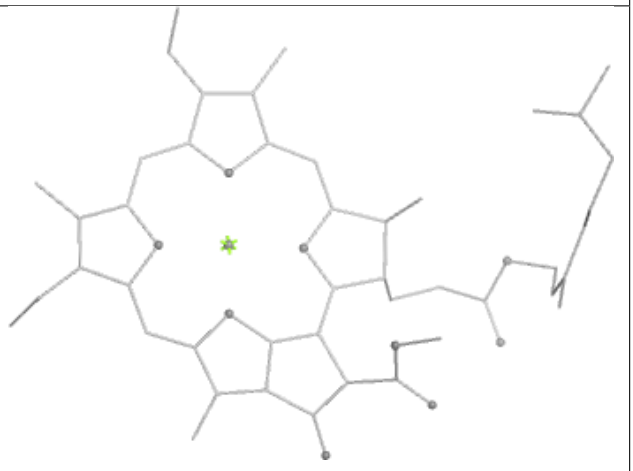
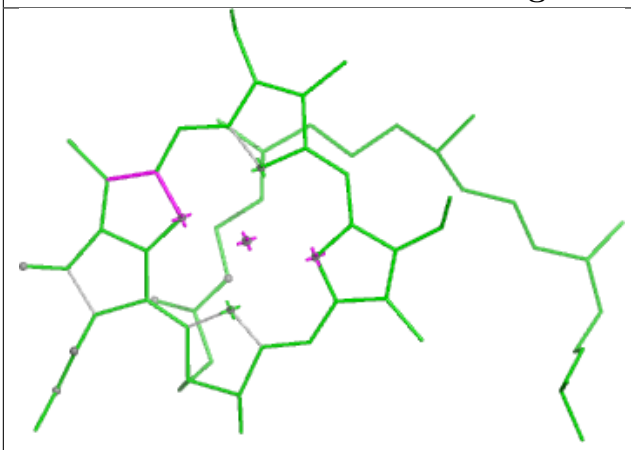


Rings

Ligand CLA 6 613



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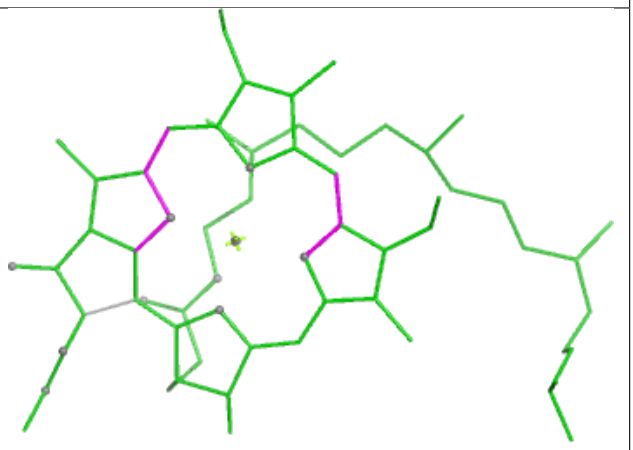
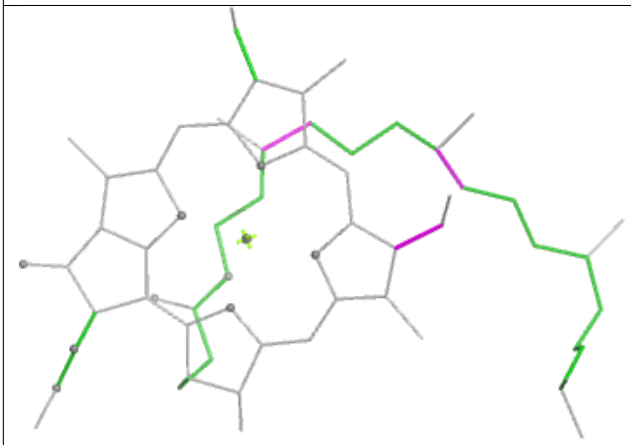


Bond angles



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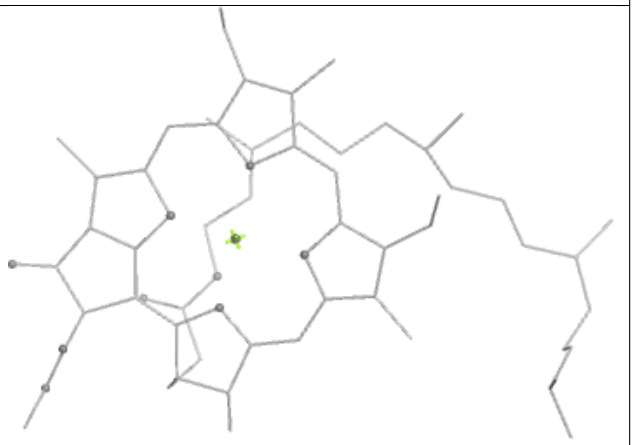
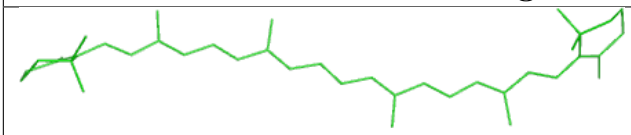


Rings

Ligand BCR 32 620



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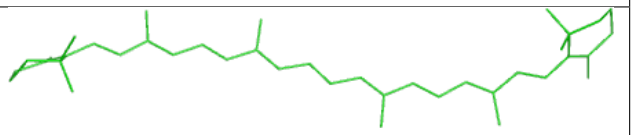

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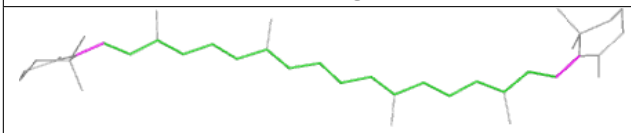

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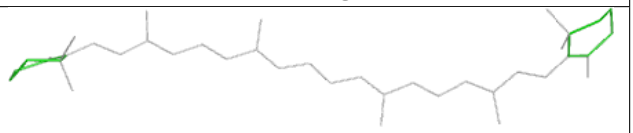
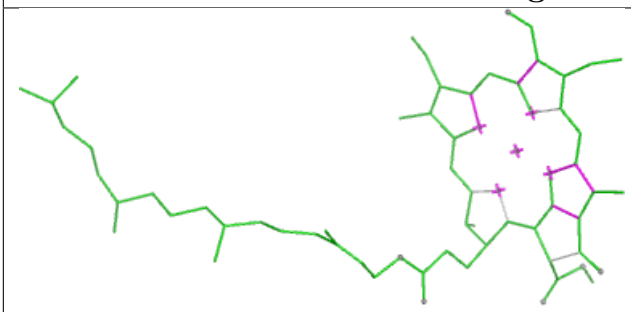


Rings

Ligand CHL 7 601



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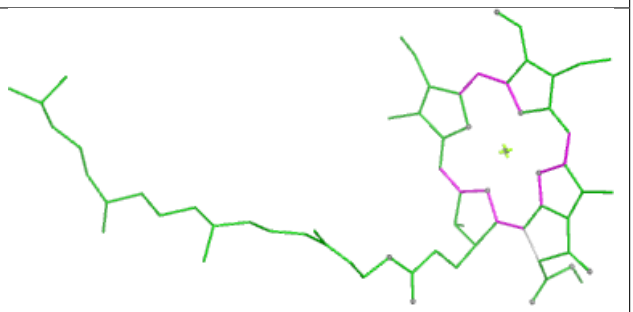
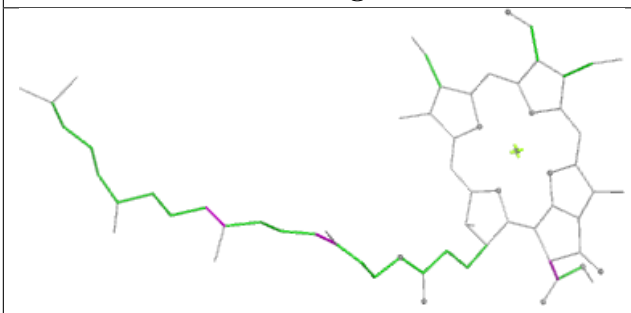


Bond angles



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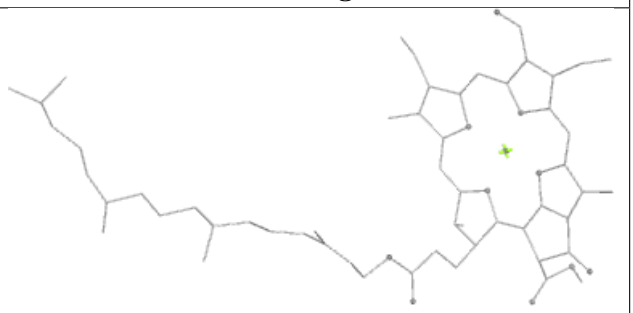
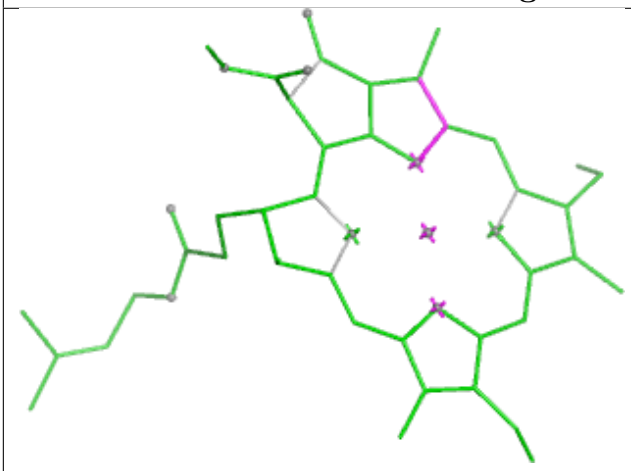


Rings

Ligand CLA 72 608



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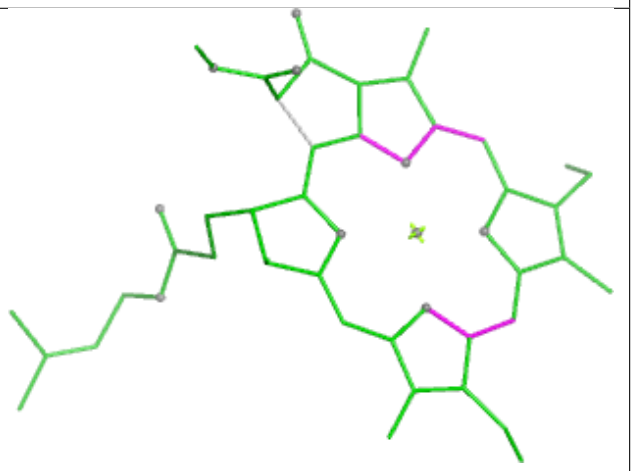
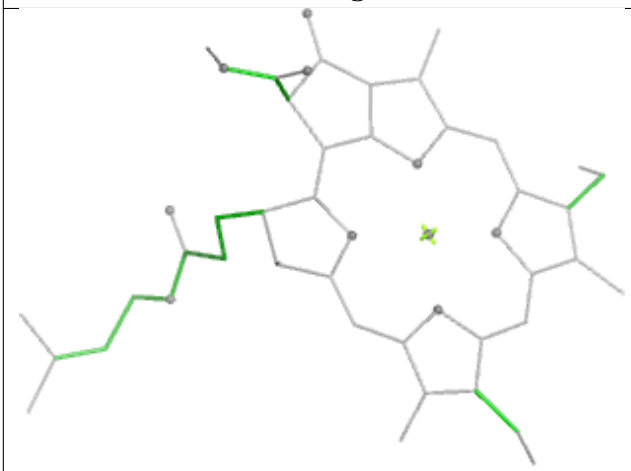


Bond angles



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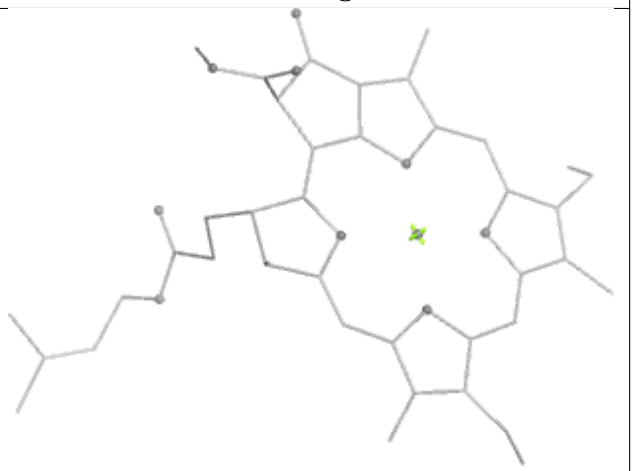
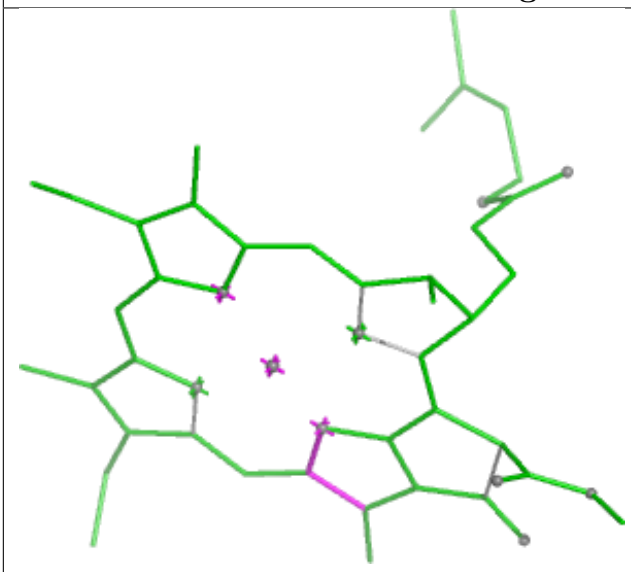


Rings

Ligand CLA 42 604



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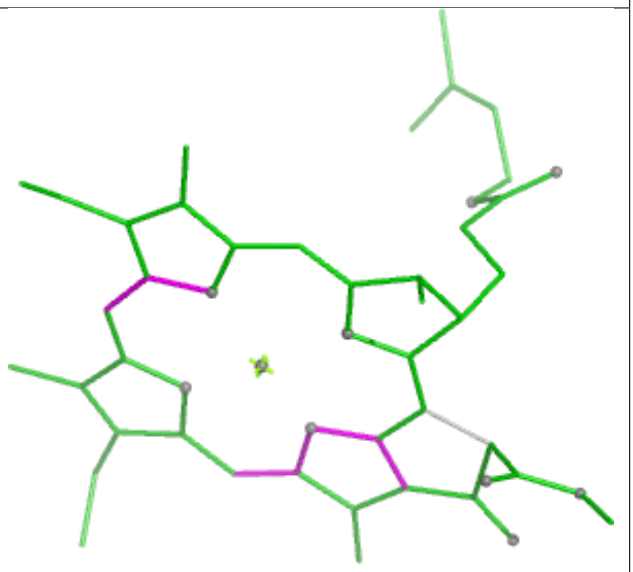
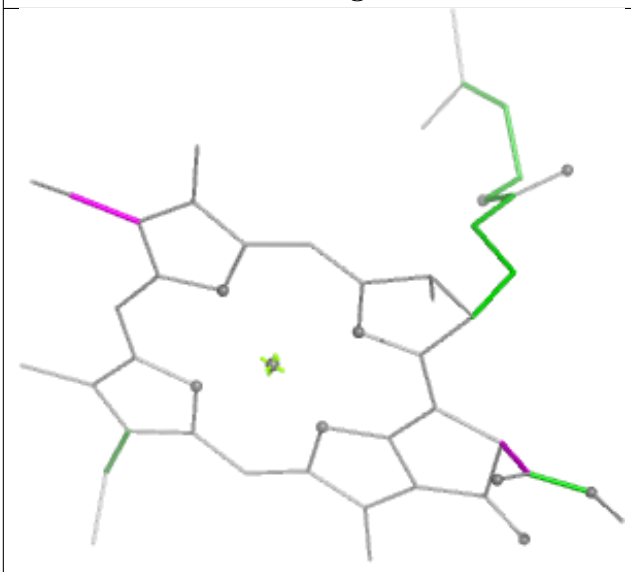


Bond angles

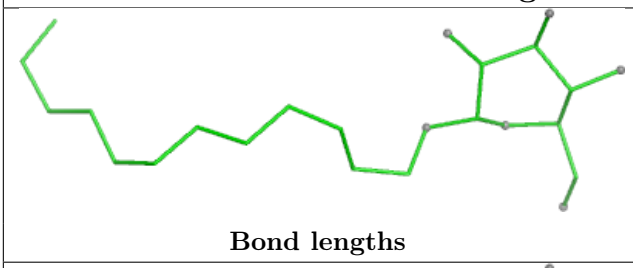


Torsions



Rings

Ligand LMU K 208



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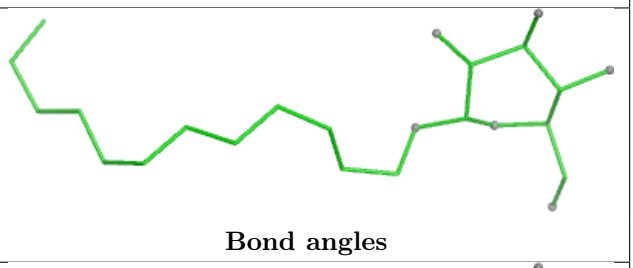

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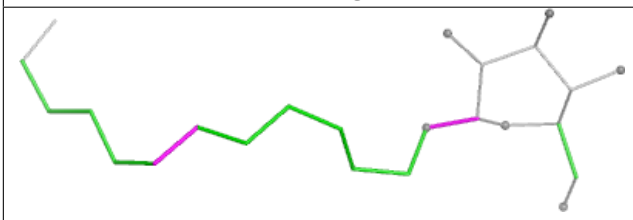
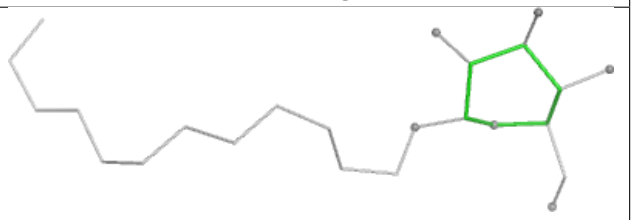
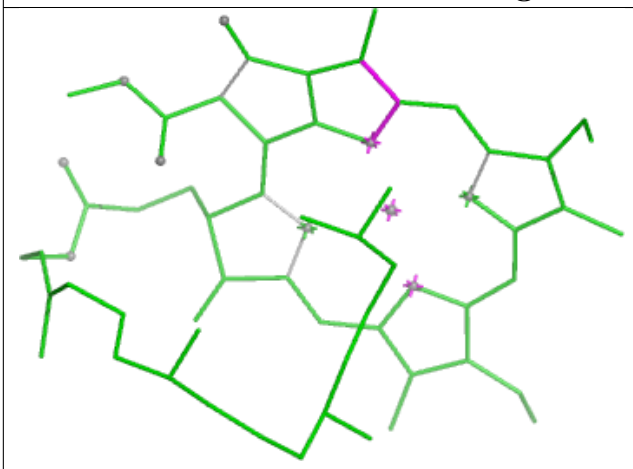


Torsions



Rings

Ligand CLA B2 806



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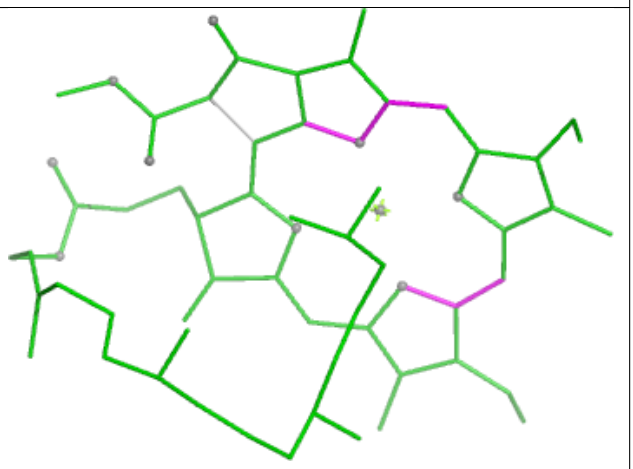

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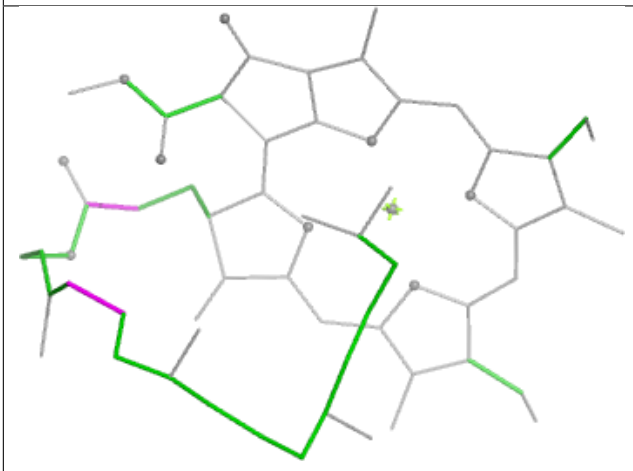

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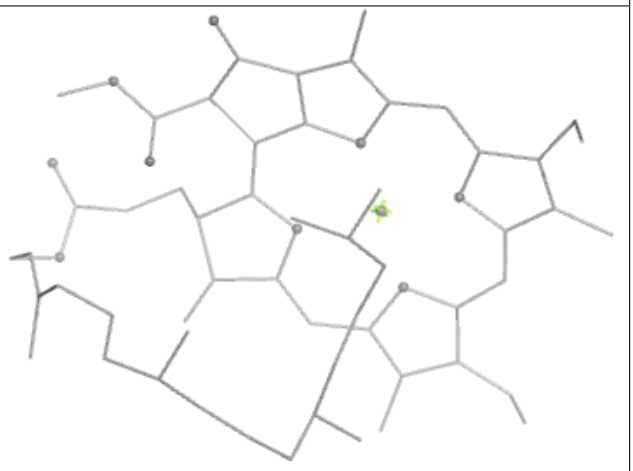
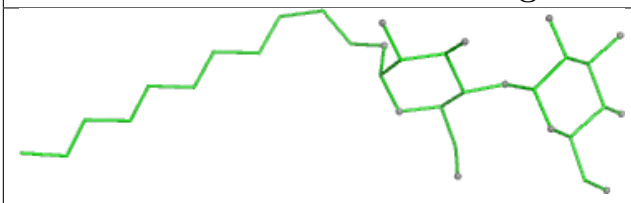


Rings

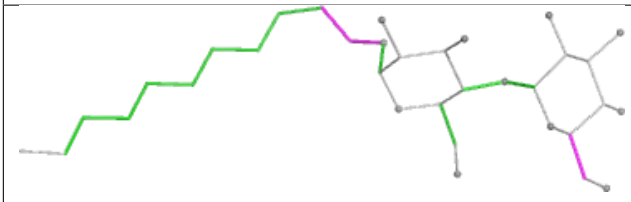
Ligand LMU A 857



Bond lengths



Bond angles



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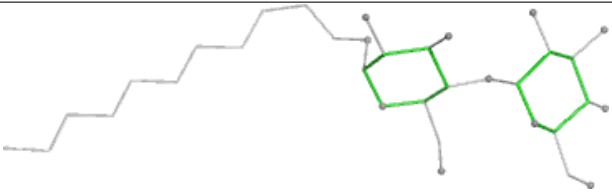
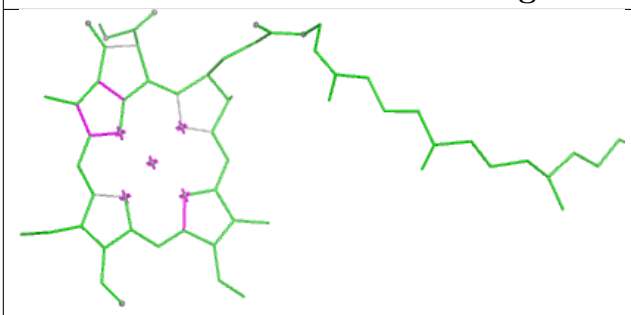


Rings

Ligand CHL 12 601



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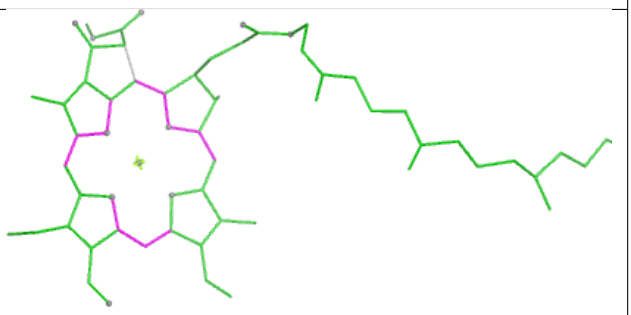

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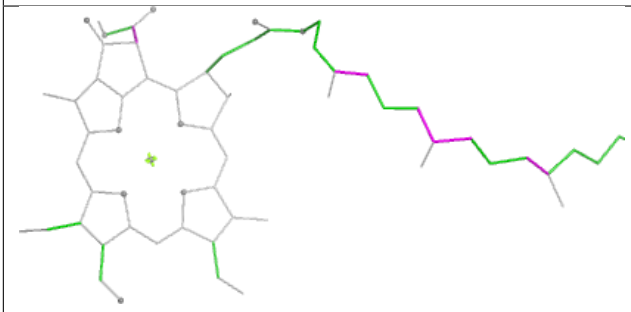

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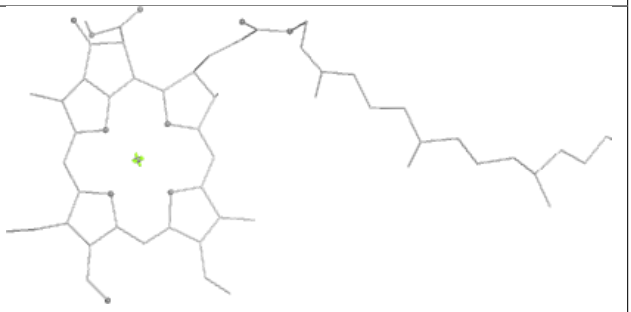
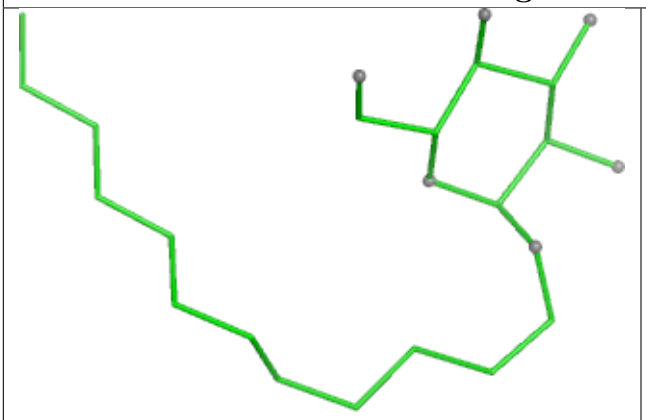


Rings

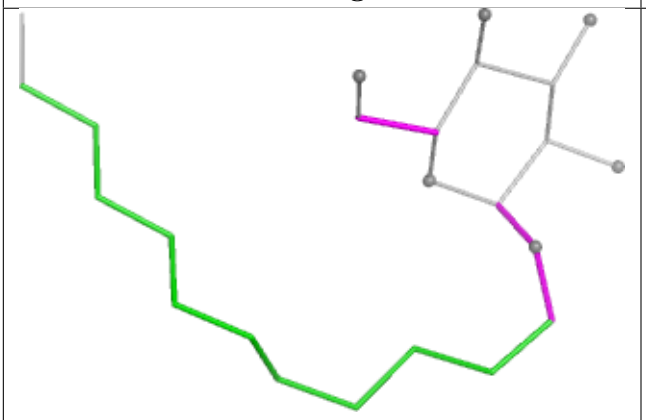
Ligand LMU 82 628



Bond lengths



Bond angles



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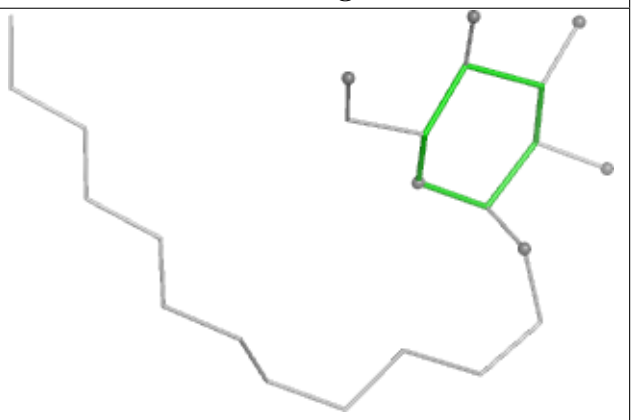

Rings

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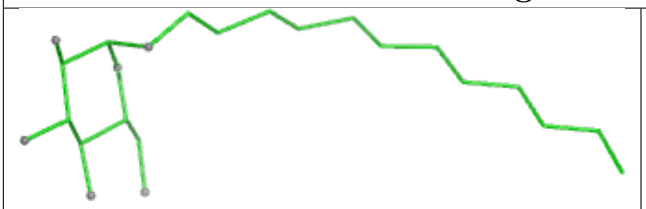

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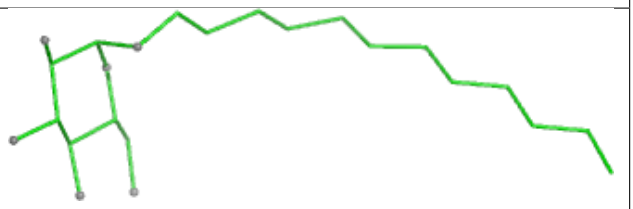

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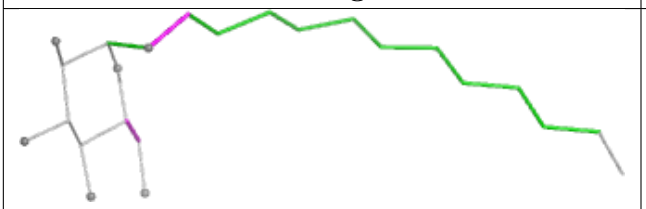

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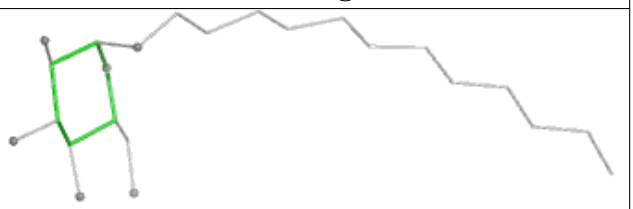
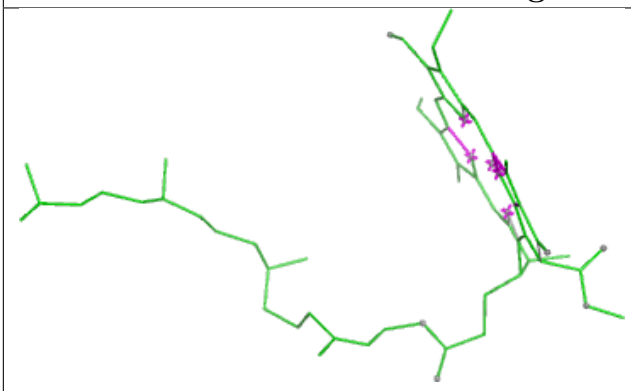


Rings

Ligand CHL 5 607



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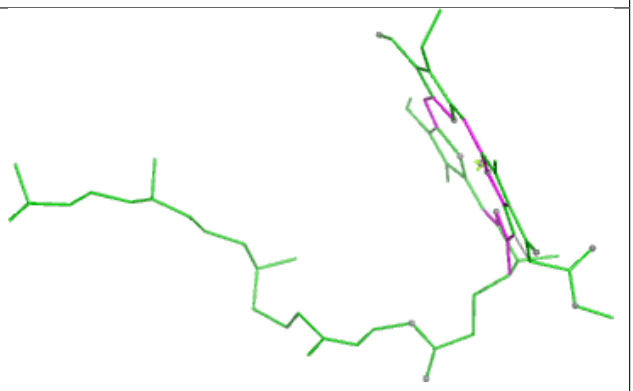

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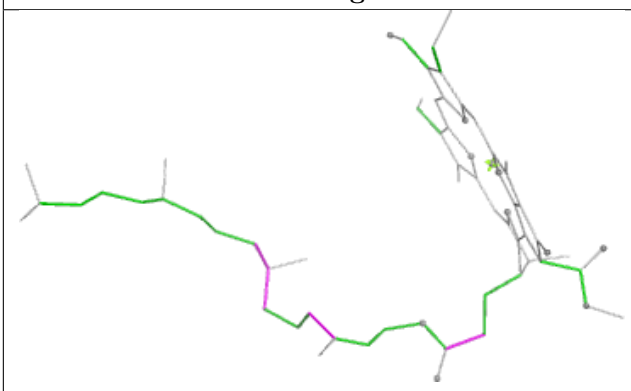
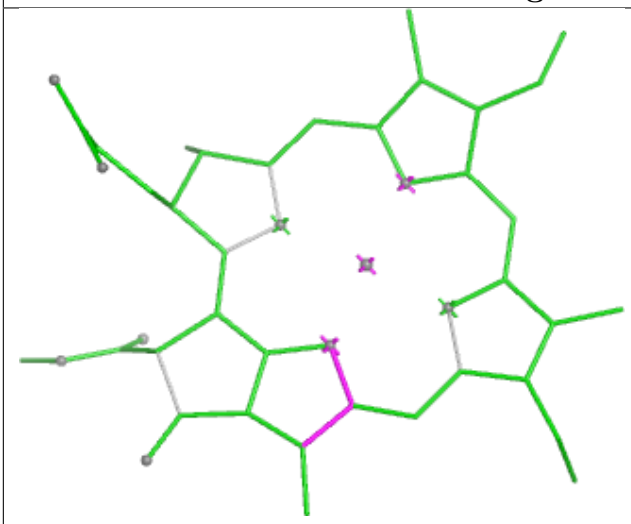


Torsions



Rings

Ligand CLA L 204



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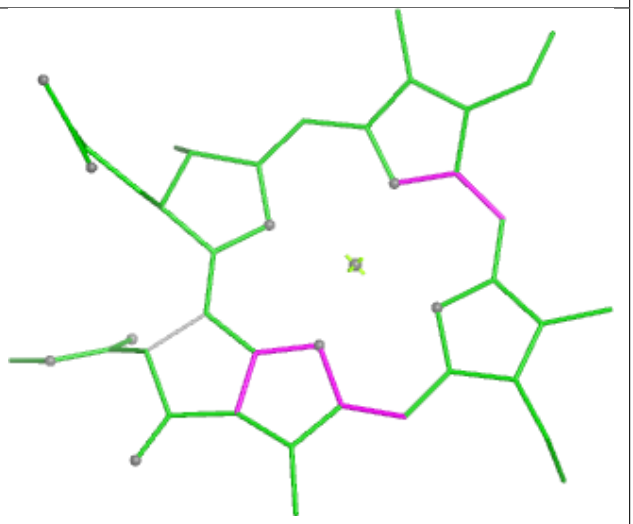

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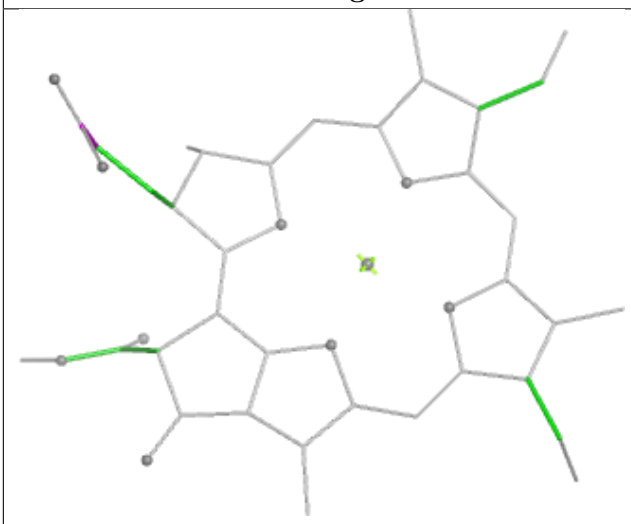

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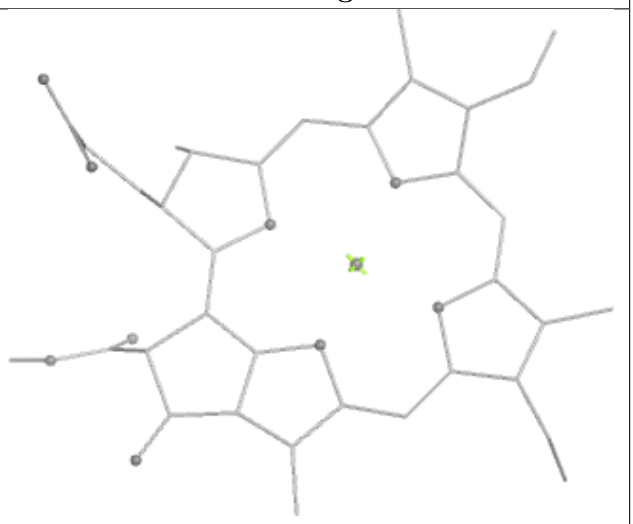
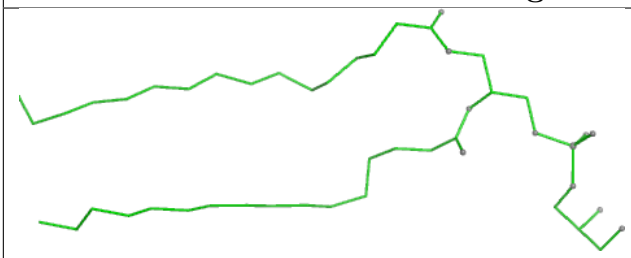


Rings

Ligand LHG 6 619



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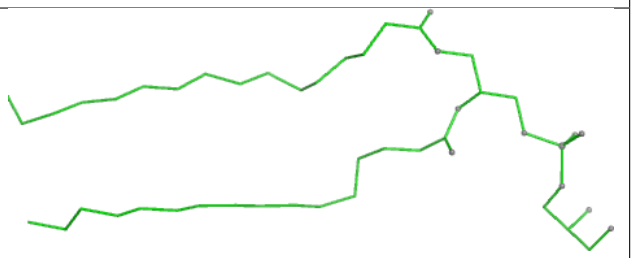

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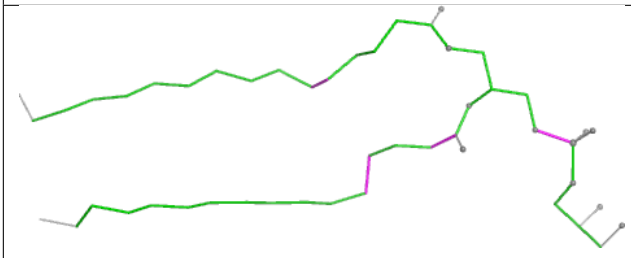
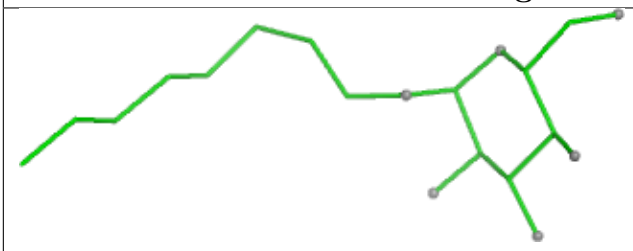


Torsions



Rings

Ligand LMU 62 632



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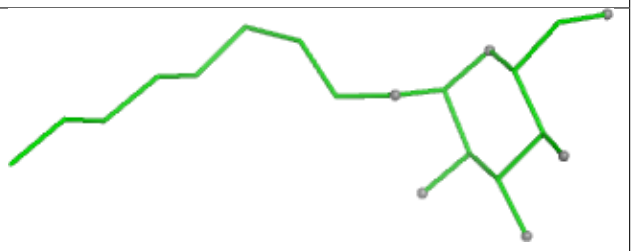

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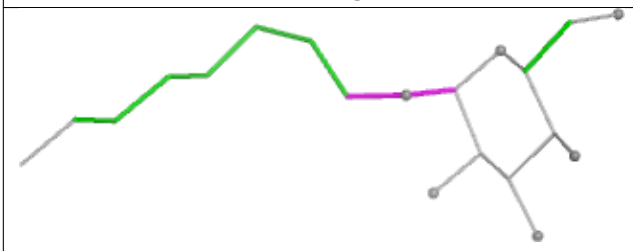

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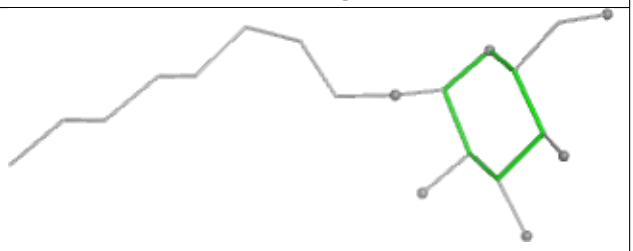
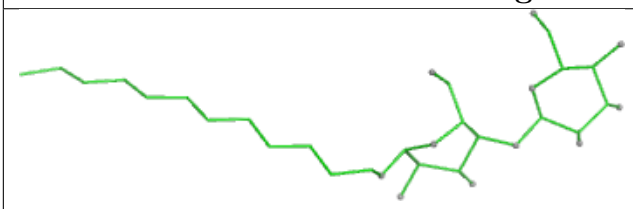


Rings

Ligand LMU 12 621



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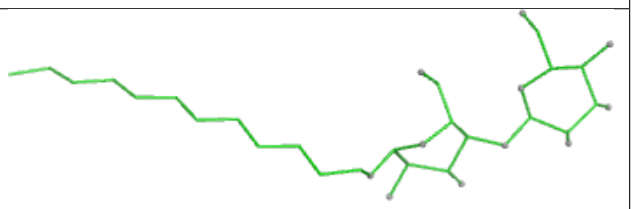

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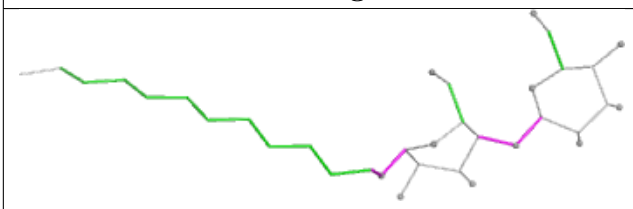

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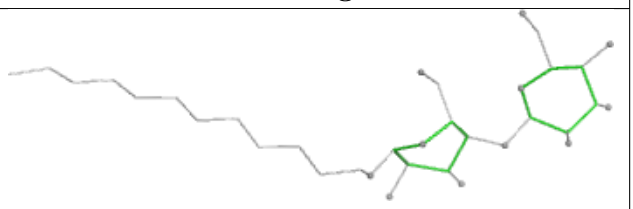
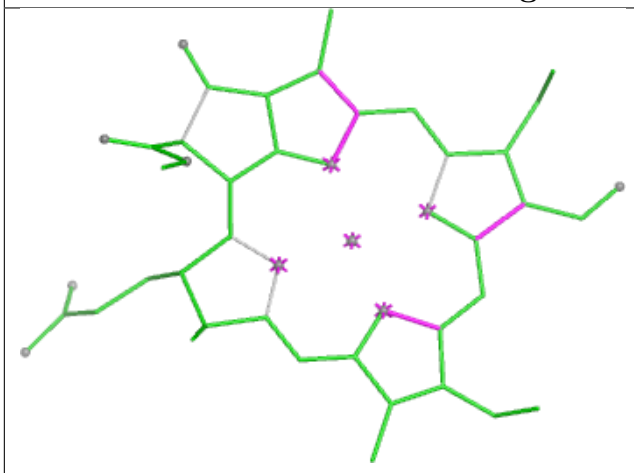


Rings

Ligand CHL 42 618



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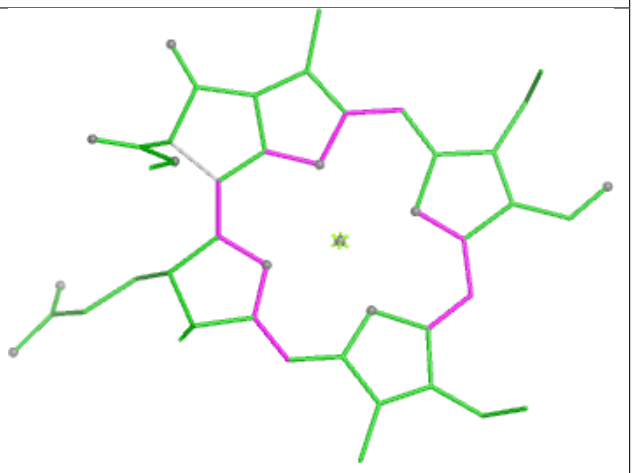

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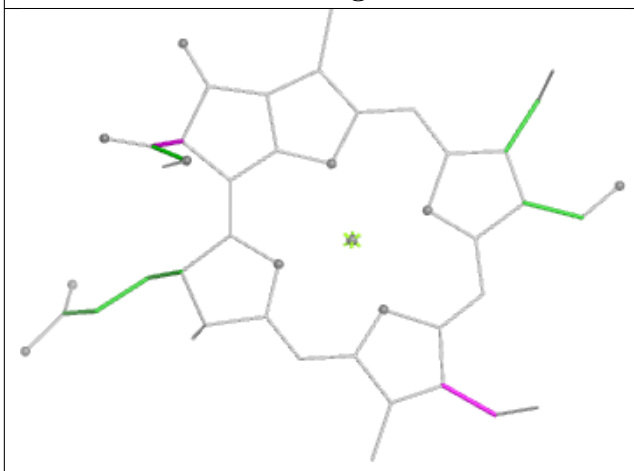

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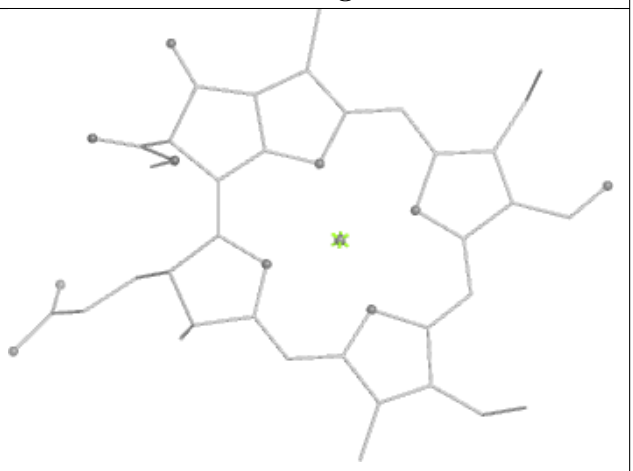


Rings

Ligand LMU 12 625



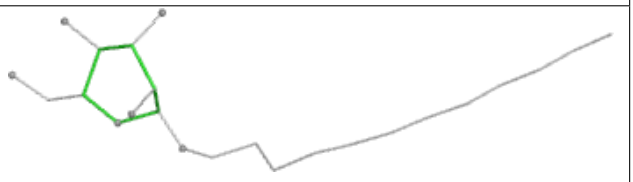
Bond lengths



Bond angles

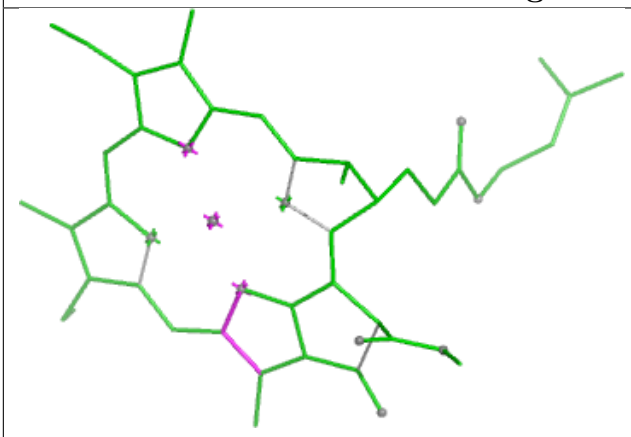


Torsions



Rings

Ligand CLA Z 608



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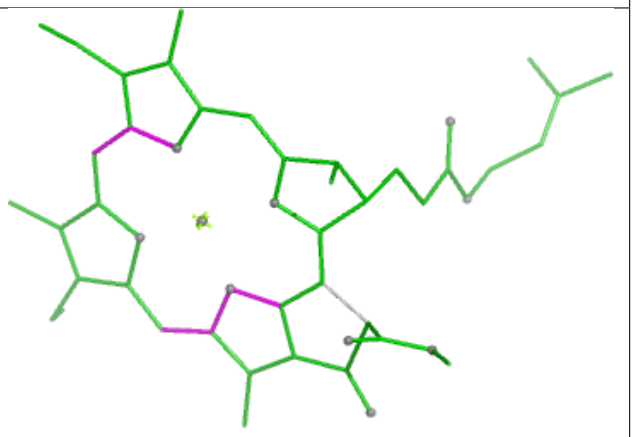
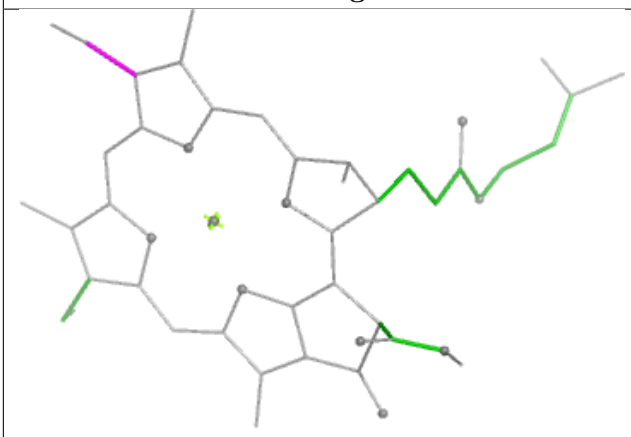


Bond angles



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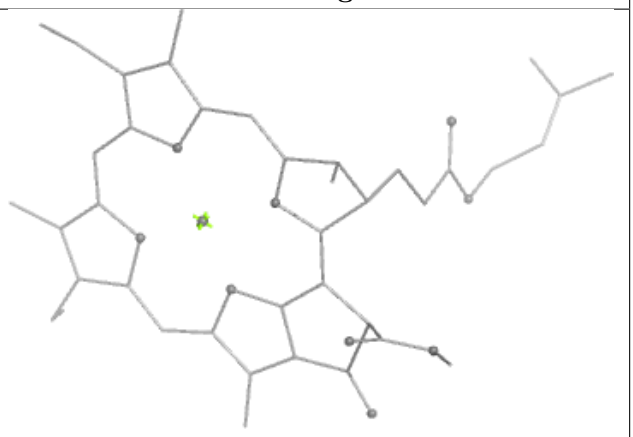
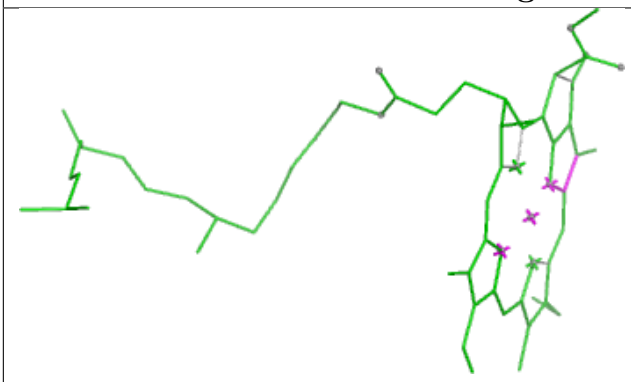


Rings

Ligand CLA L2 203



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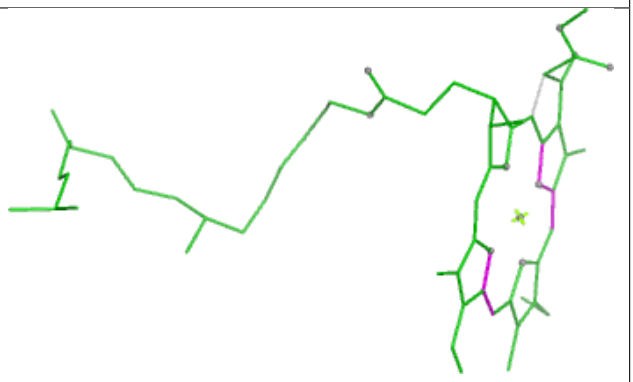
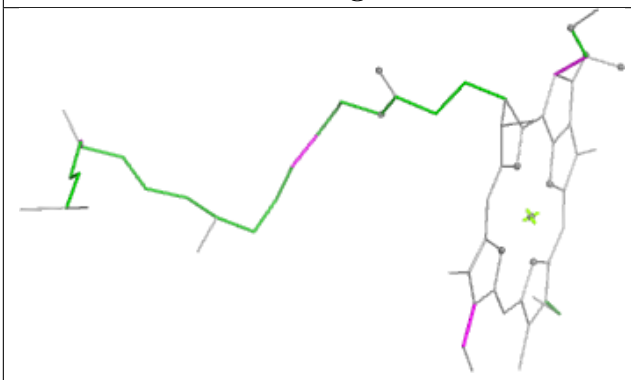


Bond angles



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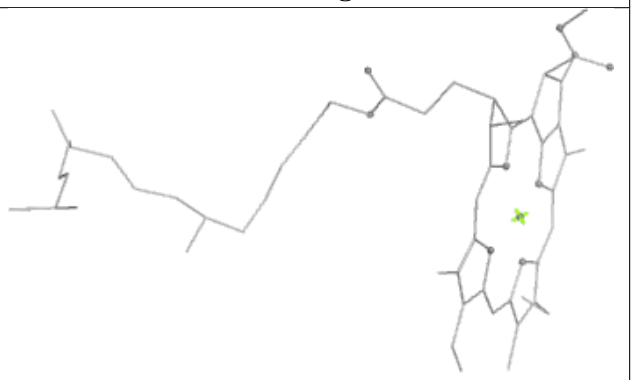
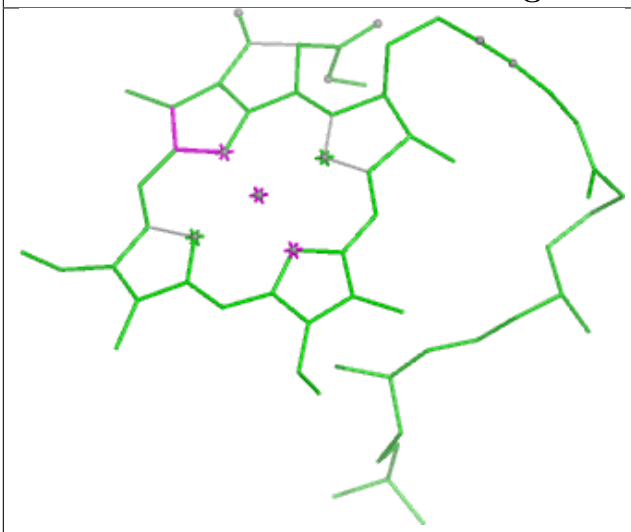


Rings

Ligand CLA A 814



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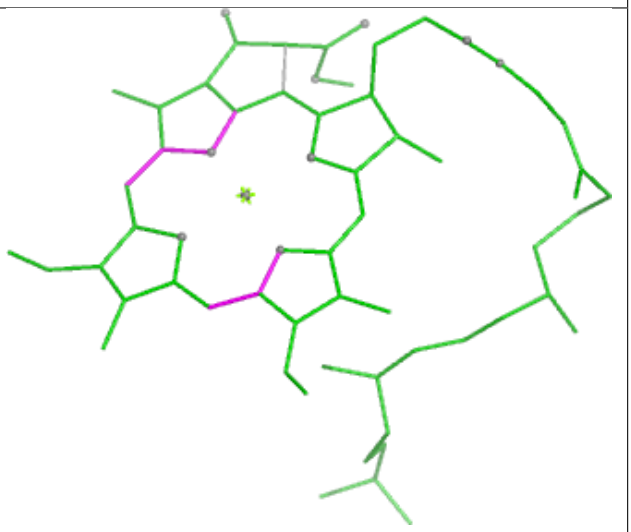

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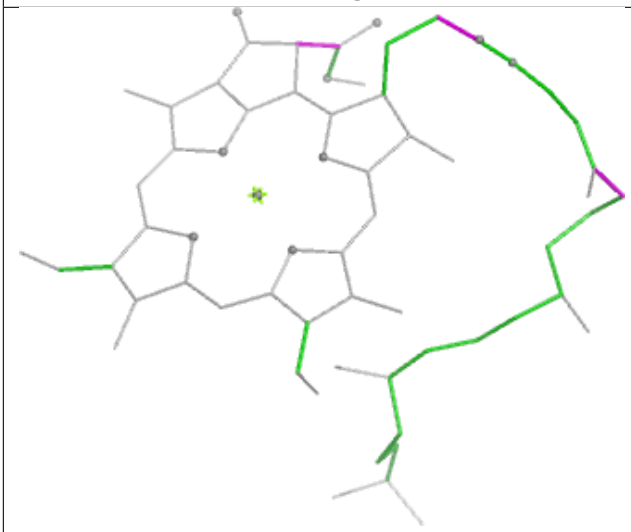
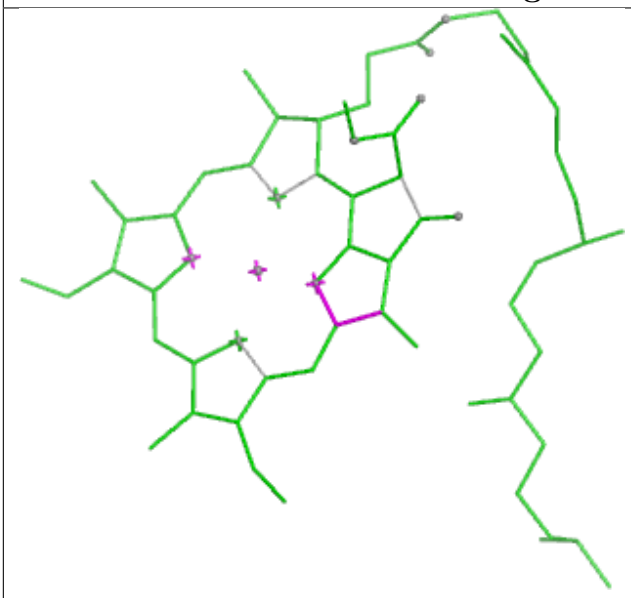


Torsions



Rings

Ligand CLA A 826



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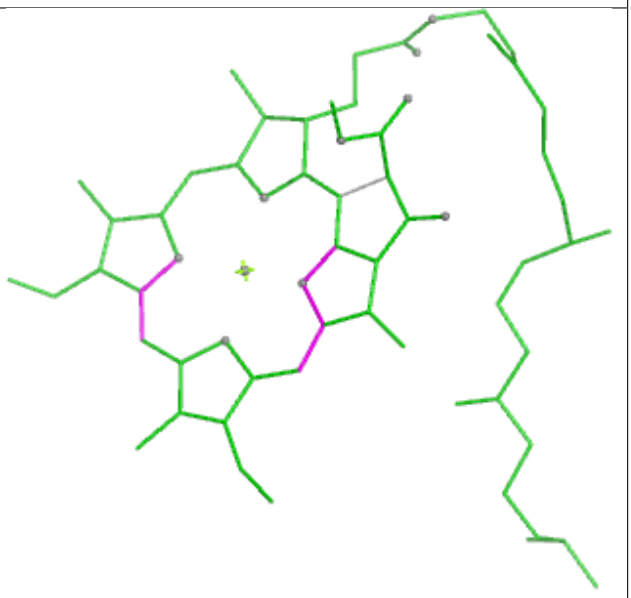
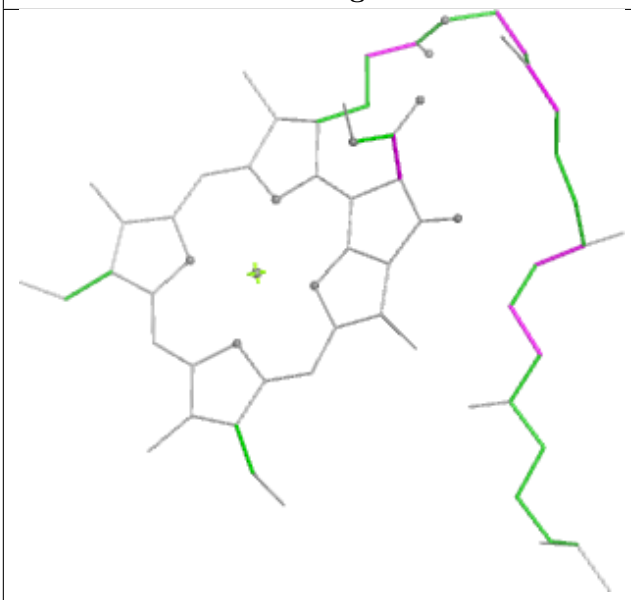
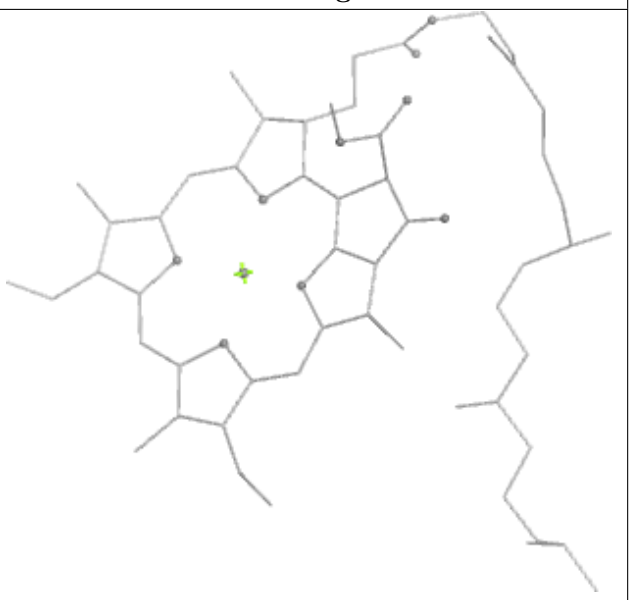


Bond angles

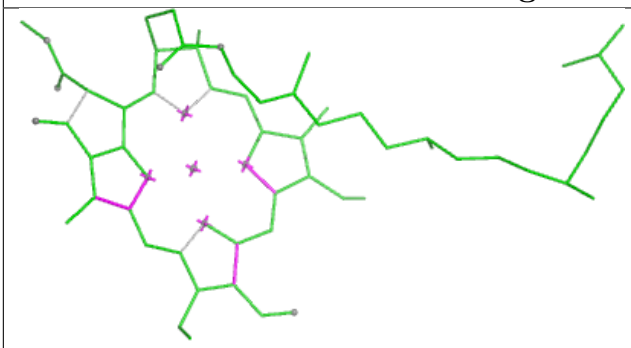


Torsions

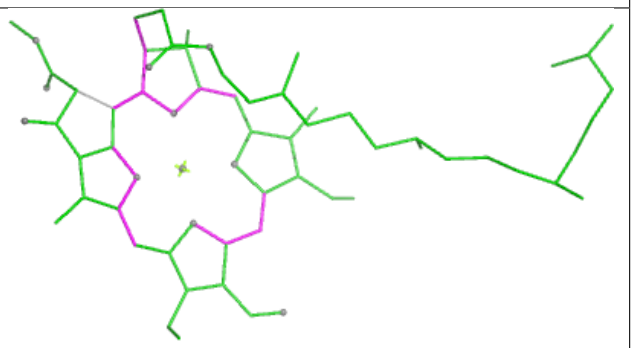


Rings

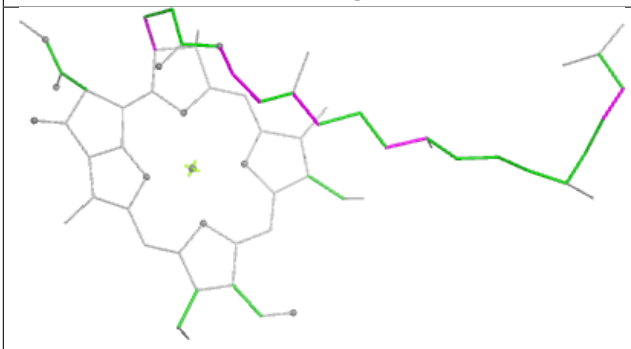
Ligand CHL 82 607



Bond lengths



Bond angles



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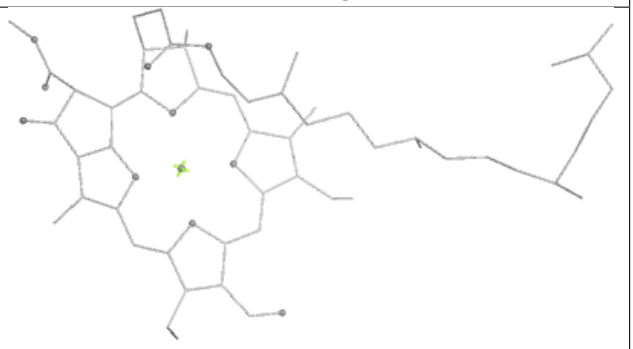
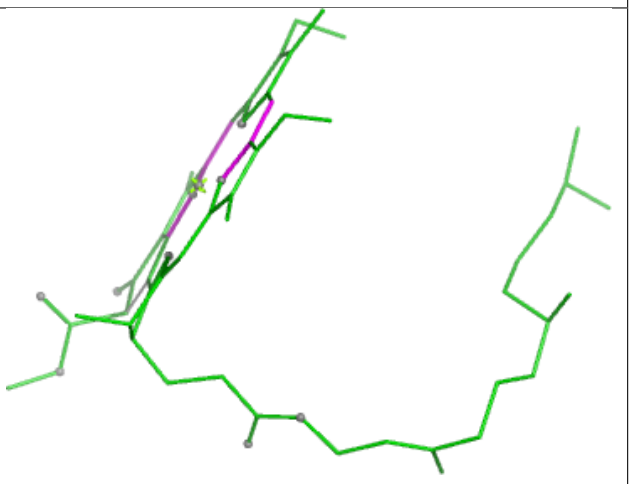


Rings

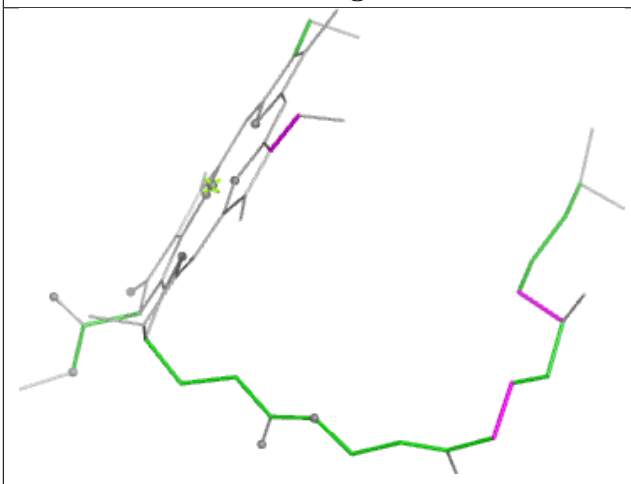
Ligand CLA B 819



Bond lengths



Bond angles

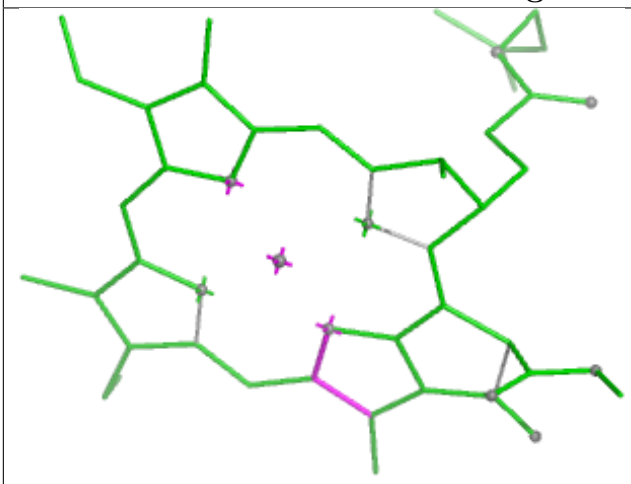


Torsions



Rings

Ligand CLA Z 614



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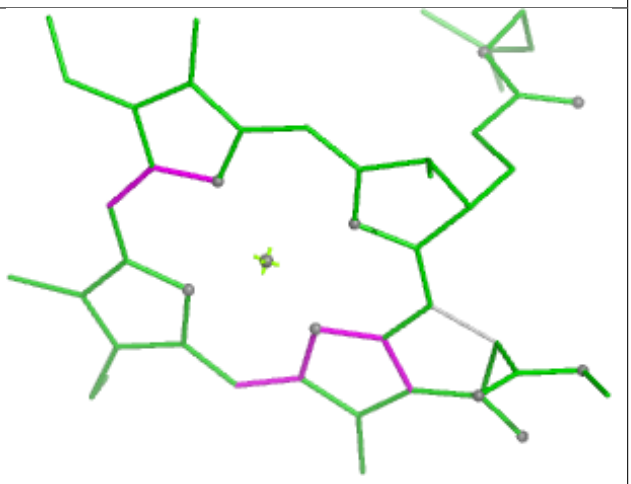
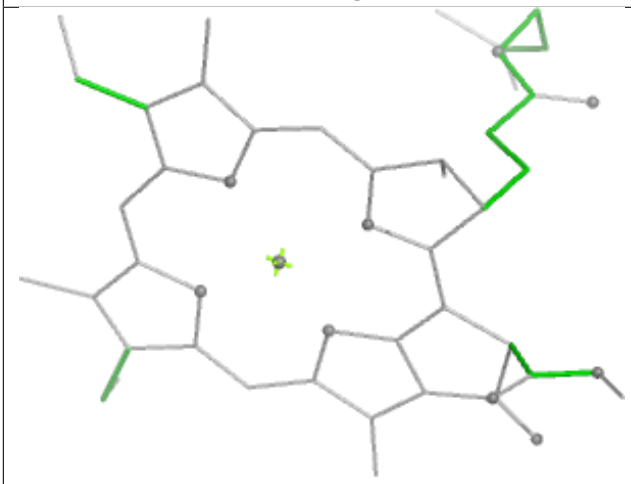


Bond angles



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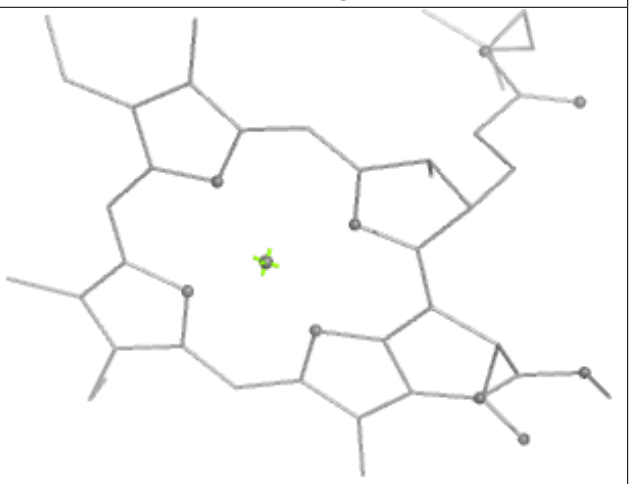
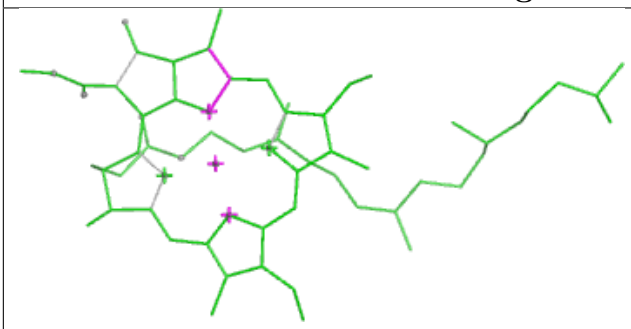


Rings

Ligand CLA B2 816



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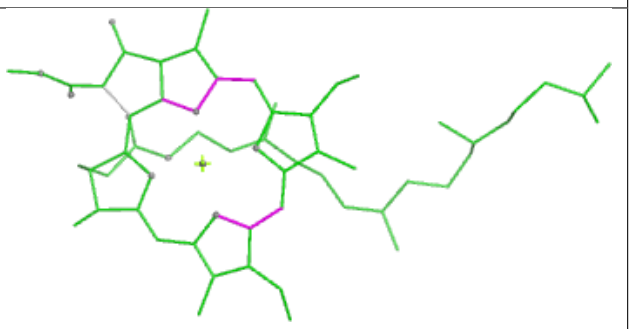
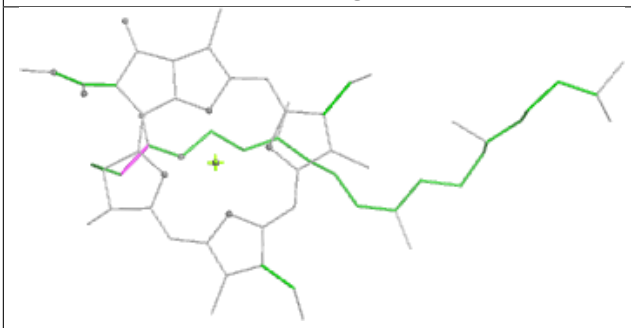


Bond angles



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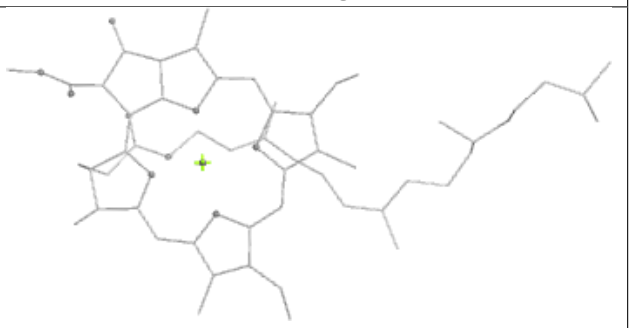
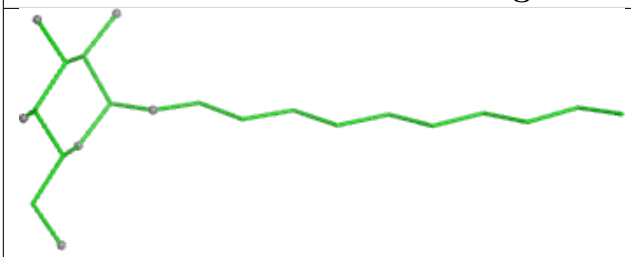


Rings

Ligand LMU Z2 621



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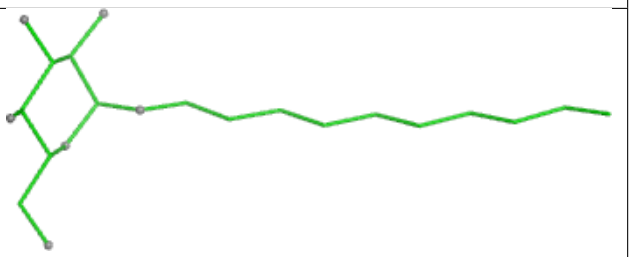
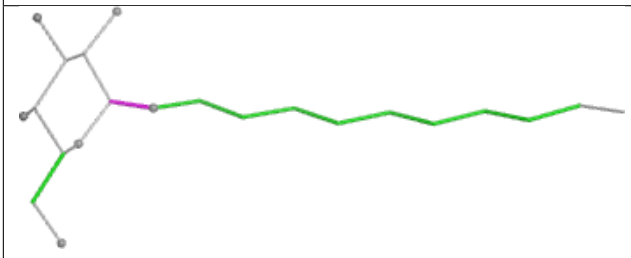


Bond angles



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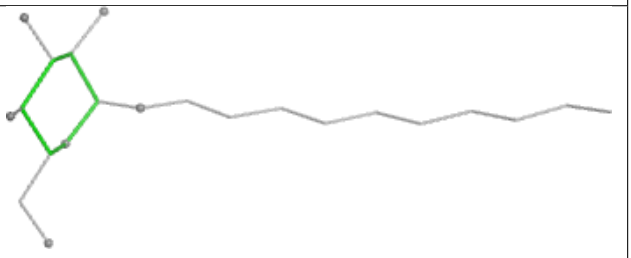
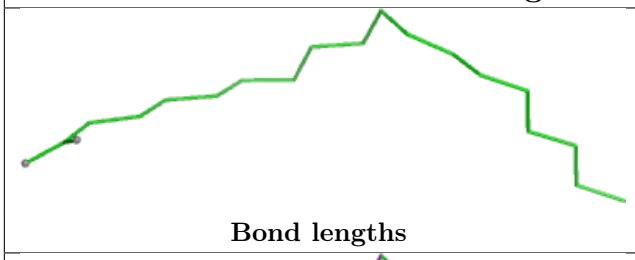


Rings

Ligand LMG 6 633



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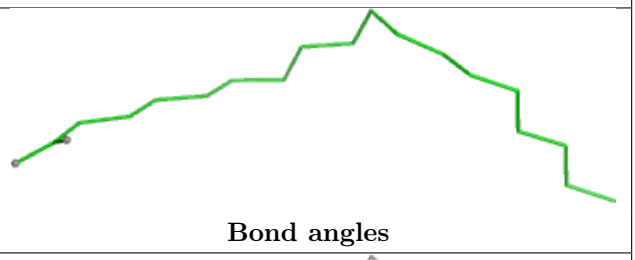
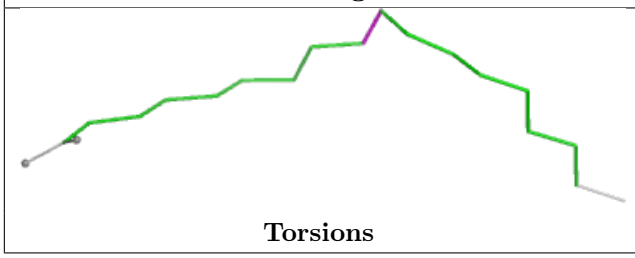


Bond angles



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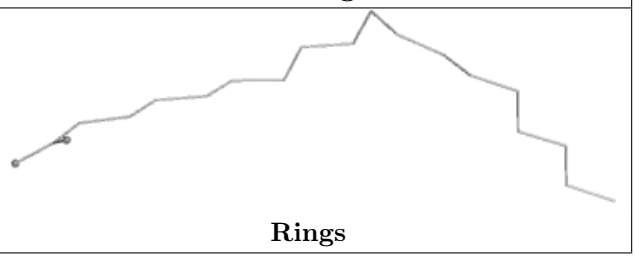
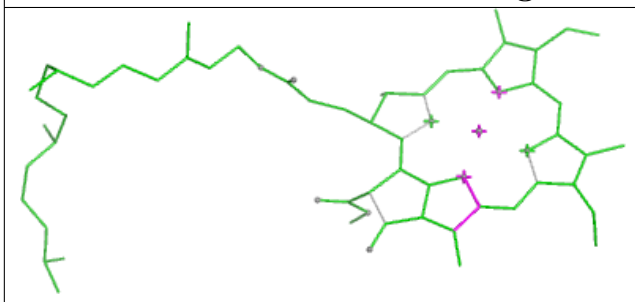


Rings

Ligand CLA B2 826



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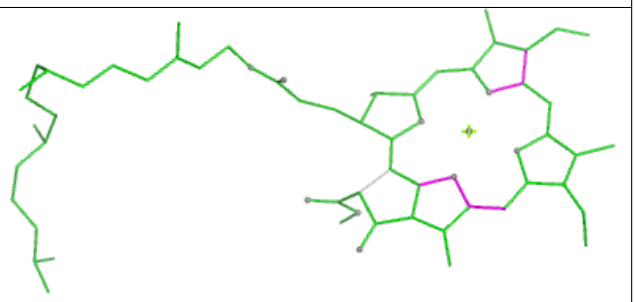
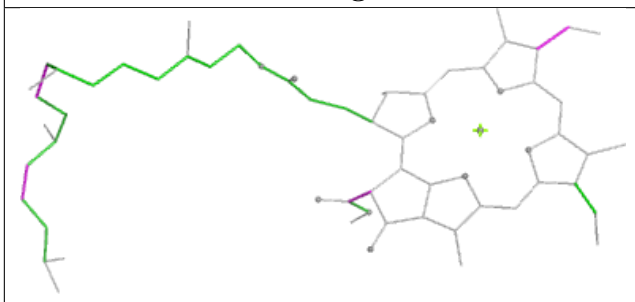


Bond angles



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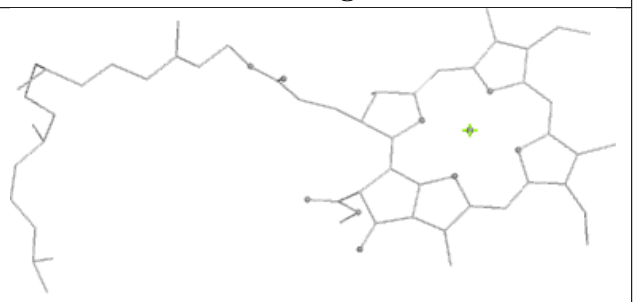
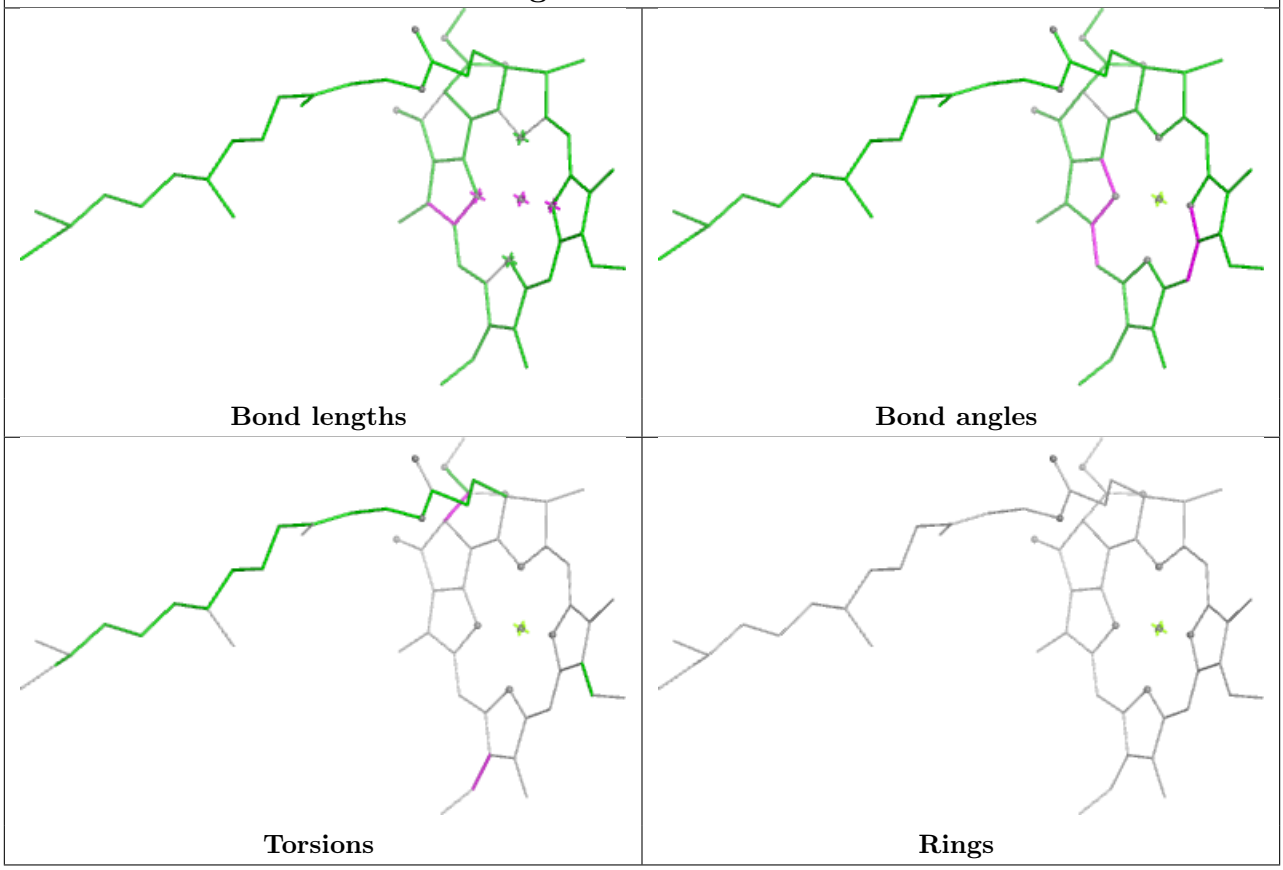


Rings

Ligand CLA 3 609



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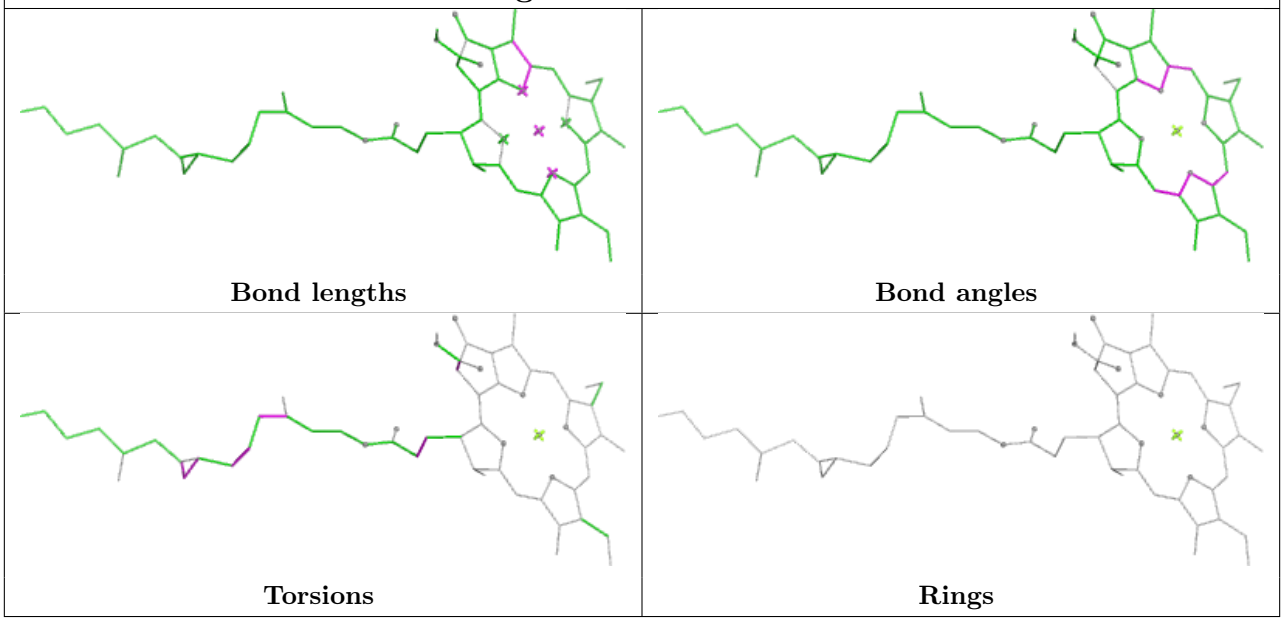

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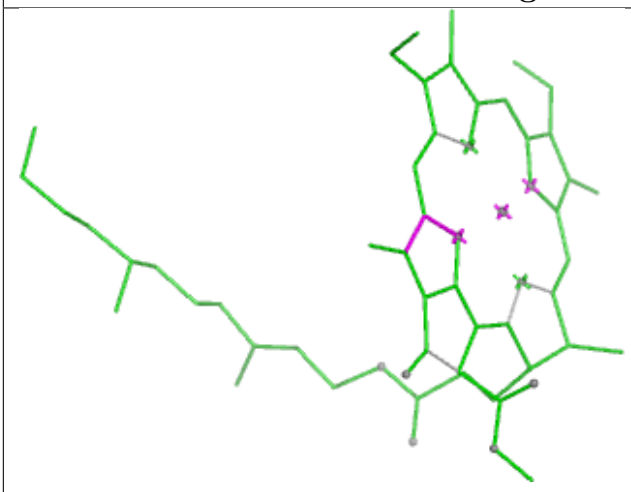

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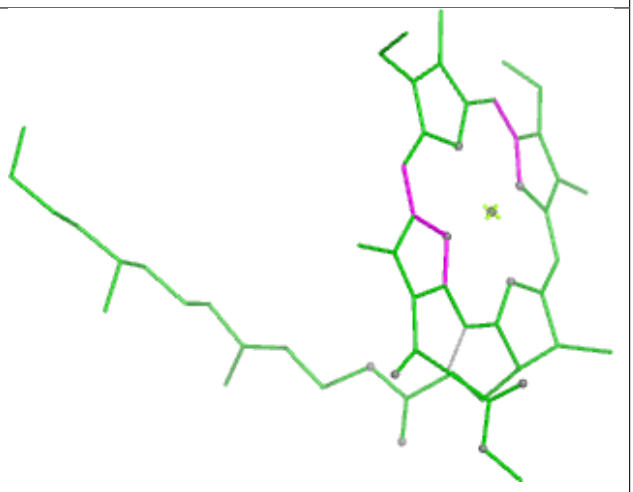
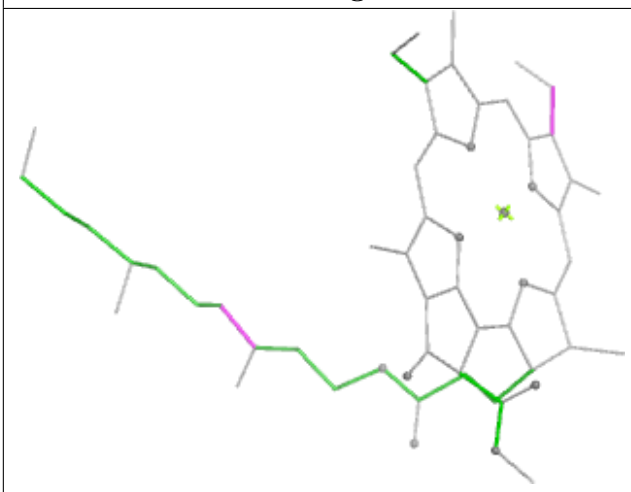


Bond angles



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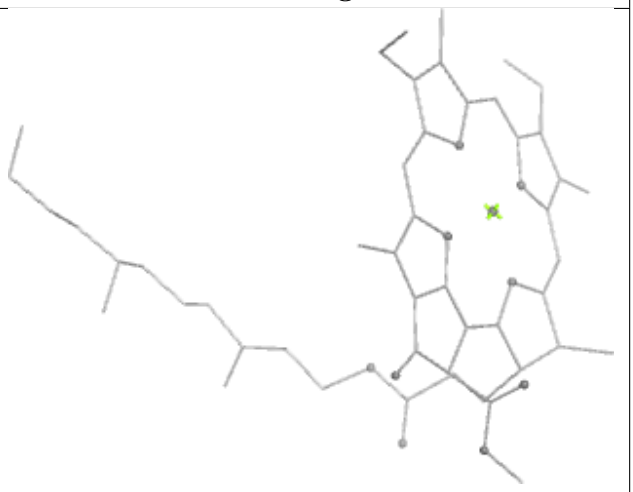
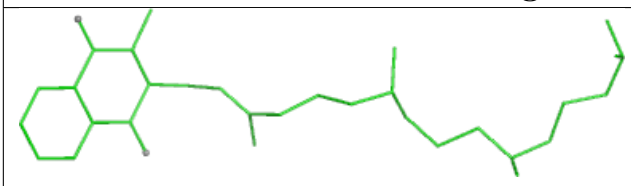


Rings

Ligand PQN A 844



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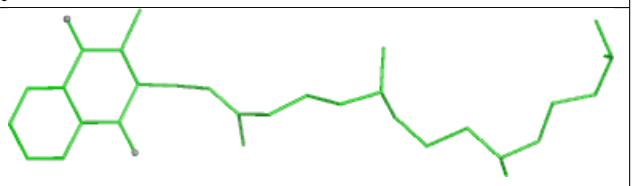
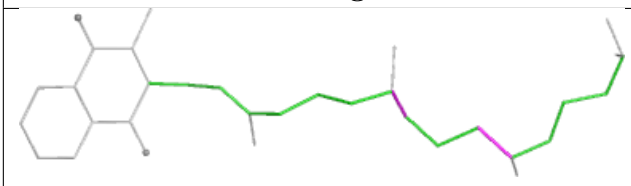


Bond angles

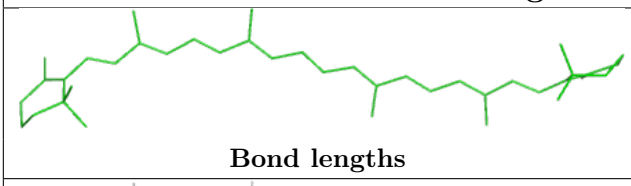


Torsions



Rings

Ligand BCR 3 620



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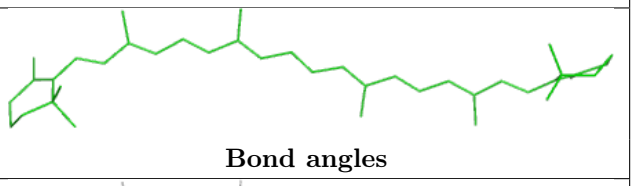
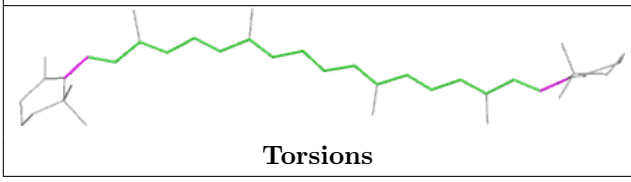


Bond angles



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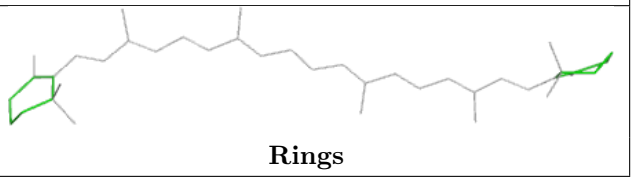
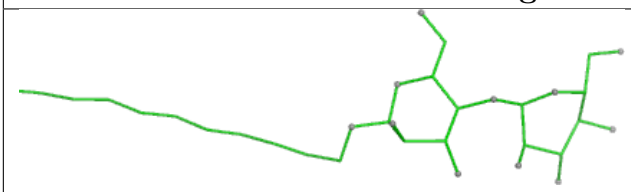


Rings

Ligand LMU A 858



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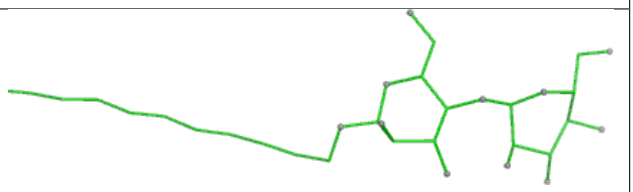
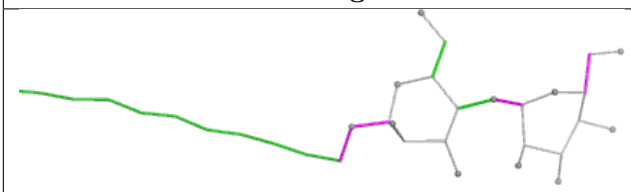


Bond angles



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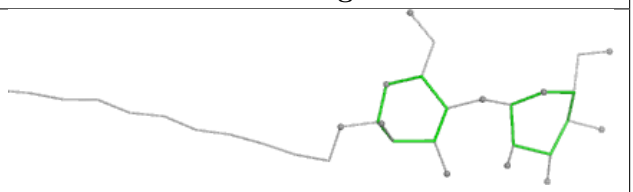
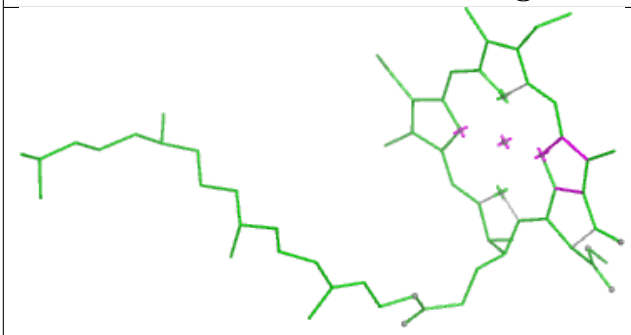


Rings

Ligand CLA A2 809



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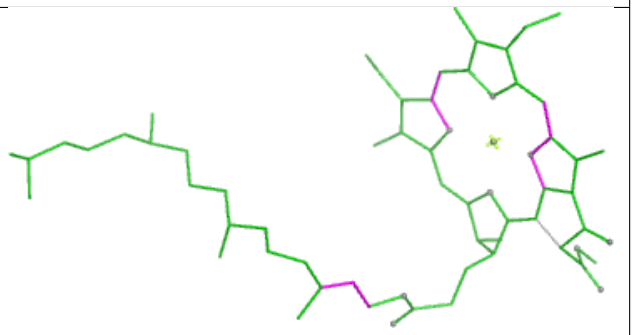
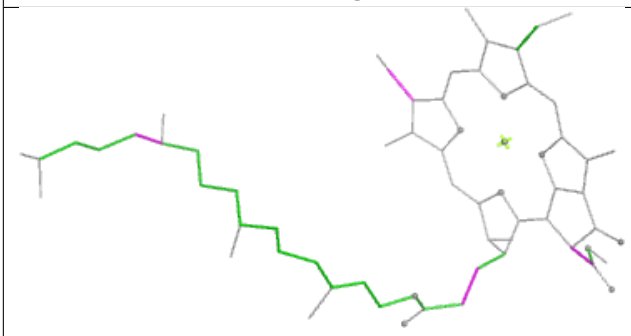


Bond angles

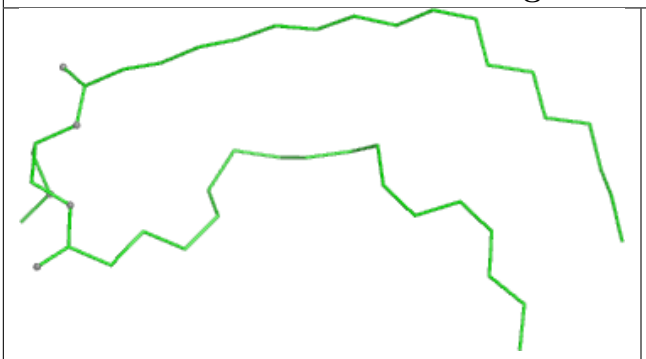


Torsions



Rings

Ligand LMG 3 722



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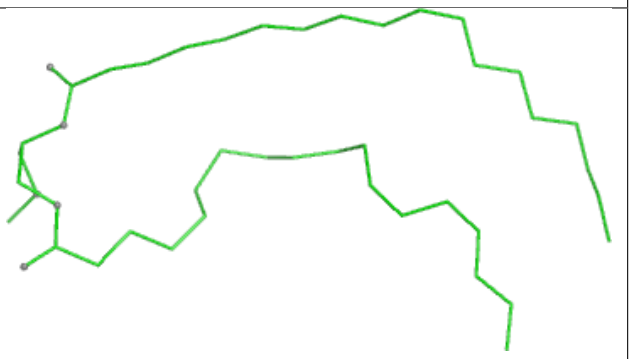
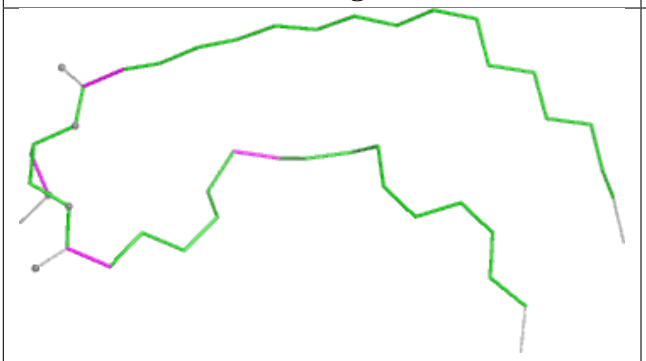


Bond angles



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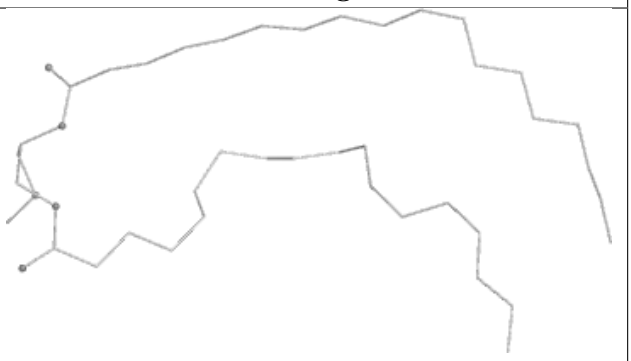
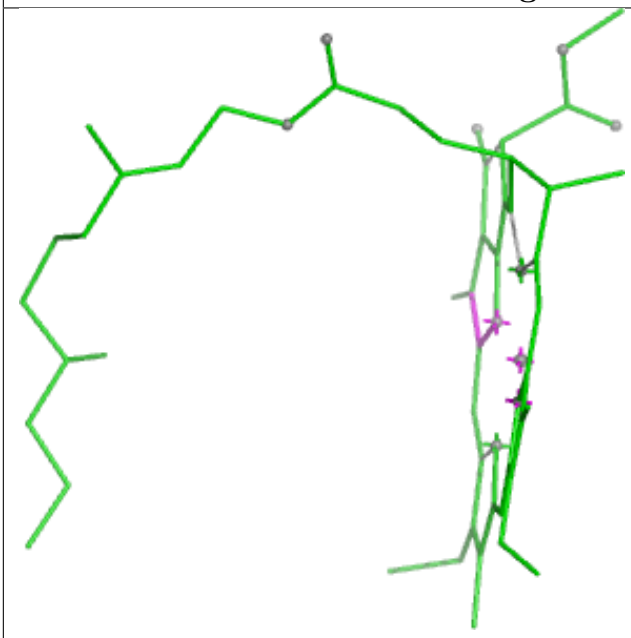


Rings

Ligand CLA 82 614



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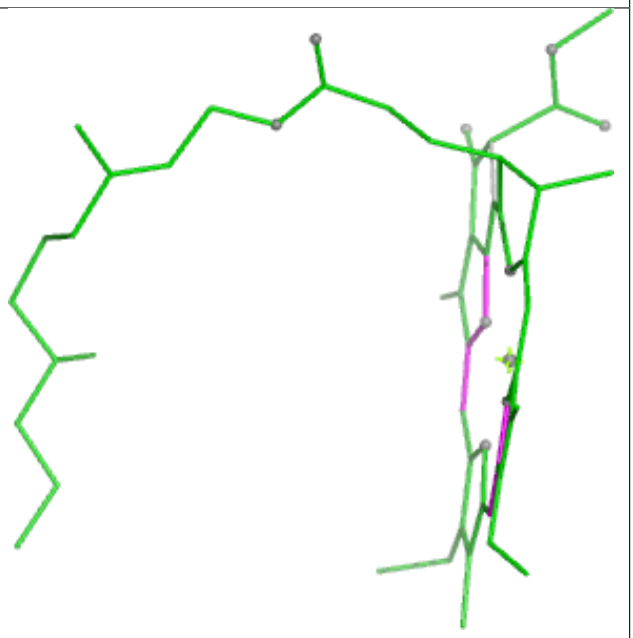
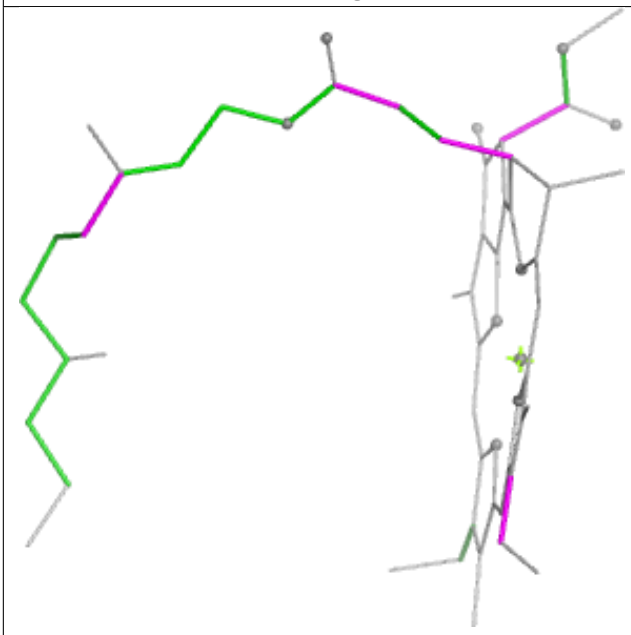


Bond angles



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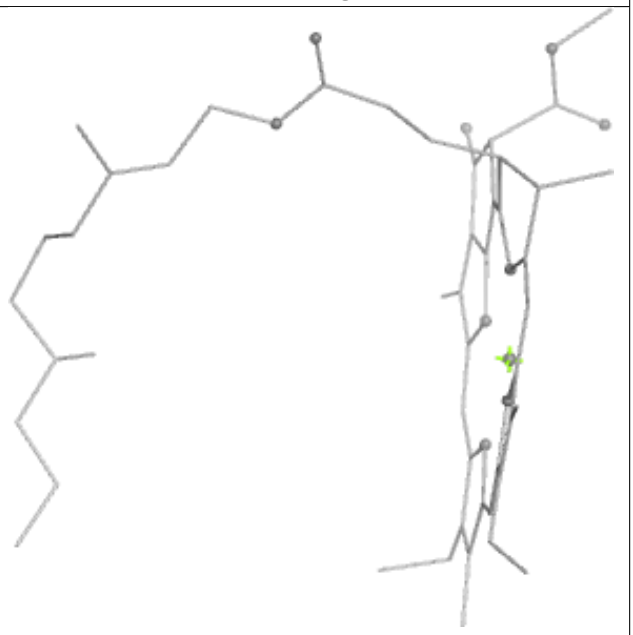
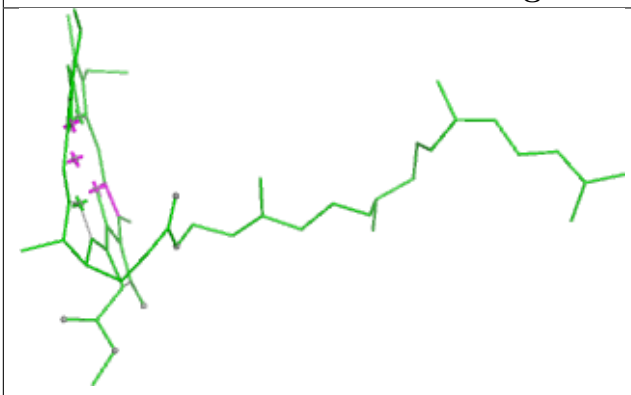
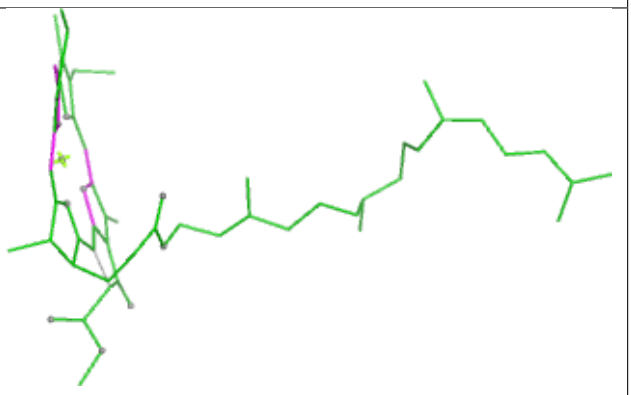


Rings

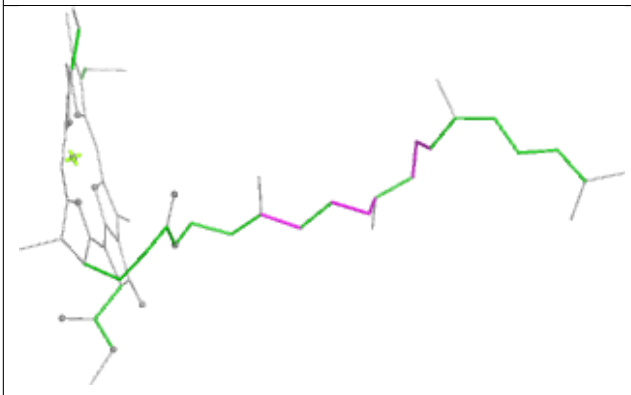
Ligand CLA A 829



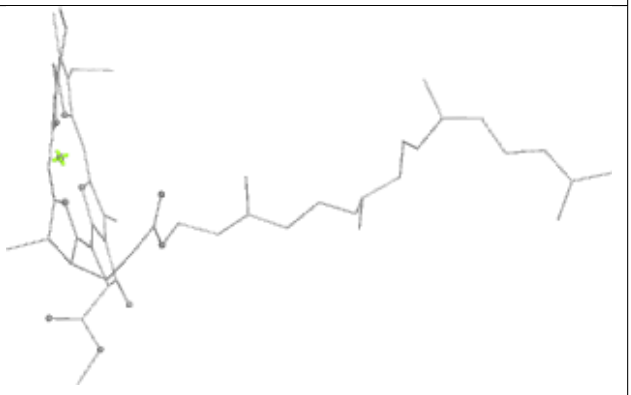
Bond lengths



Bond angles

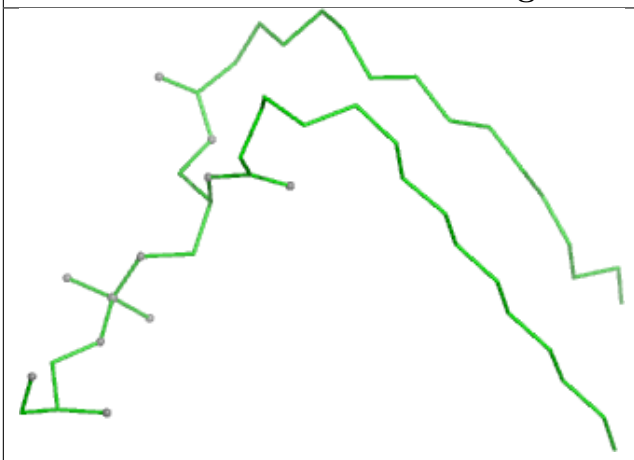


Torsions



Rings

Ligand LHG 72 625



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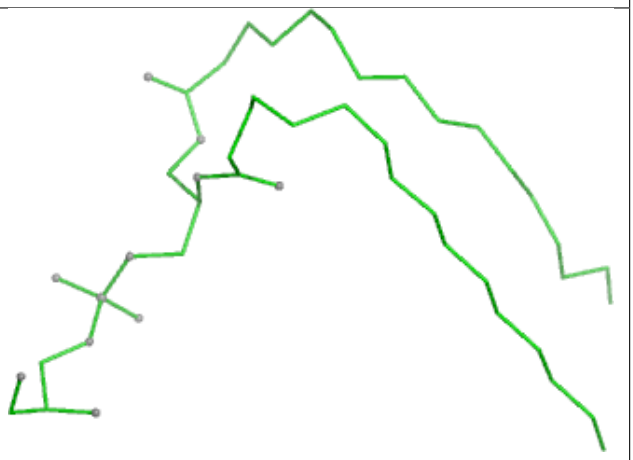
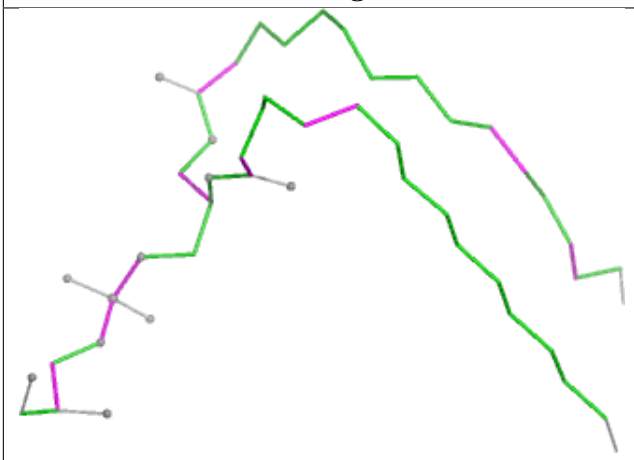


Bond angles



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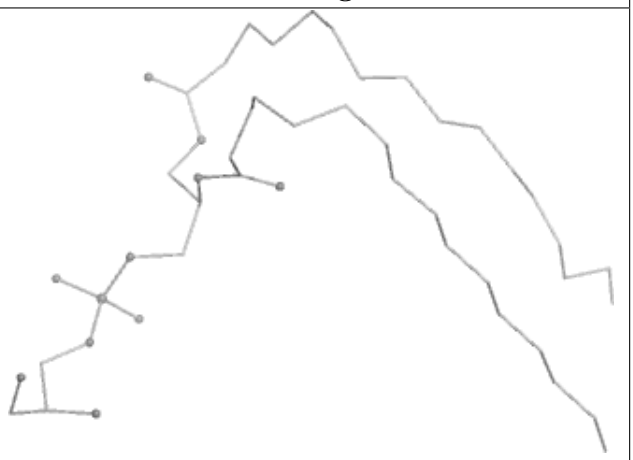
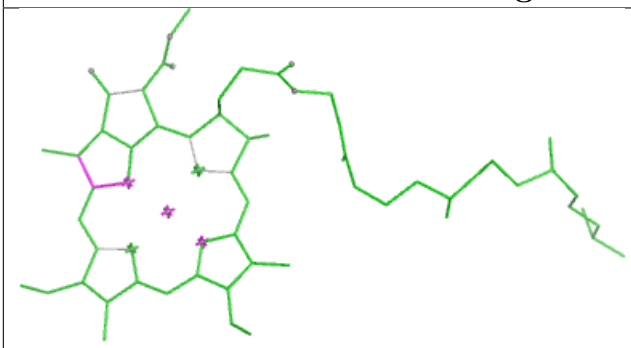


Rings

Ligand CLA B2 803



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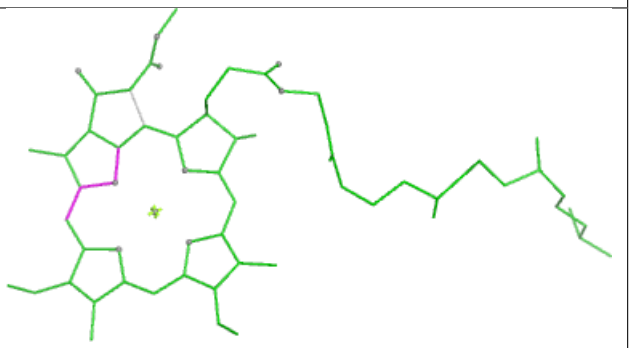

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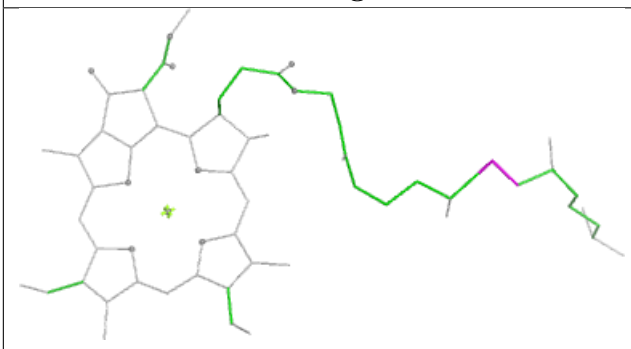

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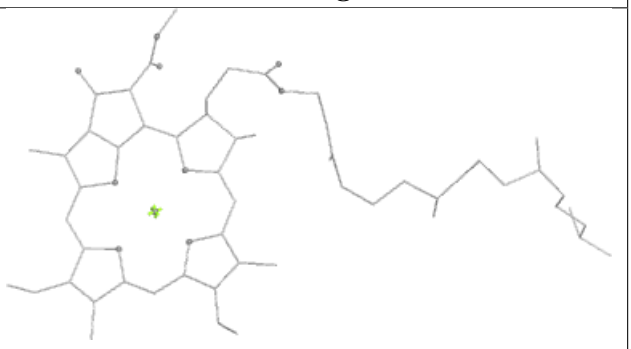
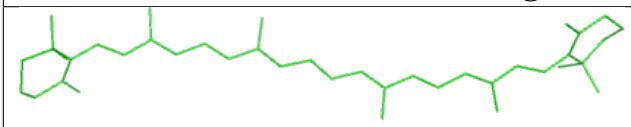


Rings

Ligand BCR A 848



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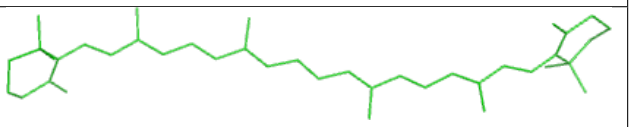
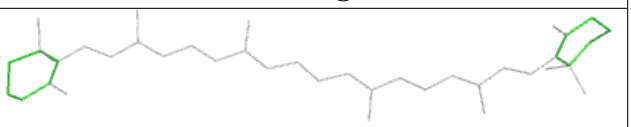


Bond angles

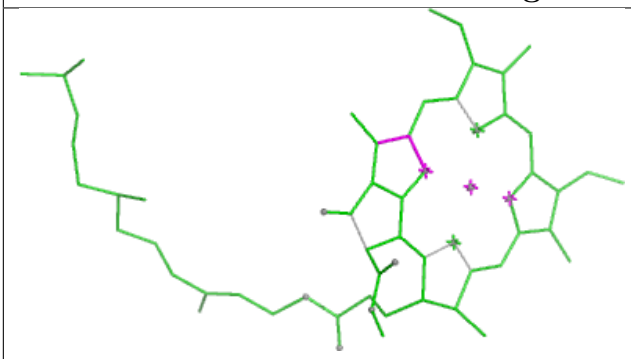


Torsions



Rings

Ligand CLA K 203



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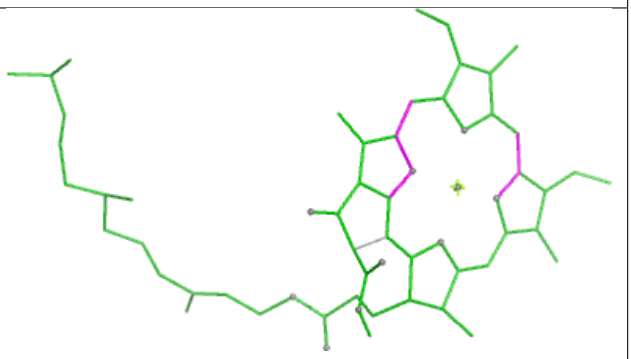
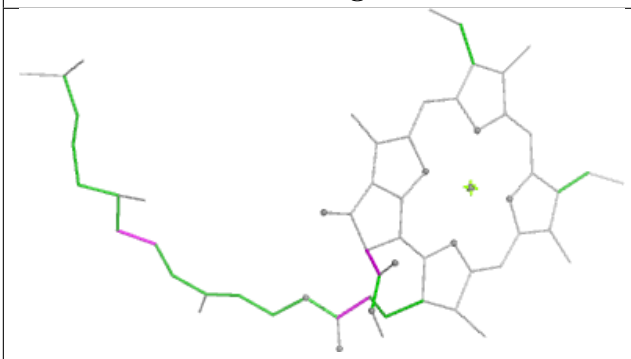


Bond angles



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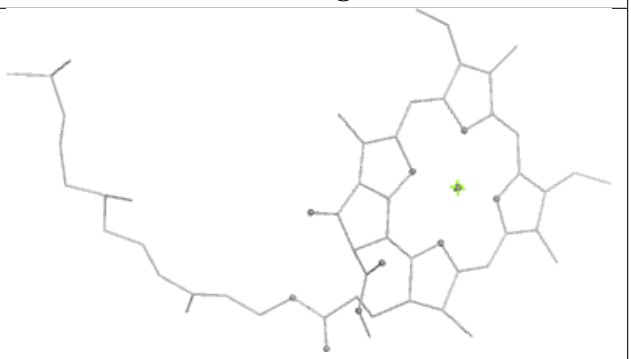
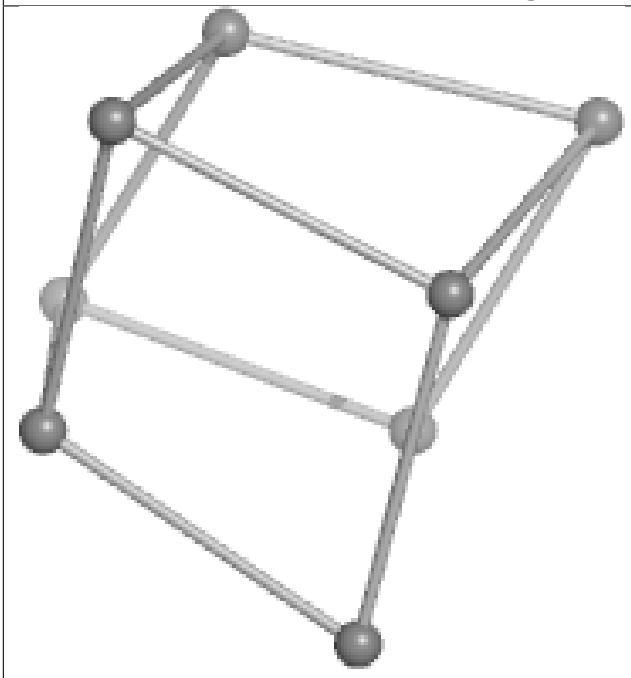


Rings

Ligand SF4 C2 101



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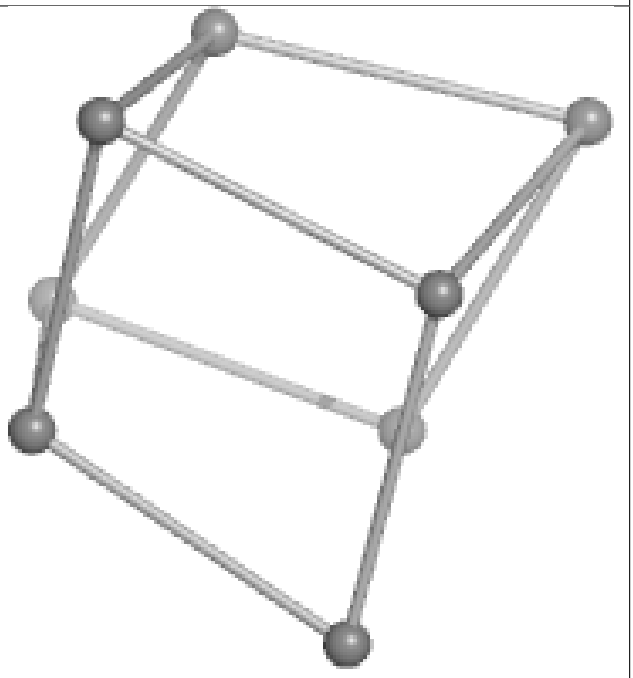

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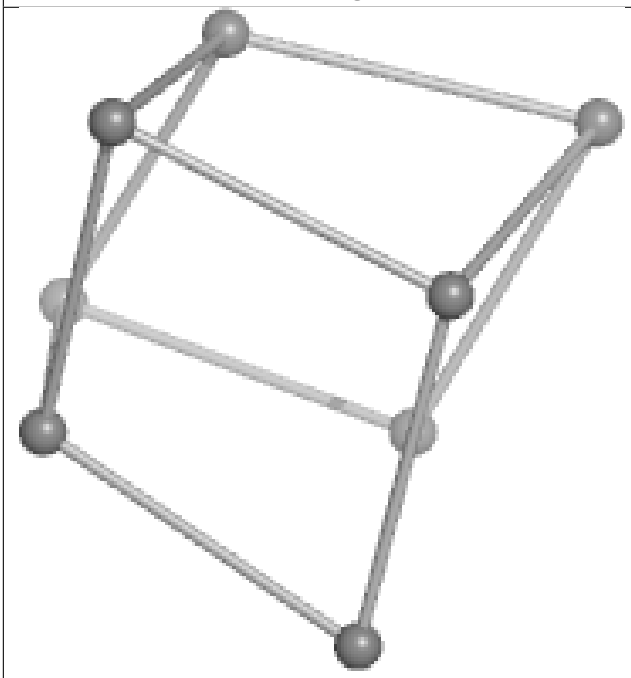

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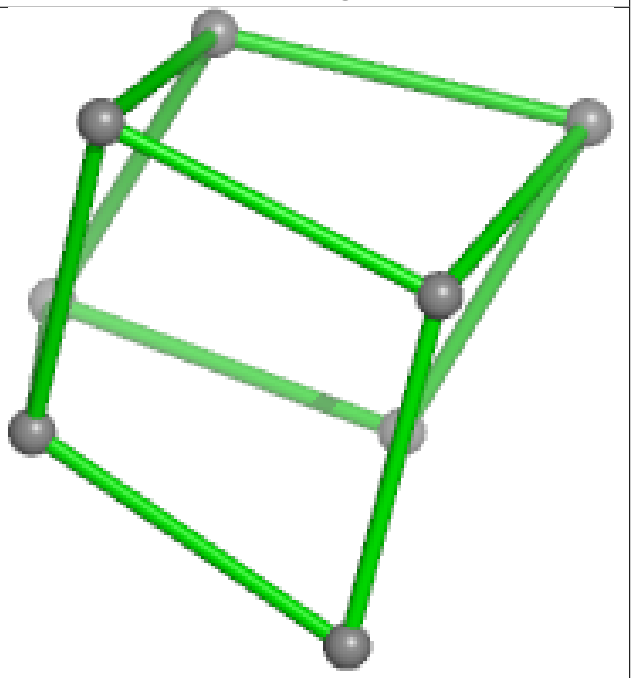
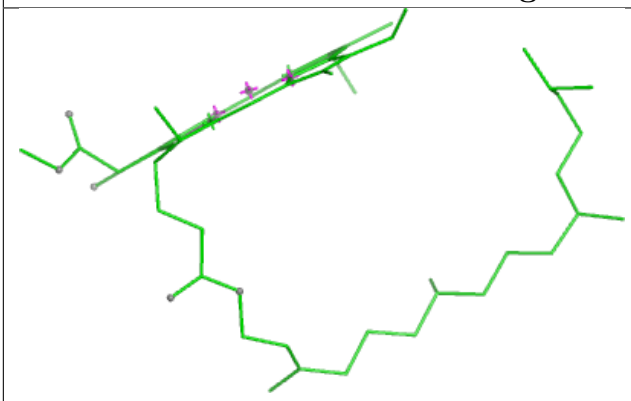


Rings

Ligand CLA 62 604



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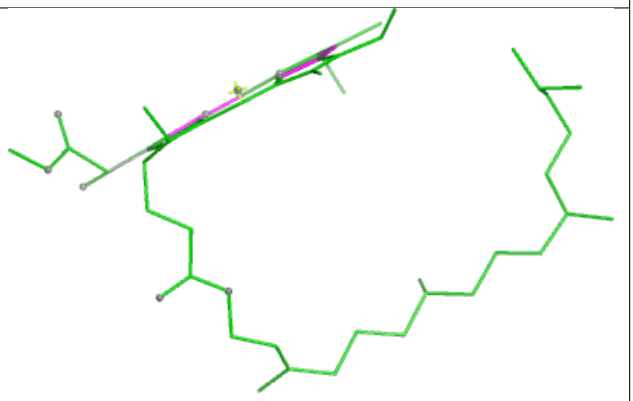
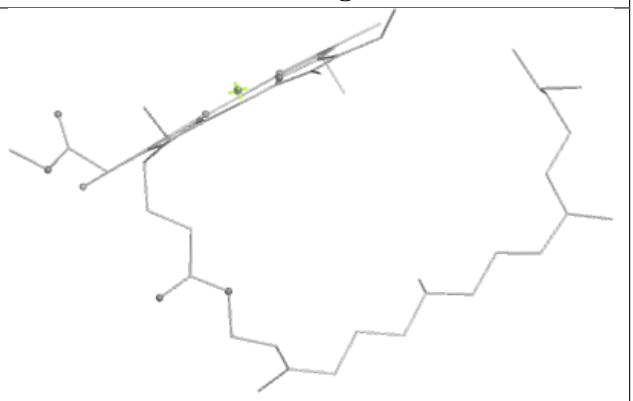


Bond angles

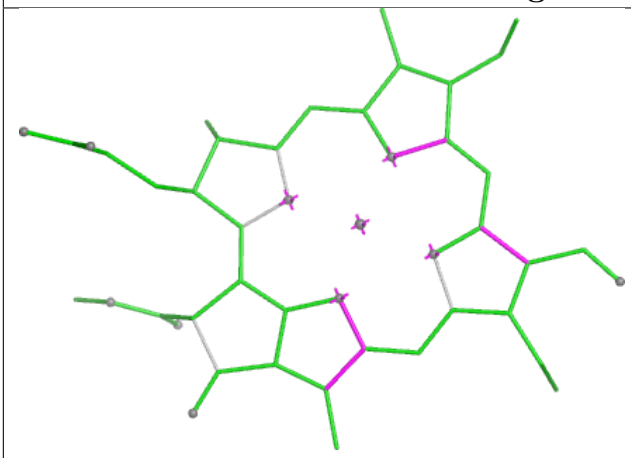


Torsions



Rings

Ligand CHL 5 606



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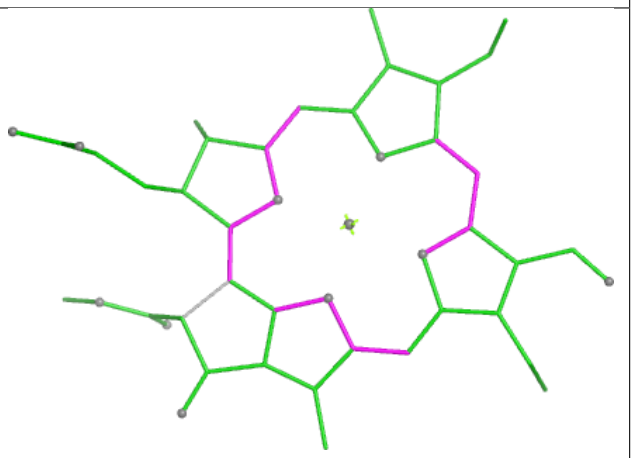
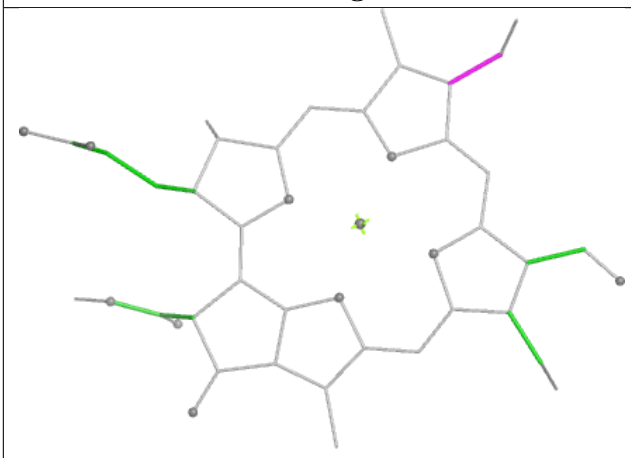


Bond angles



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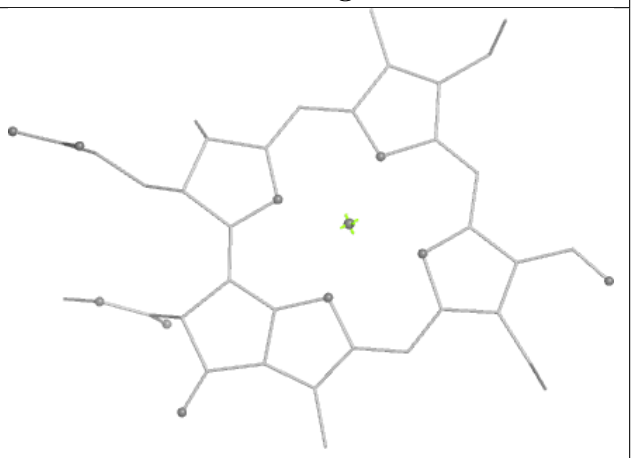
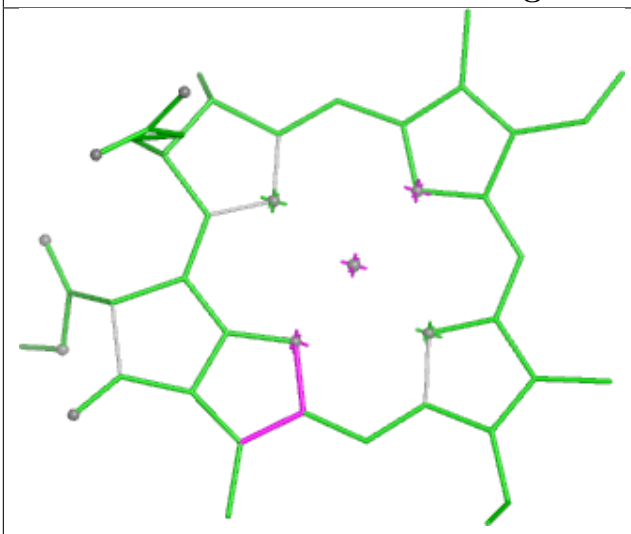


Rings

Ligand CLA A 845



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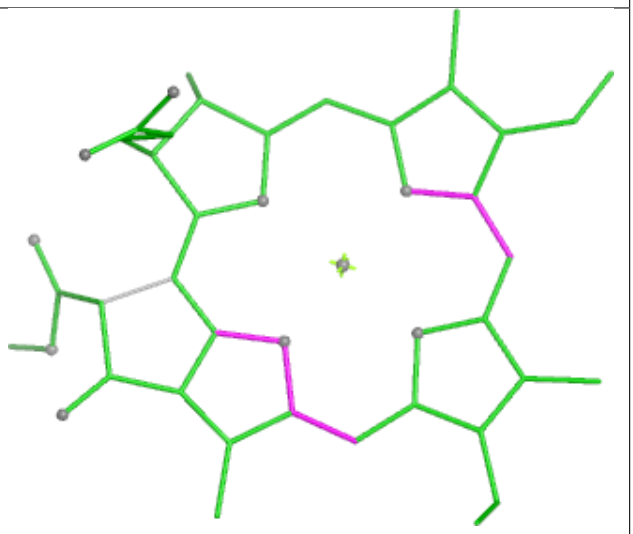

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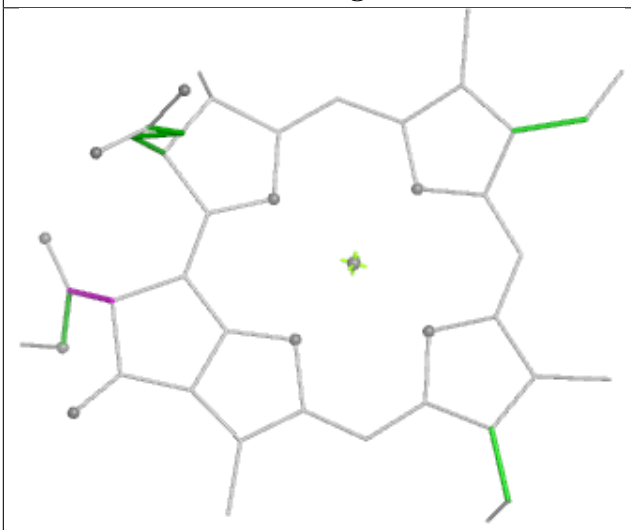

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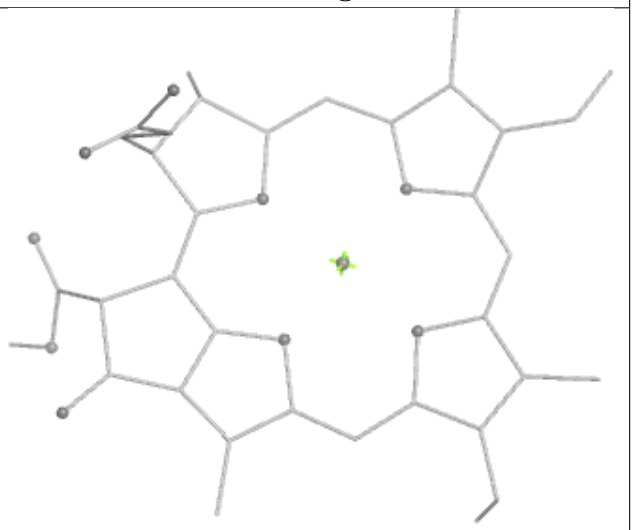
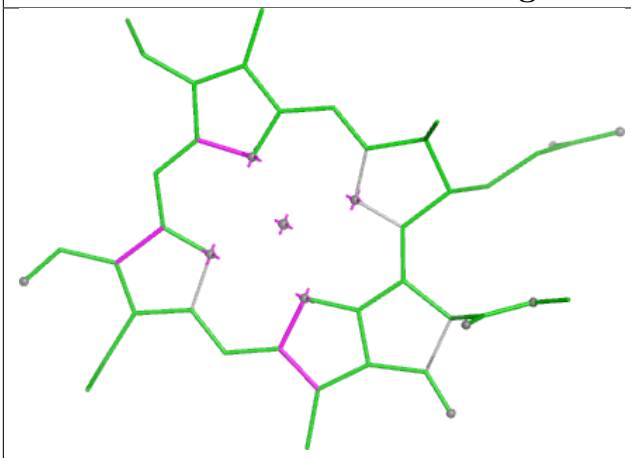


Rings

Ligand CHL 52 606



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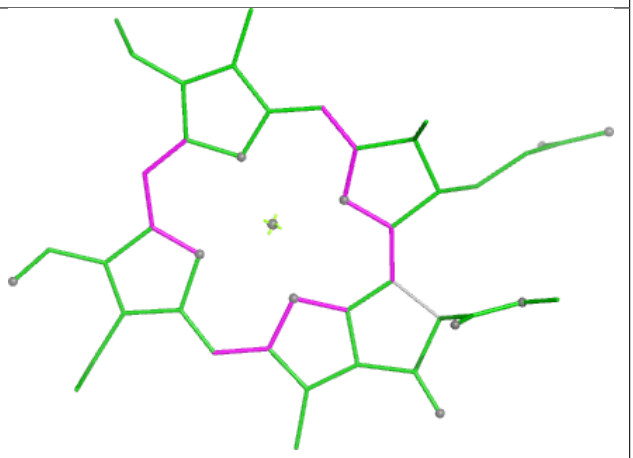

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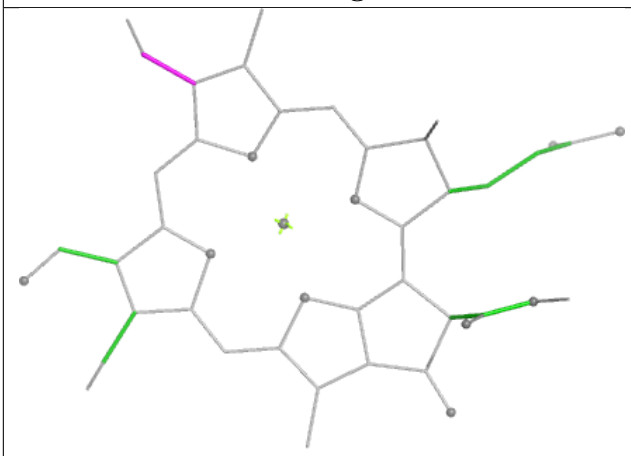

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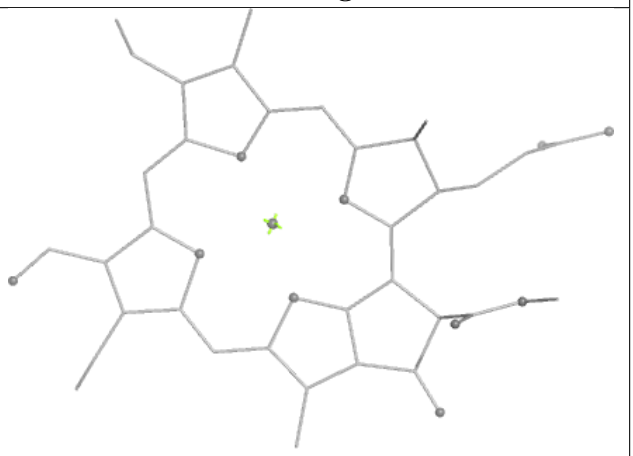
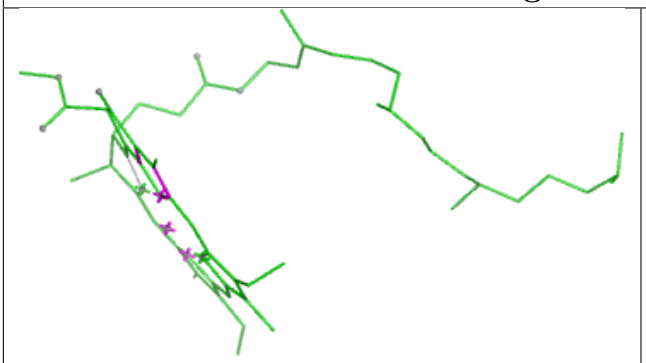


Rings

Ligand CLA A 811



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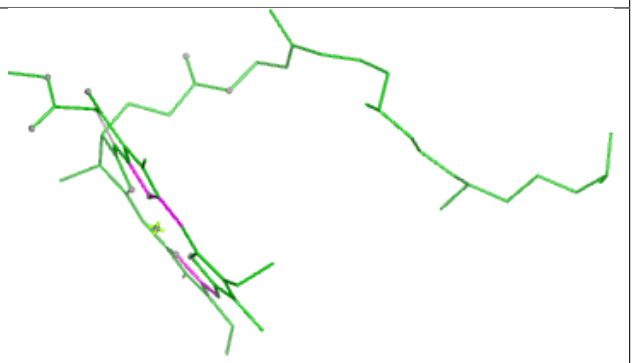

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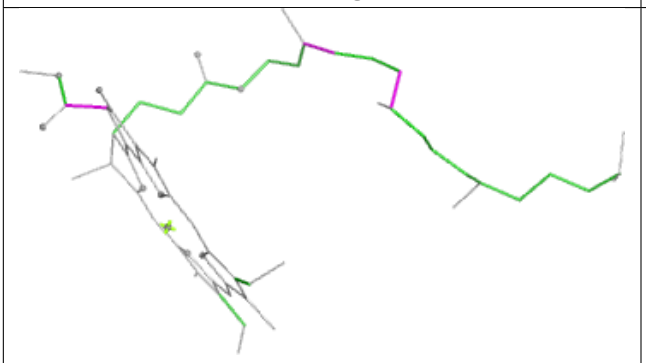
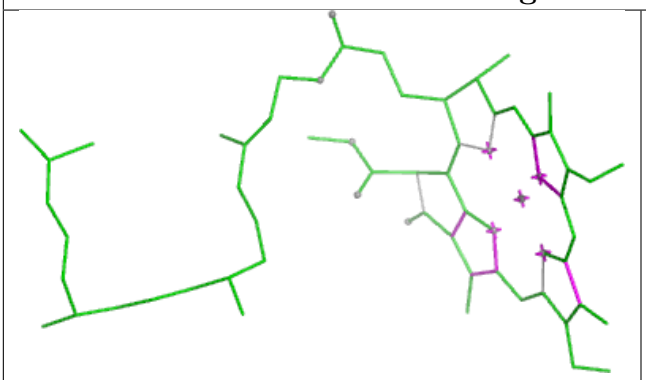


Torsions



Rings

Ligand CL0 A2 801



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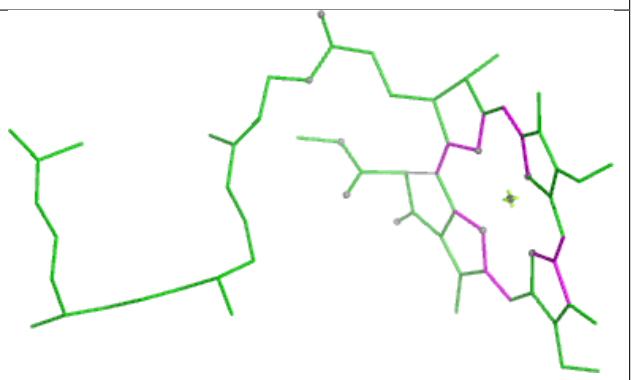

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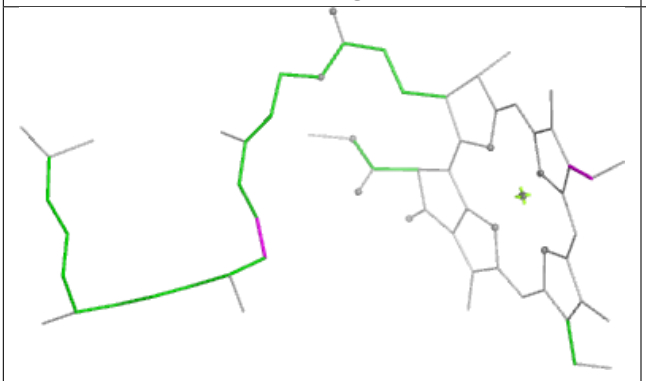
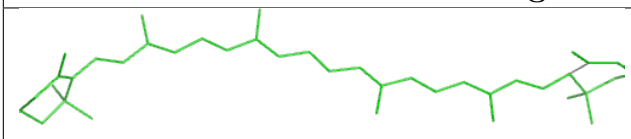


Torsions



Rings

Ligand LUT 7 621



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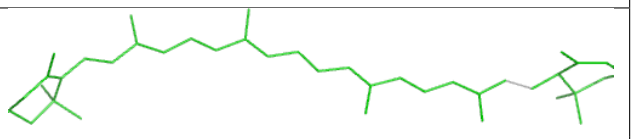

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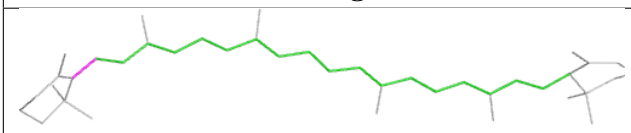

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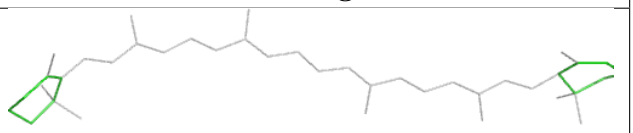
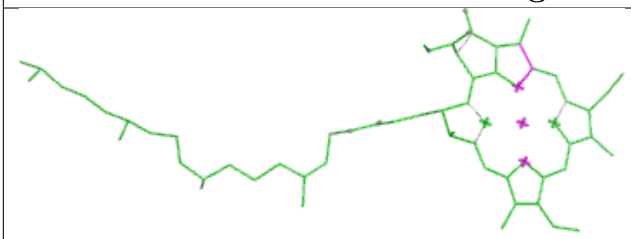


Rings

Ligand CLA 5 617



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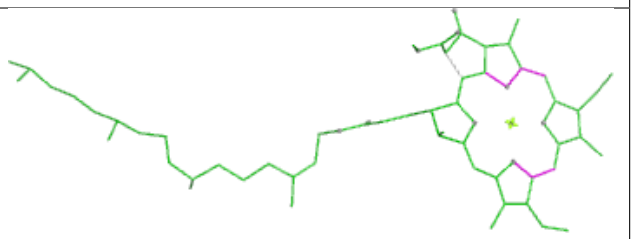
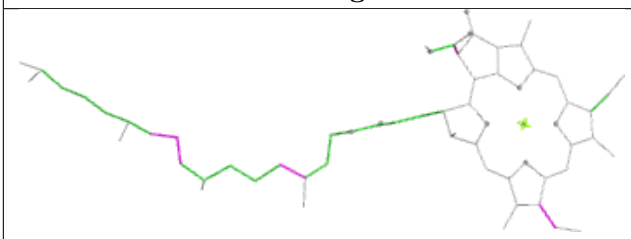


Bond angles



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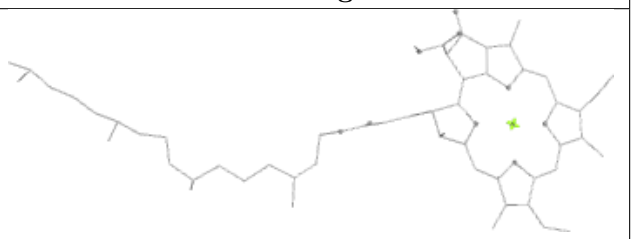
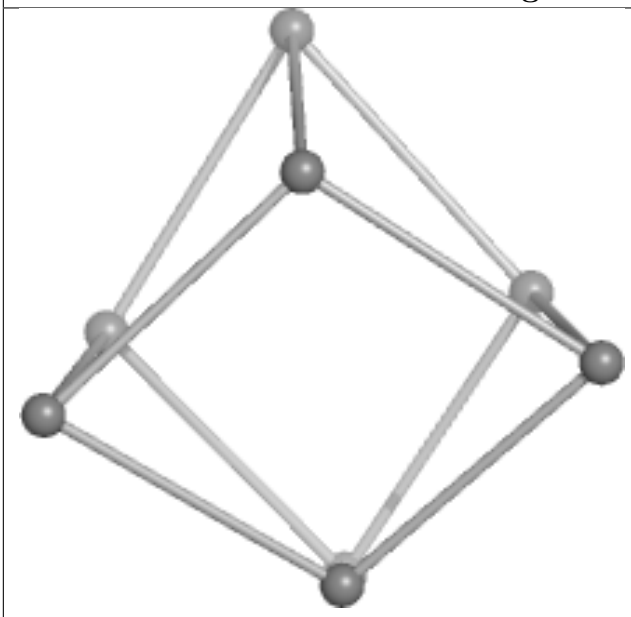


Rings

Ligand SF4 A2 853



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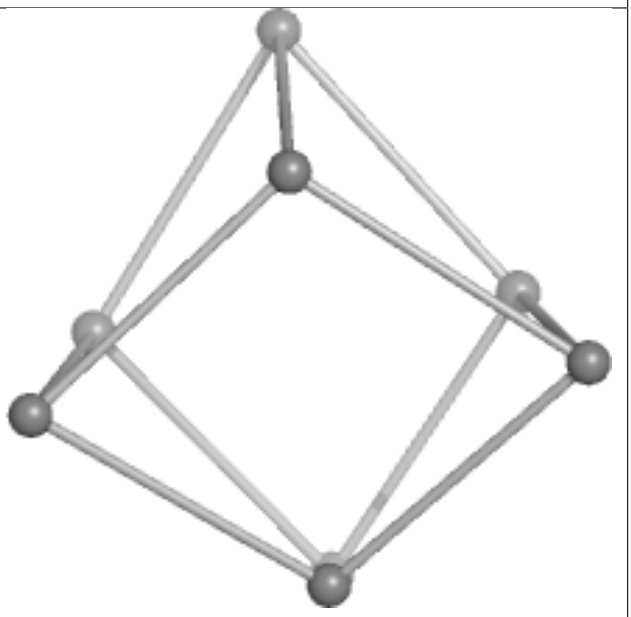
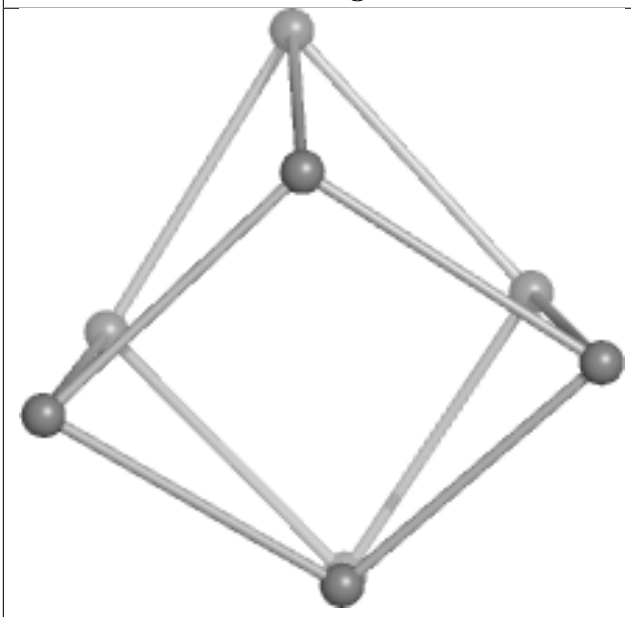


Bond angles



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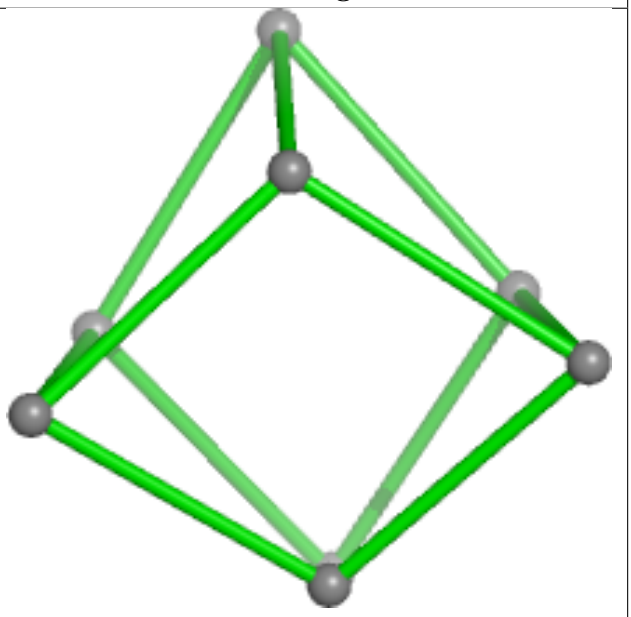
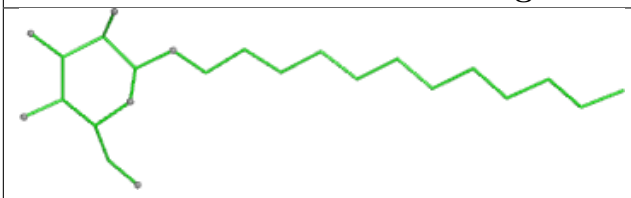


Rings

Ligand LMU 12 626



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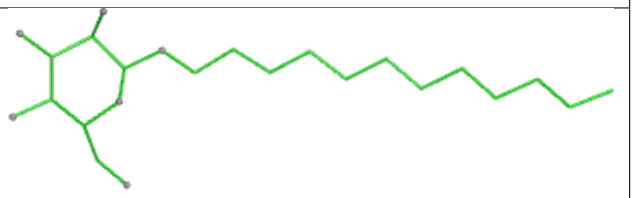
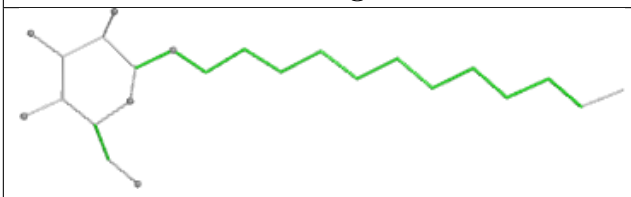


Bond angles



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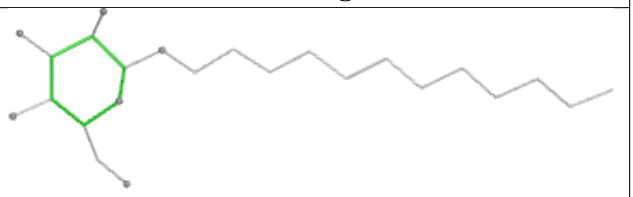
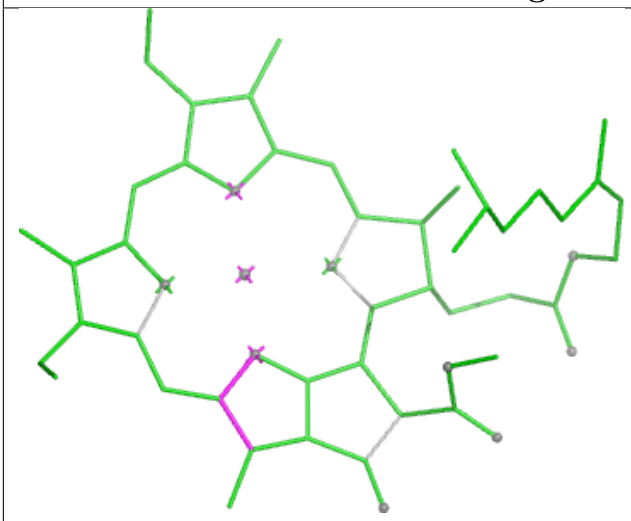
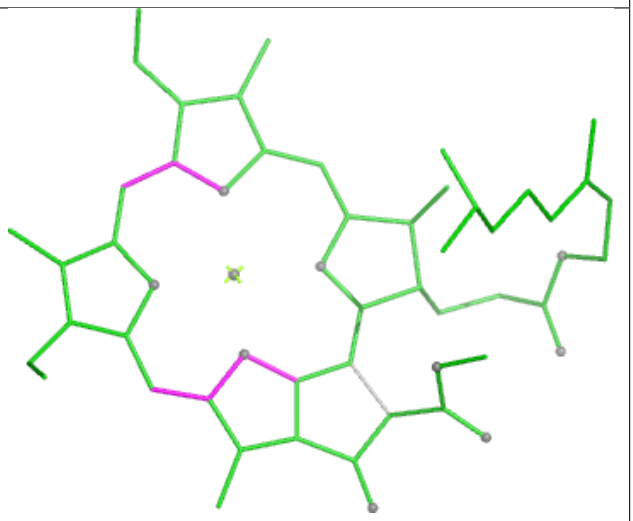


Rings

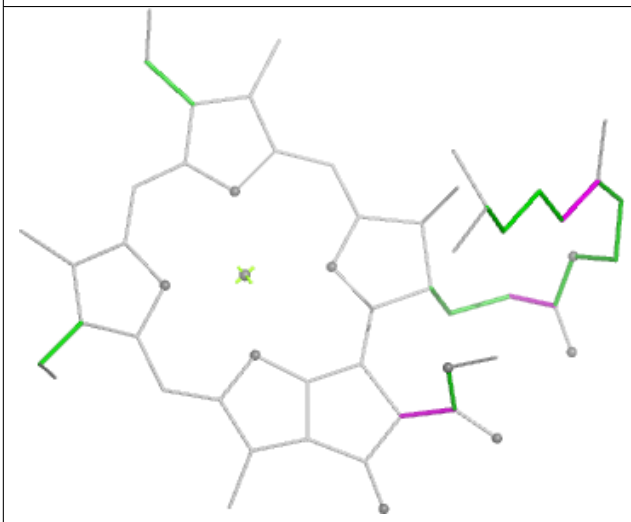
Ligand CLA 8 612



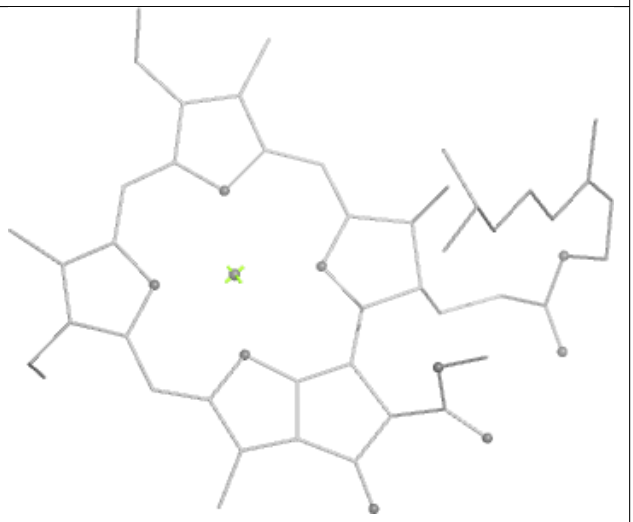
Bond lengths



Bond angles

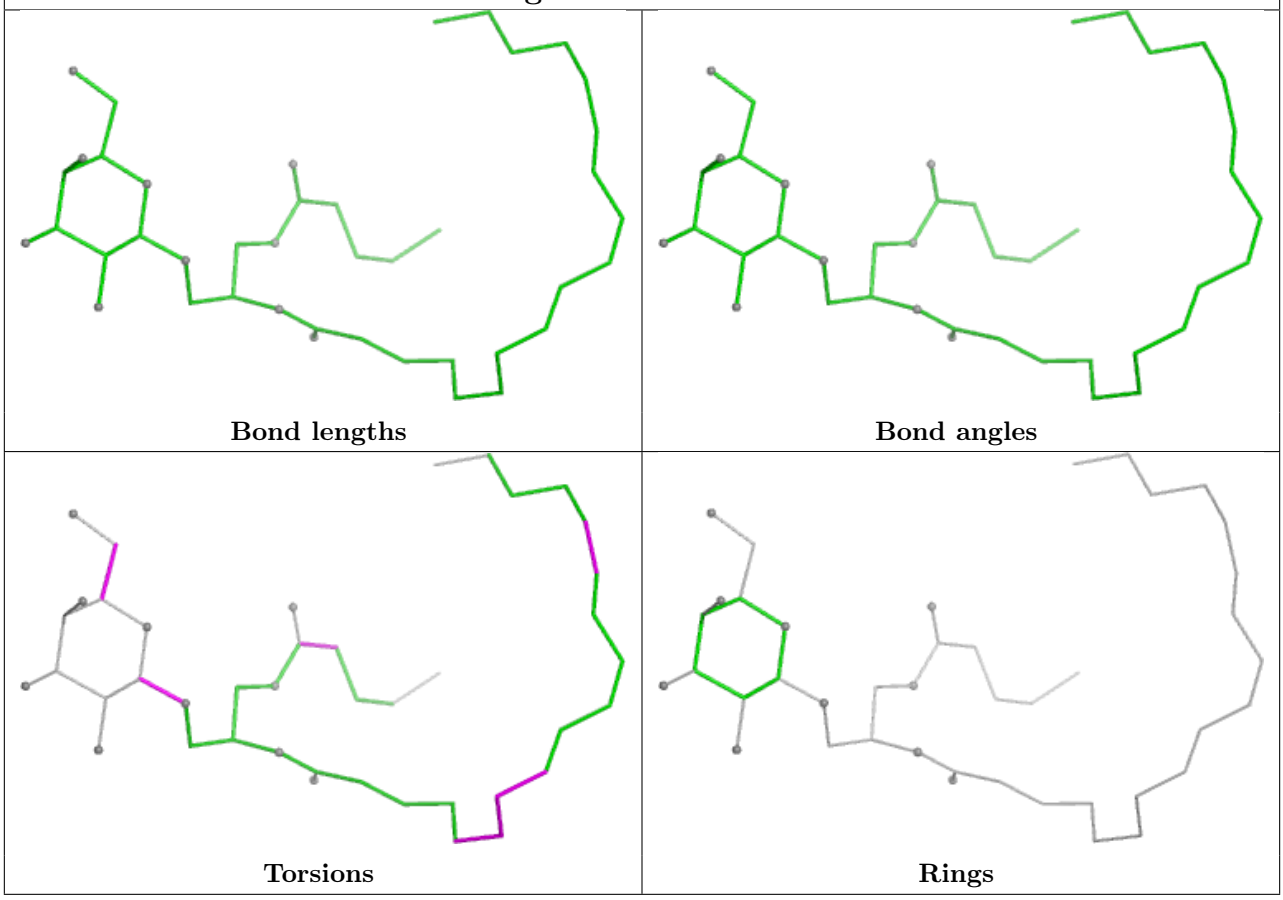


Torsions

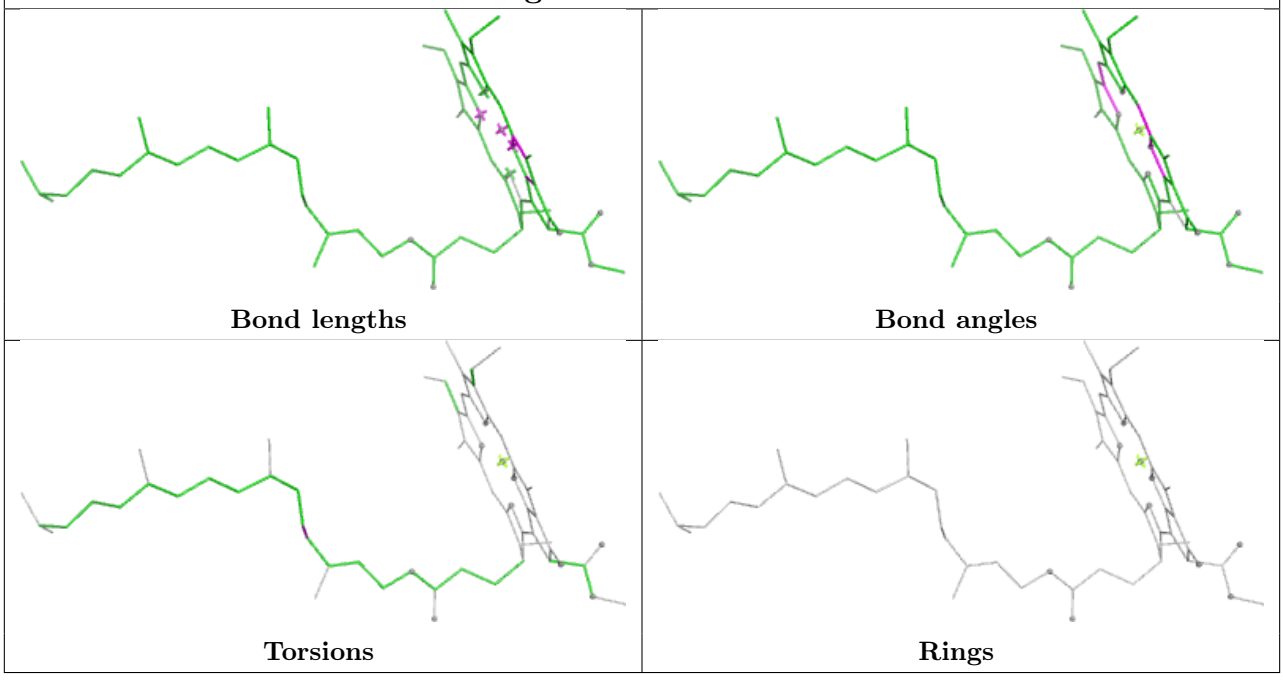


Rings

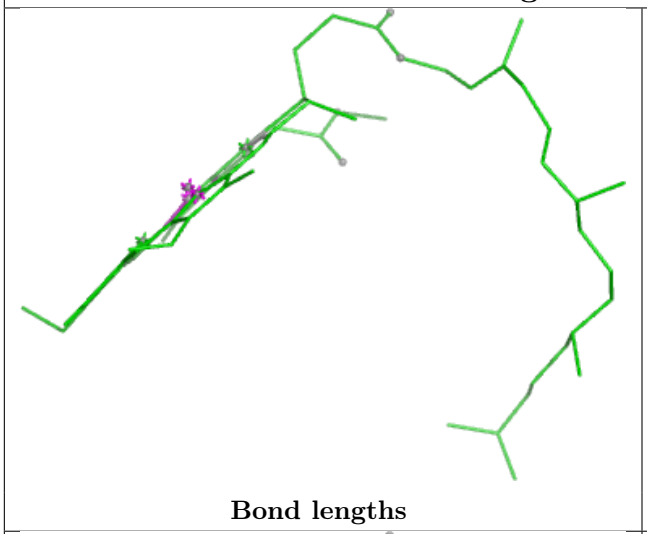
Ligand LMG 8 629



Ligand CLA A 833



Ligand CLA 42 603



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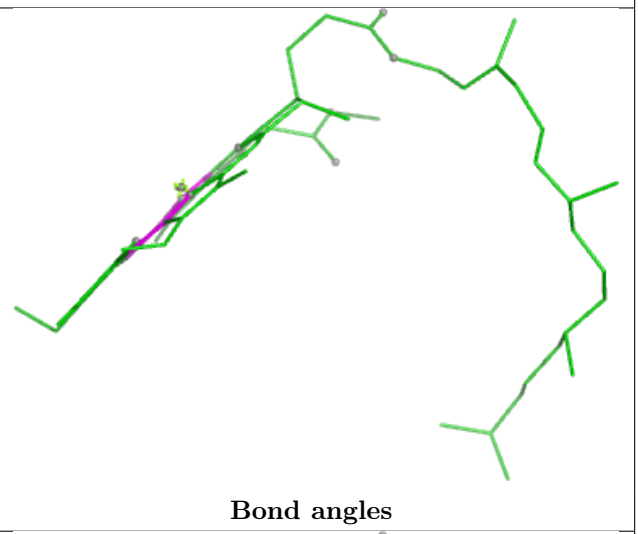

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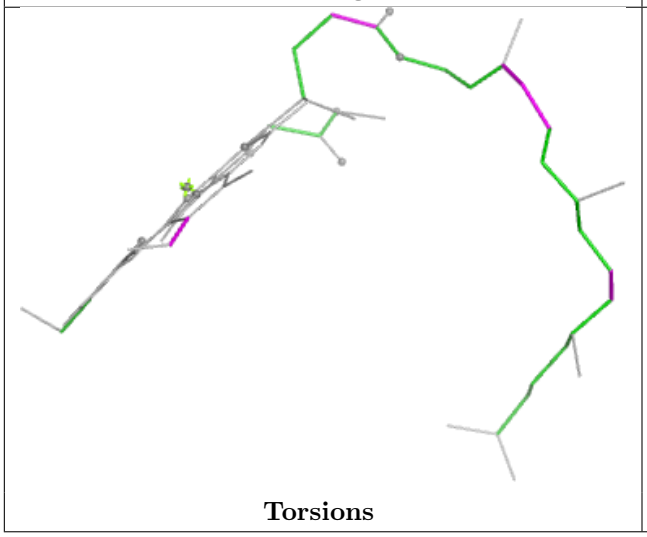

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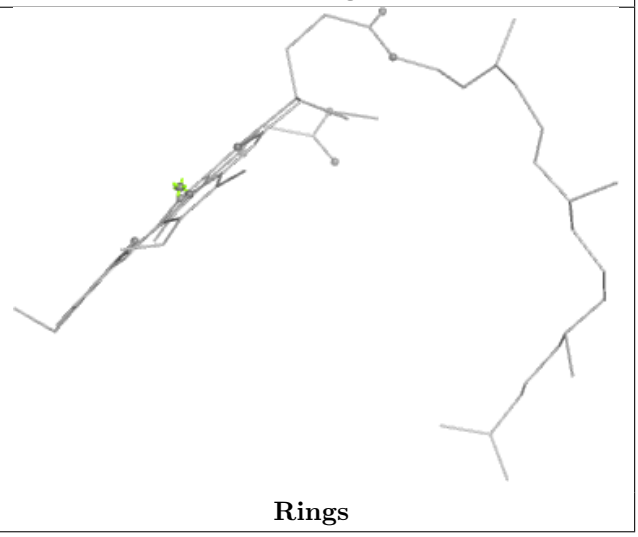
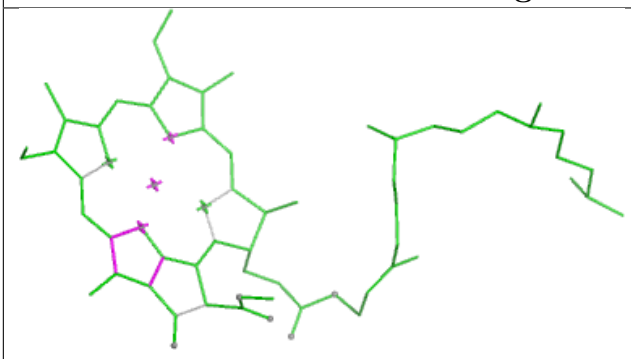


Rings

Ligand CLA A2 804



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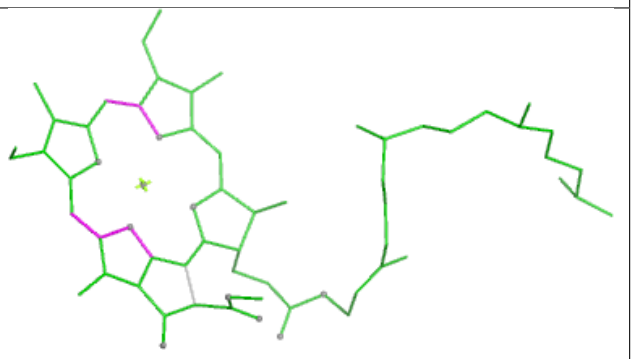
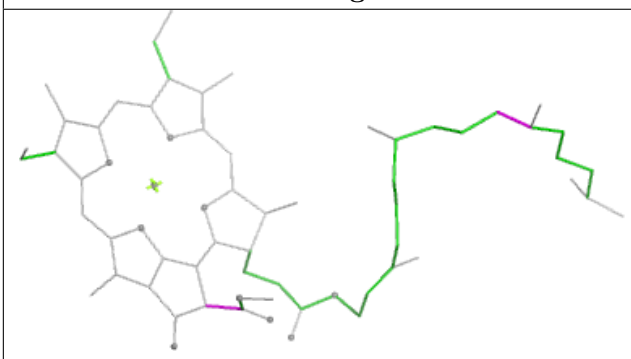


Bond angles



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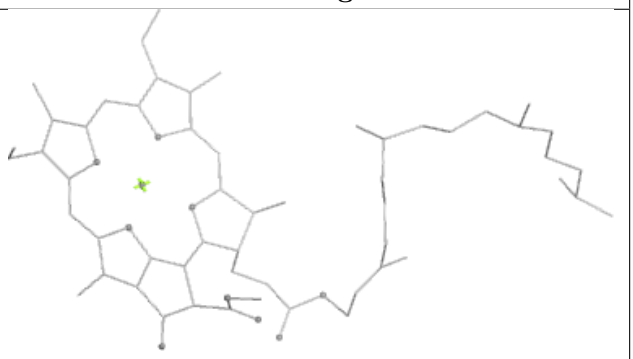
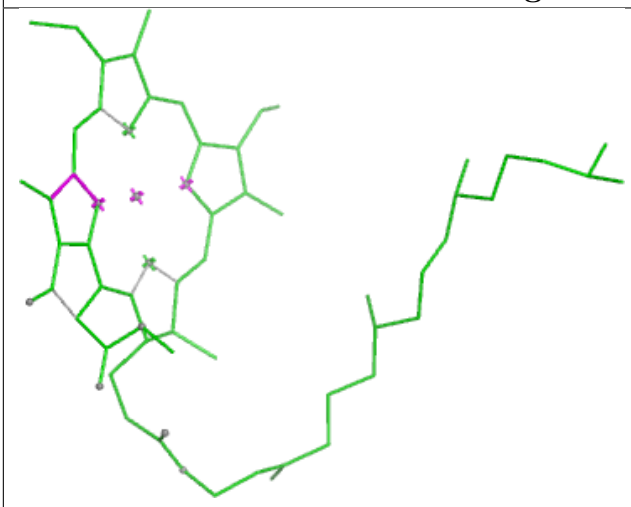


Rings

Ligand CLA B 824



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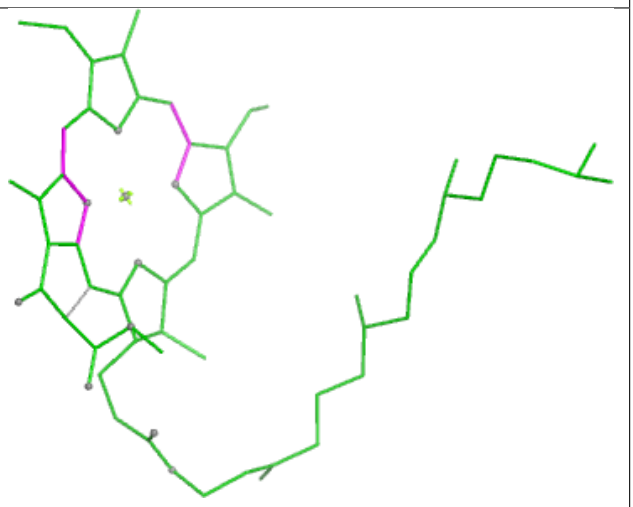
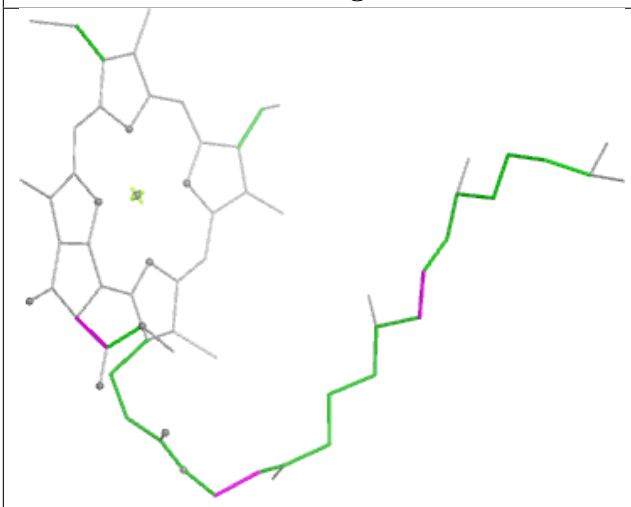


Bond angles



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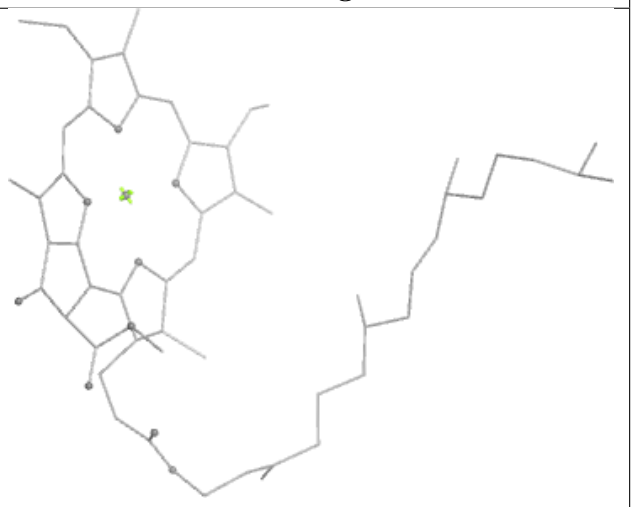
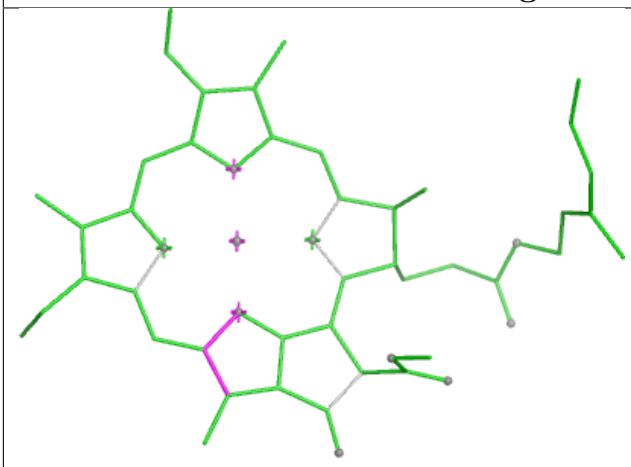


Rings

Ligand CLA 72 603



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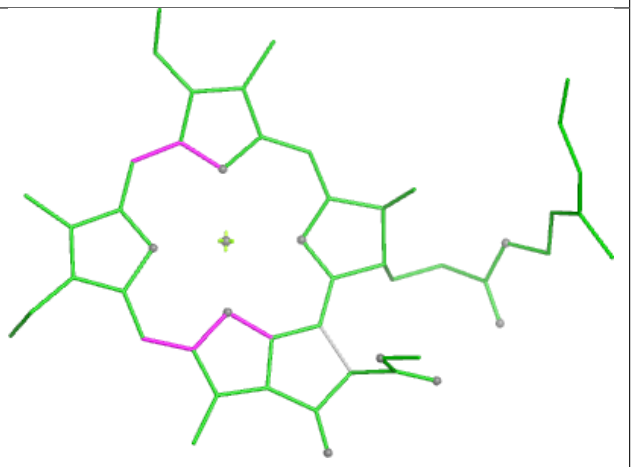
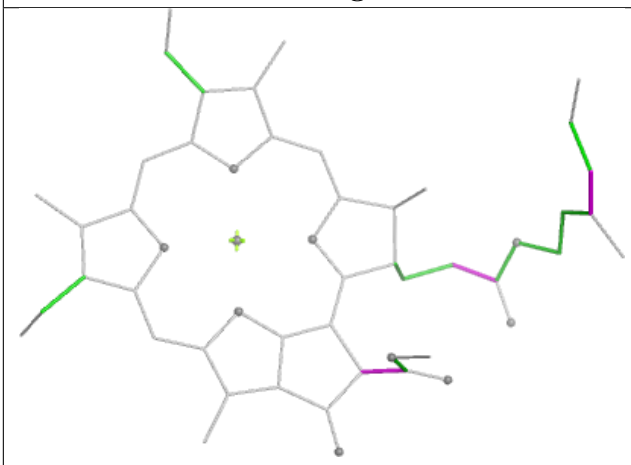


Bond angles



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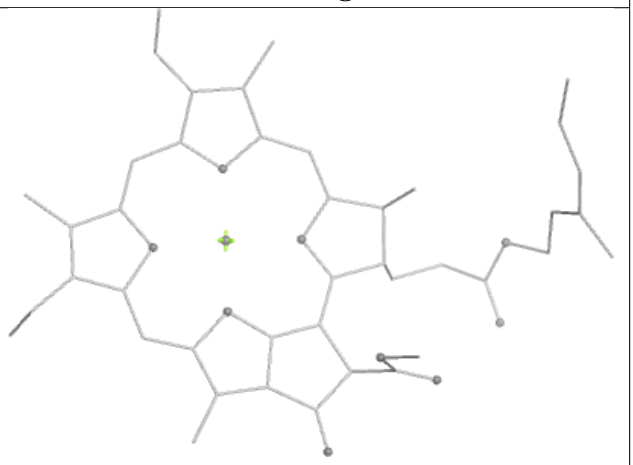
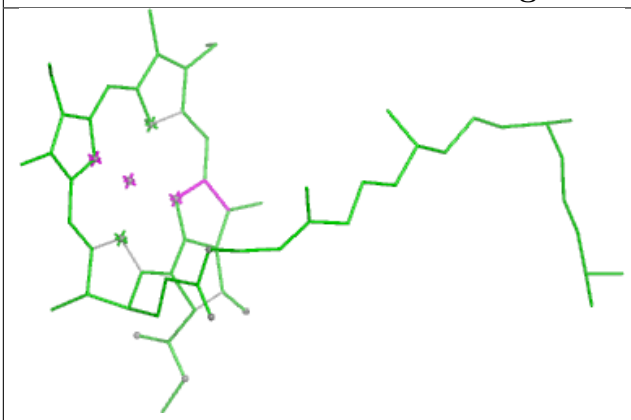


Rings

Ligand CLA 52 609



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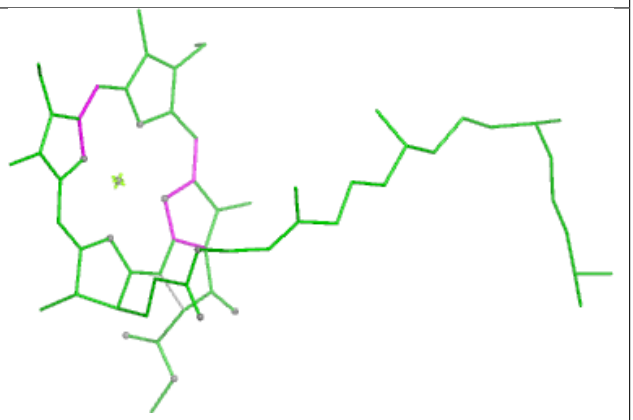
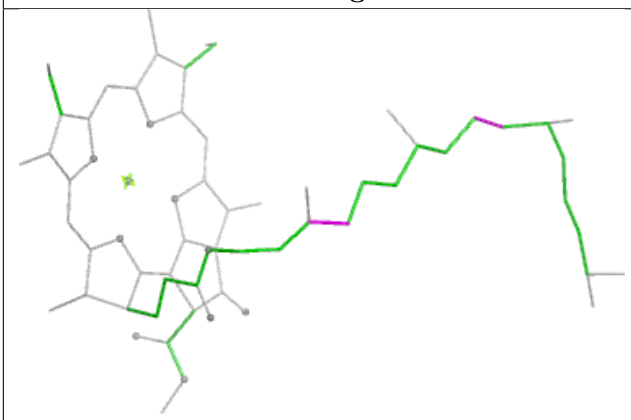


Bond angles



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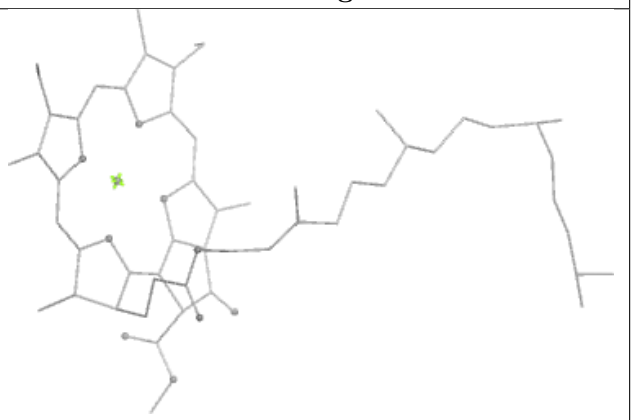
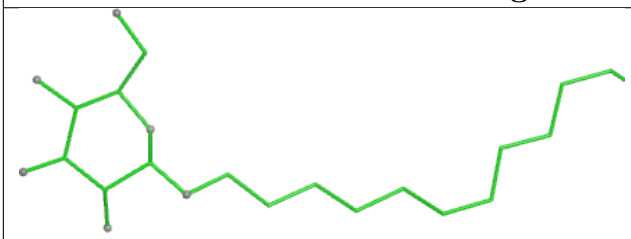


Rings

Ligand LMU A2 864



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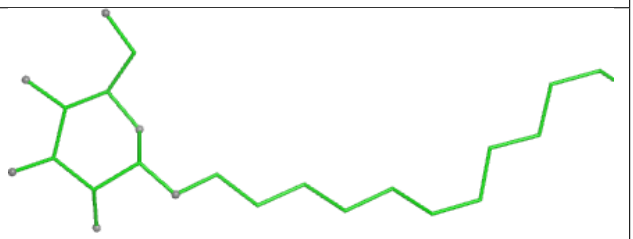
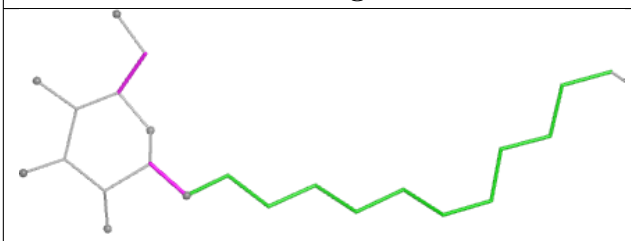


Bond angles

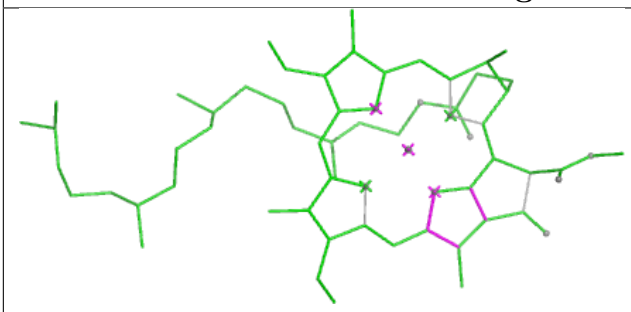


Torsions



Rings

Ligand CLA B2 837



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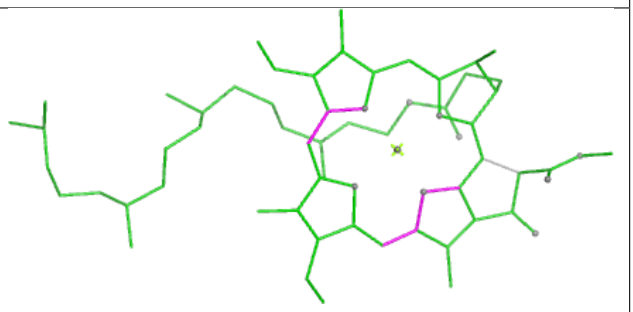
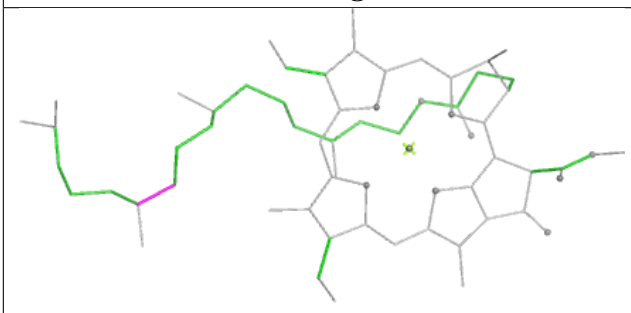


Bond angles



Torsions



Rings

Ligand LHG 1 620



Bond lengths



Bond angles

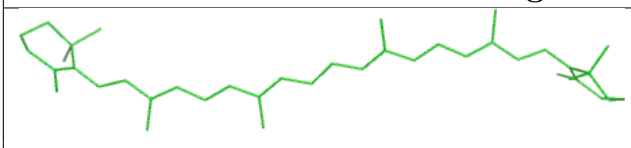


Torsions

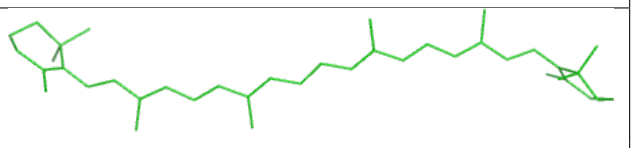


Rings

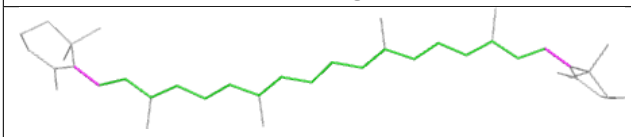
Ligand BCR 5 622



Bond lengths



Bond angles



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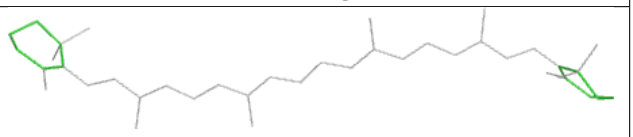
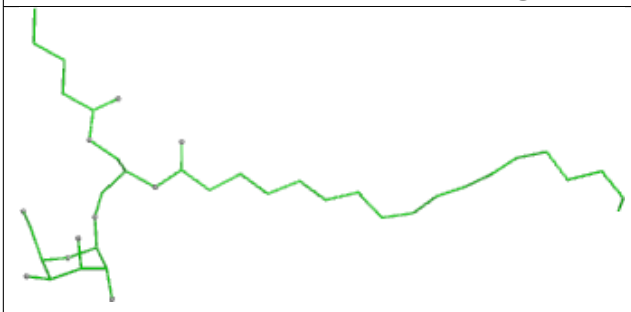
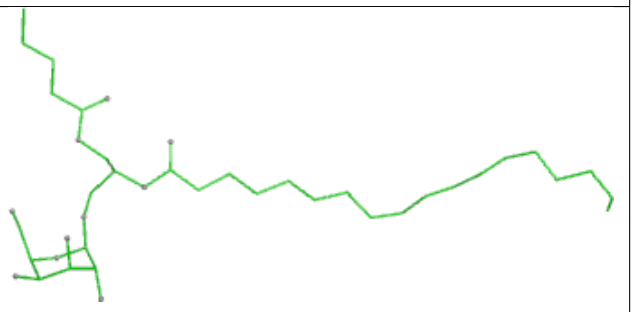


Rings

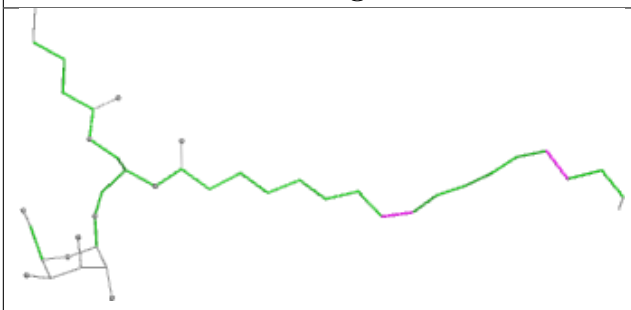
Ligand LMG J2 103



Bond lengths



Bond angles



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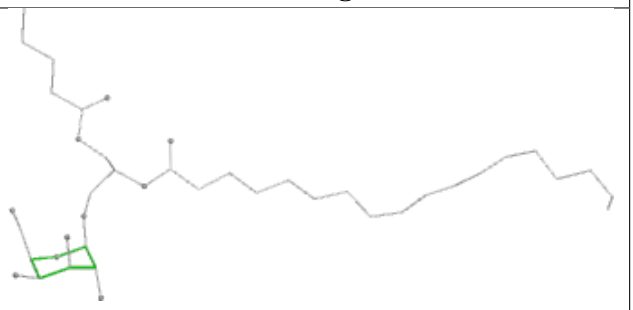


Rings

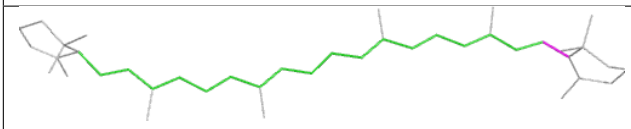
Ligand LUT 32 622



Bond lengths



Bond angles



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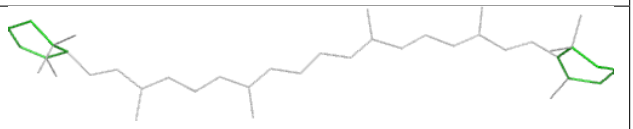
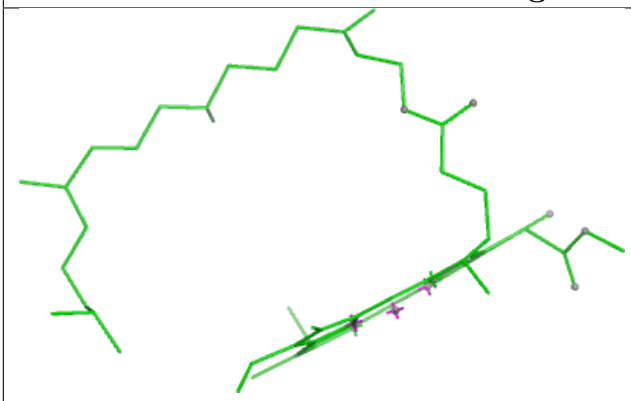


Rings

Ligand CLA 6 604



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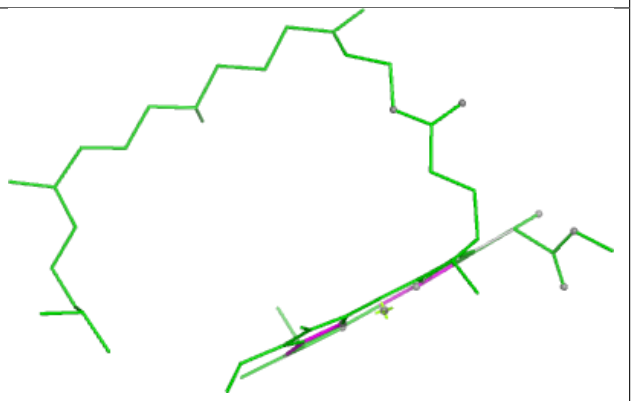
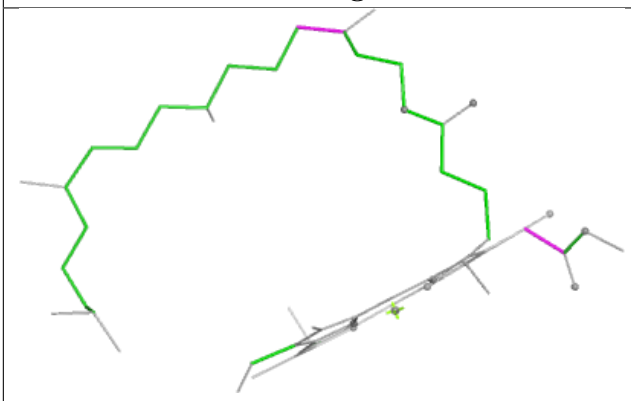


Bond angles

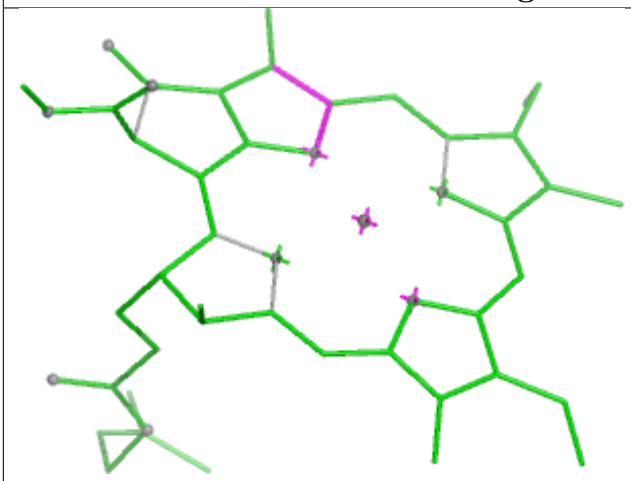


Torsions



Rings

Ligand CLA Z2 614



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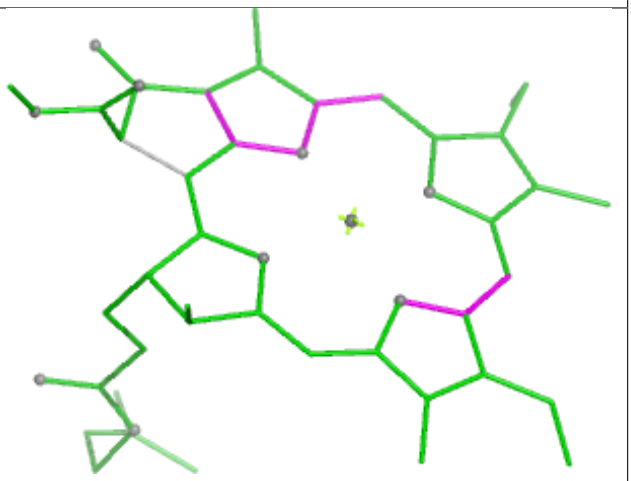
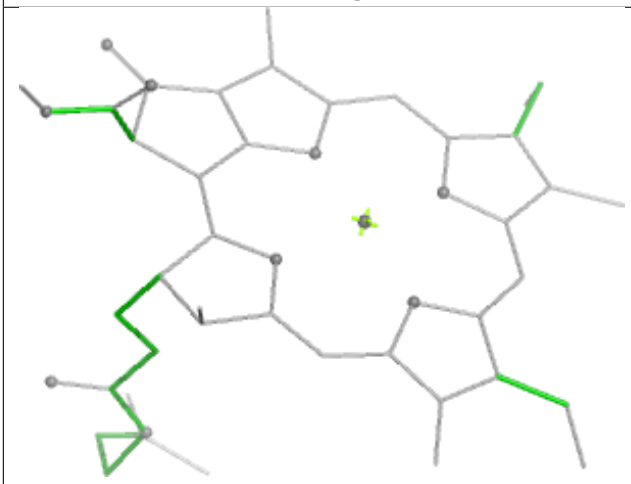


Bond angles



Torsions



Rings

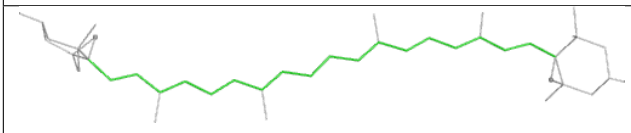
Ligand XAT 52 624



Bond lengths



Bond angles



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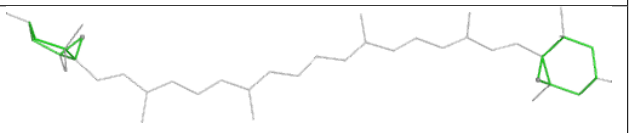
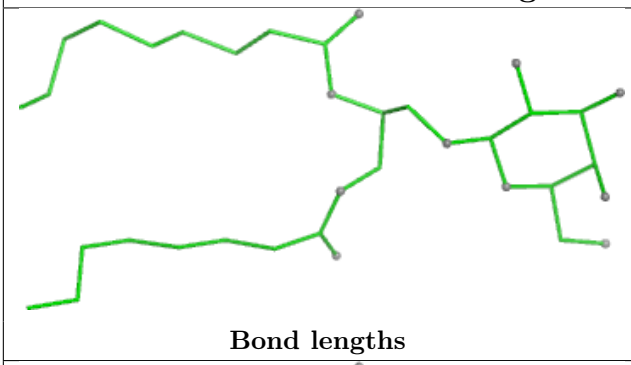
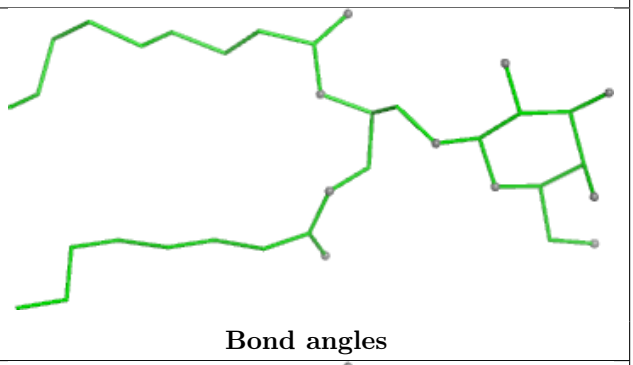


Rings

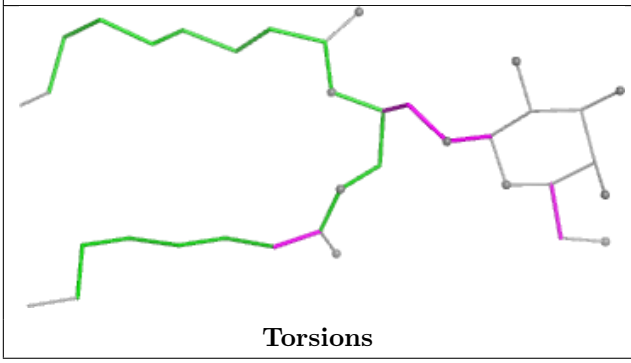
Ligand LMG A 860



Bond lengths



Bond angles



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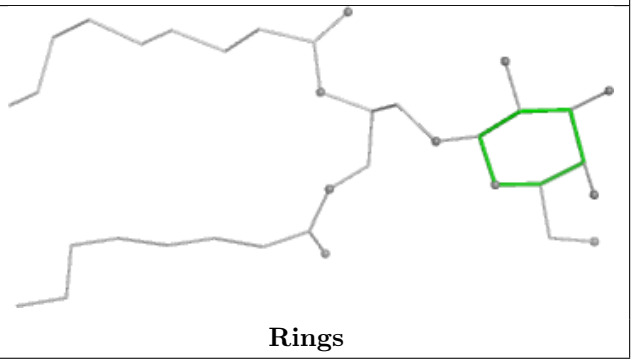
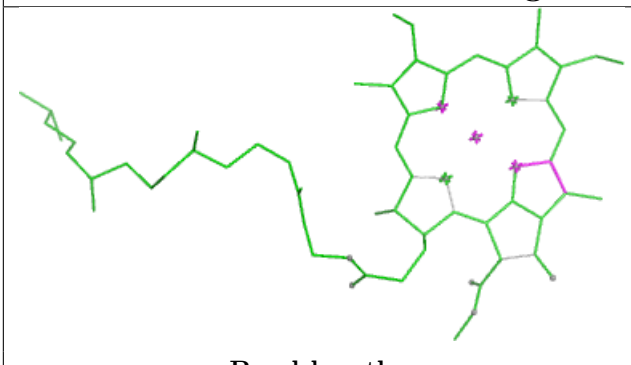
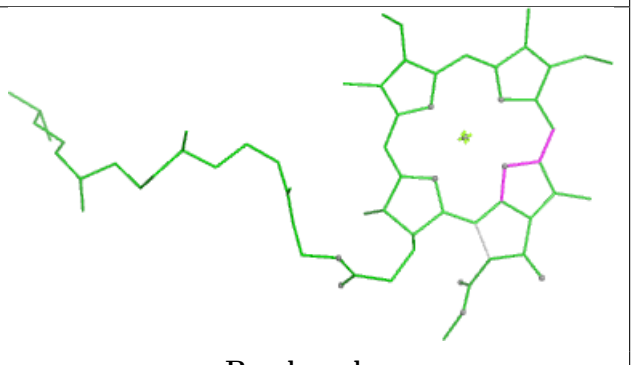


Rings

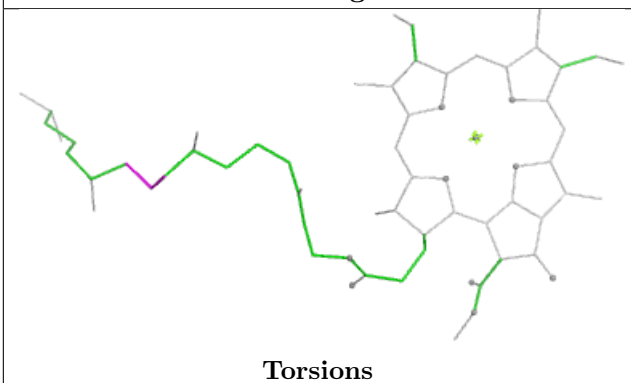
Ligand CLA B 803



Bond lengths



Bond angles



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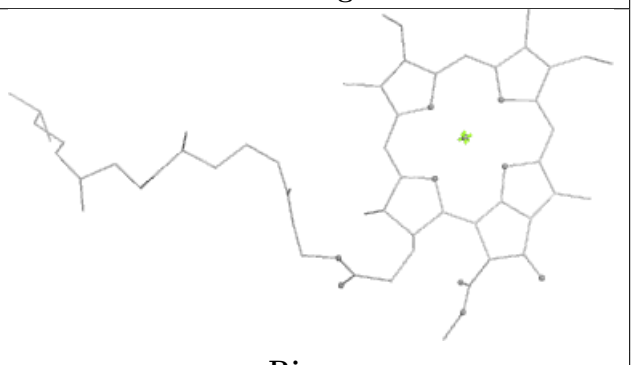
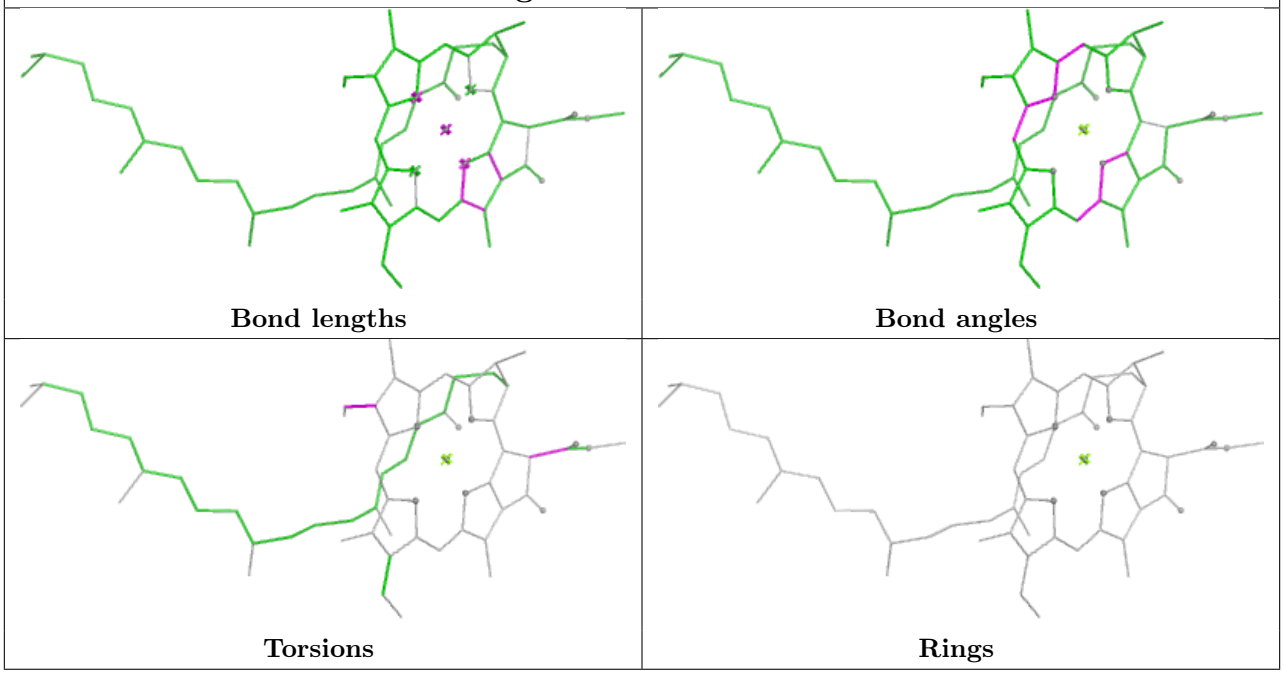
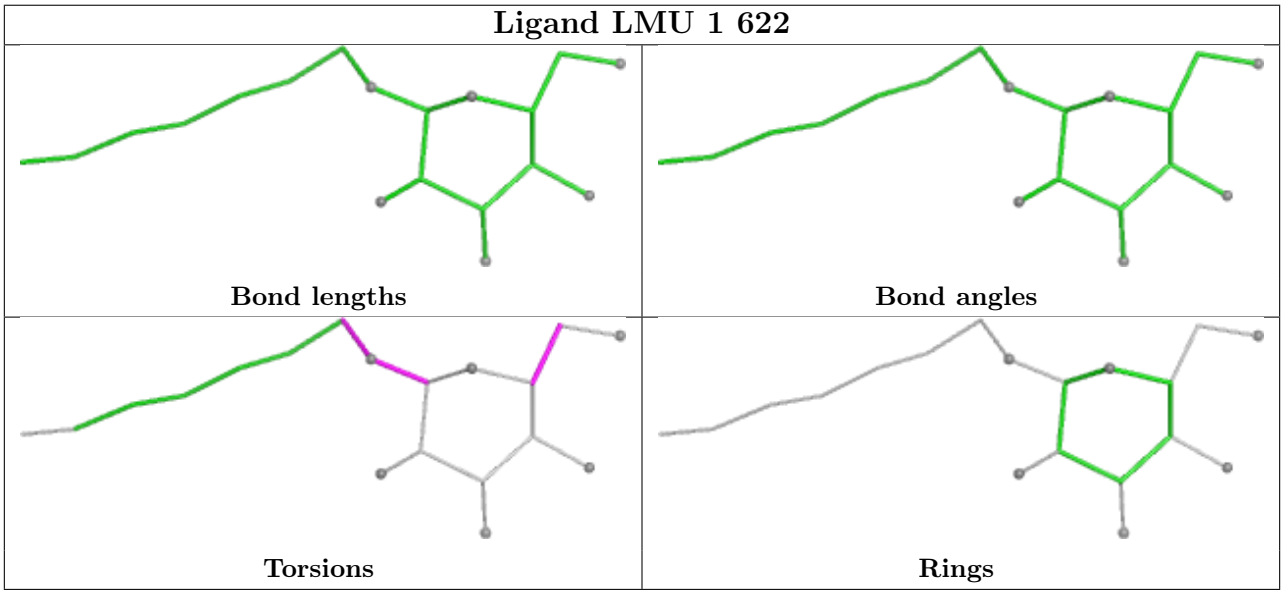


Rings

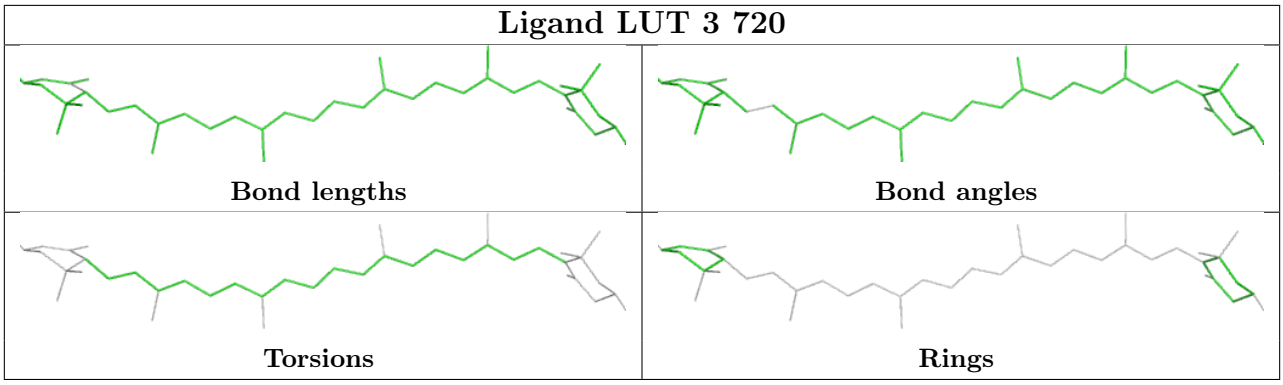
Ligand CLA A2 842



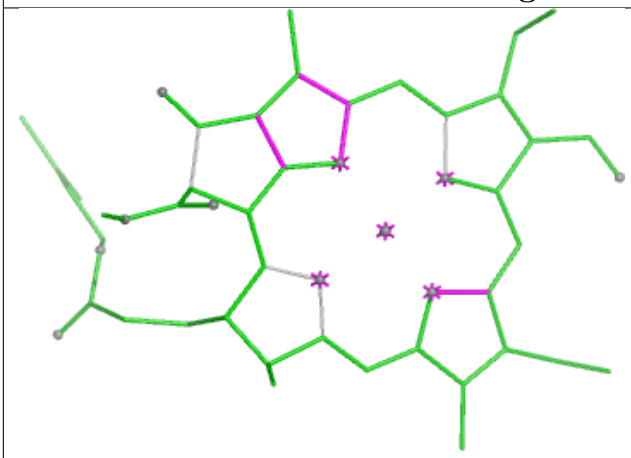
Ligand LMU 1 622



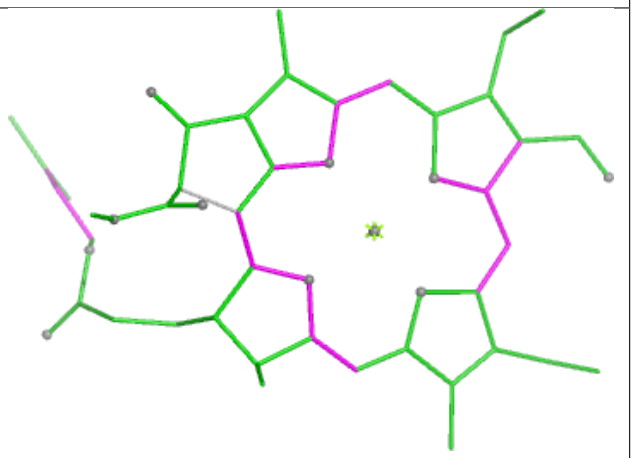
Ligand LUT 3 720



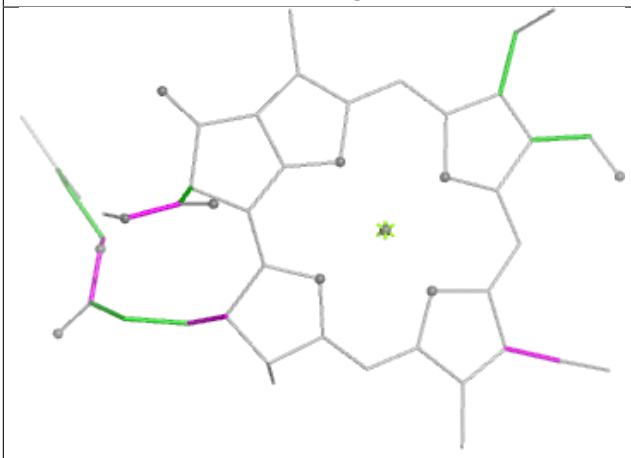
Ligand CHL 92 607



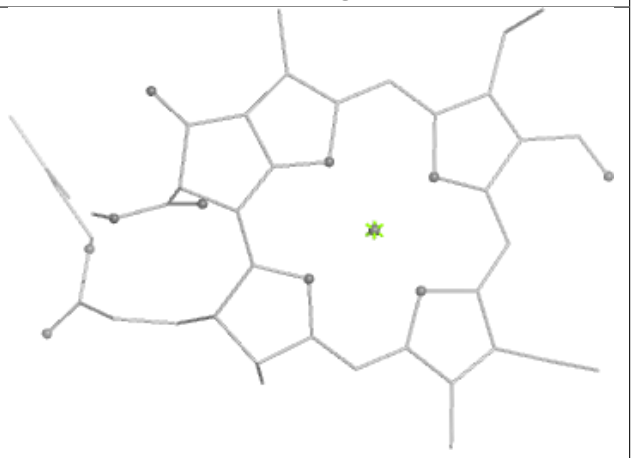
Bond lengths



Bond angles

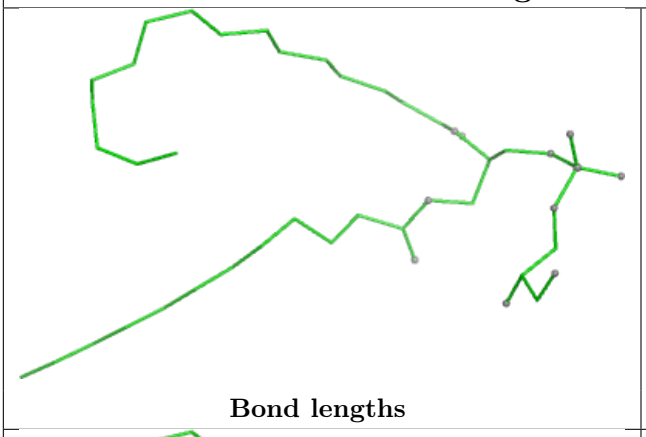


Torsions

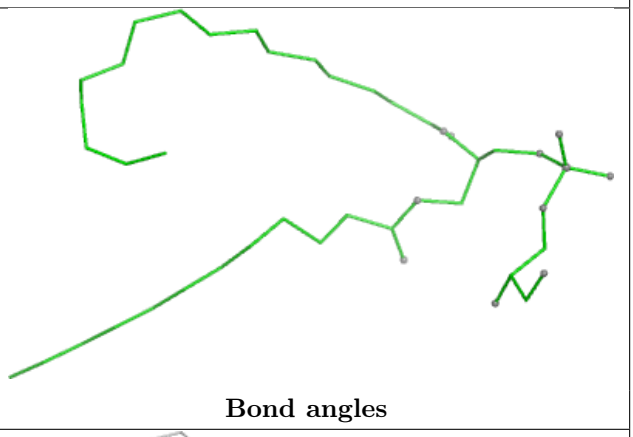


Rings

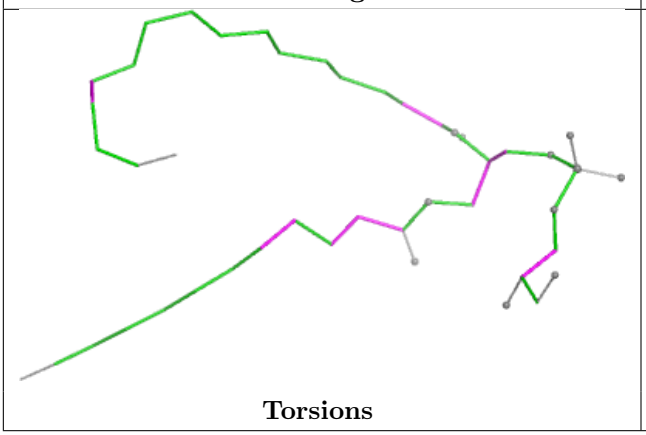
Ligand LHG B2 851



Bond lengths



Bond angles



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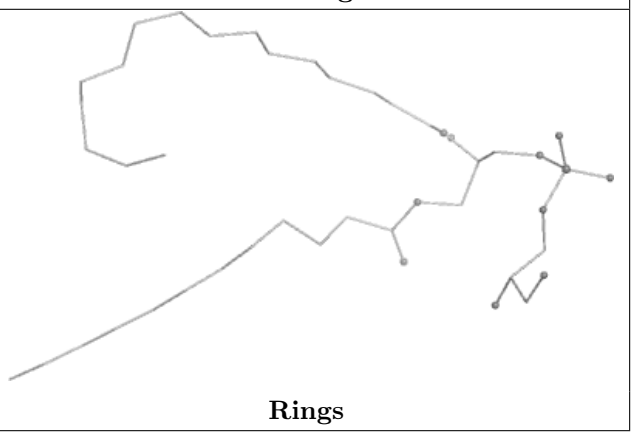


Rings

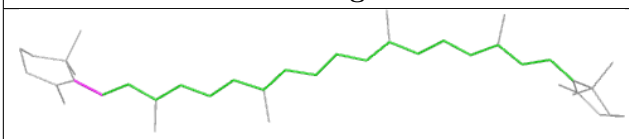
Ligand BCR 3 719



Bond lengths



Bond angles



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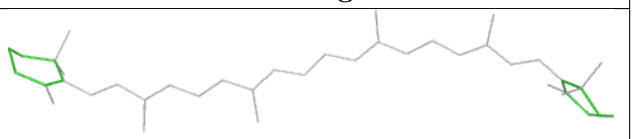
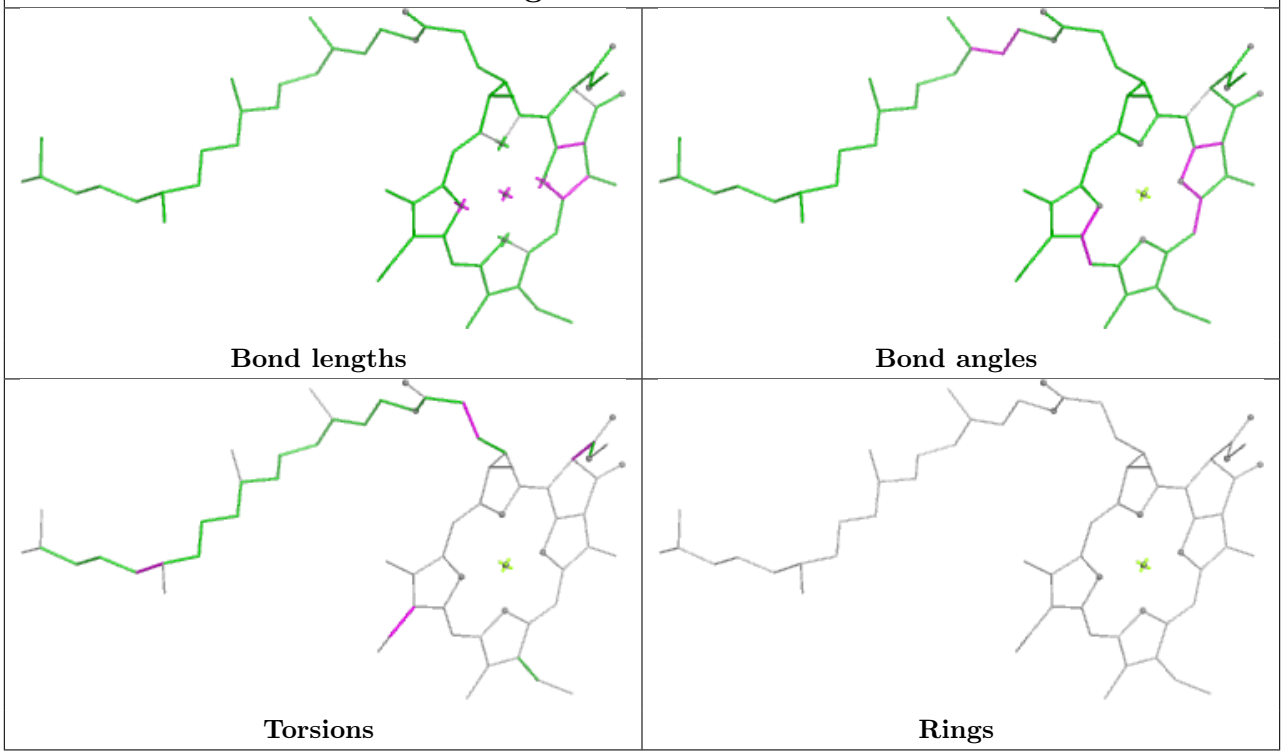
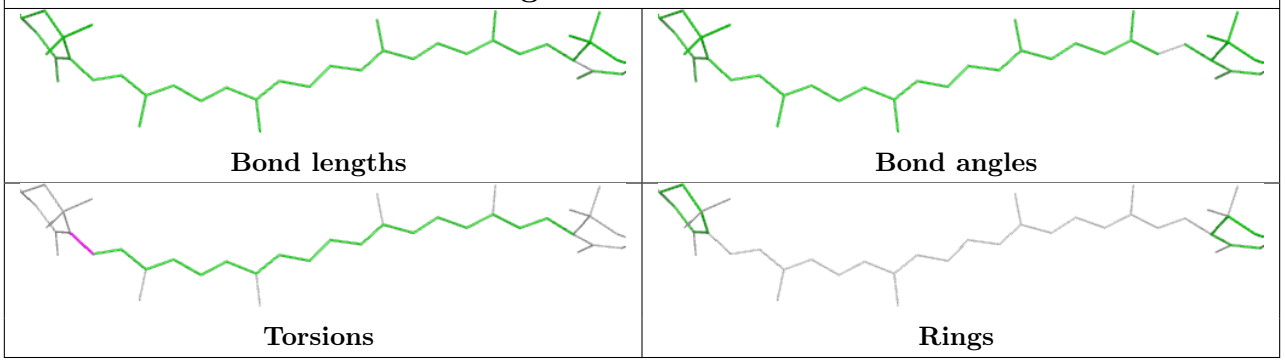


Rings

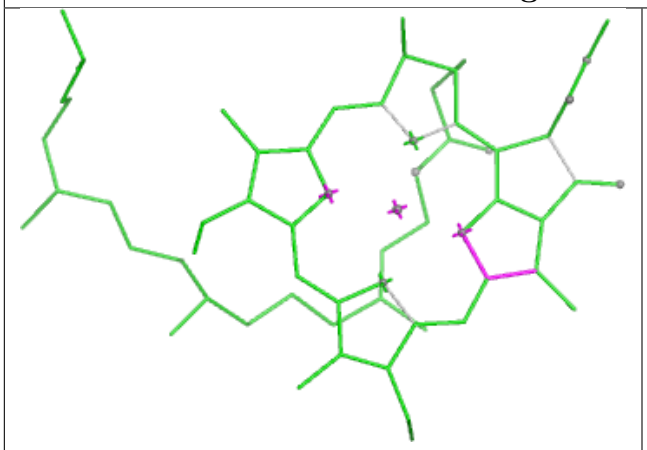
Ligand CLA A 809



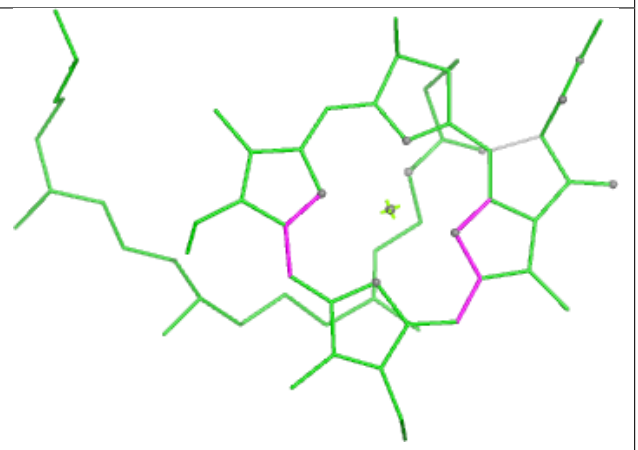
Ligand LUT 52 620



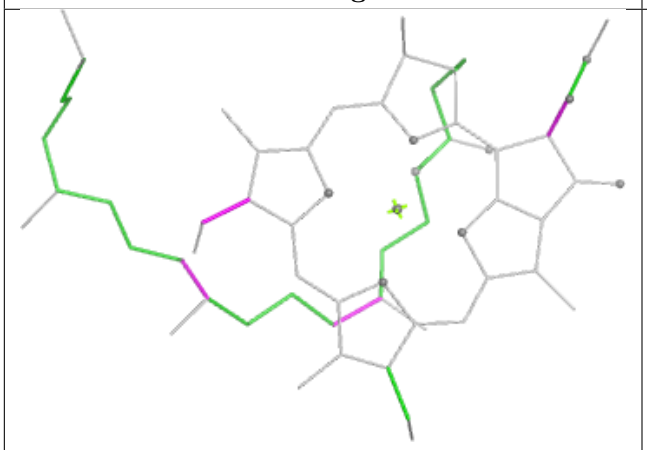
Ligand CLA 62 613



Bond lengths



Bond angles



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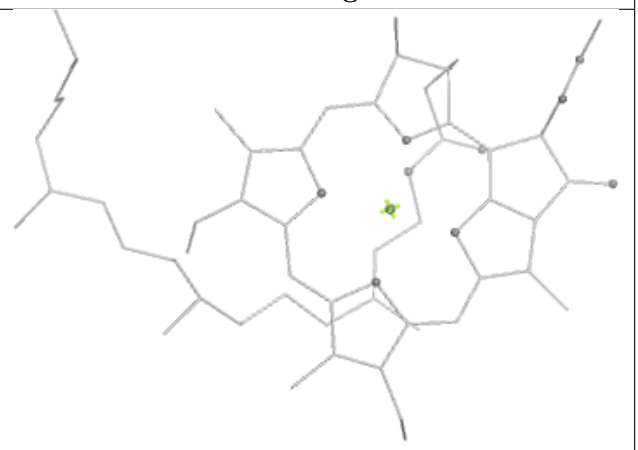
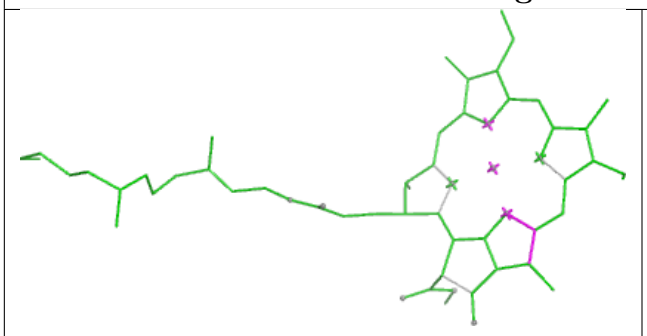


Rings

Ligand CLA G2 203



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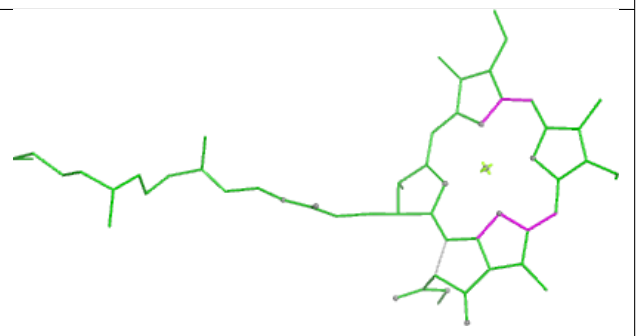
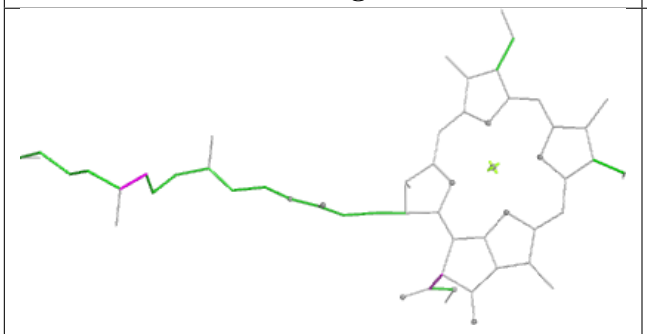


Bond angles



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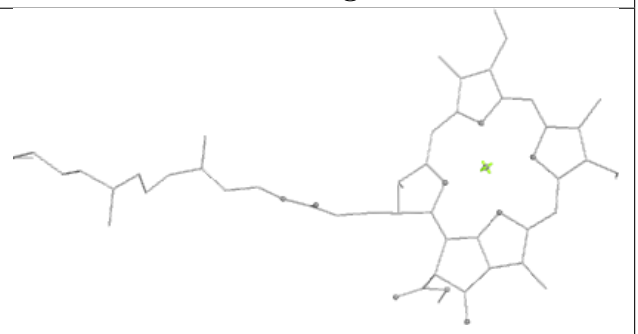
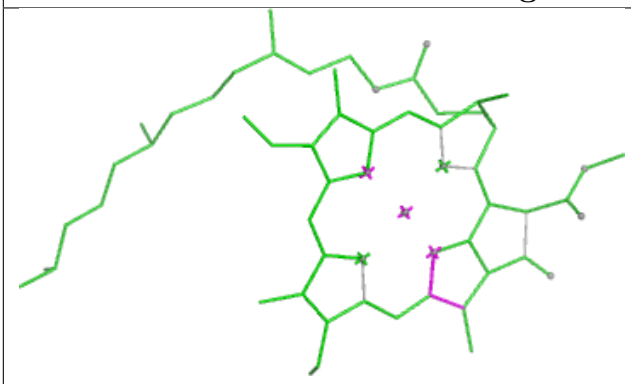


Rings

Ligand CLA 62 610



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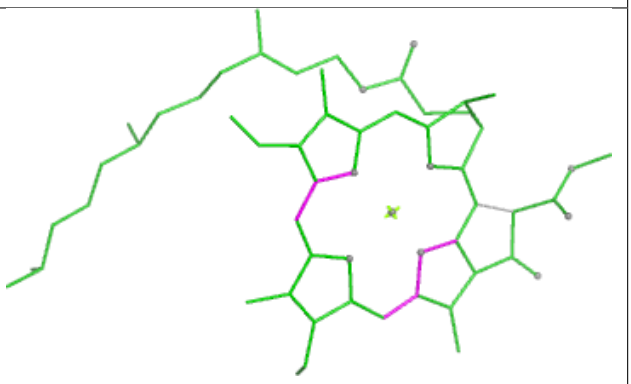
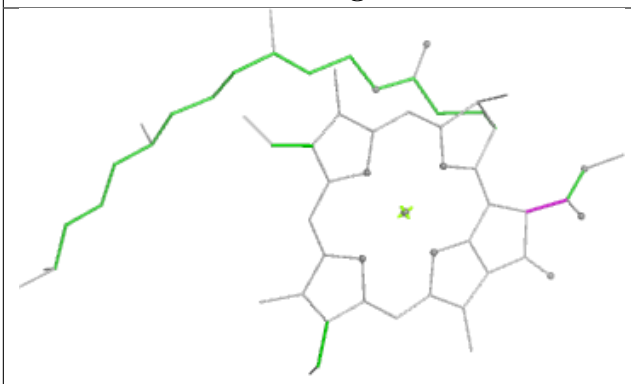


Bond angles



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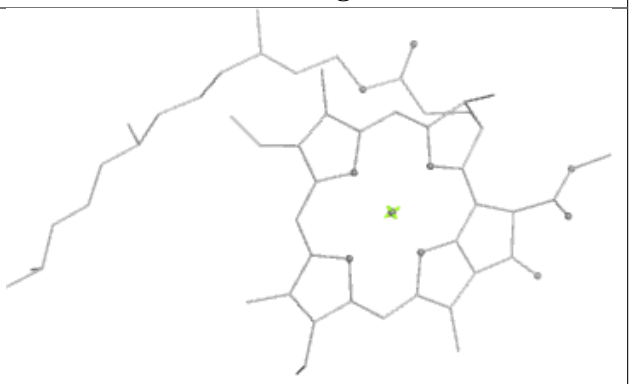
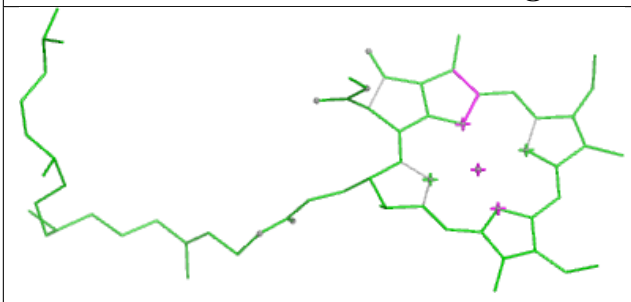
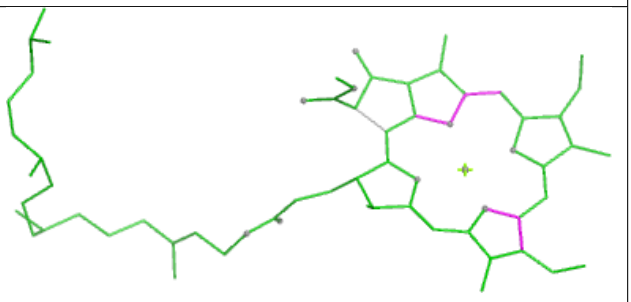


Rings

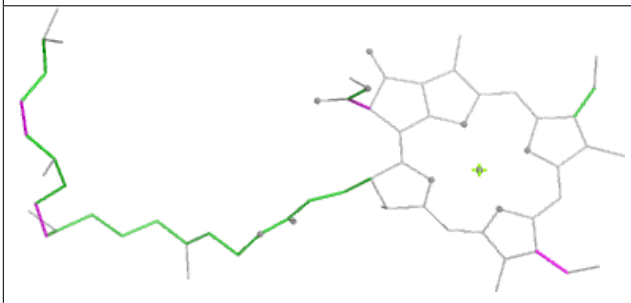
Ligand CLA B 826



Bond lengths



Bond angles



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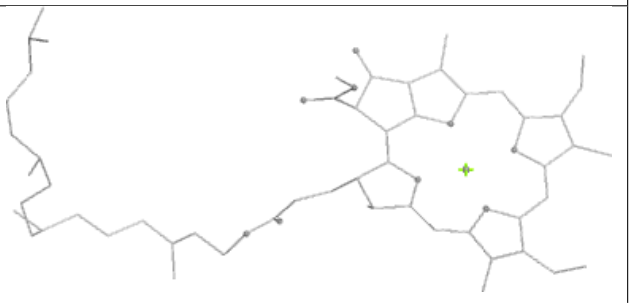
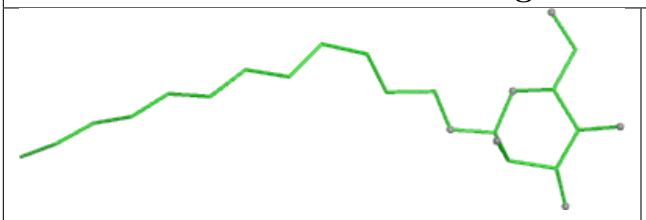


Rings

Ligand LMU 62 628



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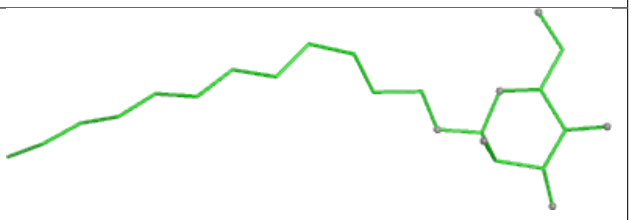
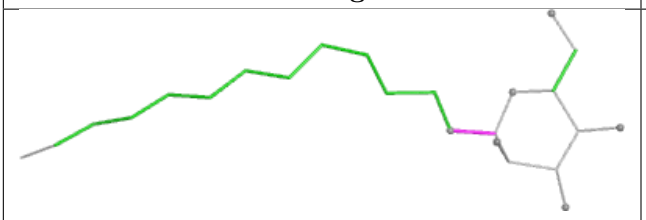


Bond angles



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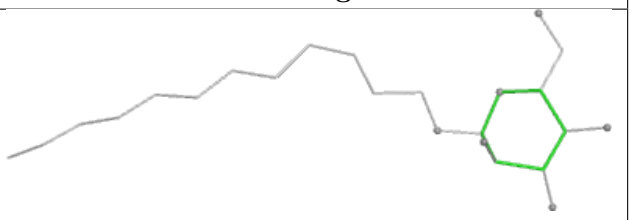
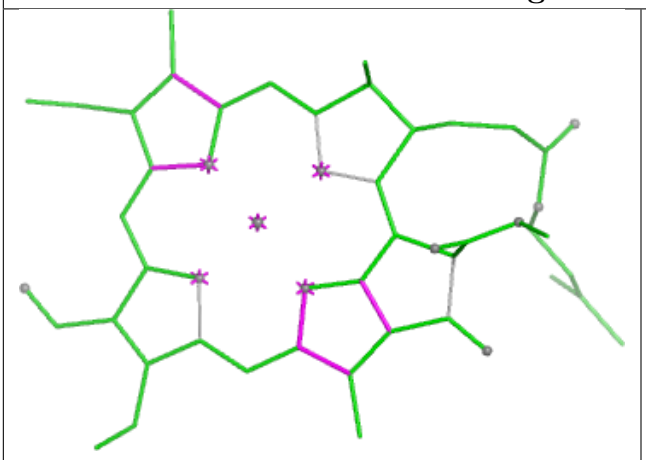


Rings

Ligand CHL 9 607



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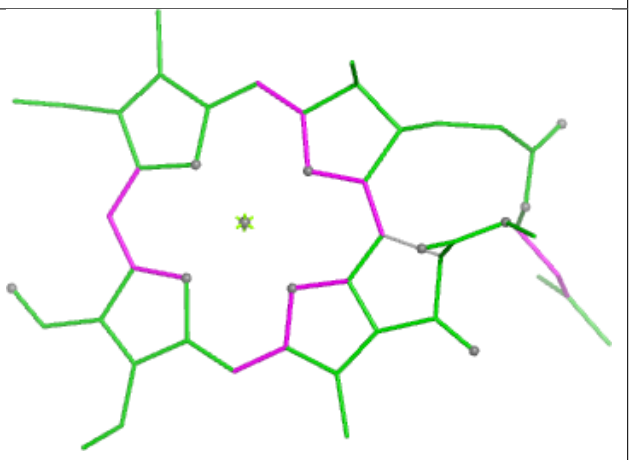
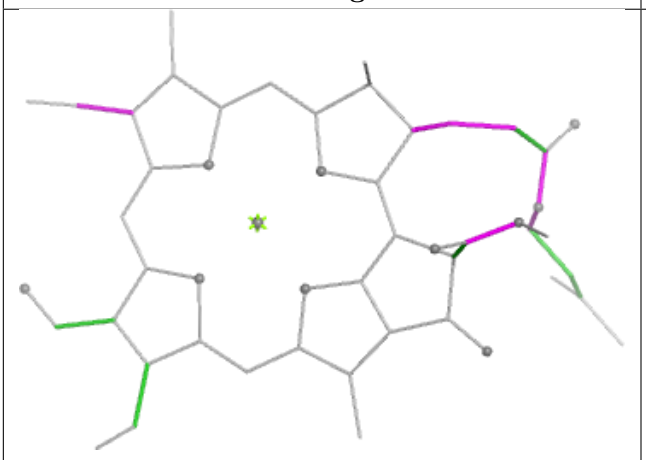


Bond angles



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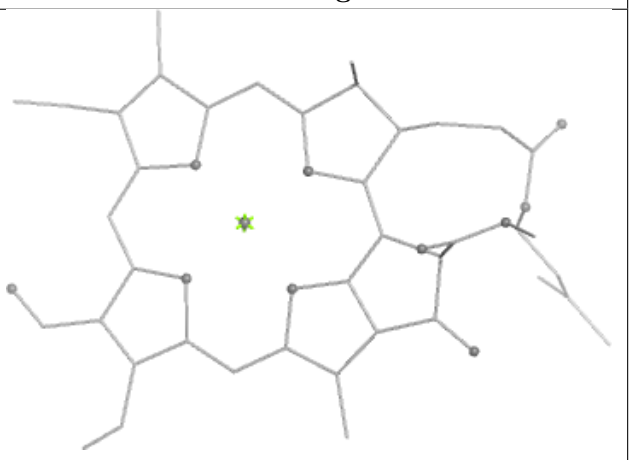
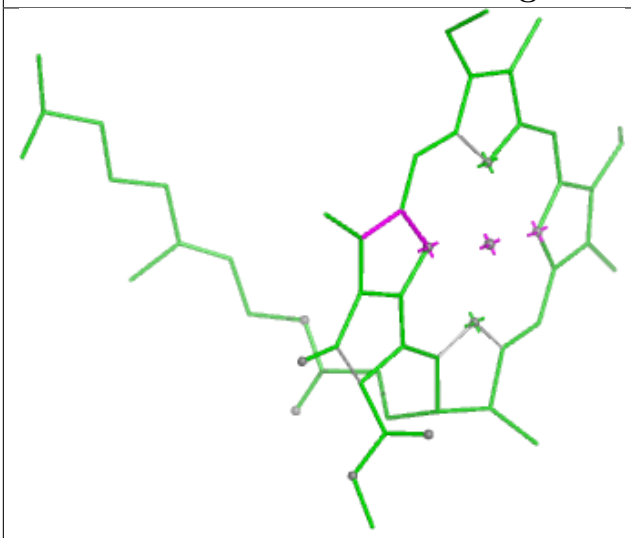


Rings

Ligand CLA 52 611



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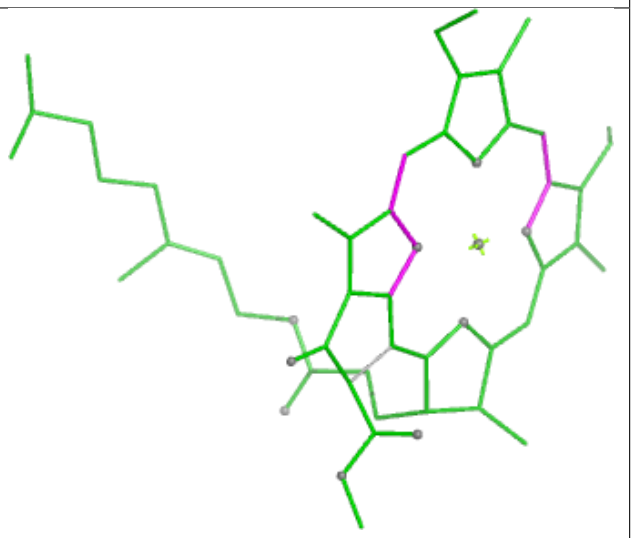
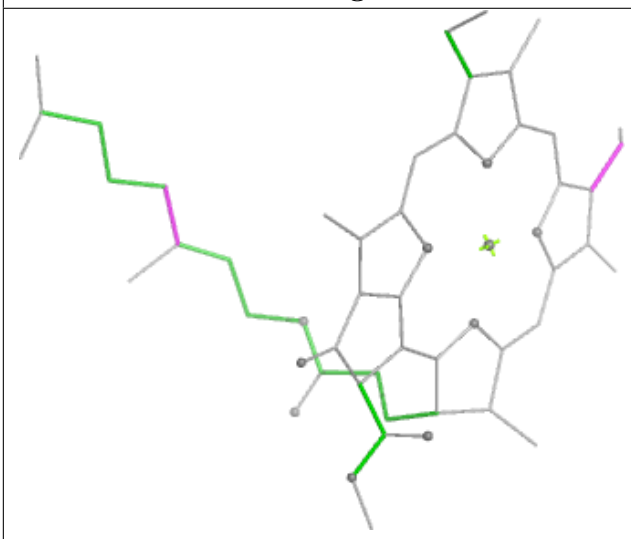


Bond angles



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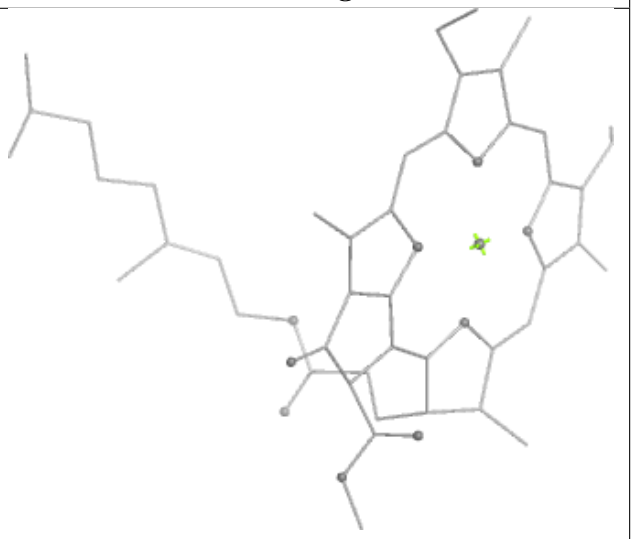
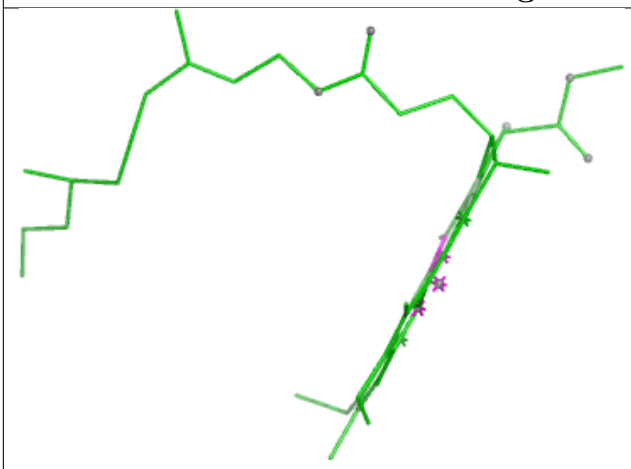


Rings

Ligand CLA Z2 604



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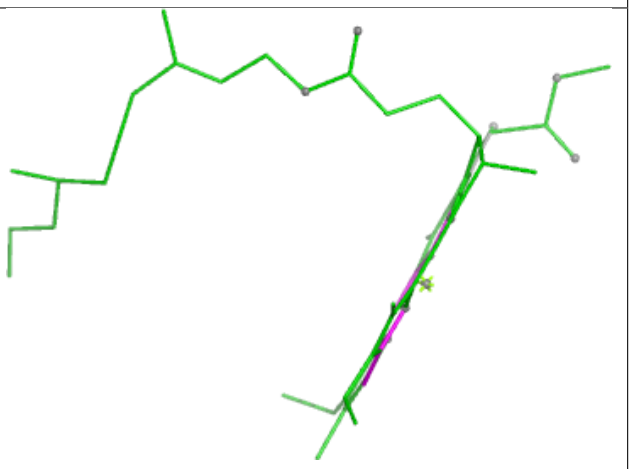
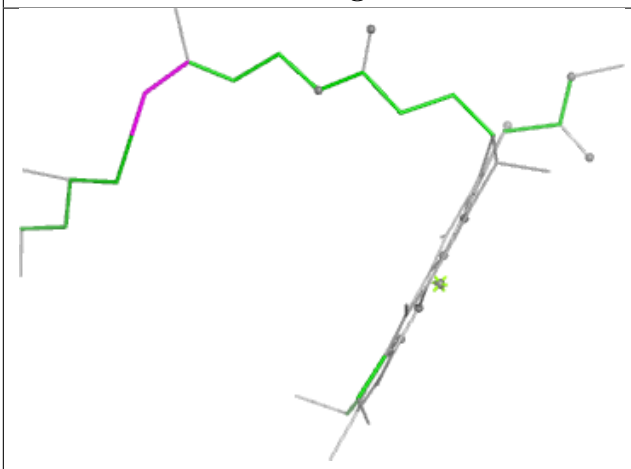


Bond angles

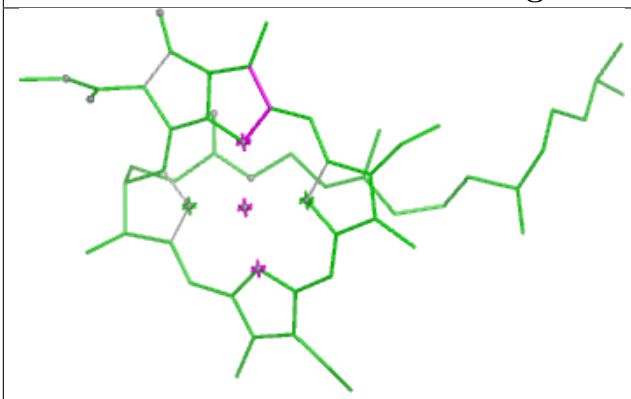


Torsions



Rings

Ligand CLA Z 616



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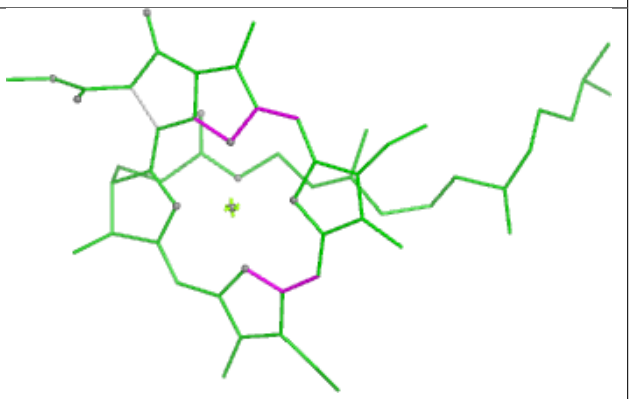
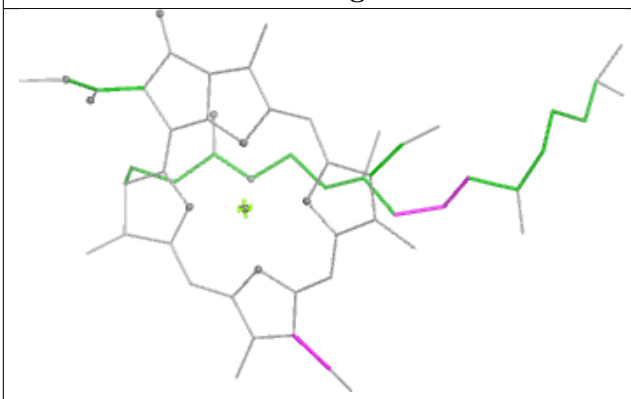


Bond angles



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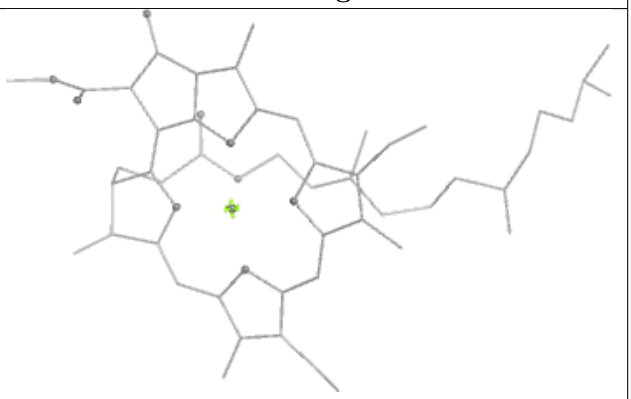
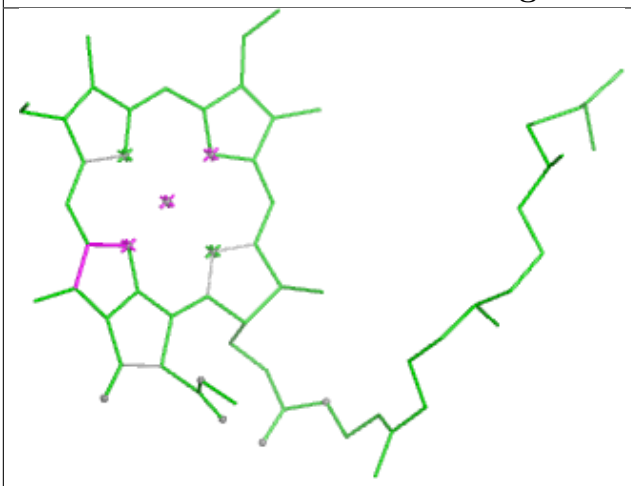


Rings

Ligand CLA 62 603



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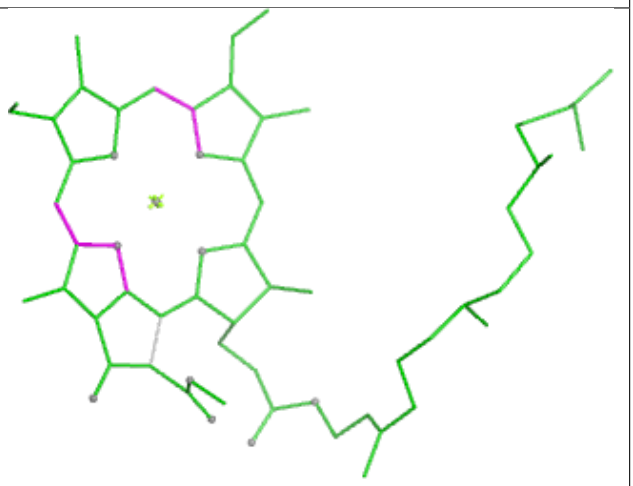
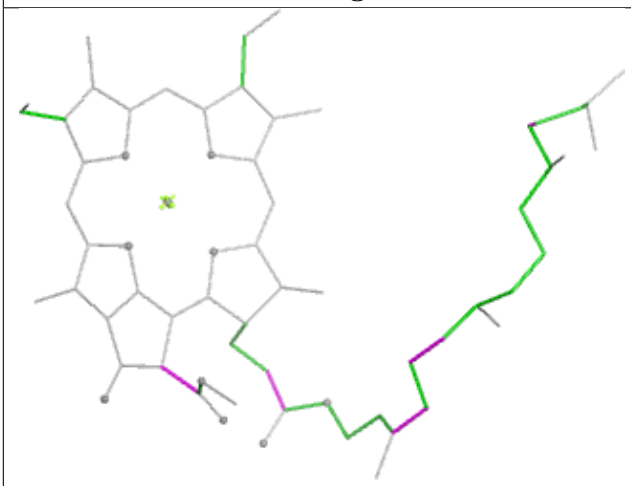


Bond angles



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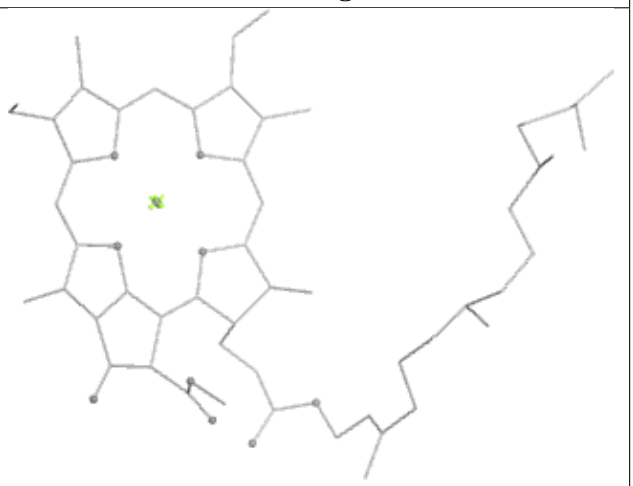
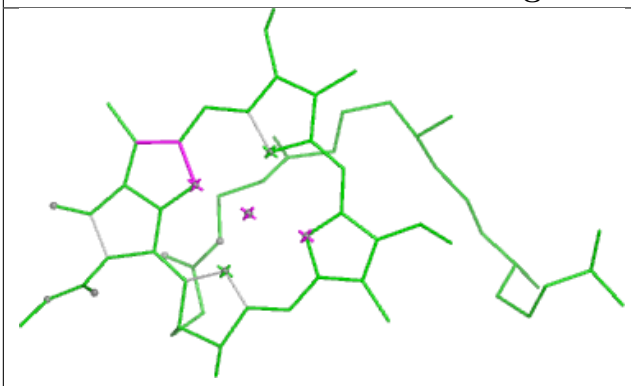
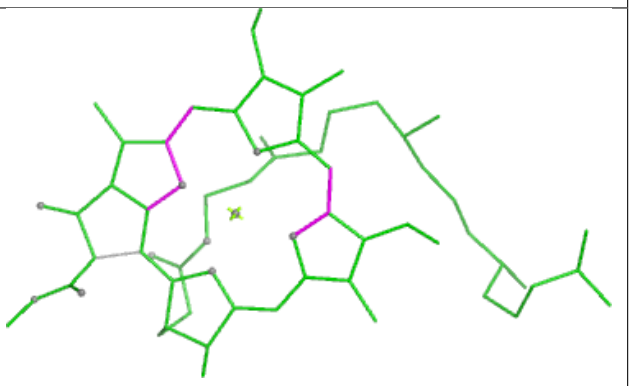


Rings

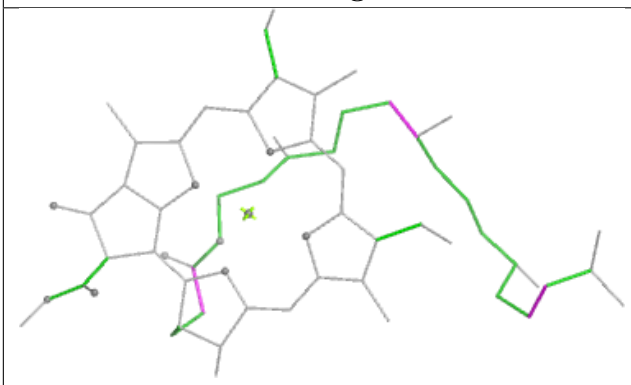
Ligand CLA A 813



Bond lengths



Bond angles



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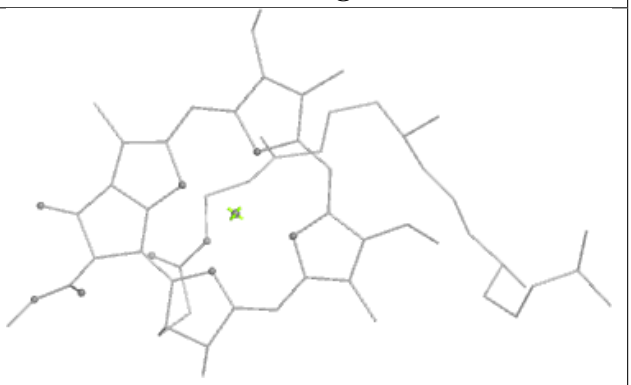
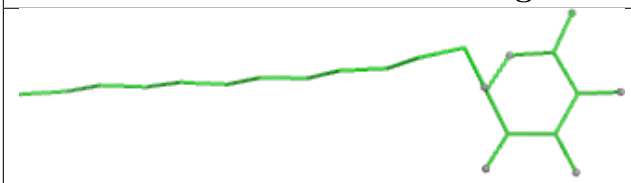
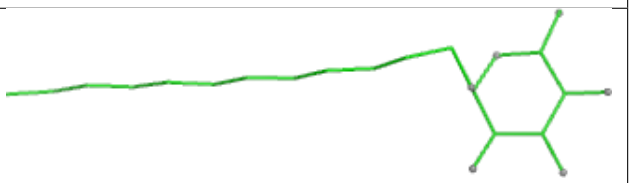


Rings

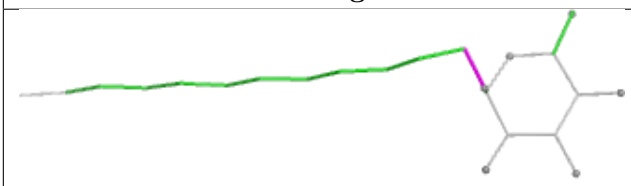
Ligand LMU 82 624



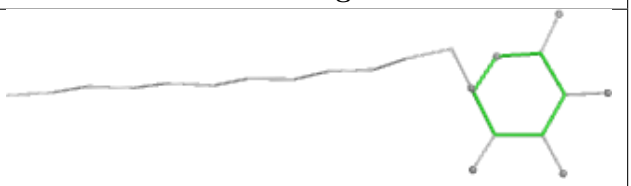
Bond lengths



Bond angles

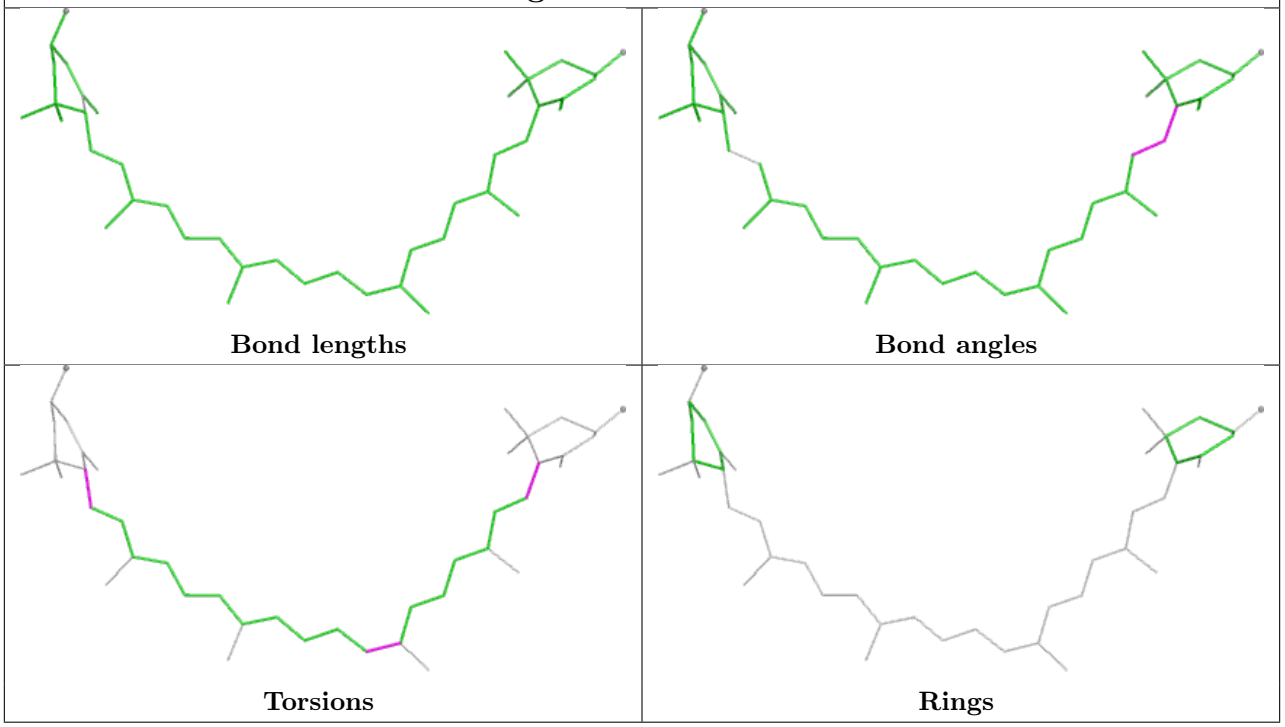


Torsions

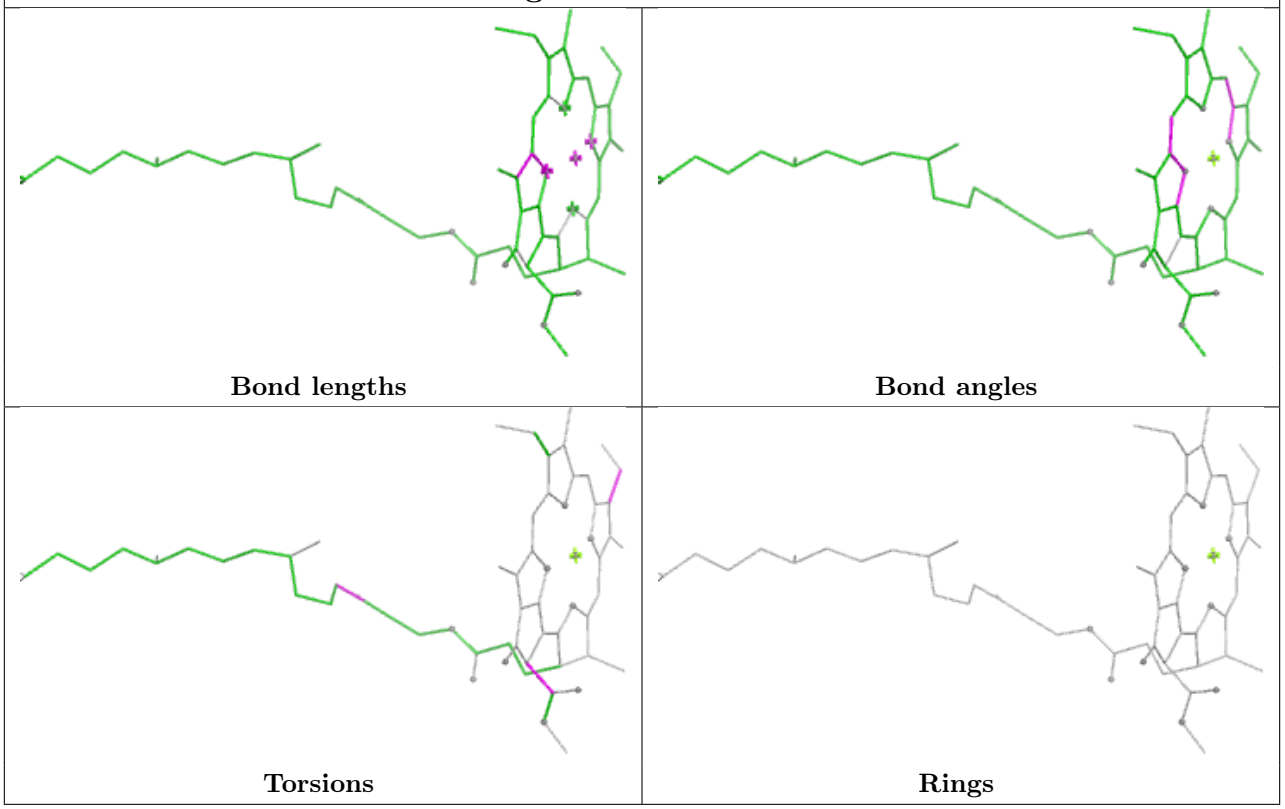


Rings

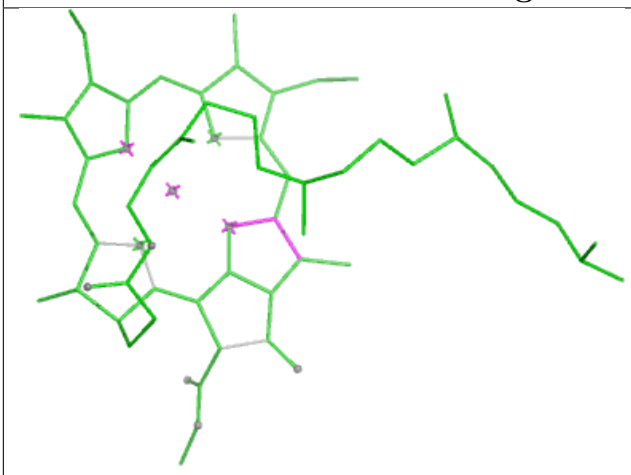
Ligand LUT F 305



Ligand CLA B 828



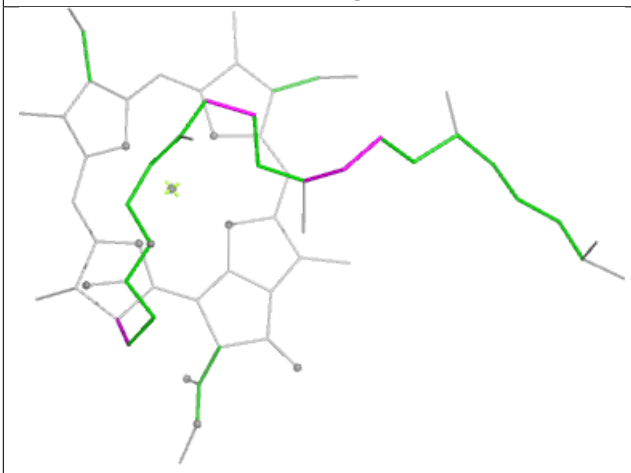
Ligand CLA B2 827



Bond lengths



Bond angles

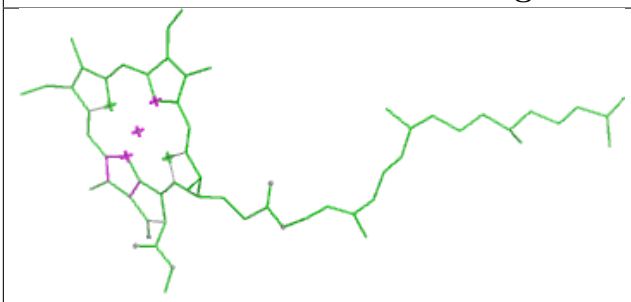


Torsions



Rings

Ligand CLA A2 803



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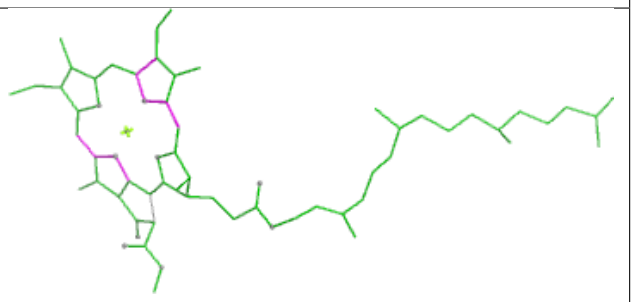
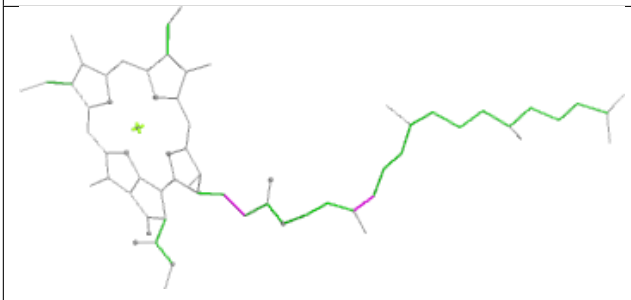
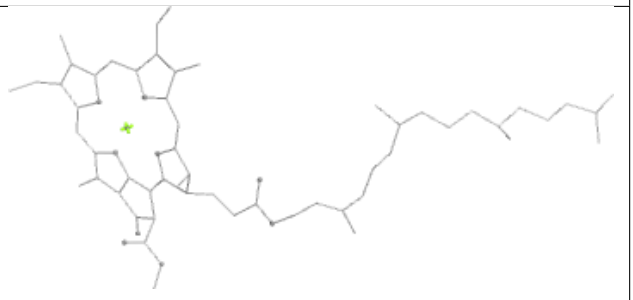


Bond angles

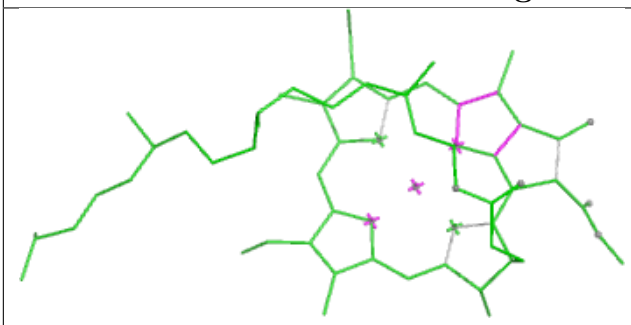


Torsions



Rings

Ligand CLA A2 841



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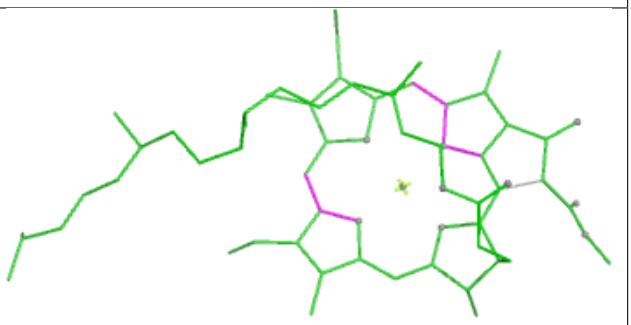
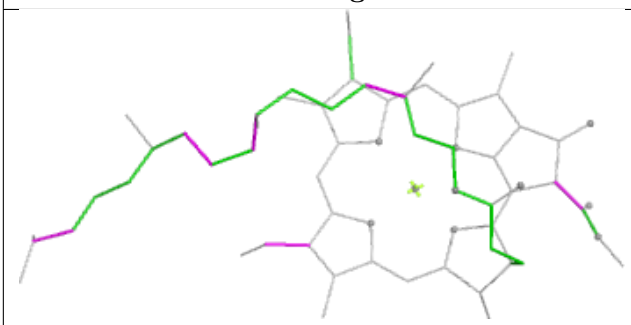


Bond angles

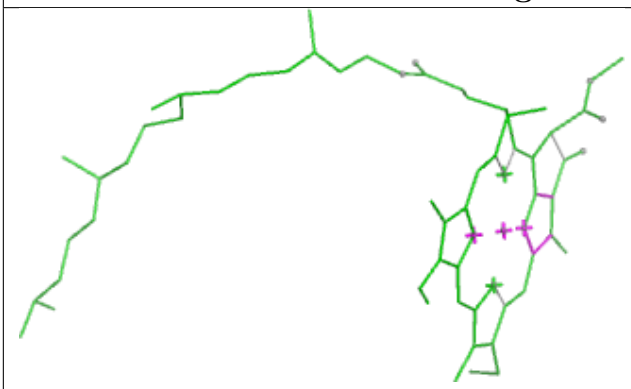


Torsions



Rings

Ligand CLA A2 836



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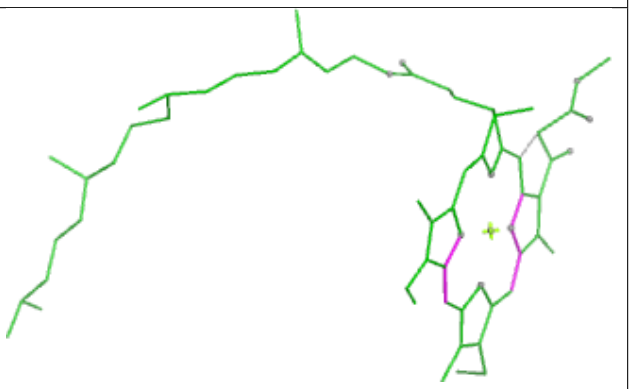
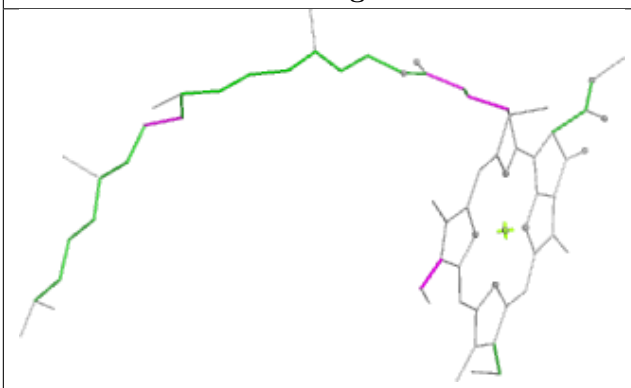


Bond angles

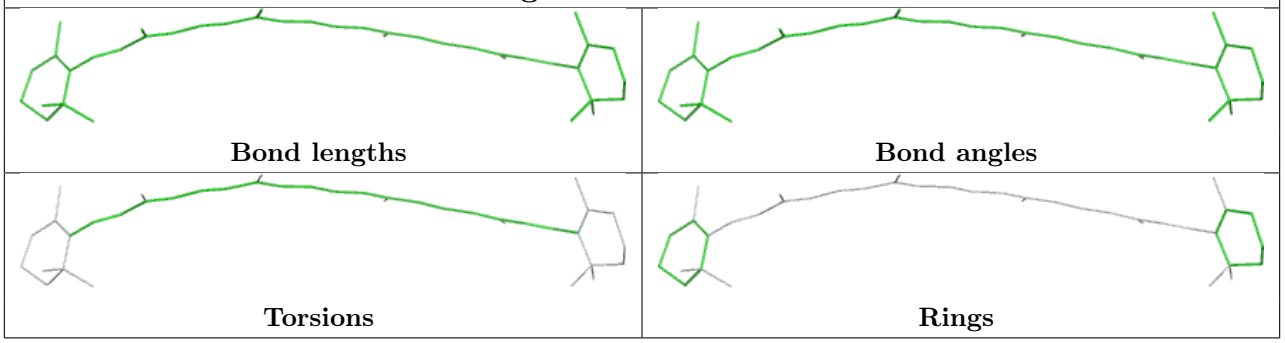


Torsions

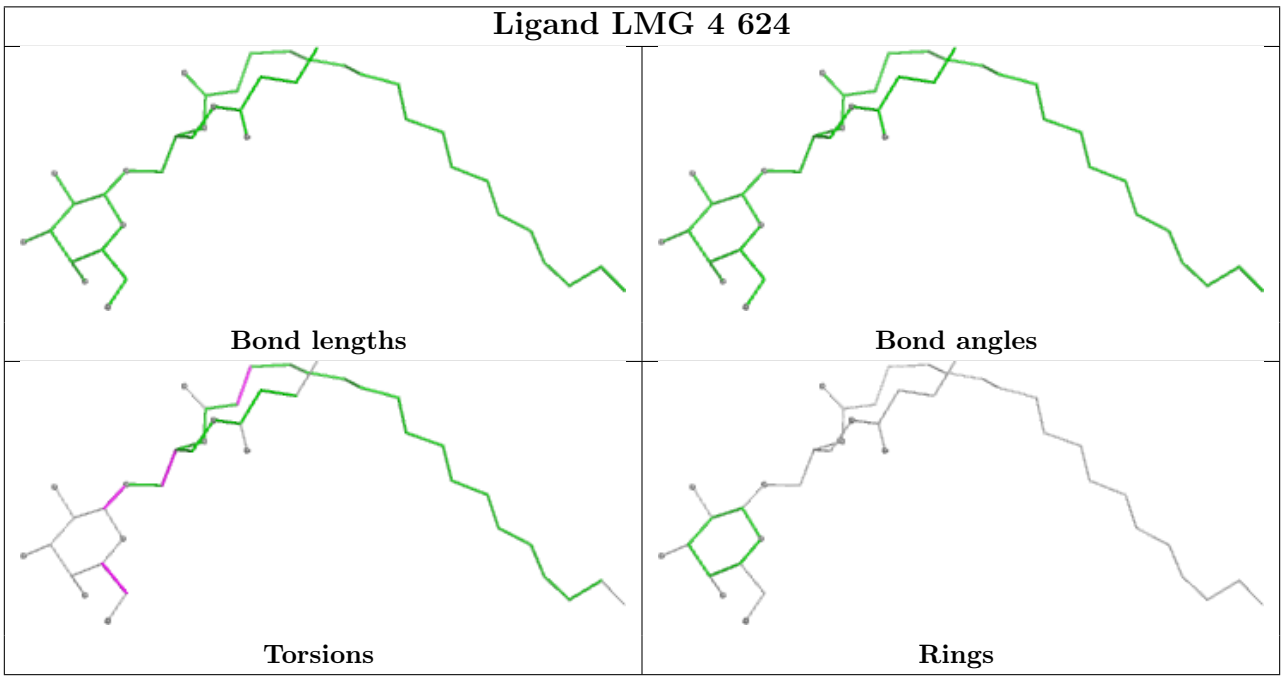


Rings

Ligand BCR I2 172



Ligand LMG 4 624



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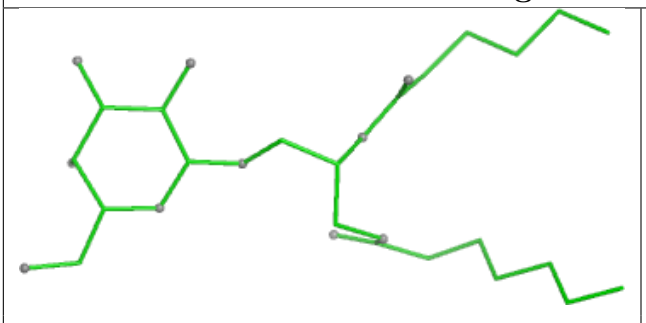

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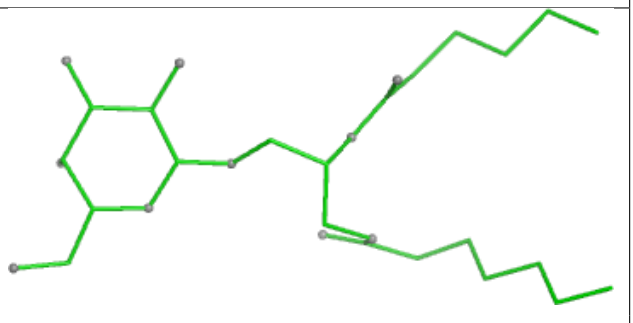
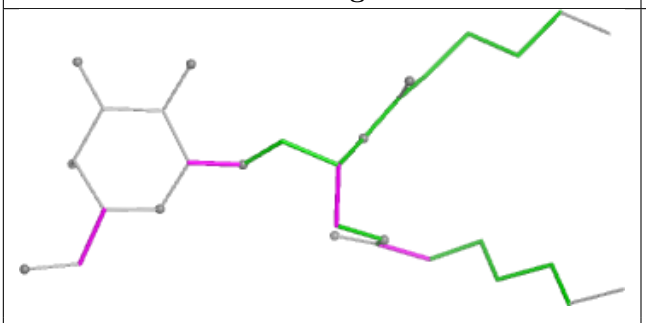


Bond angles



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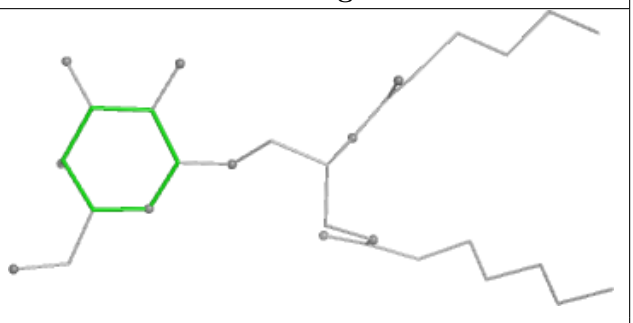

Rings

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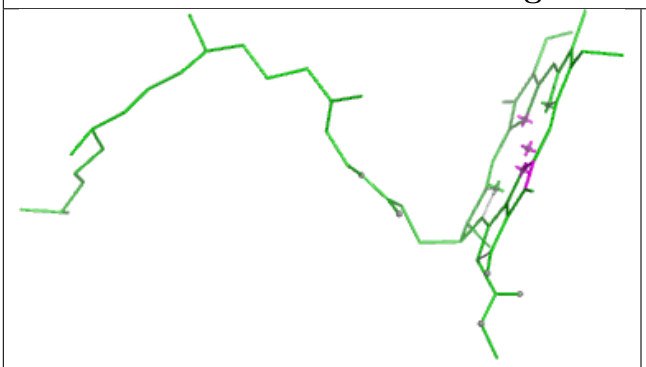

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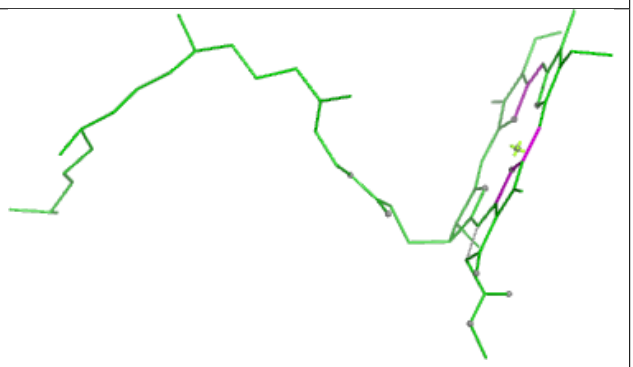
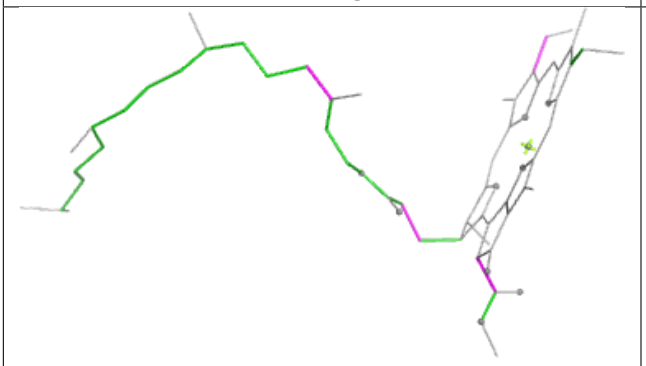


Bond angles

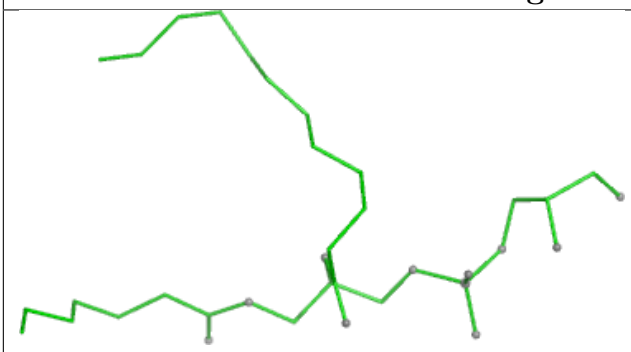


Torsions



Rings

Ligand LHG 6 629



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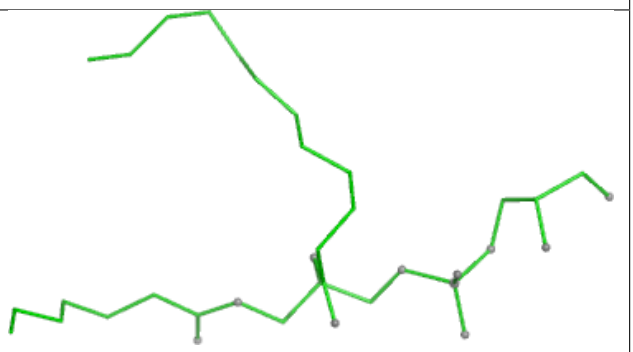
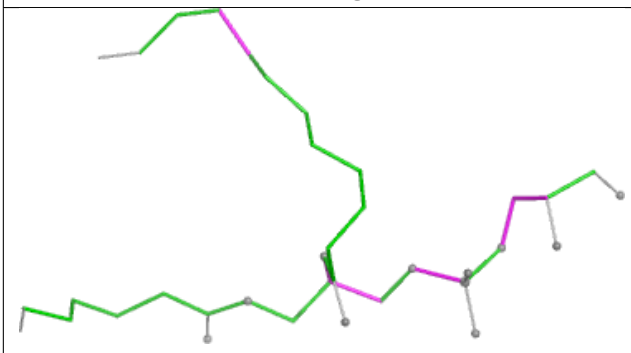


Bond angles



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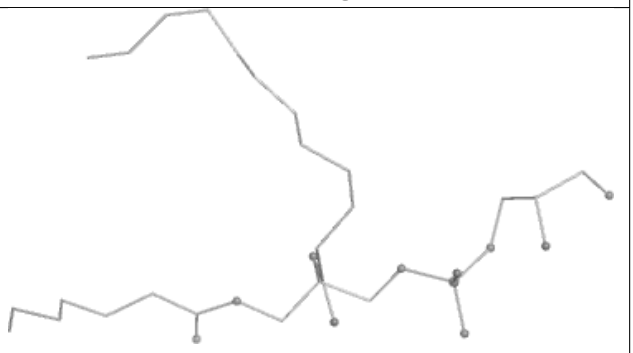
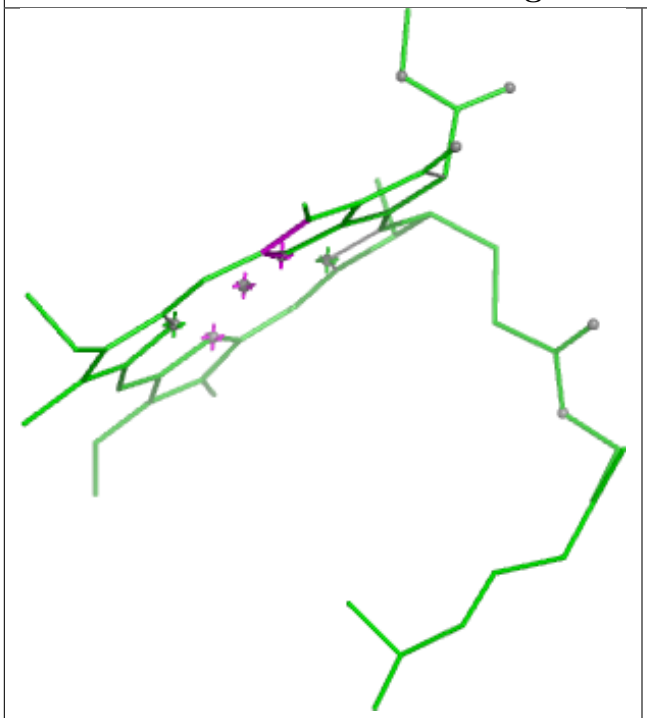


Rings

Ligand CLA A 815



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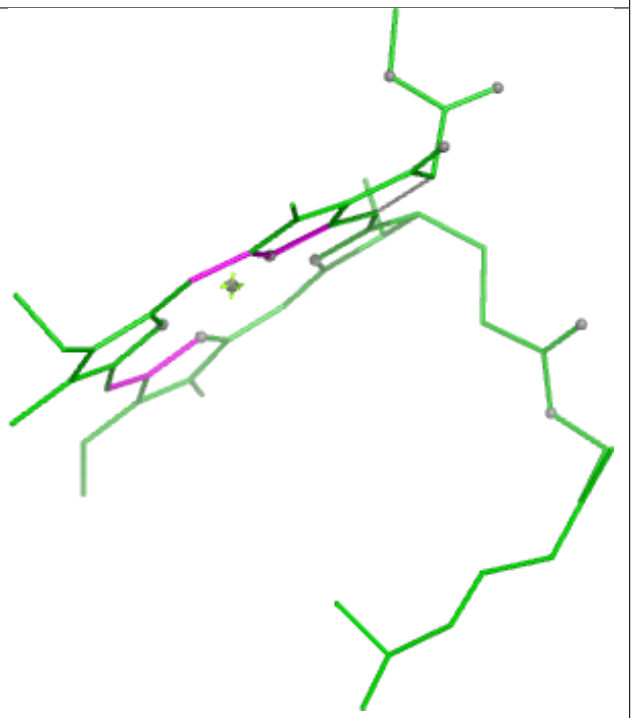
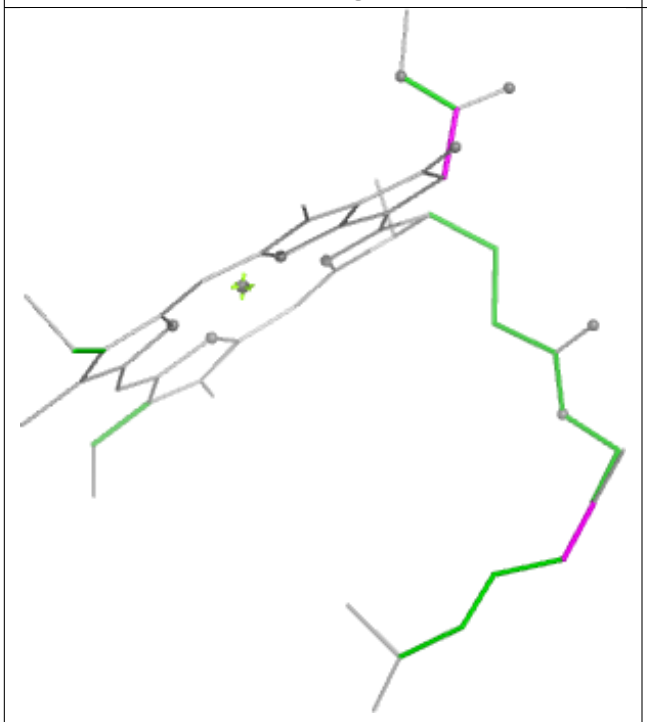


Bond angles



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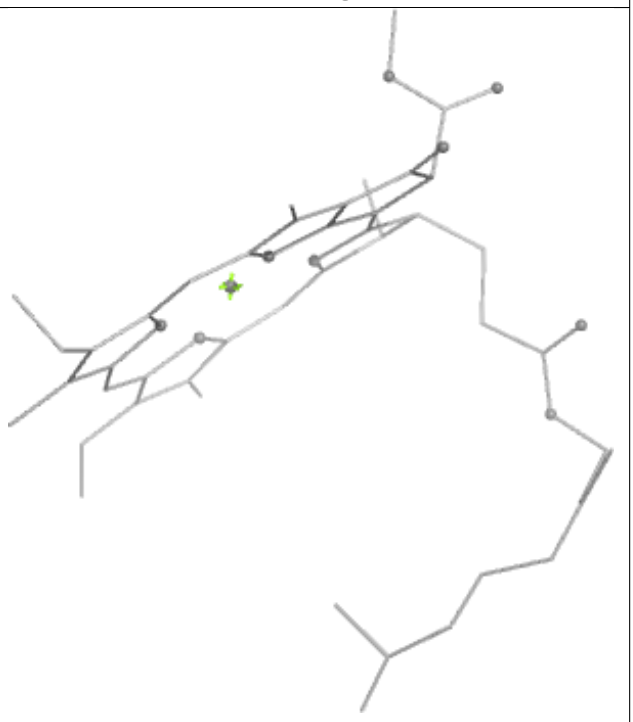
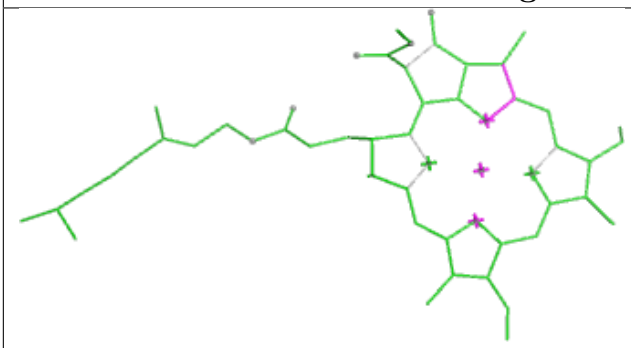


Rings

Ligand CLA 62 622



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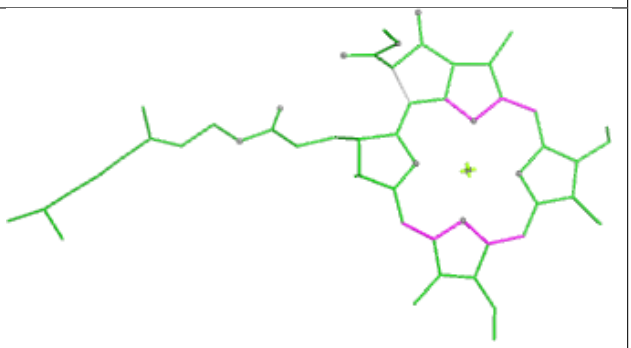
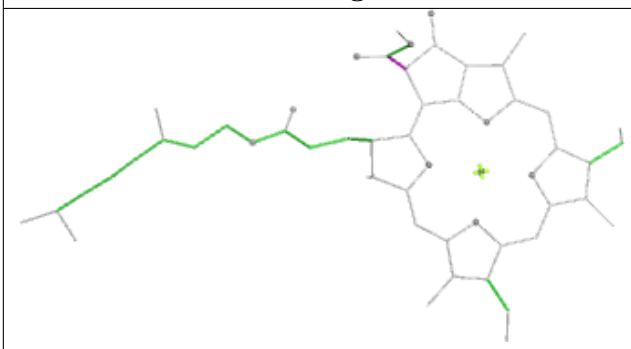


Bond angles



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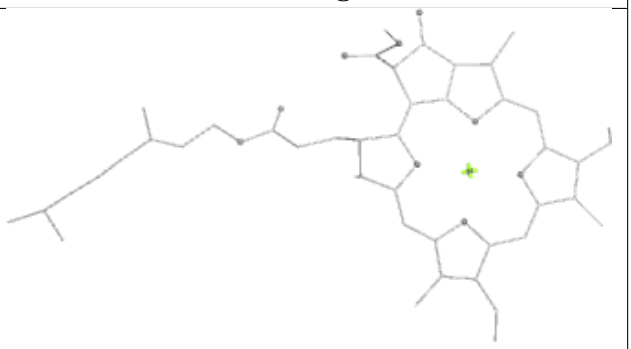
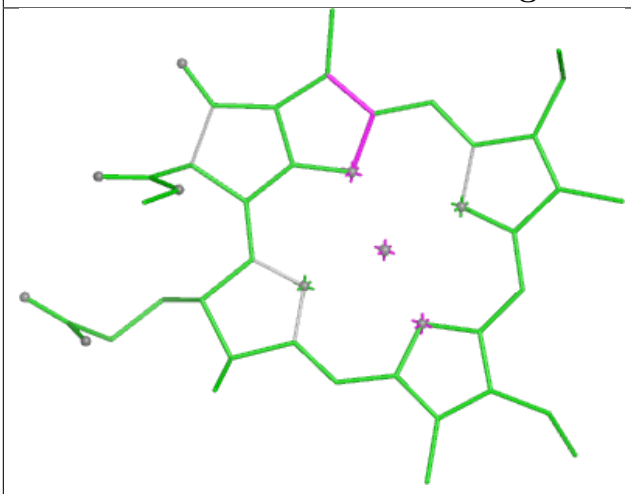


Rings

Ligand CLA 12 612



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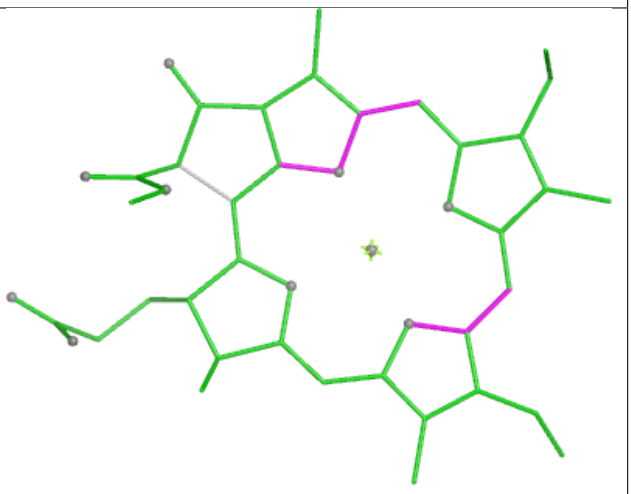

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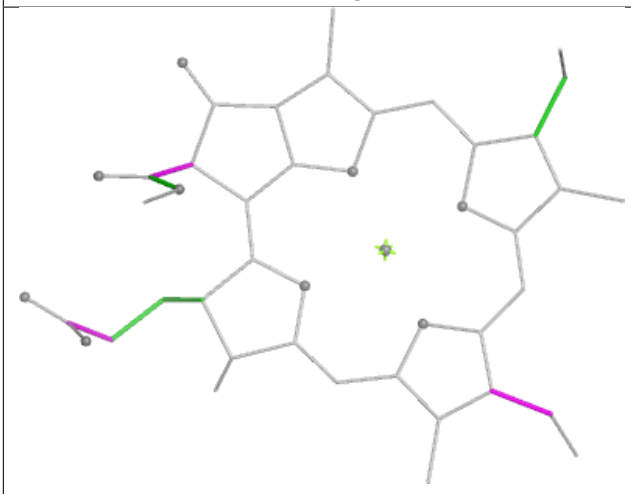

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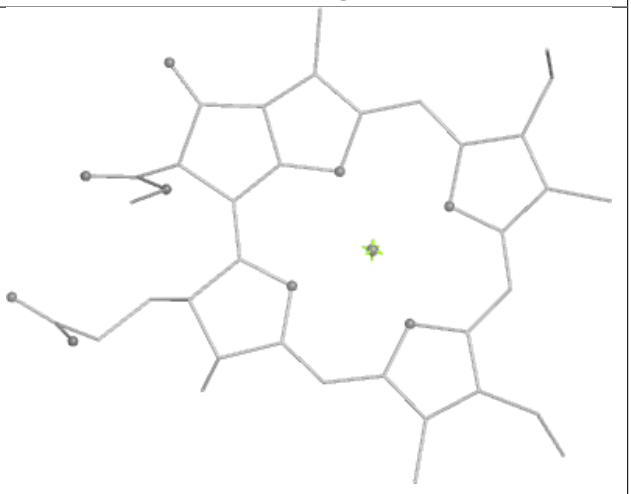
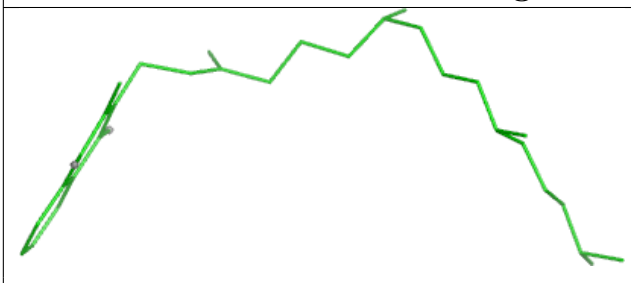


Rings

Ligand PQN B2 842



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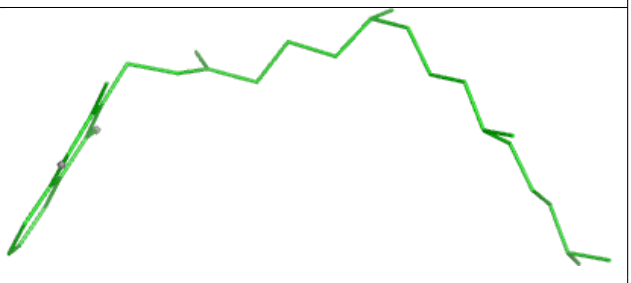
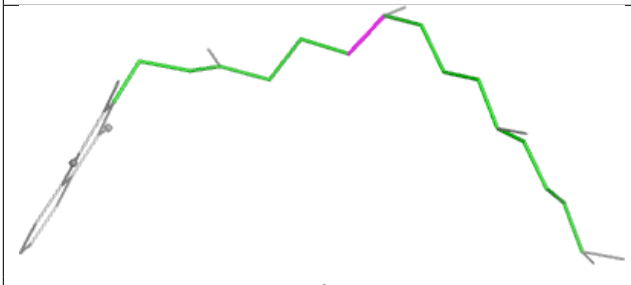


Bond angles



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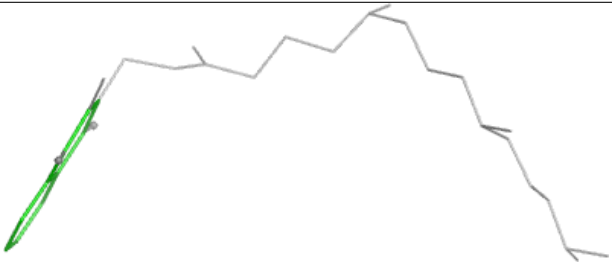
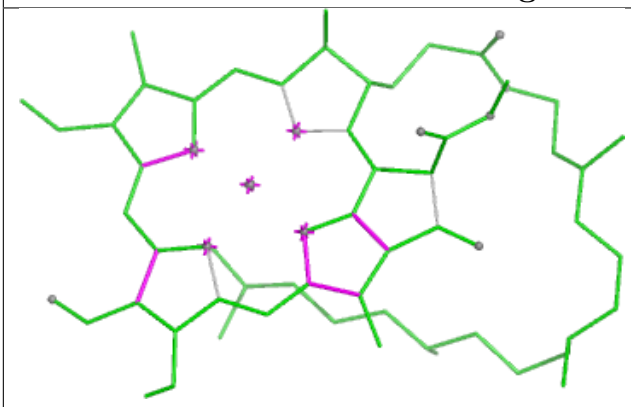


Rings

Ligand CHL 42 607



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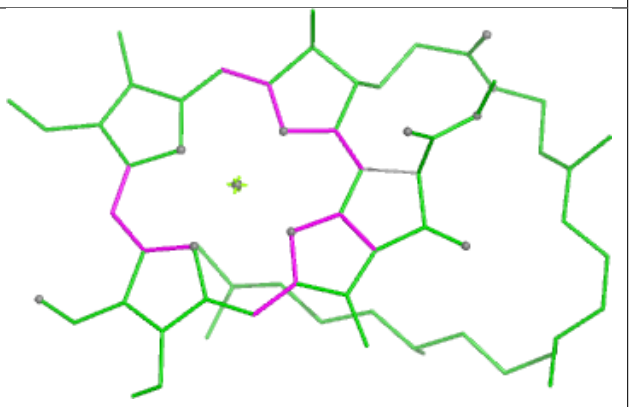
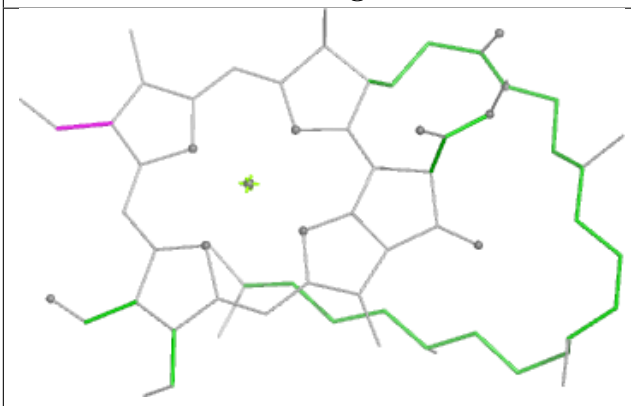


Bond angles



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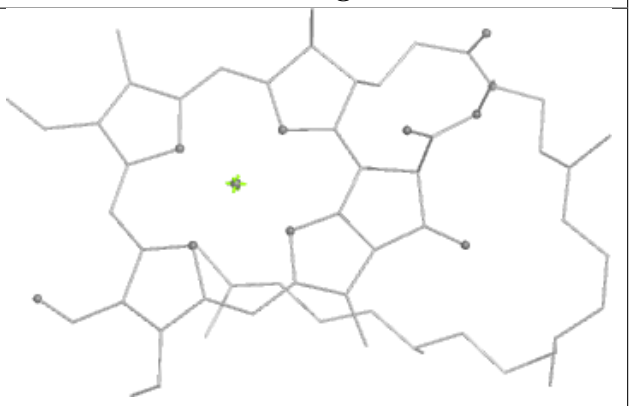
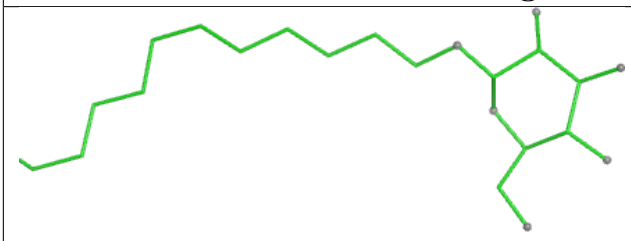


Rings

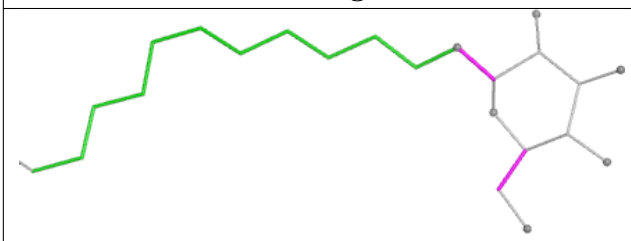
Ligand LMU A 864



Bond lengths



Bond angles



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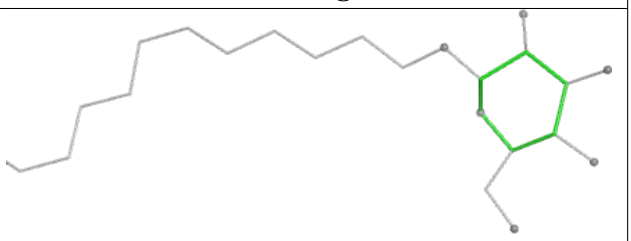
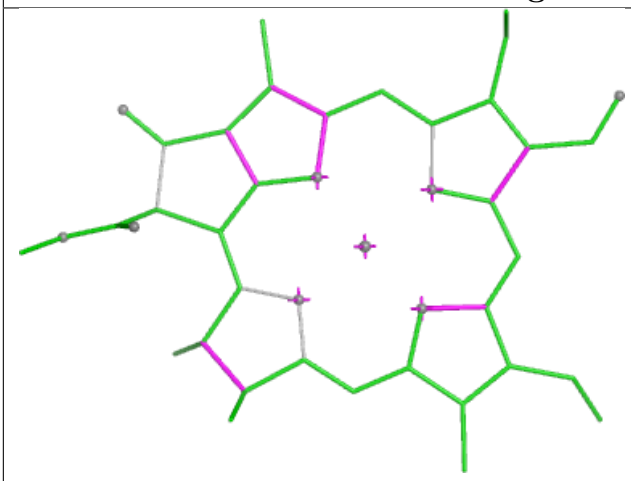


Rings

Ligand CHL 9 606



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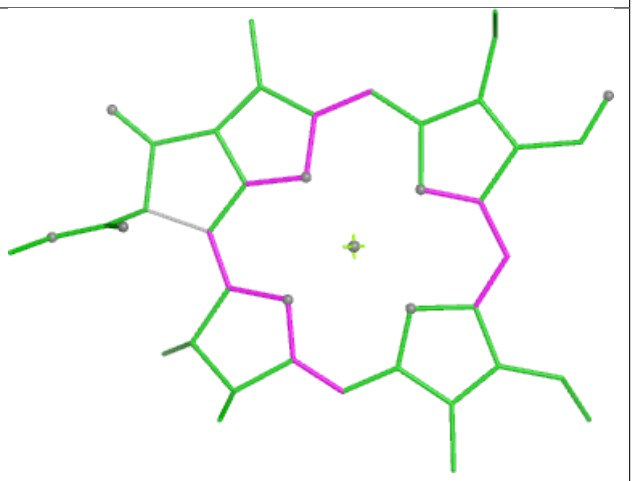
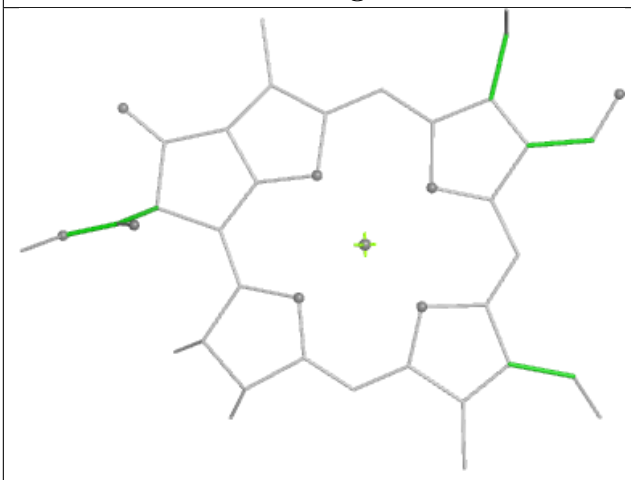


Bond angles



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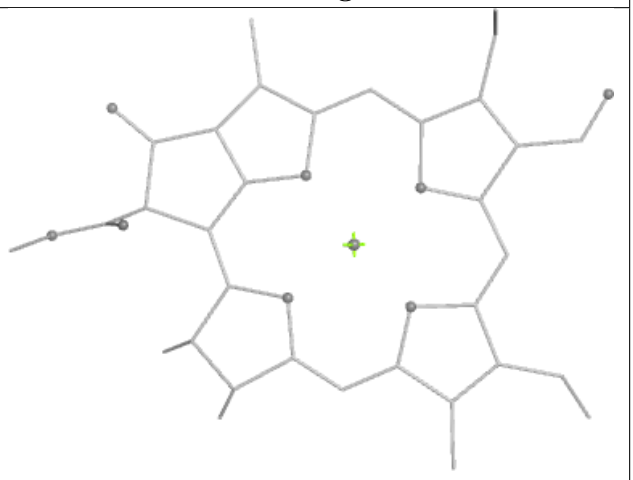
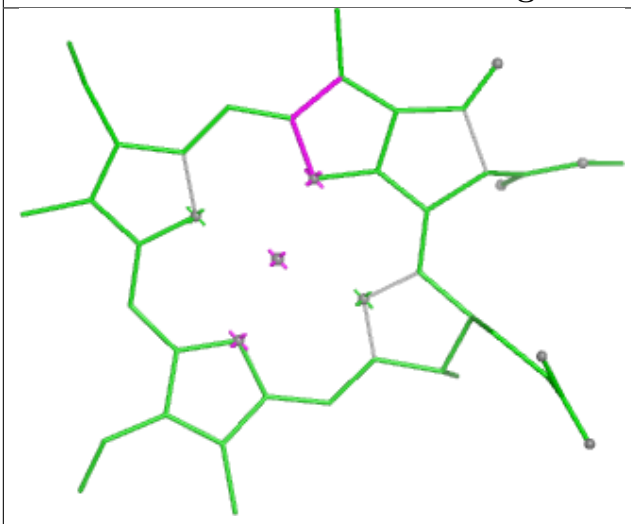
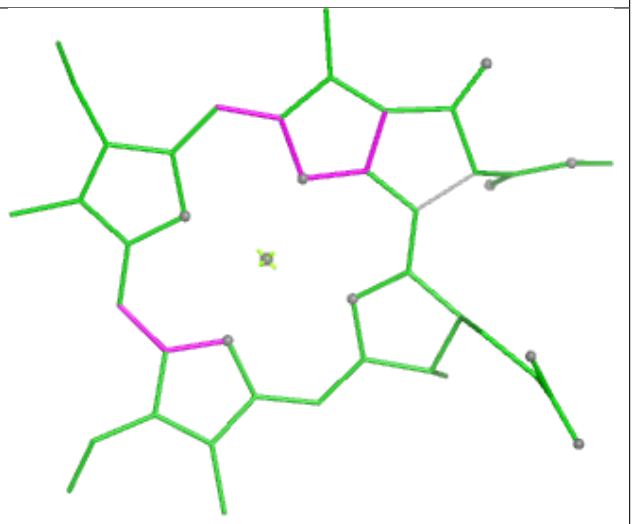


Rings

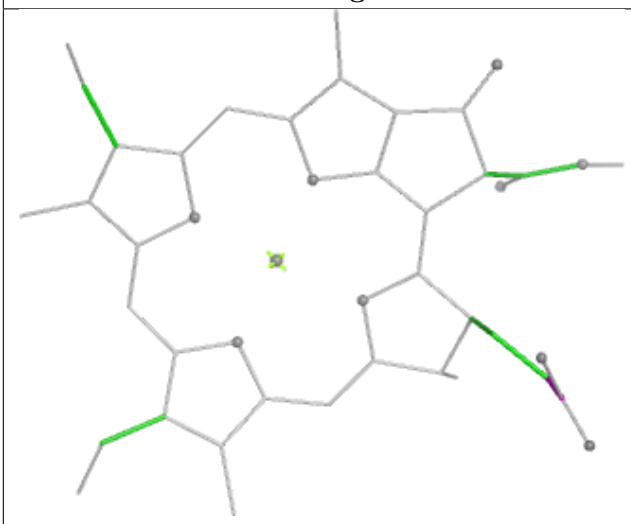
Ligand CLA L2 204



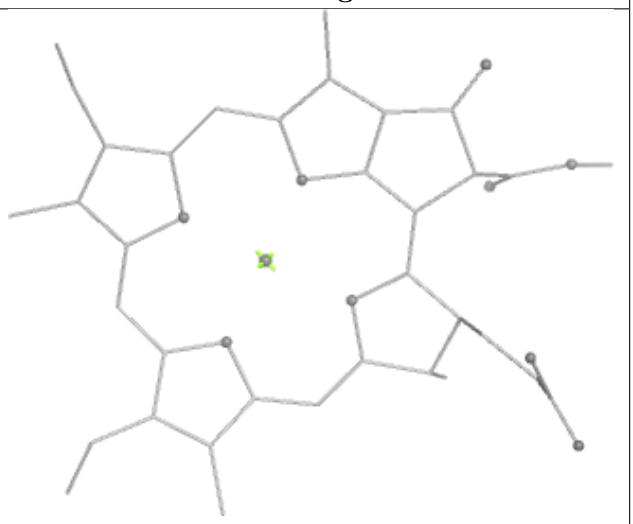
Bond lengths



Bond angles

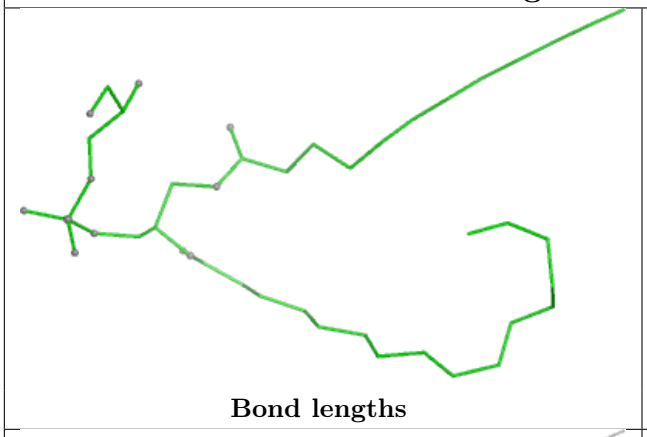


Torsions



Rings

Ligand LHG B 851



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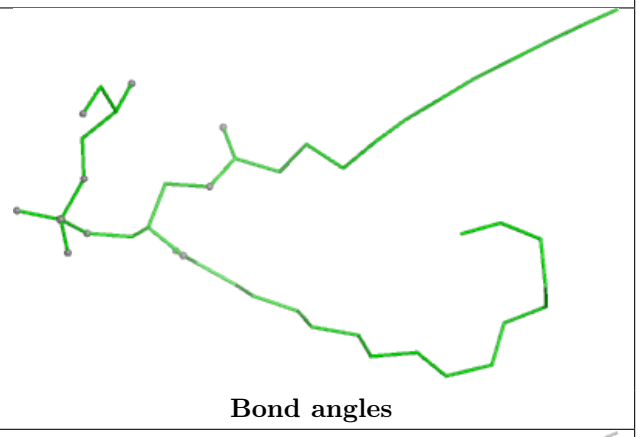

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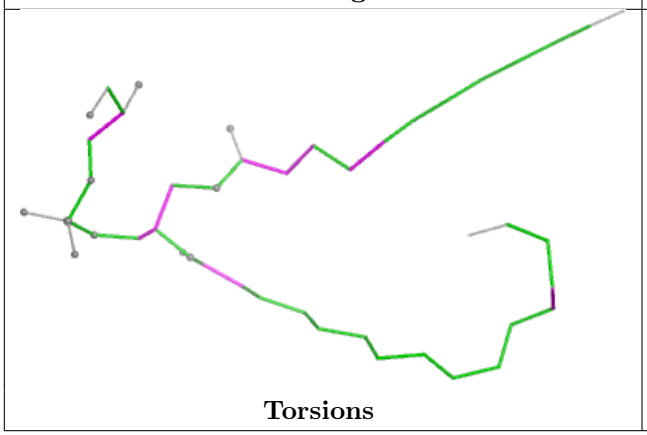

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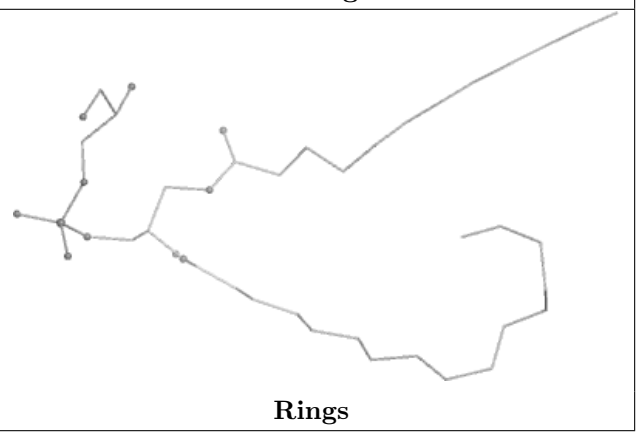
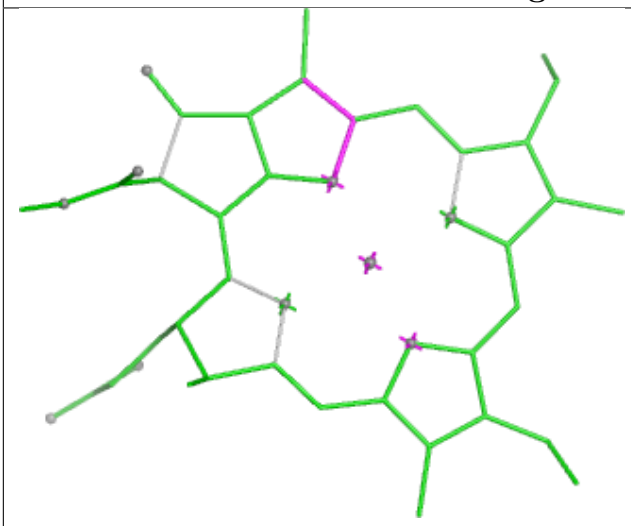


Rings

Ligand CLA 8 616



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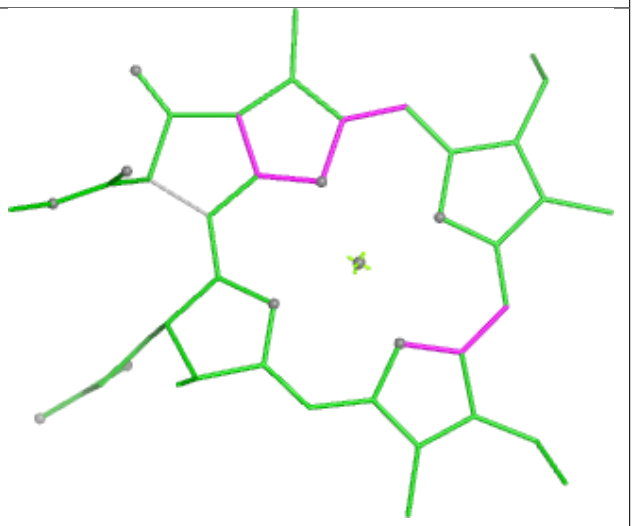
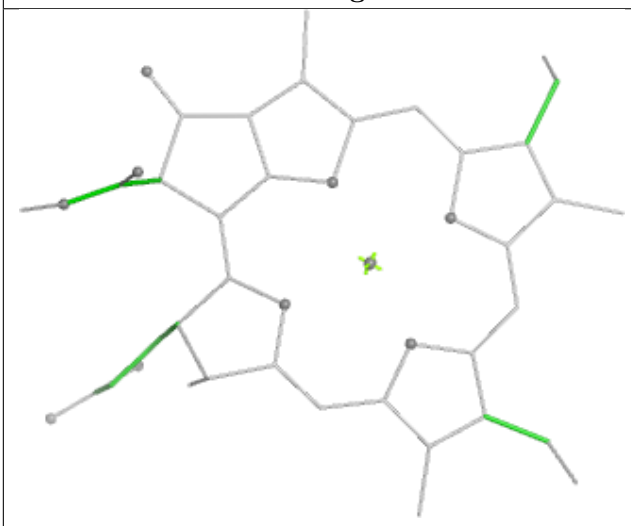


Bond angles



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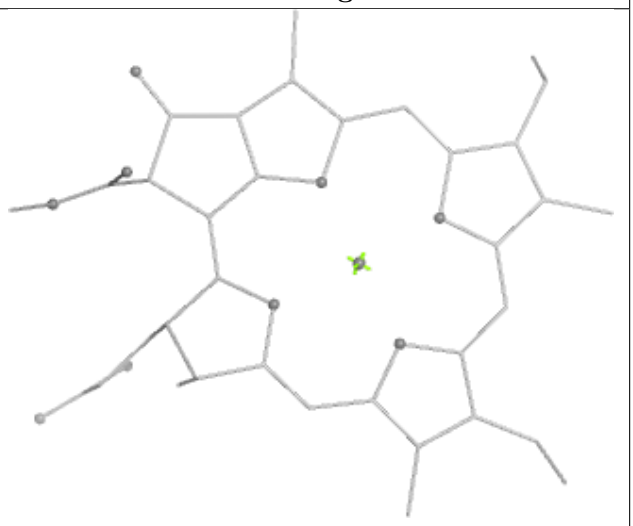
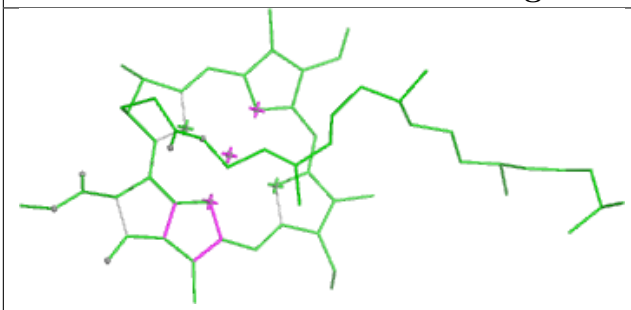


Rings

Ligand CLA B 811



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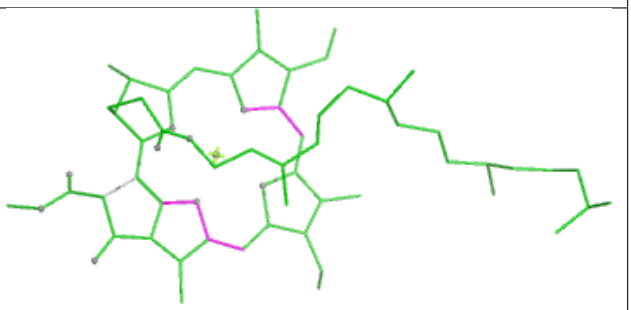
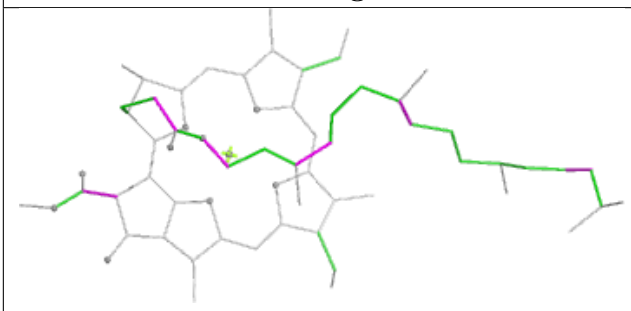


Bond angles



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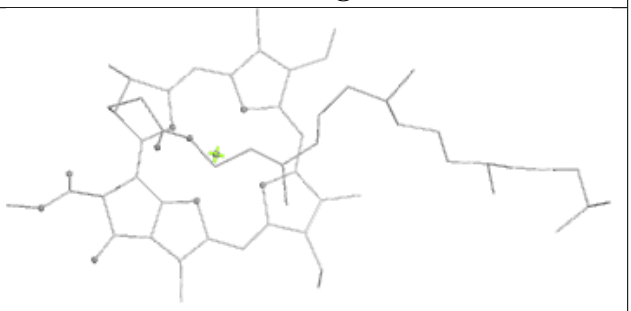
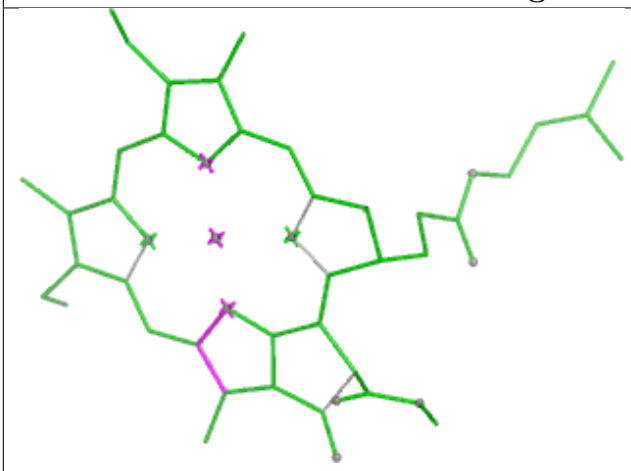
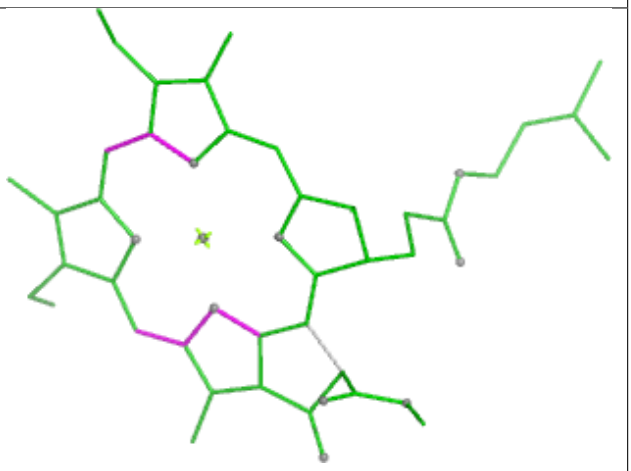


Rings

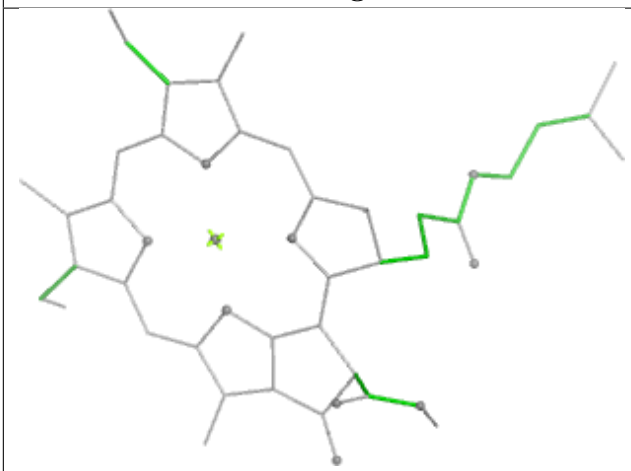
Ligand CLA 7 608



Bond lengths



Bond angles



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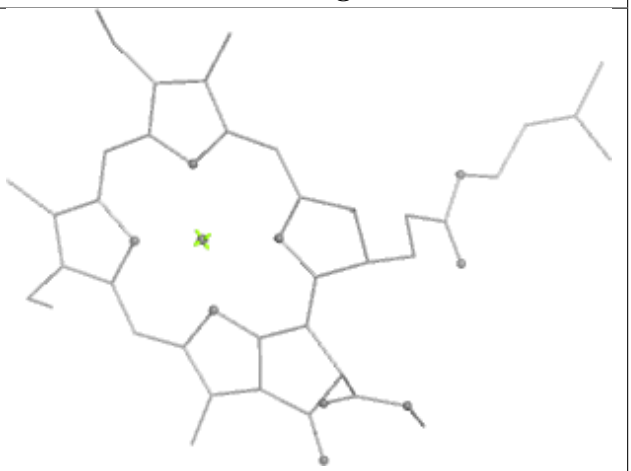
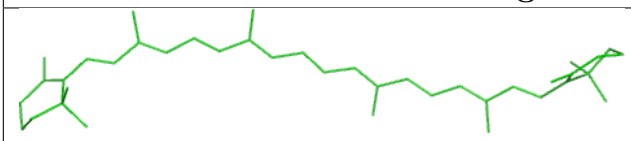
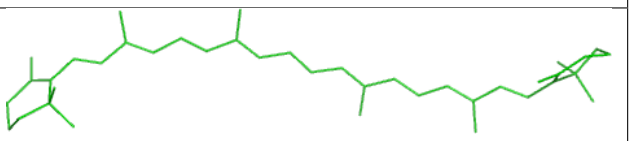
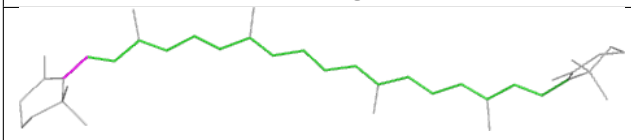
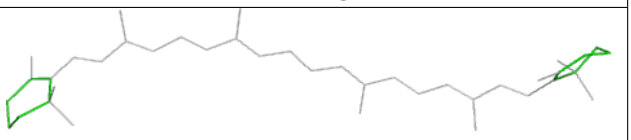


Rings

Ligand BCR 72 623	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand BCR A 850	
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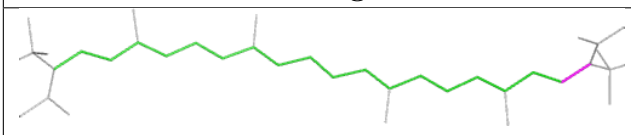
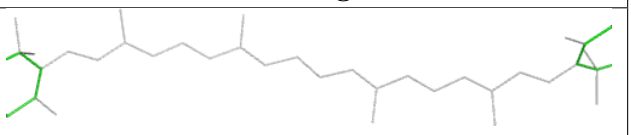
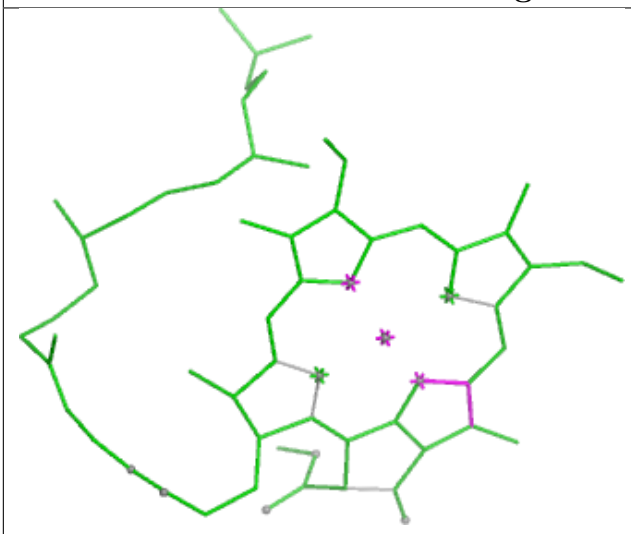
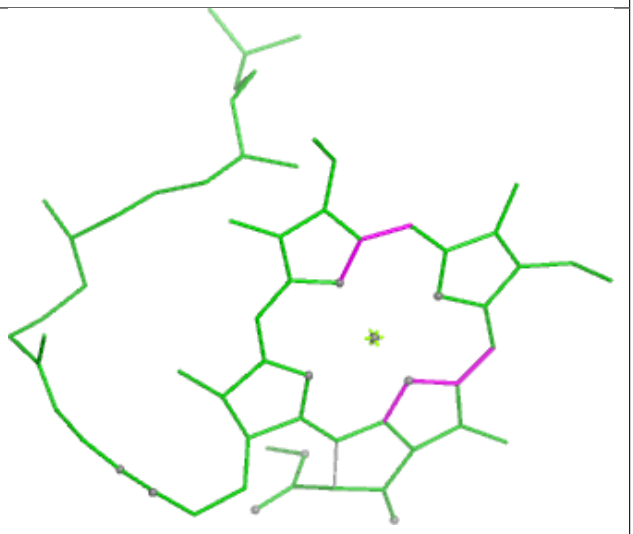
 Torsions	 Rings

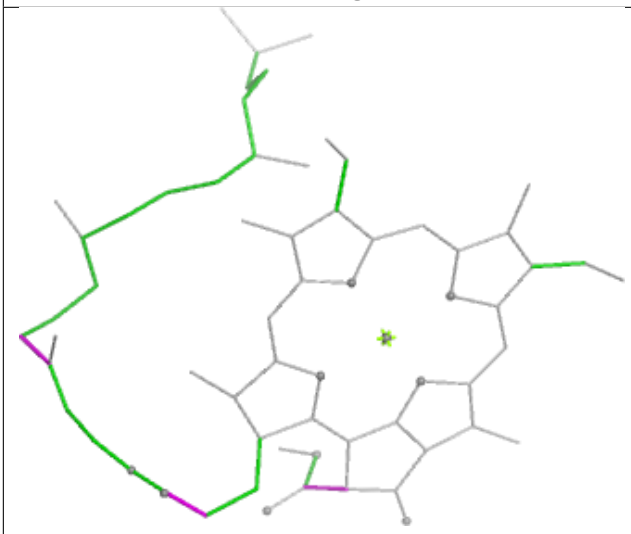
Ligand CLA A2 814



Bond lengths



Bond angles

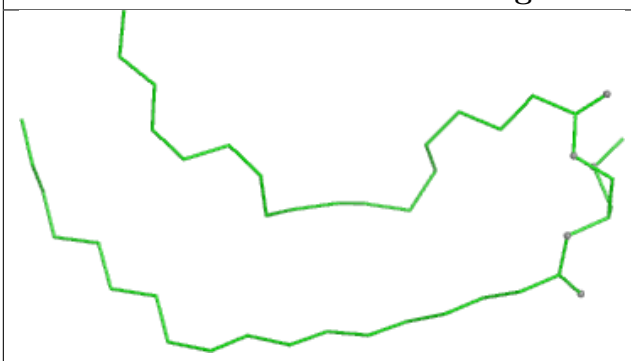


Torsions



Rings

Ligand LMG 32 722



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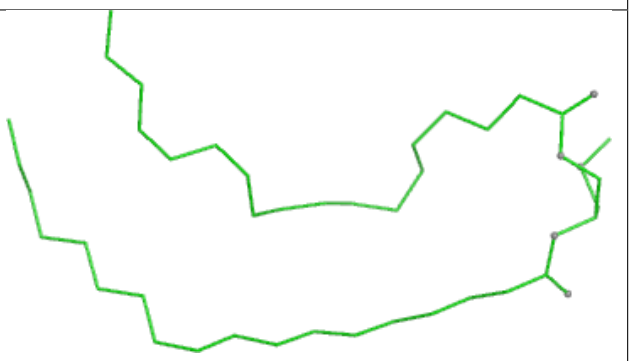
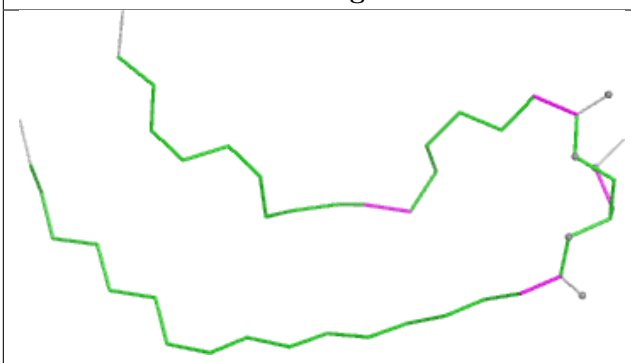


Bond angles



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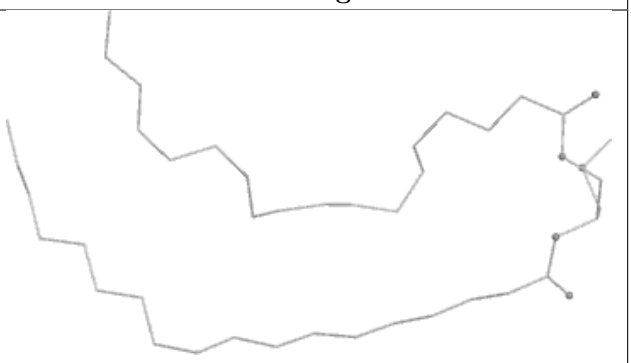
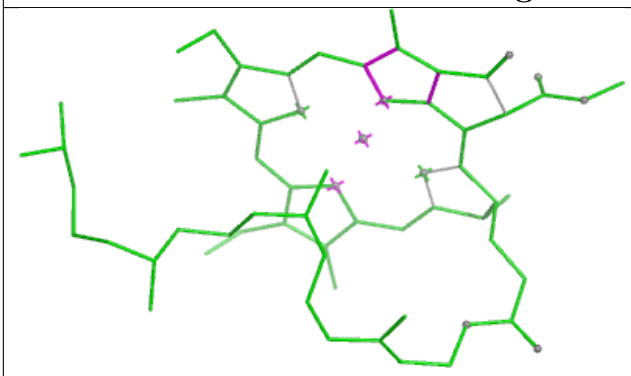


Rings

Ligand CLA B2 817



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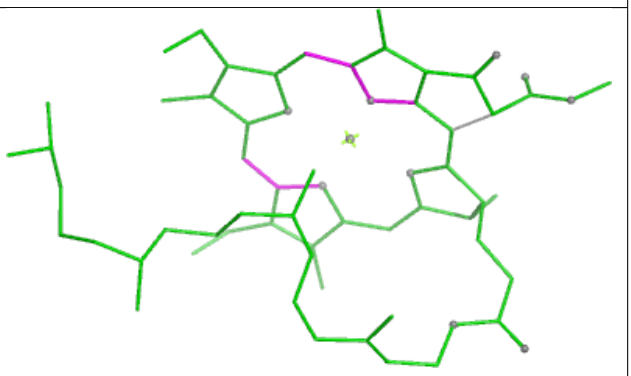
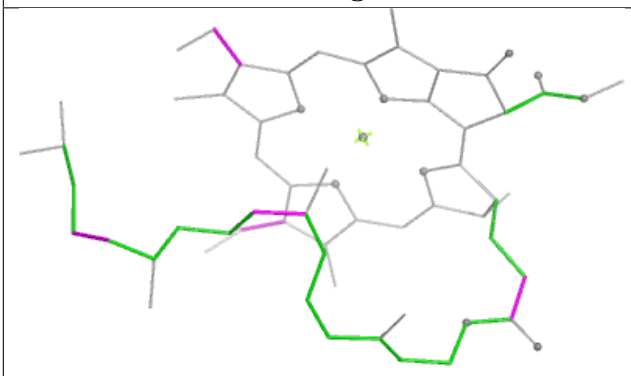


Bond angles



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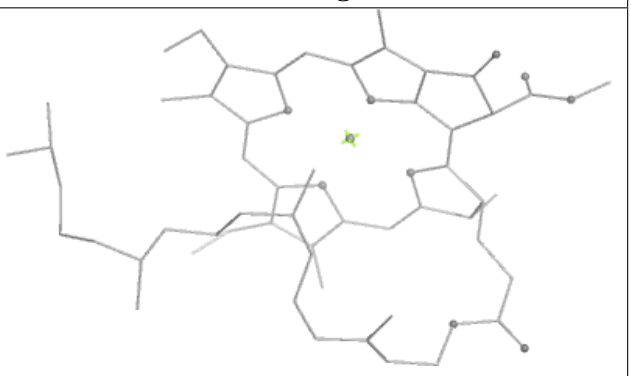
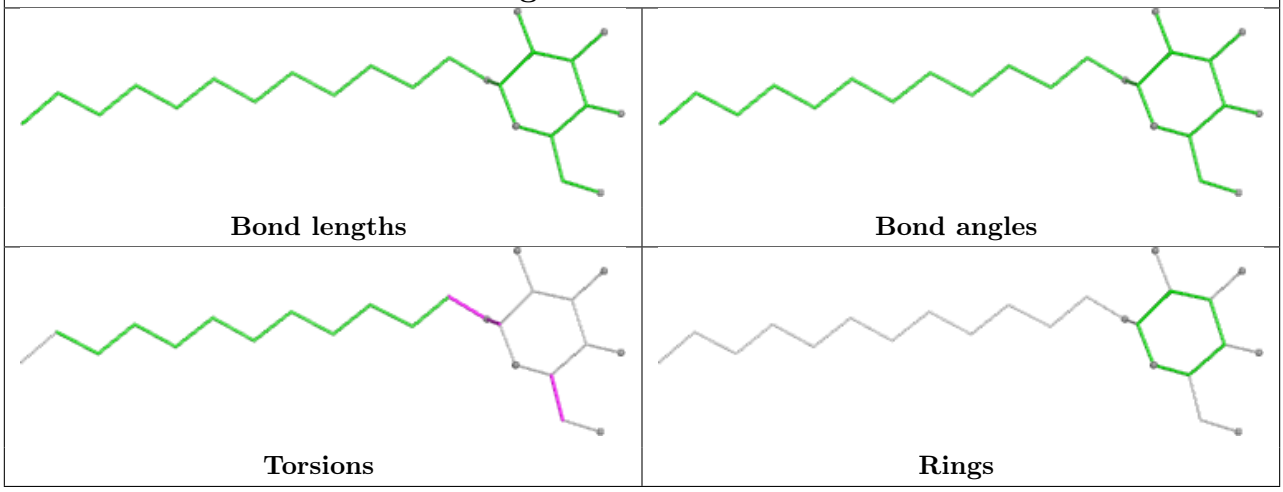
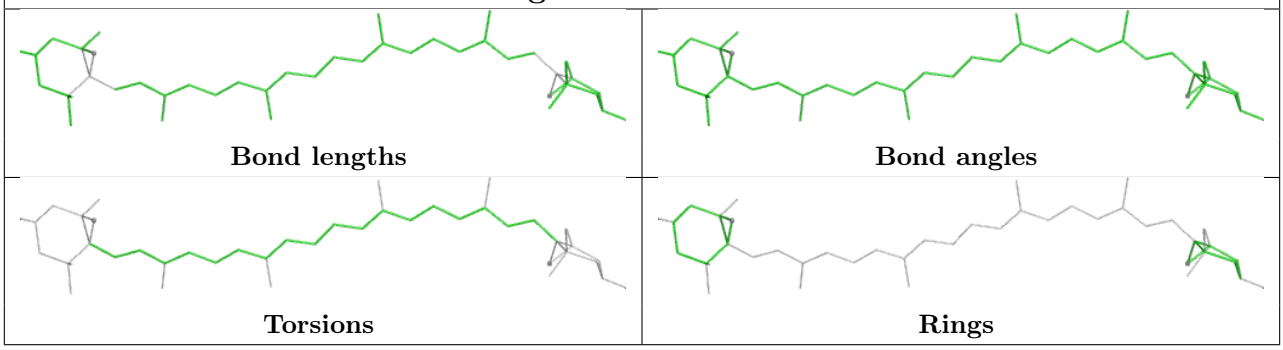


Rings

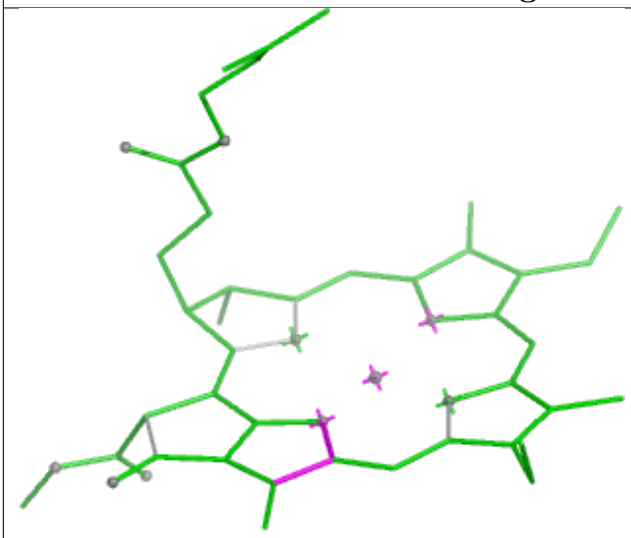
Ligand LMU G 206



Ligand XAT 5 624



Ligand CLA 12 604



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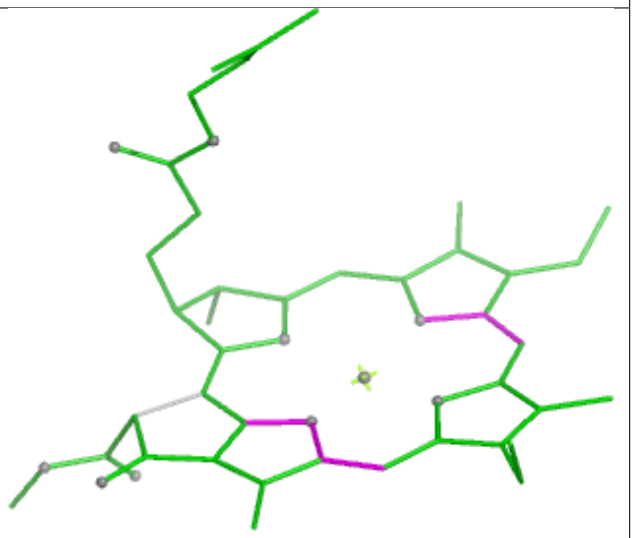
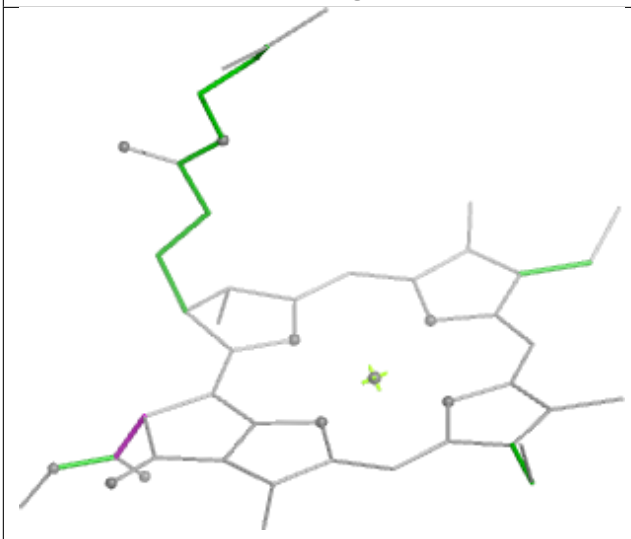


Bond angles

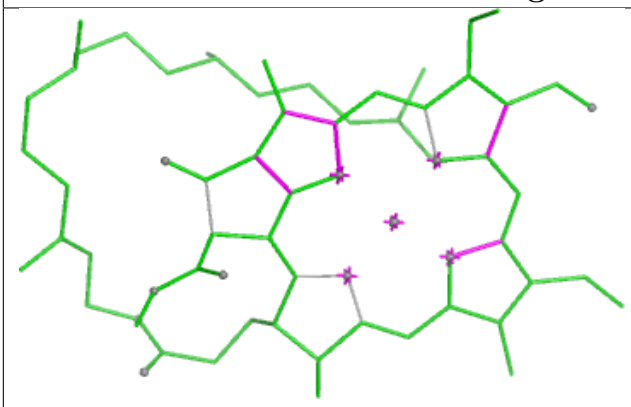


Torsions



Rings

Ligand CHL 4 607



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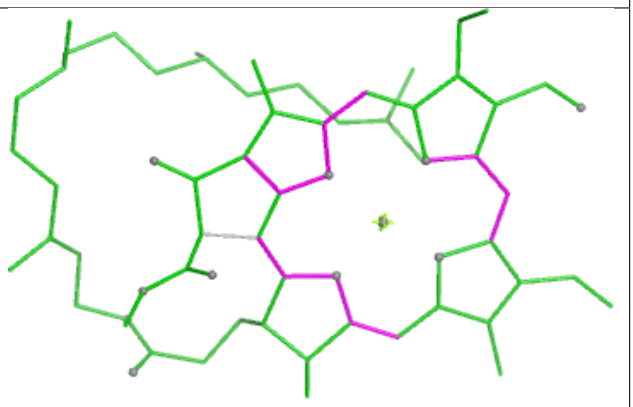
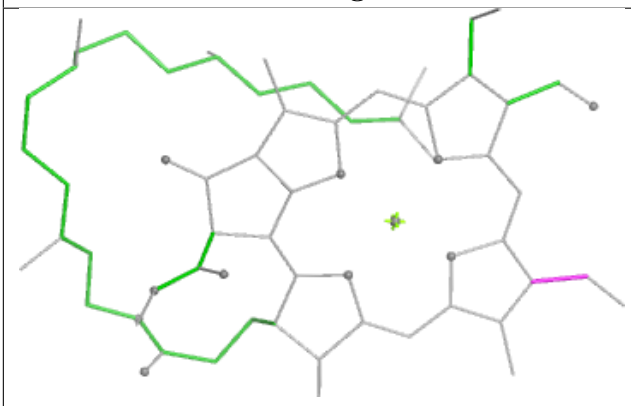


Bond angles



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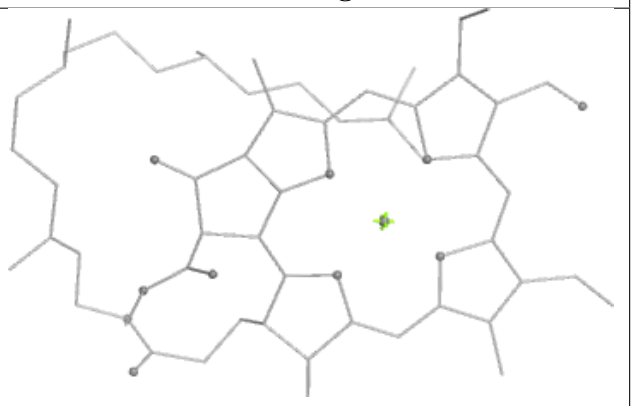


Rings

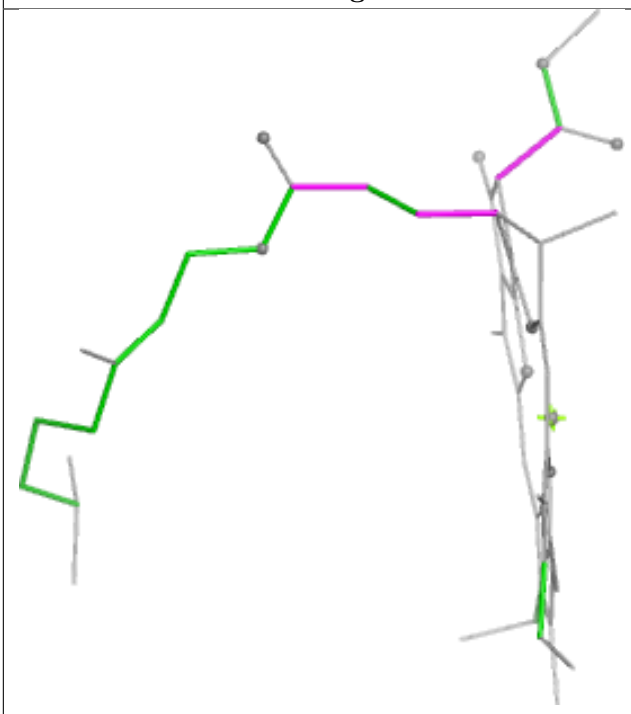
Ligand CLA 42 614



Bond lengths



Bond angles

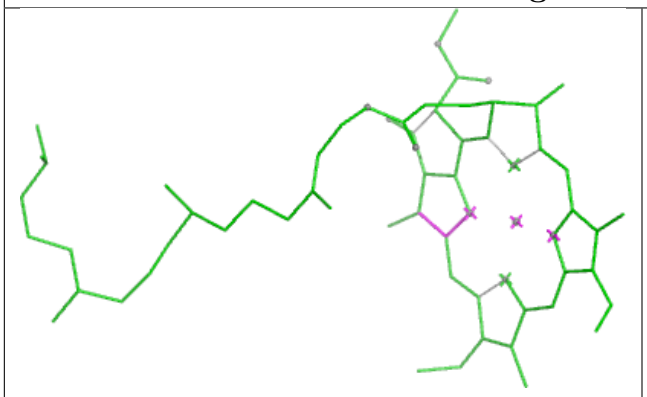


Torsions



Rings

Ligand CLA 9 611



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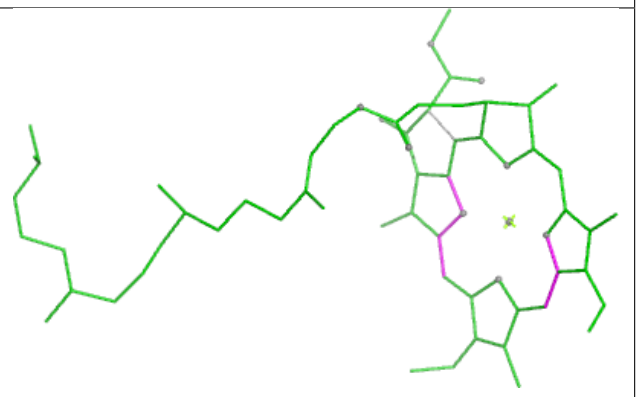
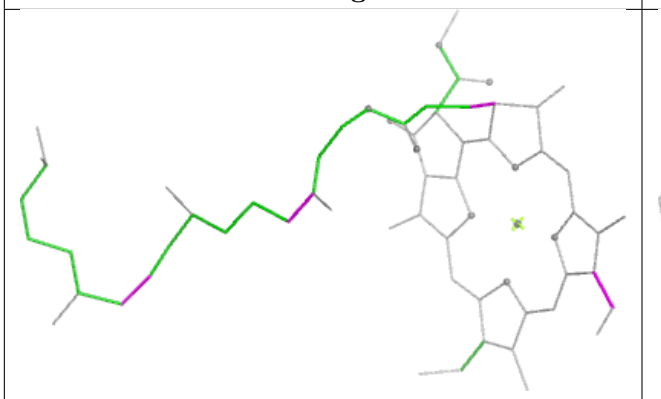


Bond angles

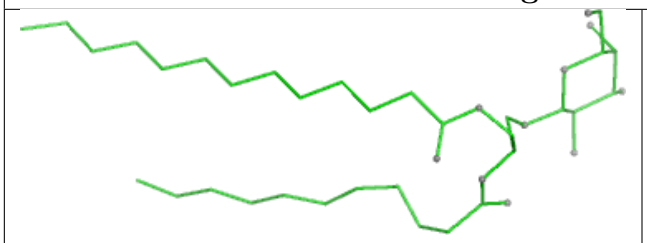


Torsions



Rings

Ligand LMG B 852



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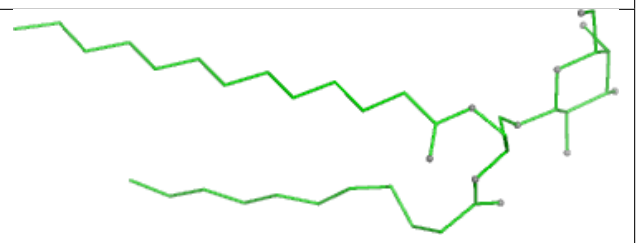
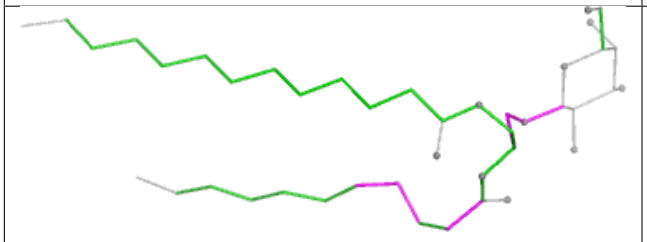
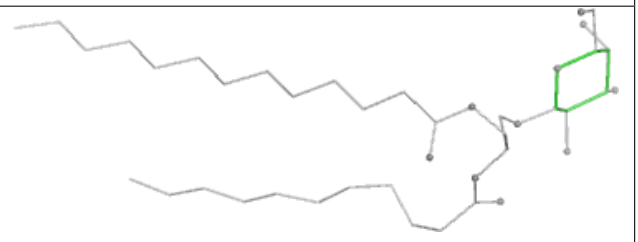


Bond angles

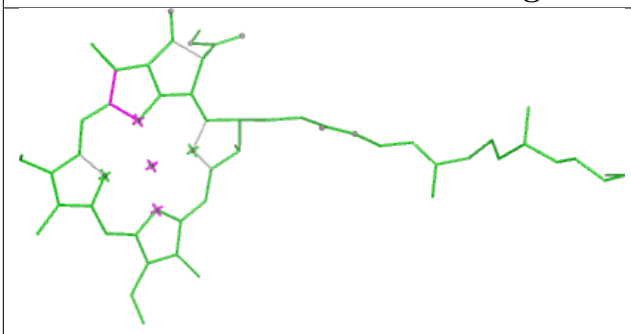


Torsions



Rings

Ligand CLA G 203



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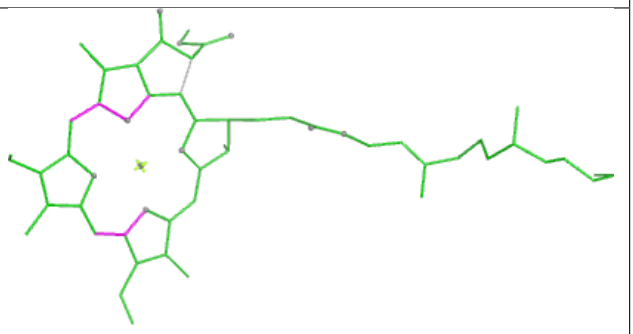
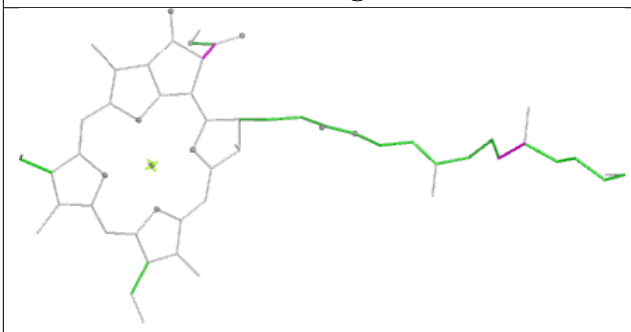


Bond angles



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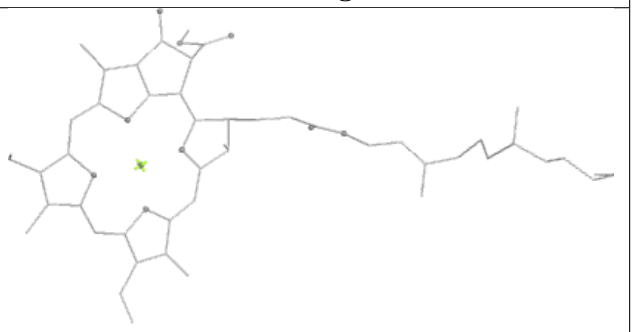
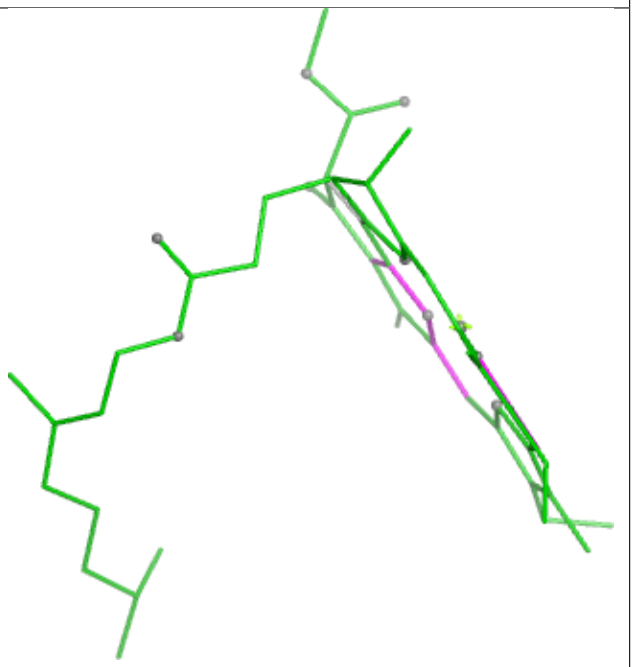


Rings

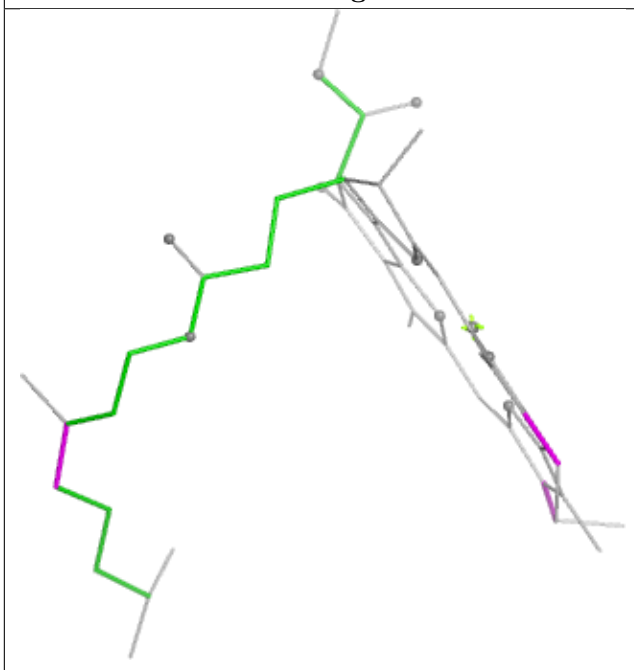
Ligand CLA 32 607



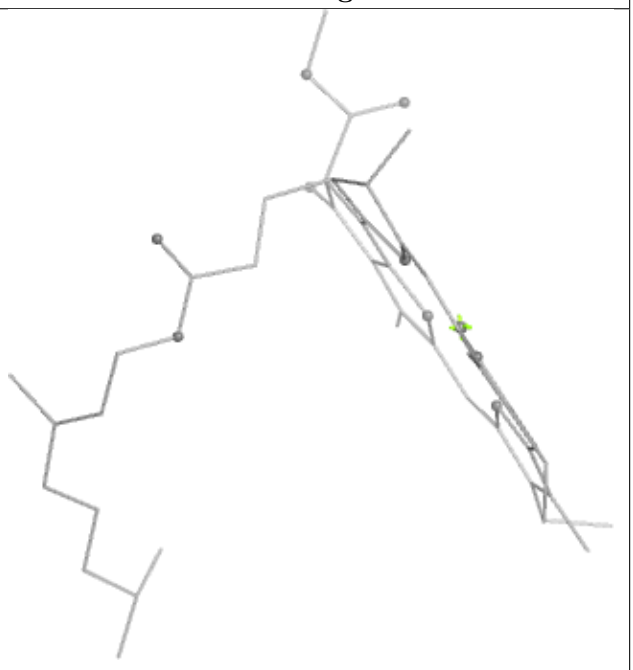
Bond lengths



Bond angles

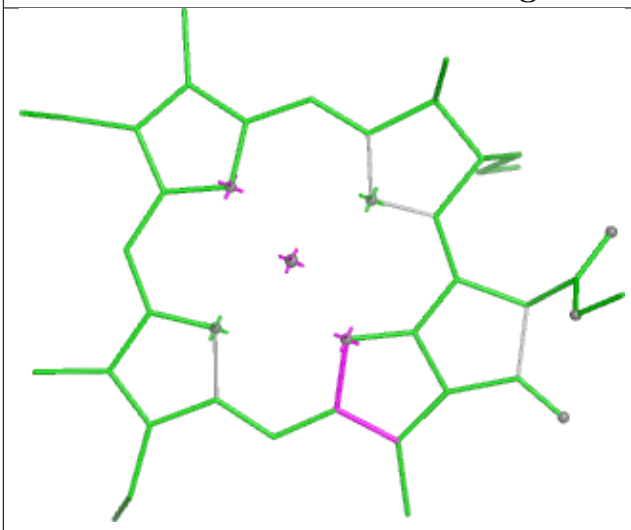


Torsions

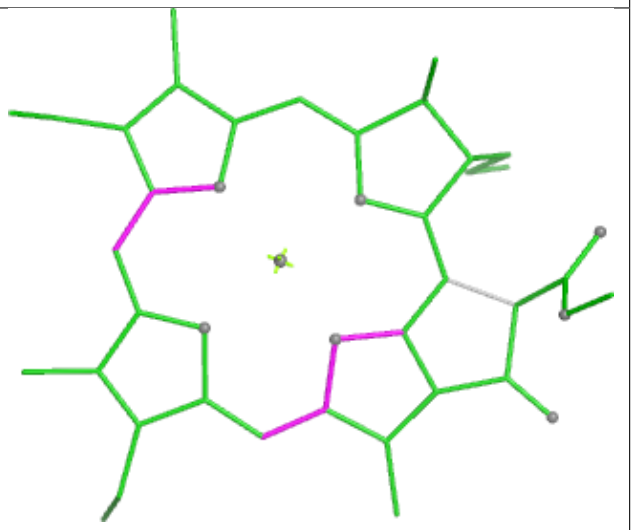


Rings

Ligand CLA 72 614



Bond lengths



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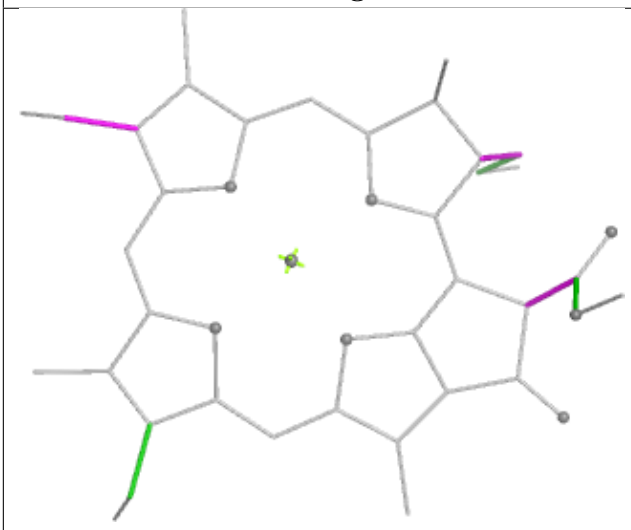

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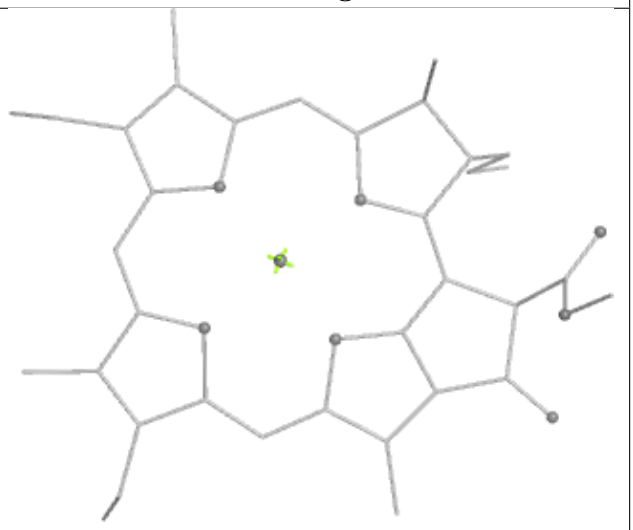
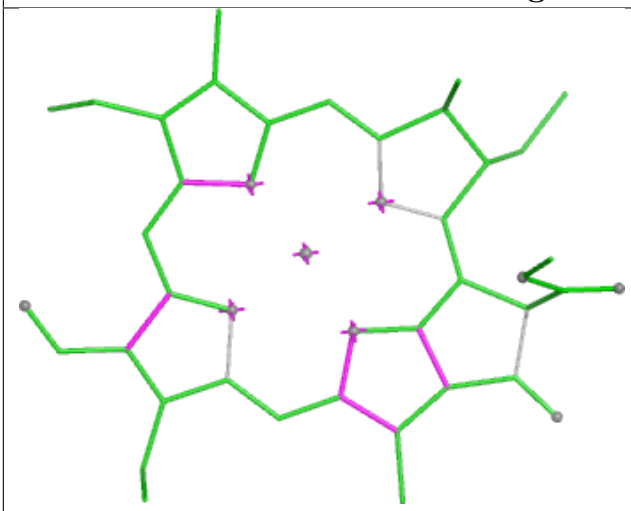


Rings

Ligand CHL 6 618



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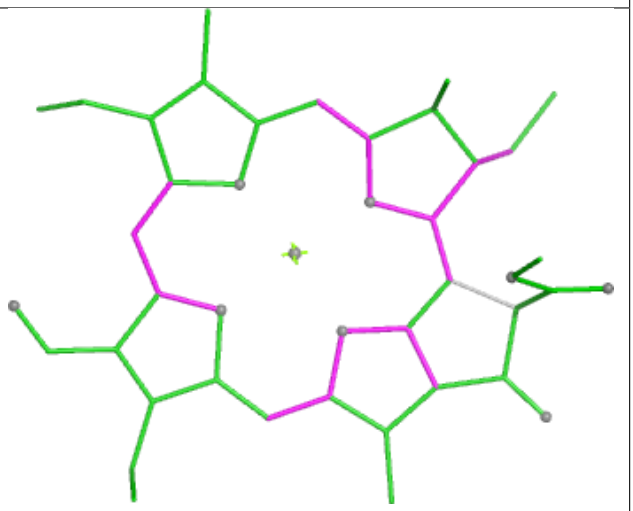
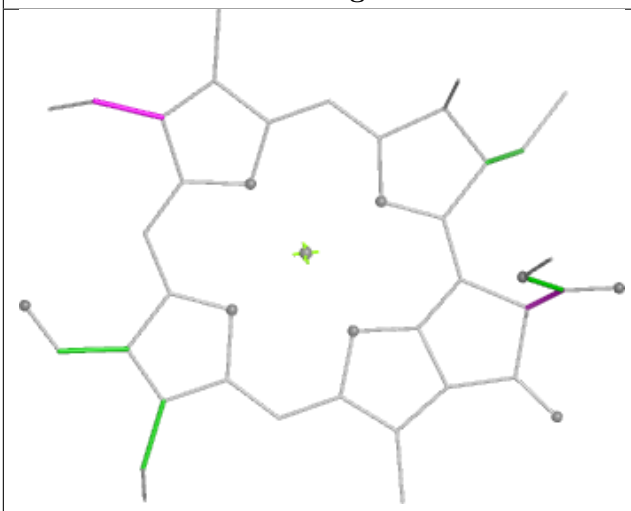


Bond angles



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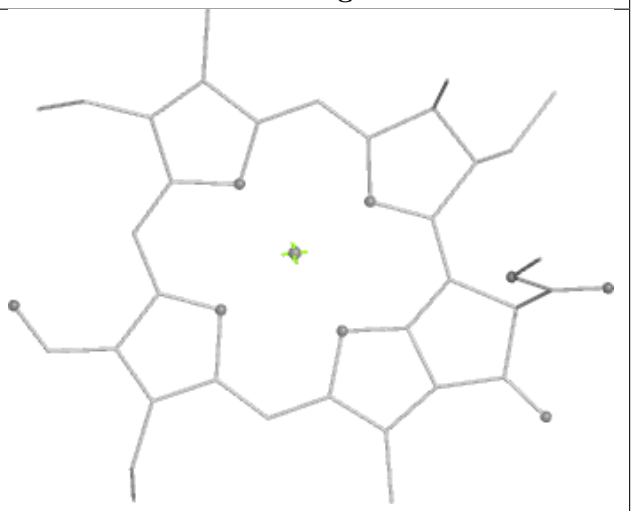
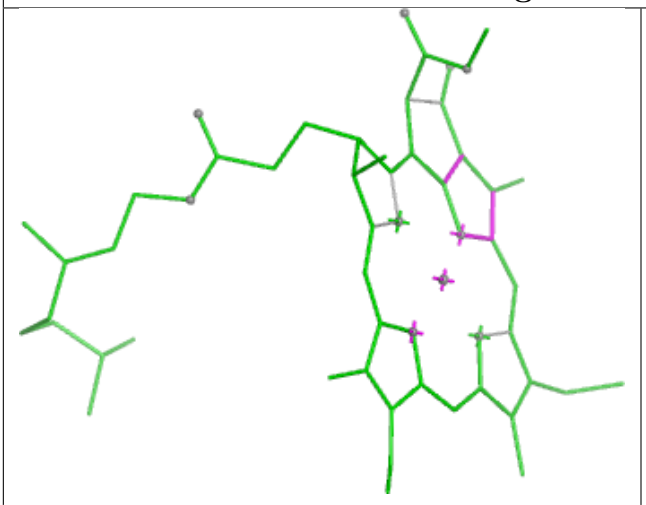


Rings

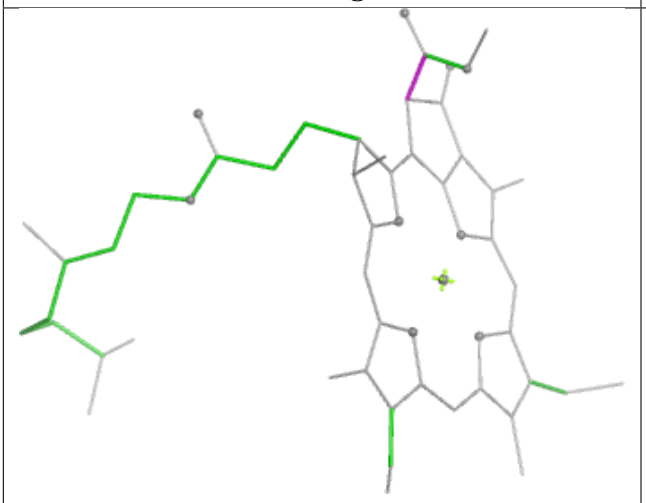
Ligand CLA A2 805



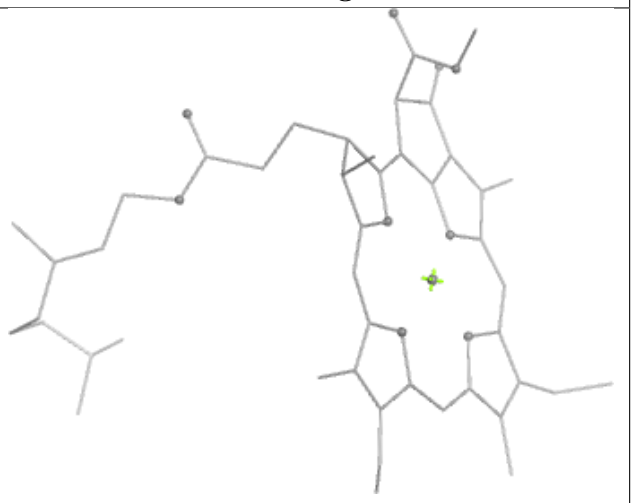
Bond lengths



Bond angles

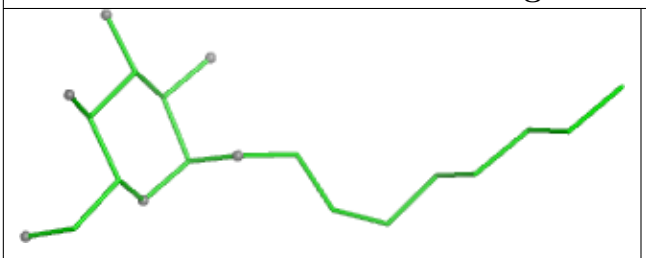


Torsions



Rings

Ligand LMU 6 632



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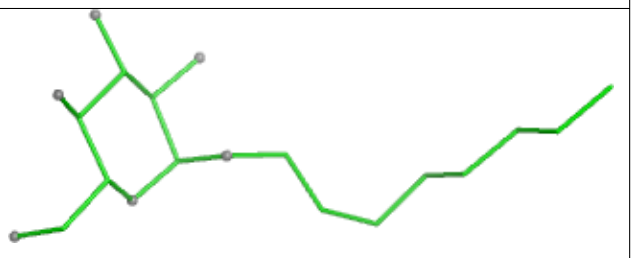
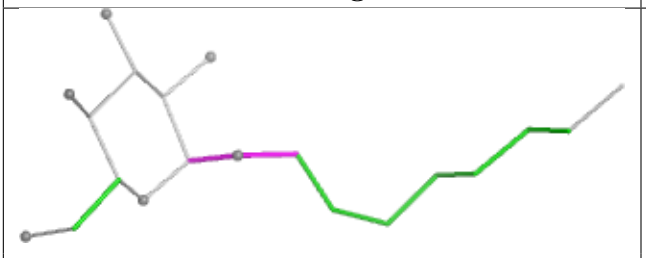
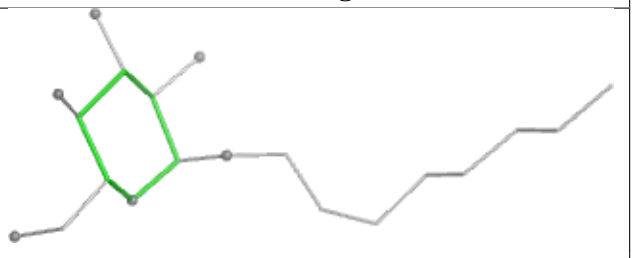


Bond angles

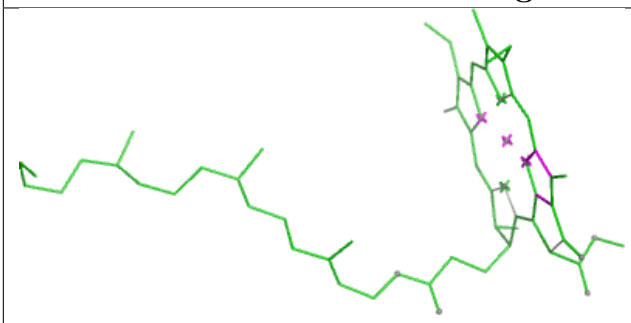


Torsions



Rings

Ligand CLA B2 821



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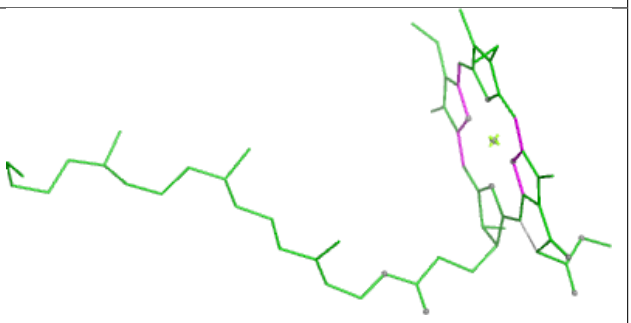
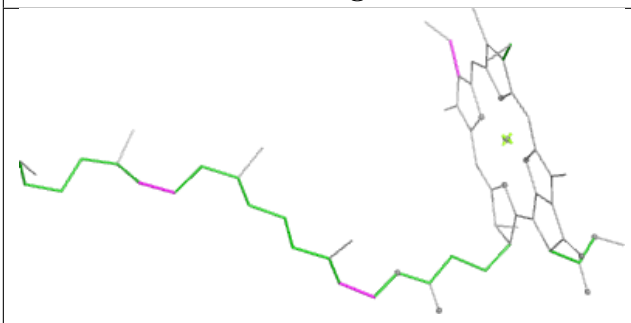


Bond angles



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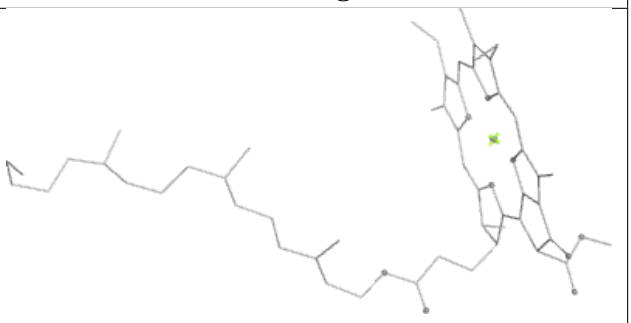
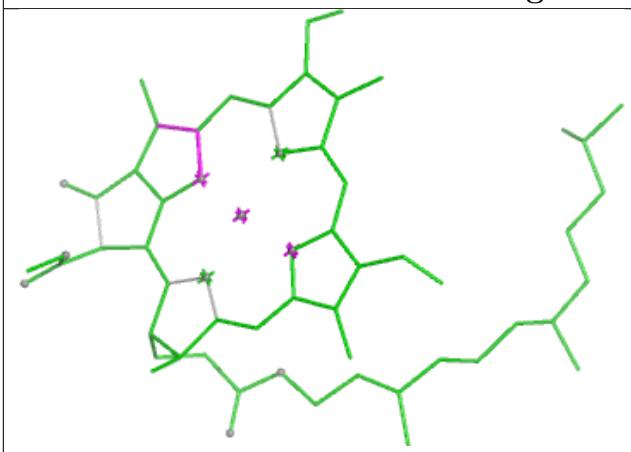


Rings

Ligand CLA Z 602



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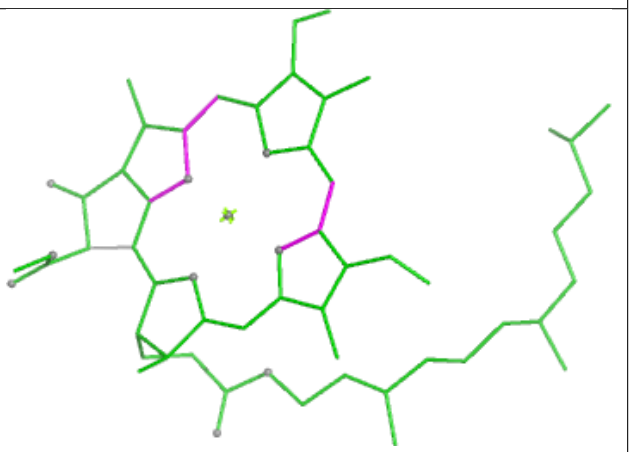
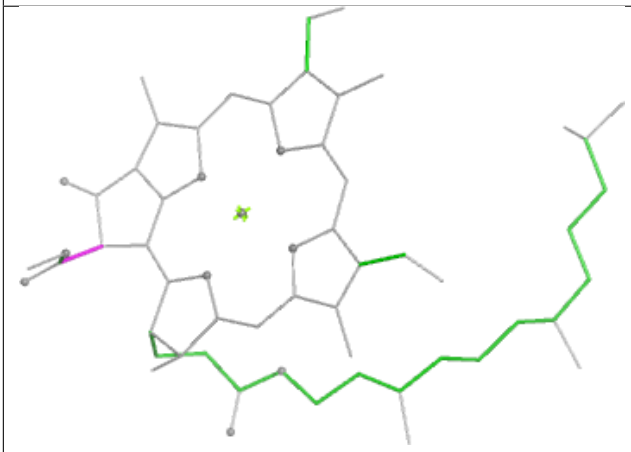


Bond angles



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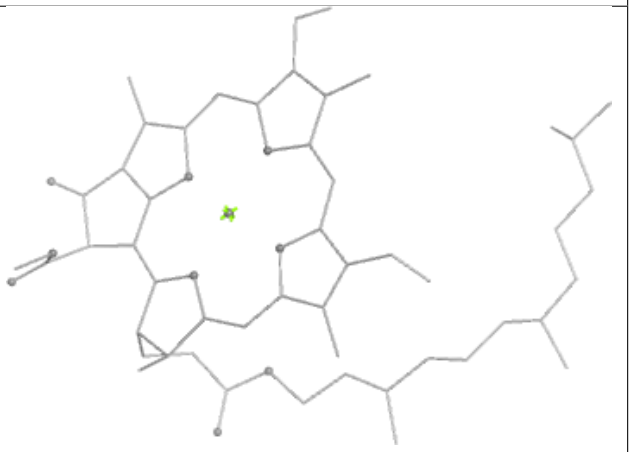
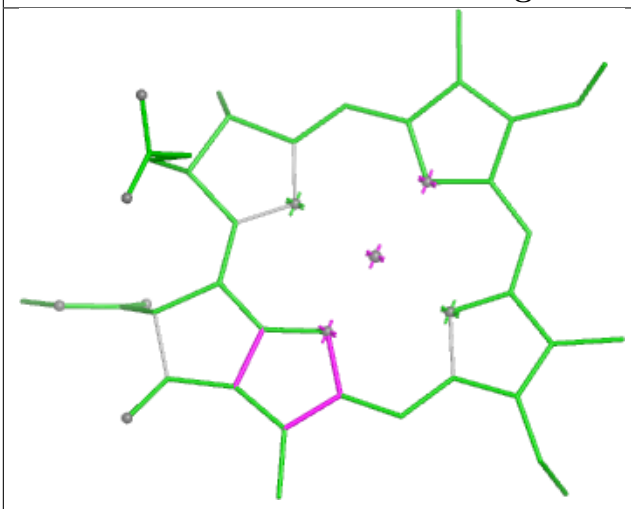


Rings

Ligand CLA A2 824



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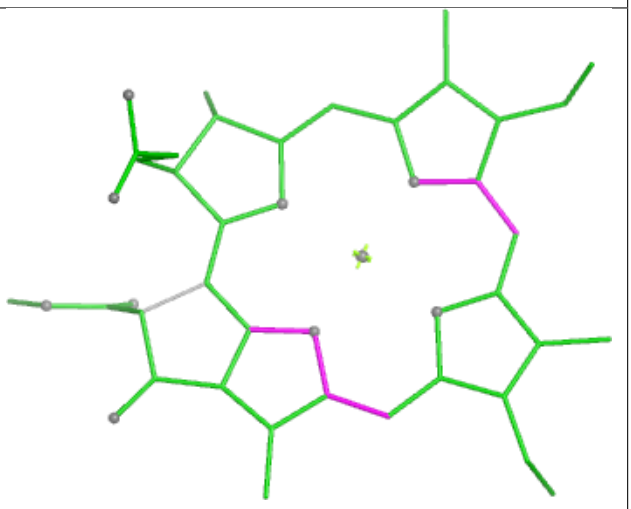
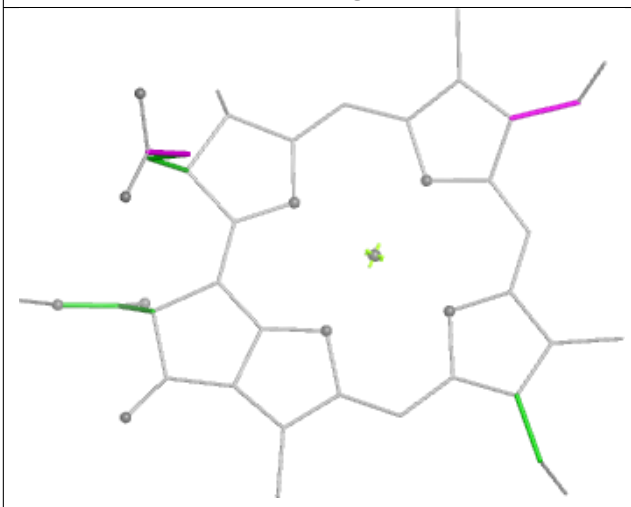


Bond angles



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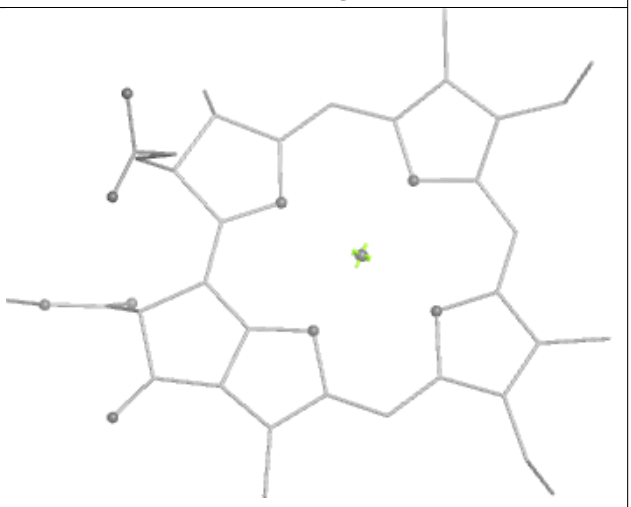
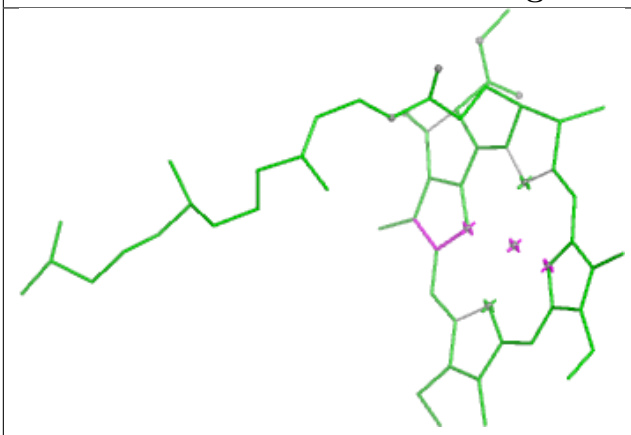


Rings

Ligand CLA Z 611



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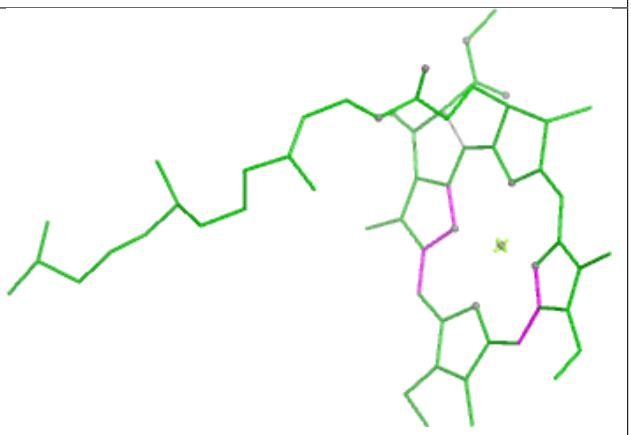
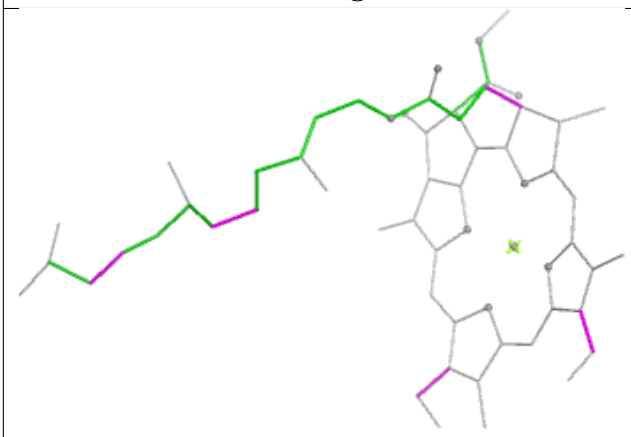


Bond angles

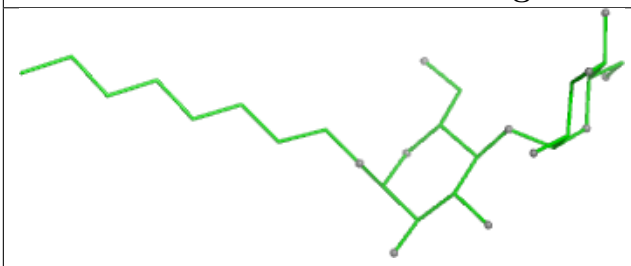


Torsions



Rings

Ligand LMU Z2 622



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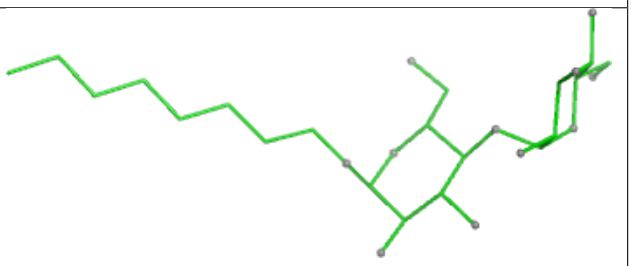
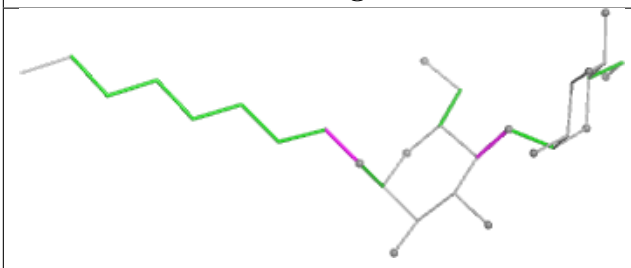


Bond angles



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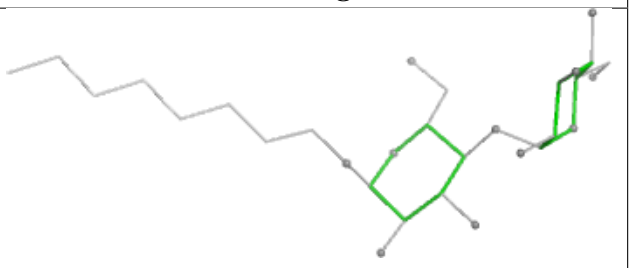
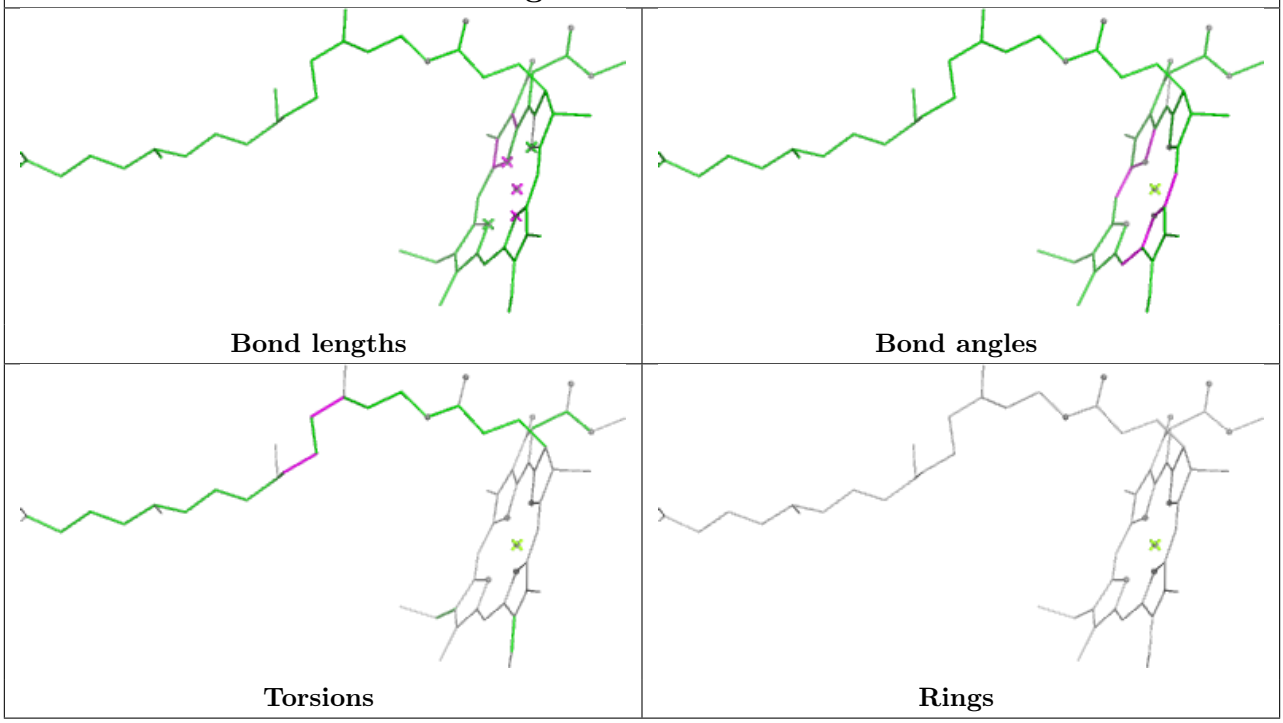
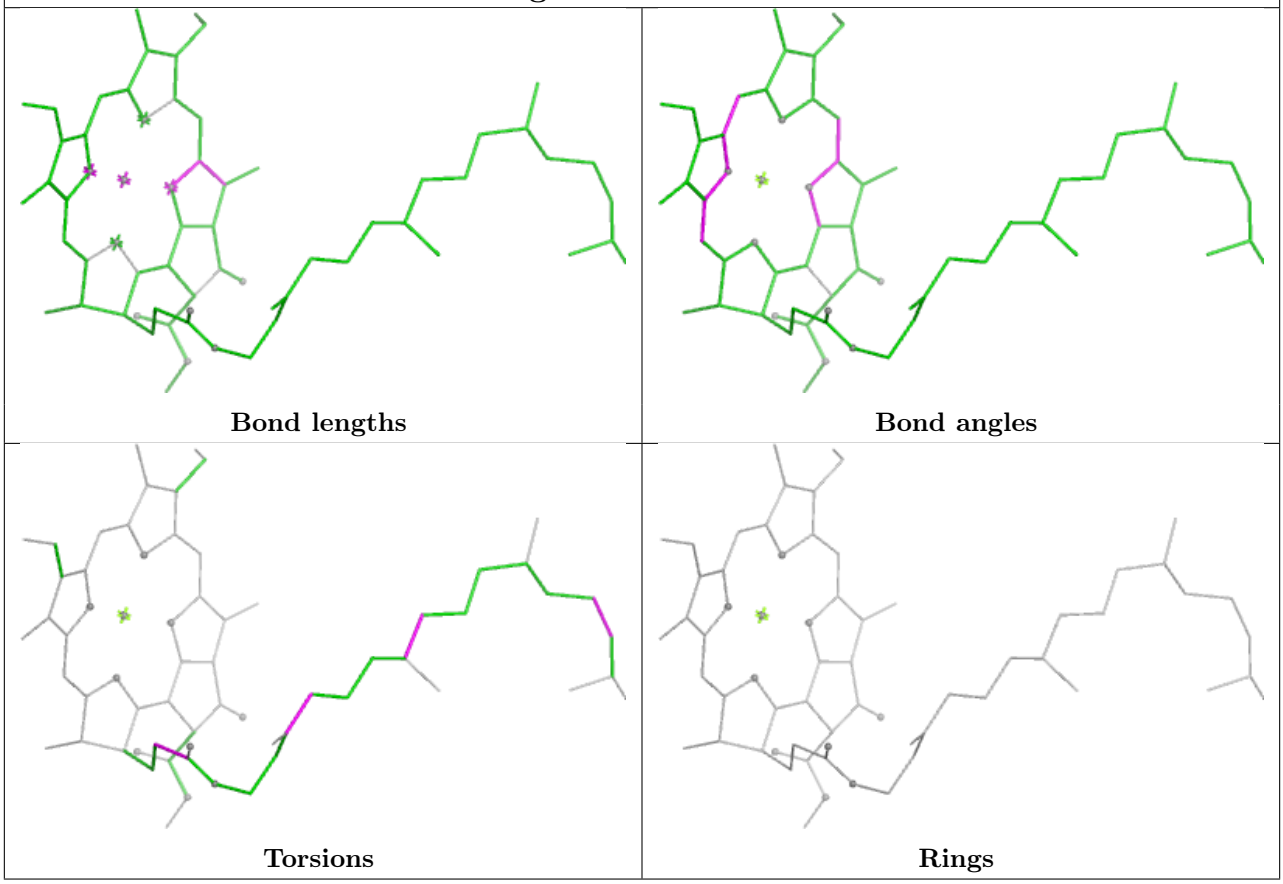


Rings

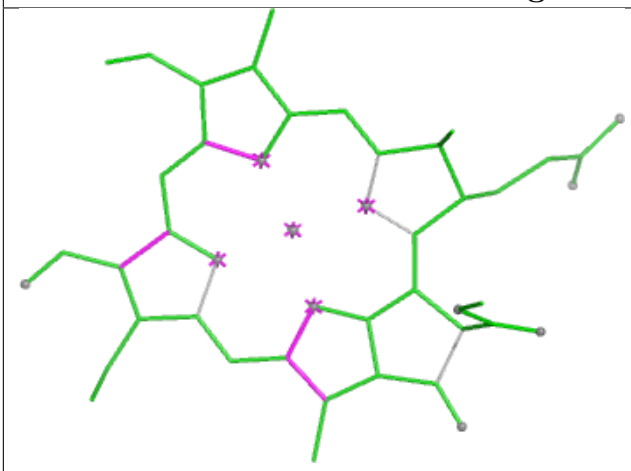
Ligand CLA B 829



Ligand CLA 1 609



Ligand CHL 4 618



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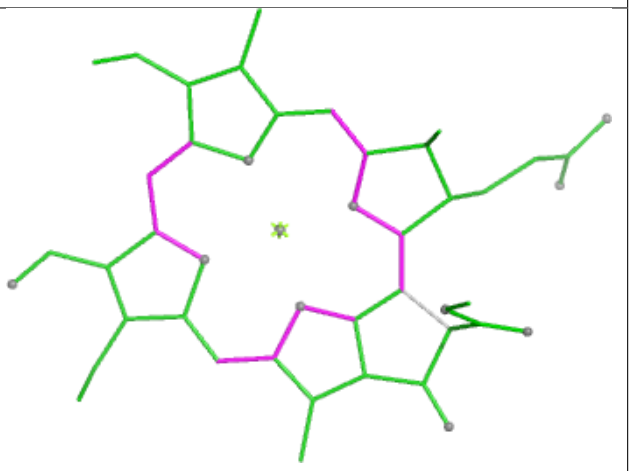
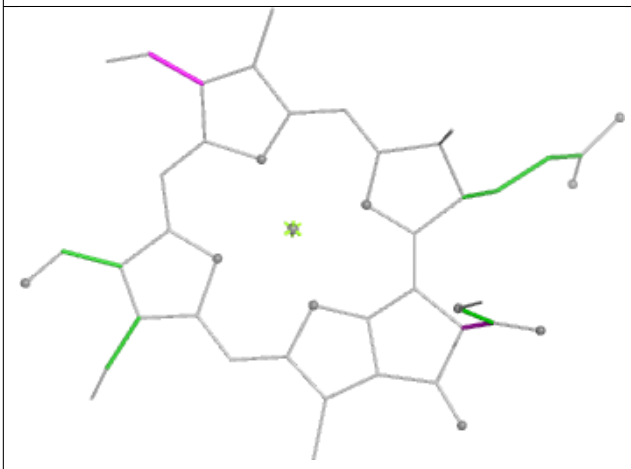


Bond angles



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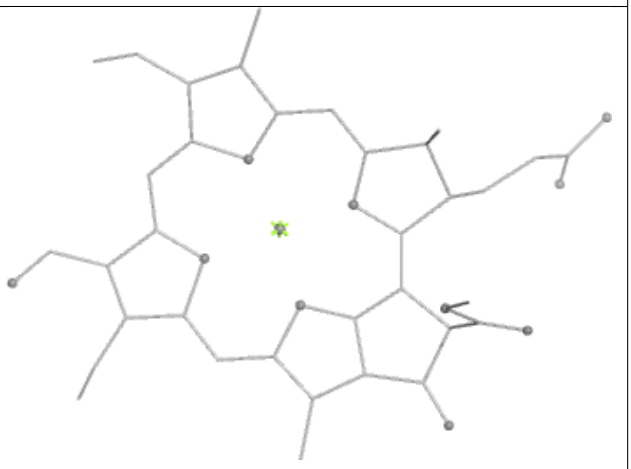
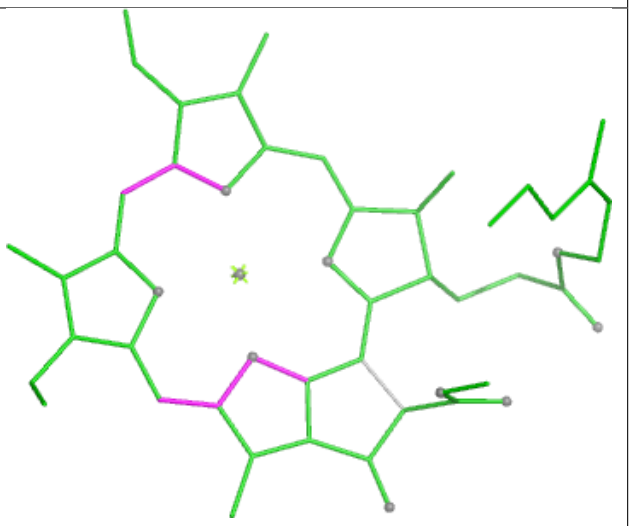


Rings

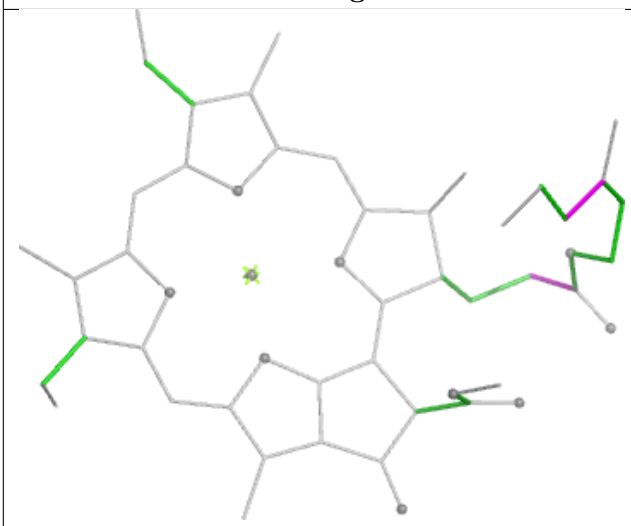
Ligand CLA 7 612



Bond lengths



Bond angles



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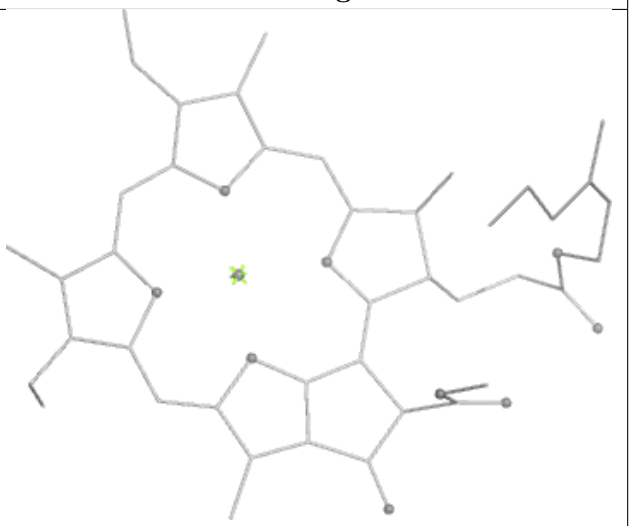
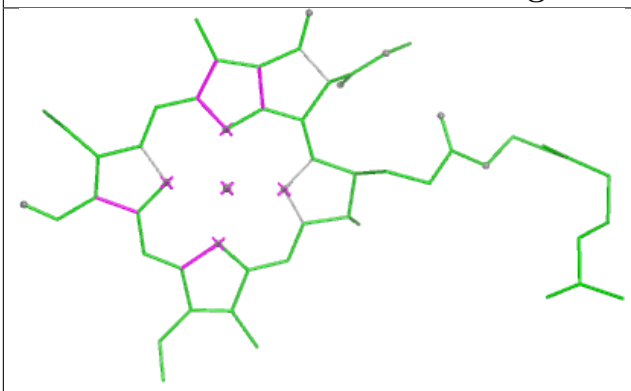


Rings

Ligand CHL 4 606



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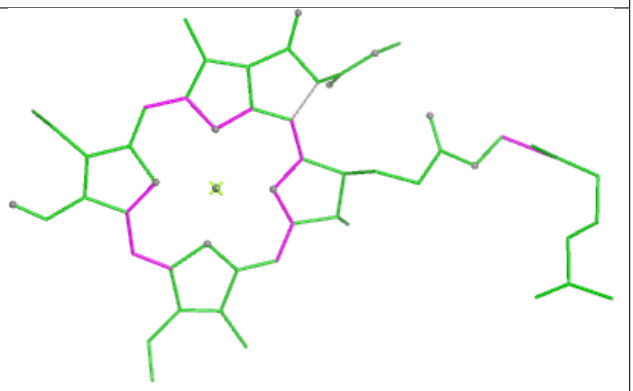
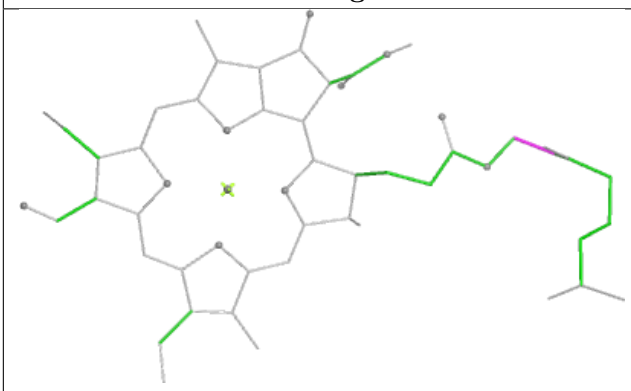


Bond angles



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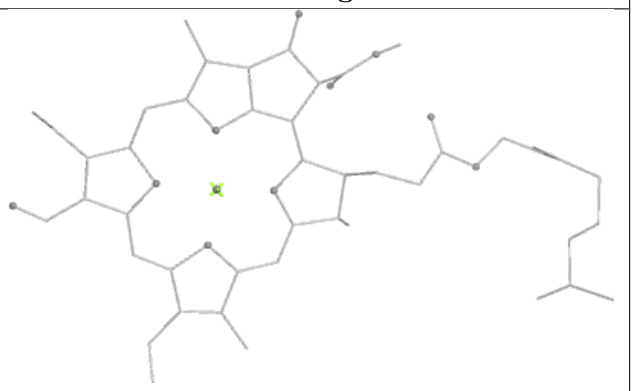
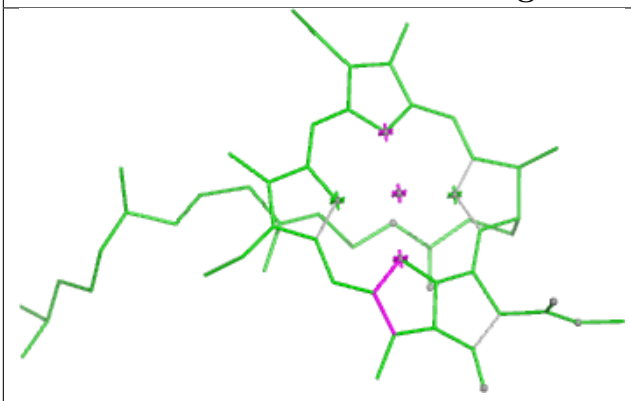


Rings

Ligand CLA Z2 616



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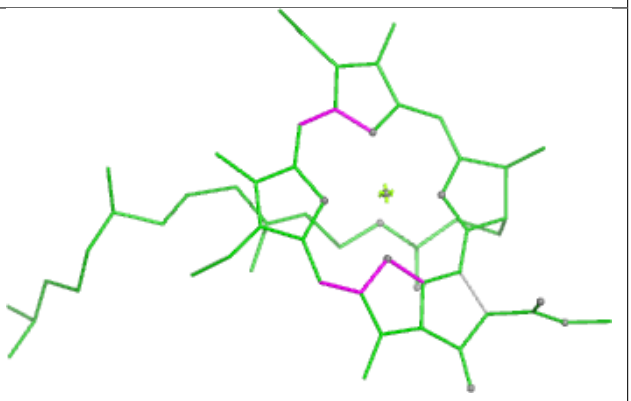
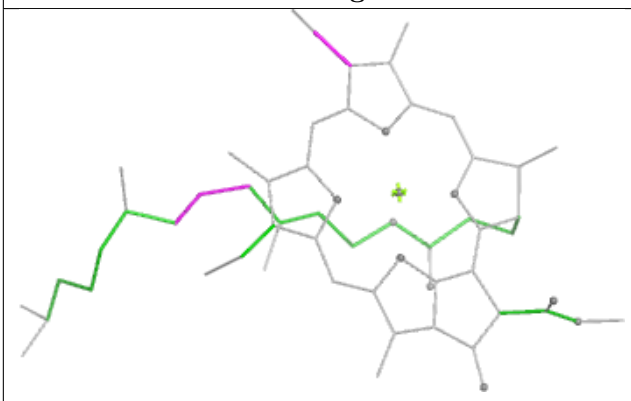


Bond angles



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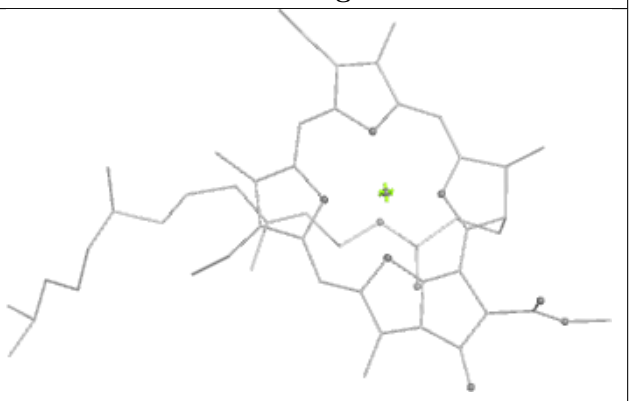
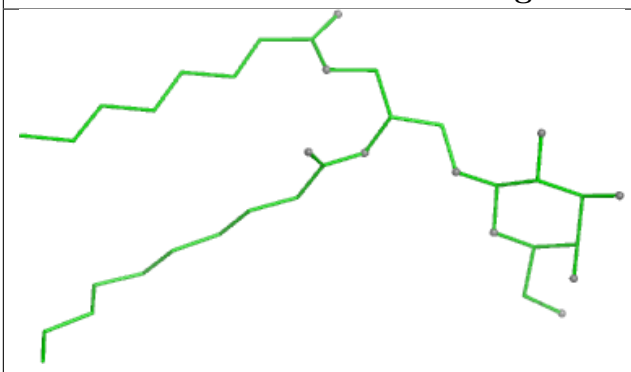


Rings

Ligand LMG 72 626



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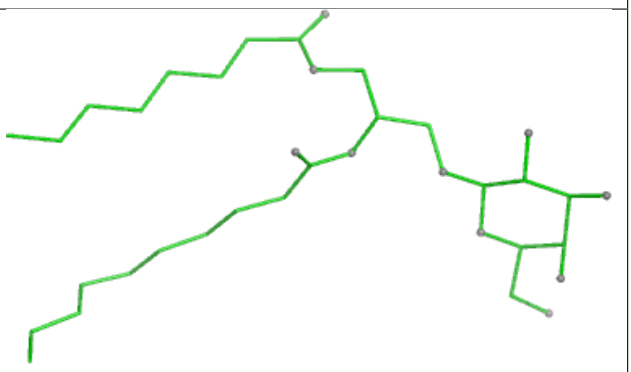
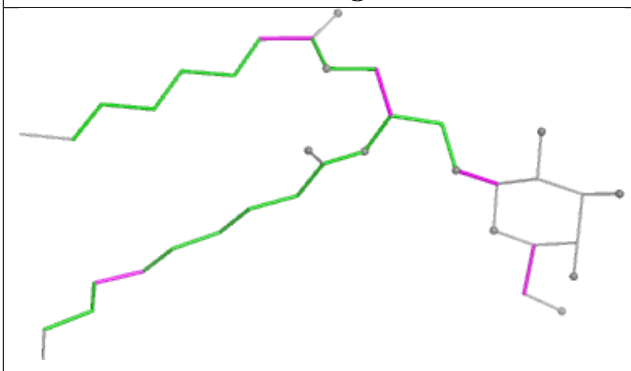


Bond angles



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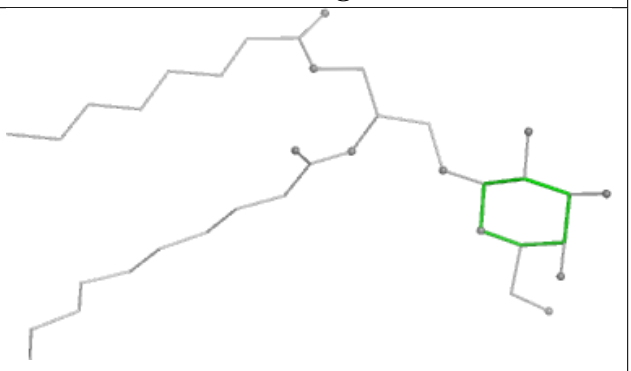
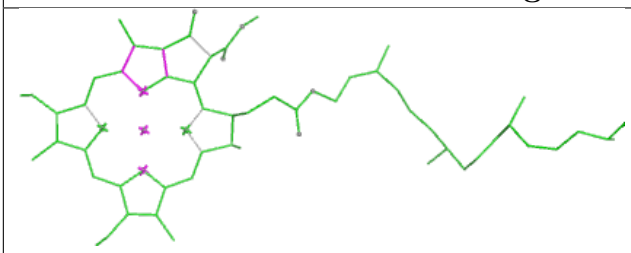
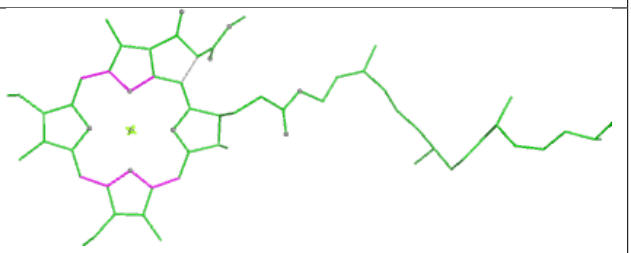


Rings

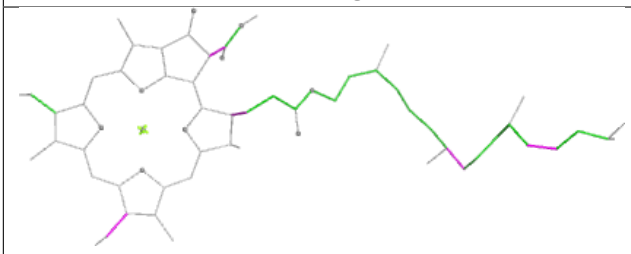
Ligand CLA A 834



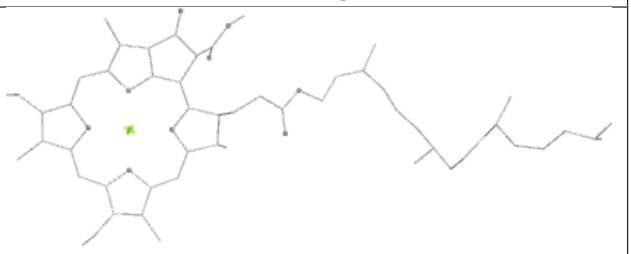
Bond lengths



Bond angles

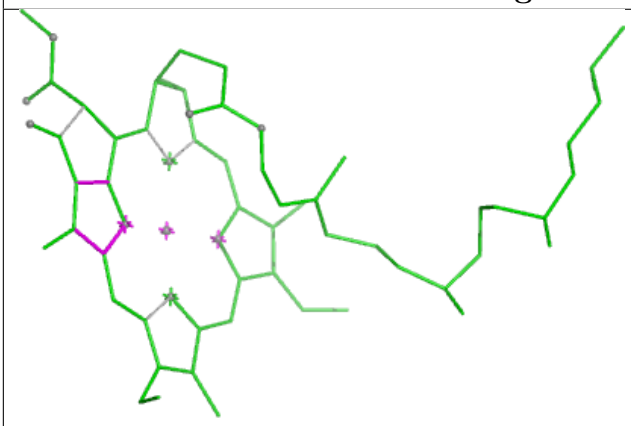


Torsions



Rings

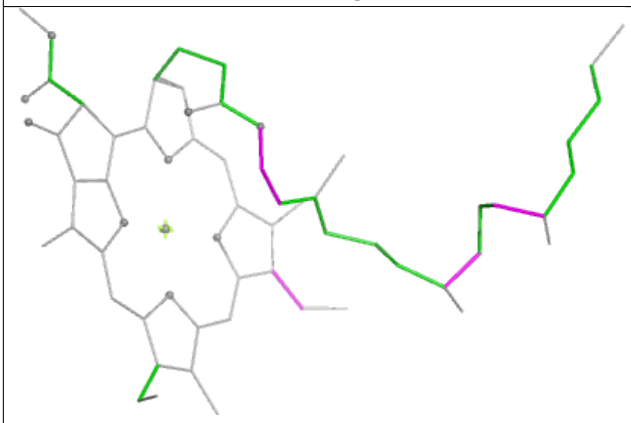
Ligand CLA A2 843



Bond lengths



Bond angles



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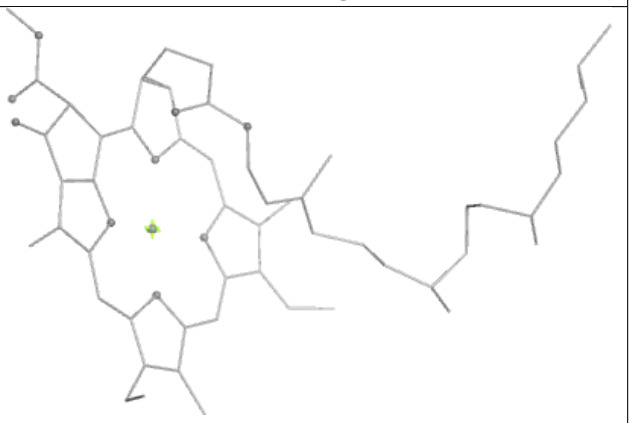
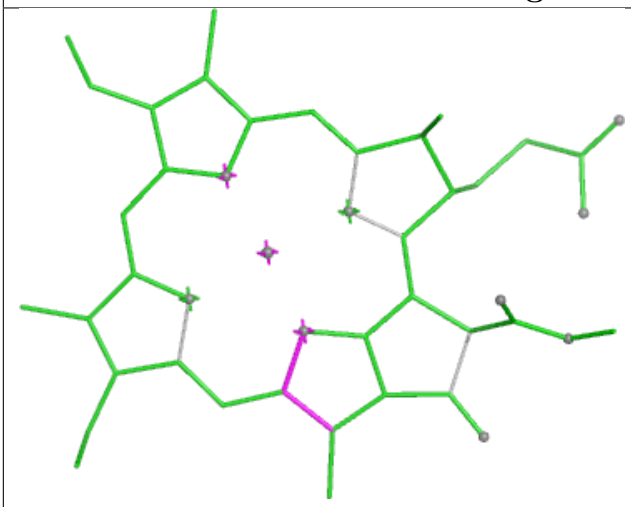


Rings

Ligand CLA F 303



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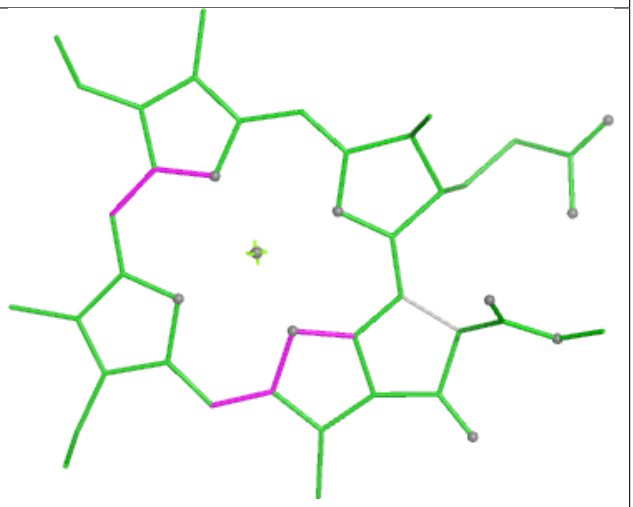
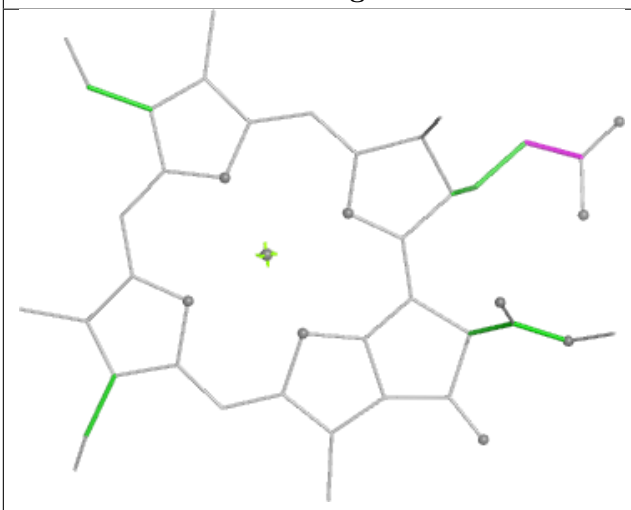


Bond angles



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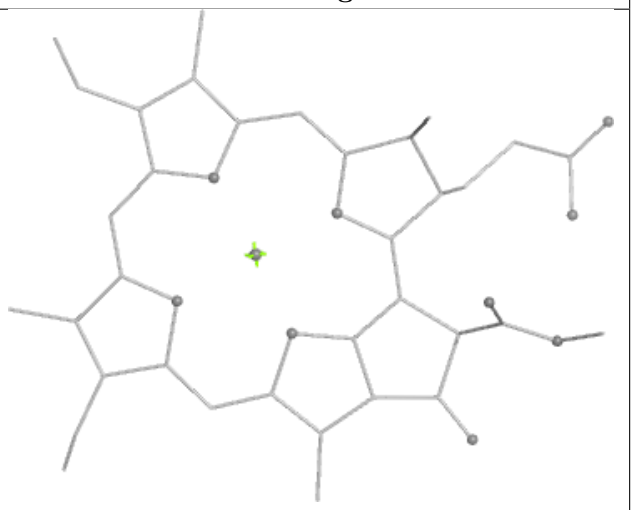
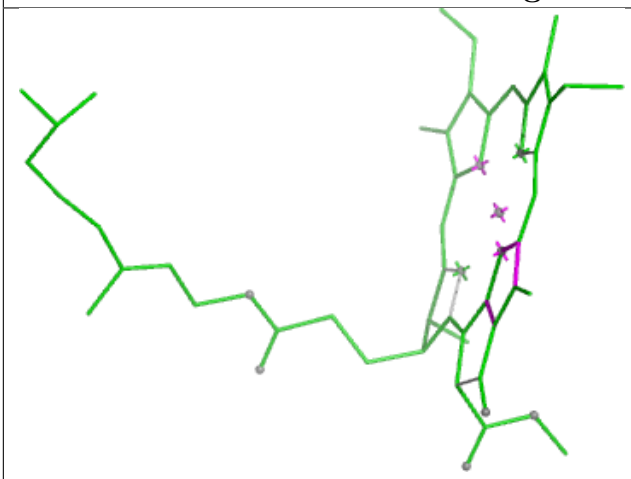


Rings

Ligand CLA A 832



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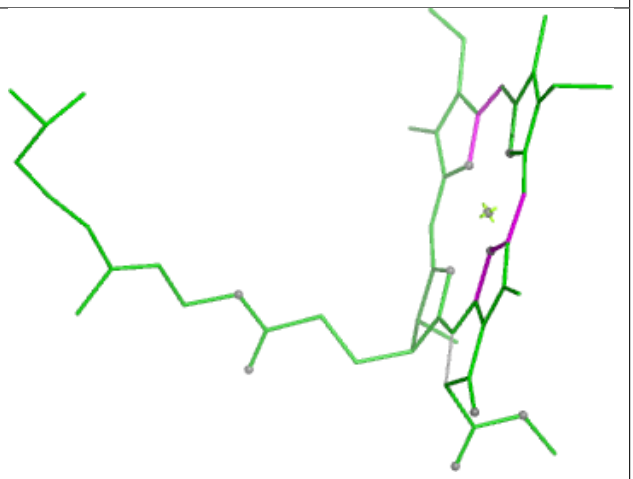
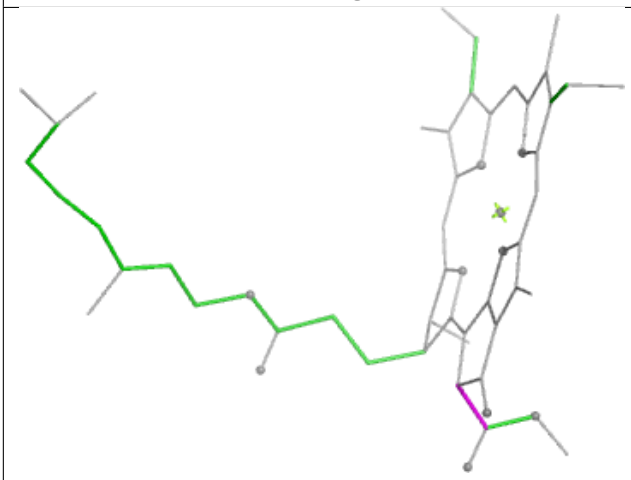


Bond angles



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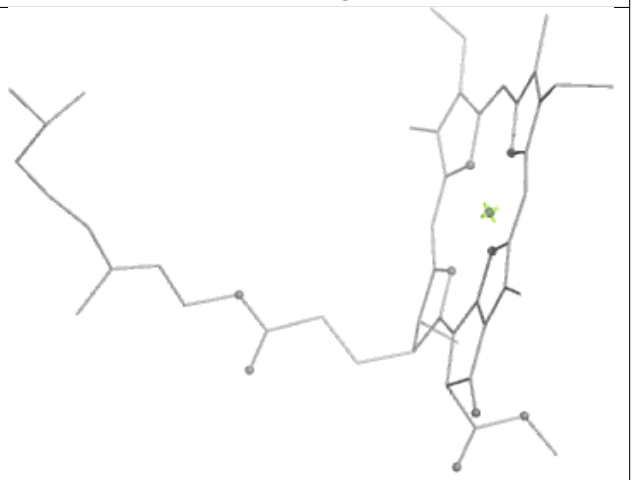
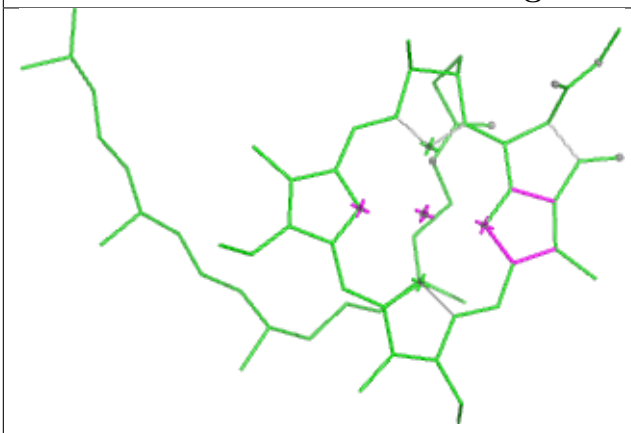
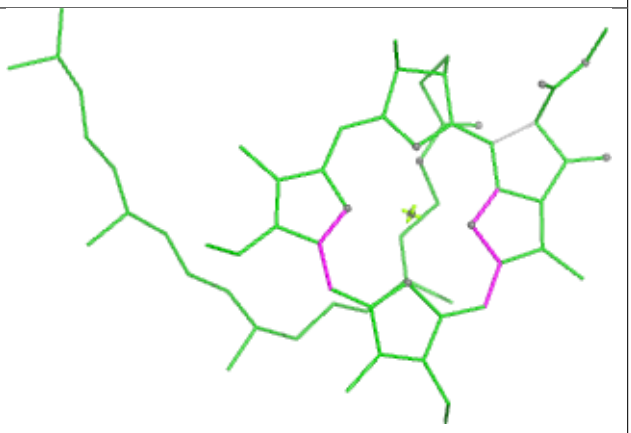


Rings

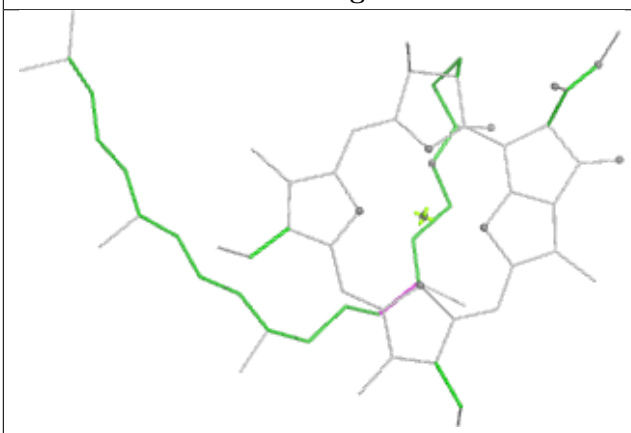
Ligand CLA B 812



Bond lengths



Bond angles



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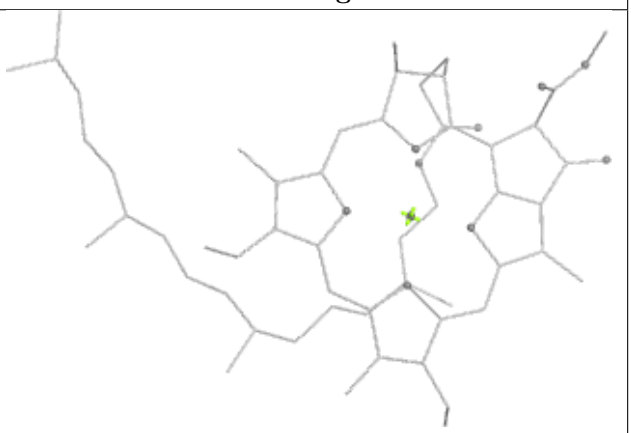


Rings

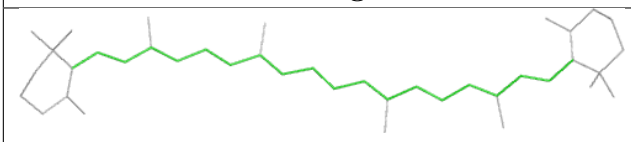
Ligand BCR B 844



Bond lengths



Bond angles



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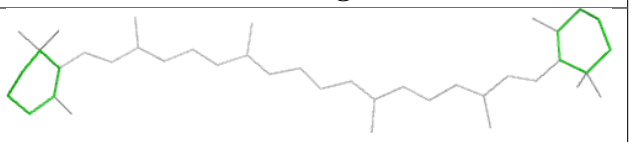
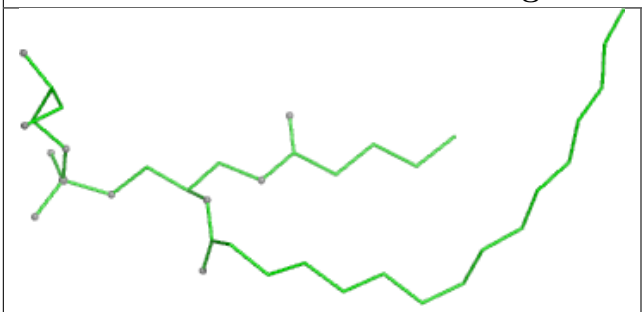


Rings

Ligand LHG A 847



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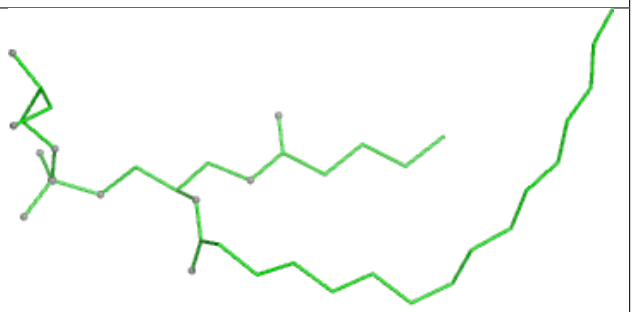
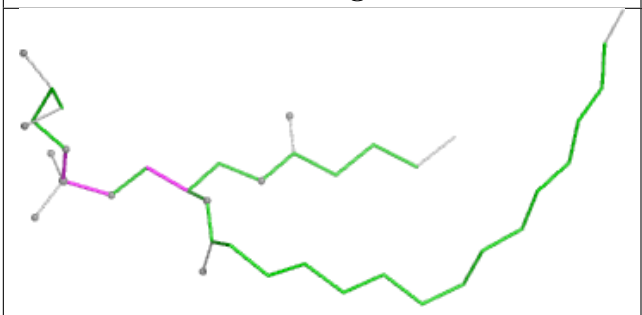


Bond angles



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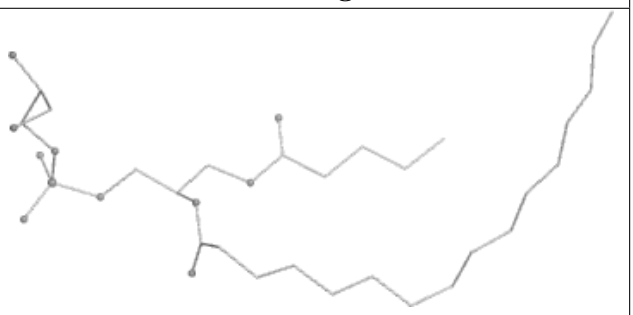
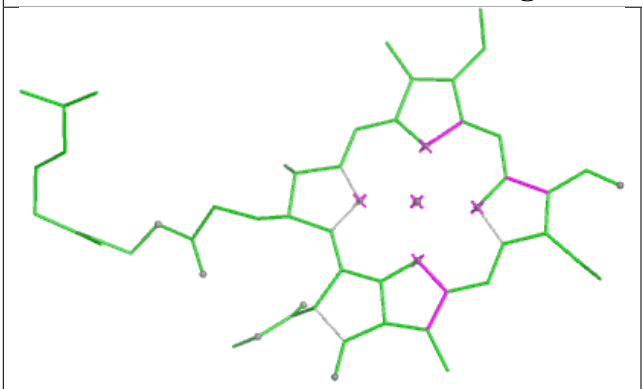


Rings

Ligand CHL 42 606



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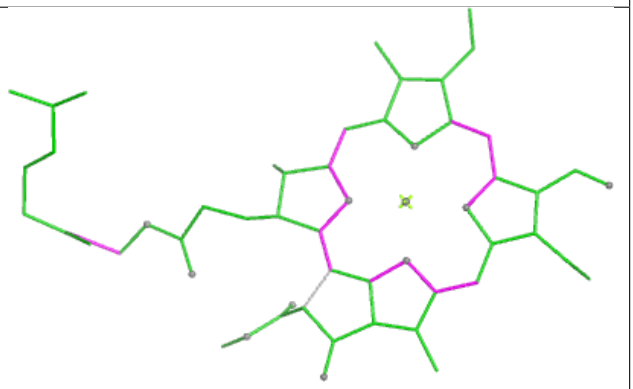
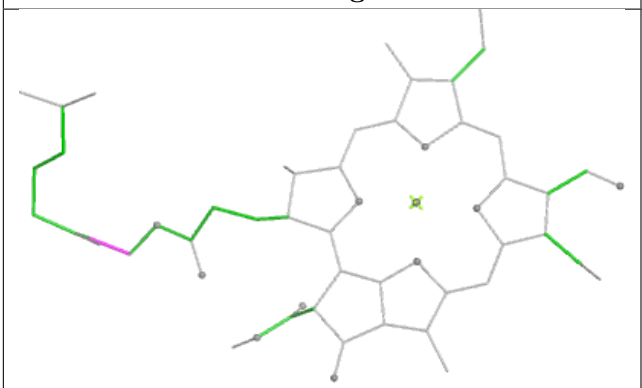


Bond angles



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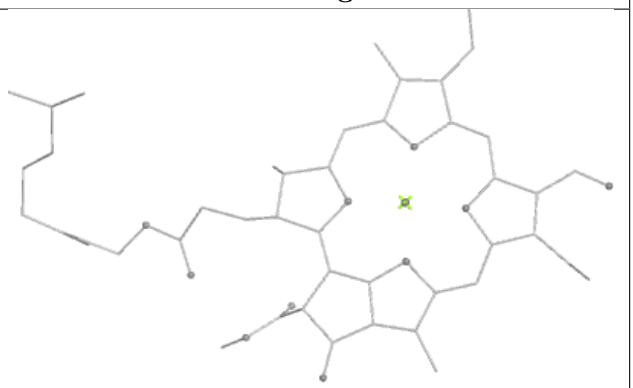
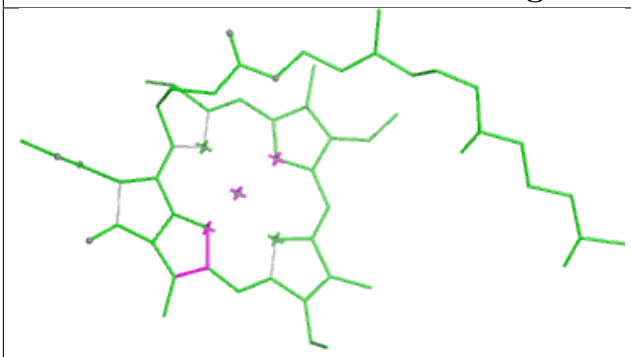


Rings

Ligand CLA Z 610



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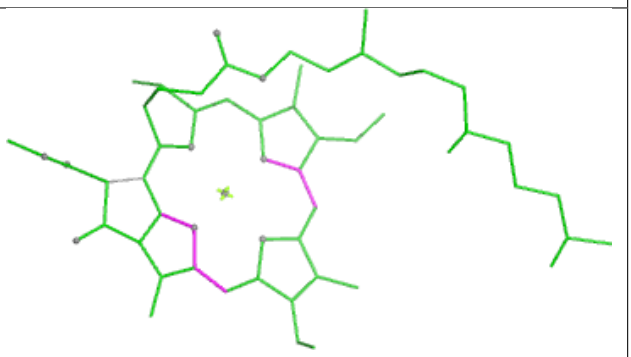
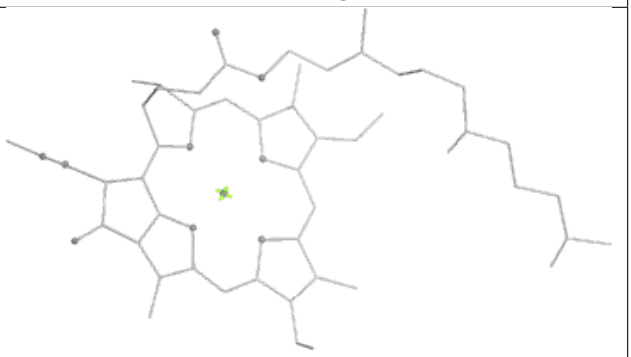


Bond angles

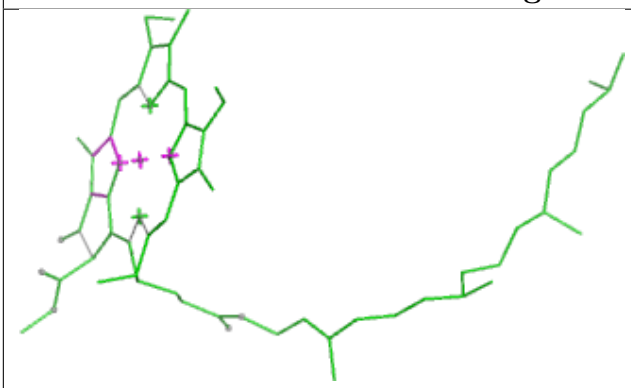


Torsions



Rings

Ligand CLA A 836



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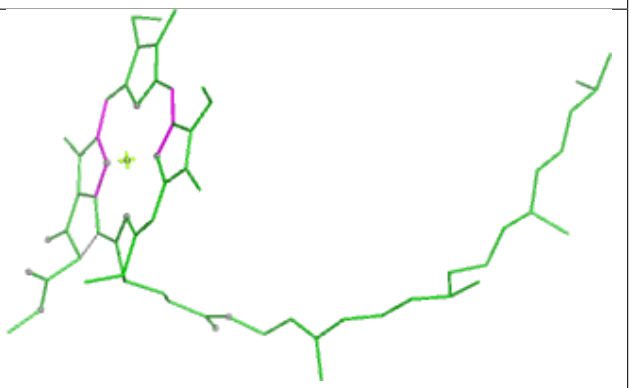
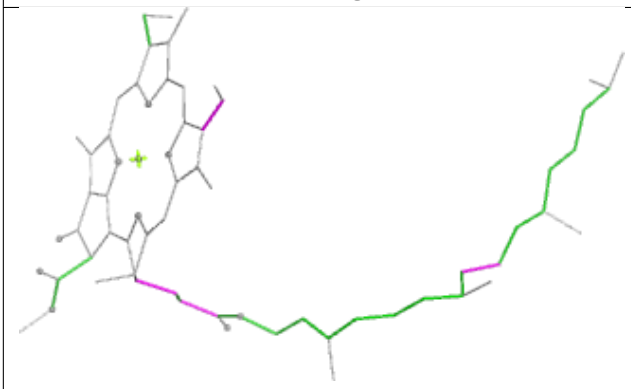


Bond angles

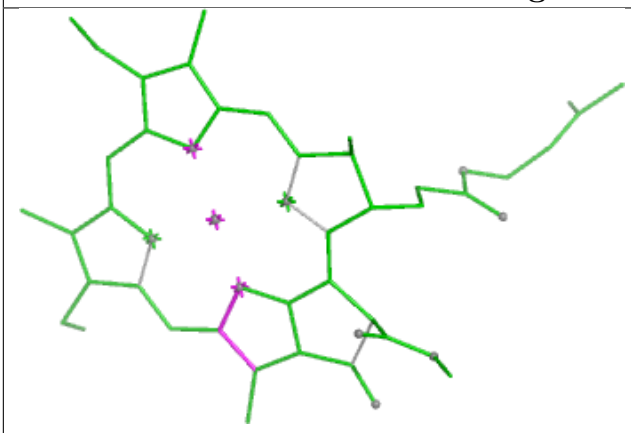


Torsions



Rings

Ligand CLA 8 608



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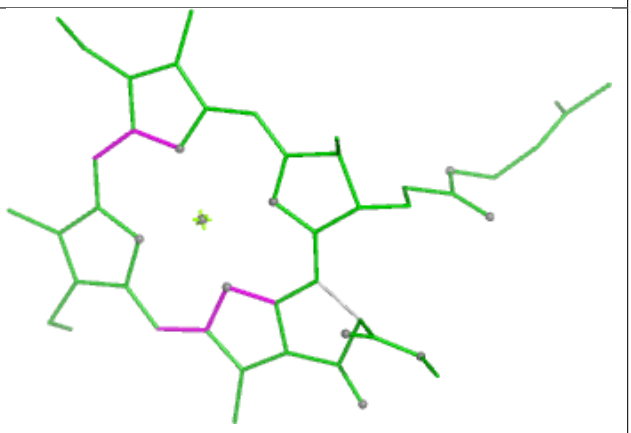
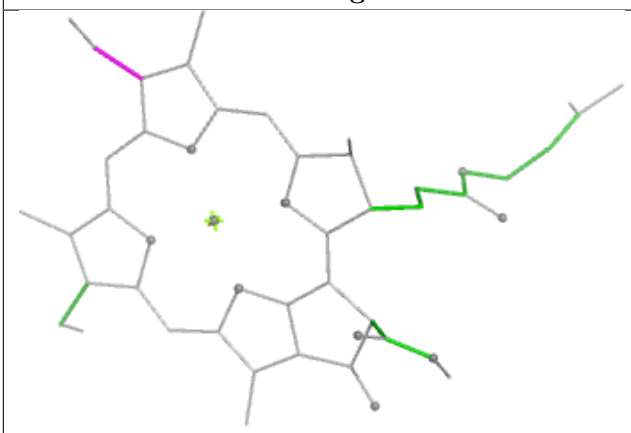


Bond angles



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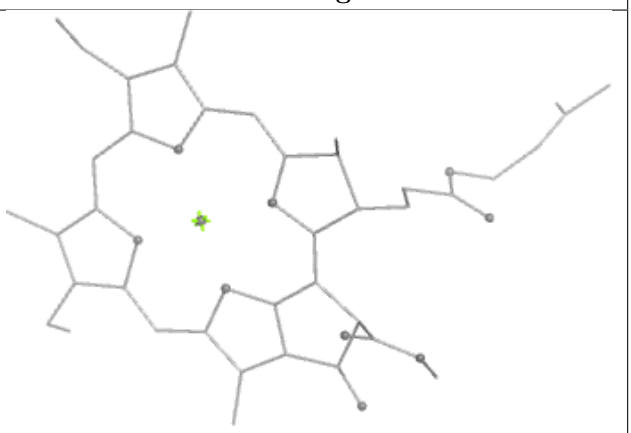
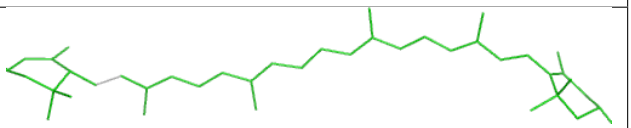


Rings

Ligand LUT 62 621



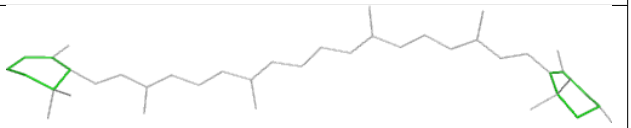
Bond lengths



Bond angles

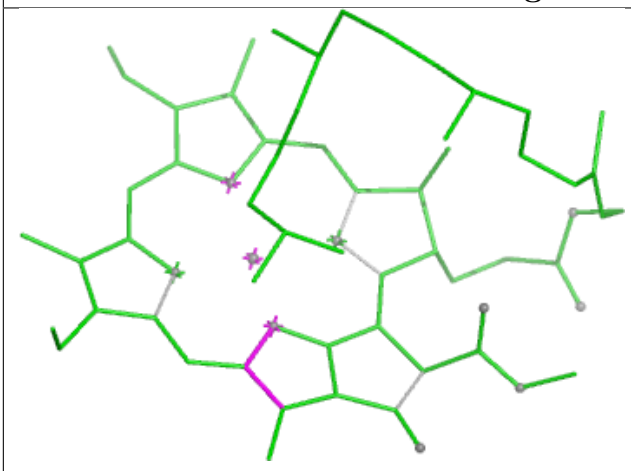


Torsions

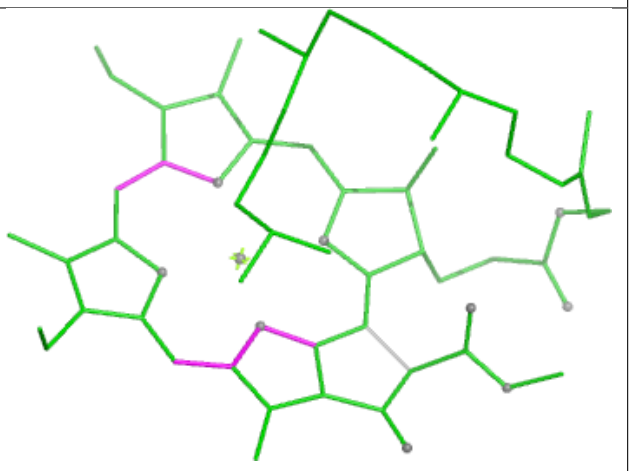


Rings

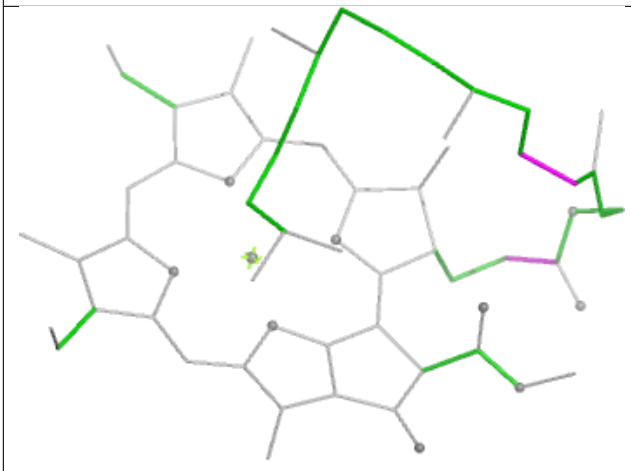
Ligand CLA B 806



Bond lengths



Bond angles



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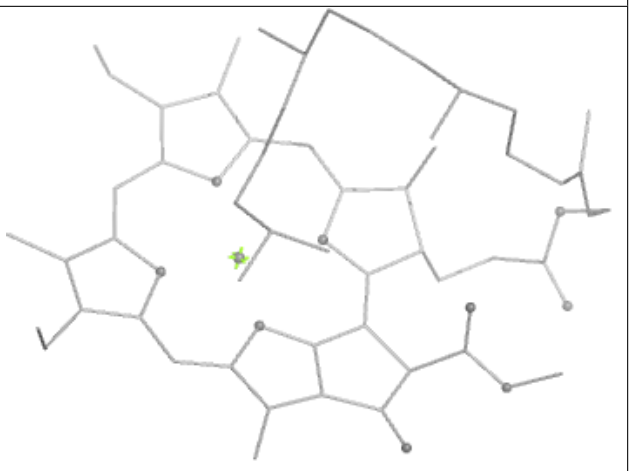
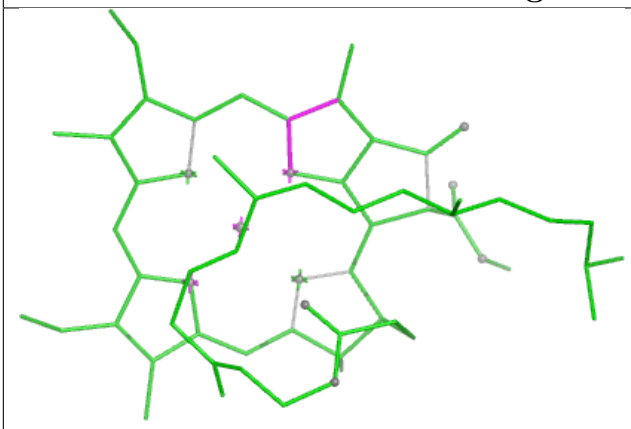


Rings

Ligand CLA F 304



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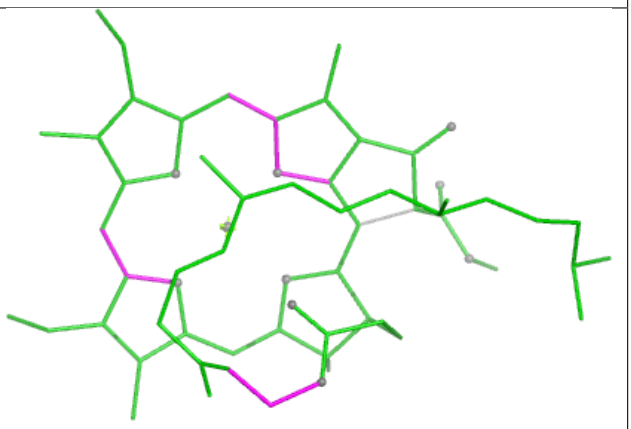
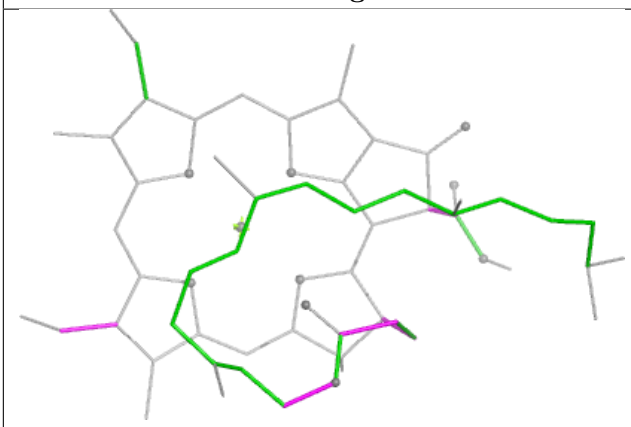


Bond angles



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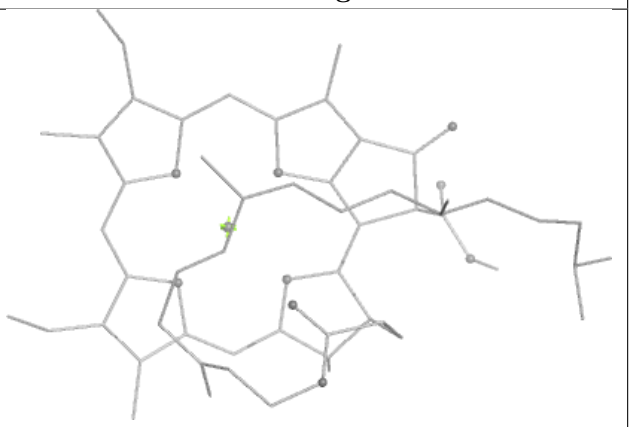
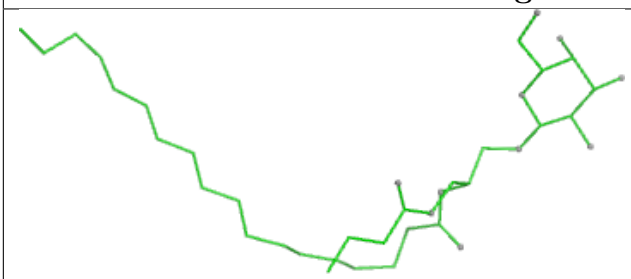


Rings

Ligand LMG 42 624



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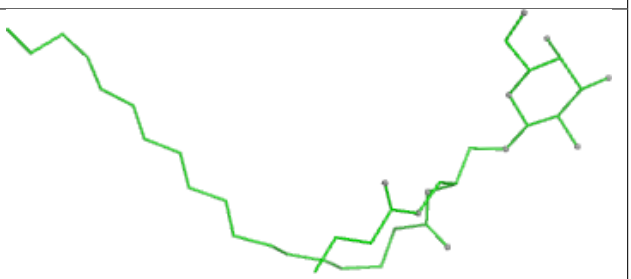
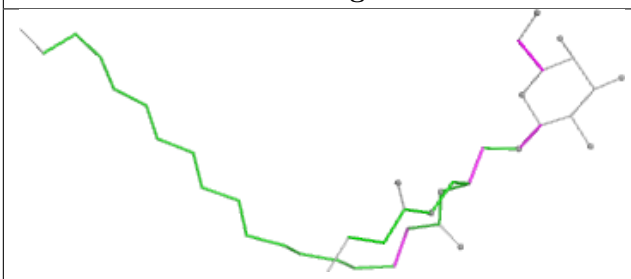


Bond angles



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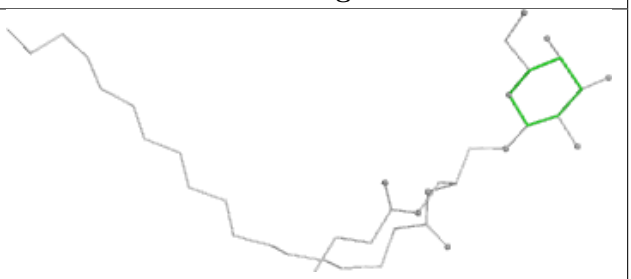
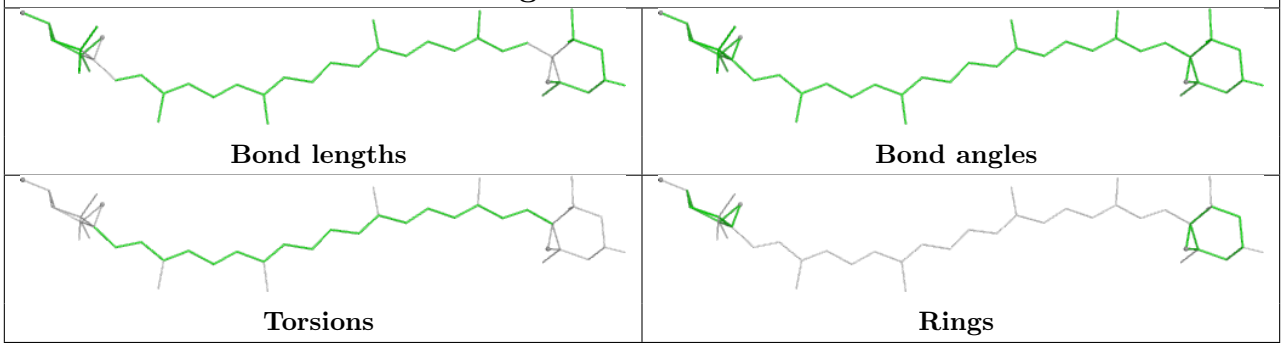


Rings

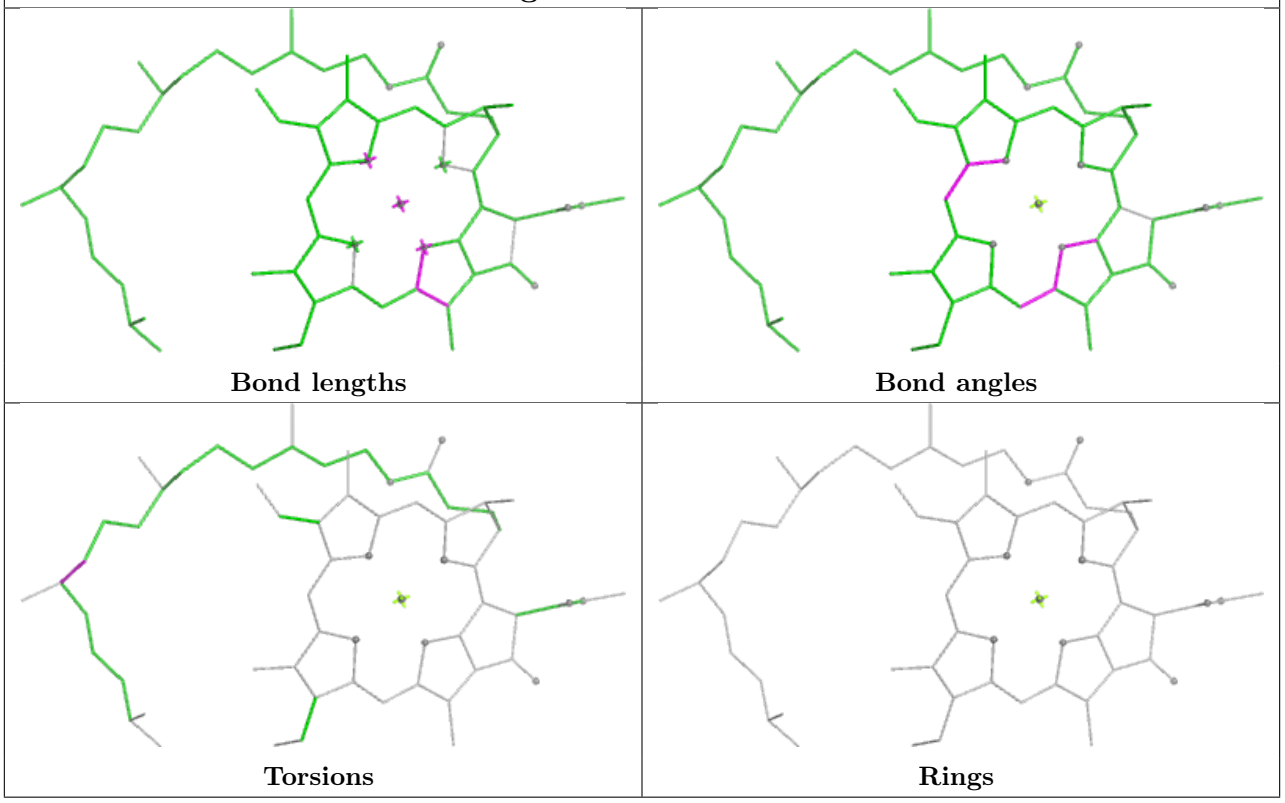
Ligand XAT 62 624



Bond lengths | Bond angles

Torsions | Rings

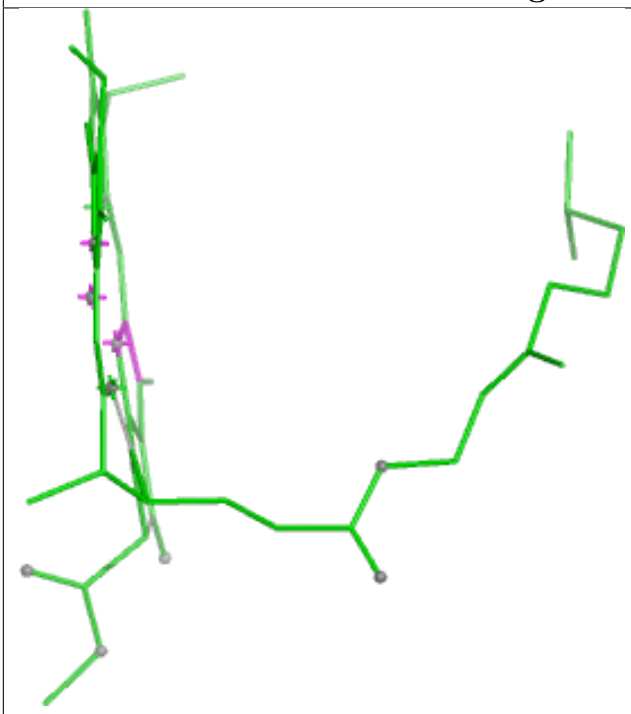
Ligand CLA 82 610



Bond lengths | Bond angles

Torsions | Rings

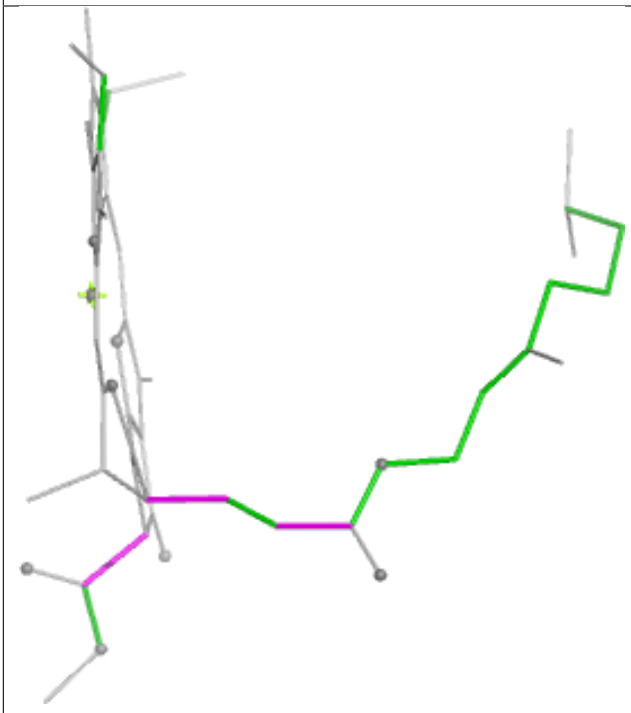
Ligand CLA 4 614



Bond lengths



Bond angles



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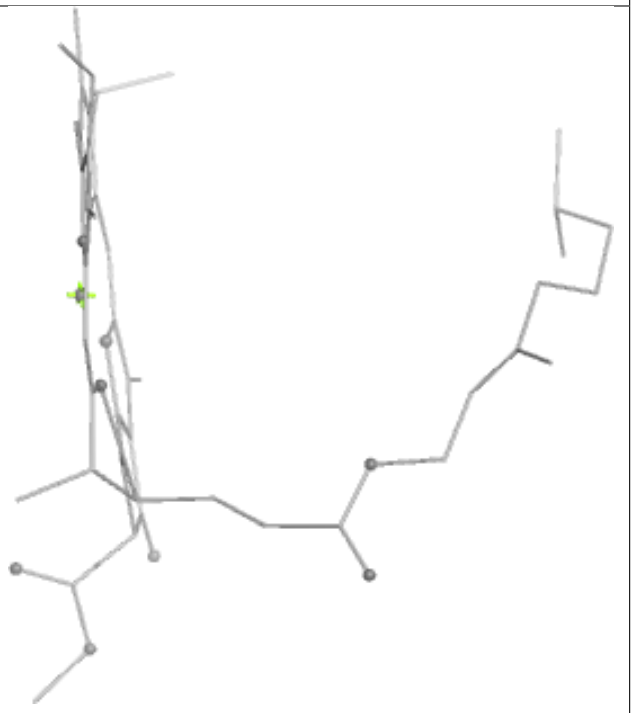
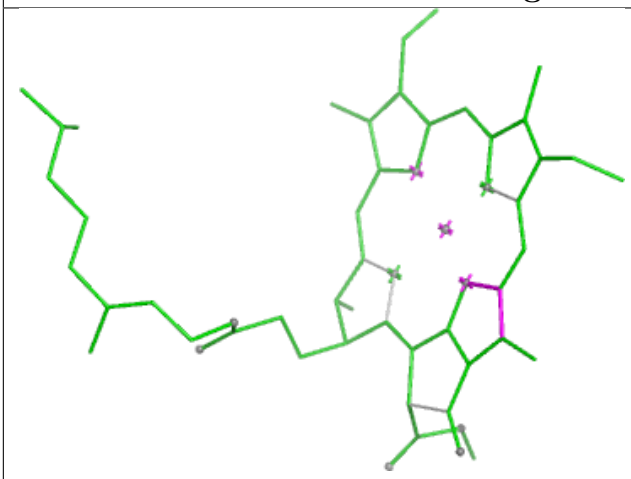
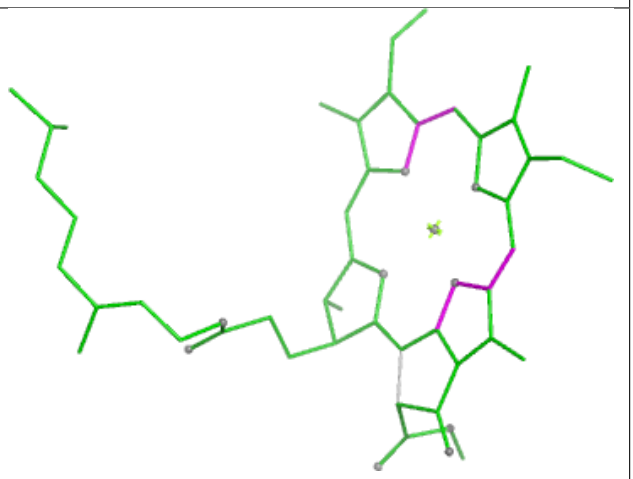


Rings

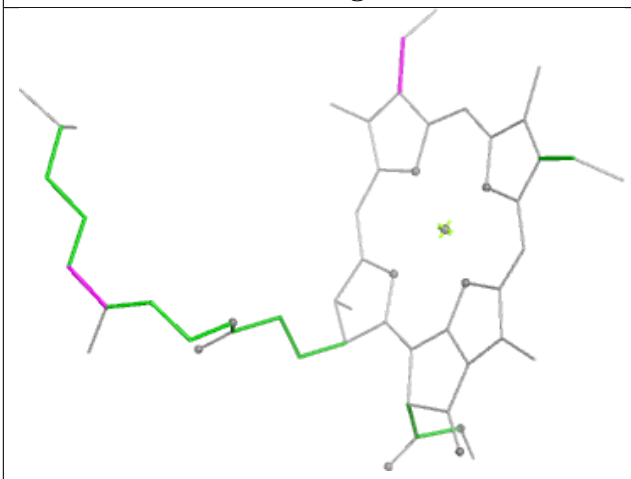
Ligand CLA A 821



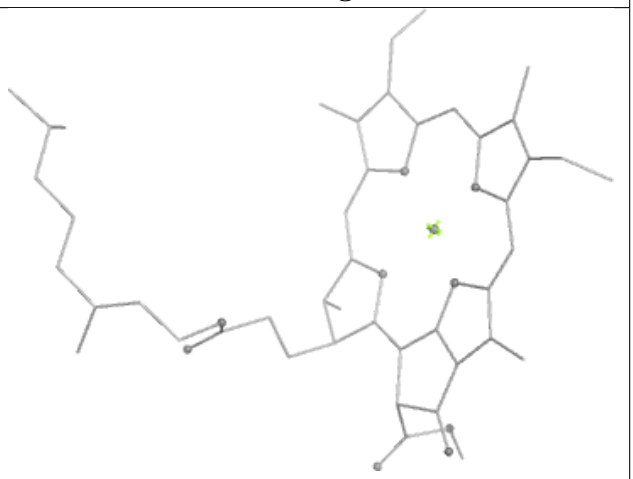
Bond lengths



Bond angles

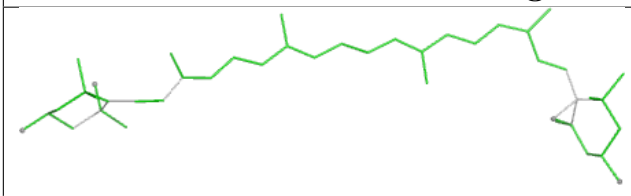


Torsions



Rings

Ligand NEX 6 625



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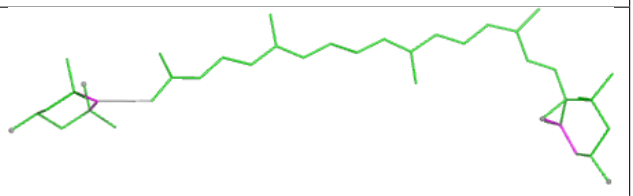
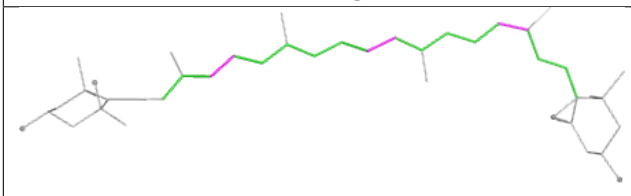


Bond angles



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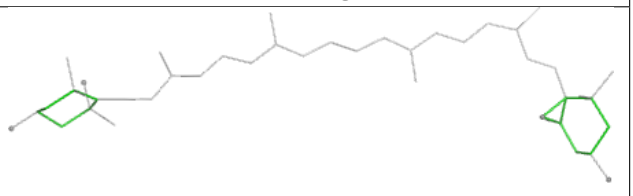
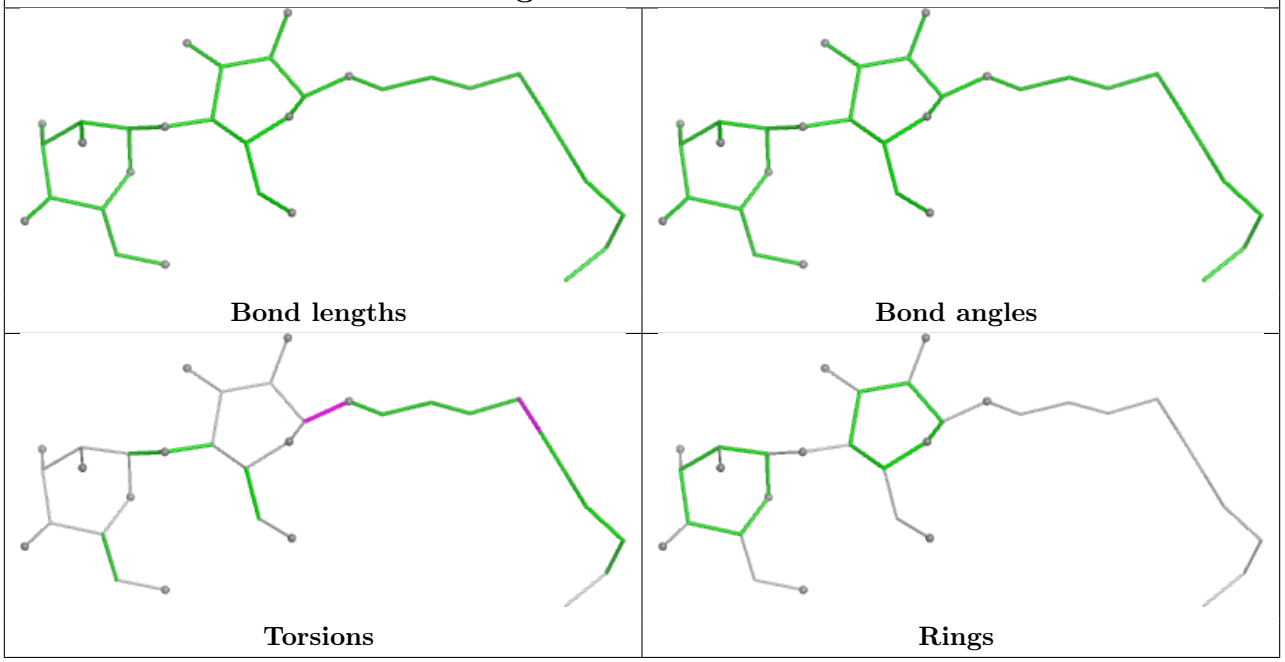
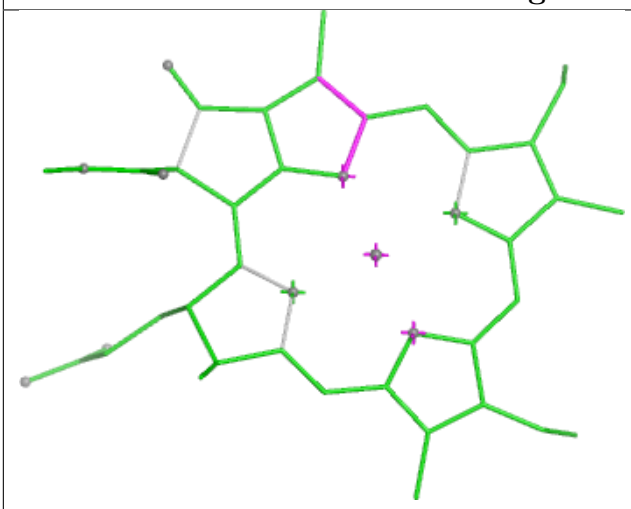


Rings

Ligand LMU 42 625



Ligand CLA 3 614



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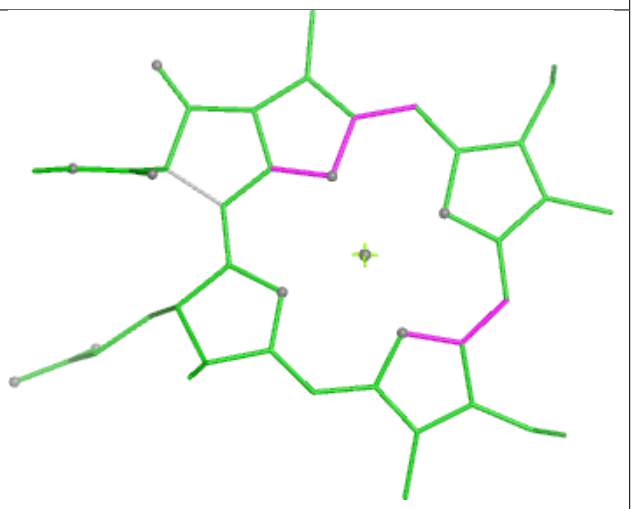
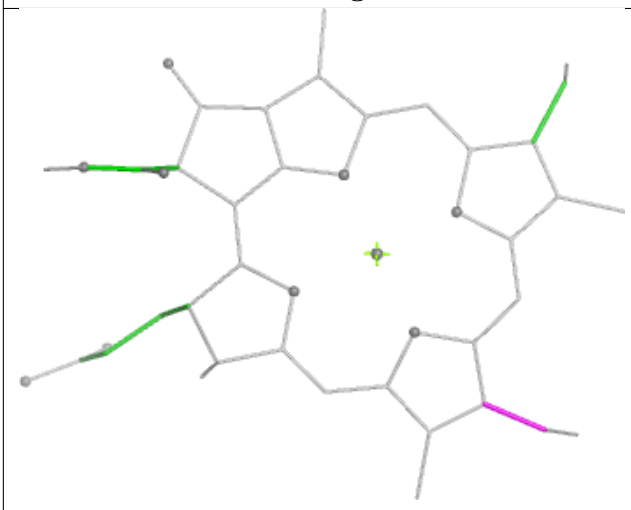


Bond angles



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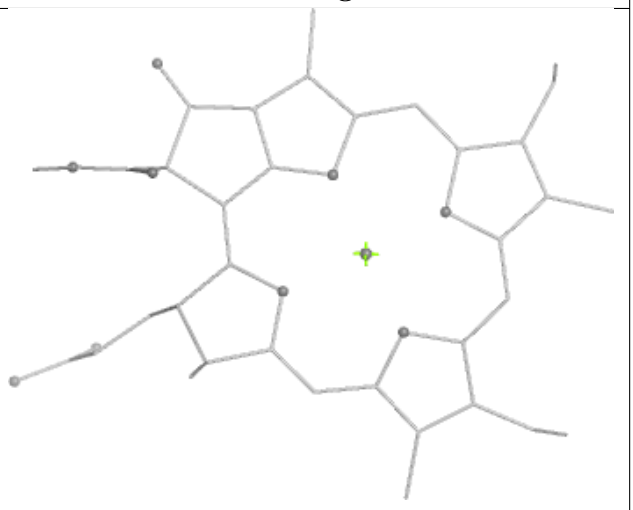
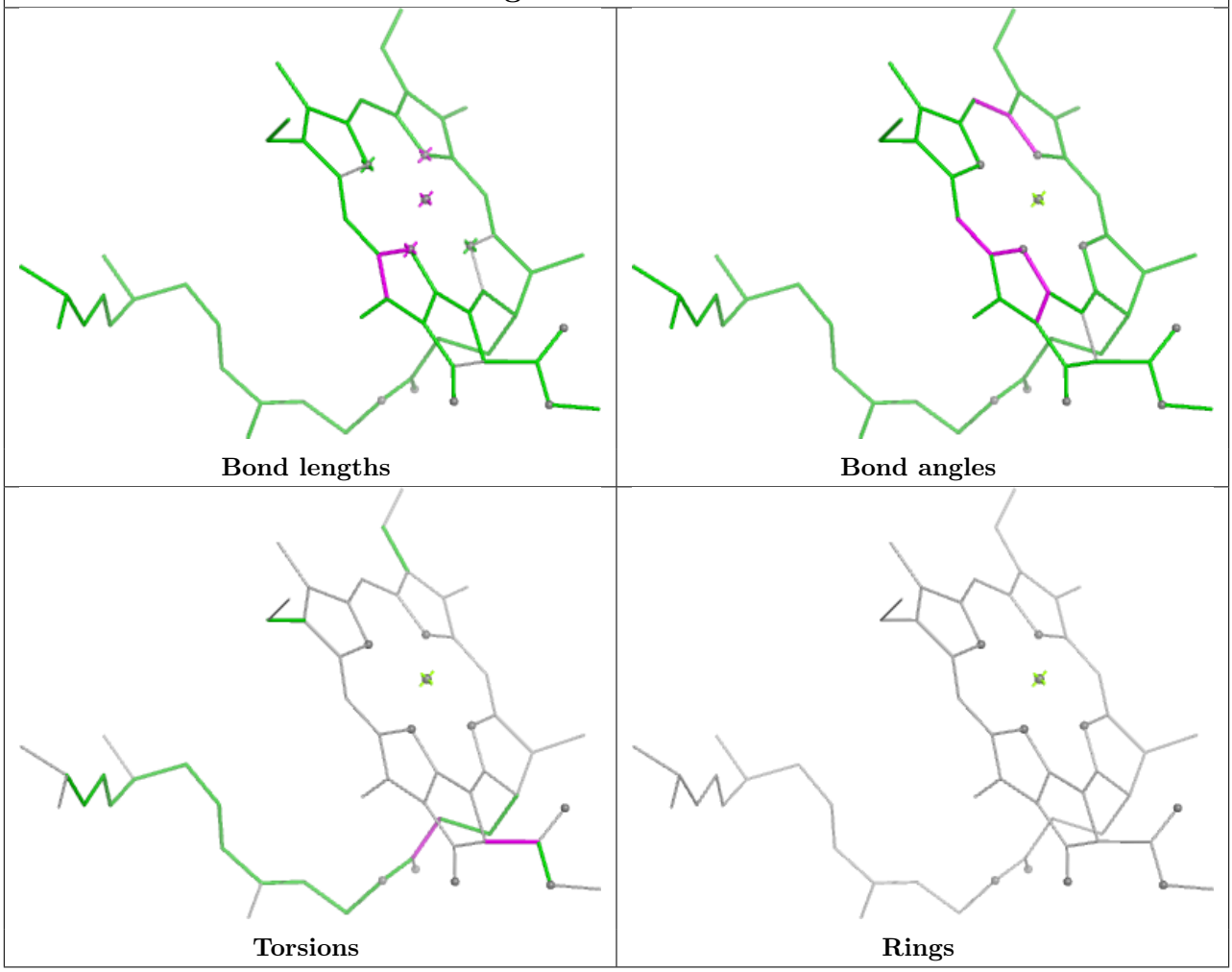
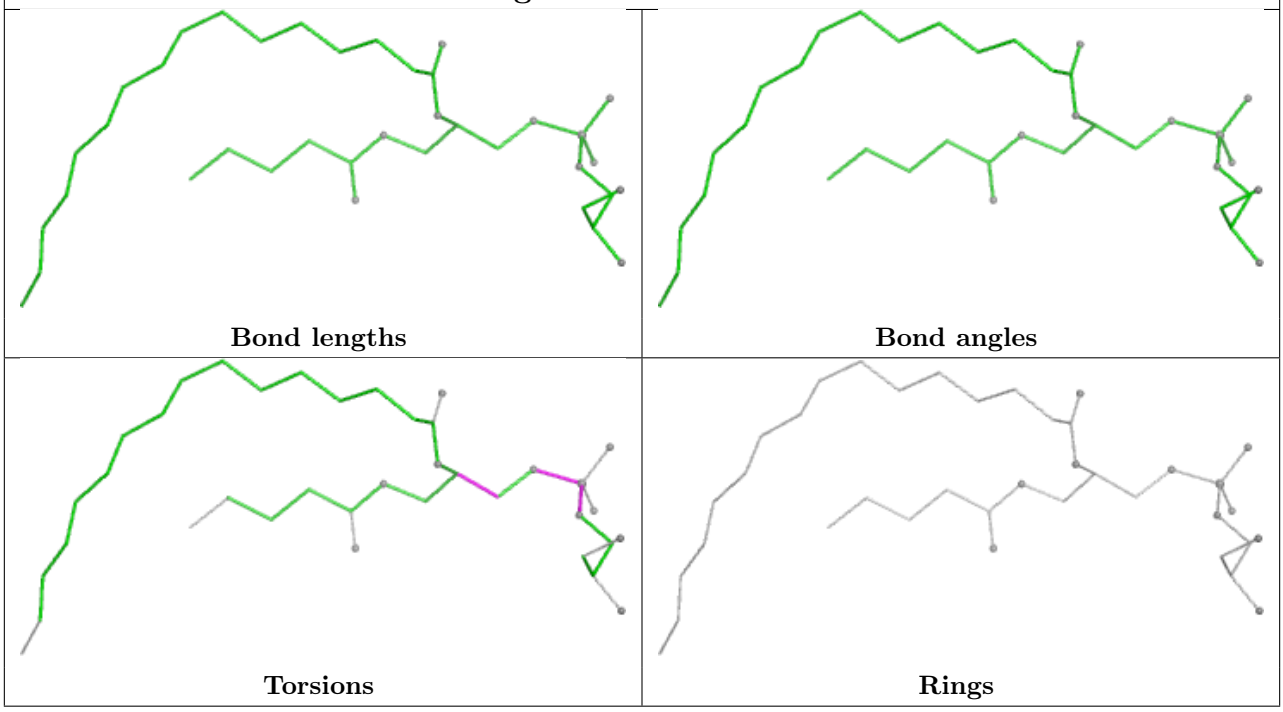


Rings

Ligand CLA B 814



Ligand LHG A2 847



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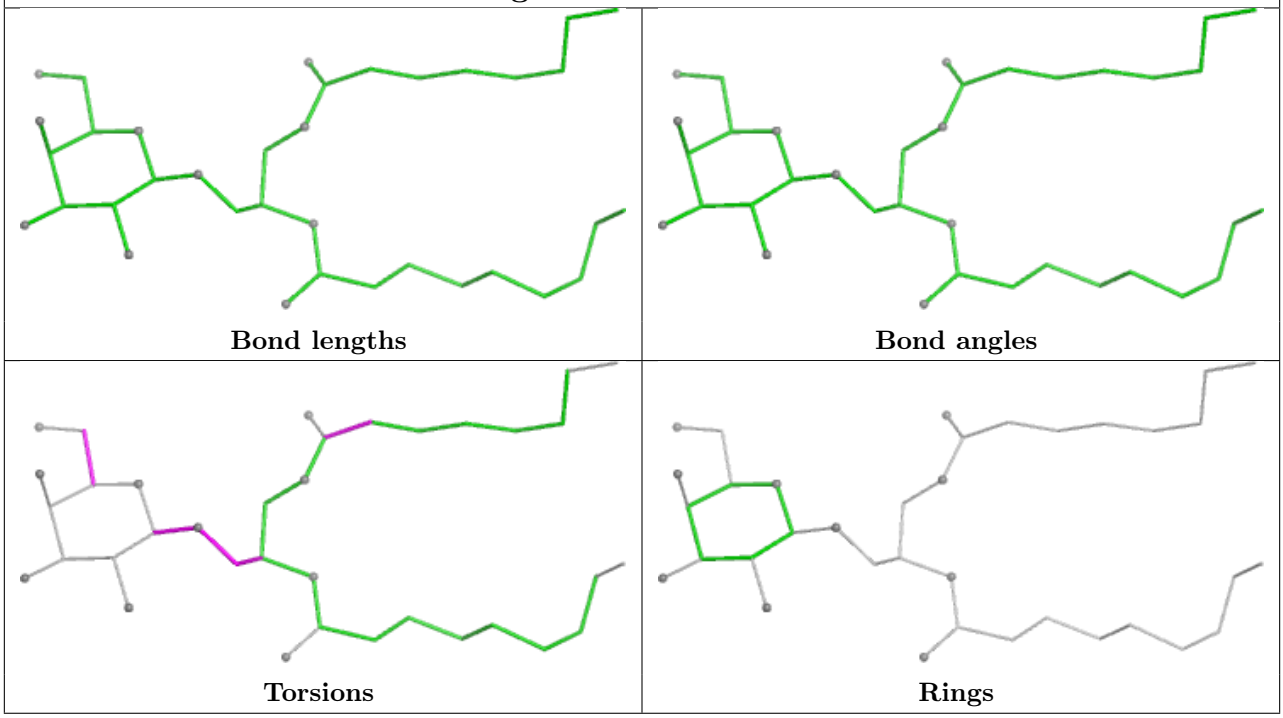
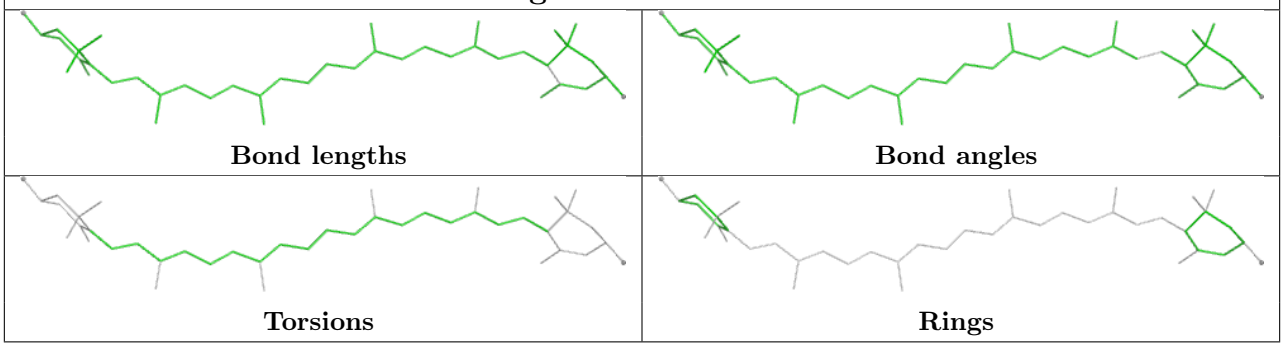
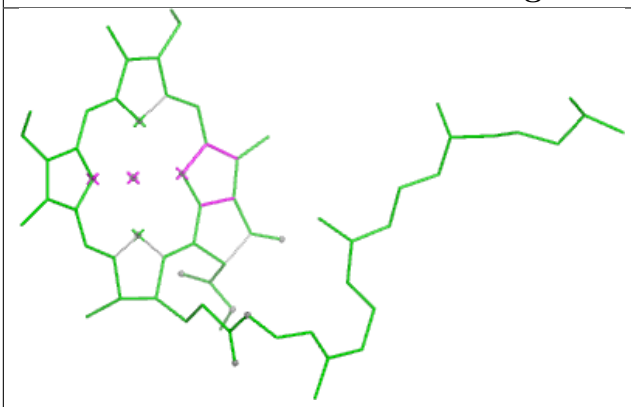


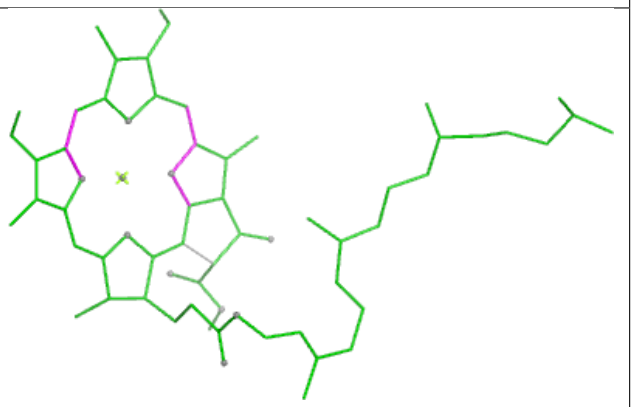
Ligand LUT 9 617



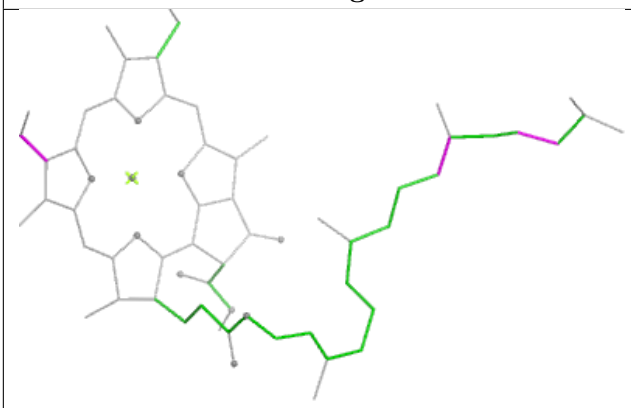
Ligand CLA B 832



Bond lengths



Bond angles



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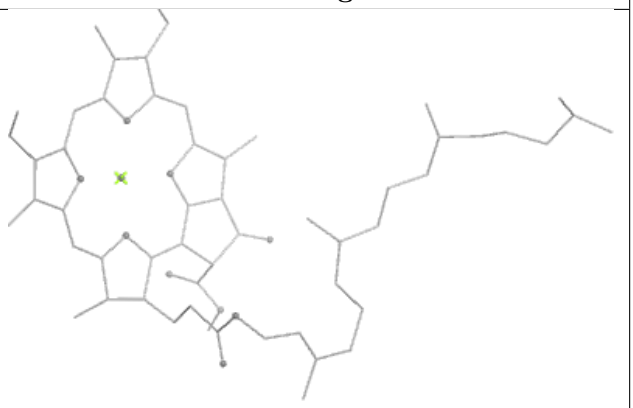
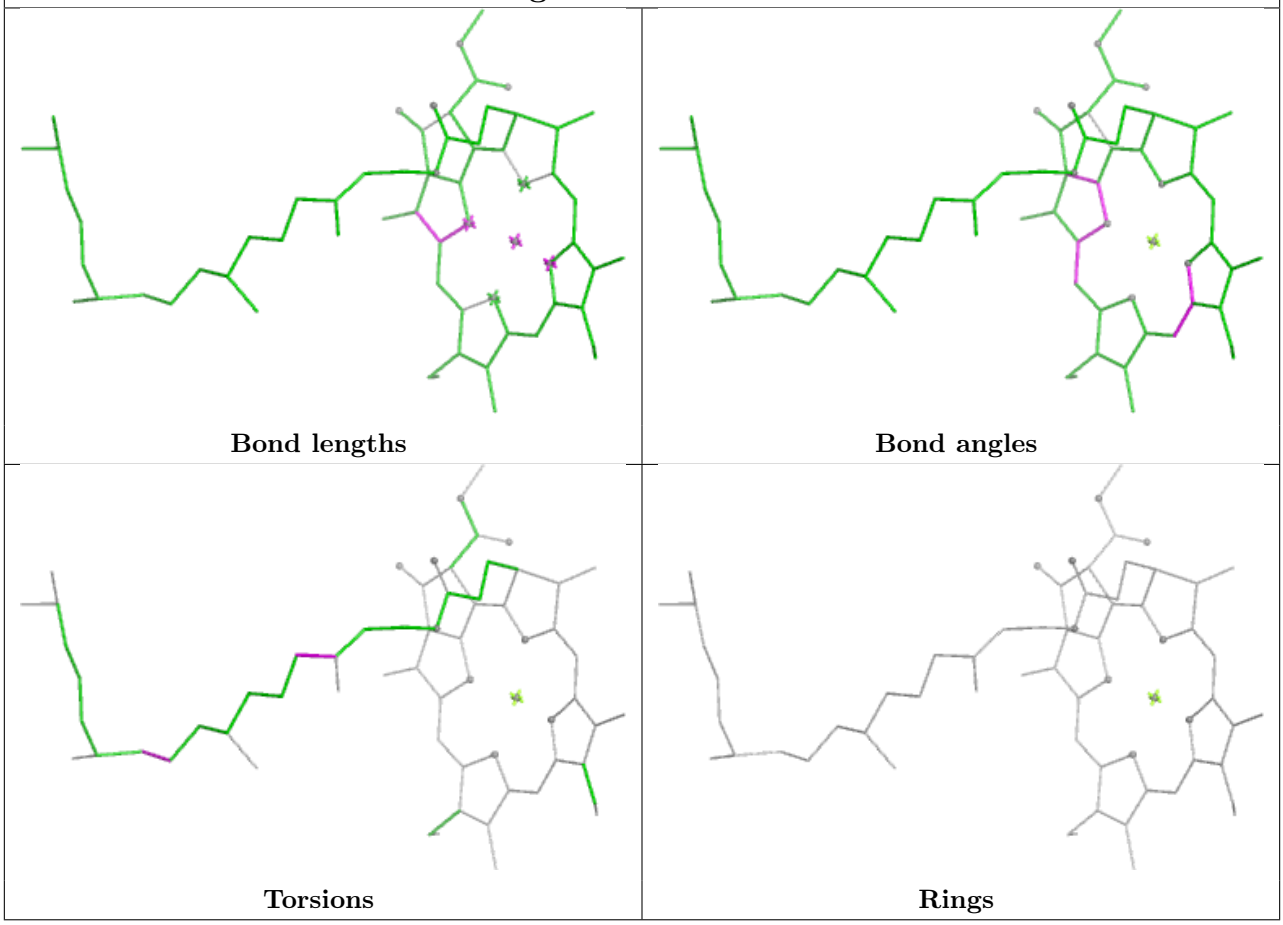


Rings

Ligand CLA 5 609



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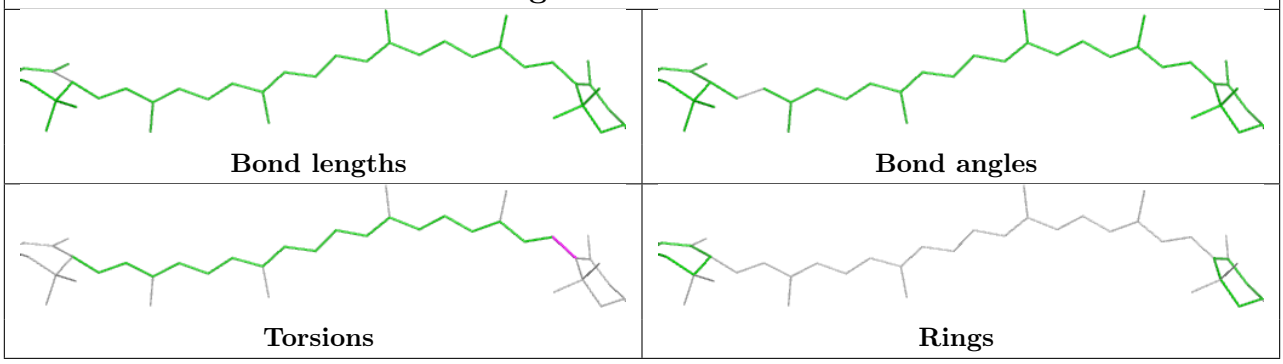

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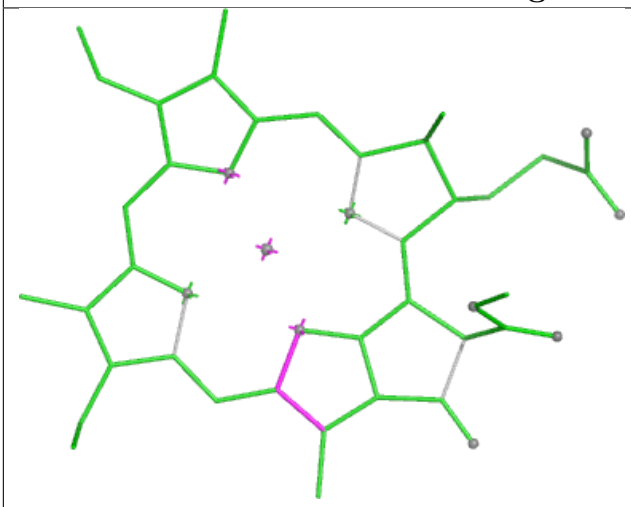

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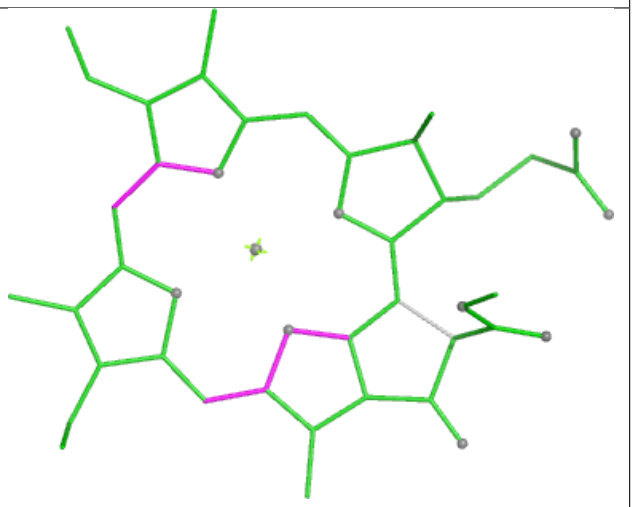
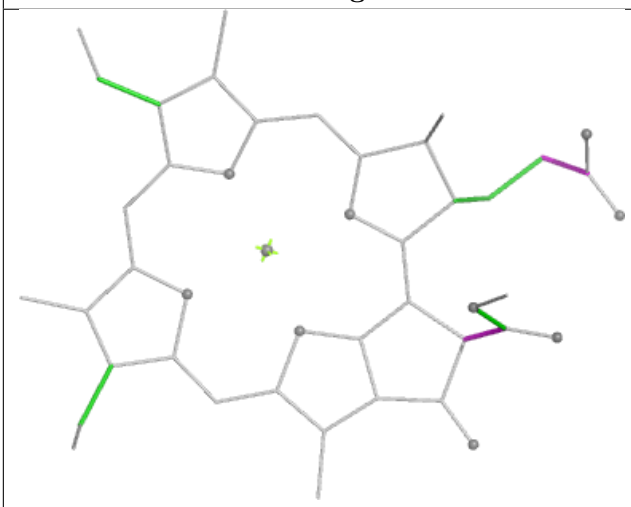


Bond angles



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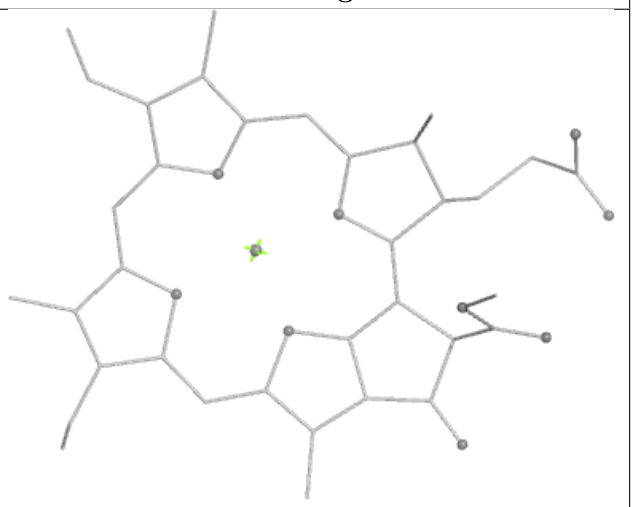
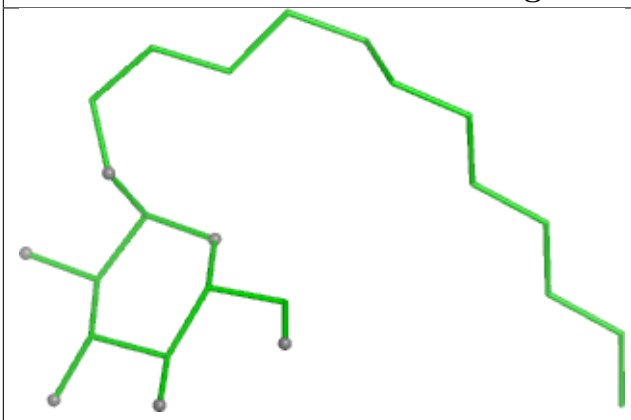


Rings

Ligand LMU 8 628



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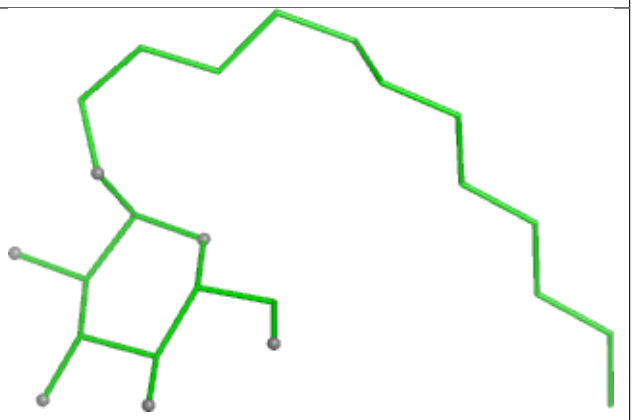
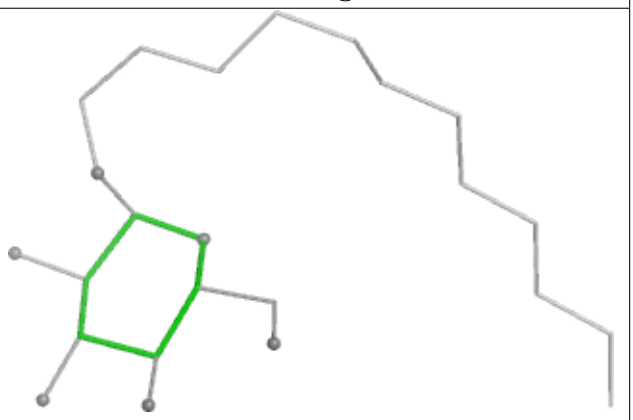


Bond angles

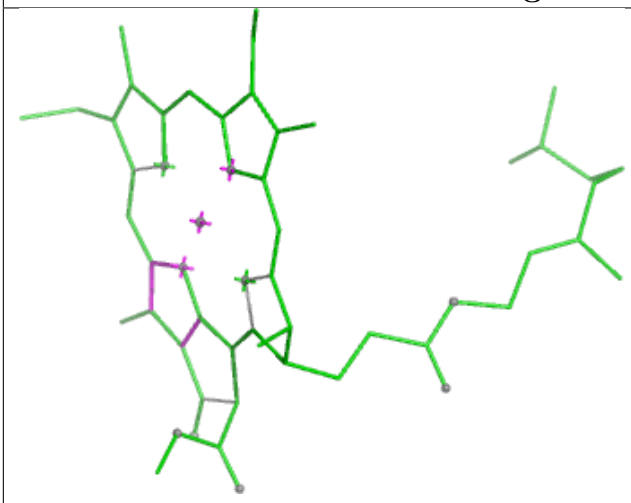


Torsions



Rings

Ligand CLA A 805



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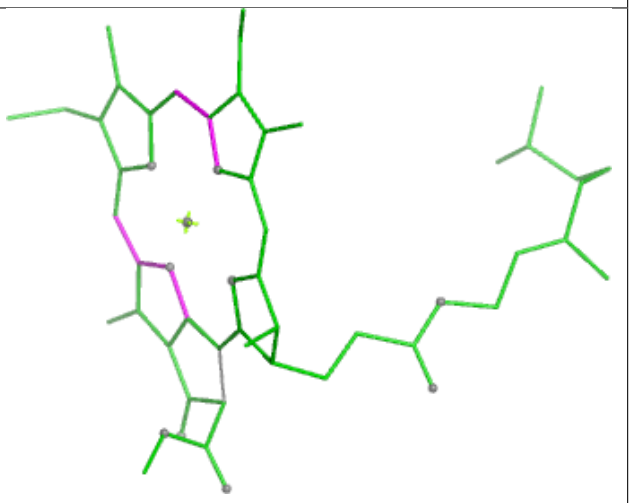
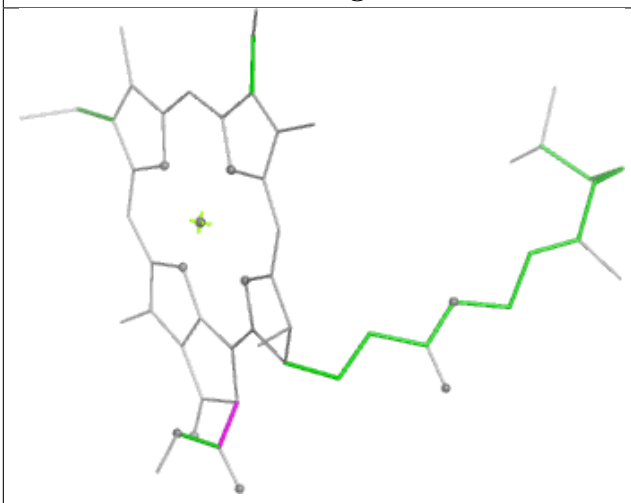


Bond angles



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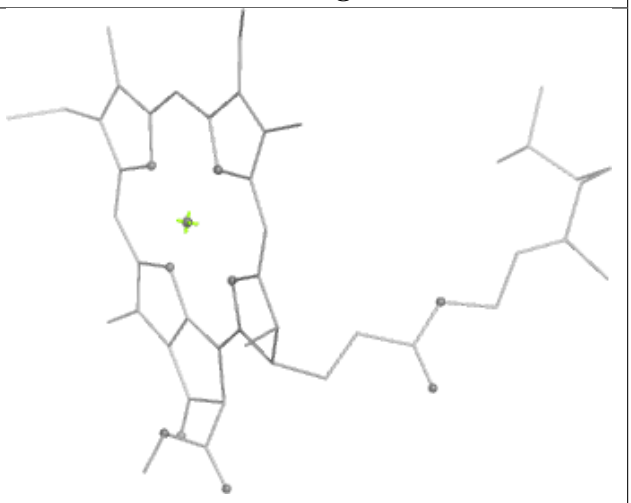
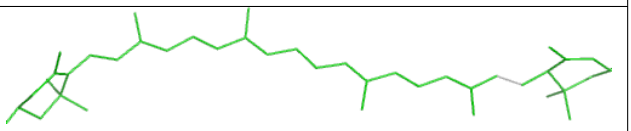


Rings

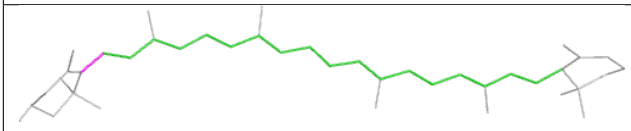
Ligand LUT 6 621



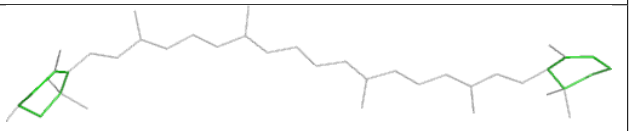
Bond lengths



Bond angles

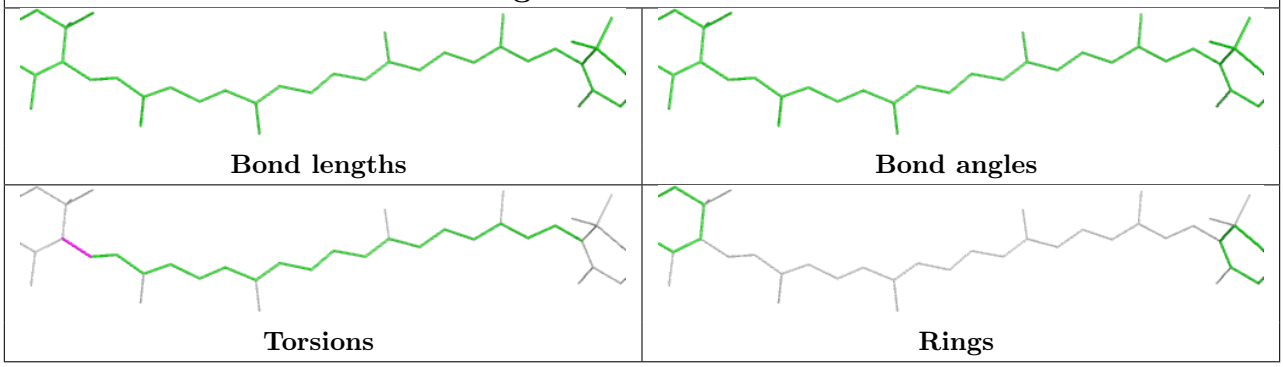


Torsions

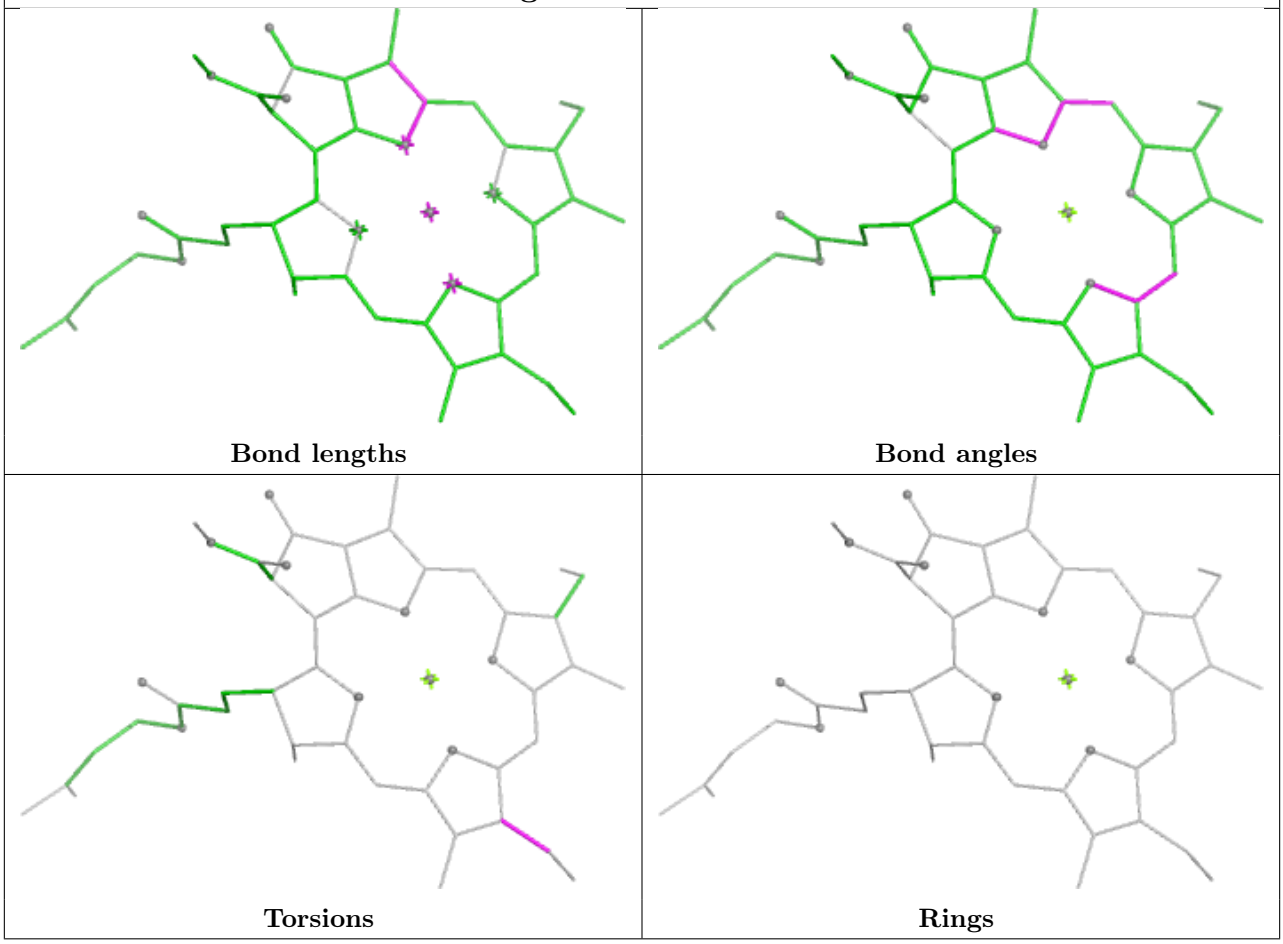


Rings

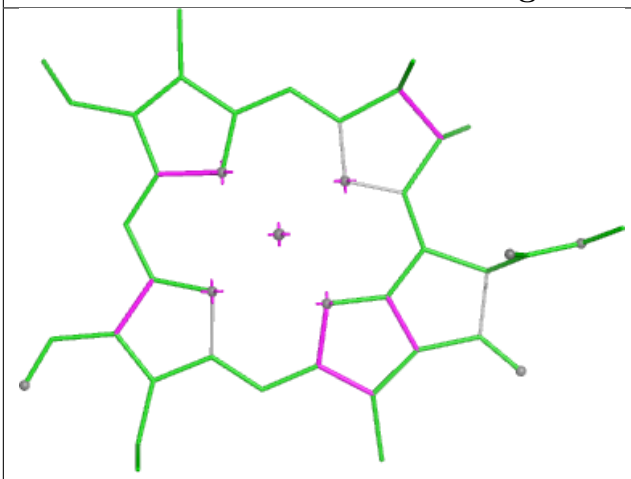
Ligand BCR K2 202



Ligand CLA 82 608



Ligand CHL 92 606



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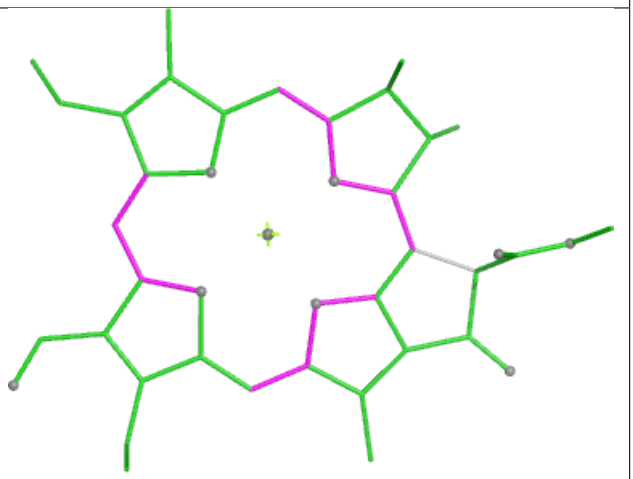
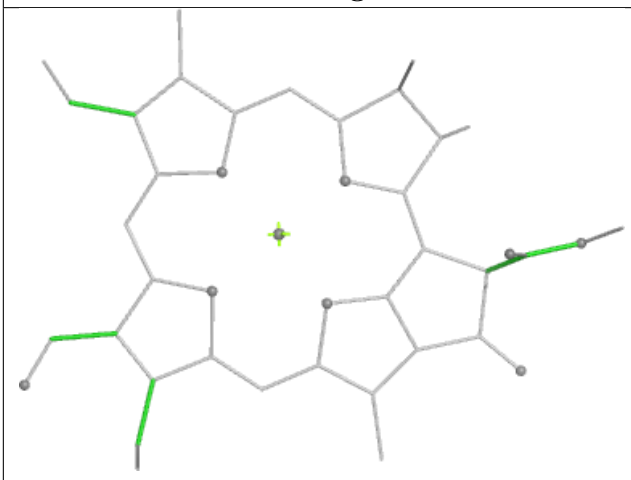


Bond angles



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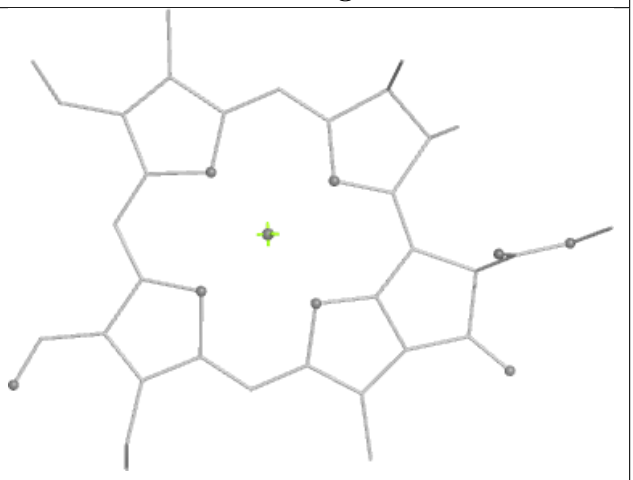
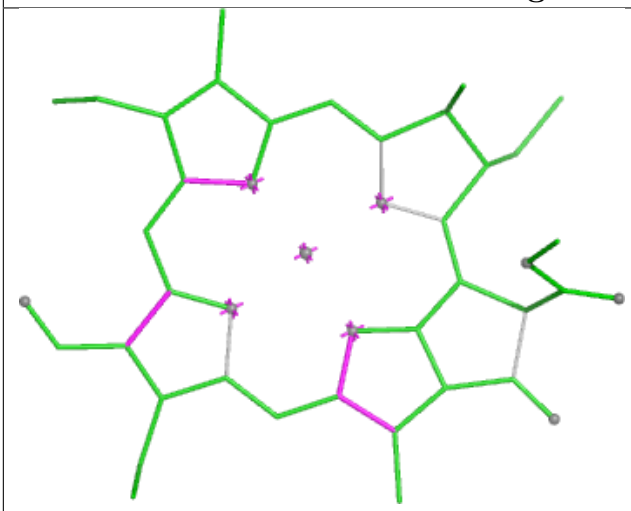


Rings

Ligand CHL 5 618



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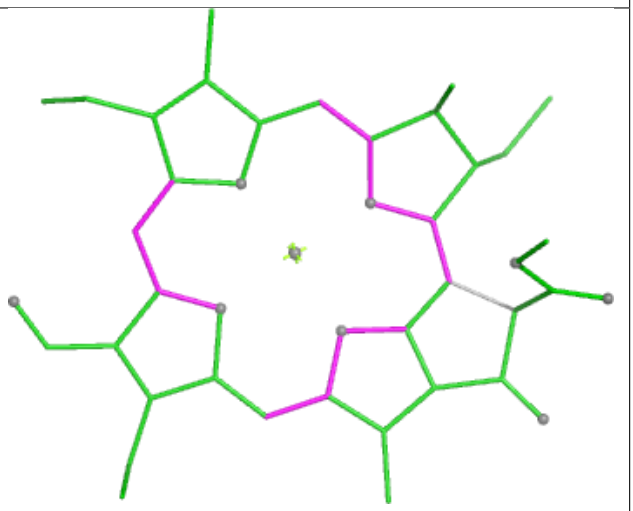
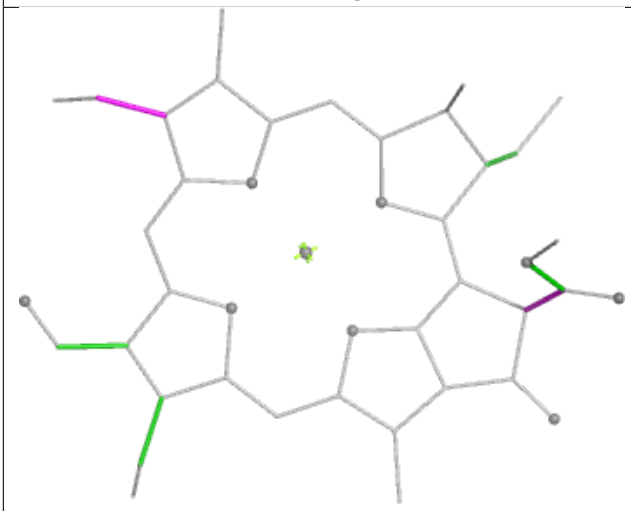


Bond angles



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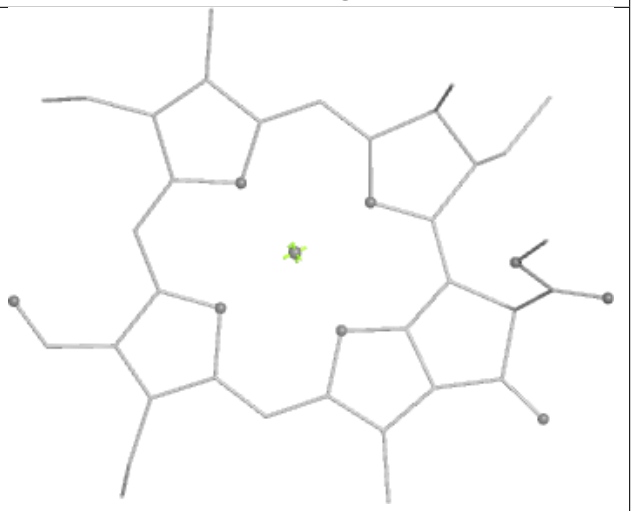
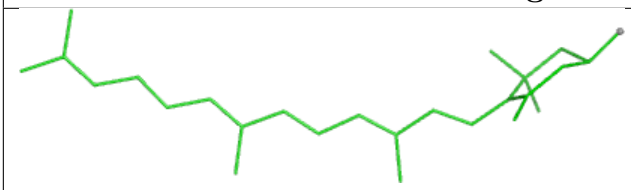


Rings

Ligand LUT Z 619



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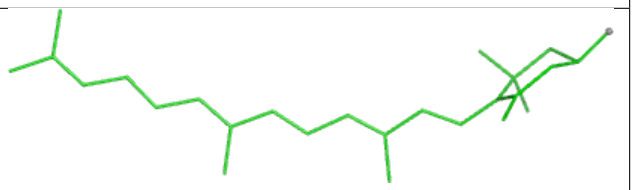
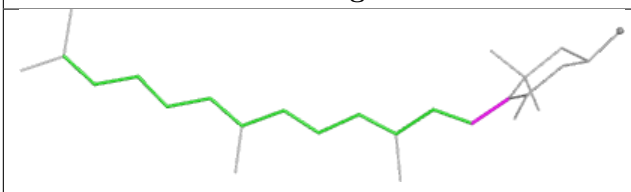


Bond angles



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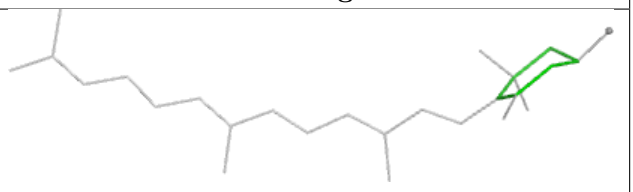
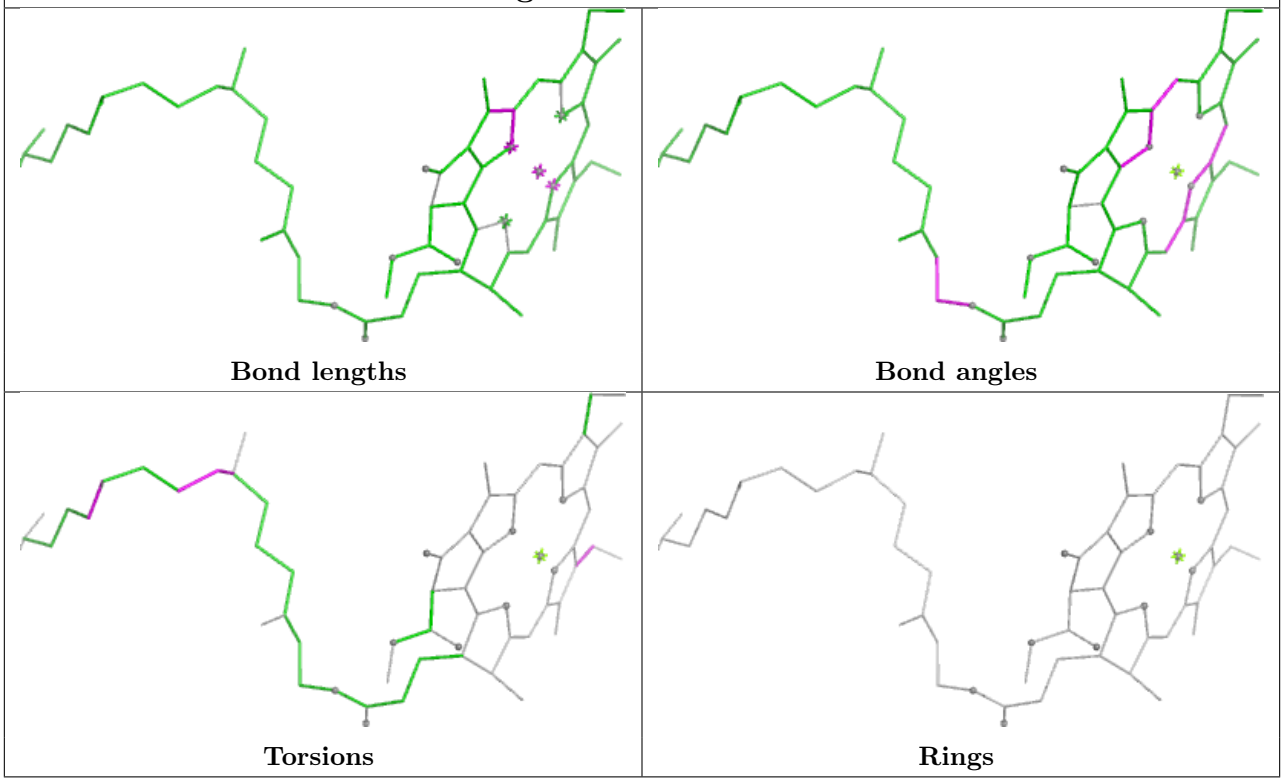
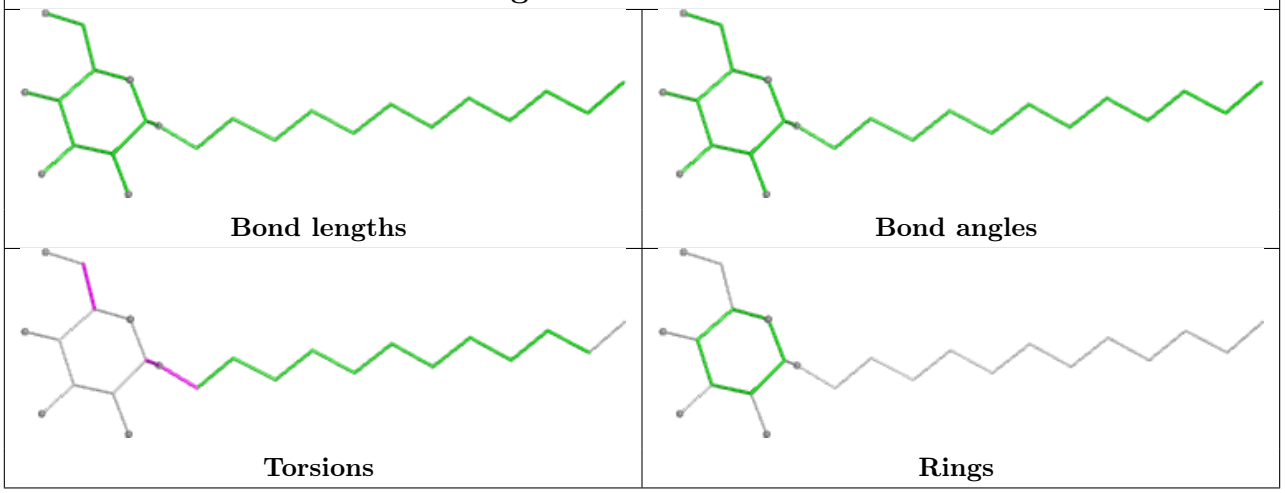


Rings

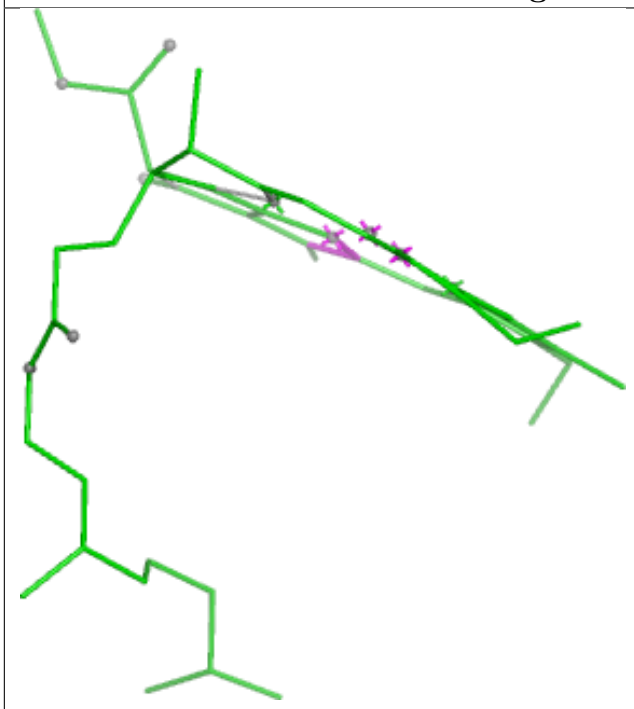
Ligand CLA B2 802



Ligand LMU G2 206



Ligand CLA 6 609



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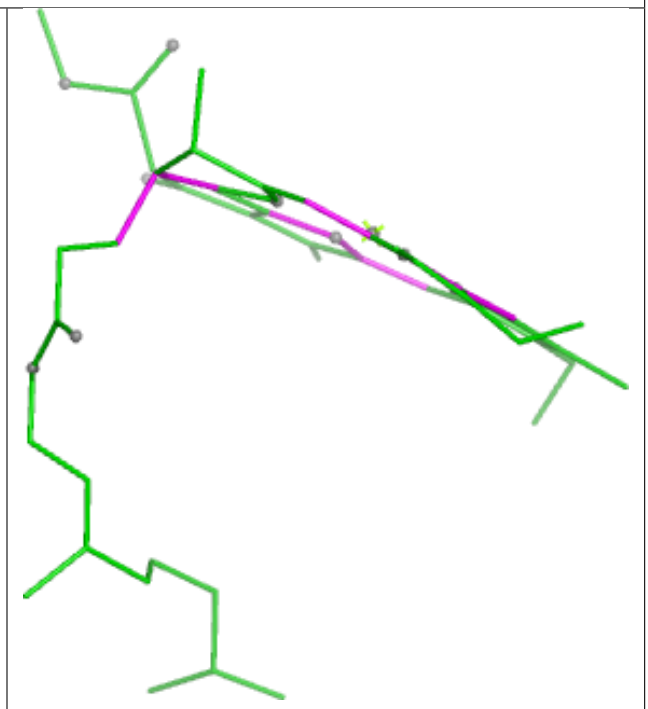
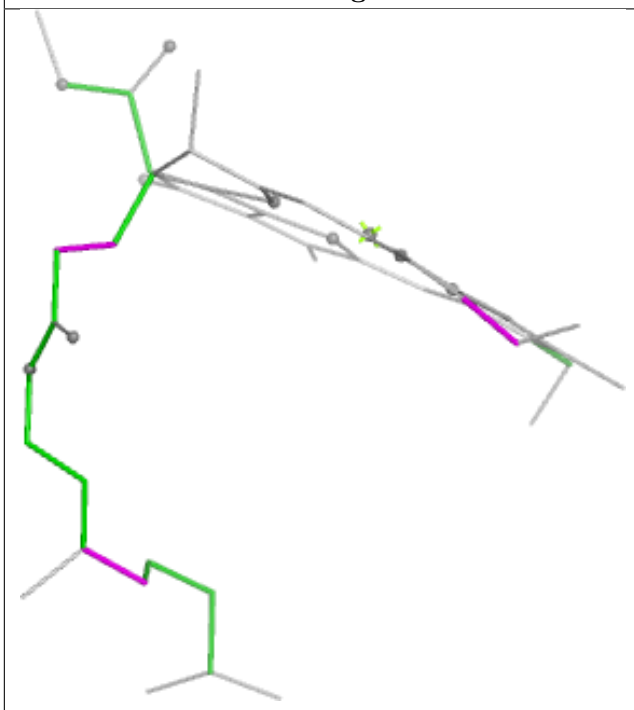


Bond angles



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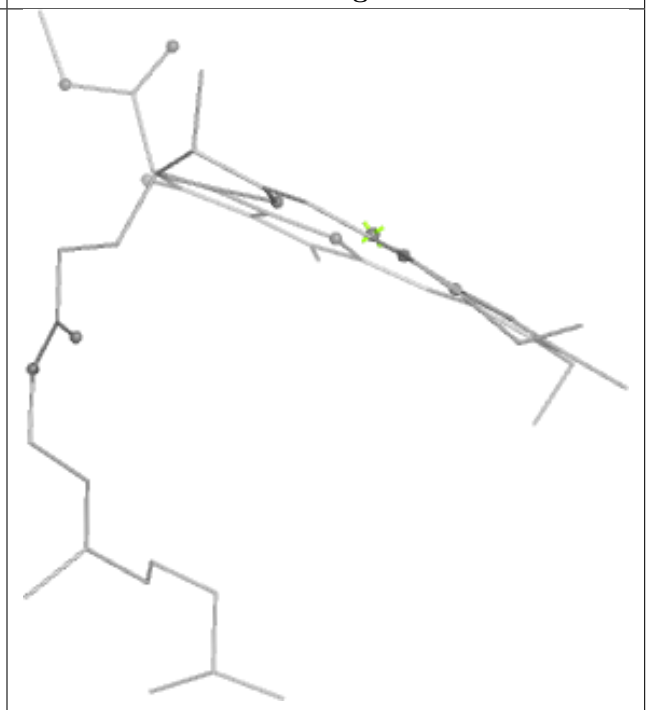
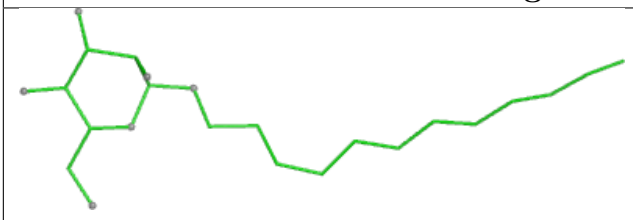
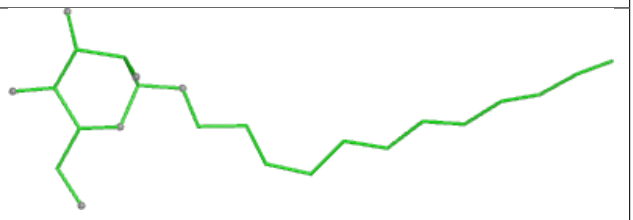


Rings

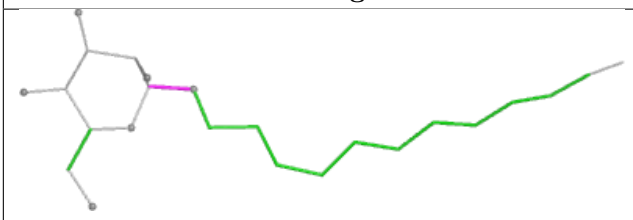
Ligand LMU 6 628



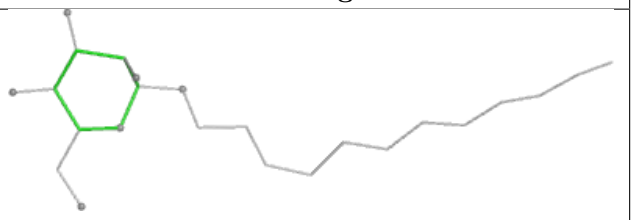
Bond lengths



Bond angles

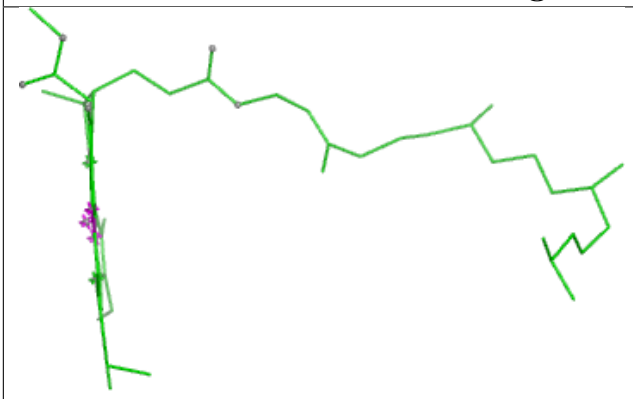


Torsions

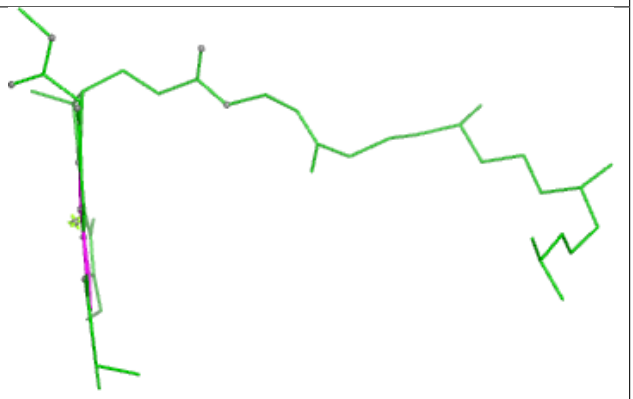


Rings

Ligand CLA 3 604



Bond lengths



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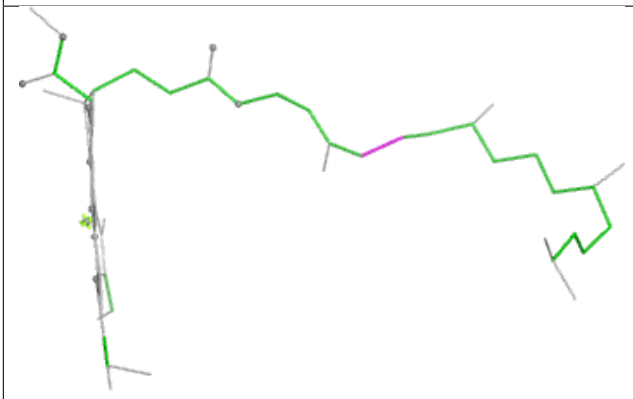

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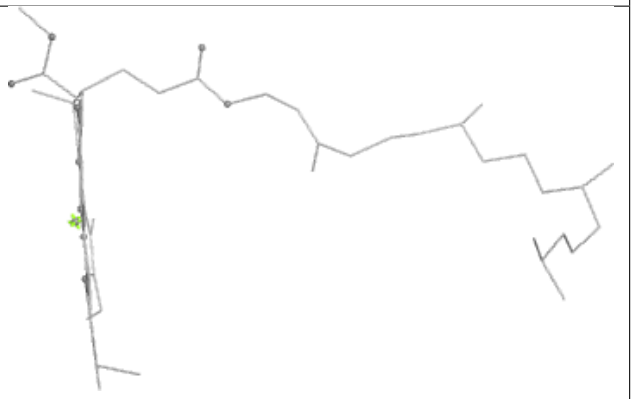
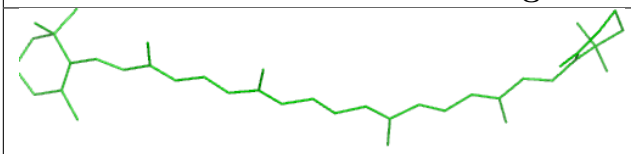


Rings

Ligand BCR B 801



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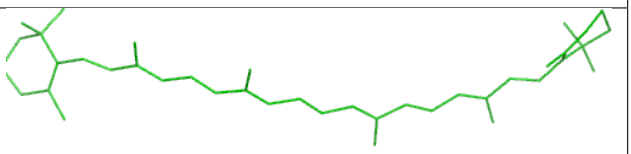

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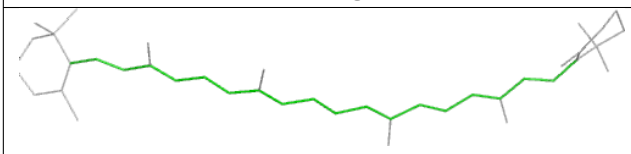

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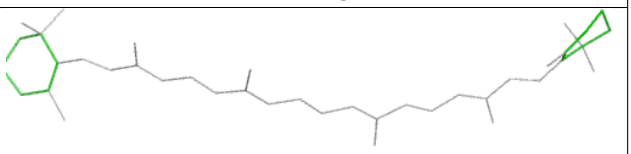
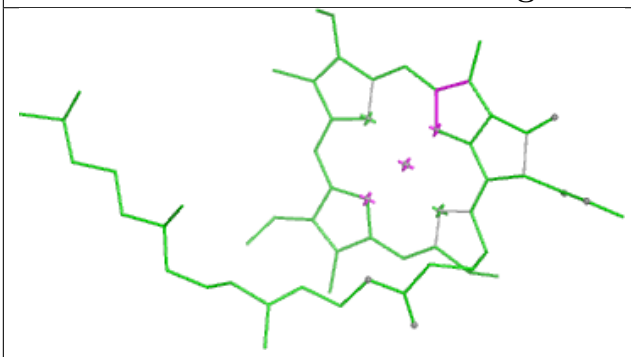


Rings

Ligand CLA Z2 610



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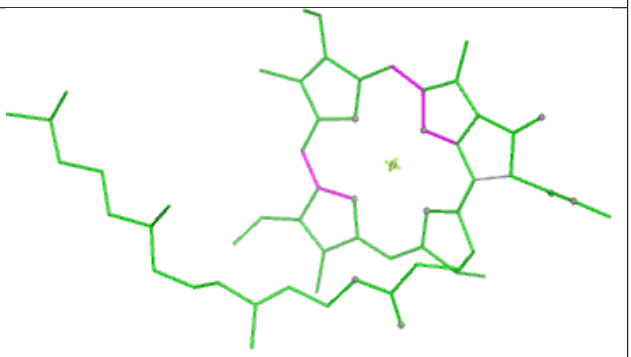

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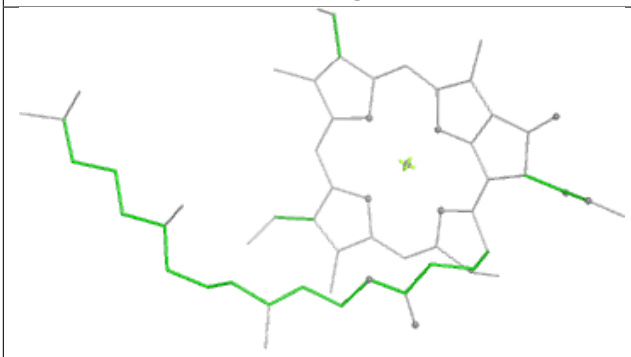

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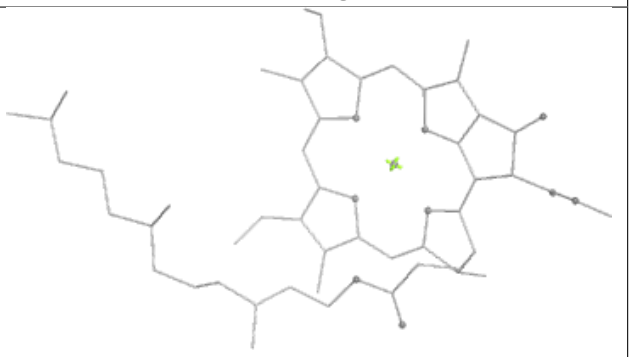
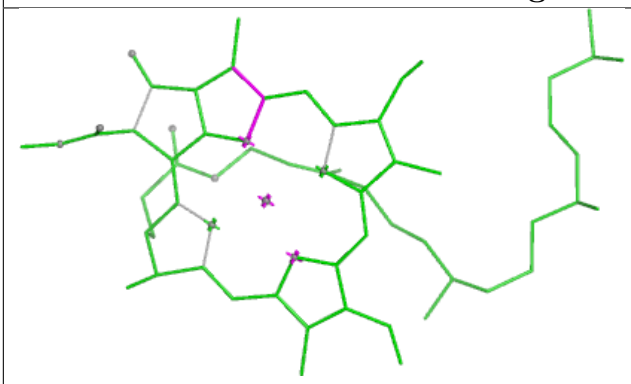


Rings

Ligand CLA 3 615



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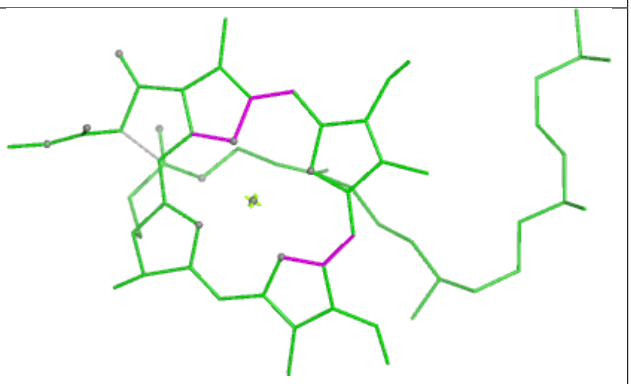
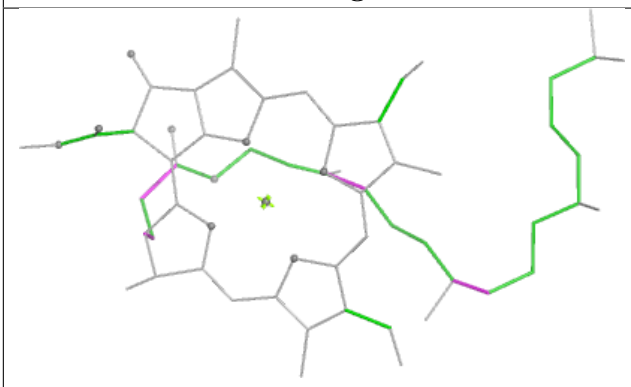


Bond angles



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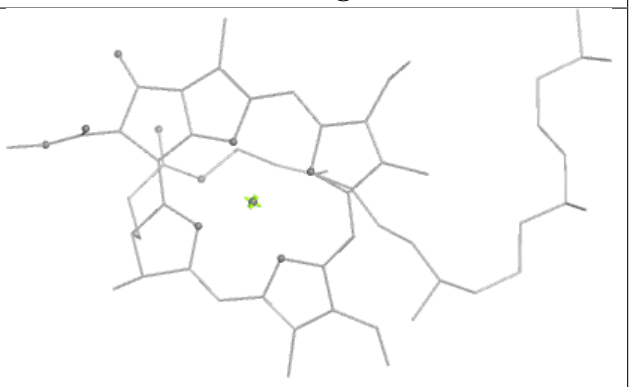
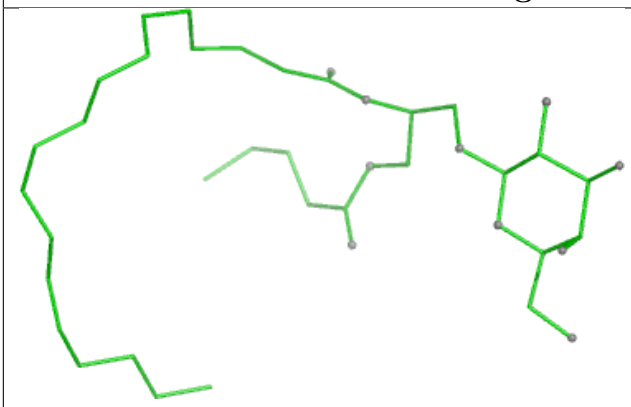


Rings

Ligand LMG 82 629



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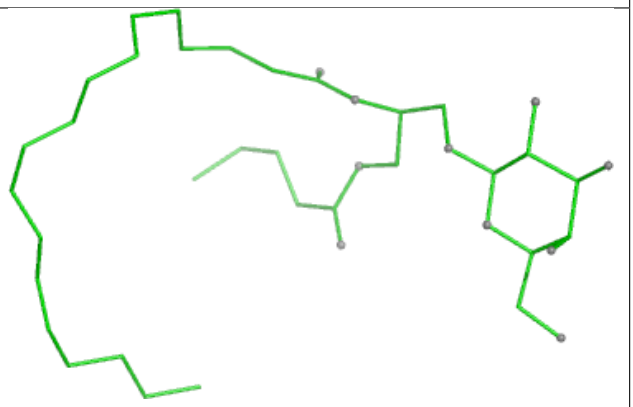
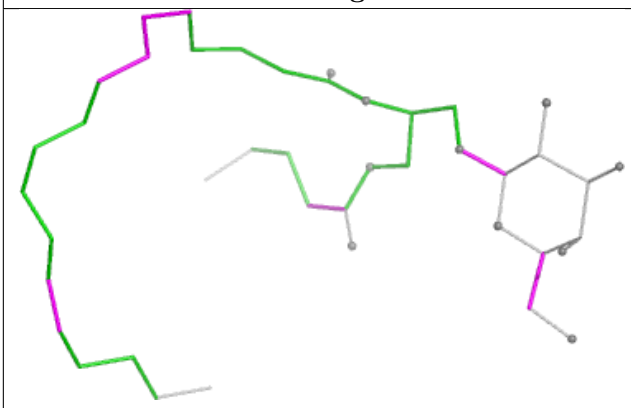


Bond angles



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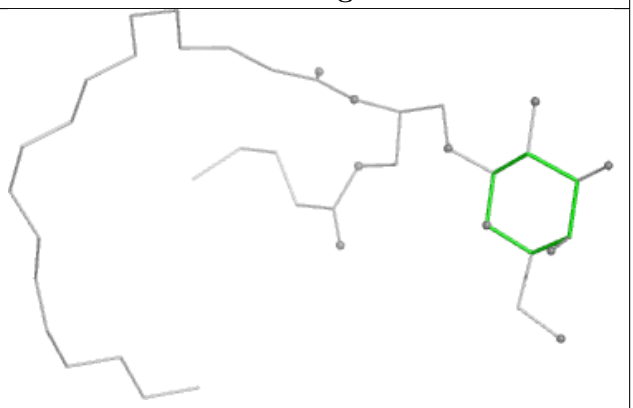
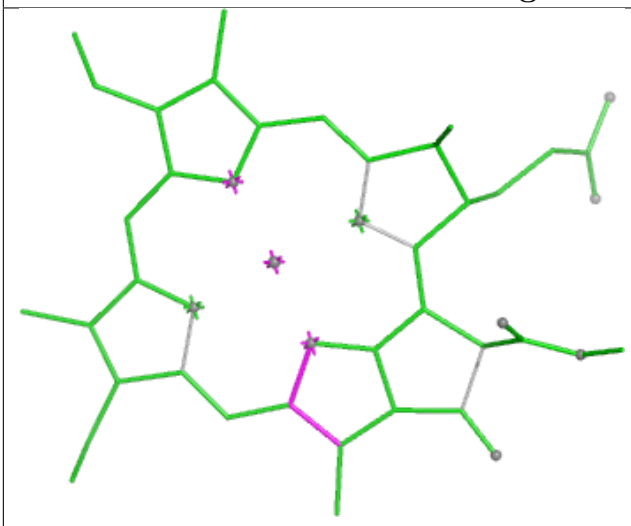


Rings

Ligand CLA 42 616



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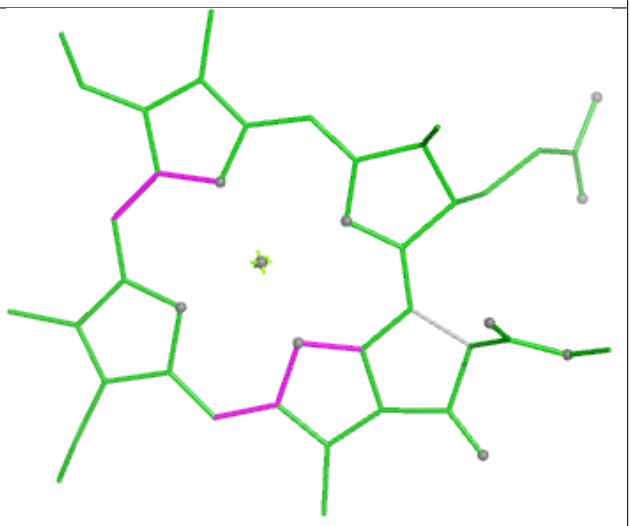

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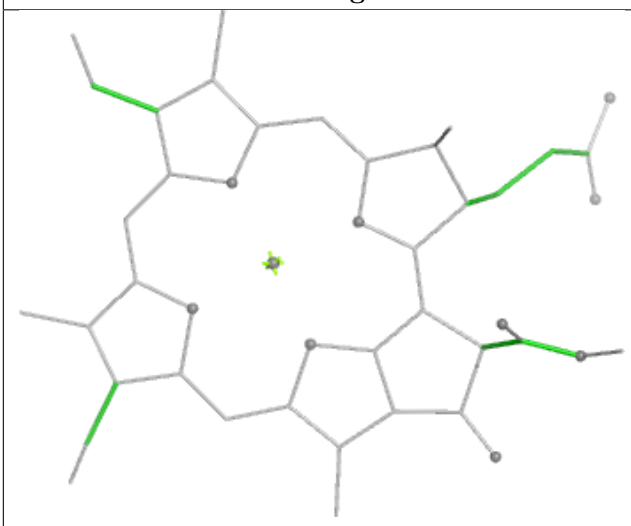

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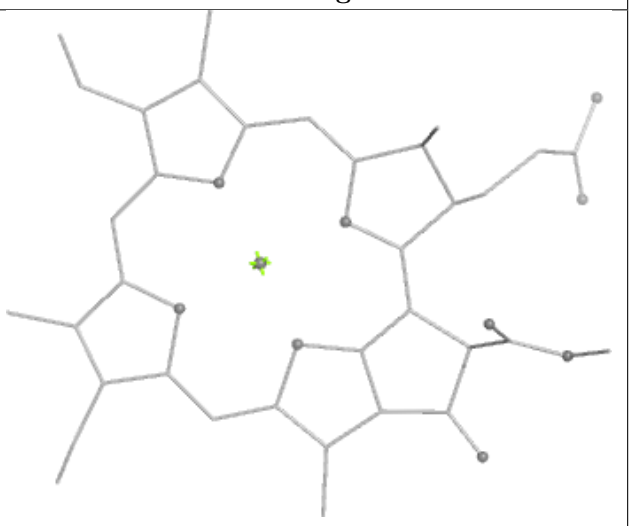
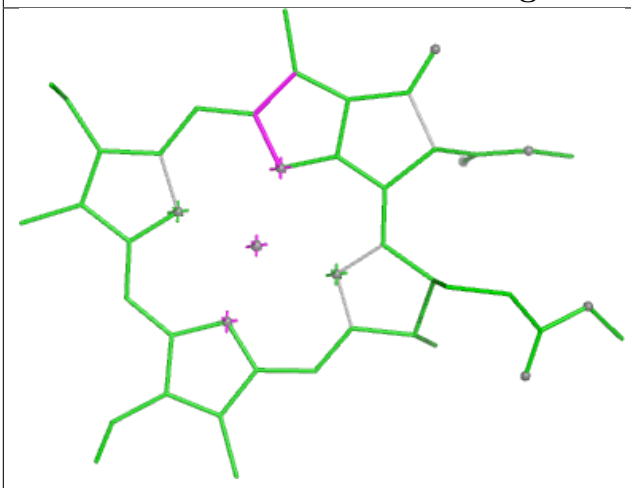


Rings

Ligand CLA 72 616



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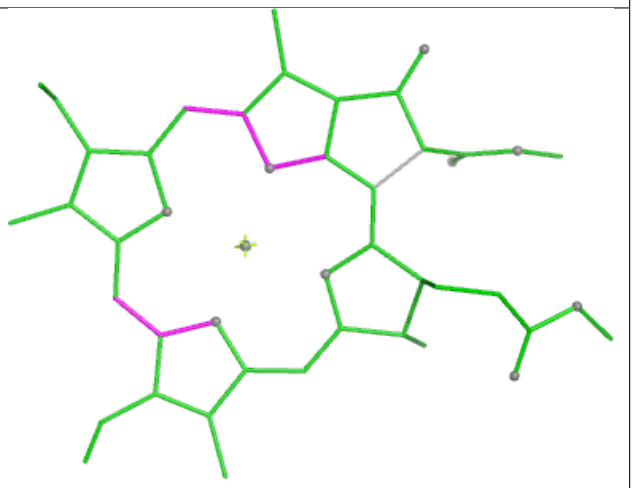

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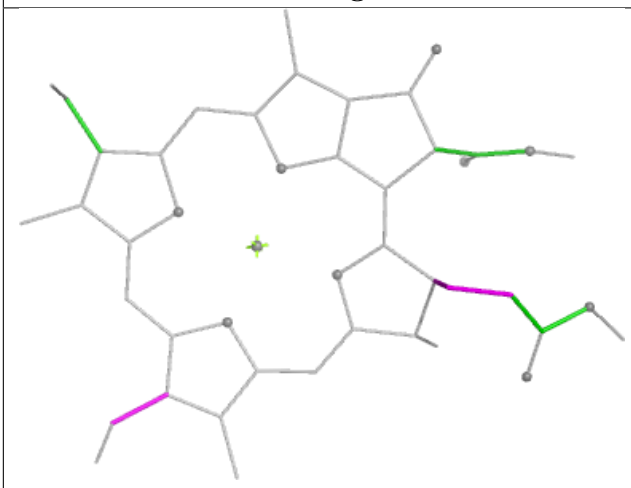

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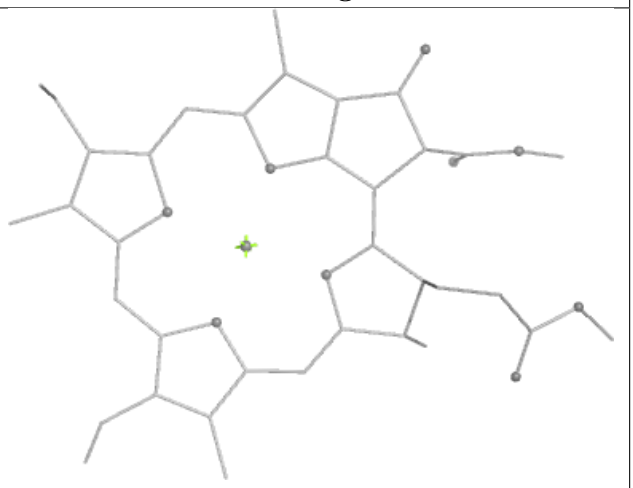
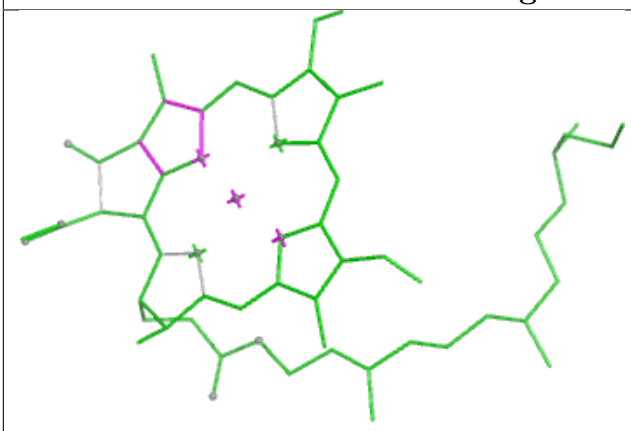


Rings

Ligand CLA 82 602



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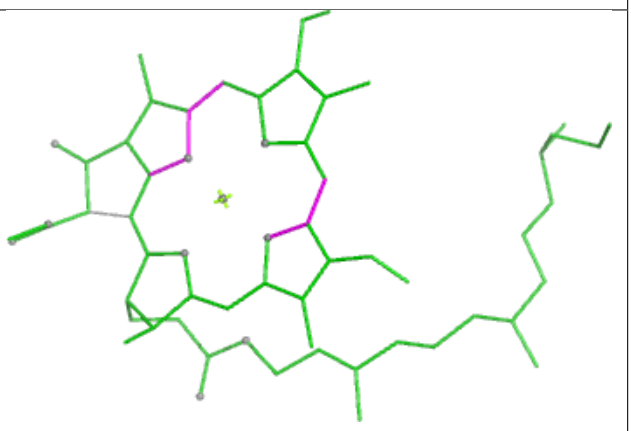
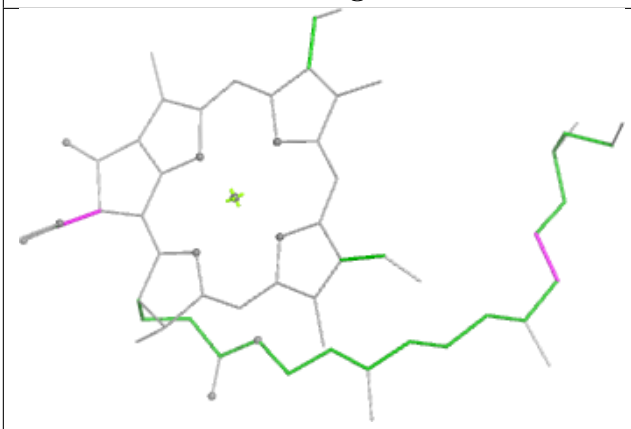


Bond angles



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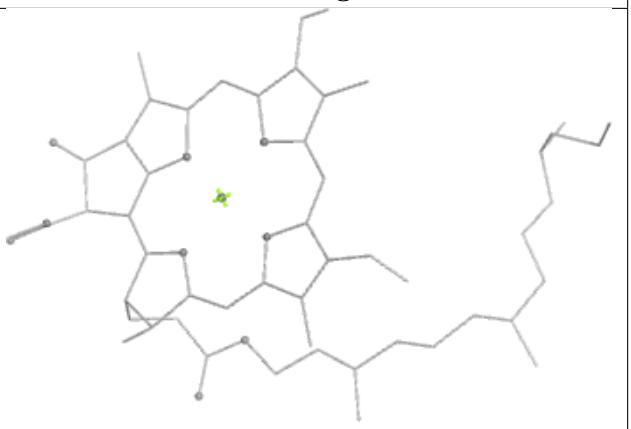
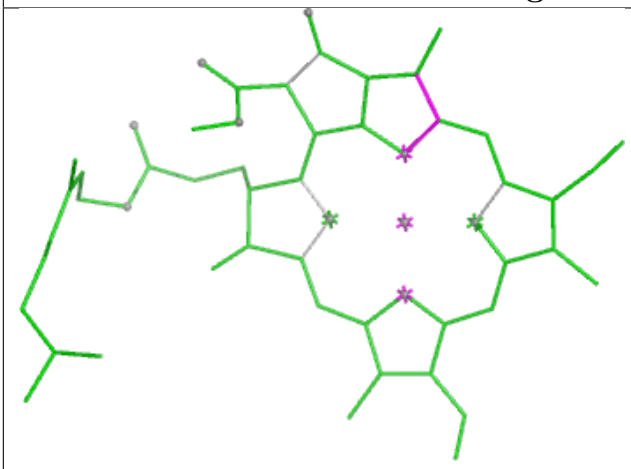


Rings

Ligand CLA Z 603



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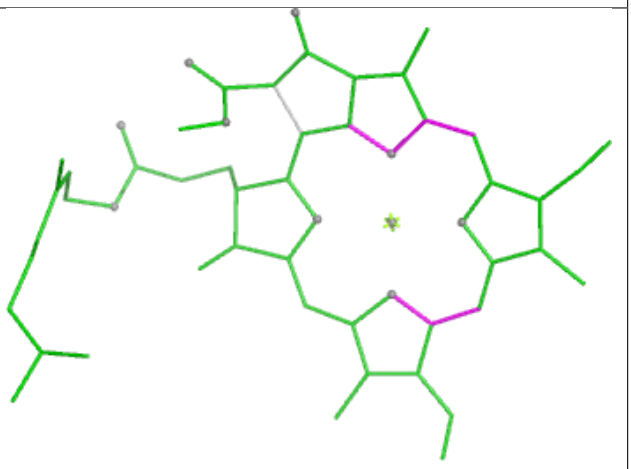
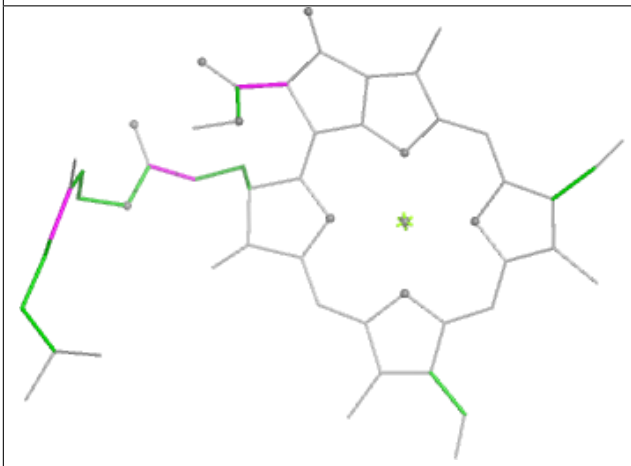


Bond angles



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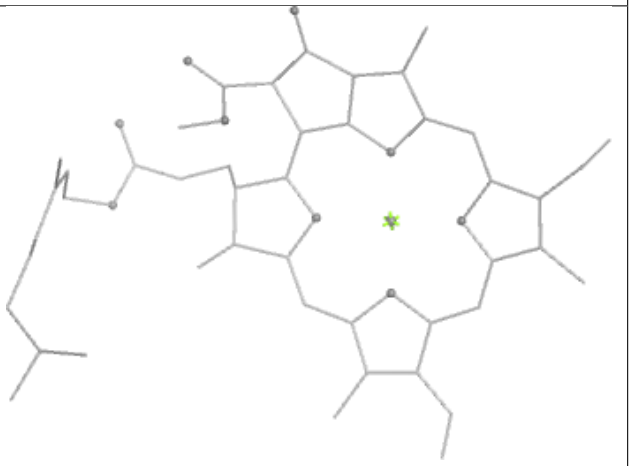
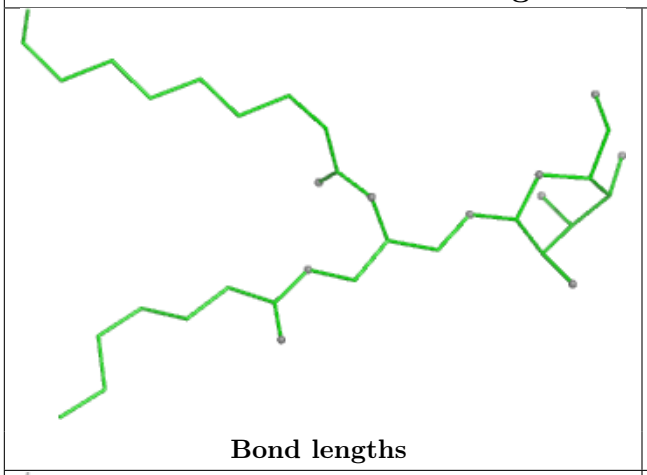


Rings

Ligand LMG B2 854



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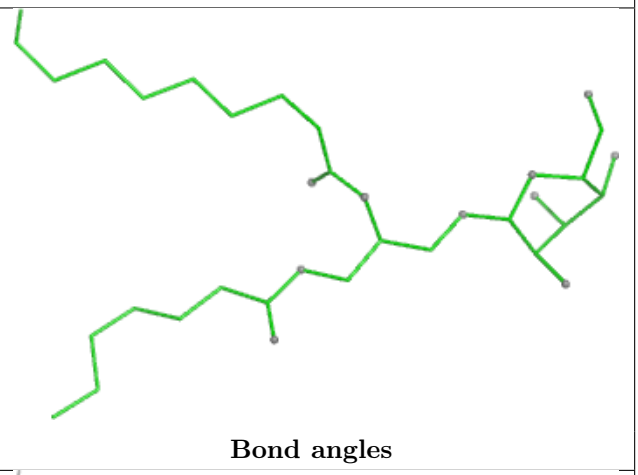
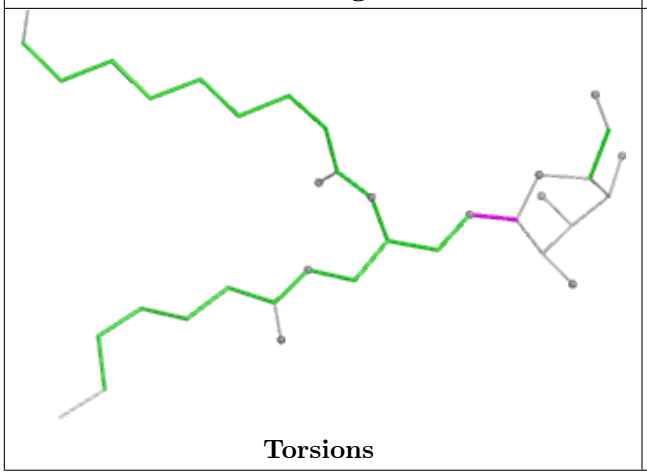


Bond angles



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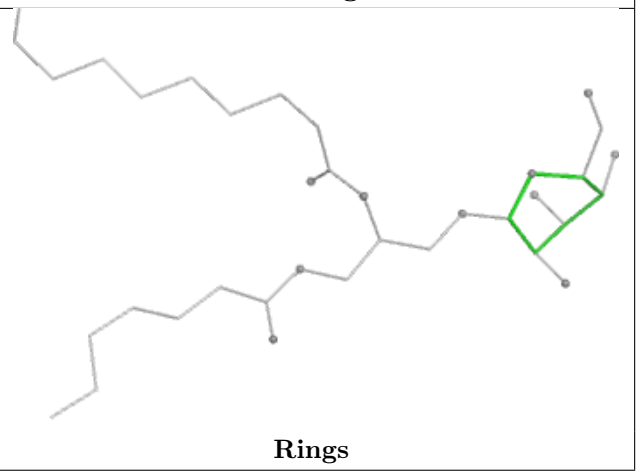
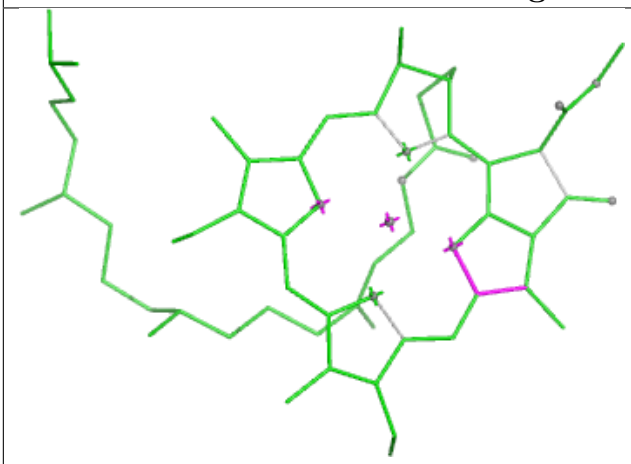


Rings

Ligand CLA 8 613



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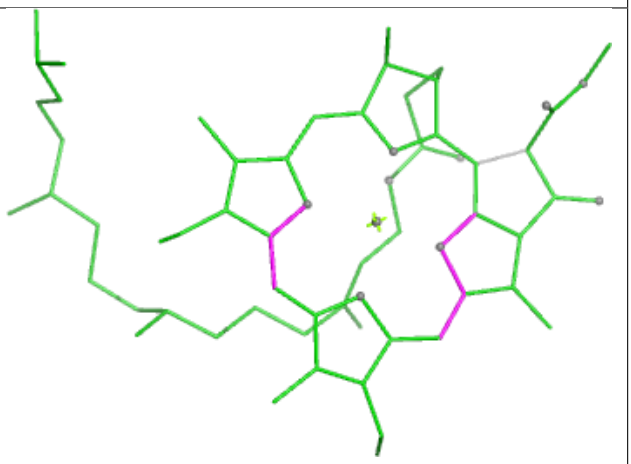
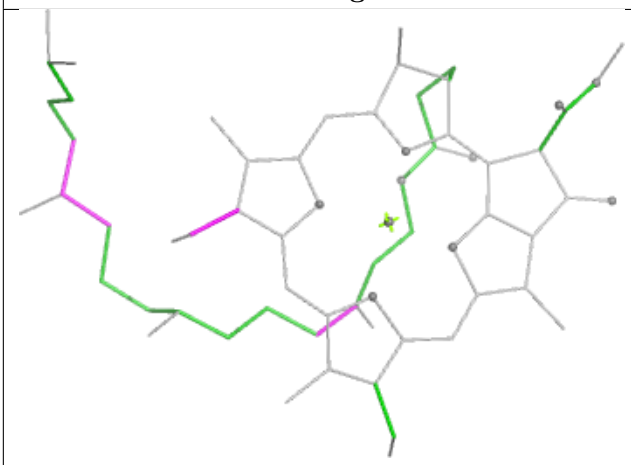


Bond angles



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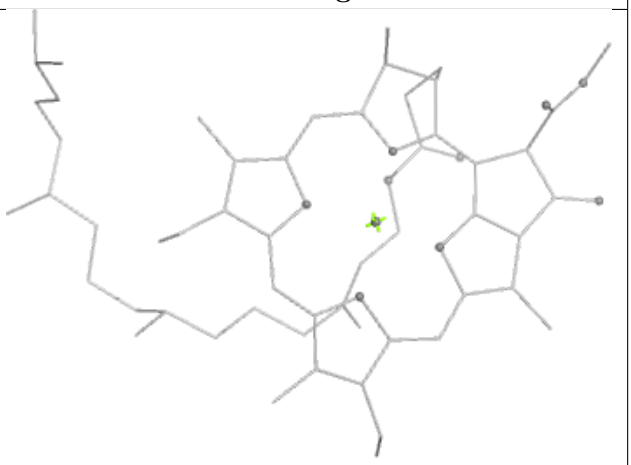
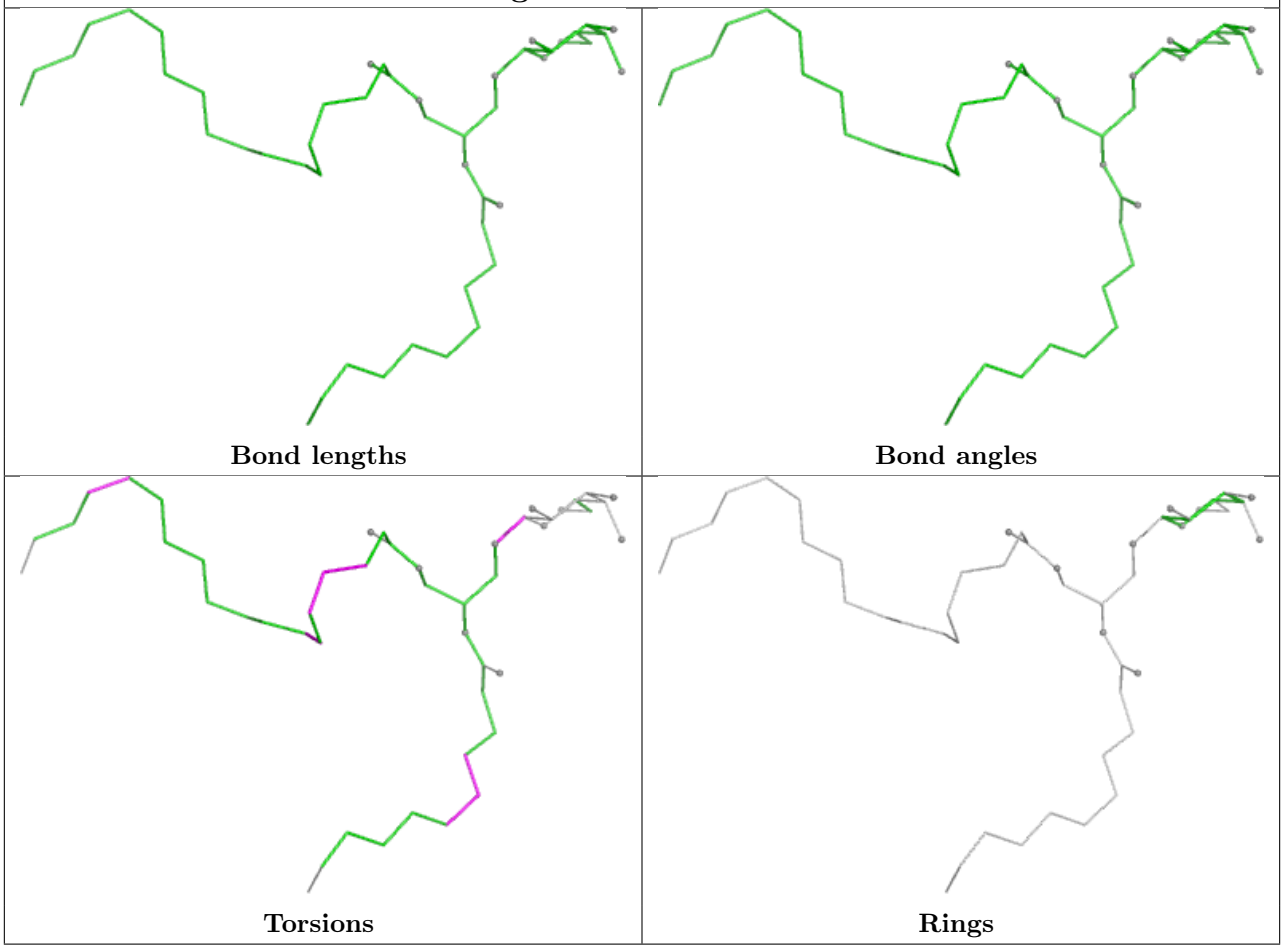
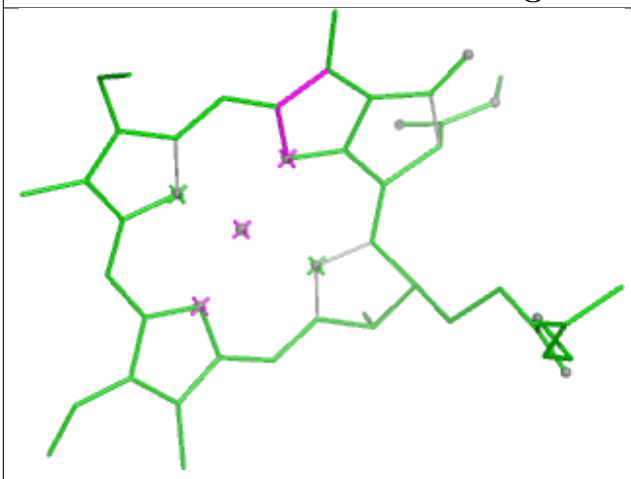


Rings

Ligand LMG A2 859



Ligand CLA B 838



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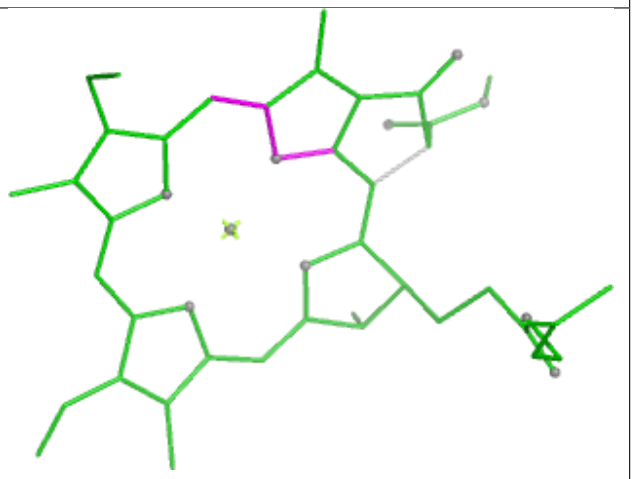
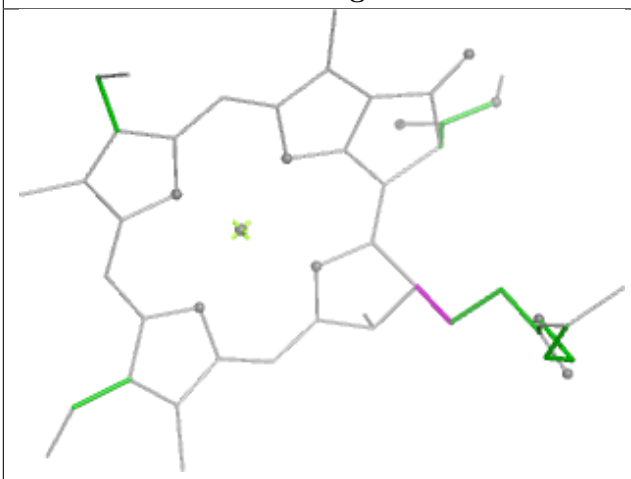


Bond angles



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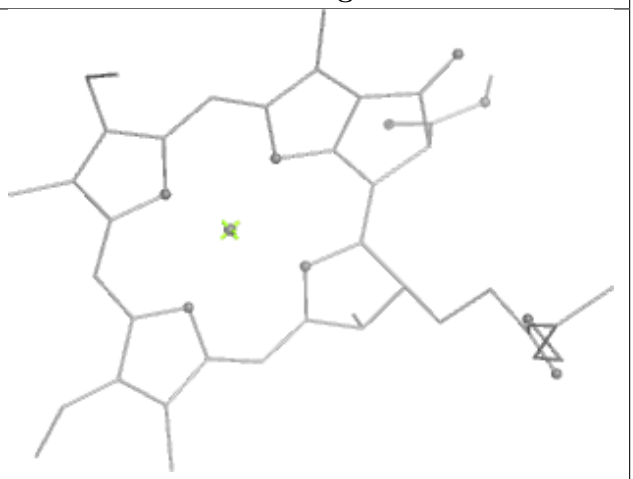
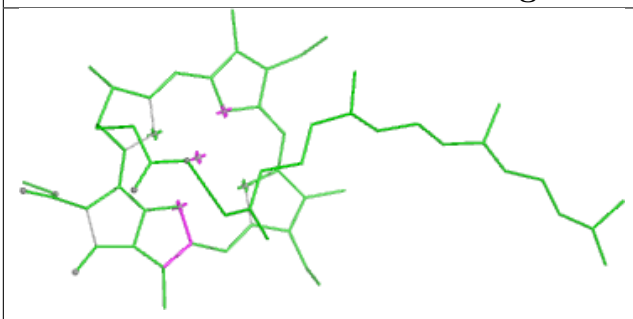


Rings

Ligand CLA 92 613



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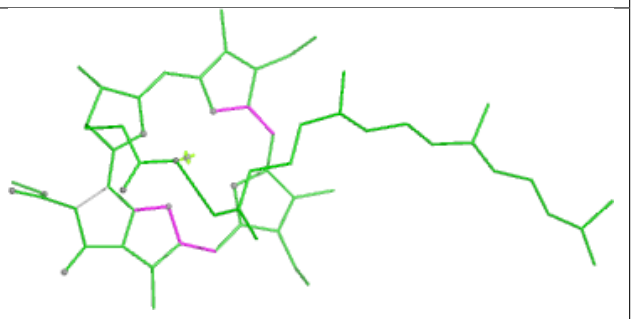
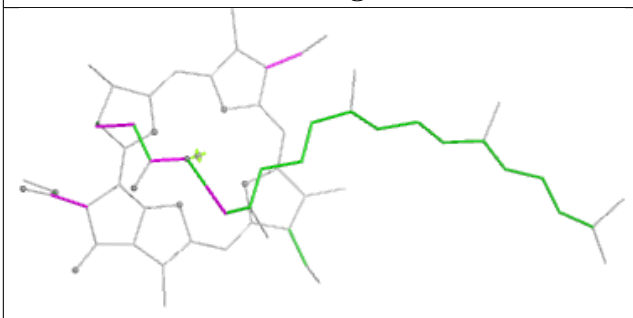


Bond angles



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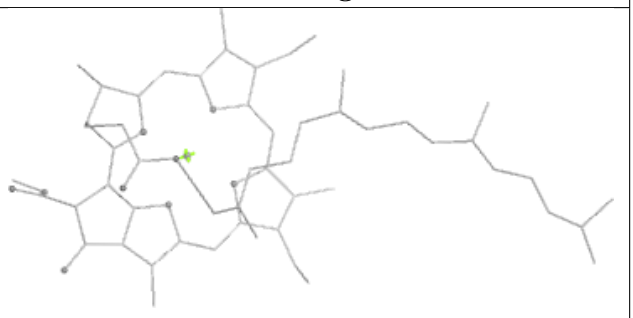
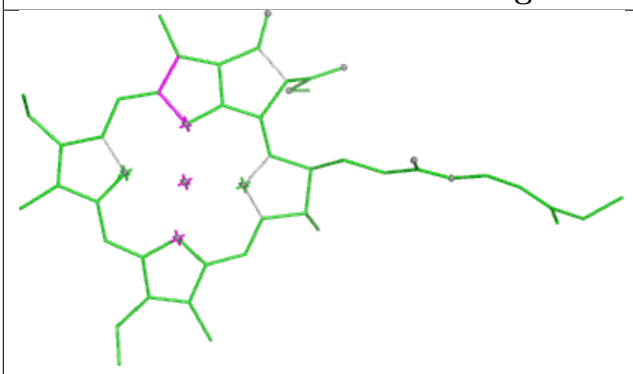


Rings

Ligand CLA A2 838



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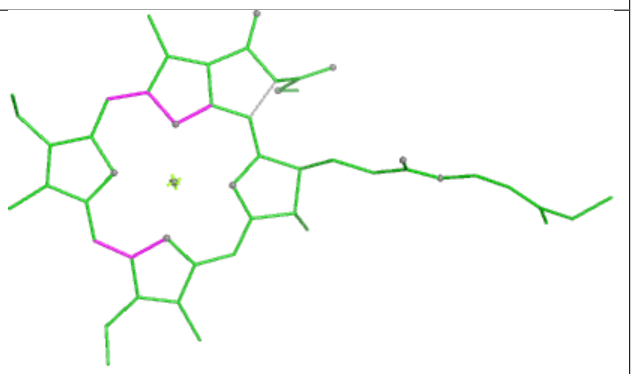
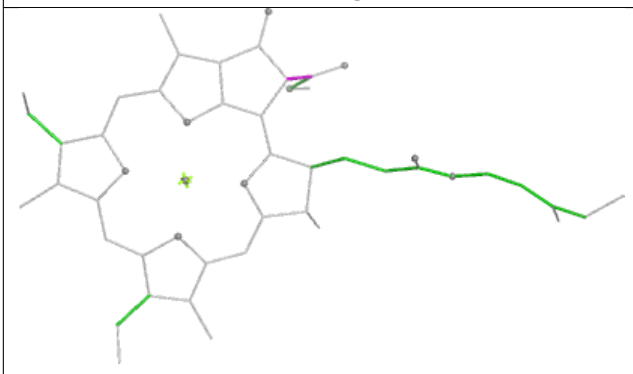
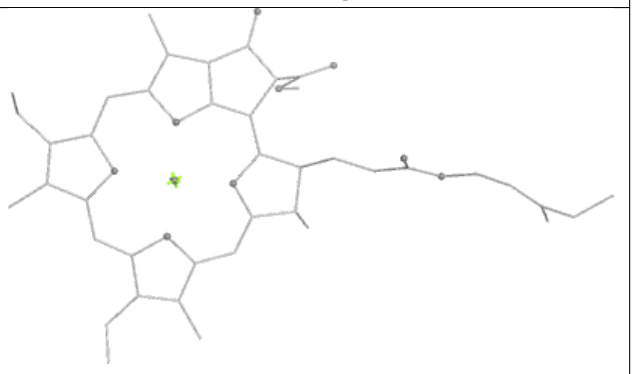


Bond angles

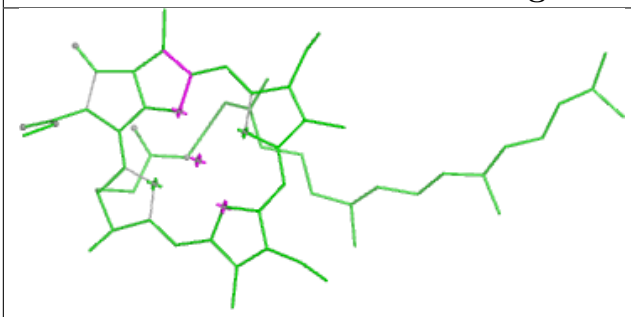


Torsions



Rings

Ligand CLA 9 613



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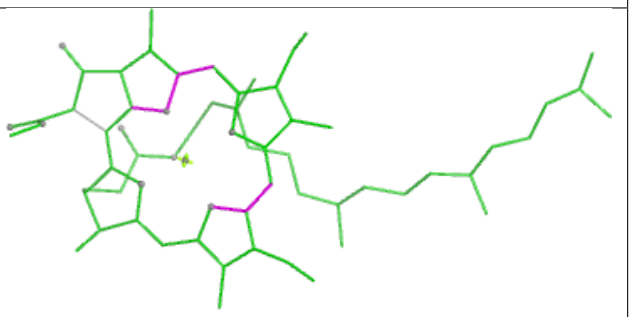
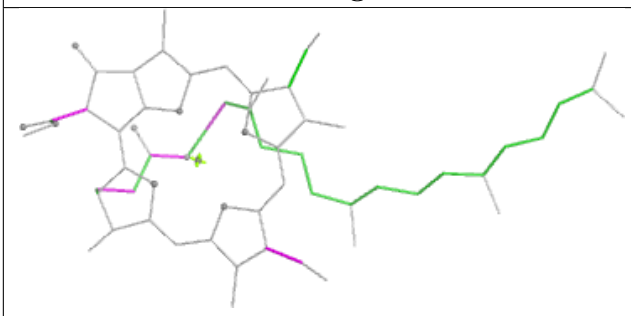


Bond angles



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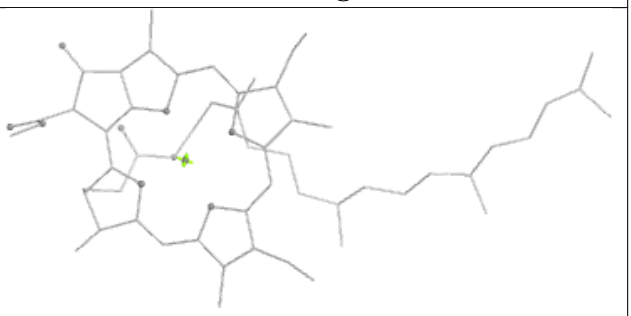
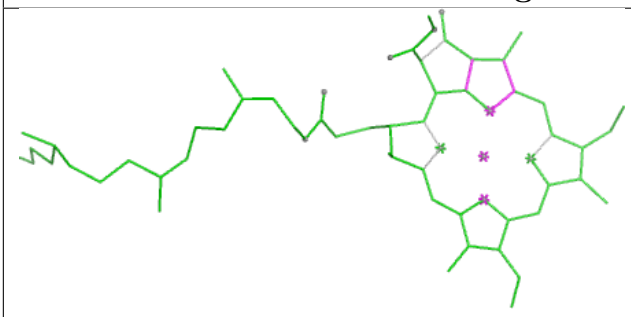


Rings

Ligand CLA A2 806



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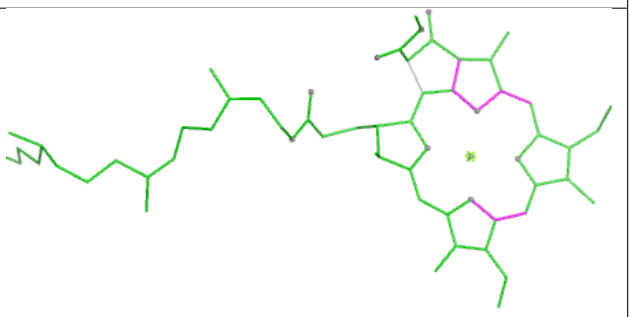

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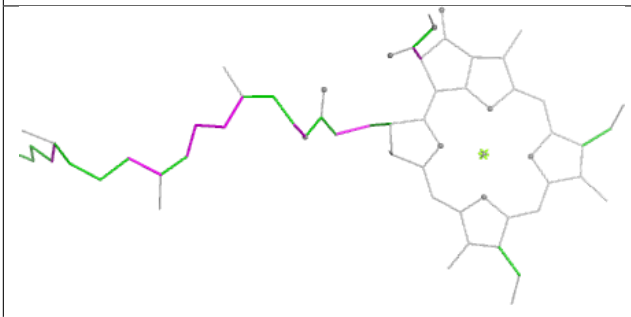

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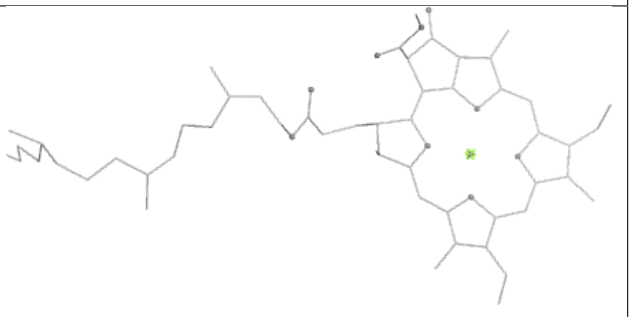
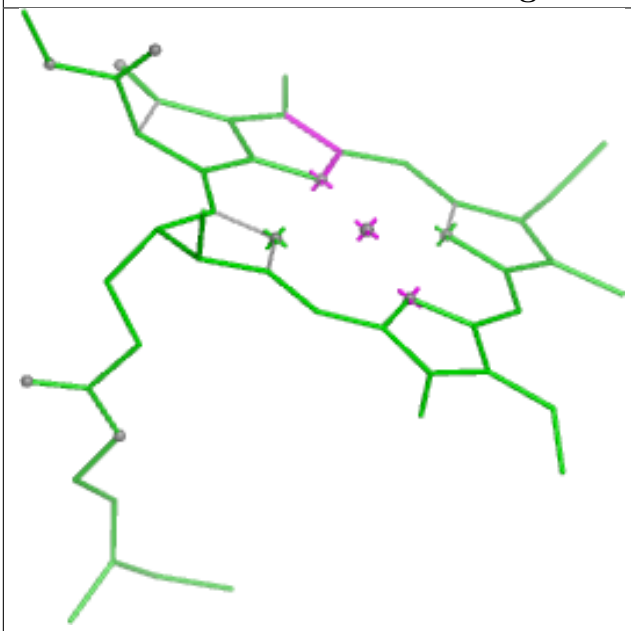


Rings

Ligand CLA 72 604



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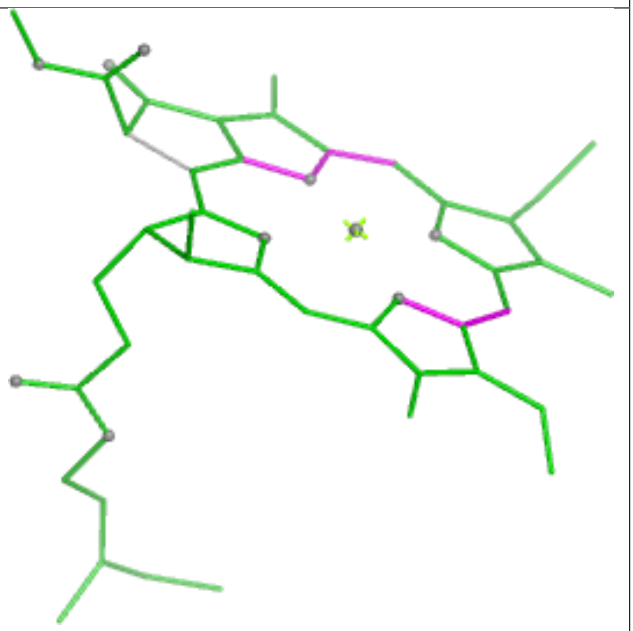

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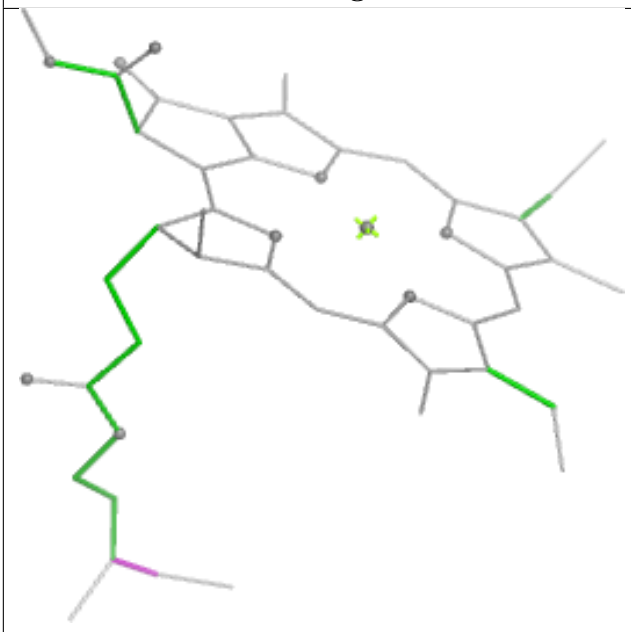

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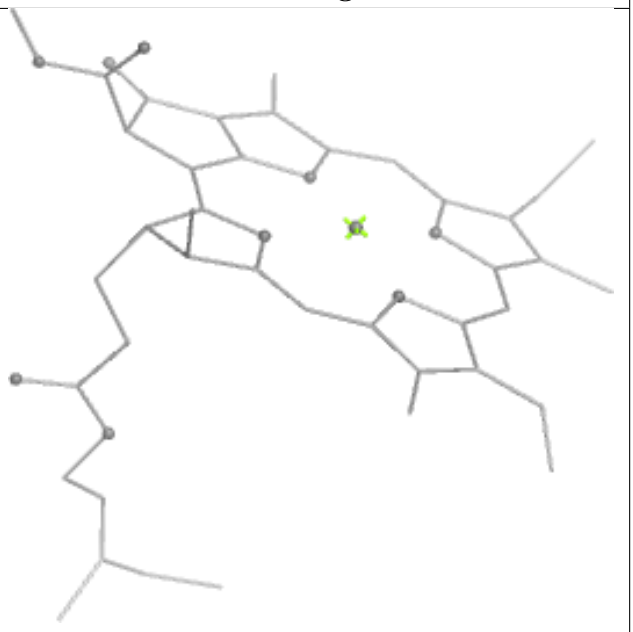
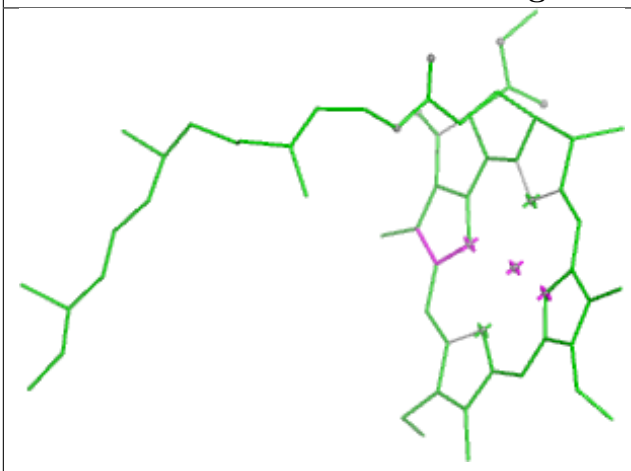


Rings

Ligand CLA 1 611



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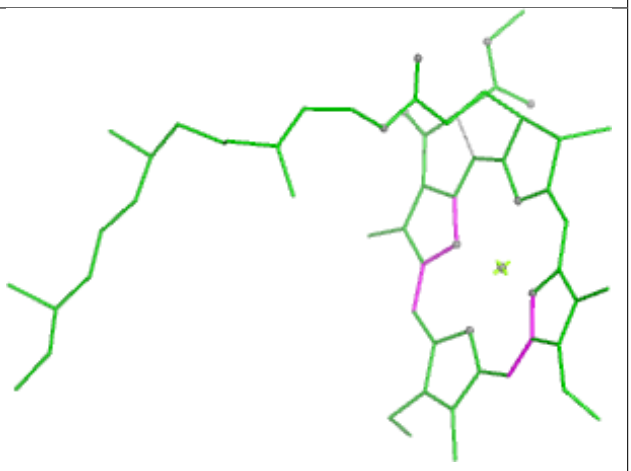

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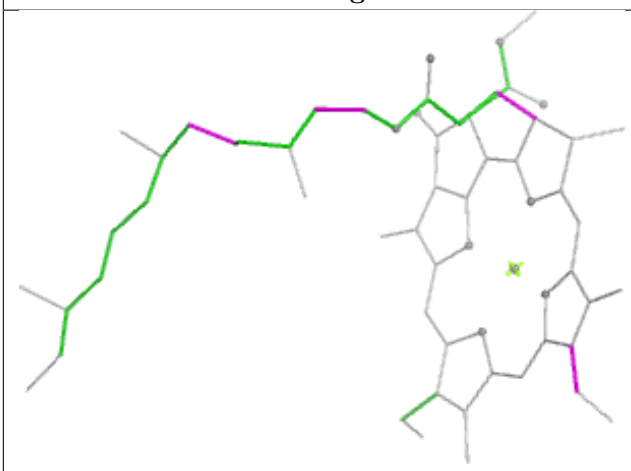

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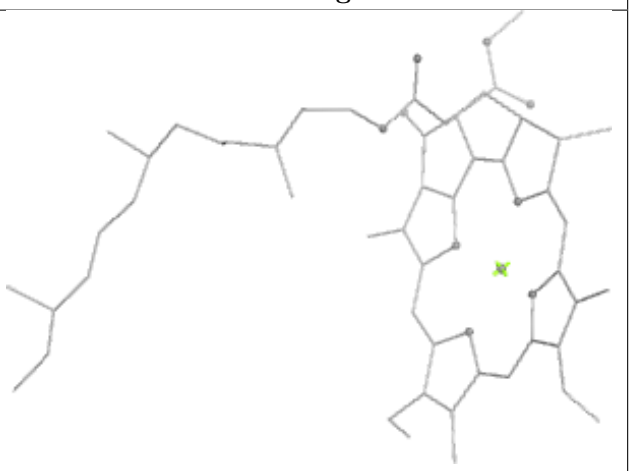
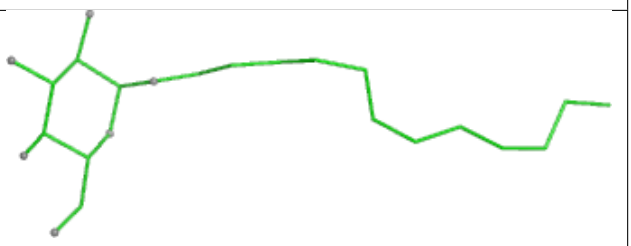


Rings

Ligand LMU 9 624



Bond lengths



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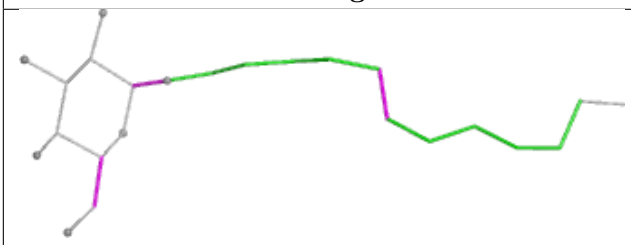

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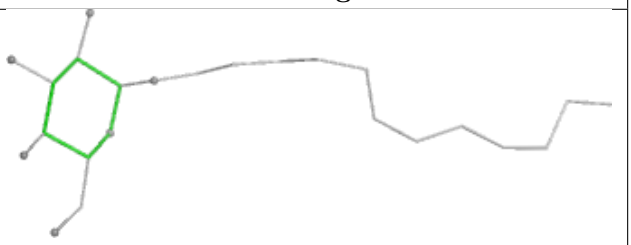
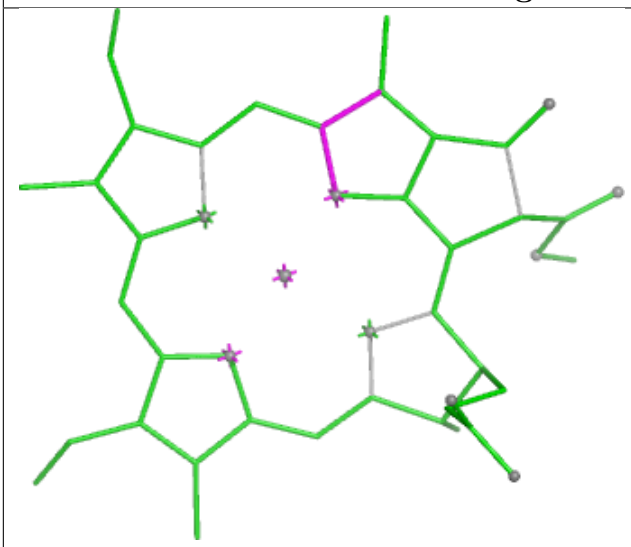


Rings

Ligand CLA B2 804



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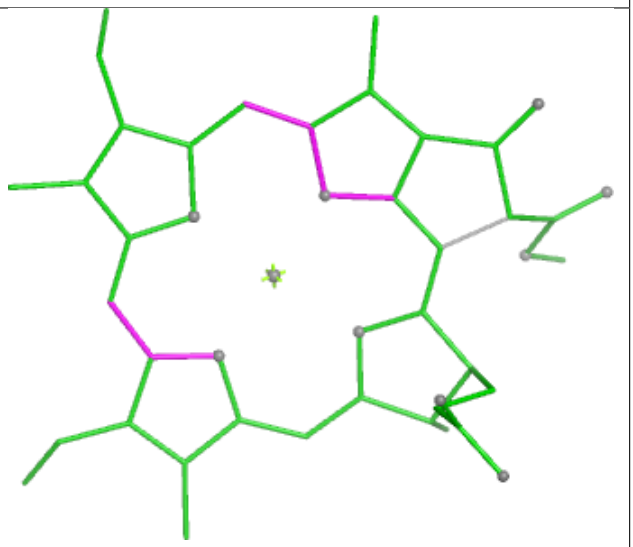
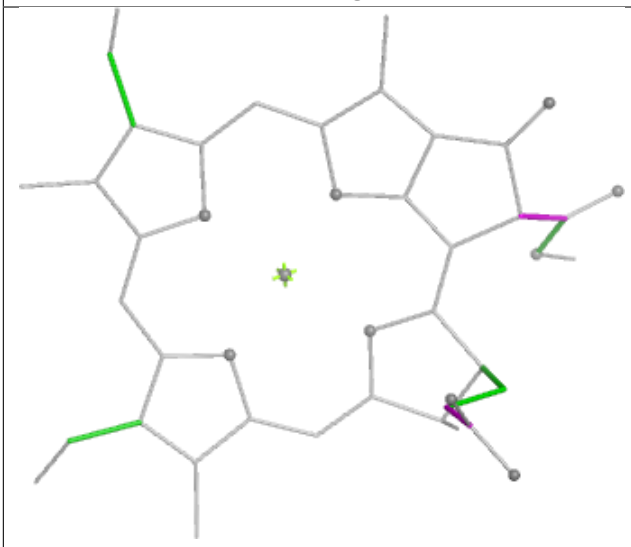


Bond angles



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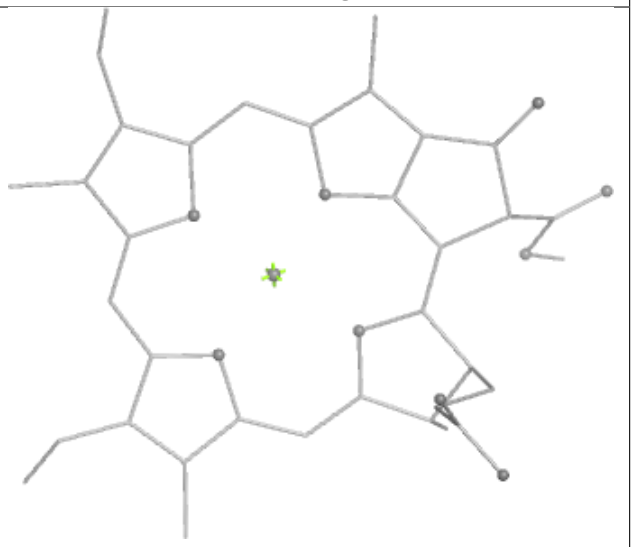
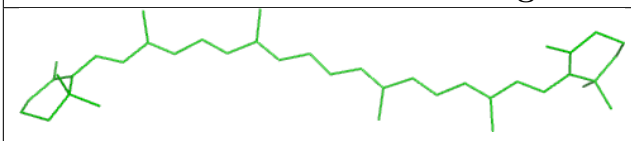


Rings

Ligand BCR 62 623



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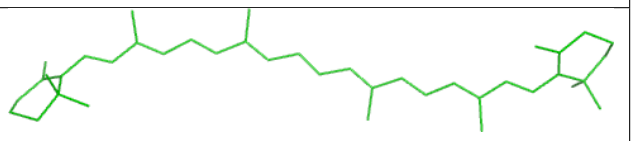

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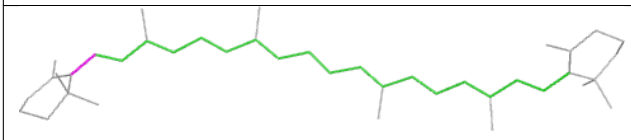

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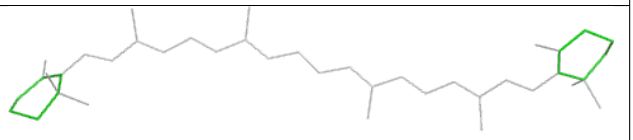
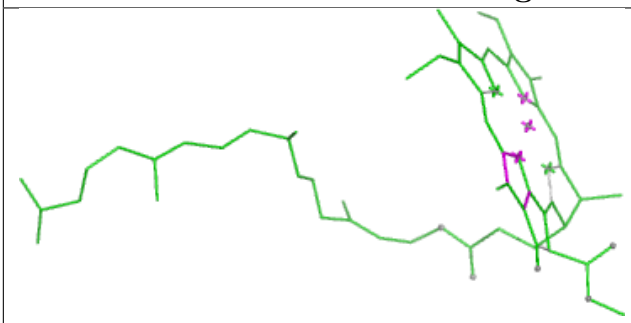


Rings

Ligand CLA A2 812



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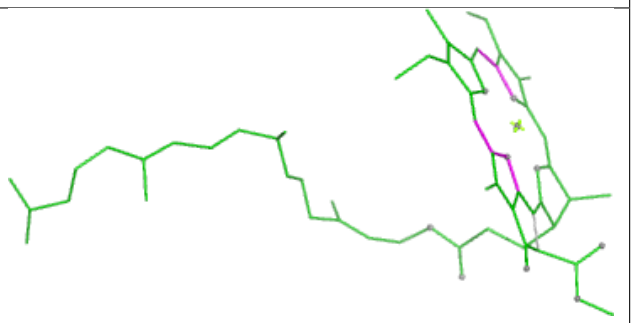

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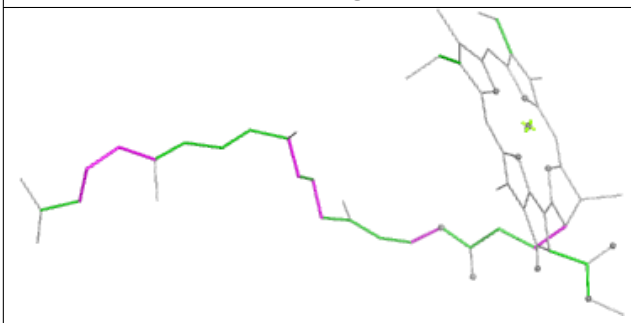
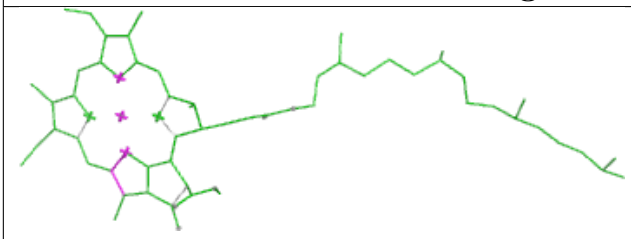


Torsions



Rings

Ligand CLA 52 617



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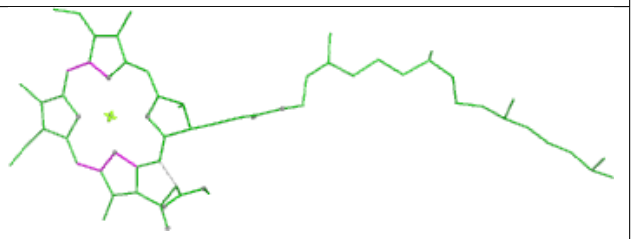
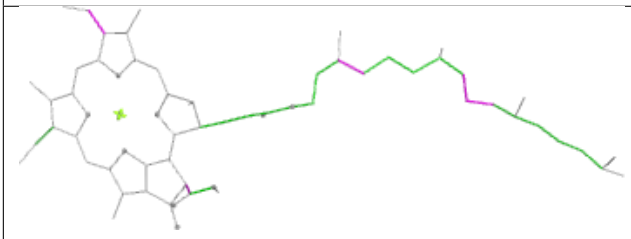


Bond angles



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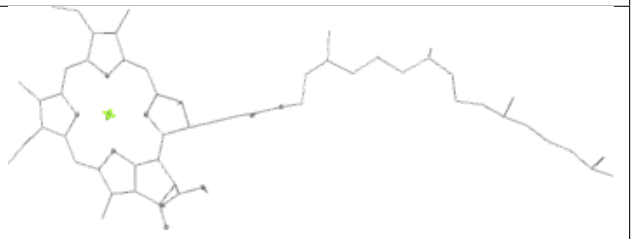
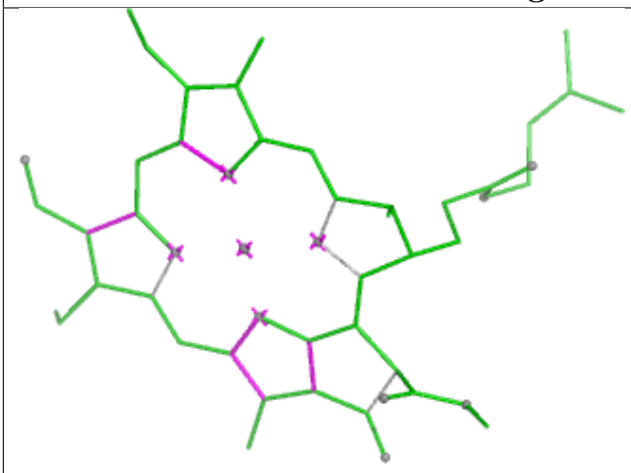


Rings

Ligand CHL 6 608



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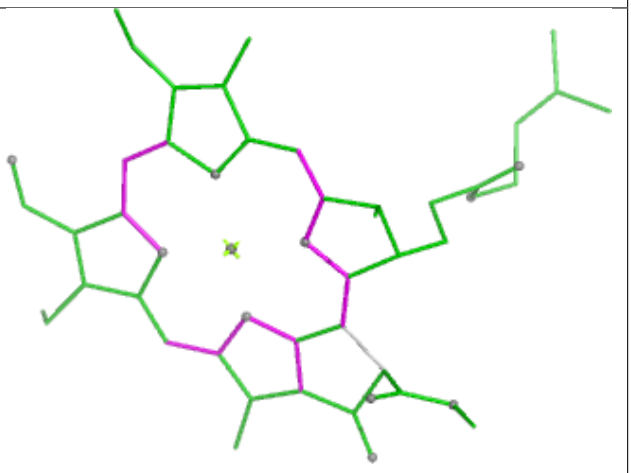

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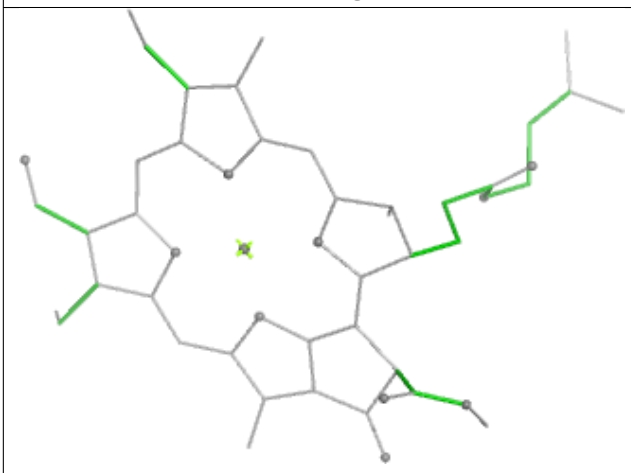

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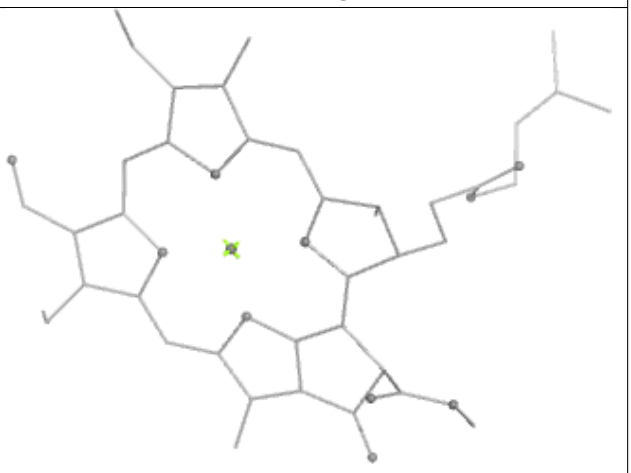
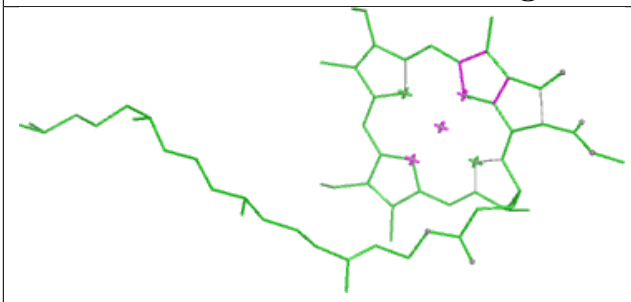


Rings

Ligand CLA 12 610



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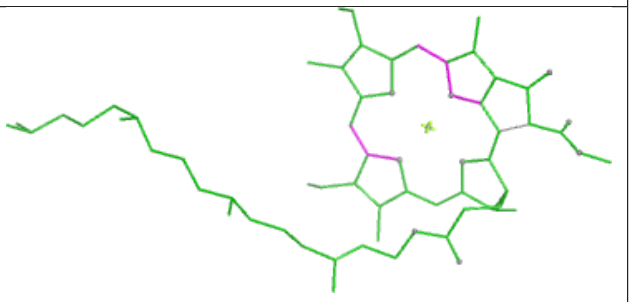
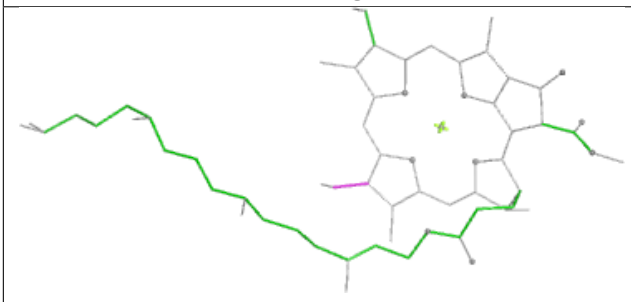


Bond angles



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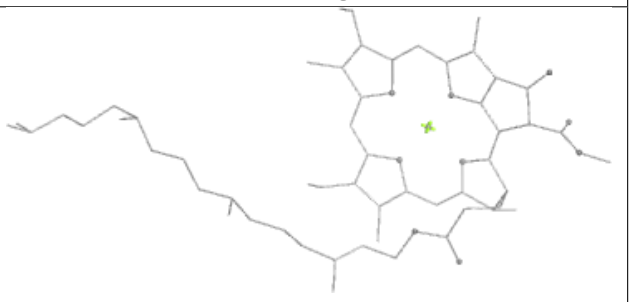
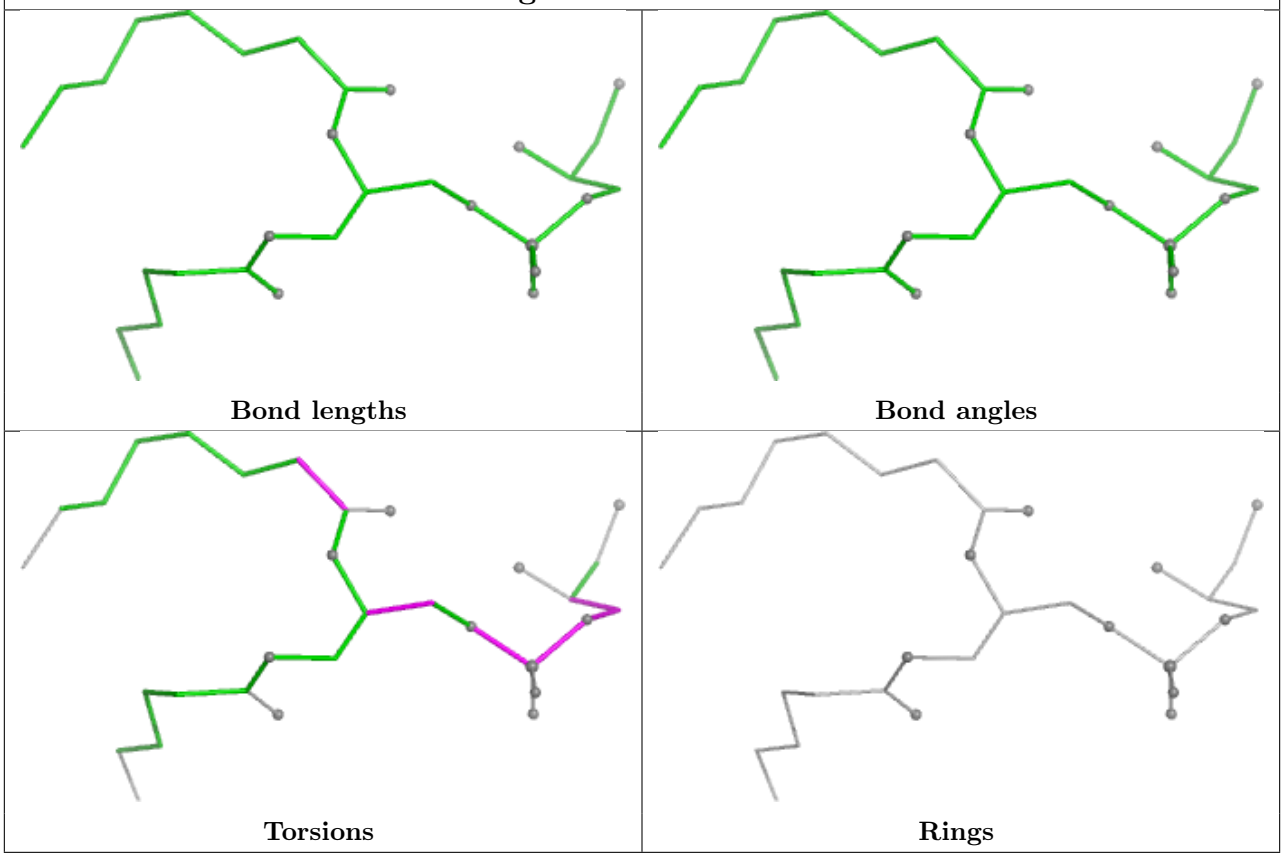
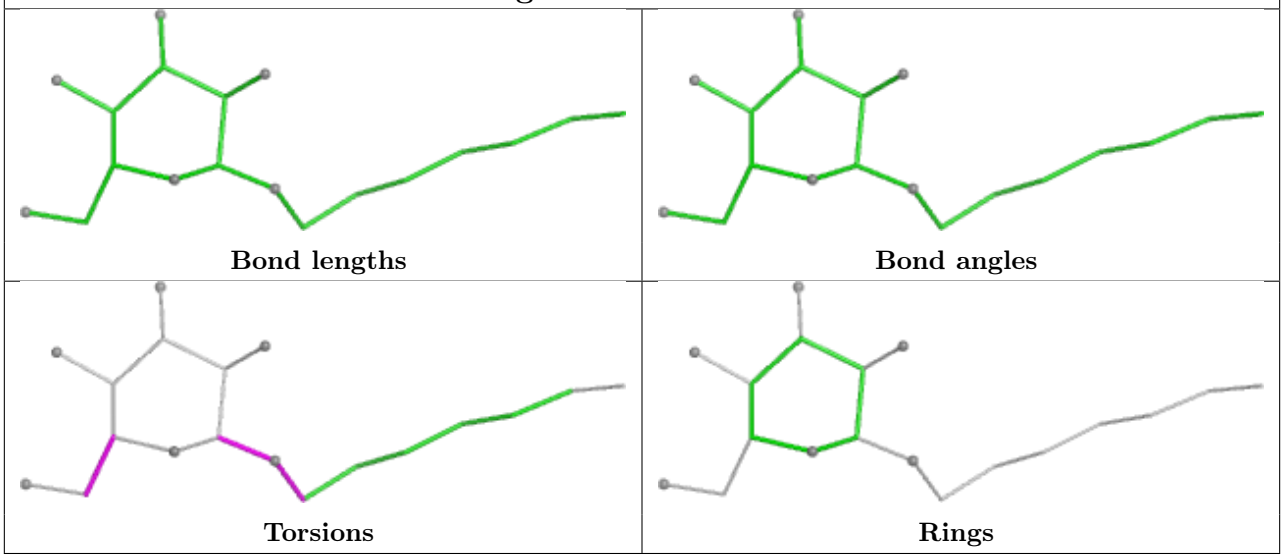


Rings

Ligand LHG 32 721



Ligand LMU 12 622



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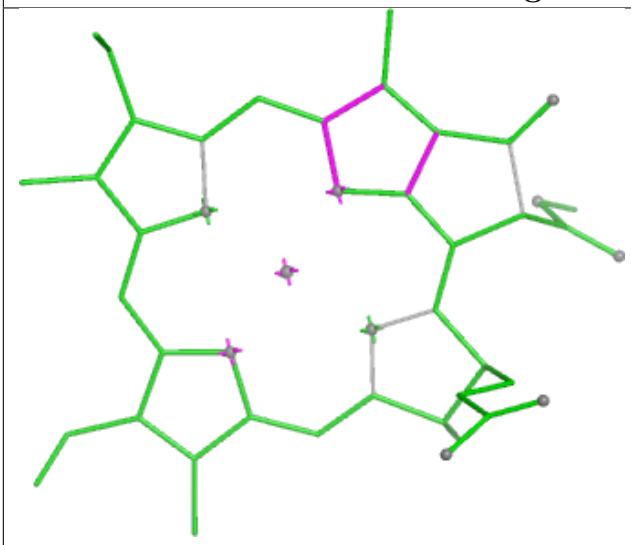

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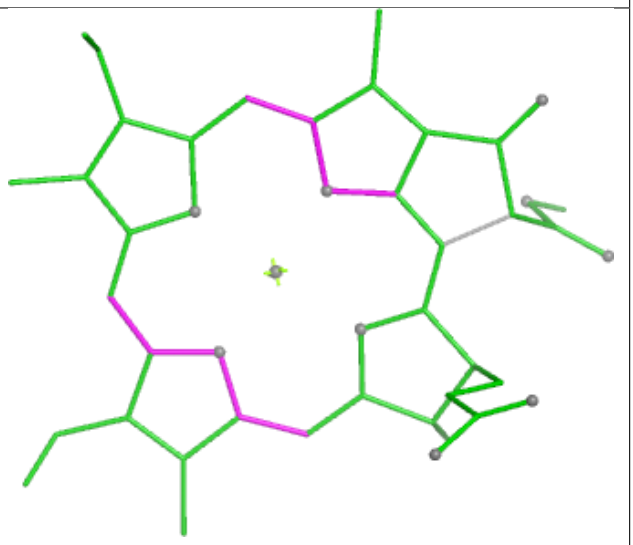

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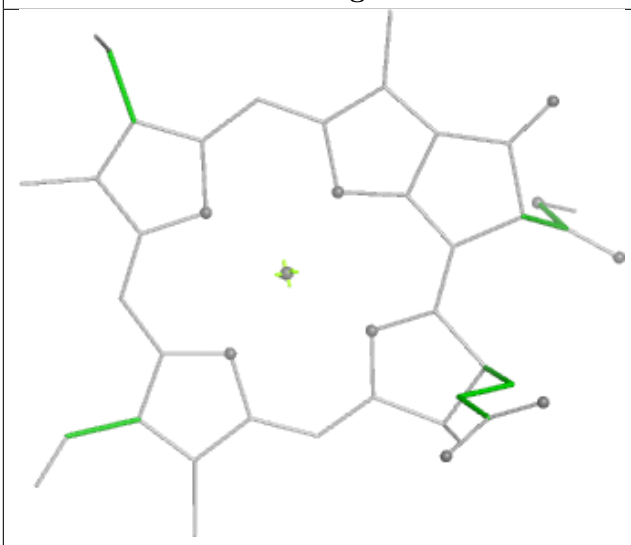

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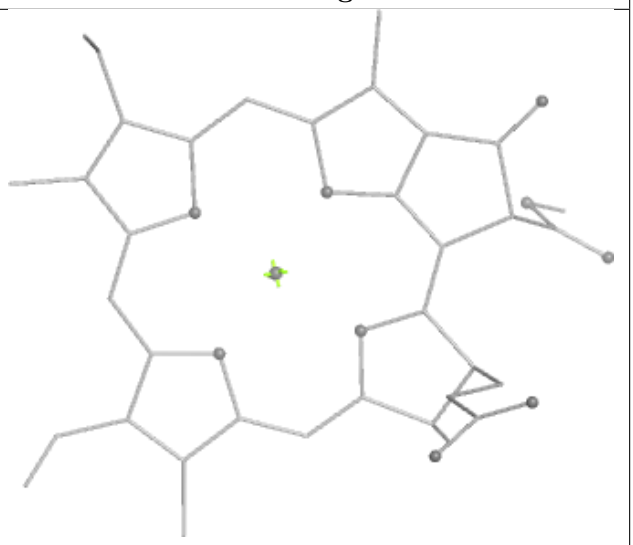
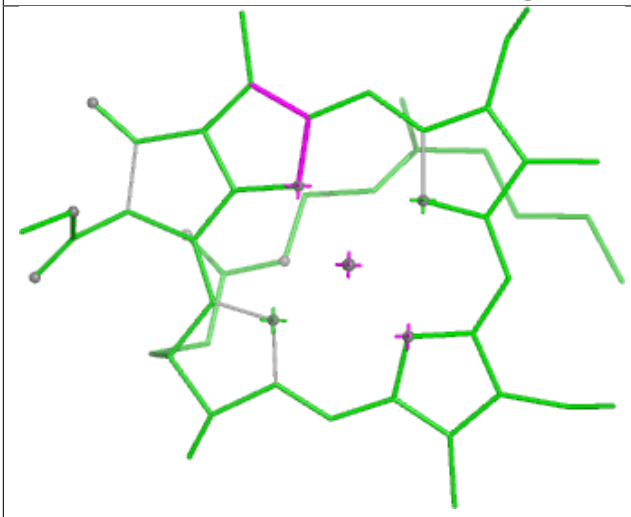


Rings

Ligand CLA 72 620



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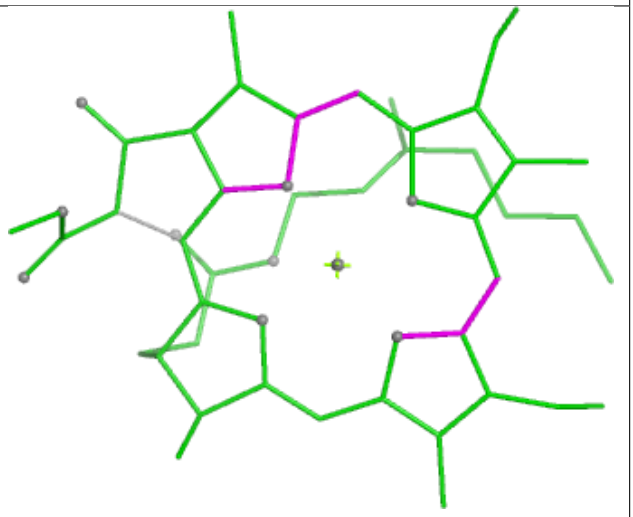
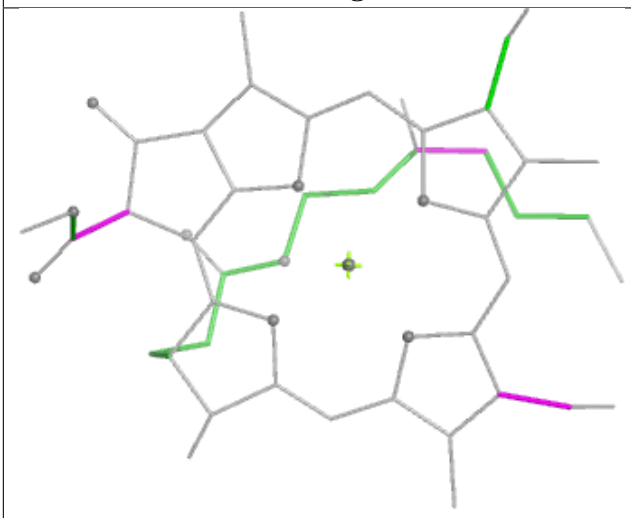


Bond angles



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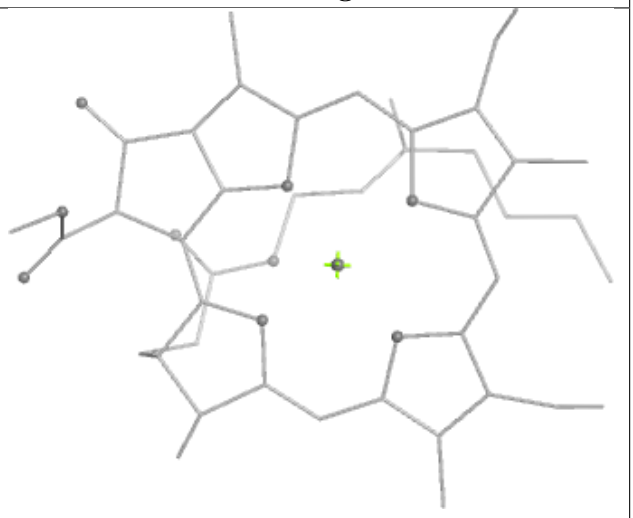
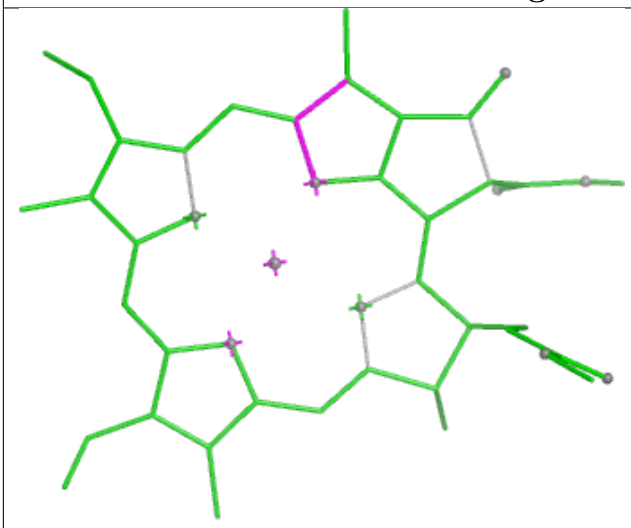


Rings

Ligand CLA 3 617



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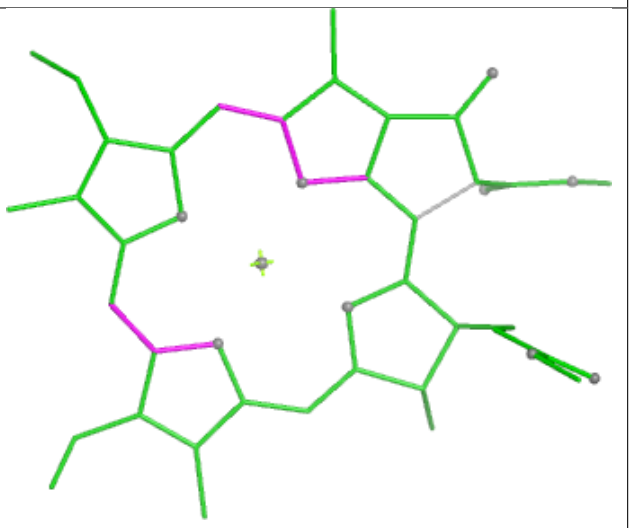
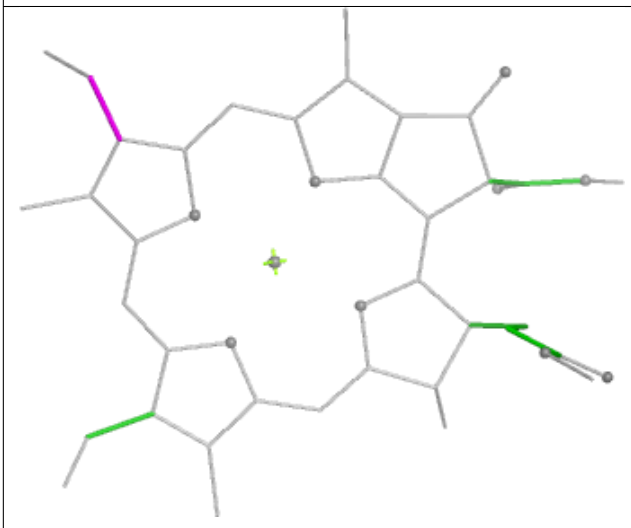


Bond angles



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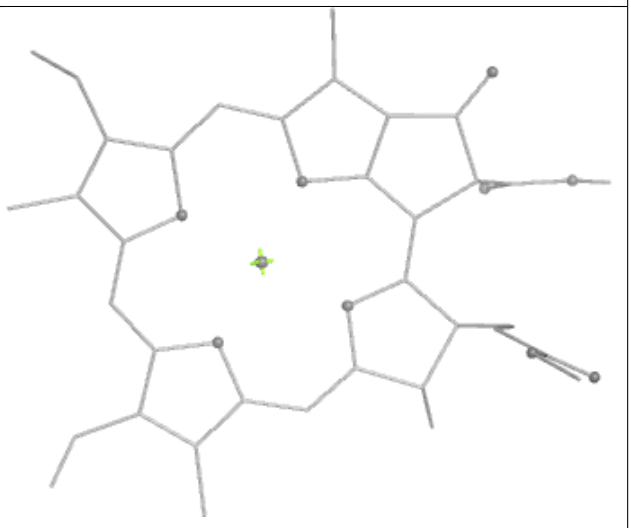


Rings

Ligand LMU 6 631



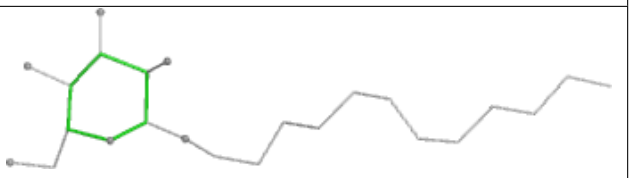
Bond lengths



Bond angles

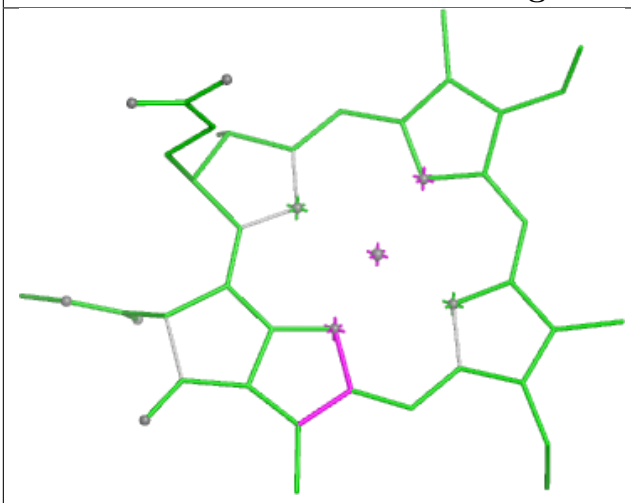


Torsions



Rings

Ligand CLA 8 609



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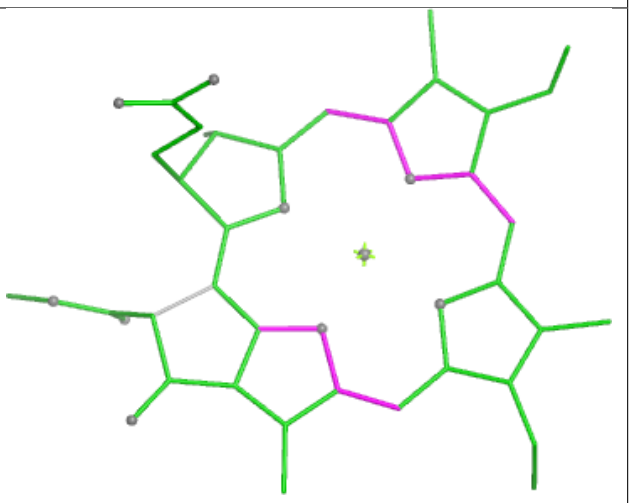

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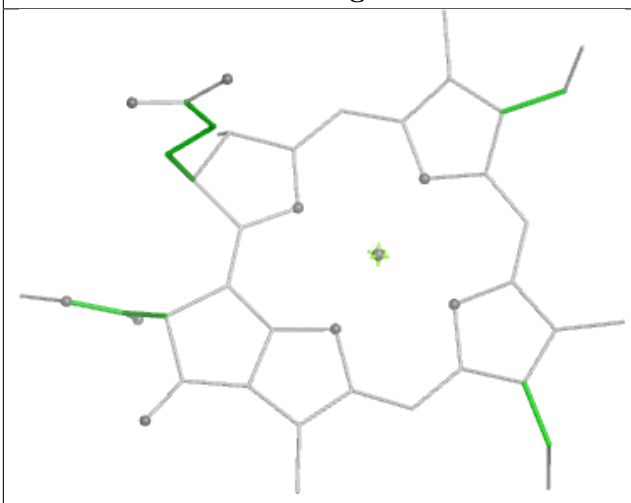

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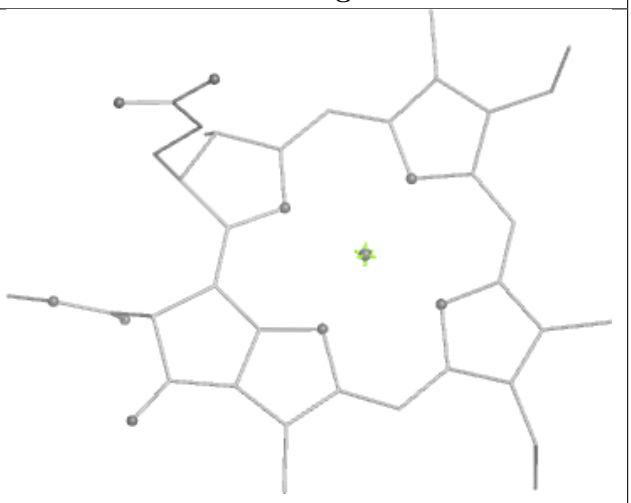
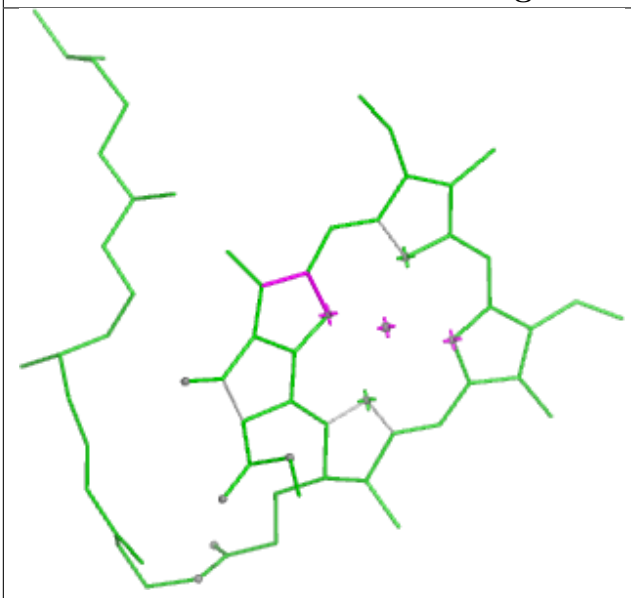


Rings

Ligand CLA A2 826



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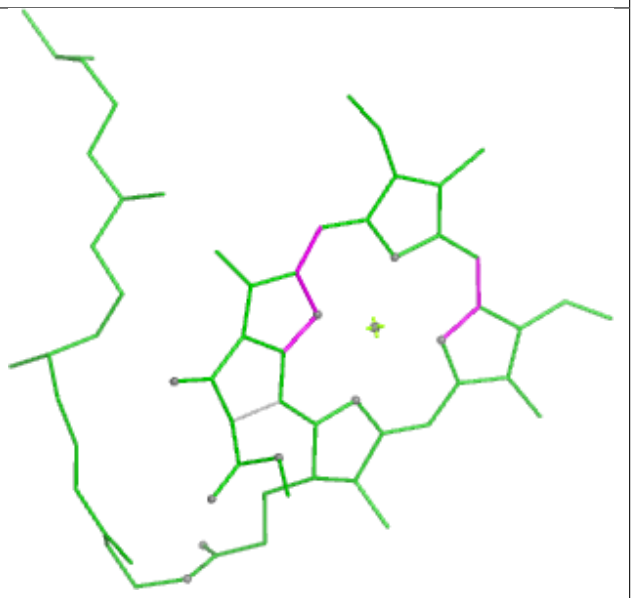

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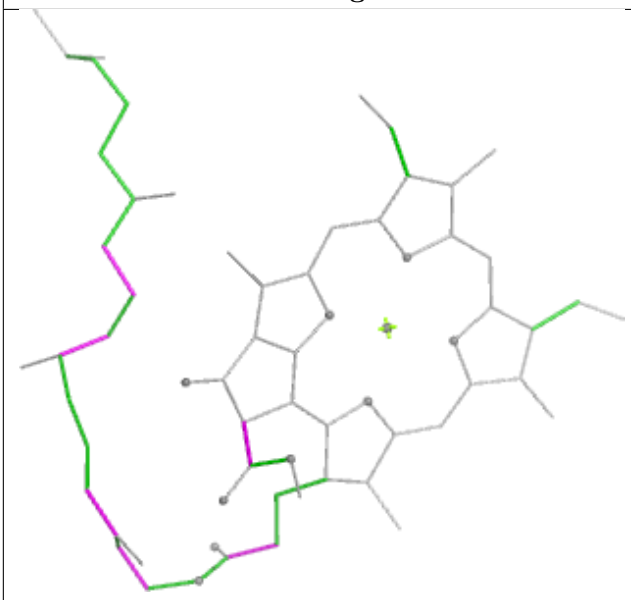

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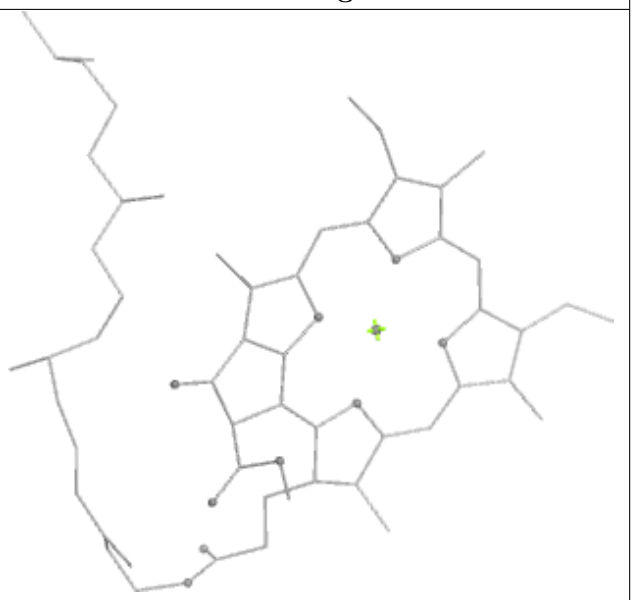
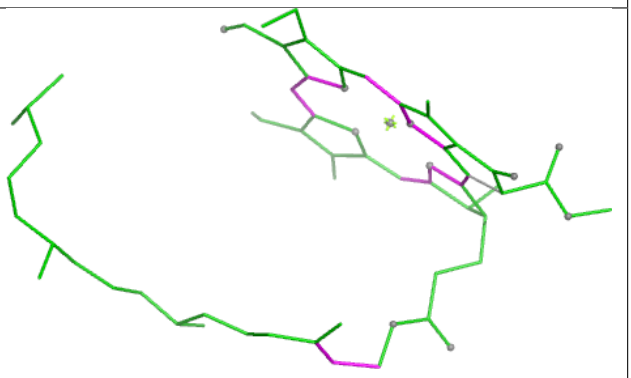


Rings

Ligand CHL 6 607



Bond lengths



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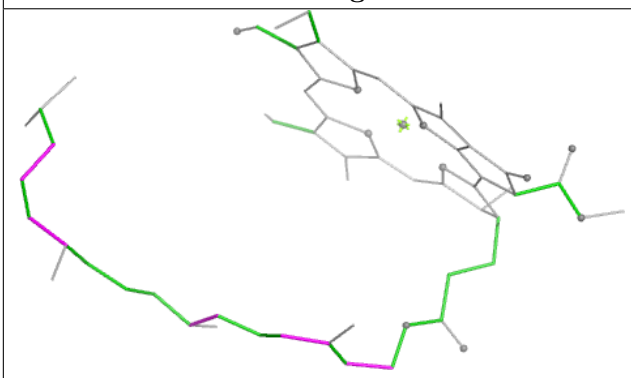
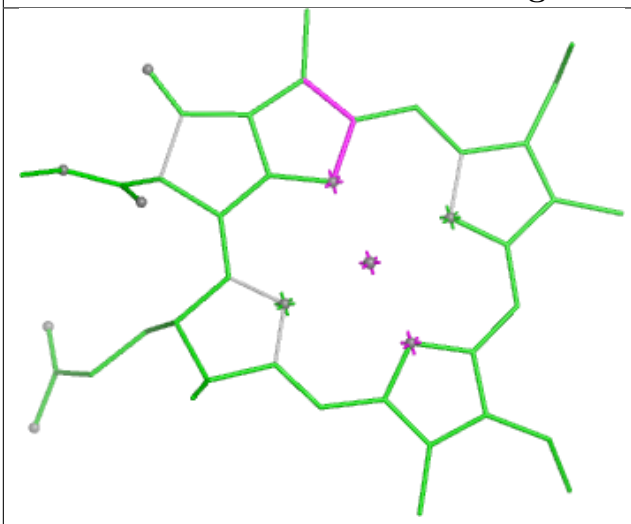


Torsions



Rings

Ligand CLA 4 616



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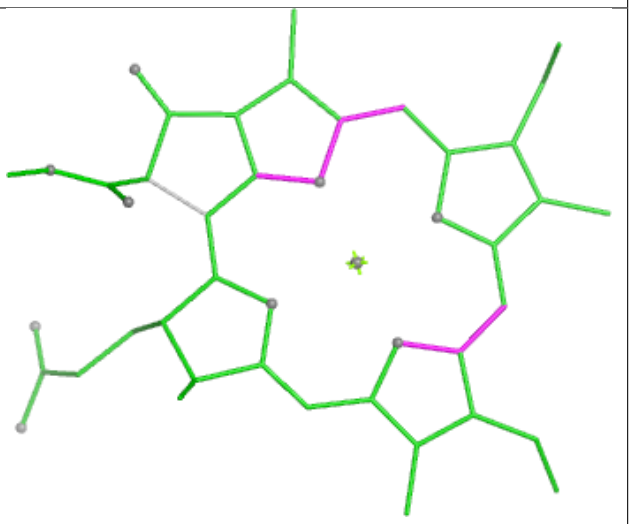

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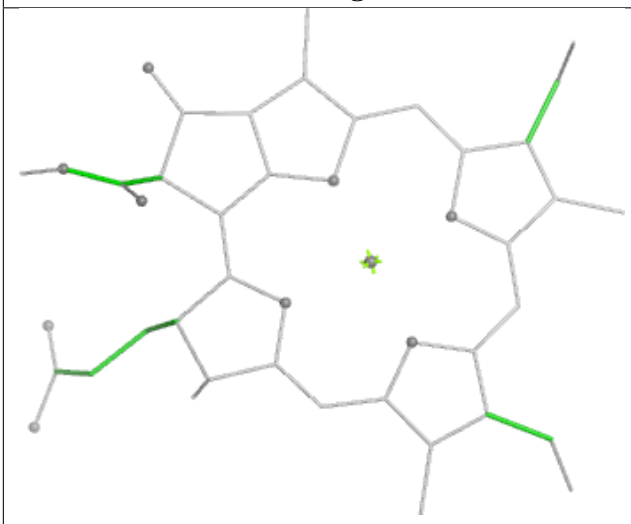

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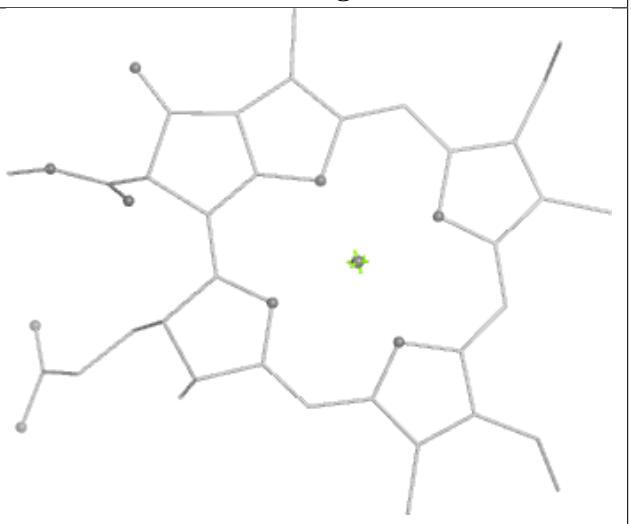
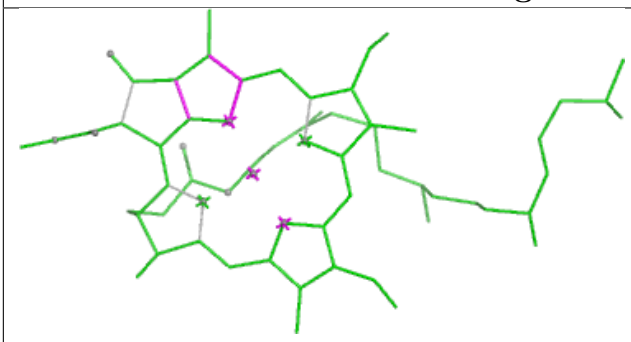


Rings

Ligand CLA A2 839



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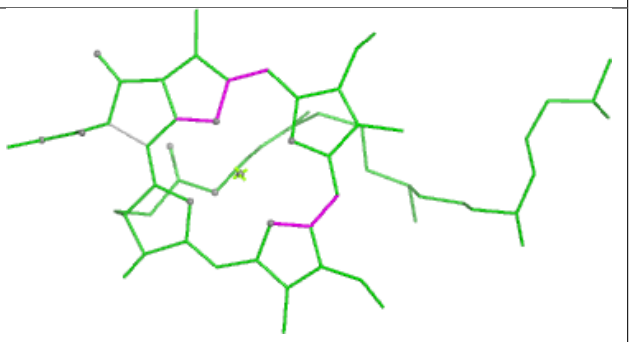

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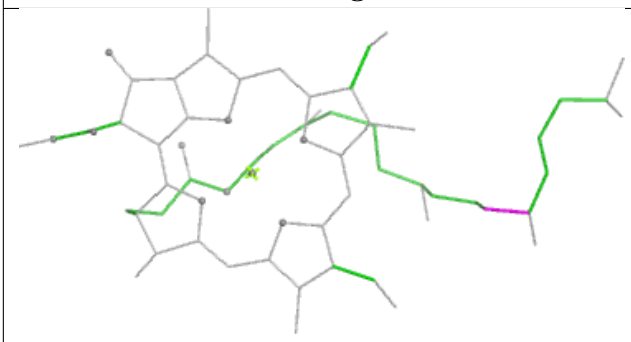
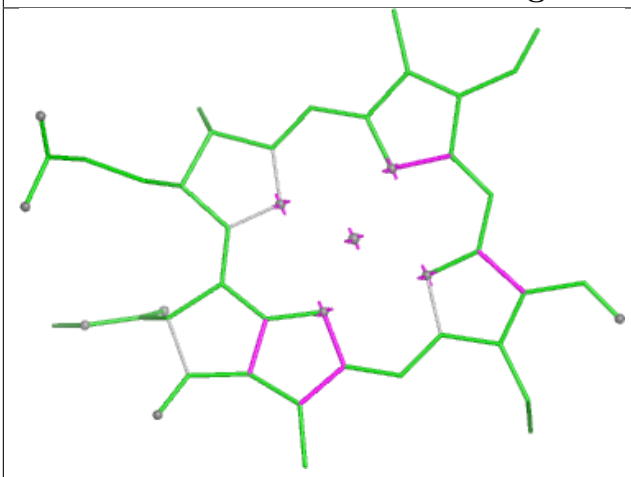


Torsions



Rings

Ligand CHL 7 606



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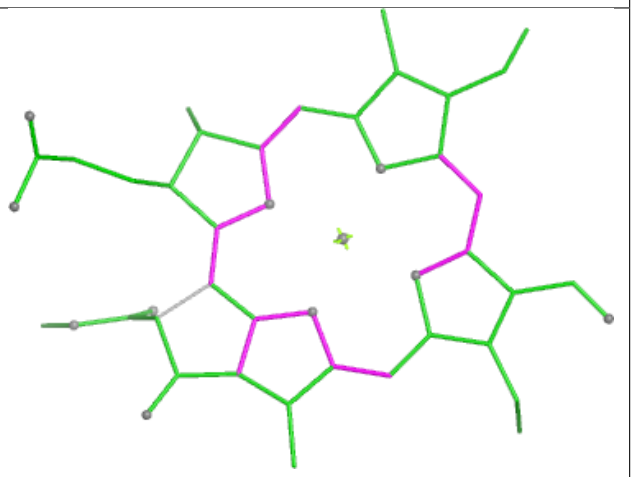

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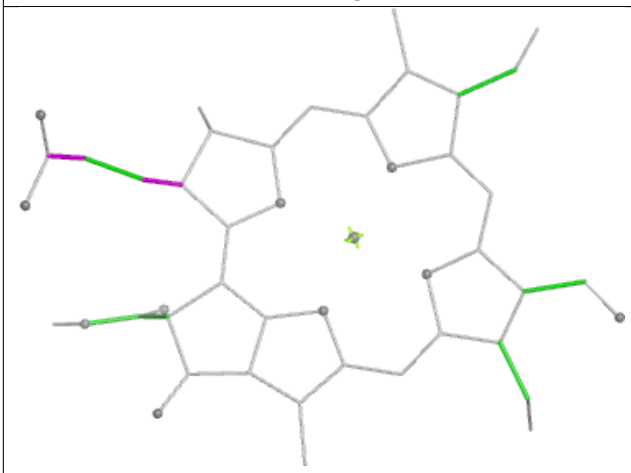

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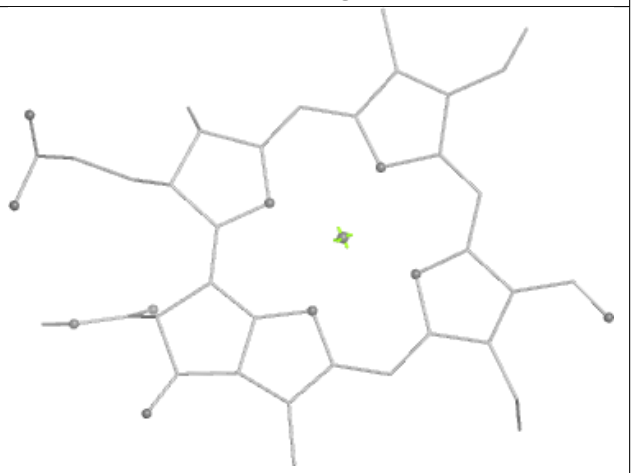

Rings

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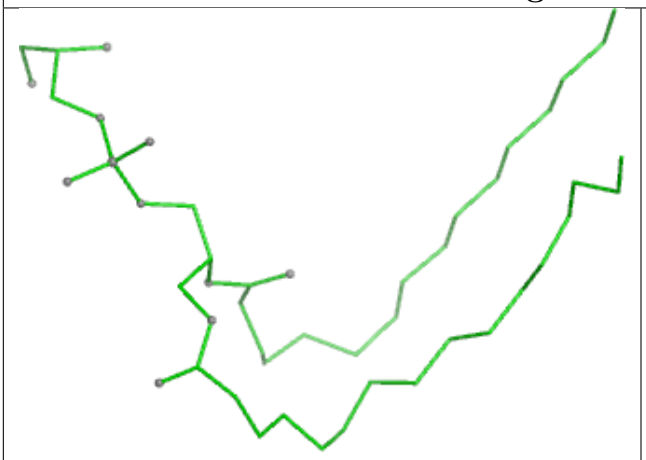

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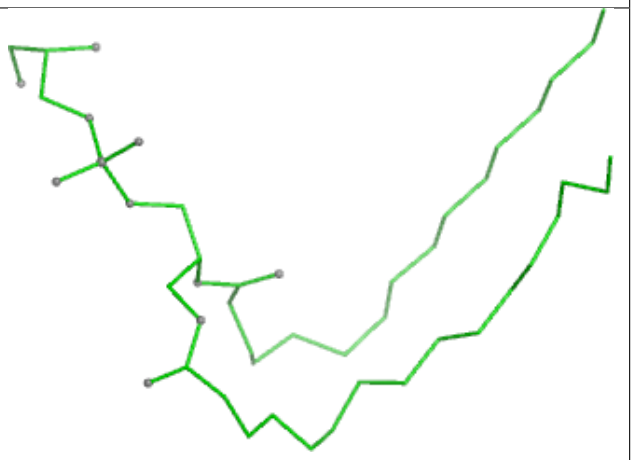

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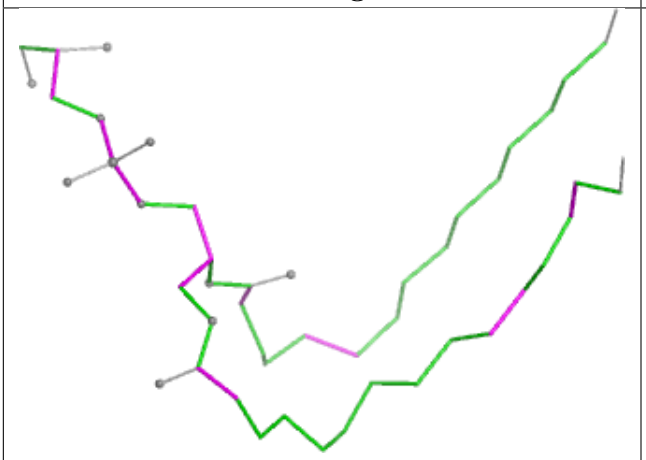

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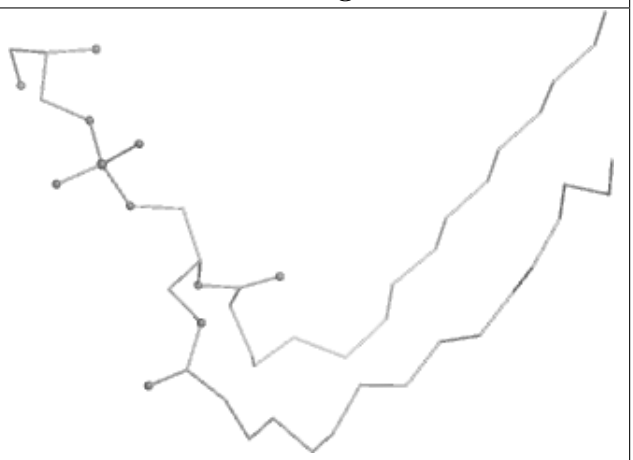
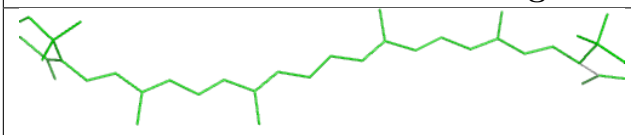


Rings

Ligand LUT 9 616



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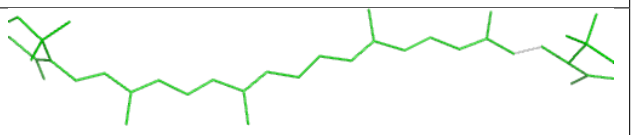
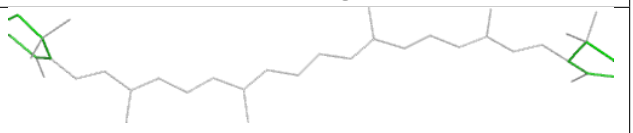


Bond angles

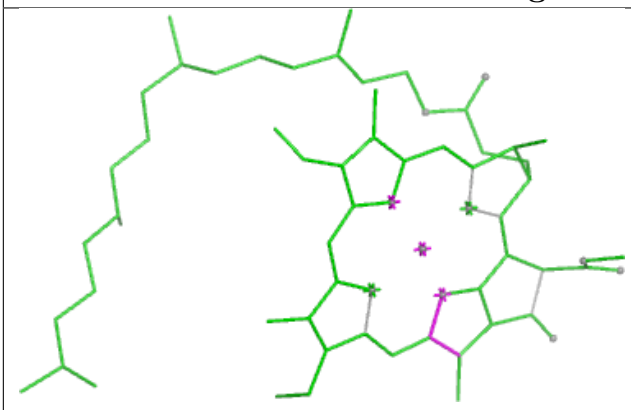


Torsions



Rings

Ligand CLA 7 602



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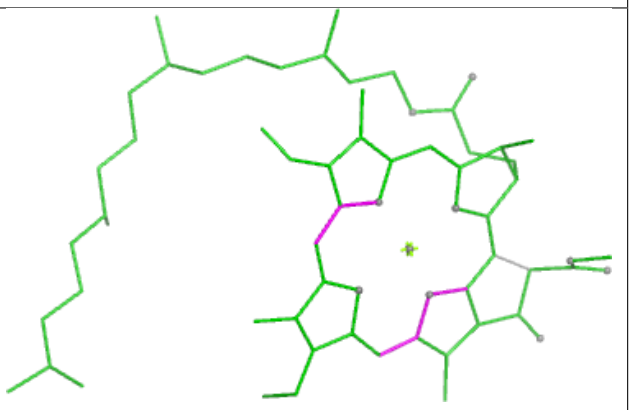

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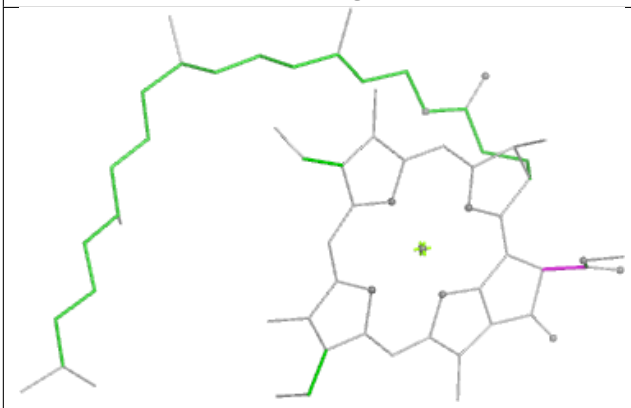

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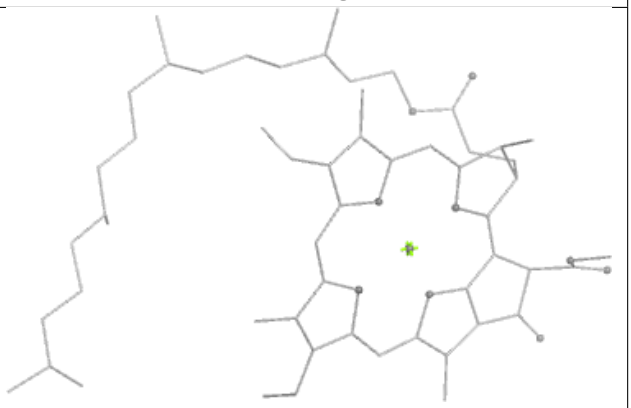
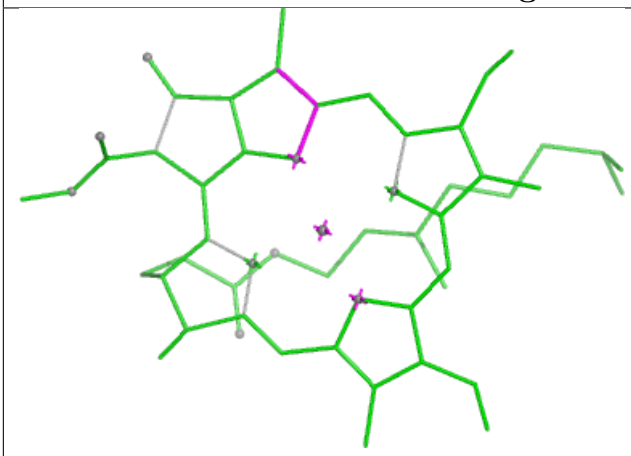


Rings

Ligand CLA J2 101



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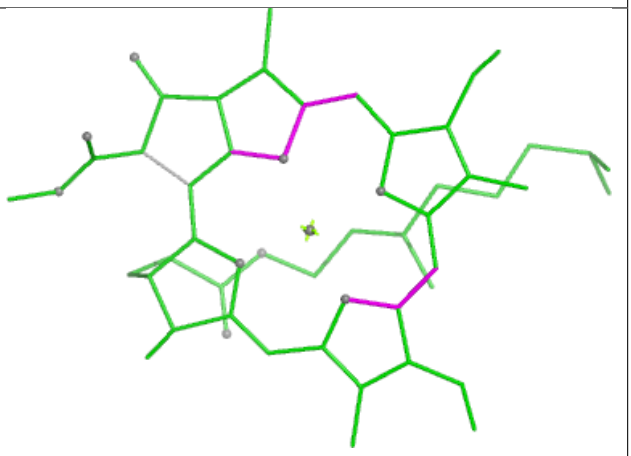

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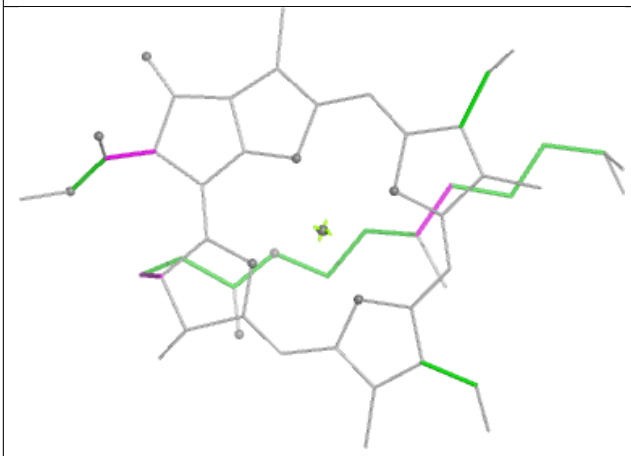

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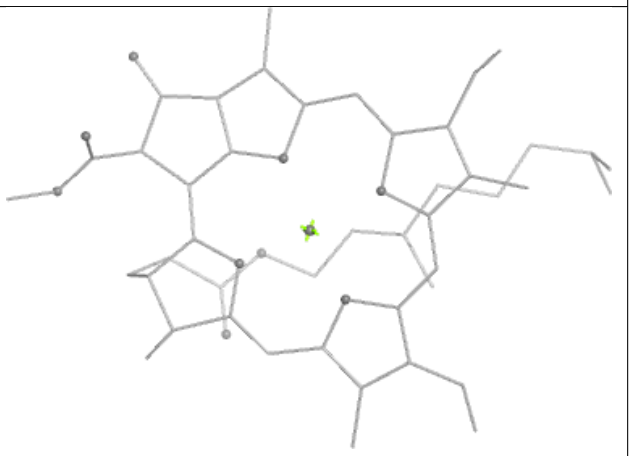
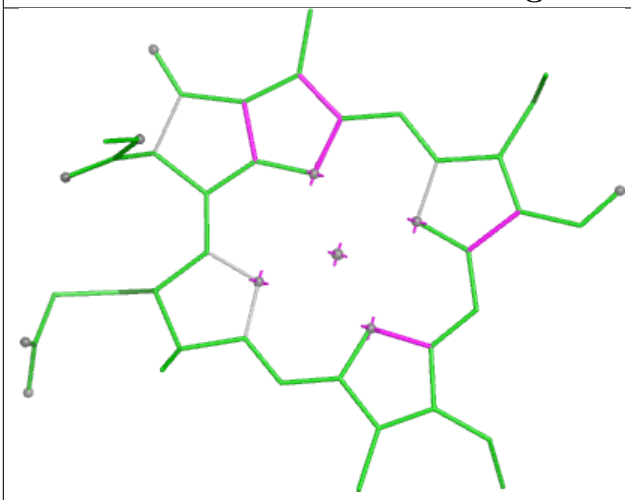


Rings

Ligand CHL Z 606



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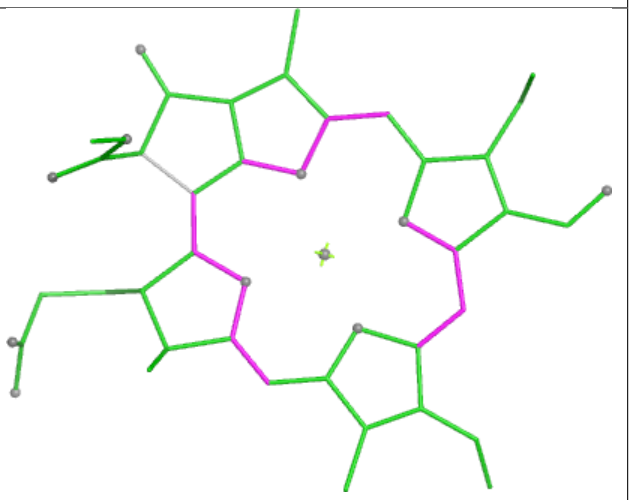

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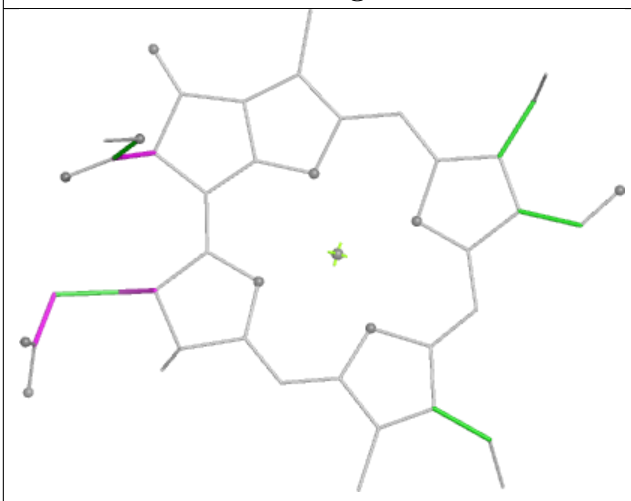

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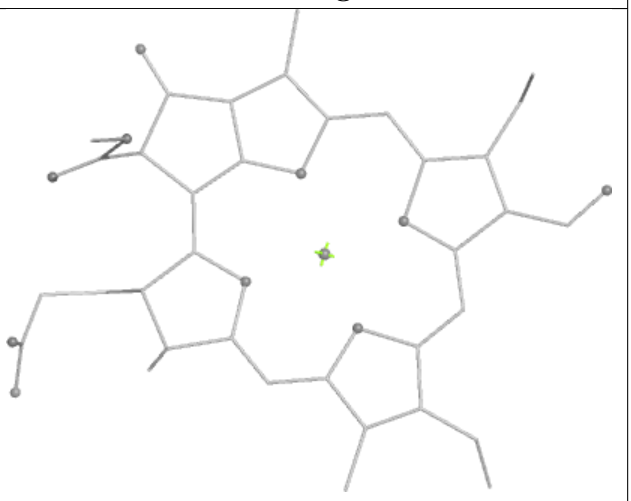


Rings

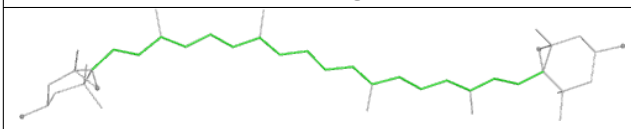
Ligand XAT Z 618



Bond lengths



Bond angles



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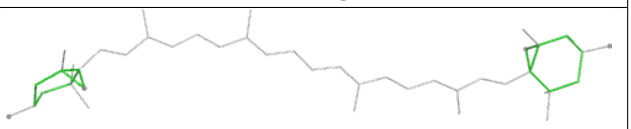

Rings

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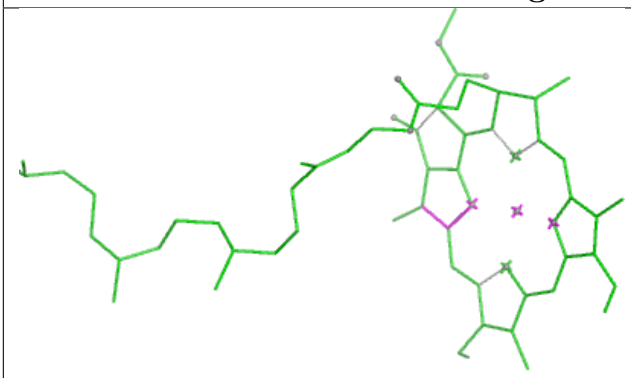

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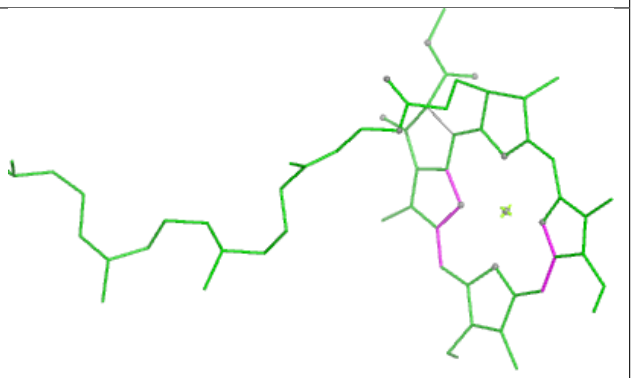
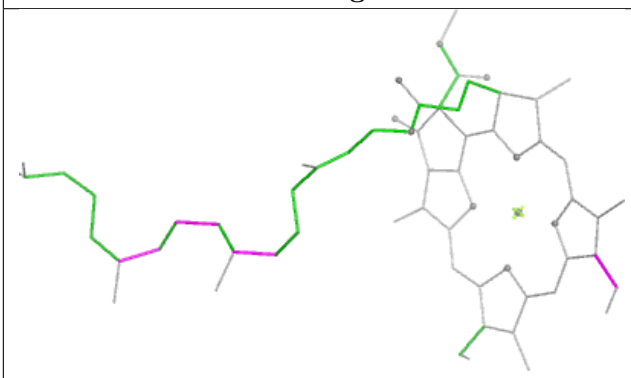


Bond angles

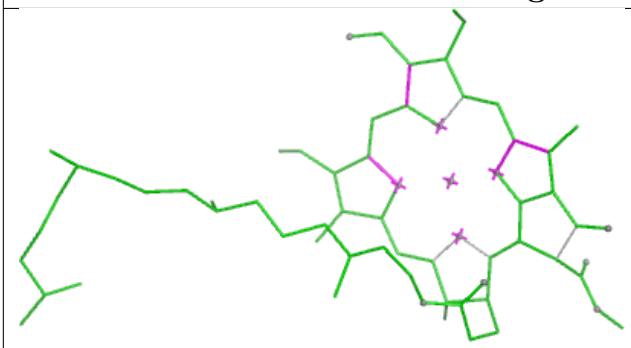


Torsions



Rings

Ligand CHL 8 607



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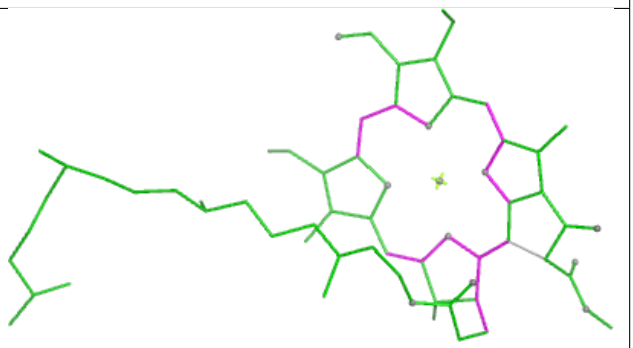

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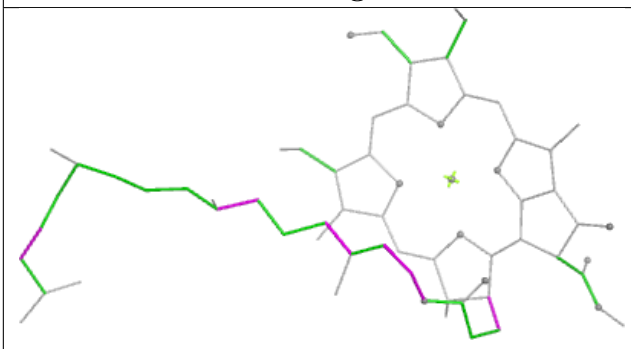

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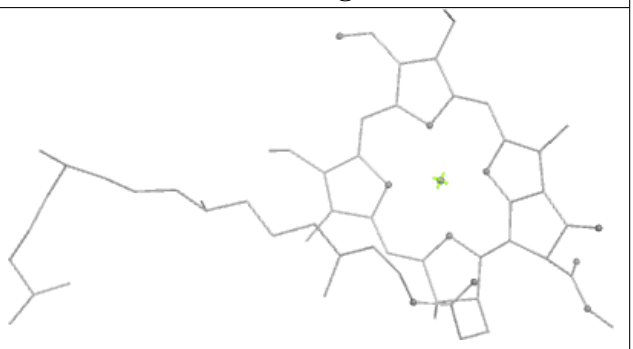
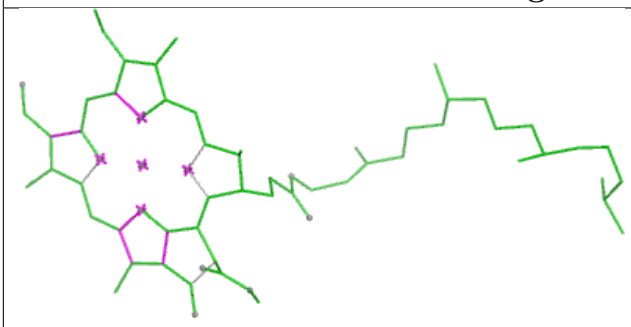


Rings

Ligand CHL 3 608



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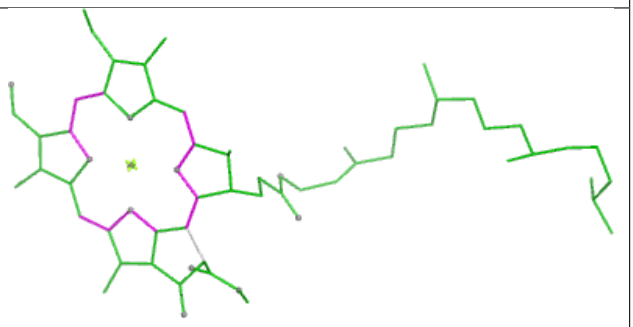

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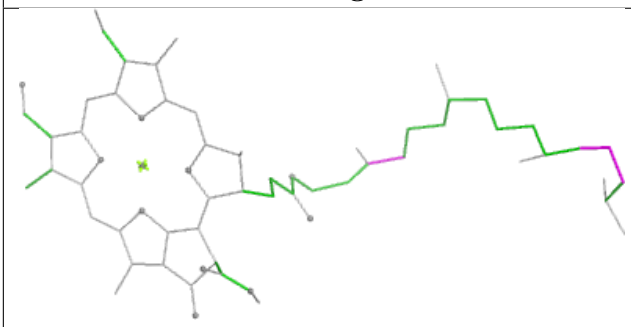

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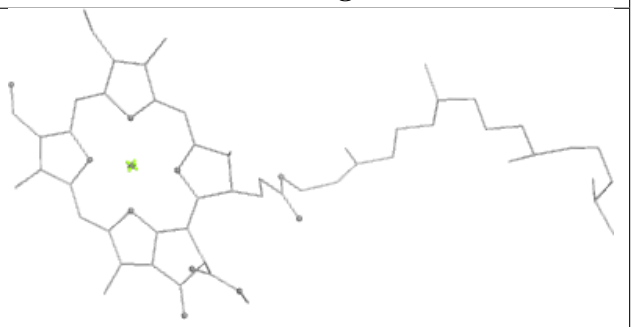
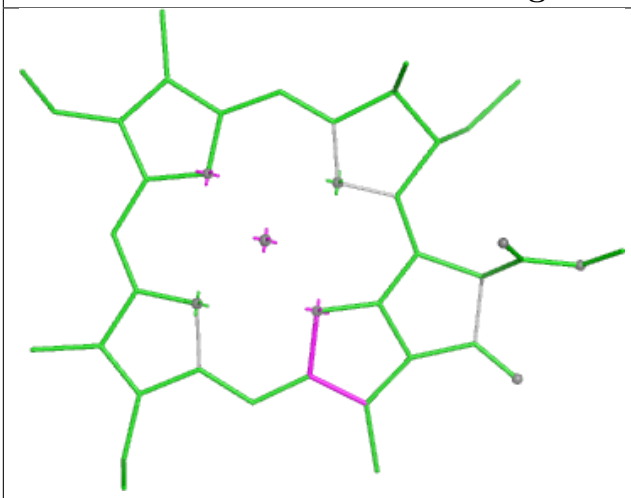


Rings

Ligand CLA 3 606



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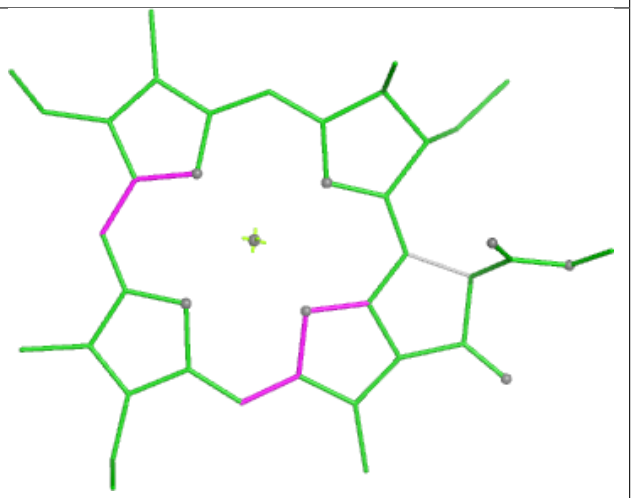
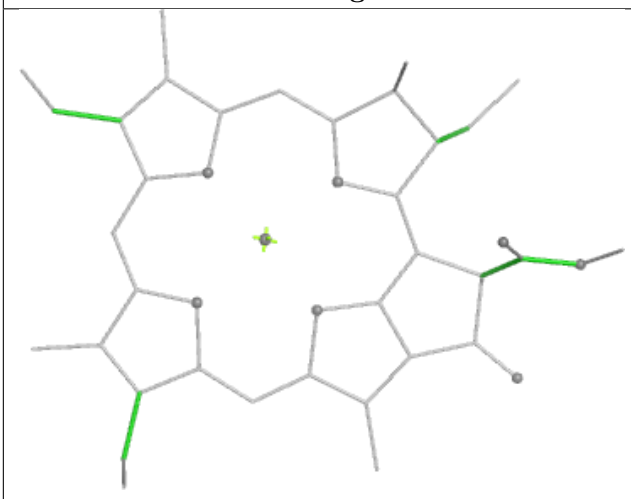


Bond angles



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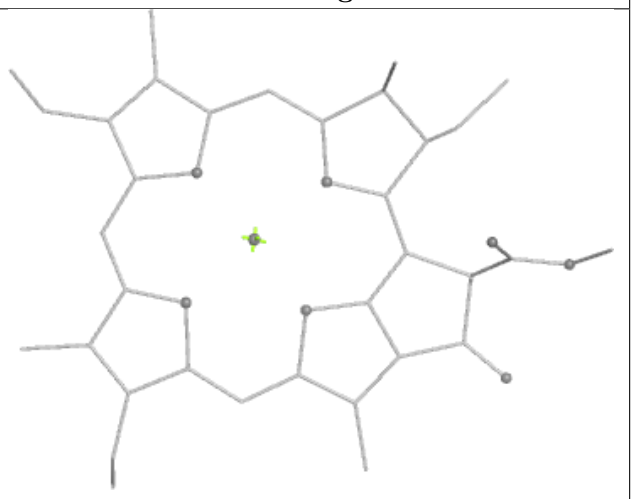
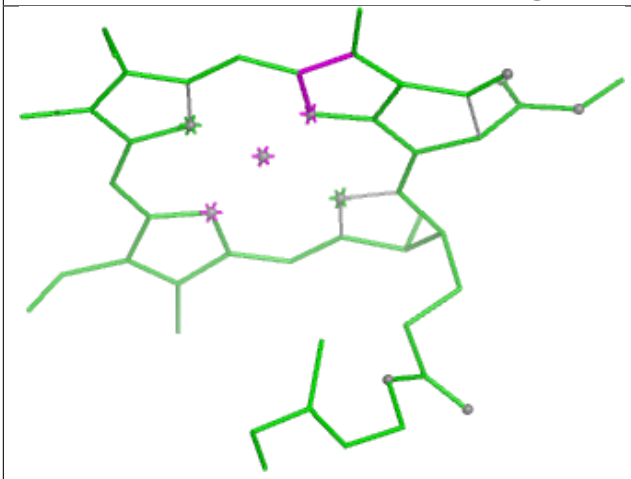


Rings

Ligand CLA 9 609



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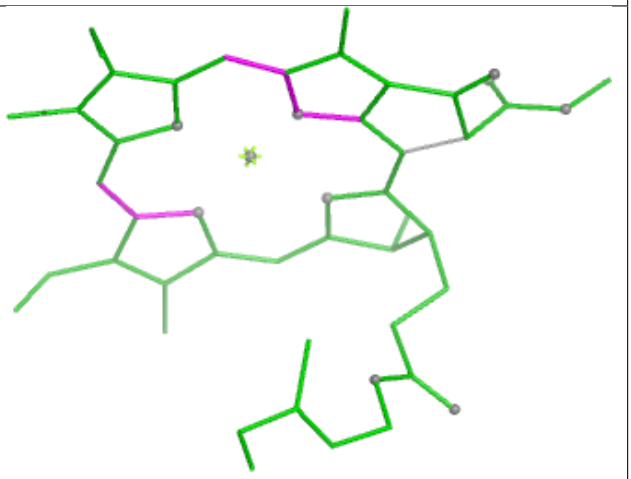
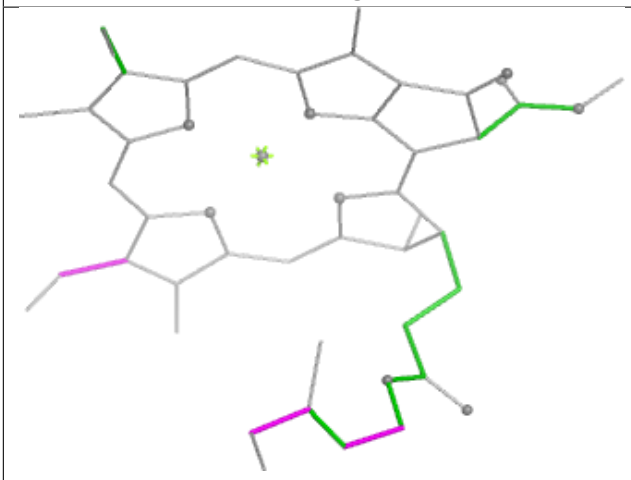
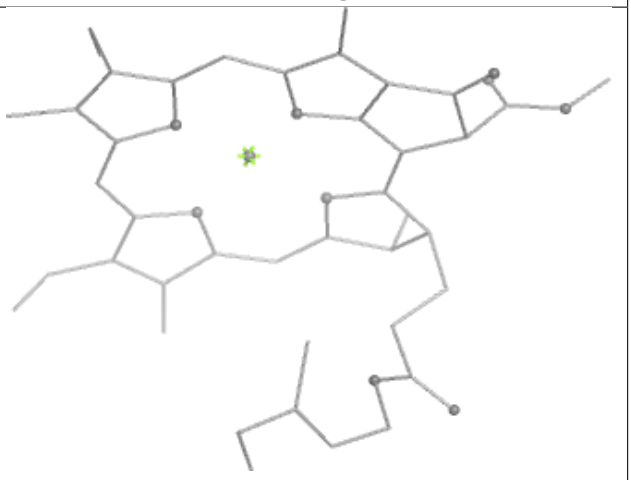


Bond angles

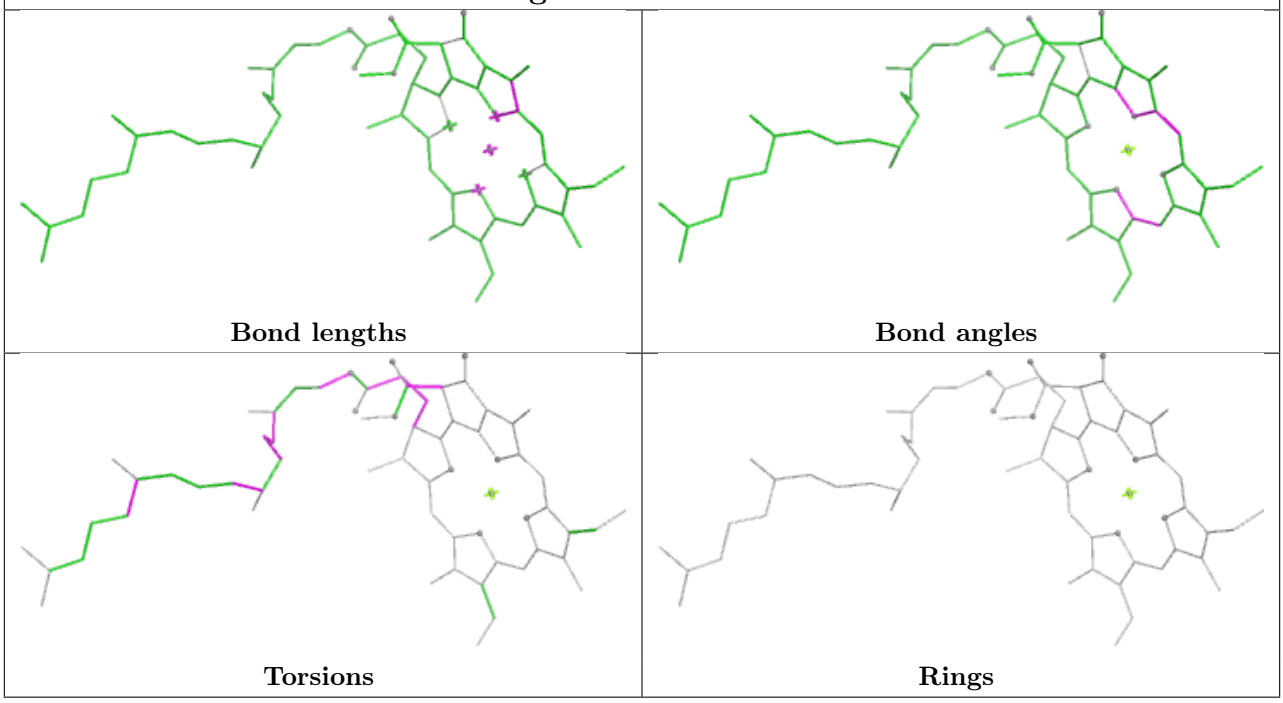


Torsions

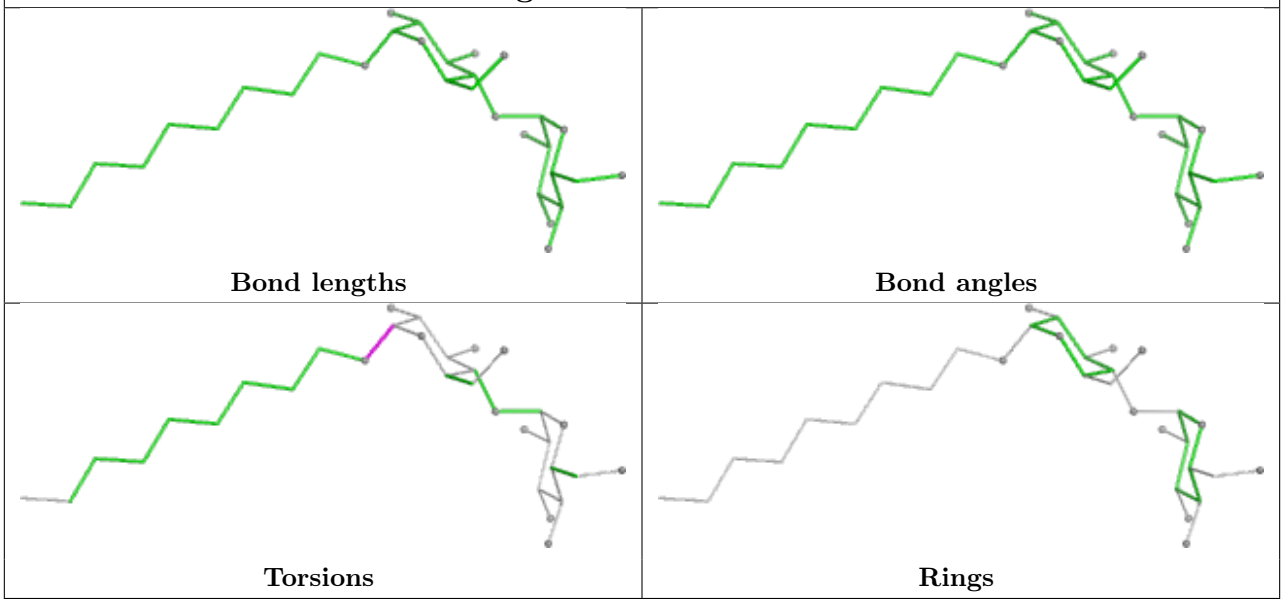


Rings

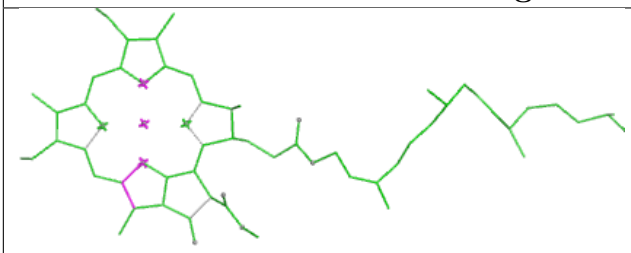
Ligand CLA 5 603



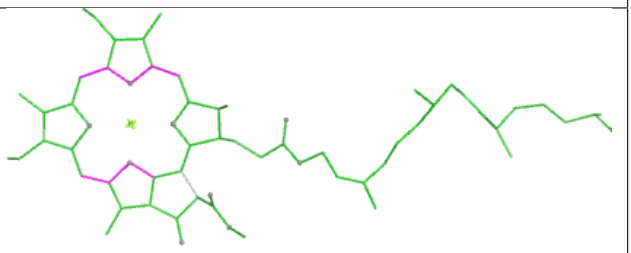
Ligand LMU 72 627



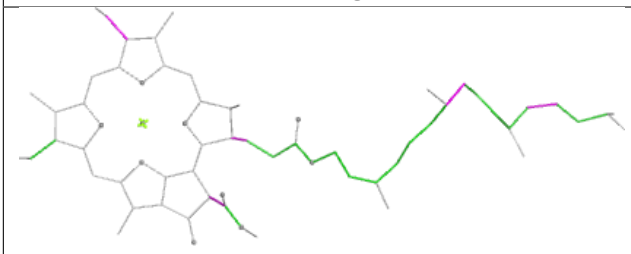
Ligand CLA A2 834



Bond lengths



Bond angles



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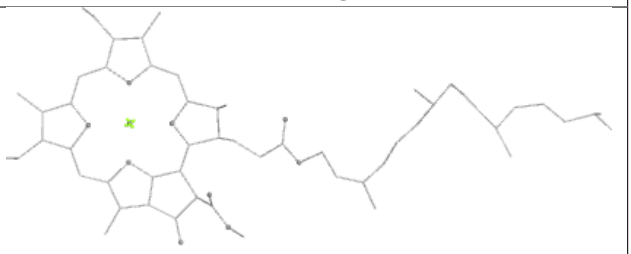
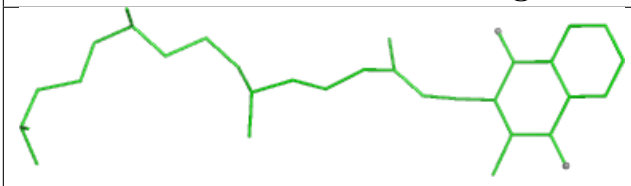


Rings

Ligand PQN A2 844



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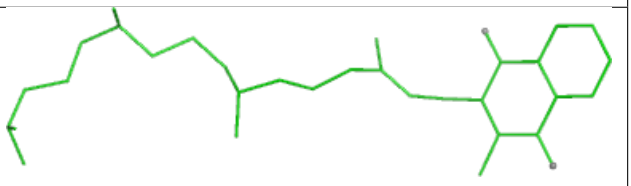
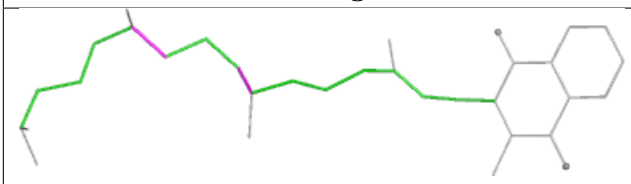


Bond angles



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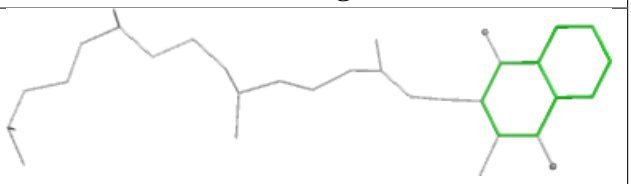
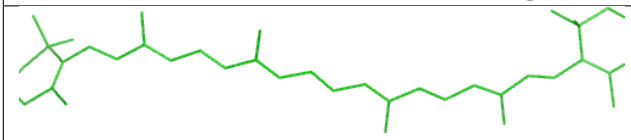


Rings

Ligand BCR K 202



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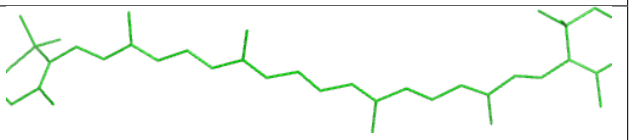
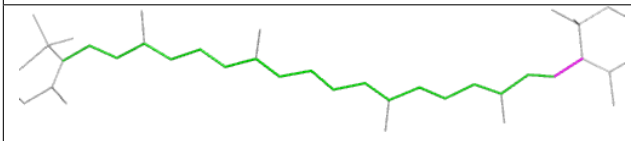


Bond angles



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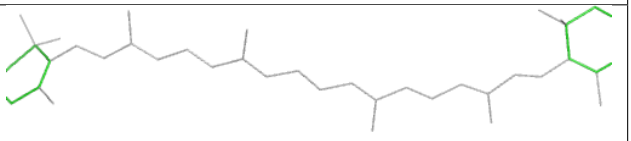
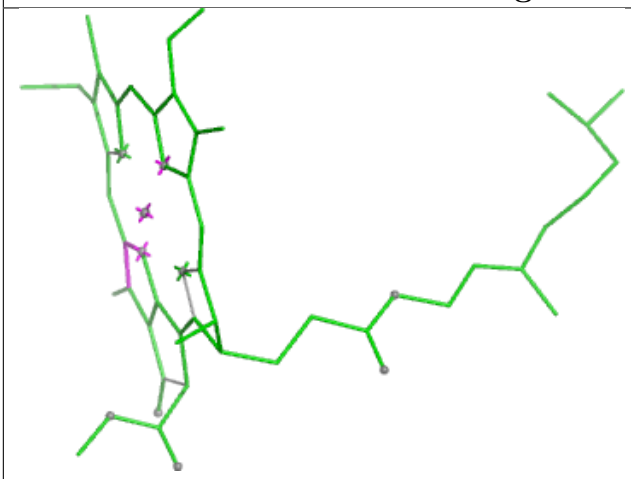


Rings

Ligand CLA A2 832



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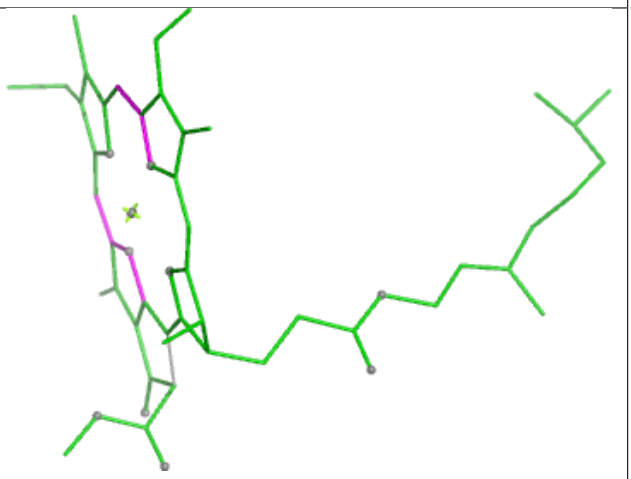
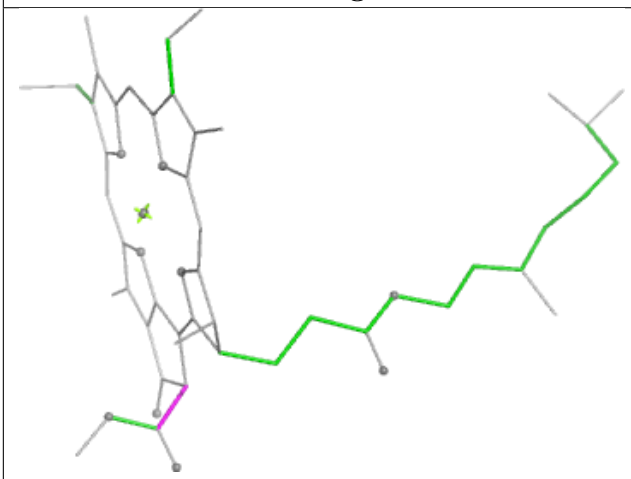


Bond angles



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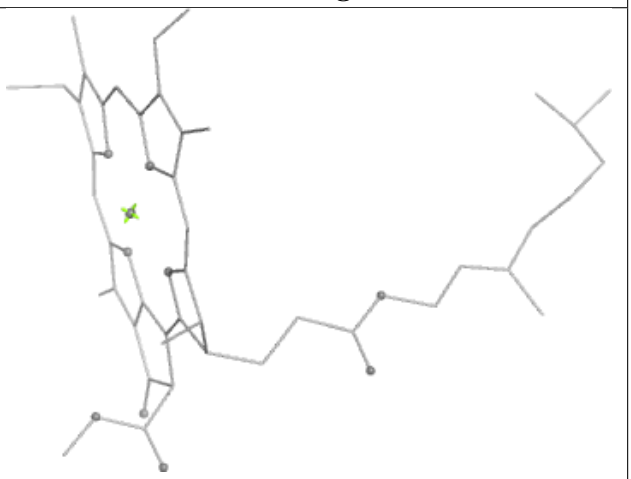
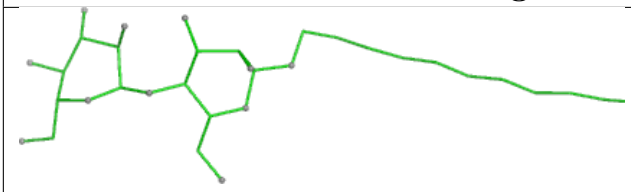


Rings

Ligand LMU A2 858



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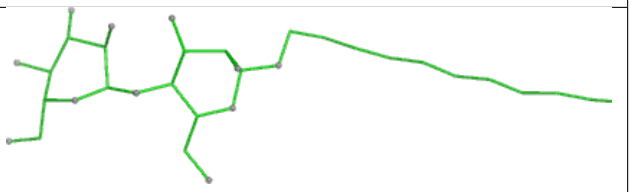
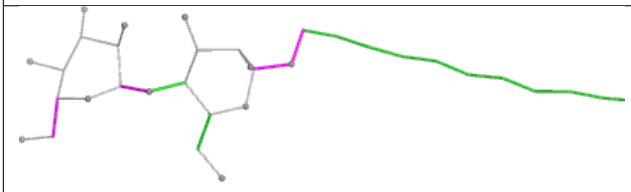


Bond angles



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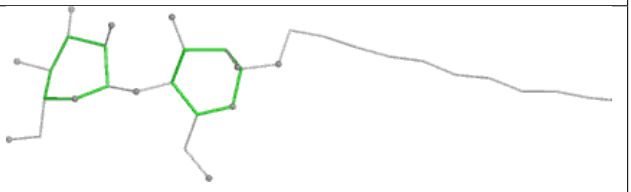
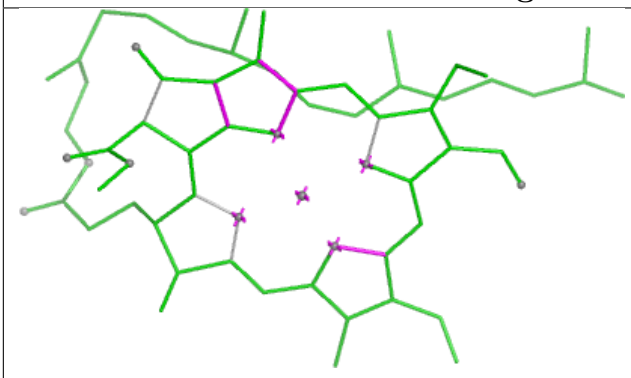


Rings

Ligand CHL Z2 607



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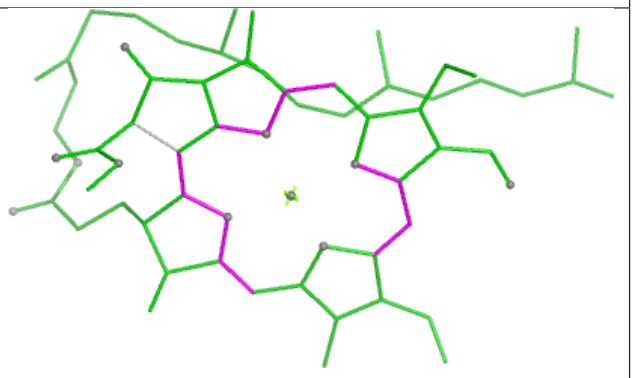
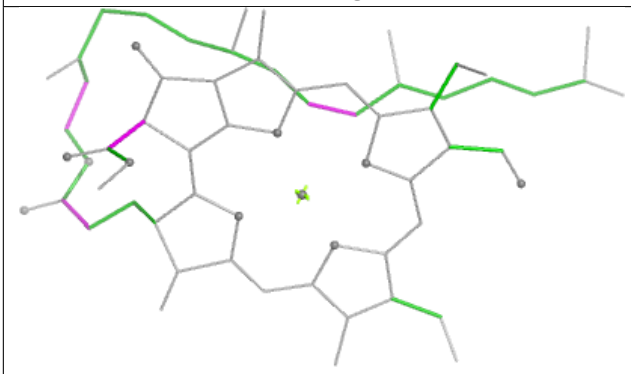


Bond angles



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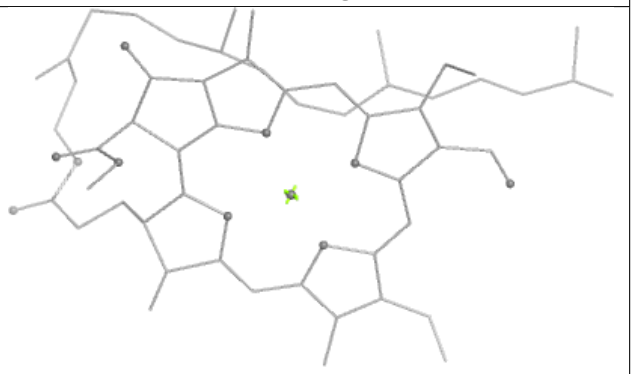
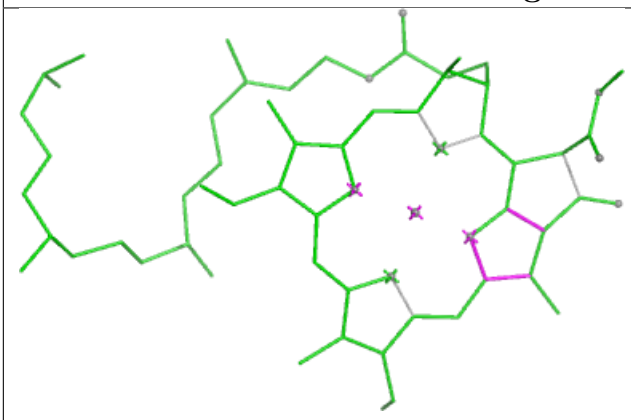


Rings

Ligand CLA A 820



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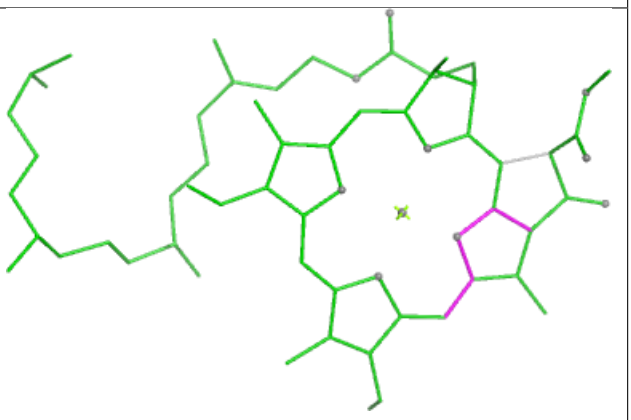
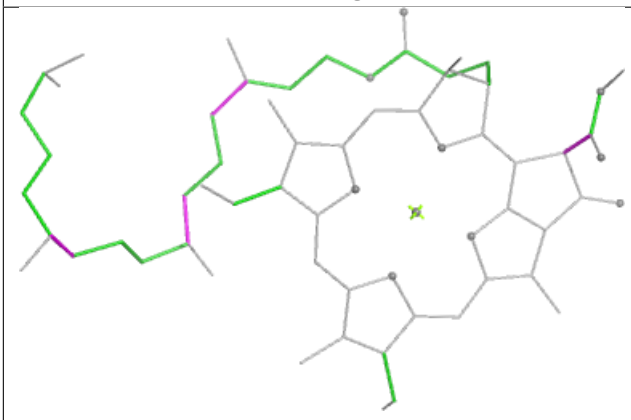


Bond angles



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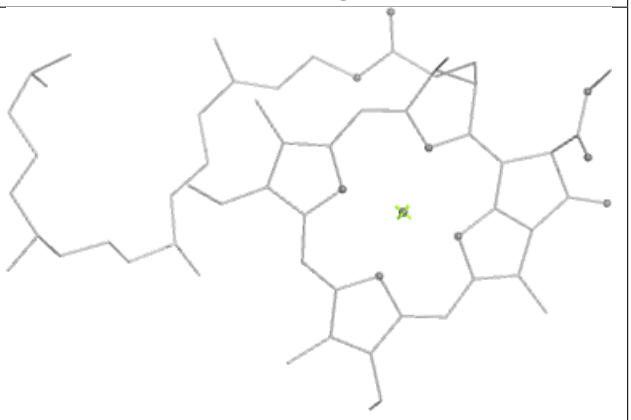
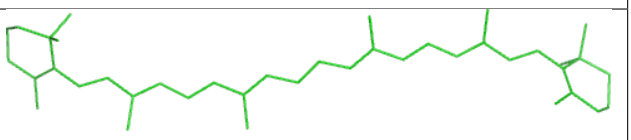


Rings

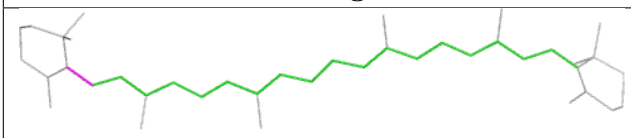
Ligand BCR A 851



Bond lengths



Bond angles



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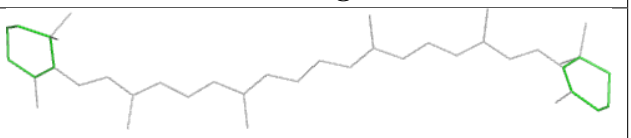
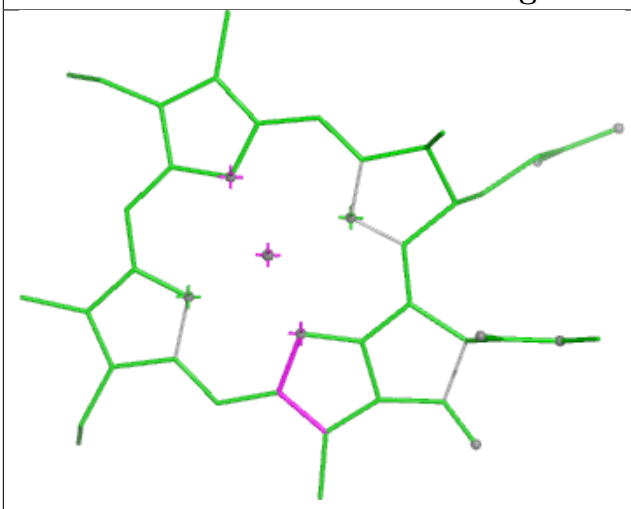


Rings

Ligand CLA 32 614



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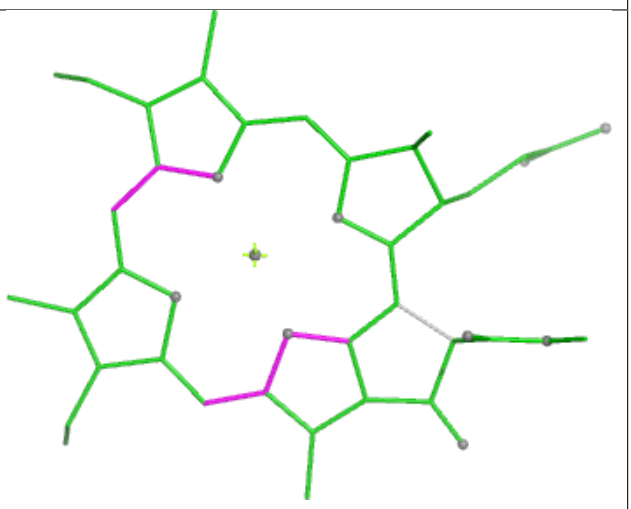
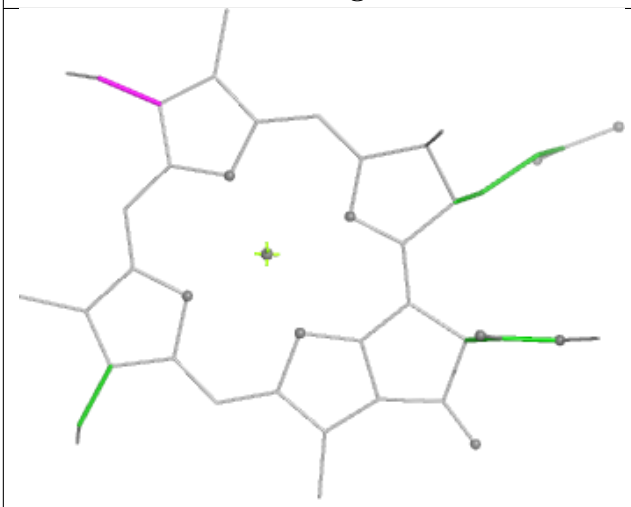


Bond angles



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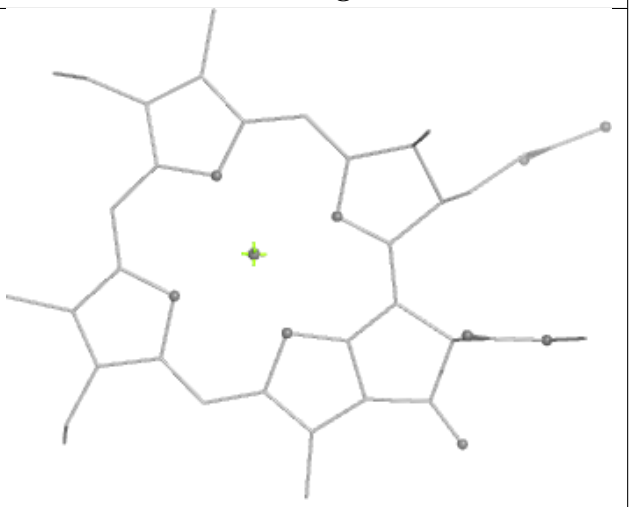
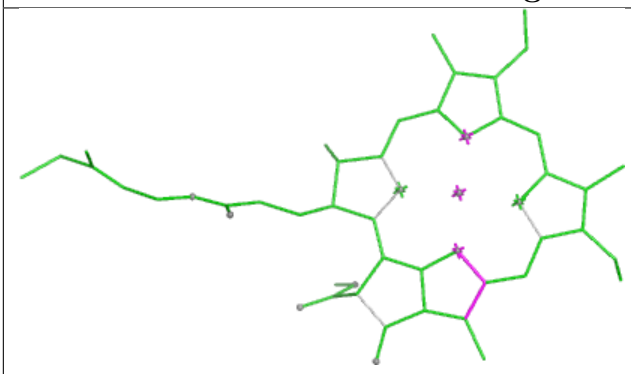


Rings

Ligand CLA A 838



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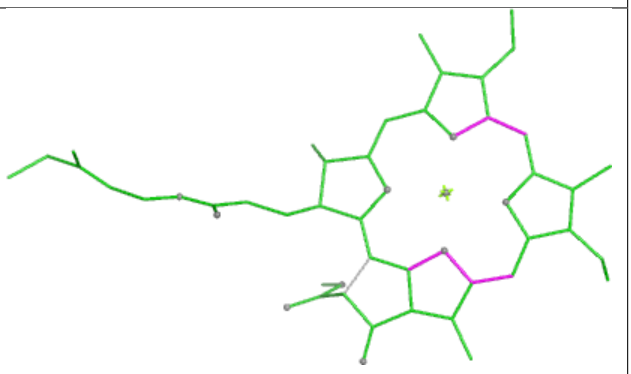
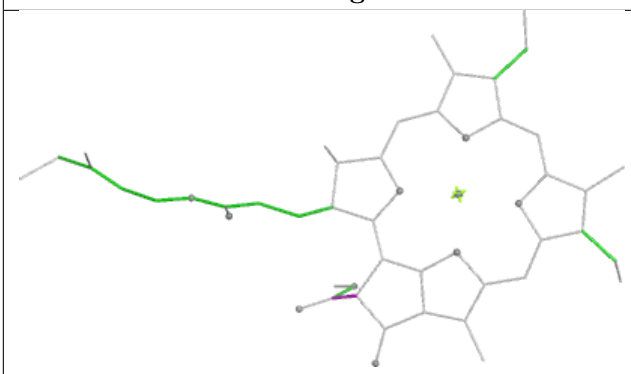


Bond angles



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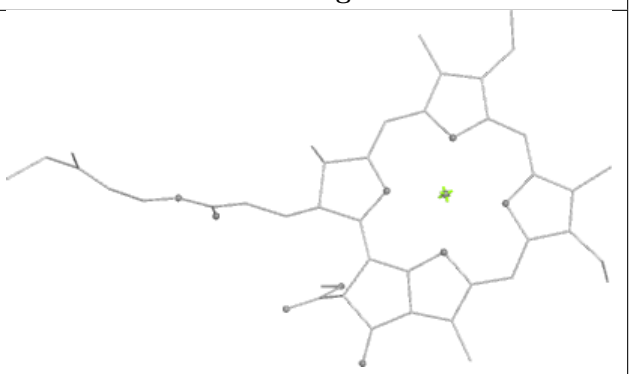
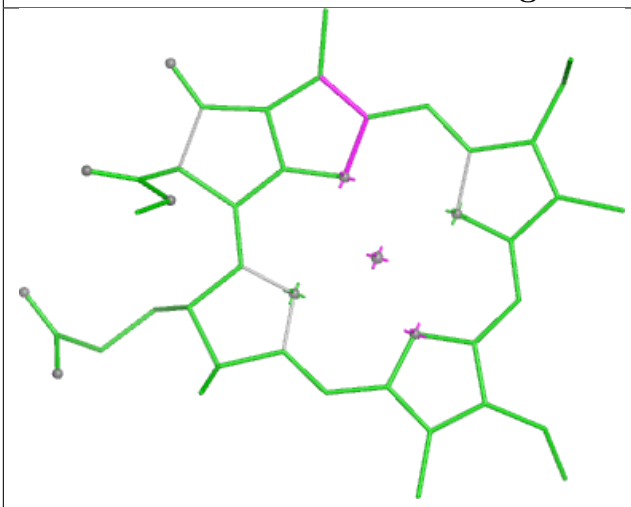


Rings

Ligand CLA 42 612



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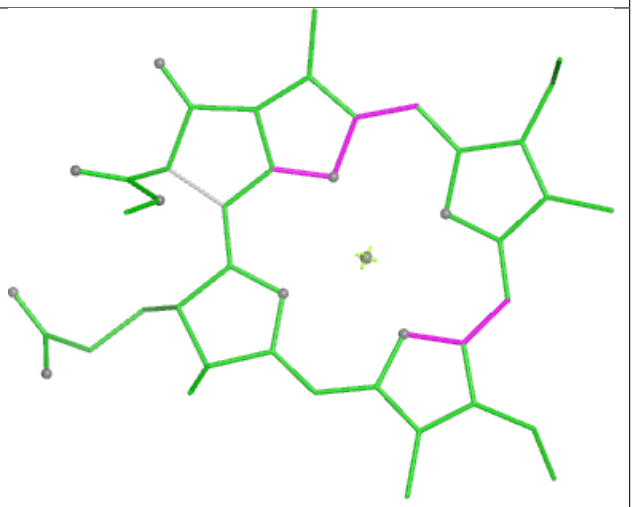
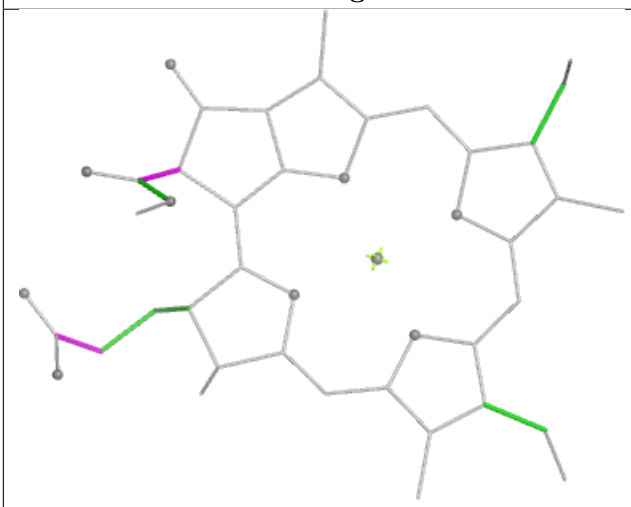


Bond angles



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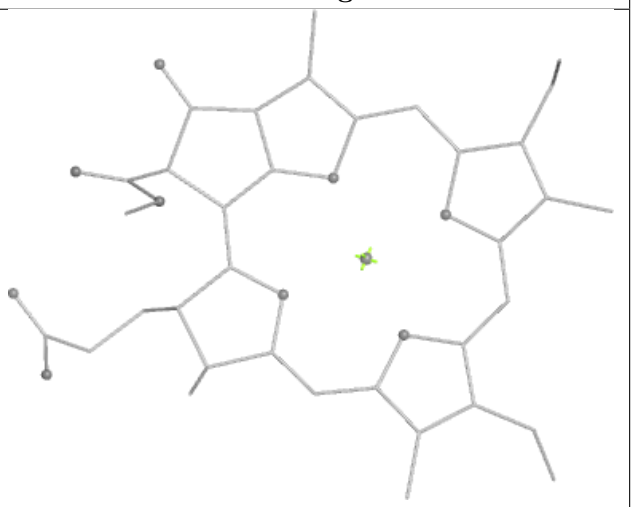
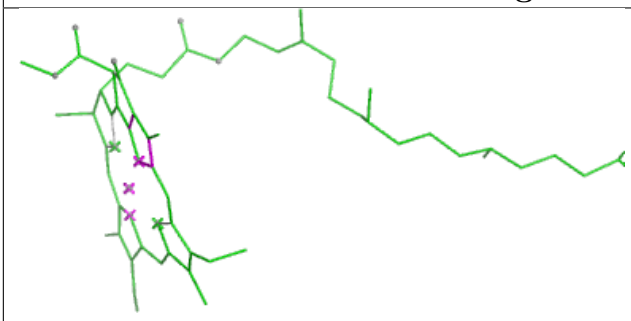


Rings

Ligand CLA B2 829



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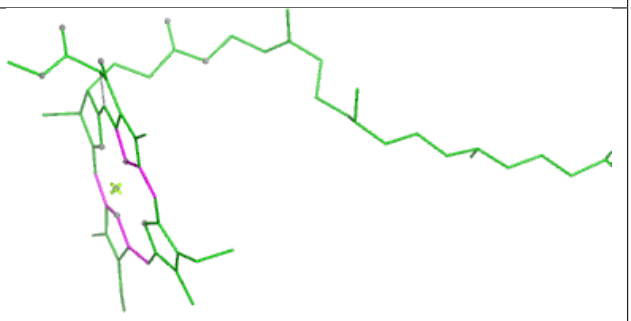
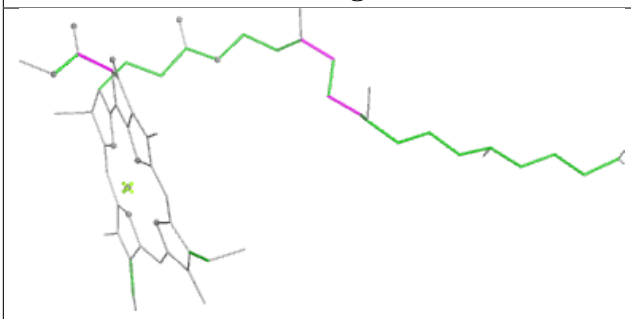


Bond angles



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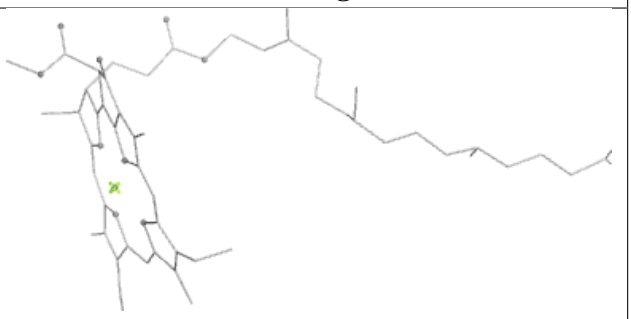
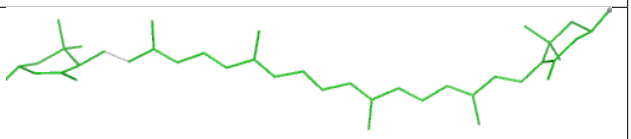


Rings

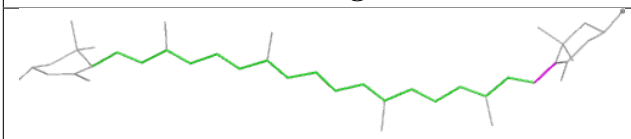
Ligand LUT 1 619



Bond lengths



Bond angles



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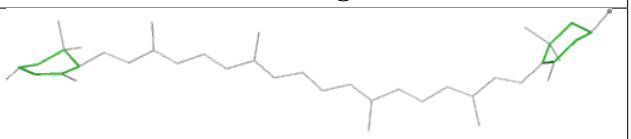
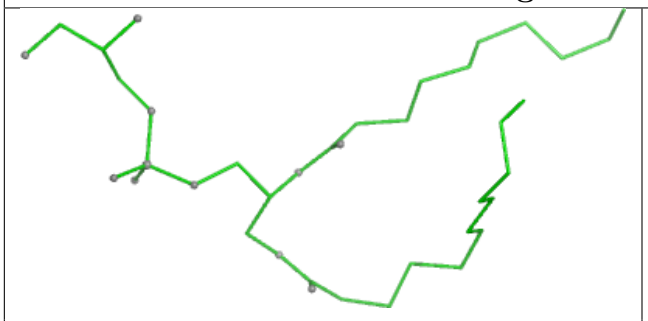


Rings

Ligand LHG Z2 620



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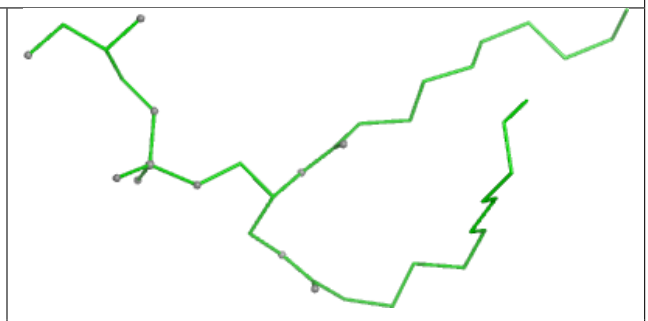
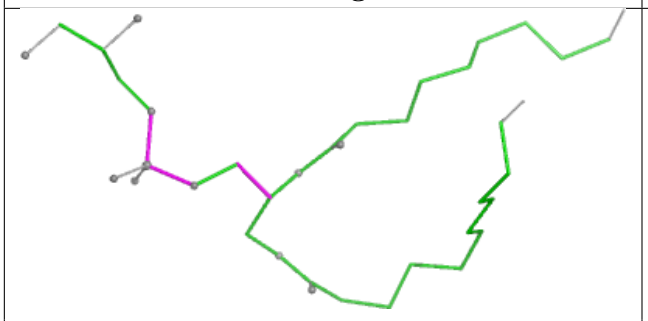


Bond angles



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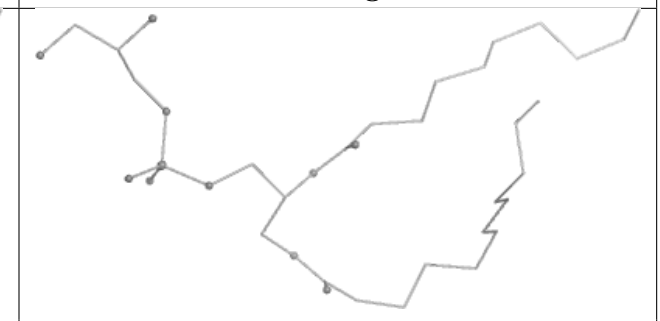
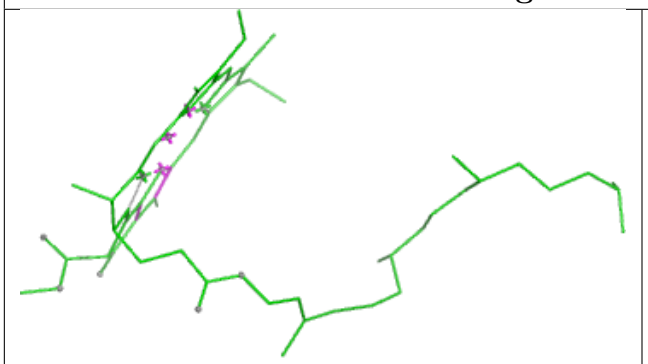
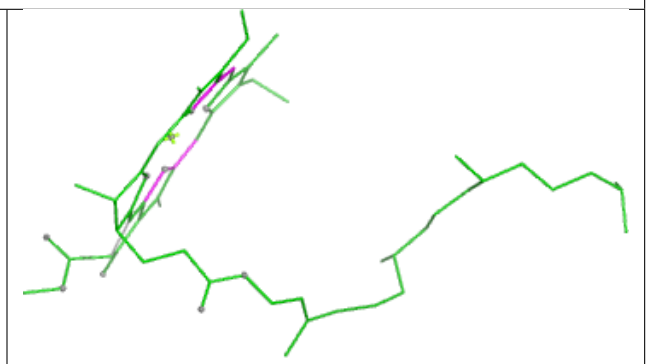


Rings

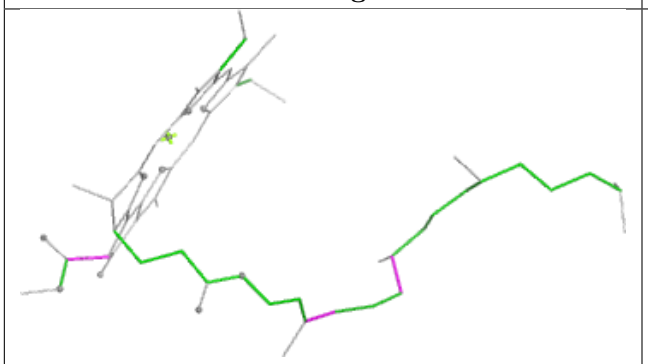
Ligand CLA A2 811



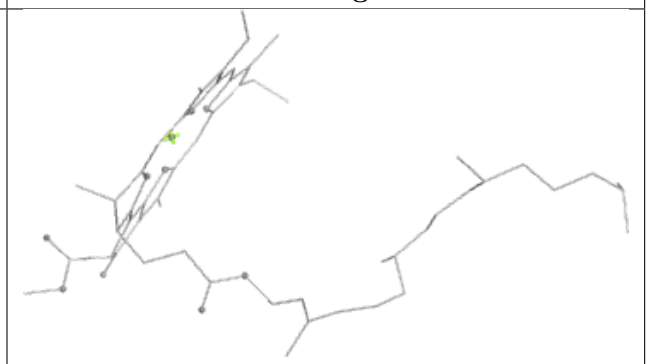
Bond lengths



Bond angles

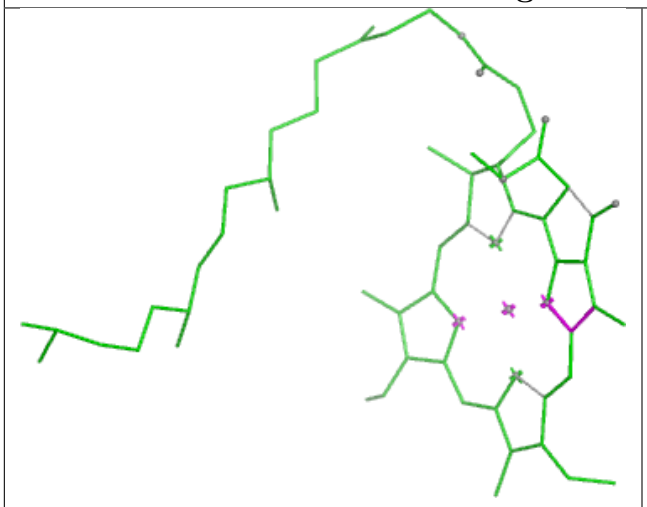


Torsions



Rings

Ligand CLA B2 824



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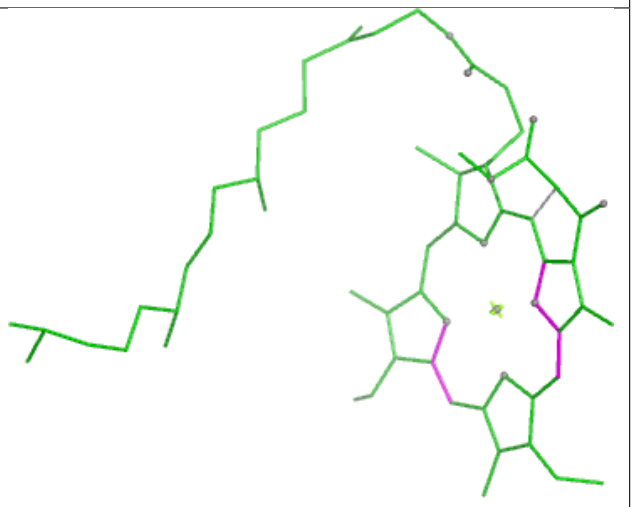

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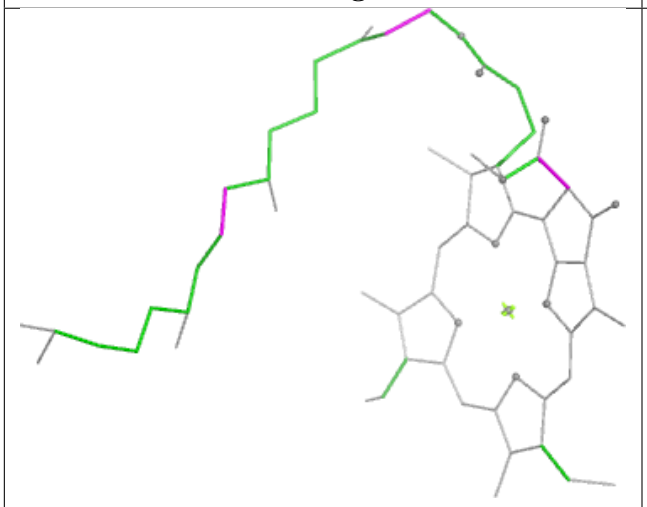

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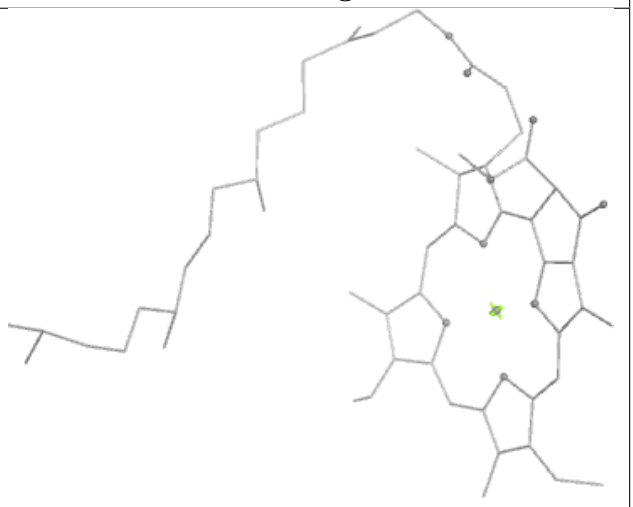
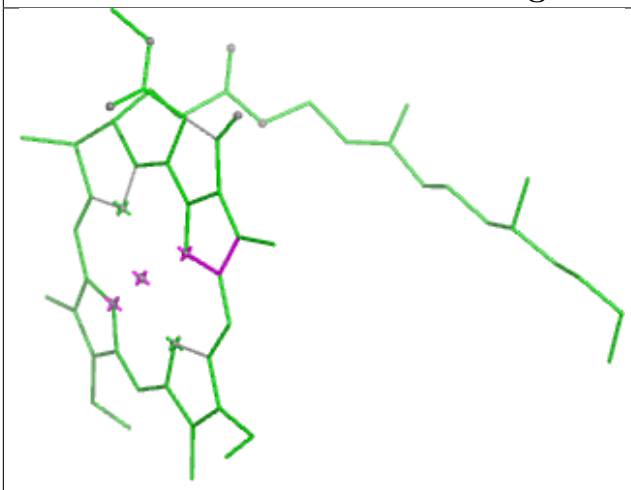


Rings

Ligand CLA 6 611



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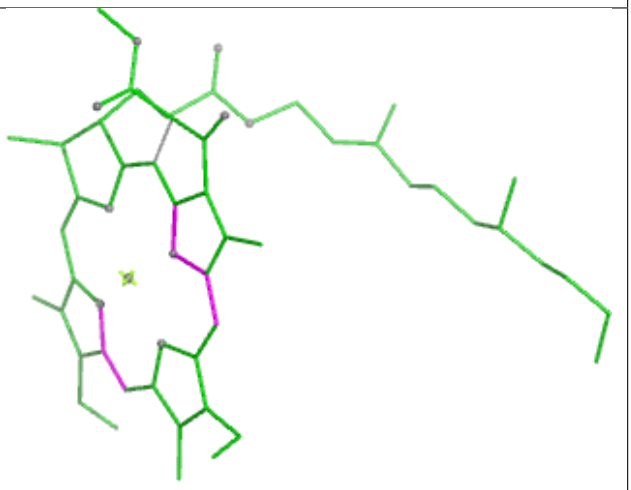

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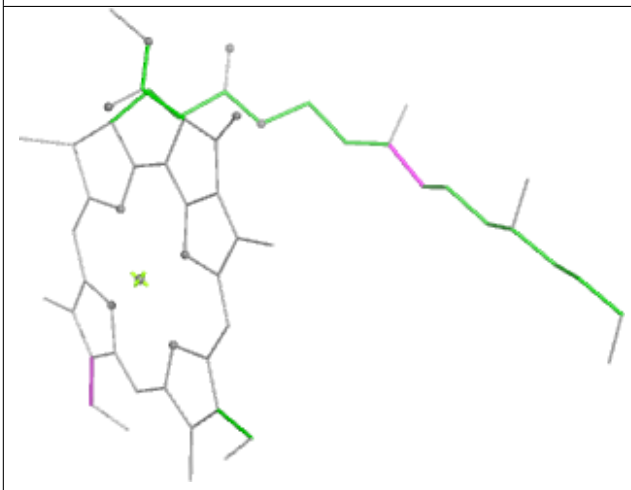

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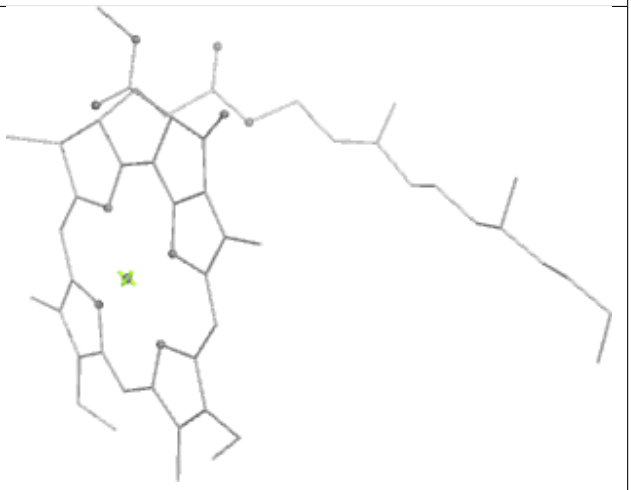
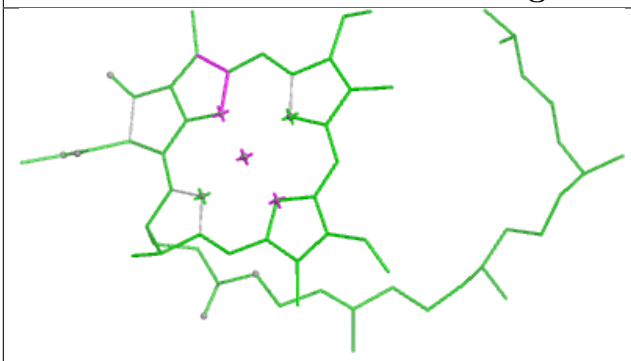


Rings

Ligand CLA 8 610



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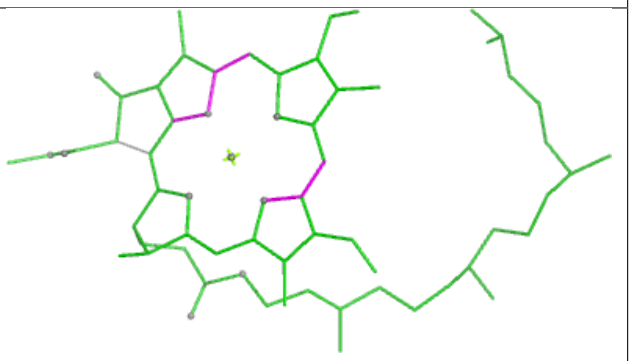
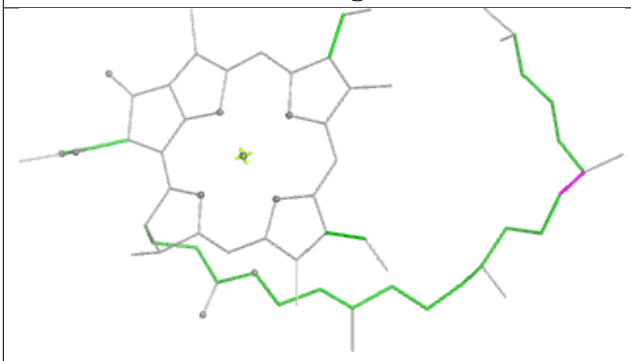


Bond angles



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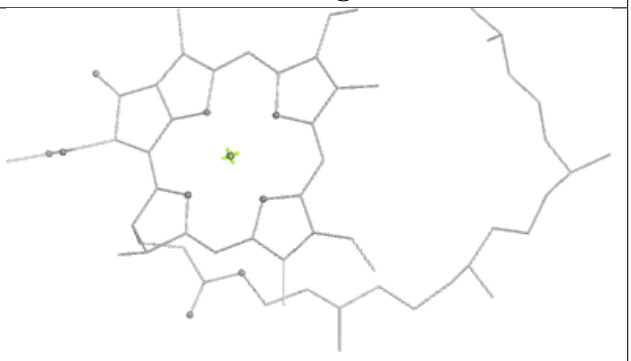
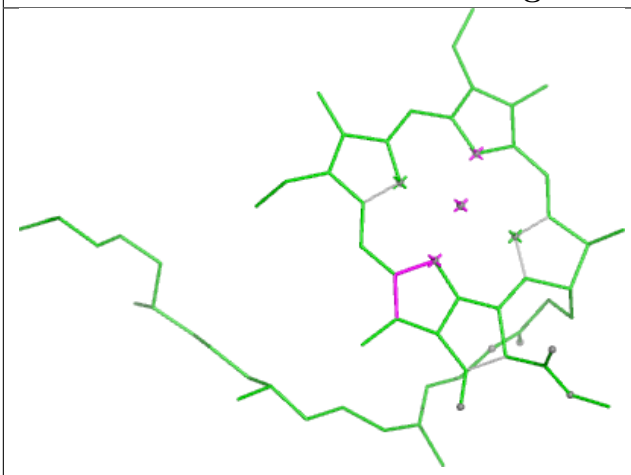


Rings

Ligand CLA A 830



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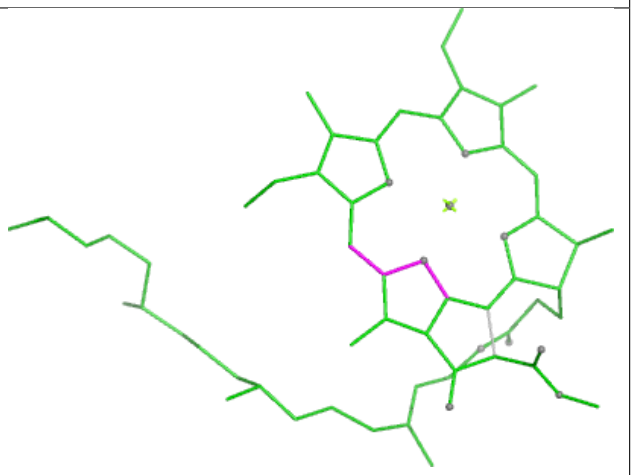

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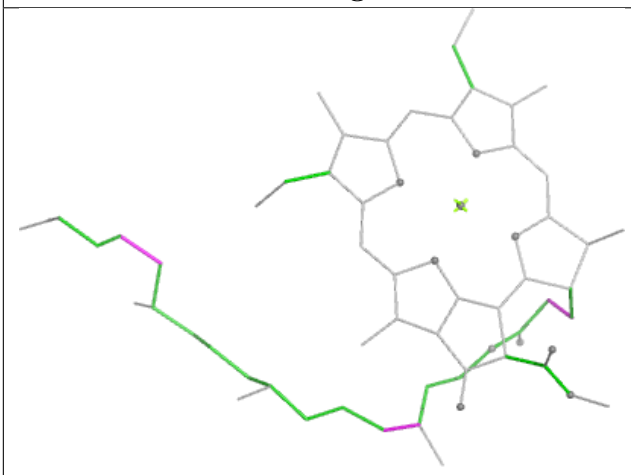

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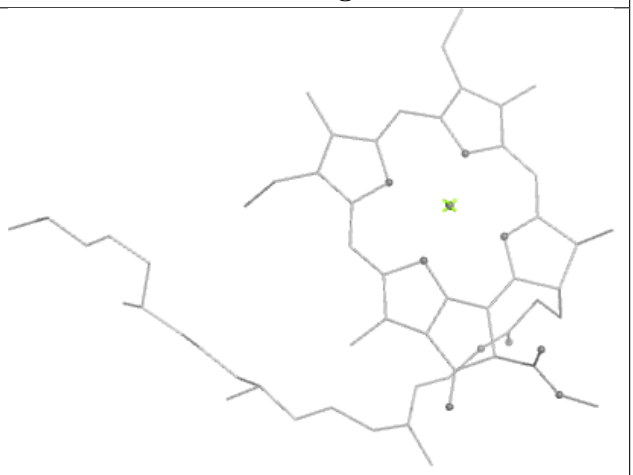
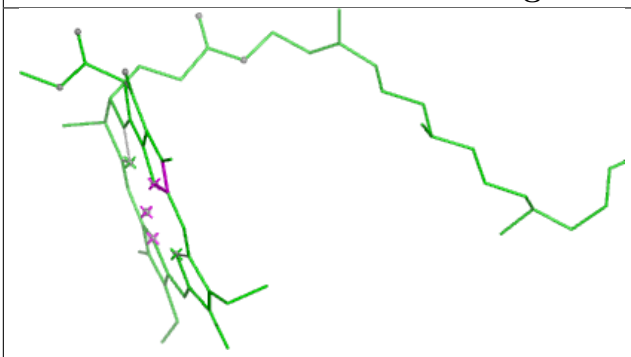


Rings

Ligand CLA A 831



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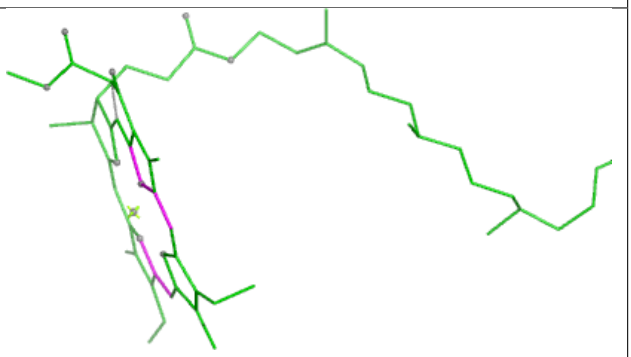

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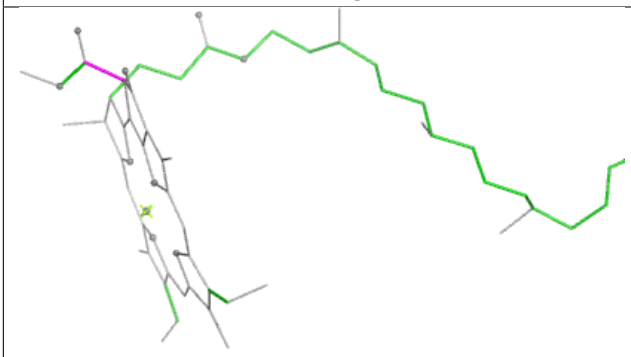
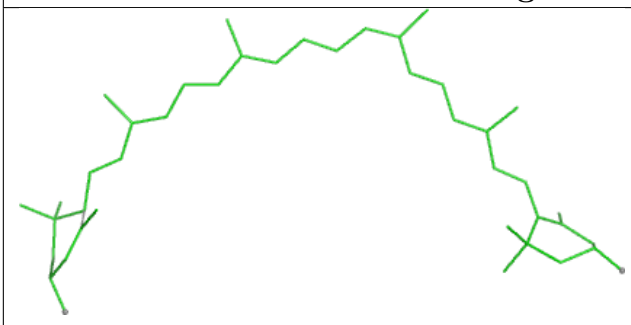


Torsions



Rings

Ligand LUT F2 305



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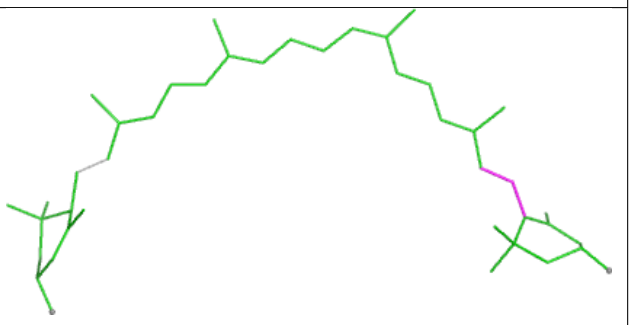

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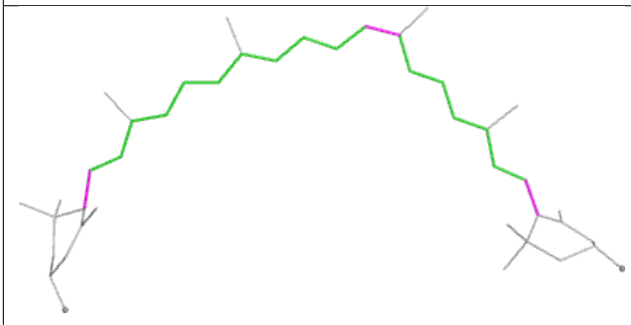

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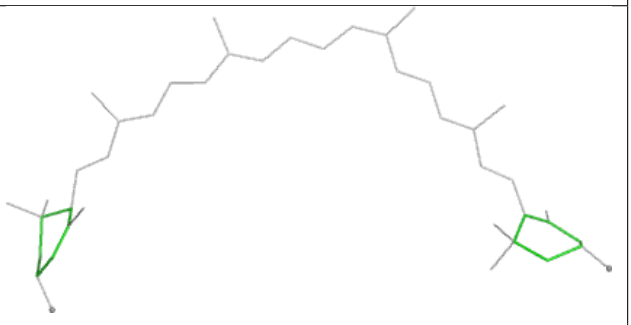
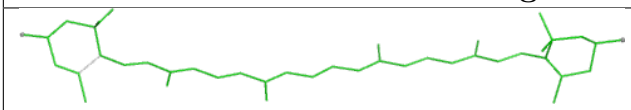


Rings

Ligand LUT 52 626



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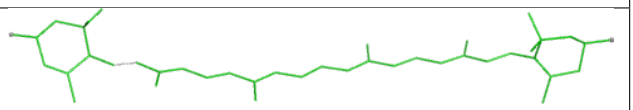
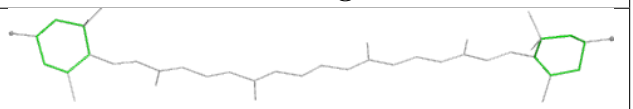


Bond angles

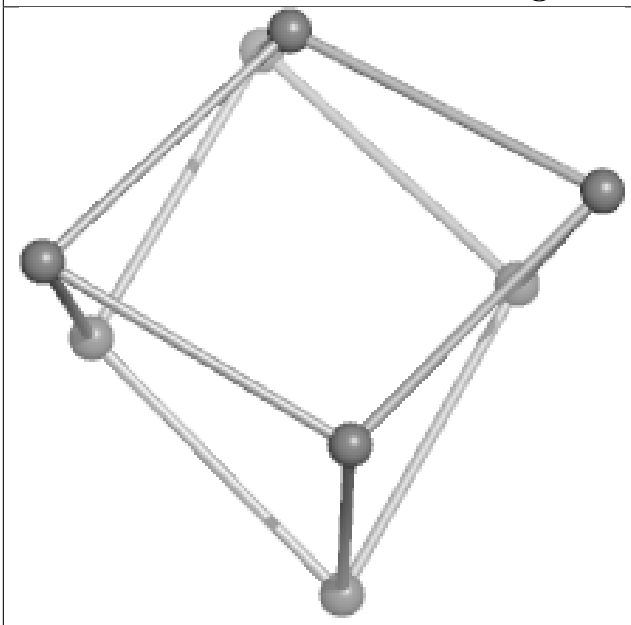


Torsions



Rings

Ligand SF4 A 853



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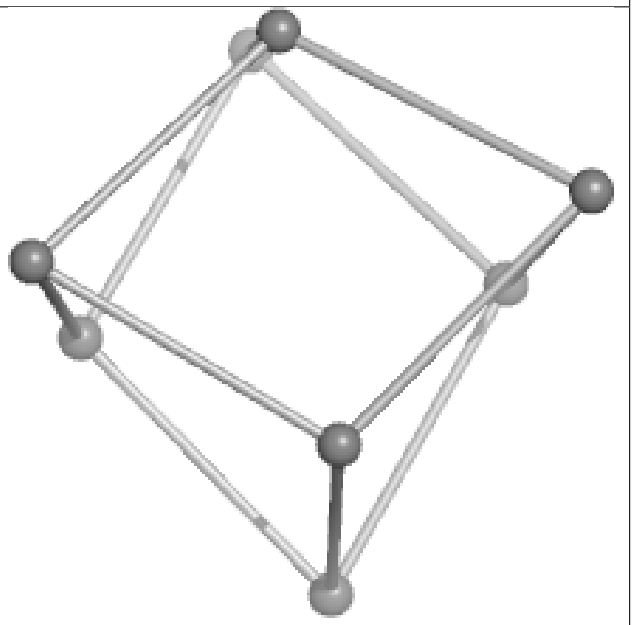
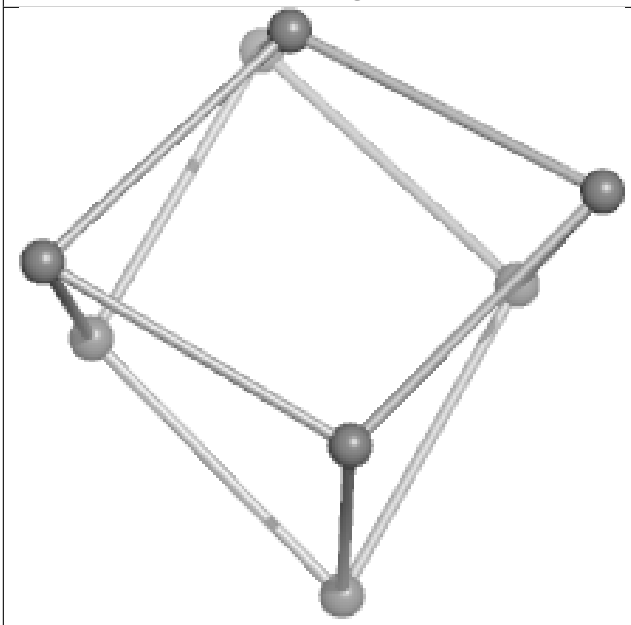


Bond angles



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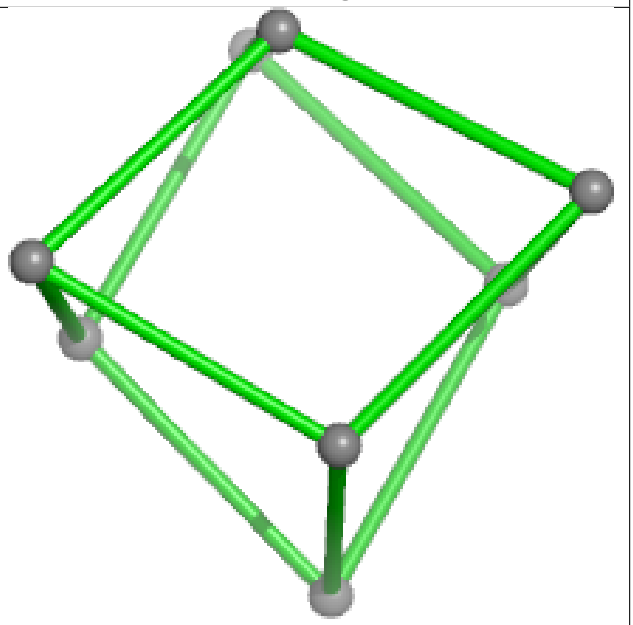
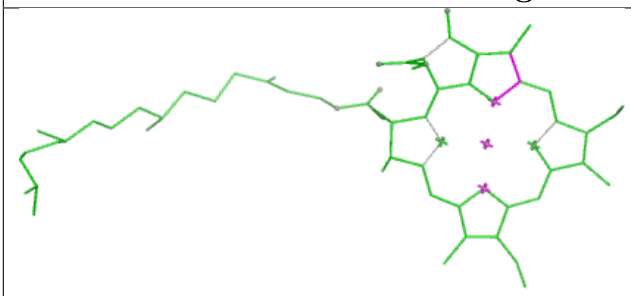


Rings

Ligand CLA B2 841



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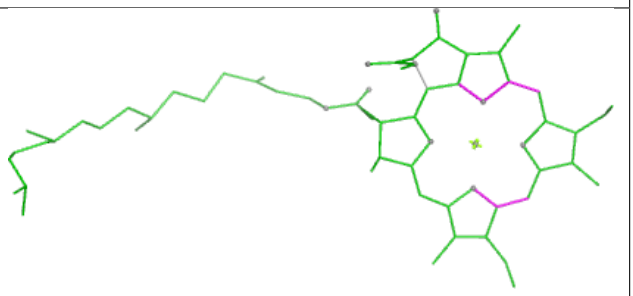
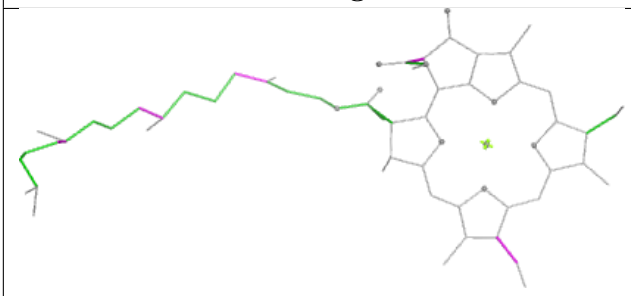


Bond angles



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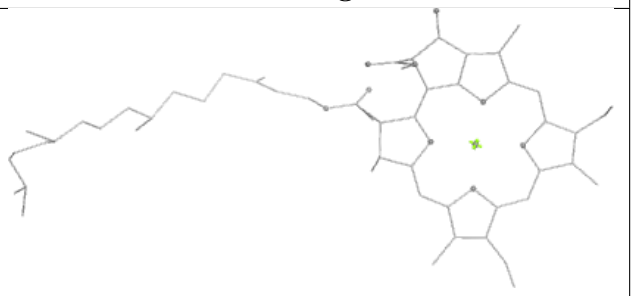
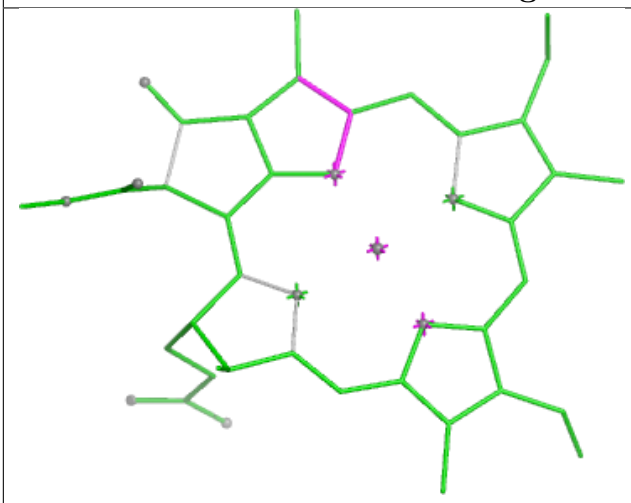


Rings

Ligand CLA 82 609



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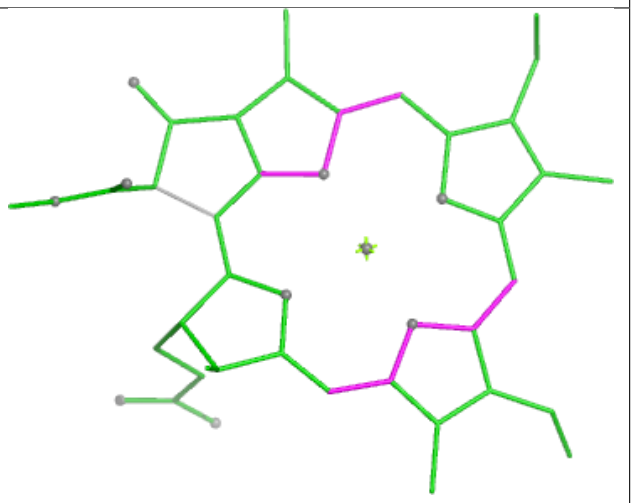

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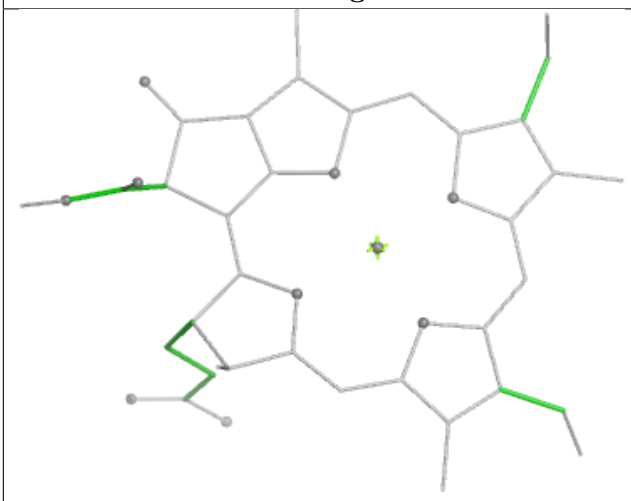

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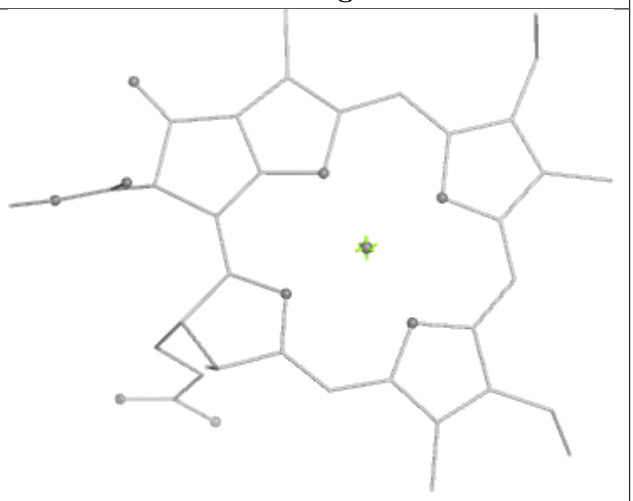
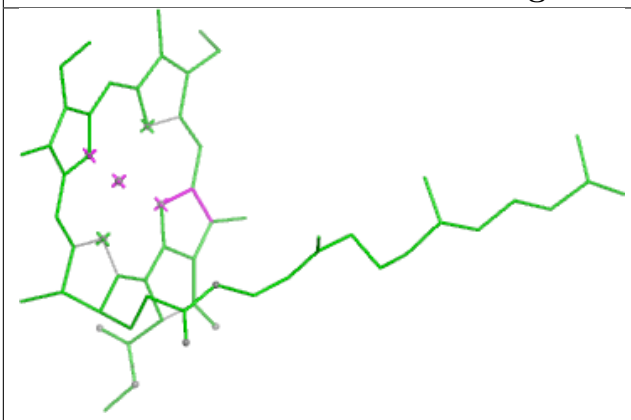


Rings

Ligand CLA 4 611



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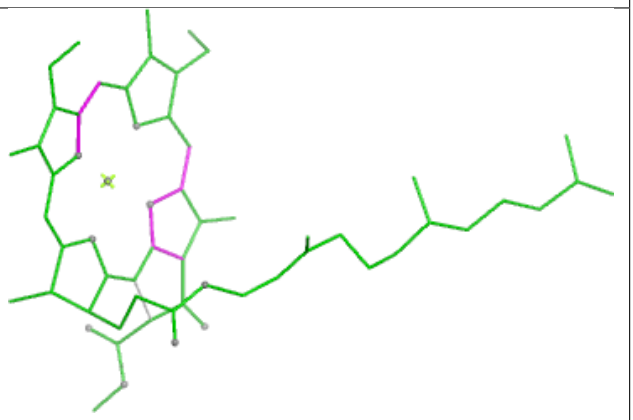

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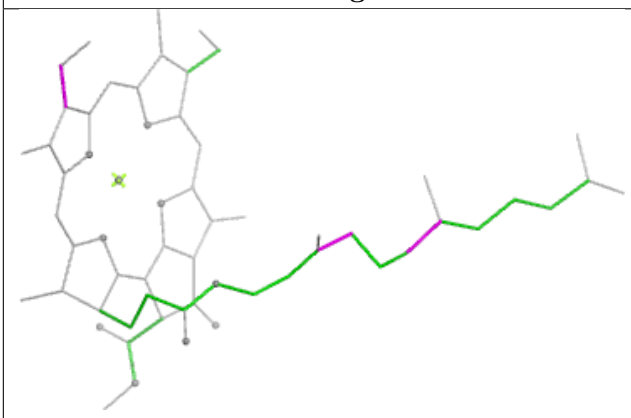

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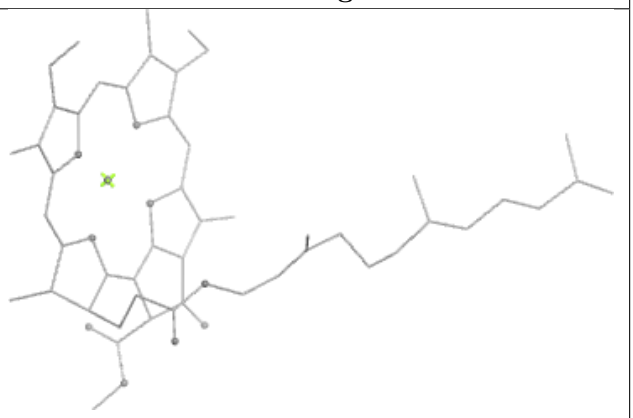
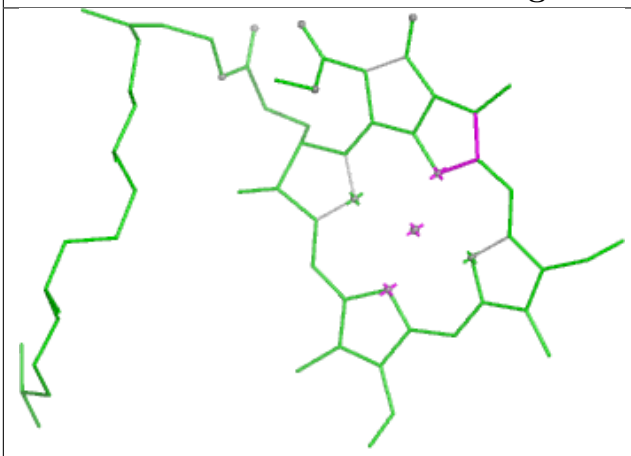


Rings

Ligand CLA 8 603



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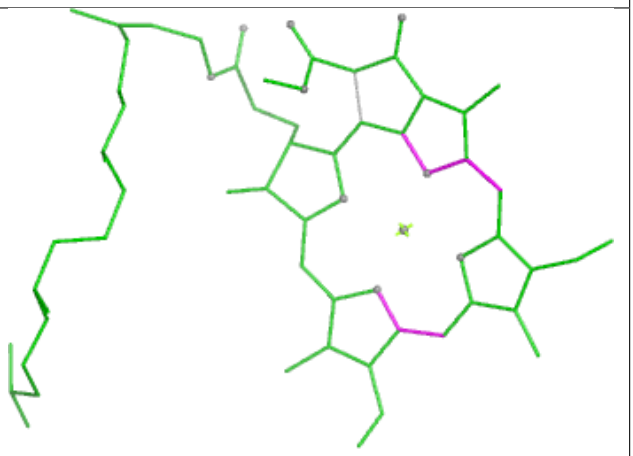
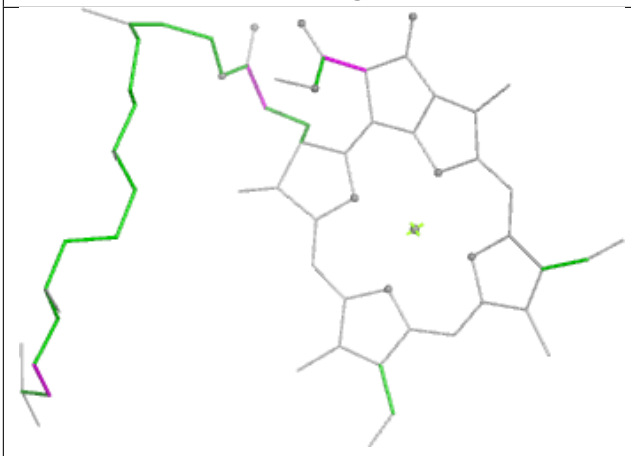


Bond angles



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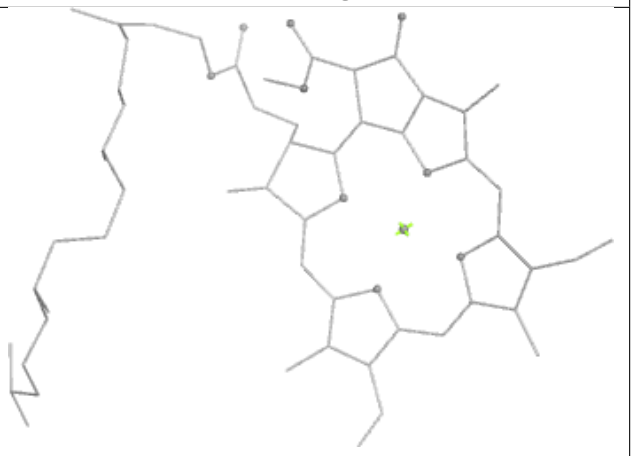
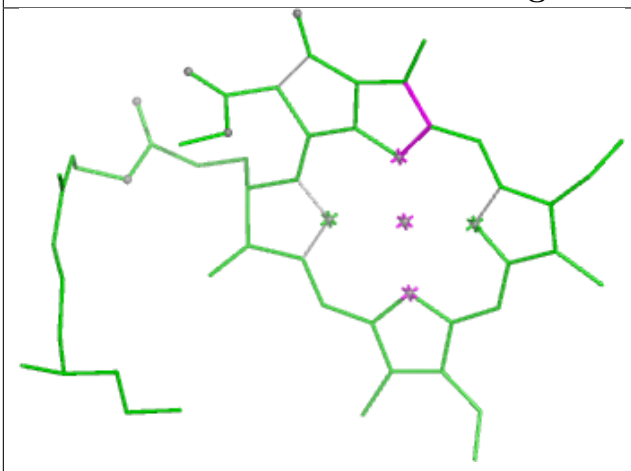


Rings

Ligand CLA 1 603



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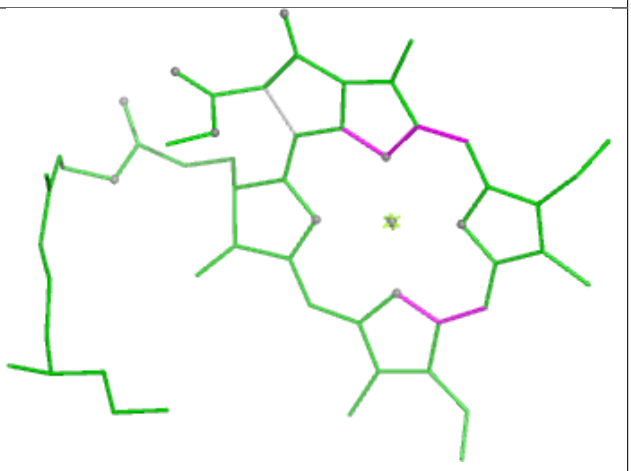
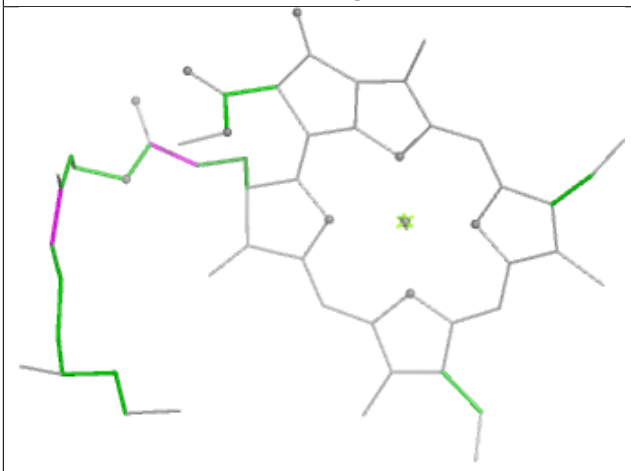


Bond angles



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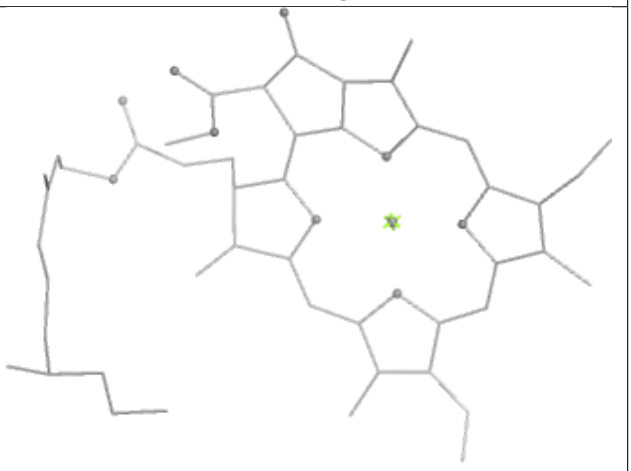
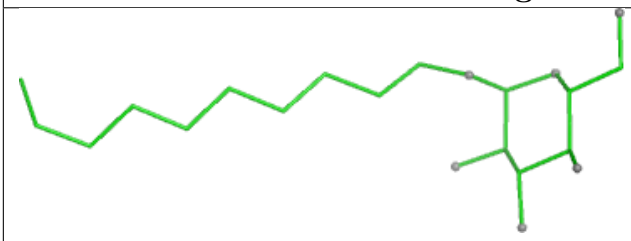


Rings

Ligand LMU 12 627



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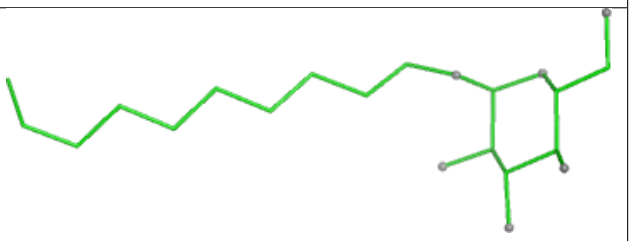
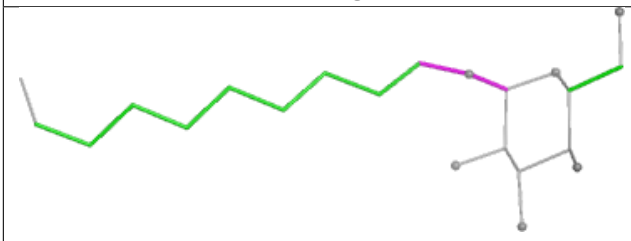


Bond angles



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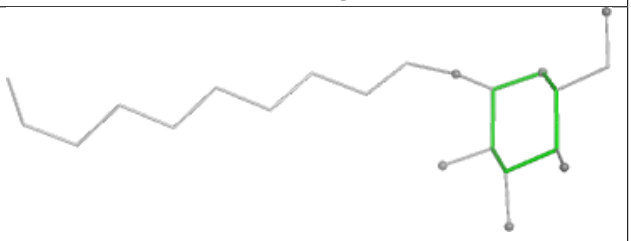
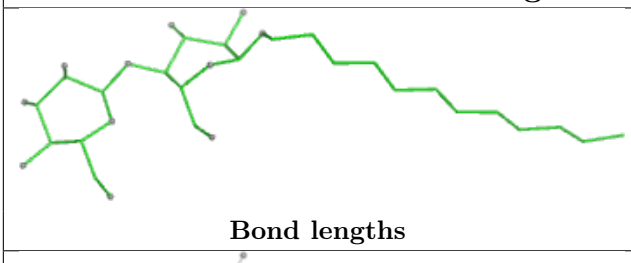
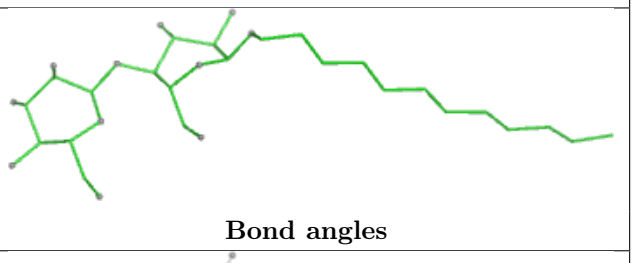


Rings

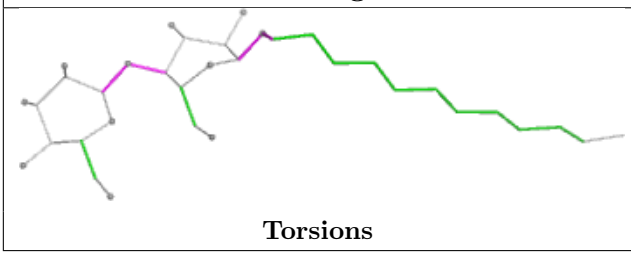
Ligand LMU 1 621



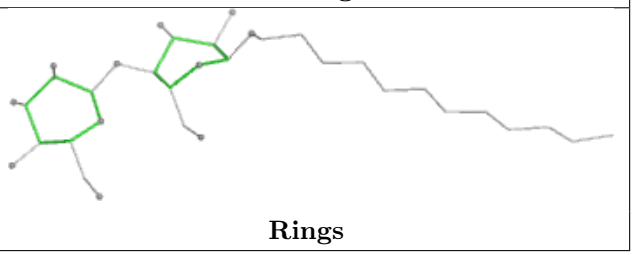
Bond lengths



Bond angles

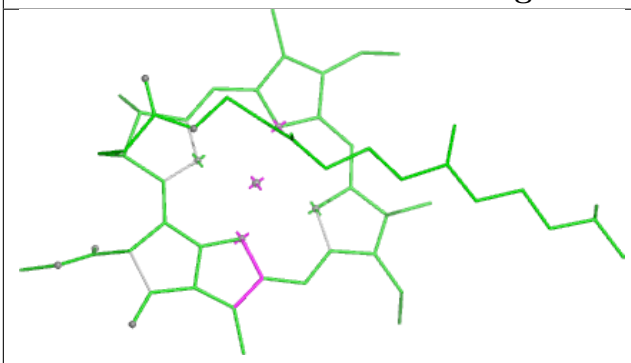


Torsions



Rings

Ligand CLA A2 819



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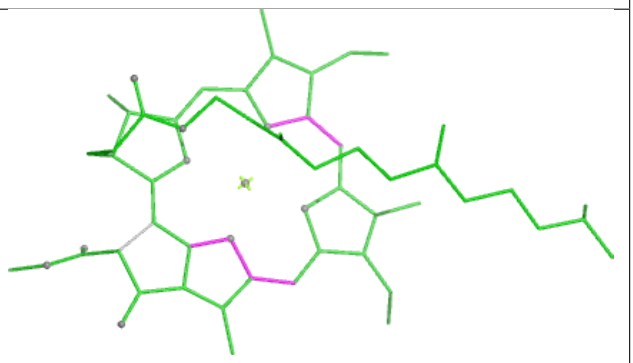

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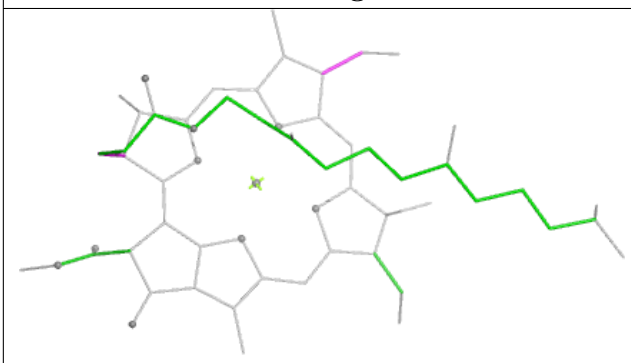

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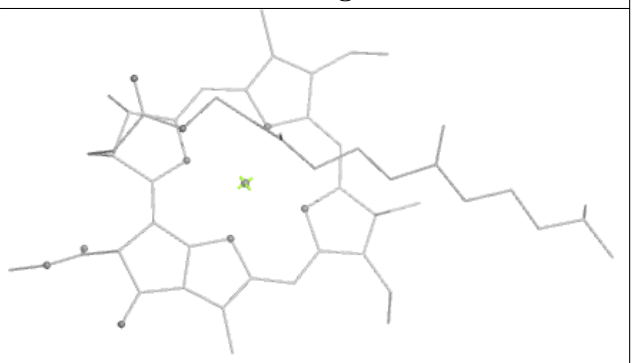
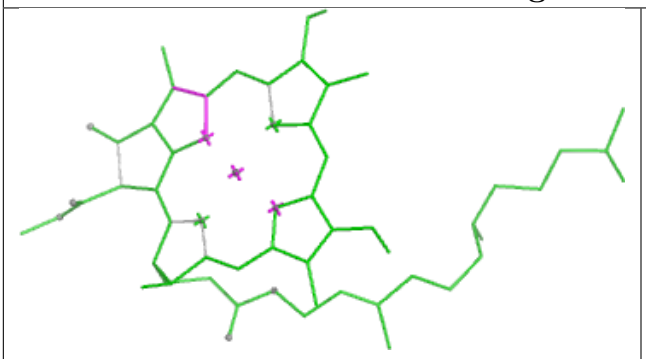


Rings

Ligand CLA 4 610



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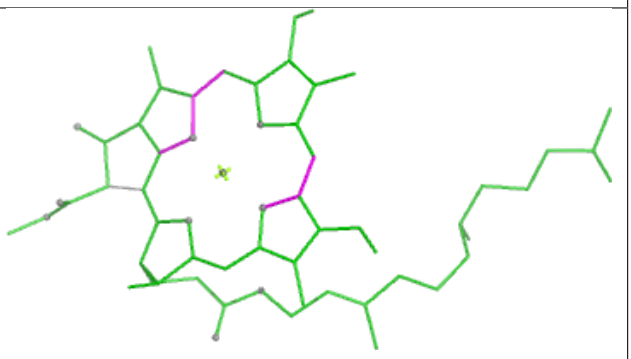

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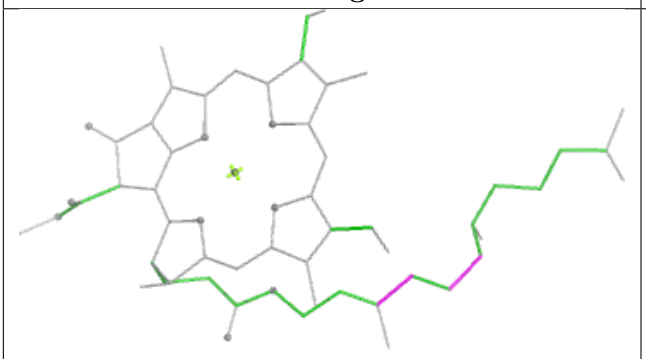

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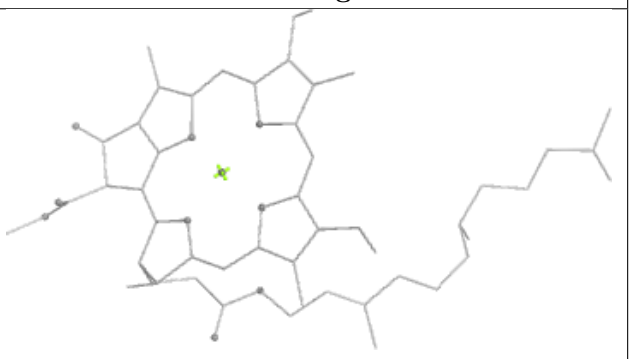


Rings

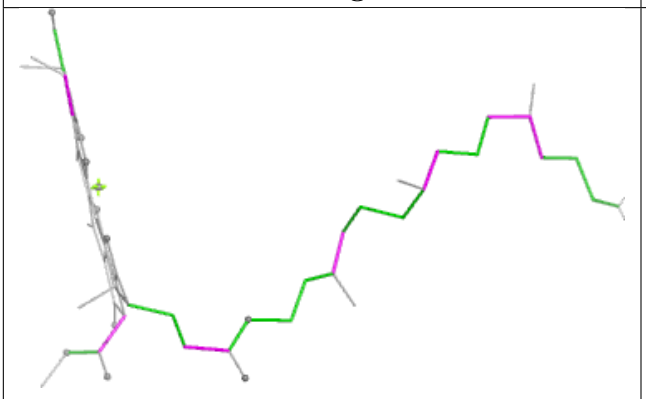
Ligand CHL 8 601



Bond lengths



Bond angles



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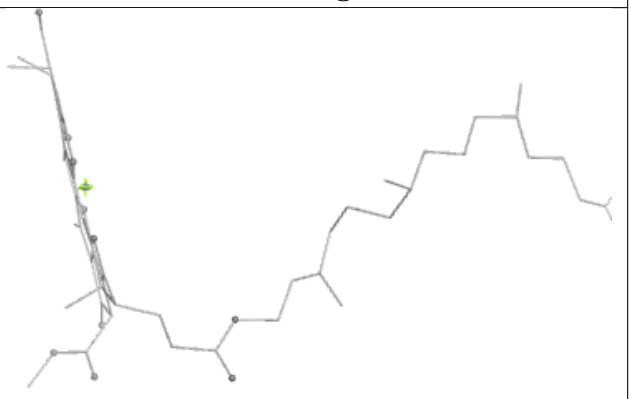
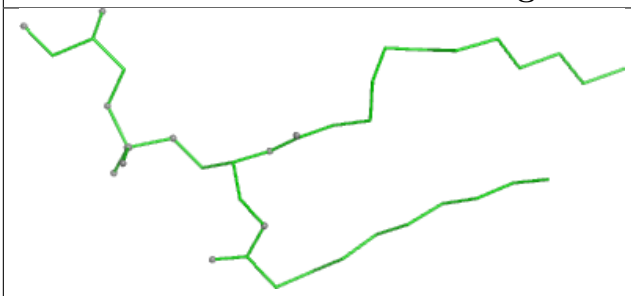


Rings

Ligand LHG 12 620



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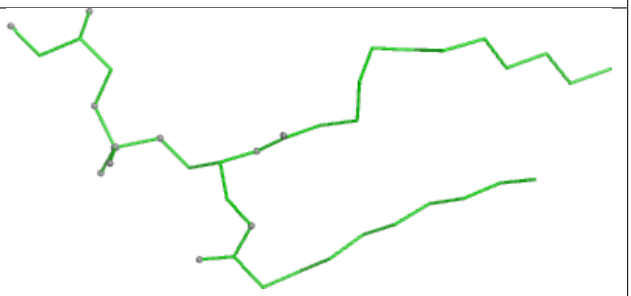

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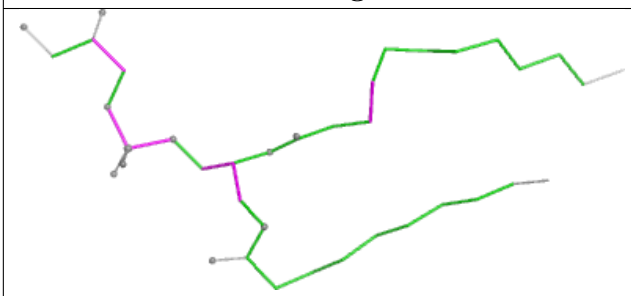

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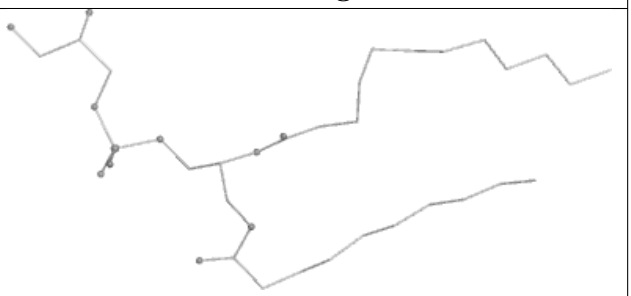
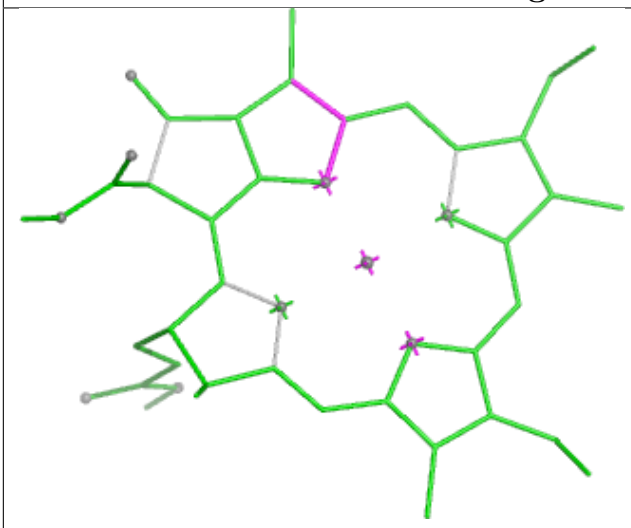


Rings

Ligand CLA 1 616



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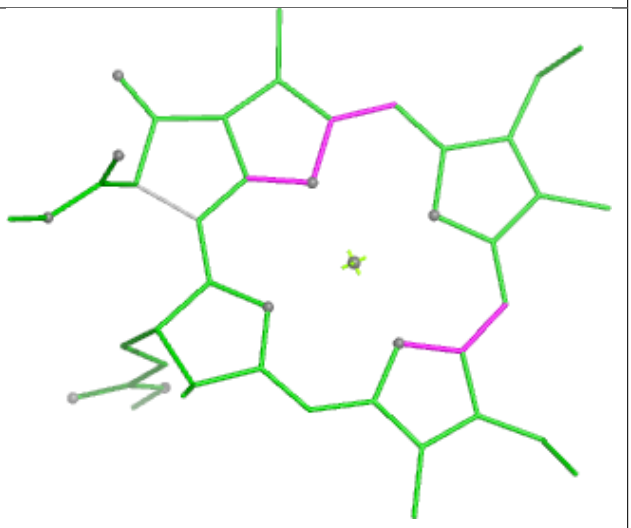

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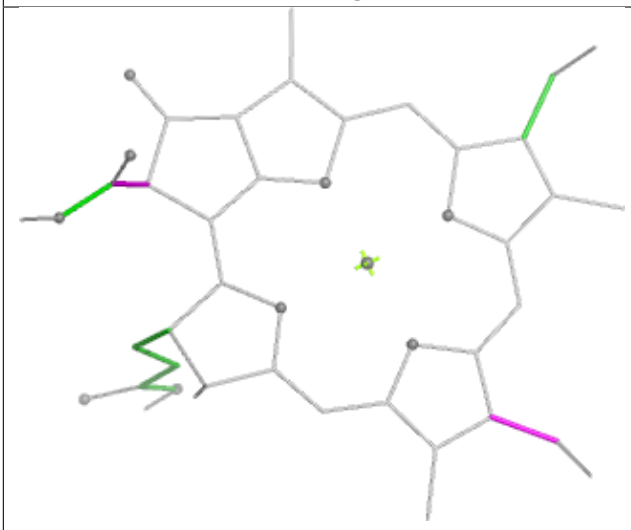

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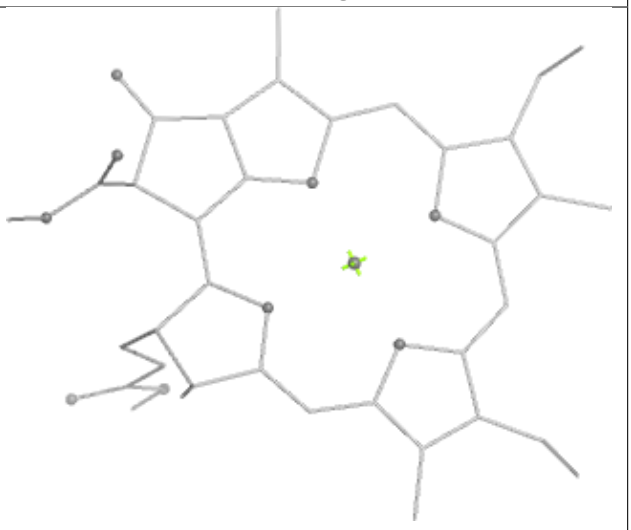
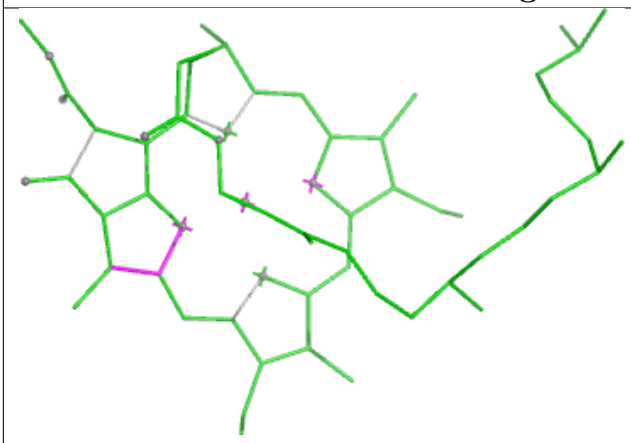


Rings

Ligand CLA 42 613



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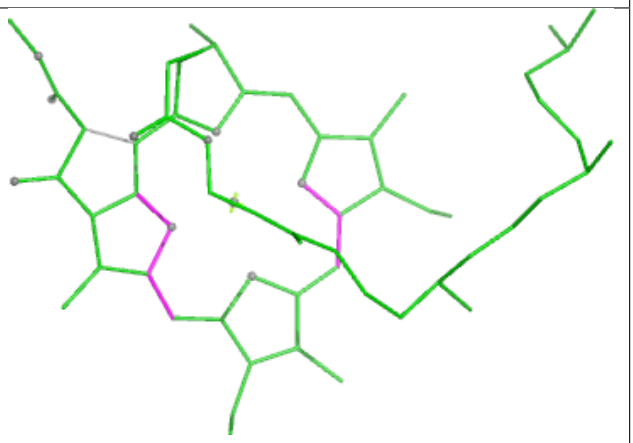
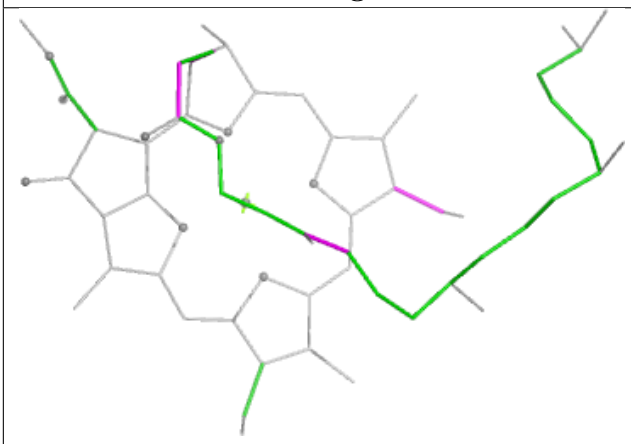


Bond angles



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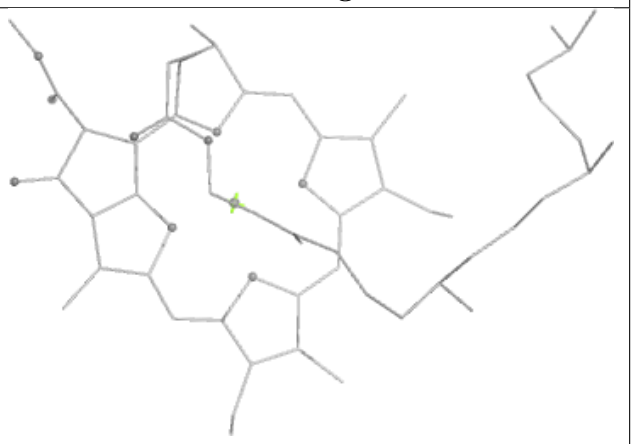
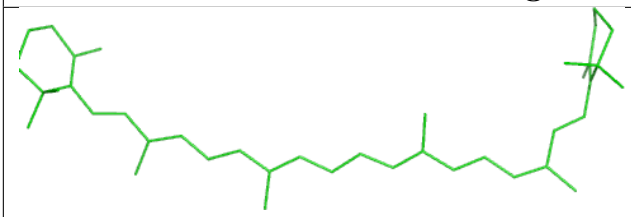


Rings

Ligand BCR L 201



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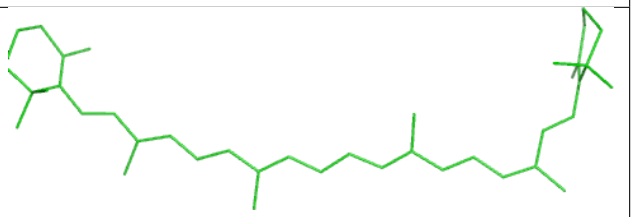
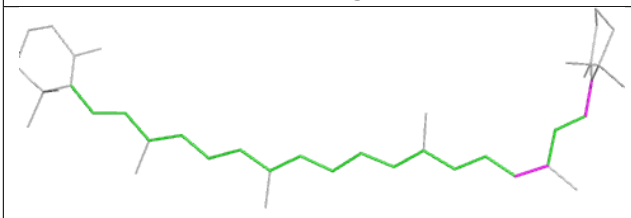


Bond angles



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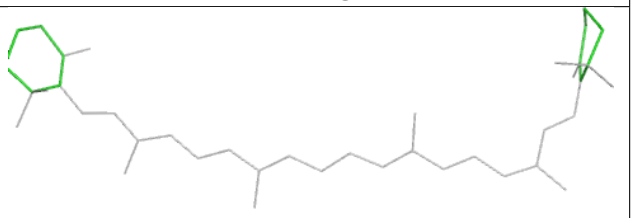
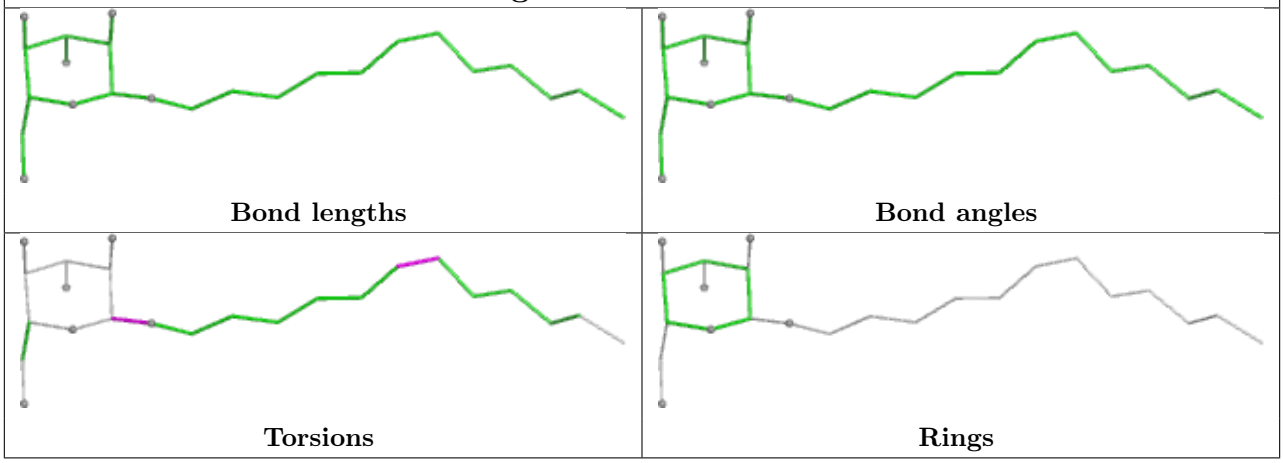
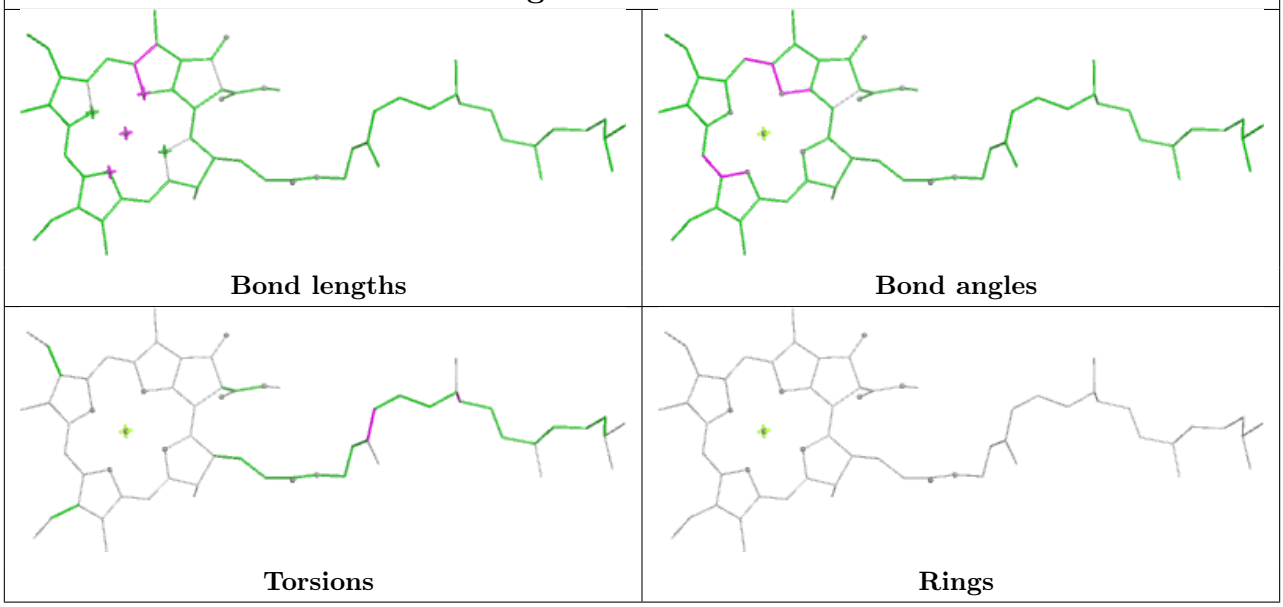


Rings

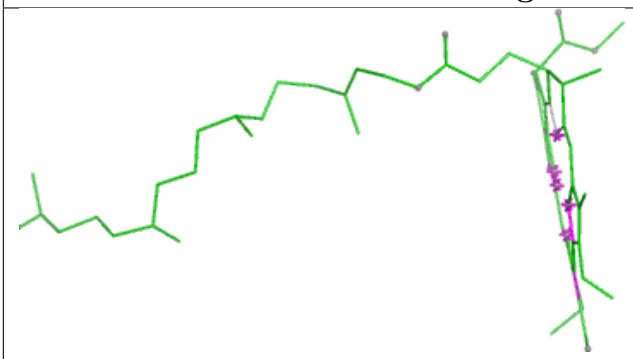
Ligand LMU A2 865



Ligand CLA F 301



Ligand CHL Z2 601



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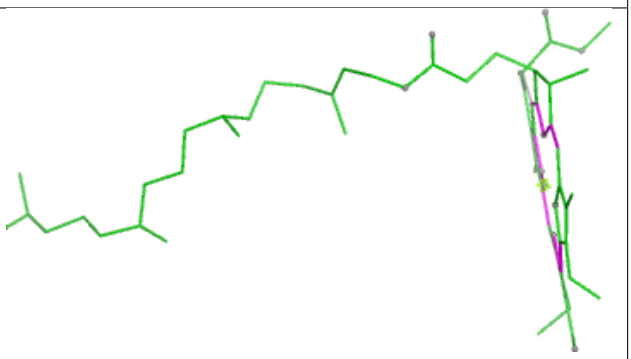
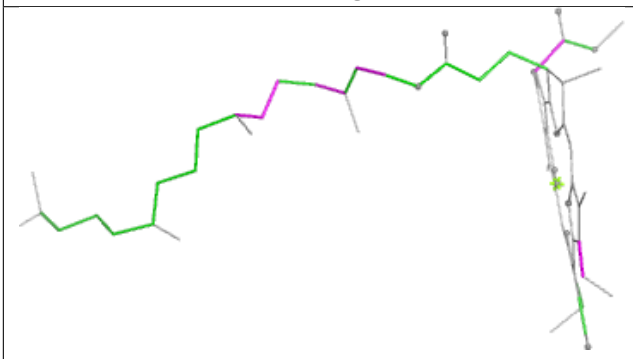


Bond angles



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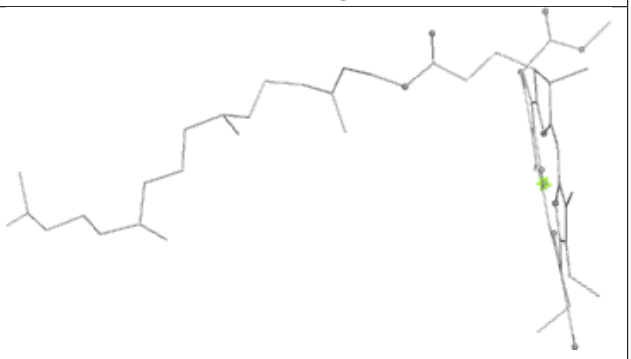
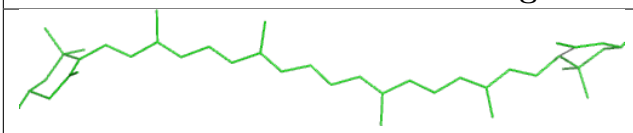


Rings

Ligand LUT 32 720



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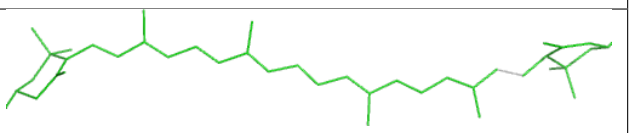

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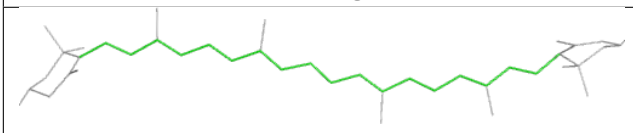
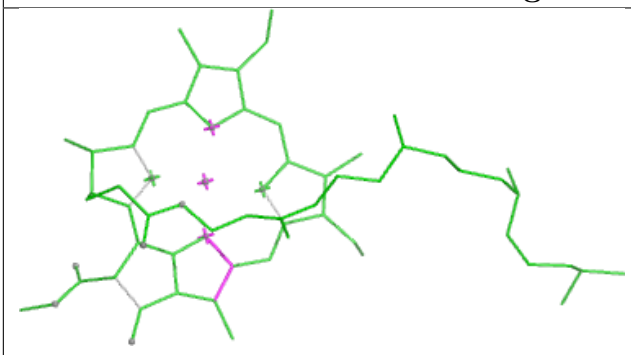


Torsions



Rings

Ligand CLA A 818



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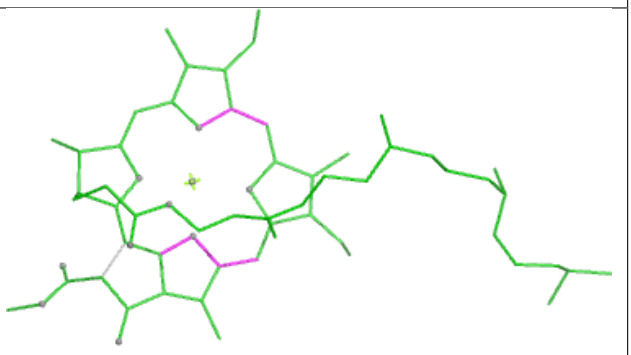
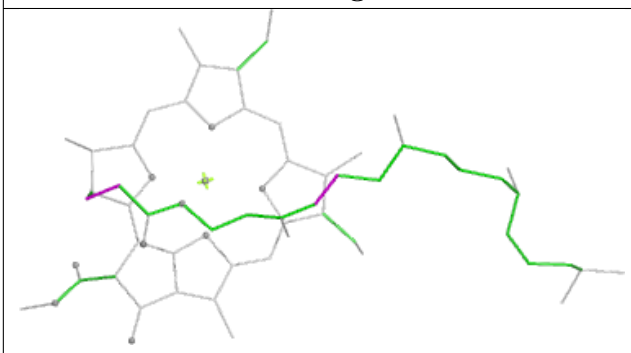


Bond angles



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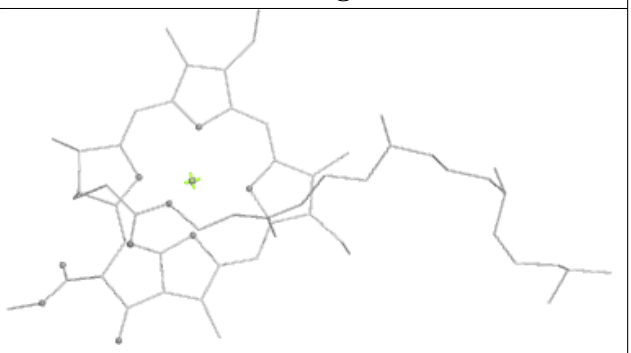
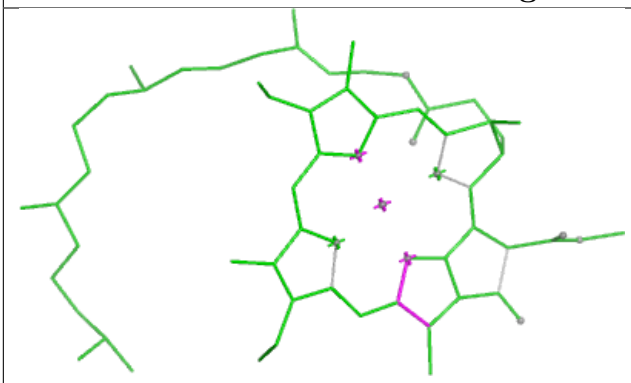


Rings

Ligand CLA 72 610



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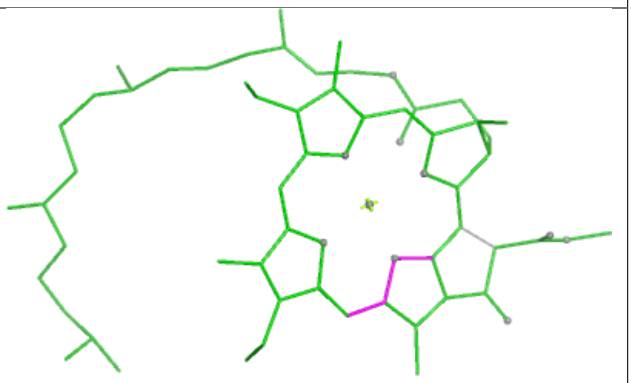
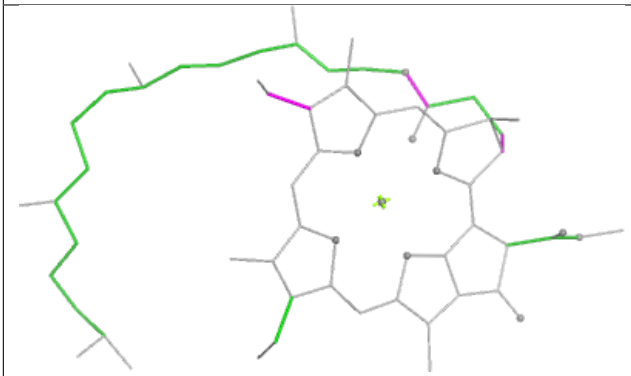


Bond angles



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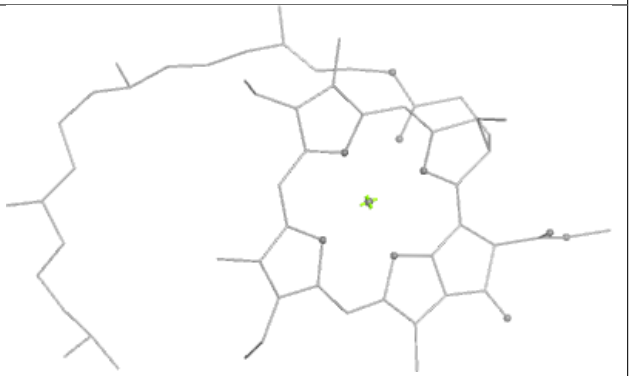
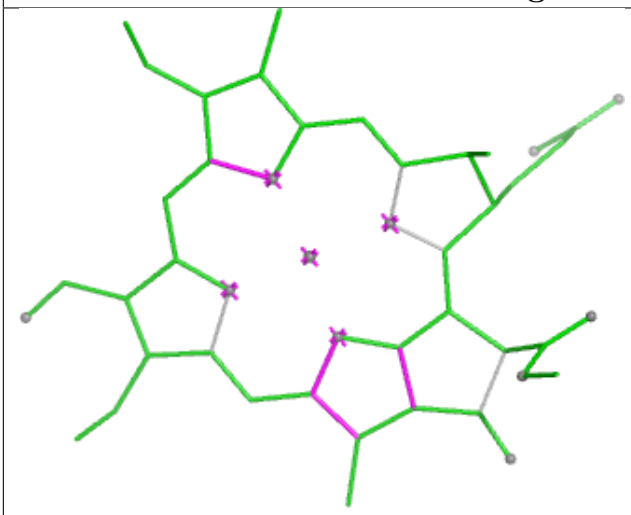


Rings

Ligand CHL 1 607



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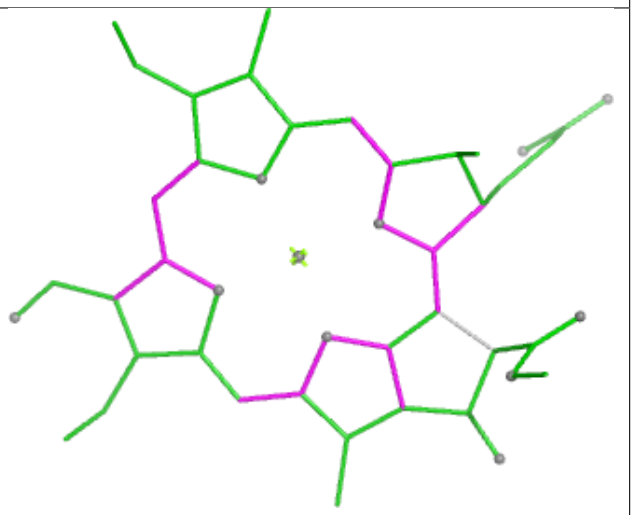
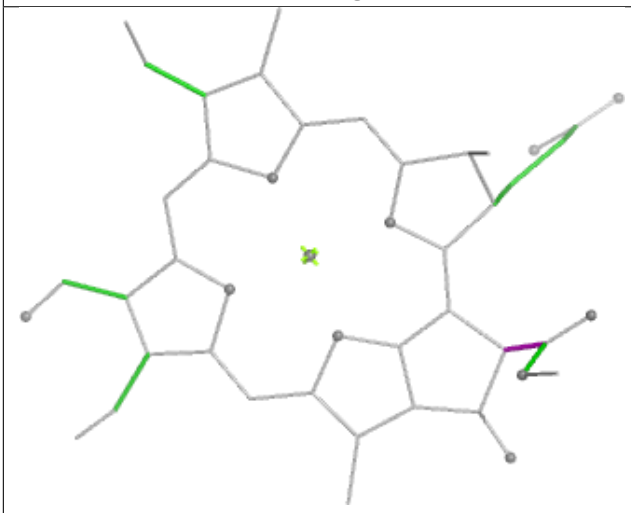


Bond angles



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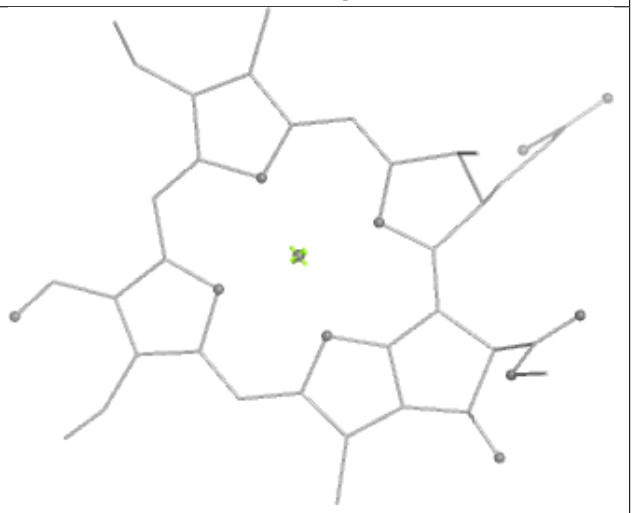
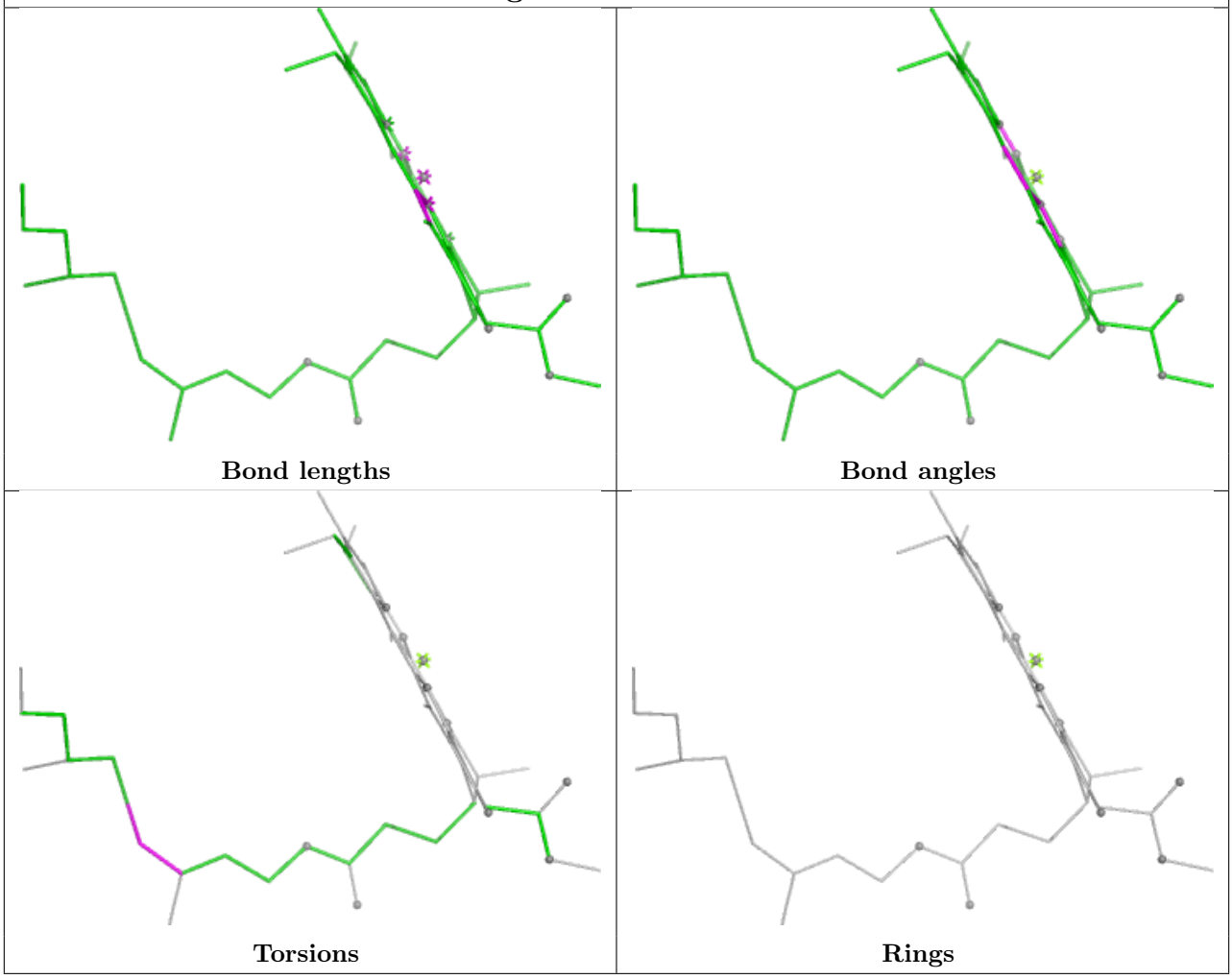
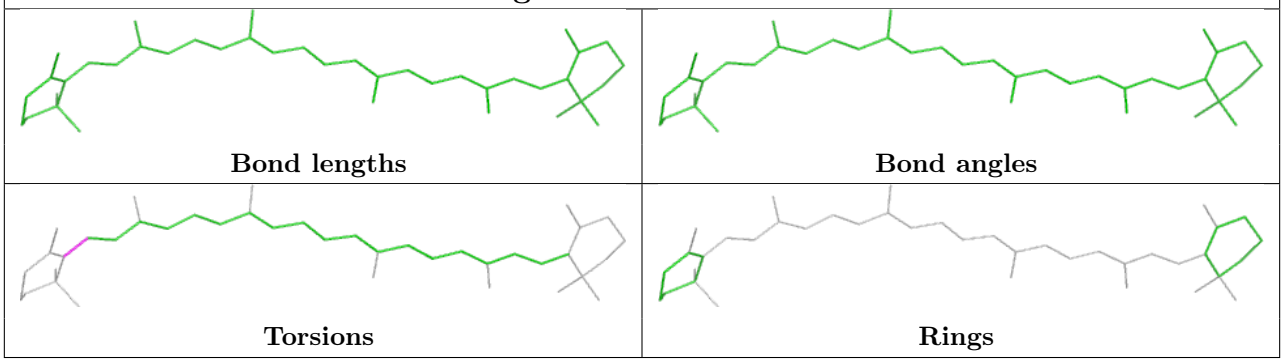


Rings

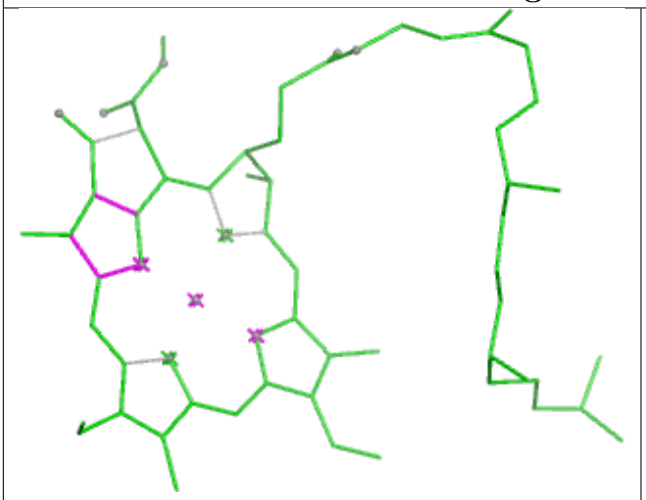
Ligand CLA Z 604



Ligand BCR G2 205



Ligand CLA B 823



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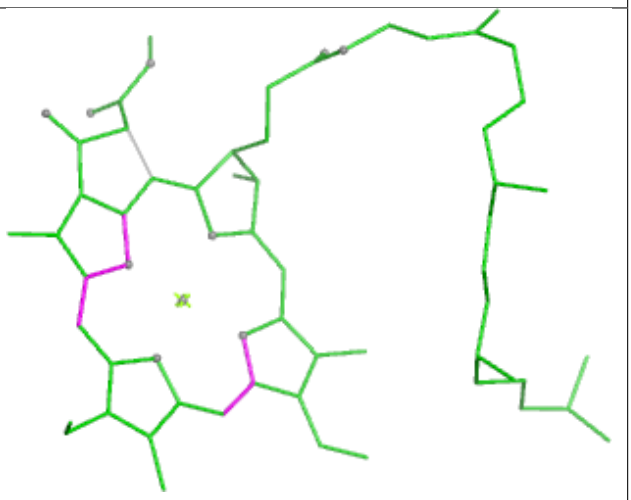
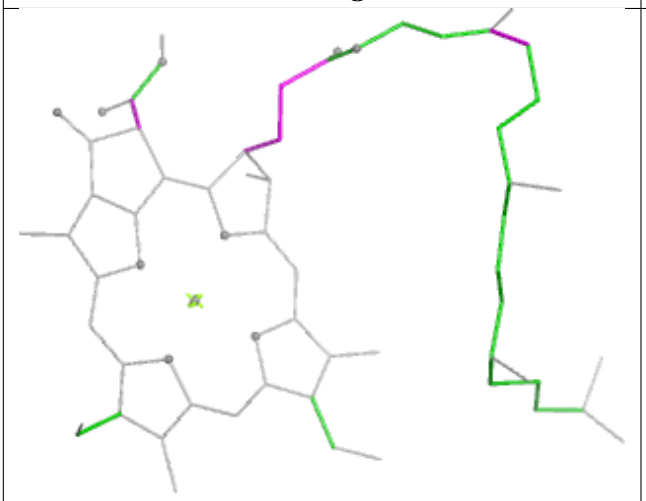


Bond angles

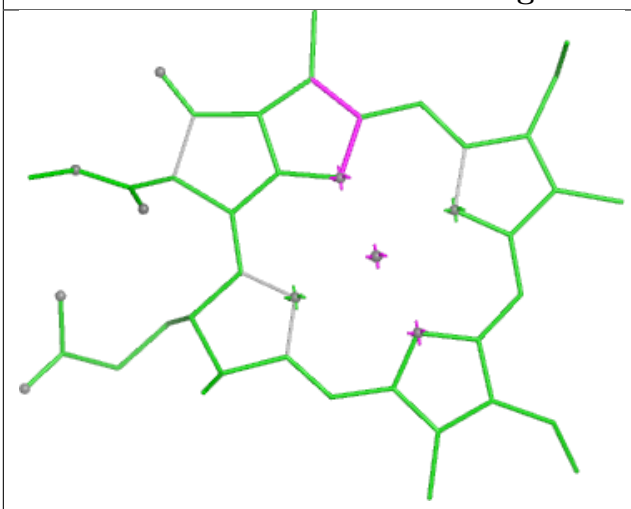


Torsions



Rings

Ligand CLA F2 303



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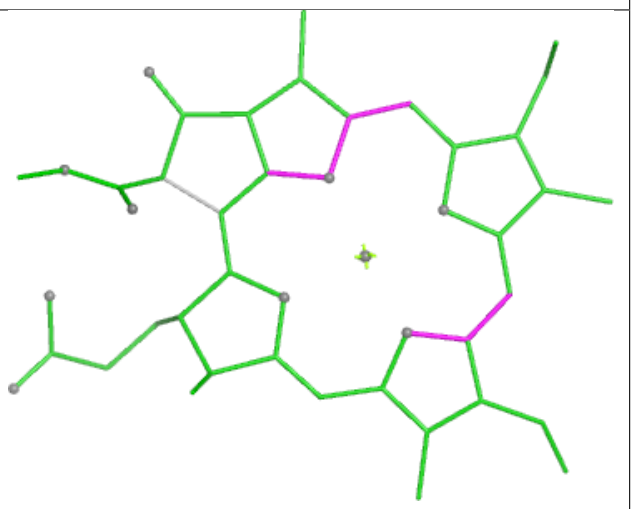
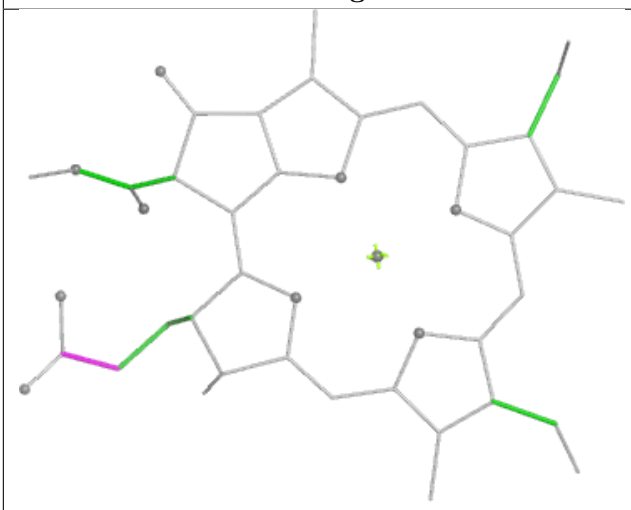
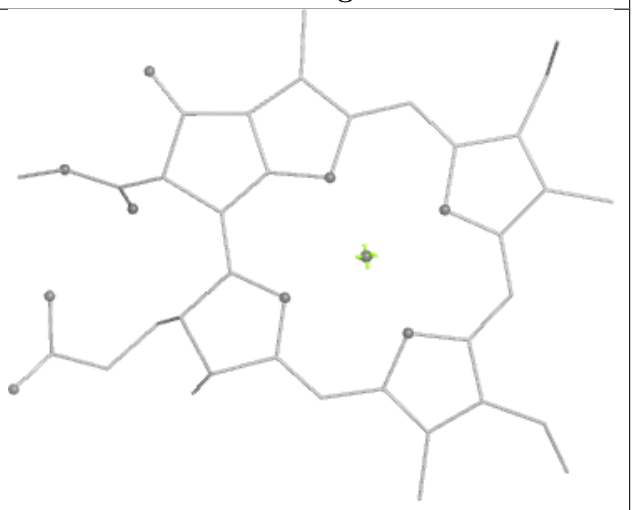


Bond angles

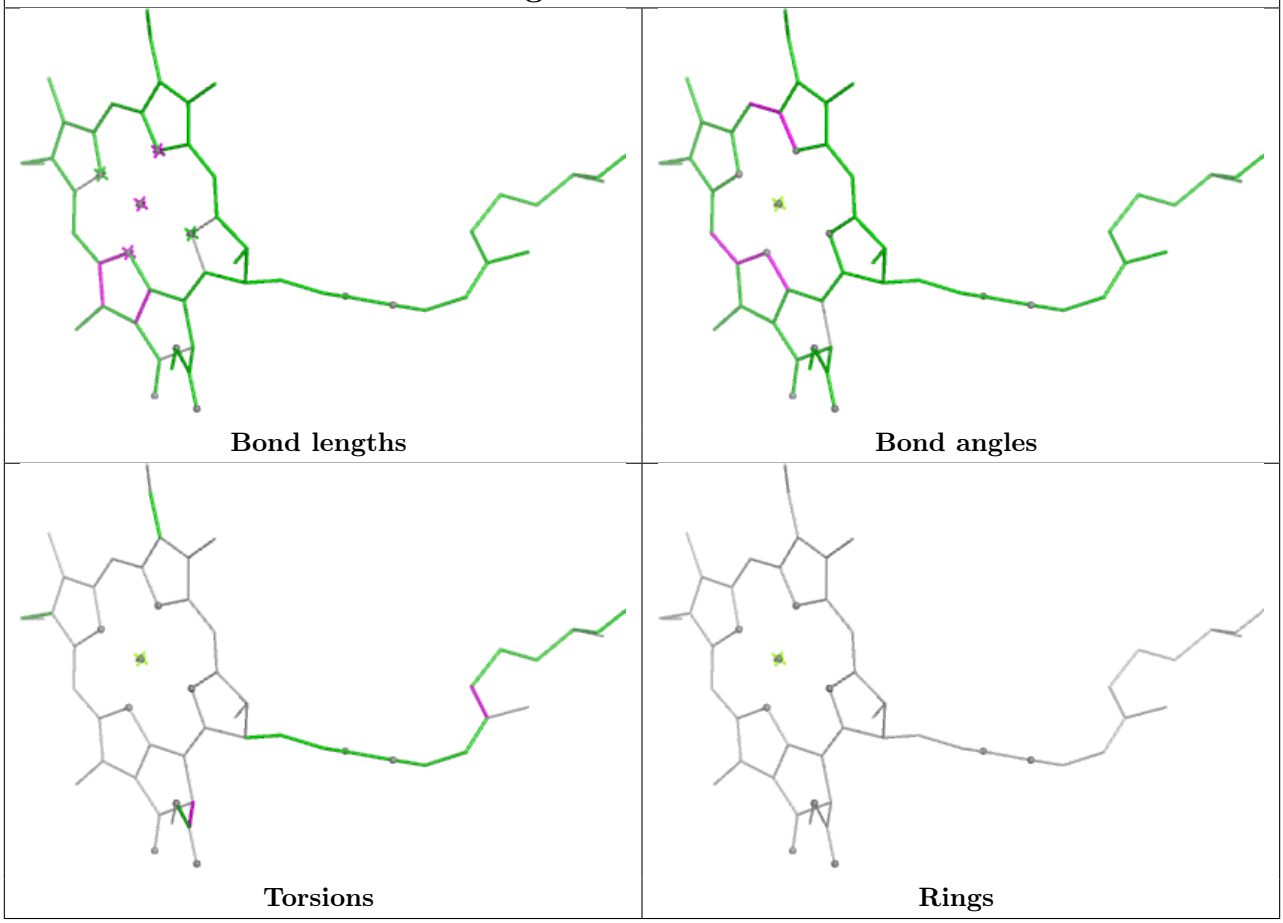


Torsions

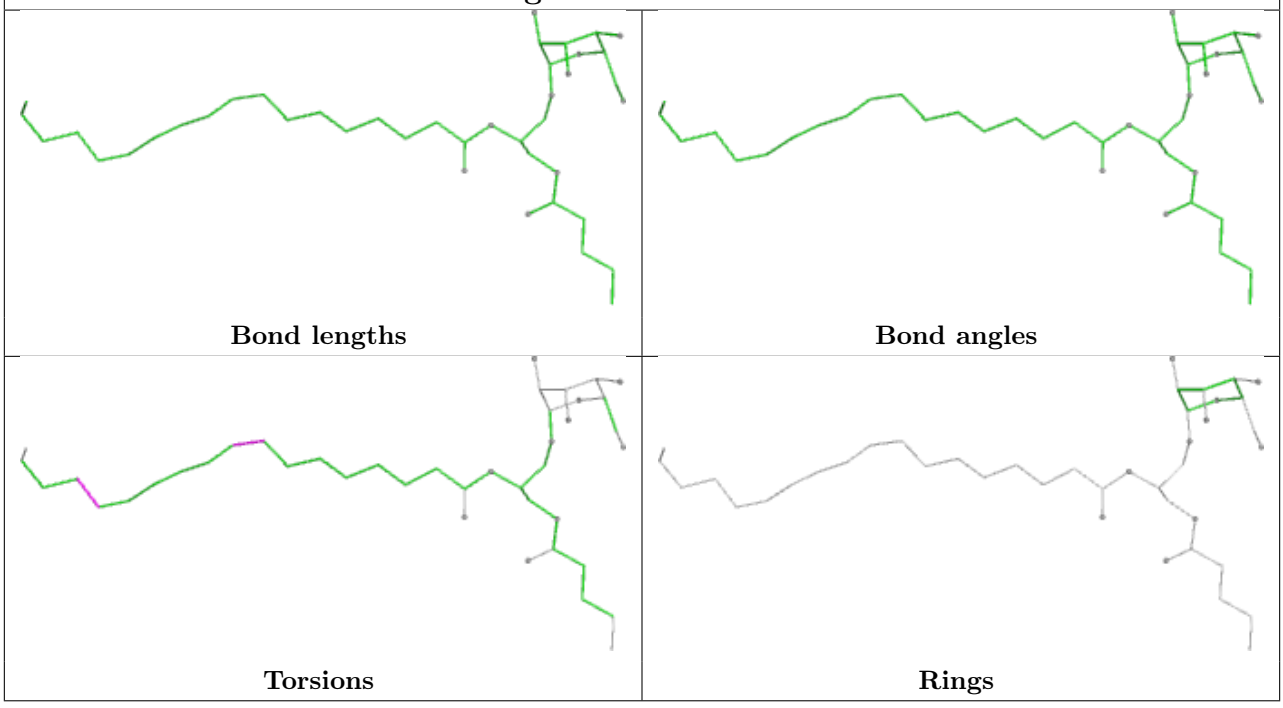


Rings

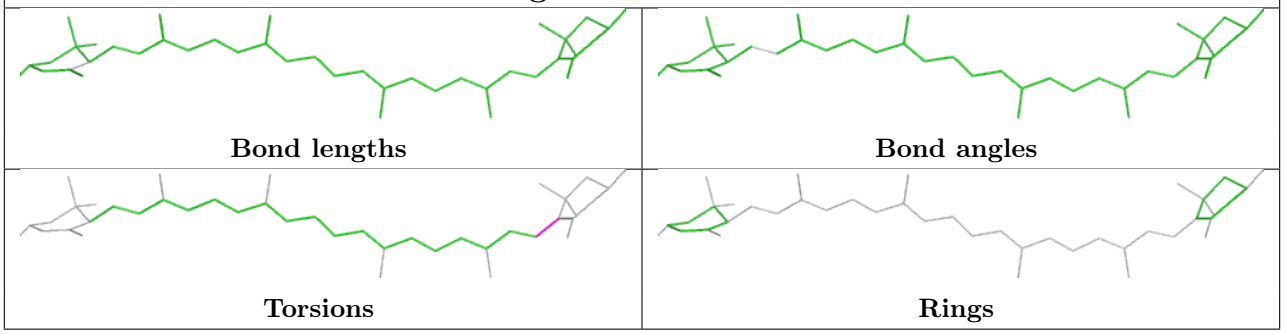
Ligand CLA B 833



Ligand LMG J 103



Ligand LUT 3 621



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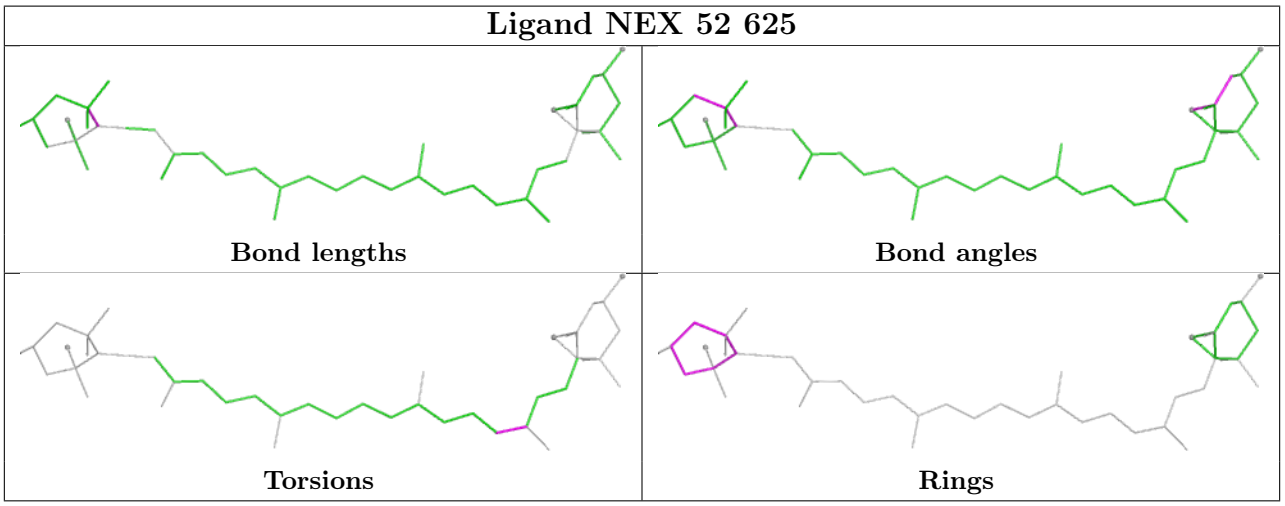
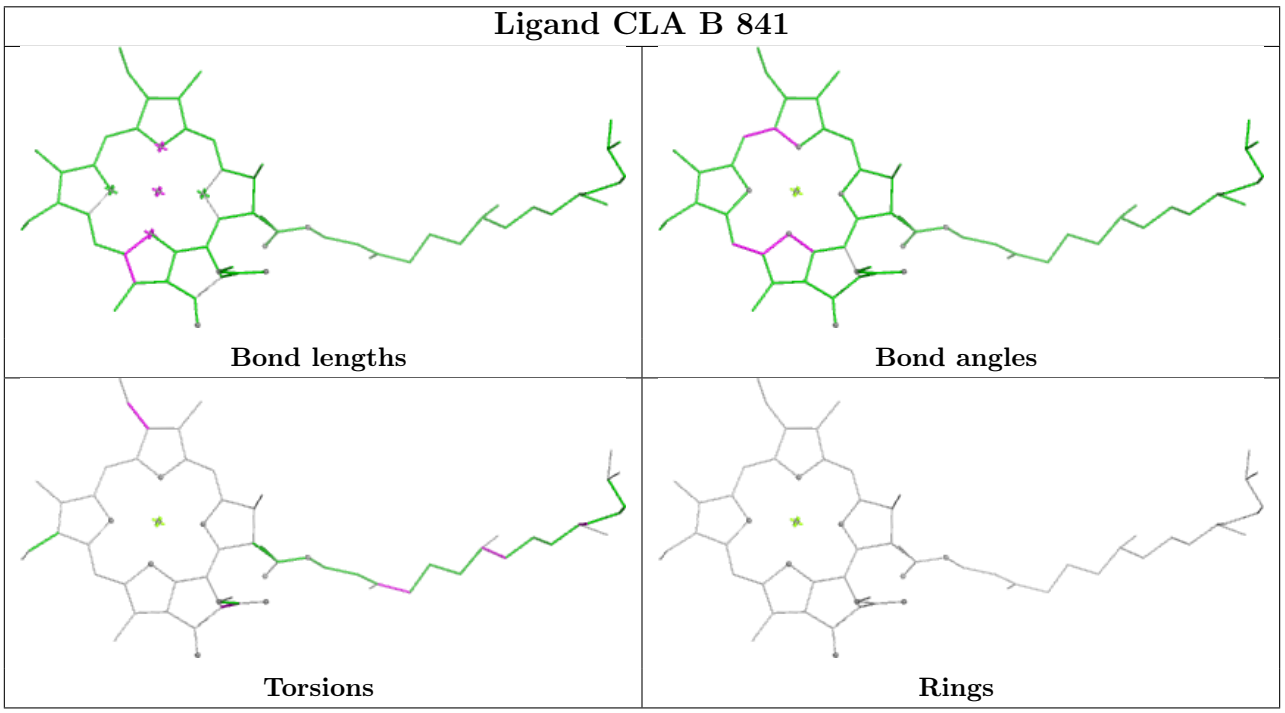
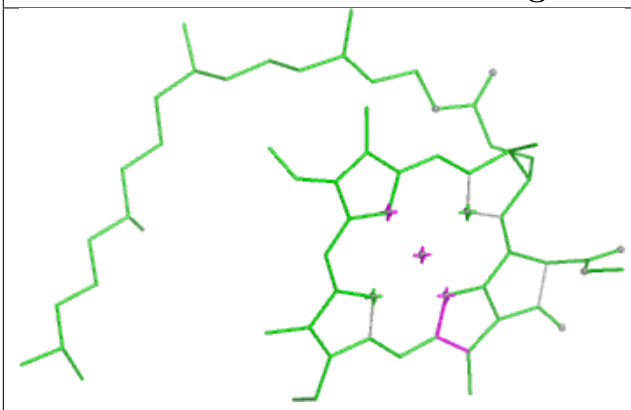


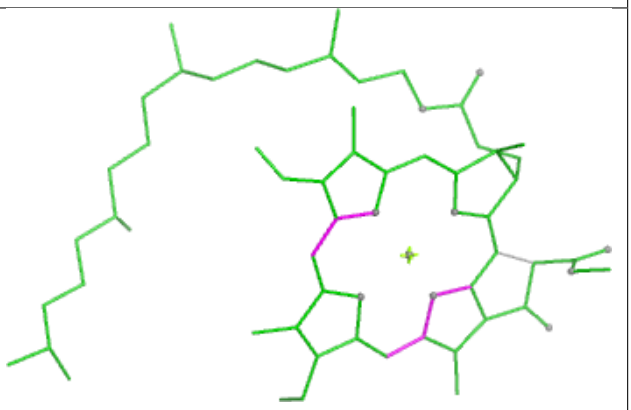
Ligand CLA B 841



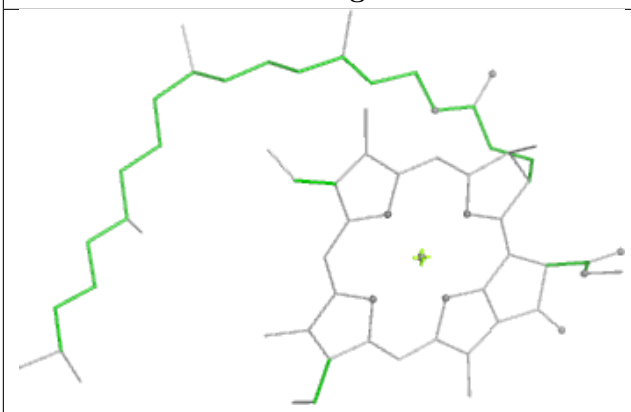
Ligand CLA 5 602



Bond lengths



Bond angles



Torsions



Rings

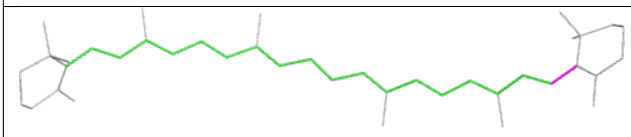
Ligand BCR A2 851



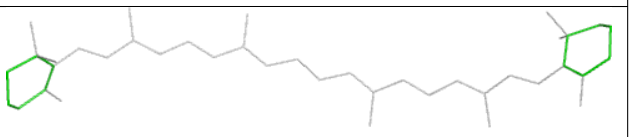
Bond lengths



Bond angles



Torsions



Rings

Ligand BCR 92 623



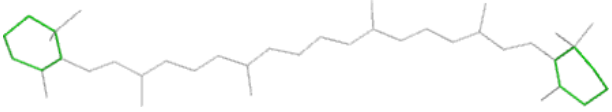
Bond lengths



Bond angles

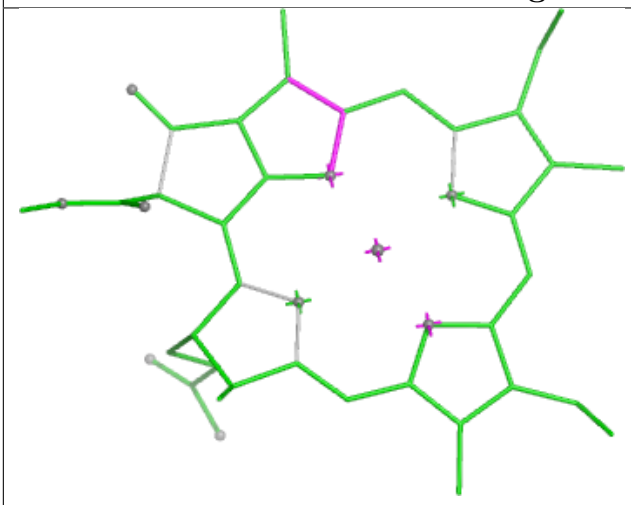


Torsions

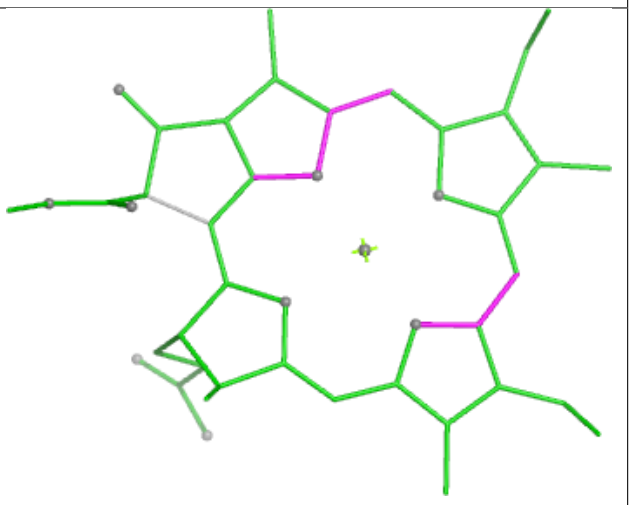


Rings

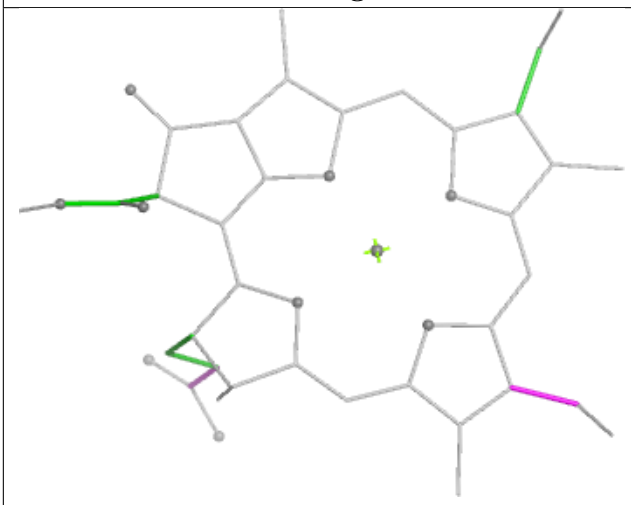
Ligand CLA 5 614



Bond lengths



Bond angles



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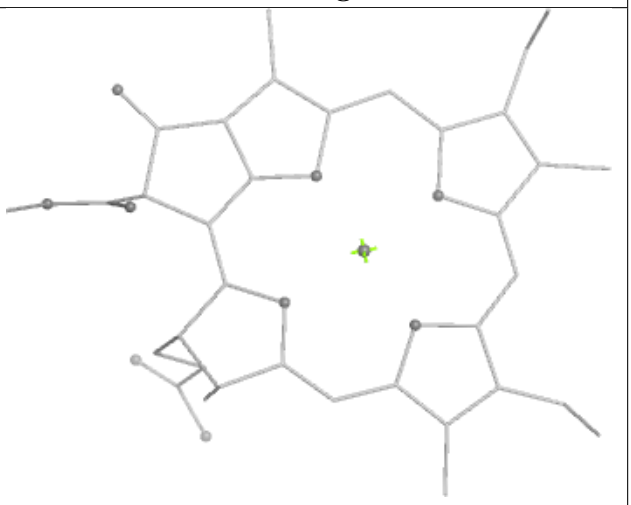


Rings

Ligand LUT 7 624



Bond lengths



Bond angles

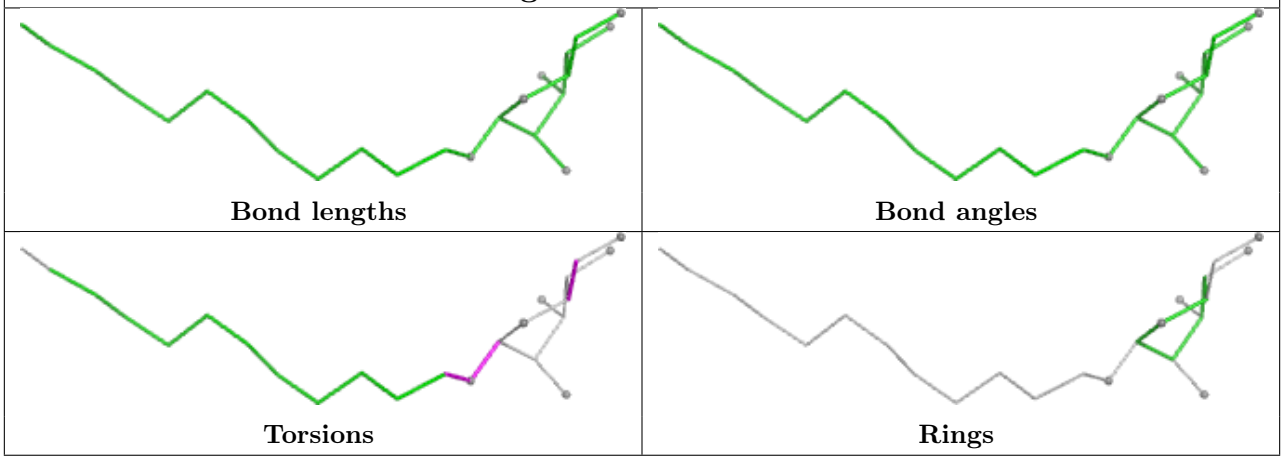


Torsions

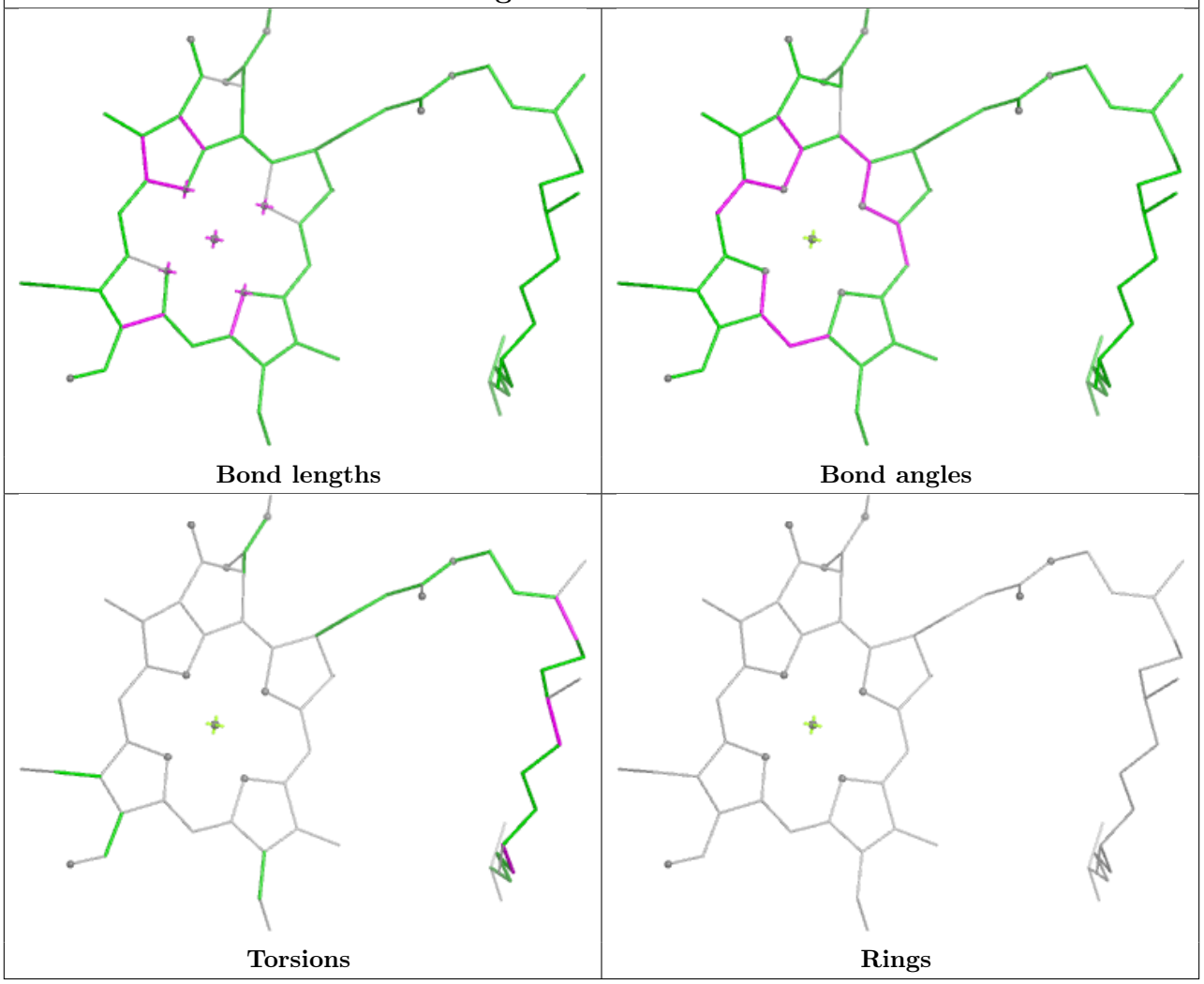


Rings

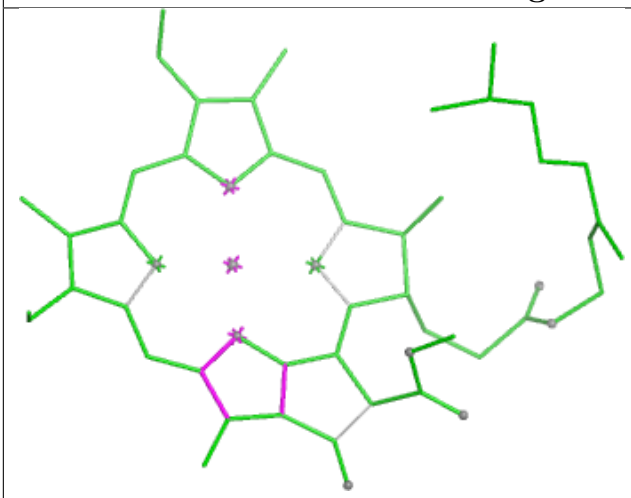
Ligand LMU A 861



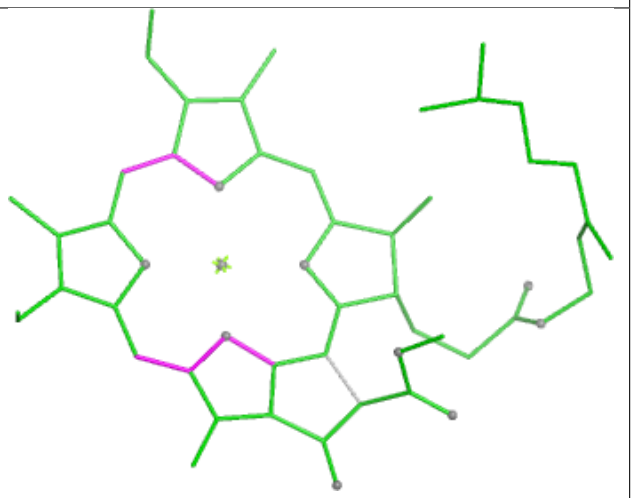
Ligand CHL 8 606



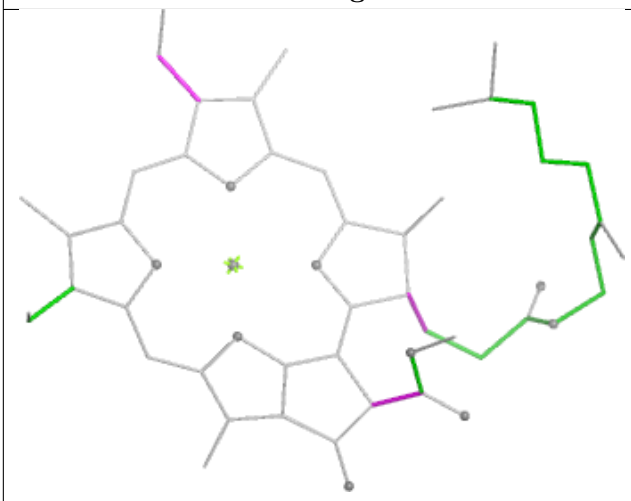
Ligand CLA 9 603



Bond lengths



Bond angles



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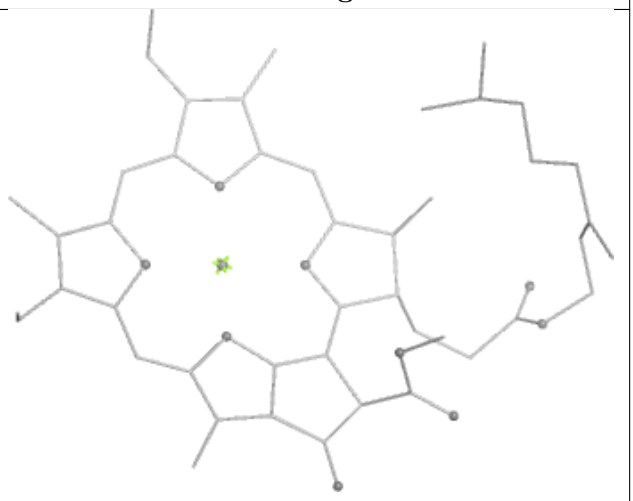
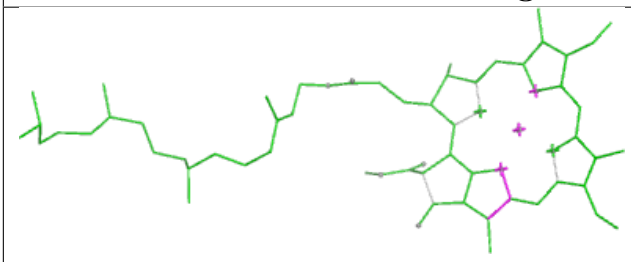


Rings

Ligand CLA F2 301



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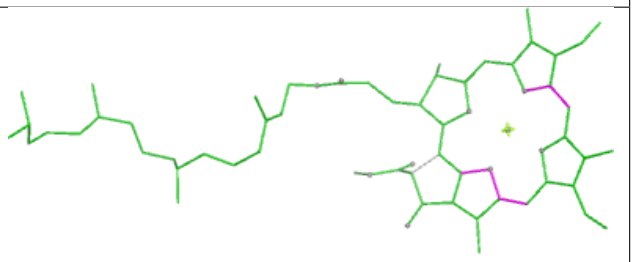
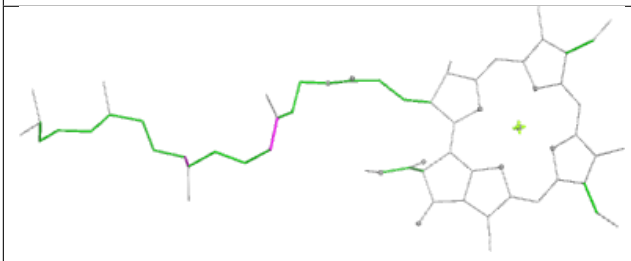


Bond angles



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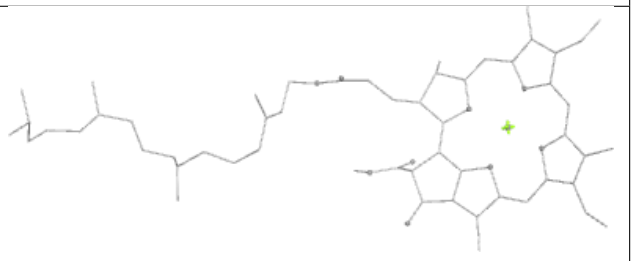
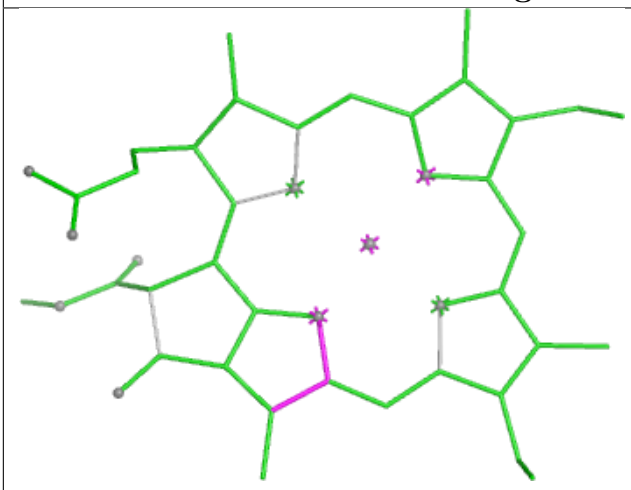


Rings

Ligand CLA K2 201



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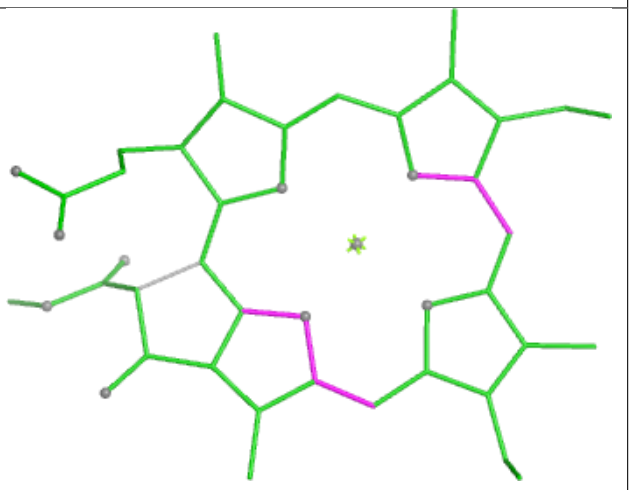
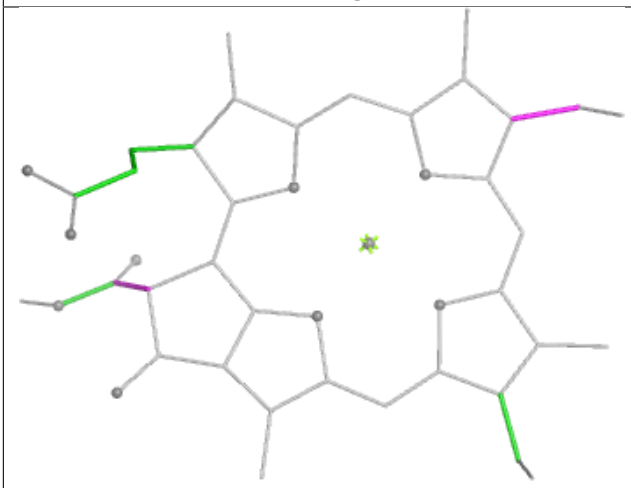


Bond angles



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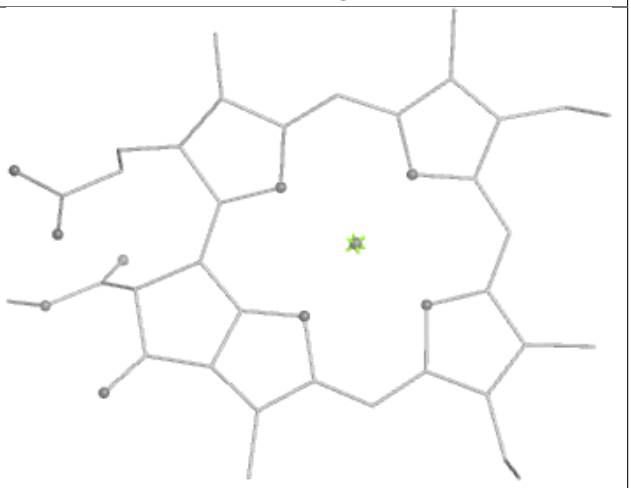
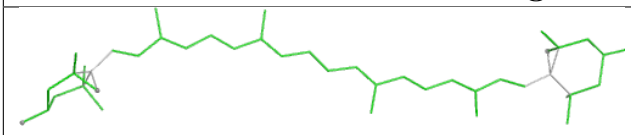
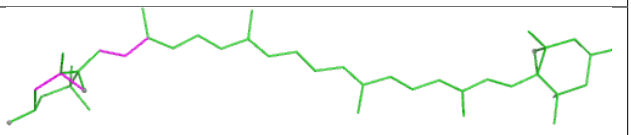


Rings

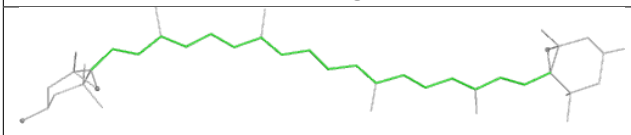
Ligand XAT 1 618



Bond lengths



Bond angles



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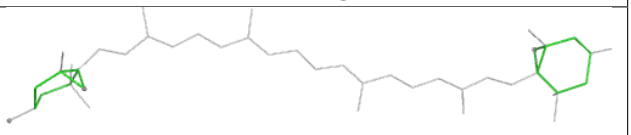
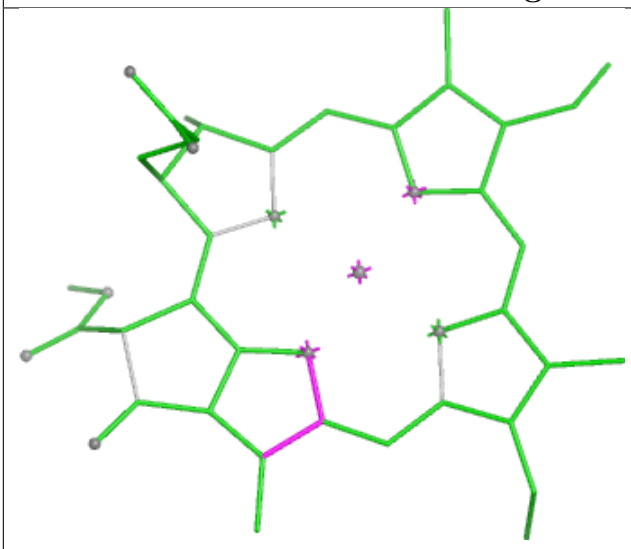
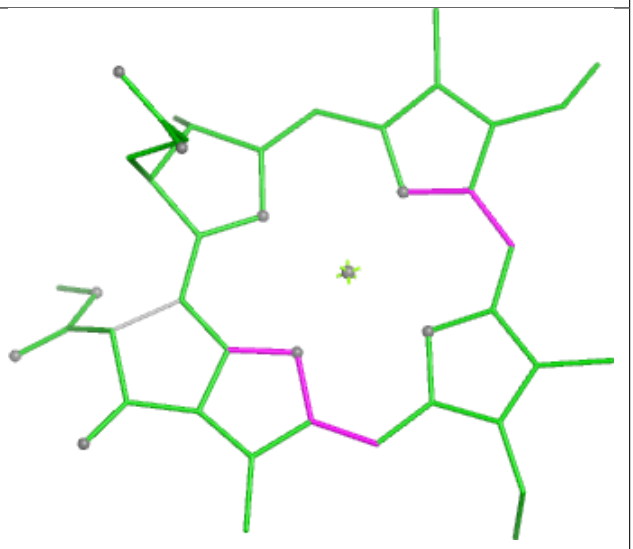


Rings

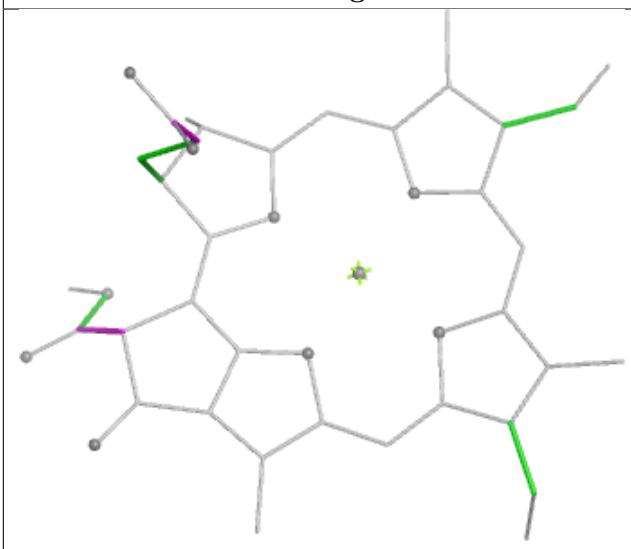
Ligand CLA B 804



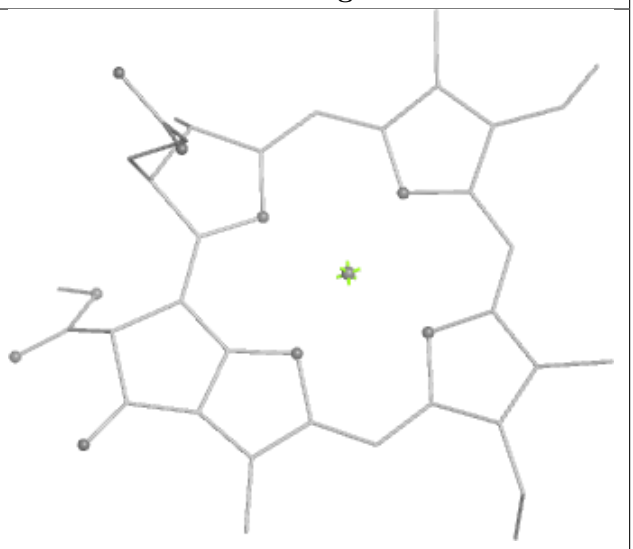
Bond lengths



Bond angles

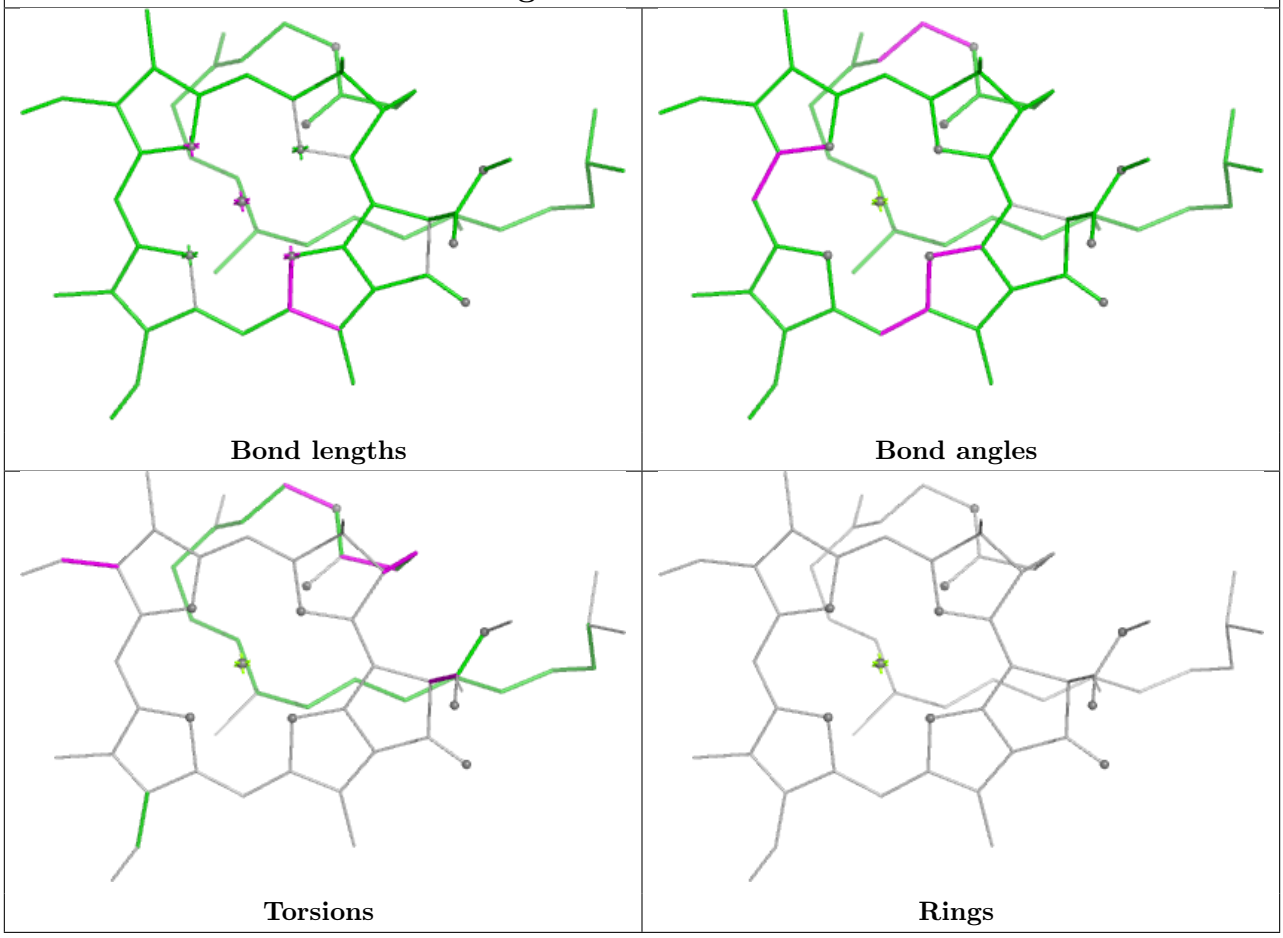


Torsions

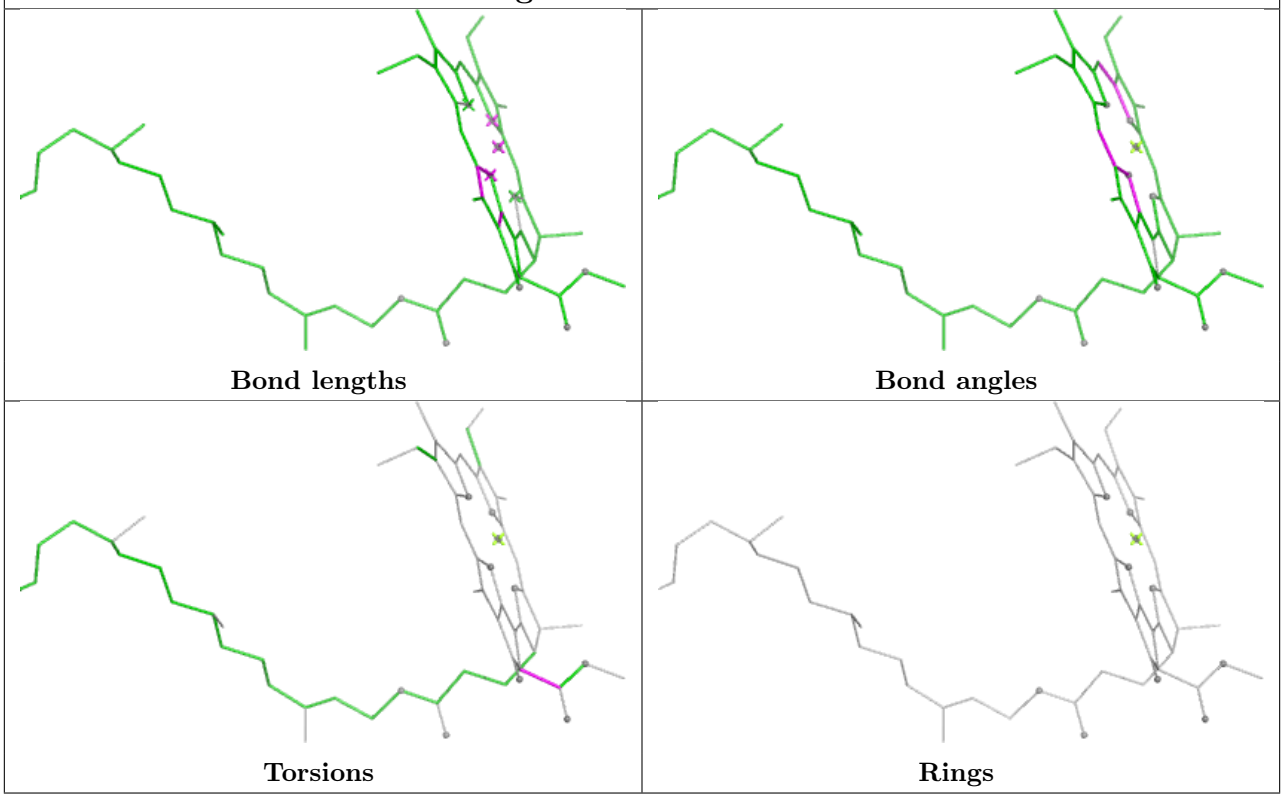


Rings

Ligand CLA F2 304



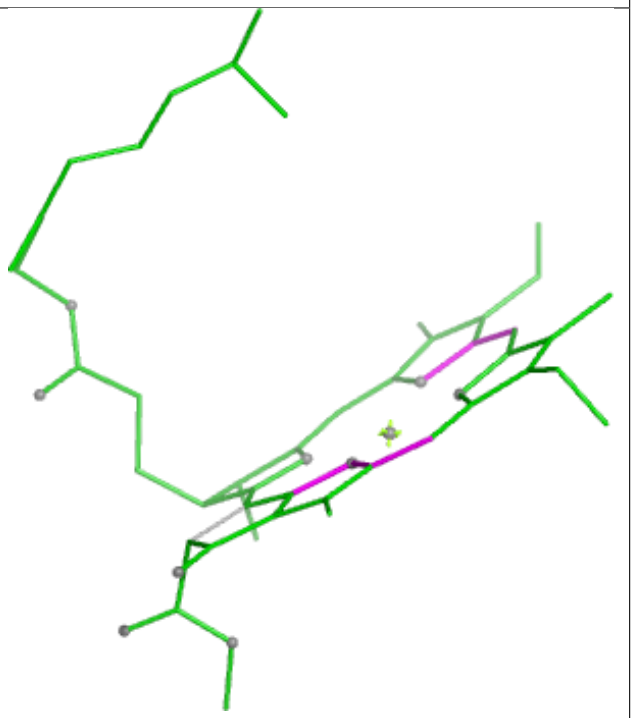
Ligand CLA A2 831



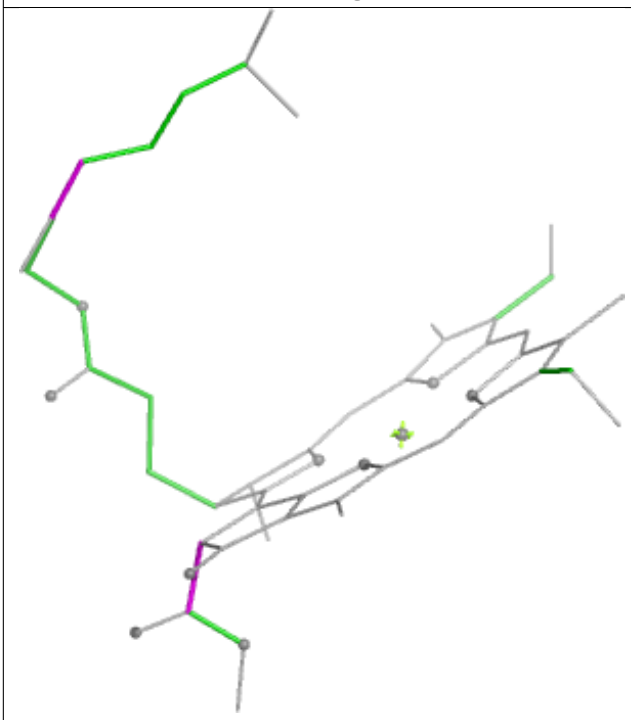
Ligand CLA A2 815



Bond lengths



Bond angles



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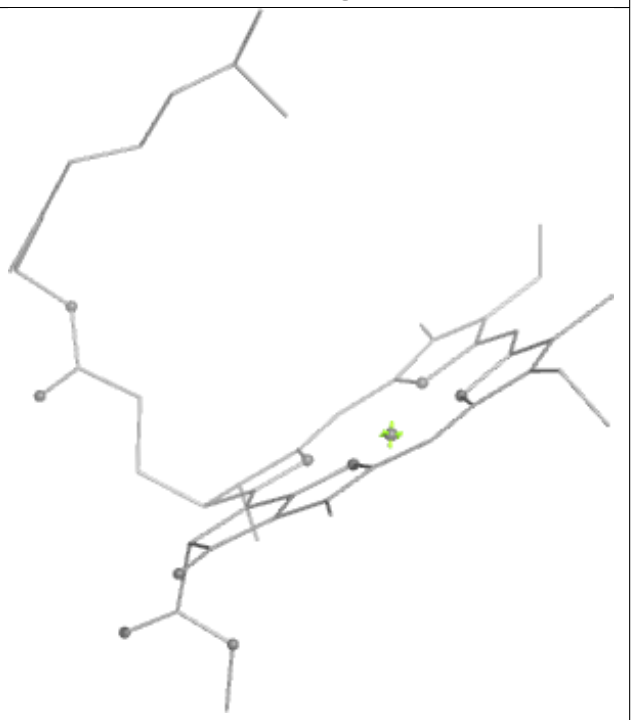
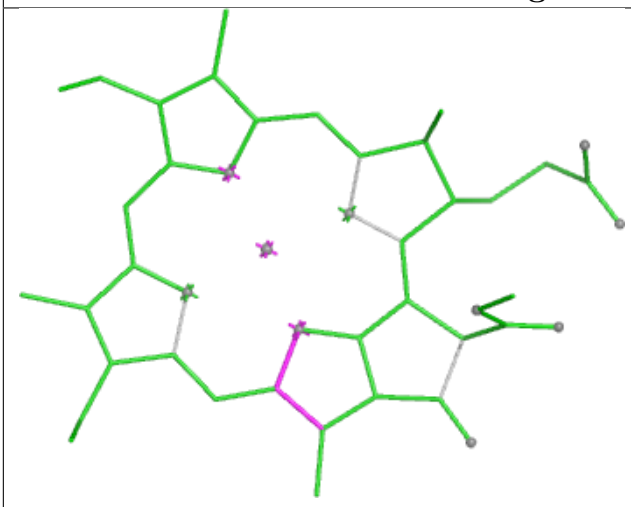


Rings

Ligand CLA 5 612



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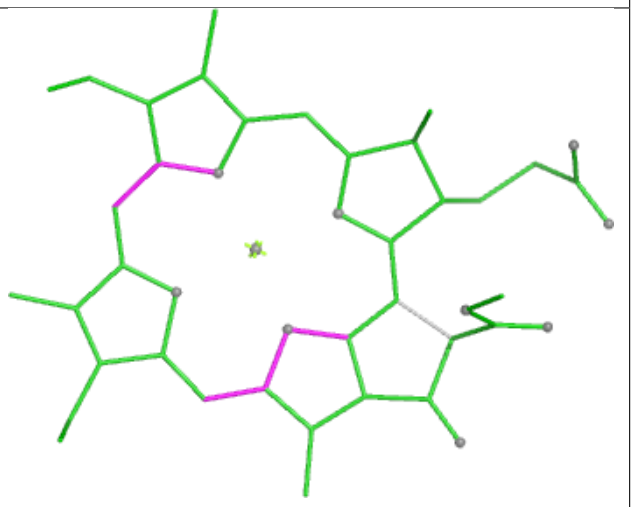
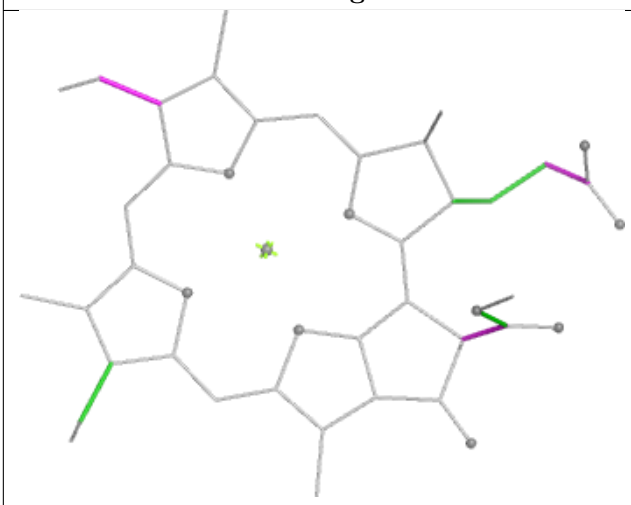


Bond angles



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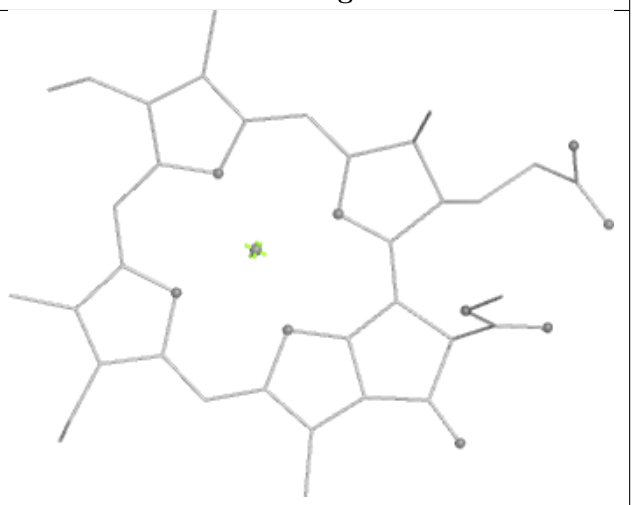
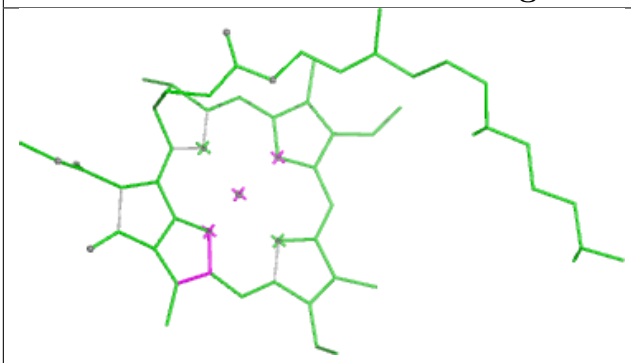


Rings

Ligand CLA 52 610



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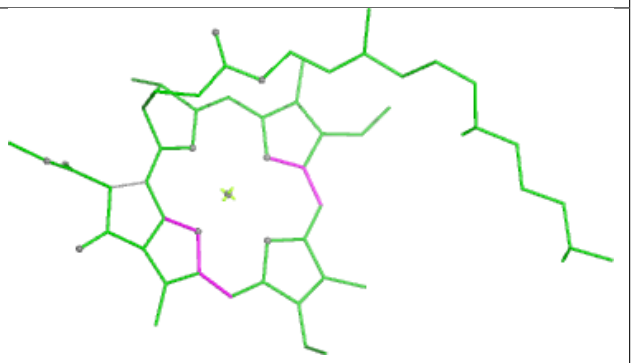
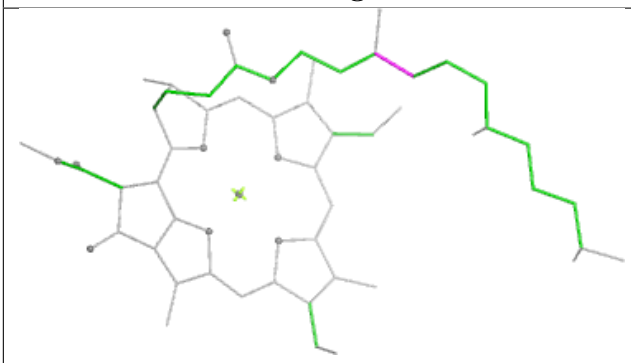


Bond angles



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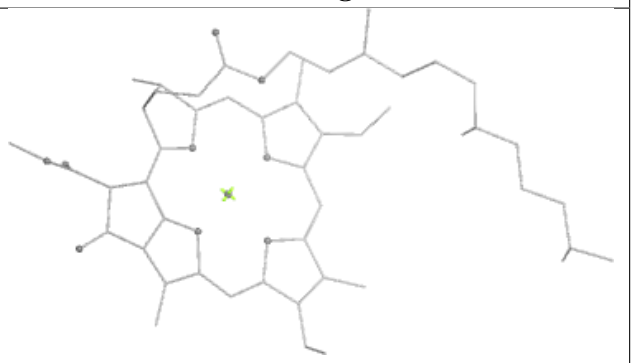
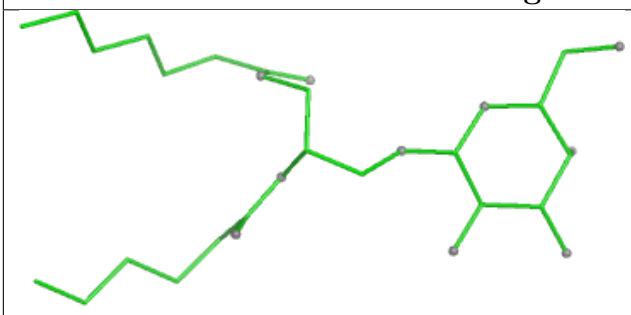
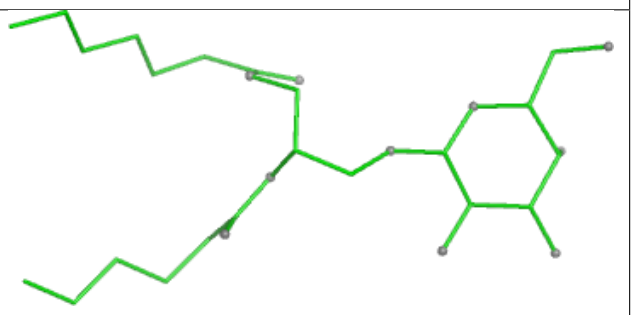


Rings

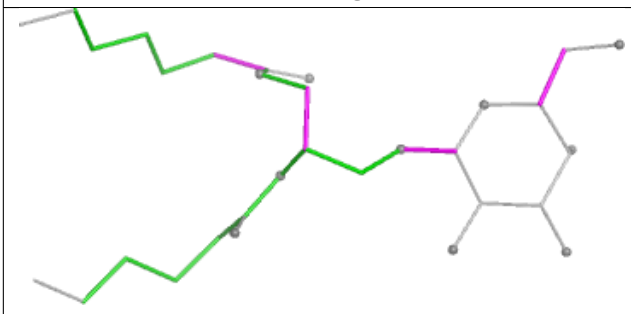
Ligand LMG 8 626



Bond lengths



Bond angles



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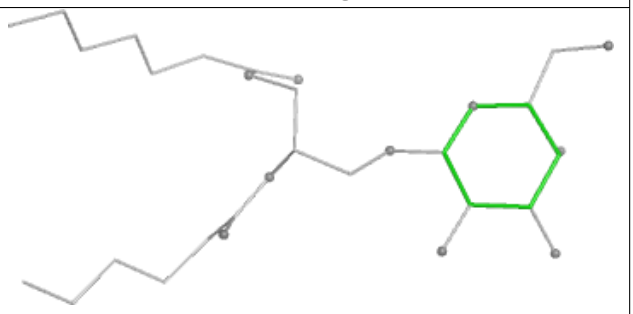
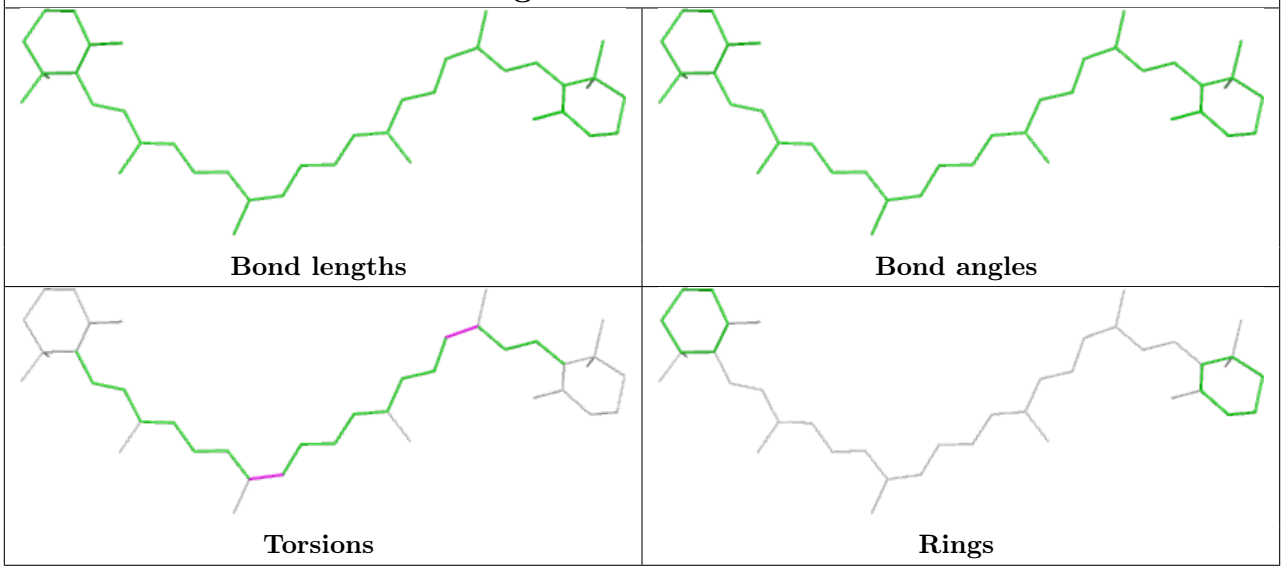
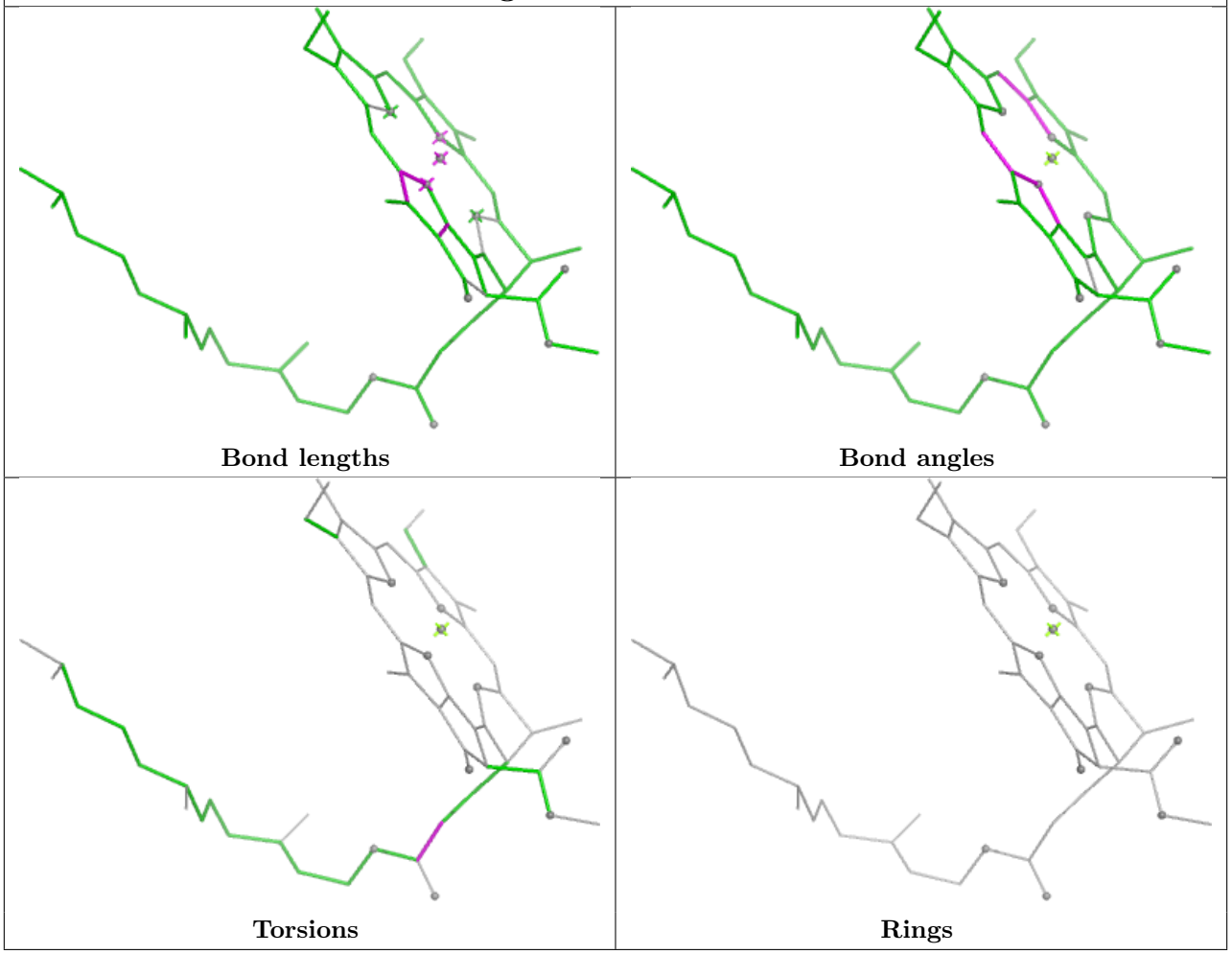


Rings

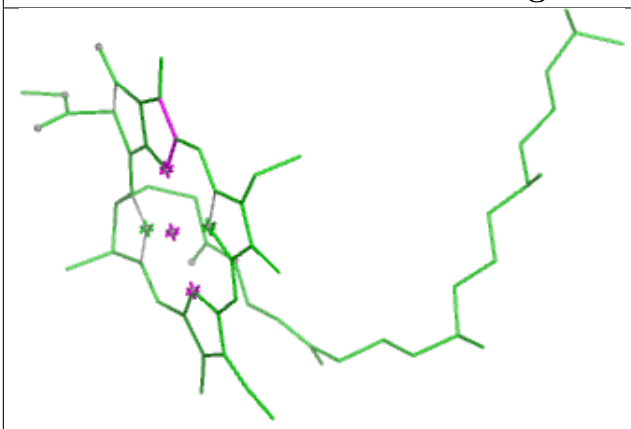
Ligand BCR A2 852



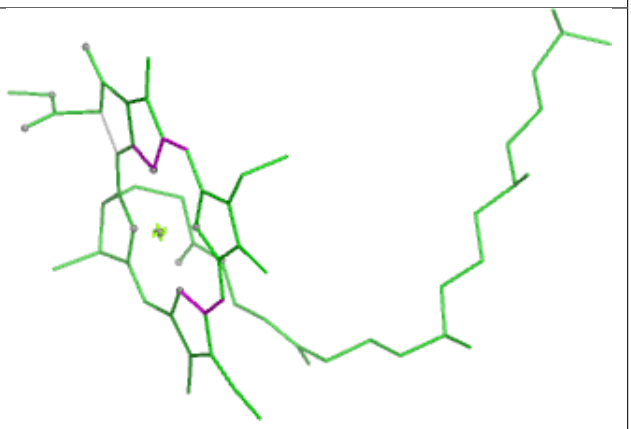
Ligand CLA 82 604



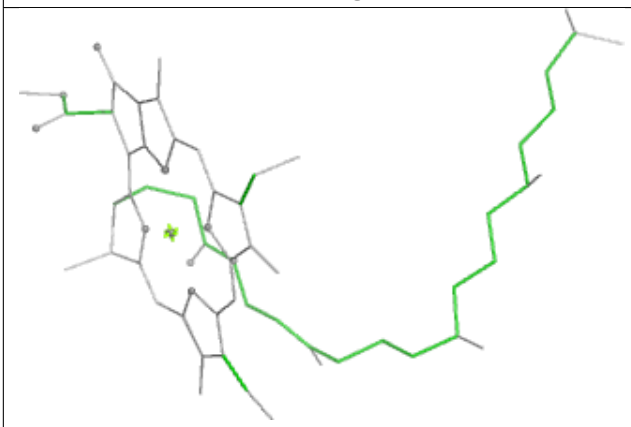
Ligand CLA 3 610



Bond lengths



Bond angles



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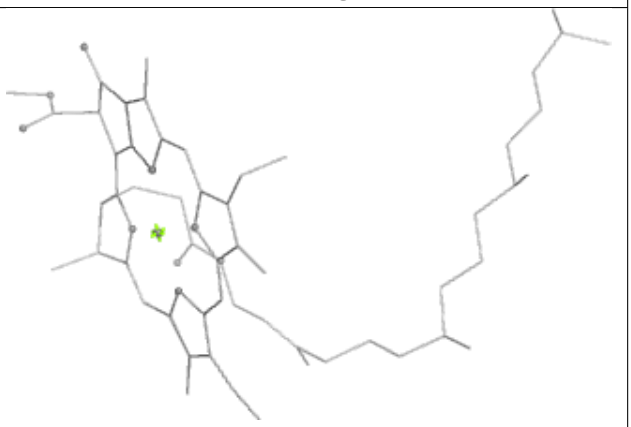
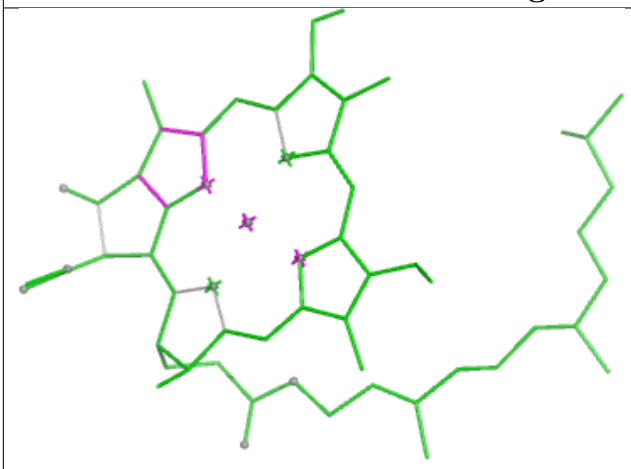


Rings

Ligand CLA 9 602



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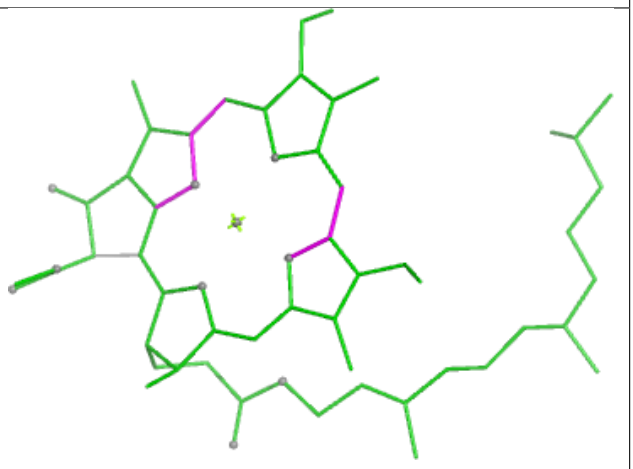

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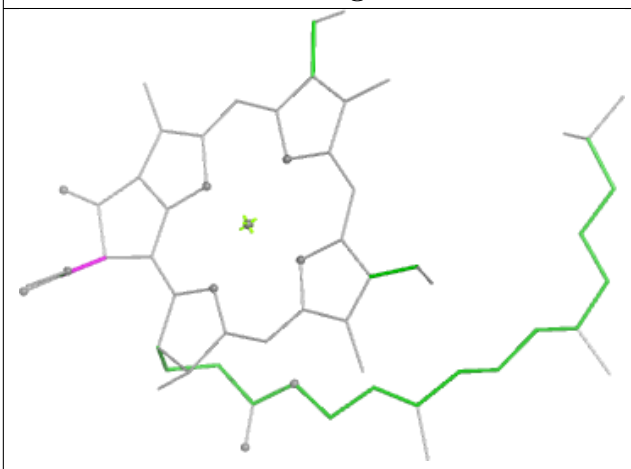

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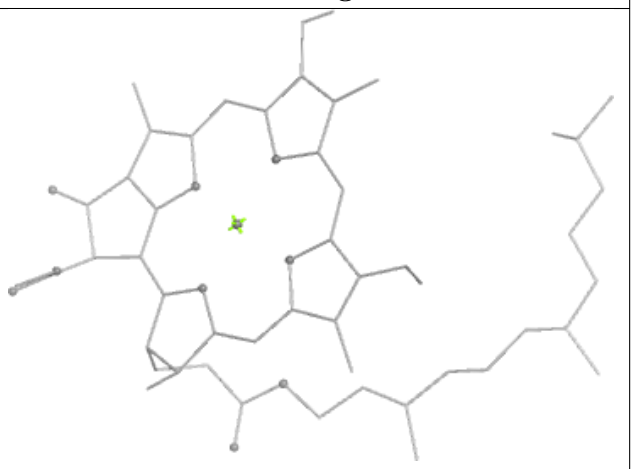
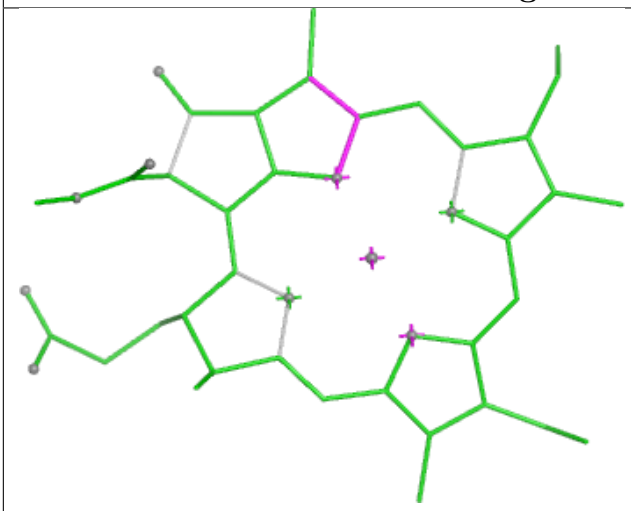


Rings

Ligand CLA 92 614



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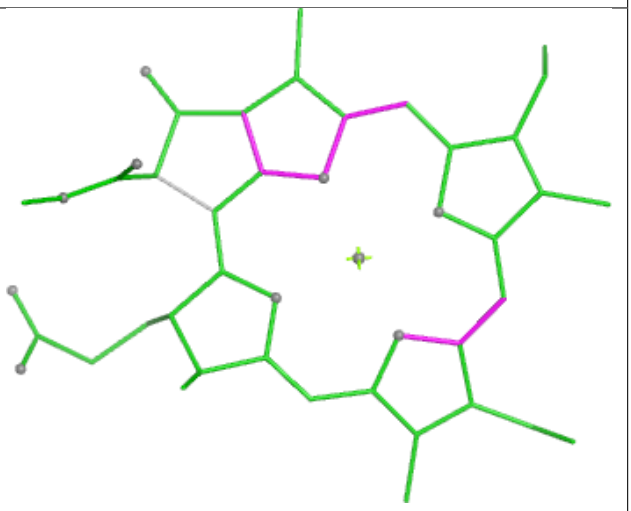

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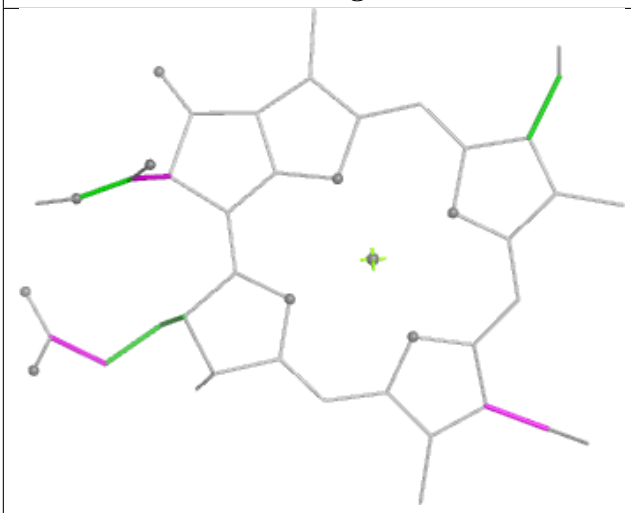

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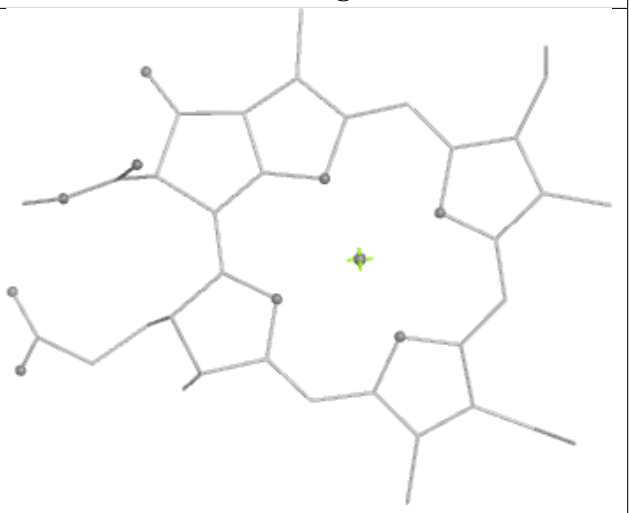


Rings

Ligand XAT 8 618



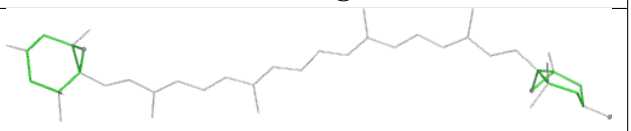
Bond lengths



Bond angles

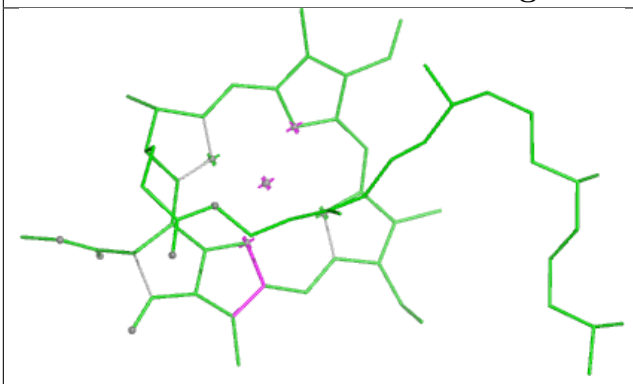


Torsions



Rings

Ligand CLA 32 615



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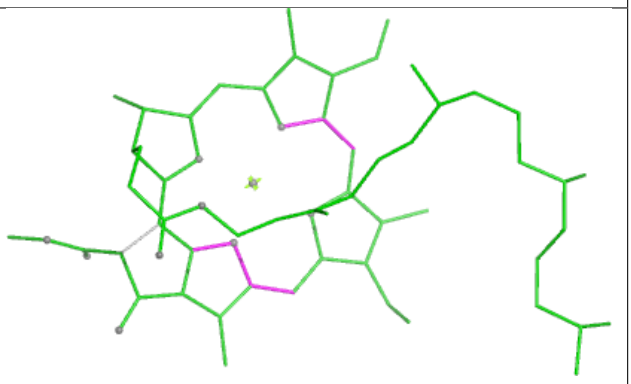
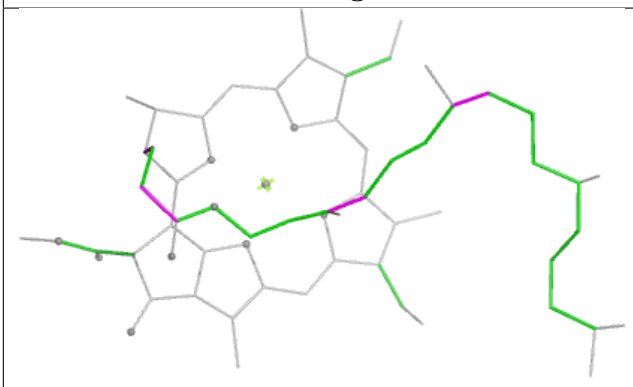


Bond angles



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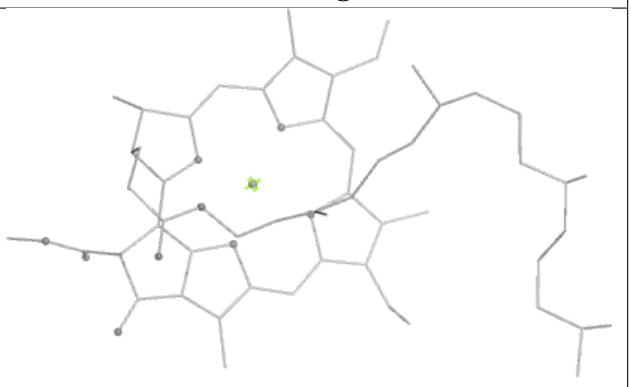
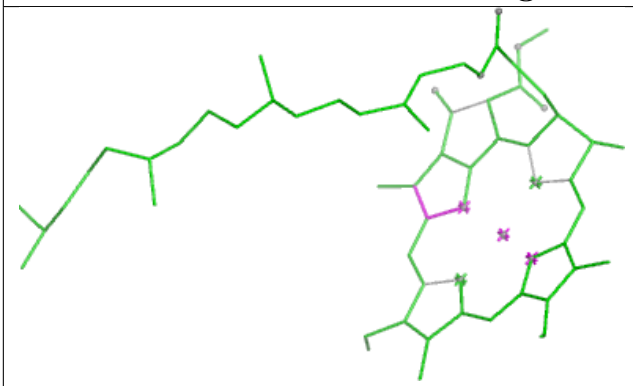


Rings

Ligand CLA Z2 609



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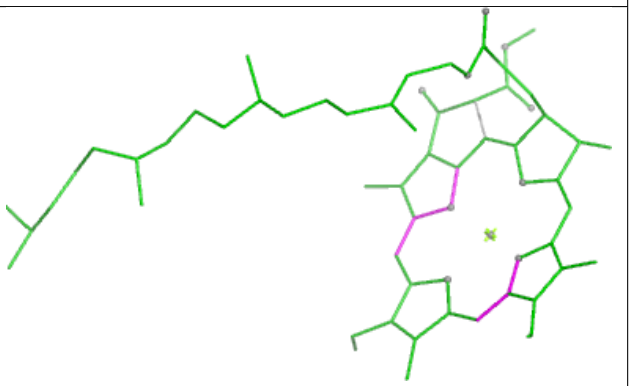
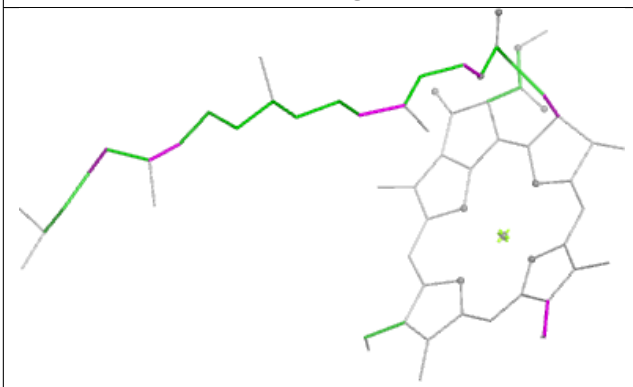


Bond angles



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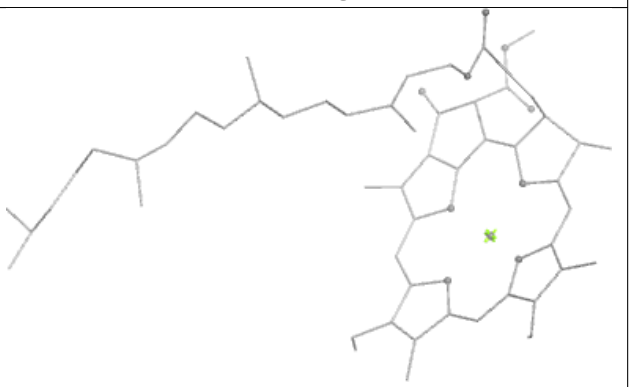
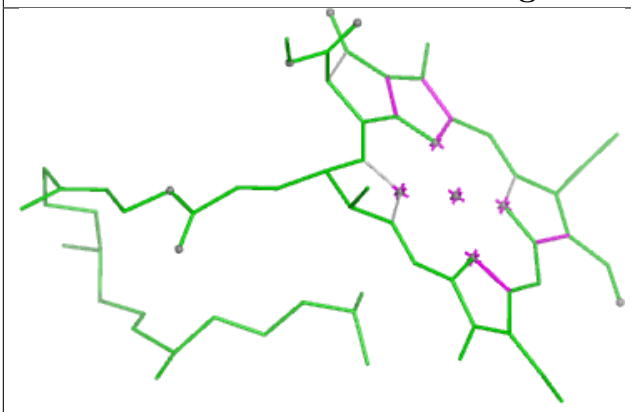


Rings

Ligand CHL 62 616



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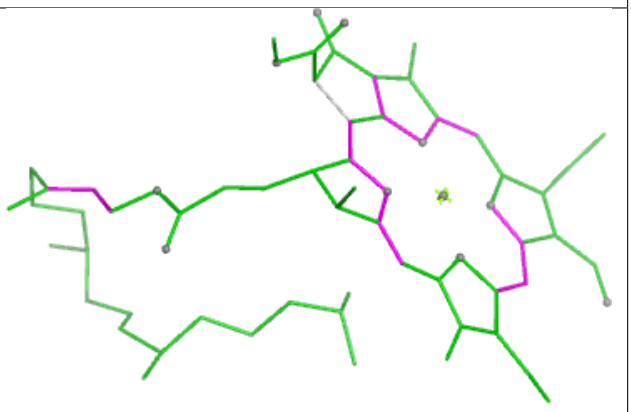
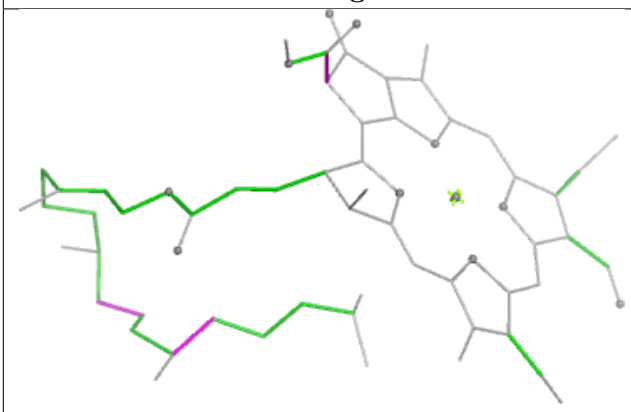


Bond angles



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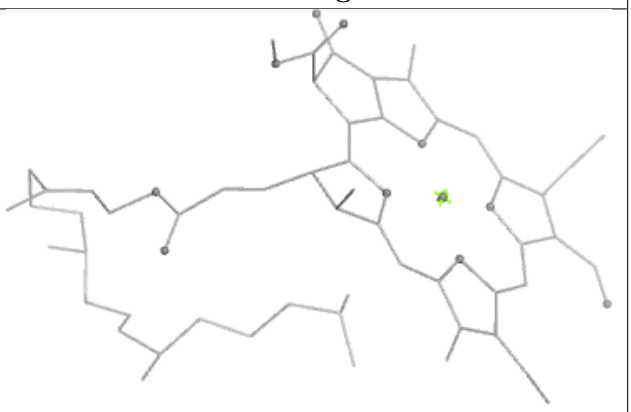
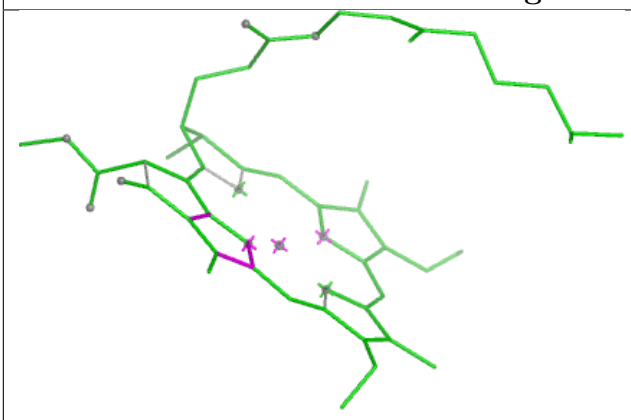


Rings

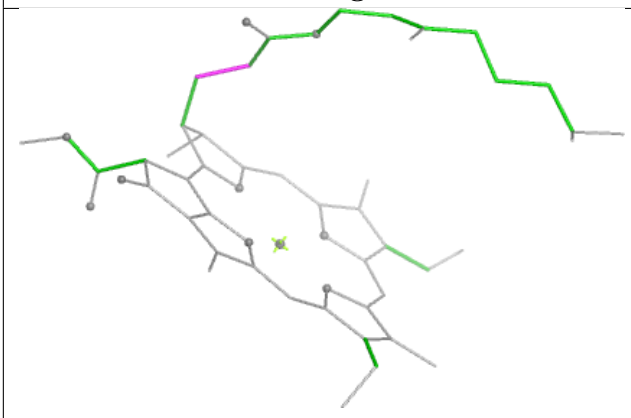
Ligand CLA B 831



Bond lengths



Bond angles



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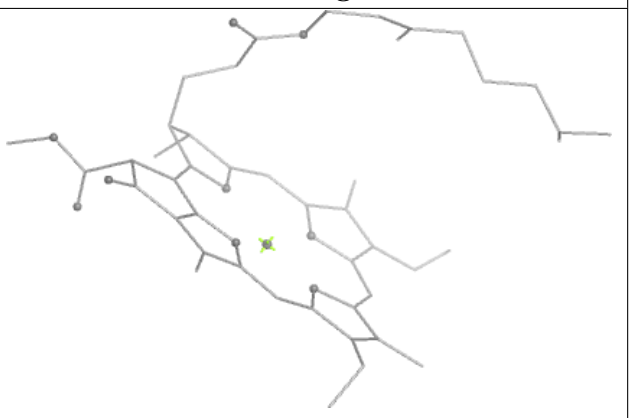
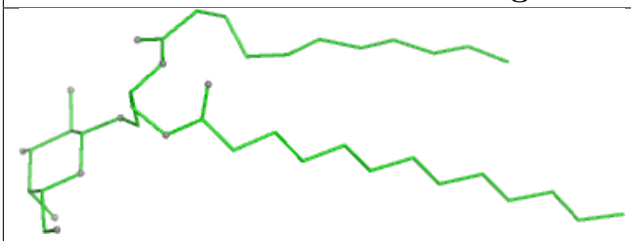
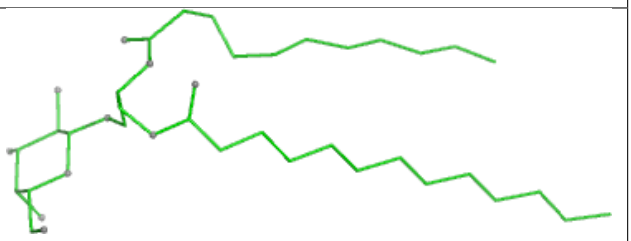


Rings

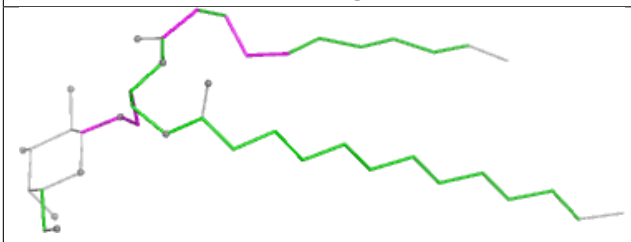
Ligand LMG B2 852



Bond lengths



Bond angles



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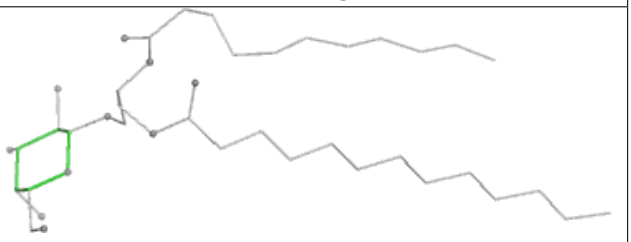
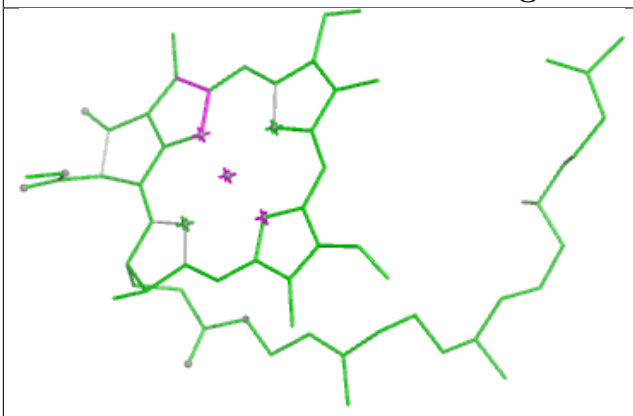


Rings

Ligand CLA 62 602



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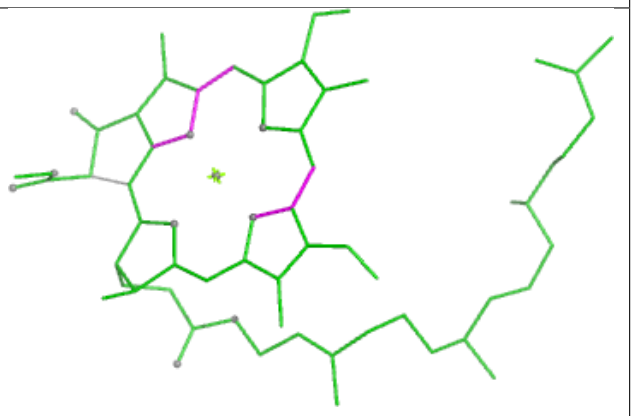
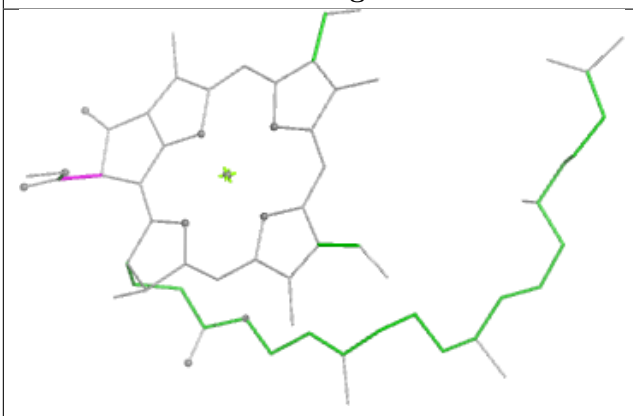


Bond angles



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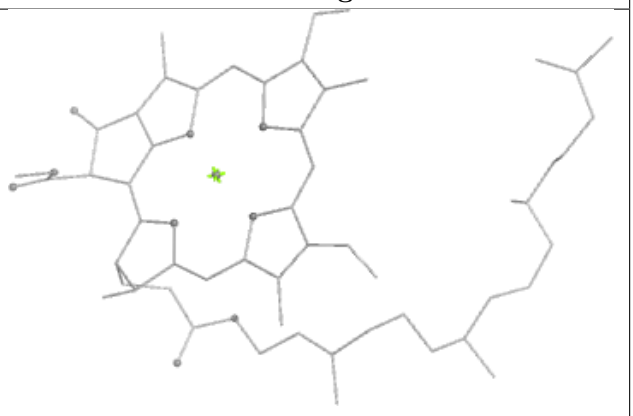


Rings

Ligand LUT 42 619



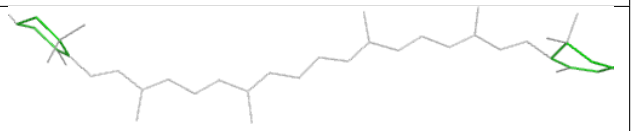
Bond lengths



Bond angles



Torsions

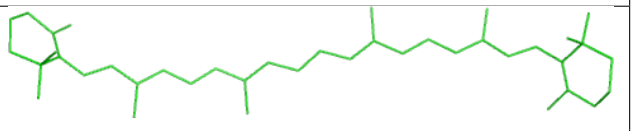


Rings

Ligand BCR B 843



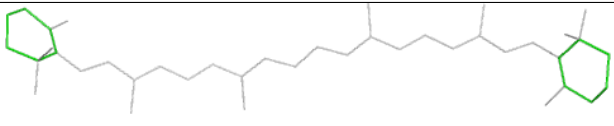
Bond lengths



Bond angles

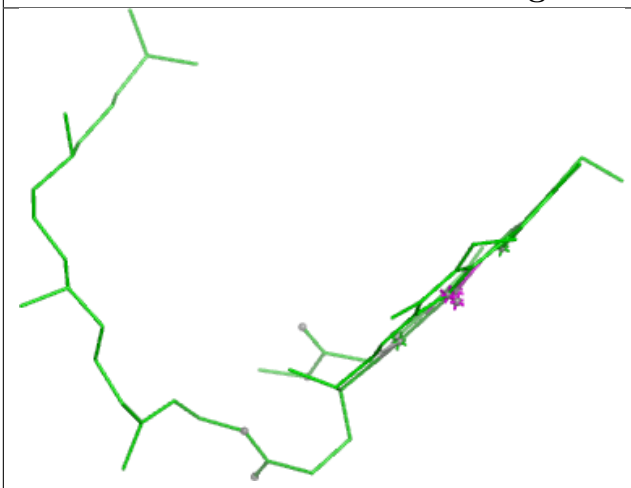


Torsions

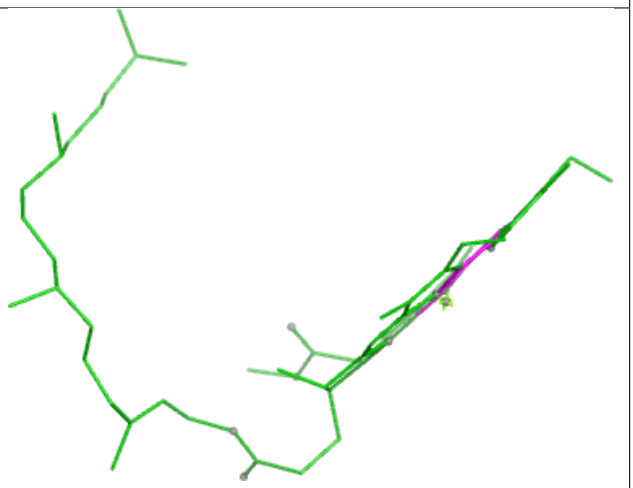


Rings

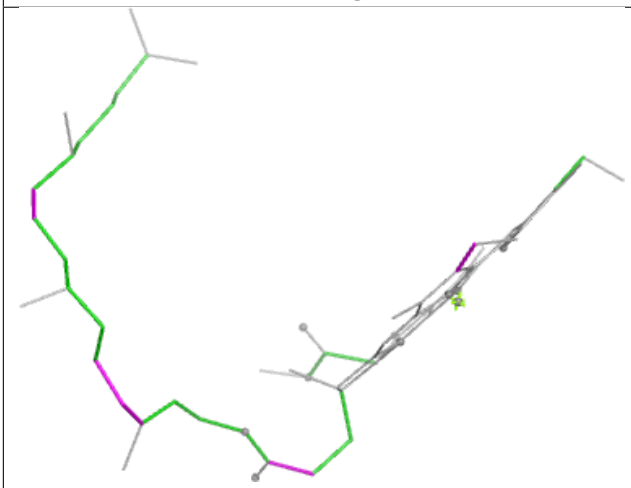
Ligand CLA 4 603



Bond lengths



Bond angles

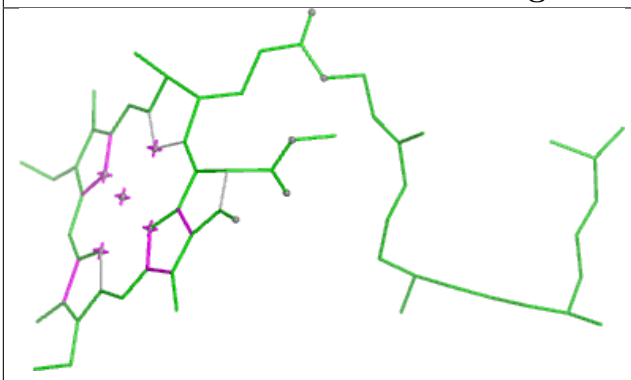


Torsions



Rings

Ligand CL0 A 801



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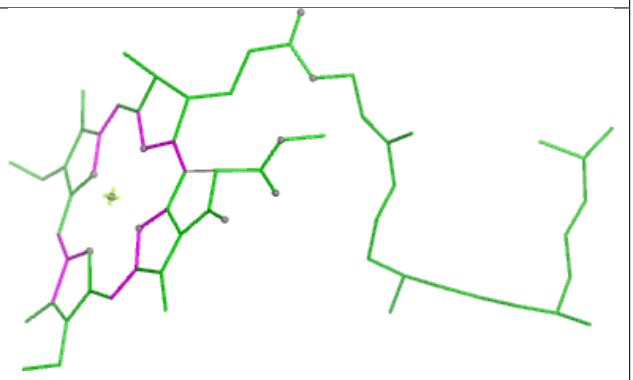
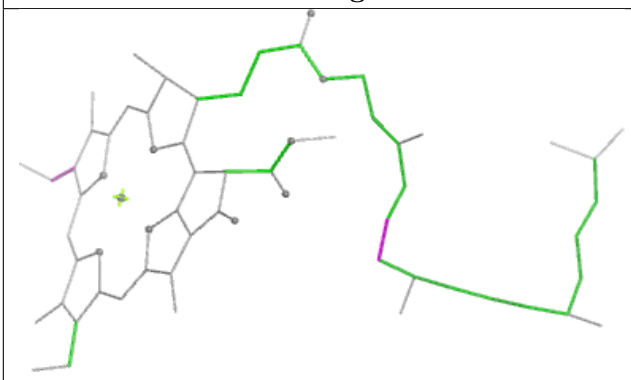


Bond angles

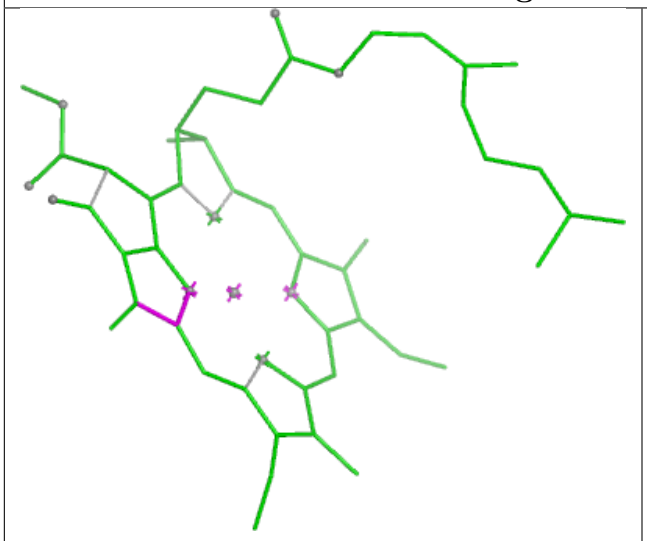


Torsions



Rings

Ligand CLA A2 825



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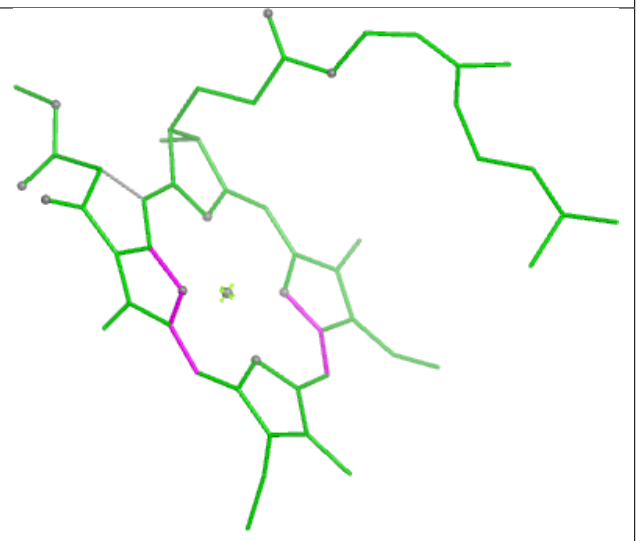
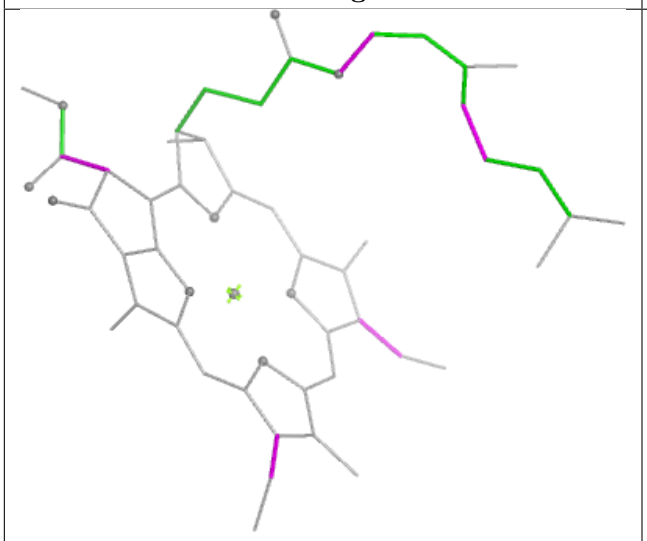


Bond angles

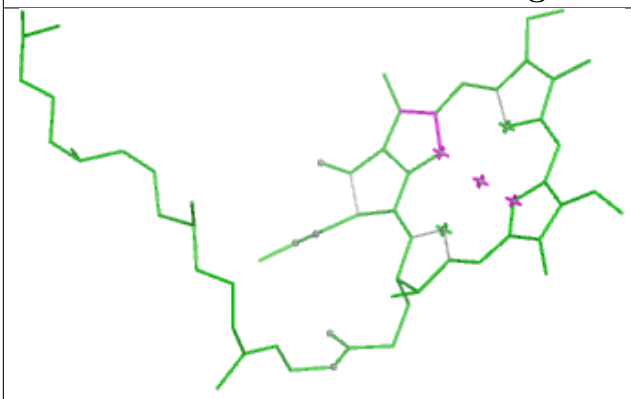


Torsions



Rings

Ligand CLA 3 603



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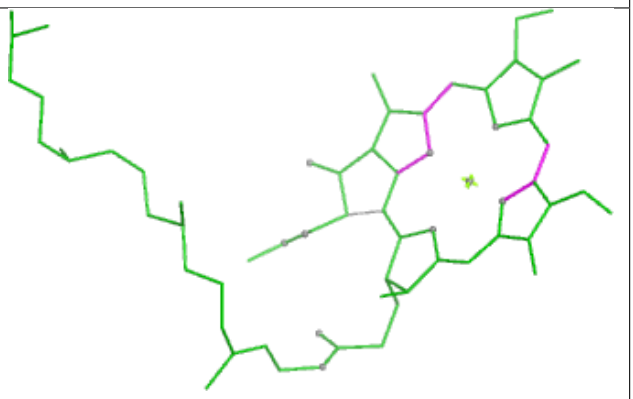
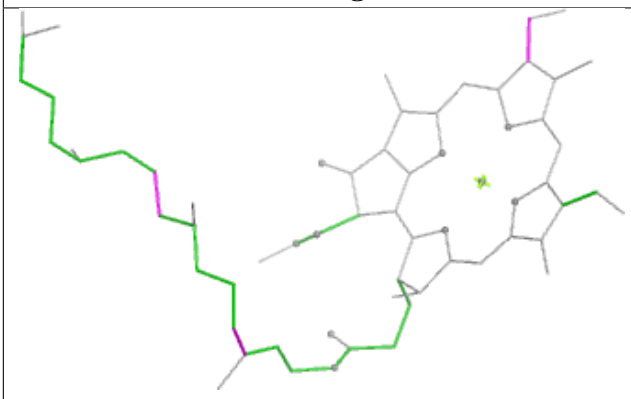


Bond angles



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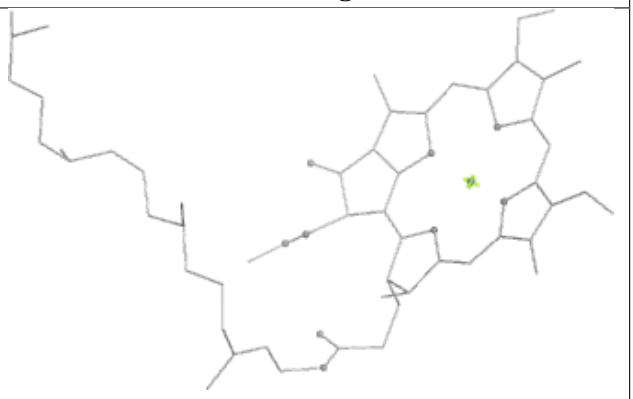
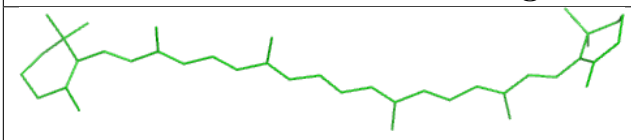


Rings

Ligand BCR G 205



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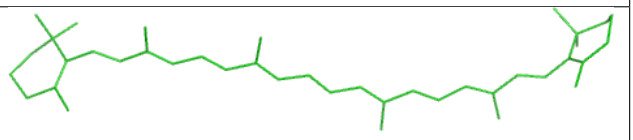
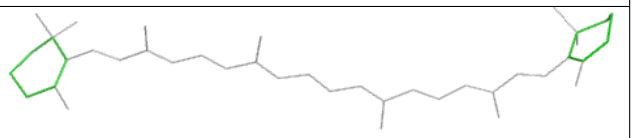


Bond angles

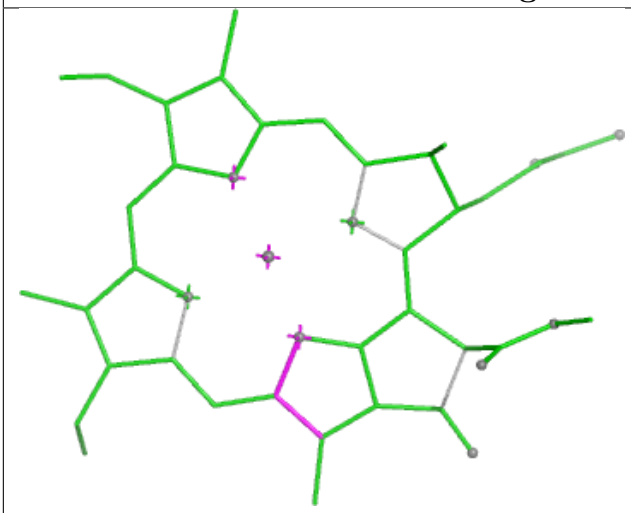


Torsions



Rings

Ligand CLA 62 617



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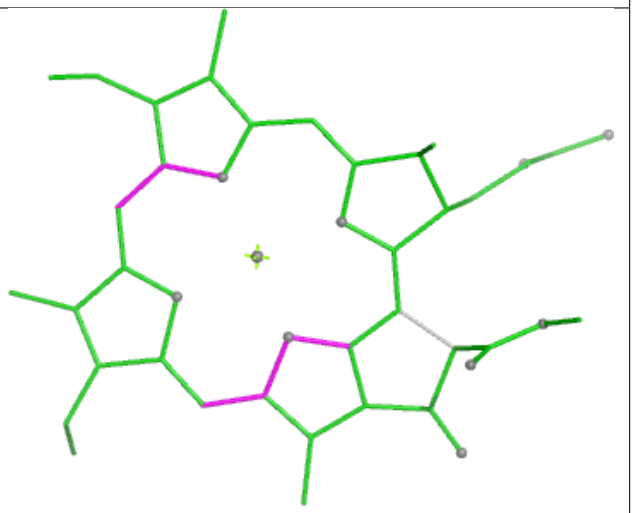
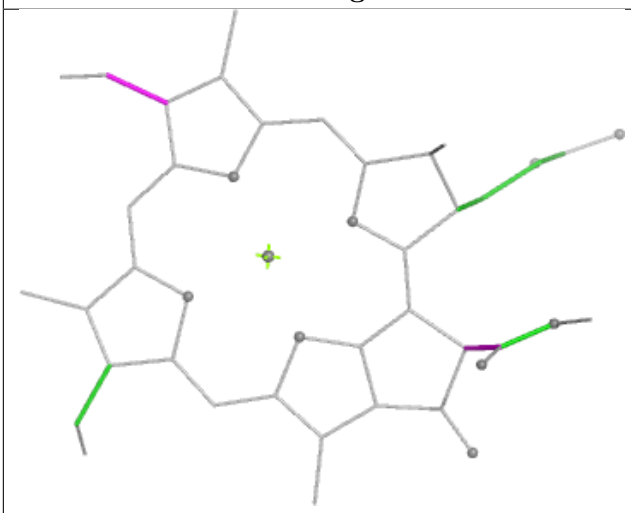


Bond angles



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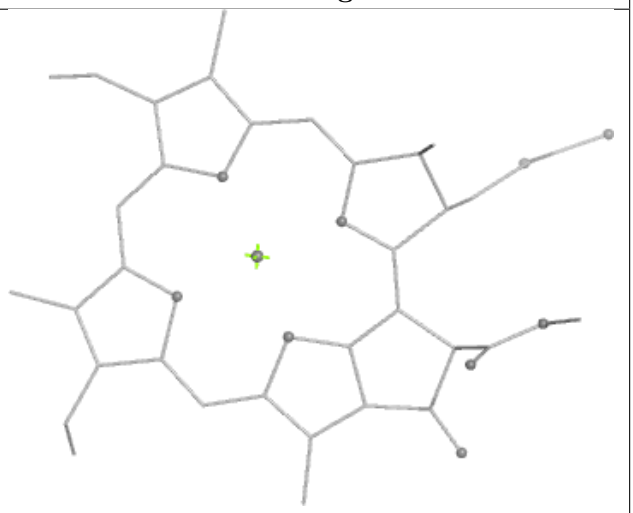
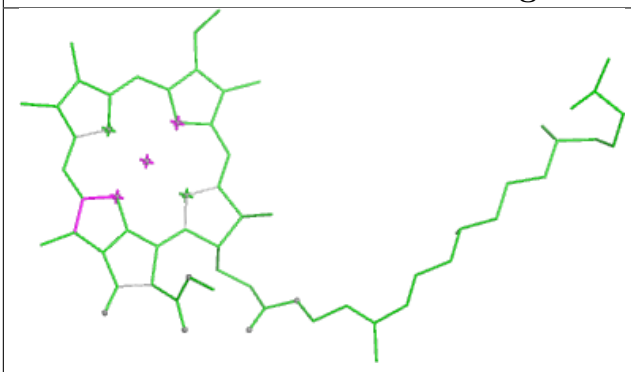


Rings

Ligand CLA 92 612



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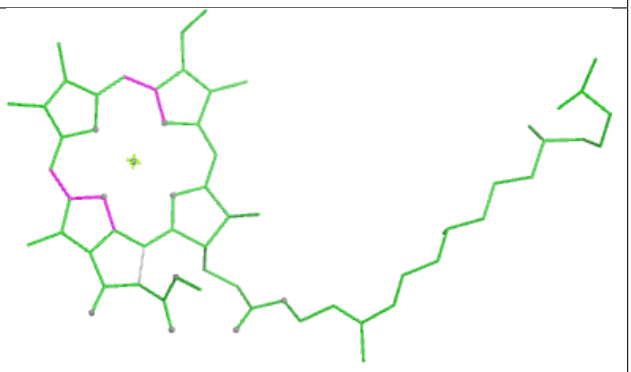
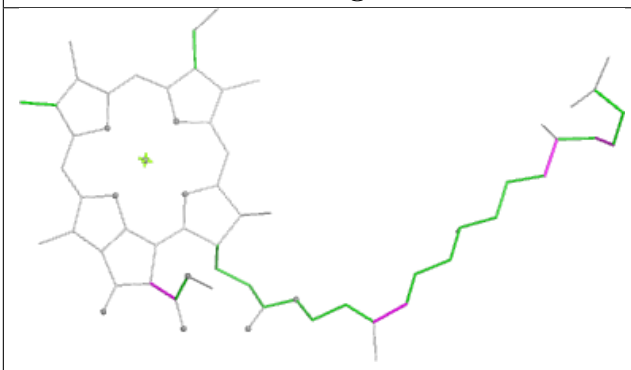
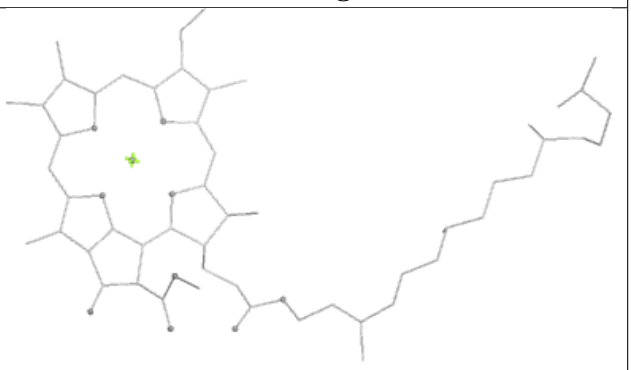


Bond angles

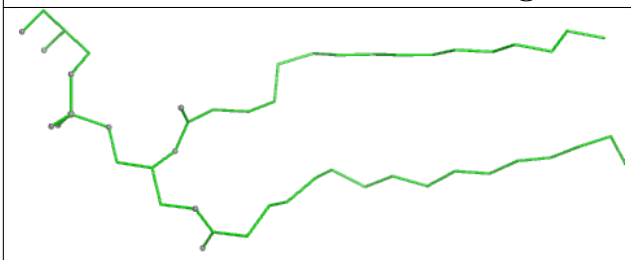


Torsions



Rings

Ligand LHG 62 619



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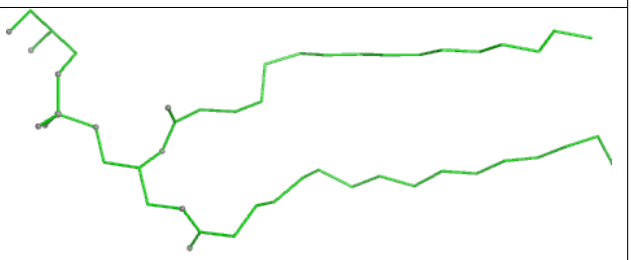

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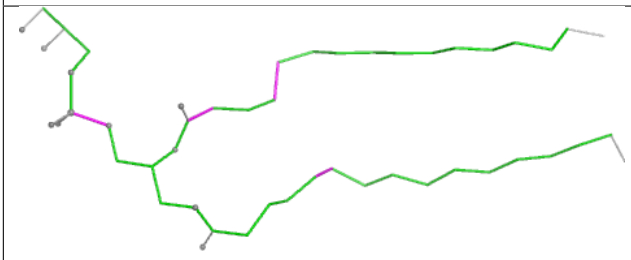

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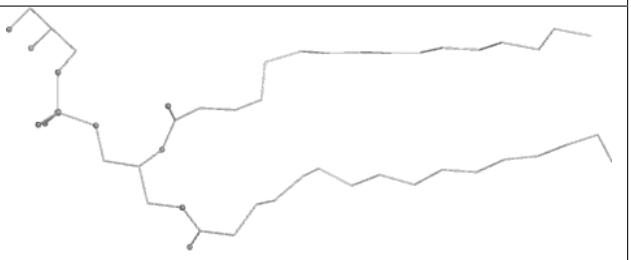
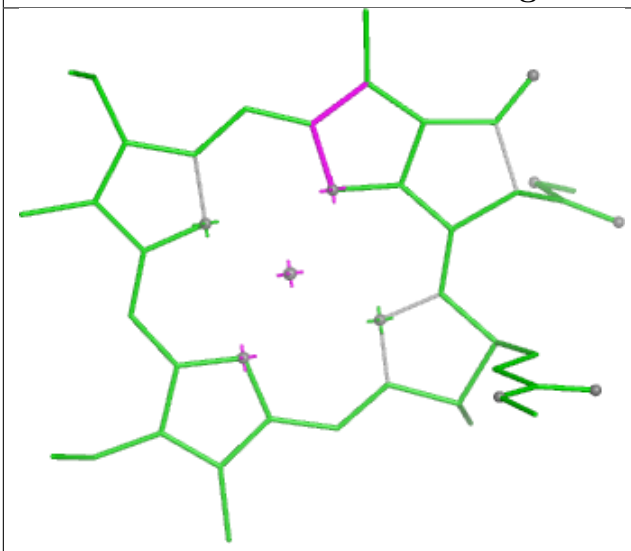


Rings

Ligand CLA 92 601



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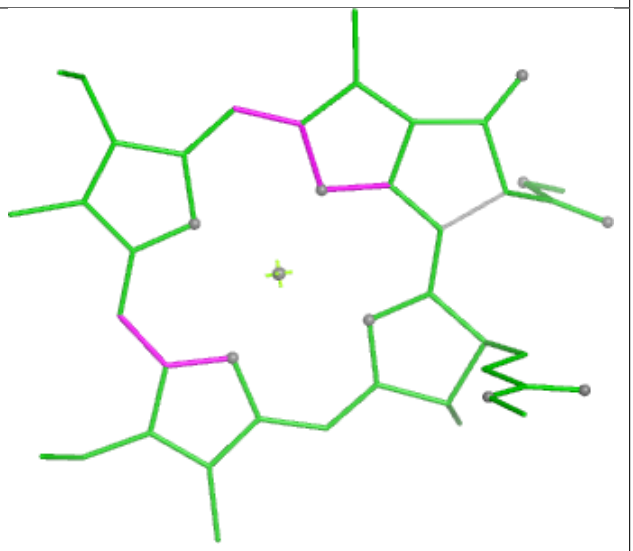

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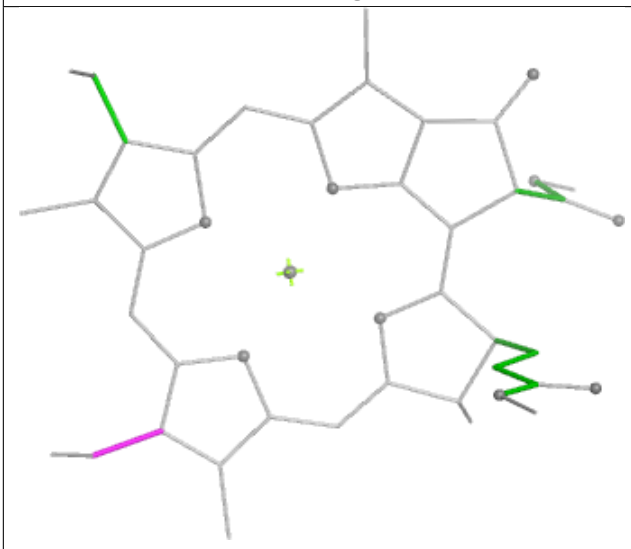

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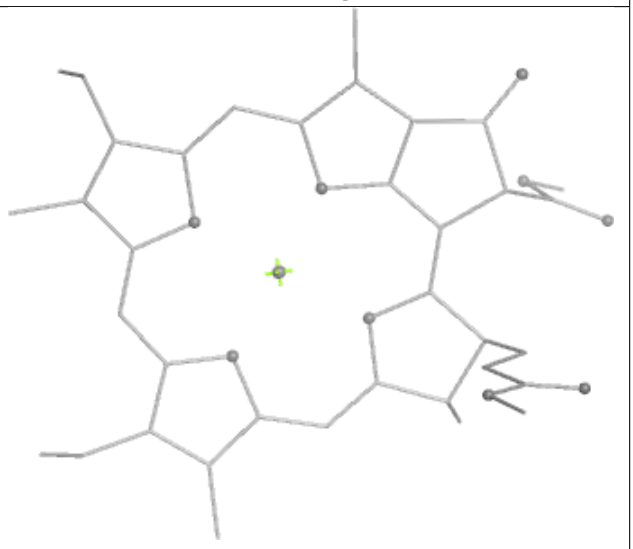
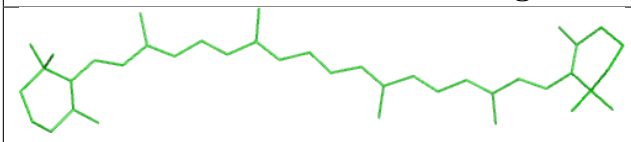


Rings

Ligand BCR B2 844



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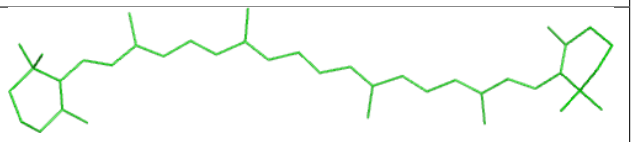

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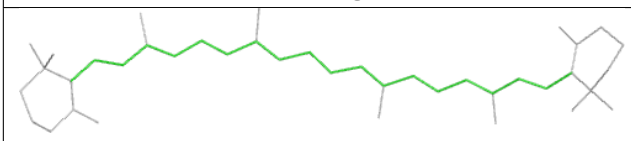

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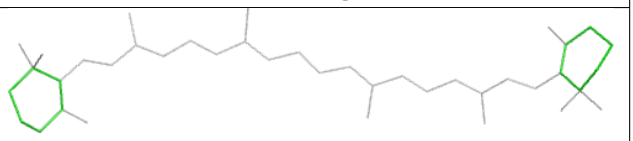
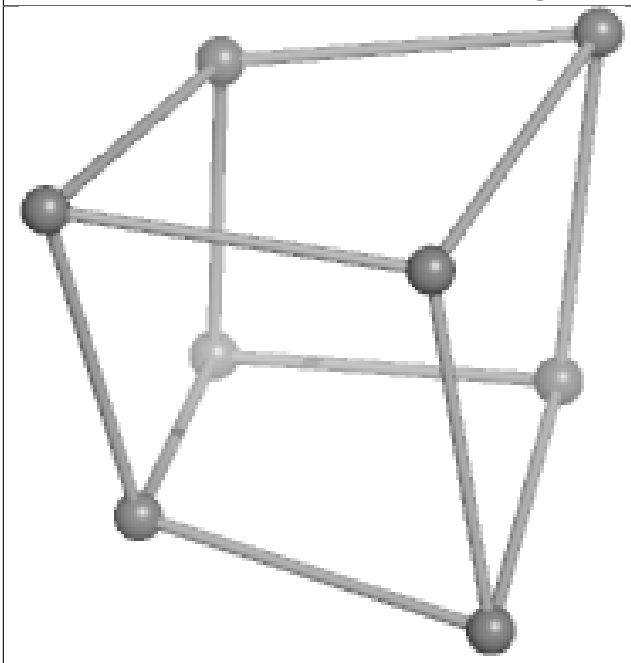


Rings

Ligand SF4 C 102



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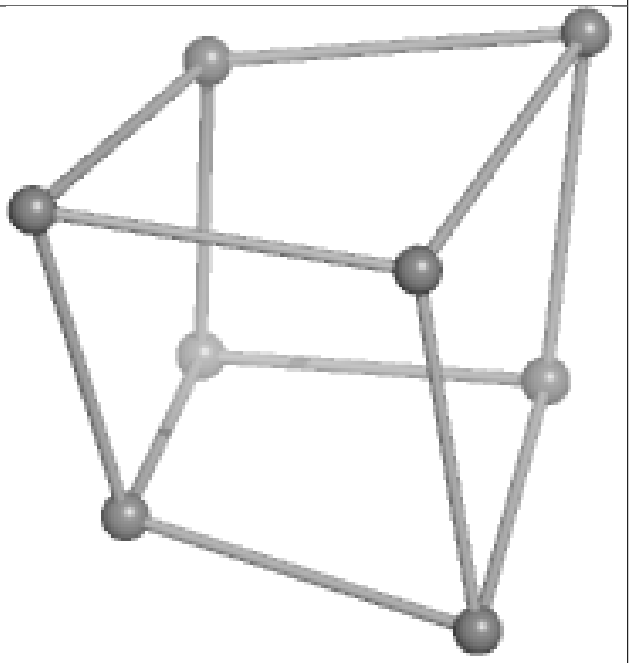

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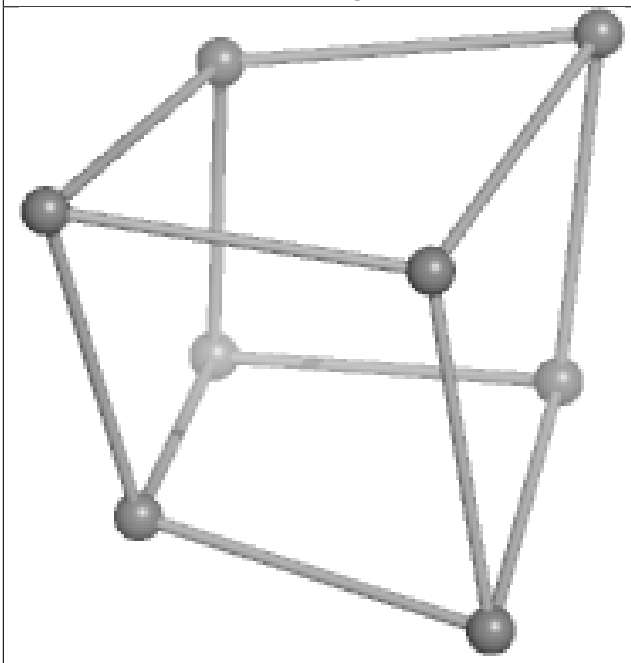

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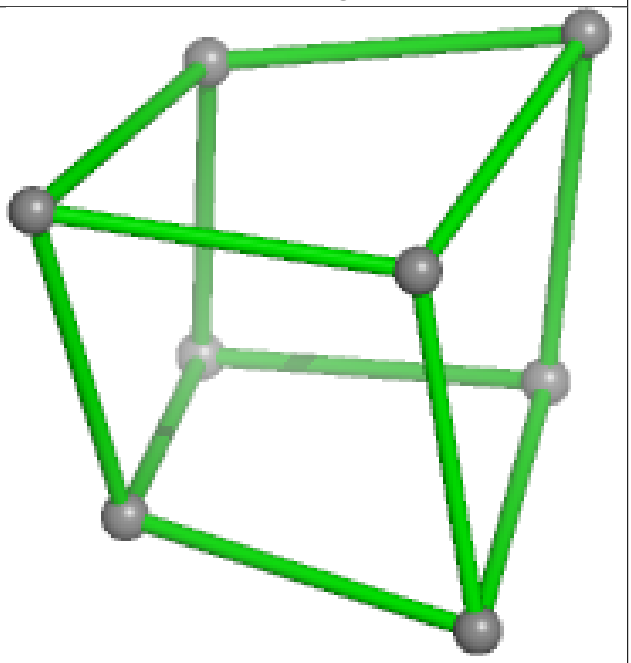
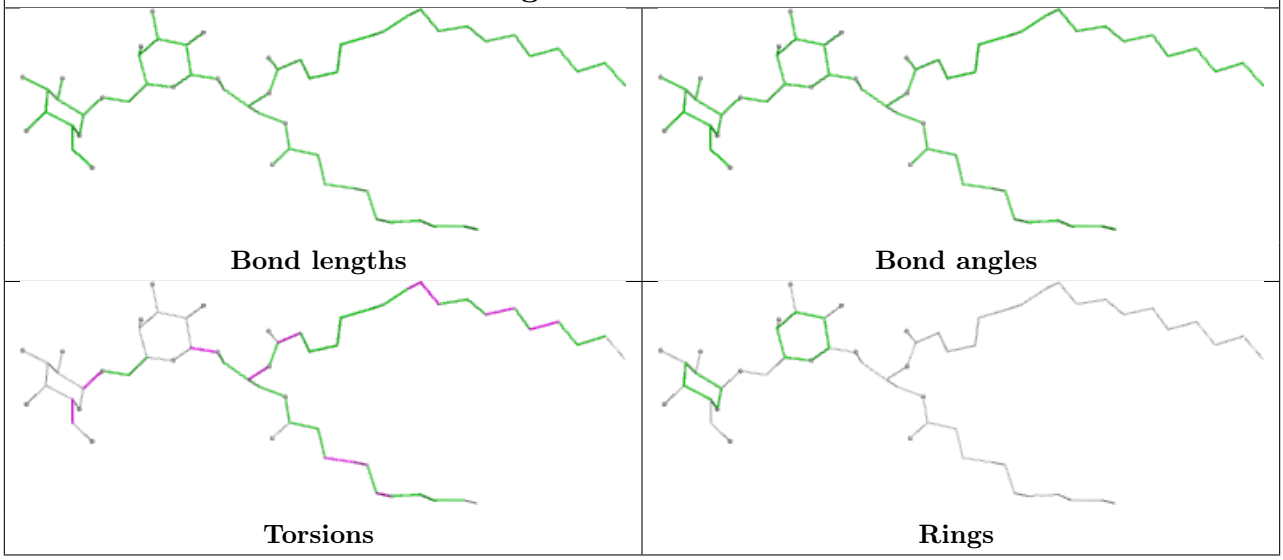
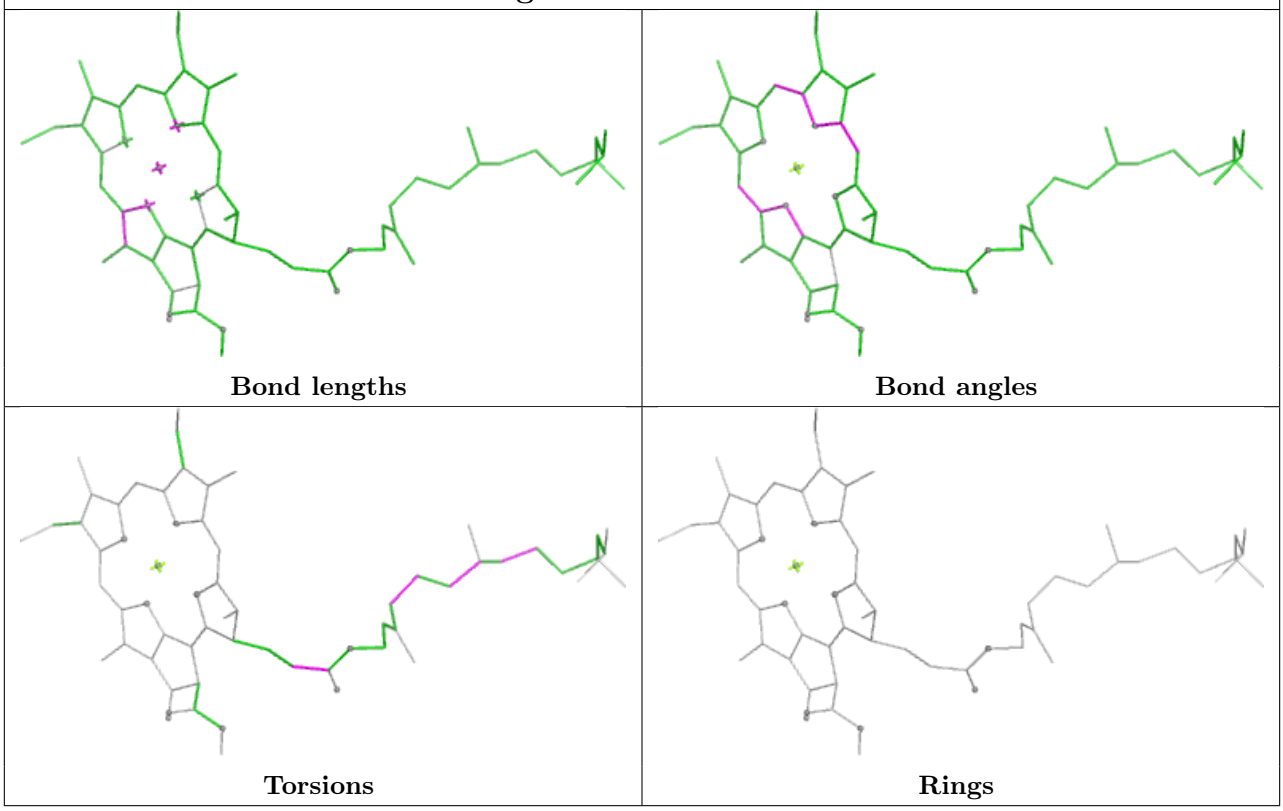


Rings

Ligand DGD B 850



Ligand CLA B2 809



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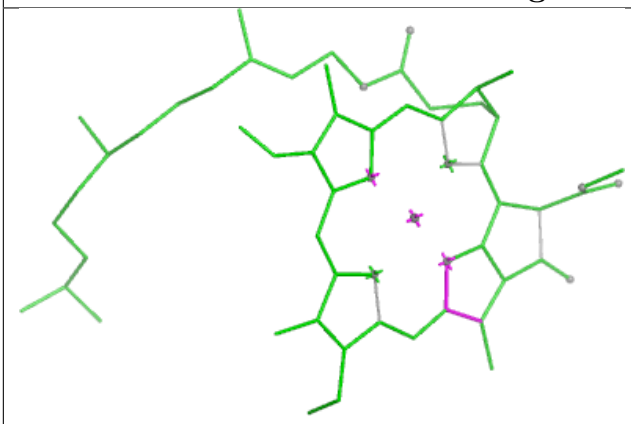

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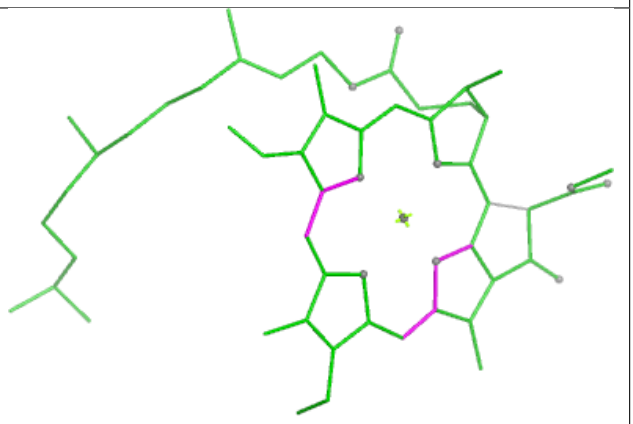
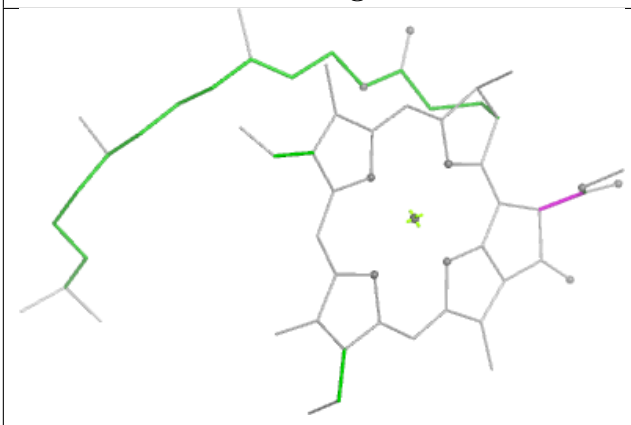


Bond angles



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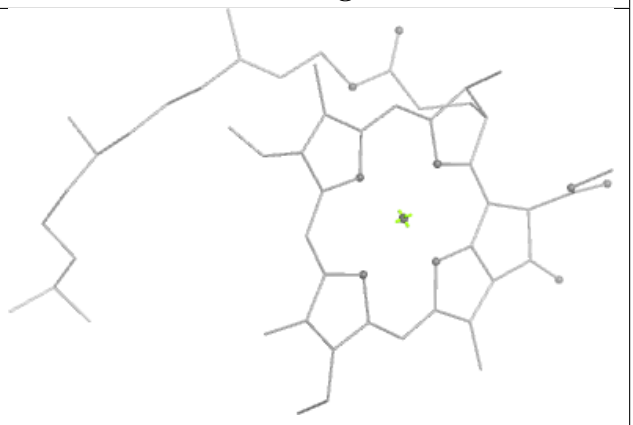
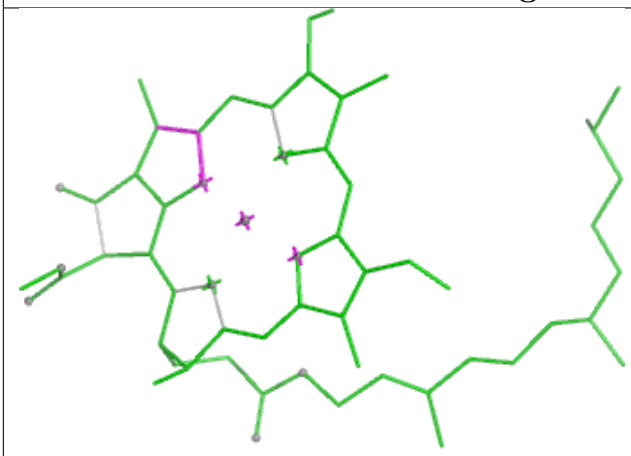


Rings

Ligand CLA 32 602



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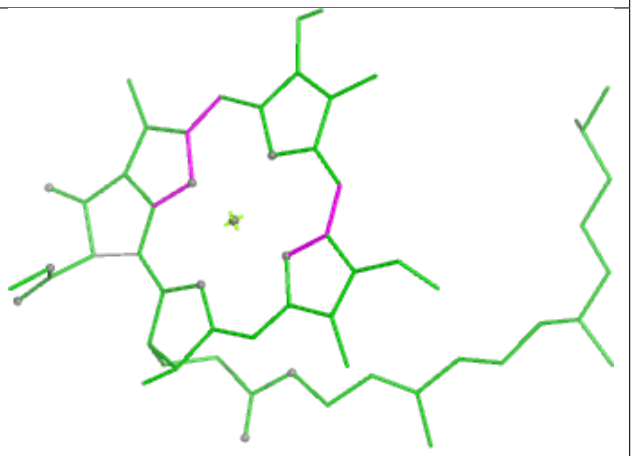
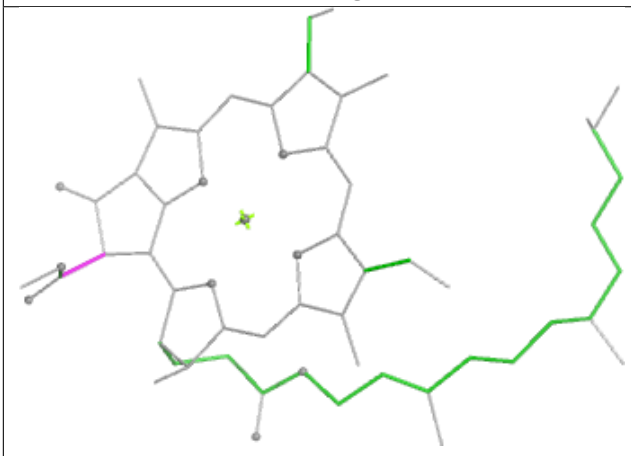


Bond angles



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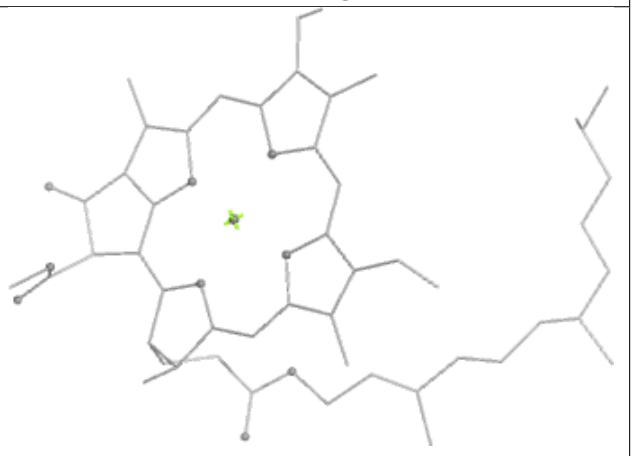

Rings

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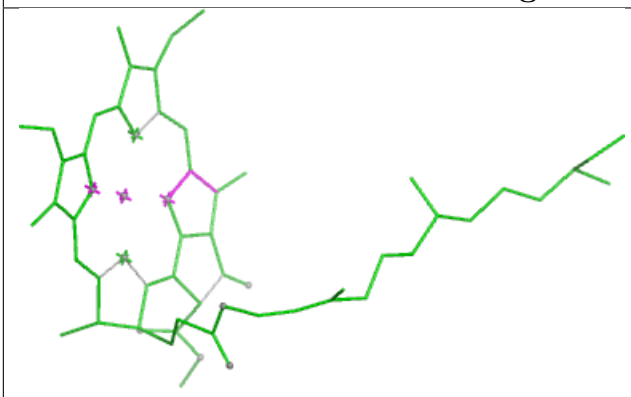

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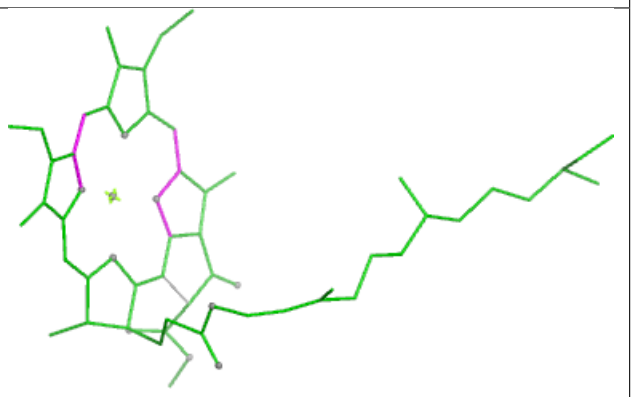
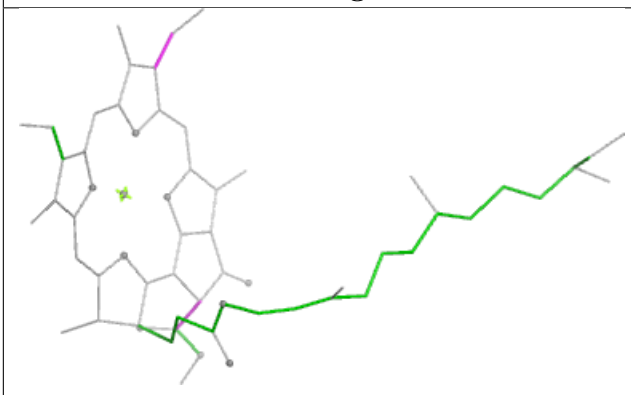


Bond angles



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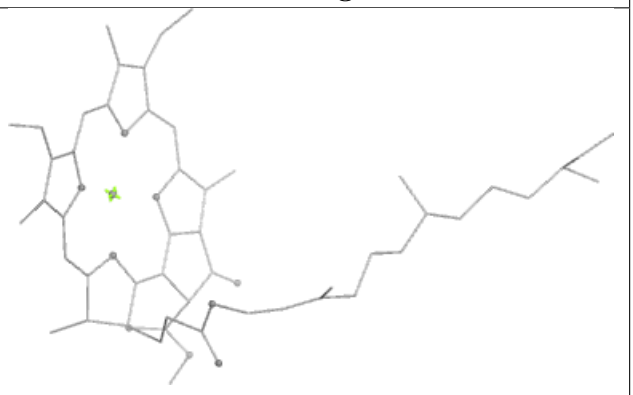
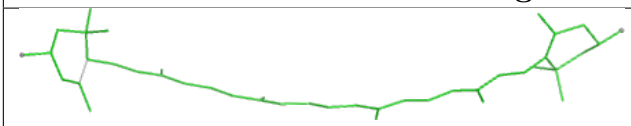


Rings

Ligand LUT A2 856



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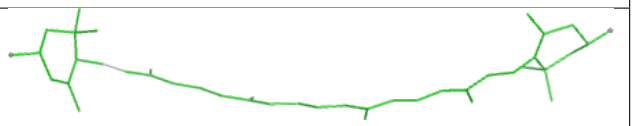


Bond angles

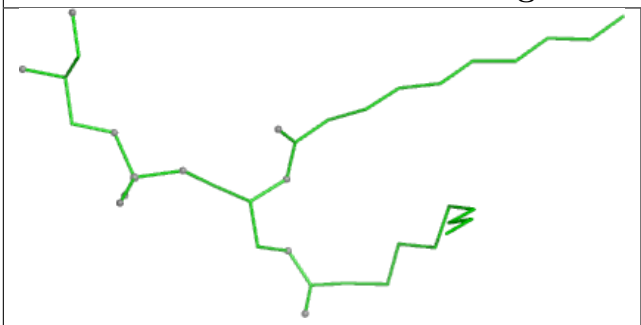


Torsions



Rings

Ligand LHG 52 623



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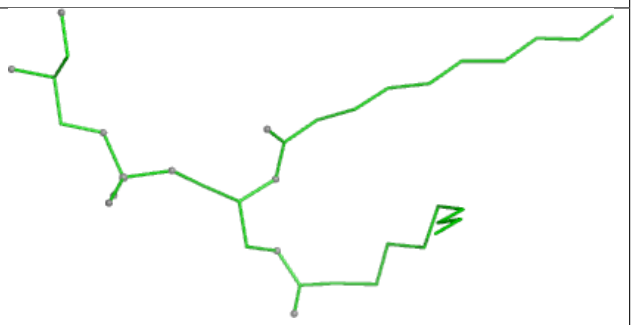
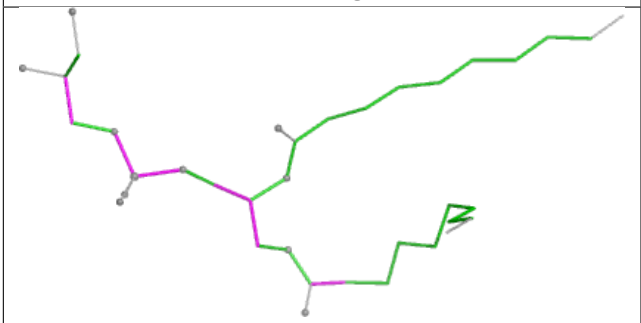


Bond angles



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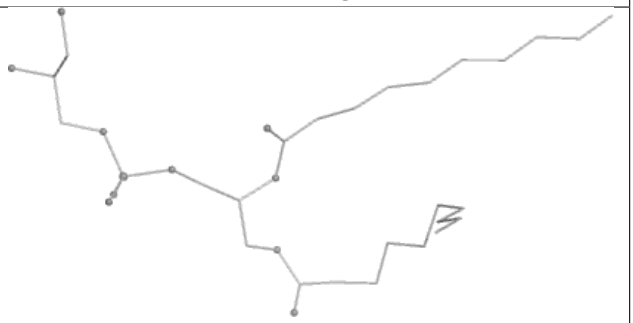
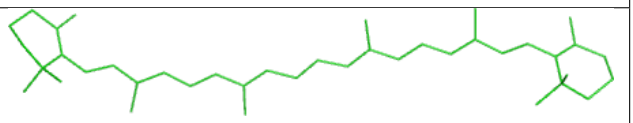


Rings

Ligand BCR 9 623



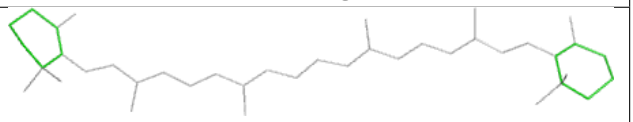
Bond lengths



Bond angles

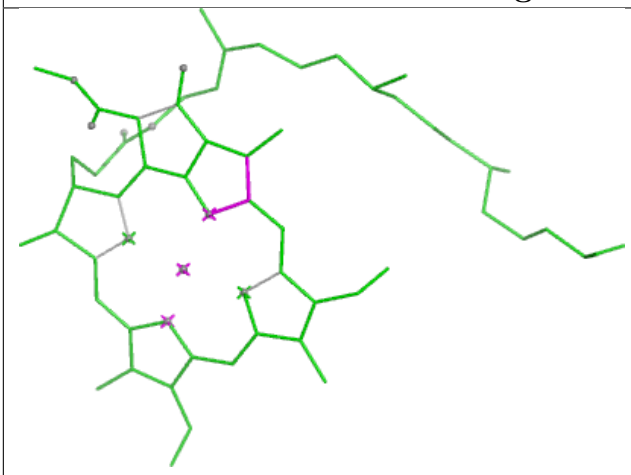


Torsions



Rings

Ligand CLA A2 830



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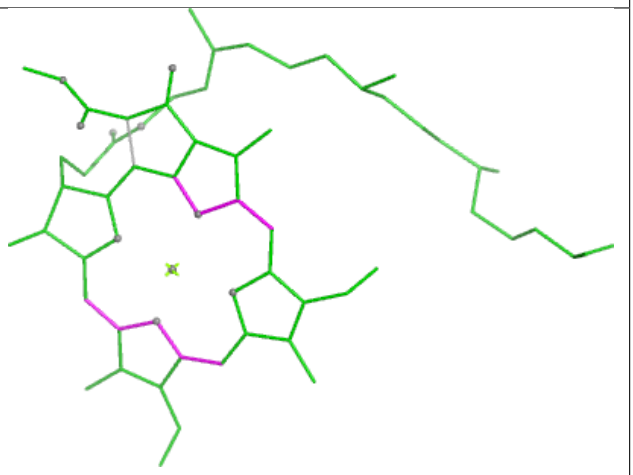
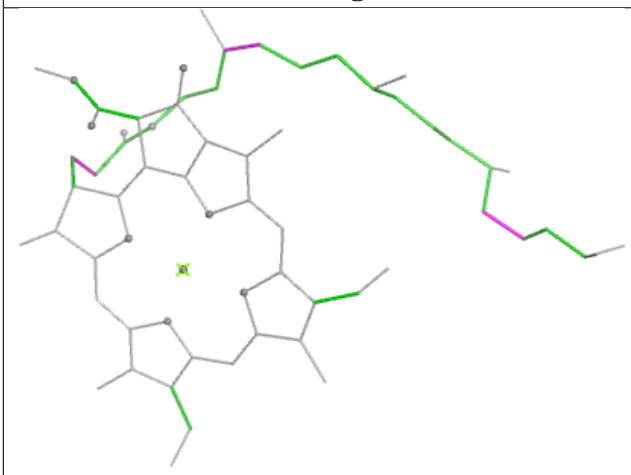


Bond angles



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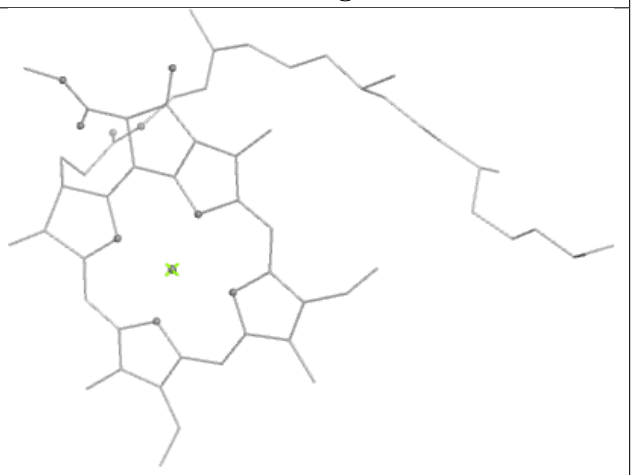
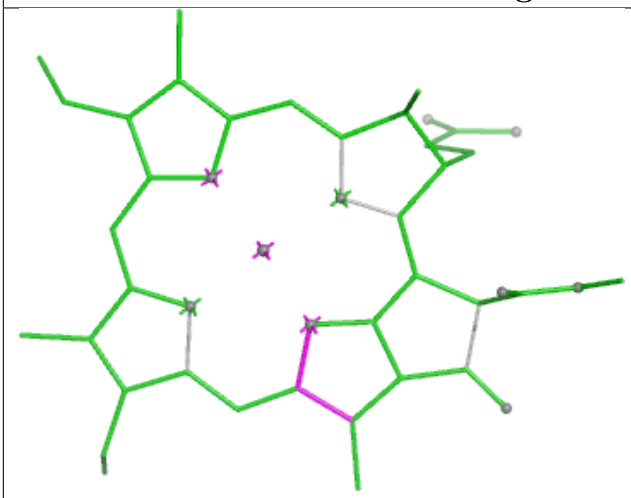


Rings

Ligand CLA B2 835



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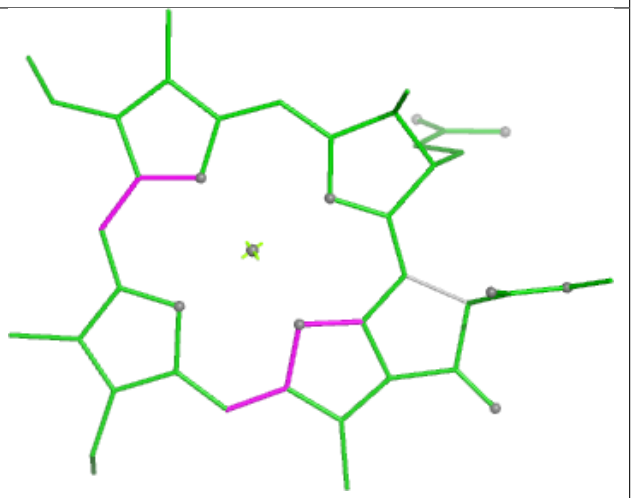
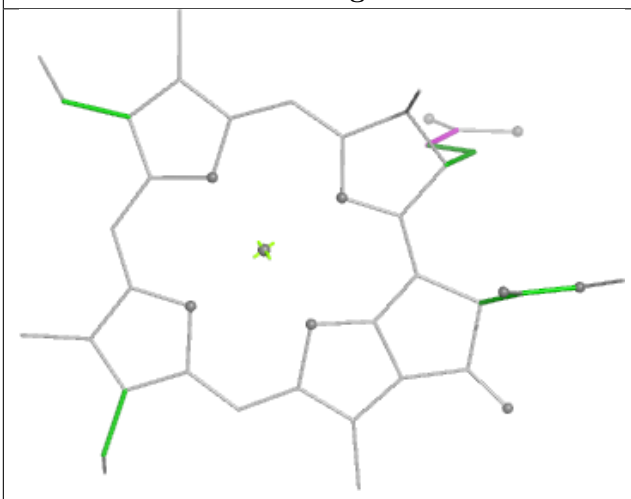


Bond angles



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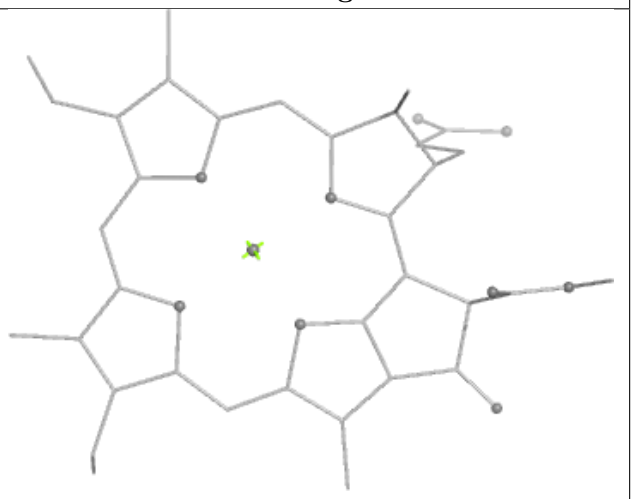
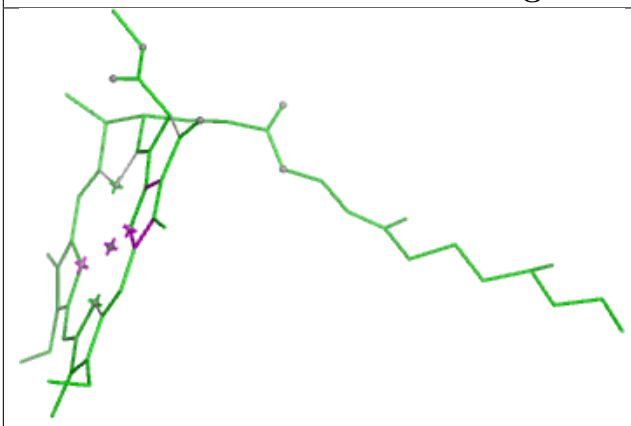
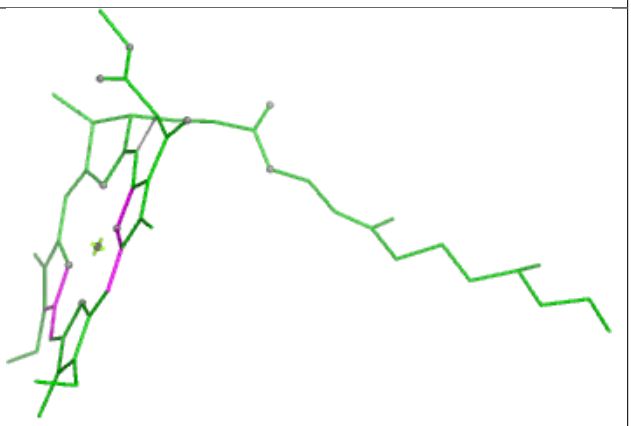


Rings

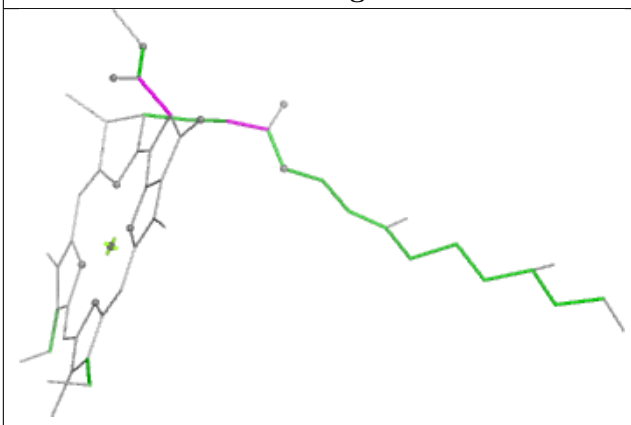
Ligand CLA A 837



Bond lengths



Bond angles



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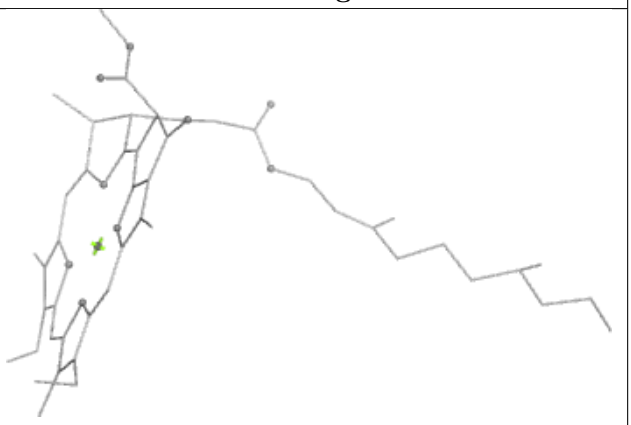
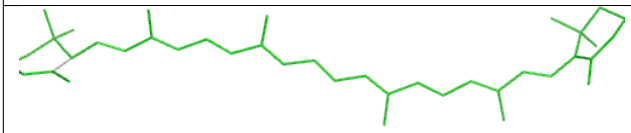


Rings

Ligand LUT Z 617



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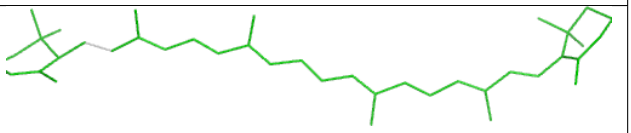
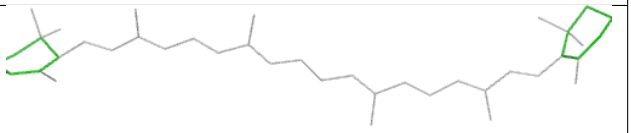


Bond angles

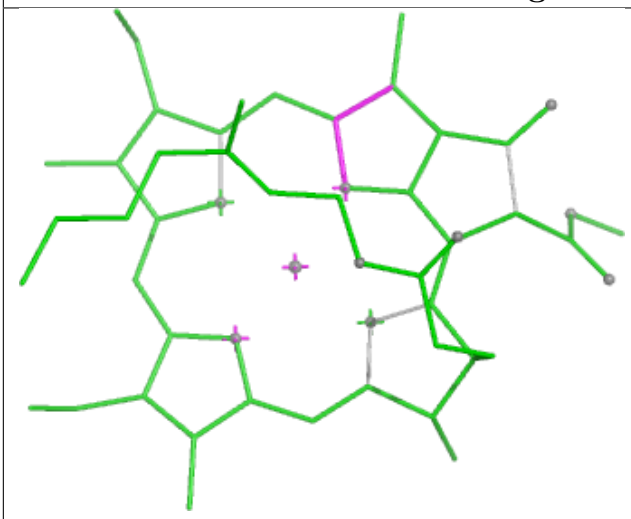


Torsions

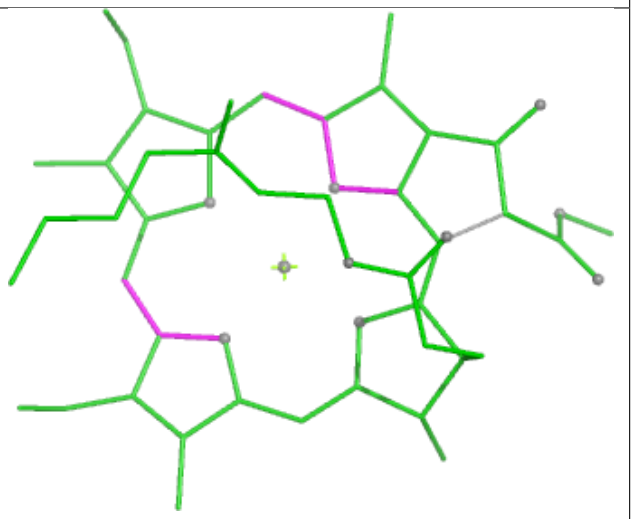


Rings

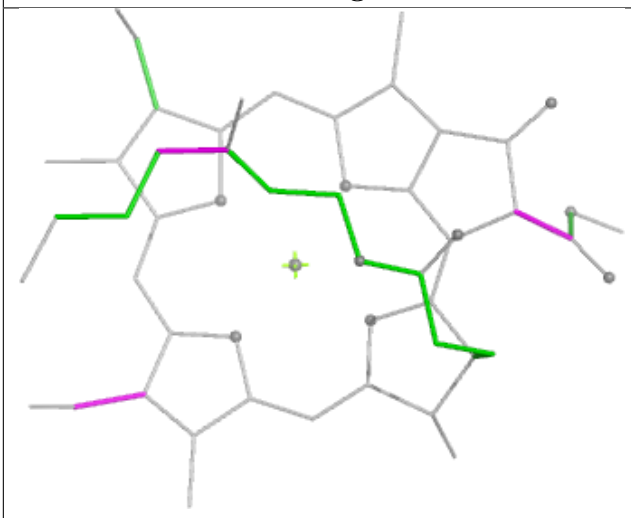
Ligand CLA 7 620



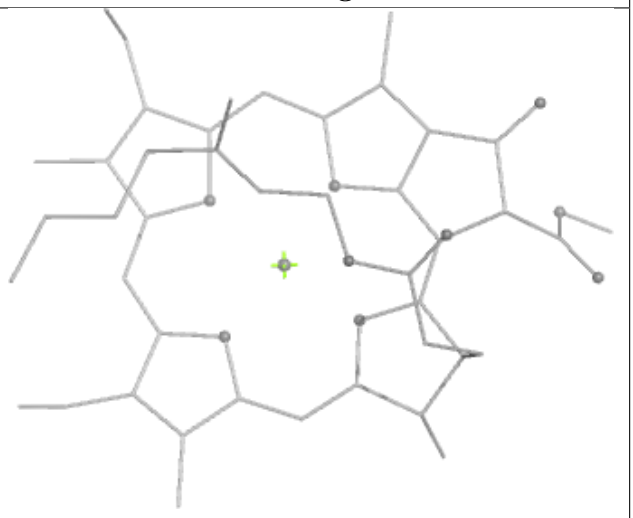
Bond lengths



Bond angles

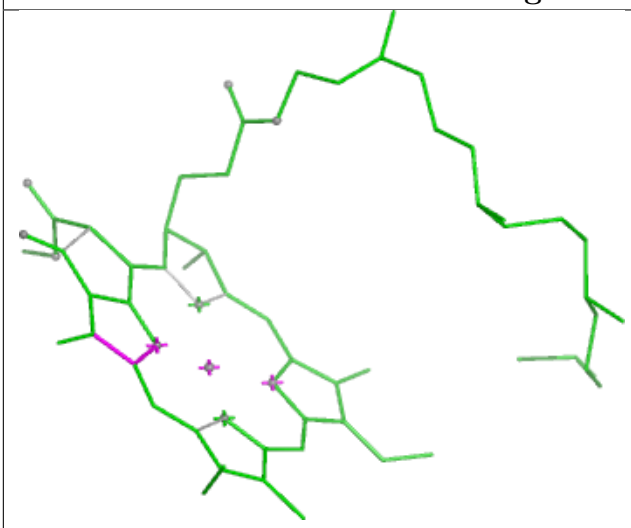


Torsions



Rings

Ligand CLA B 815



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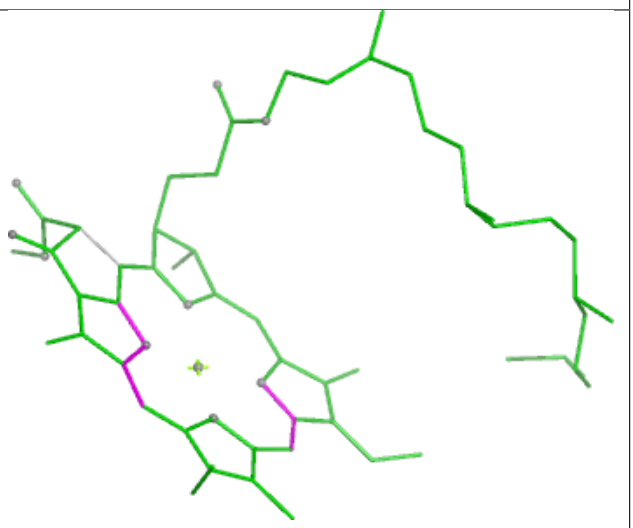

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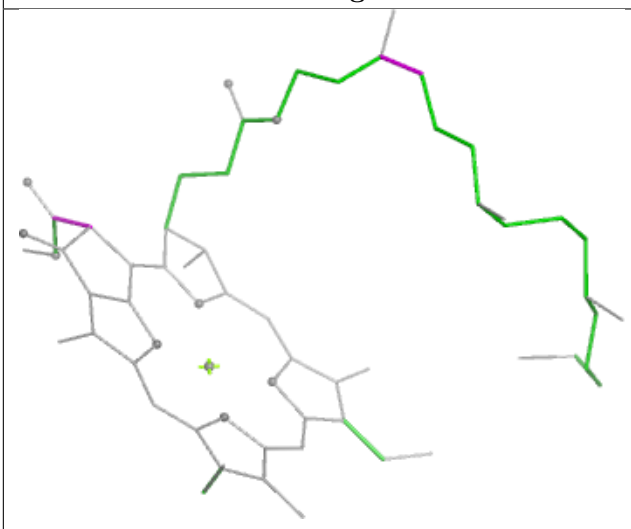
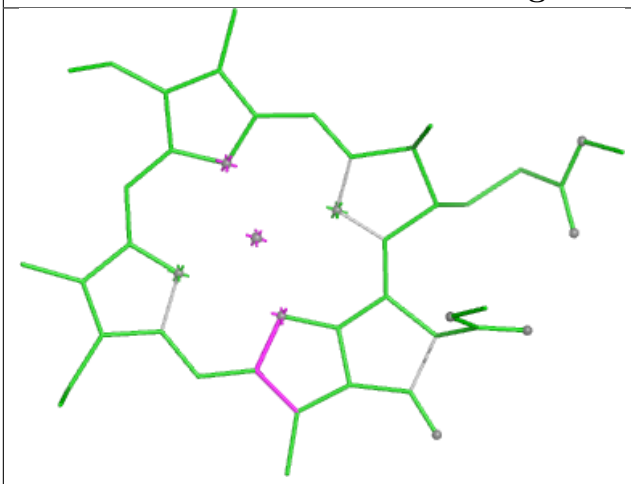


Torsions



Rings

Ligand CLA 3 612



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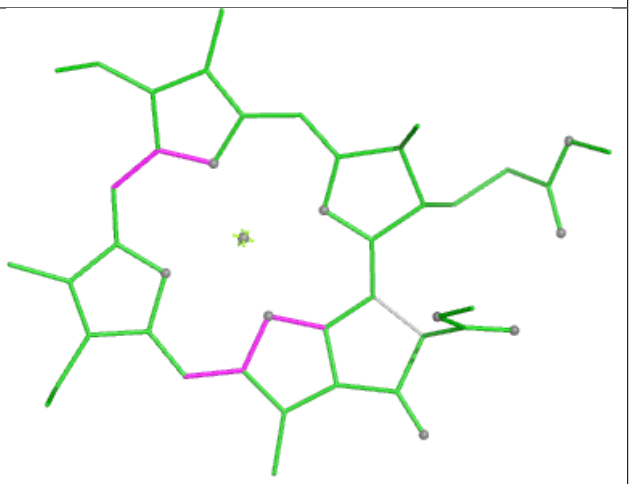
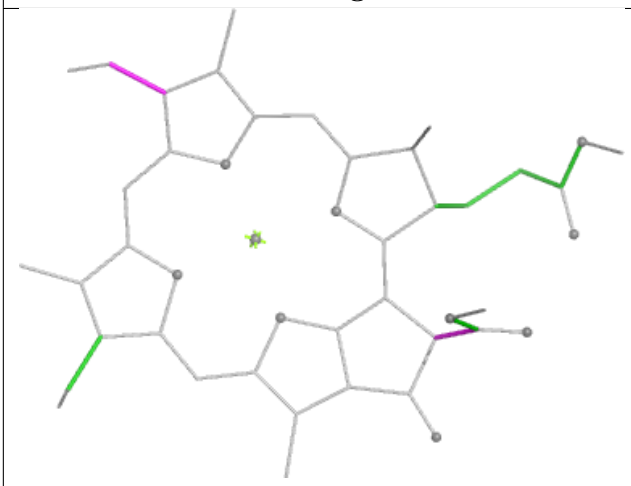


Bond angles



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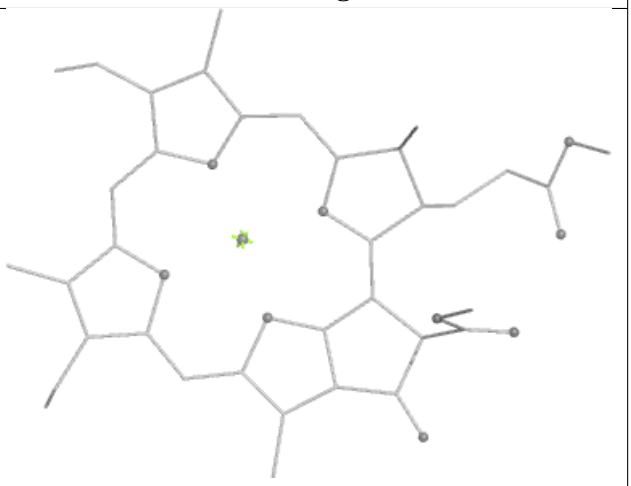
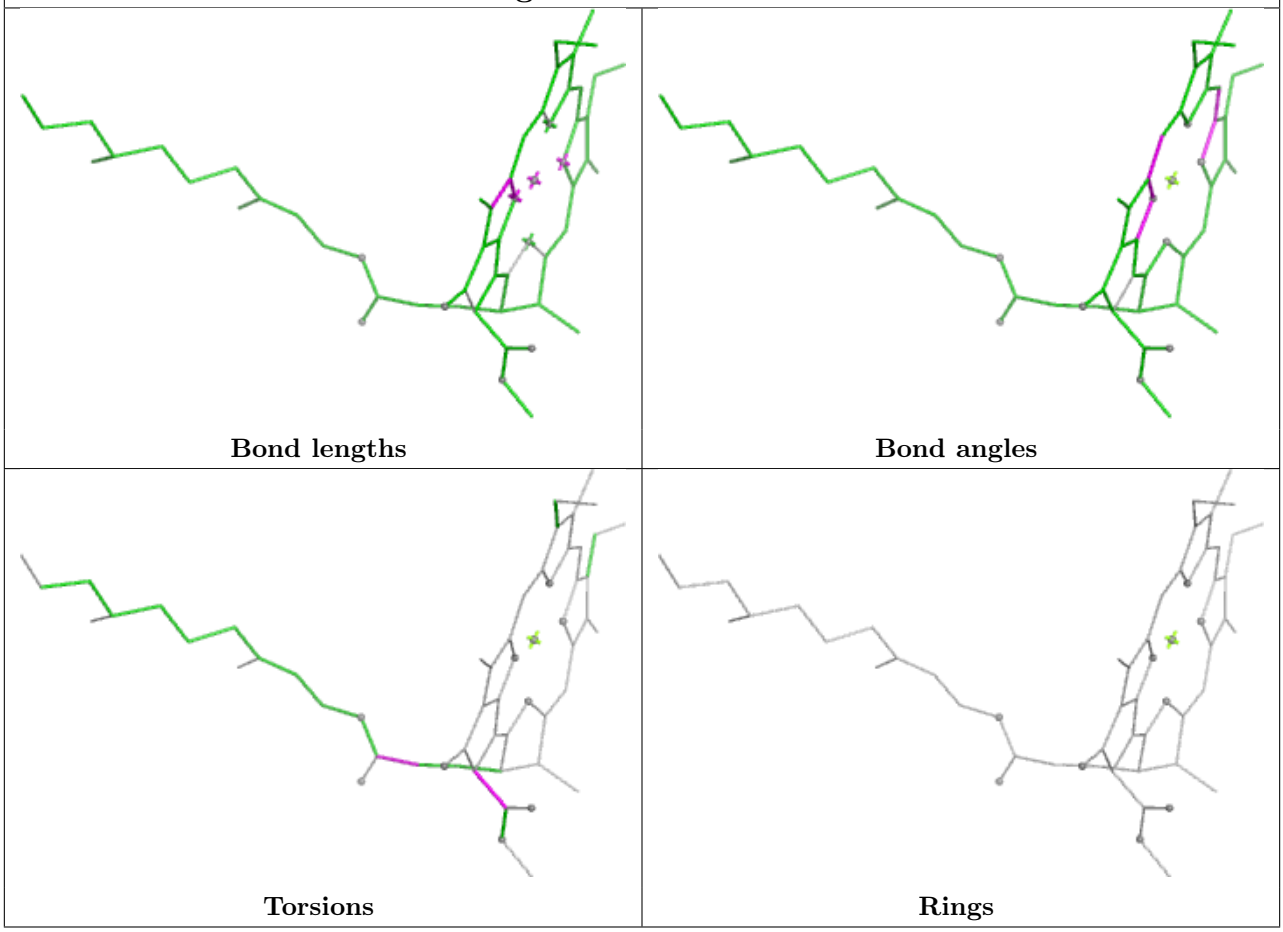
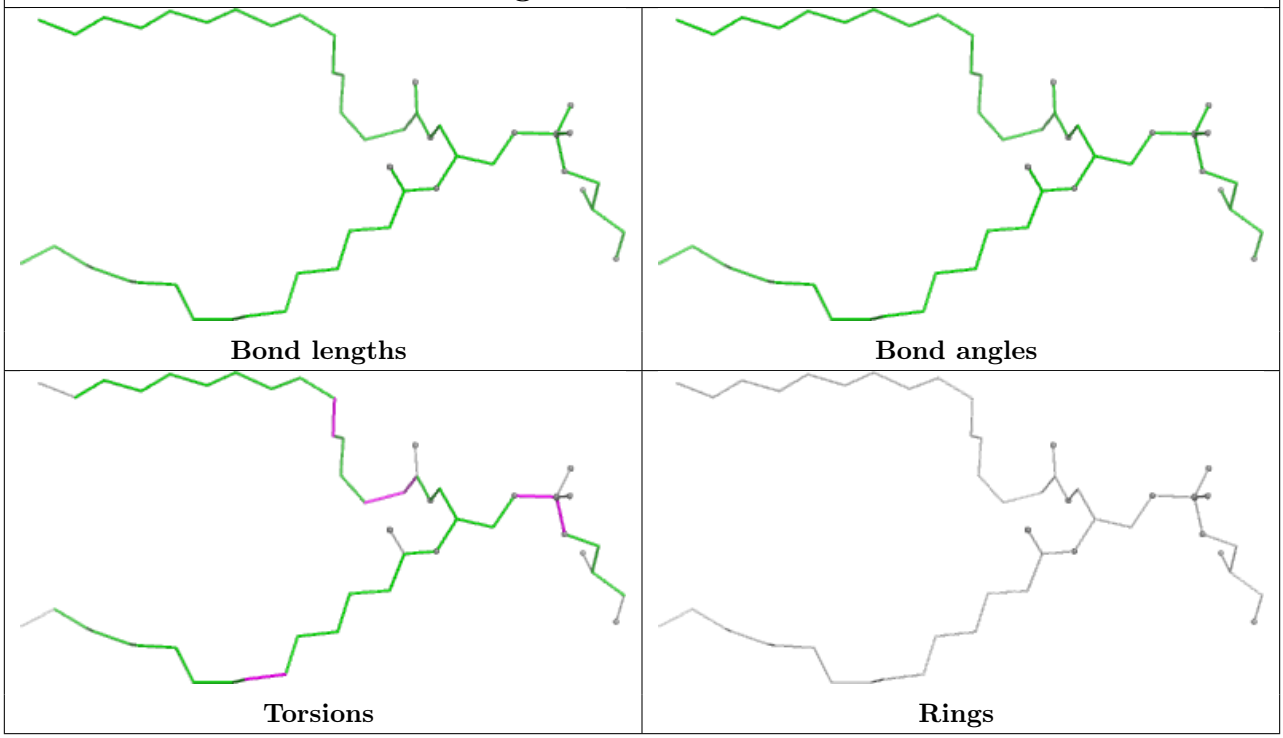


Rings

Ligand CLA A2 837



Ligand LHG A2 846



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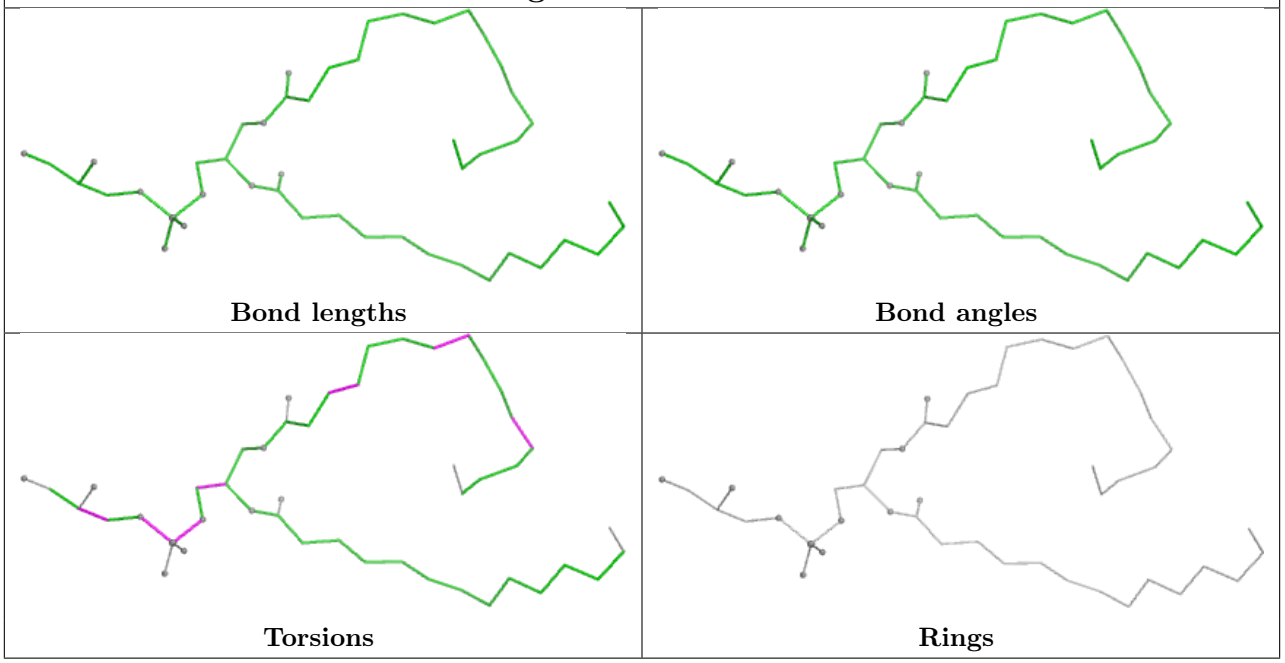

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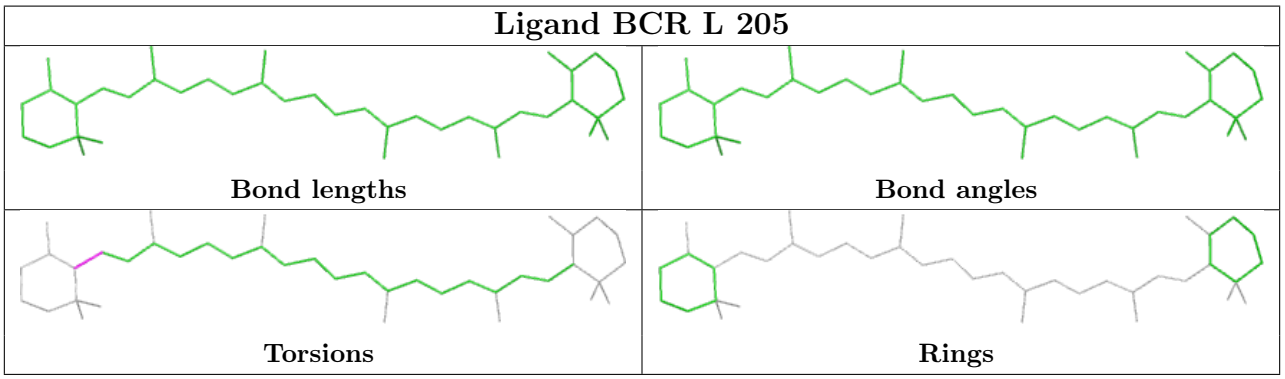

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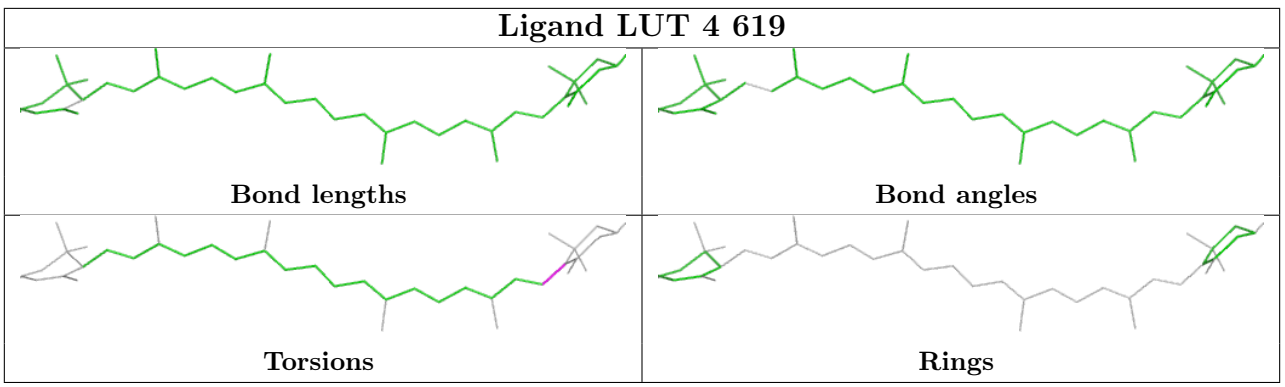

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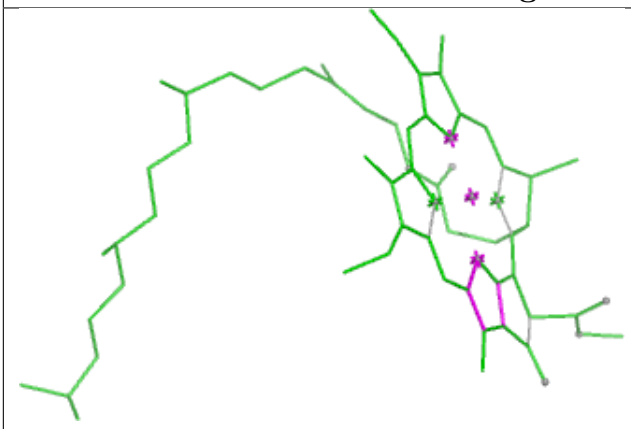
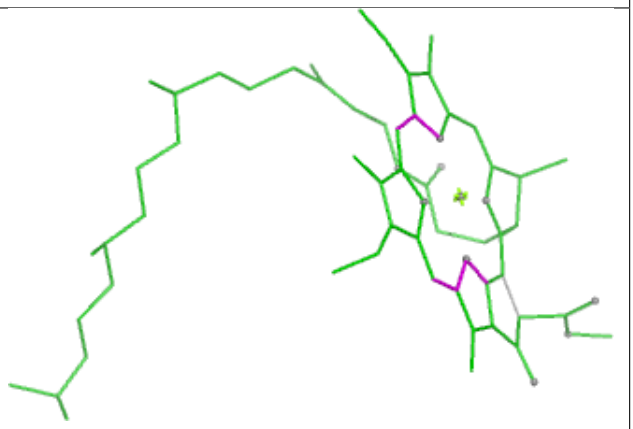


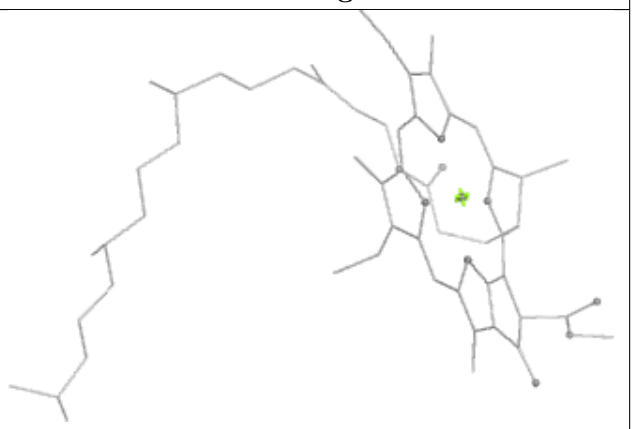
Bond lengths



Bond angles

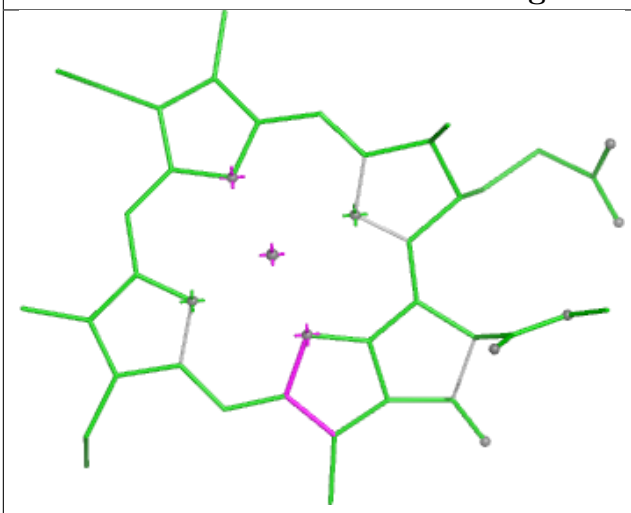


Torsions



Rings

Ligand CLA 9 614



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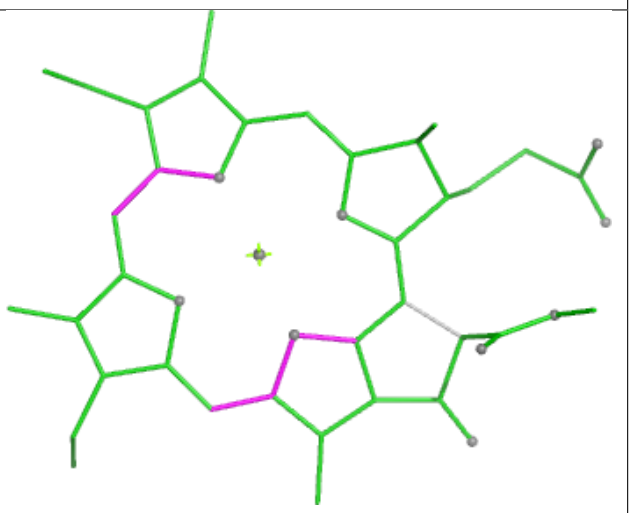
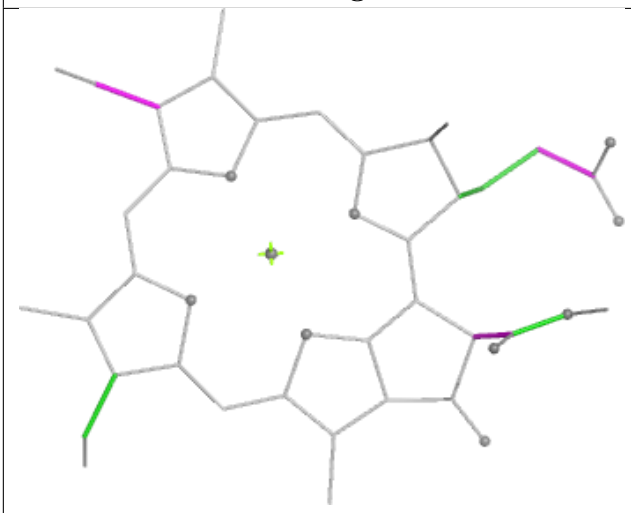


Bond angles



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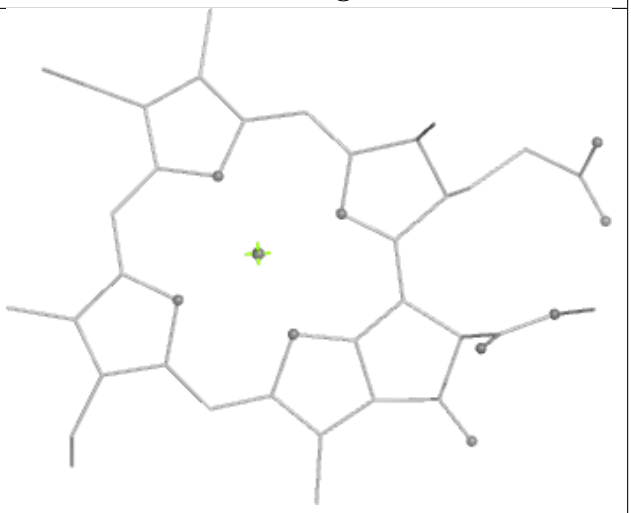
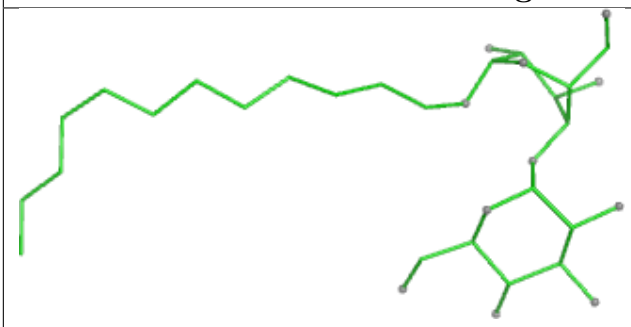


Rings

Ligand LMU 82 627



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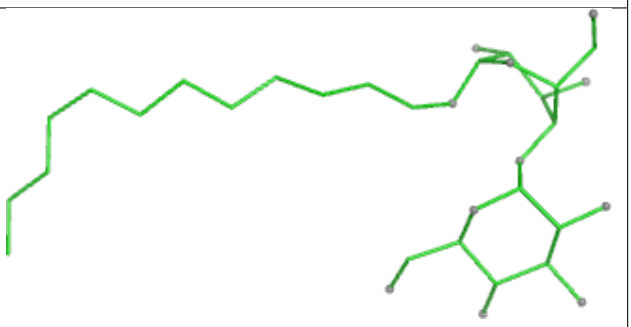
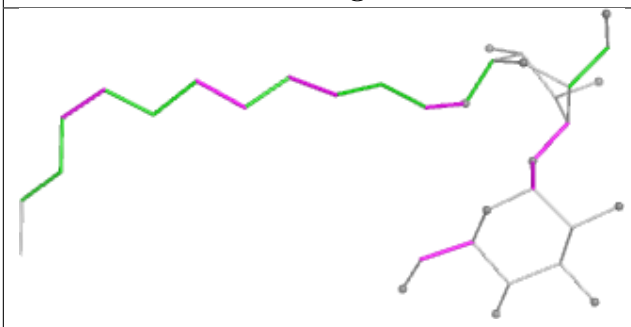


Bond angles



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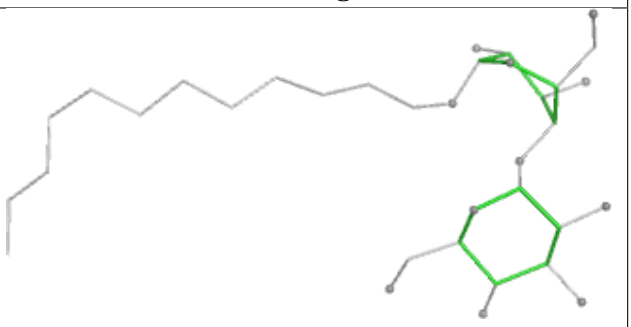
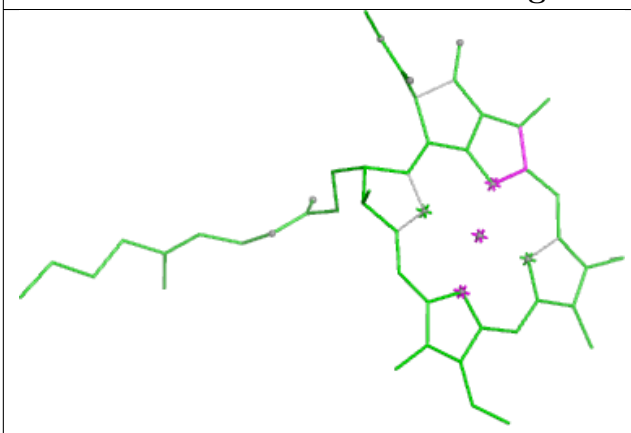


Rings

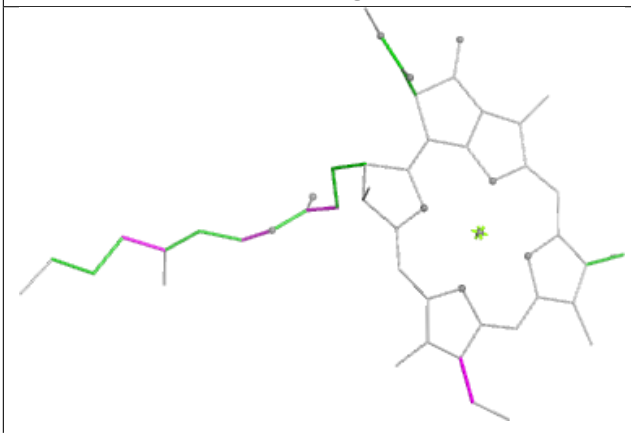
Ligand CLA 5 616



Bond lengths



Bond angles



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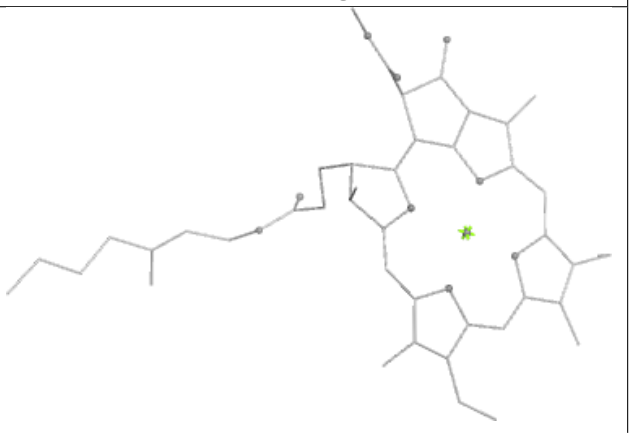
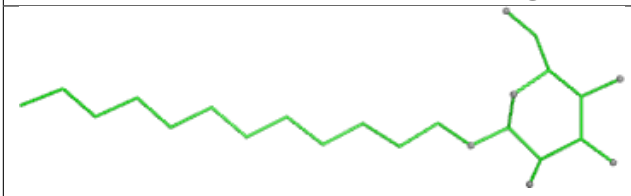


Rings

Ligand LMU 1 626



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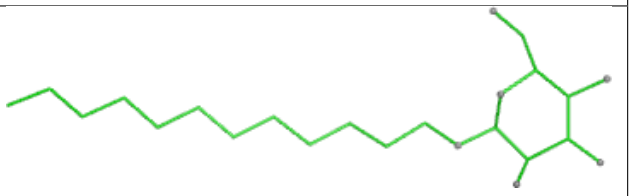
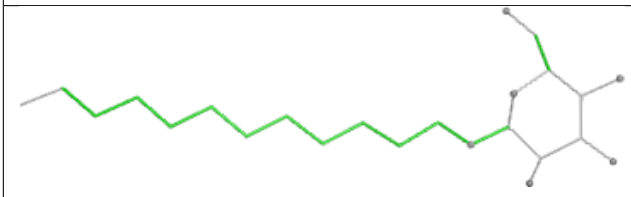


Bond angles



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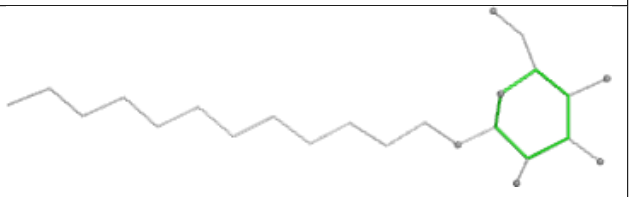
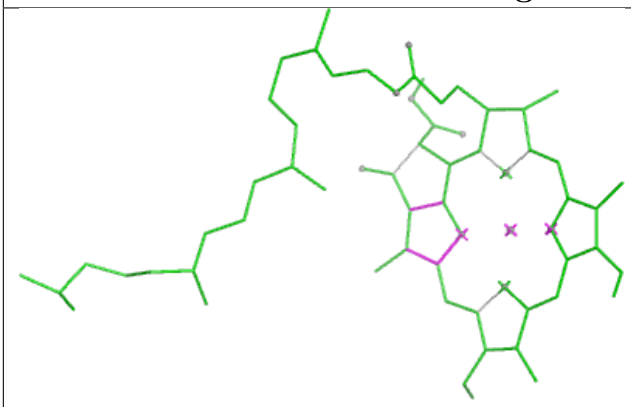


Rings

Ligand CLA B2 832



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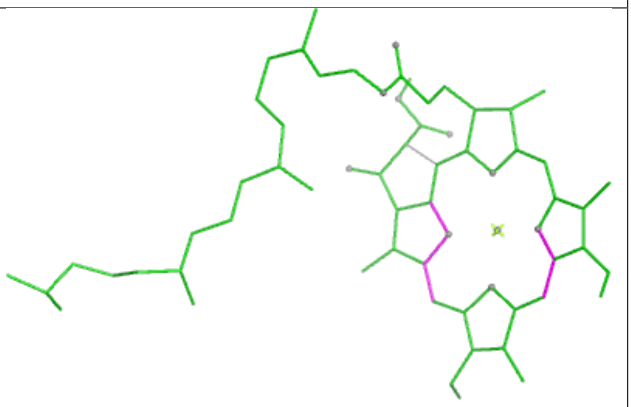
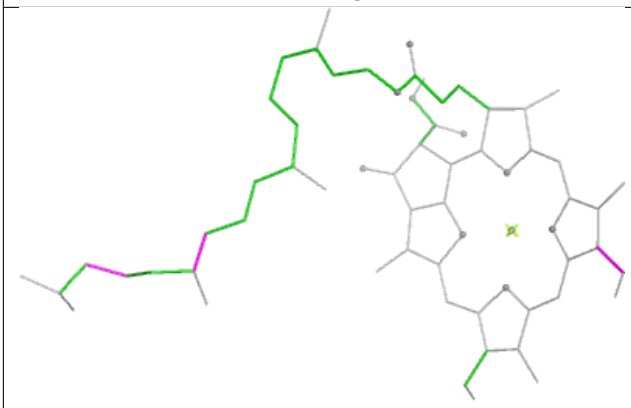


Bond angles

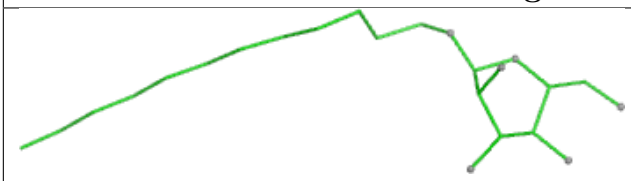


Torsions



Rings

Ligand LMU 1 625



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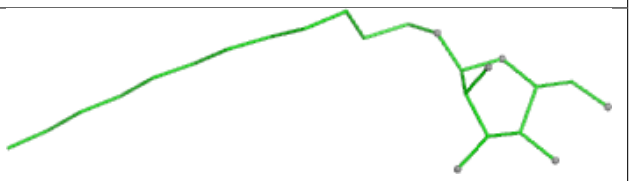
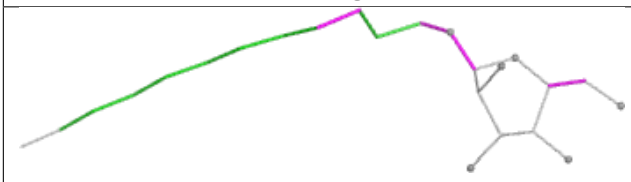


Bond angles

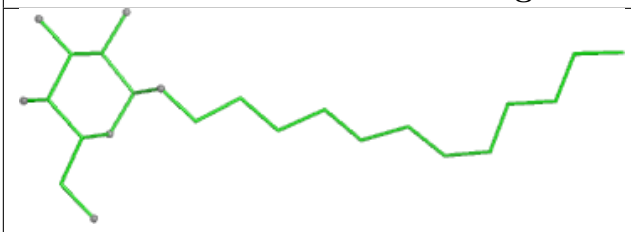


Torsions



Rings

Ligand LMU 52 627



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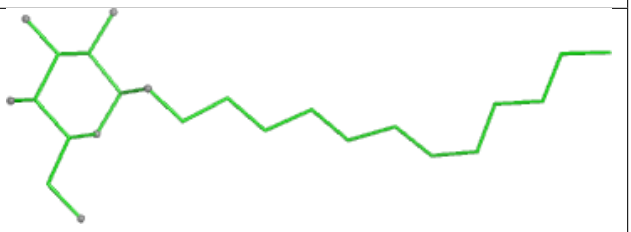
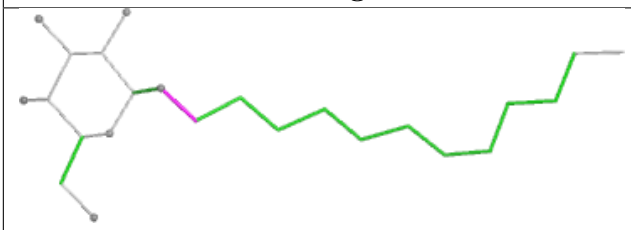
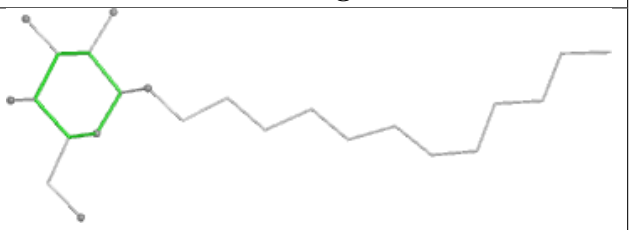


Bond angles

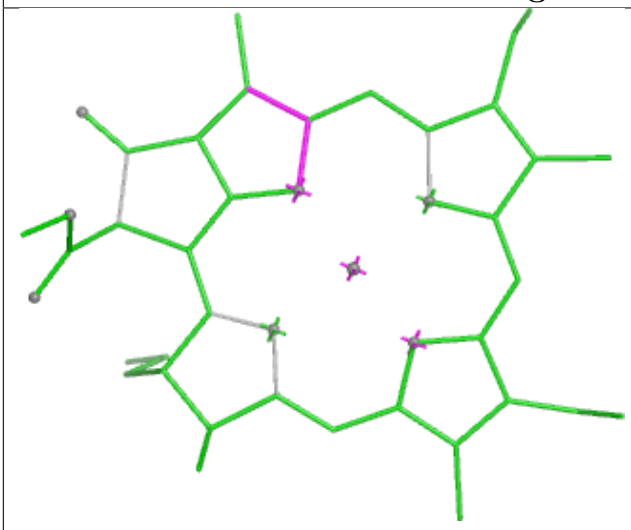


Torsions



Rings

Ligand CLA 7 614



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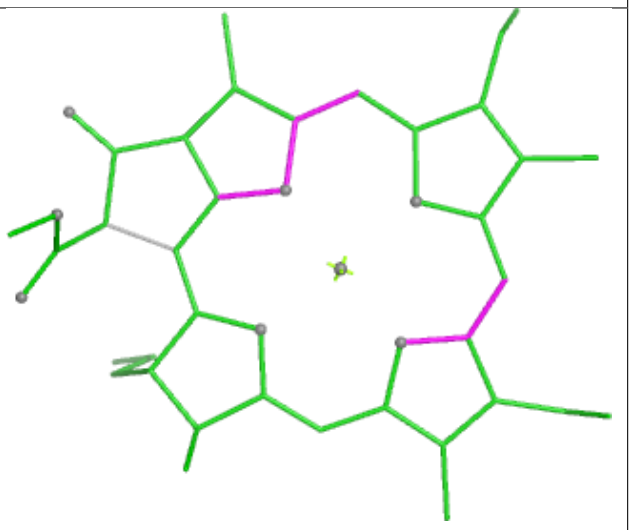
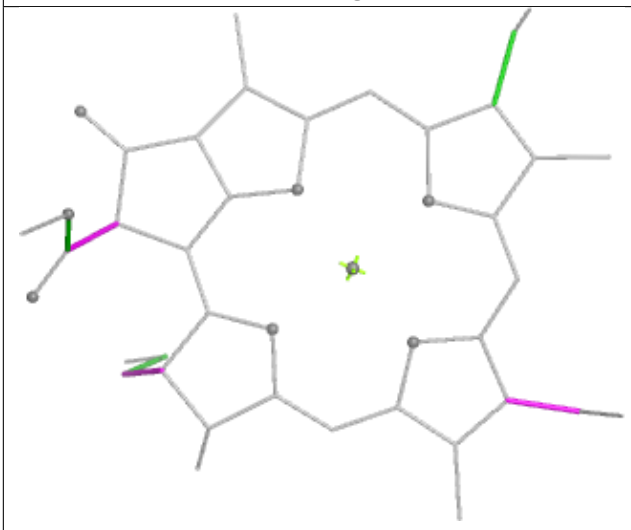


Bond angles



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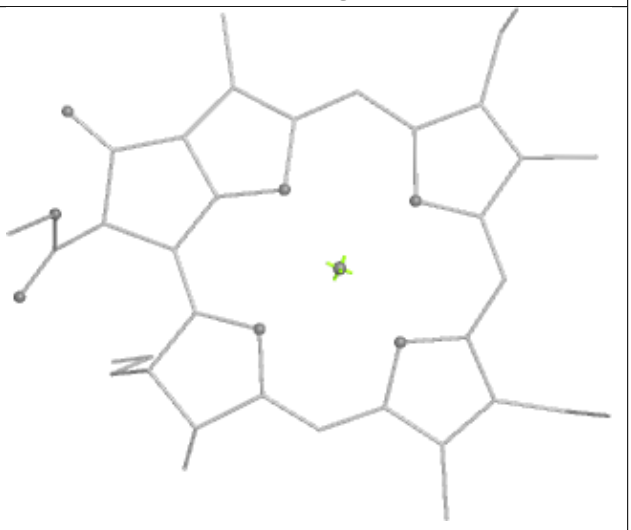
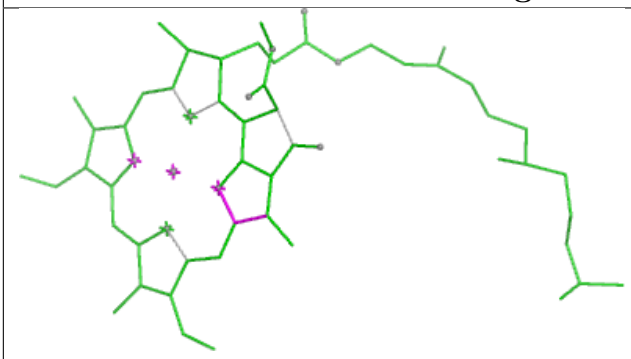


Rings

Ligand CLA K2 203



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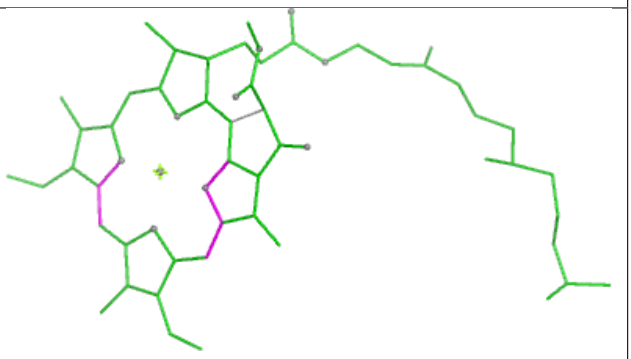
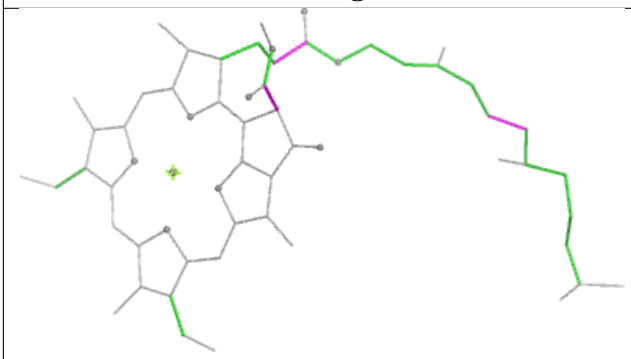


Bond angles



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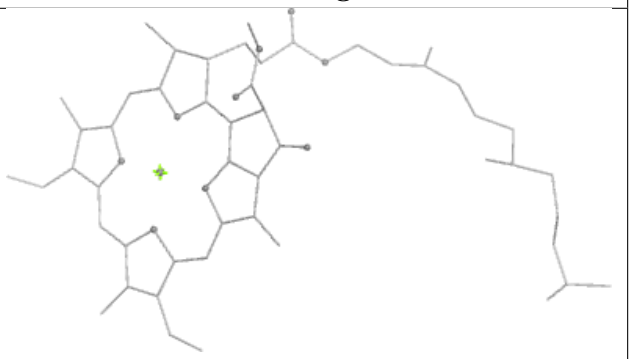
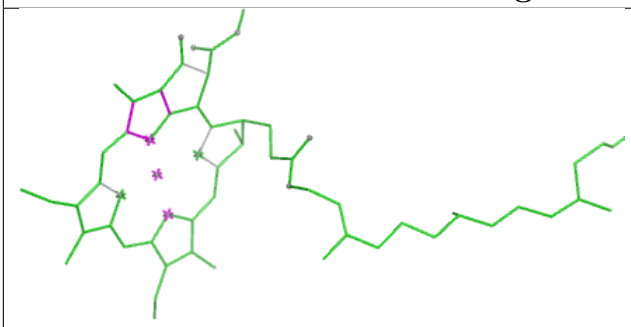


Rings

Ligand CLA A2 822



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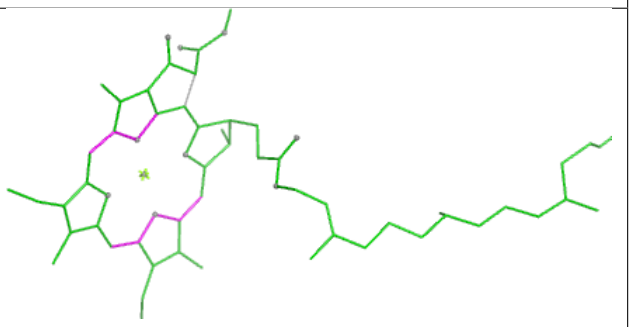
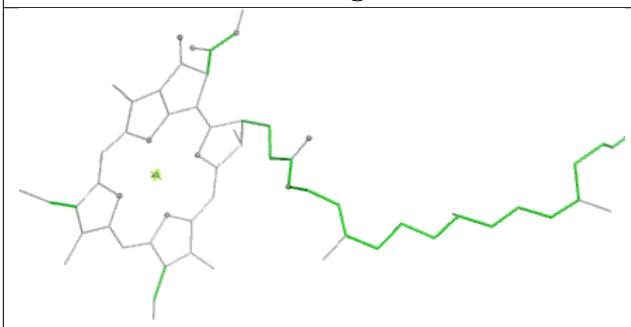


Bond angles



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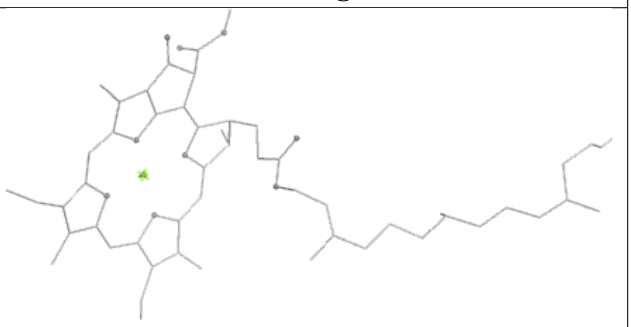
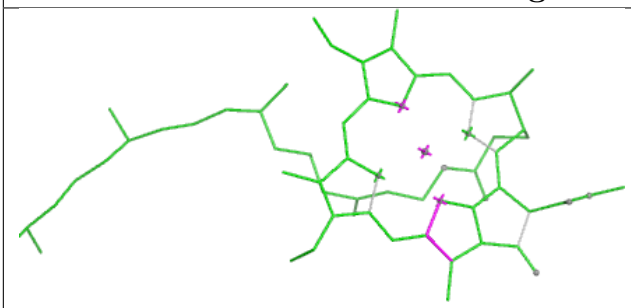
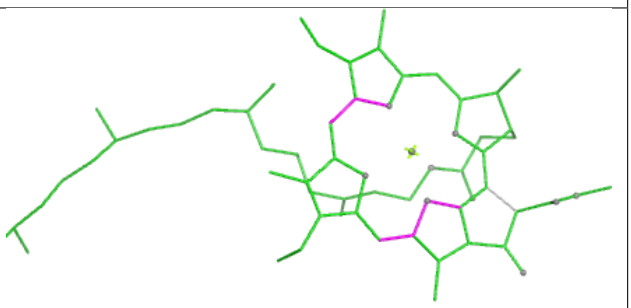
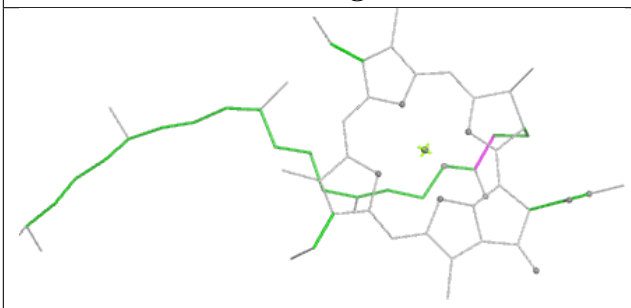
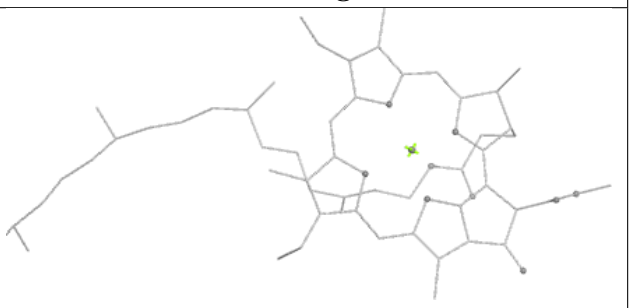


Rings

Ligand CLA 7 613	
 Bond lengths	 Bond angles
 Torsions	 Rings

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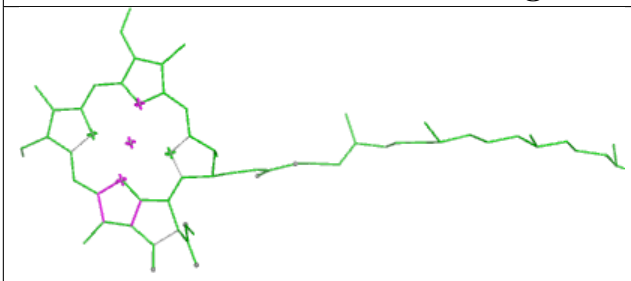
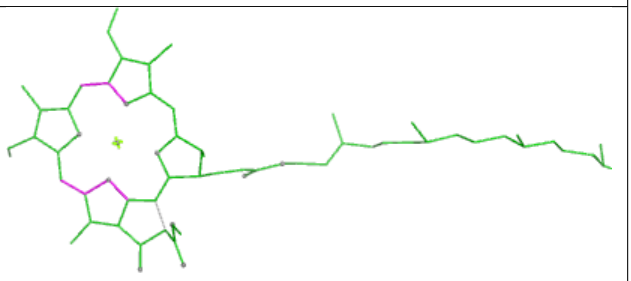
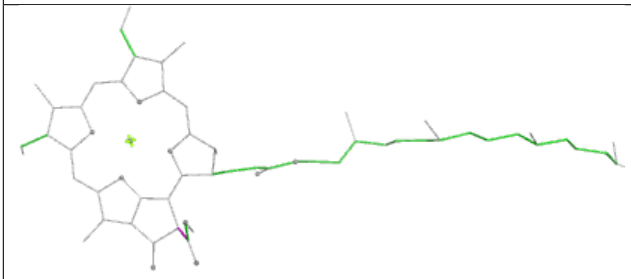
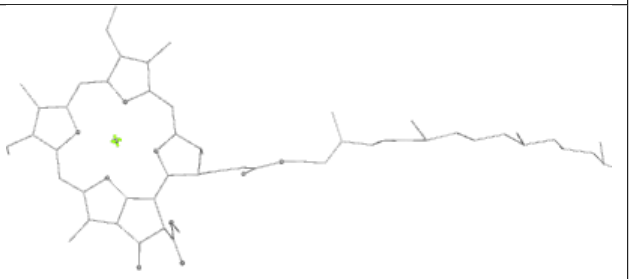
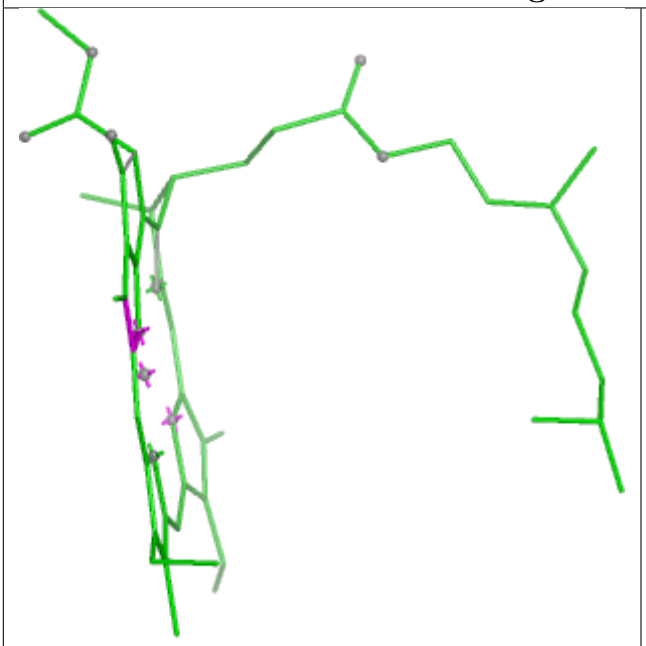
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA 5 604



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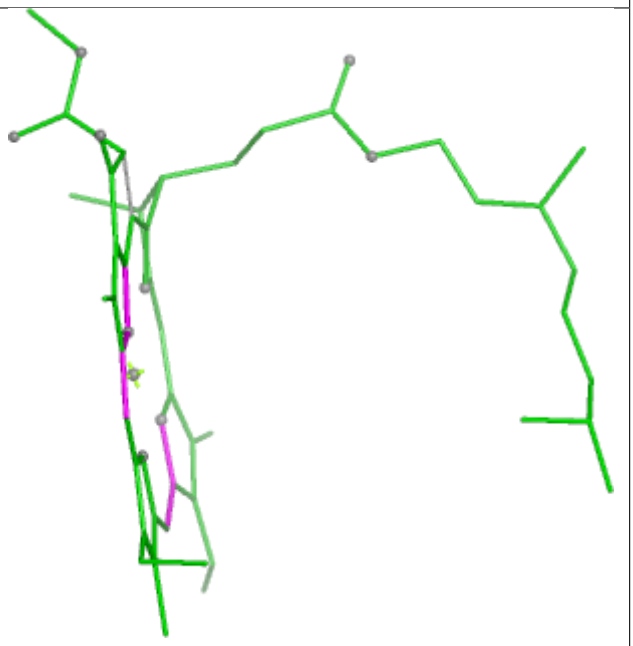

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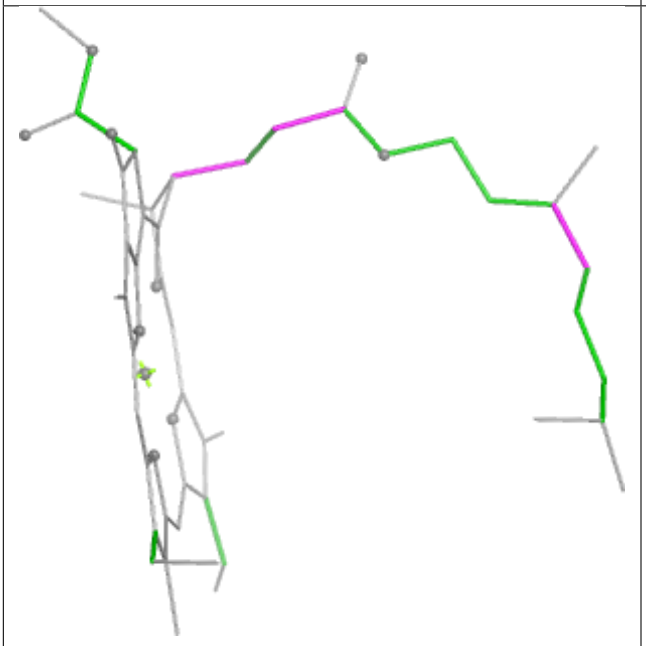

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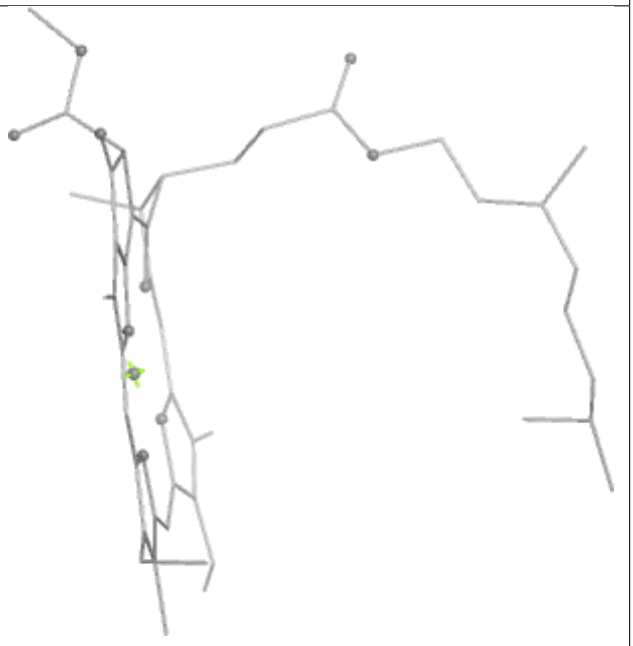

Rings

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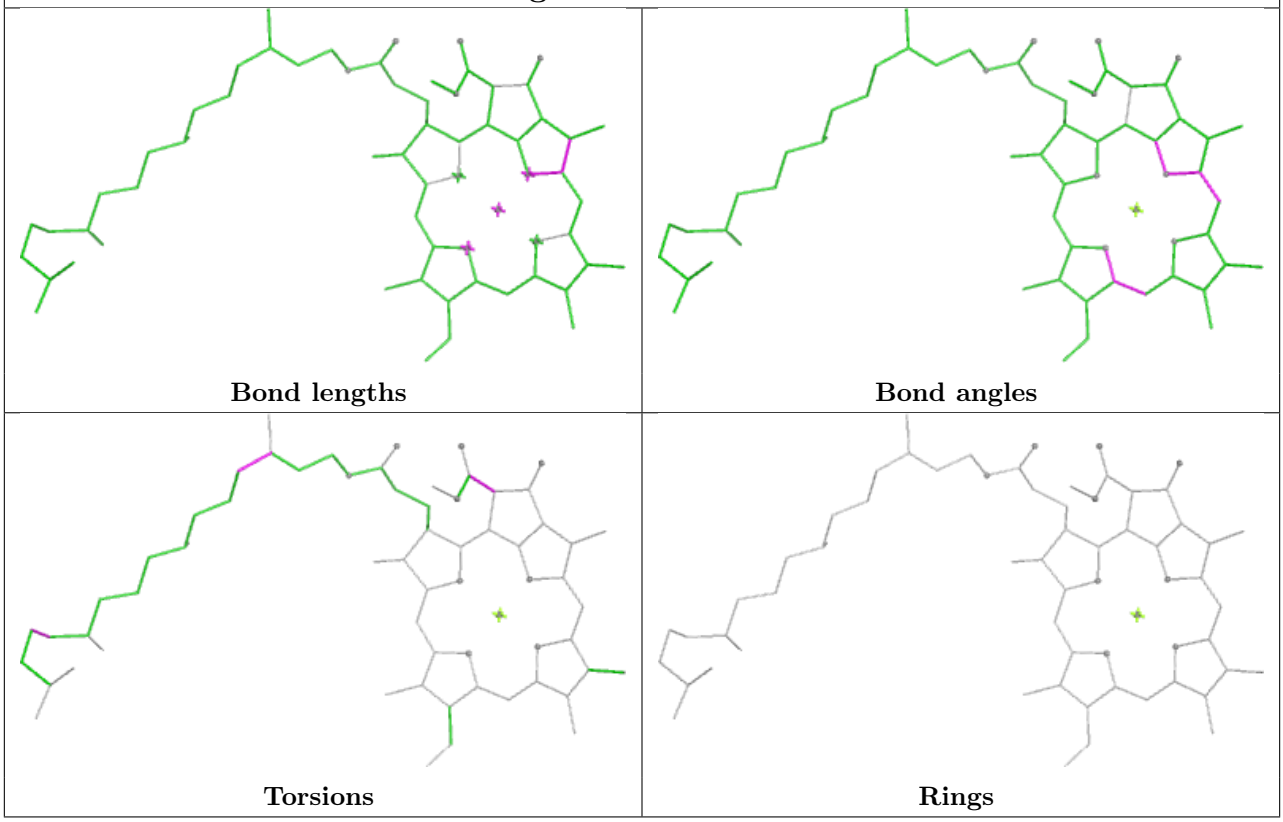

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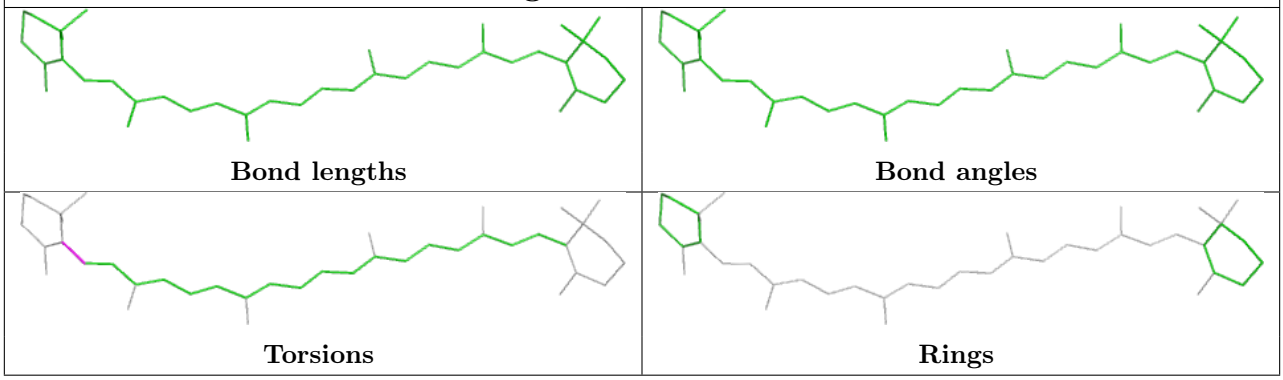

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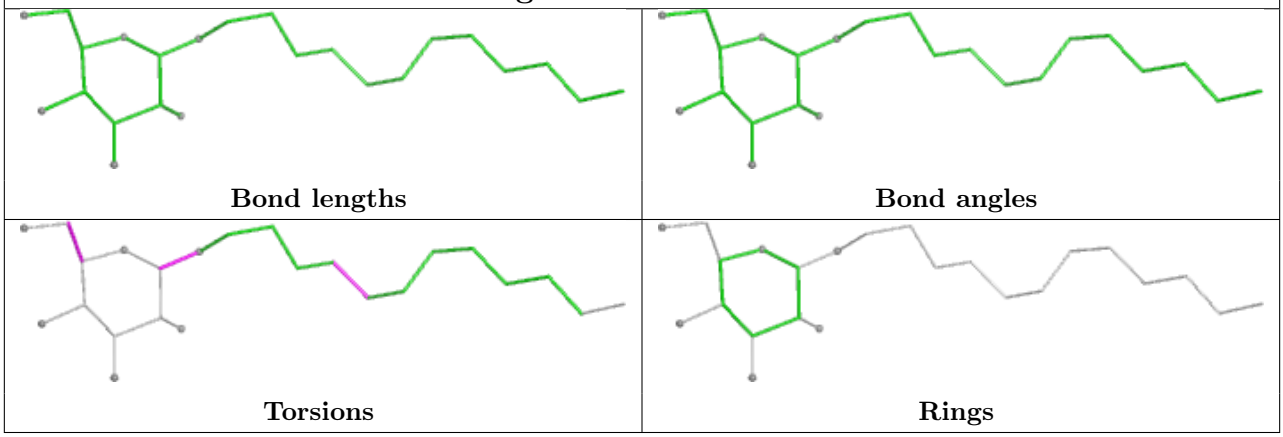

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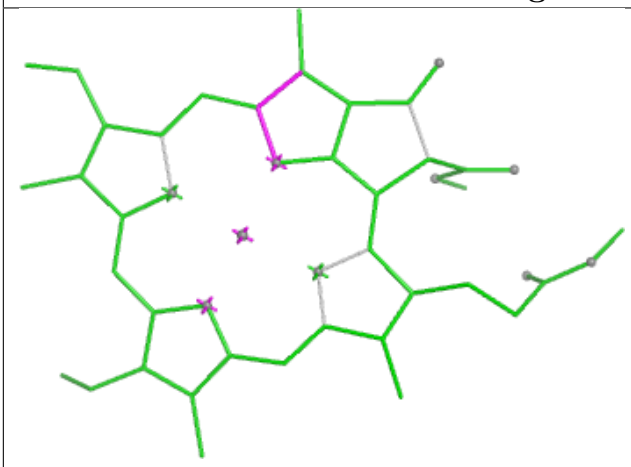

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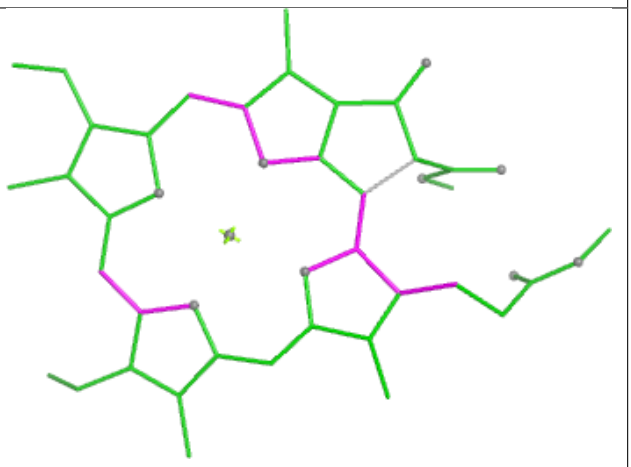

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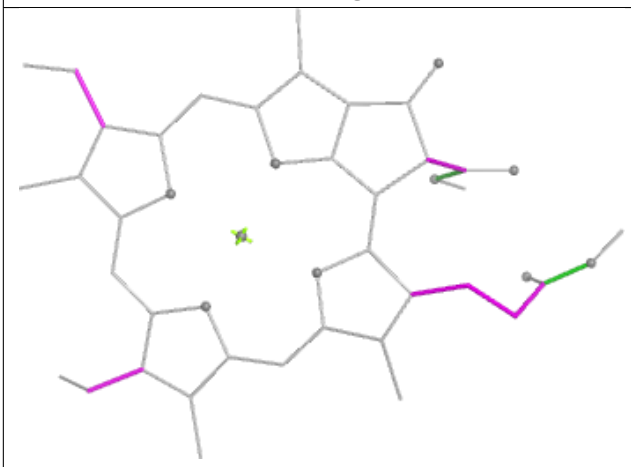

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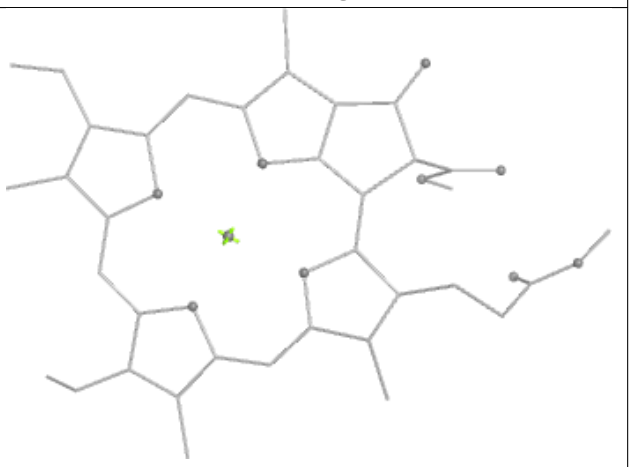

Rings

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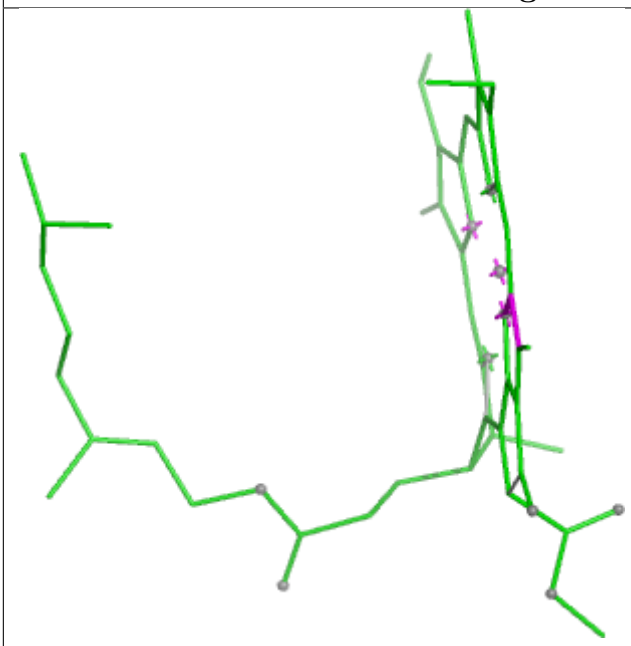

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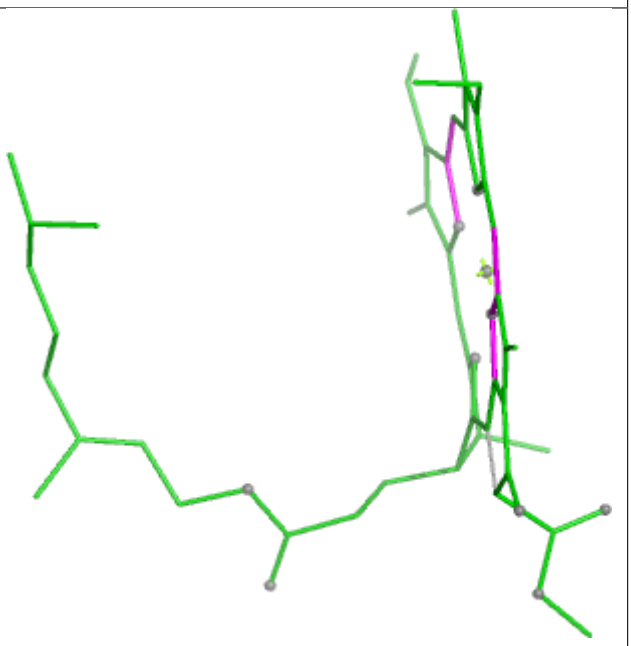

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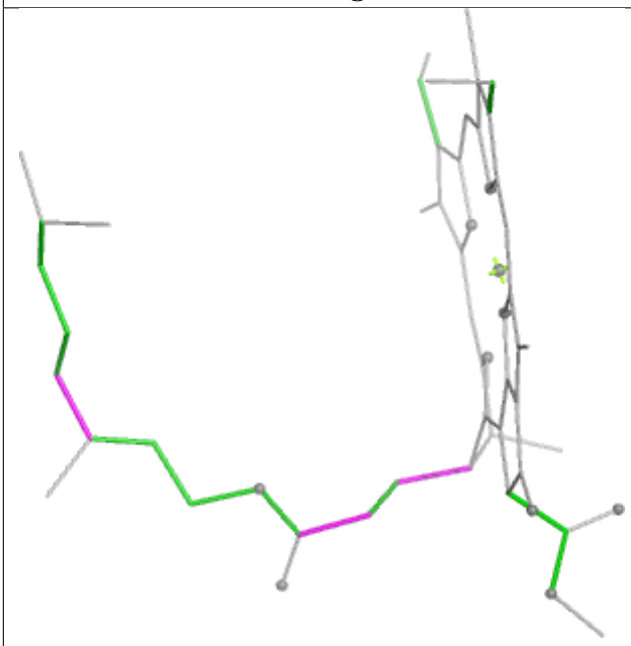

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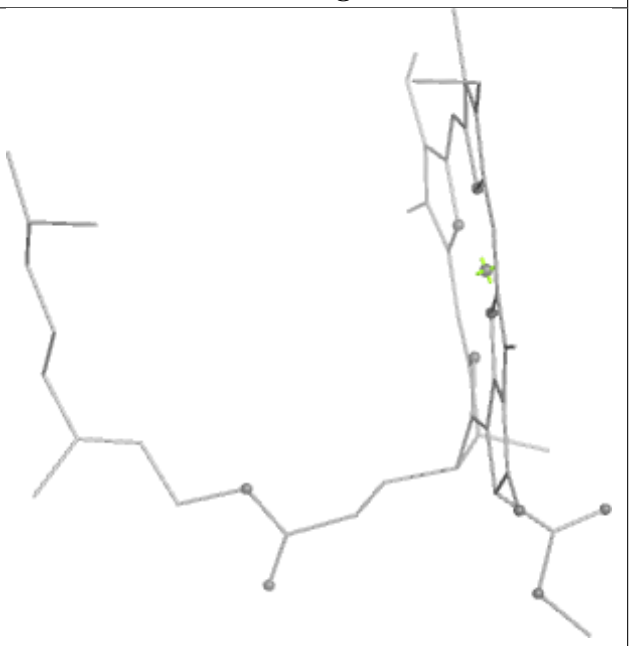


Rings

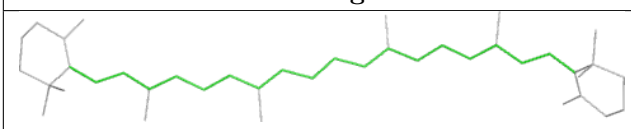
Ligand BCR B2 843



Bond lengths



Bond angles



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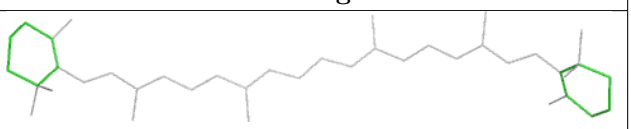
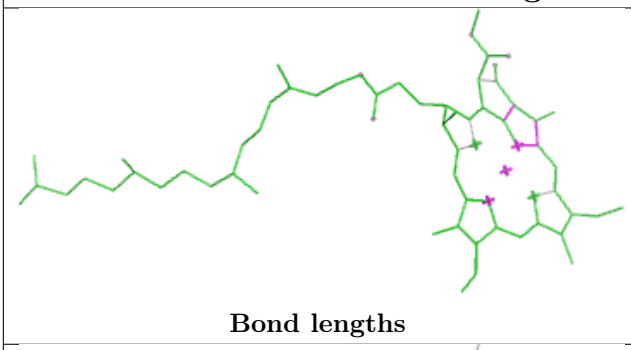


Rings

Ligand CLA A 803



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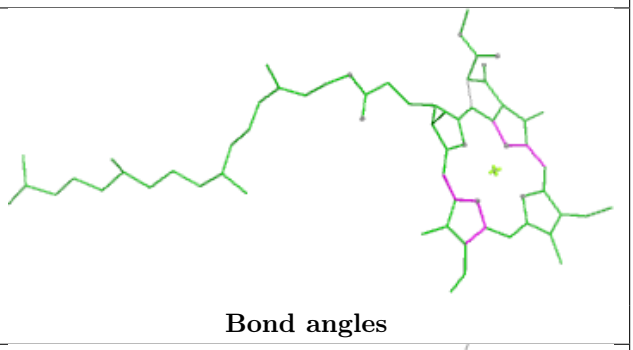

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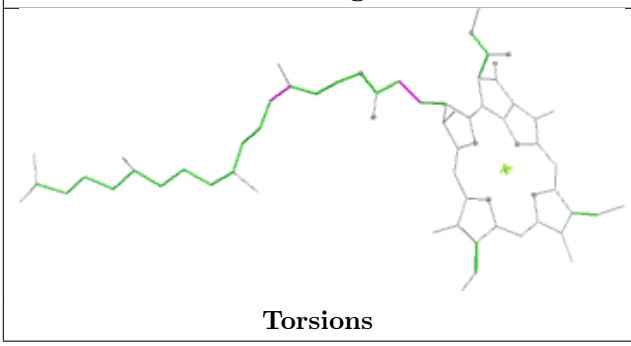

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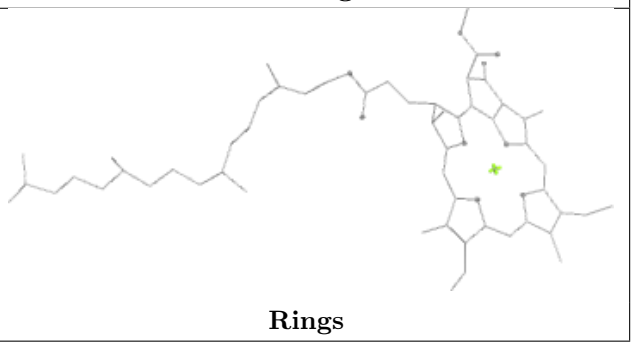
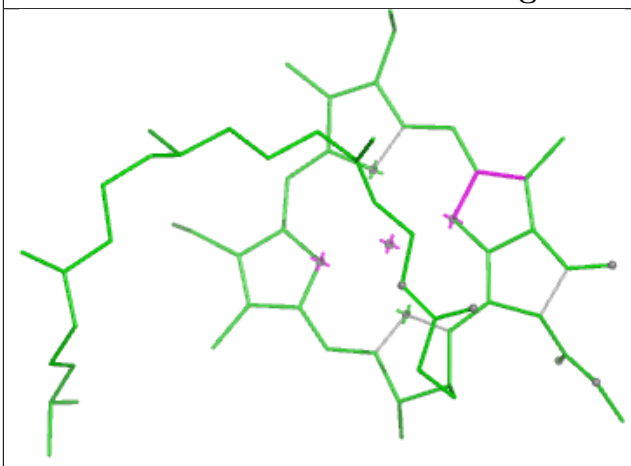


Rings

Ligand CLA 82 613



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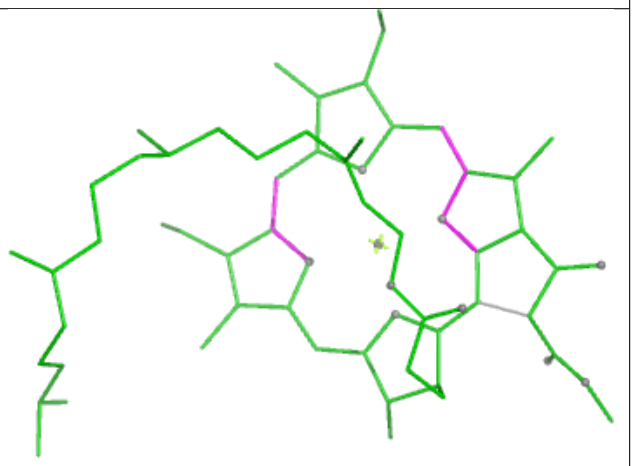

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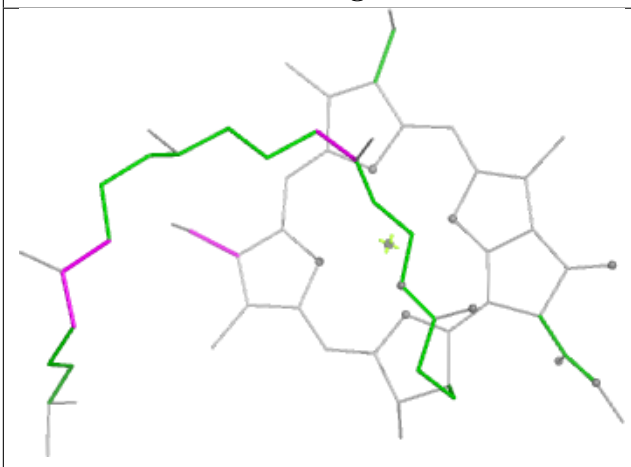

Torsions



Rings

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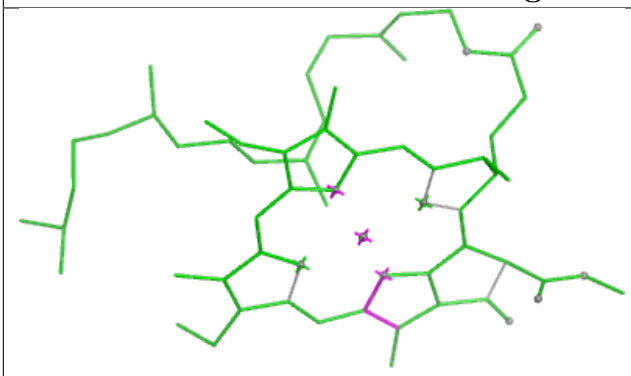

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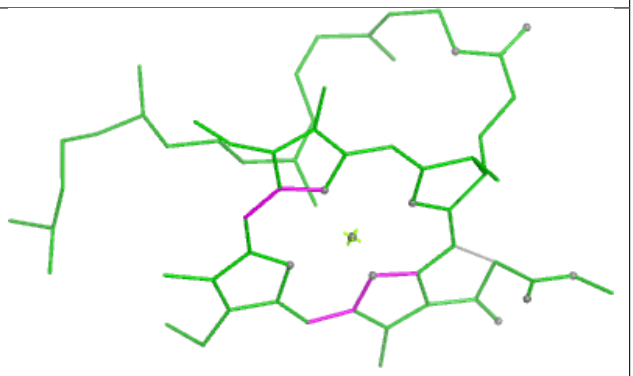

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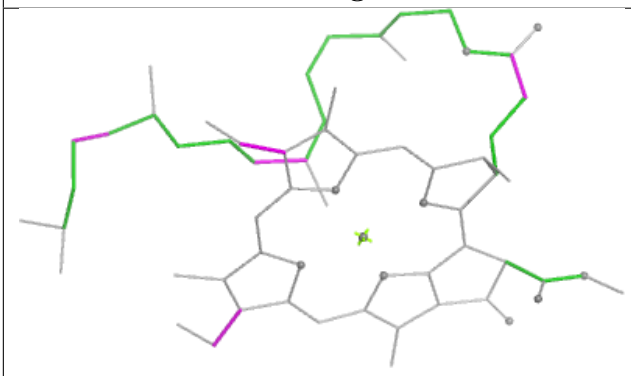

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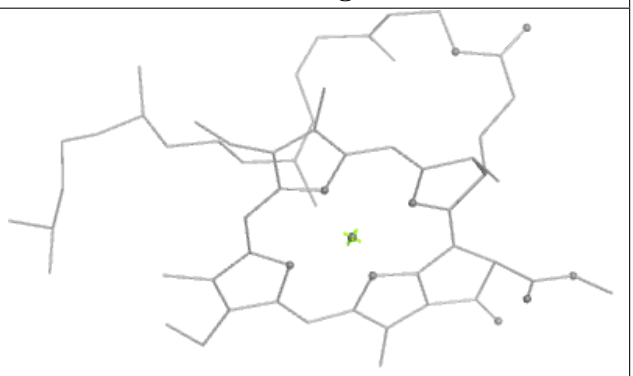
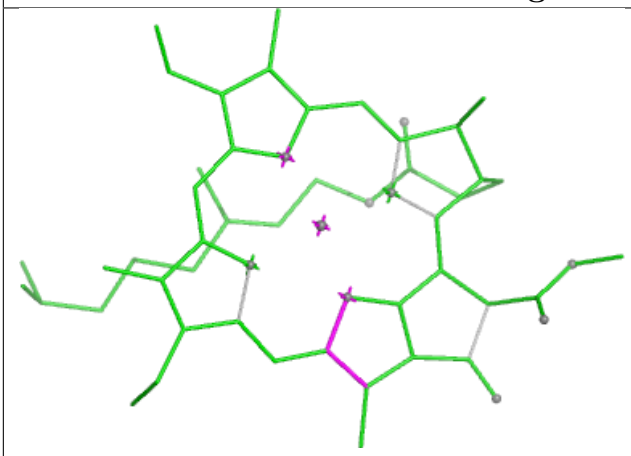


Rings

Ligand CLA J 101



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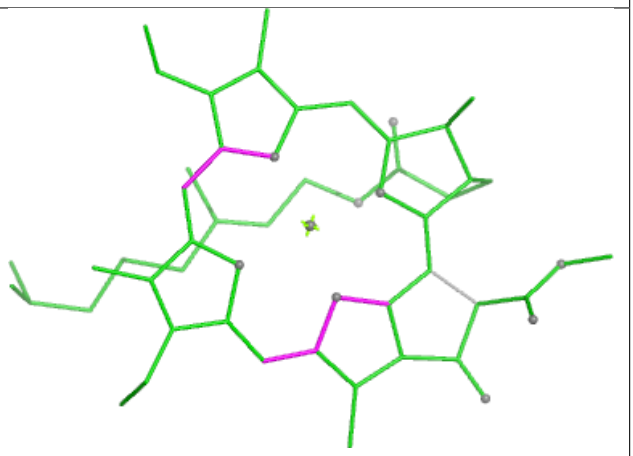

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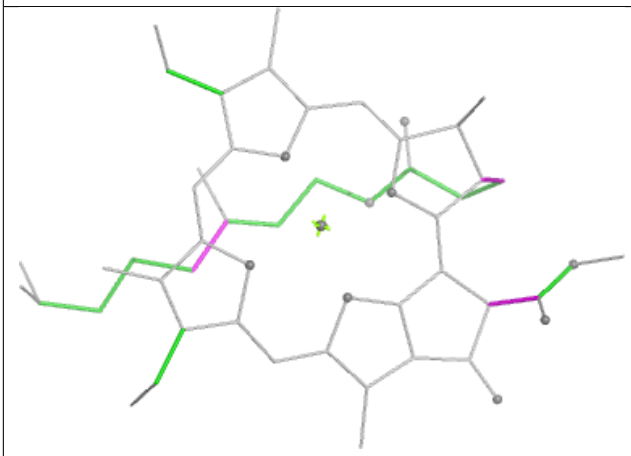

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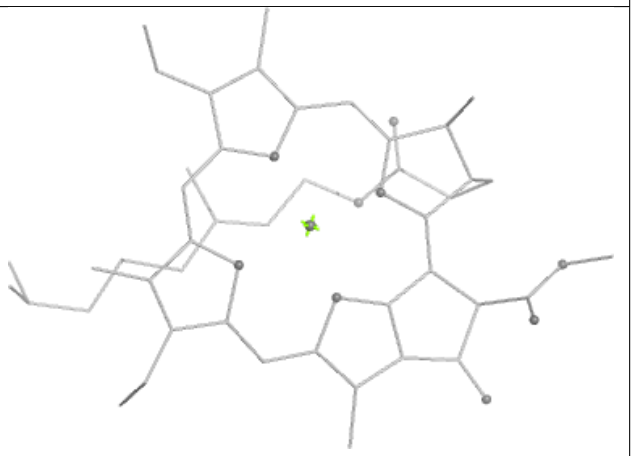
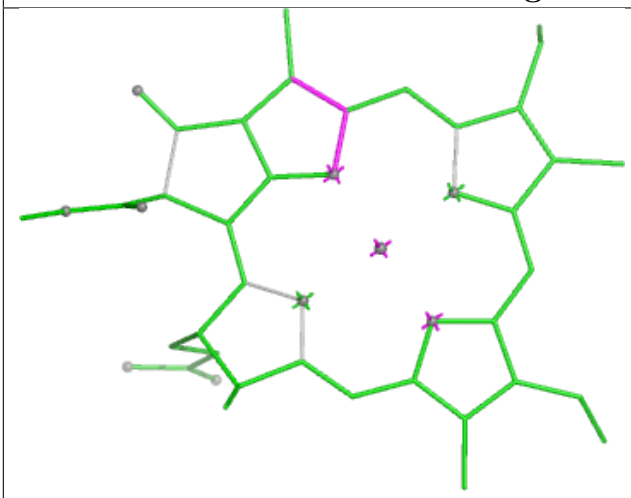


Rings

Ligand CLA B 835



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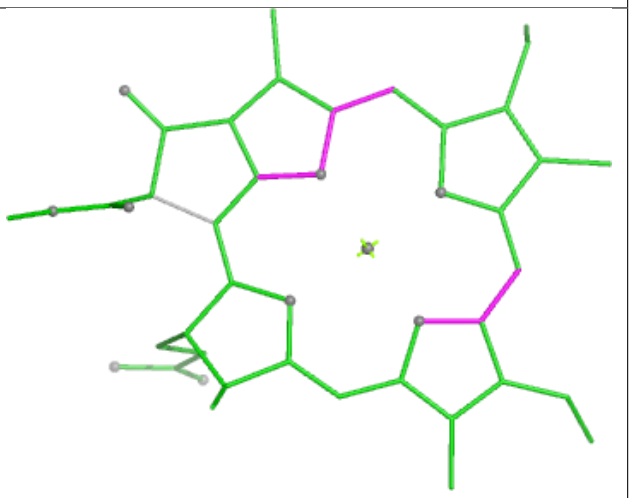

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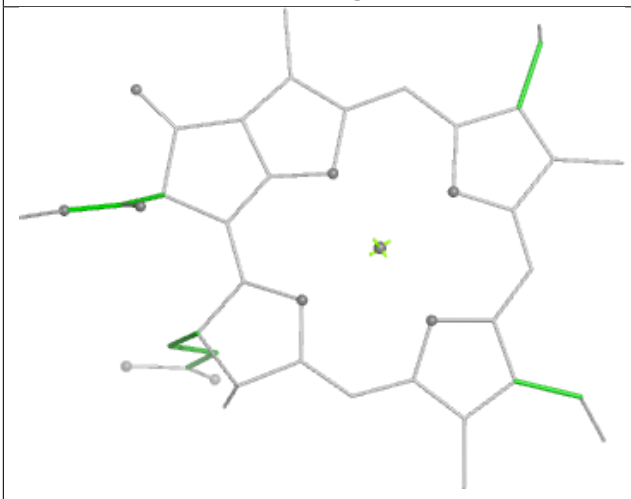

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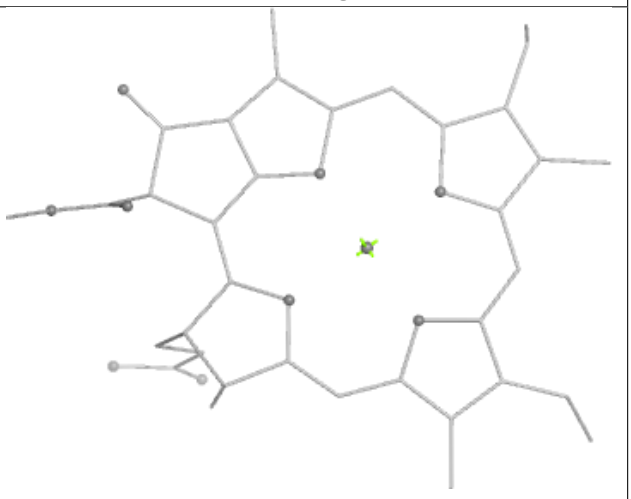
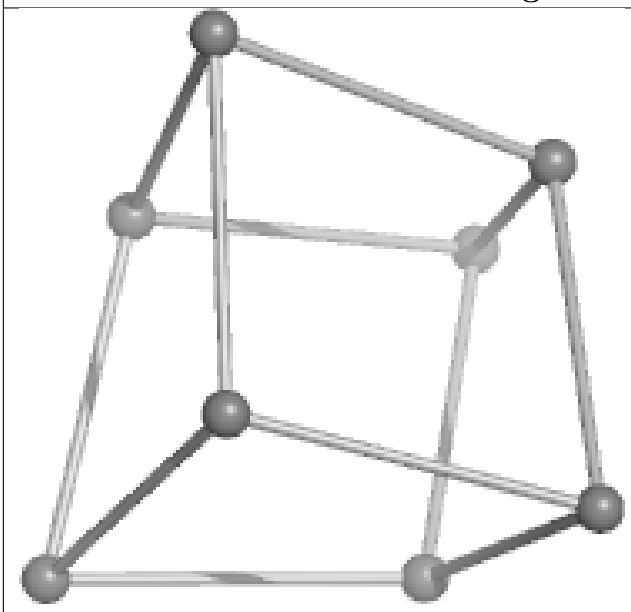


Rings

Ligand SF4 C2 102



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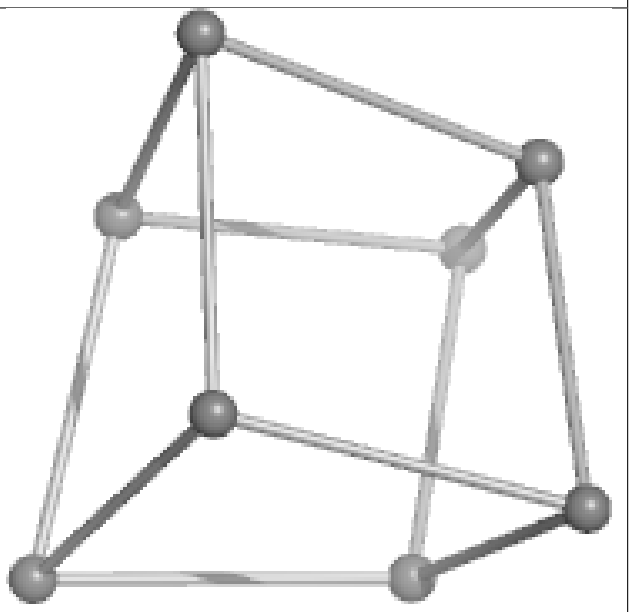

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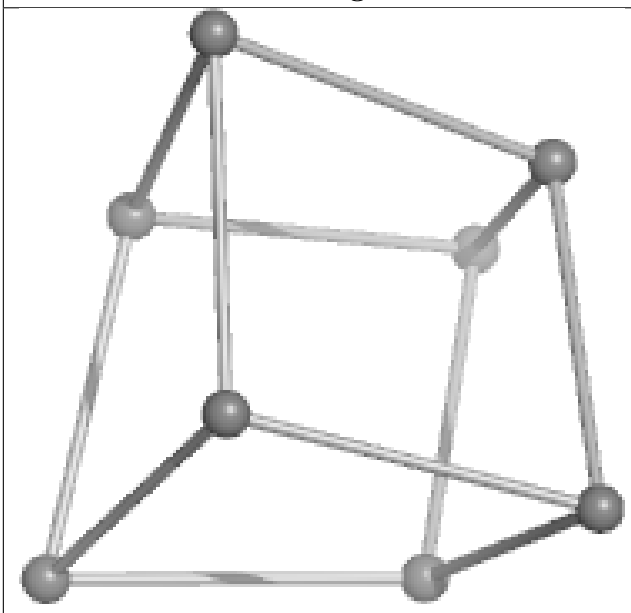

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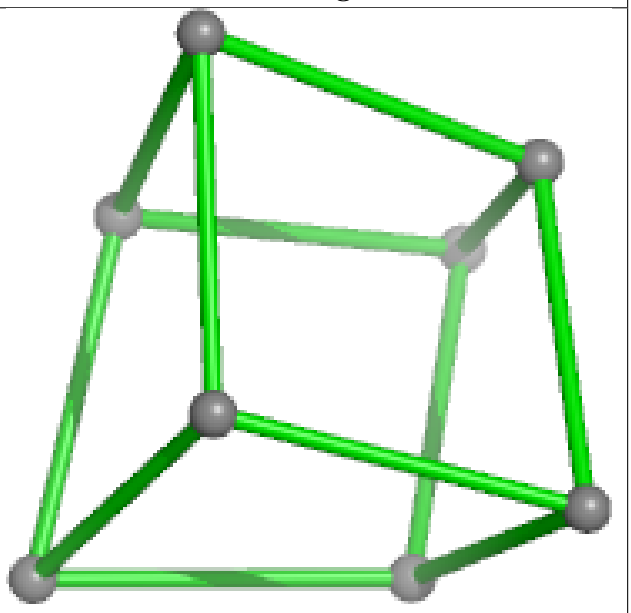
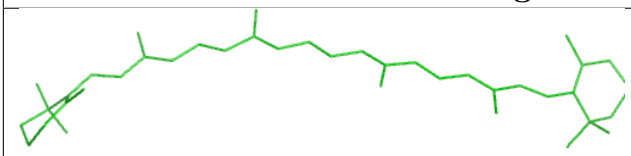


Rings

Ligand BCR B2 801



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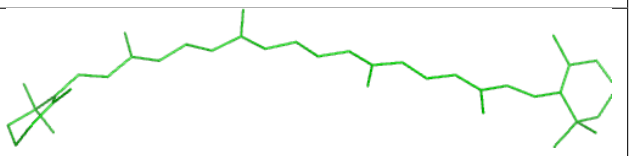

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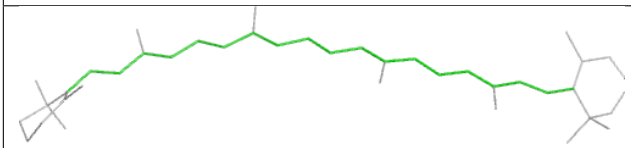

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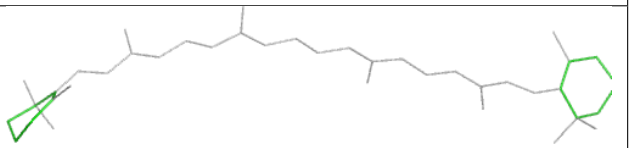

Rings

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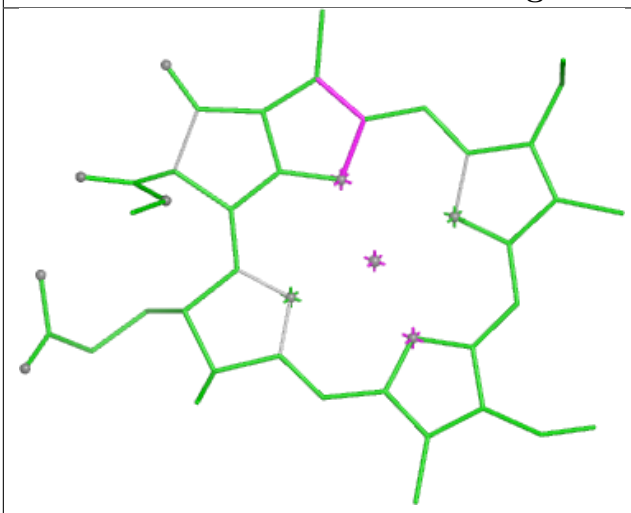

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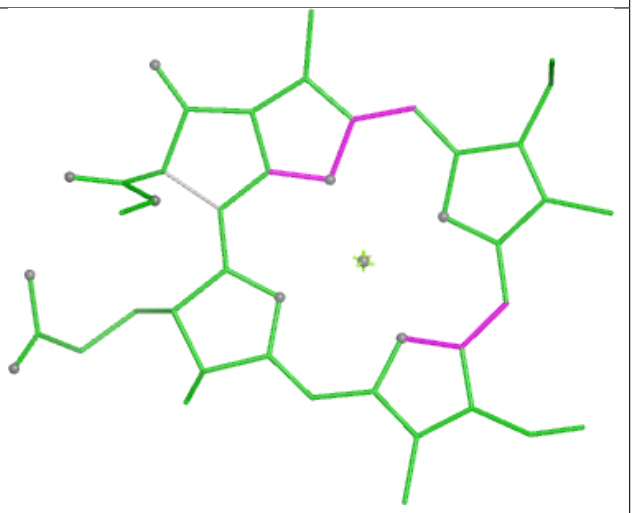

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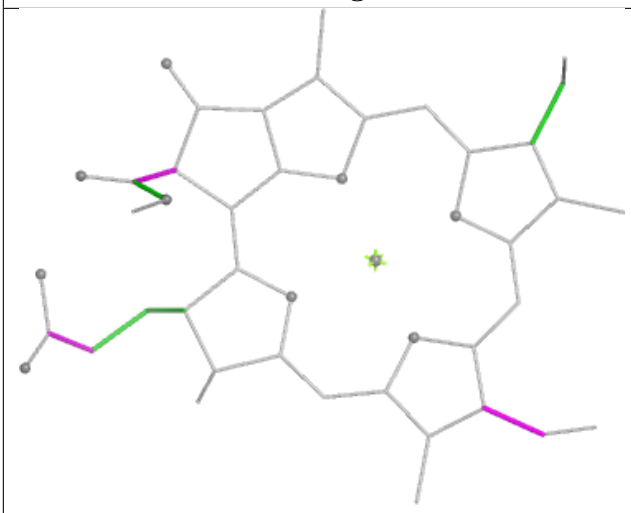

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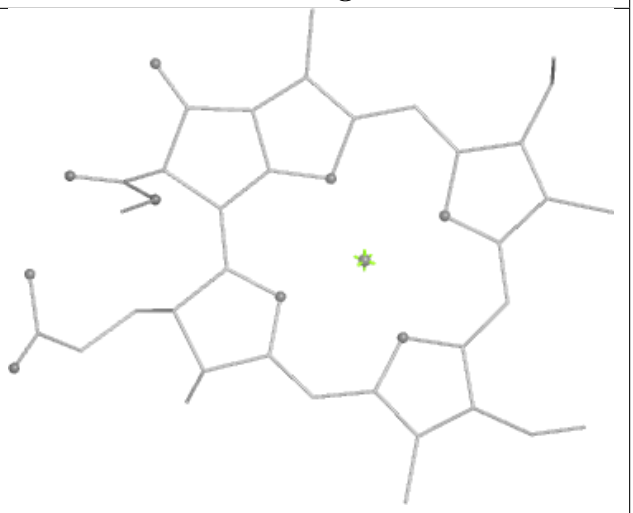

Rings

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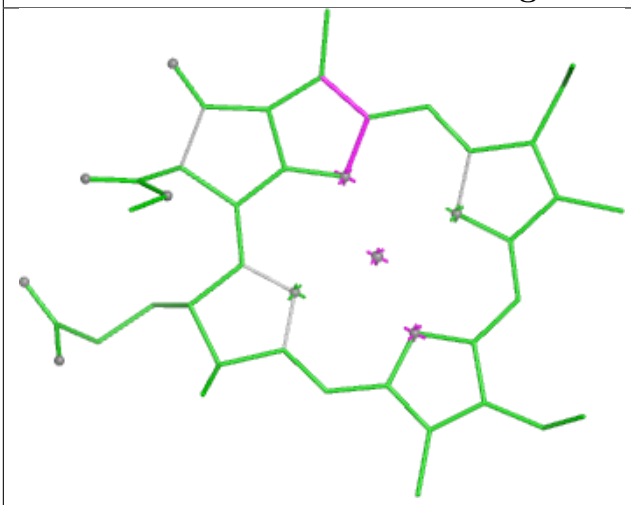

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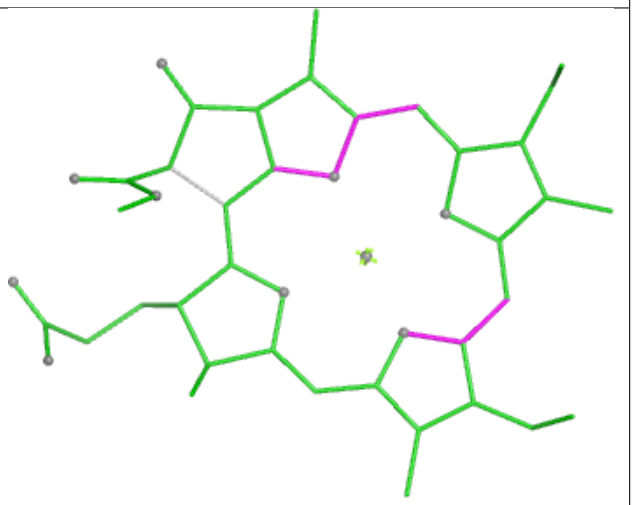
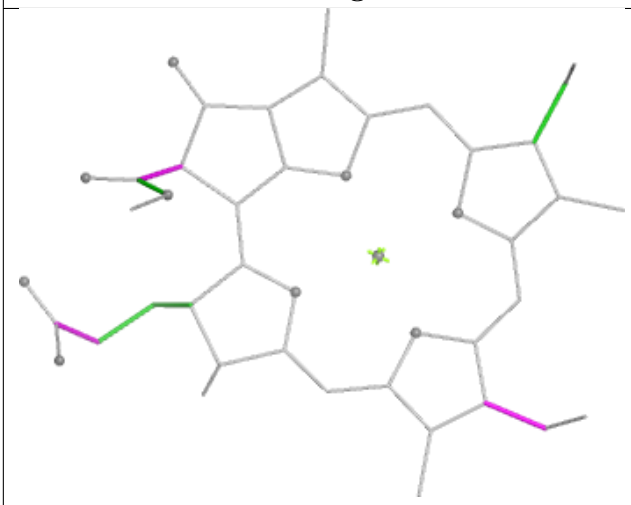
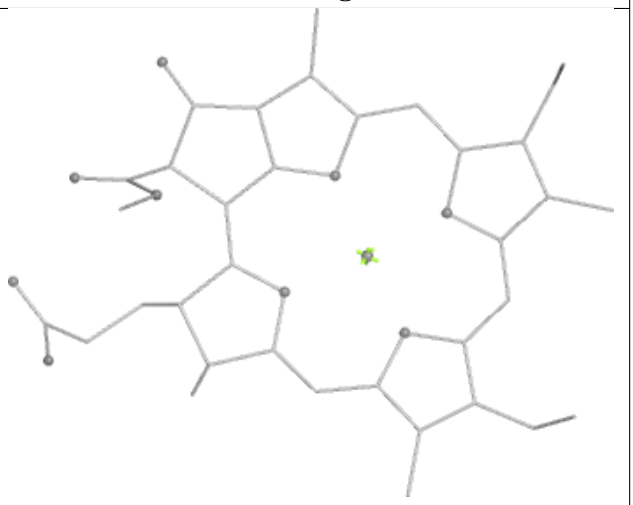


Bond angles

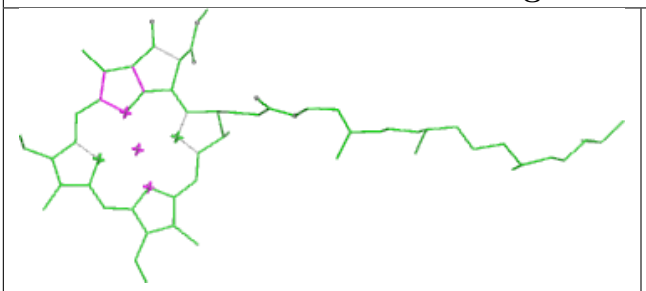


Torsions

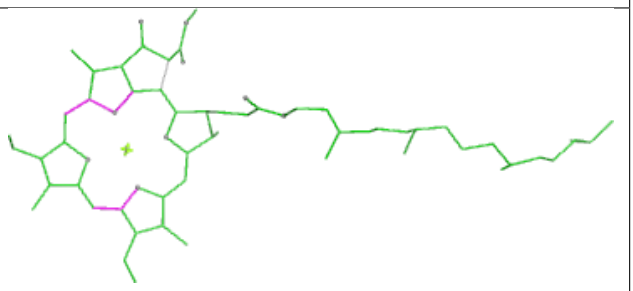


Rings

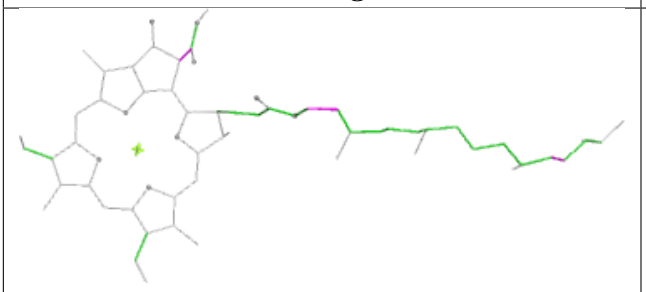
Ligand CLA A 827



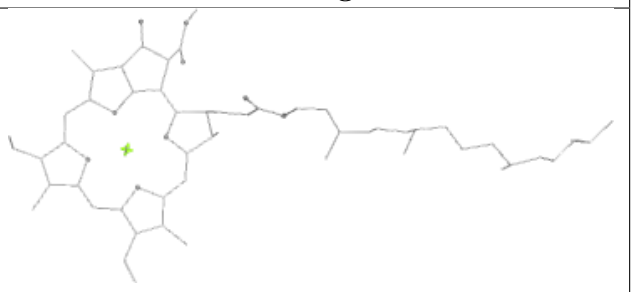
Bond lengths



Bond angles

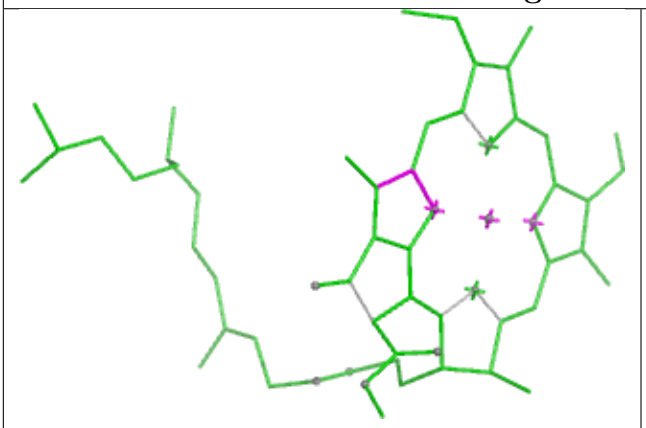


Torsions

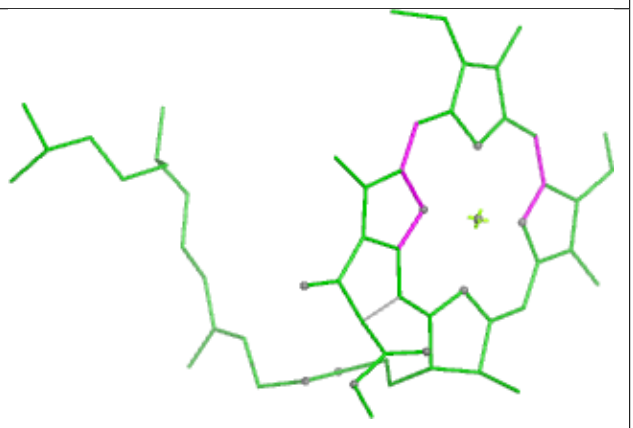


Rings

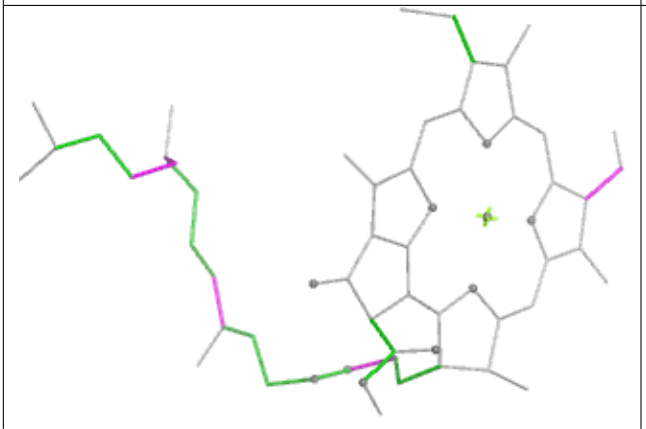
Ligand CLA B 834



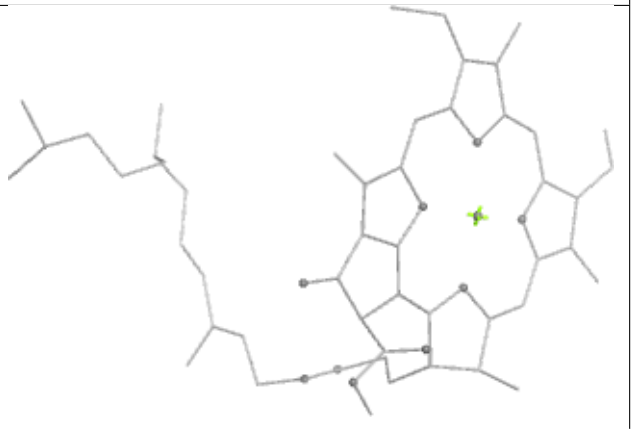
Bond lengths



Bond angles

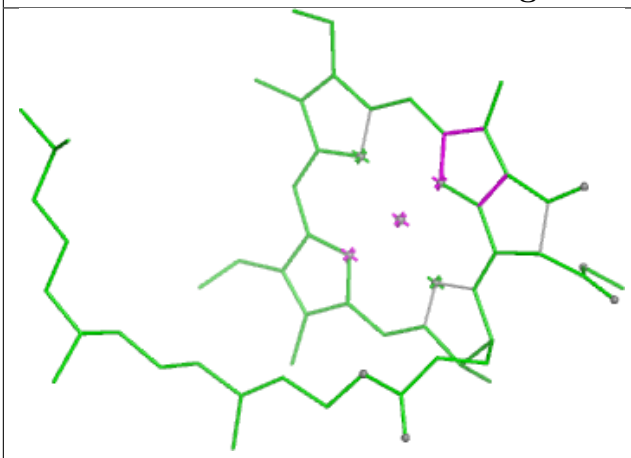


Torsions

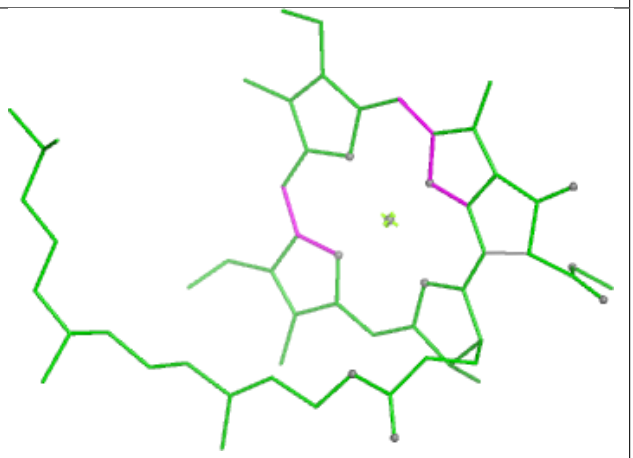


Rings

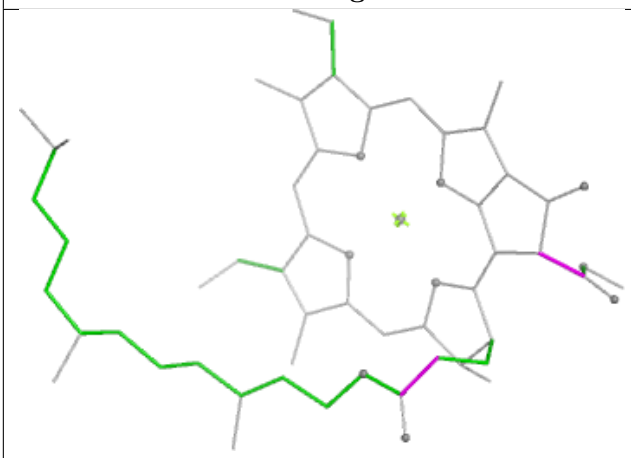
Ligand CLA 12 602



Bond lengths



Bond angles

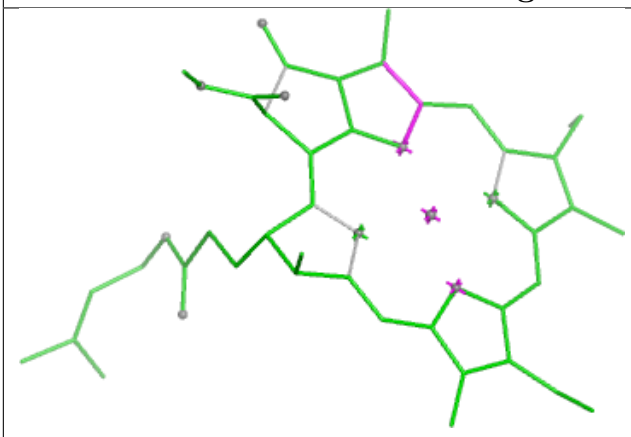


Torsions

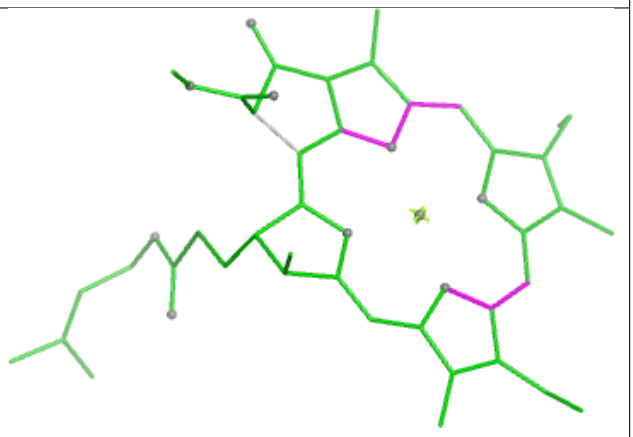


Rings

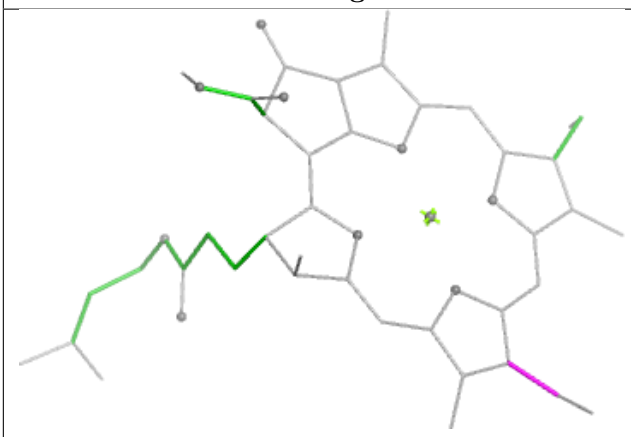
Ligand CLA Z2 608



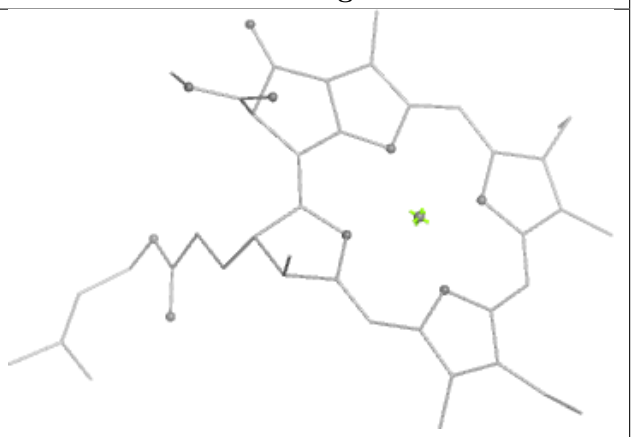
Bond lengths



Bond angles

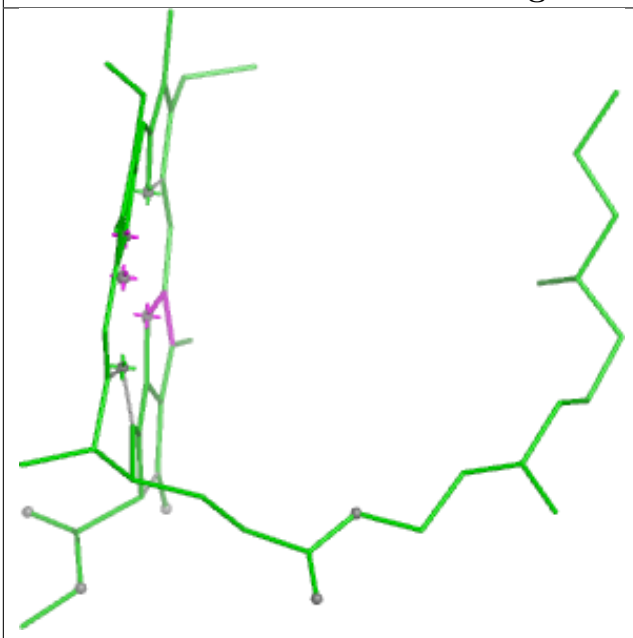


Torsions

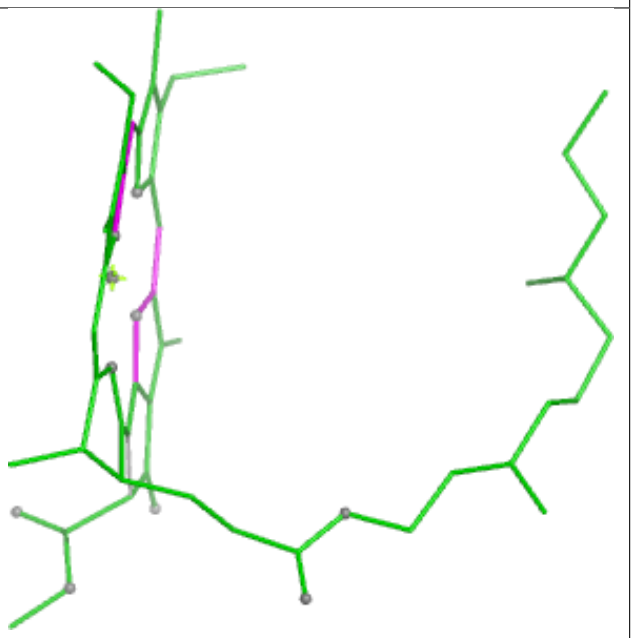


Rings

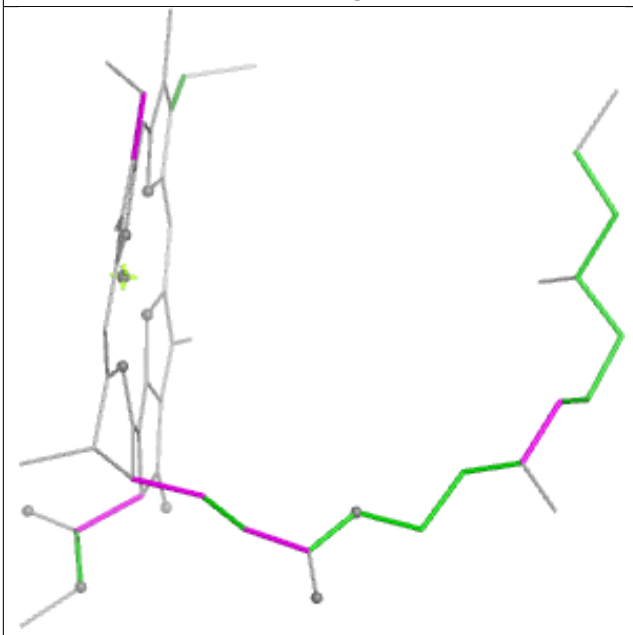
Ligand CLA 8 614



Bond lengths



Bond angles



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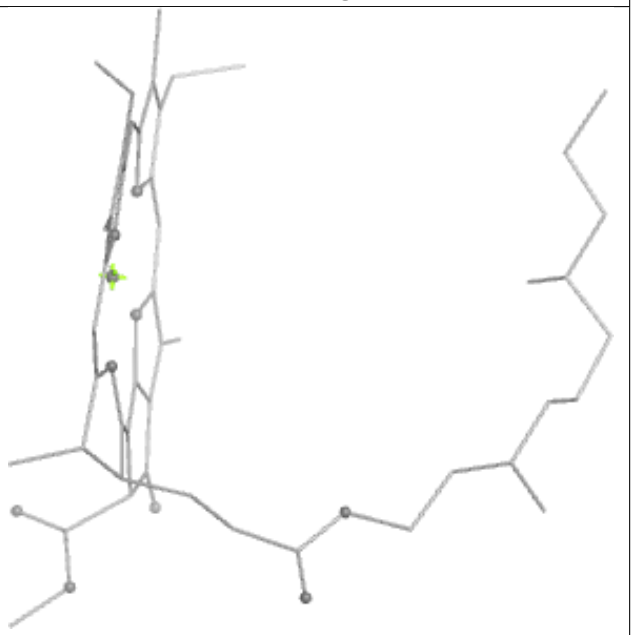
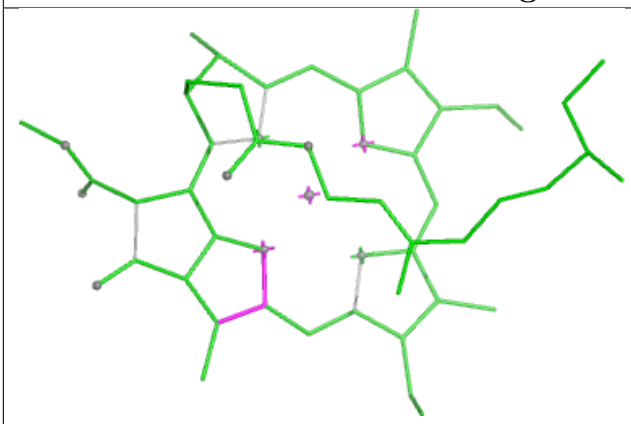
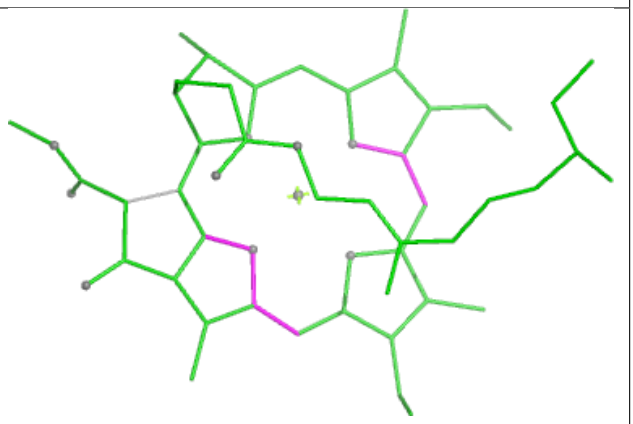


Rings

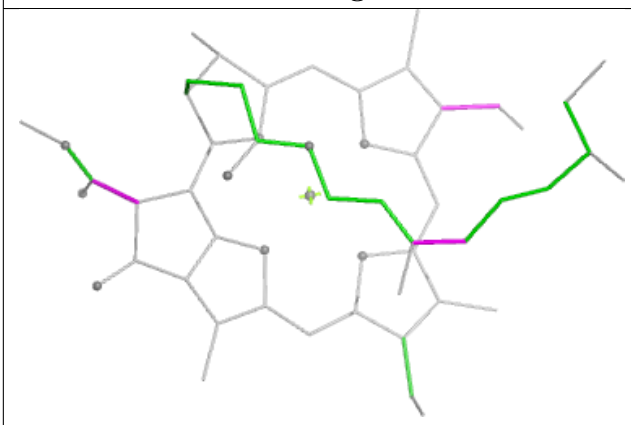
Ligand CLA 52 613



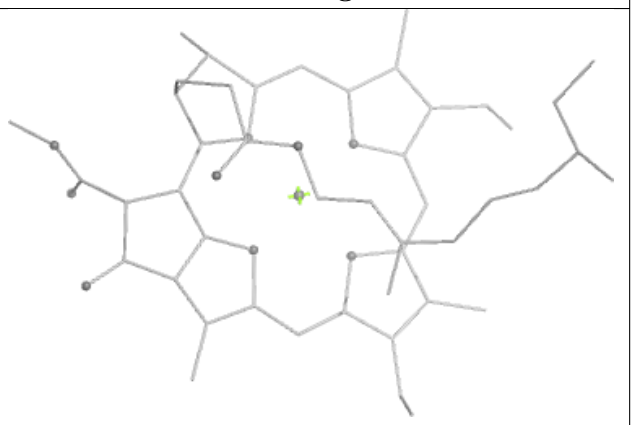
Bond lengths



Bond angles

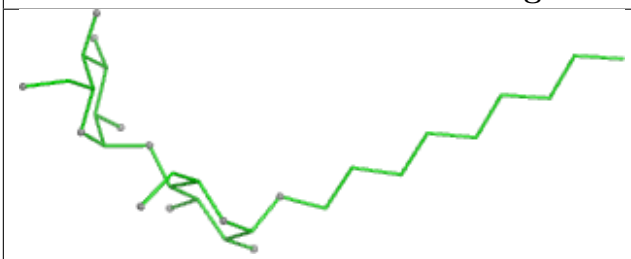


Torsions



Rings

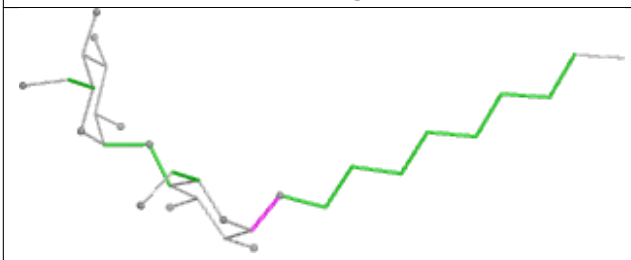
Ligand LMU 7 627



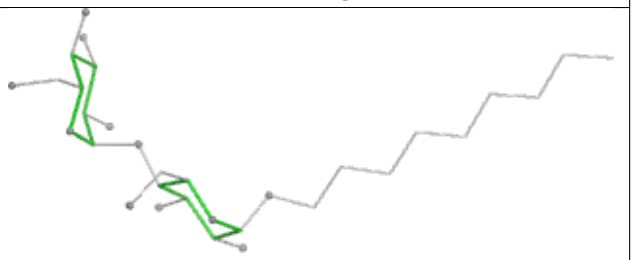
Bond lengths



Bond angles



Torsions



Rings

Ligand CLA 62 609



Bond lengths



Bond angles

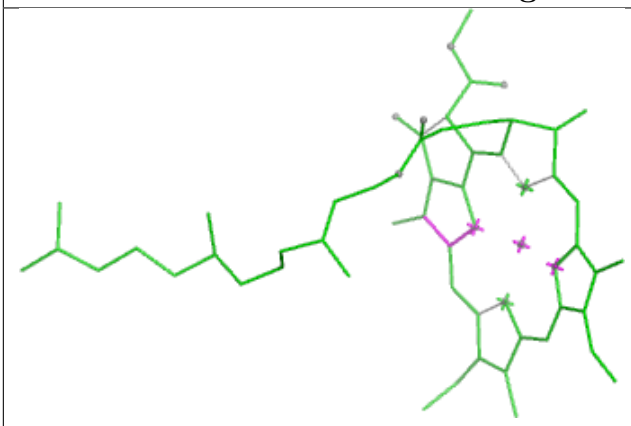


Torsions

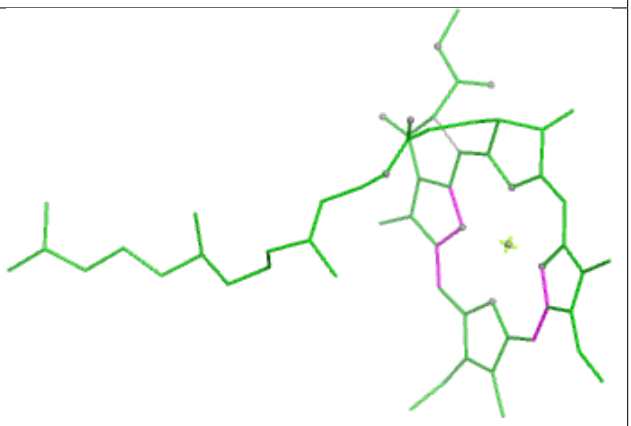


Rings

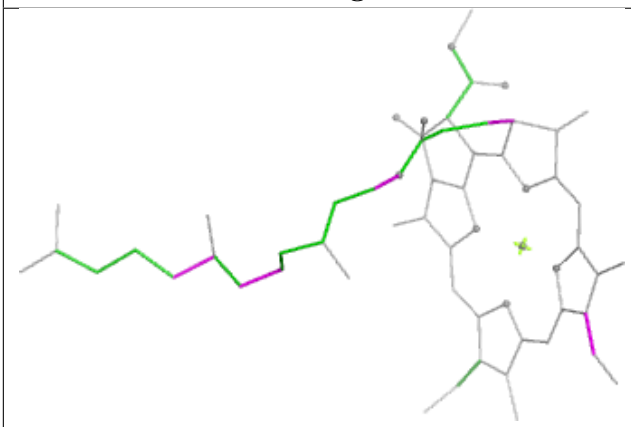
Ligand CLA 42 609



Bond lengths



Bond angles

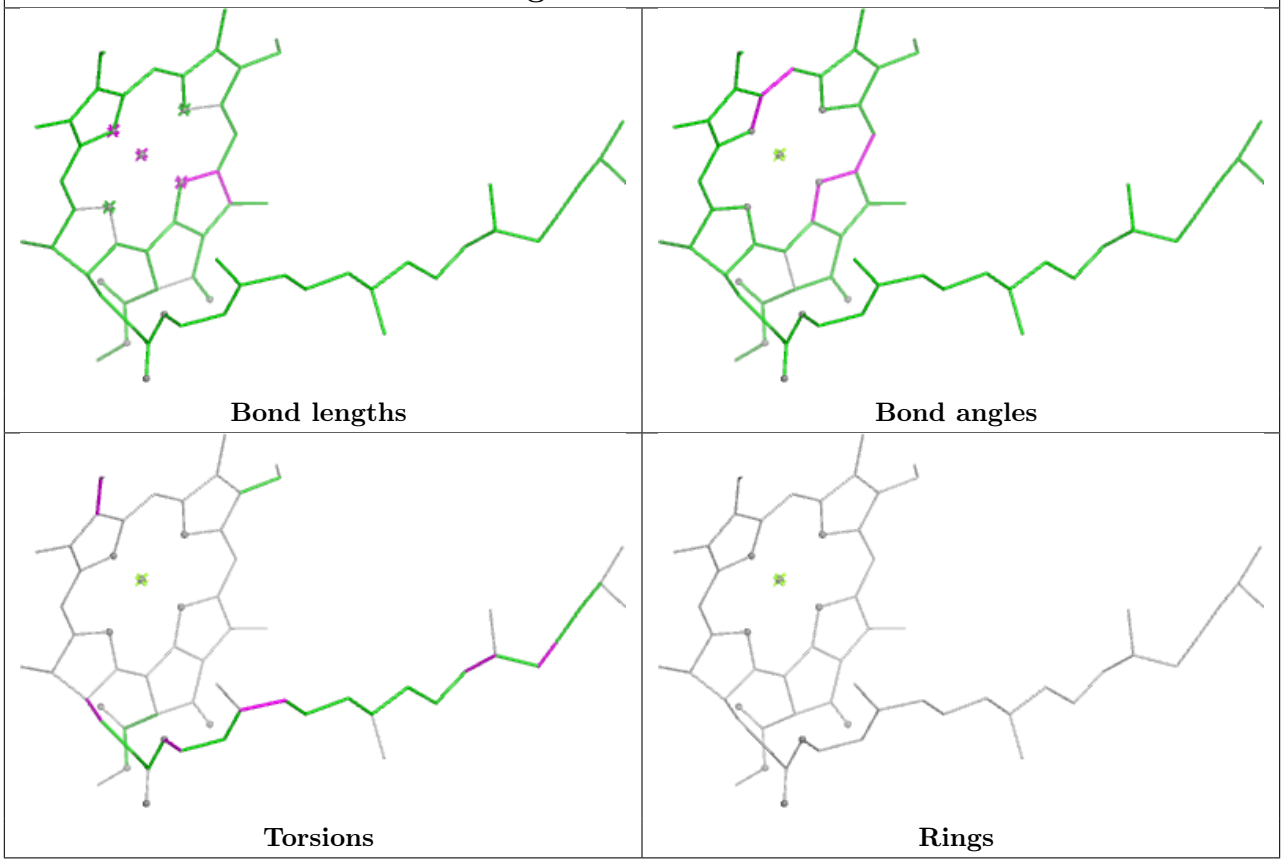


Torsions

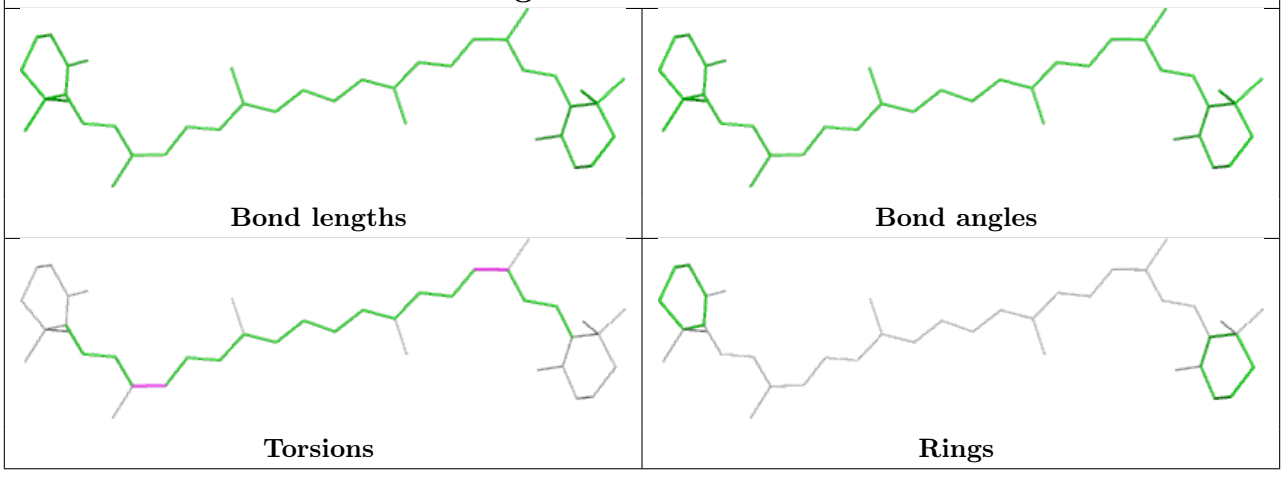


Rings

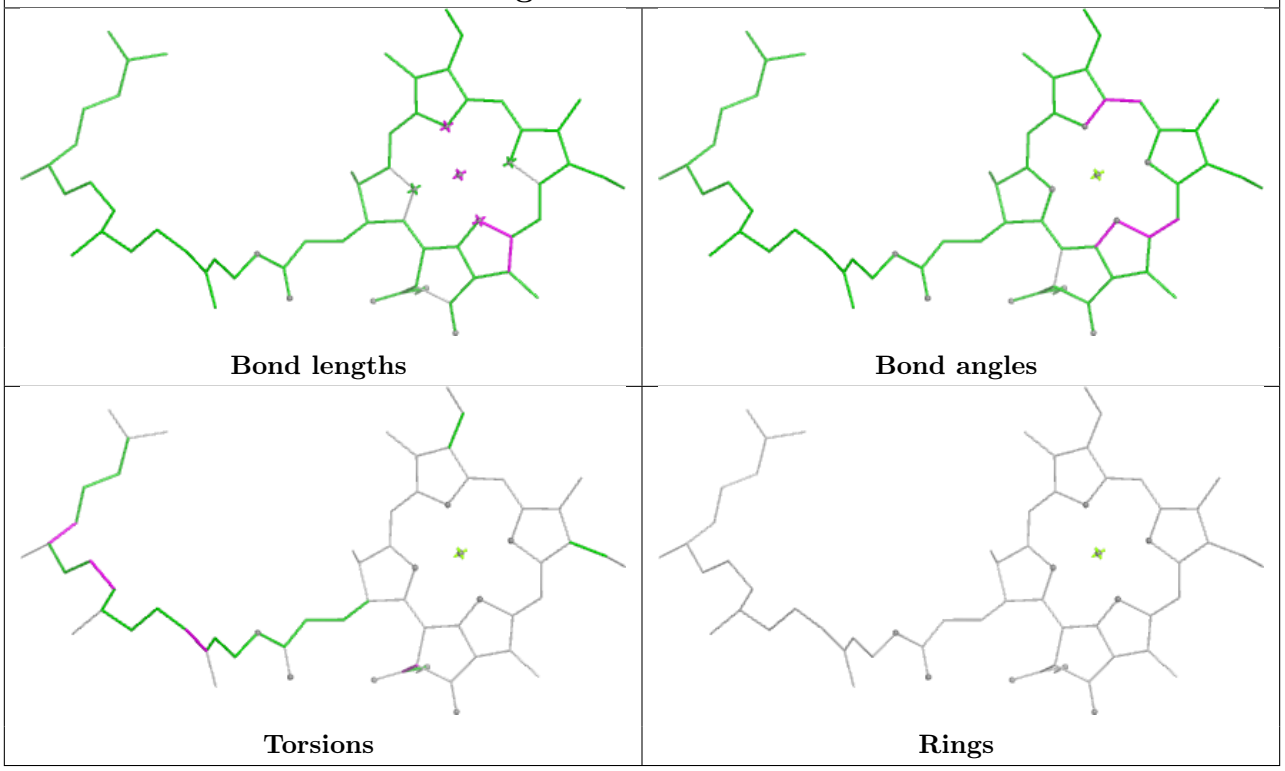
Ligand CLA Z 609



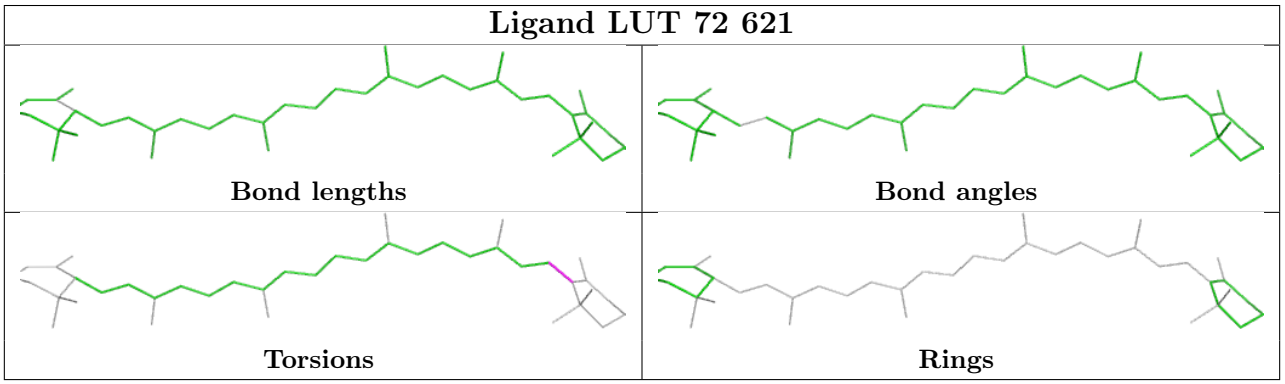
Ligand BCR B2 845



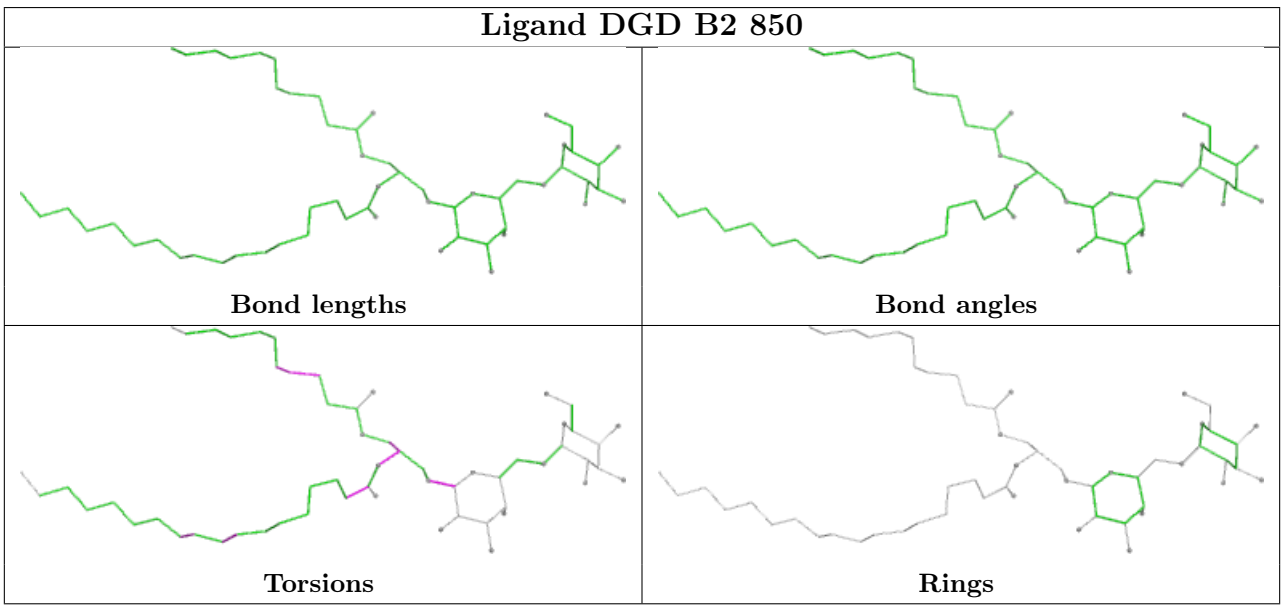
Ligand CLA A2 828



Ligand LUT 72 621



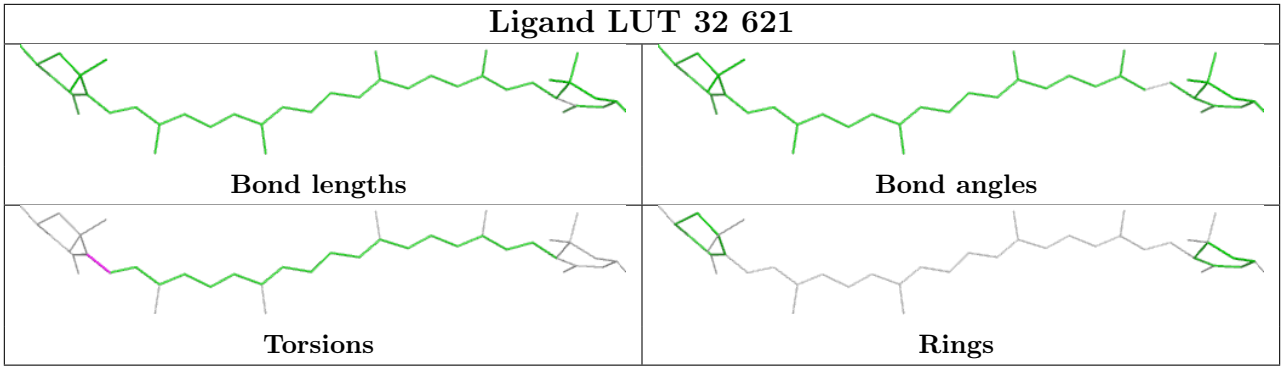
Ligand DGD B2 850



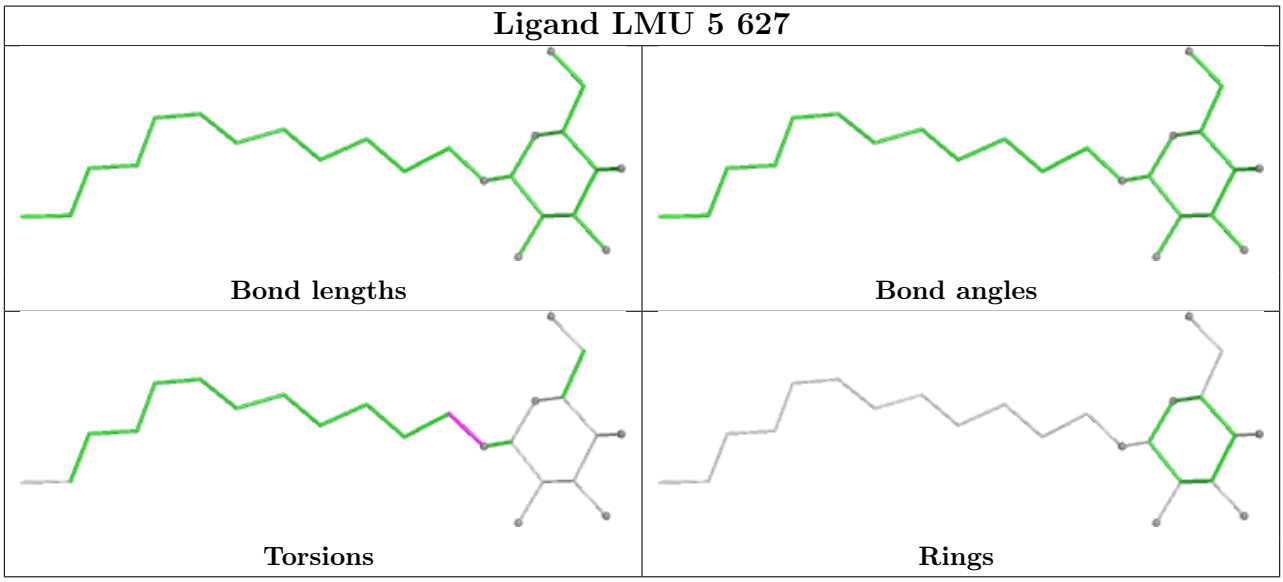
Ligand BCR 42 621



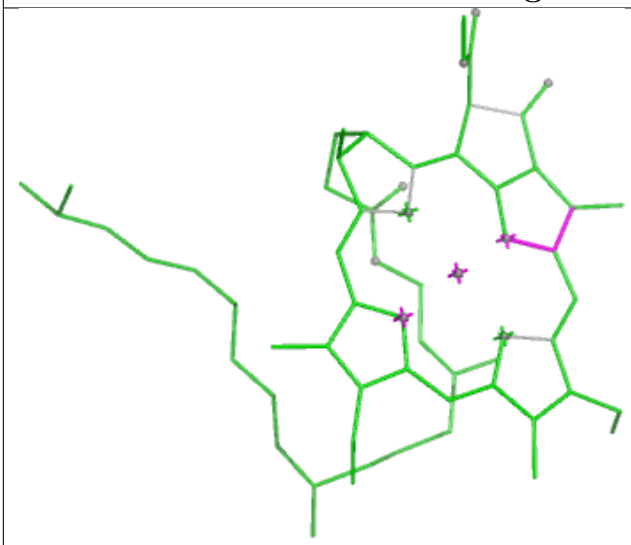
Ligand LUT 32 621



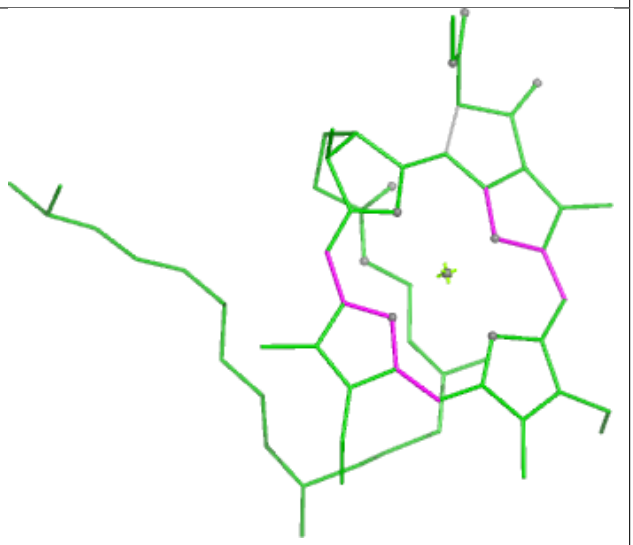
Ligand LMU 5 627



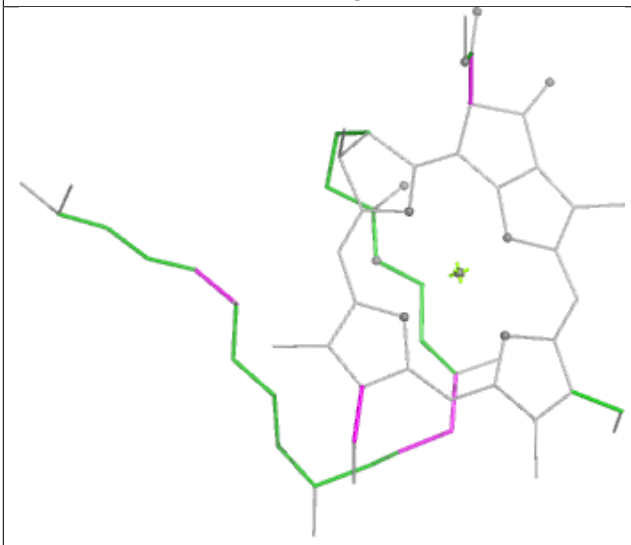
Ligand CLA B 808



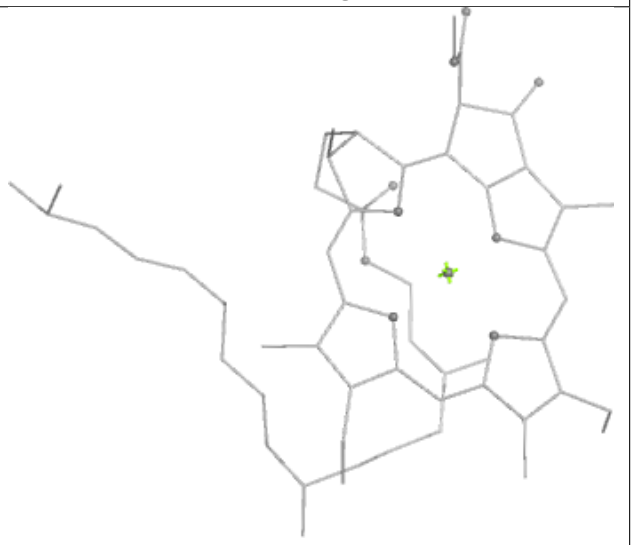
Bond lengths



Bond angles

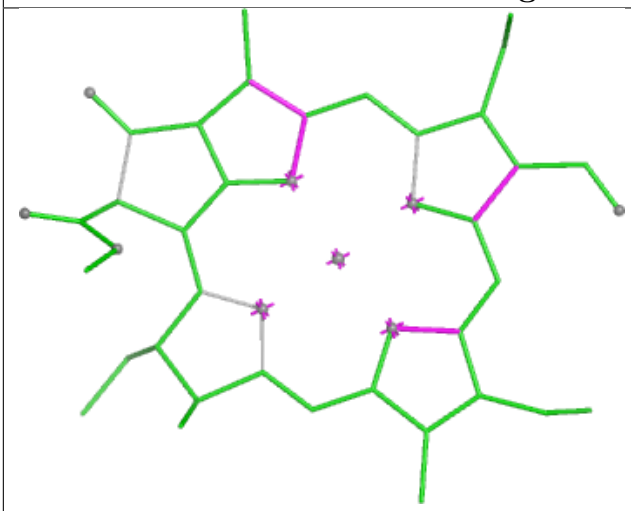


Torsions

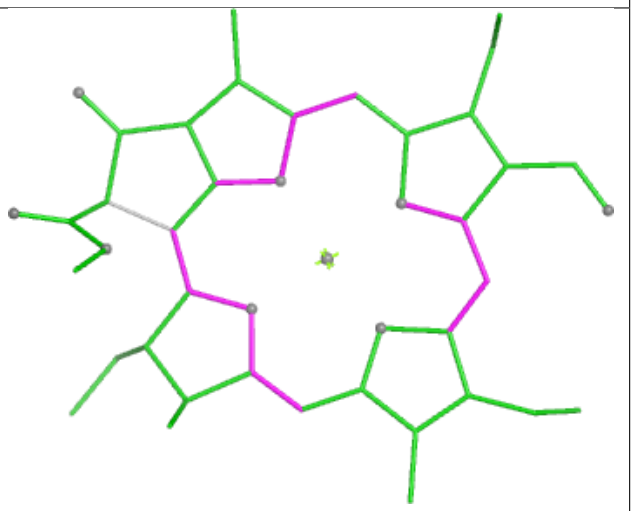


Rings

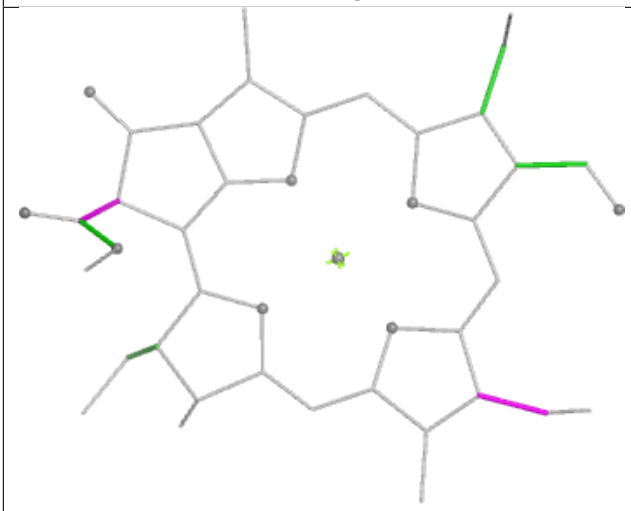
Ligand CHL 52 618



Bond lengths



Bond angles



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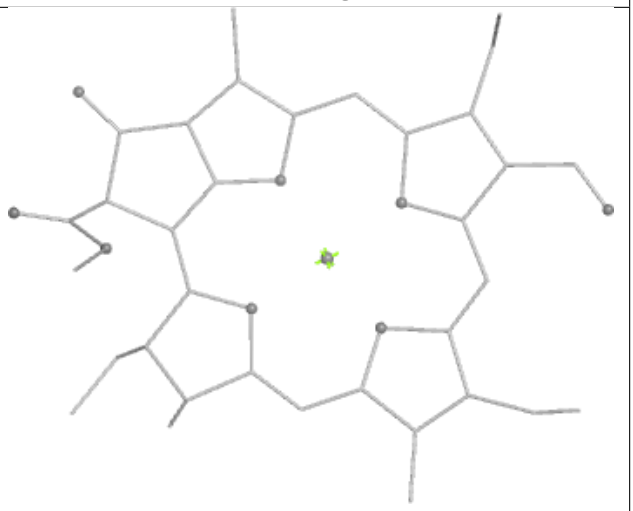
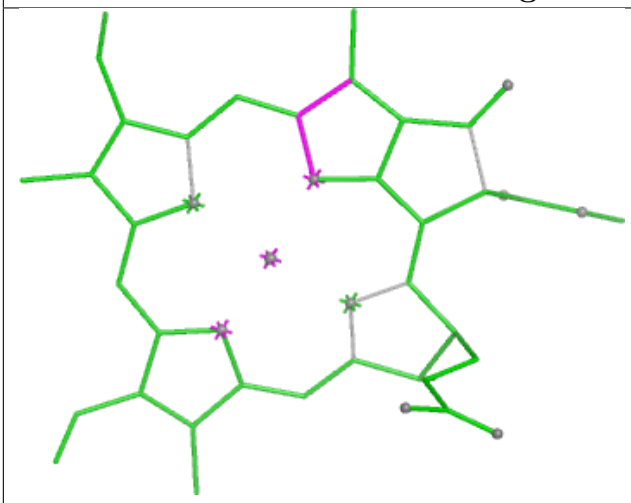
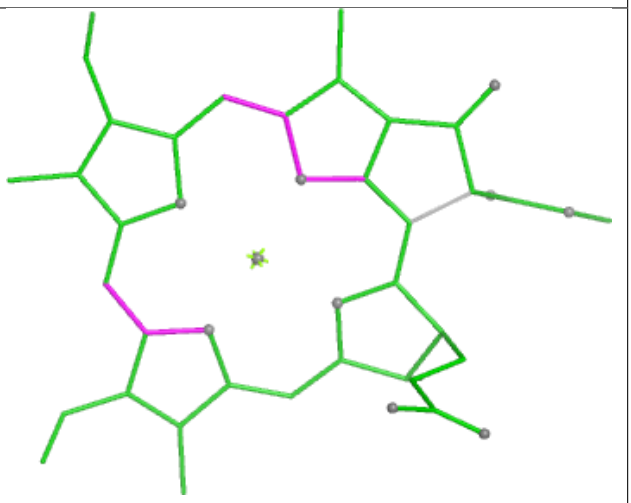


Rings

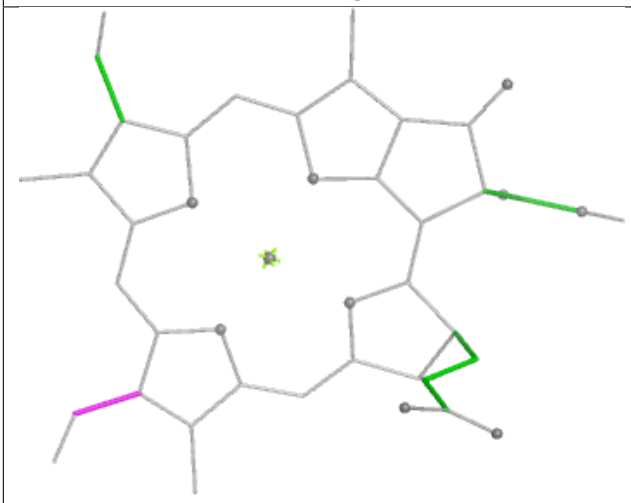
Ligand CLA 72 609



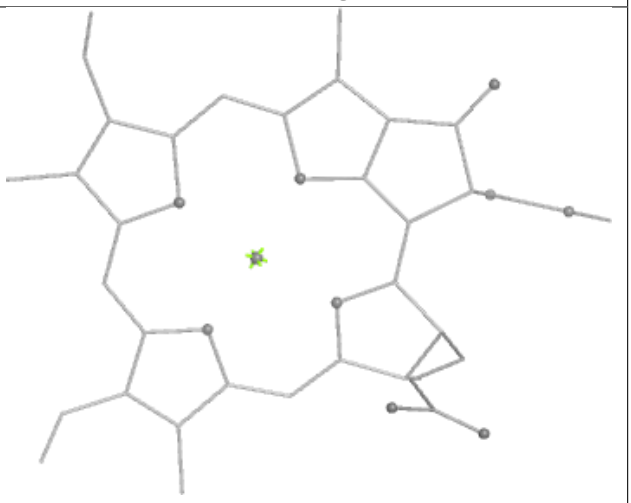
Bond lengths



Bond angles

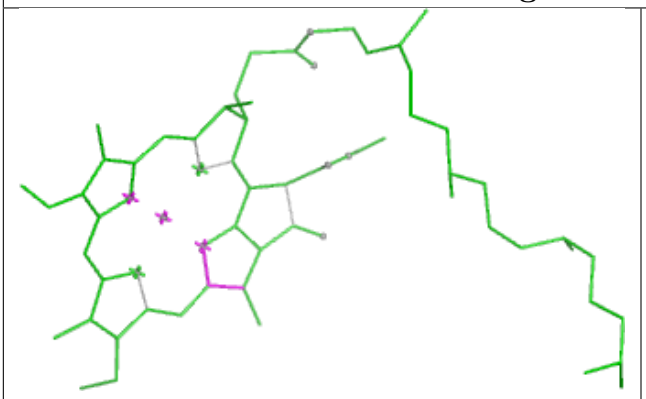


Torsions

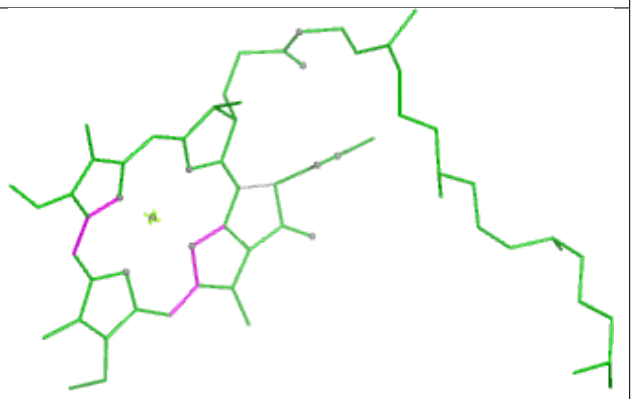


Rings

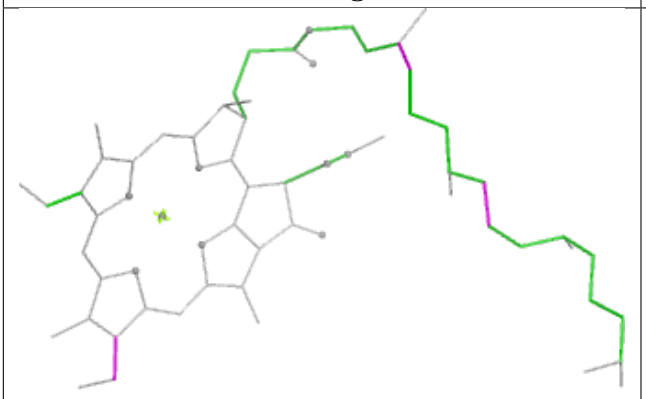
Ligand CLA 32 603



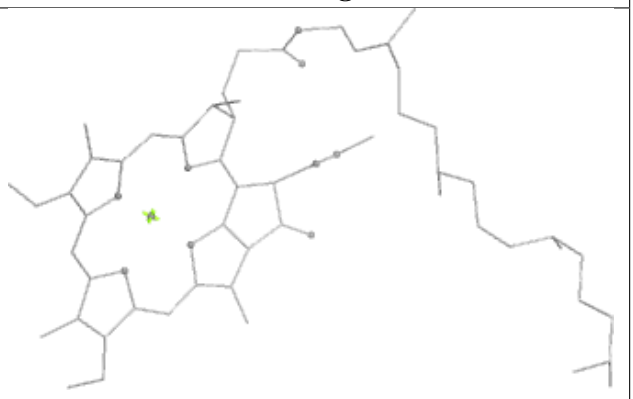
Bond lengths



Bond angles

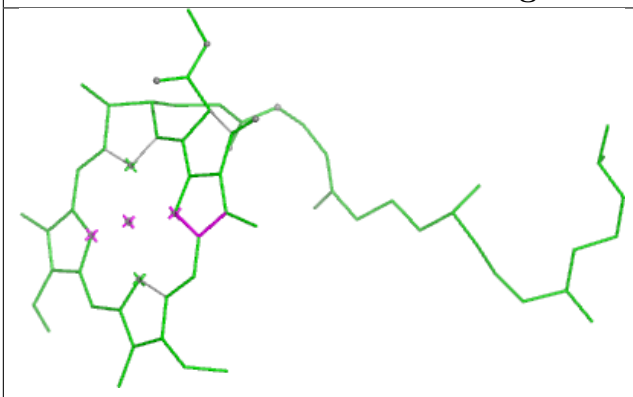


Torsions

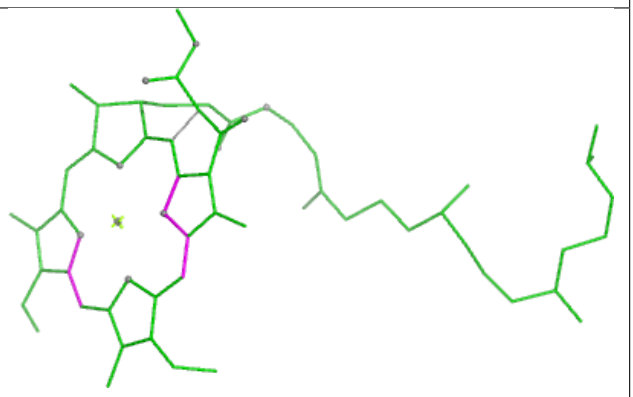


Rings

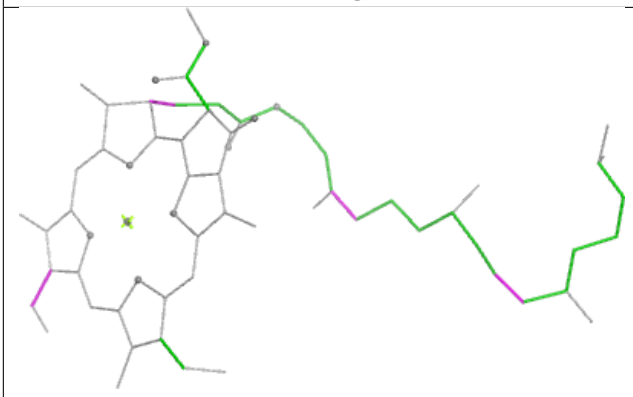
Ligand CLA 92 611



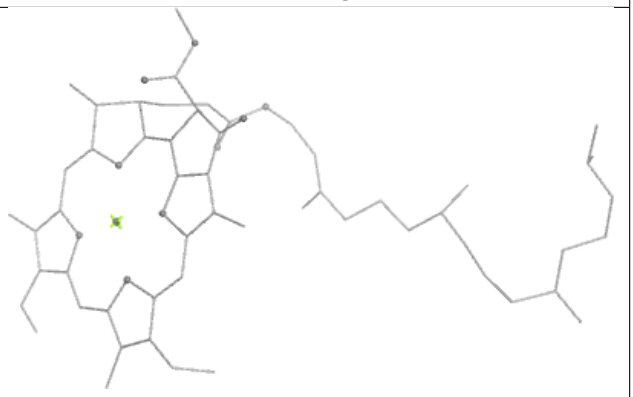
Bond lengths



Bond angles

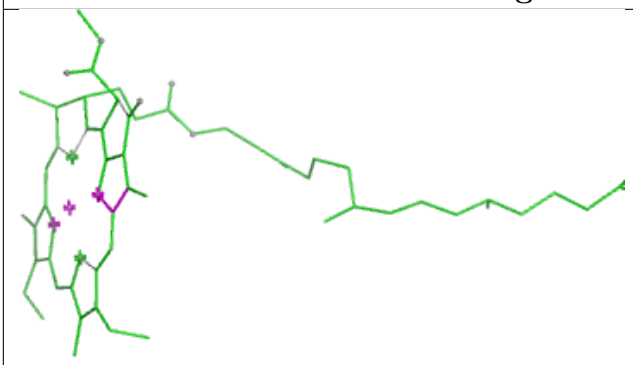


Torsions

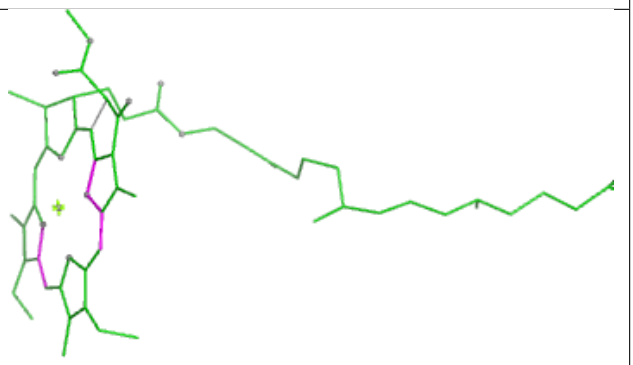


Rings

Ligand CLA B2 828



Bond lengths



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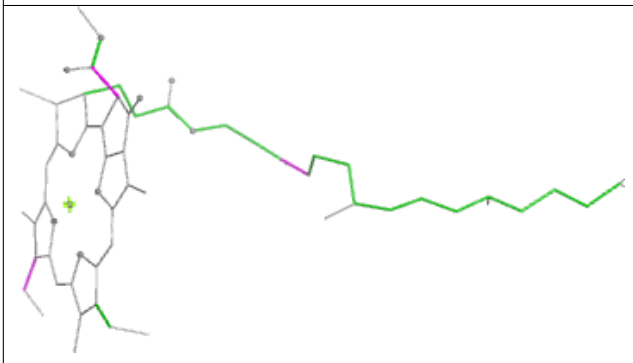
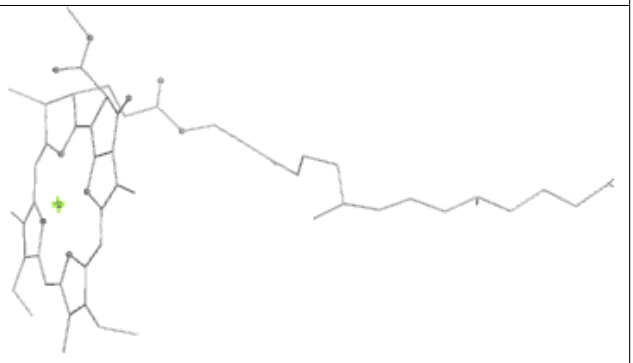
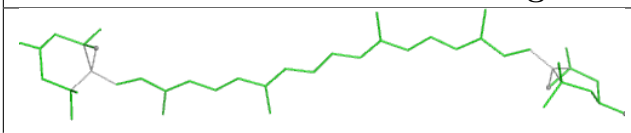


Torsions



Rings

Ligand XAT 7 622



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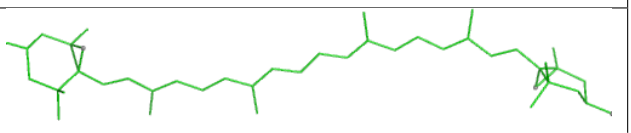

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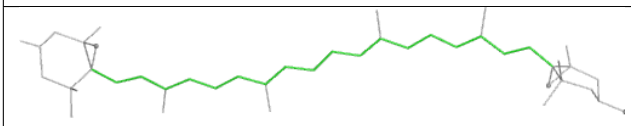

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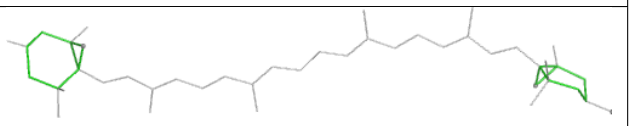
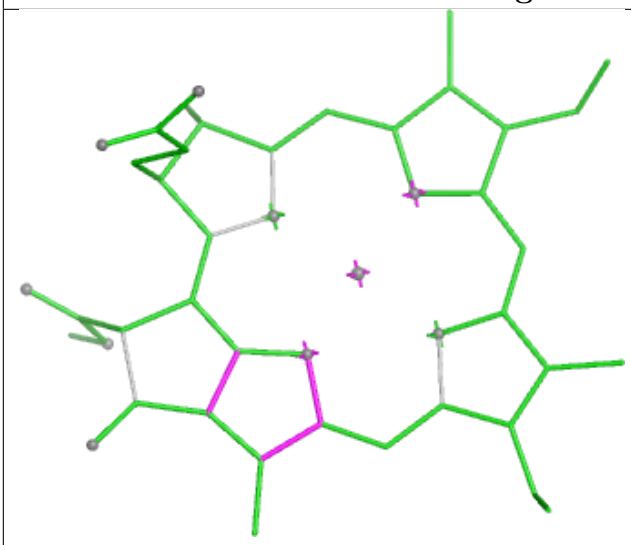


Rings

Ligand CLA B2 830



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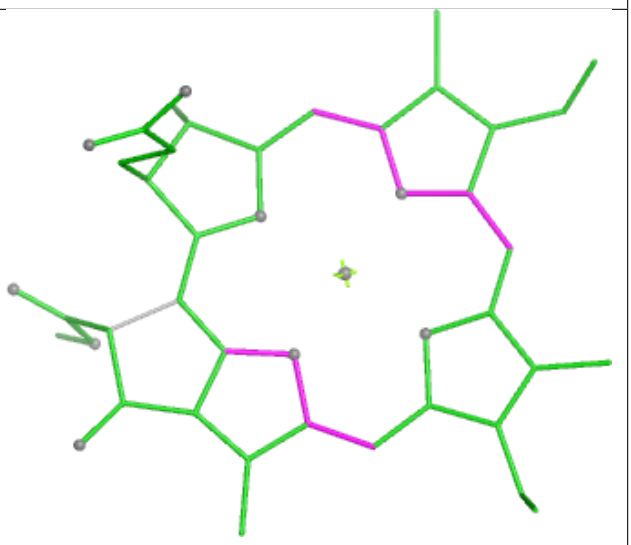

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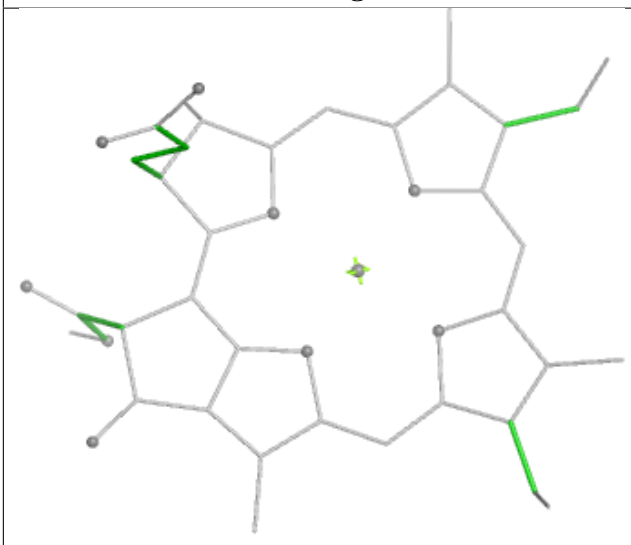

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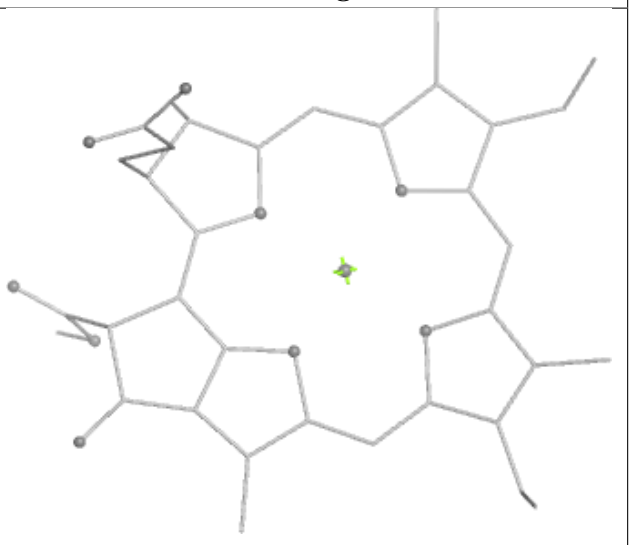
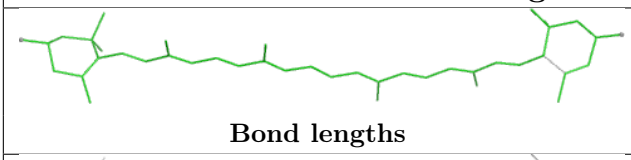


Rings

Ligand LUT 5 626



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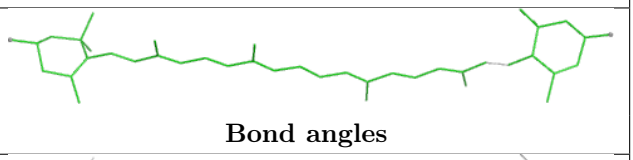

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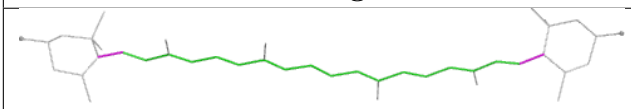
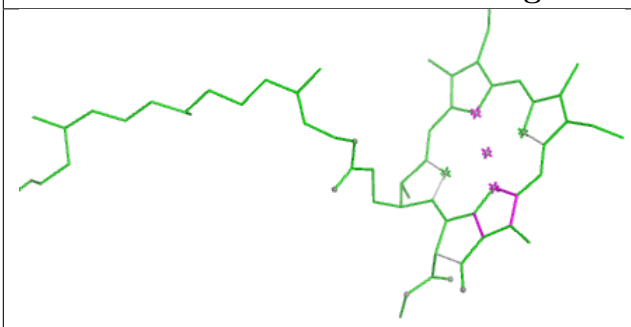


Torsions



Rings

Ligand CLA A 822



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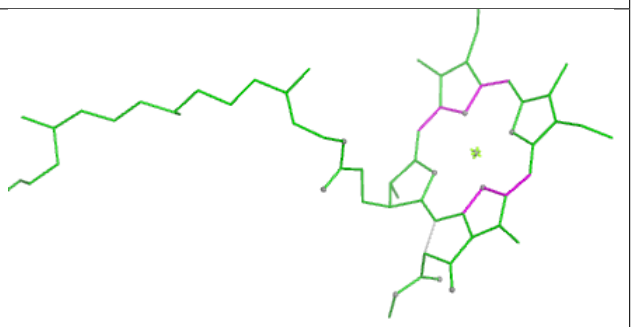

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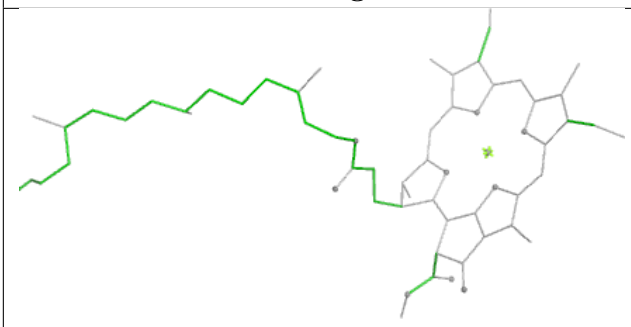
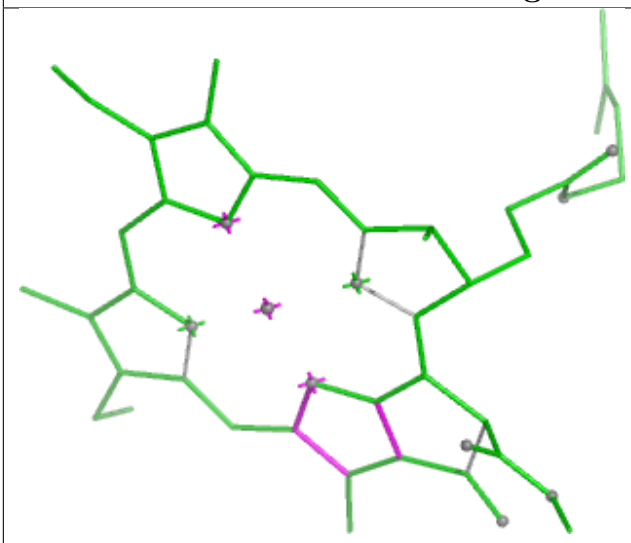


Torsions



Rings

Ligand CLA A 808



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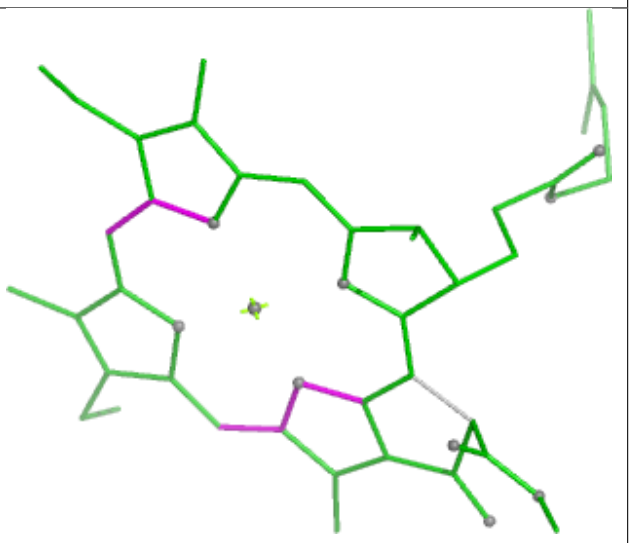

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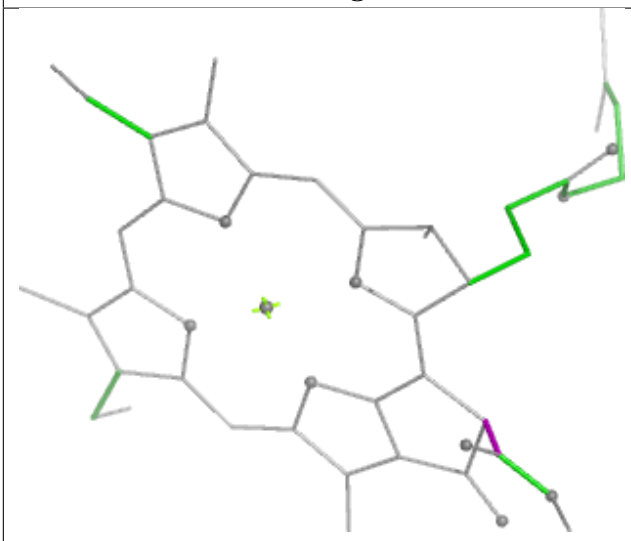

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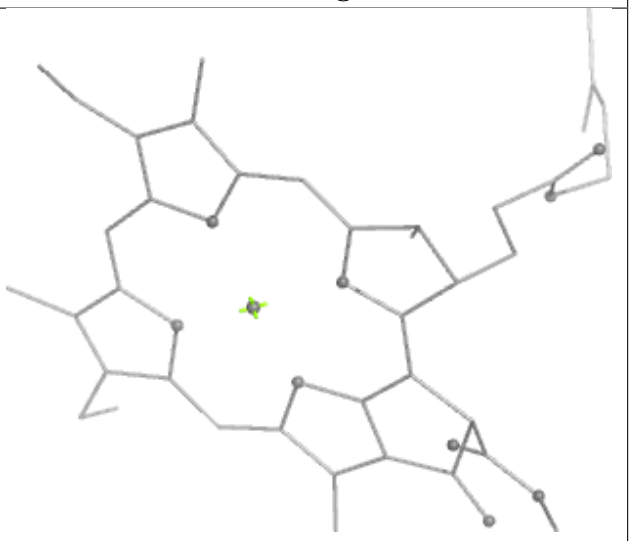
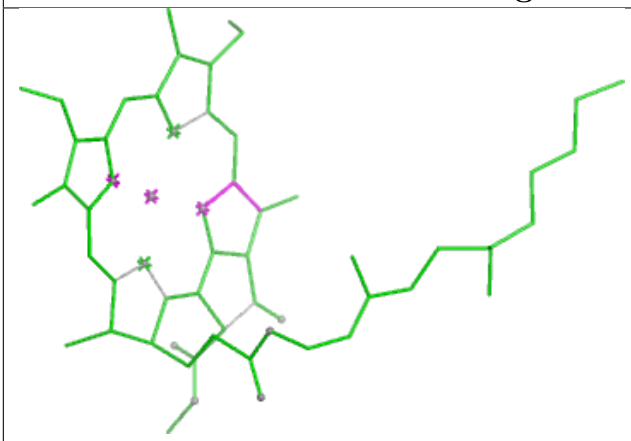


Rings

Ligand CLA B2 822



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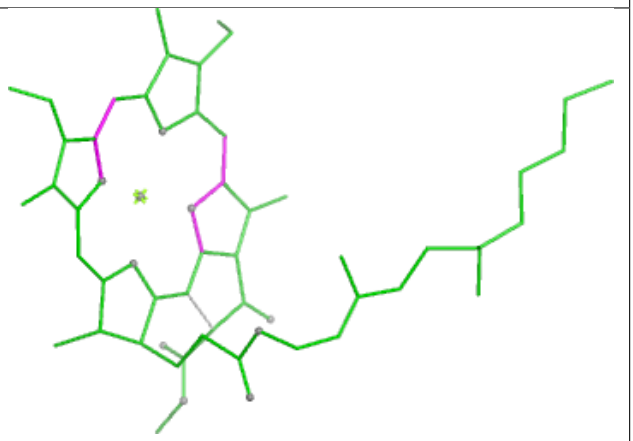

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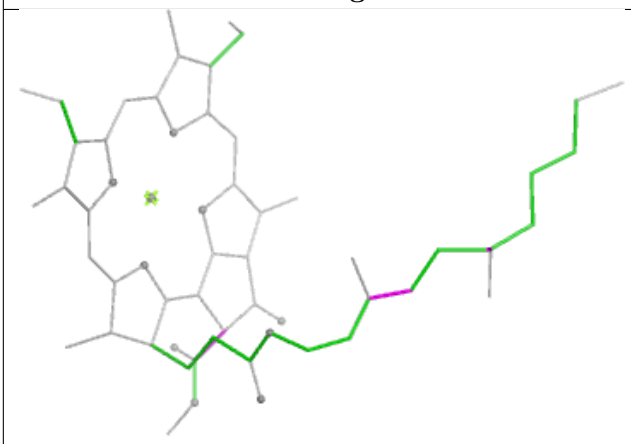

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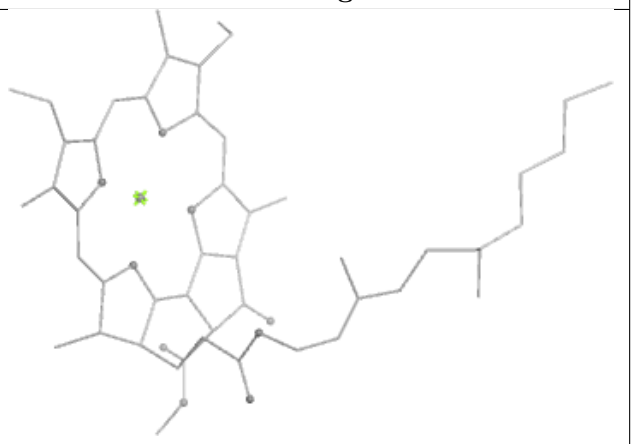
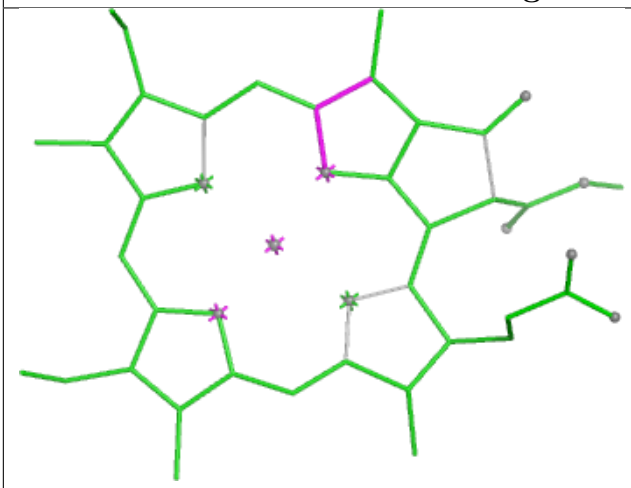


Rings

Ligand CLA K 201



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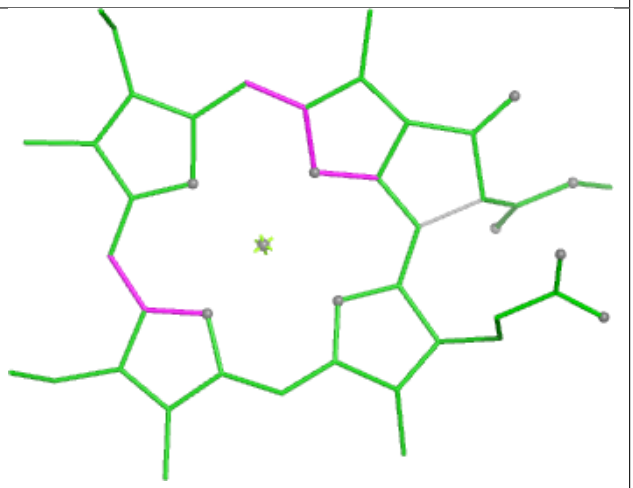

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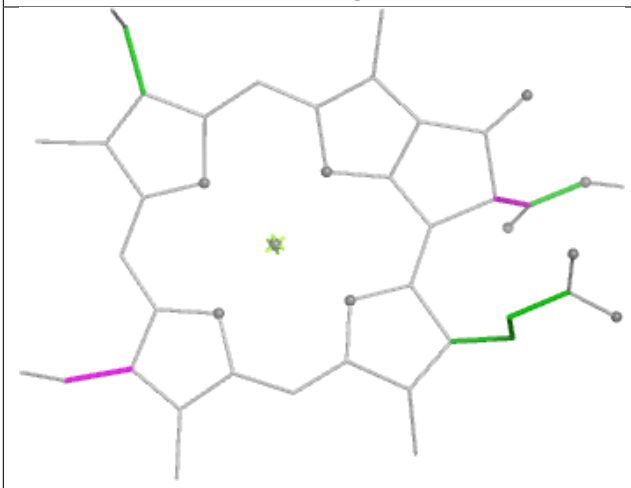

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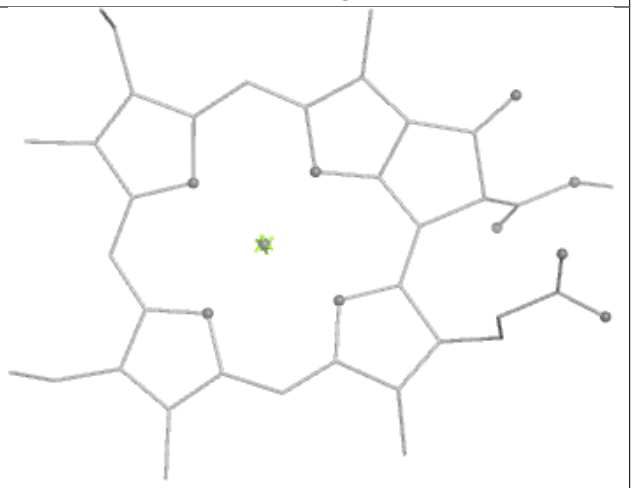
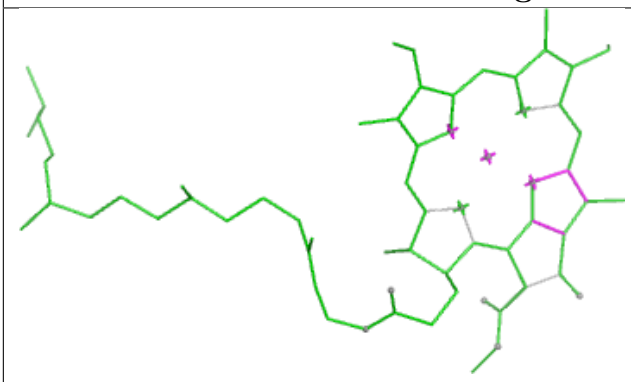


Rings

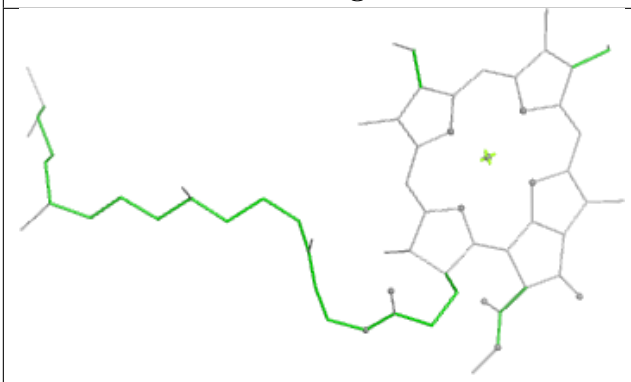
Ligand CLA A2 802



Bond lengths



Bond angles



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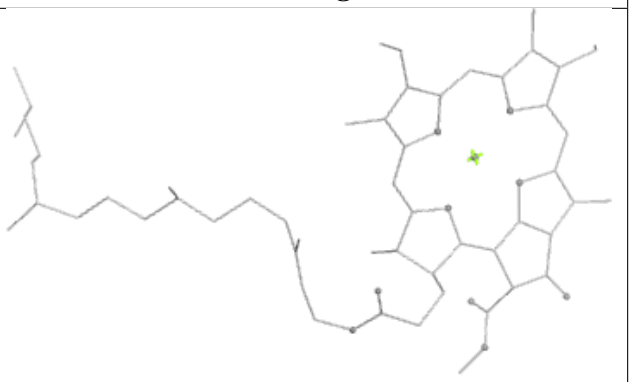

Rings

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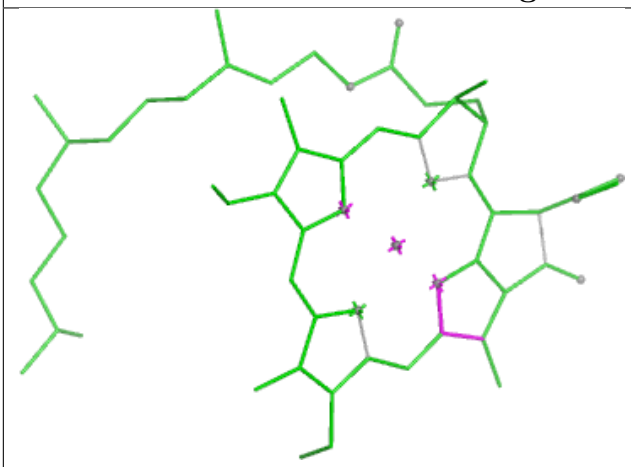

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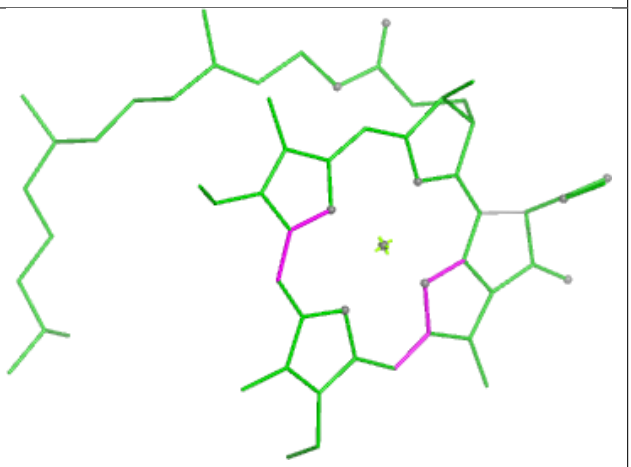
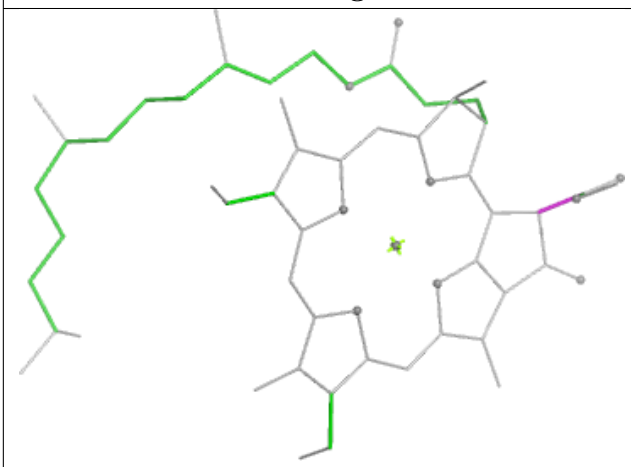


Bond angles



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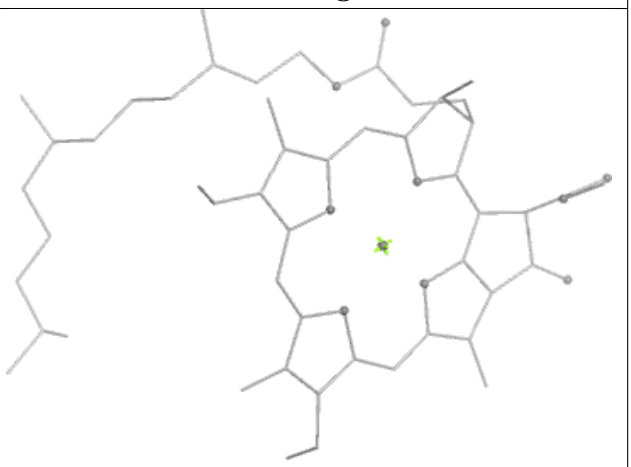
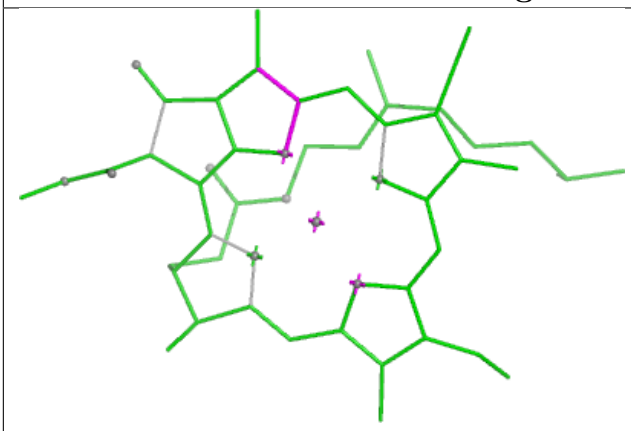


Rings

Ligand CLA B2 807



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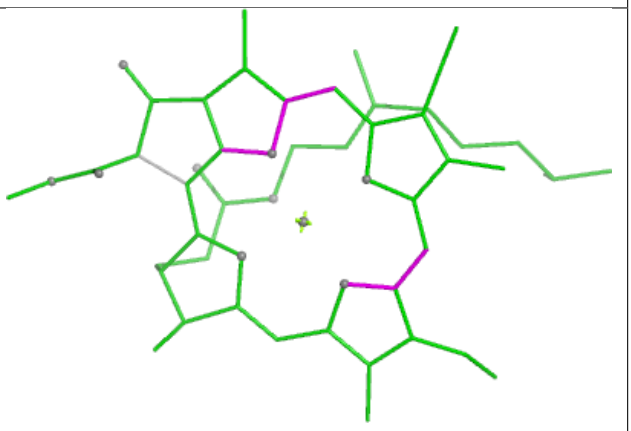

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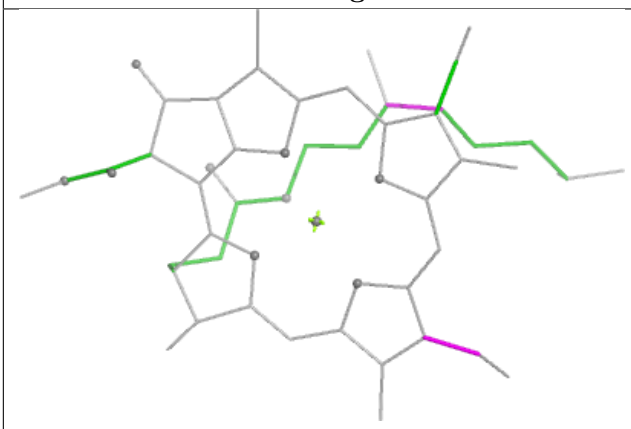

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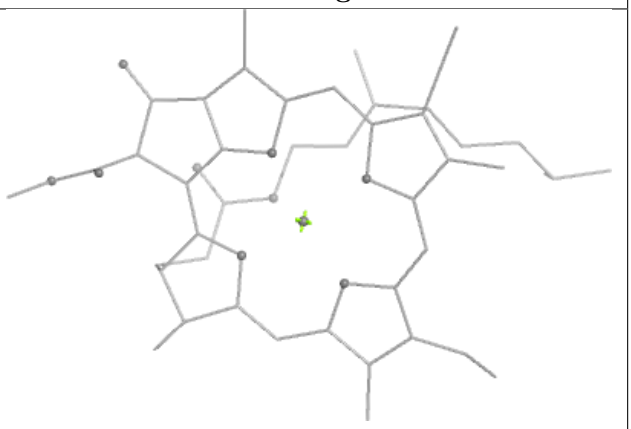
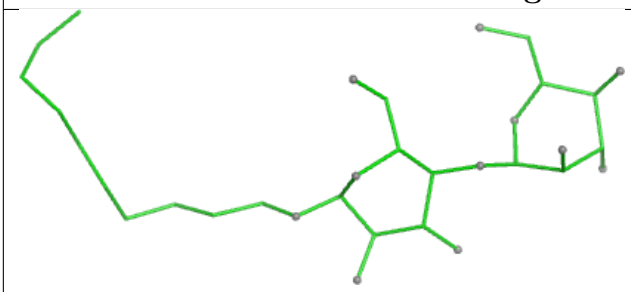


Rings

Ligand LMU 4 625



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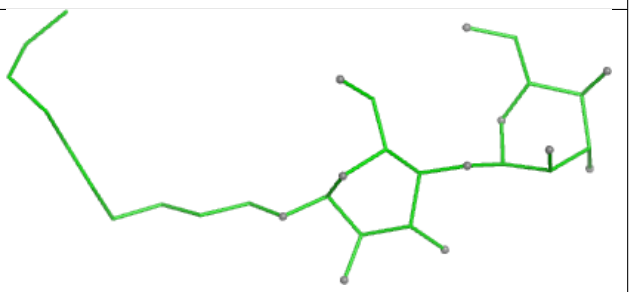
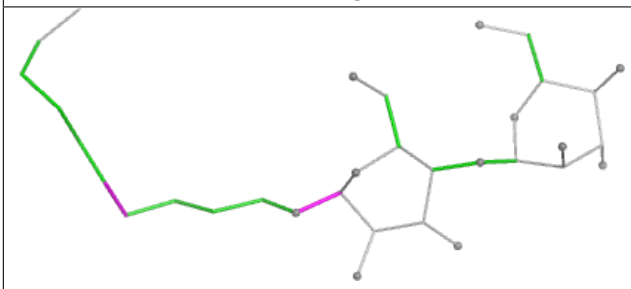


Bond angles



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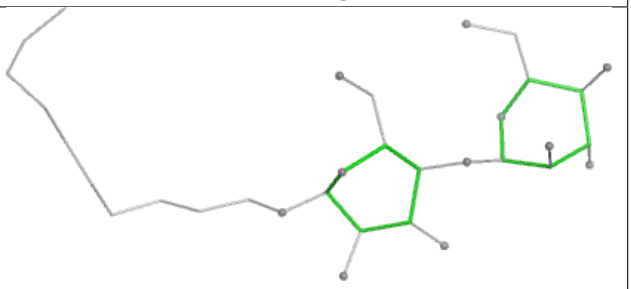
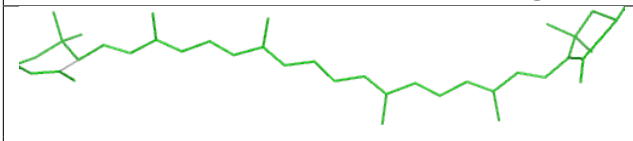


Rings

Ligand LUT 1 617



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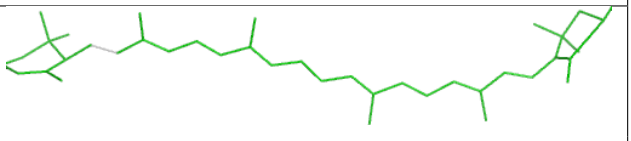
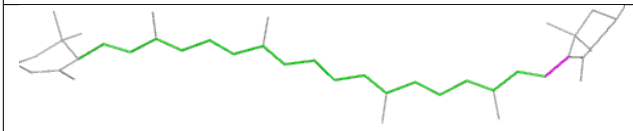


Bond angles



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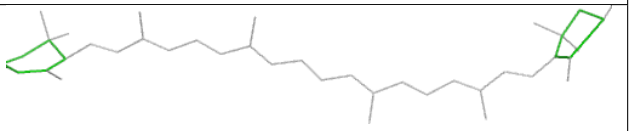

Rings

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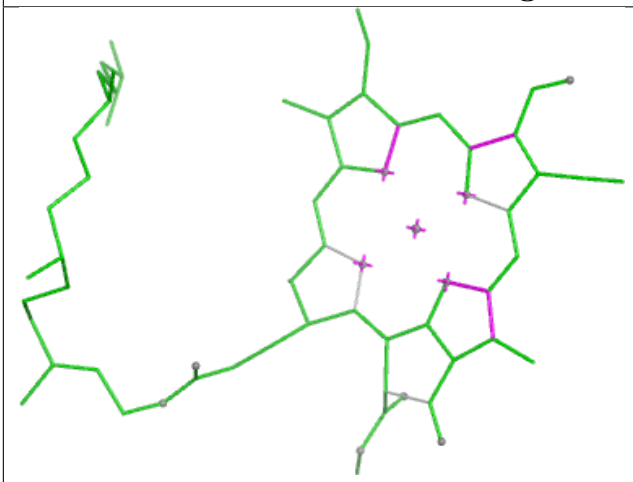

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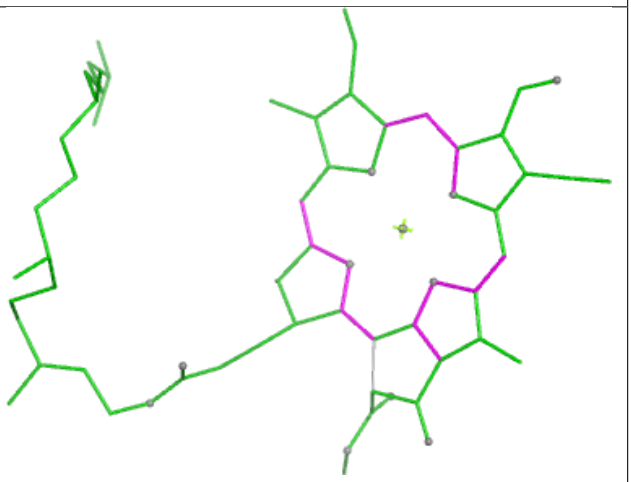
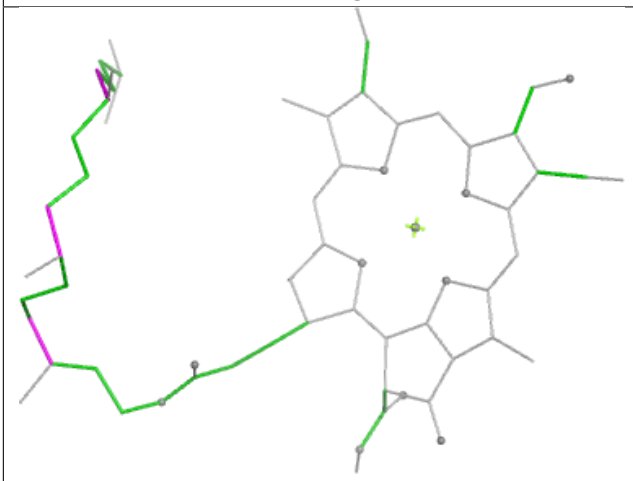


Bond angles

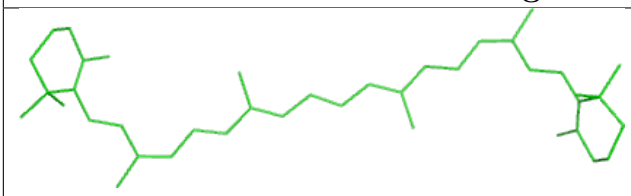


Torsions



Rings

Ligand BCR B 845



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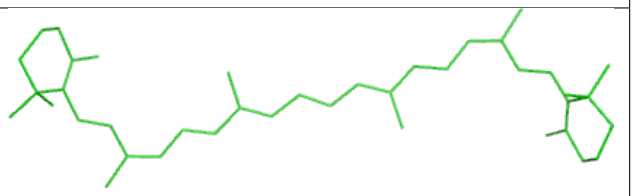
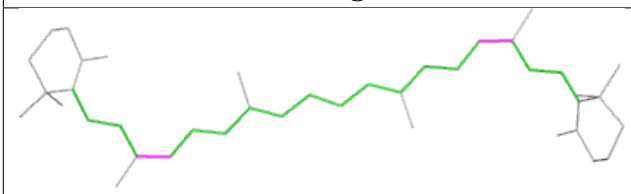


Bond angles



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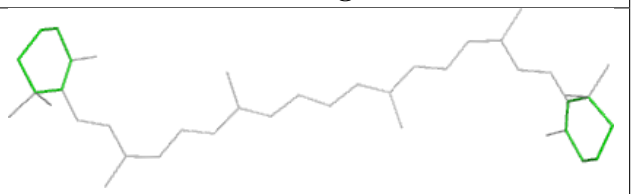
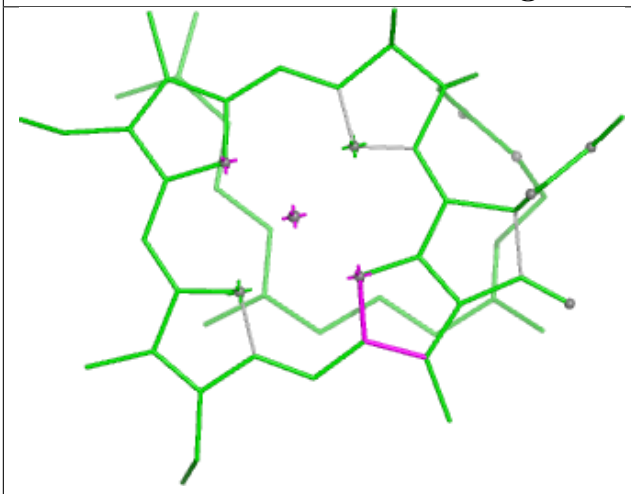


Rings

Ligand CLA 12 614



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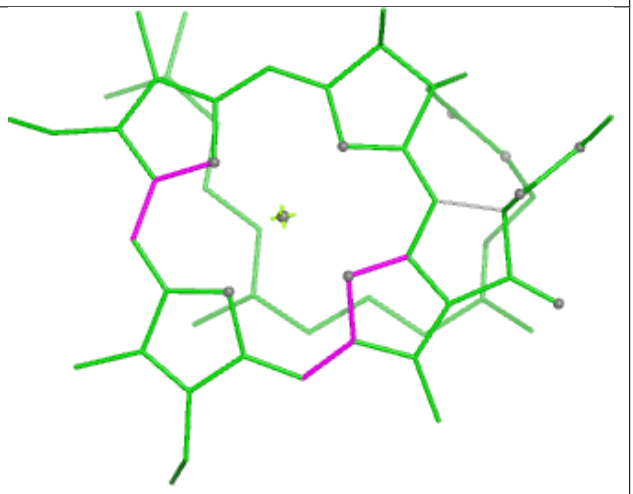
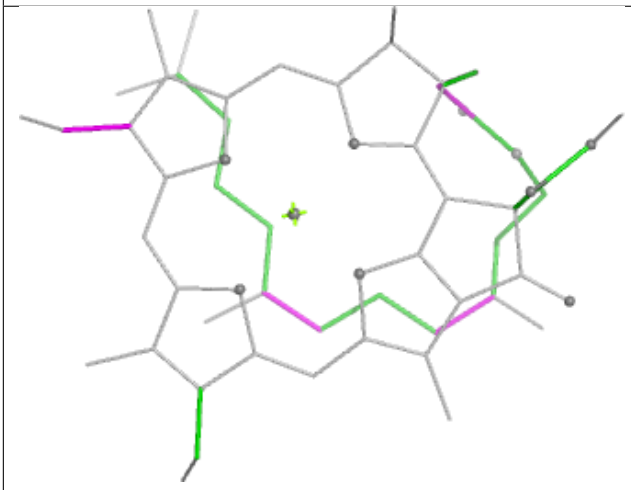
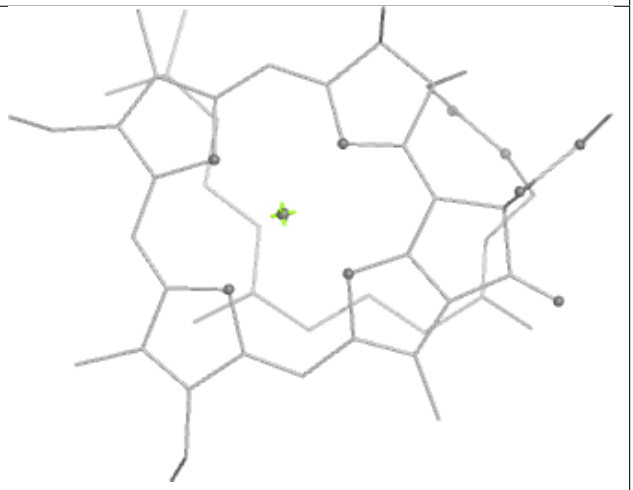


Bond angles

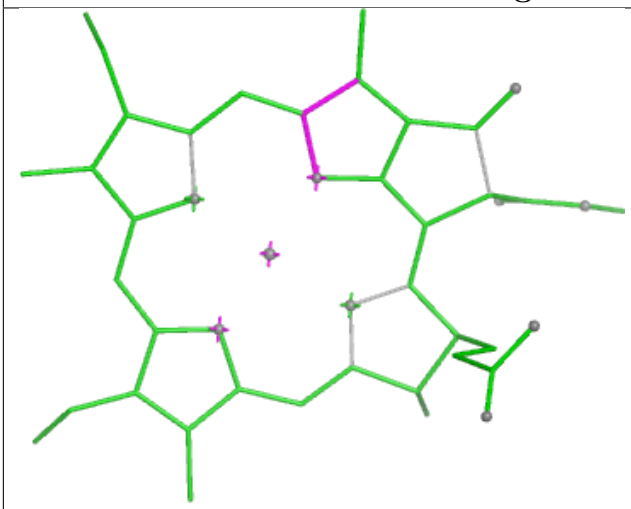


Torsions



Rings

Ligand CLA K2 206



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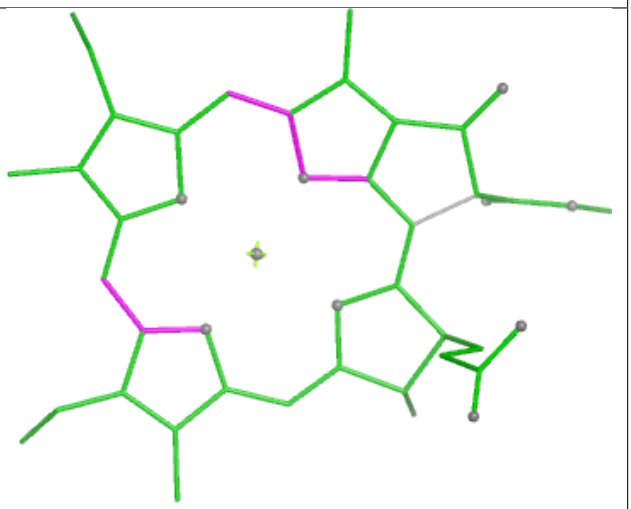
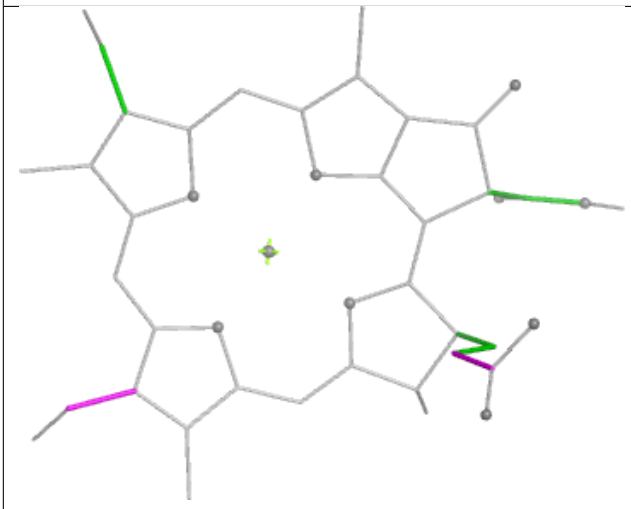


Bond angles



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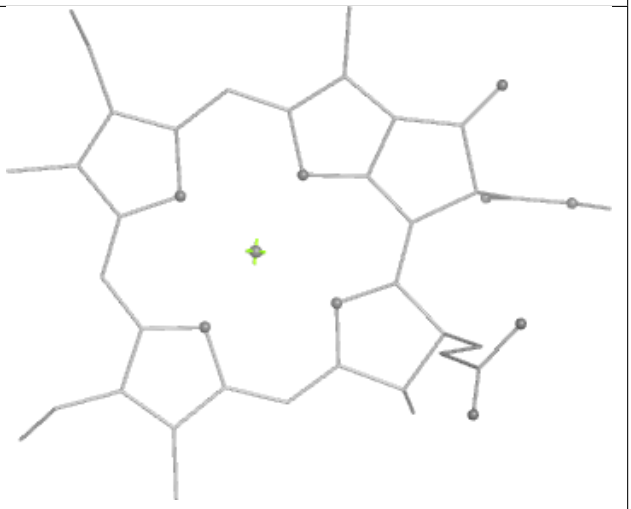
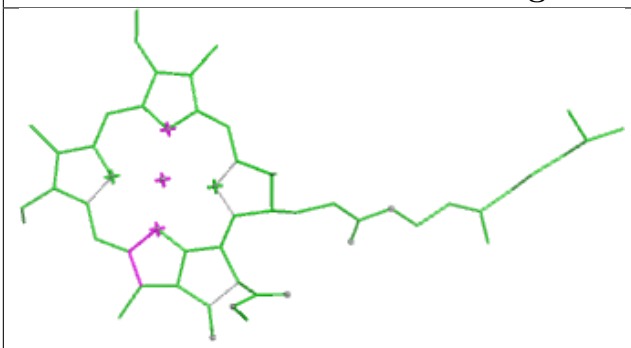


Rings

Ligand CLA 6 622



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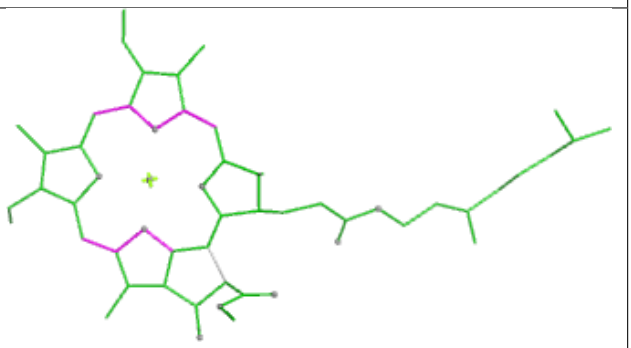
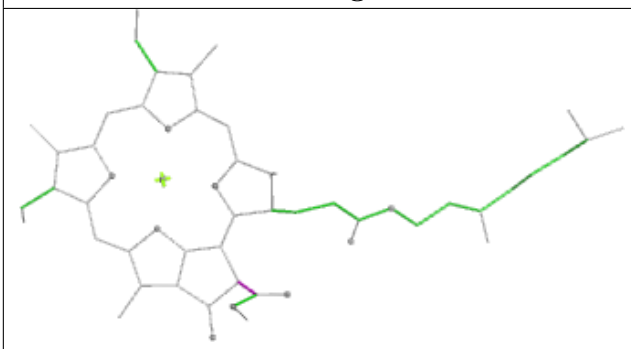


Bond angles



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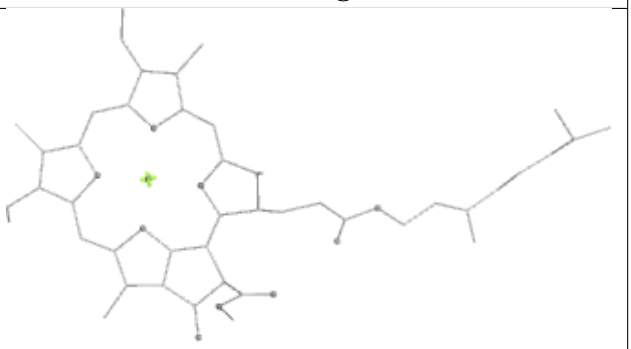
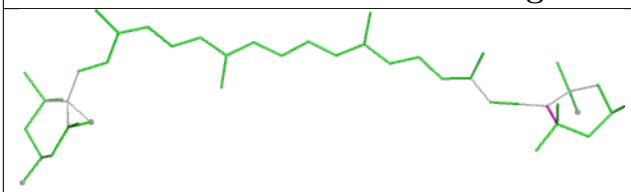


Rings

Ligand NEX 5 625



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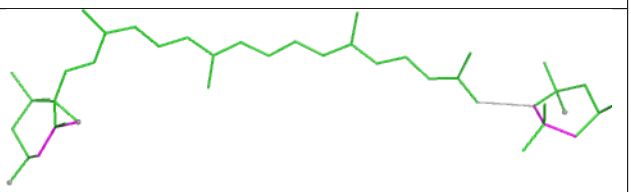

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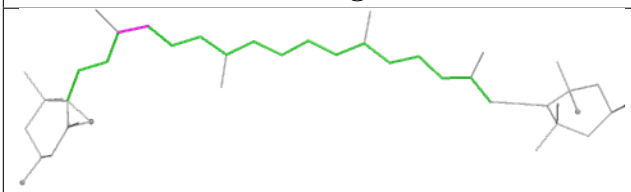

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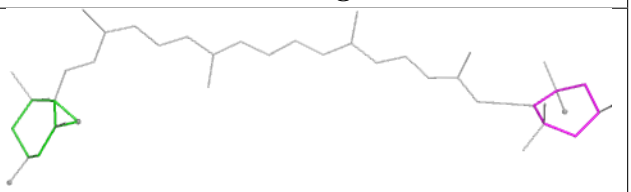
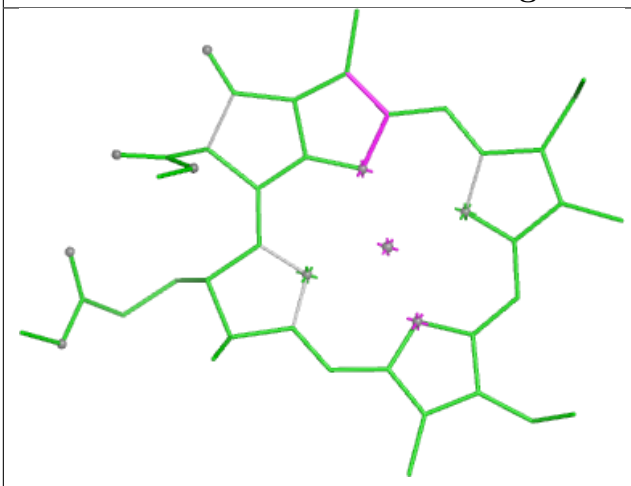


Rings

Ligand CLA 32 612



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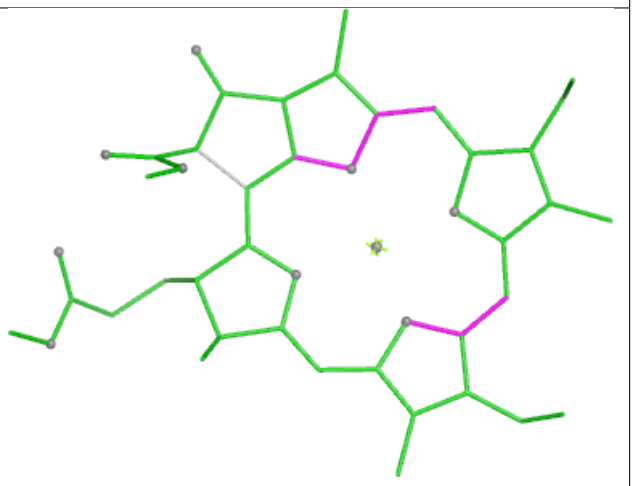

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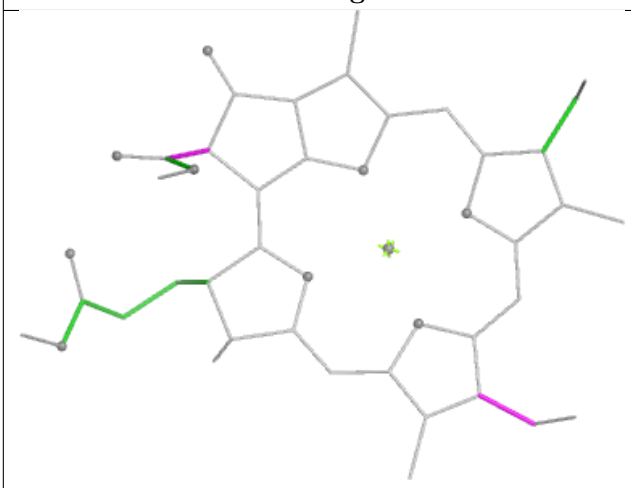

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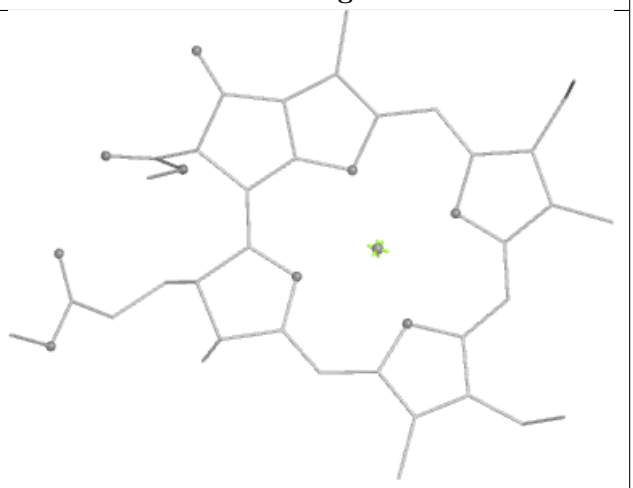
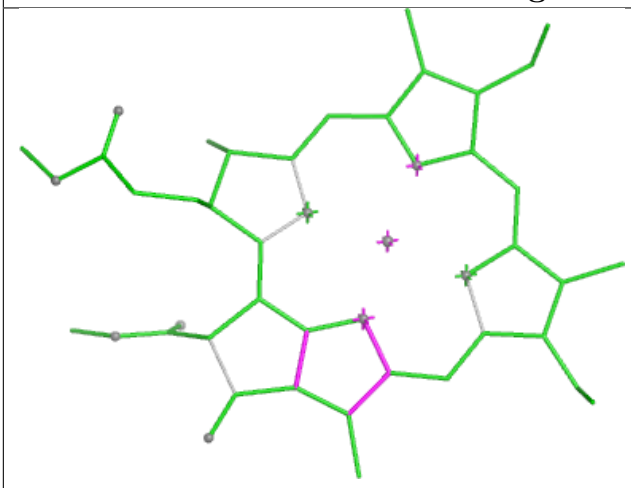


Rings

Ligand CLA 7 616



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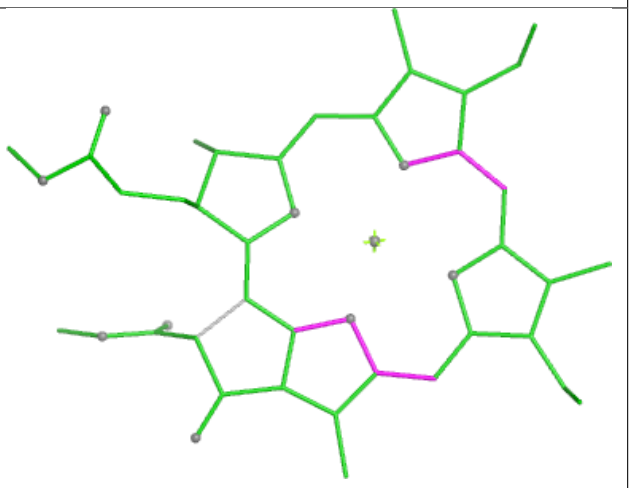

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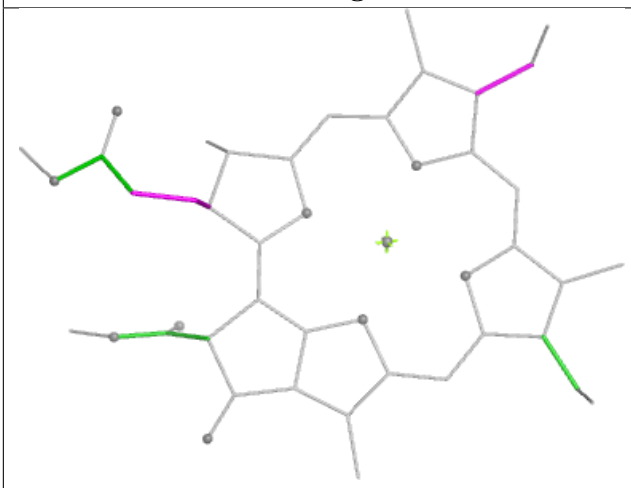

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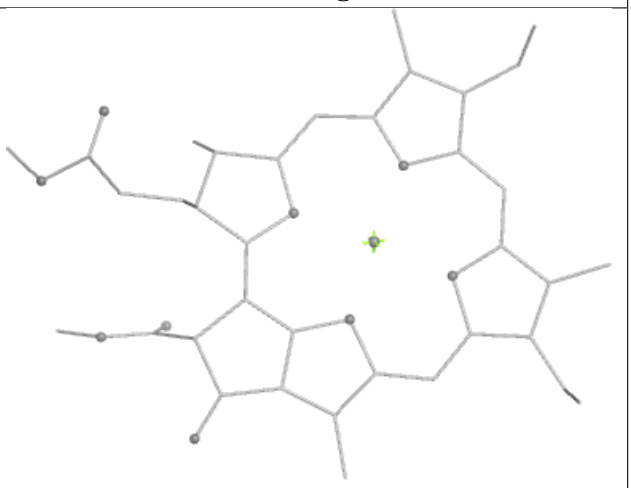
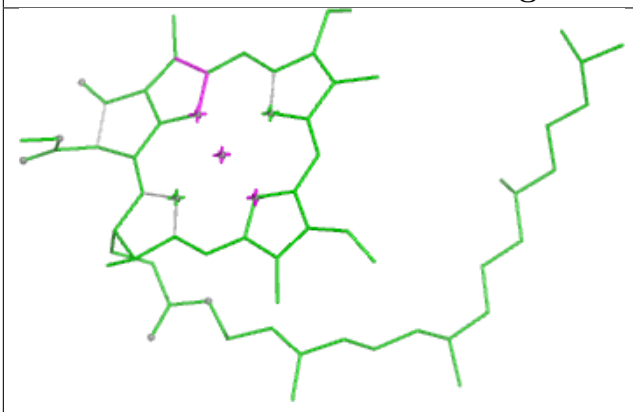


Rings

Ligand CLA 52 602



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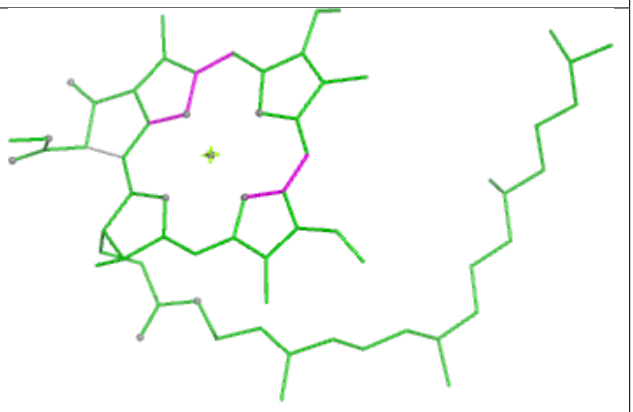

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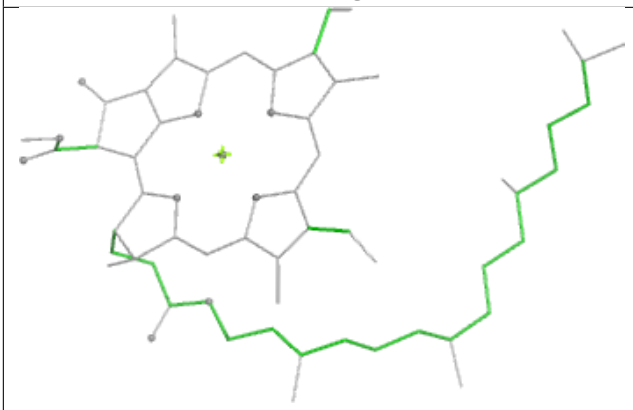

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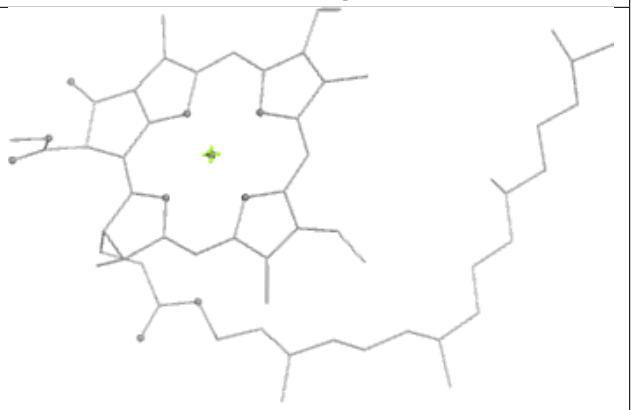
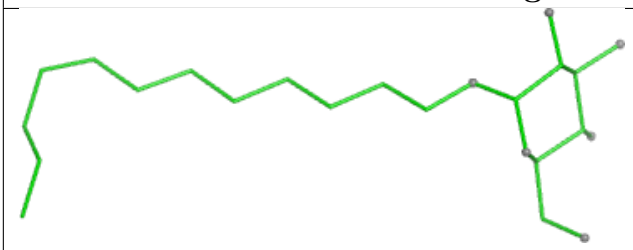


Rings

Ligand LMU 1 623



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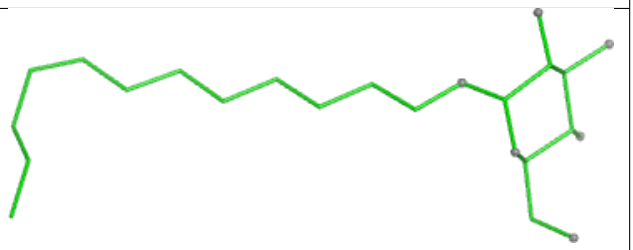

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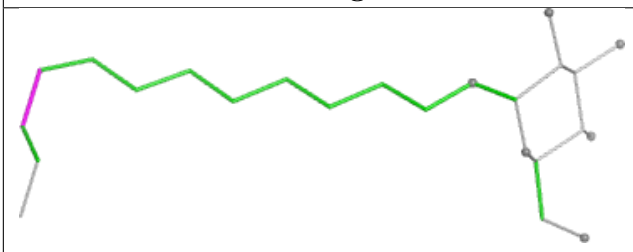

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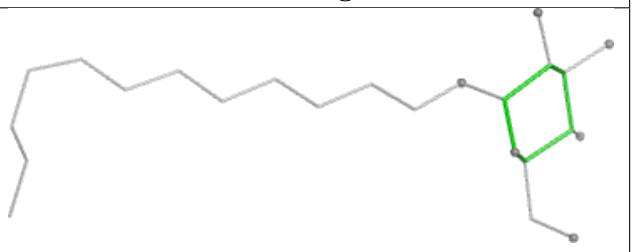
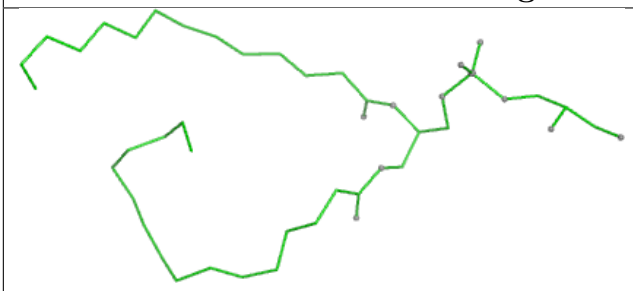


Rings

Ligand LHG 32 623



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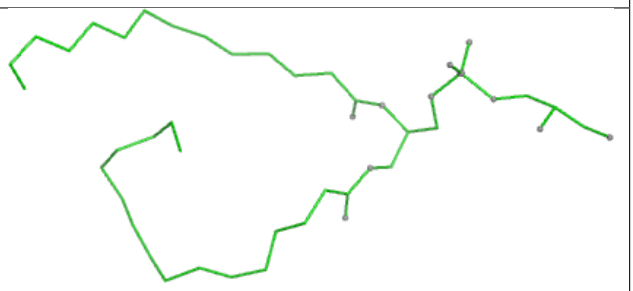
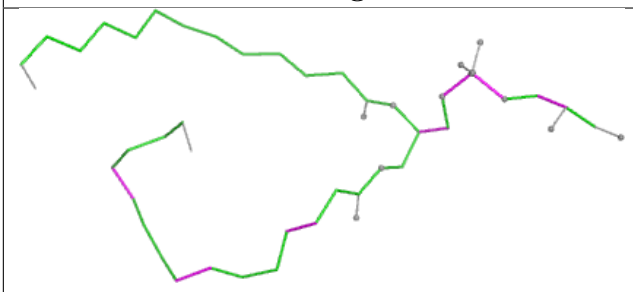


Bond angles



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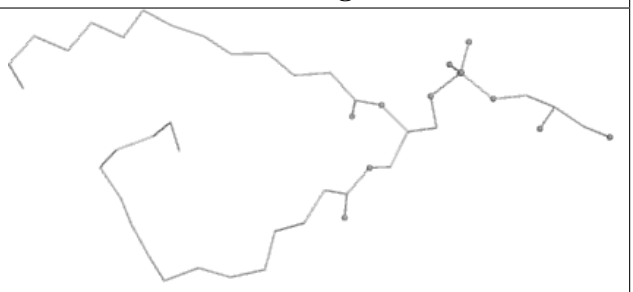
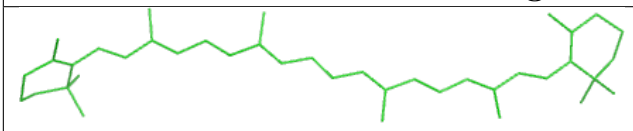


Rings

Ligand BCR J 102



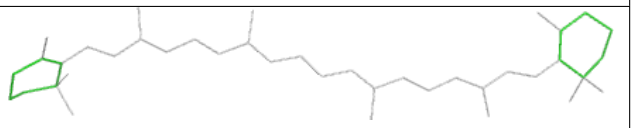
Bond lengths



Bond angles

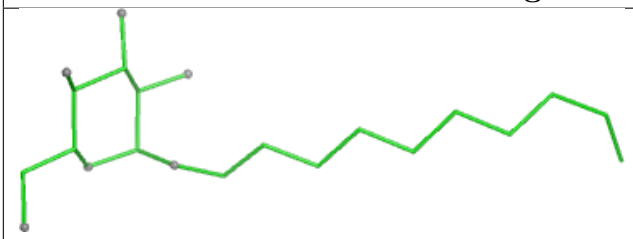


Torsions



Rings

Ligand LMU 1 627



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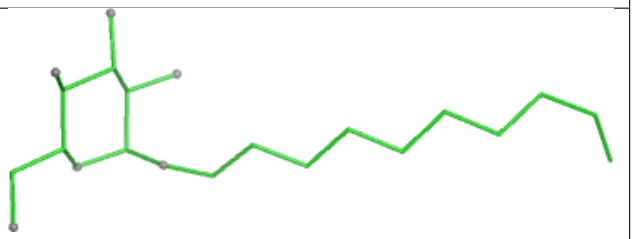
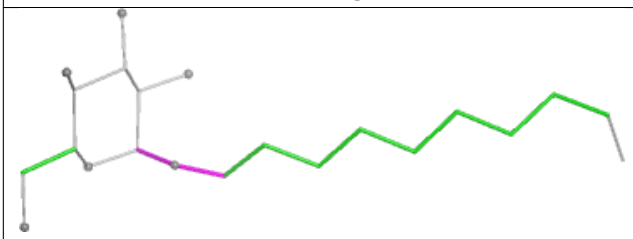


Bond angles



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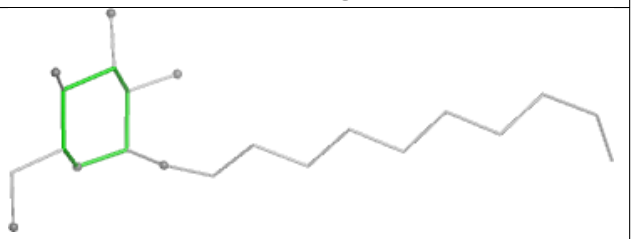
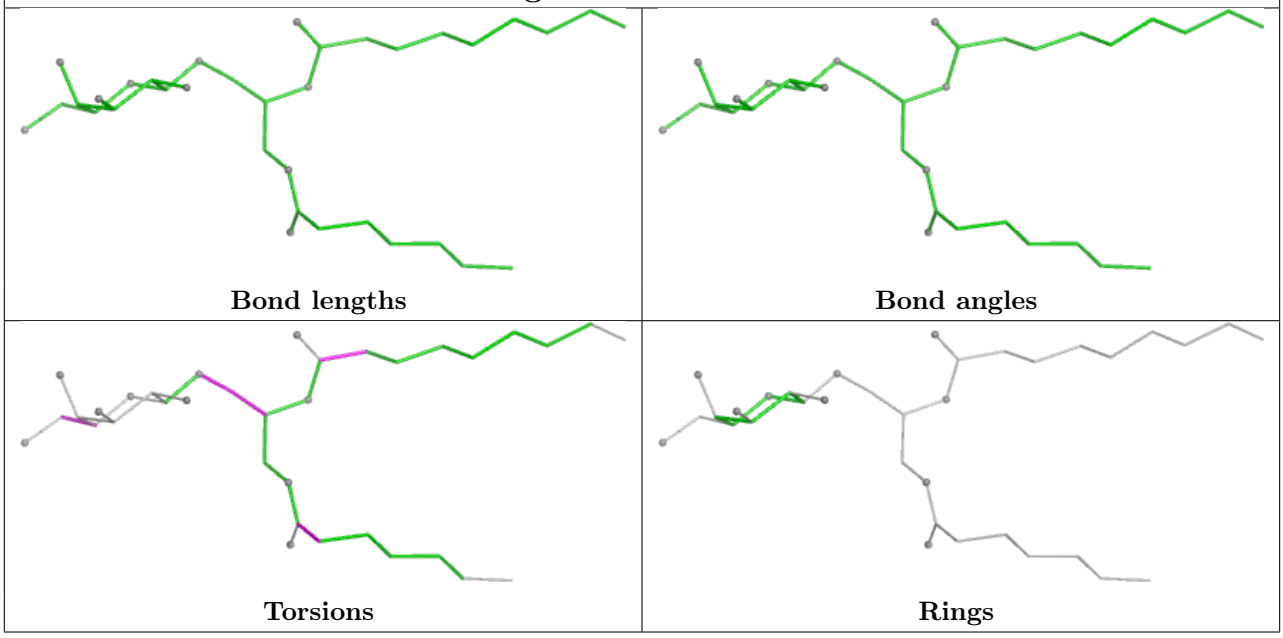
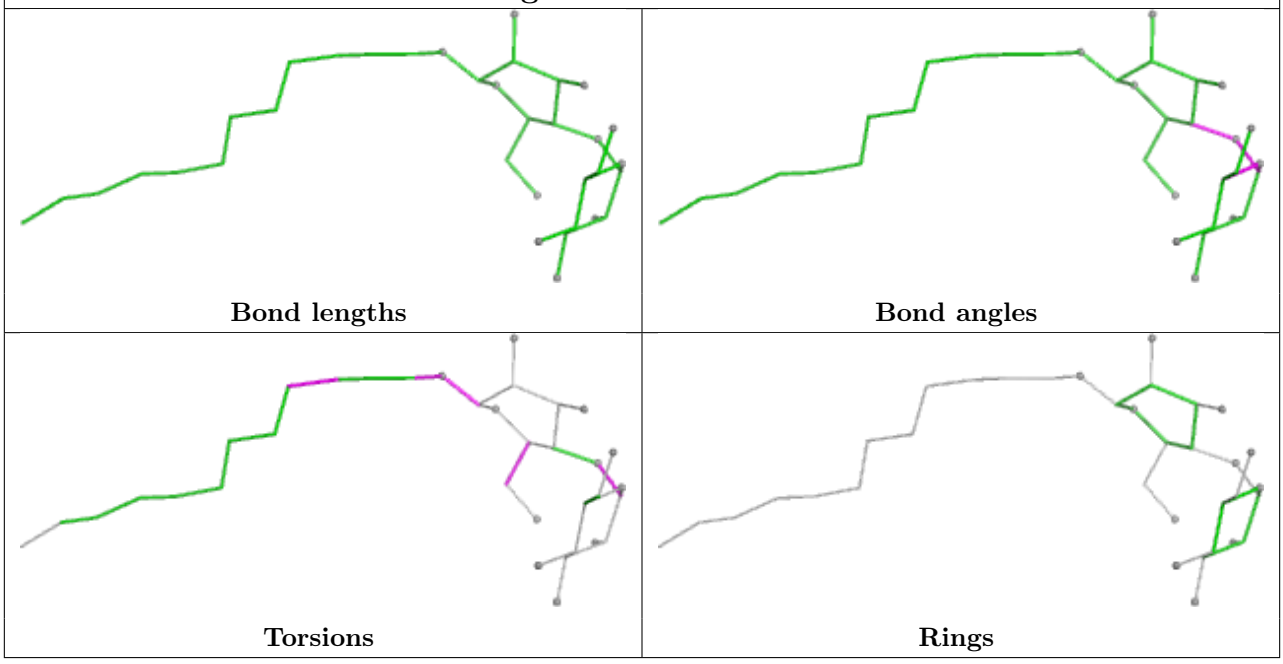


Rings

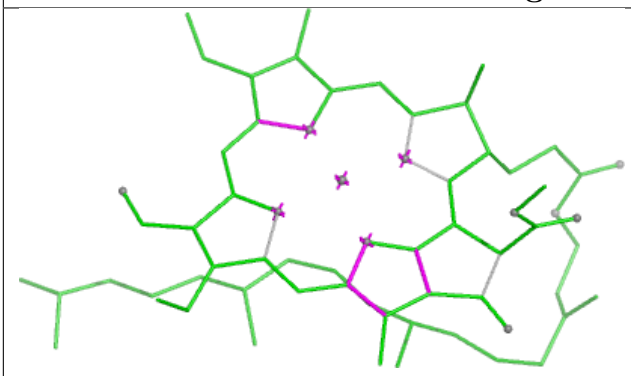
Ligand LMG J 104



Ligand LMU B 853



Ligand CHL Z 607



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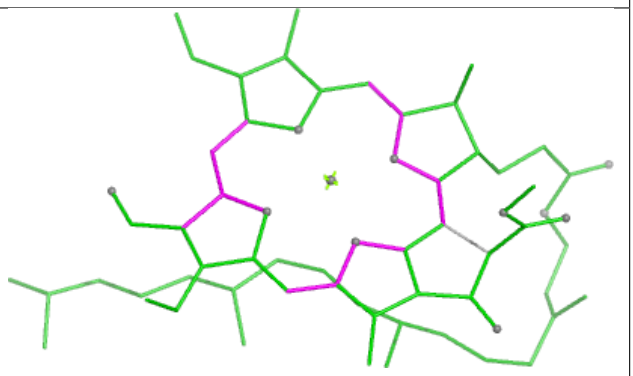
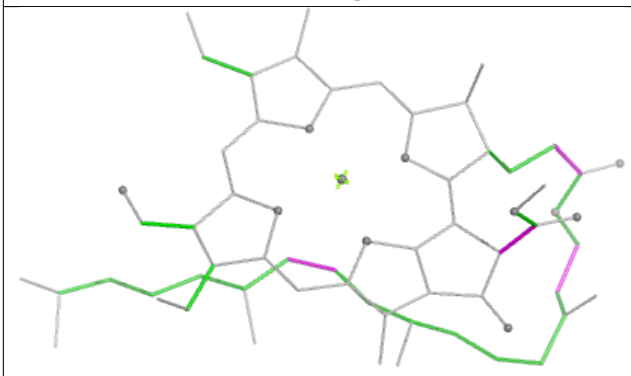


Bond angles



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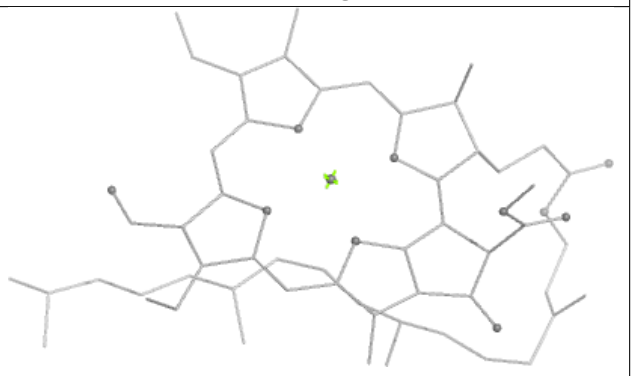
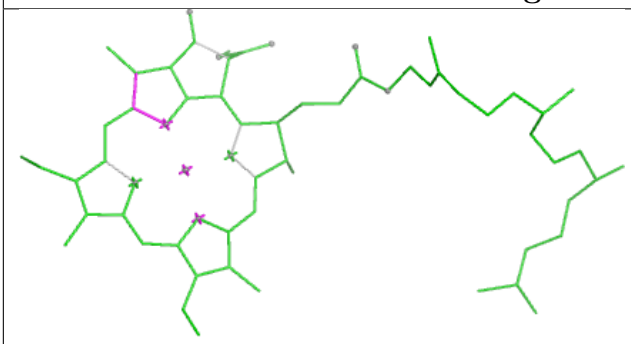


Rings

Ligand CLA A 828



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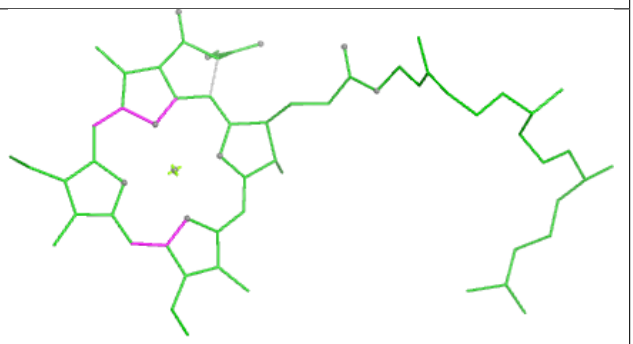
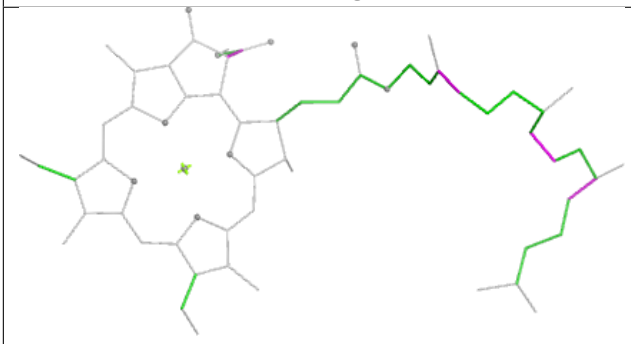


Bond angles



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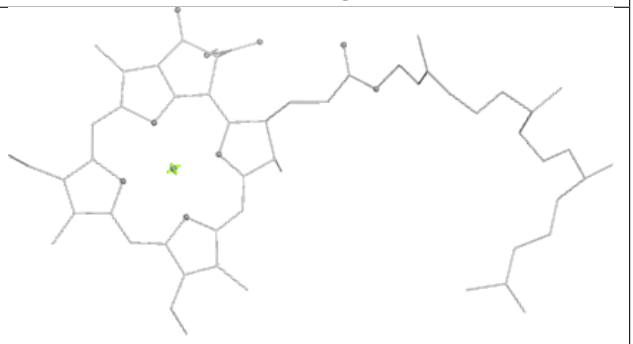
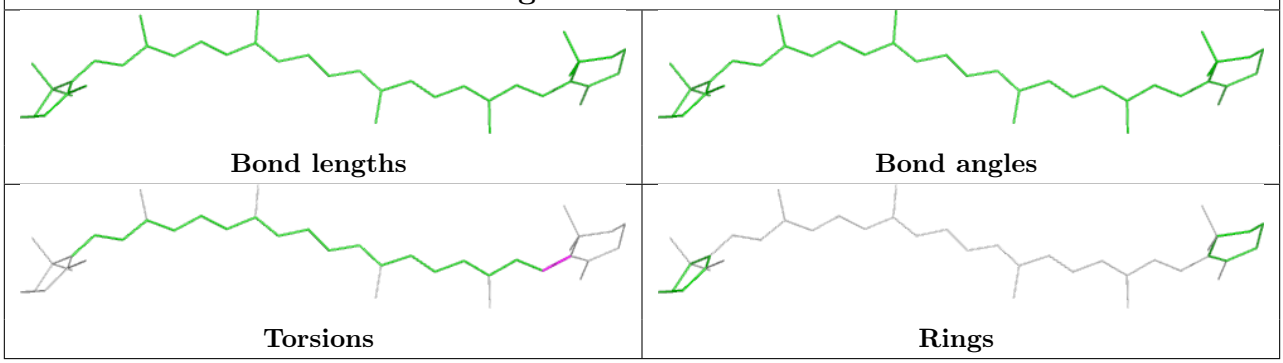
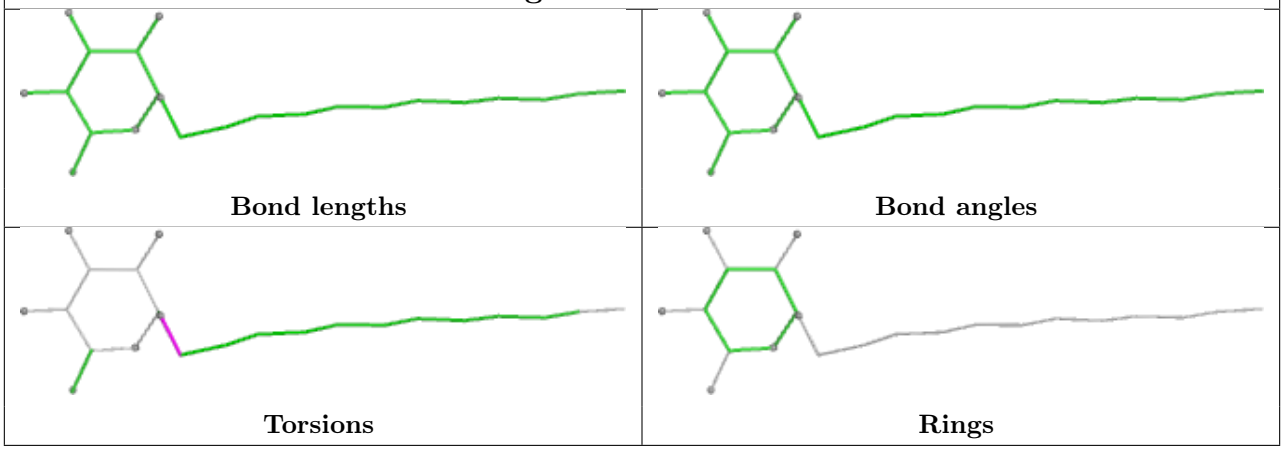


Rings

Ligand BCR 32 719



Ligand LMU 8 624



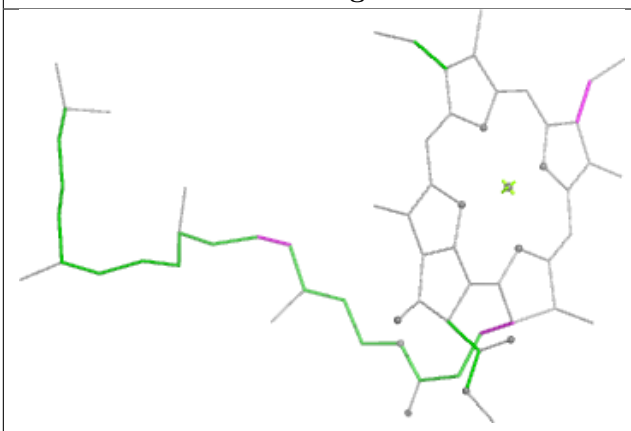
Ligand CLA 3 611



Bond lengths



Bond angles



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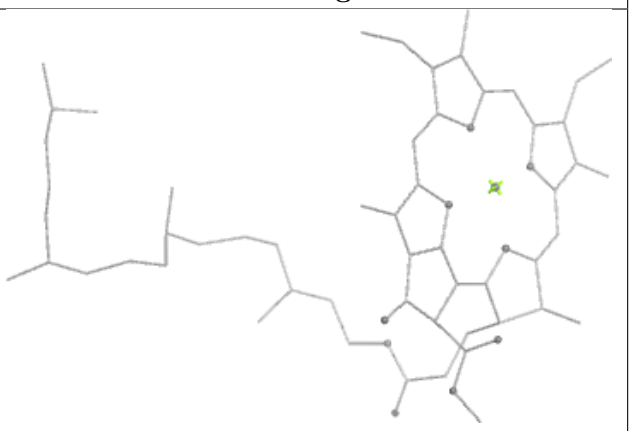
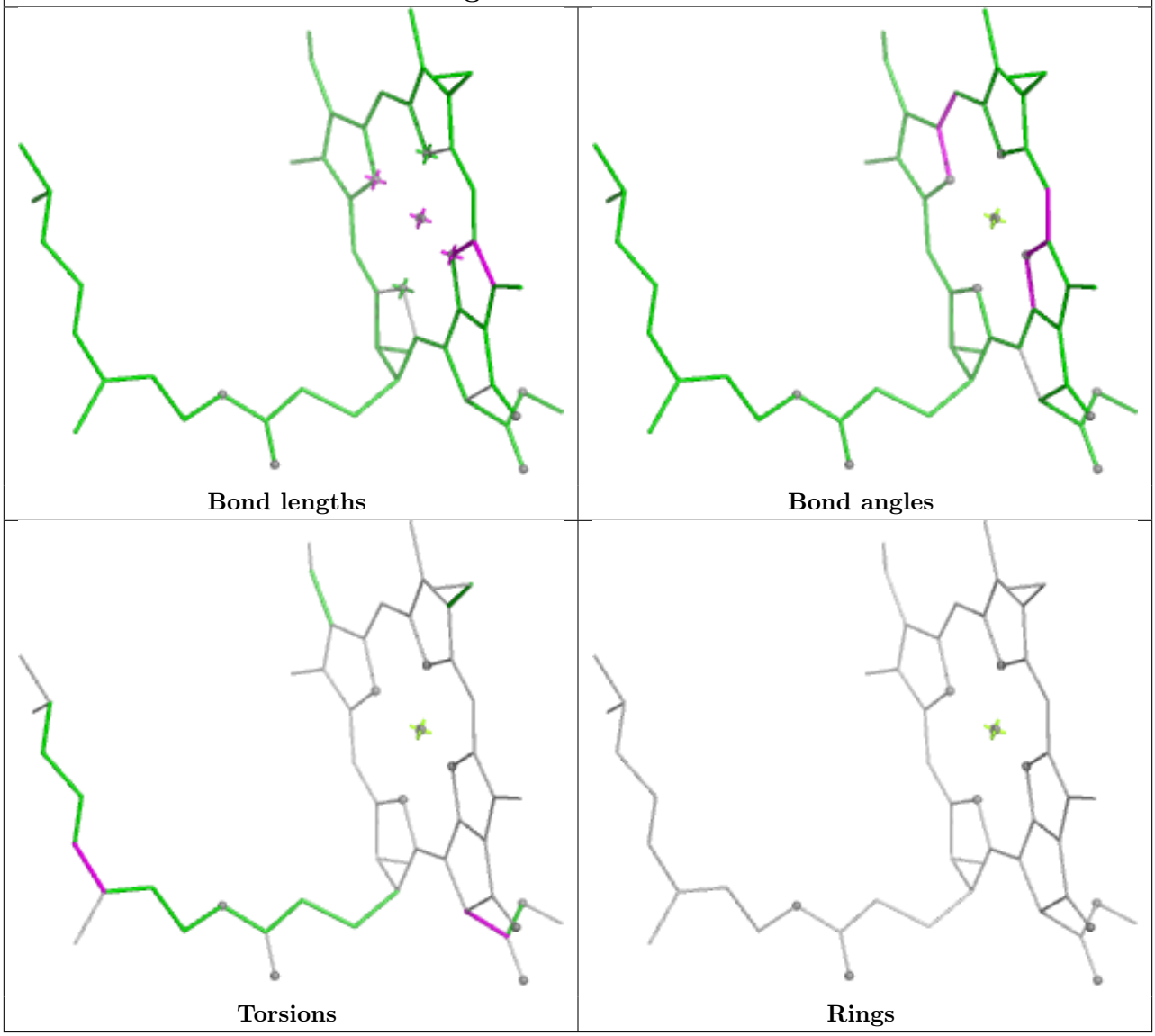


Rings

Ligand CLA A2 817



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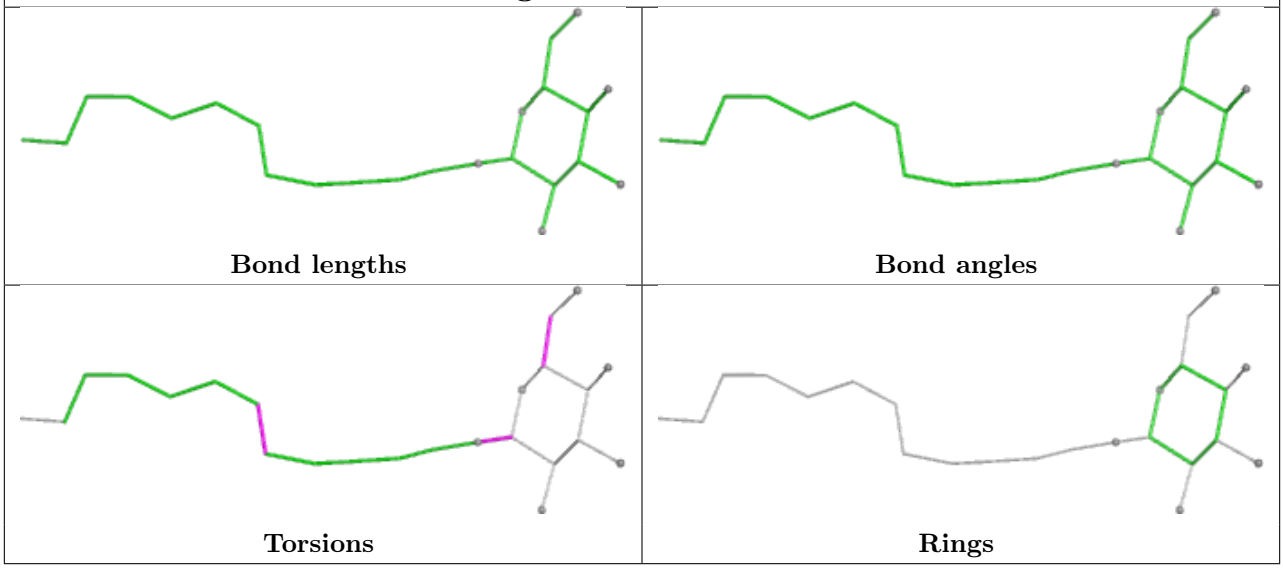

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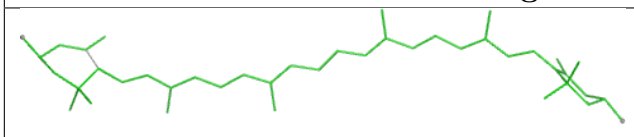
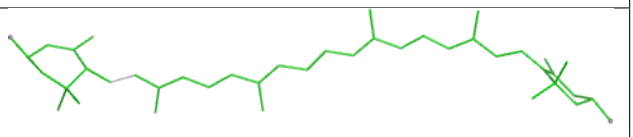
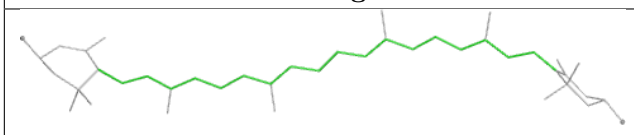


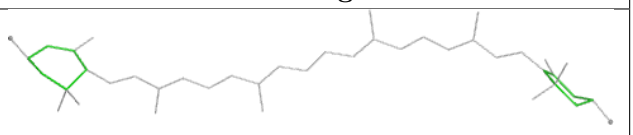
Bond lengths



Bond angles

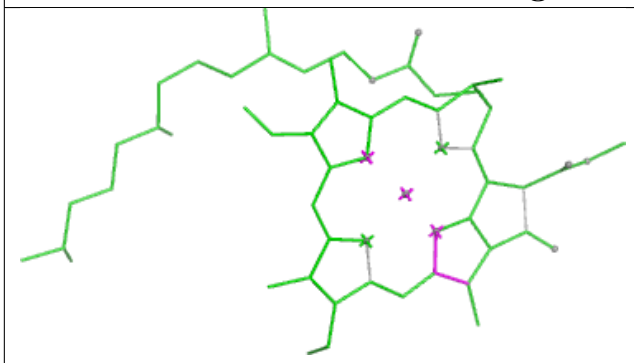


Torsions



Rings

Ligand CLA 5 610



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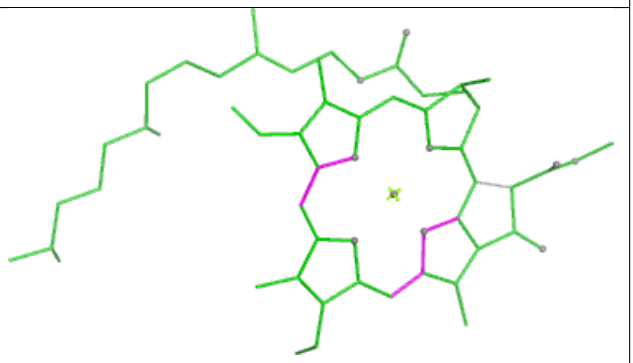
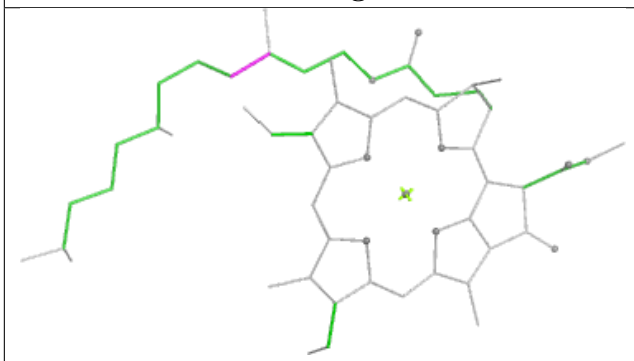


Bond angles



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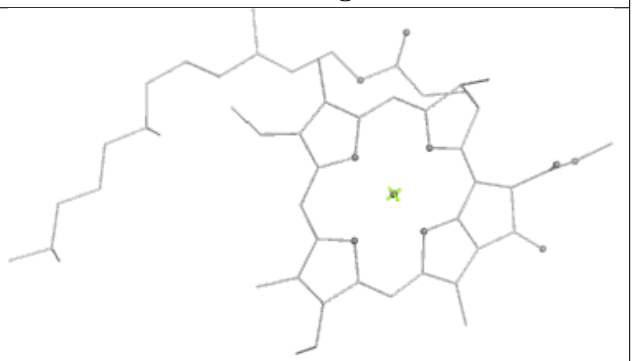
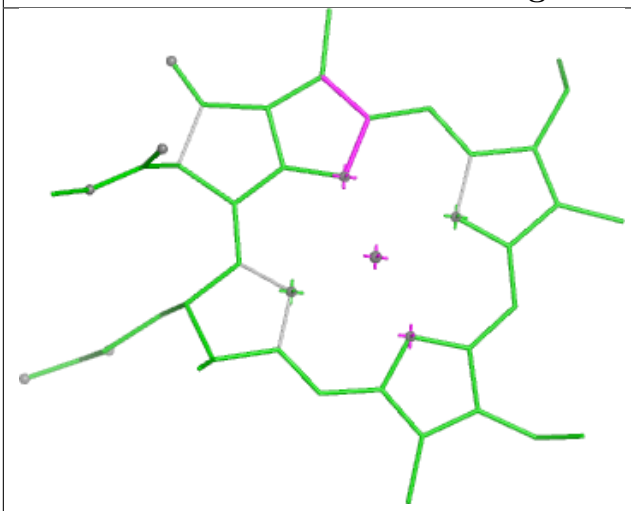


Rings

Ligand CLA 6 617



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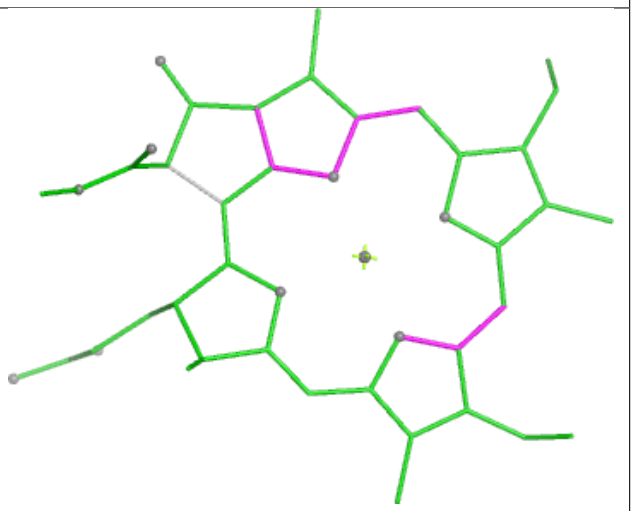
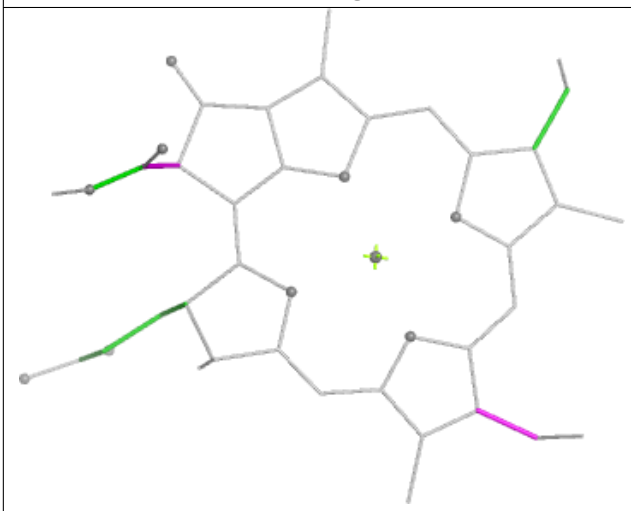


Bond angles



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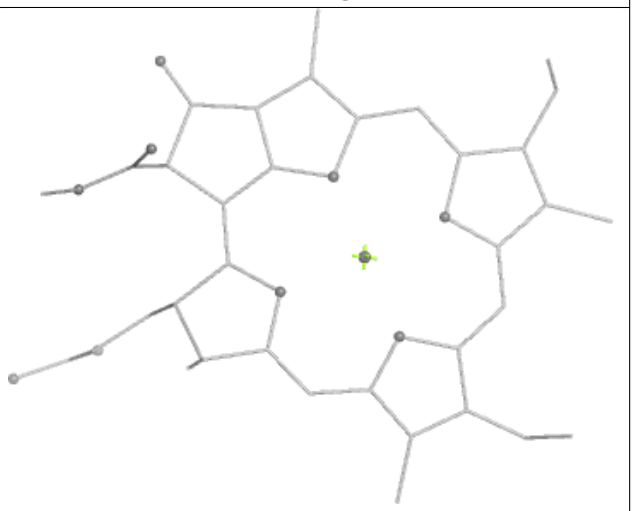
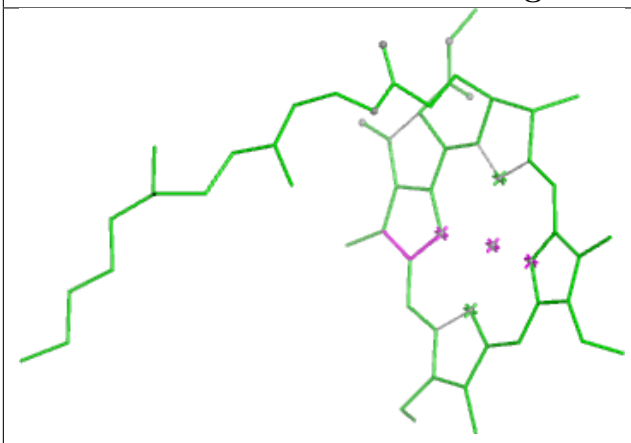


Rings

Ligand CLA B 822



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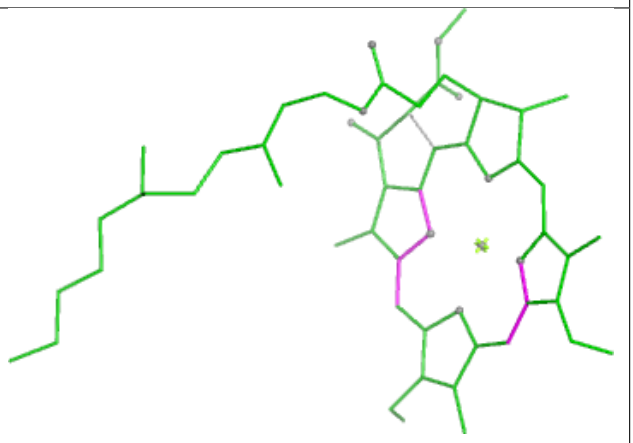
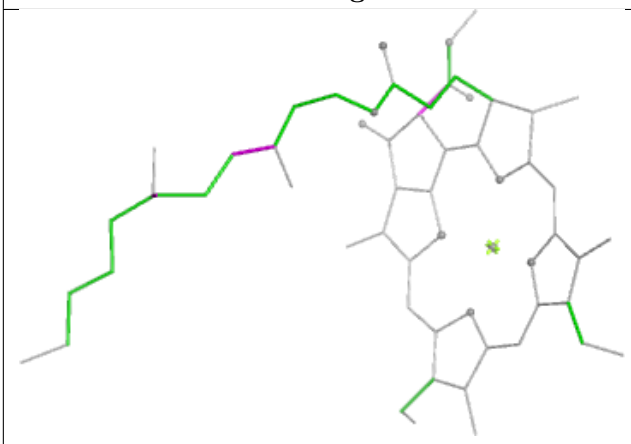


Bond angles



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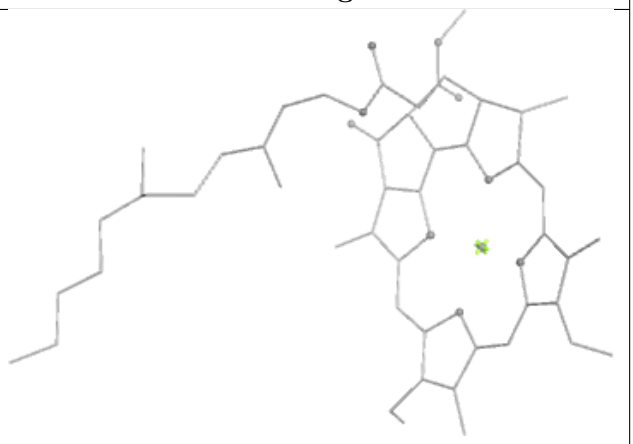
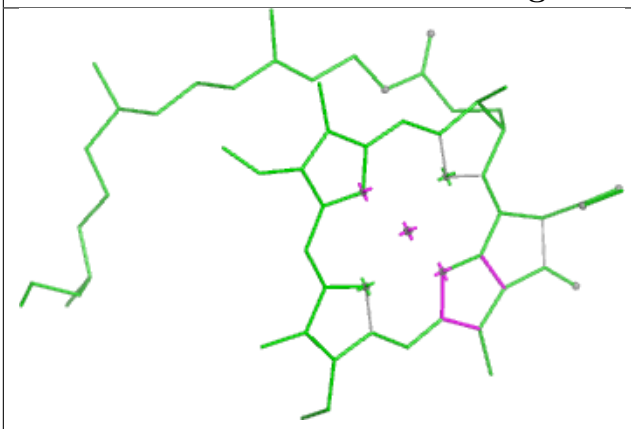


Rings

Ligand CLA 8 602



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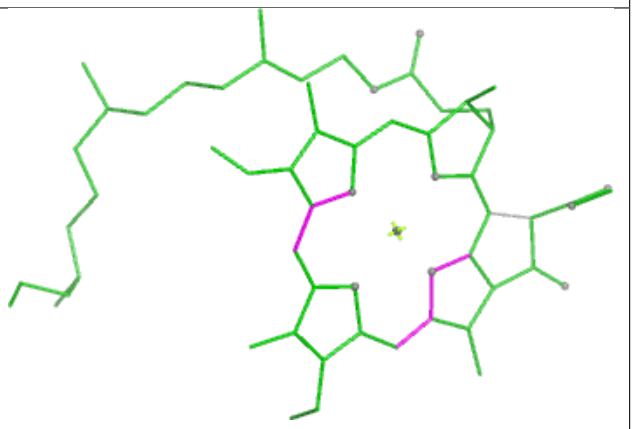
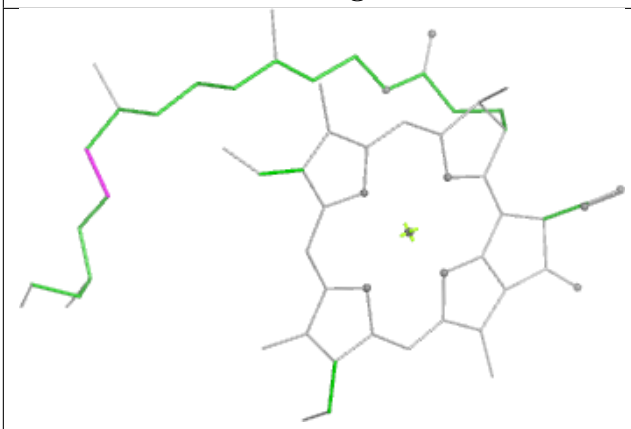


Bond angles

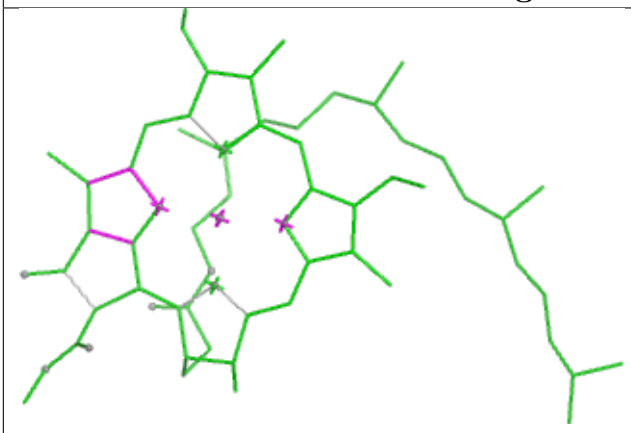


Torsions



Rings

Ligand CLA B2 812



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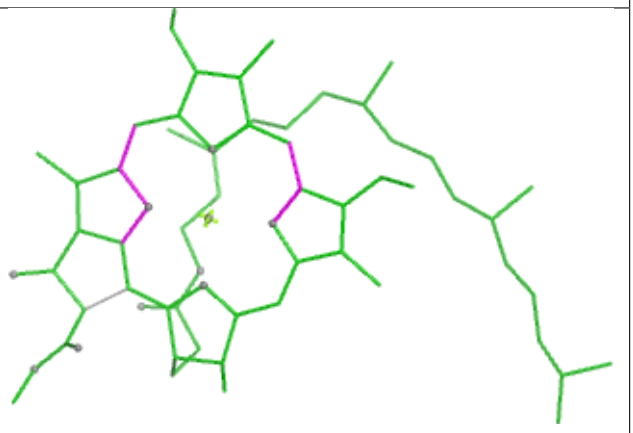

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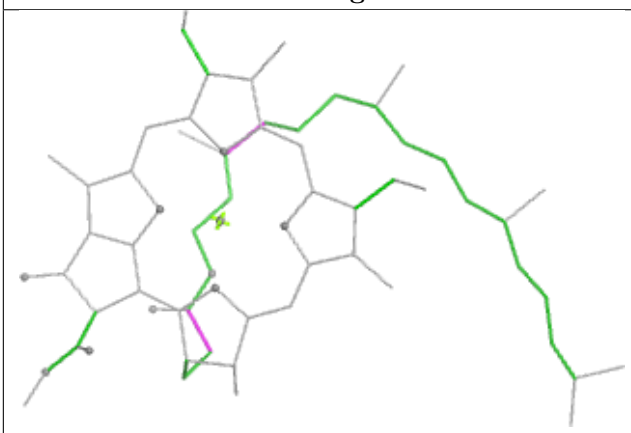

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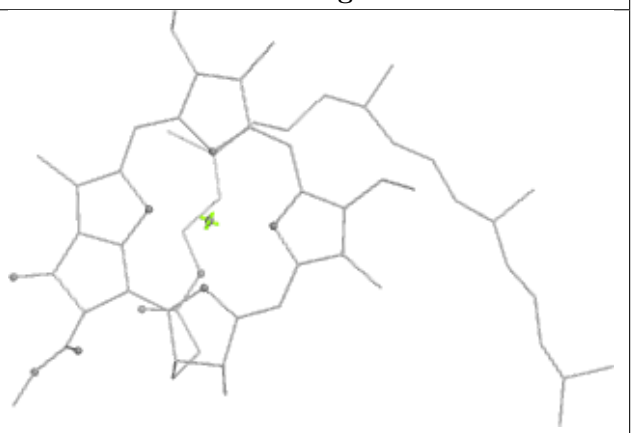
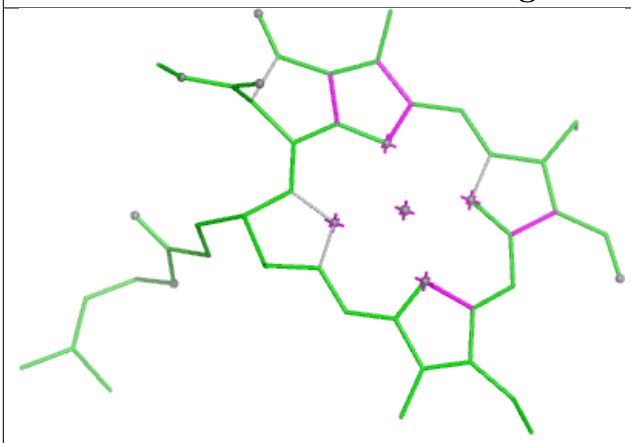


Rings

Ligand CHL 52 608



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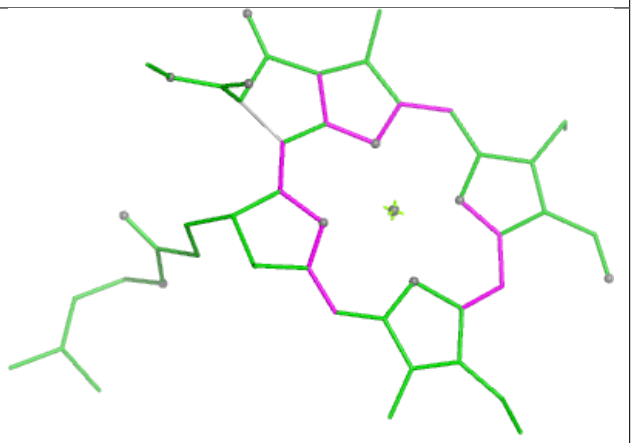
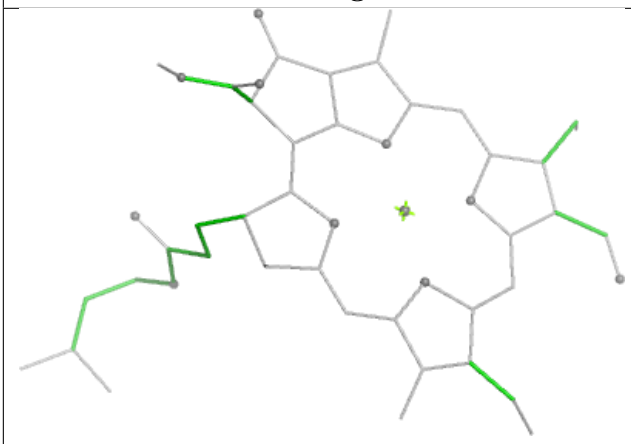


Bond angles

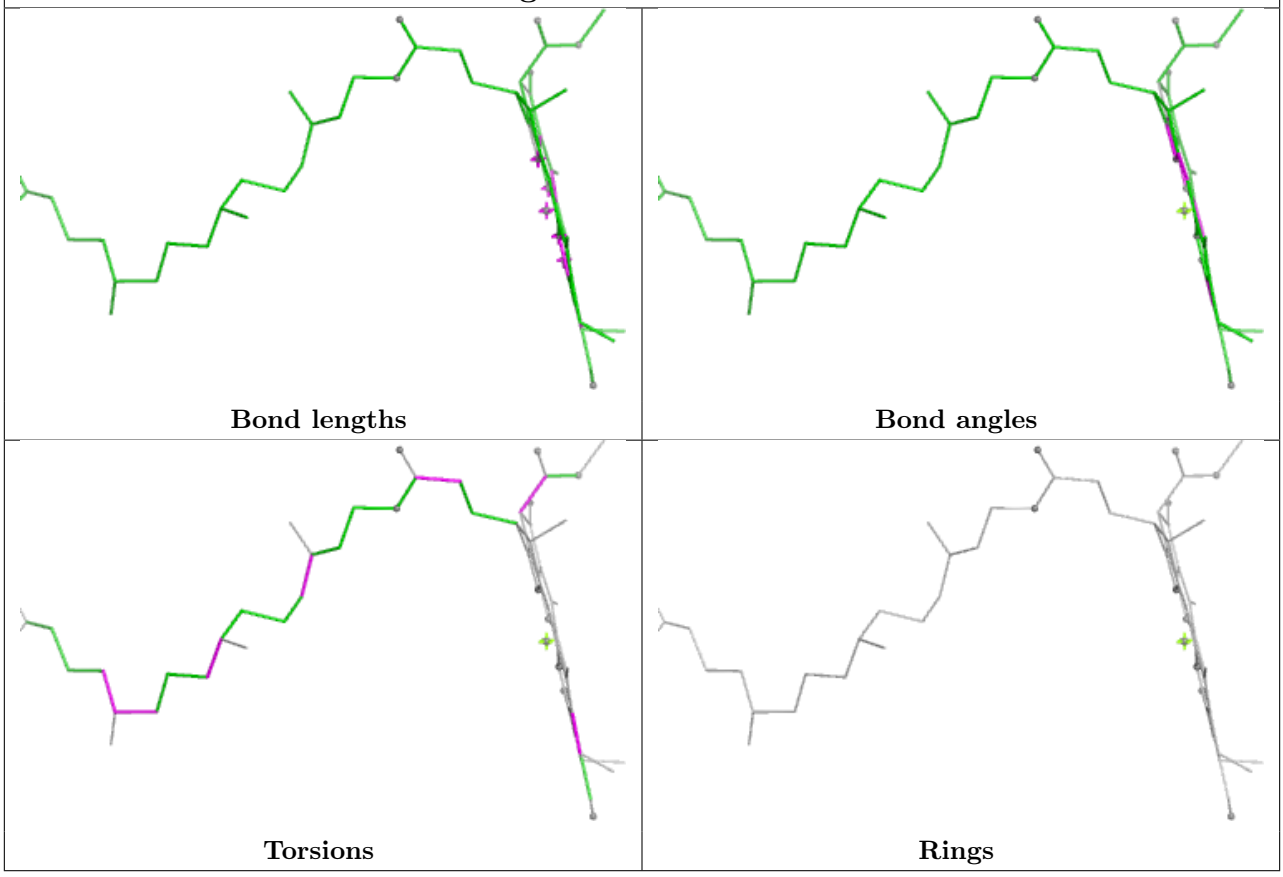


Torsions

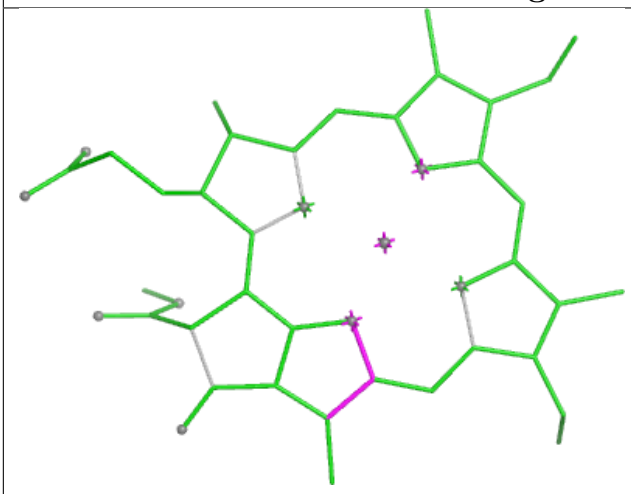


Rings

Ligand CHL 82 601



Ligand CLA 1 612



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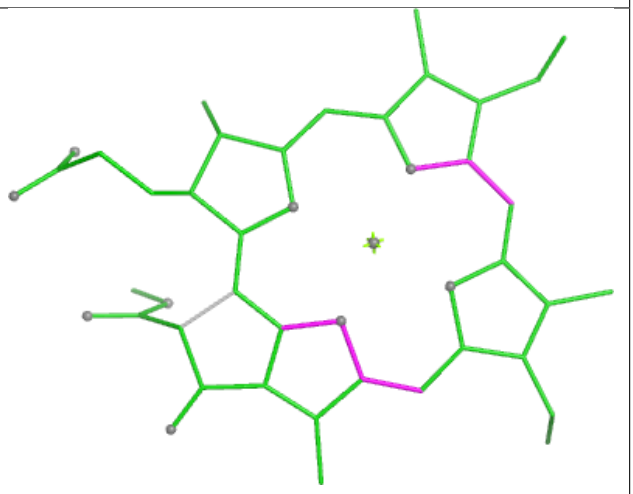
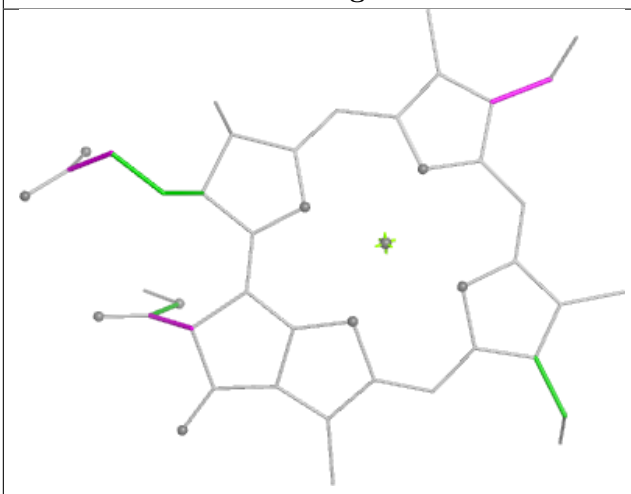


Bond angles



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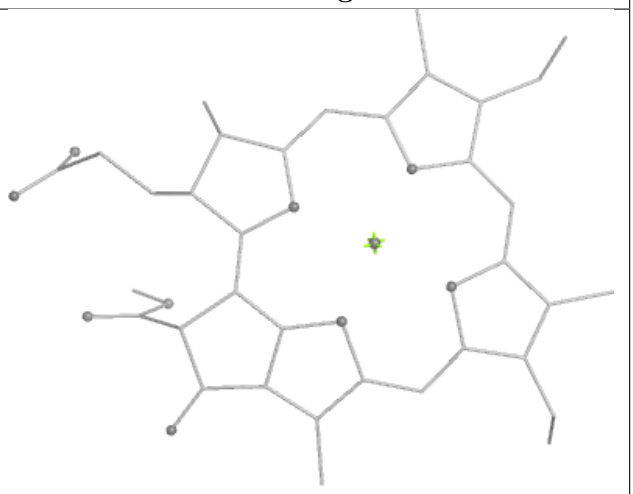
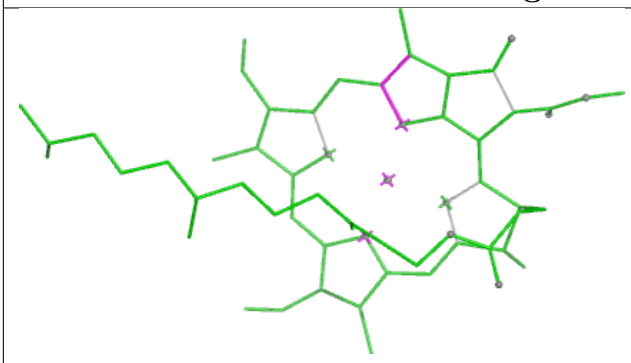


Rings

Ligand CLA A 819



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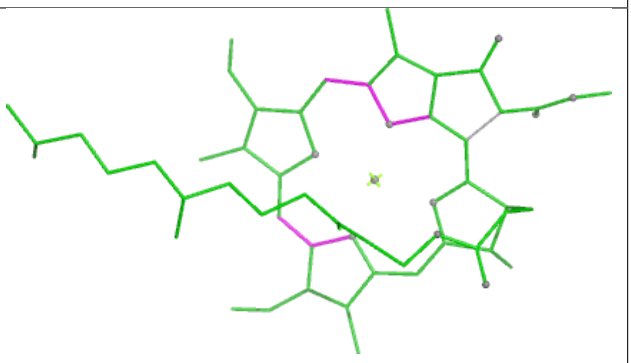

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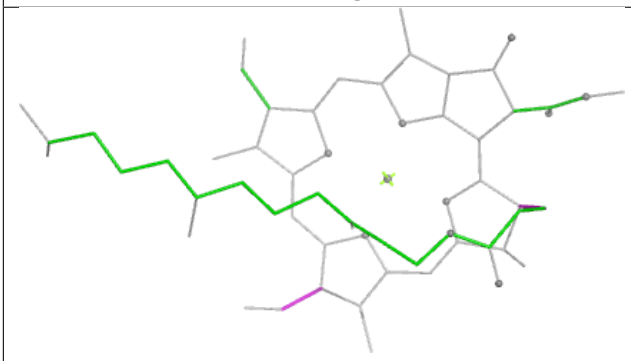
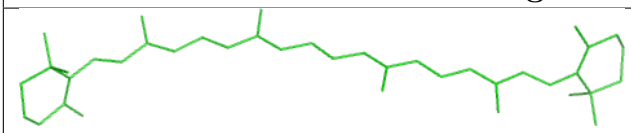


Torsions



Rings

Ligand BCR 3 718



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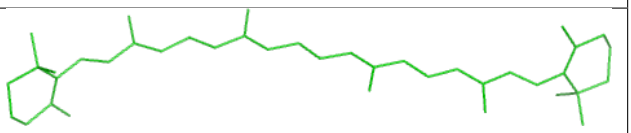
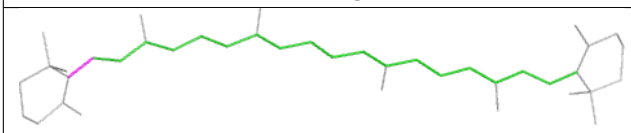


Bond angles



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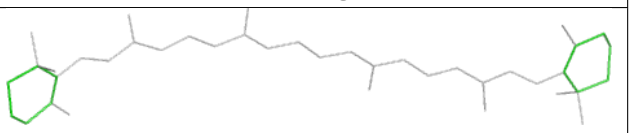
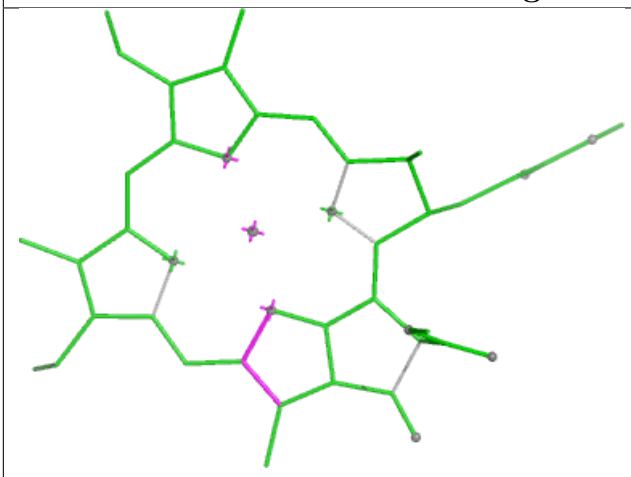


Rings

Ligand CLA K 204



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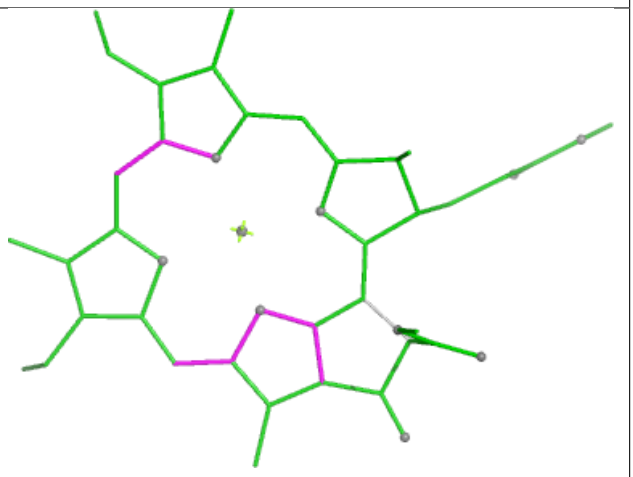
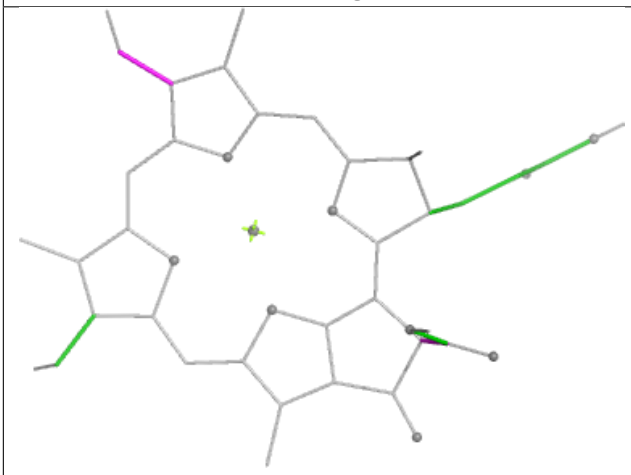


Bond angles



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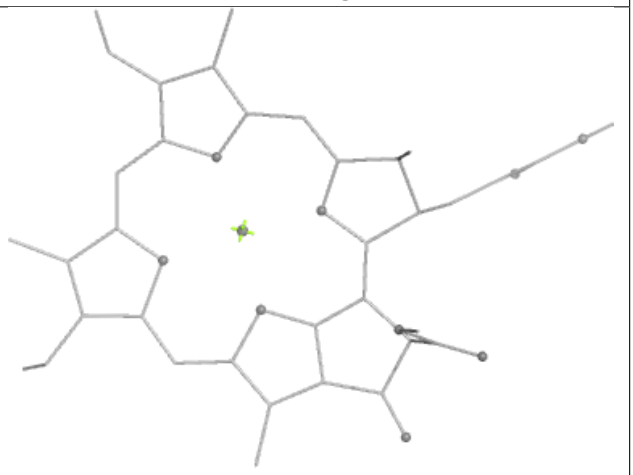
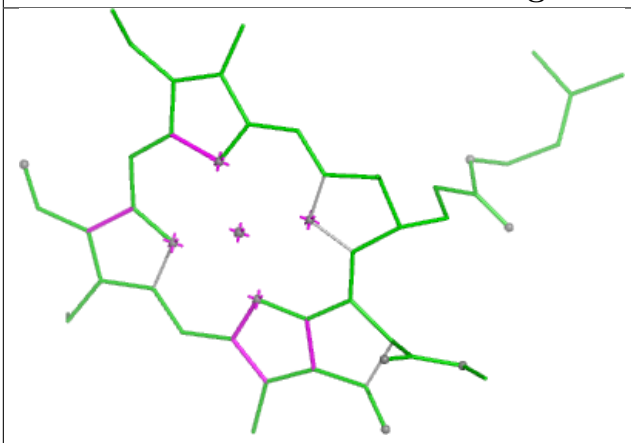


Rings

Ligand CHL 5 608



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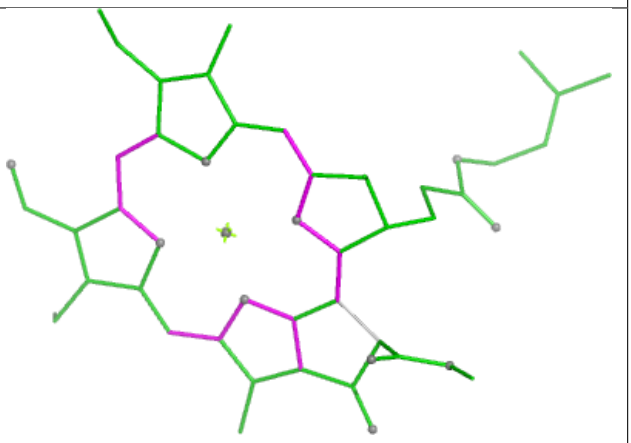

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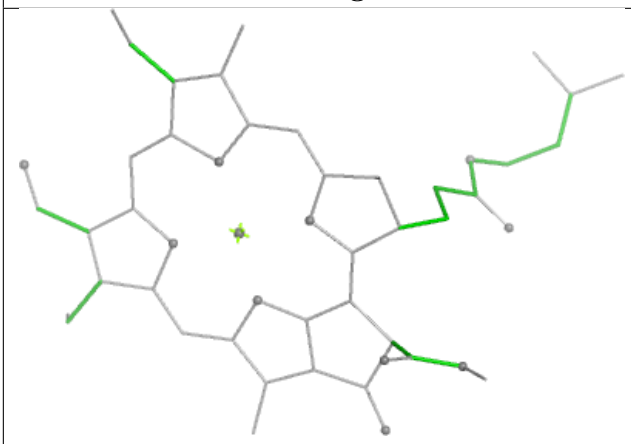

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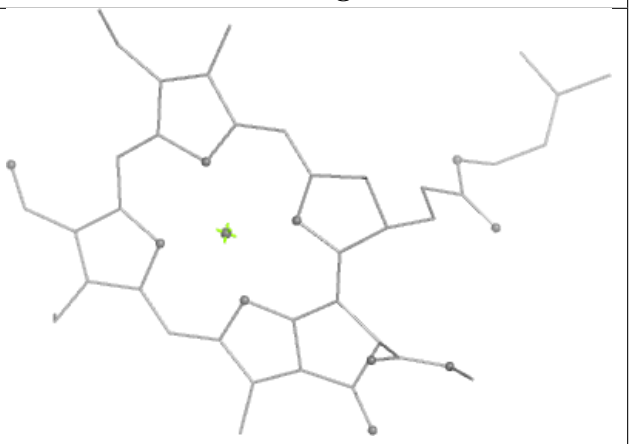
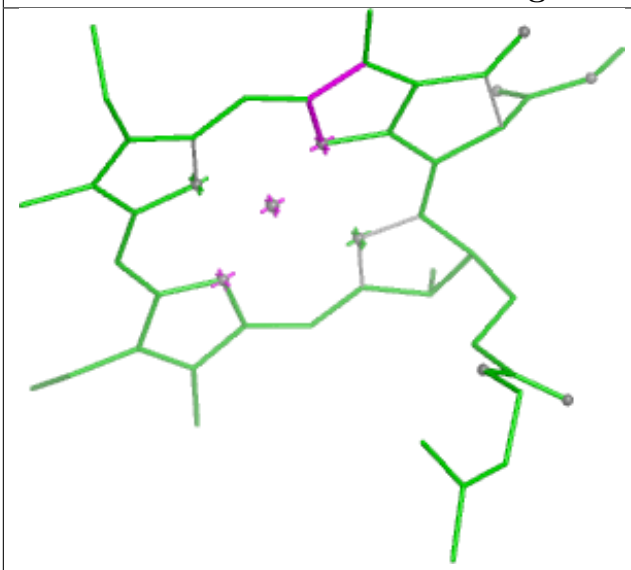


Rings

Ligand CLA 4 604



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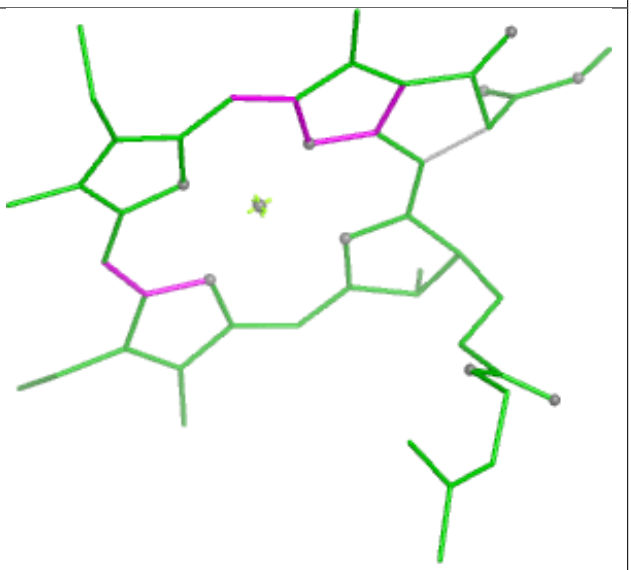

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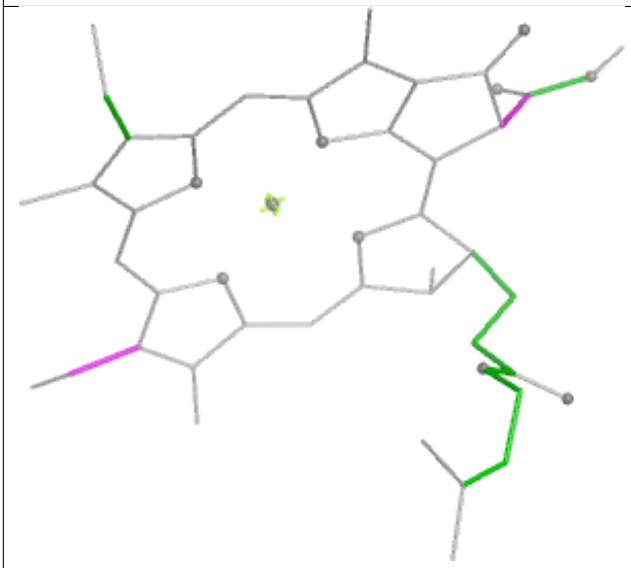

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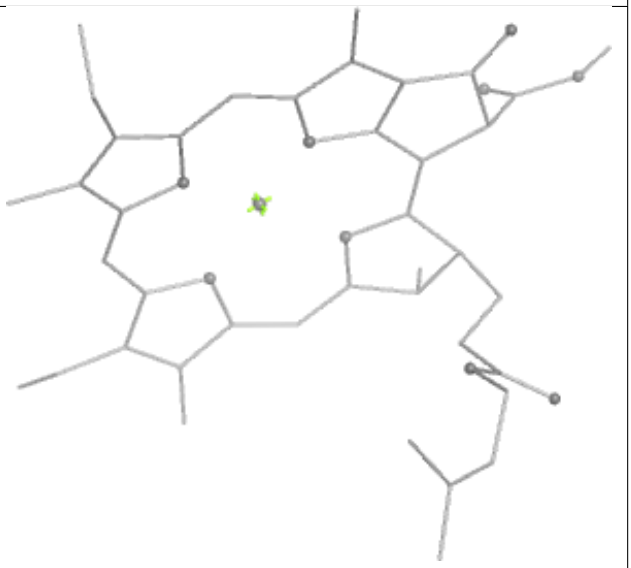
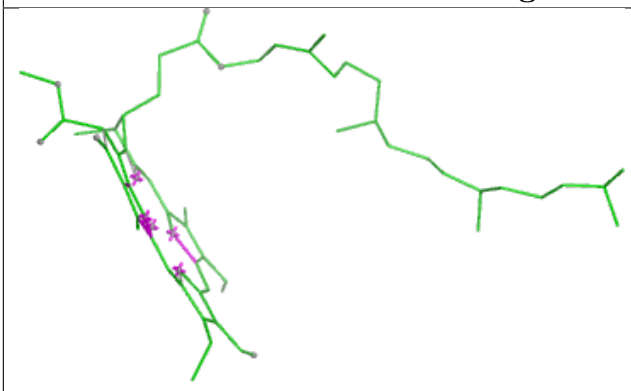


Rings

Ligand CHL 52 607



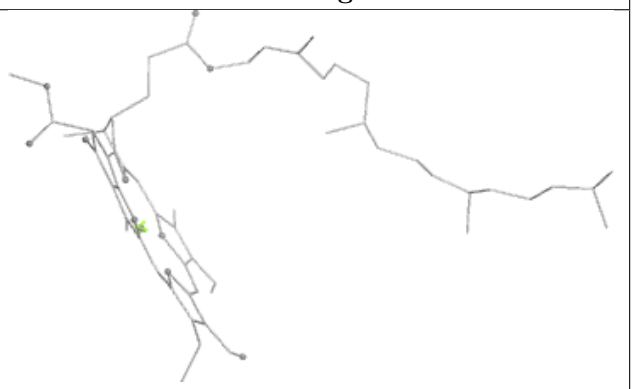
Bond lengths



Bond angles

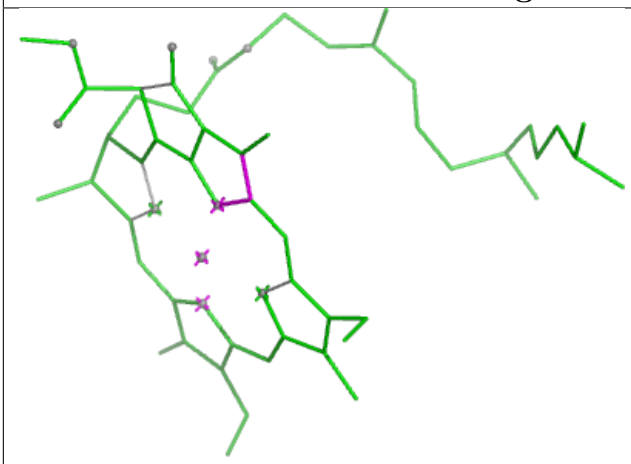


Torsions



Rings

Ligand CLA B2 814



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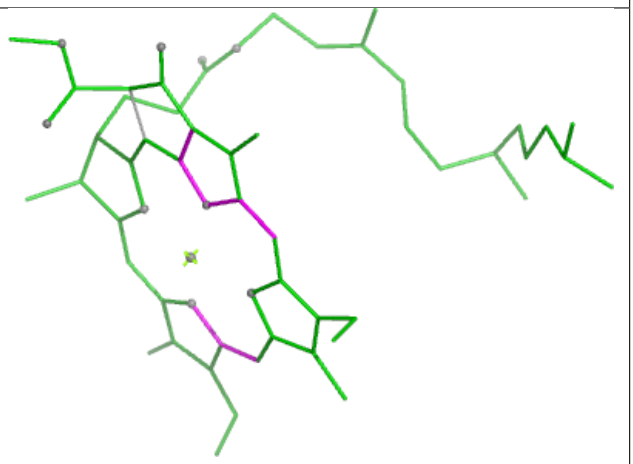
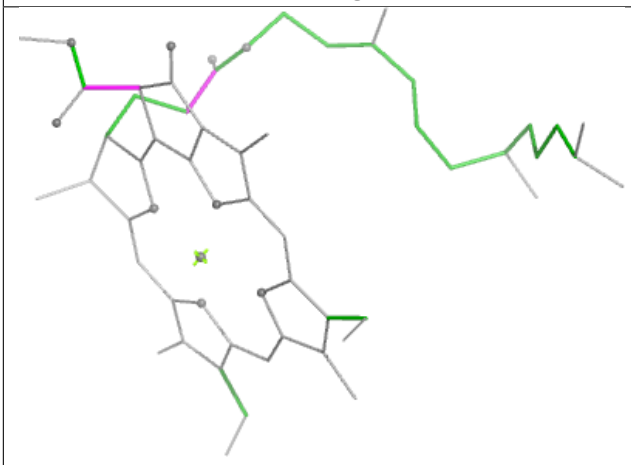


Bond angles

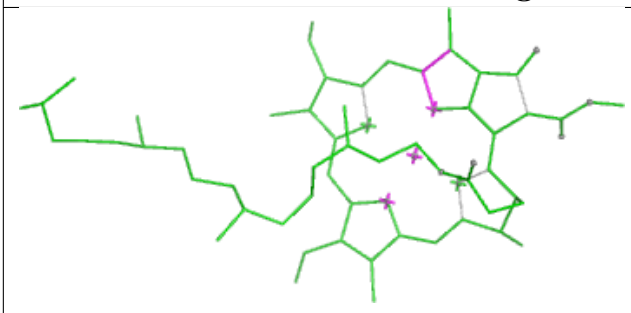


Torsions



Rings

Ligand CLA B2 811



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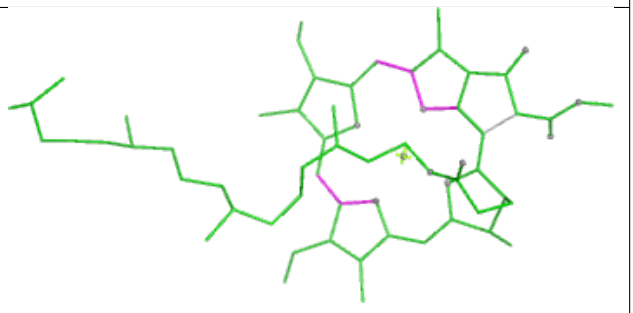
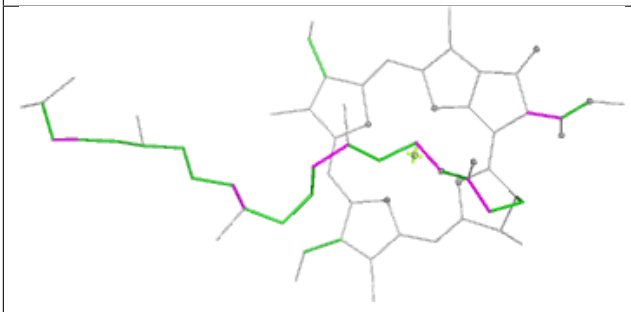


Bond angles

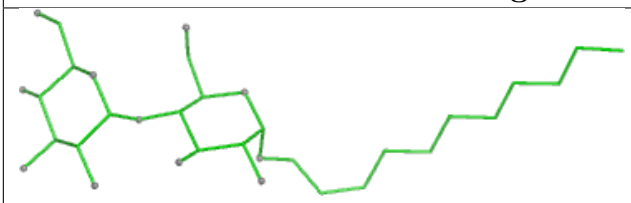


Torsions



Rings

Ligand LMU A2 857



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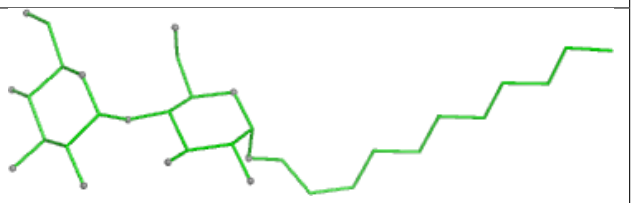
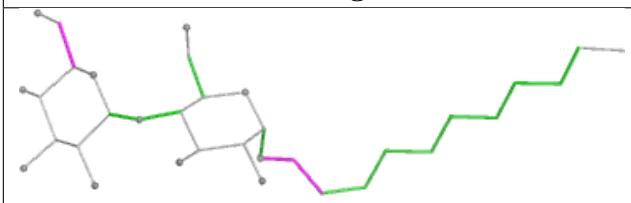
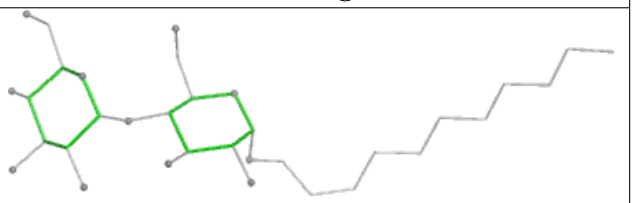


Bond angles

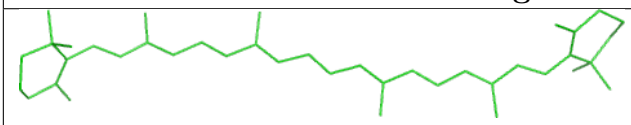


Torsions



Rings

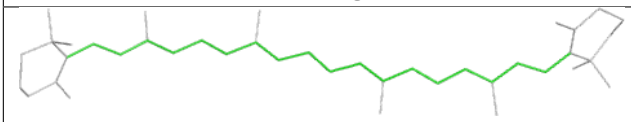
Ligand BCR A2 849



Bond lengths



Bond angles



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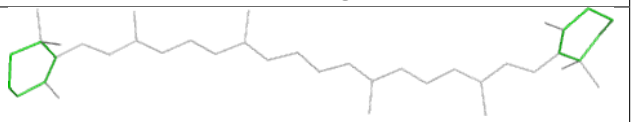
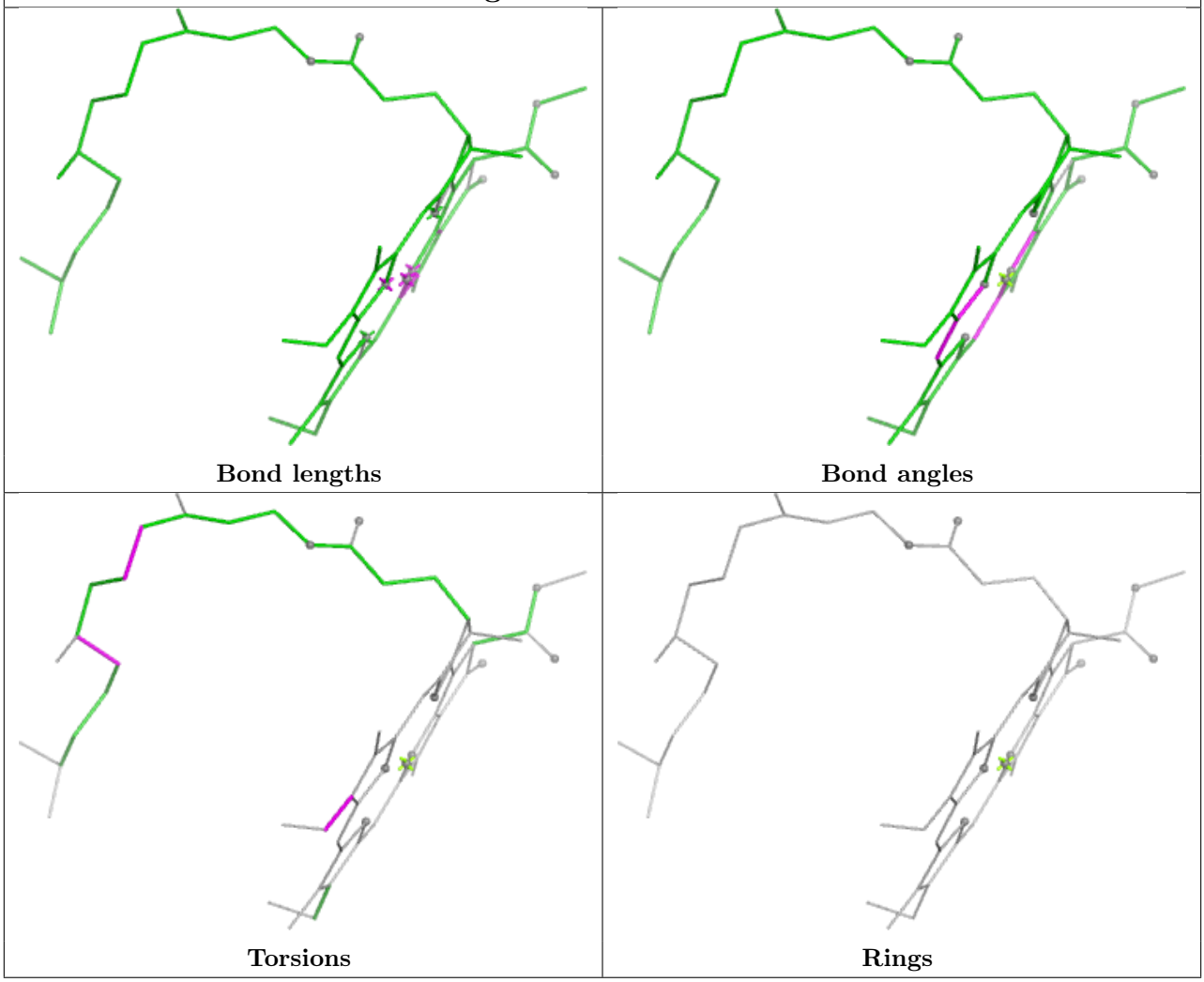
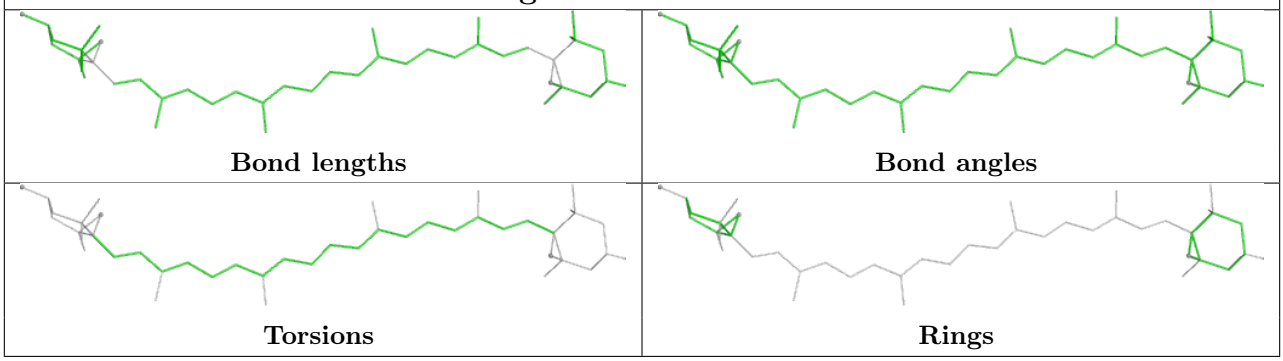


Rings

Ligand CLA B2 819



Ligand XAT 42 620



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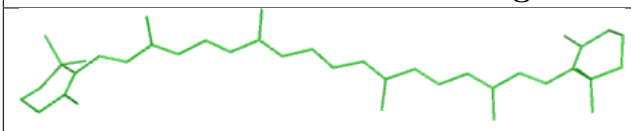
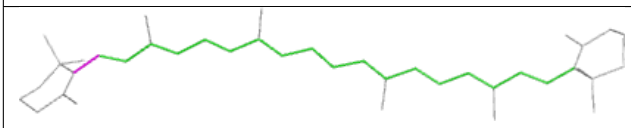


Bond lengths



Bond angles



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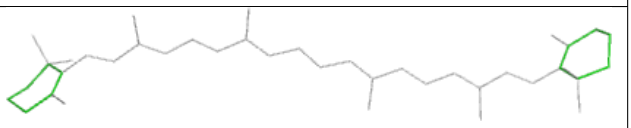
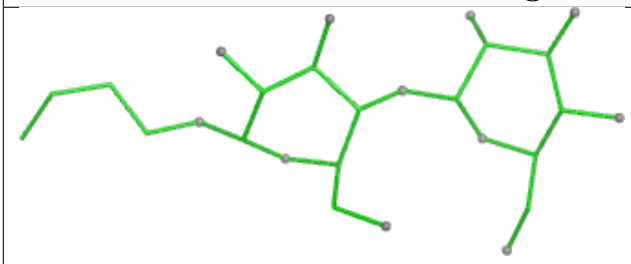


Rings

Ligand LMU 7 629



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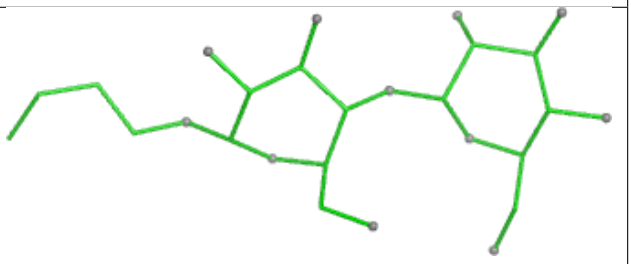
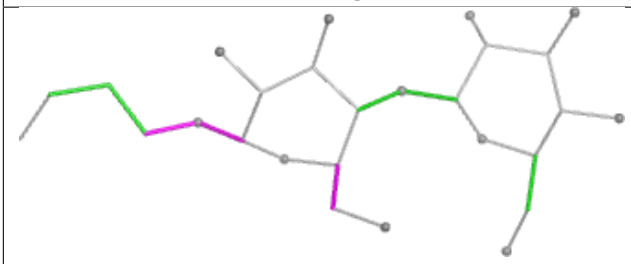


Bond angles



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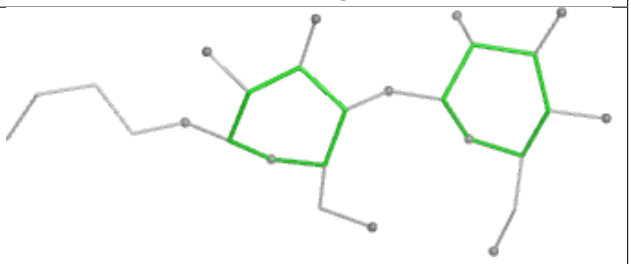
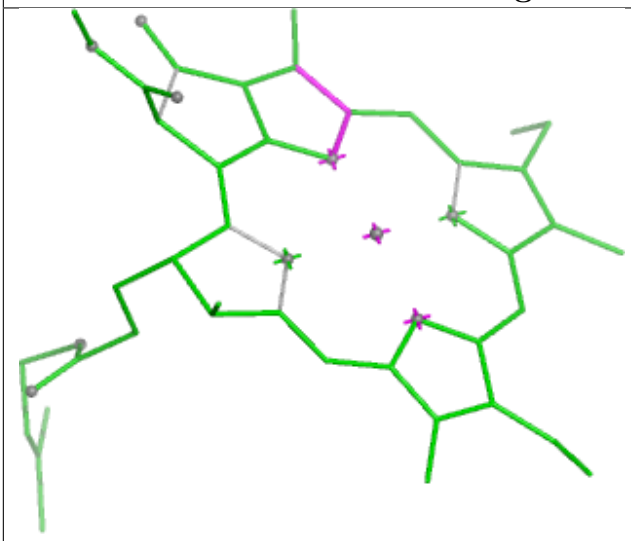


Rings

Ligand CLA A2 808



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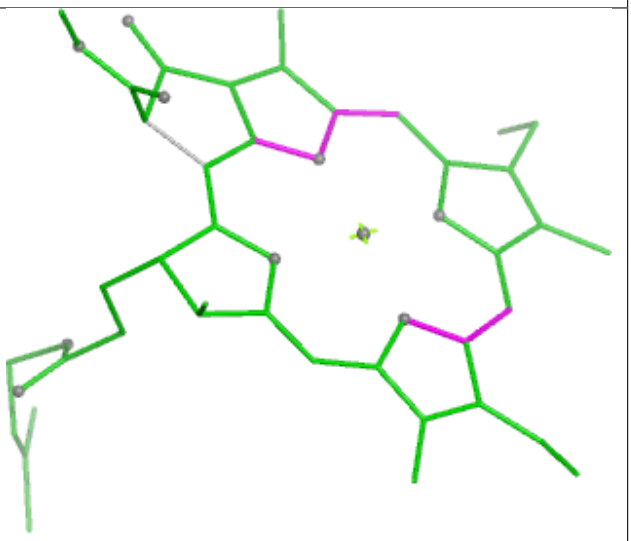
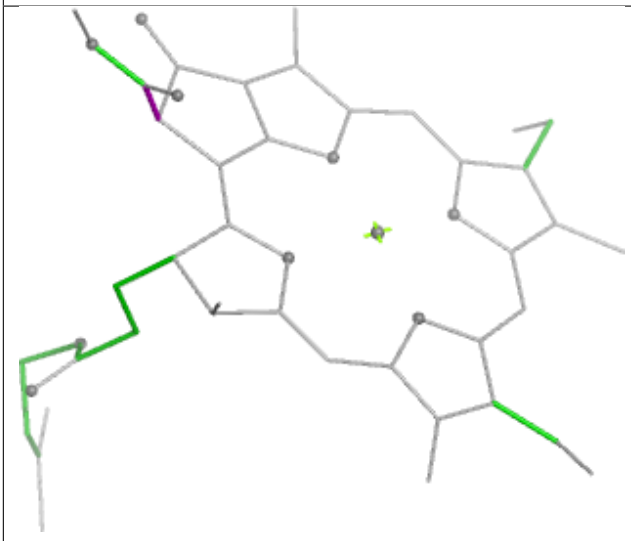


Bond angles



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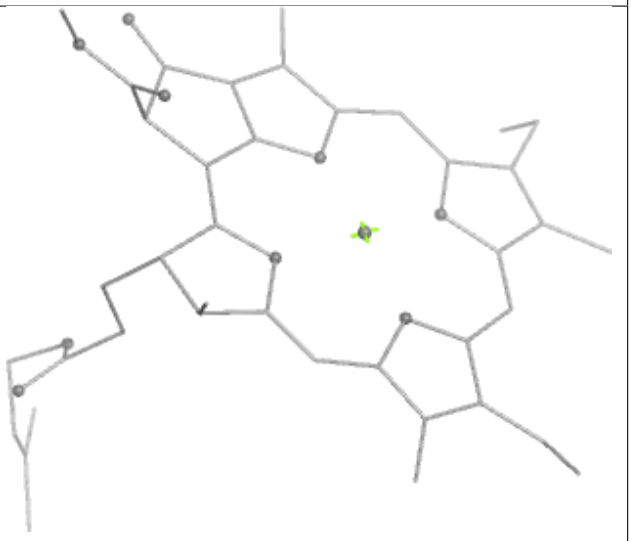
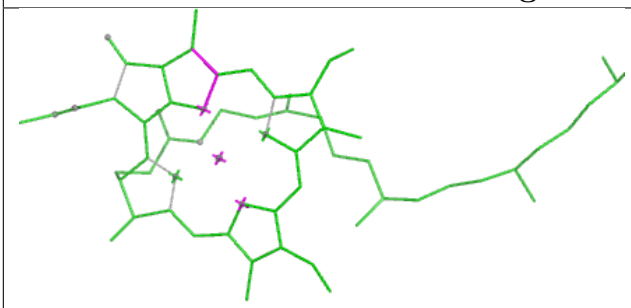


Rings

Ligand CLA 72 613



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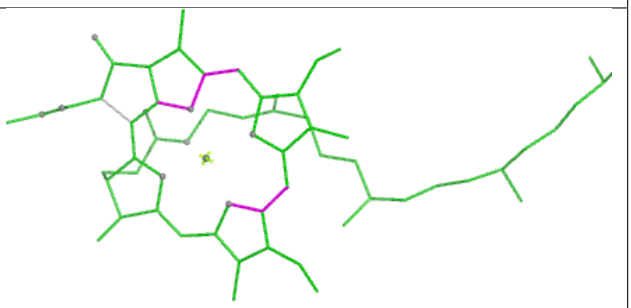
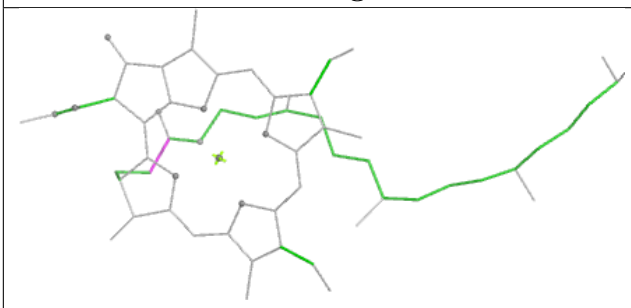


Bond angles



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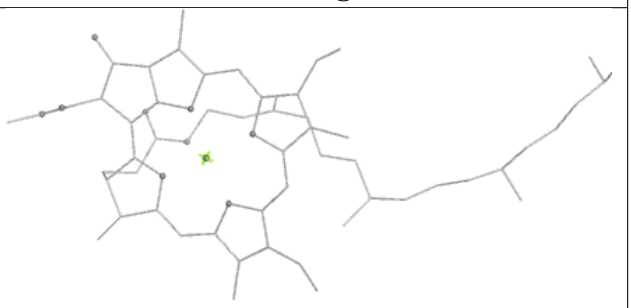
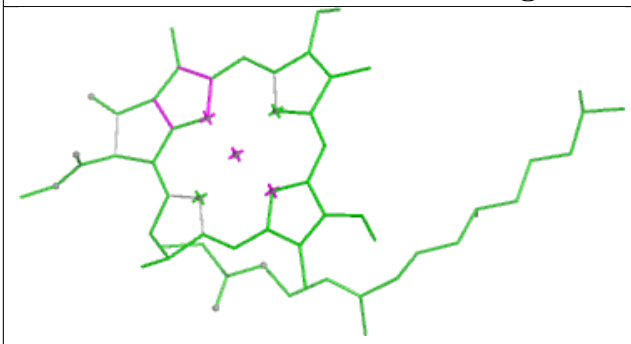


Rings

Ligand CLA 92 610



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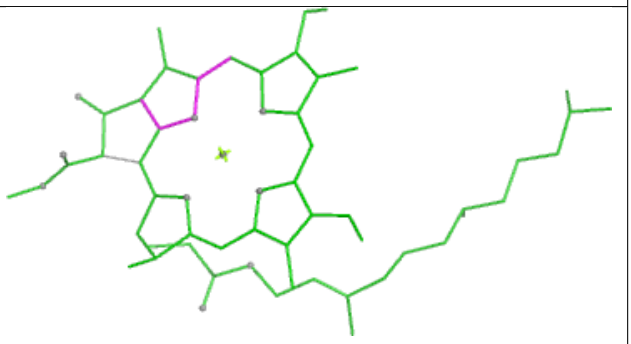

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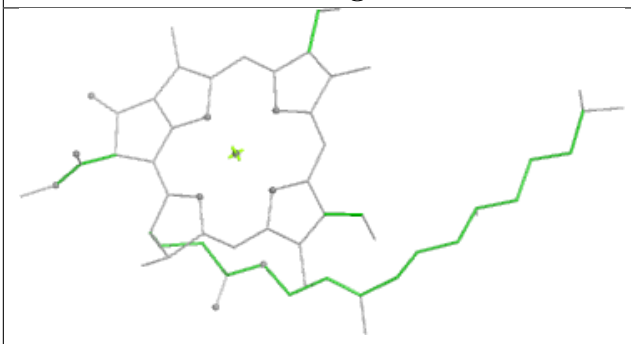

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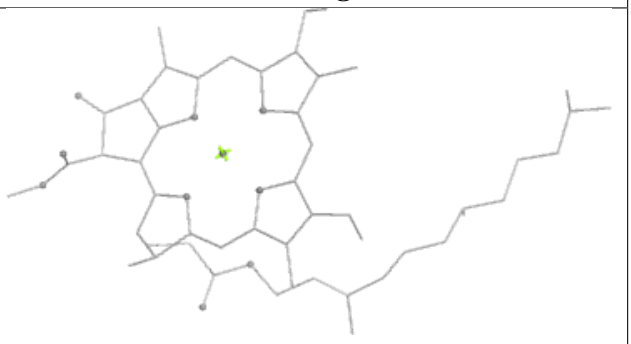

Rings

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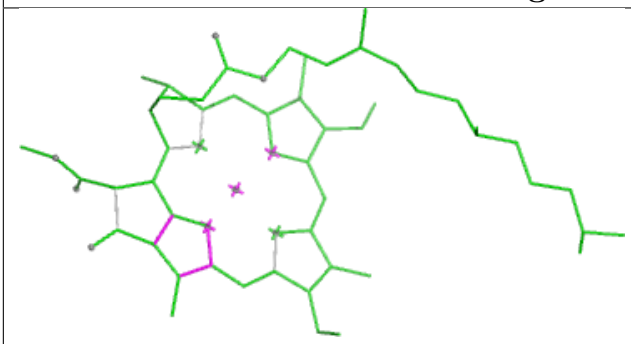

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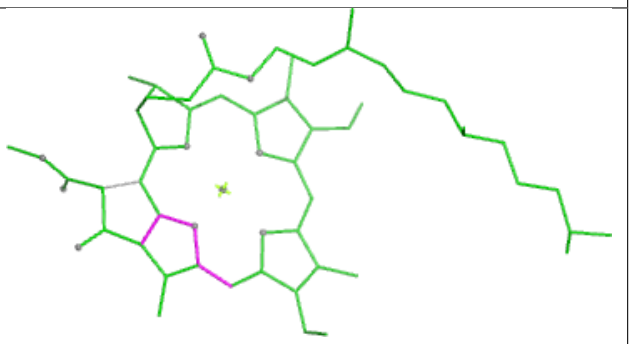
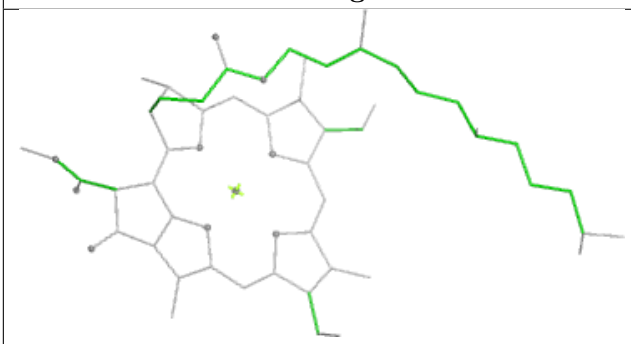


Bond angles



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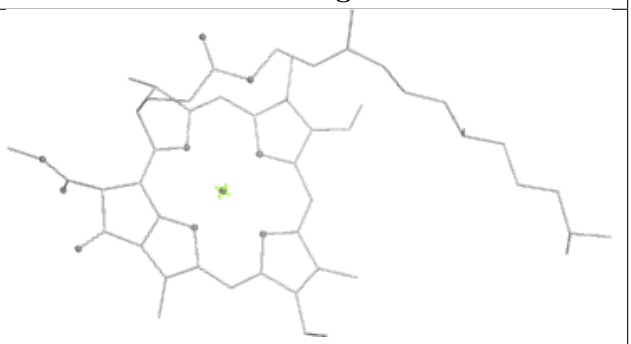
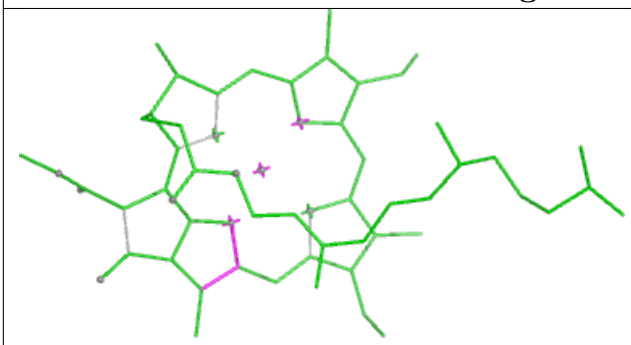


Rings

Ligand CLA 32 613



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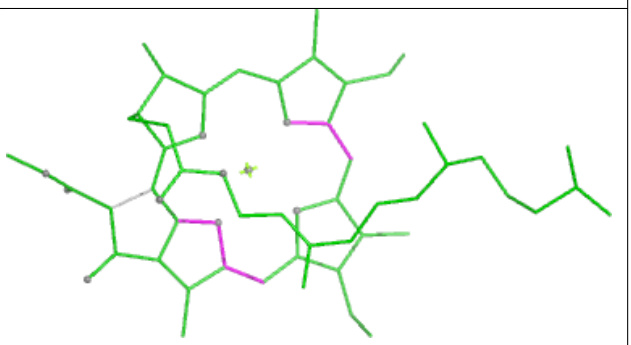
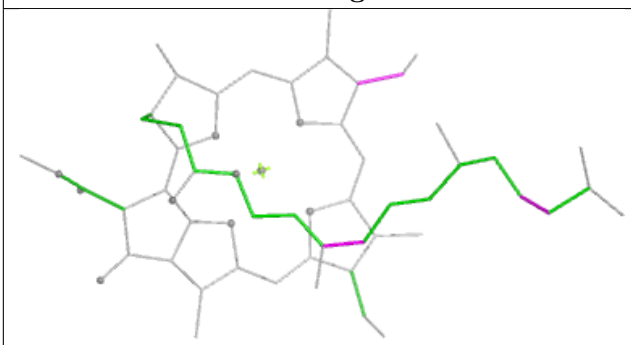


Bond angles



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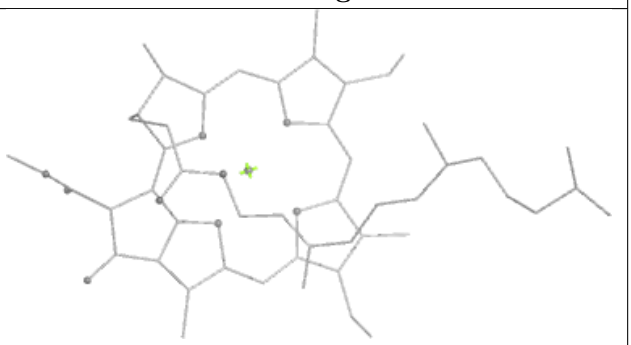
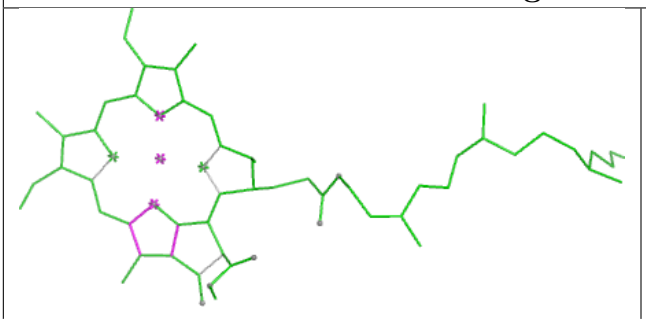


Rings

Ligand CLA A 806



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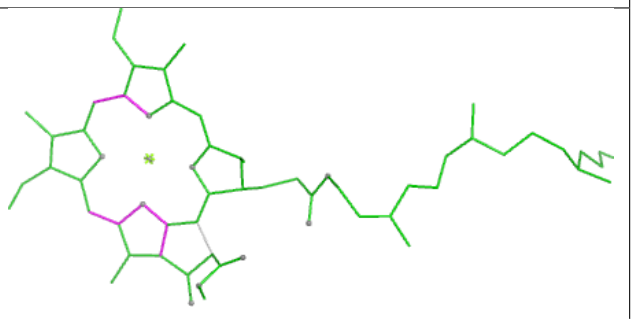
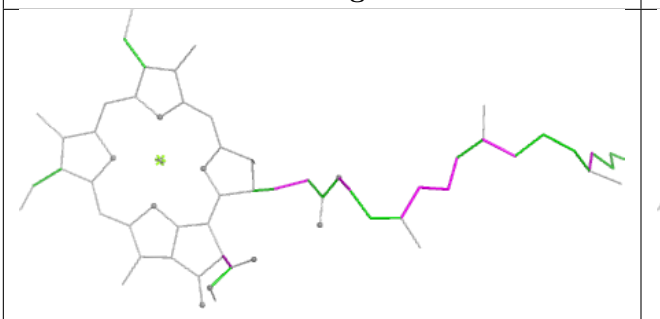


Bond angles



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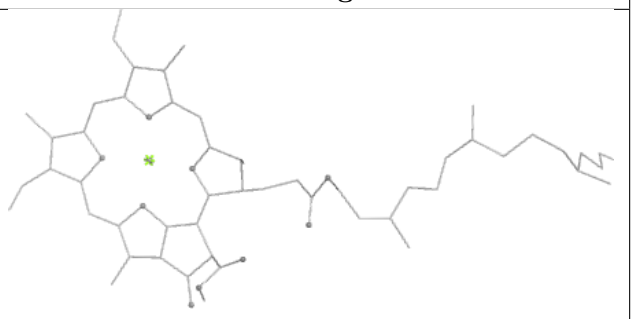
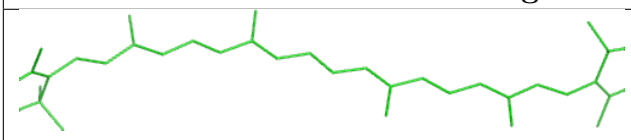


Rings

Ligand BCR K 207



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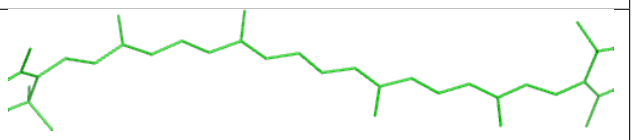
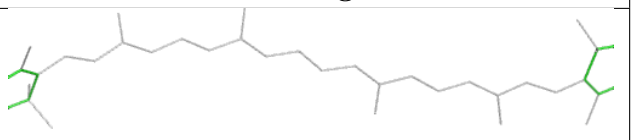


Bond angles

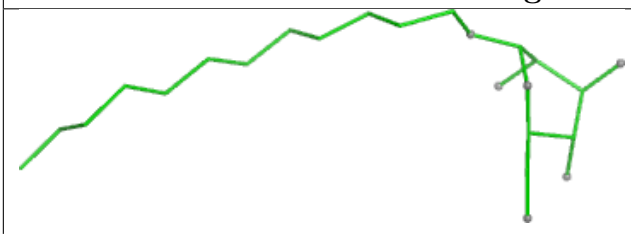


Torsions



Rings

Ligand LMU 6 630



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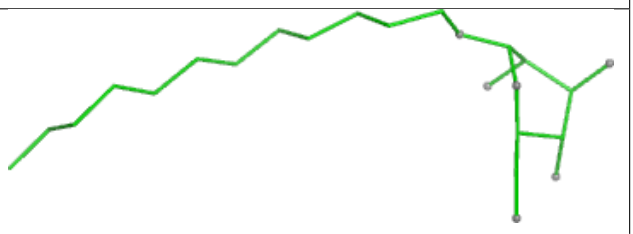
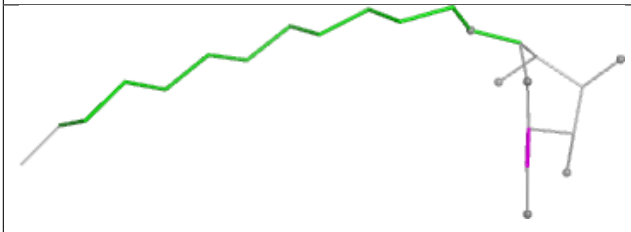


Bond angles



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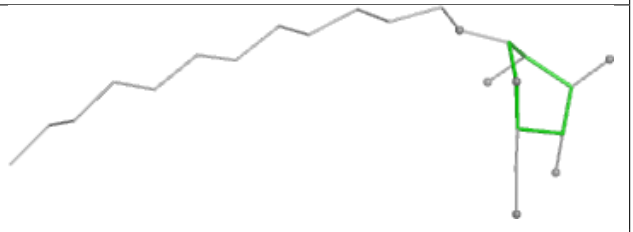
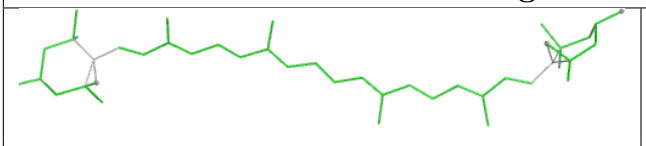


Rings

Ligand XAT 12 618



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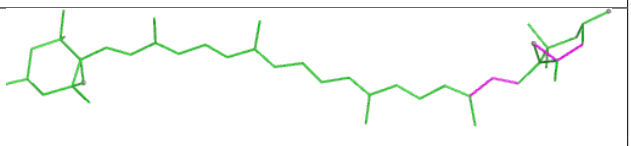
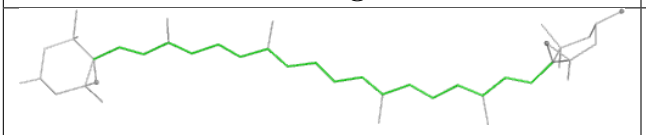


Bond angles



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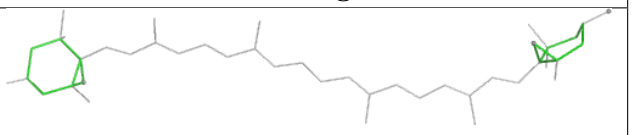
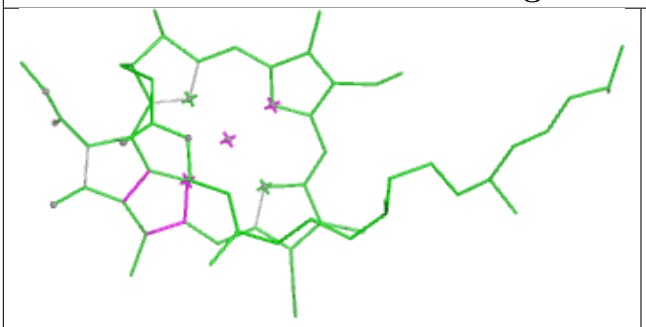


Rings

Ligand CLA A 841



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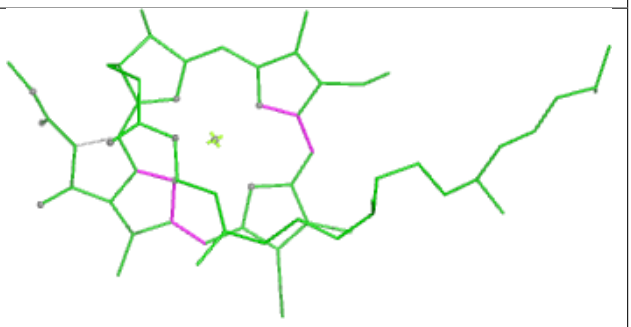
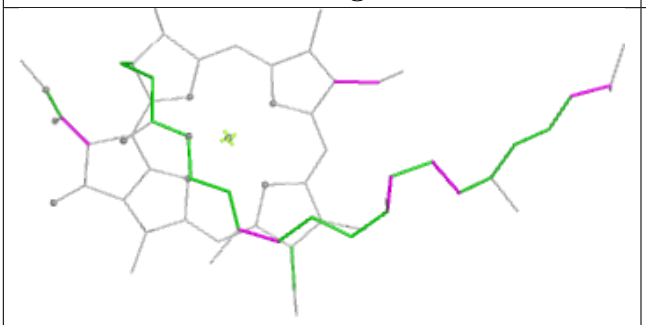


Bond angles

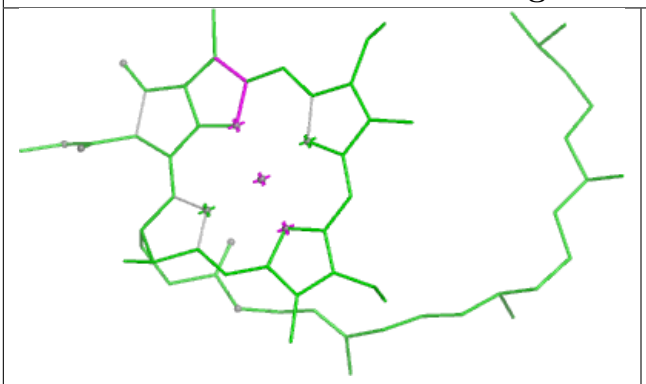


Torsions



Rings

Ligand CLA 7 610



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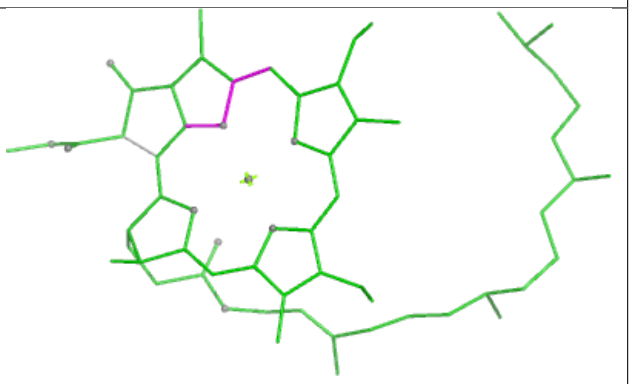
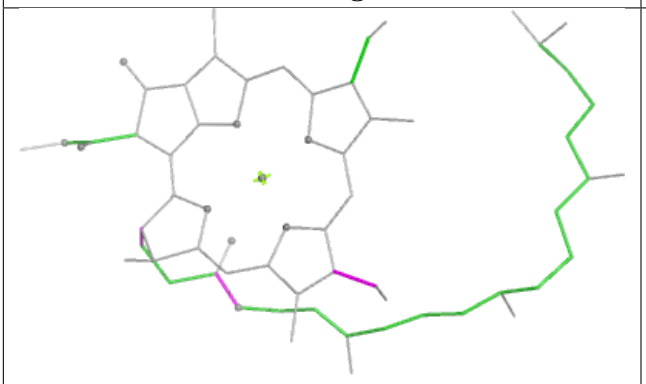


Bond angles



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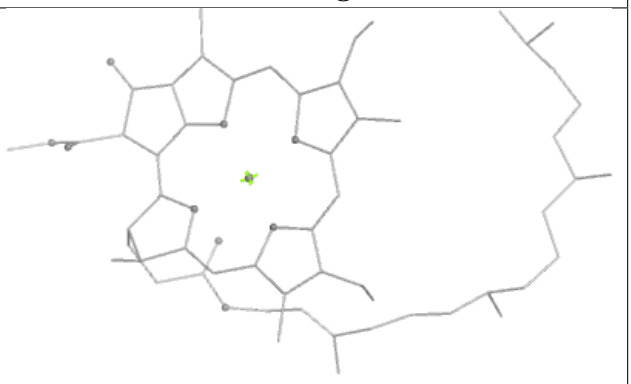
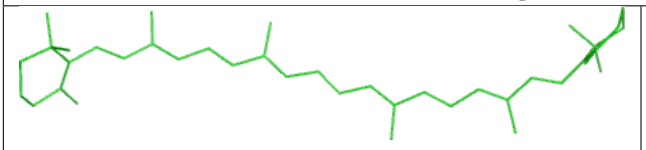


Rings

Ligand BCR B2 848



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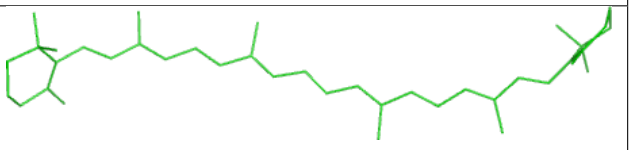
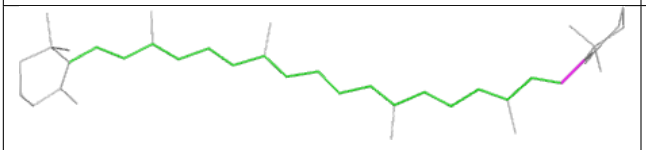
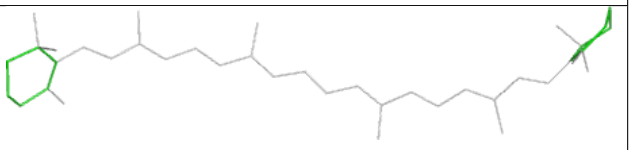


Bond angles

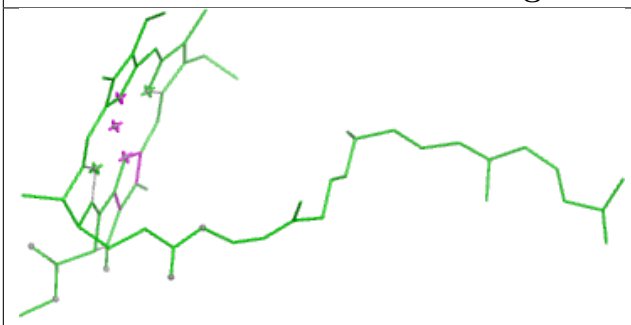


Torsions

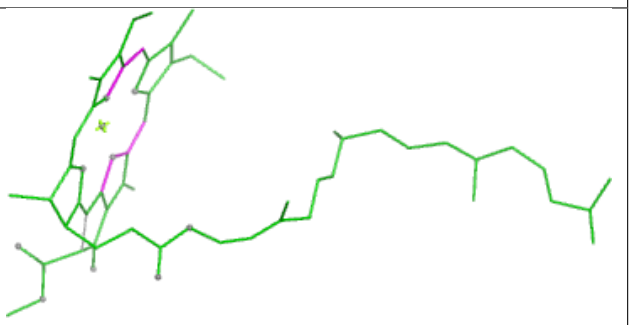


Rings

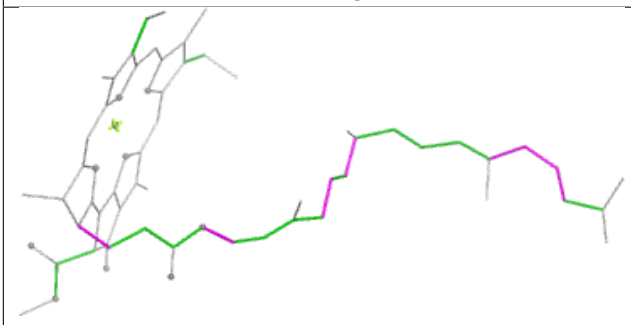
Ligand CLA A 812



Bond lengths



Bond angles



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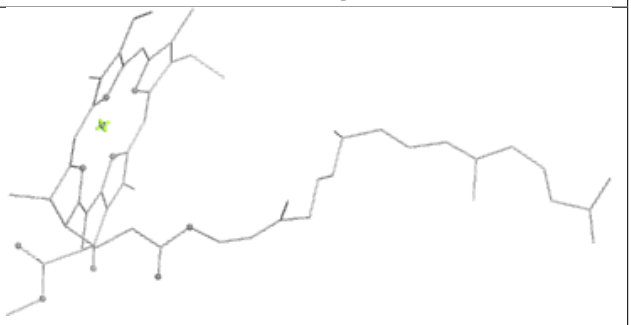
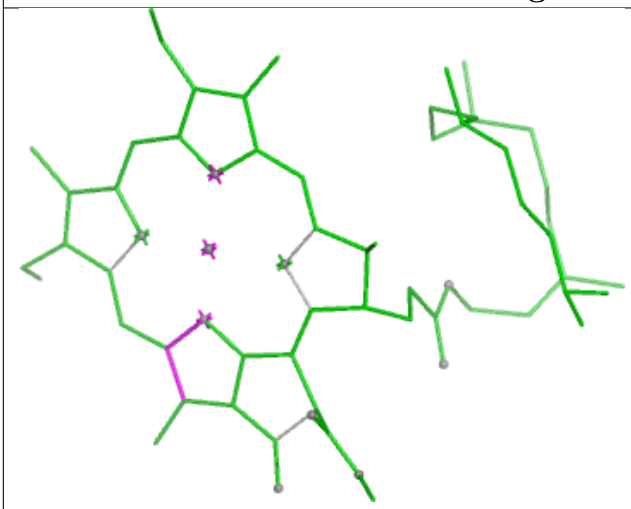


Rings

Ligand CLA 1 608



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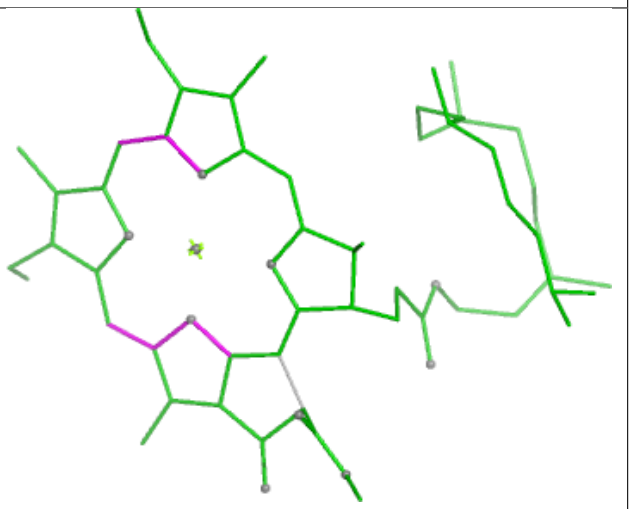

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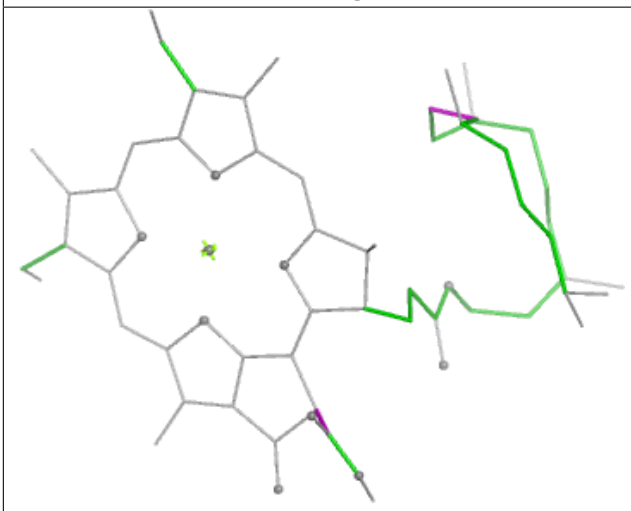

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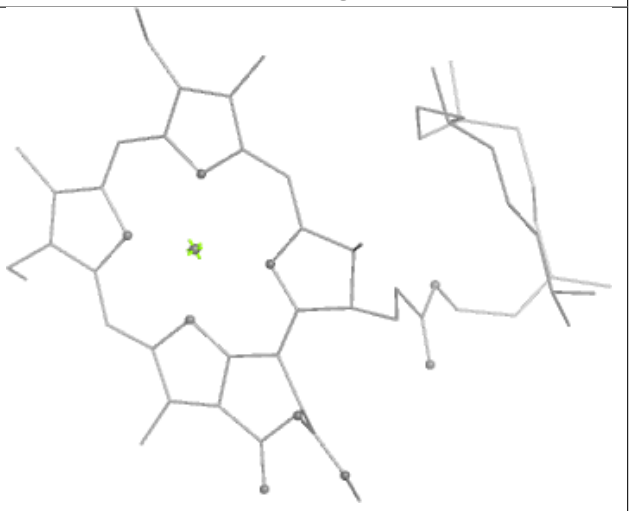
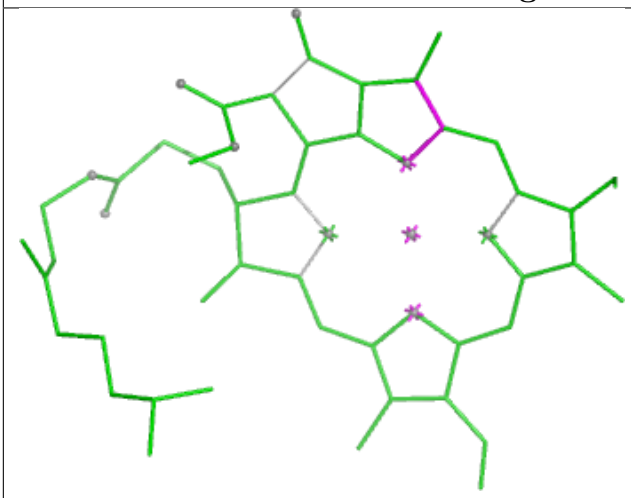


Rings

Ligand CLA 92 603



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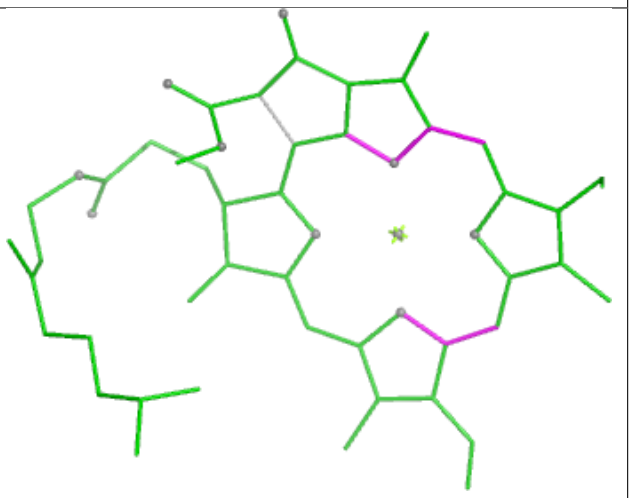

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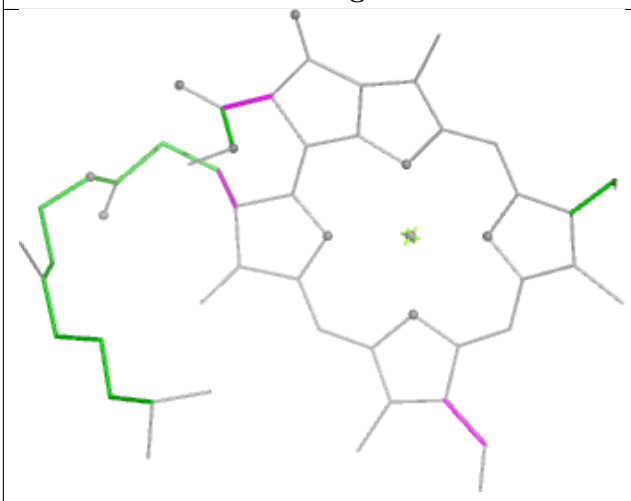

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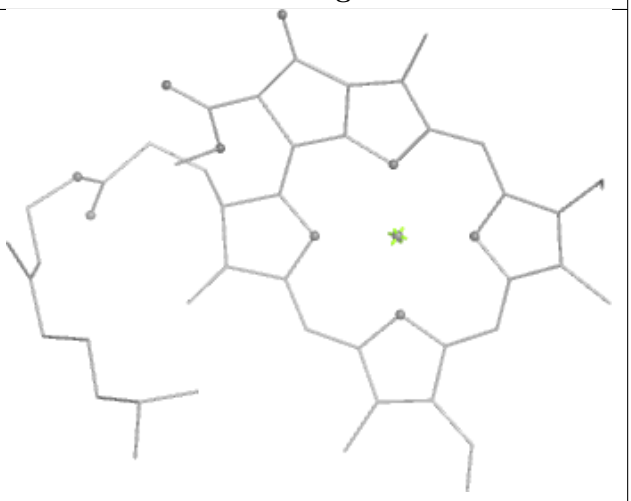
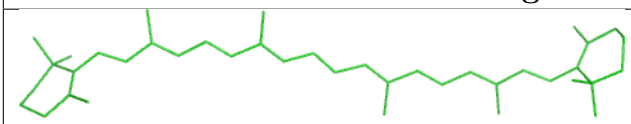


Rings

Ligand BCR A 849



Bond lengths



Bond angles

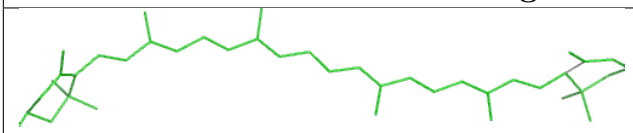


Torsions



Rings

Ligand LUT 12 617



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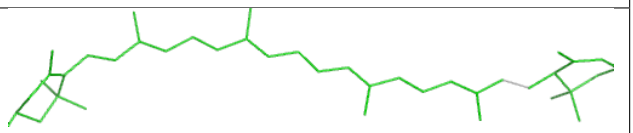
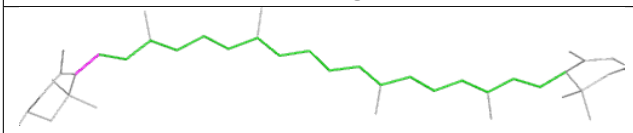


Bond angles



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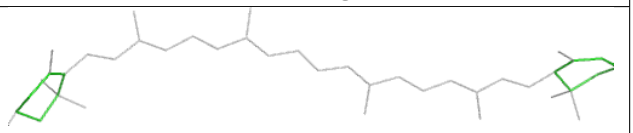
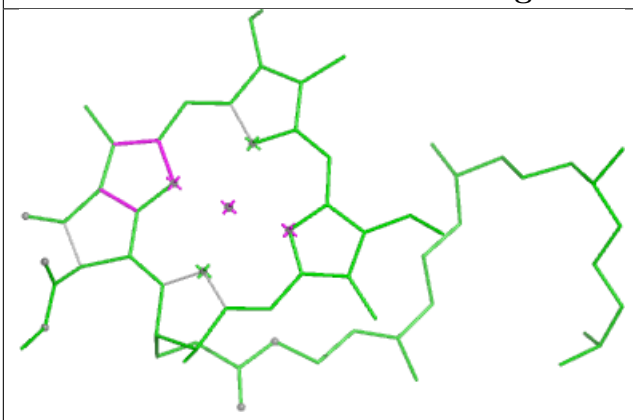


Rings

Ligand CLA A2 820



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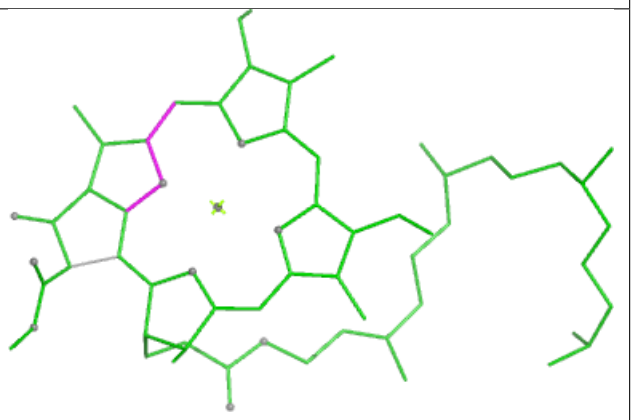
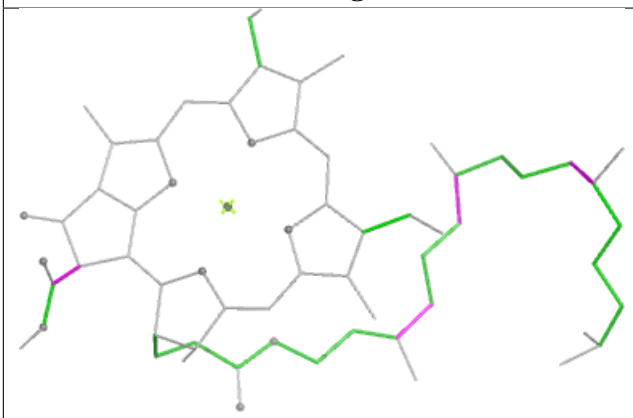


Bond angles



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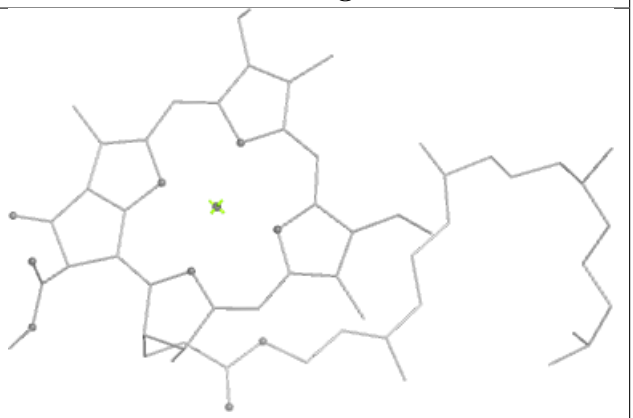
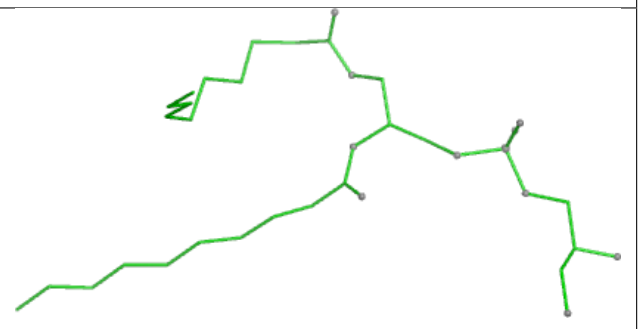


Rings

Ligand LHG 5 623



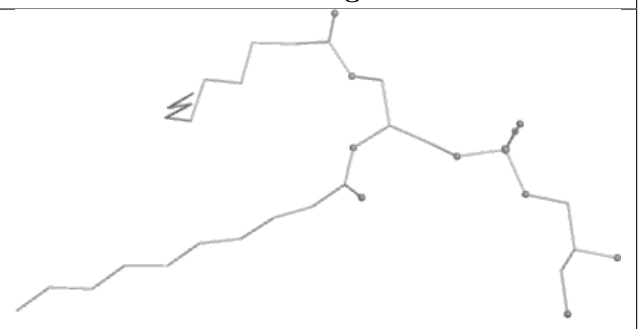
Bond lengths



Bond angles

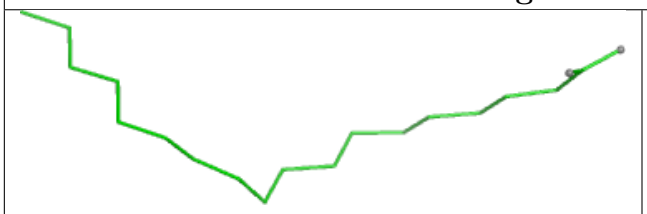


Torsions



Rings

Ligand LMG 62 633



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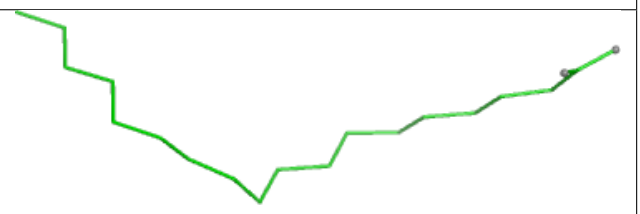
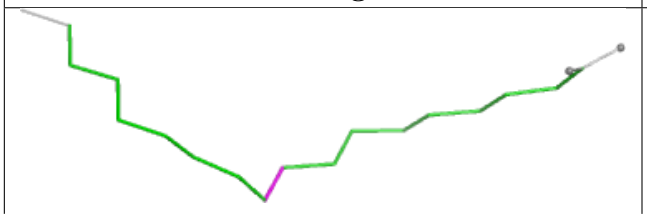


Bond angles

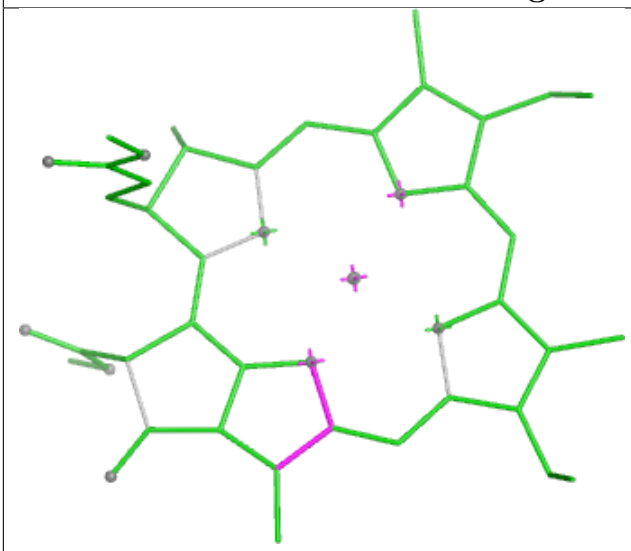


Torsions



Rings

Ligand CLA 9 601



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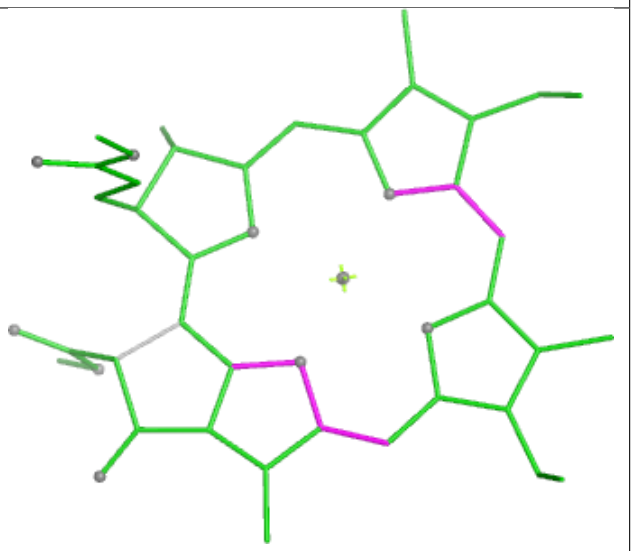

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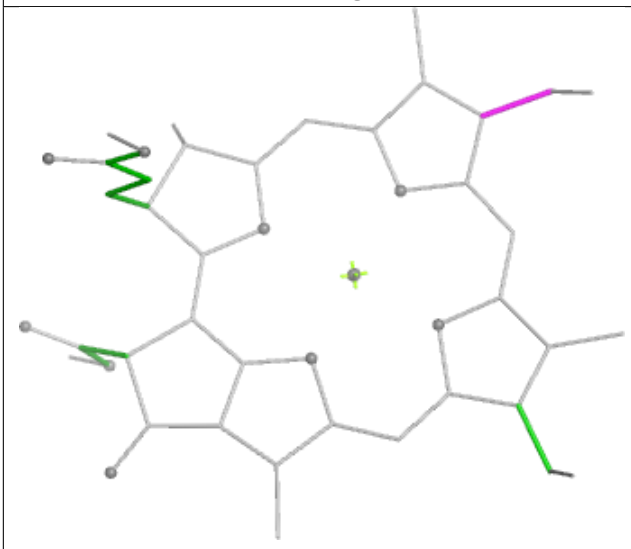

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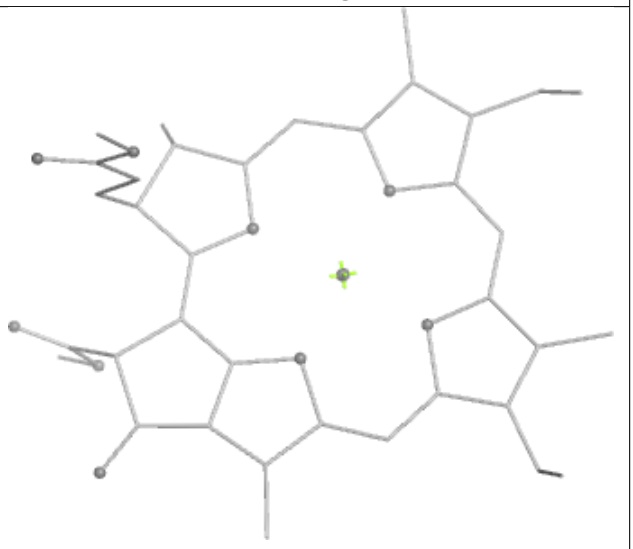
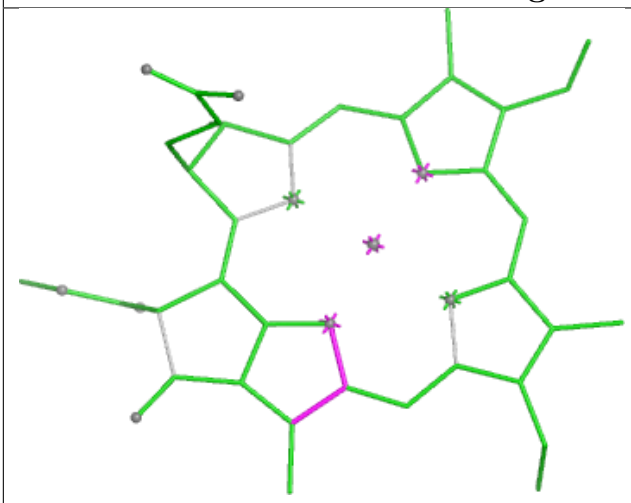


Rings

Ligand CLA 7 609



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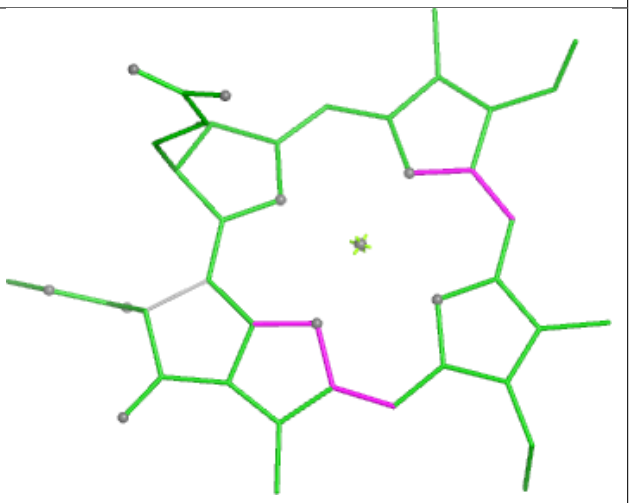
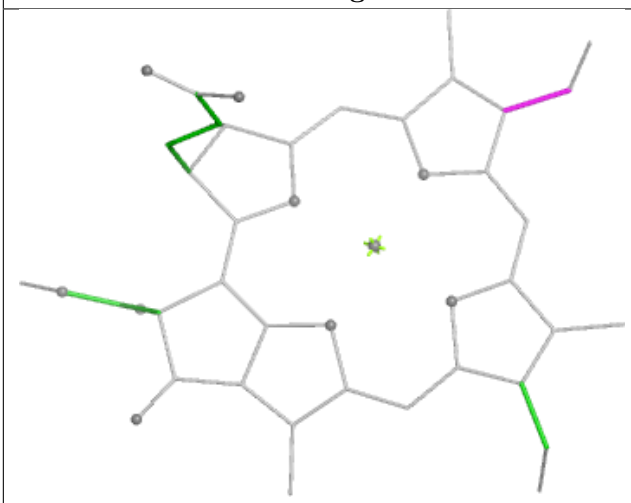


Bond angles



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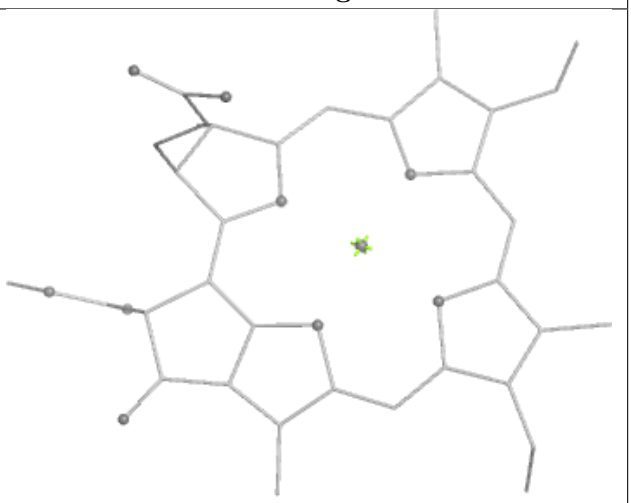
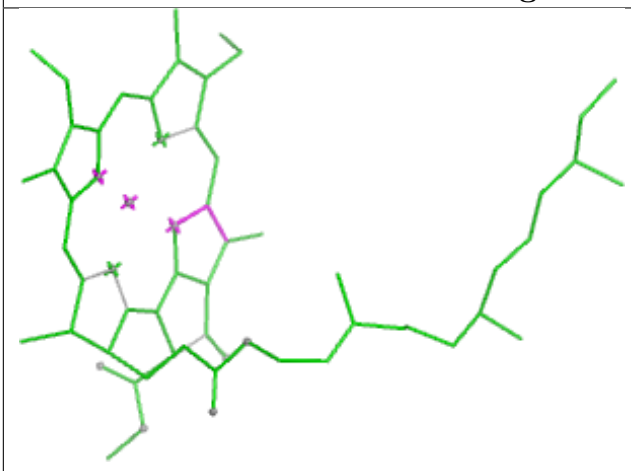


Rings

Ligand CLA 12 611



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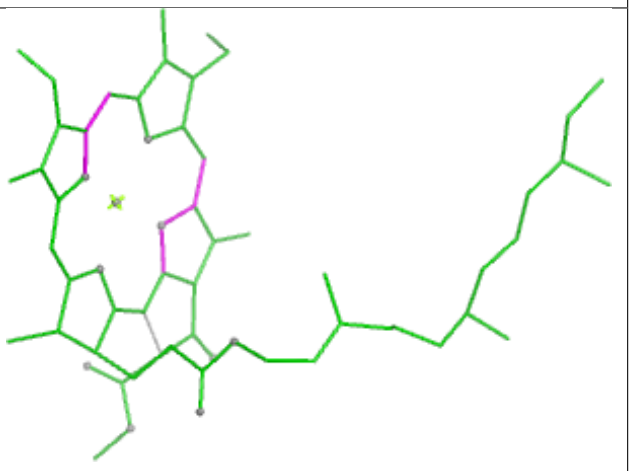
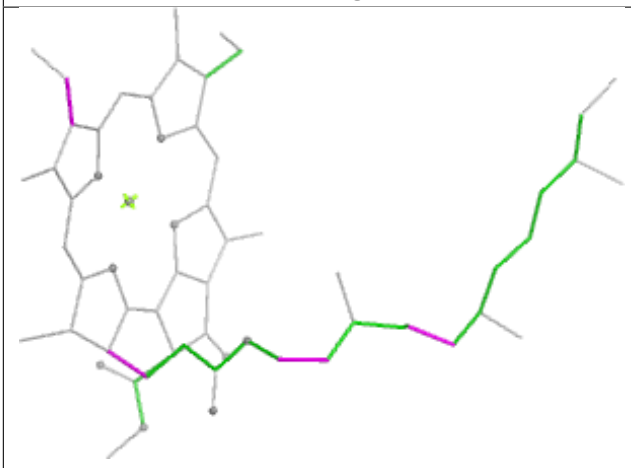


Bond angles

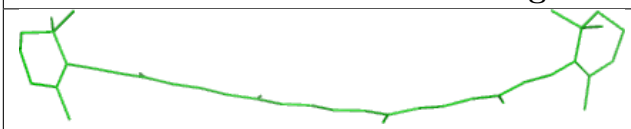


Torsions



Rings

Ligand BCR I 172



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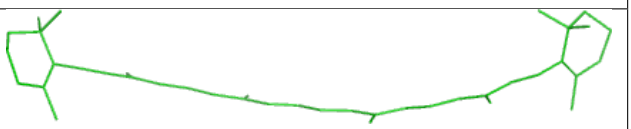
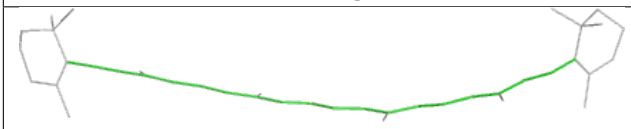


Bond angles



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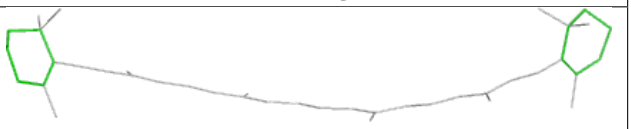
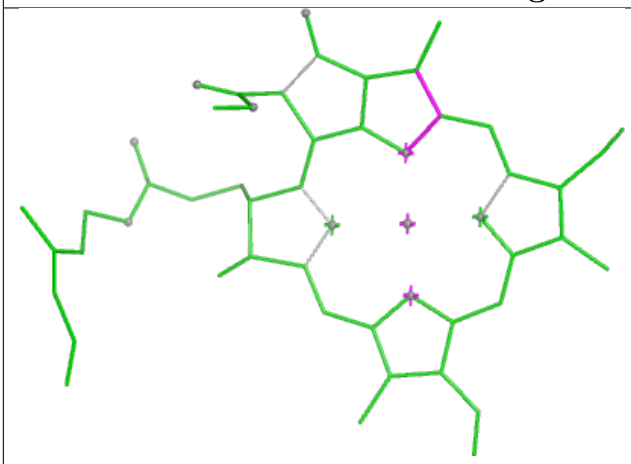


Rings

Ligand CLA 7 603



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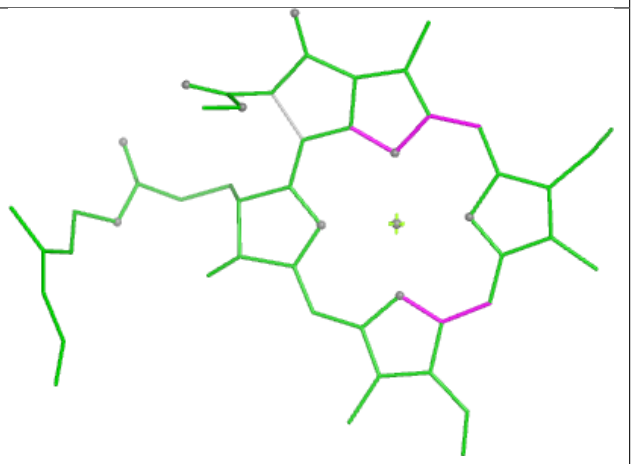

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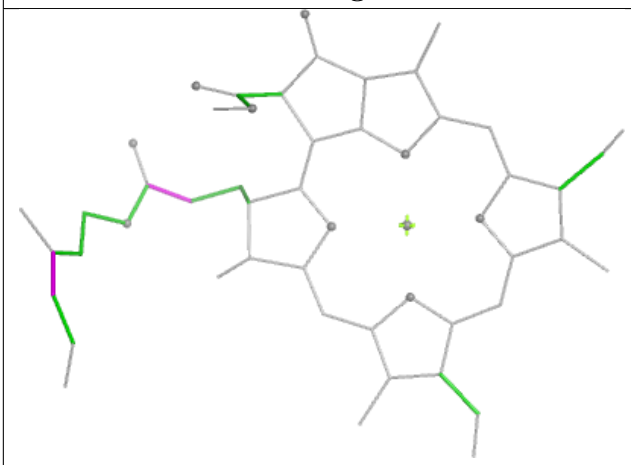

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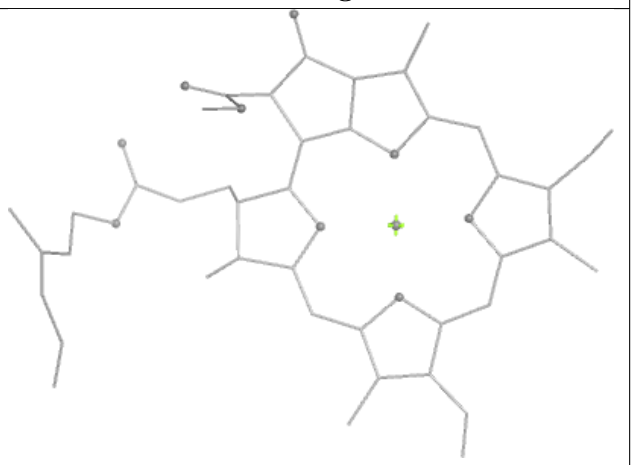
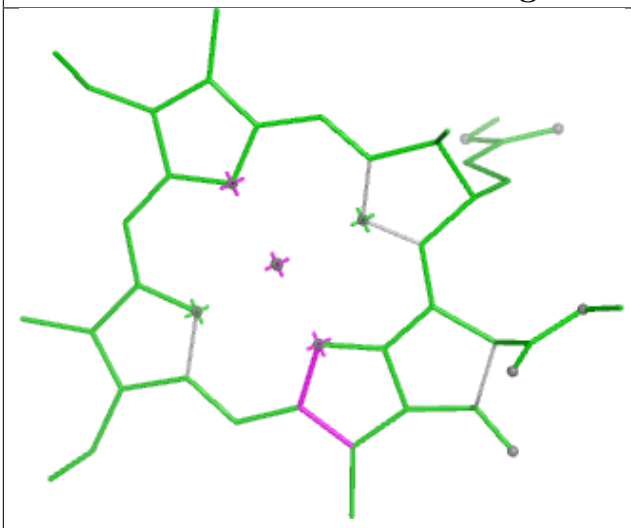


Rings

Ligand CLA 12 616



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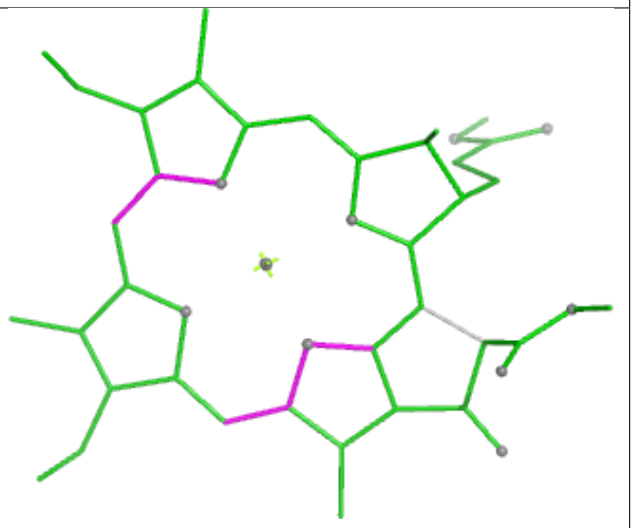
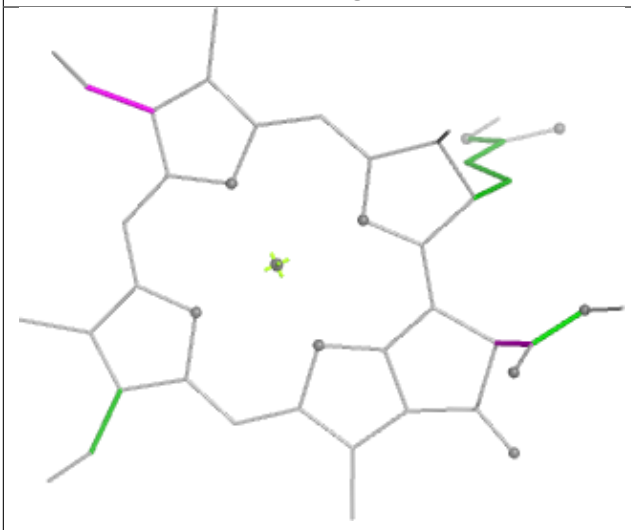


Bond angles



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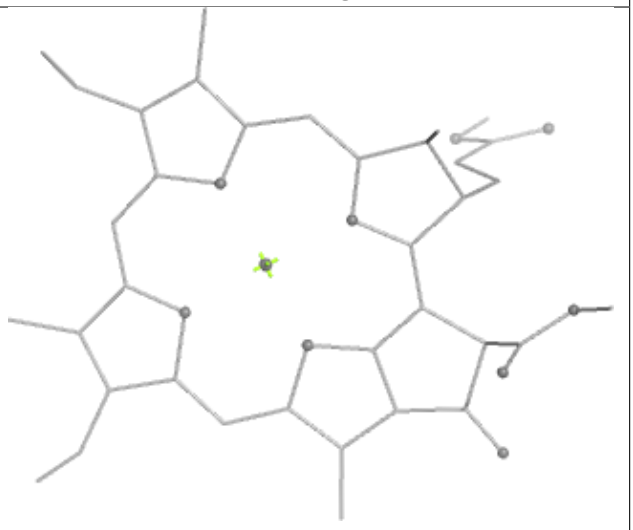
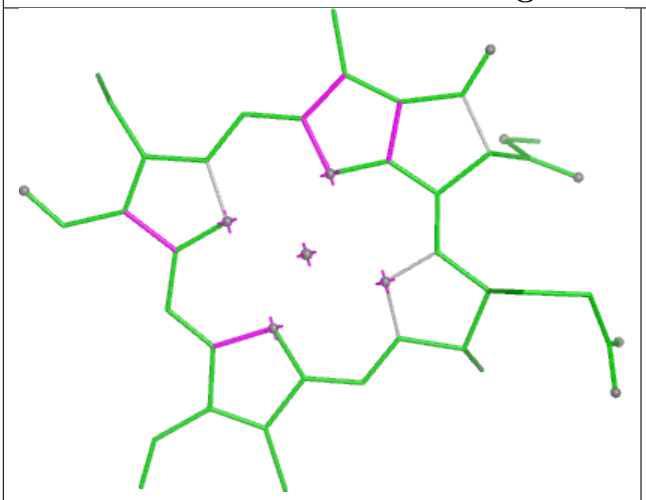


Rings

Ligand CHL Z2 606



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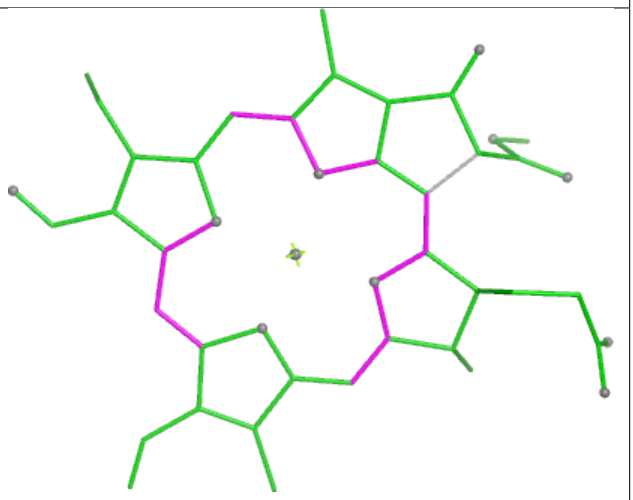
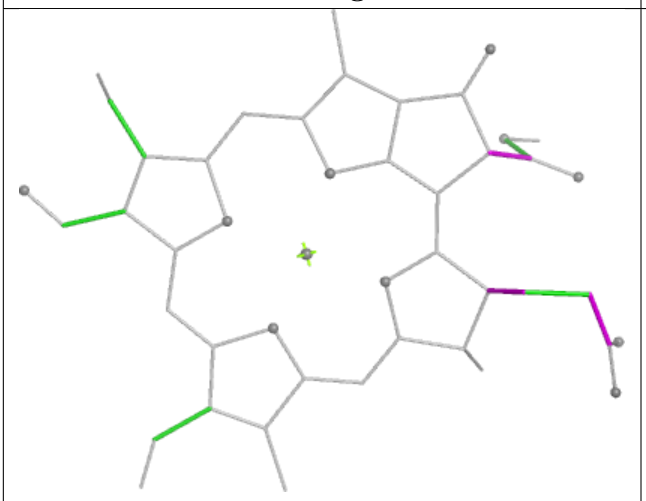


Bond angles



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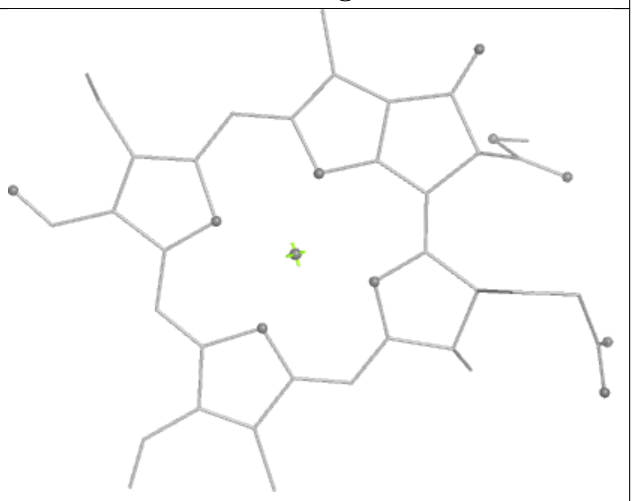
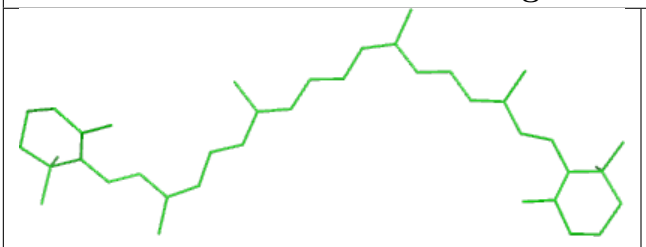


Rings

Ligand BCR A 852



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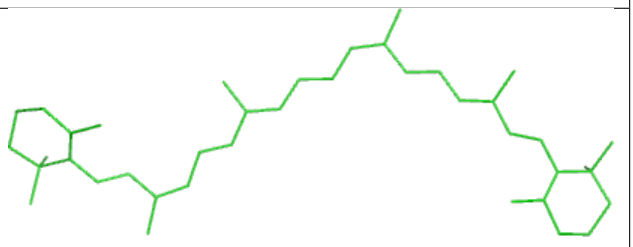
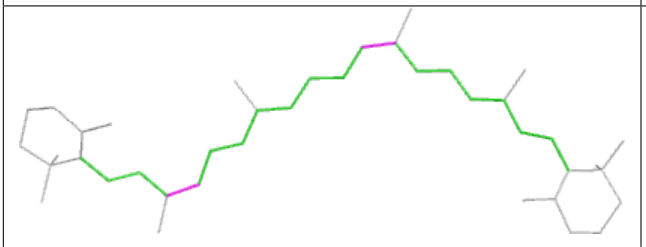


Bond angles

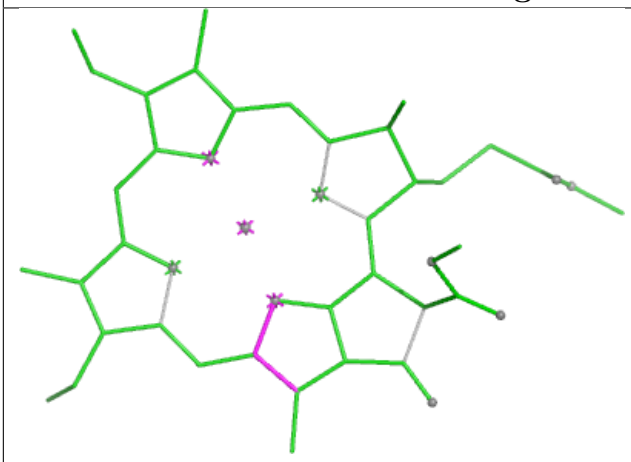


Torsions

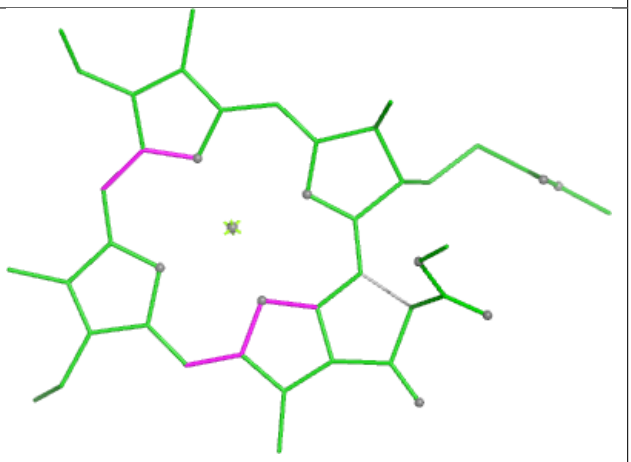


Rings

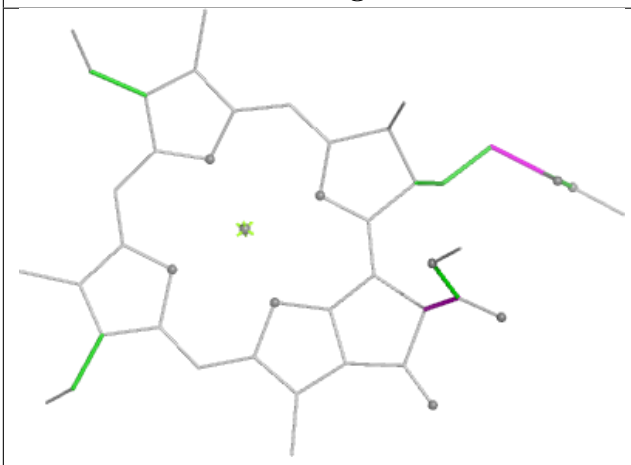
Ligand CLA G2 204



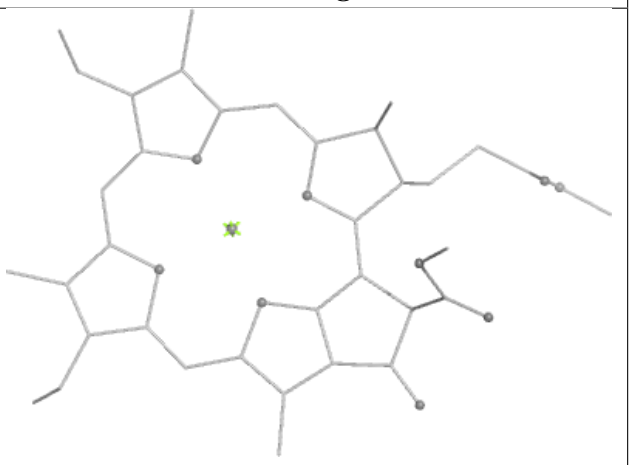
Bond lengths



Bond angles

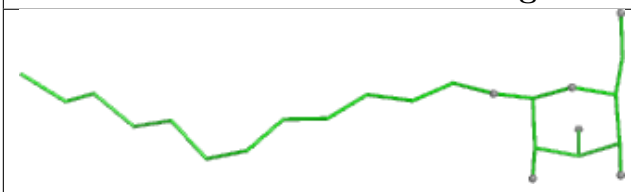


Torsions



Rings

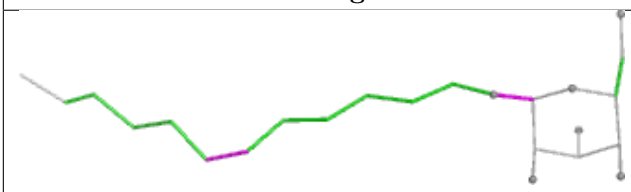
Ligand LMU A 865



Bond lengths



Bond angles



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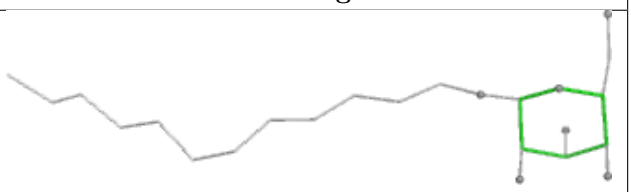
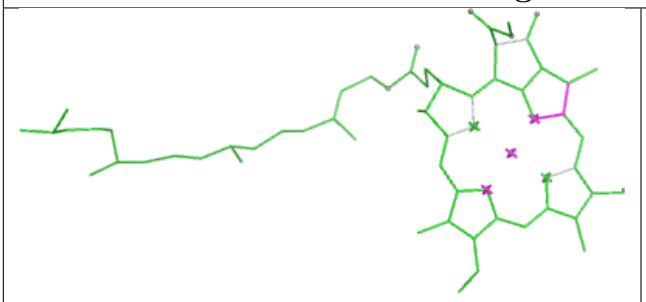


Rings

Ligand CLA A2 816



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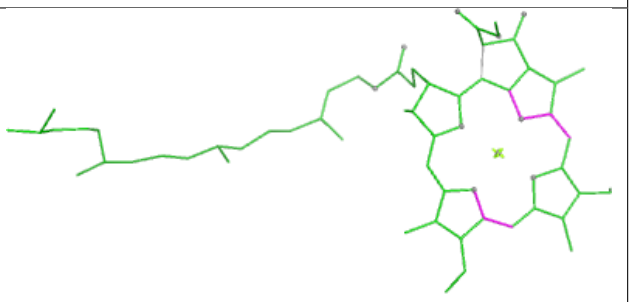

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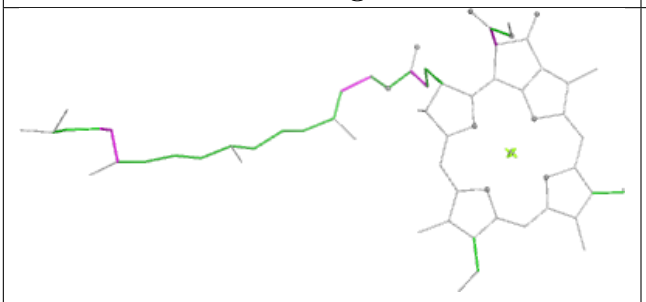

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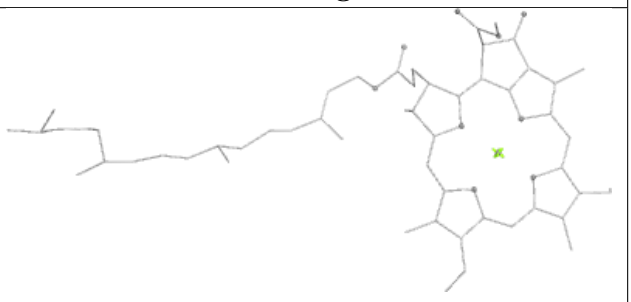
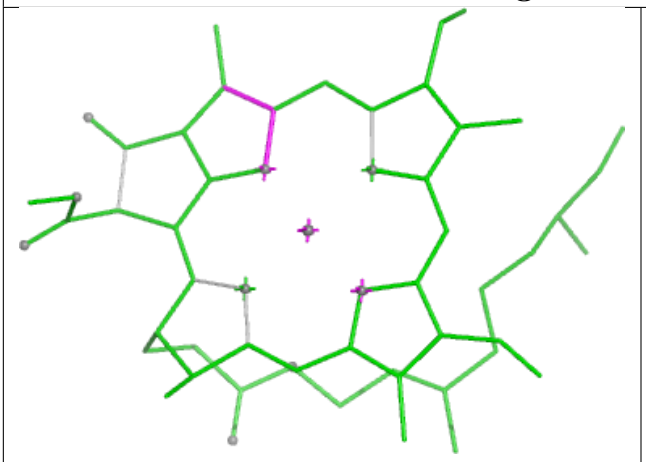


Rings

Ligand CLA B2 820



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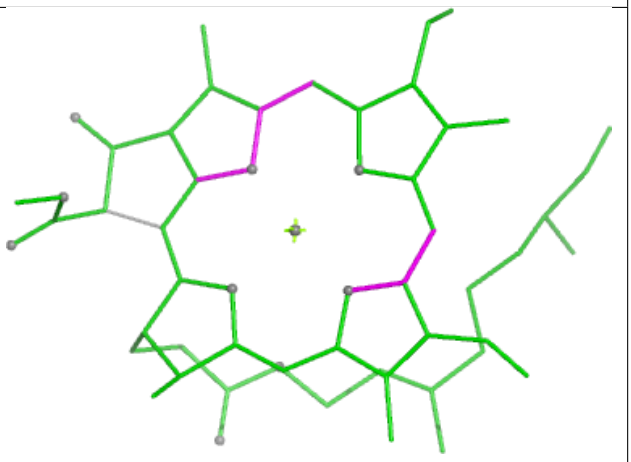

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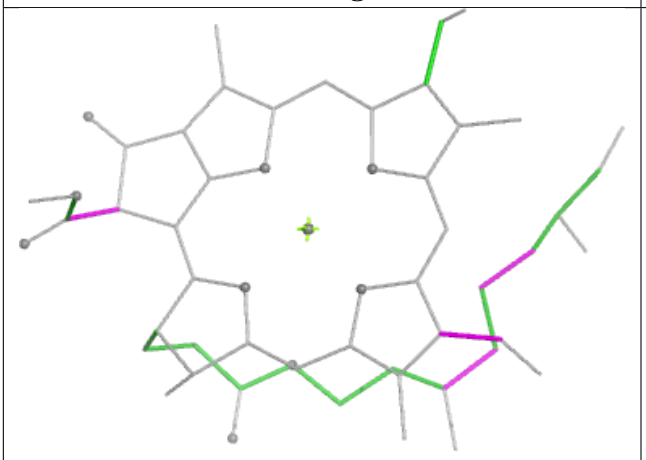

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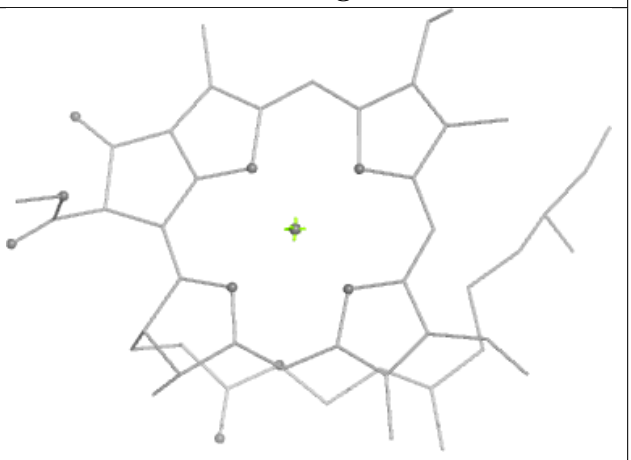
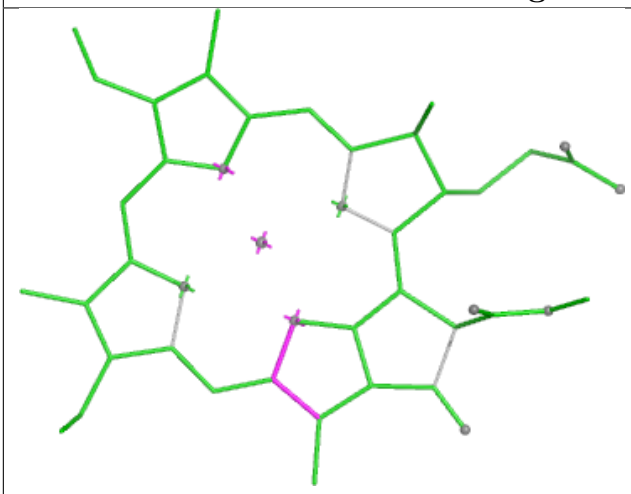


Rings

Ligand CLA 6 612



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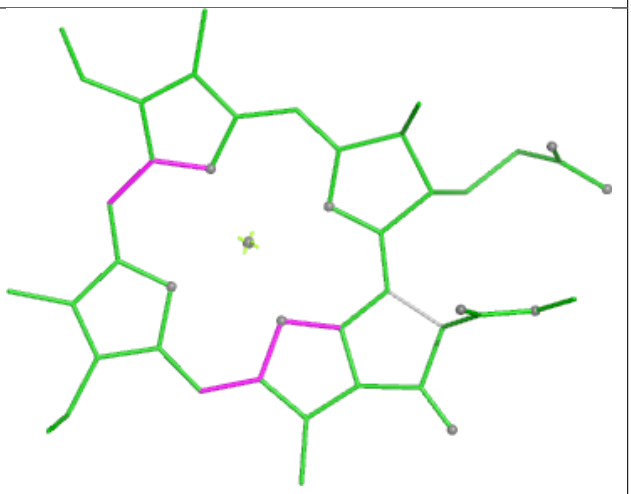

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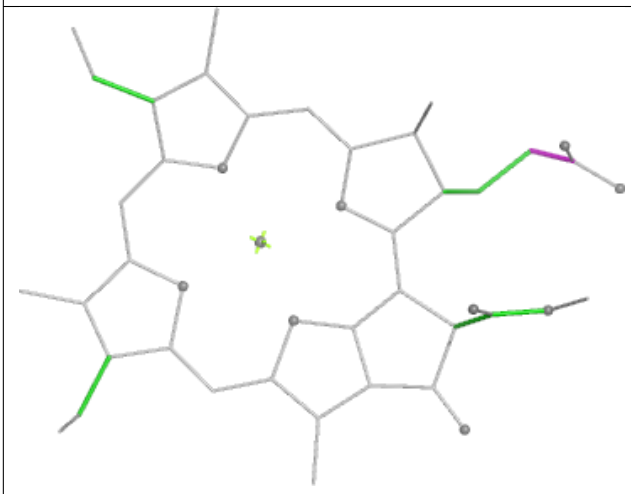

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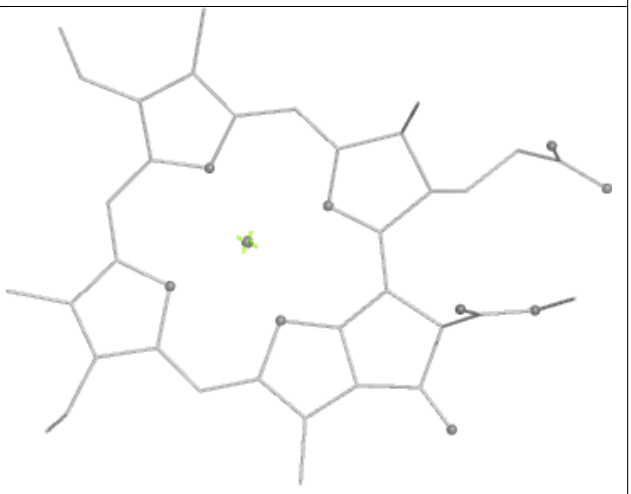
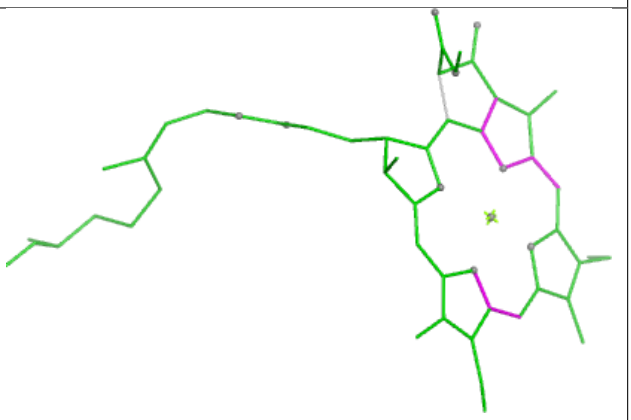


Rings

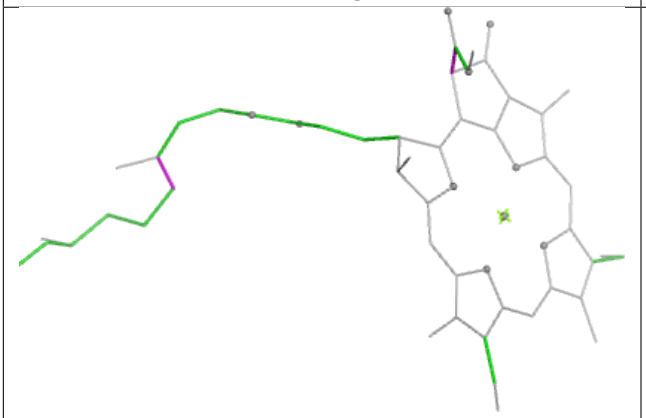
Ligand CLA B2 833



Bond lengths



Bond angles



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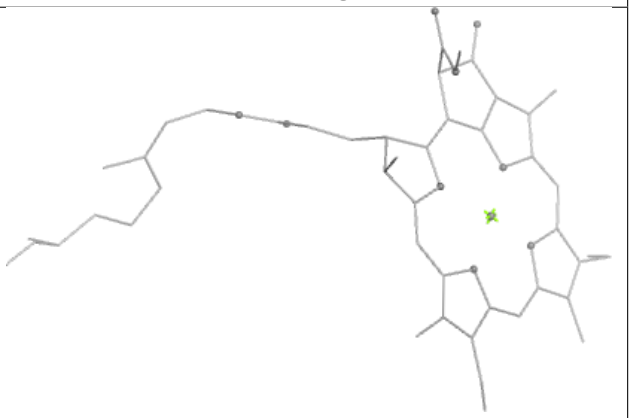
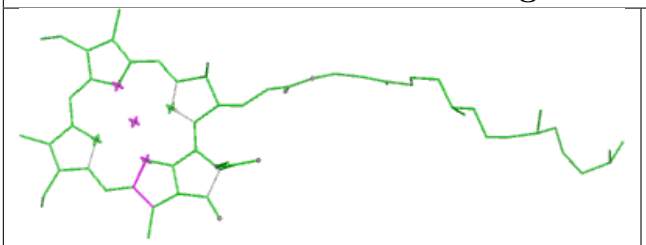


Rings

Ligand CLA 52 601



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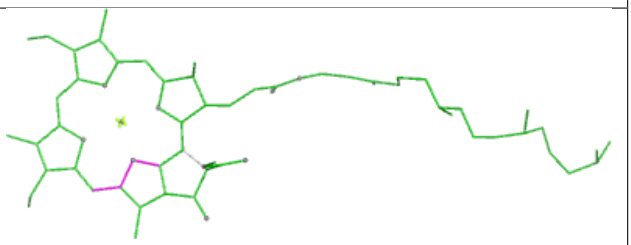
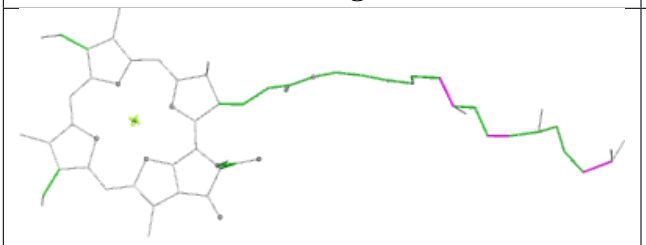


Bond angles



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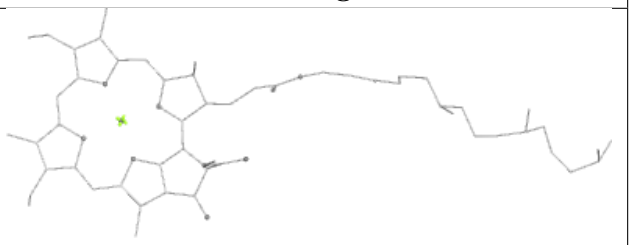
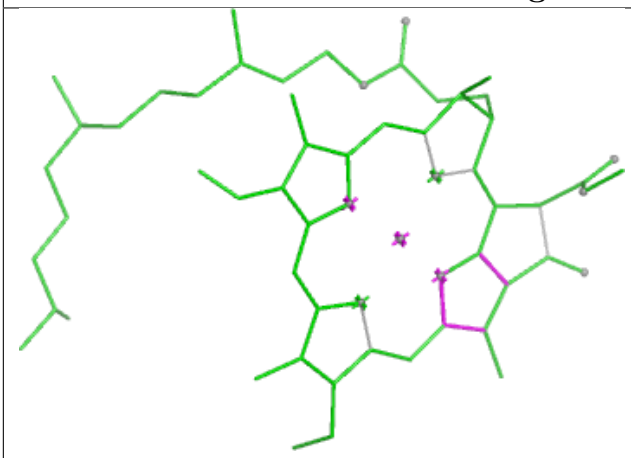


Rings

Ligand CLA 1 602



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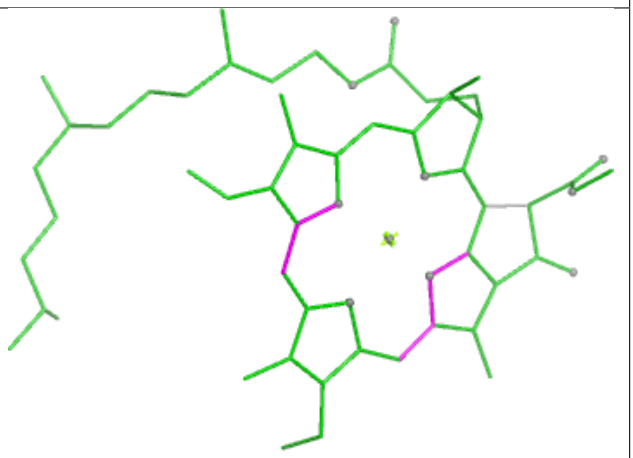
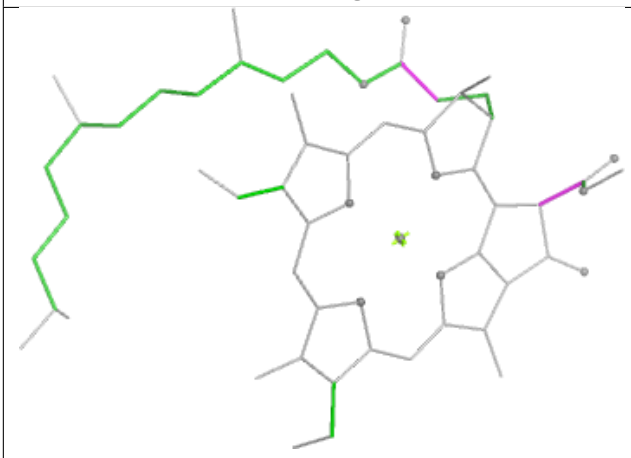


Bond angles

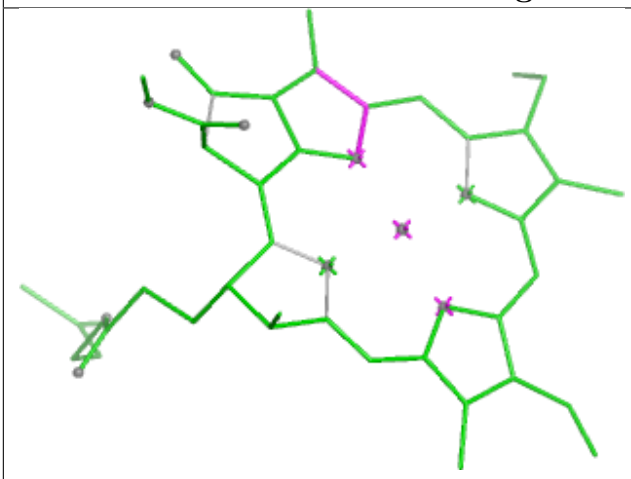


Torsions



Rings

Ligand CLA B2 838



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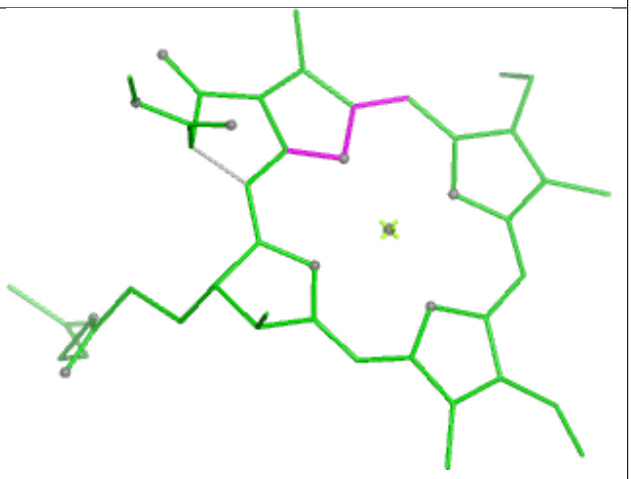

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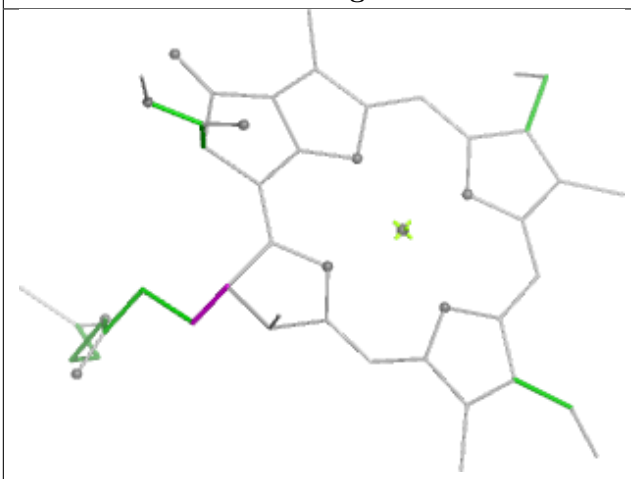

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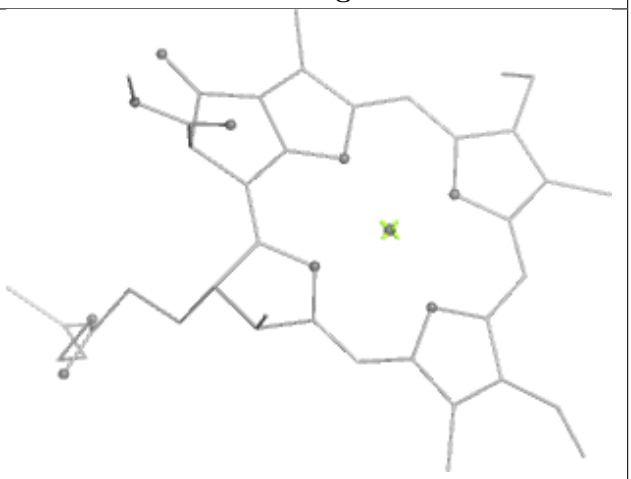
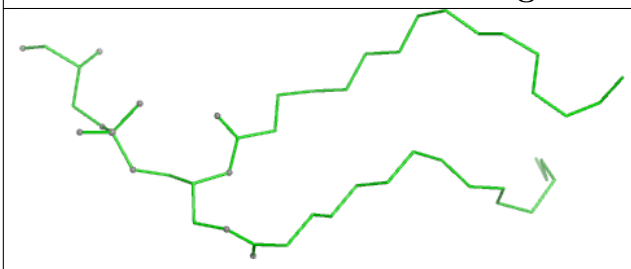


Rings

Ligand LHG 42 622



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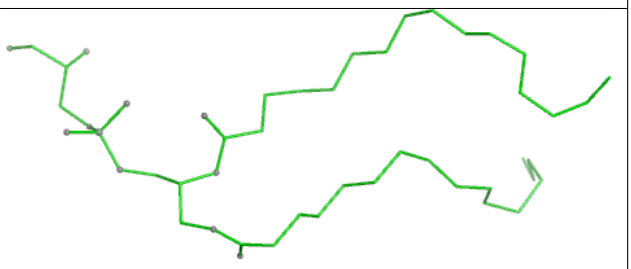
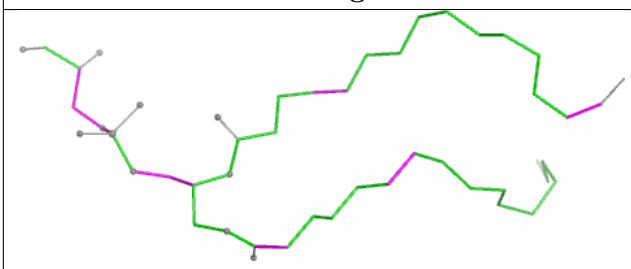


Bond angles



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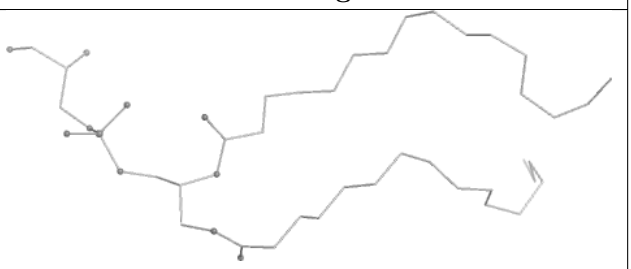
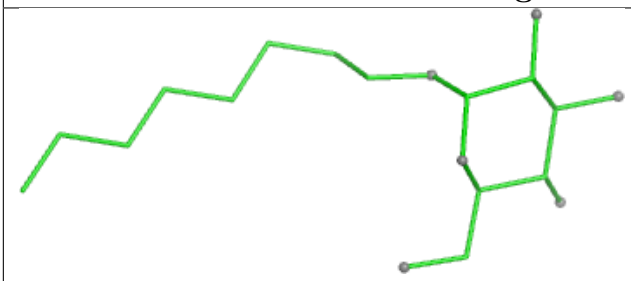


Rings

Ligand LMU 42 626



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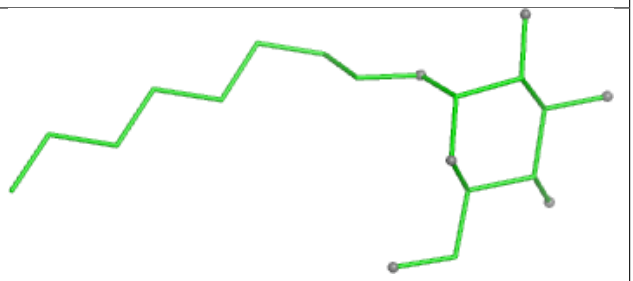

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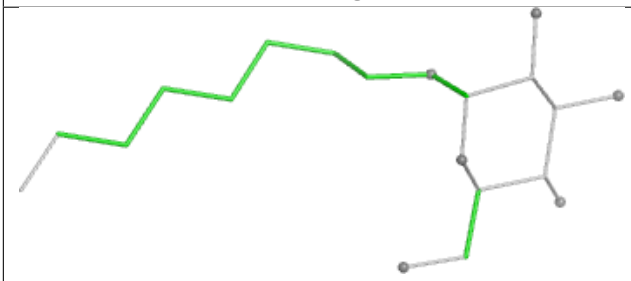

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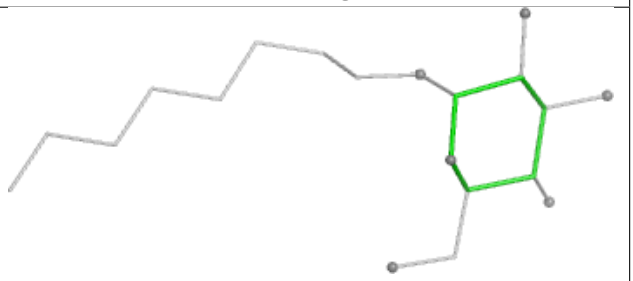
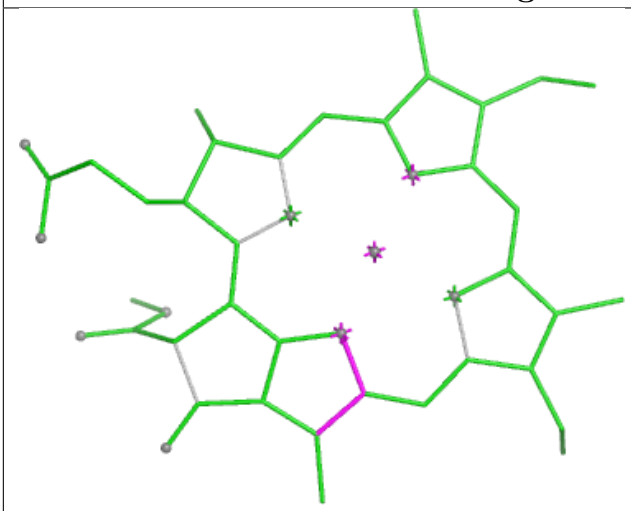


Rings

Ligand CLA Z2 612



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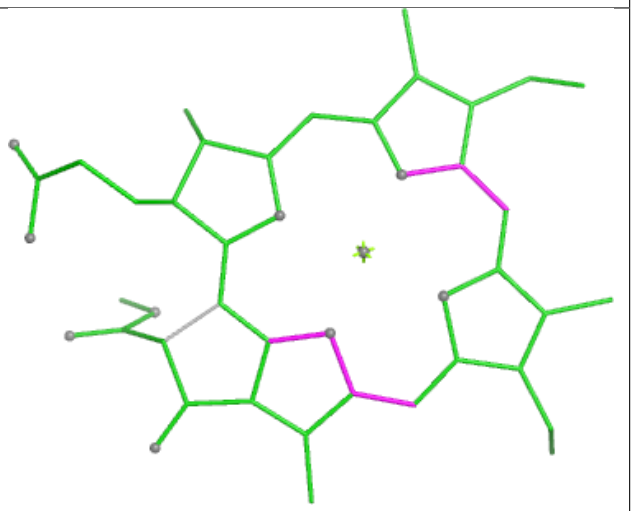
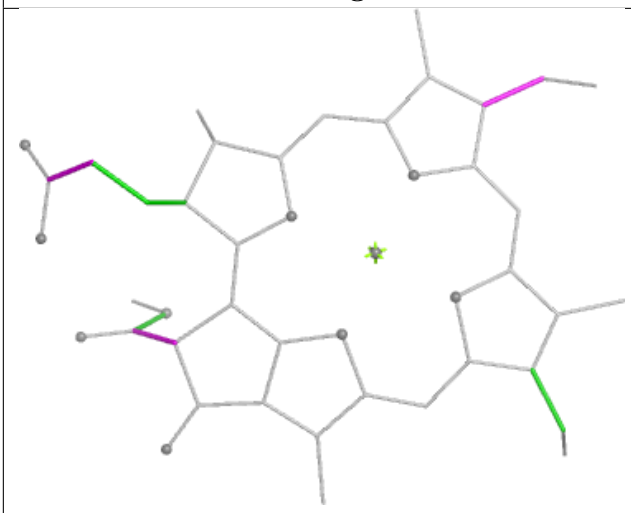


Bond angles



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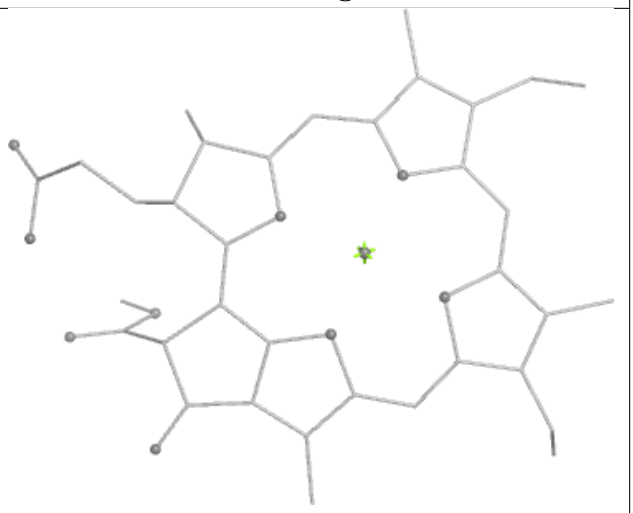
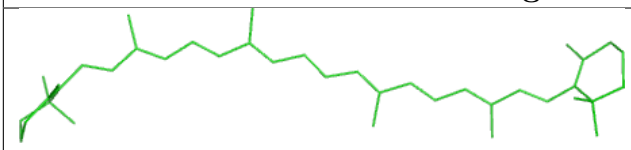


Rings

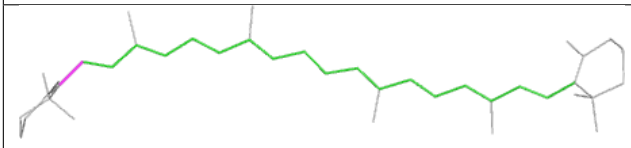
Ligand BCR B 848



Bond lengths



Bond angles



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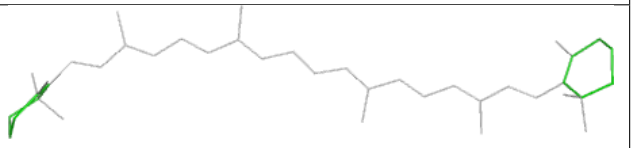
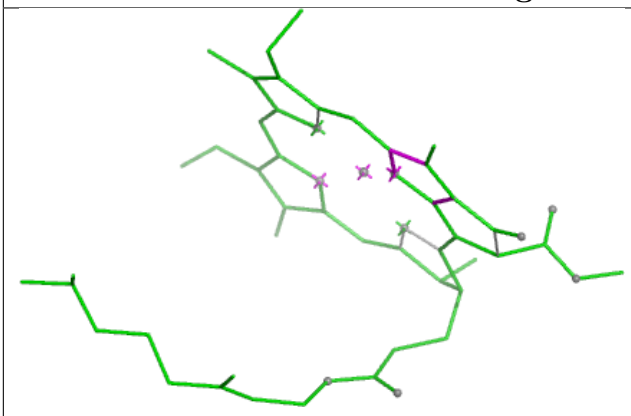
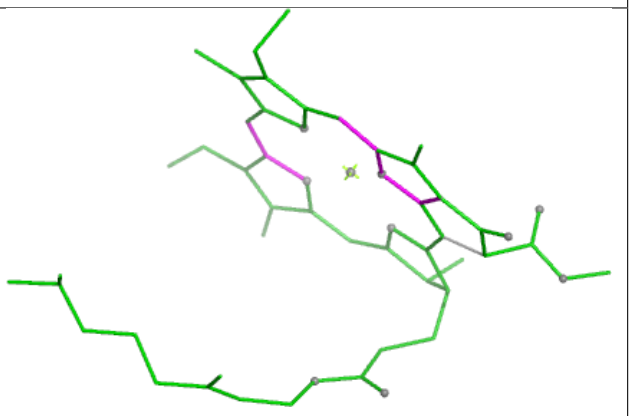


Rings

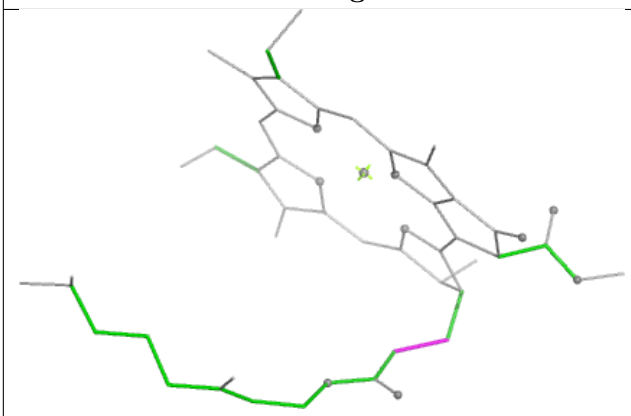
Ligand CLA B2 831



Bond lengths



Bond angles



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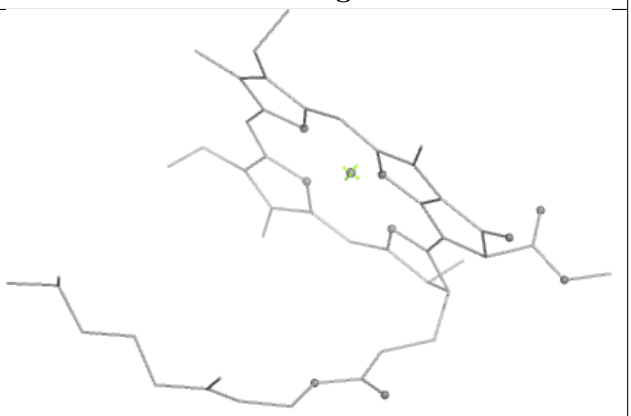
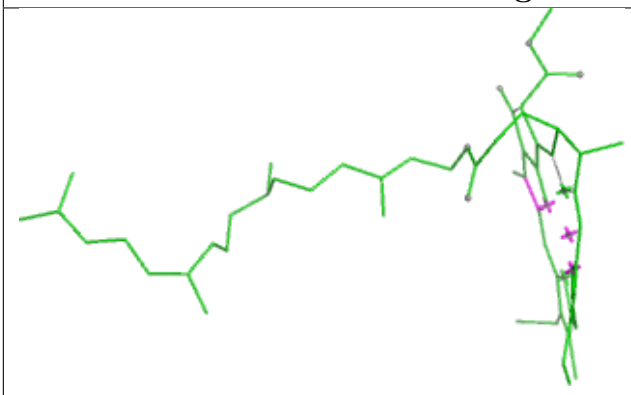


Rings

Ligand CLA A2 829



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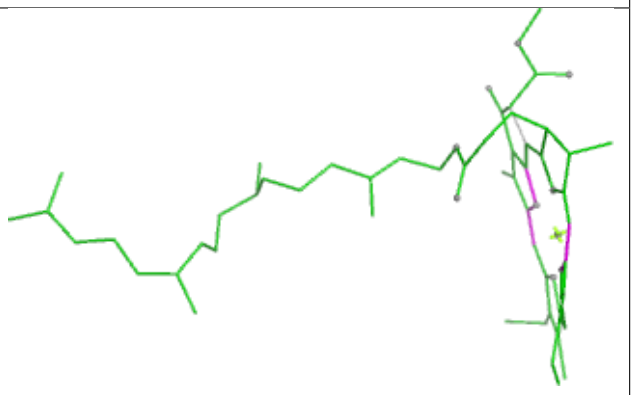
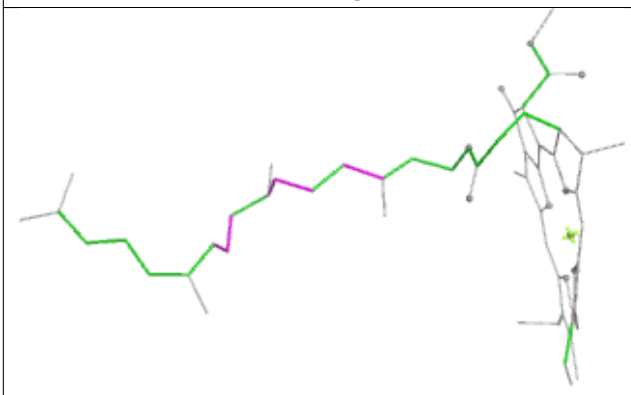


Bond angles



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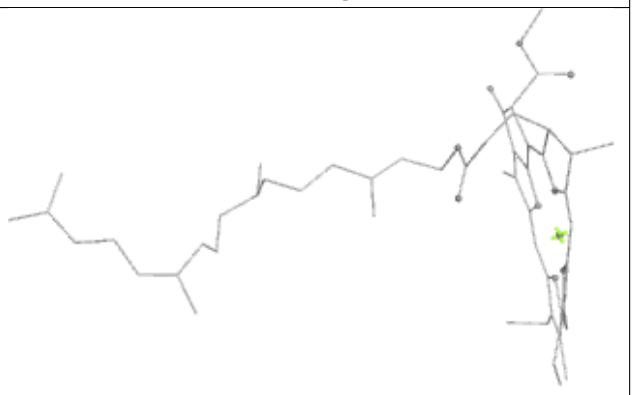
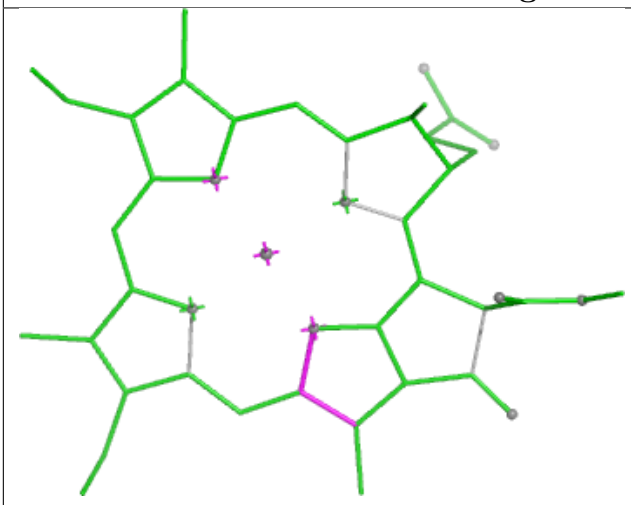
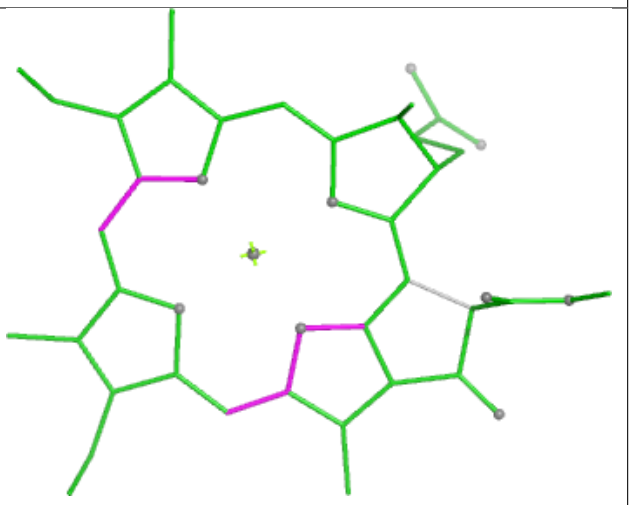


Rings

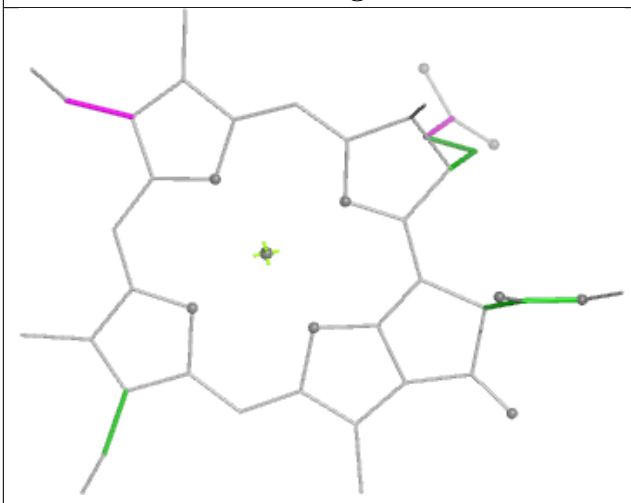
Ligand CLA 52 614



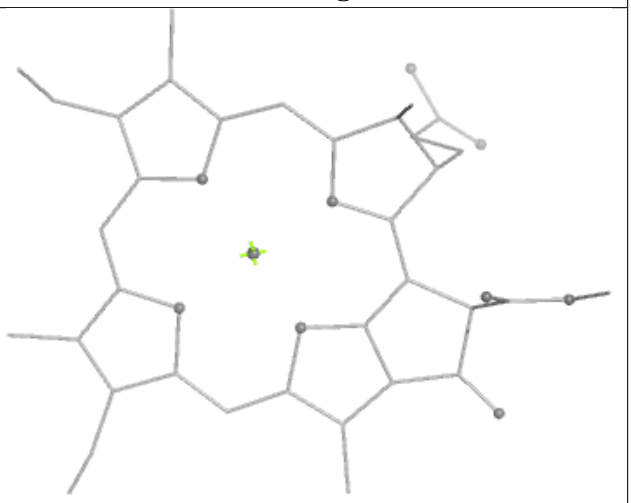
Bond lengths



Bond angles

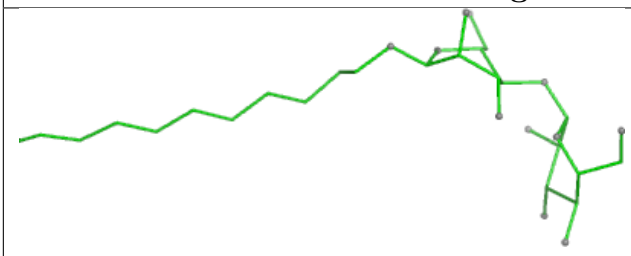


Torsions

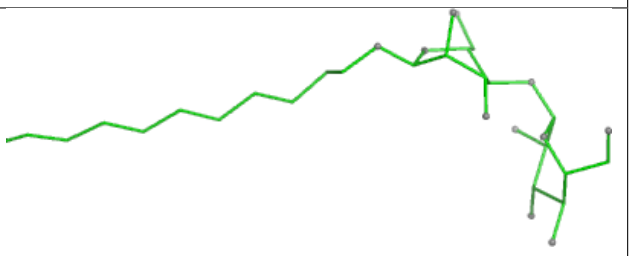


Rings

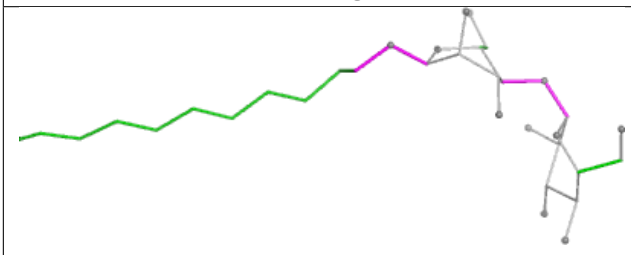
Ligand LMU A2 863



Bond lengths



Bond angles



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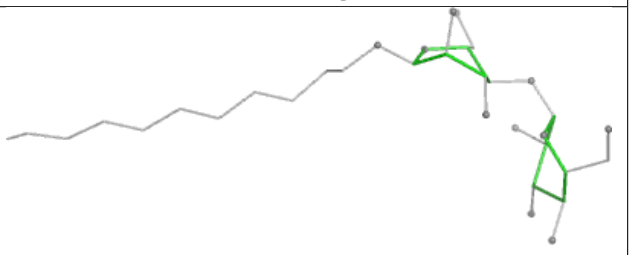
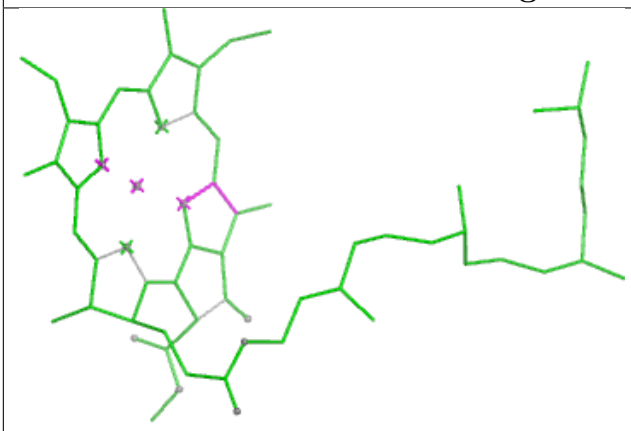


Rings

Ligand CLA 32 611



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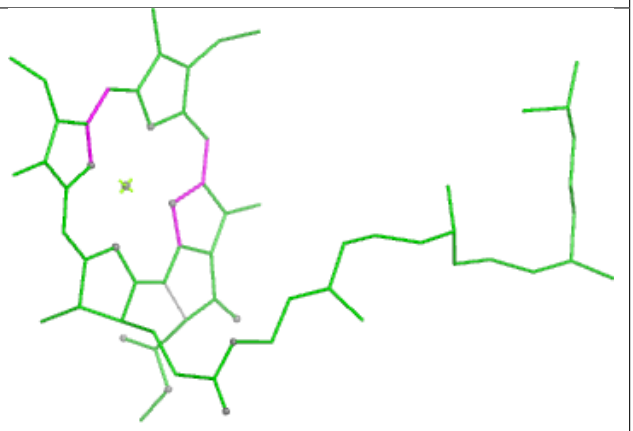

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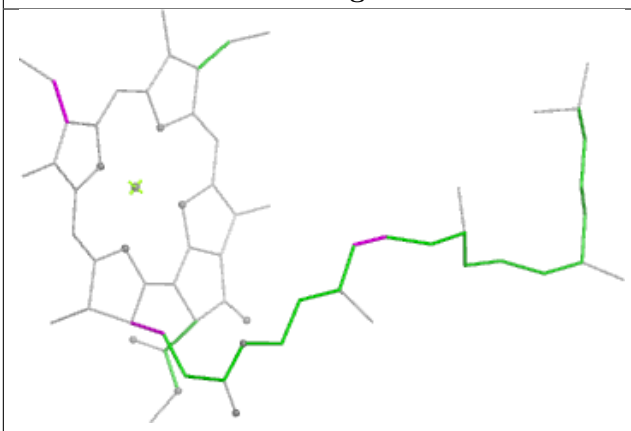
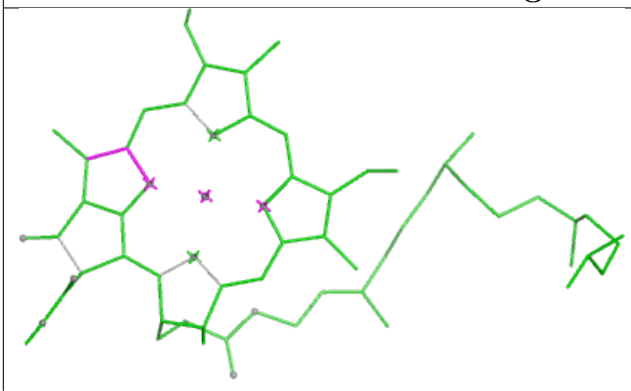


Torsions



Rings

Ligand CLA B 818



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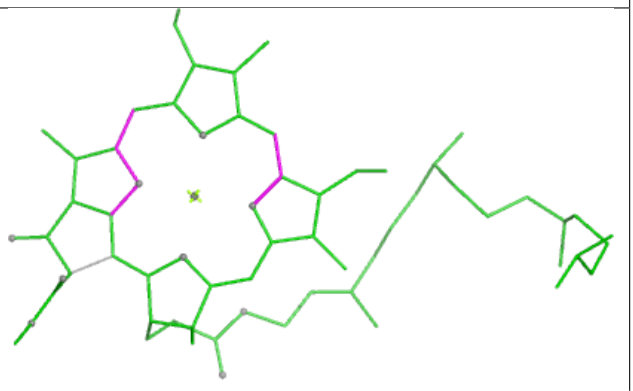
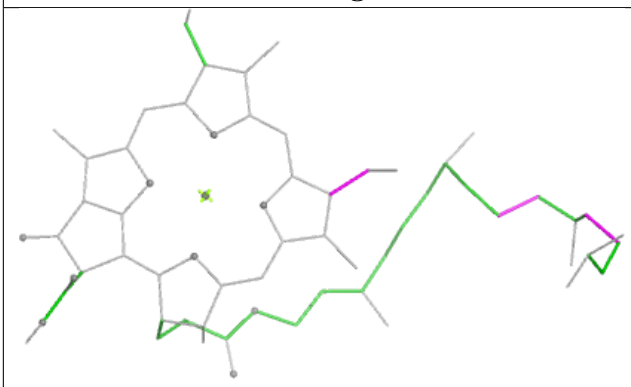


Bond angles



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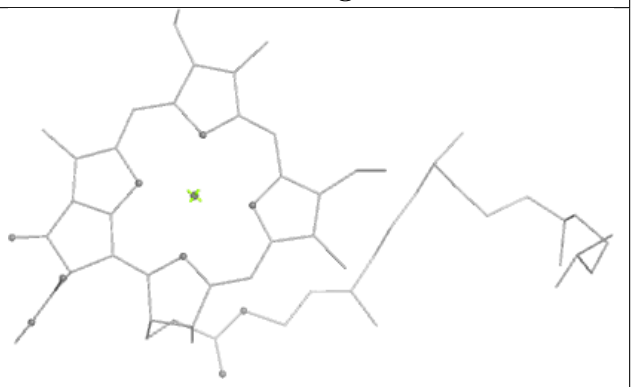
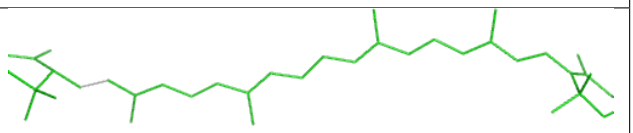


Rings

Ligand LUT 92 616



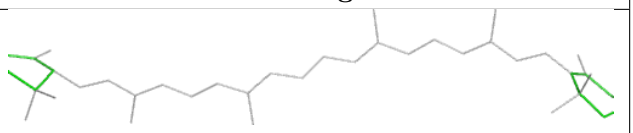
Bond lengths



Bond angles

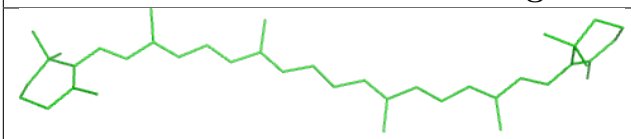


Torsions



Rings

Ligand BCR 6 623



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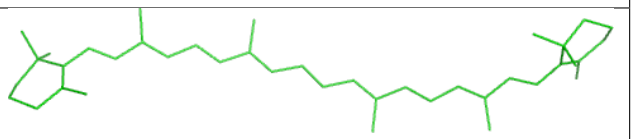
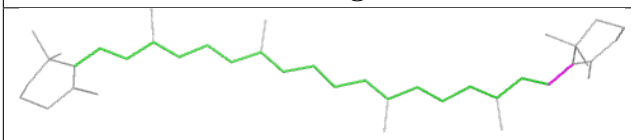


Bond angles



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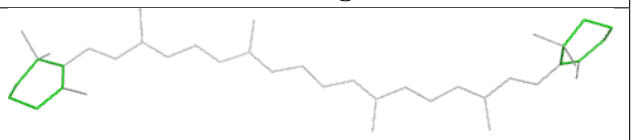
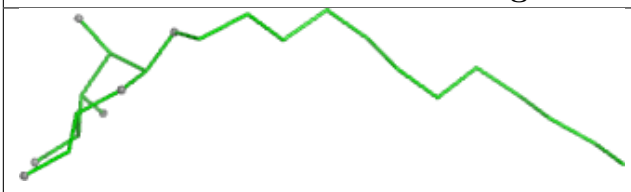


Rings

Ligand LMU A2 861



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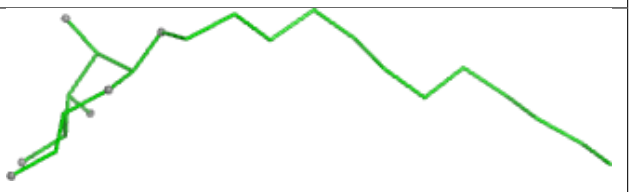
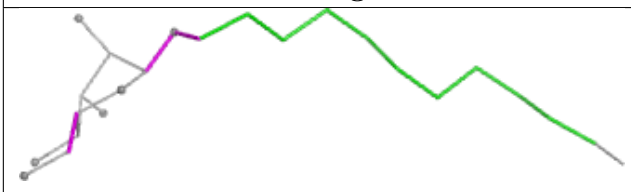


Bond angles



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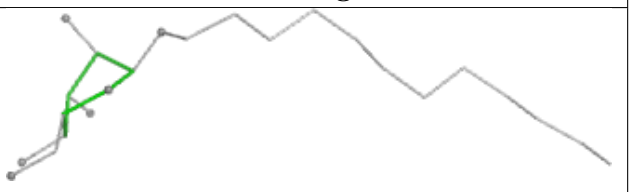
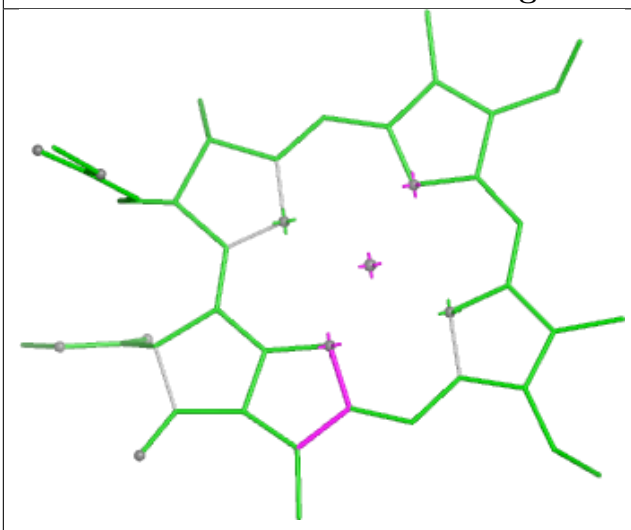


Rings

Ligand CLA 32 617



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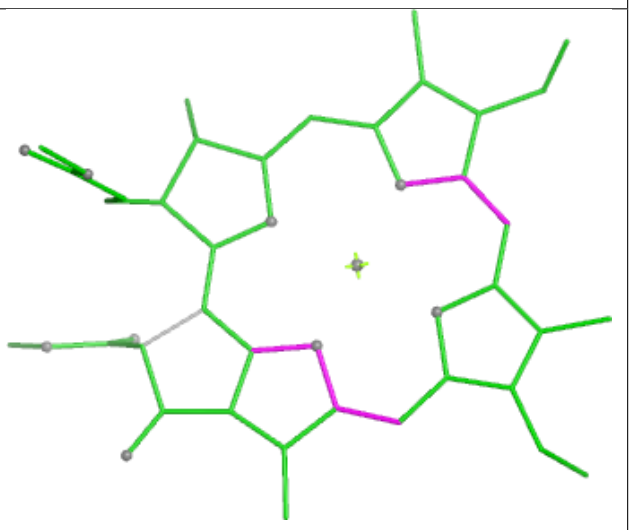
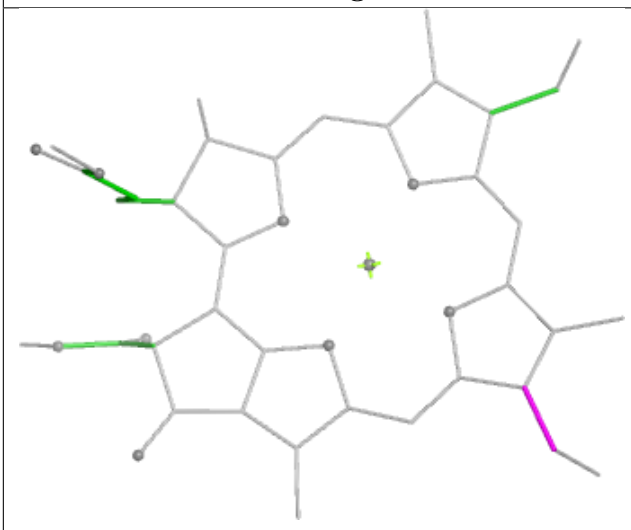


Bond angles



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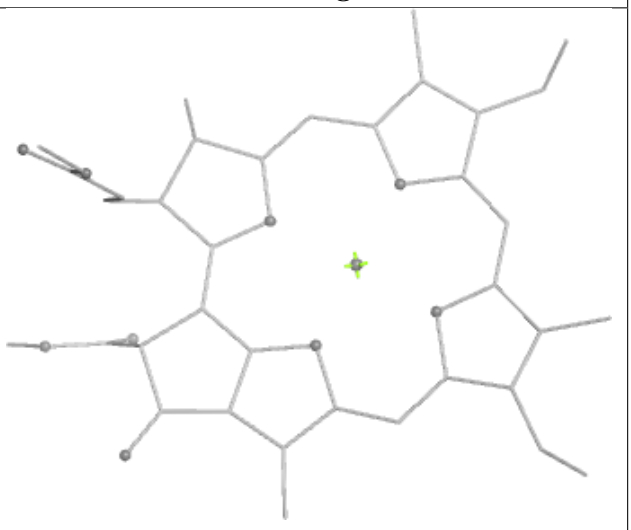
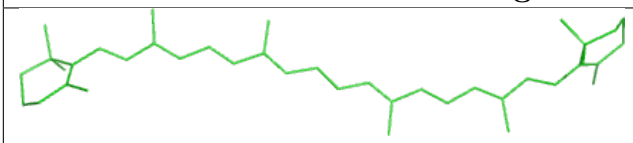


Rings

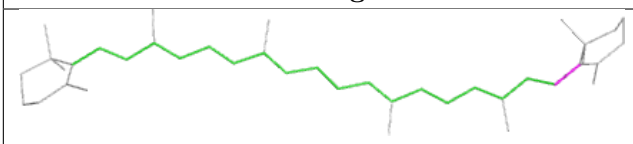
Ligand BCR B2 846



Bond lengths



Bond angles



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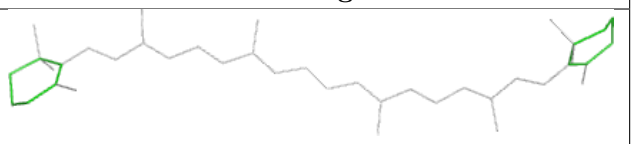
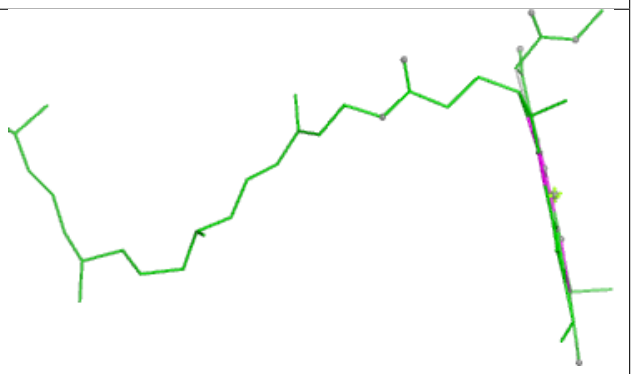


Rings

Ligand CHL 42 601



Bond lengths



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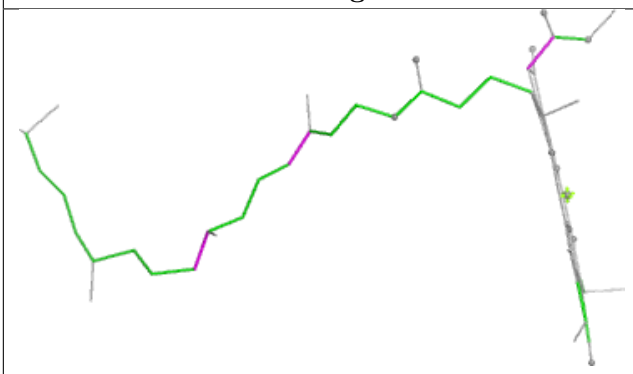

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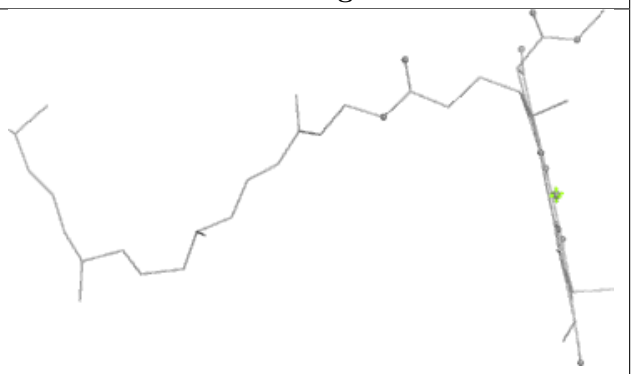
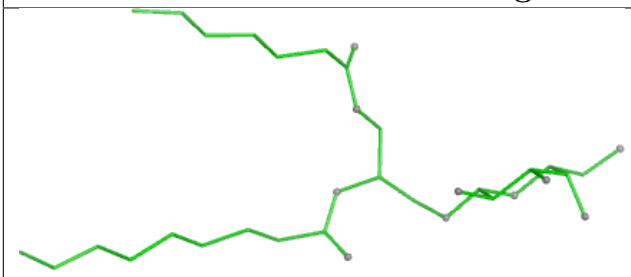


Rings

Ligand LMG J2 104



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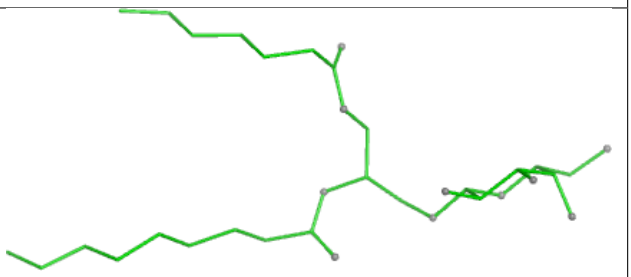
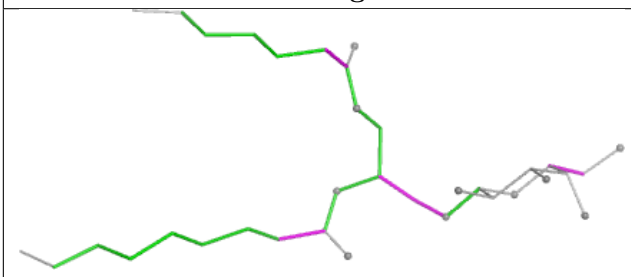


Bond angles



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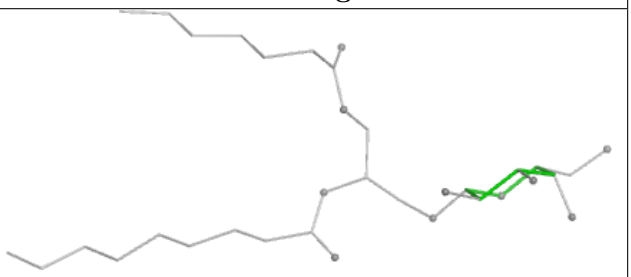
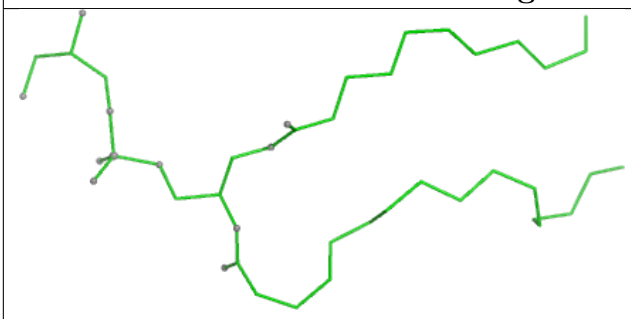


Rings

Ligand LHG 82 620



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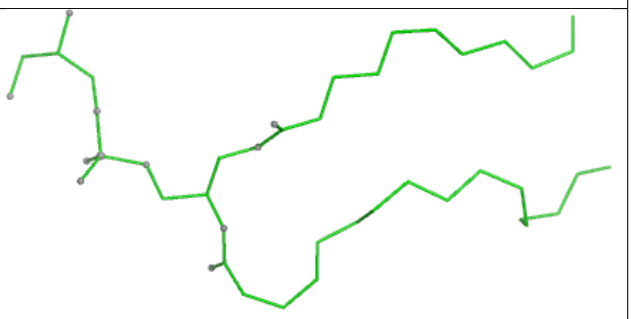
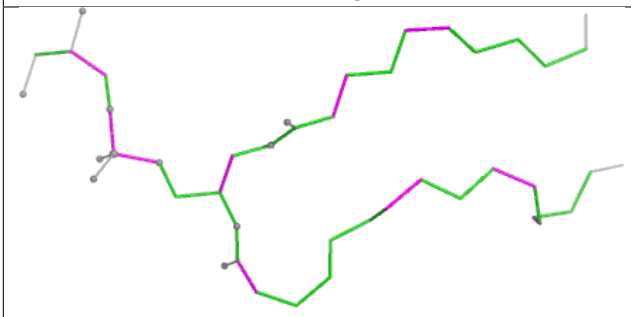


Bond angles



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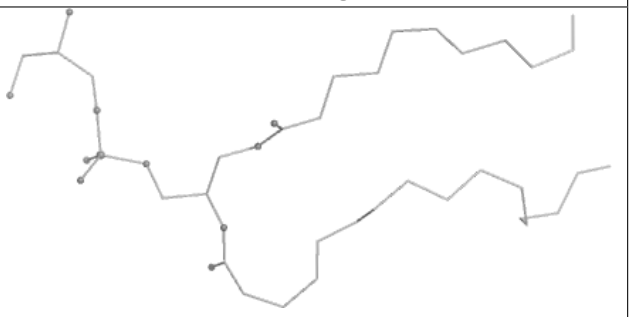
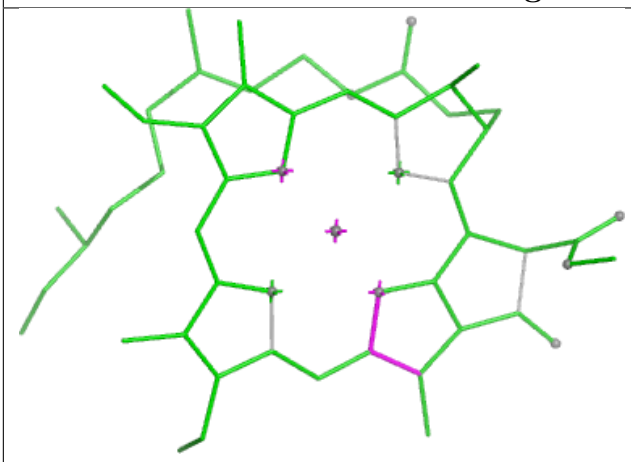


Rings

Ligand CLA B 820



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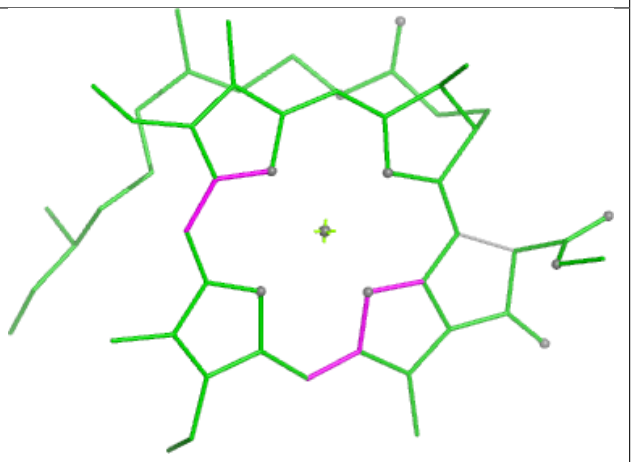
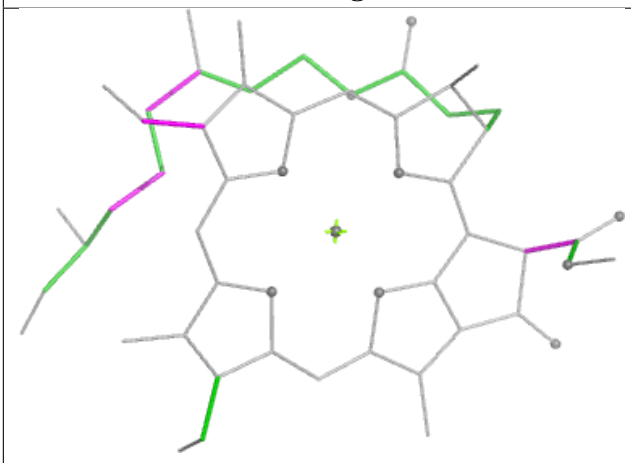


Bond angles



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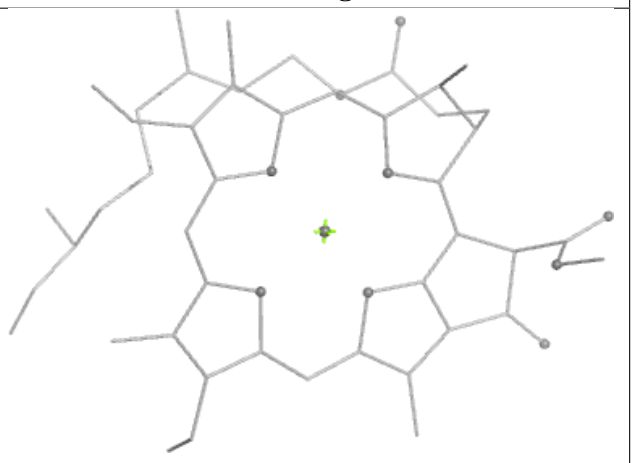
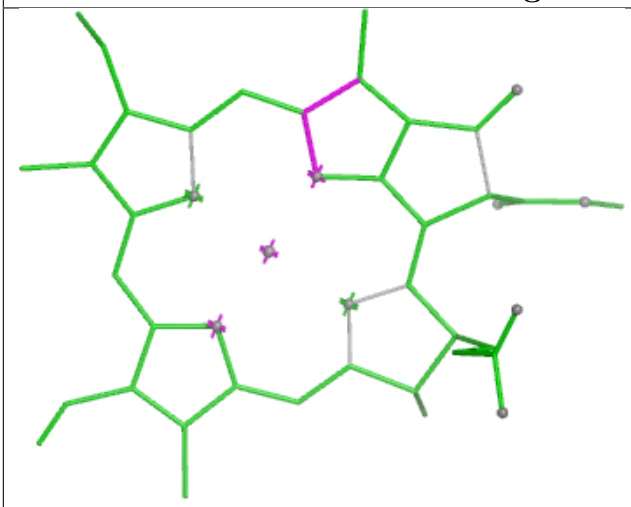


Rings

Ligand CLA A 824



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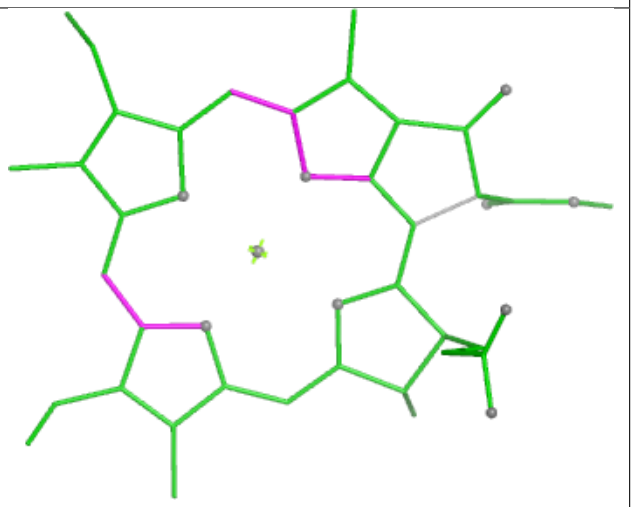
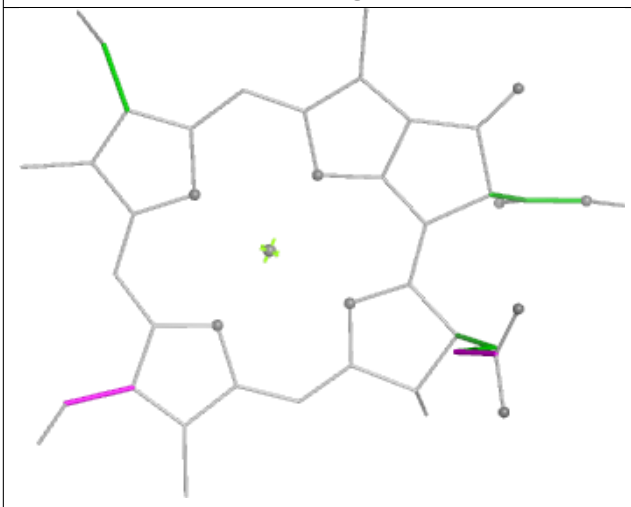


Bond angles



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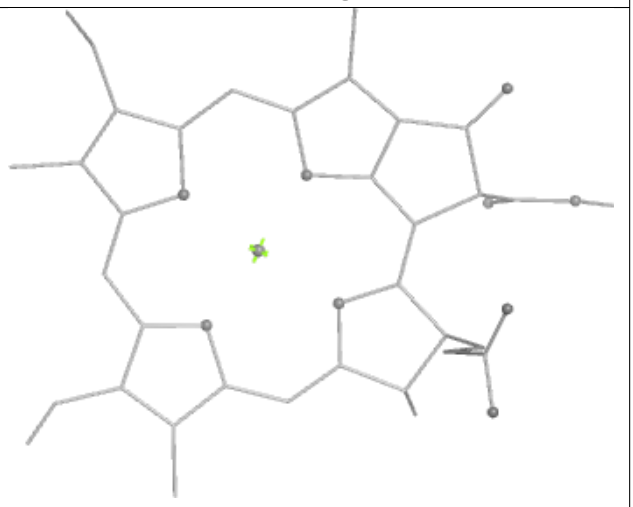
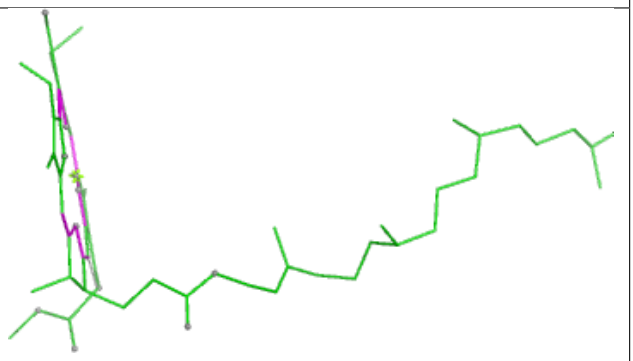


Rings

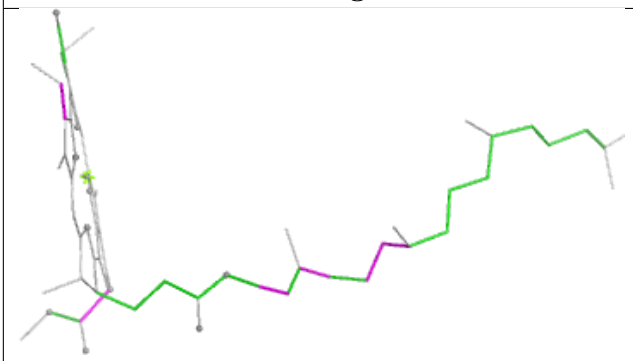
Ligand CHL Z 601



Bond lengths



Bond angles

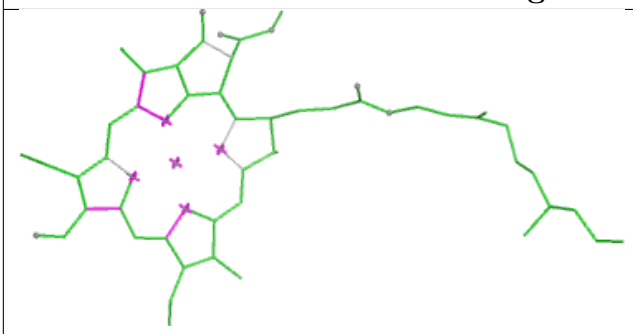


Torsions



Rings

Ligand CHL 6 606



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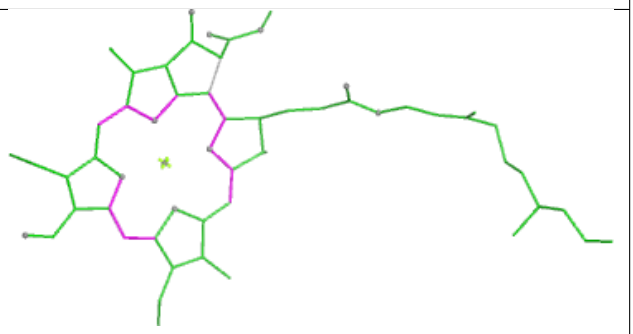
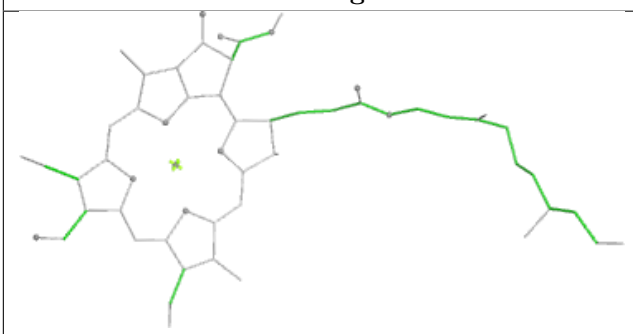


Bond angles



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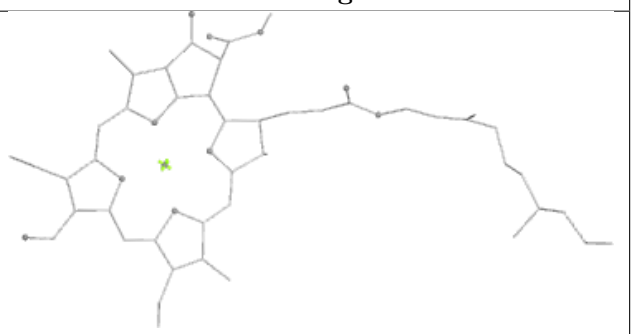
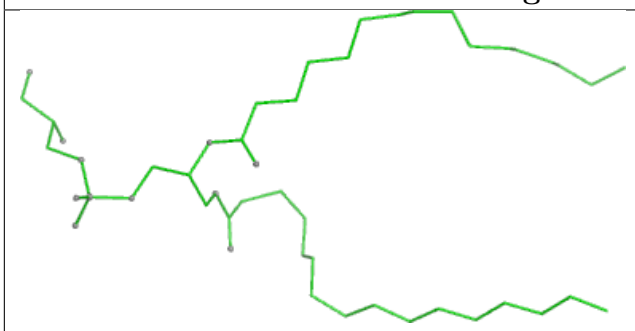


Rings

Ligand LHG A 846



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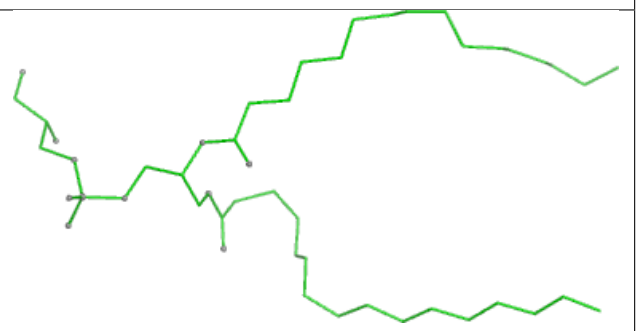
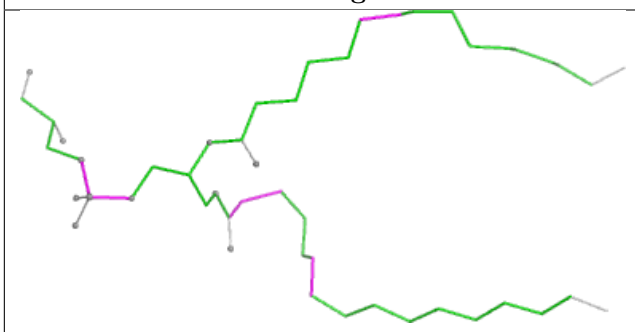


Bond angles



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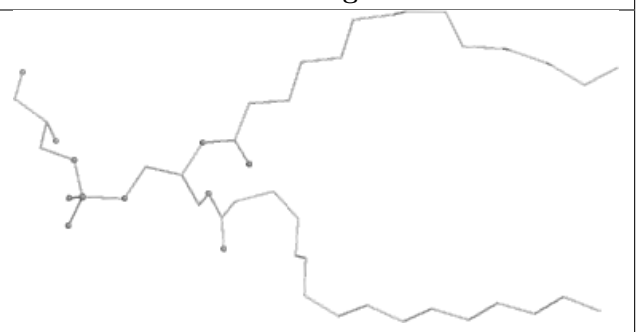
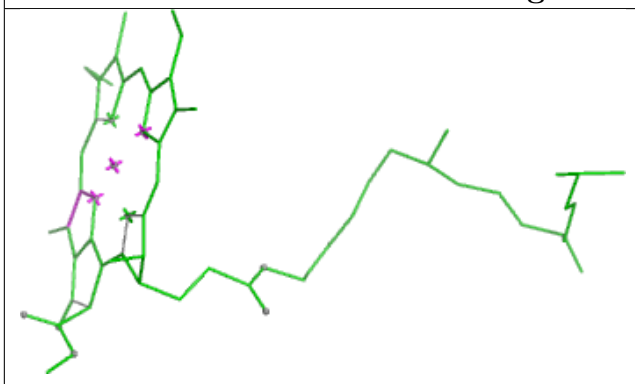
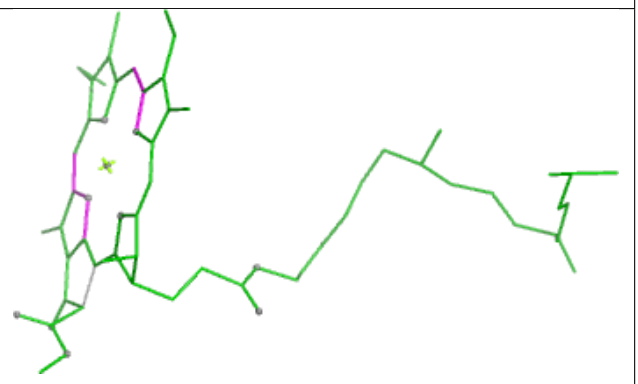


Rings

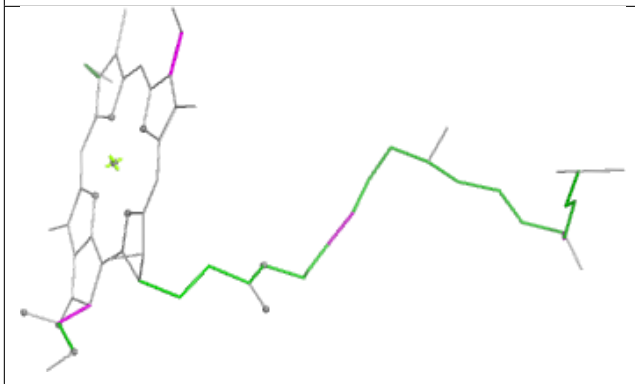
Ligand CLA L 203



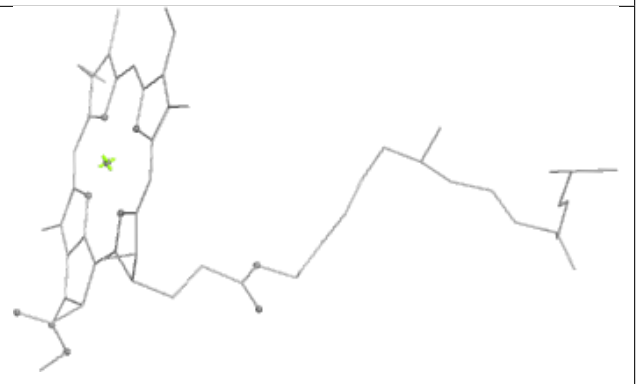
Bond lengths



Bond angles

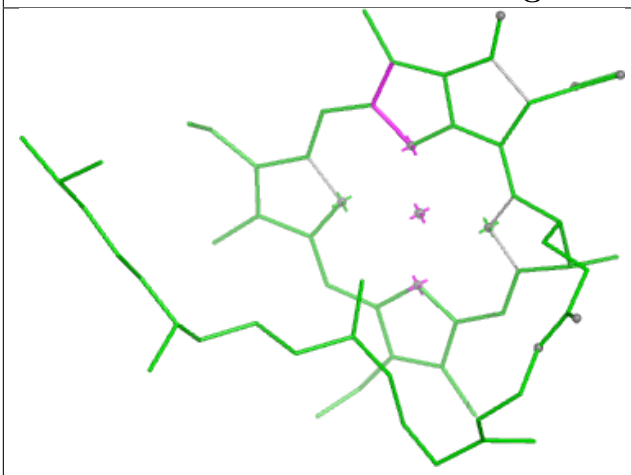


Torsions



Rings

Ligand CLA A 823



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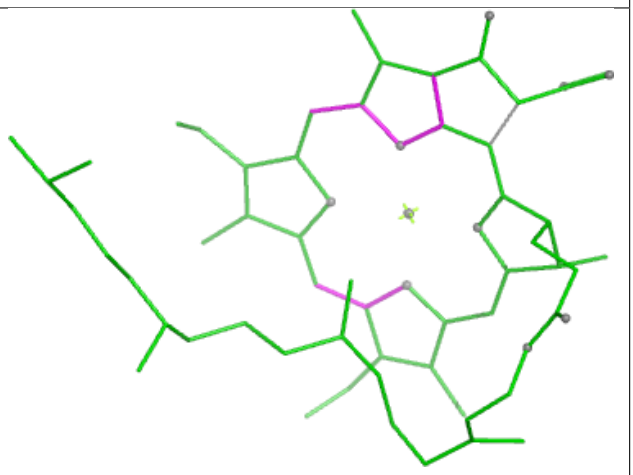

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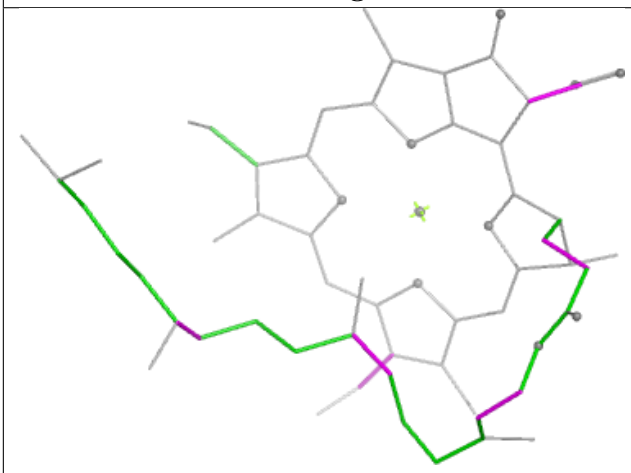

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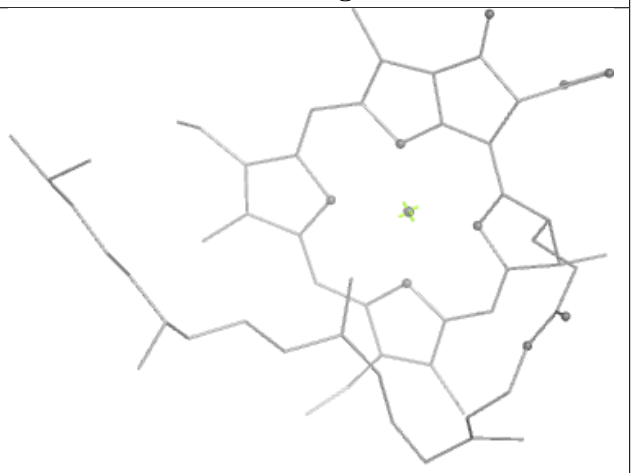
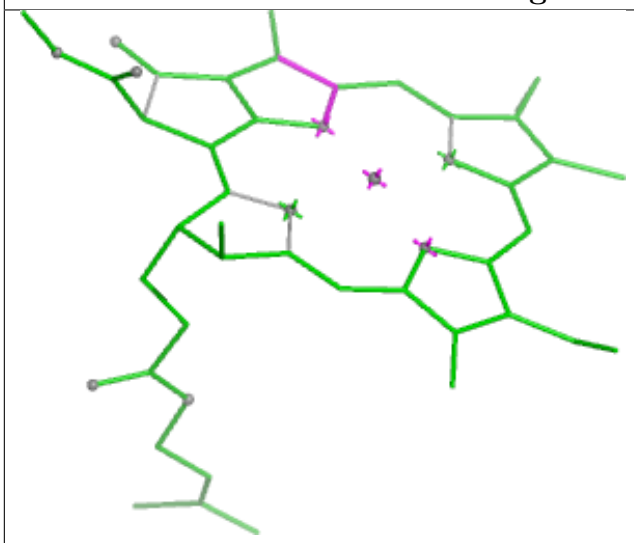


Rings

Ligand CLA 6 614



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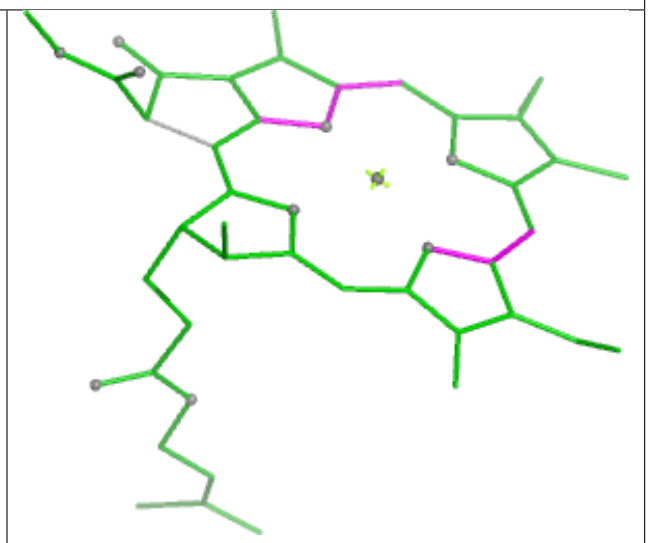

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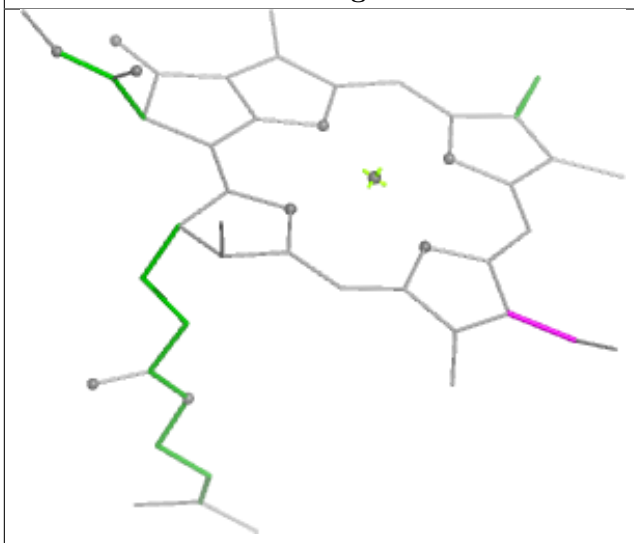

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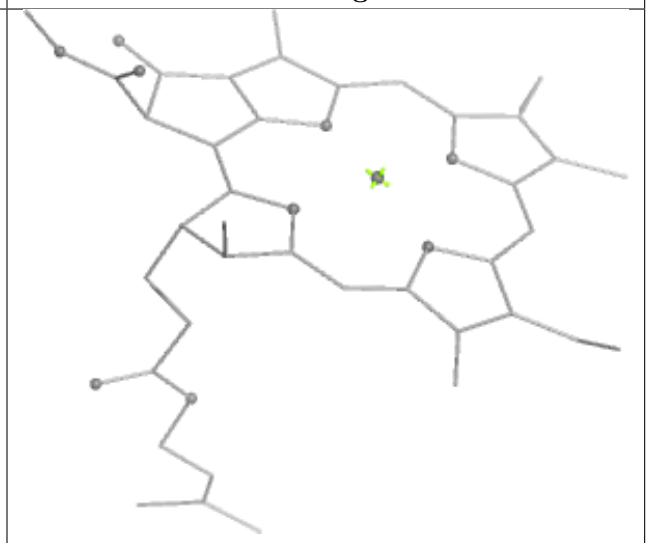
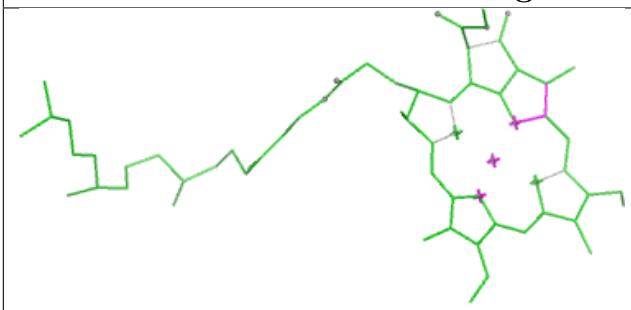


Rings

Ligand CLA B2 813



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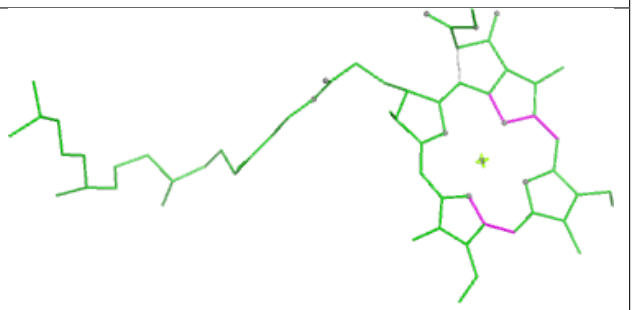

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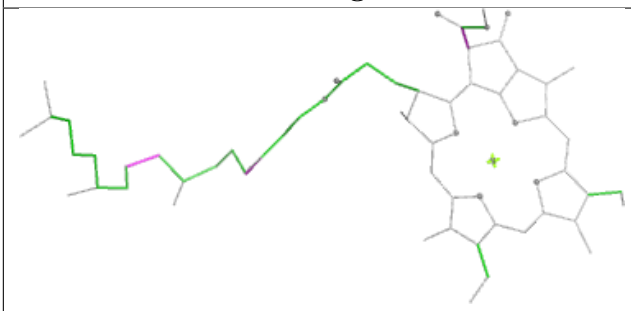

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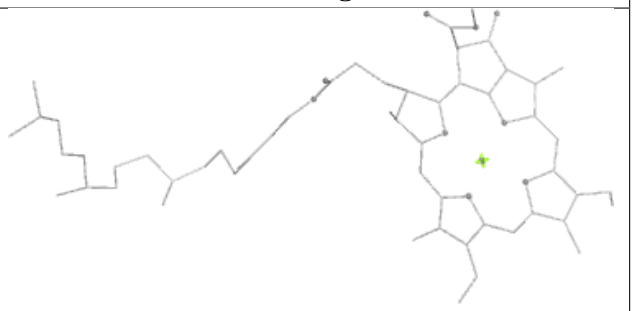
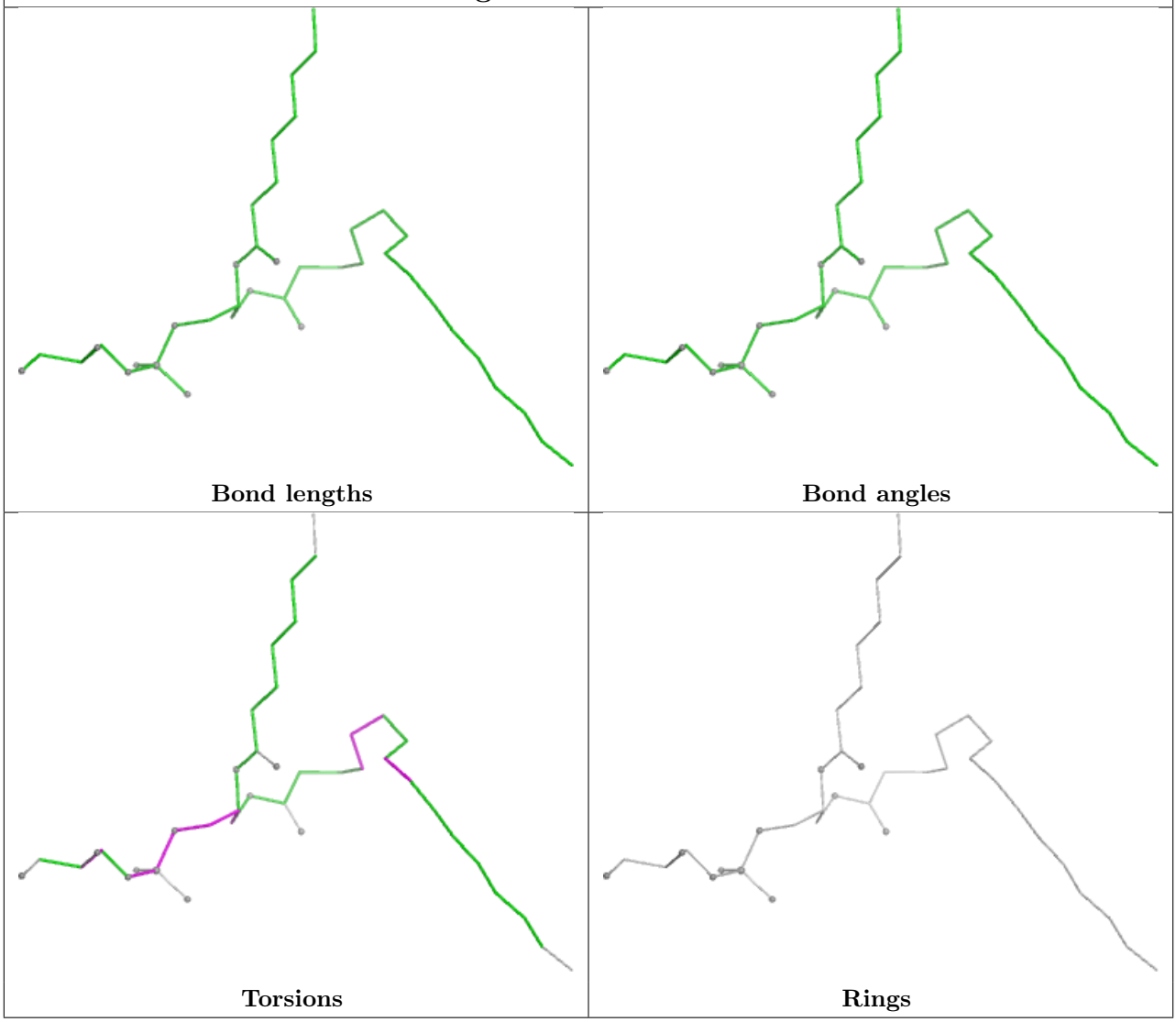
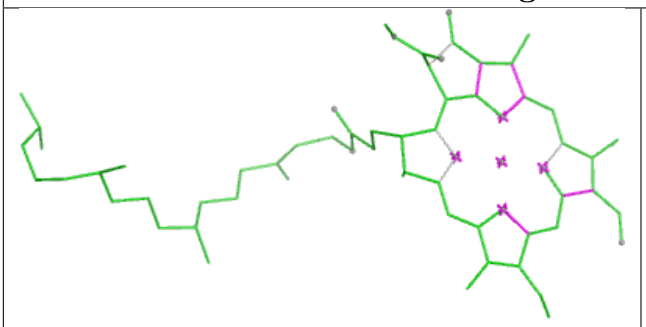


Rings

Ligand LHG 92 622



Ligand CHL 32 608



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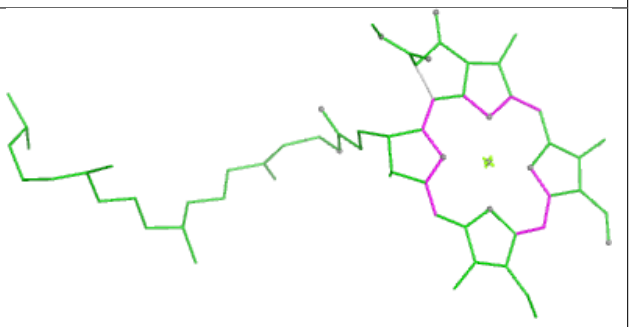
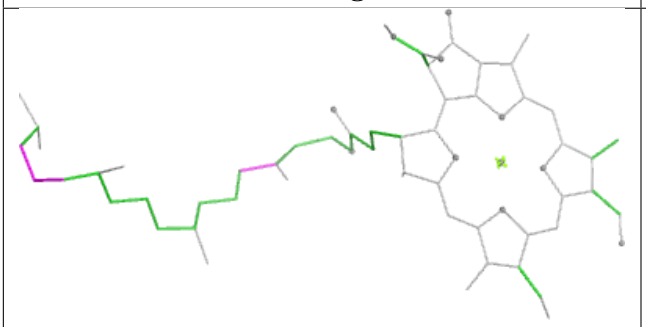


Bond angles



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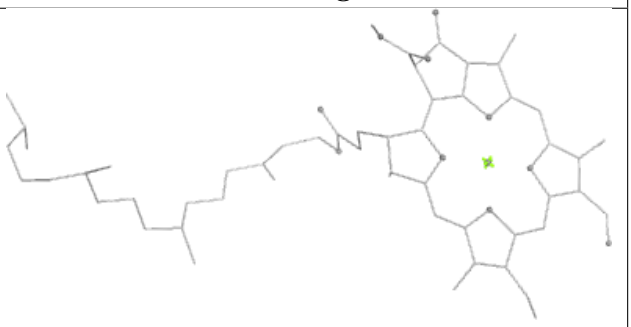

Rings

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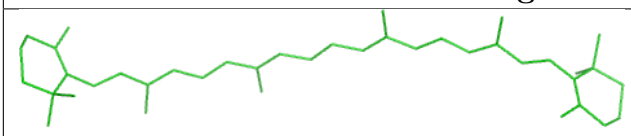

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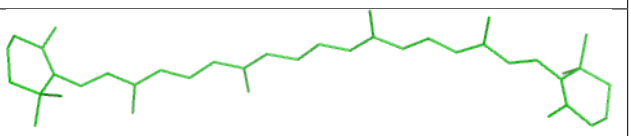
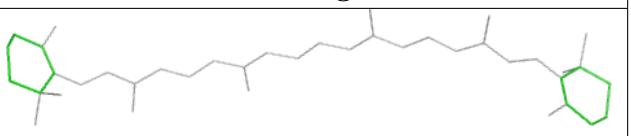


Bond angles



Torsions

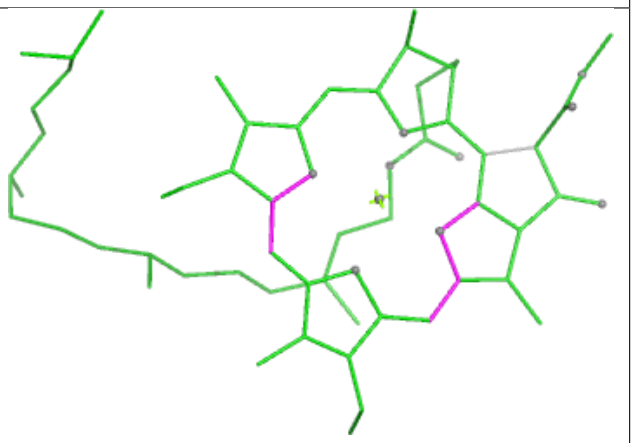


Rings

Ligand CLA 12 613



Bond lengths



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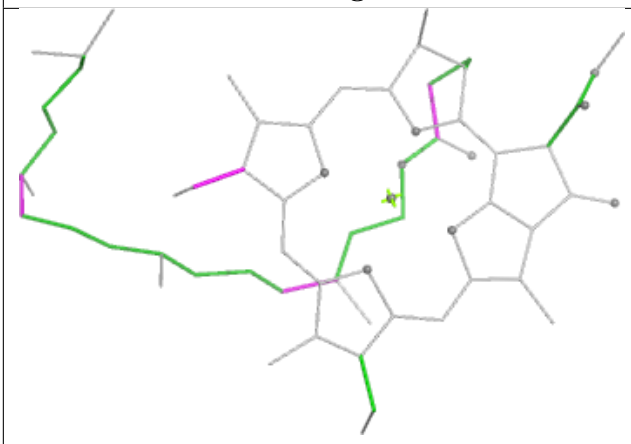

Torsions



Rings

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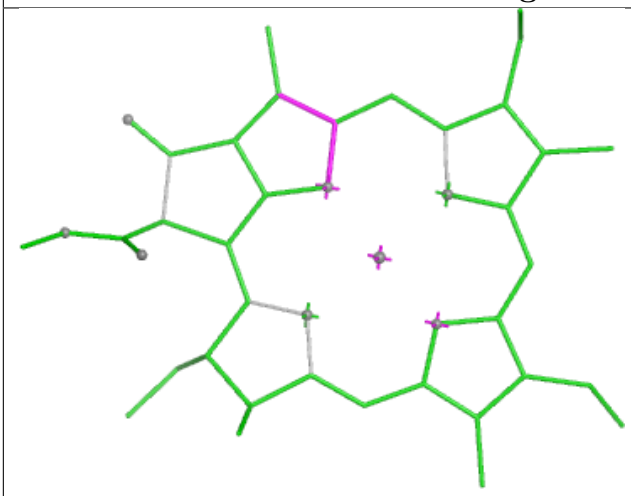

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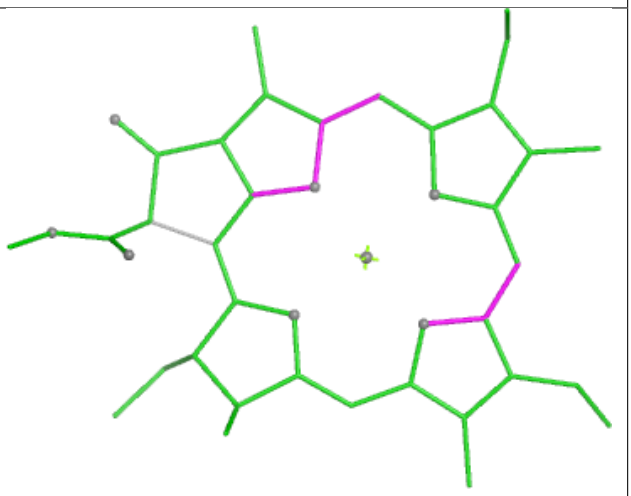

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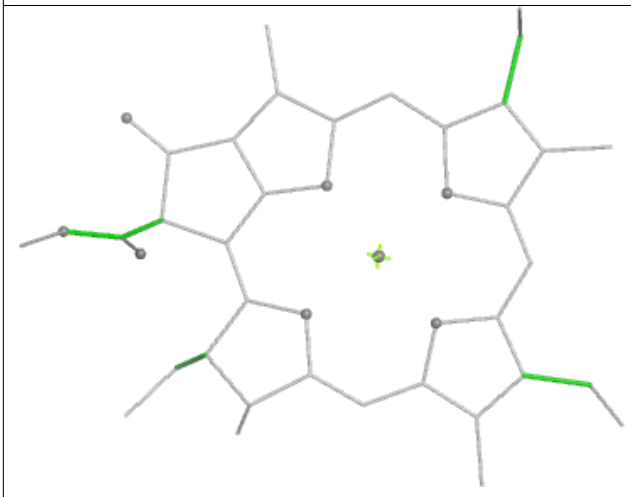

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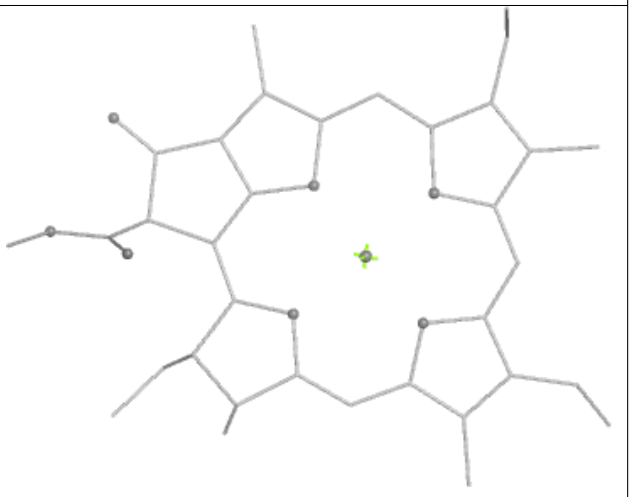
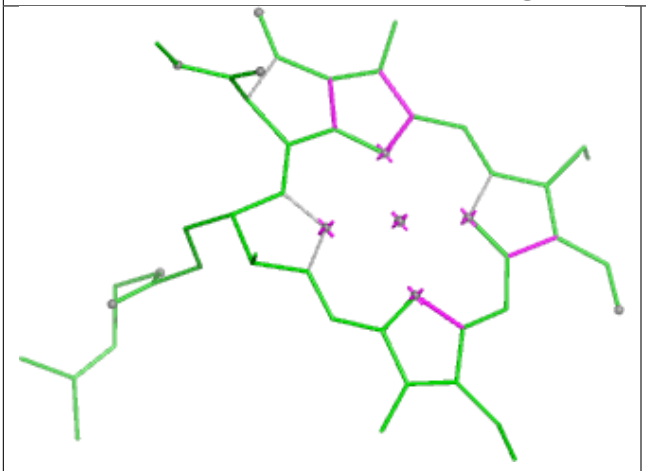


Rings

Ligand CHL 62 608



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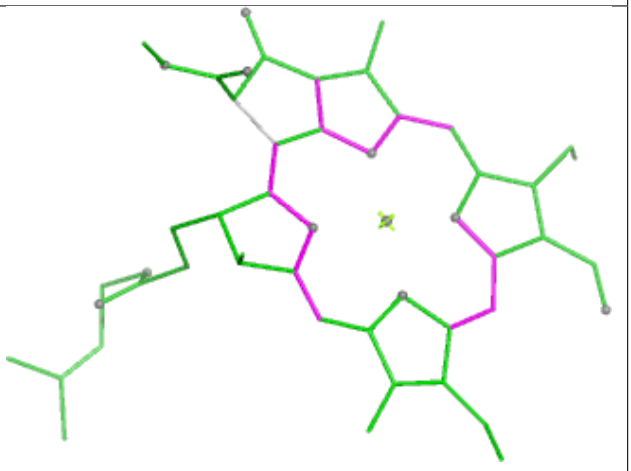

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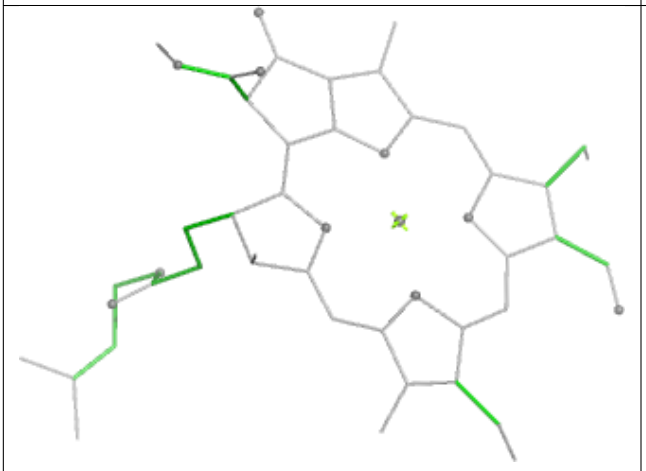

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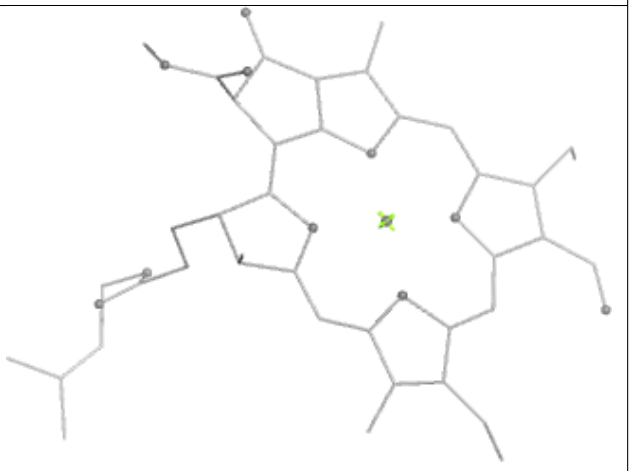
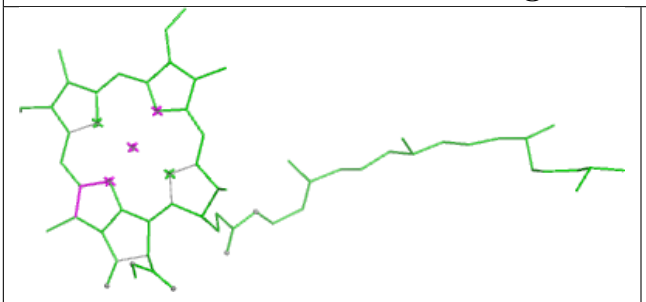


Rings

Ligand CLA A 816



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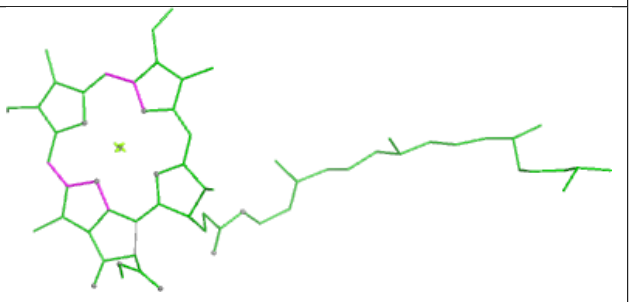

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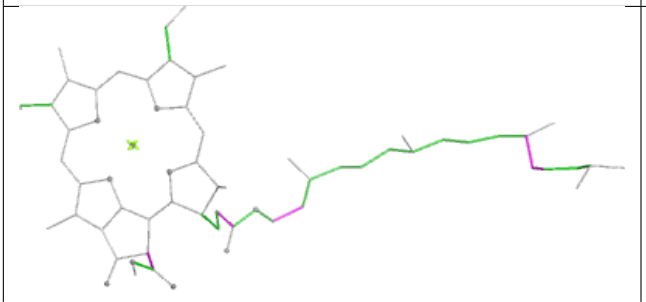

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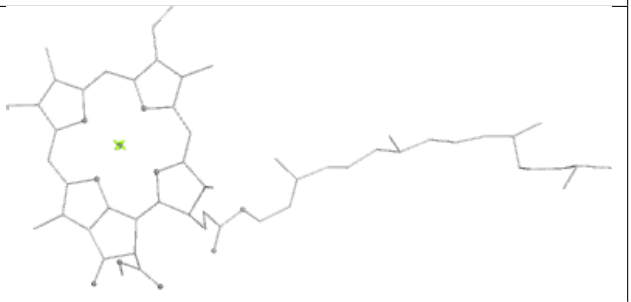

Rings

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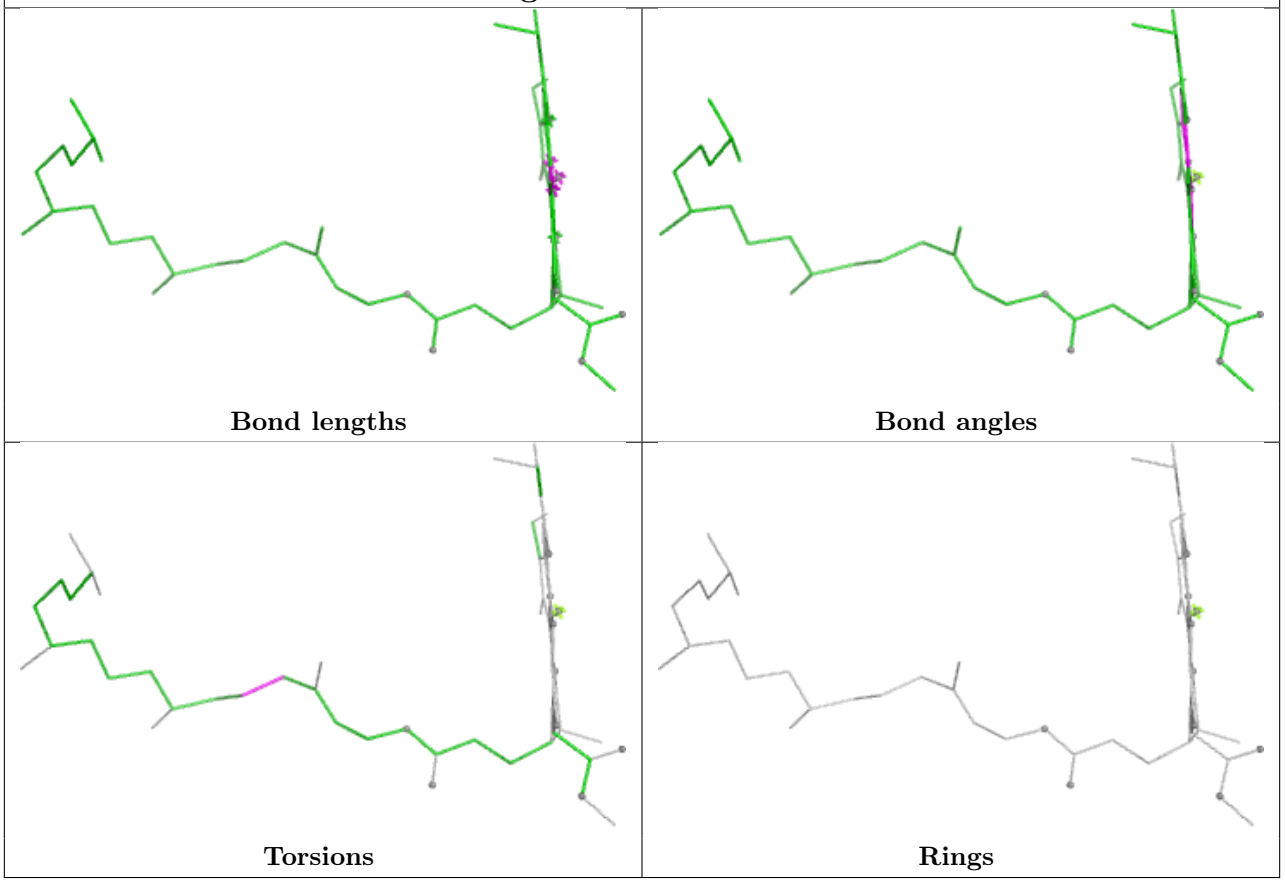

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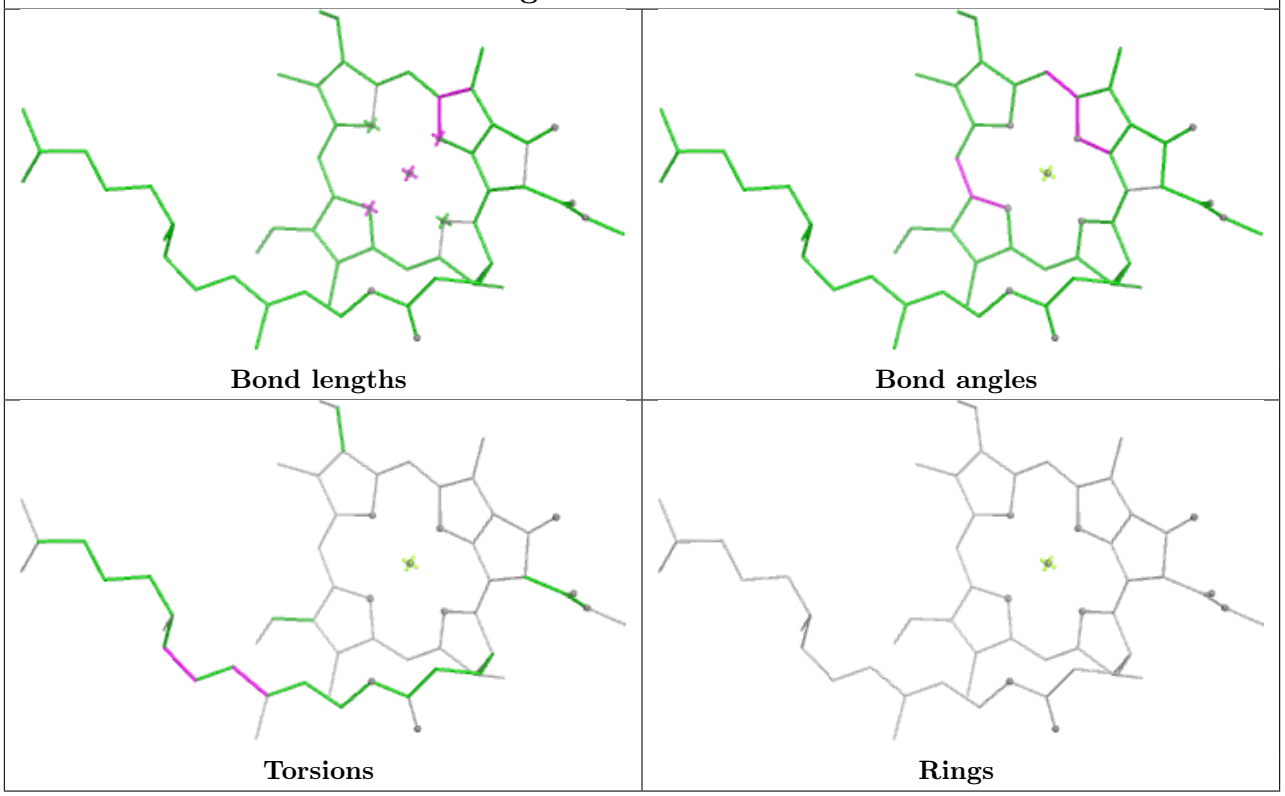
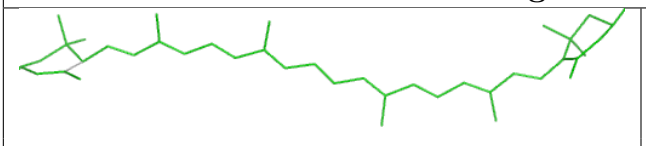


Ligand LUT 8 617



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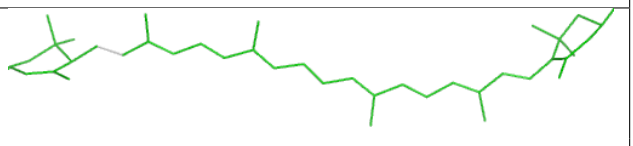

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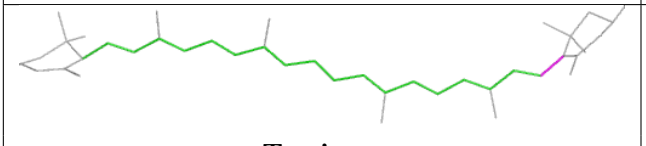

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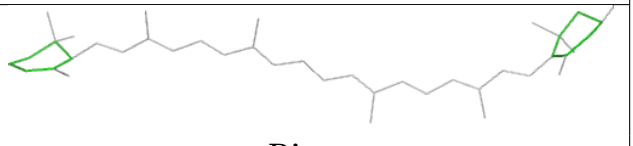
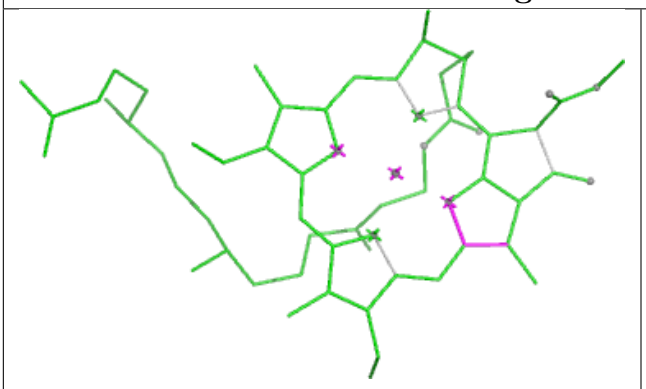


Rings

Ligand CLA A2 813



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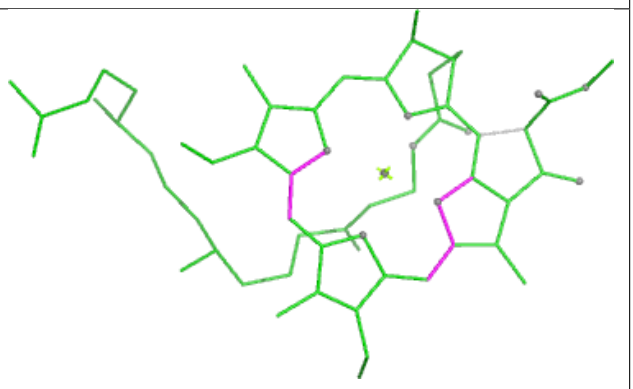

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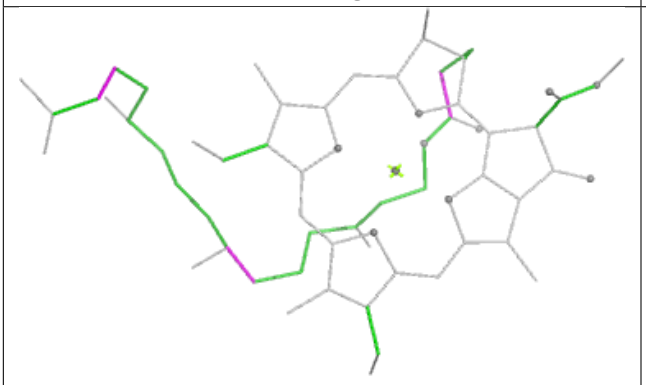

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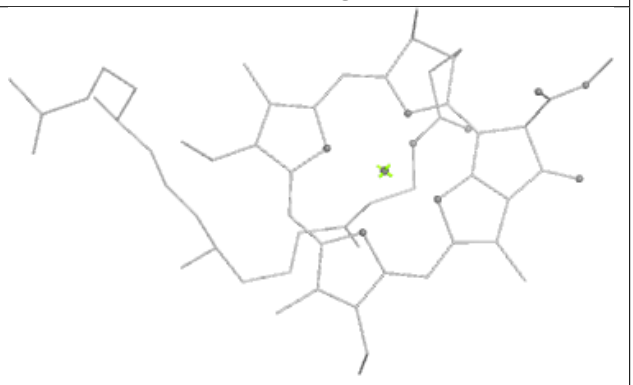
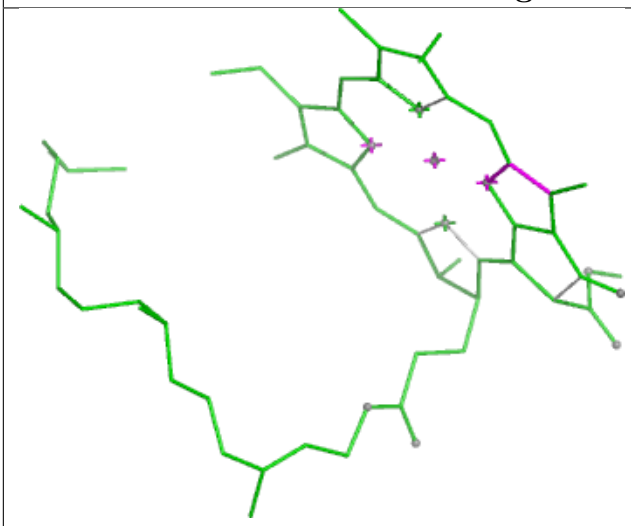


Rings

Ligand CLA B2 815



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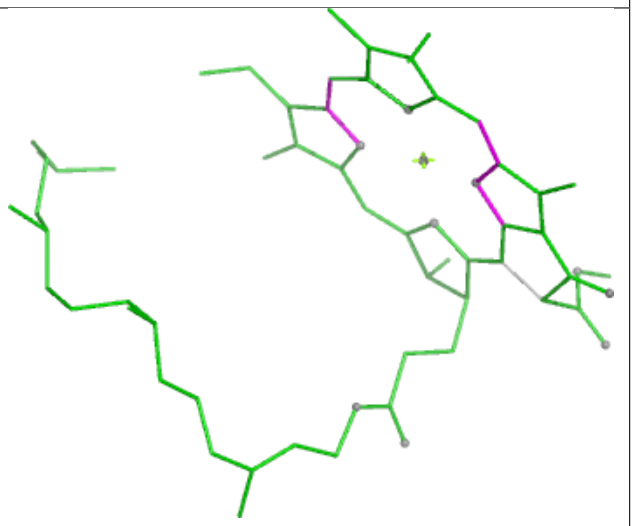
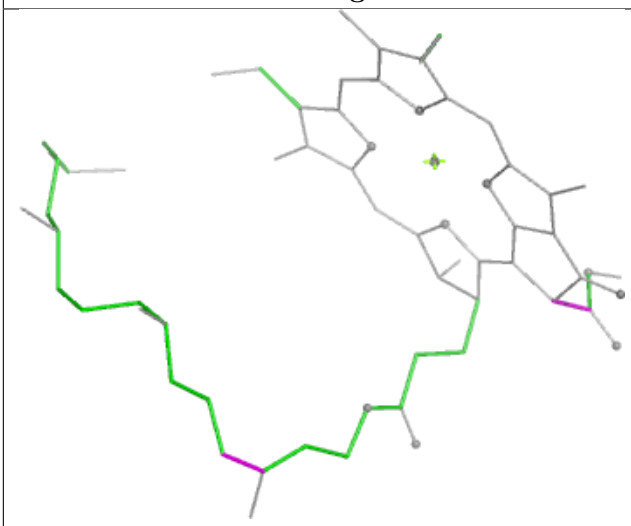


Bond angles



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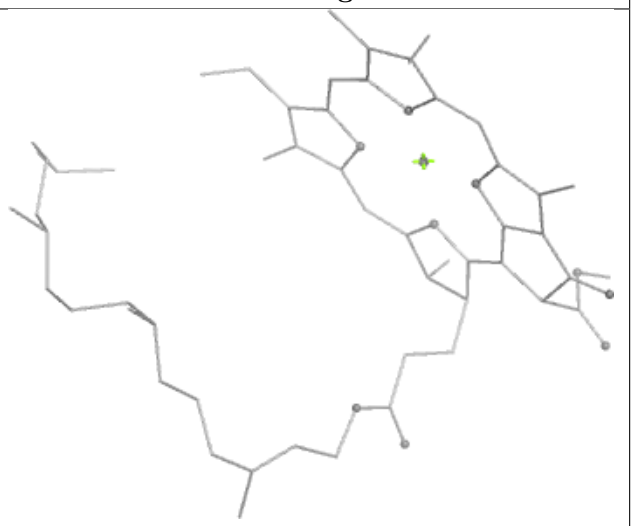
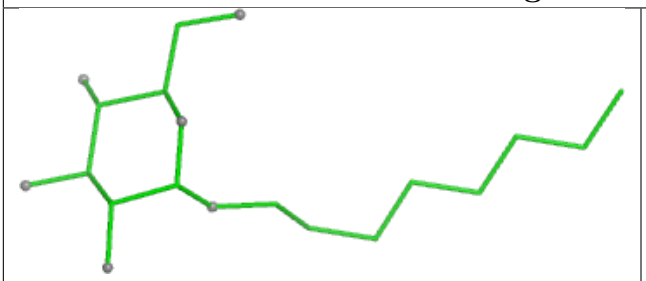


Rings

Ligand LMU 4 626



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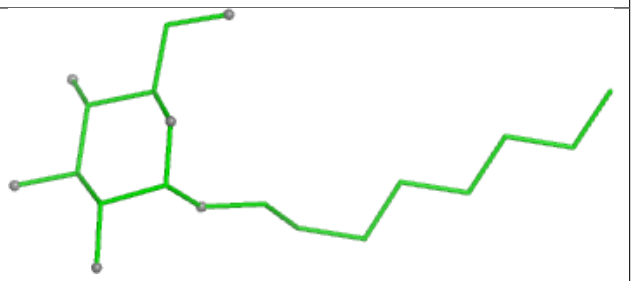
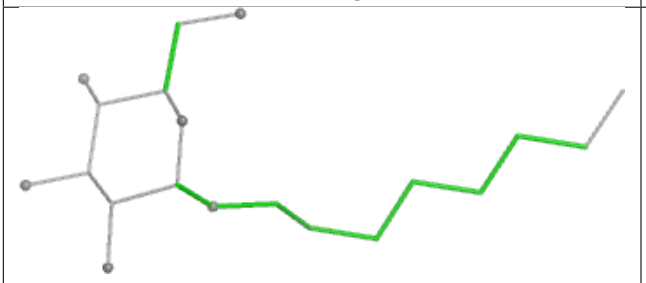


Bond angles

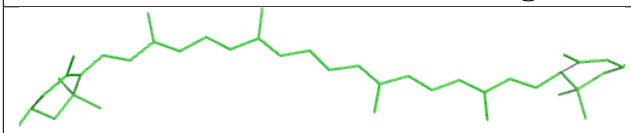


Torsions



Rings

Ligand LUT 82 617



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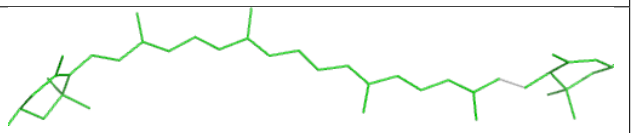
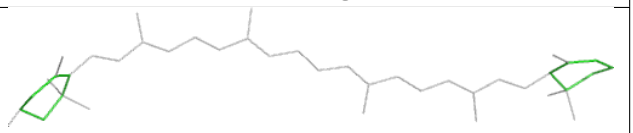


Bond angles

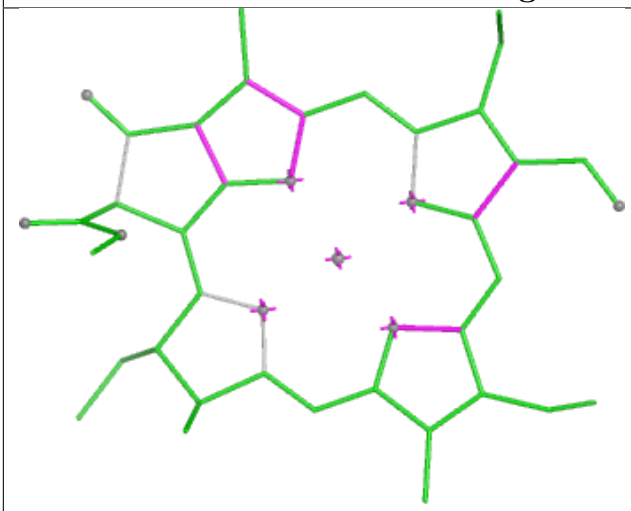


Torsions

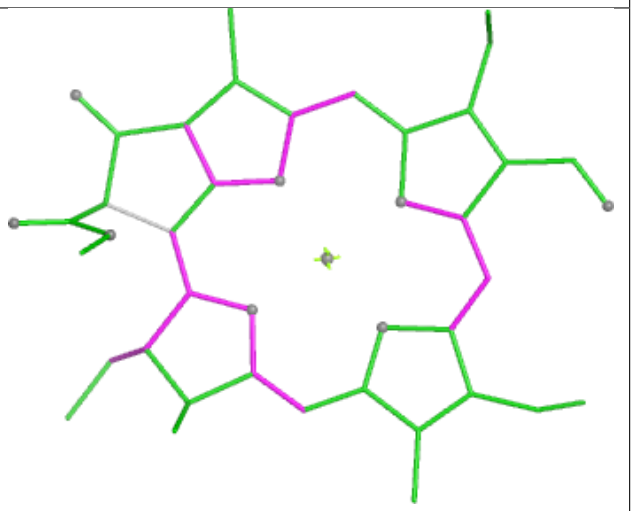


Rings

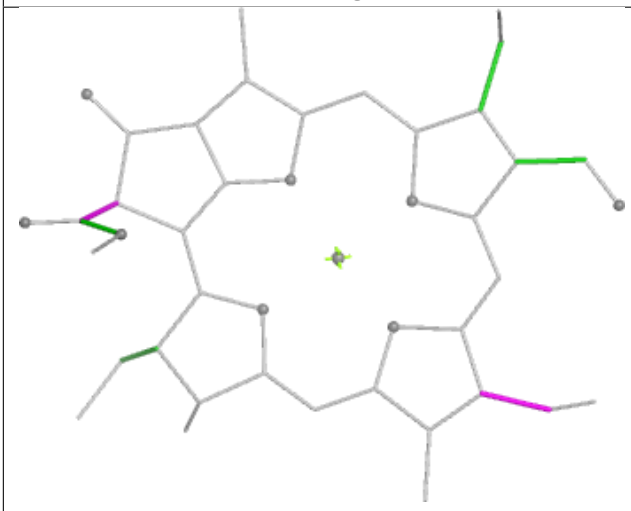
Ligand CHL 62 618



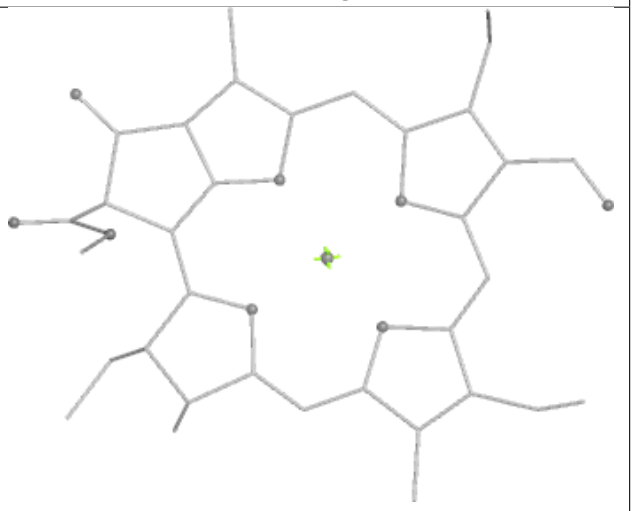
Bond lengths



Bond angles

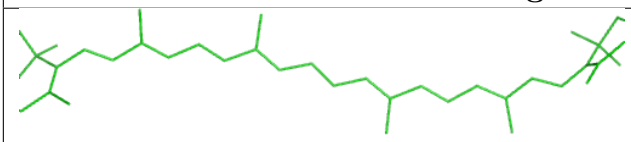


Torsions



Rings

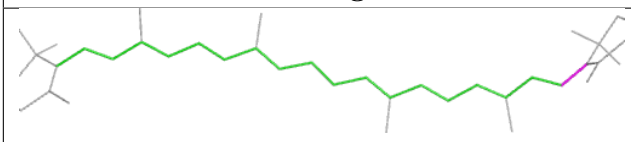
Ligand BCR 4 621



Bond lengths



Bond angles



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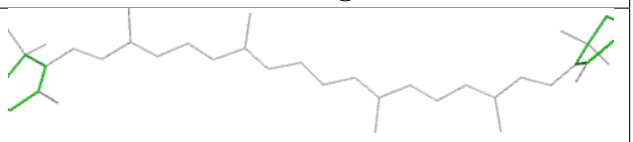
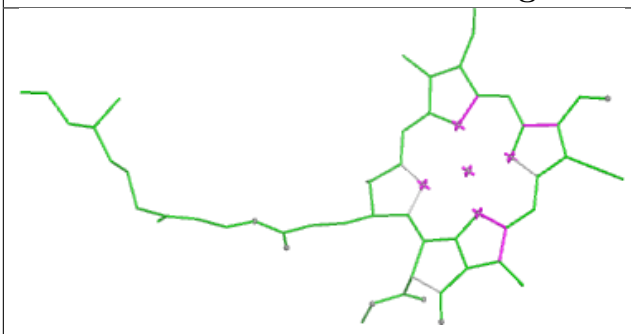
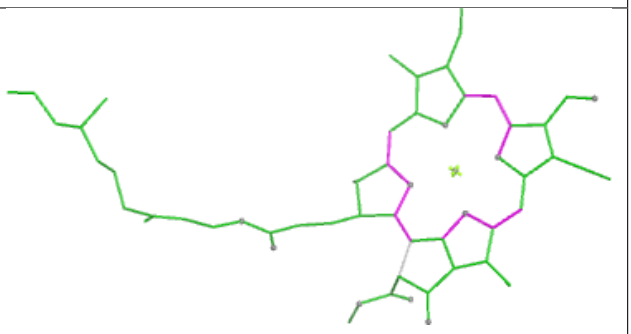


Rings

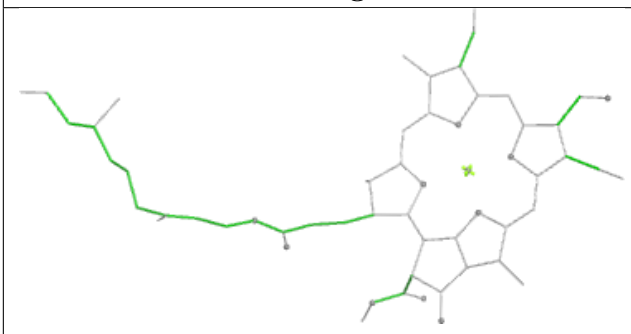
Ligand CHL 62 606



Bond lengths



Bond angles



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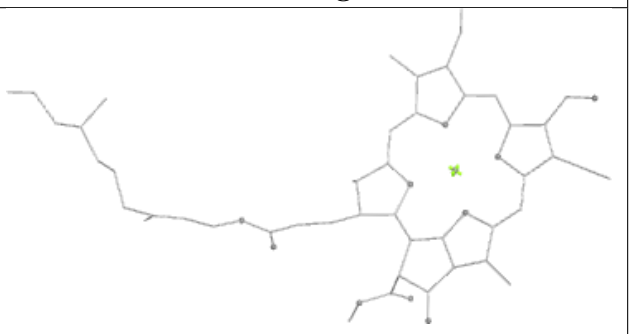
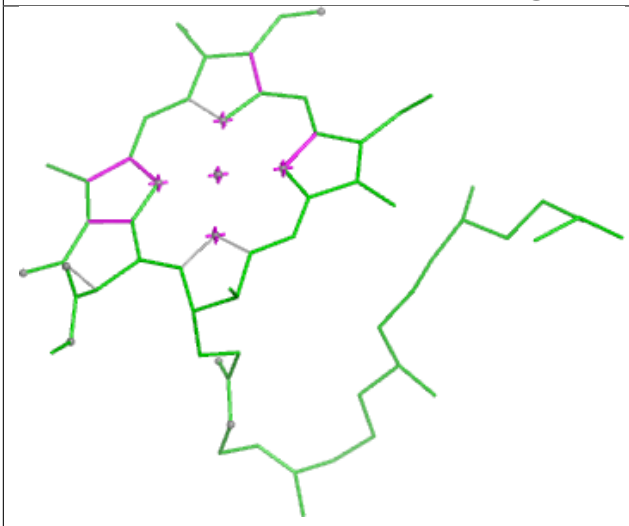
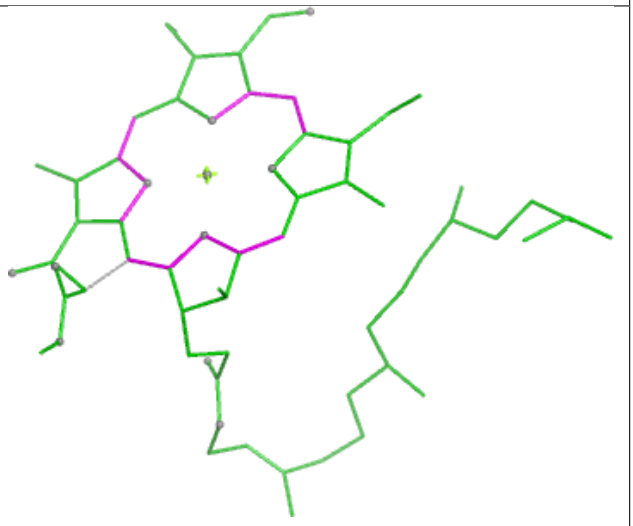


Rings

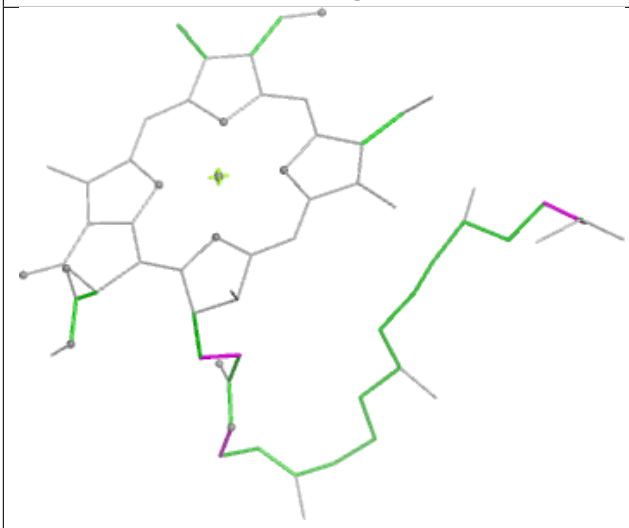
Ligand CHL 4 608



Bond lengths



Bond angles

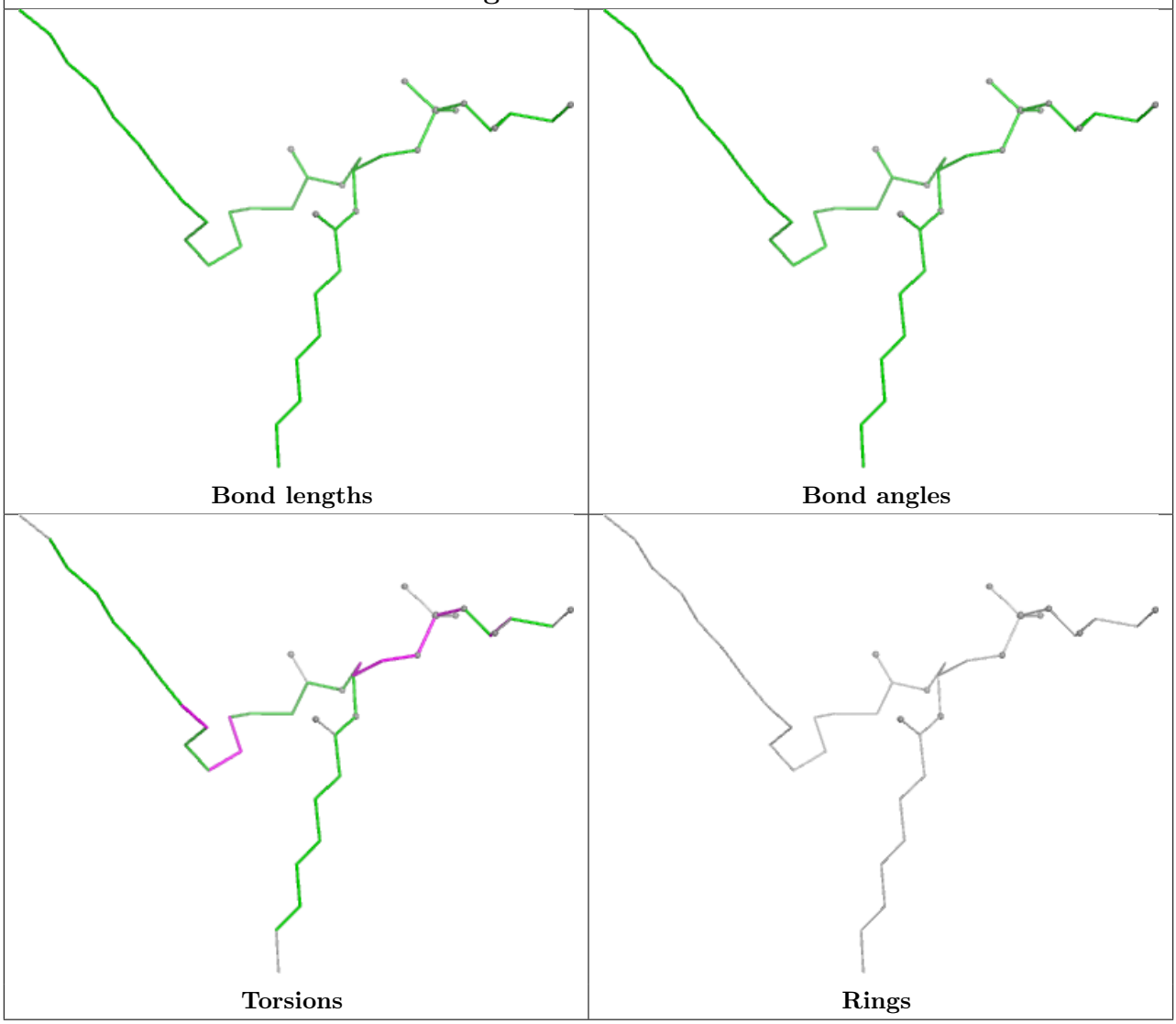


Torsions



Rings

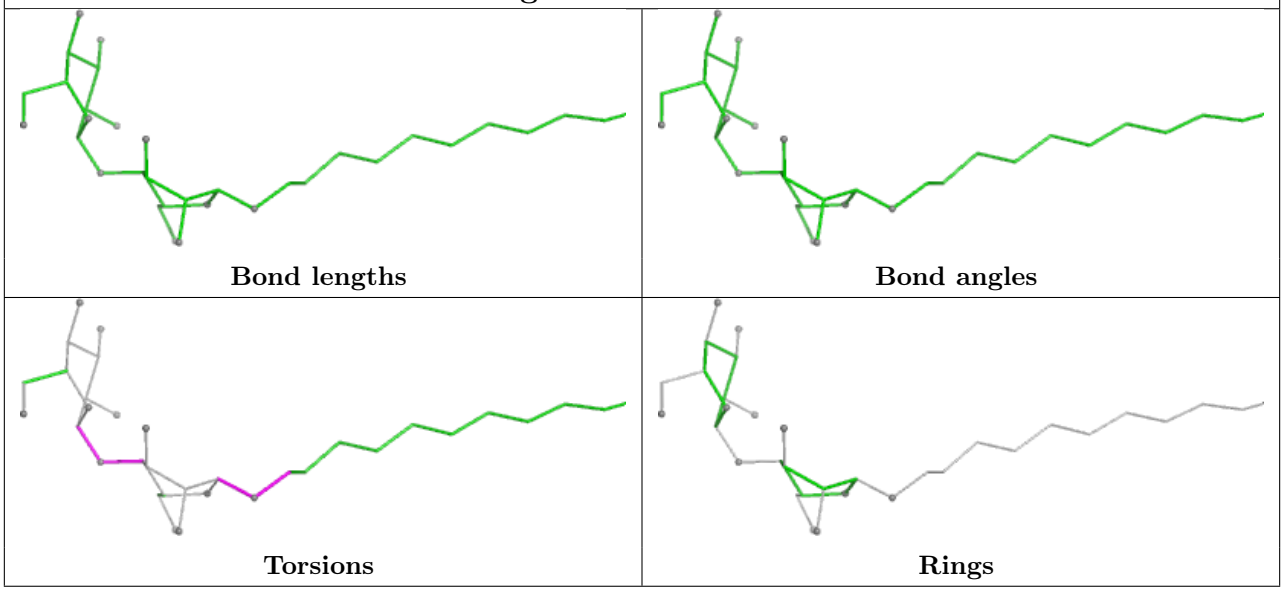
Ligand LHG 9 622



Bond lengths | Bond angles

Torsions | Rings

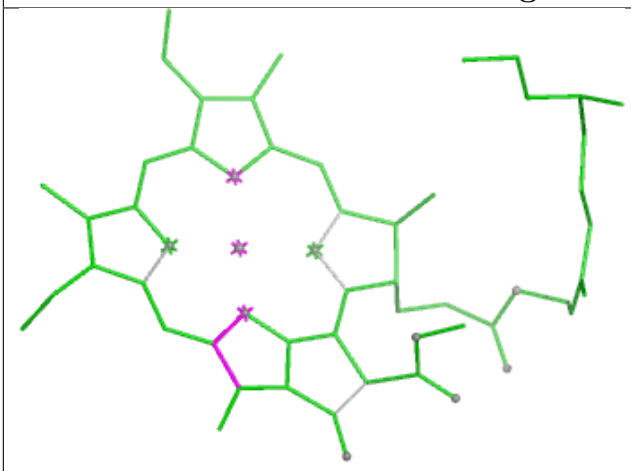
Ligand LMU A 863



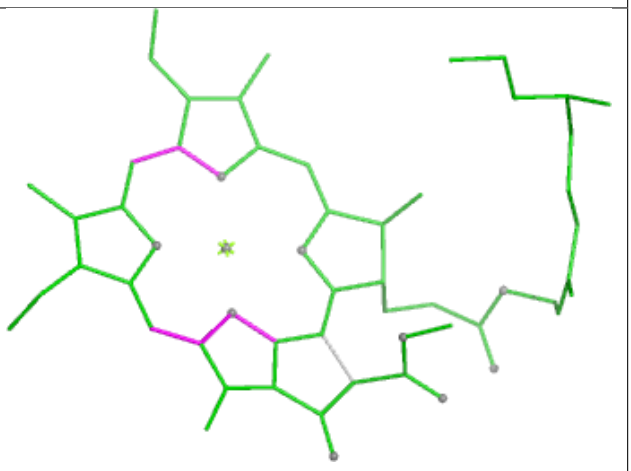
Bond lengths | Bond angles

Torsions | Rings

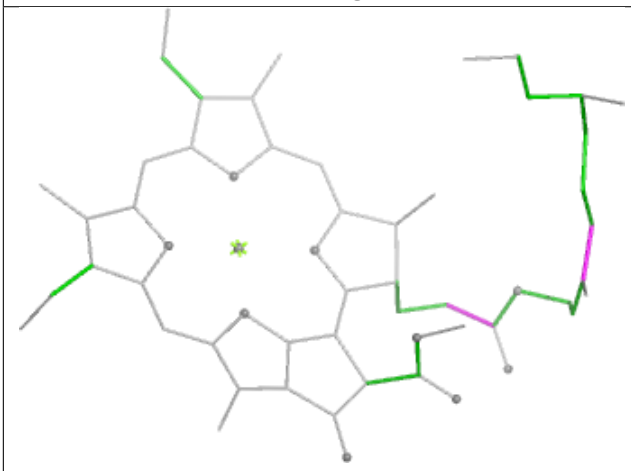
Ligand CLA 12 603



Bond lengths



Bond angles



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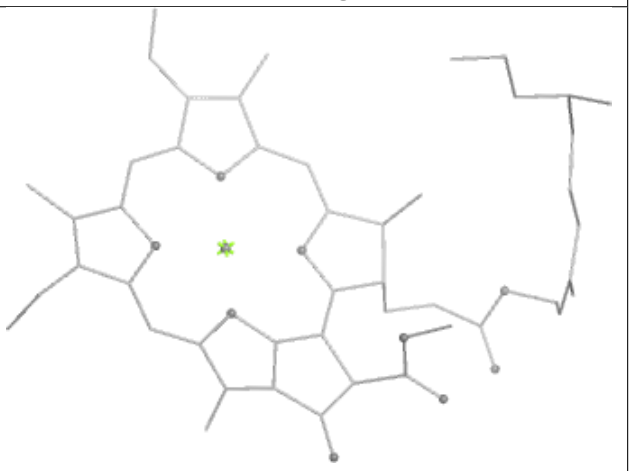
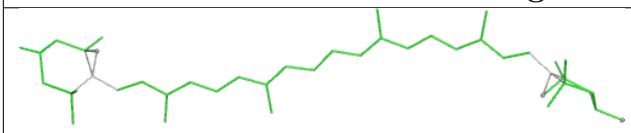


Rings

Ligand XAT 6 624



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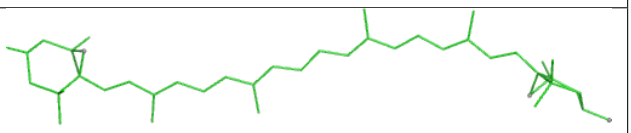
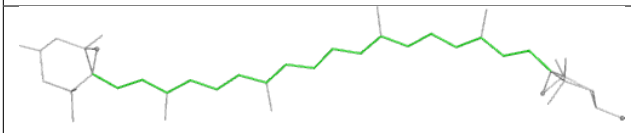


Bond angles



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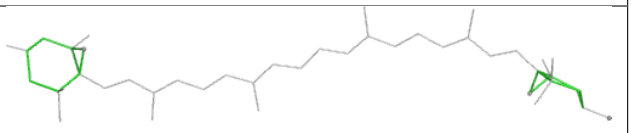
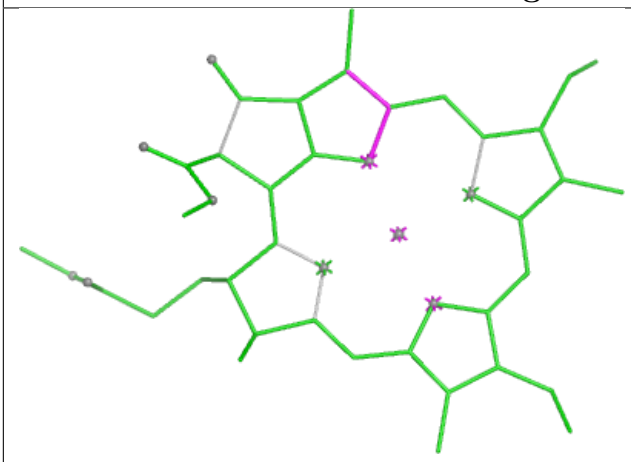


Rings

Ligand CLA G 204



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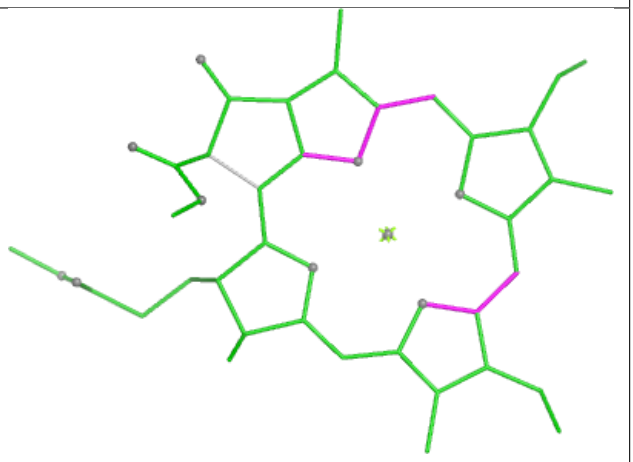
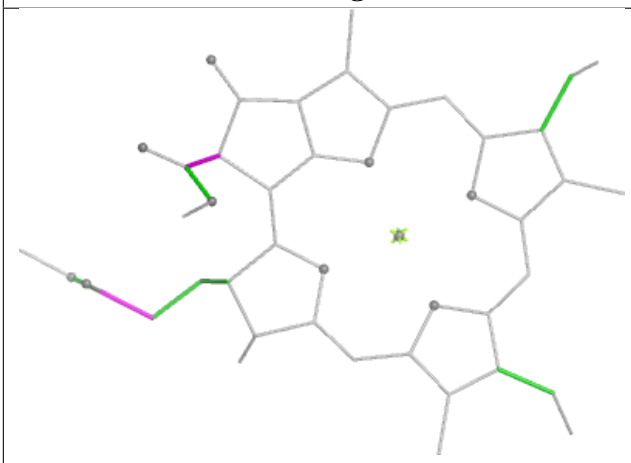
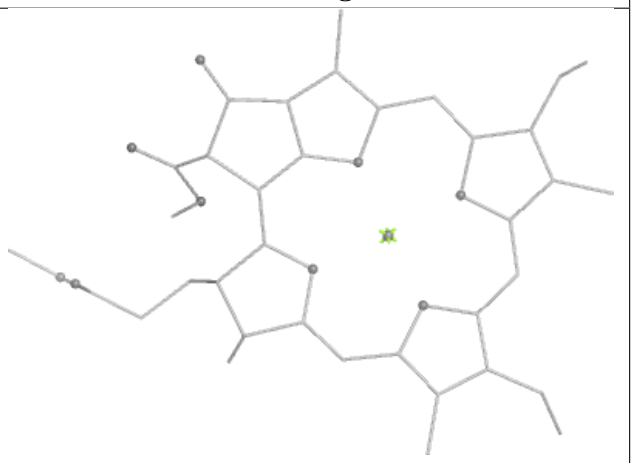


Bond angles

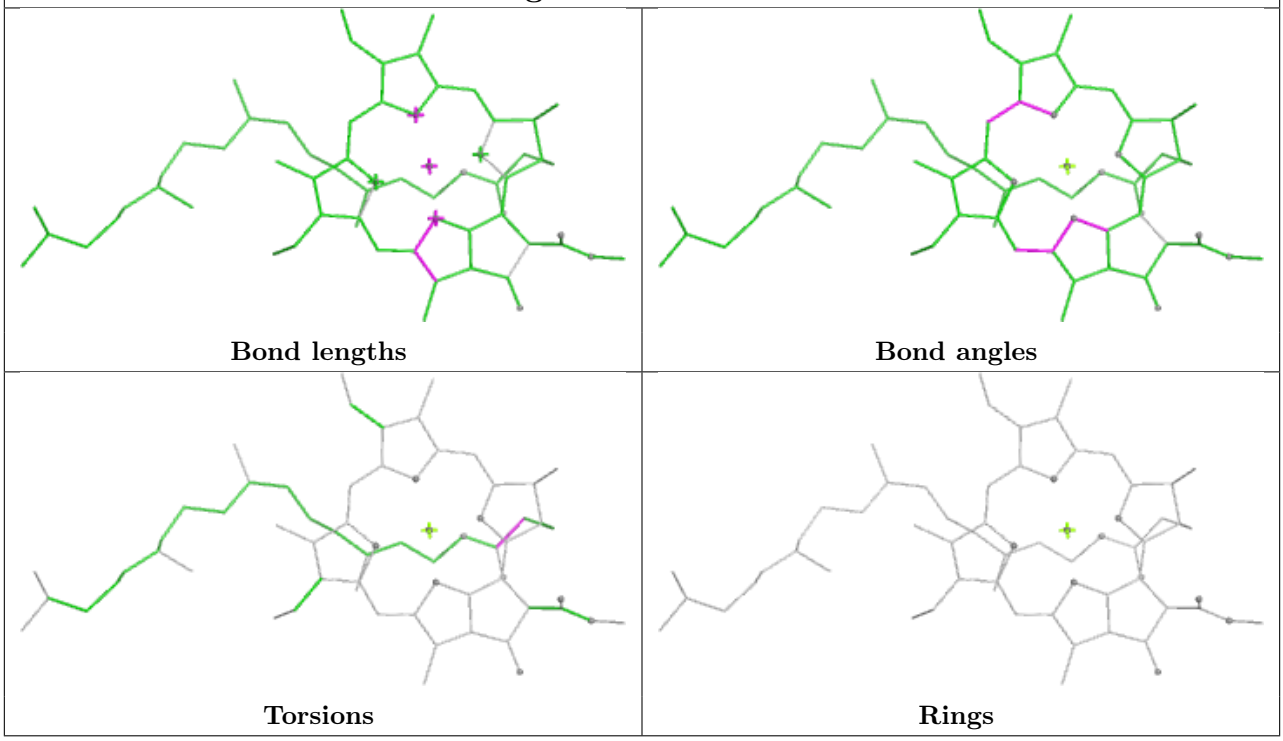


Torsions

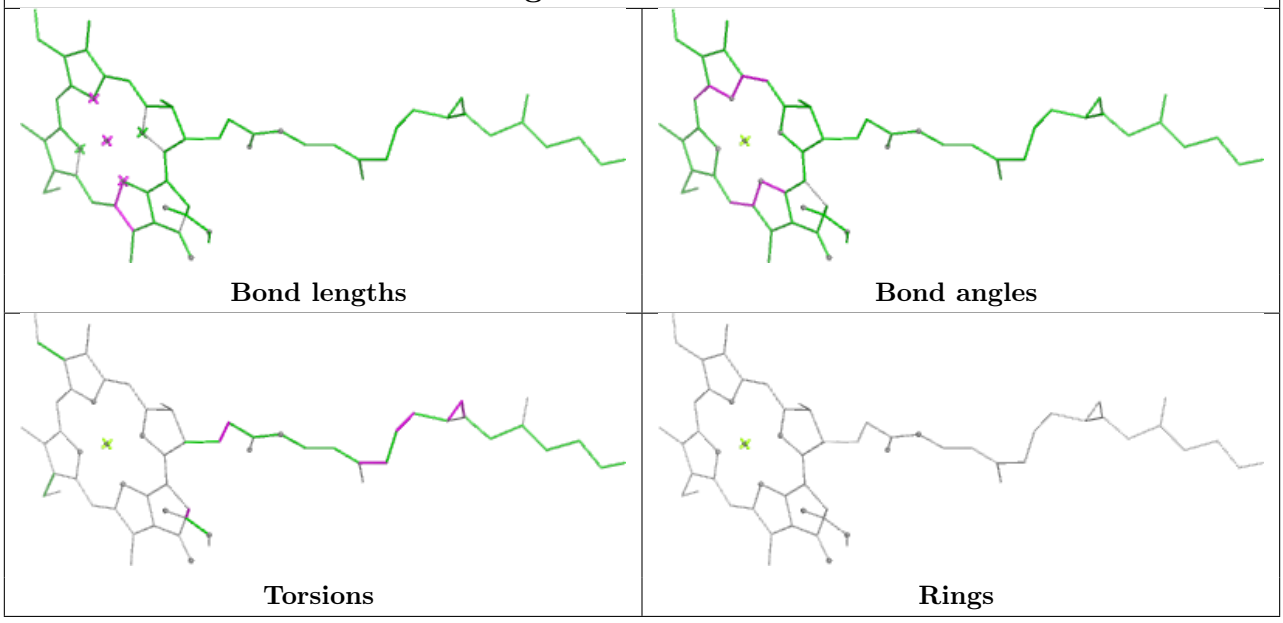


Rings

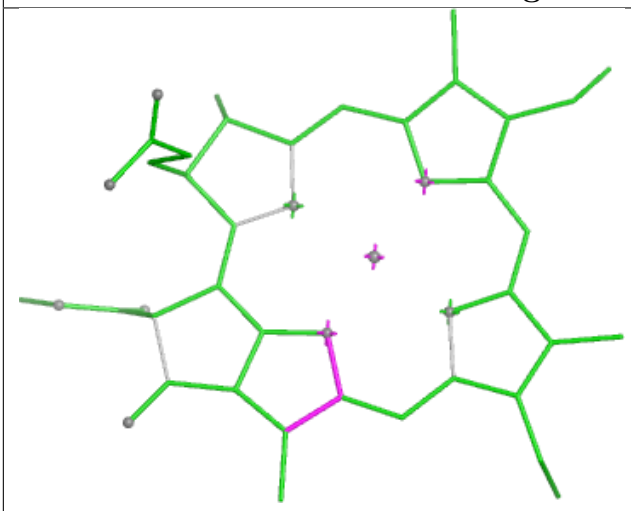
Ligand CLA B 816



Ligand CLA A 810



Ligand CLA K 206



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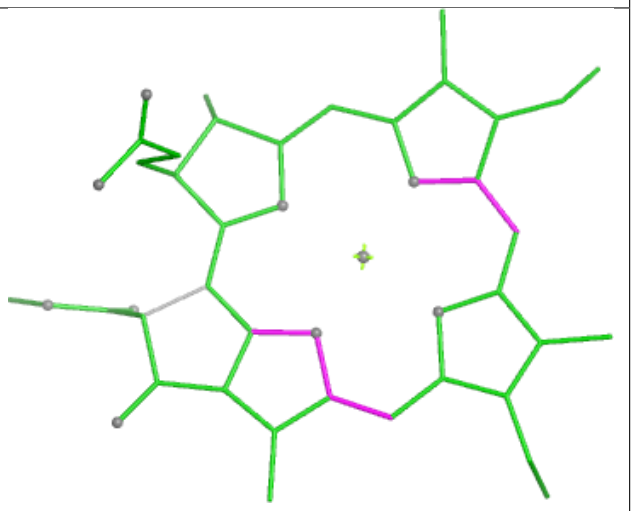
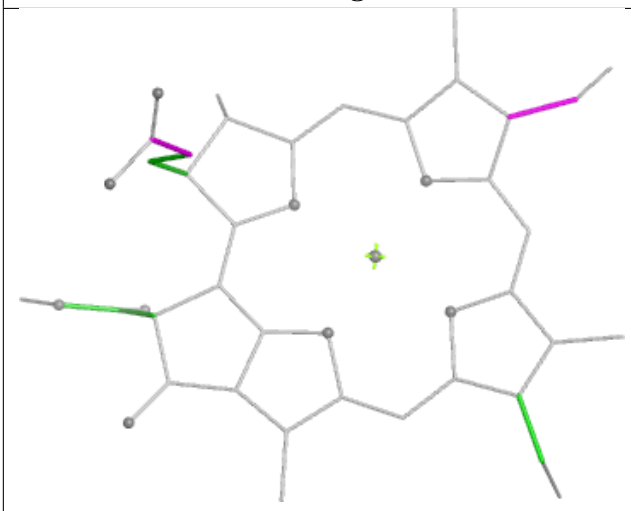


Bond angles



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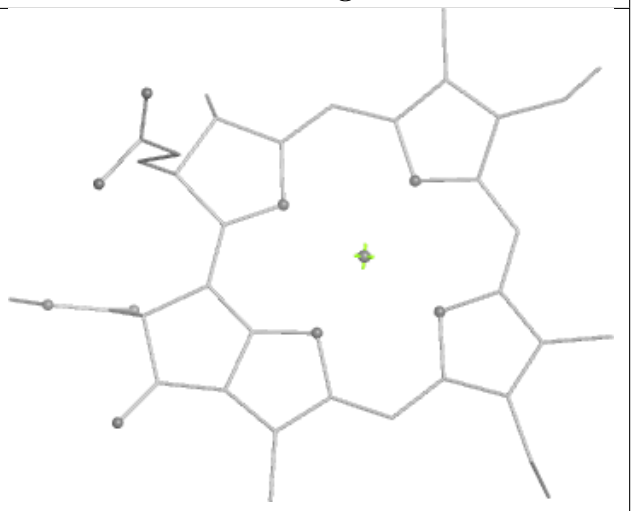
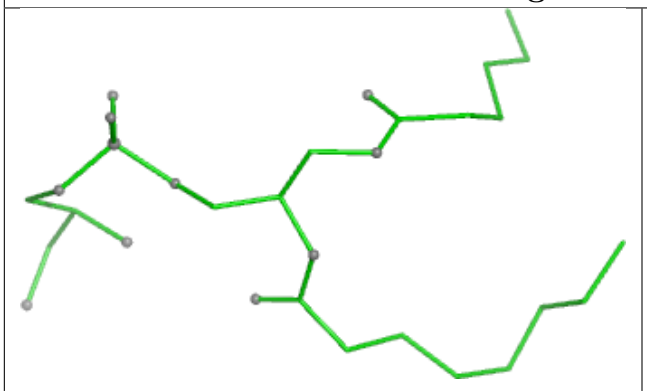
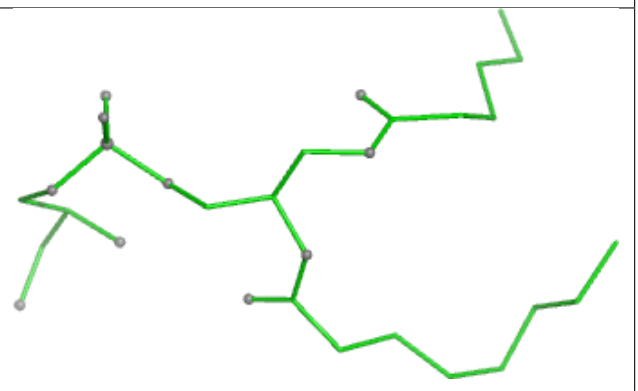


Rings

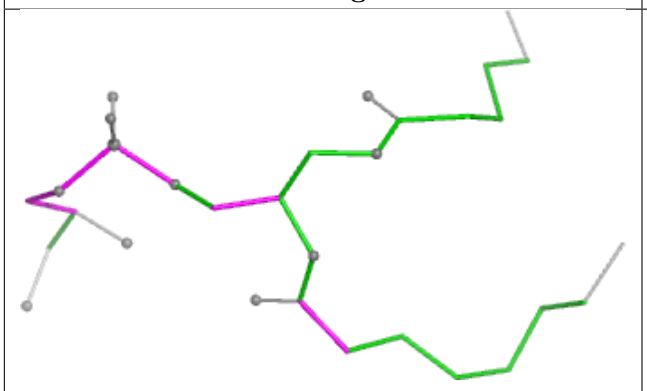
Ligand LHG 3 721



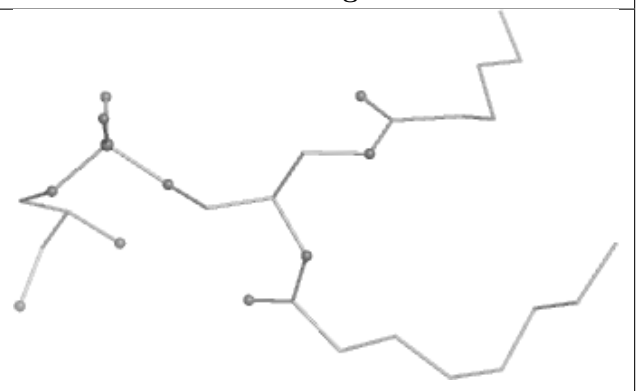
Bond lengths



Bond angles

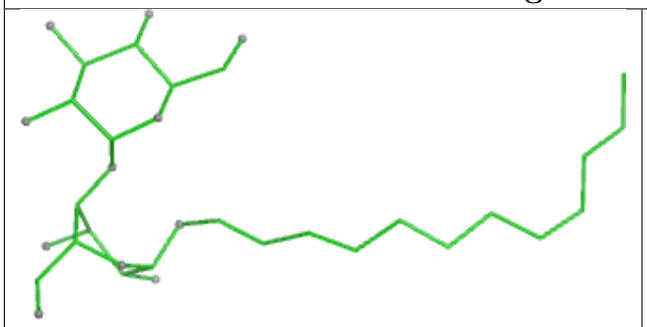


Torsions



Rings

Ligand LMU 8 627



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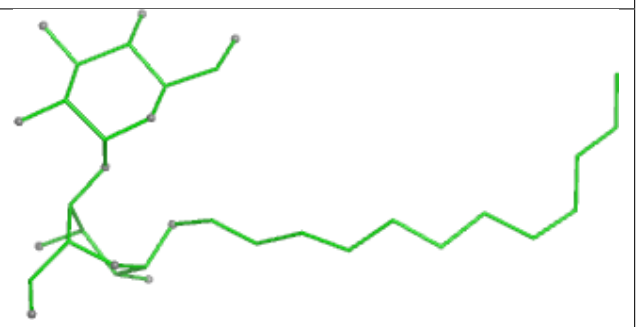
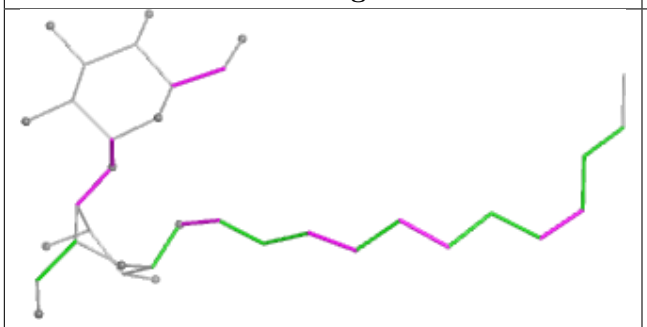


Bond angles



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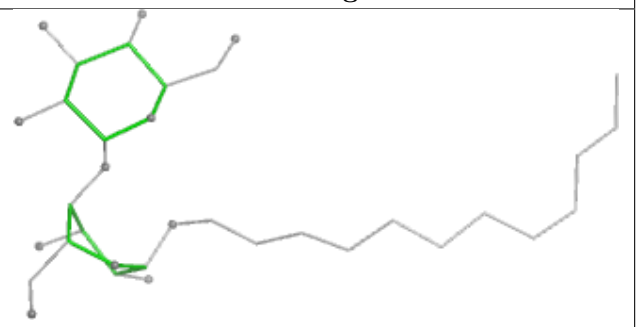
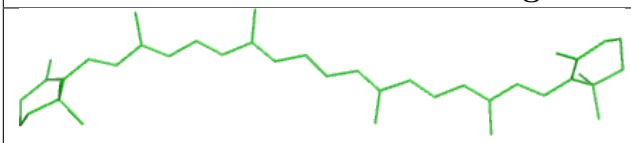


Rings

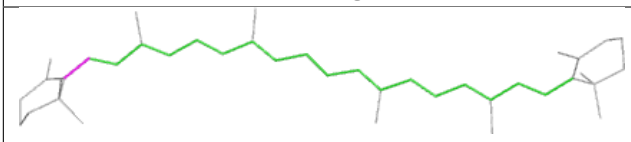
Ligand BCR B 846



Bond lengths



Bond angles



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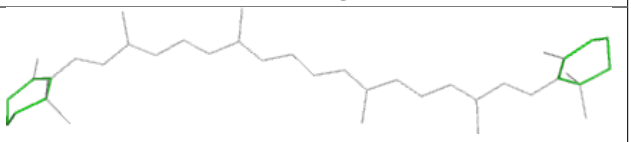
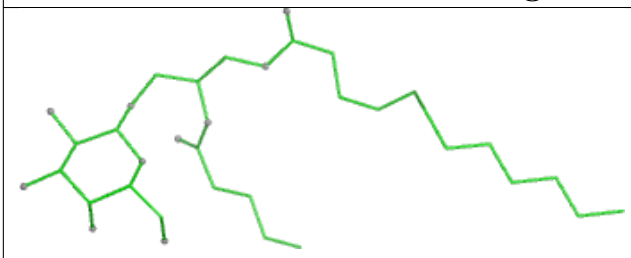


Rings

Ligand LMG 1 624



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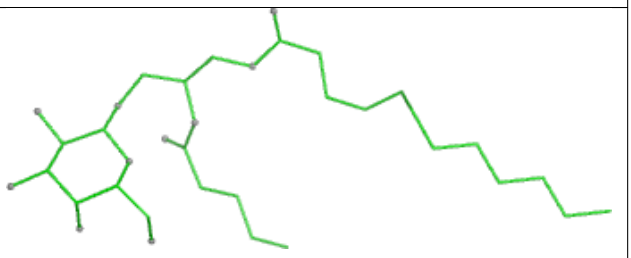
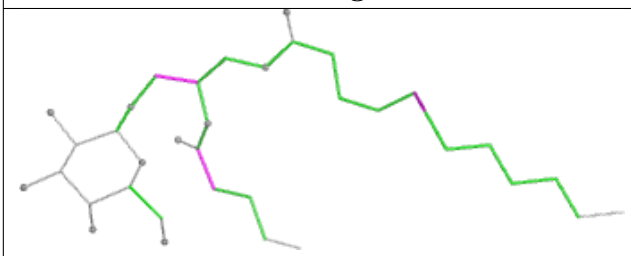


Bond angles



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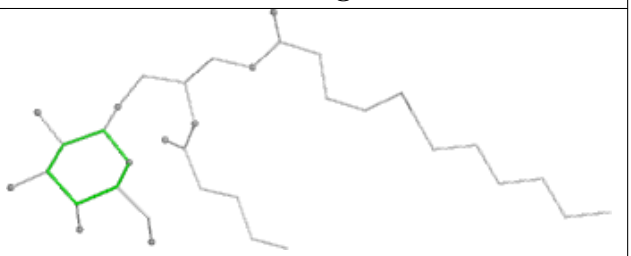
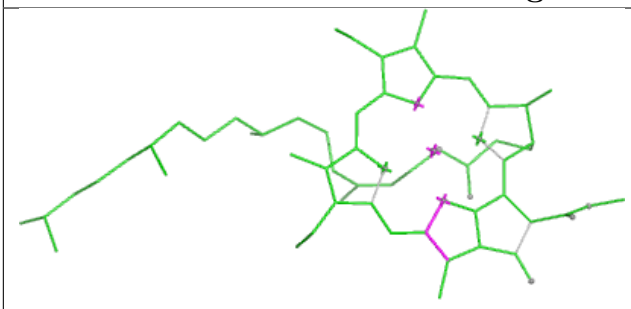
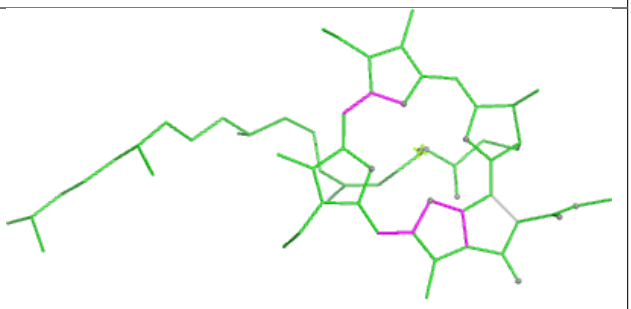


Rings

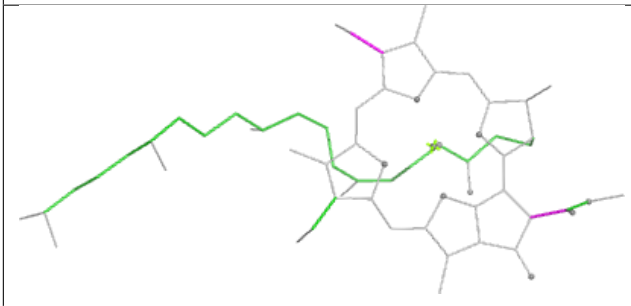
Ligand CLA Z 613



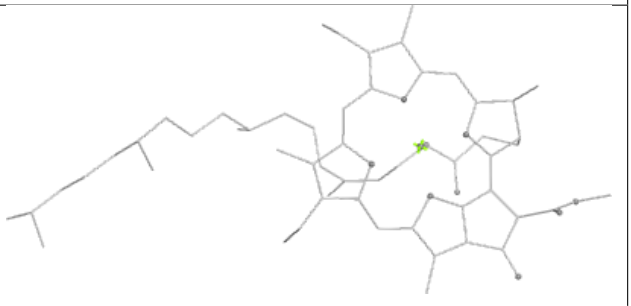
Bond lengths



Bond angles

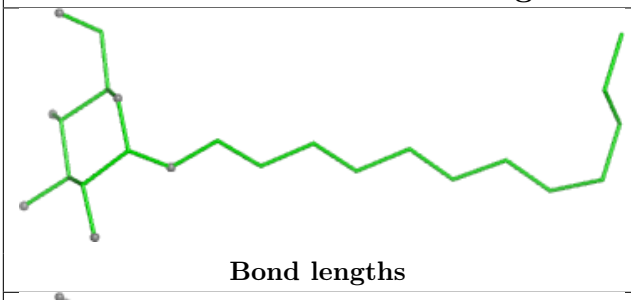


Torsions

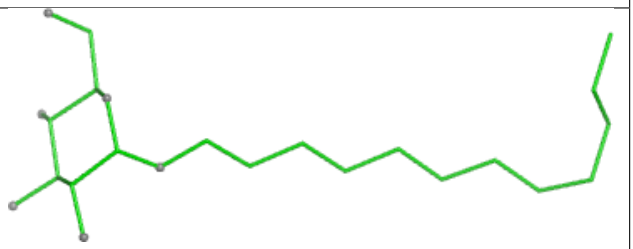


Rings

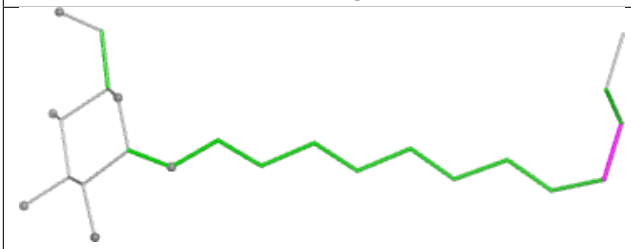
Ligand LMU 12 623



Bond lengths



Bond angles



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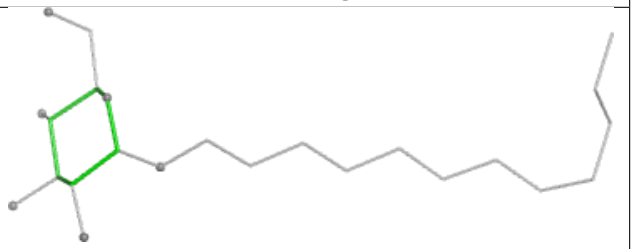
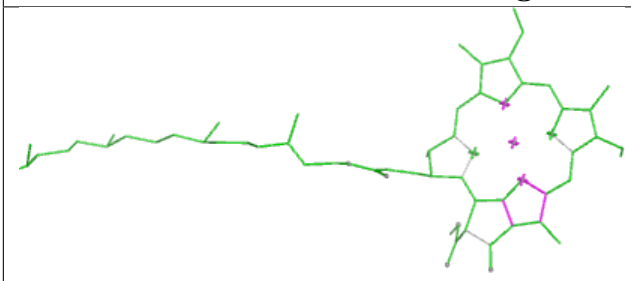
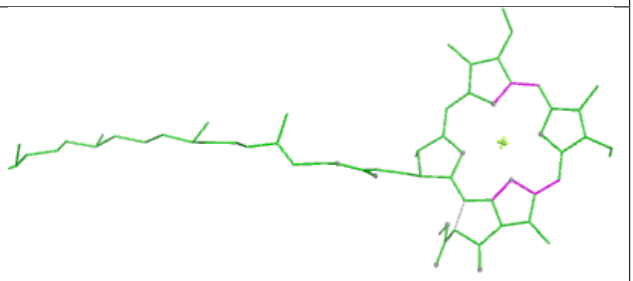


Rings

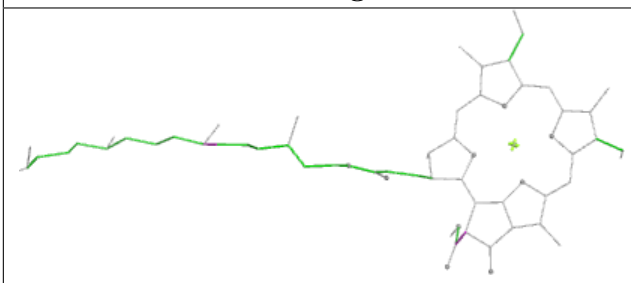
Ligand CLA B2 825



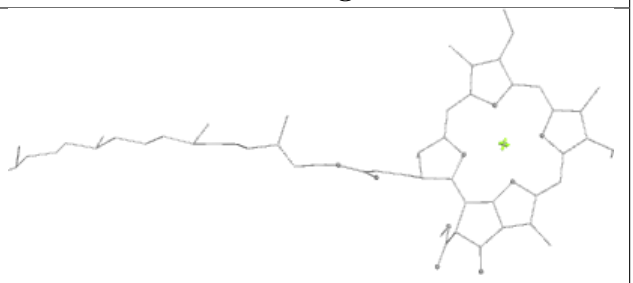
Bond lengths



Bond angles

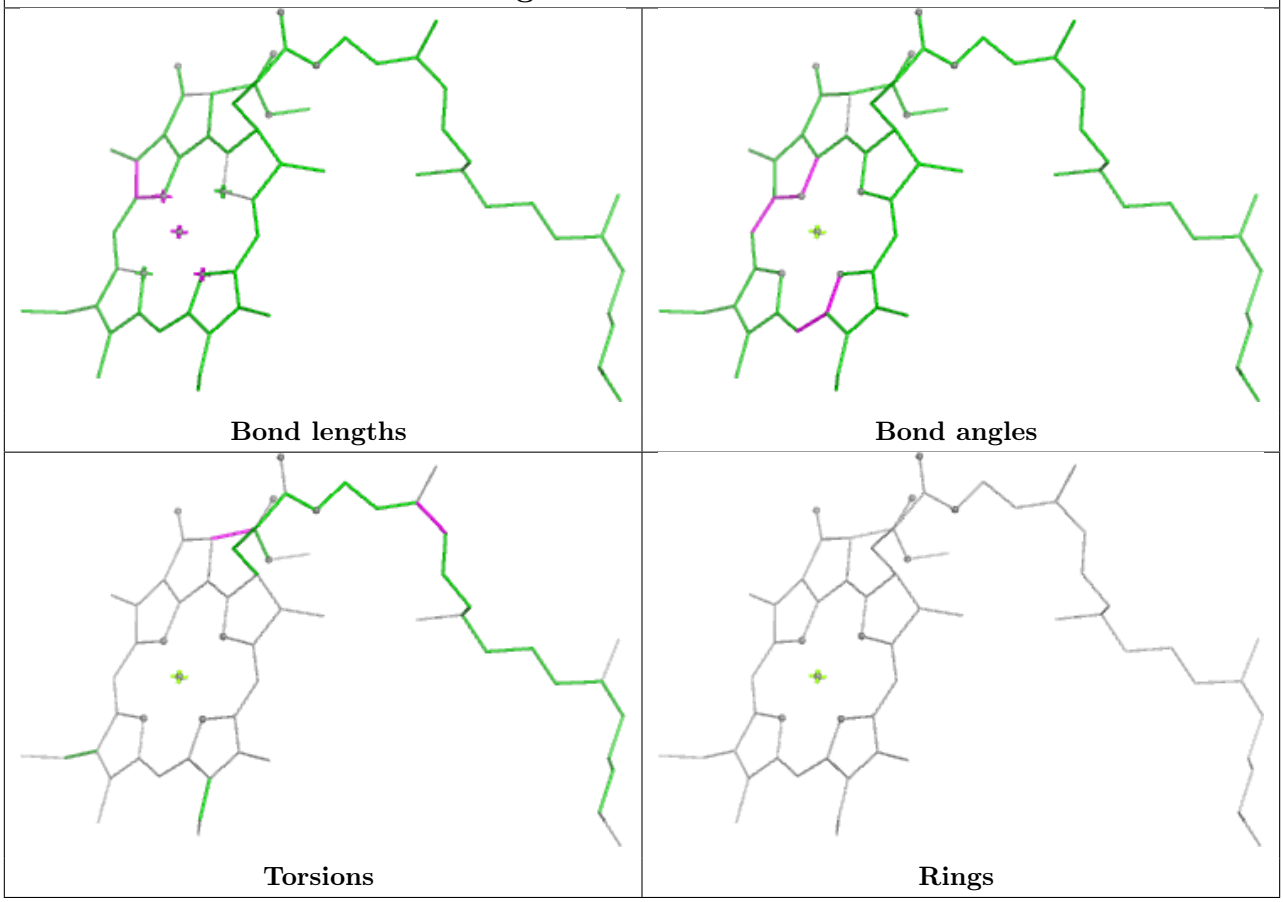


Torsions

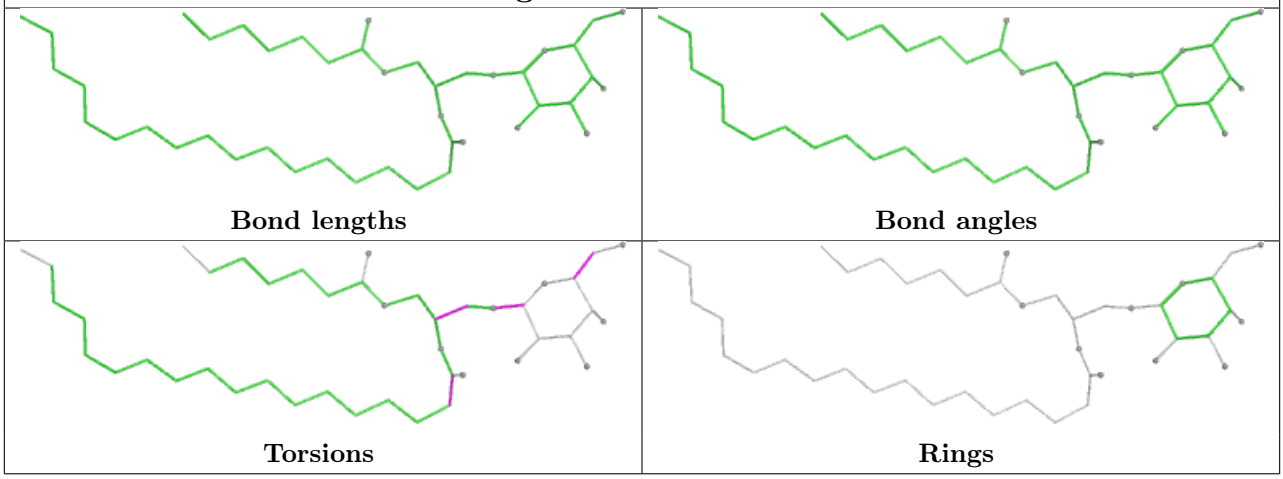


Rings

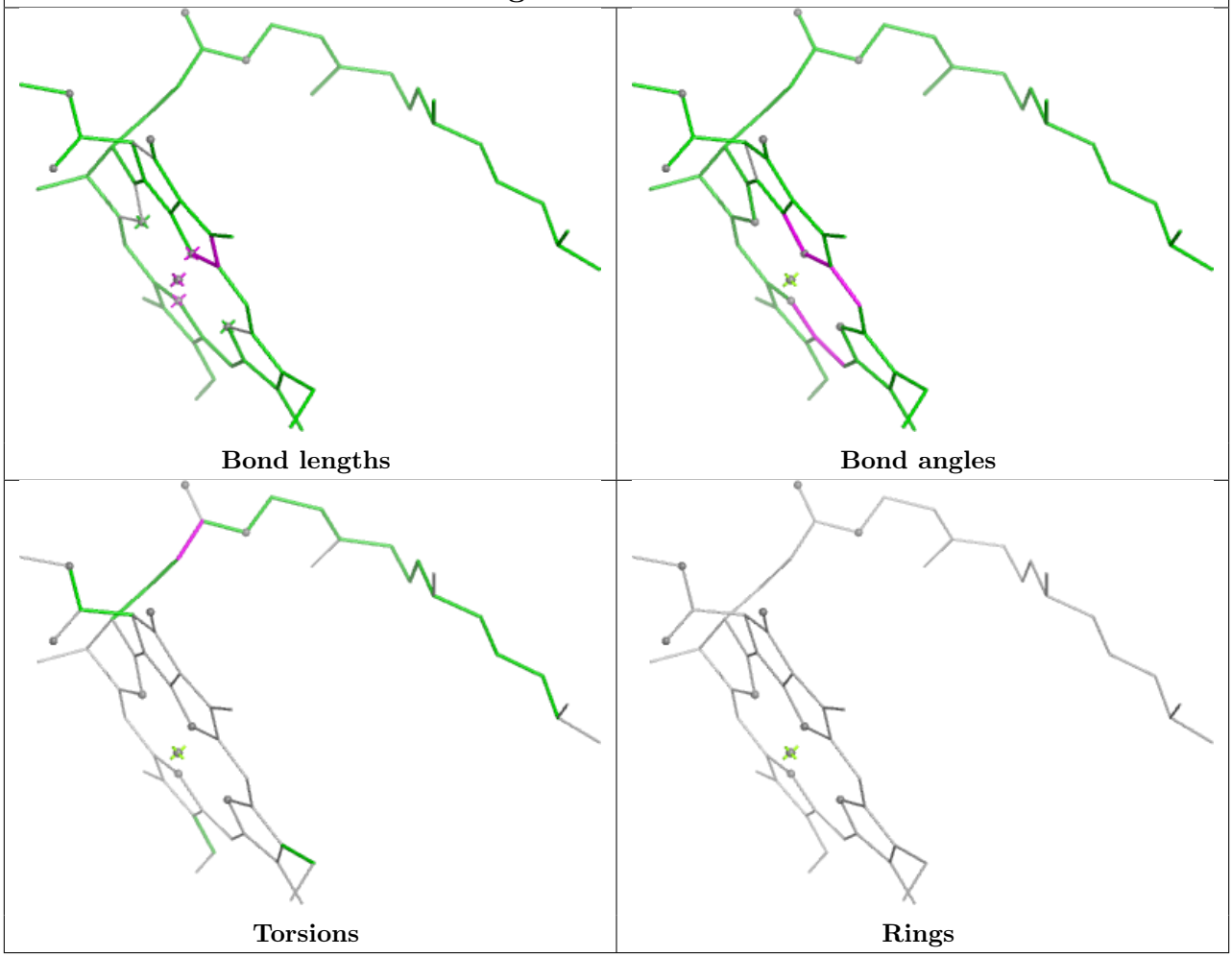
Ligand CLA B2 810



Ligand LMG 92 620



Ligand CLA 8 604



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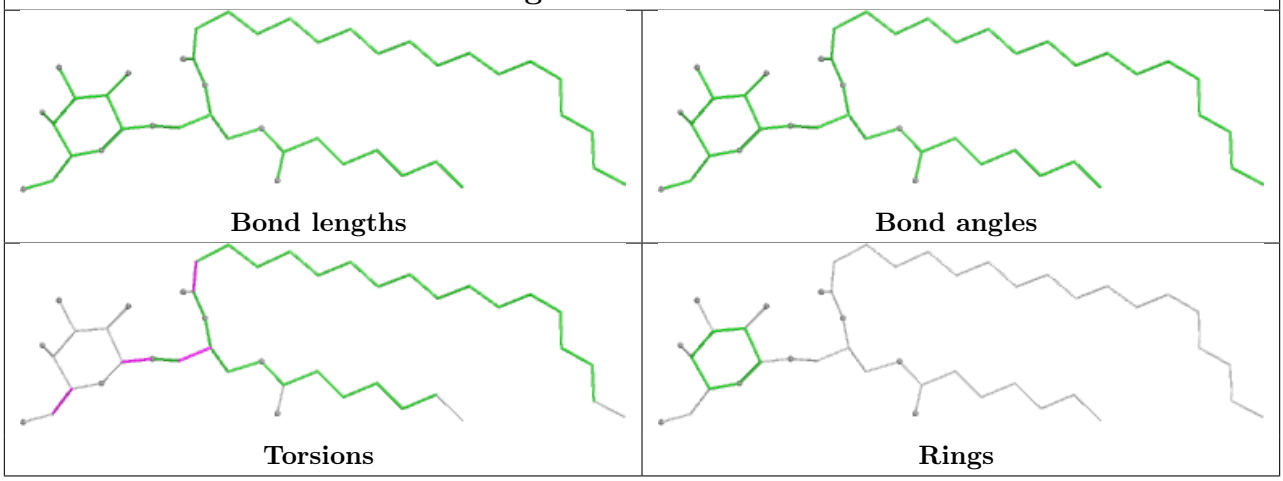
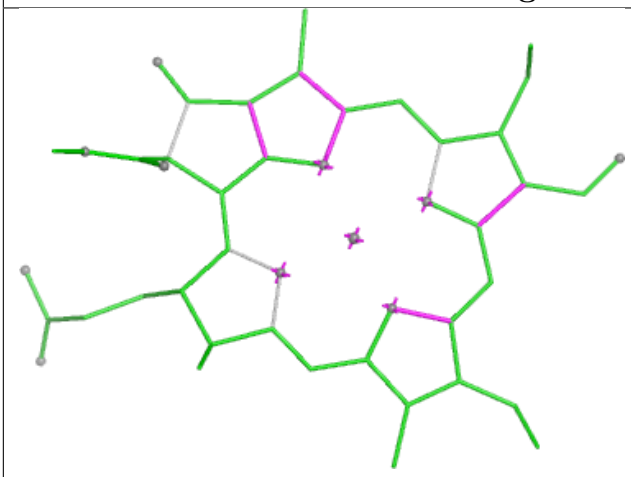
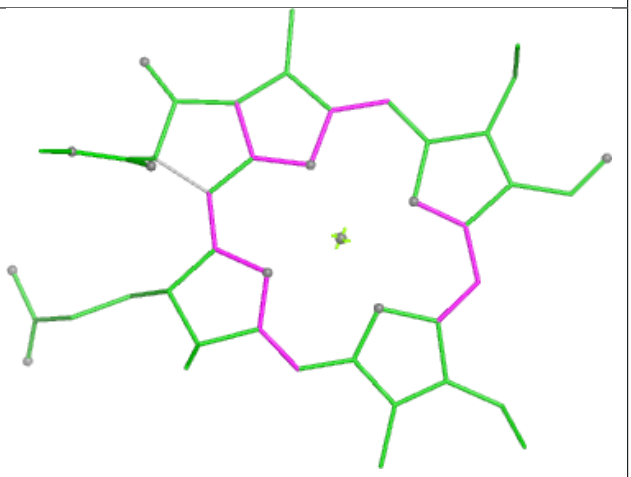


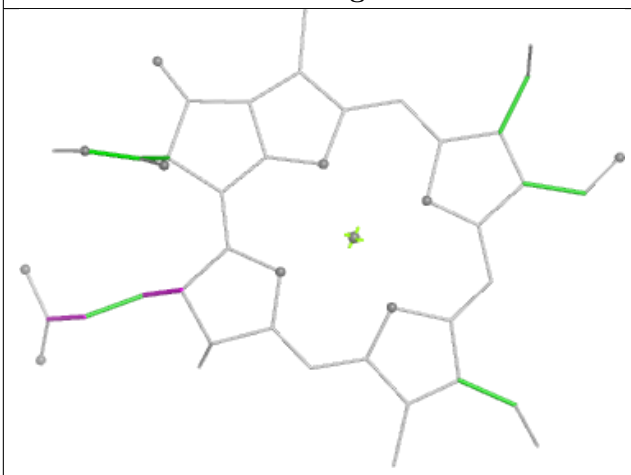
Ligand CHL 72 606



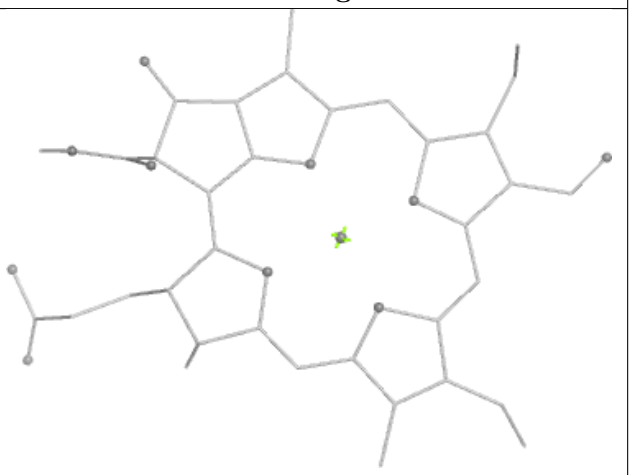
Bond lengths



Bond angles

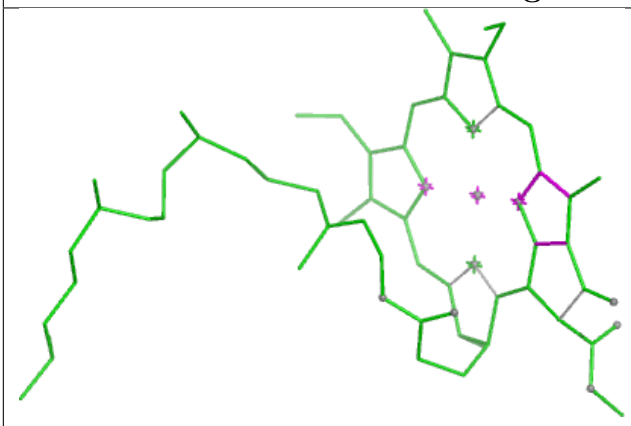


Torsions



Rings

Ligand CLA A 843



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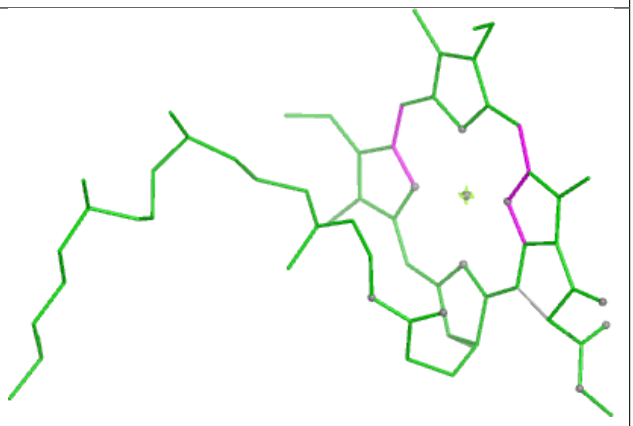
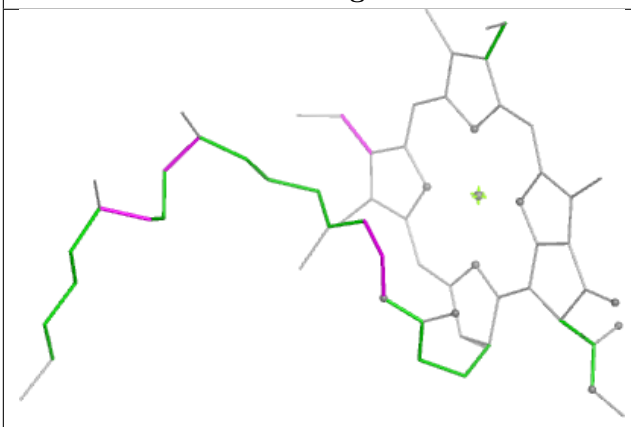
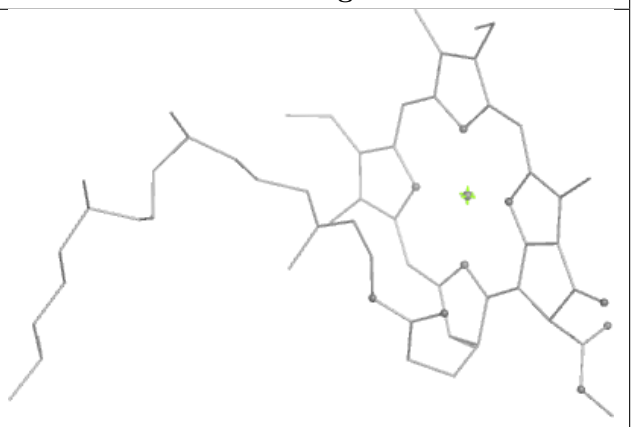


Bond angles

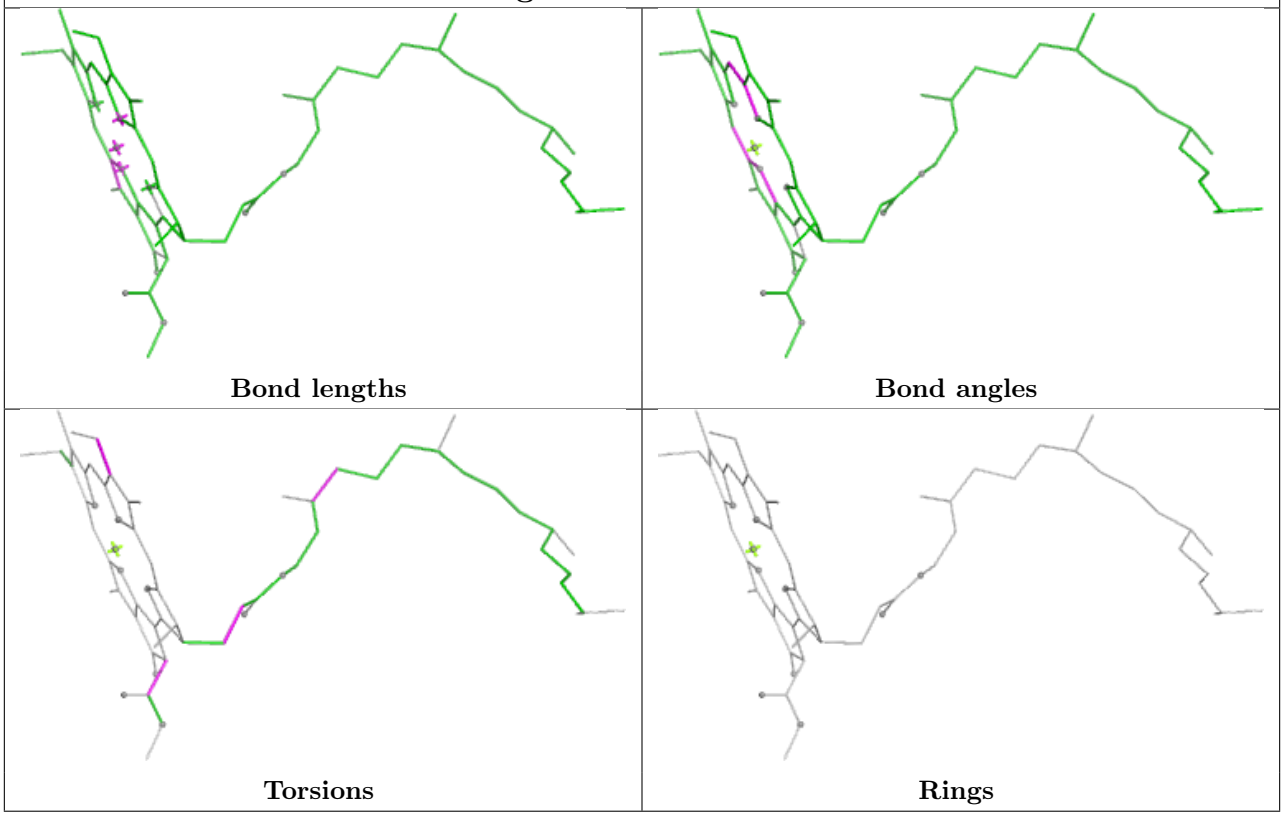


Torsions

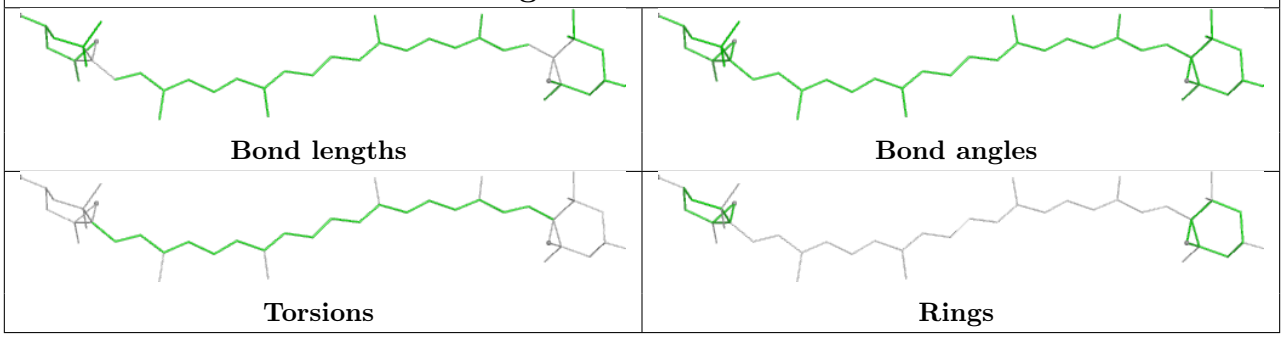


Rings

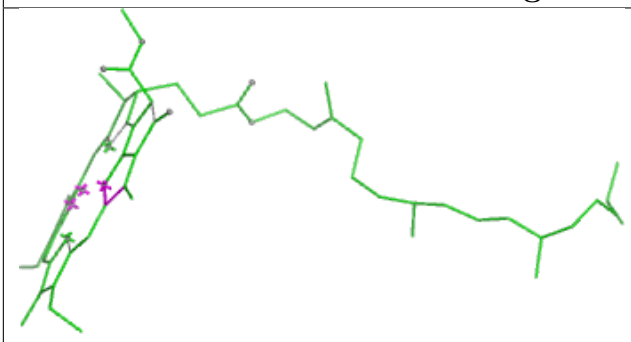
Ligand CLA B2 839



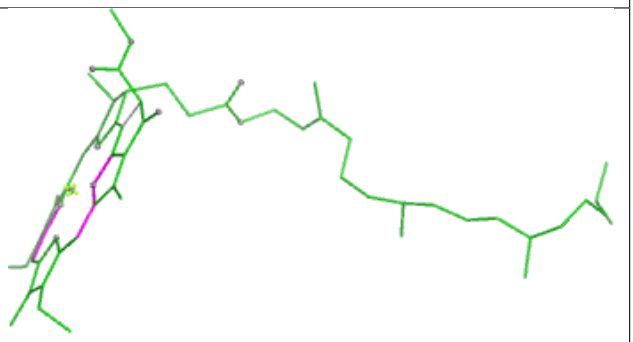
Ligand XAT 72 622



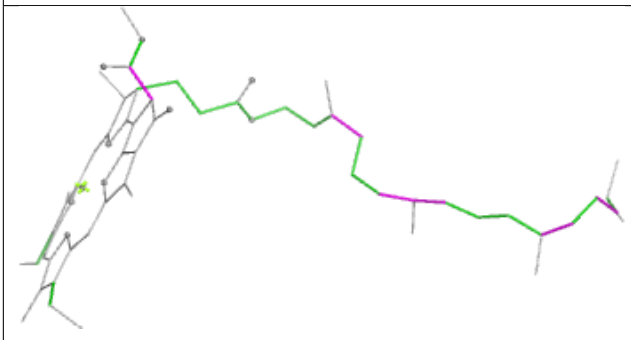
Ligand CLA A 840



Bond lengths



Bond angles



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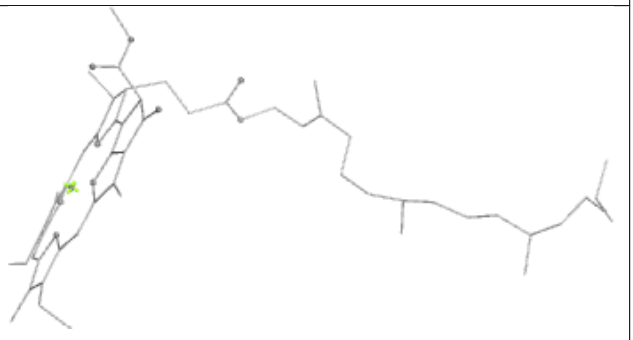
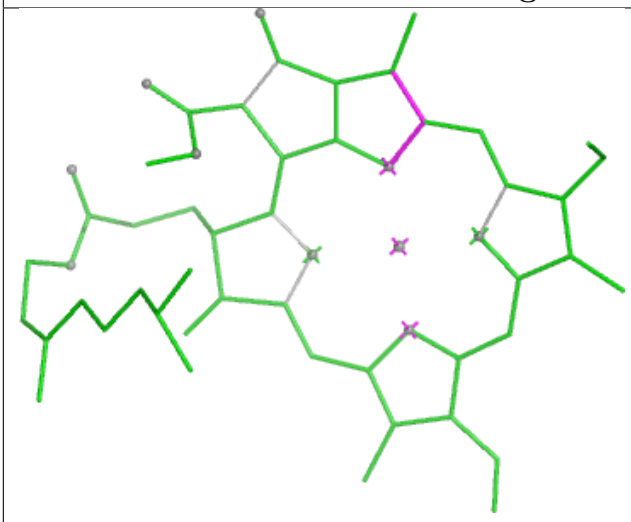
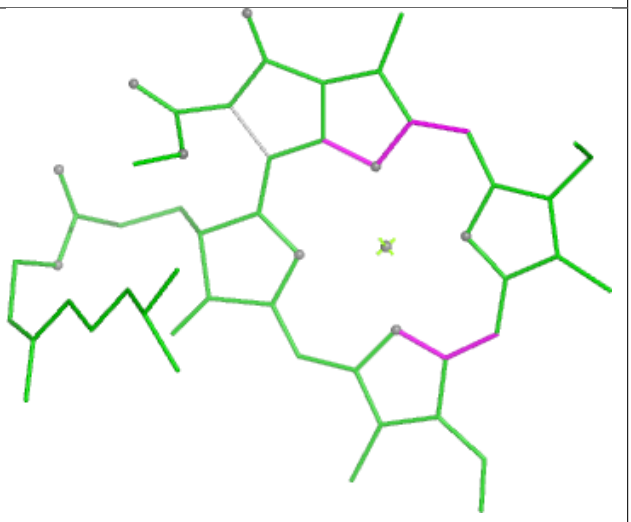


Rings

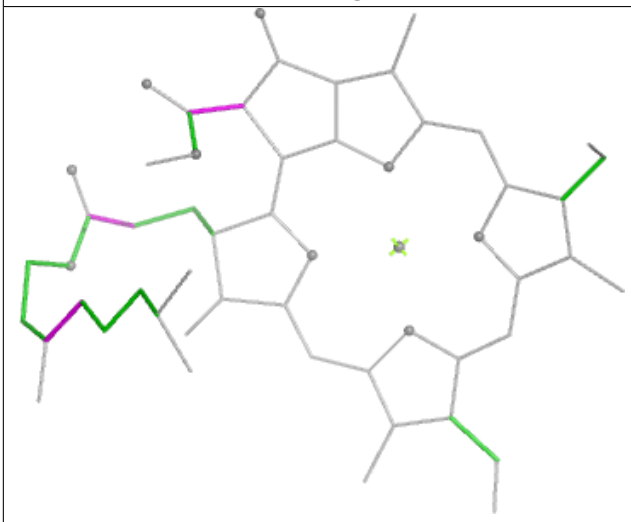
Ligand CLA 82 612



Bond lengths



Bond angles



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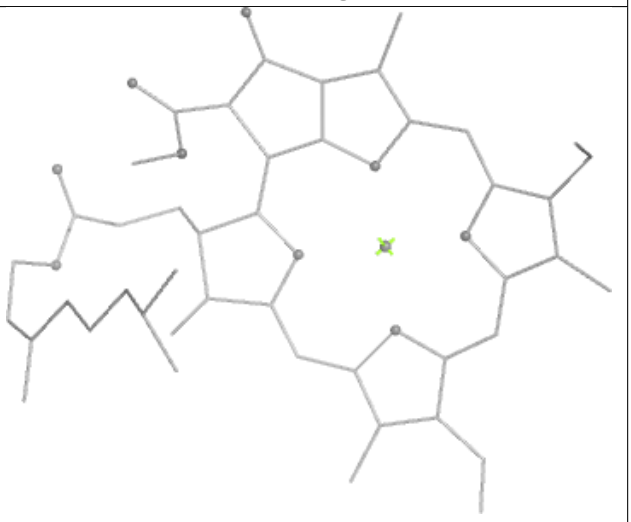
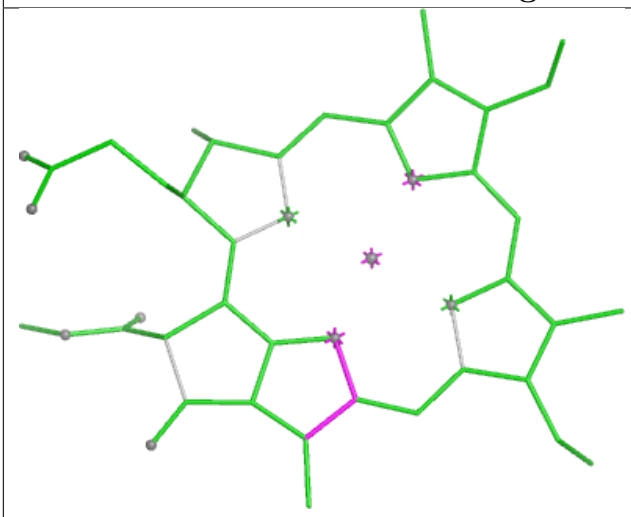


Rings

Ligand CLA 82 611



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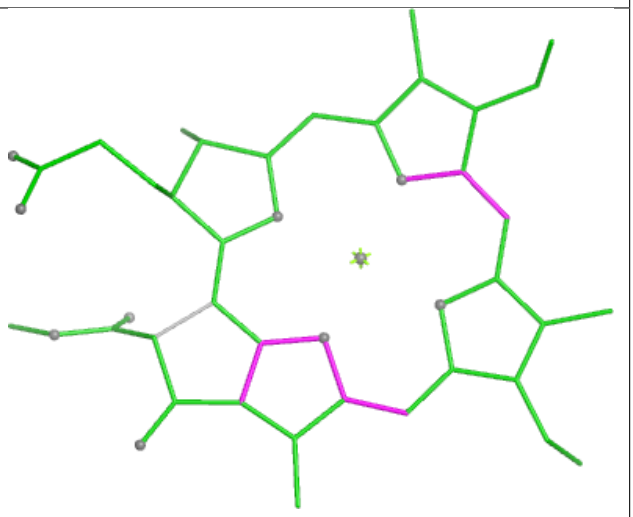
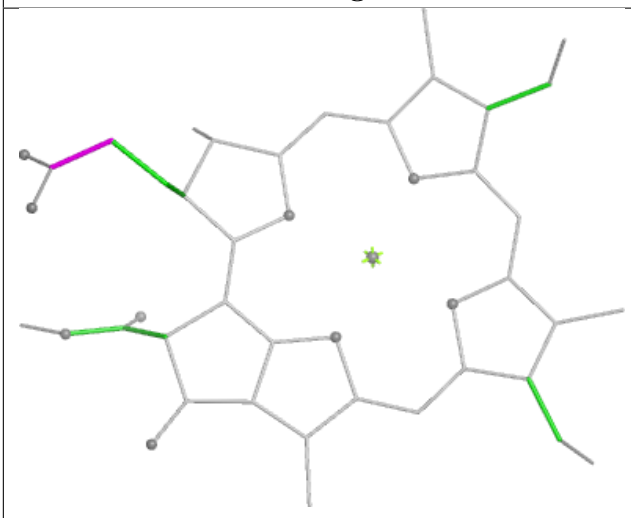


Bond angles



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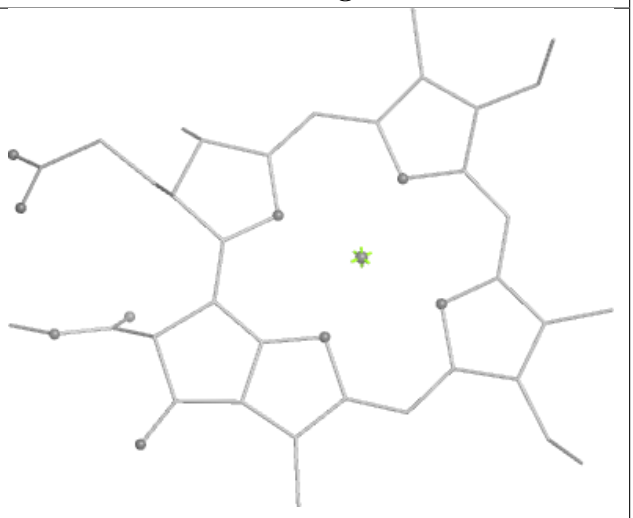
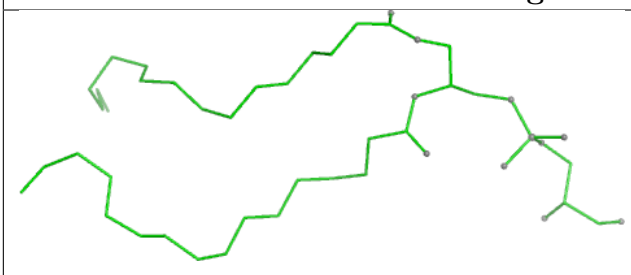


Rings

Ligand LHG 4 622



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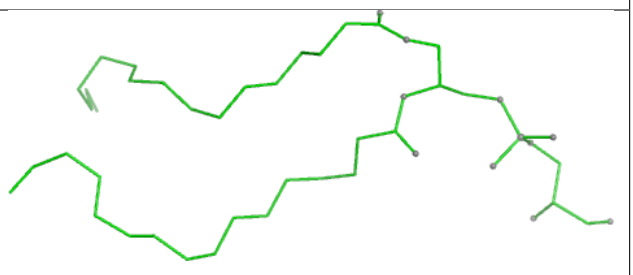
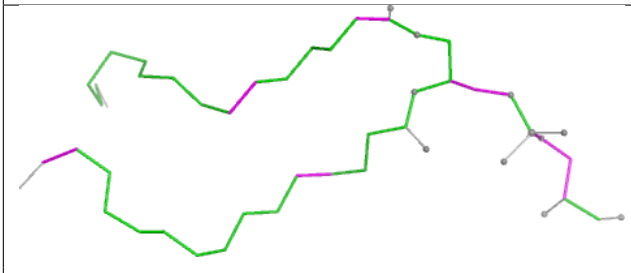


Bond angles



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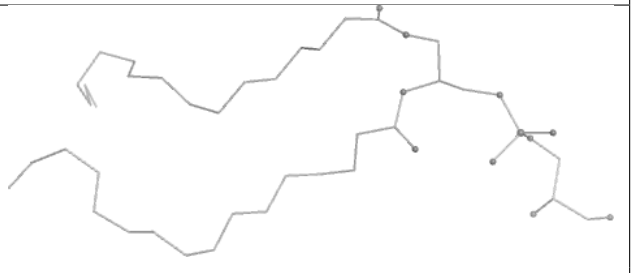
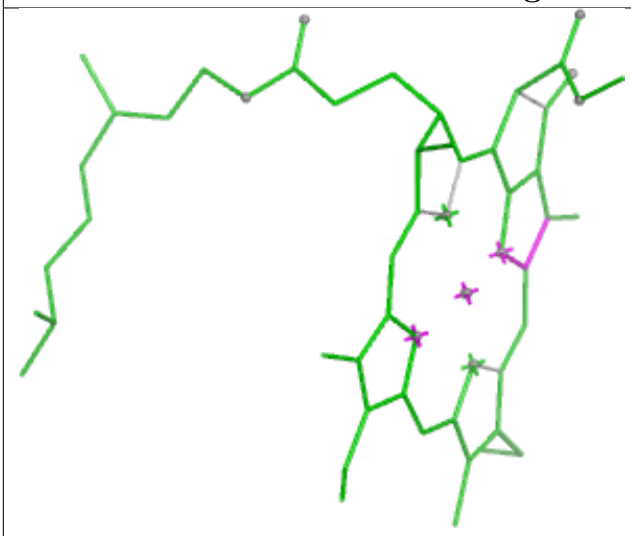


Rings

Ligand CLA A 817



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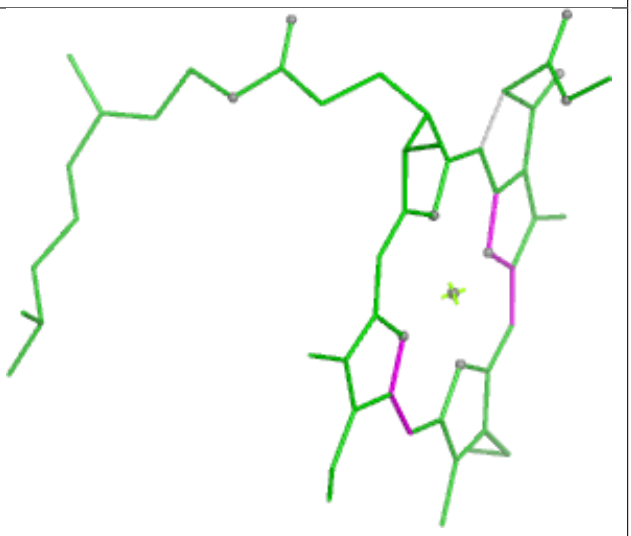
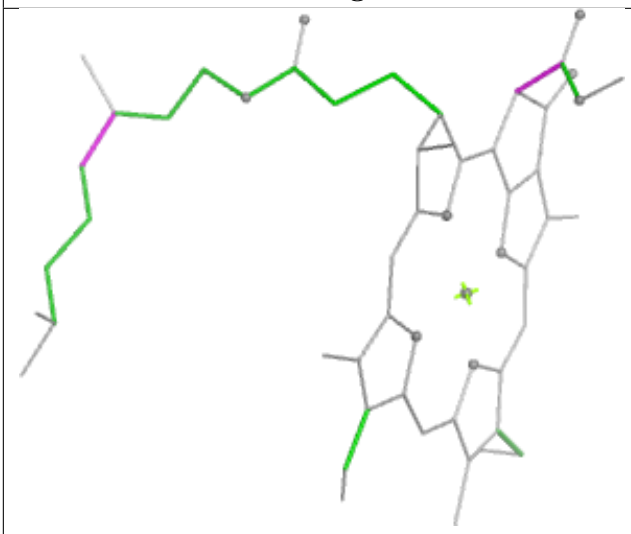


Bond angles



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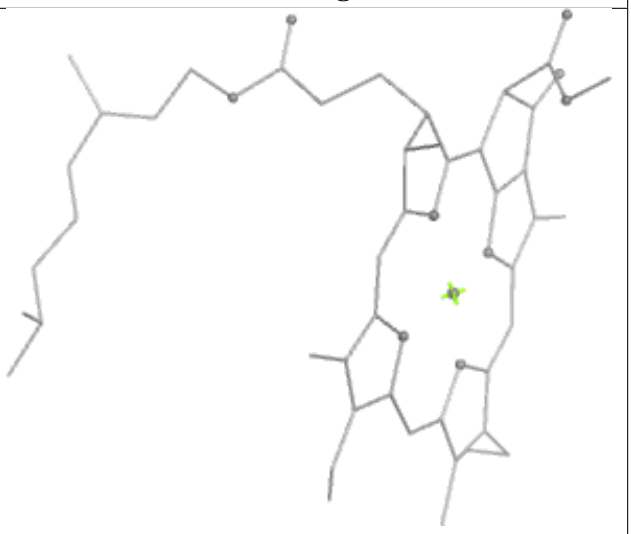
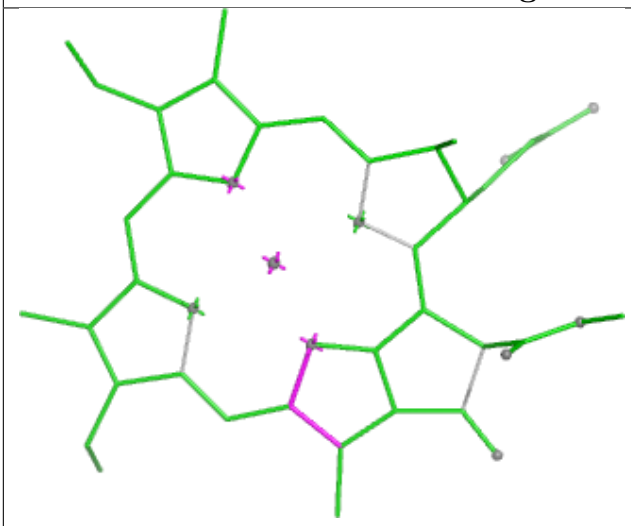


Rings

Ligand CLA 82 616



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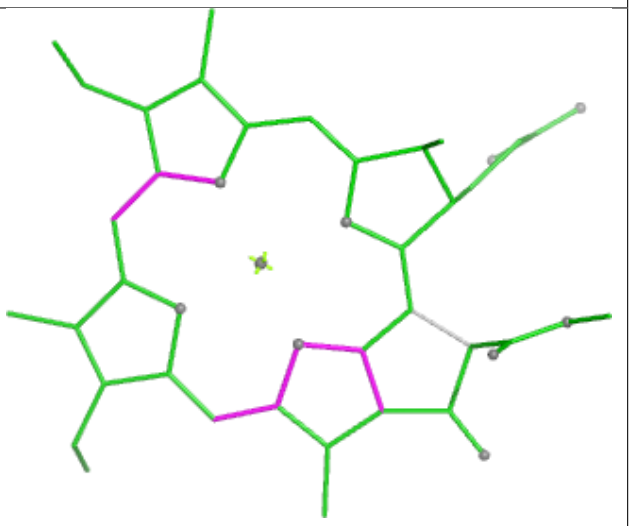
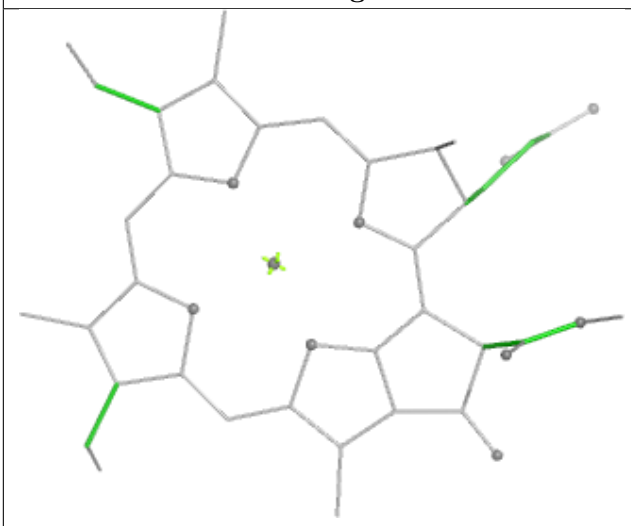


Bond angles



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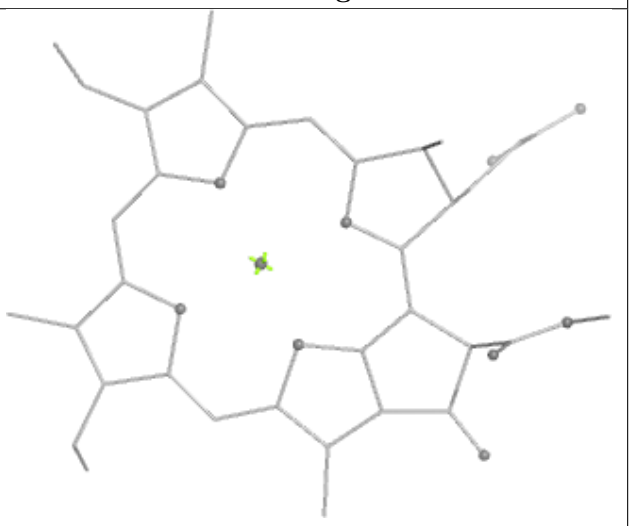
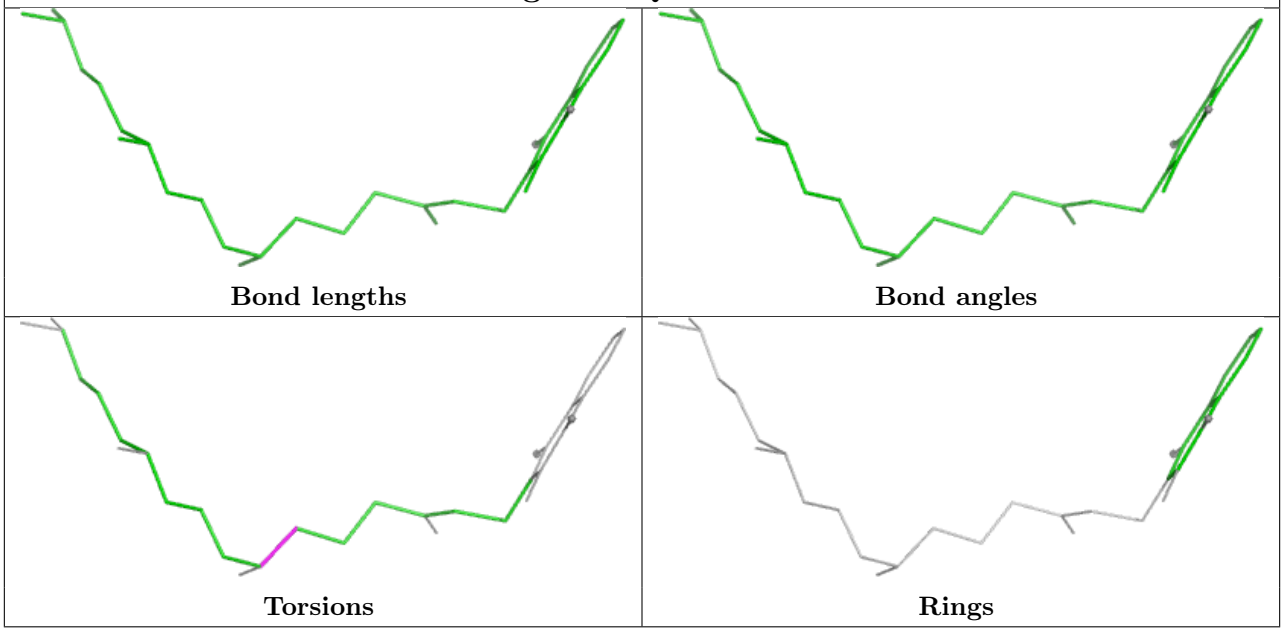
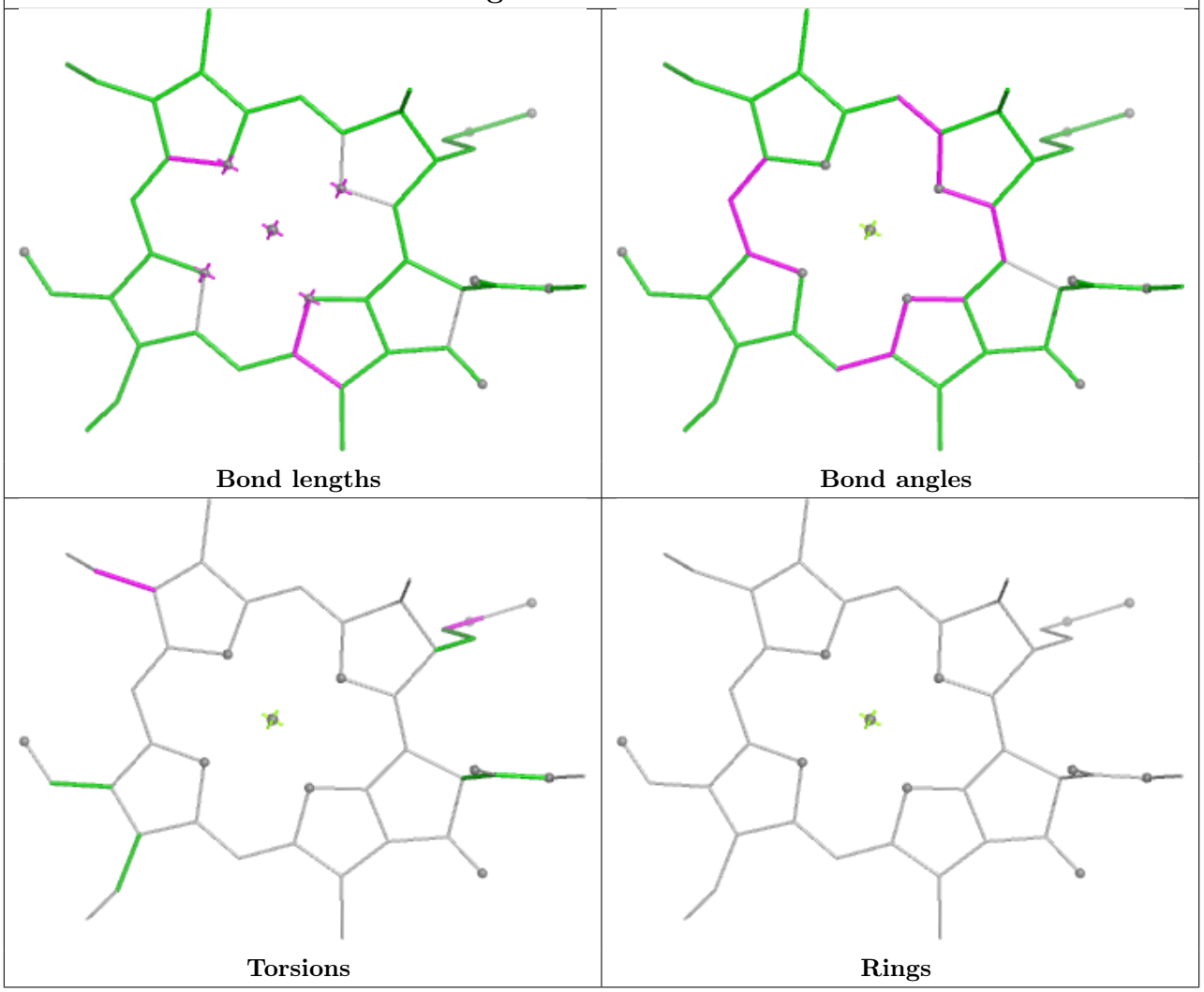


Rings

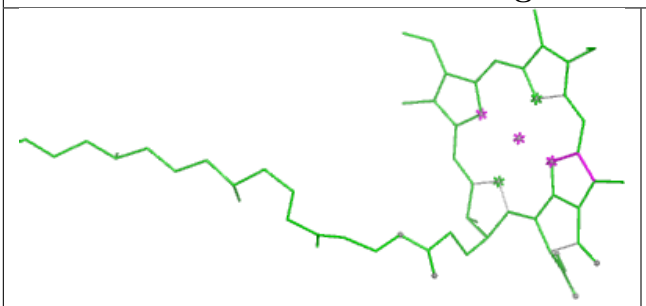
Ligand PQN B 842



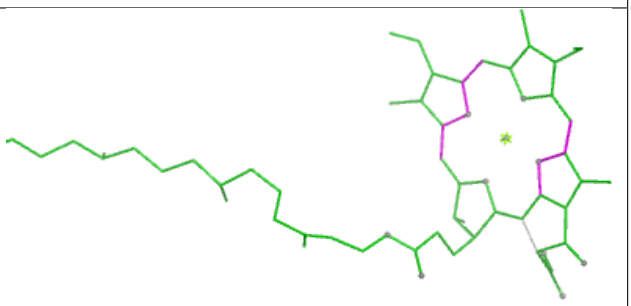
Ligand CHL 72 607



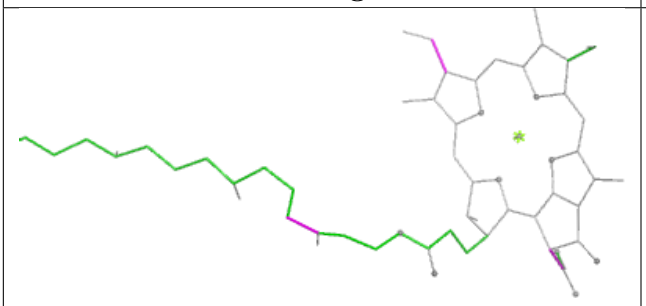
Ligand CLA A2 835



Bond lengths



Bond angles



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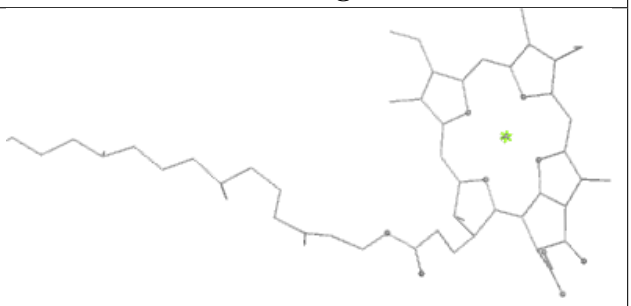
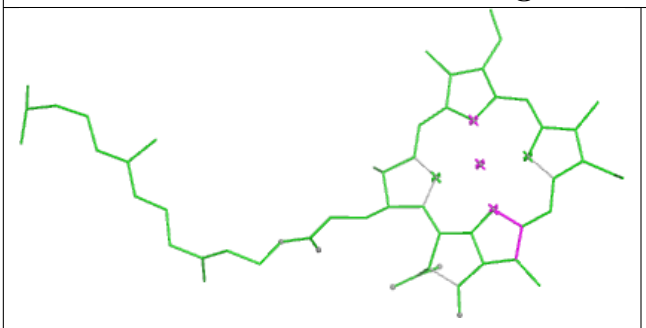
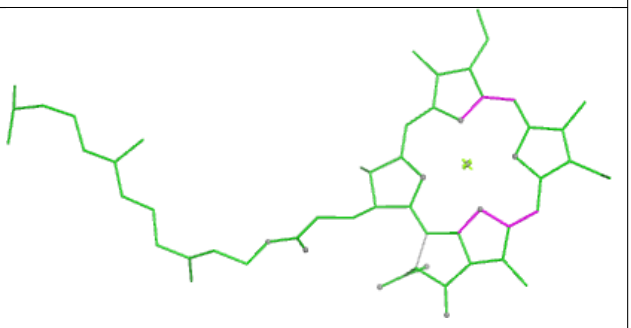


Rings

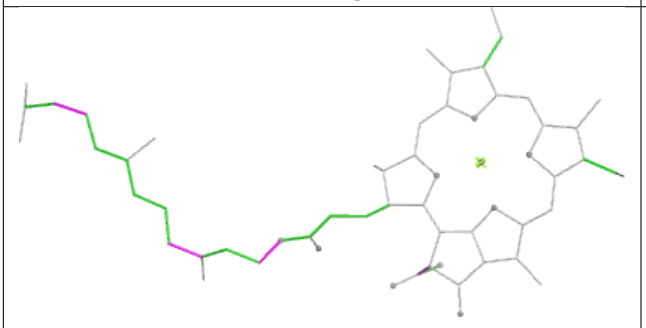
Ligand CLA B2 836



Bond lengths



Bond angles



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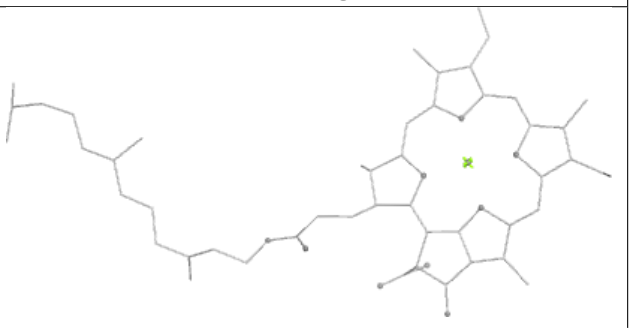
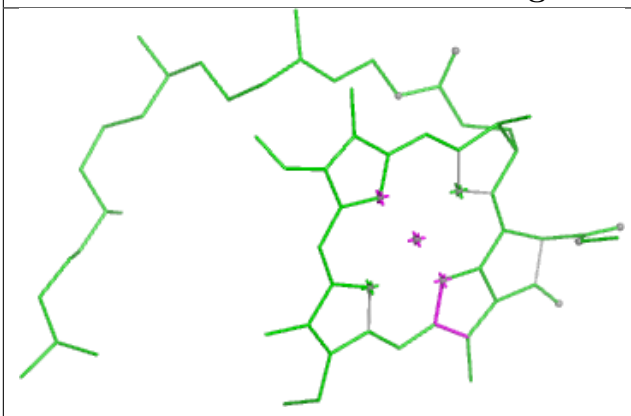
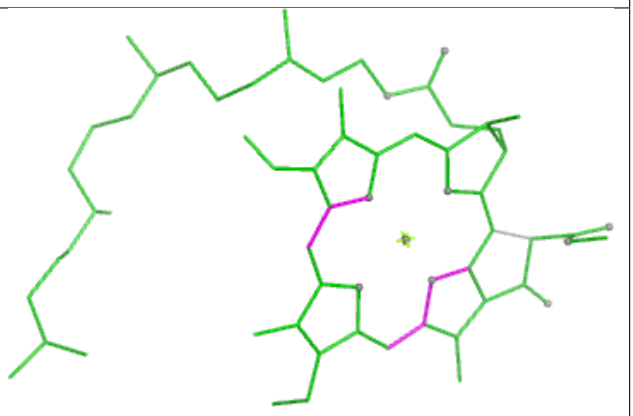


Rings

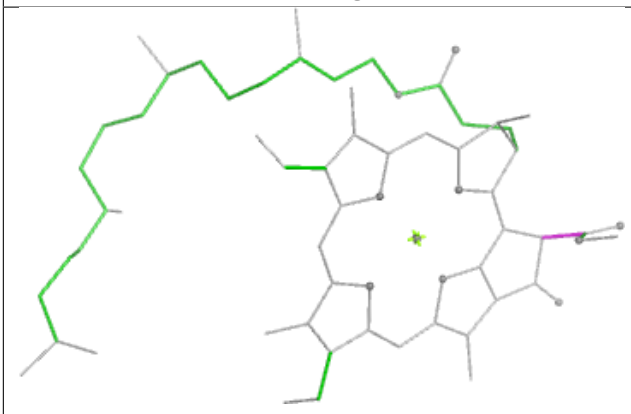
Ligand CLA 6 602



Bond lengths



Bond angles



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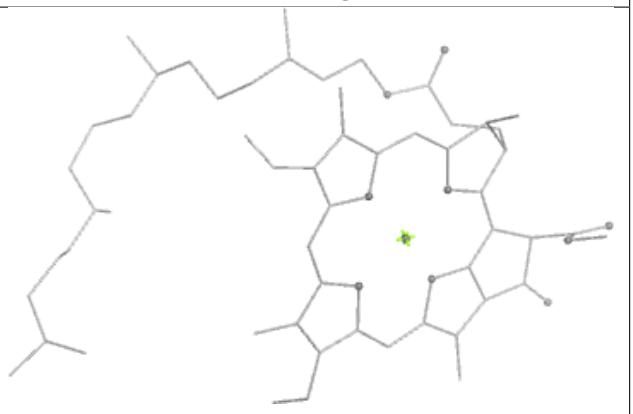
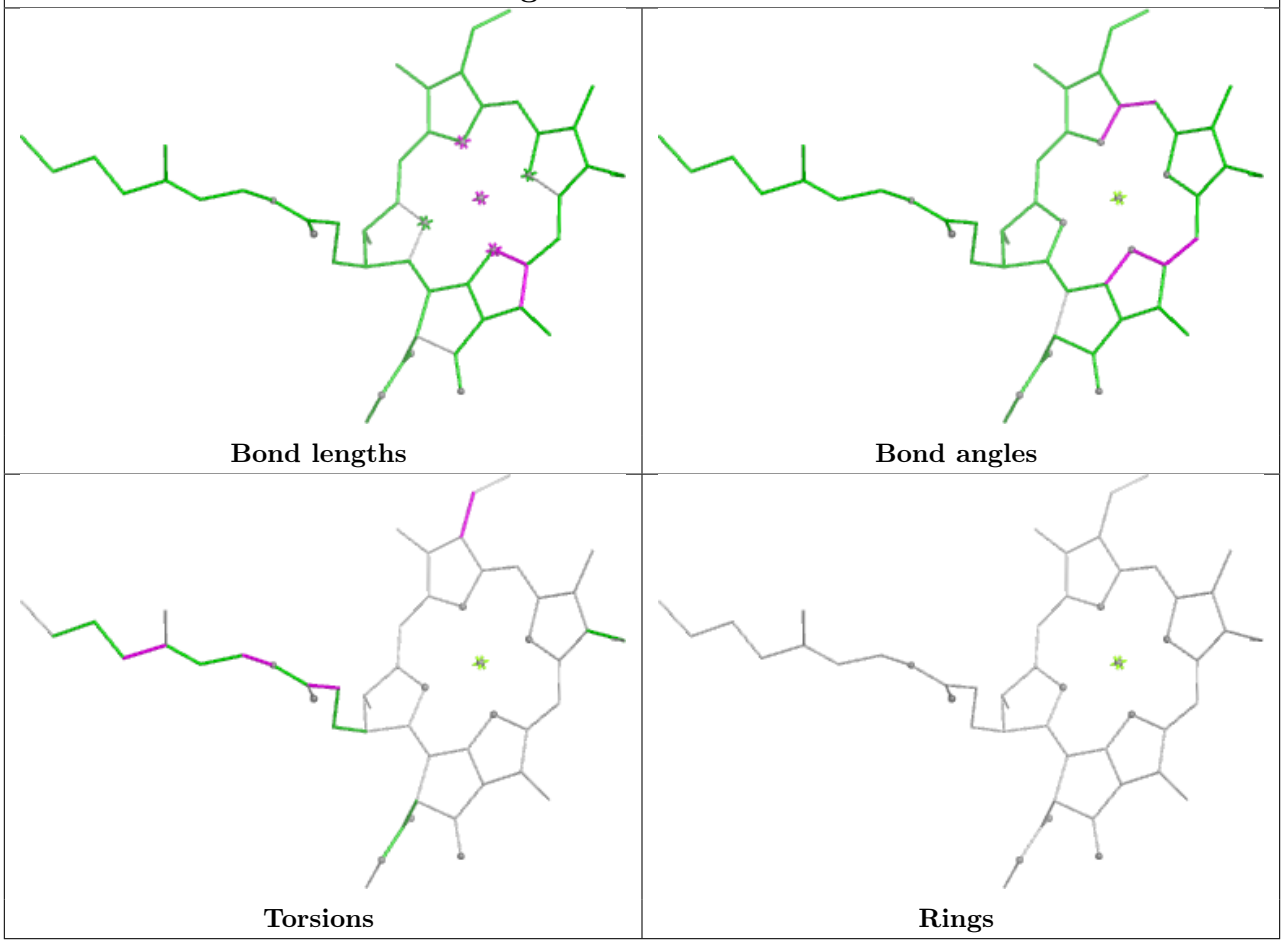


Rings

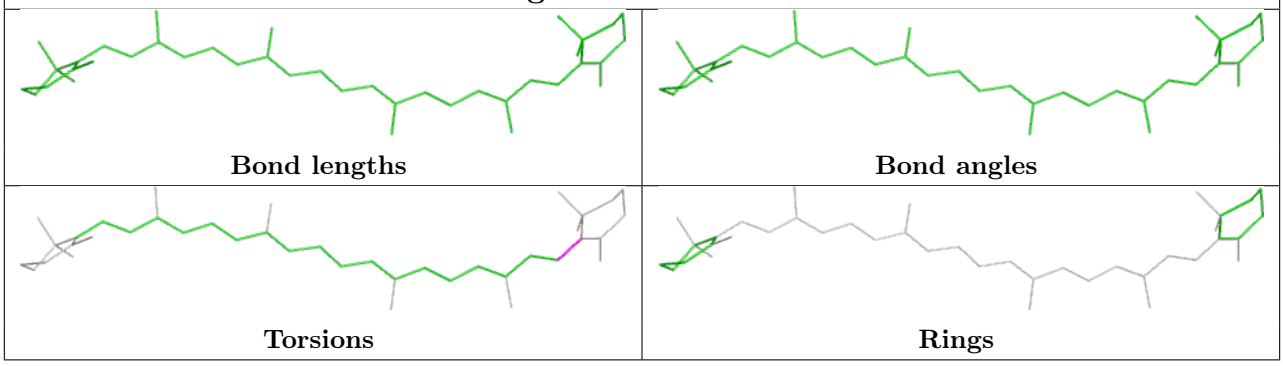
Ligand CLA 52 616



Bond lengths | Bond angles

Torsions | Rings

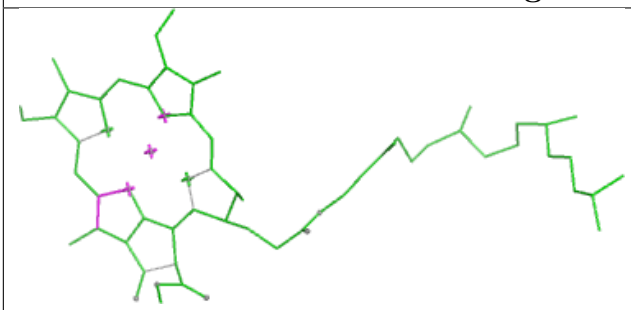
Ligand BCR 7 623



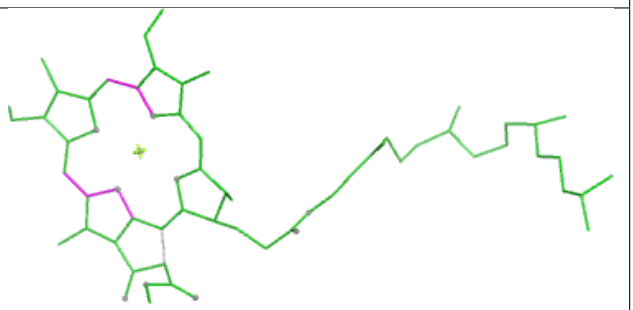
Bond lengths | Bond angles

Torsions | Rings

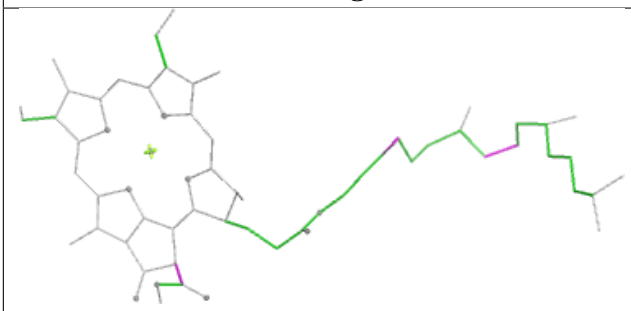
Ligand CLA B 813



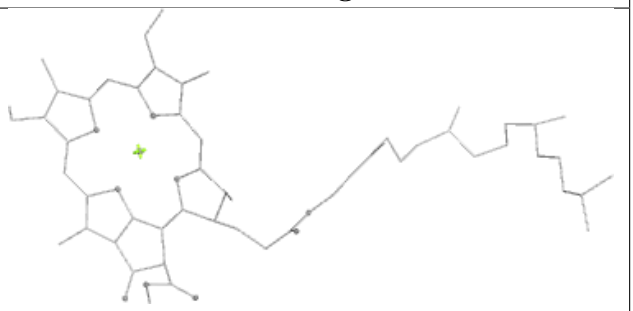
Bond lengths



Bond angles

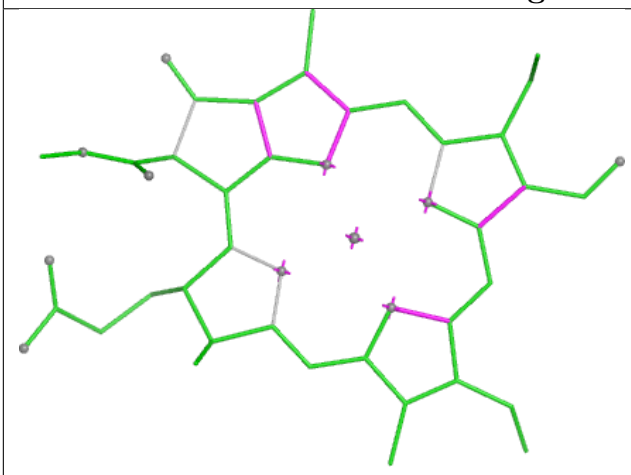


Torsions

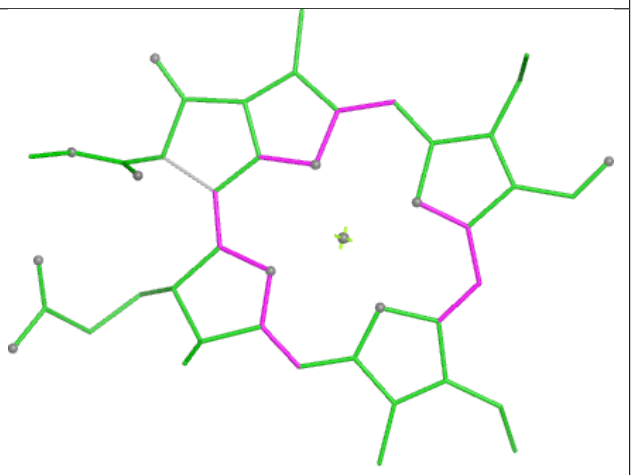


Rings

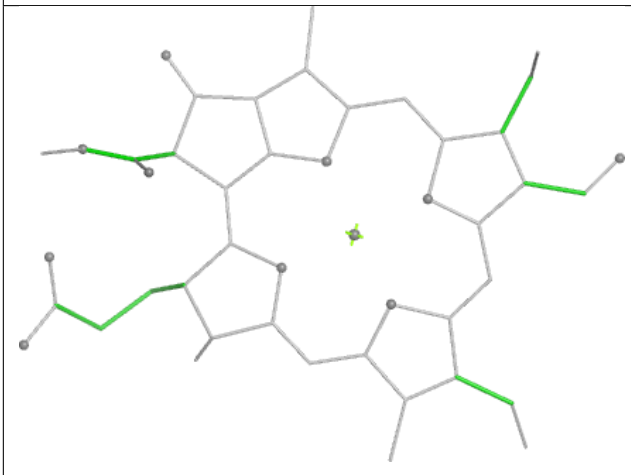
Ligand CHL 1 606



Bond lengths



Bond angles



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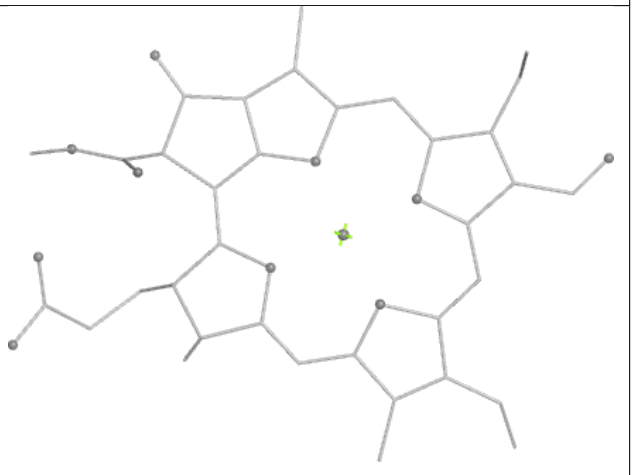
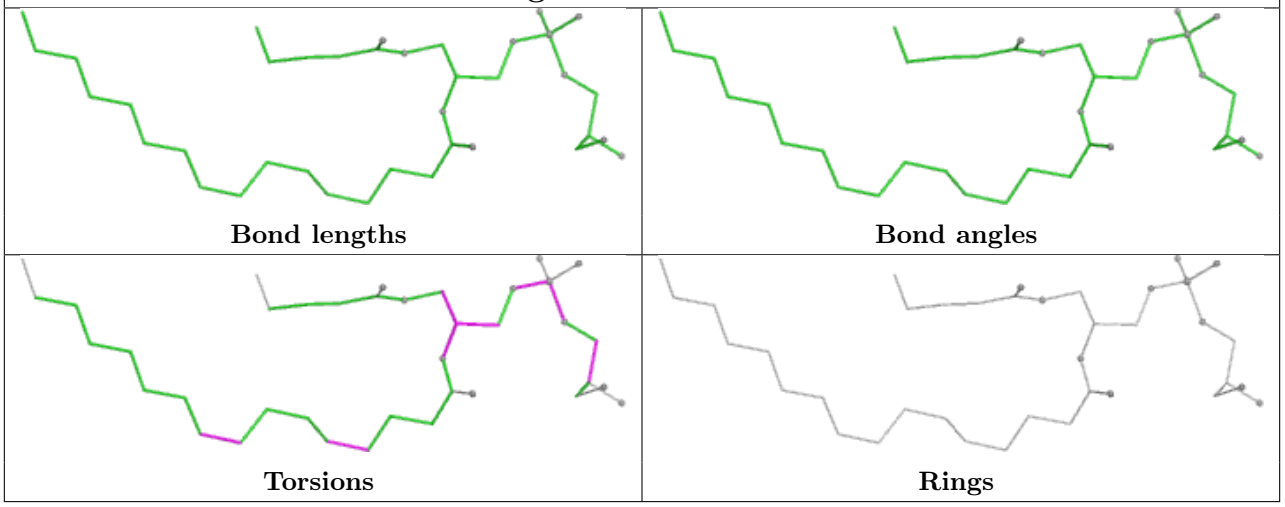
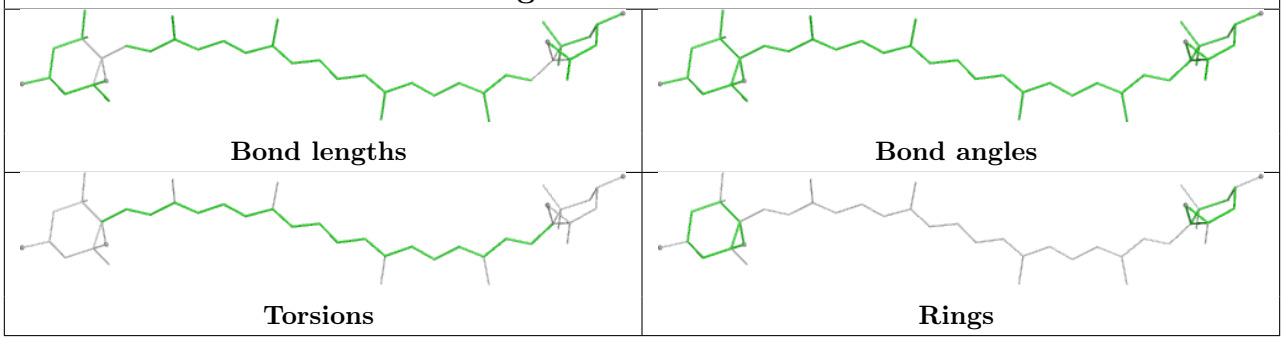


Rings

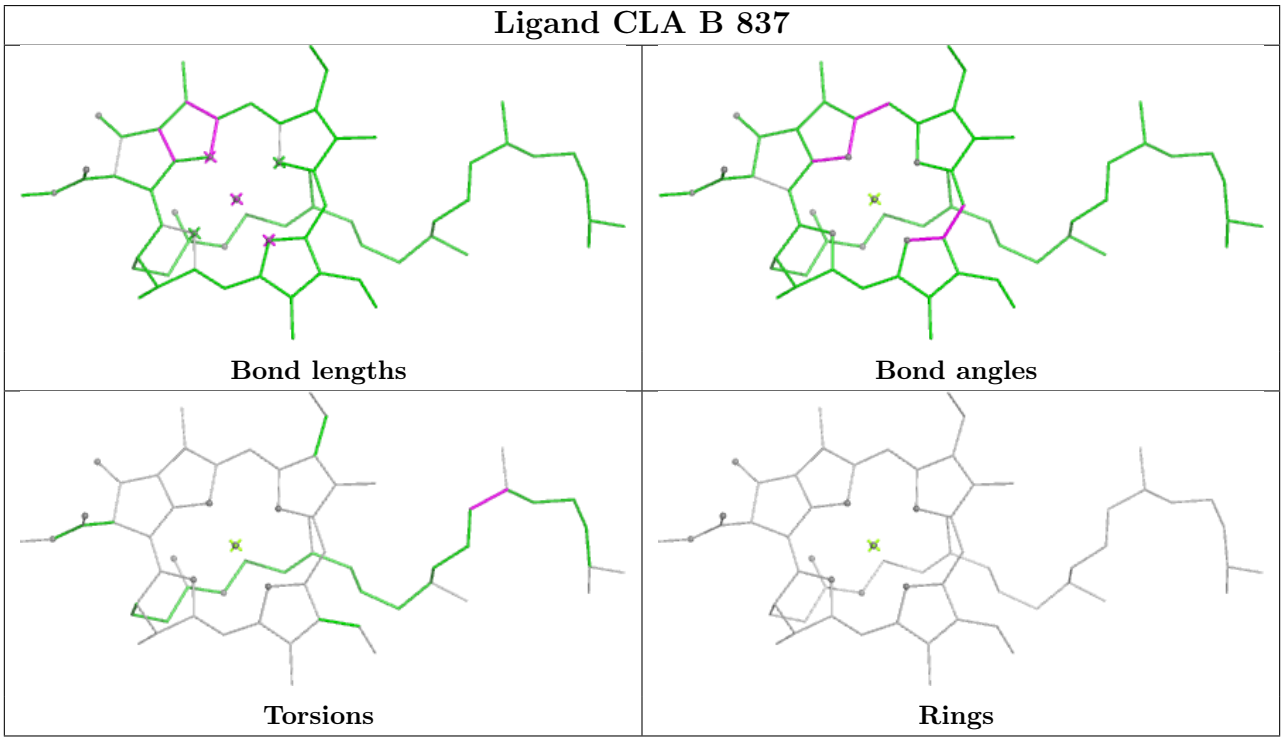
Ligand LHG 4 623



Ligand XAT Z2 618



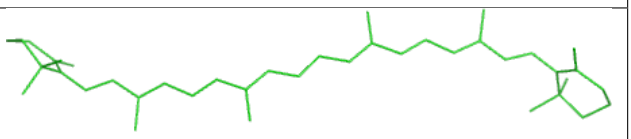
Ligand CLA B 837



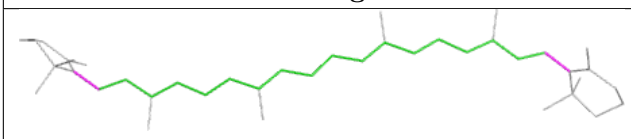
Ligand BCR 52 622



Bond lengths



Bond angles



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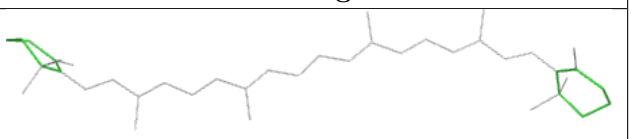
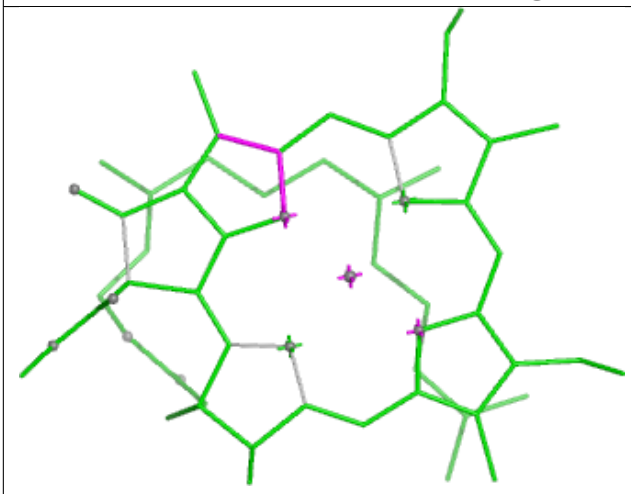
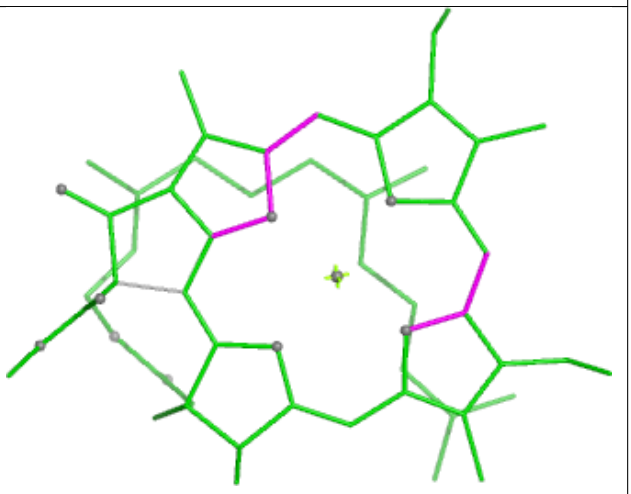


Rings

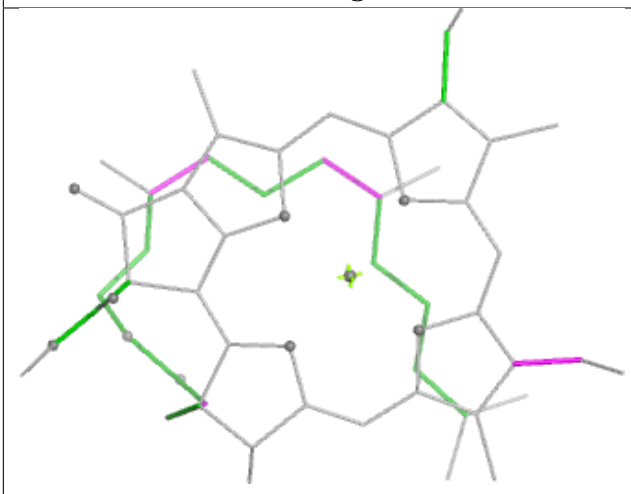
Ligand CLA 1 614



Bond lengths



Bond angles



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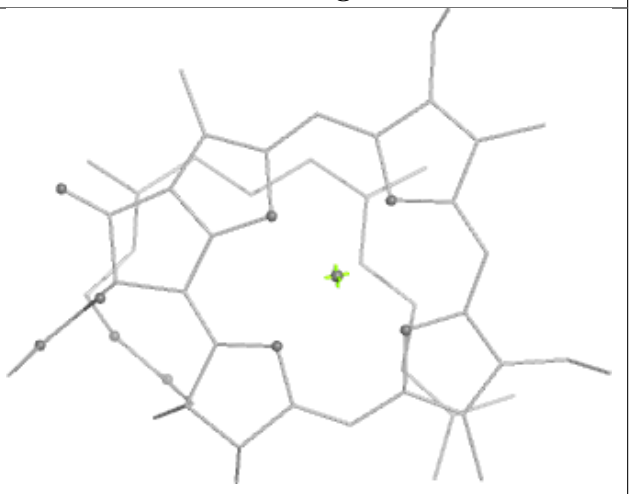
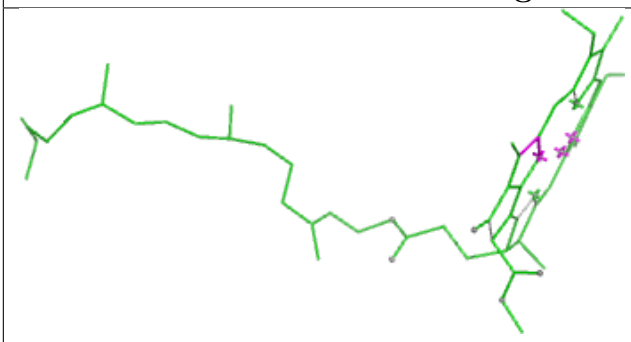


Rings

Ligand CLA A2 840



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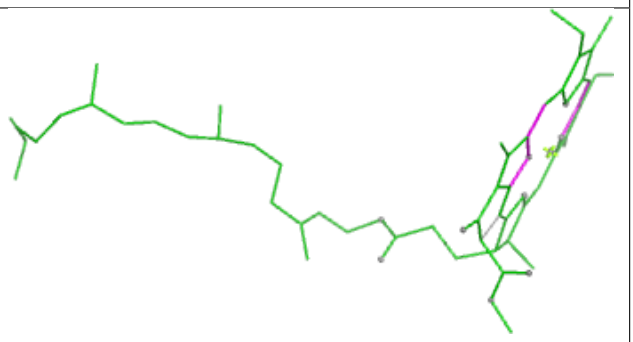
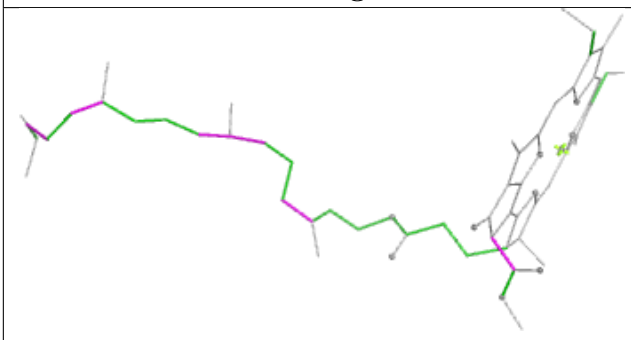


Bond angles

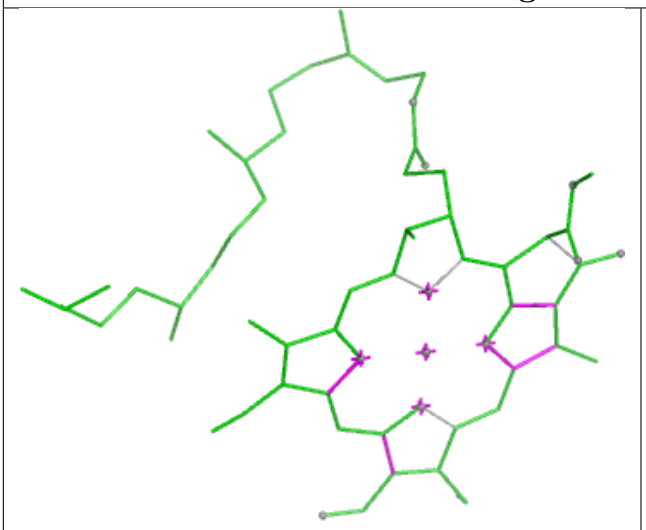


Torsions



Rings

Ligand CHL 42 608



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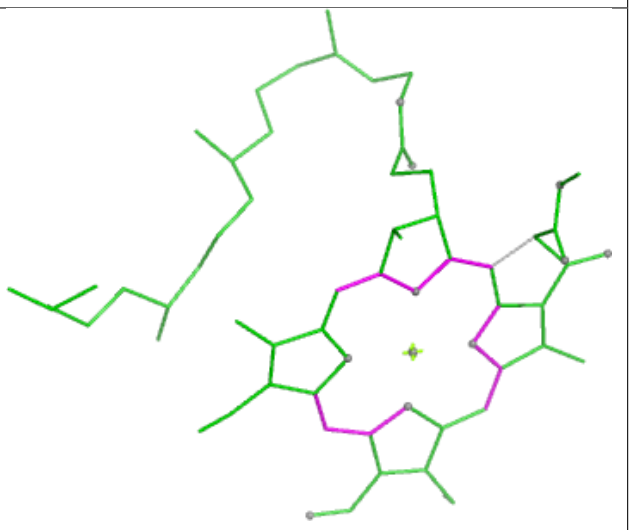
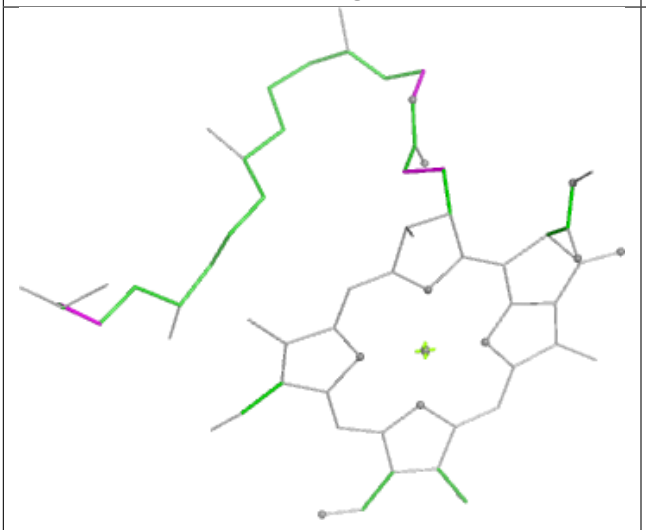


Bond angles



Torsions



Rings

Ligand BCR J2 102



Bond lengths



Bond angles

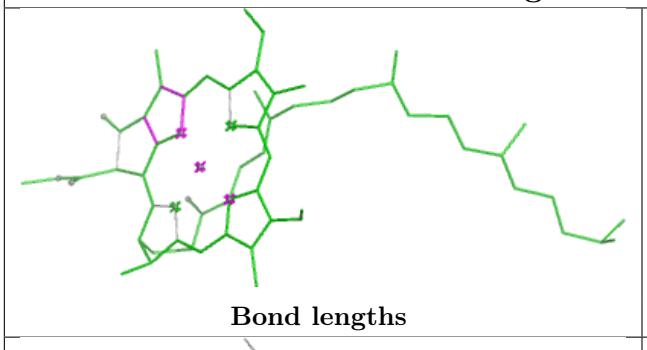


Torsions

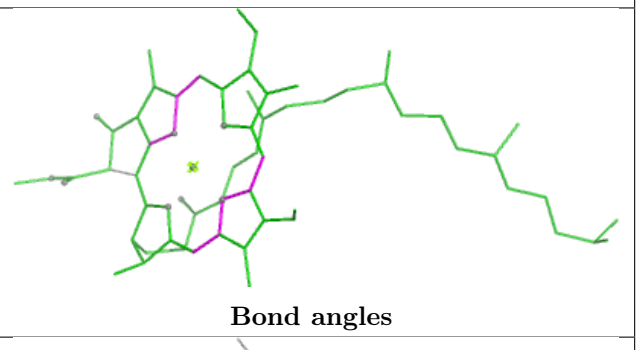


Rings

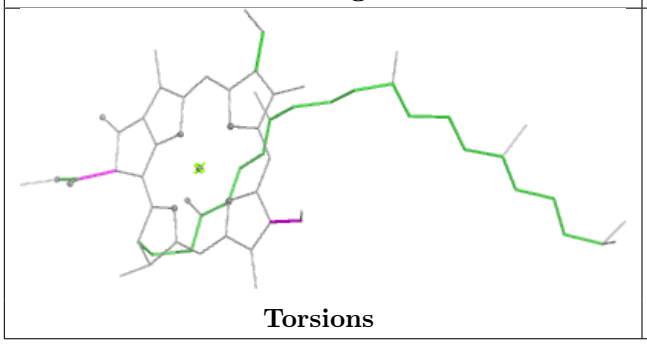
Ligand CLA A 842



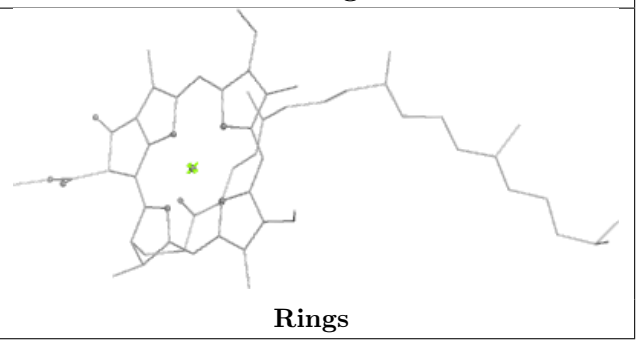
Bond lengths



Bond angles

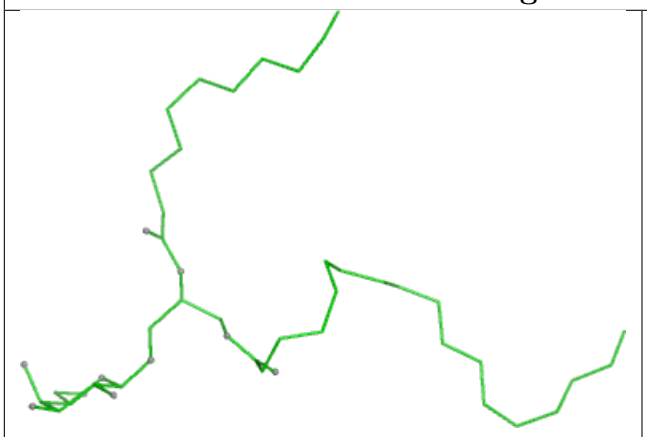


Torsions



Rings

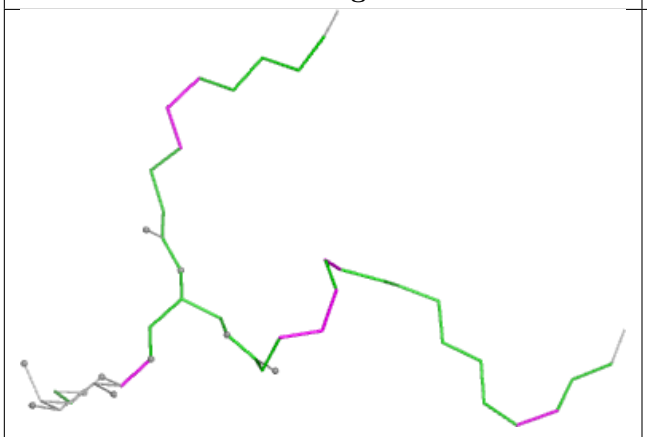
Ligand LMG A 859



Bond lengths



Bond angles

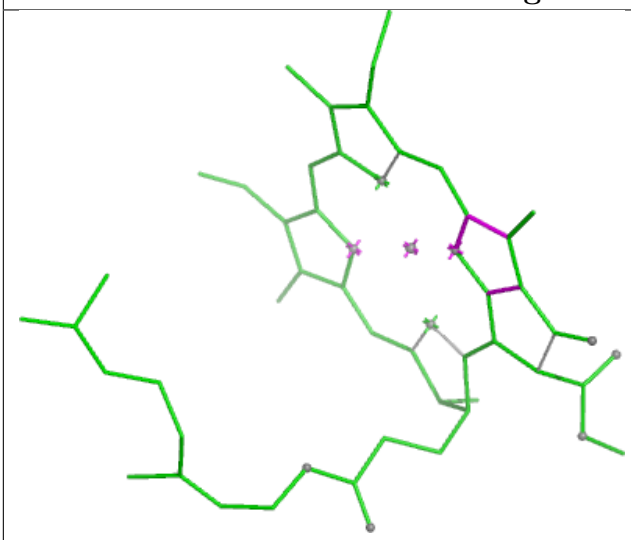


Torsions



Rings

Ligand CLA A 825



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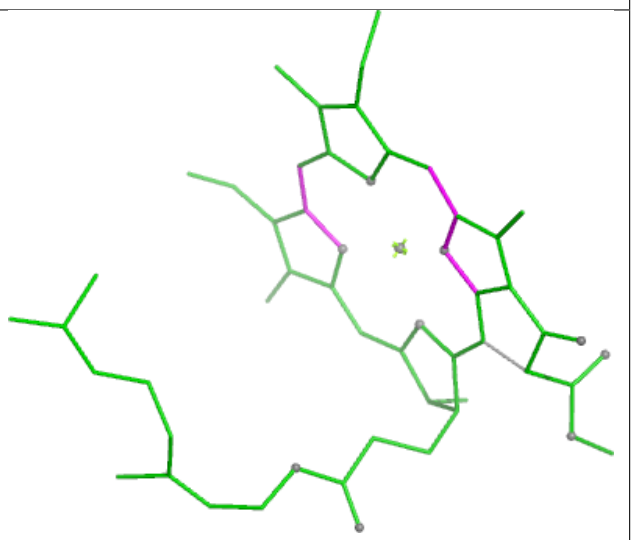
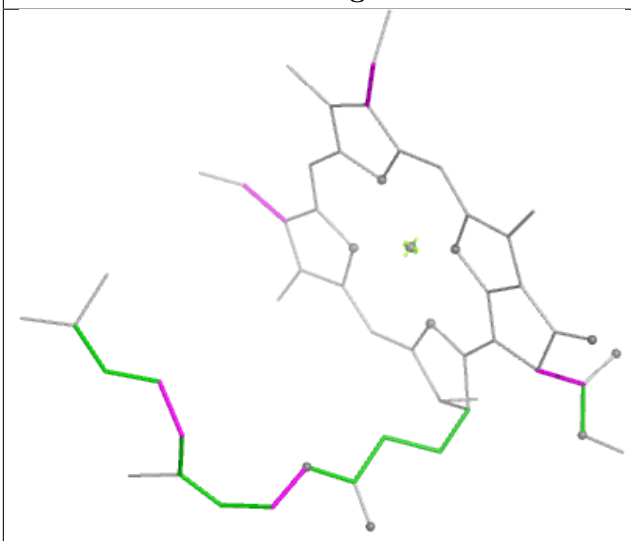


Bond angles



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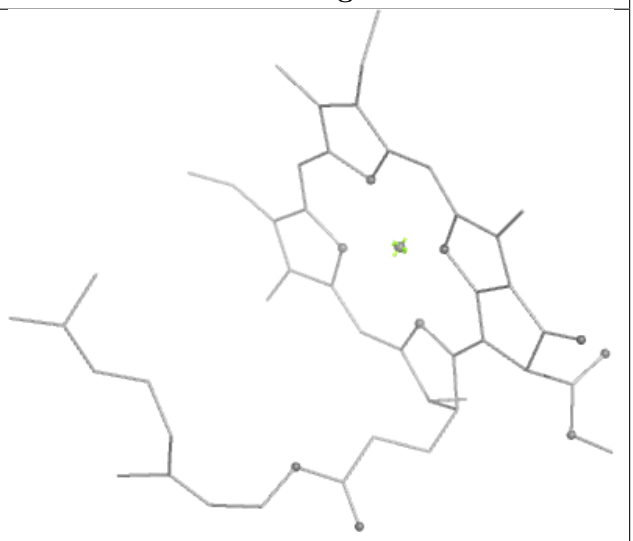
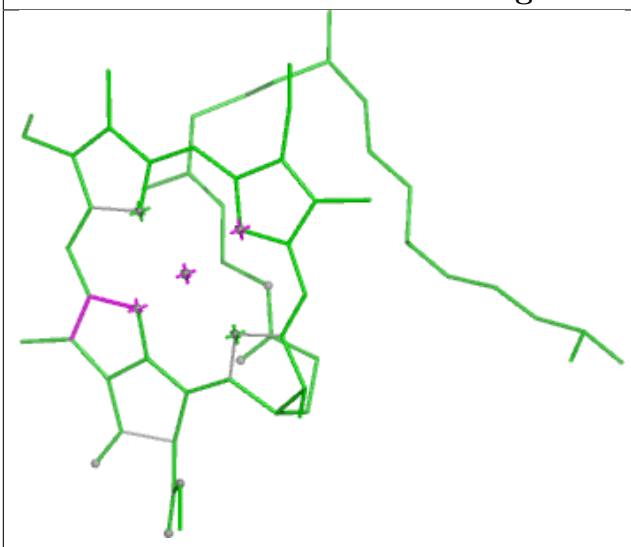


Rings

Ligand CLA B2 808



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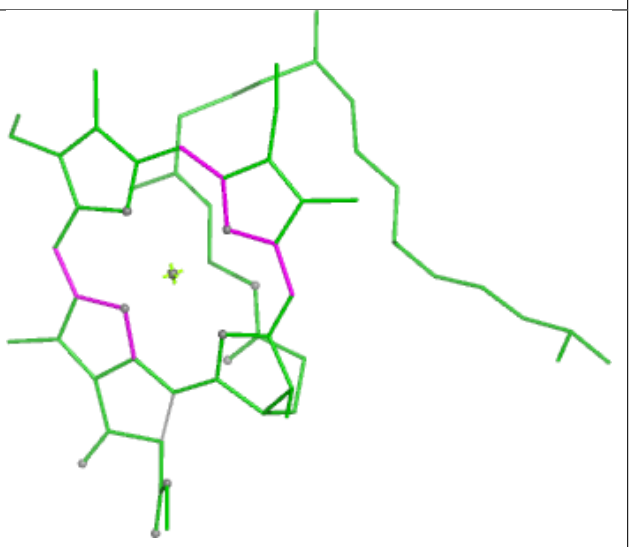
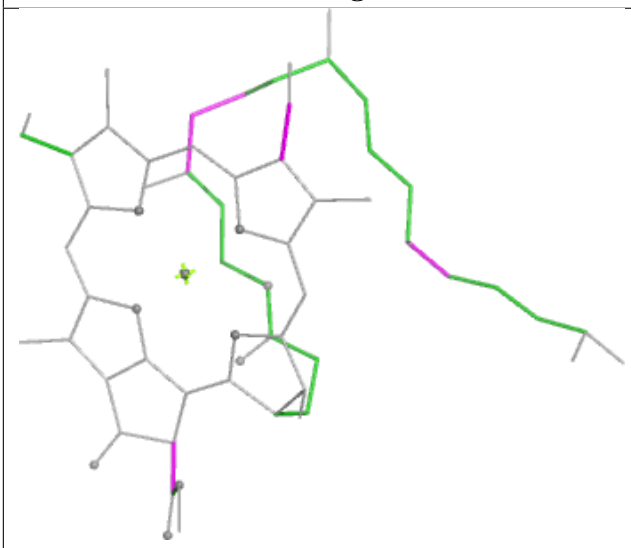


Bond angles

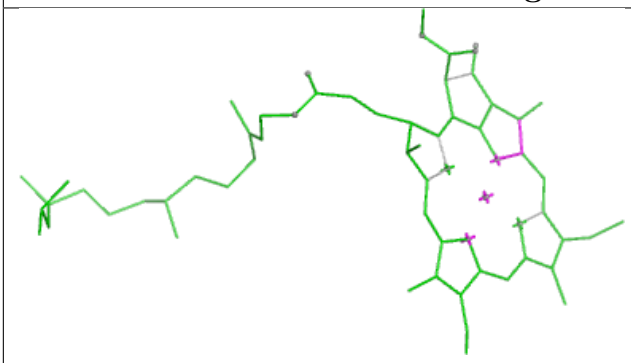


Torsions

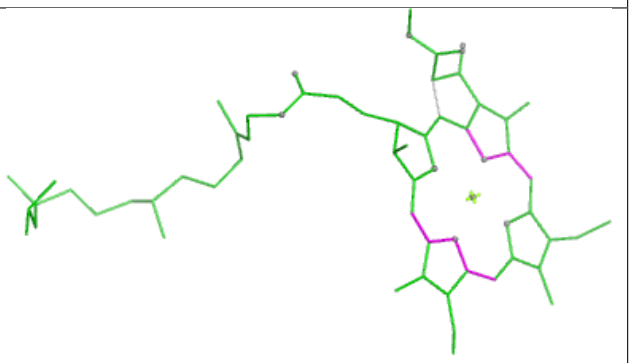


Rings

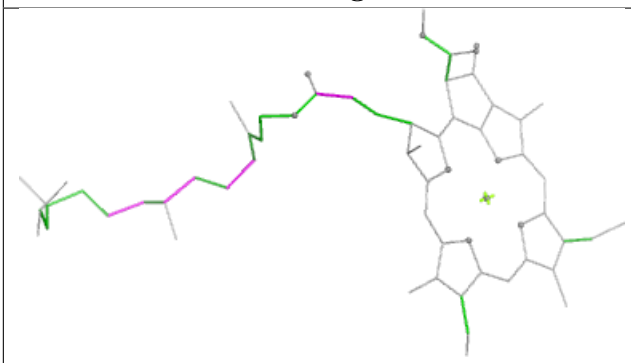
Ligand CLA B 809



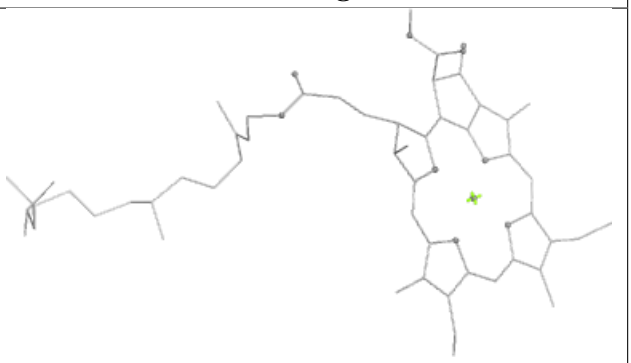
Bond lengths



Bond angles

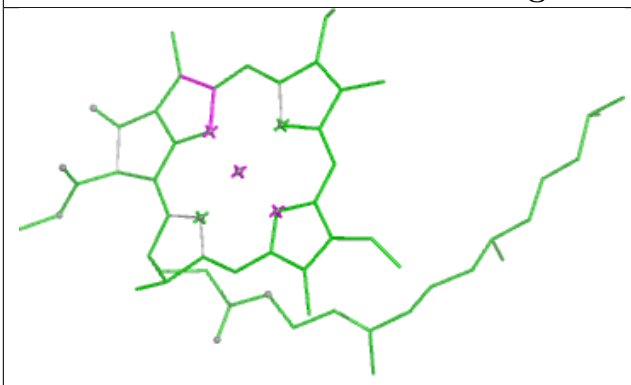


Torsions



Rings

Ligand CLA 6 610



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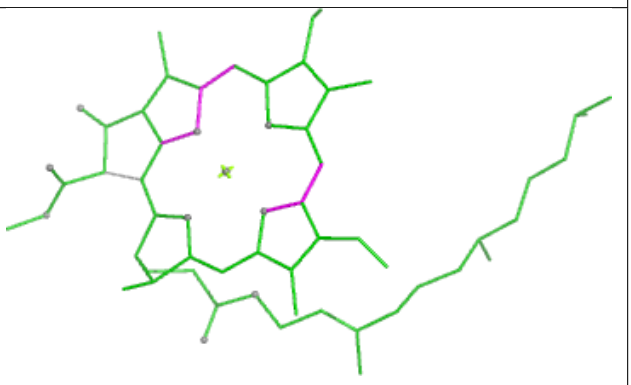
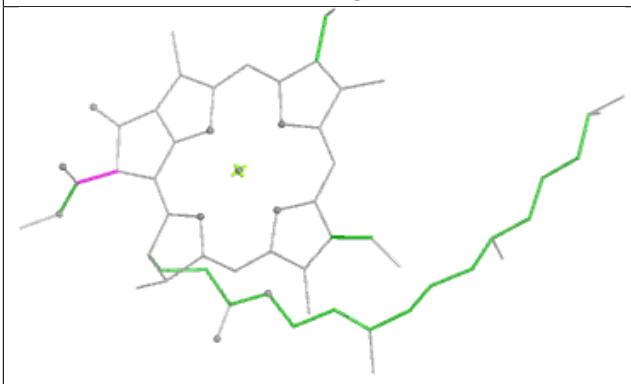


Bond angles



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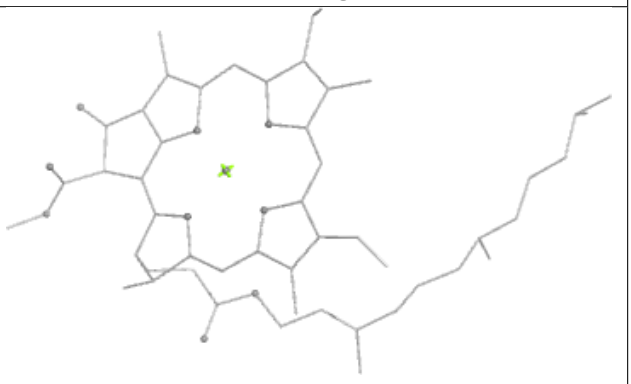
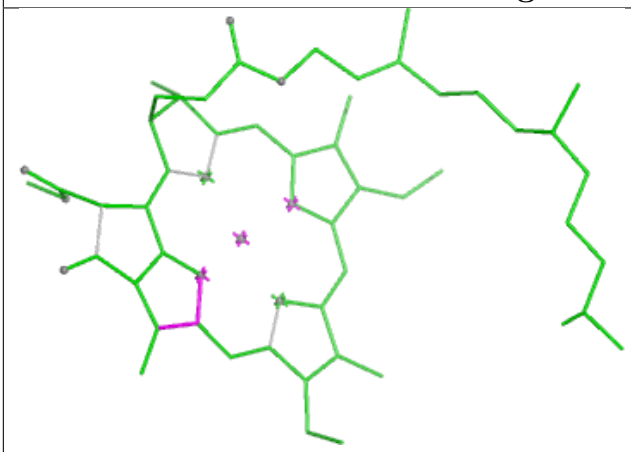


Rings

Ligand CLA Z2 602



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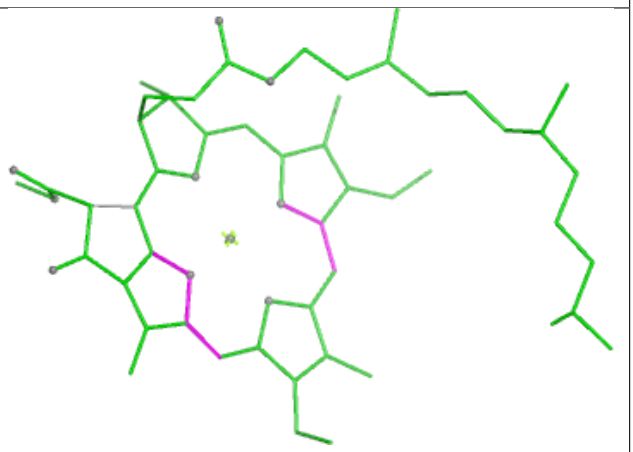
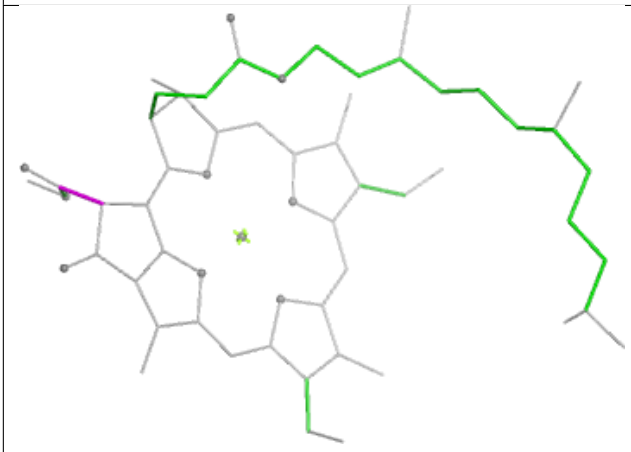


Bond angles

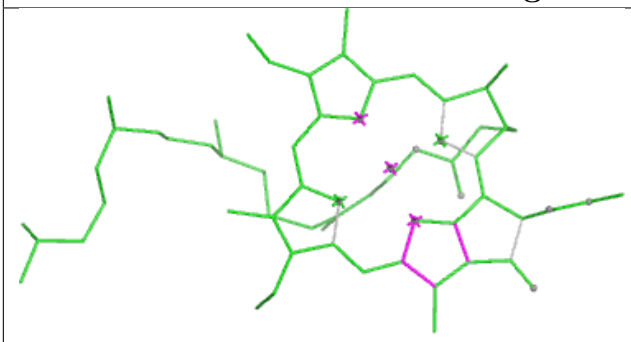


Torsions



Rings

Ligand CLA A 839



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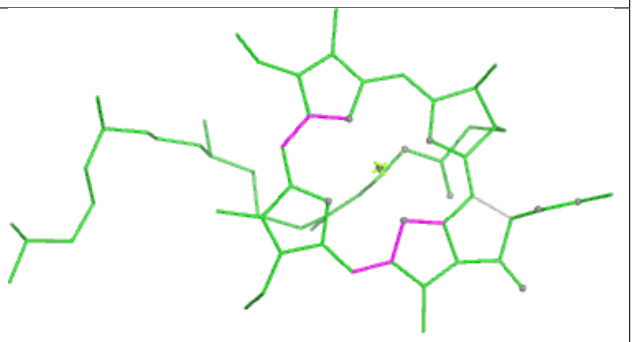
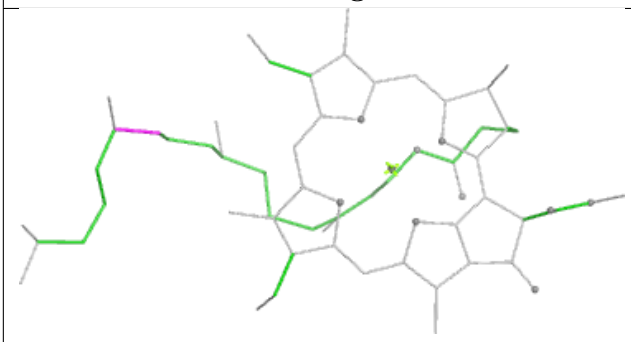


Bond angles

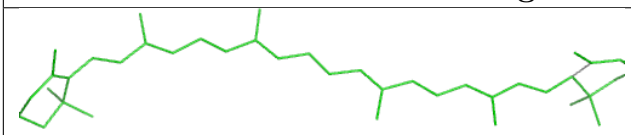


Torsions



Rings

Ligand LUT Z2 617



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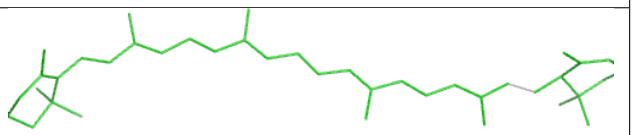
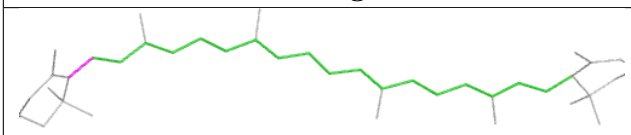
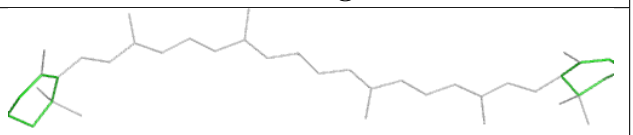


Bond angles

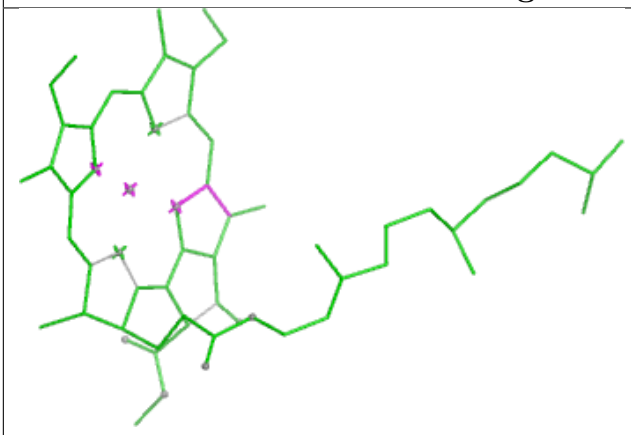


Torsions

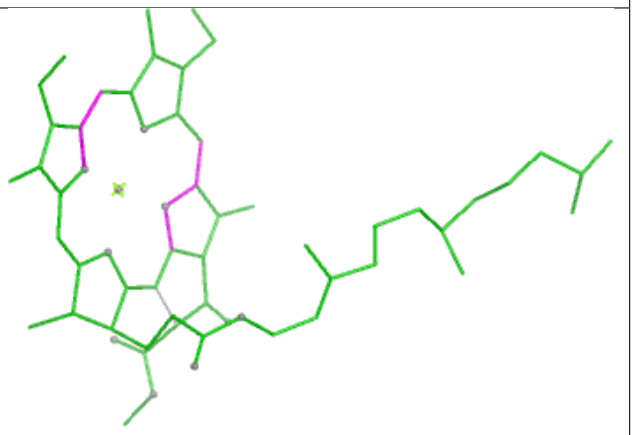


Rings

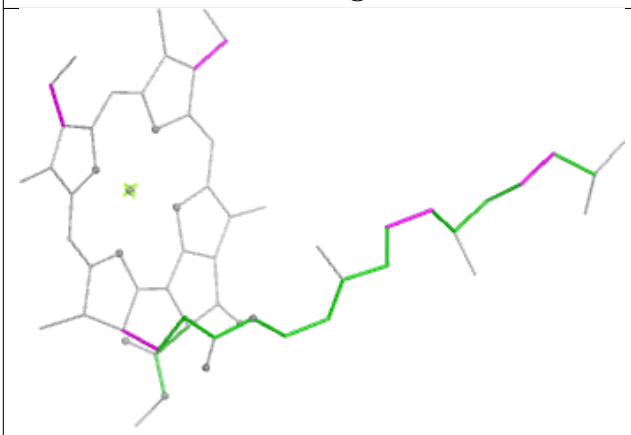
Ligand CLA Z2 611



Bond lengths



Bond angles

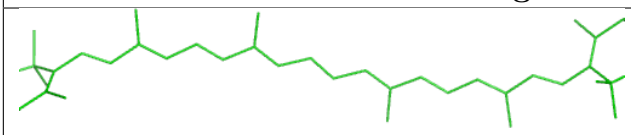


Torsions



Rings

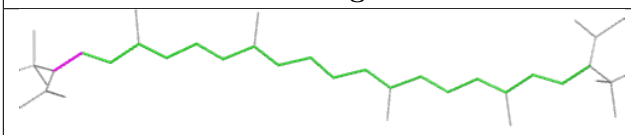
Ligand BCR A2 850



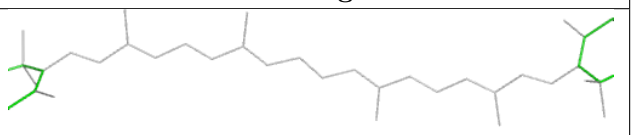
Bond lengths



Bond angles

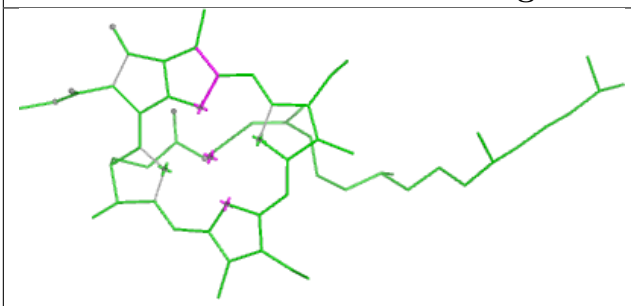


Torsions

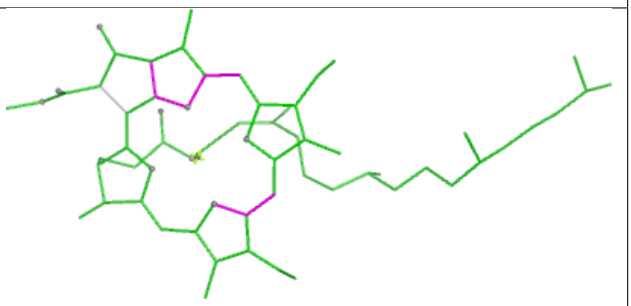


Rings

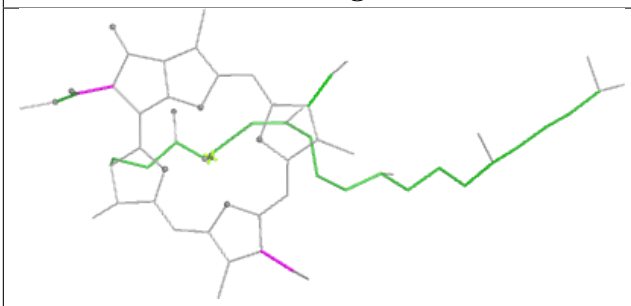
Ligand CLA Z2 613



Bond lengths



Bond angles



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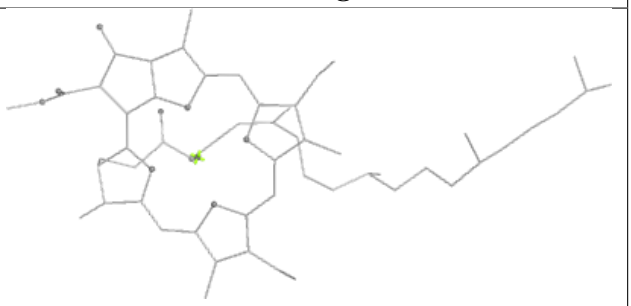
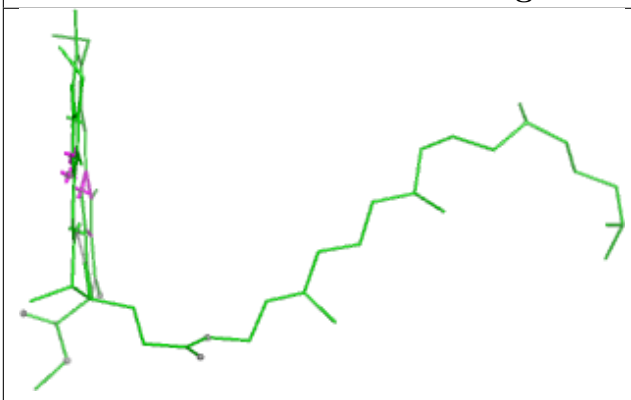


Rings

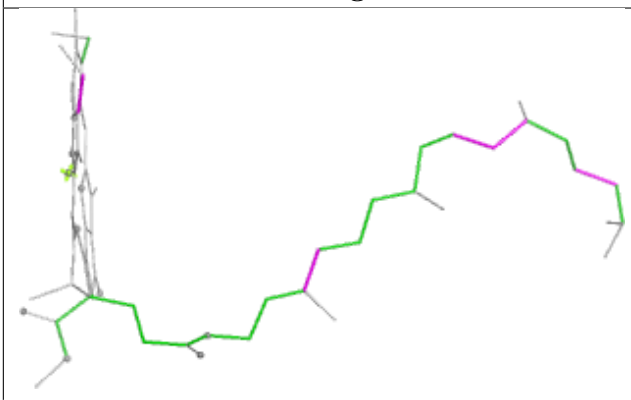
Ligand CLA B2 840



Bond lengths



Bond angles



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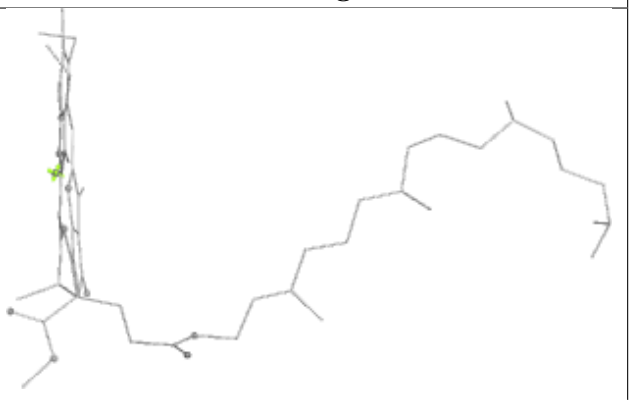
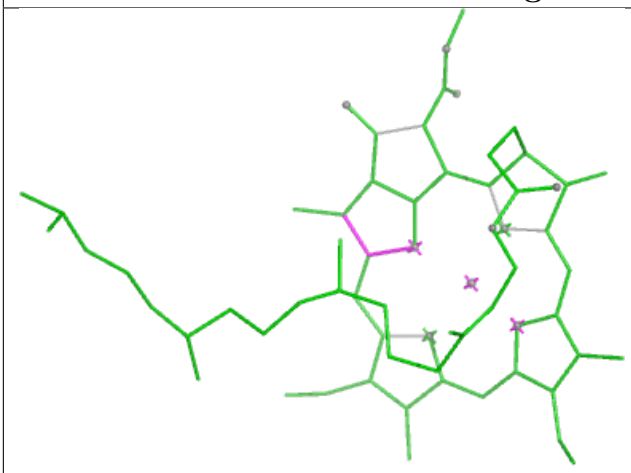


Rings

Ligand CLA B 827



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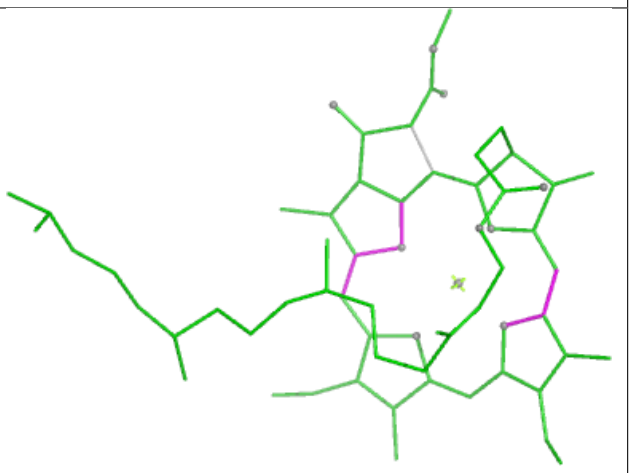
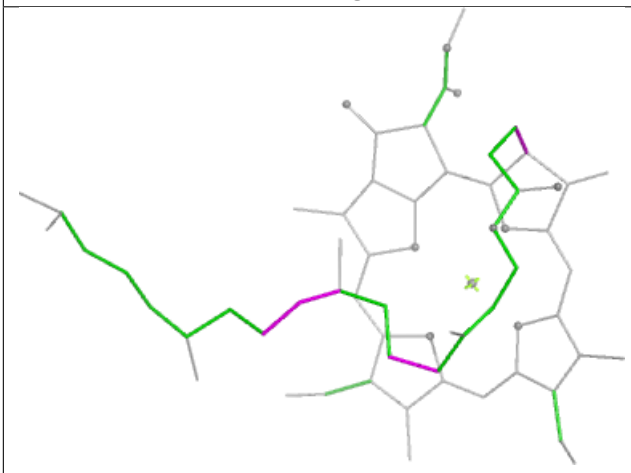


Bond angles

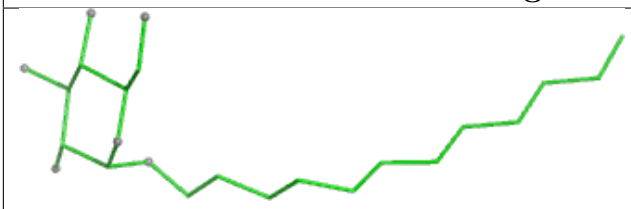


Torsions



Rings

Ligand LMU 8 625



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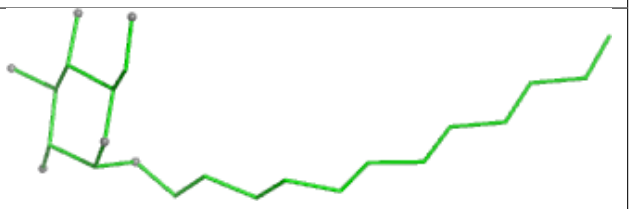

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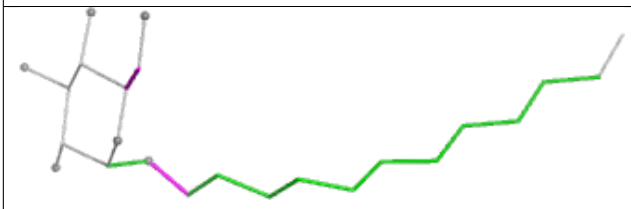
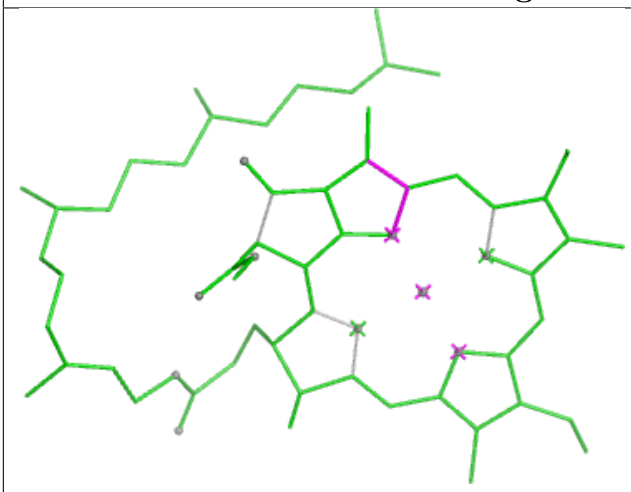


Torsions



Rings

Ligand CLA B2 805



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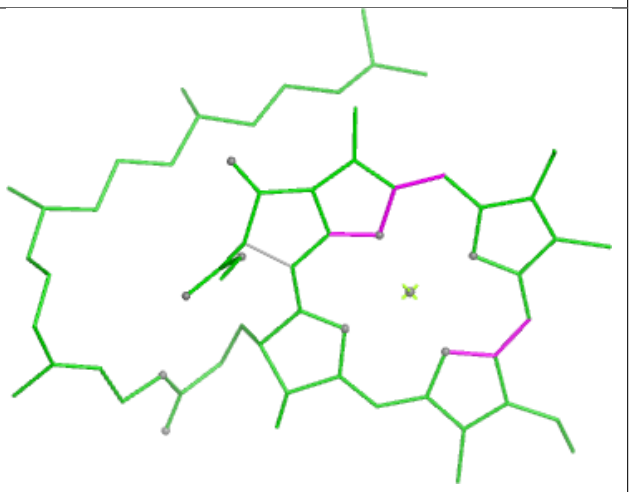
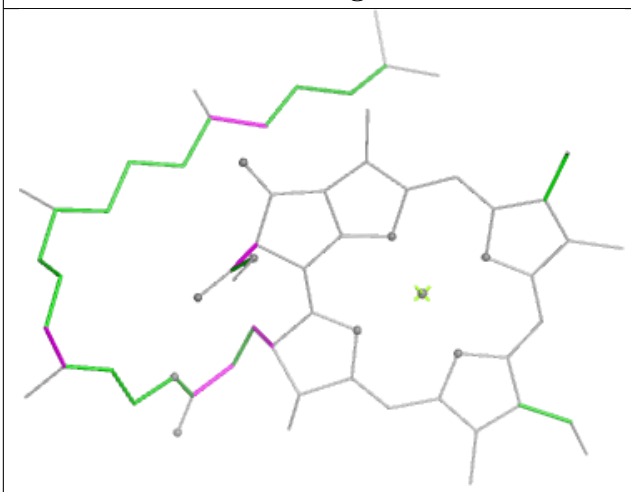


Bond angles



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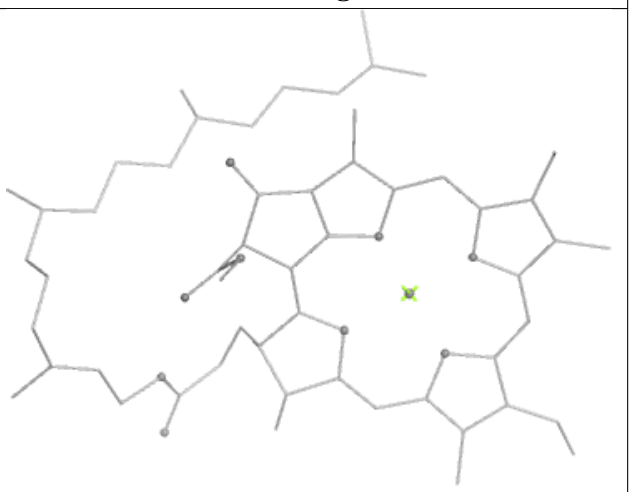
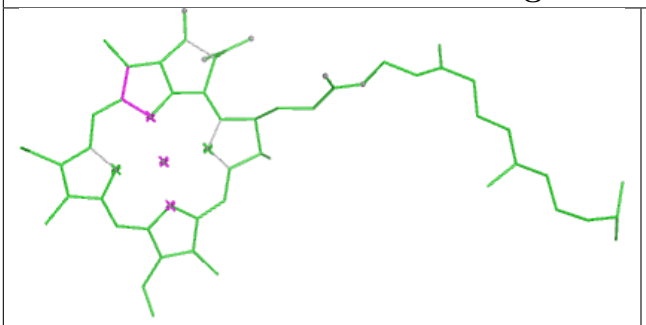


Rings

Ligand CLA B 836



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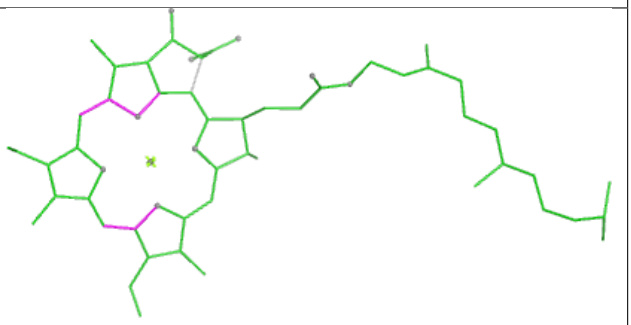
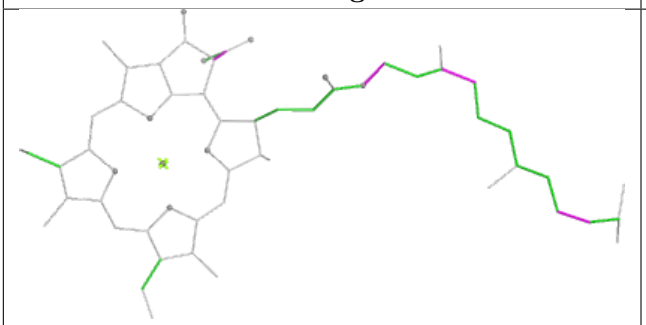


Bond angles



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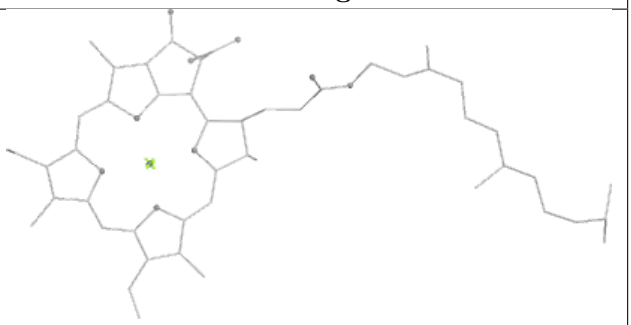
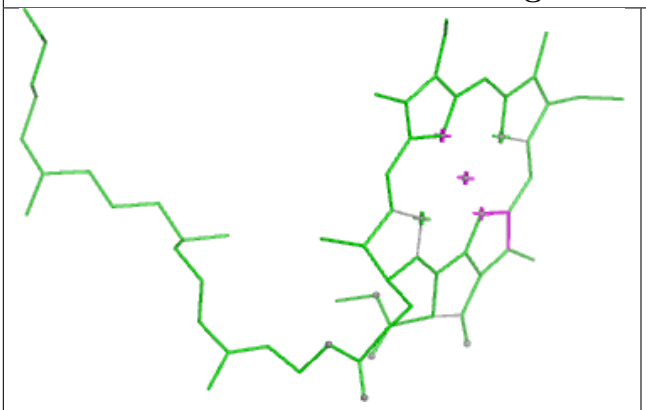


Rings

Ligand CLA B 810



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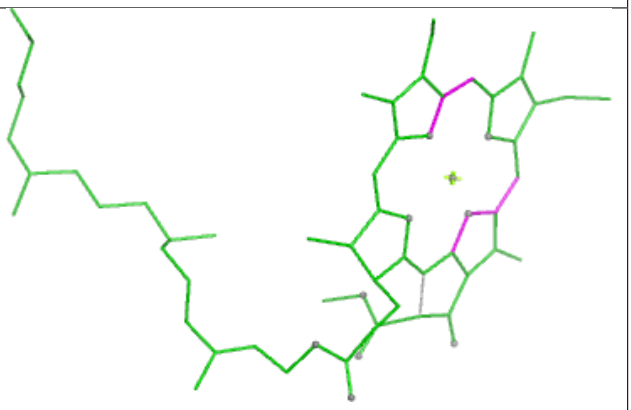
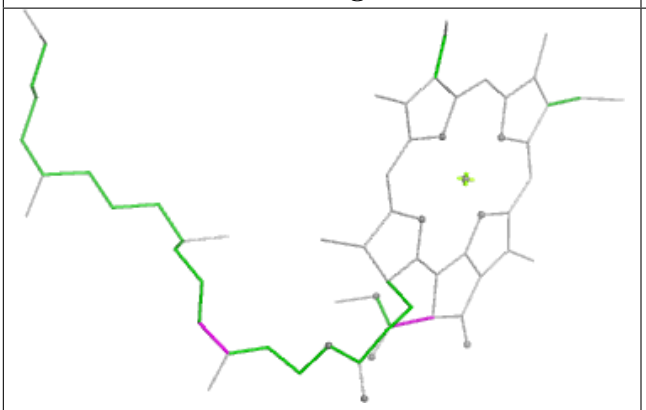


Bond angles



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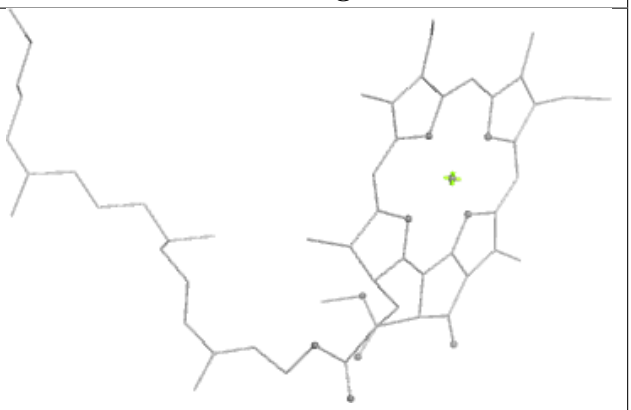
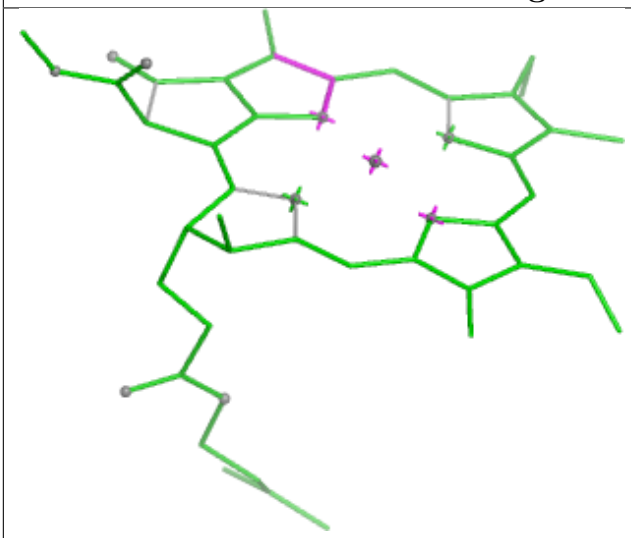


Rings

Ligand CLA 1 604



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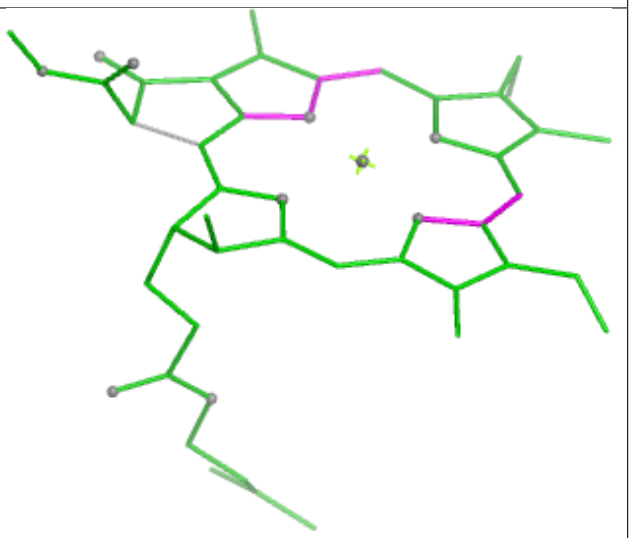


Bond angles



Torsions

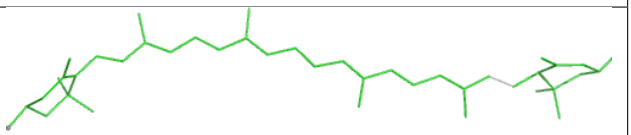


Rings

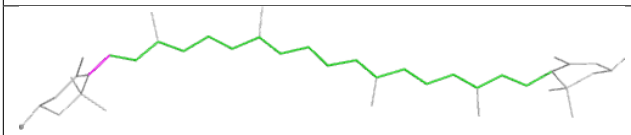
Ligand LUT 12 619



Bond lengths



Bond angles



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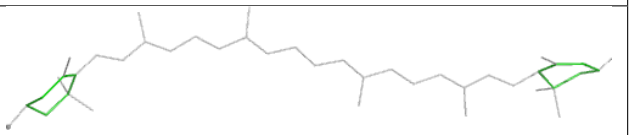
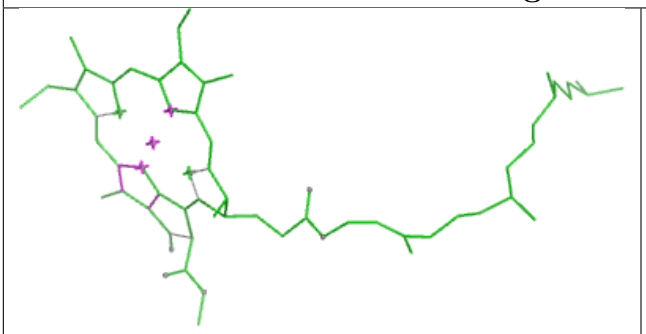


Rings

Ligand CLA A 854



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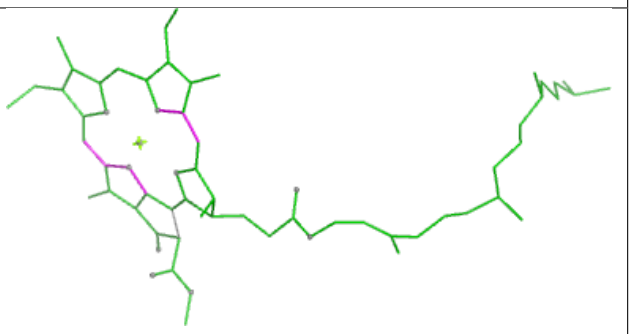
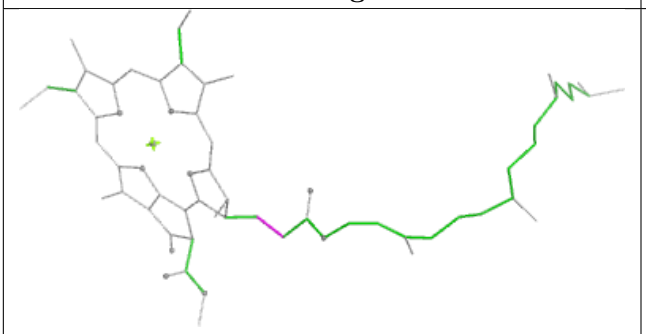


Bond angles



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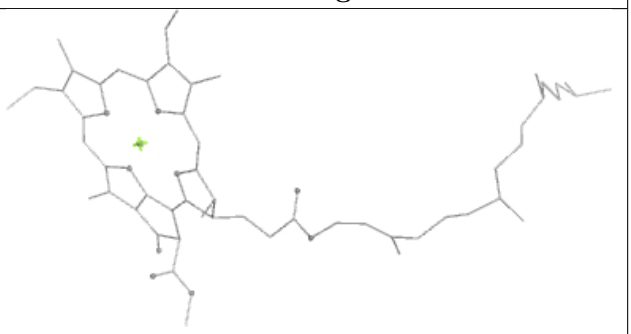
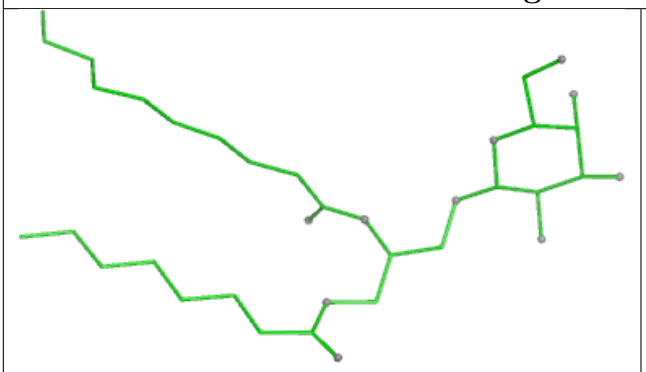


Rings

Ligand LMG 7 626



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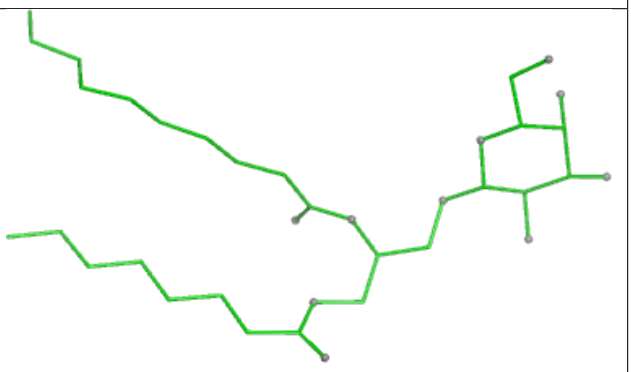

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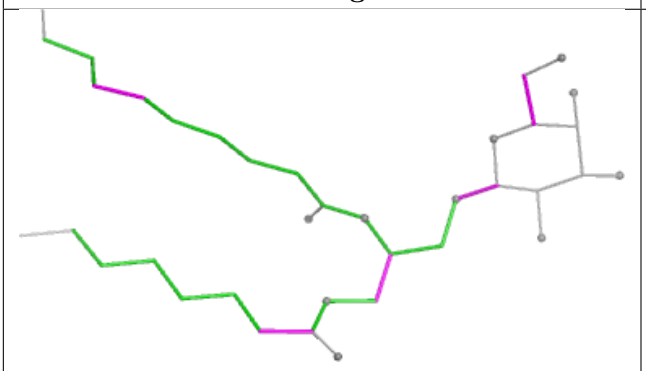
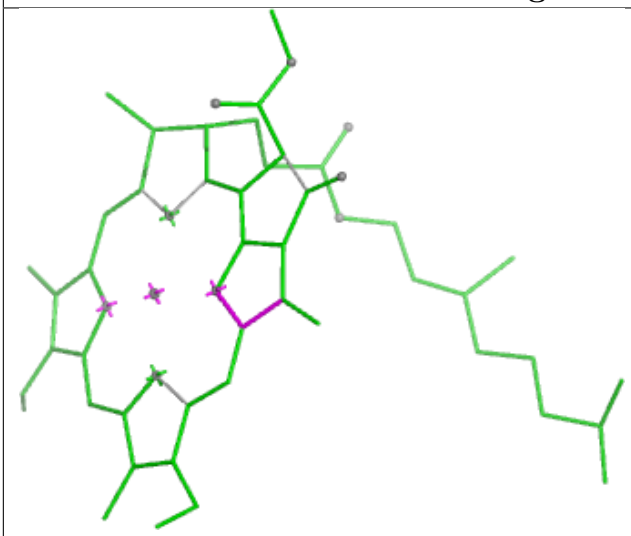


Torsions



Rings

Ligand CLA 5 611



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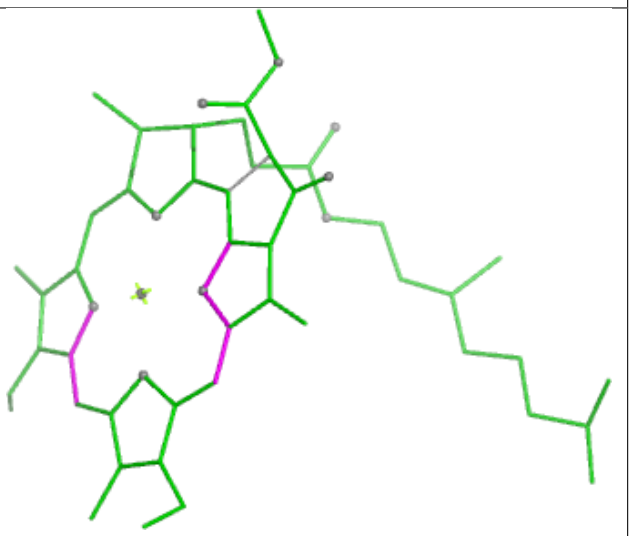
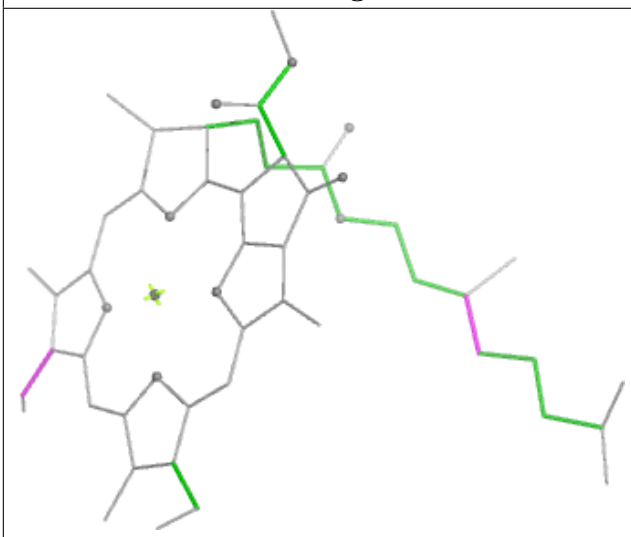


Bond angles



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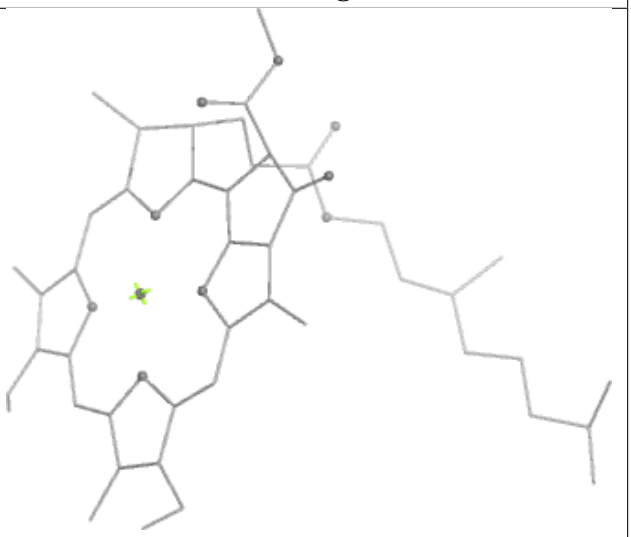
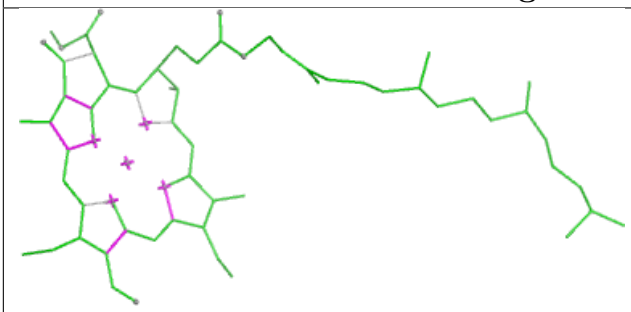


Rings

Ligand CHL 72 601



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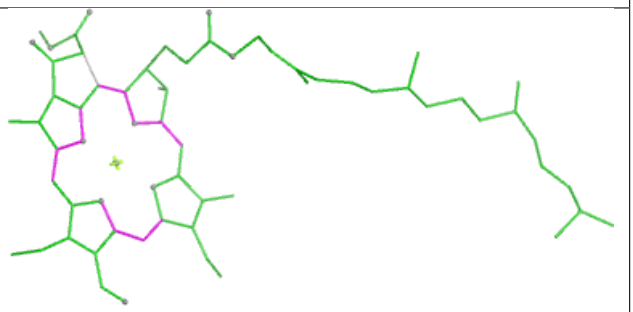

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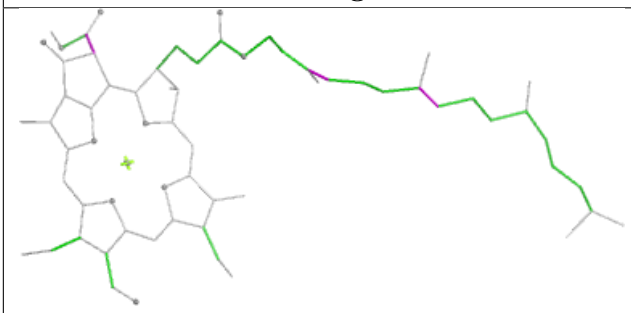

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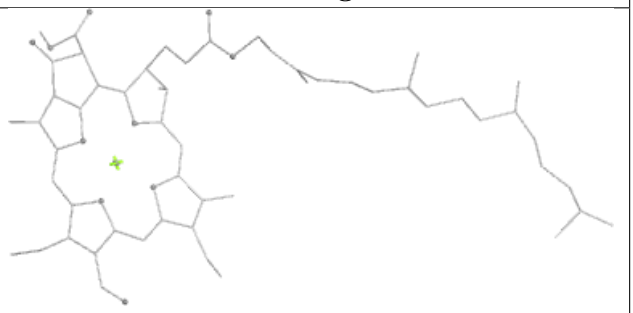
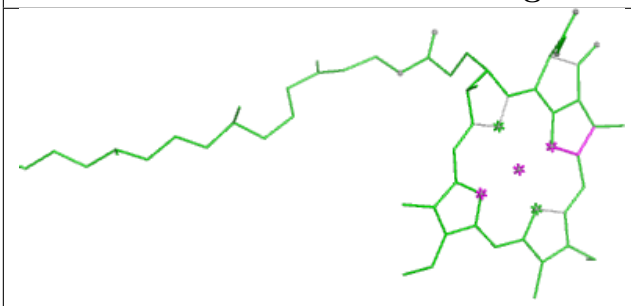


Rings

Ligand CLA A 835



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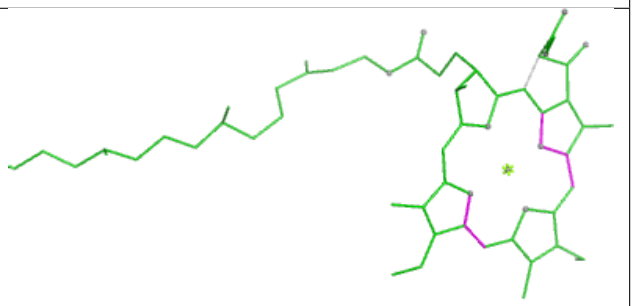
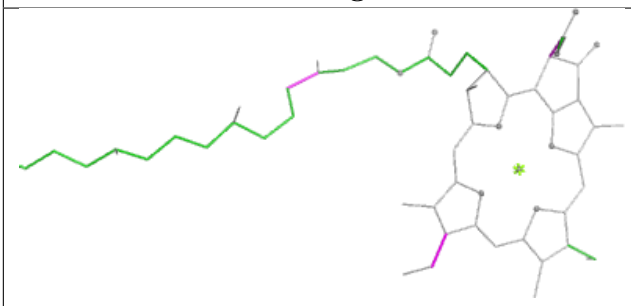


Bond angles



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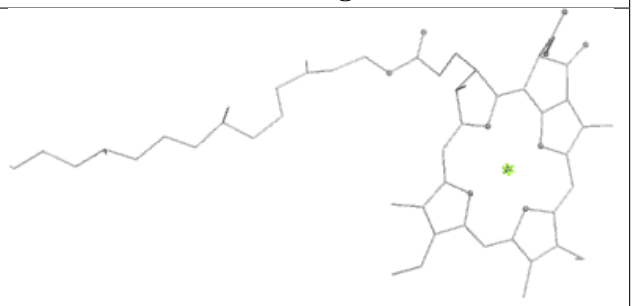
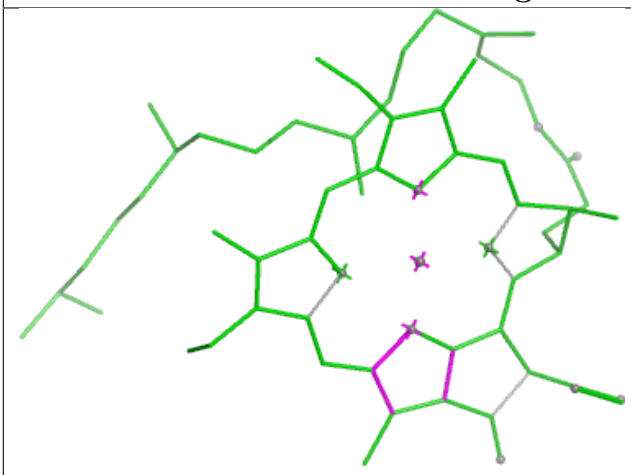


Rings

Ligand CLA A2 823



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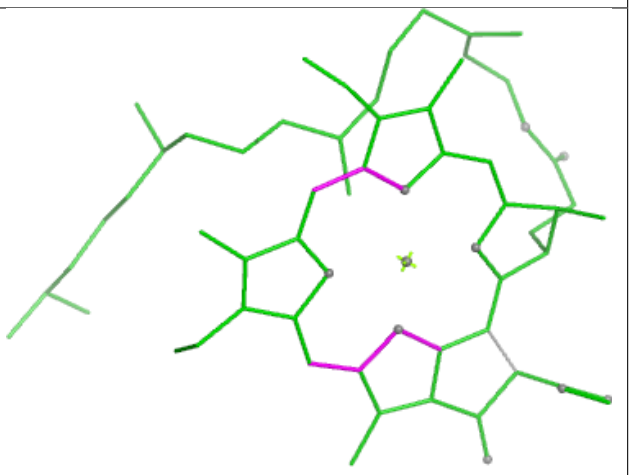
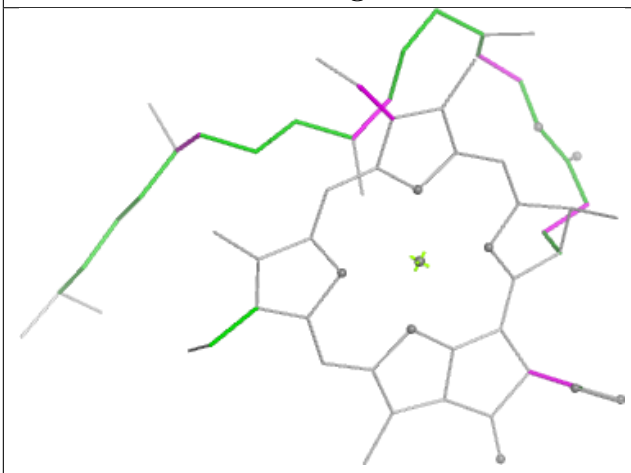


Bond angles



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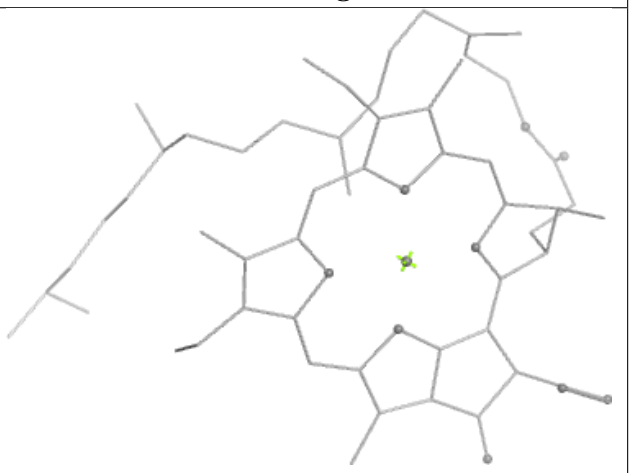
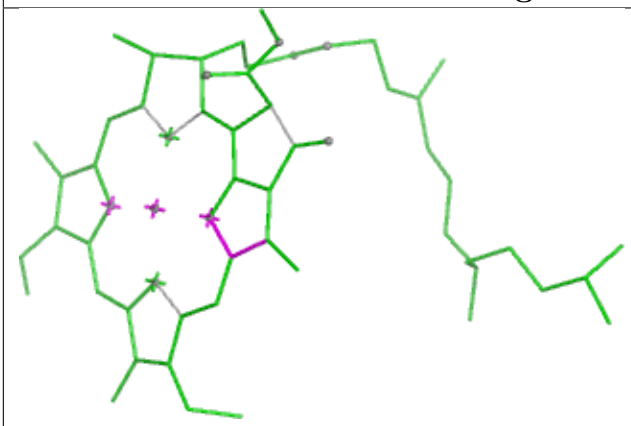


Rings

Ligand CLA B2 834



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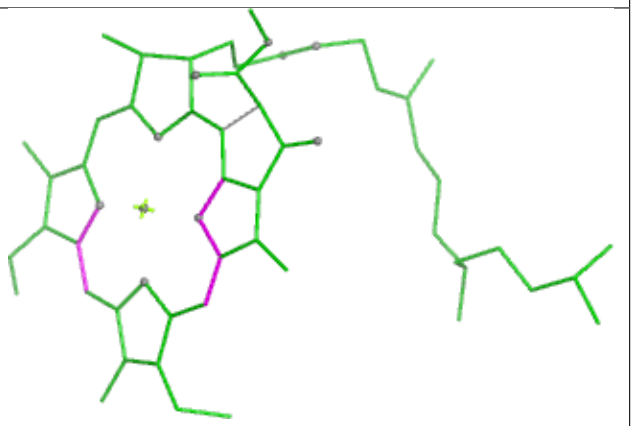
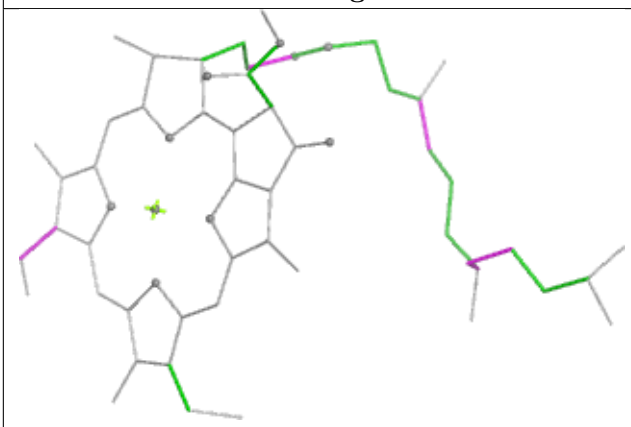


Bond angles



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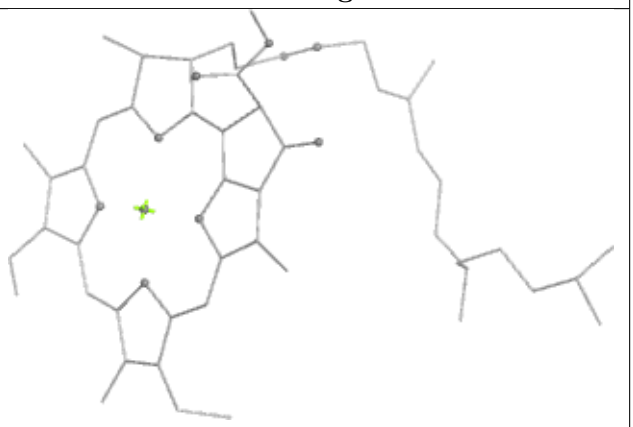
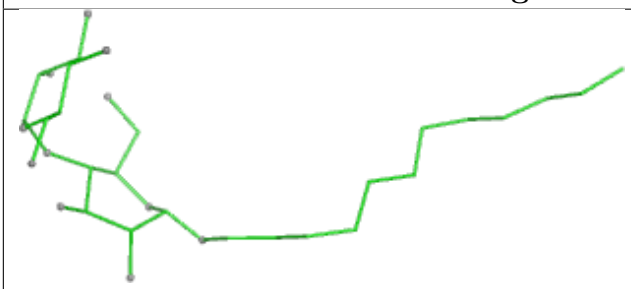
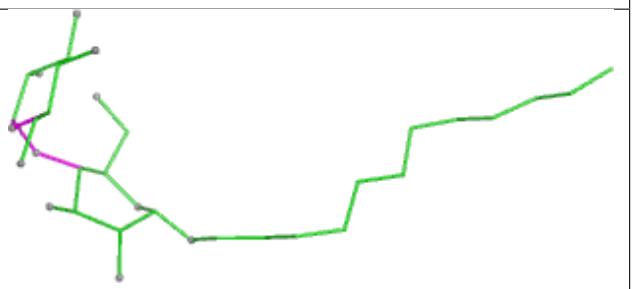


Rings

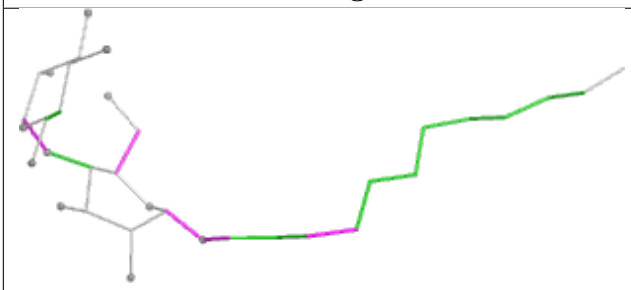
Ligand LMU B2 853



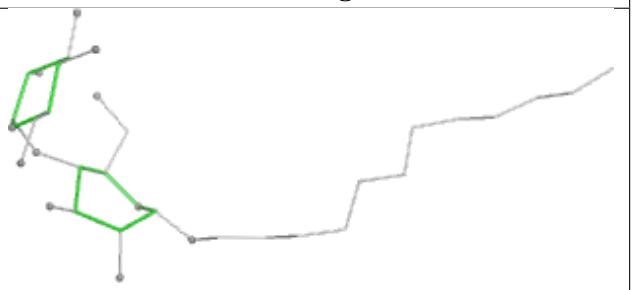
Bond lengths



Bond angles

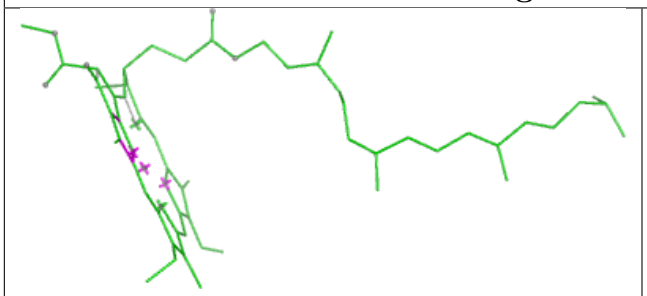


Torsions



Rings

Ligand CLA A2 833



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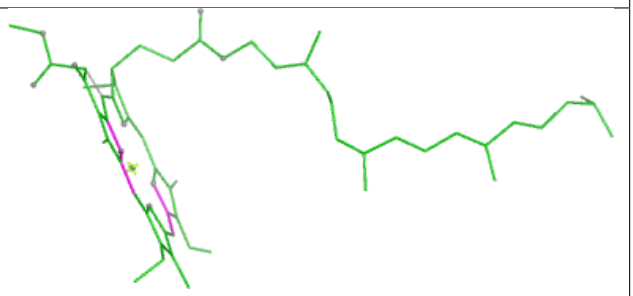

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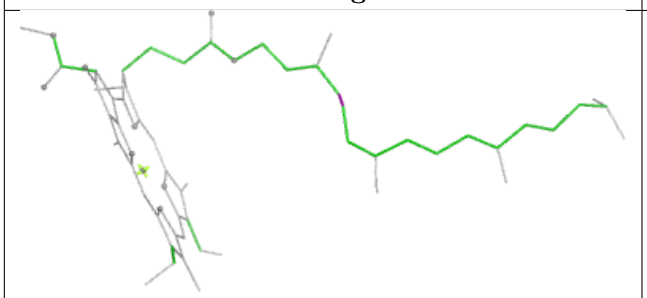

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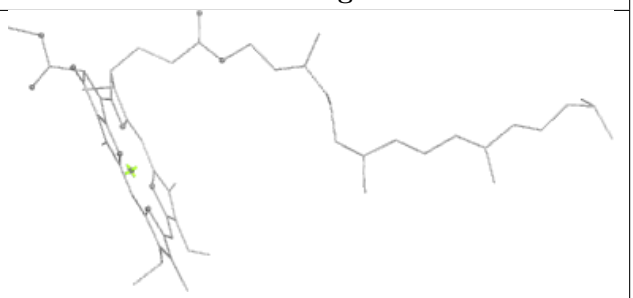
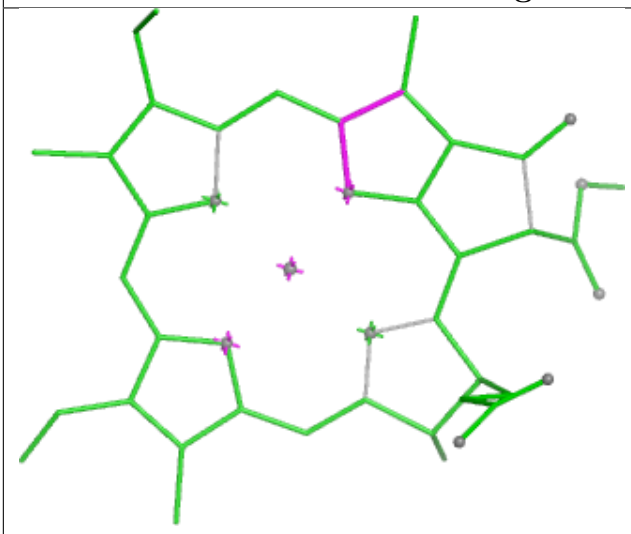


Rings

Ligand CLA A2 845



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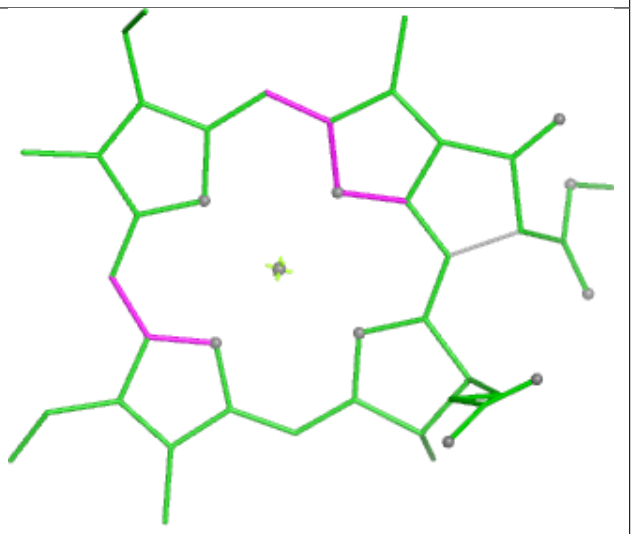

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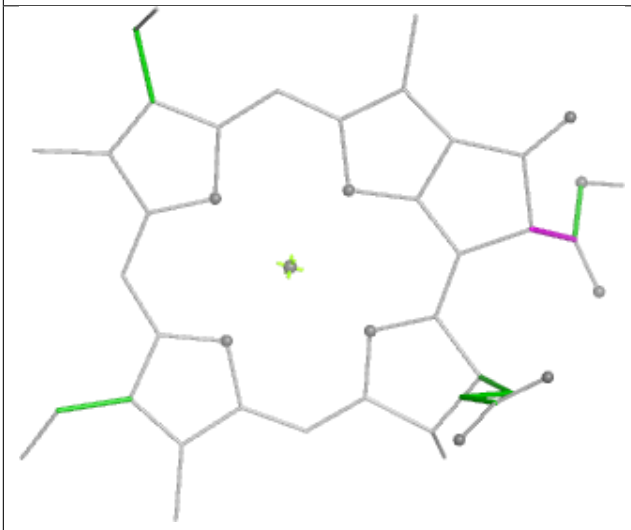

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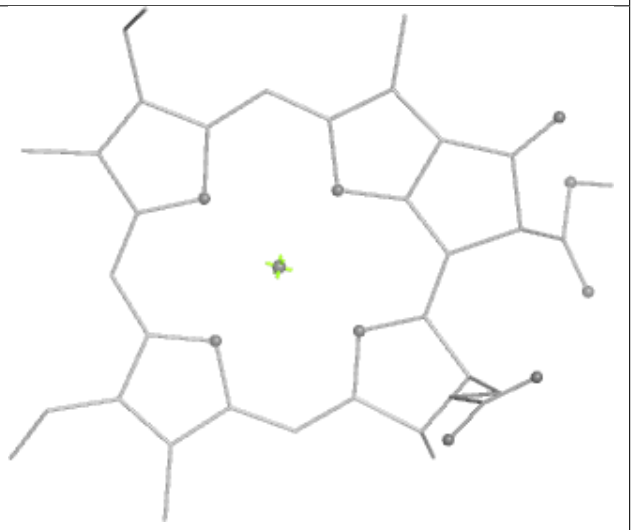
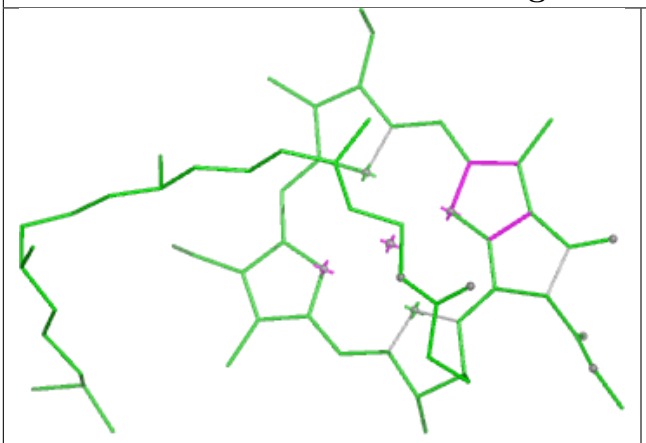


Rings

Ligand CLA 1 613



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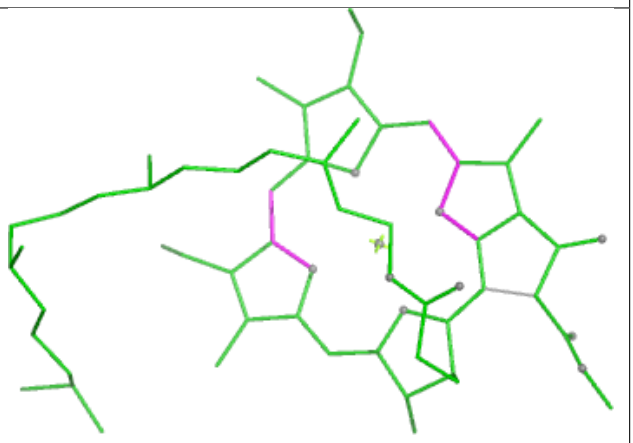

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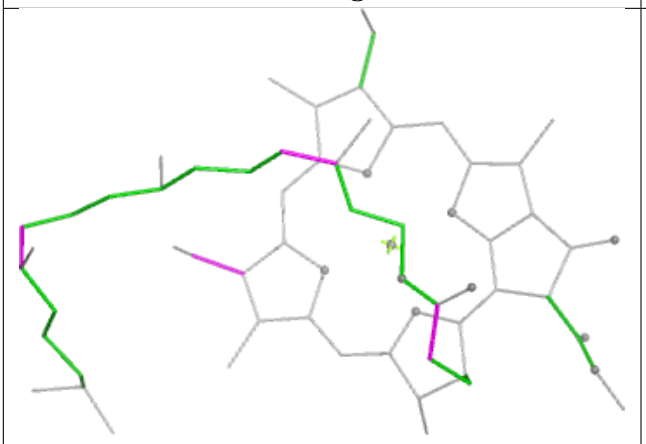
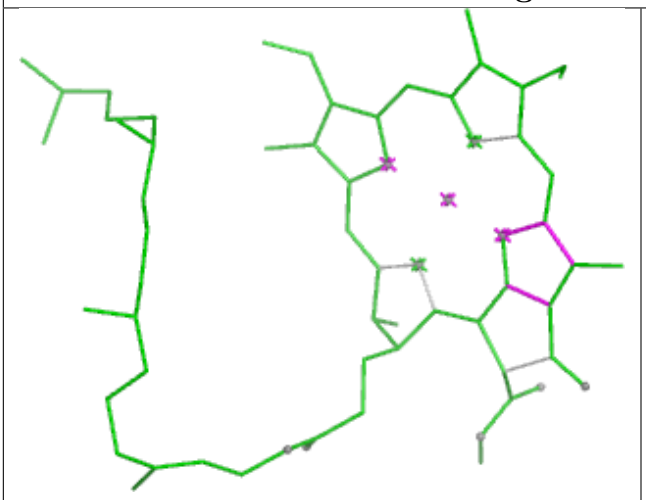


Torsions



Rings

Ligand CLA B2 823



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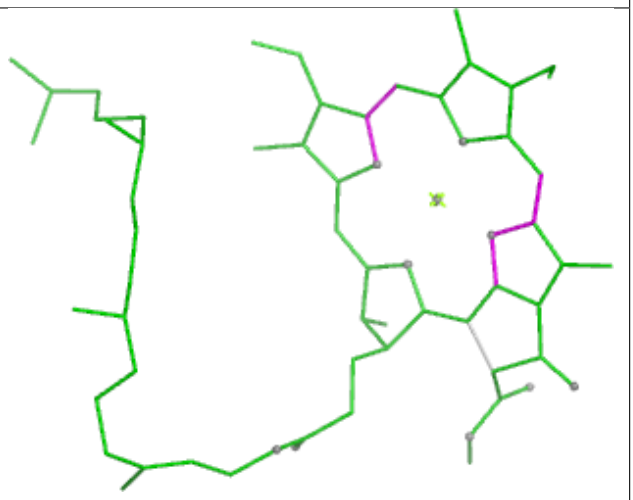

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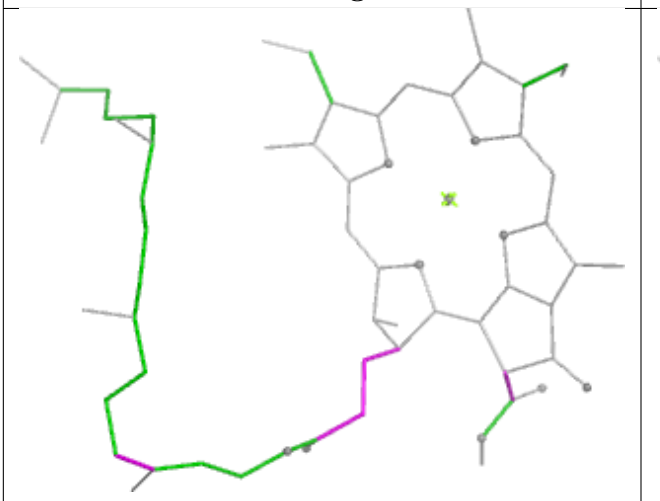
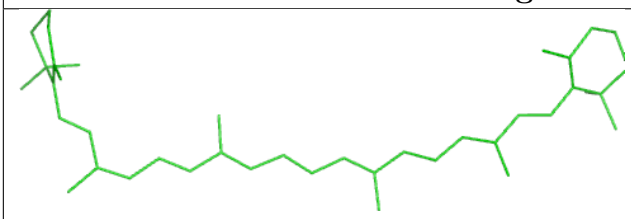


Torsions



Rings

Ligand BCR L2 201



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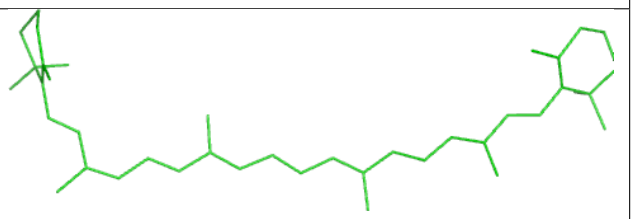

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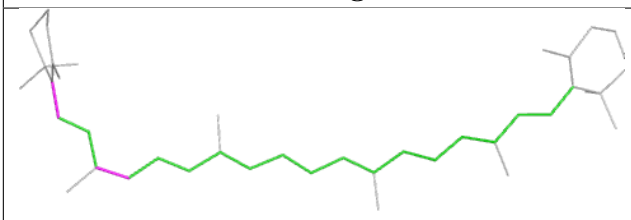

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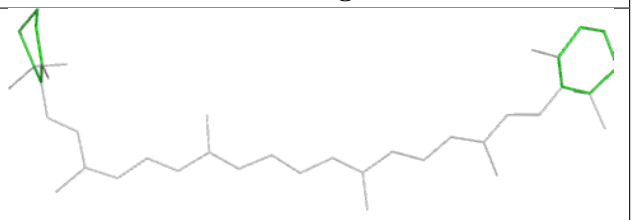
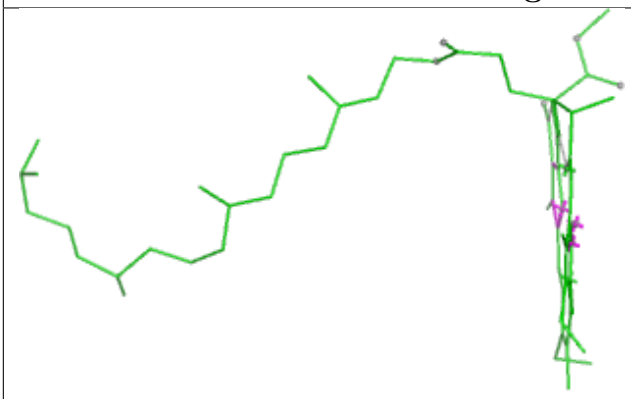


Rings

Ligand CLA B 840



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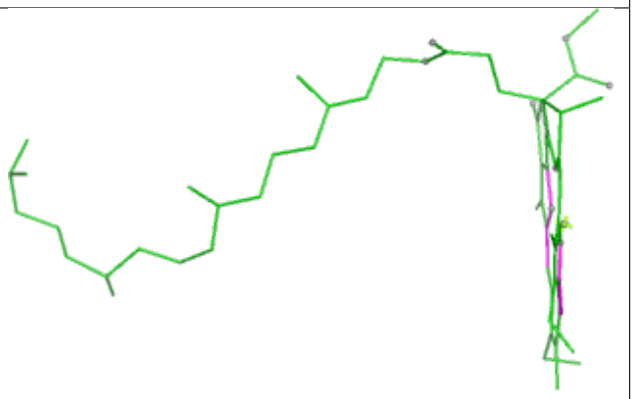

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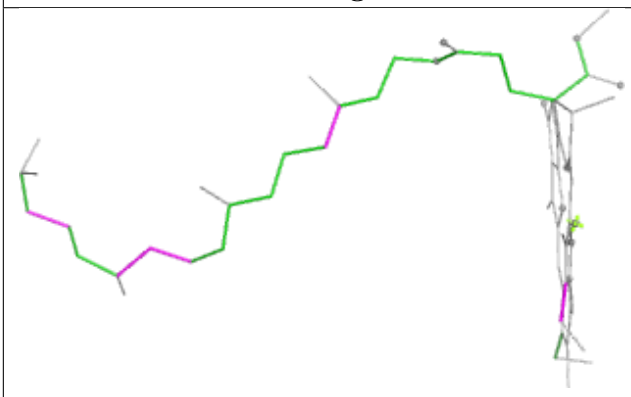

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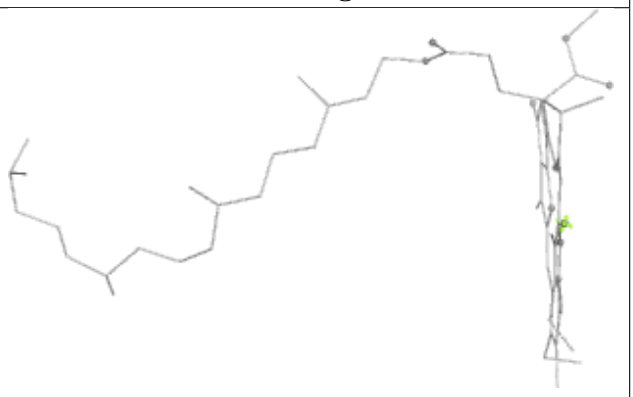
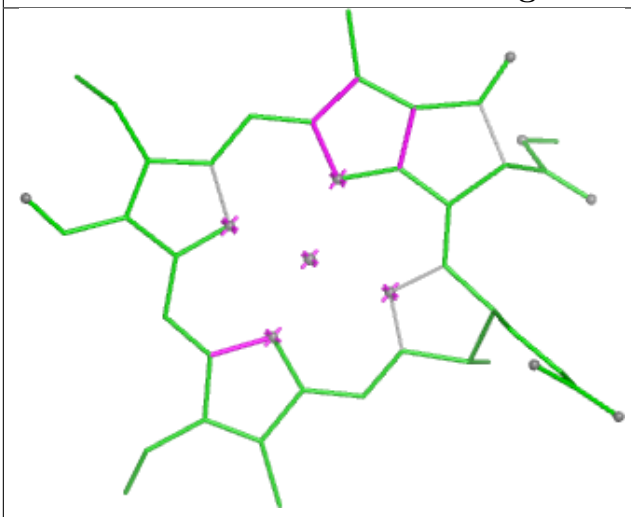


Rings

Ligand CHL 12 607



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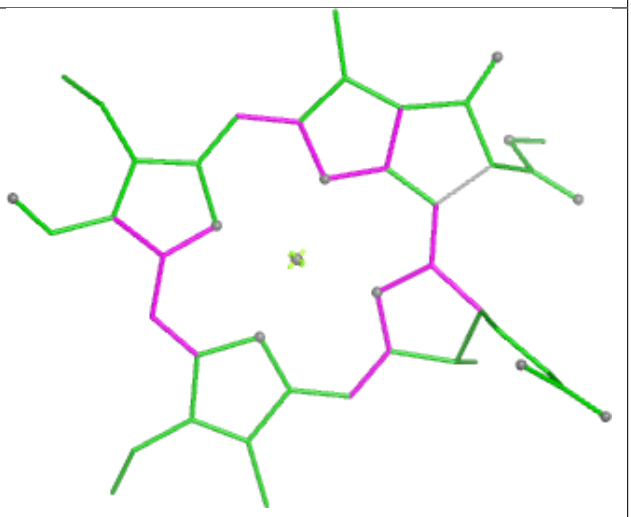

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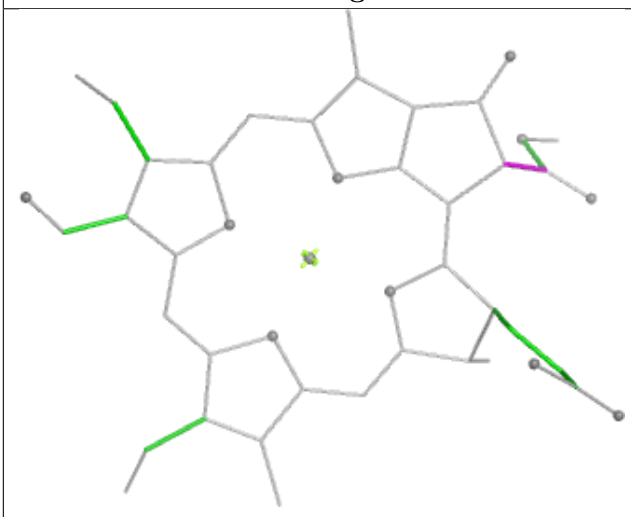

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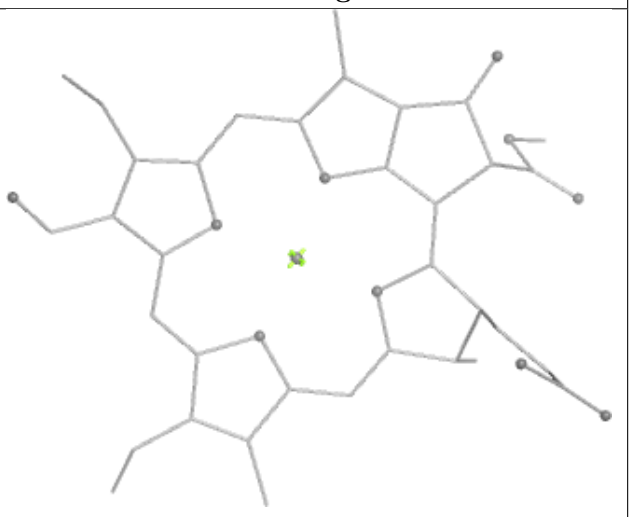
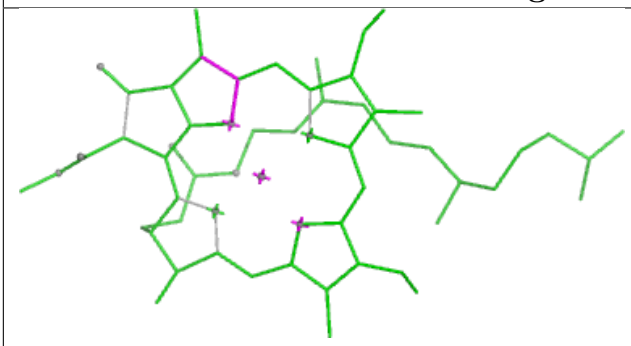


Rings

Ligand CLA 3 613



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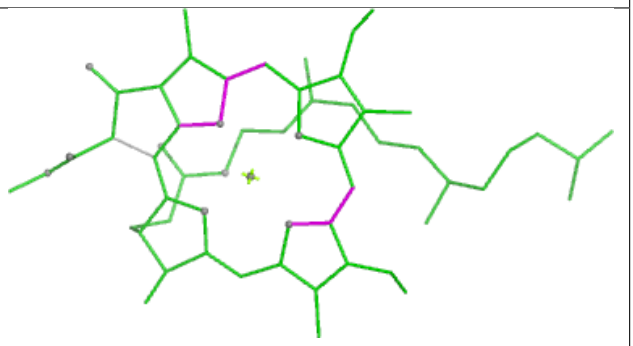
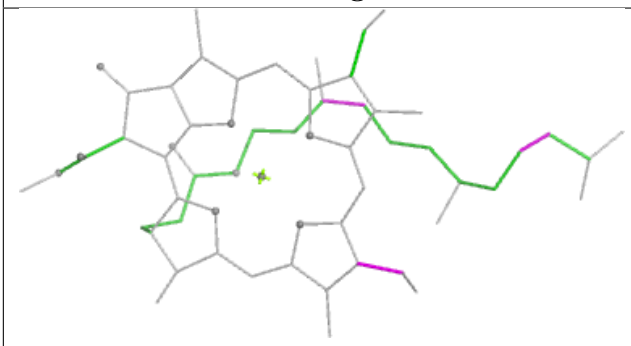


Bond angles



Torsions



Rings

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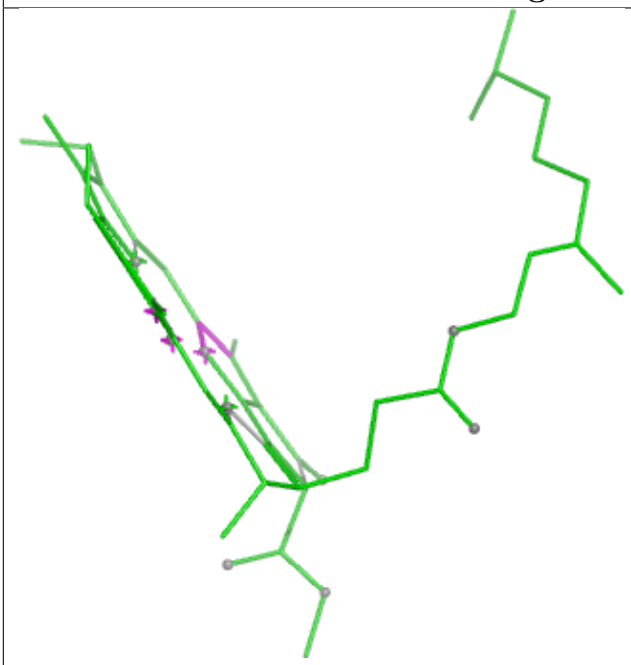

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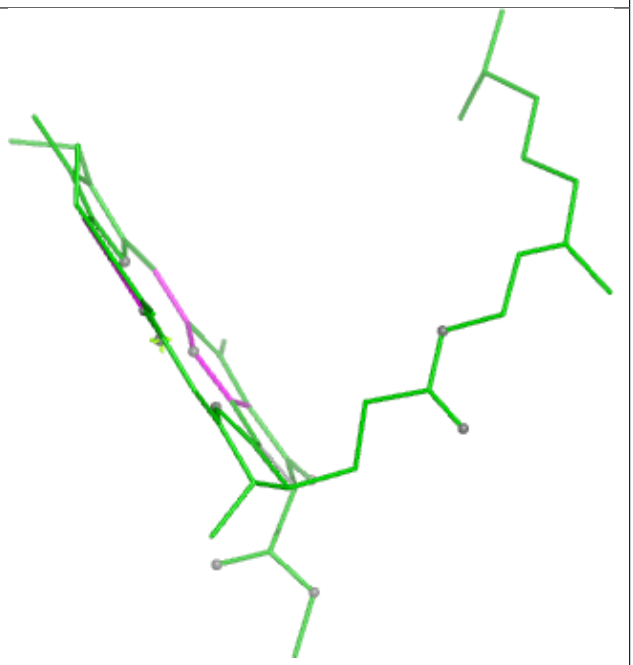

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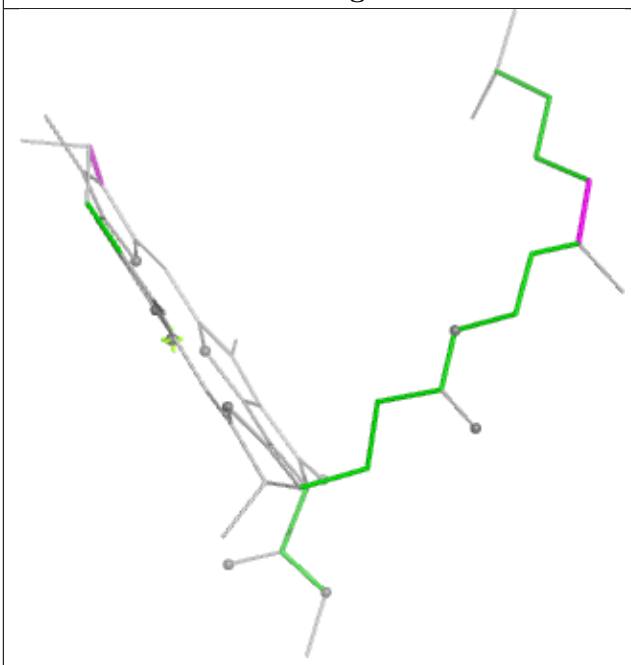

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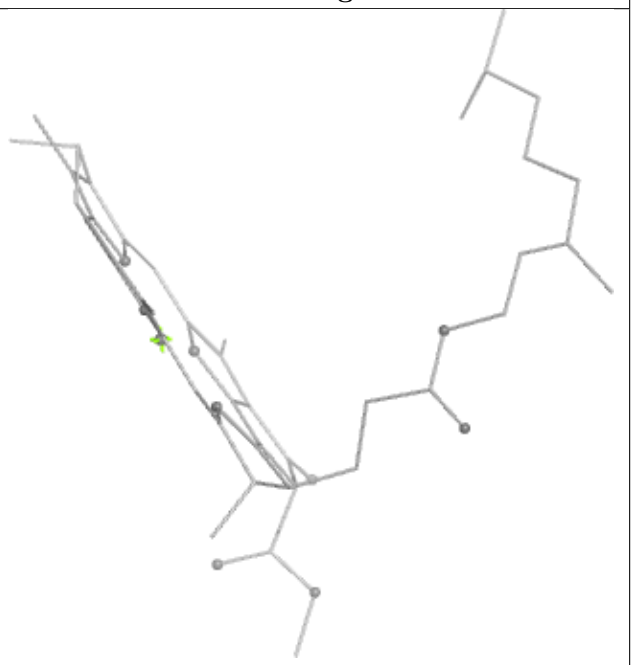
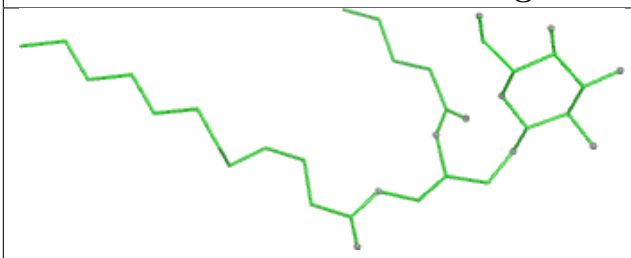


Rings

Ligand LMG 12 624



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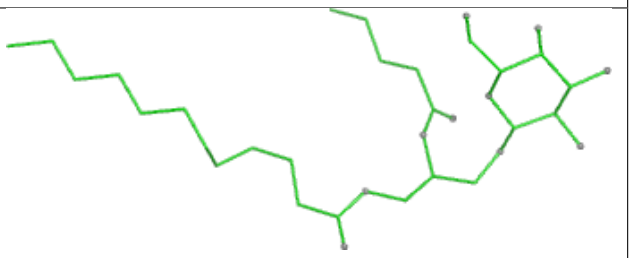
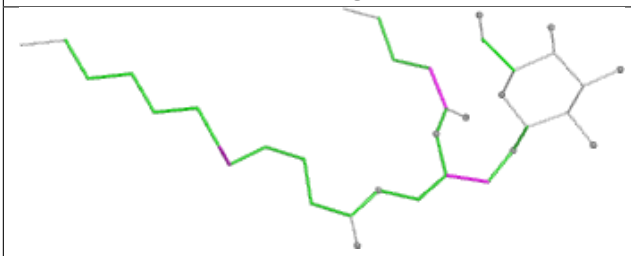


Bond angles



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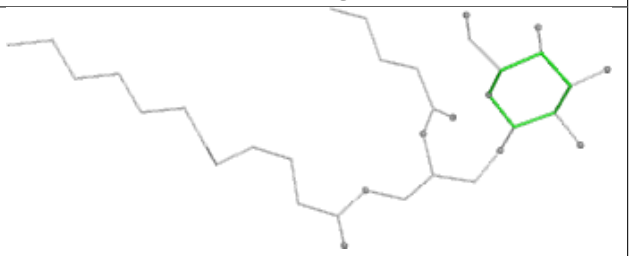
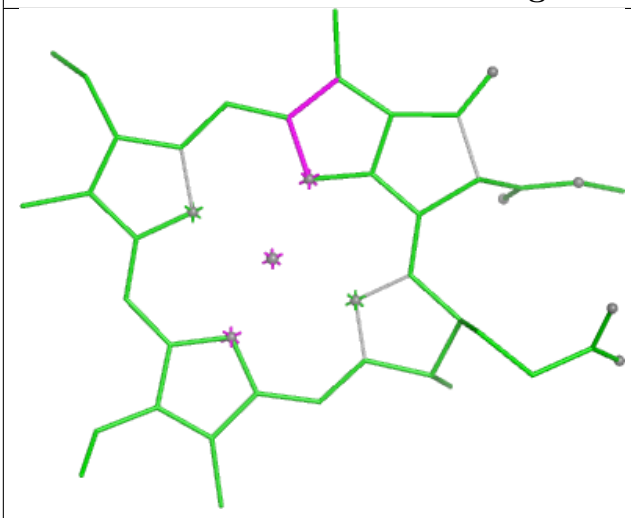


Rings

Ligand CLA 8 611



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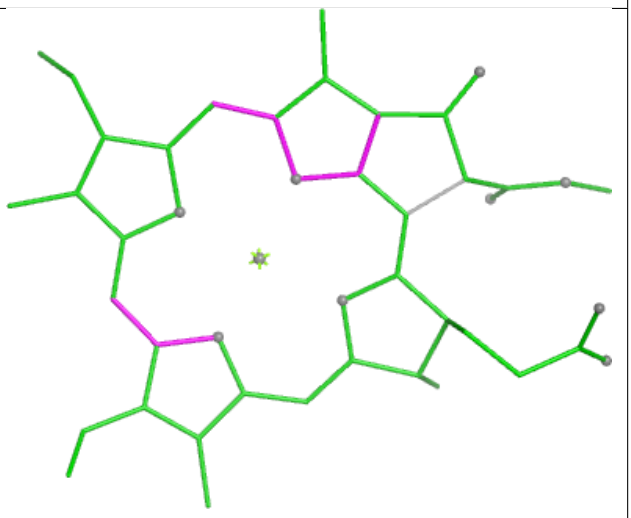

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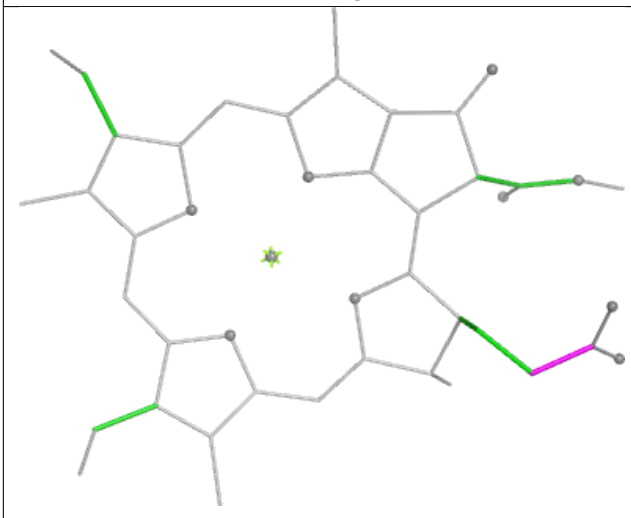

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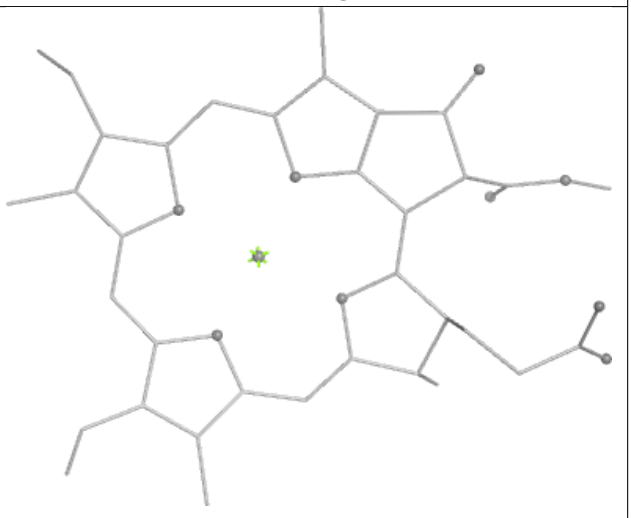

Rings

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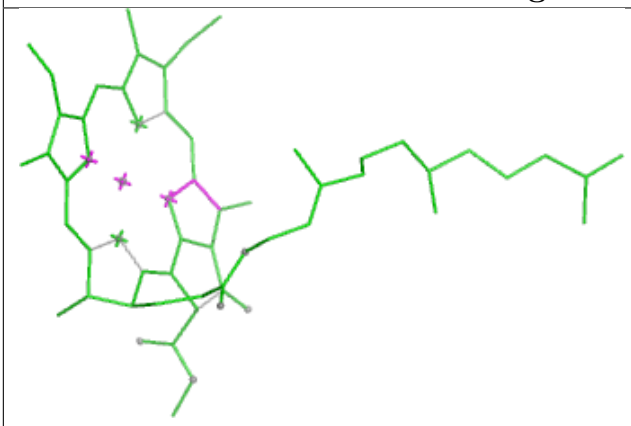

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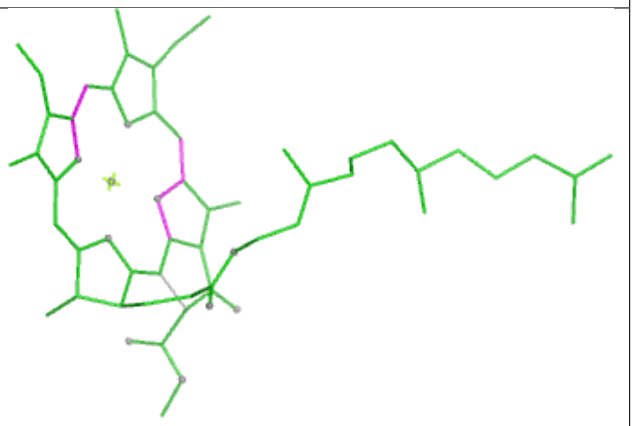
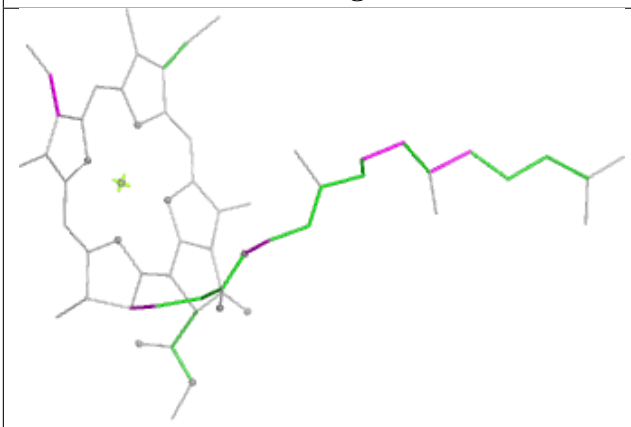


Bond angles

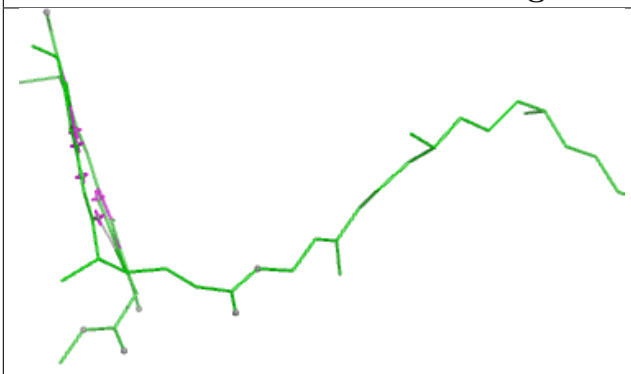


Torsions



Rings

Ligand CHL 6 601



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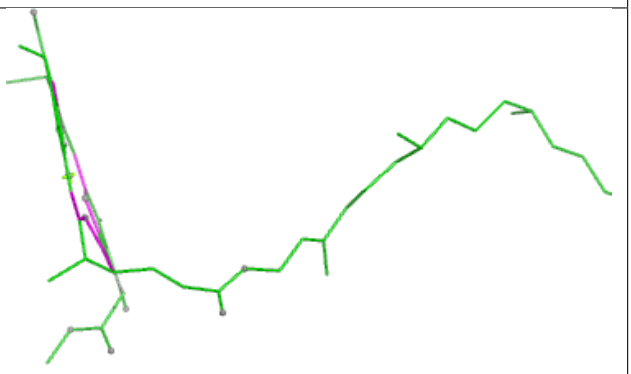
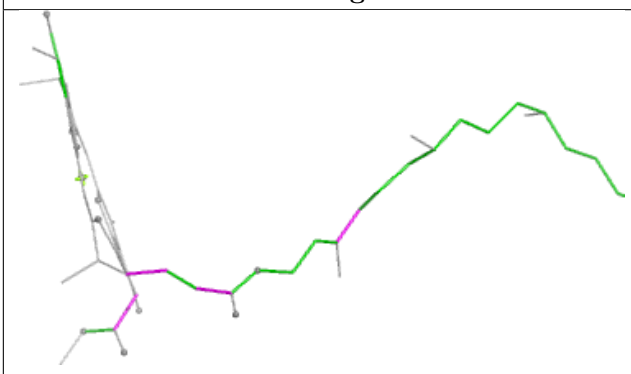
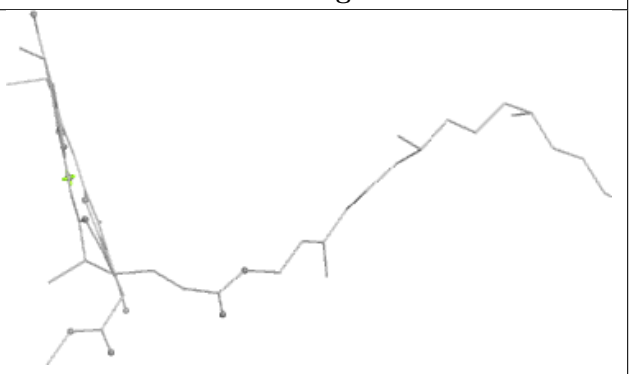


Bond angles

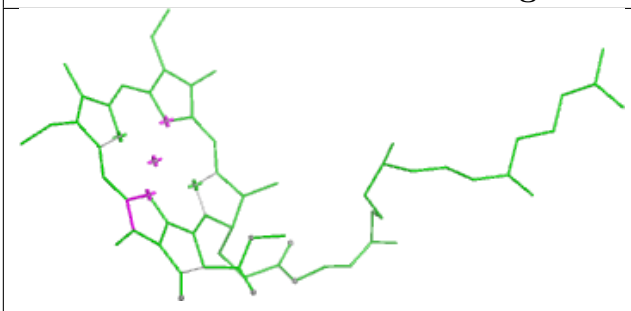


Torsions



Rings

Ligand CLA 52 603



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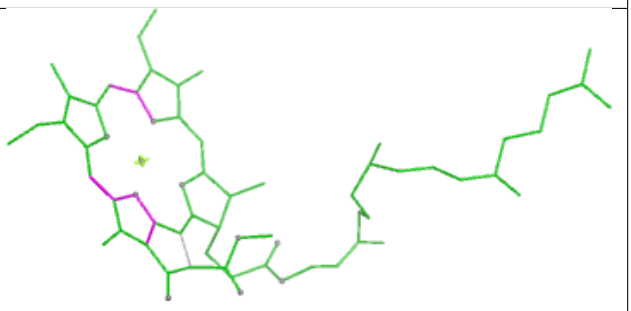
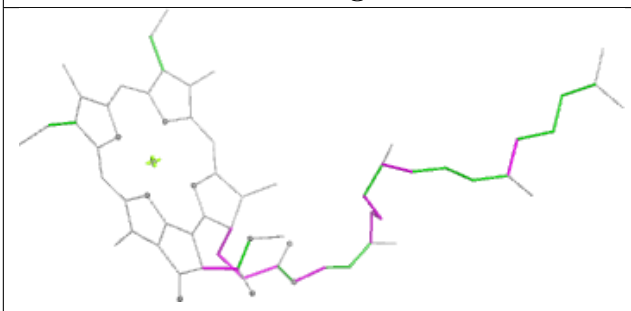


Bond angles



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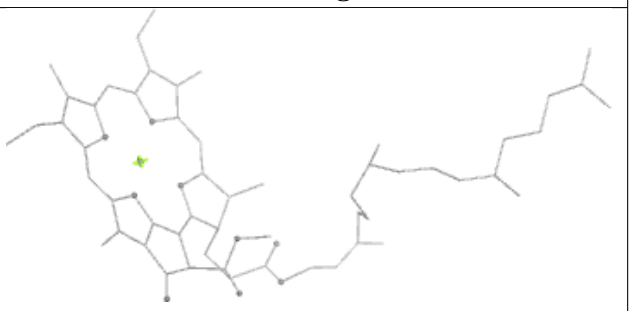
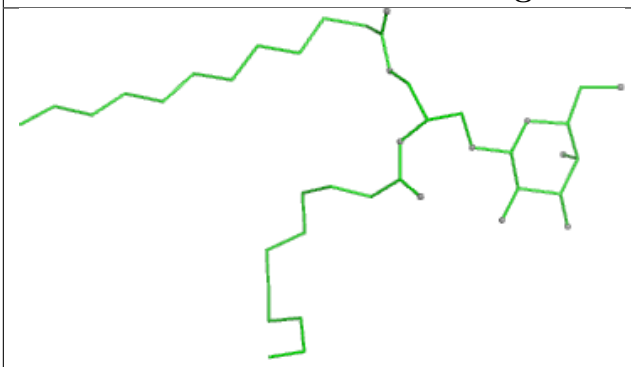


Rings

Ligand LMG 12 628



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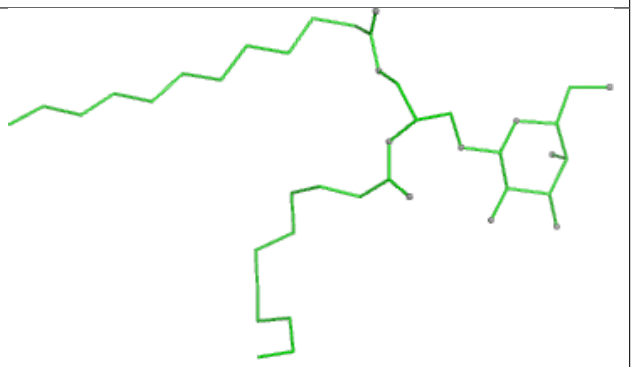


Bond angles

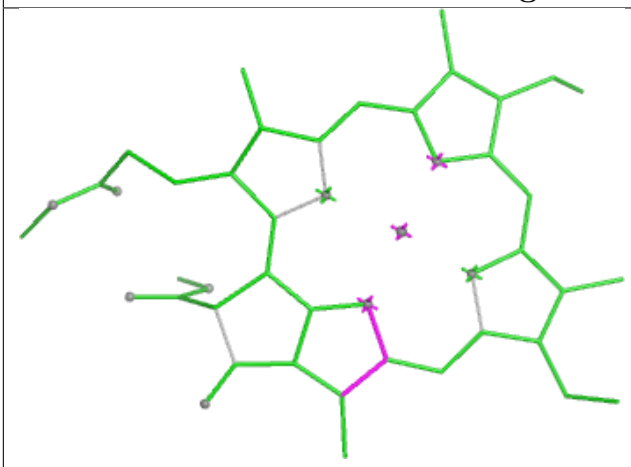


Torsions

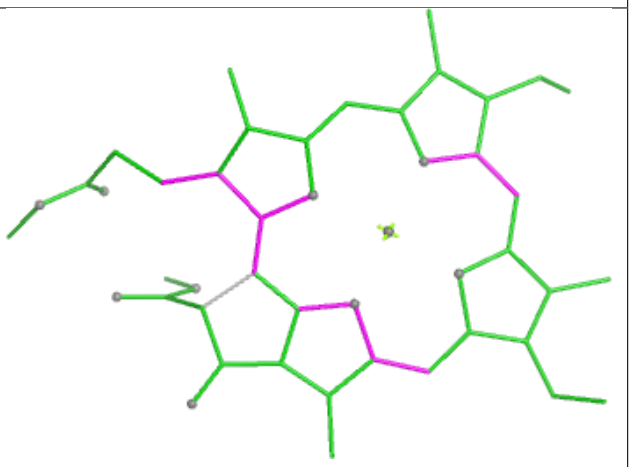


Rings

Ligand CLA 52 621



Bond lengths



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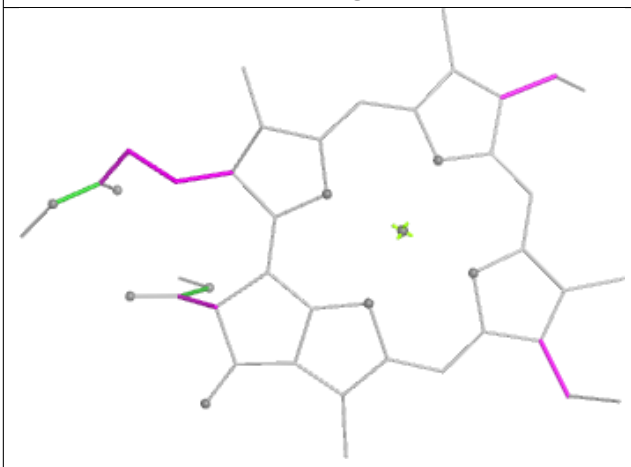
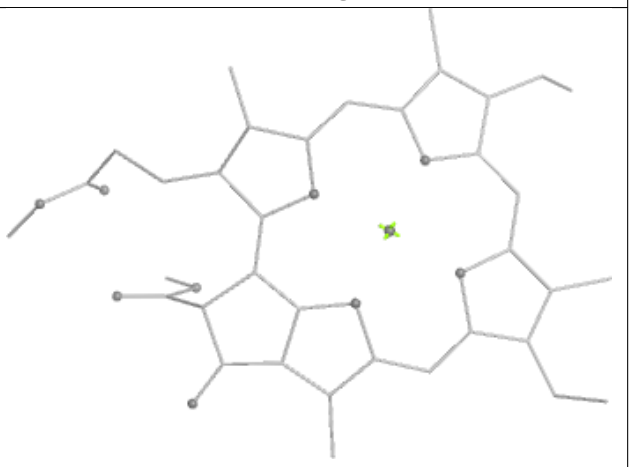


Torsions

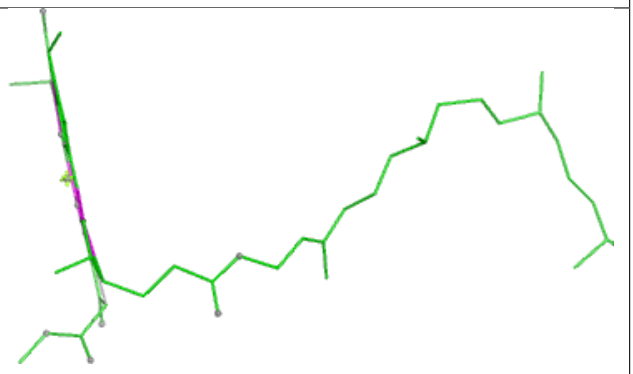


Rings

Ligand CHL 4 601



Bond lengths



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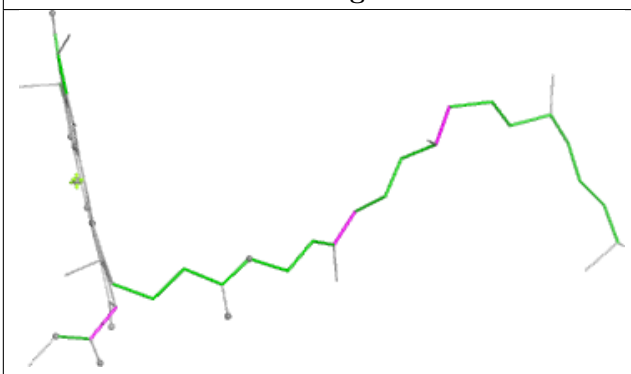

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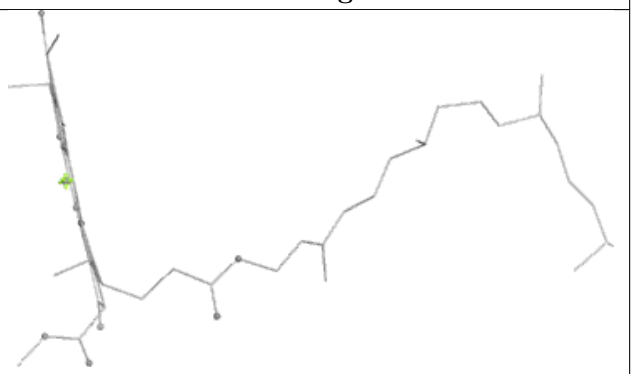
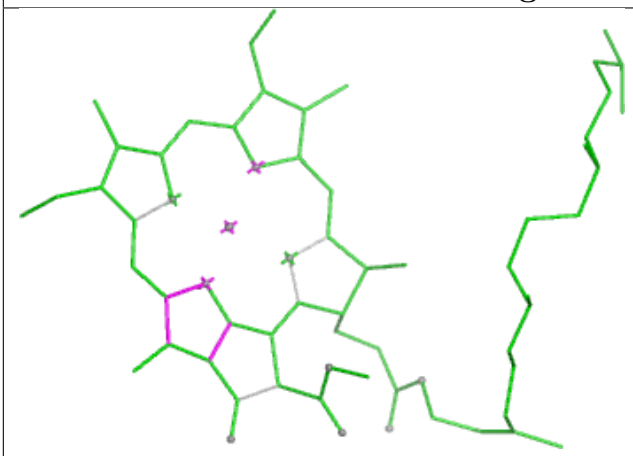


Rings

Ligand CLA 82 603



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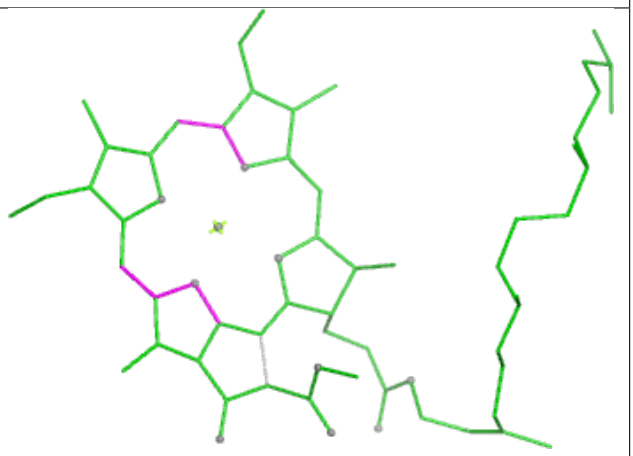

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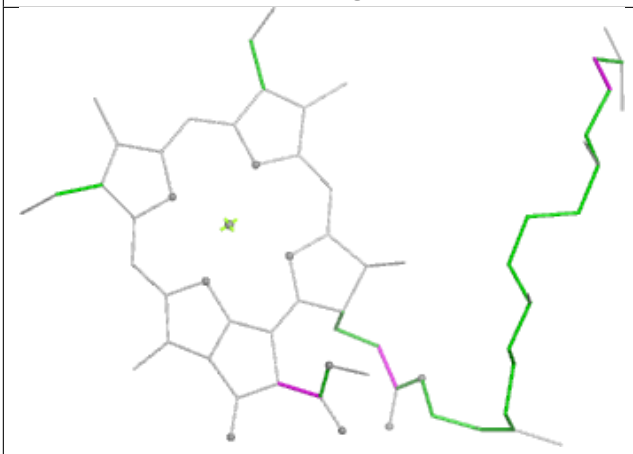
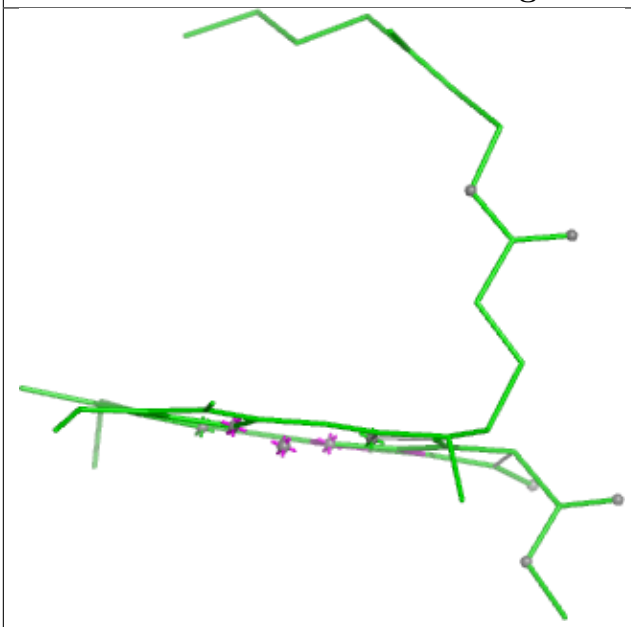


Torsions



Rings

Ligand CLA 92 604



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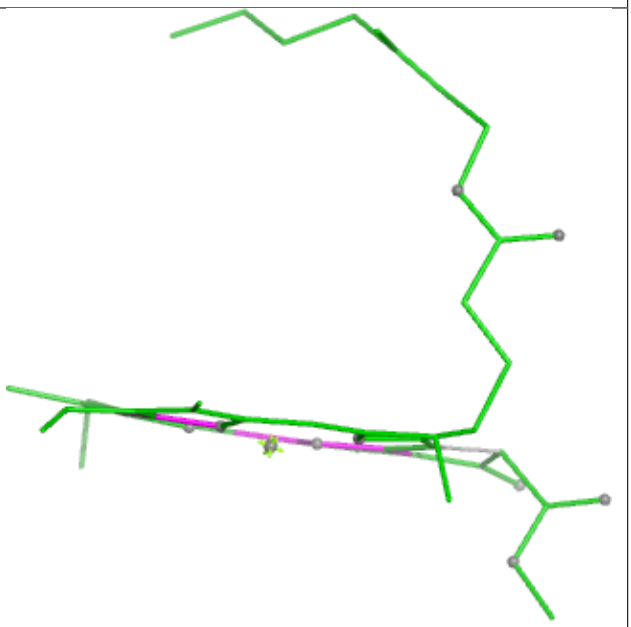
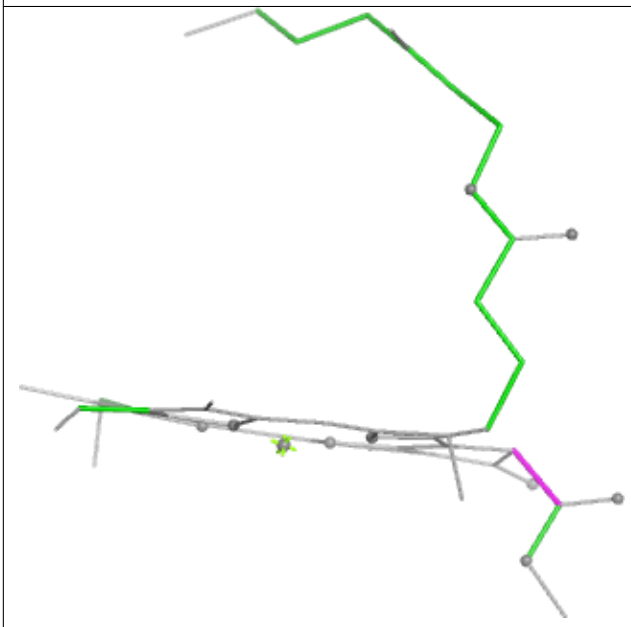


Bond angles

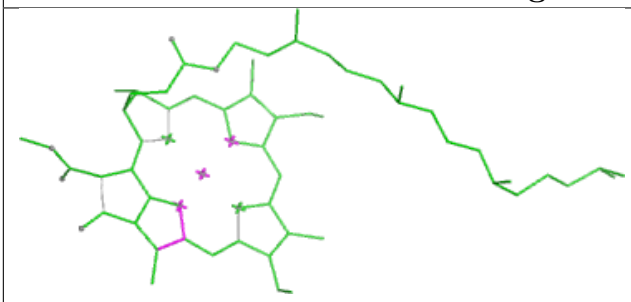


Torsions



Rings

Ligand CLA 1 610



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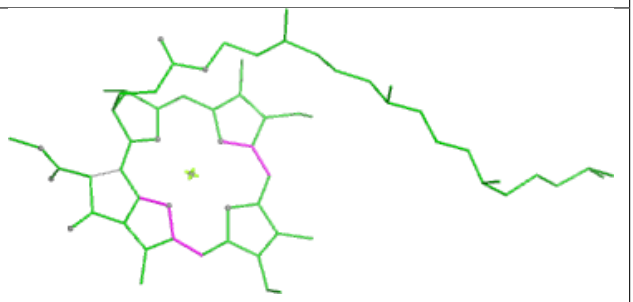

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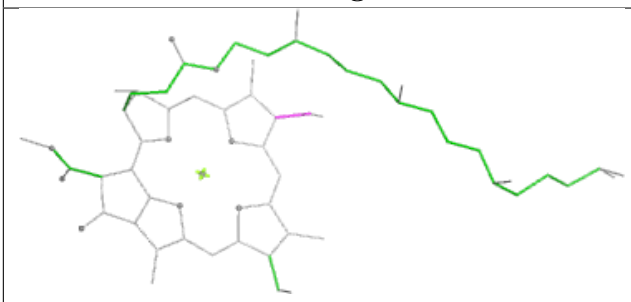

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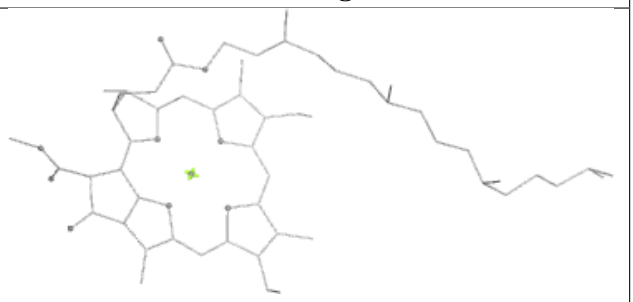
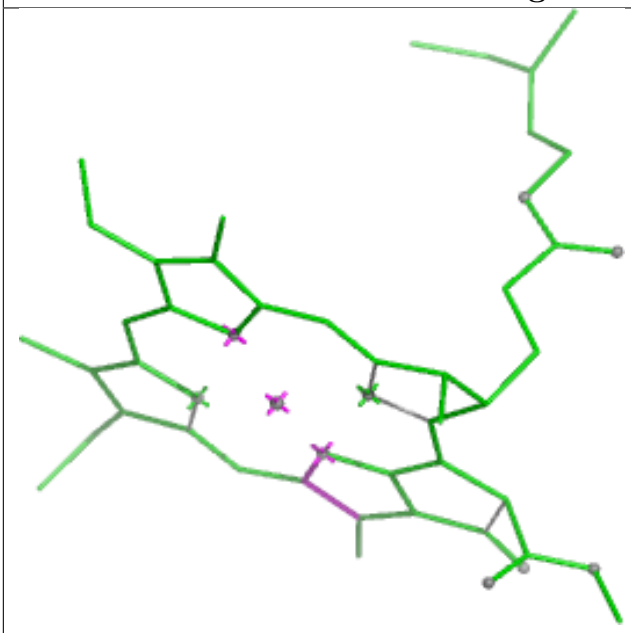


Rings

Ligand CLA 9 604



Ligand CLA 7 604



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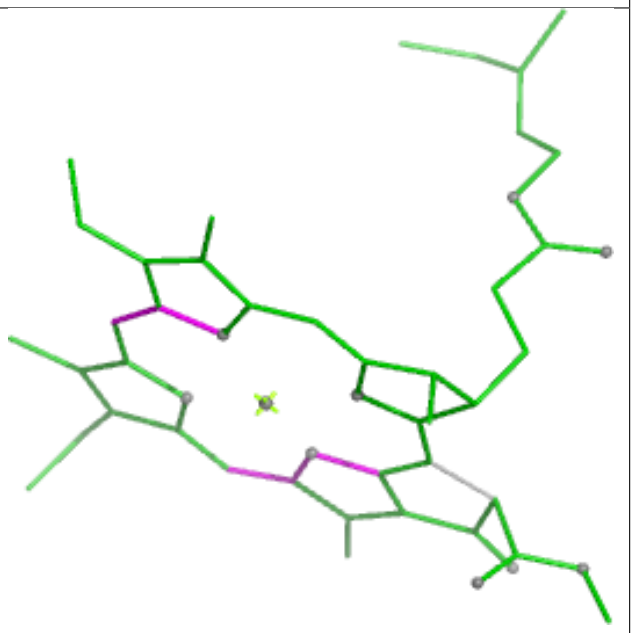

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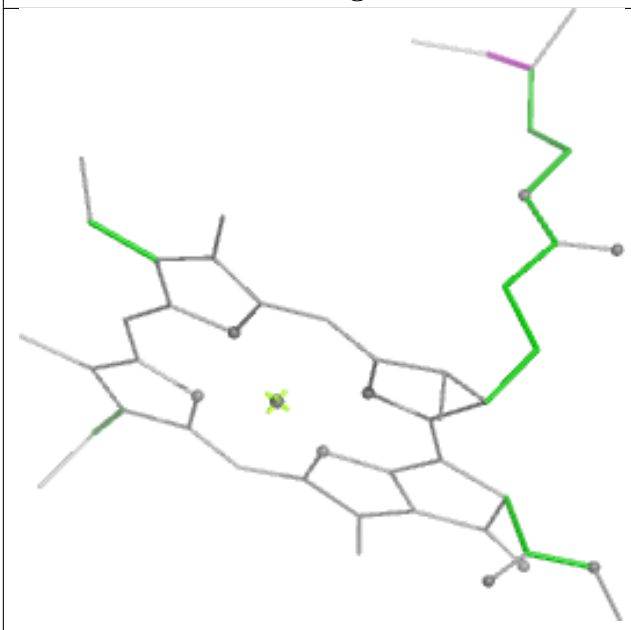

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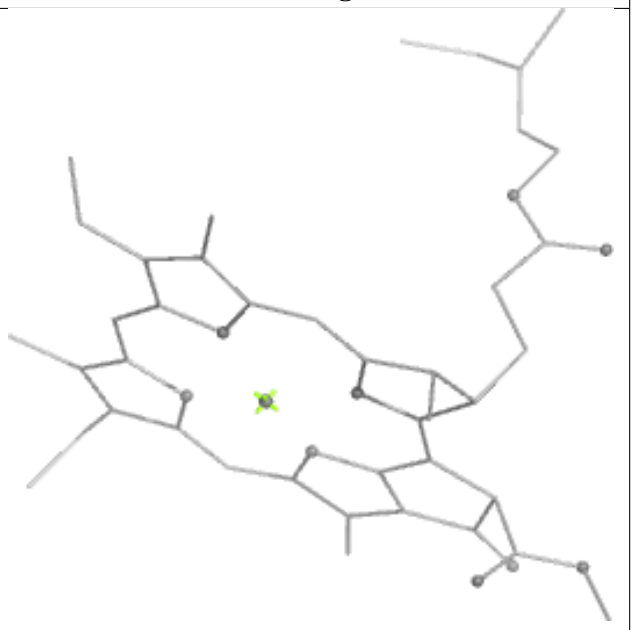
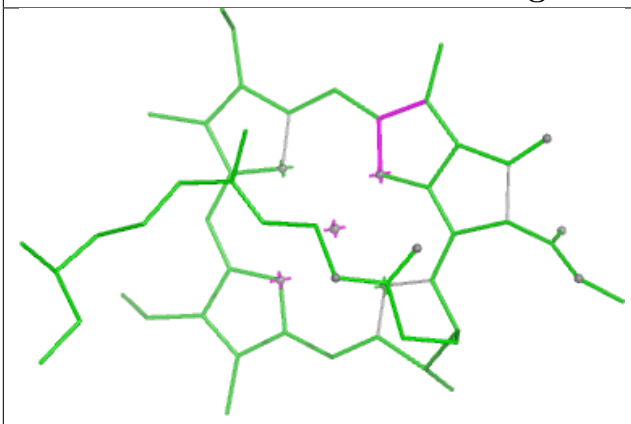


Rings

Ligand CLA 5 613



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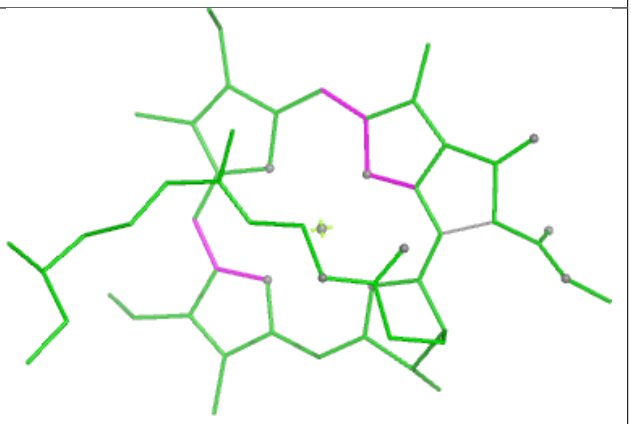
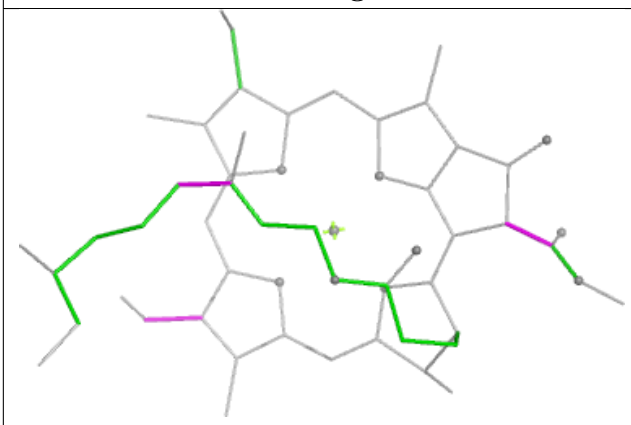


Bond angles



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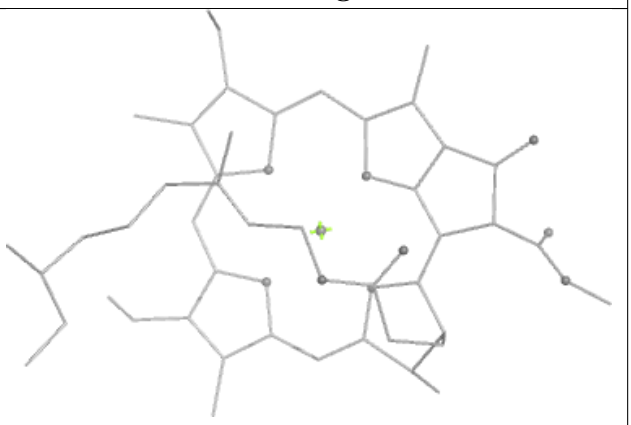
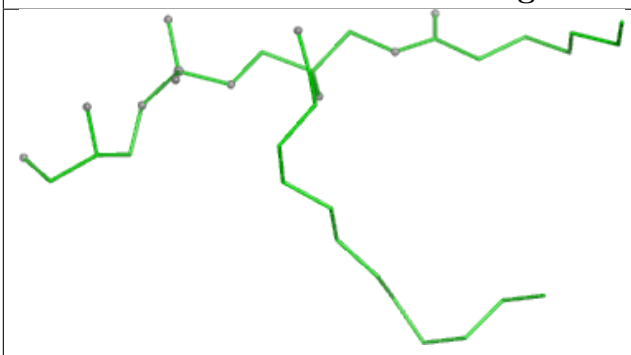


Rings

Ligand LHG 62 629



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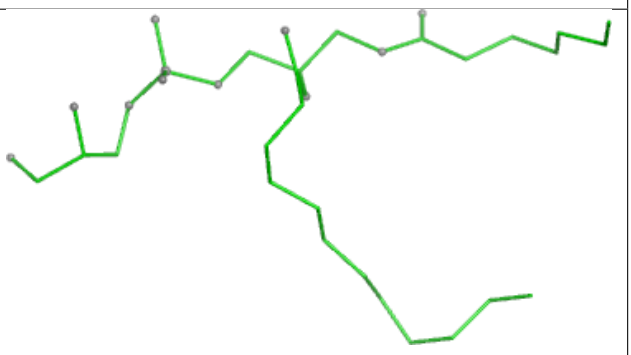

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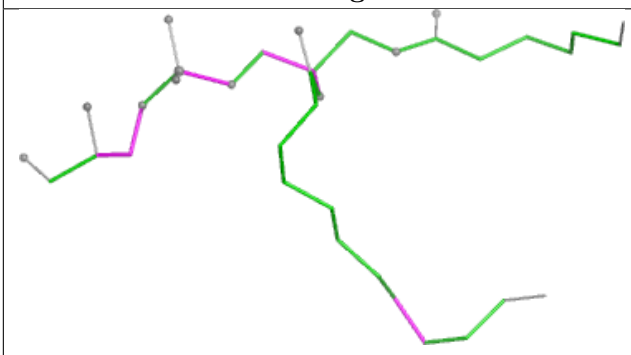

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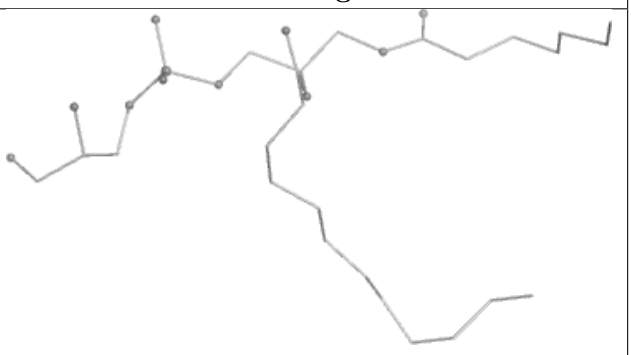
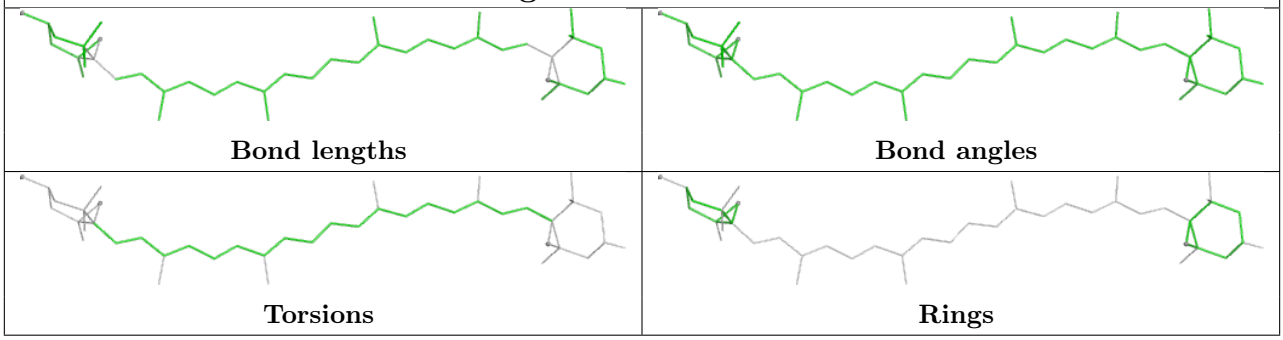
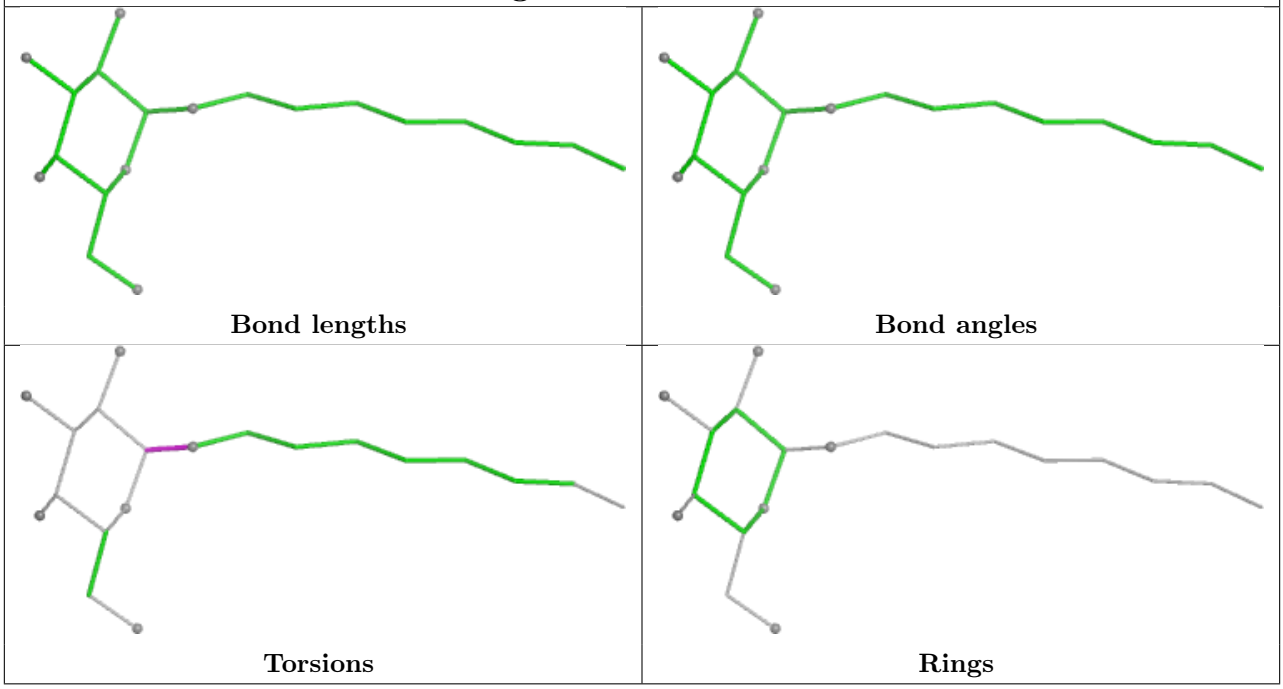


Rings

Ligand XAT 82 618



Ligand LMU A2 862



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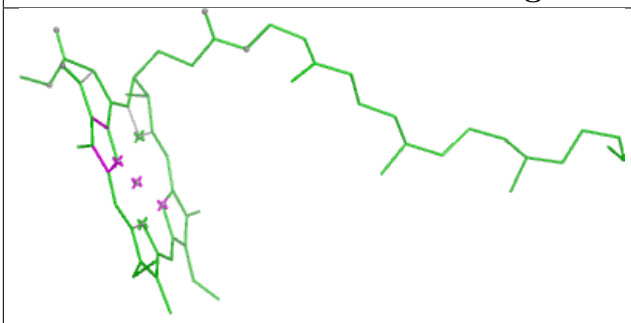

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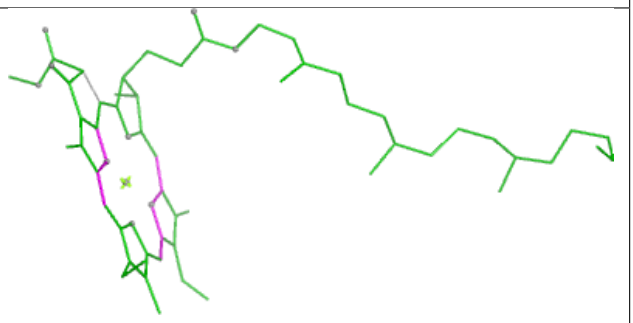
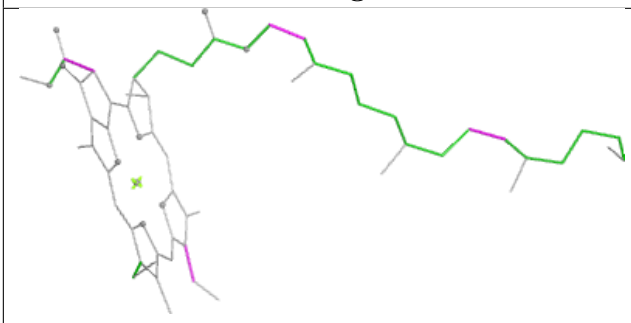


Bond angles

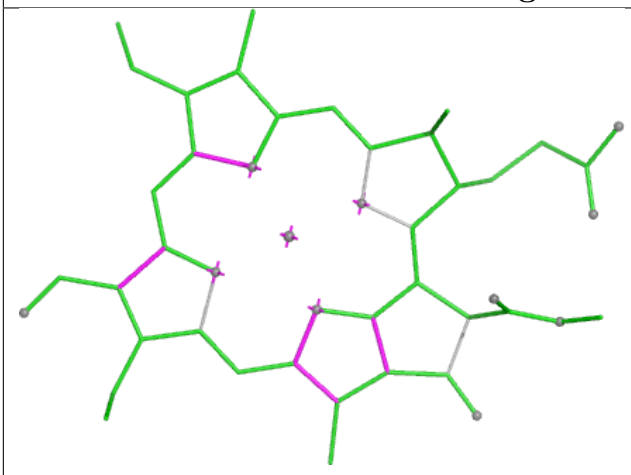


Torsions



Rings

Ligand CHL 12 606



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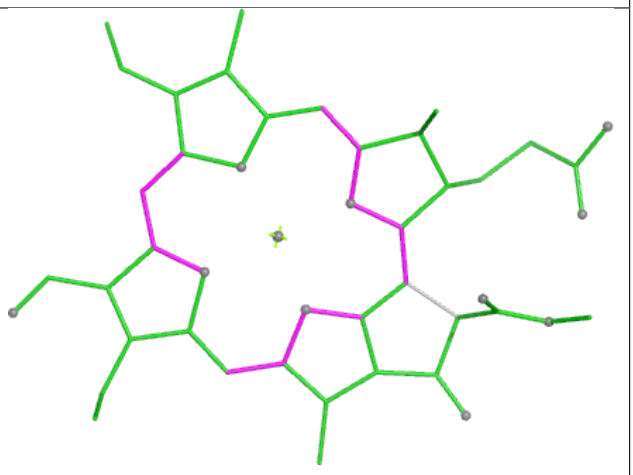

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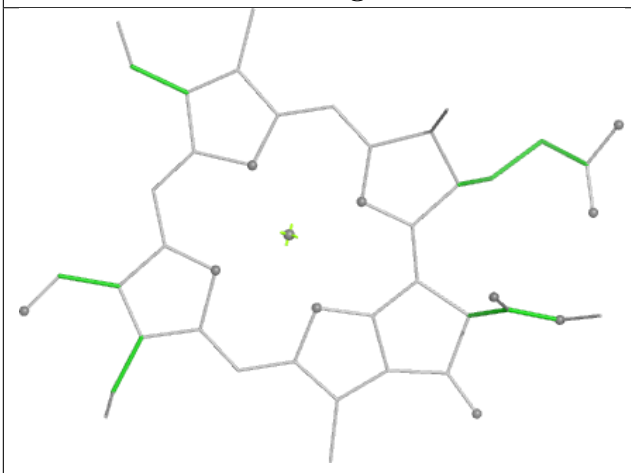

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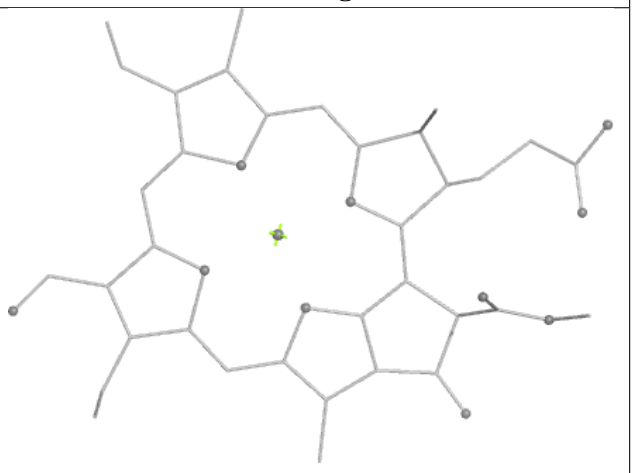

Rings

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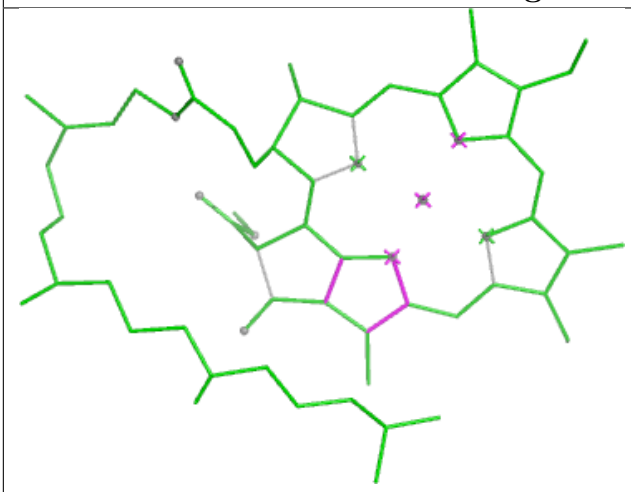

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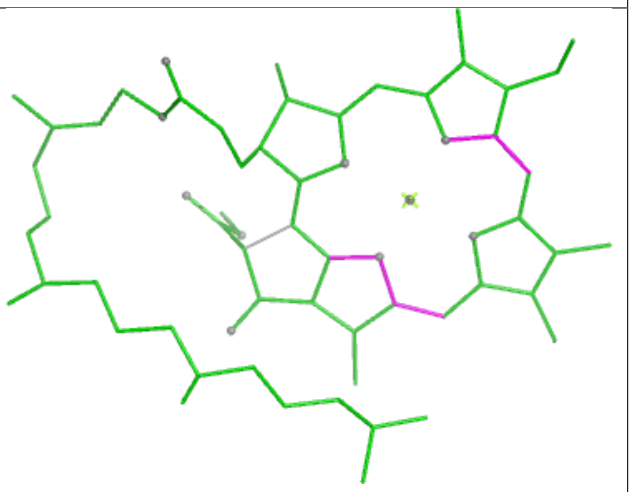
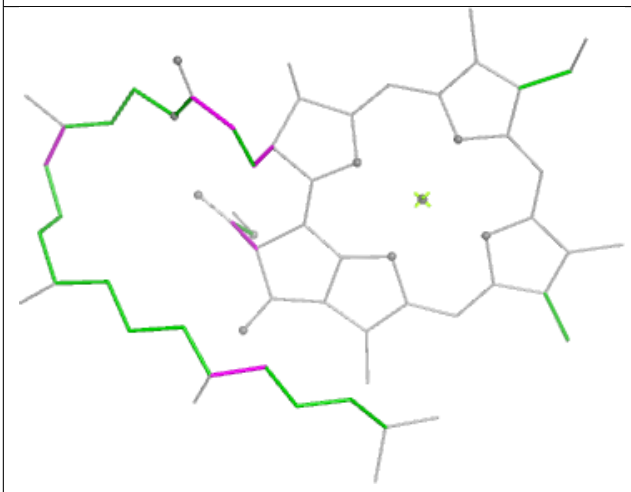


Bond angles



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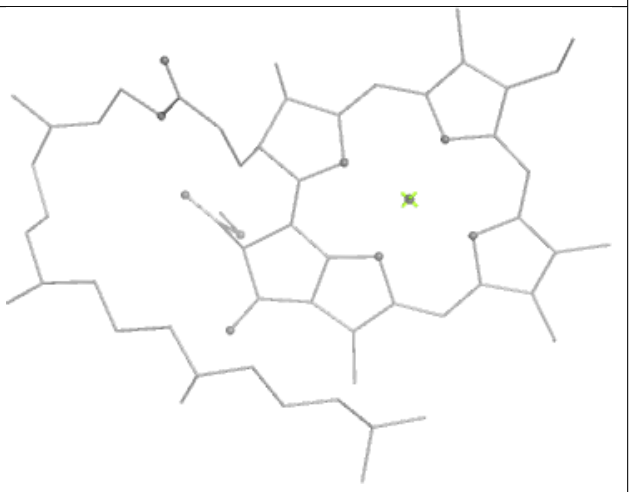
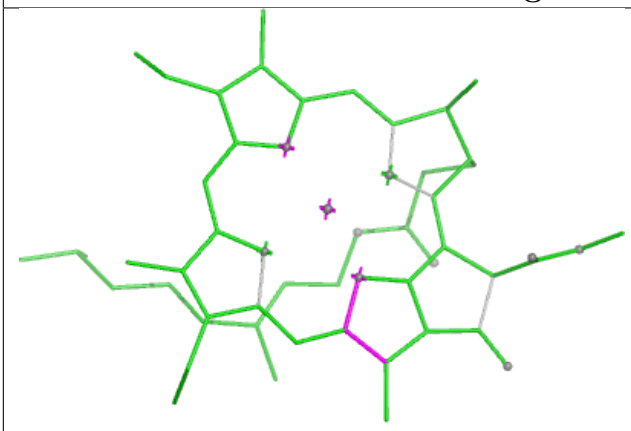


Rings

Ligand CLA B 807



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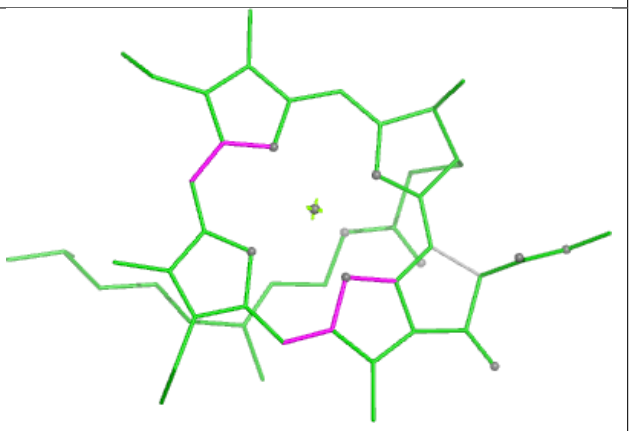
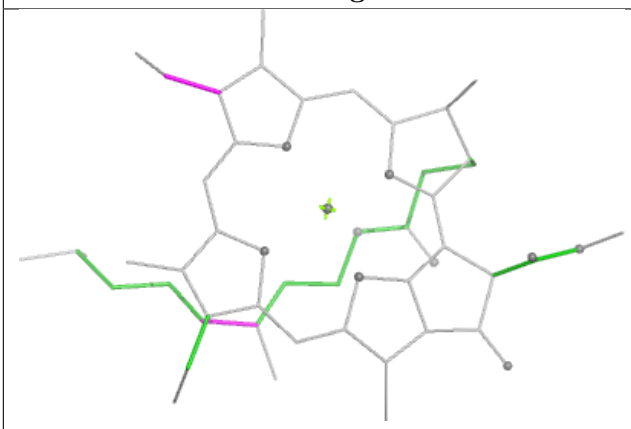


Bond angles



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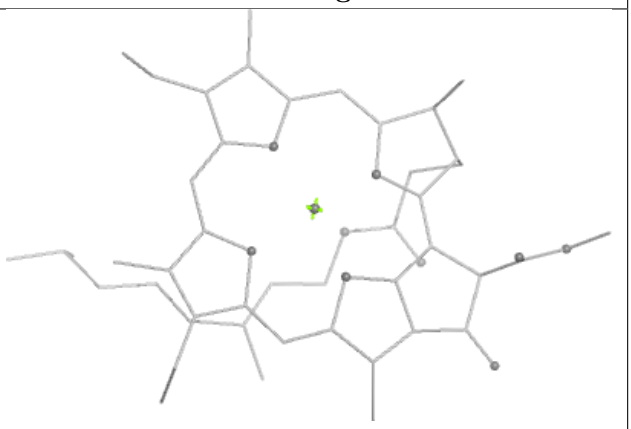
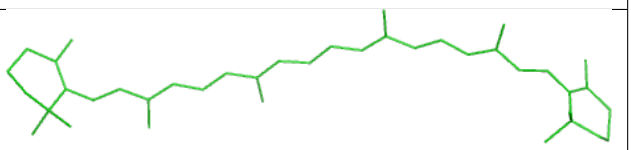


Rings

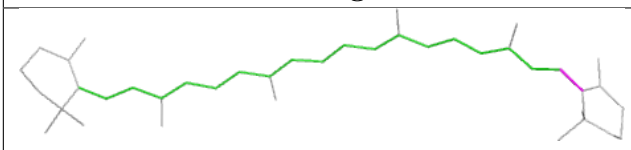
Ligand BCR B2 847



Bond lengths



Bond angles



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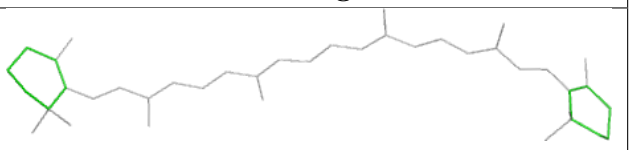
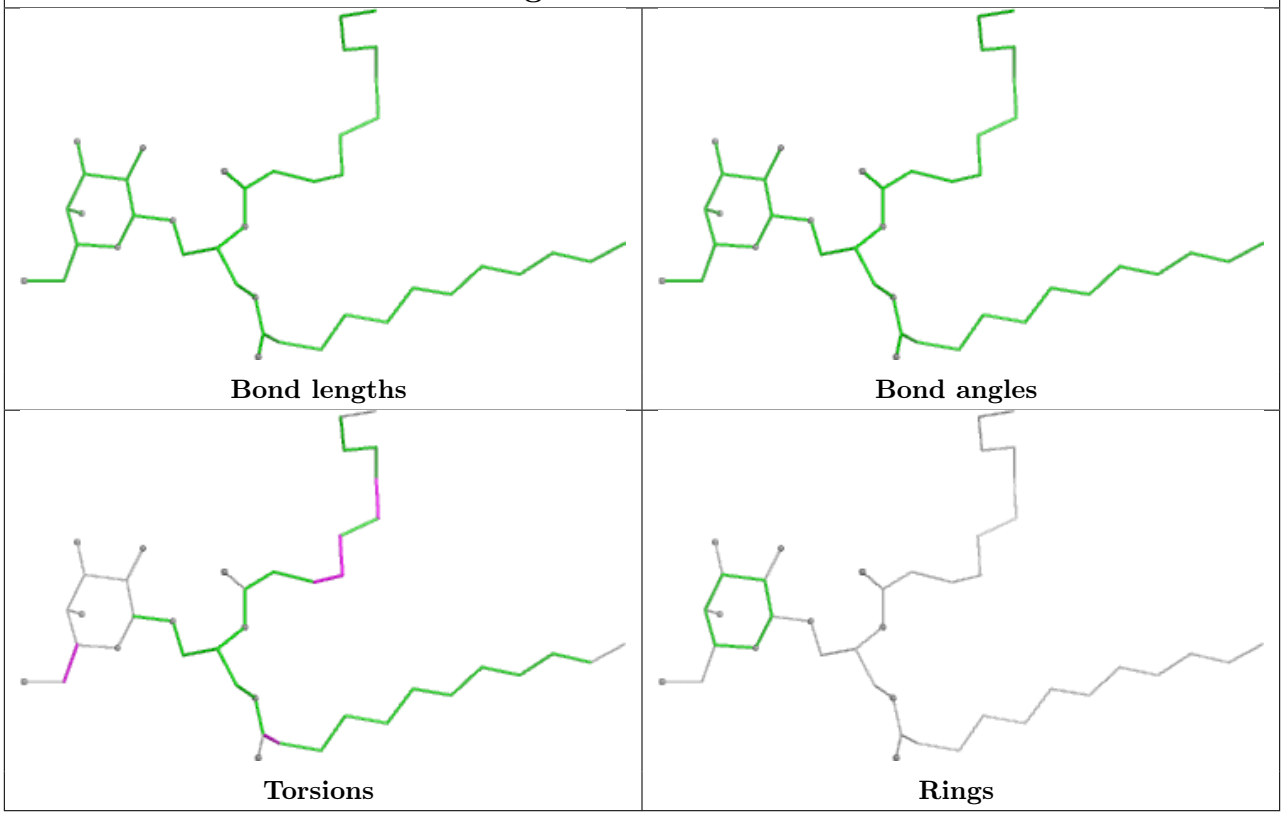
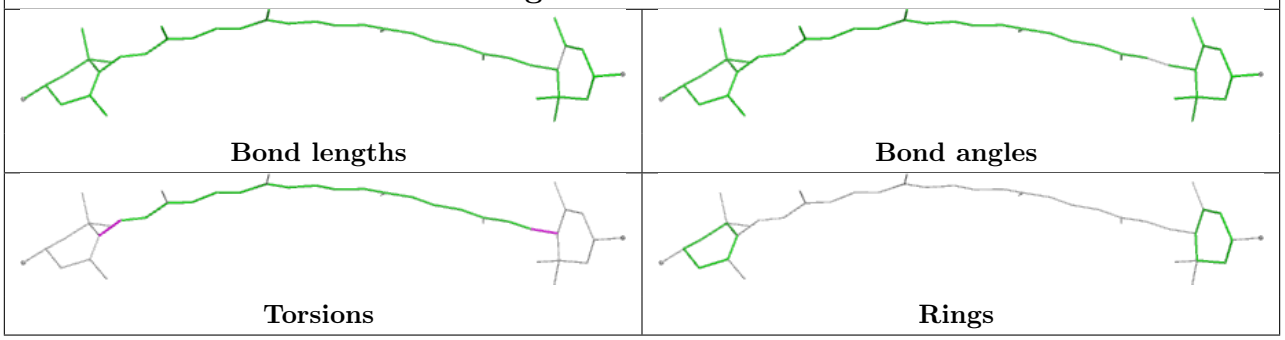


Rings

Ligand LMG 1 628



Ligand LUT A 856



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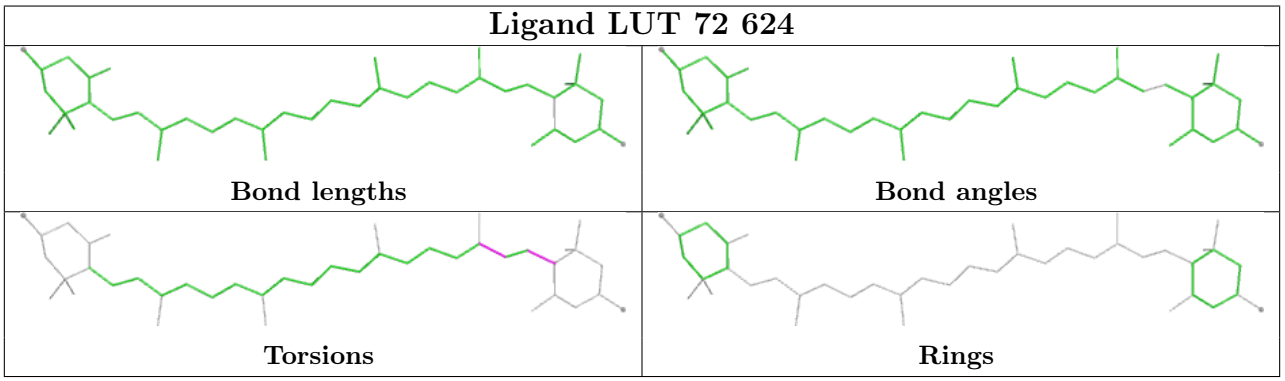
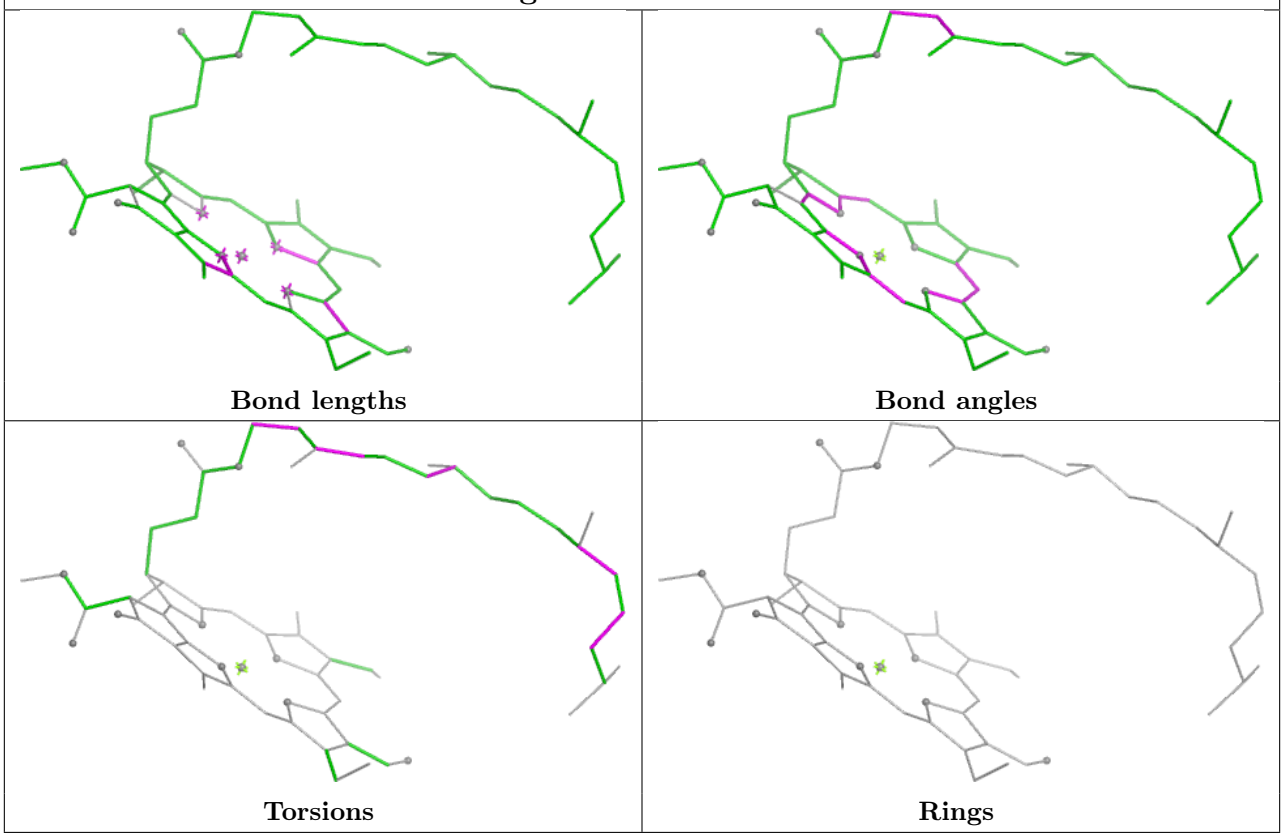


Ligand CHL 62 607



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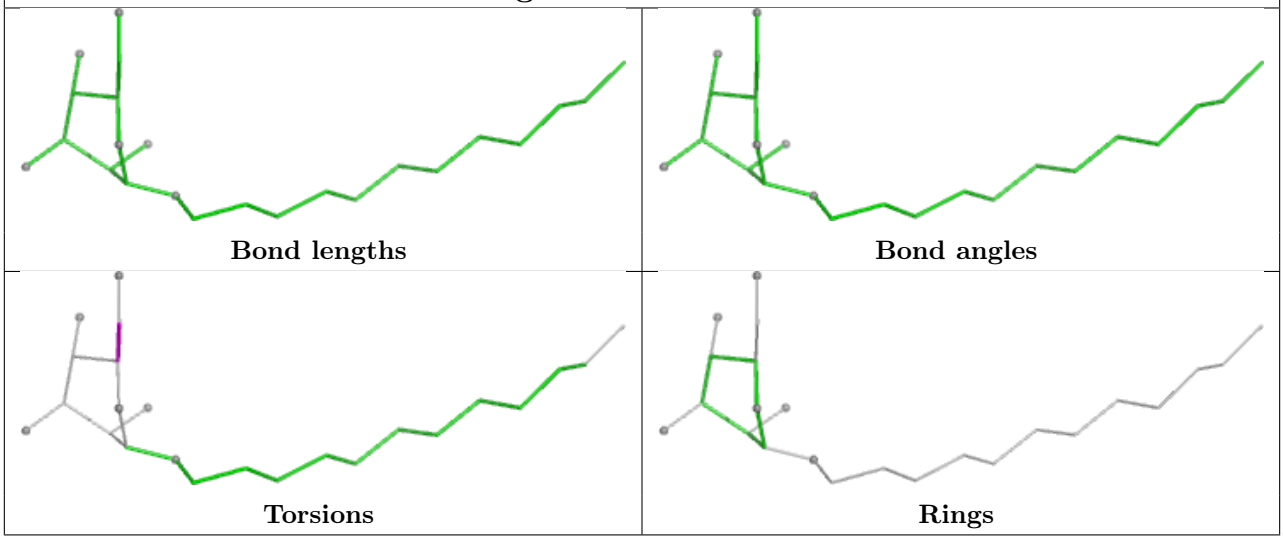
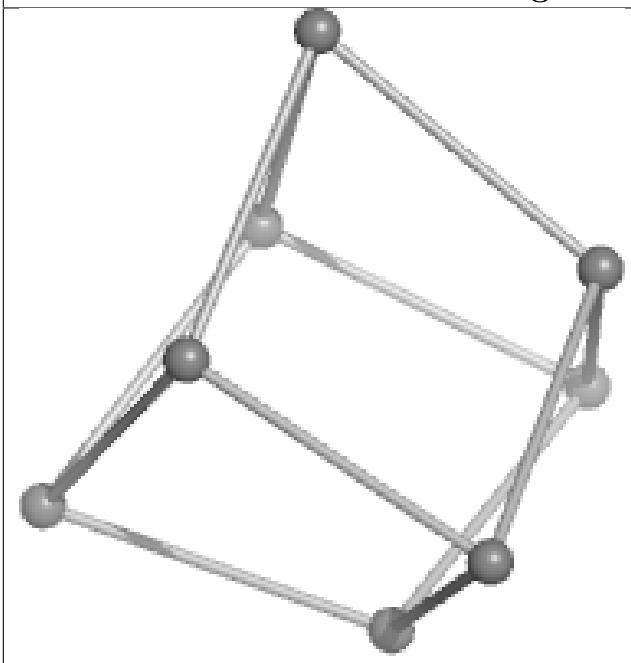
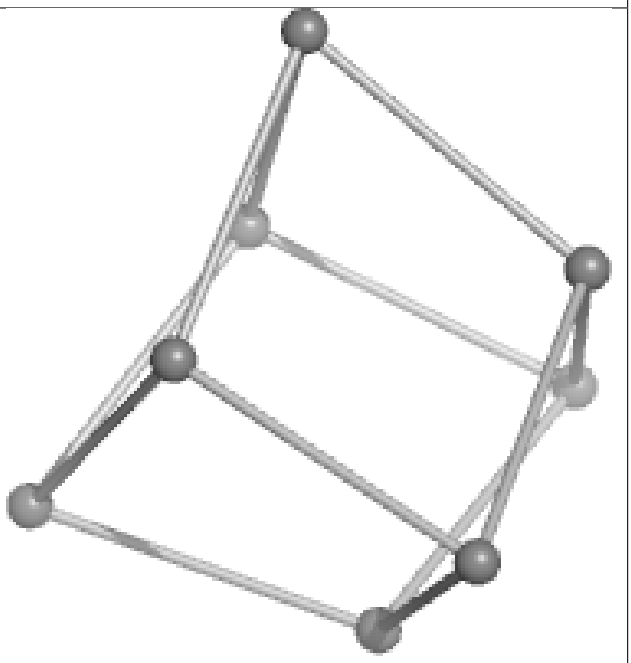


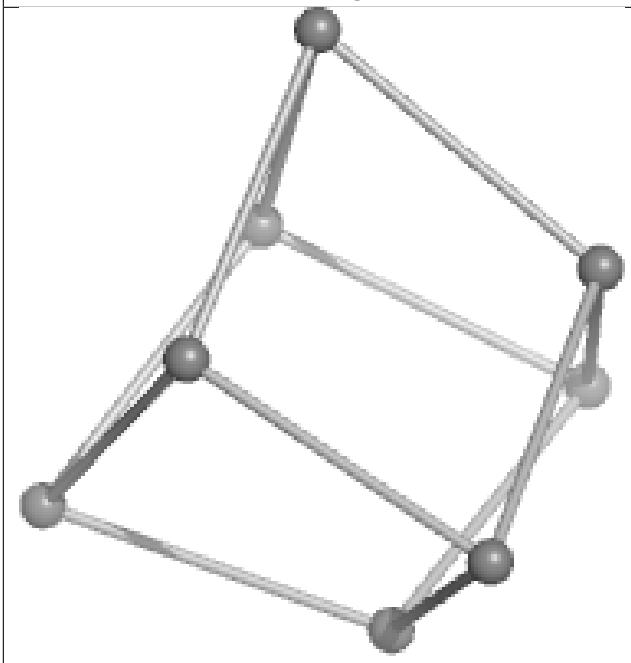
Ligand SF4 C 101



Bond lengths



Bond angles



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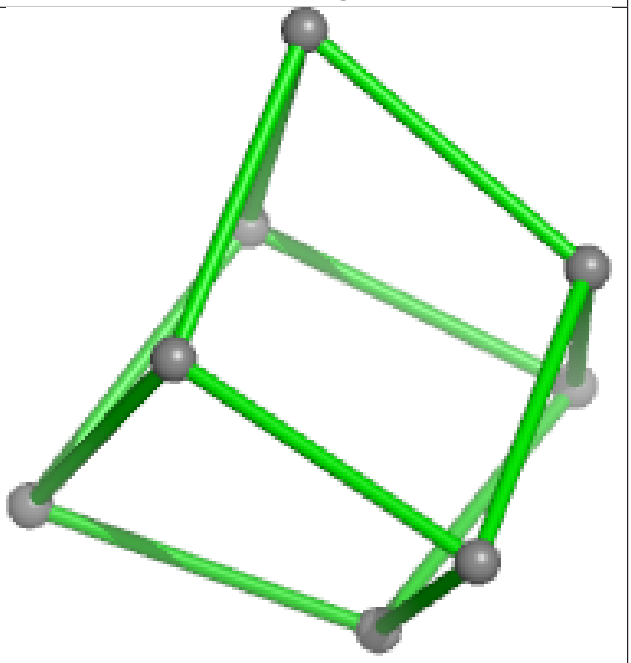
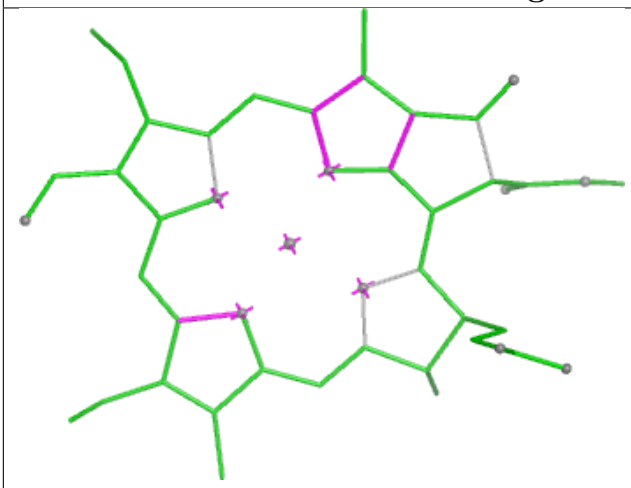
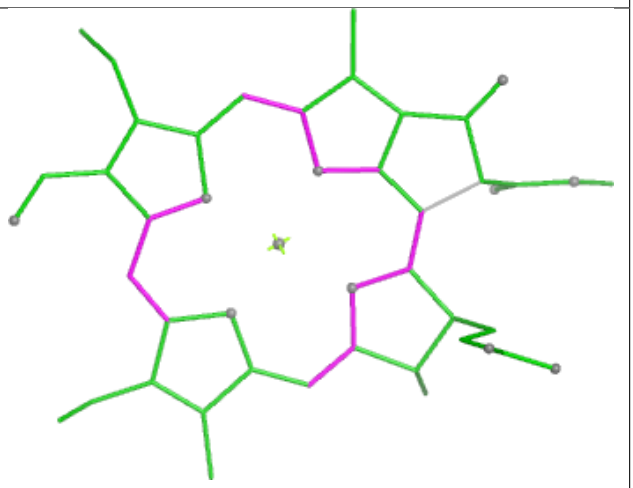


Rings

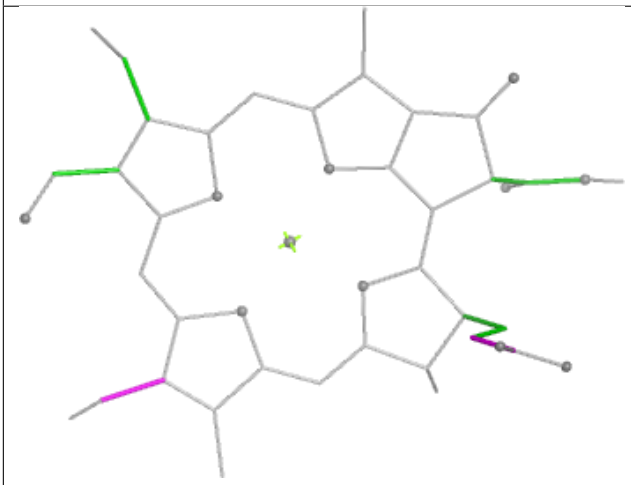
Ligand CHL 7 607



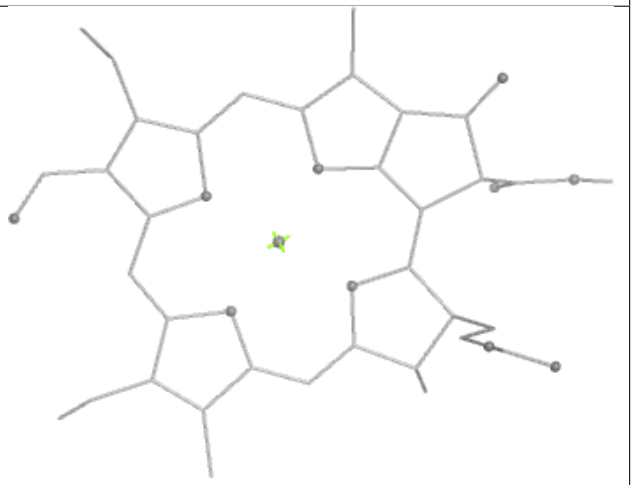
Bond lengths



Bond angles

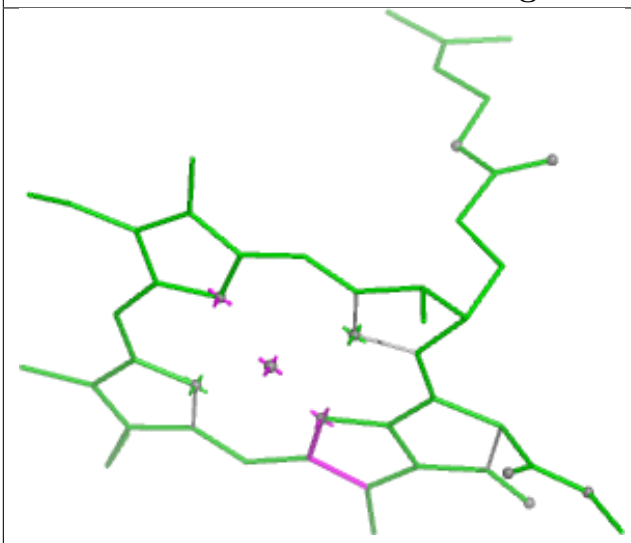


Torsions



Rings

Ligand CLA 62 614



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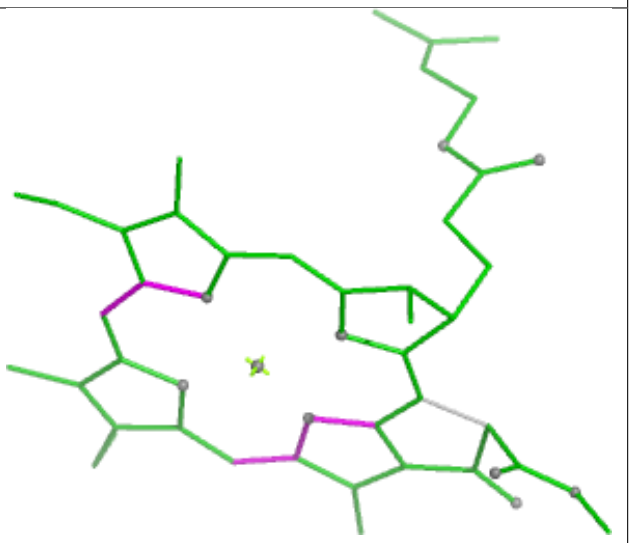

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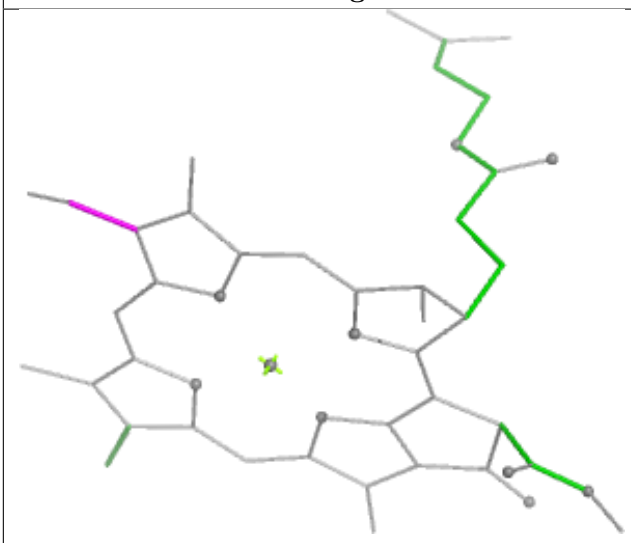

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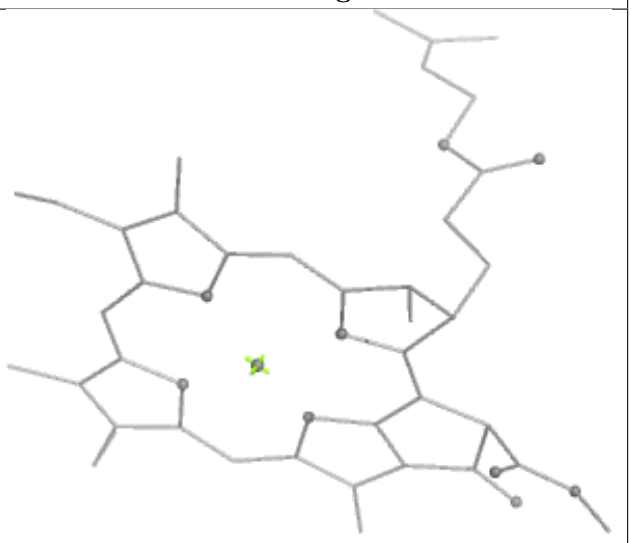
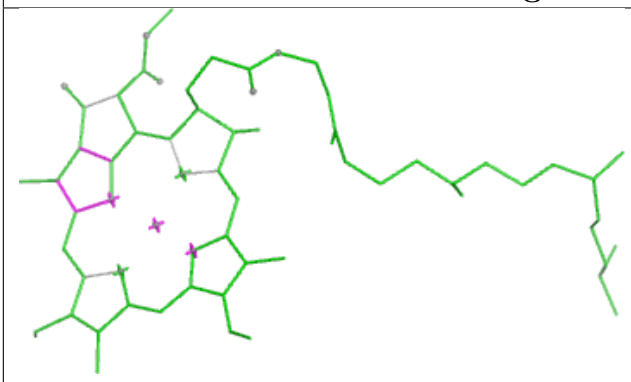


Rings

Ligand CLA A 802



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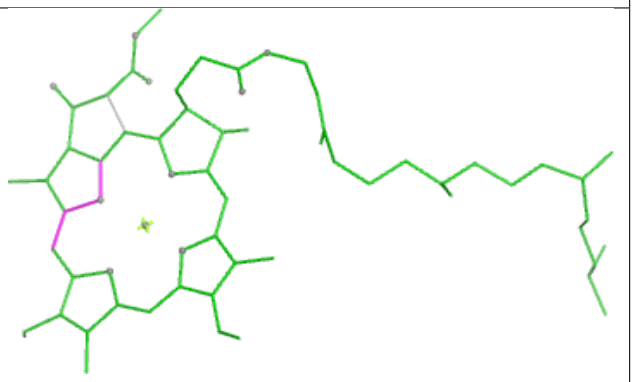

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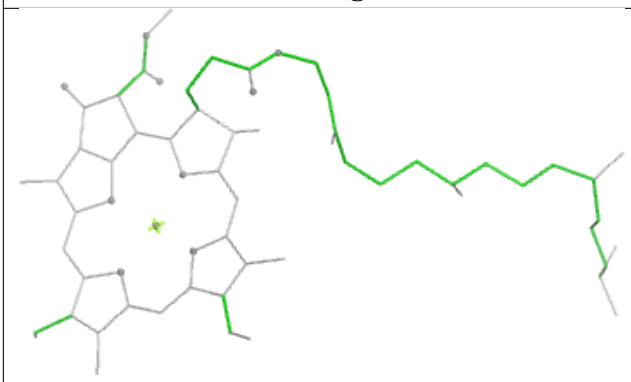

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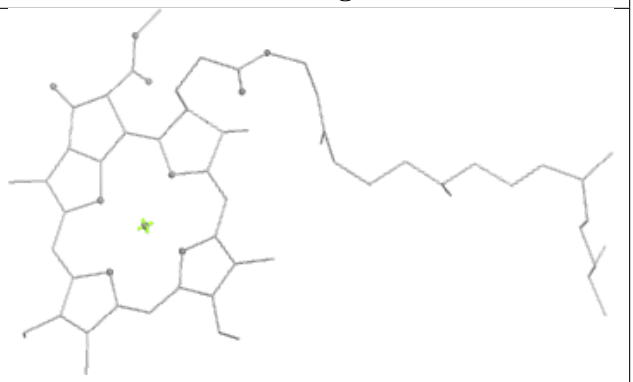
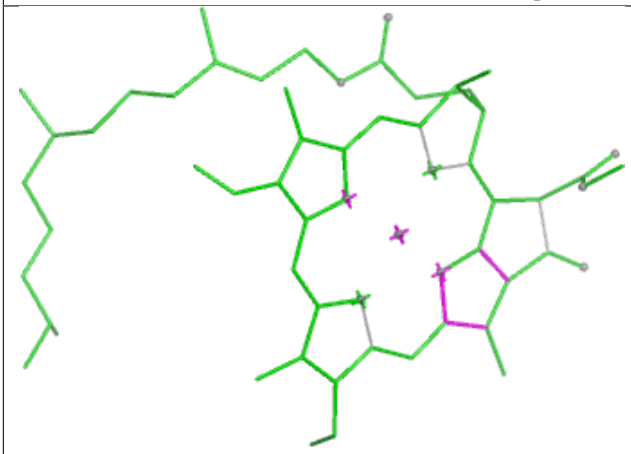


Rings

Ligand CLA 3 602



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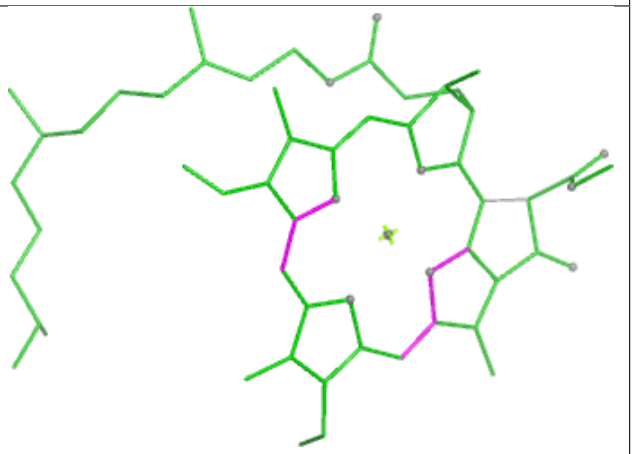

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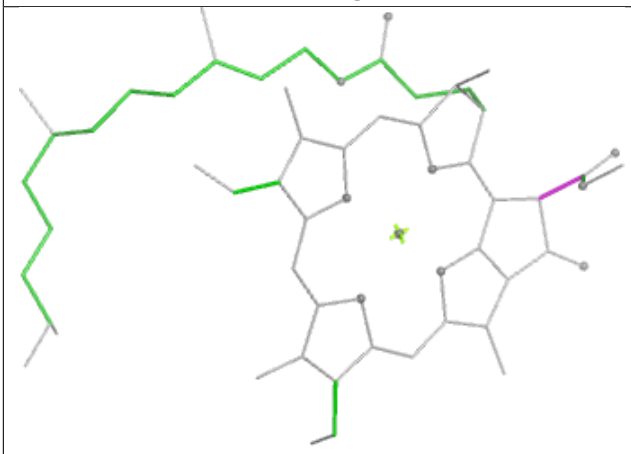

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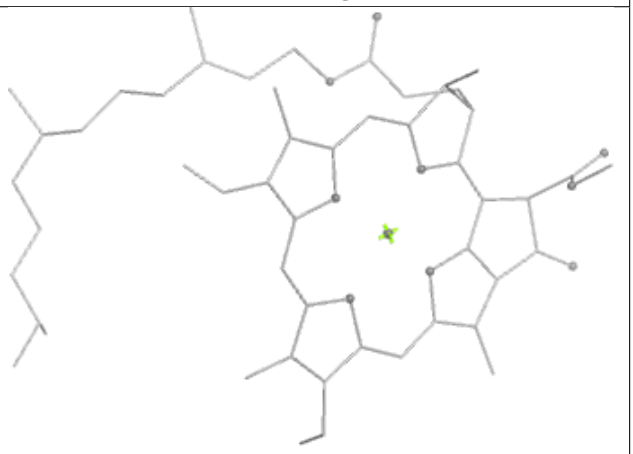
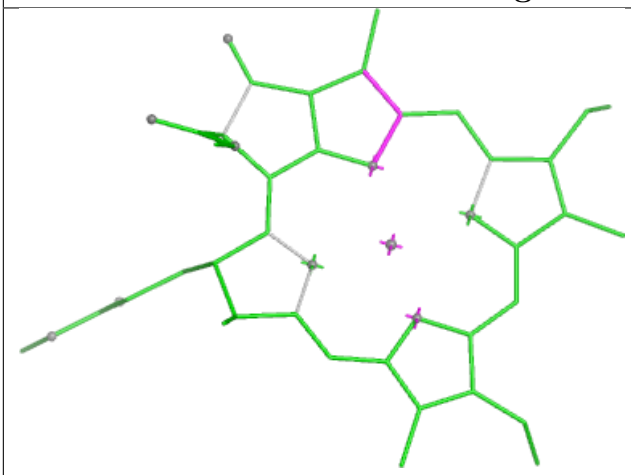


Rings

Ligand CLA K2 204



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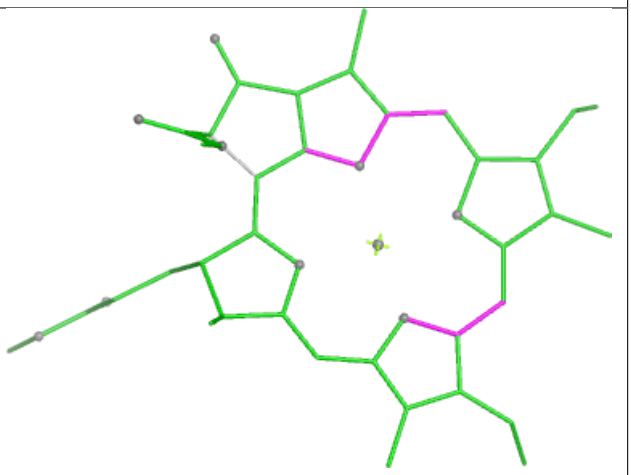

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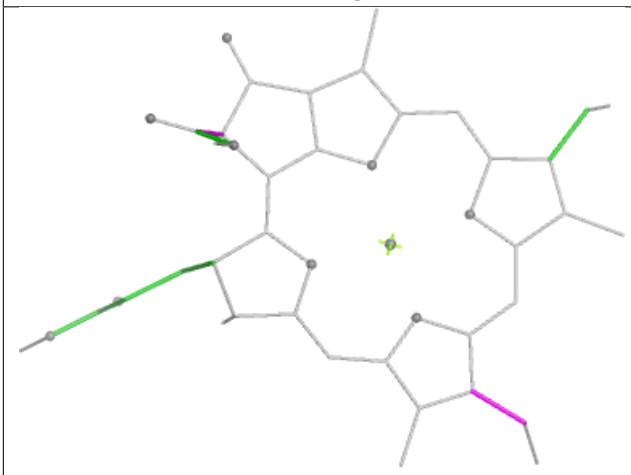

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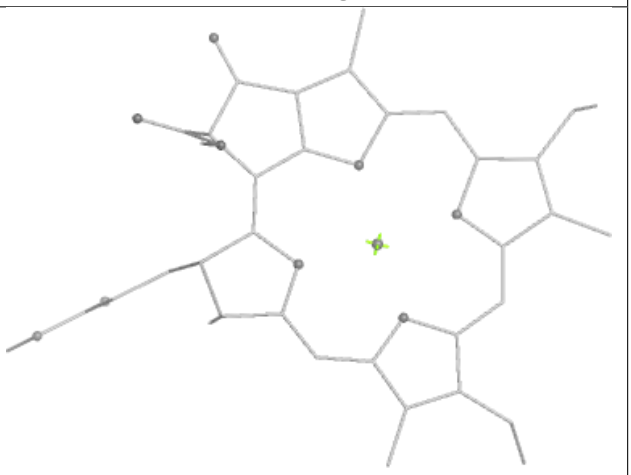
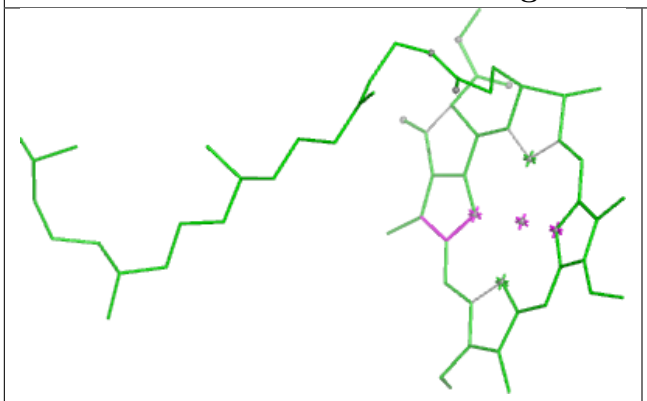


Rings

Ligand CLA 12 609



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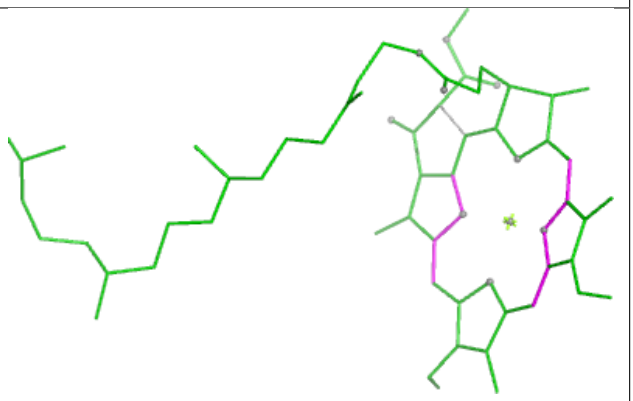

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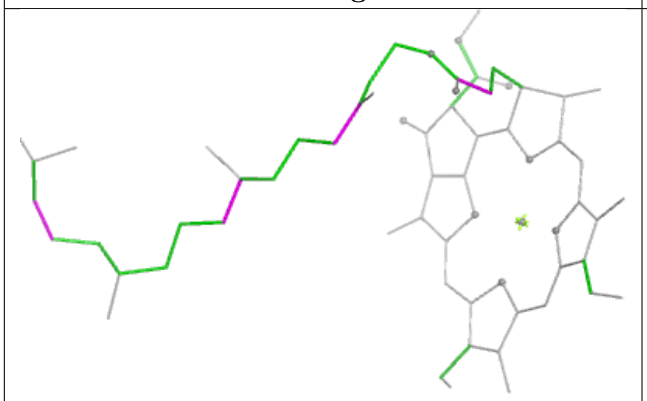

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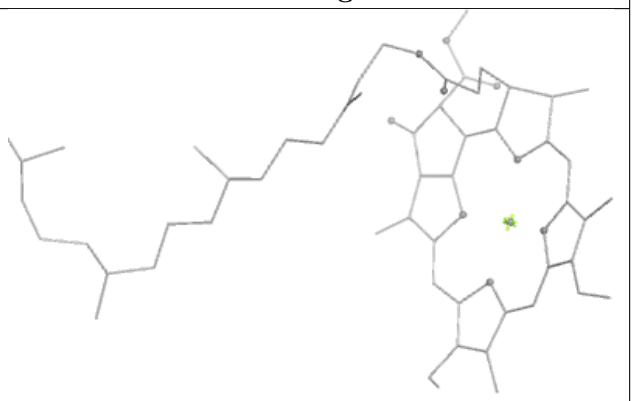

Rings

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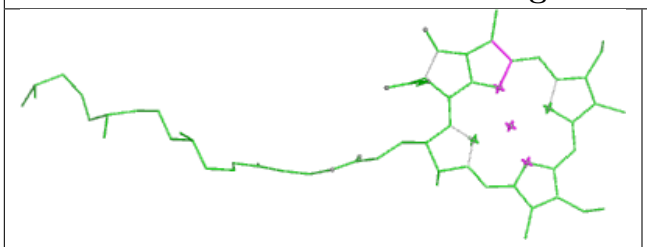

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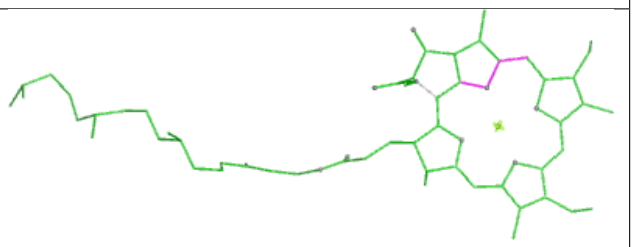
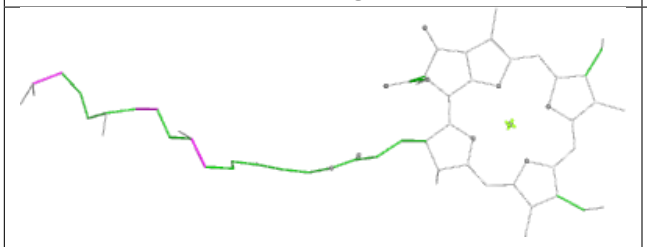


Bond angles



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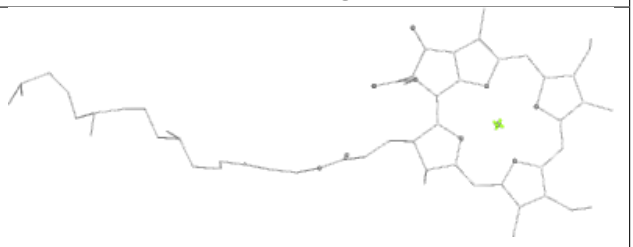
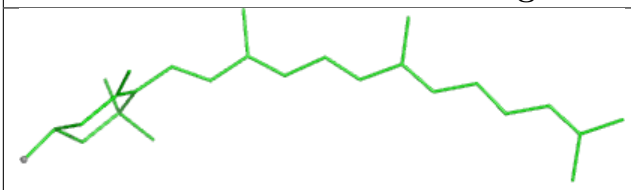
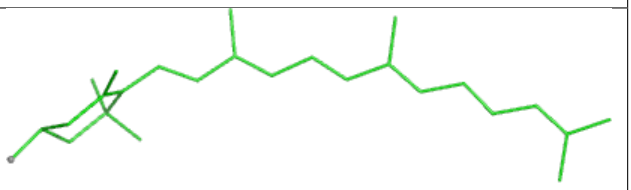
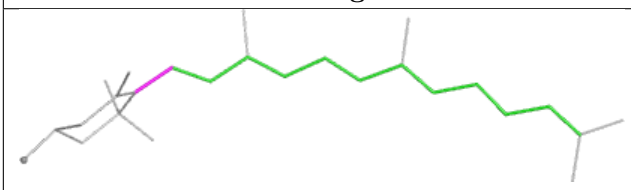
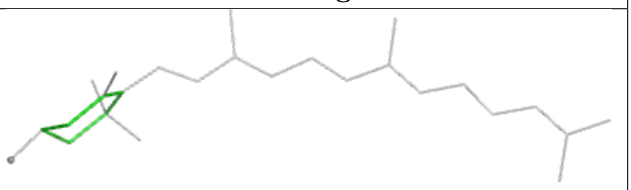


Rings

Ligand LUT Z2 619	
 Bond lengths	 Bond angles
 Torsions	 Rings

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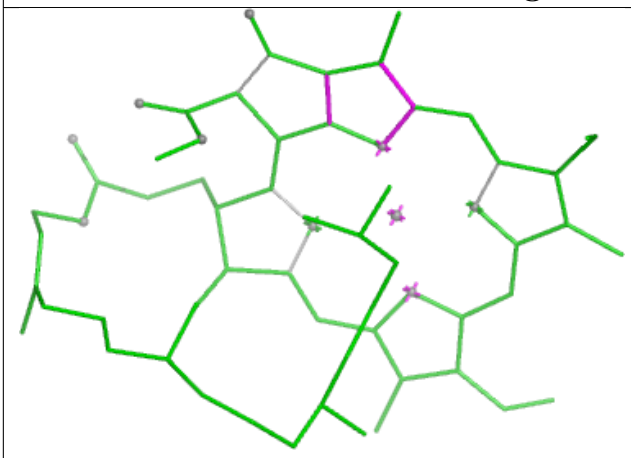
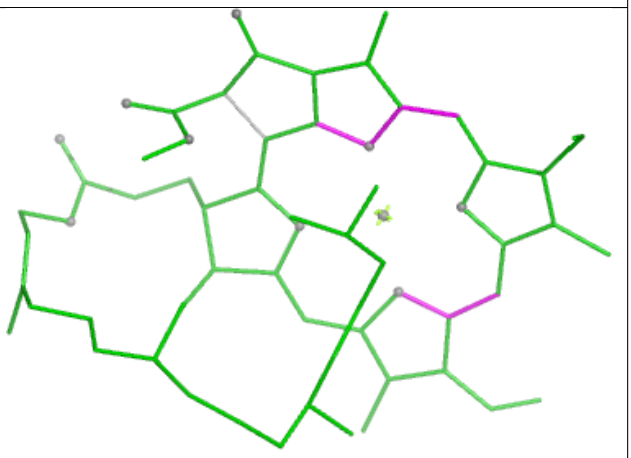
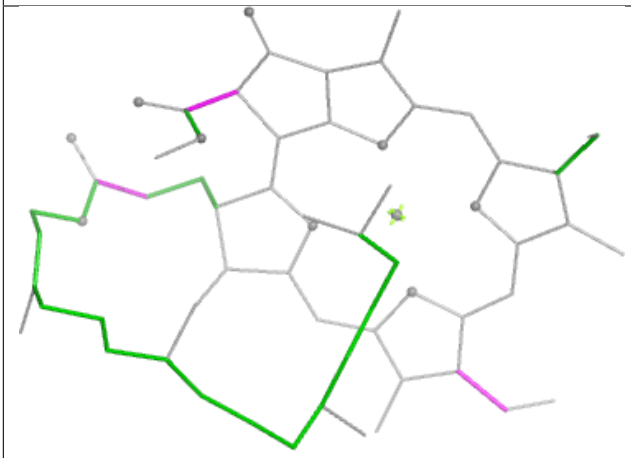
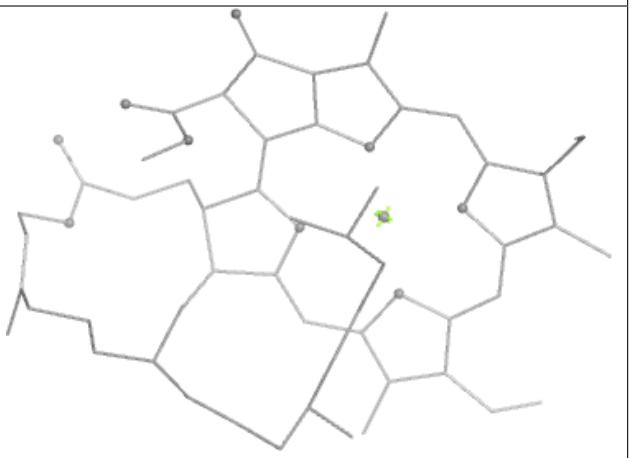
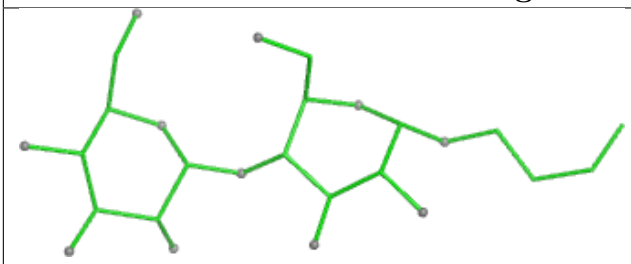
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand LMU 72 629



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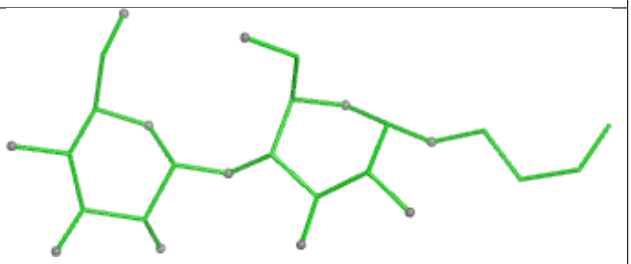
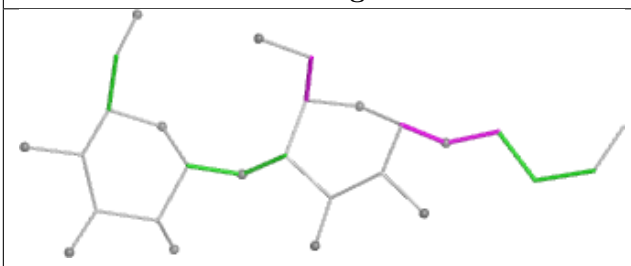


Bond angles



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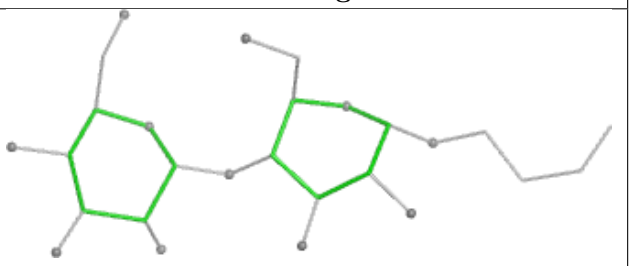
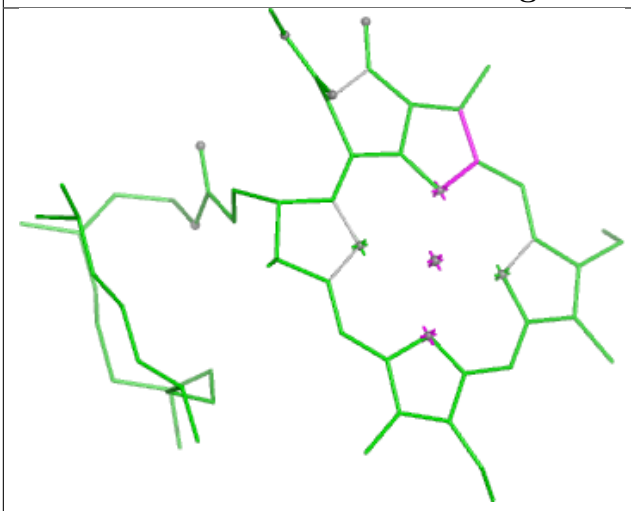


Rings

Ligand CLA 12 608



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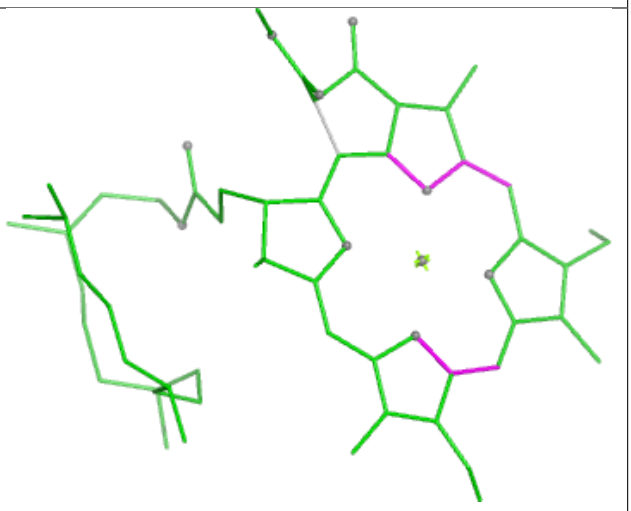

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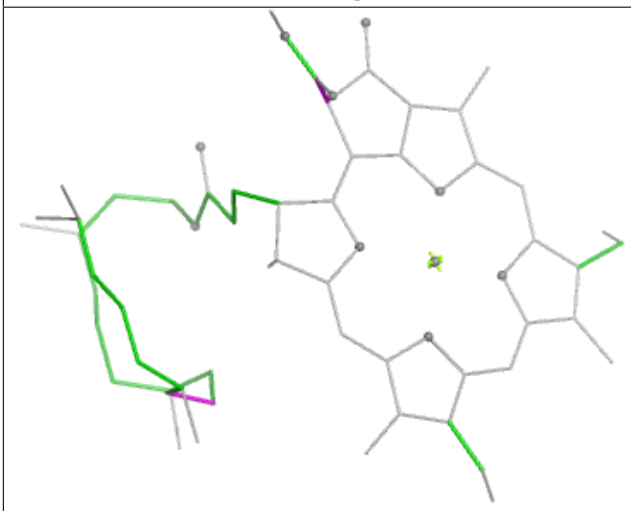

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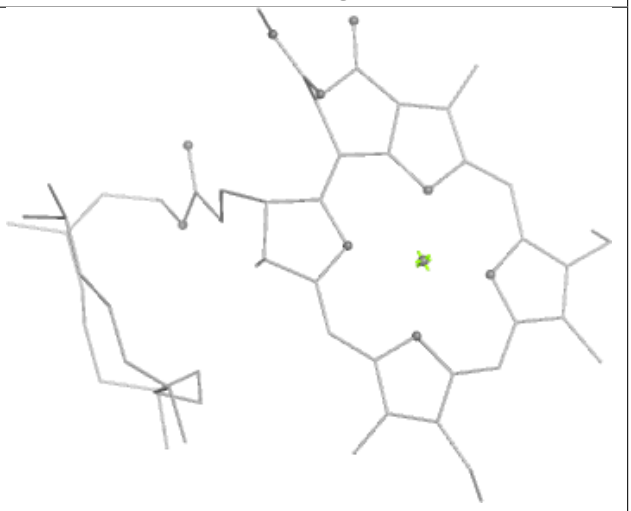
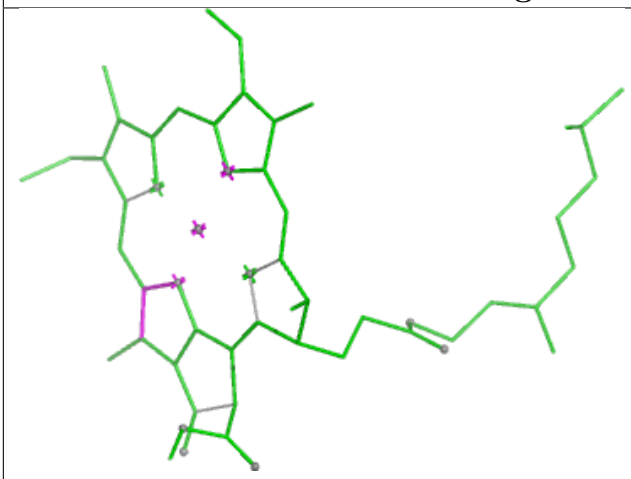


Rings

Ligand CLA A2 821



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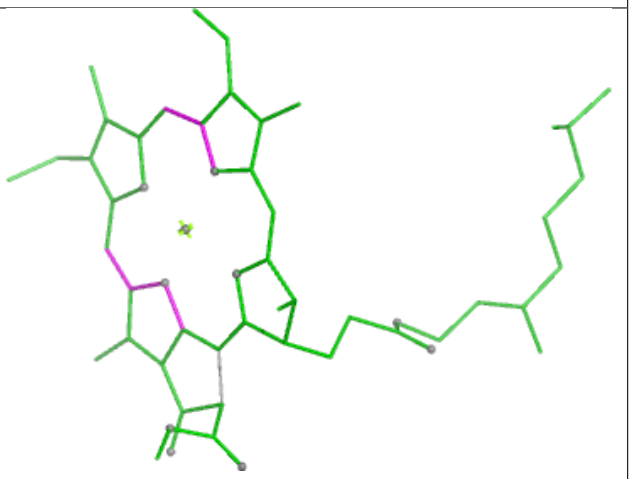
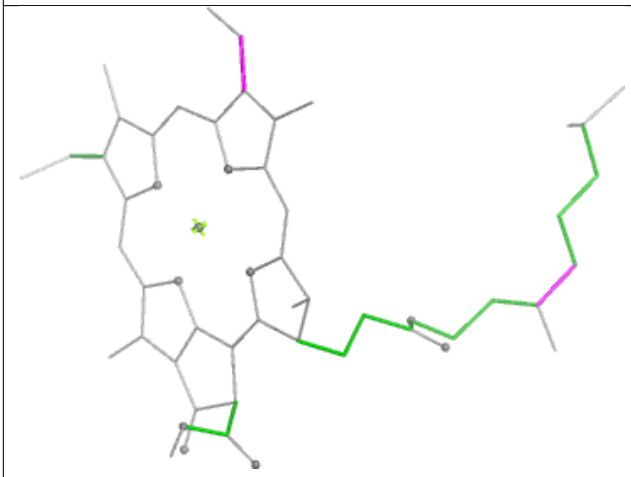


Bond angles



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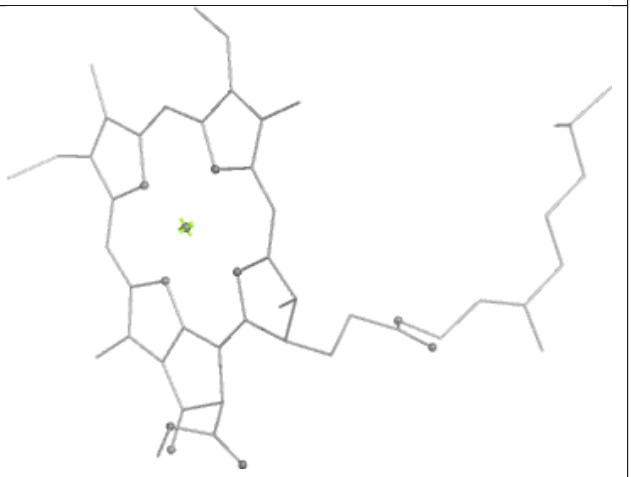
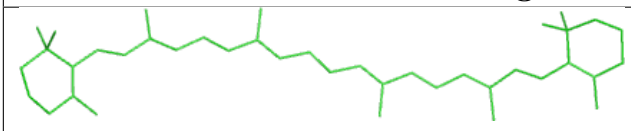


Rings

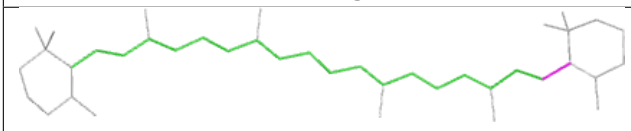
Ligand BCR L2 205



Bond lengths



Bond angles



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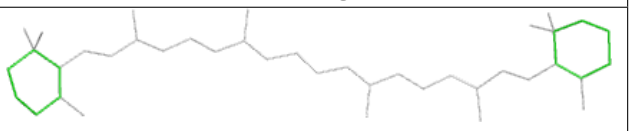
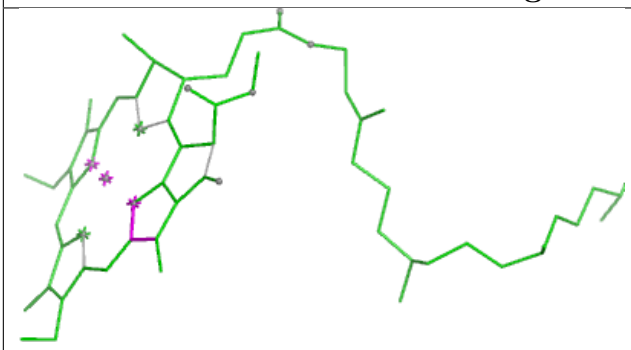


Rings

Ligand CLA B 802



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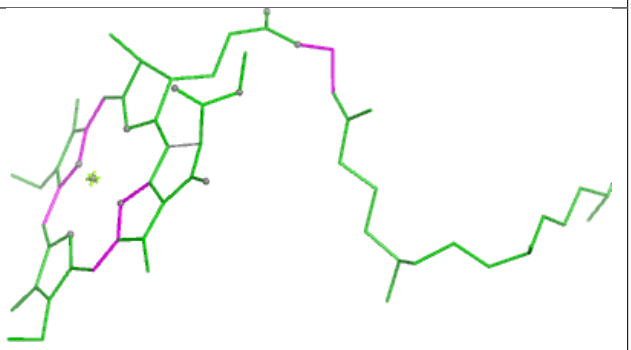
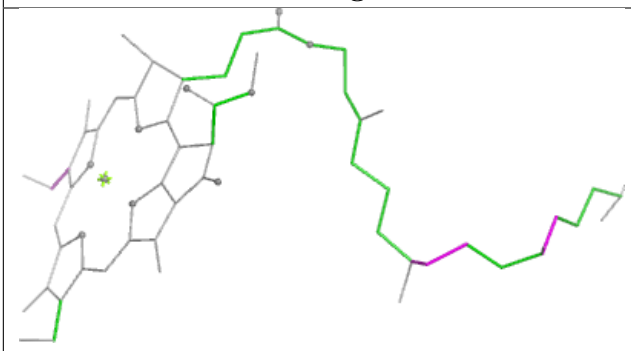


Bond angles



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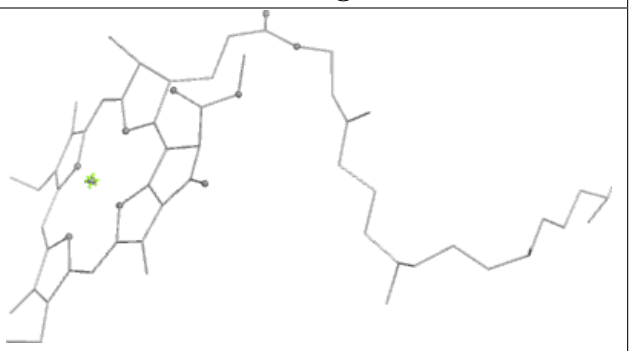
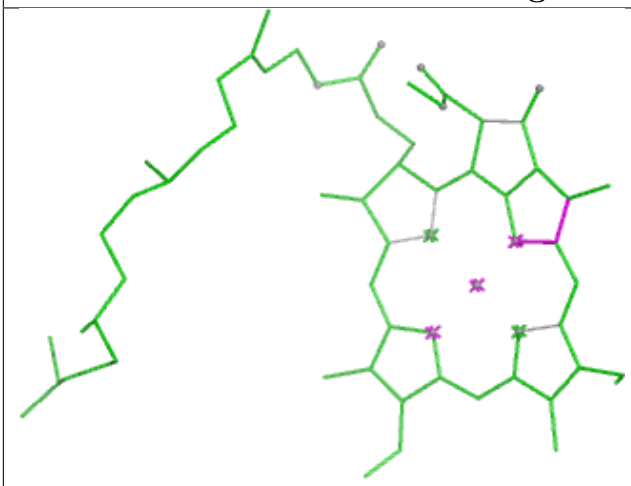


Rings

Ligand CLA 6 603



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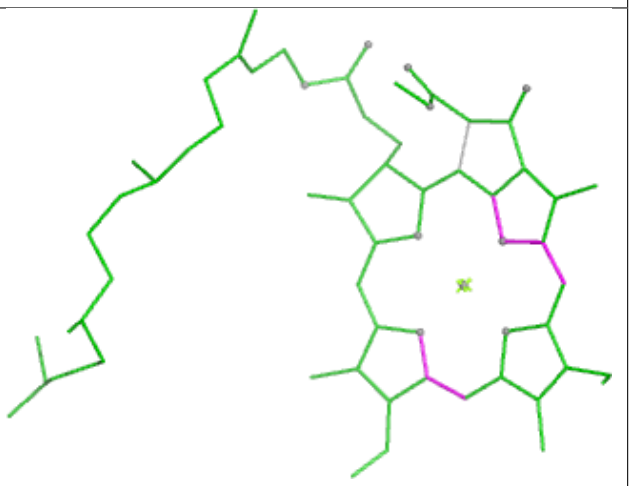
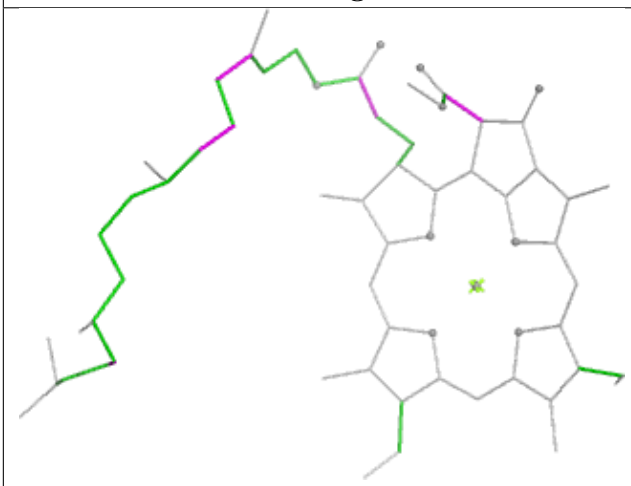


Bond angles



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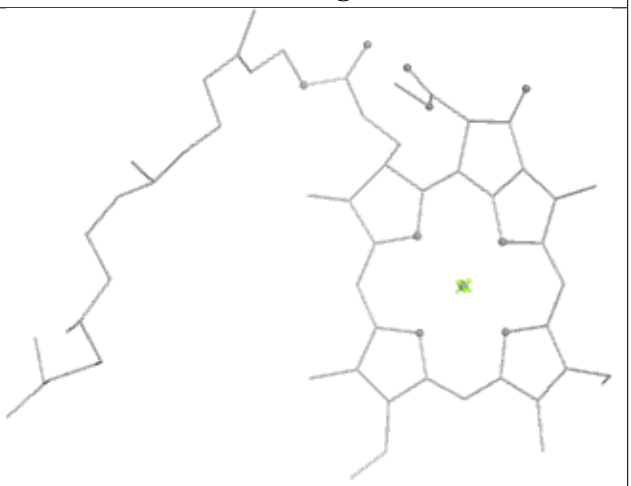
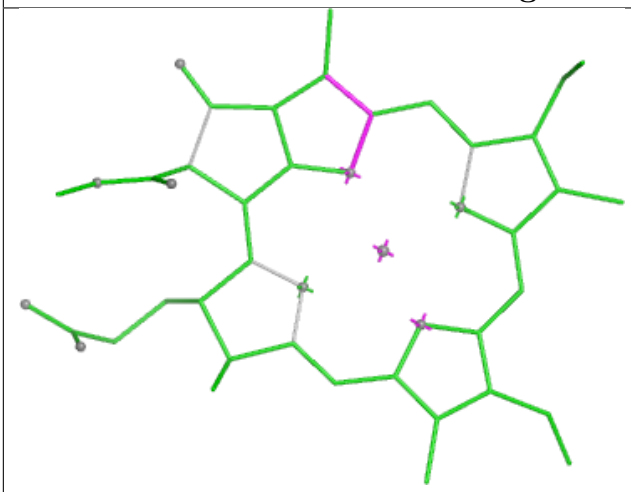
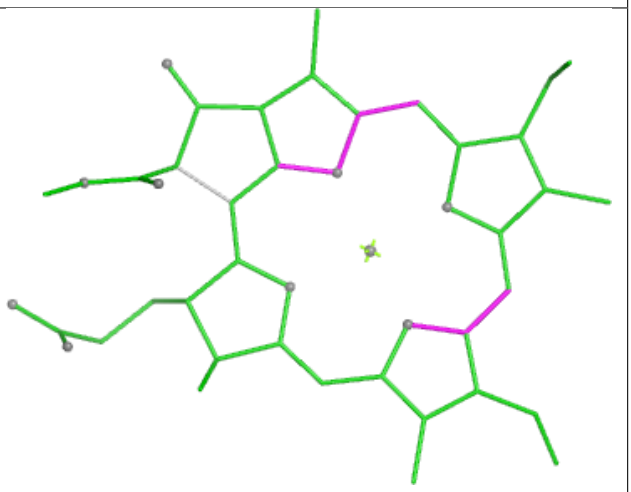


Rings

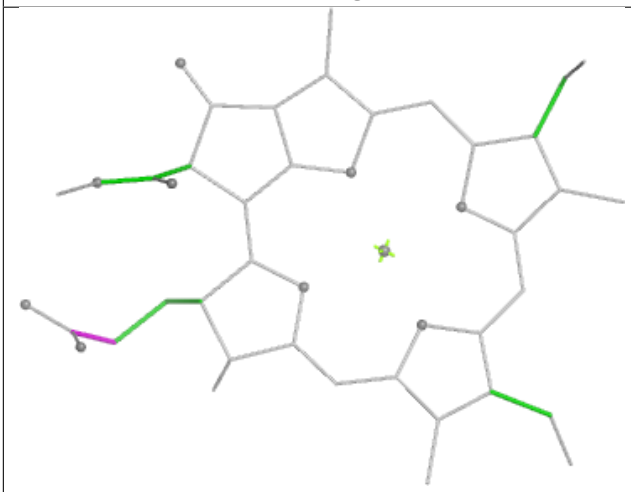
Ligand CLA 62 612



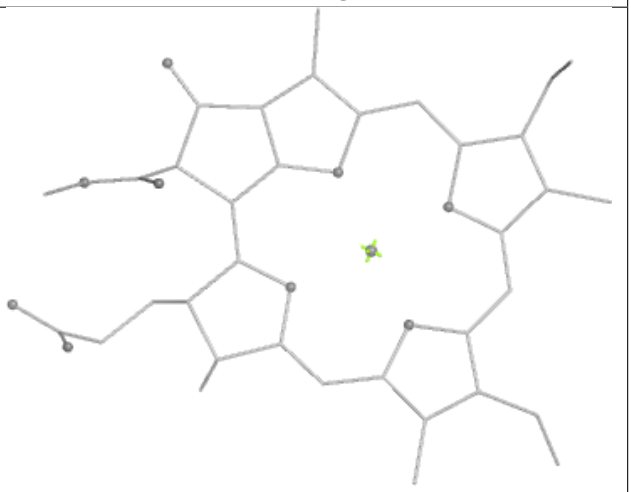
Bond lengths



Bond angles

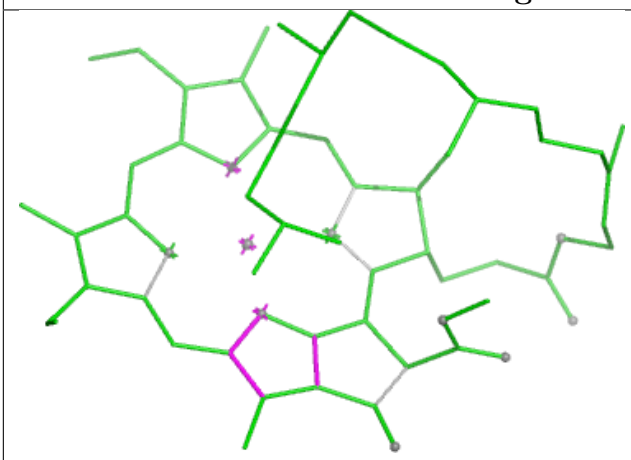


Torsions

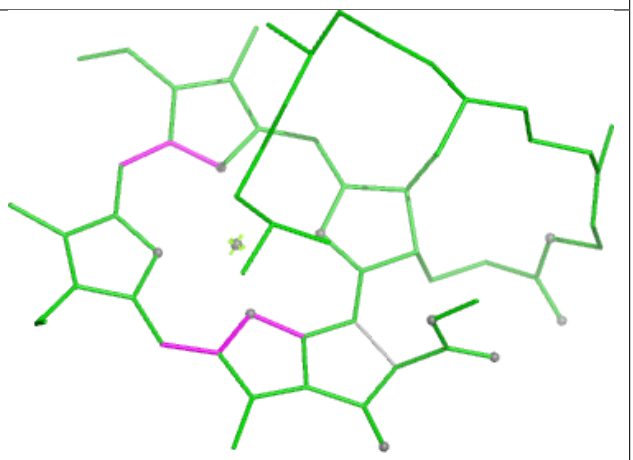


Rings

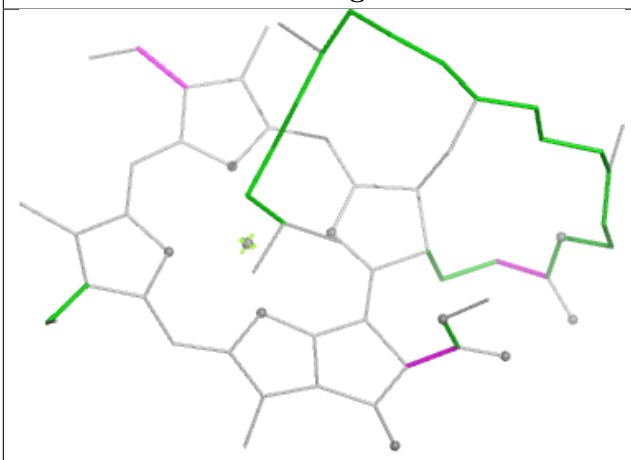
Ligand CLA A2 807



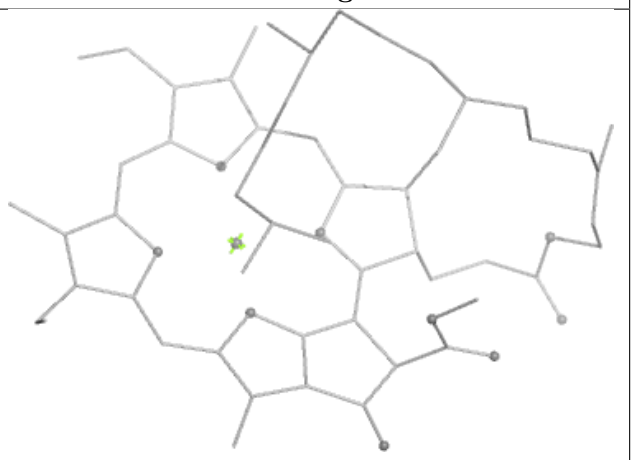
Bond lengths



Bond angles

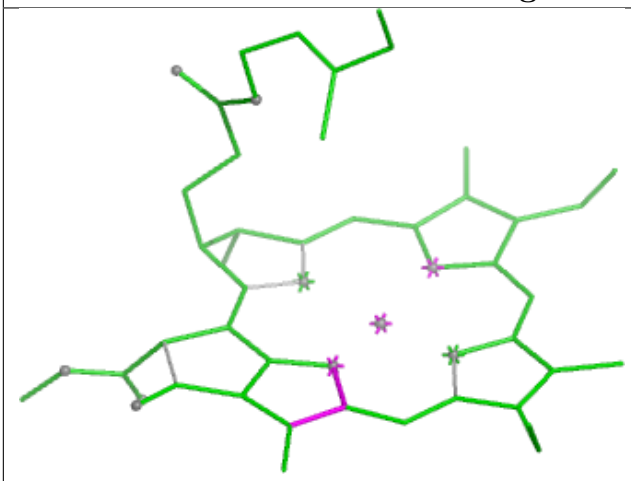


Torsions

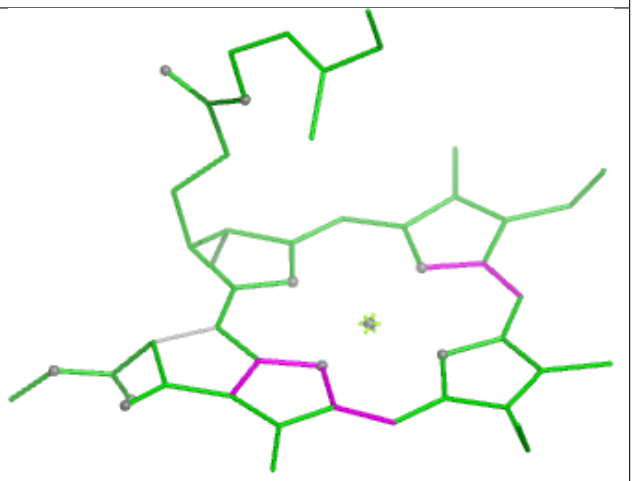


Rings

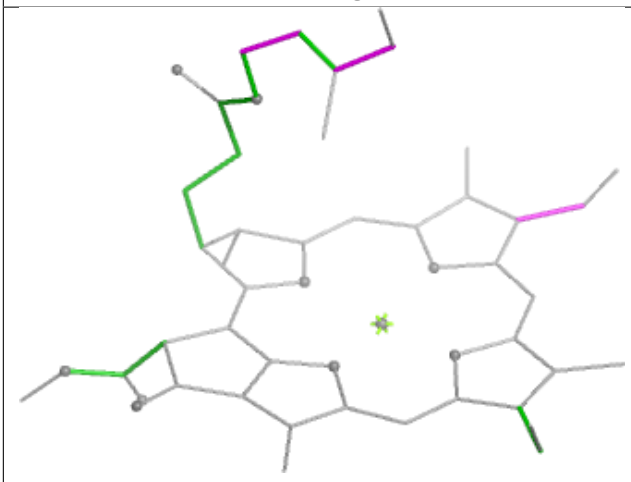
Ligand CLA 92 609



Bond lengths



Bond angles

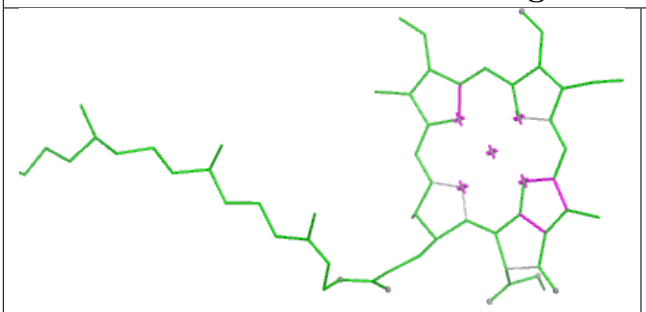


Torsions

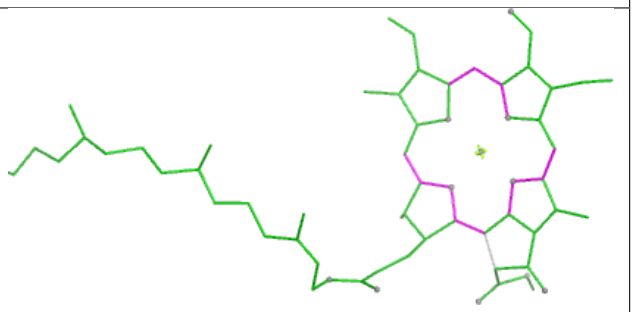


Rings

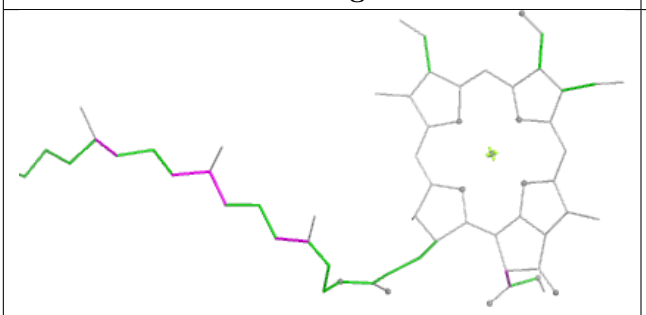
Ligand CHL 1 601



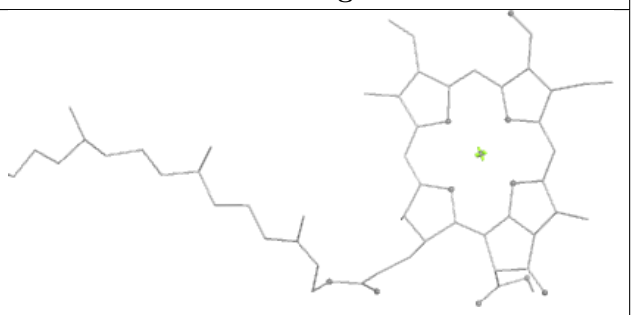
Bond lengths



Bond angles

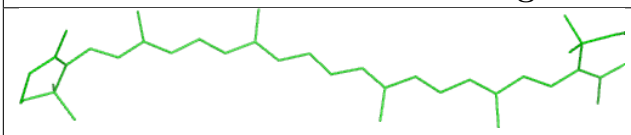


Torsions

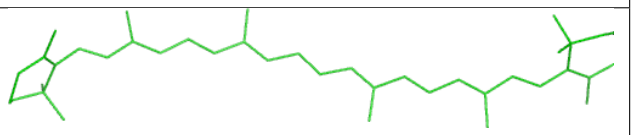


Rings

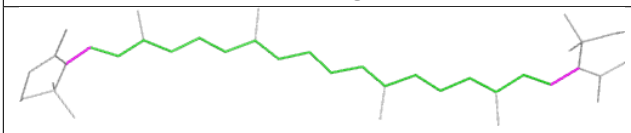
Ligand BCR 82 619



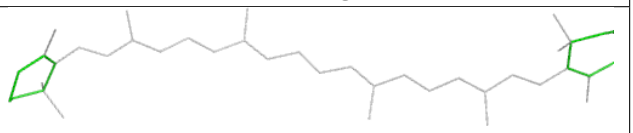
Bond lengths



Bond angles



Torsions

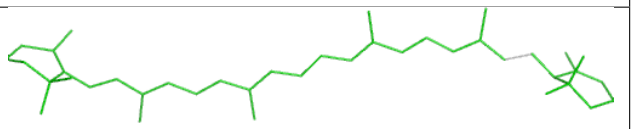


Rings

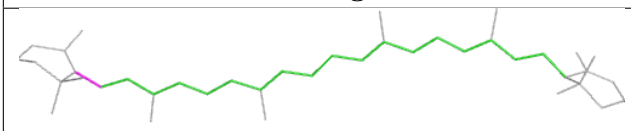
Ligand LUT 3 622



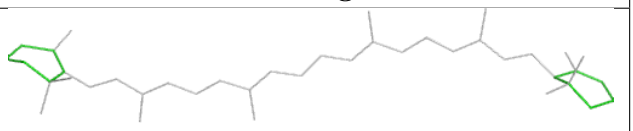
Bond lengths



Bond angles

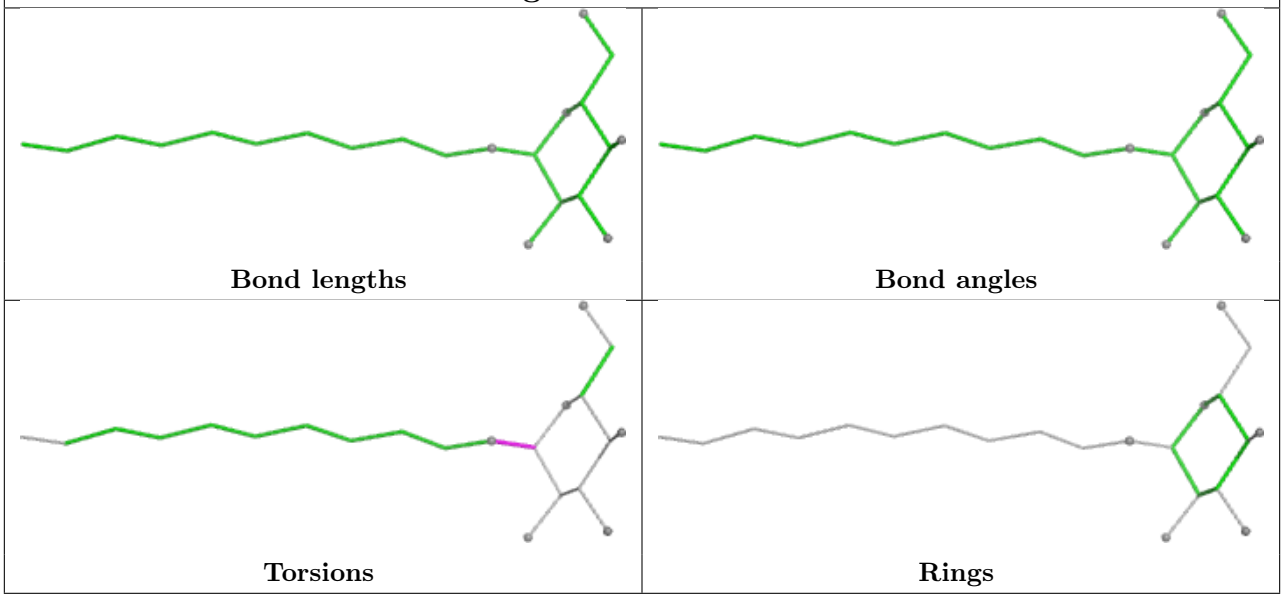


Torsions



Rings

Ligand LMU Z 621



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

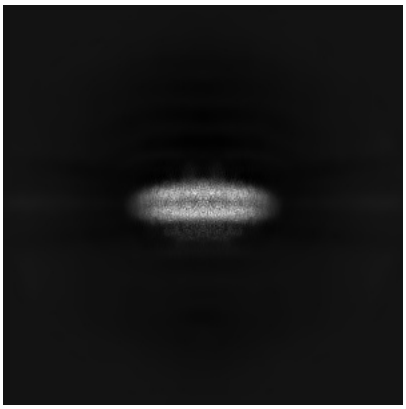
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-14871. These allow visual inspection of the internal detail of the map and identification of artifacts.

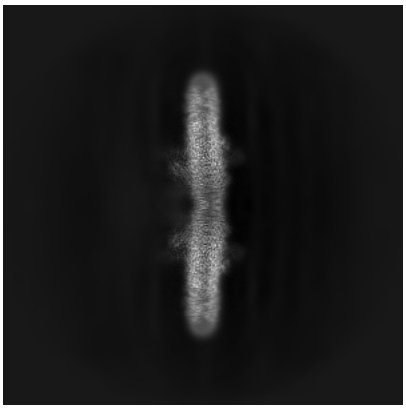
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

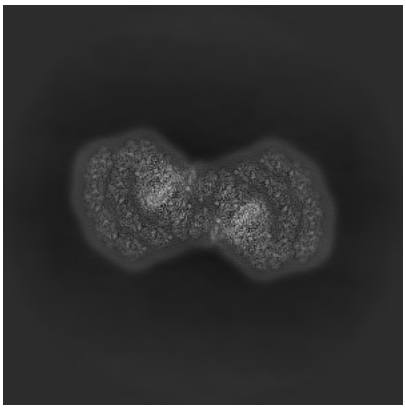
6.1.1 Primary map



X

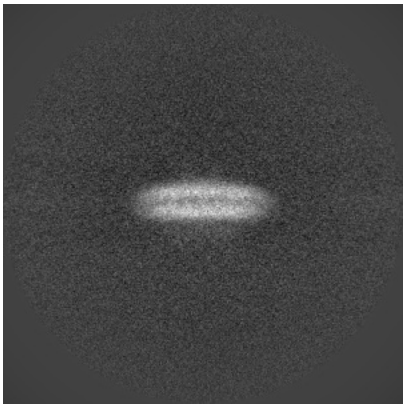


Y

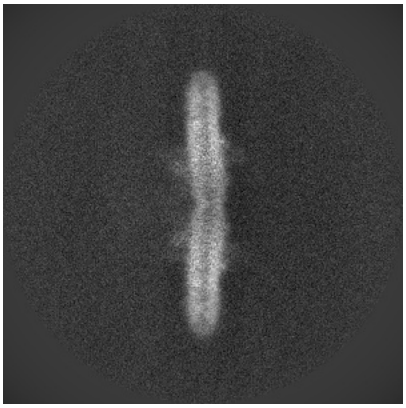


Z

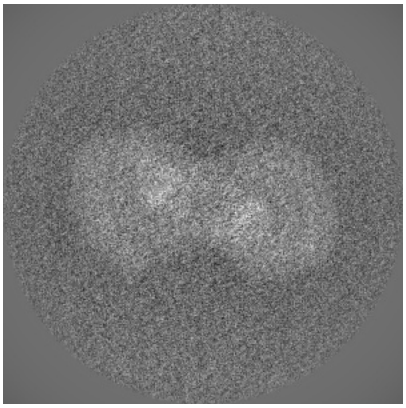
6.1.2 Raw map



X



Y

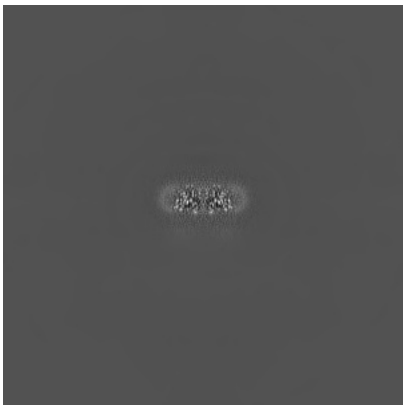


Z

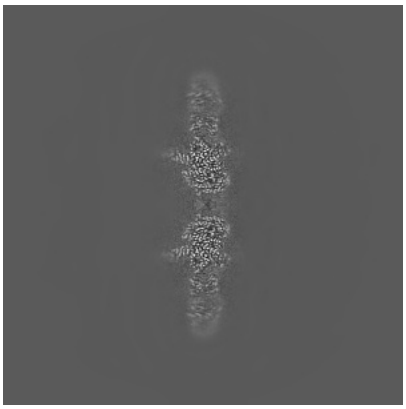
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

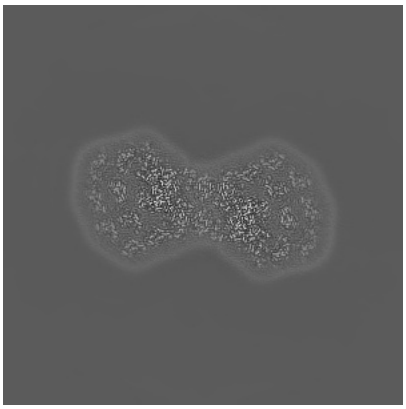
6.2.1 Primary map



X Index: 350

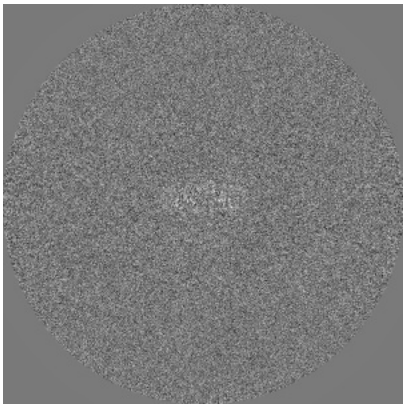


Y Index: 350

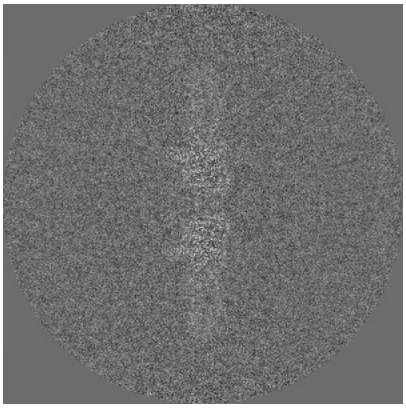


Z Index: 350

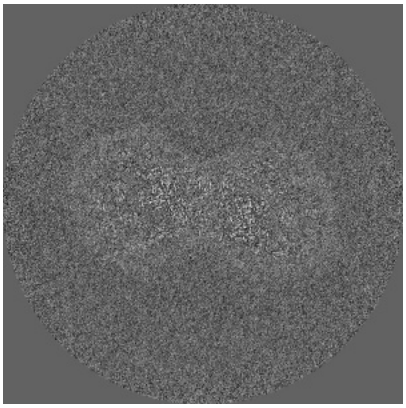
6.2.2 Raw map



X Index: 350



Y Index: 350

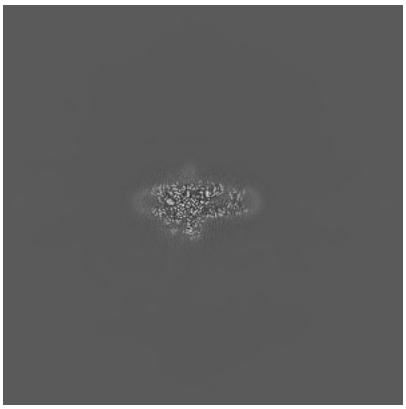


Z Index: 350

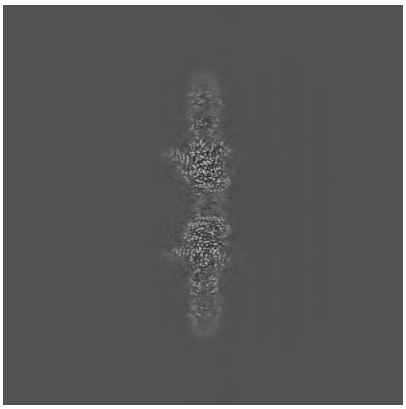
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

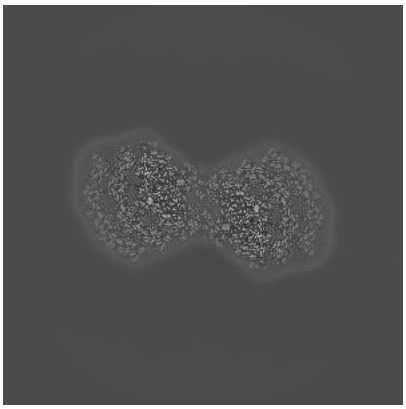
6.3.1 Primary map



X Index: 422

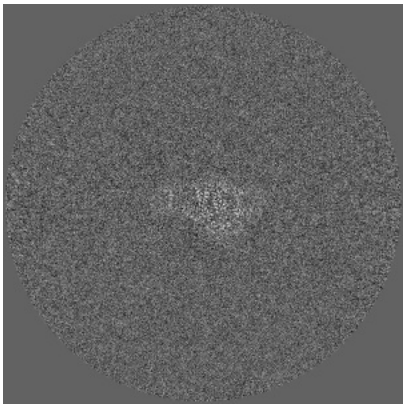


Y Index: 349

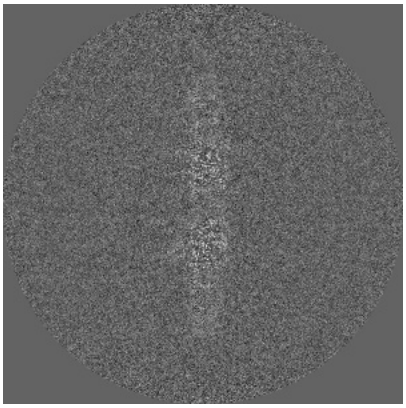


Z Index: 340

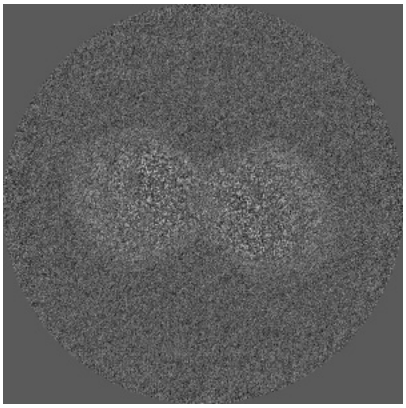
6.3.2 Raw map



X Index: 292



Y Index: 355

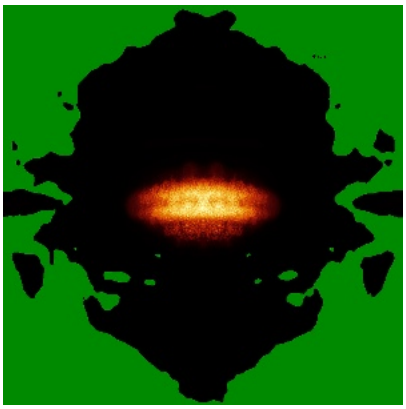


Z Index: 339

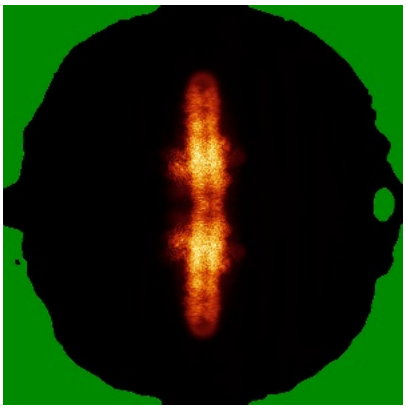
The images above show the largest variance slices of the map in three orthogonal directions.

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

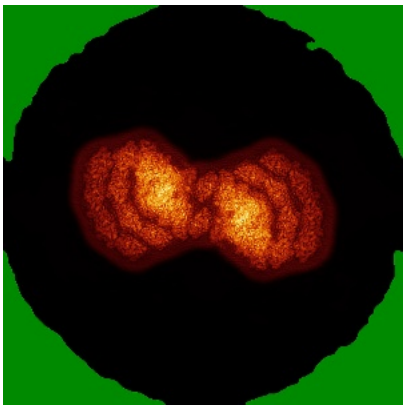
6.4.1 Primary map



X

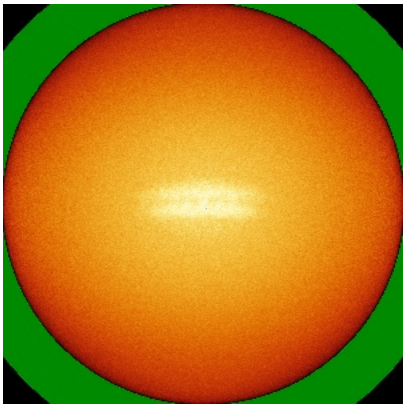


Y

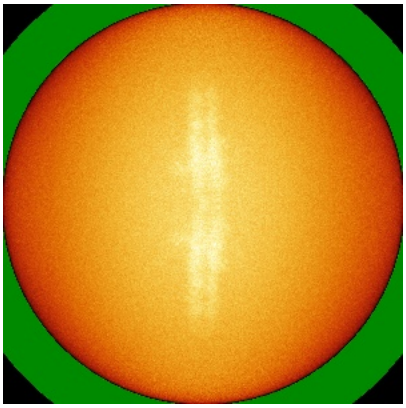


Z

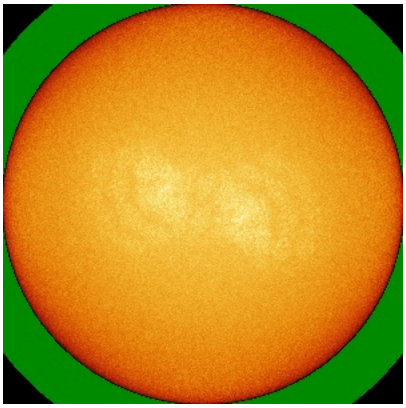
6.4.2 Raw map



X



Y

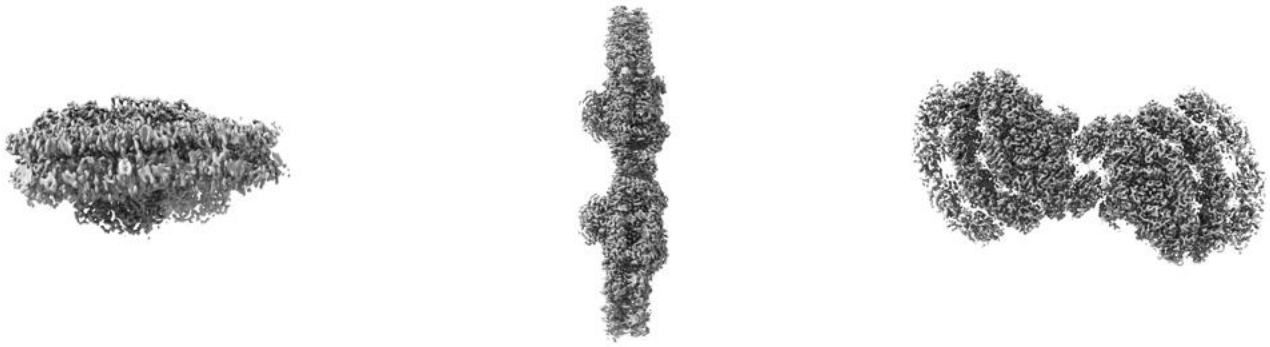


Z

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 0.036. 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.

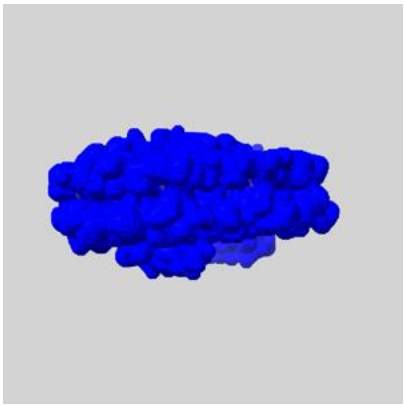
6.6 Mask visualisation (i)

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

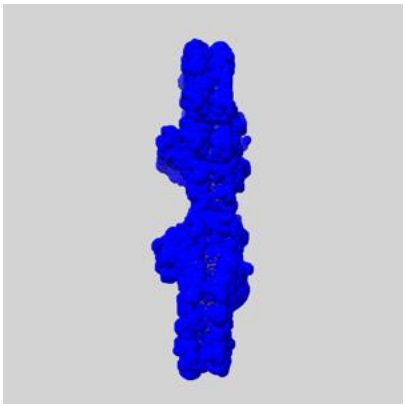
A mask typically either:

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

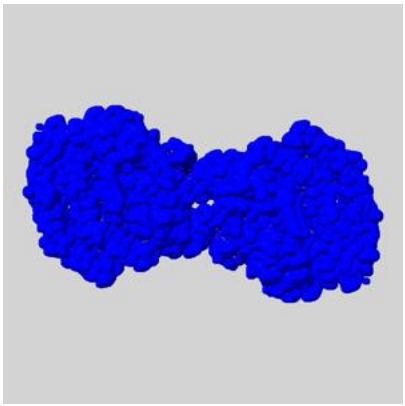
6.6.1 emd_14871_msk_1.map (i)



X



Y

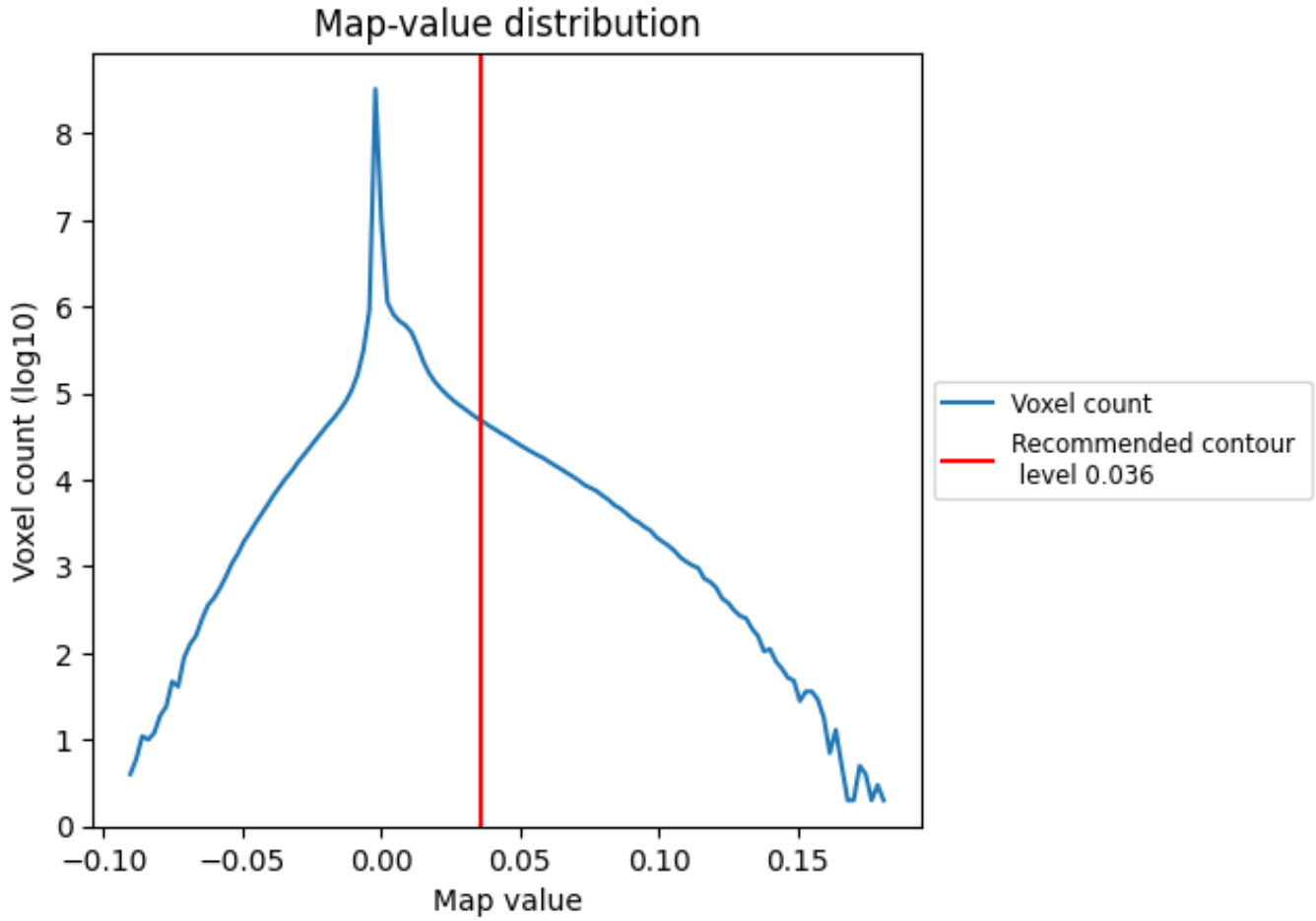


Z

7 Map analysis

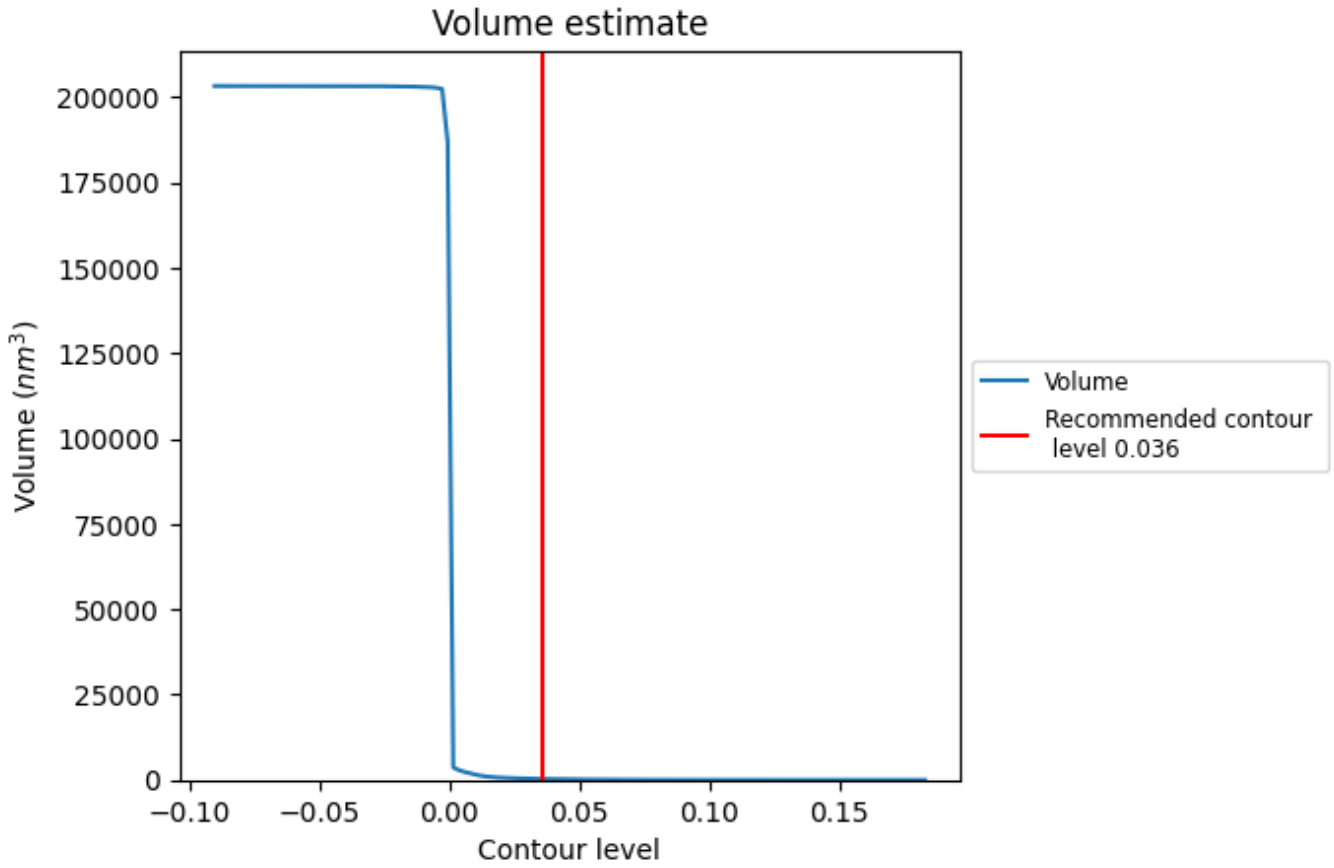
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

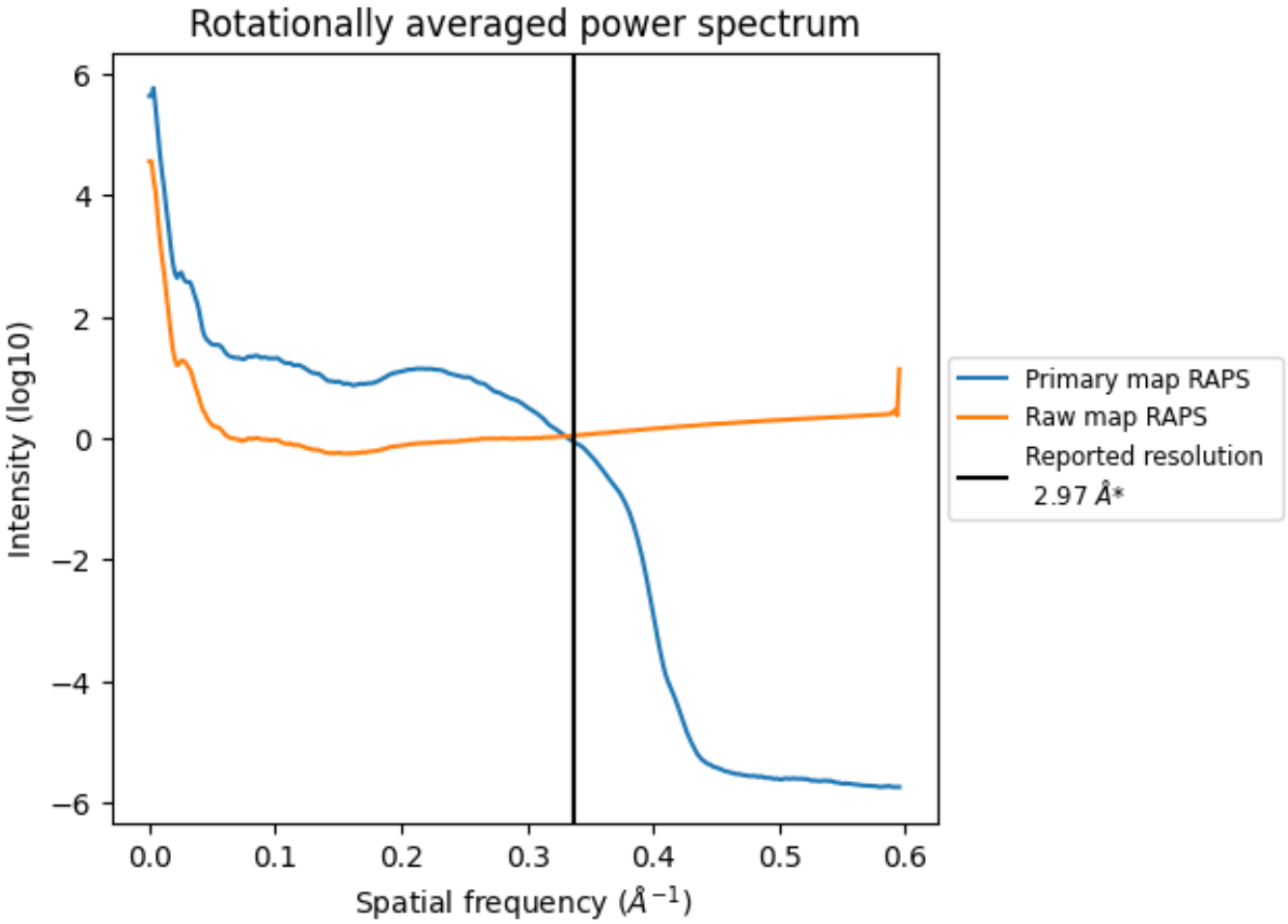
7.2 Volume estimate



The volume at the recommended contour level is 297 nm^3; this corresponds to an approximate mass of 268 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)

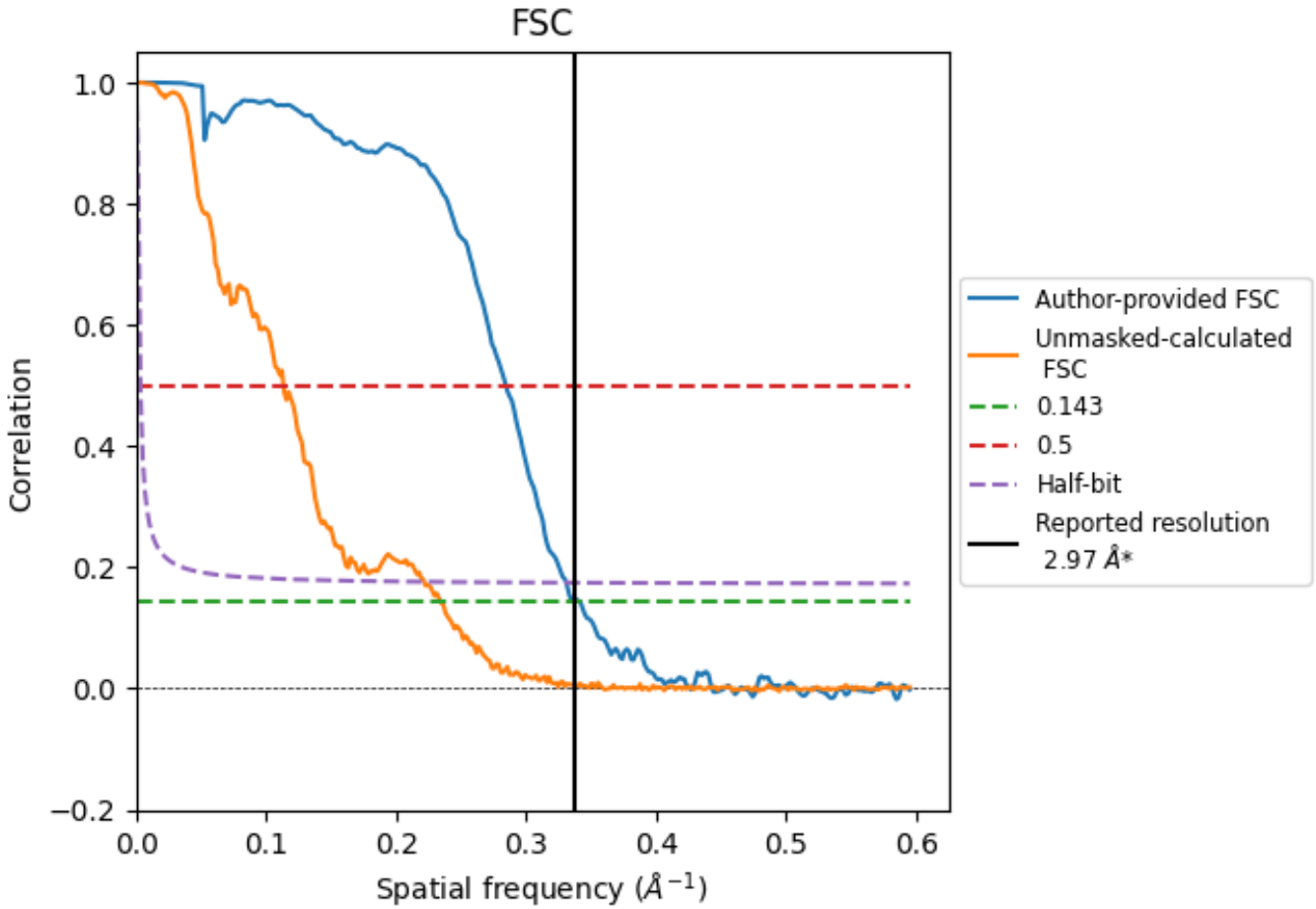


*Reported resolution corresponds to spatial frequency of 0.337 Å^{-1}

8 Fourier-Shell correlation

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

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.337 Å^{-1}

8.2 Resolution estimates (i)

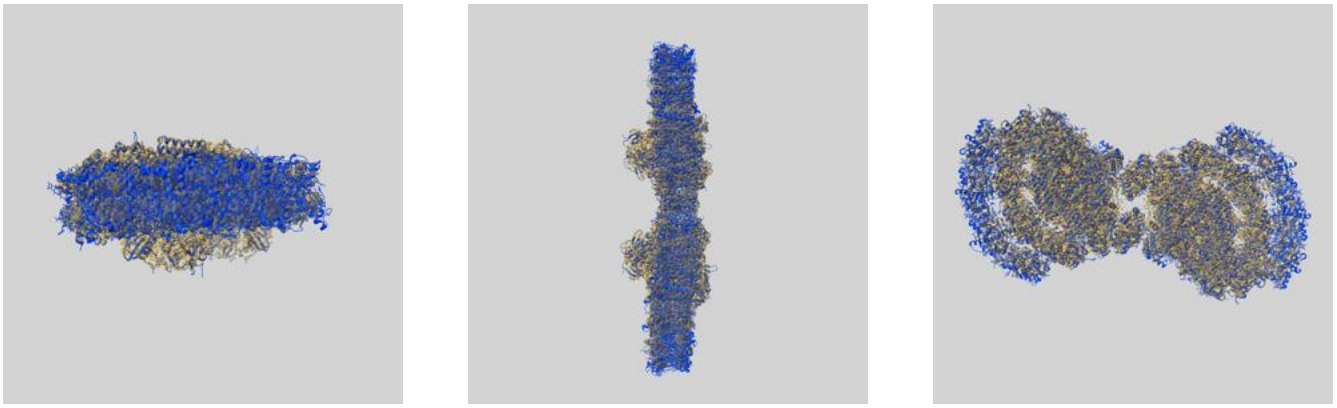
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.97	-	-
Author-provided FSC curve	2.92	3.51	3.02
Unmasked-calculated*	4.27	8.82	4.51

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.27 differs from the reported value 2.97 by more than 10 %

9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-14871 and PDB model 7ZQD. Per-residue inclusion information can be found in section 3 on page 51.

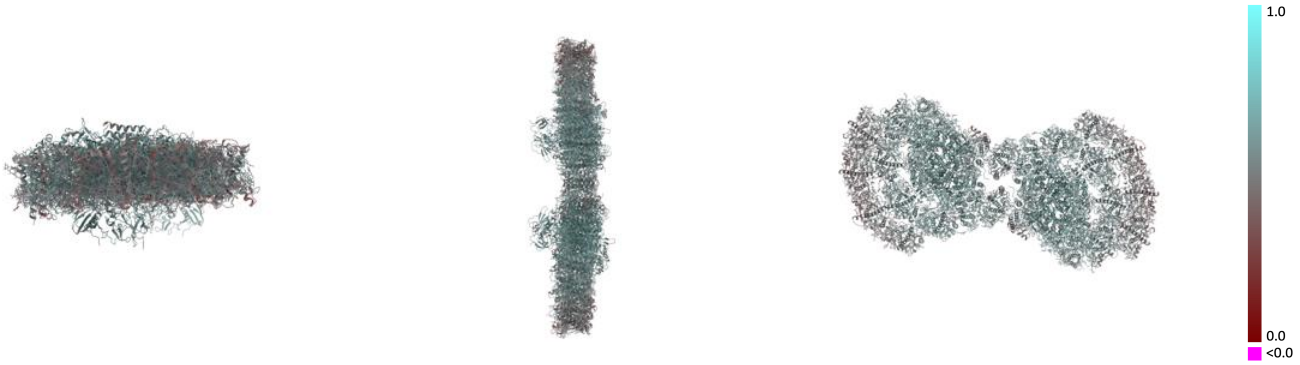
9.1 Map-model overlay



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.036 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

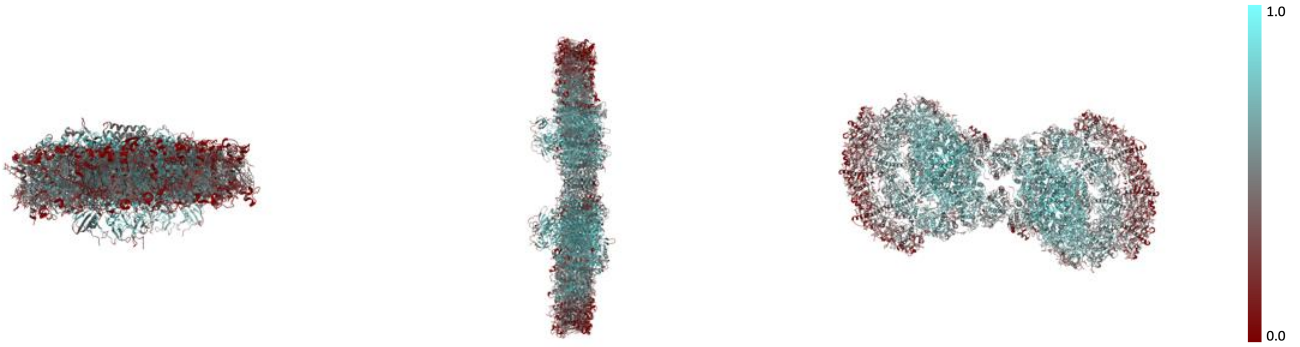
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

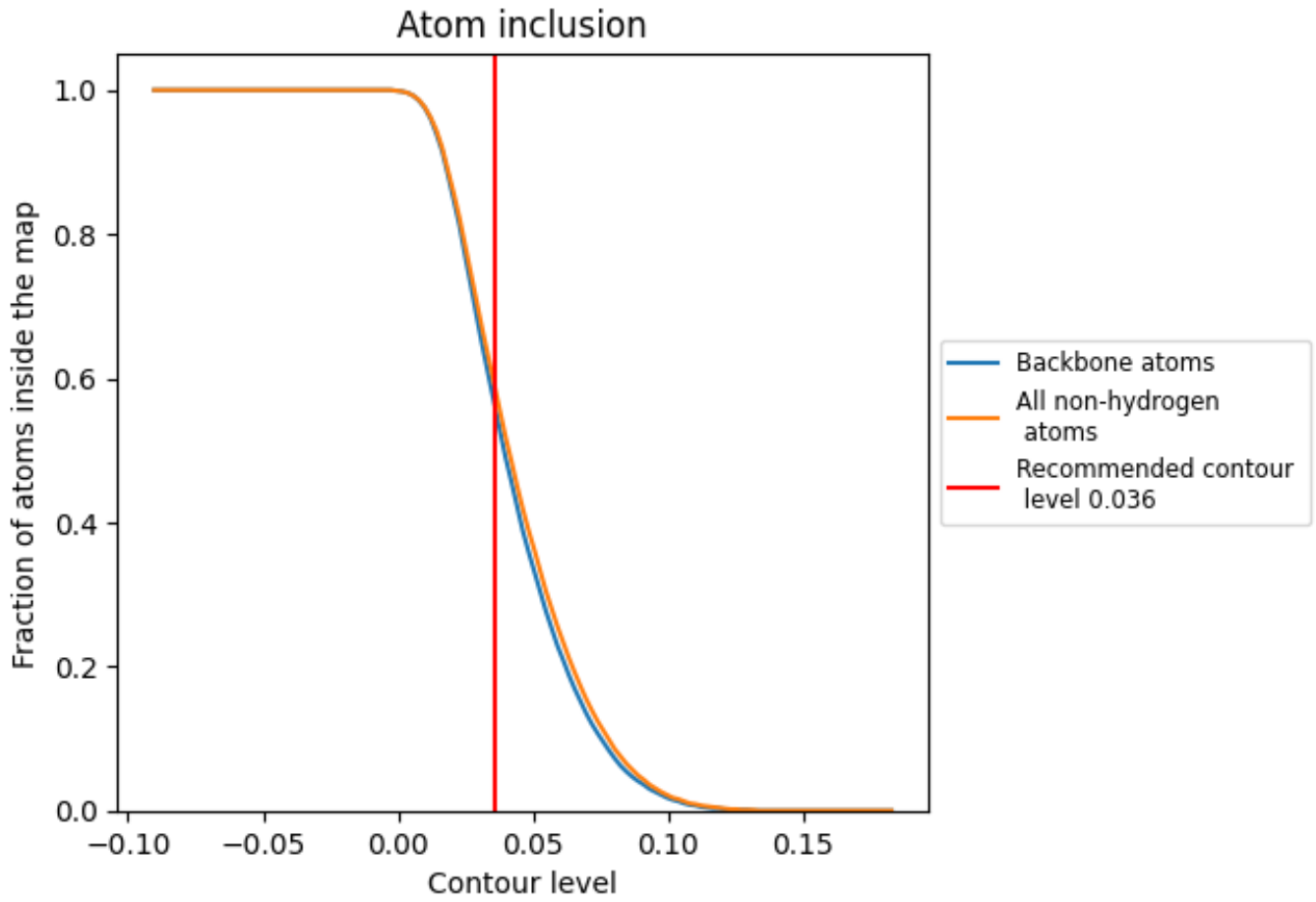
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.036).

9.4 Atom inclusion (i)



At the recommended contour level, 56% of all backbone atoms, 59% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.036) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5860	0.5590
1	0.5840	0.5670
12	0.5940	0.5700
3	0.5550	0.5510
32	0.5540	0.5520
4	0.2170	0.4530
42	0.2180	0.4540
5	0.2790	0.4730
52	0.2720	0.4740
6	0.1970	0.4450
62	0.2040	0.4470
7	0.5830	0.5540
72	0.5770	0.5510
8	0.6230	0.5710
82	0.6220	0.5700
9	0.5400	0.5400
92	0.5430	0.5420
A	0.7970	0.6210
A2	0.7980	0.6200
B	0.8060	0.6190
B2	0.8070	0.6190
C	0.7500	0.6000
C2	0.7510	0.5950
D	0.5600	0.5630
D2	0.5610	0.5590
E	0.6130	0.5730
E2	0.6050	0.5720
F	0.6940	0.5900
F2	0.6890	0.5870
G	0.5060	0.5480
G2	0.5050	0.5490
I	0.5740	0.5470
I2	0.5740	0.5440
J	0.7280	0.5920
J2	0.7340	0.5950



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Chain	Atom inclusion	Q-score
K	0.3470	0.5380
K2	0.3190	0.5390
L	0.3930	0.5010
L2	0.3890	0.5010
Z	0.3190	0.4950
Z2	0.3190	0.4960