wwPDB EM Validation Summary Report

Sep 29, 2026 – 06:15 PM JST

PDB ID	:	8JW0 / pdb_00008jw0
EMDB ID	:	EMD-36678
Title	:	PSI-AcpPCI supercomplex from Amphidinium carterae
Authors	:	Li, Z.H.; Li, X.Y.; Wang, W.D.
Deposited on	:	2023-06-28
Resolution	:	2.90 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 ⓘ 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 ⓘ) were used in the production of this report:

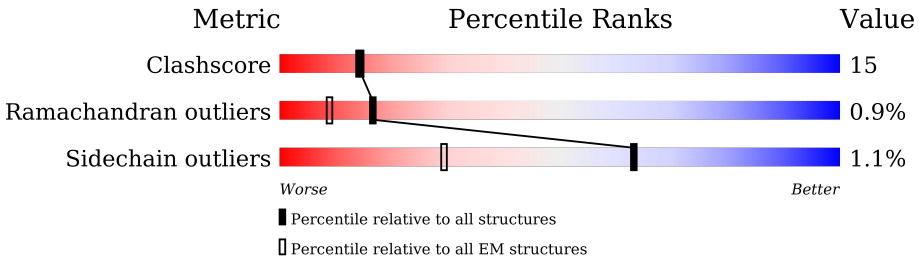
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.2
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.51

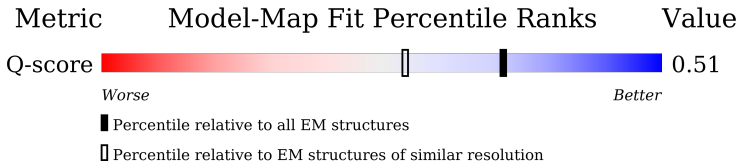
1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.90 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	13054 (2.40 - 3.40)

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	645	5% 74% 26%
2	b	617	70% 30%
3	c	86	76% 23%
4	d	257	75% 25%

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Mol	Chain	Length	Quality of chain
5	e	74	81% 19%
6	f	185	71% 29%
7	h	132	80% 15% 5%
8	i	126	70% 29%
9	j	70	69% 31%
10	l	253	69% 31%
11	m	89	74% 26%
12	A	180	73% 27%
13	G	215	73% 26%
14	I	194	69% 29%
15	K	172	66% 34%
16	F	176	61% 38%
17	J	165	67% 33%
18	M	168	5% 67% 32%
19	L	185	68% 31%
20	D	160	9% 62% 36%
21	B	172	69% 29%
22	H	160	52% 59% 39%
23	N	160	39% 59% 38%
24	O	161	14% 61% 39%
25	C	160	72% 28%
25	T	160	18% 69% 28%
26	Q	162	69% 29%
27	P	160	73% 64% 34%
28	E	142	68% 30%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
33	SF4	a	836	-	-	X	-
33	SF4	c	102	-	-	X	-

2 Entry composition (i)

There are 40 unique types of molecules in this entry. The entry contains 63119 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Photosystem I PsaA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	a	645	Total	C	N	O	S	0	0
			4980	3267	825	874	14		

- Molecule 2 is a protein called Photosystem I PsaB.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	b	617	Total	C	N	O	S	0	0
			4813	3185	765	848	15		

- Molecule 3 is a protein called Photosystem I PsaC.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	c	86	Total	C	N	O	S	0	0
			647	401	109	128	9		

- Molecule 4 is a protein called Photosystem I PsaD.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	d	257	Total	C	N	O	S	0	0
			1985	1259	340	375	11		

- Molecule 5 is a protein called Photosystem I PsaE.

Mol	Chain	Residues	Atoms				AltConf	Trace
5	e	74	Total	C	N	O	0	0
			607	392	102	113		

- Molecule 6 is a protein called Photosystem I PsaF.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	f	185	Total	C	N	O	S	0	0
			1455	926	257	263	9		

- Molecule 7 is a protein called Photosystem I PsaR.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	h	132	Total	C	N	O	S	0	0
			1056	693	167	191	5		

- Molecule 8 is a protein called Photosystem I PsaI.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	i	126	Total	C	N	O	S	0	0
			1001	651	164	183	3		

- Molecule 9 is a protein called Photosystem I PsaJ.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	j	70	Total	C	N	O	S	0	0
			549	362	86	100	1		

- Molecule 10 is a protein called Photosystem I PsaL.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	l	253	Total	C	N	O	S	0	0
			1961	1274	321	355	11		

- Molecule 11 is a protein called Photosystem I PsaM.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	m	89	Total	C	N	O	S	0	0
			679	438	109	131	1		

- Molecule 12 is a protein called Chlorophyll a-chlorophyll c-peridinin-protein-complex I-10, acpPCI-10.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	A	180	Total	C	N	O	S	0	0
			1358	882	221	245	10		

- Molecule 13 is a protein called Chlorophyll a-chlorophyll c-peridinin-protein-complex I-8, acpPCI-8.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	G	215	Total	C	N	O	S	0	0
			1675	1086	278	299	12		

- Molecule 14 is a protein called Chlorophyll a-chlorophyll c-peridinin-protein-complex I-7, acpPCI-7.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	I	194	Total	C	N	O	S	0	0
			1455	946	244	253	12		

- Molecule 15 is a protein called Chlorophyll a-chlorophyll c-peridinin-protein-complex I-6, acpPCI-6.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	K	172	Total	C	N	O	S	0	0
			1325	857	222	234	12		

- Molecule 16 is a protein called Chlorophyll a-chlorophyll c-peridinin-protein-complex I-2, acpPCI-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	F	176	Total	C	N	O	S	0	0
			1356	869	226	249	12		

- Molecule 17 is a protein called Chlorophyll a-chlorophyll c-peridinin-protein-complex I-3, acpPCI-3.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	J	165	Total	C	N	O	S	0	0
			1282	828	207	239	8		

- Molecule 18 is a protein called Chlorophyll a-chlorophyll c-peridinin-protein-complex I-4, acpPCI-4.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	M	168	Total	C	N	O	S	0	0
			1346	885	224	232	5		

- Molecule 19 is a protein called Chlorophyll a-chlorophyll c-peridinin-protein-complex I-5, acpPCI-5.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	L	185	Total	C	N	O	S	0	0
			1453	942	242	263	6		

- Molecule 20 is a protein called Chlorophyll a-chlorophyll c-peridinin-protein-complex I-9, acpPCI-9.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	D	160	Total	C	N	O	S	0	0
			1198	761	200	230	7		

- Molecule 21 is a protein called Chlorophyll a-chlorophyll c-peridinin-protein-complex I-11, acpPCI-11.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	B	172	Total	C	N	O	S	0	0
			1371	888	226	245	12		

- Molecule 22 is a protein called Chlorophyll a-chlorophyll c-peridinin-protein-complex I-12, acpPCI-12.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	H	160	Total	C	N	O	S	0	0
			1202	769	198	228	7		

- Molecule 23 is a protein called Chlorophyll a-chlorophyll c-peridinin-protein-complex I-13, acpPCI-13.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	N	160	Total	C	N	O	S	0	0
			1203	767	200	229	7		

- Molecule 24 is a protein called Chlorophyll a-chlorophyll c-peridinin-protein-complex I-15, acpPCI-15.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	O	161	Total	C	N	O	S	0	0
			1226	789	204	226	7		

- Molecule 25 is a protein called Chlorophyll a-chlorophyll c-peridinin-protein-complex I-16, acpPCI-16.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	T	159	Total	C	N	O	S	0	0
			1189	756	199	226	8		
25	C	160	Total	C	N	O	S	0	0
			1200	765	200	227	8		

- Molecule 26 is a protein called Chlorophyll a-chlorophyll c-peridinin-protein-complex I-17, acpPCI-17.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	Q	162	Total	C	N	O	S	0	0
			1219	787	204	219	9		

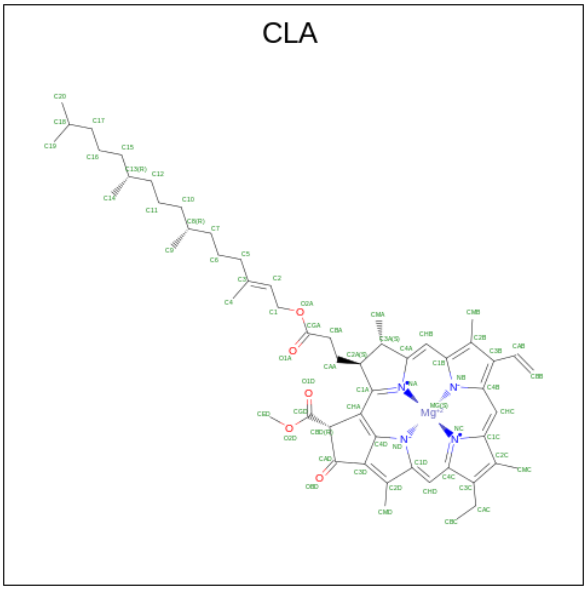
- Molecule 27 is a protein called Chlorophyll a-chlorophyll c-peridinin-protein-complex I-14, acpPCI-14.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	P	160	Total	C	N	O	S	0	0
			1218	778	204	228	8		

- Molecule 28 is a protein called Chlorophyll a-chlorophyll c-peridinin-protein-complex I-1, acpPCI-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	E	142	Total	C	N	O	S	0	0
			1071	684	178	201	8		

- Molecule 29 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
29	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
29	a	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
29	a	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
29	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	a	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
29	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	a	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
29	a	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
29	a	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
29	a	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
29	a	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
29	a	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
29	a	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
29	a	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
29	a	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
29	a	1	Total	C	Mg	N	O	0
			57	47	1	4	5	
29	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	a	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
29	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	a	1	Total	C	Mg	N	O	0
			58	48	1	4	5	
29	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
29	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	a	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
29	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	a	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
29	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	a	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
29	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	b	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
29	b	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
29	b	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
29	b	1	Total	C	Mg	N	O	0
			58	48	1	4	5	
29	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	b	1	Total	C	Mg	N	O	0
			53	43	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
29	b	1	Total	C	Mg	N	O	0
			64	54	1	4	5	
29	b	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
29	b	1	Total	C	Mg	N	O	0
			53	43	1	4	5	
29	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	b	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
29	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	b	1	Total	C	Mg	N	O	0
			58	48	1	4	5	
29	b	1	Total	C	Mg	N	O	0
			58	48	1	4	5	
29	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	b	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
29	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	b	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
29	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	f	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
29	f	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
29	f	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
29	h	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
29	i	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	i	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
29	i	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
29	j	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
29	l	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
29	l	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	l	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	l	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	l	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	l	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
29	l	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
29	l	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
29	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
29	A	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
29	A	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
29	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	A	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
29	A	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
29	A	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
29	A	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
29	A	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
29	A	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
29	A	1	Total	C	Mg	N	O	0
			51	41	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
29	A	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
29	G	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
29	G	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	G	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
29	G	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
29	G	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	G	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
29	G	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
29	G	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	G	1	Total	C	Mg	N	O	0
			53	43	1	4	5	
29	G	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
29	I	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
29	I	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
29	I	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
29	I	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
29	I	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
29	I	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	I	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
29	I	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	I	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
29	I	1	Total	C	Mg	N	O	0
			52	42	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
29	I	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
29	K	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
29	K	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
29	K	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
29	K	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
29	K	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
29	K	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
29	K	1	Total	C	Mg	N	O	0
			48	38	1	4	5	
29	K	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
29	K	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
29	K	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
29	K	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
29	F	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
29	F	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
29	F	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
29	F	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
29	F	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
29	F	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
29	F	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
29	J	1	Total	C	Mg	N	O	0
			46	36	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
29	J	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	J	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
29	J	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
29	J	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
29	J	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
29	J	1	Total	C	Mg	N	O	0
			53	43	1	4	5	
29	J	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
29	M	1	Total	C	Mg	N	O	0
			53	43	1	4	5	
29	M	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
29	M	1	Total	C	Mg	N	O	0
			48	38	1	4	5	
29	M	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
29	M	1	Total	C	Mg	N	O	0
			48	38	1	4	5	
29	M	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
29	M	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
29	M	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
29	M	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
29	L	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
29	L	1	Total	C	Mg	N	O	0
			53	43	1	4	5	
29	L	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
29	L	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
29	L	1	Total	C	Mg	N	O	0
			46	36	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
29	L	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
29	L	1	Total	C	Mg	N	O	0
			53	43	1	4	5	
29	L	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
29	L	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
29	L	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
29	D	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
29	D	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
29	D	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
29	D	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
29	D	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
29	D	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
29	D	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
29	B	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
29	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
29	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	B	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
29	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	B	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
29	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	B	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
29	B	1	Total	C	Mg	N	O	0
			46	36	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
29	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
29	H	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
29	H	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	H	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
29	H	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
29	H	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
29	H	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
29	N	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
29	N	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	N	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
29	N	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
29	N	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
29	N	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
29	O	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
29	O	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	O	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
29	O	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
29	O	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
29	O	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
29	T	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
29	T	1	Total	C	Mg	N	O	0
			46	36	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
29	T	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
29	T	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
29	T	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
29	T	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
29	Q	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
29	Q	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	Q	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	Q	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
29	Q	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
29	Q	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
29	C	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
29	C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	C	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
29	C	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
29	C	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
29	C	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
29	P	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
29	P	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	P	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
29	P	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
29	P	1	Total	C	Mg	N	O	0
			47	37	1	4	5	

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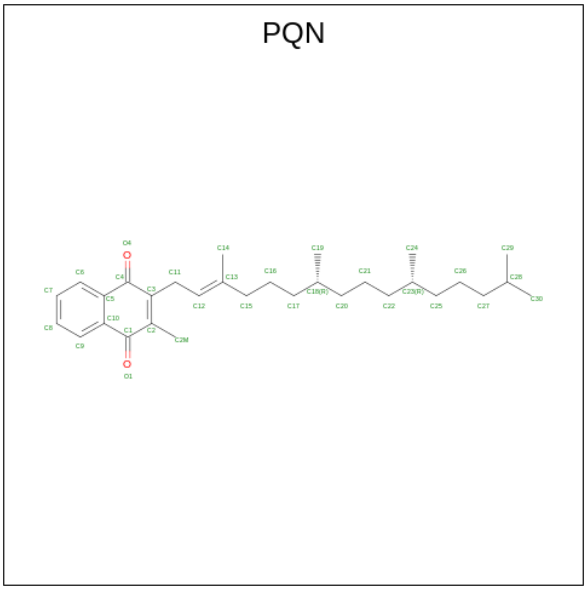
Mol	Chain	Residues	Atoms					AltConf
29	P	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
29	E	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
29	E	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	E	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	E	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
29	E	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
29	E	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	E	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
29	E	1	Total	C	Mg	N	O	0
			48	38	1	4	5	
29	E	1	Total	C	Mg	N	O	0
			57	47	1	4	5	

- Molecule 30 is PHYLLOQUINONE (CCD ID: PQN) (formula: $C_{31}H_{46}O_2$).



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

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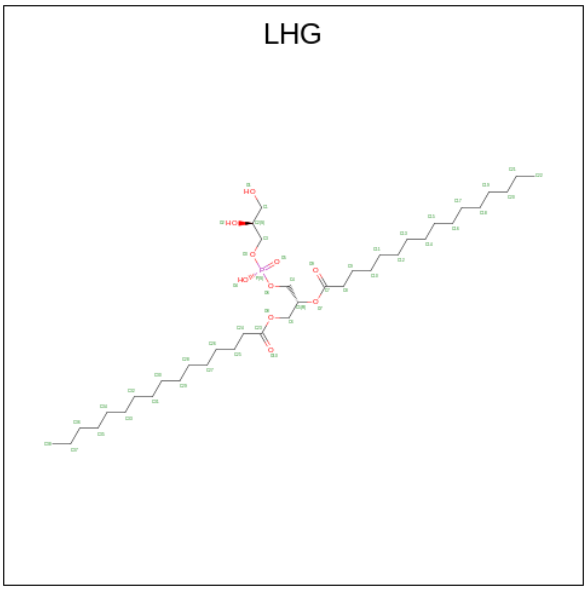
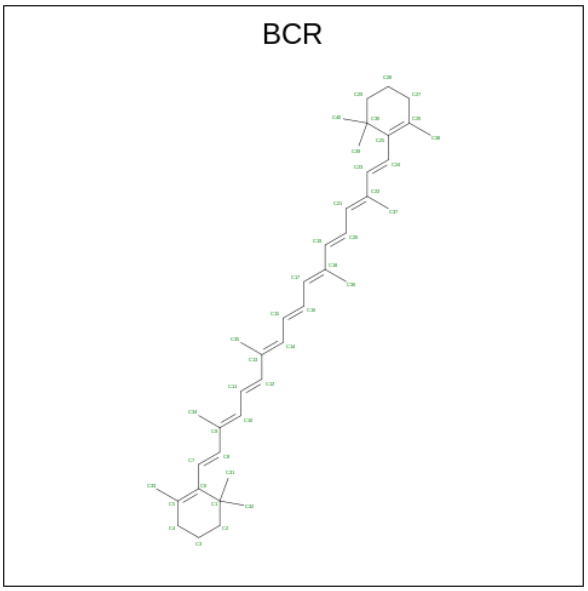
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
30	b	1	33	31	2	0

- Molecule 31 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: $C_{38}H_{75}O_{10}P$) (labeled as "Ligand of Interest" by depositor).



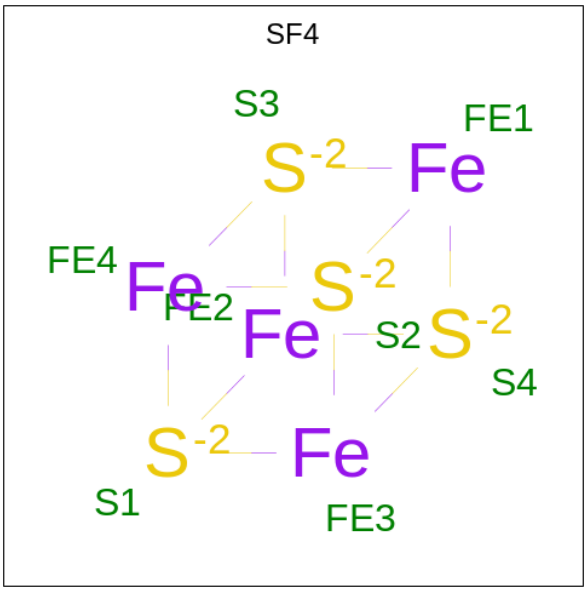
Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
31	a	1	48	37	10	1	0

- Molecule 32 is BETA-CAROTENE (CCD ID: BCR) (formula: $C_{40}H_{56}$) (labeled as "Ligand of Interest" by depositor).



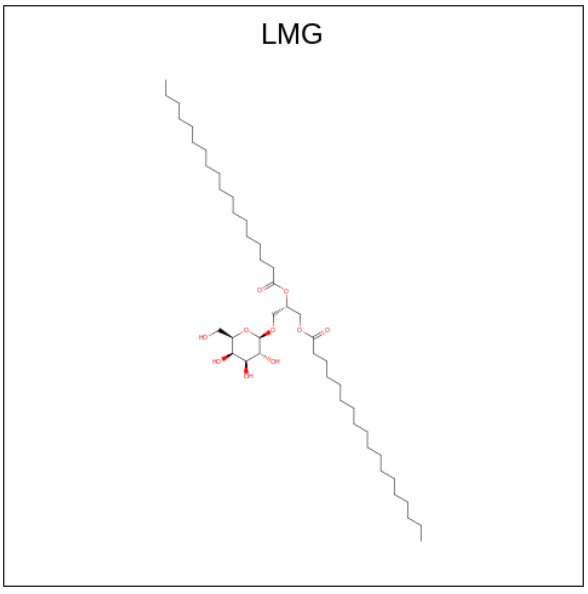
Mol	Chain	Residues	Atoms	AltConf
32	a	1	Total C 40 40	0
32	a	1	Total C 40 40	0
32	a	1	Total C 40 40	0
32	b	1	Total C 40 40	0
32	b	1	Total C 40 40	0
32	b	1	Total C 40 40	0
32	f	1	Total C 40 40	0
32	f	1	Total C 40 40	0
32	i	1	Total C 40 40	0
32	l	1	Total C 40 40	0
32	l	1	Total C 40 40	0
32	m	1	Total C 40 40	0

- Molecule 33 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



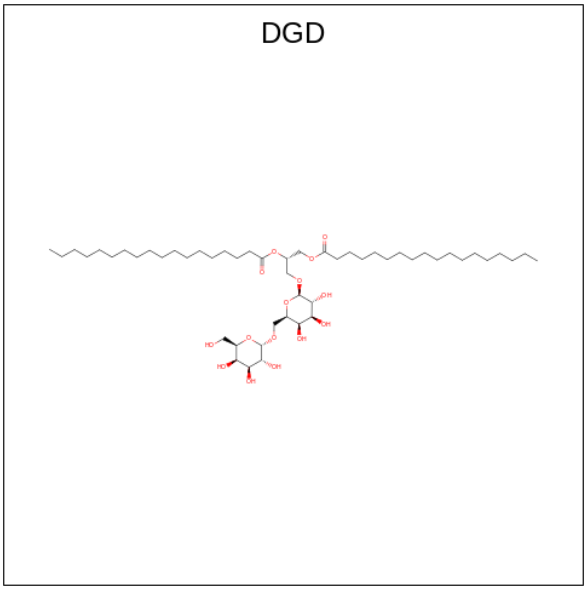
Mol	Chain	Residues	Atoms			AltConf
33	a	1	Total	Fe	S	0
			8	4	4	
33	c	1	Total	Fe	S	0
			8	4	4	
33	c	1	Total	Fe	S	0
			8	4	4	

- Molecule 34 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$) (labeled as "Ligand of Interest" by depositor).



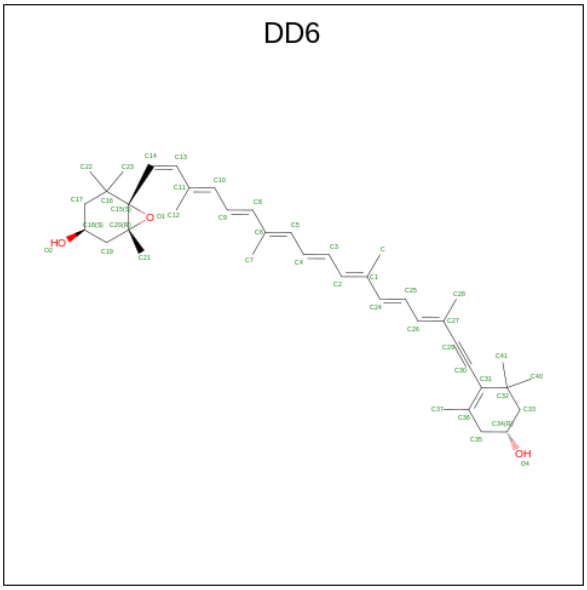
Mol	Chain	Residues	Atoms			AltConf
34	b	1	Total	C	O	0
			46	36	10	
34	b	1	Total	C	O	0
			44	34	10	
34	b	1	Total	C	O	0
			40	30	10	
34	h	1	Total	C	O	0
			28	18	10	
34	j	1	Total	C	O	0
			43	33	10	
34	A	1	Total	C	O	0
			37	27	10	
34	K	1	Total	C	O	0
			43	33	10	
34	K	1	Total	C	O	0
			35	25	10	
34	K	1	Total	C	O	0
			36	26	10	
34	P	1	Total	C	O	0
			27	17	10	
34	E	1	Total	C	O	0
			32	22	10	

- Molecule 35 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
35	b	1	Total C O 57 42 15	0
35	h	1	Total C O 54 39 15	0
35	j	1	Total C O 43 28 15	0
35	j	1	Total C O 41 26 15	0
35	j	1	Total C O 49 34 15	0
35	m	1	Total C O 66 51 15	0
35	G	1	Total C O 45 30 15	0
35	B	1	Total C O 45 30 15	0

- Molecule 36 is (3S,3'R,5R,6S,7cis)-7',8'-didehydro-5,6-dihydro-5,6-epoxy-beta,beta-carotene-3,3'-diol (CCD ID: DD6) (formula: $C_{40}H_{54}O_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	AltConf
36	h	1	Total C O 43 40 3	0
36	m	1	Total C O 43 40 3	0
36	A	1	Total C O 43 40 3	0

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Mol	Chain	Residues	Atoms	AltConf
36	A	1	Total C O 43 40 3	0
36	A	1	Total C O 43 40 3	0
36	G	1	Total C O 43 40 3	0
36	G	1	Total C O 43 40 3	0
36	G	1	Total C O 43 40 3	0
36	G	1	Total C O 43 40 3	0
36	I	1	Total C O 43 40 3	0
36	I	1	Total C O 43 40 3	0
36	I	1	Total C O 43 40 3	0
36	I	1	Total C O 43 40 3	0
36	I	1	Total C O 43 40 3	0
36	K	1	Total C O 43 40 3	0
36	K	1	Total C O 43 40 3	0
36	K	1	Total C O 43 40 3	0
36	K	1	Total C O 43 40 3	0
36	K	1	Total C O 43 40 3	0
36	K	1	Total C O 43 40 3	0
36	F	1	Total C O 43 40 3	0
36	F	1	Total C O 43 40 3	0
36	J	1	Total C O 43 40 3	0
36	J	1	Total C O 43 40 3	0

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Mol	Chain	Residues	Atoms	AltConf
36	J	1	Total C O 43 40 3	0
36	M	1	Total C O 43 40 3	0
36	M	1	Total C O 43 40 3	0
36	M	1	Total C O 43 40 3	0
36	M	1	Total C O 43 40 3	0
36	L	1	Total C O 43 40 3	0
36	L	1	Total C O 43 40 3	0
36	L	1	Total C O 43 40 3	0
36	L	1	Total C O 43 40 3	0
36	D	1	Total C O 43 40 3	0
36	D	1	Total C O 43 40 3	0
36	B	1	Total C O 42 39 3	0
36	B	1	Total C O 43 40 3	0
36	B	1	Total C O 43 40 3	0
36	B	1	Total C O 43 40 3	0
36	B	1	Total C O 43 40 3	0
36	H	1	Total C O 43 40 3	0
36	N	1	Total C O 43 40 3	0
36	O	1	Total C O 43 40 3	0
36	T	1	Total C O 43 40 3	0
36	Q	1	Total C O 43 40 3	0

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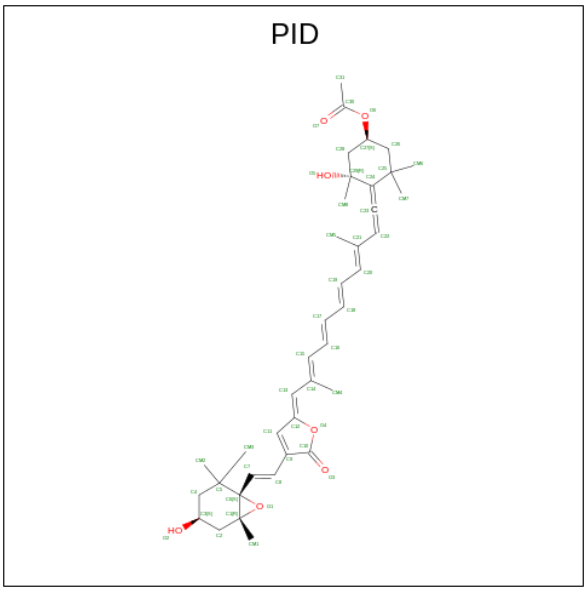
Mol	Chain	Residues	Atoms	AltConf
36	C	1	Total C O 43 40 3	0
36	P	1	Total C O 43 40 3	0
36	E	1	Total C O 43 40 3	0
36	E	1	Total C O 43 40 3	0

- Molecule 37 is PERIDININ (CCD ID: PID) (formula: $C_{39}H_{50}O_7$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	AltConf
37	h	1	Total C O 46 39 7	0
37	j	1	Total C O 46 39 7	0
37	G	1	Total C O 46 39 7	0
37	G	1	Total C O 46 39 7	0
37	G	1	Total C O 46 39 7	0
37	F	1	Total C O 46 39 7	0
37	F	1	Total C O 46 39 7	0

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Mol	Chain	Residues	Atoms	AltConf
37	F	1	Total C O 46 39 7	0
37	D	1	Total C O 46 39 7	0
37	D	1	Total C O 46 39 7	0
37	D	1	Total C O 46 39 7	0
37	D	1	Total C O 46 39 7	0
37	D	1	Total C O 46 39 7	0
37	H	1	Total C O 46 39 7	0
37	H	1	Total C O 46 39 7	0
37	H	1	Total C O 46 39 7	0
37	H	1	Total C O 46 39 7	0
37	H	1	Total C O 46 39 7	0
37	N	1	Total C O 46 39 7	0
37	N	1	Total C O 46 39 7	0
37	N	1	Total C O 46 39 7	0
37	N	1	Total C O 46 39 7	0
37	N	1	Total C O 46 39 7	0
37	O	1	Total C O 46 39 7	0
37	O	1	Total C O 46 39 7	0
37	O	1	Total C O 46 39 7	0
37	O	1	Total C O 46 39 7	0
37	O	1	Total C O 46 39 7	0

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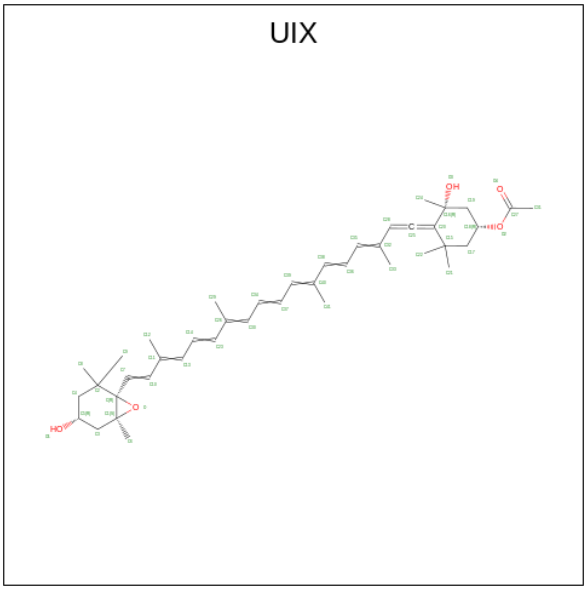
Mol	Chain	Residues	Atoms	AltConf
37	T	1	Total C O 46 39 7	0
37	T	1	Total C O 46 39 7	0
37	T	1	Total C O 46 39 7	0
37	T	1	Total C O 46 39 7	0
37	T	1	Total C O 46 39 7	0
37	T	1	Total C O 46 39 7	0
37	Q	1	Total C O 46 39 7	0
37	Q	1	Total C O 46 39 7	0
37	Q	1	Total C O 46 39 7	0
37	Q	1	Total C O 46 39 7	0
37	C	1	Total C O 46 39 7	0
37	C	1	Total C O 46 39 7	0
37	C	1	Total C O 46 39 7	0
37	C	1	Total C O 46 39 7	0
37	C	1	Total C O 46 39 7	0
37	P	1	Total C O 46 39 7	0
37	P	1	Total C O 46 39 7	0
37	P	1	Total C O 46 39 7	0
37	P	1	Total C O 46 39 7	0
37	P	1	Total C O 46 39 7	0
37	E	1	Total C O 46 39 7	0

- Molecule 38 is [(1 {S},5 {R})-3,3,5-trimethyl-5-oxidanyl-4-[(3 {E},5 {E},7 {E},9 {E},11 {E},13 {E},15 {E},17 {E})-3,7,12,16-tetramethyl-18-[(1 {S},4 {S},6 {R})-2,2,6-trimethyl-4-oxidanyl-7-oxabicyclo[4.1.0]heptan-1-yl]octadeca-1,3,5,7,9,11,13,15,17-nonaenylidene]cyclohexyl] ethanoate (CCD ID: UIX) (formula: $C_{42}H_{58}O_5$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
38	A	1	Total	C	O	0
			47	42	5	
38	F	1	Total	C	O	0
			47	42	5	
38	J	1	Total	C	O	0
			47	42	5	
38	L	1	Total	C	O	0
			47	42	5	
38	B	1	Total	C	O	0
			47	42	5	
38	N	1	Total	C	O	0
			47	42	5	
38	O	1	Total	C	O	0
			47	42	5	
38	T	1	Total	C	O	0
			47	42	5	
38	Q	1	Total	C	O	0
			47	42	5	
38	C	1	Total	C	O	0
			47	42	5	
38	P	1	Total	C	O	0
			47	42	5	

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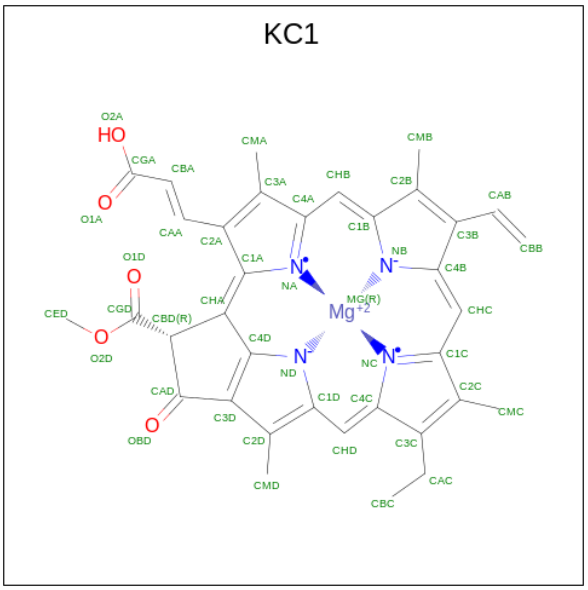
Mol	Chain	Residues	Atoms			AltConf
38	E	1	Total	C	O	0
			47	42	5	

- Molecule 39 is Chlorophyll c1 (CCD ID: KC1) (formula: $C_{35}H_{30}MgN_4O_5$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
39	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
39	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
39	G	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
39	G	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
39	I	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
39	K	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
39	F	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
39	F	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
39	J	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
39	M	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
39	M	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
39	L	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
39	L	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
39	D	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
39	D	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
39	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
39	H	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
39	H	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
39	H	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
39	N	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
39	N	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
39	N	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
39	O	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
39	O	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
39	O	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
39	T	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
39	T	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
39	T	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
39	Q	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
39	Q	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
39	Q	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

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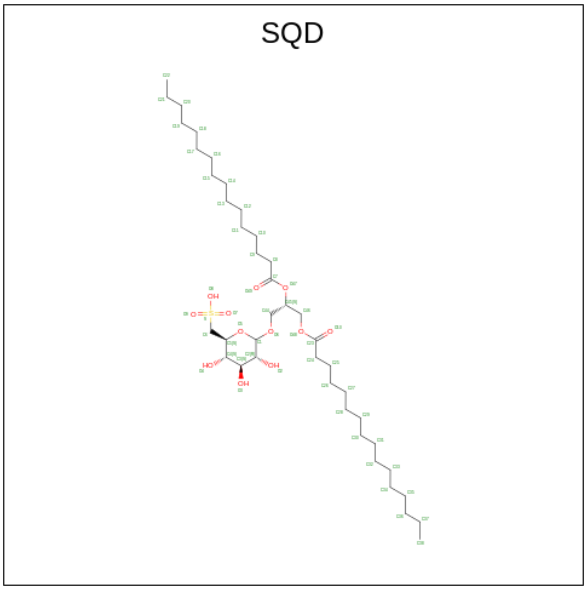
Mol	Chain	Residues	Atoms					AltConf
39	C	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
39	C	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
39	C	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
39	P	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
39	P	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
39	P	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
39	E	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
39	E	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

- Molecule 40 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (CCD ID: SQD) (formula: $C_{41}H_{78}O_{12}S$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
40	J	1	Total	C	O	S	0
			45	32	12	1	
40	B	1	Total	C	O	S	0
			42	29	12	1	

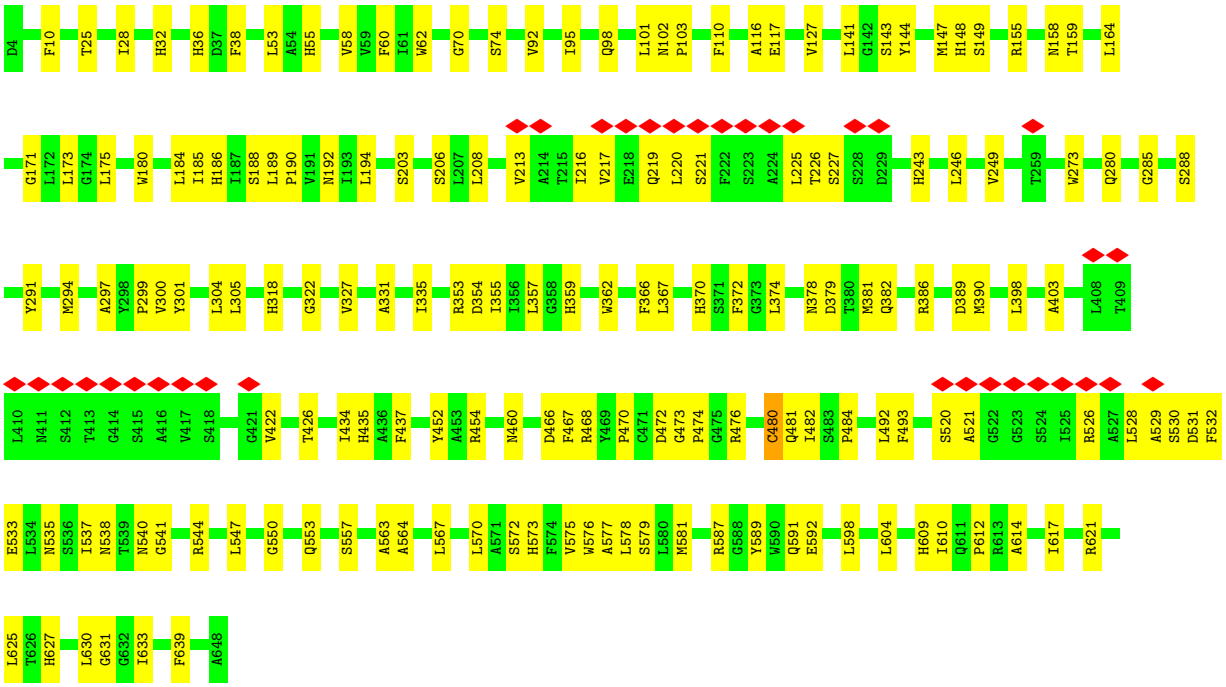
3 Residue-property plots (i)

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 PsaA

Chain a:

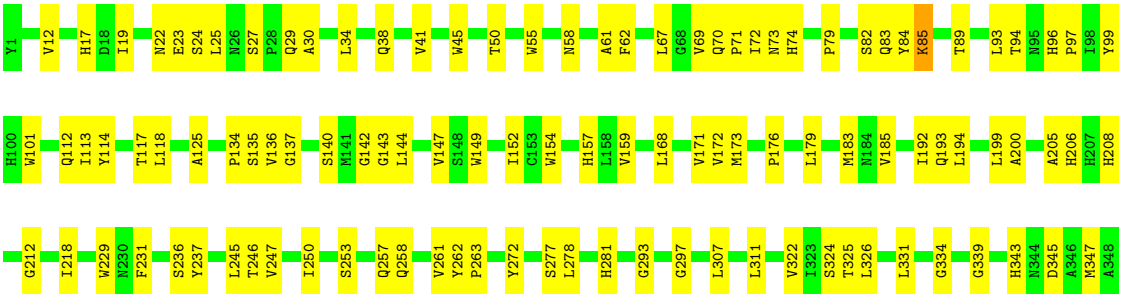


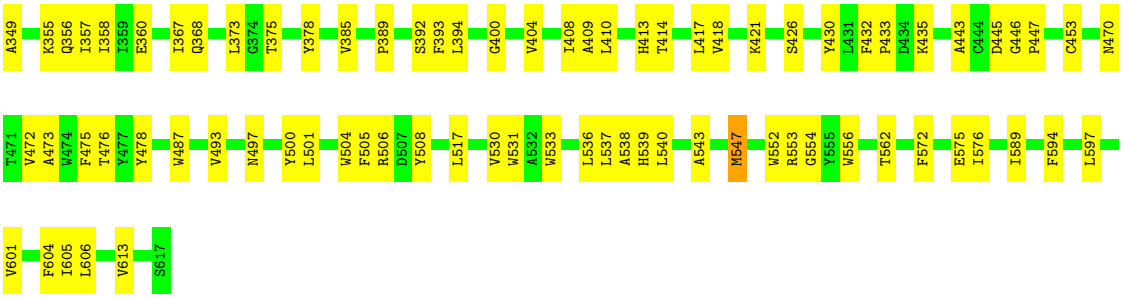


• Molecule 2: Photosystem I PsaB

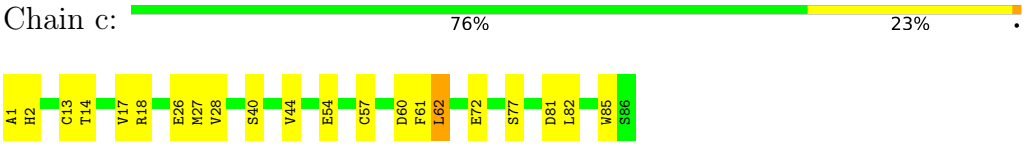
Chain b:



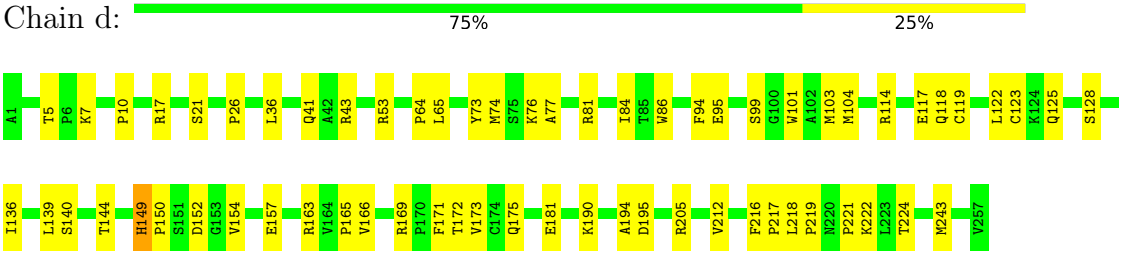




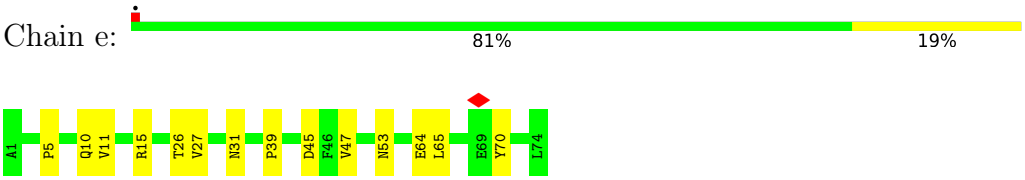
• Molecule 3: Photosystem I PsaC



• Molecule 4: Photosystem I PsaD

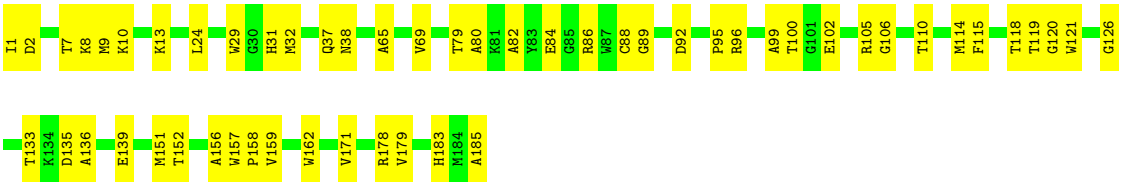


• Molecule 5: Photosystem I PsaE

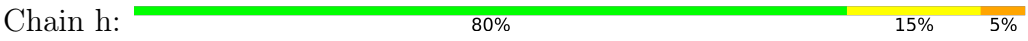


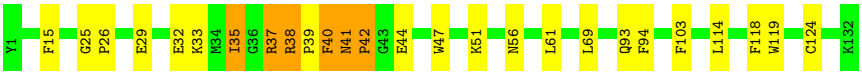
• Molecule 6: Photosystem I PsaF





• Molecule 7: Photosystem I PsaR

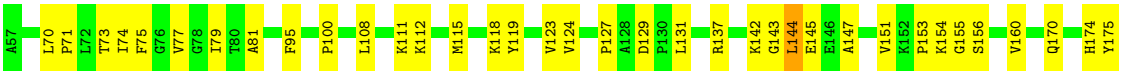


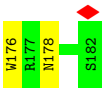


• Molecule 8: Photosystem I PsaI

Chain i:



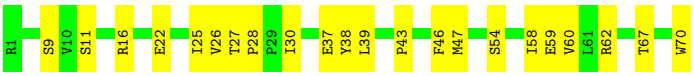




• Molecule 9: Photosystem I PsaJ

Chain j:

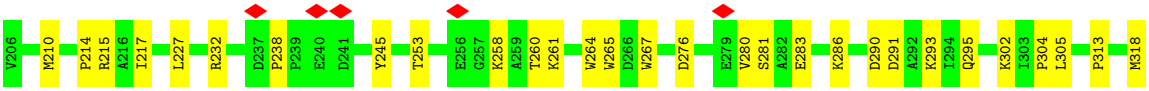




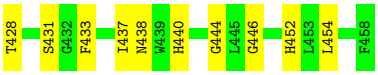
• Molecule 10: Photosystem I PsaL

Chain l:





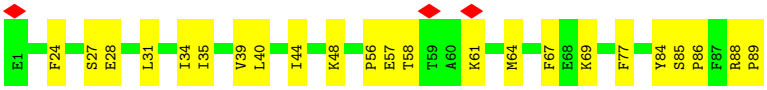




• Molecule 11: Photosystem I PsaM

Chain m:

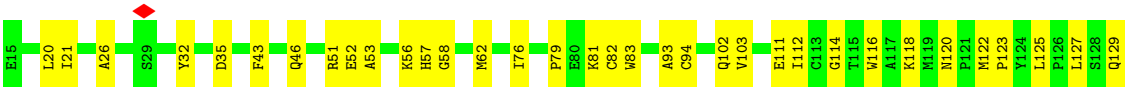




• Molecule 12: Chlorophyll a-chlorophyll c-peridinin-protein-complex I-10, acpPCI-10

Chain A:



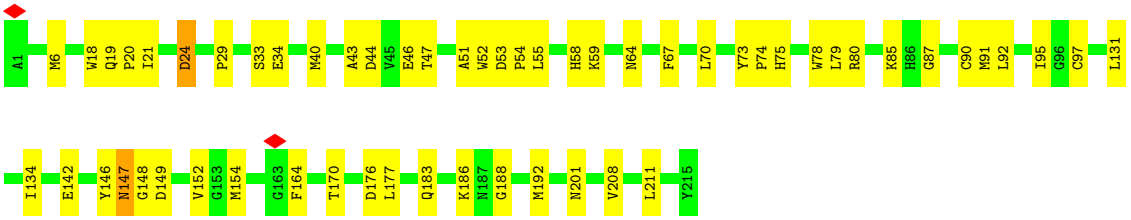




• Molecule 13: Chlorophyll a-chlorophyll c-peridinin-protein-complex I-8, acpPCI-8

Chain G:

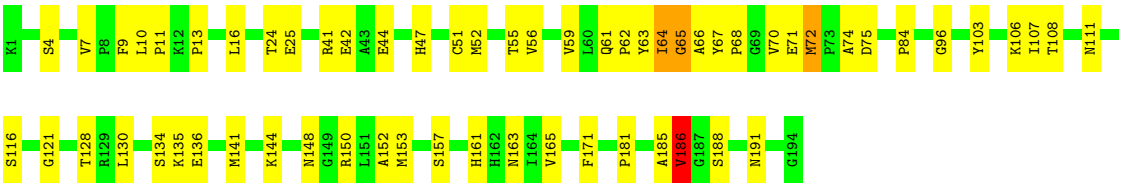




• Molecule 14: Chlorophyll a-chlorophyll c-peridinin-protein-complex I-7, acpPCI-7

Chain I:

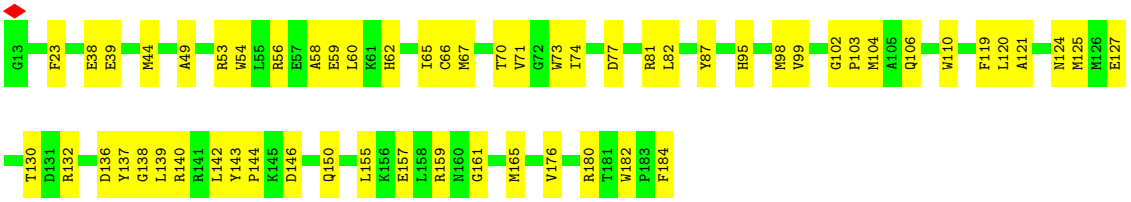




• Molecule 15: Chlorophyll a-chlorophyll c-peridinin-protein-complex I-6, acpPCI-6

Chain K:

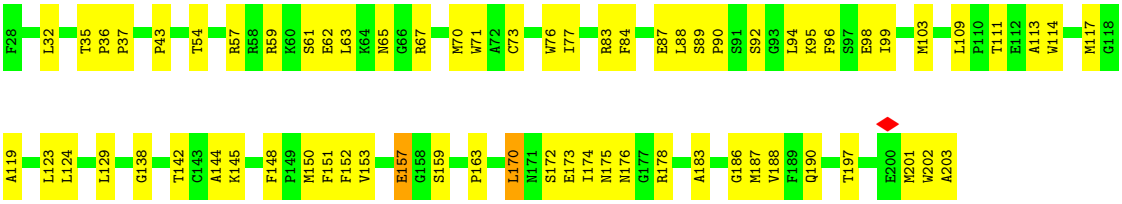




• Molecule 16: Chlorophyll a-chlorophyll c-peridinin-protein-complex I-2, acpPCI-2

Chain F:

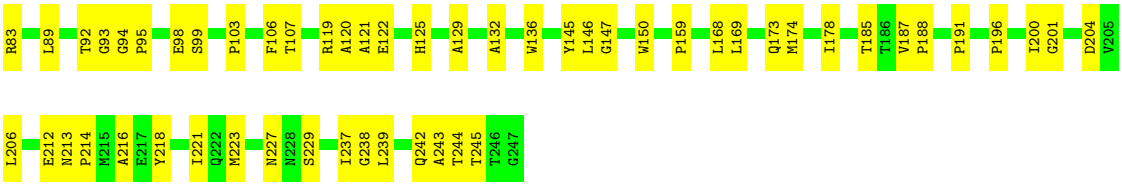




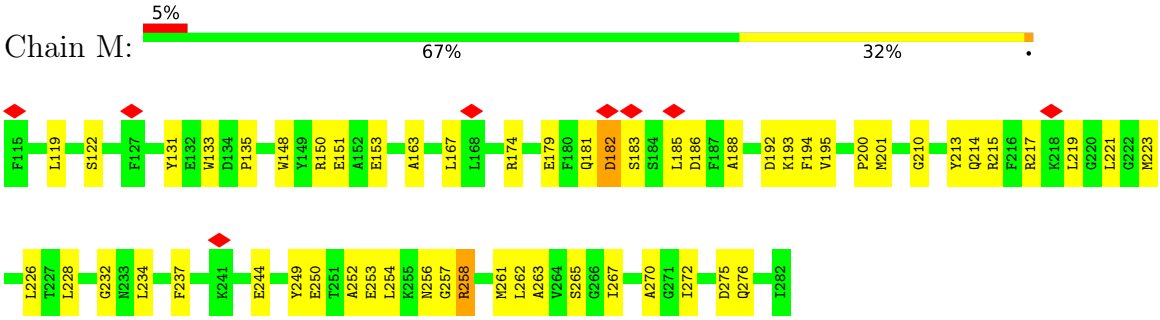
• Molecule 17: Chlorophyll a-chlorophyll c-peridinin-protein-complex I-3, acpPCI-3

Chain J:

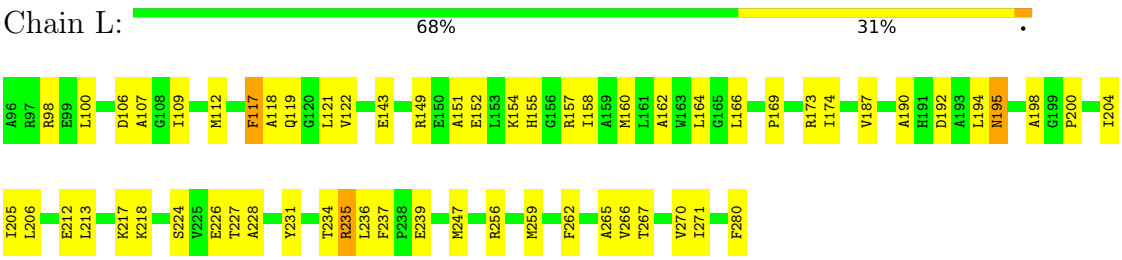




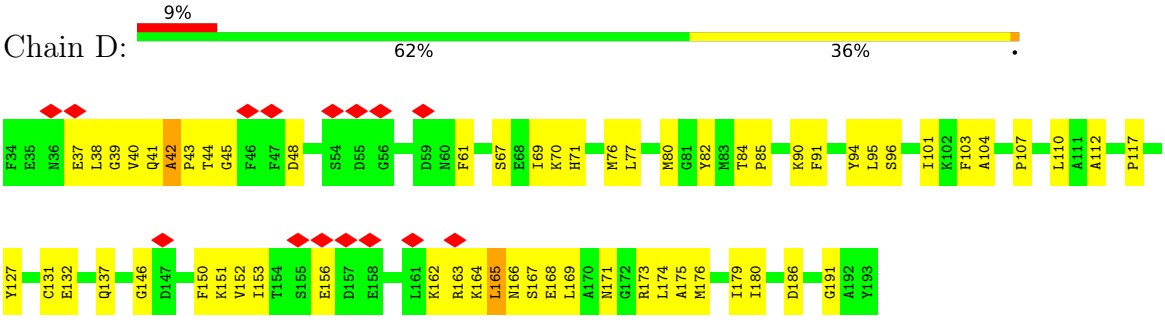
• Molecule 18: Chlorophyll a-chlorophyll c-peridinin-protein-complex I-4, acpPCI-4



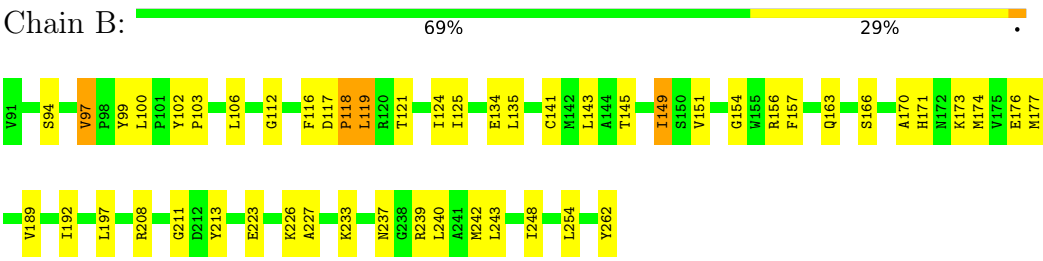
• Molecule 19: Chlorophyll a-chlorophyll c-peridinin-protein-complex I-5, acpPCI-5



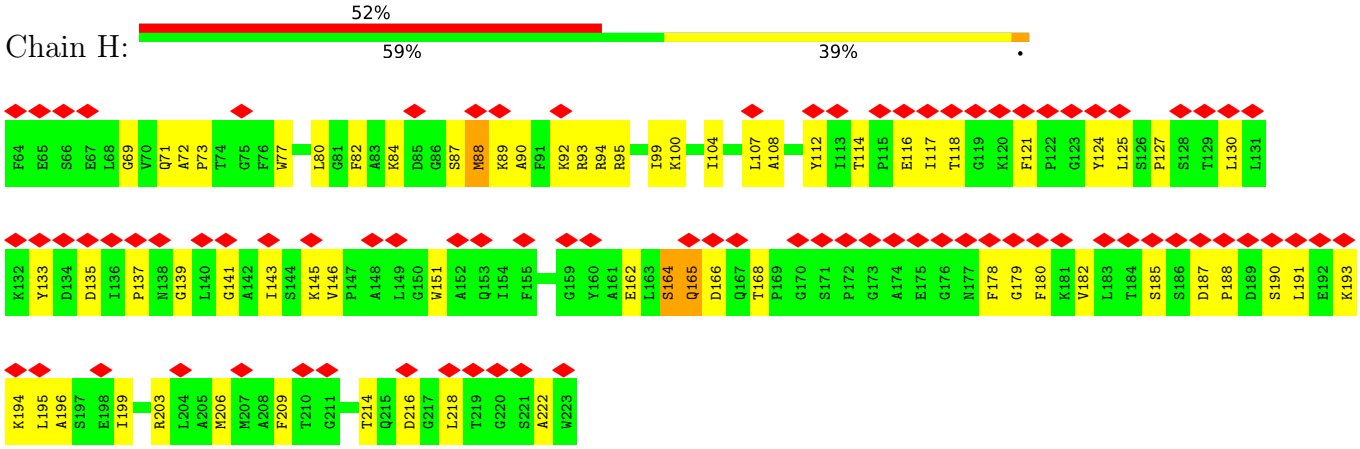
• Molecule 20: Chlorophyll a-chlorophyll c-peridinin-protein-complex I-9, acpPCI-9



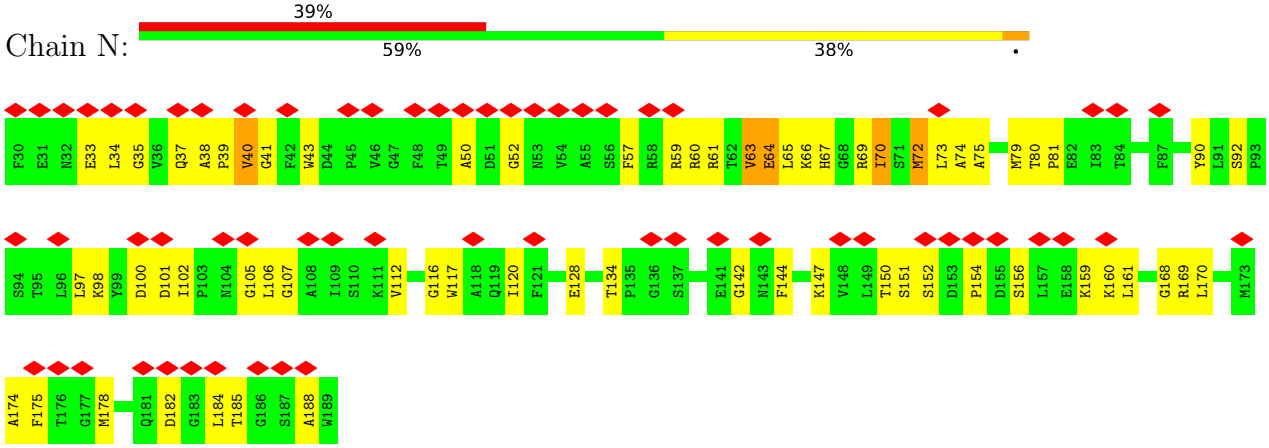
• Molecule 21: Chlorophyll a-chlorophyll c-peridinin-protein-complex I-11, acpPCI-11



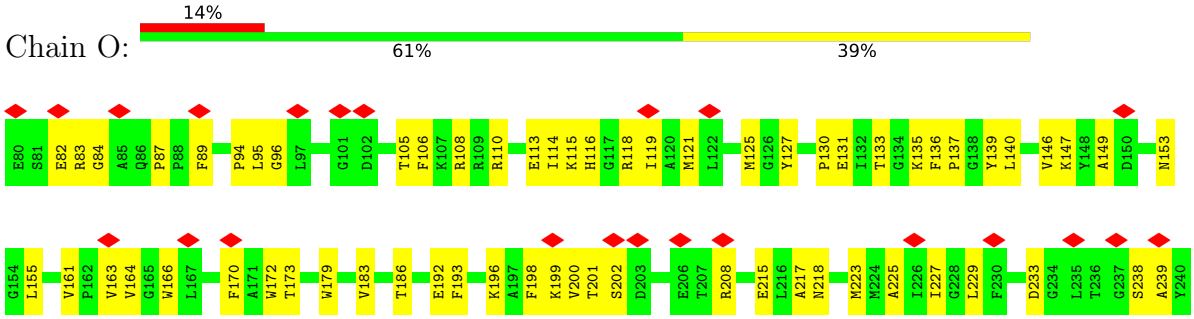
• Molecule 22: Chlorophyll a-chlorophyll c-peridinin-protein-complex I-12, acpPCI-12



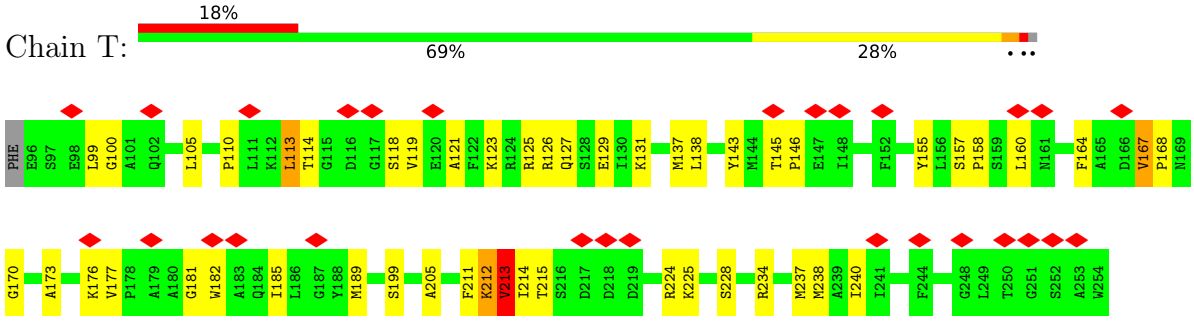
• Molecule 23: Chlorophyll a-chlorophyll c-peridinin-protein-complex I-13, acpPCI-13



• Molecule 24: Chlorophyll a-chlorophyll c-peridinin-protein-complex I-15, acpPCI-15

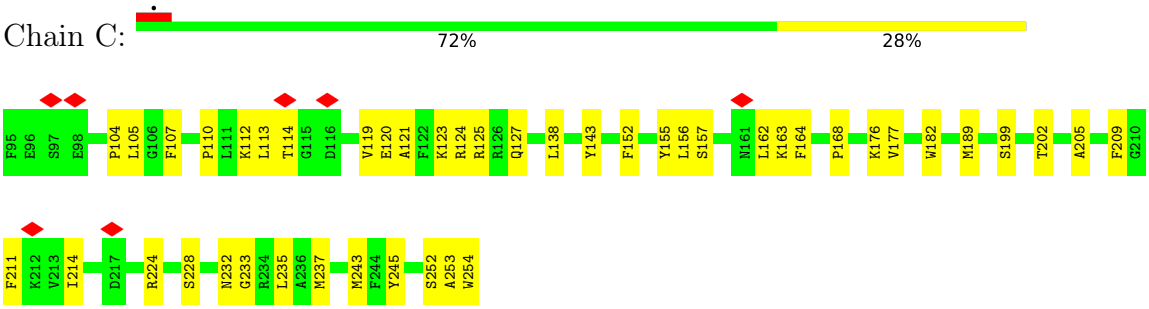


• Molecule 25: Chlorophyll a-chlorophyll c-peridinin-protein-complex I-16, acpPCI-16



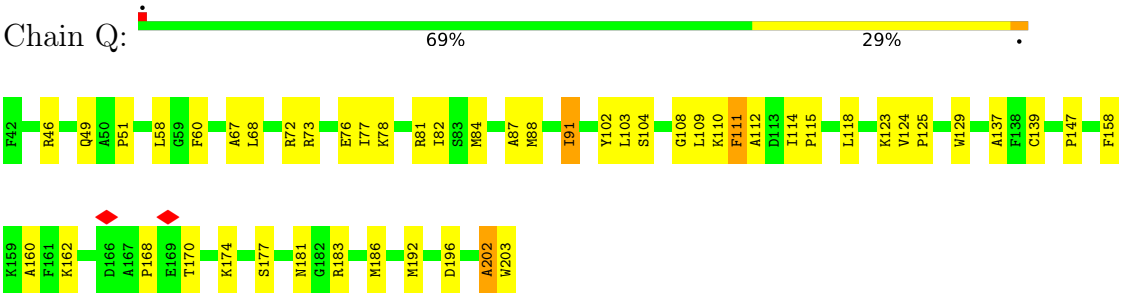
• Molecule 25: Chlorophyll a-chlorophyll c-peridinin-protein-complex I-16, acpPCI-16

Chain C:



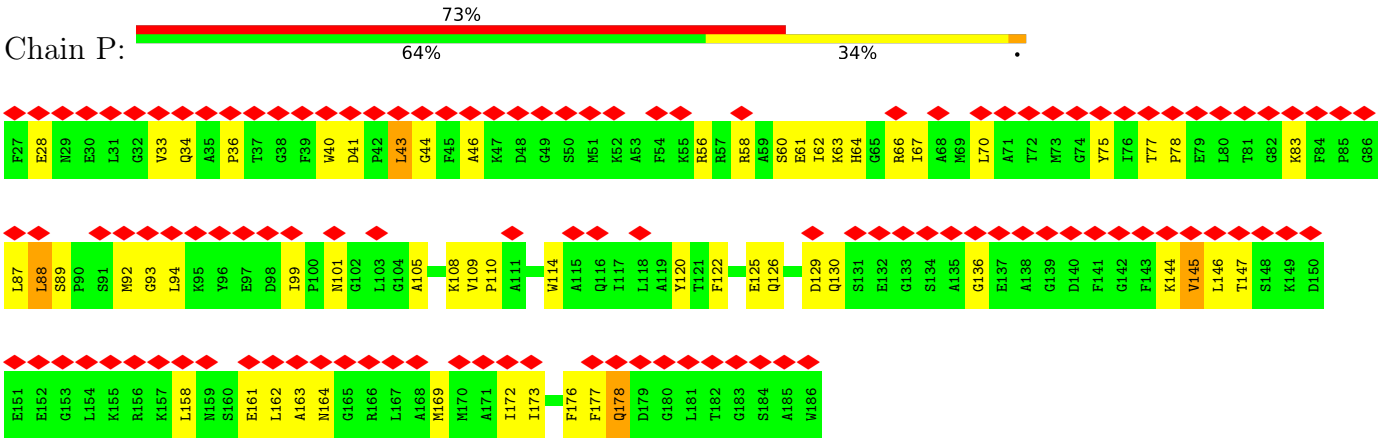
• Molecule 26: Chlorophyll a-chlorophyll c-peridinin-protein-complex I-17, acpPCI-17

Chain Q:



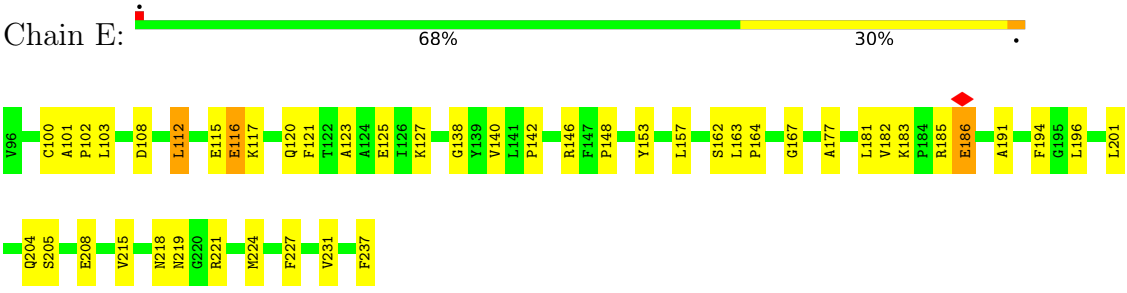
• Molecule 27: Chlorophyll a-chlorophyll c-peridinin-protein-complex I-14, acpPCI-14

Chain P:



• Molecule 28: Chlorophyll a-chlorophyll c-peridinin-protein-complex I-1, acpPCI-1

Chain E:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	356838	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	
Image detector	GATAN K2 BASE (4k x 4k)	Depositor
Maximum map value	1.883	Depositor
Minimum map value	-0.563	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.021	Depositor
Recommended contour level	0.22	Depositor
Map size (Å)	665.6, 665.6, 665.6	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.3, 1.3, 1.3	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: CLA, KC1, DD6, UIX, BCR, SQD, SF4, DGD, LHG, LMG, PID, PQN

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	0.30	1/5133 (0.0%)	0.36	0/7019
2	b	0.31	0/4968	0.39	0/6804
3	c	0.20	0/657	0.28	0/897
4	d	0.20	0/2034	0.34	0/2766
5	e	0.16	0/624	0.23	0/851
6	f	0.16	0/1484	0.26	0/1998
7	h	0.28	0/1089	0.43	0/1479
8	i	0.26	0/1030	0.45	0/1394
9	j	0.42	0/566	0.51	0/774
10	l	0.16	0/2014	0.29	0/2737
11	m	0.26	0/694	0.43	0/939
12	A	0.18	0/1395	0.31	0/1892
13	G	0.19	0/1730	0.32	0/2348
14	I	0.28	0/1499	0.42	0/2037
15	K	0.19	0/1358	0.30	0/1838
16	F	0.21	0/1395	0.45	0/1886
17	J	0.18	0/1317	0.38	0/1795
18	M	0.16	0/1395	0.45	0/1888
19	L	0.18	0/1490	0.42	0/2021
20	D	0.19	0/1223	0.46	2/1650 (0.1%)
21	B	0.28	0/1404	0.42	2/1891 (0.1%)
22	H	0.18	0/1232	0.39	0/1665
23	N	0.19	0/1233	0.45	0/1671
24	O	0.20	0/1260	0.45	0/1709
25	C	0.14	0/1226	0.33	0/1653
25	T	0.15	0/1214	0.37	0/1637
26	Q	0.18	0/1251	0.41	0/1690
27	P	0.17	0/1245	0.39	0/1673
28	E	0.19	0/1093	0.44	0/1473
All	All	0.23	1/44253 (0.0%)	0.38	4/60075 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	a	589	TYR	N-CA	-5.09	1.40	1.46

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	B	119	LEU	N-CA-C	-7.66	100.82	111.39
20	D	42	ALA	CA-C-N	-6.56	114.14	120.83
20	D	42	ALA	C-N-CA	-6.56	114.14	120.83
21	B	118	PRO	N-CA-C	-5.14	101.88	112.47

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	4980	0	4912	140	0
2	b	4813	0	4698	164	0
3	c	647	0	628	22	0
4	d	1985	0	1951	54	0
5	e	607	0	582	8	0
6	f	1455	0	1492	43	0
7	h	1056	0	1035	38	0
8	i	1001	0	999	33	0
9	j	549	0	546	20	0
10	l	1961	0	1942	68	0
11	m	679	0	685	28	0
12	A	1358	0	1328	37	0
13	G	1675	0	1614	49	0
14	I	1455	0	1392	45	0
15	K	1325	0	1317	54	0
16	F	1356	0	1315	66	0
17	J	1282	0	1255	45	0
18	M	1346	0	1263	43	0
19	L	1453	0	1423	51	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
20	D	1198	0	1176	52	0
21	B	1371	0	1372	45	0
22	H	1202	0	1182	58	0
23	N	1203	0	1172	56	0
24	O	1226	0	1200	65	0
25	C	1200	0	1185	43	0
25	T	1189	0	1176	43	0
26	Q	1219	0	1210	49	0
27	P	1218	0	1202	51	0
28	E	1071	0	1050	41	0
29	A	616	0	527	19	0
29	B	527	0	473	17	0
29	C	297	0	245	17	0
29	D	318	0	231	20	0
29	E	494	0	461	28	0
29	F	358	0	256	22	0
29	G	565	0	536	30	0
29	H	297	0	245	16	0
29	I	602	0	547	28	0
29	J	400	0	331	18	0
29	K	541	0	431	28	0
29	L	506	0	414	22	0
29	M	435	0	337	16	0
29	N	297	0	245	16	0
29	O	297	0	245	20	0
29	P	297	0	245	20	0
29	Q	311	0	276	19	0
29	T	273	0	198	18	0
29	a	1841	0	1790	120	0
29	b	1676	0	1696	119	0
29	f	152	0	125	8	0
29	h	60	0	59	7	0
29	i	185	0	193	19	0
29	j	52	0	43	0	0
29	l	447	0	438	35	0
30	a	33	0	46	6	0
30	b	33	0	46	3	0
31	a	48	0	69	5	0
32	a	120	0	168	16	0
32	b	120	0	168	19	0
32	f	80	0	112	13	0
32	i	40	0	56	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
32	l	80	0	112	8	0
32	m	40	0	56	8	0
33	a	8	0	0	2	0
33	c	16	0	0	3	0
34	A	37	0	44	2	0
34	E	32	0	34	6	0
34	K	114	0	138	7	0
34	P	27	0	24	1	0
34	b	130	0	170	13	0
34	h	28	0	26	2	0
34	j	43	0	56	3	0
35	B	45	0	48	0	0
35	G	45	0	48	2	0
35	b	57	0	72	2	0
35	h	54	0	69	9	0
35	j	133	0	140	9	0
35	m	66	0	96	5	0
36	A	129	0	0	2	0
36	B	214	0	0	8	0
36	C	43	0	0	1	0
36	D	86	0	0	3	0
36	E	86	0	0	0	0
36	F	86	0	0	2	0
36	G	172	0	0	4	0
36	H	43	0	0	0	0
36	I	215	0	0	4	0
36	J	129	0	0	5	0
36	K	258	0	0	4	0
36	L	172	0	0	2	0
36	M	172	0	0	6	0
36	N	43	0	0	1	0
36	O	43	0	0	2	0
36	P	43	0	0	1	0
36	Q	43	0	0	0	0
36	T	43	0	0	1	0
36	h	43	0	0	0	0
36	m	43	0	0	0	0
37	C	230	0	250	21	0
37	D	230	0	250	20	0
37	E	46	0	50	7	0
37	F	138	0	150	19	0
37	G	138	0	150	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
37	H	230	0	250	23	0
37	N	230	0	250	21	0
37	O	230	0	250	24	0
37	P	230	0	250	22	0
37	Q	184	0	200	17	0
37	T	276	0	300	20	0
37	h	46	0	50	1	0
37	j	46	0	50	5	0
38	A	47	0	0	0	0
38	B	47	0	0	1	0
38	C	47	0	0	0	0
38	E	47	0	0	1	0
38	F	47	0	0	2	0
38	J	47	0	0	1	0
38	L	47	0	0	0	0
38	N	47	0	0	0	0
38	O	47	0	0	0	0
38	P	47	0	0	0	0
38	Q	47	0	0	0	0
38	T	47	0	0	0	0
39	A	90	0	0	0	0
39	B	45	0	0	0	0
39	C	135	0	0	1	0
39	D	90	0	0	2	0
39	E	90	0	0	2	0
39	F	90	0	0	0	0
39	G	90	0	0	2	0
39	H	135	0	0	2	0
39	I	45	0	0	1	0
39	J	45	0	0	0	0
39	K	45	0	0	0	0
39	L	90	0	0	0	0
39	M	90	0	0	0	0
39	N	135	0	0	5	0
39	O	135	0	0	0	0
39	P	135	0	0	2	0
39	Q	135	0	0	2	0
39	T	135	0	0	0	0
40	B	42	0	48	3	0
40	J	45	0	54	7	0
All	All	63119	0	57239	1854	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 15.

The worst 5 of 1854 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)
37:F:304:PID:HM11	37:F:304:PID:H8	1.33	1.09
37:H:306:PID:HM11	37:H:306:PID:H8	1.45	0.96
7:h:38:ARG:H	7:h:39:PRO:HD2	1.31	0.95
16:F:183:ALA:HB1	37:F:304:PID:H8	1.52	0.91
37:Q:304:PID:H20	29:Q:313:CLA:HAB	1.55	0.87

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	643/645 (100%)	594 (92%)	47 (7%)	2 (0%)	36 65
2	b	615/617 (100%)	581 (94%)	34 (6%)	0	100 100
3	c	84/86 (98%)	81 (96%)	3 (4%)	0	100 100
4	d	255/257 (99%)	239 (94%)	15 (6%)	1 (0%)	30 59
5	e	72/74 (97%)	68 (94%)	4 (6%)	0	100 100
6	f	183/185 (99%)	177 (97%)	6 (3%)	0	100 100
7	h	130/132 (98%)	121 (93%)	6 (5%)	3 (2%)	5 19
8	i	124/126 (98%)	116 (94%)	8 (6%)	0	100 100
9	j	68/70 (97%)	60 (88%)	8 (12%)	0	100 100
10	l	251/253 (99%)	231 (92%)	20 (8%)	0	100 100
11	m	87/89 (98%)	79 (91%)	8 (9%)	0	100 100
12	A	178/180 (99%)	163 (92%)	15 (8%)	0	100 100
13	G	213/215 (99%)	189 (89%)	23 (11%)	1 (0%)	24 54

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
14	I	192/194 (99%)	165 (86%)	21 (11%)	6 (3%)	3	14
15	K	170/172 (99%)	153 (90%)	16 (9%)	1 (1%)	21	51
16	F	174/176 (99%)	154 (88%)	19 (11%)	1 (1%)	21	51
17	J	163/165 (99%)	144 (88%)	18 (11%)	1 (1%)	21	51
18	M	166/168 (99%)	134 (81%)	26 (16%)	6 (4%)	2	11
19	L	183/185 (99%)	152 (83%)	26 (14%)	5 (3%)	4	16
20	D	158/160 (99%)	142 (90%)	15 (10%)	1 (1%)	21	51
21	B	170/172 (99%)	153 (90%)	17 (10%)	0	100	100
22	H	158/160 (99%)	135 (85%)	19 (12%)	4 (2%)	4	17
23	N	158/160 (99%)	126 (80%)	31 (20%)	1 (1%)	21	51
24	O	159/161 (99%)	144 (91%)	12 (8%)	3 (2%)	6	23
25	C	158/160 (99%)	146 (92%)	11 (7%)	1 (1%)	21	51
25	T	157/160 (98%)	142 (90%)	11 (7%)	4 (2%)	4	17
26	Q	160/162 (99%)	138 (86%)	20 (12%)	2 (1%)	9	32
27	P	158/160 (99%)	139 (88%)	16 (10%)	3 (2%)	6	23
28	E	140/142 (99%)	120 (86%)	17 (12%)	3 (2%)	5	21
All	All	5527/5586 (99%)	4986 (90%)	492 (9%)	49 (1%)	16	41

5 of 49 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	a	520	SER
4	d	149	HIS
14	I	116	SER
14	I	135	LYS
14	I	186	VAL

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	531/535 (99%)	527 (99%)	4 (1%)	73	90
2	b	502/504 (100%)	495 (99%)	7 (1%)	59	85
3	c	73/74 (99%)	72 (99%)	1 (1%)	59	85
4	d	213/222 (96%)	213 (100%)	0	100	100
5	e	65/66 (98%)	65 (100%)	0	100	100
6	f	151/151 (100%)	150 (99%)	1 (1%)	76	92
7	h	109/109 (100%)	105 (96%)	4 (4%)	30	64
8	i	106/106 (100%)	104 (98%)	2 (2%)	50	79
9	j	60/60 (100%)	58 (97%)	2 (3%)	33	67
10	l	200/203 (98%)	200 (100%)	0	100	100
11	m	72/72 (100%)	72 (100%)	0	100	100
12	A	136/141 (96%)	136 (100%)	0	100	100
13	G	171/171 (100%)	169 (99%)	2 (1%)	63	86
14	I	141/156 (90%)	137 (97%)	4 (3%)	38	72
15	K	133/138 (96%)	133 (100%)	0	100	100
16	F	140/140 (100%)	138 (99%)	2 (1%)	59	85
17	J	136/136 (100%)	135 (99%)	1 (1%)	76	92
18	M	128/128 (100%)	126 (98%)	2 (2%)	55	83
19	L	145/145 (100%)	145 (100%)	0	100	100
20	D	123/123 (100%)	120 (98%)	3 (2%)	43	75
21	B	146/146 (100%)	144 (99%)	2 (1%)	59	85
22	H	123/123 (100%)	122 (99%)	1 (1%)	73	90
23	N	124/124 (100%)	119 (96%)	5 (4%)	28	62
24	O	124/124 (100%)	123 (99%)	1 (1%)	73	90
25	C	121/121 (100%)	121 (100%)	0	100	100
25	T	120/121 (99%)	118 (98%)	2 (2%)	53	82
26	Q	120/120 (100%)	119 (99%)	1 (1%)	73	90
27	P	123/123 (100%)	121 (98%)	2 (2%)	55	83
28	E	108/108 (100%)	107 (99%)	1 (1%)	70	90
All	All	4444/4490 (99%)	4394 (99%)	50 (1%)	63	88

5 of 50 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
16	F	170	LEU
21	B	97	VAL
28	E	112	LEU
17	J	229	SER
20	D	41	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 22 such sidechains are listed below:

Mol	Chain	Res	Type
18	M	276	GLN
22	H	71	GLN
21	B	251	GLN
23	N	133	GLN
12	A	24	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)

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

411 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	$\#\|Z\|>2$
36	DD6	h	202	-	39,45,45	2.19	5 (12%)	52,67,67	2.33	19 (36%)
29	CLA	G	311	13	55,59,73	1.38	9 (16%)	66,96,113	1.39	5 (7%)
29	CLA	Q	315	-	45,49,73	1.52	9 (20%)	54,84,113	1.53	5 (9%)
37	PID	G	309	-	41,49,49	1.33	4 (9%)	49,76,76	1.45	5 (10%)
34	LMG	E	316	-	32,32,55	0.99	1 (3%)	40,40,63	1.27	2 (5%)
39	KC1	C	310	25	49,53,53	1.43	6 (12%)	63,89,89	2.04	13 (20%)
29	CLA	b	703	-	69,73,73	1.25	10 (14%)	83,113,113	1.19	5 (6%)
29	CLA	I	211	-	69,73,73	1.23	10 (14%)	83,113,113	1.30	9 (10%)
37	PID	D	303	-	41,49,49	1.37	4 (9%)	49,76,76	1.51	8 (16%)
37	PID	Q	306	-	41,49,49	1.33	4 (9%)	49,76,76	1.52	6 (12%)
39	KC1	T	315	25	49,53,53	1.40	6 (12%)	63,89,89	1.99	13 (20%)
29	CLA	M	310	18	52,56,73	1.43	8 (15%)	62,92,113	1.40	5 (8%)
39	KC1	N	310	23	49,53,53	1.40	6 (12%)	63,89,89	2.02	13 (20%)
29	CLA	L	309	19	59,63,73	1.34	9 (15%)	71,101,113	1.35	7 (9%)
39	KC1	E	312	28	49,53,53	1.43	7 (14%)	63,89,89	1.99	15 (23%)
37	PID	D	307	-	41,49,49	1.35	4 (9%)	49,76,76	1.59	7 (14%)
29	CLA	b	708	2	56,60,73	1.39	9 (16%)	67,97,113	1.41	8 (11%)
29	CLA	b	719	-	54,58,73	1.41	9 (16%)	65,95,113	1.43	10 (15%)
37	PID	C	305	-	41,49,49	1.36	4 (9%)	49,76,76	1.95	9 (18%)
29	CLA	B	306	21	53,57,73	1.42	9 (16%)	62,93,113	1.43	7 (11%)
38	UIX	A	203	-	41,49,49	1.27	4 (9%)	52,74,74	2.39	21 (40%)
29	CLA	b	721	-	62,66,73	1.31	10 (16%)	74,104,113	1.39	7 (9%)
39	KC1	L	314	-	49,53,53	1.41	7 (14%)	63,89,89	2.00	14 (22%)
29	CLA	J	307	17	50,54,73	1.44	9 (18%)	60,90,113	1.40	5 (8%)
36	DD6	I	205	-	39,45,45	2.45	5 (12%)	52,67,67	2.18	17 (32%)
37	PID	N	304	-	41,49,49	1.34	4 (9%)	49,76,76	1.48	5 (10%)
37	PID	T	301	-	41,49,49	1.34	4 (9%)	49,76,76	1.49	5 (10%)
29	CLA	l	504	10	69,73,73	1.24	9 (13%)	83,113,113	3.92	9 (10%)
29	CLA	A	218	12	64,68,73	1.29	10 (15%)	77,107,113	1.34	7 (9%)
38	UIX	P	207	-	41,49,49	1.27	3 (7%)	52,74,74	2.56	19 (36%)
29	CLA	L	315	19	45,49,73	1.53	10 (22%)	54,84,113	1.50	6 (11%)
29	CLA	O	311	-	55,59,73	1.41	8 (14%)	66,96,113	1.39	5 (7%)
29	CLA	F	312	16	50,54,73	1.45	9 (18%)	60,90,113	1.40	4 (6%)
29	CLA	a	825	1	69,73,73	1.26	9 (13%)	83,113,113	1.38	9 (10%)
37	PID	P	206	-	41,49,49	1.36	4 (9%)	49,76,76	1.79	8 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
29	CLA	b	713	-	57,61,73	1.39	8 (14%)	68,98,113	1.35	4 (5%)
37	PID	P	205	-	41,49,49	1.34	4 (9%)	49,76,76	1.54	6 (12%)
37	PID	Q	304	-	41,49,49	1.33	4 (9%)	49,76,76	1.54	6 (12%)
39	KC1	C	315	25	49,53,53	1.42	7 (14%)	63,89,89	2.00	13 (20%)
39	KC1	N	315	-	49,53,53	1.39	6 (12%)	63,89,89	1.97	13 (20%)
29	CLA	L	316	19	56,60,73	1.41	10 (17%)	67,97,113	1.36	7 (10%)
29	CLA	a	819	1	61,65,73	1.33	10 (16%)	73,103,113	1.31	7 (9%)
29	CLA	i	202	2	69,73,73	1.24	9 (13%)	83,113,113	1.26	6 (7%)
37	PID	H	304	-	41,49,49	1.34	4 (9%)	49,76,76	1.63	5 (10%)
36	DD6	L	301	-	39,45,45	2.00	3 (7%)	52,67,67	1.97	11 (21%)
29	CLA	C	309	-	69,73,73	1.25	8 (11%)	83,113,113	1.27	4 (4%)
39	KC1	A	205	29	49,53,53	1.41	7 (14%)	63,89,89	2.03	16 (25%)
29	CLA	a	817	-	49,53,73	1.50	9 (18%)	59,89,113	1.42	5 (8%)
36	DD6	B	319	-	39,45,45	2.09	3 (7%)	52,67,67	2.26	16 (30%)
29	CLA	F	308	-	50,54,73	1.46	10 (20%)	60,90,113	1.38	5 (8%)
29	CLA	L	311	19	50,54,73	1.46	9 (18%)	60,90,113	1.36	5 (8%)
29	CLA	C	314	-	51,55,73	1.44	9 (17%)	61,91,113	1.47	6 (9%)
29	CLA	G	313	13	59,63,73	1.34	9 (15%)	71,101,113	1.37	7 (9%)
29	CLA	l	508	-	45,49,73	1.50	10 (22%)	54,84,113	1.48	5 (9%)
29	CLA	f	802	-	50,54,73	1.45	10 (20%)	60,90,113	1.39	4 (6%)
39	KC1	M	305	-	49,53,53	1.41	7 (14%)	63,89,89	2.03	15 (23%)
29	CLA	A	212	-	59,63,73	1.33	10 (16%)	71,101,113	1.34	6 (8%)
35	DGD	b	733	-	58,58,67	0.94	3 (5%)	72,72,81	1.25	7 (9%)
29	CLA	l	505	-	69,73,73	1.26	9 (13%)	83,113,113	1.27	6 (7%)
29	CLA	G	319	13	45,49,73	1.51	9 (20%)	54,84,113	1.52	5 (9%)
29	CLA	G	316	-	69,73,73	1.26	10 (14%)	83,113,113	4.72	10 (12%)
29	CLA	Q	307	-	51,55,73	1.45	9 (17%)	61,91,113	1.40	5 (8%)
29	CLA	a	805	1	59,63,73	1.34	10 (16%)	71,101,113	1.37	4 (5%)
29	CLA	K	214	-	59,63,73	1.36	10 (16%)	71,101,113	1.35	8 (11%)
37	PID	D	302	-	41,49,49	1.34	4 (9%)	49,76,76	1.45	5 (10%)
29	CLA	b	705	-	69,73,73	1.23	10 (14%)	83,113,113	1.34	5 (6%)
29	CLA	T	311	-	50,54,73	1.46	7 (14%)	60,90,113	1.42	5 (8%)
29	CLA	C	311	-	55,59,73	1.39	8 (14%)	66,96,113	1.41	7 (10%)
38	UIX	T	306	-	41,49,49	1.29	4 (9%)	52,74,74	2.77	24 (46%)
29	CLA	A	217	-	55,59,73	1.40	9 (16%)	66,96,113	1.38	7 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
36	DD6	J	303	-	39,45,45	2.10	3 (7%)	52,67,67	2.11	18 (34%)
29	CLA	A	208	12	59,63,73	1.34	9 (15%)	71,101,113	1.36	8 (11%)
29	CLA	H	307	-	51,55,73	1.45	8 (15%)	61,91,113	1.40	5 (8%)
35	DGD	B	318	-	46,46,67	1.00	2 (4%)	60,60,81	1.32	10 (16%)
29	CLA	I	208	-	50,54,73	1.45	9 (18%)	60,90,113	5.53	6 (10%)
39	KC1	P	213	27	49,53,53	1.43	6 (12%)	63,89,89	2.00	15 (23%)
37	PID	C	302	-	41,49,49	1.34	4 (9%)	49,76,76	1.44	6 (12%)
36	DD6	G	307	-	39,45,45	2.71	10 (25%)	52,67,67	2.55	19 (36%)
29	CLA	P	210	-	69,73,73	1.25	8 (11%)	83,113,113	1.25	5 (6%)
29	CLA	a	813	1	55,59,73	1.41	10 (18%)	66,96,113	1.38	5 (7%)
29	CLA	a	826	1	69,73,73	1.24	9 (13%)	83,113,113	1.31	6 (7%)
34	LMG	b	734	-	40,40,55	0.81	0	48,48,63	1.29	6 (12%)
33	SF4	c	101	3	0,12,12	-	-	-		
29	CLA	a	803	-	69,73,73	1.26	10 (14%)	83,113,113	1.22	5 (6%)
32	BCR	a	838	-	41,41,41	0.76	0	56,56,56	2.12	18 (32%)
29	CLA	L	310	-	59,63,73	1.35	9 (15%)	71,101,113	1.37	6 (8%)
36	DD6	K	221	-	39,45,45	2.14	4 (10%)	52,67,67	2.24	15 (28%)
29	CLA	J	313	-	45,49,73	1.53	8 (17%)	54,84,113	1.52	6 (11%)
39	KC1	F	314	-	49,53,53	1.40	7 (14%)	63,89,89	2.01	13 (20%)
29	CLA	L	307	39	54,58,73	1.40	10 (18%)	65,95,113	5.34	8 (12%)
29	CLA	a	828	-	50,54,73	1.46	10 (20%)	60,90,113	1.42	5 (8%)
39	KC1	A	213	-	49,53,53	1.40	6 (12%)	63,89,89	2.00	14 (22%)
39	KC1	D	315	-	49,53,53	1.41	7 (14%)	63,89,89	2.00	11 (17%)
37	PID	j	101	-	41,49,49	1.37	4 (9%)	49,76,76	1.46	9 (18%)
39	KC1	Q	309	26	49,53,53	1.40	7 (14%)	63,89,89	2.02	14 (22%)
37	PID	P	202	-	41,49,49	1.32	4 (9%)	49,76,76	1.37	8 (16%)
29	CLA	b	720	2	69,73,73	1.27	10 (14%)	83,113,113	1.27	5 (6%)
29	CLA	a	820	1	69,73,73	1.24	10 (14%)	83,113,113	1.27	6 (7%)
39	KC1	H	311	-	49,53,53	1.40	7 (14%)	63,89,89	1.99	13 (20%)
29	CLA	b	709	2	64,68,73	1.29	10 (15%)	77,107,113	1.32	7 (9%)
29	CLA	K	211	-	59,63,73	1.33	10 (16%)	71,101,113	1.39	9 (12%)
29	CLA	b	726	-	69,73,73	1.25	10 (14%)	83,113,113	1.28	7 (8%)
29	CLA	A	207	-	59,63,73	1.35	10 (16%)	71,101,113	1.35	5 (7%)
29	CLA	M	313	-	45,49,73	1.53	9 (20%)	54,84,113	1.54	6 (11%)
29	CLA	N	316	-	45,49,73	1.54	8 (17%)	54,84,113	1.50	5 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
34	LMG	K	219	-	35,35,55	0.92	1 (2%)	43,43,63	1.19	4 (9%)
29	CLA	B	310	-	69,73,73	1.24	9 (13%)	83,113,113	1.28	7 (8%)
29	CLA	a	837	-	59,63,73	1.34	9 (15%)	71,101,113	1.30	6 (8%)
29	CLA	A	216	-	45,49,73	1.51	10 (22%)	54,84,113	1.51	6 (11%)
36	DD6	L	305	-	39,45,45	2.05	3 (7%)	52,67,67	1.95	14 (26%)
37	PID	H	302	-	41,49,49	1.36	4 (9%)	49,76,76	1.40	6 (12%)
29	CLA	T	313	-	50,54,73	1.47	8 (16%)	60,90,113	1.41	4 (6%)
29	CLA	C	313	25	50,54,73	1.44	9 (18%)	60,90,113	1.40	4 (6%)
29	CLA	M	314	-	56,60,73	1.38	8 (14%)	67,97,113	1.34	6 (8%)
37	PID	O	302	-	41,49,49	1.36	4 (9%)	49,76,76	1.42	7 (14%)
37	PID	O	301	-	41,49,49	1.32	4 (9%)	49,76,76	1.62	6 (12%)
37	PID	Q	303	-	41,49,49	1.34	4 (9%)	49,76,76	1.48	6 (12%)
29	CLA	E	315	28	61,65,73	1.34	9 (14%)	73,103,113	1.35	7 (9%)
29	CLA	H	310	-	55,59,73	1.41	8 (14%)	66,96,113	1.39	6 (9%)
29	CLA	b	722	2	62,66,73	1.31	10 (16%)	74,104,113	1.37	6 (8%)
29	CLA	b	715	2	50,54,73	1.45	9 (18%)	60,90,113	1.41	5 (8%)
36	DD6	G	308	-	39,45,45	2.01	2 (5%)	52,67,67	2.12	15 (28%)
35	DGD	j	103	-	44,44,67	0.99	2 (4%)	58,58,81	1.32	9 (15%)
29	CLA	C	316	-	45,49,73	1.52	9 (20%)	54,84,113	1.57	5 (9%)
29	CLA	a	807	1	69,73,73	1.25	10 (14%)	83,113,113	1.29	7 (8%)
29	CLA	G	312	13	69,73,73	1.24	10 (14%)	83,113,113	1.29	7 (8%)
37	PID	T	304	-	41,49,49	1.33	4 (9%)	49,76,76	1.45	5 (10%)
36	DD6	P	204	-	39,45,45	1.99	3 (7%)	52,67,67	2.19	15 (28%)
29	CLA	f	803	6	50,54,73	1.45	9 (18%)	60,90,113	1.42	4 (6%)
29	CLA	I	216	-	56,60,73	1.38	10 (17%)	67,97,113	1.45	8 (11%)
32	BCR	i	204	-	41,41,41	0.76	0	56,56,56	2.35	15 (26%)
35	DGD	h	203	-	55,55,67	0.90	2 (3%)	69,69,81	0.98	3 (4%)
36	DD6	A	202	-	39,45,45	1.97	3 (7%)	52,67,67	1.81	10 (19%)
29	CLA	O	313	24	50,54,73	1.45	9 (18%)	60,90,113	1.42	7 (11%)
36	DD6	I	202	-	39,45,45	2.03	3 (7%)	52,67,67	1.92	14 (26%)
39	KC1	T	310	25	49,53,53	1.42	7 (14%)	63,89,89	1.97	13 (20%)
36	DD6	M	303	-	39,45,45	2.11	4 (10%)	52,67,67	2.03	14 (26%)
29	CLA	f	805	-	64,68,73	1.30	9 (14%)	77,107,113	1.29	5 (6%)
29	CLA	K	217	15	50,54,73	1.46	10 (20%)	60,90,113	1.43	5 (8%)
37	PID	H	305	-	41,49,49	1.33	4 (9%)	49,76,76	1.75	8 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
36	DD6	F	303	-	39,45,45	2.11	3 (7%)	52,67,67	2.09	13 (25%)
29	CLA	E	314	28	52,56,73	1.44	10 (19%)	62,92,113	1.38	7 (11%)
29	CLA	D	316	-	45,49,73	1.53	8 (17%)	54,84,113	1.54	5 (9%)
37	PID	P	203	-	41,49,49	1.36	4 (9%)	49,76,76	1.45	8 (16%)
36	DD6	N	303	-	39,45,45	1.96	3 (7%)	52,67,67	1.76	12 (23%)
29	CLA	b	711	-	62,66,73	1.32	9 (14%)	74,104,113	1.35	7 (9%)
29	CLA	O	316	-	45,49,73	1.54	8 (17%)	54,84,113	1.50	5 (9%)
29	CLA	P	217	-	45,49,73	1.54	8 (17%)	54,84,113	1.57	5 (9%)
39	KC1	L	306	29	49,53,53	1.40	7 (14%)	63,89,89	2.03	17 (26%)
36	DD6	K	202	-	39,45,45	2.15	3 (7%)	52,67,67	3.00	16 (30%)
29	CLA	K	210	15	54,58,73	1.40	8 (14%)	65,95,113	1.43	8 (12%)
29	CLA	a	814	1	50,54,73	1.46	10 (20%)	60,90,113	1.39	4 (6%)
29	CLA	Q	313	-	51,55,73	1.44	9 (17%)	61,91,113	1.42	5 (8%)
39	KC1	C	312	-	49,53,53	1.43	7 (14%)	63,89,89	2.05	15 (23%)
36	DD6	A	201	-	39,45,45	2.02	3 (7%)	52,67,67	2.02	16 (30%)
29	CLA	b	702	2	69,73,73	1.24	9 (13%)	83,113,113	1.30	4 (4%)
29	CLA	I	209	-	64,68,73	1.30	10 (15%)	77,107,113	4.91	9 (11%)
34	LMG	K	220	-	36,36,55	0.86	1 (2%)	44,44,63	1.23	4 (9%)
29	CLA	P	212	-	55,59,73	1.41	8 (14%)	66,96,113	1.39	6 (9%)
29	CLA	H	313	-	51,55,73	1.45	9 (17%)	61,91,113	1.50	6 (9%)
39	KC1	O	310	-	49,53,53	1.41	7 (14%)	63,89,89	2.01	14 (22%)
37	PID	O	305	-	41,49,49	1.35	4 (9%)	49,76,76	1.59	7 (14%)
29	CLA	G	304	-	63,67,73	1.29	10 (15%)	75,105,113	1.41	6 (8%)
34	LMG	b	732	-	44,44,55	0.80	1 (2%)	52,52,63	1.32	6 (11%)
39	KC1	P	211	-	49,53,53	1.39	7 (14%)	63,89,89	2.01	16 (25%)
29	CLA	E	311	-	69,73,73	1.25	10 (14%)	83,113,113	1.31	9 (10%)
29	CLA	M	309	-	50,54,73	1.48	9 (18%)	60,90,113	1.39	7 (11%)
39	KC1	M	312	-	49,53,53	1.40	7 (14%)	63,89,89	2.03	14 (22%)
38	UIX	C	306	-	41,49,49	1.27	4 (9%)	52,74,74	2.55	22 (42%)
37	PID	D	305	-	41,49,49	1.32	4 (9%)	49,76,76	1.48	7 (14%)
37	PID	O	307	-	41,49,49	1.33	4 (9%)	49,76,76	1.45	7 (14%)
36	DD6	M	302	-	39,45,45	2.11	4 (10%)	52,67,67	2.09	14 (26%)
29	CLA	I	214	-	59,63,73	1.33	10 (16%)	71,101,113	1.35	7 (9%)
29	CLA	E	310	28	50,54,73	1.45	8 (16%)	60,90,113	1.41	5 (8%)
39	KC1	N	312	23	49,53,53	1.40	6 (12%)	63,89,89	2.01	15 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
29	CLA	G	317	-	57,61,73	1.38	10 (17%)	68,98,113	1.34	5 (7%)
36	DD6	B	303	-	39,45,45	2.04	3 (7%)	52,67,67	1.80	14 (26%)
39	KC1	T	312	-	49,53,53	1.40	6 (12%)	63,89,89	2.05	13 (20%)
29	CLA	a	816	1	50,54,73	1.45	10 (20%)	60,90,113	1.43	5 (8%)
37	PID	G	310	-	41,49,49	1.33	4 (9%)	49,76,76	1.45	7 (14%)
29	CLA	K	207	15	53,57,73	1.42	9 (16%)	62,93,113	1.42	7 (11%)
32	BCR	a	834	-	41,41,41	0.74	0	56,56,56	2.05	16 (28%)
37	PID	O	304	-	41,49,49	1.34	4 (9%)	49,76,76	1.50	6 (12%)
29	CLA	L	313	-	57,61,73	1.36	9 (15%)	68,98,113	1.39	7 (10%)
39	KC1	B	313	21	49,53,53	1.41	7 (14%)	63,89,89	2.01	15 (23%)
29	CLA	b	704	-	69,73,73	1.24	10 (14%)	83,113,113	3.81	6 (7%)
29	CLA	K	218	-	49,53,73	1.48	9 (18%)	59,89,113	1.43	4 (6%)
38	UIX	E	304	-	41,49,49	1.30	4 (9%)	52,74,74	2.43	18 (34%)
29	CLA	i	203	2	59,63,73	1.33	9 (15%)	71,101,113	1.39	6 (8%)
29	CLA	a	829	1	69,73,73	1.25	10 (14%)	83,113,113	1.29	7 (8%)
29	CLA	l	503	10	69,73,73	1.24	10 (14%)	83,113,113	1.29	7 (8%)
29	CLA	a	801	-	69,73,73	1.25	10 (14%)	83,113,113	1.30	5 (6%)
39	KC1	F	309	-	49,53,53	1.41	7 (14%)	63,89,89	2.06	14 (22%)
29	CLA	i	201	-	69,73,73	1.23	9 (13%)	83,113,113	1.30	5 (6%)
37	PID	N	307	-	41,49,49	1.36	4 (9%)	49,76,76	1.59	9 (18%)
37	PID	H	301	-	41,49,49	1.34	4 (9%)	49,76,76	1.48	5 (10%)
35	DGD	G	320	-	46,46,67	1.01	2 (4%)	60,60,81	0.98	3 (5%)
29	CLA	b	716	2	57,61,73	1.36	10 (17%)	68,98,113	1.35	6 (8%)
36	DD6	E	302	-	39,45,45	2.11	3 (7%)	52,67,67	2.26	18 (34%)
33	SF4	c	102	3	0,12,12	-	-	-		
29	CLA	b	717	-	69,73,73	1.24	9 (13%)	83,113,113	1.26	7 (8%)
37	PID	F	302	-	41,49,49	1.34	4 (9%)	49,76,76	1.67	6 (12%)
38	UIX	F	305	-	41,49,49	1.27	3 (7%)	52,74,74	2.89	19 (36%)
29	CLA	Q	312	-	50,54,73	1.45	9 (18%)	60,90,113	1.41	5 (8%)
29	CLA	N	309	-	69,73,73	1.25	7 (10%)	83,113,113	1.25	6 (7%)
29	CLA	A	215	12	51,55,73	1.44	9 (17%)	61,91,113	1.43	4 (6%)
29	CLA	a	824	-	69,73,73	1.24	10 (14%)	83,113,113	1.28	5 (6%)
36	DD6	A	204	-	39,45,45	2.02	3 (7%)	52,67,67	1.87	15 (28%)
36	DD6	B	301	-	38,44,45	2.03	3 (7%)	50,65,67	2.00	14 (28%)
38	UIX	Q	305	-	41,49,49	1.26	4 (9%)	52,74,74	2.78	22 (42%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
29	CLA	A	211	-	59,63,73	1.33	9 (15%)	71,101,113	1.31	6 (8%)
29	CLA	M	306	-	57,61,73	1.37	8 (14%)	68,98,113	1.39	5 (7%)
38	UIX	O	306	-	41,49,49	1.25	3 (7%)	52,74,74	2.70	21 (40%)
36	DD6	G	305	-	39,45,45	2.20	3 (7%)	52,67,67	2.96	17 (32%)
29	CLA	a	822	-	69,73,73	1.24	9 (13%)	83,113,113	1.29	6 (7%)
29	CLA	b	701	1	69,73,73	1.24	9 (13%)	83,113,113	1.33	8 (9%)
29	CLA	a	810	1	59,63,73	1.35	9 (15%)	71,101,113	1.38	7 (9%)
36	DD6	K	203	-	39,45,45	2.04	3 (7%)	52,67,67	1.90	13 (25%)
29	CLA	b	710	-	50,54,73	1.44	10 (20%)	60,90,113	1.38	5 (8%)
32	BCR	f	801	-	41,41,41	0.71	0	56,56,56	2.03	17 (30%)
39	KC1	O	312	-	49,53,53	1.44	6 (12%)	63,89,89	2.15	15 (23%)
29	CLA	P	215	-	51,55,73	1.46	6 (11%)	61,91,113	1.55	7 (11%)
29	CLA	b	724	2	51,55,73	1.44	10 (19%)	61,91,113	1.42	7 (11%)
29	CLA	b	723	2	69,73,73	1.24	10 (14%)	83,113,113	1.28	8 (9%)
29	CLA	b	725	-	69,73,73	1.25	10 (14%)	83,113,113	1.28	5 (6%)
29	CLA	K	209	-	58,62,73	1.37	9 (15%)	69,99,113	1.36	8 (11%)
29	CLA	L	312	-	59,63,73	1.34	9 (15%)	71,101,113	1.33	5 (7%)
35	DGD	m	102	-	67,67,67	0.83	2 (2%)	81,81,81	0.91	4 (4%)
29	CLA	B	309	21	59,63,73	1.34	9 (15%)	71,101,113	1.36	7 (9%)
29	CLA	T	308	-	51,55,73	1.45	9 (17%)	61,91,113	1.40	5 (8%)
29	CLA	a	809	1	69,73,73	1.24	10 (14%)	83,113,113	1.31	6 (7%)
29	CLA	P	209	-	51,55,73	1.46	7 (13%)	61,91,113	1.41	6 (9%)
39	KC1	J	312	17	49,53,53	1.40	6 (12%)	63,89,89	2.00	13 (20%)
29	CLA	D	308	-	51,55,73	1.44	8 (15%)	61,91,113	1.42	5 (8%)
29	CLA	J	308	-	60,64,73	1.35	9 (15%)	72,102,113	1.37	8 (11%)
32	BCR	b	729	-	41,41,41	0.79	1 (2%)	56,56,56	1.88	20 (35%)
29	CLA	K	212	-	56,60,73	1.40	9 (16%)	67,97,113	1.37	7 (10%)
29	CLA	M	308	18	52,56,73	1.43	10 (19%)	62,92,113	1.40	4 (6%)
29	CLA	F	311	16	50,54,73	1.44	9 (18%)	60,90,113	1.46	4 (6%)
29	CLA	a	830	-	60,64,73	1.33	9 (15%)	72,102,113	5.06	9 (12%)
39	KC1	Q	311	-	49,53,53	1.46	7 (14%)	63,89,89	2.07	14 (22%)
29	CLA	N	311	-	55,59,73	1.40	7 (12%)	66,96,113	1.39	5 (7%)
29	CLA	C	308	-	51,55,73	1.44	8 (15%)	61,91,113	1.40	5 (8%)
36	DD6	m	101	-	39,45,45	2.04	3 (7%)	52,67,67	2.04	16 (30%)
29	CLA	N	308	-	51,55,73	1.46	8 (15%)	61,91,113	1.41	5 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
29	CLA	I	213	14	69,73,73	1.25	9 (13%)	83,113,113	3.91	11 (13%)
39	KC1	Q	314	26	49,53,53	1.42	7 (14%)	63,89,89	2.06	13 (20%)
29	CLA	P	214	27	50,54,73	1.47	8 (16%)	60,90,113	1.43	5 (8%)
36	DD6	H	303	-	39,45,45	1.94	3 (7%)	52,67,67	1.98	14 (26%)
29	CLA	B	312	-	69,73,73	1.25	9 (13%)	83,113,113	1.30	6 (7%)
29	CLA	B	314	21	45,49,73	1.50	9 (20%)	54,84,113	1.55	5 (9%)
36	DD6	J	301	-	39,45,45	2.06	3 (7%)	52,67,67	2.26	17 (32%)
37	PID	E	301	-	41,49,49	1.39	4 (9%)	49,76,76	1.95	9 (18%)
29	CLA	I	217	-	59,63,73	1.34	8 (13%)	71,101,113	1.33	5 (7%)
36	DD6	L	304	-	39,45,45	2.02	3 (7%)	52,67,67	1.98	17 (32%)
29	CLA	J	305	-	50,54,73	1.46	9 (18%)	60,90,113	1.40	6 (10%)
36	DD6	F	301	-	39,45,45	2.11	4 (10%)	52,67,67	1.99	14 (26%)
34	LMG	j	102	-	43,43,55	0.78	0	51,51,63	1.29	5 (9%)
29	CLA	b	707	-	69,73,73	1.25	10 (14%)	83,113,113	1.32	7 (8%)
29	CLA	I	210	14	59,63,73	1.35	9 (15%)	71,101,113	1.35	7 (9%)
36	DD6	I	204	-	39,45,45	2.19	5 (12%)	52,67,67	2.08	16 (30%)
29	CLA	a	821	-	51,55,73	1.45	8 (15%)	61,91,113	1.40	5 (8%)
29	CLA	a	806	1	69,73,73	1.24	10 (14%)	83,113,113	1.32	5 (6%)
36	DD6	Q	302	-	39,45,45	1.99	3 (7%)	52,67,67	1.86	12 (23%)
29	CLA	D	311	-	50,54,73	1.45	8 (16%)	60,90,113	1.43	5 (8%)
29	CLA	B	311	21	55,59,73	1.39	10 (18%)	66,96,113	1.39	5 (7%)
36	DD6	T	303	-	39,45,45	1.98	3 (7%)	52,67,67	1.97	15 (28%)
40	SQD	B	317	-	41,42,54	0.44	1 (2%)	50,53,65	0.50	0
38	UIX	B	304	-	41,49,49	1.27	3 (7%)	52,74,74	2.45	16 (30%)
29	CLA	l	510	-	49,53,73	1.49	9 (18%)	59,89,113	1.42	6 (10%)
29	CLA	Q	308	-	69,73,73	1.26	10 (14%)	83,113,113	1.29	6 (7%)
36	DD6	M	301	-	39,45,45	2.00	3 (7%)	52,67,67	1.85	15 (28%)
29	CLA	L	317	-	50,54,73	1.46	9 (18%)	60,90,113	1.43	4 (6%)
36	DD6	C	303	-	39,45,45	2.07	3 (7%)	52,67,67	2.04	15 (28%)
37	PID	T	317	-	41,49,49	1.33	4 (9%)	49,76,76	1.70	9 (18%)
29	CLA	F	310	-	50,54,73	1.43	10 (20%)	60,90,113	1.48	5 (8%)
37	PID	C	301	-	41,49,49	1.34	4 (9%)	49,76,76	1.59	6 (12%)
29	CLA	Q	310	-	69,73,73	1.25	9 (13%)	83,113,113	1.29	7 (8%)
29	CLA	A	206	39	49,53,73	1.48	9 (18%)	59,89,113	1.50	5 (8%)
29	CLA	G	301	-	53,57,73	1.41	10 (18%)	62,93,113	1.40	6 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
29	CLA	H	308	-	69,73,73	1.25	9 (13%)	83,113,113	1.32	8 (9%)
29	CLA	O	308	-	51,55,73	1.47	8 (15%)	61,91,113	1.42	5 (8%)
36	DD6	B	302	-	39,45,45	2.06	3 (7%)	52,67,67	1.92	13 (25%)
29	CLA	I	207	14	53,57,73	1.41	10 (18%)	62,93,113	1.45	6 (9%)
29	CLA	F	313	16	50,54,73	1.46	8 (16%)	60,90,113	1.45	4 (6%)
33	SF4	a	836	1,2	0,12,12	-	-	-		
29	CLA	l	501	-	64,68,73	1.29	9 (14%)	77,107,113	1.36	5 (6%)
32	BCR	l	506	-	41,41,41	0.75	0	56,56,56	1.93	14 (25%)
37	PID	F	306	-	41,49,49	1.35	4 (9%)	49,76,76	1.47	6 (12%)
29	CLA	a	831	1	69,73,73	1.25	9 (13%)	83,113,113	4.73	8 (9%)
37	PID	h	204	-	41,49,49	1.35	4 (9%)	49,76,76	1.40	6 (12%)
29	CLA	E	306	28	69,73,73	1.25	10 (14%)	83,113,113	1.29	5 (6%)
29	CLA	I	212	-	59,63,73	1.35	9 (15%)	71,101,113	6.48	12 (16%)
29	CLA	a	808	-	55,59,73	1.40	9 (16%)	66,96,113	1.41	7 (10%)
37	PID	P	208	-	41,49,49	1.37	4 (9%)	49,76,76	2.42	7 (14%)
29	CLA	a	827	1	69,73,73	1.24	10 (14%)	83,113,113	1.30	7 (8%)
32	BCR	b	735	-	41,41,41	0.77	0	56,56,56	2.04	17 (30%)
29	CLA	E	305	-	65,69,73	1.30	9 (13%)	78,108,113	1.36	5 (6%)
34	LMG	b	730	-	46,46,55	0.81	2 (4%)	54,54,63	1.32	5 (9%)
29	CLA	F	316	16	45,49,73	1.52	9 (20%)	54,84,113	1.53	5 (9%)
39	KC1	E	307	28	49,53,53	1.41	7 (14%)	63,89,89	2.05	14 (22%)
29	CLA	b	718	2	69,73,73	1.26	9 (13%)	83,113,113	1.36	8 (9%)
29	CLA	M	315	-	50,54,73	1.46	8 (16%)	60,90,113	1.40	4 (6%)
29	CLA	b	712	2	69,73,73	1.24	10 (14%)	83,113,113	3.90	9 (10%)
36	DD6	O	303	-	39,45,45	2.10	4 (10%)	52,67,67	2.19	17 (32%)
29	CLA	M	307	-	59,63,73	1.36	10 (16%)	71,101,113	1.32	6 (8%)
29	CLA	L	308	-	57,61,73	1.38	9 (15%)	68,98,113	5.22	9 (13%)
29	CLA	N	314	-	51,55,73	1.44	9 (17%)	61,91,113	1.45	5 (8%)
36	DD6	J	302	-	39,45,45	2.08	2 (5%)	52,67,67	2.19	17 (32%)
36	DD6	M	304	-	39,45,45	2.05	3 (7%)	52,67,67	1.76	13 (25%)
36	DD6	B	305	-	39,45,45	2.02	3 (7%)	52,67,67	1.91	16 (30%)
29	CLA	h	201	2	64,68,73	1.29	10 (15%)	77,107,113	1.33	9 (11%)
29	CLA	l	509	-	45,49,73	1.51	10 (22%)	54,84,113	1.48	6 (11%)
29	CLA	T	314	-	51,55,73	1.44	8 (15%)	61,91,113	1.47	7 (11%)
38	UIX	J	304	-	41,49,49	1.26	3 (7%)	52,74,74	2.40	13 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
37	PID	F	304	-	41,49,49	1.61	5 (12%)	49,76,76	1.57	7 (14%)
29	CLA	D	313	20	49,53,73	1.49	9 (18%)	59,89,113	1.42	5 (8%)
29	CLA	H	312	22	50,54,73	1.45	7 (14%)	60,90,113	1.42	6 (10%)
29	CLA	b	714	-	68,72,73	1.25	10 (14%)	81,111,113	1.30	7 (8%)
29	CLA	a	815	-	49,53,73	1.47	10 (20%)	59,89,113	1.47	6 (10%)
32	BCR	l	507	-	41,41,41	0.75	0	56,56,56	1.99	16 (28%)
29	CLA	a	823	1	62,66,73	1.31	9 (14%)	74,104,113	1.31	8 (10%)
39	KC1	D	310	-	49,53,53	1.40	6 (12%)	63,89,89	2.01	12 (19%)
34	LMG	h	205	-	28,28,55	1.02	1 (3%)	36,36,63	1.27	4 (11%)
37	PID	D	306	-	41,49,49	1.36	4 (9%)	49,76,76	1.42	8 (16%)
38	UIX	N	306	-	41,49,49	1.26	4 (9%)	52,74,74	2.60	20 (38%)
29	CLA	B	308	-	69,73,73	1.25	10 (14%)	83,113,113	1.27	8 (9%)
39	KC1	H	309	22	49,53,53	1.39	7 (14%)	63,89,89	2.04	14 (22%)
32	BCR	a	835	-	41,41,41	0.79	0	56,56,56	2.12	16 (28%)
29	CLA	a	804	1	59,63,73	1.36	10 (16%)	71,101,113	1.43	8 (11%)
29	CLA	K	208	-	50,54,73	1.45	10 (20%)	60,90,113	1.39	5 (8%)
34	LMG	K	201	-	43,43,55	0.79	0	51,51,63	1.32	5 (9%)
37	PID	N	302	-	41,49,49	1.36	4 (9%)	49,76,76	1.41	5 (10%)
29	CLA	A	214	12	45,49,73	1.51	9 (20%)	54,84,113	1.49	6 (11%)
29	CLA	J	310	-	51,55,73	1.45	9 (17%)	61,91,113	1.43	8 (13%)
37	PID	T	302	-	41,49,49	1.38	4 (9%)	49,76,76	1.51	8 (16%)
29	CLA	D	309	-	50,54,73	1.46	8 (16%)	60,90,113	1.42	4 (6%)
36	DD6	I	203	-	39,45,45	2.29	3 (7%)	52,67,67	2.41	17 (32%)
36	DD6	K	205	-	39,45,45	2.05	3 (7%)	52,67,67	1.91	17 (32%)
29	CLA	b	731	-	60,64,73	1.33	9 (15%)	72,102,113	1.35	7 (9%)
29	CLA	J	309	17	50,54,73	1.45	9 (18%)	60,90,113	1.47	5 (8%)
34	LMG	P	201	-	27,27,55	0.98	0	35,35,63	1.29	5 (14%)
29	CLA	H	315	-	45,49,73	1.52	8 (17%)	54,84,113	1.48	6 (11%)
29	CLA	j	104	29	56,60,73	1.37	10 (17%)	67,97,113	1.43	5 (7%)
29	CLA	a	812	-	64,68,73	1.29	10 (15%)	77,107,113	1.36	7 (9%)
29	CLA	M	311	-	50,54,73	1.47	9 (18%)	60,90,113	1.39	6 (10%)
36	DD6	I	206	-	39,45,45	2.03	3 (7%)	52,67,67	1.90	12 (23%)
29	CLA	b	706	-	69,73,73	1.26	9 (13%)	83,113,113	1.33	5 (6%)
29	CLA	E	308	-	69,73,73	1.25	8 (11%)	83,113,113	1.30	6 (7%)
29	CLA	E	313	-	45,49,73	1.53	8 (17%)	54,84,113	1.49	5 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
31	LHG	a	833	-	47,47,48	0.28	0	50,53,54	0.31	0
39	KC1	G	318	-	49,53,53	1.41	7 (14%)	63,89,89	1.99	13 (20%)
30	PQN	a	832	-	34,34,34	1.52	2 (5%)	42,45,45	1.23	5 (11%)
36	DD6	L	303	-	39,45,45	2.06	3 (7%)	52,67,67	1.73	13 (25%)
29	CLA	A	209	-	69,73,73	1.24	9 (13%)	83,113,113	1.30	8 (9%)
36	DD6	K	204	-	39,45,45	2.08	3 (7%)	52,67,67	1.95	18 (34%)
29	CLA	D	312	20	50,54,73	1.46	8 (16%)	60,90,113	1.40	4 (6%)
29	CLA	a	811	1	60,64,73	1.36	9 (15%)	72,102,113	1.34	6 (8%)
29	CLA	D	314	-	51,55,73	1.45	10 (19%)	61,91,113	1.48	6 (9%)
29	CLA	a	802	-	69,73,73	1.25	9 (13%)	83,113,113	1.35	10 (12%)
29	CLA	N	313	23	50,54,73	1.45	8 (16%)	60,90,113	4.50	9 (15%)
39	KC1	I	215	14	49,53,53	1.41	7 (14%)	63,89,89	2.02	14 (22%)
29	CLA	G	302	-	69,73,73	1.25	8 (11%)	83,113,113	1.30	6 (7%)
29	CLA	l	502	10	69,73,73	1.25	10 (14%)	83,113,113	1.32	8 (9%)
36	DD6	K	206	-	39,45,45	2.05	3 (7%)	52,67,67	2.01	14 (26%)
37	PID	C	307	-	41,49,49	1.34	4 (9%)	49,76,76	1.52	6 (12%)
38	UIX	L	302	-	41,49,49	1.26	3 (7%)	52,74,74	2.41	17 (32%)
29	CLA	T	309	25	50,54,73	1.45	9 (18%)	60,90,113	1.43	5 (8%)
29	CLA	E	309	-	50,54,73	1.46	8 (16%)	60,90,113	1.44	5 (8%)
37	PID	Q	301	-	41,49,49	1.34	4 (9%)	49,76,76	1.47	6 (12%)
29	CLA	I	201	29	49,53,73	1.48	8 (16%)	59,89,113	1.47	4 (6%)
29	CLA	T	316	-	45,49,73	1.53	8 (17%)	54,84,113	1.52	5 (9%)
35	DGD	j	105	-	42,42,67	1.03	2 (4%)	56,56,81	1.07	5 (8%)
32	BCR	b	728	-	41,41,41	0.78	1 (2%)	56,56,56	2.04	15 (26%)
37	PID	H	306	-	41,49,49	1.31	4 (9%)	49,76,76	1.46	6 (12%)
40	SQD	J	314	-	44,45,54	0.42	1 (2%)	53,56,65	0.61	2 (3%)
37	PID	G	303	-	41,49,49	1.37	4 (9%)	49,76,76	1.33	5 (10%)
29	CLA	F	315	-	45,49,73	1.52	7 (15%)	54,84,113	1.55	6 (11%)
39	KC1	G	315	-	49,53,53	1.50	7 (14%)	63,89,89	2.11	14 (22%)
36	DD6	D	304	-	39,45,45	2.09	4 (10%)	52,67,67	2.14	15 (28%)
39	KC1	O	315	-	49,53,53	1.40	5 (10%)	63,89,89	2.02	13 (20%)
29	CLA	F	307	-	50,54,73	1.45	8 (16%)	60,90,113	1.43	5 (8%)
29	CLA	J	311	-	57,61,73	1.37	10 (17%)	68,98,113	1.38	6 (8%)
34	LMG	A	219	-	37,37,55	0.85	0	45,45,63	1.31	5 (11%)
32	BCR	m	103	-	41,41,41	0.82	1 (2%)	56,56,56	2.35	18 (32%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
29	CLA	B	315	21	50,54,73	1.45	9 (18%)	60,90,113	1.44	5 (8%)
29	CLA	a	818	-	51,55,73	1.45	9 (17%)	61,91,113	1.40	6 (9%)
39	KC1	H	314	-	49,53,53	1.40	7 (14%)	63,89,89	2.01	13 (20%)
36	DD6	G	306	-	39,45,45	2.12	3 (7%)	52,67,67	2.19	13 (25%)
29	CLA	B	307	-	49,53,73	1.48	9 (18%)	59,89,113	1.45	5 (8%)
30	PQN	b	727	-	34,34,34	1.54	2 (5%)	42,45,45	1.19	3 (7%)
37	PID	N	305	-	41,49,49	1.37	4 (9%)	49,76,76	1.36	4 (8%)
36	DD6	E	303	-	39,45,45	2.02	3 (7%)	52,67,67	1.74	10 (19%)
29	CLA	b	736	-	69,73,73	1.25	10 (14%)	83,113,113	6.01	11 (13%)
29	CLA	G	314	-	64,68,73	1.28	9 (14%)	77,107,113	1.38	6 (7%)
35	DGD	j	106	-	50,50,67	0.97	2 (4%)	64,64,81	1.04	4 (6%)
32	BCR	f	804	-	41,41,41	0.74	0	56,56,56	1.98	16 (28%)
37	PID	T	305	-	41,49,49	1.32	4 (9%)	49,76,76	1.52	7 (14%)
29	CLA	O	314	-	51,55,73	1.48	9 (17%)	61,91,113	1.46	8 (13%)
29	CLA	J	306	-	69,73,73	1.23	9 (13%)	83,113,113	1.31	5 (6%)
29	CLA	A	210	12	50,54,73	1.46	9 (18%)	60,90,113	1.36	5 (8%)
29	CLA	K	213	-	52,56,73	1.44	10 (19%)	62,92,113	1.38	6 (9%)
39	KC1	K	215	-	49,53,53	1.44	7 (14%)	63,89,89	2.06	15 (23%)
29	CLA	O	309	-	69,73,73	1.26	8 (11%)	83,113,113	1.24	4 (4%)
37	PID	T	307	-	41,49,49	1.33	4 (9%)	49,76,76	1.58	8 (16%)
37	PID	N	301	-	41,49,49	1.34	4 (9%)	49,76,76	1.49	5 (10%)
36	DD6	D	301	-	39,45,45	2.08	3 (7%)	52,67,67	2.07	15 (28%)
39	KC1	P	216	-	49,53,53	1.39	7 (14%)	63,89,89	2.00	12 (19%)
37	PID	C	304	-	41,49,49	1.34	4 (9%)	49,76,76	1.44	6 (12%)
29	CLA	B	316	-	49,53,73	1.49	9 (18%)	59,89,113	1.44	4 (6%)
29	CLA	K	216	-	45,49,73	1.51	10 (22%)	54,84,113	1.56	5 (9%)

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
36	DD6	h	202	-	-	2/26/80/80	0/3/3/3
29	CLA	G	311	13	-	9/23/99/115	-
29	CLA	Q	315	-	-	6/10/86/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
37	PID	G	309	-	-	2/24/93/93	0/4/4/4
34	LMG	E	316	-	-	10/27/47/70	0/1/1/1
39	KC1	C	310	25	-	9/15/71/71	-
29	CLA	b	703	-	-	13/39/115/115	-
29	CLA	I	211	-	-	8/39/115/115	-
37	PID	D	303	-	-	1/24/93/93	0/4/4/4
37	PID	Q	306	-	-	3/24/93/93	0/4/4/4
39	KC1	T	315	25	-	5/15/71/71	-
29	CLA	M	310	18	-	5/19/95/115	-
39	KC1	N	310	23	-	6/15/71/71	-
29	CLA	L	309	19	-	2/27/103/115	-
39	KC1	E	312	28	-	7/15/71/71	-
37	PID	D	307	-	-	4/24/93/93	0/4/4/4
29	CLA	b	708	2	-	5/24/100/115	-
29	CLA	b	719	-	-	10/21/97/115	-
37	PID	C	305	-	-	9/24/93/93	0/4/4/4
29	CLA	B	306	21	-	7/20/96/115	-
38	UIX	A	203	-	-	4/31/87/87	0/3/3/3
29	CLA	b	721	-	-	12/31/107/115	-
39	KC1	L	314	-	-	7/15/71/71	-
29	CLA	J	307	17	-	4/17/93/115	-
36	DD6	I	205	-	-	6/26/80/80	0/3/3/3
37	PID	N	304	-	-	1/24/93/93	0/4/4/4
37	PID	T	301	-	-	2/24/93/93	0/4/4/4
29	CLA	l	504	10	-	10/39/115/115	-
29	CLA	A	218	12	-	10/33/109/115	-
38	UIX	P	207	-	-	6/31/87/87	0/3/3/3
29	CLA	L	315	19	-	6/10/86/115	-
29	CLA	O	311	-	-	3/23/99/115	-
29	CLA	F	312	16	-	5/17/93/115	-
29	CLA	a	825	1	-	13/39/115/115	-
37	PID	P	206	-	-	8/24/93/93	0/4/4/4
29	CLA	b	713	-	-	6/25/101/115	-
37	PID	P	205	-	-	1/24/93/93	0/4/4/4
37	PID	Q	304	-	-	2/24/93/93	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
39	KC1	C	315	25	-	8/15/71/71	-
39	KC1	N	315	-	-	9/15/71/71	-
29	CLA	L	316	19	-	11/24/100/115	-
29	CLA	a	819	1	-	6/30/106/115	-
29	CLA	i	202	2	-	12/39/115/115	-
37	PID	H	304	-	-	0/24/93/93	0/4/4/4
36	DD6	L	301	-	-	4/26/80/80	0/3/3/3
29	CLA	C	309	-	-	10/39/115/115	-
39	KC1	A	205	29	-	6/15/71/71	-
29	CLA	a	817	-	-	6/15/91/115	-
36	DD6	B	319	-	-	9/26/80/80	0/3/3/3
29	CLA	F	308	-	-	4/17/93/115	-
29	CLA	L	311	19	-	7/17/93/115	-
29	CLA	C	314	-	-	7/18/94/115	-
29	CLA	G	313	13	-	3/27/103/115	-
29	CLA	l	508	-	-	2/10/86/115	-
29	CLA	f	802	-	-	4/17/93/115	-
39	KC1	M	305	-	-	5/15/71/71	-
29	CLA	A	212	-	-	10/27/103/115	-
35	DGD	b	733	-	-	24/46/86/95	0/2/2/2
29	CLA	l	505	-	-	12/39/115/115	-
29	CLA	G	319	13	-	3/10/86/115	-
29	CLA	G	316	-	-	12/39/115/115	-
29	CLA	Q	307	-	-	3/18/94/115	-
29	CLA	a	805	1	-	6/27/103/115	-
29	CLA	K	214	-	-	10/27/103/115	-
37	PID	D	302	-	-	1/24/93/93	0/4/4/4
29	CLA	b	705	-	-	12/39/115/115	-
29	CLA	T	311	-	-	10/17/93/115	-
29	CLA	C	311	-	-	7/23/99/115	-
38	UIX	T	306	-	-	4/31/87/87	0/3/3/3
29	CLA	A	217	-	-	9/23/99/115	-
36	DD6	J	303	-	-	2/26/80/80	0/3/3/3
29	CLA	A	208	12	-	4/27/103/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	CLA	H	307	-	-	7/18/94/115	-
35	DGD	B	318	-	-	9/34/74/95	0/2/2/2
29	CLA	I	208	-	-	9/17/93/115	-
39	KC1	P	213	27	-	5/15/71/71	-
37	PID	C	302	-	-	2/24/93/93	0/4/4/4
36	DD6	G	307	-	-	2/26/80/80	0/3/3/3
29	CLA	P	210	-	-	10/39/115/115	-
29	CLA	a	813	1	-	12/23/99/115	-
29	CLA	a	826	1	-	12/39/115/115	-
34	LMG	b	734	-	-	10/35/55/70	0/1/1/1
33	SF4	c	101	3	-	-	0/6/5/5
29	CLA	a	803	-	-	8/39/115/115	-
32	BCR	a	838	-	-	6/29/63/63	0/2/2/2
29	CLA	L	310	-	-	9/27/103/115	-
36	DD6	K	221	-	-	5/26/80/80	0/3/3/3
29	CLA	J	313	-	-	2/10/86/115	-
39	KC1	F	314	-	-	6/15/71/71	-
29	CLA	L	307	39	-	11/21/97/115	-
29	CLA	a	828	-	-	8/17/93/115	-
39	KC1	A	213	-	-	7/15/71/71	-
39	KC1	D	315	-	-	6/15/71/71	-
37	PID	j	101	-	-	2/24/93/93	0/4/4/4
39	KC1	Q	309	26	-	7/15/71/71	-
37	PID	P	202	-	-	4/24/93/93	0/4/4/4
29	CLA	b	720	2	-	15/39/115/115	-
29	CLA	a	820	1	-	12/39/115/115	-
39	KC1	H	311	-	-	6/15/71/71	-
29	CLA	b	709	2	-	17/33/109/115	-
29	CLA	K	211	-	-	7/27/103/115	-
29	CLA	b	726	-	-	8/39/115/115	-
29	CLA	A	207	-	-	5/27/103/115	-
29	CLA	M	313	-	-	2/10/86/115	-
29	CLA	N	316	-	-	5/10/86/115	-
34	LMG	K	219	-	-	16/30/50/70	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	CLA	B	310	-	-	16/39/115/115	-
29	CLA	a	837	-	-	14/27/103/115	-
29	CLA	A	216	-	-	2/10/86/115	-
36	DD6	L	305	-	-	4/26/80/80	0/3/3/3
37	PID	H	302	-	-	2/24/93/93	0/4/4/4
29	CLA	T	313	-	-	7/17/93/115	-
29	CLA	C	313	25	-	7/17/93/115	-
29	CLA	M	314	-	-	7/24/100/115	-
37	PID	O	302	-	-	2/24/93/93	0/4/4/4
37	PID	O	301	-	-	3/24/93/93	0/4/4/4
37	PID	Q	303	-	-	0/24/93/93	0/4/4/4
29	CLA	E	315	28	-	8/30/106/115	-
29	CLA	H	310	-	-	9/23/99/115	-
29	CLA	b	722	2	-	8/31/107/115	-
29	CLA	b	715	2	-	9/17/93/115	-
36	DD6	G	308	-	-	1/26/80/80	0/3/3/3
35	DGD	j	103	-	-	10/32/72/95	0/2/2/2
29	CLA	C	316	-	-	6/10/86/115	-
29	CLA	a	807	1	-	16/39/115/115	-
29	CLA	G	312	13	-	18/39/115/115	-
37	PID	T	304	-	-	1/24/93/93	0/4/4/4
36	DD6	P	204	-	-	2/26/80/80	0/3/3/3
29	CLA	f	803	6	-	8/17/93/115	-
29	CLA	I	216	-	-	4/24/100/115	-
32	BCR	i	204	-	-	4/29/63/63	0/2/2/2
35	DGD	h	203	-	-	8/43/83/95	0/2/2/2
36	DD6	A	202	-	-	1/26/80/80	0/3/3/3
29	CLA	O	313	24	-	5/17/93/115	-
36	DD6	I	202	-	-	5/26/80/80	0/3/3/3
39	KC1	T	310	25	-	5/15/71/71	-
36	DD6	M	303	-	-	6/26/80/80	0/3/3/3
29	CLA	f	805	-	-	10/33/109/115	-
29	CLA	K	217	15	-	5/17/93/115	-
37	PID	H	305	-	-	3/24/93/93	0/4/4/4
36	DD6	F	303	-	-	0/26/80/80	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	CLA	E	314	28	-	5/19/95/115	-
29	CLA	D	316	-	-	5/10/86/115	-
37	PID	P	203	-	-	3/24/93/93	0/4/4/4
36	DD6	N	303	-	-	1/26/80/80	0/3/3/3
29	CLA	b	711	-	-	11/31/107/115	-
29	CLA	O	316	-	-	5/10/86/115	-
29	CLA	P	217	-	-	3/10/86/115	-
39	KC1	L	306	29	-	5/15/71/71	-
36	DD6	K	202	-	-	8/26/80/80	0/3/3/3
29	CLA	K	210	15	-	6/21/97/115	-
29	CLA	a	814	1	-	6/17/93/115	-
29	CLA	Q	313	-	-	8/18/94/115	-
39	KC1	C	312	-	-	8/15/71/71	-
36	DD6	A	201	-	-	3/26/80/80	0/3/3/3
29	CLA	b	702	2	-	18/39/115/115	-
29	CLA	I	209	-	-	14/33/109/115	-
34	LMG	K	220	-	-	13/31/51/70	0/1/1/1
29	CLA	P	212	-	-	10/23/99/115	-
29	CLA	H	313	-	-	8/18/94/115	-
39	KC1	O	310	-	-	6/15/71/71	-
37	PID	O	305	-	-	7/24/93/93	0/4/4/4
29	CLA	G	304	-	-	14/32/108/115	-
34	LMG	b	732	-	-	20/39/59/70	0/1/1/1
39	KC1	P	211	-	-	7/15/71/71	-
29	CLA	E	311	-	-	11/39/115/115	-
29	CLA	M	309	-	-	6/17/93/115	-
39	KC1	M	312	-	-	6/15/71/71	-
38	UIX	C	306	-	-	6/31/87/87	0/3/3/3
37	PID	D	305	-	-	5/24/93/93	0/4/4/4
37	PID	O	307	-	-	4/24/93/93	0/4/4/4
36	DD6	M	302	-	-	1/26/80/80	0/3/3/3
29	CLA	I	214	-	-	5/27/103/115	-
29	CLA	E	310	28	-	4/17/93/115	-
39	KC1	N	312	23	-	6/15/71/71	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	CLA	G	317	-	-	8/25/101/115	-
36	DD6	B	303	-	-	0/26/80/80	0/3/3/3
39	KC1	T	312	-	-	5/15/71/71	-
29	CLA	a	816	1	-	10/17/93/115	-
37	PID	G	310	-	-	2/24/93/93	0/4/4/4
29	CLA	K	207	15	-	8/20/96/115	-
32	BCR	a	834	-	-	0/29/63/63	0/2/2/2
37	PID	O	304	-	-	3/24/93/93	0/4/4/4
29	CLA	L	313	-	-	8/25/101/115	-
39	KC1	B	313	21	-	8/15/71/71	-
29	CLA	b	704	-	-	12/39/115/115	-
29	CLA	K	218	-	-	9/15/91/115	-
38	UIX	E	304	-	-	2/31/87/87	0/3/3/3
29	CLA	i	203	2	-	12/27/103/115	-
29	CLA	a	829	1	-	16/39/115/115	-
29	CLA	l	503	10	-	17/39/115/115	-
29	CLA	a	801	-	-	12/39/115/115	-
39	KC1	F	309	-	-	7/15/71/71	-
29	CLA	i	201	-	-	16/39/115/115	-
37	PID	N	307	-	-	6/24/93/93	0/4/4/4
37	PID	H	301	-	-	2/24/93/93	0/4/4/4
35	DGD	G	320	-	-	9/34/74/95	0/2/2/2
29	CLA	b	716	2	-	7/25/101/115	-
36	DD6	E	302	-	-	2/26/80/80	0/3/3/3
33	SF4	c	102	3	-	-	0/6/5/5
29	CLA	b	717	-	-	15/39/115/115	-
37	PID	F	302	-	-	3/24/93/93	0/4/4/4
38	UIX	F	305	-	-	12/31/87/87	0/3/3/3
29	CLA	Q	312	-	-	5/17/93/115	-
29	CLA	N	309	-	-	15/39/115/115	-
29	CLA	A	215	12	-	5/18/94/115	-
29	CLA	a	824	-	-	9/39/115/115	-
36	DD6	A	204	-	-	2/26/80/80	0/3/3/3
36	DD6	B	301	-	-	4/24/78/80	0/3/3/3
38	UIX	Q	305	-	-	5/31/87/87	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	CLA	A	211	-	-	5/27/103/115	-
29	CLA	M	306	-	-	6/25/101/115	-
38	UIX	O	306	-	-	6/31/87/87	0/3/3/3
36	DD6	G	305	-	-	7/26/80/80	0/3/3/3
29	CLA	a	822	-	-	10/39/115/115	-
29	CLA	b	701	1	-	13/39/115/115	-
29	CLA	a	810	1	-	10/27/103/115	-
36	DD6	K	203	-	-	6/26/80/80	0/3/3/3
29	CLA	b	710	-	-	7/17/93/115	-
32	BCR	f	801	-	-	5/29/63/63	0/2/2/2
39	KC1	O	312	-	-	4/15/71/71	-
29	CLA	P	215	-	-	8/18/94/115	-
29	CLA	b	724	2	-	2/18/94/115	-
29	CLA	b	723	2	-	5/39/115/115	-
29	CLA	b	725	-	-	11/39/115/115	-
29	CLA	K	209	-	-	10/26/102/115	-
29	CLA	L	312	-	-	11/27/103/115	-
35	DGD	m	102	-	-	8/55/95/95	0/2/2/2
29	CLA	B	309	21	-	6/27/103/115	-
29	CLA	T	308	-	-	4/18/94/115	-
29	CLA	a	809	1	-	17/39/115/115	-
29	CLA	P	209	-	-	10/18/94/115	-
39	KC1	J	312	17	-	5/15/71/71	-
29	CLA	D	308	-	-	6/18/94/115	-
29	CLA	J	308	-	-	8/29/105/115	-
32	BCR	b	729	-	-	6/29/63/63	0/2/2/2
29	CLA	K	212	-	-	7/24/100/115	-
29	CLA	M	308	18	-	9/19/95/115	-
29	CLA	F	311	16	-	5/17/93/115	-
29	CLA	a	830	-	-	5/29/105/115	-
39	KC1	Q	311	-	-	6/15/71/71	-
29	CLA	N	311	-	-	6/23/99/115	-
29	CLA	C	308	-	-	9/18/94/115	-
36	DD6	m	101	-	-	1/26/80/80	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	CLA	N	308	-	-	9/18/94/115	-
29	CLA	I	213	14	-	15/39/115/115	-
39	KC1	Q	314	26	-	8/15/71/71	-
29	CLA	P	214	27	-	9/17/93/115	-
36	DD6	H	303	-	-	1/26/80/80	0/3/3/3
29	CLA	B	312	-	-	10/39/115/115	-
29	CLA	B	314	21	-	6/10/86/115	-
36	DD6	J	301	-	-	3/26/80/80	0/3/3/3
37	PID	E	301	-	-	6/24/93/93	0/4/4/4
29	CLA	I	217	-	-	9/27/103/115	-
36	DD6	L	304	-	-	2/26/80/80	0/3/3/3
29	CLA	J	305	-	-	4/17/93/115	-
36	DD6	F	301	-	-	8/26/80/80	0/3/3/3
34	LMG	j	102	-	-	24/38/58/70	0/1/1/1
29	CLA	b	707	-	-	13/39/115/115	-
29	CLA	I	210	14	-	6/27/103/115	-
36	DD6	I	204	-	-	3/26/80/80	0/3/3/3
29	CLA	a	821	-	-	9/18/94/115	-
29	CLA	a	806	1	-	16/39/115/115	-
36	DD6	Q	302	-	-	1/26/80/80	0/3/3/3
29	CLA	D	311	-	-	12/17/93/115	-
29	CLA	B	311	21	-	4/23/99/115	-
36	DD6	T	303	-	-	7/26/80/80	0/3/3/3
40	SQD	B	317	-	-	4/37/57/69	0/1/1/1
38	UIX	B	304	-	-	2/31/87/87	0/3/3/3
29	CLA	l	510	-	-	7/15/91/115	-
29	CLA	Q	308	-	-	21/39/115/115	-
36	DD6	M	301	-	-	2/26/80/80	0/3/3/3
29	CLA	L	317	-	-	7/17/93/115	-
36	DD6	C	303	-	-	0/26/80/80	0/3/3/3
37	PID	T	317	-	-	10/24/93/93	1/4/4/4
29	CLA	F	310	-	-	8/17/93/115	-
37	PID	C	301	-	-	4/24/93/93	0/4/4/4
29	CLA	Q	310	-	-	13/39/115/115	-
29	CLA	A	206	39	-	5/15/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	CLA	G	301	-	-	6/20/96/115	-
29	CLA	H	308	-	-	9/39/115/115	-
29	CLA	O	308	-	-	8/18/94/115	-
36	DD6	B	302	-	-	2/26/80/80	0/3/3/3
29	CLA	I	207	14	-	7/20/96/115	-
29	CLA	F	313	16	-	8/17/93/115	-
37	PID	F	306	-	-	0/24/93/93	0/4/4/4
29	CLA	l	501	-	-	13/33/109/115	-
32	BCR	l	506	-	-	9/29/63/63	0/2/2/2
33	SF4	a	836	1,2	-	-	0/6/5/5
29	CLA	a	831	1	-	14/39/115/115	-
37	PID	h	204	-	-	2/24/93/93	1/4/4/4
29	CLA	E	306	28	-	16/39/115/115	-
29	CLA	I	212	-	-	12/27/103/115	-
29	CLA	a	808	-	-	6/23/99/115	-
37	PID	P	208	-	-	4/24/93/93	0/4/4/4
29	CLA	a	827	1	-	14/39/115/115	-
32	BCR	b	735	-	-	4/29/63/63	0/2/2/2
29	CLA	E	305	-	-	16/35/111/115	-
34	LMG	b	730	-	-	19/41/61/70	0/1/1/1
29	CLA	F	316	16	-	5/10/86/115	-
39	KC1	E	307	28	-	6/15/71/71	-
29	CLA	b	718	2	-	14/39/115/115	-
29	CLA	M	315	-	-	5/17/93/115	-
29	CLA	b	712	2	-	12/39/115/115	-
36	DD6	O	303	-	-	4/26/80/80	0/3/3/3
29	CLA	M	307	-	-	6/27/103/115	-
29	CLA	L	308	-	-	10/25/101/115	-
29	CLA	N	314	-	-	7/18/94/115	-
36	DD6	J	302	-	-	2/26/80/80	0/3/3/3
36	DD6	M	304	-	-	3/26/80/80	0/3/3/3
36	DD6	B	305	-	-	2/26/80/80	0/3/3/3
29	CLA	h	201	2	-	7/33/109/115	-
29	CLA	l	509	-	-	2/10/86/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	CLA	T	314	-	-	7/18/94/115	-
38	UIX	J	304	-	-	3/31/87/87	0/3/3/3
37	PID	F	304	-	-	15/24/93/93	1/4/4/4
29	CLA	D	313	20	-	4/15/91/115	-
29	CLA	H	312	22	-	7/17/93/115	-
29	CLA	b	714	-	-	7/38/114/115	-
29	CLA	a	815	-	-	4/15/91/115	-
32	BCR	l	507	-	-	5/29/63/63	0/2/2/2
29	CLA	a	823	1	-	11/31/107/115	-
39	KC1	D	310	-	-	5/15/71/71	-
34	LMG	h	205	-	-	3/23/43/70	0/1/1/1
37	PID	D	306	-	-	3/24/93/93	0/4/4/4
38	UIX	N	306	-	-	9/31/87/87	0/3/3/3
29	CLA	B	308	-	-	13/39/115/115	-
39	KC1	H	309	22	-	8/15/71/71	-
32	BCR	a	835	-	-	2/29/63/63	0/2/2/2
29	CLA	a	804	1	-	1/27/103/115	-
29	CLA	K	208	-	-	5/17/93/115	-
34	LMG	K	201	-	-	17/38/58/70	0/1/1/1
37	PID	N	302	-	-	2/24/93/93	0/4/4/4
29	CLA	A	214	12	-	6/10/86/115	-
29	CLA	J	310	-	-	6/18/94/115	-
37	PID	T	302	-	-	1/24/93/93	0/4/4/4
29	CLA	D	309	-	-	2/17/93/115	-
36	DD6	I	203	-	-	7/26/80/80	0/3/3/3
36	DD6	K	205	-	-	1/26/80/80	0/3/3/3
29	CLA	b	731	-	-	3/29/105/115	-
29	CLA	J	309	17	-	5/17/93/115	-
34	LMG	P	201	-	-	6/22/42/70	0/1/1/1
29	CLA	H	315	-	-	3/10/86/115	-
29	CLA	j	104	29	-	4/24/100/115	-
29	CLA	a	812	-	-	16/33/109/115	-
29	CLA	M	311	-	-	8/17/93/115	-
36	DD6	I	206	-	-	2/26/80/80	0/3/3/3
29	CLA	b	706	-	-	11/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	CLA	E	308	-	-	11/39/115/115	-
29	CLA	E	313	-	-	2/10/86/115	-
31	LHG	a	833	-	-	8/52/52/53	-
39	KC1	G	318	-	-	5/15/71/71	-
30	PQN	a	832	-	-	6/23/43/43	0/2/2/2
36	DD6	L	303	-	-	0/26/80/80	0/3/3/3
29	CLA	A	209	-	-	20/39/115/115	-
36	DD6	K	204	-	-	5/26/80/80	0/3/3/3
29	CLA	D	312	20	-	7/17/93/115	-
29	CLA	a	811	1	-	8/29/105/115	-
29	CLA	D	314	-	-	7/18/94/115	-
29	CLA	a	802	-	-	10/39/115/115	-
29	CLA	N	313	23	-	9/17/93/115	-
39	KC1	I	215	14	-	10/15/71/71	-
29	CLA	G	302	-	-	15/39/115/115	-
29	CLA	l	502	10	-	15/39/115/115	-
36	DD6	K	206	-	-	1/26/80/80	0/3/3/3
37	PID	C	307	-	-	2/24/93/93	0/4/4/4
38	UIX	L	302	-	-	2/31/87/87	0/3/3/3
29	CLA	T	309	25	-	5/17/93/115	-
29	CLA	E	309	-	-	10/17/93/115	-
37	PID	Q	301	-	-	2/24/93/93	0/4/4/4
29	CLA	I	201	29	-	4/15/91/115	-
29	CLA	T	316	-	-	6/10/86/115	-
35	DGD	j	105	-	-	0/30/70/95	0/2/2/2
32	BCR	b	728	-	-	7/29/63/63	0/2/2/2
37	PID	H	306	-	-	4/24/93/93	0/4/4/4
40	SQD	J	314	-	-	9/40/60/69	0/1/1/1
37	PID	G	303	-	-	6/24/93/93	0/4/4/4
29	CLA	F	315	-	-	3/10/86/115	-
39	KC1	G	315	-	-	6/15/71/71	-
36	DD6	D	304	-	-	6/26/80/80	0/3/3/3
39	KC1	O	315	-	-	9/15/71/71	-
29	CLA	F	307	-	-	4/17/93/115	-
29	CLA	J	311	-	-	10/25/101/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
34	LMG	A	219	-	-	17/32/52/70	0/1/1/1
32	BCR	m	103	-	-	5/29/63/63	0/2/2/2
29	CLA	B	315	21	-	3/17/93/115	-
29	CLA	a	818	-	-	6/18/94/115	-
39	KC1	H	314	-	-	6/15/71/71	-
36	DD6	G	306	-	-	1/26/80/80	0/3/3/3
29	CLA	B	307	-	-	4/15/91/115	-
30	PQN	b	727	-	-	4/23/43/43	0/2/2/2
37	PID	N	305	-	-	19/24/93/93	0/4/4/4
36	DD6	E	303	-	-	1/26/80/80	0/3/3/3
29	CLA	b	736	-	-	18/39/115/115	-
29	CLA	G	314	-	-	8/33/109/115	-
35	DGD	j	106	-	-	16/38/78/95	0/2/2/2
32	BCR	f	804	-	-	2/29/63/63	0/2/2/2
37	PID	T	305	-	-	0/24/93/93	0/4/4/4
29	CLA	O	314	-	-	6/18/94/115	-
29	CLA	J	306	-	-	17/39/115/115	-
29	CLA	A	210	12	-	8/17/93/115	-
29	CLA	K	213	-	-	7/19/95/115	-
39	KC1	K	215	-	-	6/15/71/71	-
29	CLA	O	309	-	-	10/39/115/115	-
37	PID	T	307	-	-	4/24/93/93	0/4/4/4
37	PID	N	301	-	-	4/24/93/93	0/4/4/4
36	DD6	D	301	-	-	8/26/80/80	0/3/3/3
39	KC1	P	216	-	-	6/15/71/71	-
37	PID	C	304	-	-	3/24/93/93	0/4/4/4
29	CLA	B	316	-	-	6/15/91/115	-
29	CLA	K	216	-	-	3/10/86/115	-

The worst 5 of 2723 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	G	307	DD6	C29-C27	-9.45	1.24	1.42
36	I	203	DD6	C29-C27	-9.14	1.25	1.42
36	K	202	DD6	C29-C27	-9.12	1.25	1.42
36	G	306	DD6	C29-C27	-9.01	1.25	1.42
36	K	221	DD6	C29-C27	-8.93	1.25	1.42

The worst 5 of 3486 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	L	308	CLA	O2D-CGD-CBD	26.55	158.46	111.27
29	b	736	CLA	O2D-CGD-CBD	26.54	158.43	111.27
29	I	209	CLA	O2D-CGD-CBD	26.47	158.31	111.27
29	I	212	CLA	O2D-CGD-CBD	26.29	157.99	111.27
29	a	831	CLA	O2D-CGD-CBD	26.25	157.91	111.27

There are no chirality outliers.

5 of 2853 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
29	a	801	CLA	CHA-CBD-CGD-O1D
29	a	801	CLA	CHA-CBD-CGD-O2D
29	a	801	CLA	CBD-CGD-O2D-CED
29	a	805	CLA	C1A-C2A-CAA-CBA
29	a	805	CLA	C3A-C2A-CAA-CBA

All (3) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
37	h	204	PID	C24-C25-C26-C27-C28-C29
37	T	317	PID	C24-C25-C26-C27-C28-C29
37	F	304	PID	C24-C25-C26-C27-C28-C29

331 monomers are involved in 958 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
29	Q	315	CLA	2	0
37	G	309	PID	2	0
34	E	316	LMG	6	0
39	C	310	KC1	1	0
29	b	703	CLA	7	0
29	I	211	CLA	3	0
37	D	303	PID	10	0
37	Q	306	PID	5	0
39	N	310	KC1	2	0
37	D	307	PID	2	0
29	b	708	CLA	3	0
29	b	719	CLA	10	0
37	C	305	PID	10	0
29	B	306	CLA	1	0
29	b	721	CLA	5	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
29	J	307	CLA	2	0
36	I	205	DD6	3	0
37	N	304	PID	2	0
37	T	301	PID	4	0
29	l	504	CLA	10	0
29	A	218	CLA	2	0
29	L	315	CLA	2	0
29	F	312	CLA	4	0
29	a	825	CLA	4	0
37	P	206	PID	9	0
29	b	713	CLA	1	0
37	P	205	PID	3	0
37	Q	304	PID	5	0
39	N	315	KC1	3	0
29	L	316	CLA	4	0
29	a	819	CLA	4	0
29	i	202	CLA	8	0
37	H	304	PID	4	0
36	L	301	DD6	1	0
29	C	309	CLA	3	0
29	a	817	CLA	1	0
36	B	319	DD6	4	0
29	F	308	CLA	1	0
29	L	311	CLA	1	0
29	C	314	CLA	6	0
29	G	313	CLA	1	0
29	f	802	CLA	1	0
29	A	212	CLA	3	0
35	b	733	DGD	2	0
29	l	505	CLA	6	0
29	G	316	CLA	1	0
29	Q	307	CLA	3	0
29	a	805	CLA	2	0
29	K	214	CLA	7	0
37	D	302	PID	1	0
29	b	705	CLA	9	0
29	T	311	CLA	1	0
29	C	311	CLA	2	0
29	A	217	CLA	2	0
36	J	303	DD6	1	0
29	A	208	CLA	2	0
29	I	208	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
37	C	302	PID	4	0
36	G	307	DD6	3	0
29	P	210	CLA	7	0
29	a	813	CLA	2	0
29	a	826	CLA	5	0
34	b	734	LMG	1	0
29	a	803	CLA	8	0
32	a	838	BCR	5	0
29	L	310	CLA	3	0
36	K	221	DD6	2	0
29	J	313	CLA	1	0
29	L	307	CLA	1	0
29	a	828	CLA	4	0
39	D	315	KC1	2	0
37	j	101	PID	5	0
37	P	202	PID	4	0
29	b	720	CLA	5	0
29	a	820	CLA	4	0
29	b	709	CLA	3	0
29	K	211	CLA	3	0
29	b	726	CLA	6	0
29	A	207	CLA	1	0
29	M	313	CLA	1	0
34	K	219	LMG	2	0
29	B	310	CLA	5	0
29	a	837	CLA	5	0
29	A	216	CLA	2	0
36	L	305	DD6	1	0
37	H	302	PID	3	0
29	T	313	CLA	2	0
29	C	313	CLA	1	0
29	M	314	CLA	1	0
37	O	302	PID	8	0
37	O	301	PID	2	0
37	Q	303	PID	2	0
29	E	315	CLA	5	0
29	H	310	CLA	3	0
29	b	722	CLA	2	0
29	b	715	CLA	4	0
35	j	103	DGD	2	0
29	C	316	CLA	3	0
29	a	807	CLA	7	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
29	G	312	CLA	4	0
37	T	304	PID	4	0
36	P	204	DD6	1	0
29	f	803	CLA	2	0
29	I	216	CLA	2	0
32	i	204	BCR	7	0
35	h	203	DGD	9	0
36	A	202	DD6	1	0
29	O	313	CLA	3	0
36	M	303	DD6	1	0
29	f	805	CLA	5	0
29	K	217	CLA	1	0
37	H	305	PID	7	0
36	F	303	DD6	2	0
29	E	314	CLA	1	0
29	D	316	CLA	1	0
37	P	203	PID	5	0
36	N	303	DD6	1	0
29	b	711	CLA	6	0
29	O	316	CLA	1	0
29	P	217	CLA	2	0
29	K	210	CLA	4	0
29	a	814	CLA	1	0
29	Q	313	CLA	4	0
29	b	702	CLA	11	0
29	I	209	CLA	4	0
34	K	220	LMG	1	0
29	P	212	CLA	2	0
29	H	313	CLA	4	0
37	O	305	PID	7	0
29	G	304	CLA	7	0
34	b	732	LMG	6	0
39	P	211	KC1	1	0
29	E	311	CLA	3	0
29	M	309	CLA	2	0
37	D	305	PID	5	0
37	O	307	PID	5	0
36	M	302	DD6	3	0
29	I	214	CLA	4	0
29	E	310	CLA	1	0
29	G	317	CLA	2	0
36	B	303	DD6	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
29	a	816	CLA	1	0
37	G	310	PID	3	0
32	a	834	BCR	8	0
37	O	304	PID	3	0
29	L	313	CLA	4	0
29	b	704	CLA	2	0
29	K	218	CLA	3	0
38	E	304	UIX	1	0
29	i	203	CLA	5	0
29	a	829	CLA	5	0
29	l	503	CLA	6	0
29	a	801	CLA	4	0
29	i	201	CLA	6	0
37	N	307	PID	6	0
37	H	301	PID	4	0
35	G	320	DGD	2	0
29	b	716	CLA	5	0
33	c	102	SF4	3	0
29	b	717	CLA	5	0
37	F	302	PID	1	0
38	F	305	UIX	2	0
29	Q	312	CLA	3	0
29	N	309	CLA	8	0
29	A	215	CLA	2	0
29	a	824	CLA	10	0
36	A	204	DD6	1	0
36	B	301	DD6	2	0
29	A	211	CLA	2	0
29	M	306	CLA	1	0
36	G	305	DD6	1	0
29	a	822	CLA	2	0
29	b	701	CLA	5	0
29	a	810	CLA	7	0
32	f	801	BCR	8	0
29	P	215	CLA	5	0
29	b	724	CLA	7	0
29	b	723	CLA	6	0
29	b	725	CLA	3	0
29	K	209	CLA	2	0
29	L	312	CLA	4	0
35	m	102	DGD	5	0
29	B	309	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
29	a	809	CLA	6	0
29	P	209	CLA	2	0
29	D	308	CLA	1	0
32	b	729	BCR	5	0
29	K	212	CLA	4	0
29	M	308	CLA	1	0
29	F	311	CLA	4	0
29	a	830	CLA	1	0
29	N	311	CLA	1	0
29	C	308	CLA	2	0
29	N	308	CLA	1	0
29	I	213	CLA	3	0
39	Q	314	KC1	2	0
29	P	214	CLA	2	0
29	B	312	CLA	2	0
37	E	301	PID	7	0
29	I	217	CLA	4	0
29	J	305	CLA	1	0
34	j	102	LMG	3	0
29	b	707	CLA	7	0
29	I	210	CLA	3	0
29	a	821	CLA	3	0
29	a	806	CLA	11	0
29	D	311	CLA	1	0
36	T	303	DD6	1	0
40	B	317	SQD	3	0
38	B	304	UIX	1	0
29	l	510	CLA	3	0
29	Q	308	CLA	4	0
36	M	301	DD6	1	0
29	L	317	CLA	1	0
36	C	303	DD6	1	0
37	T	317	PID	3	0
29	F	310	CLA	5	0
37	C	301	PID	2	0
29	Q	310	CLA	3	0
29	A	206	CLA	2	0
29	G	301	CLA	2	0
29	H	308	CLA	5	0
29	I	207	CLA	2	0
29	F	313	CLA	4	0
33	a	836	SF4	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
29	l	501	CLA	9	0
32	l	506	BCR	4	0
37	F	306	PID	5	0
29	a	831	CLA	4	0
37	h	204	PID	1	0
29	E	306	CLA	9	0
29	I	212	CLA	3	0
29	a	808	CLA	3	0
37	P	208	PID	3	0
29	a	827	CLA	4	0
32	b	735	BCR	8	0
29	E	305	CLA	6	0
34	b	730	LMG	6	0
39	E	307	KC1	2	0
29	b	718	CLA	5	0
29	M	315	CLA	1	0
29	b	712	CLA	5	0
36	O	303	DD6	2	0
29	M	307	CLA	2	0
29	L	308	CLA	2	0
29	N	314	CLA	5	0
36	J	302	DD6	4	0
36	M	304	DD6	1	0
36	B	305	DD6	1	0
29	h	201	CLA	7	0
29	l	509	CLA	2	0
29	T	314	CLA	8	0
38	J	304	UIX	1	0
37	F	304	PID	15	0
29	D	313	CLA	2	0
29	H	312	CLA	2	0
29	b	714	CLA	4	0
29	a	815	CLA	1	0
32	l	507	BCR	4	0
29	a	823	CLA	5	0
34	h	205	LMG	2	0
37	D	306	PID	3	0
29	B	308	CLA	5	0
39	H	309	KC1	1	0
32	a	835	BCR	4	0
29	a	804	CLA	6	0
34	K	201	LMG	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
37	N	302	PID	4	0
29	A	214	CLA	2	0
29	J	310	CLA	3	0
37	T	302	PID	4	0
29	D	309	CLA	2	0
29	b	731	CLA	2	0
29	J	309	CLA	5	0
34	P	201	LMG	1	0
29	H	315	CLA	2	0
29	a	812	CLA	5	0
29	M	311	CLA	8	0
36	I	206	DD6	1	0
29	b	706	CLA	3	0
29	E	308	CLA	3	0
29	E	313	CLA	2	0
31	a	833	LHG	5	0
39	G	318	KC1	1	0
30	a	832	PQN	6	0
29	A	209	CLA	1	0
36	K	204	DD6	2	0
29	D	312	CLA	4	0
29	a	811	CLA	2	0
29	D	314	CLA	9	0
29	a	802	CLA	4	0
29	N	313	CLA	1	0
39	I	215	KC1	1	0
29	G	302	CLA	9	0
29	l	502	CLA	1	0
37	C	307	PID	3	0
29	T	309	CLA	4	0
37	Q	301	PID	5	0
29	T	316	CLA	3	0
35	j	105	DGD	4	0
32	b	728	BCR	6	0
37	H	306	PID	7	0
40	J	314	SQD	7	0
37	G	303	PID	3	0
29	F	315	CLA	1	0
39	G	315	KC1	1	0
36	D	304	DD6	3	0
29	F	307	CLA	3	0
29	J	311	CLA	2	0

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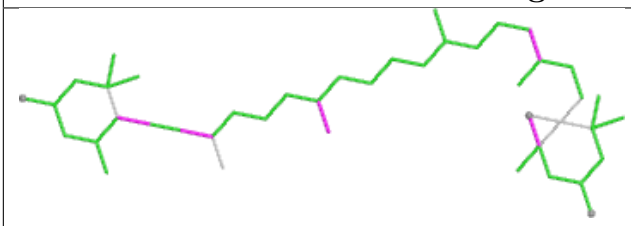
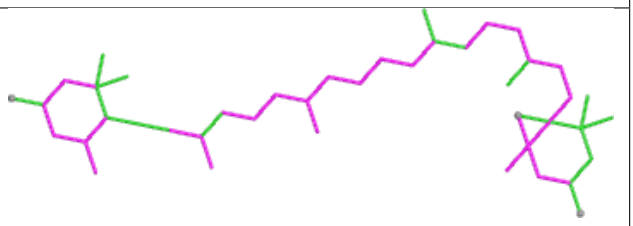
Mol	Chain	Res	Type	Clashes	Symm-Clashes
34	A	219	LMG	2	0
32	m	103	BCR	8	0
29	B	315	CLA	1	0
29	a	818	CLA	1	0
39	H	314	KC1	1	0
29	B	307	CLA	2	0
30	b	727	PQN	3	0
37	N	305	PID	7	0
29	b	736	CLA	4	0
29	G	314	CLA	4	0
35	j	106	DGD	4	0
32	f	804	BCR	5	0
37	T	305	PID	5	0
29	O	314	CLA	10	0
29	J	306	CLA	5	0
29	K	213	CLA	6	0
29	O	309	CLA	6	0
37	T	307	PID	3	0
37	N	301	PID	2	0
39	P	216	KC1	1	0
37	C	304	PID	4	0
29	B	316	CLA	1	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.

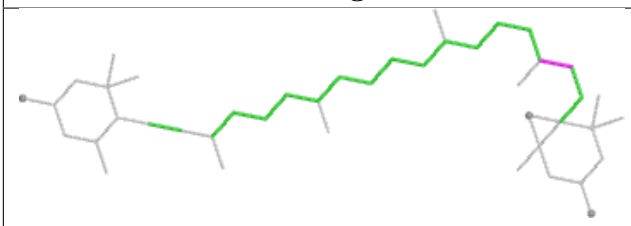
Ligand DD6 h 202



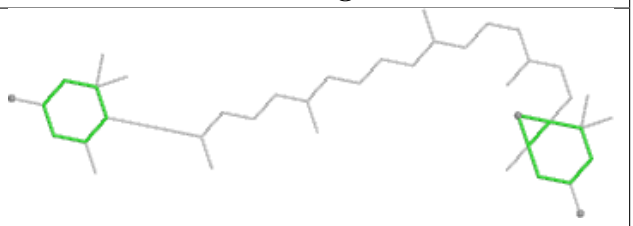
Bond lengths



Bond angles

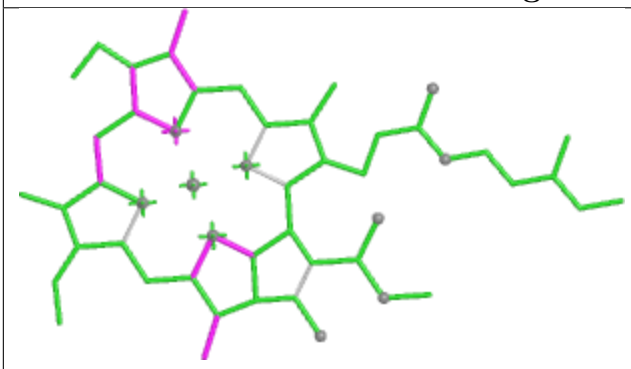


Torsions



Rings

Ligand CLA G 311



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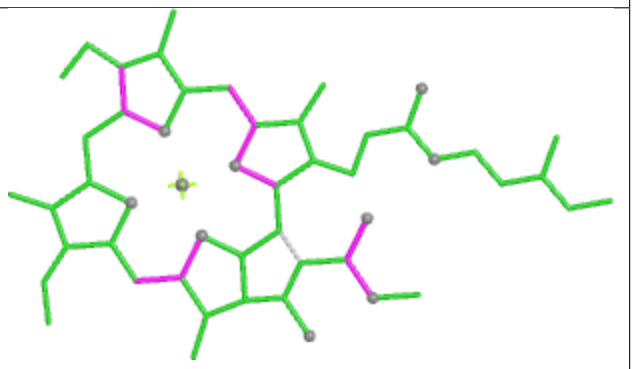

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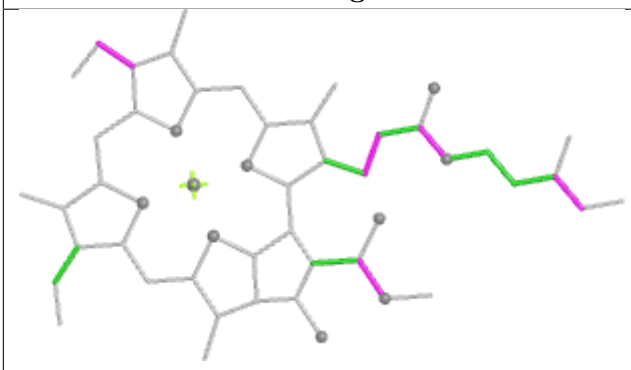

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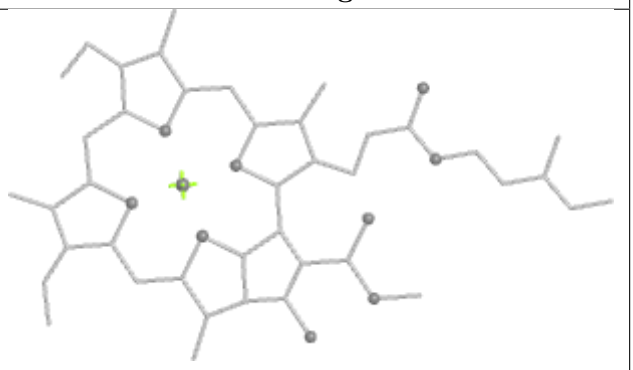
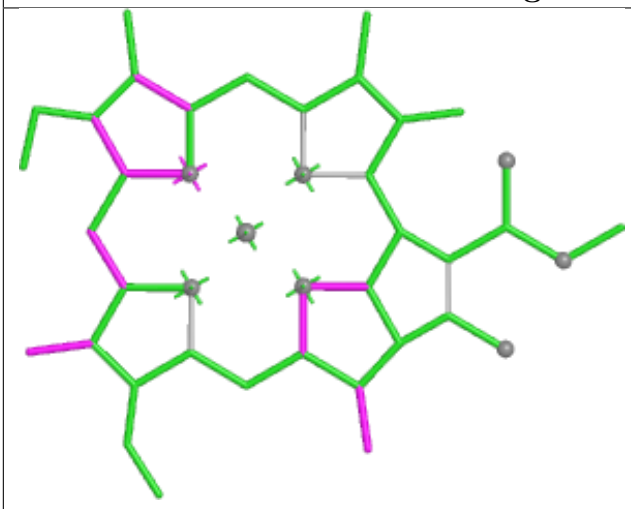


Rings

Ligand CLA Q 315



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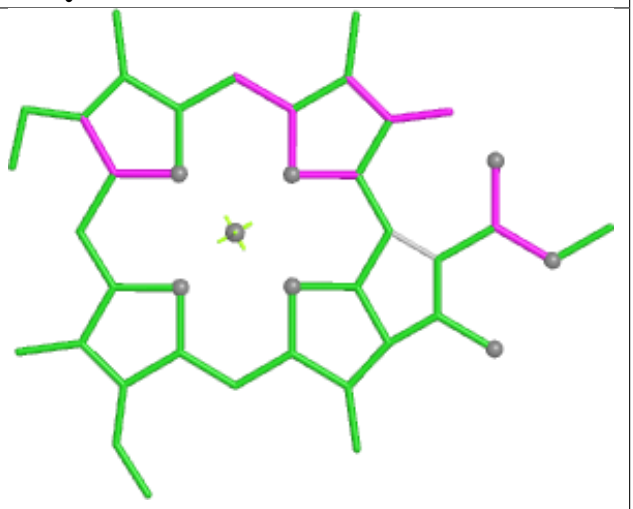

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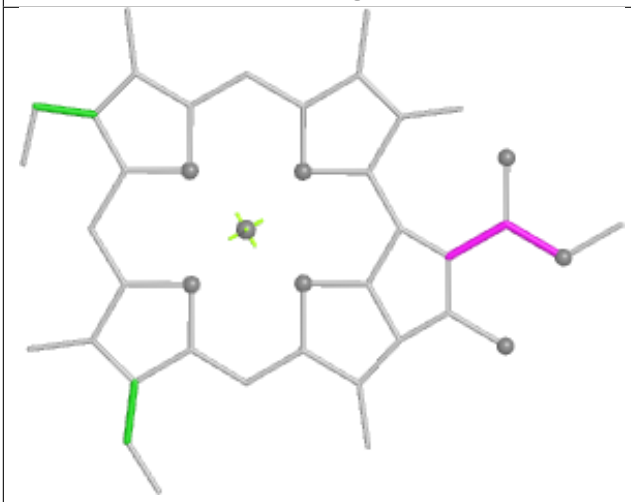

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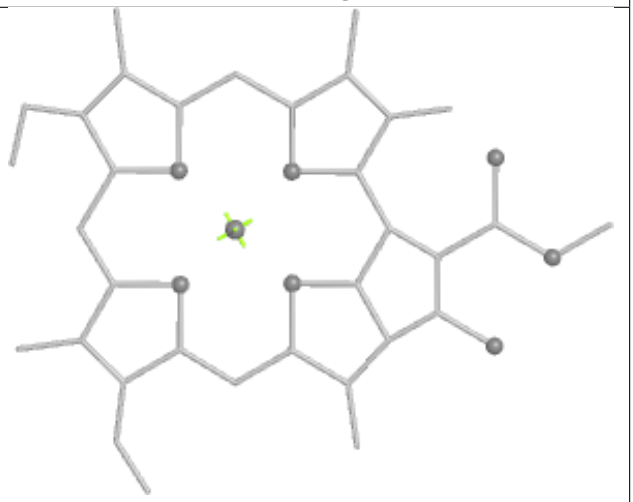
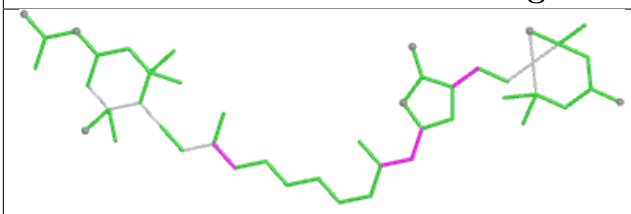


Rings

Ligand PID G 309



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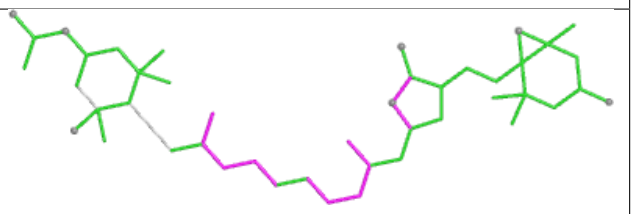

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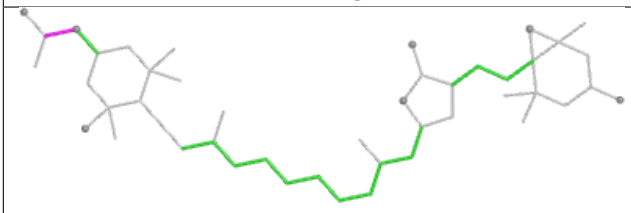

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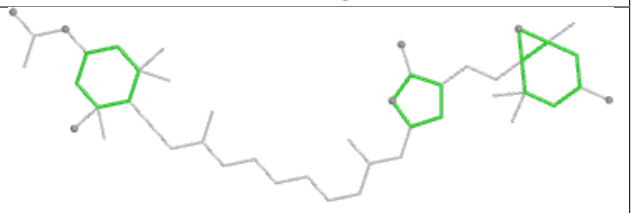
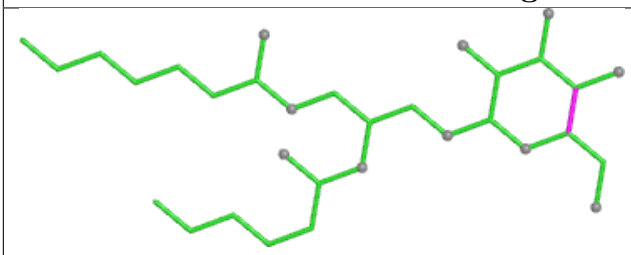


Rings

Ligand LMG E 316



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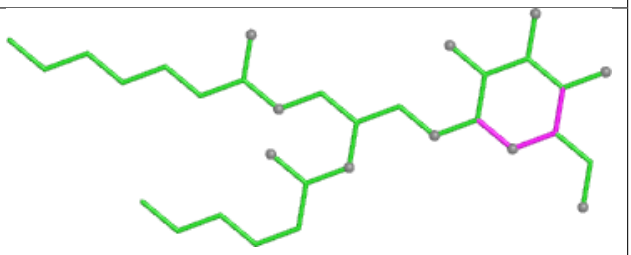

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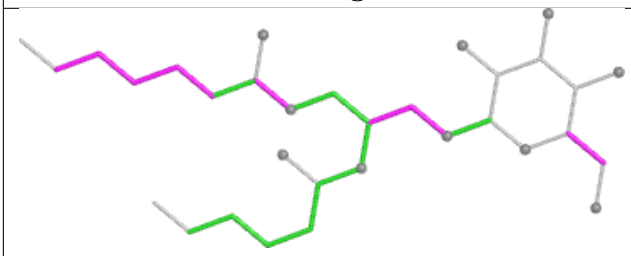

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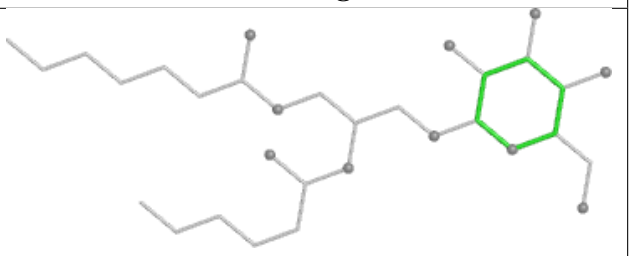
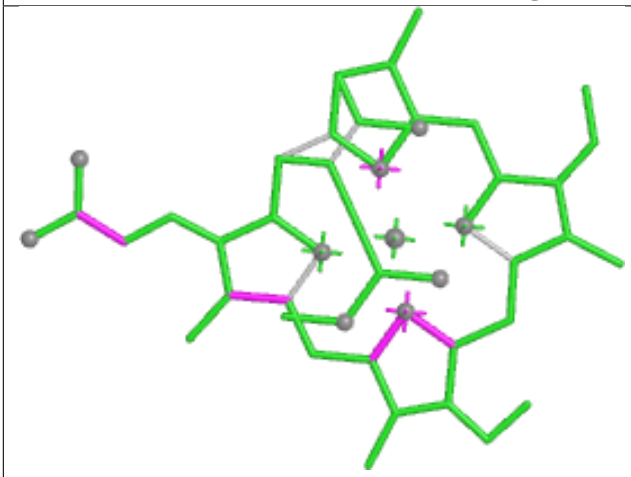


Rings

Ligand KC1 C 310



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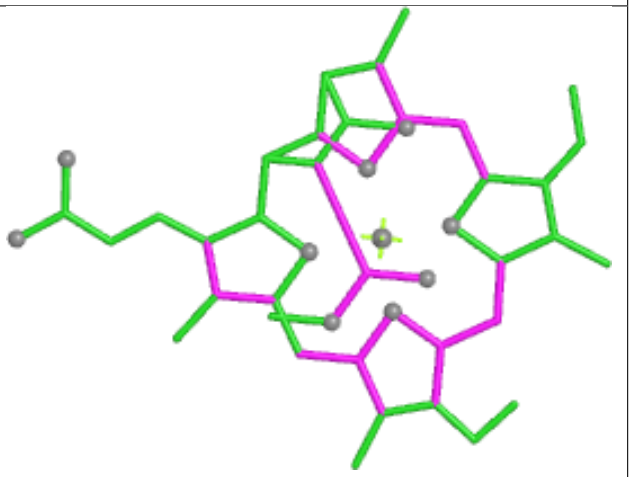

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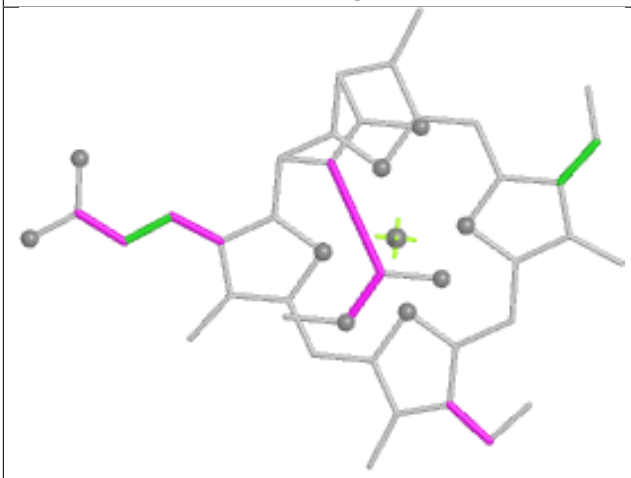

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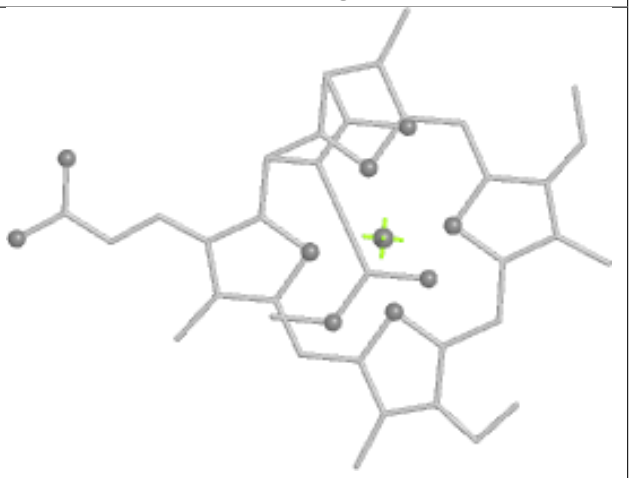
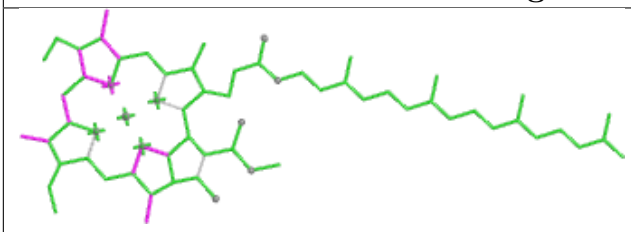


Rings

Ligand CLA b 703



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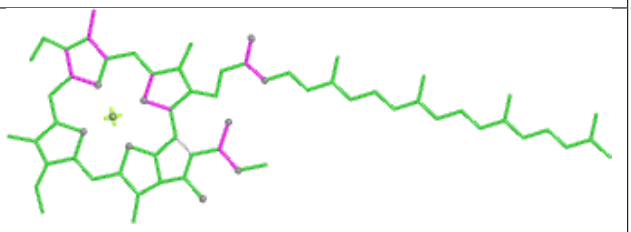

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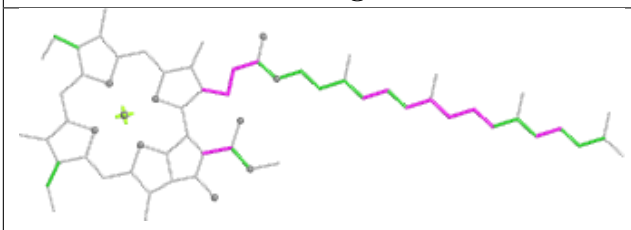

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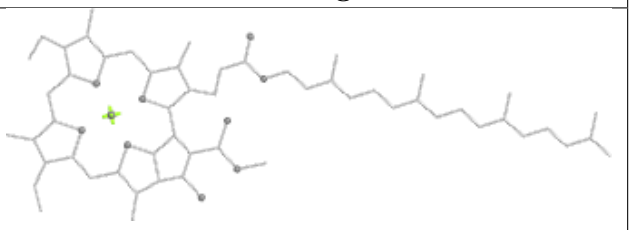
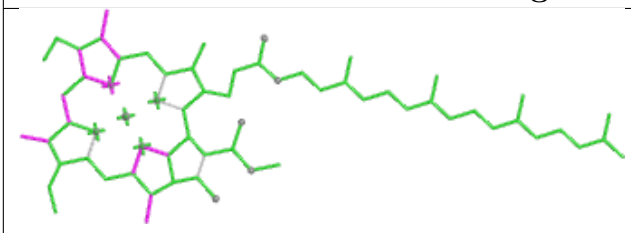


Rings

Ligand CLA I 211



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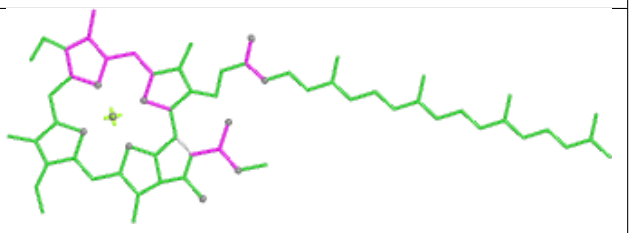

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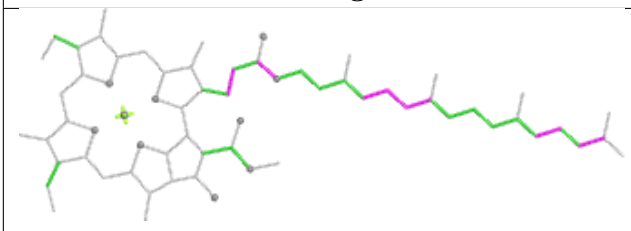

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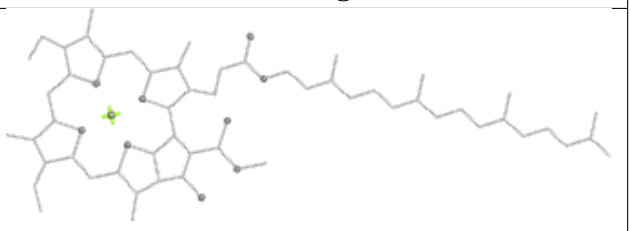
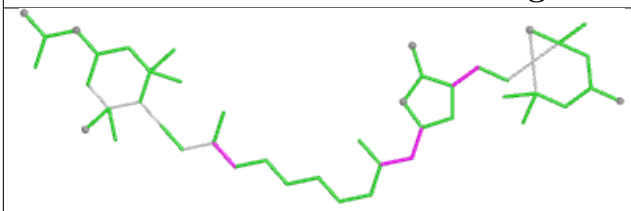


Rings

Ligand PID D 303



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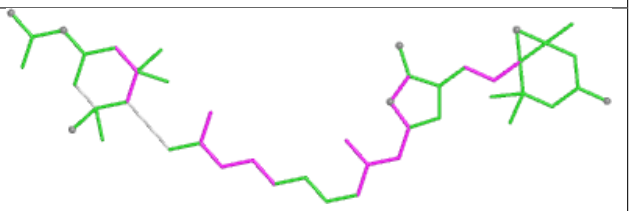

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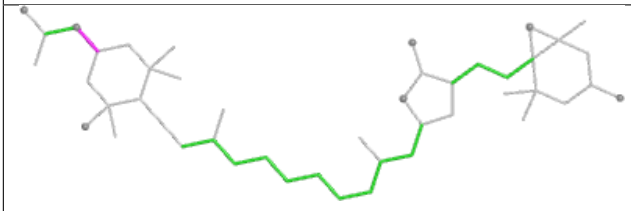

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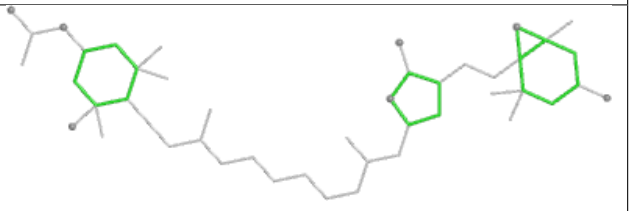
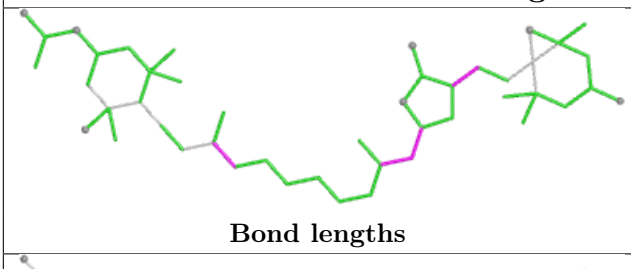


Rings

Ligand PID Q 306



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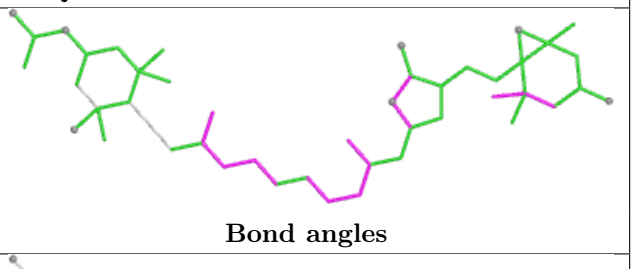

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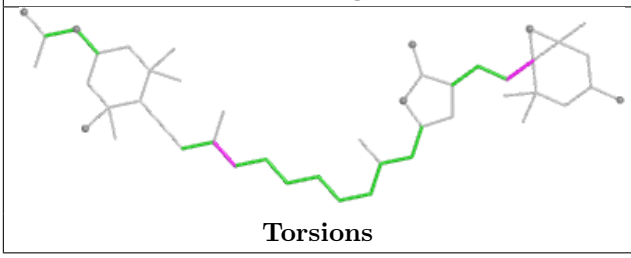

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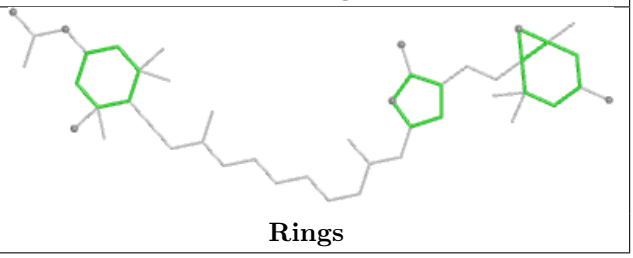
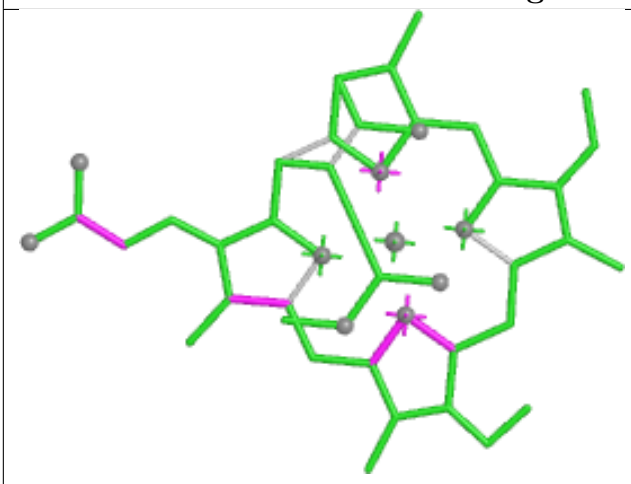


Rings

Ligand KC1 T 315



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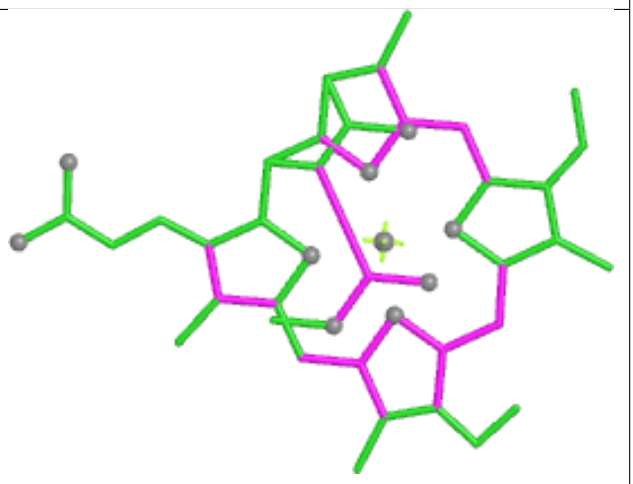

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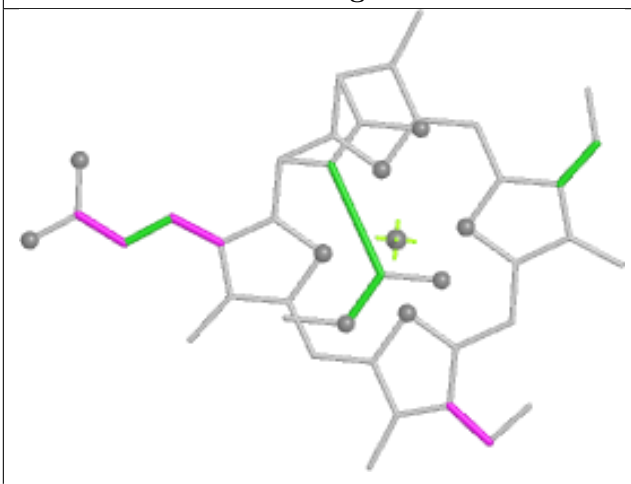

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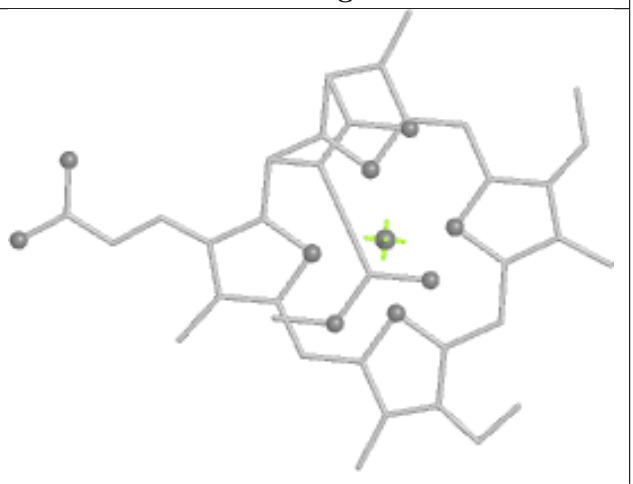
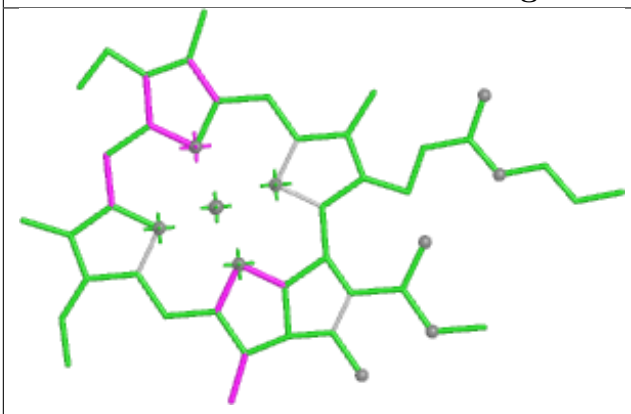


Rings

Ligand CLA M 310



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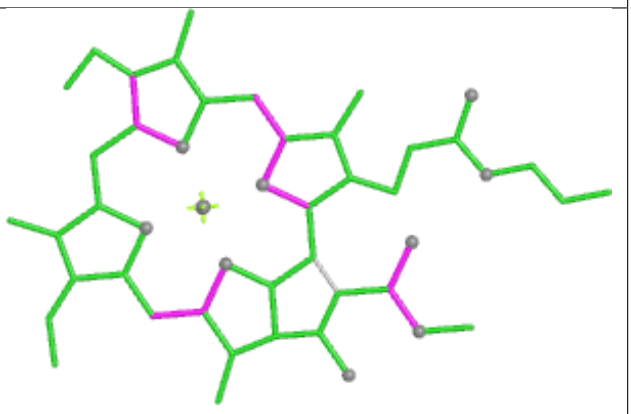

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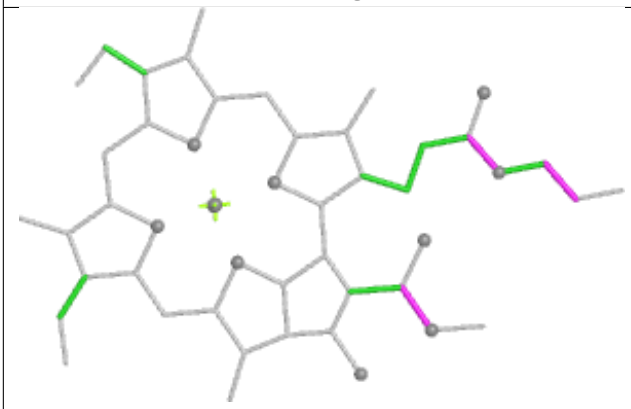

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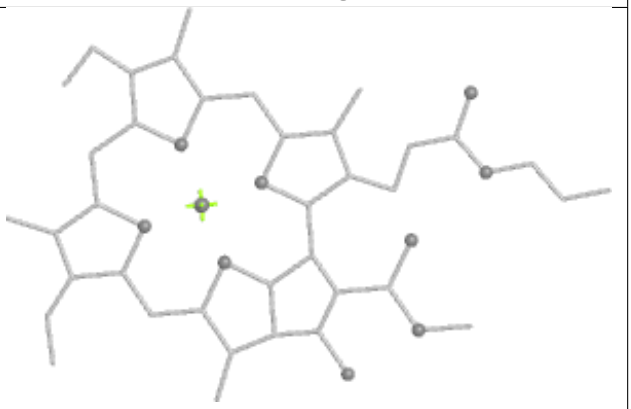
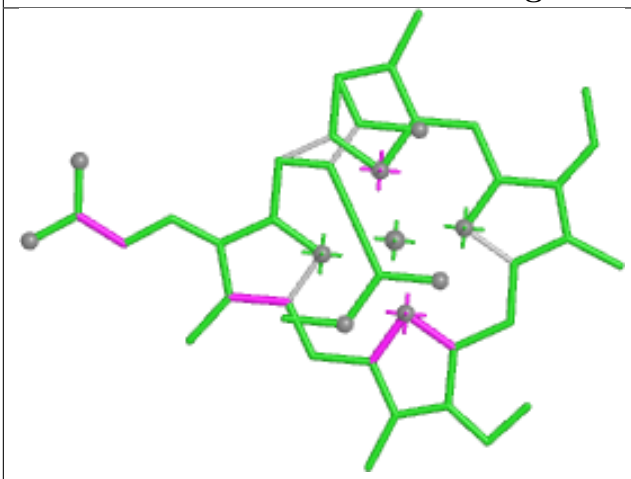


Rings

Ligand KC1 N 310



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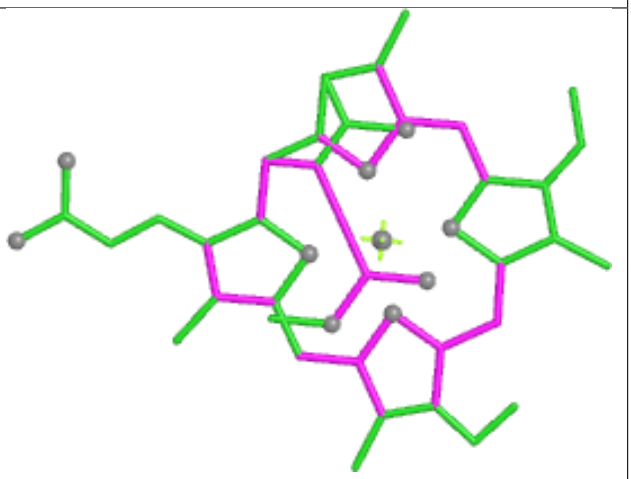

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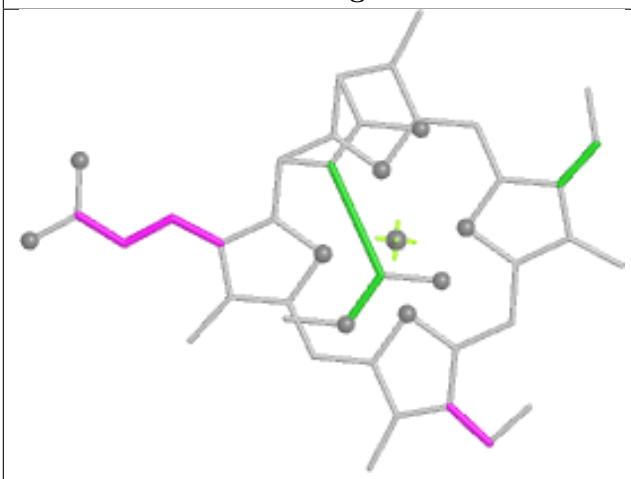

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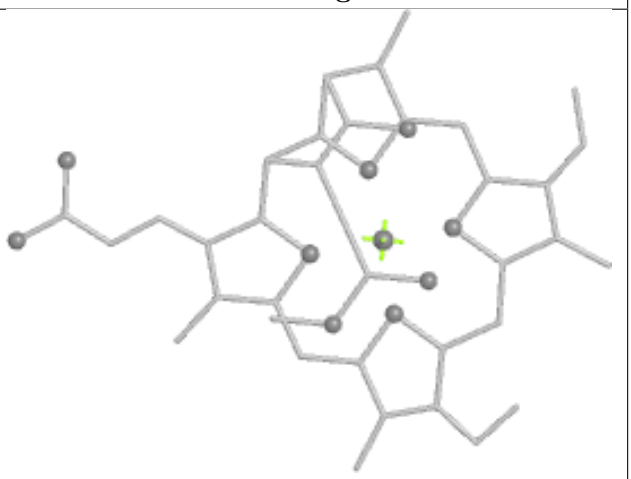
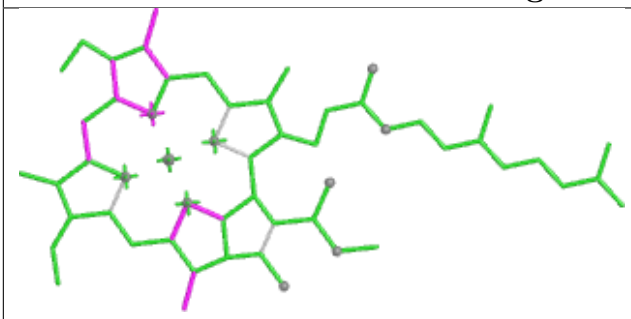


Rings

Ligand CLA L 309



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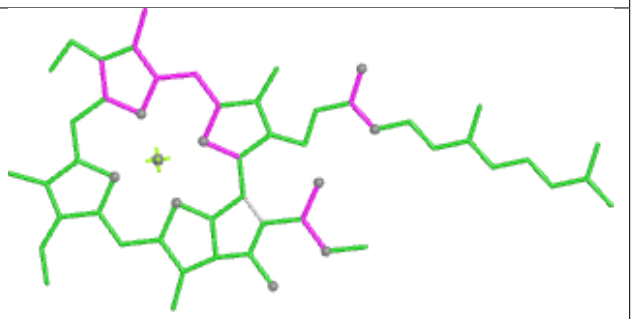
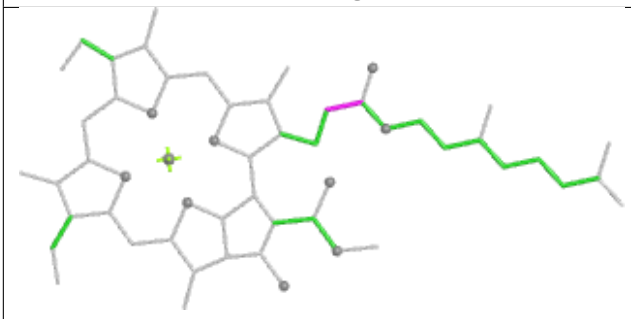


Bond angles



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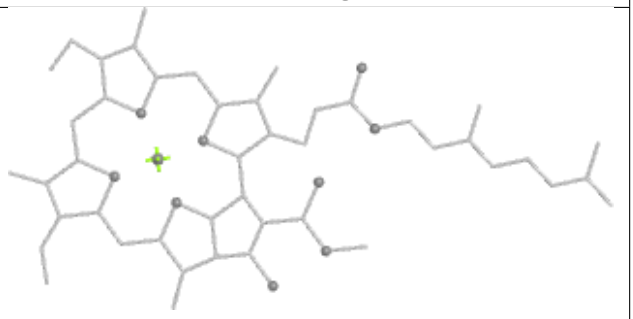
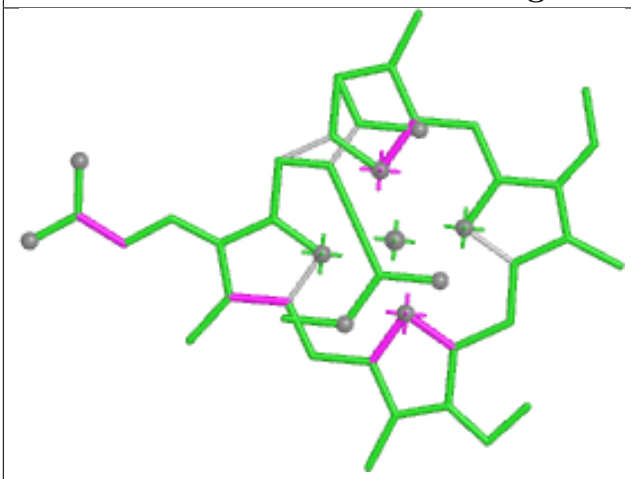


Rings

Ligand KC1 E 312



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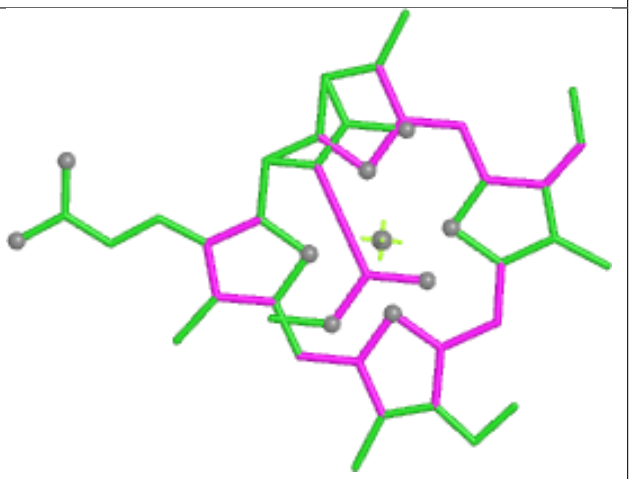
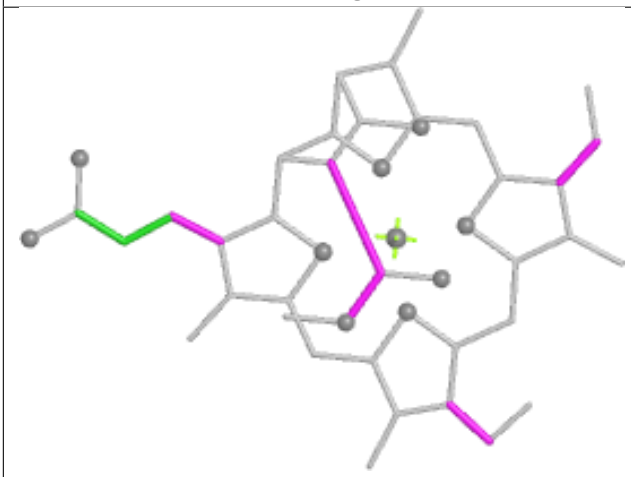
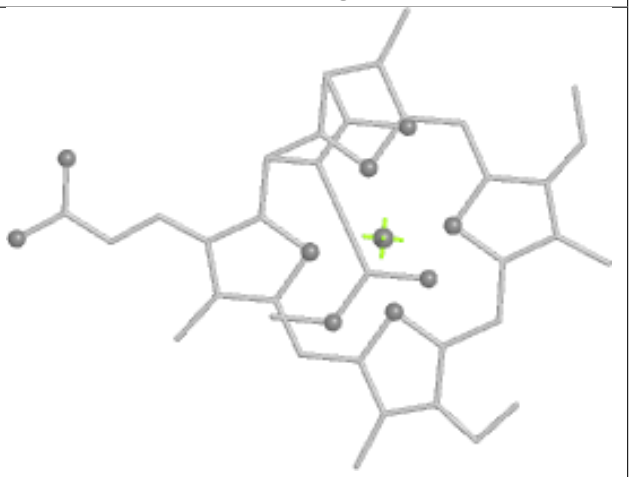


Bond angles

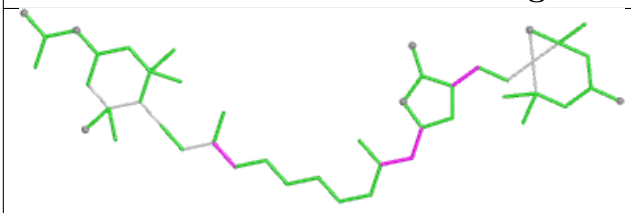


Torsions

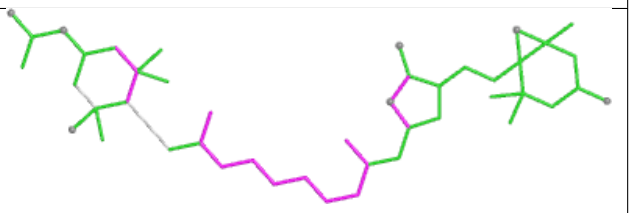


Rings

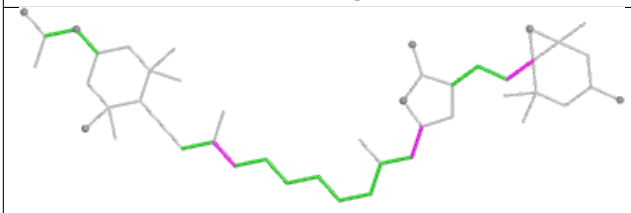
Ligand PID D 307



Bond lengths



Bond angles



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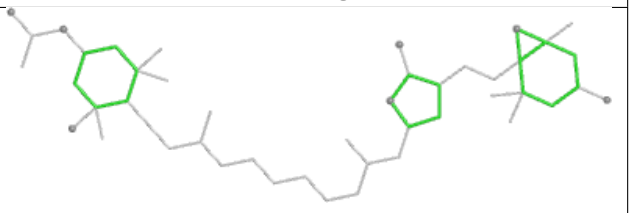
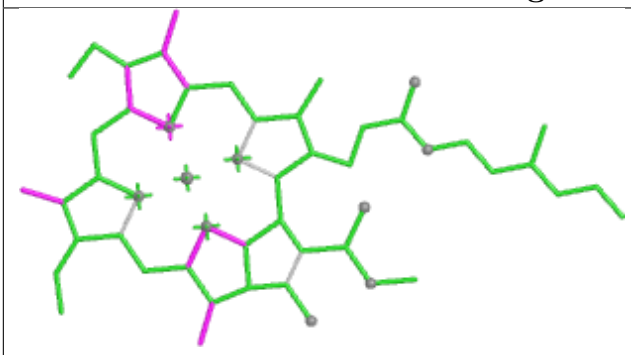
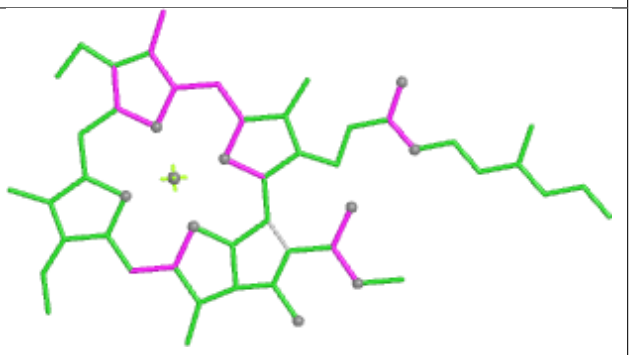


Rings

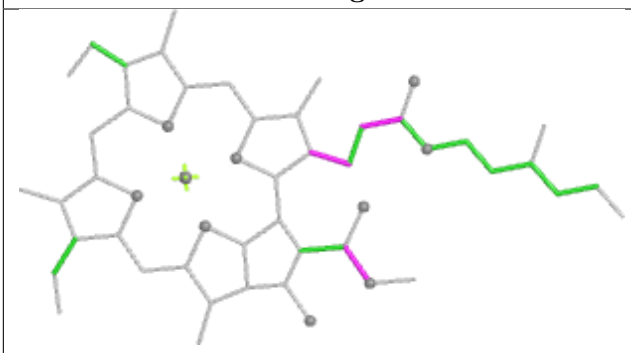
Ligand CLA b 708



Bond lengths



Bond angles



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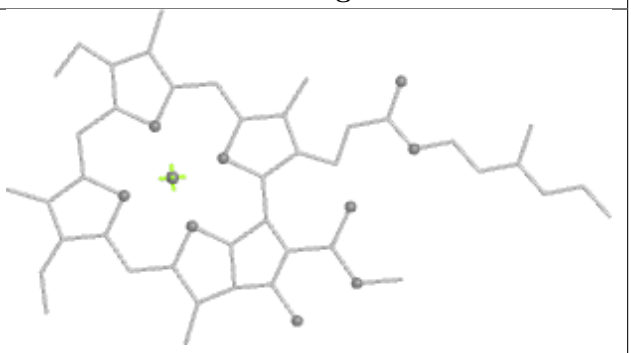
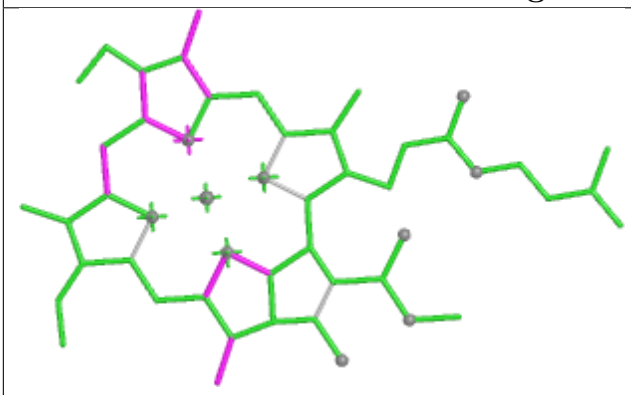


Rings

Ligand CLA b 719



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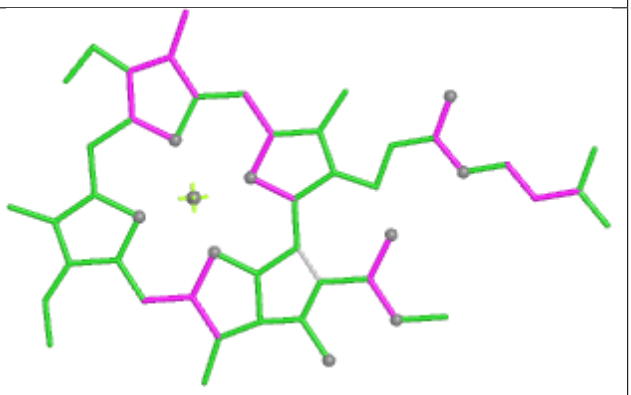
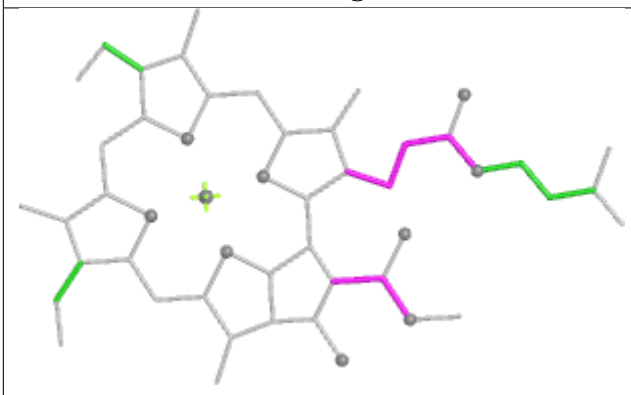


Bond angles



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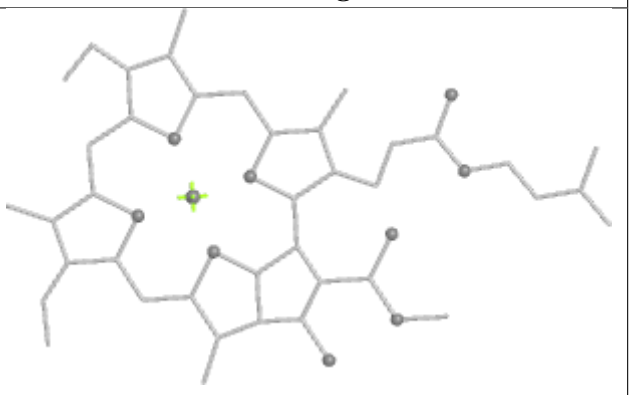
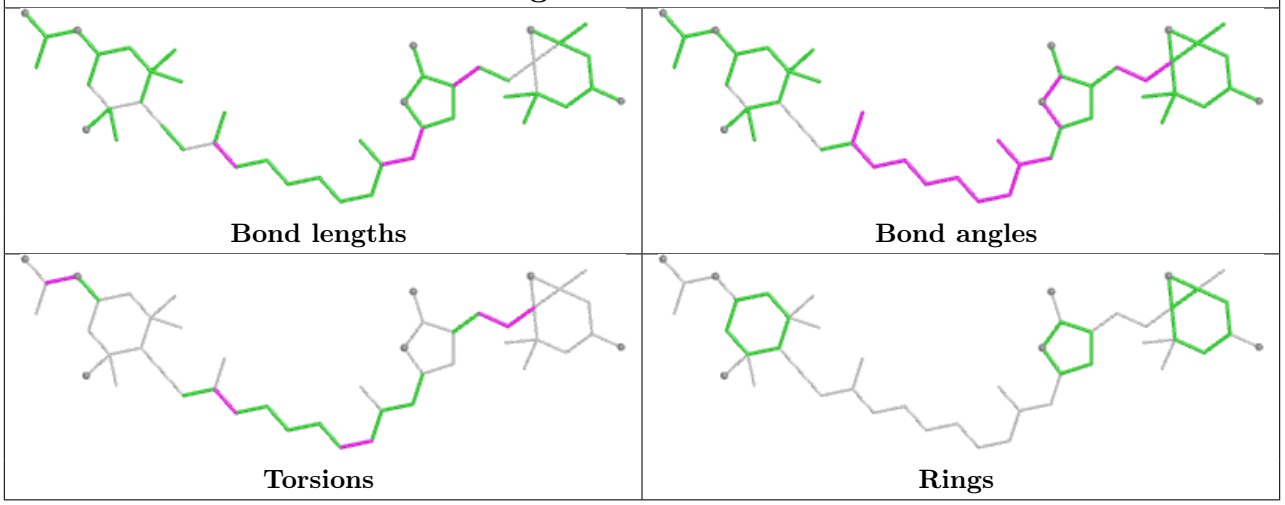
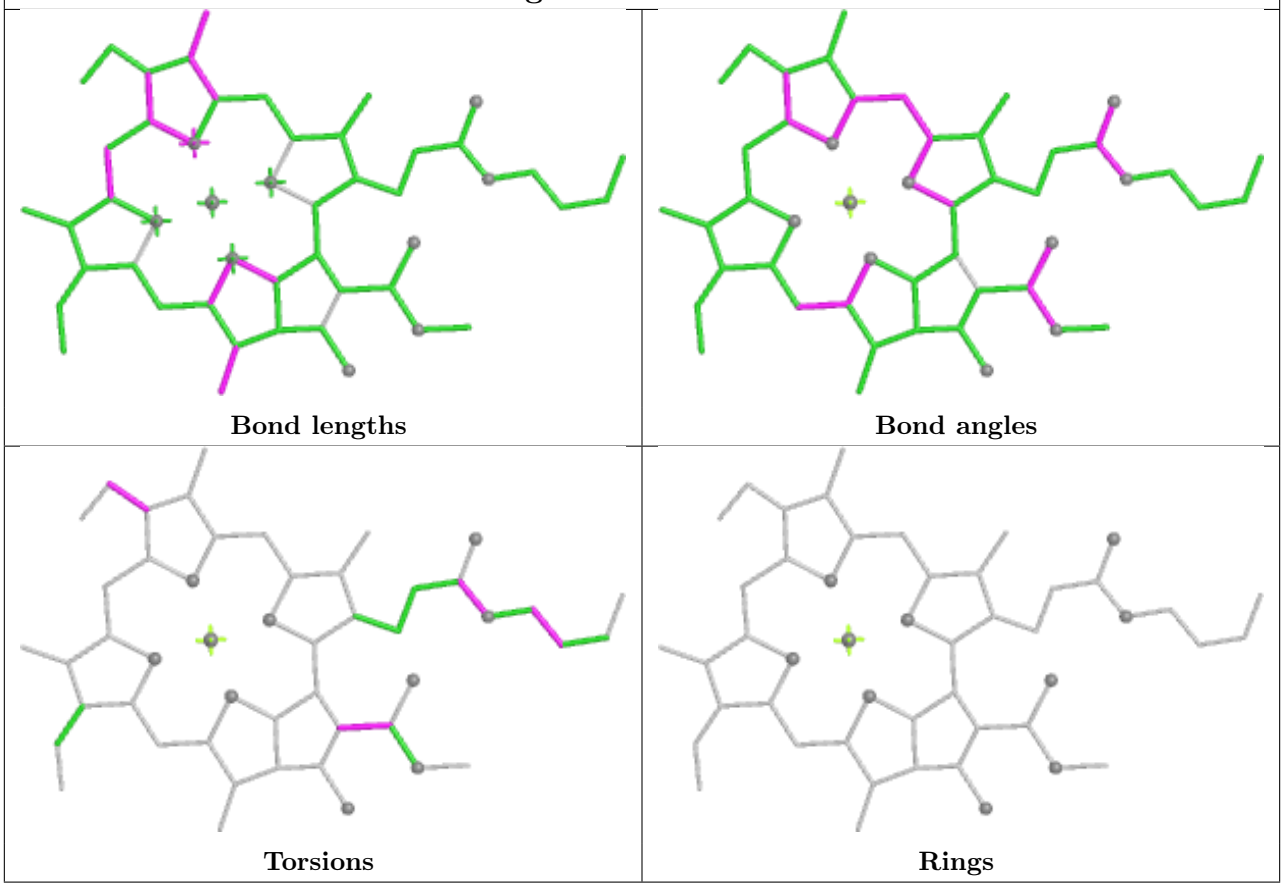


Rings

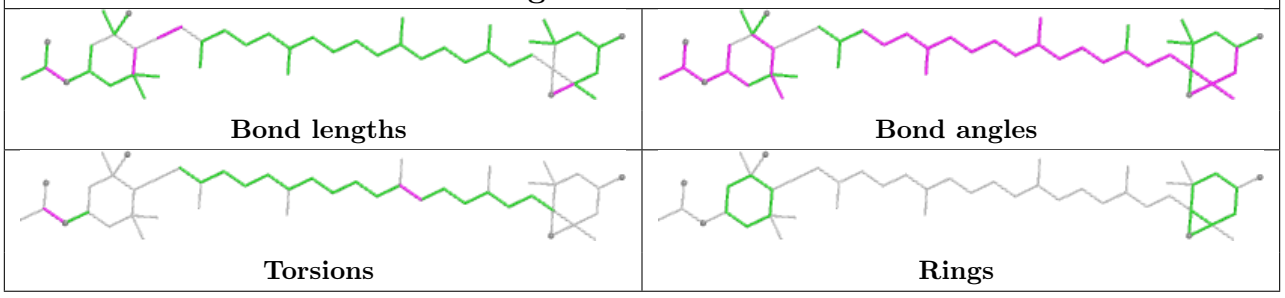
Ligand PID C 305



Ligand CLA B 306



Ligand UIX A 203



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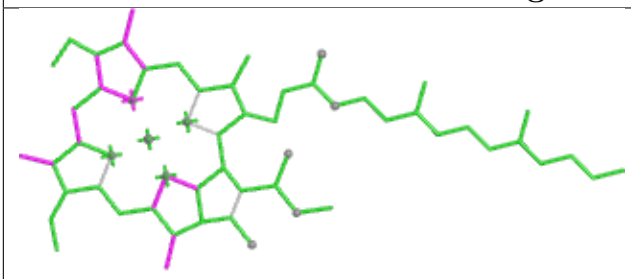
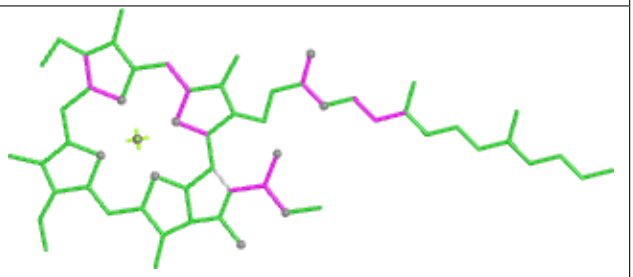
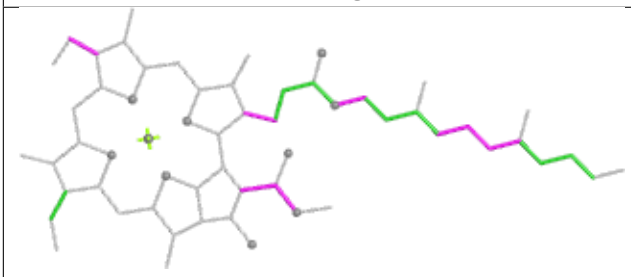


Bond lengths



Bond angles



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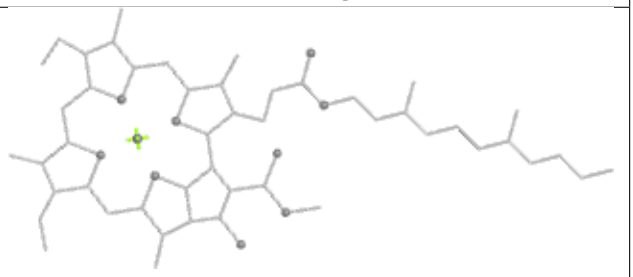
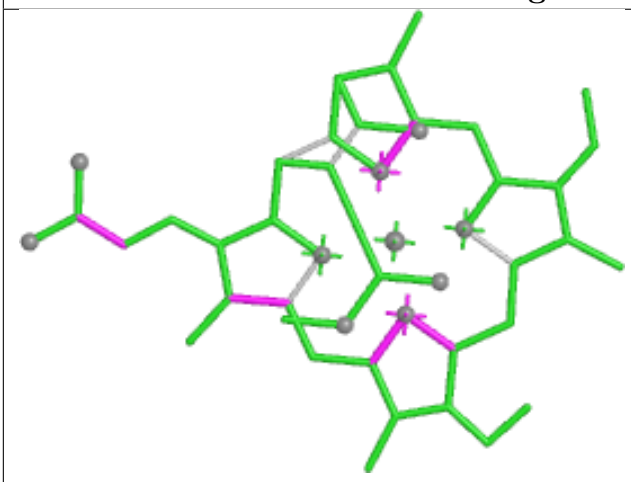


Rings

Ligand KC1 L 314



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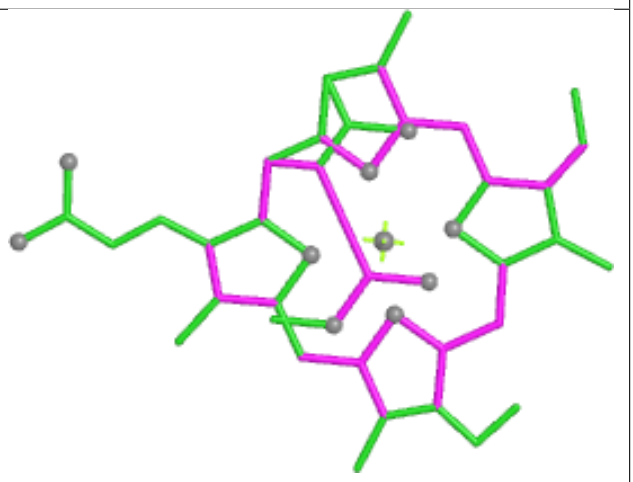
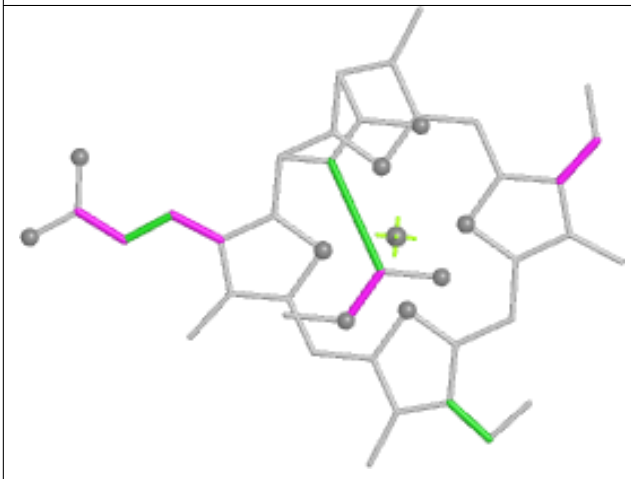


Bond angles



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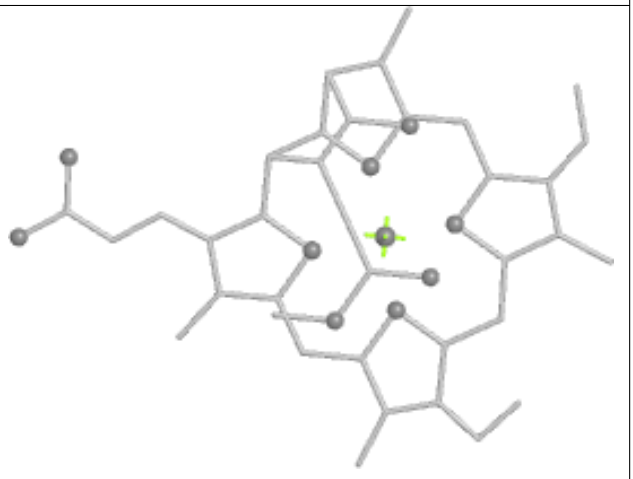
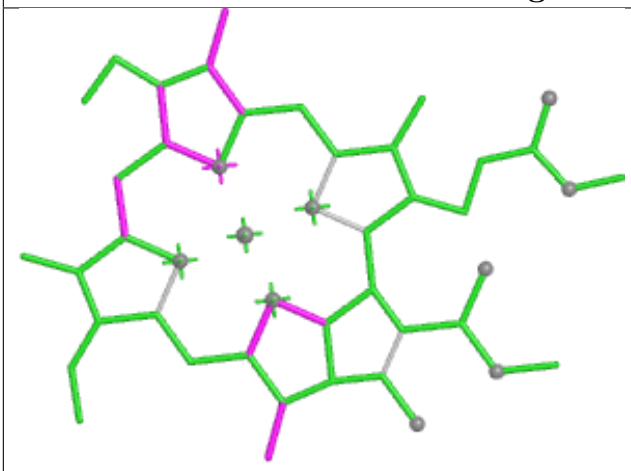


Rings

Ligand CLA J 307



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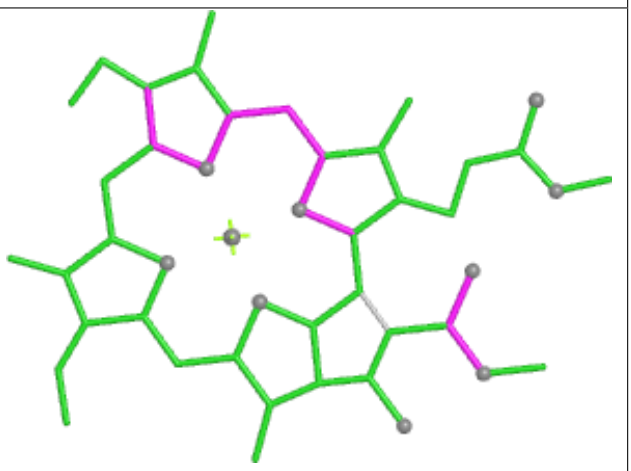
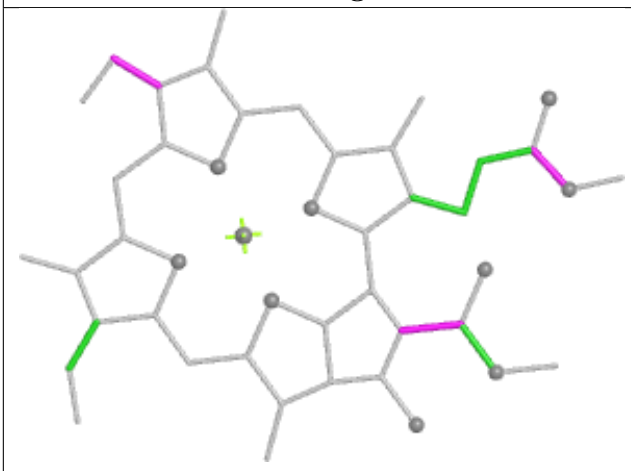


Bond angles



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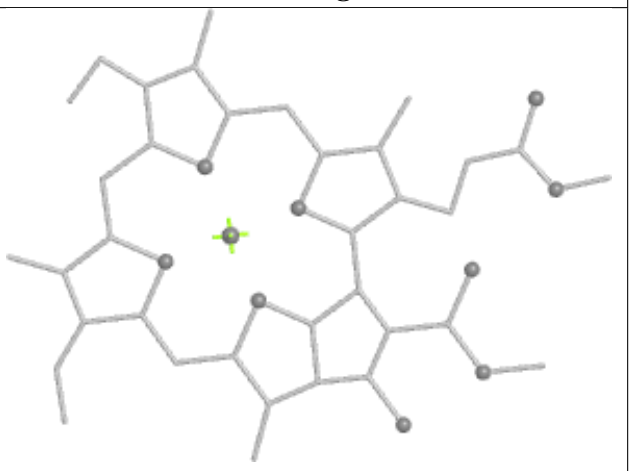
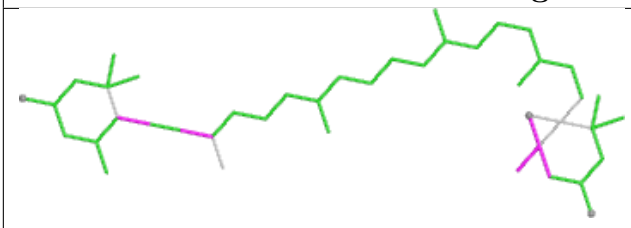


Rings

Ligand DD6 I 205



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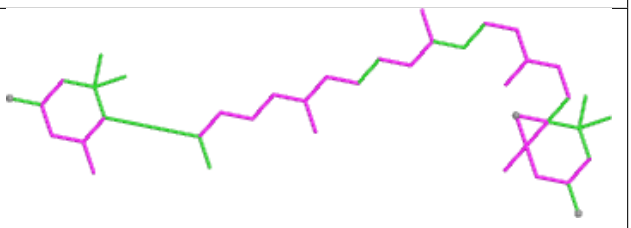
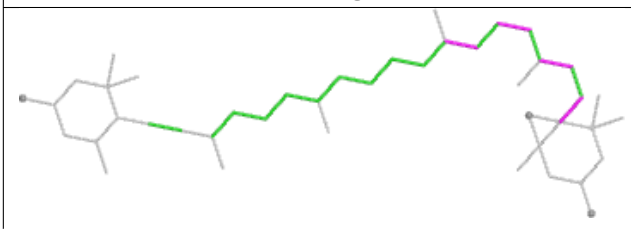
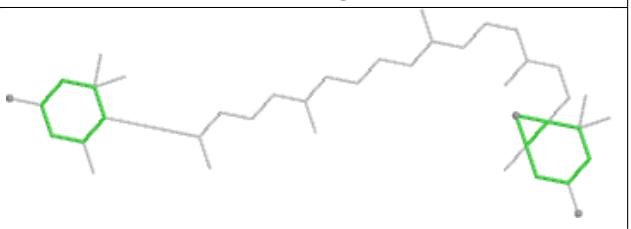


Bond angles

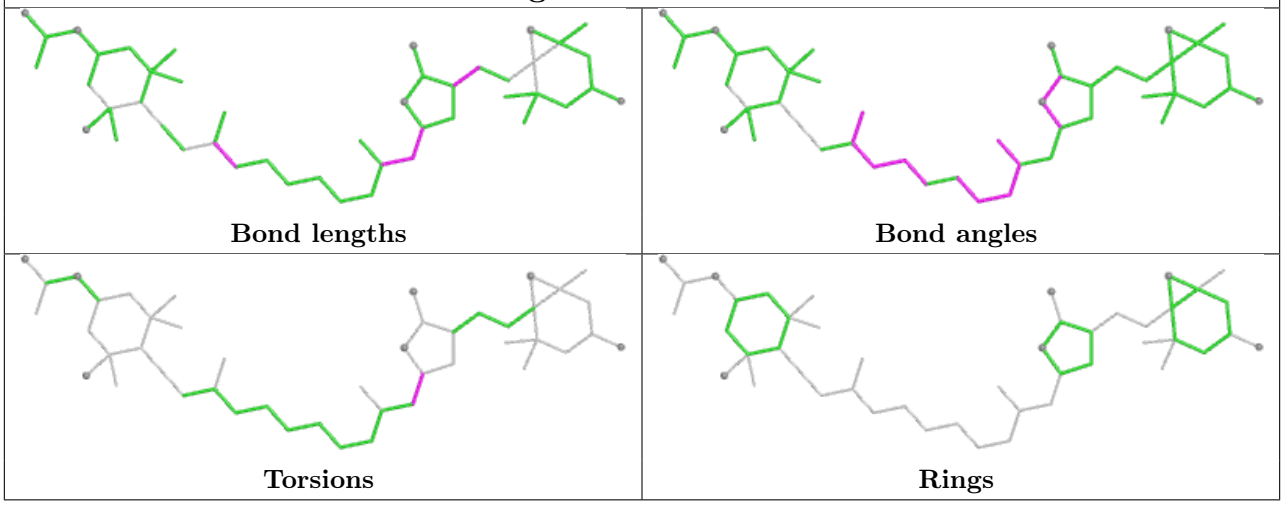


Torsions

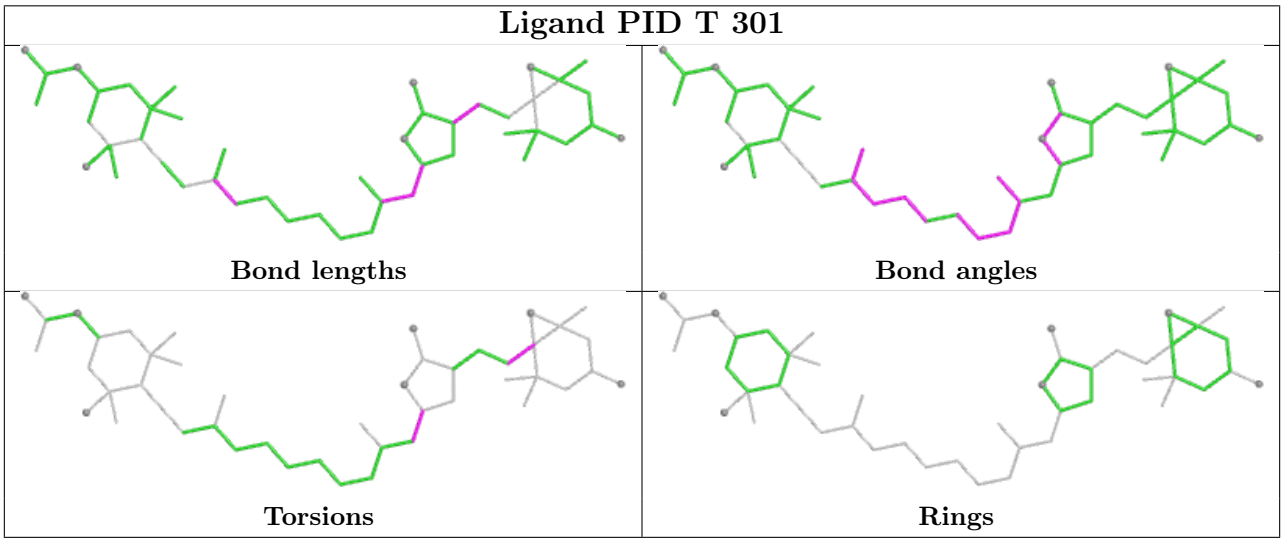


Rings

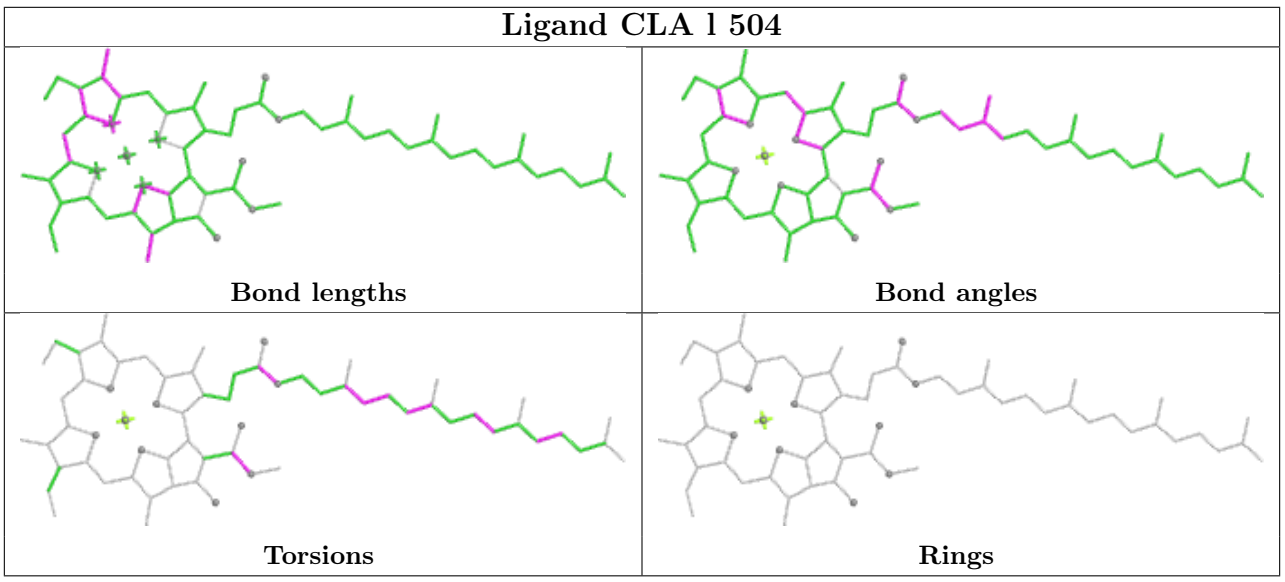
Ligand PID N 304



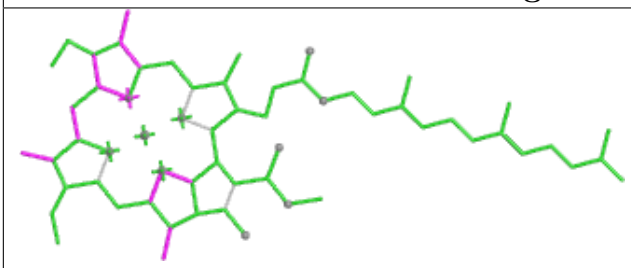
Ligand PID T 301



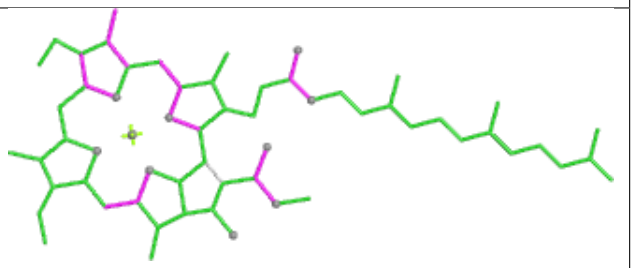
Ligand CLA l 504



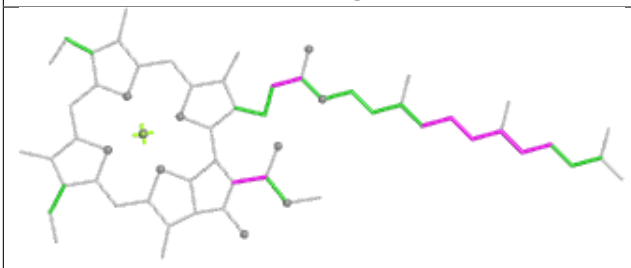
Ligand CLA A 218



Bond lengths



Bond angles



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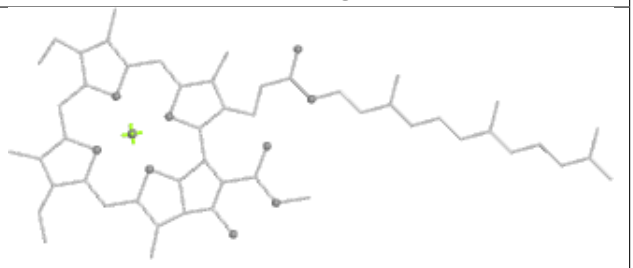
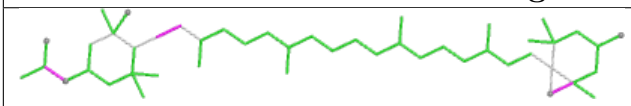


Rings

Ligand UIX P 207



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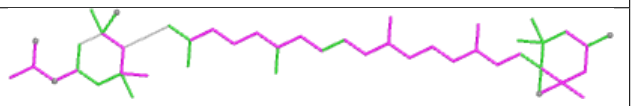
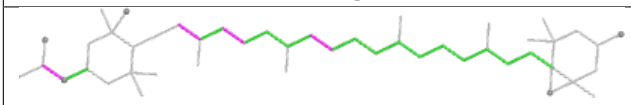


Bond angles



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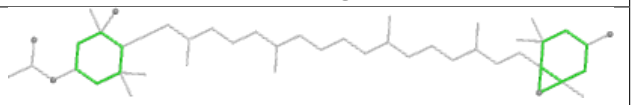
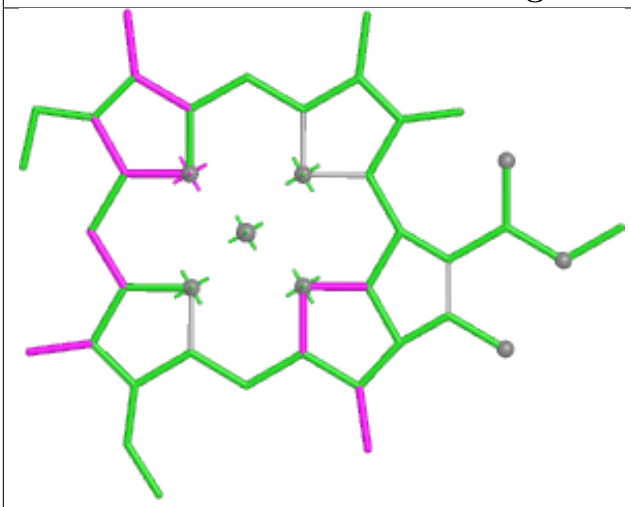


Rings

Ligand CLA L 315



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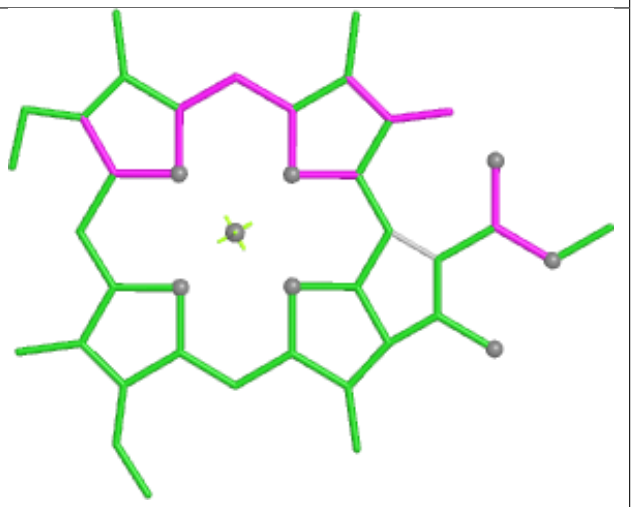
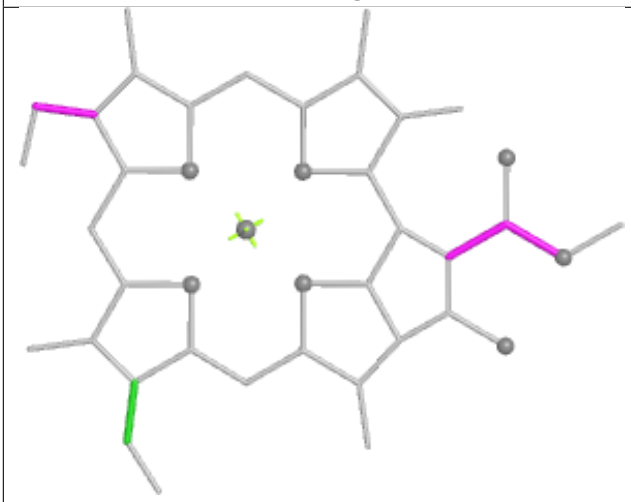


Bond angles



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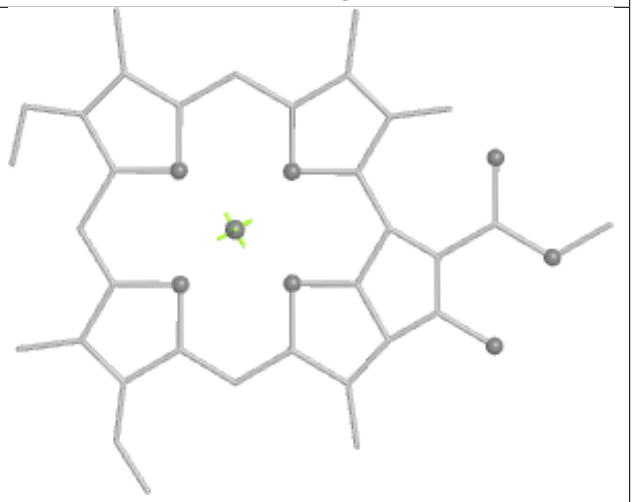
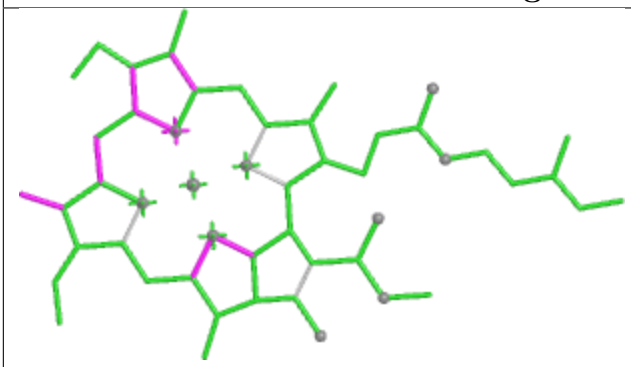
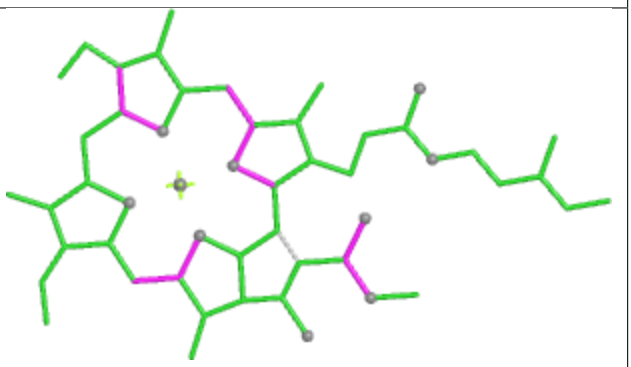


Rings

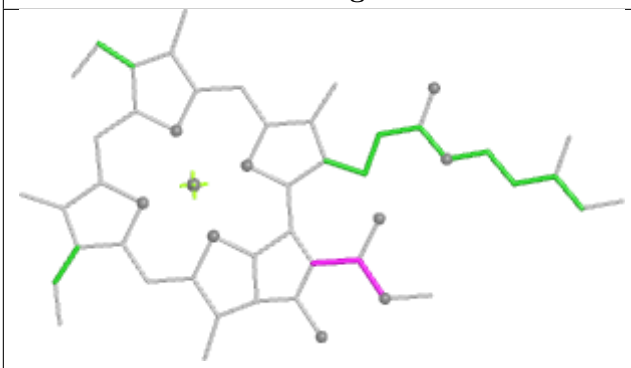
Ligand CLA O 311



Bond lengths



Bond angles



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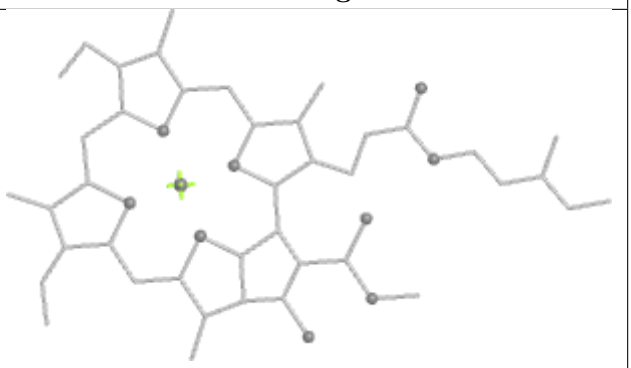
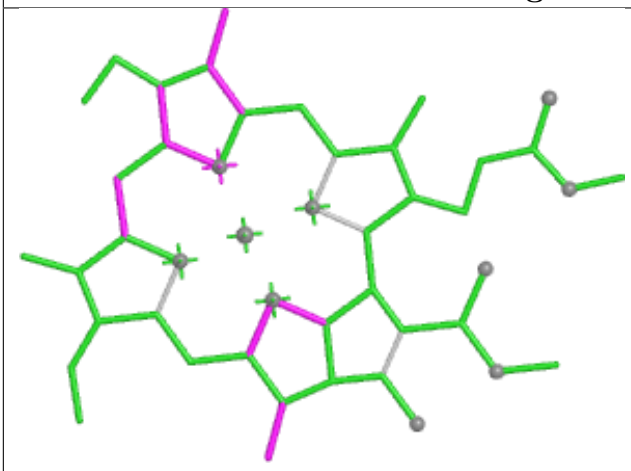


Rings

Ligand CLA F 312



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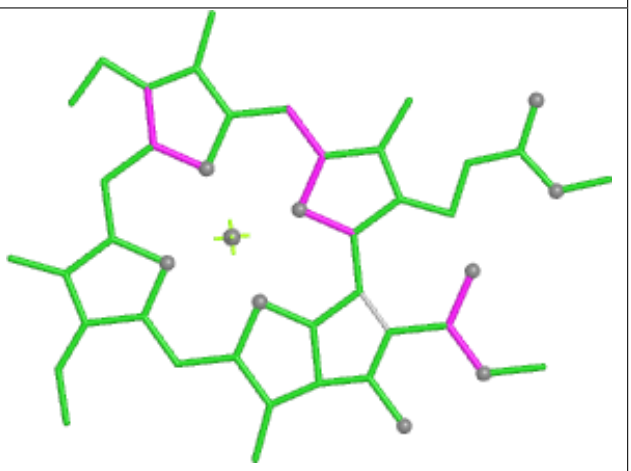
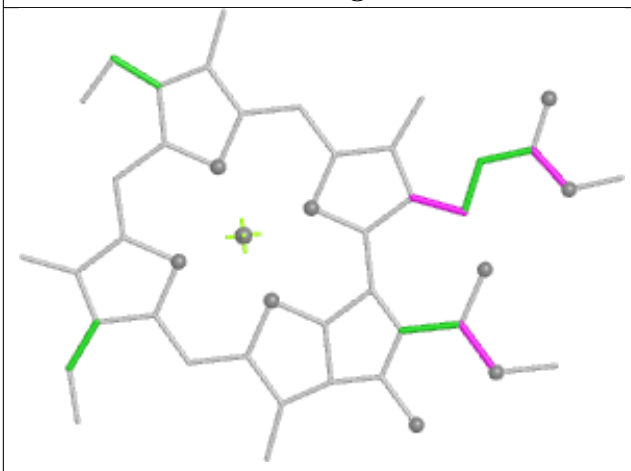
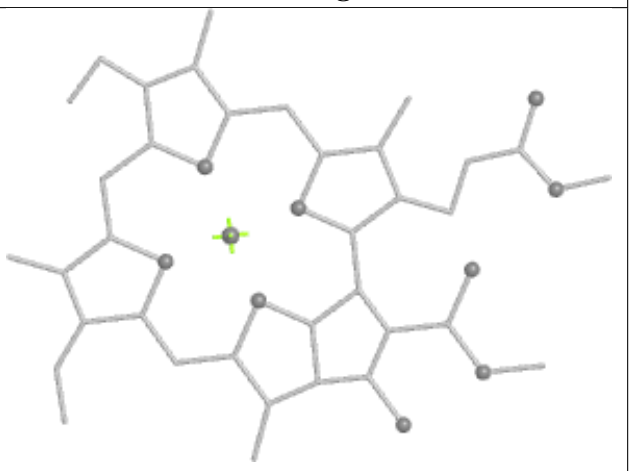


Bond angles

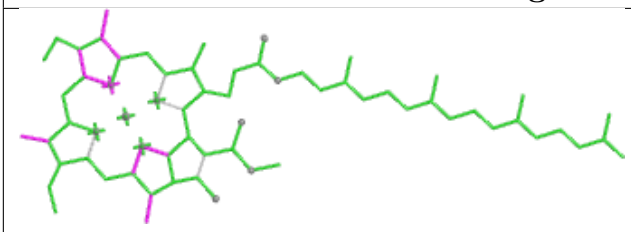


Torsions

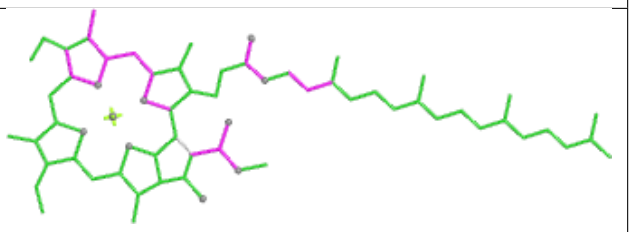


Rings

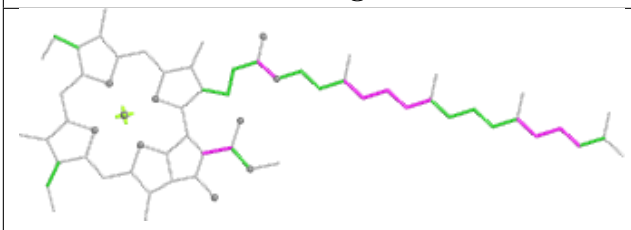
Ligand CLA a 825



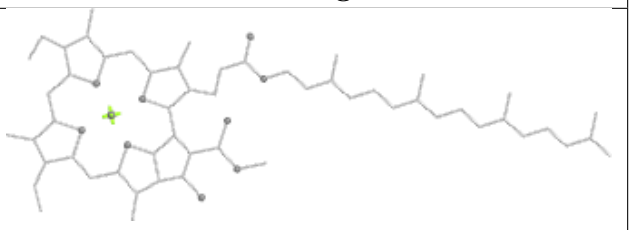
Bond lengths



Bond angles

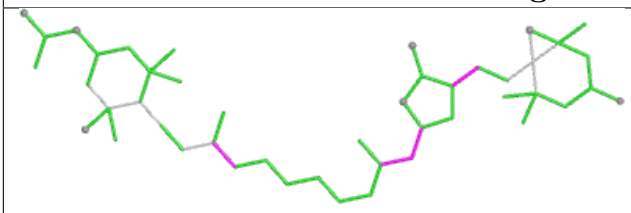


Torsions

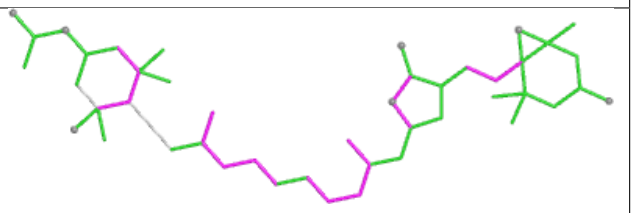


Rings

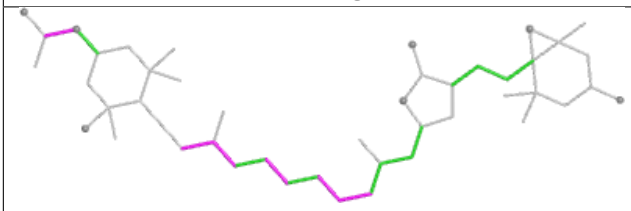
Ligand PID P 206



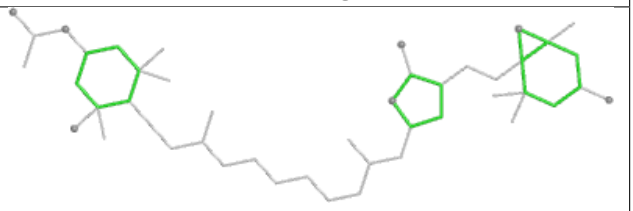
Bond lengths



Bond angles

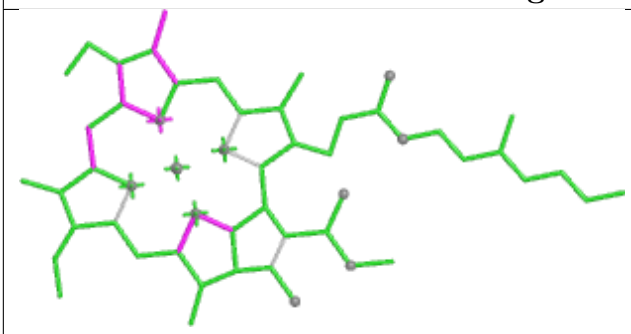


Torsions



Rings

Ligand CLA b 713



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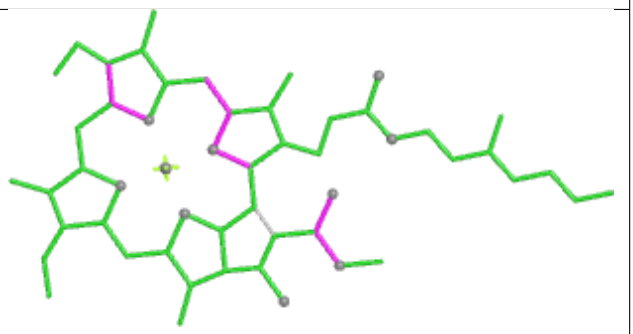
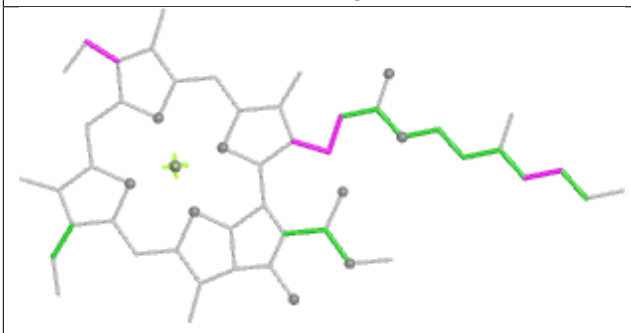


Bond angles



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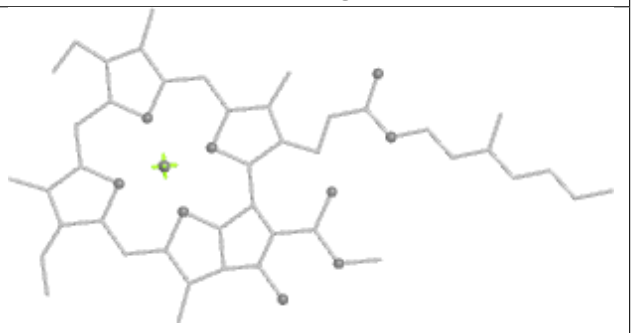
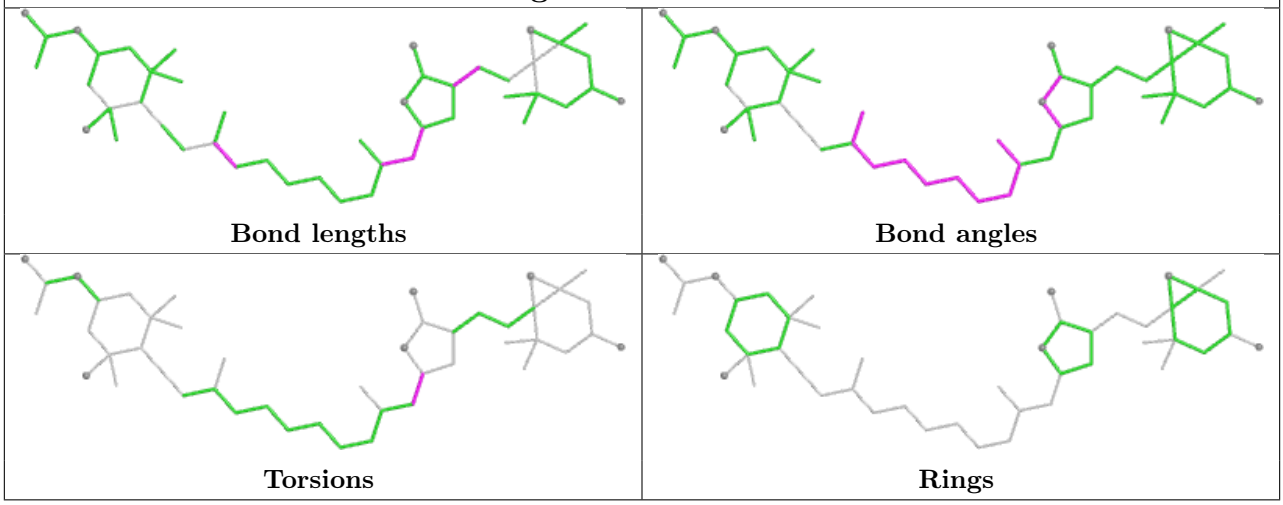
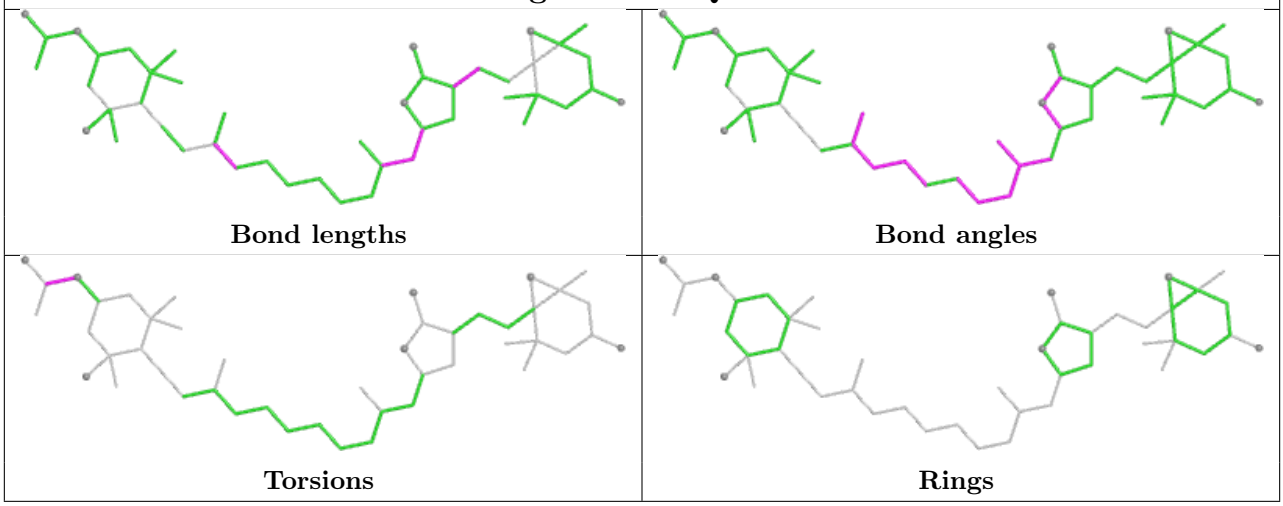


Rings

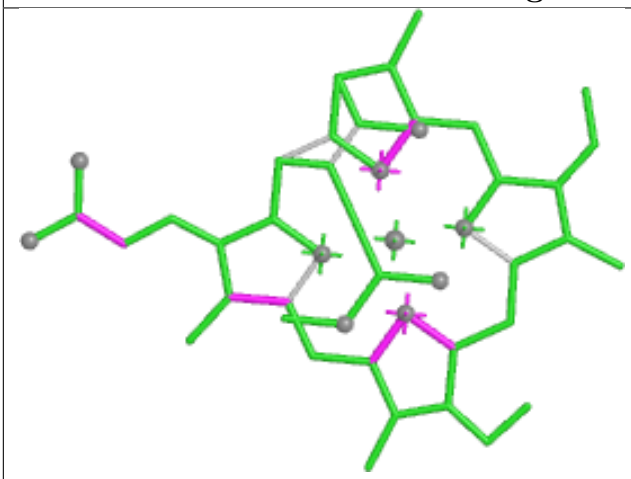
Ligand PID P 205



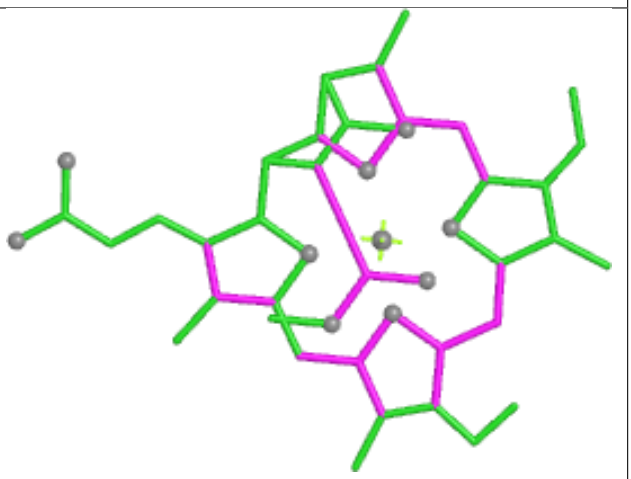
Ligand PID Q 304



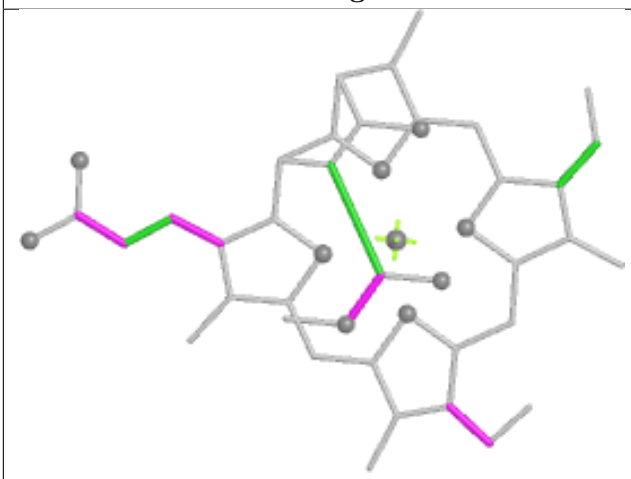
Ligand KC1 C 315



Bond lengths



Bond angles



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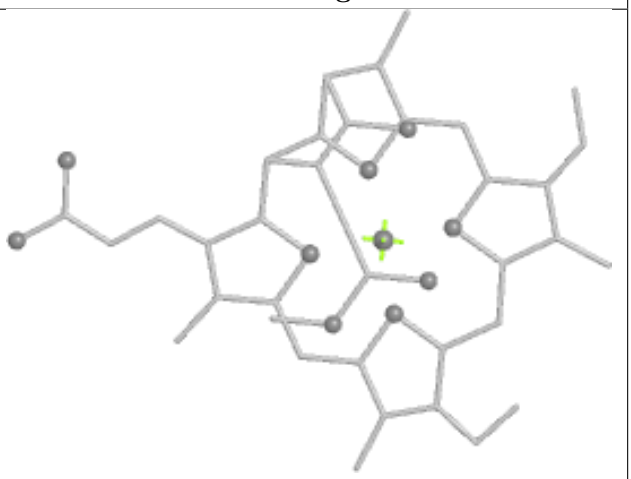
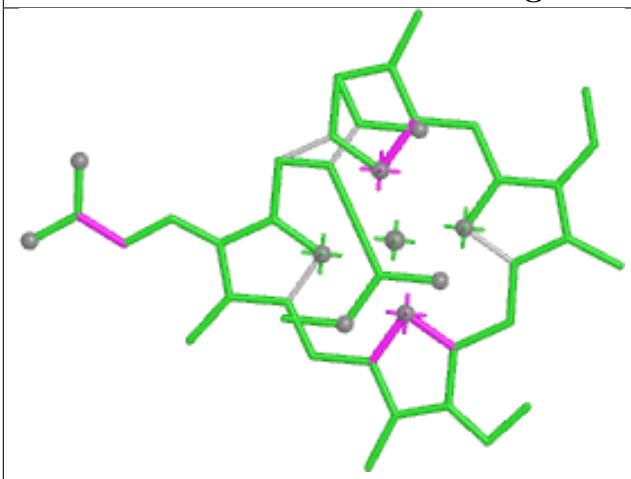
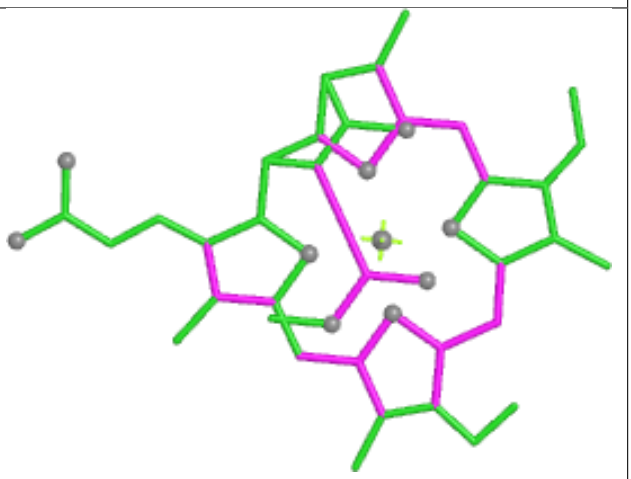


Rings

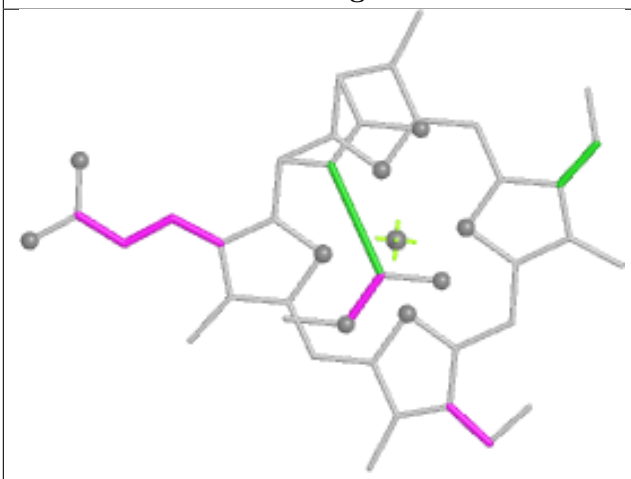
Ligand KC1 N 315



Bond lengths



Bond angles



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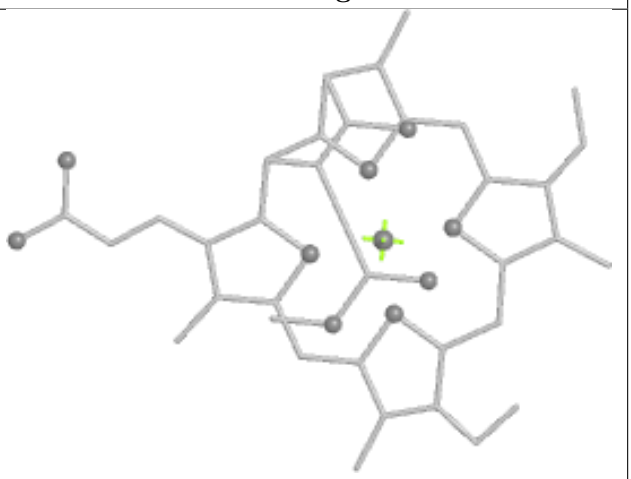
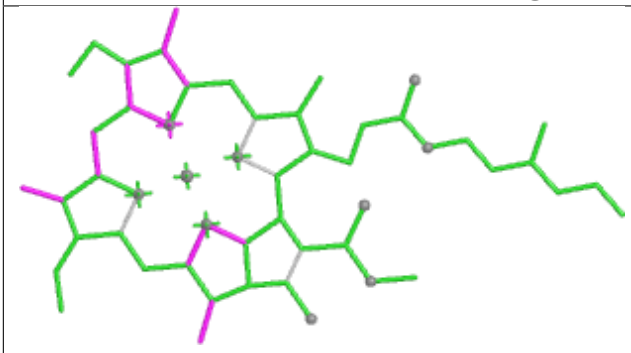
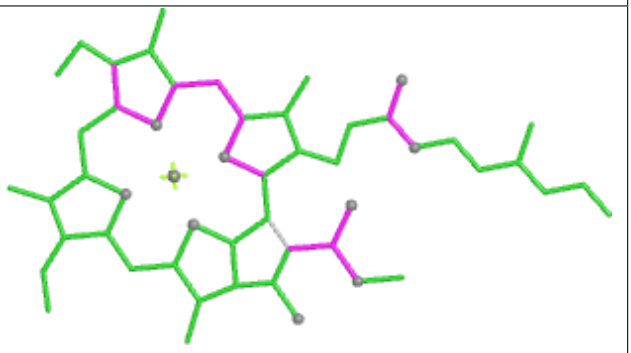
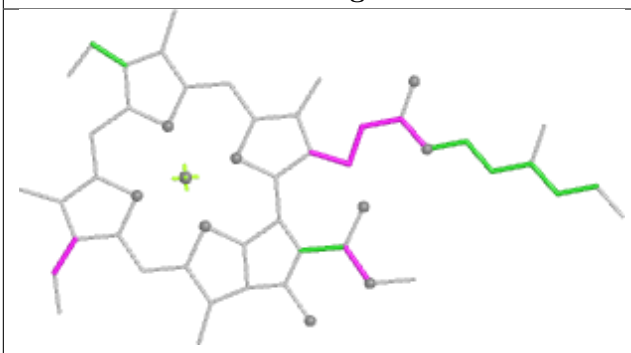
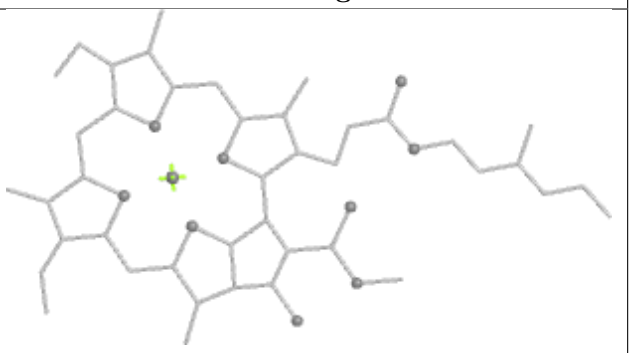
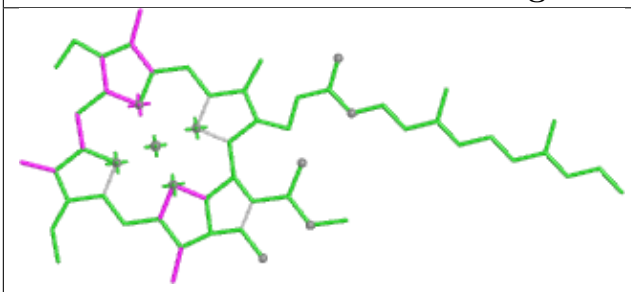
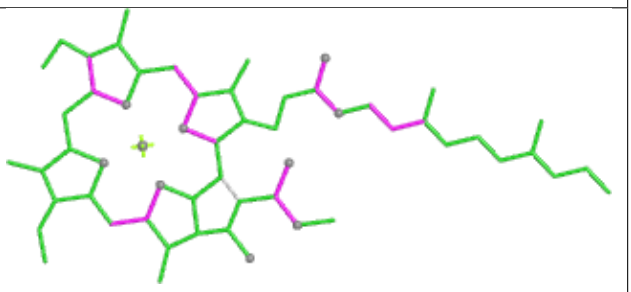
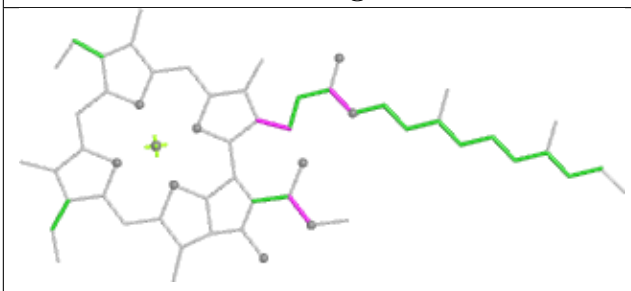
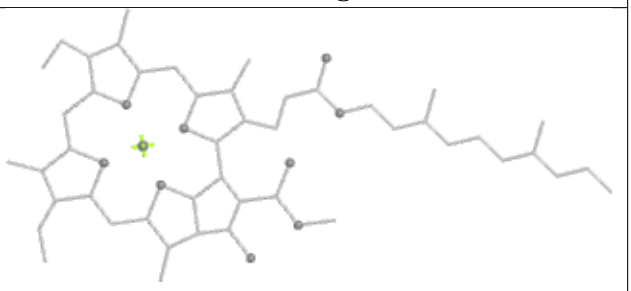
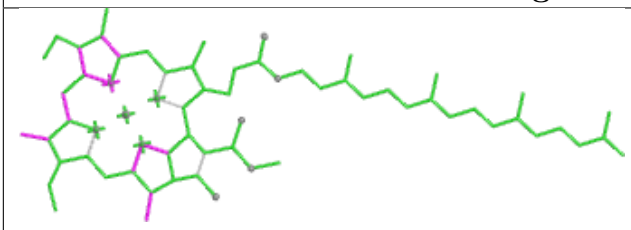


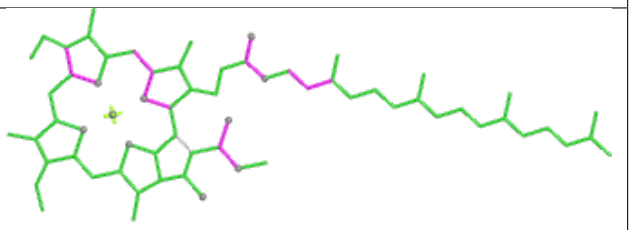
Rings

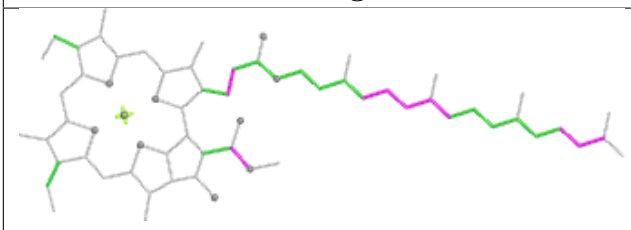
Ligand CLA L 316	
	
Bond lengths	Bond angles
	
Torsions	Rings

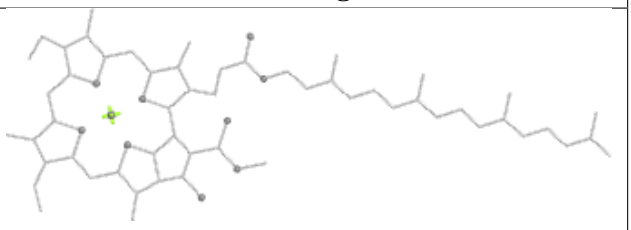
Ligand CLA a 819	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA i 202

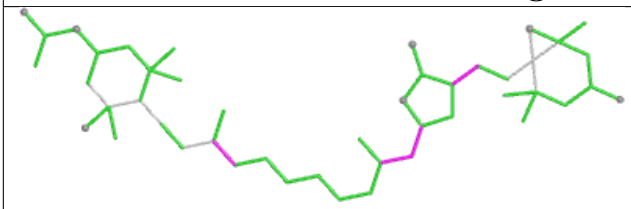

Bond lengths


Bond angles


Torsions


Rings

Ligand PID H 304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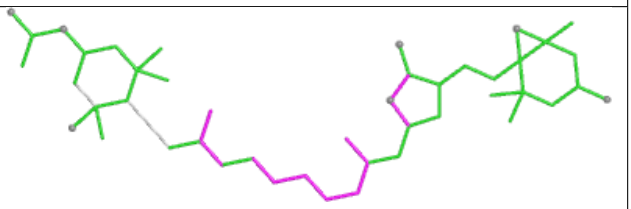
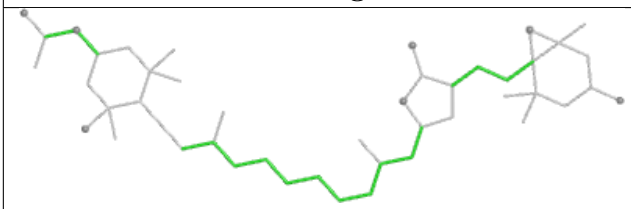

Bond angles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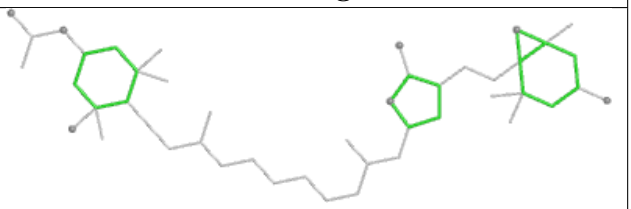
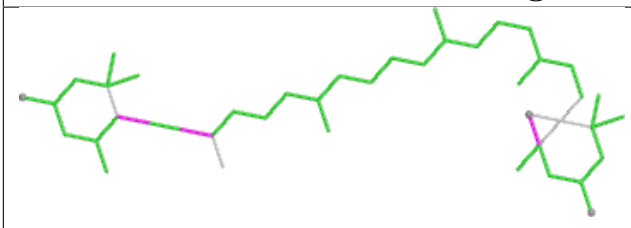

Rings

Ligand DD6 L 301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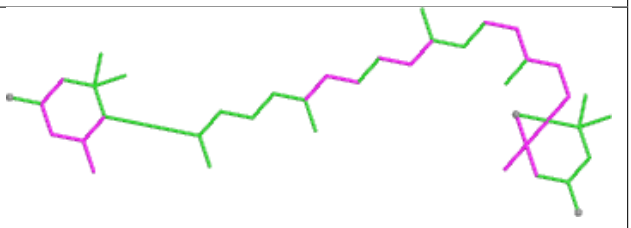
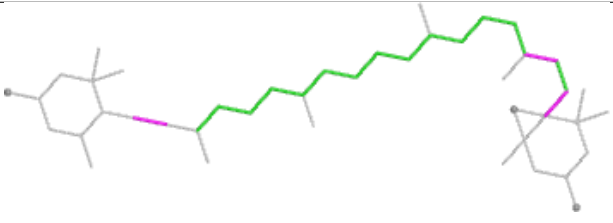

Bond angles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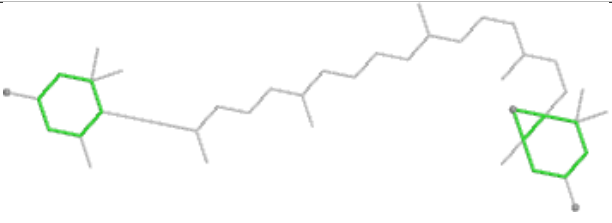
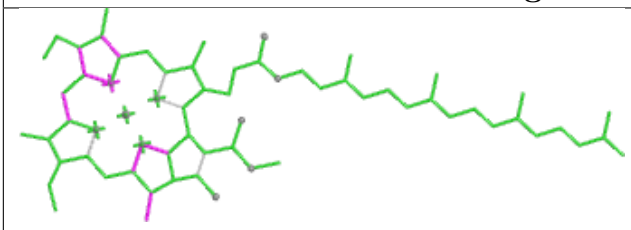
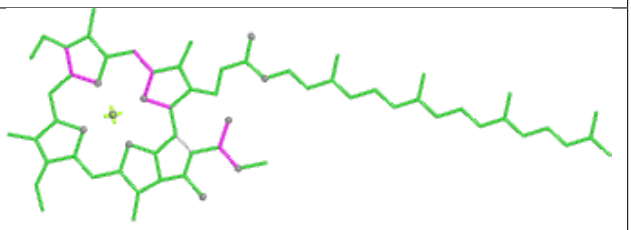

Rings

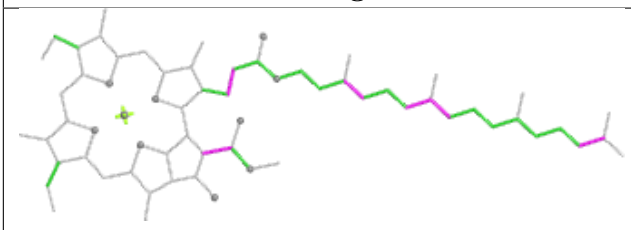
Ligand CLA C 309



Bond lengths



Bond angles



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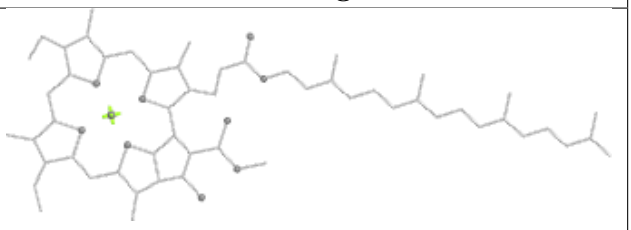
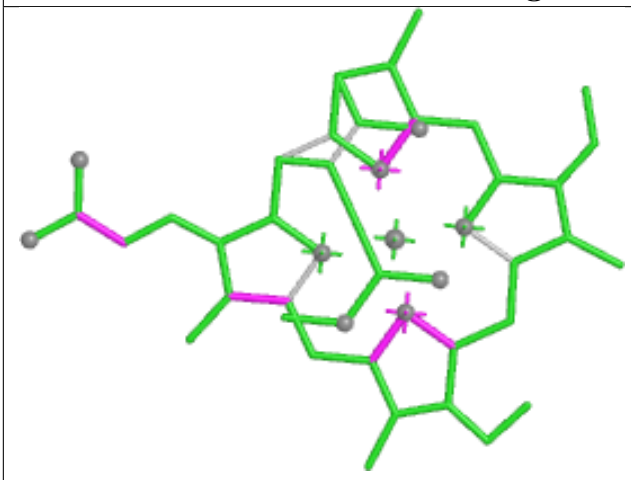


Rings

Ligand KC1 A 205



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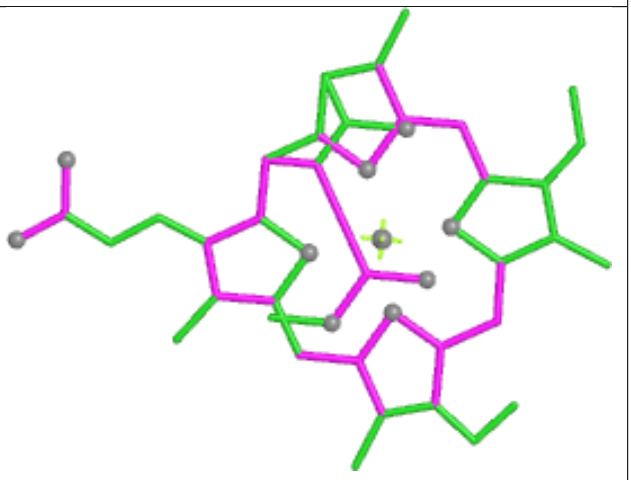
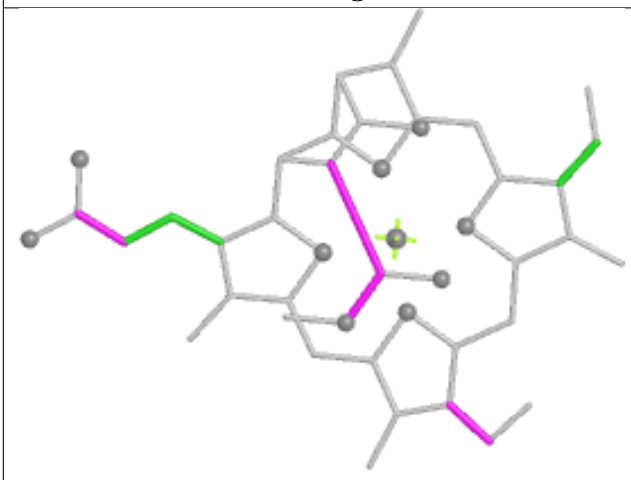


Bond angles



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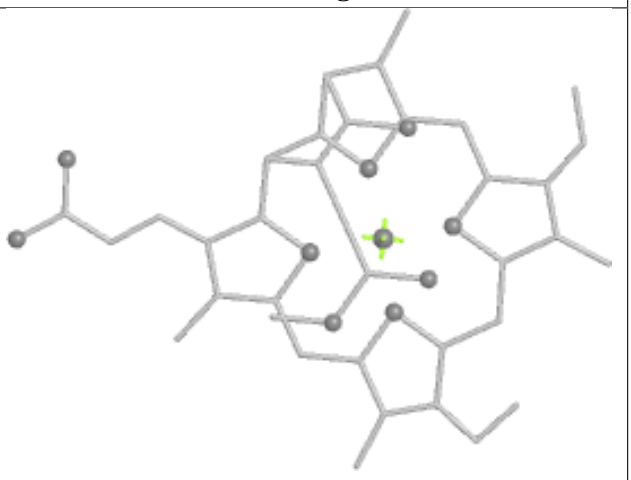
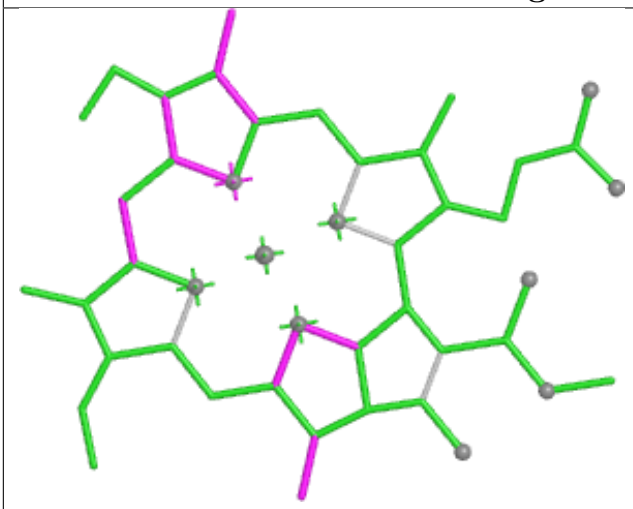


Rings

Ligand CLA a 817



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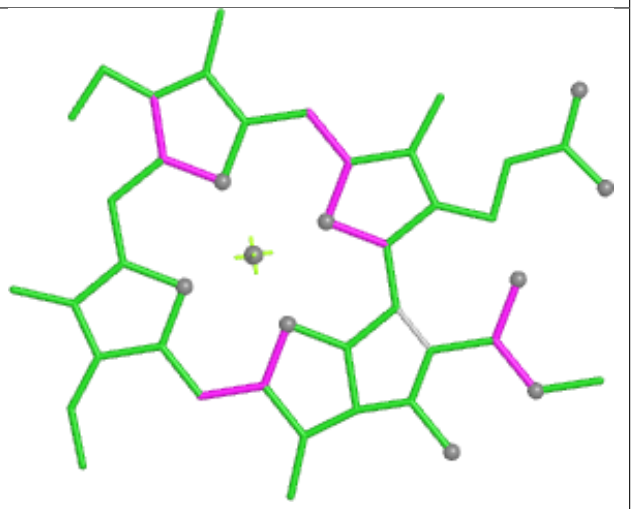
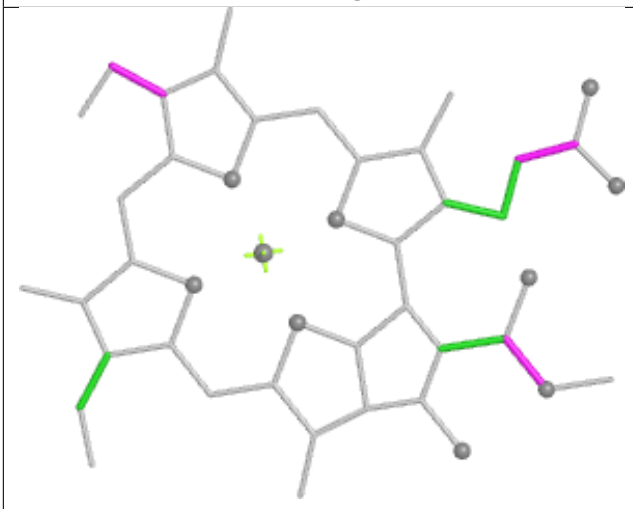


Bond angles

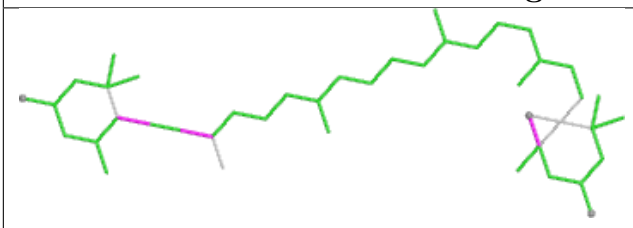


Torsions



Rings

Ligand DD6 B 319



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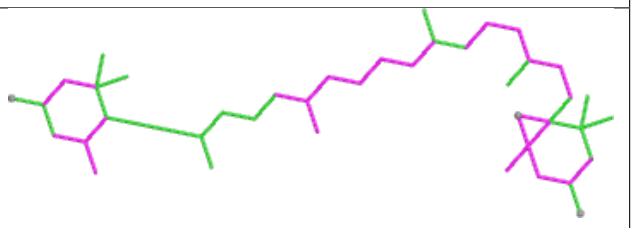
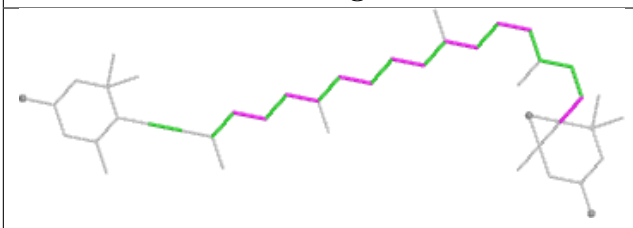
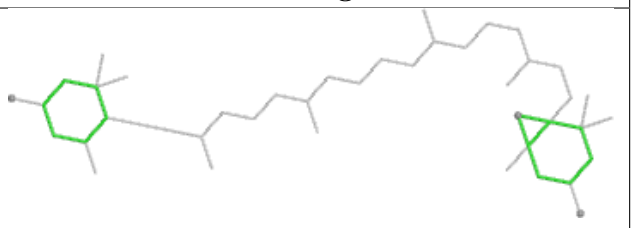


Bond angles

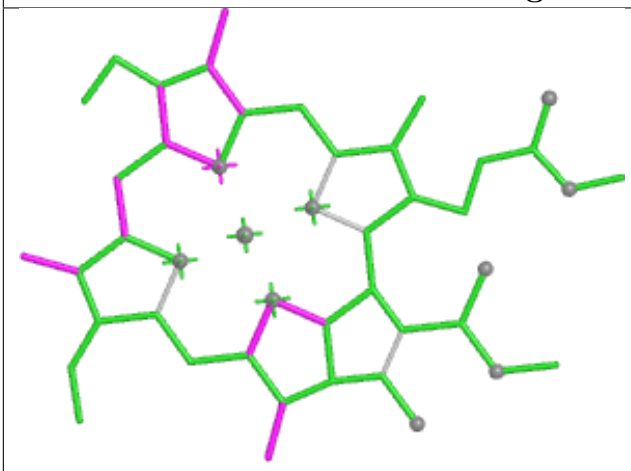


Torsions

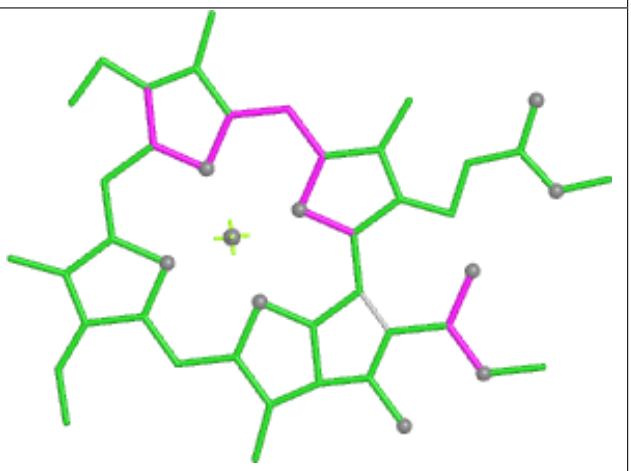


Rings

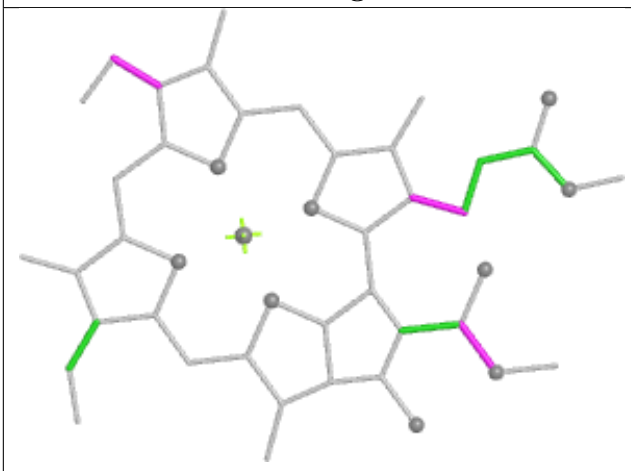
Ligand CLA F 308



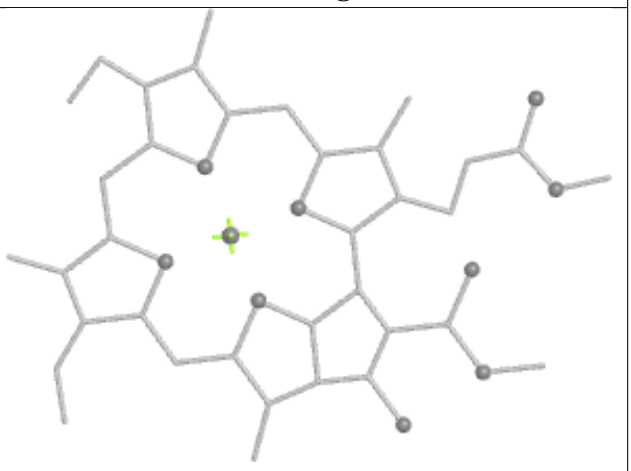
Bond lengths



Bond angles

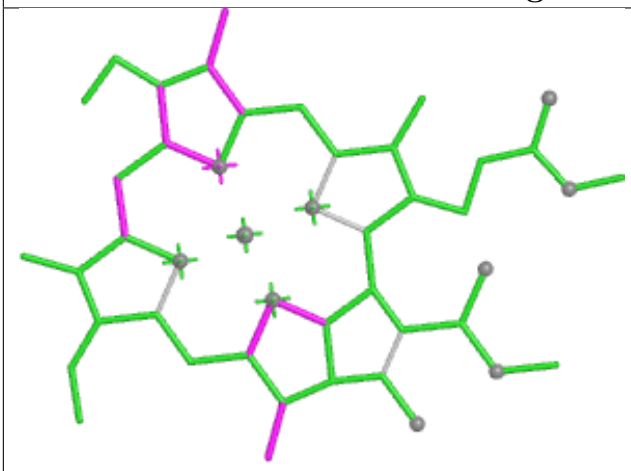


Torsions



Rings

Ligand CLA L 311



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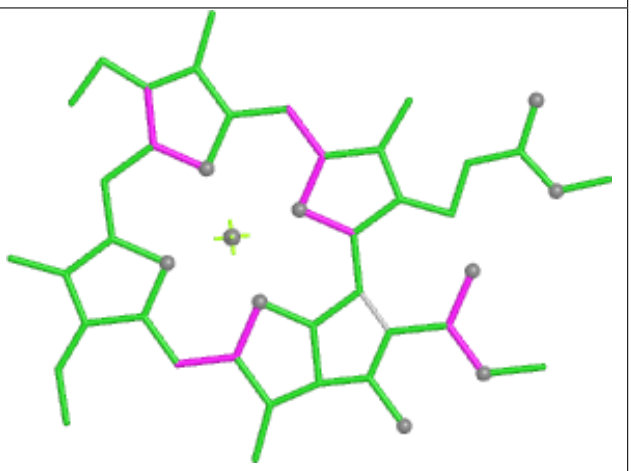
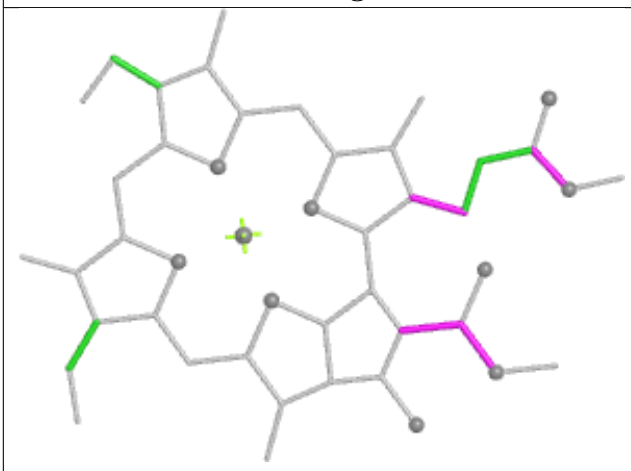


Bond angles



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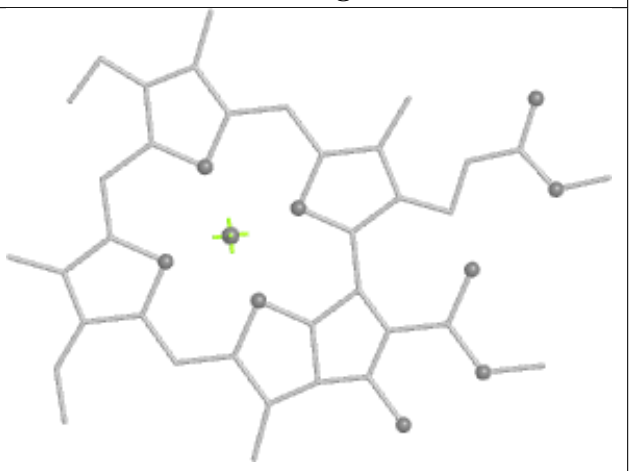
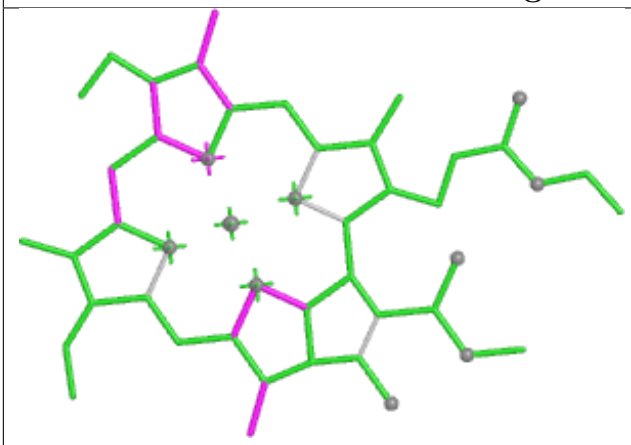


Rings

Ligand CLA C 314



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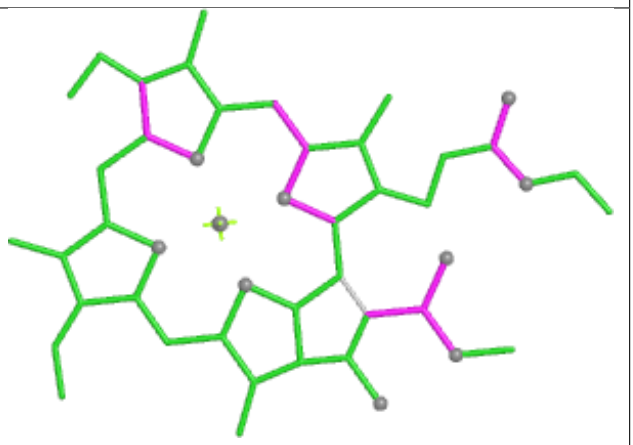

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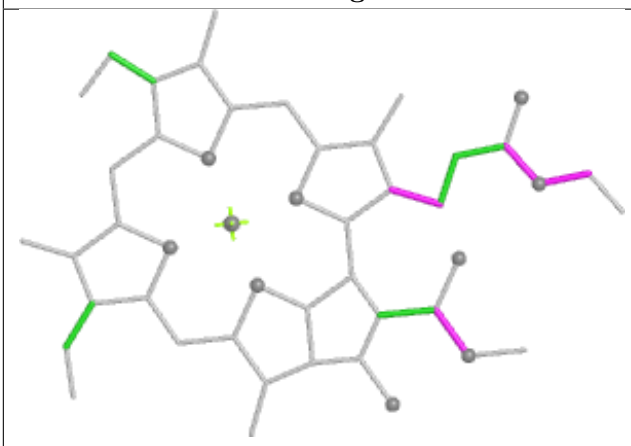

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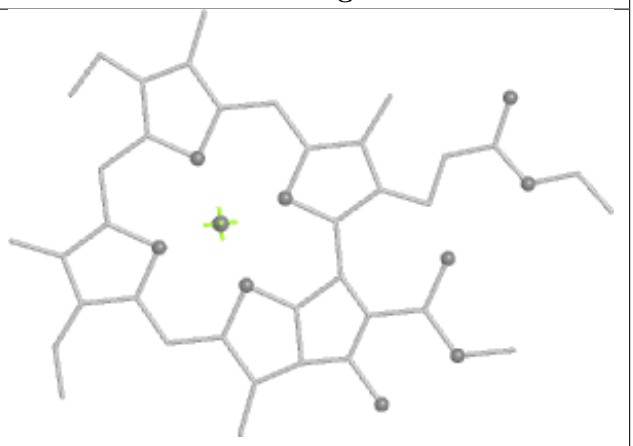
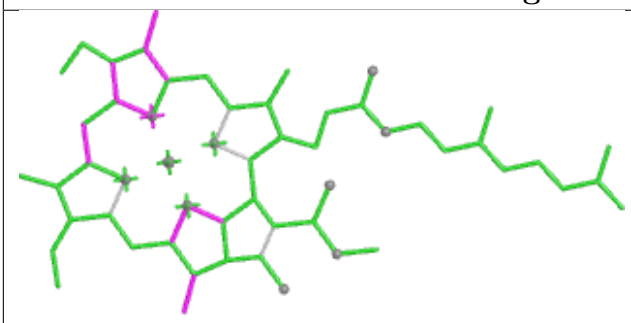


Rings

Ligand CLA G 313



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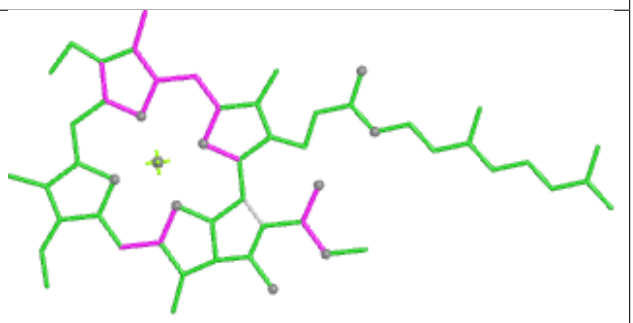
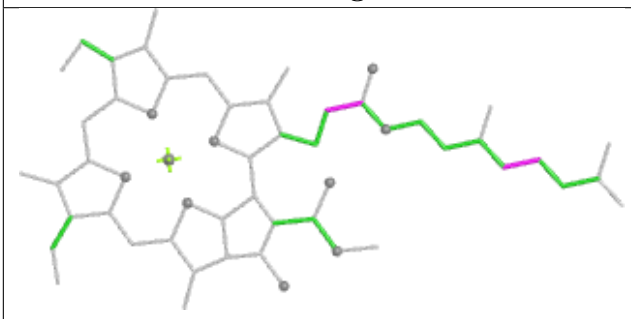


Bond angles



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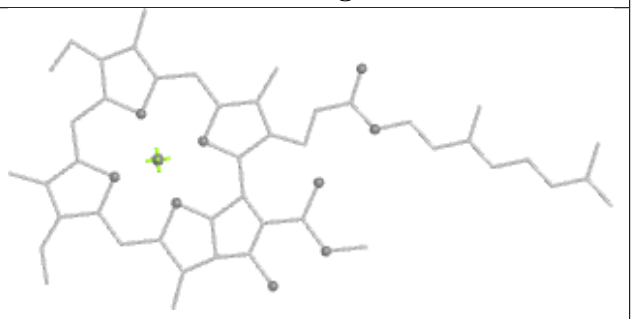
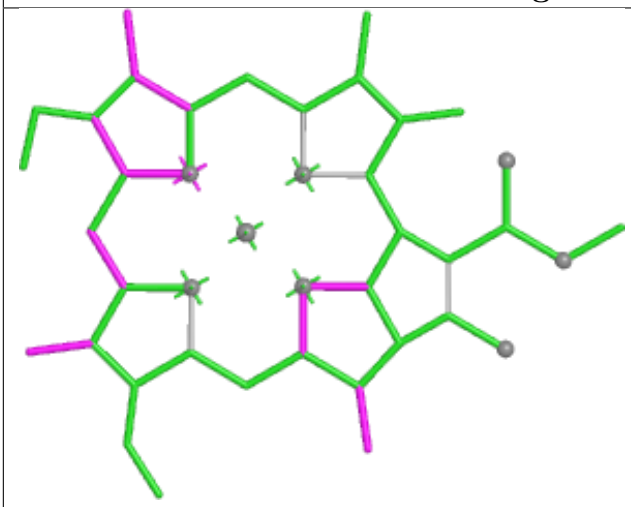


Rings

Ligand CLA l 508



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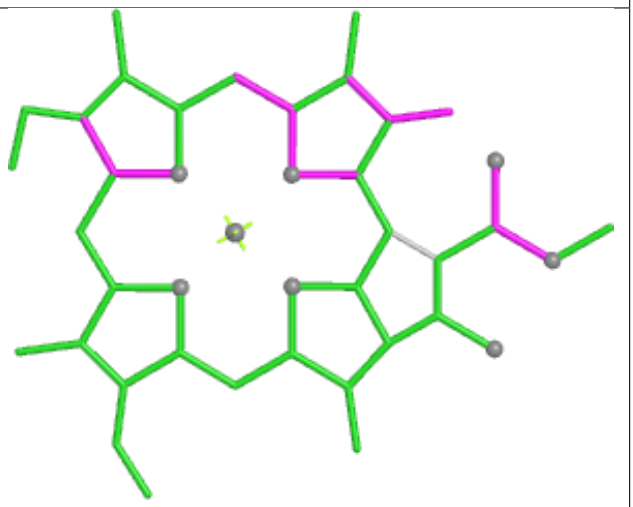
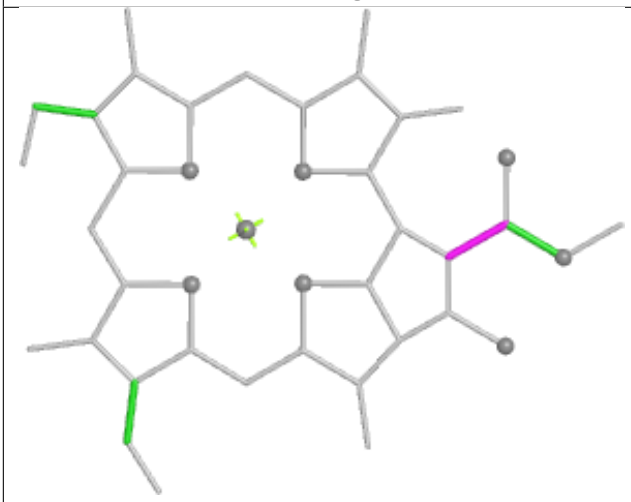


Bond angles



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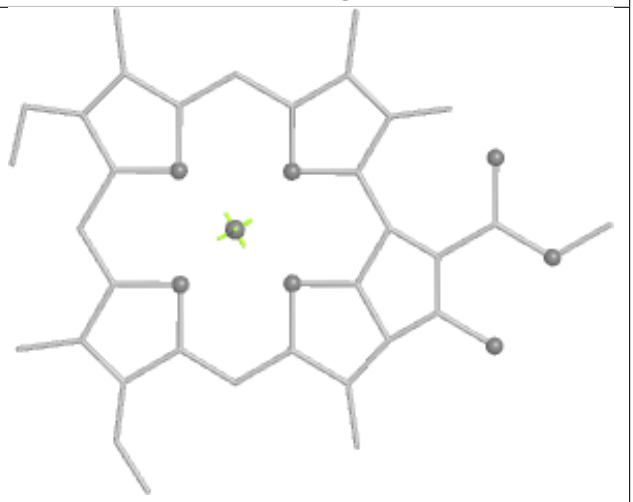
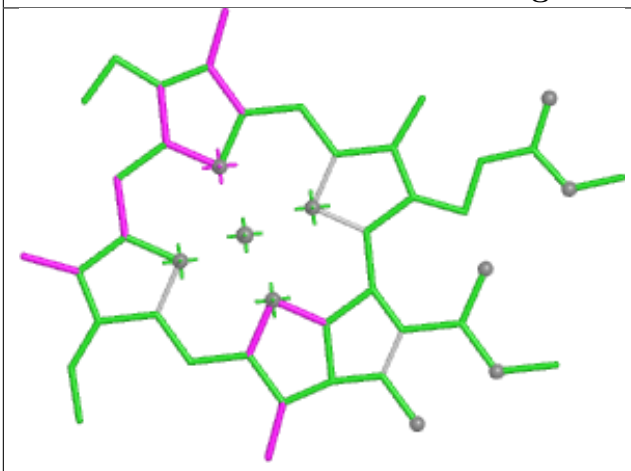


Rings

Ligand CLA f 802



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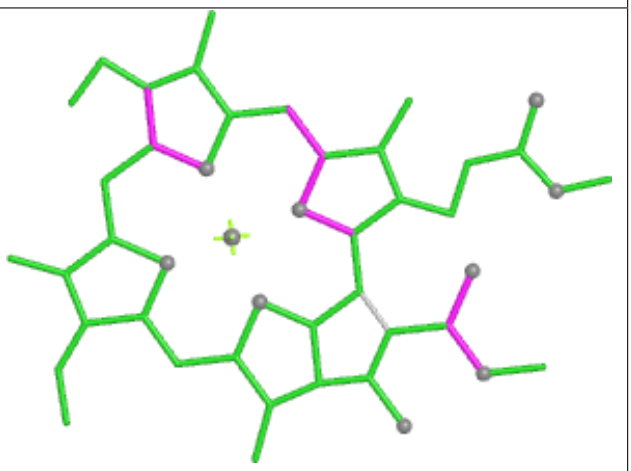
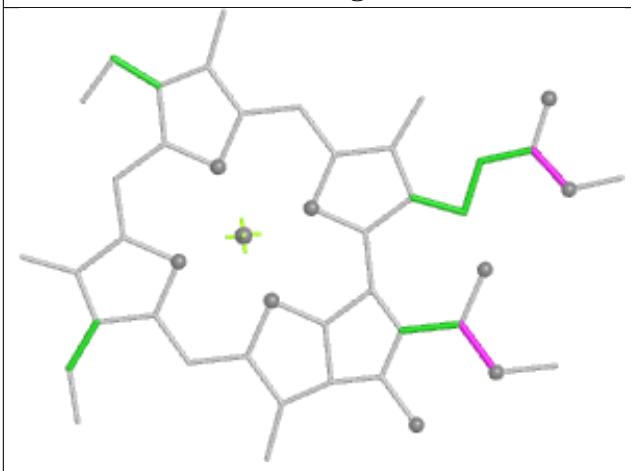


Bond angles



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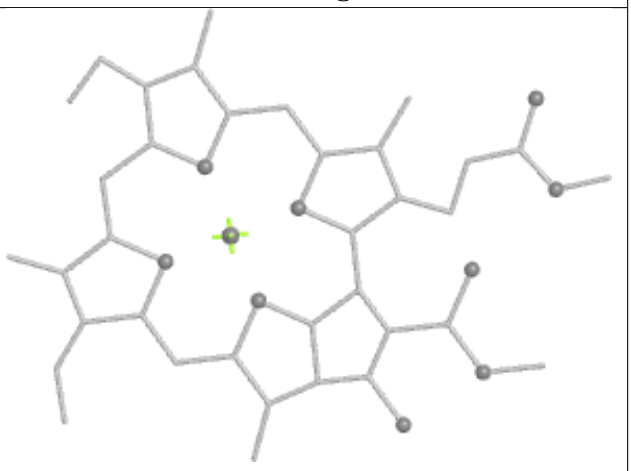
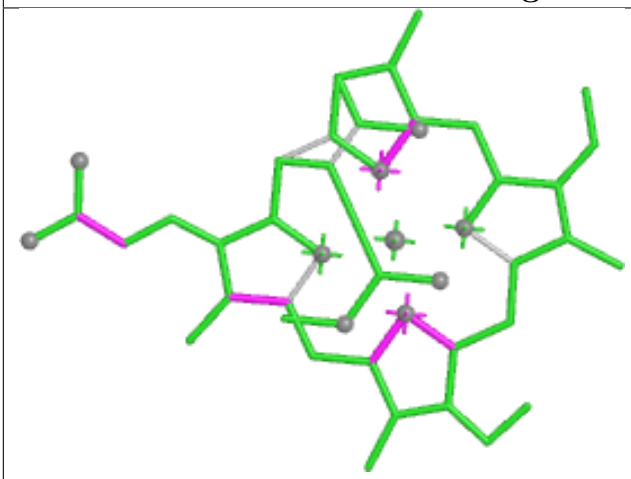


Rings

Ligand KC1 M 305



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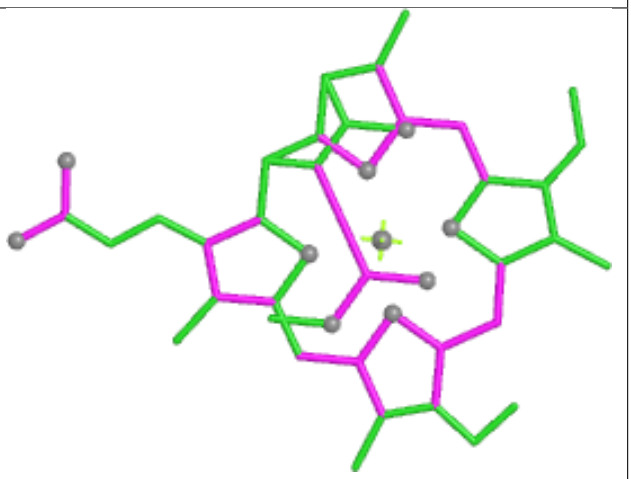
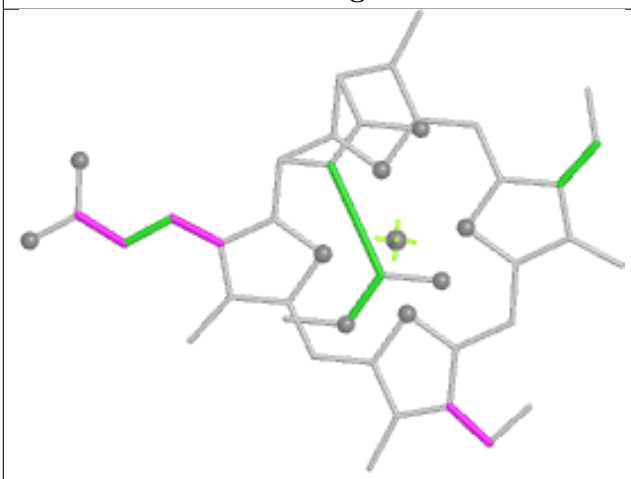


Bond angles



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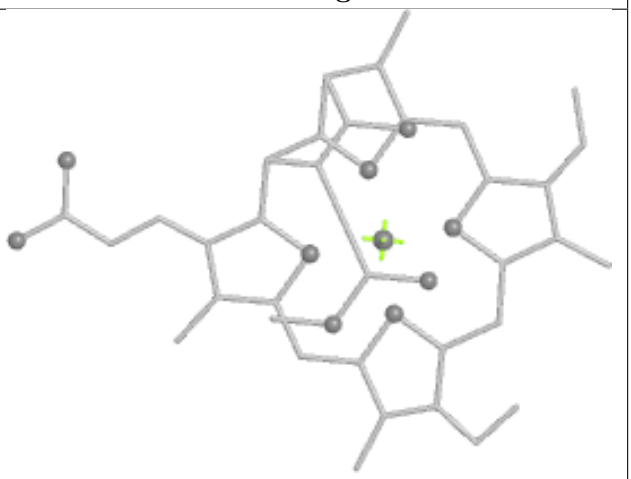
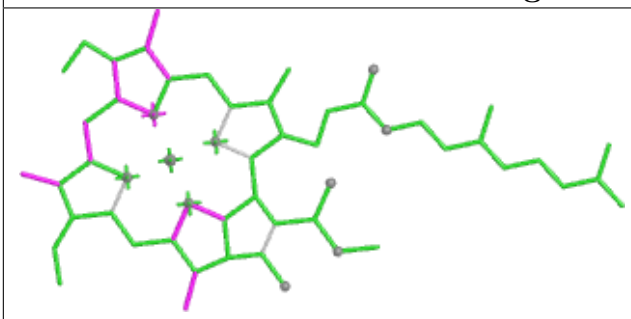


Rings

Ligand CLA A 212



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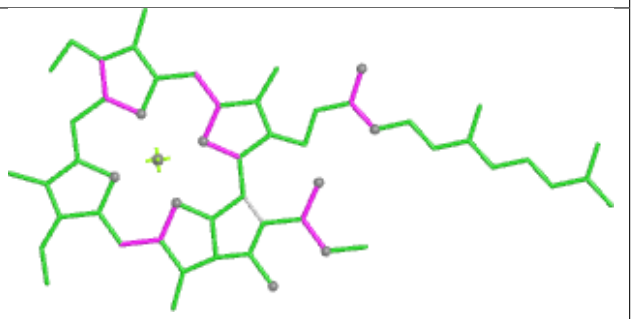

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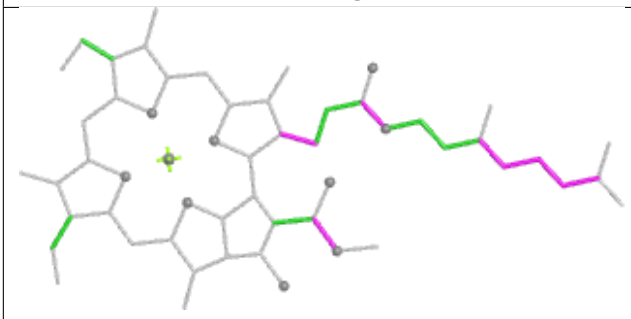

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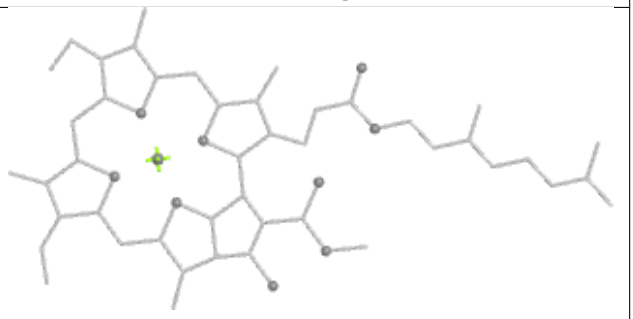
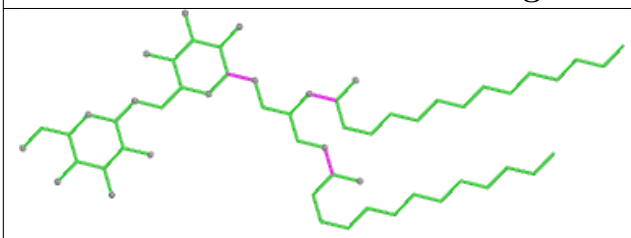


Rings

Ligand DGD b 733



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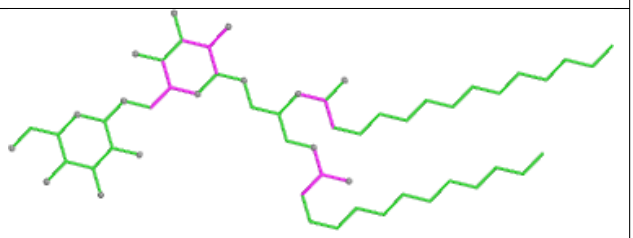
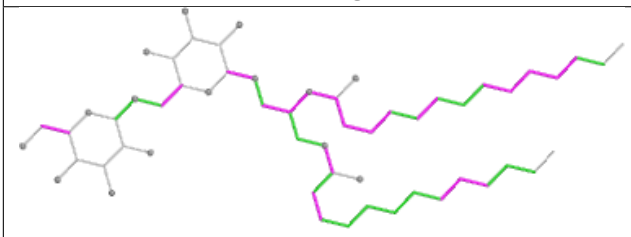


Bond angles



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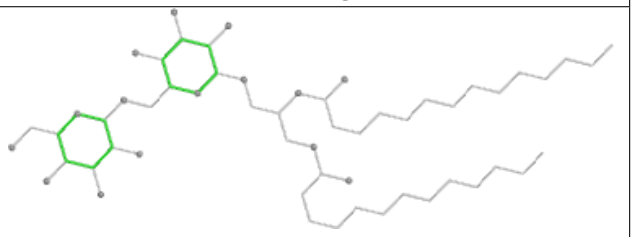
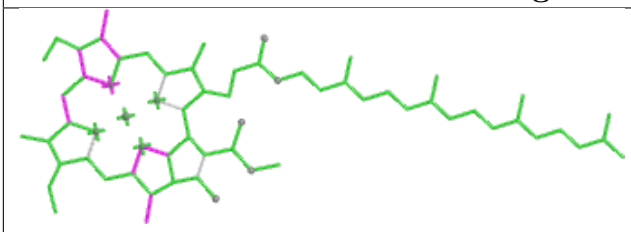


Rings

Ligand CLA l 505



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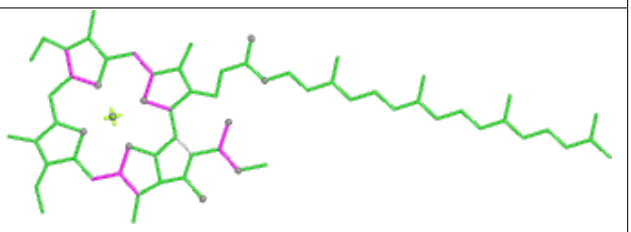
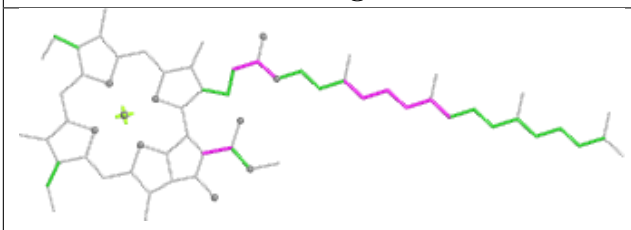


Bond angles



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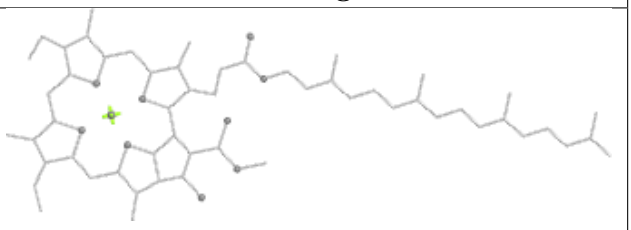
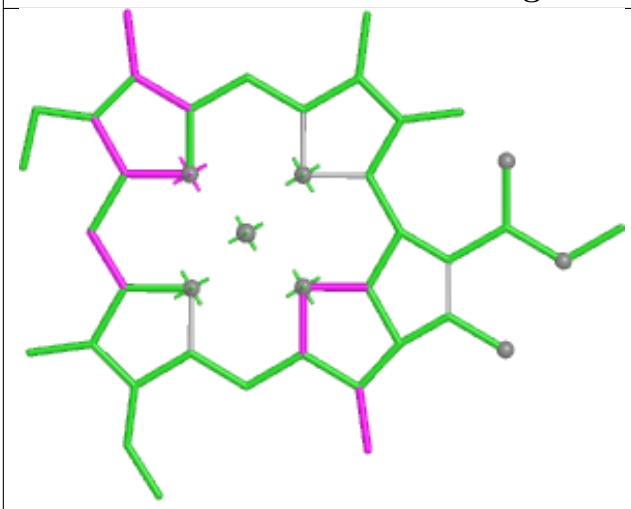


Rings

Ligand CLA G 319



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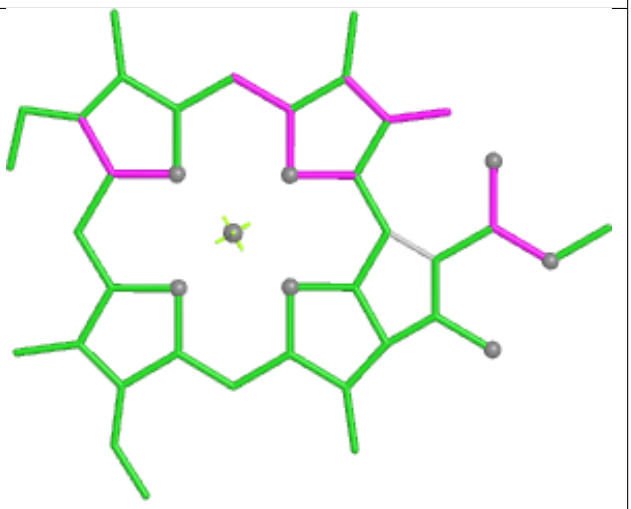
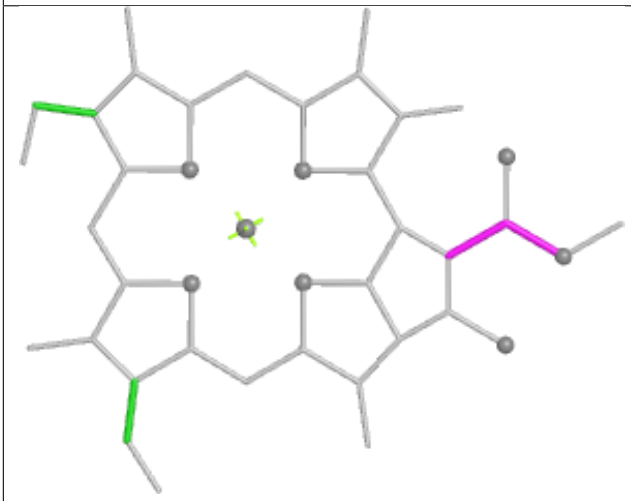


Bond angles



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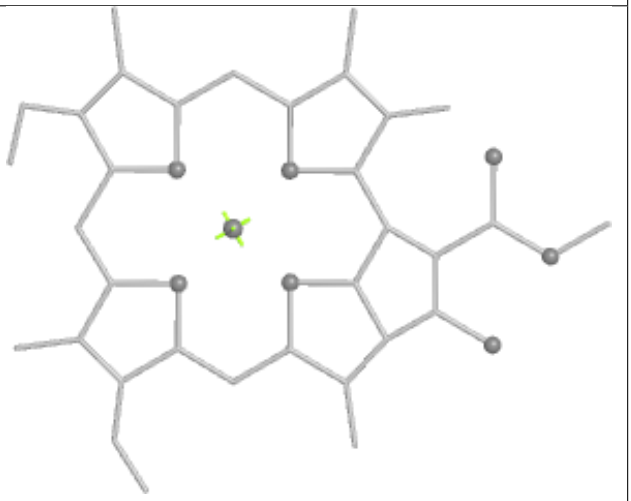
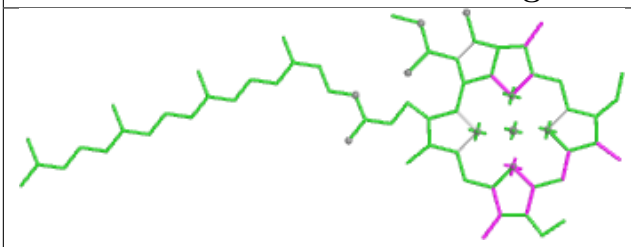


Rings

Ligand CLA G 316



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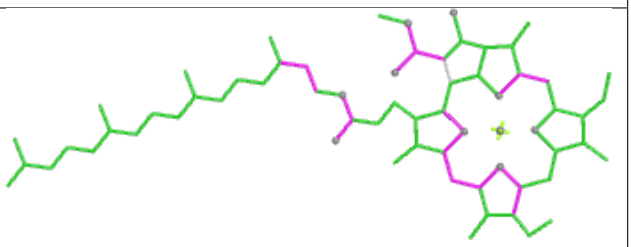
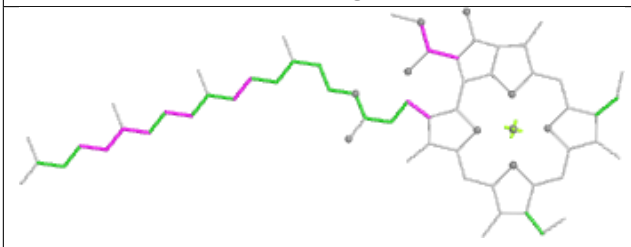


Bond angles



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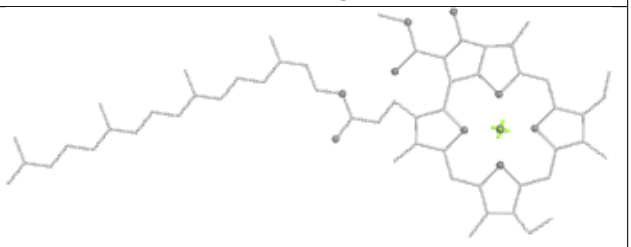
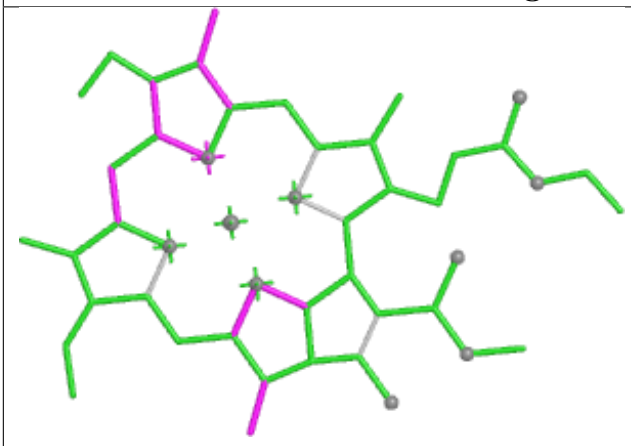


Rings

Ligand CLA Q 307



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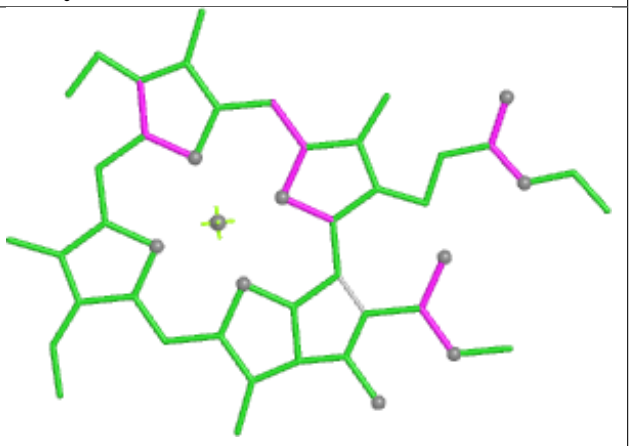
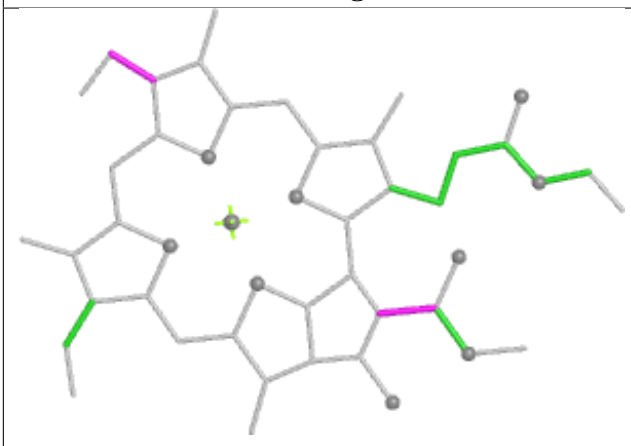


Bond angles



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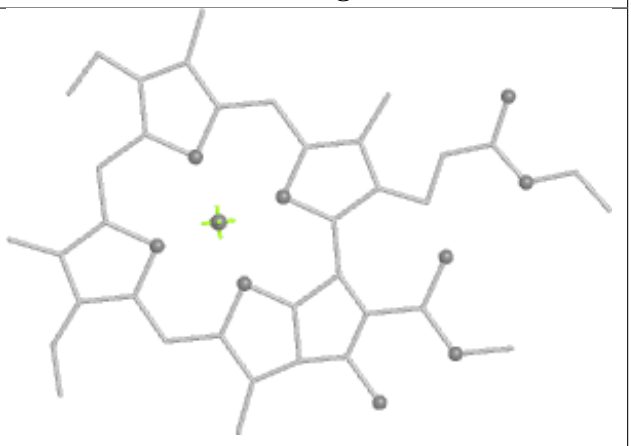
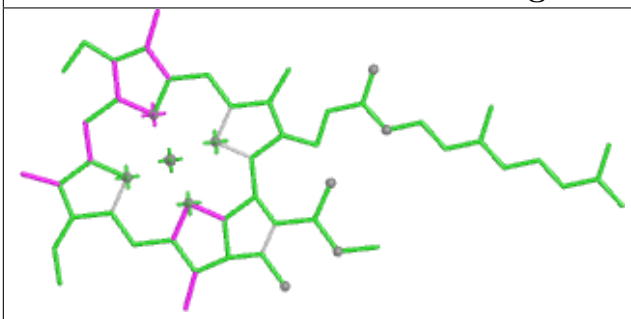


Rings

Ligand CLA a 805



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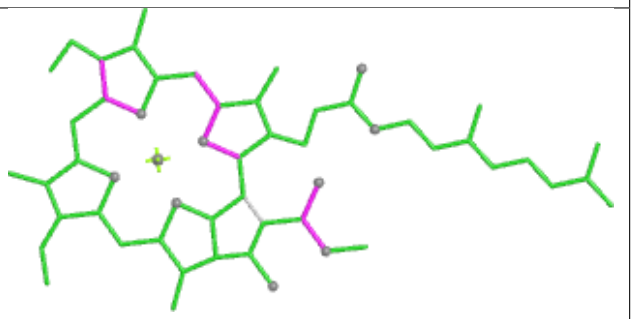
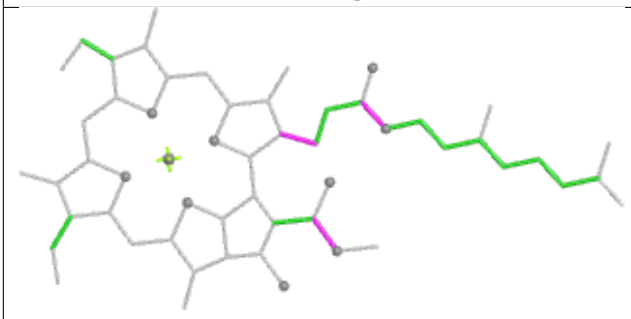


Bond angles



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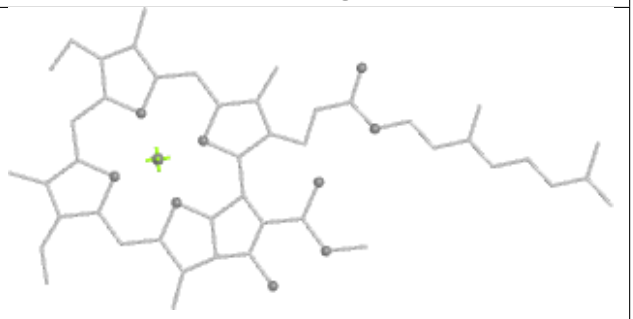
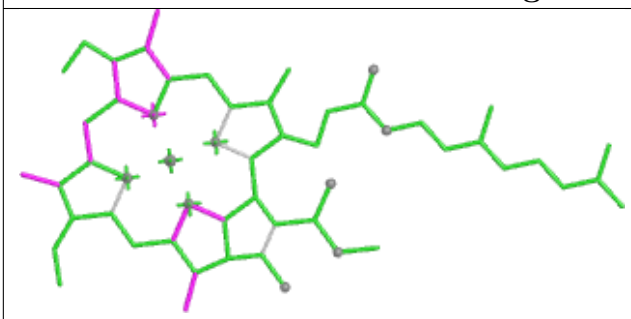


Rings

Ligand CLA K 214



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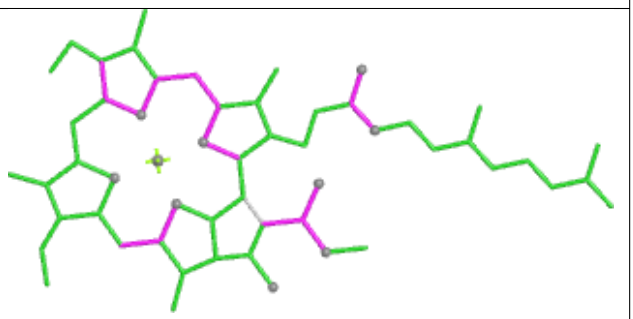
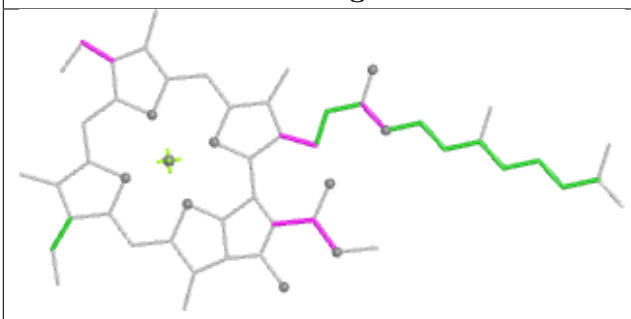


Bond angles



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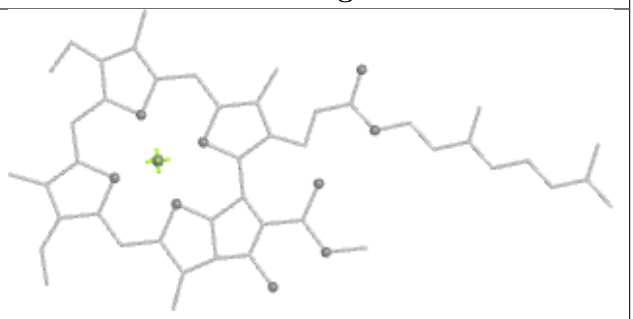
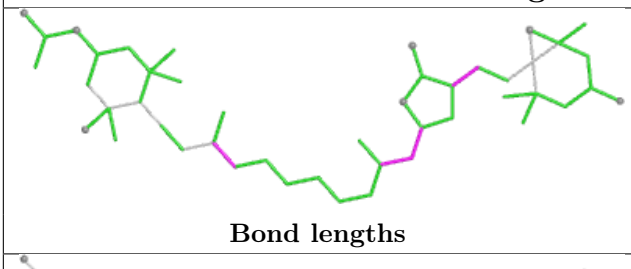
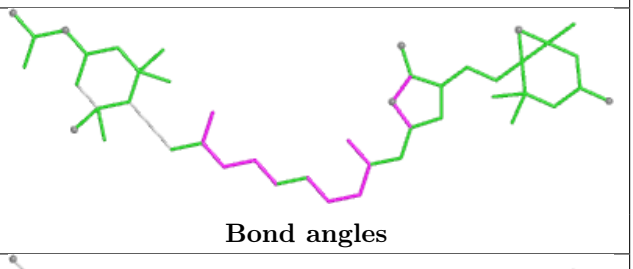


Rings

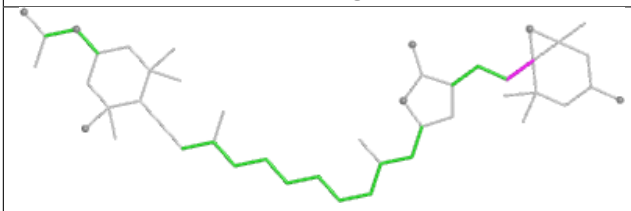
Ligand PID D 302



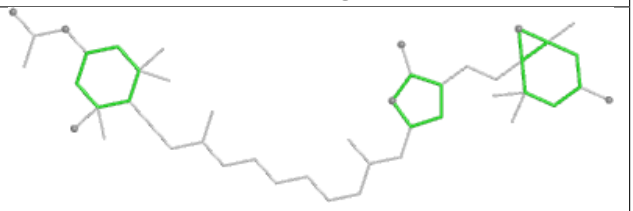
Bond lengths



Bond angles

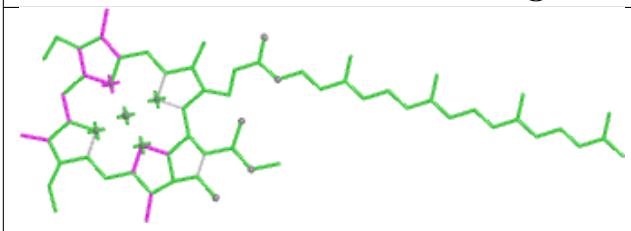


Torsions



Rings

Ligand CLA b 705



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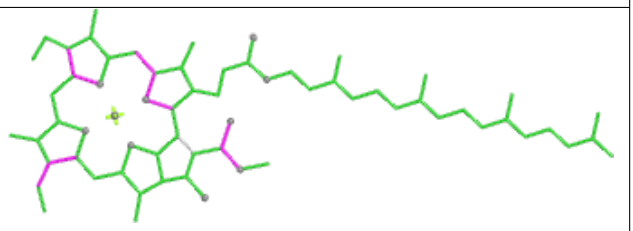

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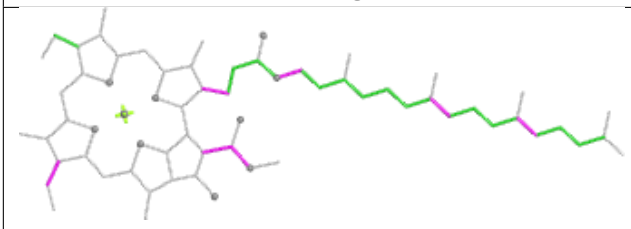

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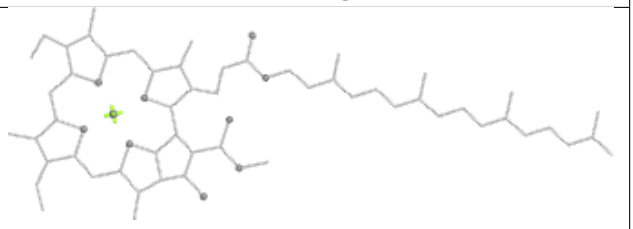
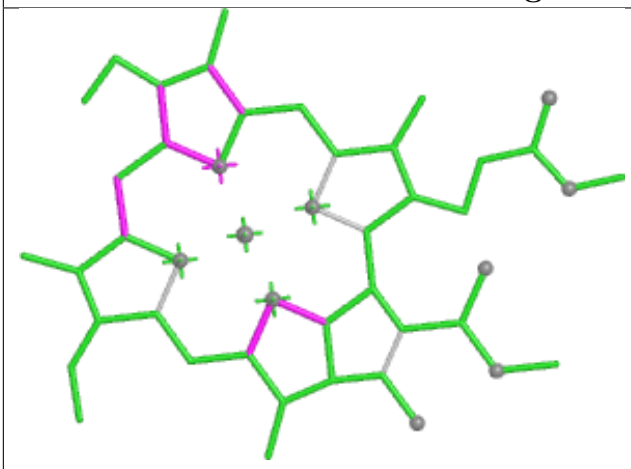


Rings

Ligand CLA T 311



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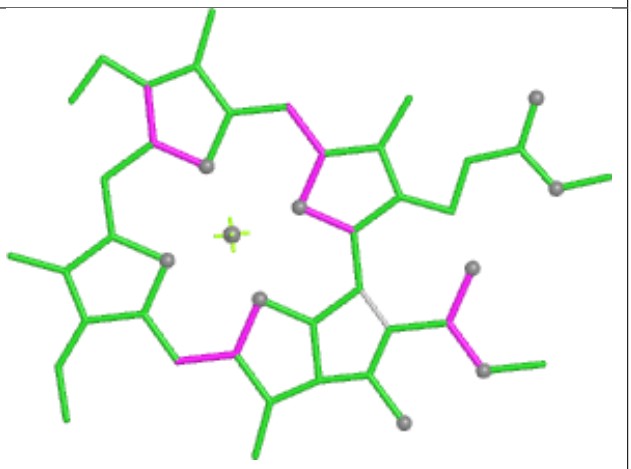

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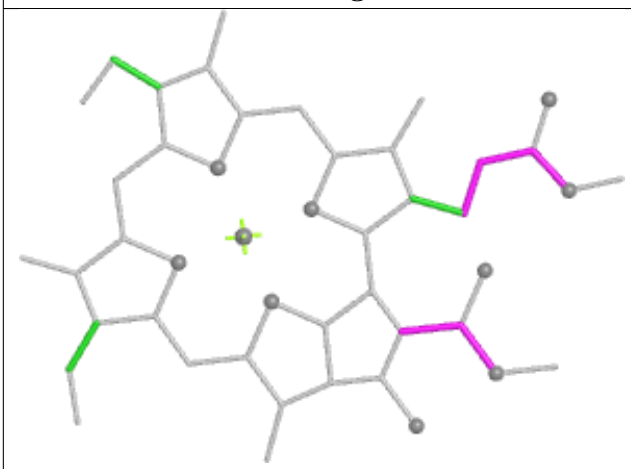

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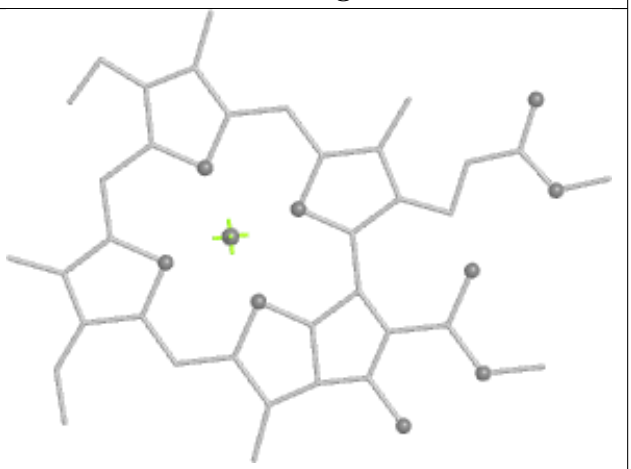
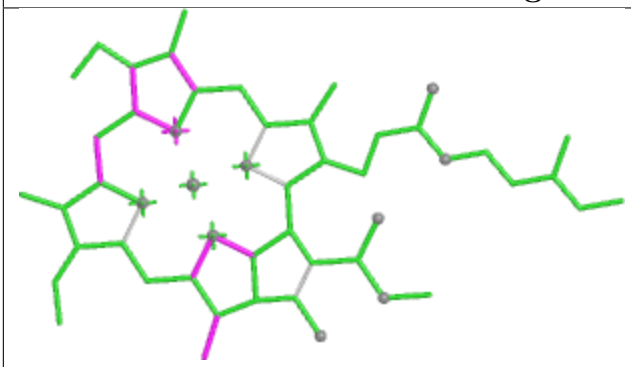


Rings

Ligand CLA C 311



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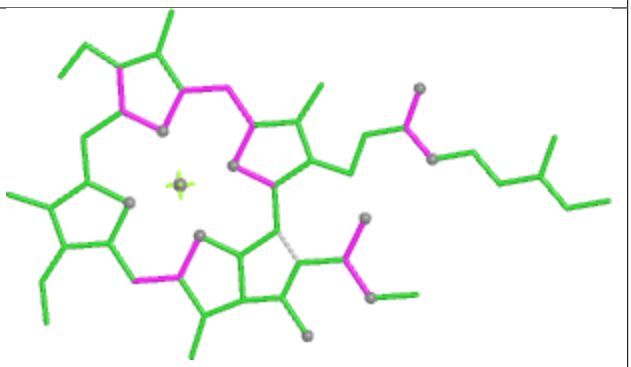

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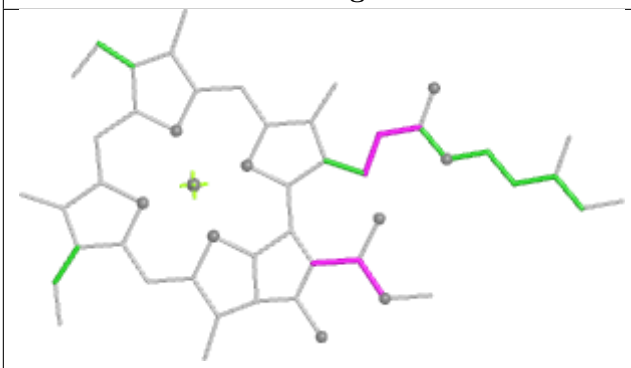

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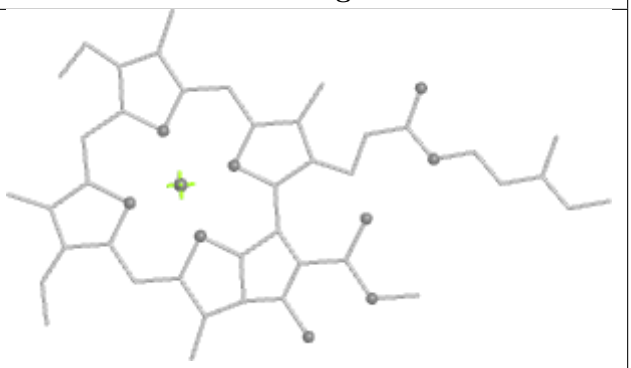
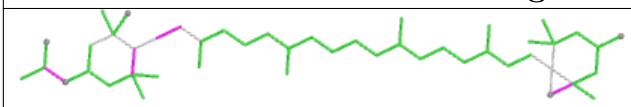


Rings

Ligand UIX T 306



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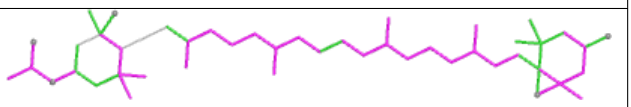

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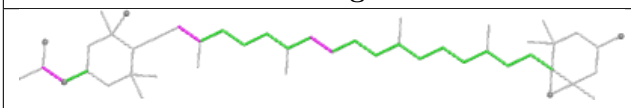

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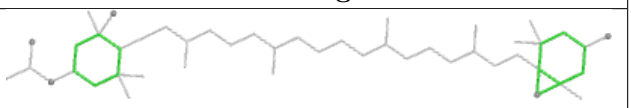
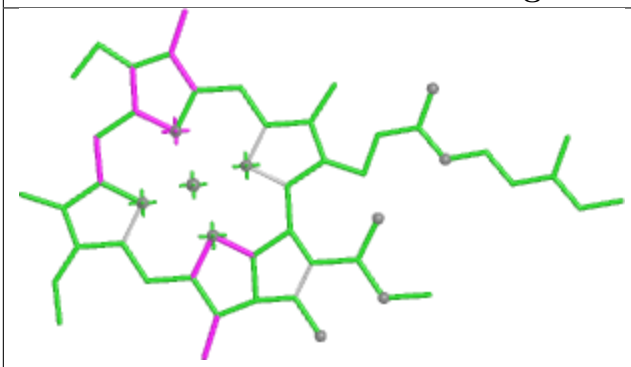


Rings

Ligand CLA A 217



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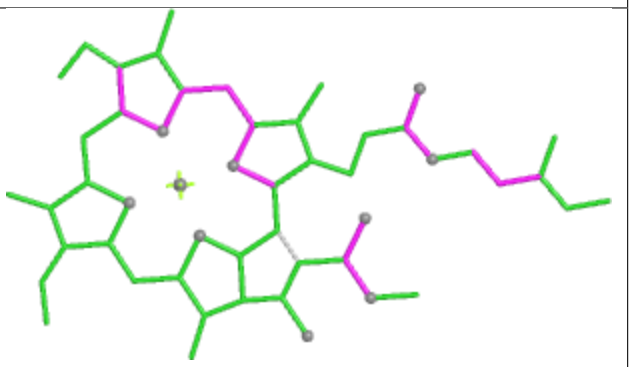

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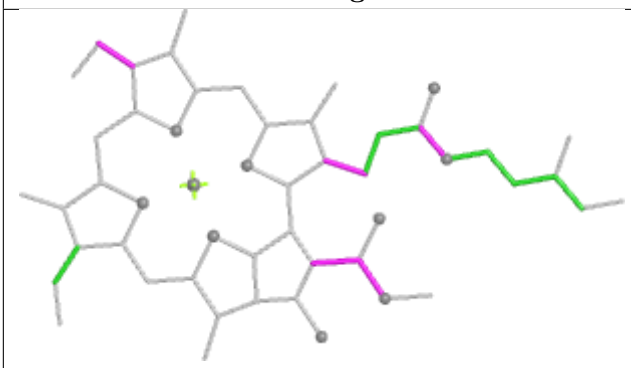

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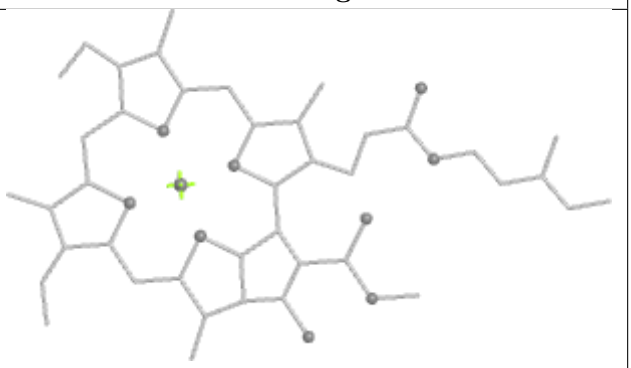
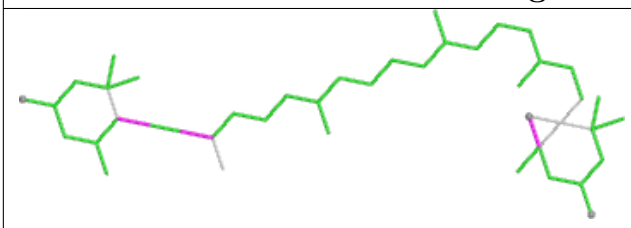


Rings

Ligand DD6 J 303



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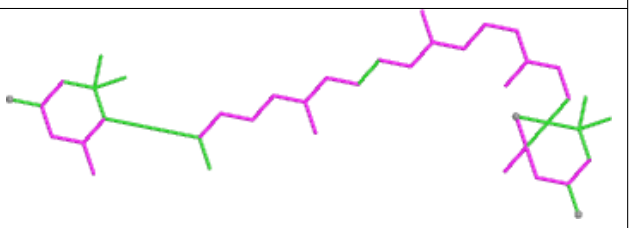

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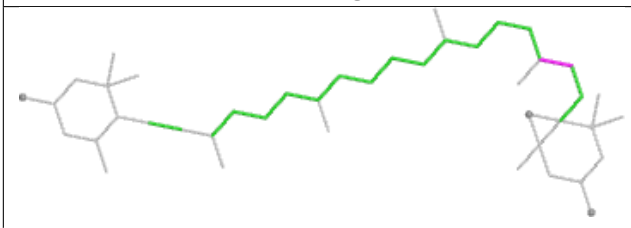

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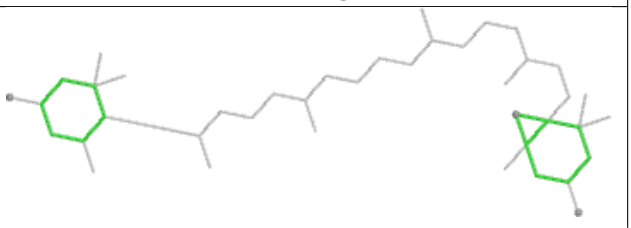
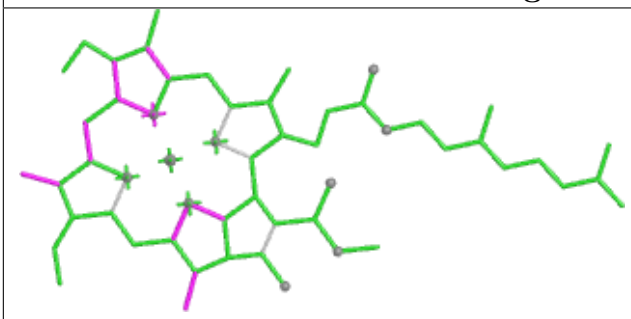


Rings

Ligand CLA A 208



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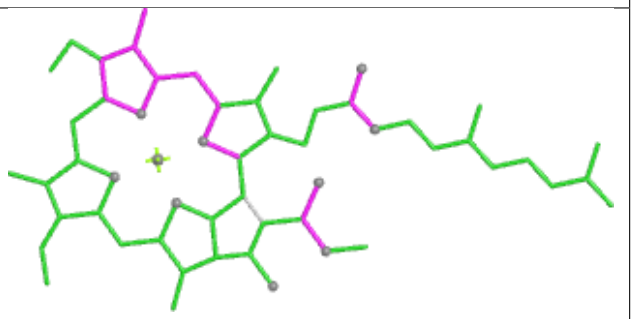

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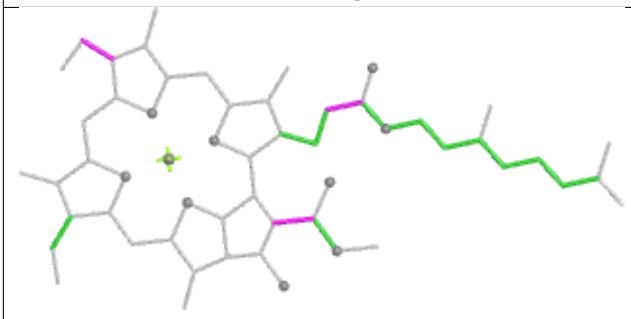

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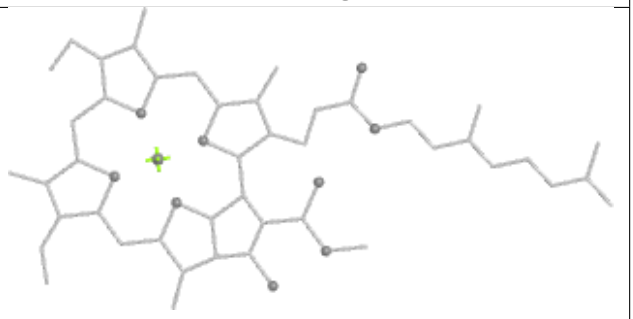
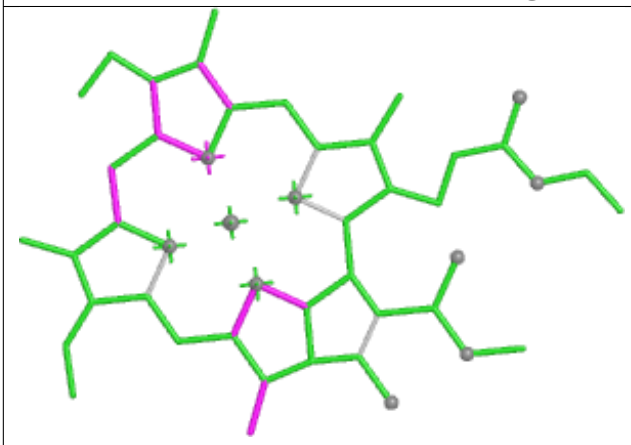


Rings

Ligand CLA H 307



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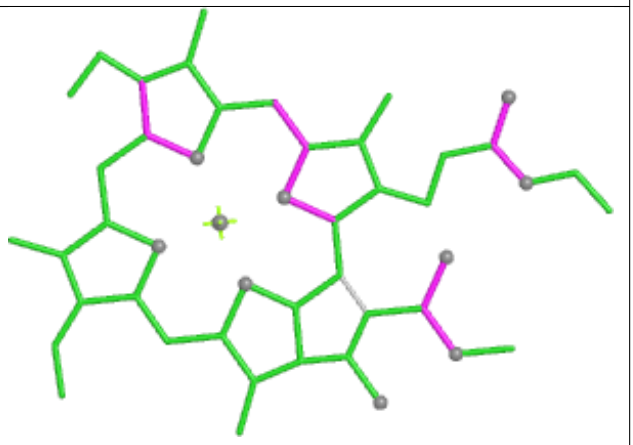
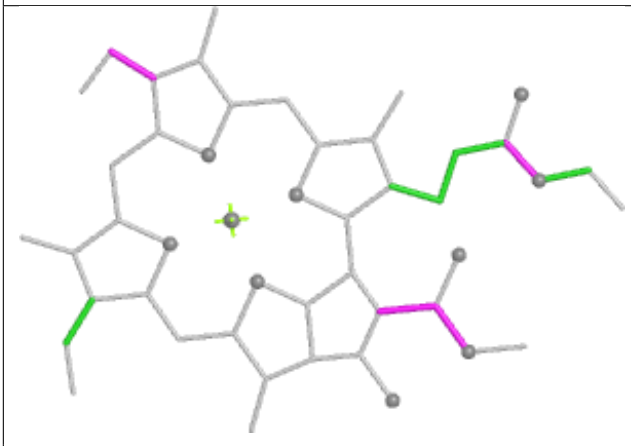


Bond angles



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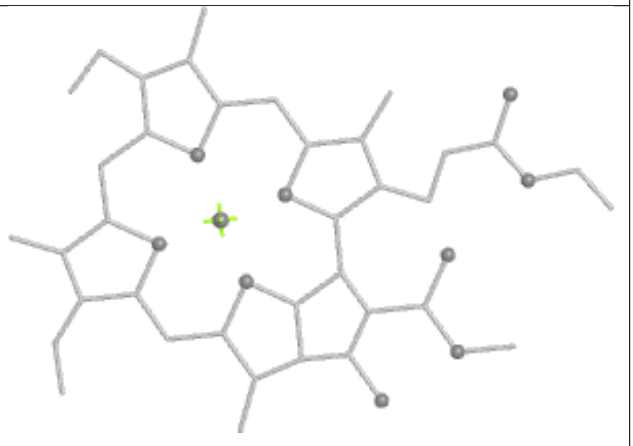
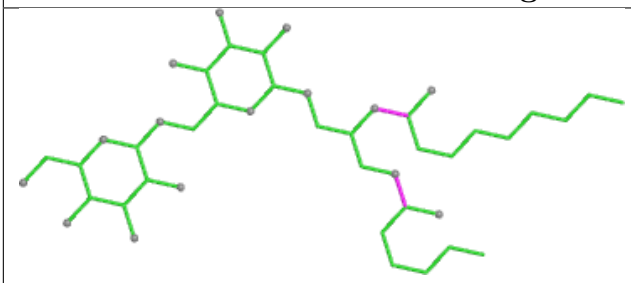


Rings

Ligand DGD B 318



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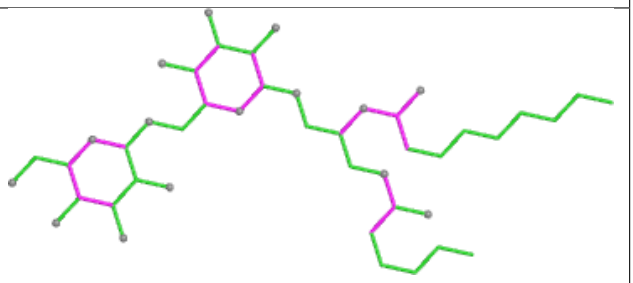

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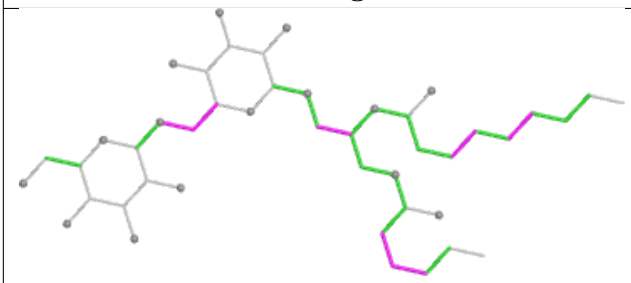

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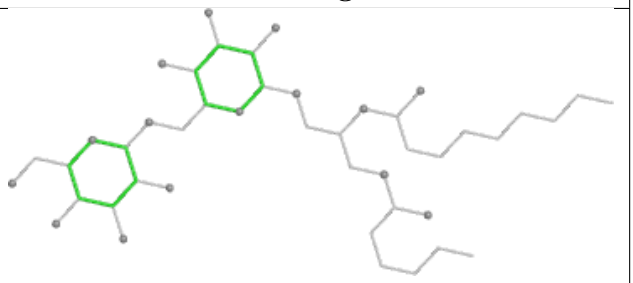
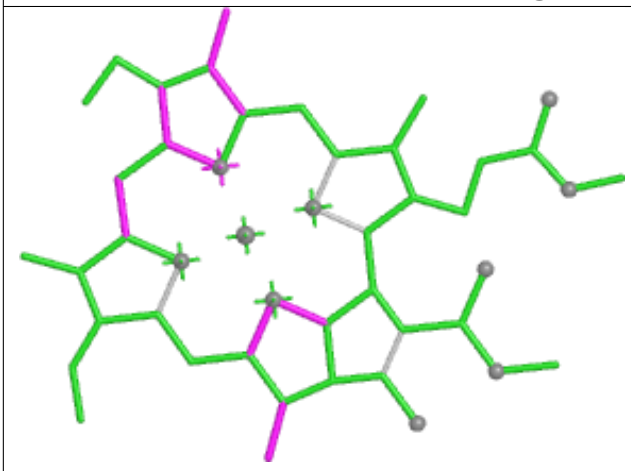


Rings

Ligand CLA I 208



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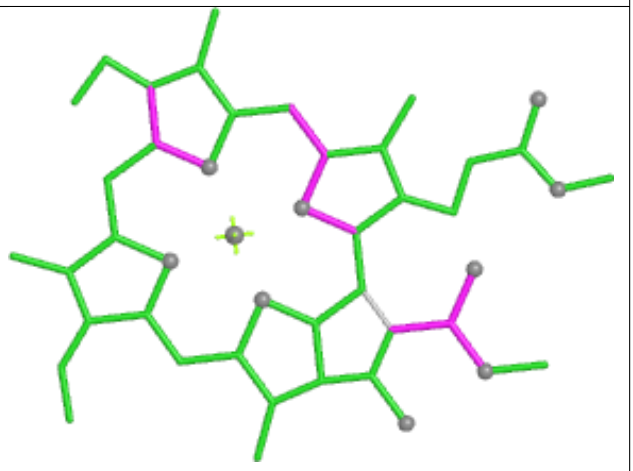
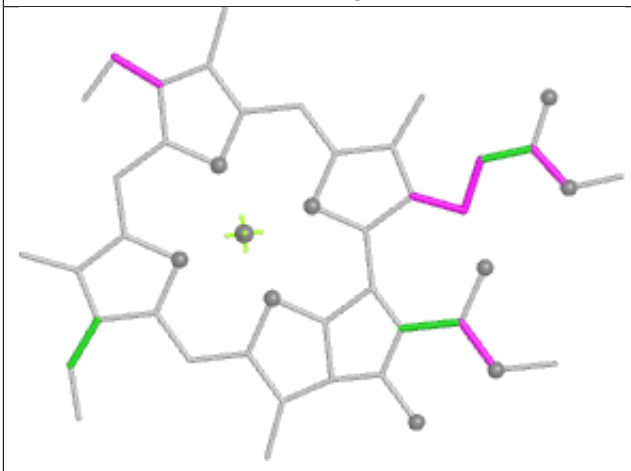


Bond angles



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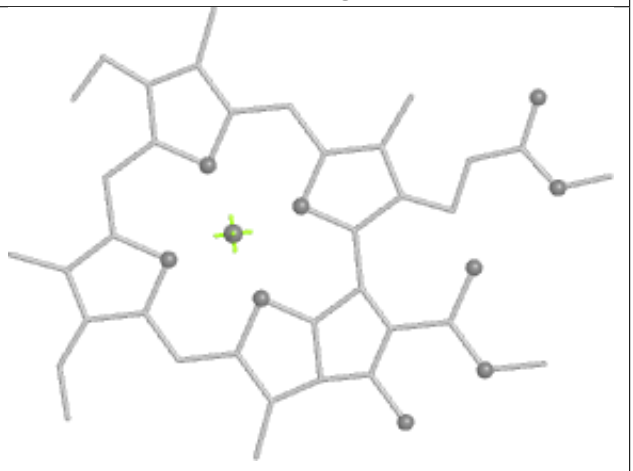
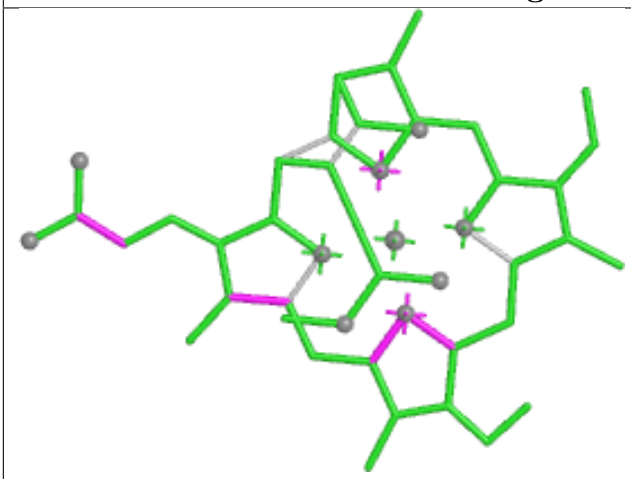


Rings

Ligand KC1 P 213



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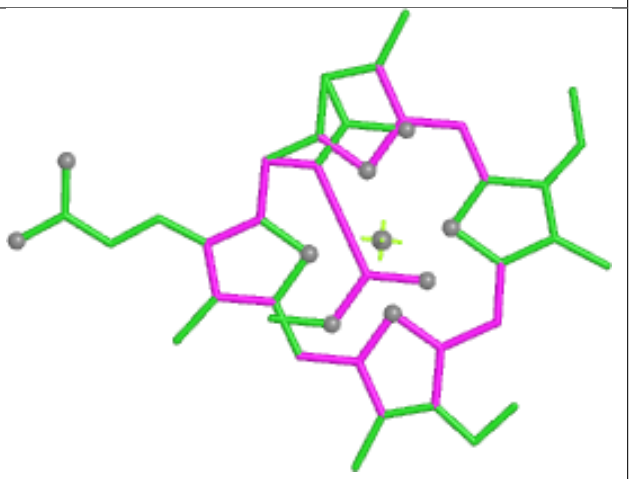

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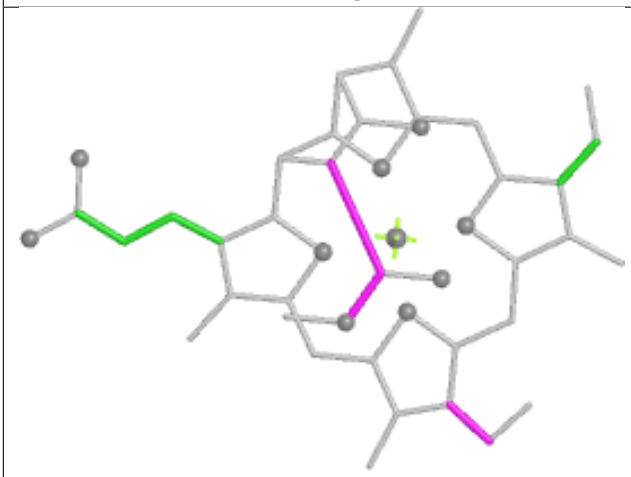

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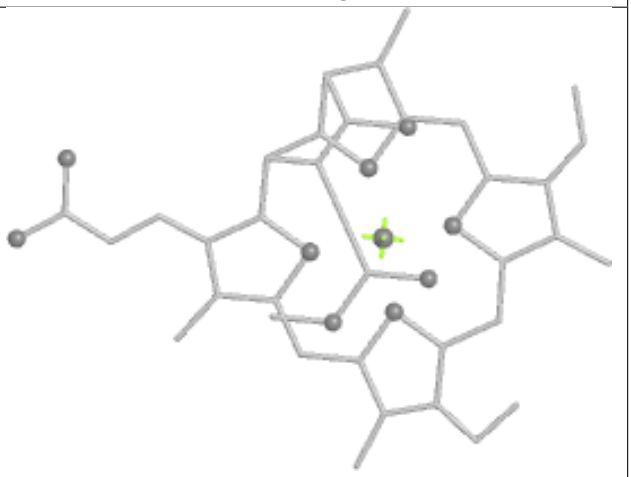
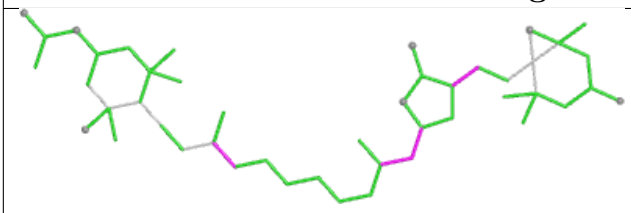


Rings

Ligand PID C 302



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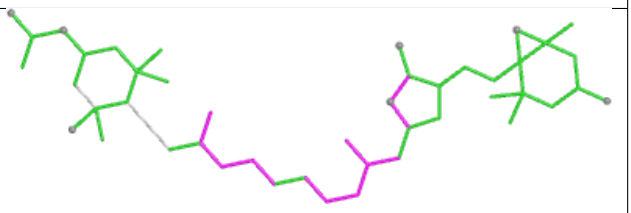
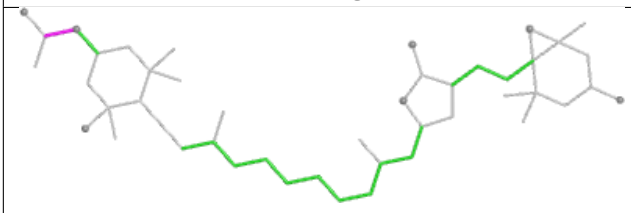


Bond angles



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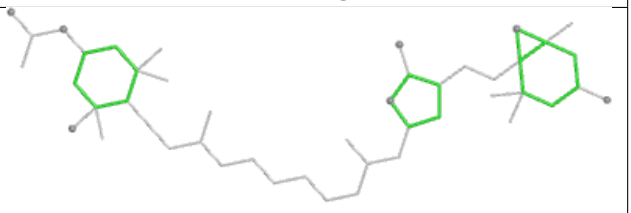
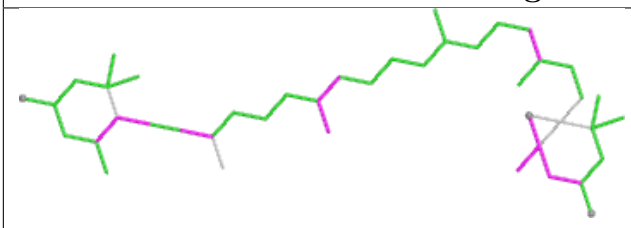


Rings

Ligand DD6 G 307



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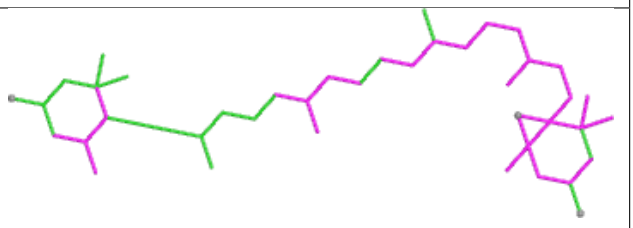
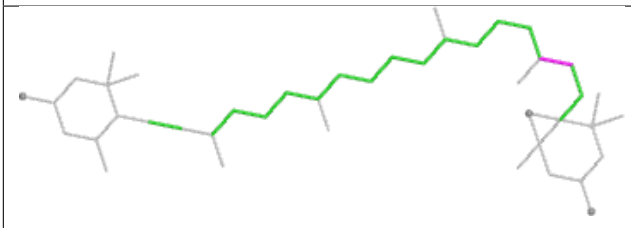


Bond angles

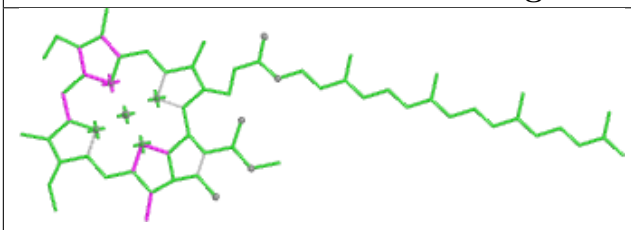


Torsions



Rings

Ligand CLA P 210



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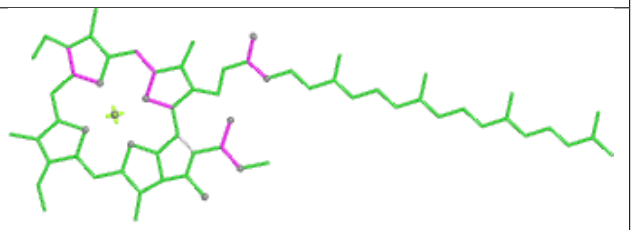
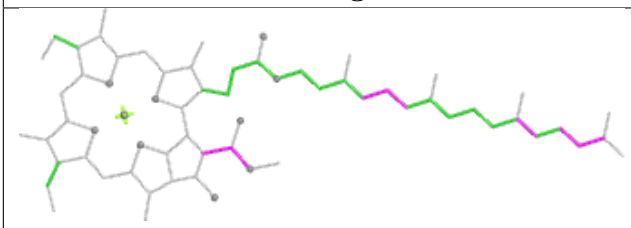


Bond angles



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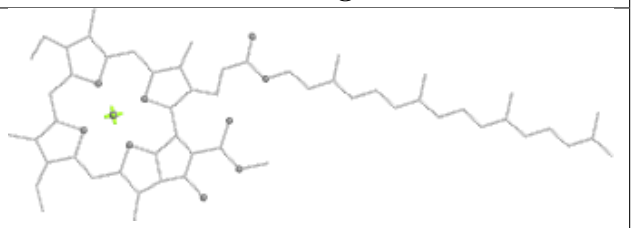
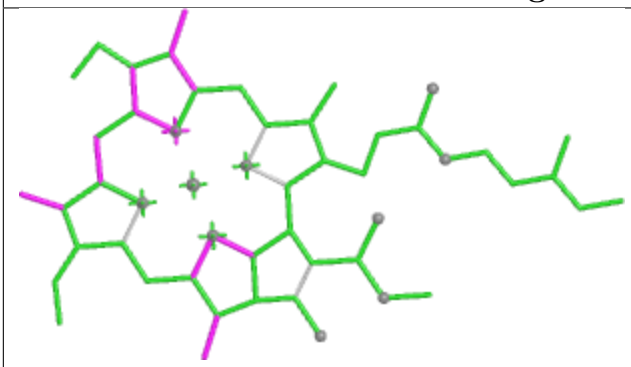
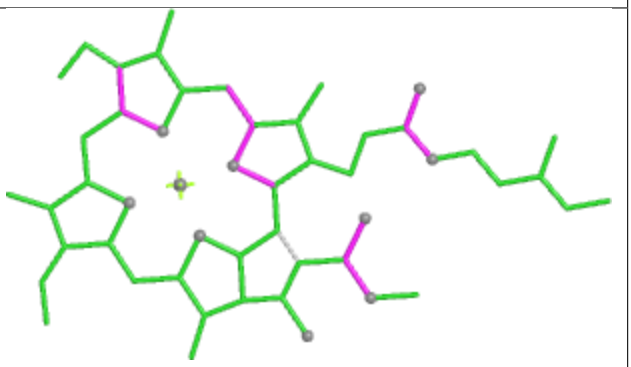


Rings

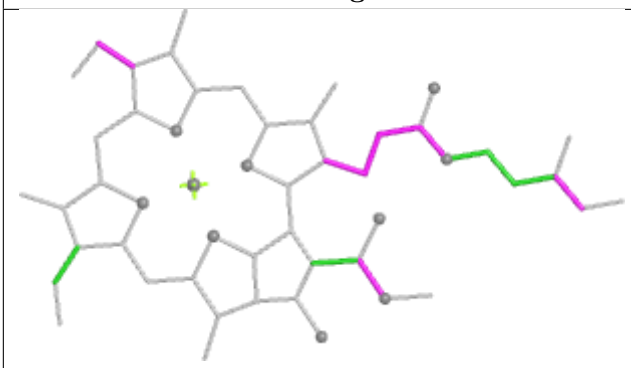
Ligand CLA a 813



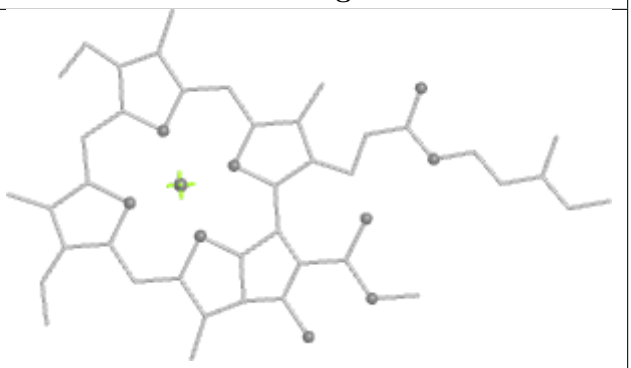
Bond lengths



Bond angles

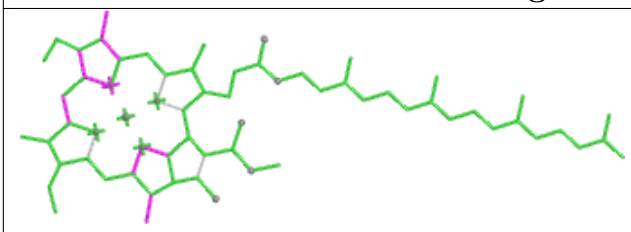


Torsions



Rings

Ligand CLA a 826



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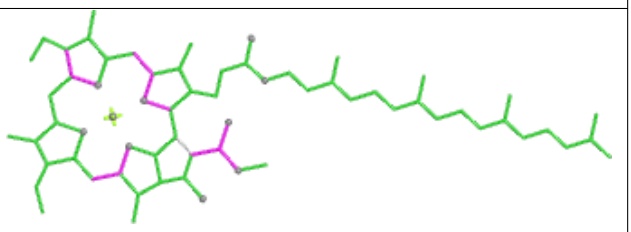
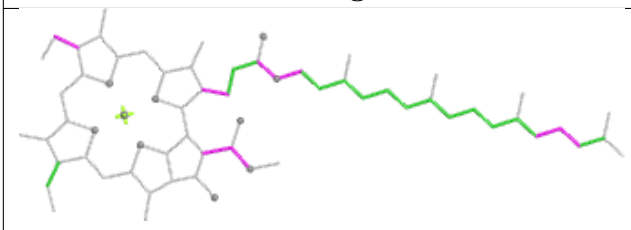


Bond angles



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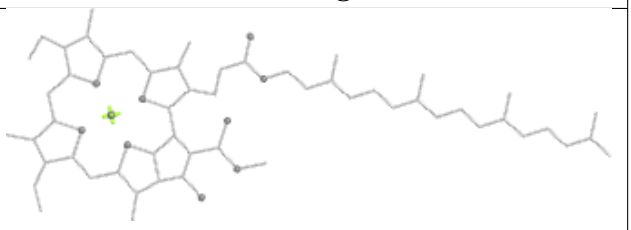
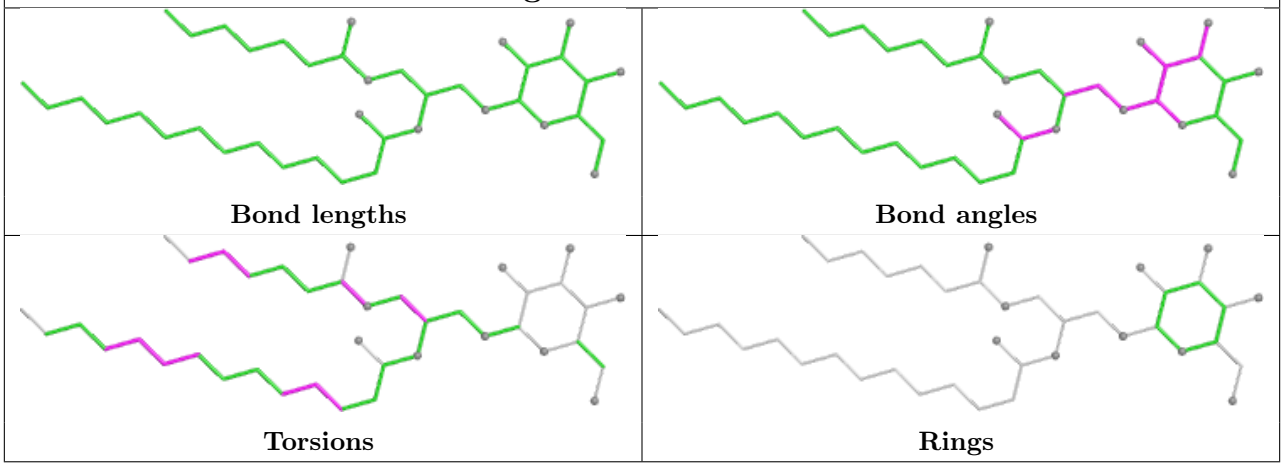
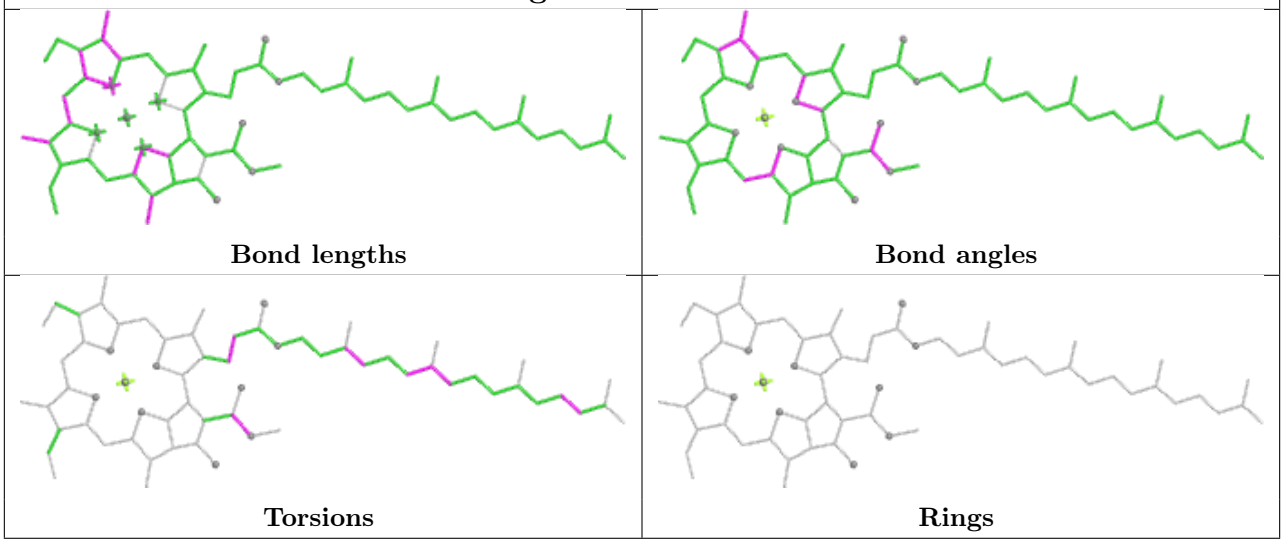


Rings

Ligand LMG b 734



Ligand CLA a 803



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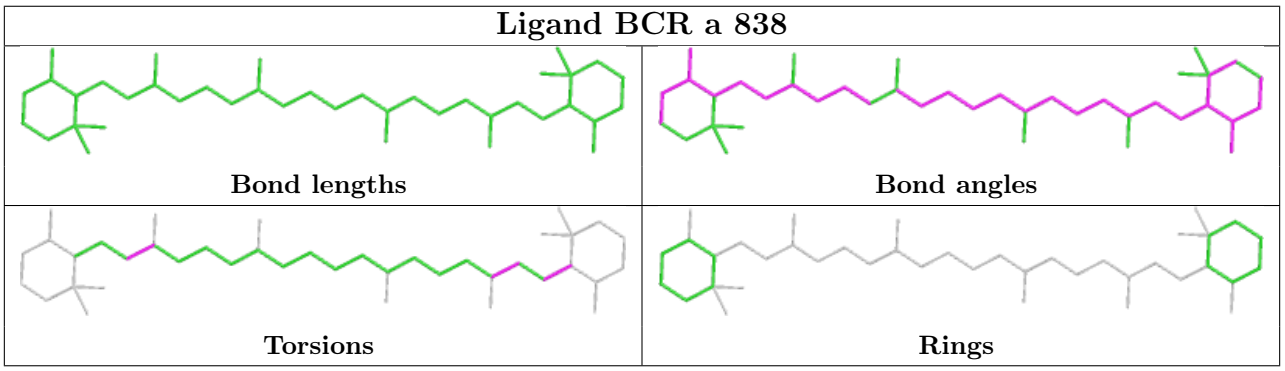
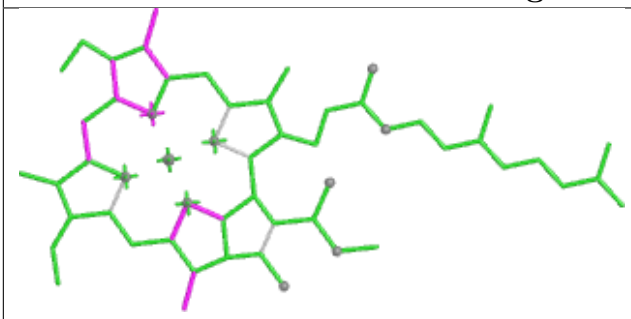
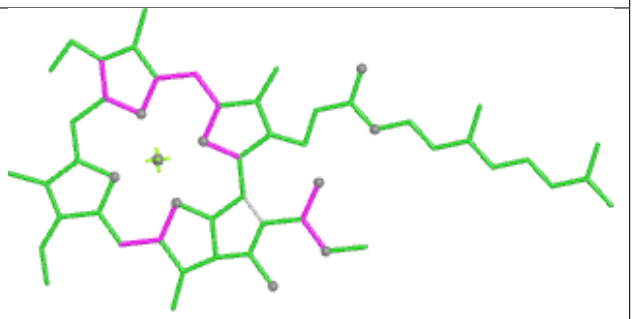


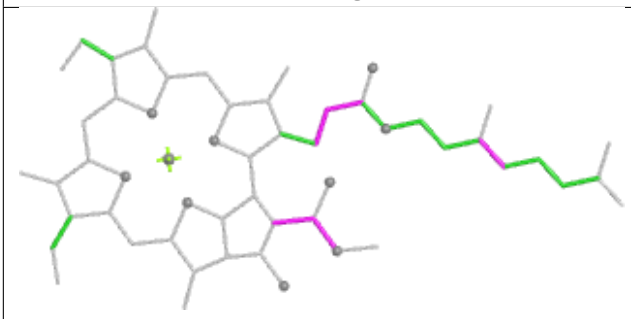
Ligand CLA L 310



Bond lengths



Bond angles



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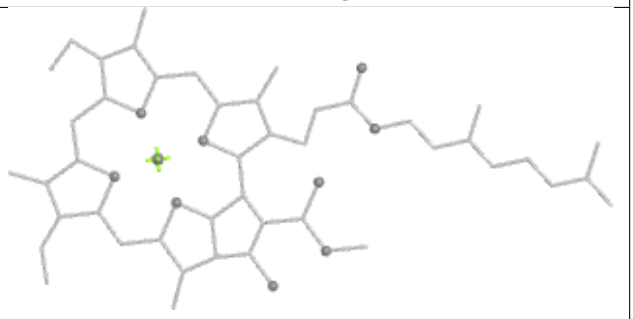
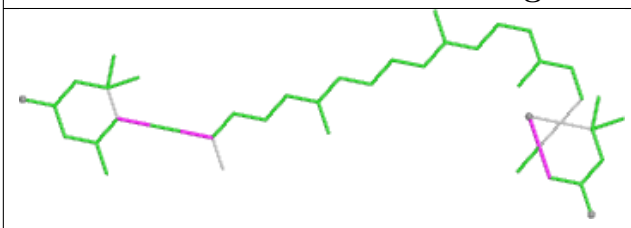


Rings

Ligand DD6 K 221



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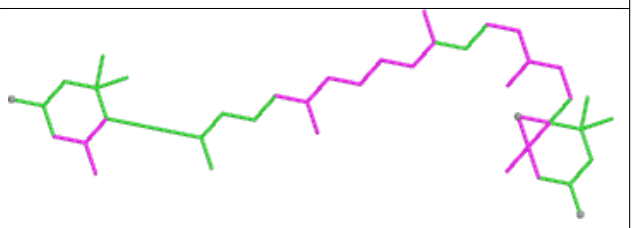
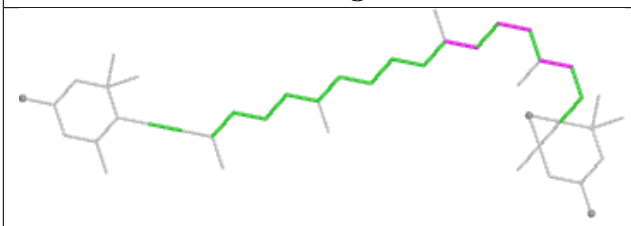


Bond angles



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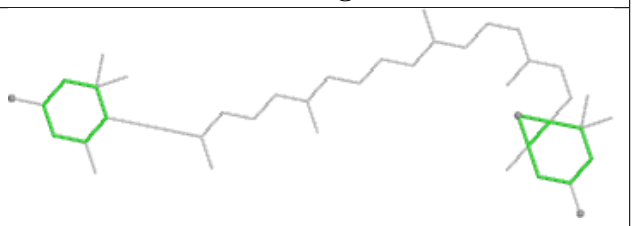
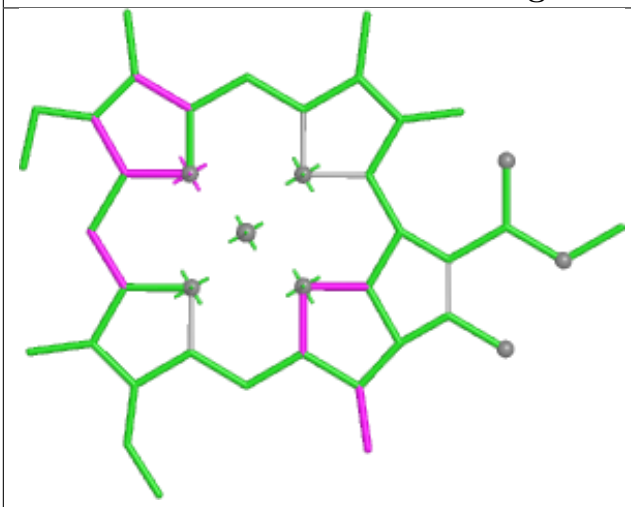


Rings

Ligand CLA J 313



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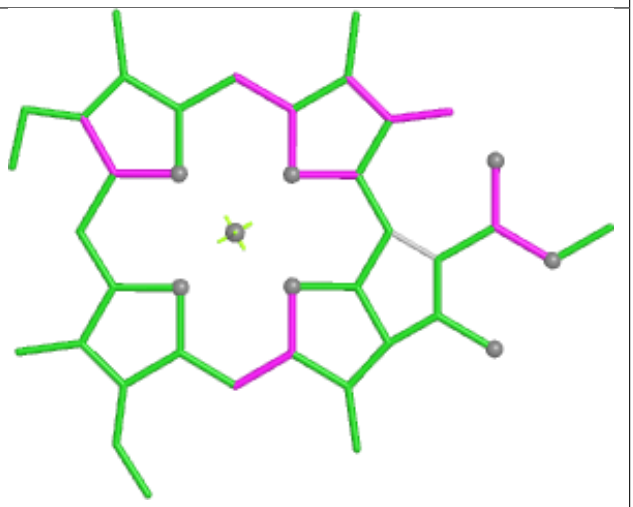

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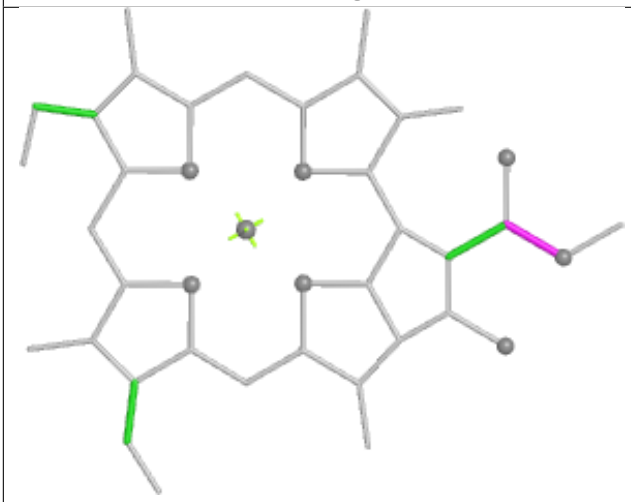

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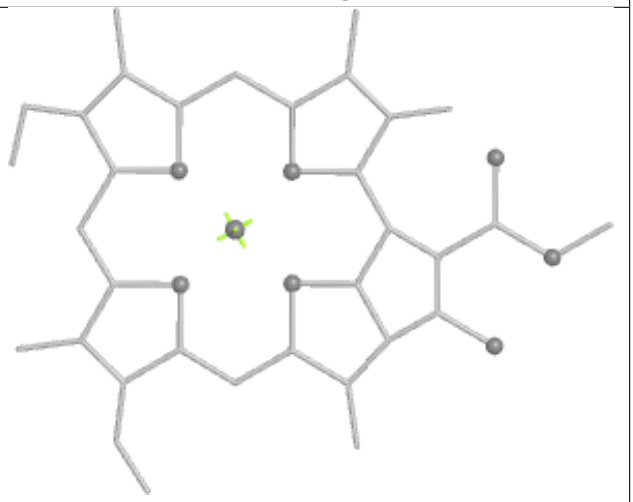
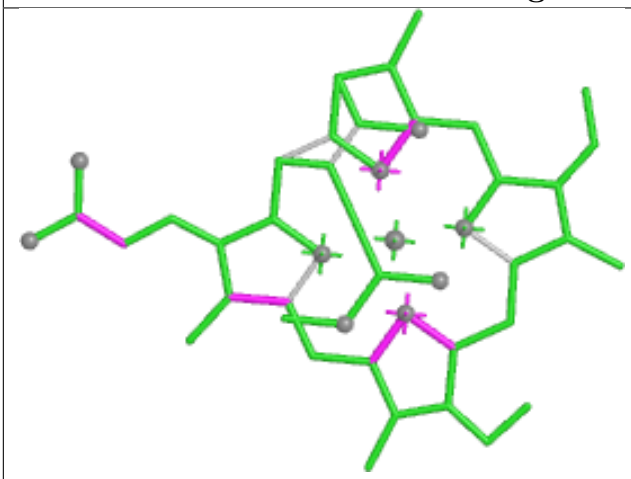


Rings

Ligand KC1 F 314



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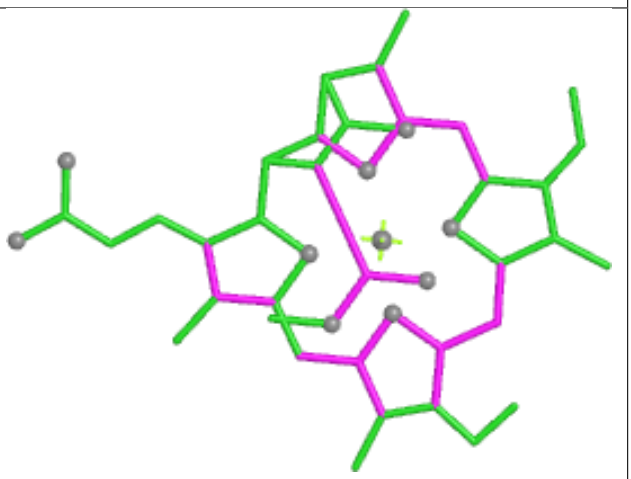
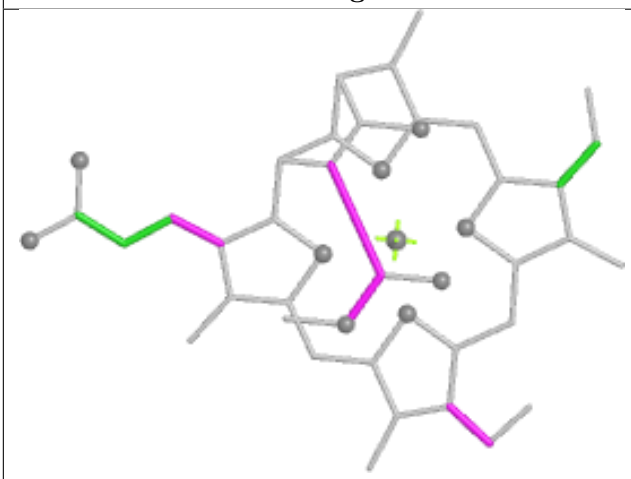


Bond angles



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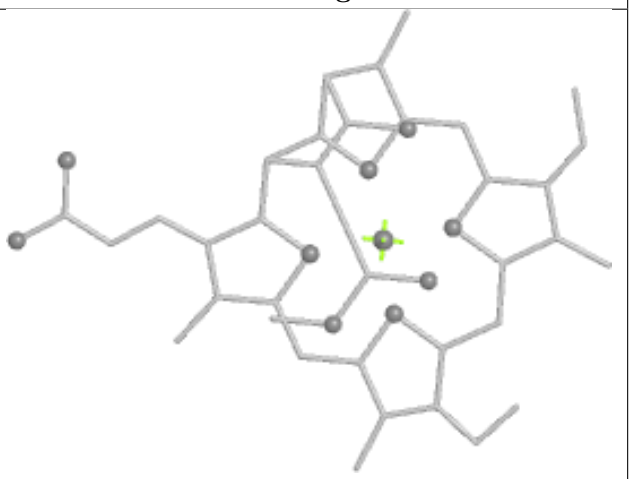
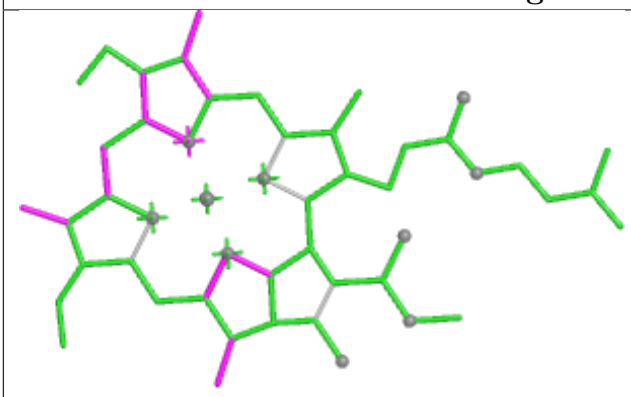


Rings

Ligand CLA L 307



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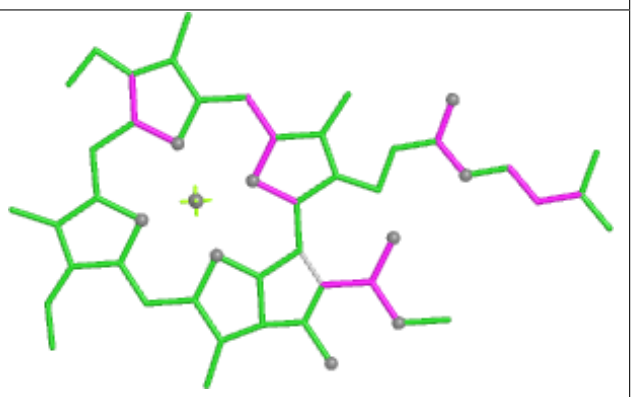

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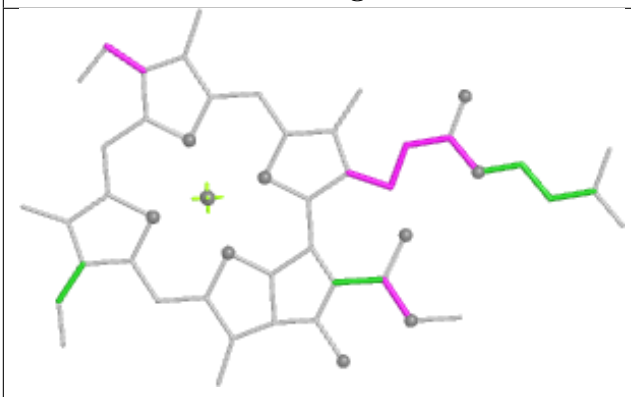

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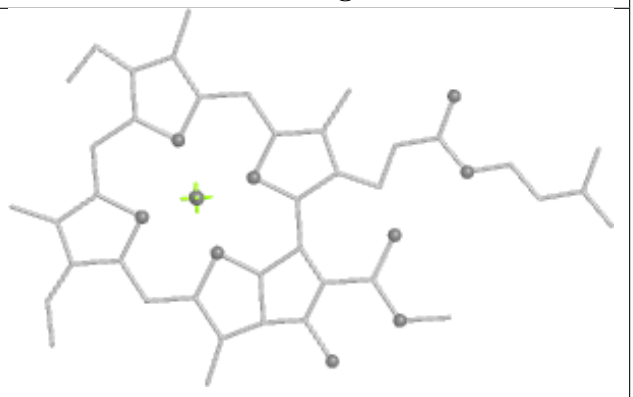
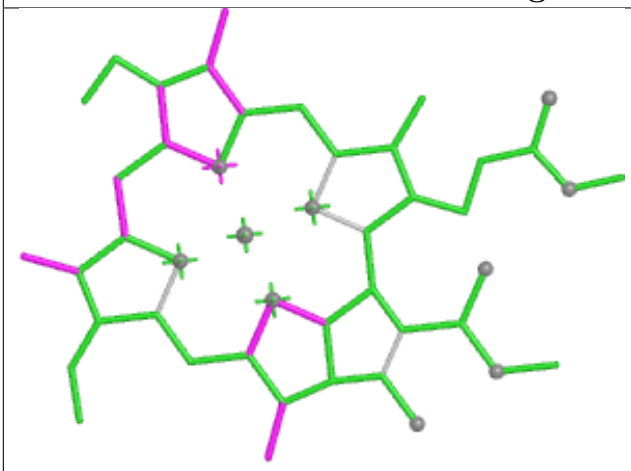


Rings

Ligand CLA a 828



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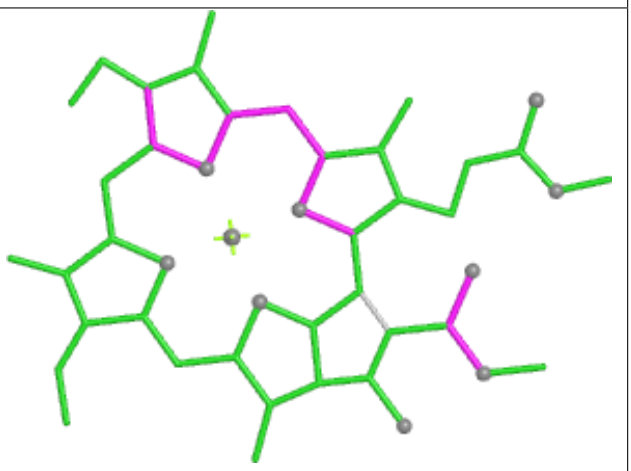
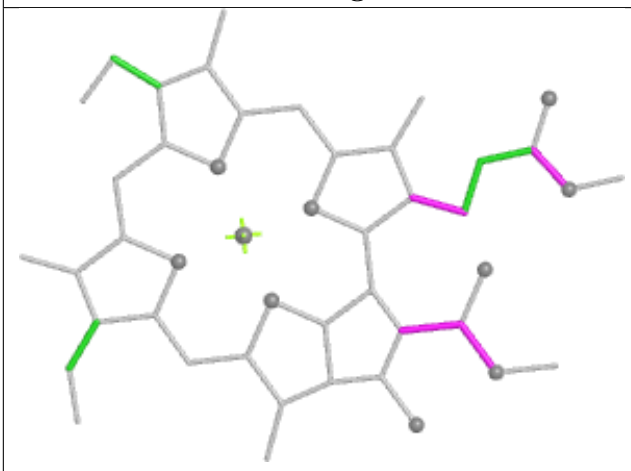


Bond angles



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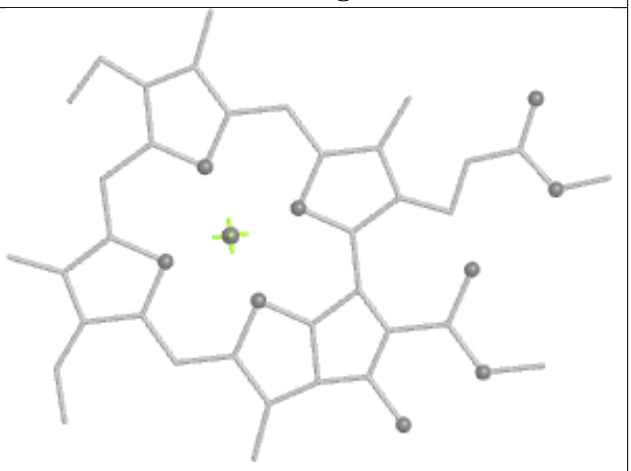
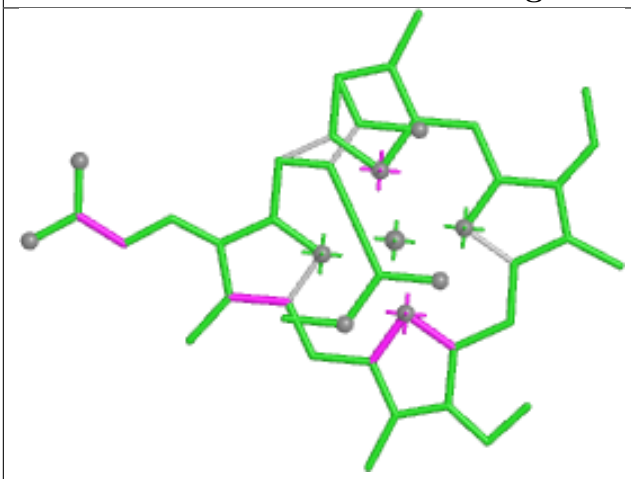


Rings

Ligand KC1 A 213



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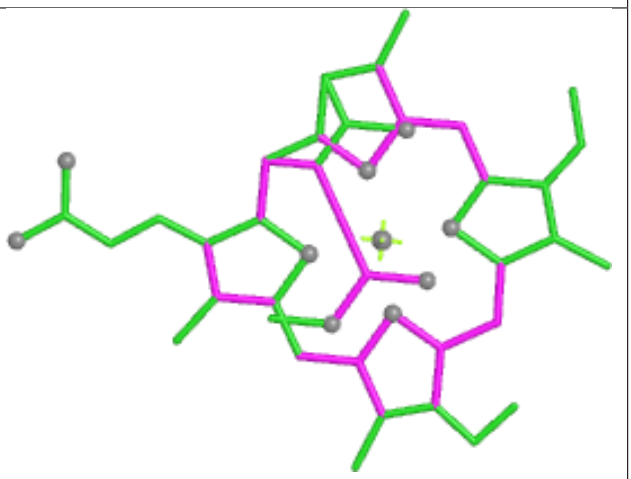
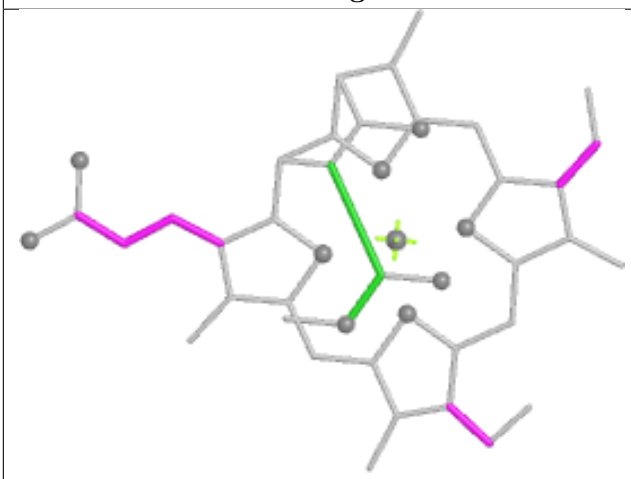


Bond angles



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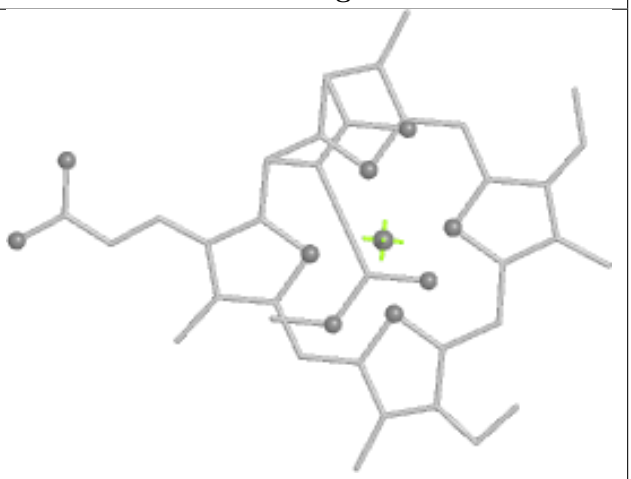
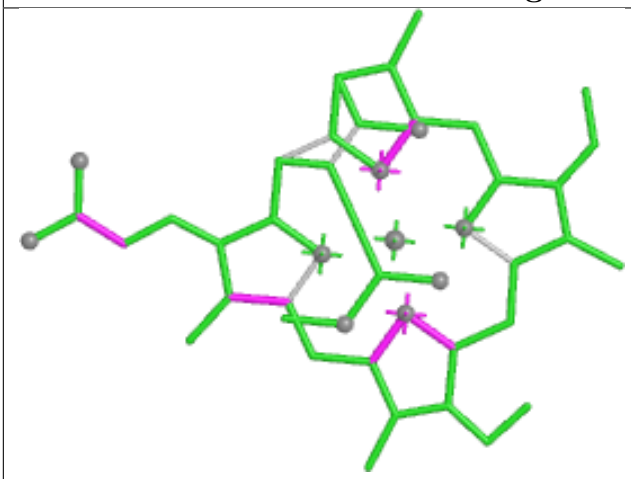


Rings

Ligand KC1 D 315



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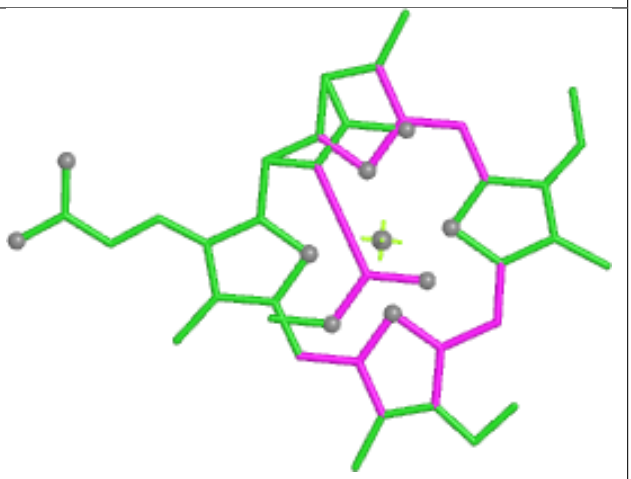

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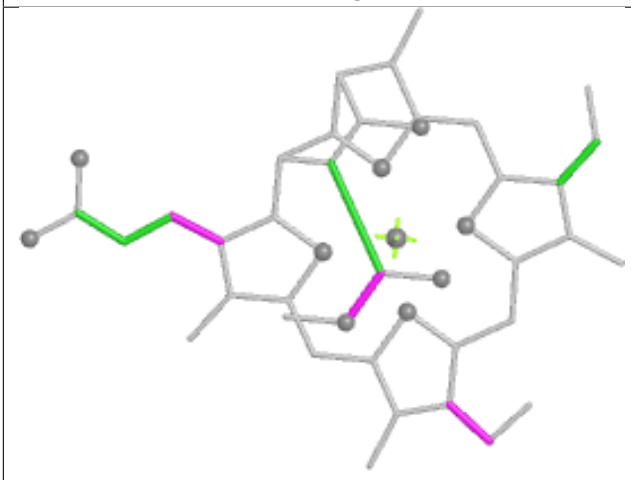

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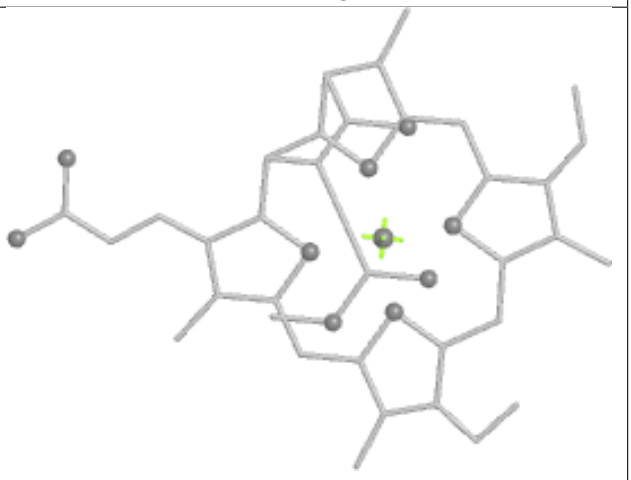
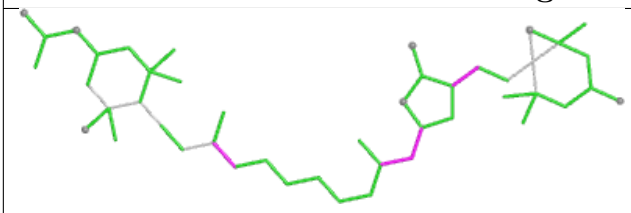


Rings

Ligand PID j 101



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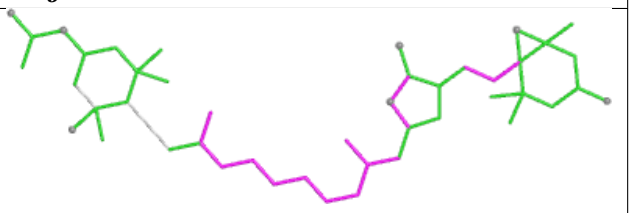
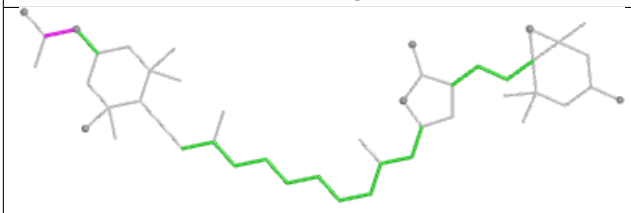


Bond angles



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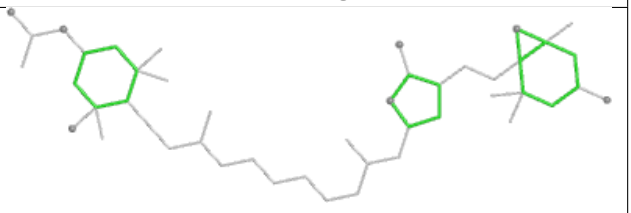
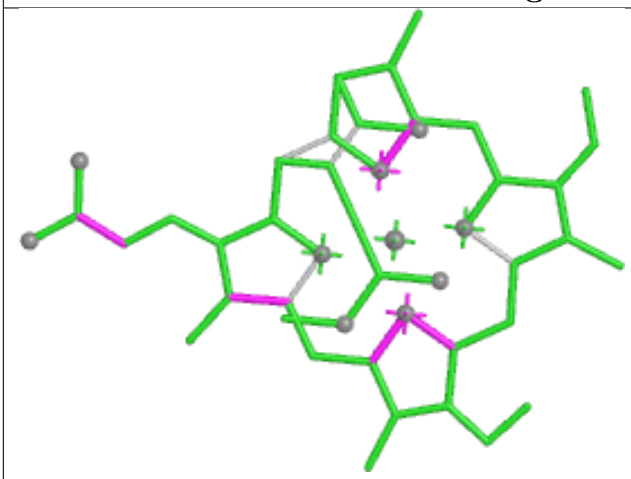
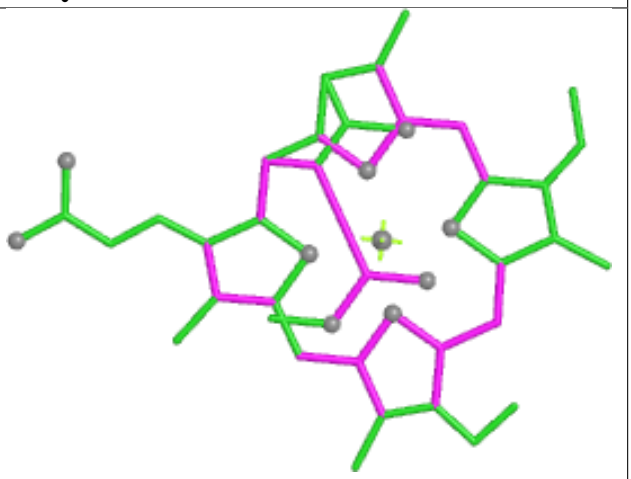


Rings

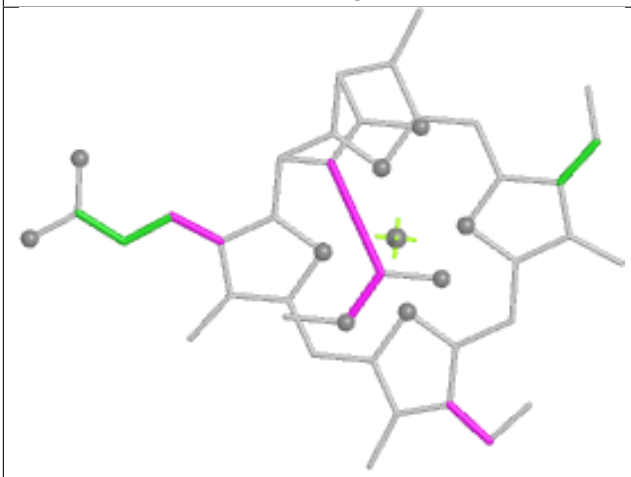
Ligand KC1 Q 309



Bond lengths



Bond angles



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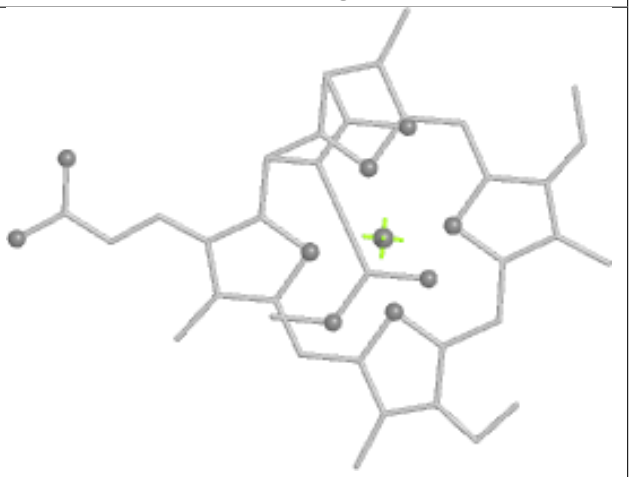
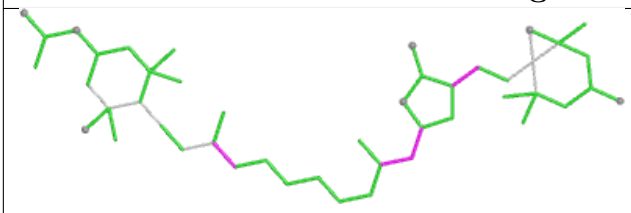


Rings

Ligand PID P 202



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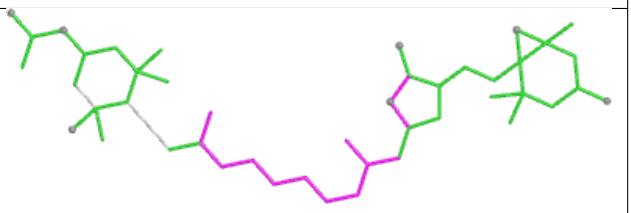
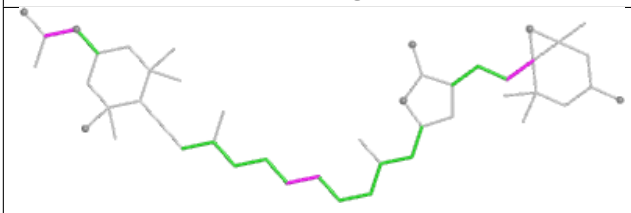


Bond angles



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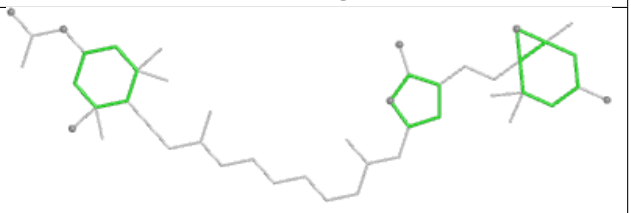
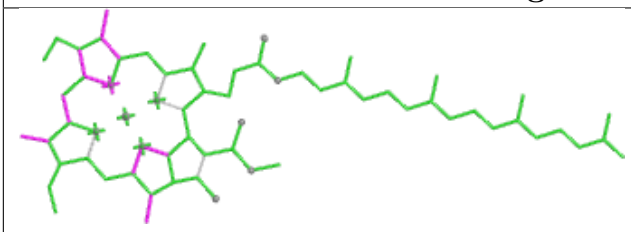
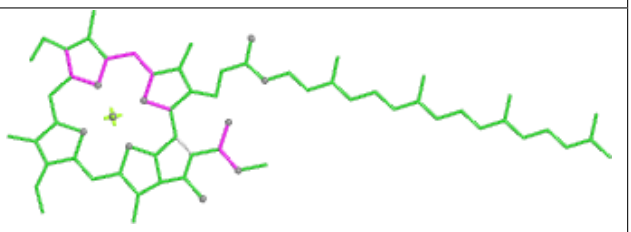
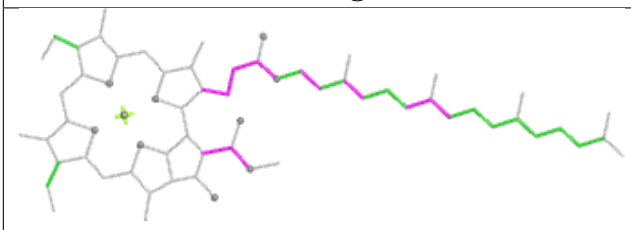
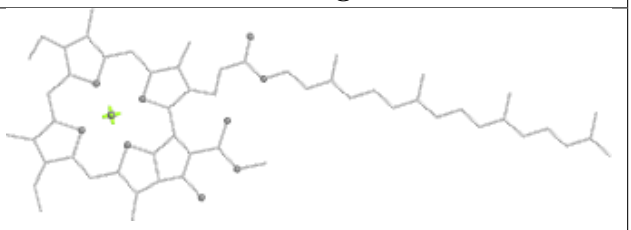
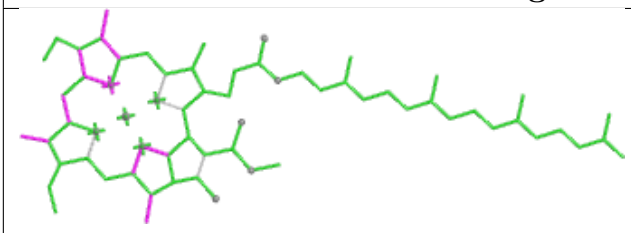
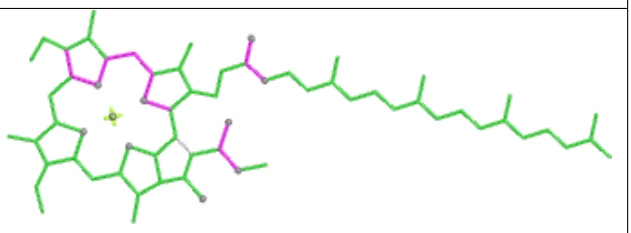
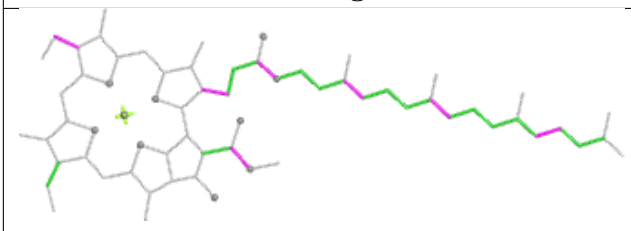
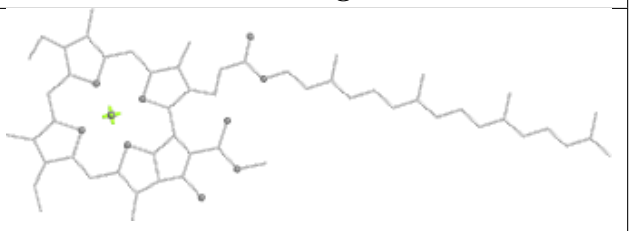
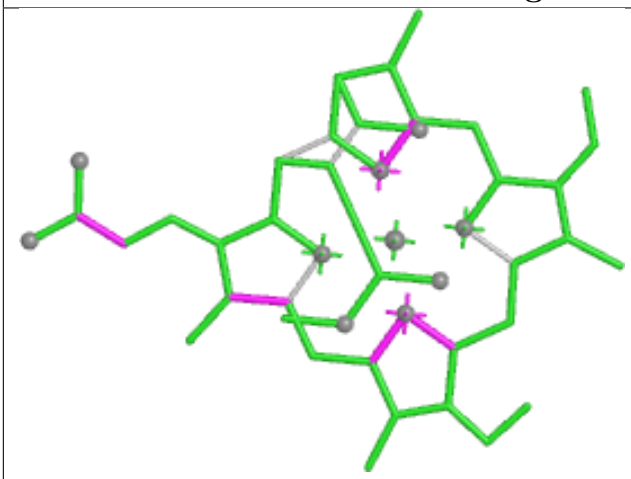


Rings

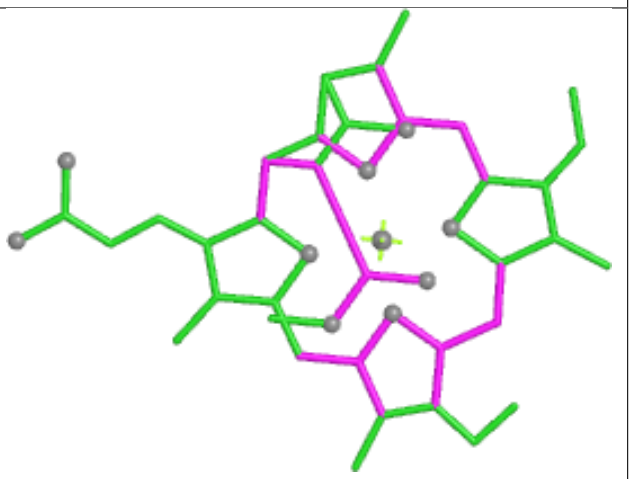
Ligand CLA b 720	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA a 820	
	
Bond lengths	Bond angles
	
Torsions	Rings

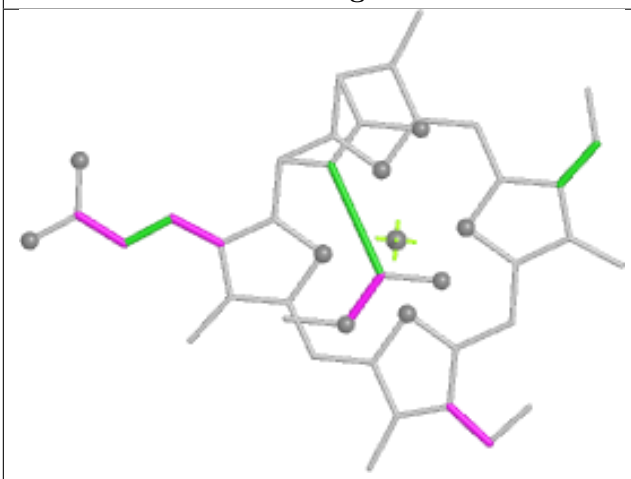
Ligand KC1 H 311



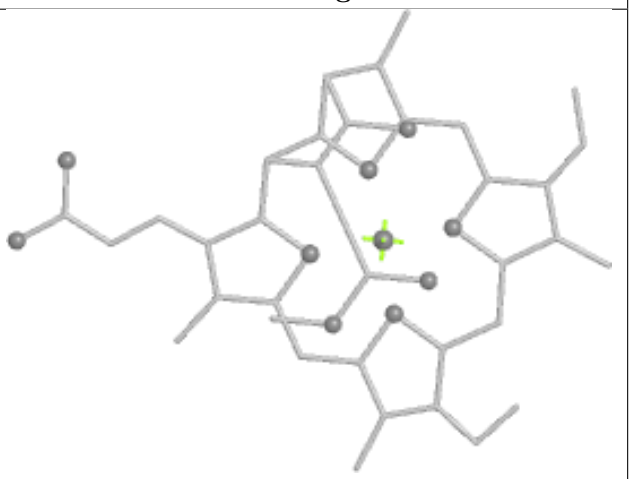
Bond lengths



Bond angles

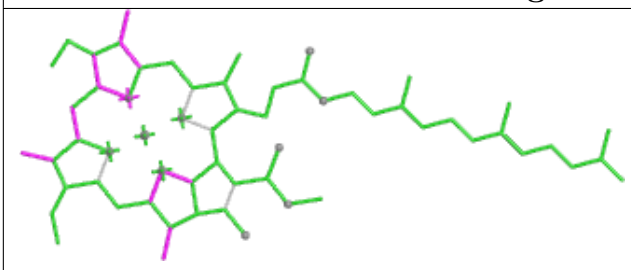


Torsions

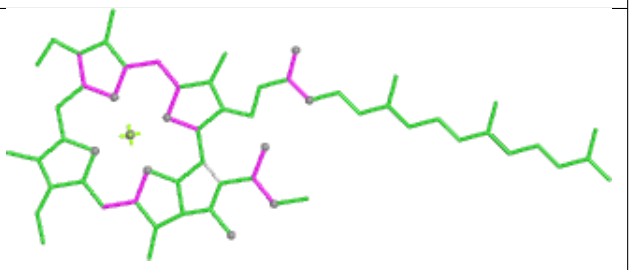


Rings

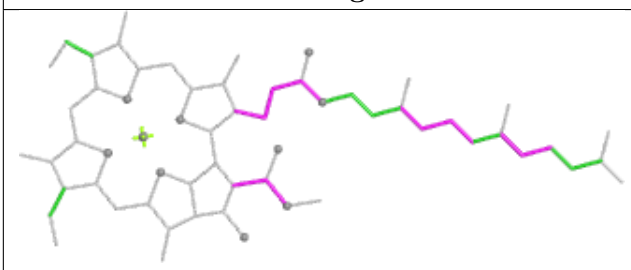
Ligand CLA b 709



Bond lengths



Bond angles



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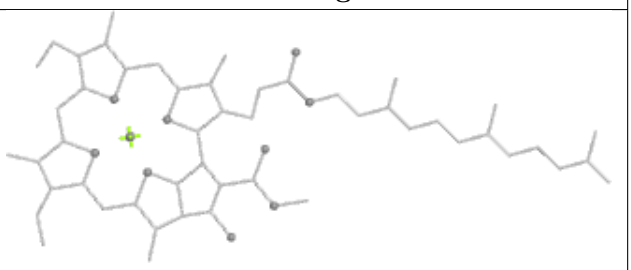
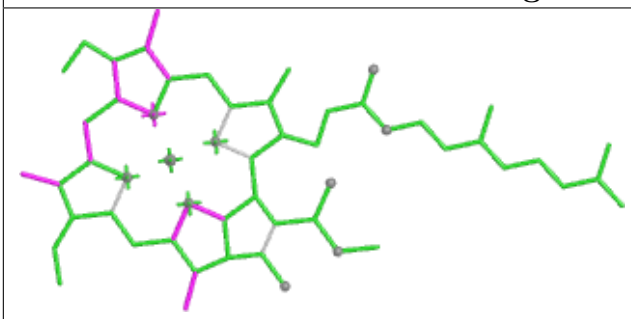
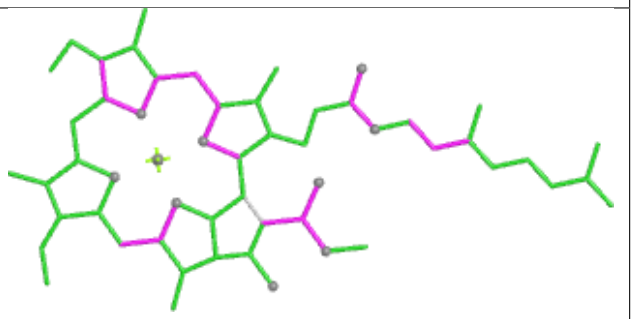


Rings

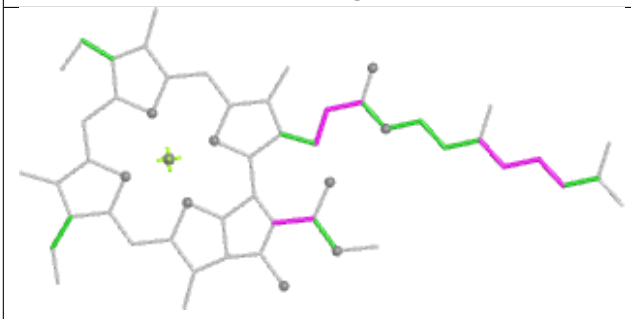
Ligand CLA K 211



Bond lengths



Bond angles



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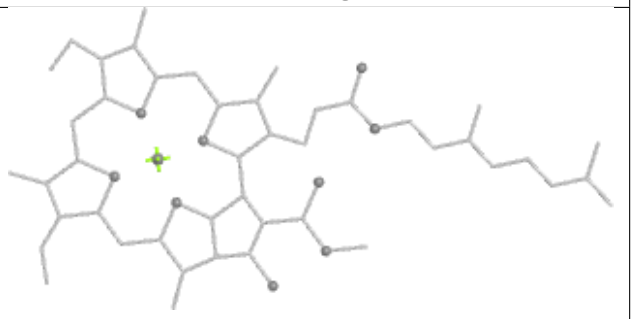
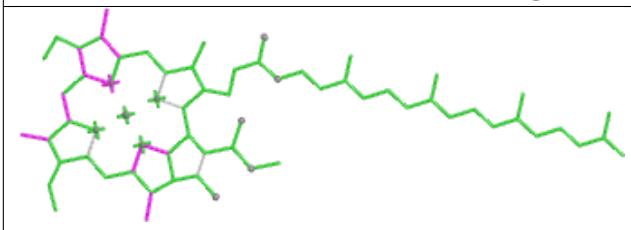
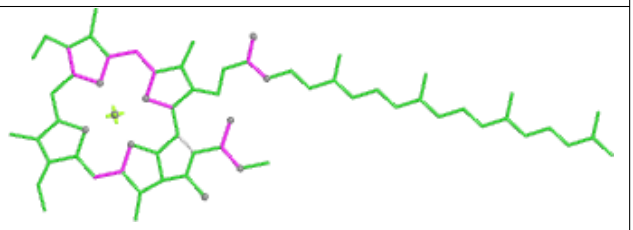


Rings

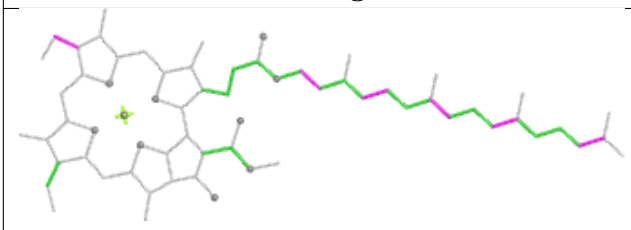
Ligand CLA b 726



Bond lengths



Bond angles



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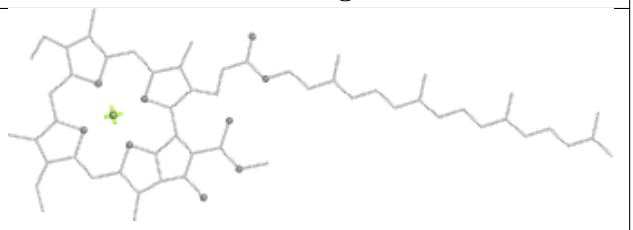
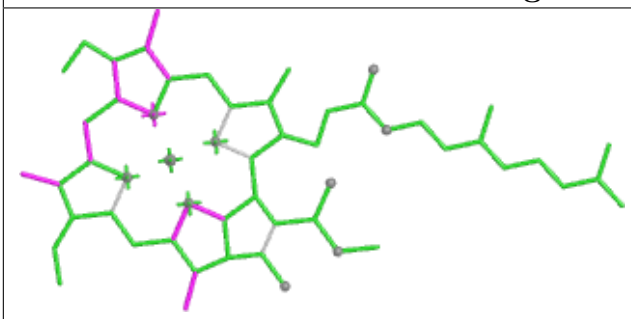
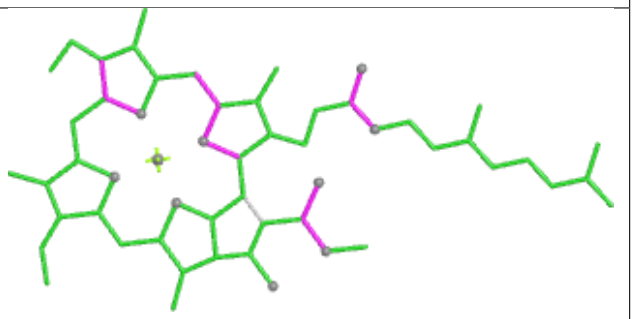
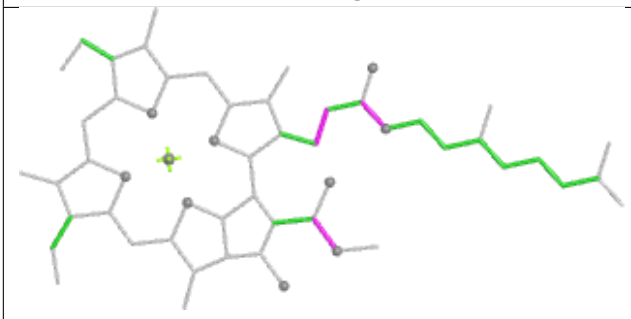
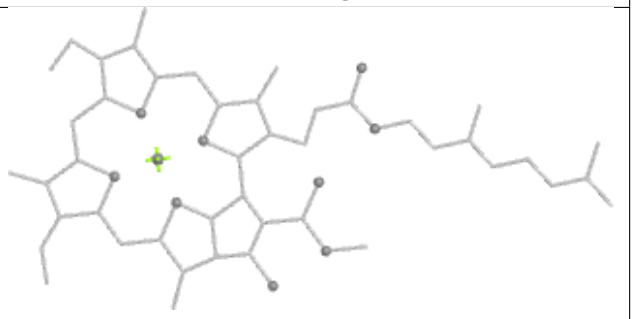
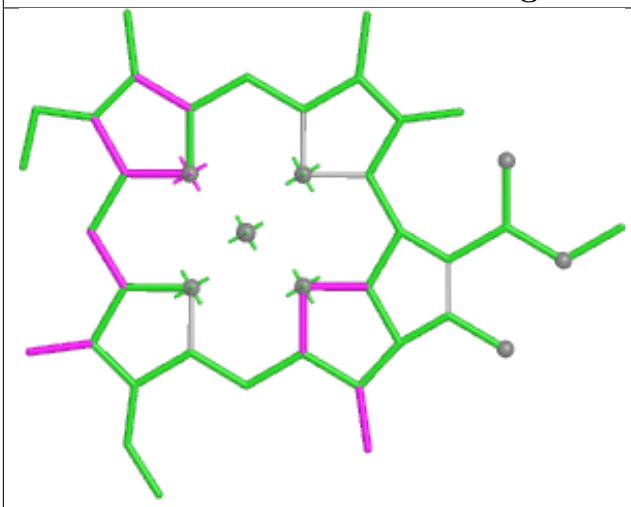


Rings

Ligand CLA A 207	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

Ligand CLA M 313



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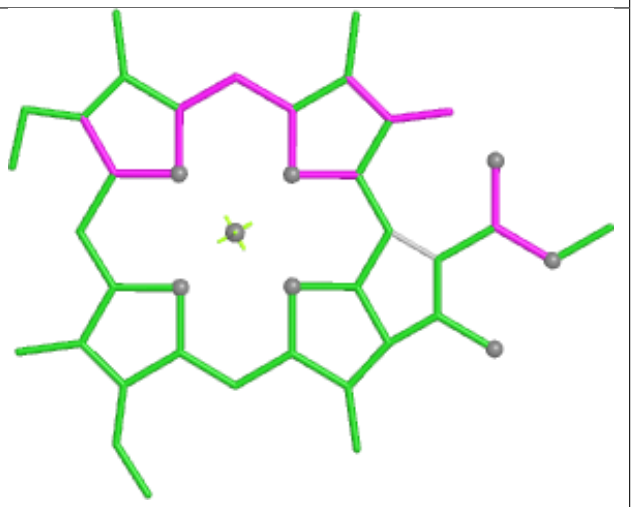
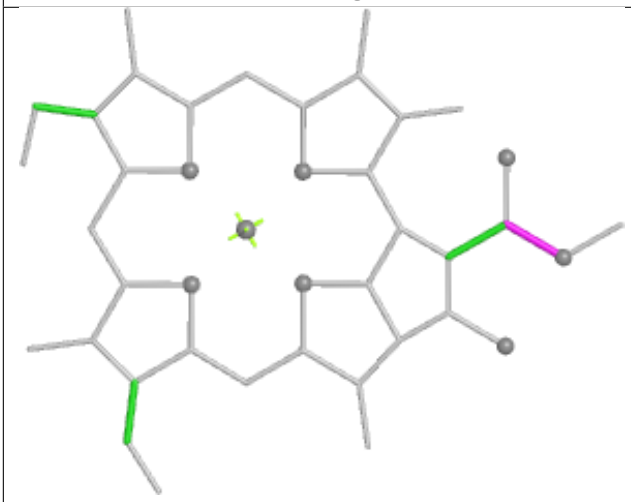


Bond angles



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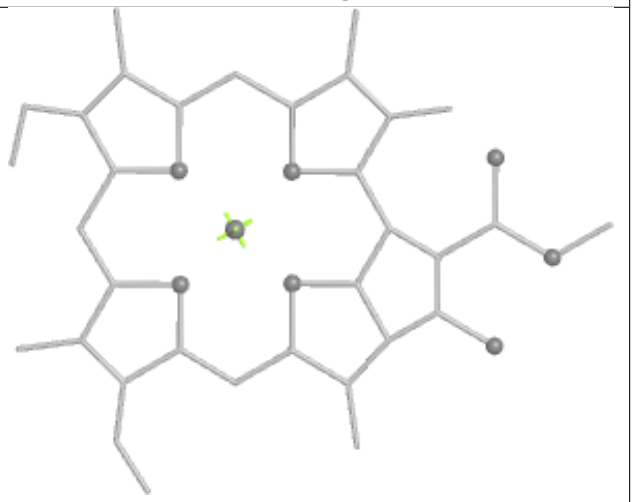
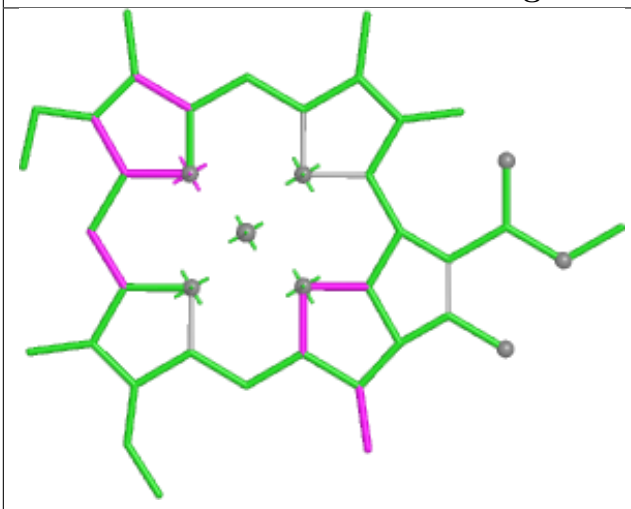


Rings

Ligand CLA N 316



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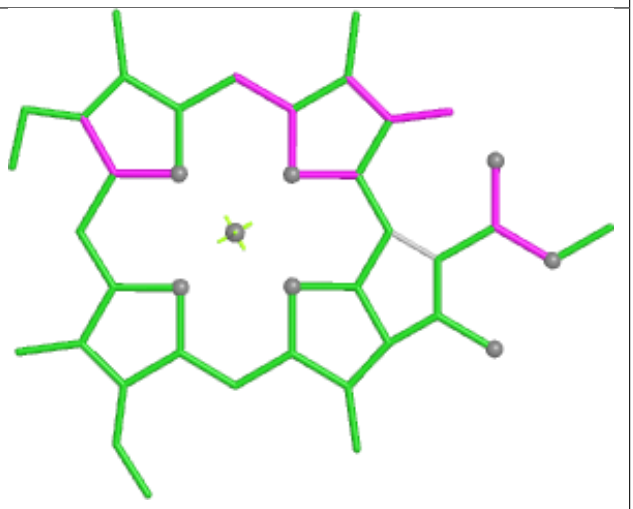
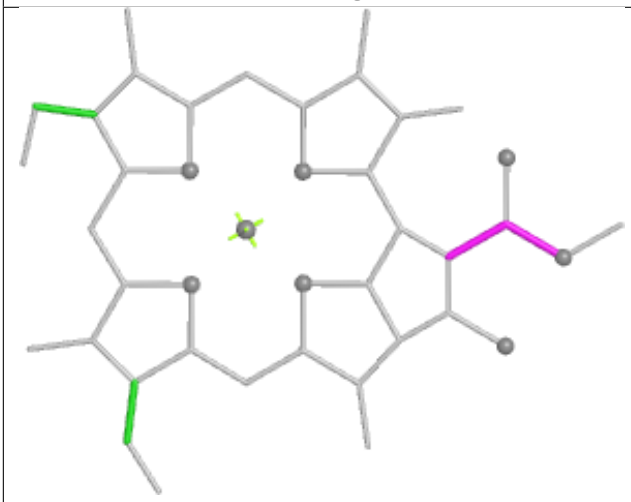


Bond angles



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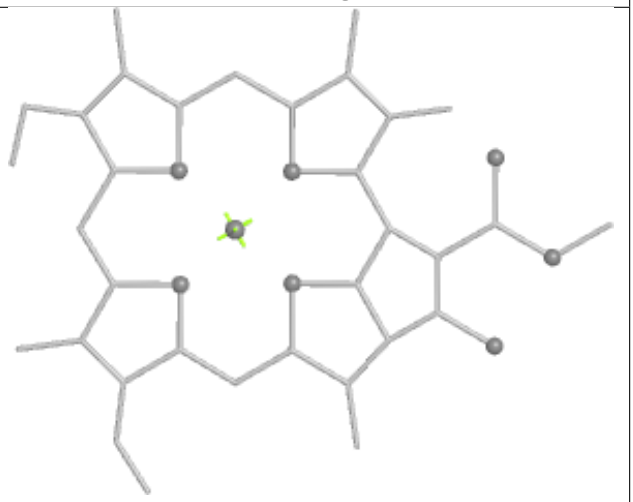
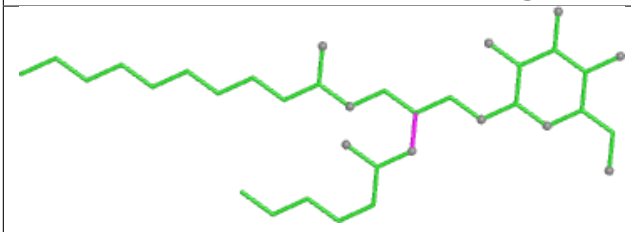


Rings

Ligand LMG K 219



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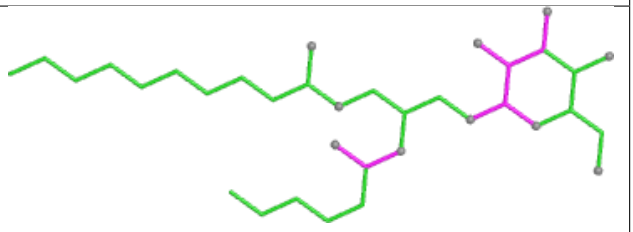
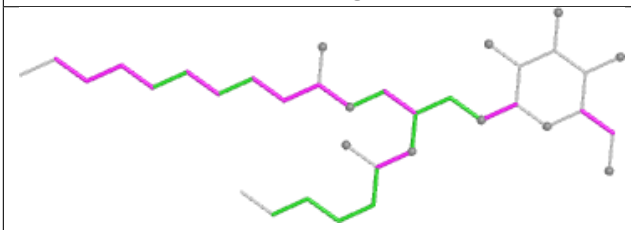


Bond angles



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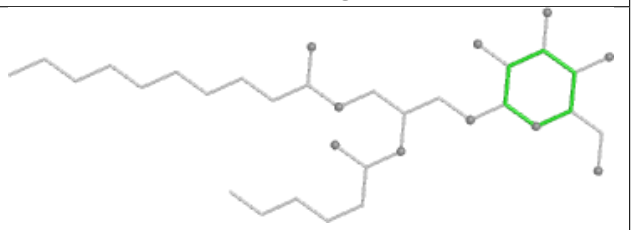
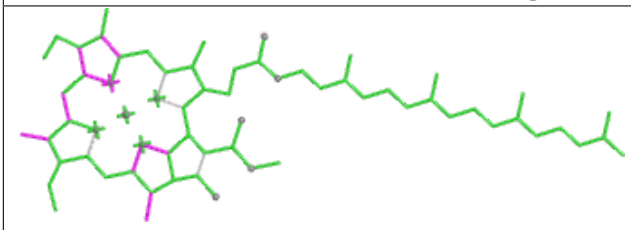


Rings

Ligand CLA B 310



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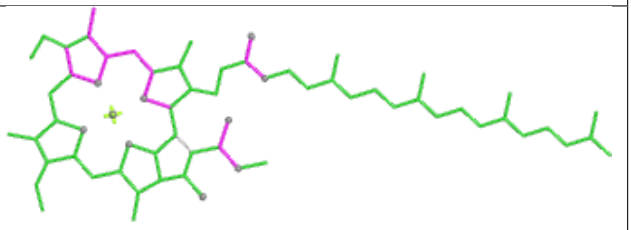
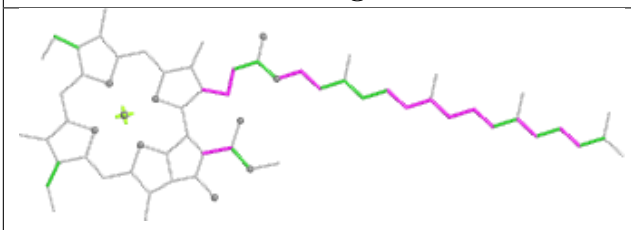


Bond angles



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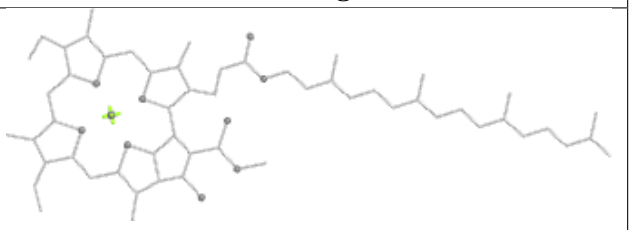
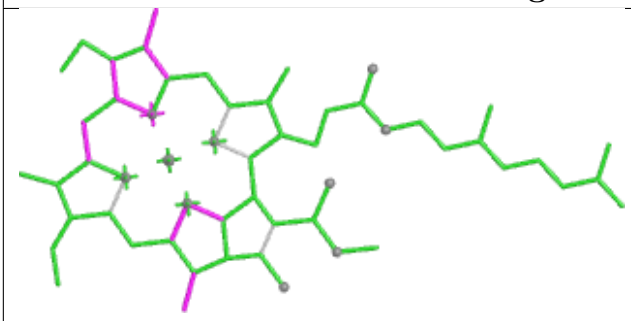


Rings

Ligand CLA a 837



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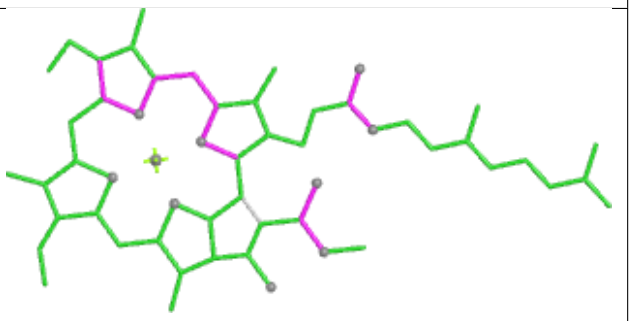
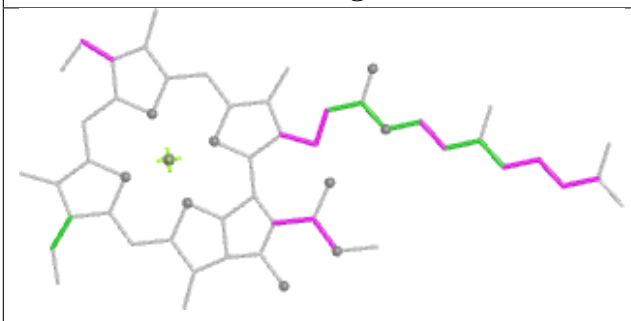


Bond angles



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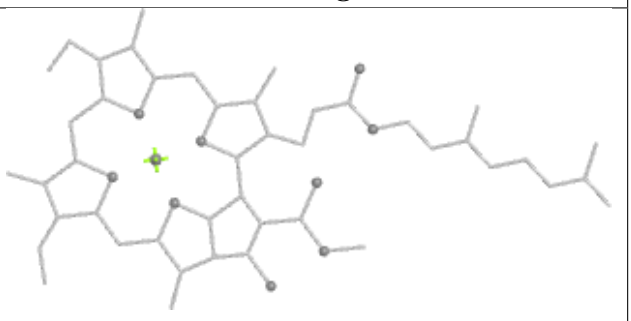
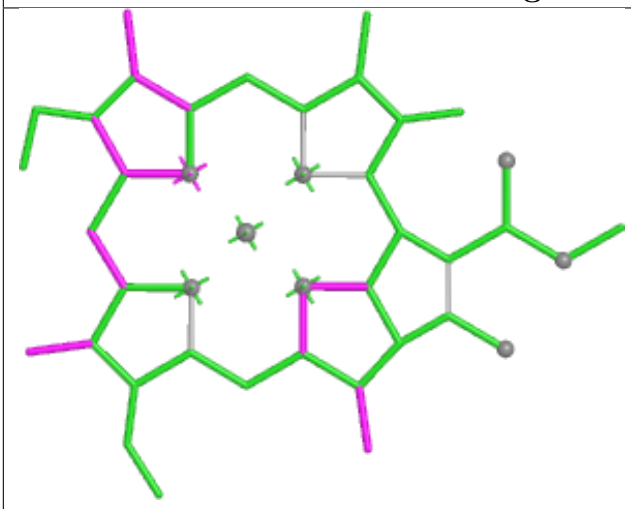


Rings

Ligand CLA A 216



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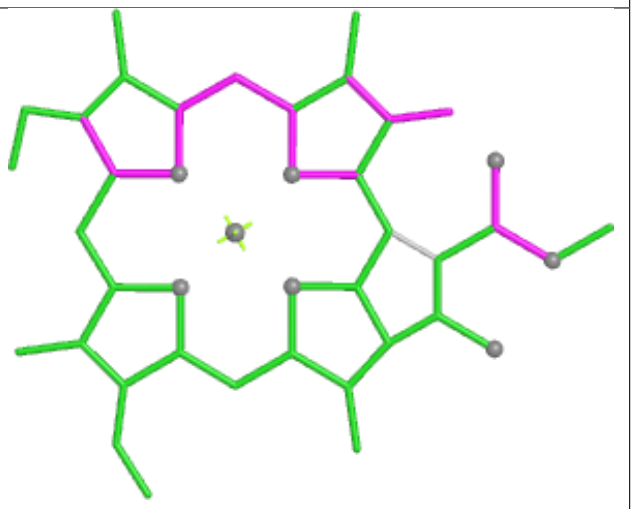
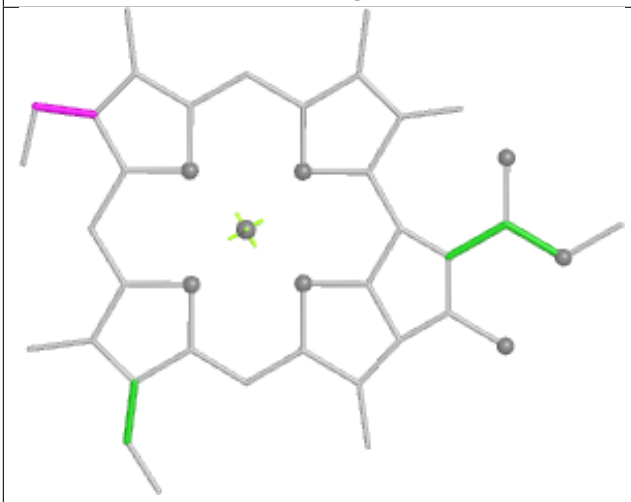


Bond angles



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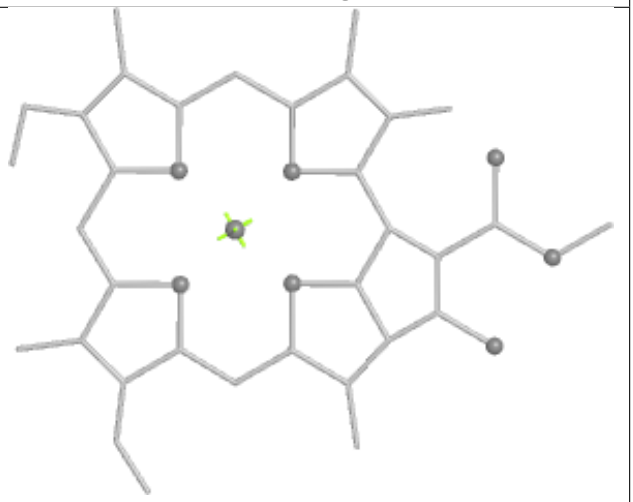
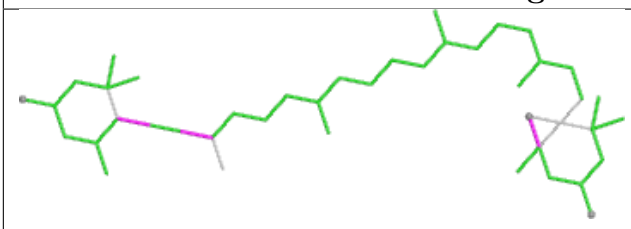


Rings

Ligand DD6 L 305



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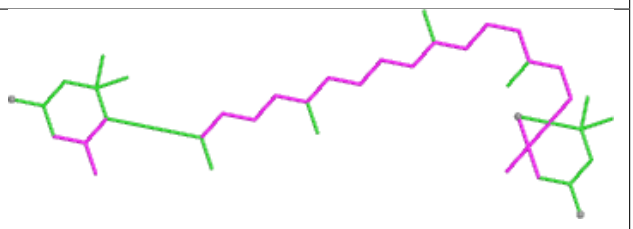
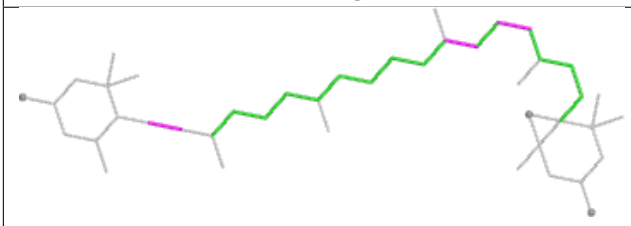


Bond angles

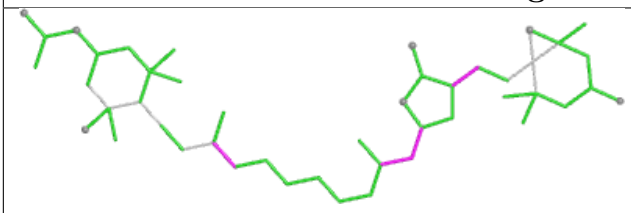


Torsions

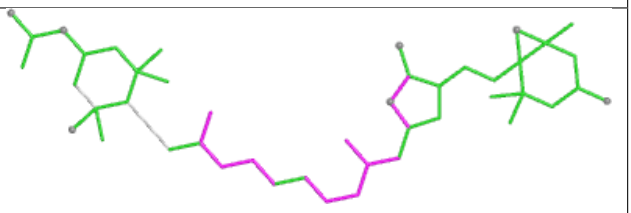


Rings

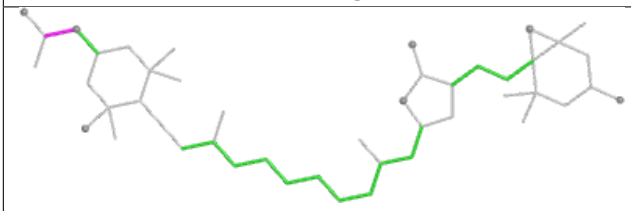
Ligand PID H 302



Bond lengths



Bond angles



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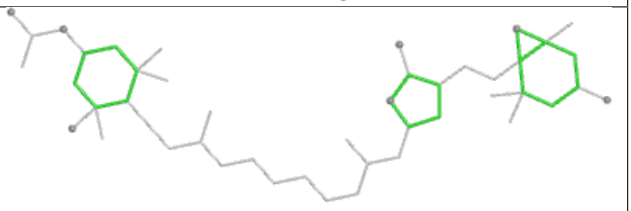
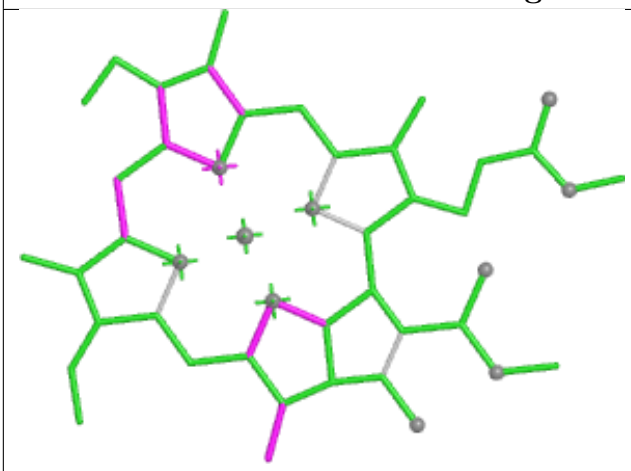
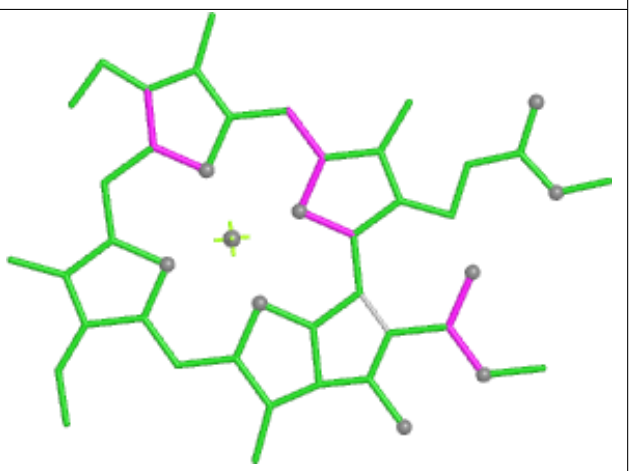


Rings

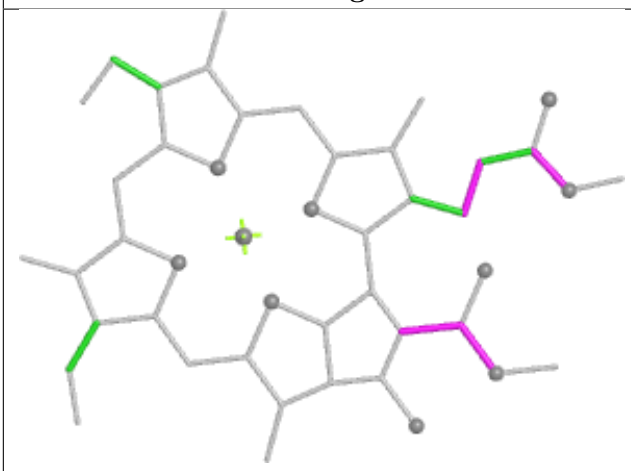
Ligand CLA T 313



Bond lengths



Bond angles

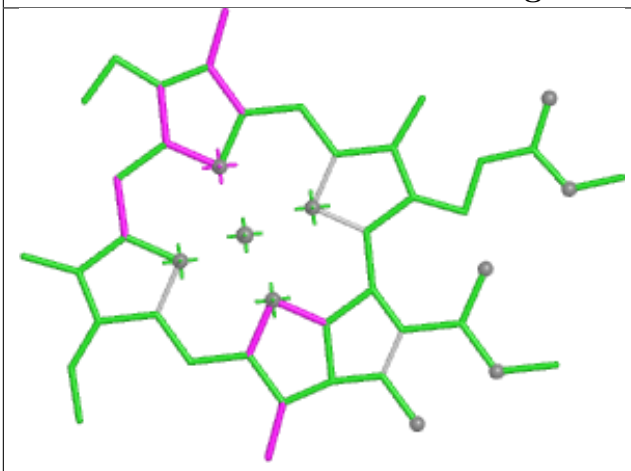


Torsions

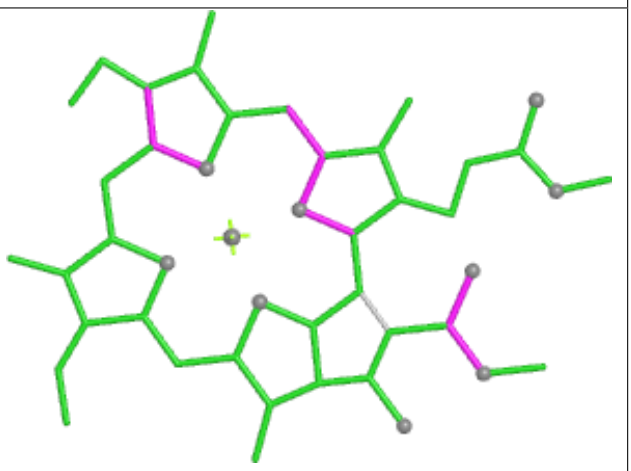


Rings

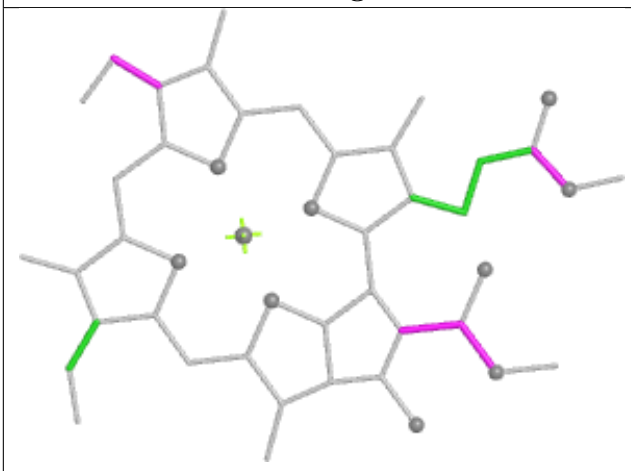
Ligand CLA C 313



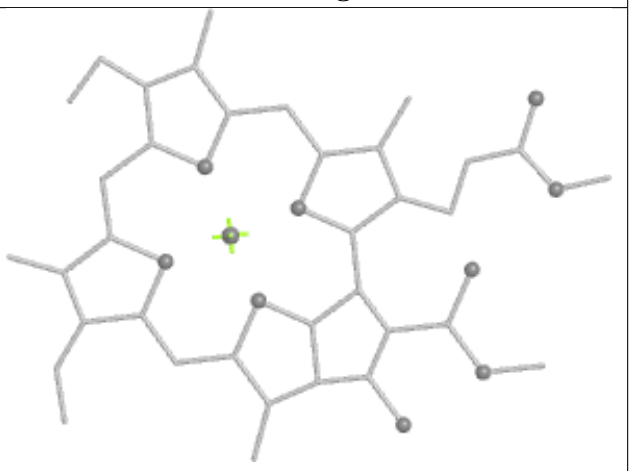
Bond lengths



Bond angles

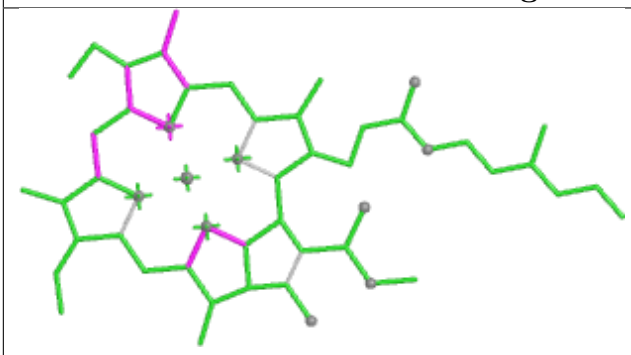


Torsions



Rings

Ligand CLA M 314



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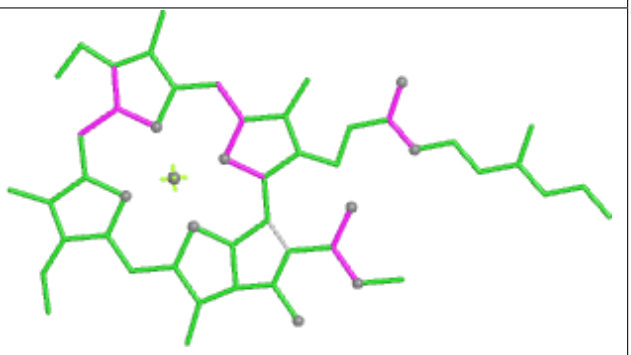
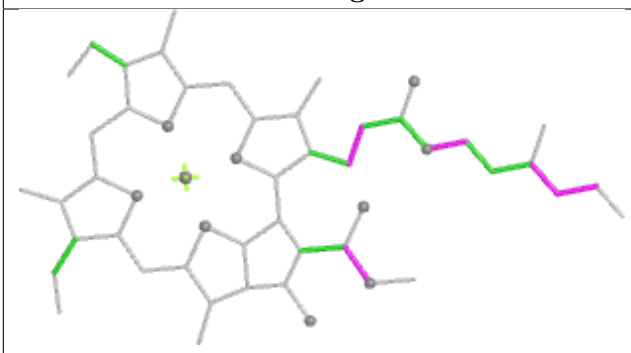


Bond angles



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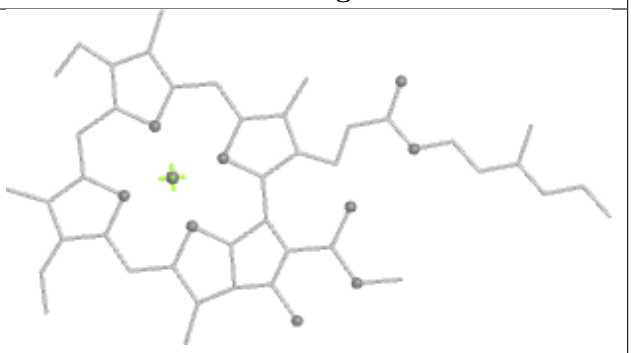
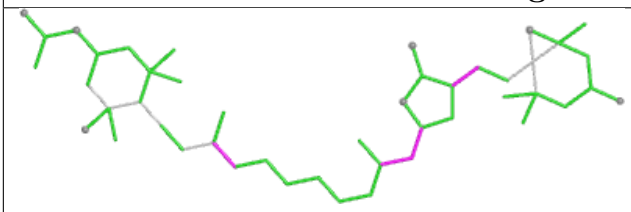
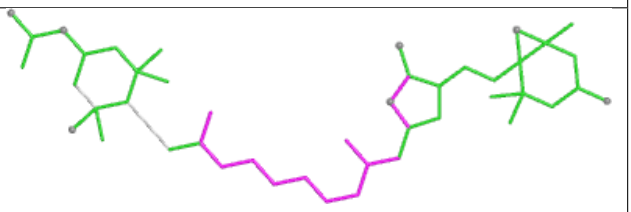


Rings

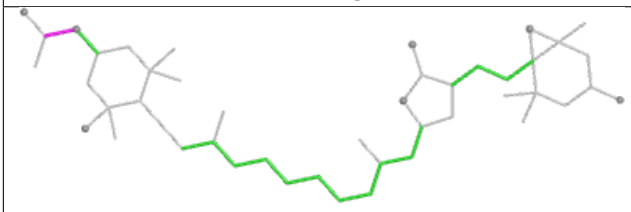
Ligand PID O 302



Bond lengths



Bond angles



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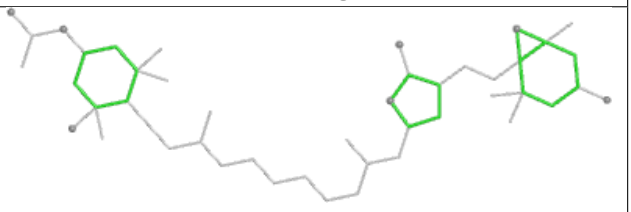
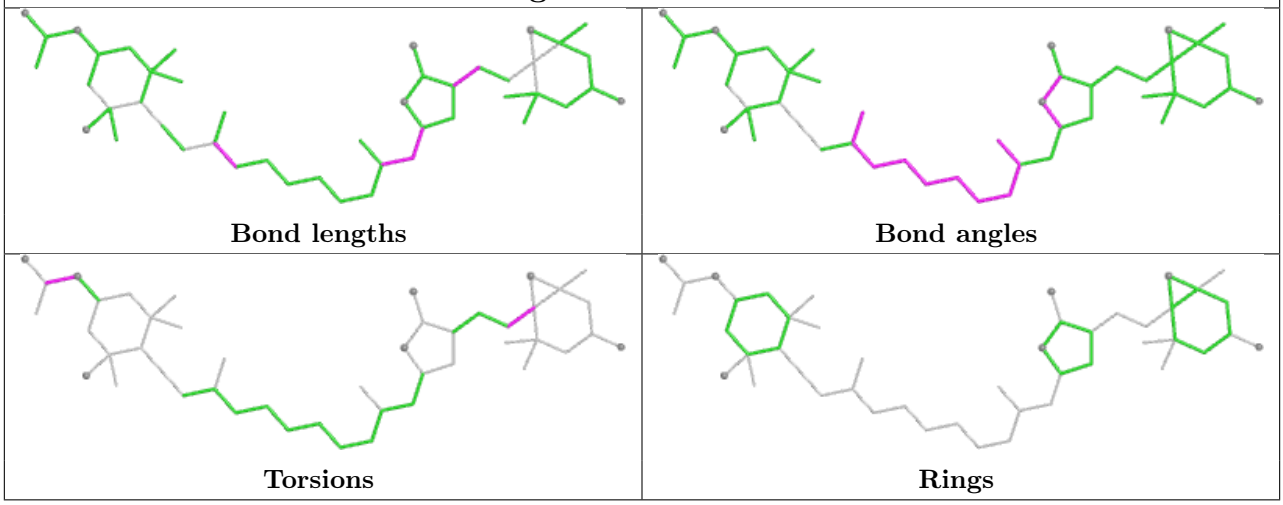
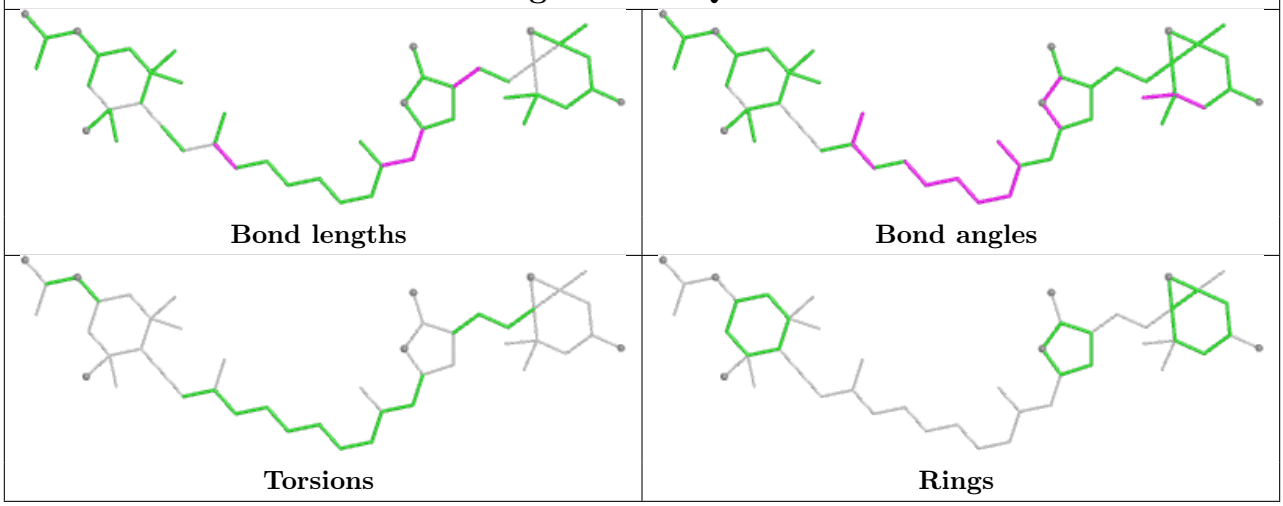


Rings

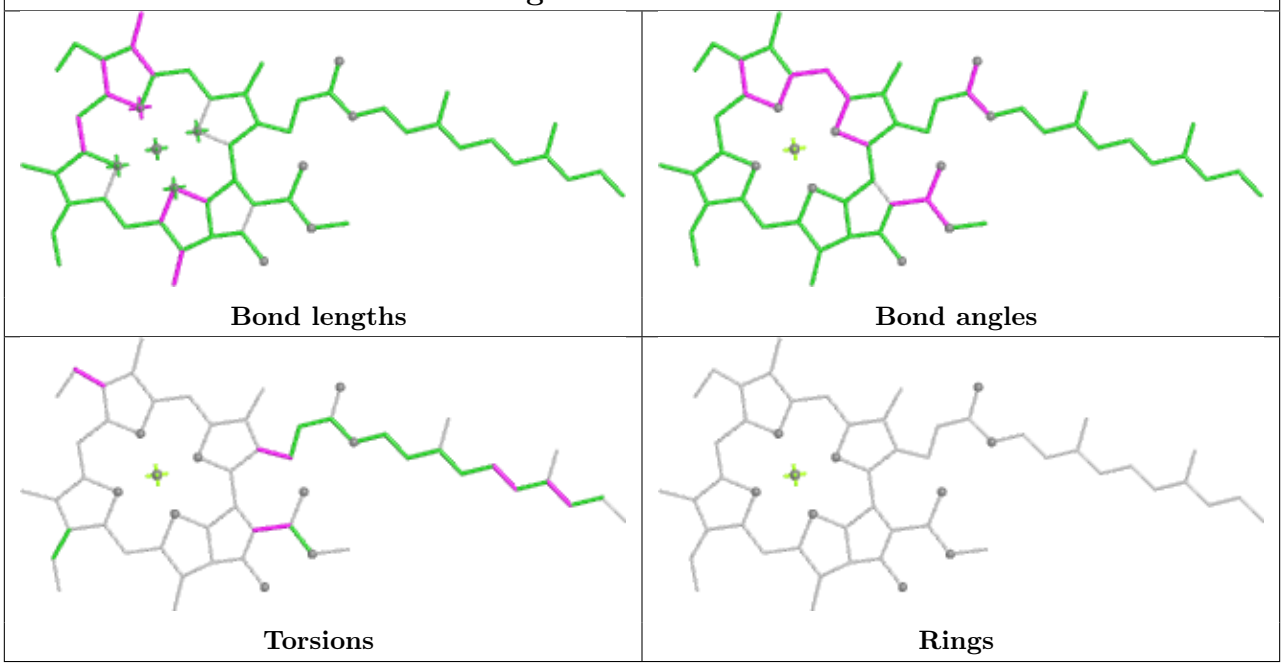
Ligand PID O 301



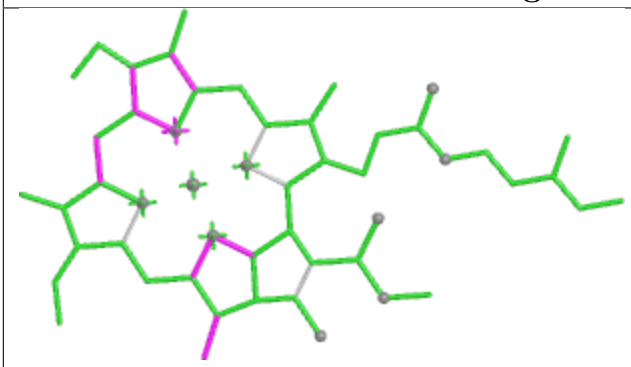
Ligand PID Q 303



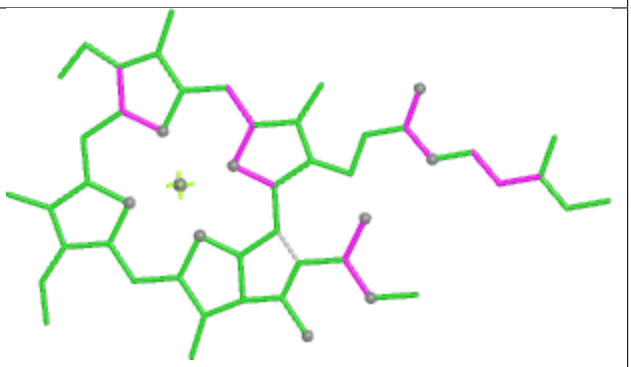
Ligand CLA E 315



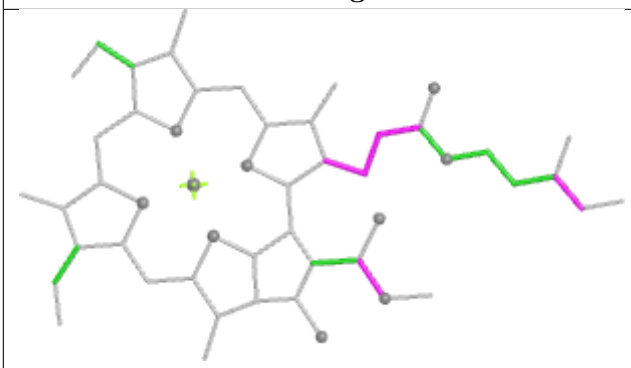
Ligand CLA H 310



Bond lengths



Bond angles



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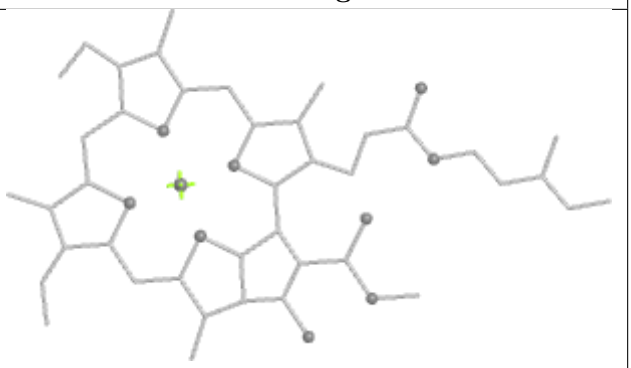
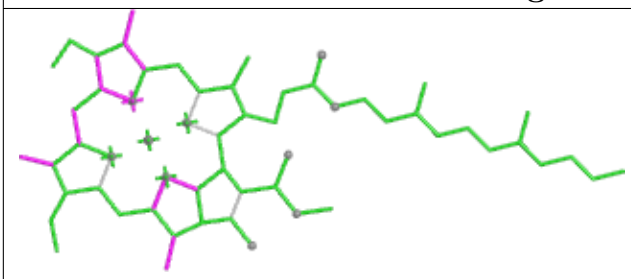


Rings

Ligand CLA b 722



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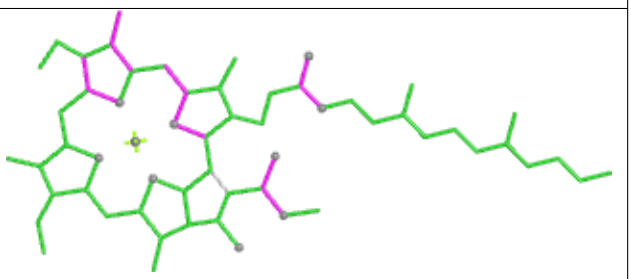
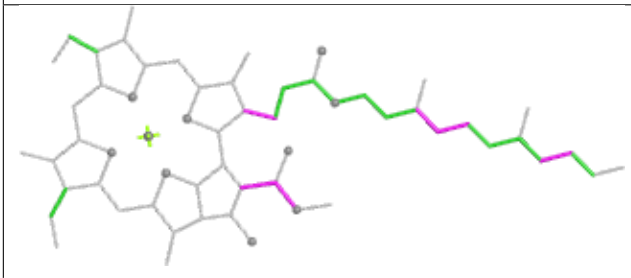


Bond angles



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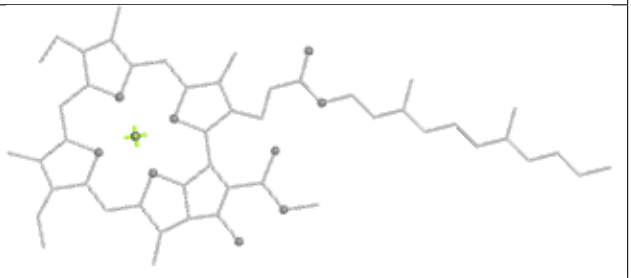
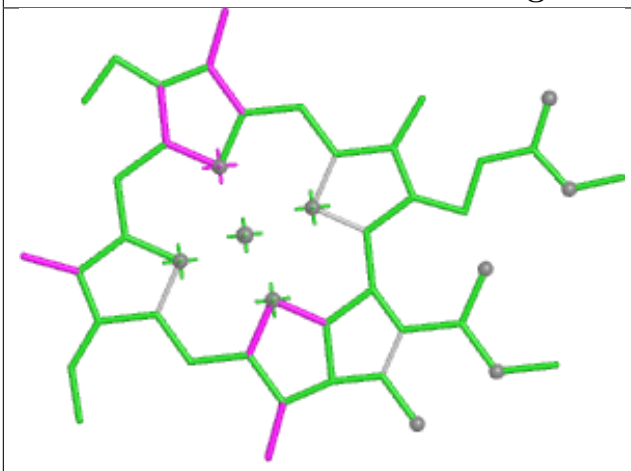


Rings

Ligand CLA b 715



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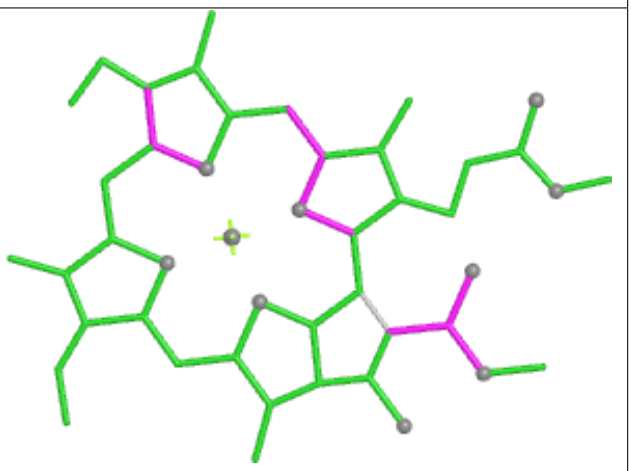
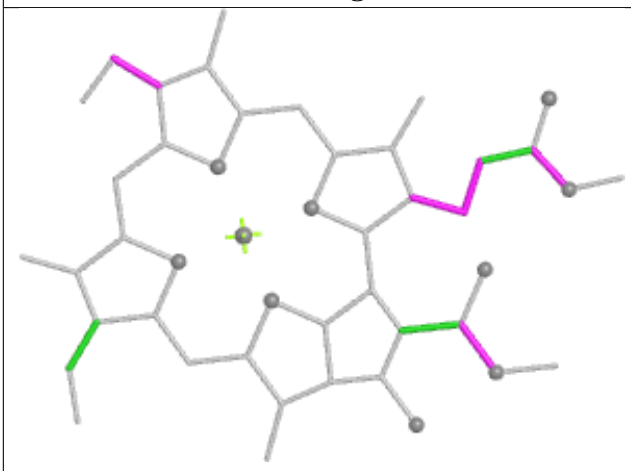


Bond angles



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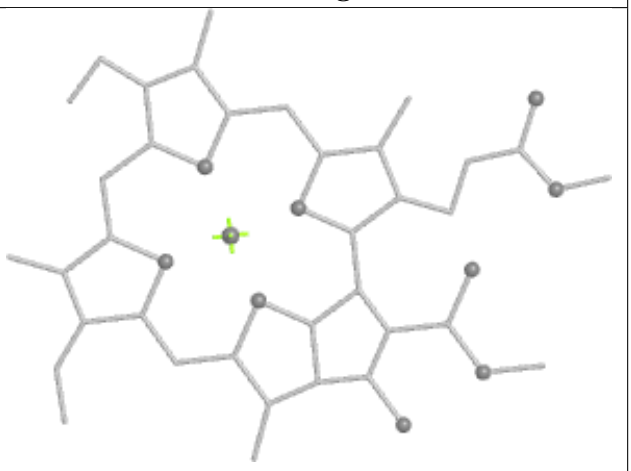
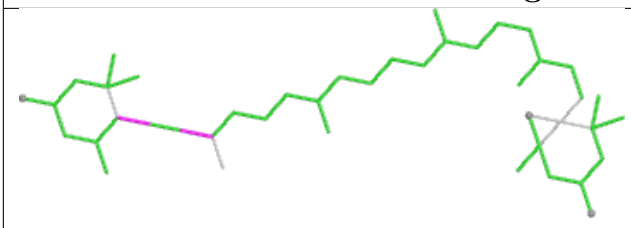


Rings

Ligand DD6 G 308



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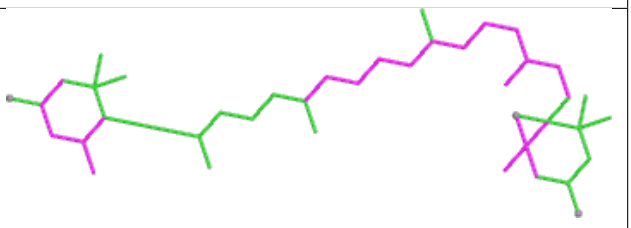
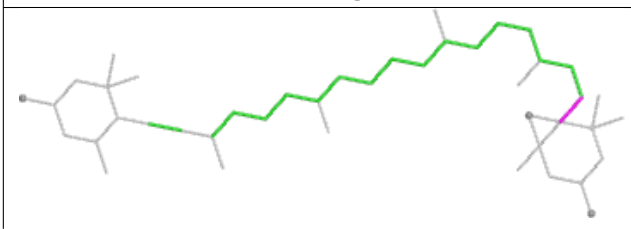


Bond angles



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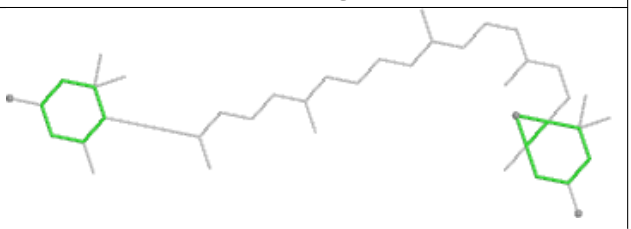
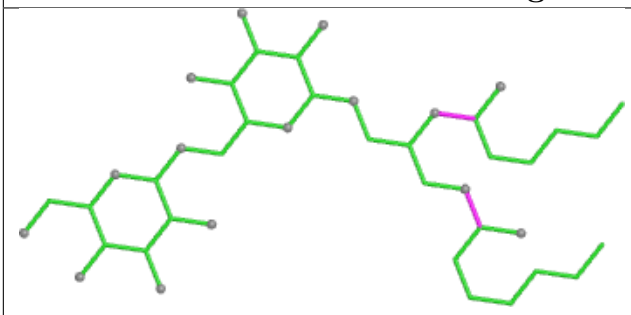


Rings

Ligand DGD j 103



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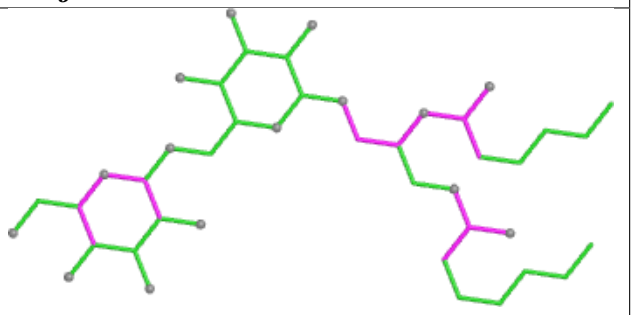
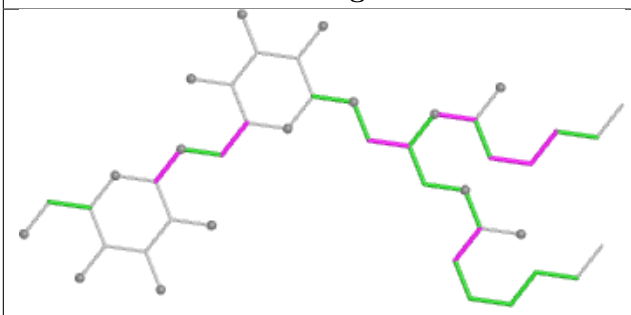


Bond angles



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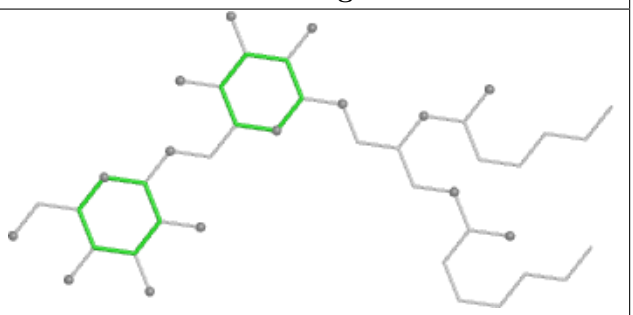
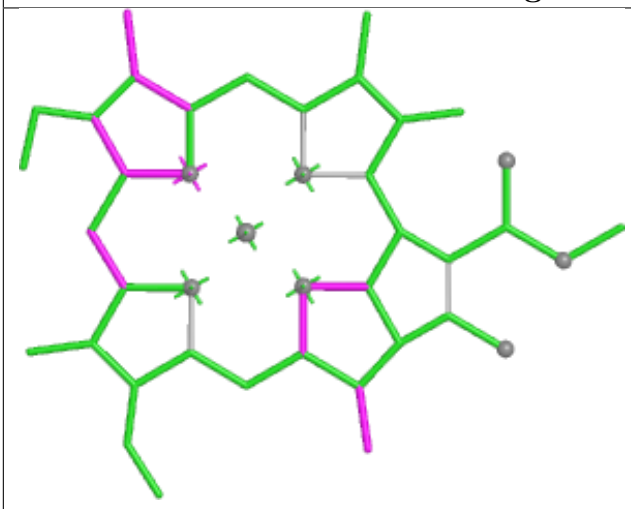


Rings

Ligand CLA C 316



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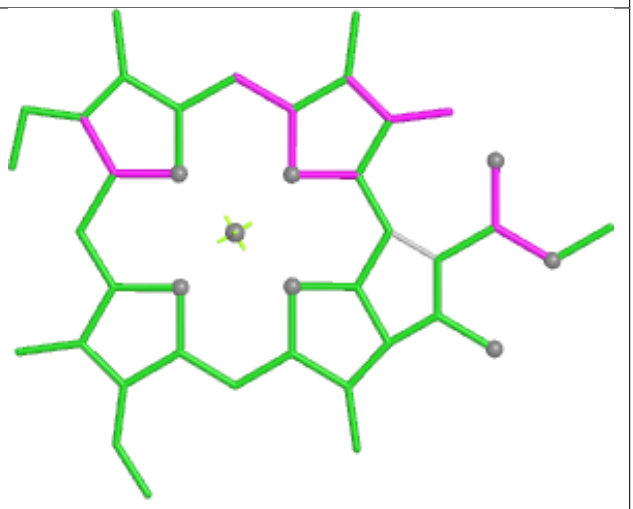
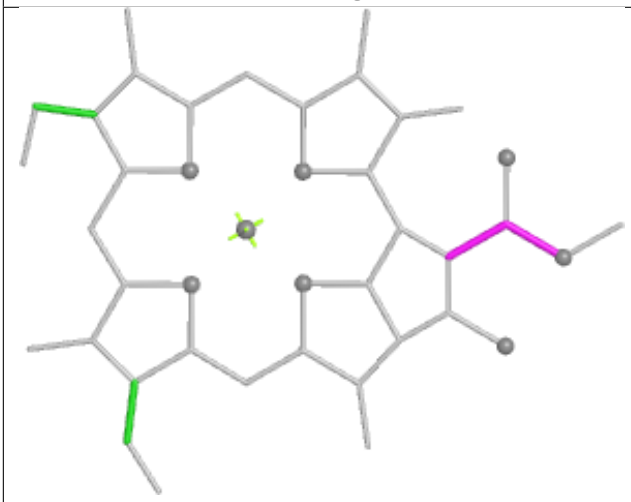


Bond angles



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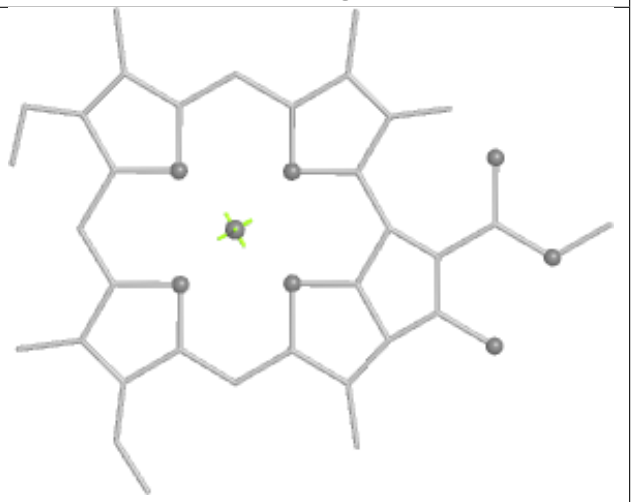
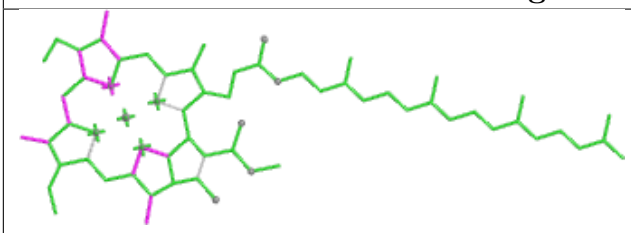


Rings

Ligand CLA a 807



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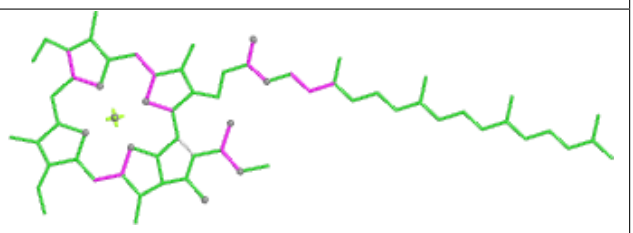
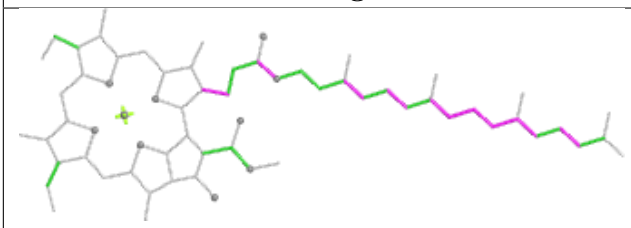


Bond angles



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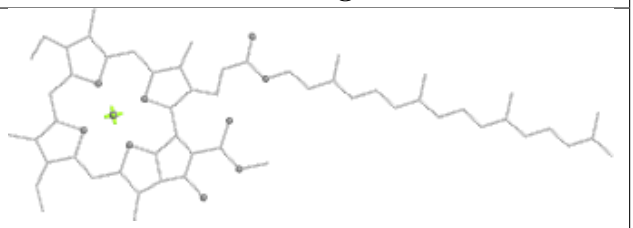
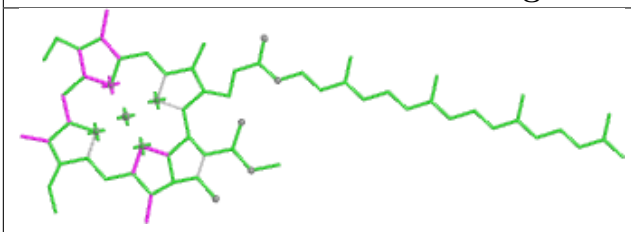


Rings

Ligand CLA G 312



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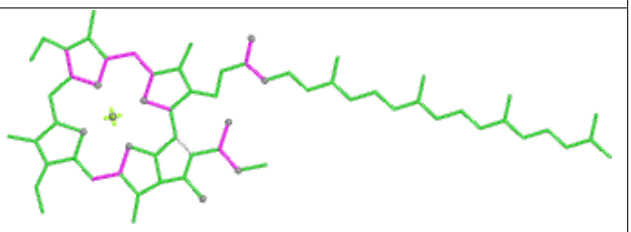
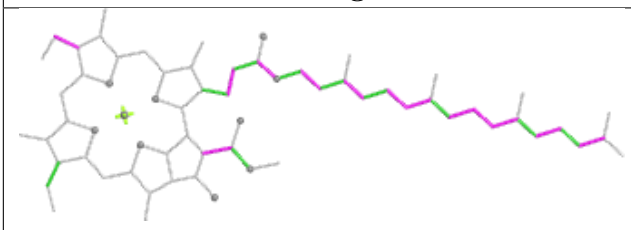


Bond angles



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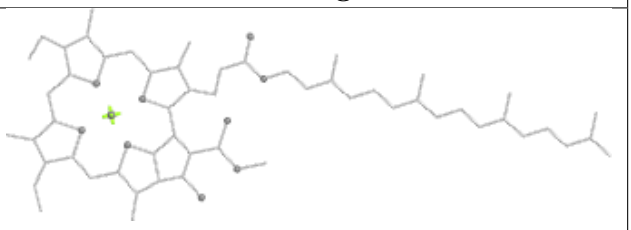
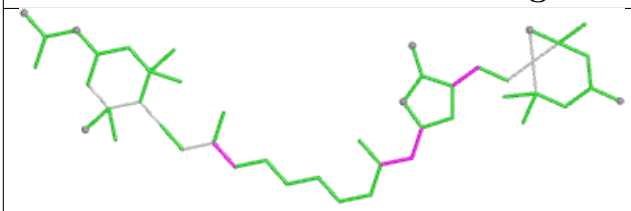


Rings

Ligand PID T 304



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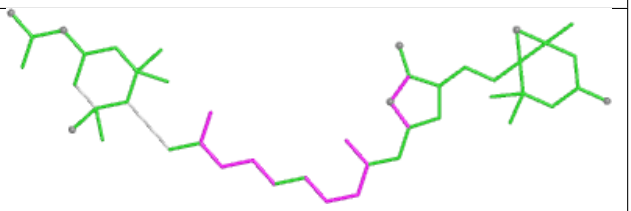
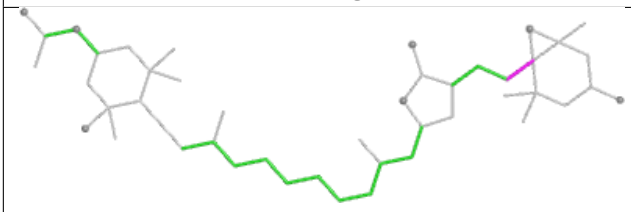


Bond angles



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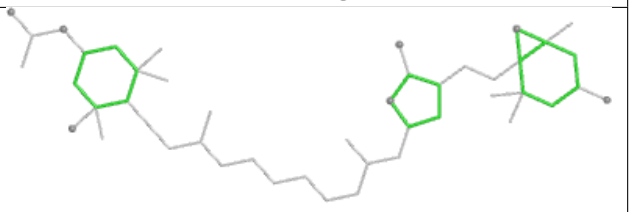
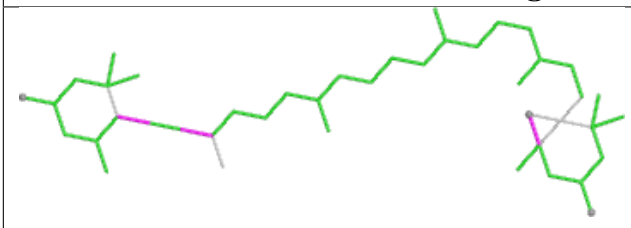


Rings

Ligand DD6 P 204



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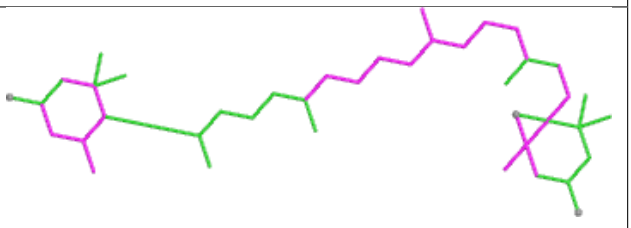
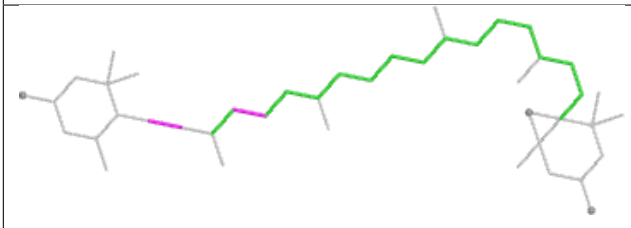


Bond angles

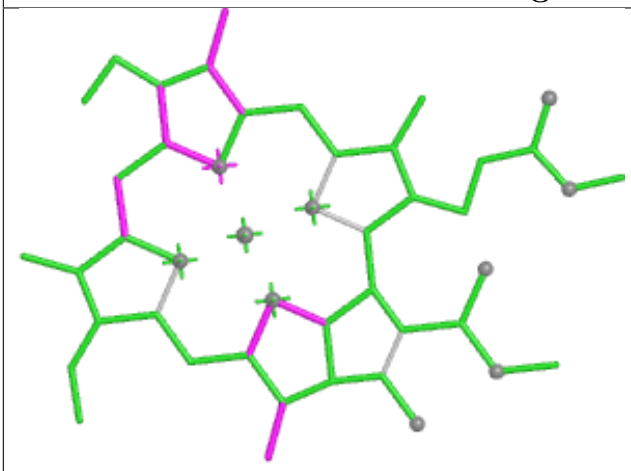


Torsions



Rings

Ligand CLA f 803



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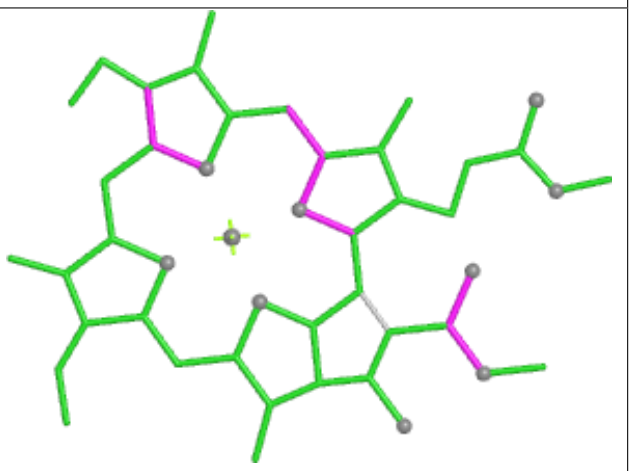
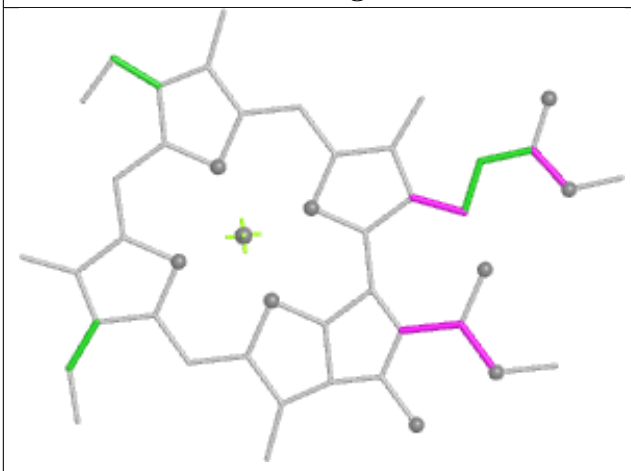
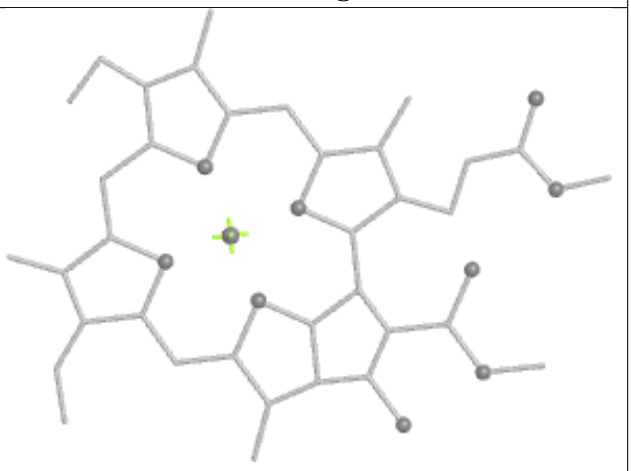


Bond angles

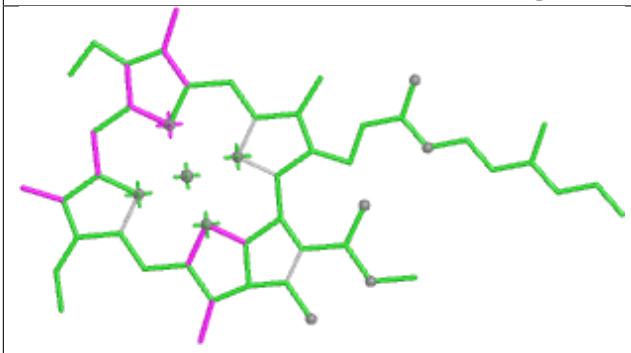


Torsions

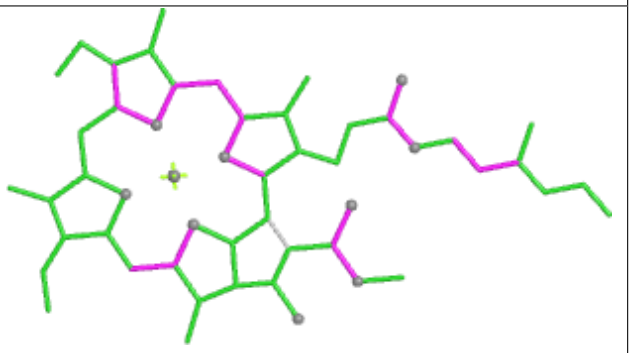


Rings

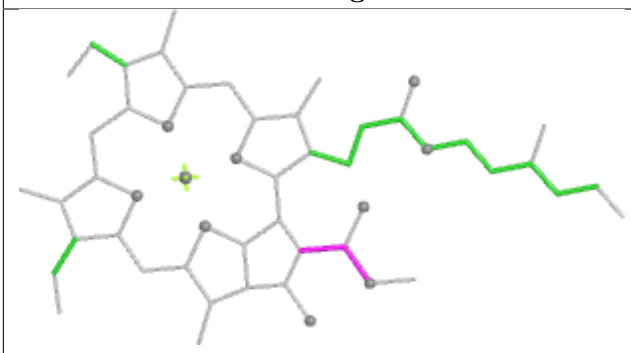
Ligand CLA I 216



Bond lengths



Bond angles



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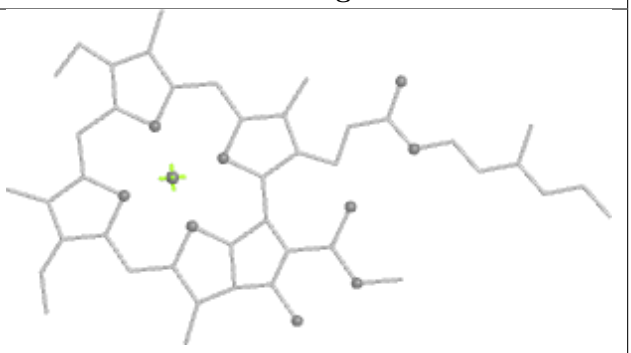
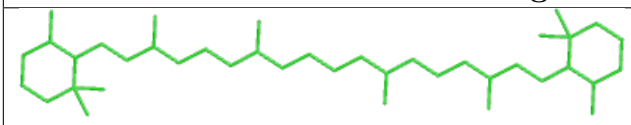


Rings

Ligand BCR i 204



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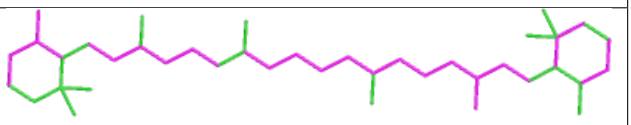

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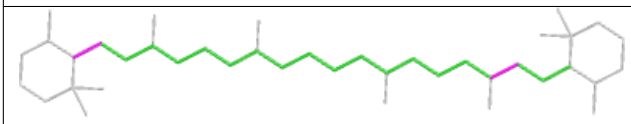

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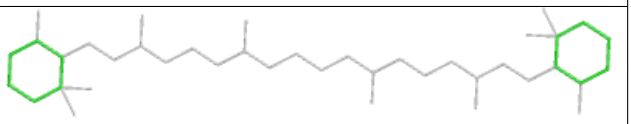

Rings

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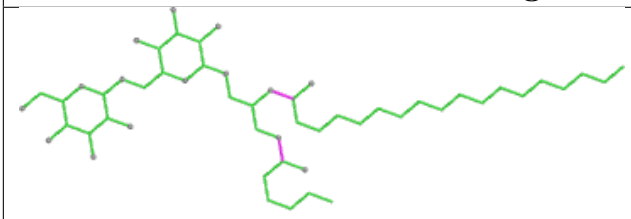

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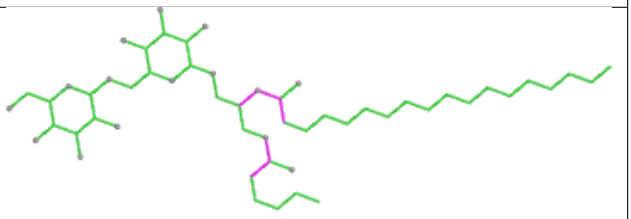

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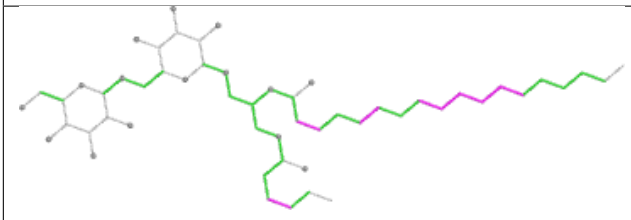

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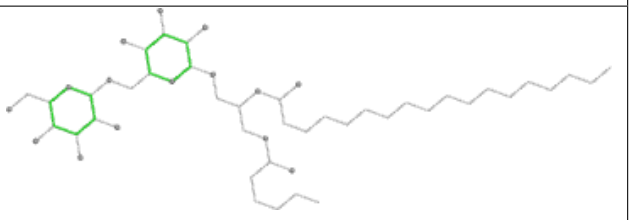

Rings

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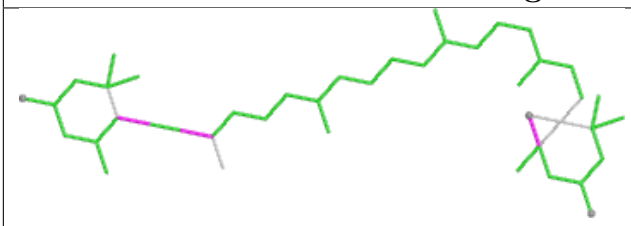

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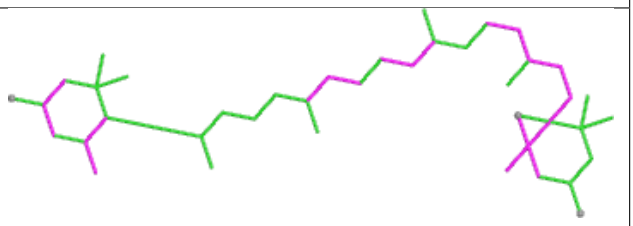

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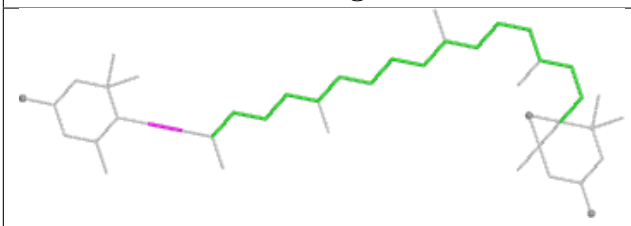

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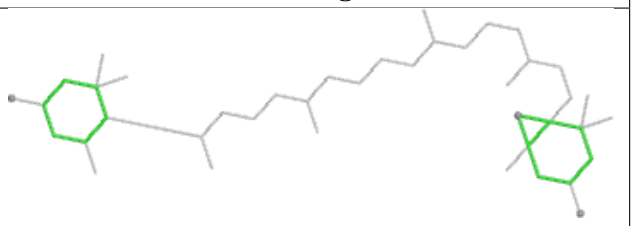
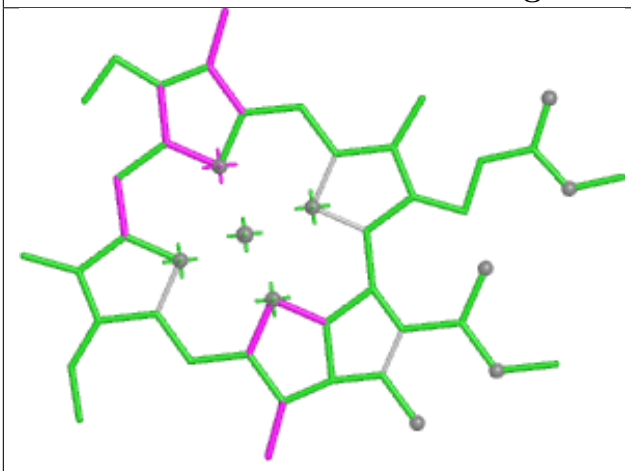


Rings

Ligand CLA O 313



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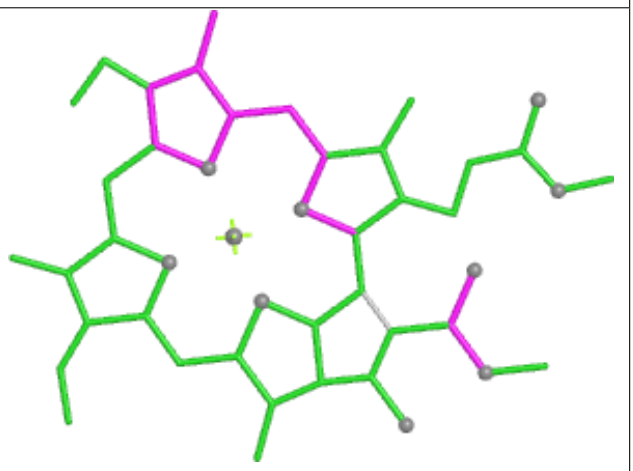

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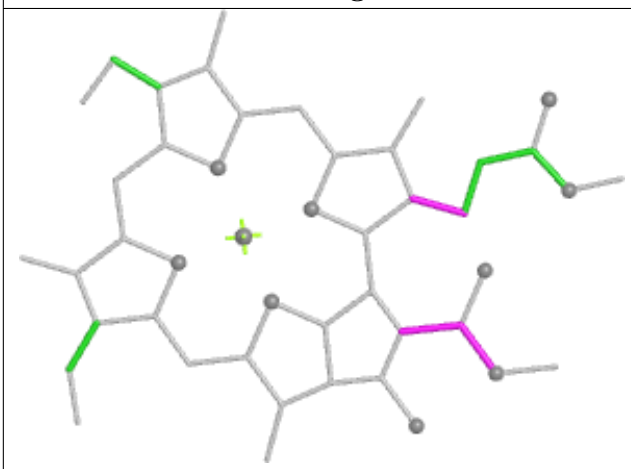

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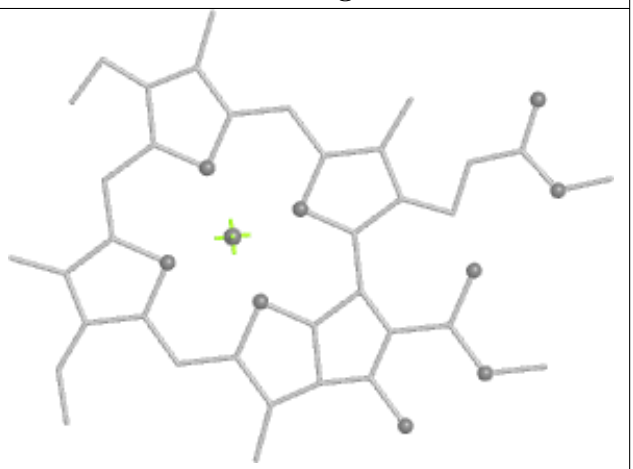

Rings

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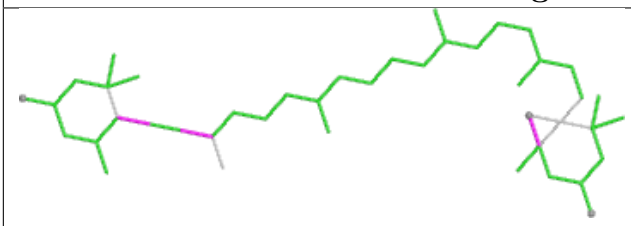

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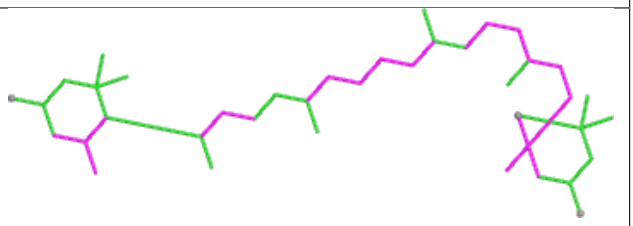

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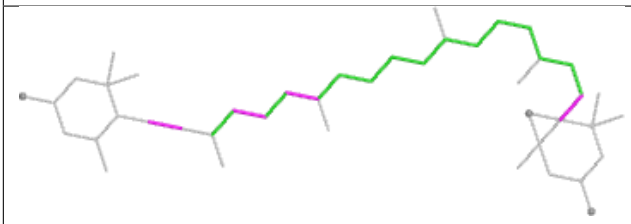

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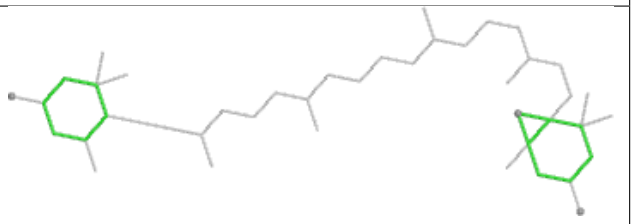

Rings

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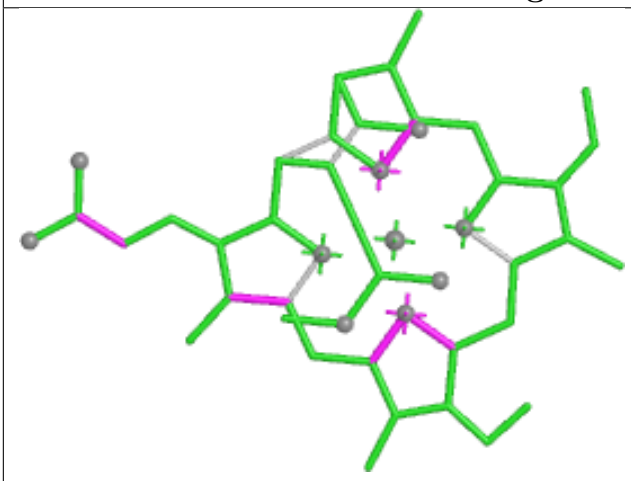

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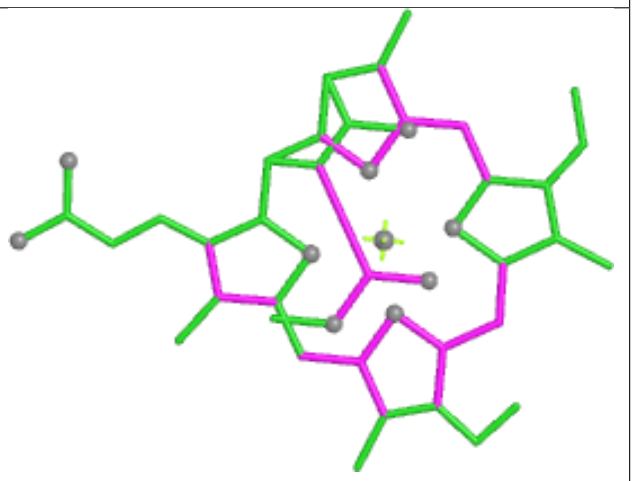

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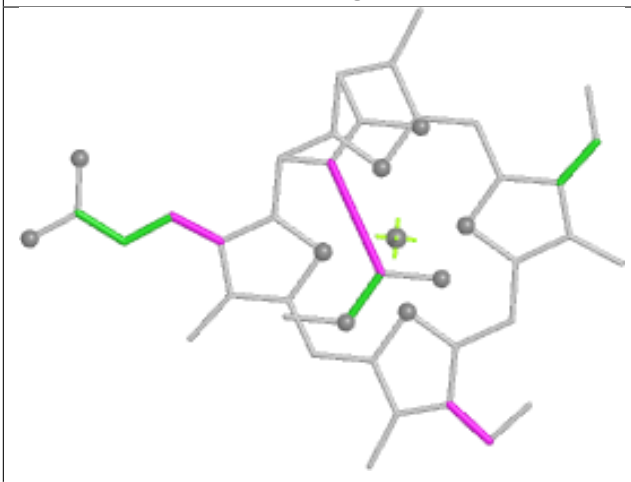

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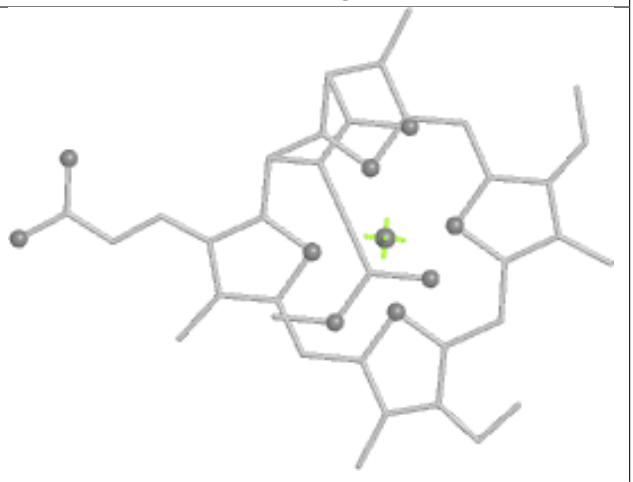
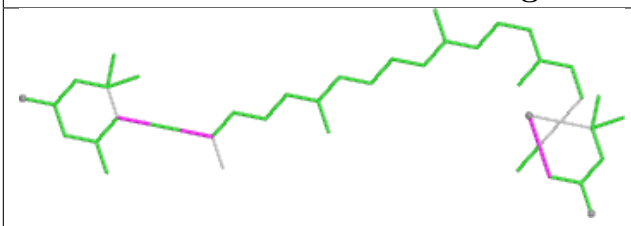


Rings

Ligand DD6 M 303



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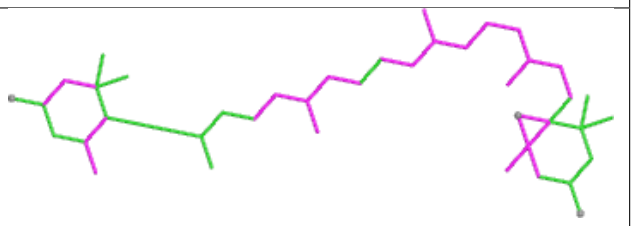

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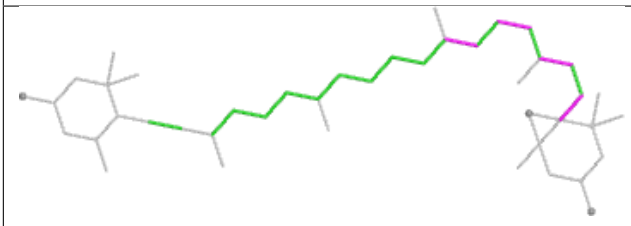

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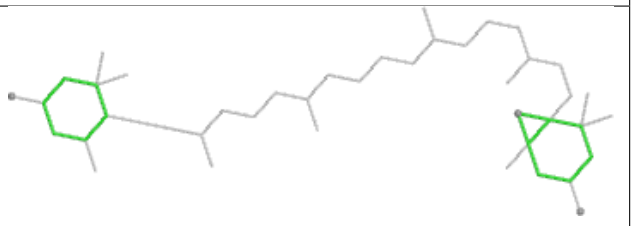
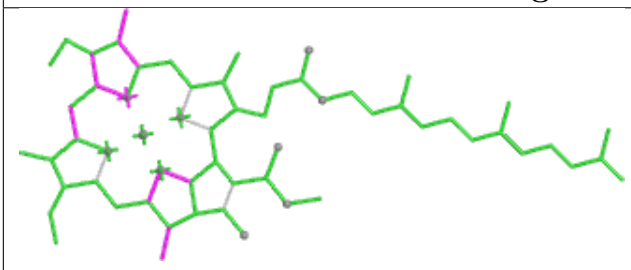


Rings

Ligand CLA f 805



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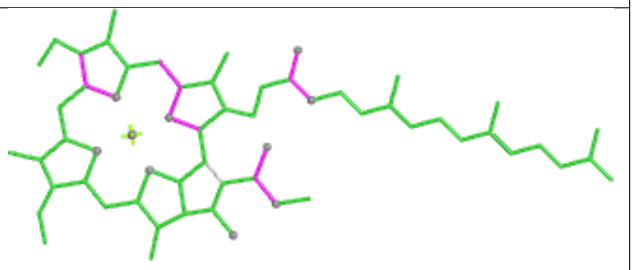

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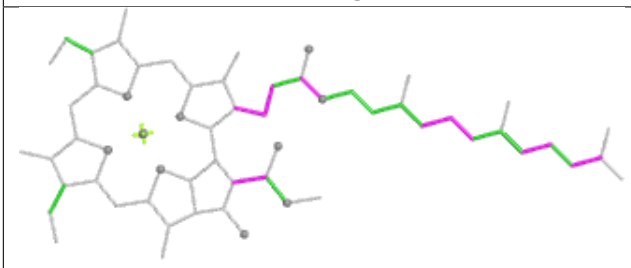

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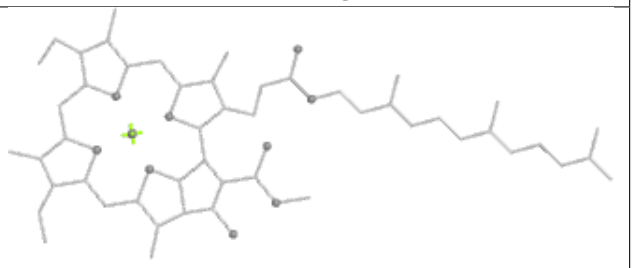
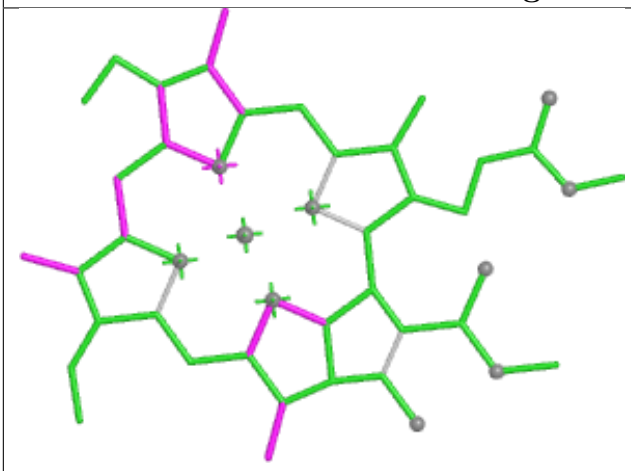


Rings

Ligand CLA K 217



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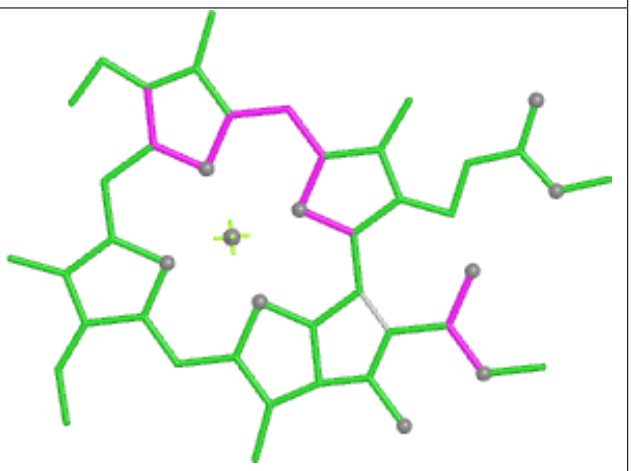
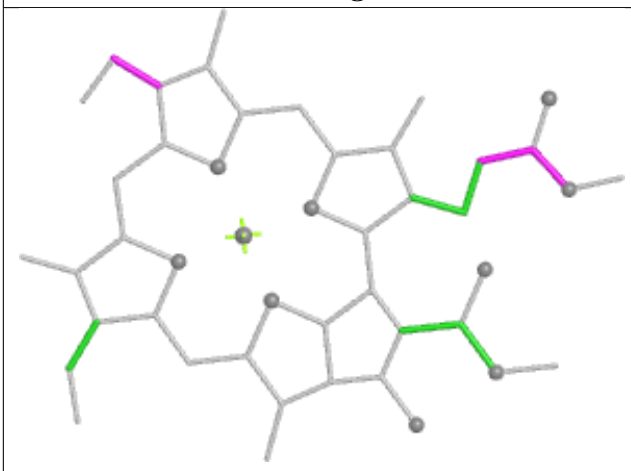


Bond angles



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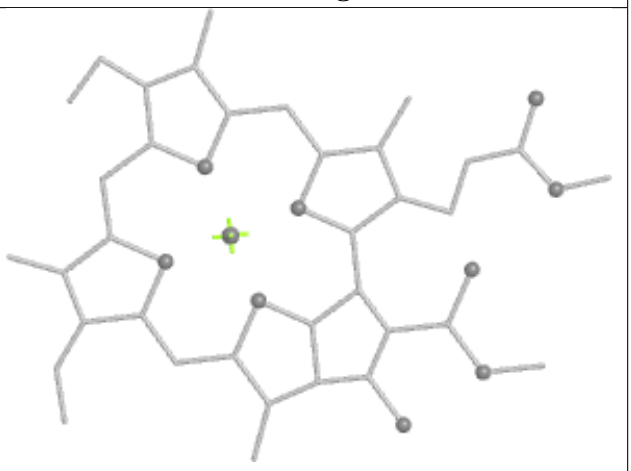
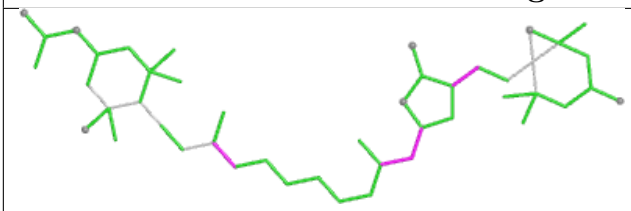


Rings

Ligand PID H 305



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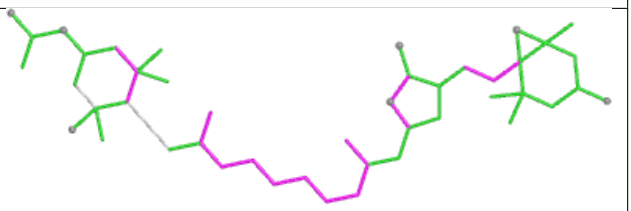

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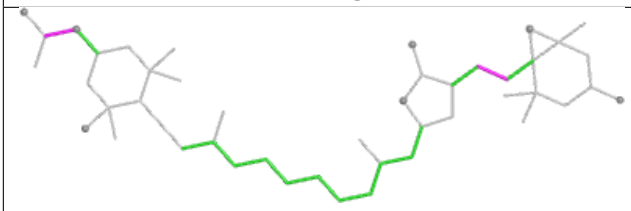

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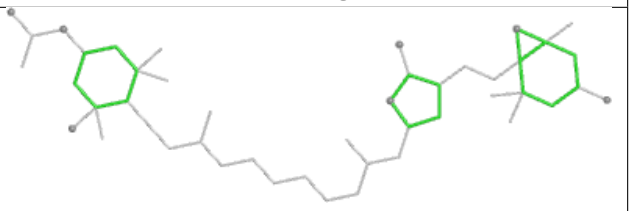
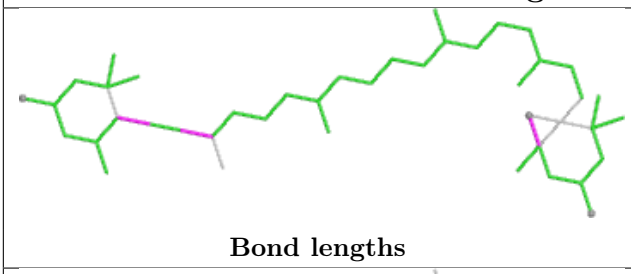


Rings

Ligand DD6 F 303



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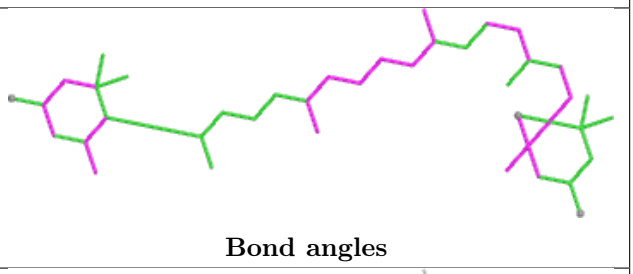
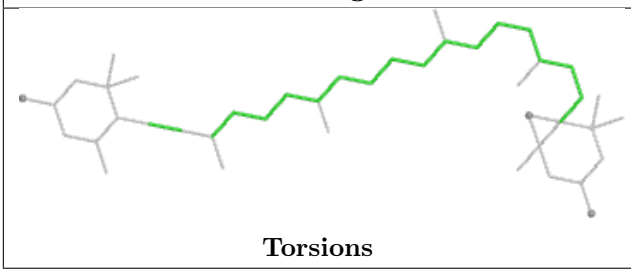


Bond angles



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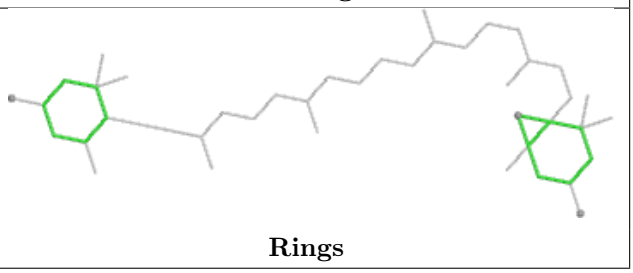
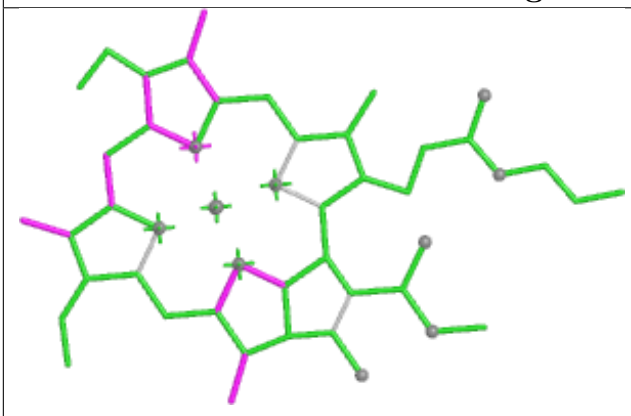


Rings

Ligand CLA E 314



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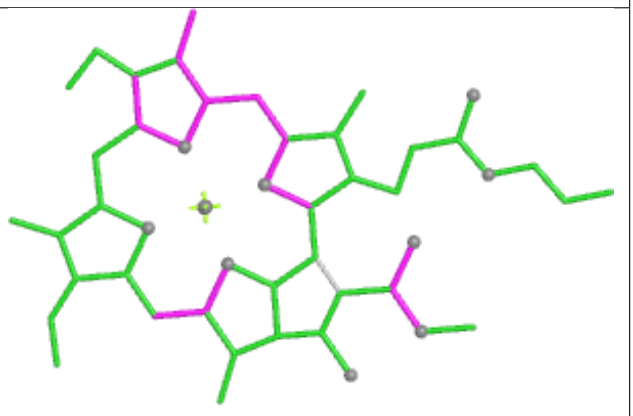
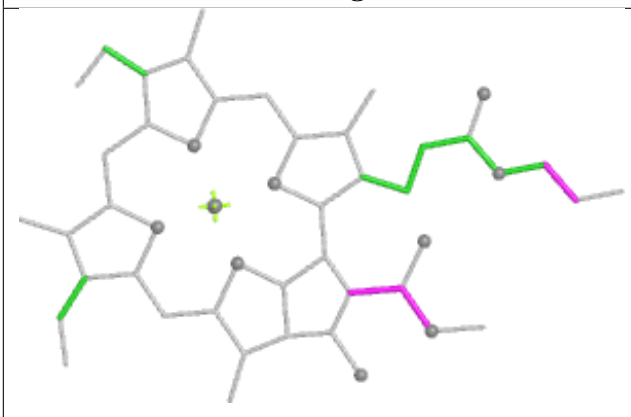


Bond angles



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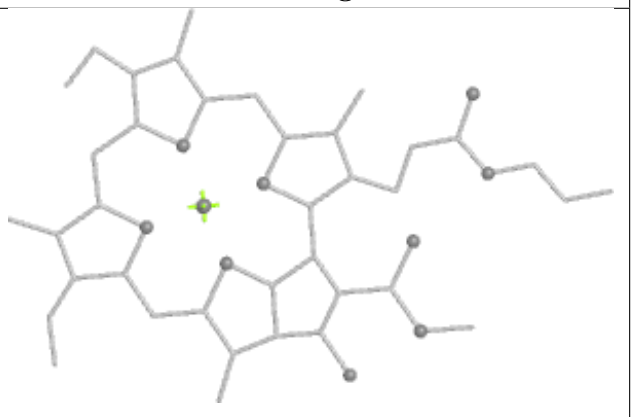
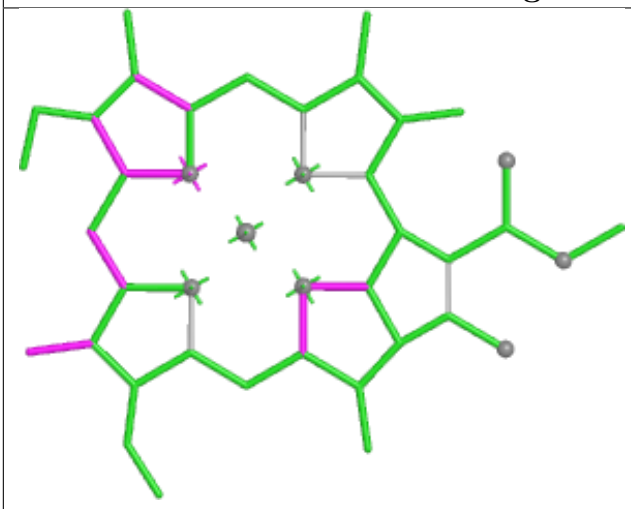


Rings

Ligand CLA D 316



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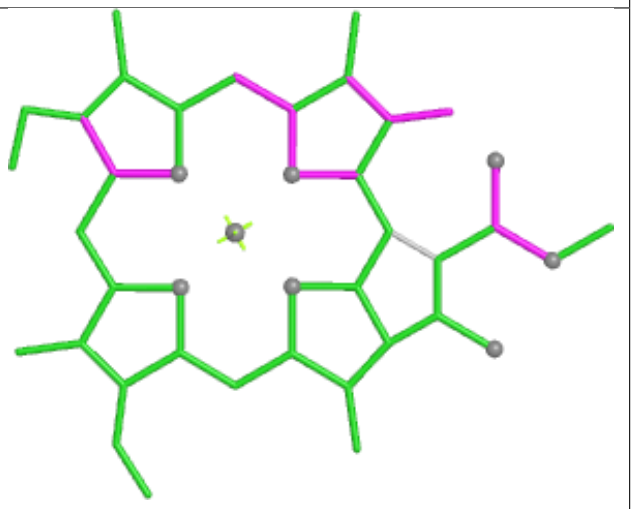
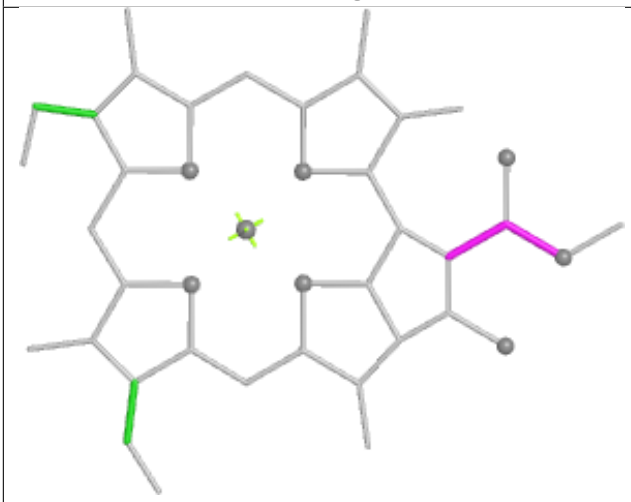


Bond angles



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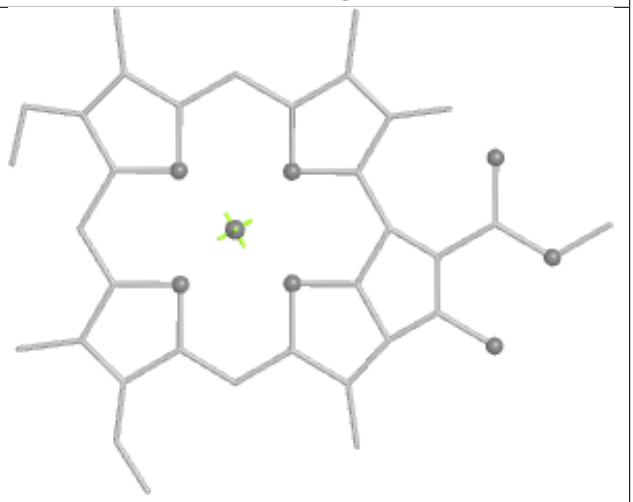
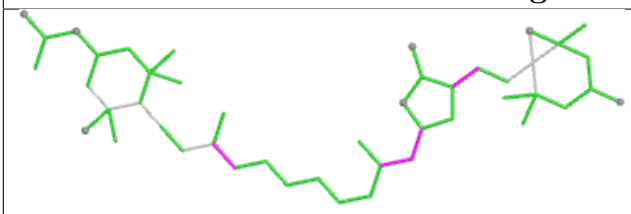


Rings

Ligand PID P 203



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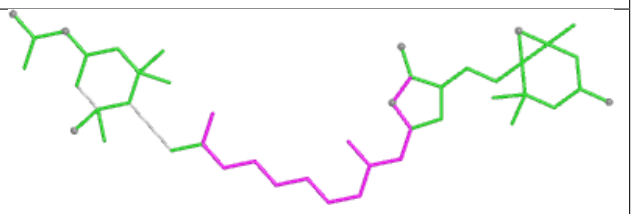
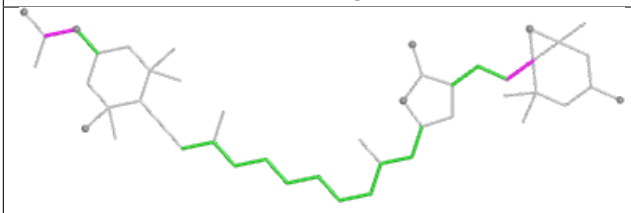


Bond angles



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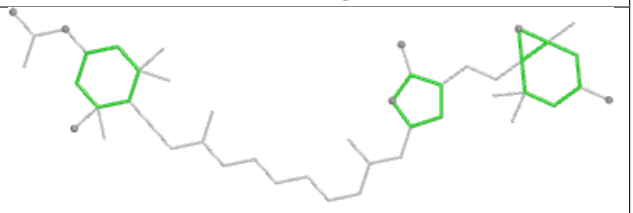
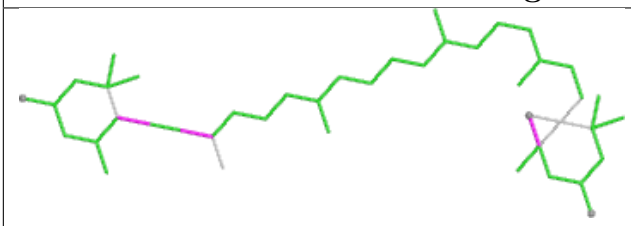
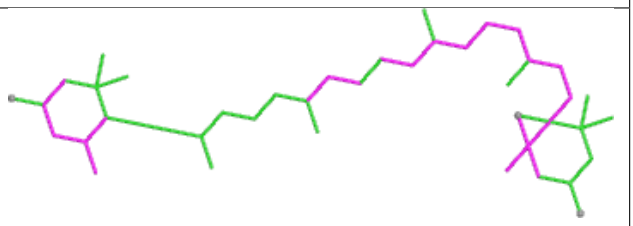


Rings

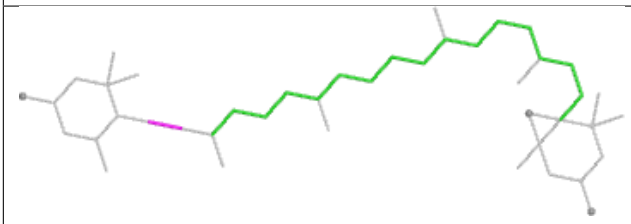
Ligand DD6 N 303



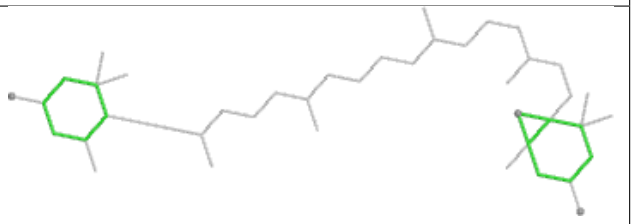
Bond lengths



Bond angles

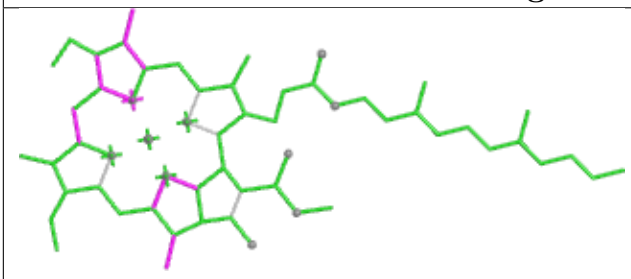


Torsions



Rings

Ligand CLA b 711



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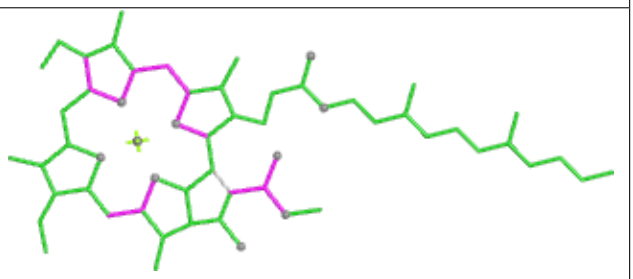

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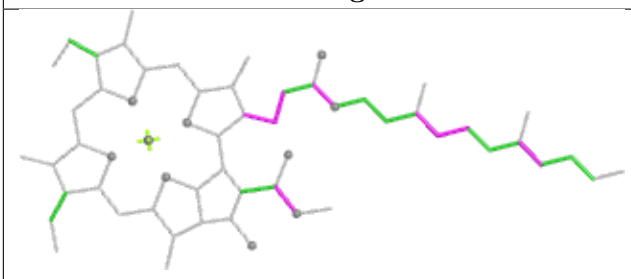

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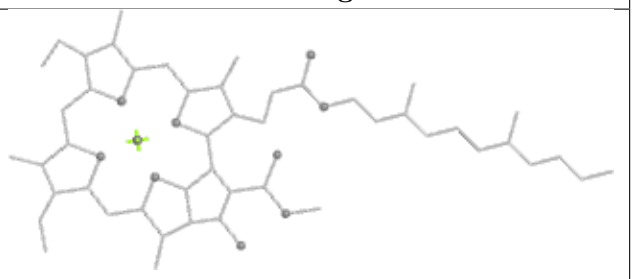
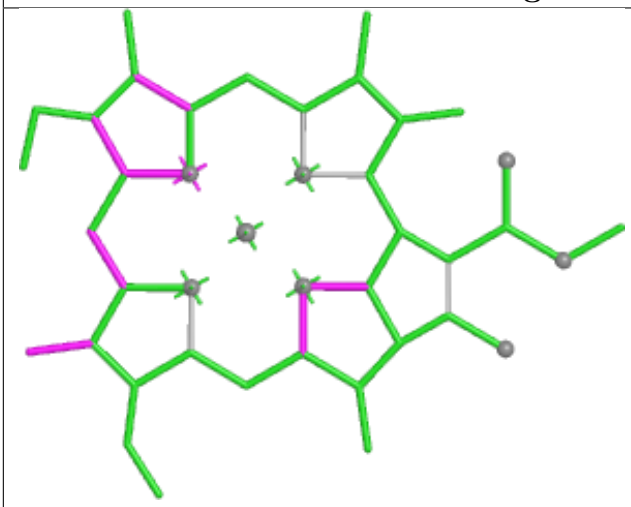


Rings

Ligand CLA O 316



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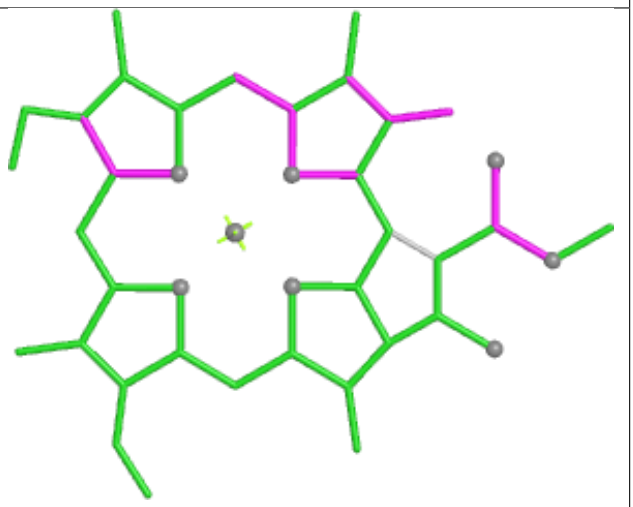

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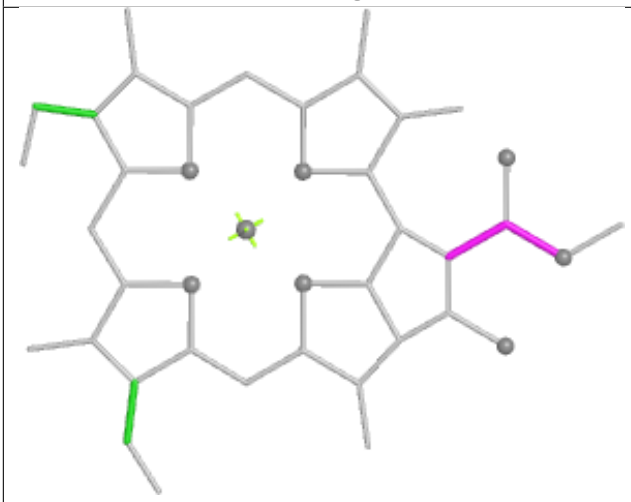

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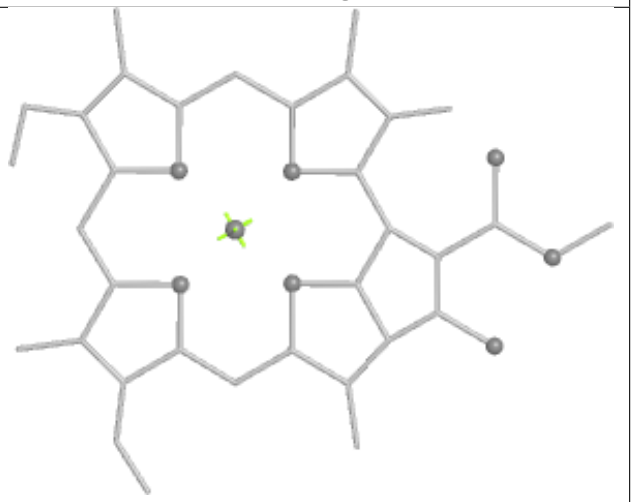
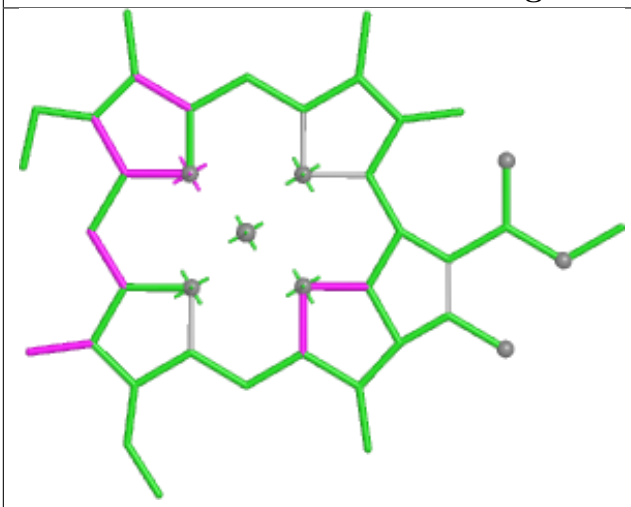


Rings

Ligand CLA P 217



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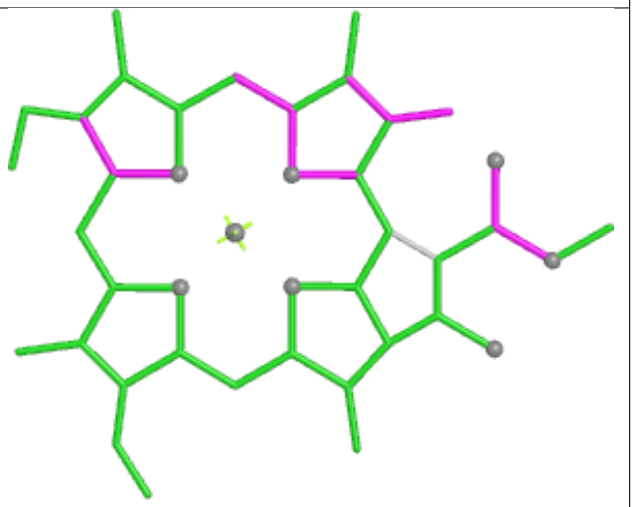

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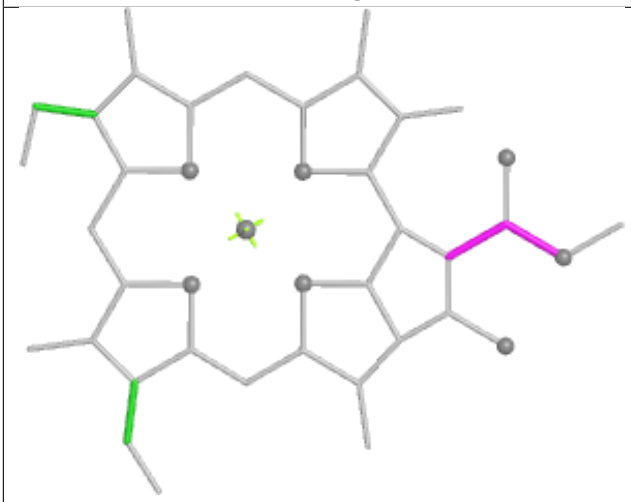

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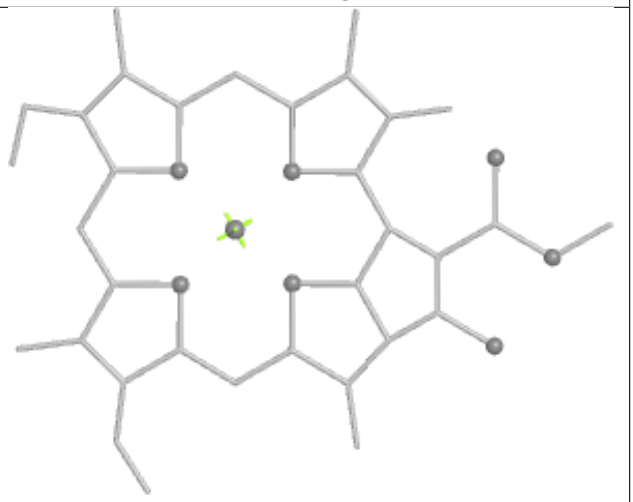
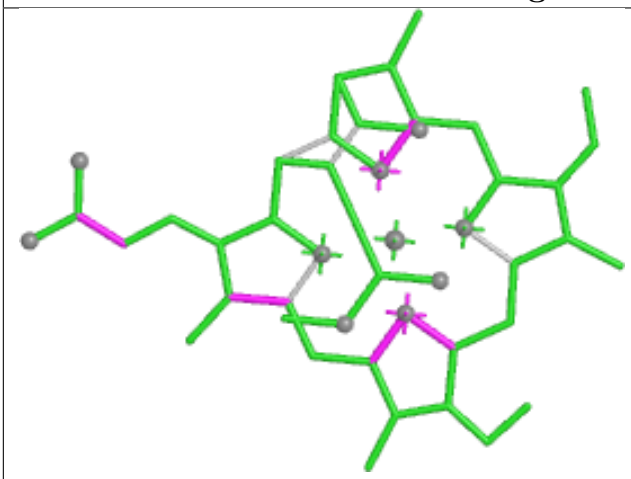


Rings

Ligand KC1 L 306



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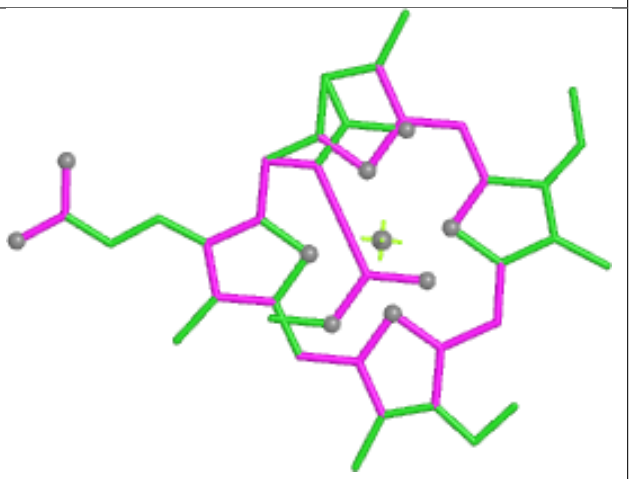

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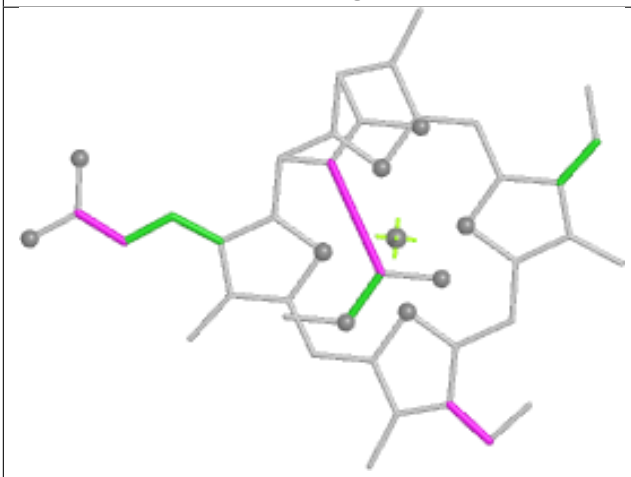

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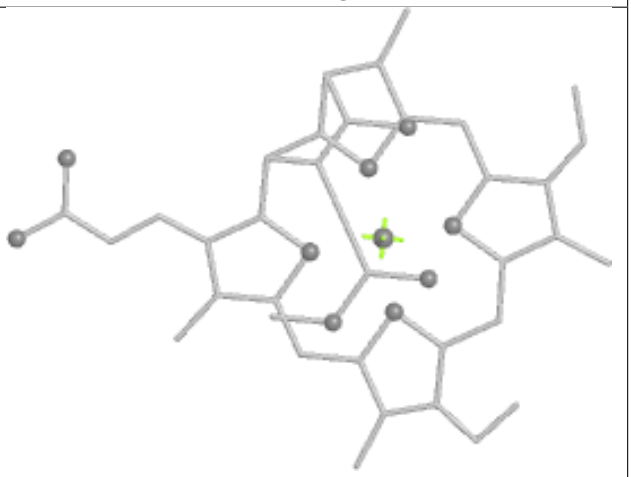
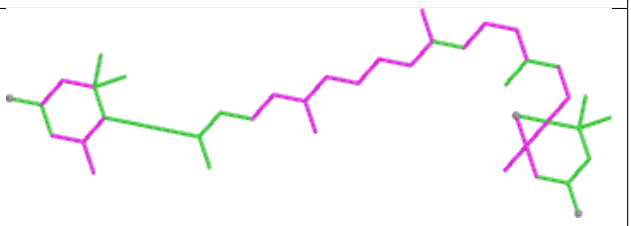


Rings

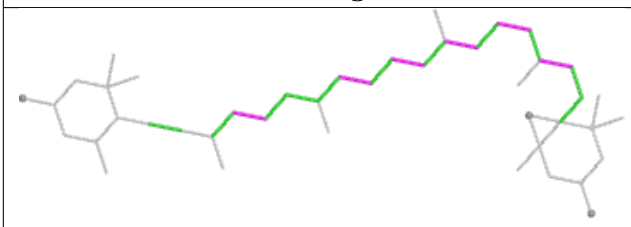
Ligand DD6 K 202



Bond lengths



Bond angles



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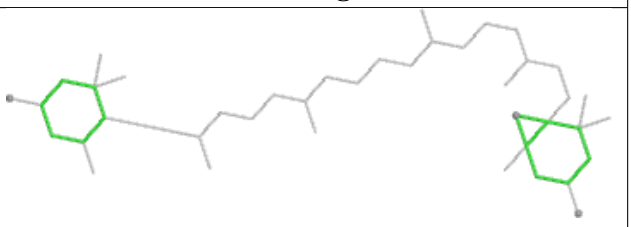
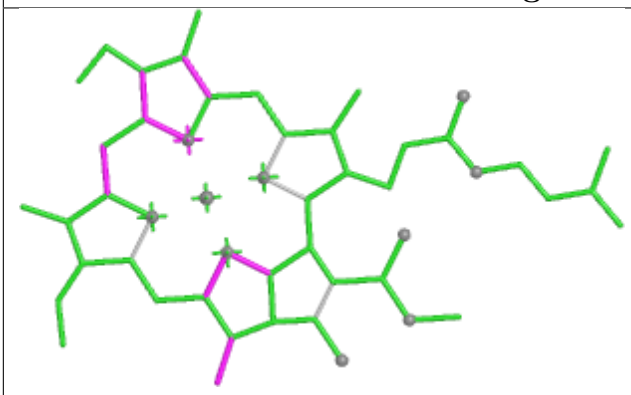


Rings

Ligand CLA K 210



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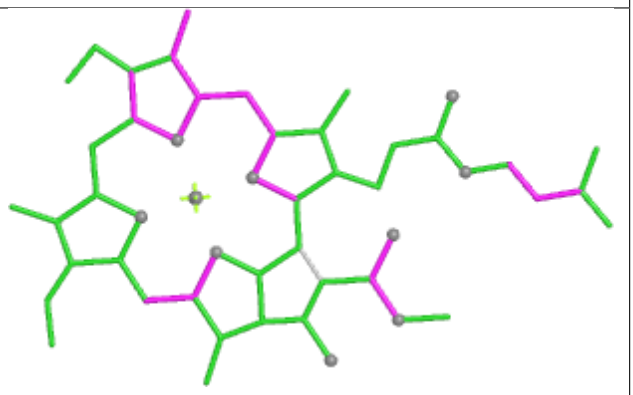
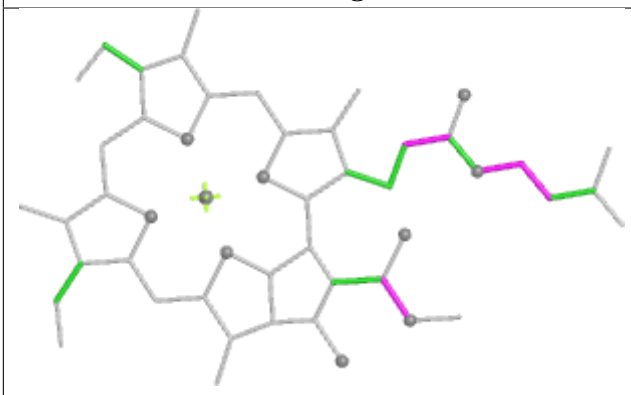


Bond angles



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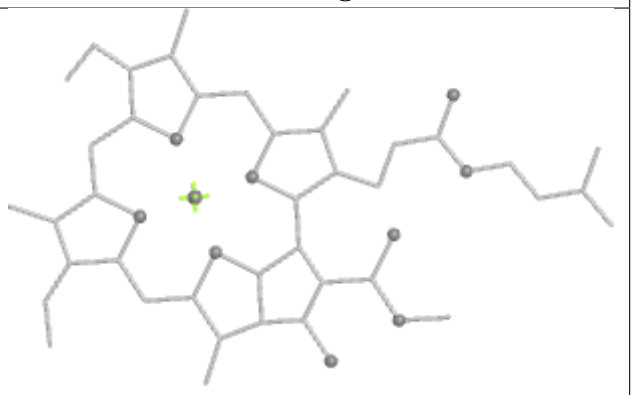
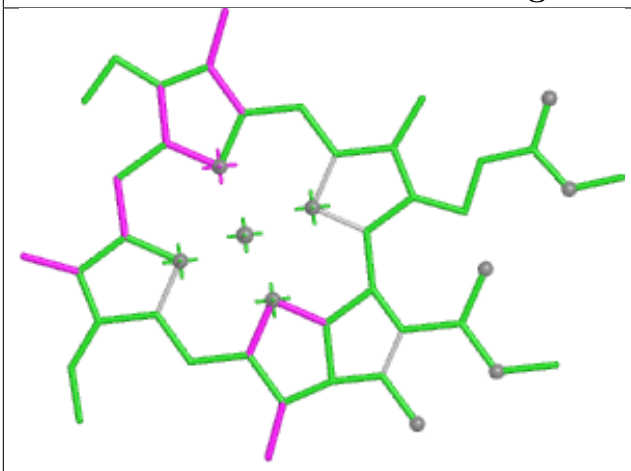


Rings

Ligand CLA a 814



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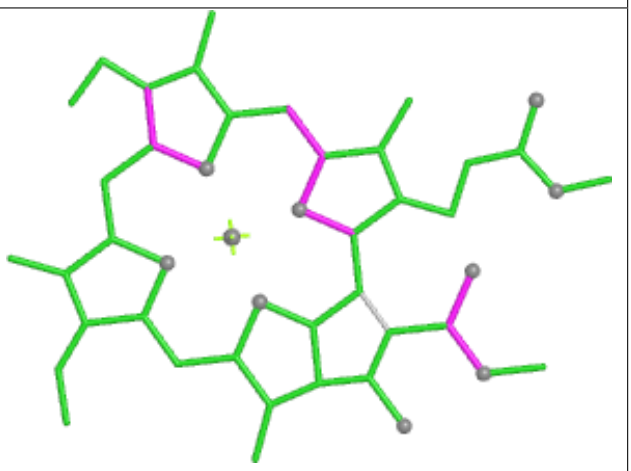
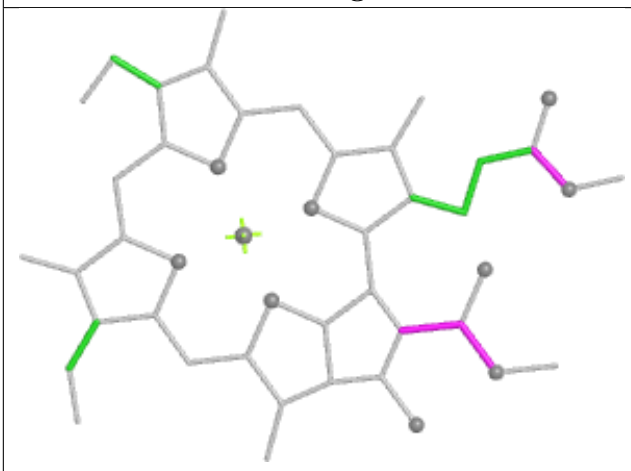


Bond angles



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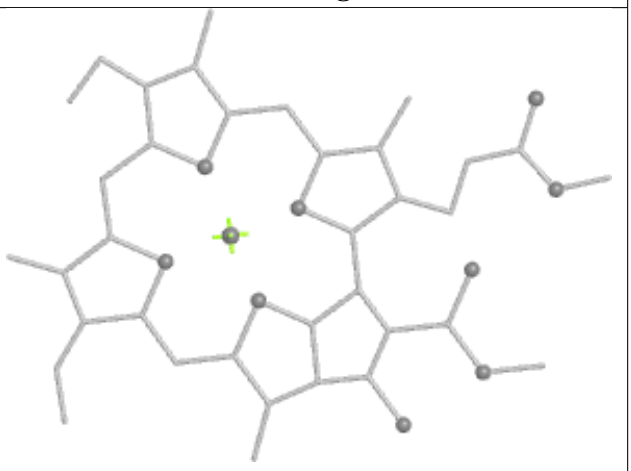
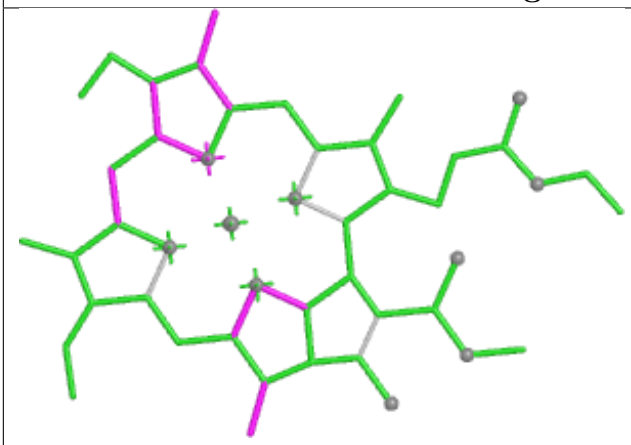


Rings

Ligand CLA Q 313



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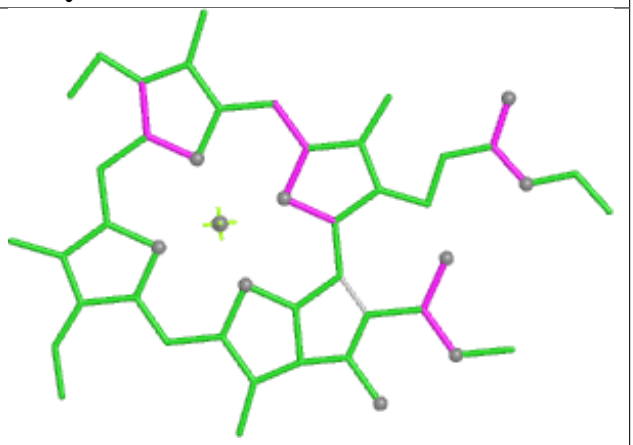
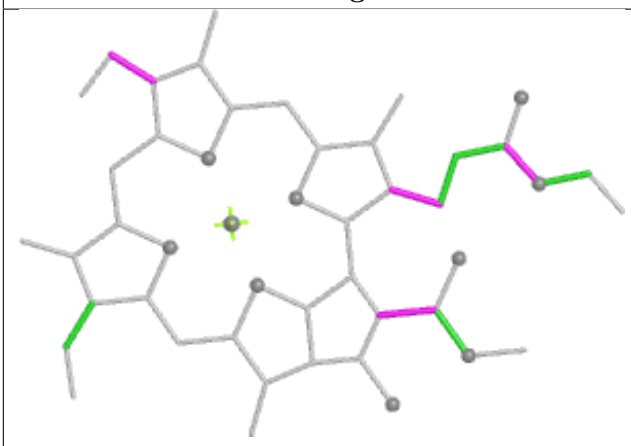


Bond angles



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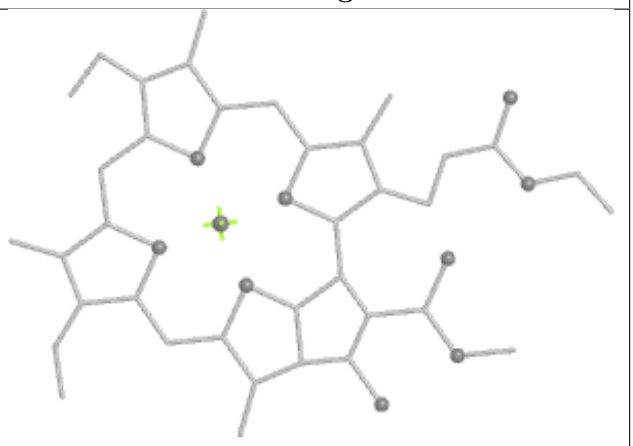
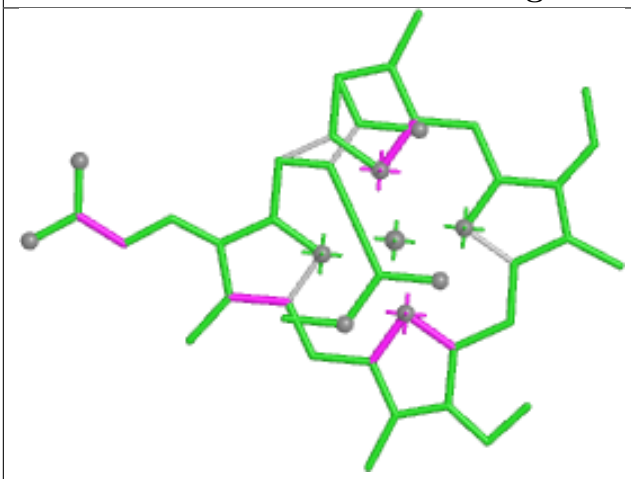


Rings

Ligand KC1 C 312



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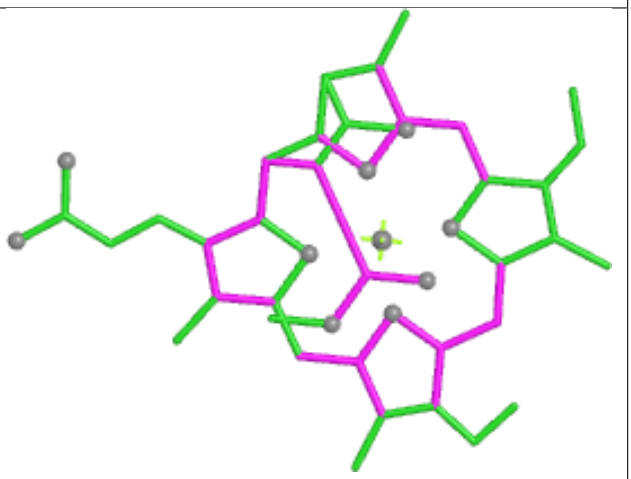
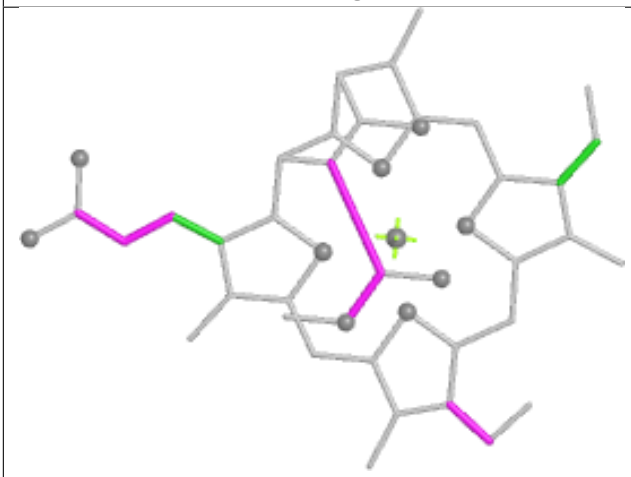


Bond angles



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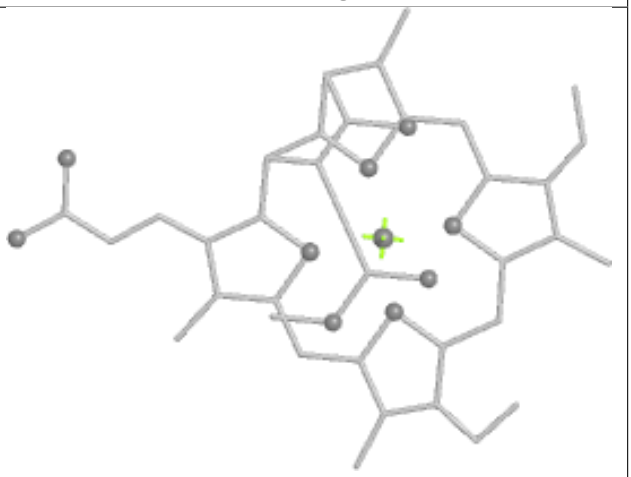
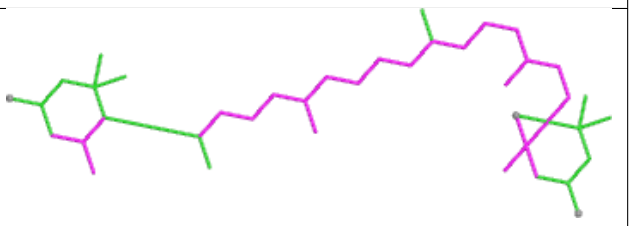


Rings

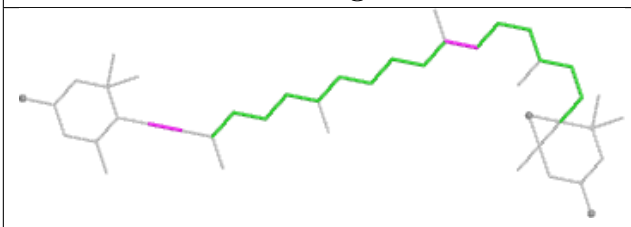
Ligand DD6 A 201



Bond lengths



Bond angles



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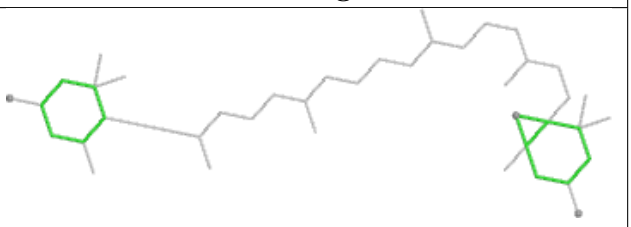
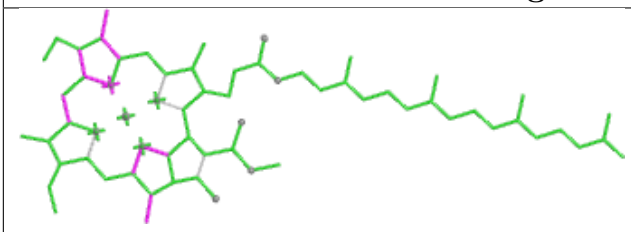


Rings

Ligand CLA b 702



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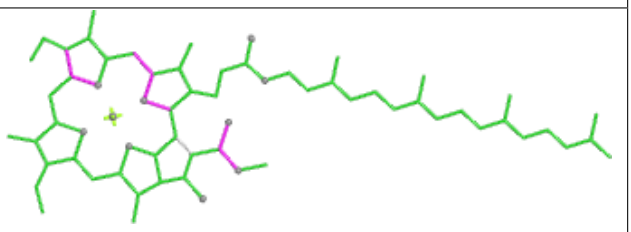
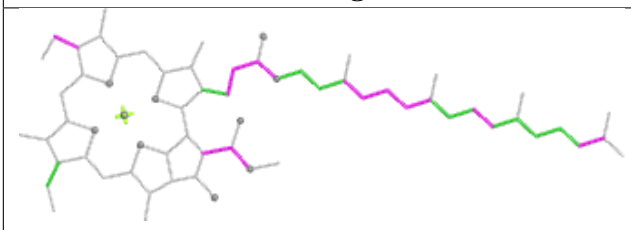


Bond angles



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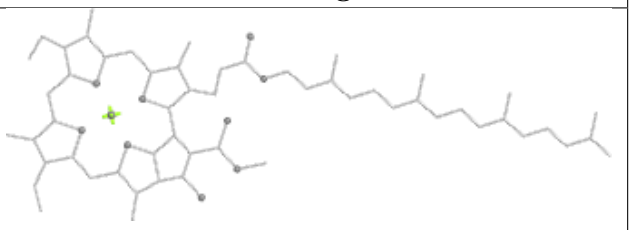
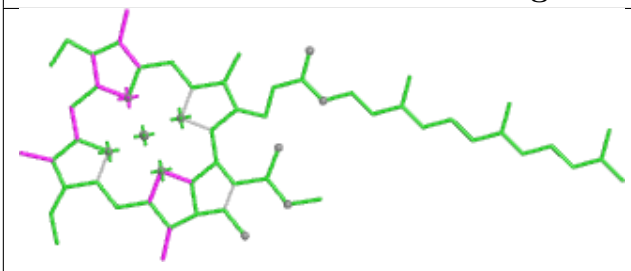


Rings

Ligand CLA I 209



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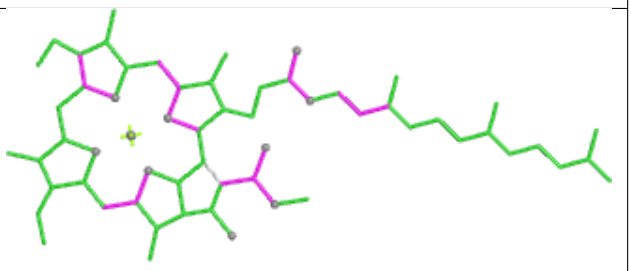
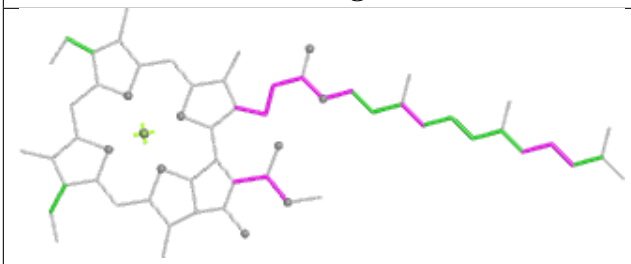


Bond angles



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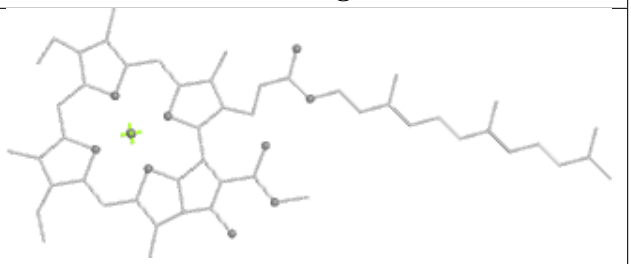
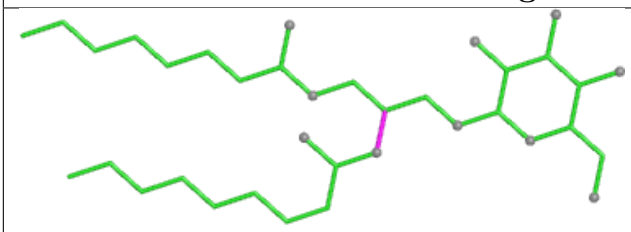


Rings

Ligand LMG K 220



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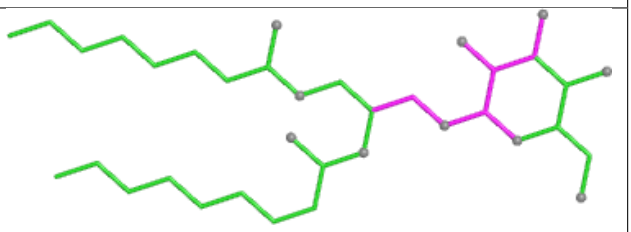
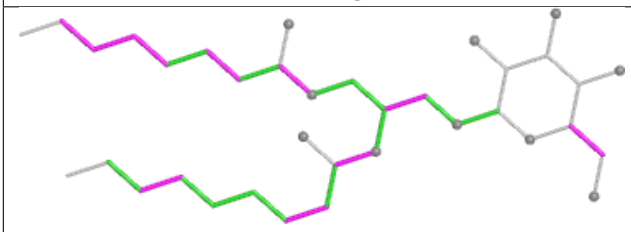


Bond angles



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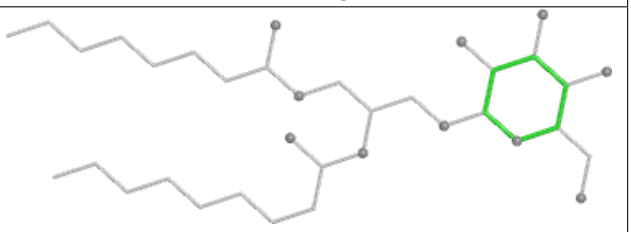
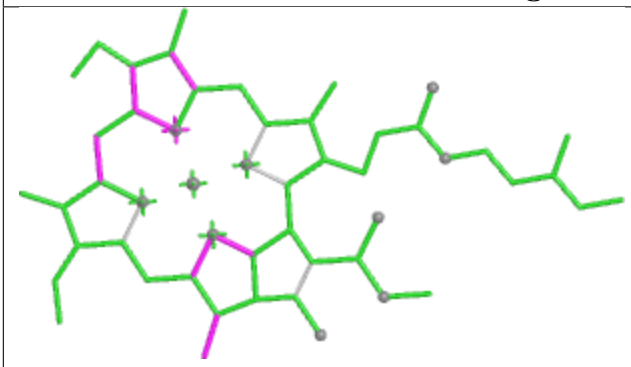


Rings

Ligand CLA P 212



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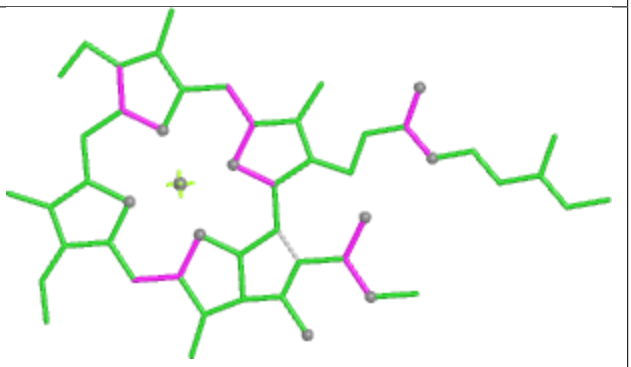
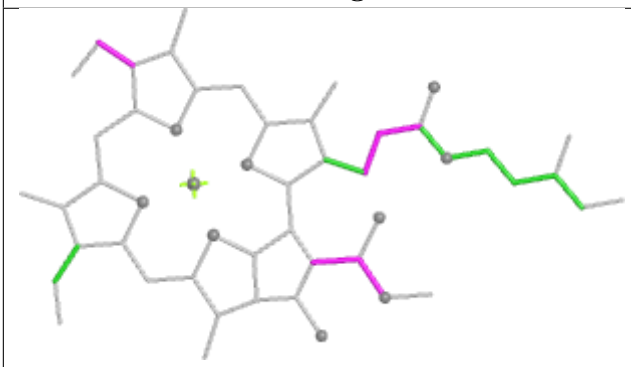


Bond angles



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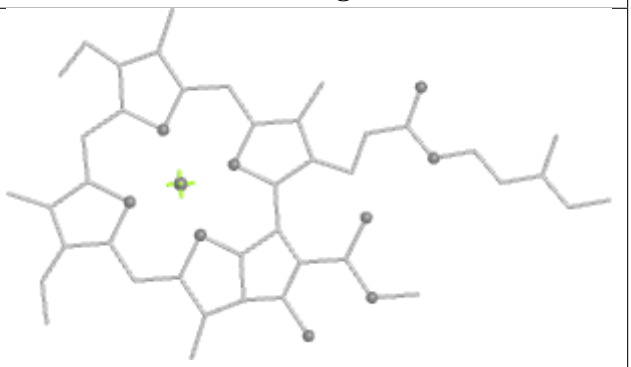
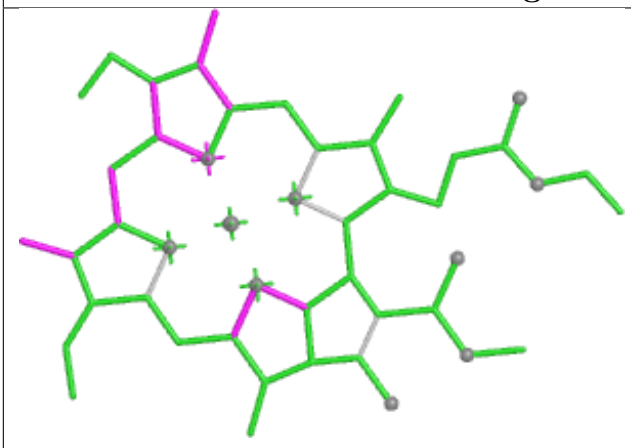
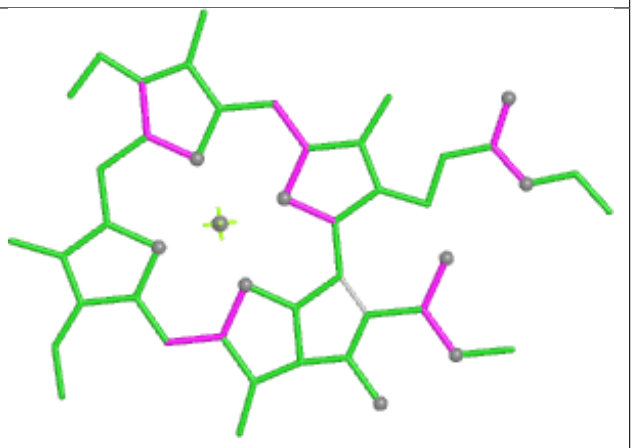


Rings

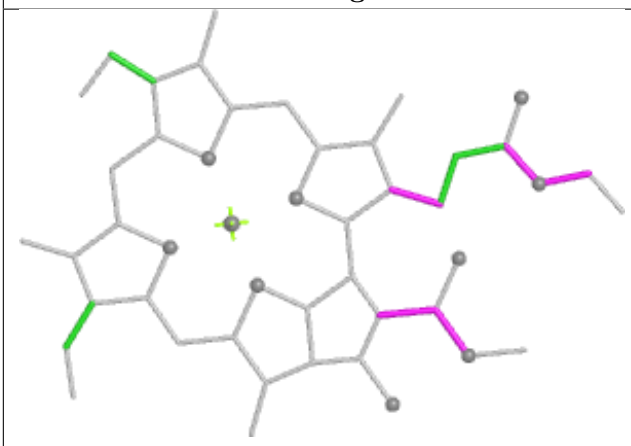
Ligand CLA H 313



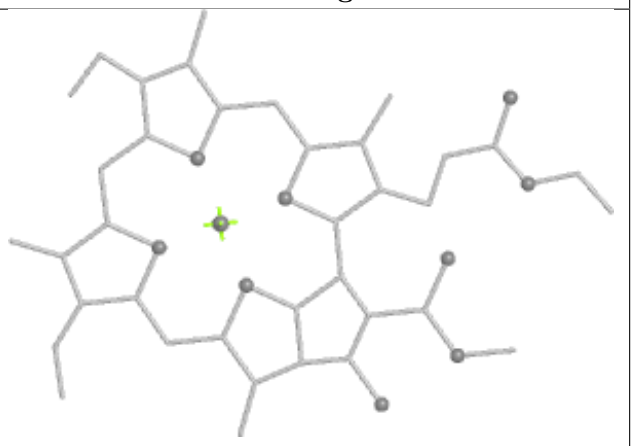
Bond lengths



Bond angles

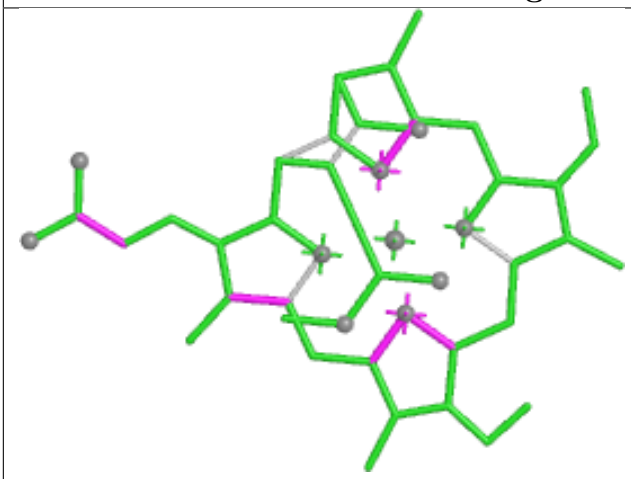


Torsions



Rings

Ligand KC1 O 310



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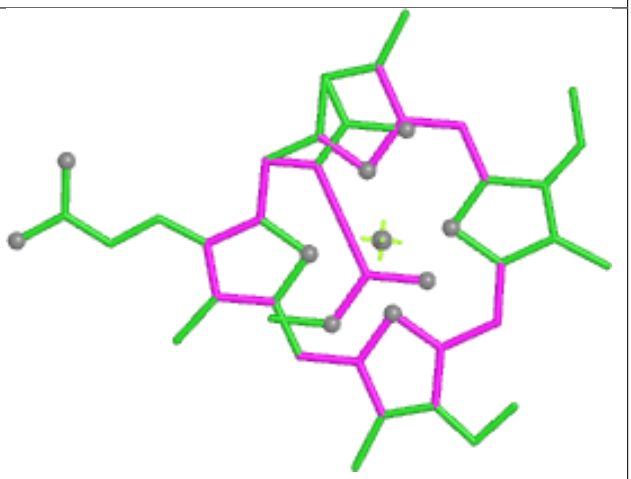
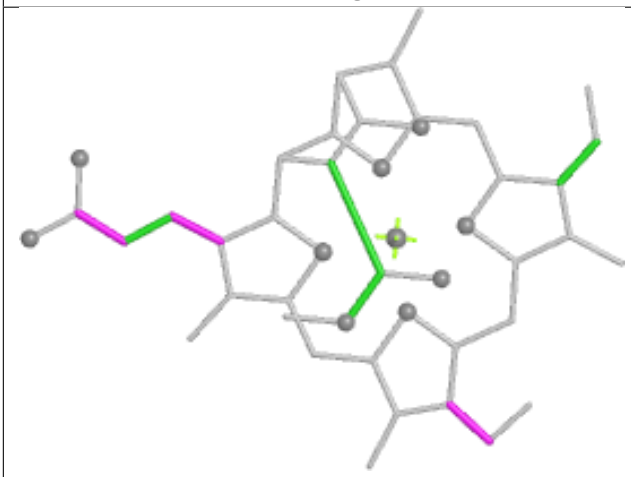


Bond angles



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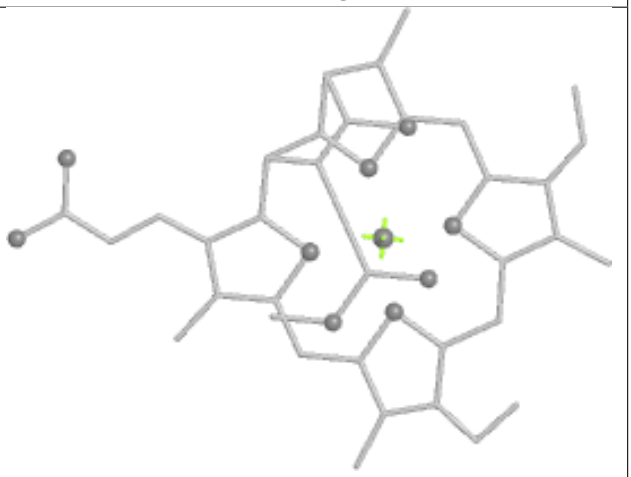
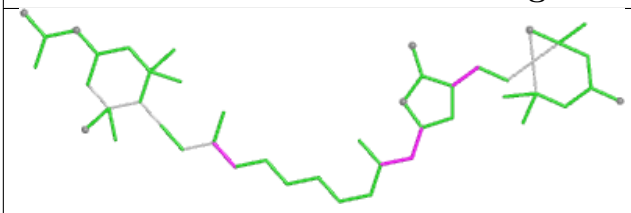


Rings

Ligand PID O 305



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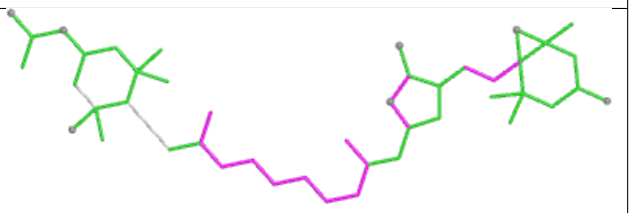
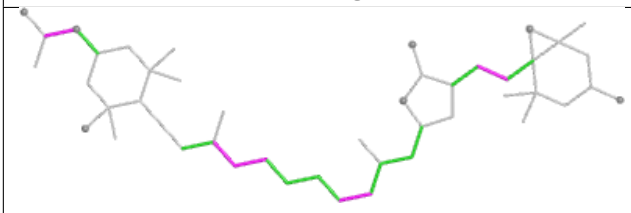


Bond angles



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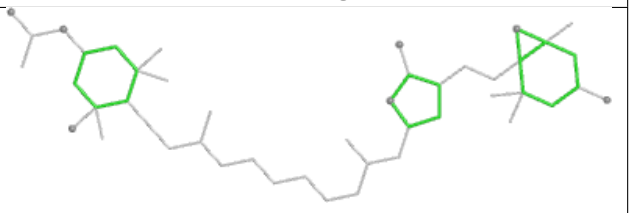
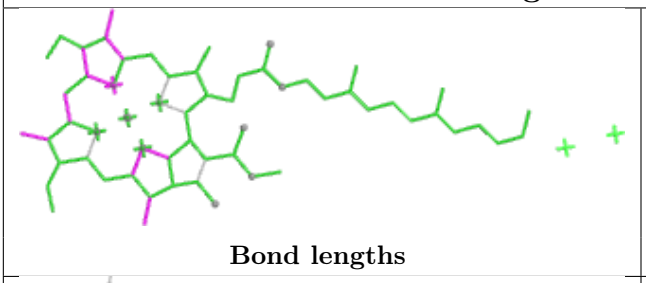


Rings

Ligand CLA G 304



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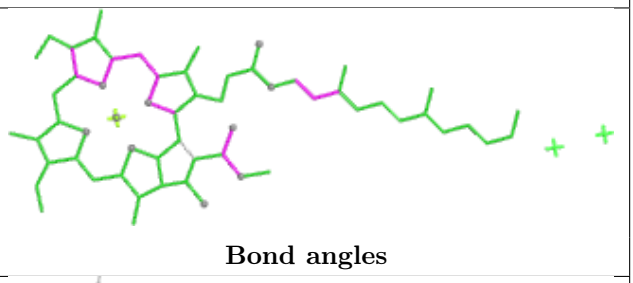
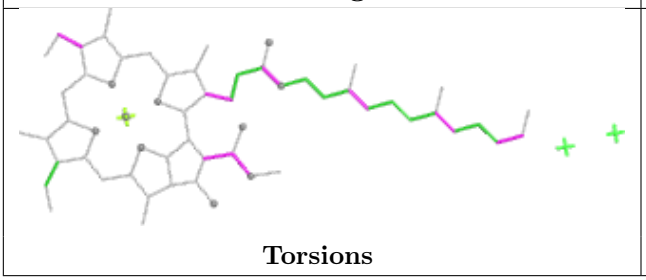


Bond angles



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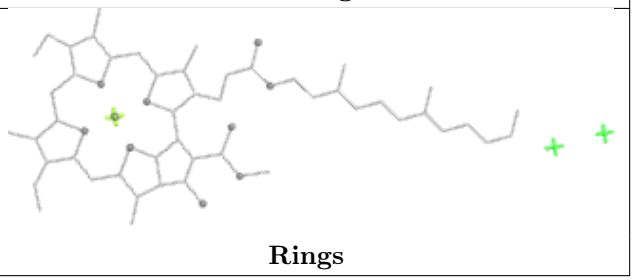
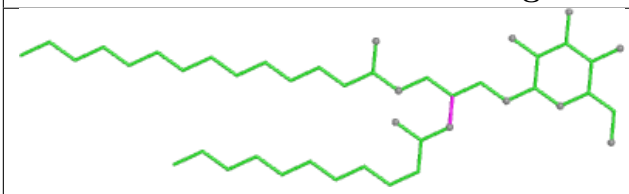


Rings

Ligand LMG b 732



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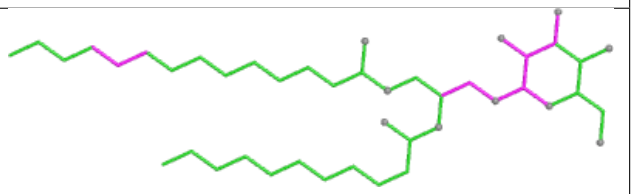
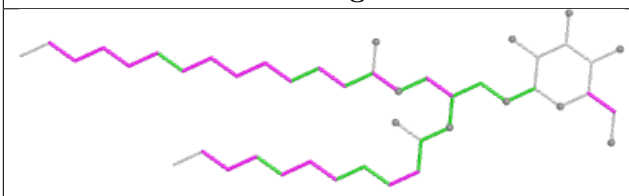


Bond angles



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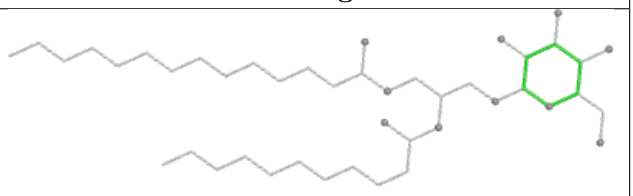
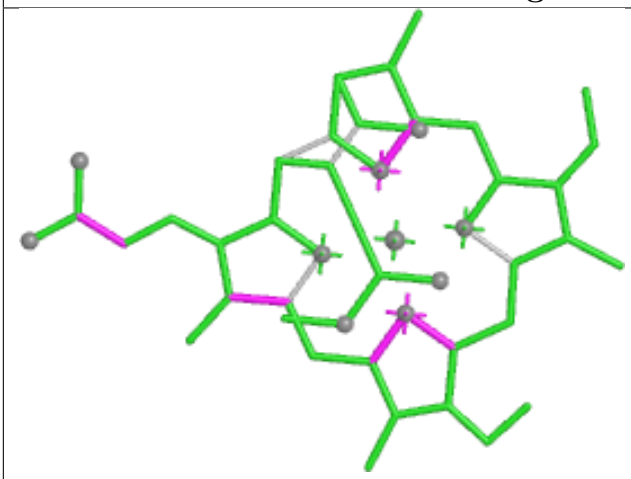


Rings

Ligand KC1 P 211



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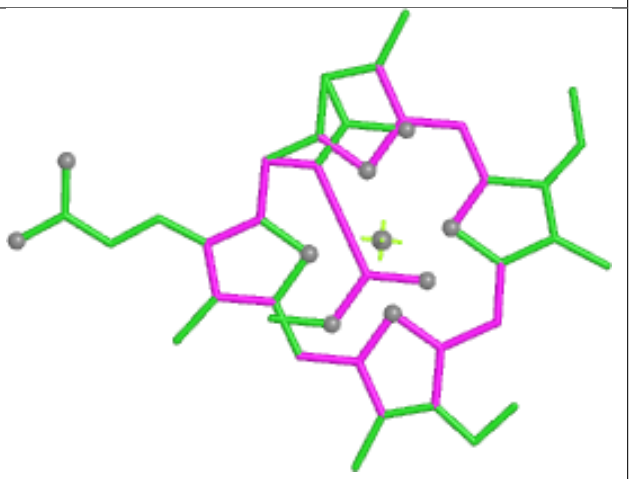
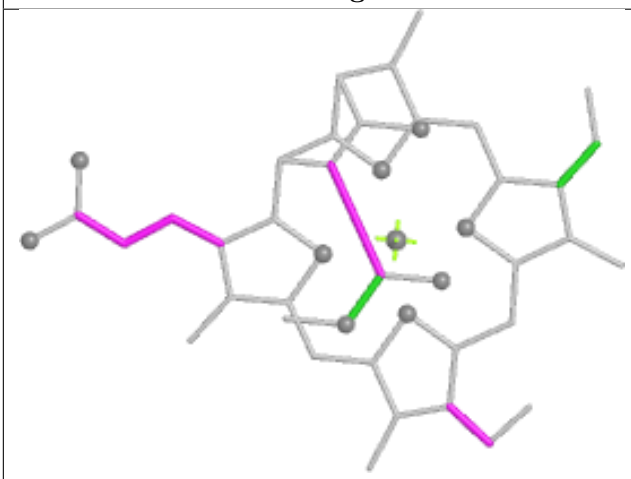


Bond angles



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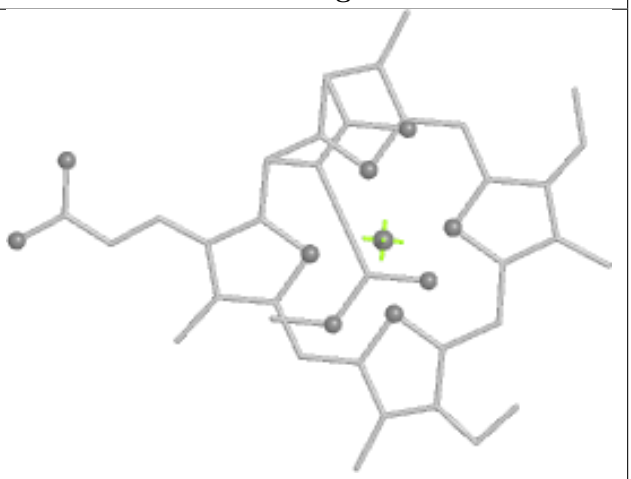
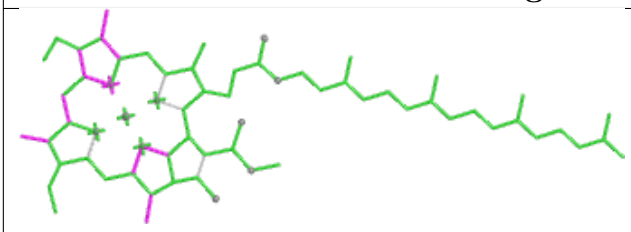


Rings

Ligand CLA E 311



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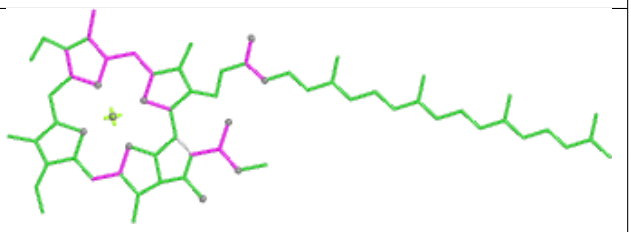
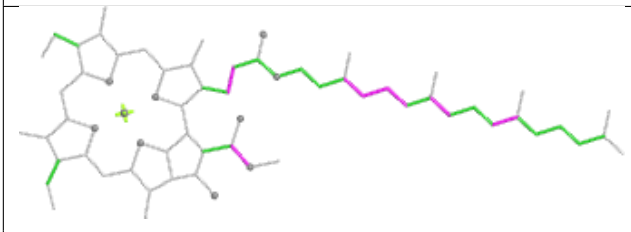


Bond angles



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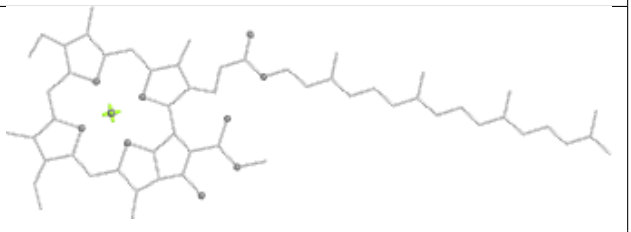
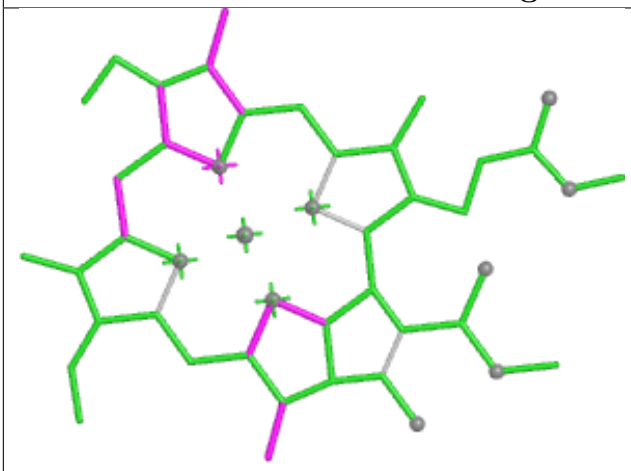


Rings

Ligand CLA M 309



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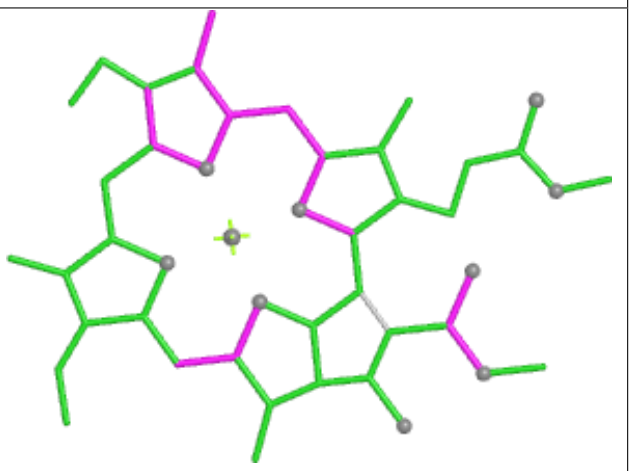
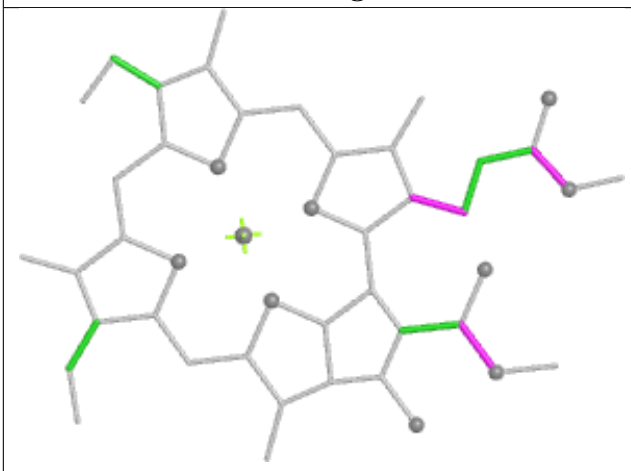


Bond angles



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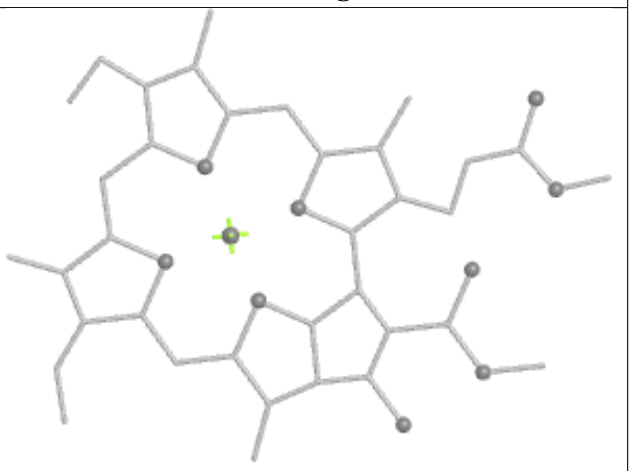
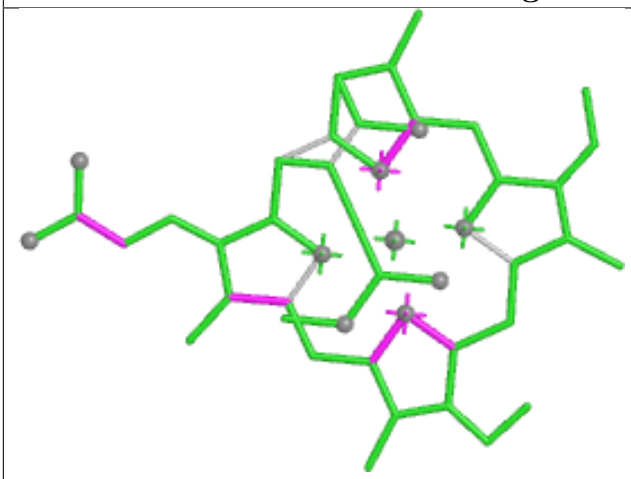


Rings

Ligand KC1 M 312



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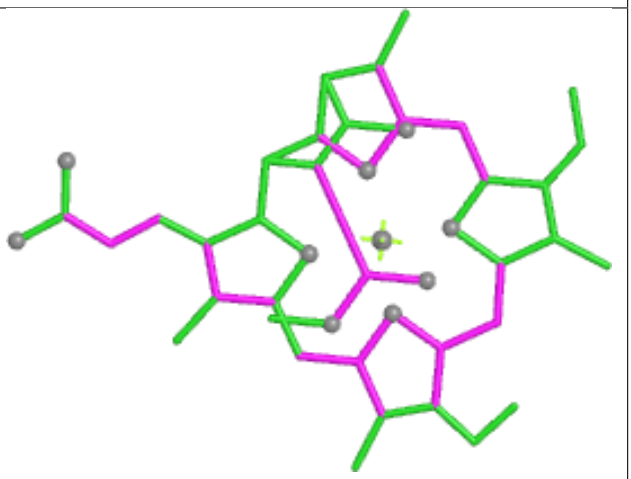
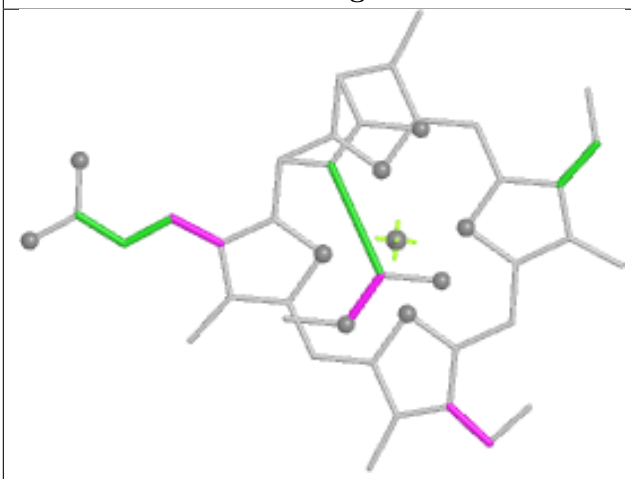


Bond angles



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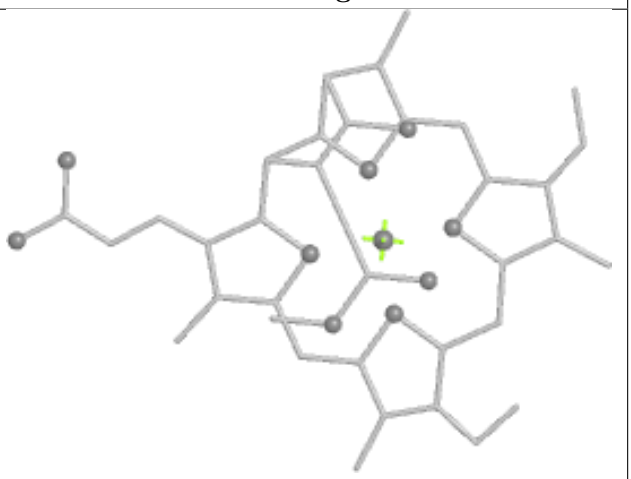


Rings

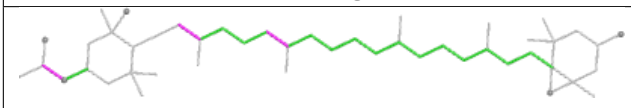
Ligand UIX C 306



Bond lengths



Bond angles



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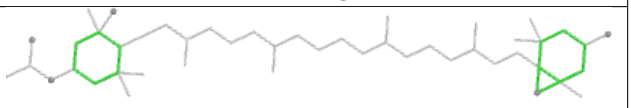
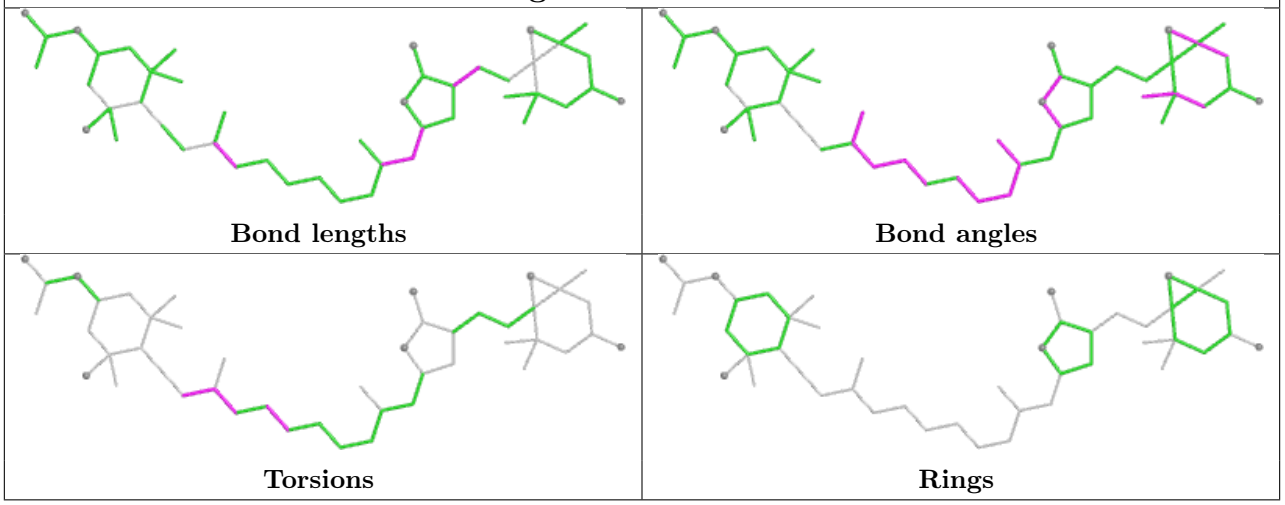
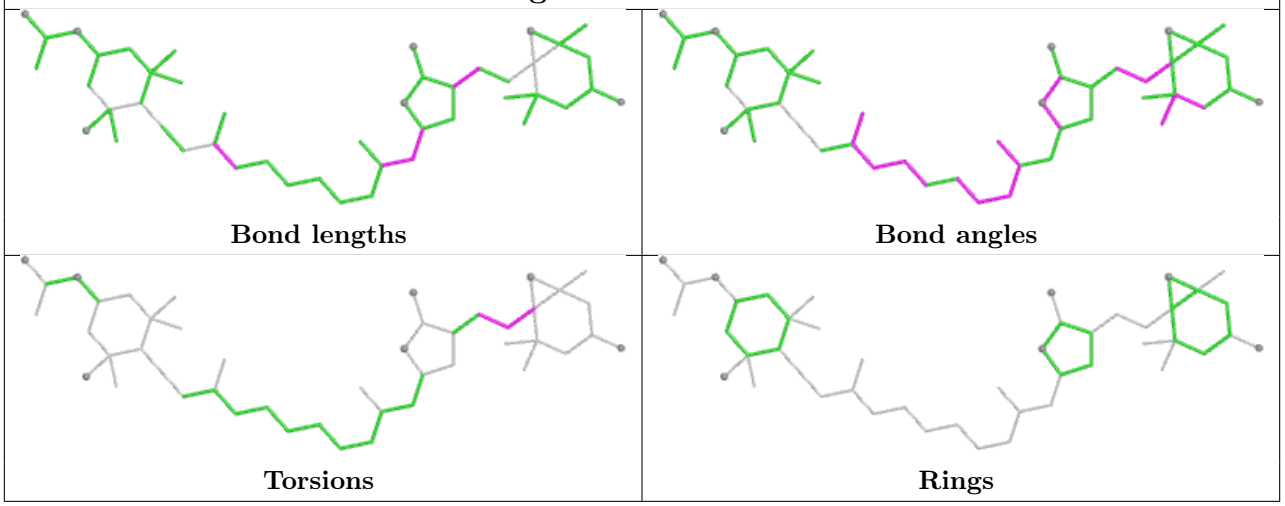


Rings

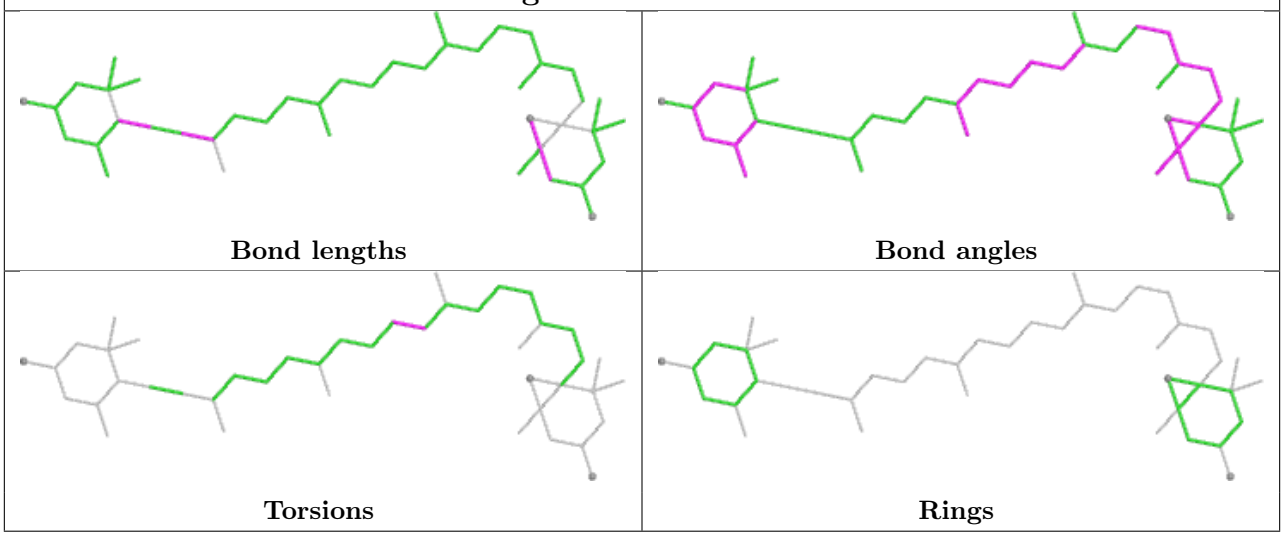
Ligand PID D 305



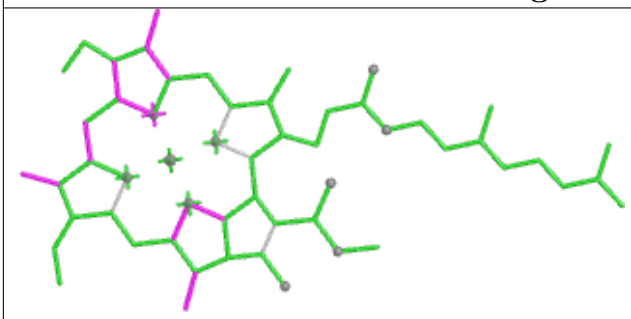
Ligand PID O 307



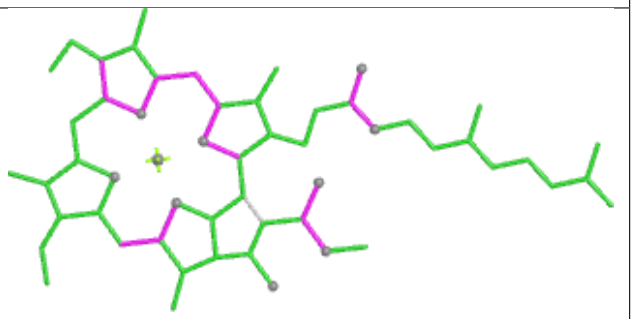
Ligand DD6 M 302



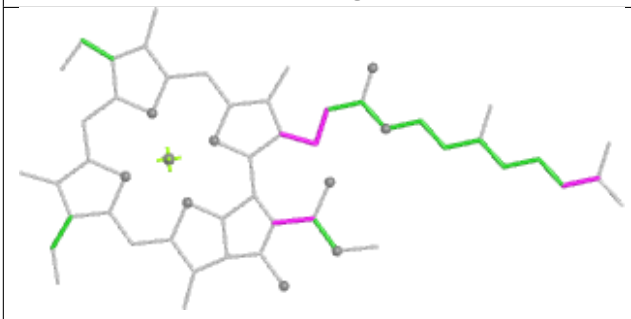
Ligand CLA I 214



Bond lengths



Bond angles



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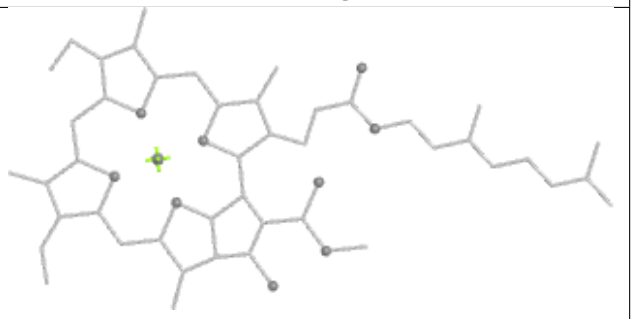
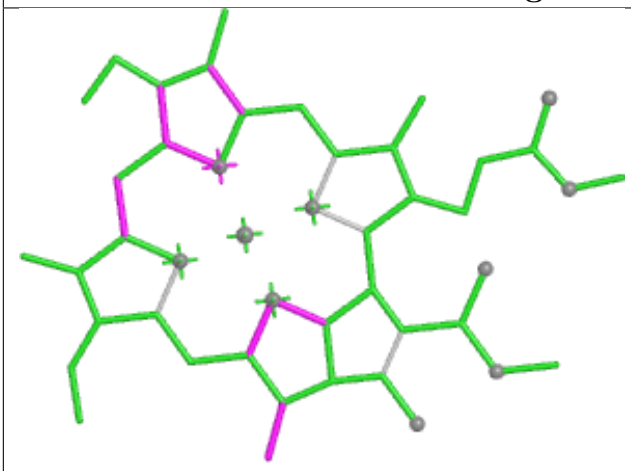


Rings

Ligand CLA E 310



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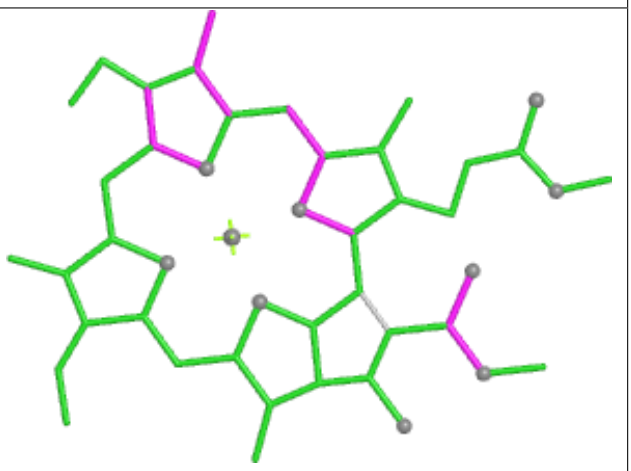
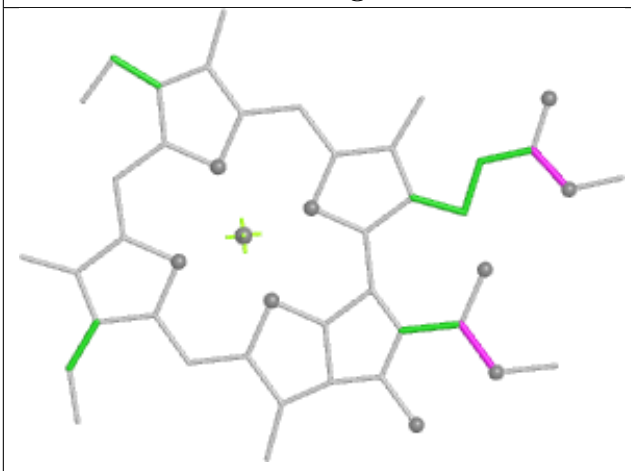


Bond angles



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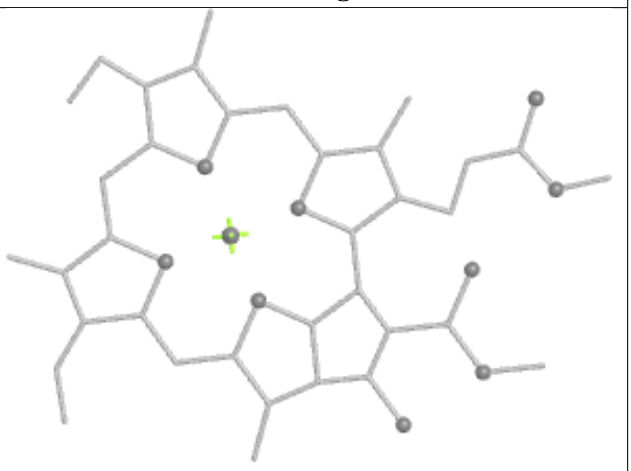
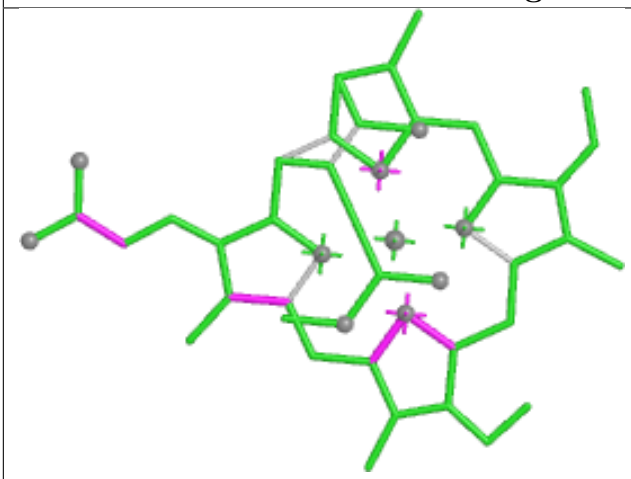


Rings

Ligand KC1 N 312



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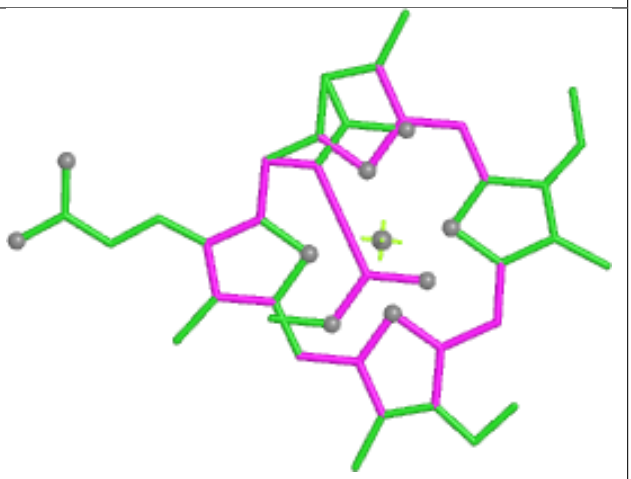
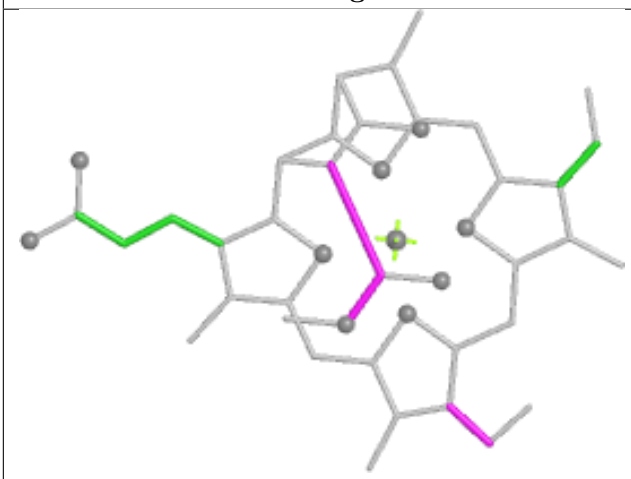


Bond angles



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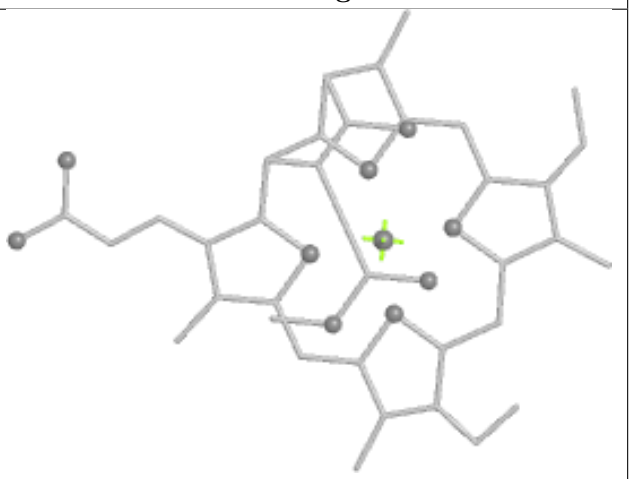
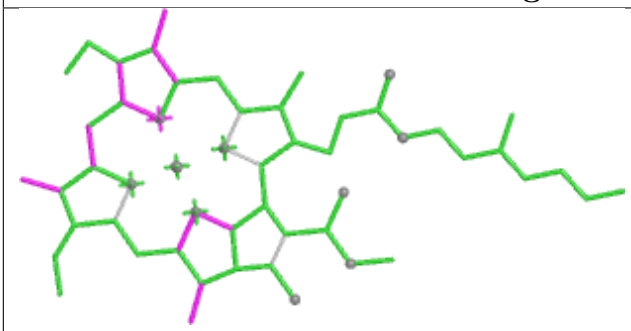
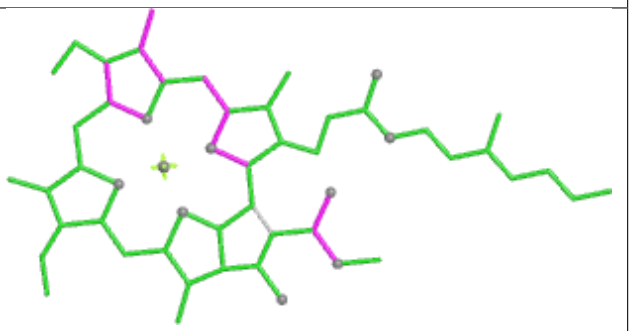


Rings

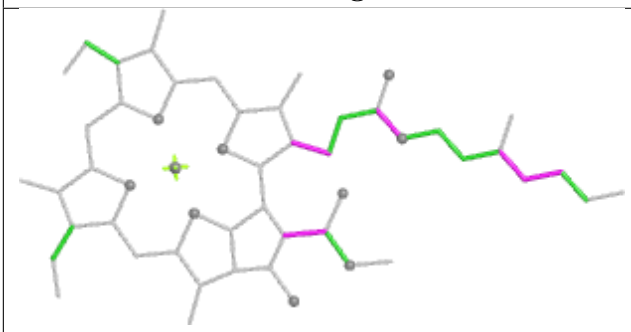
Ligand CLA G 317



Bond lengths



Bond angles



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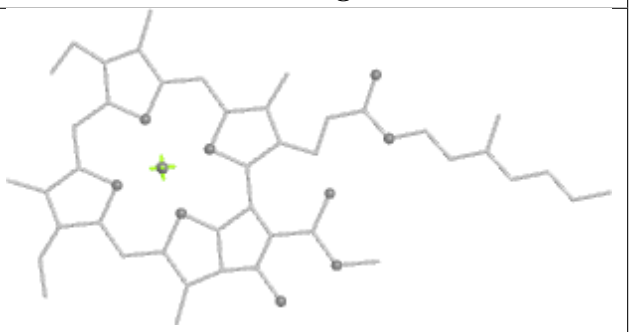
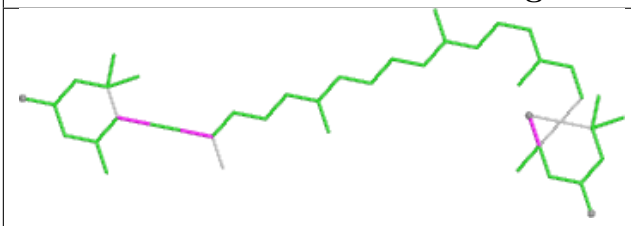


Rings

Ligand DD6 B 303



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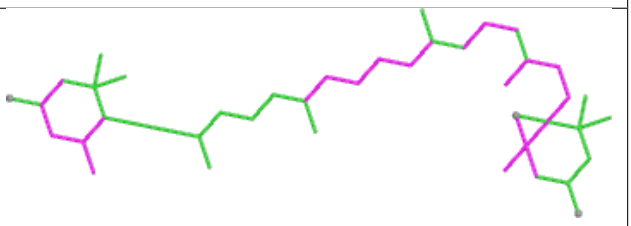
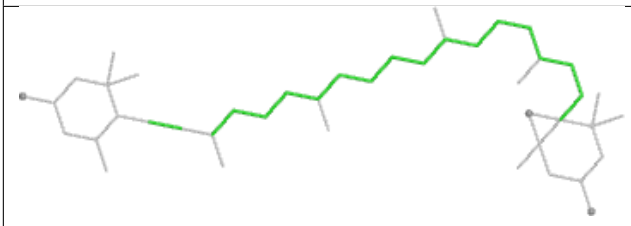


Bond angles

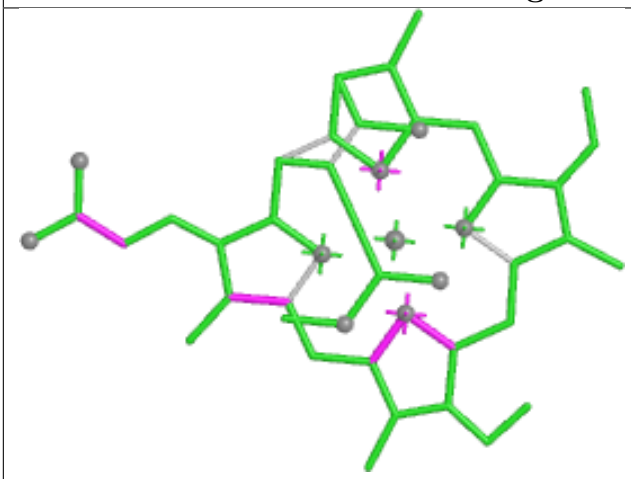


Torsions



Rings

Ligand KC1 T 312



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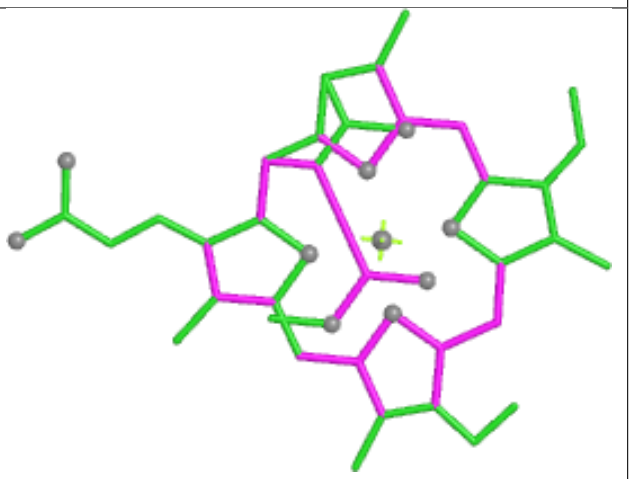

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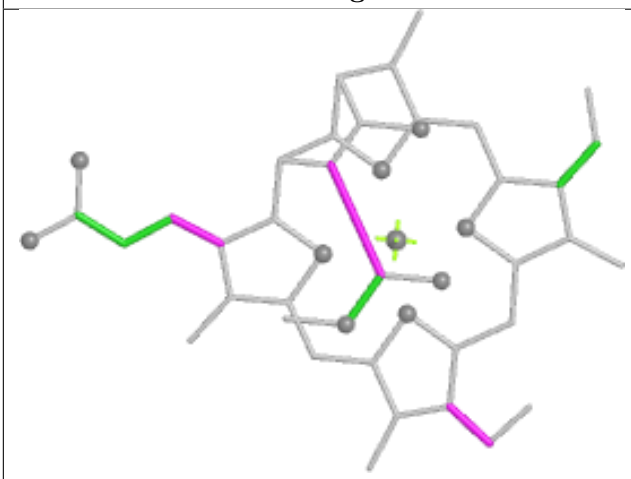
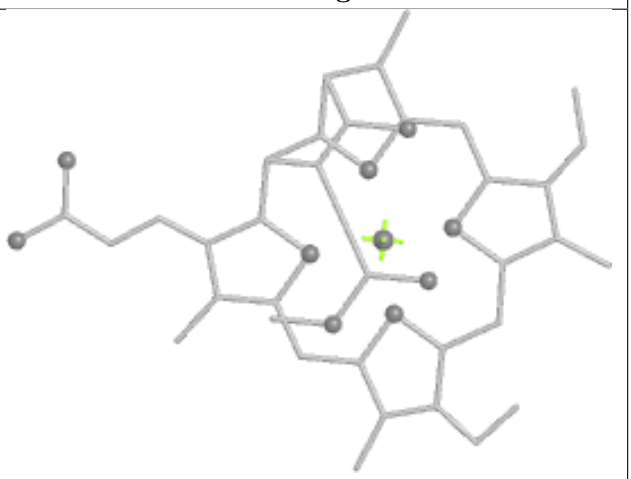
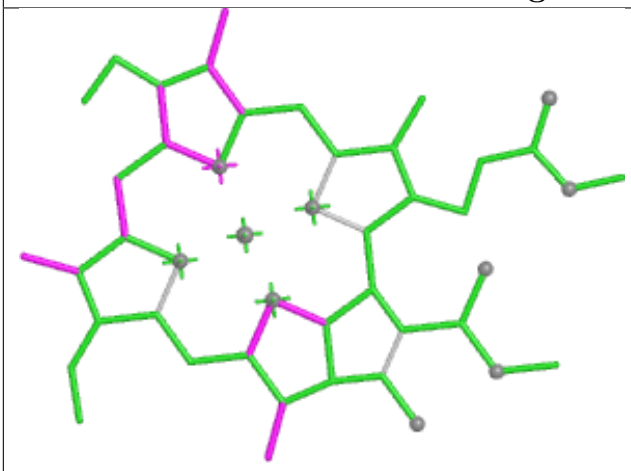


Torsions



Rings

Ligand CLA a 816



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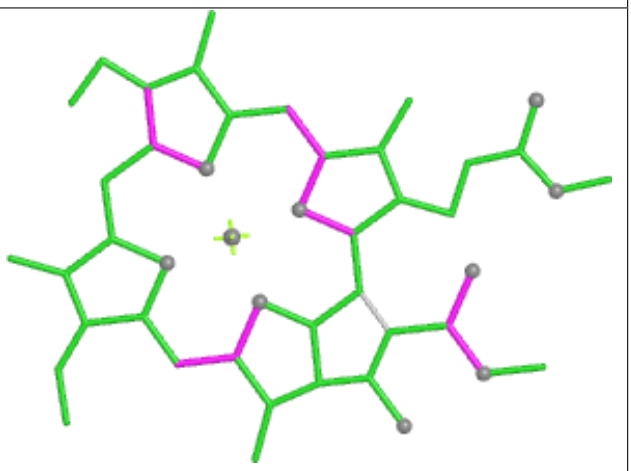

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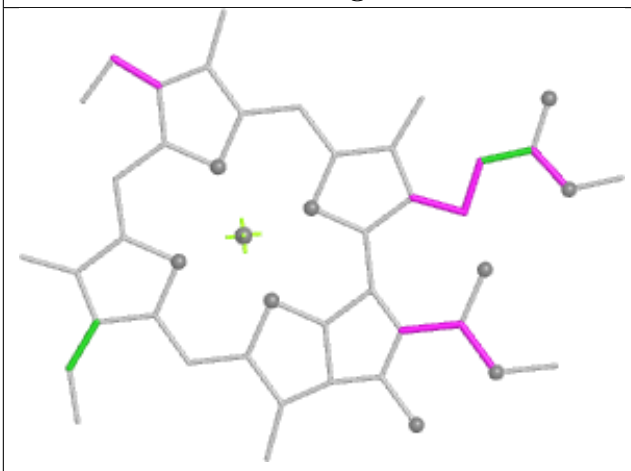

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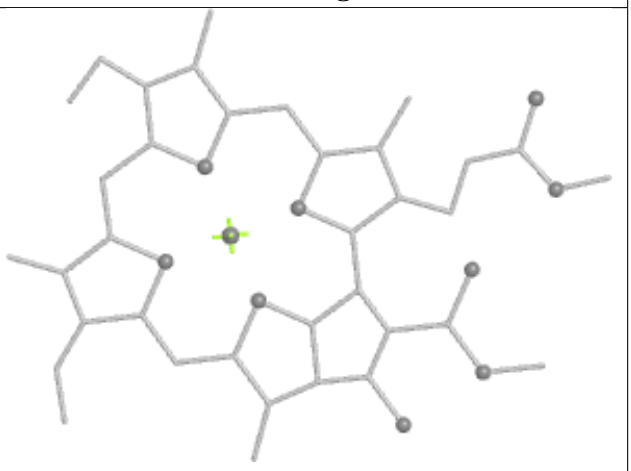
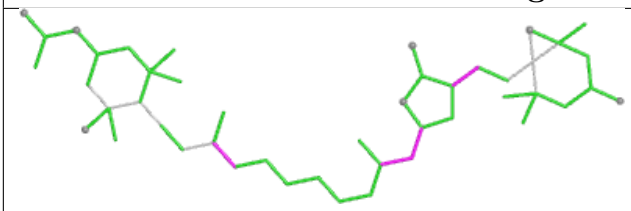


Rings

Ligand PID G 310



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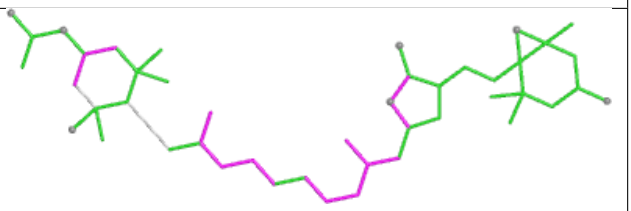

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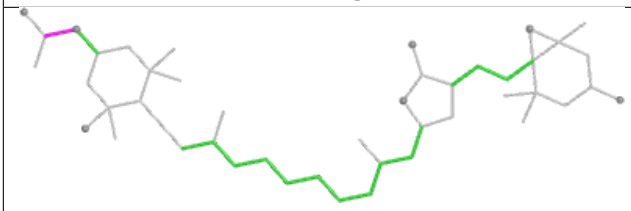

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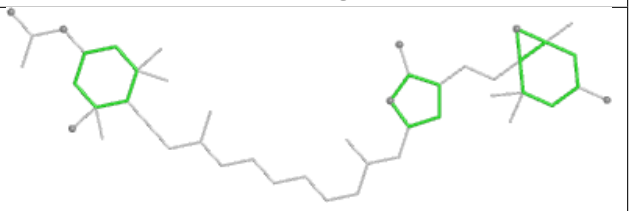
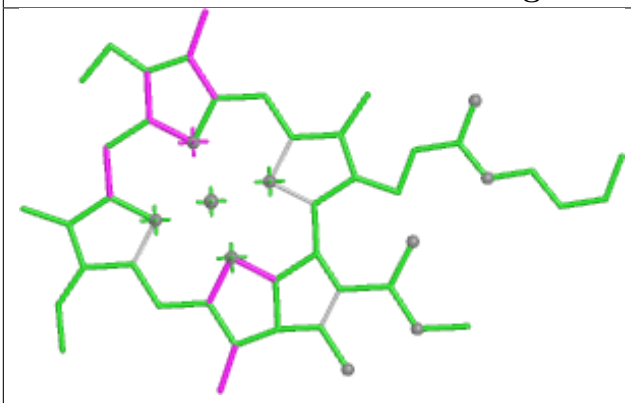


Rings

Ligand CLA K 207



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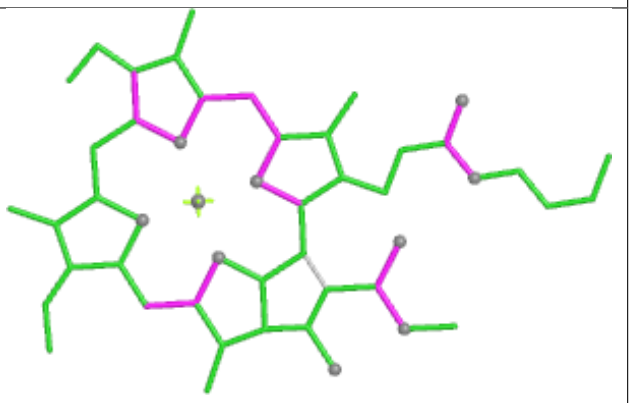

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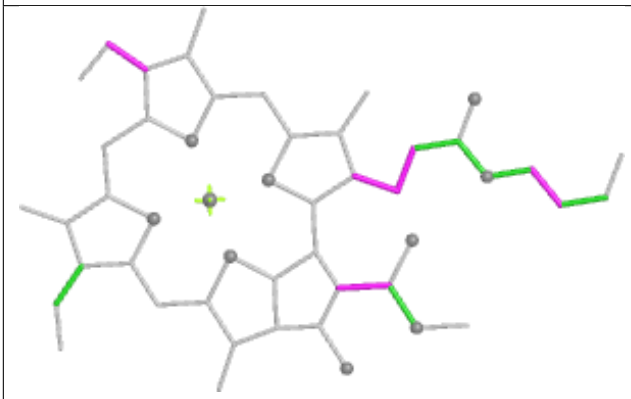

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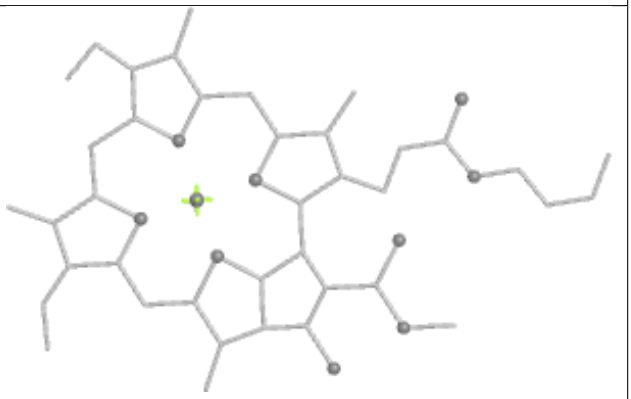
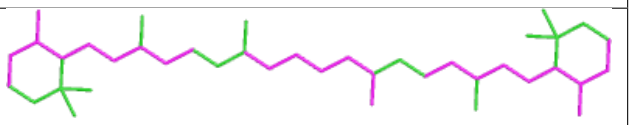


Rings

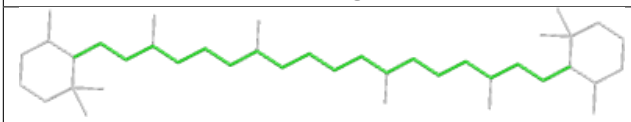
Ligand BCR a 834



Bond lengths



Bond angles



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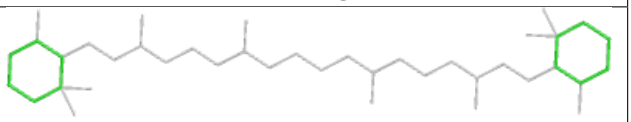
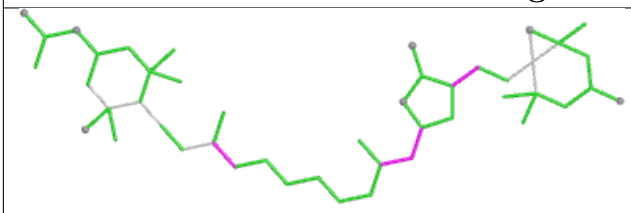


Rings

Ligand PID O 304



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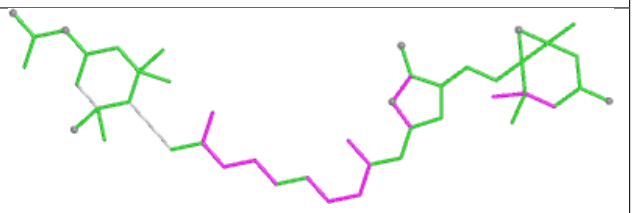
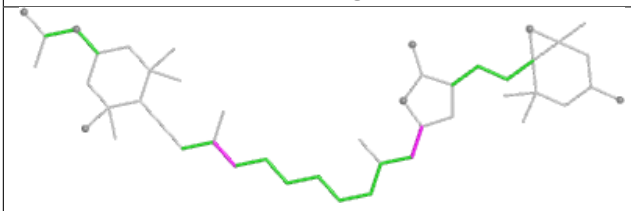


Bond angles



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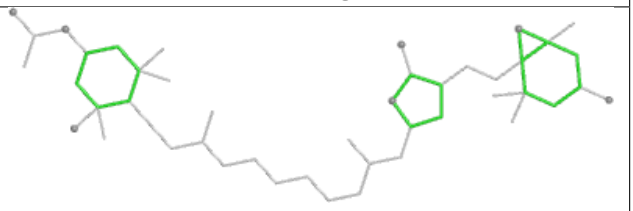
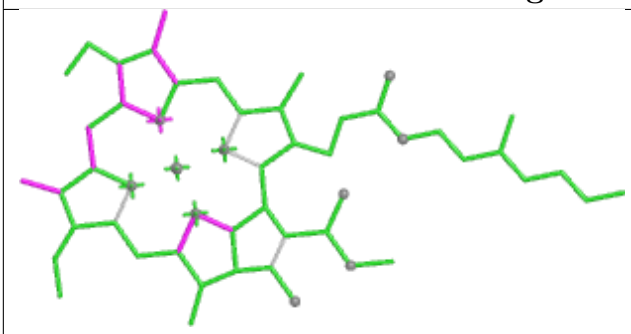


Rings

Ligand CLA L 313



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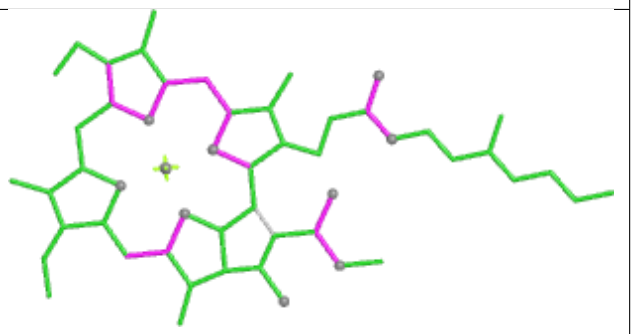
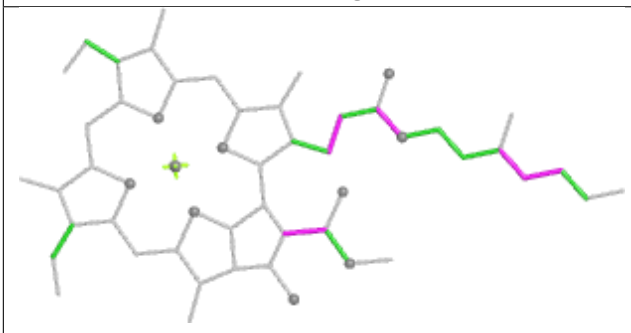


Bond angles



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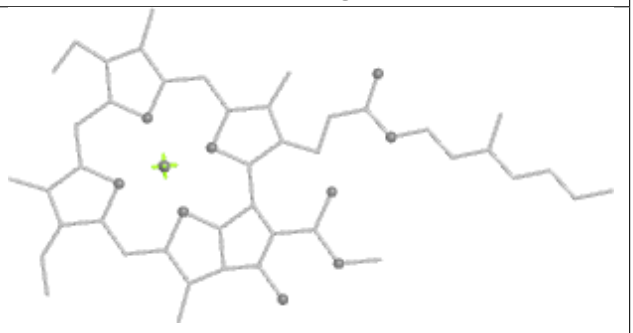
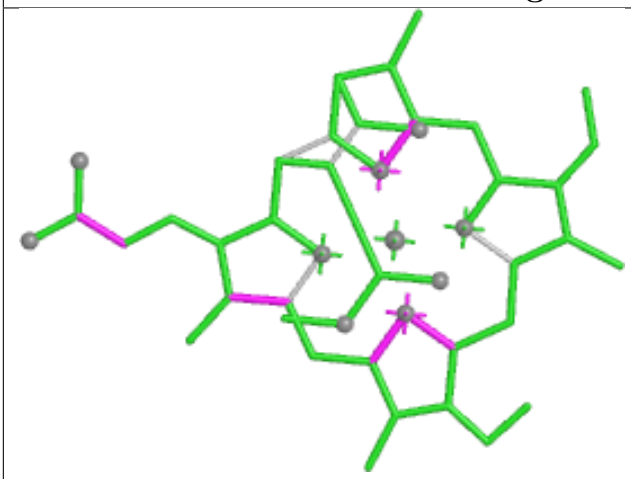


Rings

Ligand KC1 B 313



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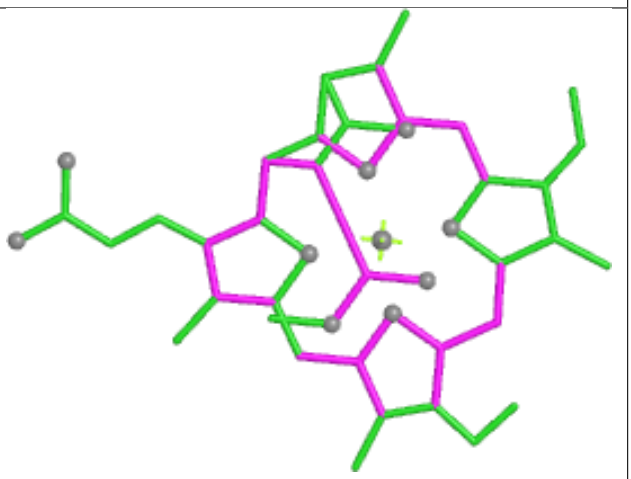
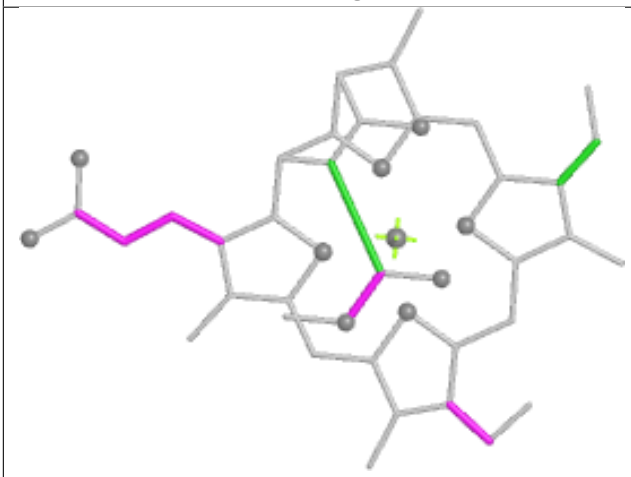


Bond angles



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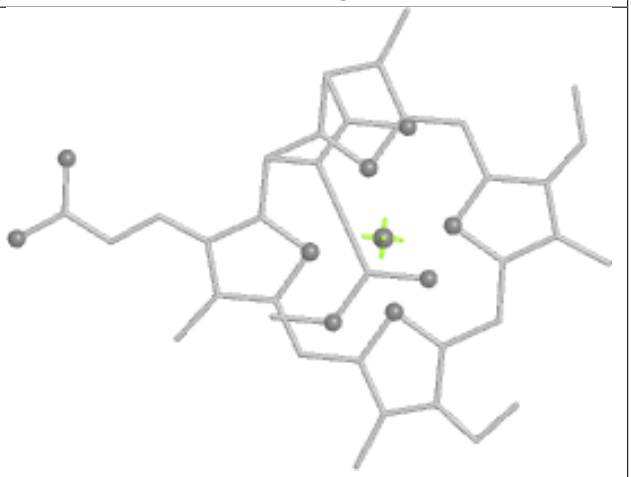
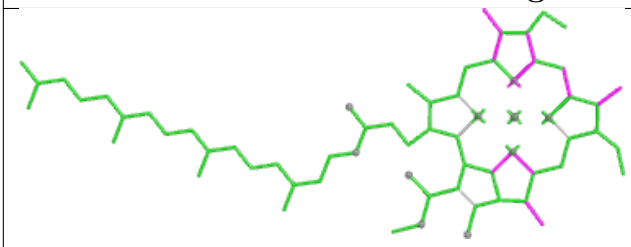


Rings

Ligand CLA b 704



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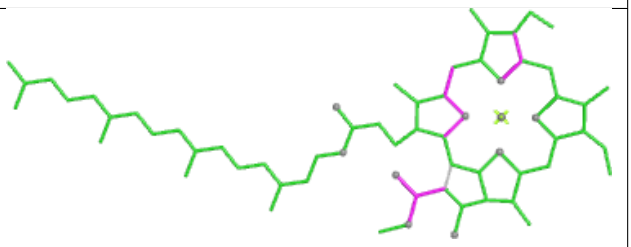
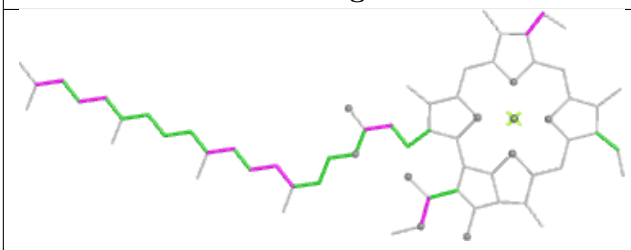


Bond angles



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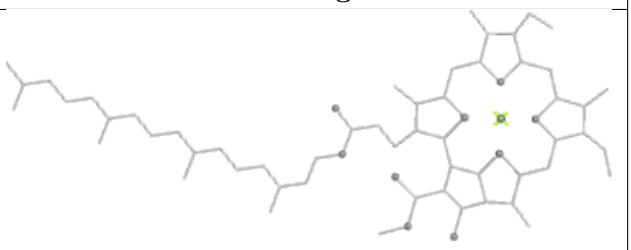
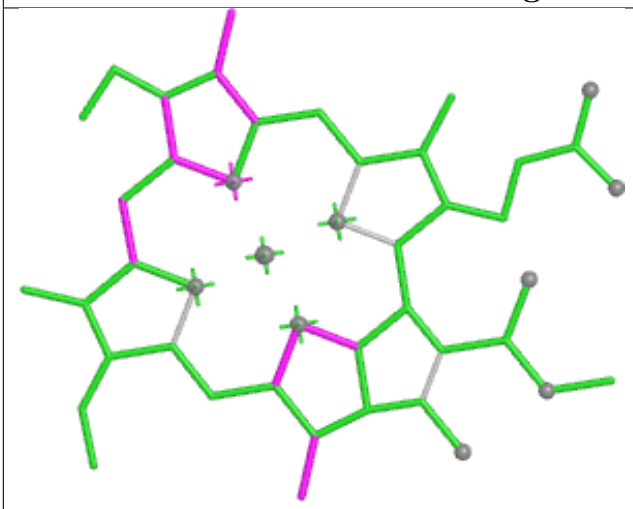


Rings

Ligand CLA K 218



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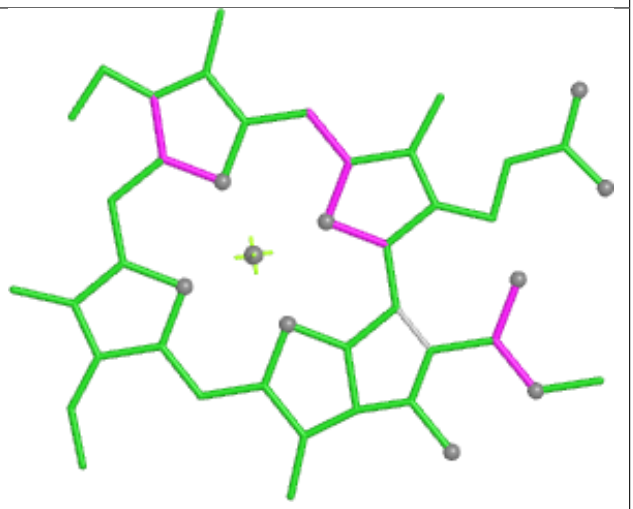
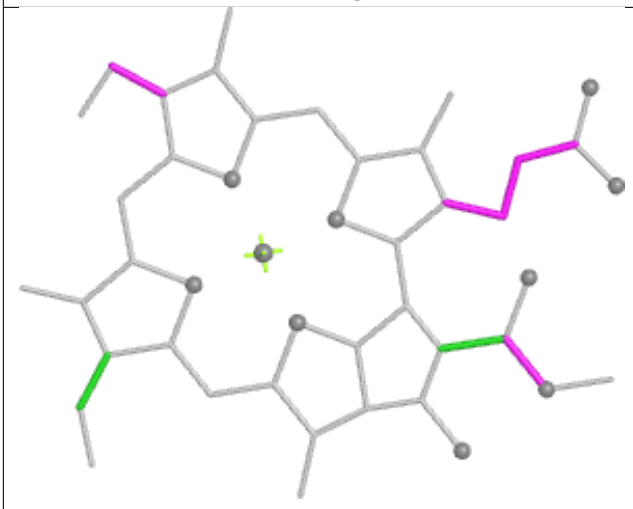


Bond angles

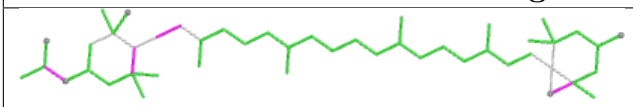


Torsions



Rings

Ligand UIX E 304



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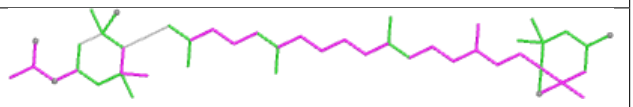
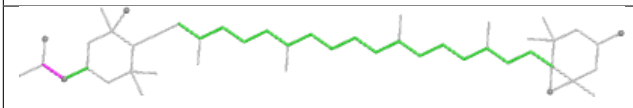


Bond angles



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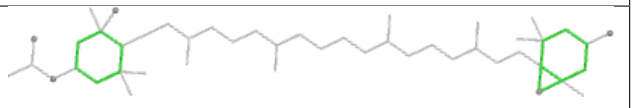
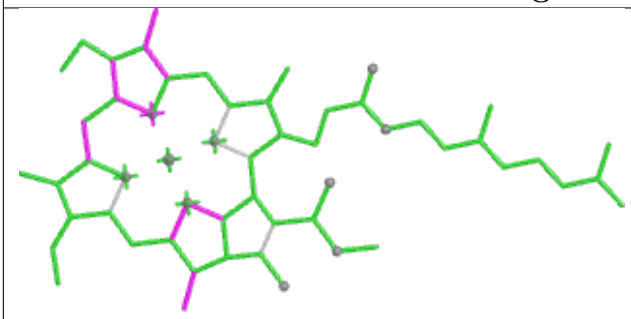


Rings

Ligand CLA i 203



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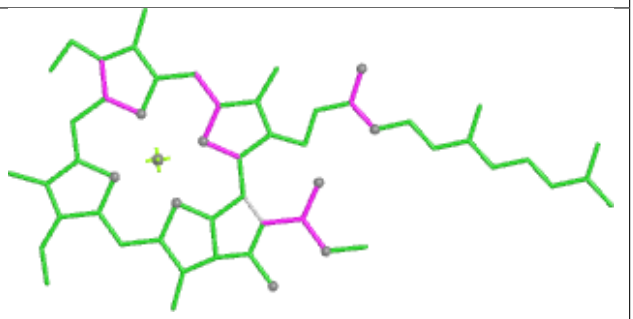
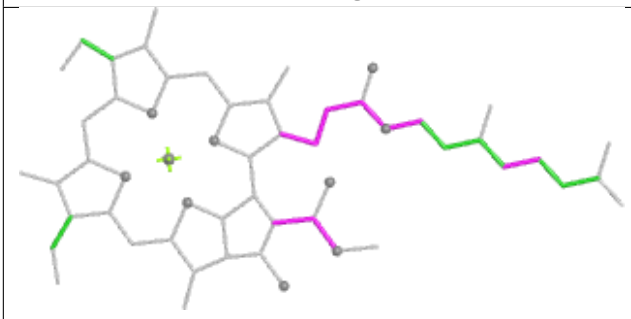


Bond angles



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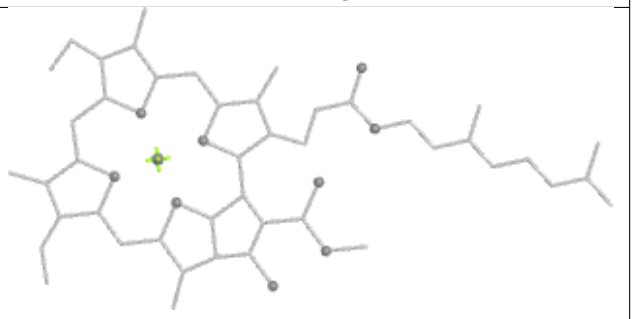
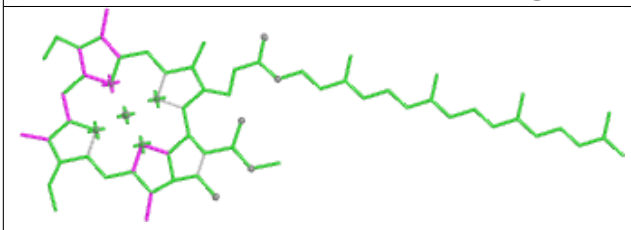


Rings

Ligand CLA a 829



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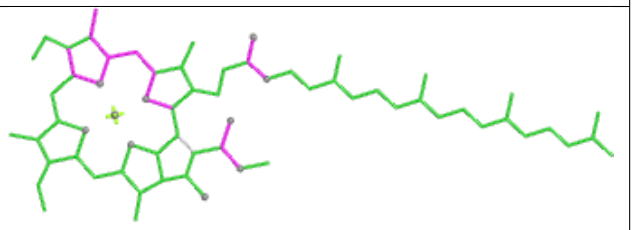
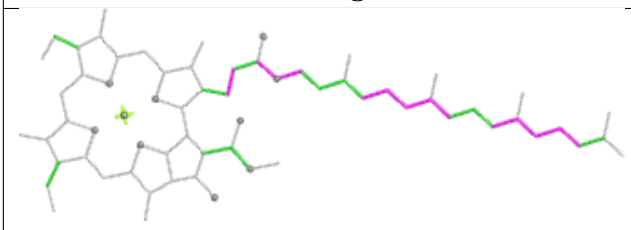


Bond angles



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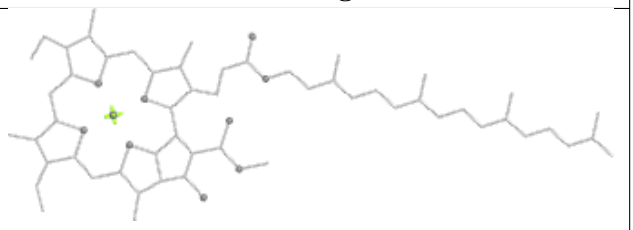
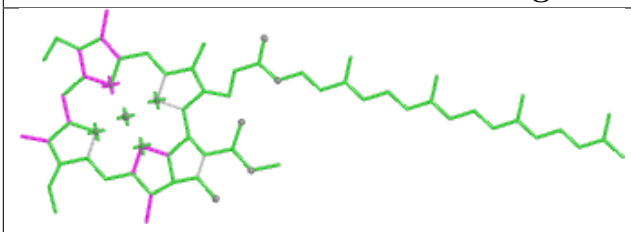
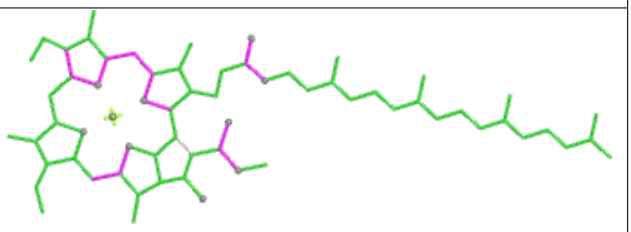


Rings

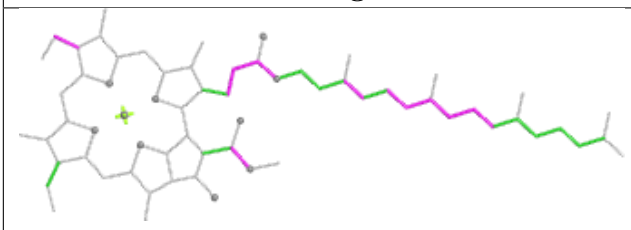
Ligand CLA l 503



Bond lengths



Bond angles



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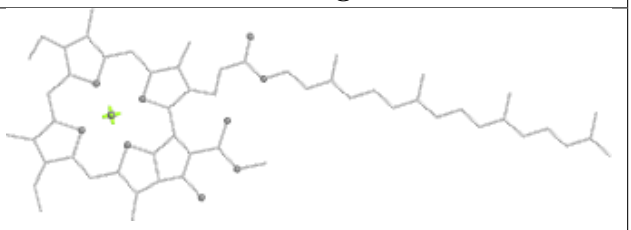
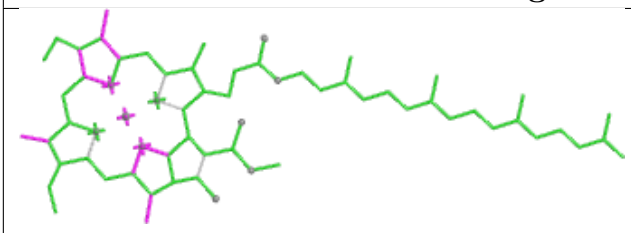


Rings

Ligand CLA a 801



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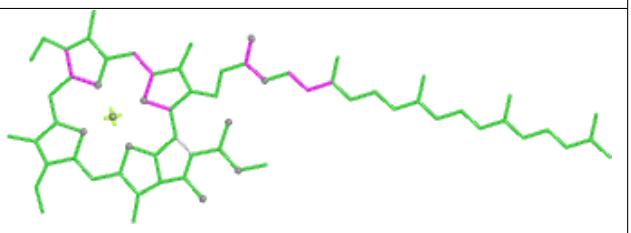
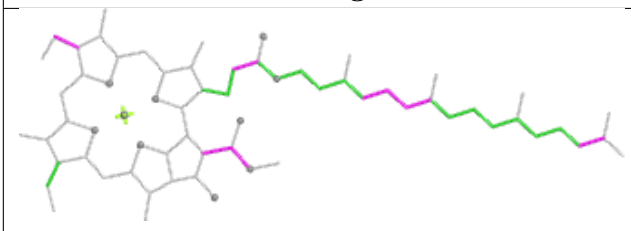
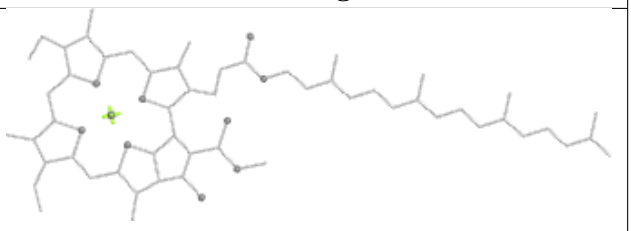


Bond angles

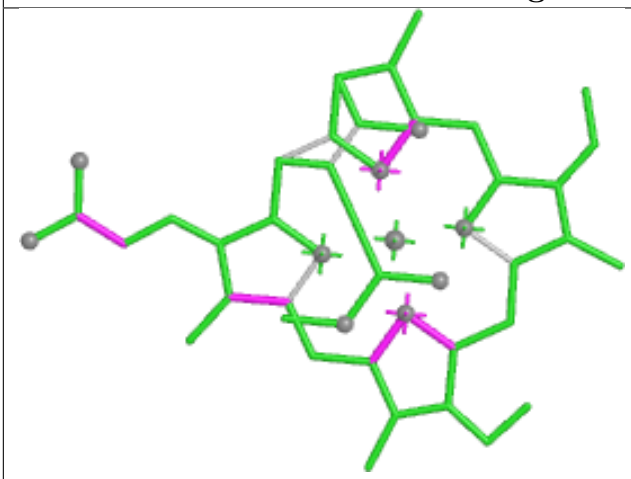


Torsions

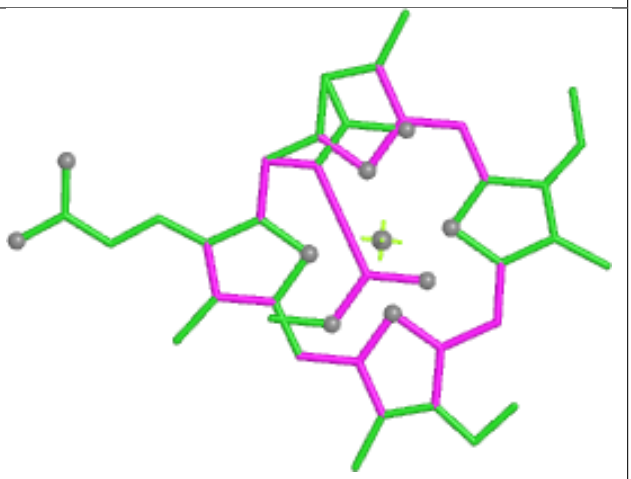


Rings

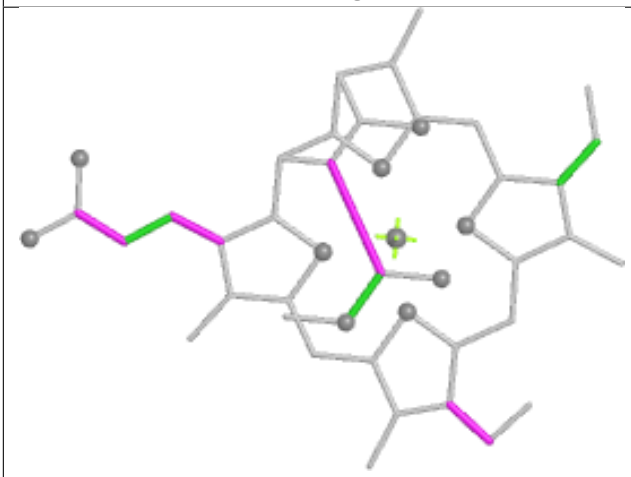
Ligand KC1 F 309



Bond lengths



Bond angles



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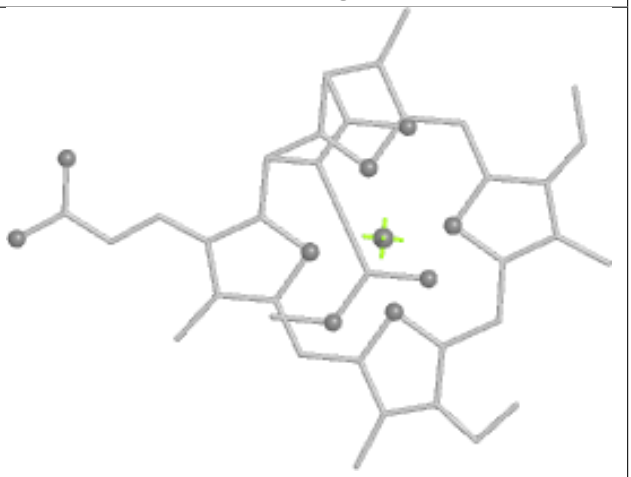
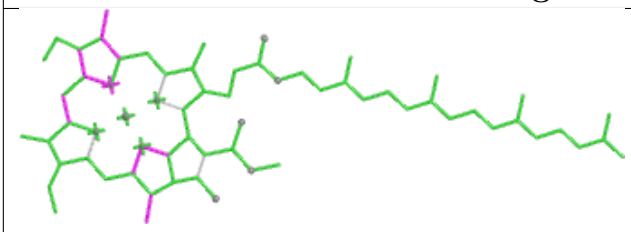


Rings

Ligand CLA i 201



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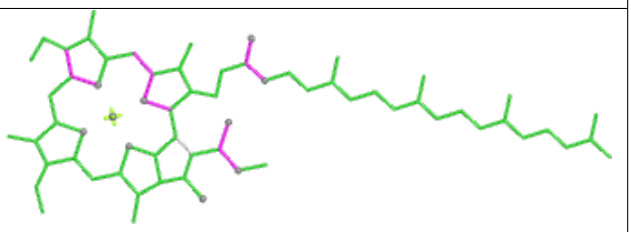
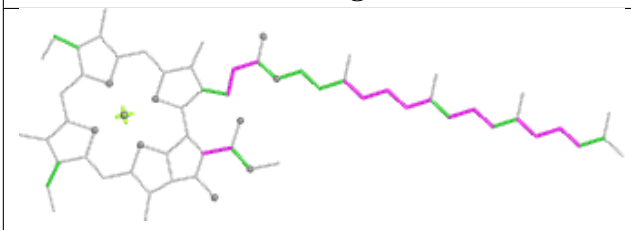


Bond angles



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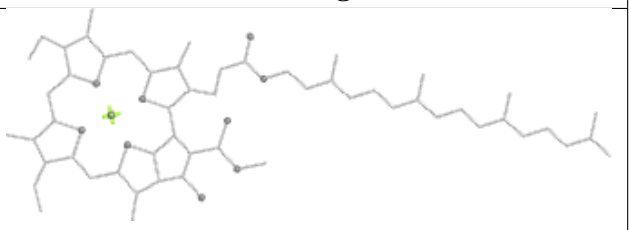
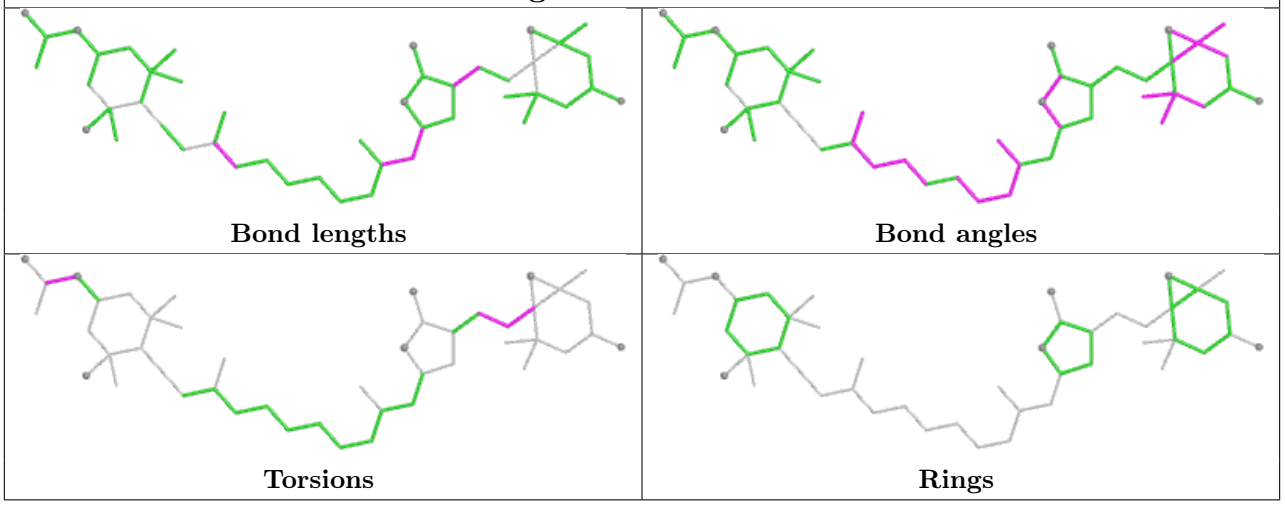
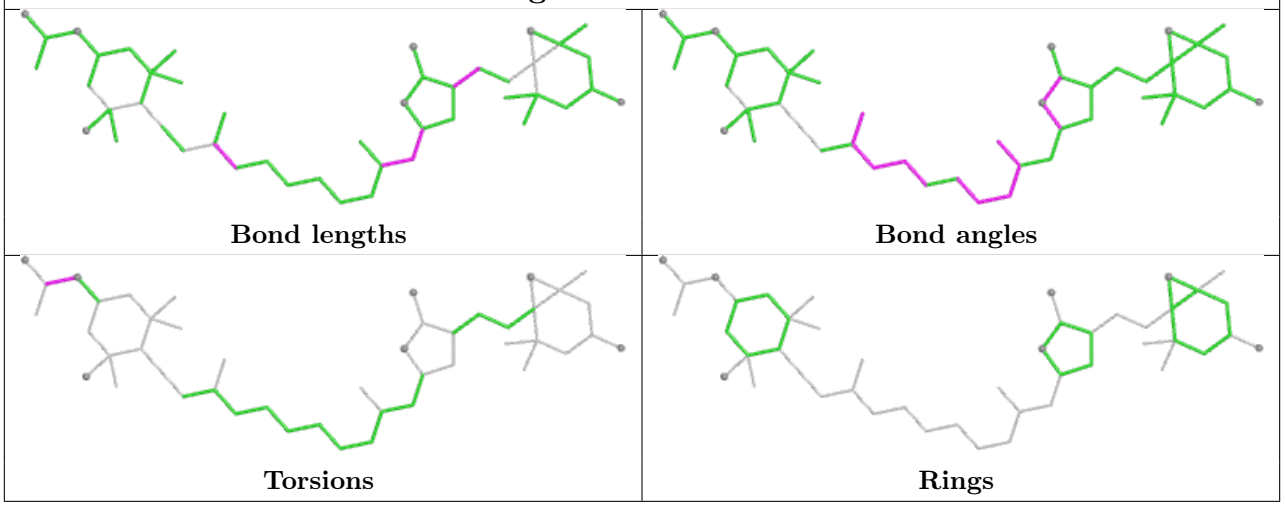


Rings

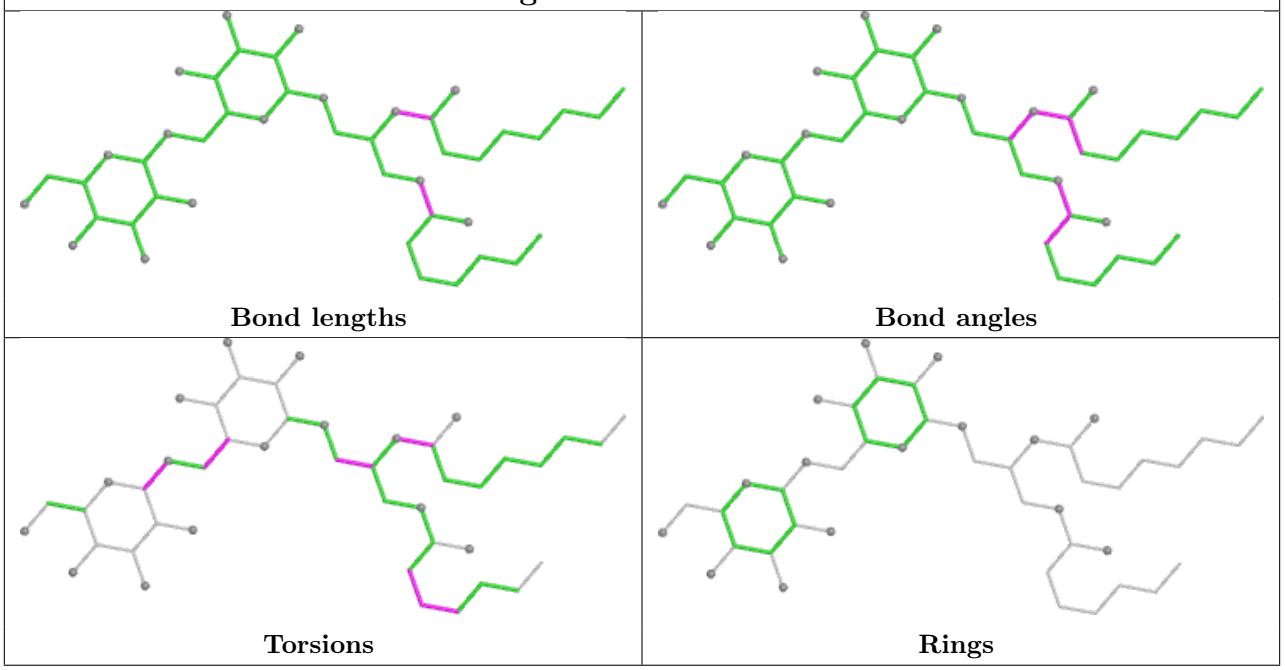
Ligand PID N 307



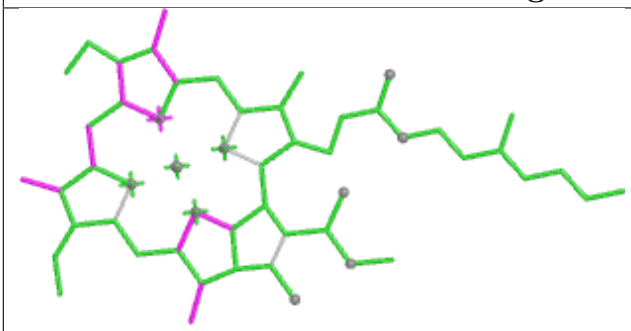
Ligand PID H 301



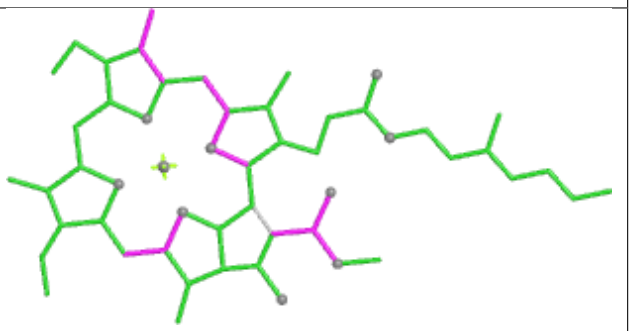
Ligand DGD G 320



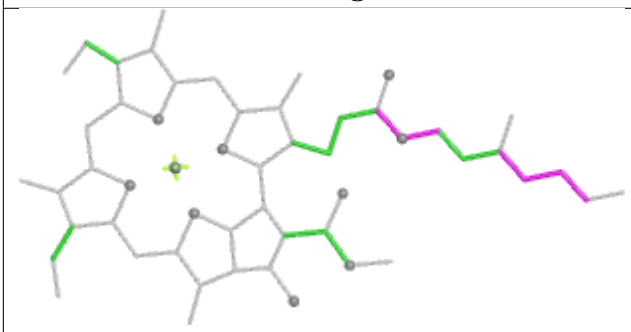
Ligand CLA b 716



Bond lengths



Bond angles



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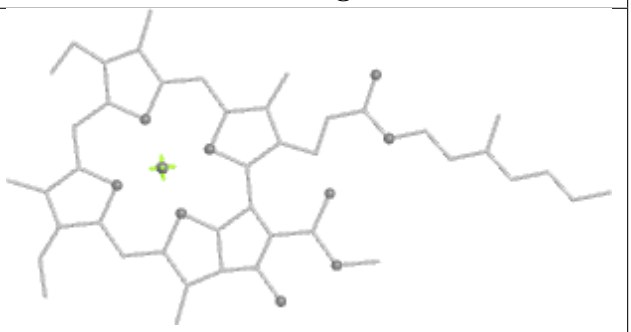
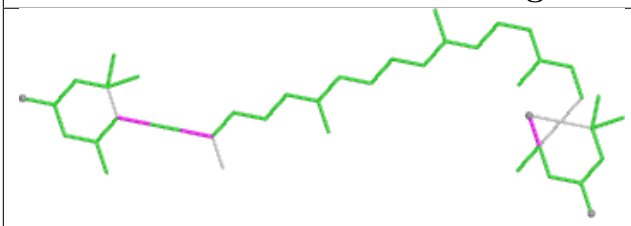


Rings

Ligand DD6 E 302



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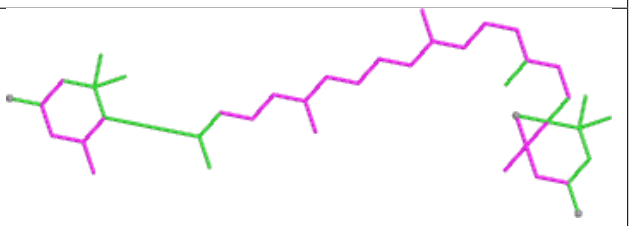


Bond angles

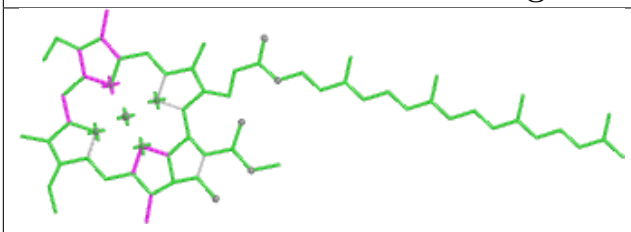


Torsions



Rings

Ligand CLA b 717



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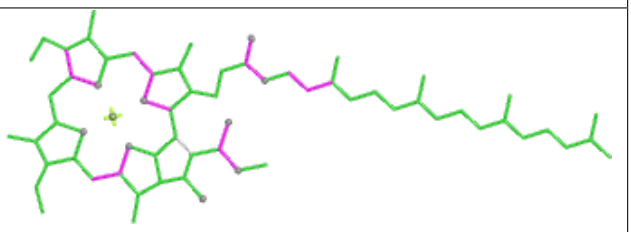
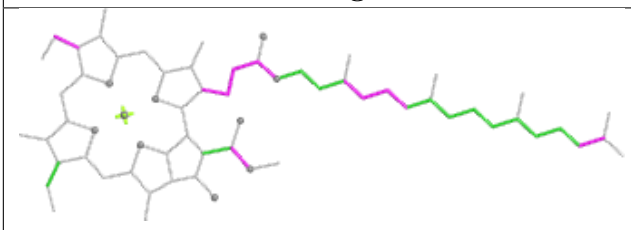


Bond angles



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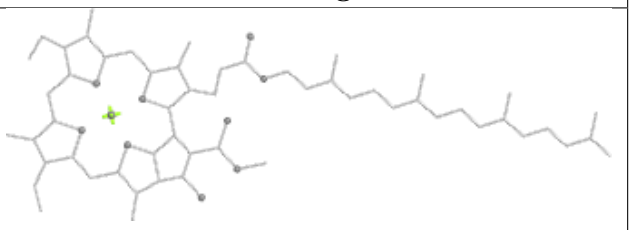
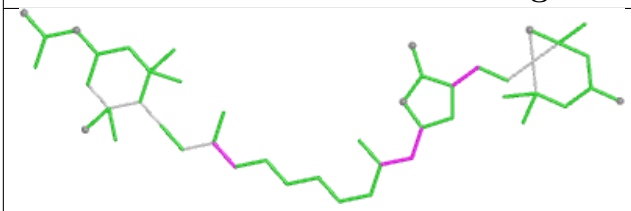


Rings

Ligand PID F 302



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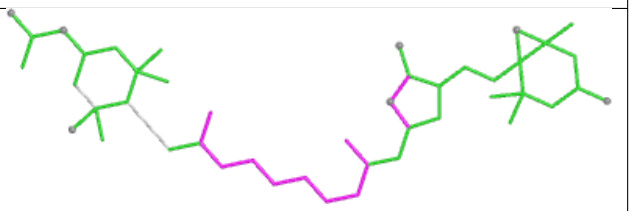
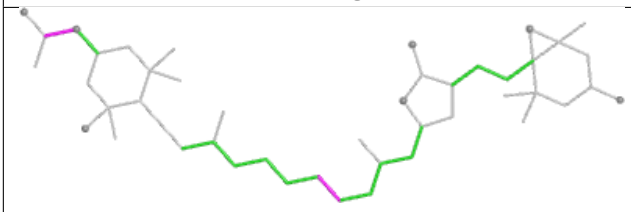


Bond angles



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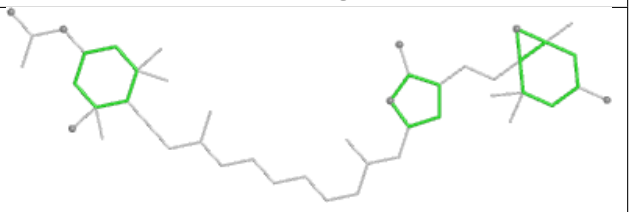
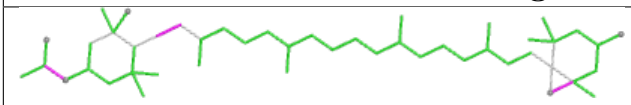


Rings

Ligand UIX F 305



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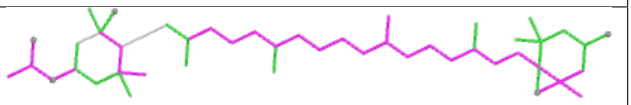
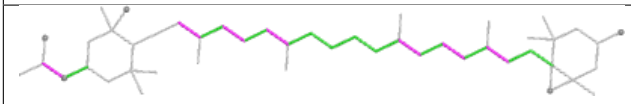


Bond angles



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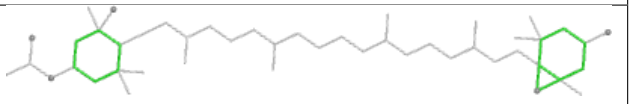
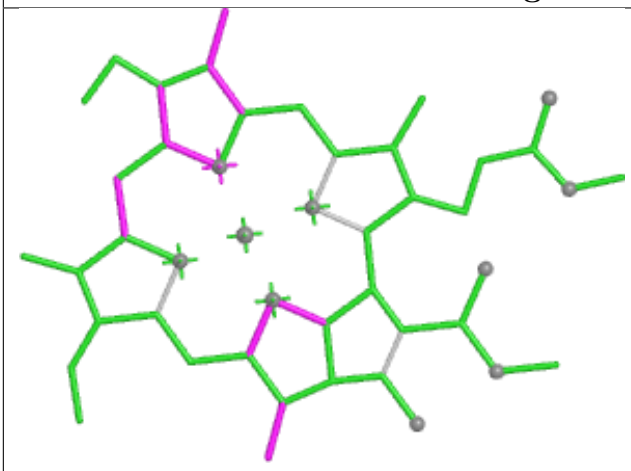


Rings

Ligand CLA Q 312



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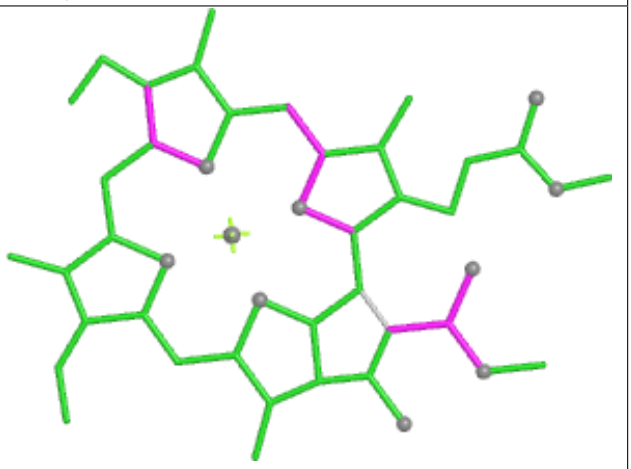
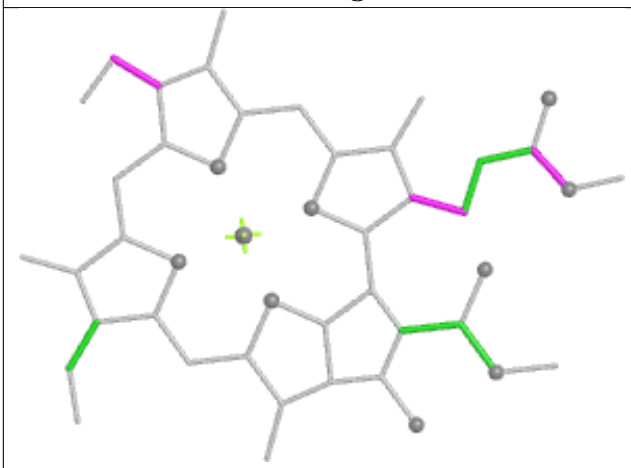


Bond angles



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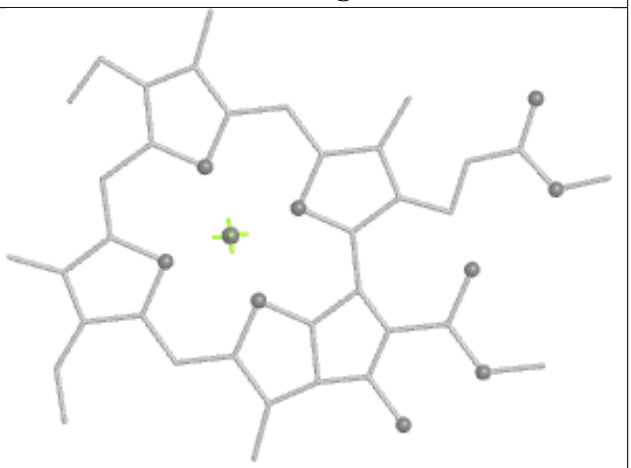
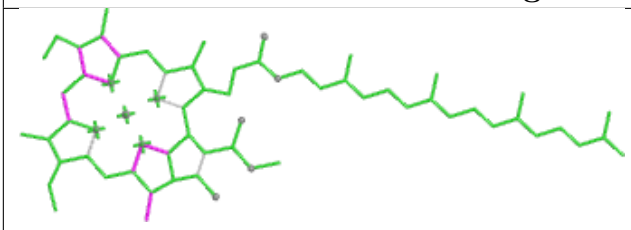


Rings

Ligand CLA N 309



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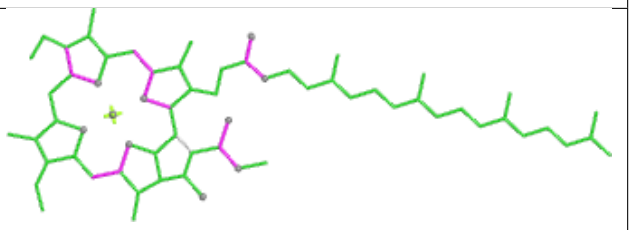
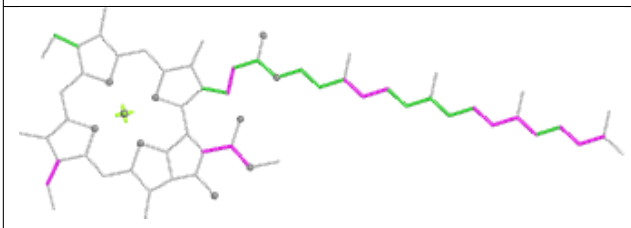


Bond angles



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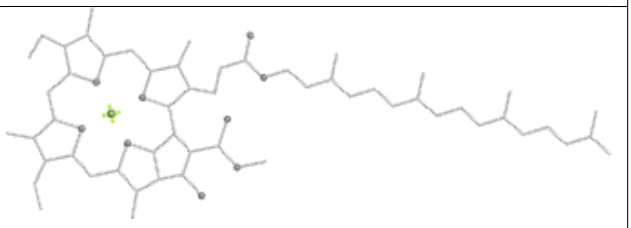
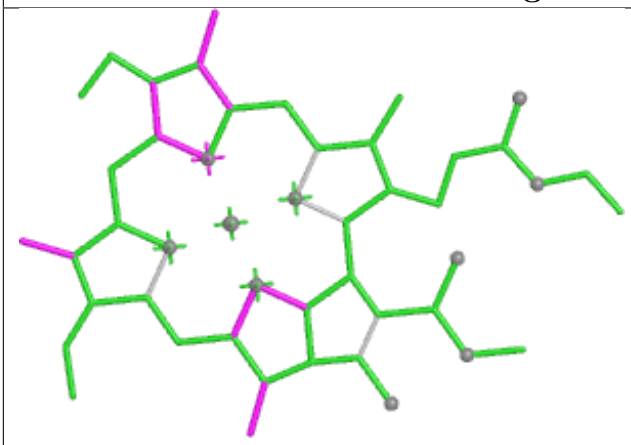


Rings

Ligand CLA A 215



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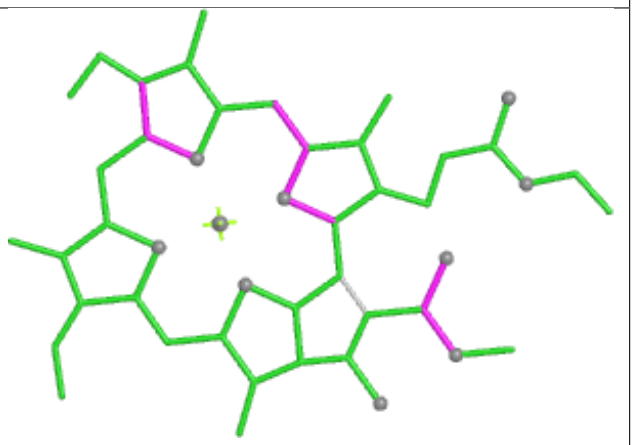
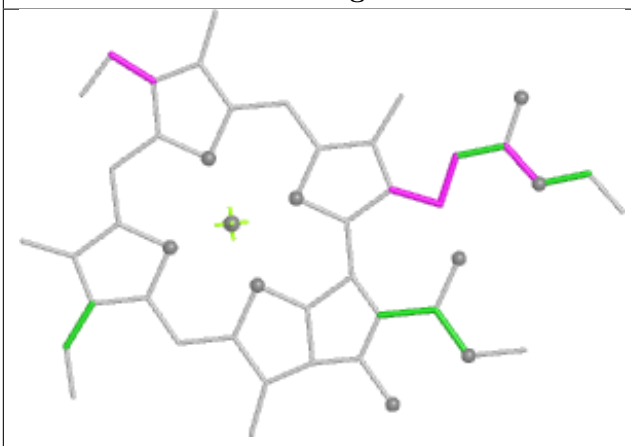


Bond angles



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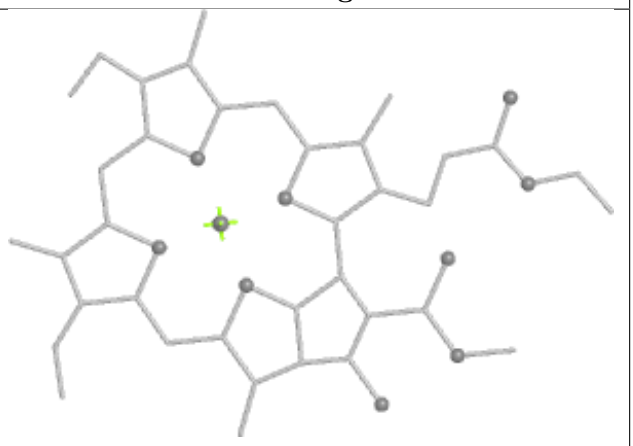
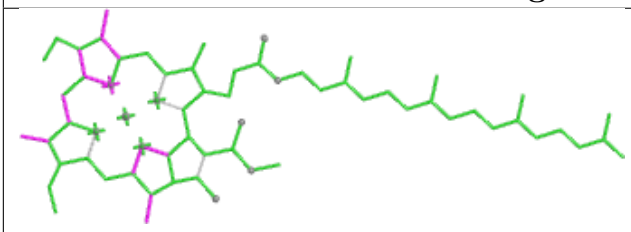


Rings

Ligand CLA a 824



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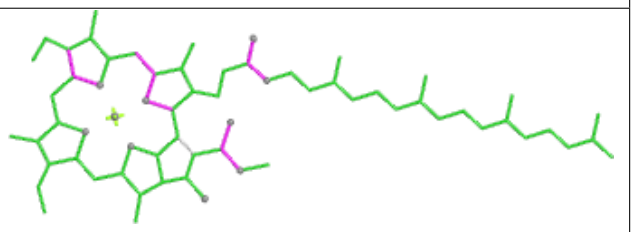
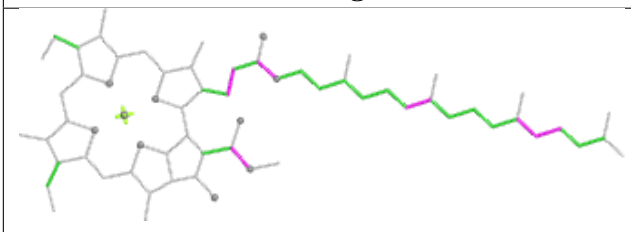


Bond angles



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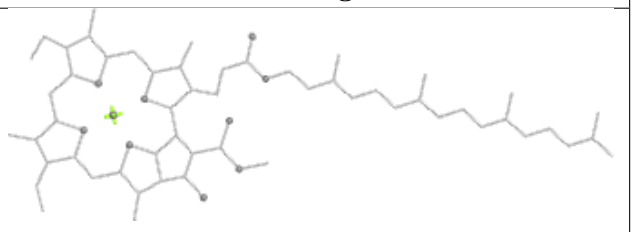
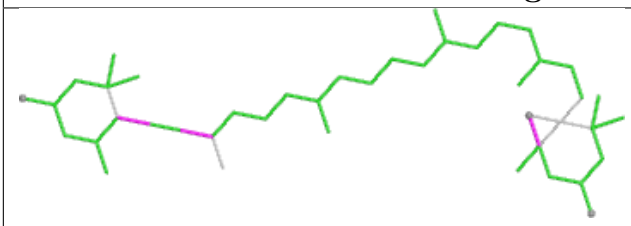


Rings

Ligand DD6 A 204



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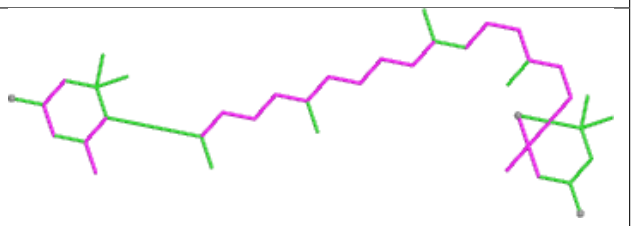
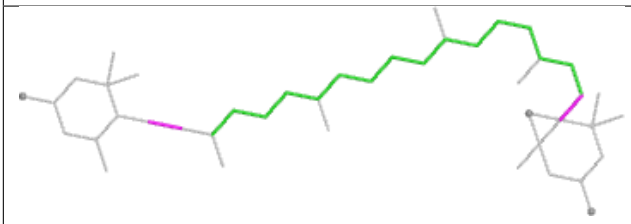


Bond angles



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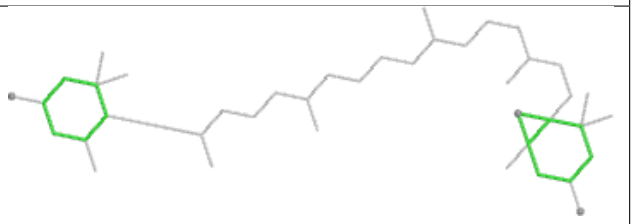
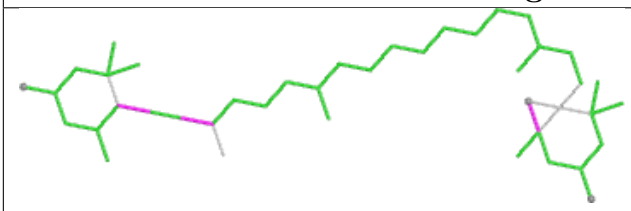


Rings

Ligand DD6 B 301



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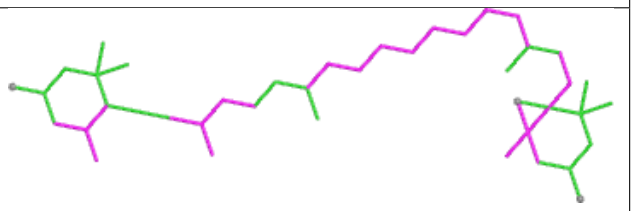
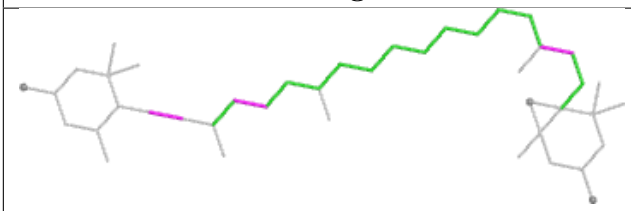


Bond angles

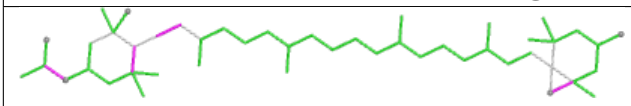


Torsions



Rings

Ligand UIX Q 305



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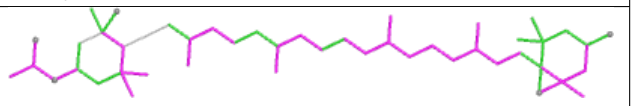
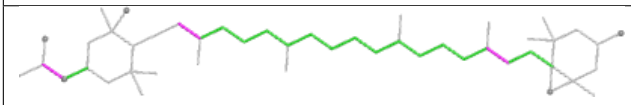


Bond angles



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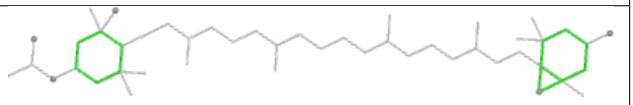
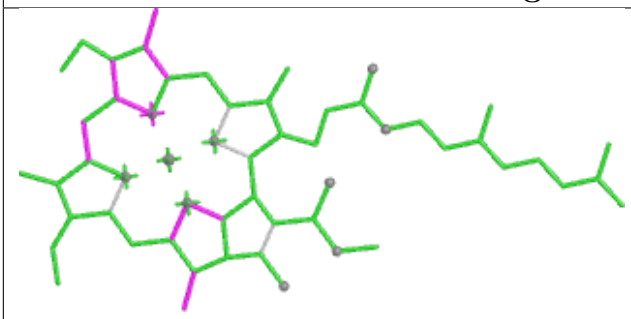
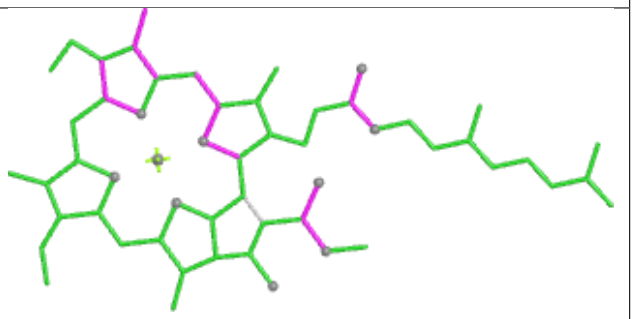


Rings

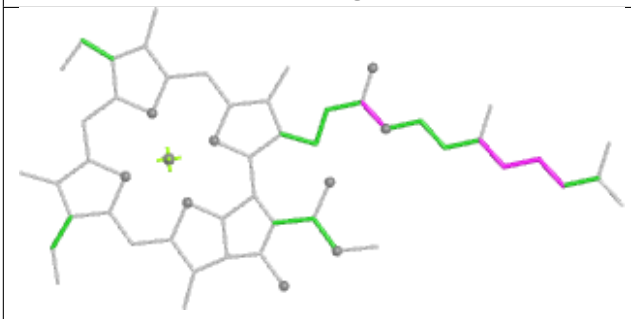
Ligand CLA A 211



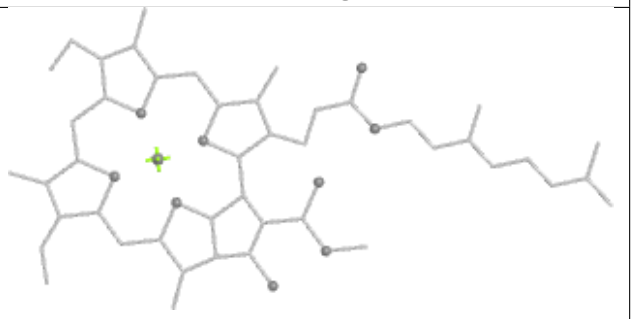
Bond lengths



Bond angles

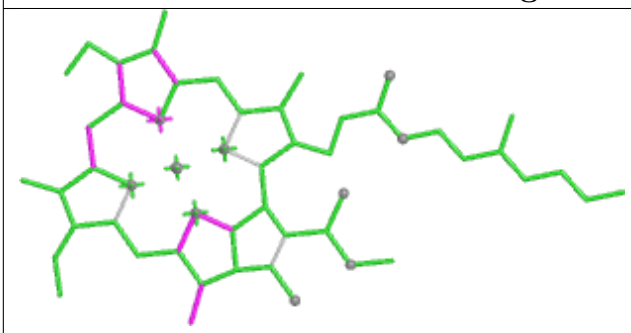


Torsions



Rings

Ligand CLA M 306



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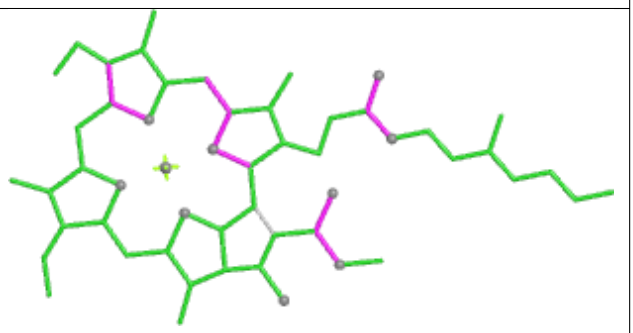

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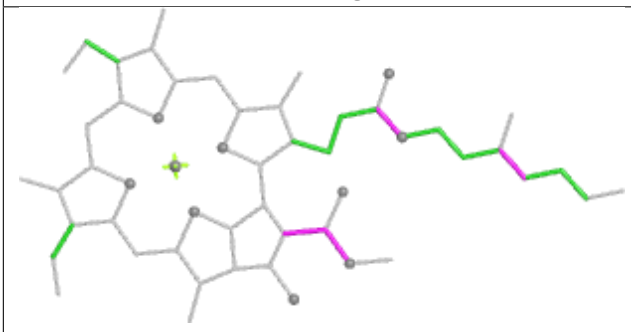

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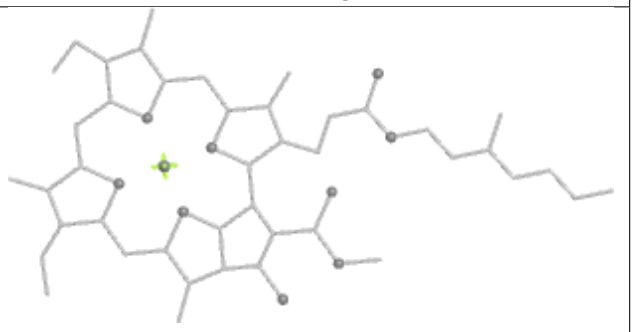
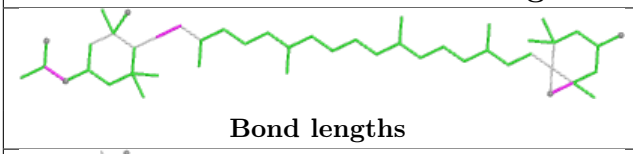


Rings

Ligand UIX O 306



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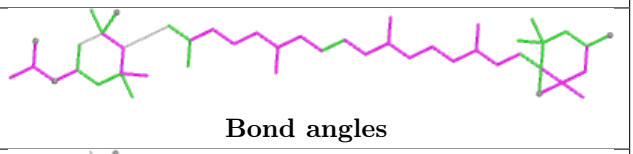

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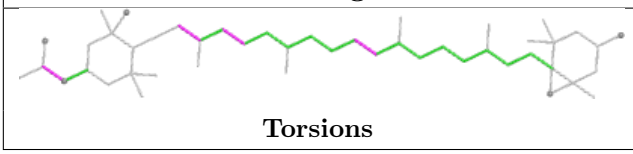

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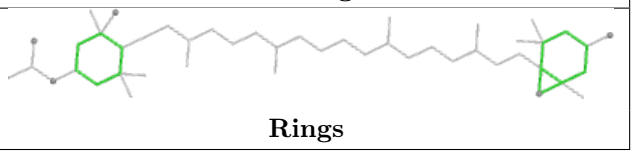
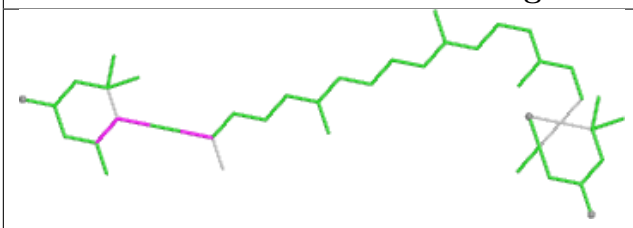


Rings

Ligand DD6 G 305



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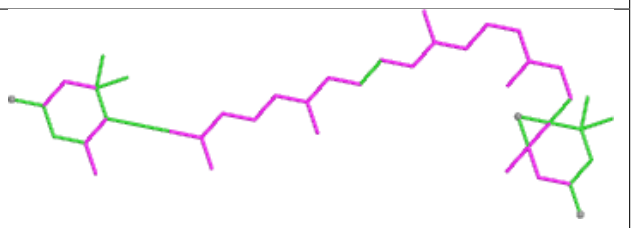

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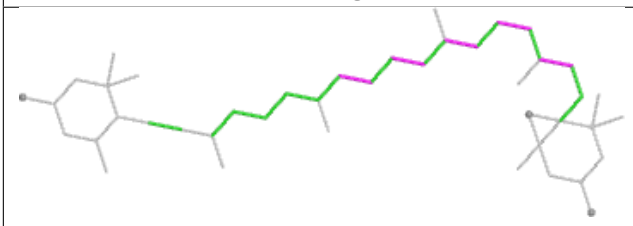
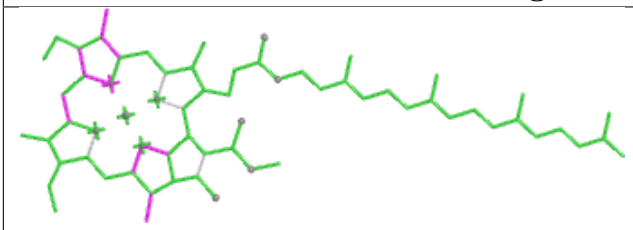


Torsions



Rings

Ligand CLA a 822



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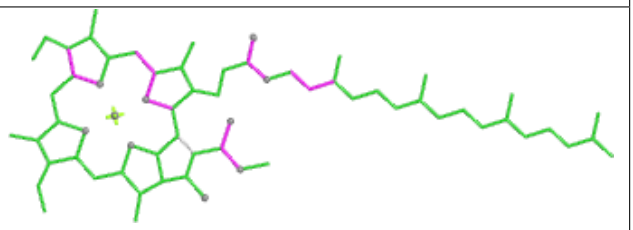
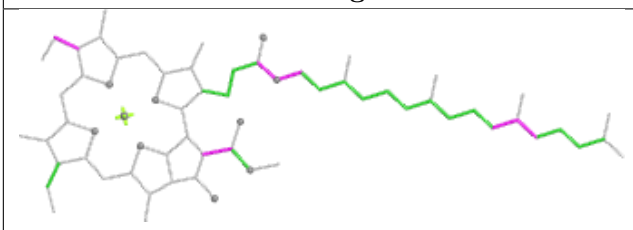


Bond angles



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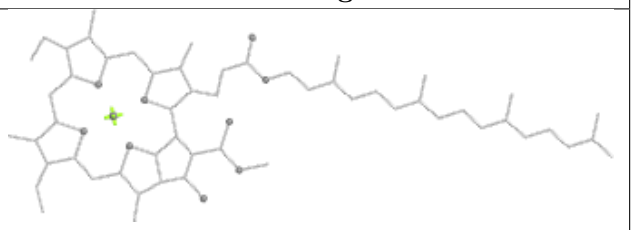
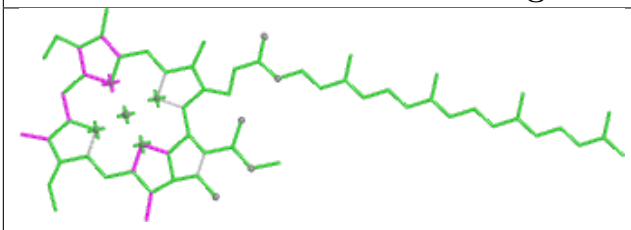


Rings

Ligand CLA b 701



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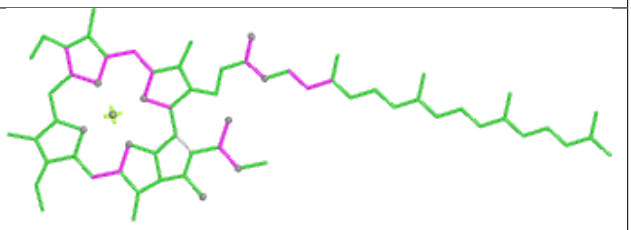
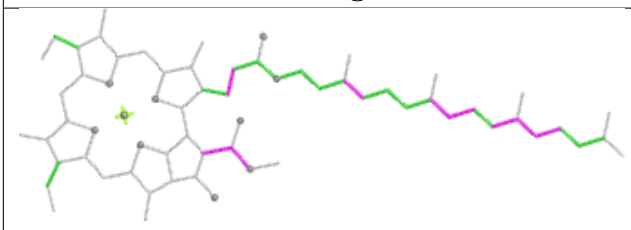


Bond angles



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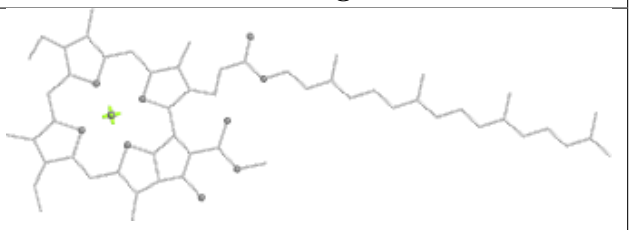
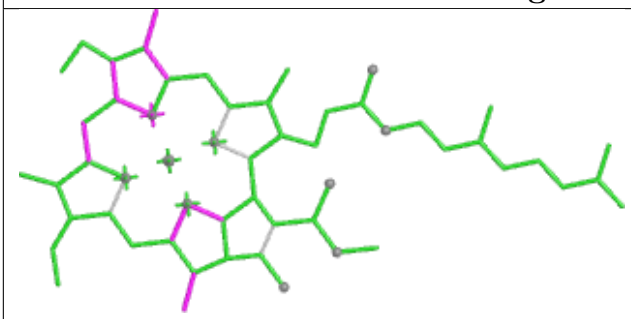


Rings

Ligand CLA a 810



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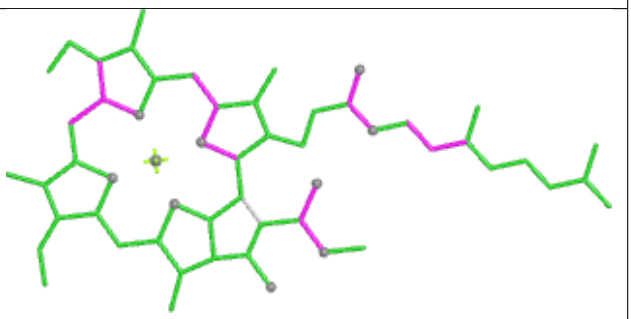
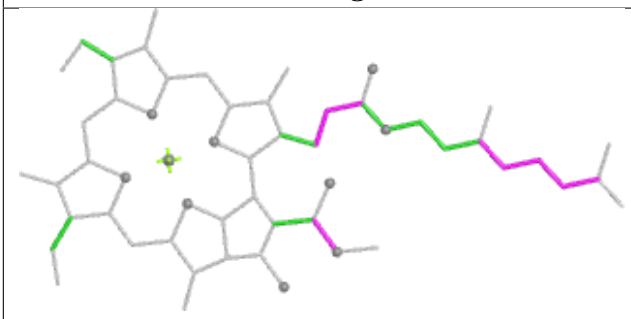


Bond angles



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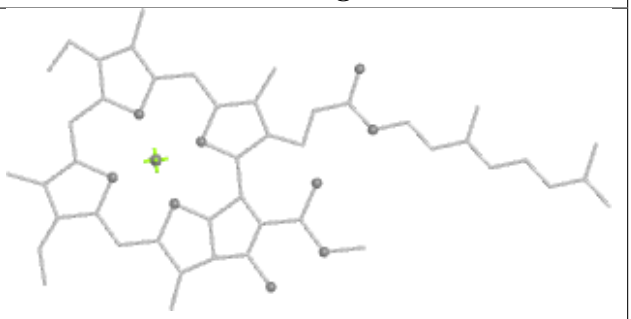
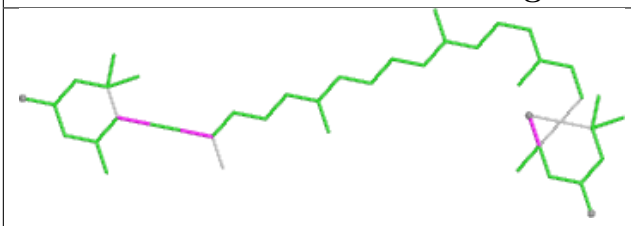


Rings

Ligand DD6 K 203



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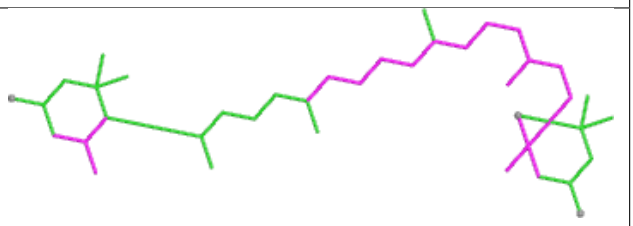
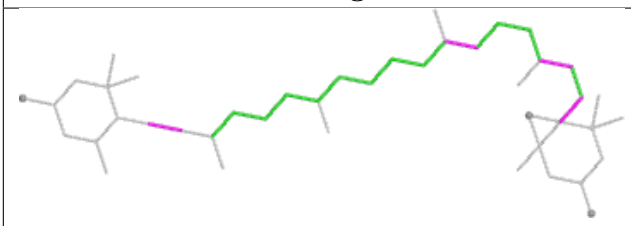


Bond angles



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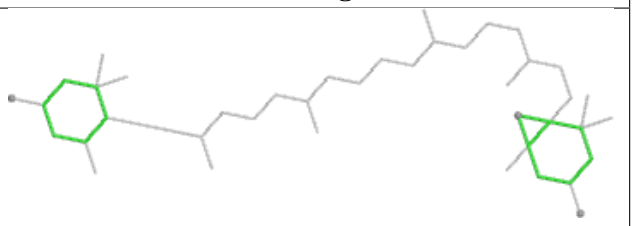
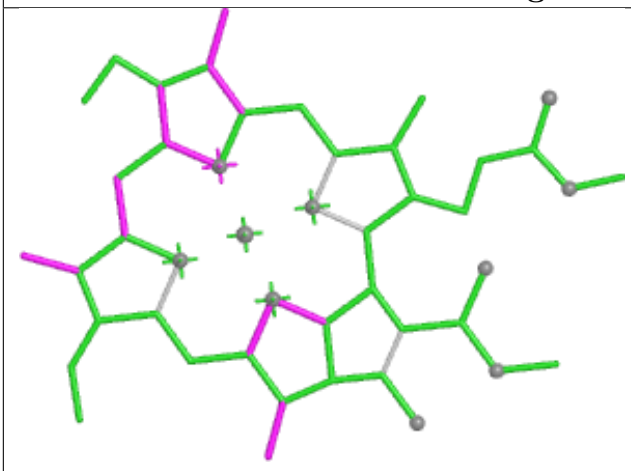


Rings

Ligand CLA b 710



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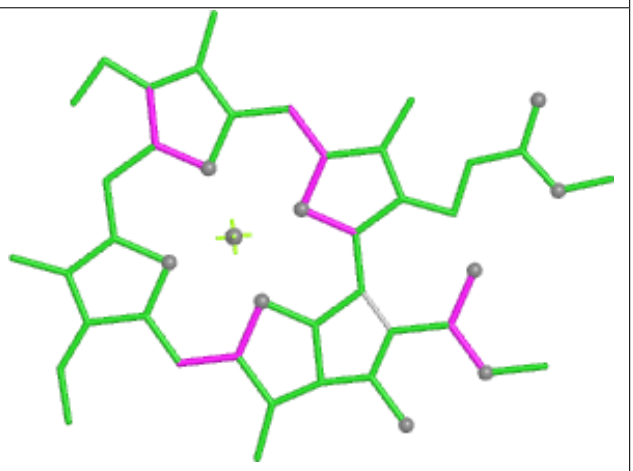
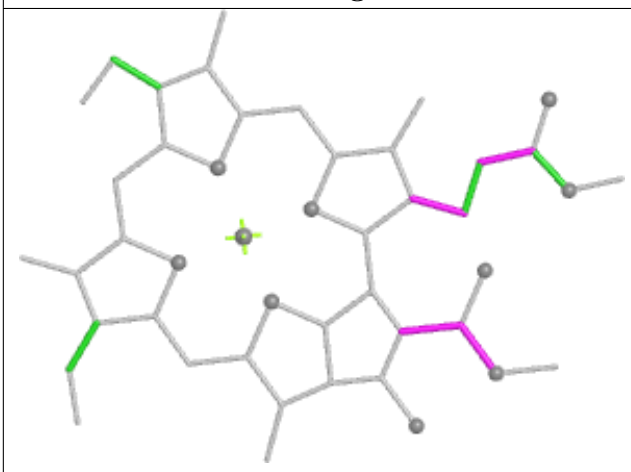


Bond angles



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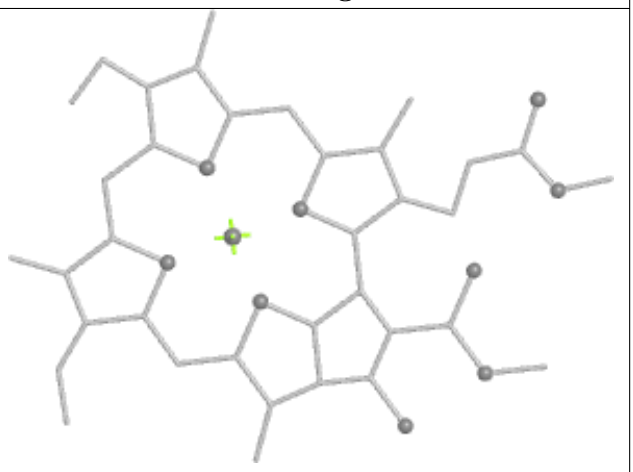
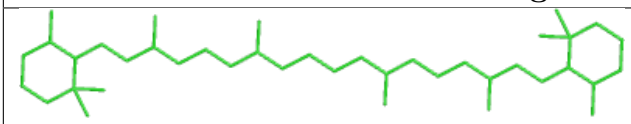


Rings

Ligand BCR f 801



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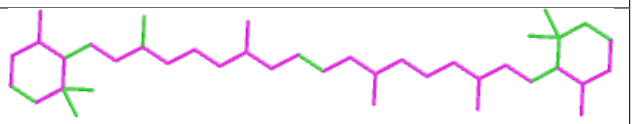
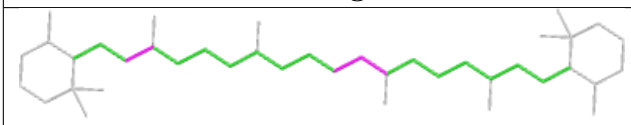


Bond angles



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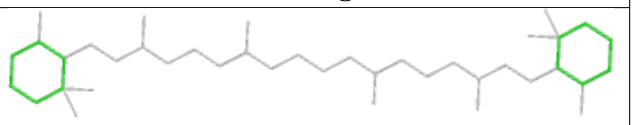
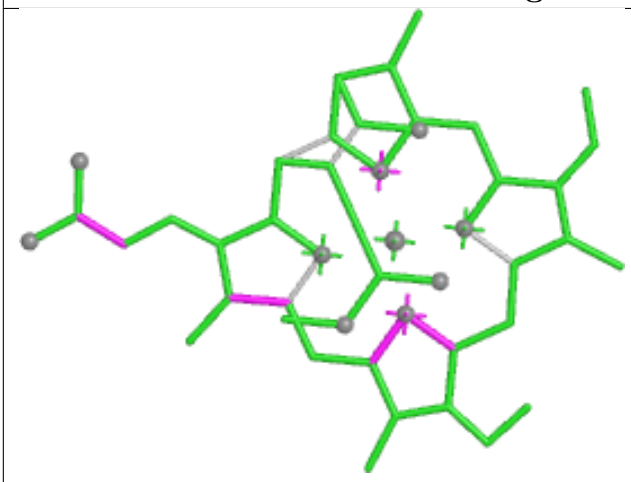


Rings

Ligand KC1 O 312



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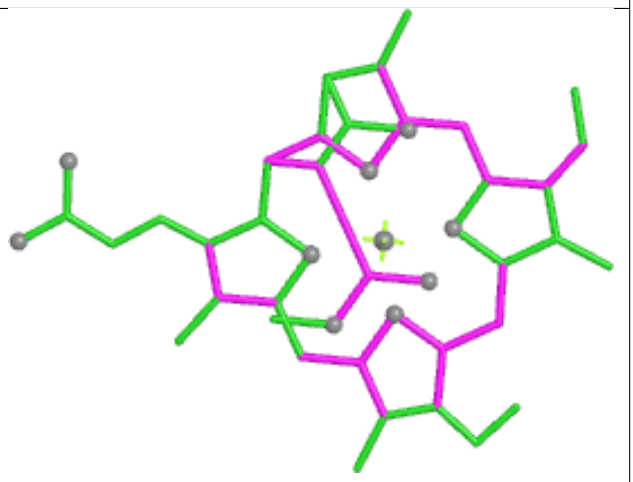
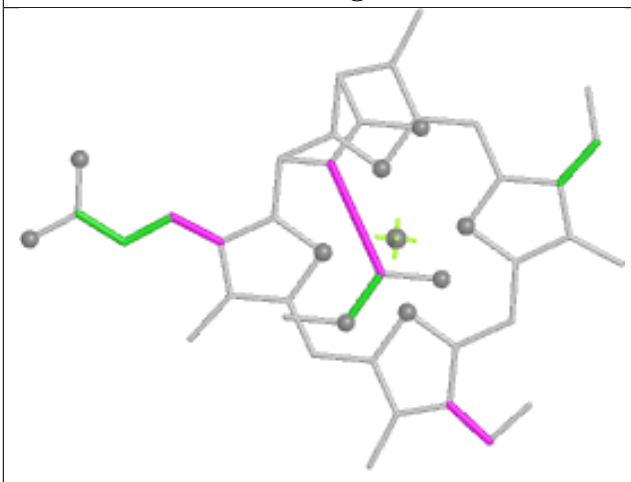


Bond angles



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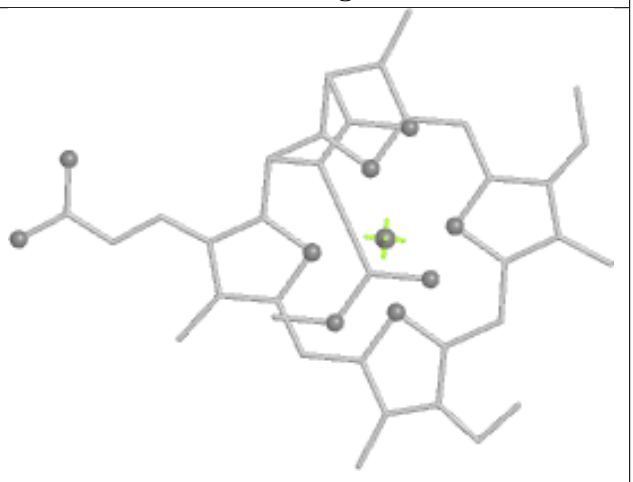
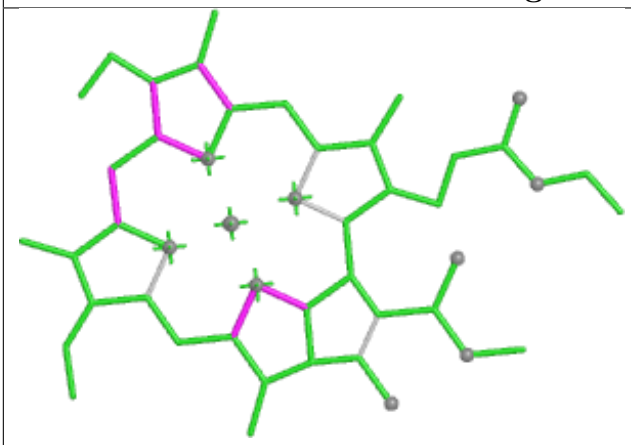


Rings

Ligand CLA P 215



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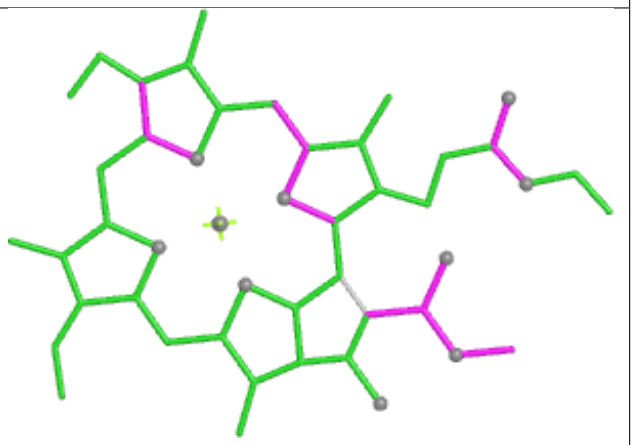
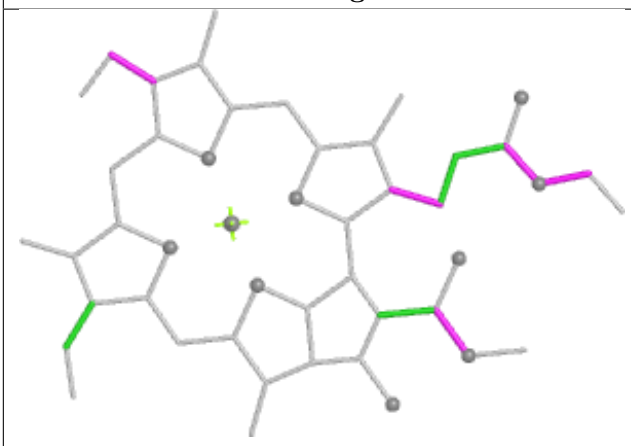


Bond angles



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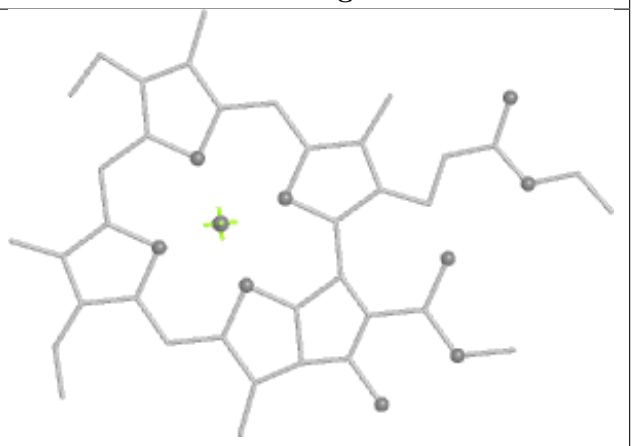
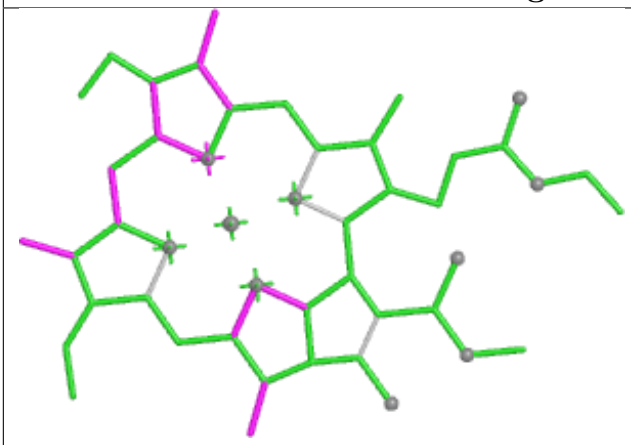


Rings

Ligand CLA b 724



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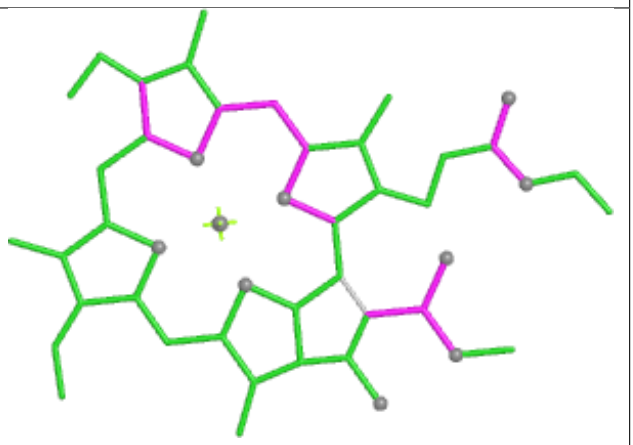
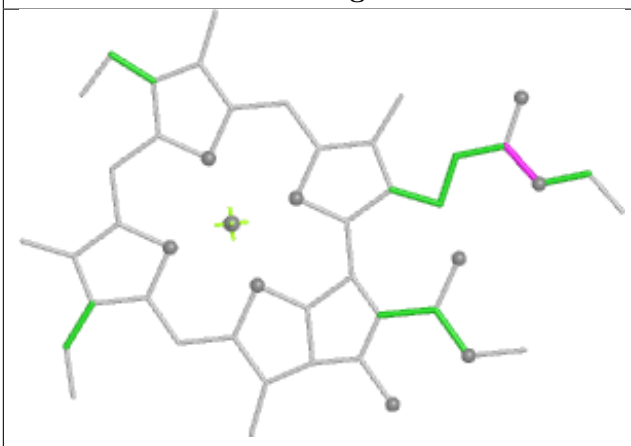


Bond angles



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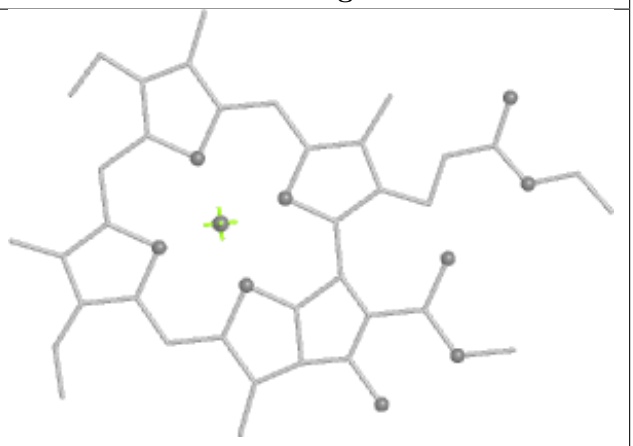
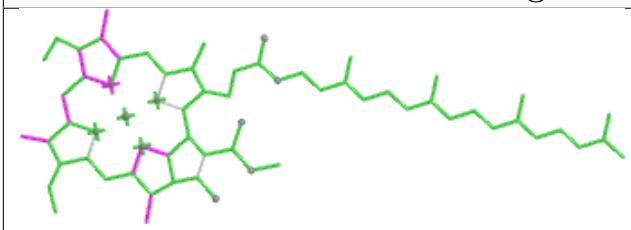
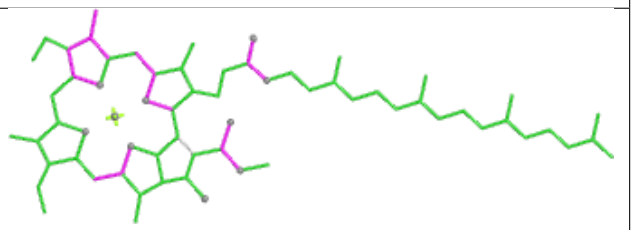


Rings

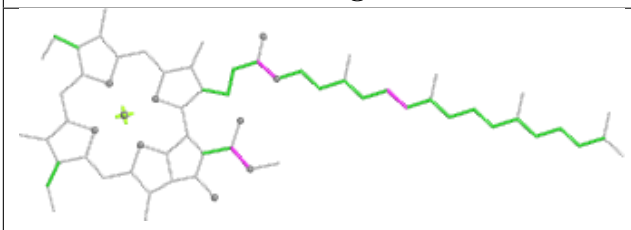
Ligand CLA b 723



Bond lengths



Bond angles



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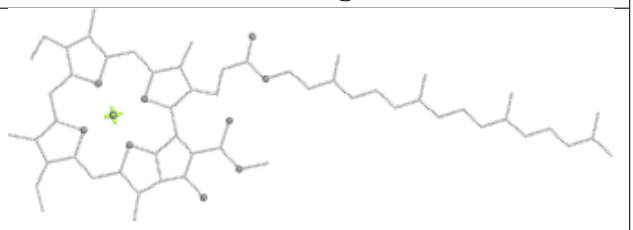
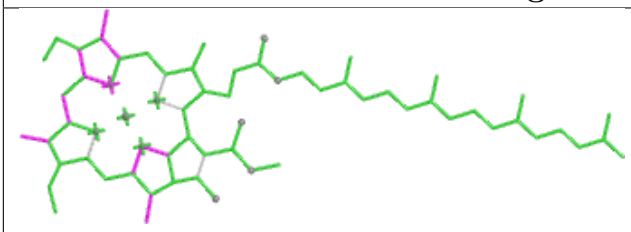
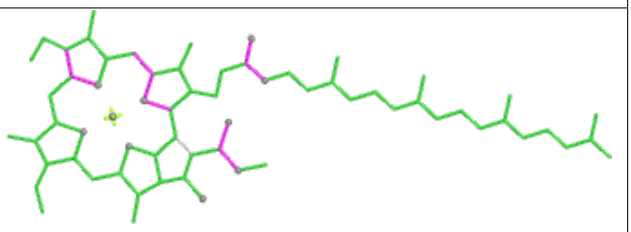


Rings

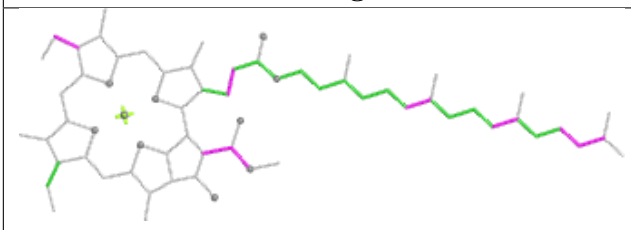
Ligand CLA b 725



Bond lengths



Bond angles



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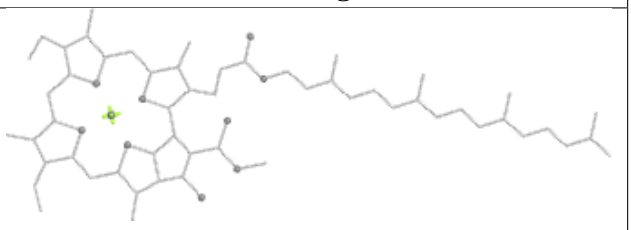
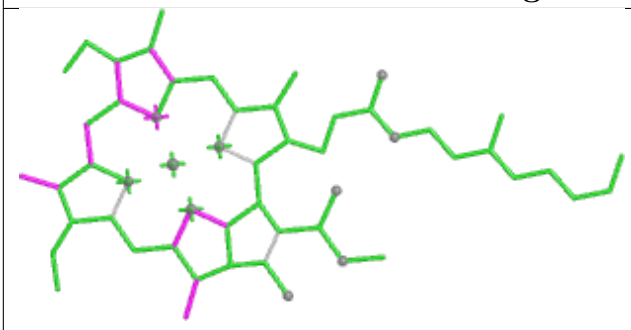


Rings

Ligand CLA K 209



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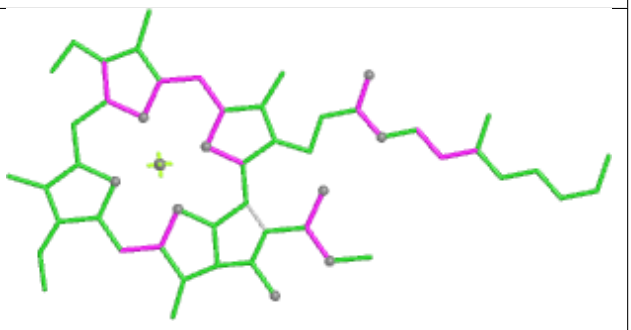

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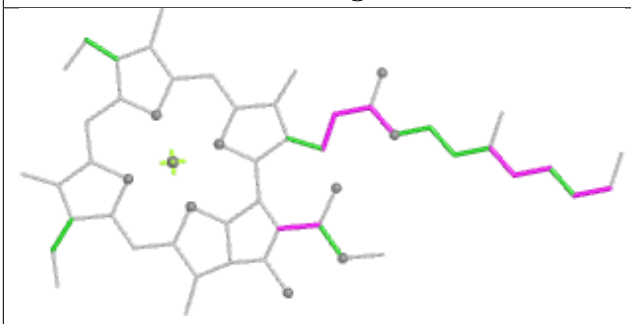
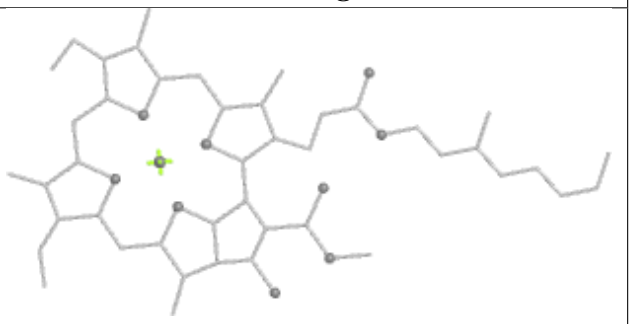
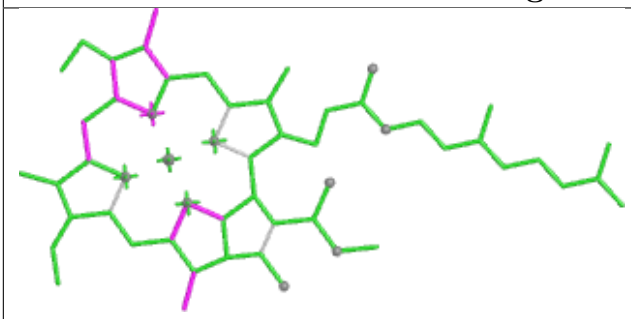


Torsions



Rings

Ligand CLA L 312



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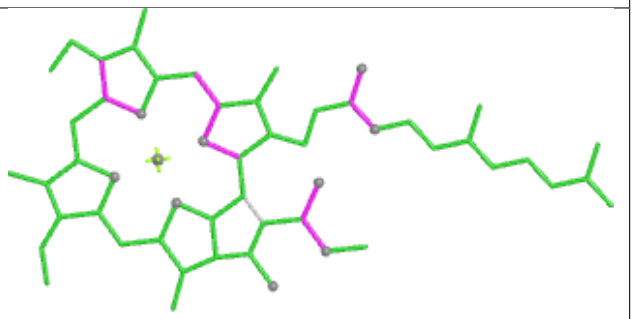

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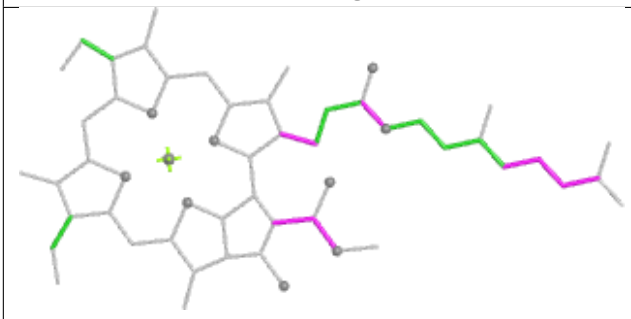

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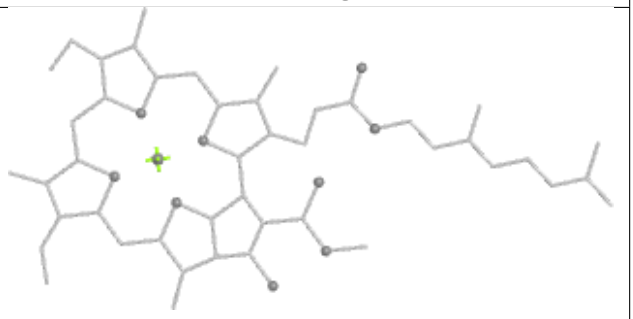
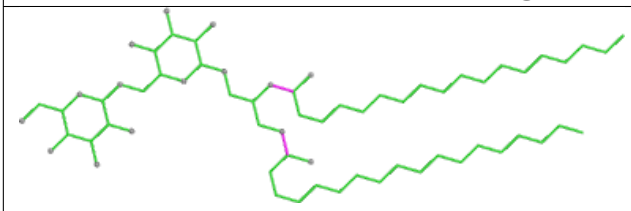


Rings

Ligand DGD m 102



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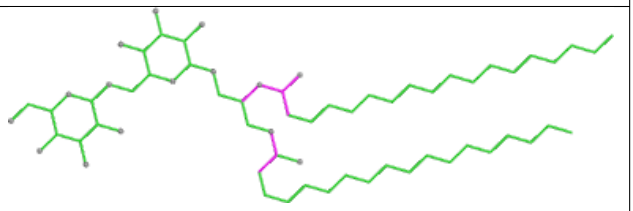

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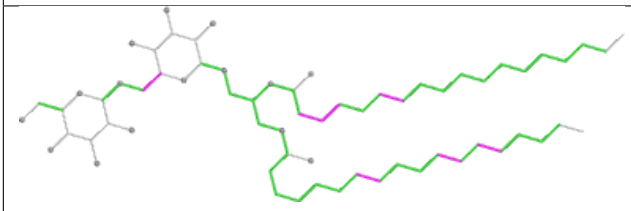

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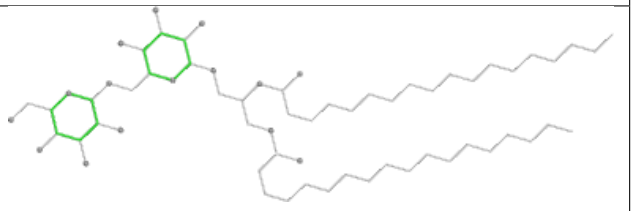
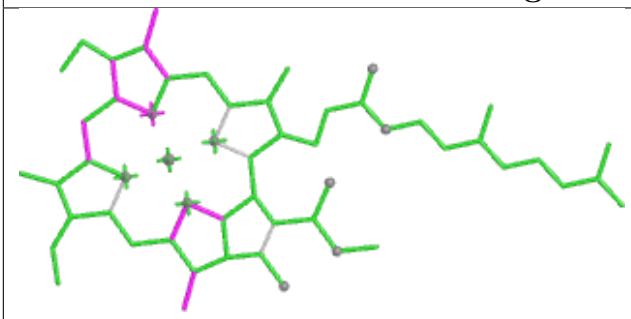


Rings

Ligand CLA B 309



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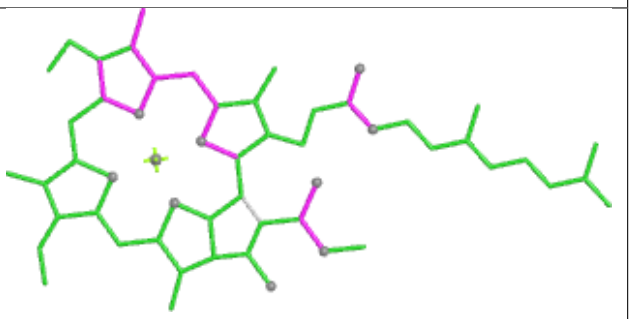

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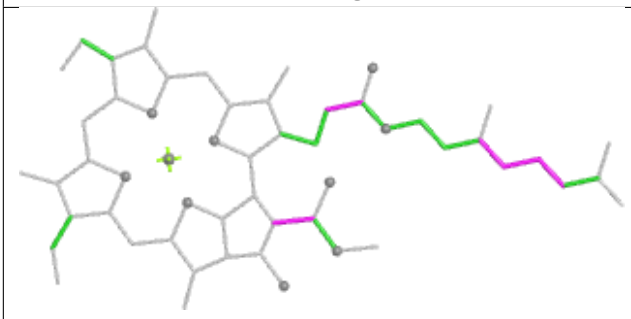

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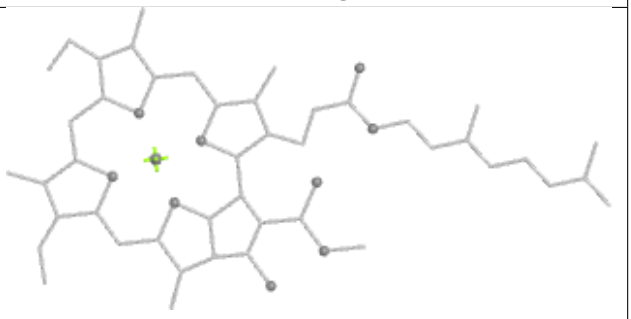
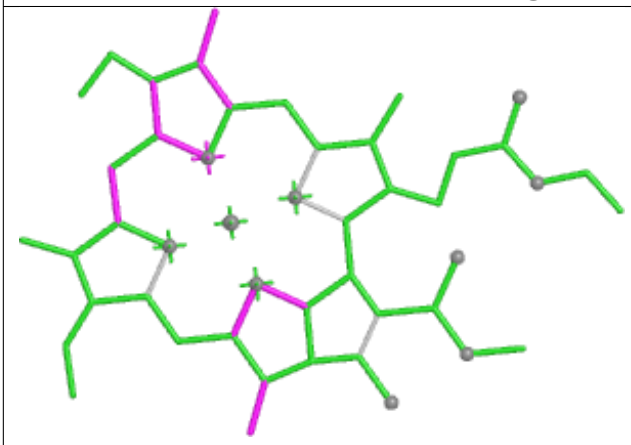


Rings

Ligand CLA T 308



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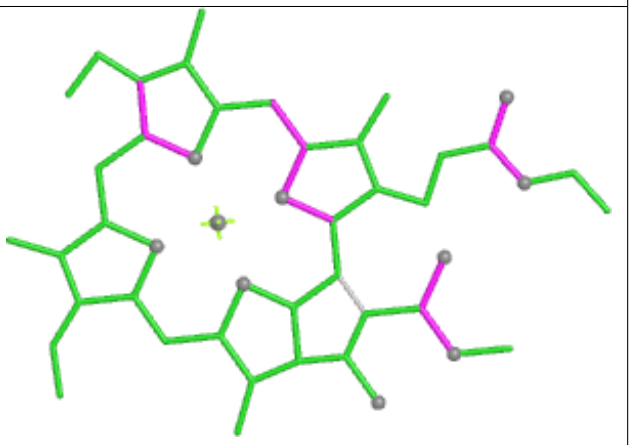

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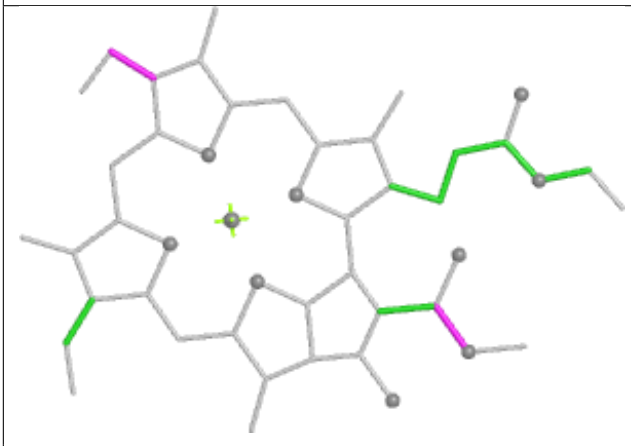

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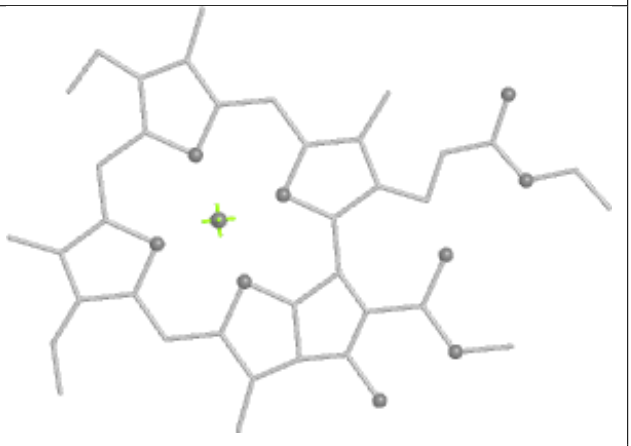
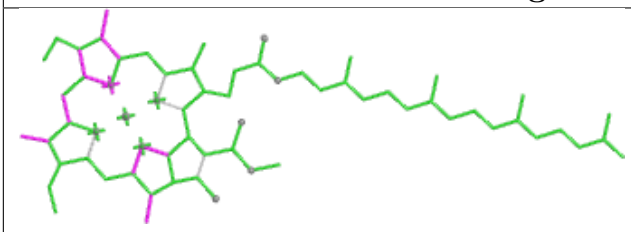


Rings

Ligand CLA a 809



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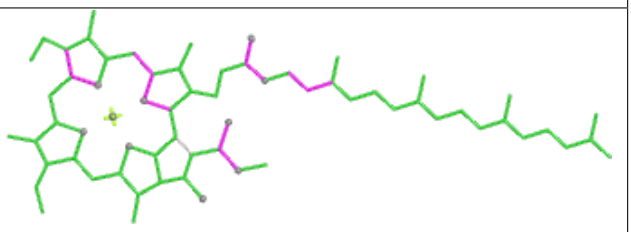

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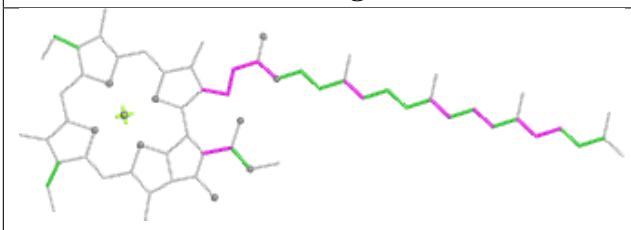

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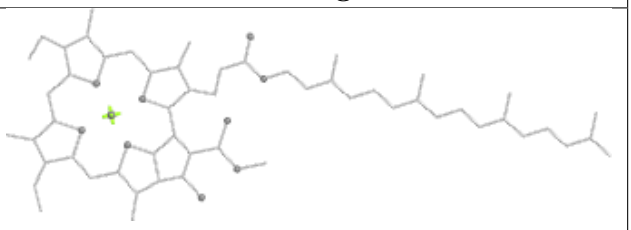
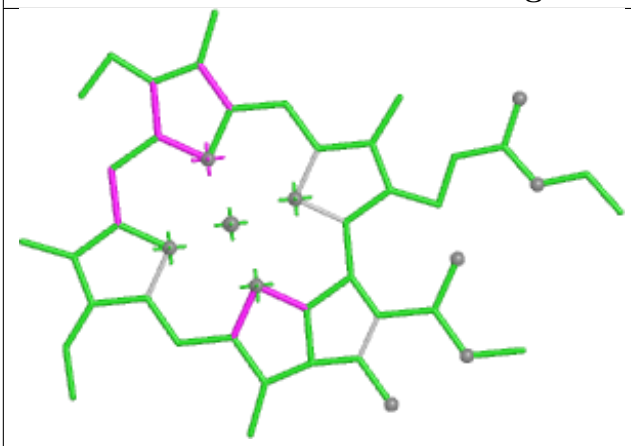


Rings

Ligand CLA P 209



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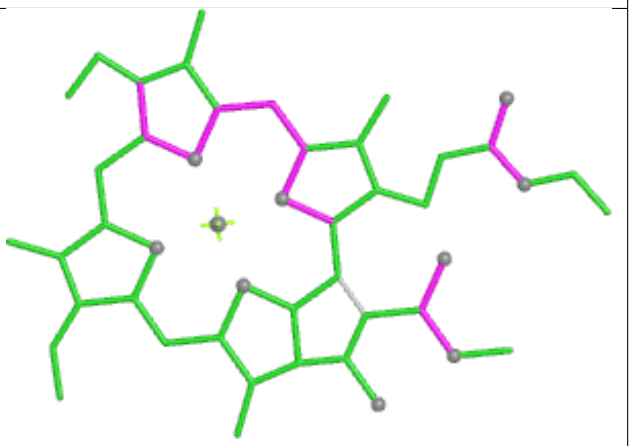

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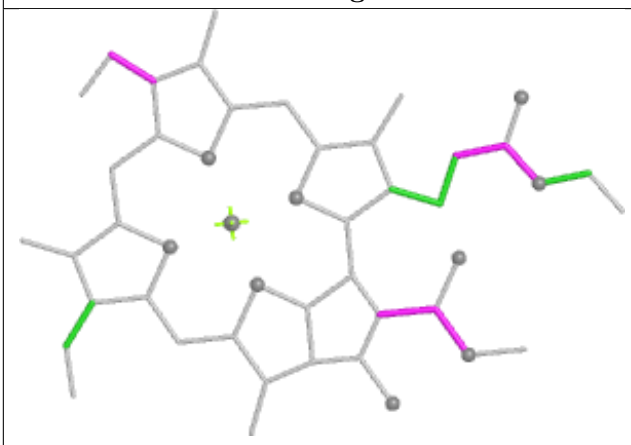

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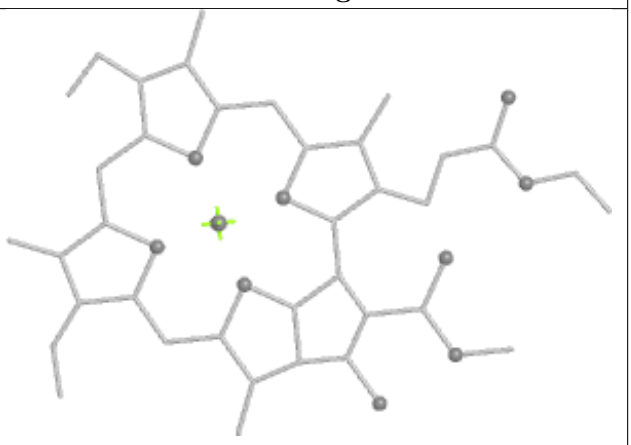
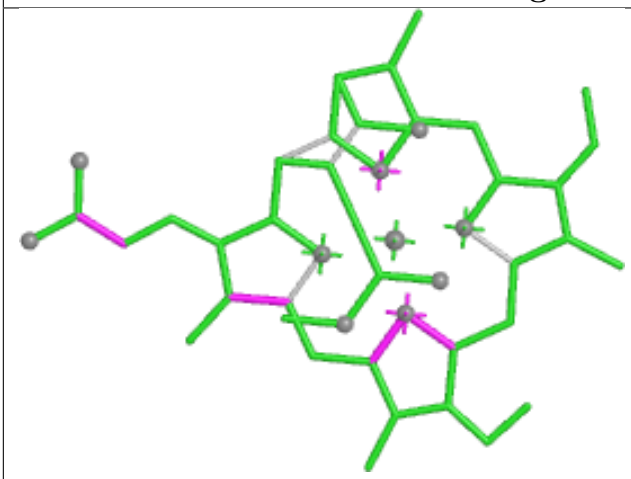


Rings

Ligand KC1 J 312



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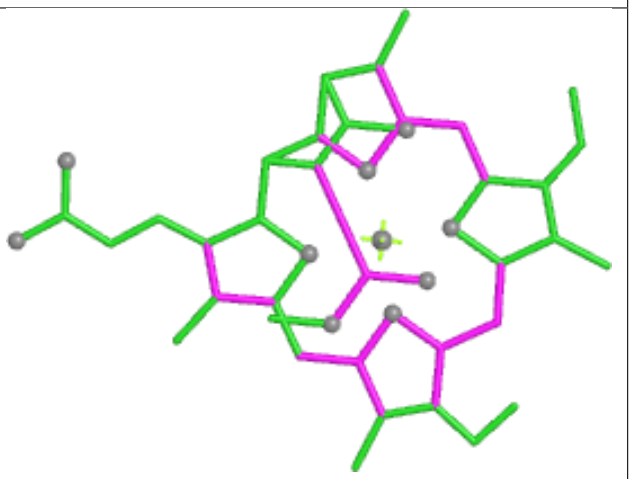

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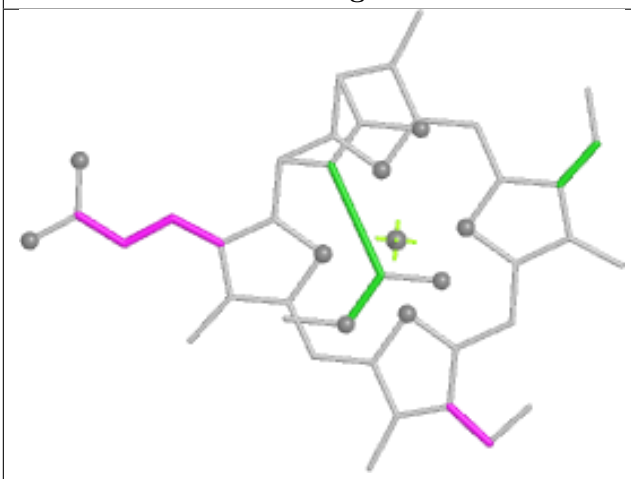

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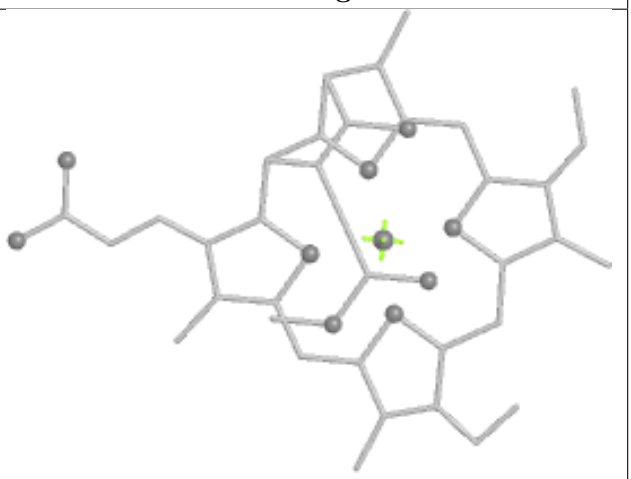
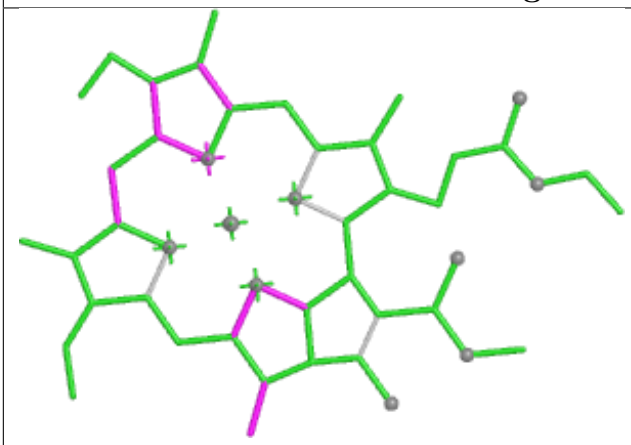


Rings

Ligand CLA D 308



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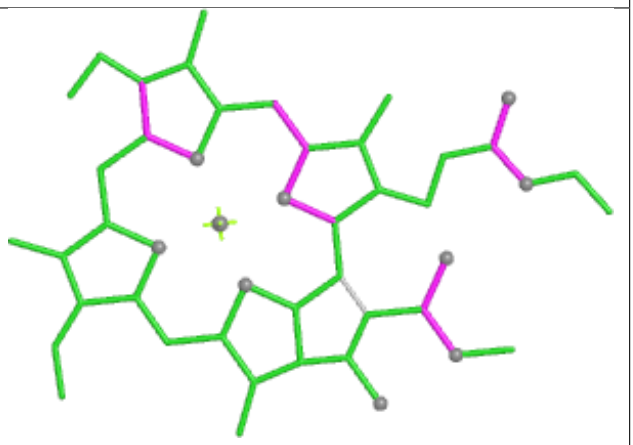

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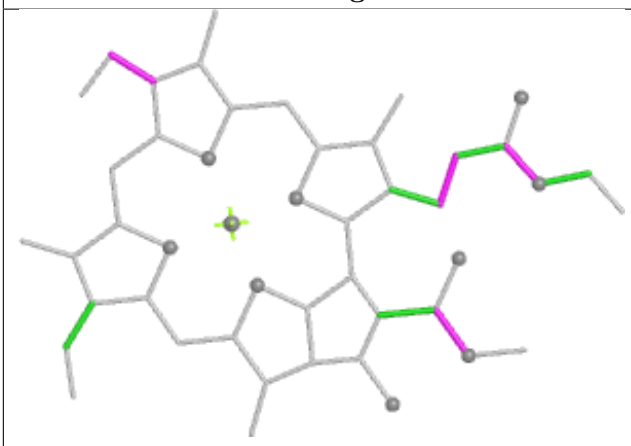

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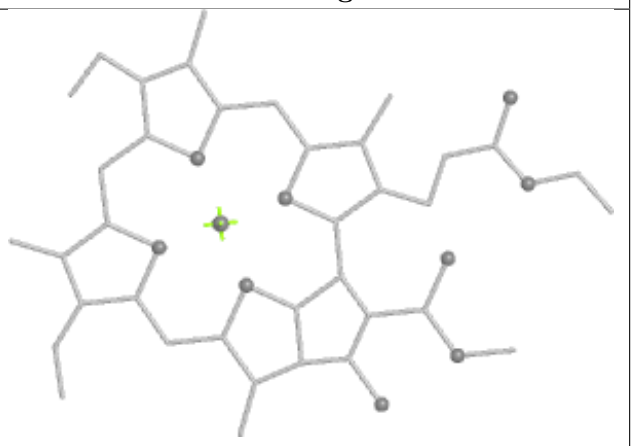
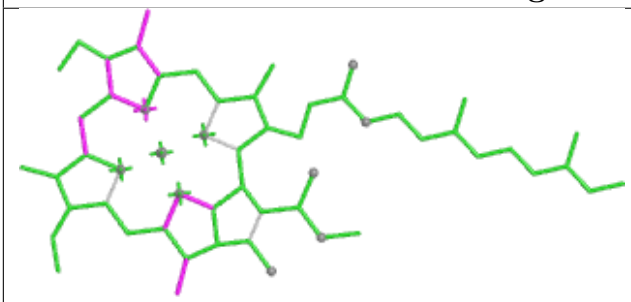


Rings

Ligand CLA J 308



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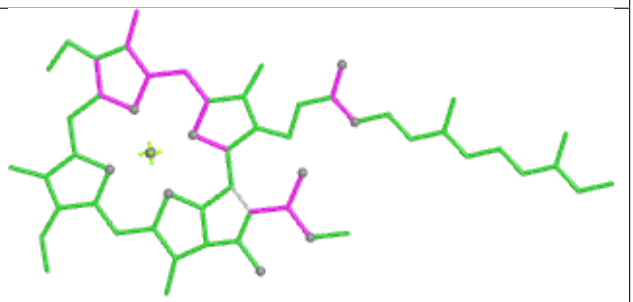

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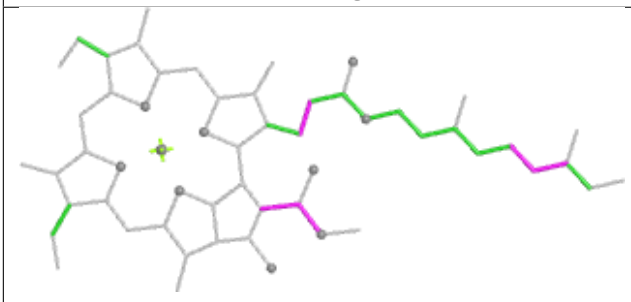

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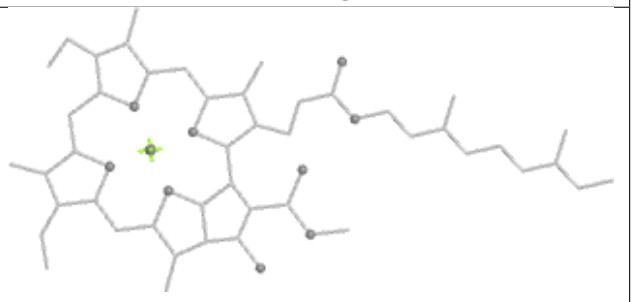
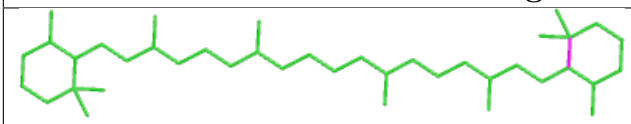


Rings

Ligand BCR b 729



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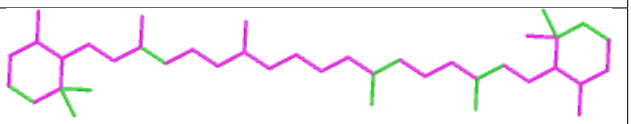

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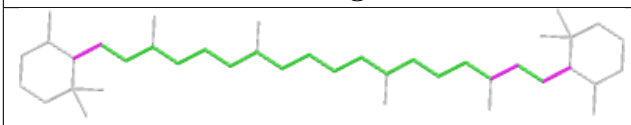

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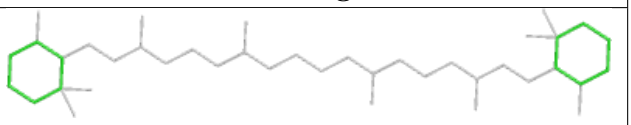
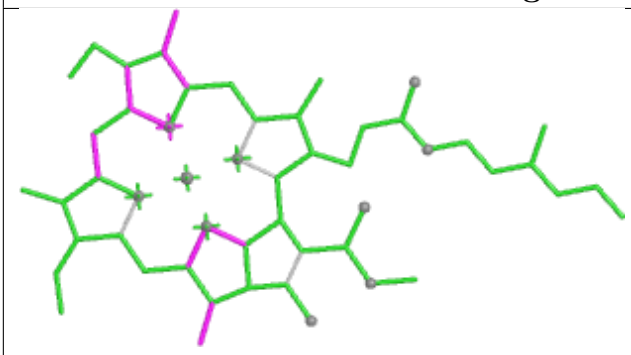


Rings

Ligand CLA K 212



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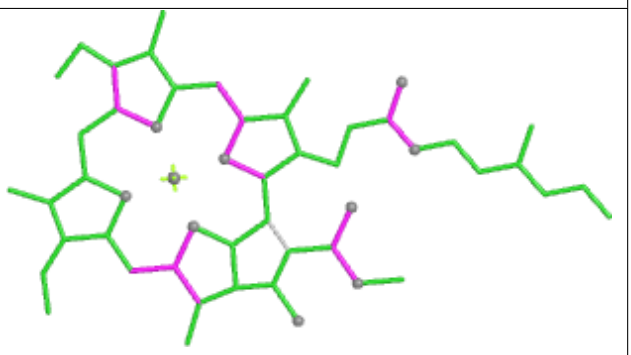
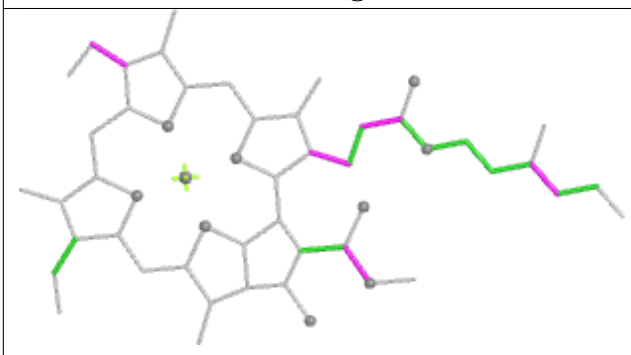


Bond angles



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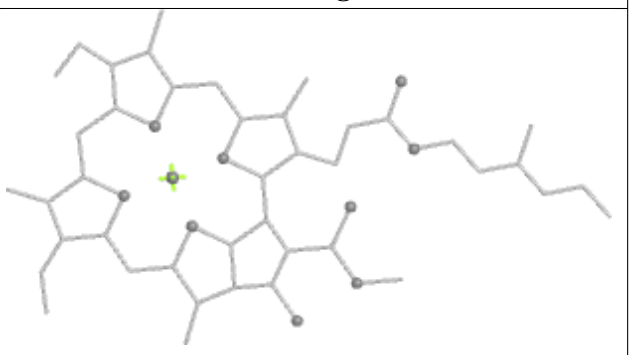
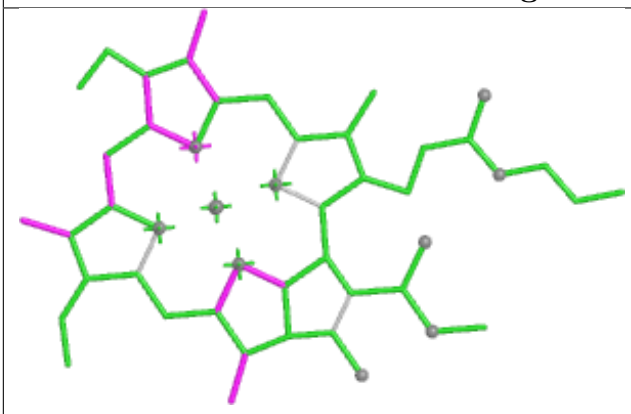


Rings

Ligand CLA M 308



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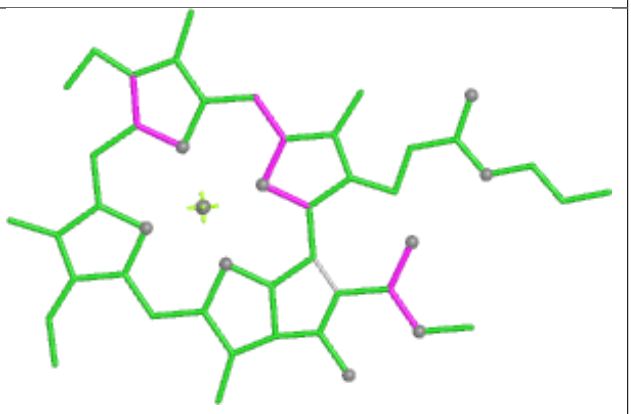
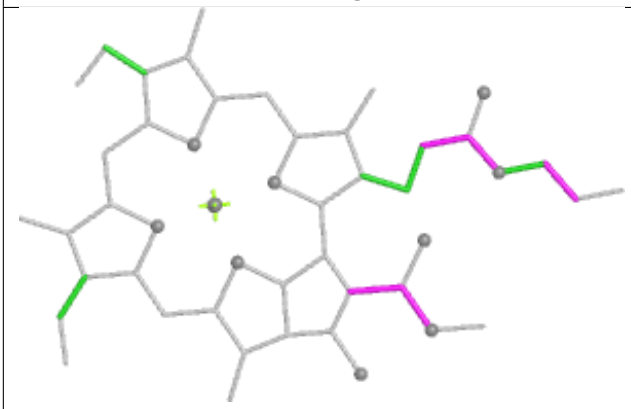


Bond angles



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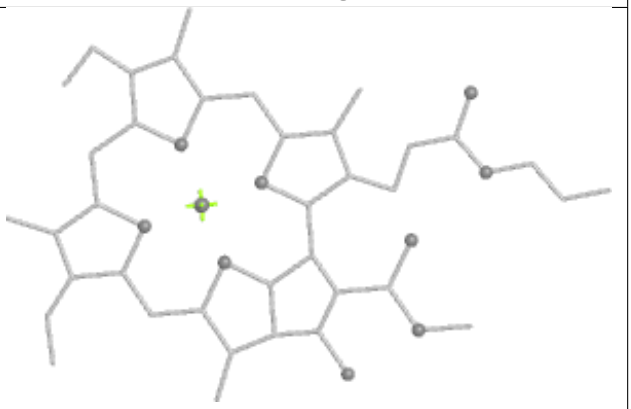
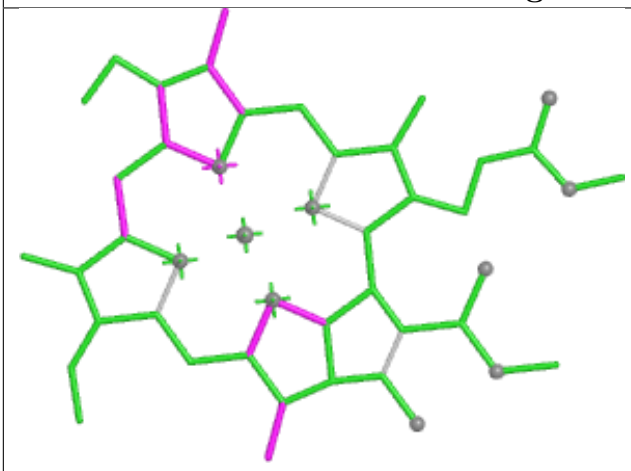


Rings

Ligand CLA F 311



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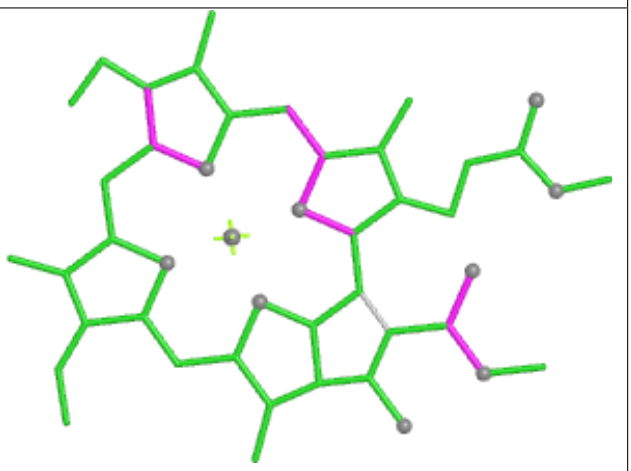
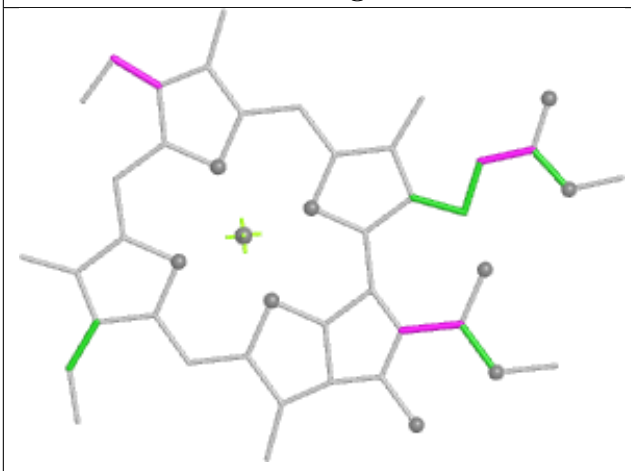


Bond angles



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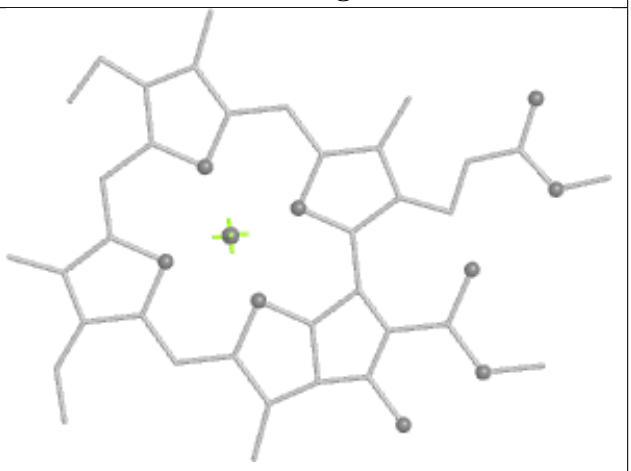
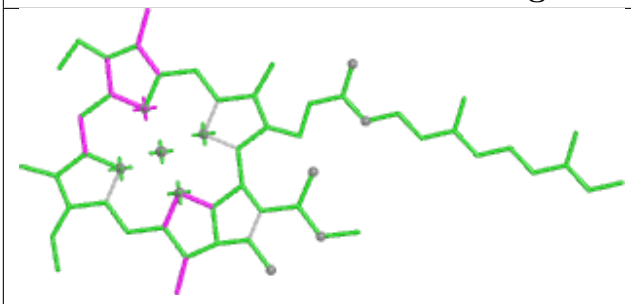
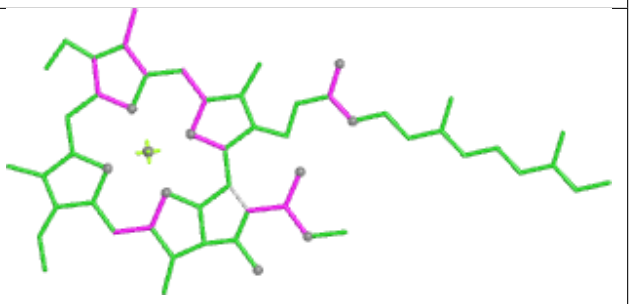


Rings

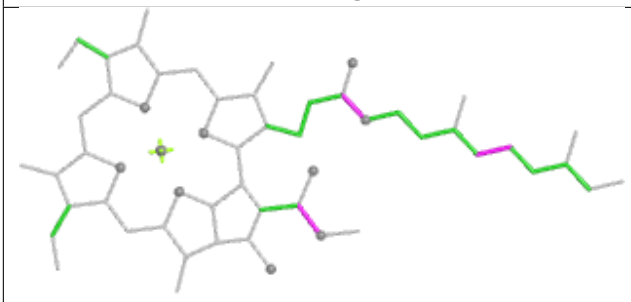
Ligand CLA a 830



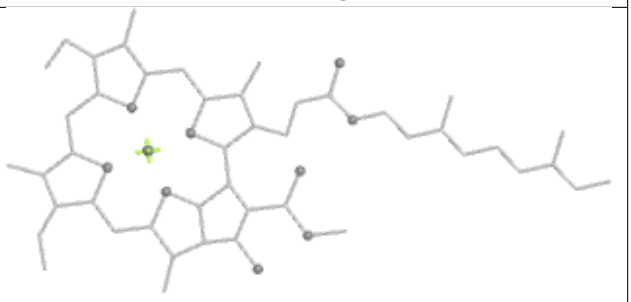
Bond lengths



Bond angles

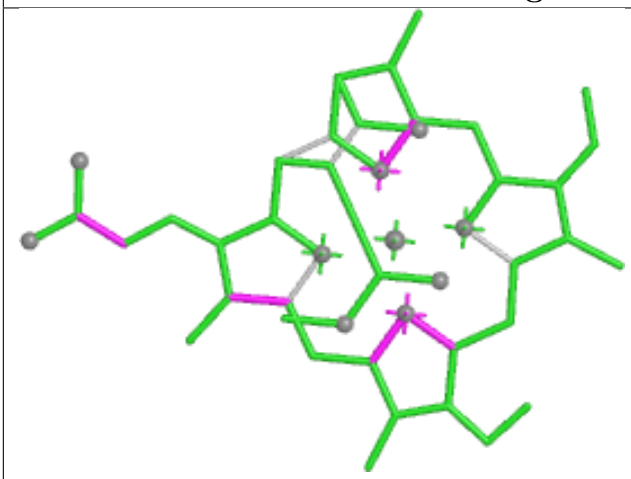


Torsions

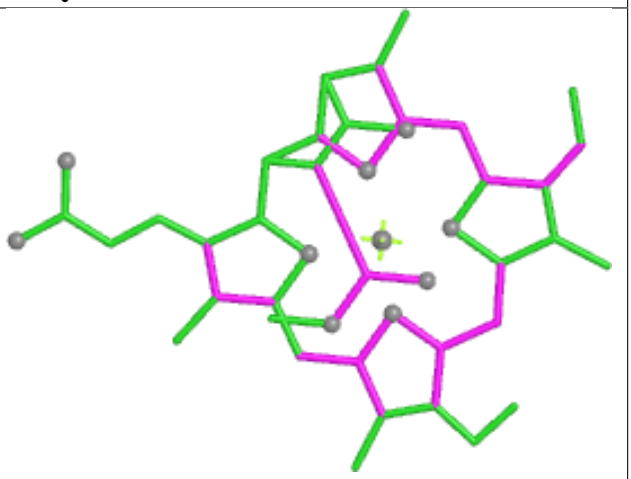


Rings

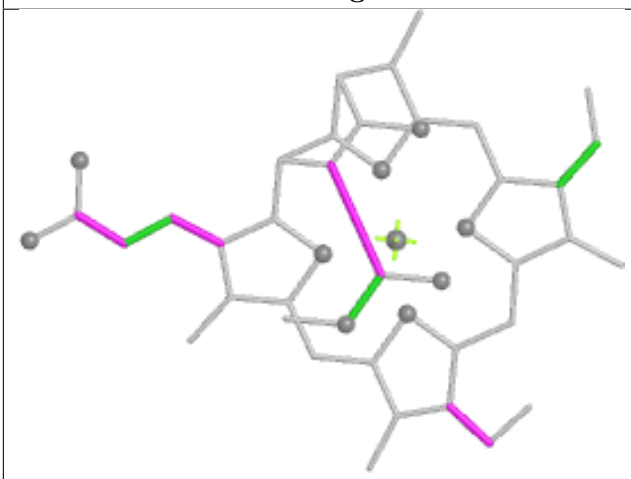
Ligand KC1 Q 311



Bond lengths



Bond angles



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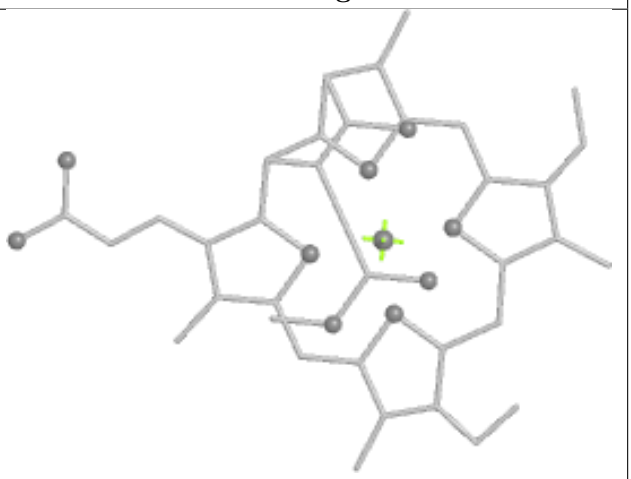
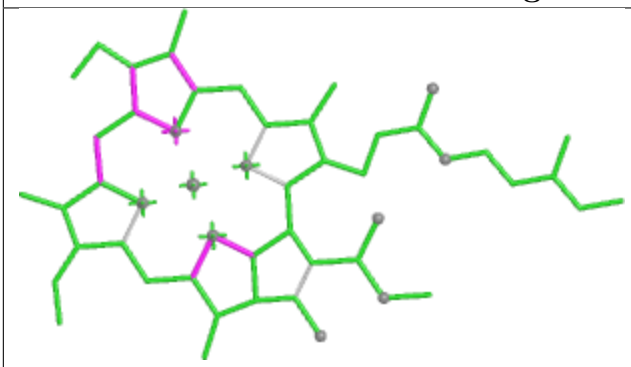


Rings

Ligand CLA N 311



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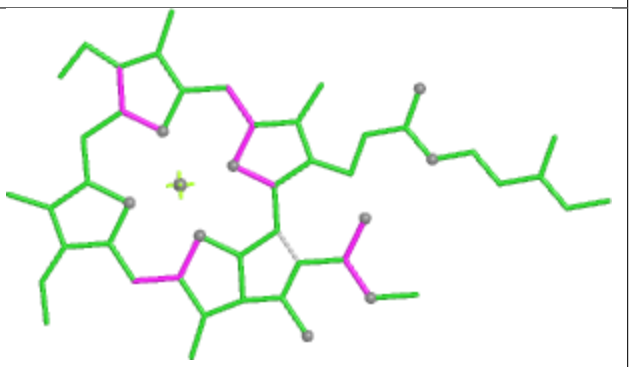
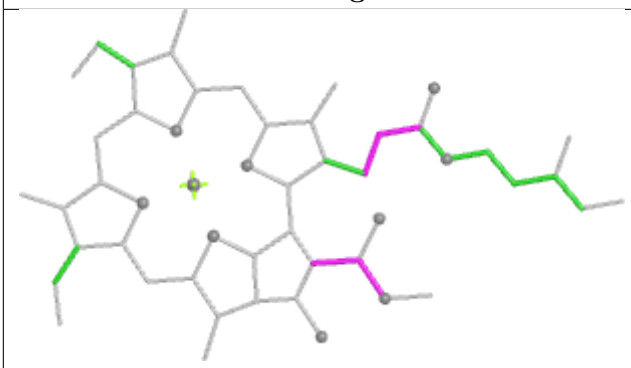


Bond angles



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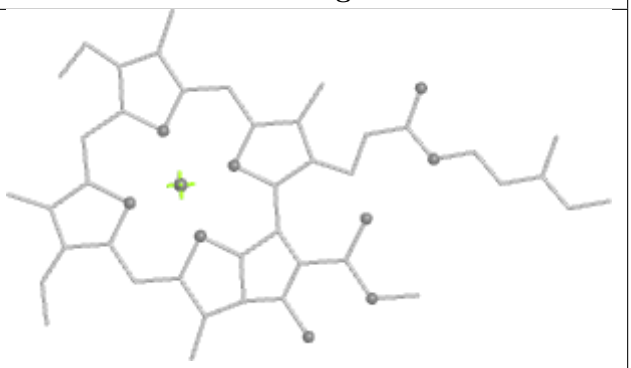
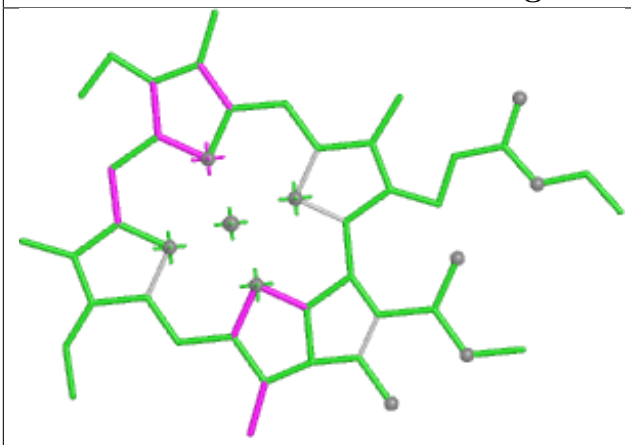


Rings

Ligand CLA C 308



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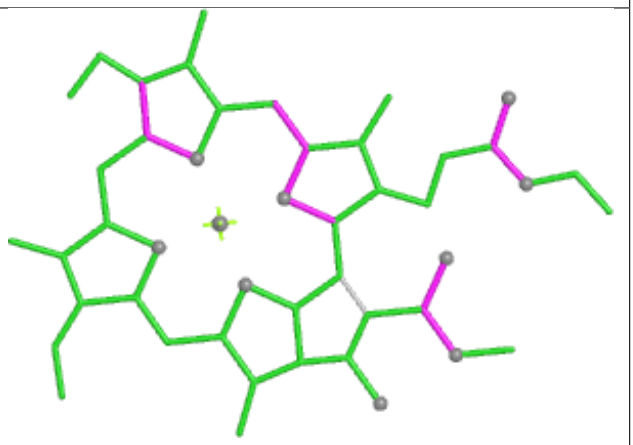

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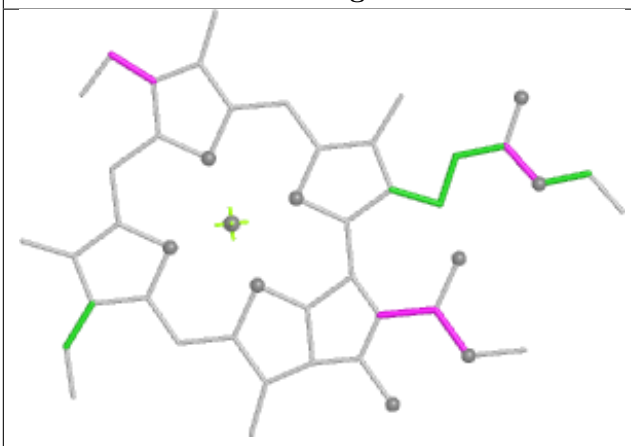

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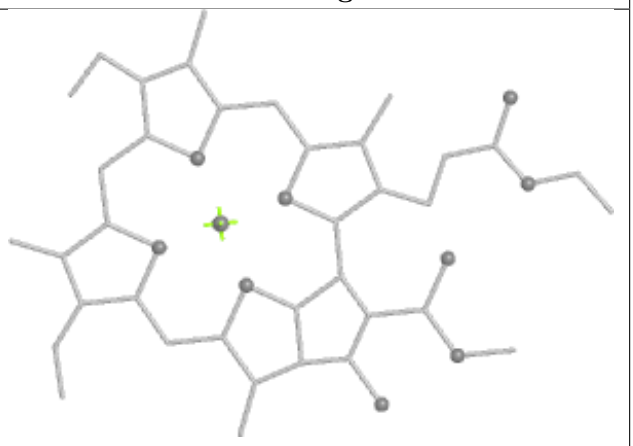
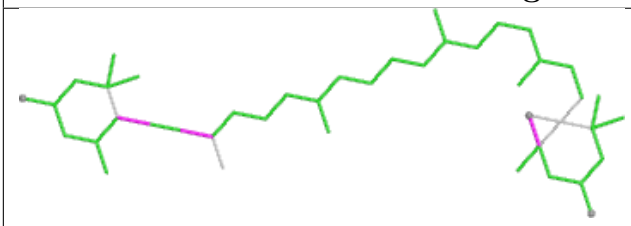


Rings

Ligand DD6 m 101



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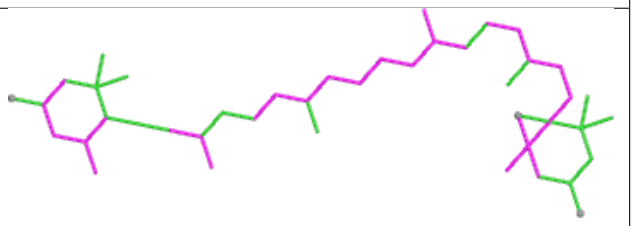
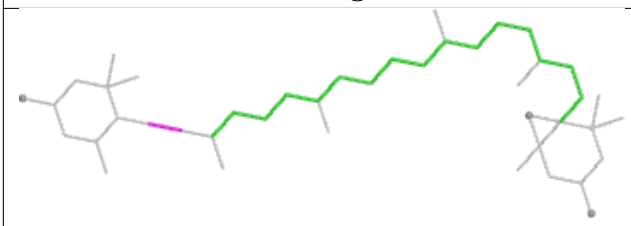


Bond angles

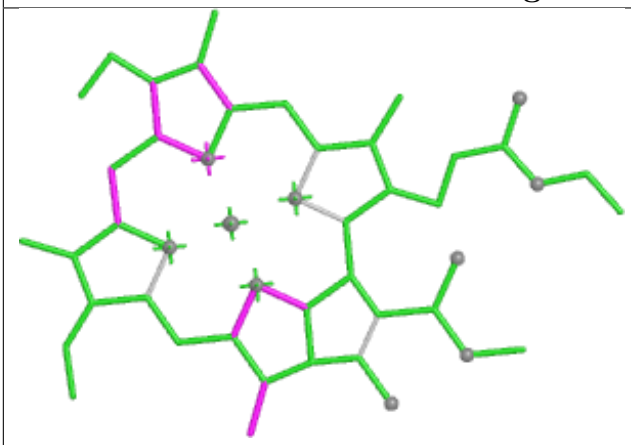


Torsions



Rings

Ligand CLA N 308



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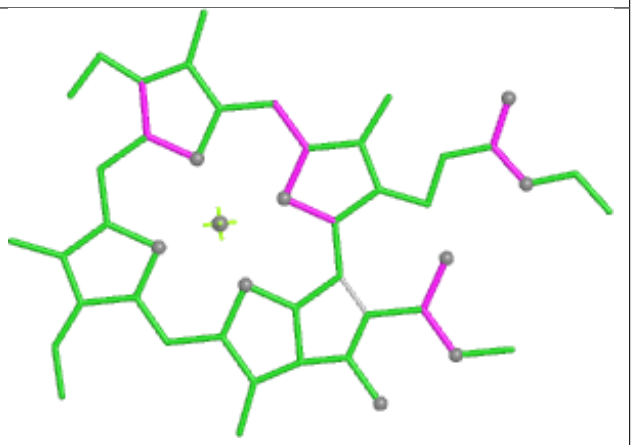
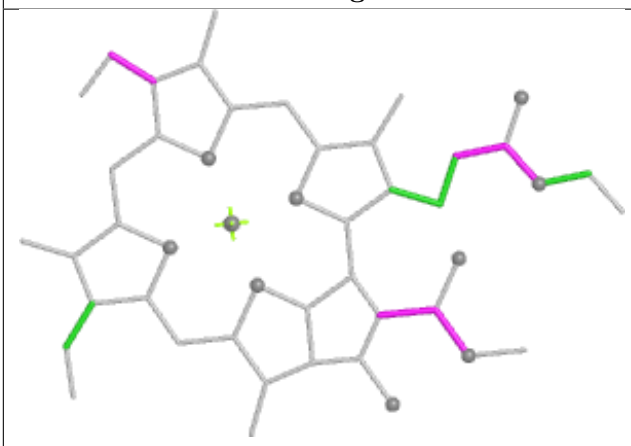


Bond angles



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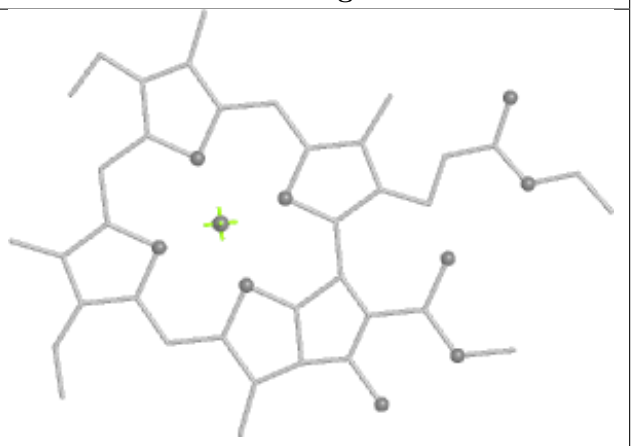
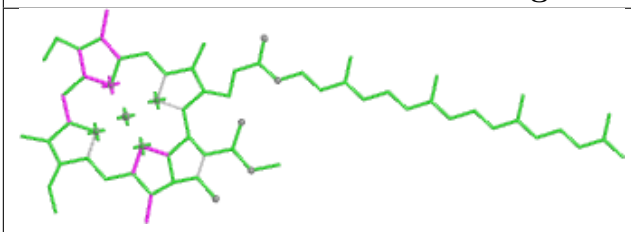


Rings

Ligand CLA I 213



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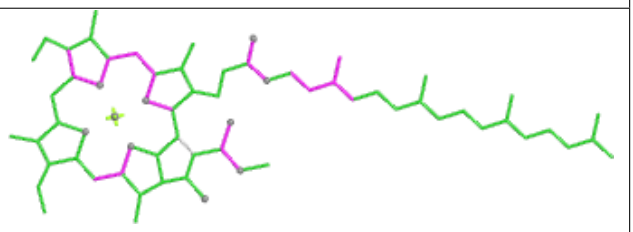
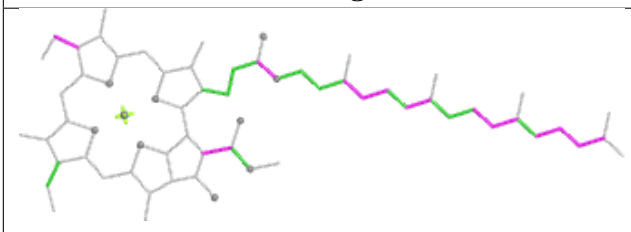


Bond angles



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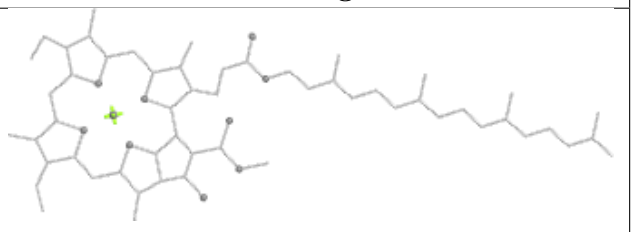
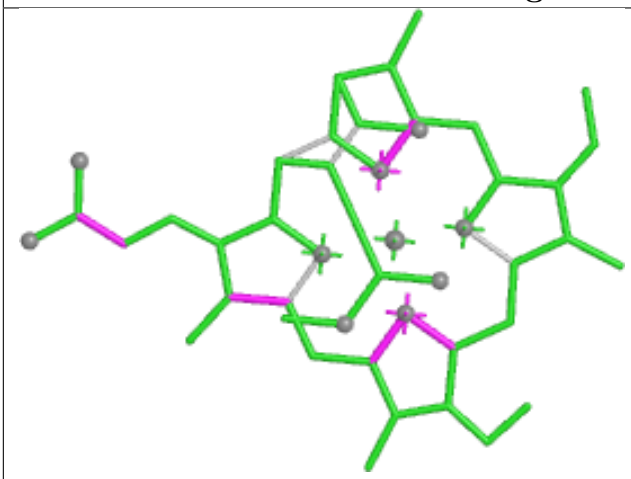


Rings

Ligand KC1 Q 314



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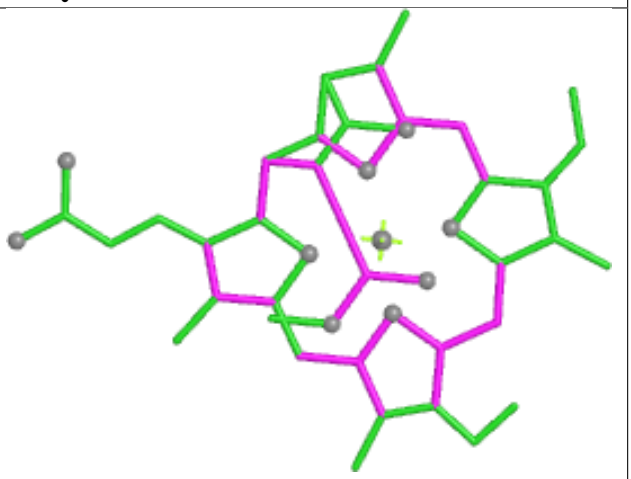
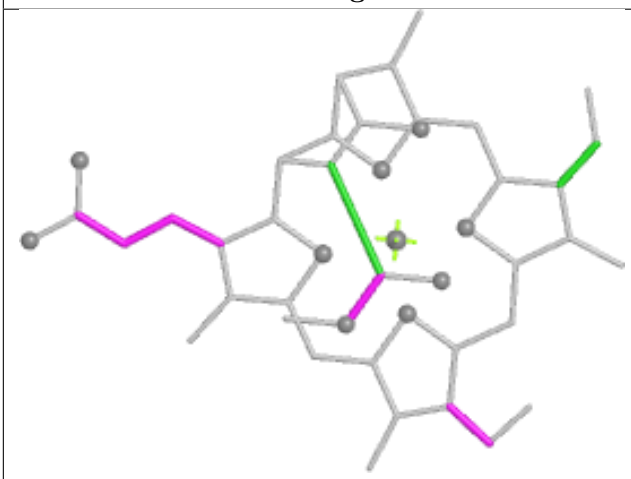


Bond angles



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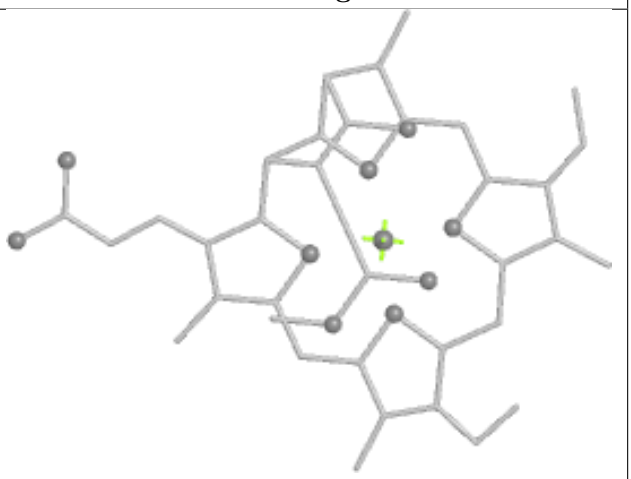
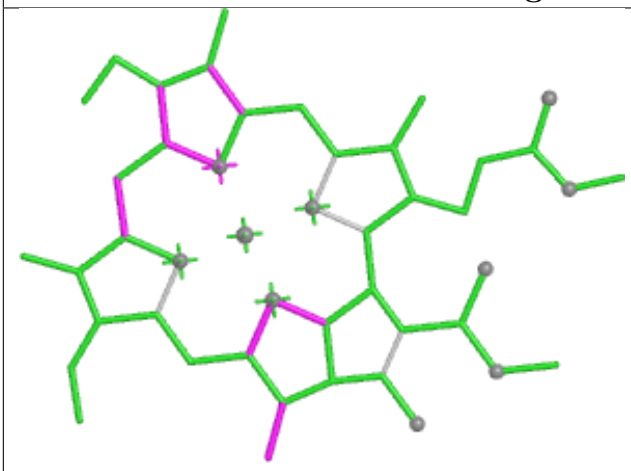


Rings

Ligand CLA P 214



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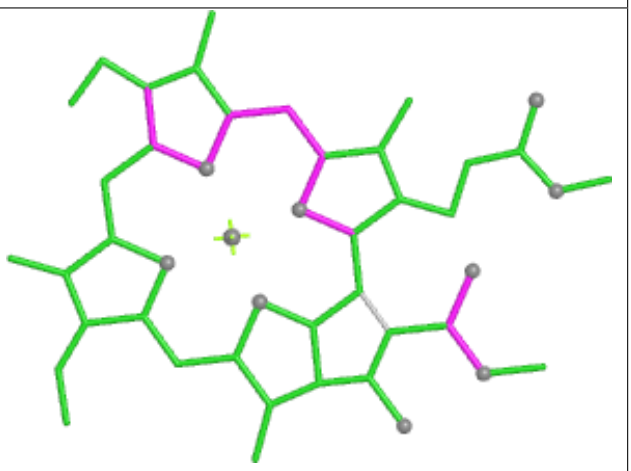
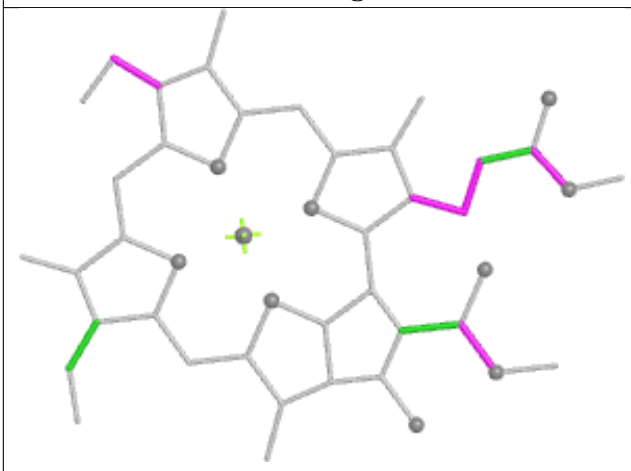


Bond angles



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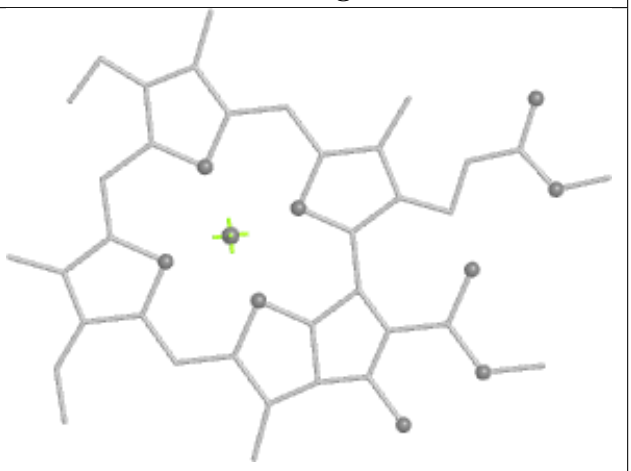
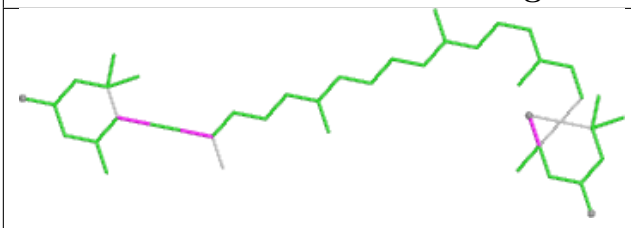


Rings

Ligand DD6 H 303



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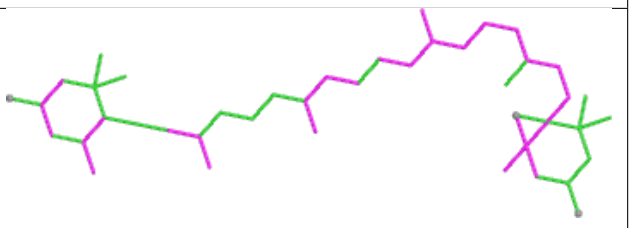
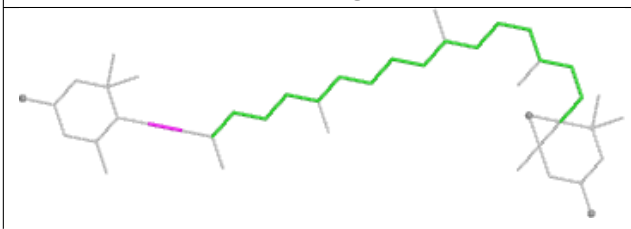


Bond angles



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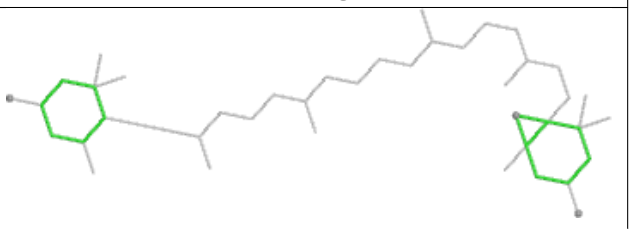
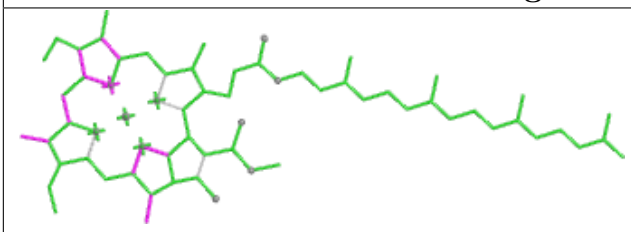


Rings

Ligand CLA B 312



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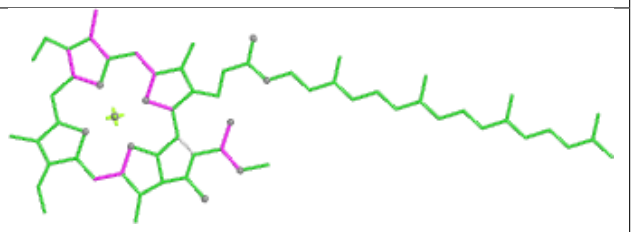
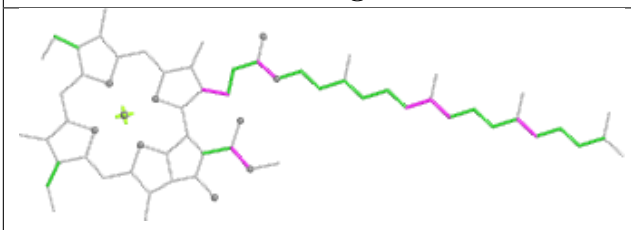


Bond angles



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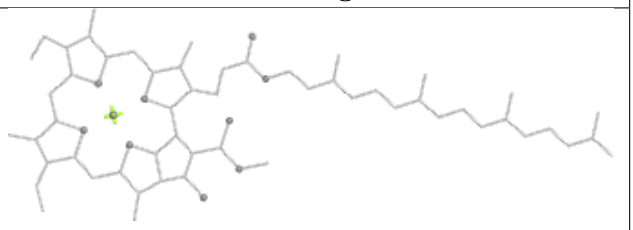
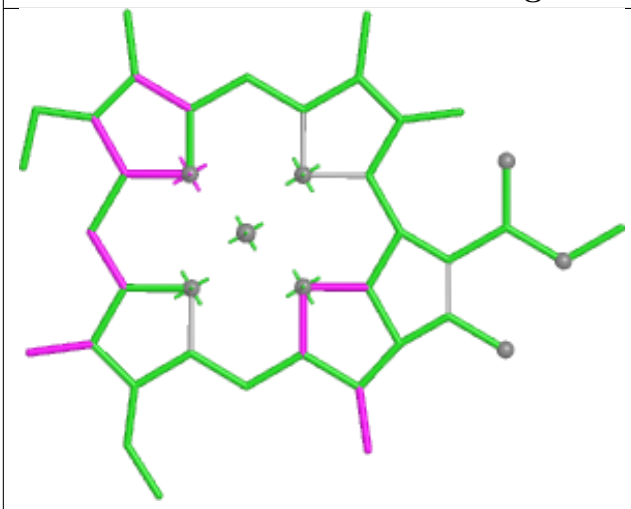


Rings

Ligand CLA B 314



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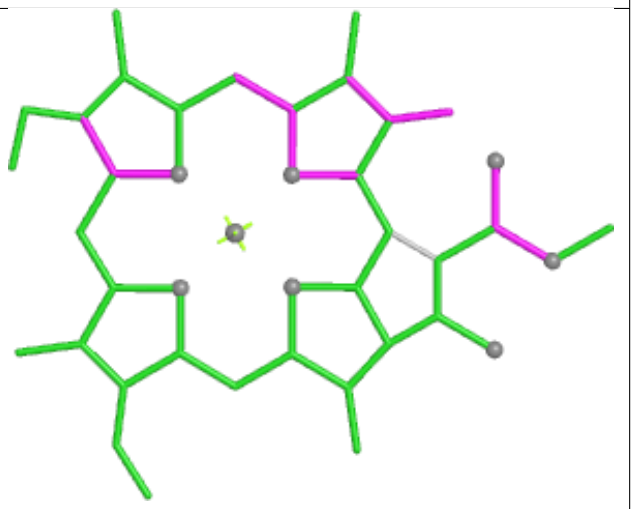

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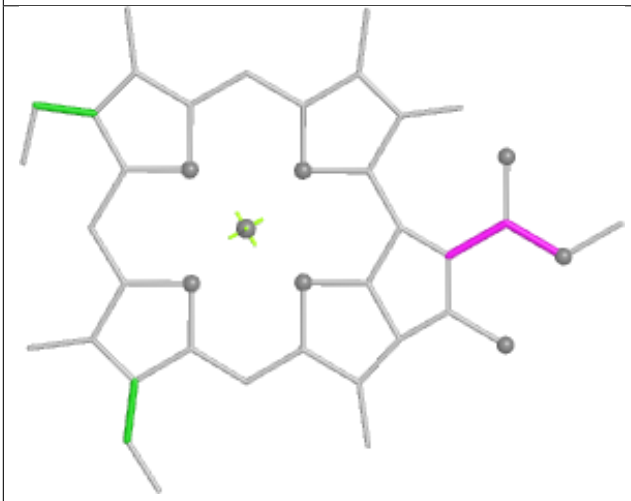

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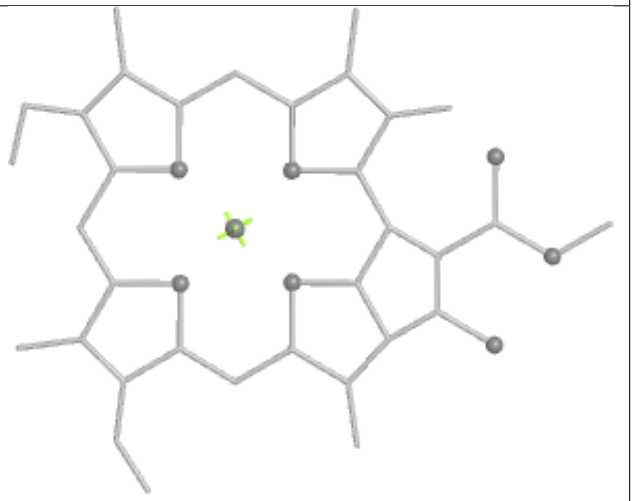
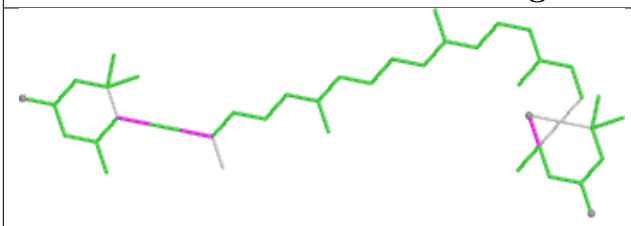


Rings

Ligand DD6 J 301



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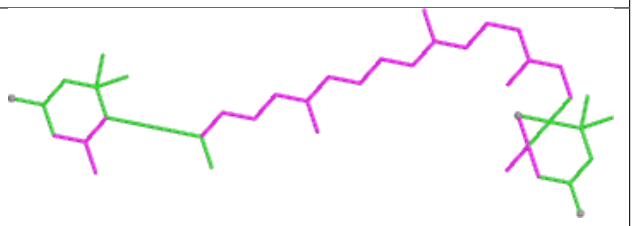
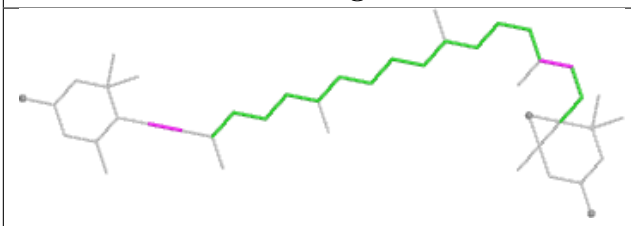


Bond angles



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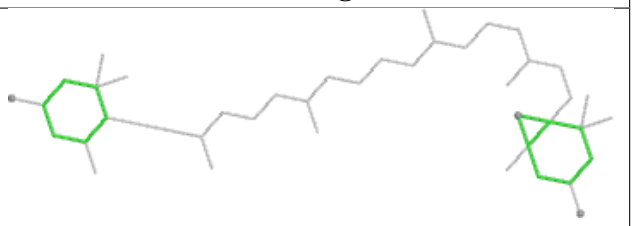
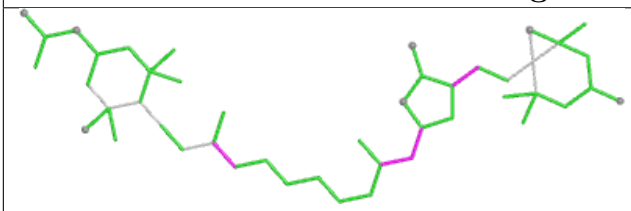


Rings

Ligand PID E 301



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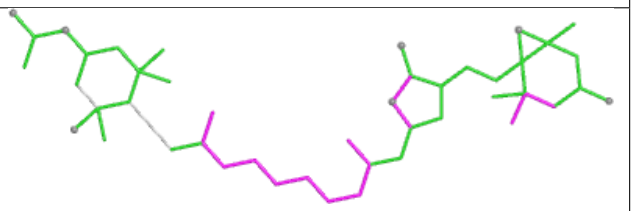
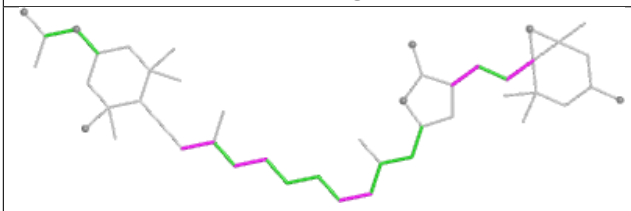


Bond angles



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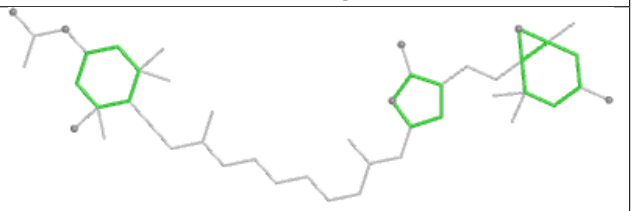
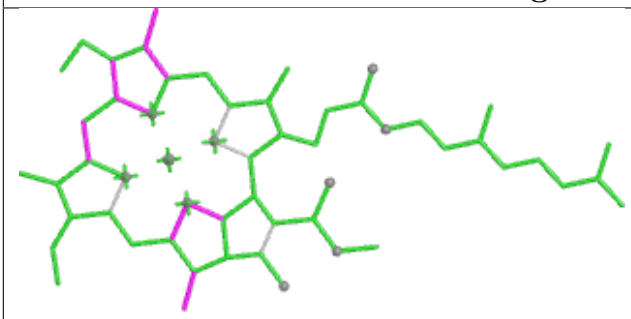
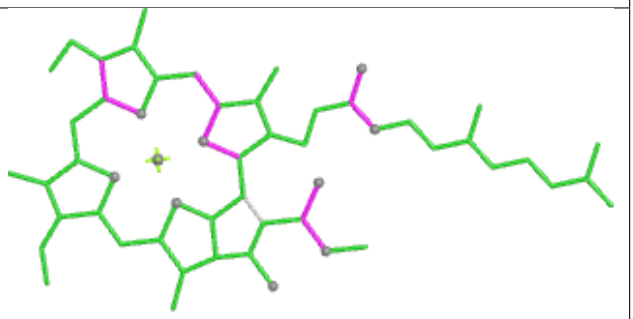


Rings

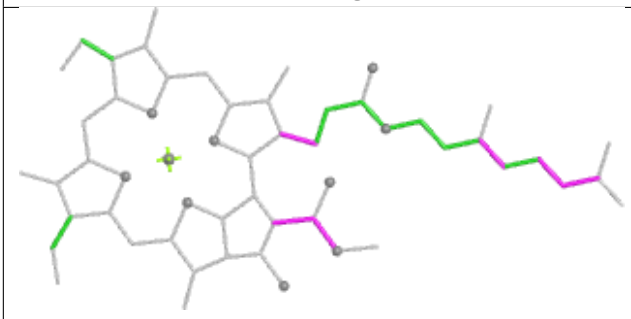
Ligand CLA I 217



Bond lengths



Bond angles



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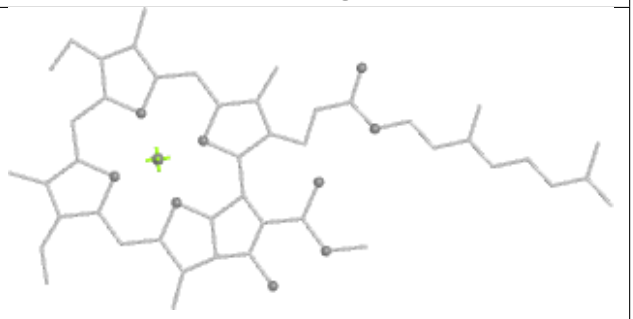
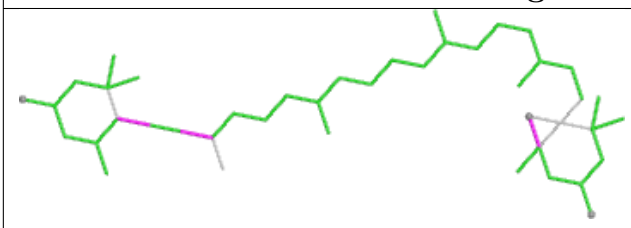
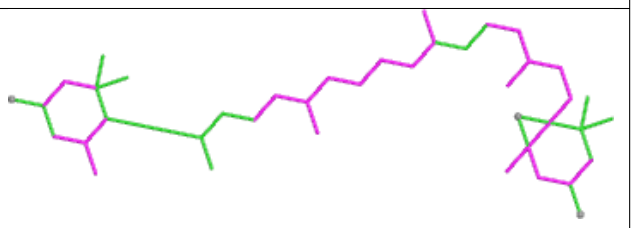


Rings

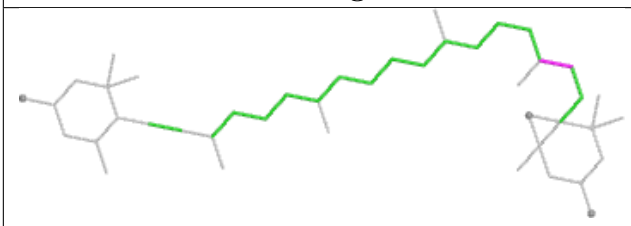
Ligand DD6 L 304



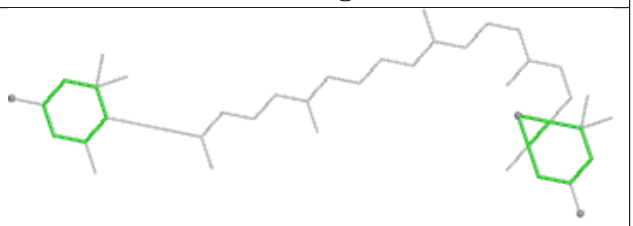
Bond lengths



Bond angles

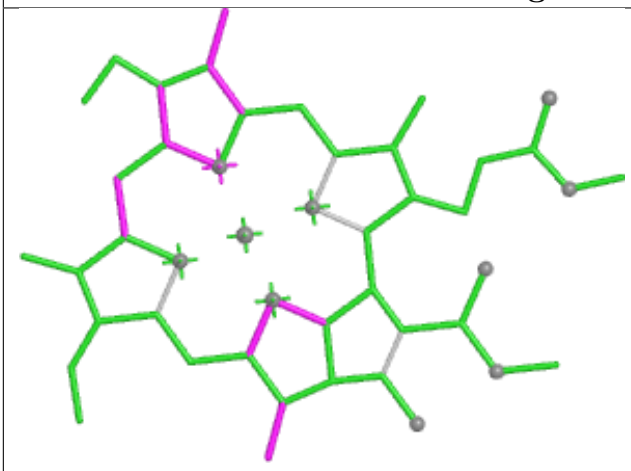


Torsions



Rings

Ligand CLA J 305



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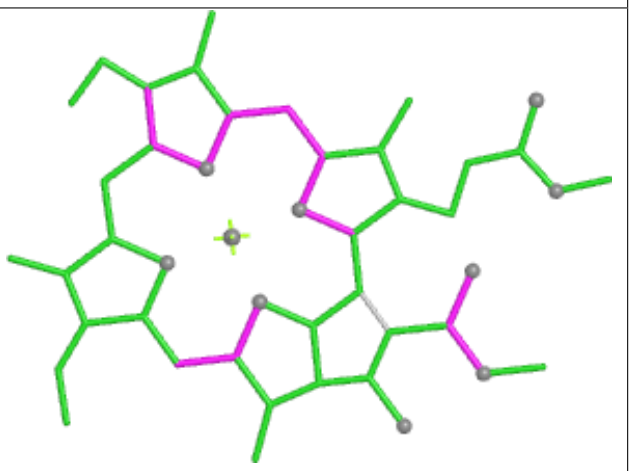

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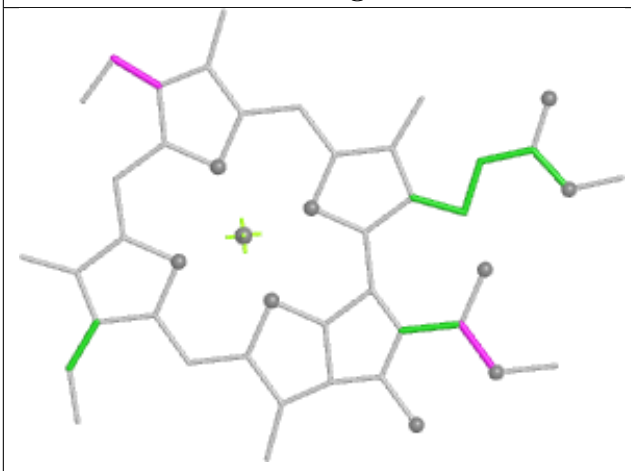

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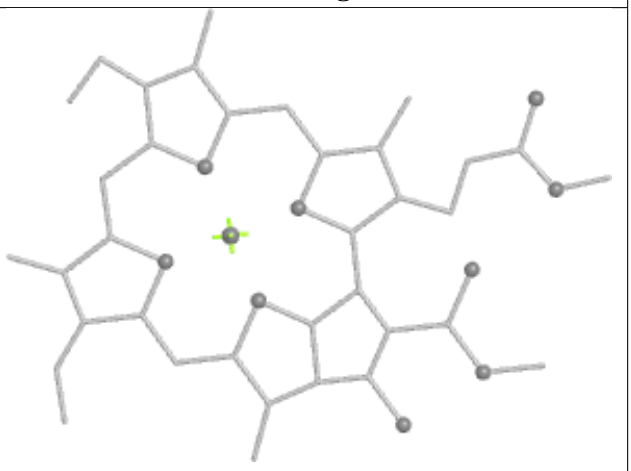
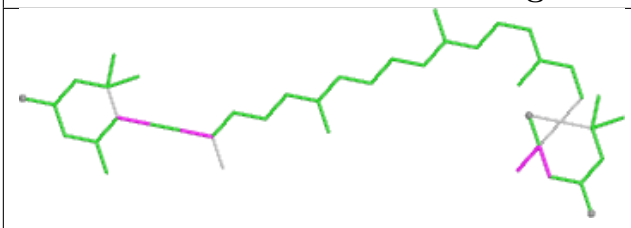


Rings

Ligand DD6 F 301



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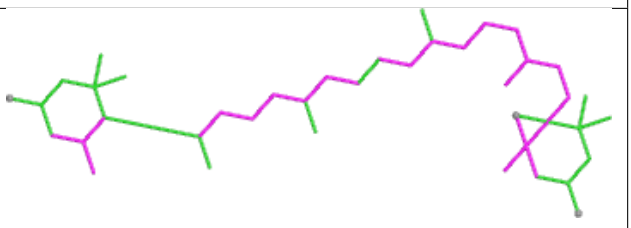
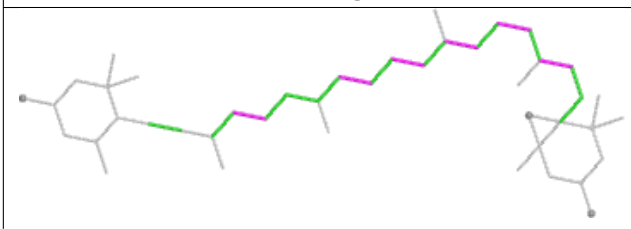


Bond angles



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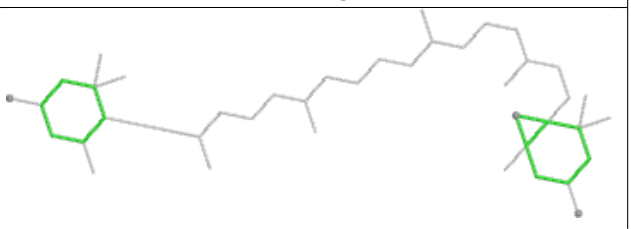
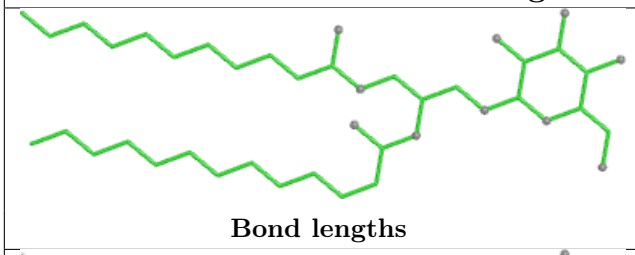


Rings

Ligand LMG j 102



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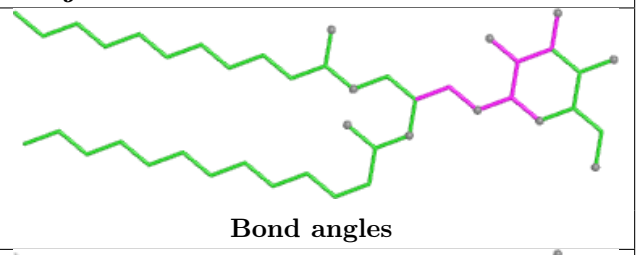

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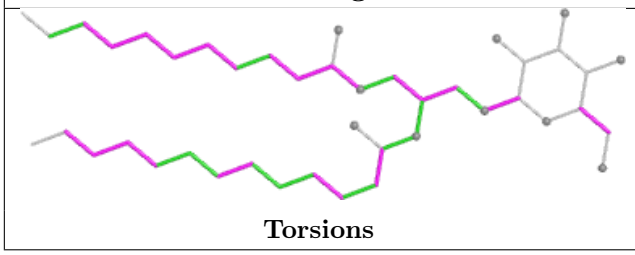

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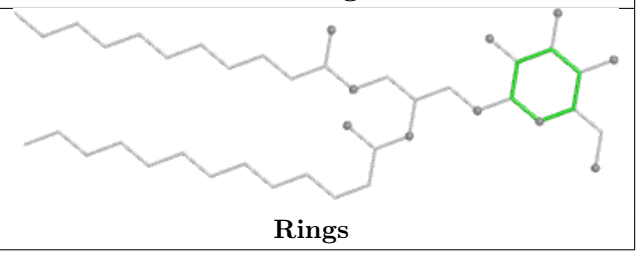
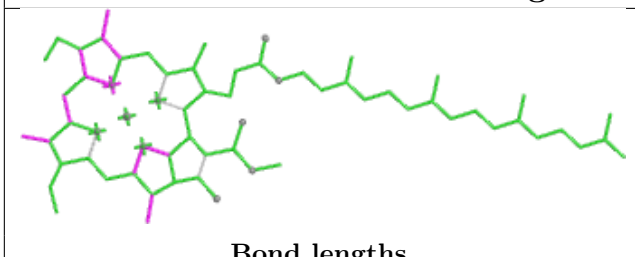


Rings

Ligand CLA b 707



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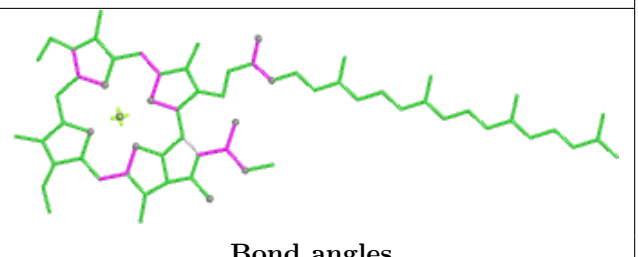
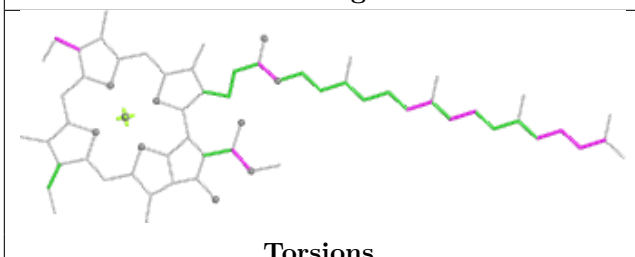


Bond angles



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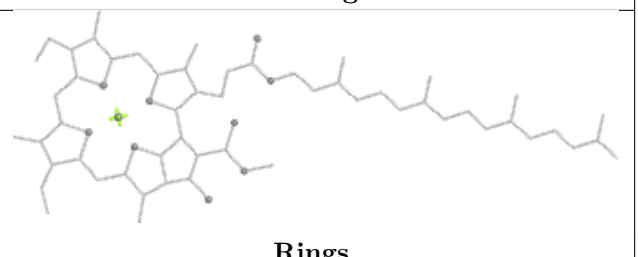
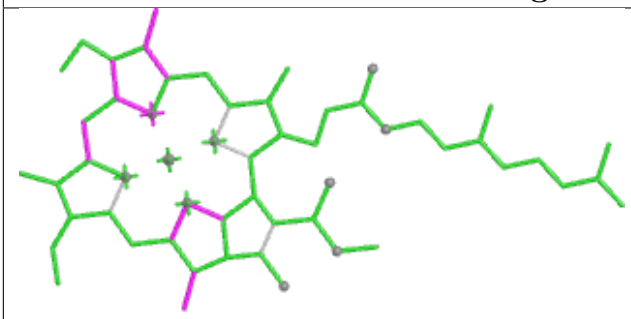


Rings

Ligand CLA I 210



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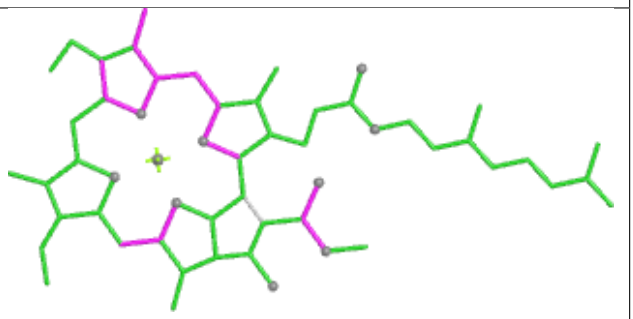
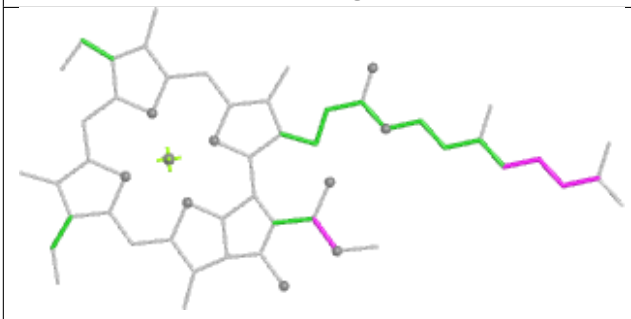


Bond angles



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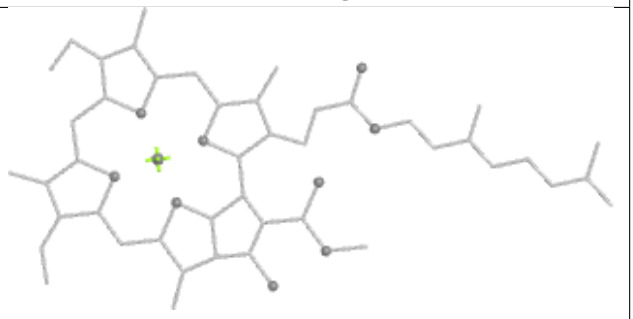
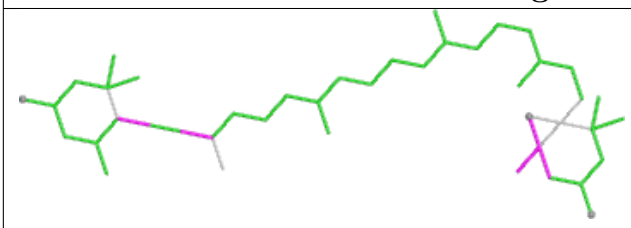


Rings

Ligand DD6 I 204



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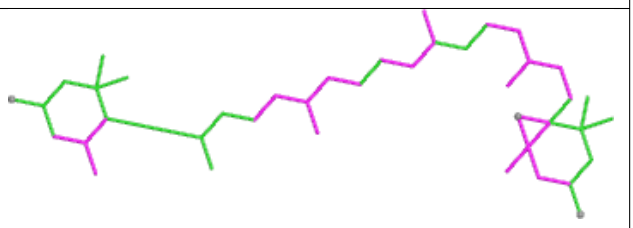
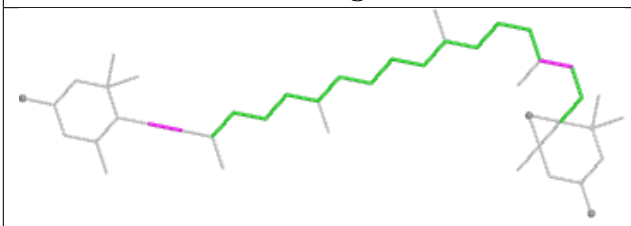


Bond angles



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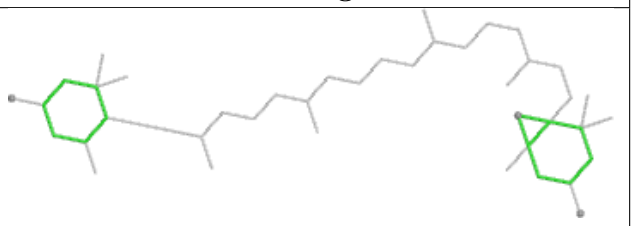
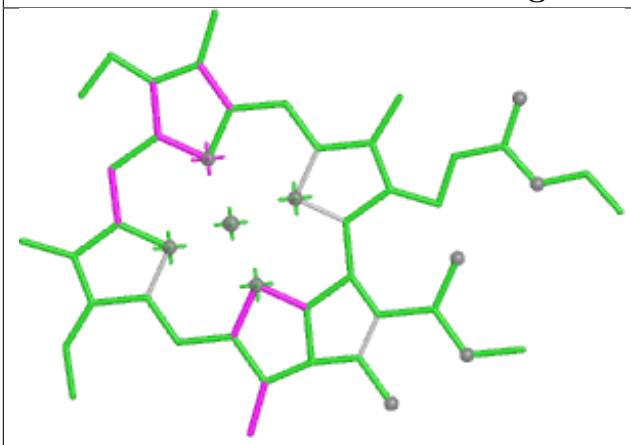


Rings

Ligand CLA a 821



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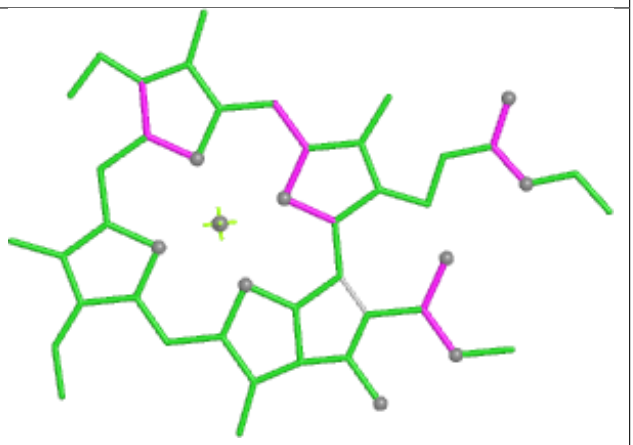
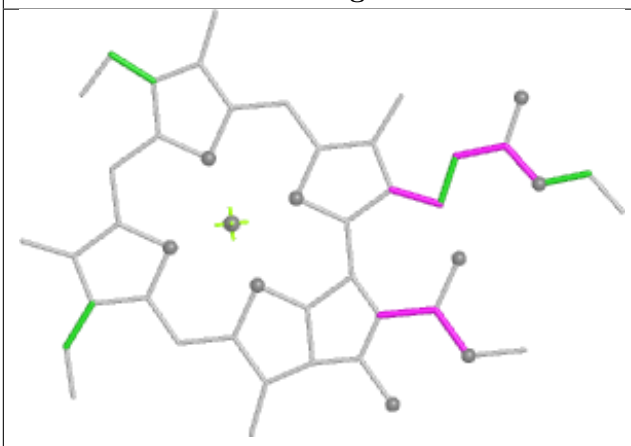


Bond angles



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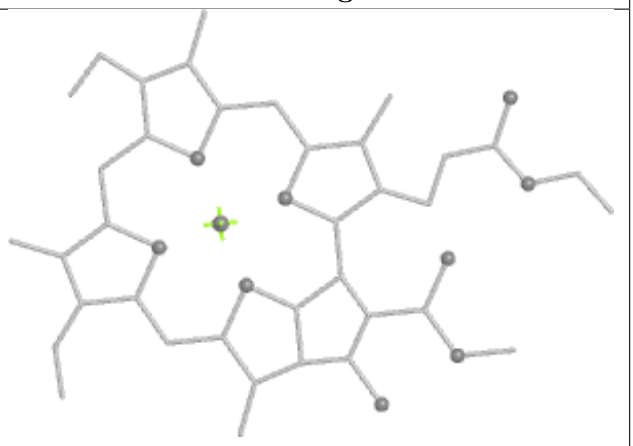
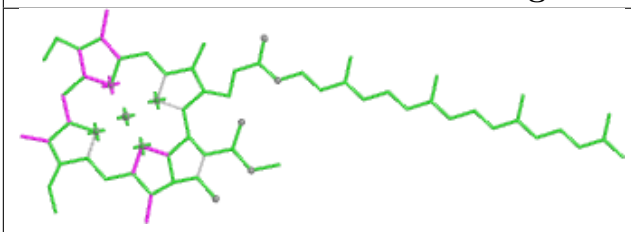


Rings

Ligand CLA a 806



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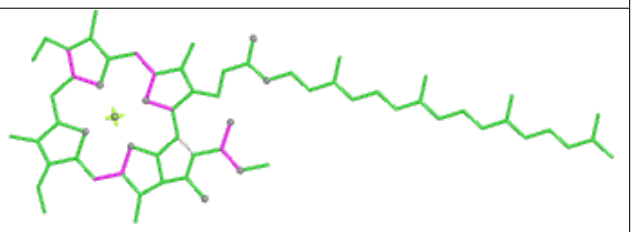
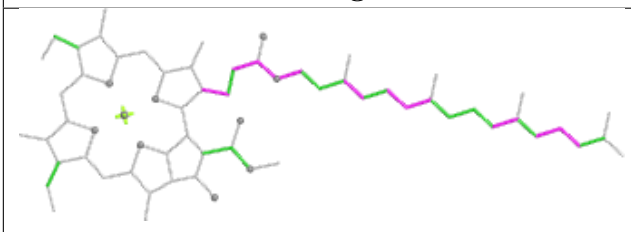


Bond angles



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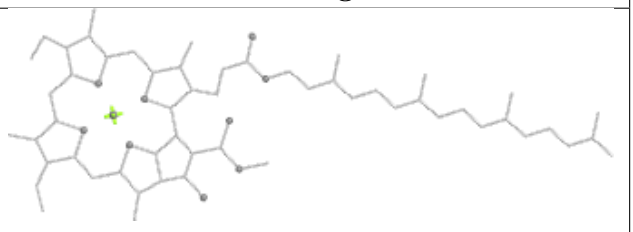
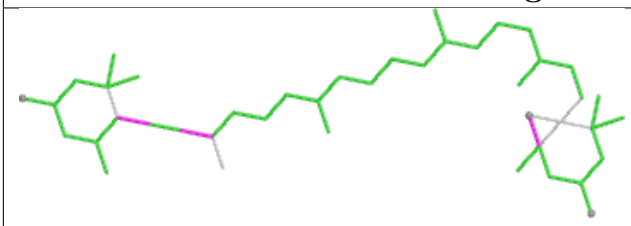


Rings

Ligand DD6 Q 302



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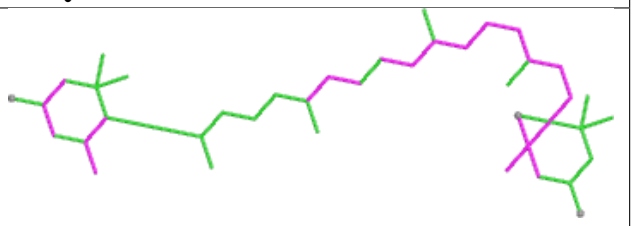
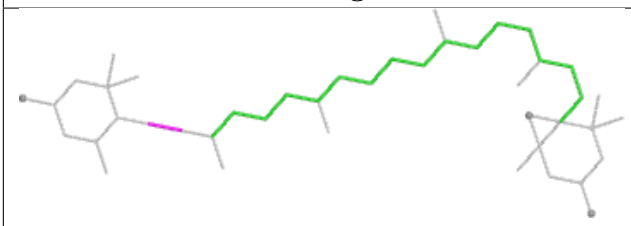


Bond angles



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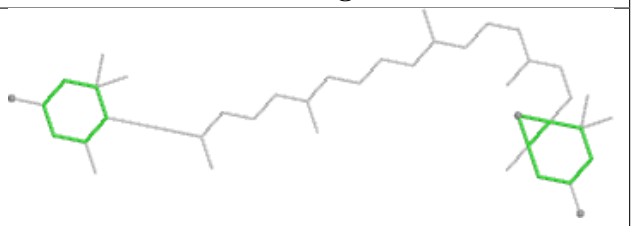
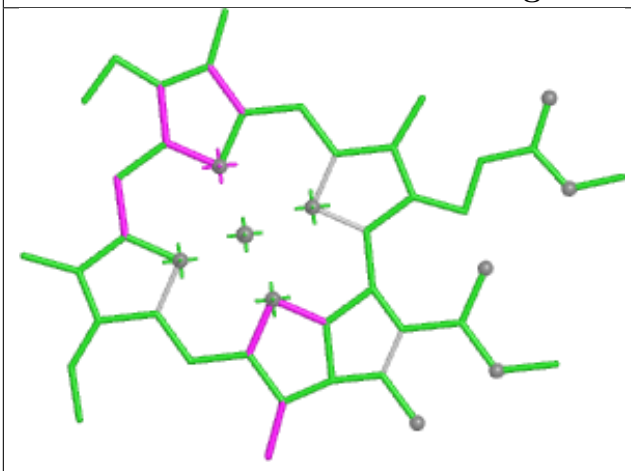


Rings

Ligand CLA D 311



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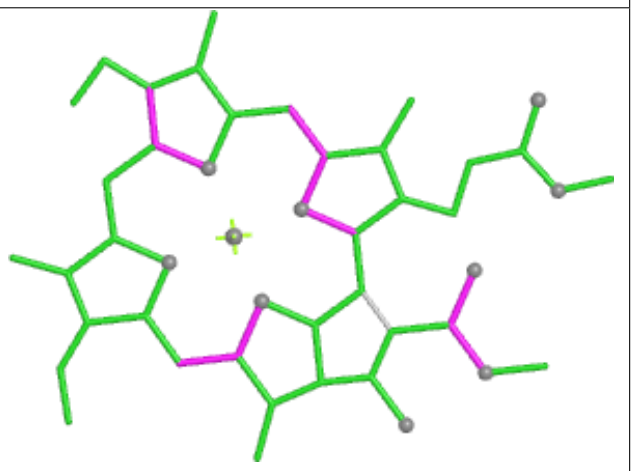
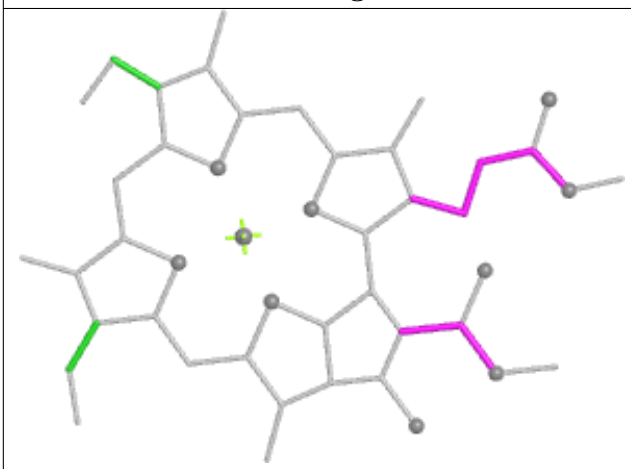


Bond angles



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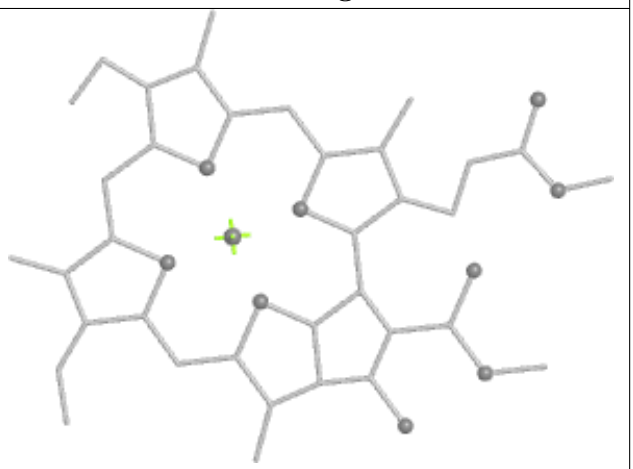
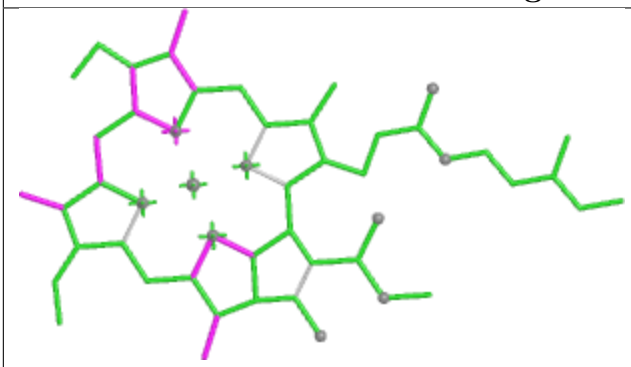


Rings

Ligand CLA B 311



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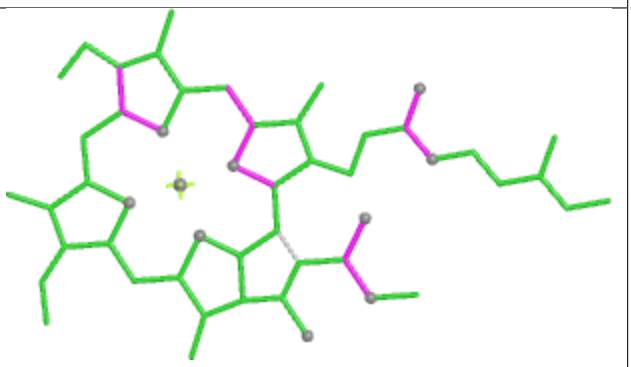
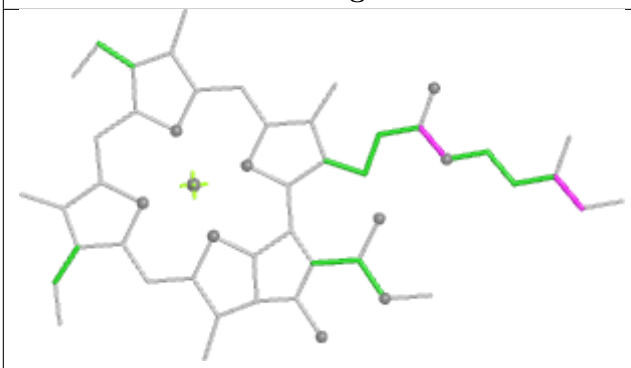


Bond angles



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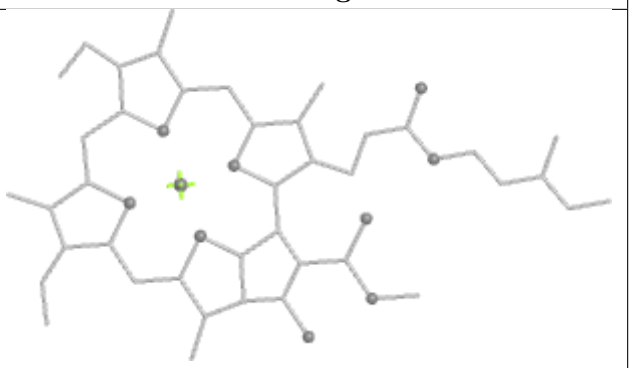
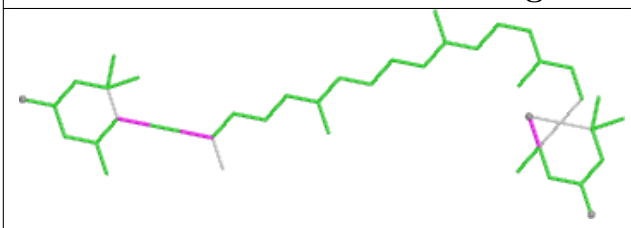


Rings

Ligand DD6 T 303



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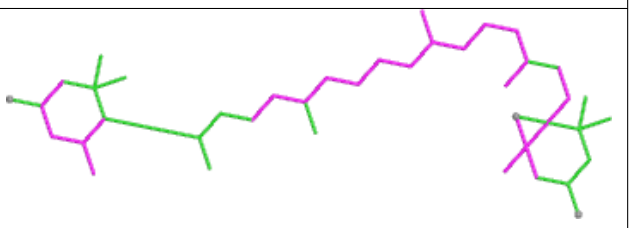
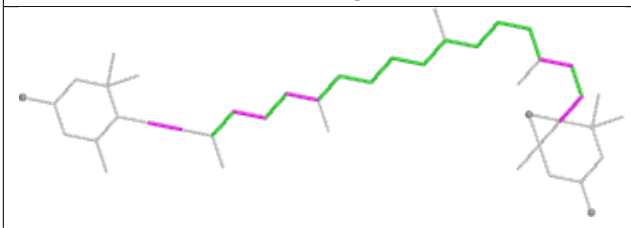


Bond angles



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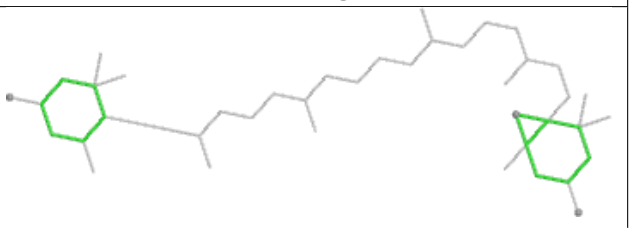
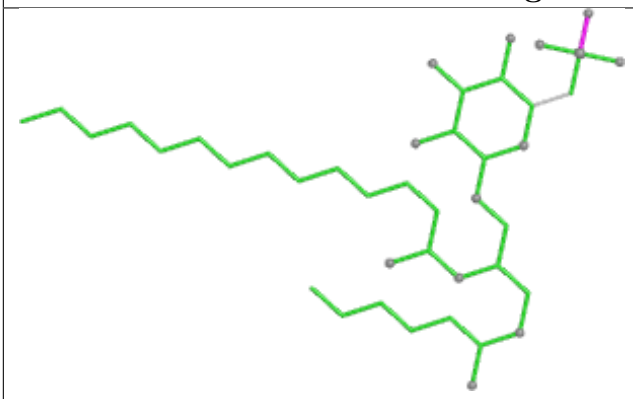


Rings

Ligand SQD B 317



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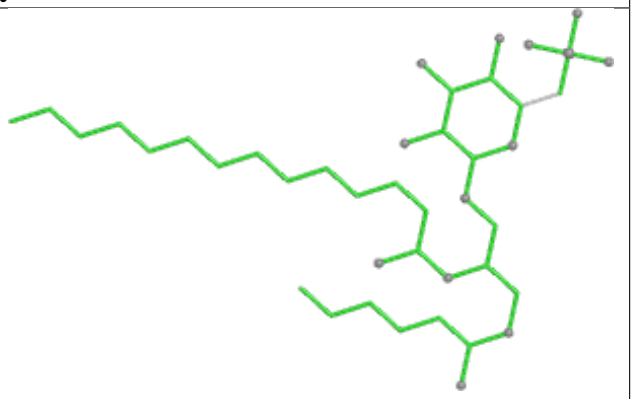
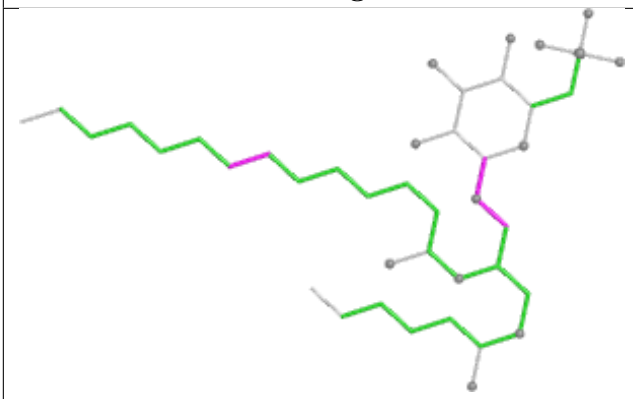


Bond angles



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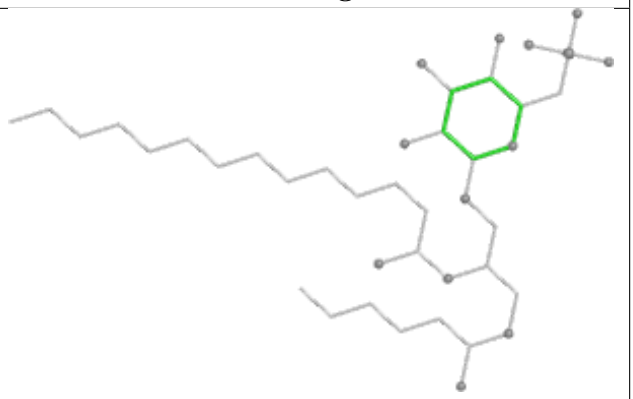
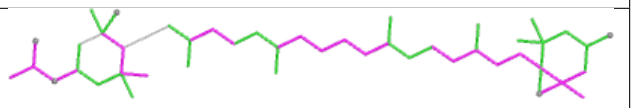


Rings

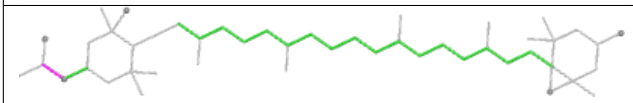
Ligand UIX B 304



Bond lengths



Bond angles



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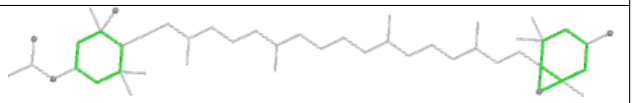
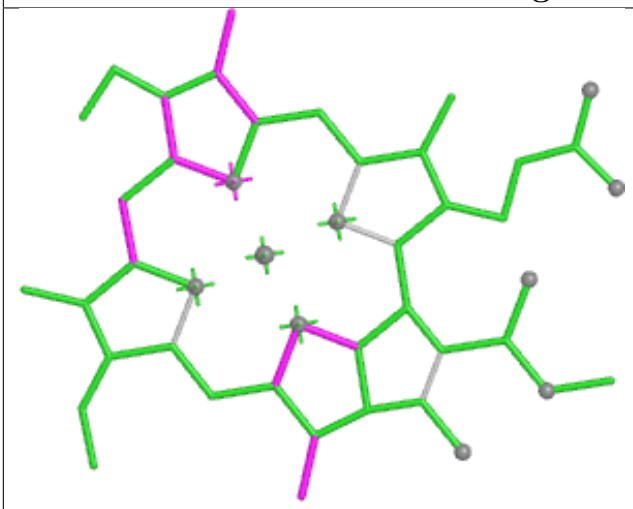
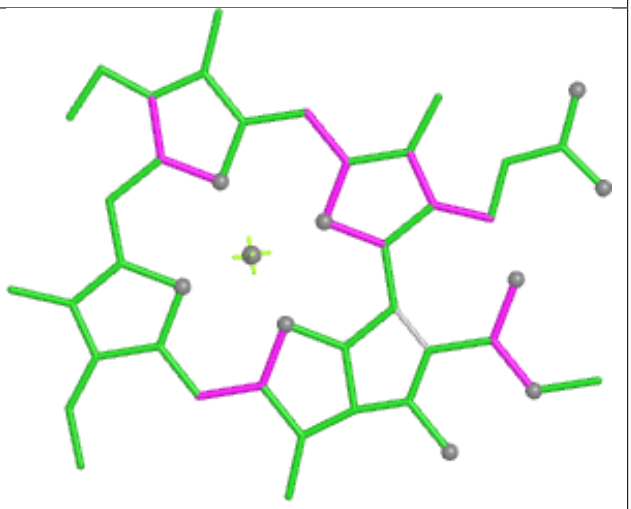


Rings

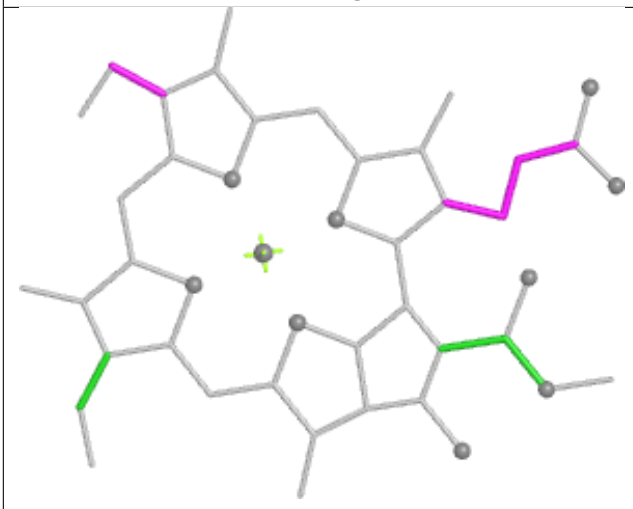
Ligand CLA l 510



Bond lengths



Bond angles

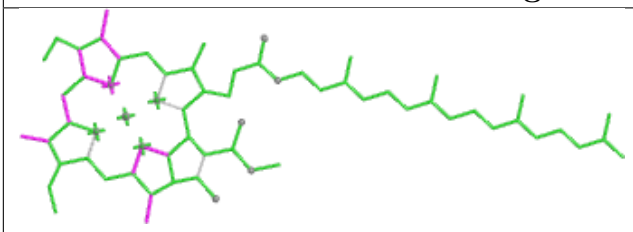


Torsions



Rings

Ligand CLA Q 308



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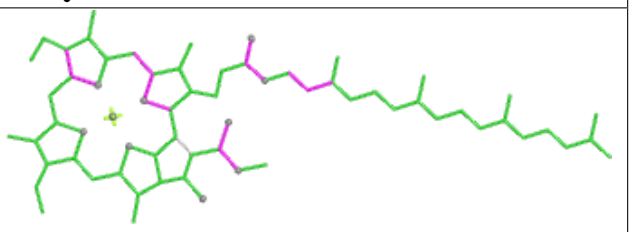

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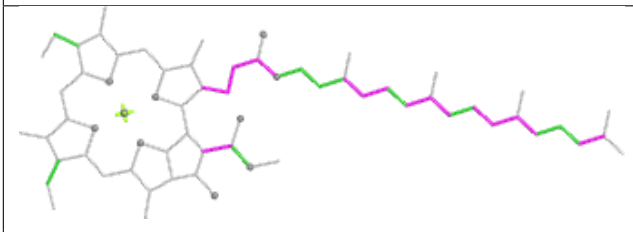

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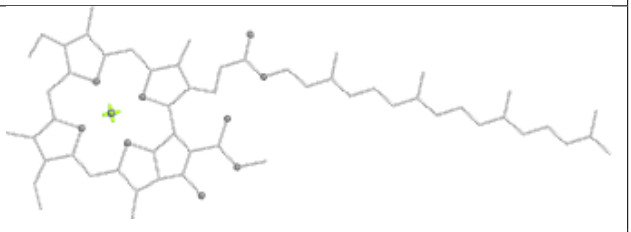
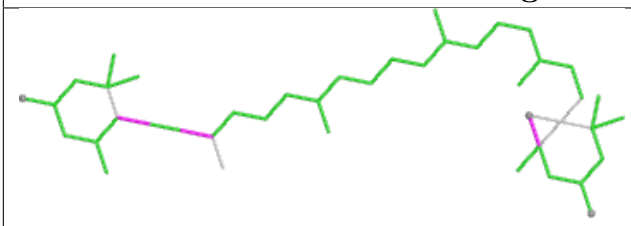


Rings

Ligand DD6 M 301



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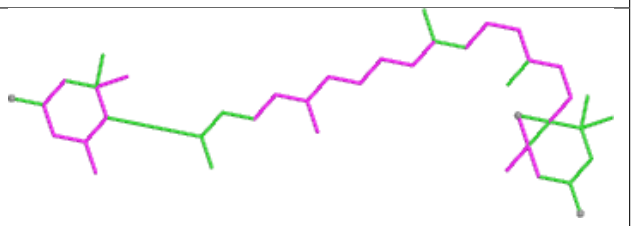

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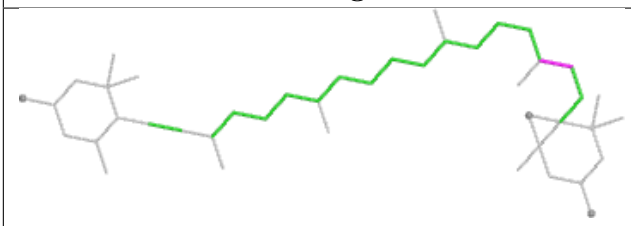

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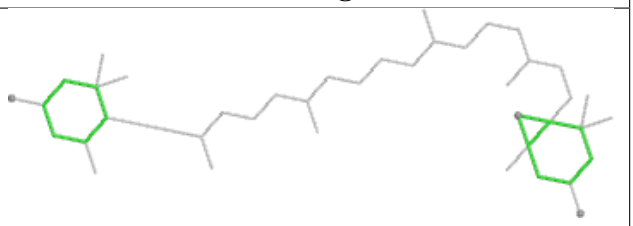
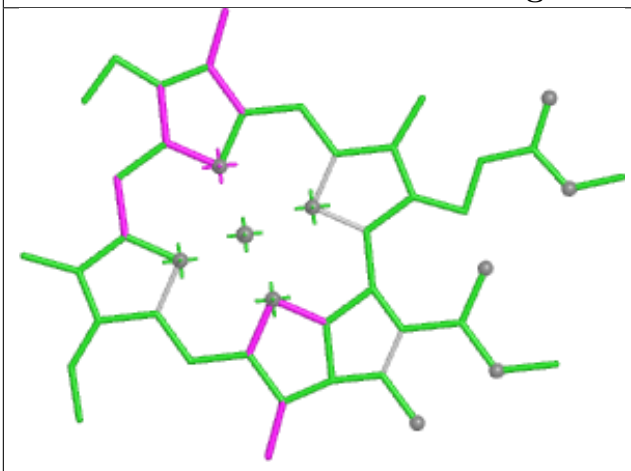


Rings

Ligand CLA L 317



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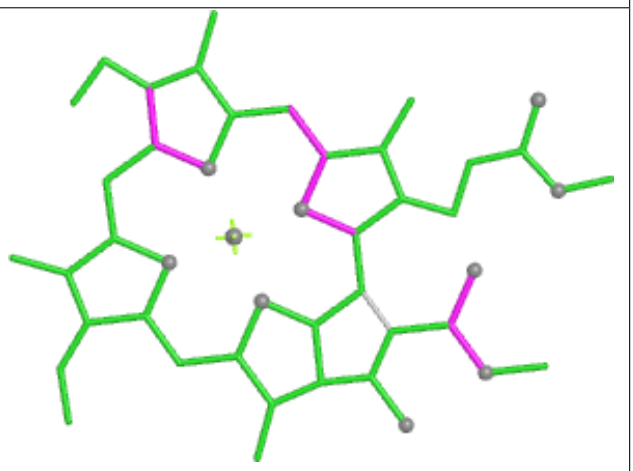

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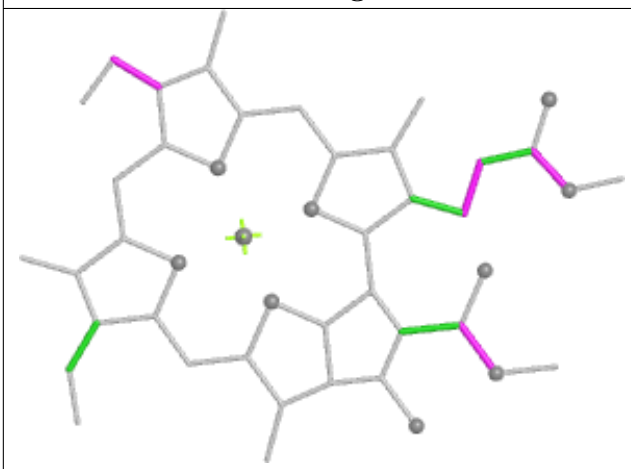

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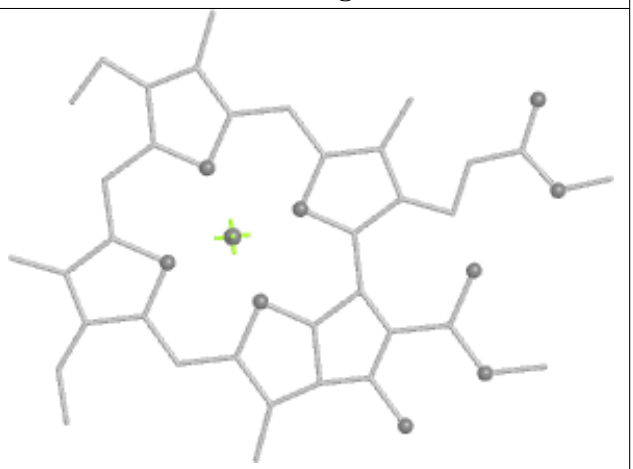
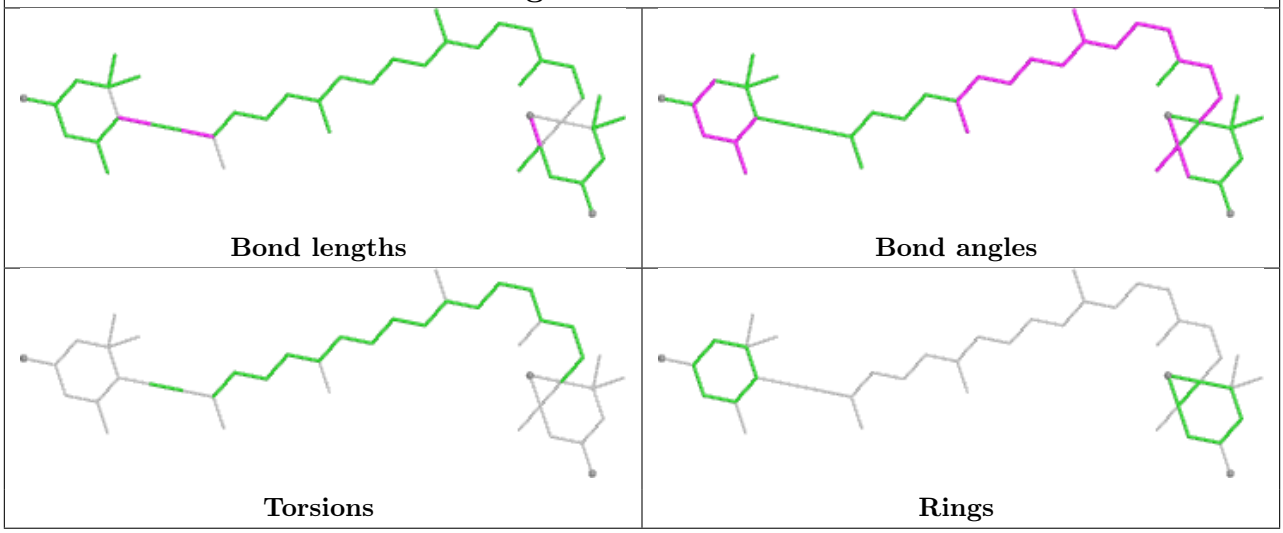
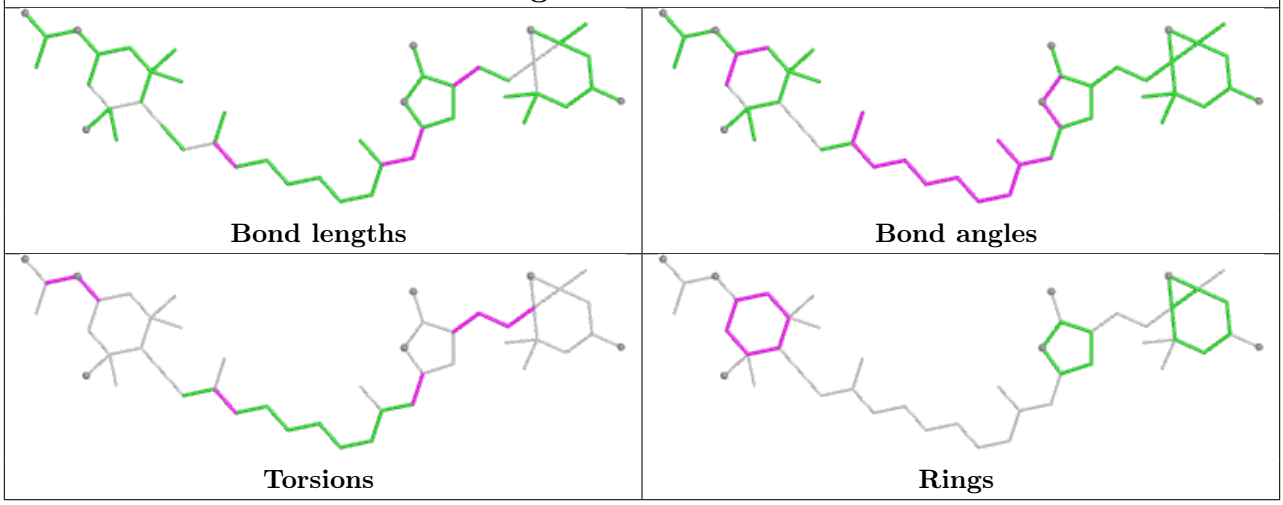


Rings

Ligand DD6 C 303



Ligand PID T 317



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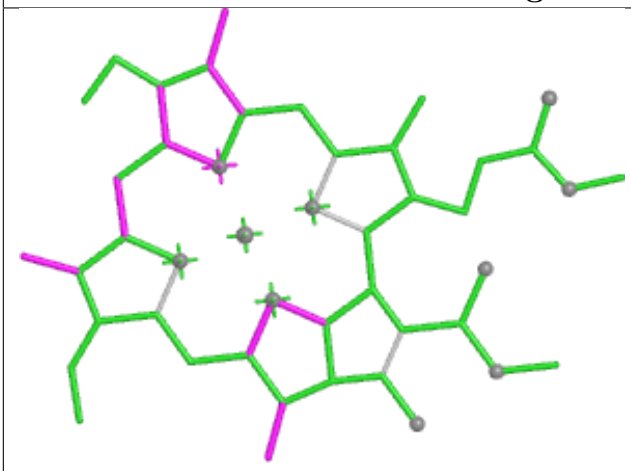

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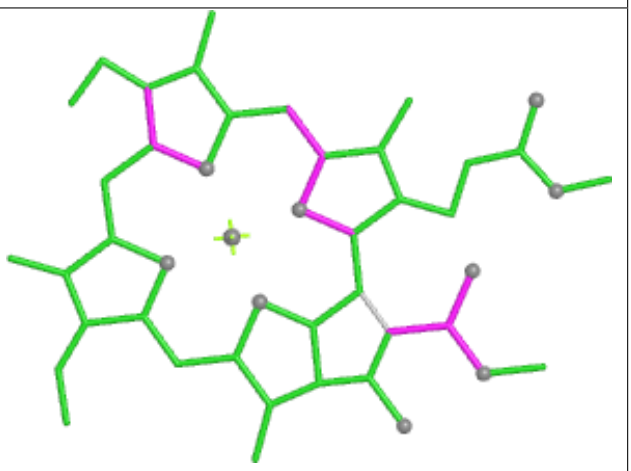
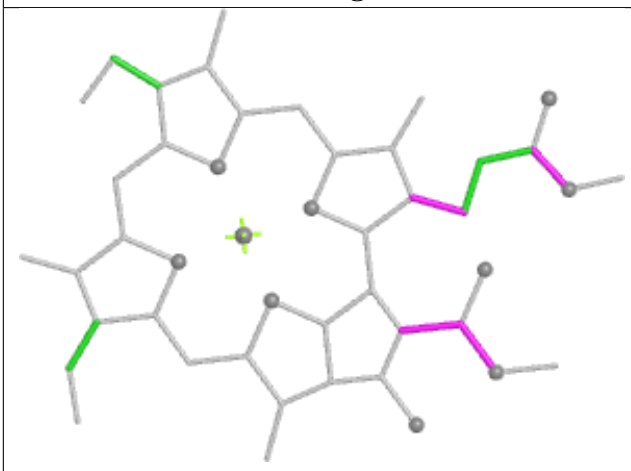


Bond angles



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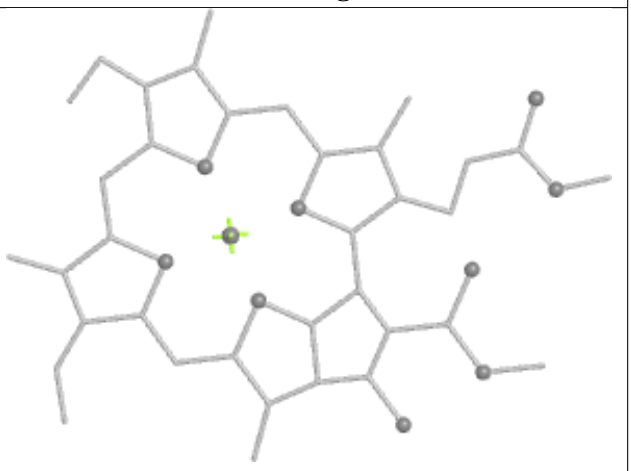

Rings

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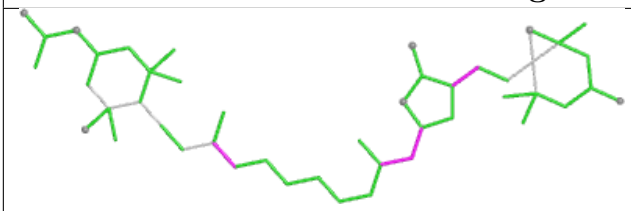

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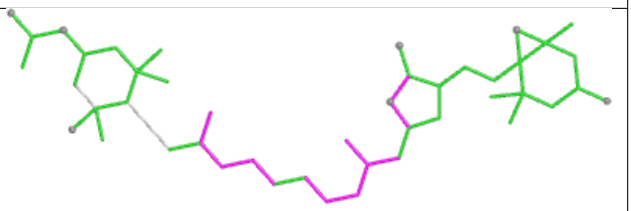
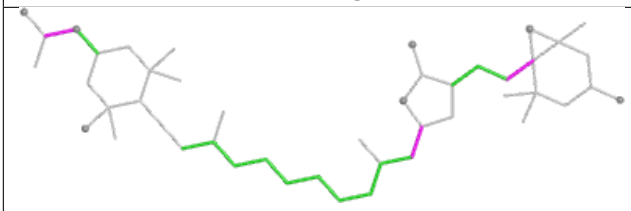


Bond angles



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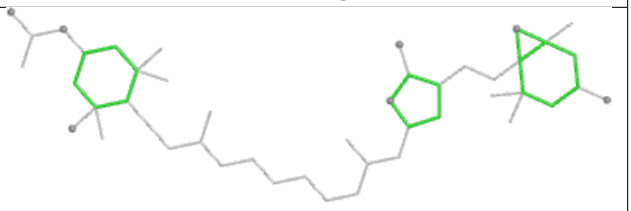
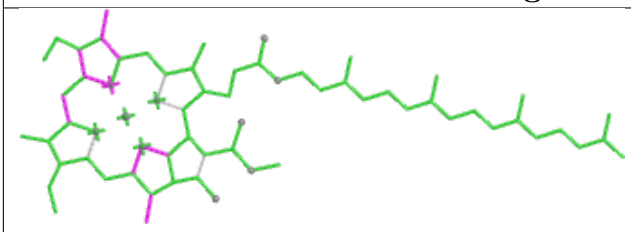


Rings

Ligand CLA Q 310



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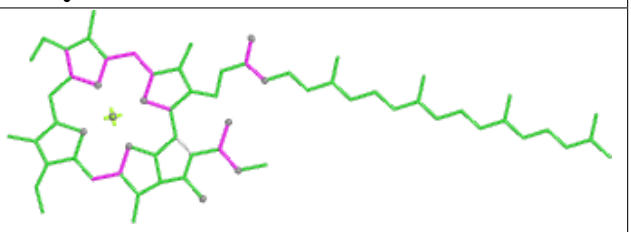
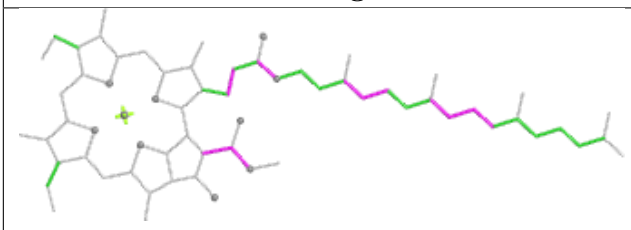


Bond angles



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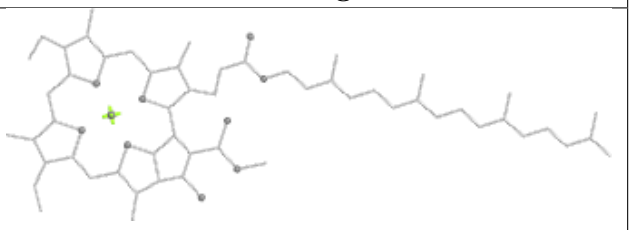
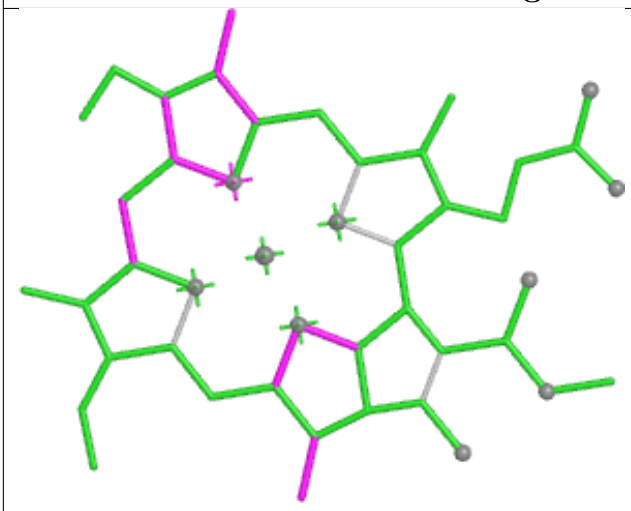


Rings

Ligand CLA A 206



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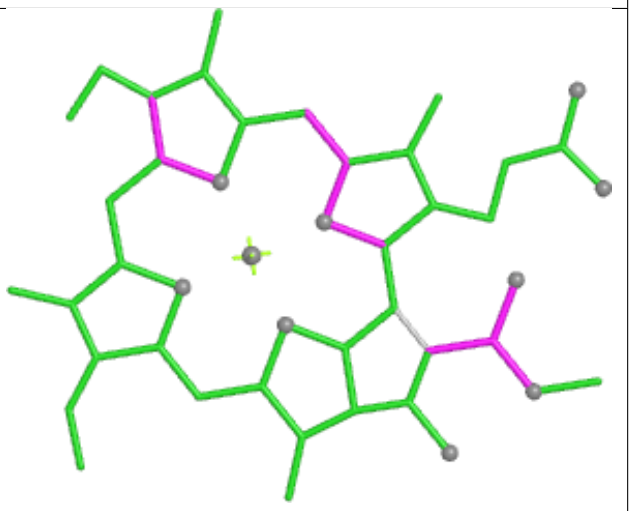
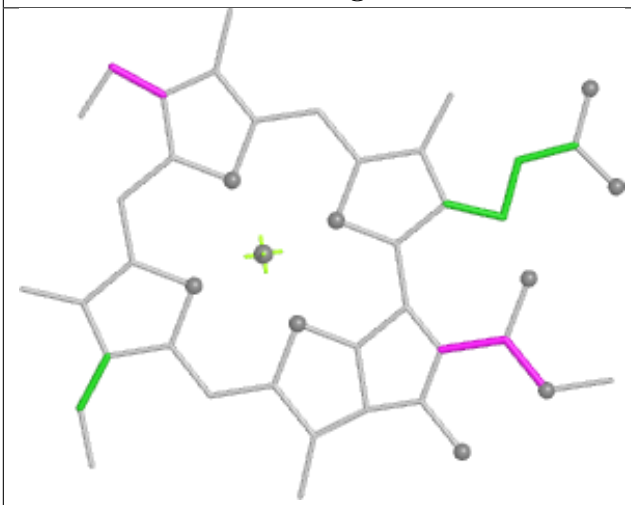


Bond angles



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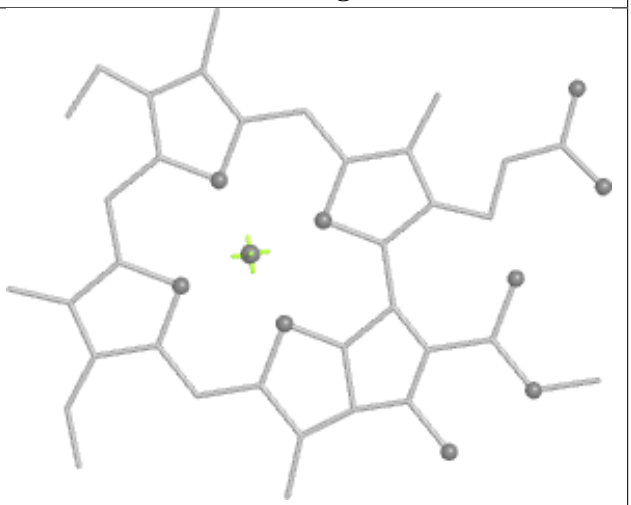
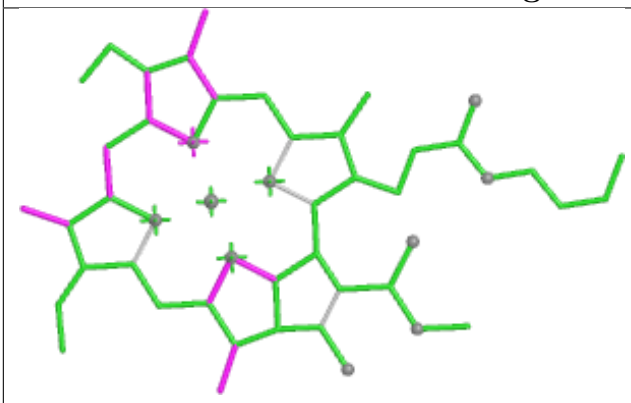


Rings

Ligand CLA G 301



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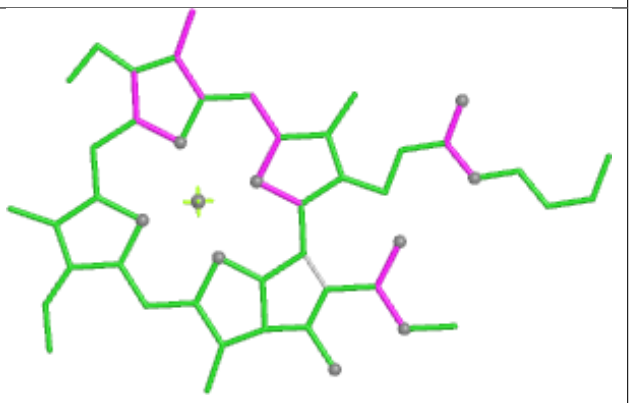

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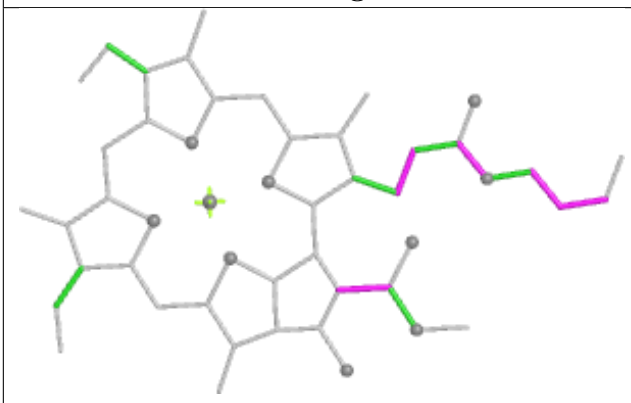

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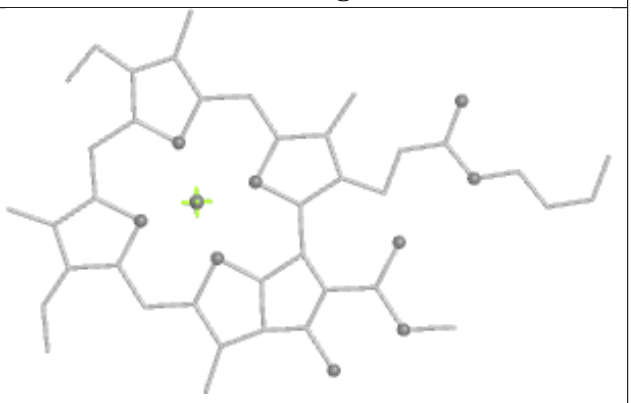
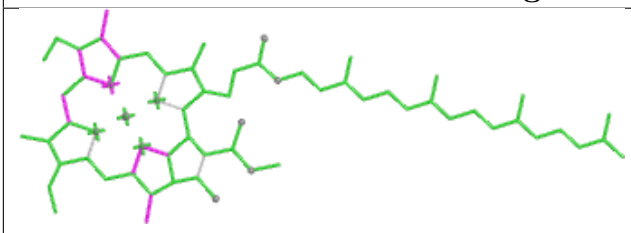


Rings

Ligand CLA H 308



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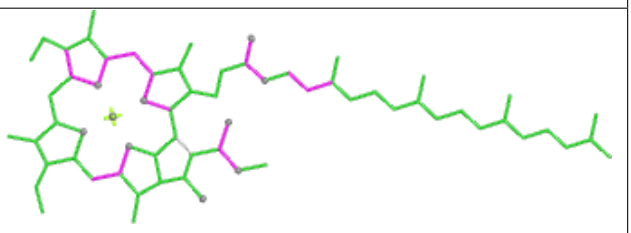

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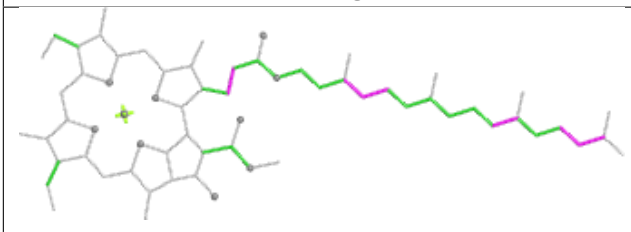

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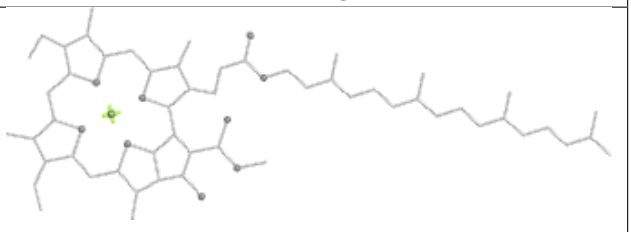
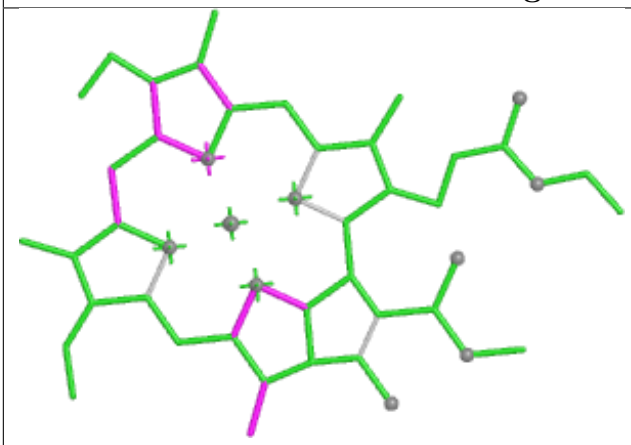


Rings

Ligand CLA O 308



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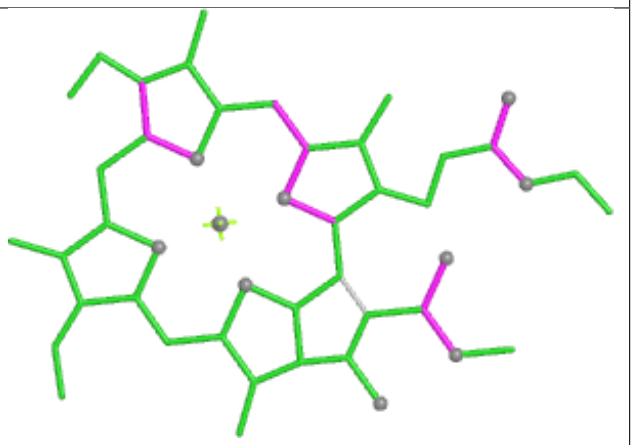

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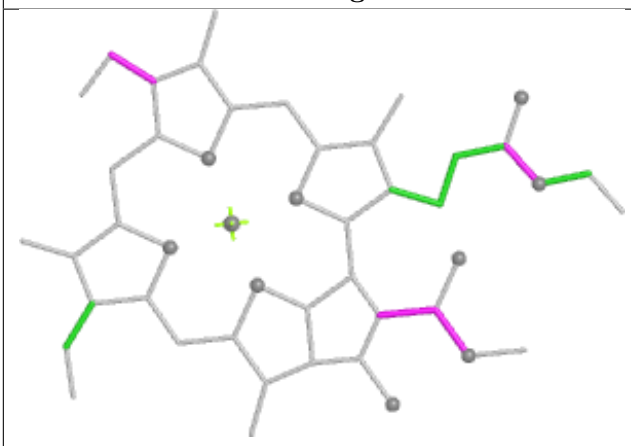

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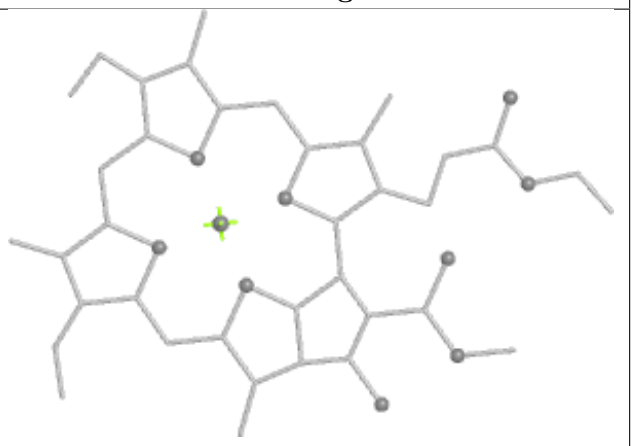
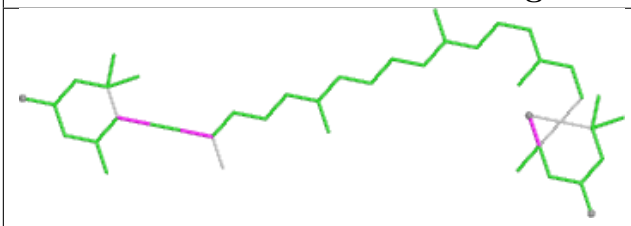


Rings

Ligand DD6 B 302



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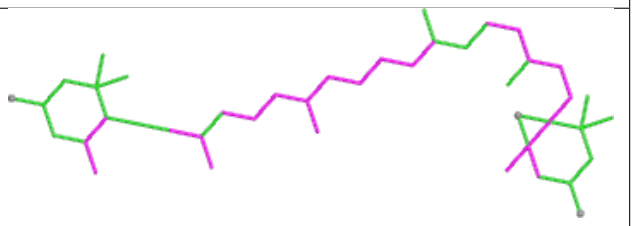
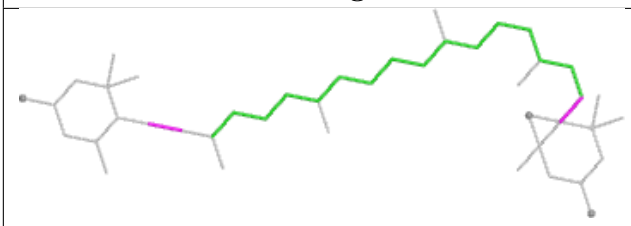


Bond angles

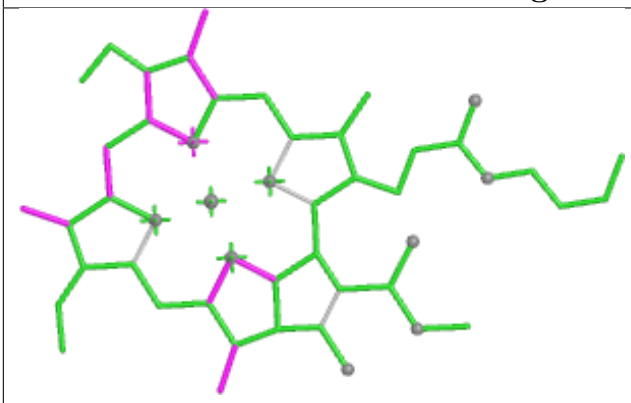


Torsions



Rings

Ligand CLA I 207



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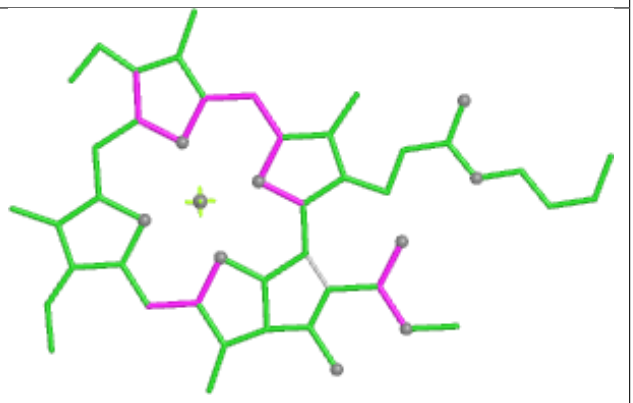
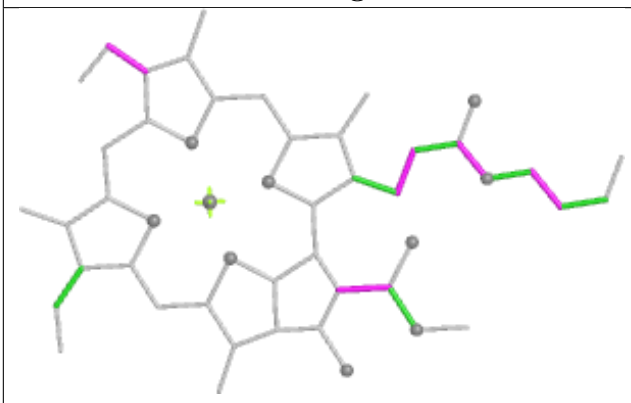


Bond angles



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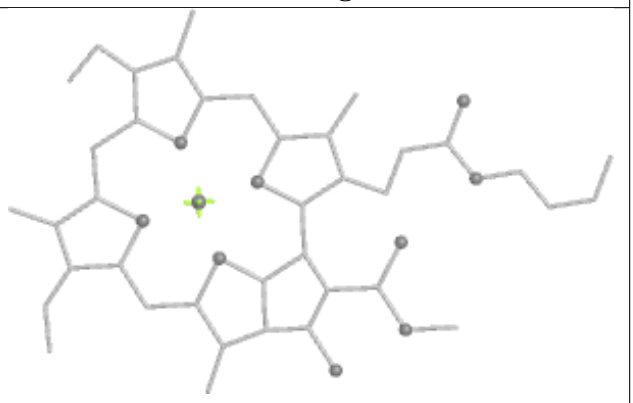
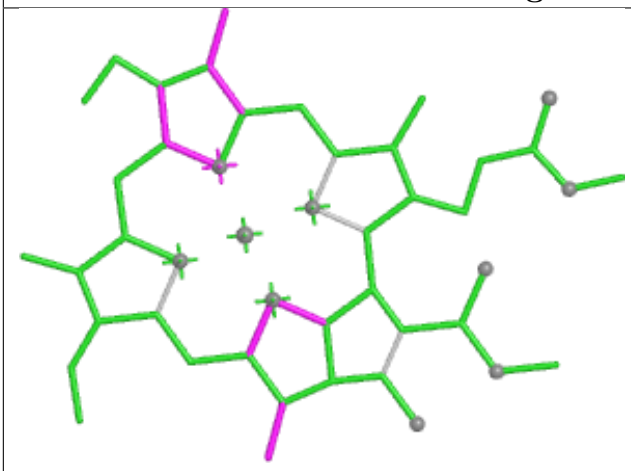


Rings

Ligand CLA F 313



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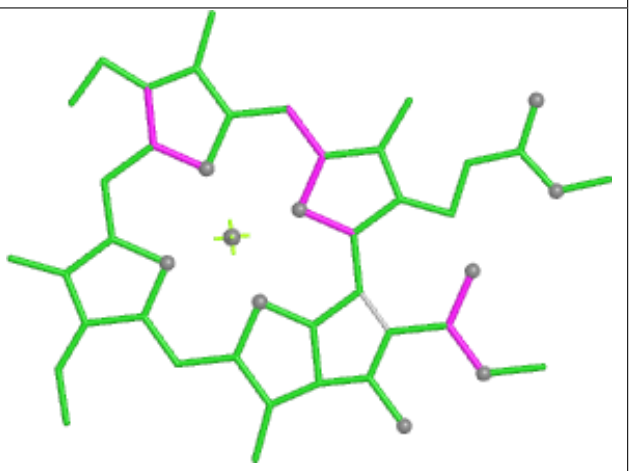
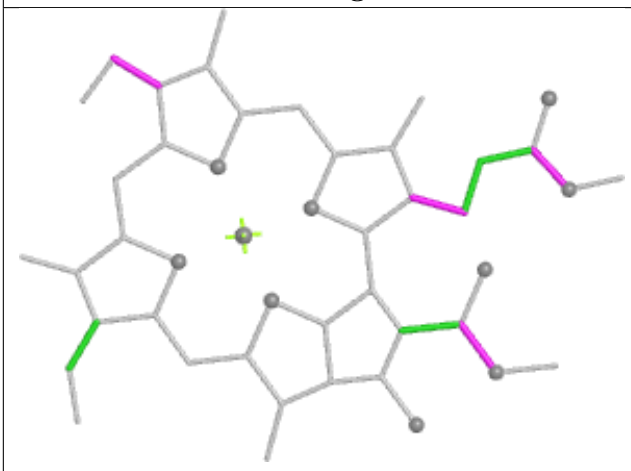


Bond angles



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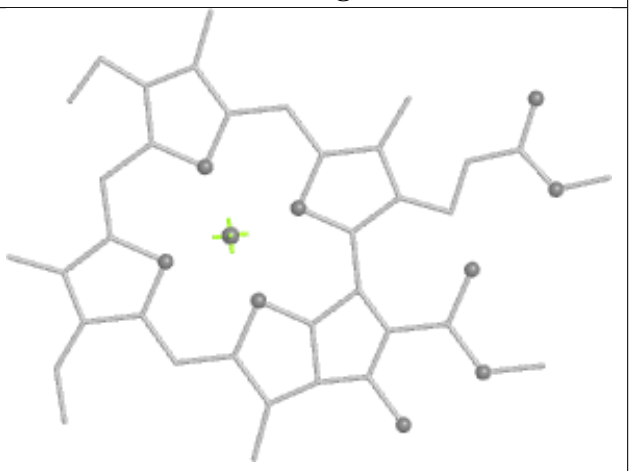
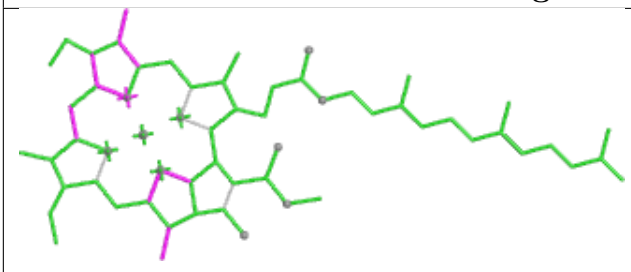
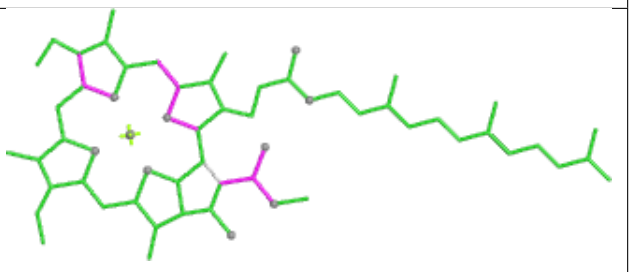


Rings

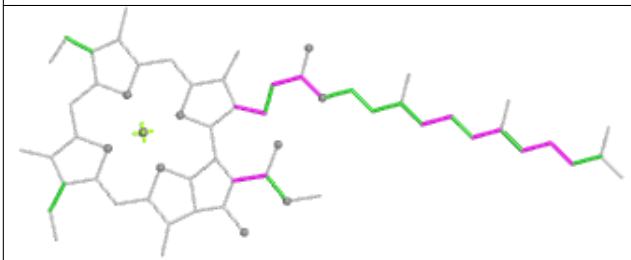
Ligand CLA l 501



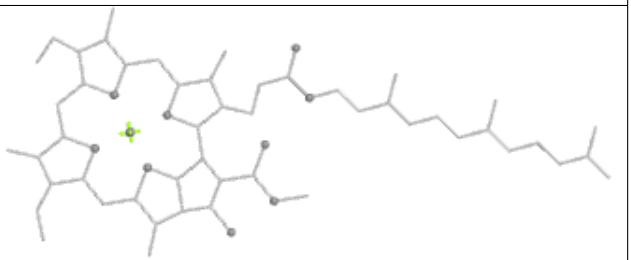
Bond lengths



Bond angles

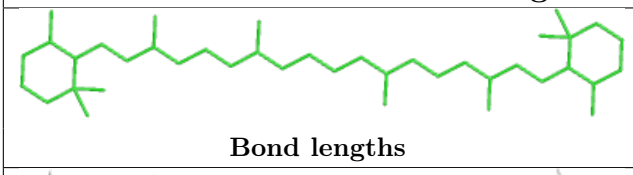


Torsions

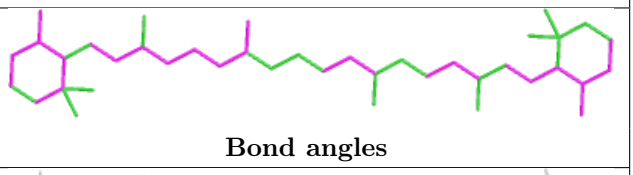


Rings

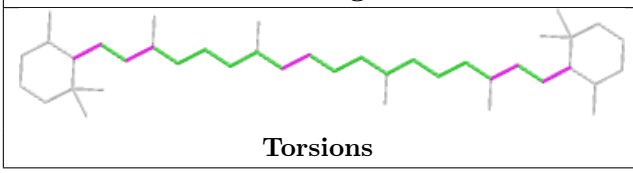
Ligand BCR l 506



Bond lengths



Bond angles



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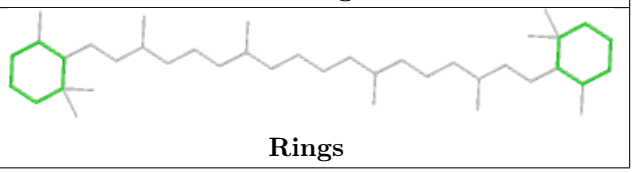
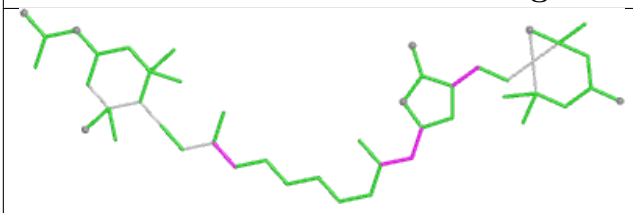


Rings

Ligand PID F 306



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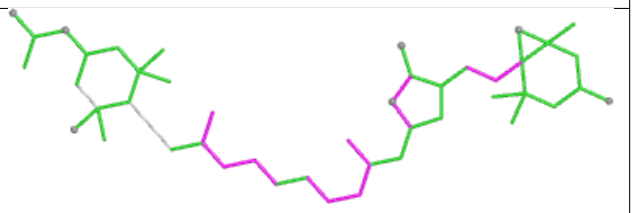
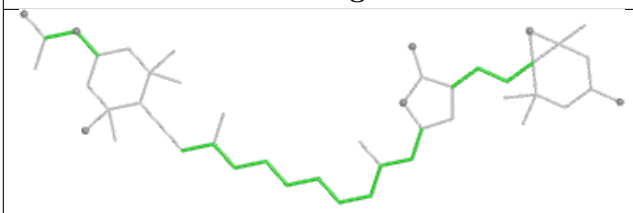


Bond angles



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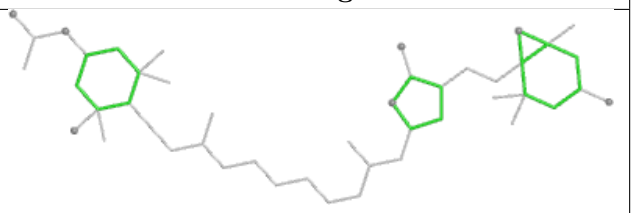
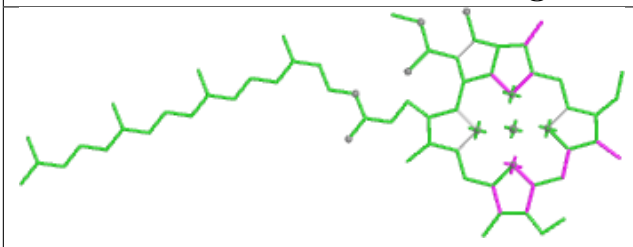


Rings

Ligand CLA a 831



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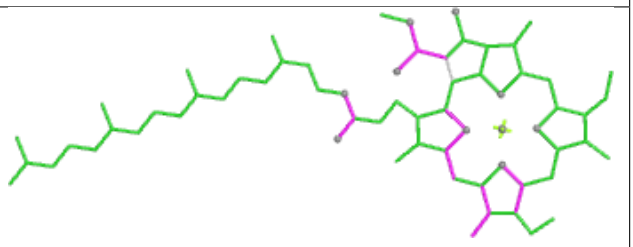
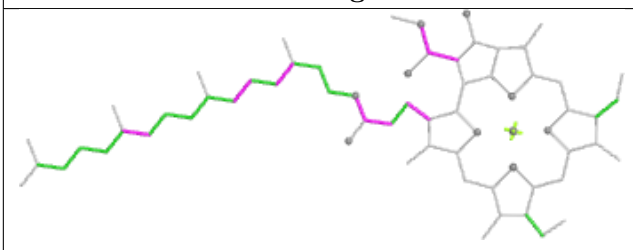


Bond angles



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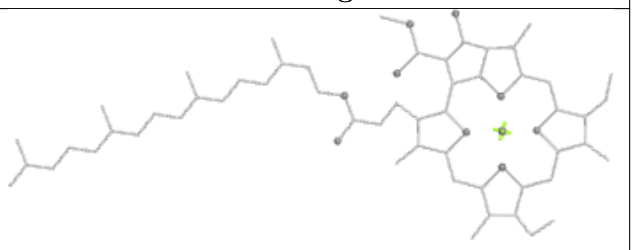
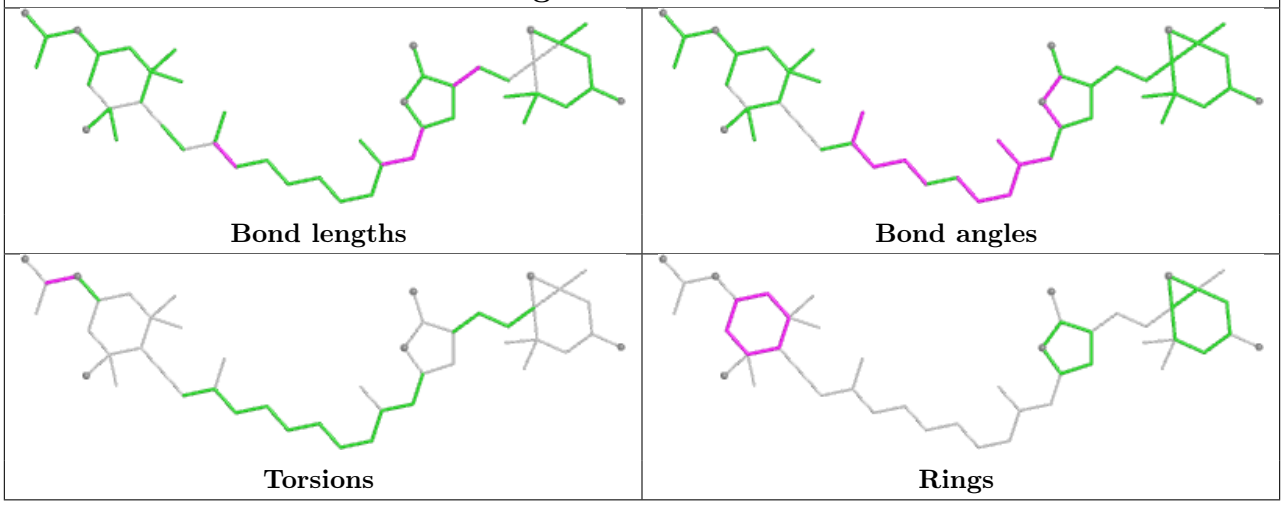
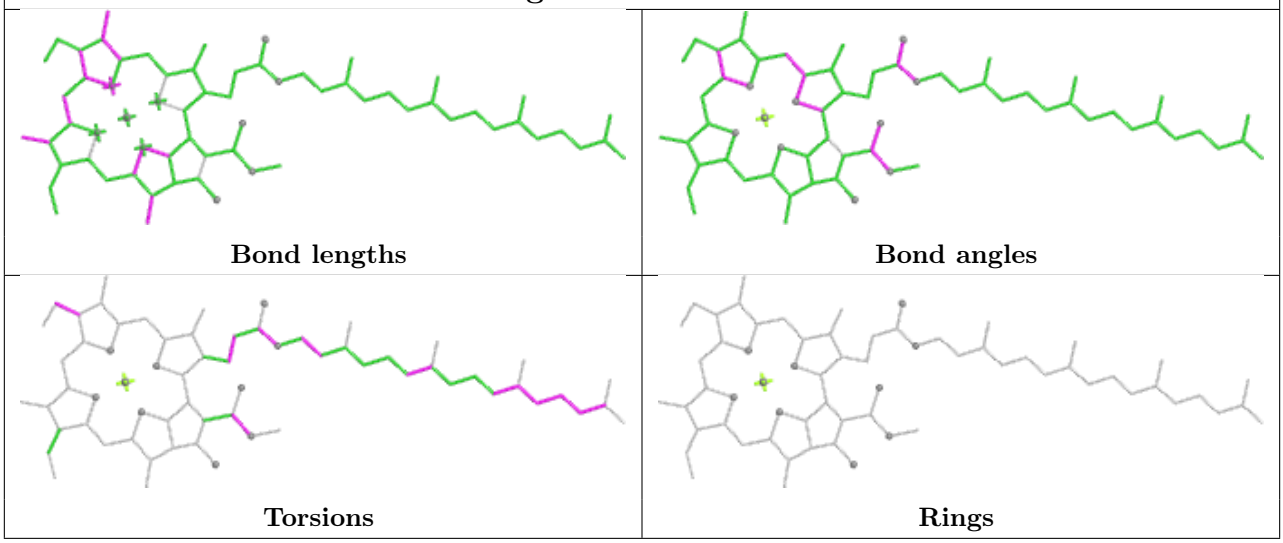


Rings

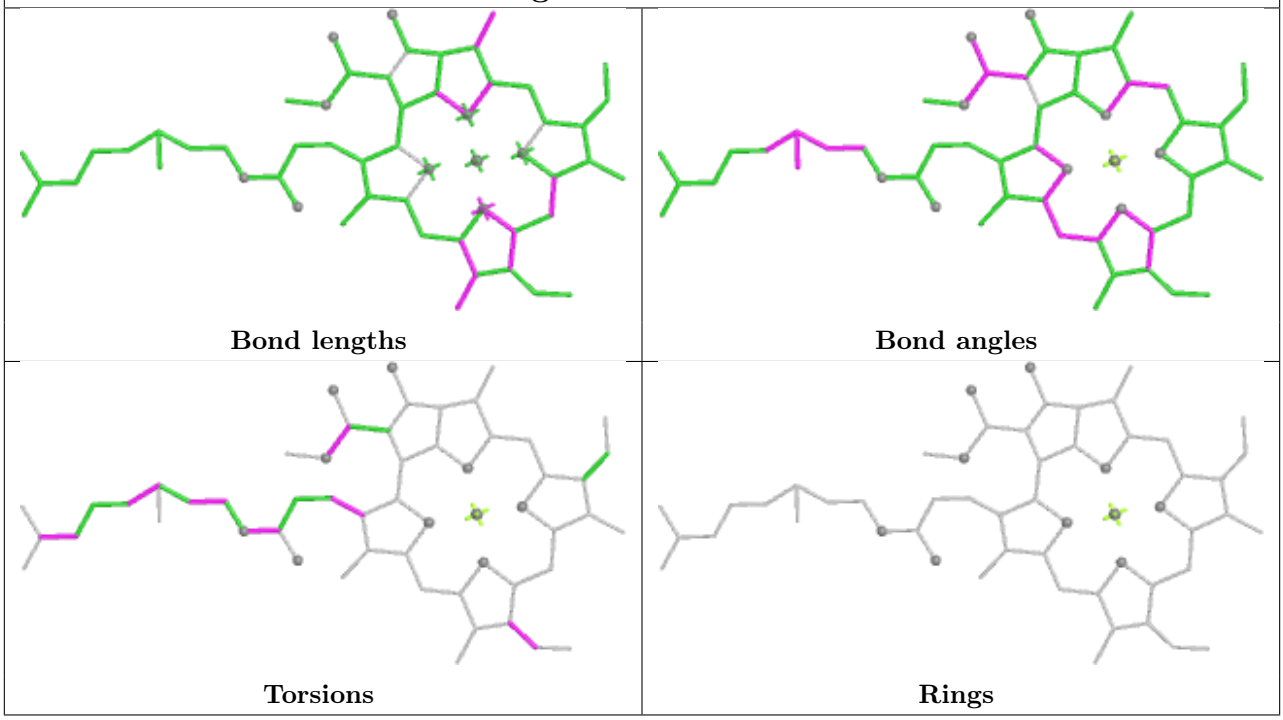
Ligand PID h 204



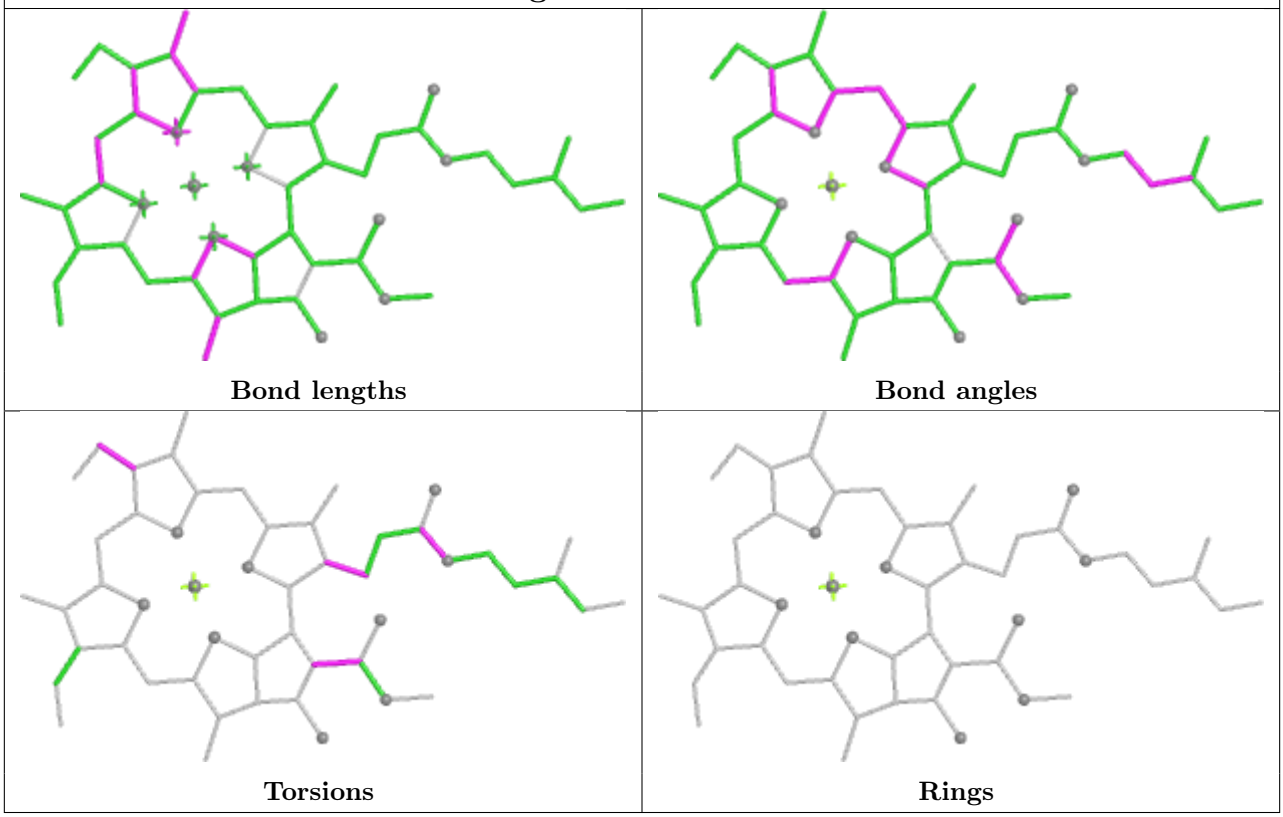
Ligand CLA E 306



Ligand CLA I 212



Ligand CLA a 808



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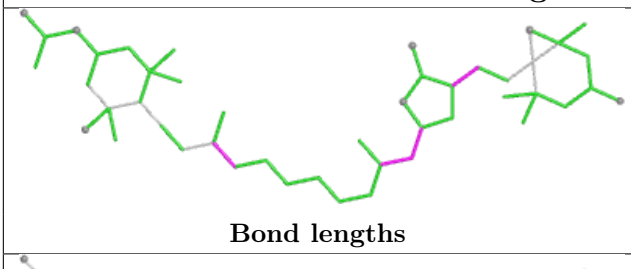
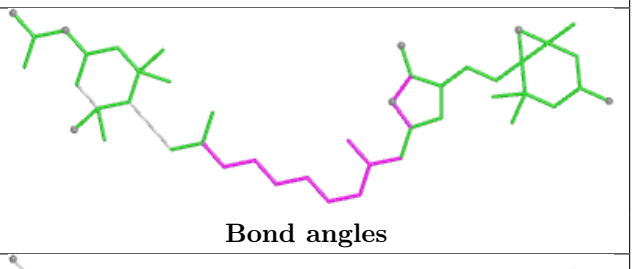
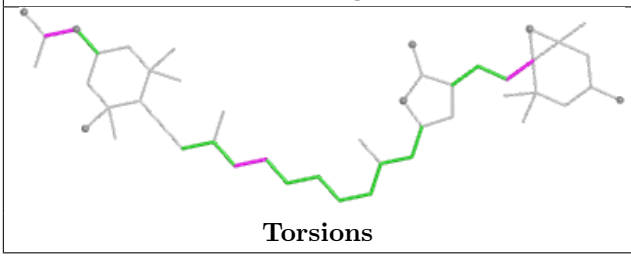


Bond lengths



Bond angles



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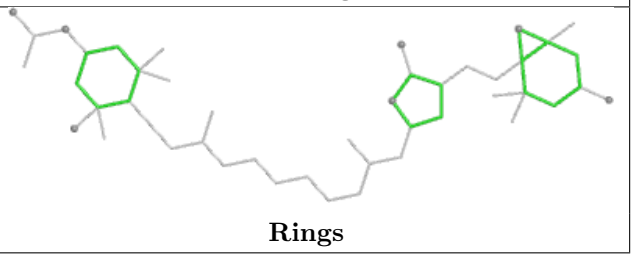
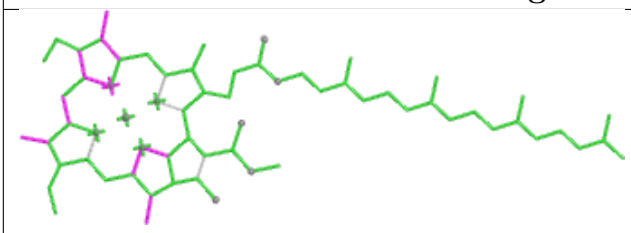


Rings

Ligand CLA a 827



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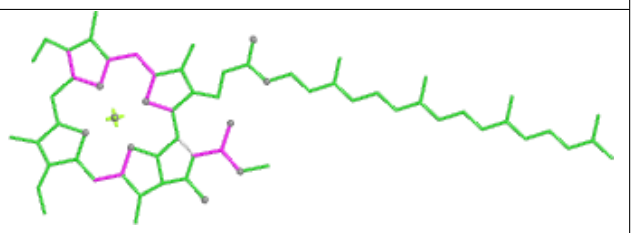
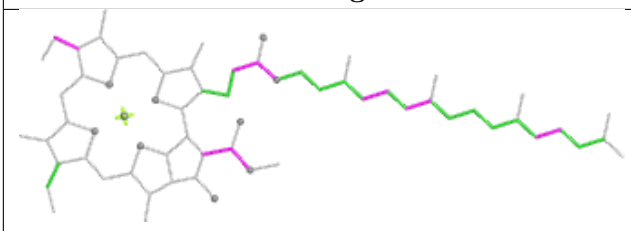


Bond angles



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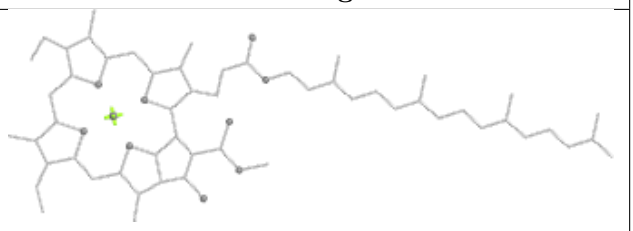
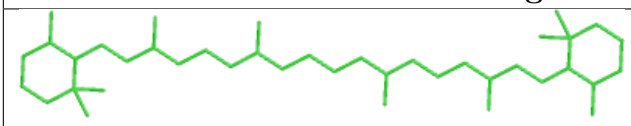


Rings

Ligand BCR b 735



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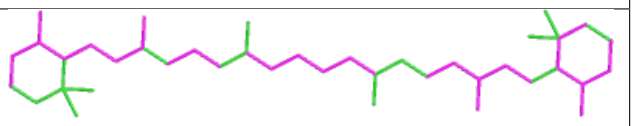
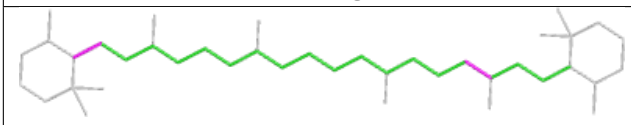


Bond angles



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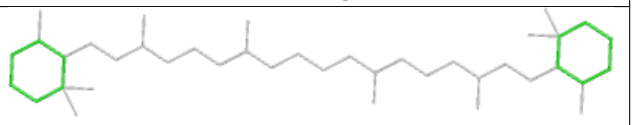
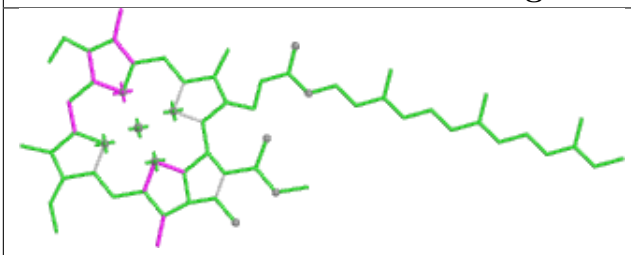
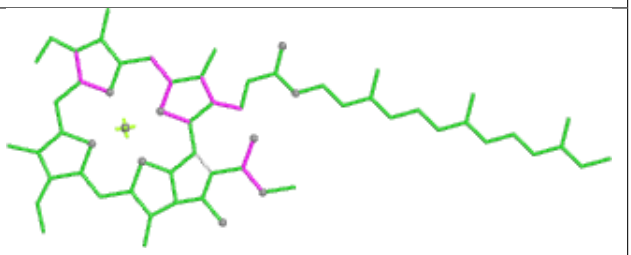
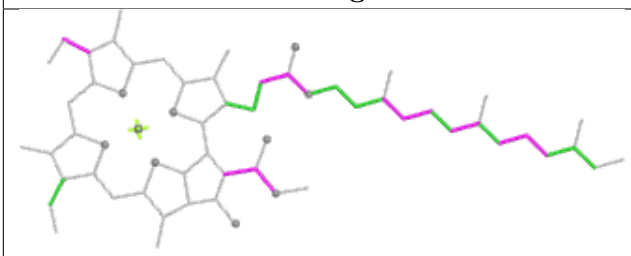
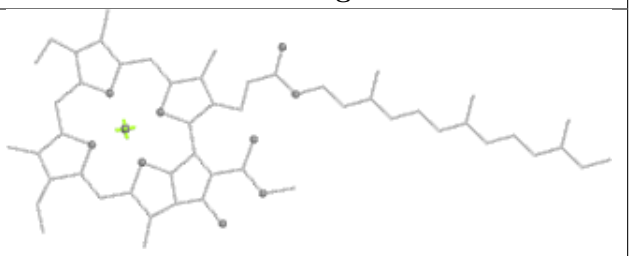
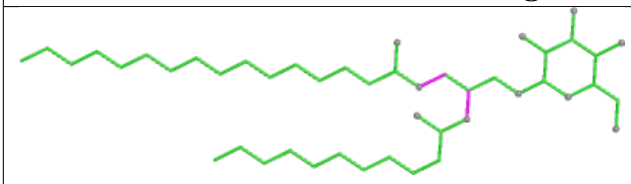
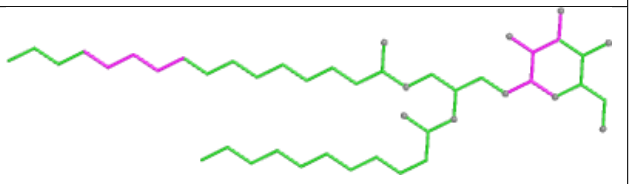
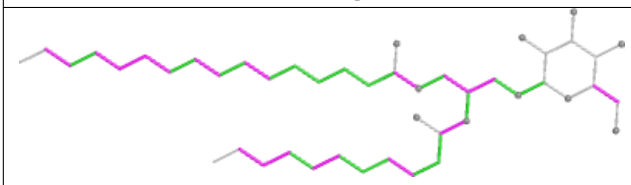
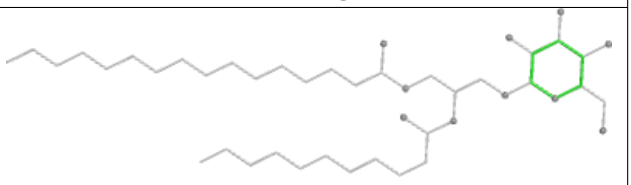
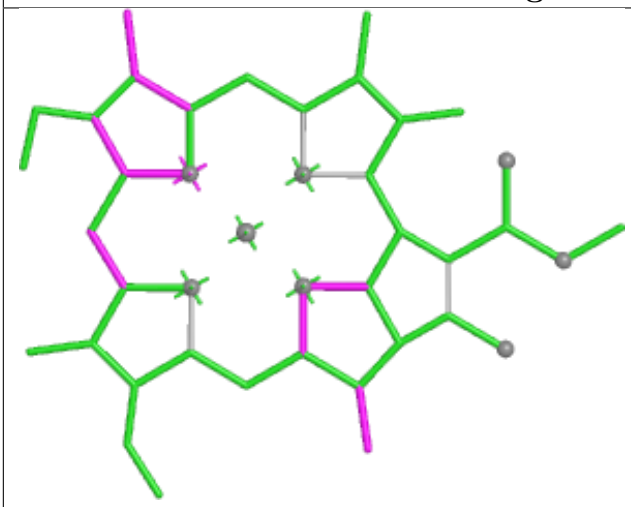


Rings

Ligand CLA E 305	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand LMG b 730	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA F 316



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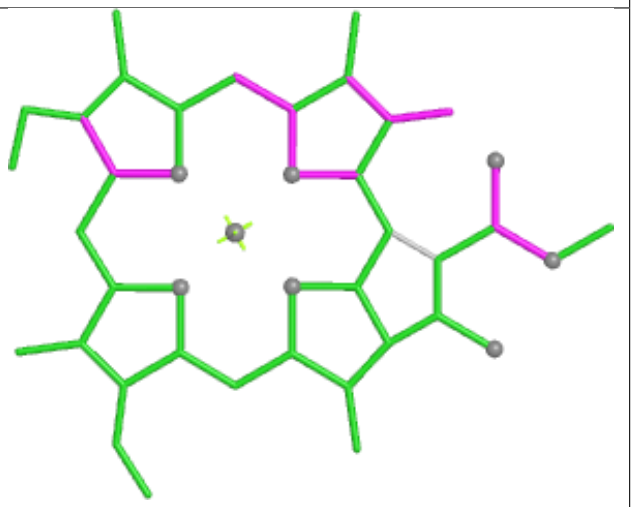
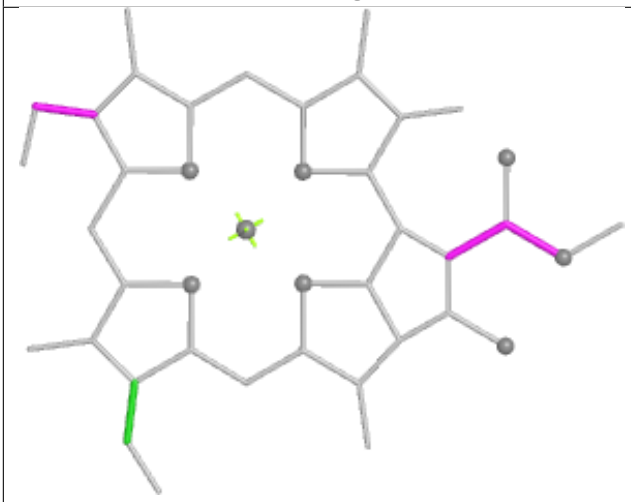


Bond angles



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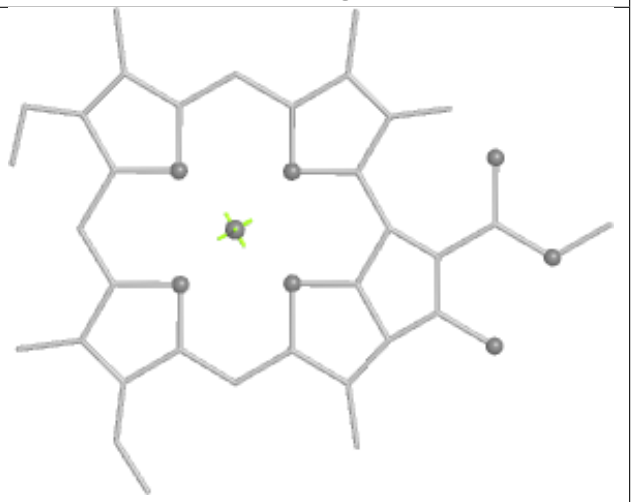
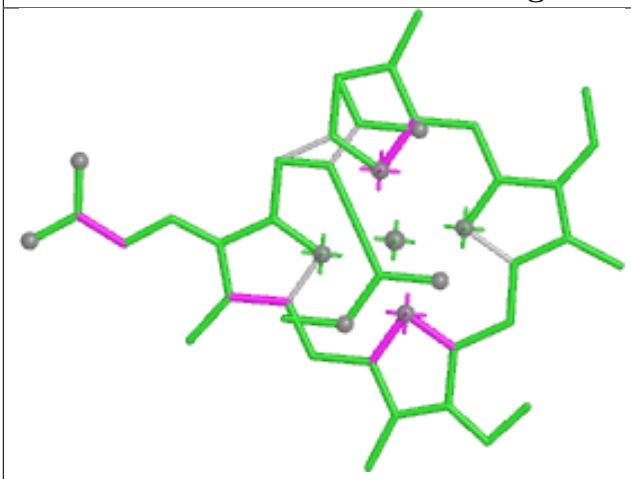


Rings

Ligand KC1 E 307



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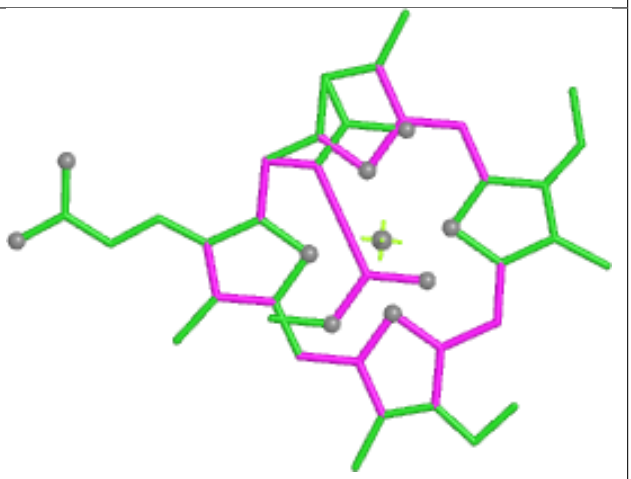
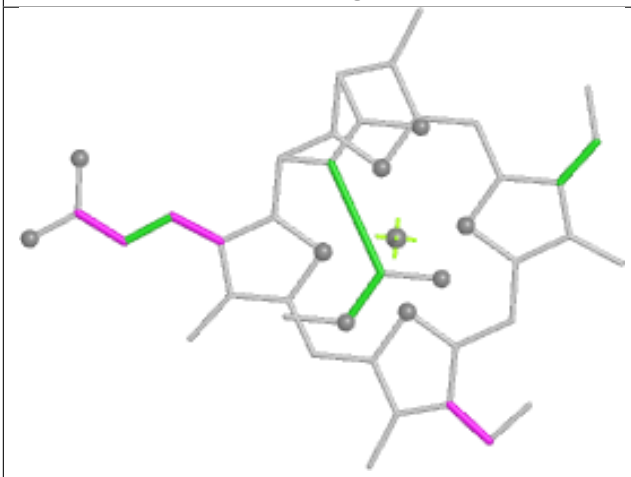


Bond angles



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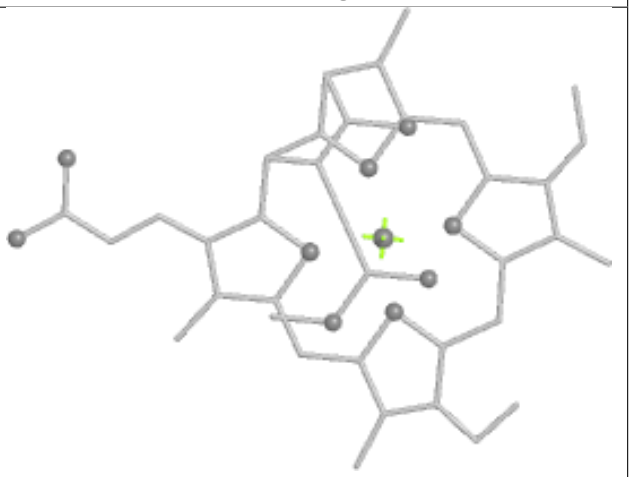
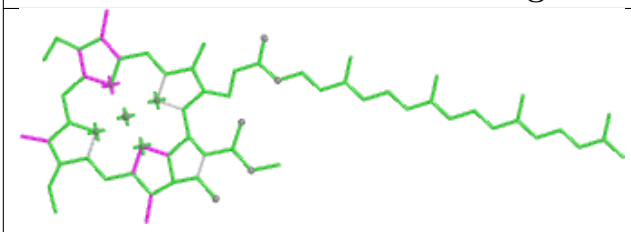


Rings

Ligand CLA b 718



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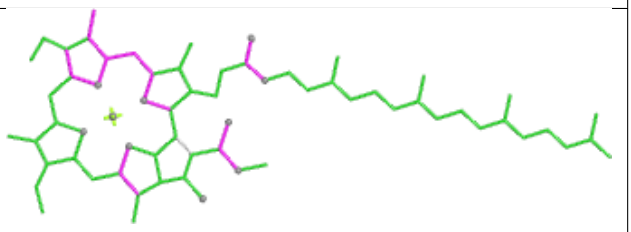
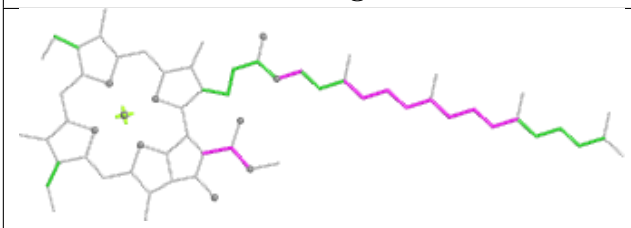


Bond angles



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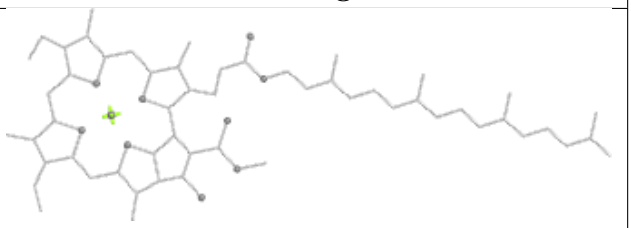
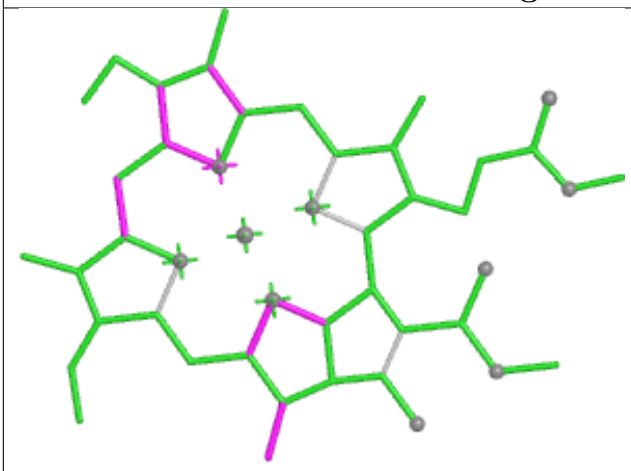


Rings

Ligand CLA M 315



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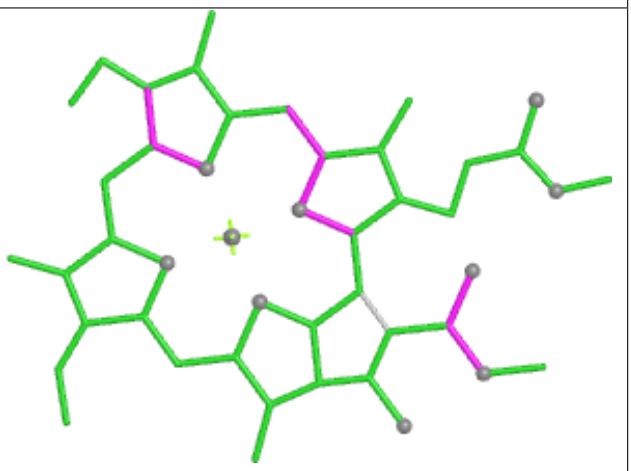
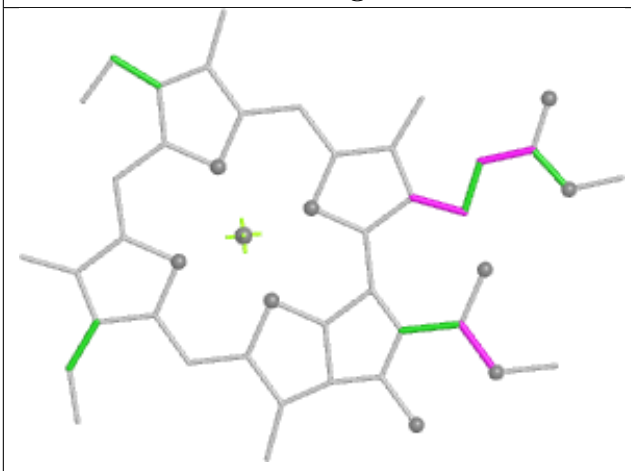


Bond angles



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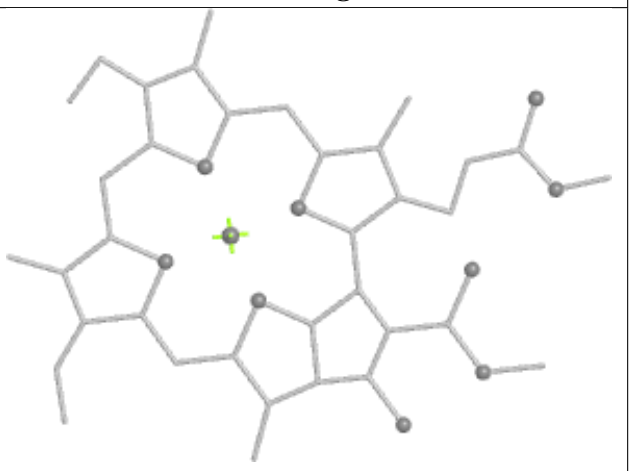
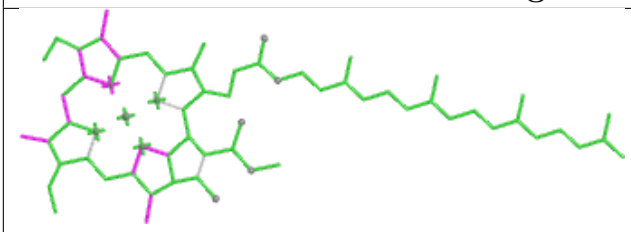
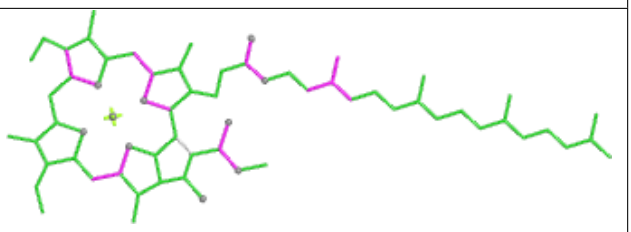


Rings

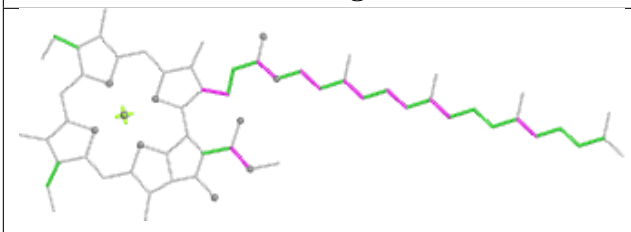
Ligand CLA b 712



Bond lengths



Bond angles



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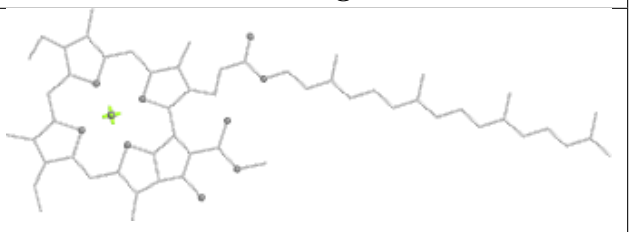
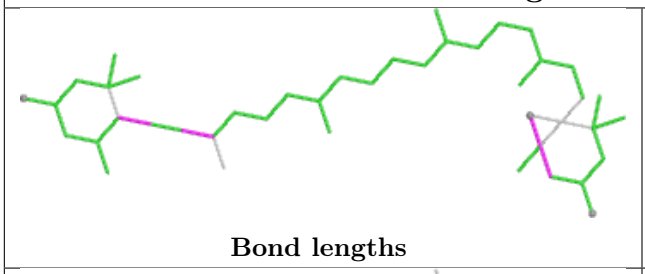
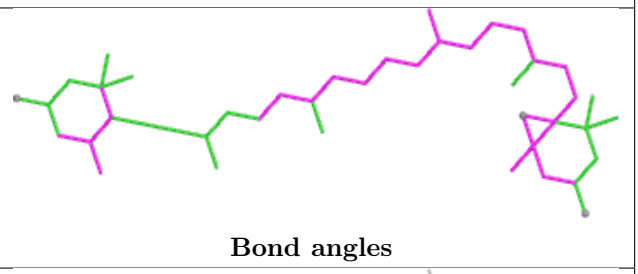


Rings

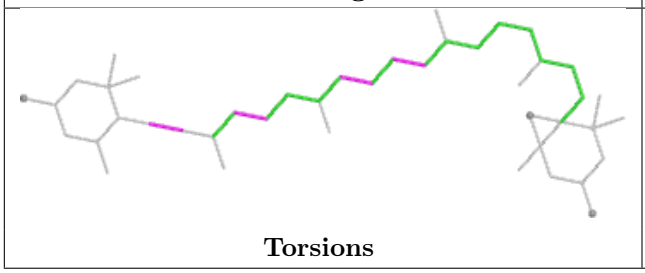
Ligand DD6 O 303



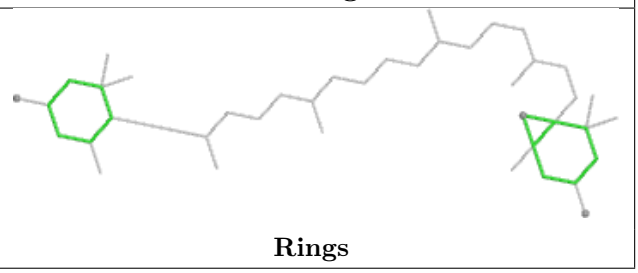
Bond lengths



Bond angles

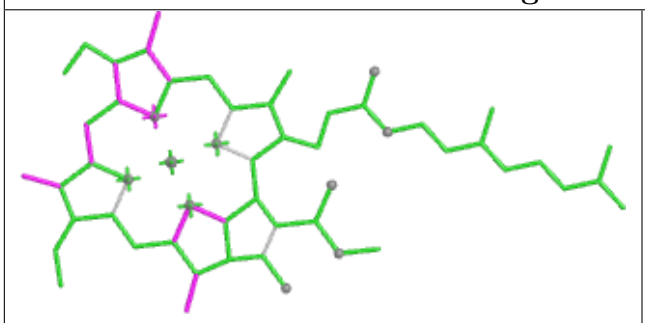


Torsions



Rings

Ligand CLA M 307



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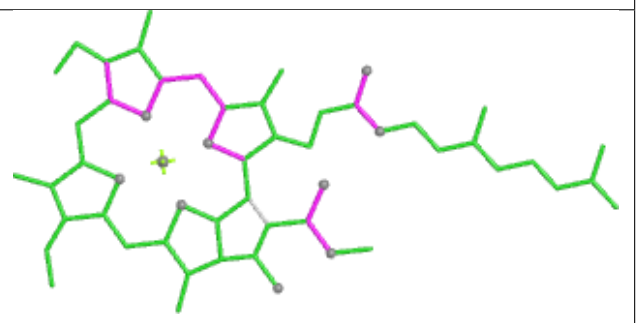

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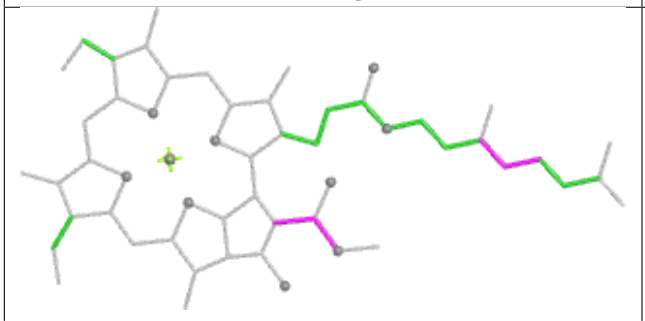

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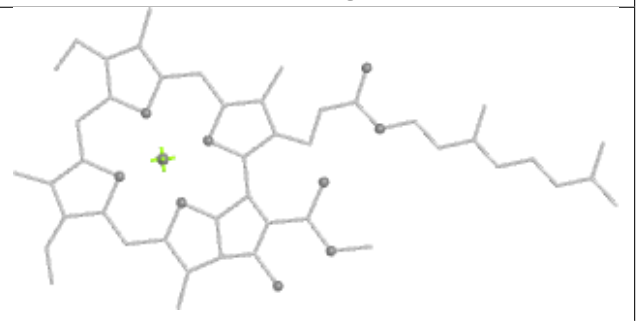
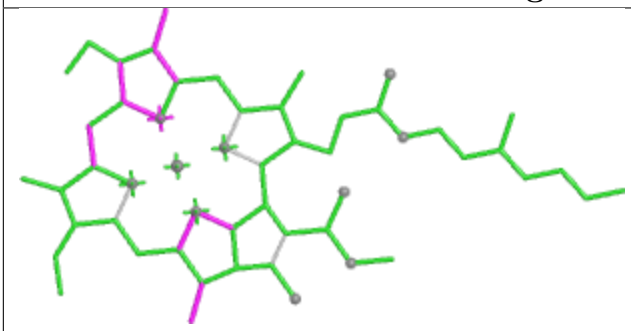


Rings

Ligand CLA L 308



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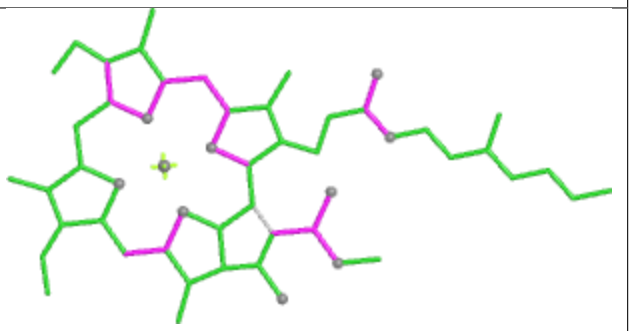

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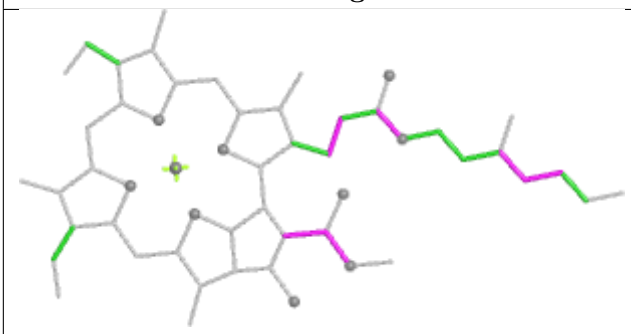

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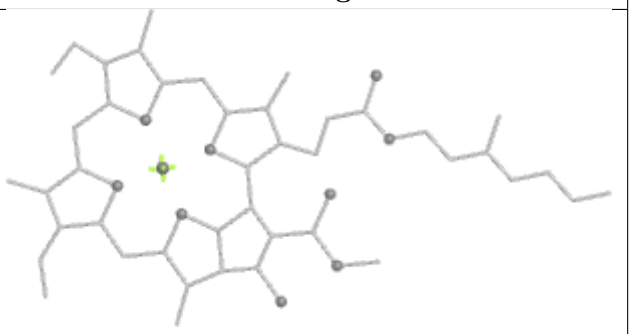
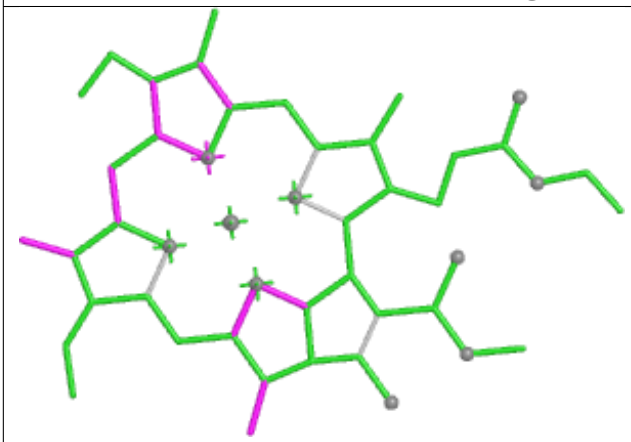


Rings

Ligand CLA N 314



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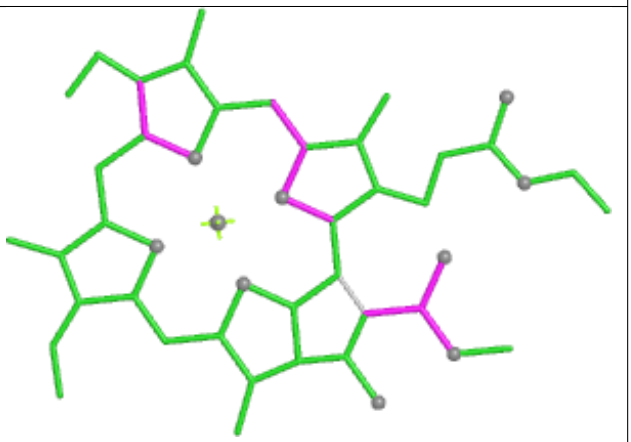

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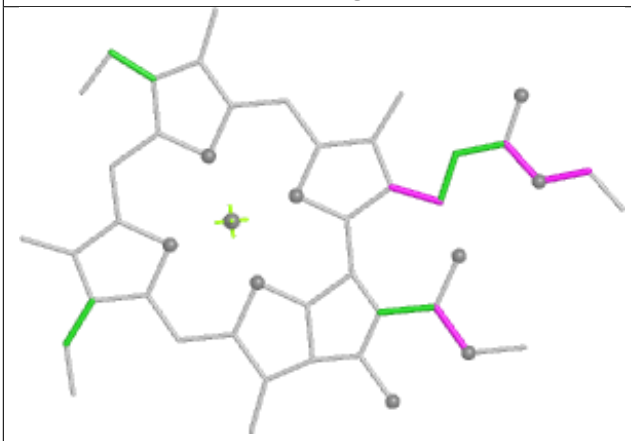

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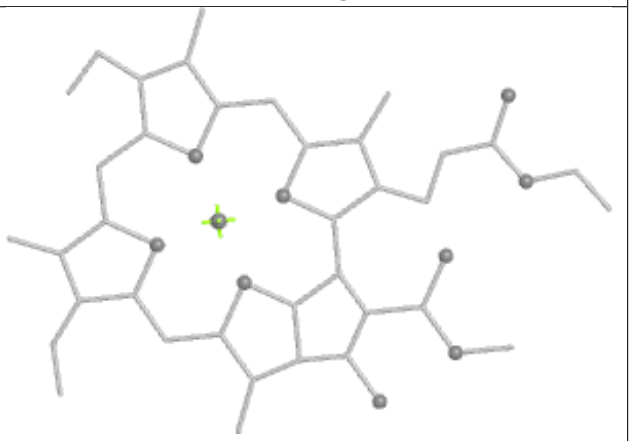
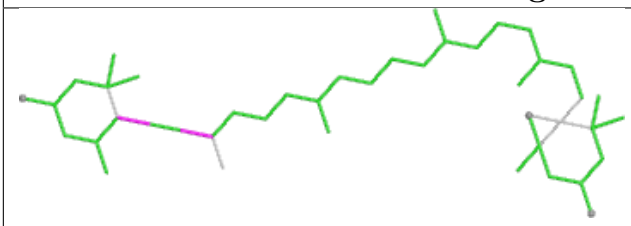


Rings

Ligand DD6 J 302



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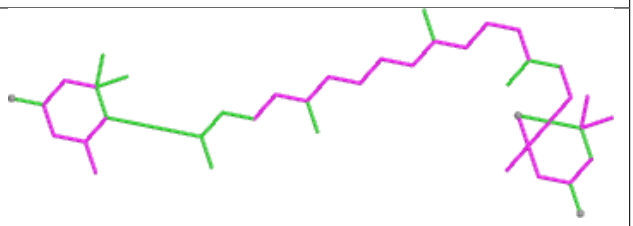
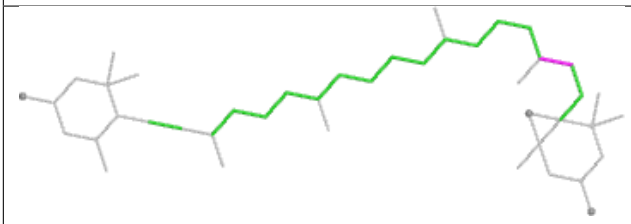


Bond angles



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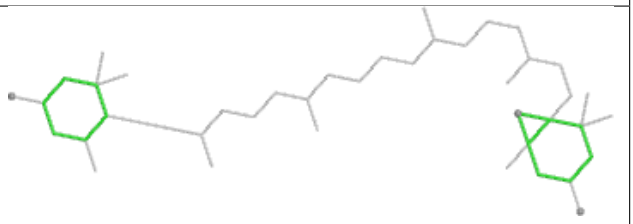
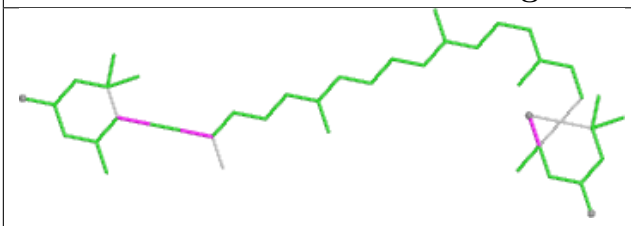


Rings

Ligand DD6 M 304



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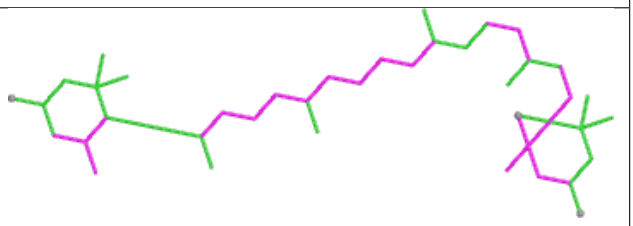

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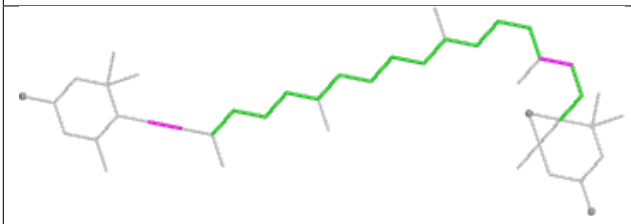
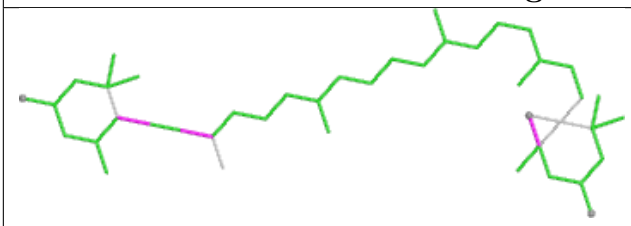


Torsions



Rings

Ligand DD6 B 305



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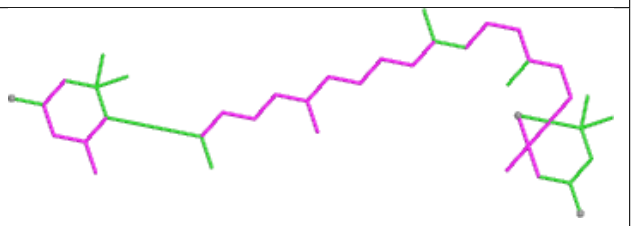
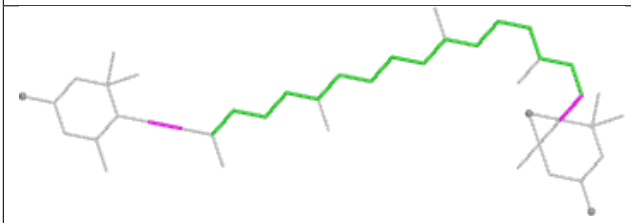


Bond angles



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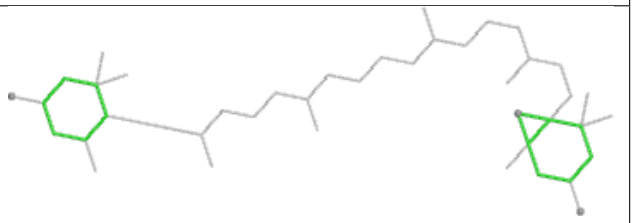
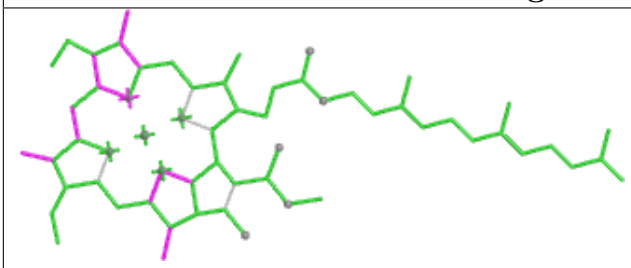


Rings

Ligand CLA h 201



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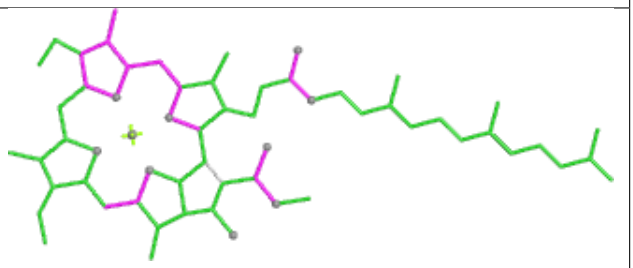
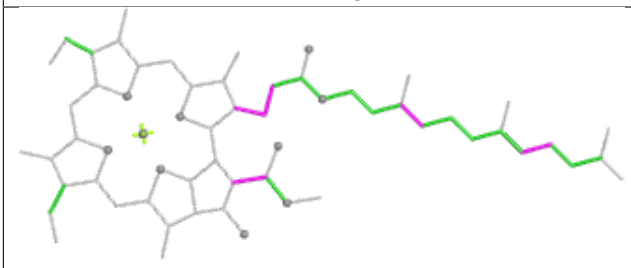


Bond angles



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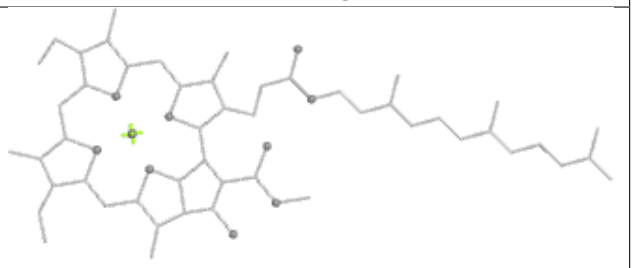
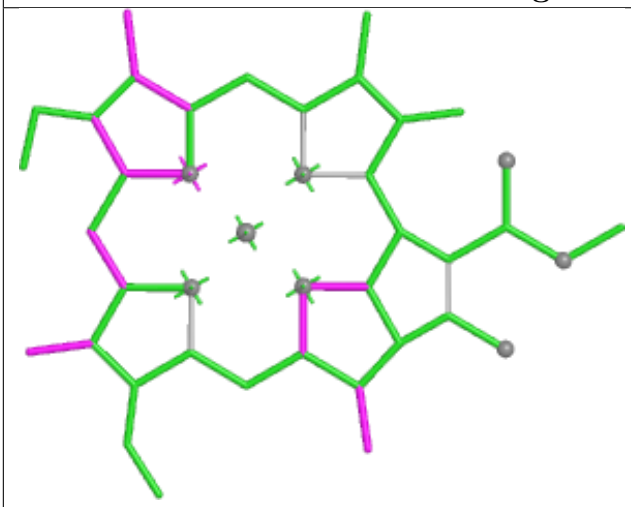


Rings

Ligand CLA l 509



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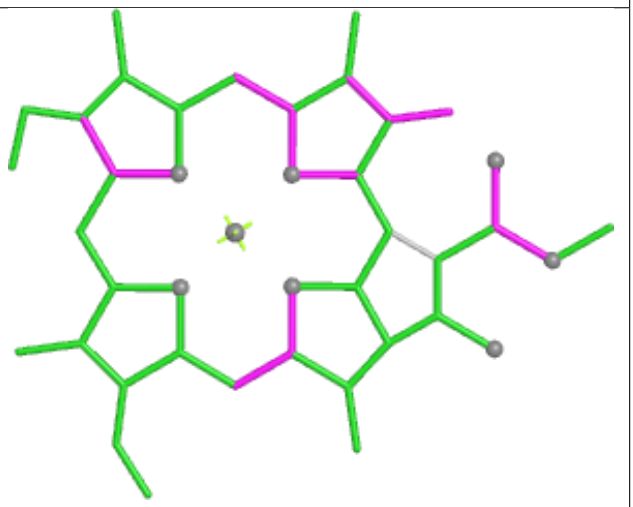
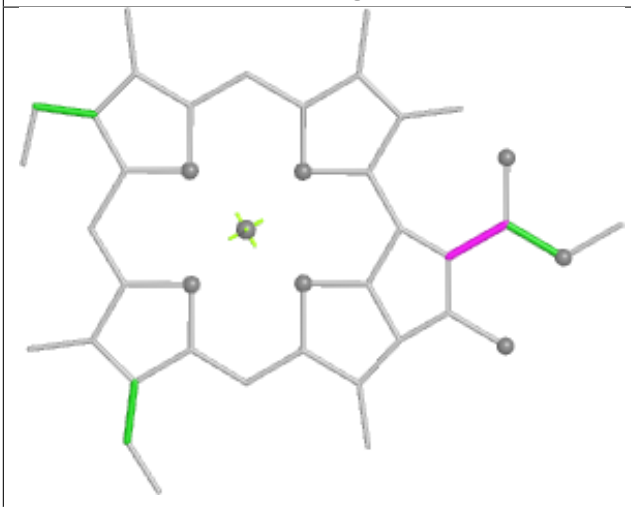


Bond angles



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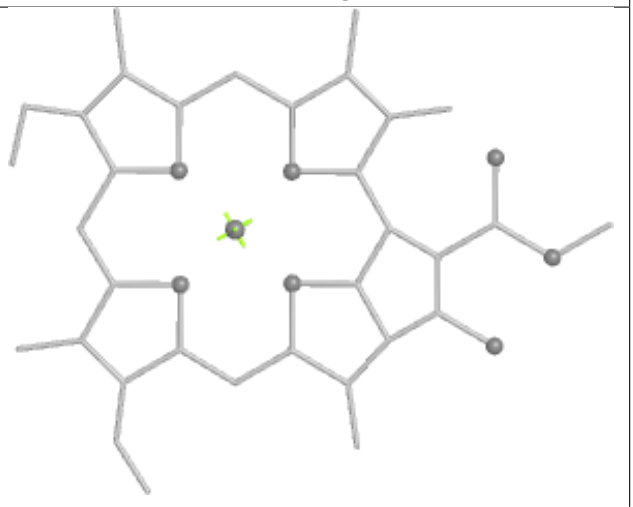
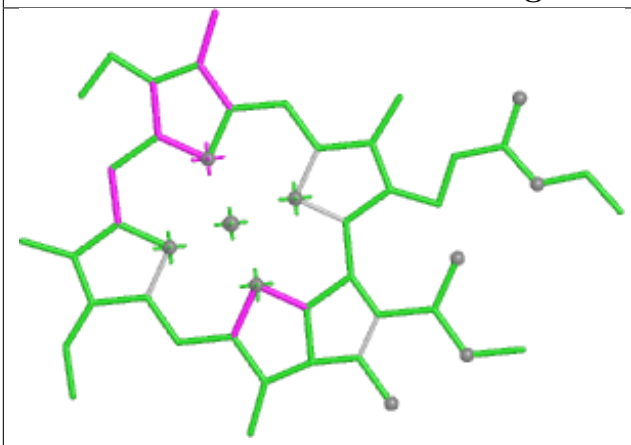


Rings

Ligand CLA T 314



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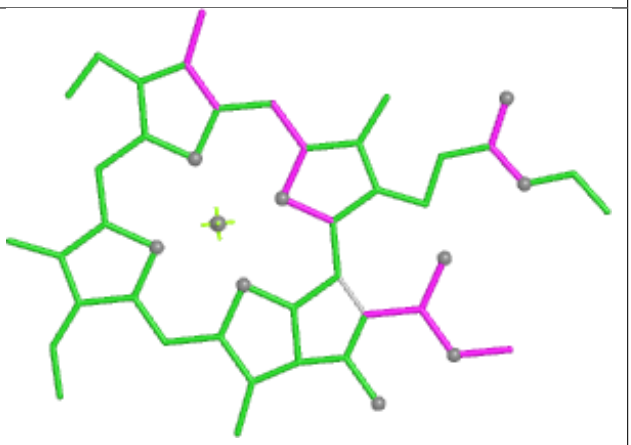
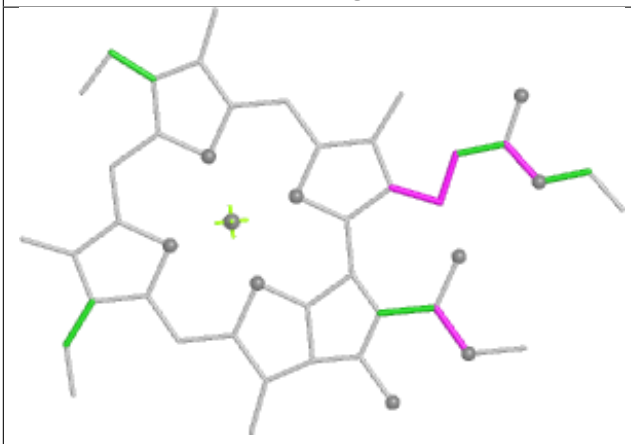
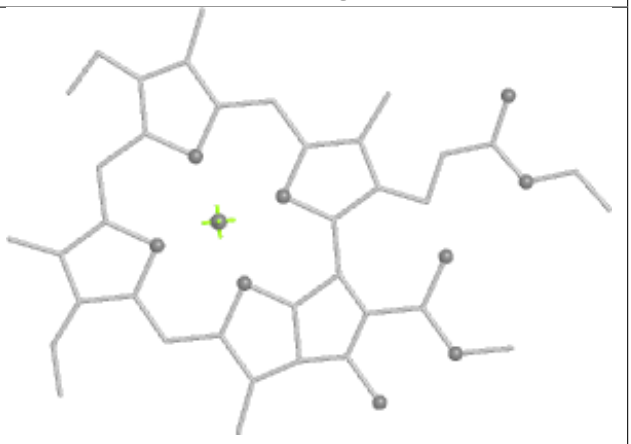


Bond angles



Torsions

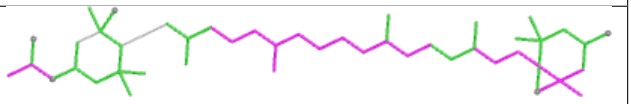


Rings

Ligand UIX J 304



Bond lengths



Bond angles

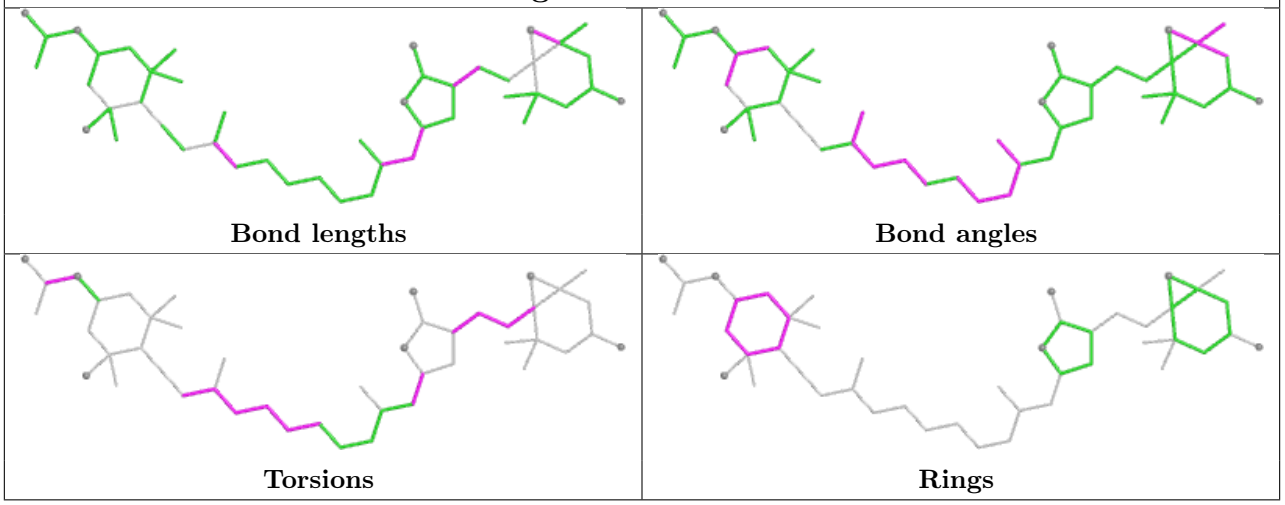


Torsions



Rings

Ligand PID F 304



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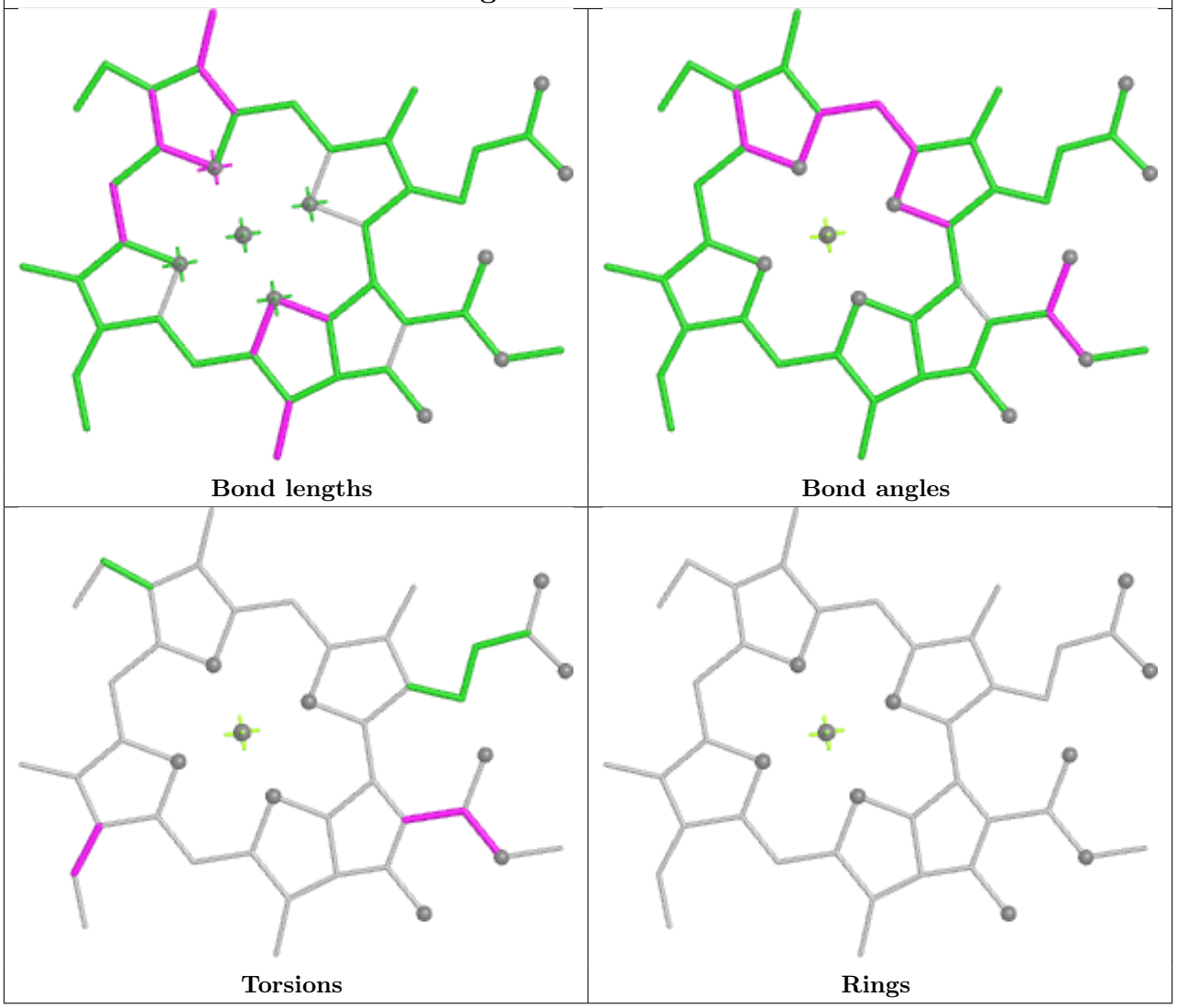

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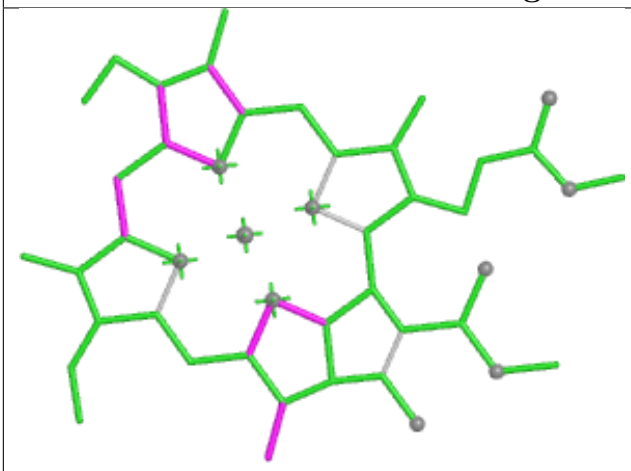

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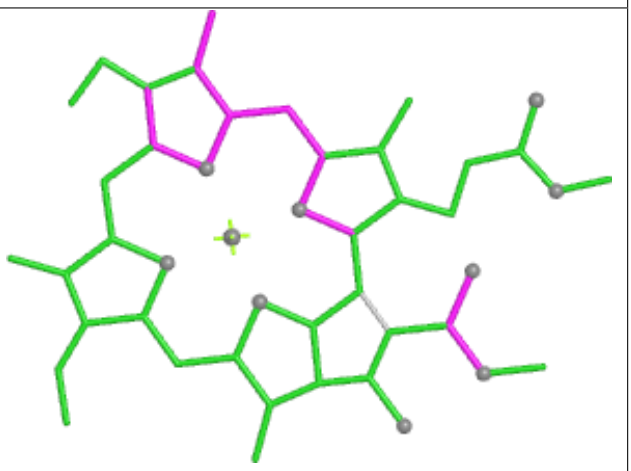
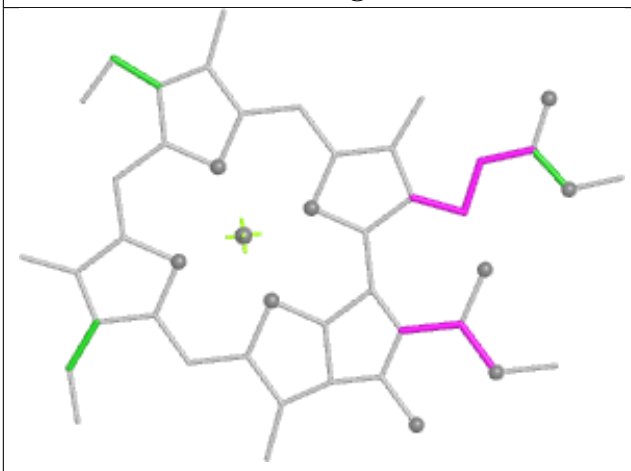


Bond angles



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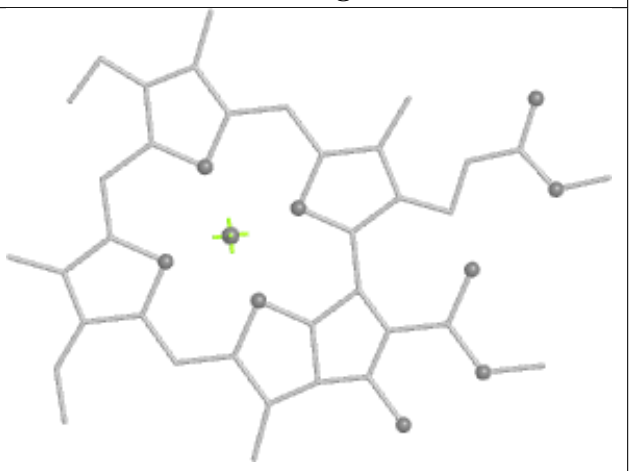
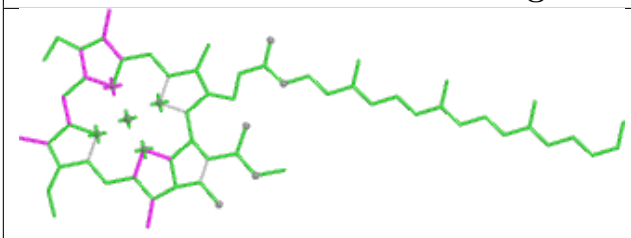


Rings

Ligand CLA b 714



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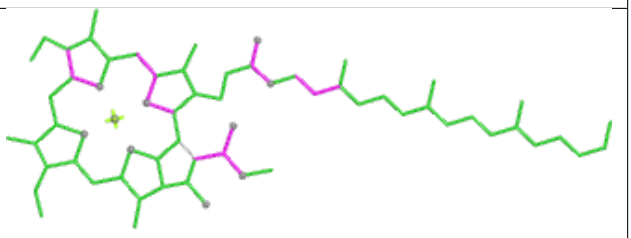
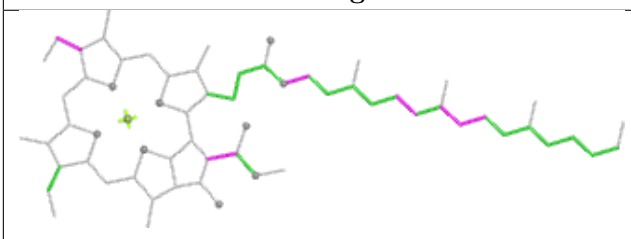


Bond angles



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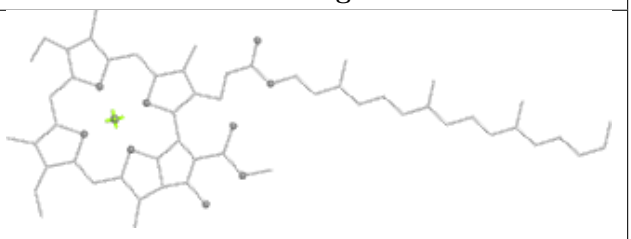
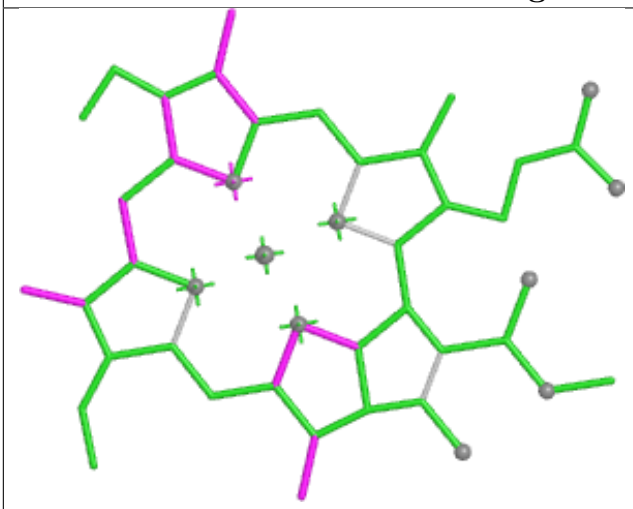


Rings

Ligand CLA a 815



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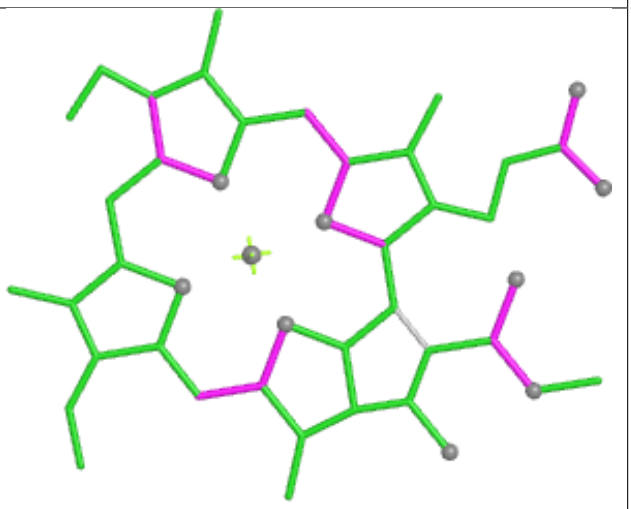
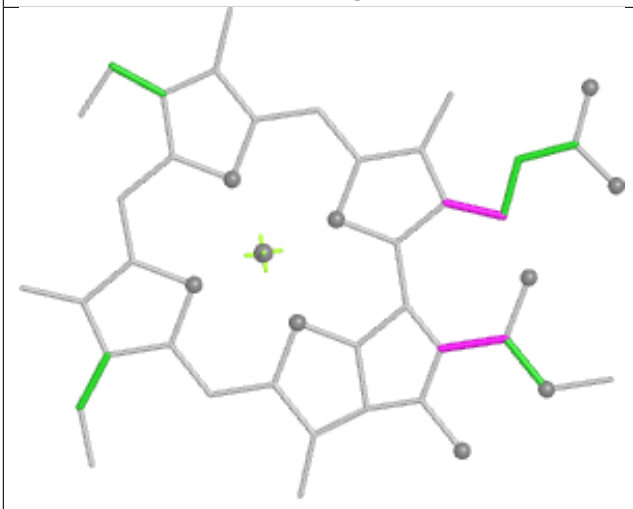


Bond angles

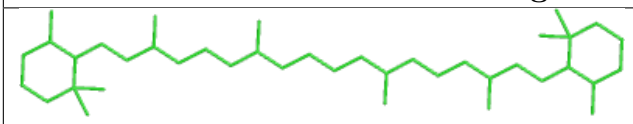


Torsions



Rings

Ligand BCR l 507



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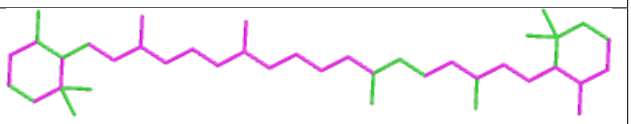
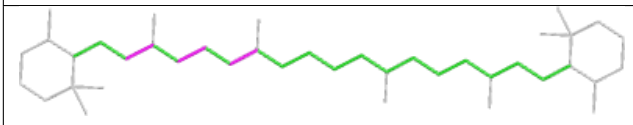


Bond angles



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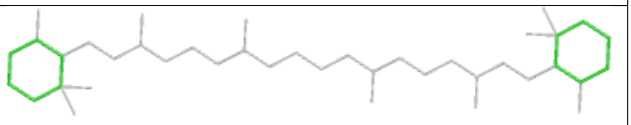
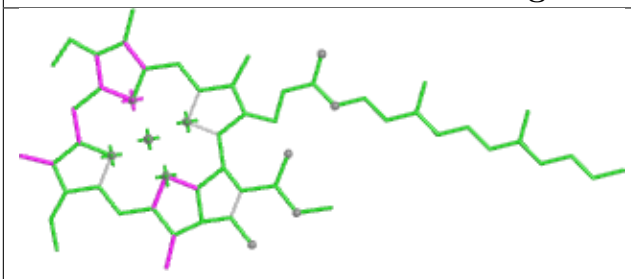


Rings

Ligand CLA a 823



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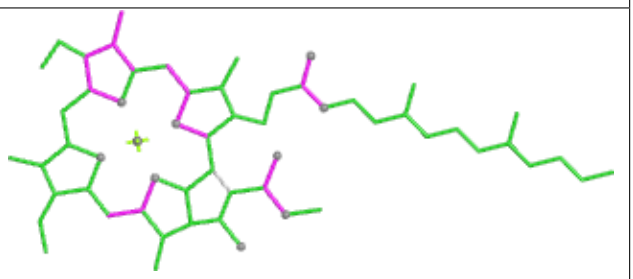
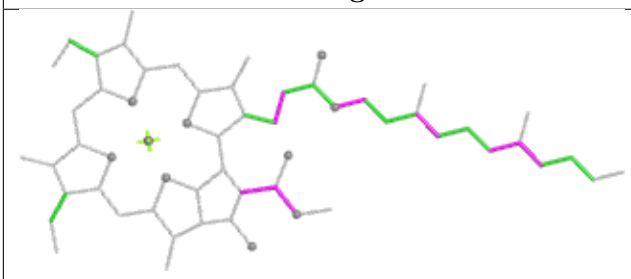
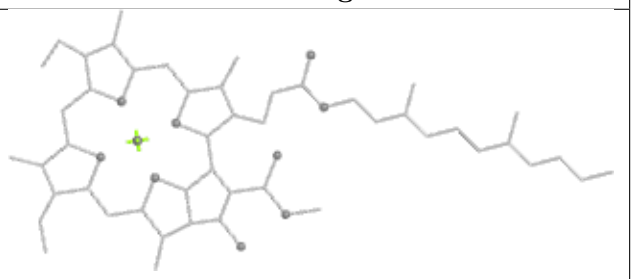


Bond angles

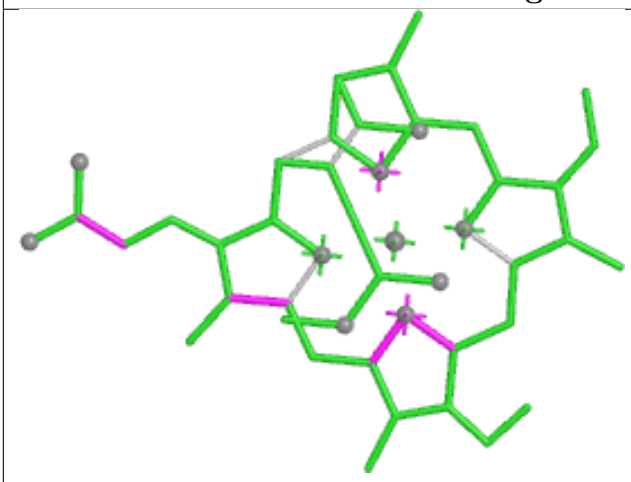


Torsions

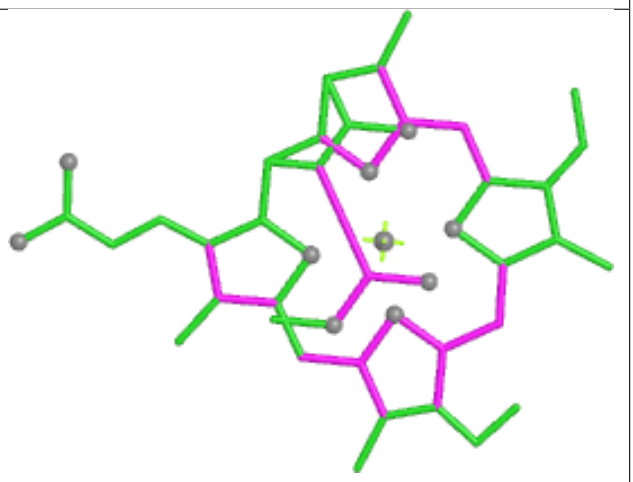


Rings

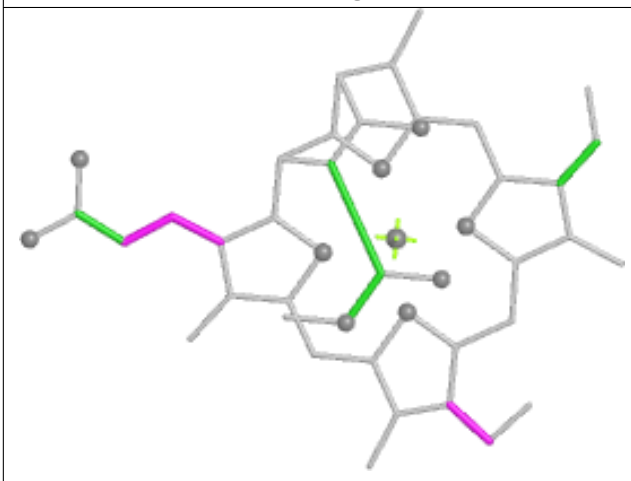
Ligand KC1 D 310



Bond lengths



Bond angles



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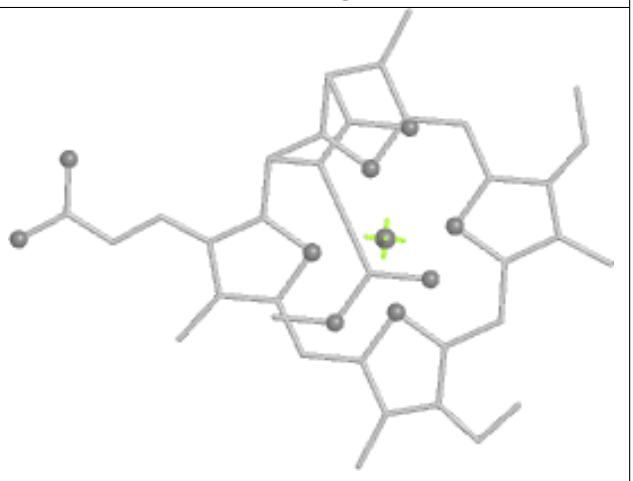
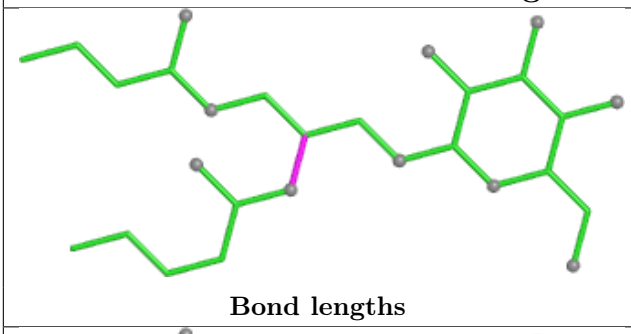


Rings

Ligand LMG h 205



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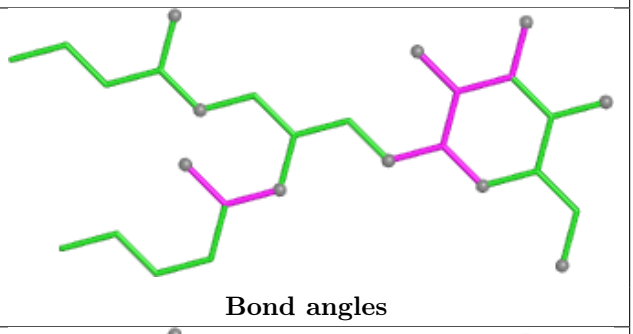
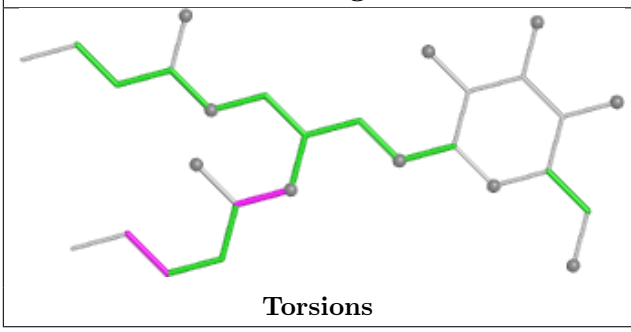


Bond angles



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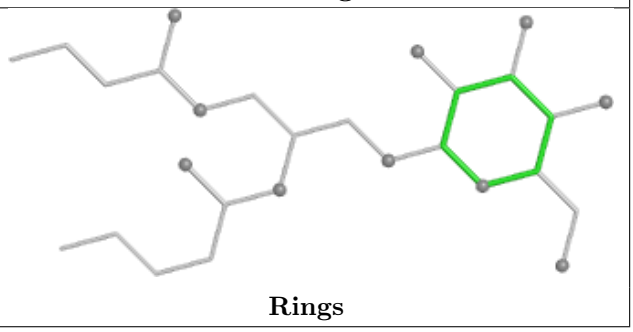
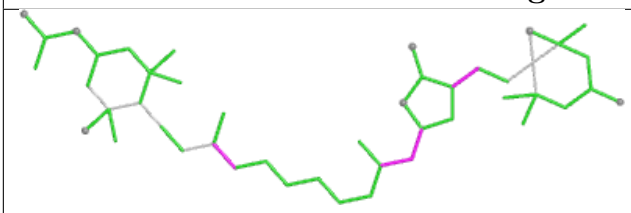


Rings

Ligand PID D 306



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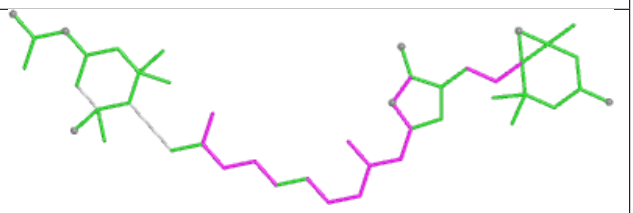
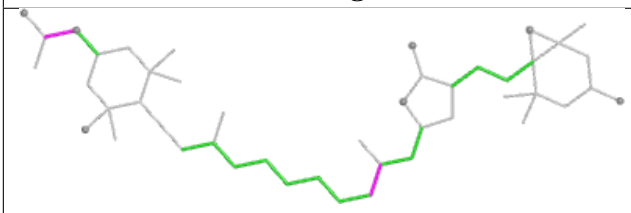


Bond angles



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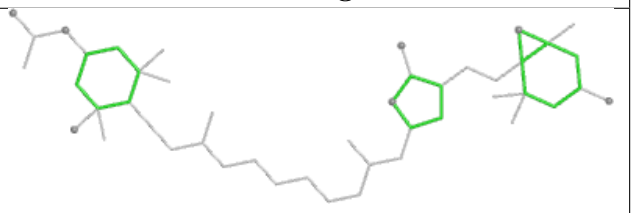
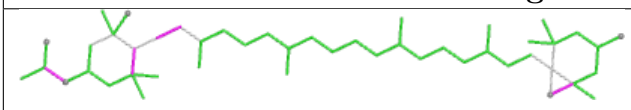


Rings

Ligand UIX N 306



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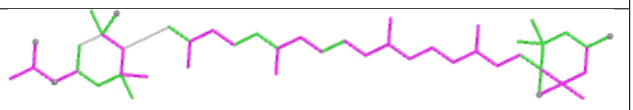
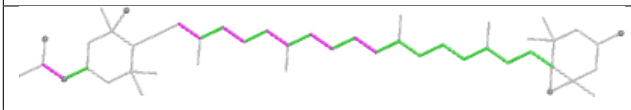


Bond angles



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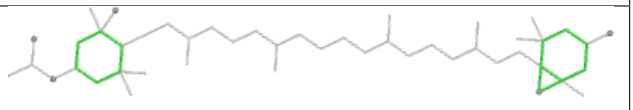
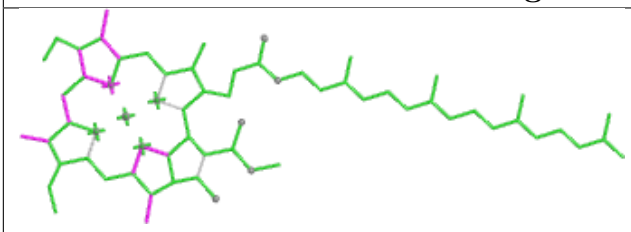


Rings

Ligand CLA B 308



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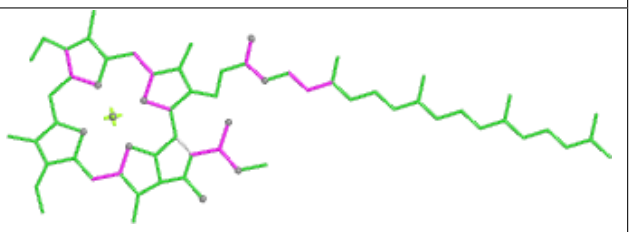
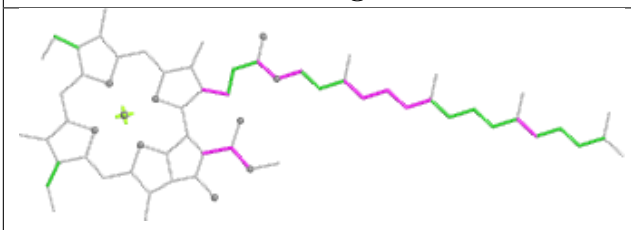


Bond angles



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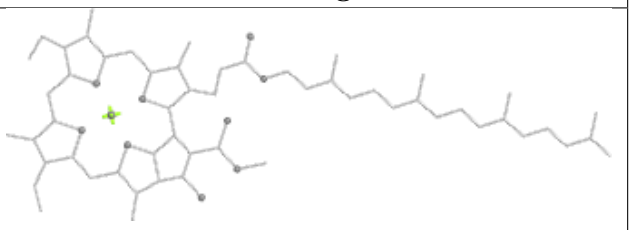
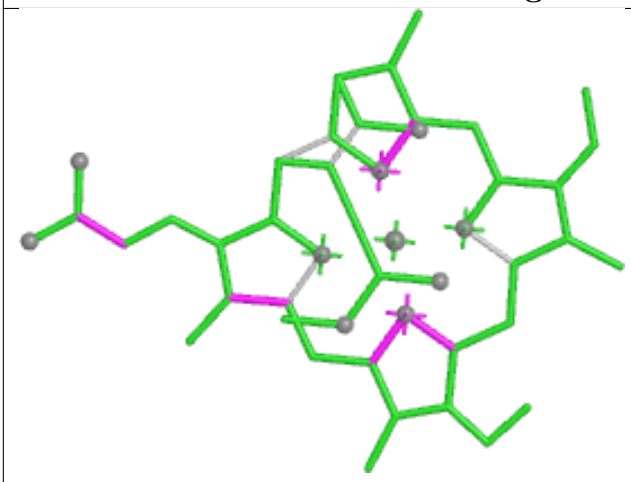
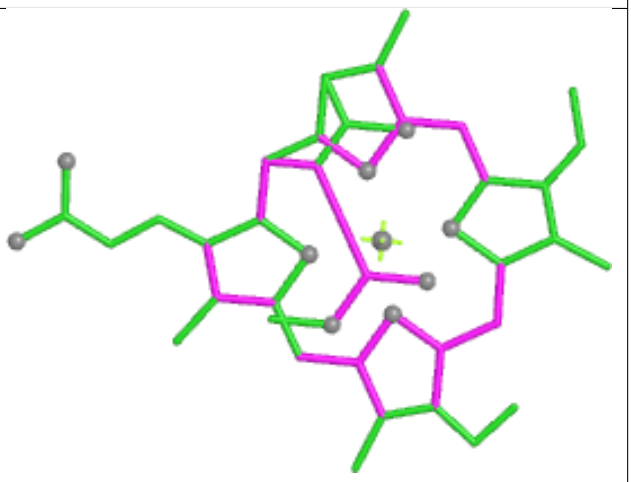


Rings

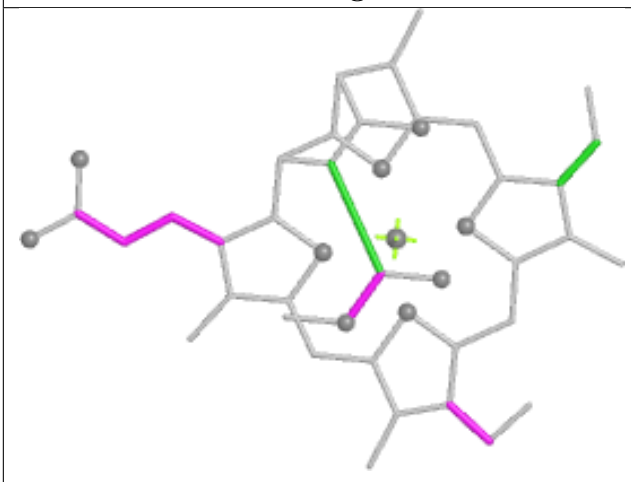
Ligand KC1 H 309



Bond lengths



Bond angles



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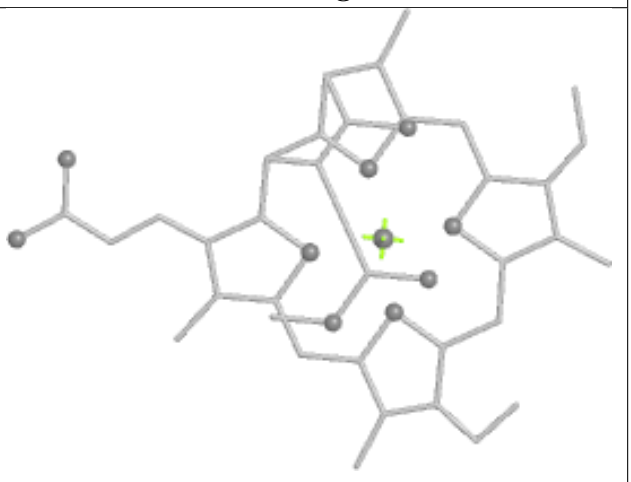
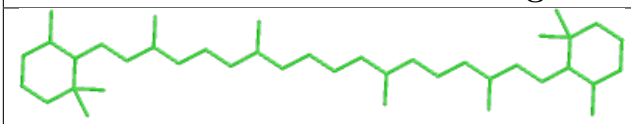
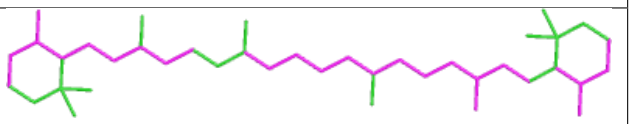
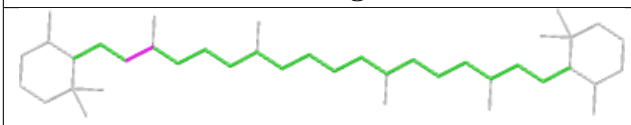
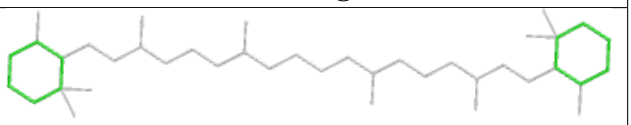


Rings

Ligand BCR a 835	
 Bond lengths	 Bond angles
 Torsions	 Rings

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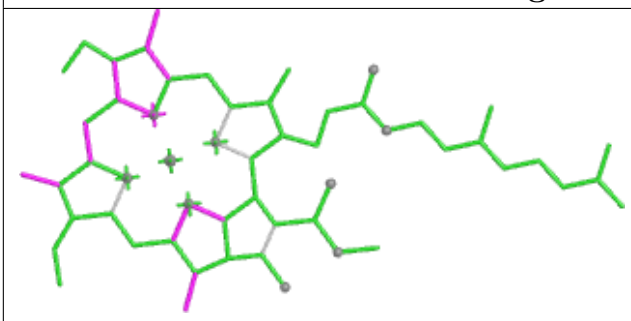
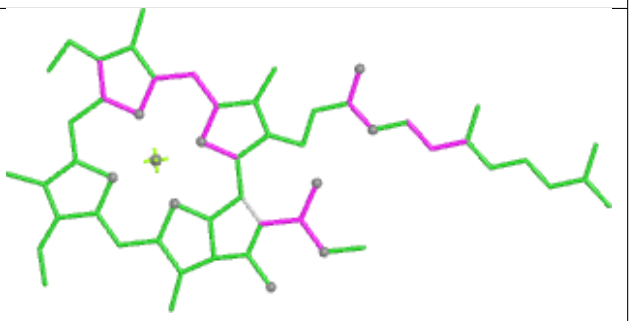
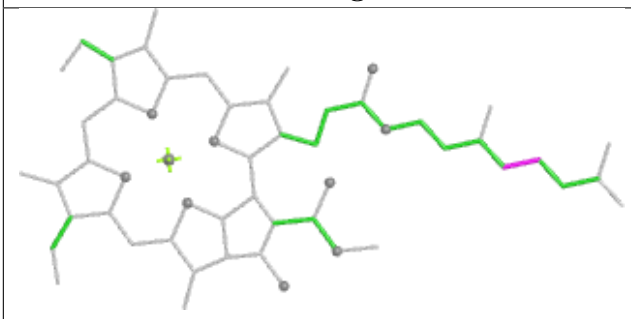
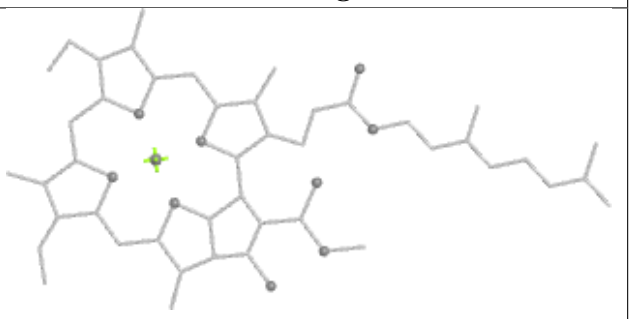
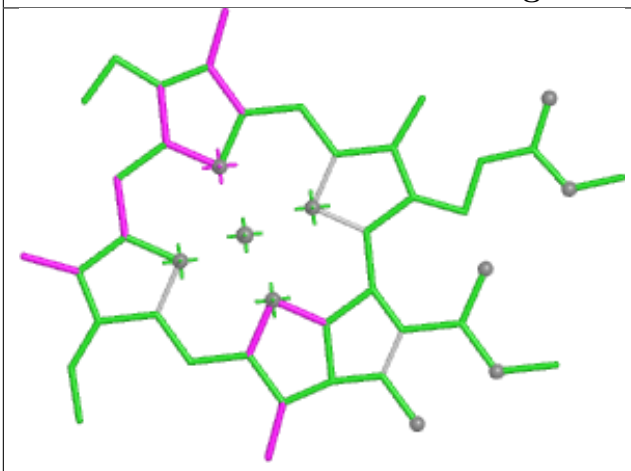
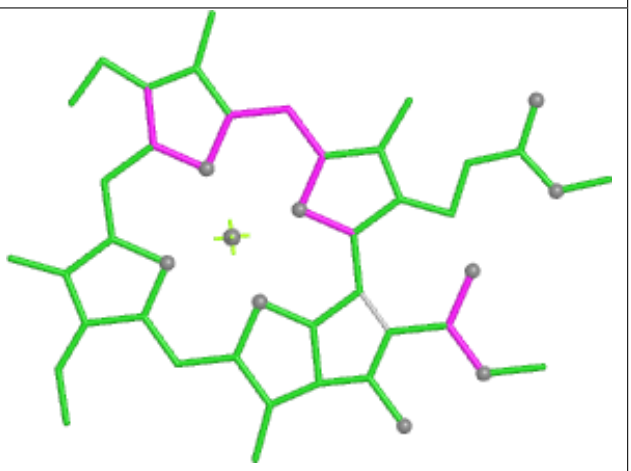
 Bond lengths	 Bond angles
 Torsions	 Rings

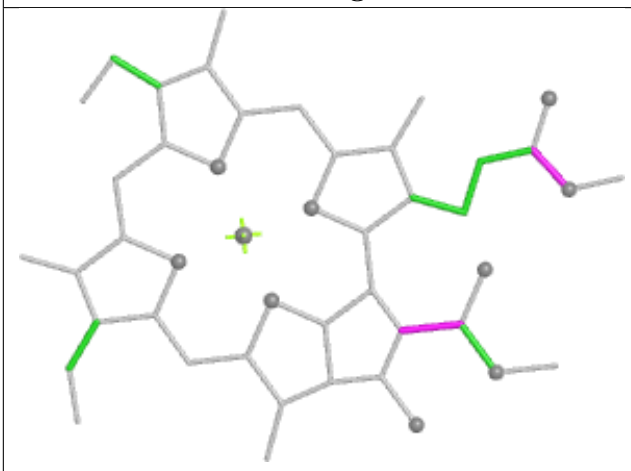
Ligand CLA K 208



Bond lengths



Bond angles



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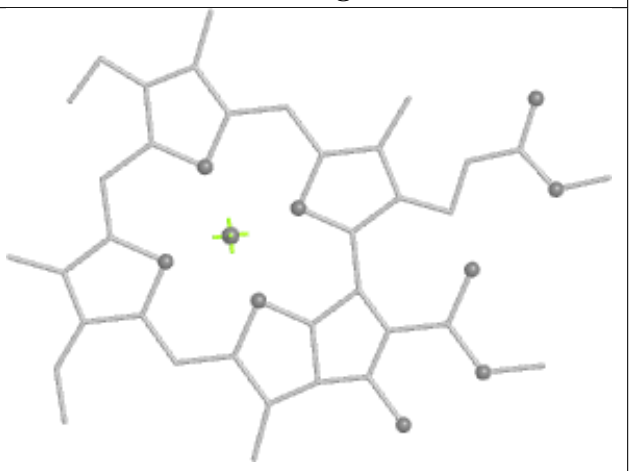
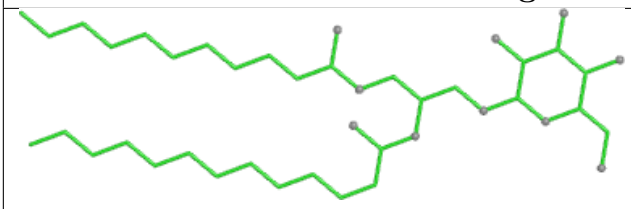


Rings

Ligand LMG K 201



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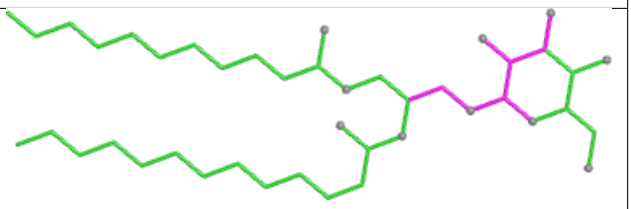
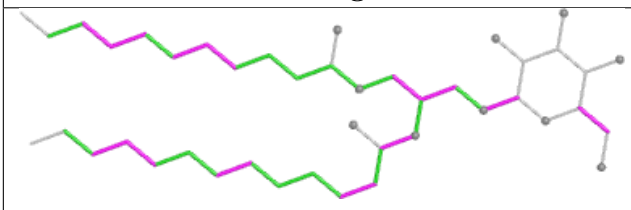


Bond angles



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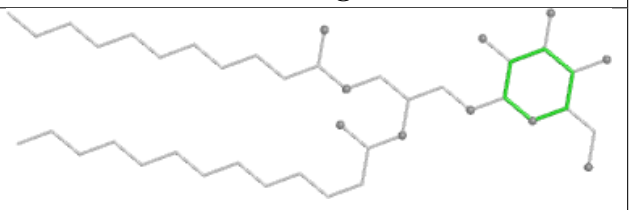
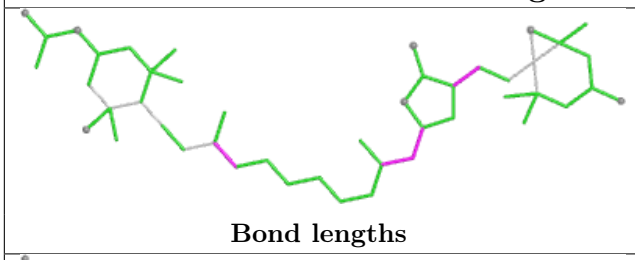


Rings

Ligand PID N 302



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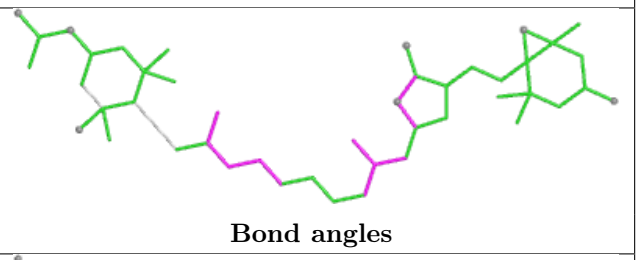
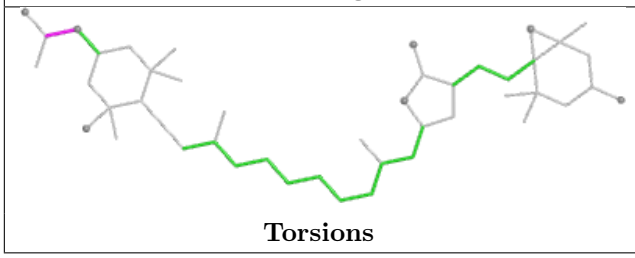


Bond angles



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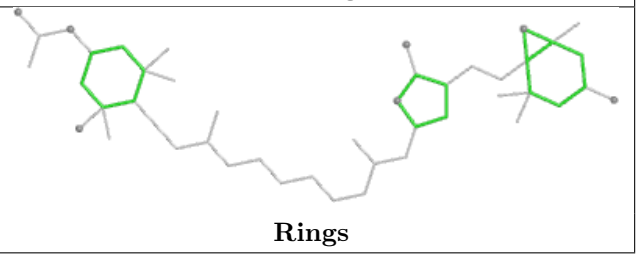
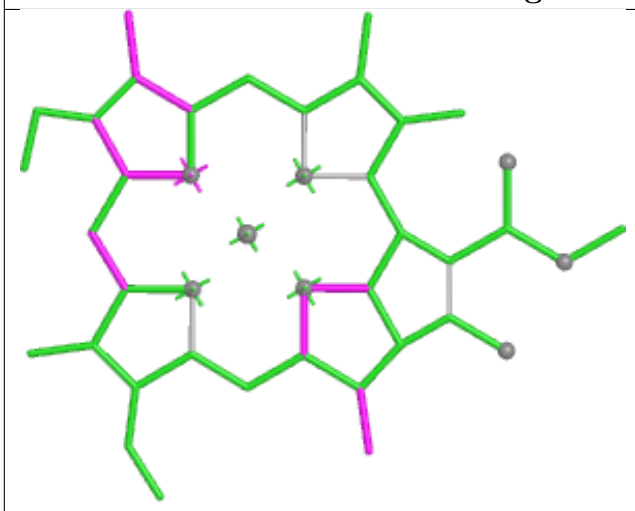


Rings

Ligand CLA A 214



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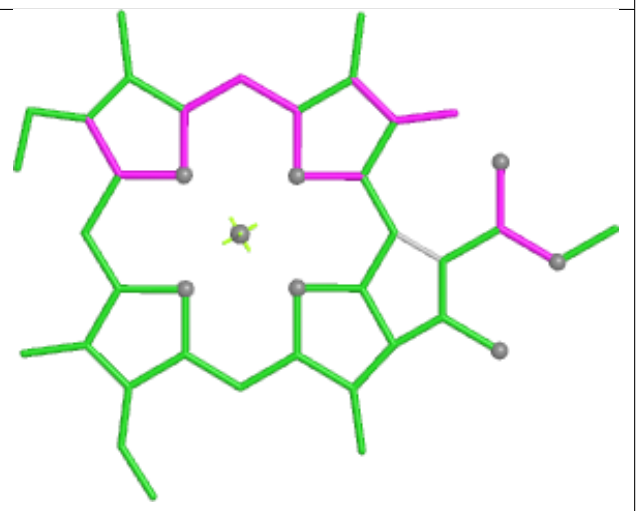
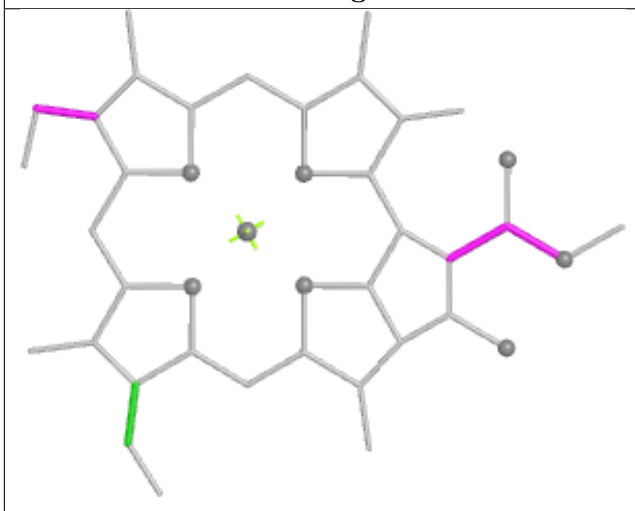


Bond angles



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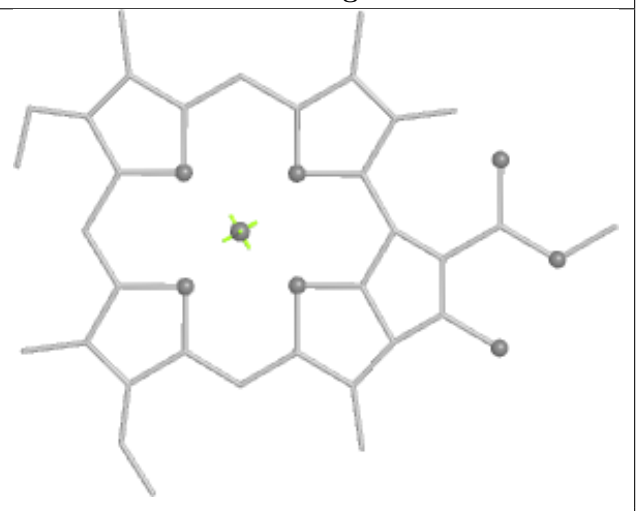
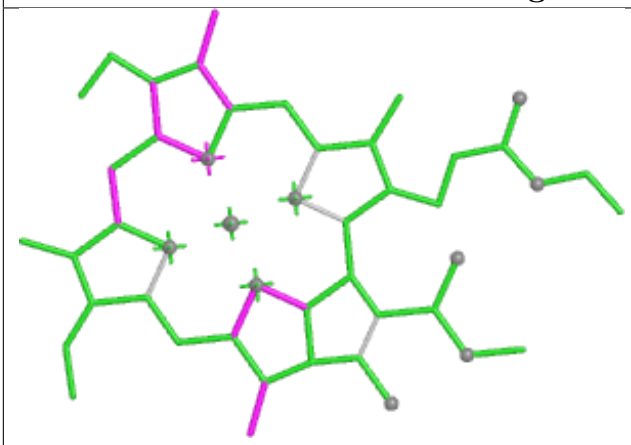


Rings

Ligand CLA J 310



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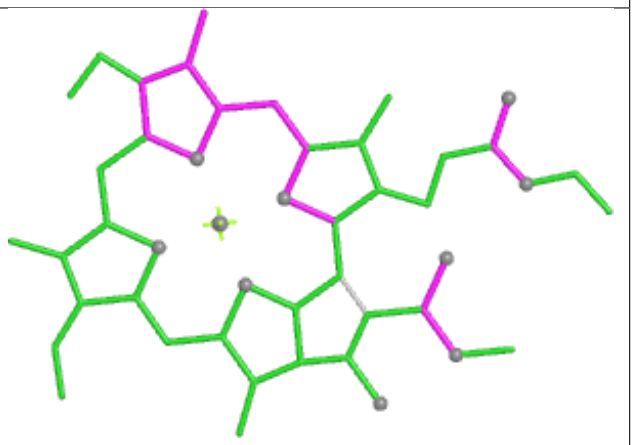
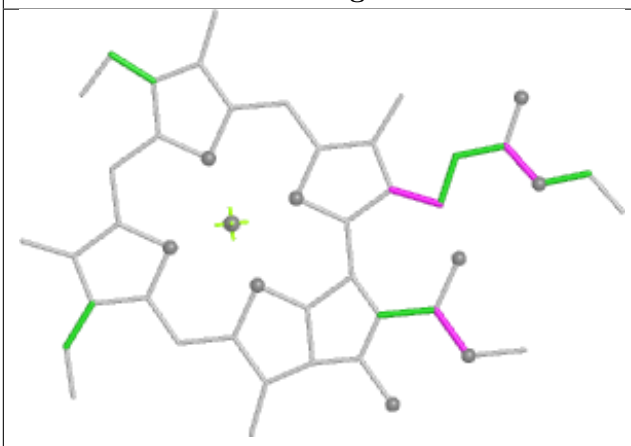


Bond angles



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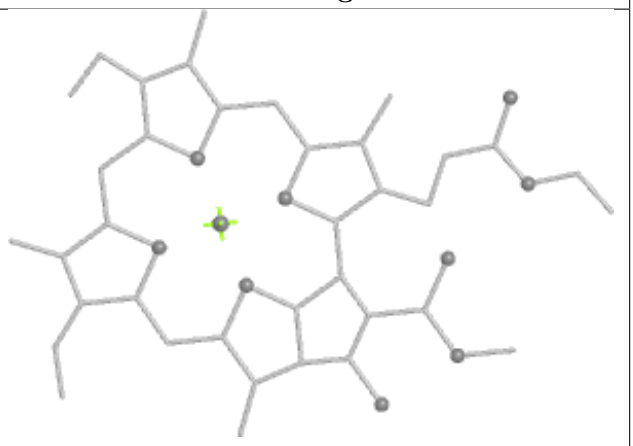
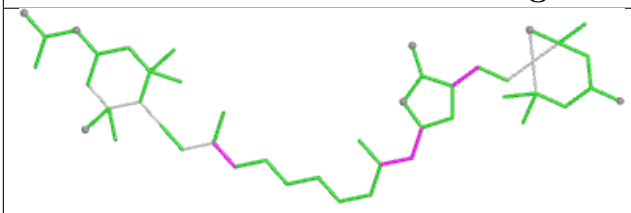


Rings

Ligand PID T 302



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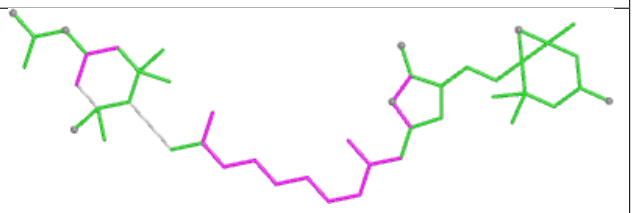
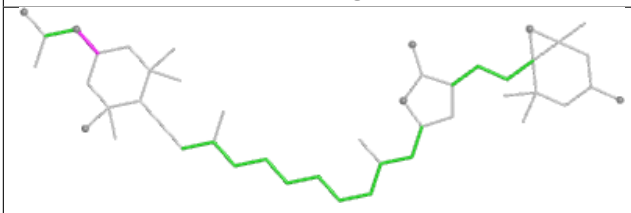


Bond angles



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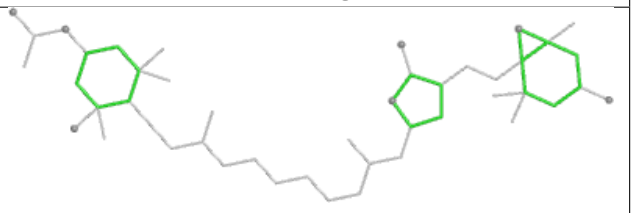
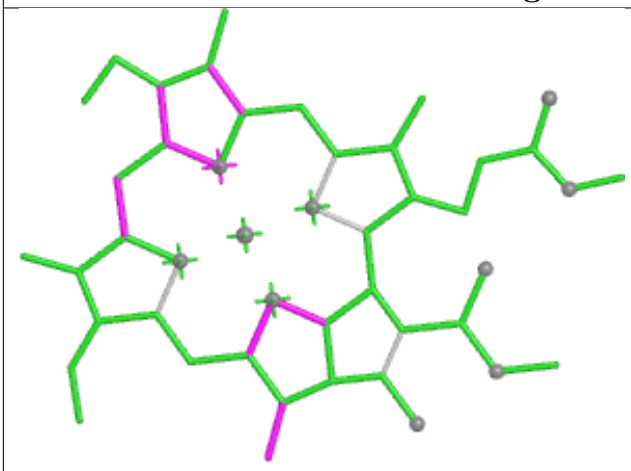
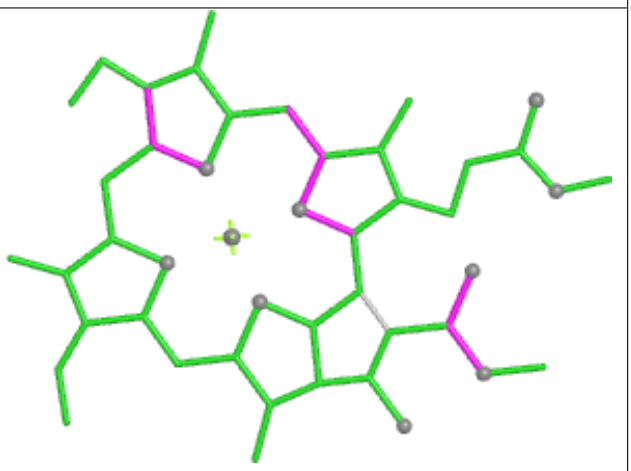


Rings

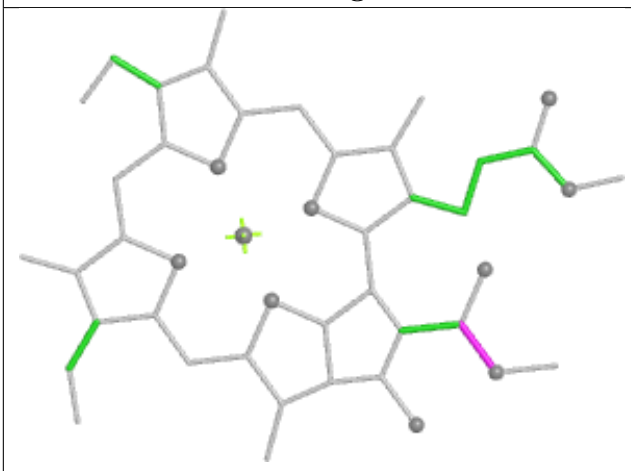
Ligand CLA D 309



Bond lengths



Bond angles



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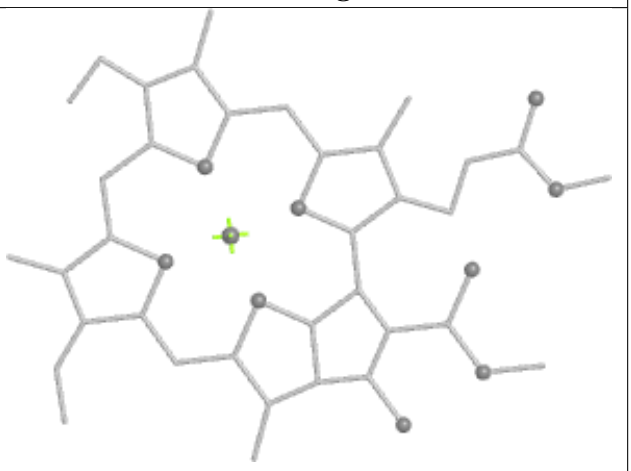
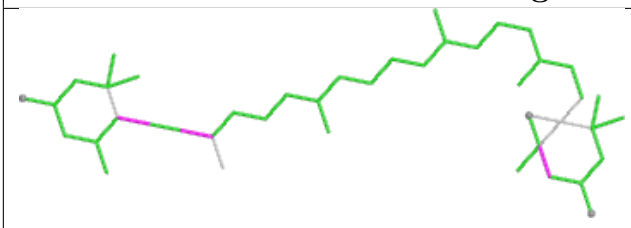


Rings

Ligand DD6 I 203



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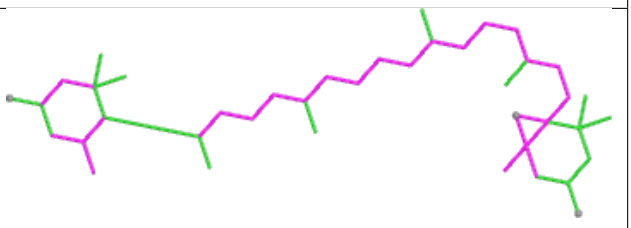

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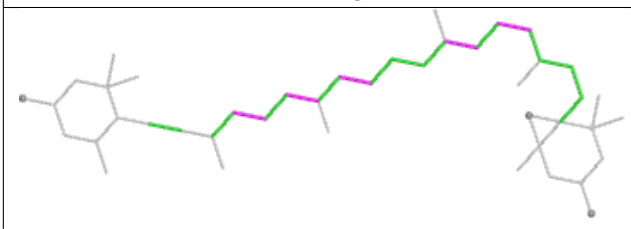

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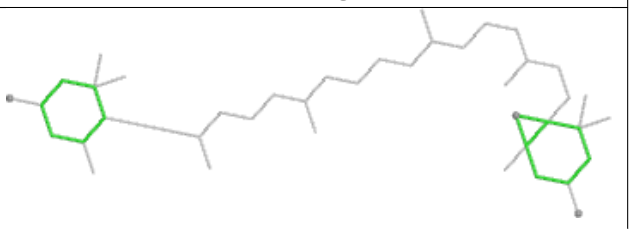
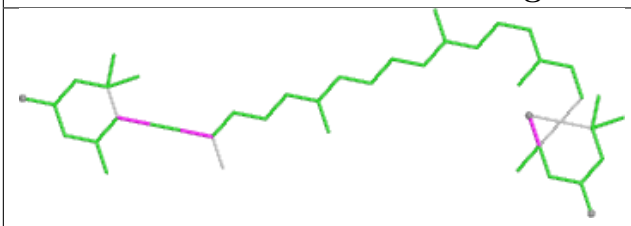


Rings

Ligand DD6 K 205



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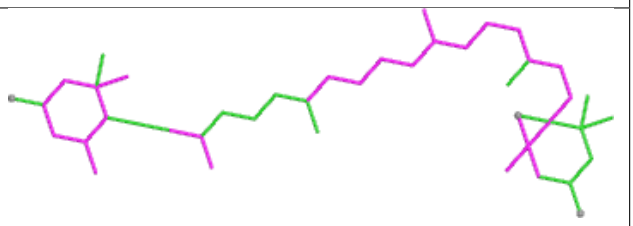

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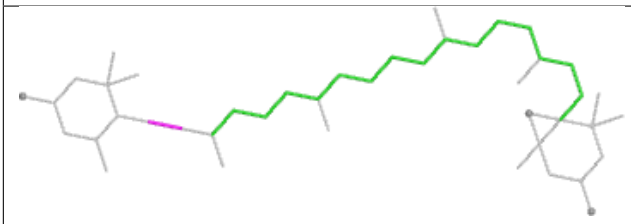

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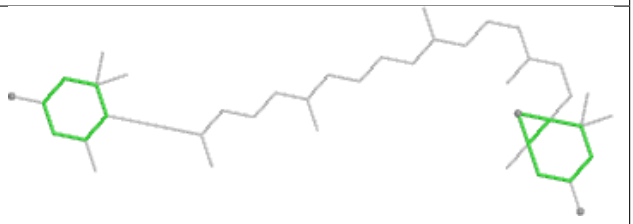
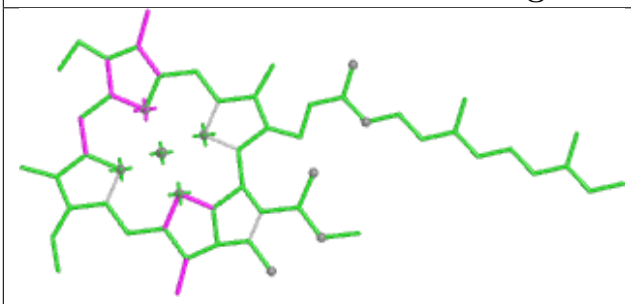


Rings

Ligand CLA b 731



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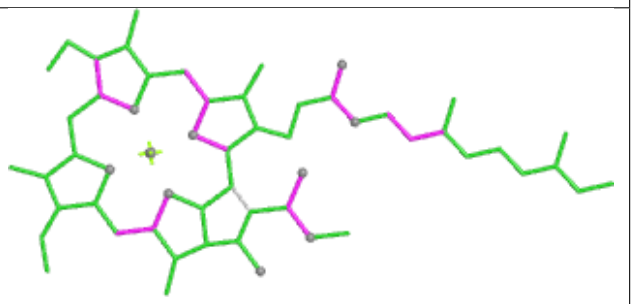

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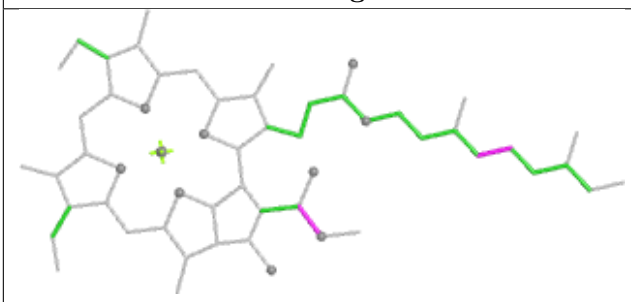

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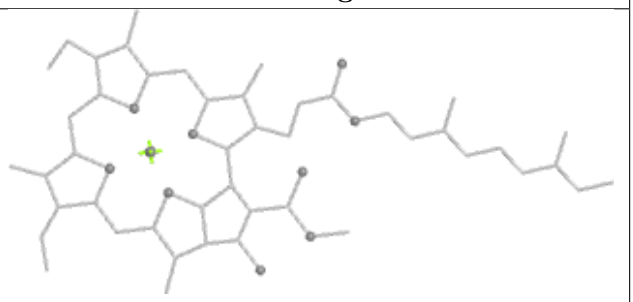
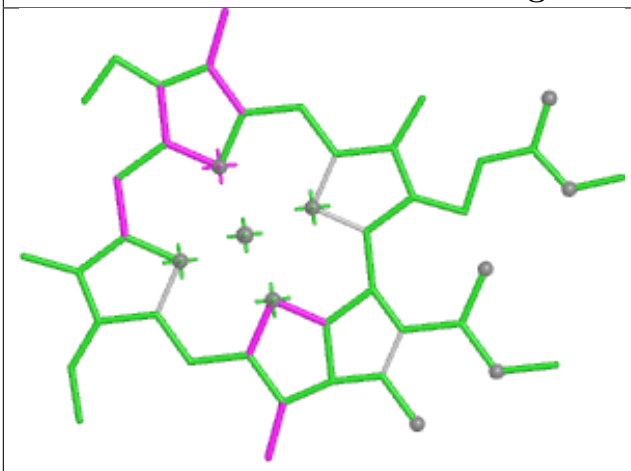


Rings

Ligand CLA J 309



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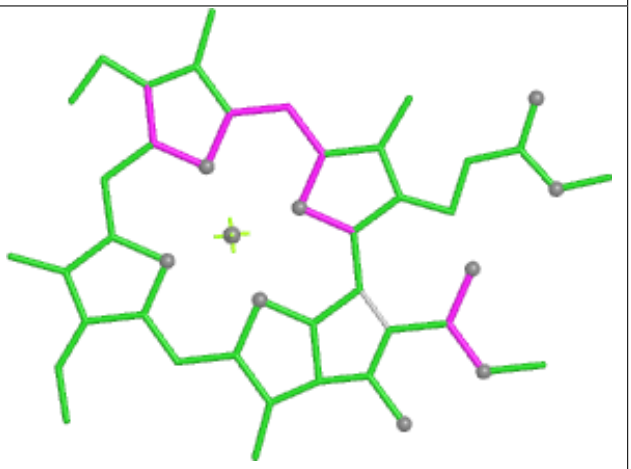

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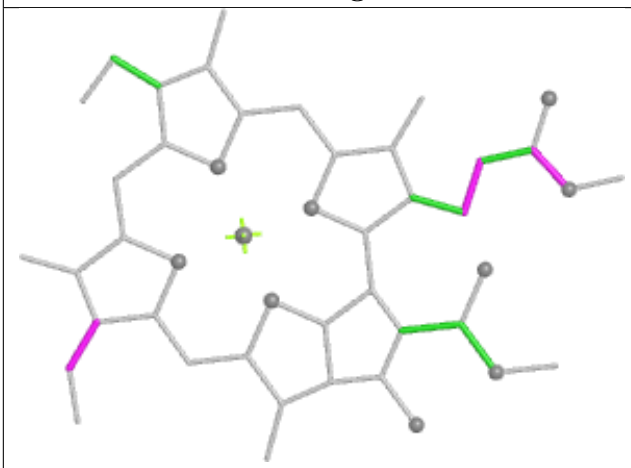

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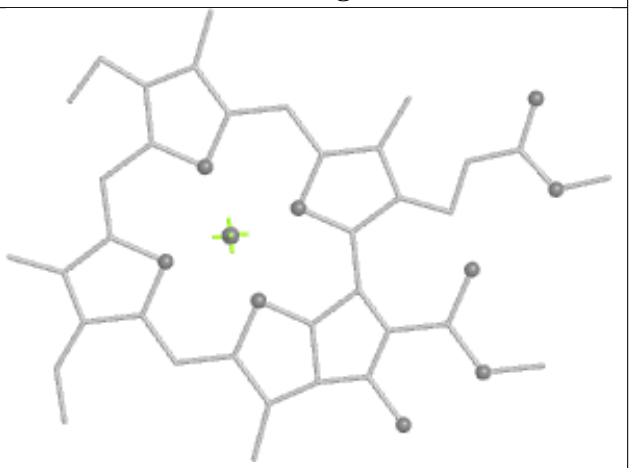
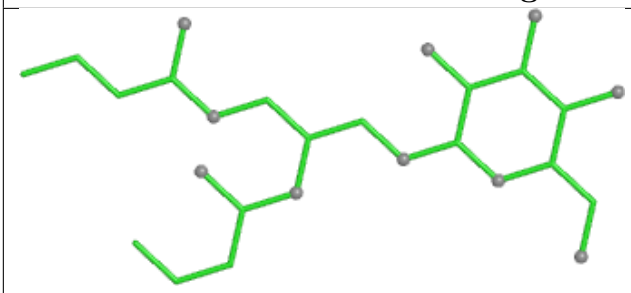


Rings

Ligand LMG P 201



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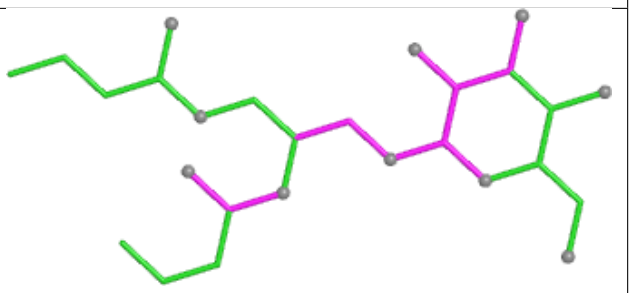

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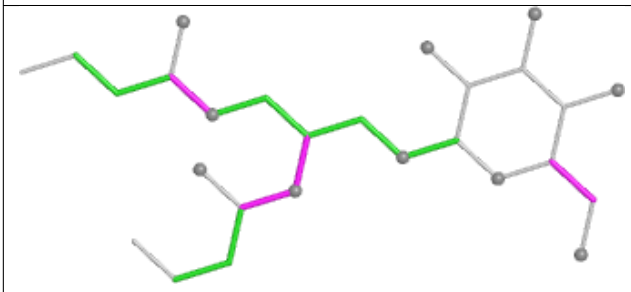

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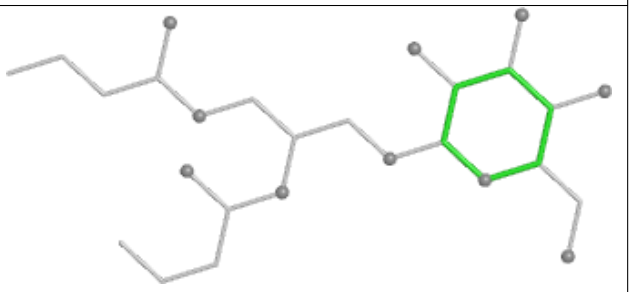
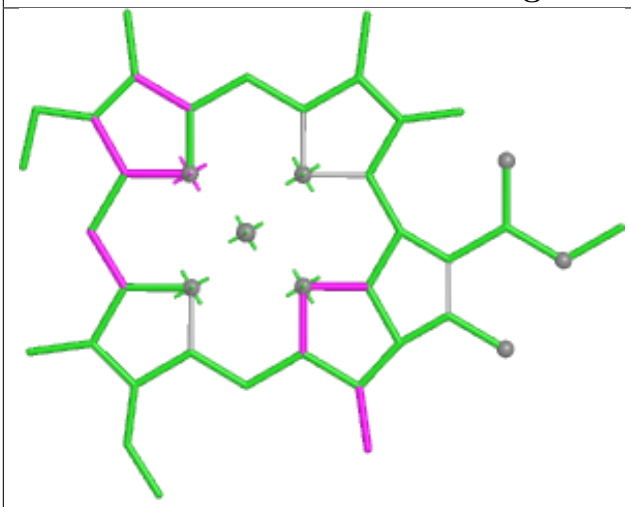


Rings

Ligand CLA H 315



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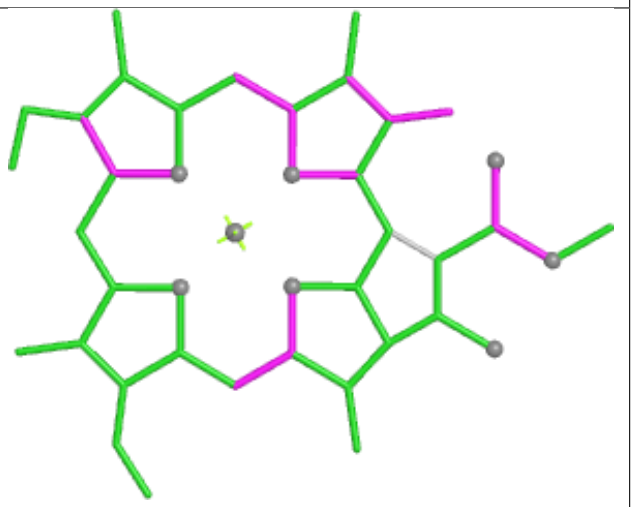
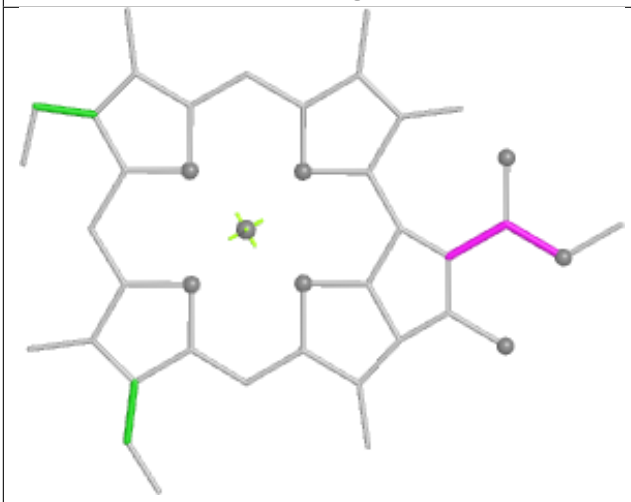


Bond angles



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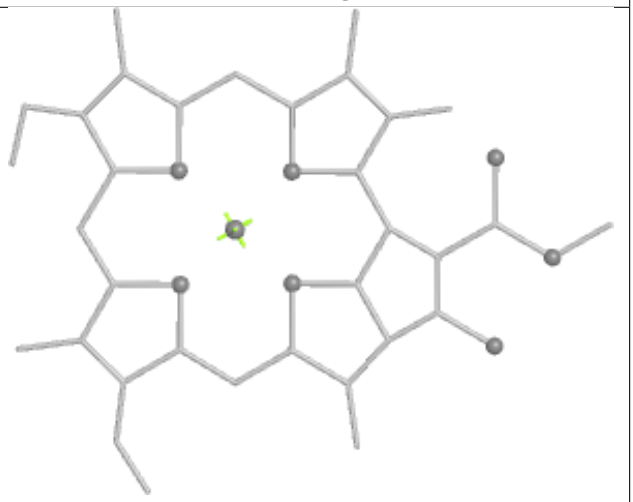
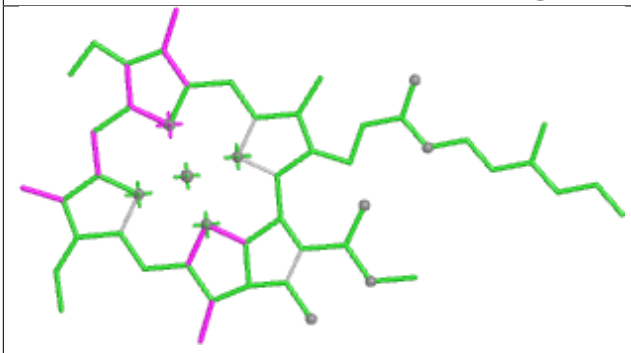


Rings

Ligand CLA j 104



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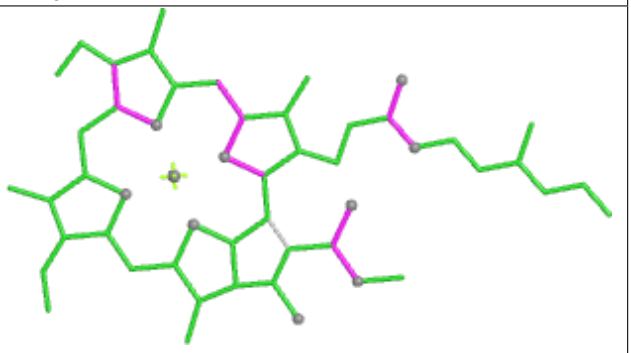

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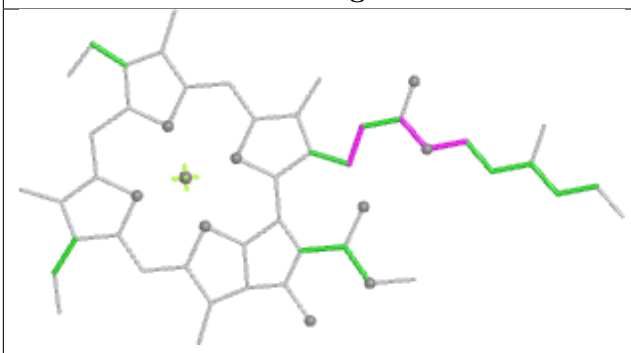

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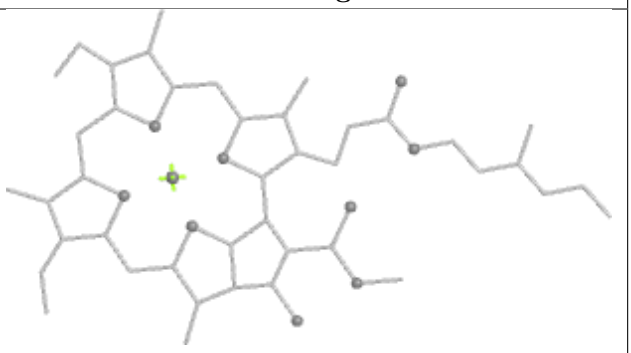
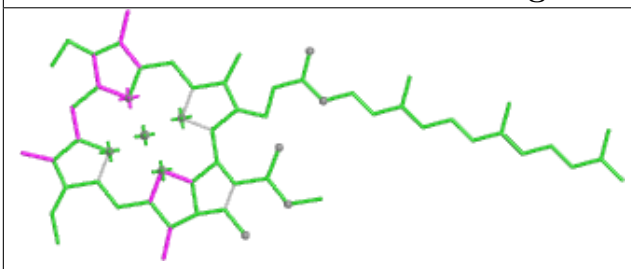


Rings

Ligand CLA a 812



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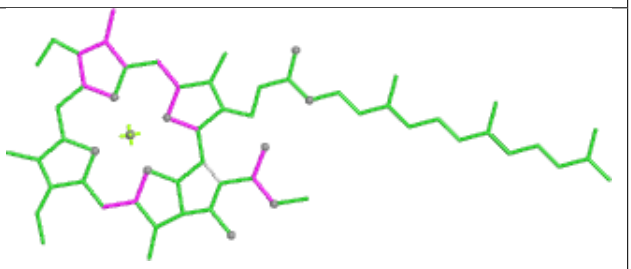

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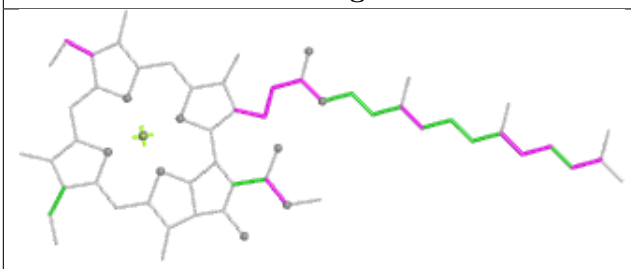

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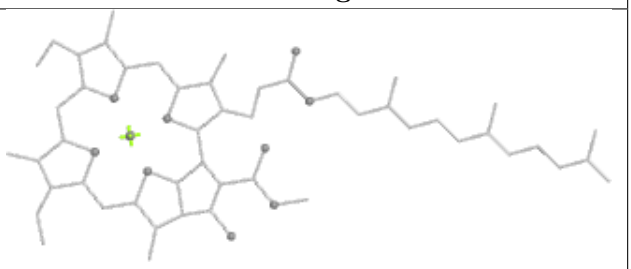
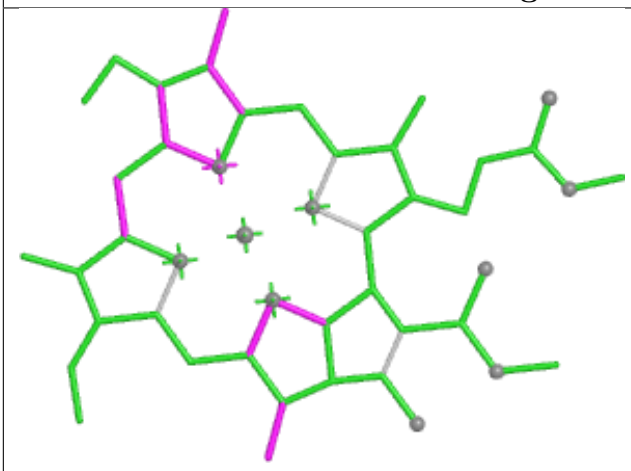


Rings

Ligand CLA M 311



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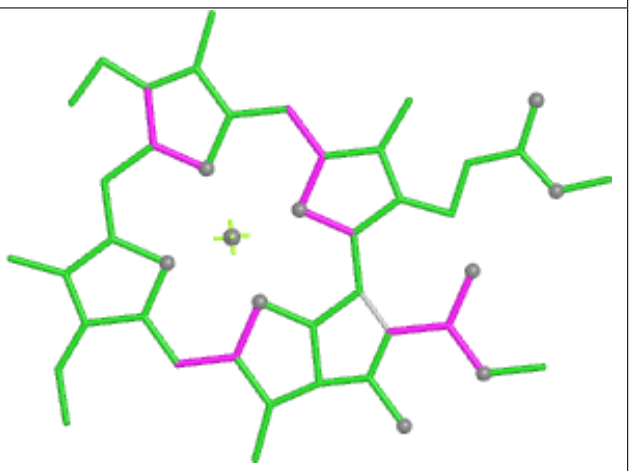
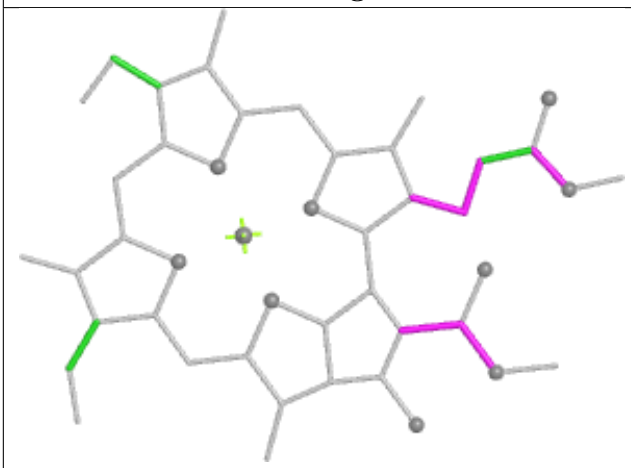


Bond angles



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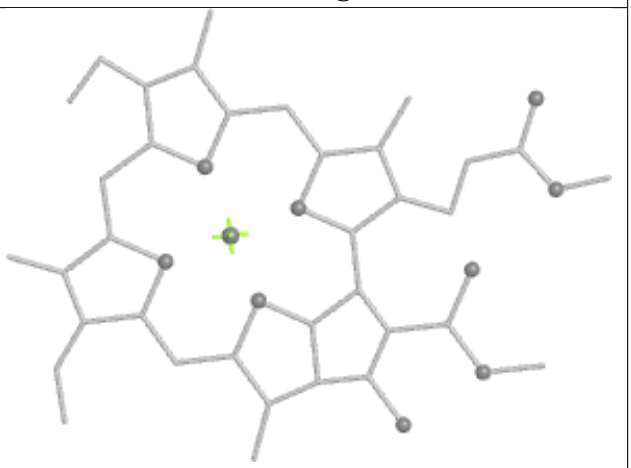
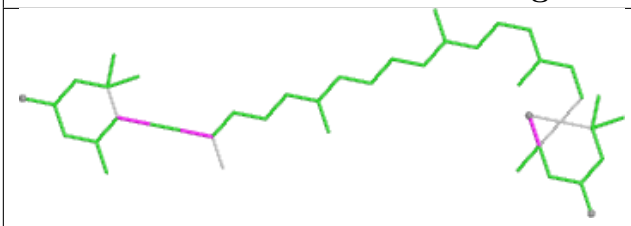


Rings

Ligand DD6 I 206



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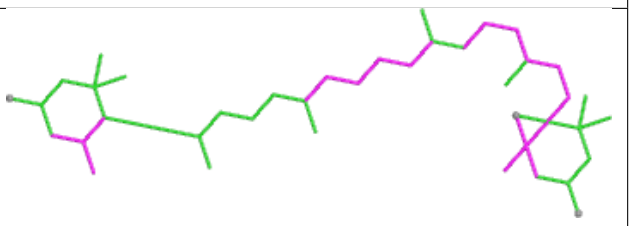
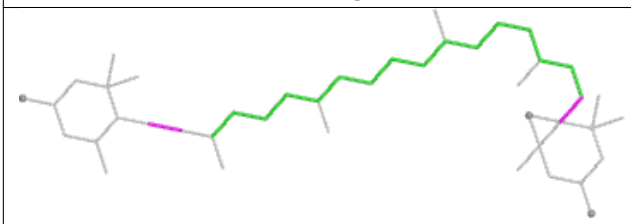


Bond angles



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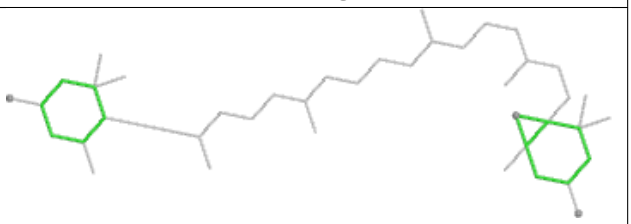
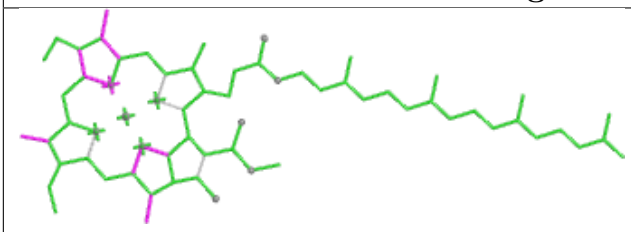


Rings

Ligand CLA b 706



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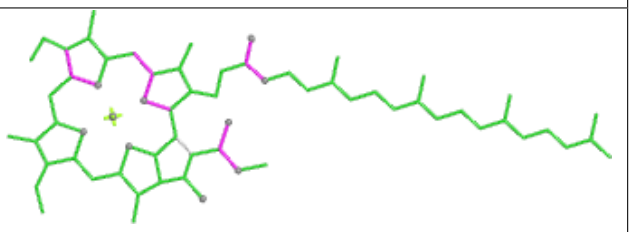
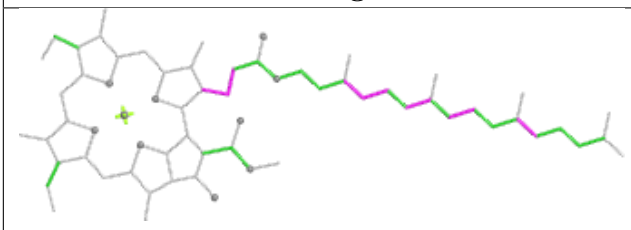


Bond angles



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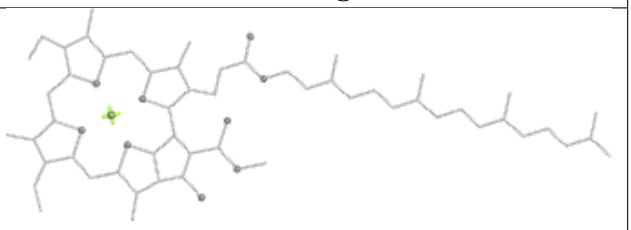
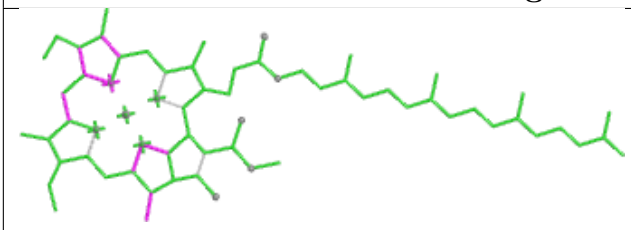


Rings

Ligand CLA E 308



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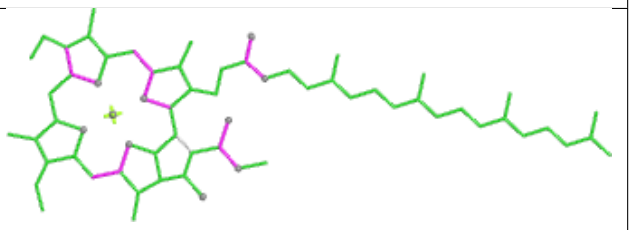
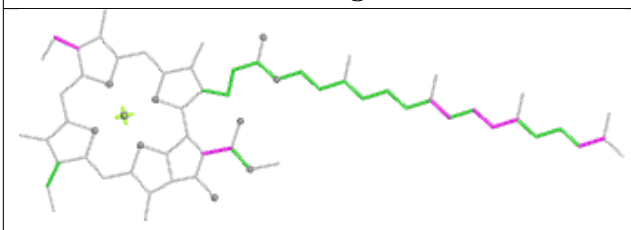


Bond angles



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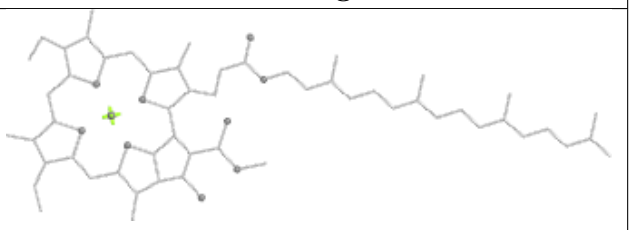
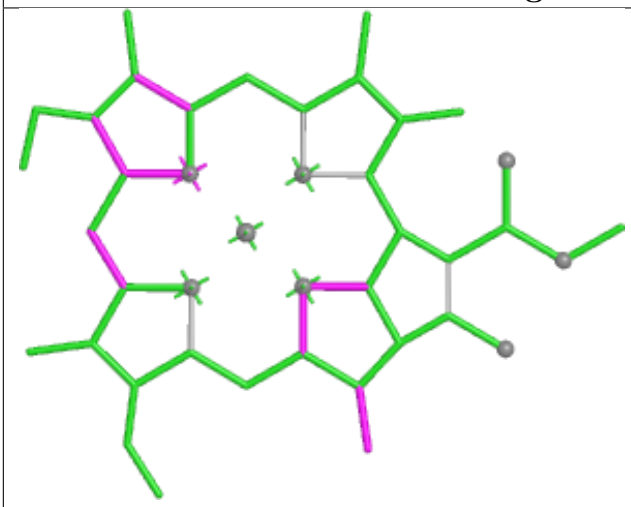


Rings

Ligand CLA E 313



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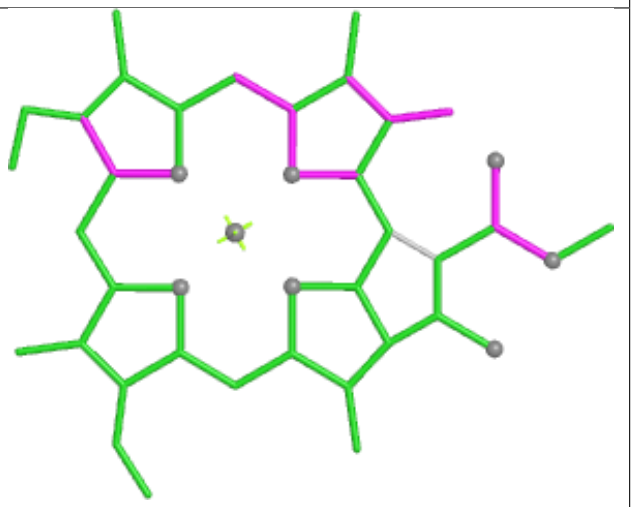
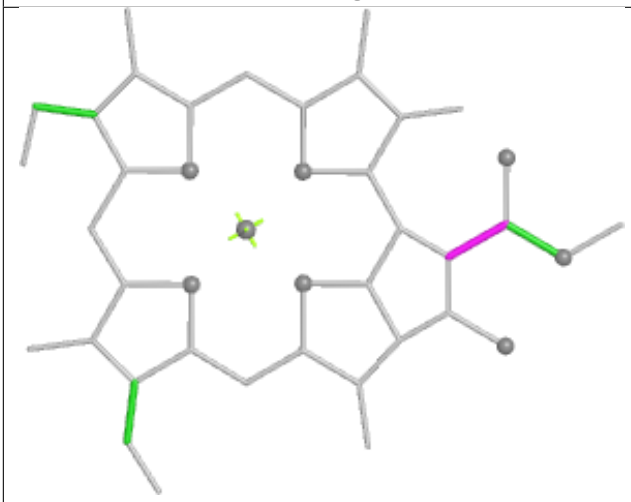


Bond angles



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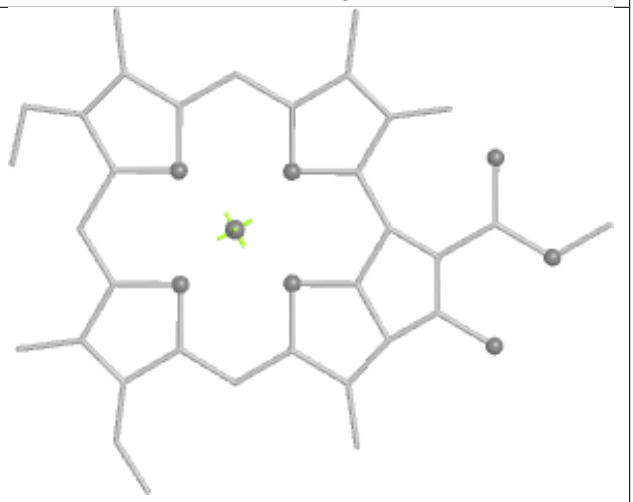
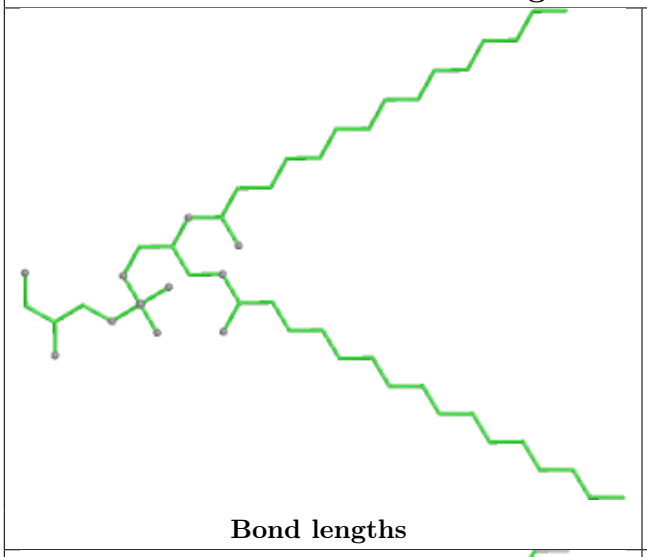


Rings

Ligand LHG a 833



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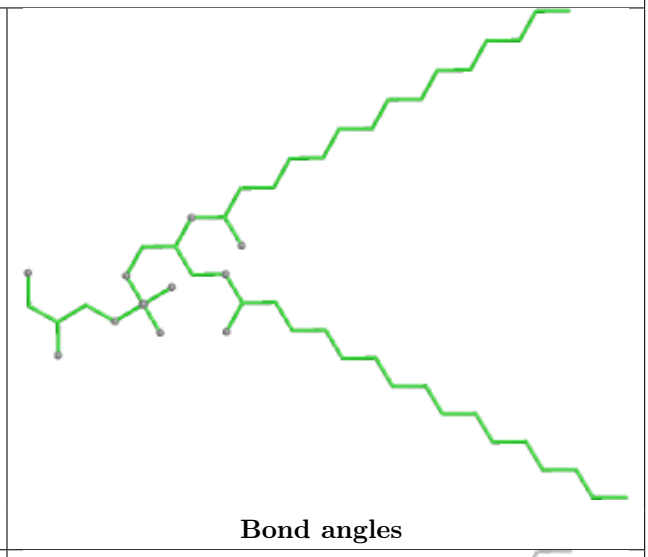
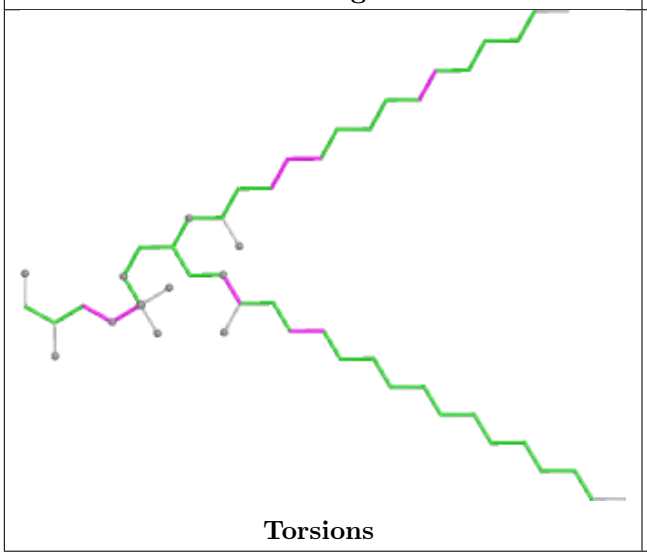


Bond angles



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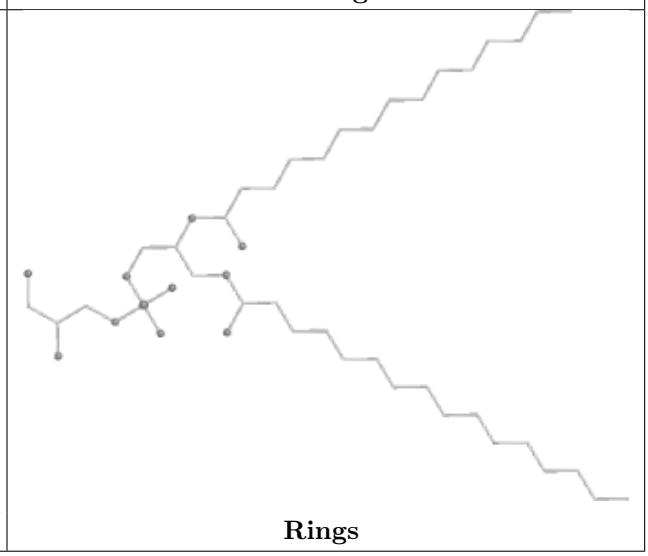
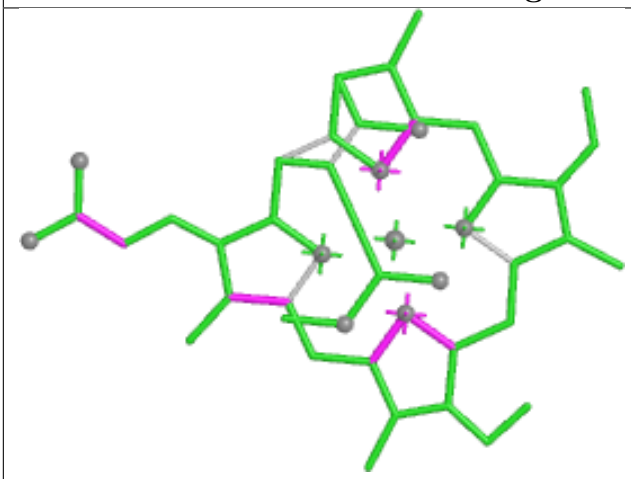


Rings

Ligand KC1 G 318



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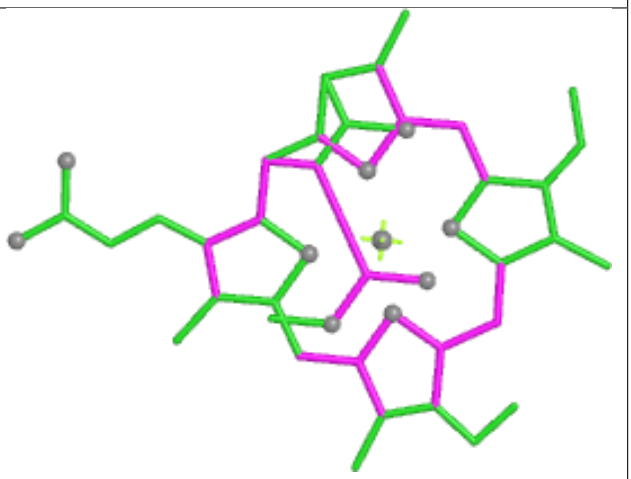

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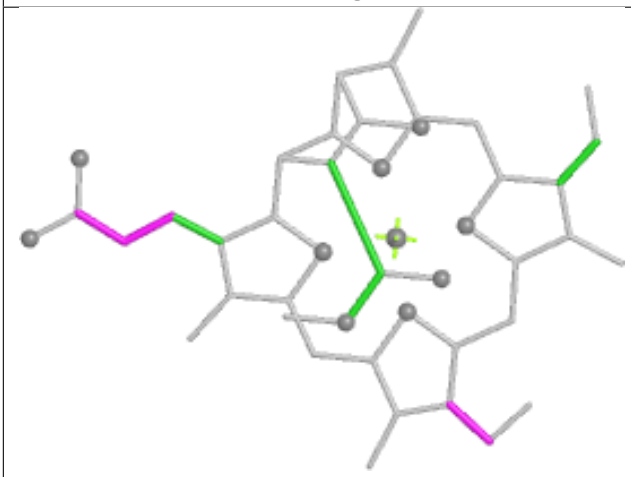
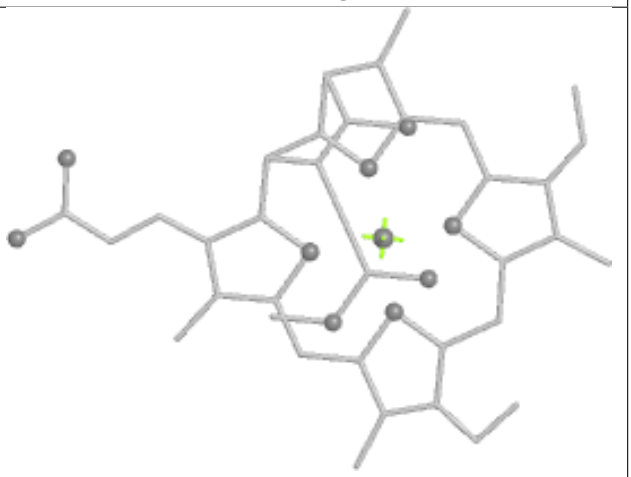
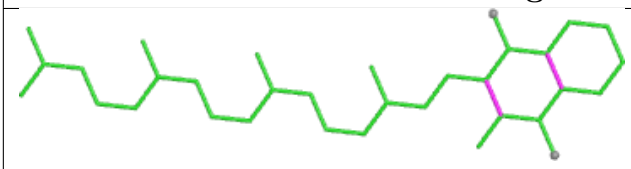


Torsions



Rings

Ligand PQN a 832



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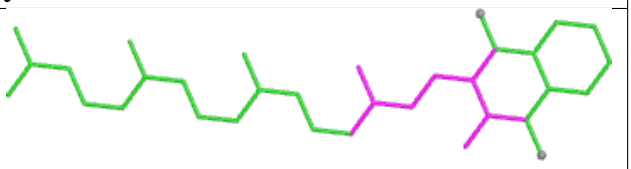

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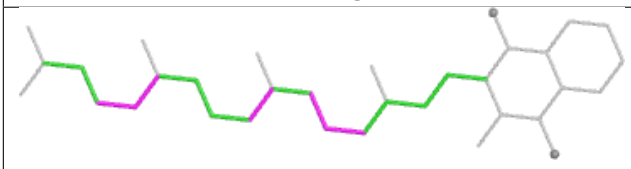

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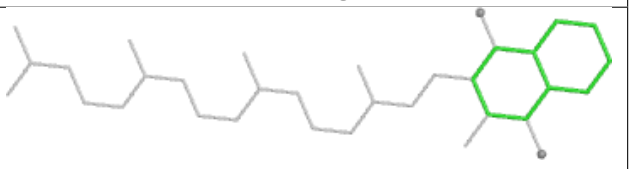
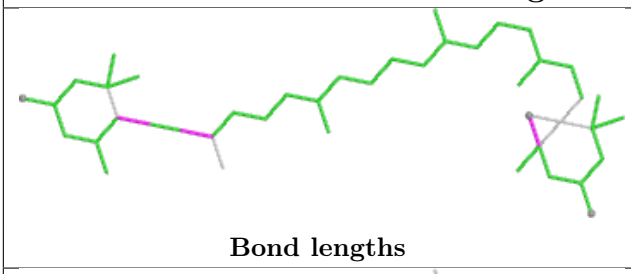


Rings

Ligand DD6 L 303



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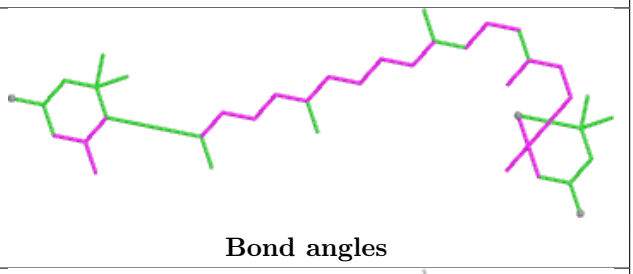

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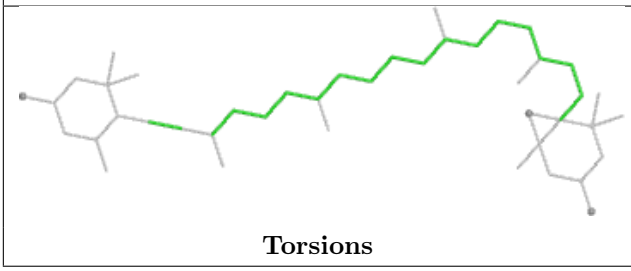

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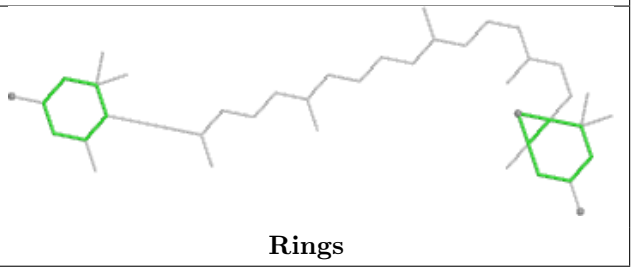
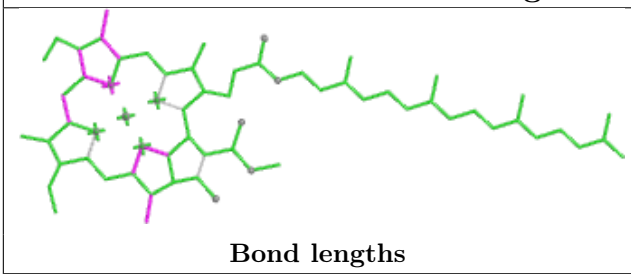


Rings

Ligand CLA A 209



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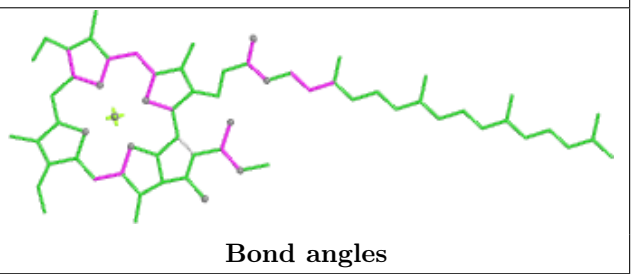

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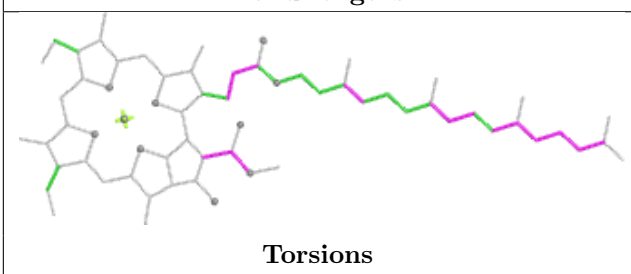

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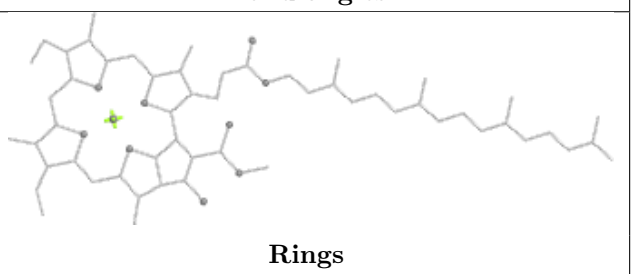
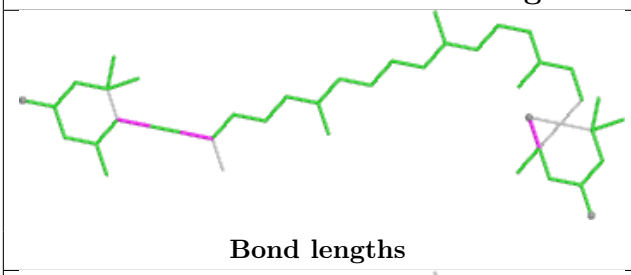


Rings

Ligand DD6 K 204



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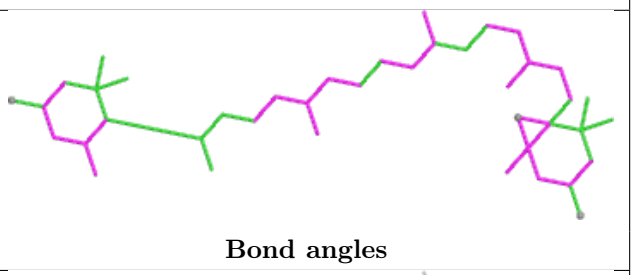

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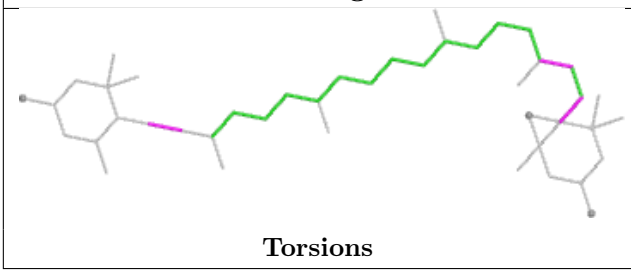

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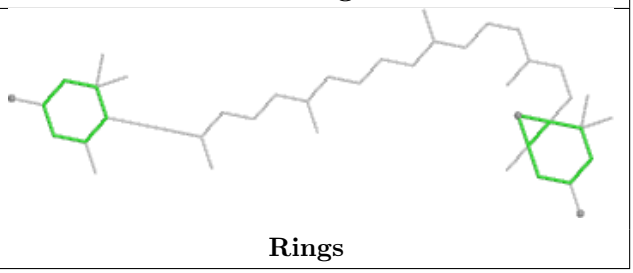
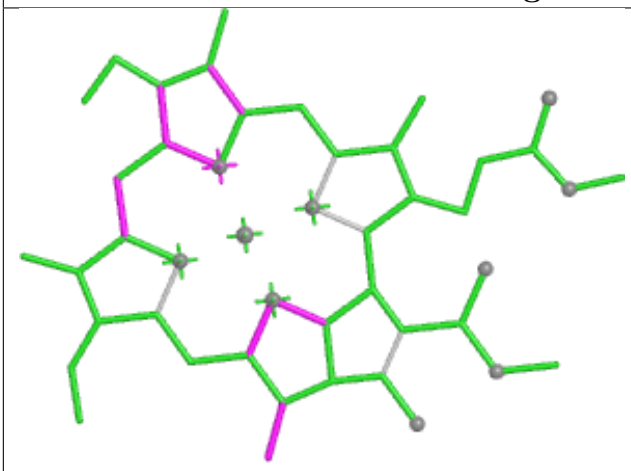


Rings

Ligand CLA D 312



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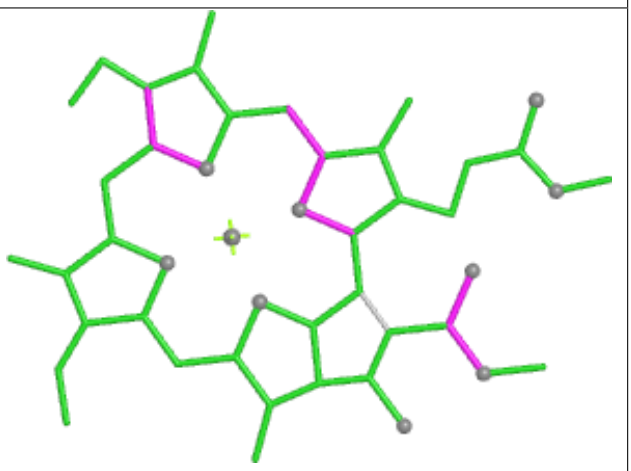

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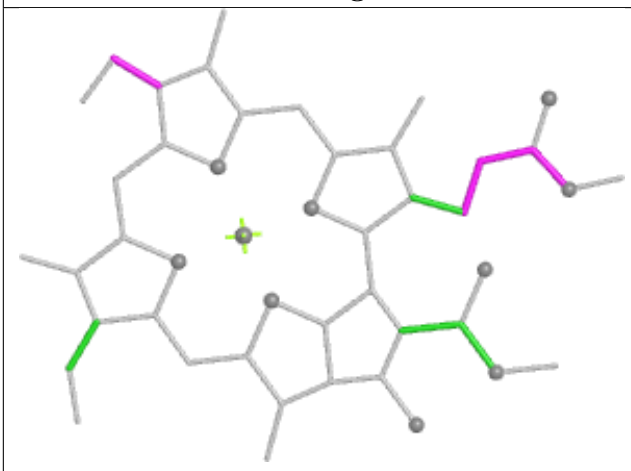

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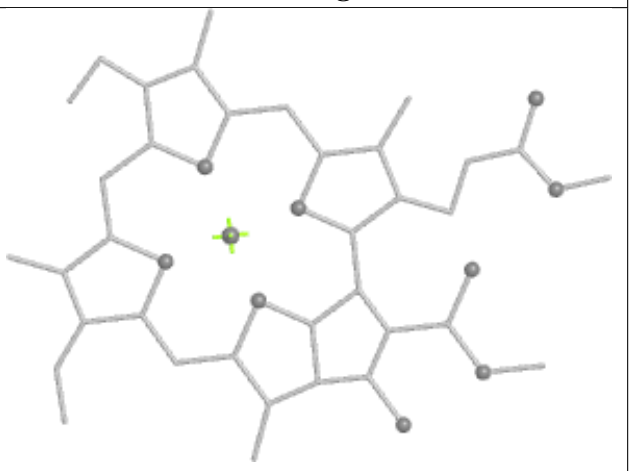
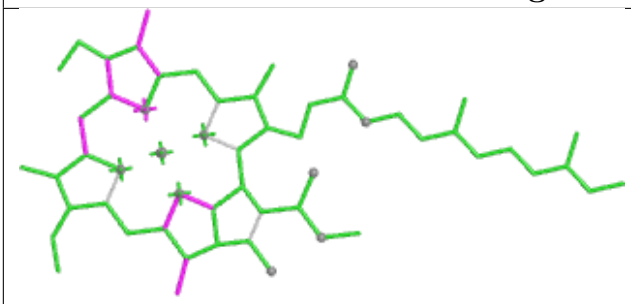


Rings

Ligand CLA a 811



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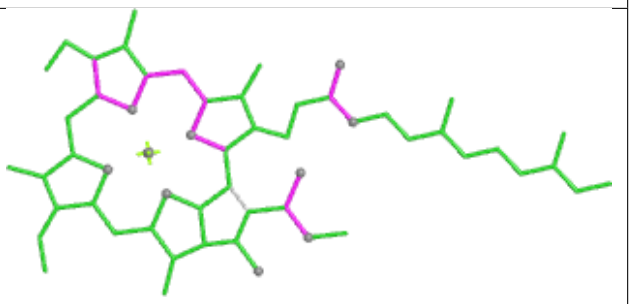

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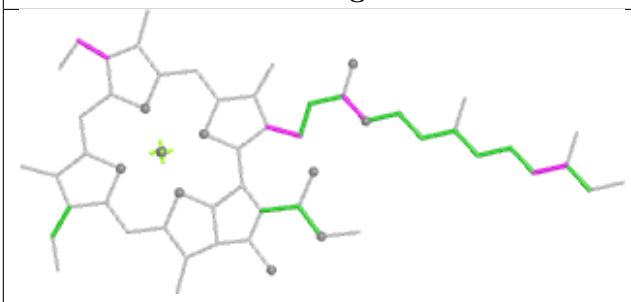

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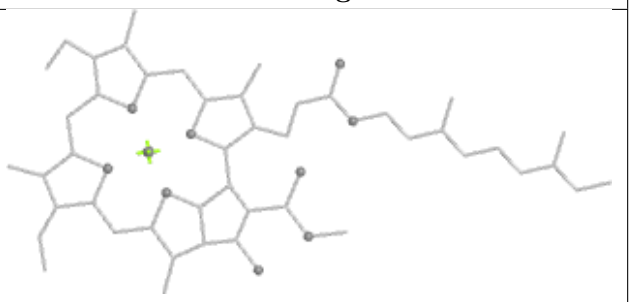
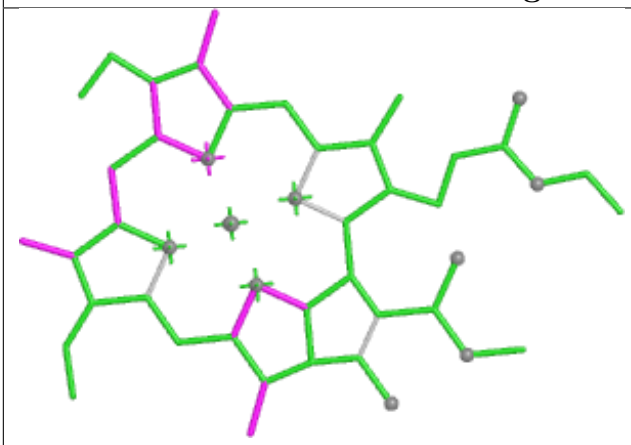


Rings

Ligand CLA D 314



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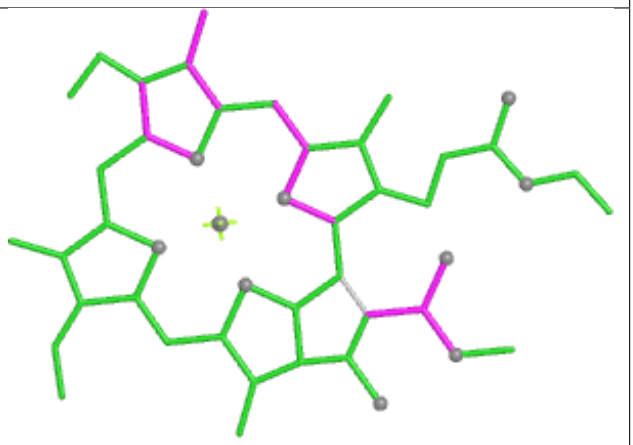

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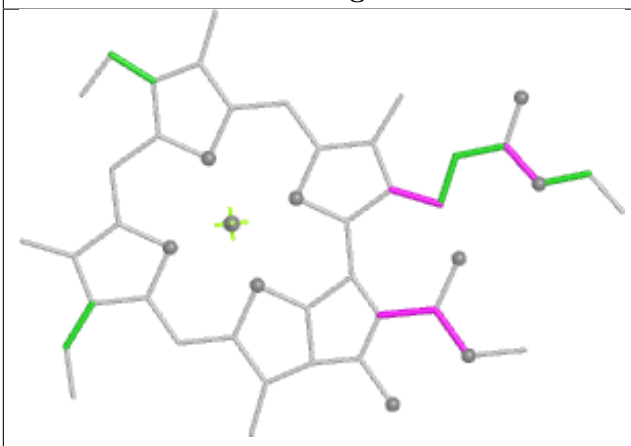

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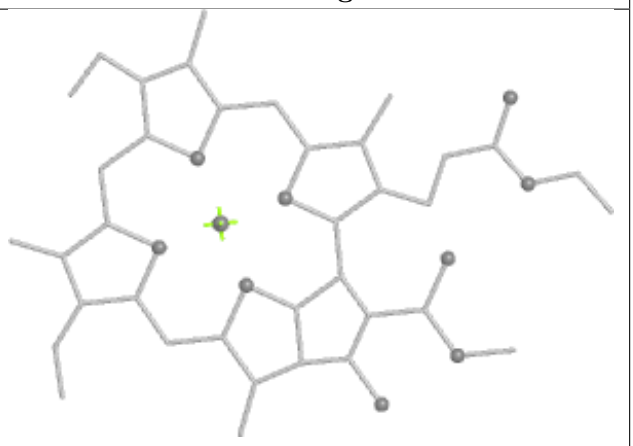
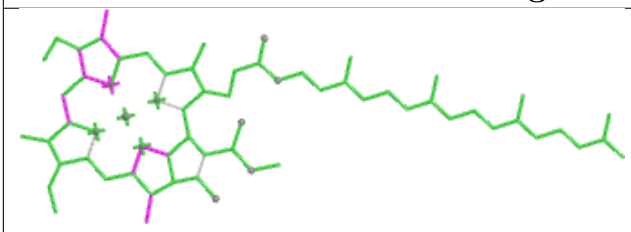


Rings

Ligand CLA a 802



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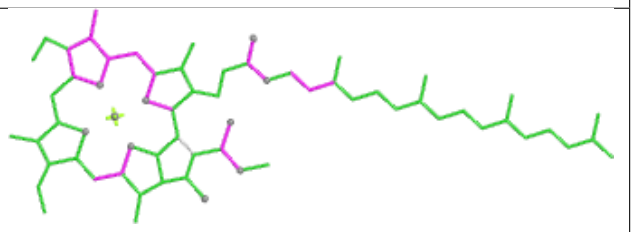

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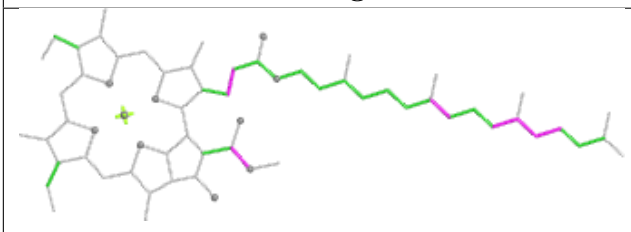

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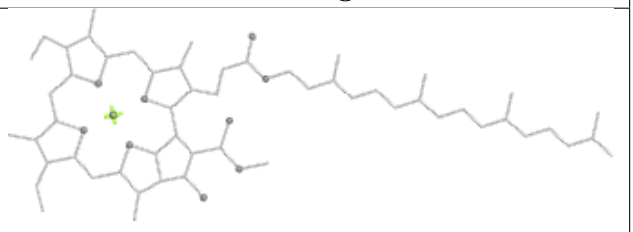
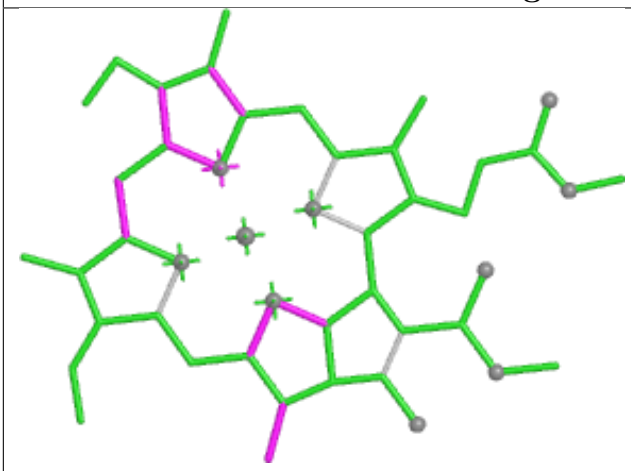


Rings

Ligand CLA N 313



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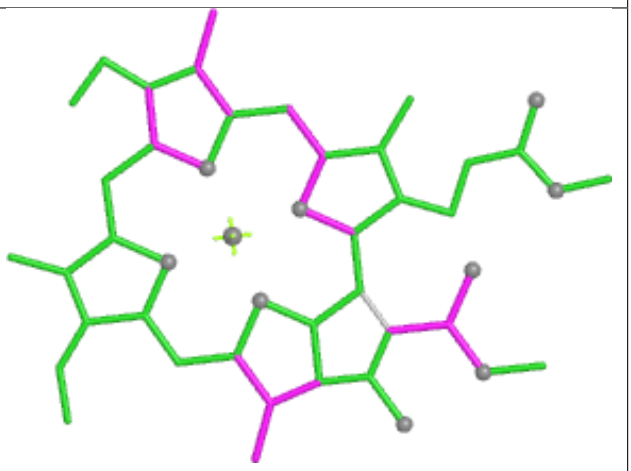

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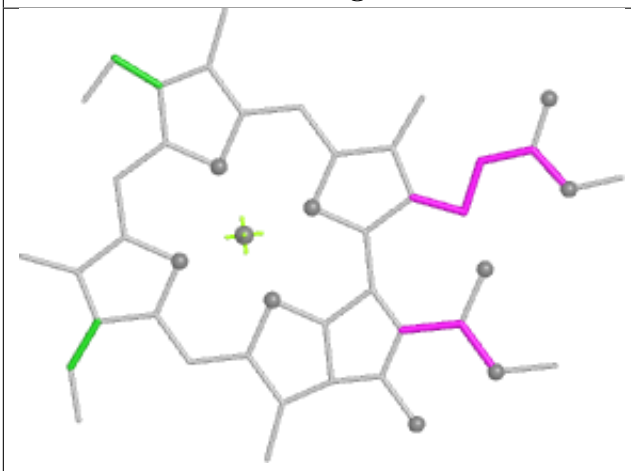

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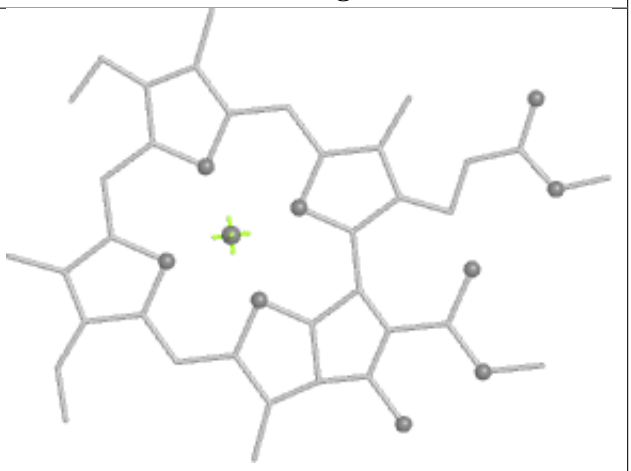
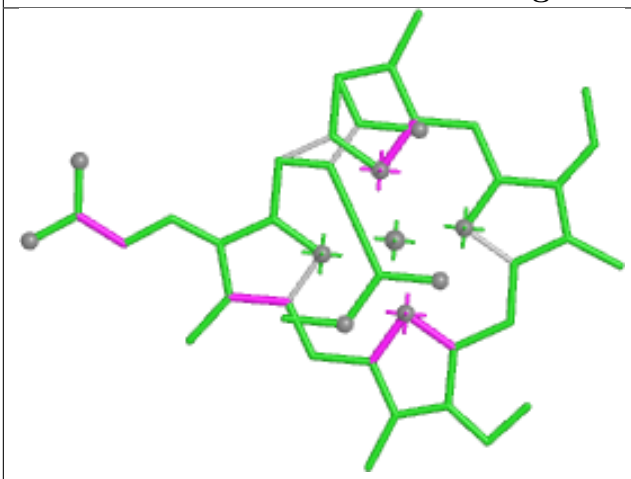


Rings

Ligand KC1 I 215



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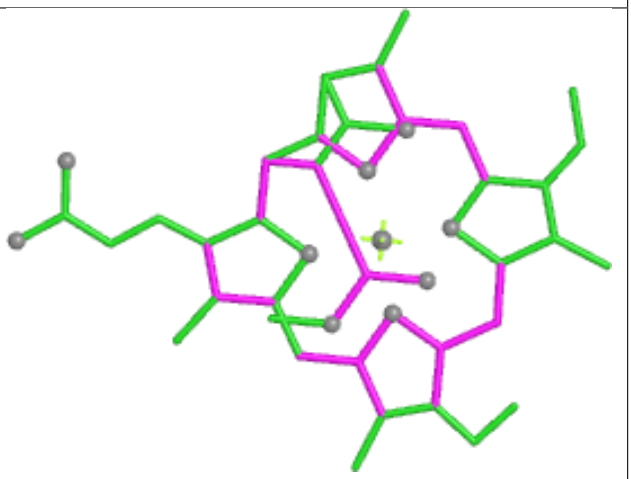

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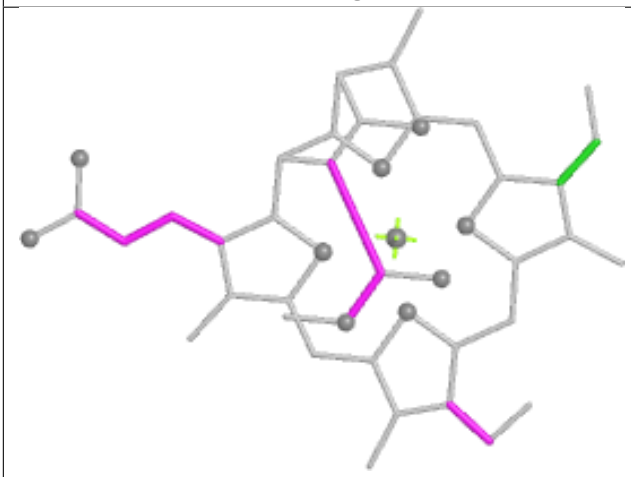

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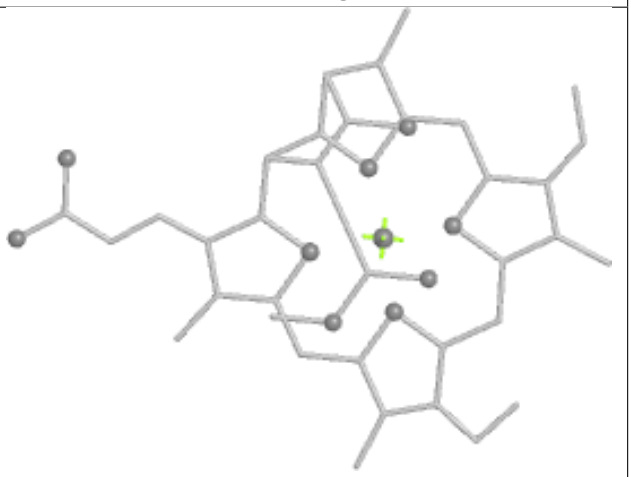
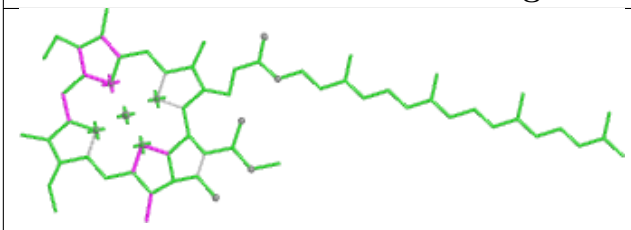


Rings

Ligand CLA G 302



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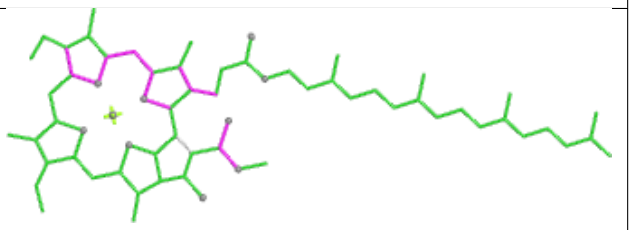
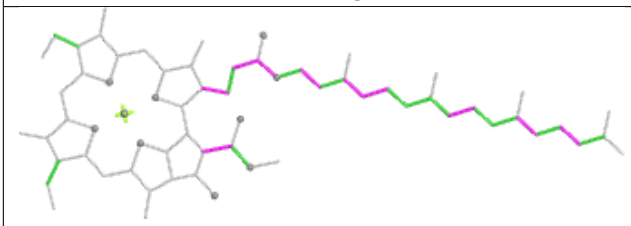


Bond angles



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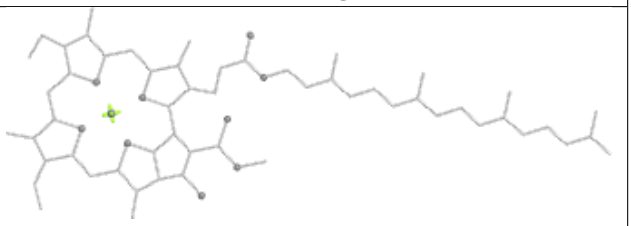
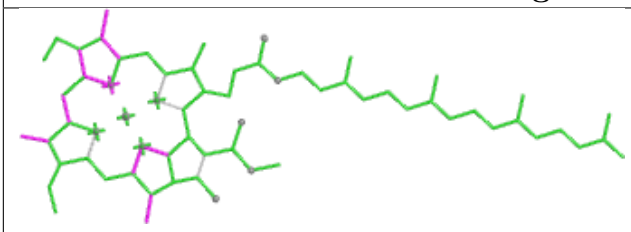


Rings

Ligand CLA l 502



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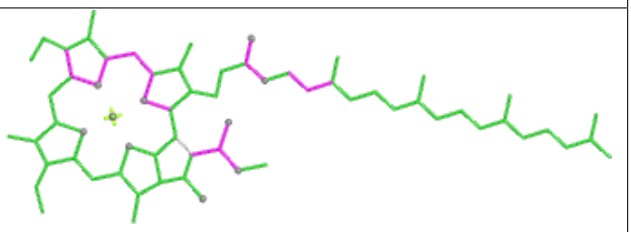
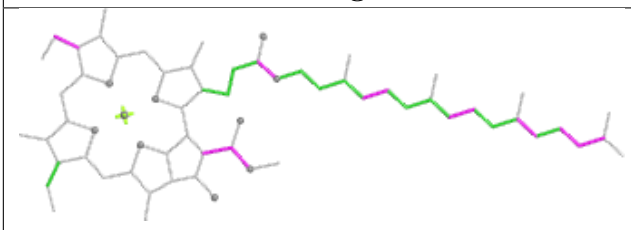


Bond angles



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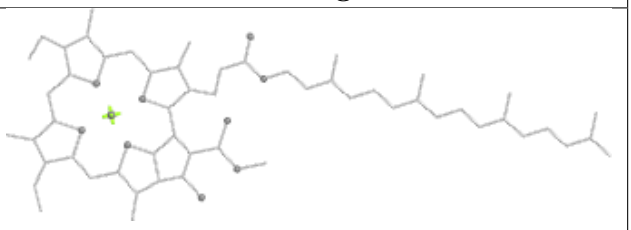
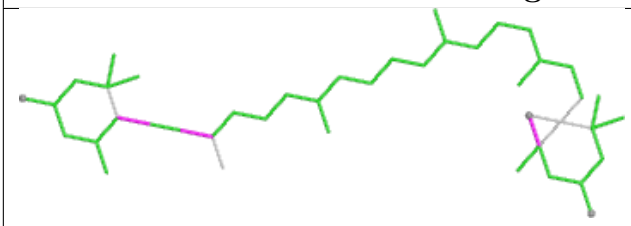


Rings

Ligand DD6 K 206



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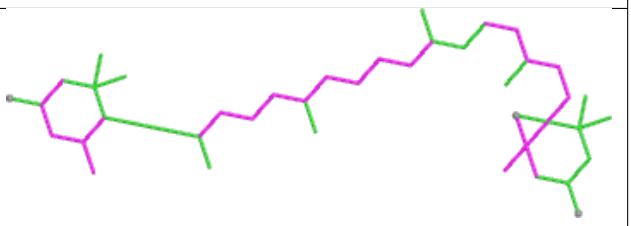
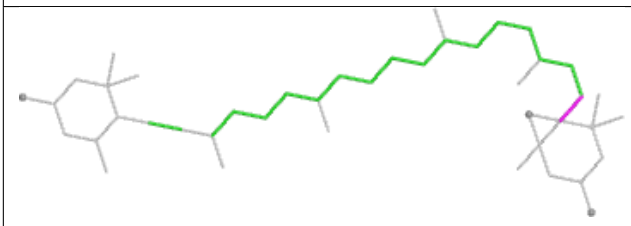


Bond angles



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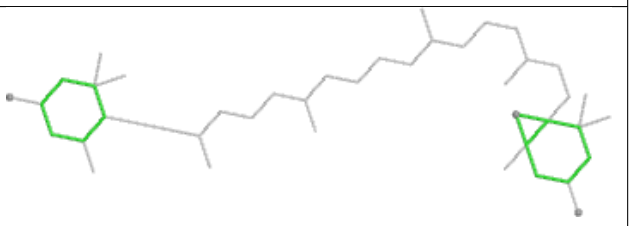
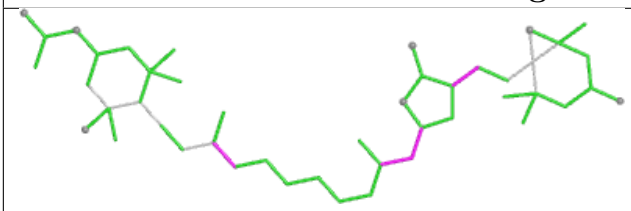


Rings

Ligand PID C 307



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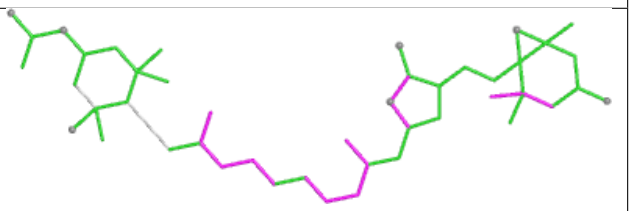
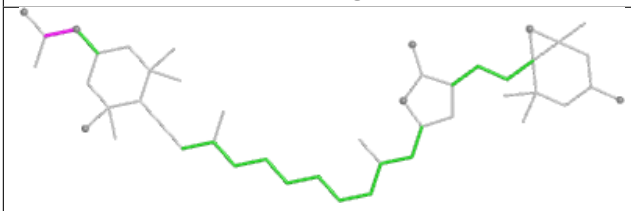
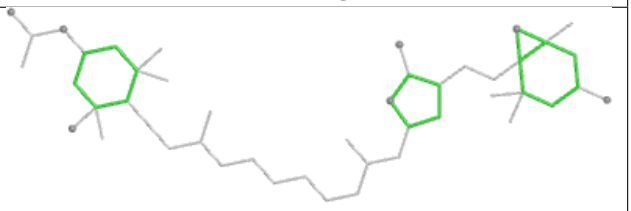


Bond angles

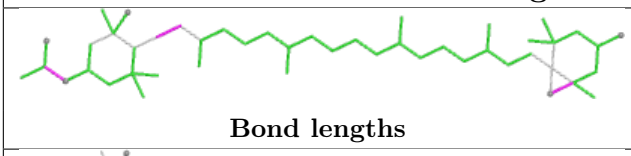


Torsions

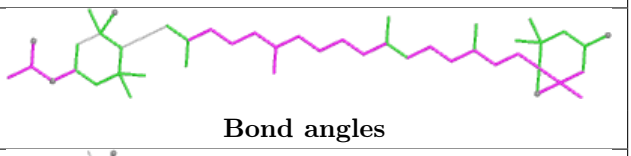


Rings

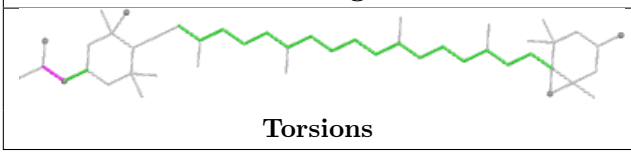
Ligand UIX L 302



Bond lengths



Bond angles



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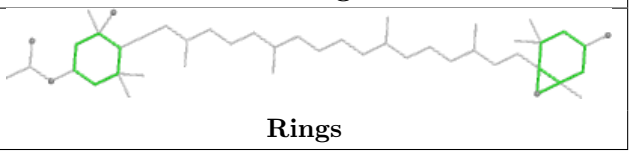
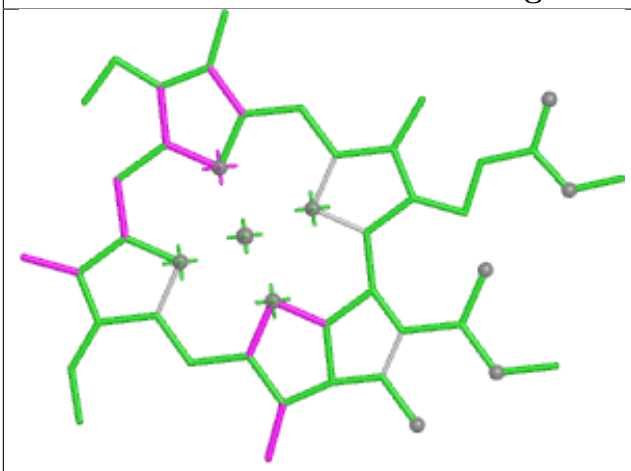


Rings

Ligand CLA T 309



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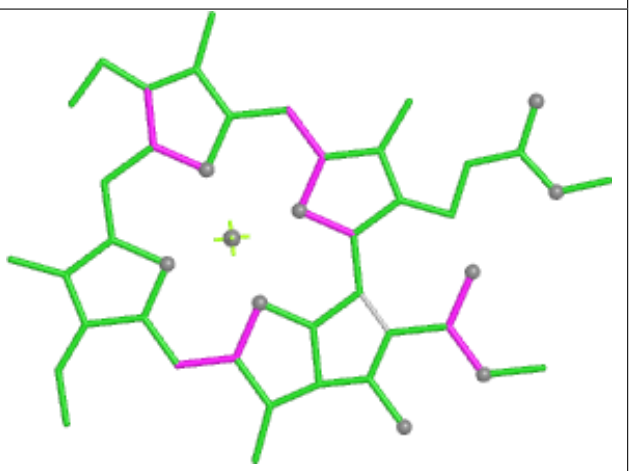

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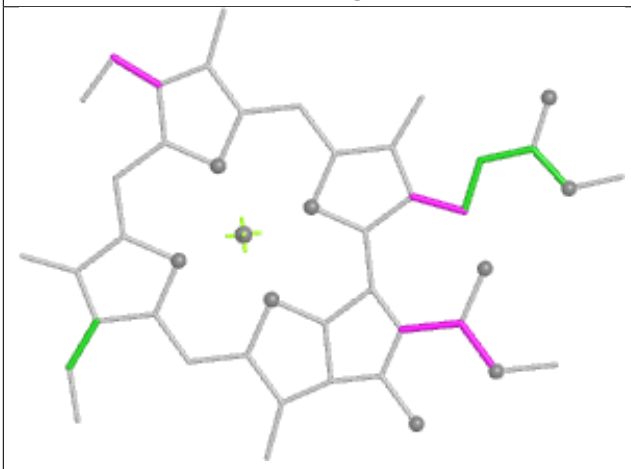

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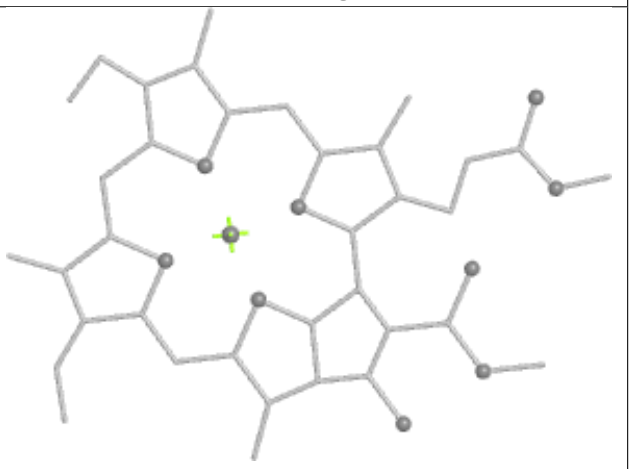
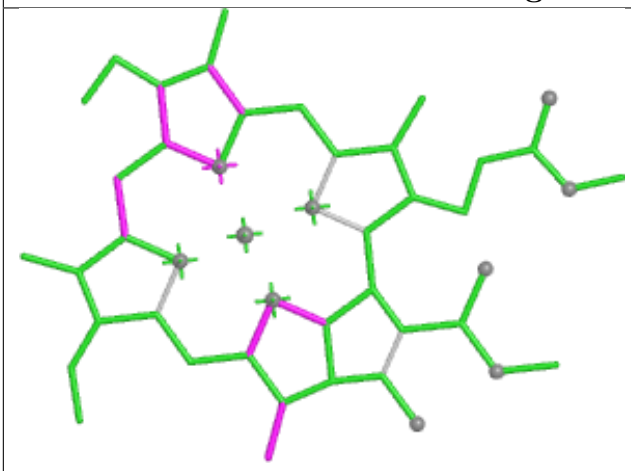


Rings

Ligand CLA E 309



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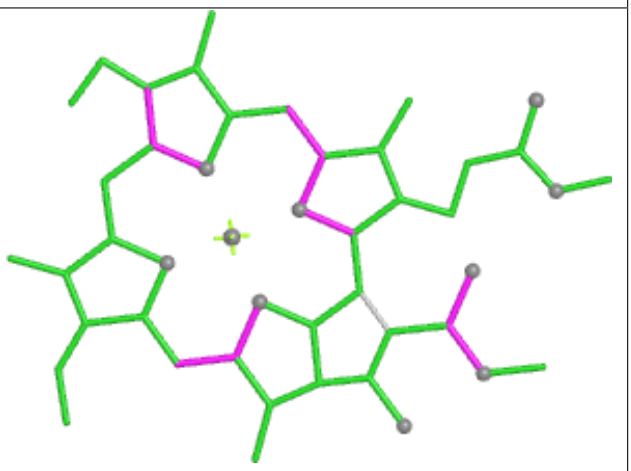
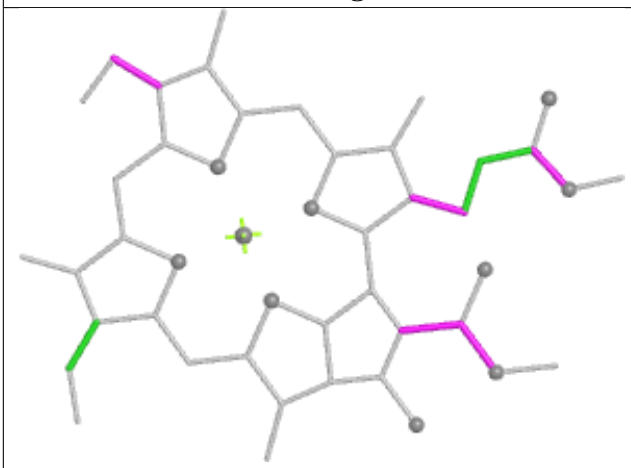


Bond angles



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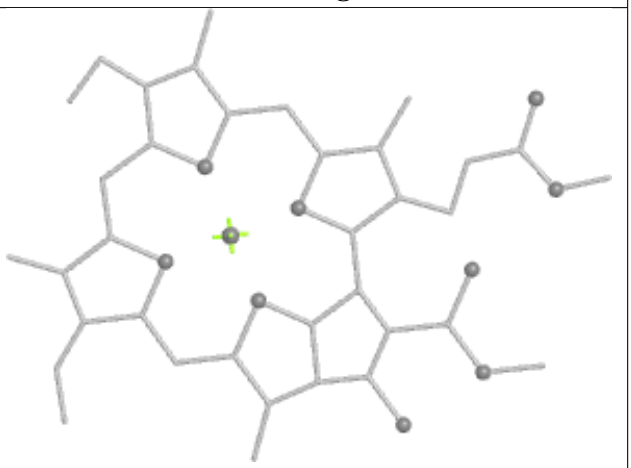
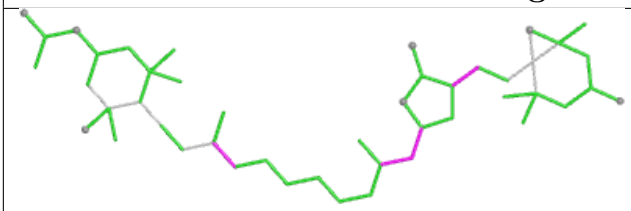


Rings

Ligand PID Q 301



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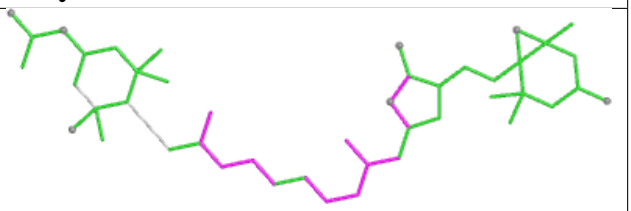

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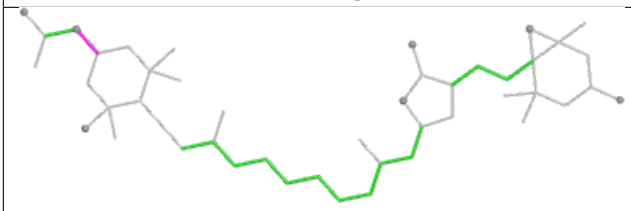

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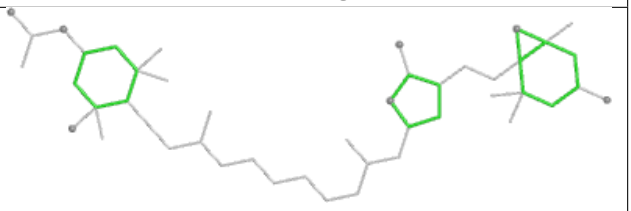
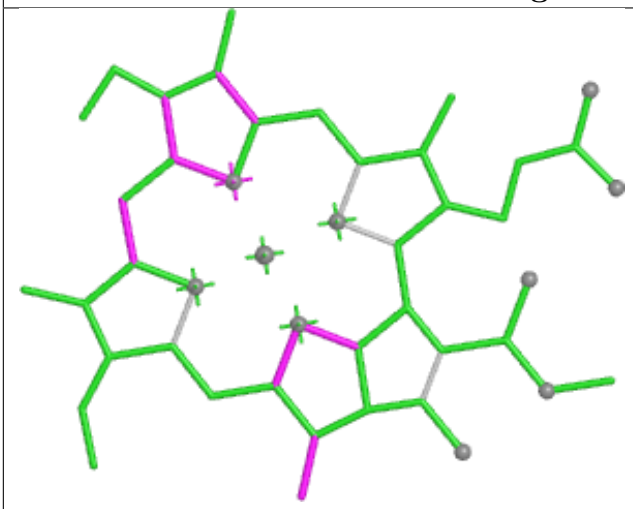


Rings

Ligand CLA I 201



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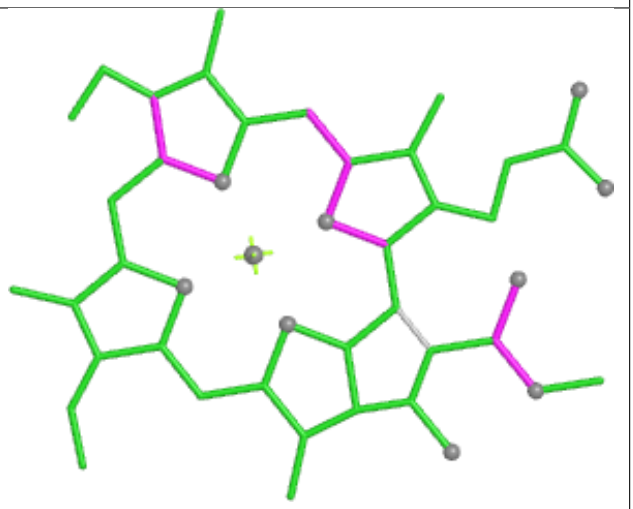

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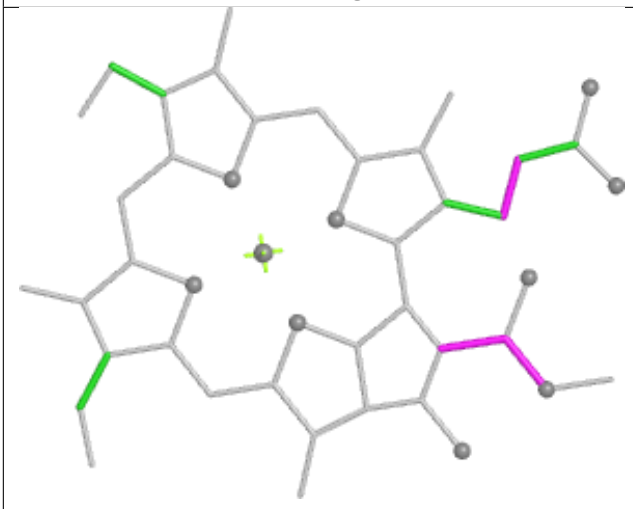
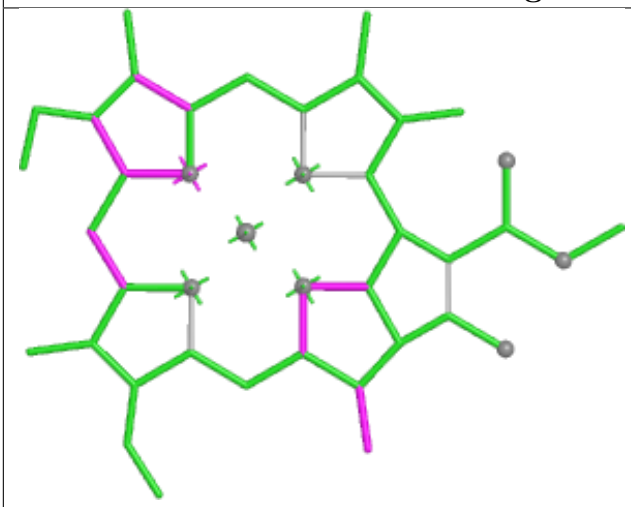


Torsions



Rings

Ligand CLA T 316



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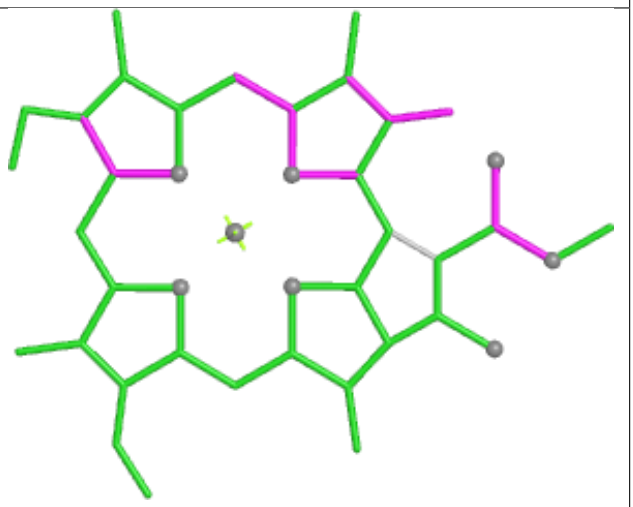
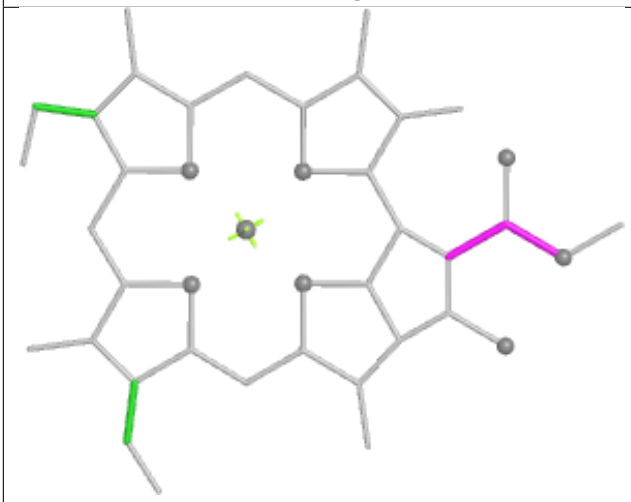


Bond angles



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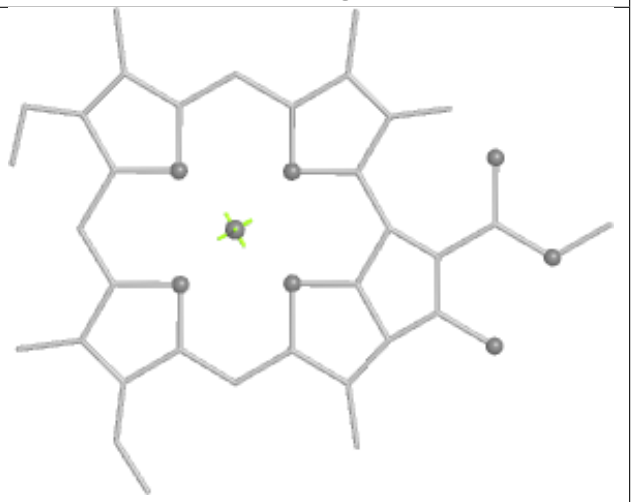
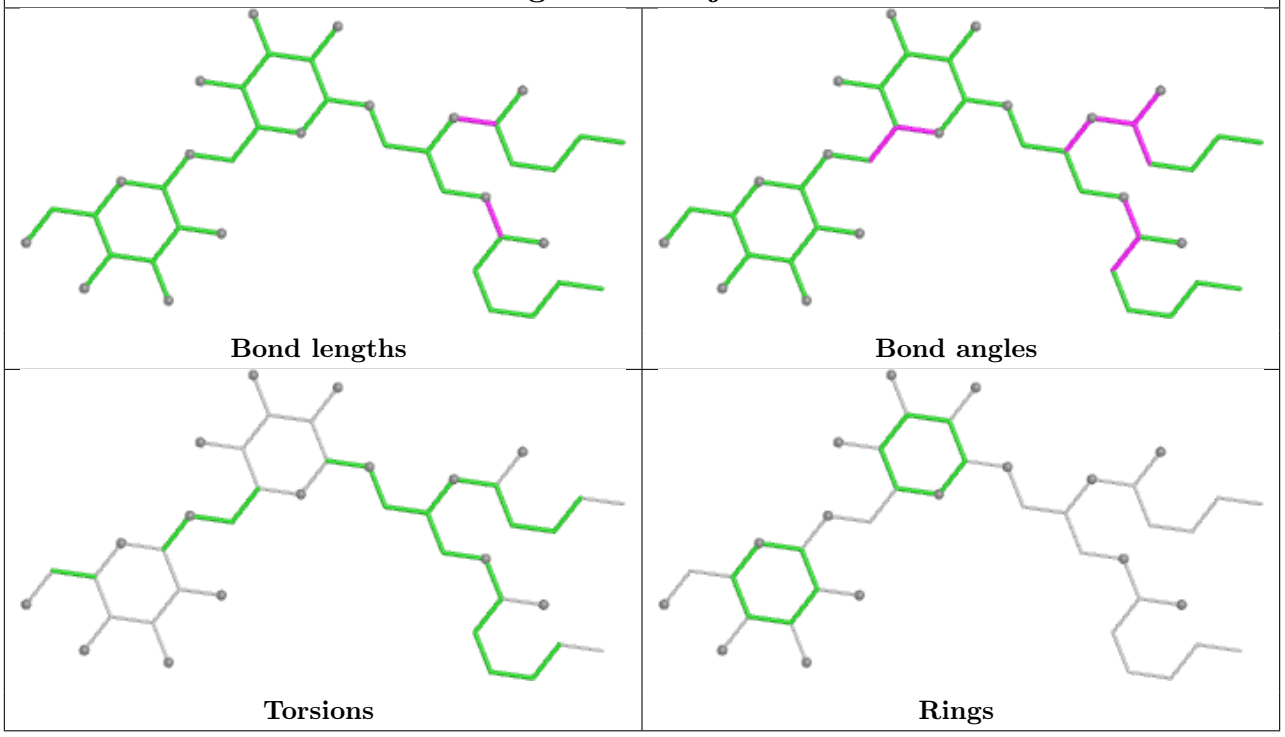
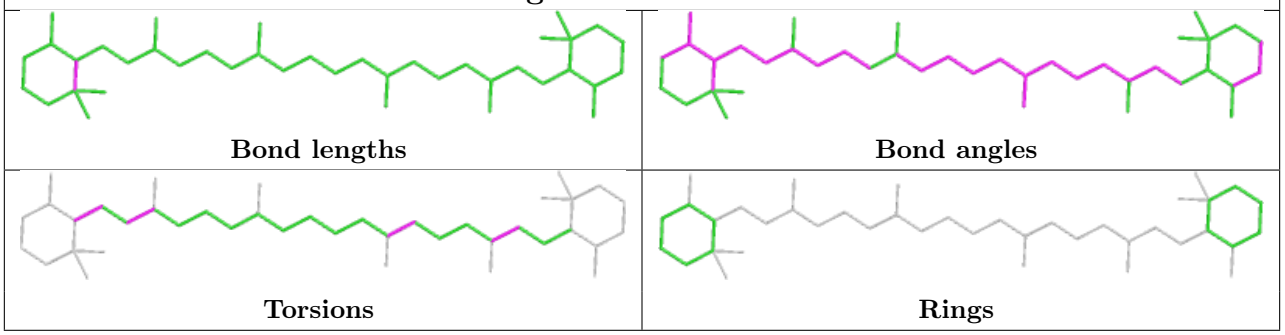


Rings

Ligand DGD j 105



Ligand BCR b 728



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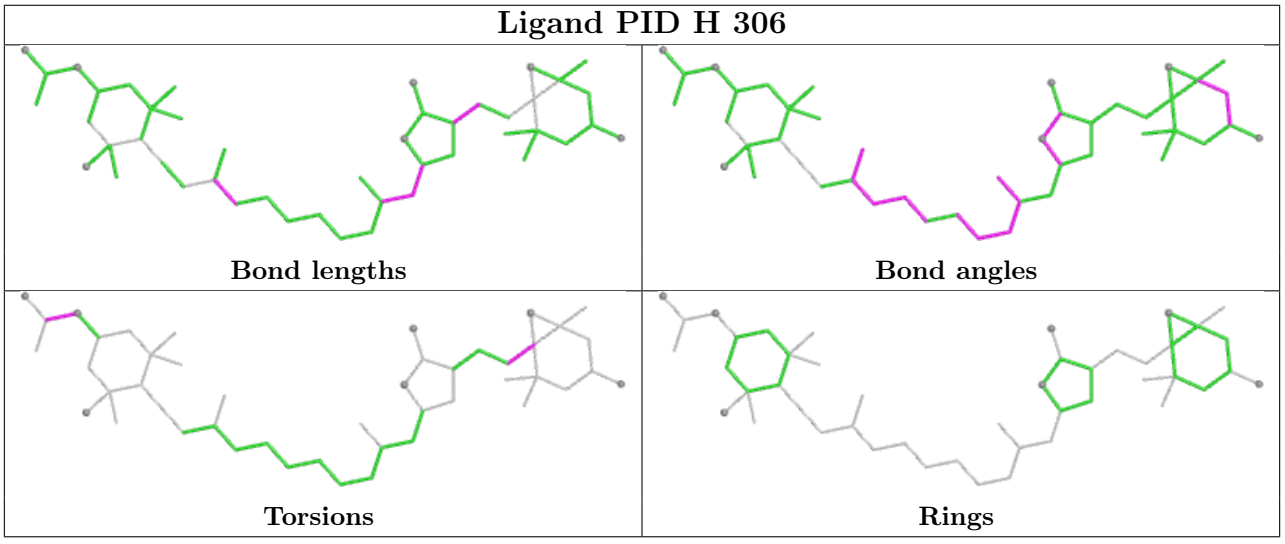

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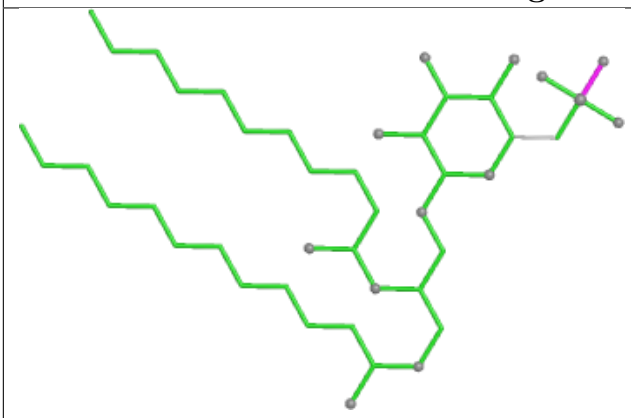

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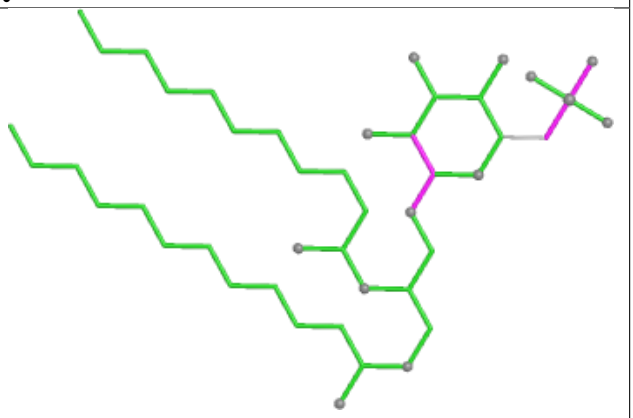
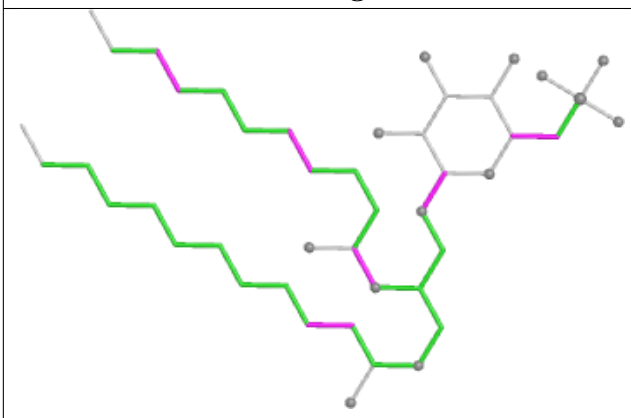


Bond angles



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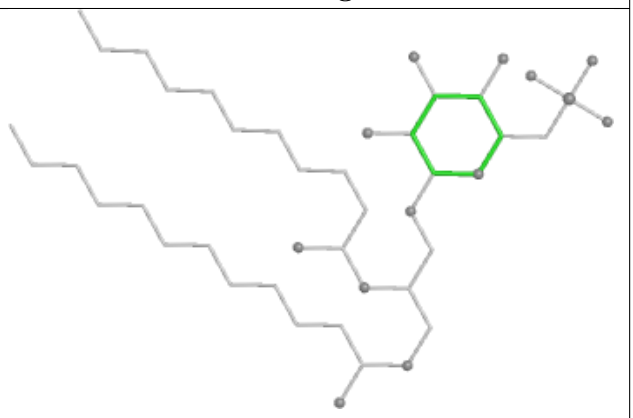
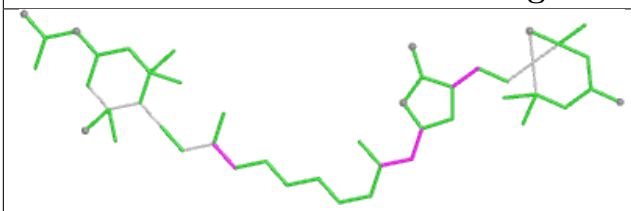


Rings

Ligand PID G 303



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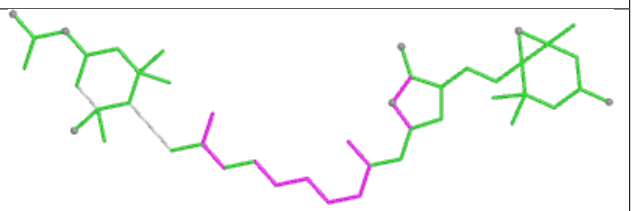
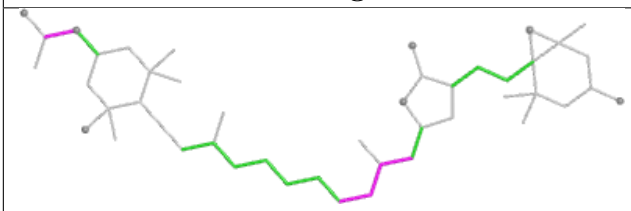


Bond angles



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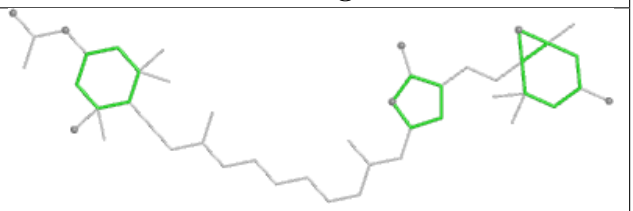
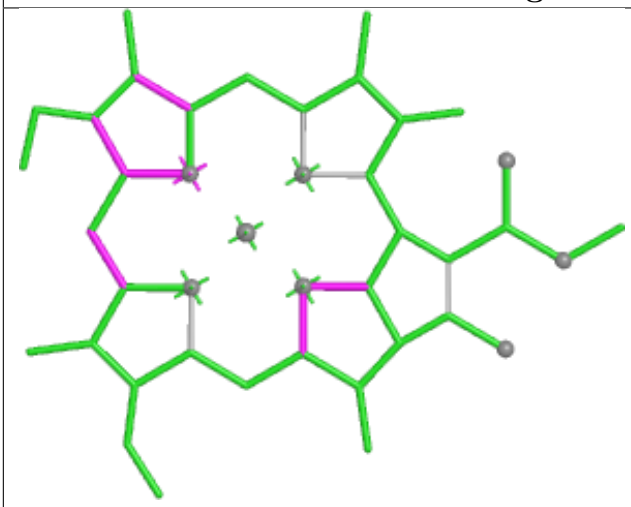


Rings

Ligand CLA F 315



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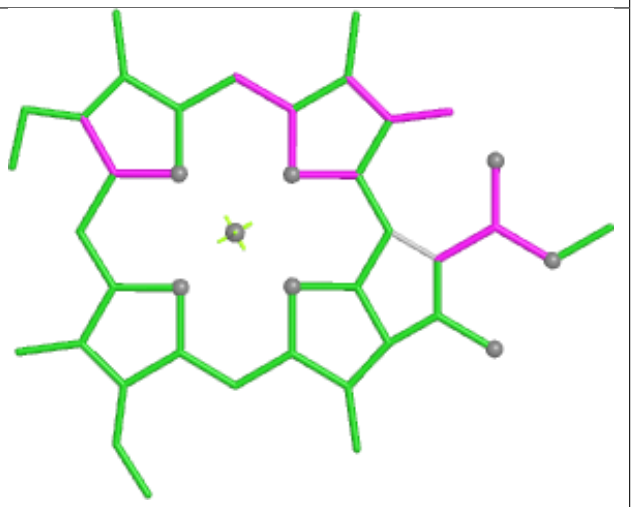

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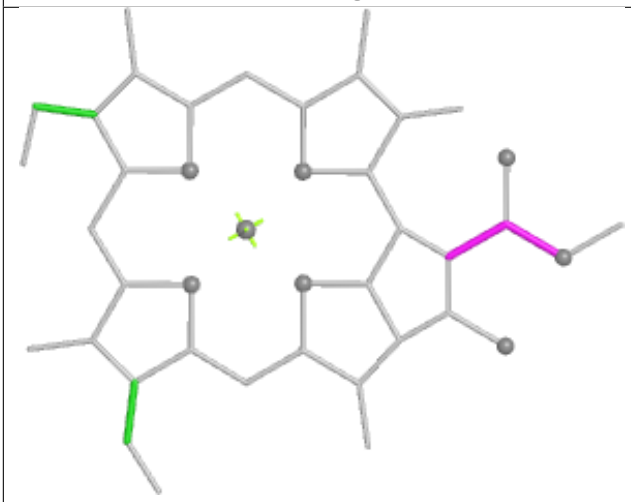

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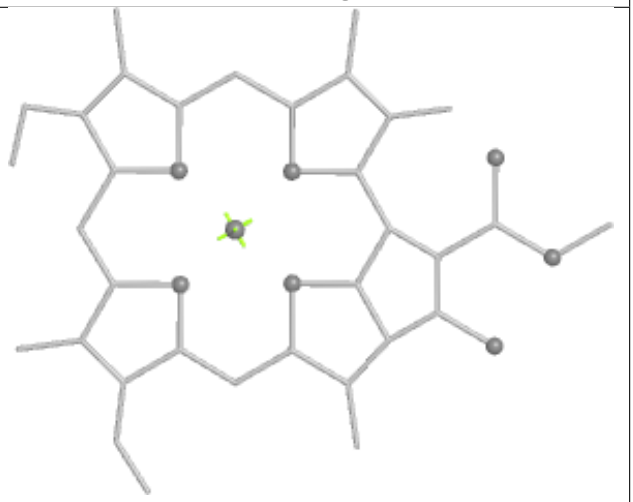
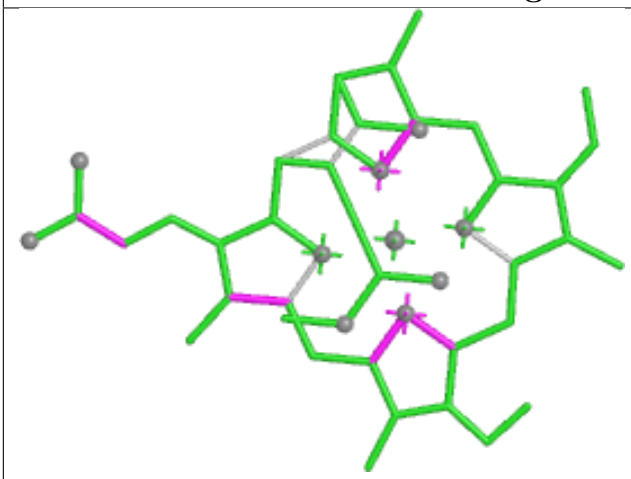


Rings

Ligand KC1 G 315



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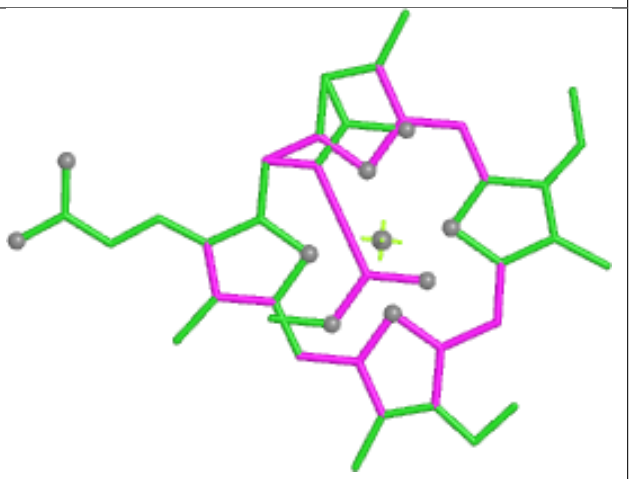
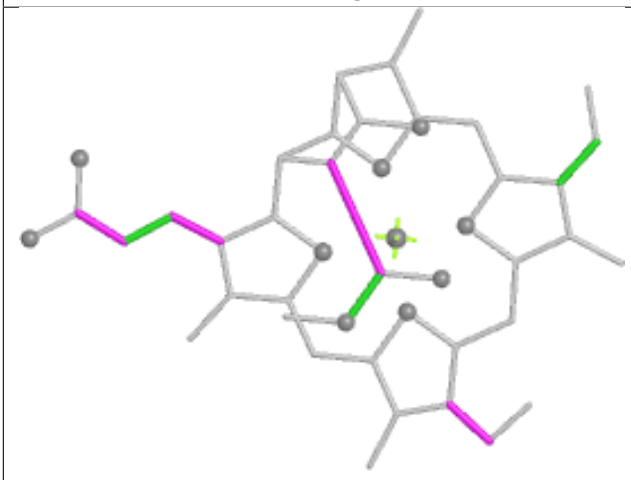


Bond angles



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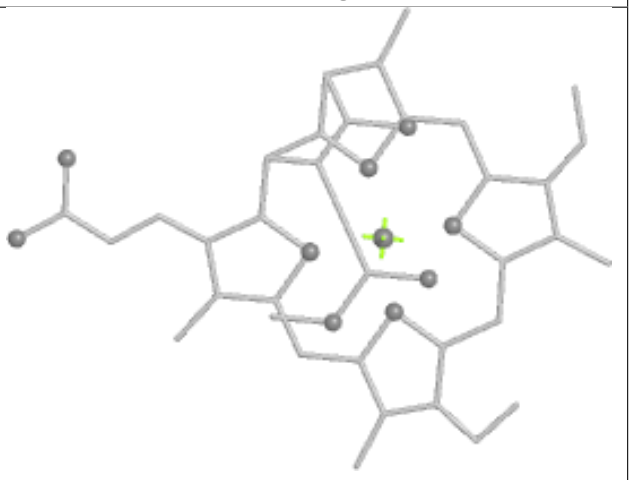
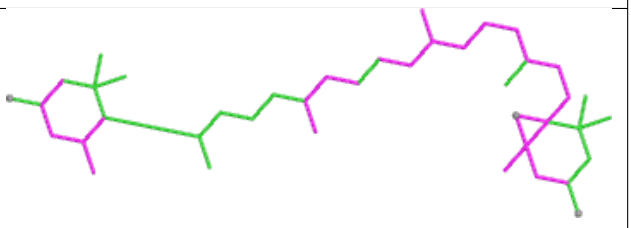


Rings

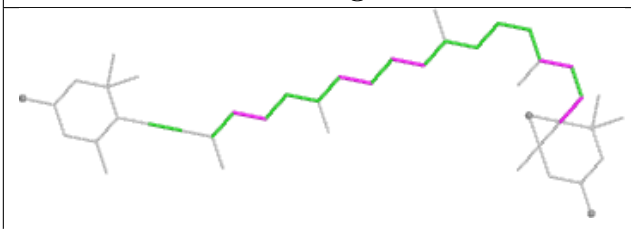
Ligand DD6 D 304



Bond lengths



Bond angles



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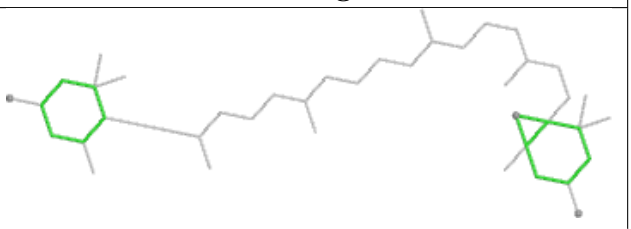
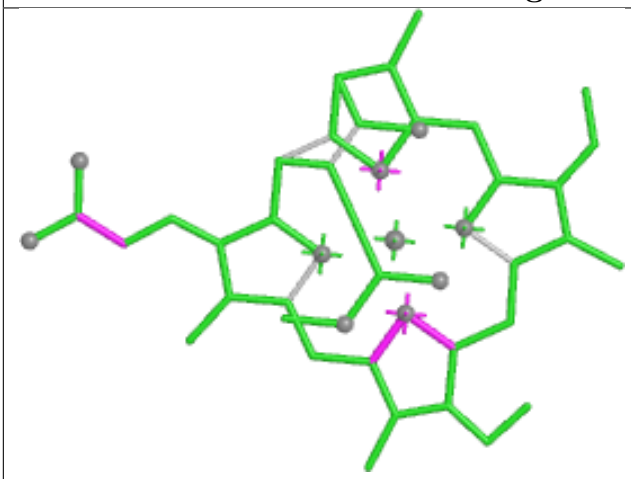


Rings

Ligand KC1 O 315



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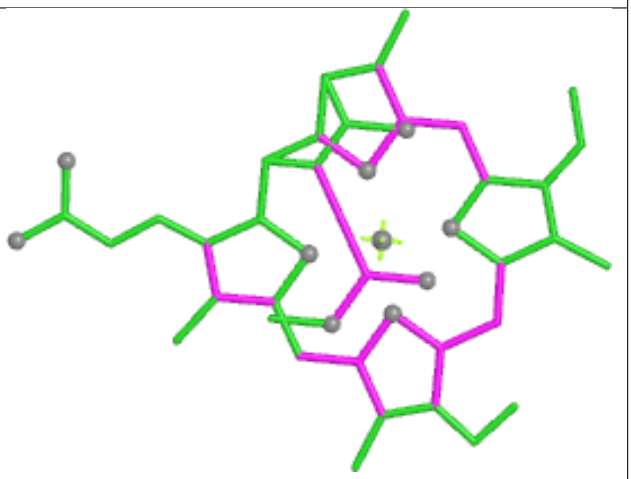
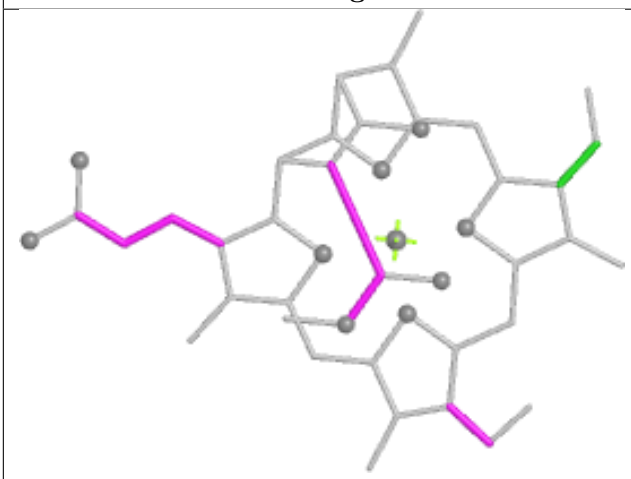


Bond angles



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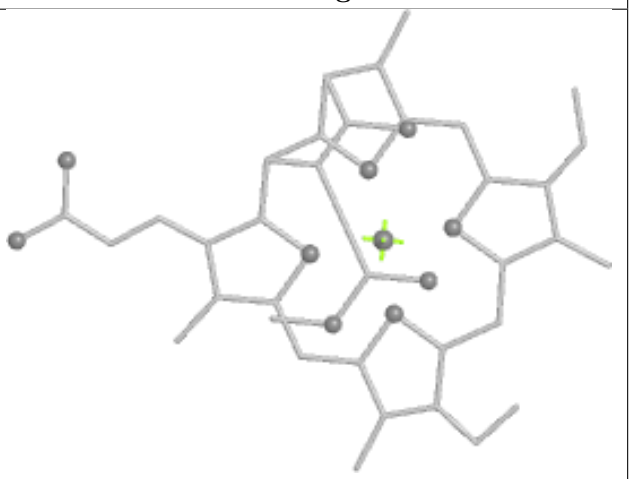
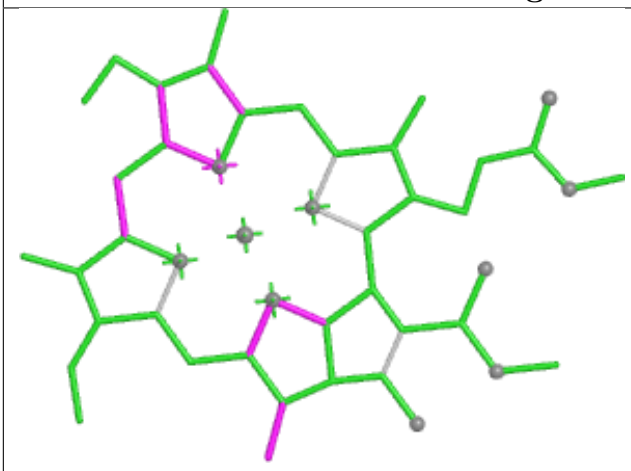


Rings

Ligand CLA F 307



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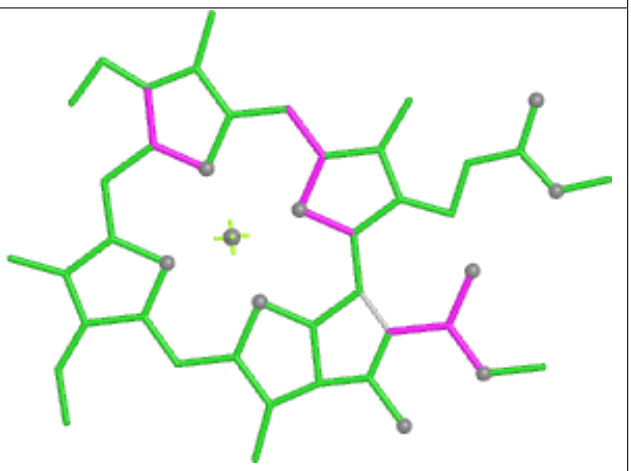
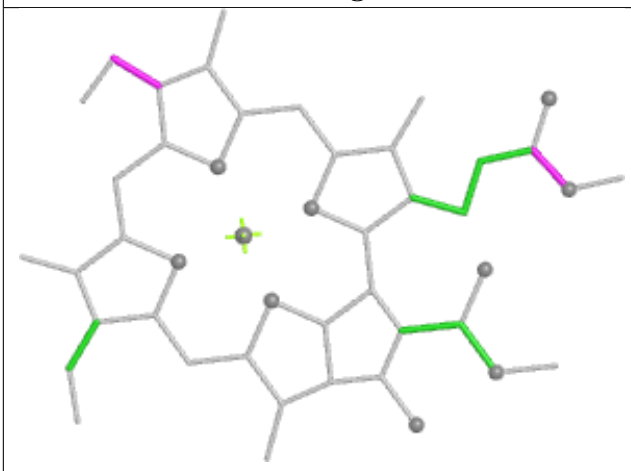


Bond angles



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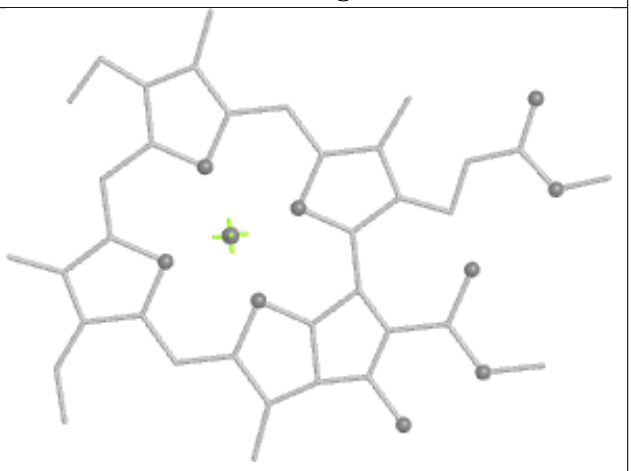
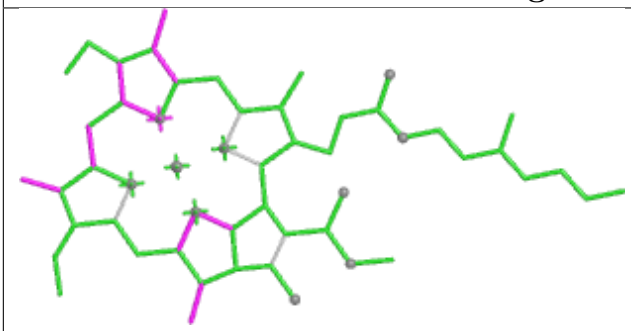


Rings

Ligand CLA J 311



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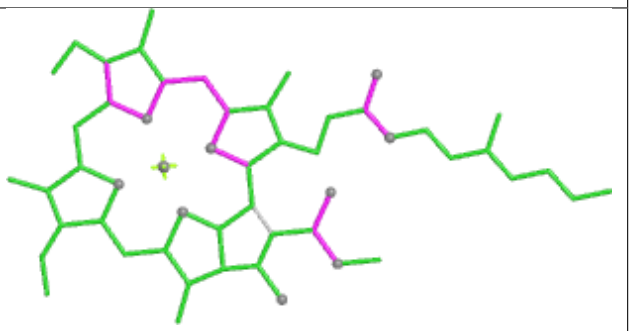
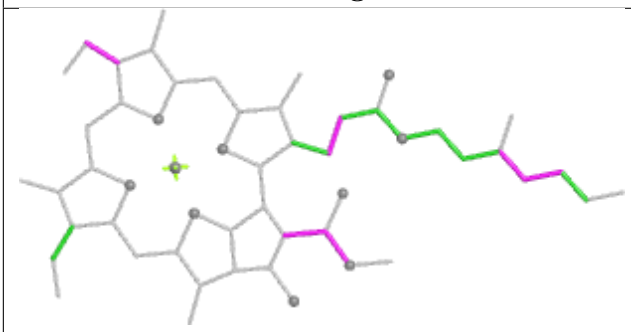


Bond angles



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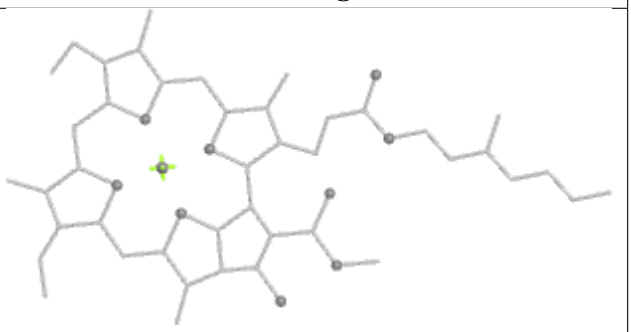
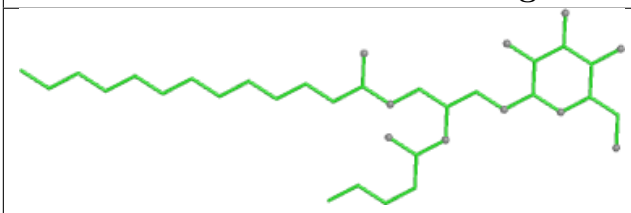
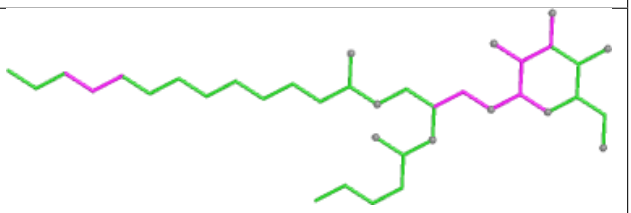


Rings

Ligand LMG A 219



Bond lengths



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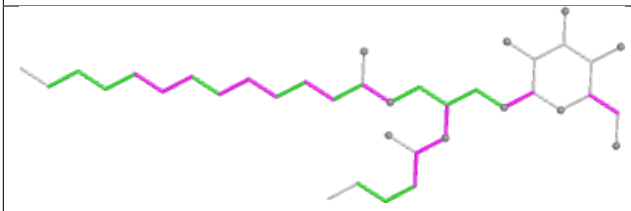
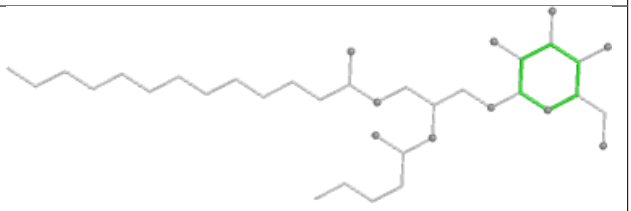


Torsions

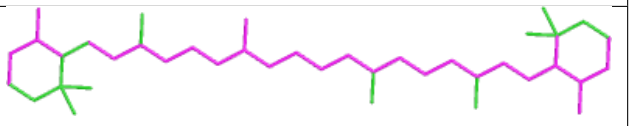


Rings

Ligand BCR m 103



Bond lengths



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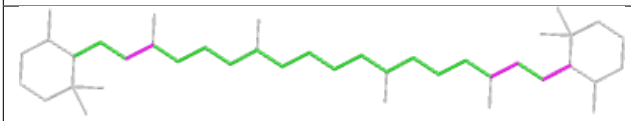

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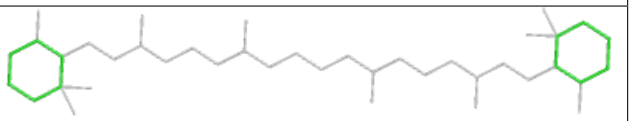
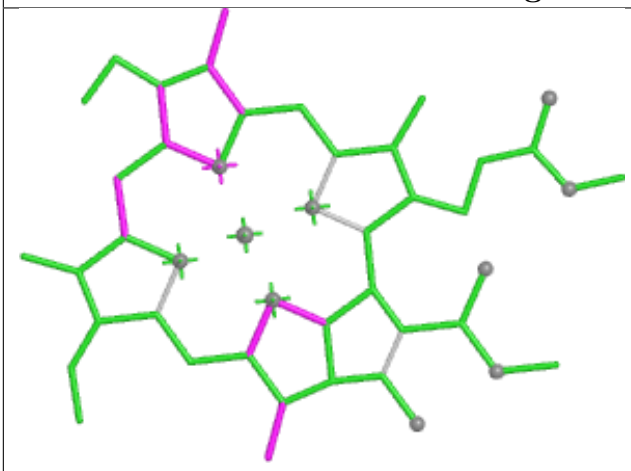


Rings

Ligand CLA B 315



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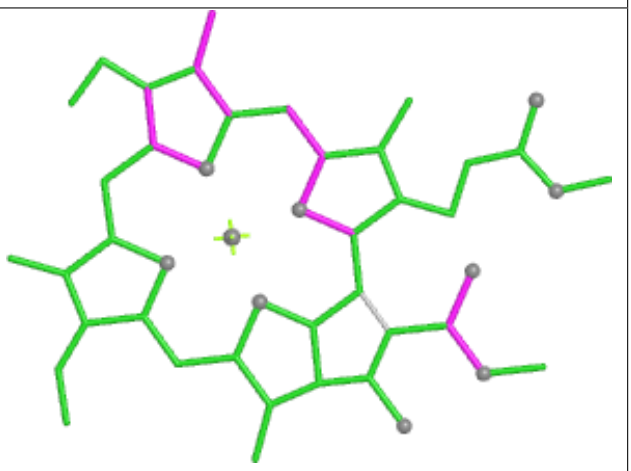

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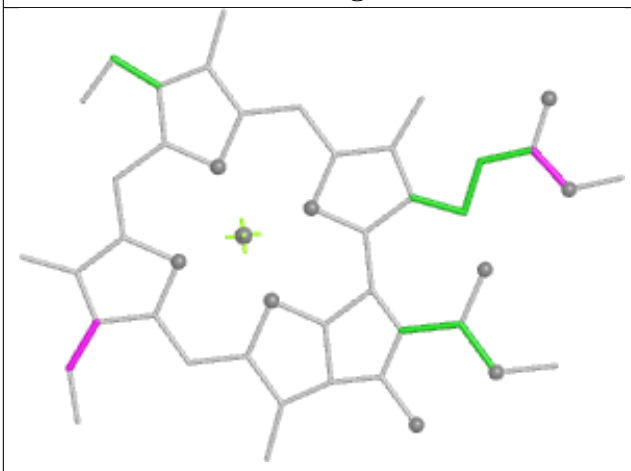

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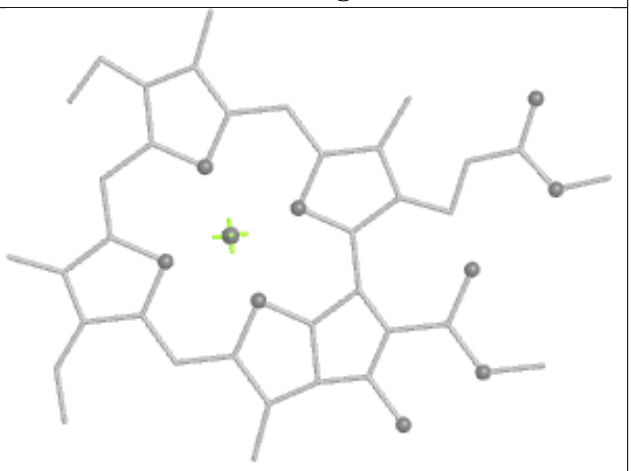
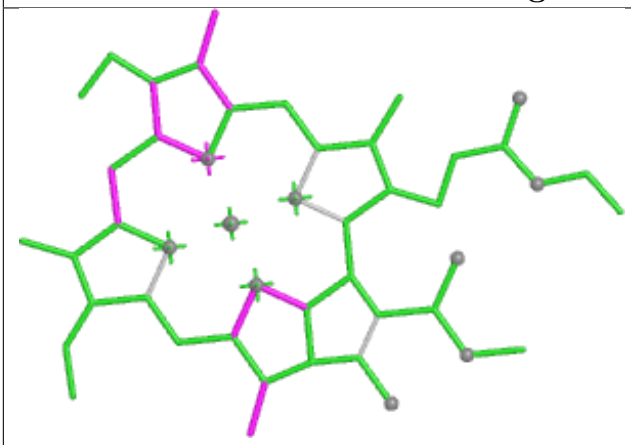


Rings

Ligand CLA a 818



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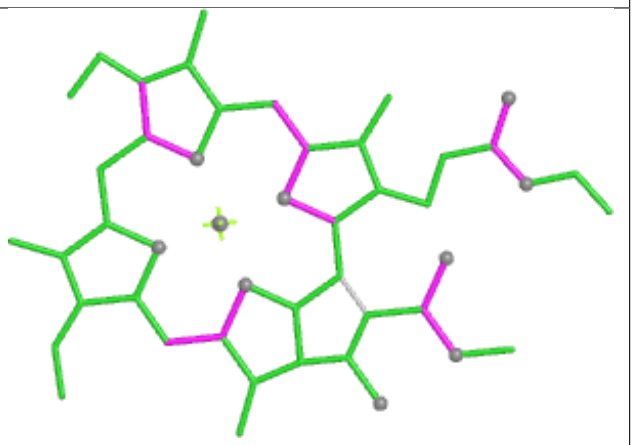

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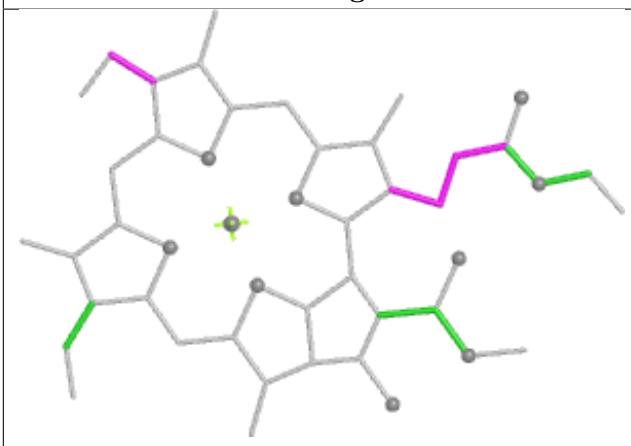

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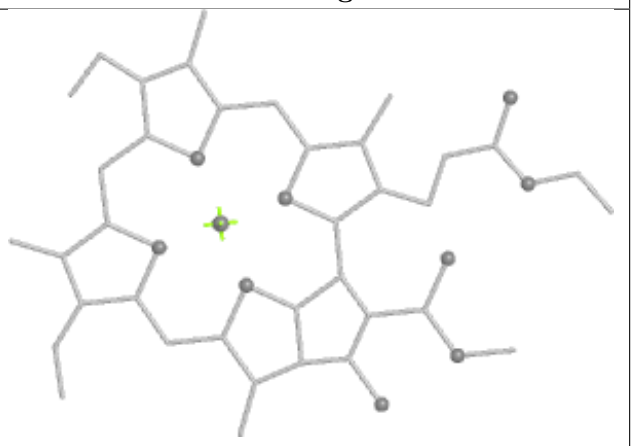
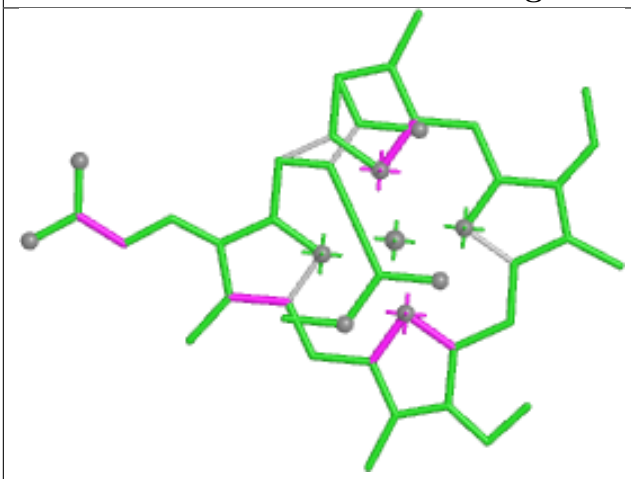


Rings

Ligand KC1 H 314



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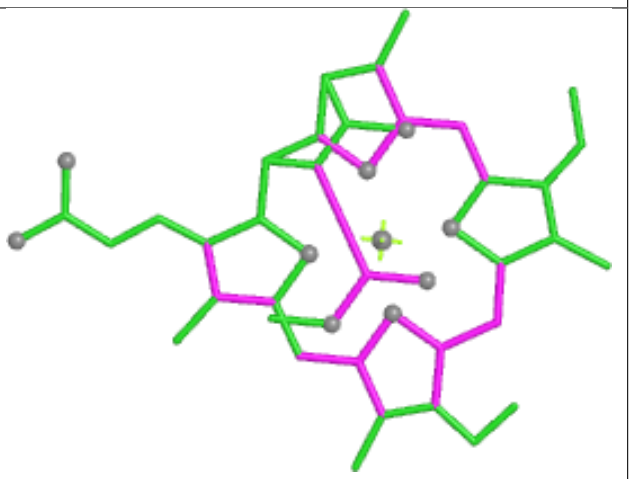

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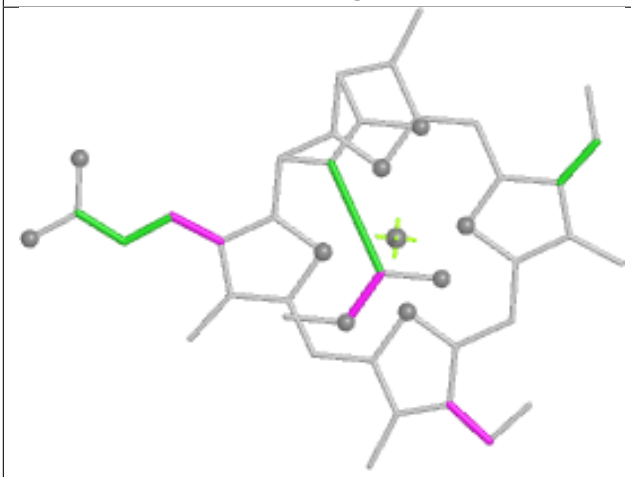

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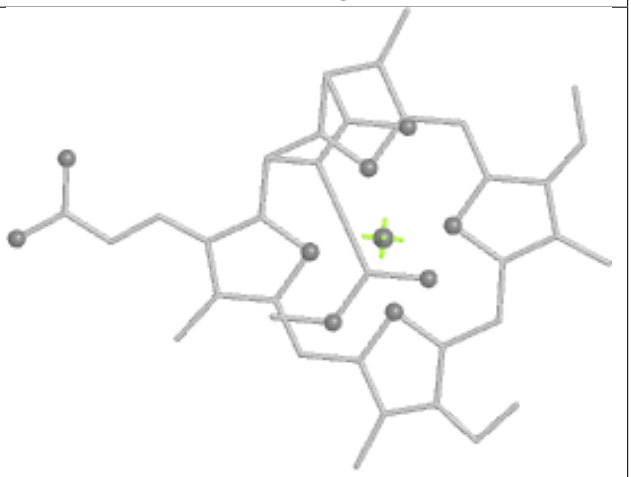
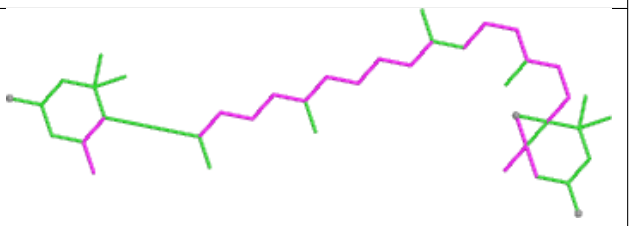


Rings

Ligand DD6 G 306



Bond lengths



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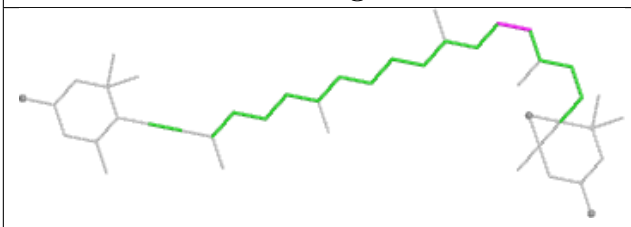

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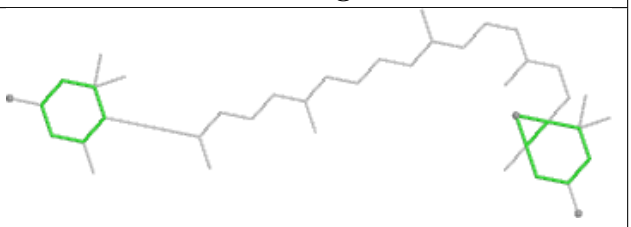
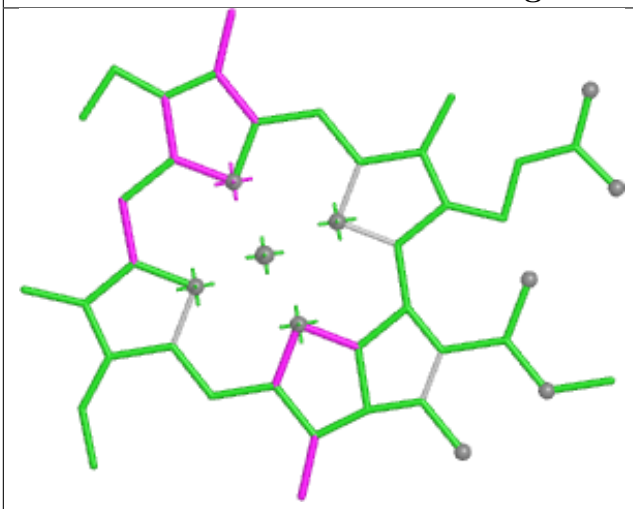


Rings

Ligand CLA B 307



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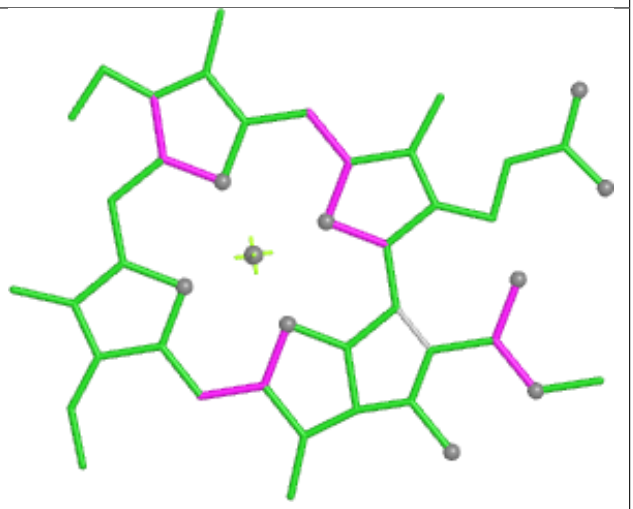

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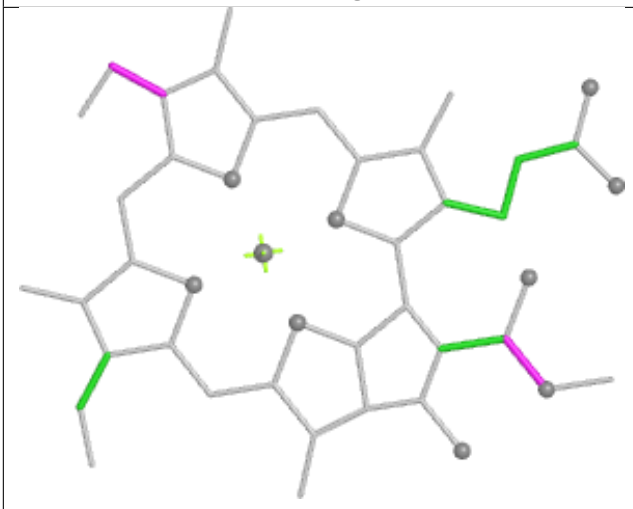
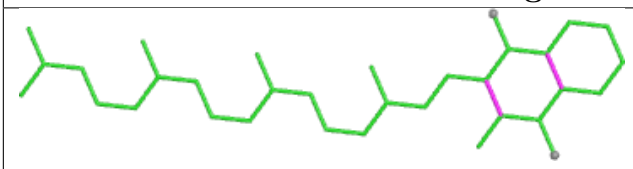


Torsions



Rings

Ligand PQN b 727



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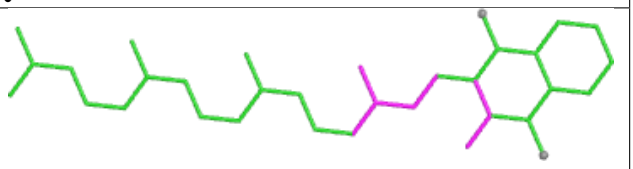

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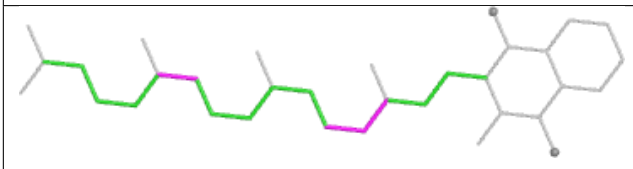

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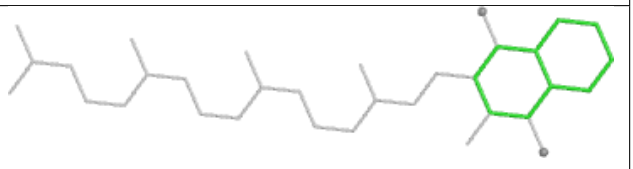
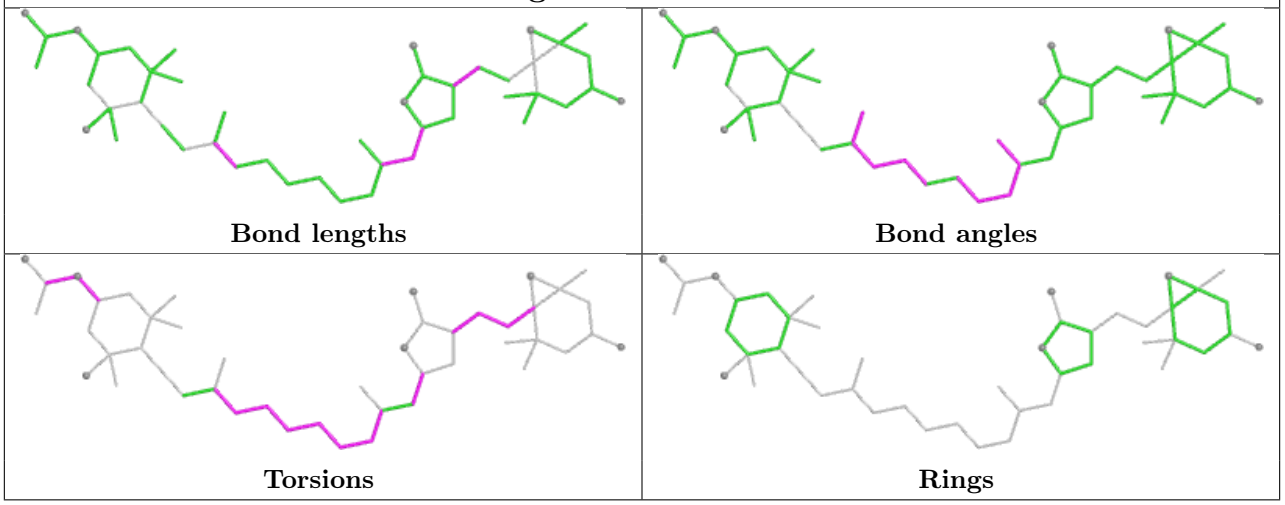
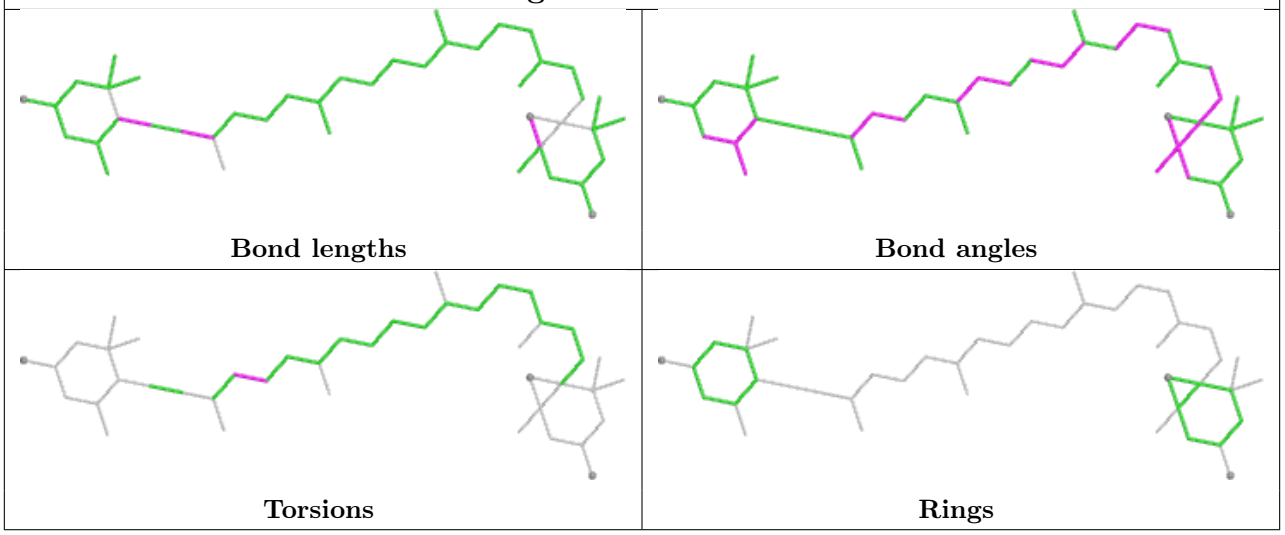


Rings

Ligand PID N 305



Ligand DD6 E 303



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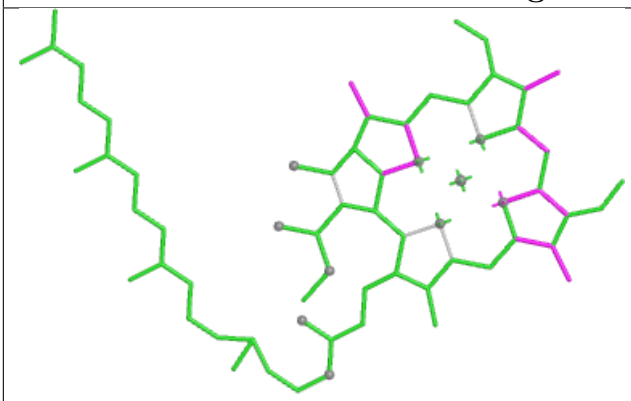

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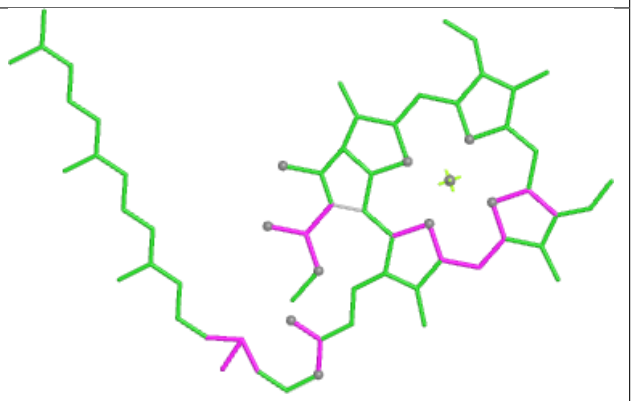
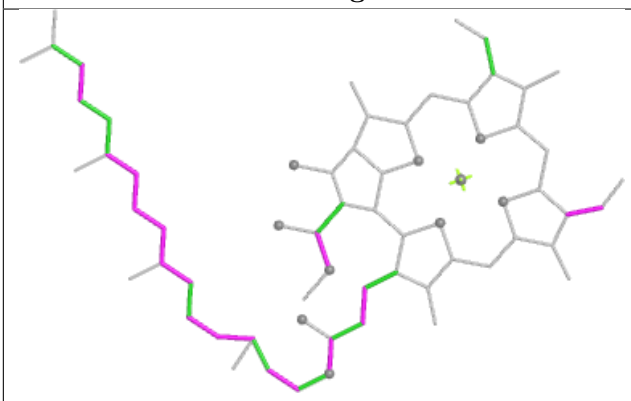


Bond angles



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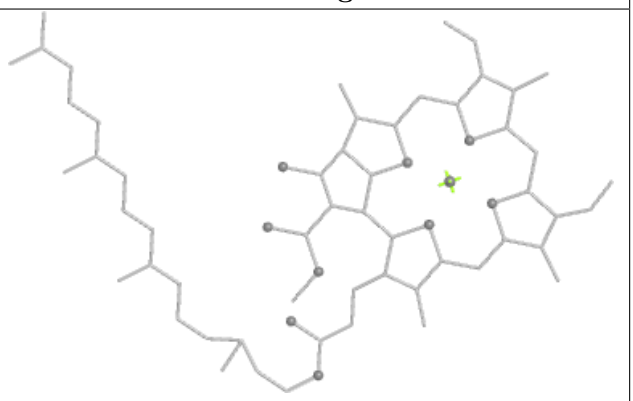
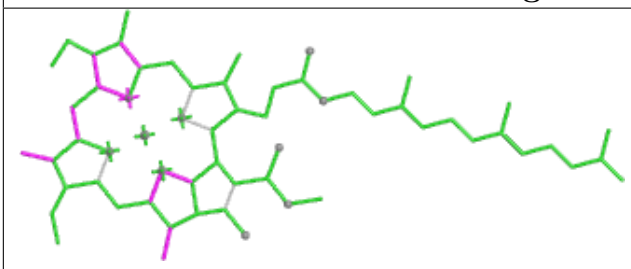


Rings

Ligand CLA G 314



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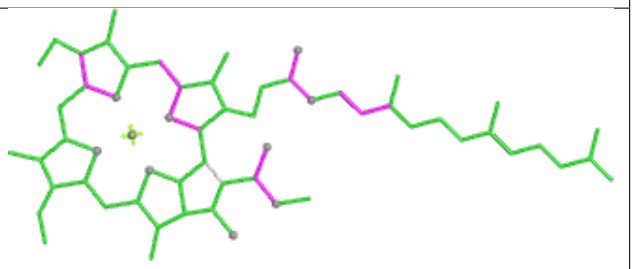
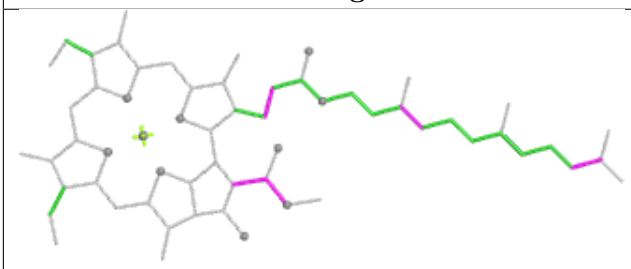


Bond angles



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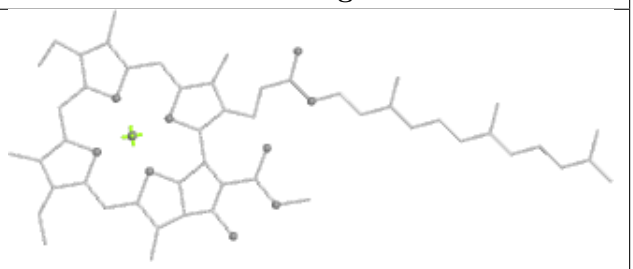
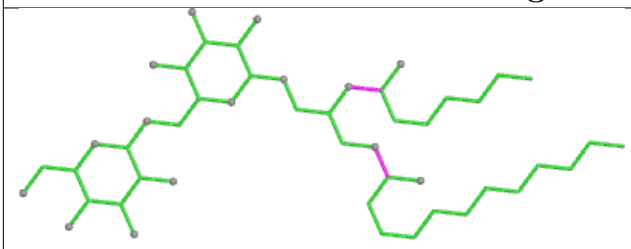


Rings

Ligand DGD j 106



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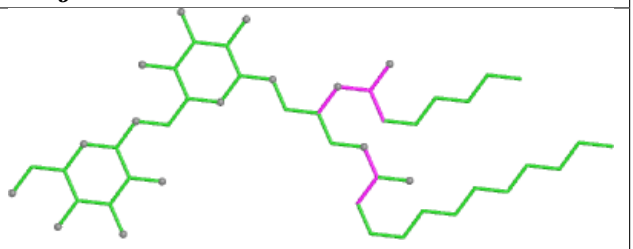

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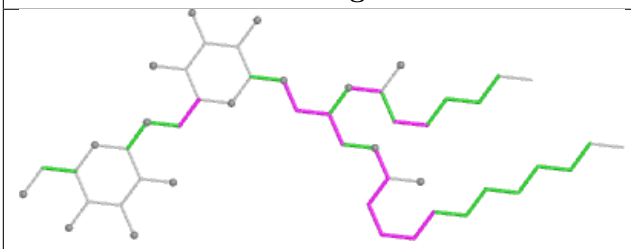

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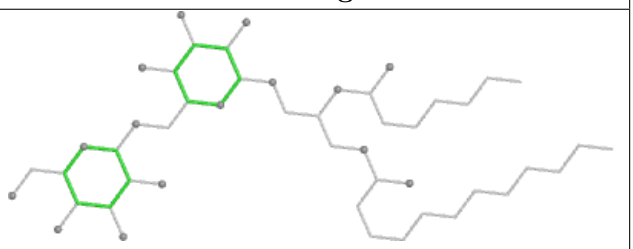
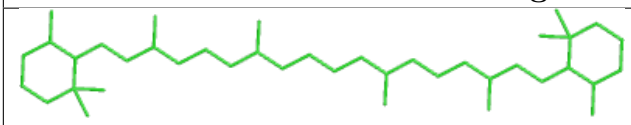


Rings

Ligand BCR f 804



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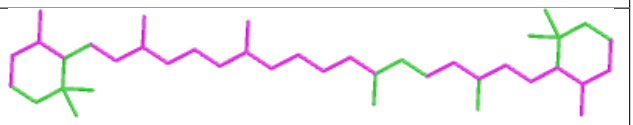
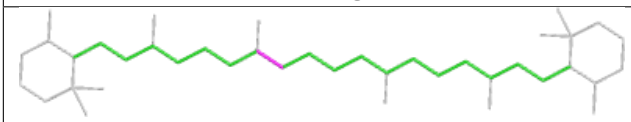


Bond angles



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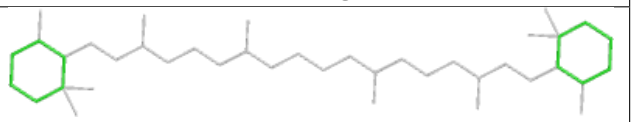
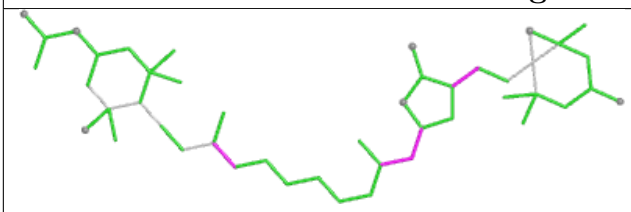


Rings

Ligand PID T 305



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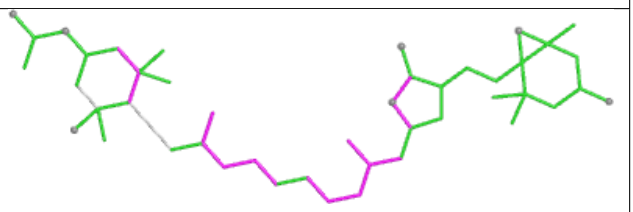
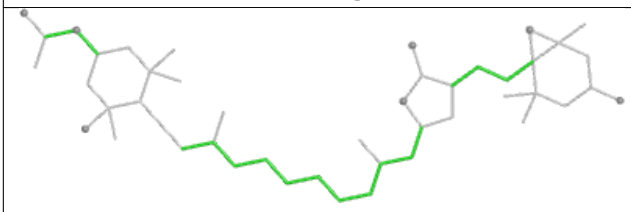


Bond angles



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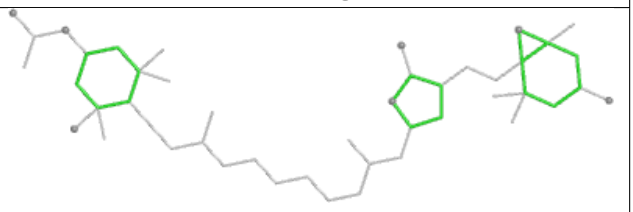
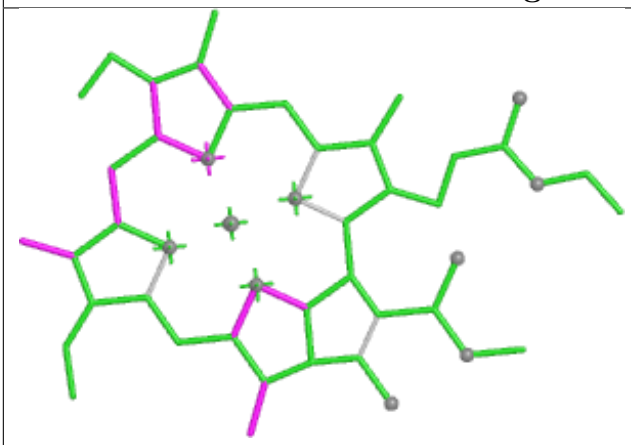


Rings

Ligand CLA O 314



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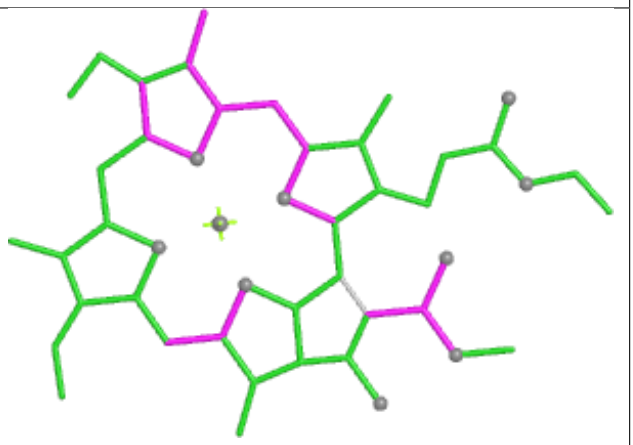
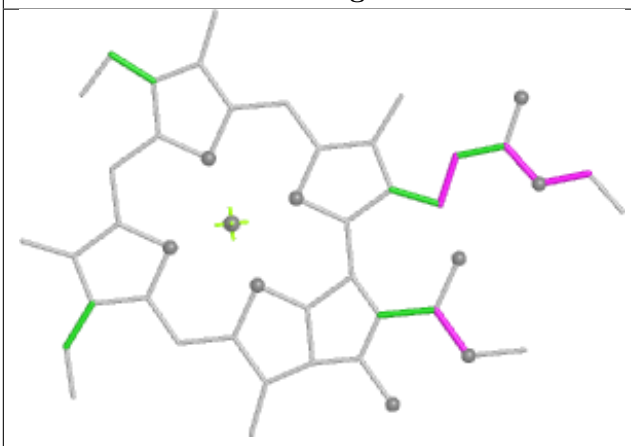


Bond angles



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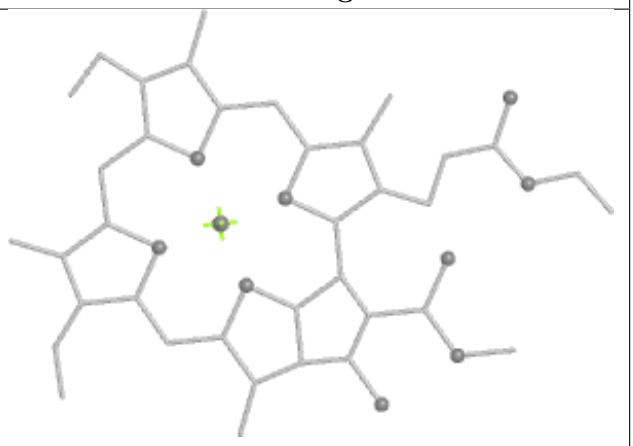
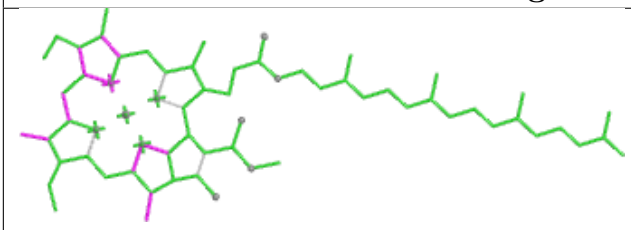


Rings

Ligand CLA J 306



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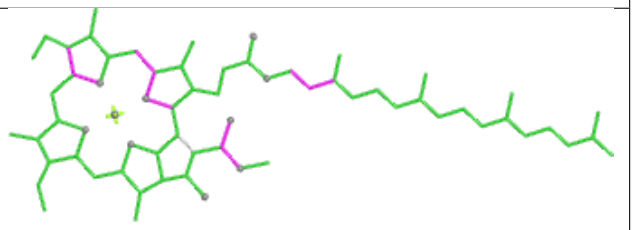
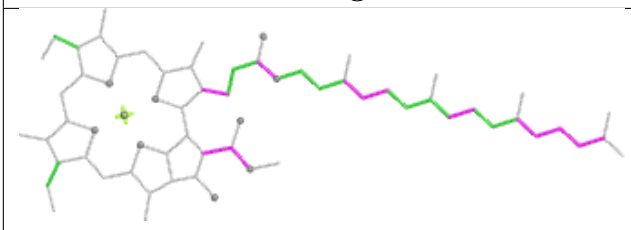


Bond angles



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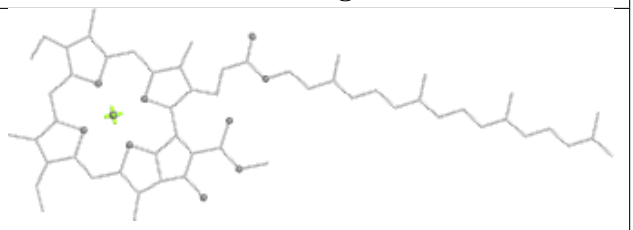
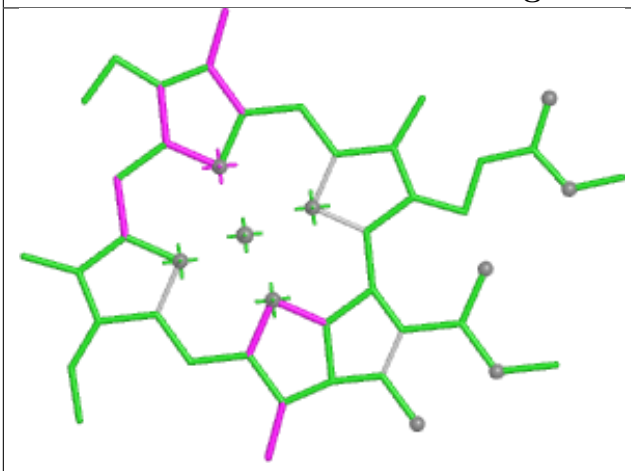
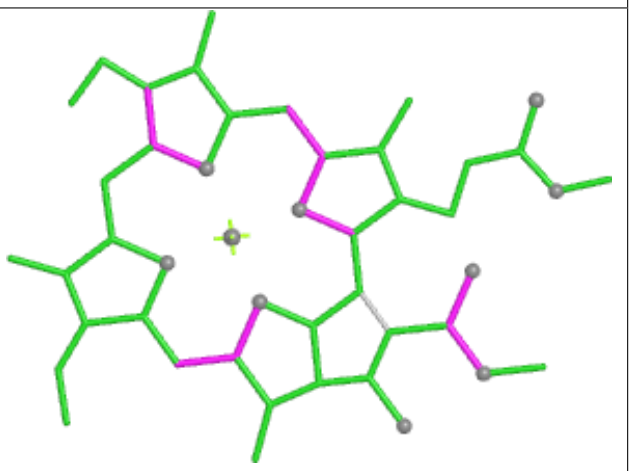


Rings

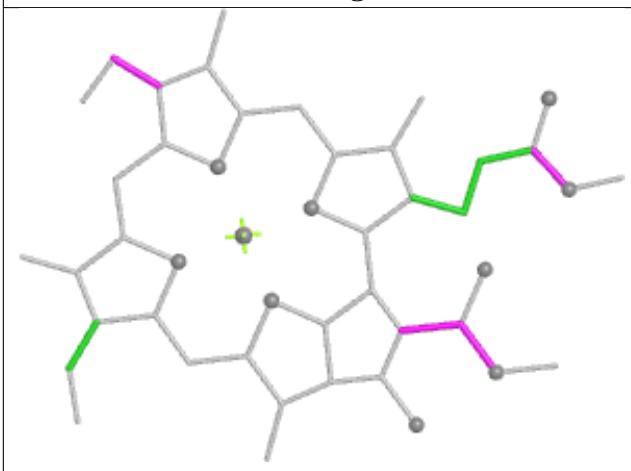
Ligand CLA A 210



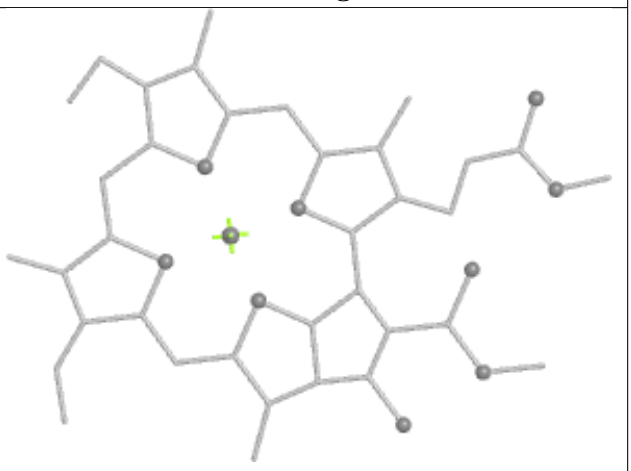
Bond lengths



Bond angles

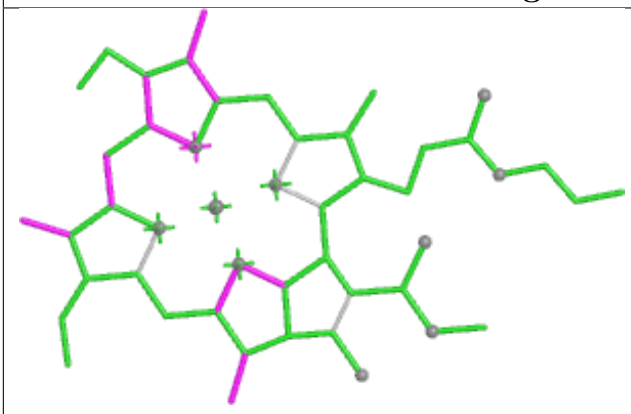


Torsions

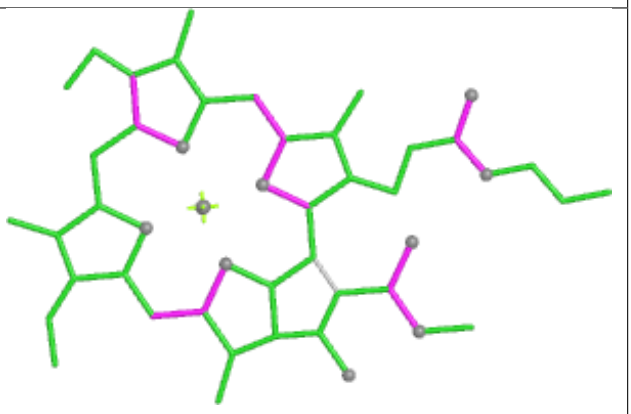


Rings

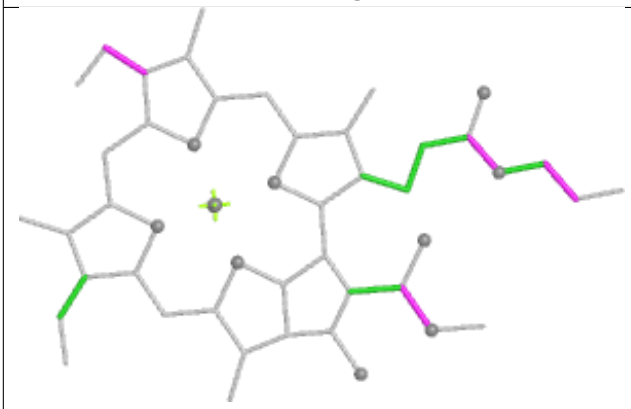
Ligand CLA K 213



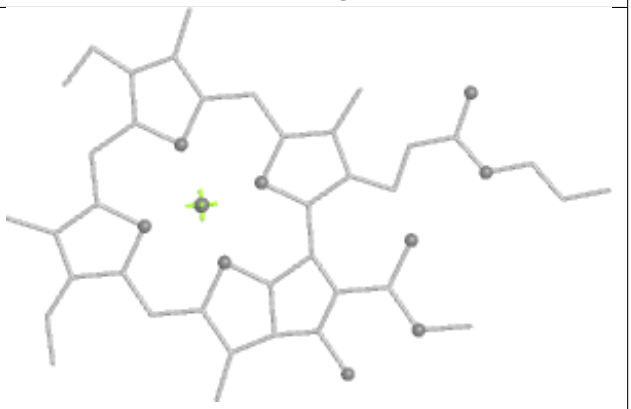
Bond lengths



Bond angles

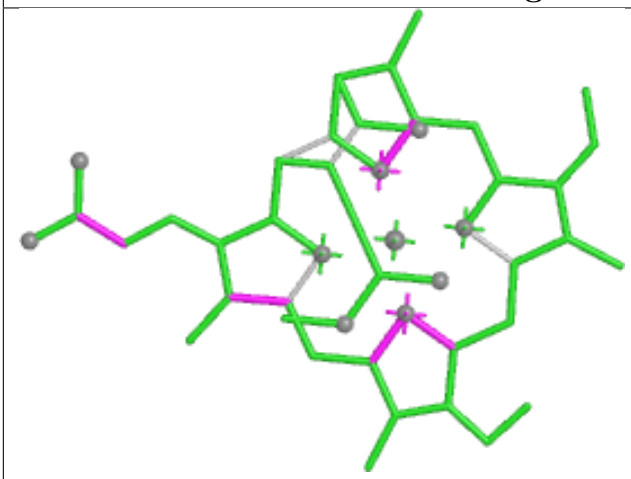


Torsions

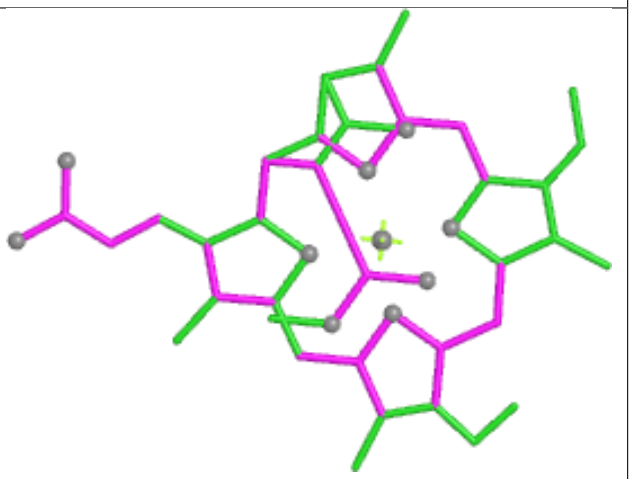


Rings

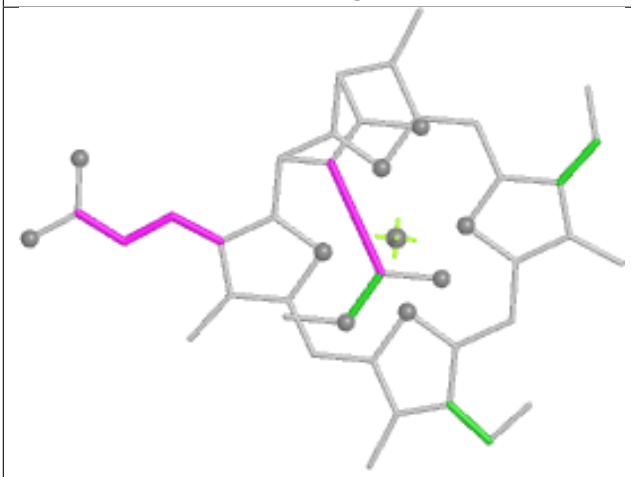
Ligand KC1 K 215



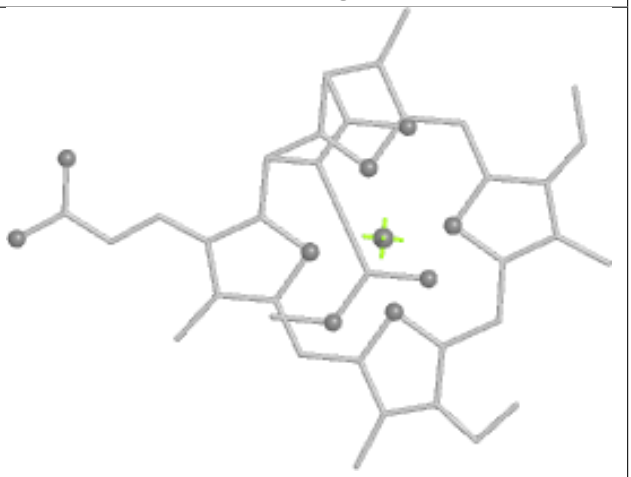
Bond lengths



Bond angles

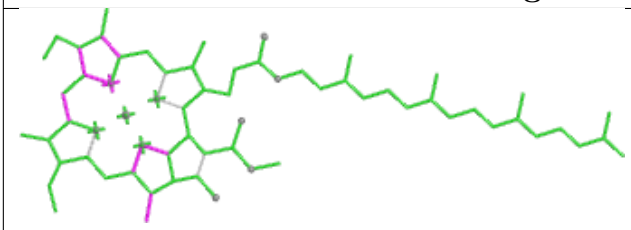


Torsions

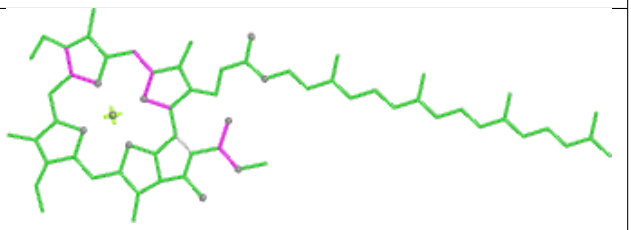


Rings

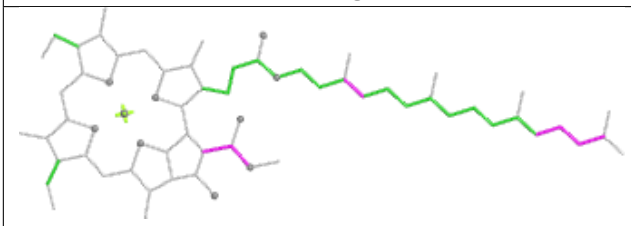
Ligand CLA O 309



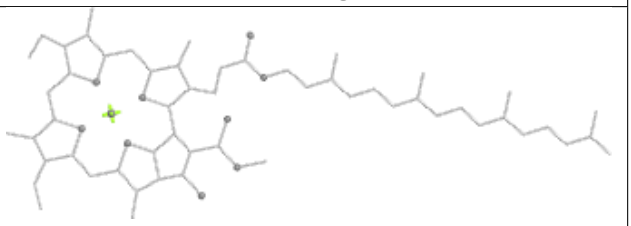
Bond lengths



Bond angles

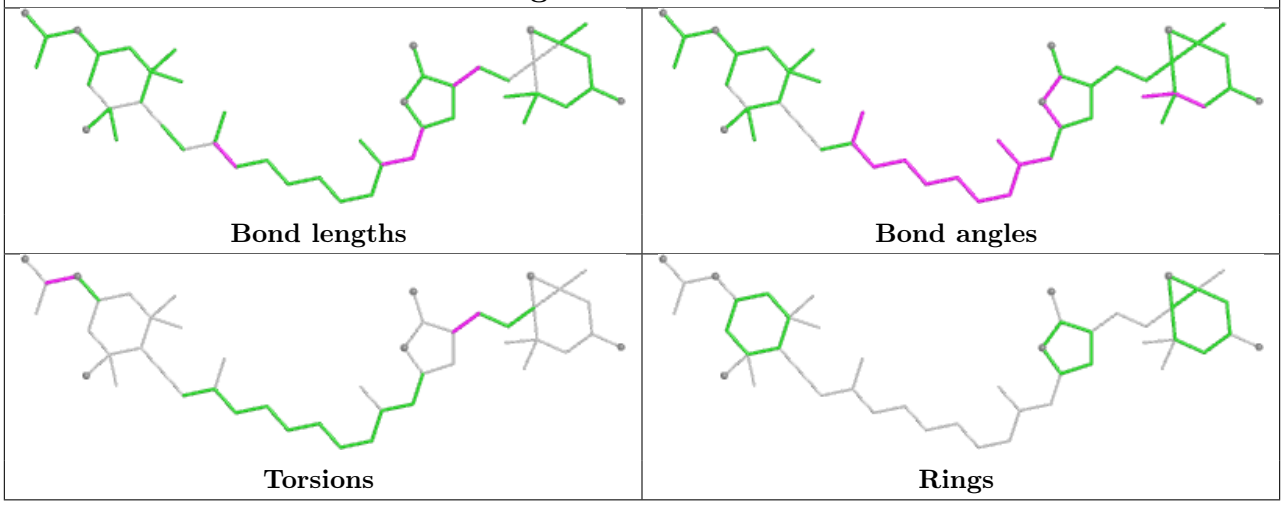


Torsions

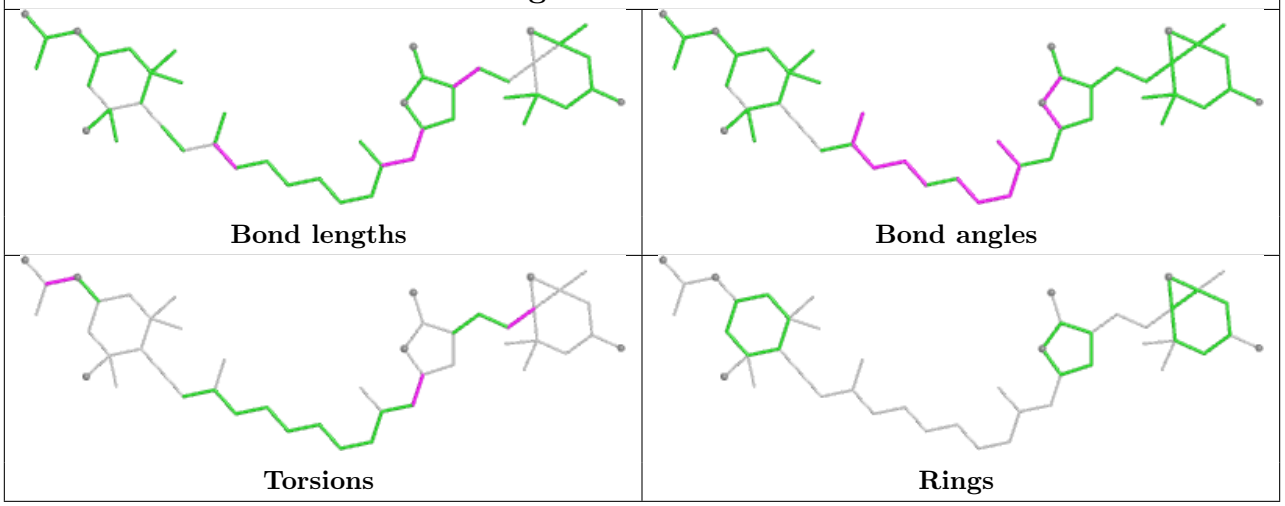


Rings

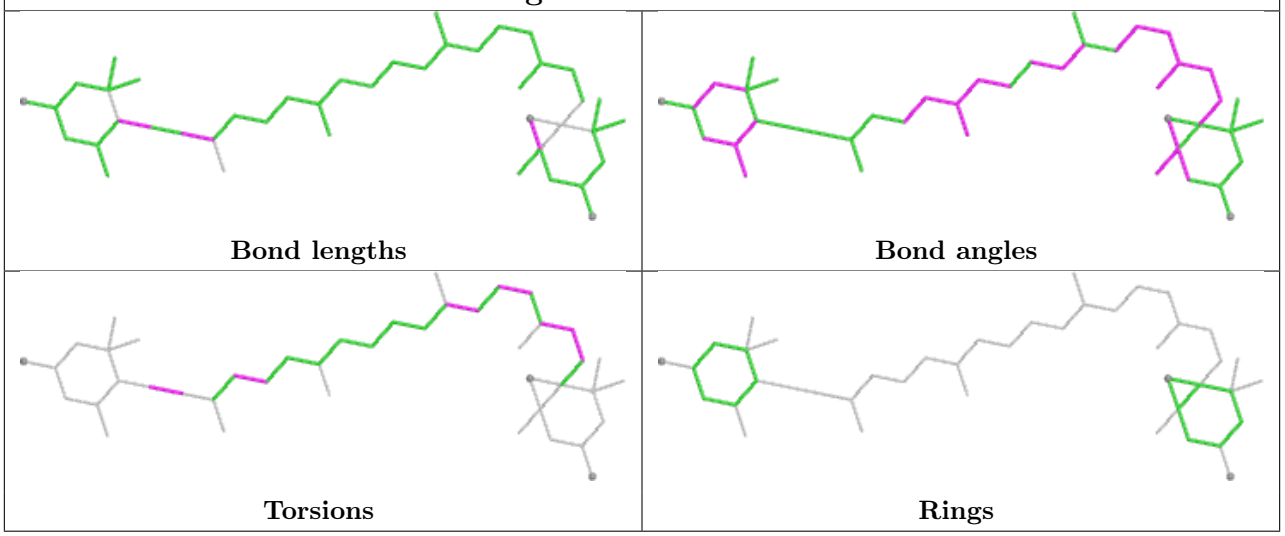
Ligand PID T 307



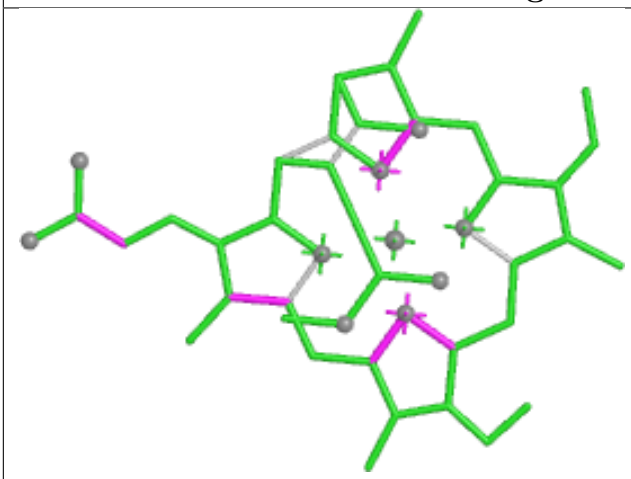
Ligand PID N 301



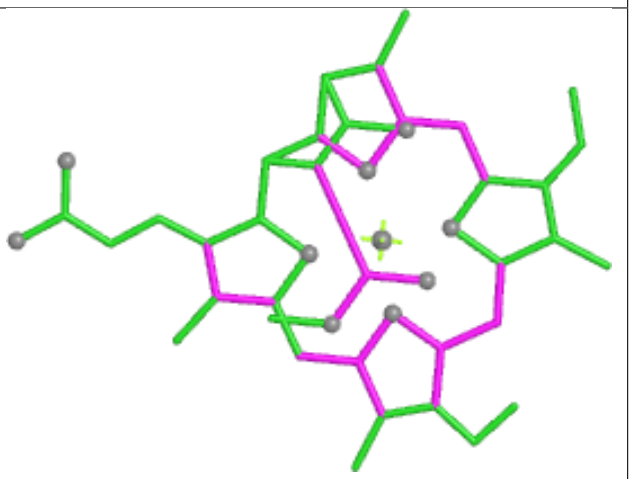
Ligand DD6 D 301



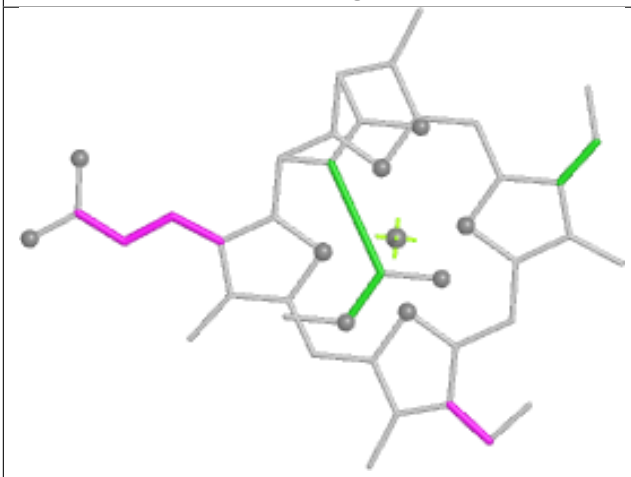
Ligand KC1 P 216



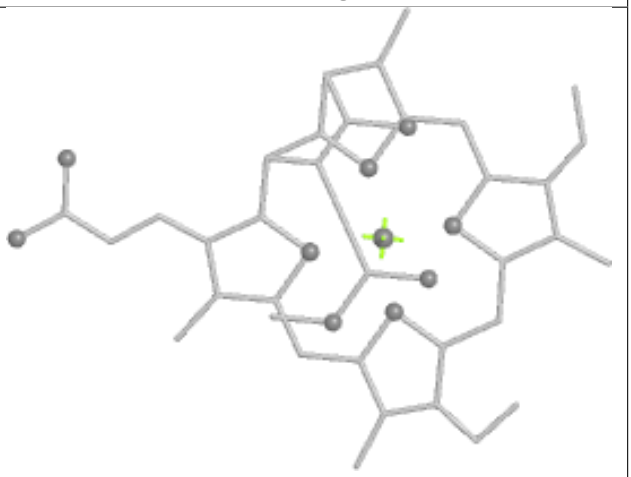
Bond lengths



Bond angles

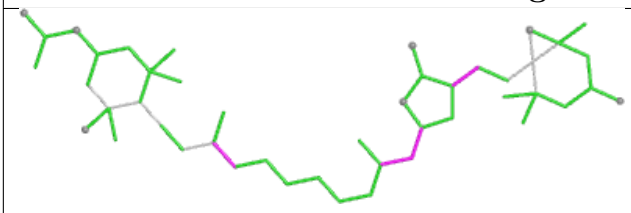


Torsions

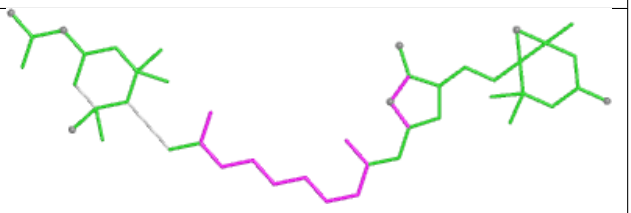


Rings

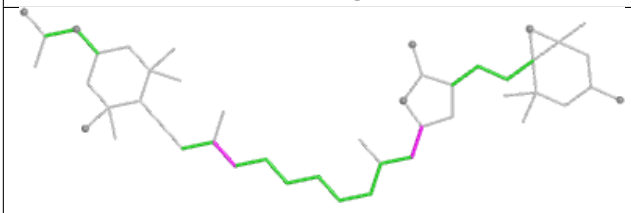
Ligand PID C 304



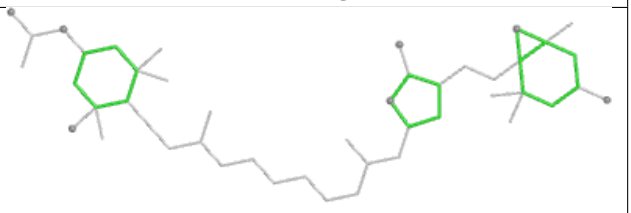
Bond lengths



Bond angles

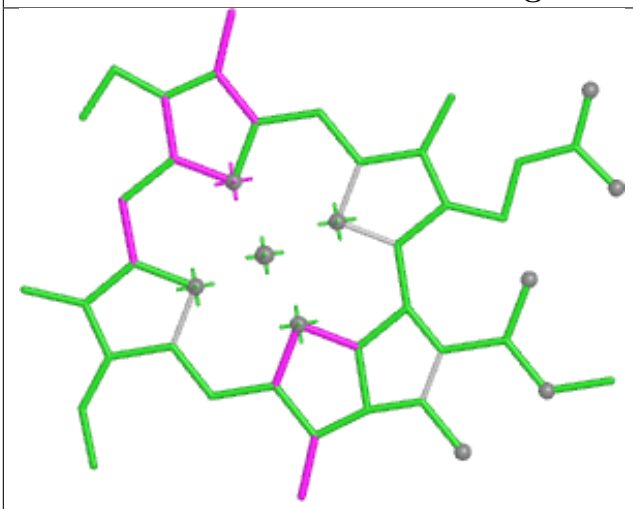


Torsions

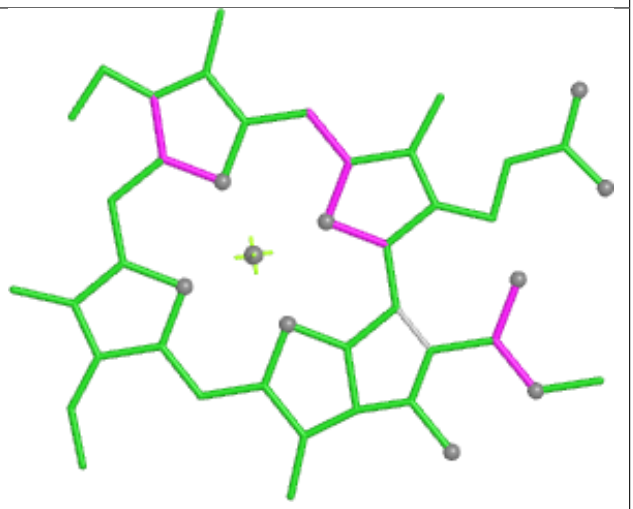


Rings

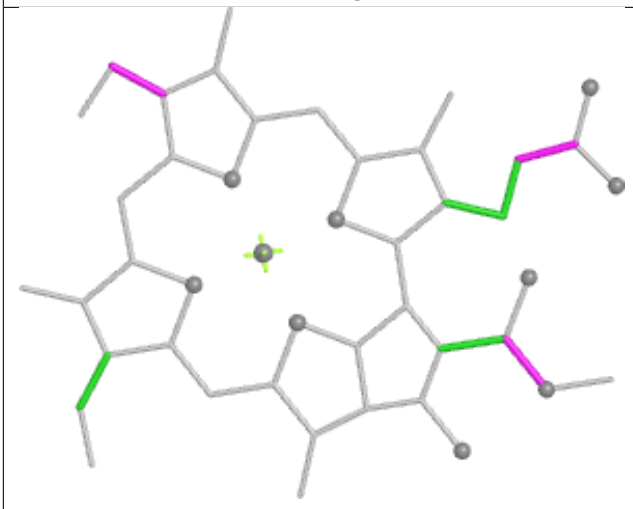
Ligand CLA B 316



Bond lengths



Bond angles

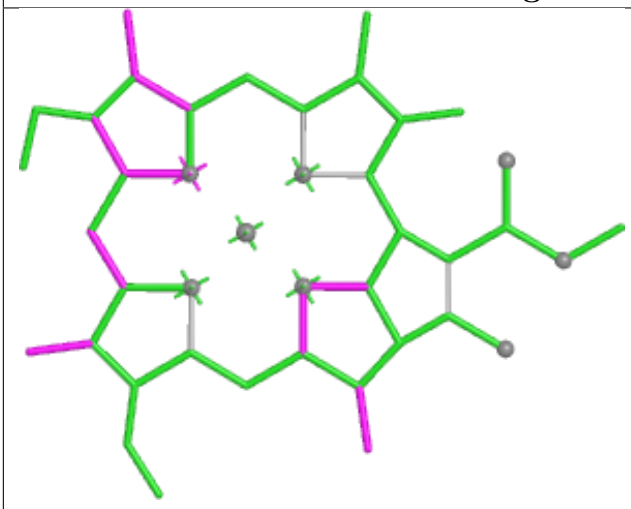


Torsions

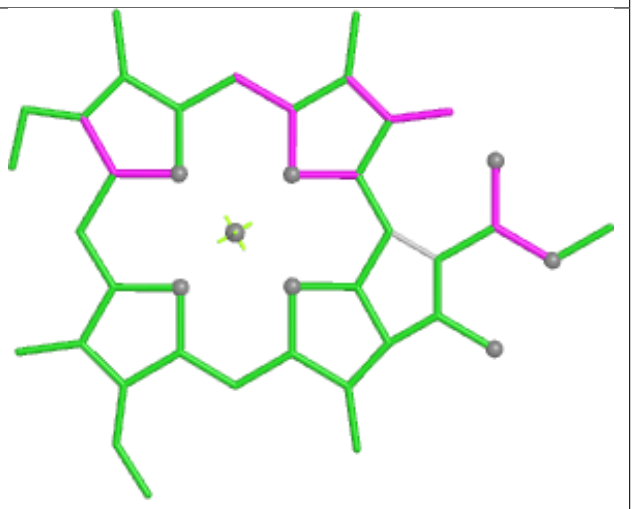


Rings

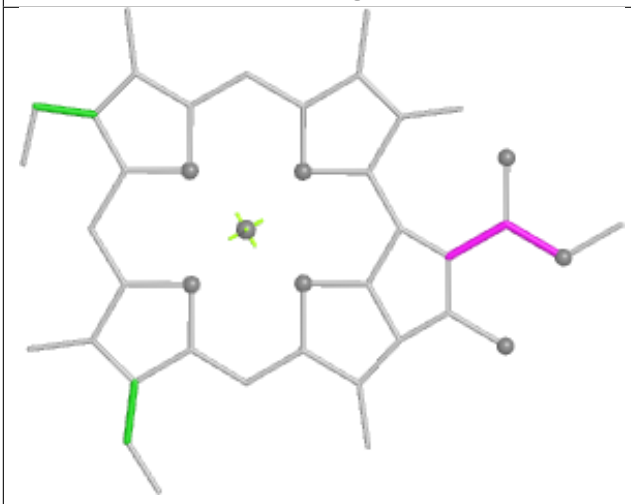
Ligand CLA K 216



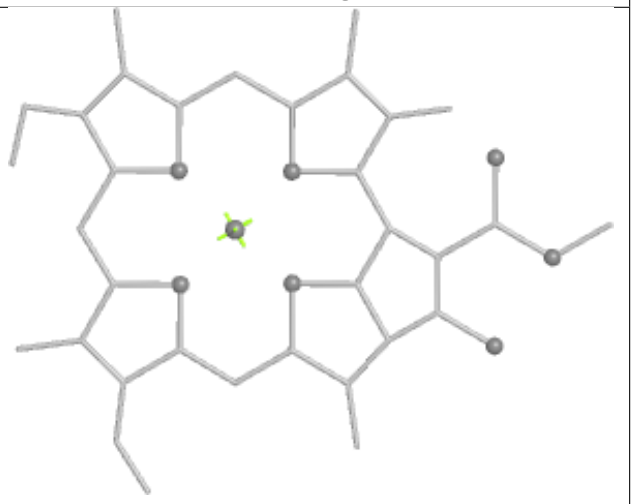
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

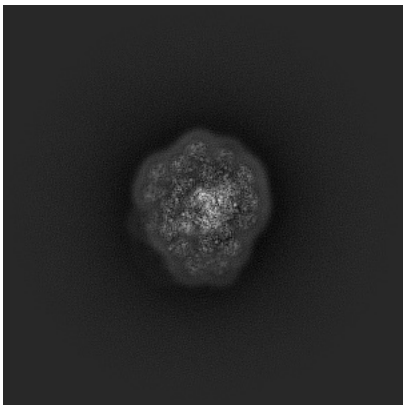
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-36678. These allow visual inspection of the internal detail of the map and identification of artifacts.

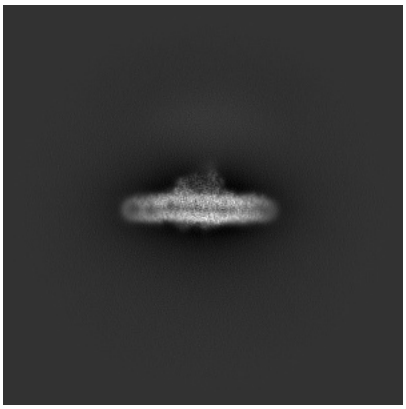
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

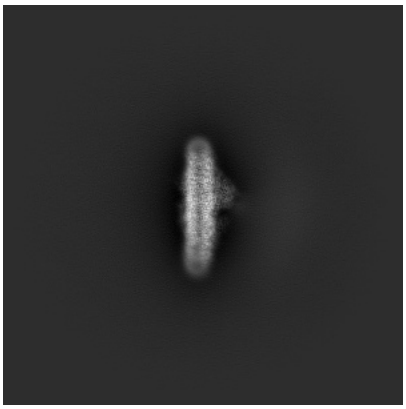
6.1.1 Primary map



X

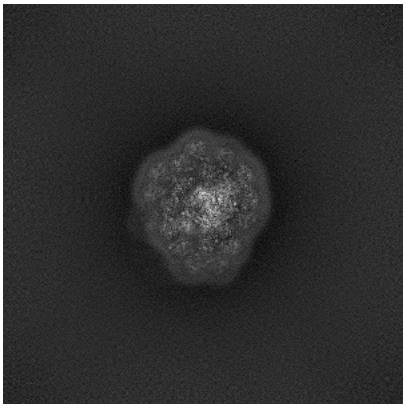


Y

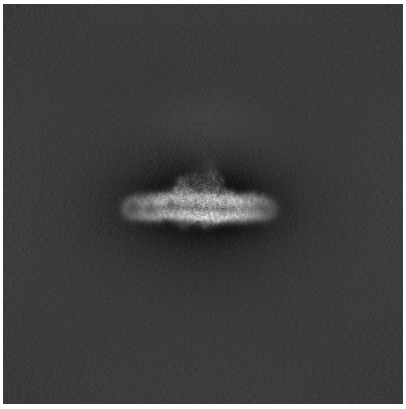


Z

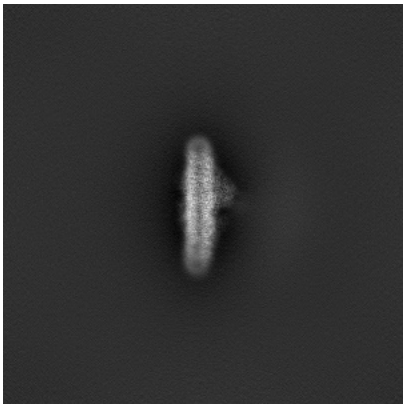
6.1.2 Raw map



X



Y

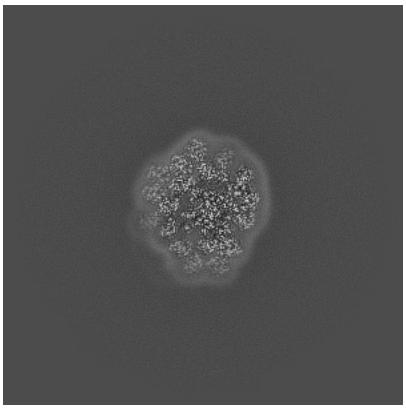


Z

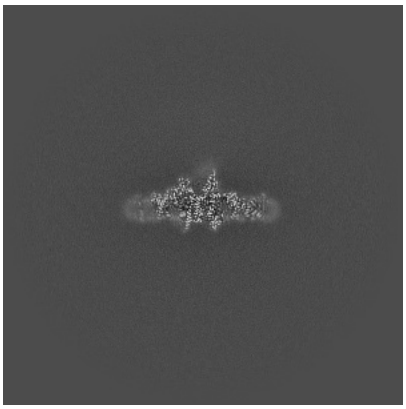
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

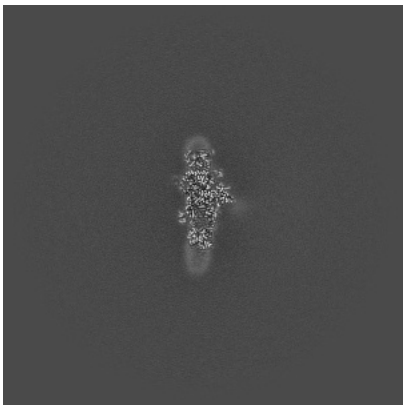
6.2.1 Primary map



X Index: 256

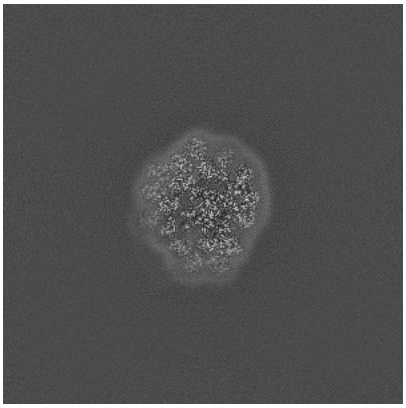


Y Index: 256

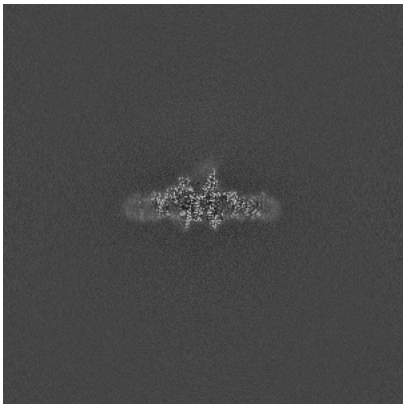


Z Index: 256

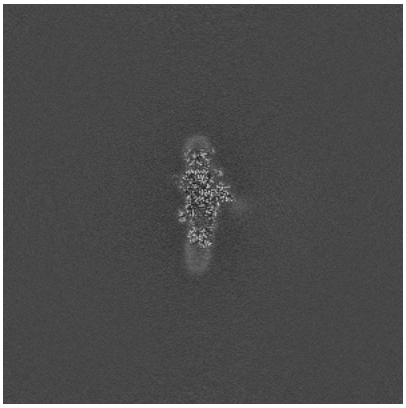
6.2.2 Raw map



X Index: 256



Y Index: 256

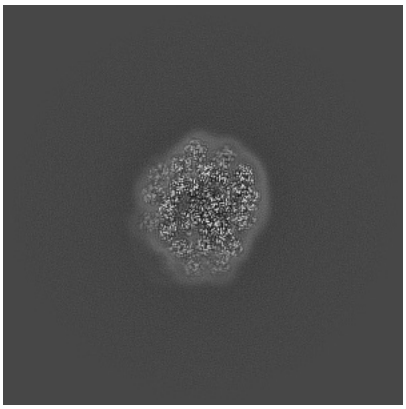


Z Index: 256

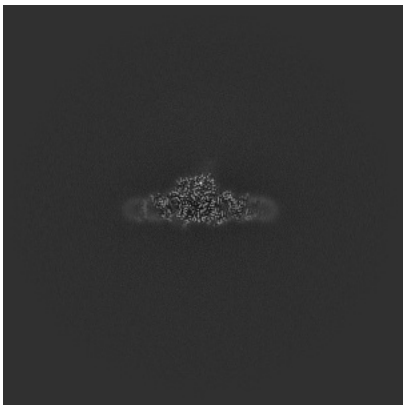
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

6.3.1 Primary map



X Index: 259

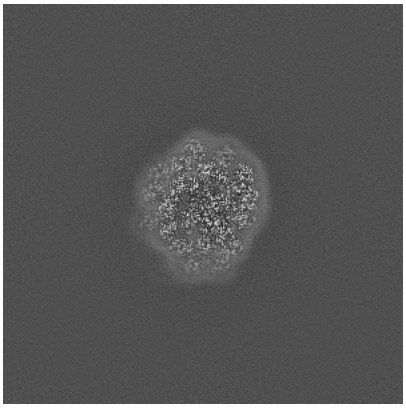


Y Index: 262

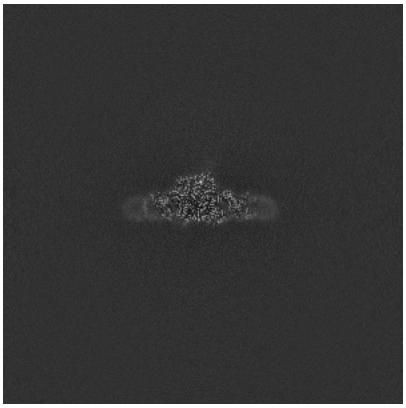


Z Index: 262

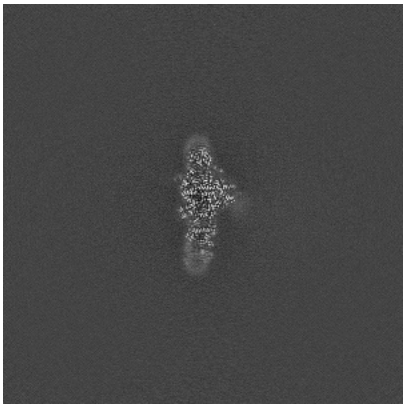
6.3.2 Raw map



X Index: 259



Y Index: 262

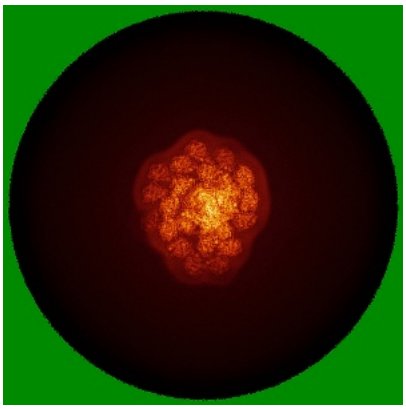


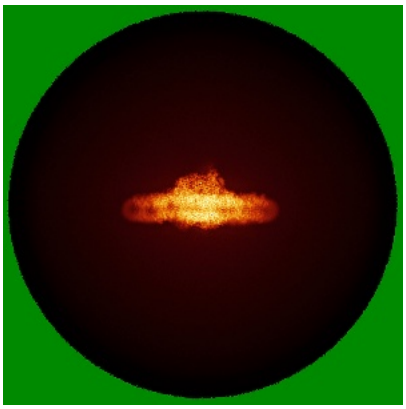
Z Index: 262

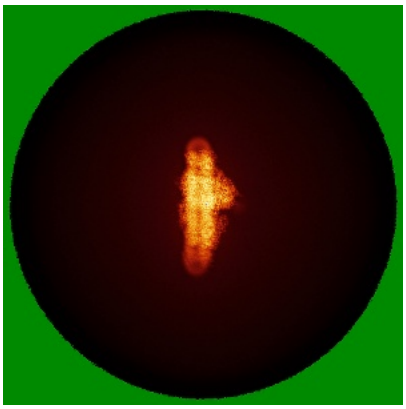
The images above show the largest variance slices of the map in three orthogonal directions.

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

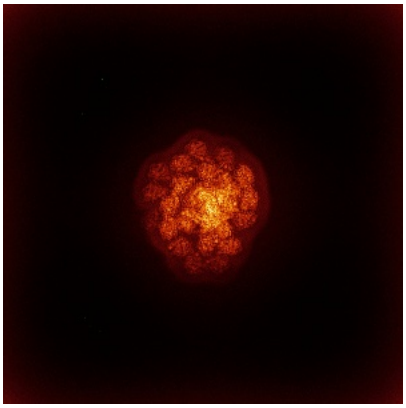
6.4.1 Primary map

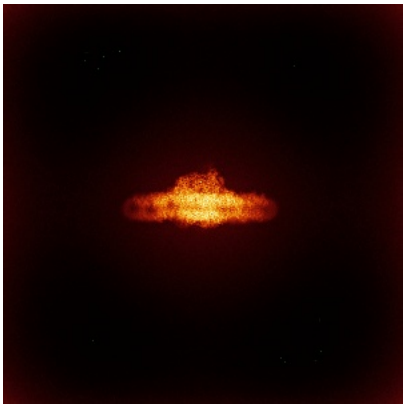

X

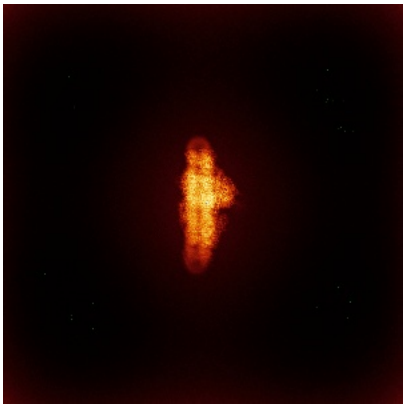

Y


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 0.22. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X Y Z

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

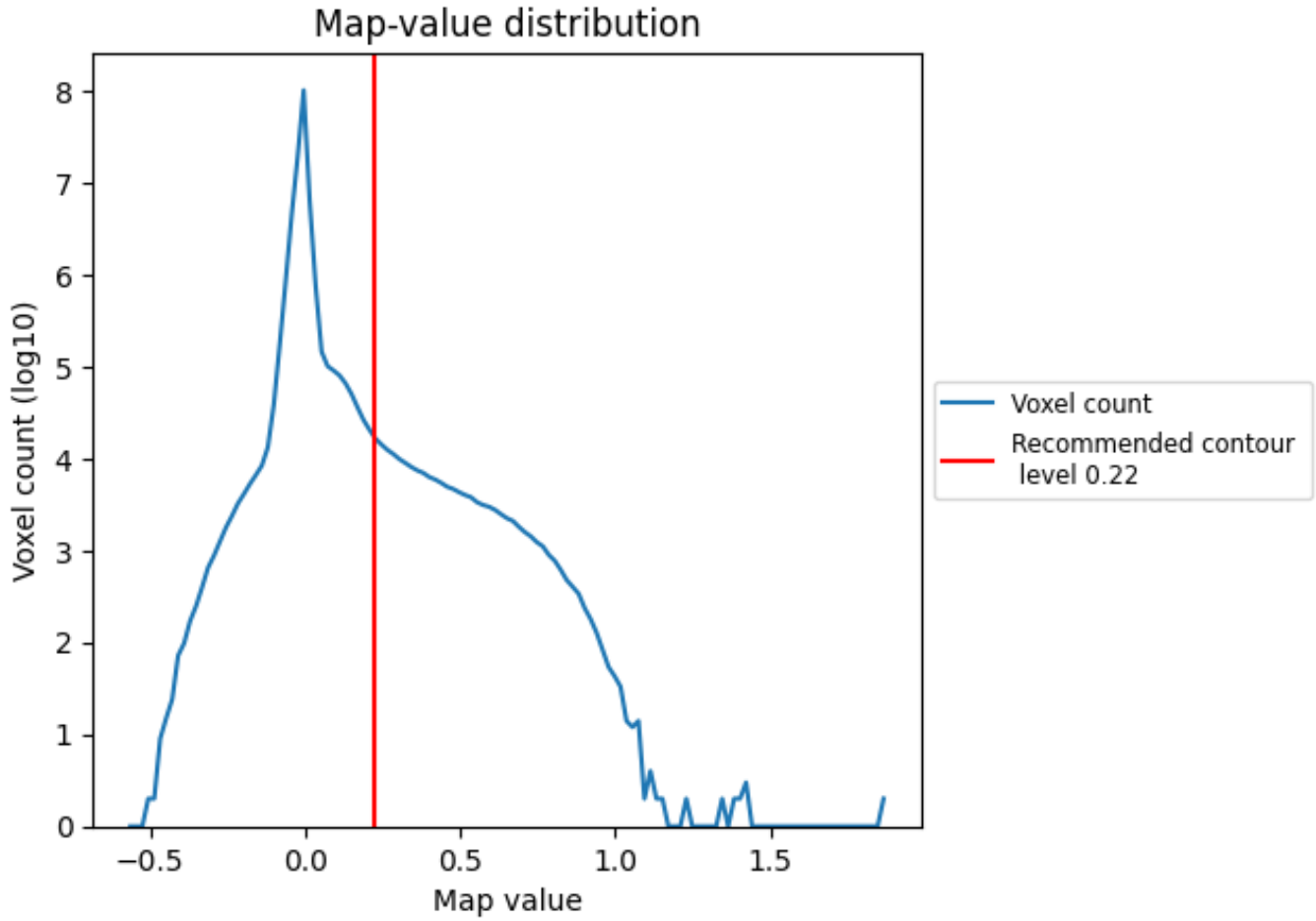
6.6 Mask visualisation (i)

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

7 Map analysis

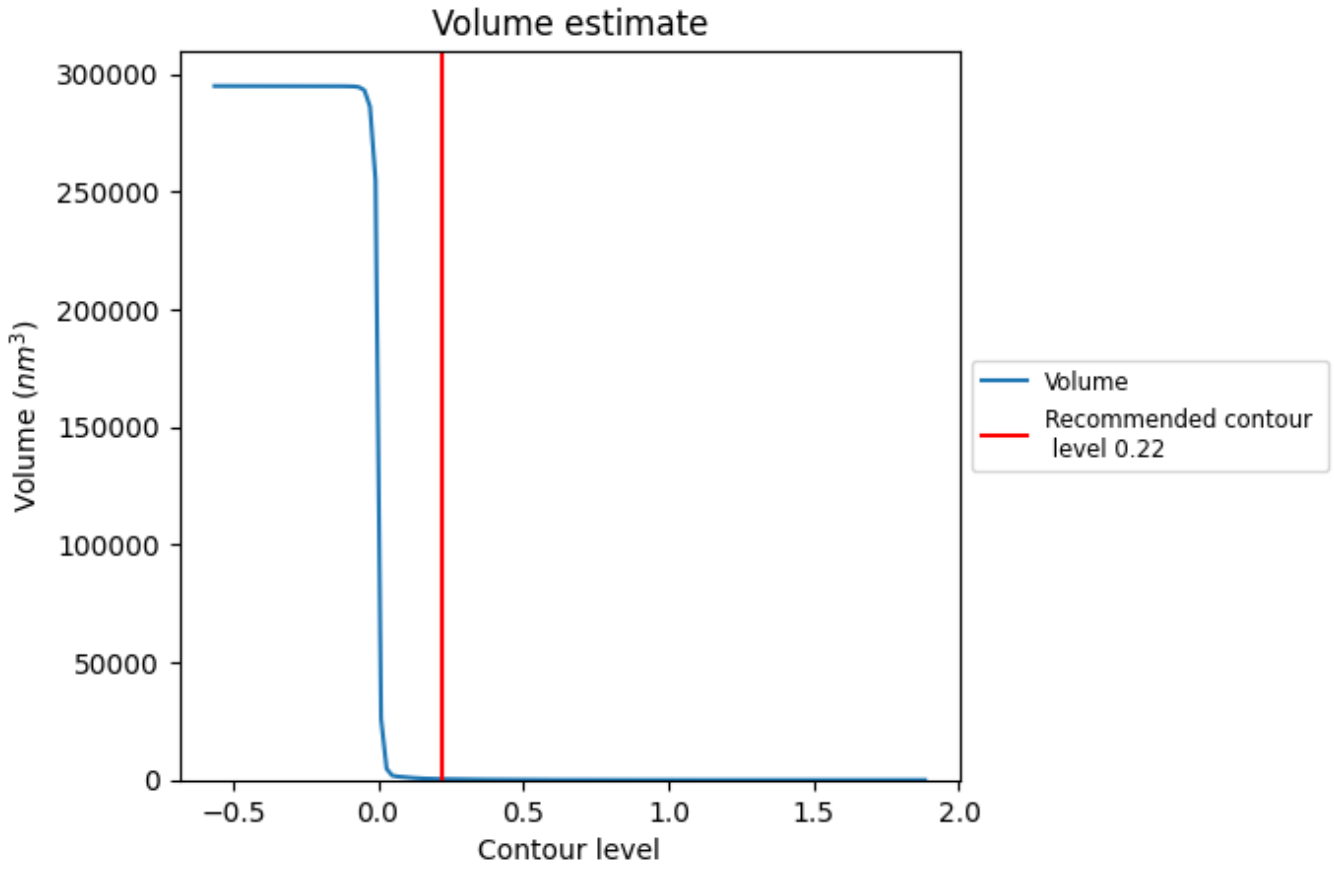
This section contains the results of statistical analysis of the map.

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.

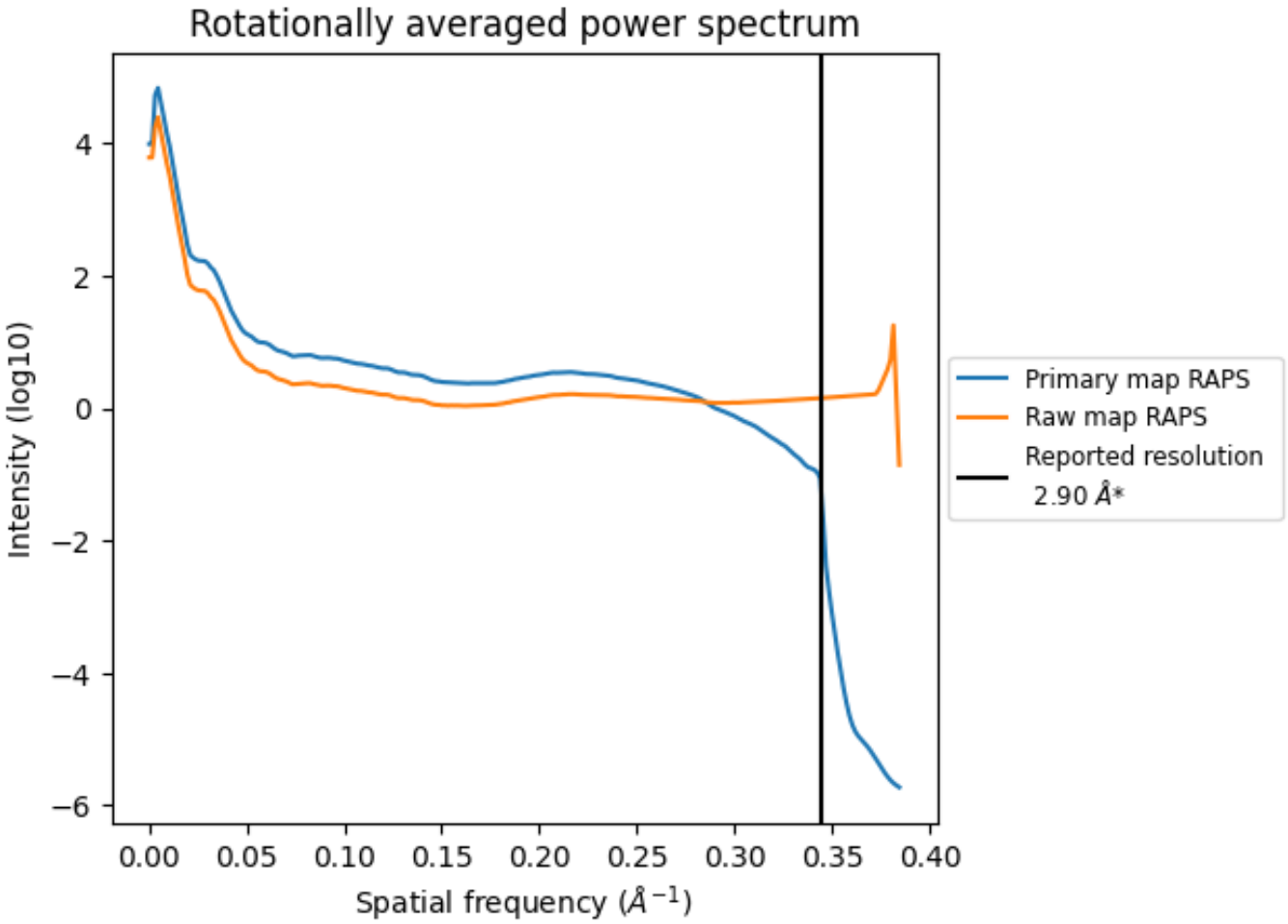
7.2 Volume estimate (i)



The volume at the recommended contour level is 378 nm^3; this corresponds to an approximate mass of 342 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)

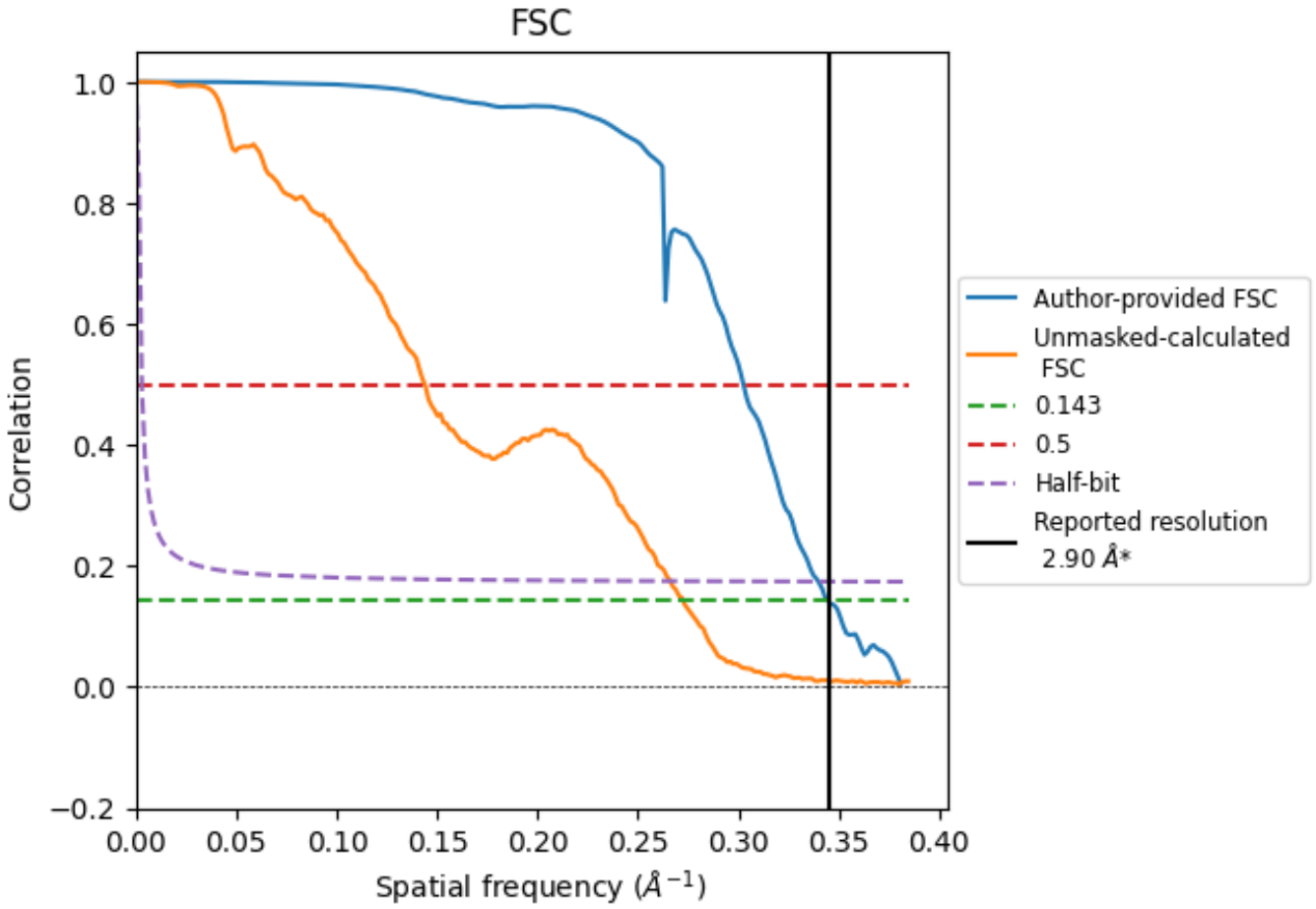


*Reported resolution corresponds to spatial frequency of 0.345 Å^{-1}

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 0.345 Å^{-1}

8.2 Resolution estimates (i)

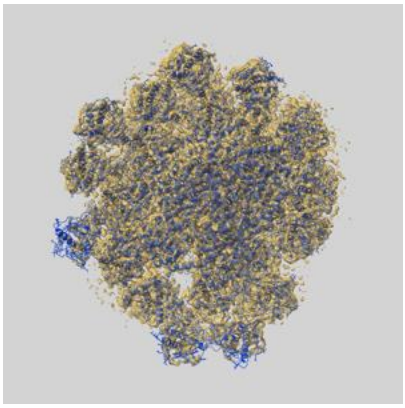
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.90	-	-
Author-provided FSC curve	2.90	3.31	2.94
Unmasked-calculated*	3.67	6.95	3.76

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.67 differs from the reported value 2.9 by more than 10 %

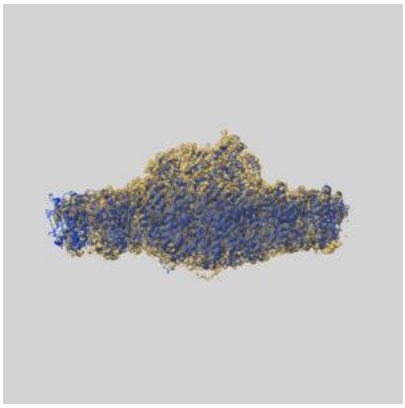
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-36678 and PDB model 8JW0. Per-residue inclusion information can be found in section 3 on page 35.

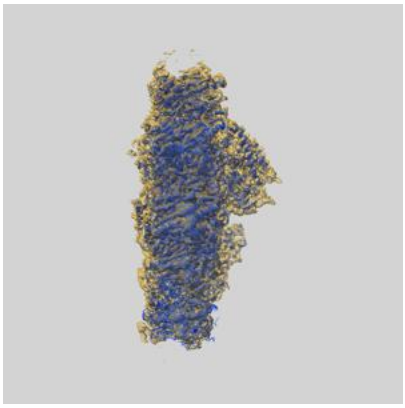
9.1 Map-model overlay



X



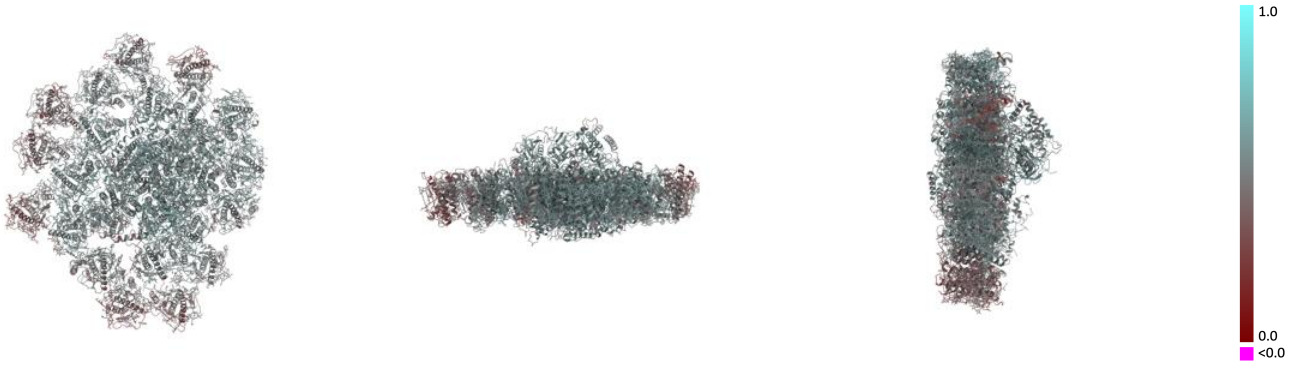
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.22 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.

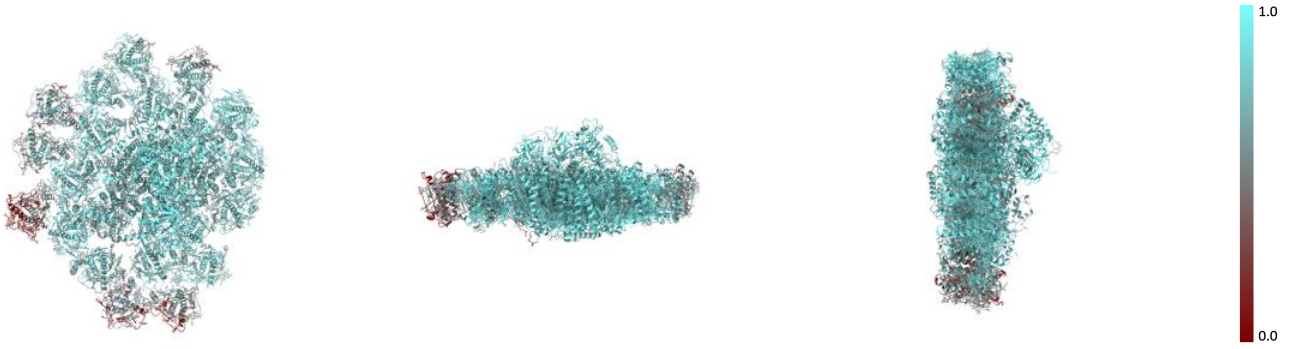
9.2 Q-score mapped to coordinate model



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.

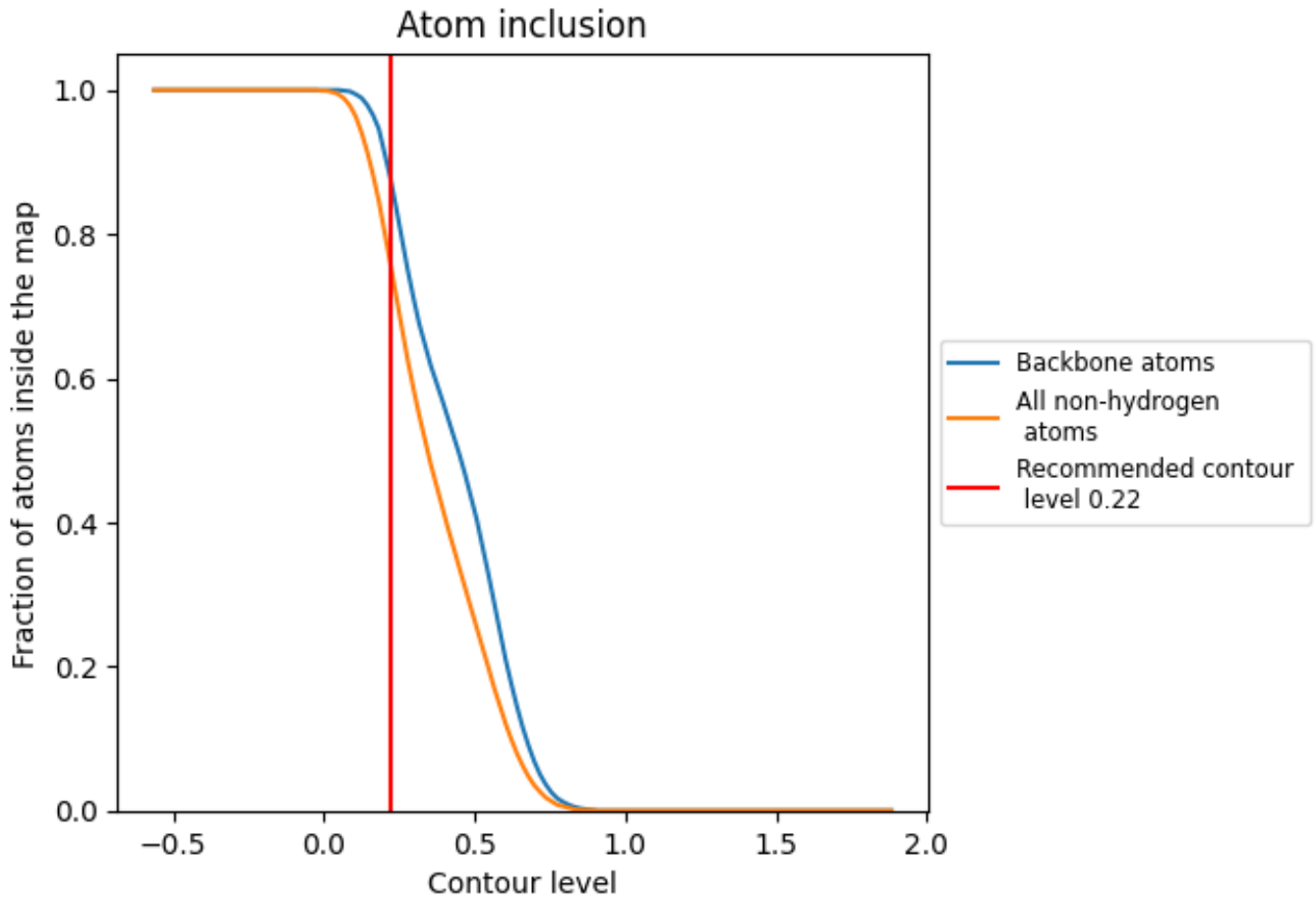
9.3 Atom inclusion mapped to coordinate model



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 (0.22).

9.4 Atom inclusion (i)



At the recommended contour level, 88% of all backbone atoms, 76% 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 (0.22) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7610	0.5100
A	0.8530	0.5420
B	0.8250	0.5400
C	0.7340	0.4710
D	0.6420	0.4360
E	0.7510	0.5040
F	0.7860	0.5010
G	0.8350	0.5470
H	0.3850	0.3860
I	0.8550	0.5520
J	0.8020	0.5160
K	0.8480	0.5520
L	0.8120	0.5330
M	0.7040	0.4660
N	0.4320	0.3830
O	0.5950	0.4070
P	0.2580	0.3780
Q	0.8000	0.5110
T	0.5580	0.3790
a	0.8120	0.5450
b	0.8740	0.5690
c	0.9430	0.5590
d	0.8890	0.5480
e	0.9090	0.5690
f	0.8360	0.5440
h	0.8700	0.5530
i	0.8300	0.5450
j	0.8020	0.5450
l	0.8340	0.5370
m	0.7750	0.5380

