wwPDB EM Validation Summary Report

Feb 18, 2024 – 07:39 PM JST

PDB ID	:	8JW0
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:

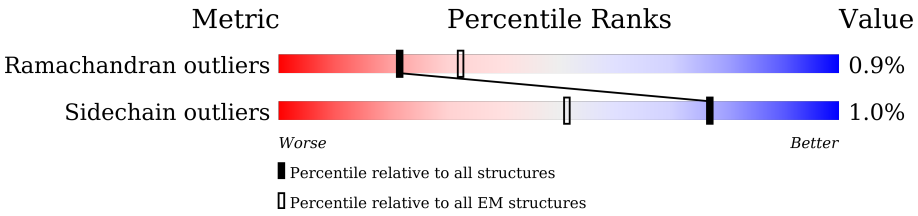
EMDB validation analysis	:	0.0.1.dev70
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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% 99%
2	b	617	99%
3	c	86	100%
4	d	257	99%
5	e	74	100%
6	f	185	100%
7	h	132	95% 5%
8	i	126	98%
9	j	70	97%

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Mol	Chain	Length	Quality of chain
10	l	253	100%
11	m	89	99%
12	A	180	100%
13	G	215	99%
14	I	194	95% 5%
15	K	172	99%
16	F	176	99%
17	J	165	99%
18	M	168	5% 95% 5%
19	L	185	97%
20	D	160	9% 98%
21	B	172	99%
22	H	160	52% 97%
23	N	160	39% 96%
24	O	161	14% 98%
25	C	160	99%
25	T	160	18% 96%
26	Q	162	99%
27	P	160	73% 96%
28	E	142	97%

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
29	CLA	A	206	X	-	-	-
29	CLA	A	207	X	-	-	-
29	CLA	A	208	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
29	CLA	A	209	X	-	-	-
29	CLA	A	210	X	-	-	-
29	CLA	A	211	X	-	-	-
29	CLA	A	212	X	-	-	-
29	CLA	A	214	X	-	-	-
29	CLA	A	215	X	-	-	-
29	CLA	A	216	X	-	-	-
29	CLA	A	217	X	-	-	-
29	CLA	A	218	X	-	-	-
29	CLA	B	306	X	-	-	-
29	CLA	B	307	X	-	-	-
29	CLA	B	308	X	-	-	-
29	CLA	B	309	X	-	-	-
29	CLA	B	310	X	-	-	-
29	CLA	B	311	X	-	-	-
29	CLA	B	312	X	-	-	-
29	CLA	B	314	X	-	-	-
29	CLA	B	315	X	-	-	-
29	CLA	B	316	X	-	-	-
29	CLA	C	308	X	-	-	-
29	CLA	C	309	X	-	-	-
29	CLA	C	311	X	-	-	-
29	CLA	C	313	X	-	-	-
29	CLA	C	314	X	-	-	-
29	CLA	C	316	X	-	-	-
29	CLA	D	308	X	-	-	-
29	CLA	D	309	X	-	-	-
29	CLA	D	311	X	-	-	-
29	CLA	D	312	X	-	-	-
29	CLA	D	313	X	-	-	-
29	CLA	D	314	X	-	-	-
29	CLA	D	316	X	-	-	-
29	CLA	E	305	X	-	-	-
29	CLA	E	306	X	-	-	-
29	CLA	E	308	X	-	-	-
29	CLA	E	309	X	-	-	-
29	CLA	E	310	X	-	-	-
29	CLA	E	311	X	-	-	-
29	CLA	E	313	X	-	-	-
29	CLA	E	315	X	-	-	-
29	CLA	F	307	X	-	-	-
29	CLA	F	308	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
29	CLA	F	310	X	-	-	-
29	CLA	F	311	X	-	-	-
29	CLA	F	312	X	-	-	-
29	CLA	F	313	X	-	-	-
29	CLA	F	315	X	-	-	-
29	CLA	F	316	X	-	-	-
29	CLA	G	301	X	-	-	-
29	CLA	G	302	X	-	-	-
29	CLA	G	304	X	-	-	-
29	CLA	G	311	X	-	-	-
29	CLA	G	312	X	-	-	-
29	CLA	G	313	X	-	-	-
29	CLA	G	314	X	-	-	-
29	CLA	G	316	X	-	-	-
29	CLA	G	317	X	-	-	-
29	CLA	G	319	X	-	-	-
29	CLA	H	307	X	-	-	-
29	CLA	H	308	X	-	-	-
29	CLA	H	310	X	-	-	-
29	CLA	H	312	X	-	-	-
29	CLA	H	313	X	-	-	-
29	CLA	H	315	X	-	-	-
29	CLA	I	201	X	-	-	-
29	CLA	I	207	X	-	-	-
29	CLA	I	208	X	-	-	-
29	CLA	I	209	X	-	-	-
29	CLA	I	210	X	-	-	-
29	CLA	I	211	X	-	-	-
29	CLA	I	212	X	-	-	-
29	CLA	I	213	X	-	-	-
29	CLA	I	214	X	-	-	-
29	CLA	I	216	X	-	-	-
29	CLA	I	217	X	-	-	-
29	CLA	J	305	X	-	-	-
29	CLA	J	306	X	-	-	-
29	CLA	J	307	X	-	-	-
29	CLA	J	308	X	-	-	-
29	CLA	J	309	X	-	-	-
29	CLA	J	310	X	-	-	-
29	CLA	J	311	X	-	-	-
29	CLA	J	313	X	-	-	-
29	CLA	K	207	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
29	CLA	K	208	X	-	-	-
29	CLA	K	209	X	-	-	-
29	CLA	K	210	X	-	-	-
29	CLA	K	211	X	-	-	-
29	CLA	K	212	X	-	-	-
29	CLA	K	213	X	-	-	-
29	CLA	K	214	X	-	-	-
29	CLA	K	216	X	-	-	-
29	CLA	K	217	X	-	-	-
29	CLA	K	218	X	-	-	-
29	CLA	L	307	X	-	-	-
29	CLA	L	308	X	-	-	-
29	CLA	L	309	X	-	-	-
29	CLA	L	310	X	-	-	-
29	CLA	L	311	X	-	-	-
29	CLA	L	312	X	-	-	-
29	CLA	L	313	X	-	-	-
29	CLA	L	315	X	-	-	-
29	CLA	L	316	X	-	-	-
29	CLA	L	317	X	-	-	-
29	CLA	M	306	X	-	-	-
29	CLA	M	307	X	-	-	-
29	CLA	M	308	X	-	-	-
29	CLA	M	309	X	-	-	-
29	CLA	M	310	X	-	-	-
29	CLA	M	311	X	-	-	-
29	CLA	M	313	X	-	-	-
29	CLA	M	314	X	-	-	-
29	CLA	M	315	X	-	-	-
29	CLA	N	308	X	-	-	-
29	CLA	N	309	X	-	-	-
29	CLA	N	311	X	-	-	-
29	CLA	N	313	X	-	-	-
29	CLA	N	314	X	-	-	-
29	CLA	N	316	X	-	-	-
29	CLA	O	308	X	-	-	-
29	CLA	O	311	X	-	-	-
29	CLA	O	313	X	-	-	-
29	CLA	O	316	X	-	-	-
29	CLA	P	209	X	-	-	-
29	CLA	P	210	X	-	-	-
29	CLA	P	212	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
29	CLA	P	214	X	-	-	-
29	CLA	P	215	X	-	-	-
29	CLA	P	217	X	-	-	-
29	CLA	Q	307	X	-	-	-
29	CLA	Q	308	X	-	-	-
29	CLA	Q	310	X	-	-	-
29	CLA	Q	312	X	-	-	-
29	CLA	Q	313	X	-	-	-
29	CLA	Q	315	X	-	-	-
29	CLA	T	308	X	-	-	-
29	CLA	T	309	X	-	-	-
29	CLA	T	311	X	-	-	-
29	CLA	T	313	X	-	-	-
29	CLA	T	314	X	-	-	-
29	CLA	T	316	X	-	-	-
29	CLA	a	801	X	-	-	-
29	CLA	a	802	X	-	-	-
29	CLA	a	803	X	-	-	-
29	CLA	a	804	X	-	-	-
29	CLA	a	805	X	-	-	-
29	CLA	a	806	X	-	-	-
29	CLA	a	807	X	-	-	-
29	CLA	a	808	X	-	-	-
29	CLA	a	809	X	-	-	-
29	CLA	a	810	X	-	-	-
29	CLA	a	811	X	-	-	-
29	CLA	a	812	X	-	-	-
29	CLA	a	813	X	-	-	-
29	CLA	a	814	X	-	-	-
29	CLA	a	815	X	-	-	-
29	CLA	a	816	X	-	-	-
29	CLA	a	817	X	-	-	-
29	CLA	a	818	X	-	-	-
29	CLA	a	819	X	-	-	-
29	CLA	a	820	X	-	-	-
29	CLA	a	821	X	-	-	-
29	CLA	a	822	X	-	-	-
29	CLA	a	823	X	-	-	-
29	CLA	a	824	X	-	-	-
29	CLA	a	825	X	-	-	-
29	CLA	a	826	X	-	-	-
29	CLA	a	827	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
29	CLA	a	828	X	-	-	-
29	CLA	a	829	X	-	-	-
29	CLA	a	830	X	-	-	-
29	CLA	a	831	X	-	-	-
29	CLA	a	837	X	-	-	-
29	CLA	b	701	X	-	-	-
29	CLA	b	702	X	-	-	-
29	CLA	b	703	X	-	-	-
29	CLA	b	704	X	-	-	-
29	CLA	b	705	X	-	-	-
29	CLA	b	706	X	-	-	-
29	CLA	b	707	X	-	-	-
29	CLA	b	708	X	-	-	-
29	CLA	b	709	X	-	-	-
29	CLA	b	710	X	-	-	-
29	CLA	b	711	X	-	-	-
29	CLA	b	712	X	-	-	-
29	CLA	b	713	X	-	-	-
29	CLA	b	714	X	-	-	-
29	CLA	b	715	X	-	-	-
29	CLA	b	716	X	-	-	-
29	CLA	b	717	X	-	-	-
29	CLA	b	718	X	-	-	-
29	CLA	b	719	X	-	-	-
29	CLA	b	720	X	-	-	-
29	CLA	b	721	X	-	-	-
29	CLA	b	722	X	-	-	-
29	CLA	b	723	X	-	-	-
29	CLA	b	724	X	-	-	-
29	CLA	b	725	X	-	-	-
29	CLA	b	726	X	-	-	-
29	CLA	b	731	X	-	-	-
29	CLA	b	736	X	-	-	-
29	CLA	f	802	X	-	-	-
29	CLA	f	803	X	-	-	-
29	CLA	f	805	X	-	-	-
29	CLA	h	201	X	-	-	-
29	CLA	i	201	X	-	-	-
29	CLA	i	202	X	-	-	-
29	CLA	i	203	X	-	-	-
29	CLA	j	104	X	-	-	-
29	CLA	l	501	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
29	CLA	l	502	X	-	-	-
29	CLA	l	503	X	-	-	-
29	CLA	l	504	X	-	-	-
29	CLA	l	505	X	-	-	-
29	CLA	l	508	X	-	-	-
29	CLA	l	509	X	-	-	-
29	CLA	l	510	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		

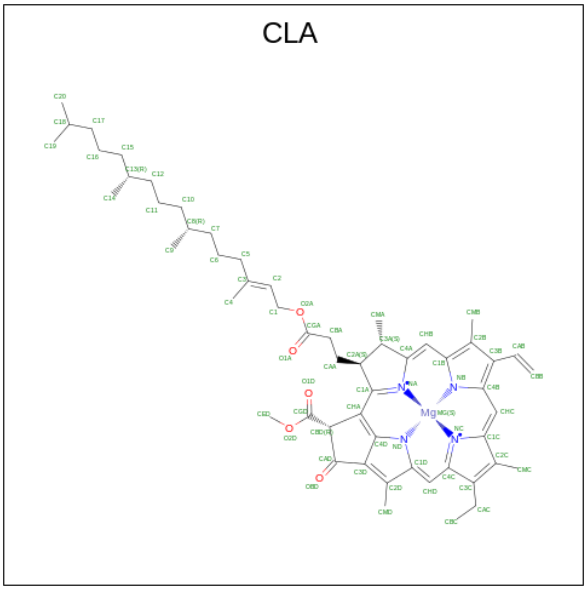
- Molecule 27 is a protein called Chlorophyll a-chlorophyll c-peridinin-protein-complex I-14, acpPCI-14.

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 (three-letter code: 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 65	C 55	Mg 1	N 4	O 5	0
29	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	a	1	Total 46	C 36	Mg 1	N 4	O 5	0
29	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	a	1	Total 56	C 46	Mg 1	N 4	O 5	0
29	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	a	1	Total 55	C 45	Mg 1	N 4	O 5	0
29	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	b	1	Total 52	C 42	Mg 1	N 4	O 5	0
29	b	1	Total 60	C 50	Mg 1	N 4	O 5	0
29	b	1	Total 46	C 36	Mg 1	N 4	O 5	0
29	b	1	Total 58	C 48	Mg 1	N 4	O 5	0
29	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	b	1	Total 53	C 43	Mg 1	N 4	O 5	0

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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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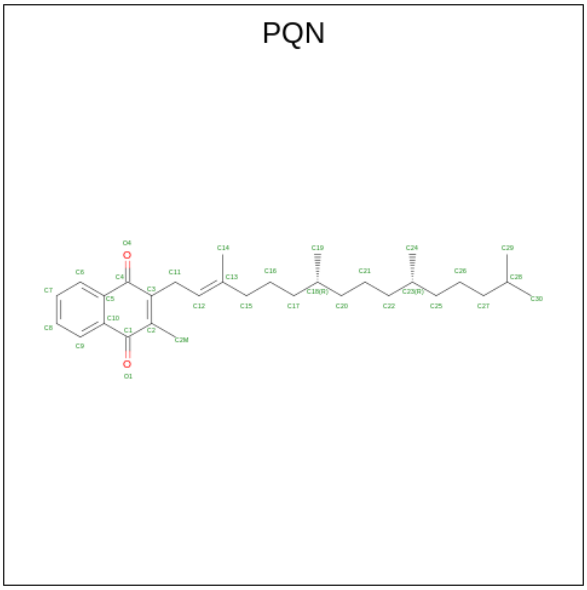
Mol	Chain	Residues	Atoms					AltConf
29	P	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
29	E	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
29	E	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	E	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
29	E	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
29	E	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
29	E	1	Total	C	Mg	N	O	0
			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 (three-letter code: 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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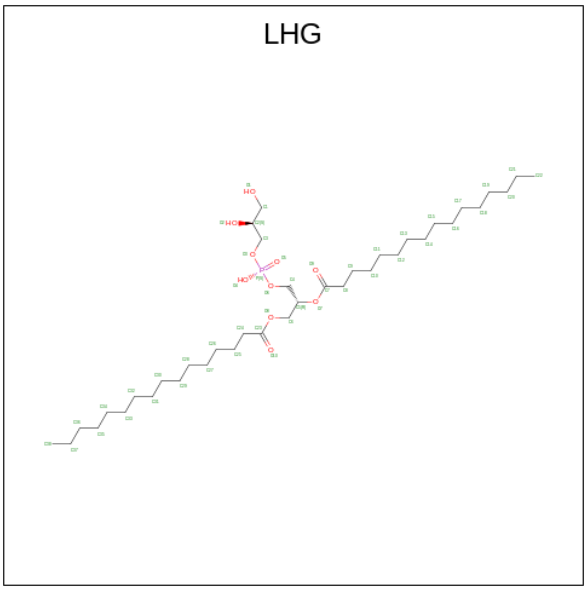
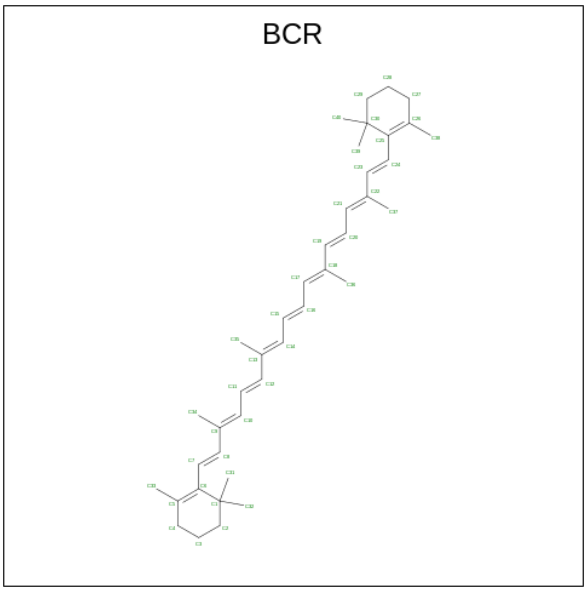
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
30	b	1	33	31	2	0

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



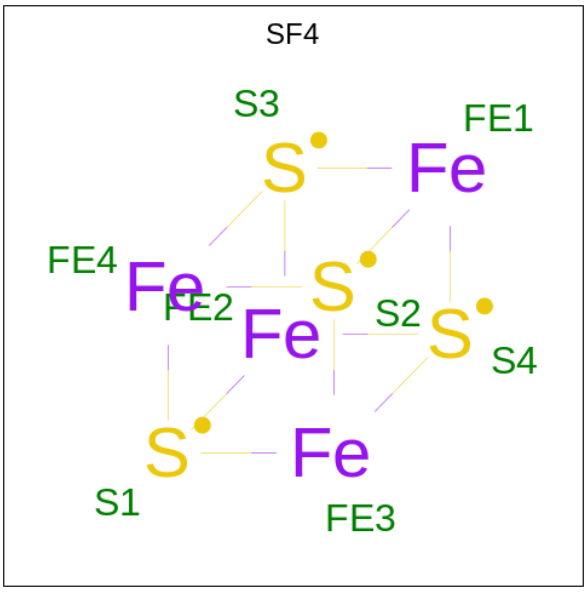
Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
31	a	1	48	37	10	1	0

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



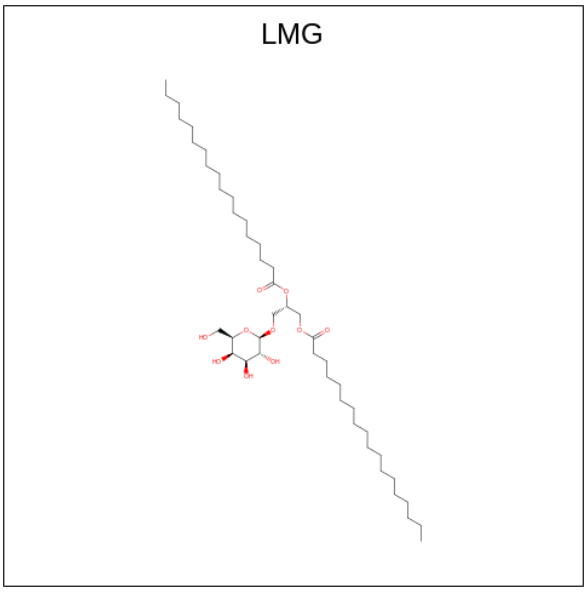
Mol	Chain	Residues	Atoms	AltConf
32	a	1	Total C 40 40	0
32	a	1	Total C 40 40	0
32	a	1	Total C 40 40	0
32	b	1	Total C 40 40	0
32	b	1	Total C 40 40	0
32	b	1	Total C 40 40	0
32	f	1	Total C 40 40	0
32	f	1	Total C 40 40	0
32	i	1	Total C 40 40	0
32	l	1	Total C 40 40	0
32	l	1	Total C 40 40	0
32	m	1	Total C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

- Molecule 33 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).



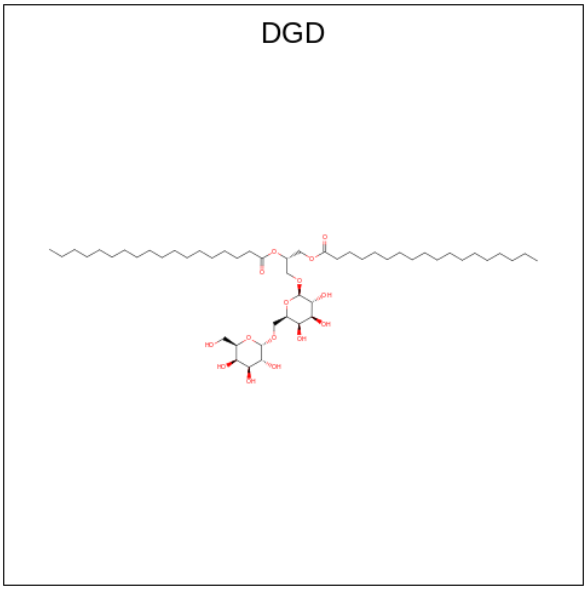
Mol	Chain	Residues	Atoms	AltConf
33	a	1	Total Fe S 8 4 4	0
33	c	1	Total Fe S 8 4 4	0
33	c	1	Total Fe S 8 4 4	0

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



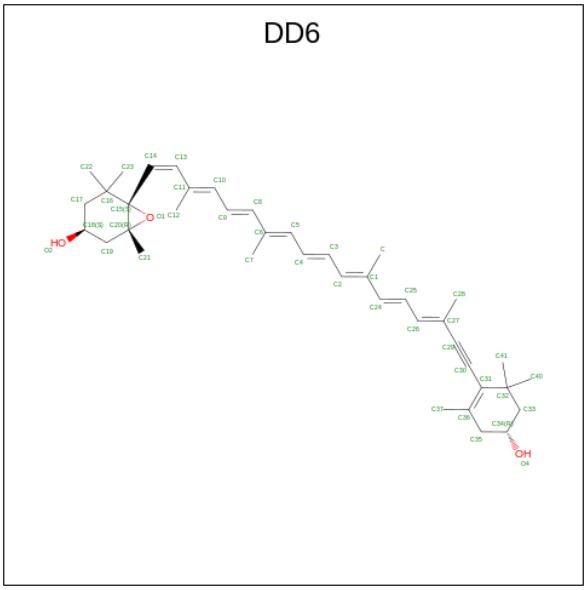
Mol	Chain	Residues	Atoms			AltConf
34	b	1	Total	C	O	0
			46	36	10	
34	b	1	Total	C	O	0
			44	34	10	
34	b	1	Total	C	O	0
			40	30	10	
34	h	1	Total	C	O	0
			28	18	10	
34	j	1	Total	C	O	0
			43	33	10	
34	A	1	Total	C	O	0
			37	27	10	
34	K	1	Total	C	O	0
			43	33	10	
34	K	1	Total	C	O	0
			35	25	10	
34	K	1	Total	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) (three-letter code: 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 (three-letter code: 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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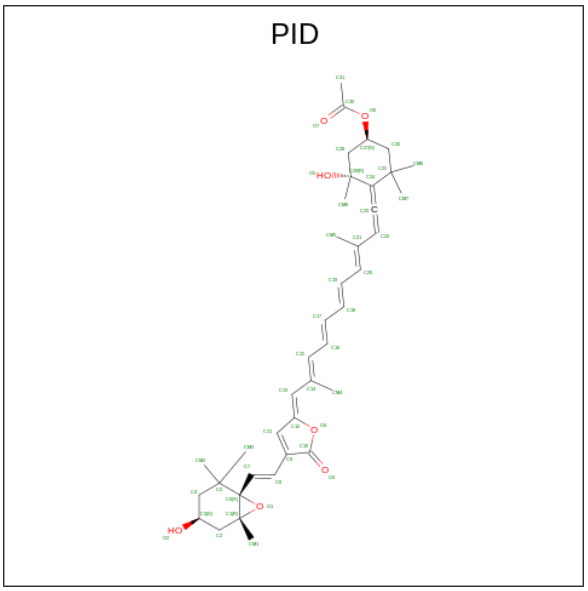
Mol	Chain	Residues	Atoms	AltConf
36	C	1	Total C O 43 40 3	0
36	P	1	Total C O 43 40 3	0
36	E	1	Total C O 43 40 3	0
36	E	1	Total C O 43 40 3	0

- Molecule 37 is PERIDININ (three-letter code: 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	0
			46	39	7	
37	D	1	Total	C	O	0
			46	39	7	
37	D	1	Total	C	O	0
			46	39	7	
37	D	1	Total	C	O	0
			46	39	7	
37	D	1	Total	C	O	0
			46	39	7	
37	D	1	Total	C	O	0
			46	39	7	
37	H	1	Total	C	O	0
			46	39	7	
37	H	1	Total	C	O	0
			46	39	7	
37	H	1	Total	C	O	0
			46	39	7	
37	H	1	Total	C	O	0
			46	39	7	
37	H	1	Total	C	O	0
			46	39	7	
37	N	1	Total	C	O	0
			46	39	7	
37	N	1	Total	C	O	0
			46	39	7	
37	N	1	Total	C	O	0
			46	39	7	
37	N	1	Total	C	O	0
			46	39	7	
37	N	1	Total	C	O	0
			46	39	7	
37	O	1	Total	C	O	0
			46	39	7	
37	O	1	Total	C	O	0
			46	39	7	
37	O	1	Total	C	O	0
			46	39	7	
37	O	1	Total	C	O	0
			46	39	7	
37	O	1	Total	C	O	0
			46	39	7	

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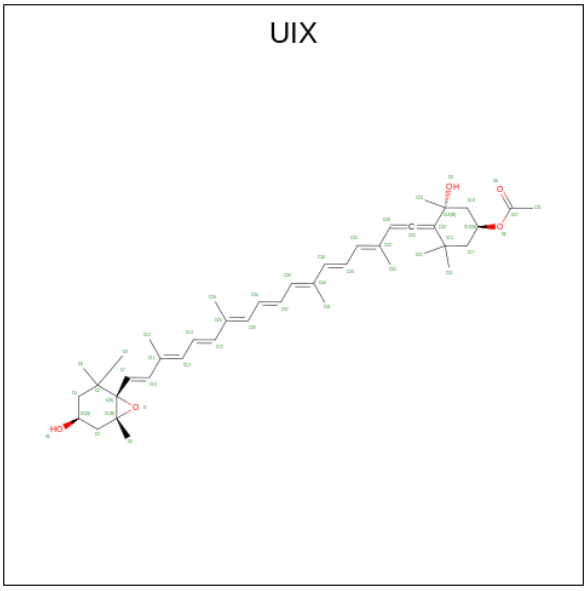
Mol	Chain	Residues	Atoms			AltConf
37	T	1	Total	C	O	0
			46	39	7	
37	T	1	Total	C	O	0
			46	39	7	
37	T	1	Total	C	O	0
			46	39	7	
37	T	1	Total	C	O	0
			46	39	7	
37	T	1	Total	C	O	0
			46	39	7	
37	T	1	Total	C	O	0
			46	39	7	
37	Q	1	Total	C	O	0
			46	39	7	
37	Q	1	Total	C	O	0
			46	39	7	
37	Q	1	Total	C	O	0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

- 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 (three-letter code: 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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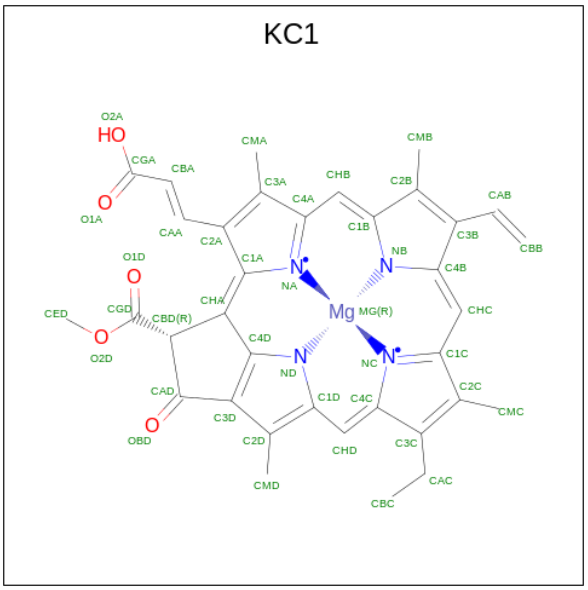
Mol	Chain	Residues	Atoms	AltConf
38	E	1	Total C O 47 42 5	0

- Molecule 39 is Chlorophyll c1 (three-letter code: 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 45 35 1 4 5	0
39	A	1	Total C Mg N O 45 35 1 4 5	0
39	G	1	Total C Mg N O 45 35 1 4 5	0
39	G	1	Total C Mg N O 45 35 1 4 5	0
39	I	1	Total C Mg N O 45 35 1 4 5	0
39	K	1	Total C Mg N O 45 35 1 4 5	0
39	F	1	Total C Mg N O 45 35 1 4 5	0
39	F	1	Total C Mg N O 45 35 1 4 5	0
39	J	1	Total C Mg N O 45 35 1 4 5	0
39	M	1	Total C Mg N O 45 35 1 4 5	0

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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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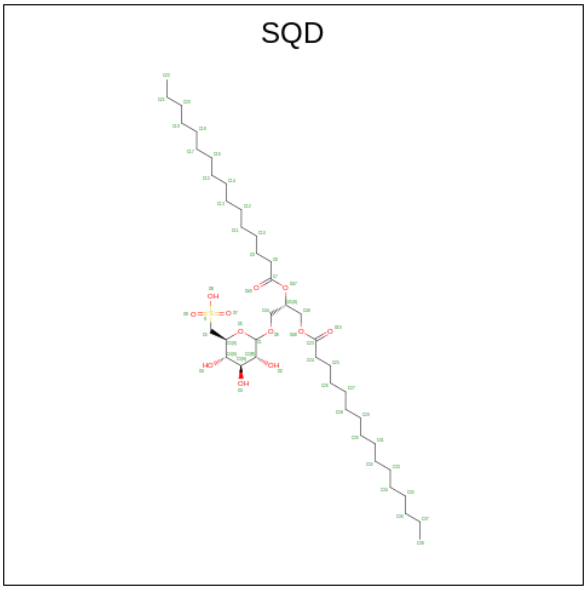
Mol	Chain	Residues	Atoms					AltConf
39	C	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
39	C	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
39	C	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
39	P	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
39	P	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
39	P	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
39	E	1	Total	C	Mg	N	O	0
			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 (three-letter code: SQD) (formula: $C_{41}H_{78}O_{12}S$) (labeled as "Ligand of Interest" by depositor).



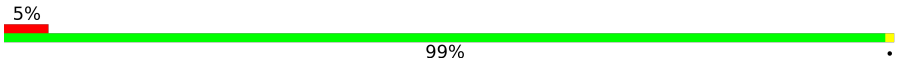
Mol	Chain	Residues	Atoms				AltConf
40	J	1	Total	C	O	S	0
			45	32	12	1	
40	B	1	Total	C	O	S	0
			42	29	12	1	

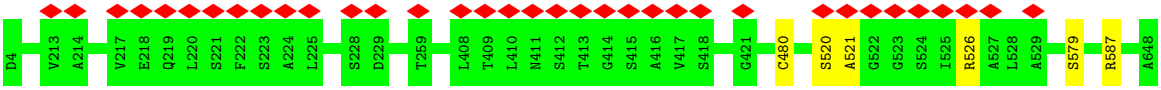
3 Residue-property plots (i)

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

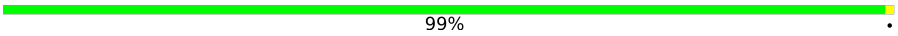
Chain a:





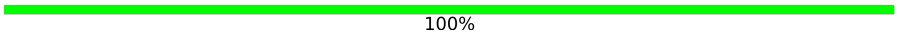
• Molecule 2: Photosystem I PsaB

Chain b:



• Molecule 3: Photosystem I PsaC

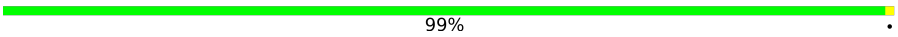
Chain c:



There are no outlier residues recorded for this chain.

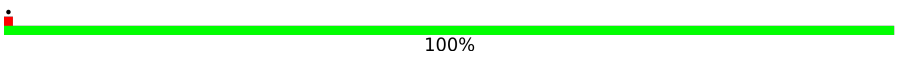
• Molecule 4: Photosystem I PsaD

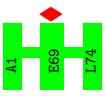
Chain d:



• Molecule 5: Photosystem I PsaE

Chain e:





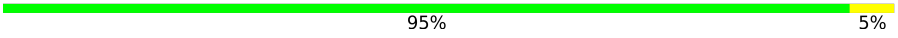
• Molecule 6: Photosystem I PsaF

Chain f:

There are no outlier residues recorded for this chain.

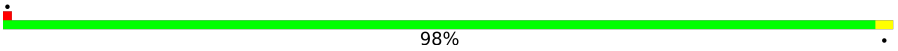
• Molecule 7: Photosystem I PsaR

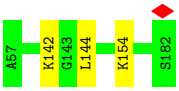
Chain h:



• Molecule 8: Photosystem I PsaI

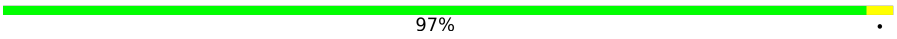
Chain i:





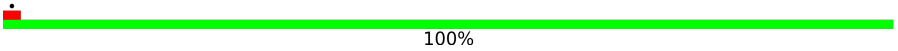
• Molecule 9: Photosystem I PsaJ

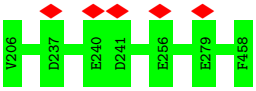
Chain j:



• Molecule 10: Photosystem I PsaL

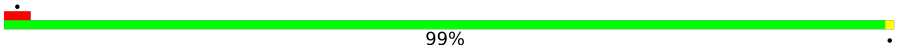
Chain l:

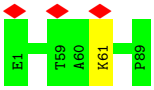




• Molecule 11: Photosystem I PsaM

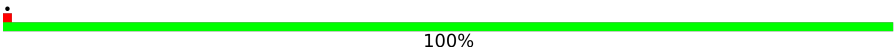
Chain m:

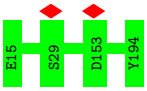




• Molecule 12: Chlorophyll a-chlorophyll c-peridinin-protein-complex I-10, acpPCI-10

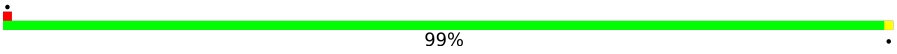
Chain A:

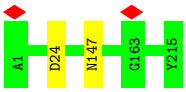




• Molecule 13: Chlorophyll a-chlorophyll c-peridinin-protein-complex I-8, acpPCI-8

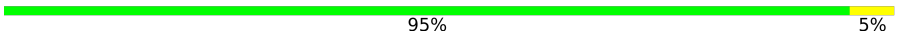
Chain G:





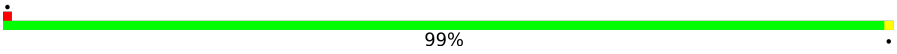
• Molecule 14: Chlorophyll a-chlorophyll c-peridinin-protein-complex I-7, acpPCI-7

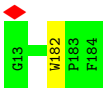
Chain I:



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

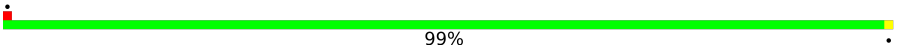
Chain K:

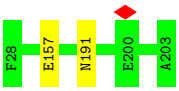




• Molecule 16: Chlorophyll a-chlorophyll c-peridinin-protein-complex I-2, acpPCI-2

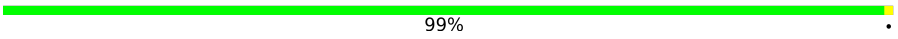
Chain F:





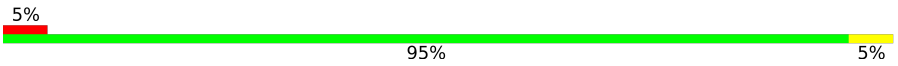
• Molecule 17: Chlorophyll a-chlorophyll c-peridinin-protein-complex I-3, acpPCI-3

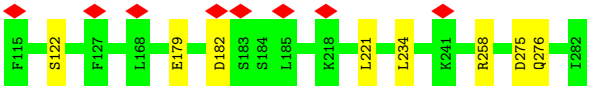
Chain J:



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

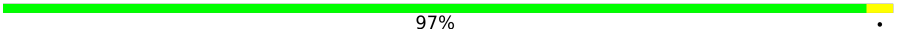
Chain M:





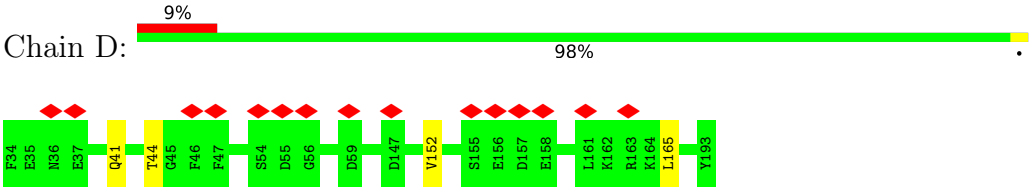
• Molecule 19: Chlorophyll a-chlorophyll c-peridinin-protein-complex I-5, acpPCI-5

Chain L:



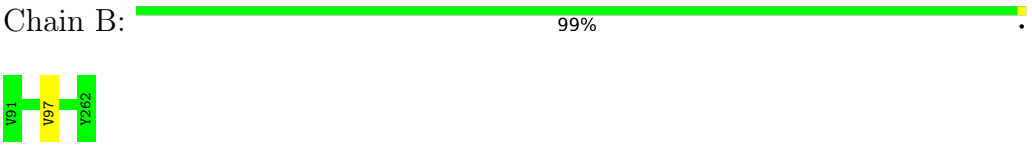
• Molecule 20: Chlorophyll a-chlorophyll c-peridinin-protein-complex I-9, acpPCI-9

Chain D:



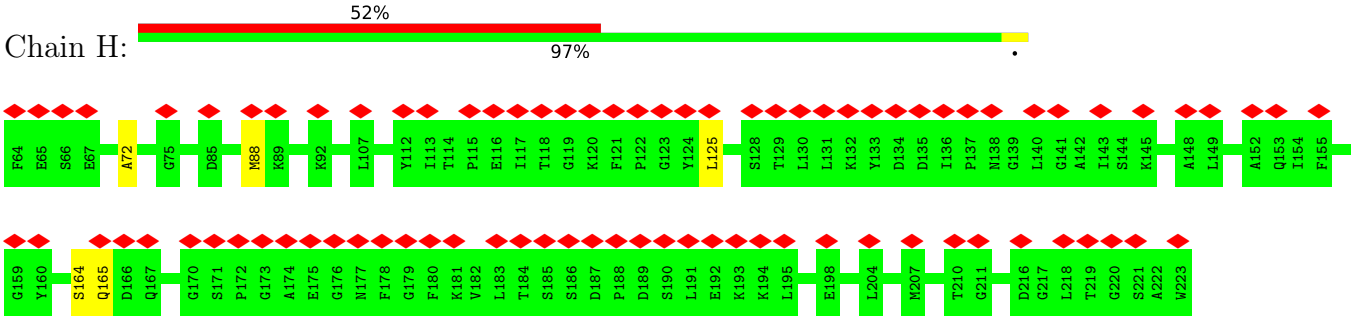
• Molecule 21: Chlorophyll a-chlorophyll c-peridinin-protein-complex I-11, acpPCI-11

Chain B:



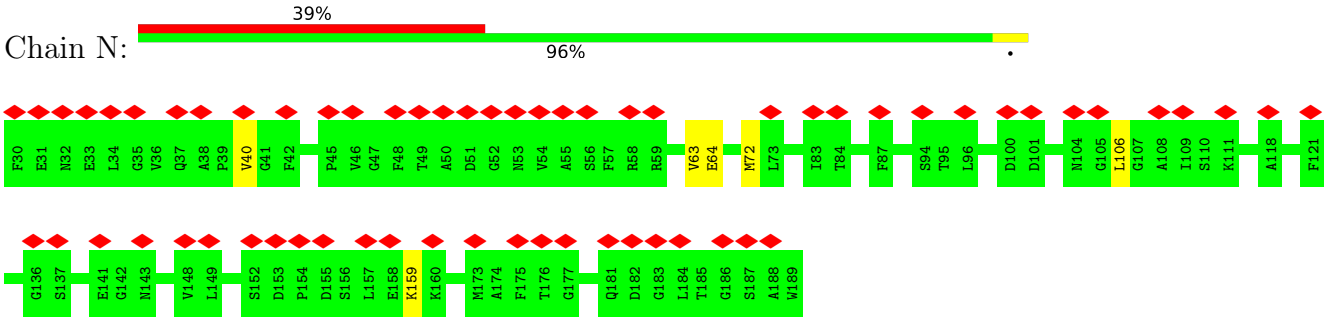
• Molecule 22: Chlorophyll a-chlorophyll c-peridinin-protein-complex I-12, acpPCI-12

Chain H:



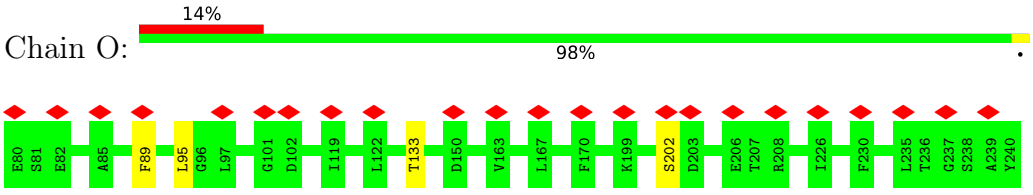
• Molecule 23: Chlorophyll a-chlorophyll c-peridinin-protein-complex I-13, acpPCI-13

Chain N:



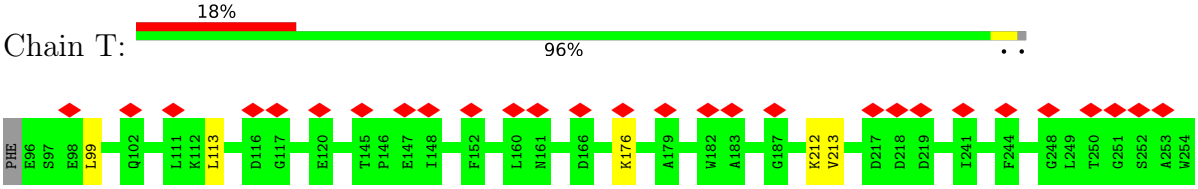
• Molecule 24: Chlorophyll a-chlorophyll c-peridinin-protein-complex I-15, acpPCI-15

Chain O:



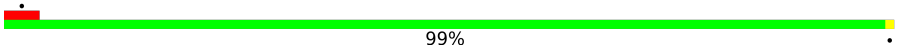
• Molecule 25: Chlorophyll a-chlorophyll c-peridinin-protein-complex I-16, acpPCI-16

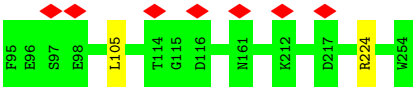
Chain T:



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

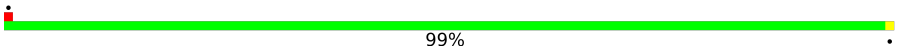
Chain C:

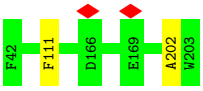




• Molecule 26: Chlorophyll a-chlorophyll c-peridinin-protein-complex I-17, acpPCI-17

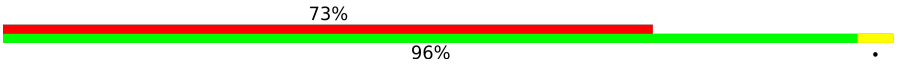
Chain Q:

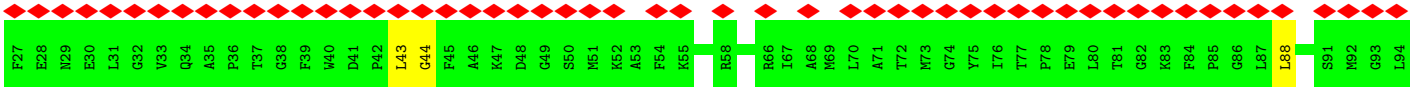


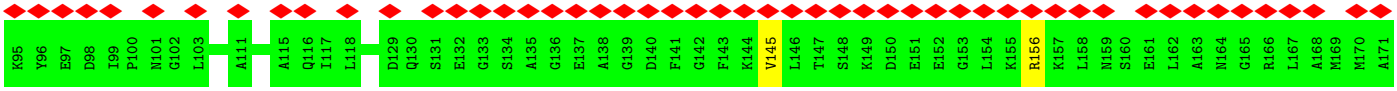


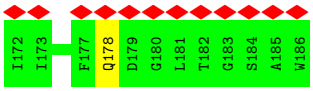
• Molecule 27: Chlorophyll a-chlorophyll c-peridinin-protein-complex I-14, acpPCI-14

Chain P:



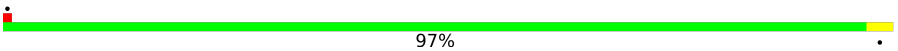


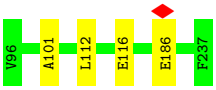




• Molecule 28: Chlorophyll a-chlorophyll c-peridinin-protein-complex I-1, acpPCI-1

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: BCR, SQD, KC1, UIX, LMG, DD6, PID, DGD, PQN, LHG, SF4, CLA

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	a	0.33	0/5133	0.46	0/7019
2	b	0.35	0/4968	0.46	0/6804
3	c	0.31	0/657	0.50	0/897
4	d	0.30	0/2034	0.50	0/2766
5	e	0.30	0/624	0.43	0/851
6	f	0.28	0/1484	0.48	0/1998
7	h	0.31	0/1089	0.46	0/1479
8	i	0.30	0/1030	0.44	0/1394
9	j	0.36	0/566	0.52	0/774
10	l	0.28	0/2014	0.46	0/2737
11	m	0.30	0/694	0.48	0/939
12	A	0.28	0/1395	0.45	0/1892
13	G	0.30	0/1730	0.43	0/2348
14	I	0.31	0/1499	0.47	0/2037
15	K	0.29	0/1358	0.48	0/1838
16	F	0.29	0/1395	0.50	0/1886
17	J	0.27	0/1317	0.46	0/1795
18	M	0.27	0/1395	0.49	0/1888
19	L	0.28	0/1490	0.52	0/2021
20	D	0.27	0/1223	0.51	0/1650
21	B	0.30	0/1404	0.49	0/1891
22	H	0.28	0/1232	0.49	0/1665
23	N	0.27	0/1233	0.50	0/1671
24	O	0.28	0/1260	0.50	0/1709
25	C	0.26	0/1226	0.50	0/1653
25	T	0.27	0/1214	0.50	0/1637
26	Q	0.28	0/1251	0.50	0/1690
27	P	0.28	0/1245	0.49	0/1673
28	E	0.28	0/1093	0.52	0/1473
All	All	0.30	0/44253	0.48	0/60075

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

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%)	41 71
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%)	34 66
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%)	6 23
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%)	29 61
14	I	192/194 (99%)	165 (86%)	21 (11%)	6 (3%)	4 16
15	K	170/172 (99%)	153 (90%)	16 (9%)	1 (1%)	25 58
16	F	174/176 (99%)	154 (88%)	19 (11%)	1 (1%)	25 58

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
17	J	163/165 (99%)	144 (88%)	18 (11%)	1 (1%)	25 58
18	M	166/168 (99%)	134 (81%)	26 (16%)	6 (4%)	3 14
19	L	183/185 (99%)	152 (83%)	26 (14%)	5 (3%)	5 19
20	D	158/160 (99%)	142 (90%)	15 (10%)	1 (1%)	25 58
21	B	170/172 (99%)	153 (90%)	17 (10%)	0	100 100
22	H	158/160 (99%)	135 (85%)	19 (12%)	4 (2%)	5 21
23	N	158/160 (99%)	126 (80%)	31 (20%)	1 (1%)	25 58
24	O	159/161 (99%)	144 (91%)	12 (8%)	3 (2%)	8 28
25	C	158/160 (99%)	146 (92%)	11 (7%)	1 (1%)	25 58
25	T	157/160 (98%)	142 (90%)	11 (7%)	4 (2%)	5 21
26	Q	160/162 (99%)	138 (86%)	20 (12%)	2 (1%)	12 37
27	P	158/160 (99%)	139 (88%)	16 (10%)	3 (2%)	8 28
28	E	140/142 (99%)	120 (86%)	17 (12%)	3 (2%)	7 26
All	All	5527/5586 (99%)	4986 (90%)	492 (9%)	49 (1%)	21 48

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%)	81 94
2	b	502/504 (100%)	498 (99%)	4 (1%)	81 94
3	c	73/74 (99%)	73 (100%)	0	100 100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
4	d	213/222 (96%)	212 (100%)	1 (0%)	88 96
5	e	65/66 (98%)	65 (100%)	0	100 100
6	f	151/151 (100%)	151 (100%)	0	100 100
7	h	109/109 (100%)	106 (97%)	3 (3%)	43 76
8	i	106/106 (100%)	103 (97%)	3 (3%)	43 76
9	j	60/60 (100%)	58 (97%)	2 (3%)	38 72
10	l	200/203 (98%)	200 (100%)	0	100 100
11	m	72/72 (100%)	71 (99%)	1 (1%)	67 89
12	A	136/141 (96%)	136 (100%)	0	100 100
13	G	171/171 (100%)	170 (99%)	1 (1%)	86 96
14	I	141/156 (90%)	138 (98%)	3 (2%)	53 81
15	K	133/138 (96%)	133 (100%)	0	100 100
16	F	140/140 (100%)	139 (99%)	1 (1%)	84 95
17	J	136/136 (100%)	135 (99%)	1 (1%)	84 95
18	M	128/128 (100%)	126 (98%)	2 (2%)	62 86
19	L	145/145 (100%)	144 (99%)	1 (1%)	84 95
20	D	123/123 (100%)	120 (98%)	3 (2%)	49 79
21	B	146/146 (100%)	145 (99%)	1 (1%)	84 95
22	H	123/123 (100%)	122 (99%)	1 (1%)	81 94
23	N	124/124 (100%)	119 (96%)	5 (4%)	31 65
24	O	124/124 (100%)	123 (99%)	1 (1%)	81 94
25	C	121/121 (100%)	120 (99%)	1 (1%)	81 94
25	T	120/121 (99%)	119 (99%)	1 (1%)	81 94
26	Q	120/120 (100%)	120 (100%)	0	100 100
27	P	123/123 (100%)	120 (98%)	3 (2%)	49 79
28	E	108/108 (100%)	107 (99%)	1 (1%)	78 93
All	All	4444/4490 (99%)	4400 (99%)	44 (1%)	77 92

5 of 44 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
20	D	44	THR
23	N	72	MET

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Mol	Chain	Res	Type
20	D	165	LEU
23	N	40	VAL
24	O	133	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 7 such sidechains are listed below:

Mol	Chain	Res	Type
17	J	227	ASN
18	M	191	HIS
24	O	218	ASN
22	H	71	GLN
16	F	176	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides 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	$\#\|Z\| > 2$
39	KC1	G	315	-	48,53,53	1.54	7 (14%)	55,89,89	1.90	11 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
37	PID	P	208	-	41,49,49	1.37	4 (9%)	49,76,76	2.42	7 (14%)
32	BCR	m	103	-	41,41,41	0.82	1 (2%)	56,56,56	2.35	18 (32%)
36	DD6	B	303	-	39,45,45	2.04	3 (7%)	52,67,67	1.80	14 (26%)
29	CLA	b	719	-	50,58,73	1.69	6 (12%)	58,95,113	1.60	10 (17%)
29	CLA	A	206	39	45,53,73	1.76	6 (13%)	52,89,113	1.63	7 (13%)
29	CLA	a	827	-	65,73,73	1.48	9 (13%)	76,113,113	1.37	8 (10%)
29	CLA	a	829	-	65,73,73	1.46	7 (10%)	76,113,113	1.40	7 (9%)
36	DD6	I	206	-	39,45,45	2.03	3 (7%)	52,67,67	1.90	12 (23%)
29	CLA	G	316	-	65,73,73	1.50	8 (12%)	76,113,113	4.94	11 (14%)
29	CLA	F	308	-	46,54,73	1.74	7 (15%)	53,90,113	1.52	6 (11%)
29	CLA	G	302	-	65,73,73	1.47	6 (9%)	76,113,113	1.40	7 (9%)
32	BCR	l	506	-	41,41,41	0.75	0	56,56,56	1.93	14 (25%)
29	CLA	M	314	-	52,60,73	1.65	5 (9%)	60,97,113	1.49	7 (11%)
32	BCR	b	735	-	41,41,41	0.77	0	56,56,56	2.04	17 (30%)
39	KC1	E	312	28	48,53,53	1.56	7 (14%)	55,89,89	1.84	12 (21%)
29	CLA	a	807	-	65,73,73	1.48	7 (10%)	76,113,113	1.42	9 (11%)
29	CLA	I	210	-	55,63,73	1.58	6 (10%)	64,101,113	1.47	7 (10%)
29	CLA	A	209	-	65,73,73	1.47	6 (9%)	76,113,113	1.39	9 (11%)
37	PID	N	301	-	41,49,49	1.34	4 (9%)	49,76,76	1.49	5 (10%)
39	KC1	A	213	-	48,53,53	1.53	7 (14%)	55,89,89	1.84	11 (20%)
39	KC1	O	310	-	48,53,53	1.53	7 (14%)	55,89,89	1.86	12 (21%)
36	DD6	J	303	-	39,45,45	2.10	3 (7%)	52,67,67	2.11	18 (34%)
36	DD6	N	303	-	39,45,45	1.96	3 (7%)	52,67,67	1.76	12 (23%)
29	CLA	P	215	-	47,55,73	1.77	5 (10%)	54,91,113	1.70	9 (16%)
29	CLA	C	313	25	46,54,73	1.73	6 (13%)	53,90,113	1.53	6 (11%)
29	CLA	h	201	-	60,68,73	1.51	7 (11%)	70,107,113	1.46	8 (11%)
29	CLA	A	208	-	55,63,73	1.58	7 (12%)	64,101,113	1.50	7 (10%)
36	DD6	I	205	-	39,45,45	2.45	5 (12%)	52,67,67	2.18	17 (32%)
29	CLA	G	314	-	60,68,73	1.52	7 (11%)	70,107,113	1.49	8 (11%)
29	CLA	D	313	20	45,53,73	1.76	6 (13%)	52,89,113	1.55	6 (11%)
36	DD6	G	308	-	39,45,45	2.01	2 (5%)	52,67,67	2.12	15 (28%)
36	DD6	h	202	-	39,45,45	2.19	5 (12%)	52,67,67	2.33	19 (36%)
29	CLA	b	701	-	65,73,73	1.45	7 (10%)	76,113,113	1.44	9 (11%)
37	PID	T	305	-	41,49,49	1.32	4 (9%)	49,76,76	1.52	7 (14%)
29	CLA	T	308	-	47,55,73	1.75	6 (12%)	54,91,113	1.52	7 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
29	CLA	a	809	1	65,73,73	1.46	7 (10%)	76,113,113	1.41	8 (10%)
37	PID	T	317	-	41,49,49	1.33	4 (9%)	49,76,76	1.70	9 (18%)
39	KC1	H	314	-	48,53,53	1.51	7 (14%)	55,89,89	1.86	10 (18%)
29	CLA	B	312	-	65,73,73	1.45	7 (10%)	76,113,113	1.41	7 (9%)
38	UIX	E	304	-	41,49,49	1.30	4 (9%)	52,74,74	2.43	18 (34%)
29	CLA	f	803	6	46,54,73	1.73	6 (13%)	53,90,113	1.56	6 (11%)
29	CLA	L	309	-	55,63,73	1.59	6 (10%)	64,101,113	1.48	7 (10%)
29	CLA	a	806	1	65,73,73	1.45	7 (10%)	76,113,113	1.44	7 (9%)
29	CLA	a	801	-	65,73,73	1.44	10 (15%)	76,113,113	1.40	7 (9%)
29	CLA	l	509	-	41,49,73	1.83	7 (17%)	47,84,113	1.65	8 (17%)
32	BCR	l	507	-	41,41,41	0.75	0	56,56,56	1.99	16 (28%)
29	CLA	E	308	-	65,73,73	1.47	6 (9%)	76,113,113	1.39	8 (10%)
29	CLA	P	214	27	46,54,73	1.77	6 (13%)	53,90,113	1.55	6 (11%)
29	CLA	B	315	-	46,54,73	1.73	6 (13%)	53,90,113	1.59	6 (11%)
29	CLA	O	314	-	47,55,73	1.78	7 (14%)	54,91,113	1.58	8 (14%)
29	CLA	H	312	22	46,54,73	1.73	6 (13%)	53,90,113	1.59	6 (11%)
29	CLA	K	216	-	41,49,73	1.81	7 (17%)	47,84,113	1.74	7 (14%)
29	CLA	B	310	-	65,73,73	1.45	7 (10%)	76,113,113	1.38	7 (9%)
39	KC1	C	315	25	48,53,53	1.52	7 (14%)	55,89,89	1.82	10 (18%)
36	DD6	I	202	-	39,45,45	2.03	3 (7%)	52,67,67	1.92	14 (26%)
39	KC1	C	310	-	48,53,53	1.54	7 (14%)	55,89,89	1.89	10 (18%)
39	KC1	A	205	29	48,53,53	1.53	7 (14%)	55,89,89	1.87	13 (23%)
29	CLA	F	311	-	46,54,73	1.73	6 (13%)	53,90,113	1.59	6 (11%)
39	KC1	D	315	-	48,53,53	1.52	7 (14%)	55,89,89	1.84	8 (14%)
32	BCR	a	835	-	41,41,41	0.79	0	56,56,56	2.12	16 (28%)
29	CLA	b	721	-	58,66,73	1.56	8 (13%)	67,104,113	1.48	9 (13%)
29	CLA	b	702	-	65,73,73	1.47	6 (9%)	76,113,113	1.40	6 (7%)
29	CLA	C	316	-	41,49,73	1.82	6 (14%)	47,84,113	1.73	7 (14%)
36	DD6	L	305	-	39,45,45	2.05	3 (7%)	52,67,67	1.95	14 (26%)
29	CLA	b	706	-	65,73,73	1.48	7 (10%)	76,113,113	1.41	7 (9%)
29	CLA	l	502	10	65,73,73	1.49	9 (13%)	76,113,113	1.39	9 (11%)
29	CLA	L	310	-	55,63,73	1.60	6 (10%)	64,101,113	1.48	7 (10%)
39	KC1	K	215	-	48,53,53	1.56	7 (14%)	55,89,89	1.89	13 (23%)
29	CLA	D	316	-	41,49,73	1.84	6 (14%)	47,84,113	1.71	7 (14%)
37	PID	O	301	-	41,49,49	1.32	4 (9%)	49,76,76	1.62	6 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
29	CLA	T	309	25	46,54,73	1.74	7 (15%)	53,90,113	1.58	7 (13%)
29	CLA	b	723	-	65,73,73	1.45	7 (10%)	76,113,113	1.41	8 (10%)
36	DD6	F	303	-	39,45,45	2.11	3 (7%)	52,67,67	2.09	13 (25%)
29	CLA	a	802	-	65,73,73	1.47	6 (9%)	76,113,113	1.47	9 (11%)
36	DD6	K	221	-	39,45,45	2.14	4 (10%)	52,67,67	2.24	15 (28%)
29	CLA	F	312	16	46,54,73	1.73	6 (13%)	53,90,113	1.53	6 (11%)
37	PID	D	303	-	41,49,49	1.37	4 (9%)	49,76,76	1.51	8 (16%)
39	KC1	H	309	-	48,53,53	1.53	7 (14%)	55,89,89	1.87	11 (20%)
36	DD6	G	307	-	39,45,45	2.71	10 (25%)	52,67,67	2.55	19 (36%)
29	CLA	A	212	-	55,63,73	1.56	7 (12%)	64,101,113	1.47	8 (12%)
38	UIX	L	302	-	41,49,49	1.26	3 (7%)	52,74,74	2.41	17 (32%)
29	CLA	T	316	-	41,49,73	1.84	6 (14%)	47,84,113	1.67	7 (14%)
29	CLA	b	722	-	58,66,73	1.53	7 (12%)	67,104,113	1.50	7 (10%)
29	CLA	b	731	-	56,64,73	1.57	6 (10%)	65,102,113	1.47	9 (13%)
29	CLA	K	210	-	50,58,73	1.65	6 (12%)	58,95,113	1.58	8 (13%)
39	KC1	D	310	-	48,53,53	1.51	7 (14%)	55,89,89	1.84	9 (16%)
36	DD6	J	301	-	39,45,45	2.06	3 (7%)	52,67,67	2.26	17 (32%)
34	LMG	K	201	-	43,43,55	0.79	0	51,51,63	1.32	5 (9%)
38	UIX	N	306	-	41,49,49	1.26	4 (9%)	52,74,74	2.60	20 (38%)
29	CLA	F	310	-	46,54,73	1.70	7 (15%)	53,90,113	1.63	7 (13%)
29	CLA	I	216	-	52,60,73	1.64	7 (13%)	60,97,113	1.58	9 (15%)
29	CLA	K	218	-	45,53,73	1.79	6 (13%)	52,89,113	1.56	6 (11%)
29	CLA	L	316	-	52,60,73	1.68	7 (13%)	60,97,113	1.48	8 (13%)
29	CLA	b	736	-	65,73,73	1.48	9 (13%)	76,113,113	6.29	12 (15%)
29	CLA	a	812	-	60,68,73	1.51	7 (11%)	70,107,113	1.50	7 (10%)
29	CLA	A	207	-	55,63,73	1.60	7 (12%)	64,101,113	1.48	7 (10%)
37	PID	C	307	-	41,49,49	1.34	4 (9%)	49,76,76	1.52	6 (12%)
29	CLA	B	309	-	55,63,73	1.58	6 (10%)	64,101,113	1.49	7 (10%)
29	CLA	L	313	-	53,61,73	1.61	6 (11%)	61,98,113	1.52	8 (13%)
34	LMG	b	734	-	40,40,55	0.81	0	48,48,63	1.29	6 (12%)
29	CLA	i	203	-	55,63,73	1.56	6 (10%)	64,101,113	1.51	8 (12%)
29	CLA	a	822	-	65,73,73	1.46	6 (9%)	76,113,113	1.38	8 (10%)
29	CLA	K	207	15	49,57,73	1.70	6 (12%)	55,93,113	1.54	8 (14%)
37	PID	F	302	-	41,49,49	1.34	4 (9%)	49,76,76	1.67	6 (12%)
29	CLA	C	314	-	47,55,73	1.74	6 (12%)	54,91,113	1.64	8 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
29	CLA	J	305	-	46,54,73	1.76	6 (13%)	53,90,113	1.53	7 (13%)
31	LHG	a	833	-	47,47,48	0.28	0	50,53,54	0.31	0
35	DGD	b	733	-	58,58,67	0.94	3 (5%)	72,72,81	1.25	7 (9%)
37	PID	O	304	-	41,49,49	1.34	4 (9%)	49,76,76	1.50	6 (12%)
29	CLA	F	315	-	41,49,73	1.84	5 (12%)	47,84,113	1.71	8 (17%)
29	CLA	J	306	-	65,73,73	1.44	7 (10%)	76,113,113	1.42	7 (9%)
39	KC1	H	311	-	48,53,53	1.52	7 (14%)	55,89,89	1.82	10 (18%)
29	CLA	D	314	-	47,55,73	1.72	7 (14%)	54,91,113	1.65	7 (12%)
29	CLA	N	309	-	65,73,73	1.48	6 (9%)	76,113,113	1.36	8 (10%)
37	PID	T	307	-	41,49,49	1.33	4 (9%)	49,76,76	1.58	8 (16%)
29	CLA	b	725	-	65,73,73	1.47	8 (12%)	76,113,113	1.35	7 (9%)
29	CLA	E	315	-	57,65,73	1.60	6 (10%)	66,103,113	1.45	8 (12%)
29	CLA	J	308	-	56,64,73	1.57	6 (10%)	65,102,113	1.49	8 (12%)
36	DD6	G	306	-	39,45,45	2.12	3 (7%)	52,67,67	2.19	13 (25%)
37	PID	h	204	-	41,49,49	1.35	4 (9%)	49,76,76	1.40	6 (12%)
29	CLA	f	802	-	46,54,73	1.73	7 (15%)	53,90,113	1.54	6 (11%)
29	CLA	l	503	10	65,73,73	1.48	8 (12%)	76,113,113	1.40	8 (10%)
29	CLA	M	311	-	46,54,73	1.76	6 (13%)	53,90,113	1.55	8 (15%)
36	DD6	F	301	-	39,45,45	2.11	4 (10%)	52,67,67	1.99	14 (26%)
36	DD6	K	206	-	39,45,45	2.05	3 (7%)	52,67,67	2.01	14 (26%)
29	CLA	J	313	-	41,49,73	1.83	6 (14%)	47,84,113	1.67	8 (17%)
38	UIX	P	207	-	41,49,49	1.27	3 (7%)	52,74,74	2.56	19 (36%)
29	CLA	b	720	-	65,73,73	1.49	8 (12%)	76,113,113	1.36	6 (7%)
29	CLA	a	814	-	46,54,73	1.74	7 (15%)	53,90,113	1.53	6 (11%)
37	PID	N	305	-	41,49,49	1.37	4 (9%)	49,76,76	1.36	4 (8%)
36	DD6	M	303	-	39,45,45	2.11	4 (10%)	52,67,67	2.03	14 (26%)
29	CLA	a	803	-	65,73,73	1.49	7 (10%)	76,113,113	1.38	6 (7%)
38	UIX	B	304	-	41,49,49	1.27	3 (7%)	52,74,74	2.45	16 (30%)
37	PID	O	302	-	41,49,49	1.36	4 (9%)	49,76,76	1.42	7 (14%)
29	CLA	J	311	-	53,61,73	1.64	9 (16%)	61,98,113	1.48	7 (11%)
29	CLA	l	508	-	41,49,73	1.82	7 (17%)	47,84,113	1.66	7 (14%)
29	CLA	N	311	-	51,59,73	1.67	5 (9%)	59,96,113	1.53	7 (11%)
37	PID	j	101	-	41,49,49	1.37	4 (9%)	49,76,76	1.46	9 (18%)
36	DD6	A	201	-	39,45,45	2.02	3 (7%)	52,67,67	2.02	16 (30%)
37	PID	H	302	-	41,49,49	1.36	4 (9%)	49,76,76	1.40	6 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
29	CLA	b	704	-	65,73,73	1.47	8 (12%)	76,113,113	3.99	8 (10%)
29	CLA	b	715	-	46,54,73	1.75	7 (15%)	53,90,113	1.55	7 (13%)
29	CLA	l	501	-	60,68,73	1.54	6 (10%)	70,107,113	1.48	7 (10%)
39	KC1	P	211	-	48,53,53	1.54	7 (14%)	55,89,89	1.86	13 (23%)
29	CLA	H	308	-	65,73,73	1.48	6 (9%)	76,113,113	1.41	9 (11%)
36	DD6	O	303	-	39,45,45	2.10	4 (10%)	52,67,67	2.19	17 (32%)
29	CLA	E	310	28	46,54,73	1.72	6 (13%)	53,90,113	1.57	6 (11%)
37	PID	D	306	-	41,49,49	1.36	4 (9%)	49,76,76	1.42	8 (16%)
29	CLA	I	214	-	55,63,73	1.57	7 (12%)	64,101,113	1.48	8 (12%)
29	CLA	L	315	-	41,49,73	1.87	7 (17%)	47,84,113	1.63	7 (14%)
39	KC1	O	315	-	48,53,53	1.51	6 (12%)	55,89,89	1.87	10 (18%)
29	CLA	B	316	-	45,53,73	1.78	6 (13%)	52,89,113	1.57	6 (11%)
35	DGD	j	105	-	42,42,67	1.03	2 (4%)	56,56,81	1.07	5 (8%)
29	CLA	A	210	12	46,54,73	1.77	7 (15%)	53,90,113	1.51	7 (13%)
29	CLA	G	304	-	59,67,73	1.54	8 (13%)	68,105,113	1.51	7 (10%)
29	CLA	K	214	-	55,63,73	1.62	9 (16%)	64,101,113	1.45	9 (14%)
37	PID	G	303	-	41,49,49	1.37	4 (9%)	49,76,76	1.33	5 (10%)
29	CLA	I	209	-	60,68,73	1.52	7 (11%)	70,107,113	5.16	11 (15%)
29	CLA	a	813	-	51,59,73	1.69	7 (13%)	59,96,113	1.50	7 (11%)
32	BCR	i	204	-	41,41,41	0.76	0	56,56,56	2.35	15 (26%)
29	CLA	b	726	-	65,73,73	1.48	7 (10%)	76,113,113	1.37	8 (10%)
36	DD6	L	301	-	39,45,45	2.00	3 (7%)	52,67,67	1.97	11 (21%)
37	PID	P	202	-	41,49,49	1.32	4 (9%)	49,76,76	1.37	8 (16%)
37	PID	Q	304	-	41,49,49	1.33	4 (9%)	49,76,76	1.54	6 (12%)
29	CLA	b	711	-	58,66,73	1.56	7 (12%)	67,104,113	1.44	8 (11%)
29	CLA	F	316	16	41,49,73	1.82	6 (14%)	47,84,113	1.68	7 (14%)
29	CLA	I	213	14	65,73,73	1.48	6 (9%)	76,113,113	4.10	12 (15%)
29	CLA	C	308	-	47,55,73	1.73	6 (12%)	54,91,113	1.52	7 (12%)
29	CLA	a	831	-	65,73,73	1.46	7 (10%)	76,113,113	4.96	9 (11%)
29	CLA	B	314	21	41,49,73	1.80	7 (17%)	47,84,113	1.72	7 (14%)
29	CLA	C	309	-	65,73,73	1.47	6 (9%)	76,113,113	1.37	6 (7%)
36	DD6	A	204	-	39,45,45	2.02	3 (7%)	52,67,67	1.87	15 (28%)
37	PID	C	304	-	41,49,49	1.34	4 (9%)	49,76,76	1.44	6 (12%)
29	CLA	K	208	-	46,54,73	1.74	7 (15%)	53,90,113	1.52	6 (11%)
29	CLA	b	707	-	65,73,73	1.48	7 (10%)	76,113,113	1.42	9 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
29	CLA	a	805	-	55,63,73	1.59	7 (12%)	64,101,113	1.50	6 (9%)
29	CLA	b	703	-	65,73,73	1.48	7 (10%)	76,113,113	1.34	6 (7%)
29	CLA	K	213	-	48,56,73	1.71	7 (14%)	55,92,113	1.51	8 (14%)
34	LMG	A	219	-	37,37,55	0.85	0	45,45,63	1.31	5 (11%)
29	CLA	A	216	-	41,49,73	1.83	7 (17%)	47,84,113	1.66	7 (14%)
29	CLA	a	830	-	56,64,73	1.56	6 (10%)	65,102,113	5.34	10 (15%)
29	CLA	b	718	-	65,73,73	1.47	7 (10%)	76,113,113	1.48	8 (10%)
37	PID	Q	303	-	41,49,49	1.34	4 (9%)	49,76,76	1.48	6 (12%)
29	CLA	M	315	-	46,54,73	1.73	6 (13%)	53,90,113	1.53	6 (11%)
36	DD6	M	302	-	39,45,45	2.11	4 (10%)	52,67,67	2.09	14 (26%)
39	KC1	F	309	-	48,53,53	1.53	7 (14%)	55,89,89	1.88	11 (20%)
29	CLA	Q	307	-	47,55,73	1.74	6 (12%)	54,91,113	1.52	7 (12%)
32	BCR	a	838	-	41,41,41	0.76	0	56,56,56	2.12	18 (32%)
29	CLA	P	210	-	65,73,73	1.47	6 (9%)	76,113,113	1.36	7 (9%)
37	PID	G	309	-	41,49,49	1.33	4 (9%)	49,76,76	1.45	5 (10%)
39	KC1	I	215	14	48,53,53	1.54	7 (14%)	55,89,89	1.87	11 (20%)
29	CLA	L	307	39	50,58,73	1.68	7 (14%)	58,95,113	5.67	10 (17%)
29	CLA	b	709	-	60,68,73	1.52	7 (11%)	70,107,113	1.43	8 (11%)
29	CLA	l	505	-	65,73,73	1.48	6 (9%)	76,113,113	1.37	8 (10%)
29	CLA	P	209	-	47,55,73	1.75	5 (10%)	54,91,113	1.53	7 (12%)
34	LMG	E	316	-	32,32,55	0.99	1 (3%)	40,40,63	1.27	2 (5%)
29	CLA	G	301	-	49,57,73	1.69	7 (14%)	55,93,113	1.57	7 (12%)
29	CLA	I	208	-	46,54,73	1.74	6 (13%)	53,90,113	5.89	8 (15%)
38	UIX	A	203	-	41,49,49	1.27	4 (9%)	52,74,74	2.39	21 (40%)
37	PID	C	301	-	41,49,49	1.34	4 (9%)	49,76,76	1.59	6 (12%)
29	CLA	a	828	-	46,54,73	1.75	7 (15%)	53,90,113	1.54	6 (11%)
29	CLA	M	313	-	41,49,73	1.85	7 (17%)	47,84,113	1.69	7 (14%)
32	BCR	a	834	-	41,41,41	0.74	0	56,56,56	2.05	16 (28%)
29	CLA	i	201	-	65,73,73	1.43	6 (9%)	76,113,113	1.42	7 (9%)
38	UIX	F	305	-	41,49,49	1.27	3 (7%)	52,74,74	2.89	19 (36%)
29	CLA	a	826	-	65,73,73	1.48	6 (9%)	76,113,113	1.40	8 (10%)
29	CLA	N	308	-	47,55,73	1.75	6 (12%)	54,91,113	1.53	7 (12%)
29	CLA	T	313	-	46,54,73	1.76	6 (13%)	53,90,113	1.55	6 (11%)
37	PID	P	206	-	41,49,49	1.36	4 (9%)	49,76,76	1.79	8 (16%)
37	PID	T	304	-	41,49,49	1.33	4 (9%)	49,76,76	1.45	5 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
29	CLA	b	717	-	65,73,73	1.48	6 (9%)	76,113,113	1.37	9 (11%)
29	CLA	a	818	-	47,55,73	1.74	6 (12%)	54,91,113	1.53	8 (14%)
29	CLA	a	820	-	65,73,73	1.47	8 (12%)	76,113,113	1.36	7 (9%)
29	CLA	a	837	-	55,63,73	1.60	6 (10%)	64,101,113	1.40	7 (10%)
29	CLA	a	815	-	45,53,73	1.75	7 (15%)	52,89,113	1.63	8 (15%)
37	PID	O	307	-	41,49,49	1.33	4 (9%)	49,76,76	1.45	7 (14%)
29	CLA	D	311	-	46,54,73	1.72	6 (13%)	53,90,113	1.58	7 (13%)
39	KC1	M	305	-	48,53,53	1.52	7 (14%)	55,89,89	1.89	12 (21%)
29	CLA	a	821	-	47,55,73	1.73	6 (12%)	54,91,113	1.53	7 (12%)
29	CLA	M	309	-	46,54,73	1.76	6 (13%)	53,90,113	1.53	7 (13%)
29	CLA	Q	312	-	46,54,73	1.74	6 (13%)	53,90,113	1.54	7 (13%)
29	CLA	I	201	29	45,53,73	1.77	6 (13%)	52,89,113	1.62	6 (11%)
39	KC1	T	310	-	48,53,53	1.53	7 (14%)	55,89,89	1.79	10 (18%)
40	SQD	B	317	-	41,42,54	0.44	1 (2%)	50,53,65	0.50	0
32	BCR	b	728	-	41,41,41	0.78	1 (2%)	56,56,56	2.04	15 (26%)
29	CLA	P	217	-	41,49,73	1.84	6 (14%)	47,84,113	1.74	7 (14%)
32	BCR	f	804	-	41,41,41	0.74	0	56,56,56	1.98	16 (28%)
29	CLA	L	311	19	46,54,73	1.75	6 (13%)	53,90,113	1.49	7 (13%)
30	PQN	b	727	-	34,34,34	1.54	2 (5%)	42,45,45	1.19	3 (7%)
29	CLA	A	215	-	47,55,73	1.72	7 (14%)	54,91,113	1.55	6 (11%)
29	CLA	b	713	-	53,61,73	1.65	5 (9%)	61,98,113	1.45	6 (9%)
39	KC1	T	315	25	48,53,53	1.51	7 (14%)	55,89,89	1.83	10 (18%)
29	CLA	a	824	-	65,73,73	1.46	7 (10%)	76,113,113	1.37	7 (9%)
29	CLA	M	310	18	48,56,73	1.71	6 (12%)	55,92,113	1.55	7 (12%)
29	CLA	F	313	16	46,54,73	1.75	6 (13%)	53,90,113	1.59	6 (11%)
29	CLA	N	313	23	46,54,73	1.72	6 (13%)	53,90,113	4.81	10 (18%)
36	DD6	Q	302	-	39,45,45	1.99	3 (7%)	52,67,67	1.86	12 (23%)
29	CLA	a	808	-	51,59,73	1.67	8 (15%)	59,96,113	1.50	8 (13%)
29	CLA	I	212	-	55,63,73	1.61	6 (10%)	64,101,113	6.83	13 (20%)
36	DD6	B	302	-	39,45,45	2.06	3 (7%)	52,67,67	1.92	13 (25%)
37	PID	P	203	-	41,49,49	1.36	4 (9%)	49,76,76	1.45	8 (16%)
29	CLA	A	218	12	60,68,73	1.52	7 (11%)	70,107,113	1.46	8 (11%)
36	DD6	E	303	-	39,45,45	2.02	3 (7%)	52,67,67	1.74	10 (19%)
36	DD6	G	305	-	39,45,45	2.20	3 (7%)	52,67,67	2.96	17 (32%)
29	CLA	G	312	13	65,73,73	1.47	8 (12%)	76,113,113	1.39	8 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
37	PID	N	302	-	41,49,49	1.36	4 (9%)	49,76,76	1.41	5 (10%)
36	DD6	B	305	-	39,45,45	2.02	3 (7%)	52,67,67	1.91	16 (30%)
37	PID	O	305	-	41,49,49	1.35	4 (9%)	49,76,76	1.59	7 (14%)
29	CLA	E	314	28	48,56,73	1.72	7 (14%)	55,92,113	1.54	7 (12%)
36	DD6	C	303	-	39,45,45	2.07	3 (7%)	52,67,67	2.04	15 (28%)
29	CLA	b	716	-	53,61,73	1.62	7 (13%)	61,98,113	1.53	8 (13%)
36	DD6	B	319	-	39,45,45	2.09	3 (7%)	52,67,67	2.26	16 (30%)
37	PID	D	307	-	41,49,49	1.35	4 (9%)	49,76,76	1.59	7 (14%)
37	PID	F	306	-	41,49,49	1.35	4 (9%)	49,76,76	1.47	6 (12%)
29	CLA	a	810	1	55,63,73	1.61	7 (12%)	64,101,113	1.46	8 (12%)
36	DD6	M	304	-	39,45,45	2.05	3 (7%)	52,67,67	1.76	13 (25%)
37	PID	Q	301	-	41,49,49	1.34	4 (9%)	49,76,76	1.47	6 (12%)
29	CLA	a	825	-	65,73,73	1.49	8 (12%)	76,113,113	1.48	9 (11%)
37	PID	P	205	-	41,49,49	1.34	4 (9%)	49,76,76	1.54	6 (12%)
29	CLA	a	811	-	56,64,73	1.62	6 (10%)	65,102,113	1.43	7 (10%)
37	PID	F	304	-	41,49,49	1.61	5 (12%)	49,76,76	1.57	7 (14%)
29	CLA	H	315	-	41,49,73	1.84	6 (14%)	47,84,113	1.66	8 (17%)
29	CLA	P	212	-	51,59,73	1.68	6 (11%)	59,96,113	1.50	8 (13%)
38	UIX	J	304	-	41,49,49	1.26	3 (7%)	52,74,74	2.40	13 (25%)
29	CLA	b	708	2	52,60,73	1.66	7 (13%)	60,97,113	1.55	8 (13%)
36	DD6	J	302	-	39,45,45	2.08	2 (5%)	52,67,67	2.19	17 (32%)
29	CLA	J	309	17	46,54,73	1.72	6 (13%)	53,90,113	1.61	6 (11%)
35	DGD	h	203	-	55,55,67	0.90	2 (3%)	69,69,81	0.98	3 (4%)
29	CLA	B	306	21	49,57,73	1.70	6 (12%)	55,93,113	1.55	8 (14%)
29	CLA	H	310	-	51,59,73	1.69	6 (11%)	59,96,113	1.54	8 (13%)
29	CLA	G	311	13	51,59,73	1.64	6 (11%)	59,96,113	1.50	7 (11%)
29	CLA	F	307	-	46,54,73	1.74	6 (13%)	53,90,113	1.56	7 (13%)
29	CLA	b	724	-	47,55,73	1.73	9 (19%)	54,91,113	1.54	8 (14%)
29	CLA	L	317	-	46,54,73	1.75	6 (13%)	53,90,113	1.55	6 (11%)
37	PID	Q	306	-	41,49,49	1.33	4 (9%)	49,76,76	1.52	6 (12%)
29	CLA	a	804	-	55,63,73	1.62	7 (12%)	64,101,113	1.54	9 (14%)
30	PQN	a	832	-	34,34,34	1.52	2 (5%)	42,45,45	1.23	5 (11%)
39	KC1	B	313	21	48,53,53	1.53	7 (14%)	55,89,89	1.86	12 (21%)
37	PID	G	310	-	41,49,49	1.33	4 (9%)	49,76,76	1.45	7 (14%)
39	KC1	N	310	-	48,53,53	1.52	7 (14%)	55,89,89	1.86	10 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
34	LMG	h	205	-	28,28,55	1.02	1 (3%)	36,36,63	1.27	4 (11%)
29	CLA	T	314	-	47,55,73	1.73	5 (10%)	54,91,113	1.66	9 (16%)
29	CLA	D	308	-	47,55,73	1.73	6 (12%)	54,91,113	1.55	7 (12%)
35	DGD	j	106	-	50,50,67	0.97	2 (4%)	64,64,81	1.04	4 (6%)
34	LMG	b	732	-	44,44,55	0.80	1 (2%)	52,52,63	1.32	6 (11%)
39	KC1	Q	314	26	48,53,53	1.54	7 (14%)	55,89,89	1.87	10 (18%)
39	KC1	Q	309	-	48,53,53	1.54	7 (14%)	55,89,89	1.88	11 (20%)
39	KC1	P	216	-	48,53,53	1.51	7 (14%)	55,89,89	1.84	9 (16%)
39	KC1	P	213	27	48,53,53	1.52	7 (14%)	55,89,89	1.78	12 (21%)
35	DGD	m	102	-	67,67,67	0.83	2 (2%)	81,81,81	0.91	4 (4%)
29	CLA	O	309	-	65,73,73	1.51	6 (9%)	76,113,113	1.34	6 (7%)
29	CLA	G	317	-	53,61,73	1.62	7 (13%)	61,98,113	1.47	6 (9%)
29	CLA	E	309	-	46,54,73	1.76	6 (13%)	53,90,113	1.56	7 (13%)
29	CLA	a	816	-	46,54,73	1.73	7 (15%)	53,90,113	1.56	7 (13%)
29	CLA	I	211	-	65,73,73	1.44	7 (10%)	76,113,113	1.43	8 (10%)
29	CLA	G	319	13	41,49,73	1.81	6 (14%)	47,84,113	1.69	7 (14%)
29	CLA	K	212	-	52,60,73	1.69	7 (13%)	60,97,113	1.50	9 (15%)
37	PID	H	304	-	41,49,49	1.34	4 (9%)	49,76,76	1.63	5 (10%)
29	CLA	Q	310	-	65,73,73	1.48	6 (9%)	76,113,113	1.39	8 (10%)
29	CLA	Q	308	-	65,73,73	1.48	7 (10%)	76,113,113	1.41	8 (10%)
29	CLA	Q	313	-	47,55,73	1.73	6 (12%)	54,91,113	1.53	7 (12%)
39	KC1	N	315	-	48,53,53	1.50	6 (12%)	55,89,89	1.81	10 (18%)
29	CLA	H	313	-	47,55,73	1.74	6 (12%)	54,91,113	1.64	8 (14%)
29	CLA	O	316	-	41,49,73	1.85	6 (14%)	47,84,113	1.68	7 (14%)
35	DGD	G	320	-	46,46,67	1.01	2 (4%)	60,60,81	0.98	3 (5%)
29	CLA	K	209	-	54,62,73	1.61	7 (12%)	62,99,113	1.50	9 (14%)
29	CLA	N	316	-	41,49,73	1.85	6 (14%)	47,84,113	1.66	7 (14%)
29	CLA	A	217	-	51,59,73	1.66	6 (11%)	59,96,113	1.49	8 (13%)
29	CLA	O	308	-	47,55,73	1.76	6 (12%)	54,91,113	1.55	7 (12%)
29	CLA	b	710	-	46,54,73	1.74	7 (15%)	53,90,113	1.53	7 (13%)
29	CLA	a	823	-	58,66,73	1.54	7 (12%)	67,104,113	1.48	8 (11%)
29	CLA	l	510	-	45,53,73	1.80	6 (13%)	52,89,113	1.54	8 (15%)
32	BCR	b	729	-	41,41,41	0.79	1 (2%)	56,56,56	1.88	20 (35%)
37	PID	C	302	-	41,49,49	1.34	4 (9%)	49,76,76	1.44	6 (12%)
29	CLA	E	305	-	61,69,73	1.54	6 (9%)	71,108,113	1.45	7 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
36	DD6	E	302	-	39,45,45	2.11	3 (7%)	52,67,67	2.26	18 (34%)
38	UIX	T	306	-	41,49,49	1.29	4 (9%)	52,74,74	2.77	24 (46%)
39	KC1	C	312	-	48,53,53	1.54	7 (14%)	55,89,89	1.87	12 (21%)
37	PID	D	302	-	41,49,49	1.34	4 (9%)	49,76,76	1.45	5 (10%)
37	PID	N	307	-	41,49,49	1.36	4 (9%)	49,76,76	1.59	9 (18%)
38	UIX	C	306	-	41,49,49	1.27	4 (9%)	52,74,74	2.55	22 (42%)
29	CLA	I	207	14	49,57,73	1.68	7 (14%)	55,93,113	1.59	7 (12%)
39	KC1	L	314	-	48,53,53	1.55	7 (14%)	55,89,89	1.86	11 (20%)
29	CLA	N	314	-	47,55,73	1.72	7 (14%)	54,91,113	1.61	7 (12%)
29	CLA	D	309	-	46,54,73	1.74	6 (13%)	53,90,113	1.57	6 (11%)
35	DGD	B	318	-	46,46,67	1.00	2 (4%)	60,60,81	1.32	10 (16%)
29	CLA	a	817	-	45,53,73	1.80	6 (13%)	52,89,113	1.55	7 (13%)
29	CLA	M	307	-	55,63,73	1.60	7 (12%)	64,101,113	1.44	7 (10%)
36	DD6	D	304	-	39,45,45	2.09	4 (10%)	52,67,67	2.14	15 (28%)
33	SF4	c	102	3	0,12,12	-	-	-		
29	CLA	E	306	28	65,73,73	1.47	7 (10%)	76,113,113	1.38	7 (9%)
39	KC1	E	307	-	48,53,53	1.52	7 (14%)	55,89,89	1.87	11 (20%)
29	CLA	L	312	-	55,63,73	1.58	6 (10%)	64,101,113	1.45	7 (10%)
39	KC1	O	312	-	48,53,53	1.48	7 (14%)	55,89,89	1.98	11 (20%)
29	CLA	f	805	-	60,68,73	1.53	6 (10%)	70,107,113	1.40	7 (10%)
36	DD6	A	202	-	39,45,45	1.97	3 (7%)	52,67,67	1.81	10 (19%)
37	PID	C	305	-	41,49,49	1.36	4 (9%)	49,76,76	1.95	9 (18%)
29	CLA	K	217	-	46,54,73	1.76	8 (17%)	53,90,113	1.55	6 (11%)
36	DD6	I	204	-	39,45,45	2.19	5 (12%)	52,67,67	2.08	16 (30%)
36	DD6	M	301	-	39,45,45	2.00	3 (7%)	52,67,67	1.85	15 (28%)
39	KC1	G	318	-	48,53,53	1.56	7 (14%)	55,89,89	1.83	10 (18%)
29	CLA	E	311	-	65,73,73	1.46	7 (10%)	76,113,113	1.43	9 (11%)
34	LMG	K	219	-	35,35,55	0.92	1 (2%)	43,43,63	1.19	4 (9%)
36	DD6	H	303	-	39,45,45	1.94	3 (7%)	52,67,67	1.98	14 (26%)
37	PID	T	302	-	41,49,49	1.38	4 (9%)	49,76,76	1.51	8 (16%)
37	PID	D	305	-	41,49,49	1.32	4 (9%)	49,76,76	1.48	7 (14%)
29	CLA	J	307	-	46,54,73	1.73	7 (15%)	53,90,113	1.52	6 (11%)
29	CLA	M	306	-	53,61,73	1.62	6 (11%)	61,98,113	1.51	7 (11%)
29	CLA	A	214	12	41,49,73	1.83	6 (14%)	47,84,113	1.62	7 (14%)
29	CLA	M	308	-	48,56,73	1.71	7 (14%)	55,92,113	1.52	6 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
29	CLA	b	714	-	64,72,73	1.47	7 (10%)	74,111,113	1.40	9 (12%)
36	DD6	P	204	-	39,45,45	1.99	3 (7%)	52,67,67	2.19	15 (28%)
29	CLA	L	308	-	53,61,73	1.62	6 (11%)	61,98,113	5.52	10 (16%)
32	BCR	f	801	-	41,41,41	0.71	0	56,56,56	2.03	17 (30%)
33	SF4	c	101	3	0,12,12	-	-	-		
36	DD6	L	304	-	39,45,45	2.02	3 (7%)	52,67,67	1.98	17 (32%)
29	CLA	O	311	-	51,59,73	1.67	6 (11%)	59,96,113	1.52	7 (11%)
39	KC1	M	312	-	48,53,53	1.53	7 (14%)	55,89,89	1.89	11 (20%)
29	CLA	K	211	-	55,63,73	1.58	7 (12%)	64,101,113	1.51	10 (15%)
38	UIX	Q	305	-	41,49,49	1.26	4 (9%)	52,74,74	2.78	22 (42%)
29	CLA	B	307	-	45,53,73	1.78	6 (13%)	52,89,113	1.58	7 (13%)
29	CLA	G	313	-	55,63,73	1.57	6 (10%)	64,101,113	1.50	7 (10%)
29	CLA	I	217	-	55,63,73	1.61	6 (10%)	64,101,113	1.45	7 (10%)
29	CLA	j	104	29	52,60,73	1.64	7 (13%)	60,97,113	1.57	7 (11%)
33	SF4	a	836	2,1	0,12,12	-	-	-		
39	KC1	T	312	-	48,53,53	1.50	7 (14%)	55,89,89	1.84	10 (18%)
29	CLA	O	313	24	46,54,73	1.73	6 (13%)	53,90,113	1.59	6 (11%)
29	CLA	C	311	-	51,59,73	1.65	6 (11%)	59,96,113	1.54	8 (13%)
36	DD6	B	301	-	38,44,45	2.03	3 (7%)	50,65,67	2.00	14 (28%)
29	CLA	i	202	-	65,73,73	1.45	7 (10%)	76,113,113	1.38	8 (10%)
39	KC1	J	312	17	48,53,53	1.52	7 (14%)	55,89,89	1.84	10 (18%)
36	DD6	L	303	-	39,45,45	2.06	3 (7%)	52,67,67	1.73	13 (25%)
37	PID	H	301	-	41,49,49	1.34	4 (9%)	49,76,76	1.48	5 (10%)
29	CLA	b	705	-	65,73,73	1.45	8 (12%)	76,113,113	1.45	7 (9%)
36	DD6	I	203	-	39,45,45	2.29	3 (7%)	52,67,67	2.41	17 (32%)
29	CLA	Q	315	-	41,49,73	1.84	7 (17%)	47,84,113	1.69	7 (14%)
37	PID	T	301	-	41,49,49	1.34	4 (9%)	49,76,76	1.49	5 (10%)
34	LMG	b	730	-	46,46,55	0.81	2 (4%)	54,54,63	1.32	5 (9%)
37	PID	H	305	-	41,49,49	1.33	4 (9%)	49,76,76	1.75	8 (16%)
37	PID	E	301	-	41,49,49	1.39	4 (9%)	49,76,76	1.95	9 (18%)
29	CLA	l	504	-	65,73,73	1.46	6 (9%)	76,113,113	4.11	11 (14%)
34	LMG	K	220	-	36,36,55	0.86	1 (2%)	44,44,63	1.23	4 (9%)
29	CLA	T	311	-	46,54,73	1.74	5 (10%)	53,90,113	1.56	7 (13%)
36	DD6	K	203	-	39,45,45	2.04	3 (7%)	52,67,67	1.90	13 (25%)
29	CLA	B	308	-	65,73,73	1.47	7 (10%)	76,113,113	1.40	10 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
35	DGD	j	103	-	44,44,67	0.99	2 (4%)	58,58,81	1.32	9 (15%)
37	PID	H	306	-	41,49,49	1.31	4 (9%)	49,76,76	1.46	6 (12%)
34	LMG	P	201	-	27,27,55	0.98	0	35,35,63	1.29	5 (14%)
29	CLA	D	312	20	46,54,73	1.76	6 (13%)	53,90,113	1.53	6 (11%)
39	KC1	N	312	23	48,53,53	1.52	7 (14%)	55,89,89	1.86	12 (21%)
39	KC1	F	314	-	48,53,53	1.50	7 (14%)	55,89,89	1.87	10 (18%)
36	DD6	D	301	-	39,45,45	2.08	3 (7%)	52,67,67	2.07	15 (28%)
36	DD6	K	202	-	39,45,45	2.15	3 (7%)	52,67,67	3.00	16 (30%)
36	DD6	T	303	-	39,45,45	1.98	3 (7%)	52,67,67	1.97	15 (28%)
36	DD6	K	205	-	39,45,45	2.05	3 (7%)	52,67,67	1.91	17 (32%)
38	UIX	O	306	-	41,49,49	1.25	3 (7%)	52,74,74	2.70	21 (40%)
29	CLA	H	307	-	47,55,73	1.74	6 (12%)	54,91,113	1.52	7 (12%)
29	CLA	a	819	-	57,65,73	1.58	7 (12%)	66,103,113	1.44	9 (13%)
37	PID	N	304	-	41,49,49	1.34	4 (9%)	49,76,76	1.48	5 (10%)
29	CLA	A	211	-	55,63,73	1.57	6 (10%)	64,101,113	1.45	7 (10%)
29	CLA	J	310	-	47,55,73	1.71	6 (12%)	54,91,113	1.59	7 (12%)
40	SQD	J	314	-	44,45,54	0.42	1 (2%)	53,56,65	0.61	2 (3%)
29	CLA	E	313	-	41,49,73	1.85	6 (14%)	47,84,113	1.67	7 (14%)
39	KC1	L	306	29	48,53,53	1.55	7 (14%)	55,89,89	1.90	14 (25%)
36	DD6	K	204	-	39,45,45	2.08	3 (7%)	52,67,67	1.95	18 (34%)
34	LMG	j	102	-	43,43,55	0.78	0	51,51,63	1.29	5 (9%)
29	CLA	B	311	21	51,59,73	1.66	7 (13%)	59,96,113	1.52	7 (11%)
39	KC1	Q	311	-	48,53,53	1.53	7 (14%)	55,89,89	1.85	11 (20%)
36	DD6	m	101	-	39,45,45	2.04	3 (7%)	52,67,67	2.04	16 (30%)
29	CLA	b	712	-	65,73,73	1.47	7 (10%)	76,113,113	4.09	11 (14%)

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
39	KC1	G	315	-	-	6/15/71/71	-
37	PID	P	208	-	-	4/24/93/93	0/4/4/4
32	BCR	m	103	-	-	5/29/63/63	0/2/2/2
36	DD6	B	303	-	-	0/26/80/80	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	CLA	b	719	-	1/1/12/20	10/19/97/115	-
29	CLA	A	206	39	1/1/11/20	3/13/91/115	-
29	CLA	a	827	-	1/1/15/20	12/37/115/115	-
29	CLA	a	829	-	1/1/15/20	16/37/115/115	-
36	DD6	I	206	-	-	2/26/80/80	0/3/3/3
29	CLA	G	316	-	1/1/15/20	12/37/115/115	-
29	CLA	F	308	-	1/1/11/20	3/15/93/115	-
29	CLA	G	302	-	1/1/15/20	15/37/115/115	-
32	BCR	l	506	-	-	9/29/63/63	0/2/2/2
29	CLA	M	314	-	1/1/12/20	7/22/100/115	-
32	BCR	b	735	-	-	4/29/63/63	0/2/2/2
39	KC1	E	312	28	-	7/15/71/71	-
29	CLA	a	807	-	1/1/15/20	16/37/115/115	-
29	CLA	I	210	-	1/1/13/20	6/25/103/115	-
29	CLA	A	209	-	1/1/15/20	20/37/115/115	-
37	PID	N	301	-	-	4/24/93/93	0/4/4/4
39	KC1	A	213	-	-	7/15/71/71	-
39	KC1	O	310	-	-	6/15/71/71	-
36	DD6	J	303	-	-	2/26/80/80	0/3/3/3
36	DD6	N	303	-	-	1/26/80/80	0/3/3/3
29	CLA	P	215	-	1/1/11/20	7/16/94/115	-
29	CLA	C	313	25	1/1/11/20	5/15/93/115	-
29	CLA	h	201	-	1/1/14/20	7/31/109/115	-
29	CLA	A	208	-	1/1/13/20	3/25/103/115	-
36	DD6	I	205	-	-	6/26/80/80	0/3/3/3
29	CLA	G	314	-	1/1/14/20	8/31/109/115	-
29	CLA	D	313	20	1/1/11/20	4/13/91/115	-
36	DD6	G	308	-	-	1/26/80/80	0/3/3/3
36	DD6	h	202	-	-	2/26/80/80	0/3/3/3
29	CLA	b	701	-	1/1/15/20	13/37/115/115	-
37	PID	T	305	-	-	0/24/93/93	0/4/4/4
29	CLA	T	308	-	1/1/11/20	2/16/94/115	-
29	CLA	a	809	1	1/1/15/20	17/37/115/115	-
37	PID	T	317	-	-	10/24/93/93	1/4/4/4
39	KC1	H	314	-	-	6/15/71/71	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	CLA	B	312	-	1/1/15/20	10/37/115/115	-
38	UIX	E	304	-	-	2/31/87/87	0/3/3/3
29	CLA	f	803	6	1/1/11/20	8/15/93/115	-
29	CLA	L	309	-	1/1/13/20	2/25/103/115	-
29	CLA	a	806	1	1/1/15/20	16/37/115/115	-
29	CLA	a	801	-	1/1/15/20	10/37/115/115	-
29	CLA	l	509	-	1/1/10/20	2/8/86/115	-
32	BCR	l	507	-	-	5/29/63/63	0/2/2/2
29	CLA	E	308	-	1/1/15/20	10/37/115/115	-
29	CLA	P	214	27	1/1/11/20	7/15/93/115	-
29	CLA	B	315	-	1/1/11/20	3/15/93/115	-
29	CLA	O	314	-	-	6/16/94/115	-
29	CLA	H	312	22	1/1/11/20	7/15/93/115	-
29	CLA	K	216	-	1/1/10/20	3/8/86/115	-
29	CLA	B	310	-	1/1/15/20	16/37/115/115	-
39	KC1	C	315	25	-	8/15/71/71	-
36	DD6	I	202	-	-	5/26/80/80	0/3/3/3
39	KC1	C	310	-	-	9/15/71/71	-
39	KC1	A	205	29	-	6/15/71/71	-
29	CLA	F	311	-	1/1/11/20	3/15/93/115	-
39	KC1	D	315	-	-	6/15/71/71	-
32	BCR	a	835	-	-	2/29/63/63	0/2/2/2
29	CLA	b	721	-	1/1/13/20	10/29/107/115	-
29	CLA	b	702	-	1/1/15/20	17/37/115/115	-
29	CLA	C	316	-	1/1/10/20	6/8/86/115	-
36	DD6	L	305	-	-	4/26/80/80	0/3/3/3
29	CLA	b	706	-	1/1/15/20	11/37/115/115	-
29	CLA	l	502	10	1/1/15/20	13/37/115/115	-
29	CLA	L	310	-	1/1/13/20	9/25/103/115	-
39	KC1	K	215	-	-	6/15/71/71	-
29	CLA	D	316	-	1/1/10/20	5/8/86/115	-
37	PID	O	301	-	-	3/24/93/93	0/4/4/4
29	CLA	T	309	25	1/1/11/20	4/15/93/115	-
29	CLA	b	723	-	1/1/15/20	5/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
36	DD6	F	303	-	-	0/26/80/80	0/3/3/3
29	CLA	a	802	-	1/1/15/20	10/37/115/115	-
36	DD6	K	221	-	-	5/26/80/80	0/3/3/3
29	CLA	F	312	16	1/1/11/20	5/15/93/115	-
37	PID	D	303	-	-	1/24/93/93	0/4/4/4
39	KC1	H	309	-	-	8/15/71/71	-
36	DD6	G	307	-	-	2/26/80/80	0/3/3/3
29	CLA	A	212	-	1/1/13/20	10/25/103/115	-
38	UIX	L	302	-	-	2/31/87/87	0/3/3/3
29	CLA	T	316	-	1/1/10/20	6/8/86/115	-
29	CLA	b	722	-	1/1/13/20	8/29/107/115	-
29	CLA	b	731	-	1/1/13/20	3/27/105/115	-
29	CLA	K	210	-	1/1/12/20	6/19/97/115	-
39	KC1	D	310	-	-	5/15/71/71	-
36	DD6	J	301	-	-	3/26/80/80	0/3/3/3
34	LMG	K	201	-	-	17/38/58/70	0/1/1/1
38	UIX	N	306	-	-	9/31/87/87	0/3/3/3
29	CLA	F	310	-	1/1/11/20	8/15/93/115	-
29	CLA	I	216	-	1/1/12/20	4/22/100/115	-
29	CLA	K	218	-	1/1/11/20	7/13/91/115	-
29	CLA	L	316	-	1/1/12/20	11/22/100/115	-
29	CLA	b	736	-	1/1/15/20	16/37/115/115	-
29	CLA	a	812	-	1/1/14/20	15/31/109/115	-
29	CLA	A	207	-	1/1/13/20	5/25/103/115	-
37	PID	C	307	-	-	2/24/93/93	0/4/4/4
29	CLA	B	309	-	1/1/13/20	6/25/103/115	-
29	CLA	L	313	-	1/1/12/20	8/23/101/115	-
34	LMG	b	734	-	-	10/35/55/70	0/1/1/1
29	CLA	i	203	-	1/1/13/20	12/25/103/115	-
29	CLA	a	822	-	1/1/15/20	8/37/115/115	-
29	CLA	K	207	15	1/1/11/20	6/18/96/115	-
37	PID	F	302	-	-	3/24/93/93	0/4/4/4
29	CLA	C	314	-	1/1/11/20	7/16/94/115	-
29	CLA	J	305	-	1/1/11/20	2/15/93/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	LHG	a	833	-	-	8/52/52/53	-
35	DGD	b	733	-	-	24/46/86/95	0/2/2/2
37	PID	O	304	-	-	3/24/93/93	0/4/4/4
29	CLA	F	315	-	1/1/10/20	3/8/86/115	-
29	CLA	J	306	-	1/1/15/20	17/37/115/115	-
39	KC1	H	311	-	-	6/15/71/71	-
29	CLA	D	314	-	1/1/11/20	7/16/94/115	-
29	CLA	N	309	-	1/1/15/20	15/37/115/115	-
37	PID	T	307	-	-	4/24/93/93	0/4/4/4
29	CLA	b	725	-	1/1/15/20	9/37/115/115	-
29	CLA	E	315	-	1/1/13/20	6/28/106/115	-
29	CLA	J	308	-	1/1/13/20	8/27/105/115	-
36	DD6	G	306	-	-	1/26/80/80	0/3/3/3
37	PID	h	204	-	-	2/24/93/93	1/4/4/4
29	CLA	f	802	-	1/1/11/20	4/15/93/115	-
29	CLA	l	503	10	1/1/15/20	15/37/115/115	-
29	CLA	M	311	-	1/1/11/20	8/15/93/115	-
36	DD6	F	301	-	-	8/26/80/80	0/3/3/3
36	DD6	K	206	-	-	1/26/80/80	0/3/3/3
29	CLA	J	313	-	1/1/10/20	2/8/86/115	-
38	UIX	P	207	-	-	6/31/87/87	0/3/3/3
29	CLA	b	720	-	1/1/15/20	15/37/115/115	-
29	CLA	a	814	-	1/1/11/20	6/15/93/115	-
37	PID	N	305	-	-	19/24/93/93	0/4/4/4
36	DD6	M	303	-	-	6/26/80/80	0/3/3/3
29	CLA	a	803	-	1/1/15/20	8/37/115/115	-
38	UIX	B	304	-	-	2/31/87/87	0/3/3/3
37	PID	O	302	-	-	2/24/93/93	0/4/4/4
29	CLA	J	311	-	1/1/12/20	8/23/101/115	-
29	CLA	l	508	-	1/1/10/20	2/8/86/115	-
29	CLA	N	311	-	1/1/12/20	6/21/99/115	-
37	PID	j	101	-	-	2/24/93/93	0/4/4/4
36	DD6	A	201	-	-	3/26/80/80	0/3/3/3
37	PID	H	302	-	-	2/24/93/93	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	CLA	b	704	-	1/1/15/20	10/37/115/115	-
29	CLA	b	715	-	1/1/11/20	7/15/93/115	-
29	CLA	l	501	-	1/1/14/20	13/31/109/115	-
39	KC1	P	211	-	-	7/15/71/71	-
29	CLA	H	308	-	1/1/15/20	9/37/115/115	-
36	DD6	O	303	-	-	4/26/80/80	0/3/3/3
29	CLA	E	310	28	1/1/11/20	4/15/93/115	-
37	PID	D	306	-	-	3/24/93/93	0/4/4/4
29	CLA	I	214	-	1/1/13/20	5/25/103/115	-
29	CLA	L	315	-	1/1/10/20	4/8/86/115	-
39	KC1	O	315	-	-	9/15/71/71	-
29	CLA	B	316	-	1/1/11/20	4/13/91/115	-
35	DGD	j	105	-	-	0/30/70/95	0/2/2/2
29	CLA	A	210	12	1/1/11/20	6/15/93/115	-
29	CLA	G	304	-	1/1/13/20	12/30/108/115	-
29	CLA	K	214	-	1/1/13/20	8/25/103/115	-
37	PID	G	303	-	-	6/24/93/93	0/4/4/4
29	CLA	I	209	-	1/1/14/20	14/31/109/115	-
29	CLA	a	813	-	1/1/12/20	10/21/99/115	-
32	BCR	i	204	-	-	4/29/63/63	0/2/2/2
29	CLA	b	726	-	1/1/15/20	6/37/115/115	-
36	DD6	L	301	-	-	4/26/80/80	0/3/3/3
37	PID	P	202	-	-	4/24/93/93	0/4/4/4
37	PID	Q	304	-	-	2/24/93/93	0/4/4/4
29	CLA	b	711	-	1/1/13/20	11/29/107/115	-
29	CLA	F	316	16	1/1/10/20	4/8/86/115	-
29	CLA	I	213	14	1/1/15/20	13/37/115/115	-
29	CLA	C	308	-	1/1/11/20	7/16/94/115	-
29	CLA	a	831	-	1/1/15/20	14/37/115/115	-
29	CLA	B	314	21	1/1/10/20	6/8/86/115	-
29	CLA	C	309	-	1/1/15/20	10/37/115/115	-
36	DD6	A	204	-	-	2/26/80/80	0/3/3/3
37	PID	C	304	-	-	3/24/93/93	0/4/4/4
29	CLA	K	208	-	1/1/11/20	5/15/93/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	CLA	b	707	-	1/1/15/20	11/37/115/115	-
29	CLA	a	805	-	1/1/13/20	6/25/103/115	-
29	CLA	b	703	-	1/1/15/20	13/37/115/115	-
29	CLA	K	213	-	1/1/11/20	5/17/95/115	-
34	LMG	A	219	-	-	17/32/52/70	0/1/1/1
29	CLA	A	216	-	1/1/10/20	0/8/86/115	-
29	CLA	a	830	-	1/1/13/20	5/27/105/115	-
29	CLA	b	718	-	1/1/15/20	14/37/115/115	-
37	PID	Q	303	-	-	0/24/93/93	0/4/4/4
29	CLA	M	315	-	1/1/11/20	5/15/93/115	-
36	DD6	M	302	-	-	1/26/80/80	0/3/3/3
39	KC1	F	309	-	-	7/15/71/71	-
29	CLA	Q	307	-	1/1/11/20	1/16/94/115	-
32	BCR	a	838	-	-	6/29/63/63	0/2/2/2
29	CLA	P	210	-	1/1/15/20	10/37/115/115	-
37	PID	G	309	-	-	2/24/93/93	0/4/4/4
39	KC1	I	215	14	-	10/15/71/71	-
29	CLA	L	307	39	1/1/12/20	9/19/97/115	-
29	CLA	b	709	-	1/1/14/20	17/31/109/115	-
29	CLA	l	505	-	1/1/15/20	12/37/115/115	-
29	CLA	P	209	-	1/1/11/20	8/16/94/115	-
34	LMG	E	316	-	-	10/27/47/70	0/1/1/1
29	CLA	G	301	-	1/1/11/20	6/18/96/115	-
29	CLA	I	208	-	1/1/11/20	7/15/93/115	-
38	UIX	A	203	-	-	4/31/87/87	0/3/3/3
37	PID	C	301	-	-	4/24/93/93	0/4/4/4
29	CLA	a	828	-	1/1/11/20	8/15/93/115	-
29	CLA	M	313	-	1/1/10/20	2/8/86/115	-
32	BCR	a	834	-	-	0/29/63/63	0/2/2/2
29	CLA	i	201	-	1/1/15/20	16/37/115/115	-
38	UIX	F	305	-	-	12/31/87/87	0/3/3/3
29	CLA	a	826	-	1/1/15/20	10/37/115/115	-
29	CLA	N	308	-	1/1/11/20	7/16/94/115	-
29	CLA	T	313	-	1/1/11/20	7/15/93/115	-
37	PID	P	206	-	-	8/24/93/93	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
37	PID	T	304	-	-	1/24/93/93	0/4/4/4
29	CLA	b	717	-	1/1/15/20	14/37/115/115	-
29	CLA	a	818	-	1/1/11/20	4/16/94/115	-
29	CLA	a	820	-	1/1/15/20	10/37/115/115	-
29	CLA	a	837	-	1/1/13/20	12/25/103/115	-
29	CLA	a	815	-	1/1/11/20	4/13/91/115	-
37	PID	O	307	-	-	4/24/93/93	0/4/4/4
29	CLA	D	311	-	1/1/11/20	12/15/93/115	-
39	KC1	M	305	-	-	5/15/71/71	-
29	CLA	a	821	-	1/1/11/20	9/16/94/115	-
29	CLA	M	309	-	1/1/11/20	6/15/93/115	-
29	CLA	Q	312	-	1/1/11/20	3/15/93/115	-
29	CLA	I	201	29	1/1/11/20	4/13/91/115	-
39	KC1	T	310	-	-	5/15/71/71	-
40	SQD	B	317	-	-	4/37/57/69	0/1/1/1
32	BCR	b	728	-	-	7/29/63/63	0/2/2/2
29	CLA	P	217	-	1/1/10/20	3/8/86/115	-
32	BCR	f	804	-	-	2/29/63/63	0/2/2/2
29	CLA	L	311	19	1/1/11/20	7/15/93/115	-
30	PQN	b	727	-	-	4/23/43/43	0/2/2/2
29	CLA	A	215	-	1/1/11/20	4/16/94/115	-
29	CLA	b	713	-	1/1/12/20	4/23/101/115	-
39	KC1	T	315	25	-	5/15/71/71	-
29	CLA	a	824	-	1/1/15/20	9/37/115/115	-
29	CLA	M	310	18	1/1/11/20	5/17/95/115	-
29	CLA	F	313	16	1/1/11/20	6/15/93/115	-
29	CLA	N	313	23	1/1/11/20	9/15/93/115	-
36	DD6	Q	302	-	-	1/26/80/80	0/3/3/3
29	CLA	a	808	-	1/1/12/20	4/21/99/115	-
29	CLA	I	212	-	1/1/13/20	10/25/103/115	-
36	DD6	B	302	-	-	2/26/80/80	0/3/3/3
37	PID	P	203	-	-	3/24/93/93	0/4/4/4
29	CLA	A	218	12	1/1/14/20	10/31/109/115	-
36	DD6	E	303	-	-	1/26/80/80	0/3/3/3
36	DD6	G	305	-	-	7/26/80/80	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	CLA	G	312	13	1/1/15/20	16/37/115/115	-
37	PID	N	302	-	-	2/24/93/93	0/4/4/4
36	DD6	B	305	-	-	2/26/80/80	0/3/3/3
37	PID	O	305	-	-	7/24/93/93	0/4/4/4
29	CLA	E	314	28	-	5/17/95/115	-
36	DD6	C	303	-	-	0/26/80/80	0/3/3/3
29	CLA	b	716	-	1/1/12/20	7/23/101/115	-
36	DD6	B	319	-	-	9/26/80/80	0/3/3/3
37	PID	D	307	-	-	4/24/93/93	0/4/4/4
37	PID	F	306	-	-	0/24/93/93	0/4/4/4
29	CLA	a	810	1	1/1/13/20	10/25/103/115	-
36	DD6	M	304	-	-	3/26/80/80	0/3/3/3
37	PID	Q	301	-	-	2/24/93/93	0/4/4/4
29	CLA	a	825	-	1/1/15/20	13/37/115/115	-
37	PID	P	205	-	-	1/24/93/93	0/4/4/4
29	CLA	a	811	-	1/1/13/20	6/27/105/115	-
37	PID	F	304	-	-	15/24/93/93	1/4/4/4
29	CLA	H	315	-	1/1/10/20	3/8/86/115	-
29	CLA	P	212	-	1/1/12/20	8/21/99/115	-
38	UIX	J	304	-	-	3/31/87/87	0/3/3/3
29	CLA	b	708	2	1/1/12/20	5/22/100/115	-
36	DD6	J	302	-	-	2/26/80/80	0/3/3/3
29	CLA	J	309	17	1/1/11/20	5/15/93/115	-
35	DGD	h	203	-	-	8/43/83/95	0/2/2/2
29	CLA	B	306	21	1/1/11/20	5/18/96/115	-
29	CLA	H	310	-	1/1/12/20	9/21/99/115	-
29	CLA	G	311	13	1/1/12/20	7/21/99/115	-
29	CLA	F	307	-	1/1/11/20	2/15/93/115	-
29	CLA	b	724	-	1/1/11/20	2/16/94/115	-
29	CLA	L	317	-	1/1/11/20	5/15/93/115	-
37	PID	Q	306	-	-	3/24/93/93	0/4/4/4
29	CLA	a	804	-	1/1/13/20	1/25/103/115	-
30	PQN	a	832	-	-	6/23/43/43	0/2/2/2
39	KC1	B	313	21	-	8/15/71/71	-
37	PID	G	310	-	-	2/24/93/93	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
39	KC1	N	310	-	-	6/15/71/71	-
34	LMG	h	205	-	-	3/23/43/70	0/1/1/1
29	CLA	T	314	-	1/1/11/20	7/16/94/115	-
29	CLA	D	308	-	1/1/11/20	5/16/94/115	-
35	DGD	j	106	-	-	16/38/78/95	0/2/2/2
34	LMG	b	732	-	-	20/39/59/70	0/1/1/1
39	KC1	Q	314	26	-	8/15/71/71	-
39	KC1	Q	309	-	-	7/15/71/71	-
39	KC1	P	216	-	-	6/15/71/71	-
39	KC1	P	213	27	-	5/15/71/71	-
35	DGD	m	102	-	-	8/55/95/95	0/2/2/2
29	CLA	O	309	-	-	10/37/115/115	-
29	CLA	G	317	-	1/1/12/20	8/23/101/115	-
29	CLA	E	309	-	1/1/11/20	8/15/93/115	-
29	CLA	a	816	-	1/1/11/20	8/15/93/115	-
29	CLA	I	211	-	1/1/15/20	8/37/115/115	-
29	CLA	G	319	13	1/1/10/20	3/8/86/115	-
29	CLA	K	212	-	1/1/12/20	5/22/100/115	-
37	PID	H	304	-	-	0/24/93/93	0/4/4/4
29	CLA	Q	310	-	1/1/15/20	13/37/115/115	-
29	CLA	Q	308	-	1/1/15/20	21/37/115/115	-
29	CLA	Q	313	-	1/1/11/20	6/16/94/115	-
39	KC1	N	315	-	-	9/15/71/71	-
29	CLA	H	313	-	1/1/11/20	8/16/94/115	-
29	CLA	O	316	-	1/1/10/20	5/8/86/115	-
35	DGD	G	320	-	-	9/34/74/95	0/2/2/2
29	CLA	K	209	-	1/1/12/20	10/24/102/115	-
29	CLA	N	316	-	1/1/10/20	5/8/86/115	-
29	CLA	A	217	-	1/1/12/20	7/21/99/115	-
29	CLA	O	308	-	1/1/11/20	6/16/94/115	-
29	CLA	b	710	-	1/1/11/20	7/15/93/115	-
29	CLA	a	823	-	1/1/13/20	11/29/107/115	-
29	CLA	l	510	-	1/1/11/20	5/13/91/115	-
32	BCR	b	729	-	-	6/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
37	PID	C	302	-	-	2/24/93/93	0/4/4/4
29	CLA	E	305	-	1/1/14/20	14/33/111/115	-
36	DD6	E	302	-	-	2/26/80/80	0/3/3/3
38	UIX	T	306	-	-	4/31/87/87	0/3/3/3
39	KC1	C	312	-	-	8/15/71/71	-
37	PID	D	302	-	-	1/24/93/93	0/4/4/4
37	PID	N	307	-	-	6/24/93/93	0/4/4/4
38	UIX	C	306	-	-	6/31/87/87	0/3/3/3
29	CLA	I	207	14	1/1/11/20	6/18/96/115	-
39	KC1	L	314	-	-	7/15/71/71	-
29	CLA	N	314	-	1/1/11/20	7/16/94/115	-
29	CLA	D	309	-	1/1/11/20	2/15/93/115	-
35	DGD	B	318	-	-	9/34/74/95	0/2/2/2
29	CLA	a	817	-	1/1/11/20	4/13/91/115	-
29	CLA	M	307	-	1/1/13/20	6/25/103/115	-
36	DD6	D	304	-	-	6/26/80/80	0/3/3/3
33	SF4	c	102	3	-	-	0/6/5/5
29	CLA	E	306	28	1/1/15/20	14/37/115/115	-
39	KC1	E	307	-	-	6/15/71/71	-
29	CLA	L	312	-	1/1/13/20	11/25/103/115	-
39	KC1	O	312	-	-	4/15/71/71	-
29	CLA	f	805	-	1/1/14/20	10/31/109/115	-
36	DD6	A	202	-	-	1/26/80/80	0/3/3/3
37	PID	C	305	-	-	9/24/93/93	0/4/4/4
29	CLA	K	217	-	1/1/11/20	4/15/93/115	-
36	DD6	I	204	-	-	3/26/80/80	0/3/3/3
36	DD6	M	301	-	-	2/26/80/80	0/3/3/3
39	KC1	G	318	-	-	5/15/71/71	-
29	CLA	E	311	-	1/1/15/20	11/37/115/115	-
34	LMG	K	219	-	-	16/30/50/70	0/1/1/1
36	DD6	H	303	-	-	1/26/80/80	0/3/3/3
37	PID	T	302	-	-	1/24/93/93	0/4/4/4
37	PID	D	305	-	-	5/24/93/93	0/4/4/4
29	CLA	J	307	-	1/1/11/20	3/15/93/115	-
29	CLA	M	306	-	1/1/12/20	6/23/101/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	CLA	A	214	12	1/1/10/20	4/8/86/115	-
29	CLA	M	308	-	1/1/11/20	9/17/95/115	-
29	CLA	b	714	-	1/1/14/20	6/36/114/115	-
36	DD6	P	204	-	-	2/26/80/80	0/3/3/3
29	CLA	L	308	-	1/1/12/20	10/23/101/115	-
32	BCR	f	801	-	-	5/29/63/63	0/2/2/2
33	SF4	c	101	3	-	-	0/6/5/5
36	DD6	L	304	-	-	2/26/80/80	0/3/3/3
29	CLA	O	311	-	1/1/12/20	3/21/99/115	-
39	KC1	M	312	-	-	6/15/71/71	-
29	CLA	K	211	-	1/1/13/20	7/25/103/115	-
38	UIX	Q	305	-	-	5/31/87/87	0/3/3/3
29	CLA	B	307	-	1/1/11/20	2/13/91/115	-
29	CLA	G	313	-	1/1/13/20	3/25/103/115	-
29	CLA	I	217	-	1/1/13/20	9/25/103/115	-
29	CLA	j	104	29	1/1/12/20	4/22/100/115	-
33	SF4	a	836	2,1	-	-	0/6/5/5
39	KC1	T	312	-	-	5/15/71/71	-
29	CLA	O	313	24	1/1/11/20	5/15/93/115	-
29	CLA	C	311	-	1/1/12/20	7/21/99/115	-
36	DD6	B	301	-	-	4/24/78/80	0/3/3/3
29	CLA	i	202	-	1/1/15/20	12/37/115/115	-
39	KC1	J	312	17	-	5/15/71/71	-
36	DD6	L	303	-	-	0/26/80/80	0/3/3/3
37	PID	H	301	-	-	2/24/93/93	0/4/4/4
29	CLA	b	705	-	1/1/15/20	12/37/115/115	-
36	DD6	I	203	-	-	7/26/80/80	0/3/3/3
29	CLA	Q	315	-	1/1/10/20	6/8/86/115	-
37	PID	T	301	-	-	2/24/93/93	0/4/4/4
34	LMG	b	730	-	-	19/41/61/70	0/1/1/1
37	PID	H	305	-	-	3/24/93/93	0/4/4/4
37	PID	E	301	-	-	6/24/93/93	0/4/4/4
29	CLA	l	504	-	1/1/15/20	10/37/115/115	-
34	LMG	K	220	-	-	13/31/51/70	0/1/1/1
29	CLA	T	311	-	1/1/11/20	10/15/93/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
36	DD6	K	203	-	-	6/26/80/80	0/3/3/3
29	CLA	B	308	-	1/1/15/20	13/37/115/115	-
35	DGD	j	103	-	-	10/32/72/95	0/2/2/2
37	PID	H	306	-	-	4/24/93/93	0/4/4/4
34	LMG	P	201	-	-	6/22/42/70	0/1/1/1
29	CLA	D	312	20	1/1/11/20	5/15/93/115	-
39	KC1	N	312	23	-	6/15/71/71	-
39	KC1	F	314	-	-	6/15/71/71	-
36	DD6	D	301	-	-	8/26/80/80	0/3/3/3
36	DD6	K	202	-	-	8/26/80/80	0/3/3/3
36	DD6	T	303	-	-	7/26/80/80	0/3/3/3
36	DD6	K	205	-	-	1/26/80/80	0/3/3/3
38	UIX	O	306	-	-	6/31/87/87	0/3/3/3
29	CLA	H	307	-	1/1/11/20	5/16/94/115	-
29	CLA	a	819	-	1/1/13/20	6/28/106/115	-
37	PID	N	304	-	-	1/24/93/93	0/4/4/4
29	CLA	A	211	-	1/1/13/20	5/25/103/115	-
29	CLA	J	310	-	1/1/11/20	6/16/94/115	-
40	SQD	J	314	-	-	9/40/60/69	0/1/1/1
29	CLA	E	313	-	1/1/10/20	2/8/86/115	-
39	KC1	L	306	29	-	5/15/71/71	-
36	DD6	K	204	-	-	5/26/80/80	0/3/3/3
34	LMG	j	102	-	-	24/38/58/70	0/1/1/1
29	CLA	B	311	21	1/1/12/20	4/21/99/115	-
39	KC1	Q	311	-	-	6/15/71/71	-
36	DD6	m	101	-	-	1/26/80/80	0/3/3/3
29	CLA	b	712	-	1/1/15/20	12/37/115/115	-

The worst 5 of 2170 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 3687 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

5 of 220 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
29	a	801	CLA	ND
29	a	802	CLA	ND
29	a	803	CLA	ND
29	a	804	CLA	ND
29	a	805	CLA	ND

5 of 2704 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:

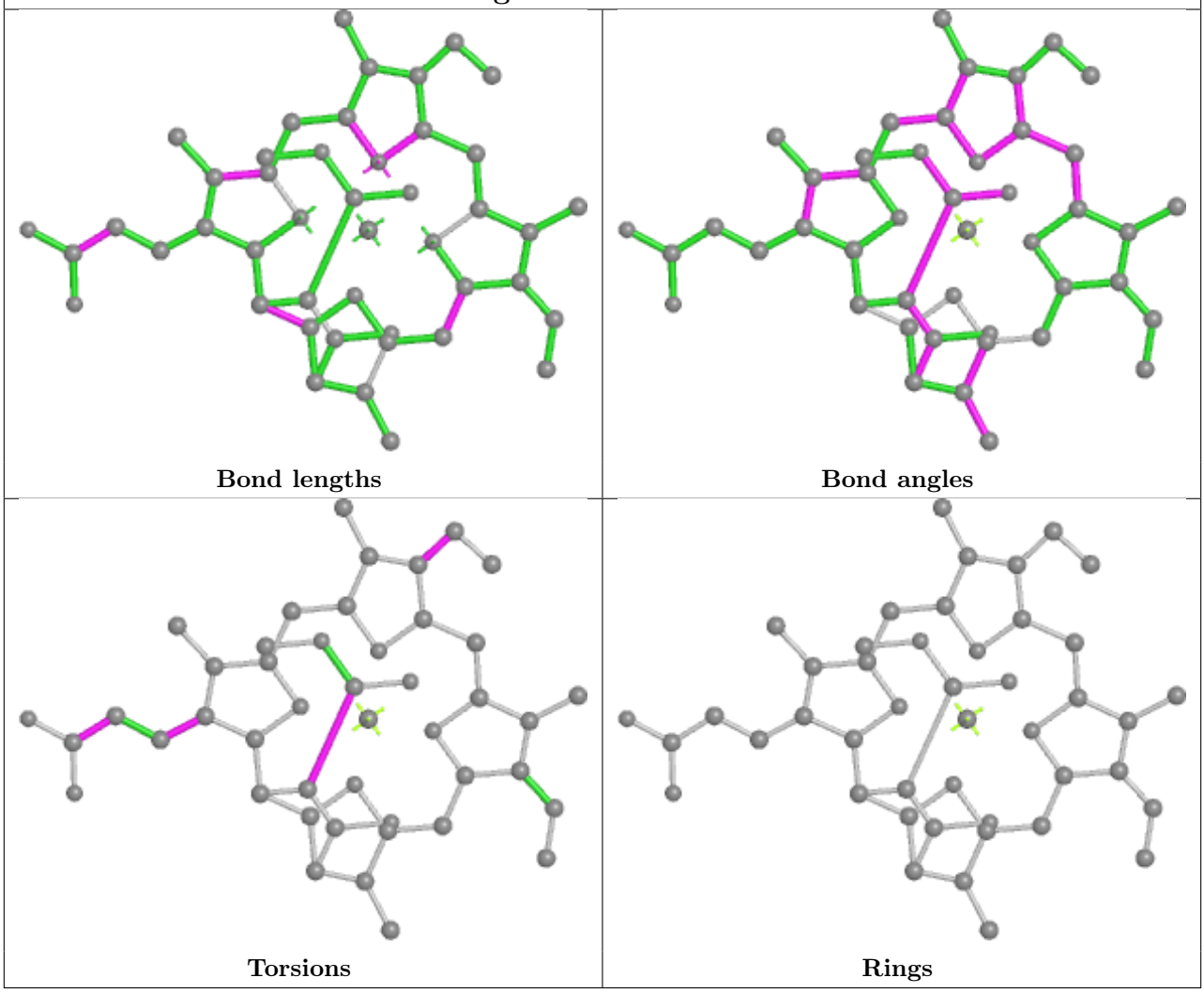
Mol	Chain	Res	Type	Atoms
37	h	204	PID	C24-C25-C26-C27-C28-C29
37	T	317	PID	C24-C25-C26-C27-C28-C29
37	F	304	PID	C24-C25-C26-C27-C28-C29

No monomer is involved in short contacts.

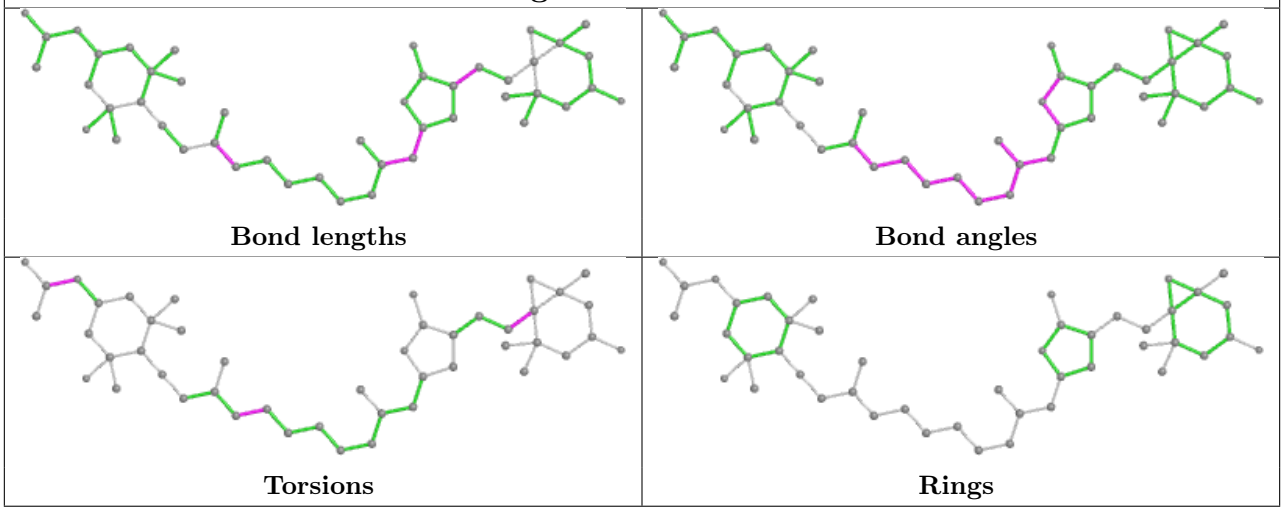
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

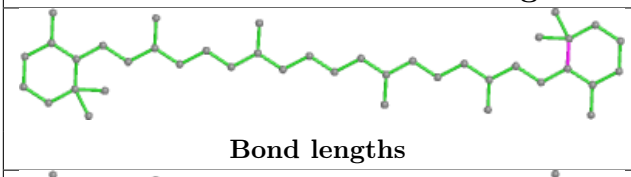
Ligand KC1 G 315



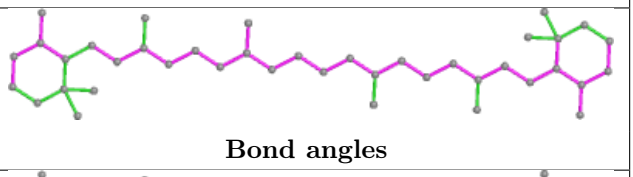
Ligand PID P 208



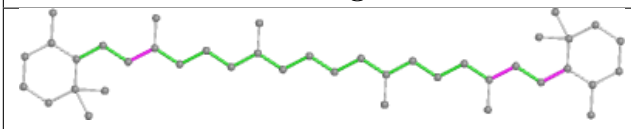
Ligand BCR m 103



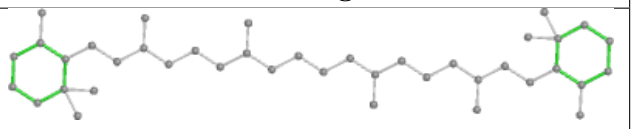
Bond lengths



Bond angles

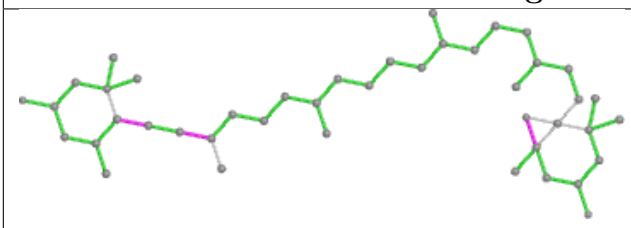


Torsions

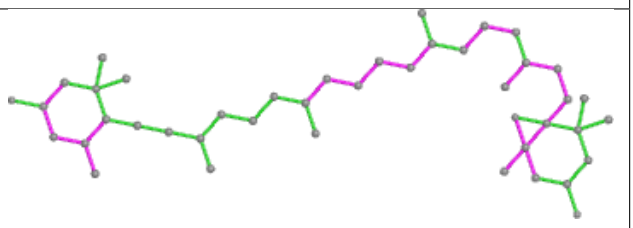


Rings

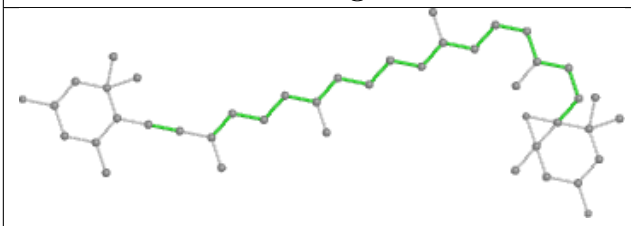
Ligand DD6 B 303



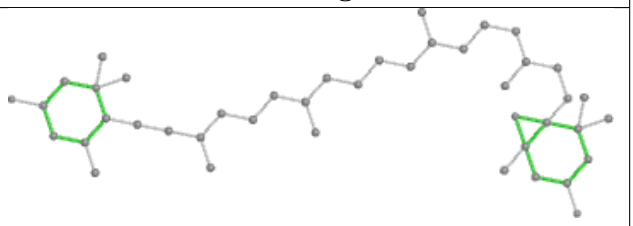
Bond lengths



Bond angles

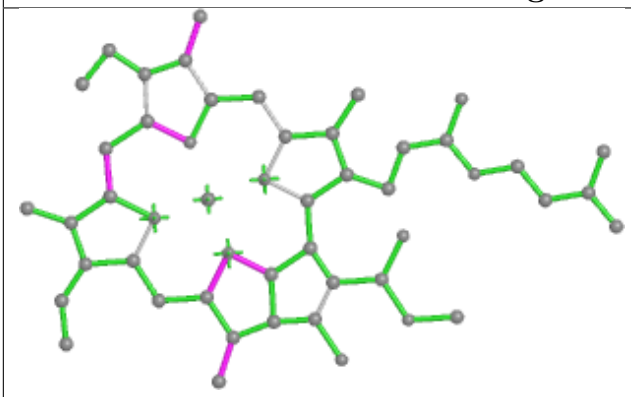


Torsions

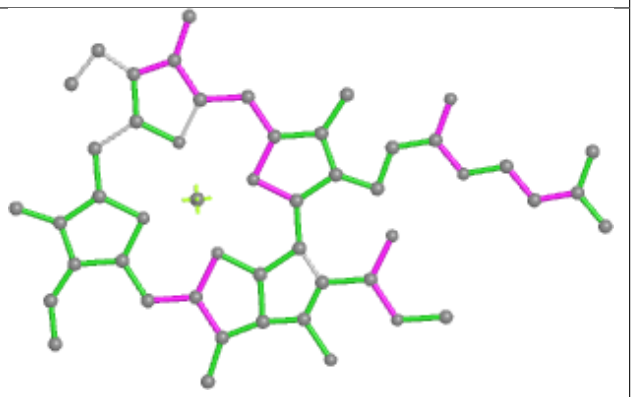


Rings

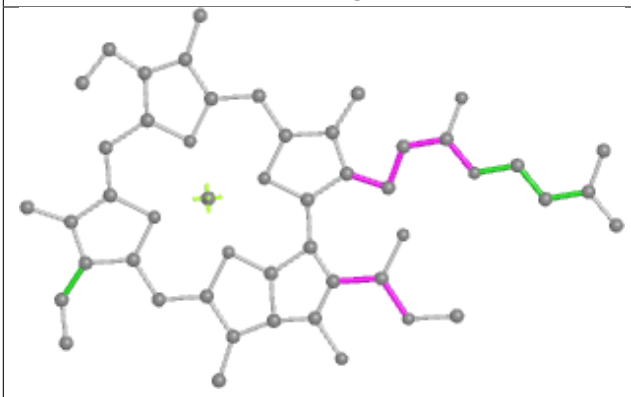
Ligand CLA b 719



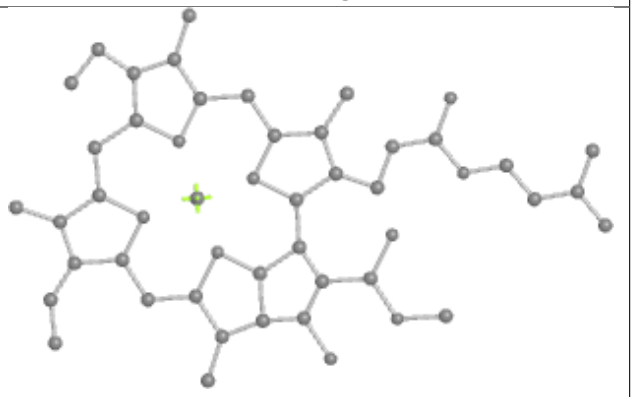
Bond lengths



Bond angles

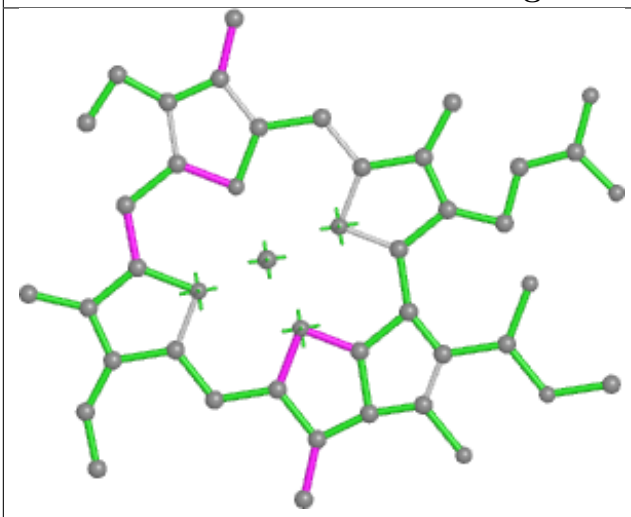


Torsions

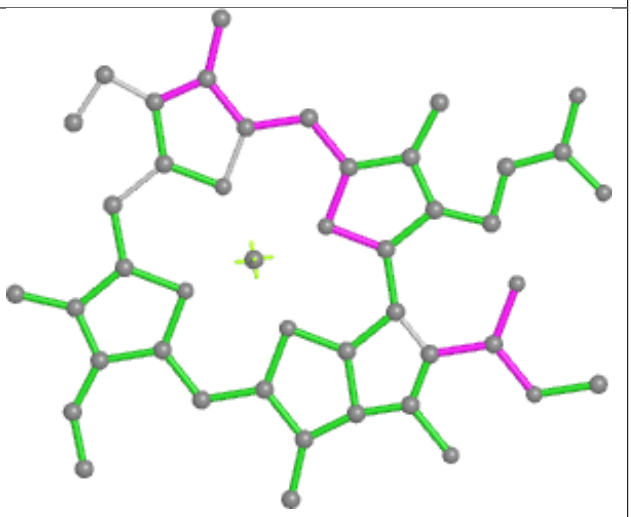


Rings

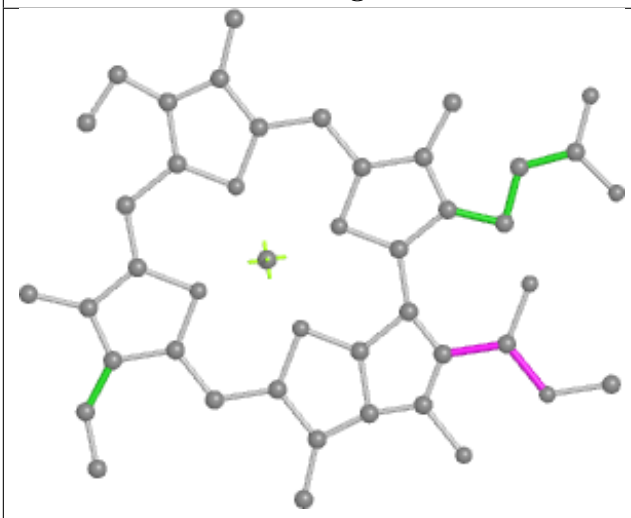
Ligand CLA A 206



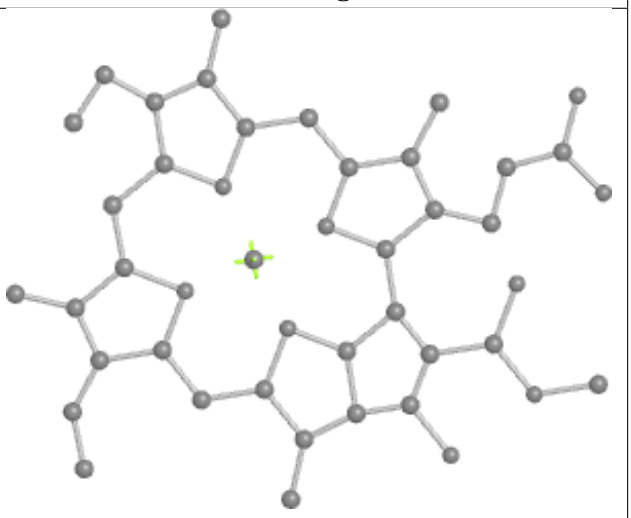
Bond lengths



Bond angles

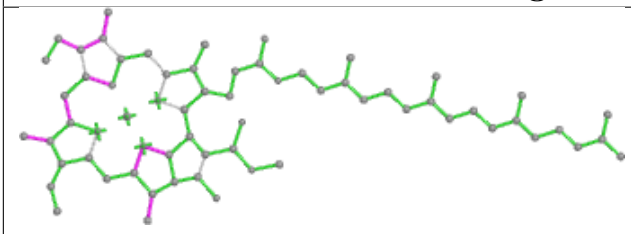


Torsions



Rings

Ligand CLA a 827



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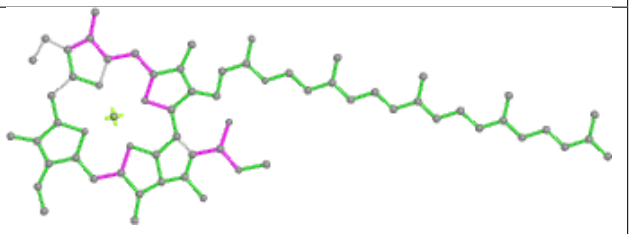
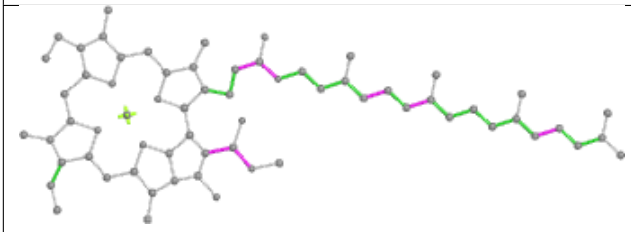
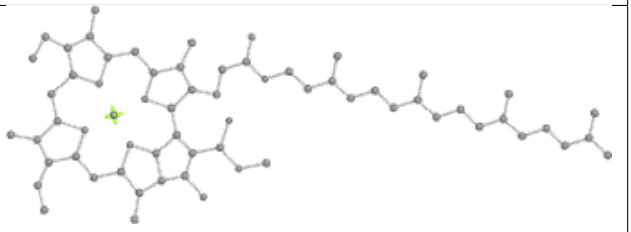


Bond angles

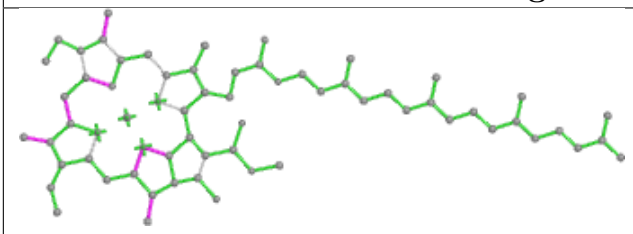


Torsions

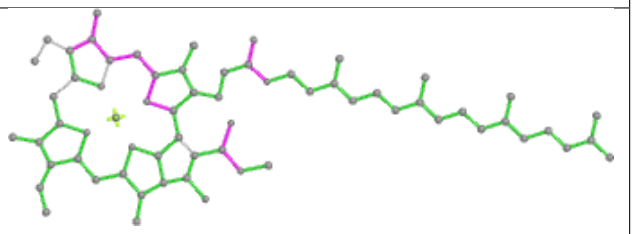


Rings

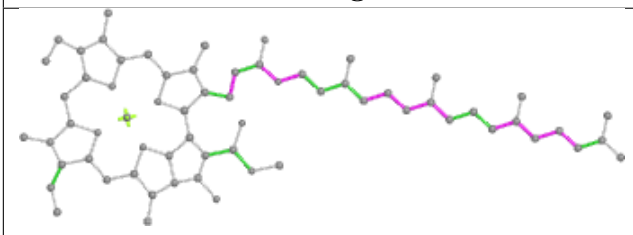
Ligand CLA a 829



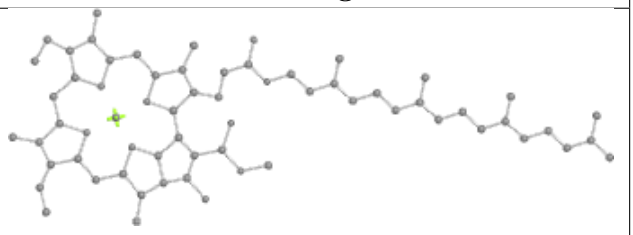
Bond lengths



Bond angles

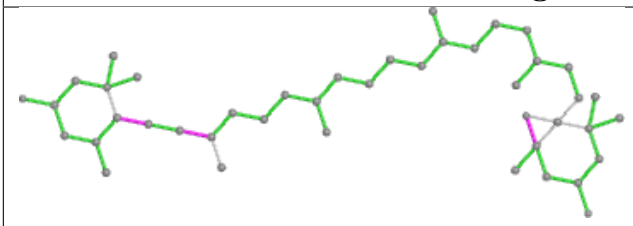


Torsions

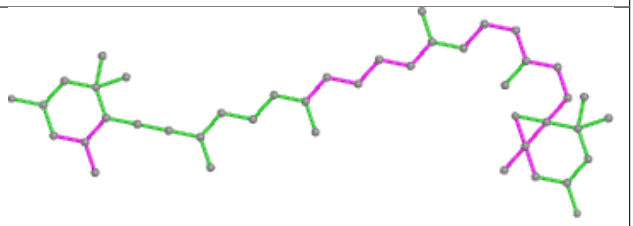


Rings

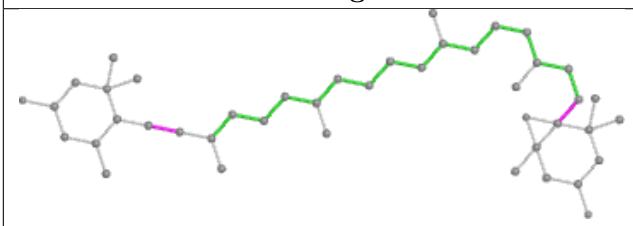
Ligand DD6 I 206



Bond lengths



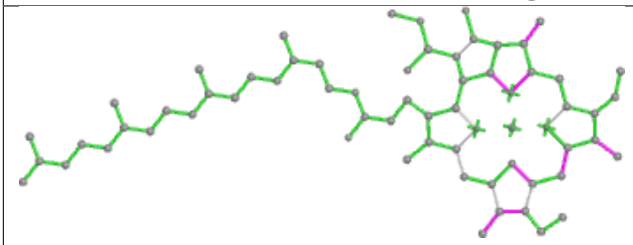
Bond angles



Torsions

Rings

Ligand CLA G 316



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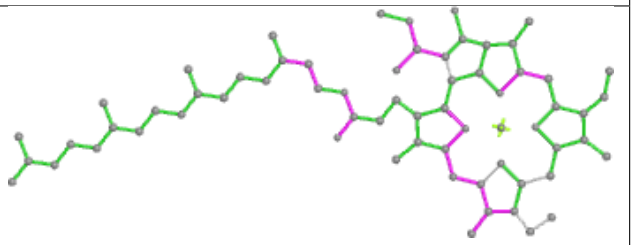
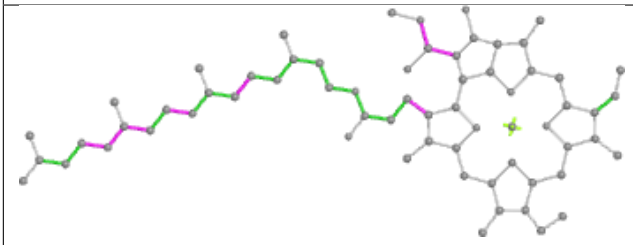


Bond angles



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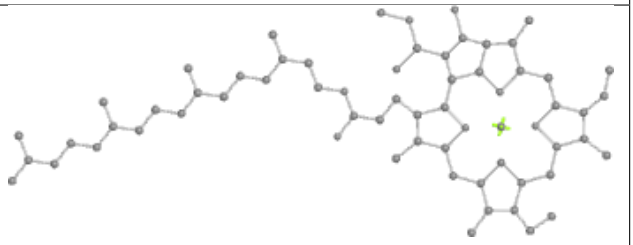
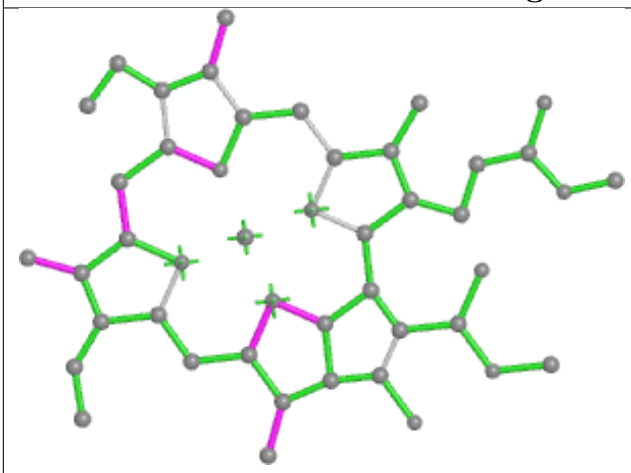


Rings

Ligand CLA F 308



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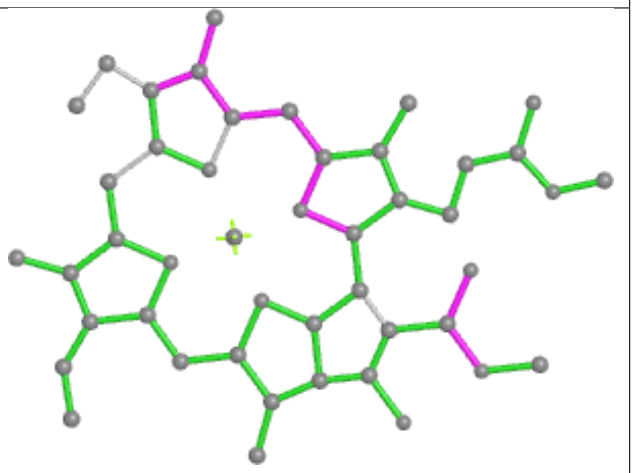
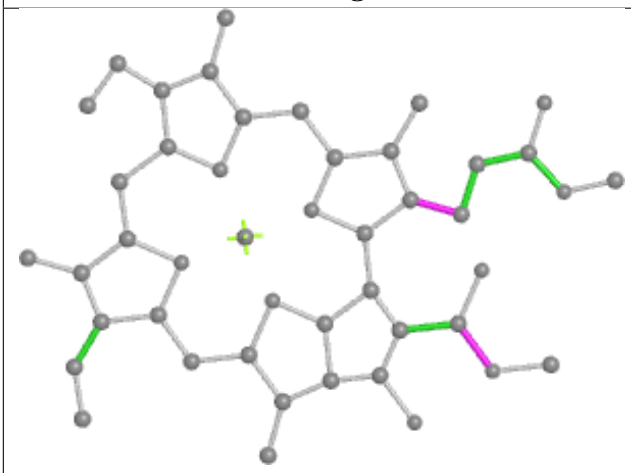


Bond angles



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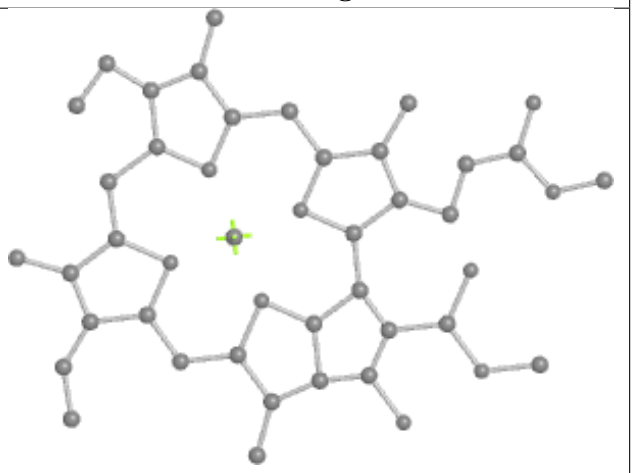
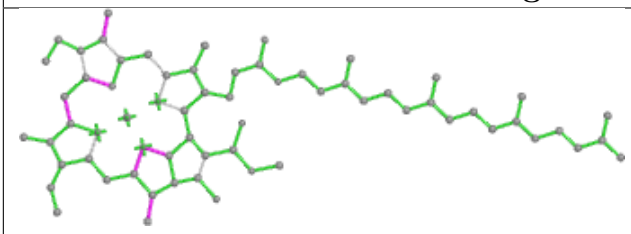


Rings

Ligand CLA G 302



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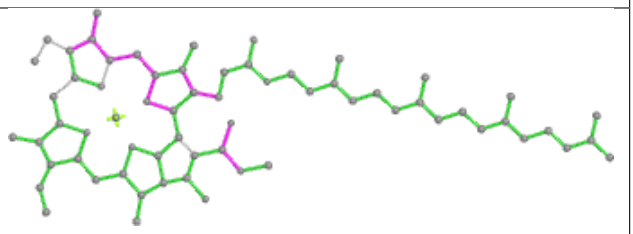
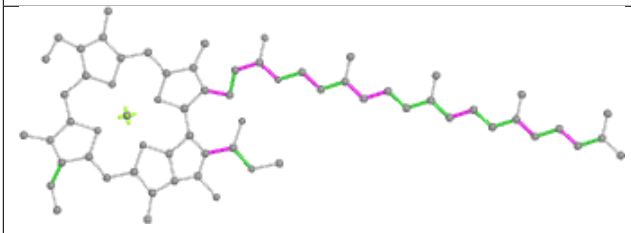


Bond angles



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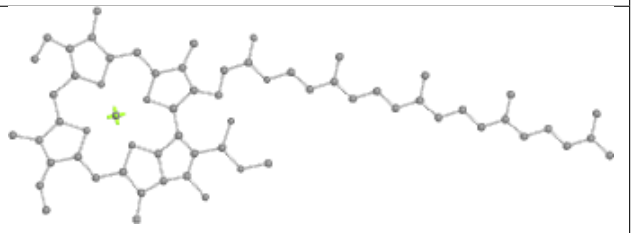
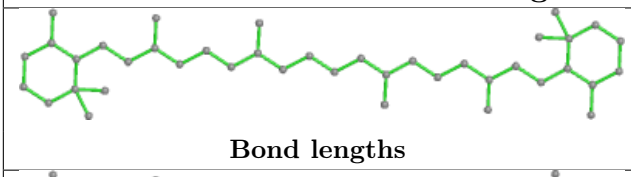
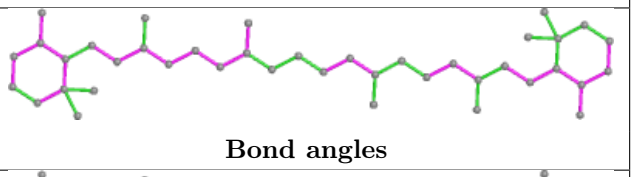


Rings

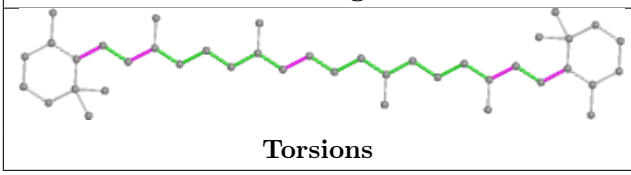
Ligand BCR l 506



Bond lengths



Bond angles



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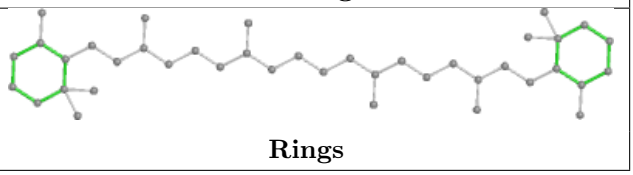
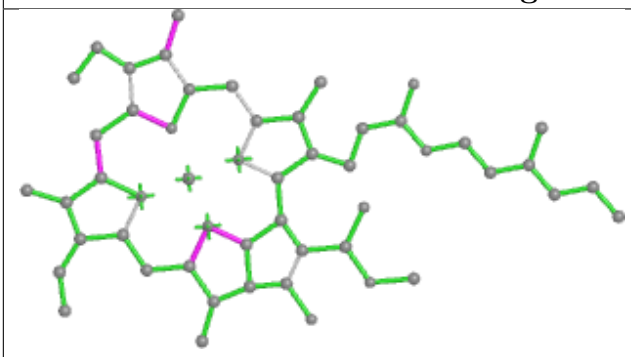


Rings

Ligand CLA M 314



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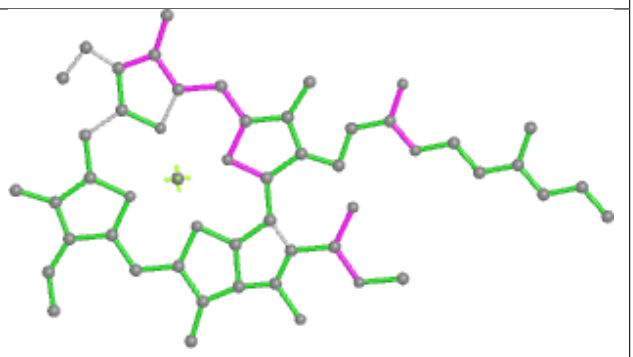
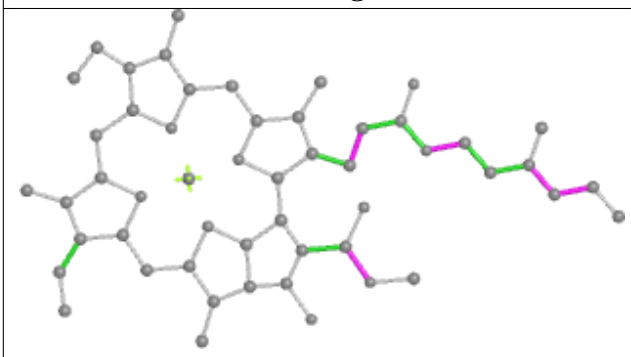
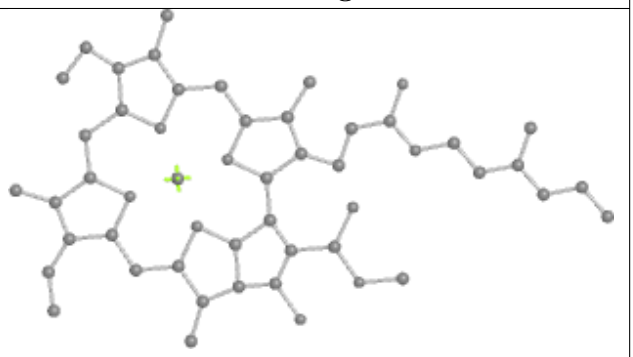


Bond angles

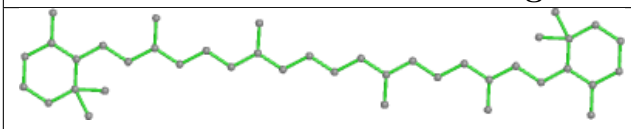


Torsions



Rings

Ligand BCR b 735



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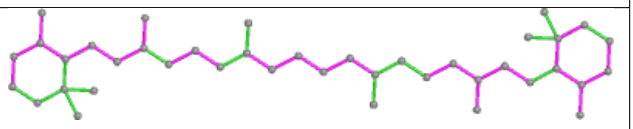
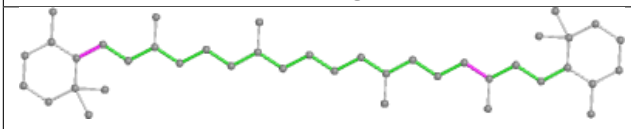
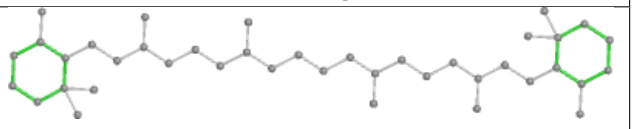


Bond angles

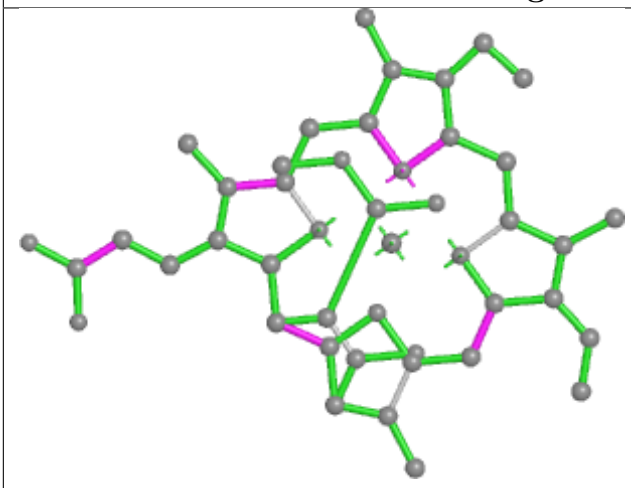


Torsions



Rings

Ligand KC1 E 312



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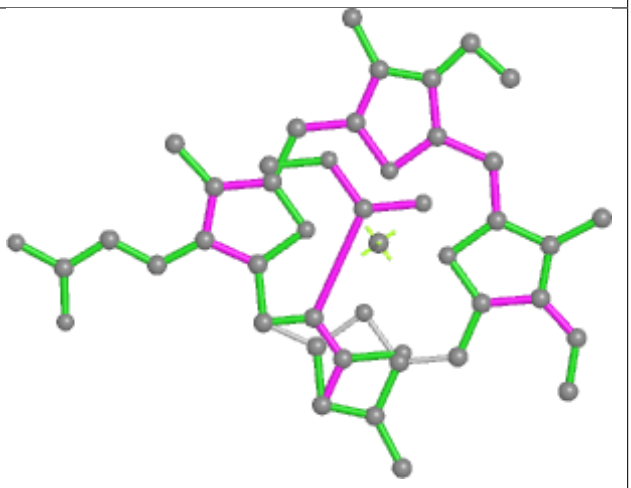
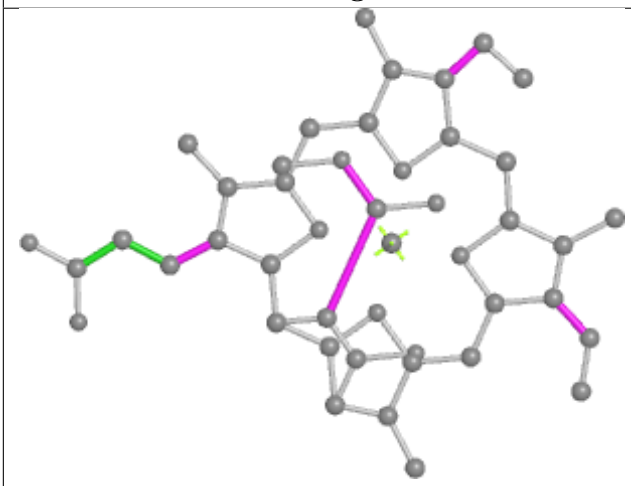
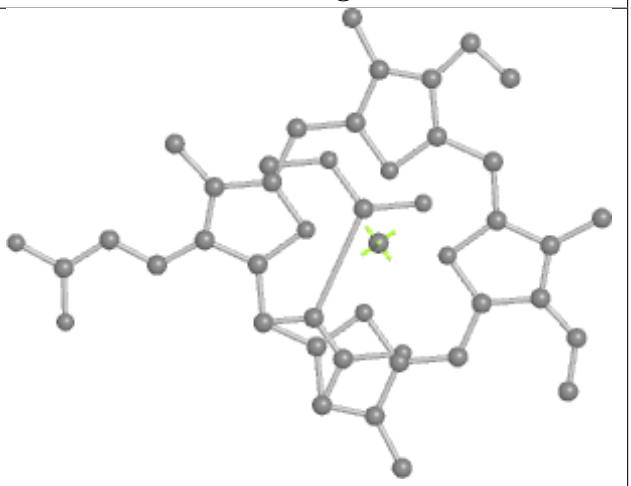


Bond angles

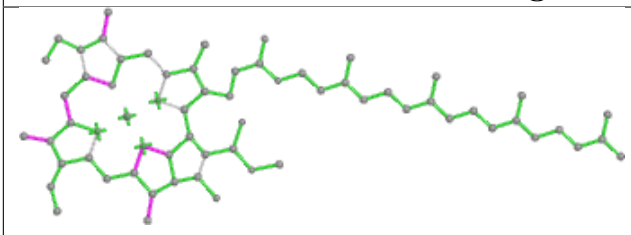


Torsions

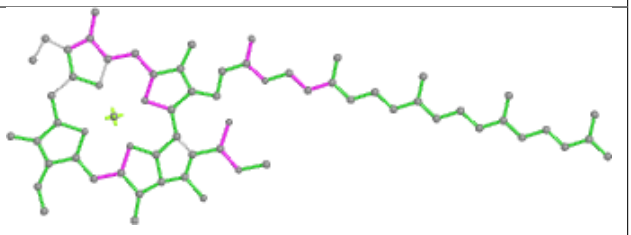


Rings

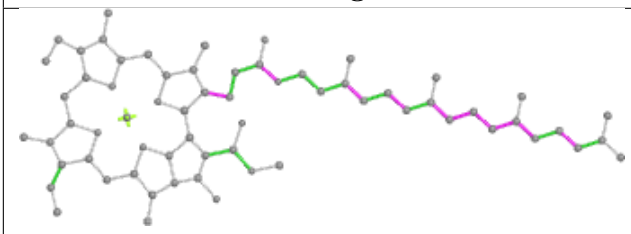
Ligand CLA a 807



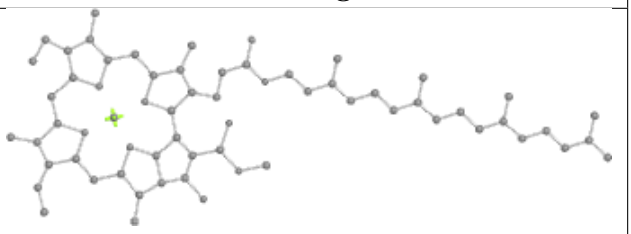
Bond lengths



Bond angles

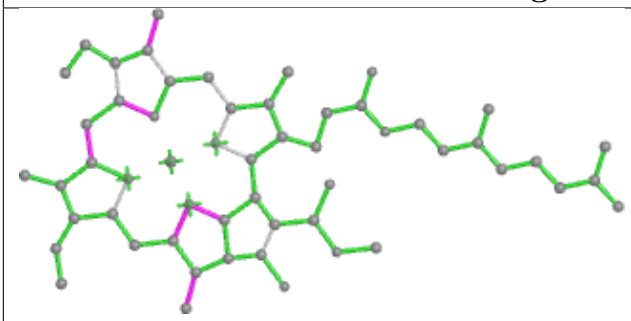


Torsions

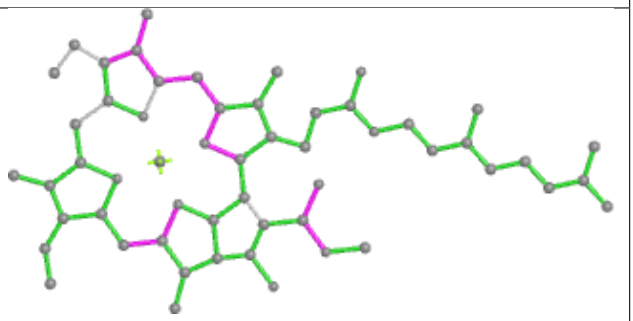


Rings

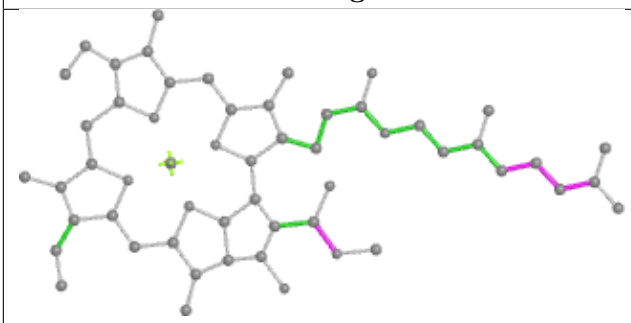
Ligand CLA I 210



Bond lengths



Bond angles



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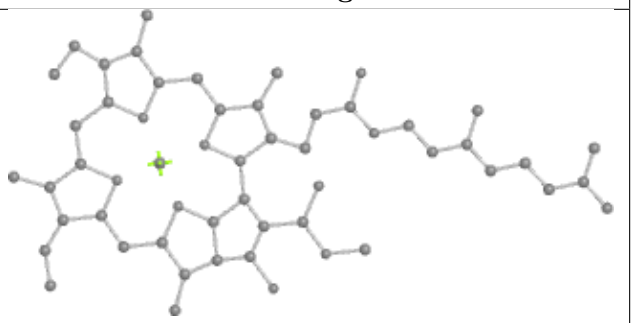
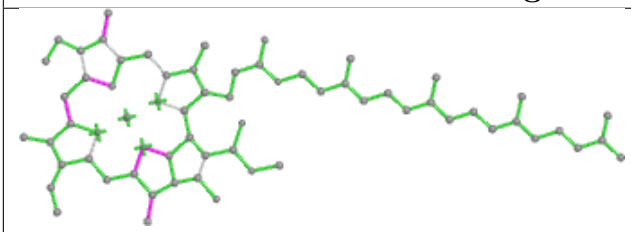
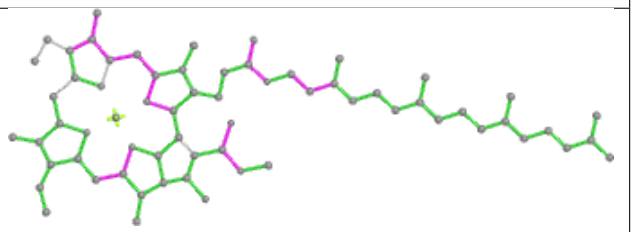


Rings

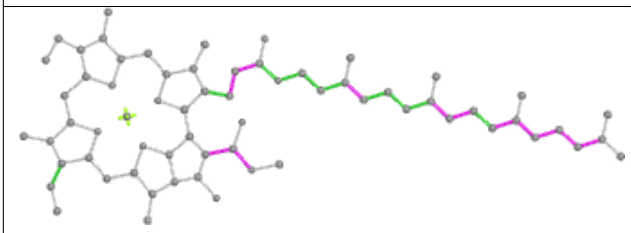
Ligand CLA A 209



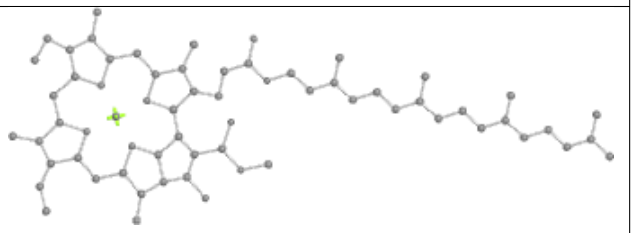
Bond lengths



Bond angles

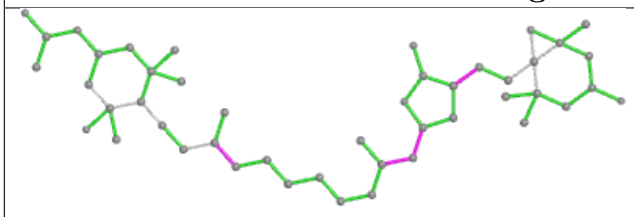


Torsions



Rings

Ligand PID N 301



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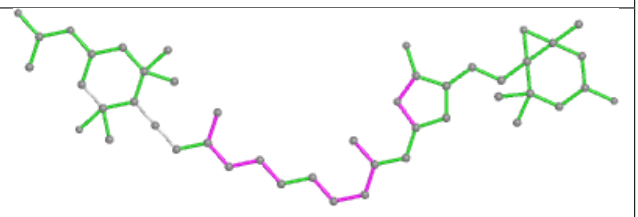
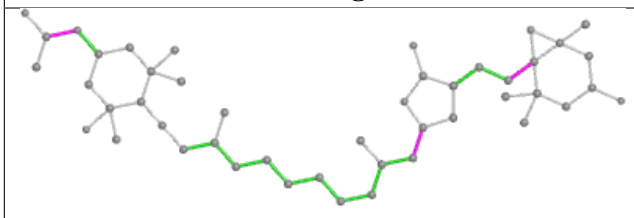


Bond angles



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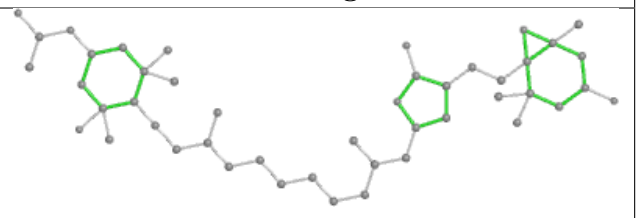
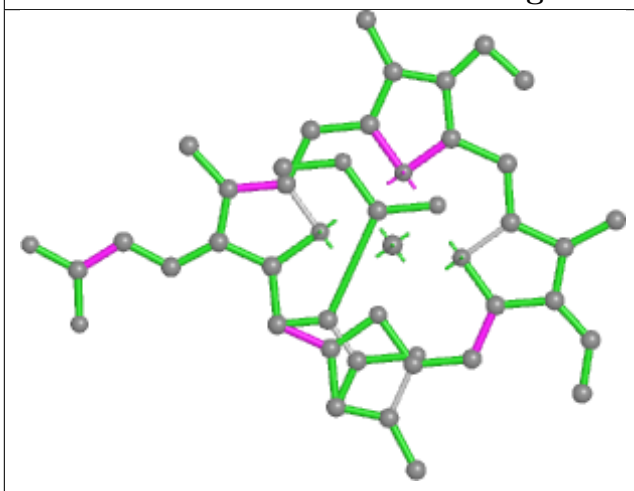


Rings

Ligand KC1 A 213



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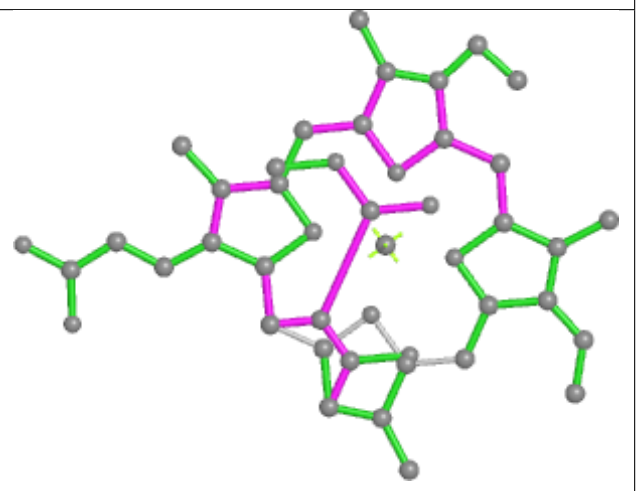
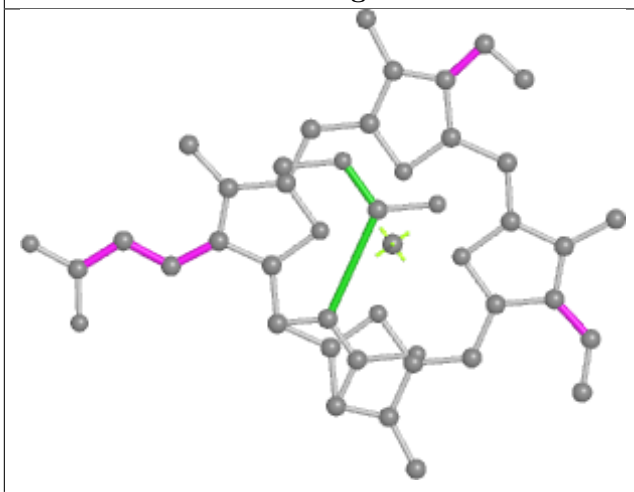
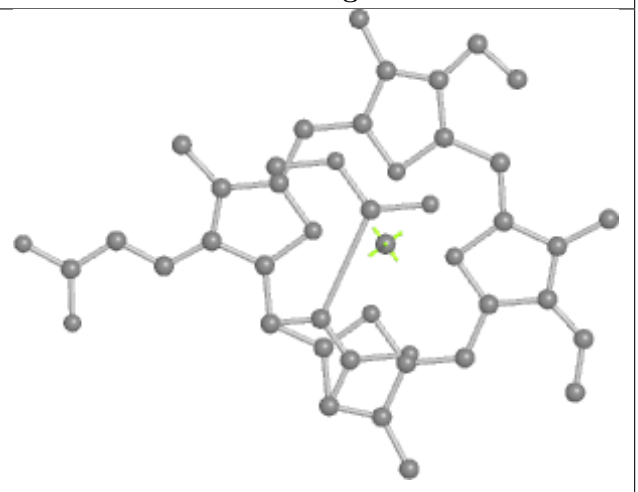


Bond angles

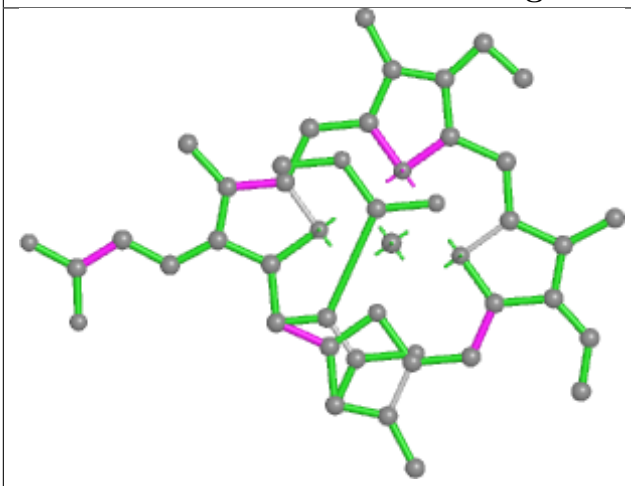


Torsions



Rings

Ligand KC1 O 310



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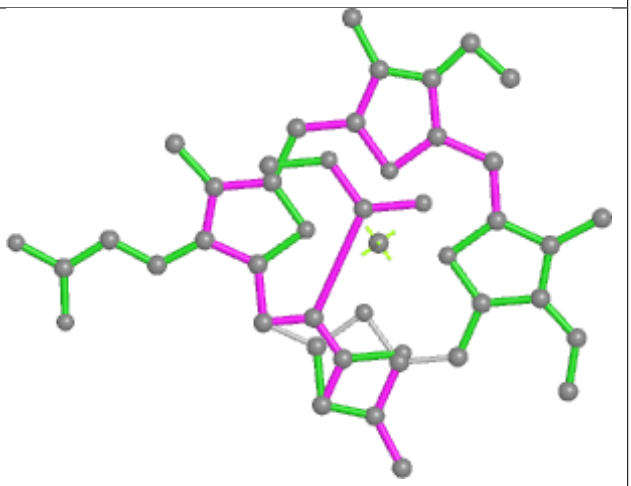
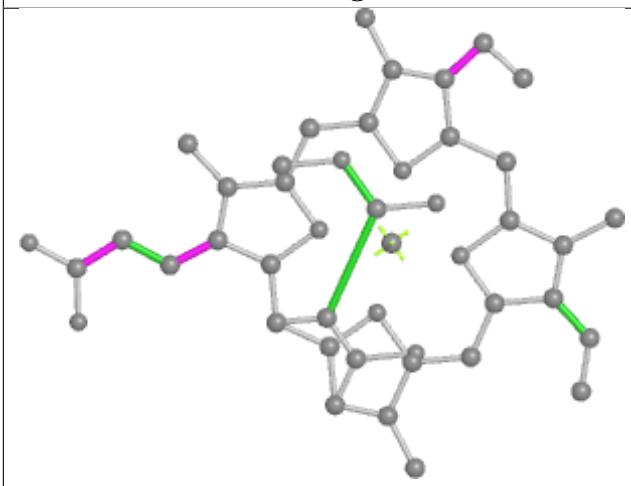


Bond angles



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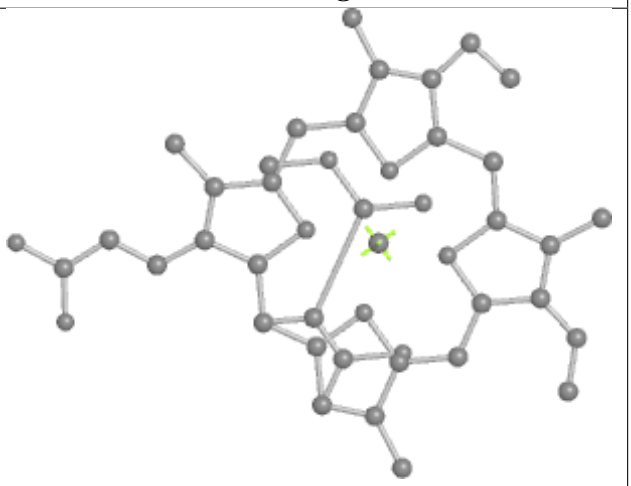
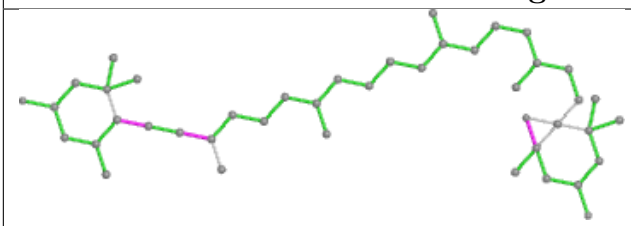


Rings

Ligand DD6 J 303



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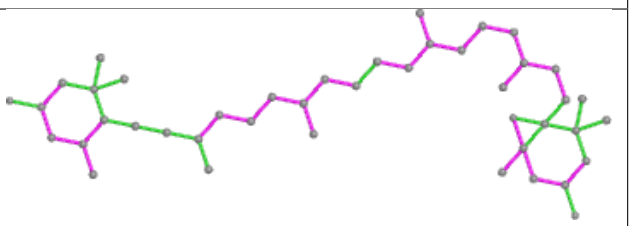
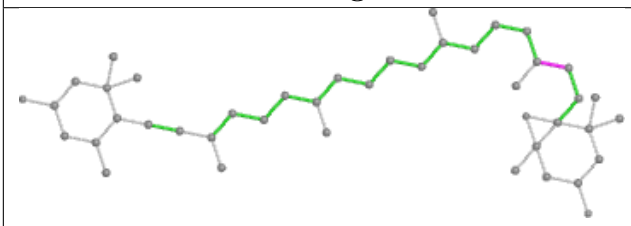


Bond angles



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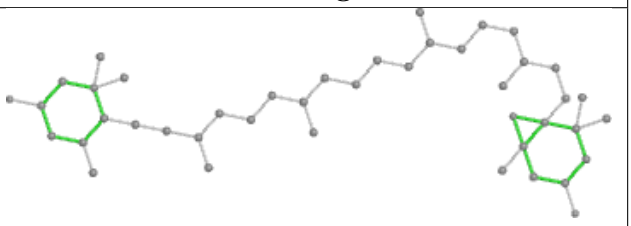
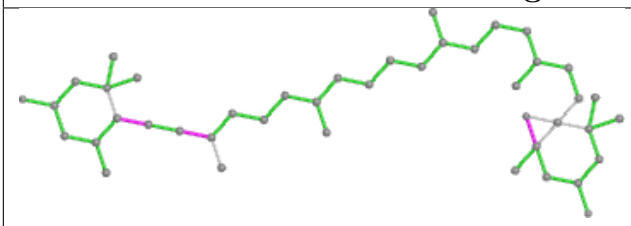


Rings

Ligand DD6 N 303



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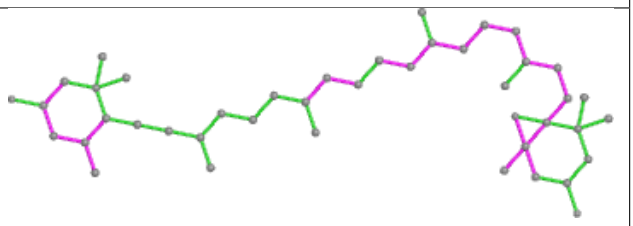
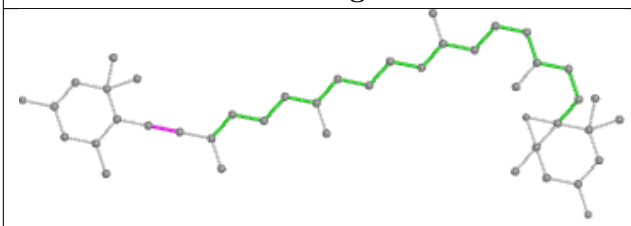


Bond angles



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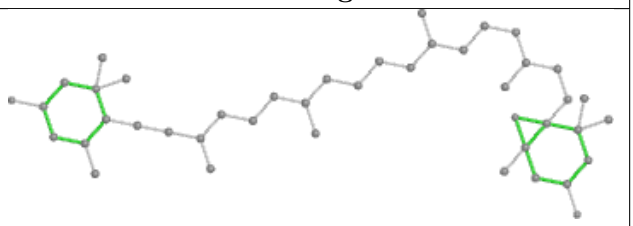
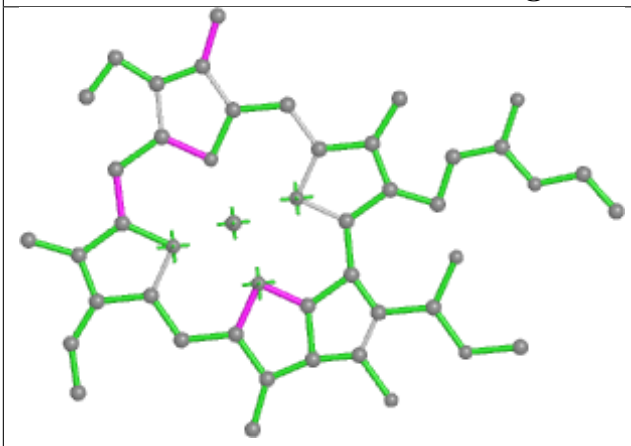


Rings

Ligand CLA P 215



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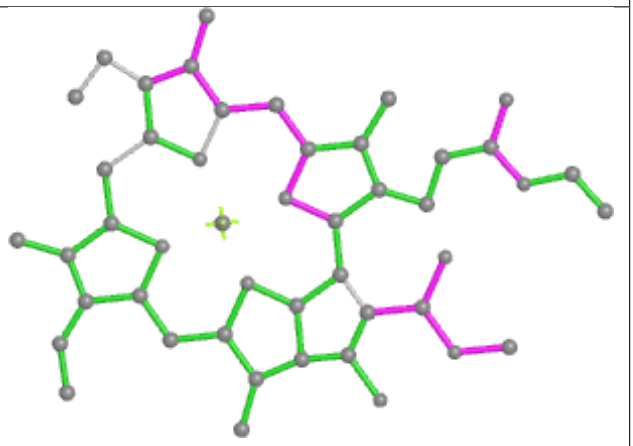
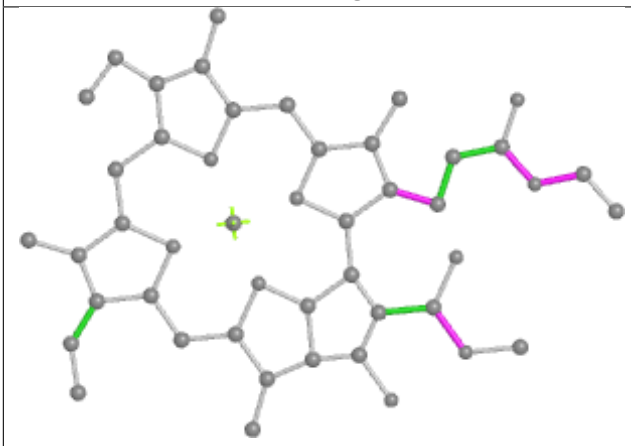


Bond angles



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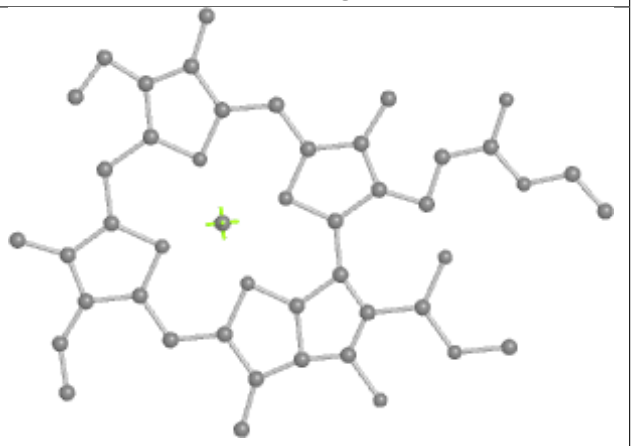
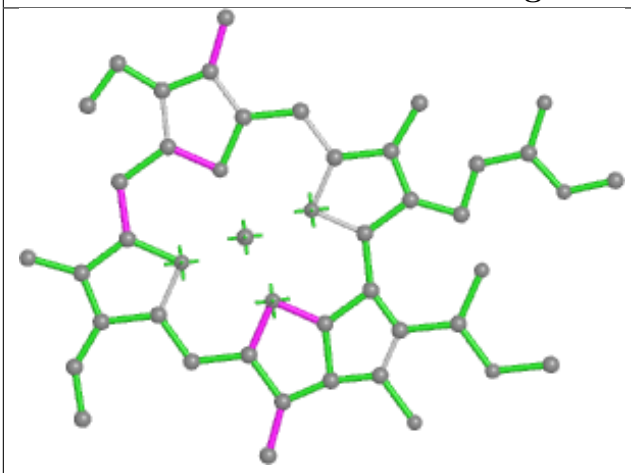


Rings

Ligand CLA C 313



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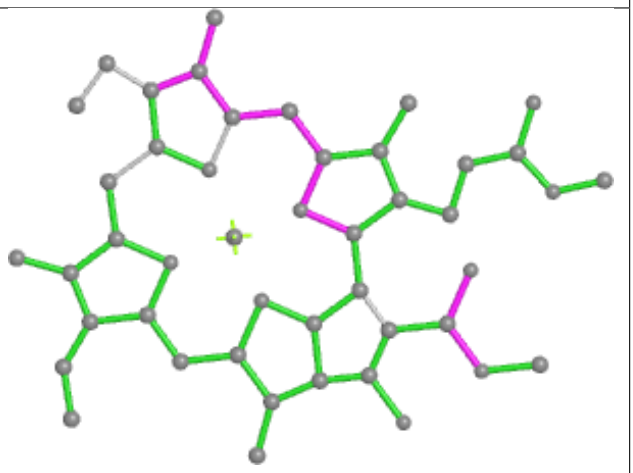
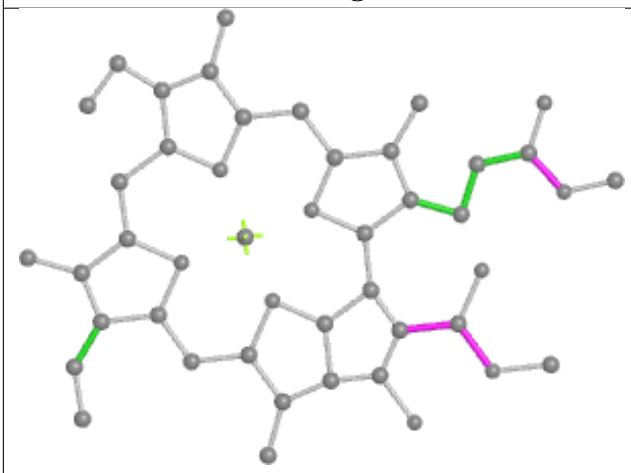


Bond angles



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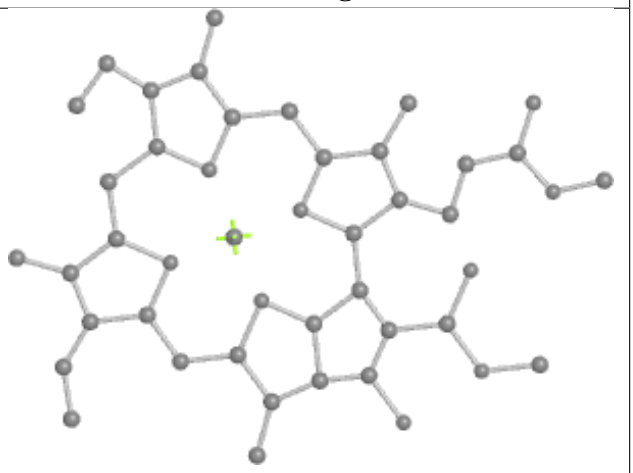
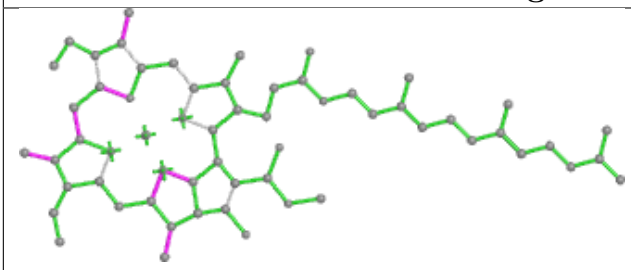
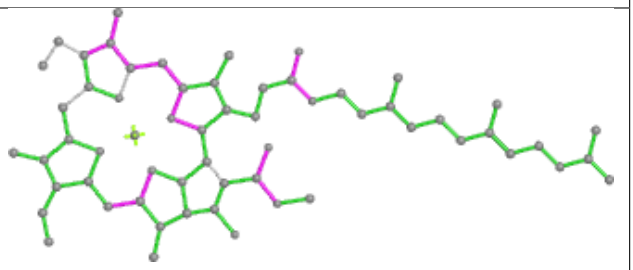


Rings

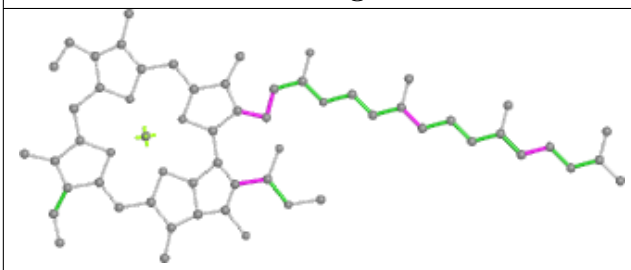
Ligand CLA h 201



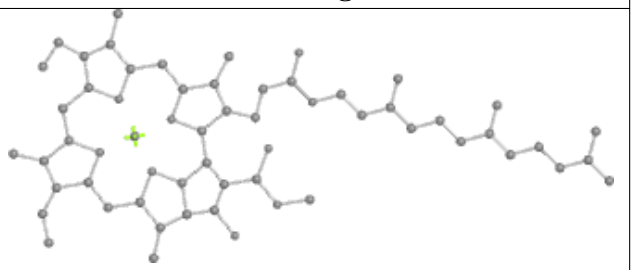
Bond lengths



Bond angles

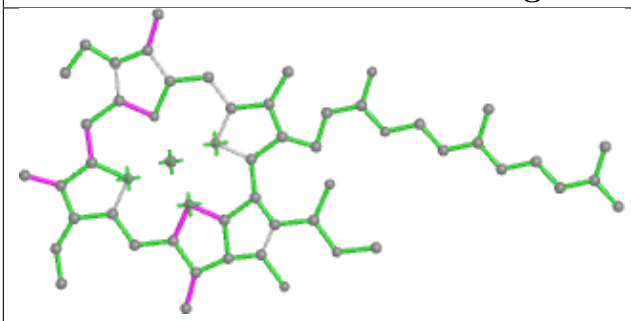


Torsions



Rings

Ligand CLA A 208



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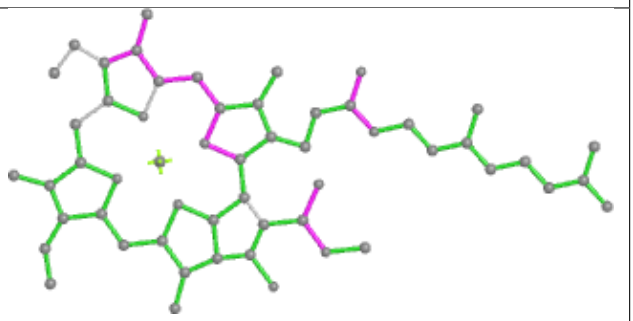
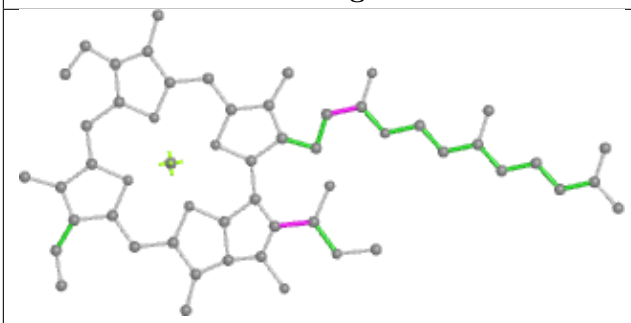
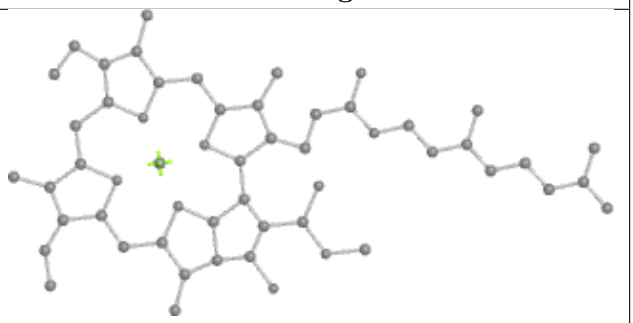


Bond angles

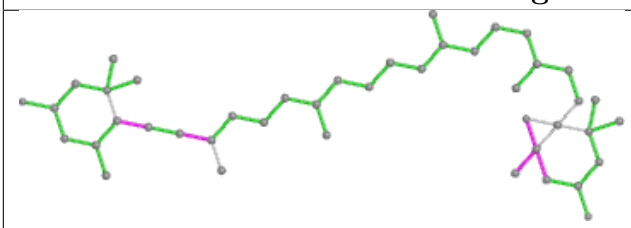


Torsions



Rings

Ligand DD6 I 205



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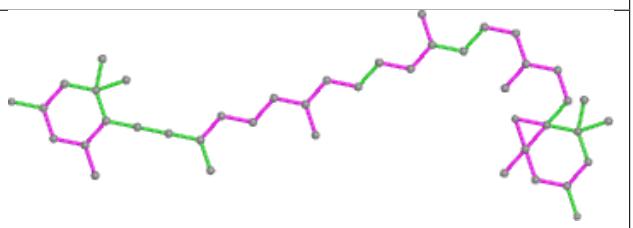
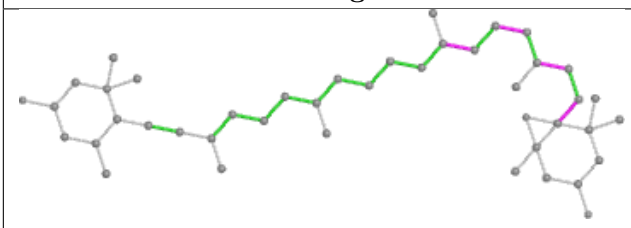


Bond angles



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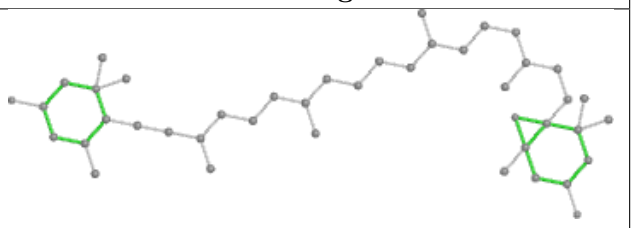
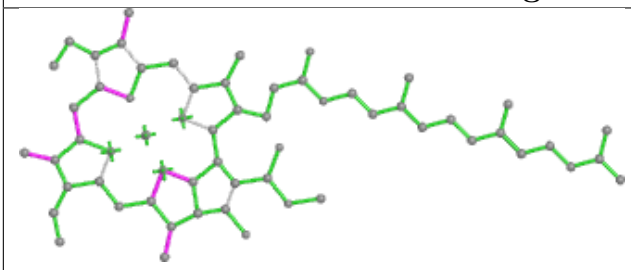


Rings

Ligand CLA G 314



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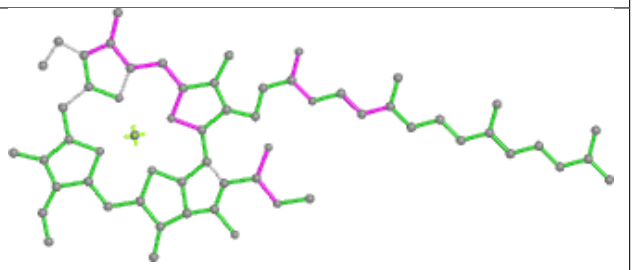
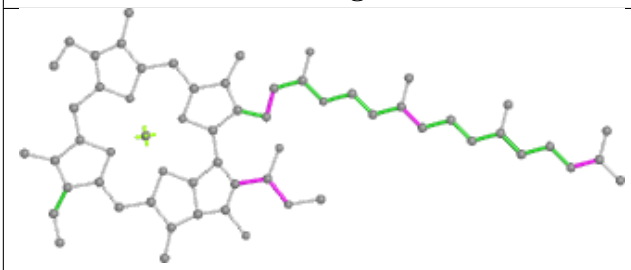
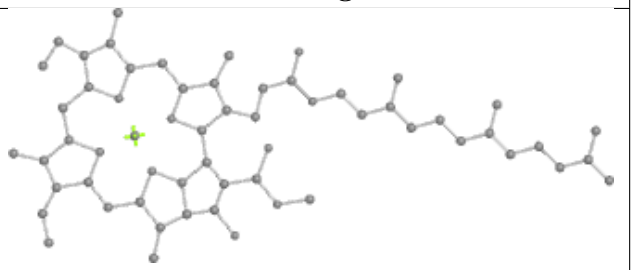


Bond angles

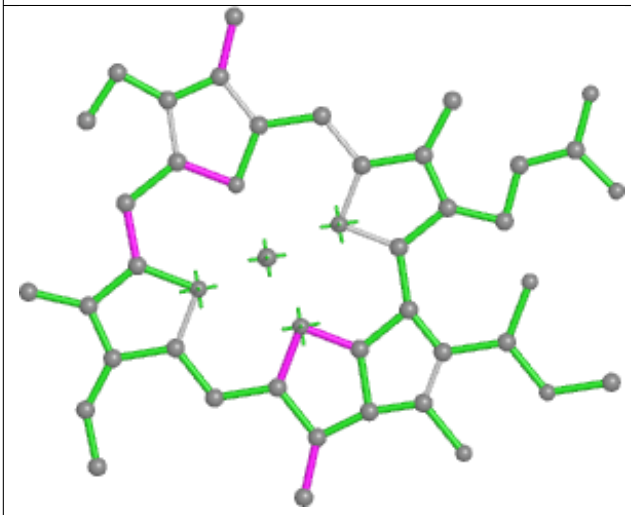


Torsions



Rings

Ligand CLA D 313



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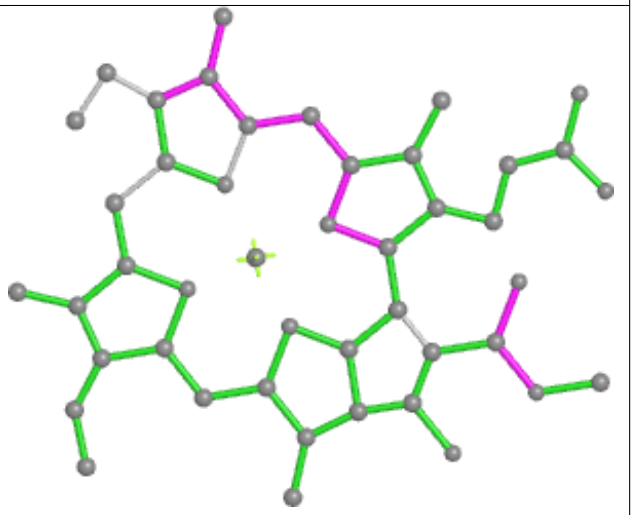
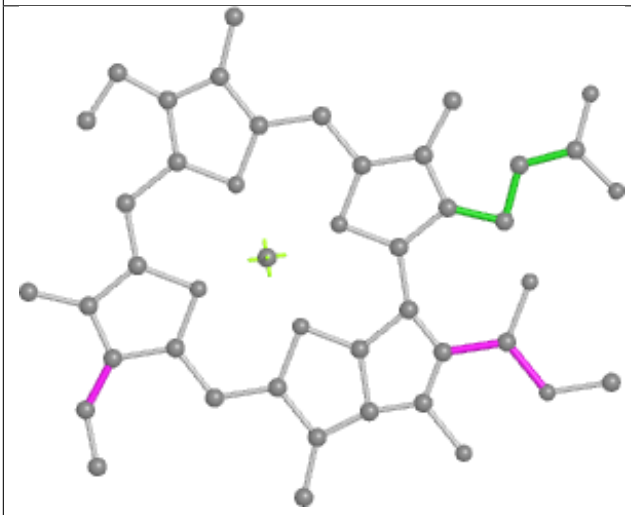
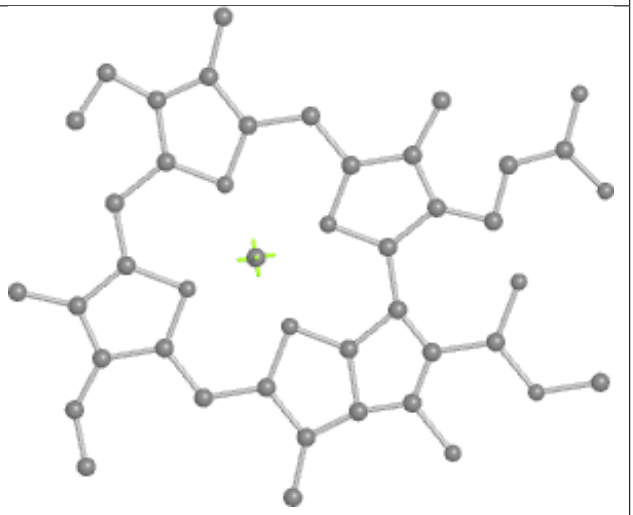


Bond angles

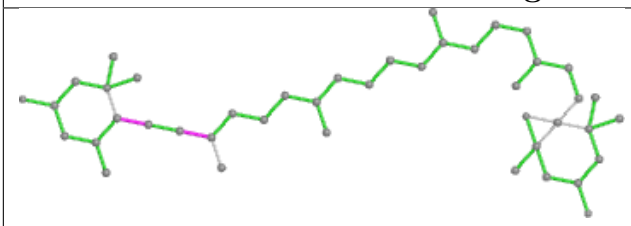


Torsions



Rings

Ligand DD6 G 308



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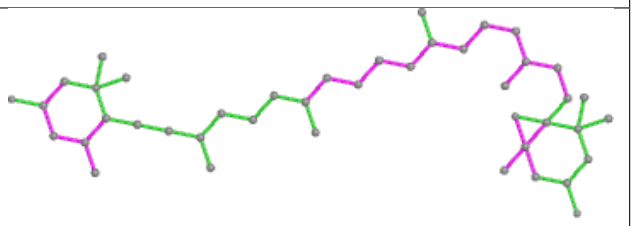
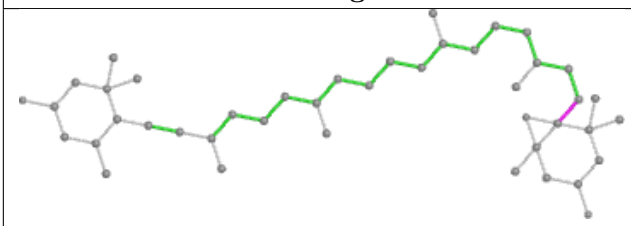
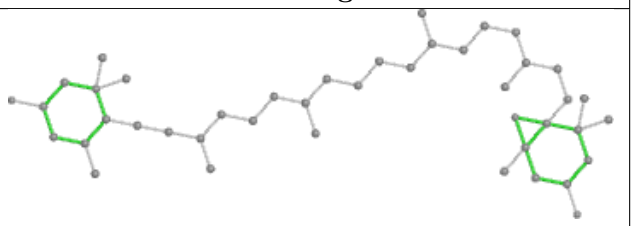


Bond angles

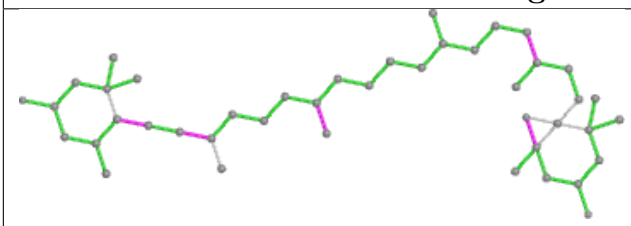


Torsions

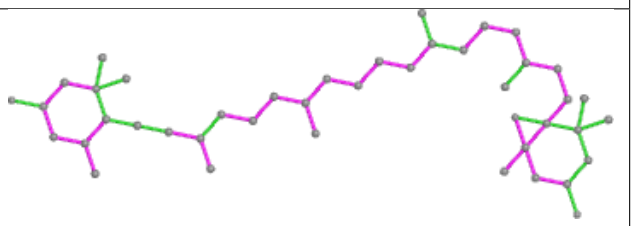


Rings

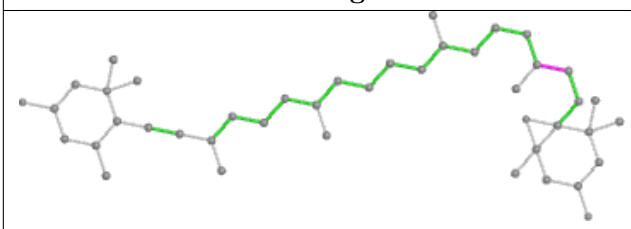
Ligand DD6 h 202



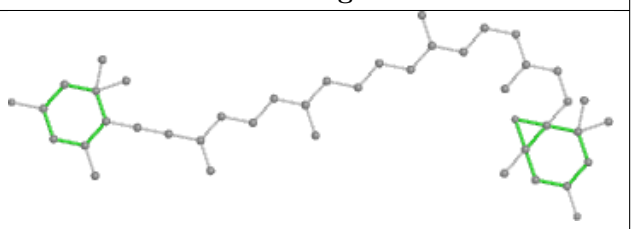
Bond lengths



Bond angles

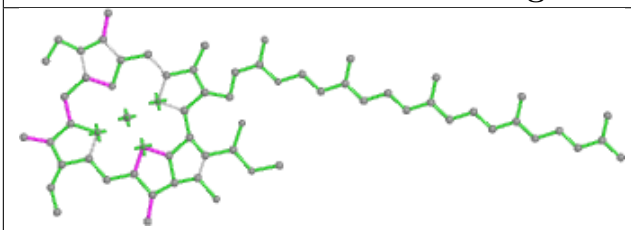


Torsions

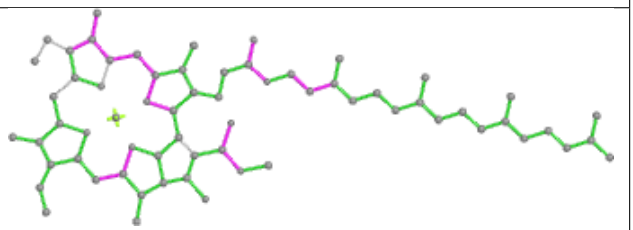


Rings

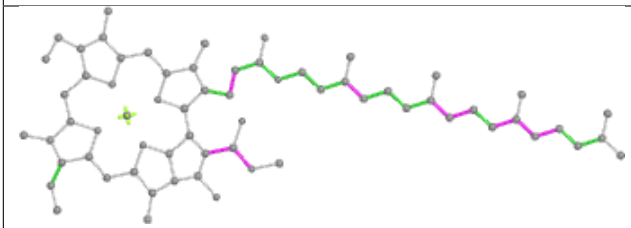
Ligand CLA b 701



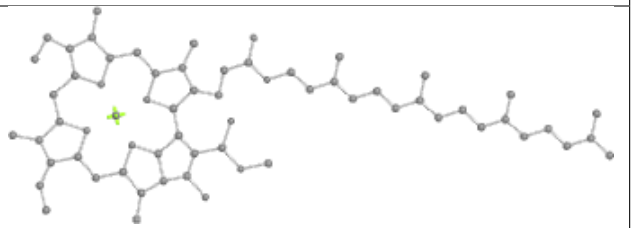
Bond lengths



Bond angles

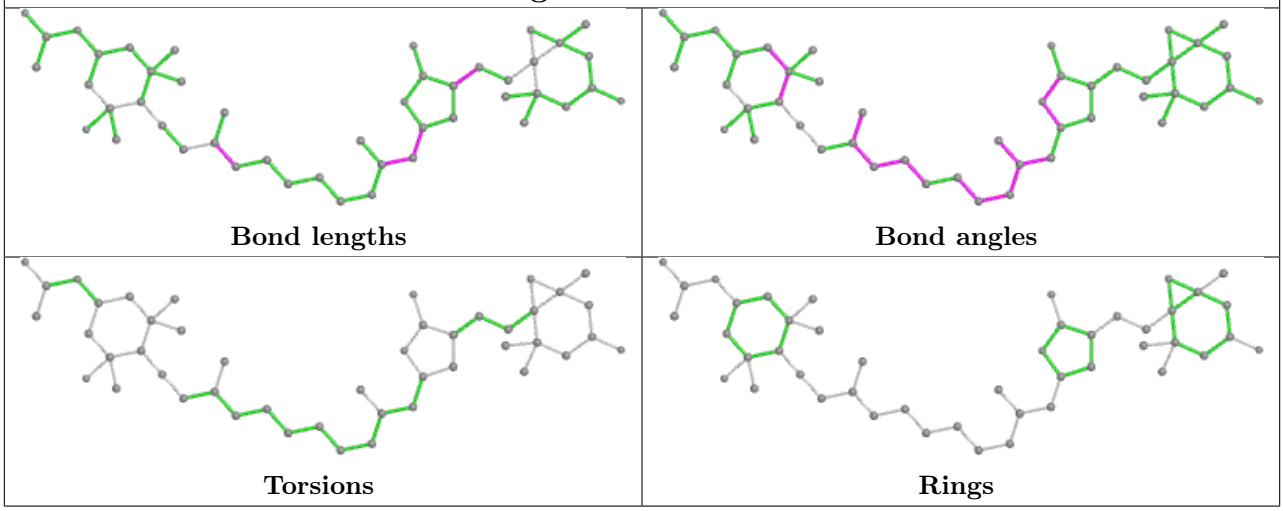


Torsions

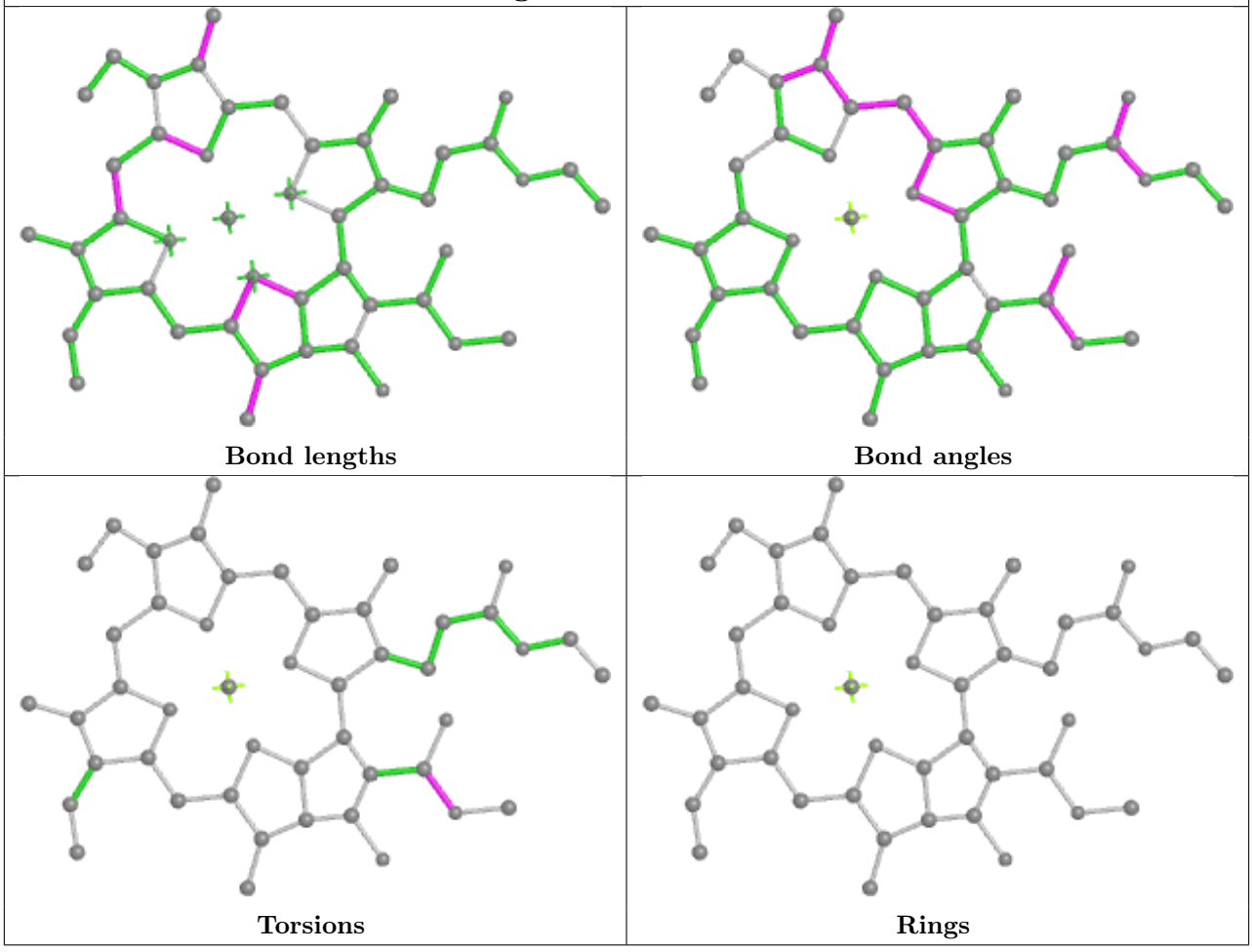


Rings

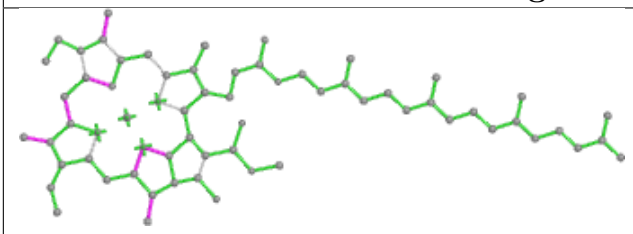
Ligand PID T 305



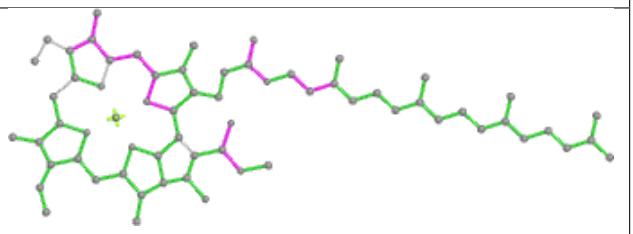
Ligand CLA T 308



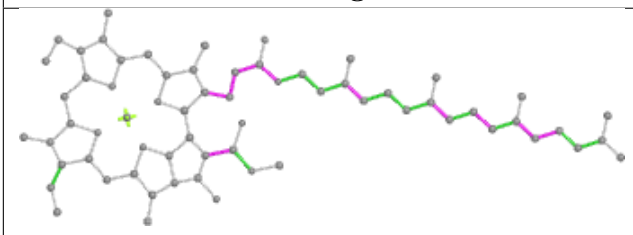
Ligand CLA a 809



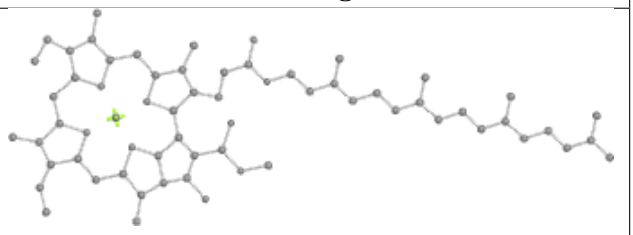
Bond lengths



Bond angles

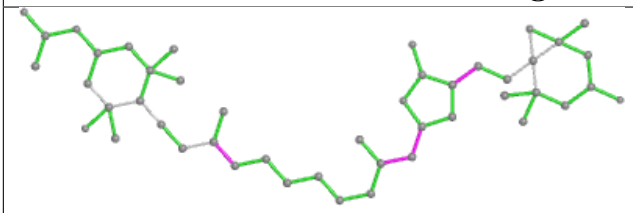


Torsions

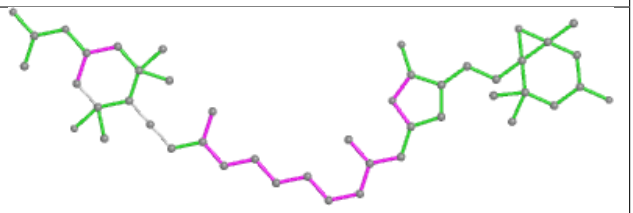


Rings

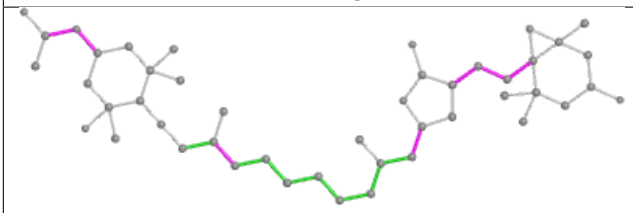
Ligand PID T 317



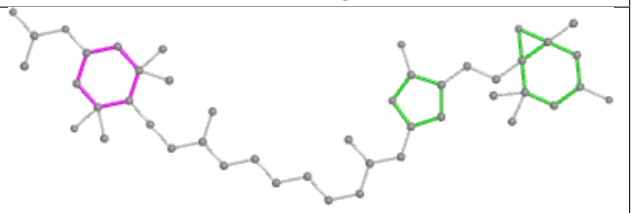
Bond lengths



Bond angles

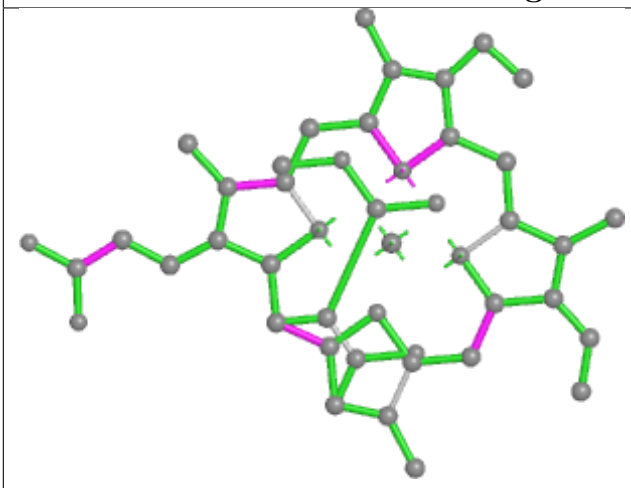


Torsions

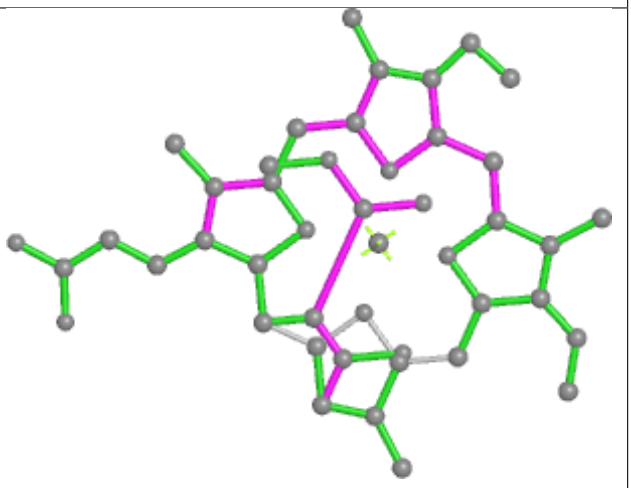


Rings

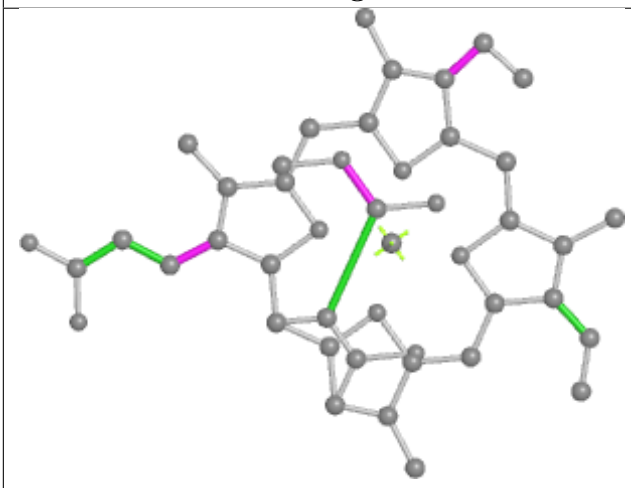
Ligand KC1 H 314



Bond lengths



Bond angles



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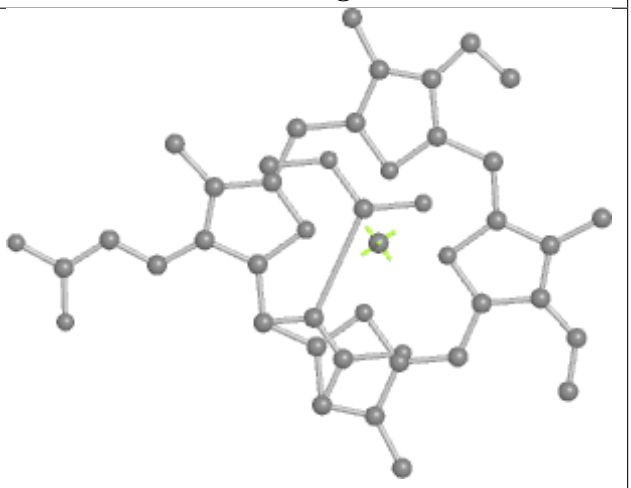
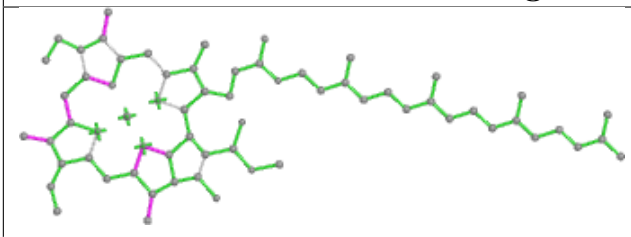


Rings

Ligand CLA B 312



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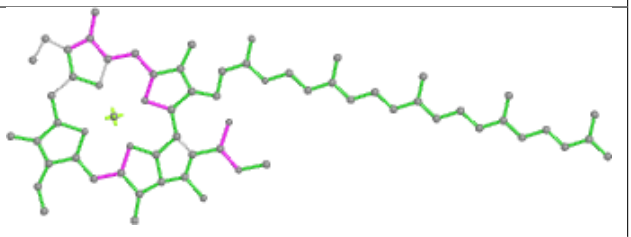
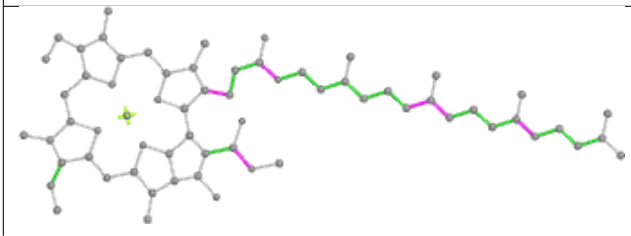


Bond angles



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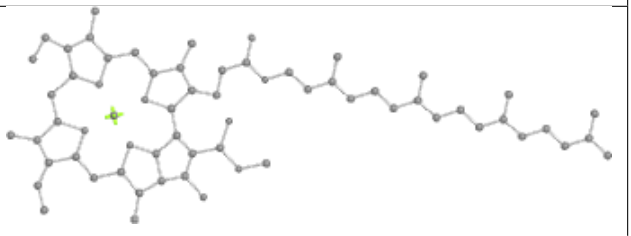
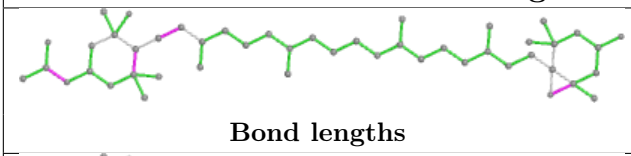


Rings

Ligand UIX E 304



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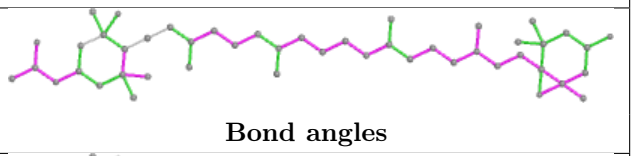

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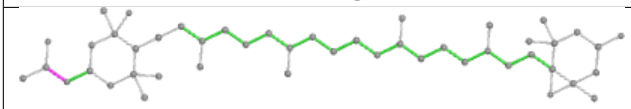
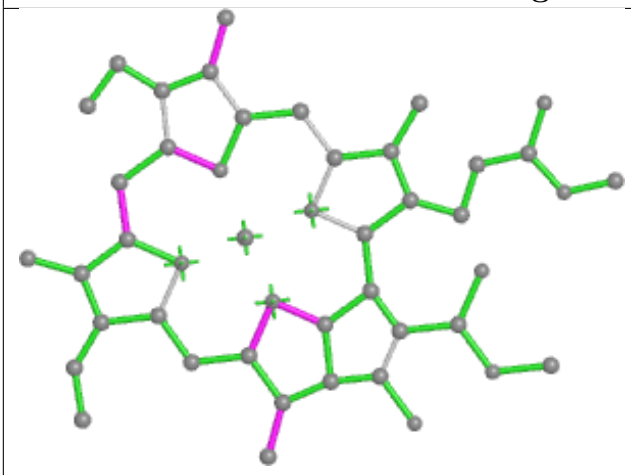


Torsions

Rings

Ligand CLA f 803



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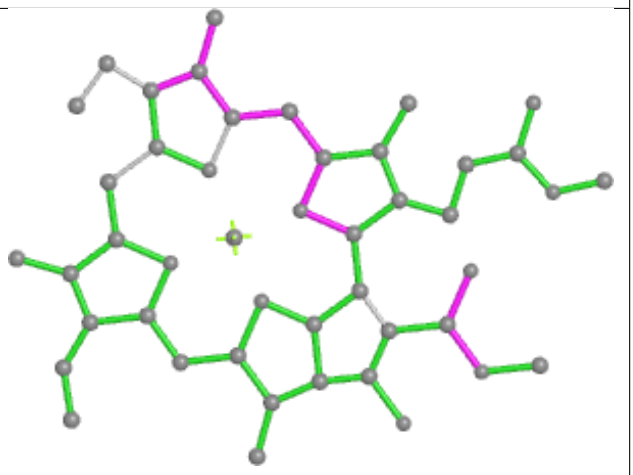
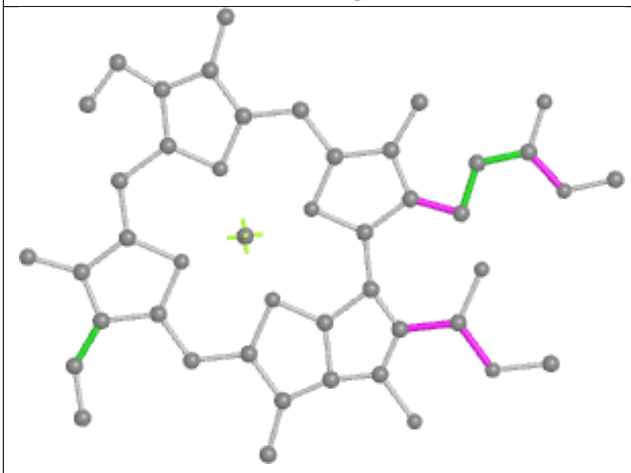
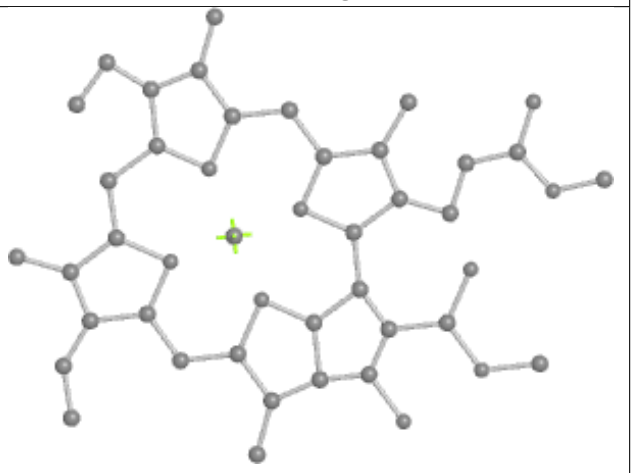


Bond angles

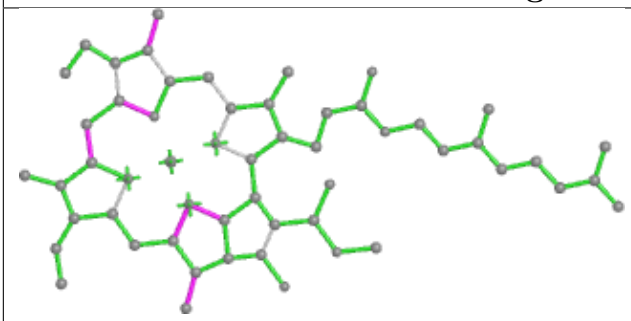


Torsions



Rings

Ligand CLA L 309



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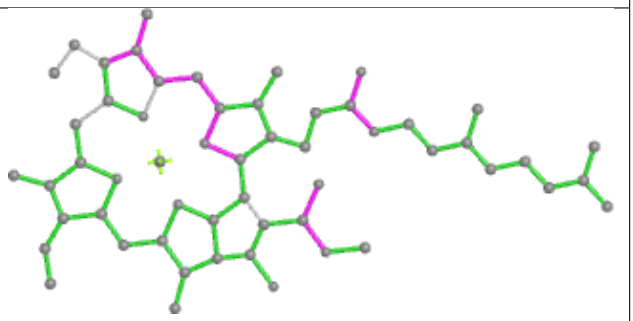
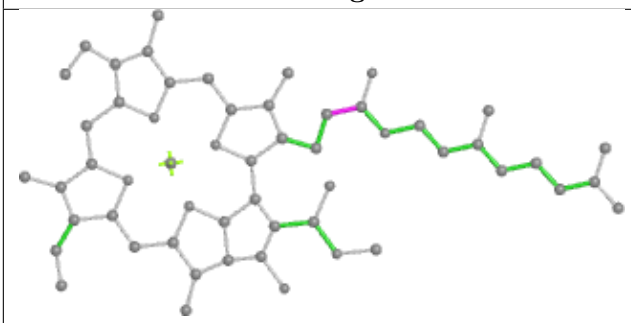
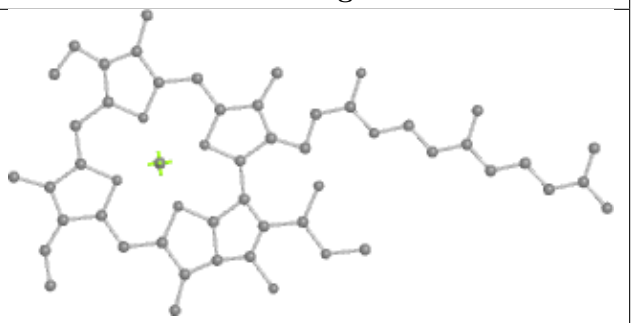


Bond angles

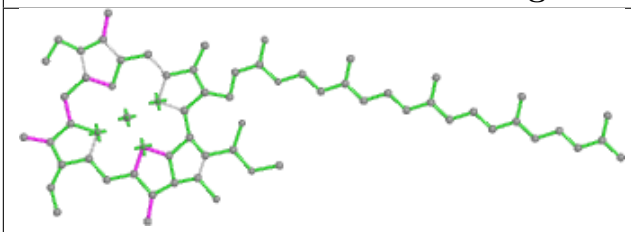


Torsions

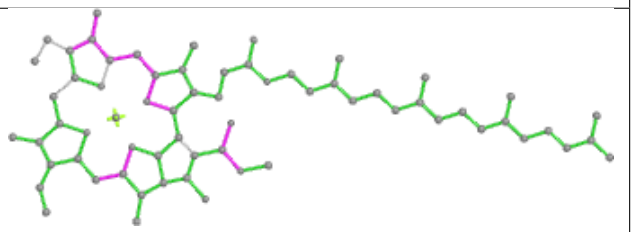


Rings

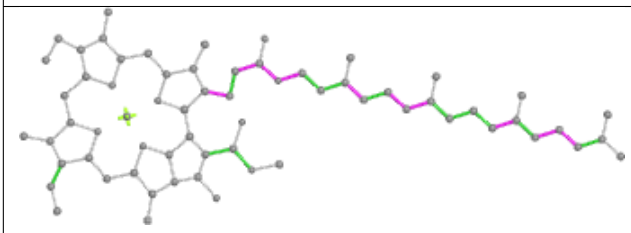
Ligand CLA a 806



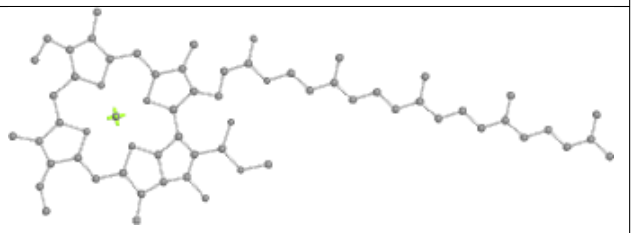
Bond lengths



Bond angles

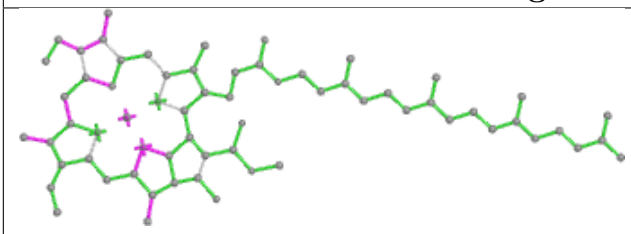


Torsions



Rings

Ligand CLA a 801



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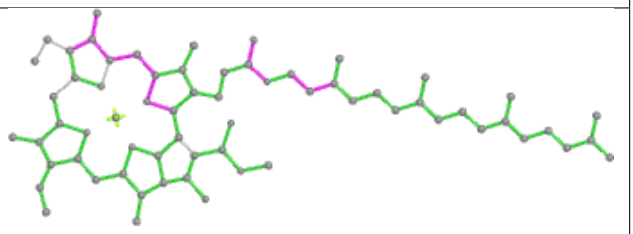
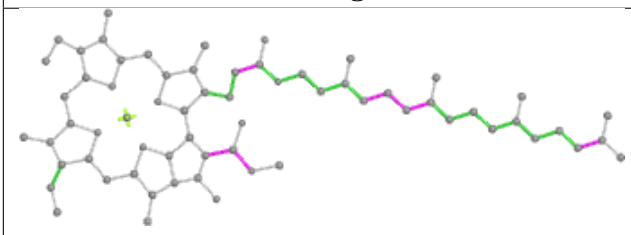
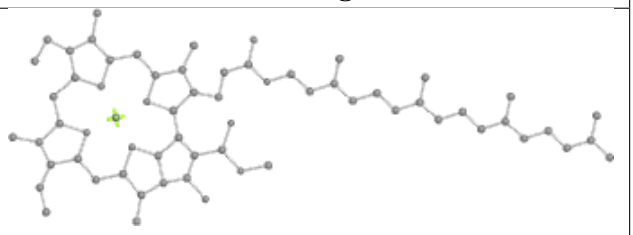


Bond angles

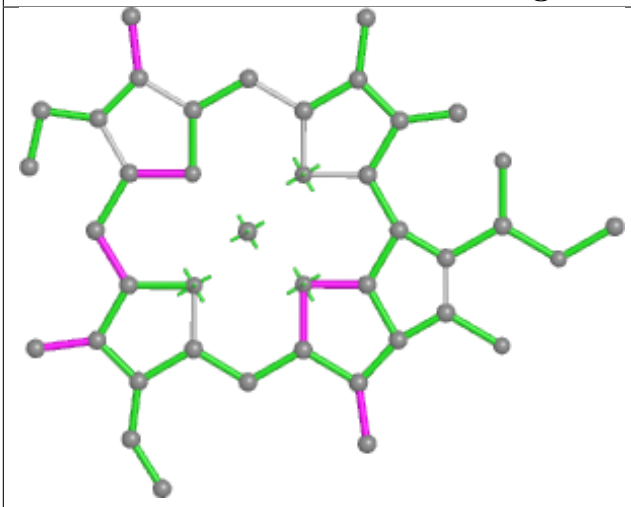


Torsions



Rings

Ligand CLA l 509



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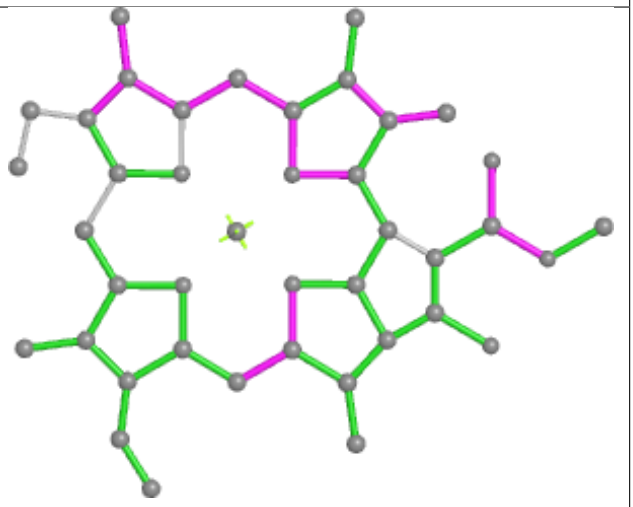
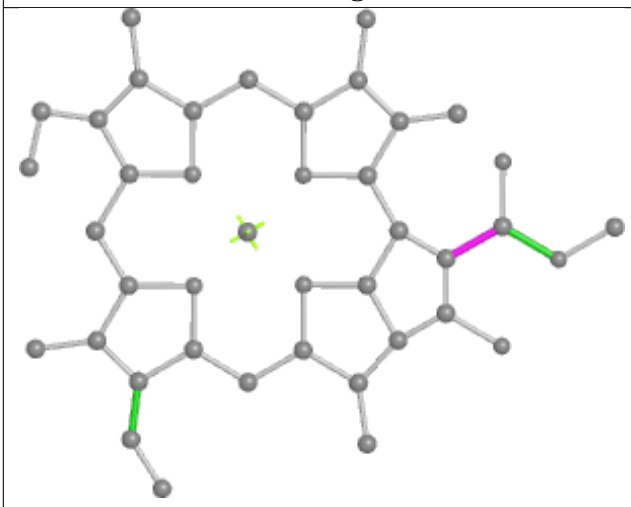
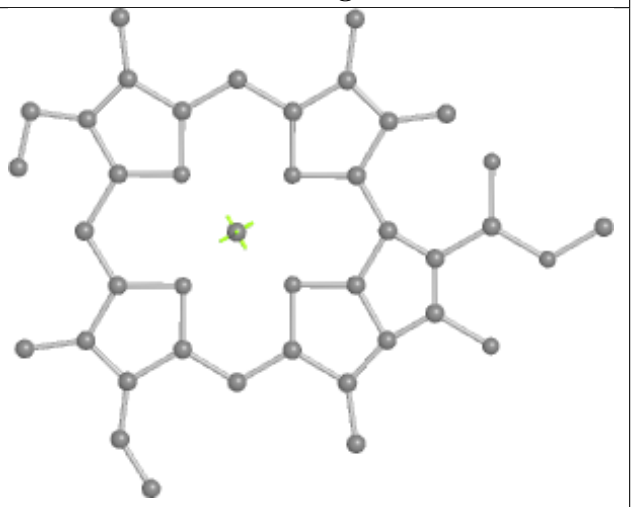


Bond angles

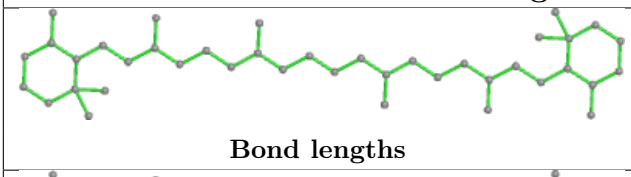


Torsions

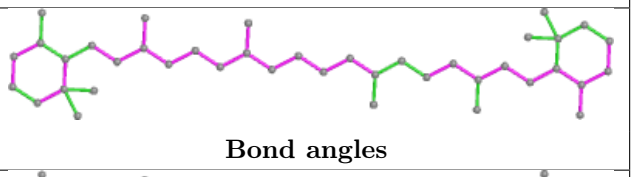


Rings

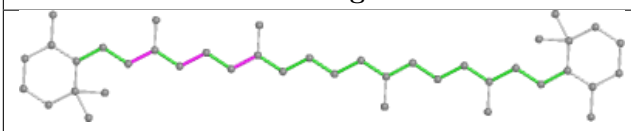
Ligand BCR l 507



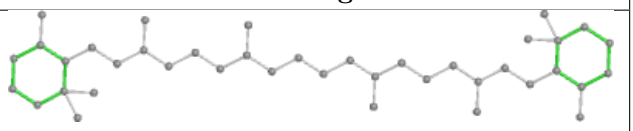
Bond lengths



Bond angles

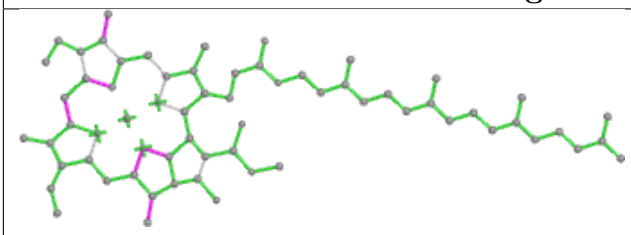


Torsions

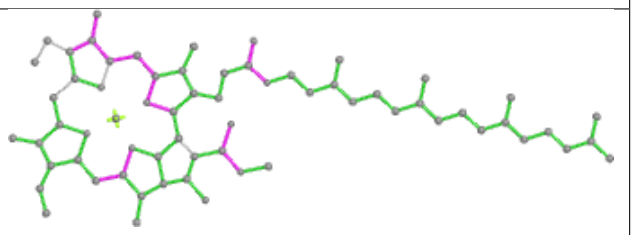


Rings

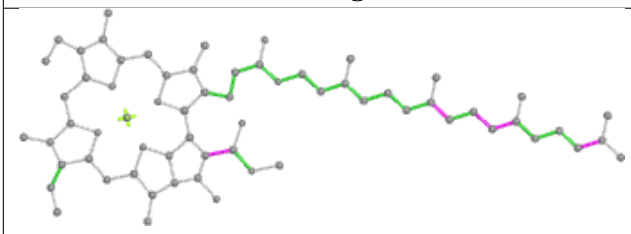
Ligand CLA E 308



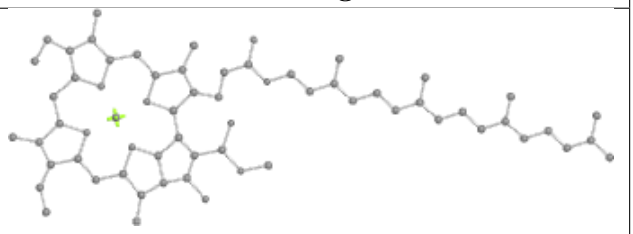
Bond lengths



Bond angles

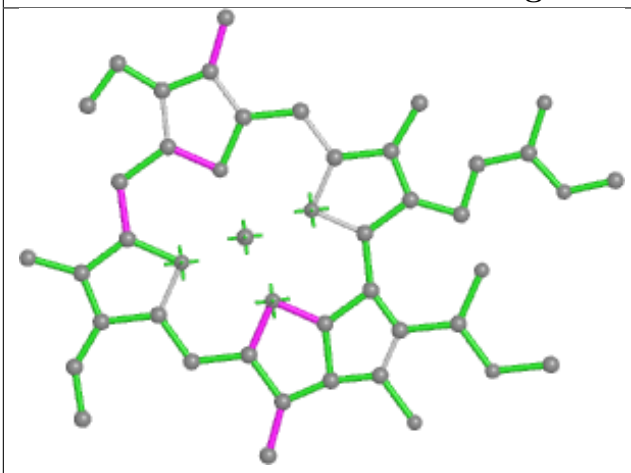


Torsions

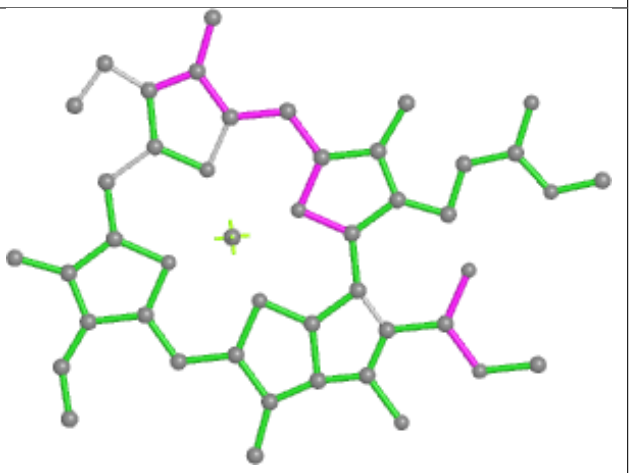


Rings

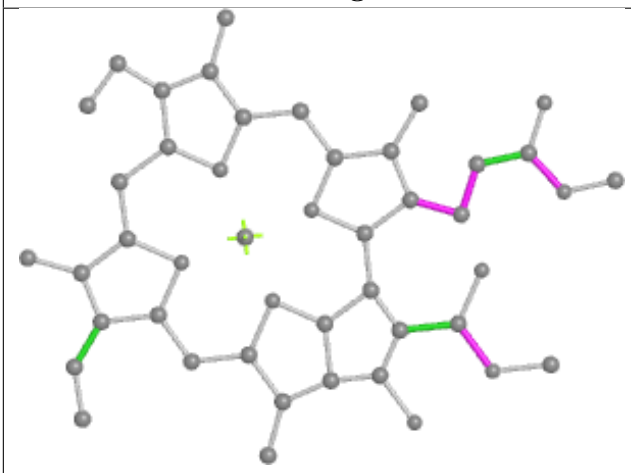
Ligand CLA P 214



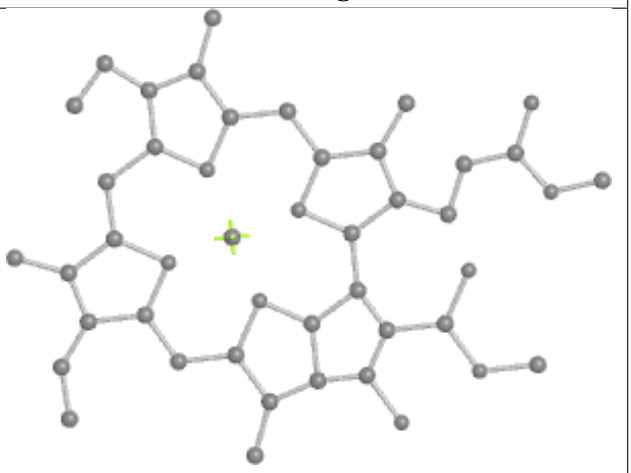
Bond lengths



Bond angles

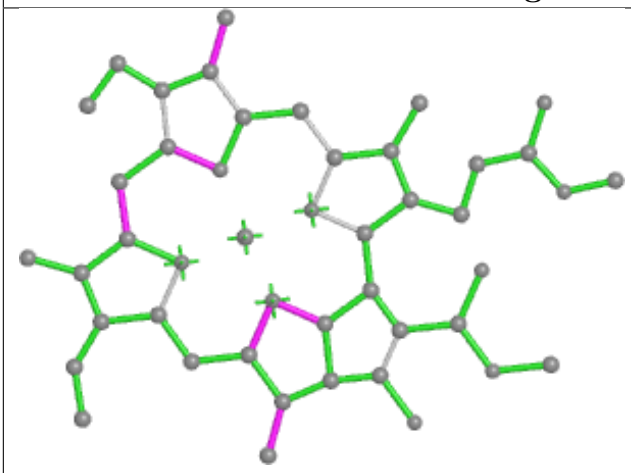


Torsions

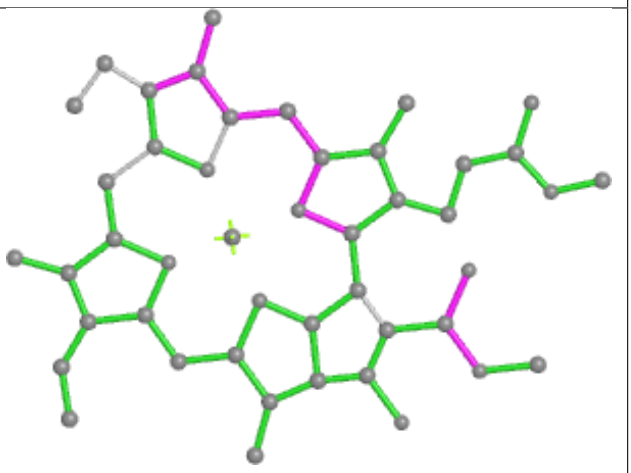


Rings

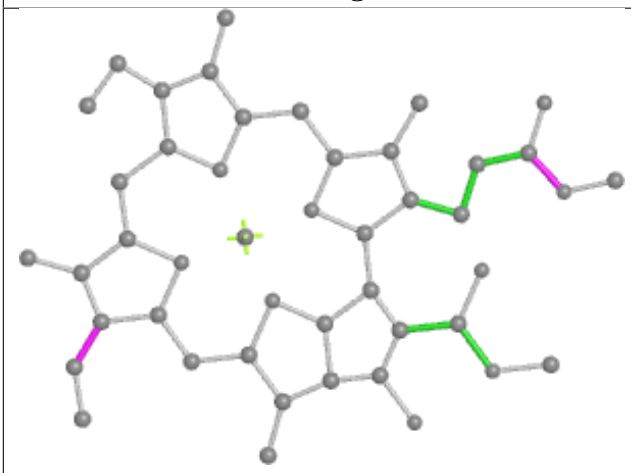
Ligand CLA B 315



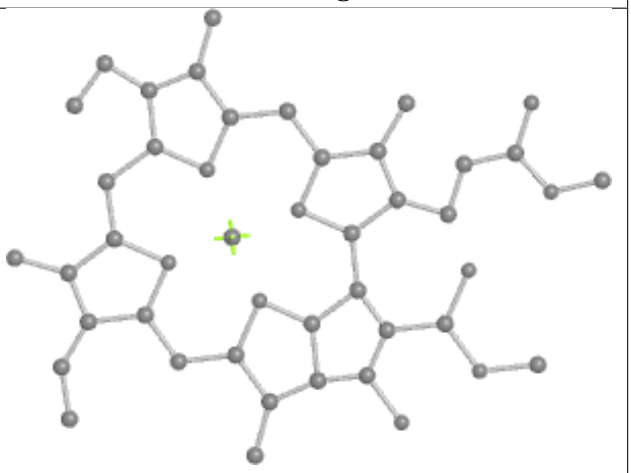
Bond lengths



Bond angles

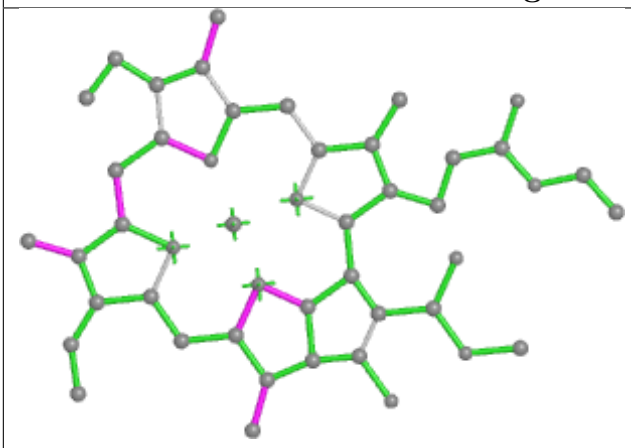


Torsions



Rings

Ligand CLA O 314



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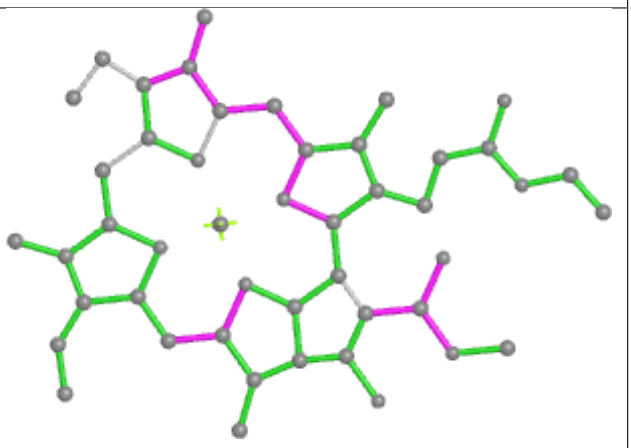
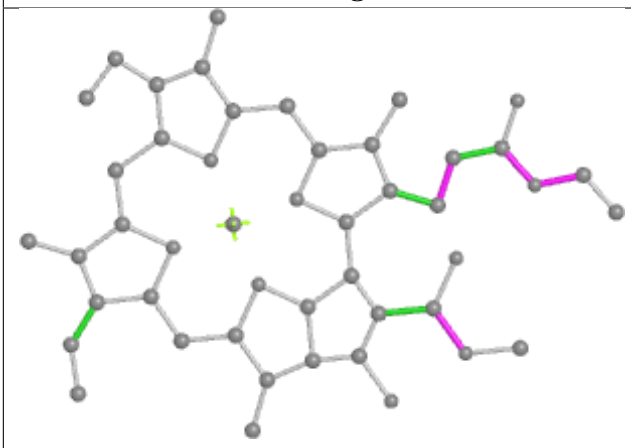


Bond angles



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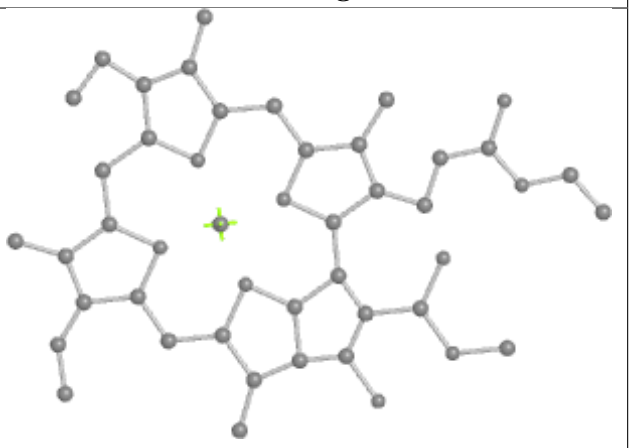
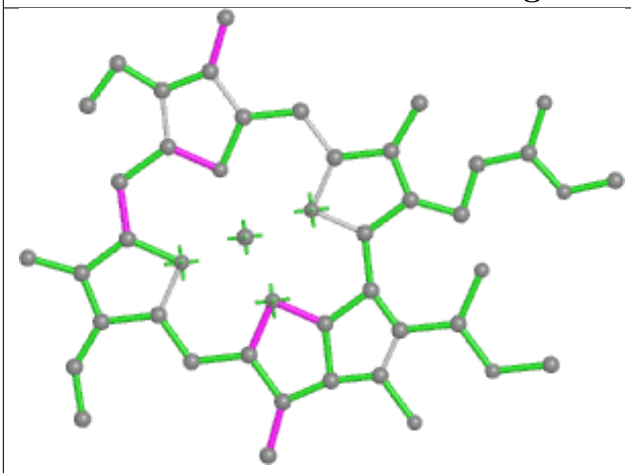
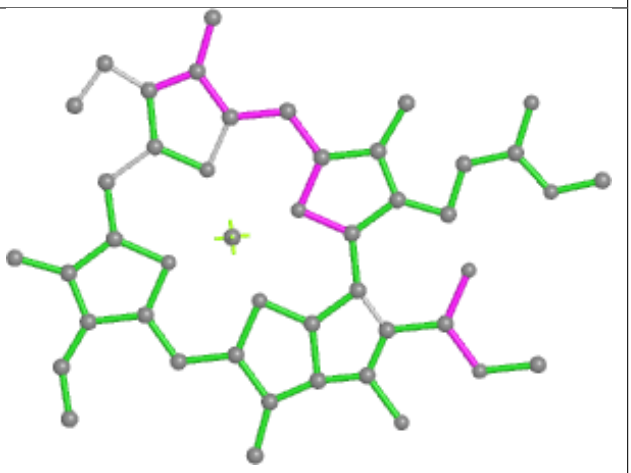


Rings

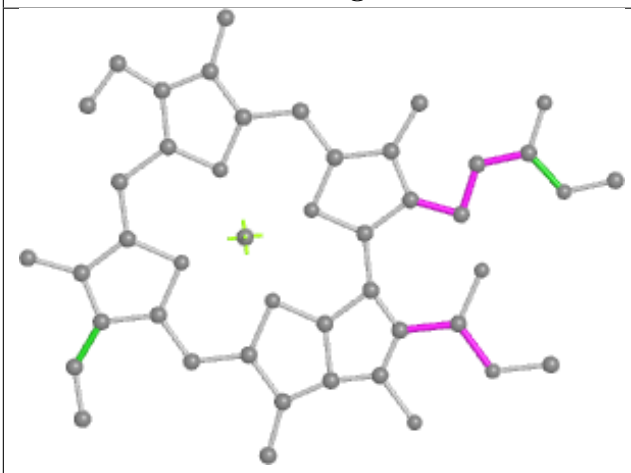
Ligand CLA H 312



Bond lengths



Bond angles



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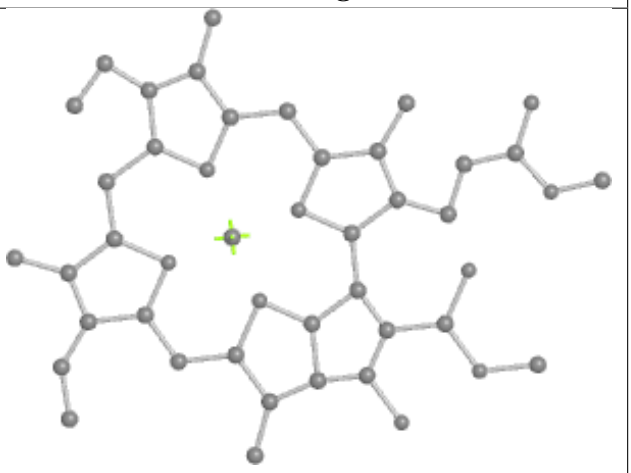
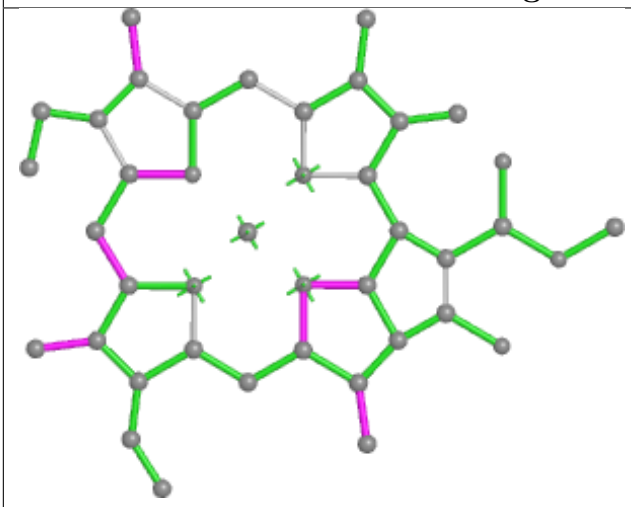


Rings

Ligand CLA K 216



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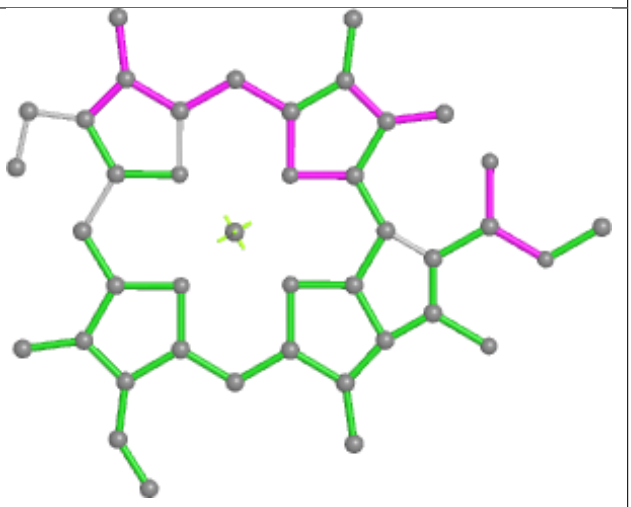

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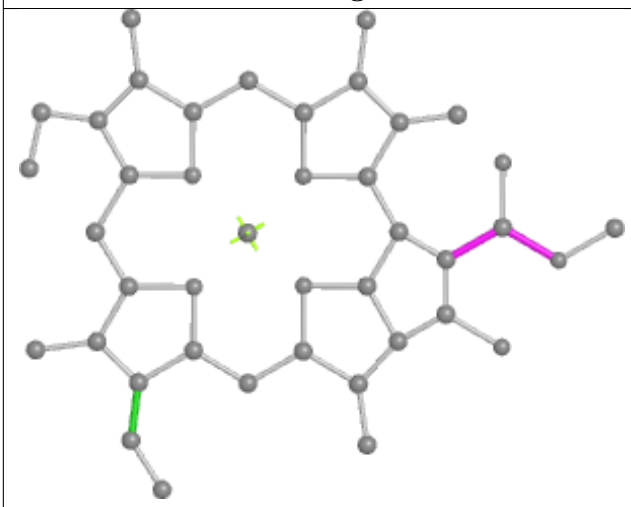

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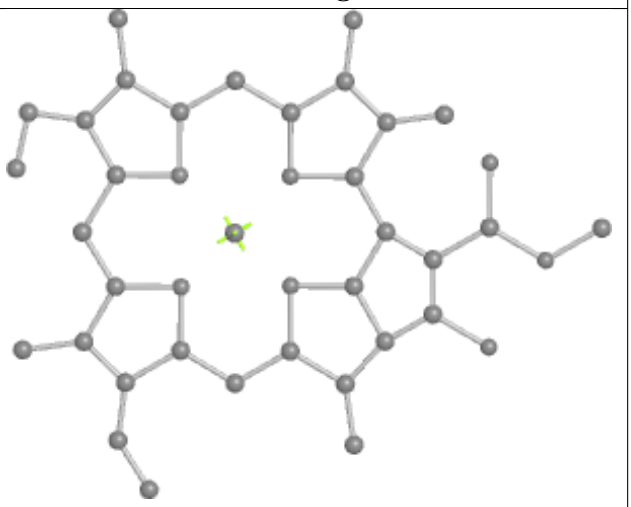
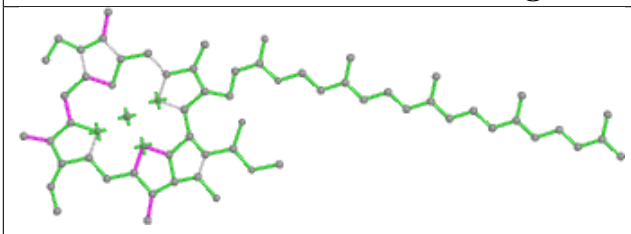


Rings

Ligand CLA B 310



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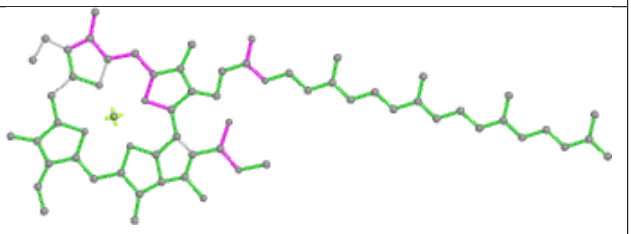
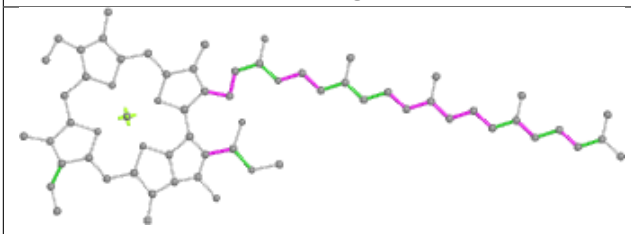


Bond angles



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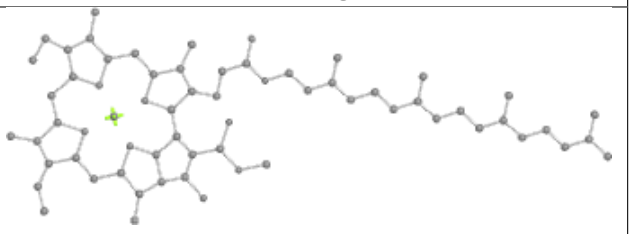
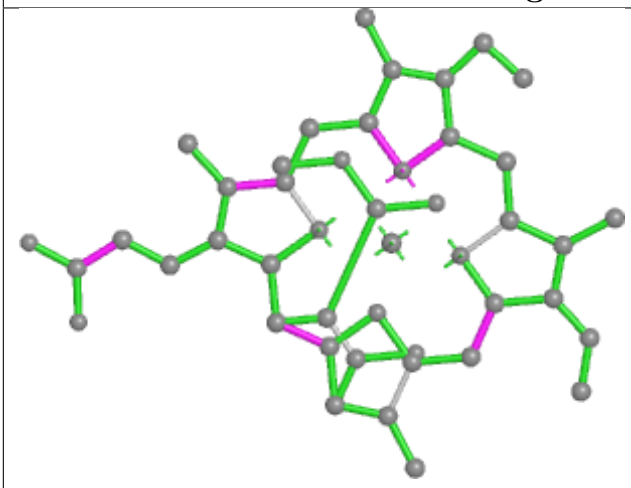


Rings

Ligand KC1 C 315



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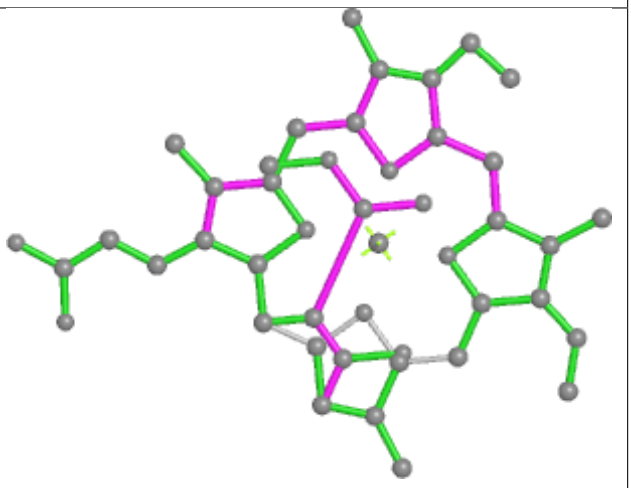

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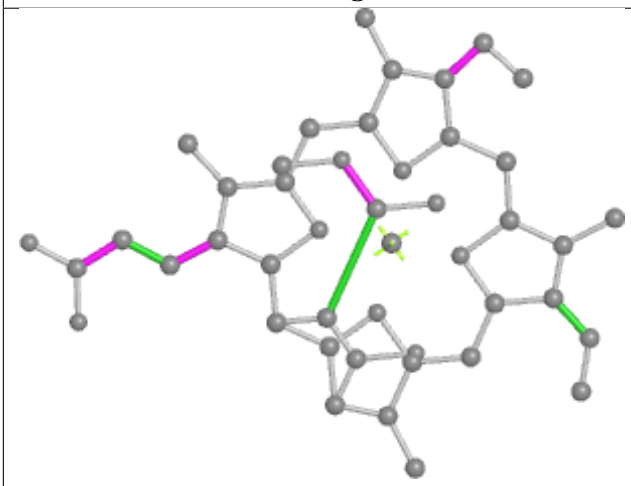

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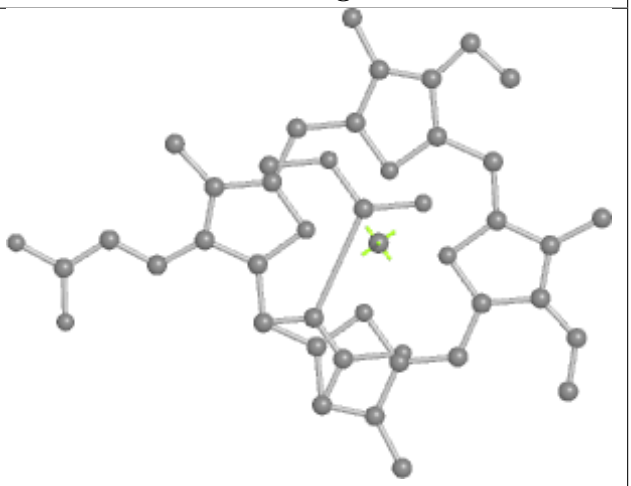
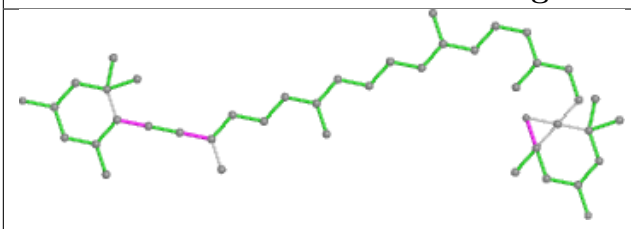


Rings

Ligand DD6 I 202



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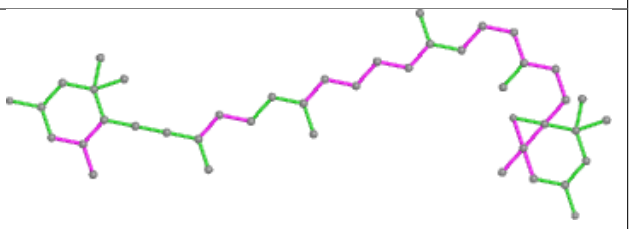
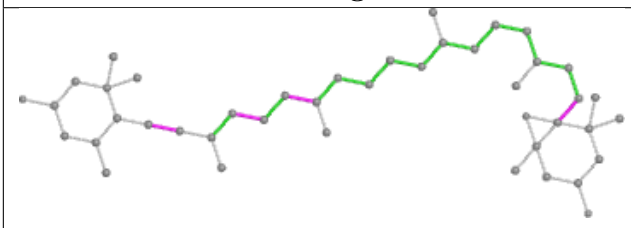


Bond angles



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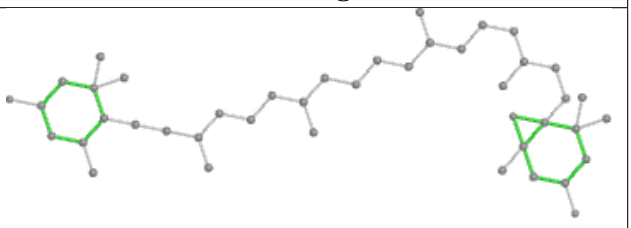
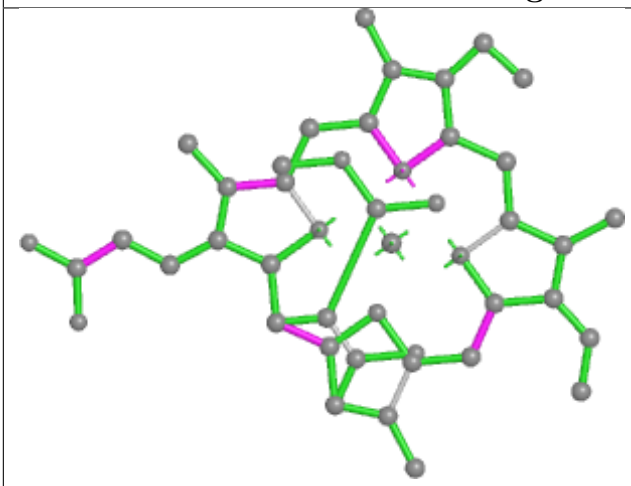


Rings

Ligand KC1 C 310



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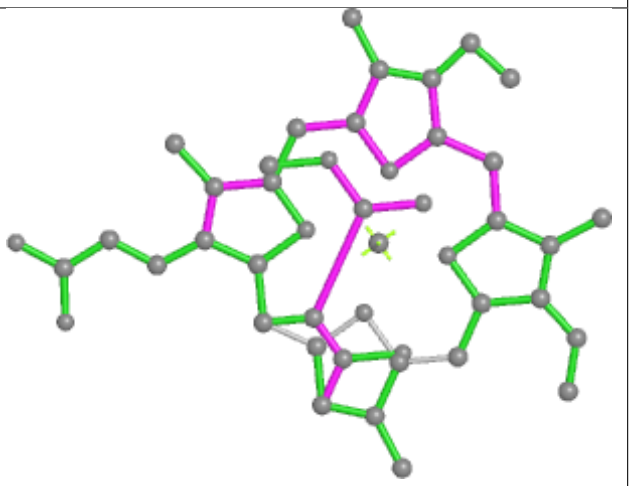
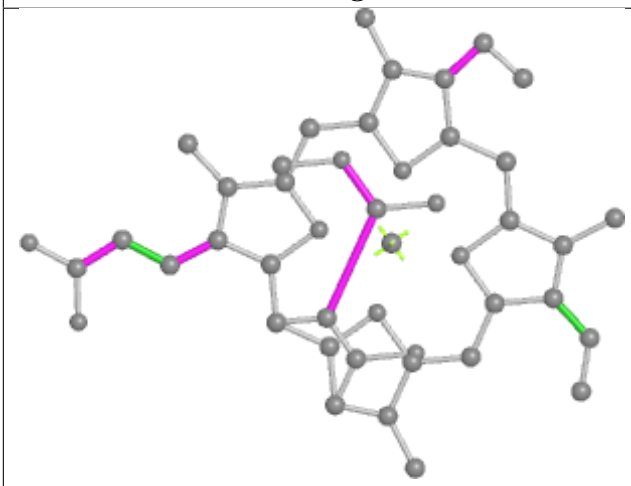


Bond angles



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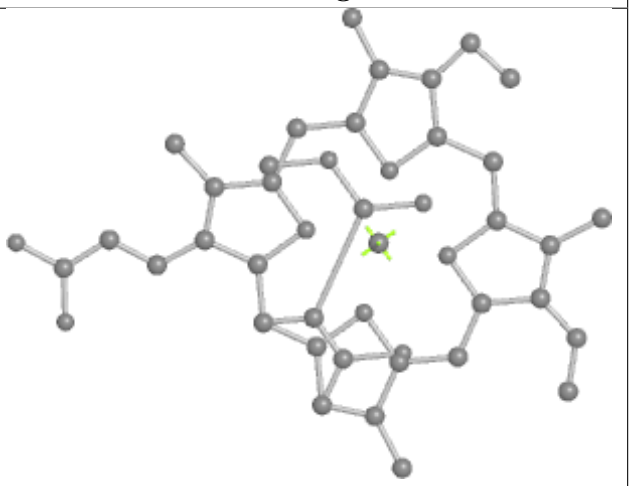
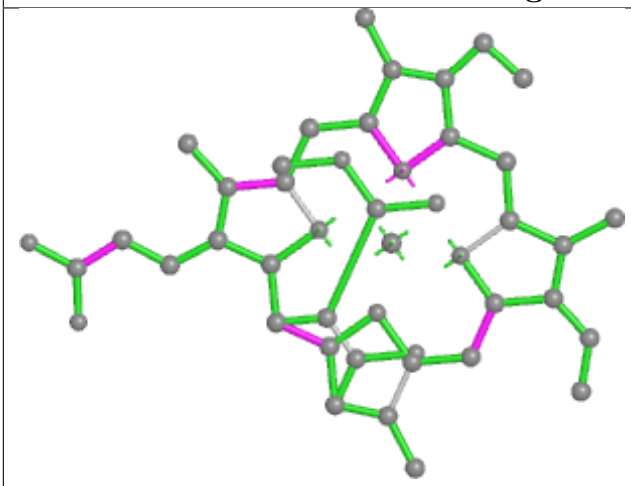


Rings

Ligand KC1 A 205



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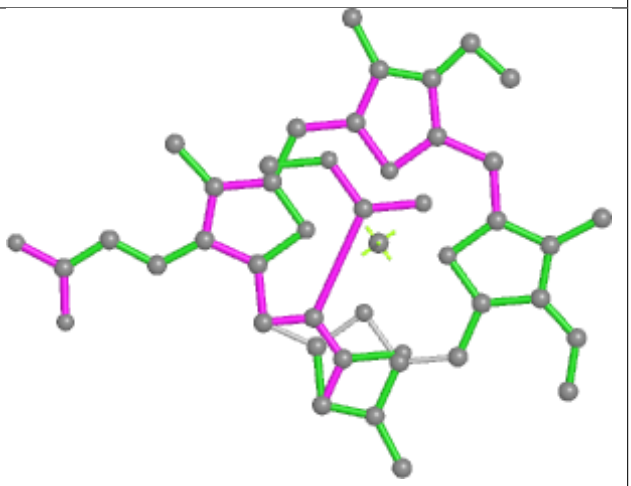
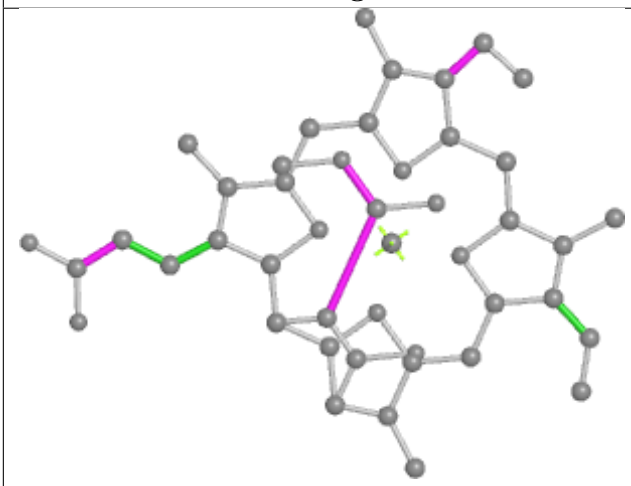


Bond angles



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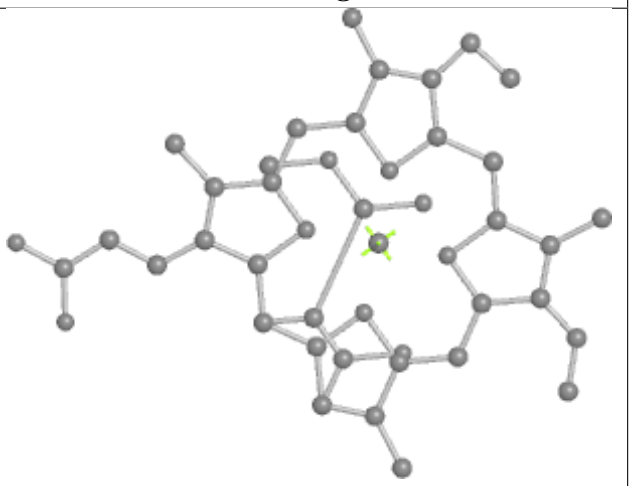
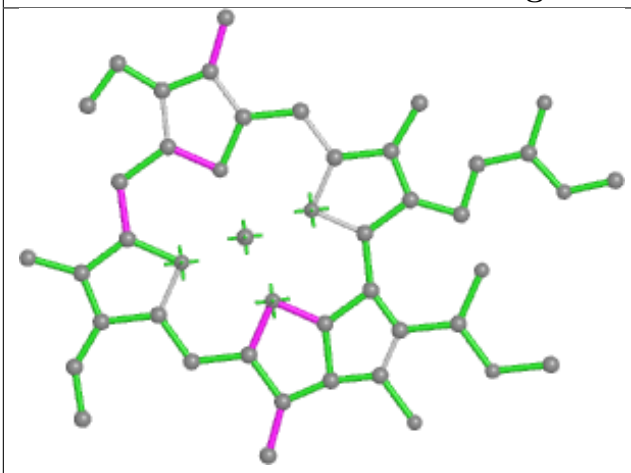


Rings

Ligand CLA F 311



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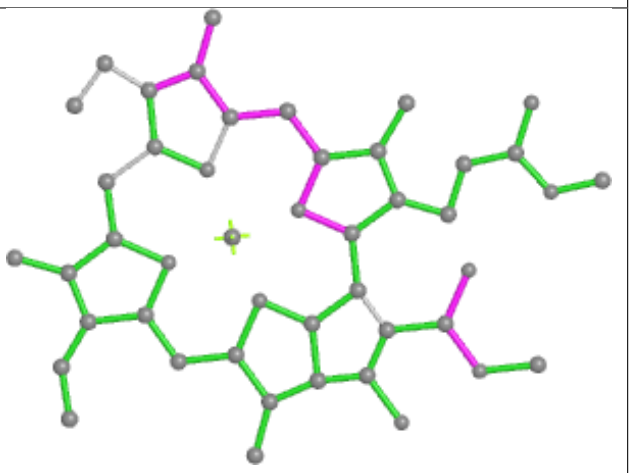
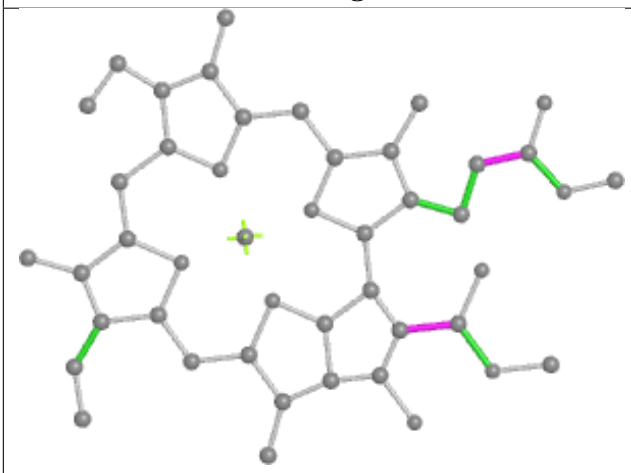


Bond angles



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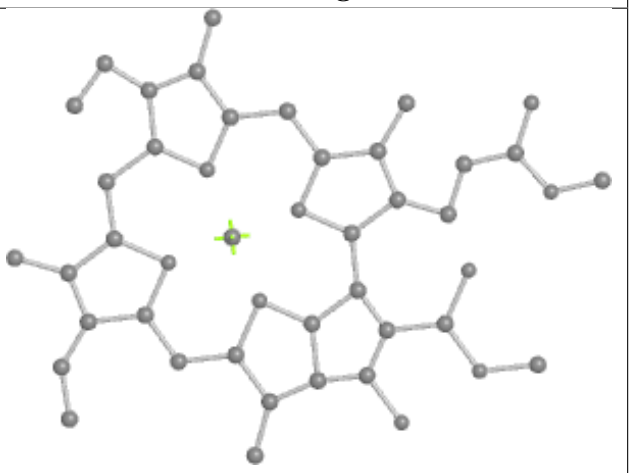
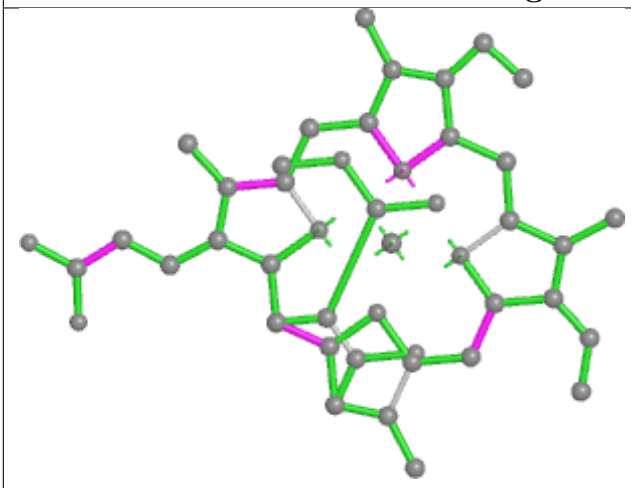


Rings

Ligand KC1 D 315



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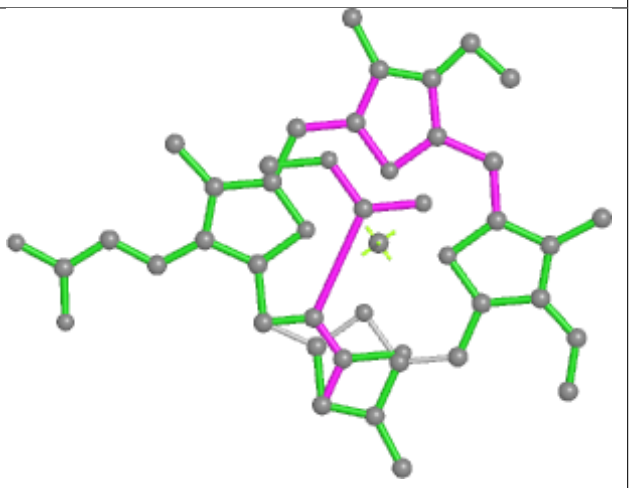

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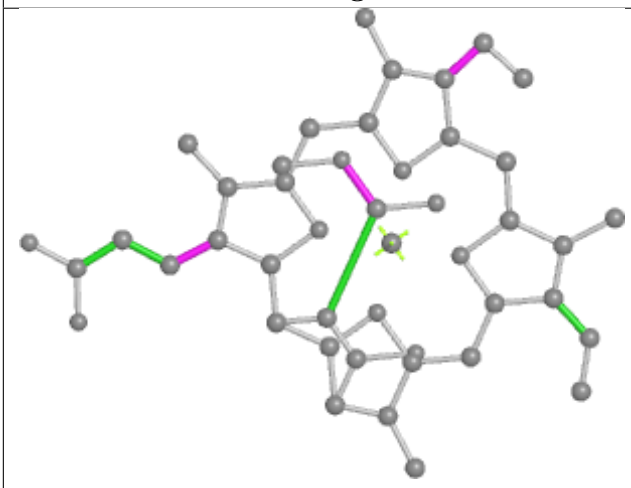

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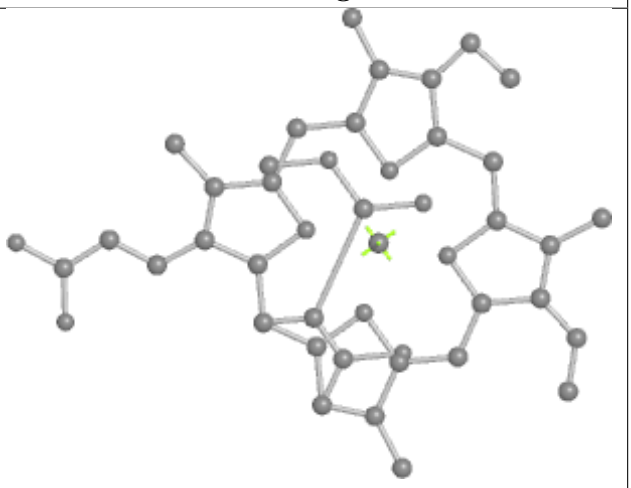
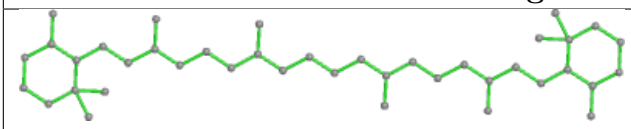


Rings

Ligand BCR a 835



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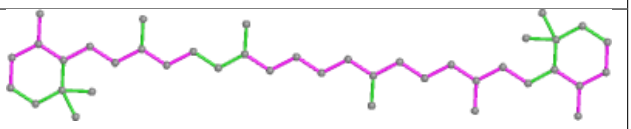
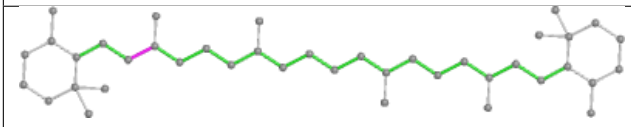
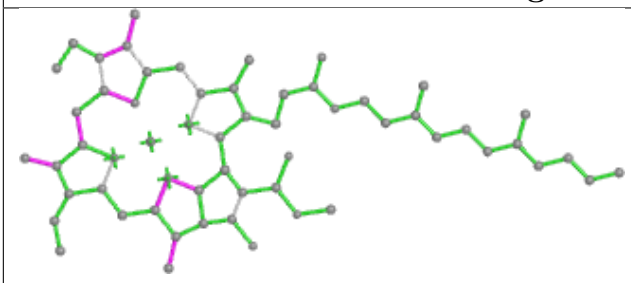
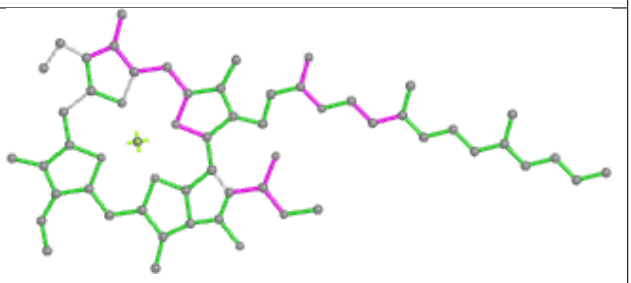
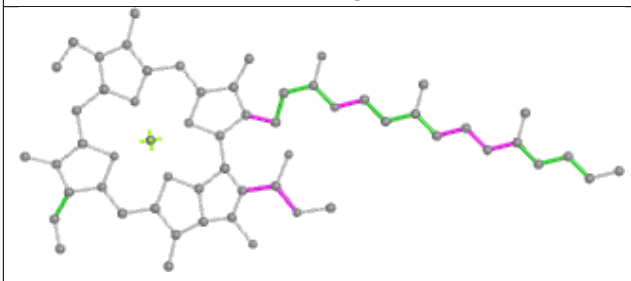
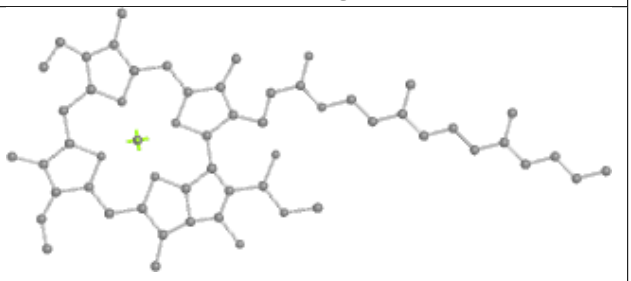


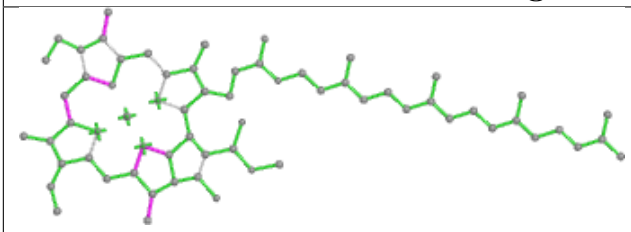
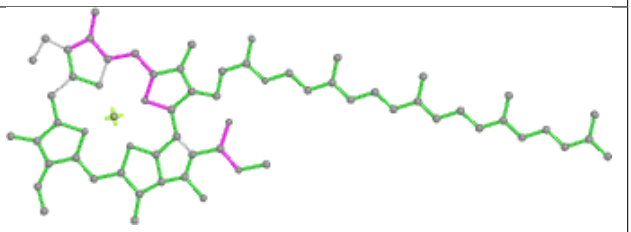
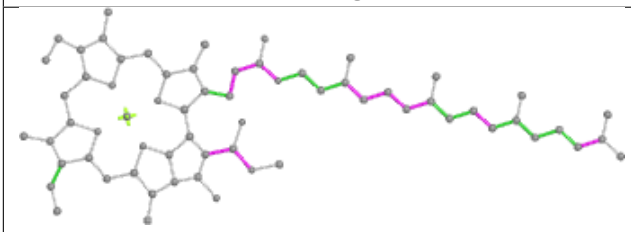
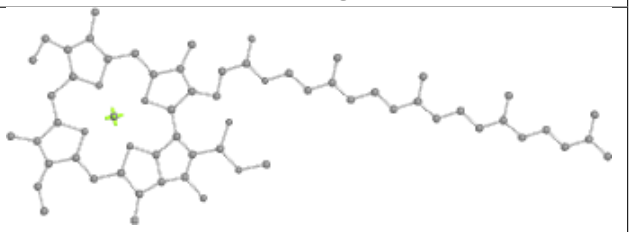
Bond angles



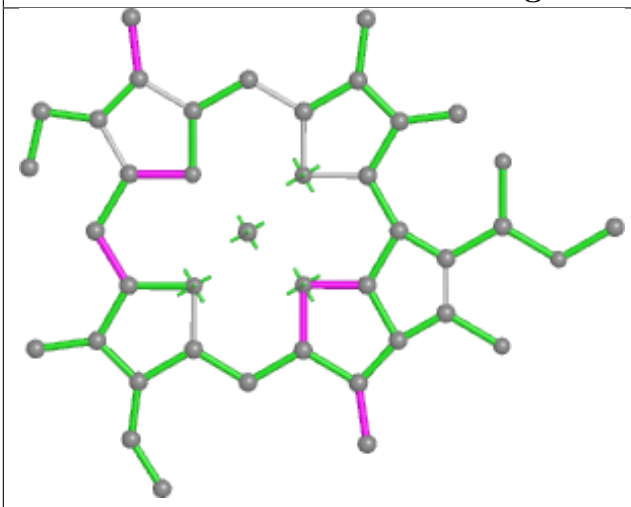
Torsions

Rings

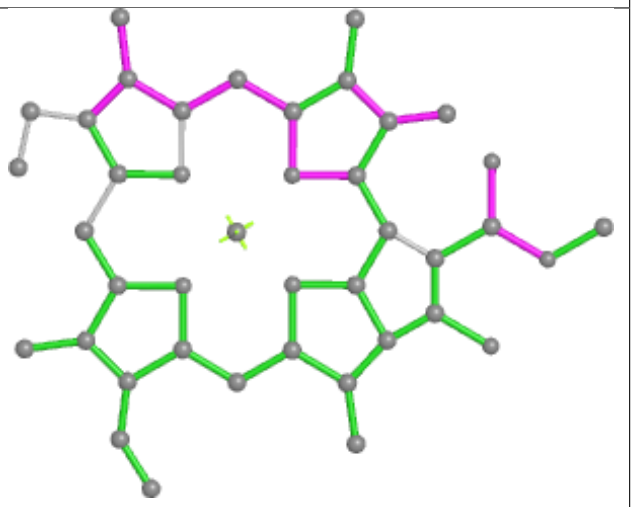
Ligand CLA b 721	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

Ligand CLA b 702	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

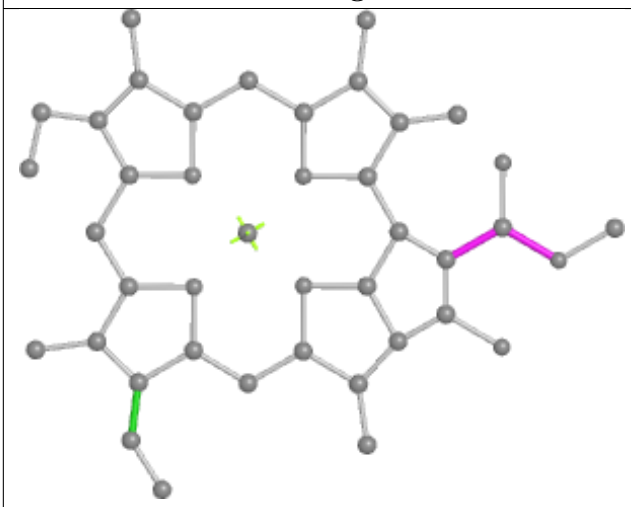
Ligand CLA C 316



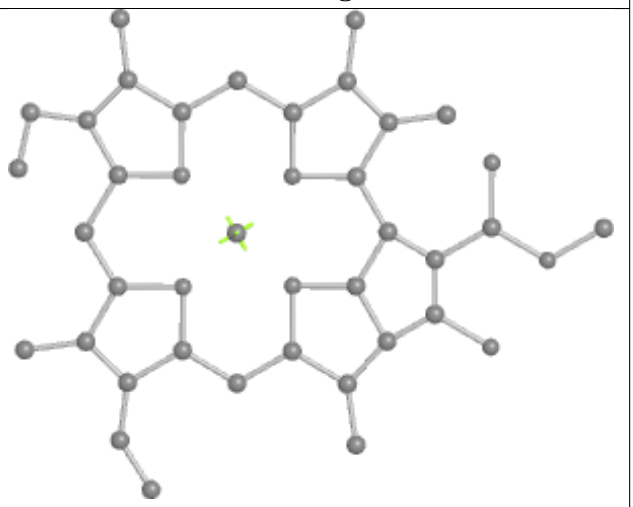
Bond lengths



Bond angles

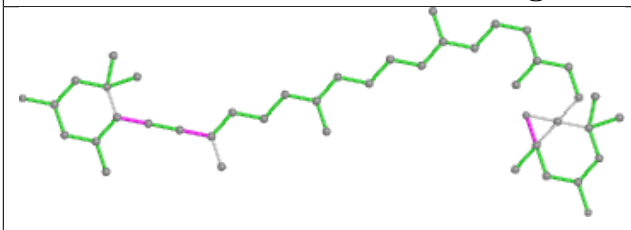


Torsions

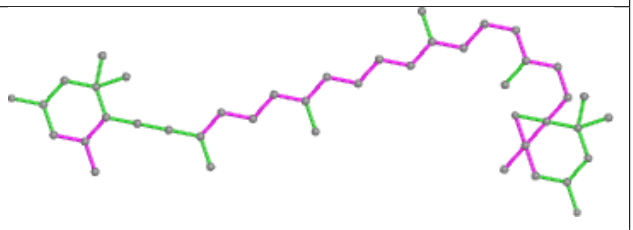


Rings

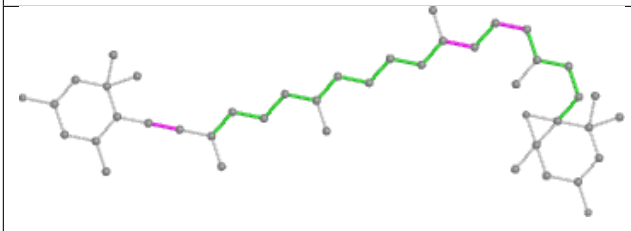
Ligand DD6 L 305



Bond lengths



Bond angles



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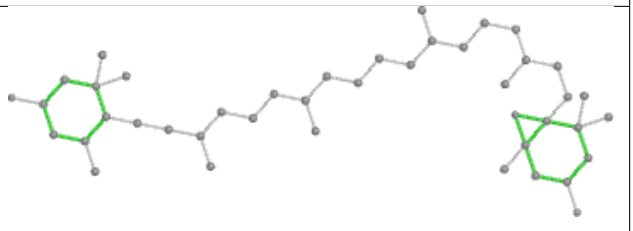
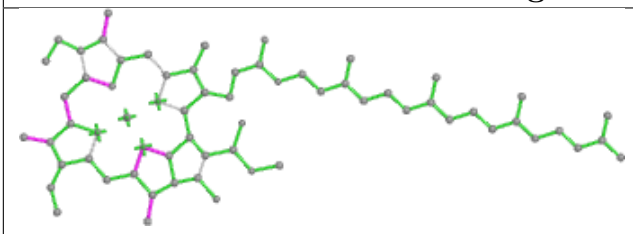


Rings

Ligand CLA b 706



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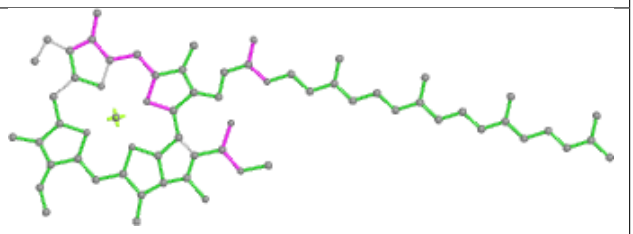
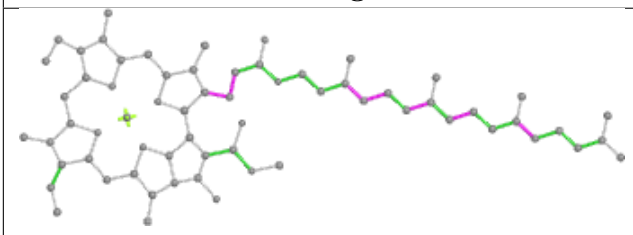
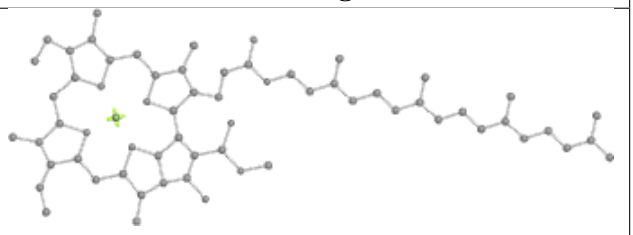


Bond angles

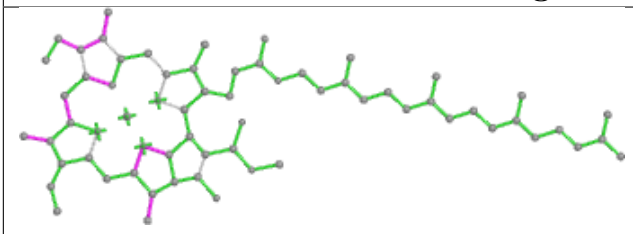


Torsions



Rings

Ligand CLA l 502



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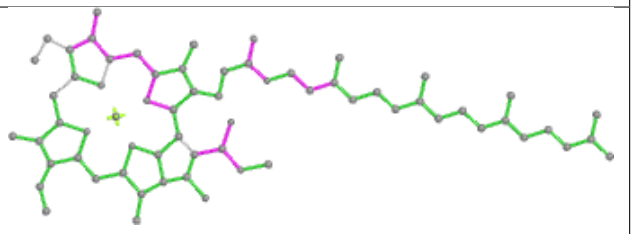
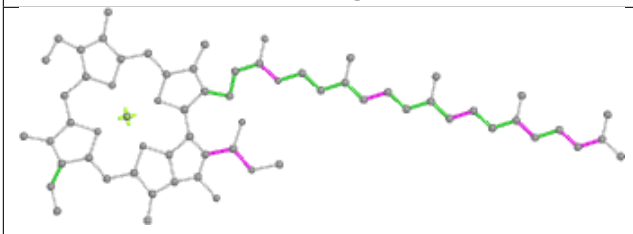


Bond angles



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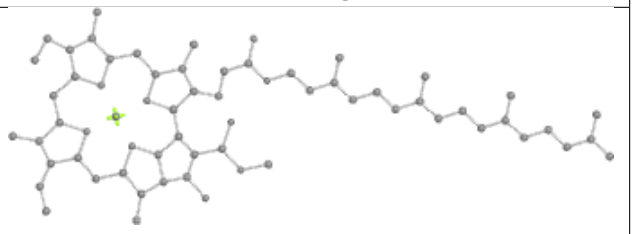
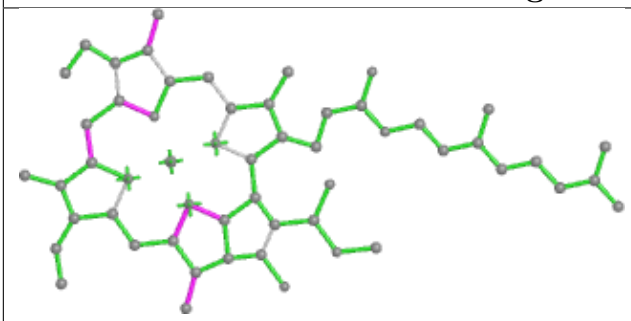


Rings

Ligand CLA L 310



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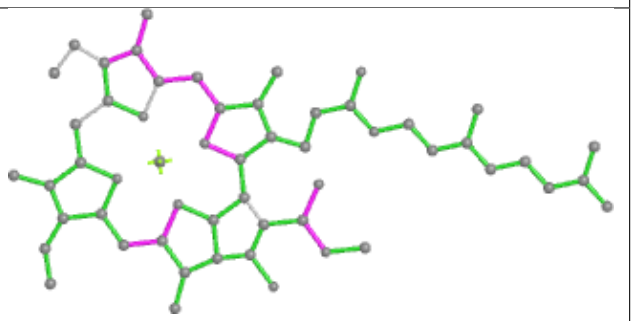
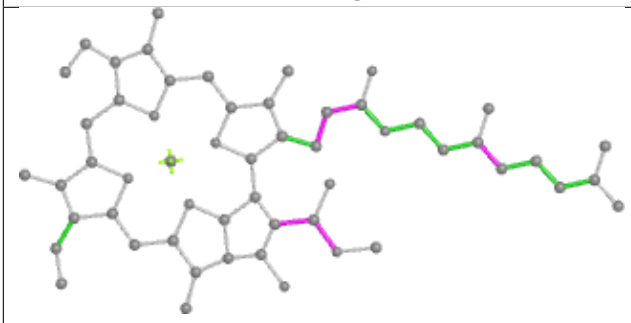


Bond angles



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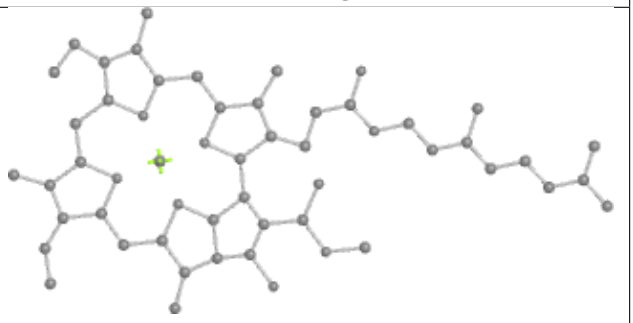
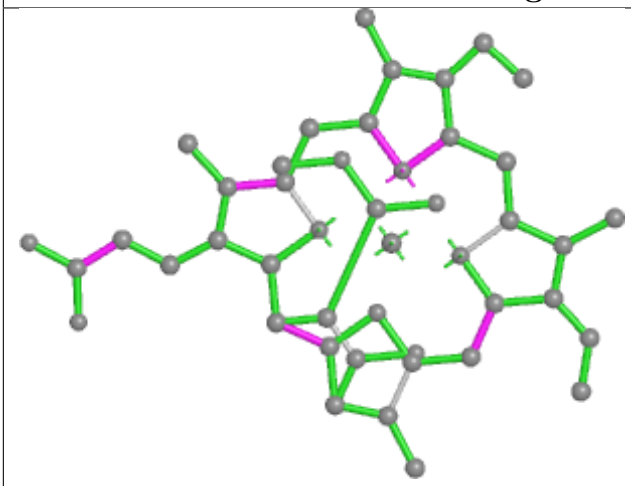


Rings

Ligand KC1 K 215



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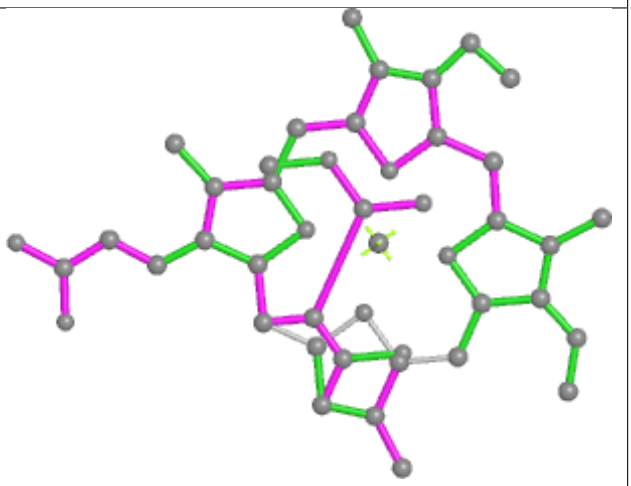
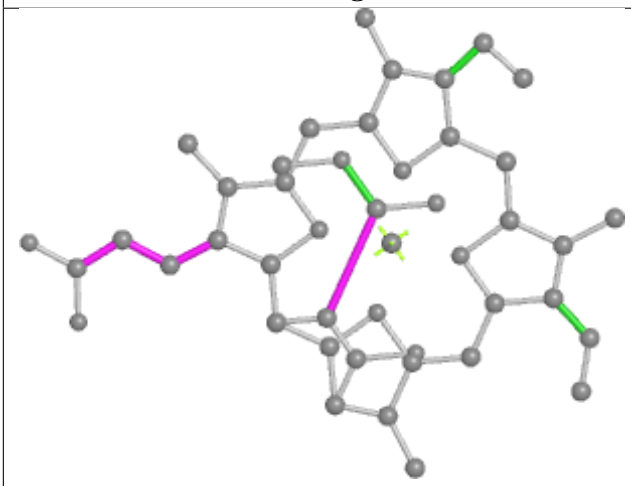


Bond angles



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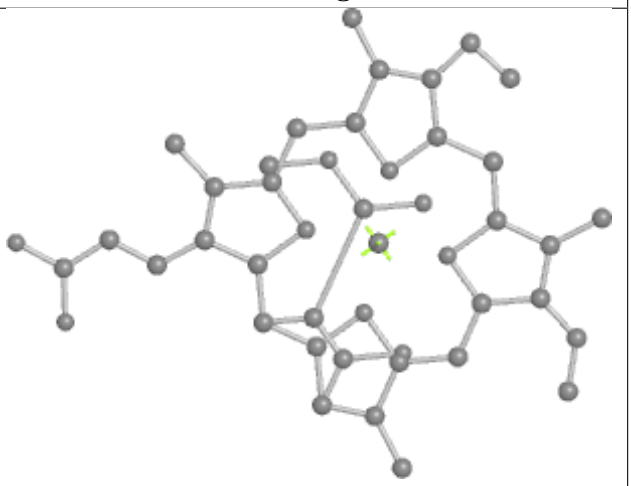
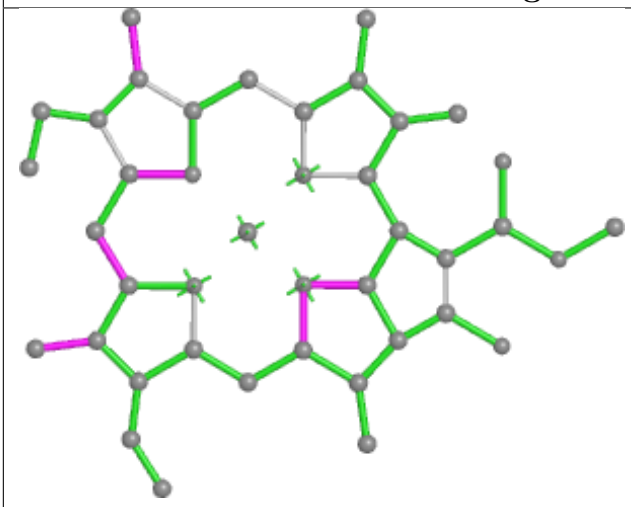


Rings

Ligand CLA D 316



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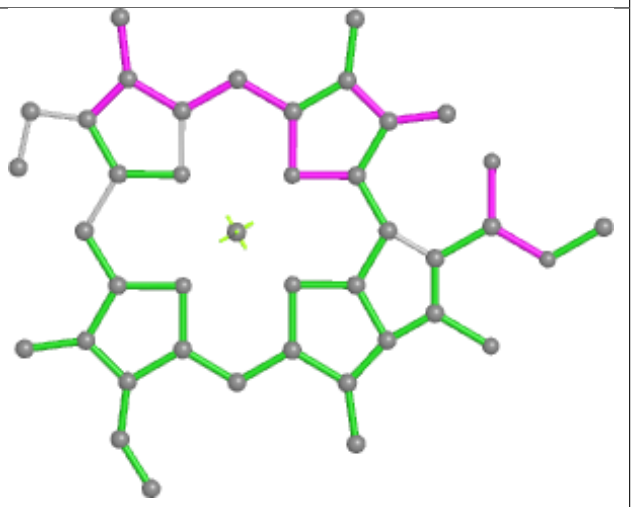
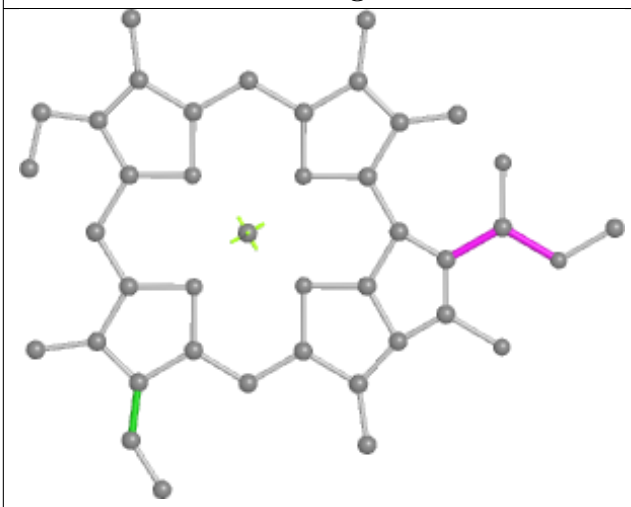


Bond angles



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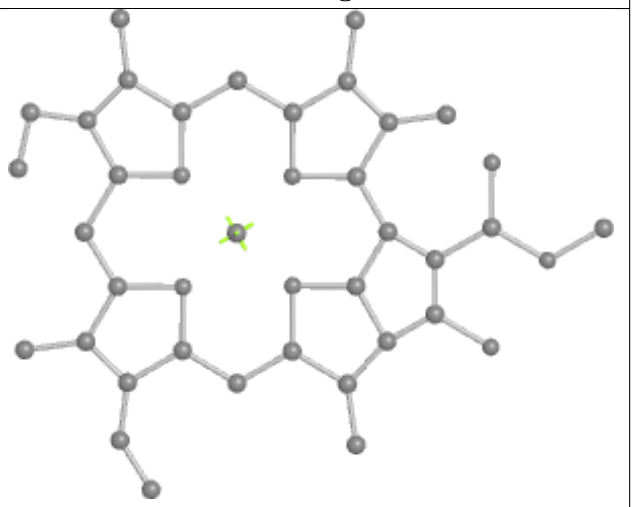
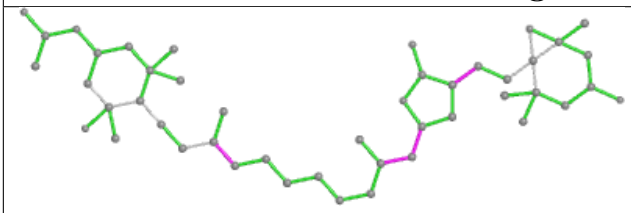


Rings

Ligand PID O 301



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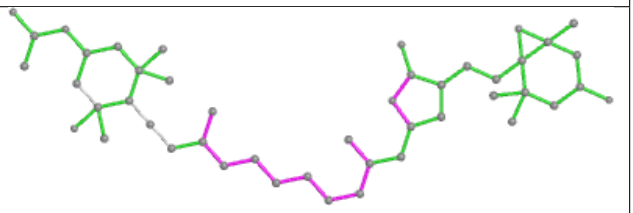
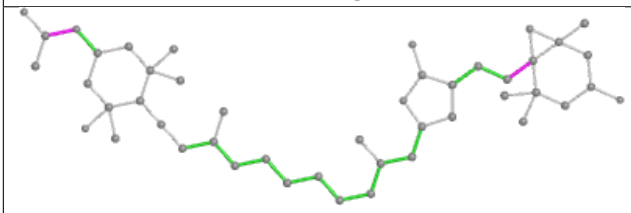


Bond angles



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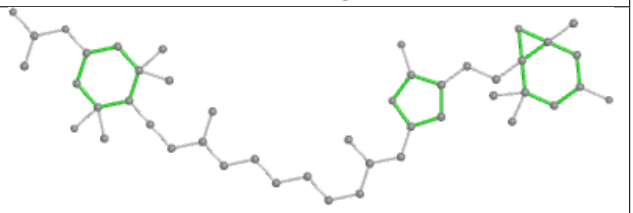
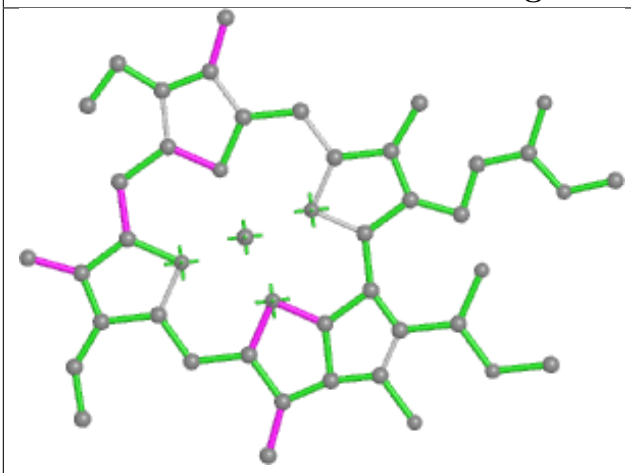


Rings

Ligand CLA T 309



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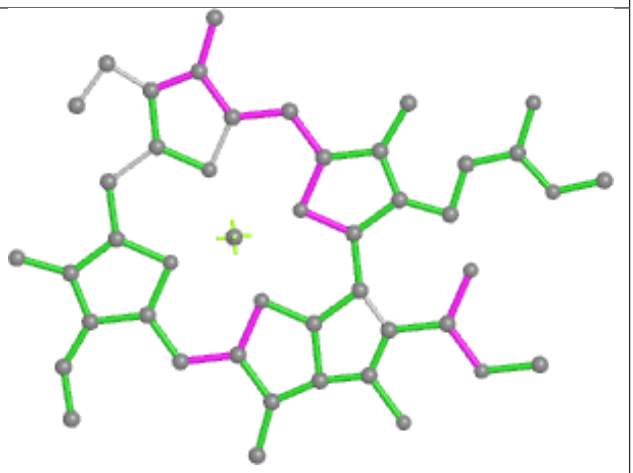
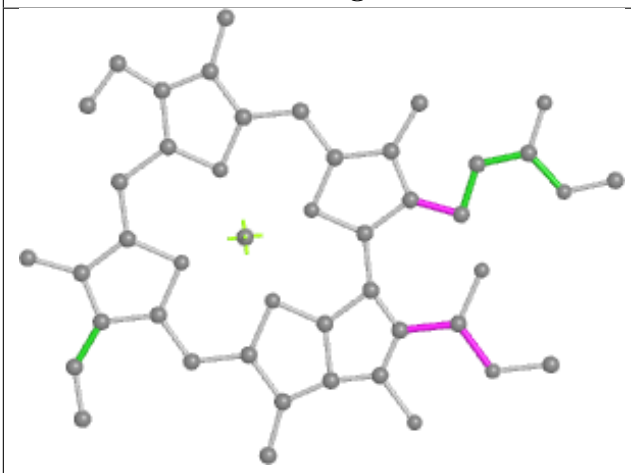


Bond angles



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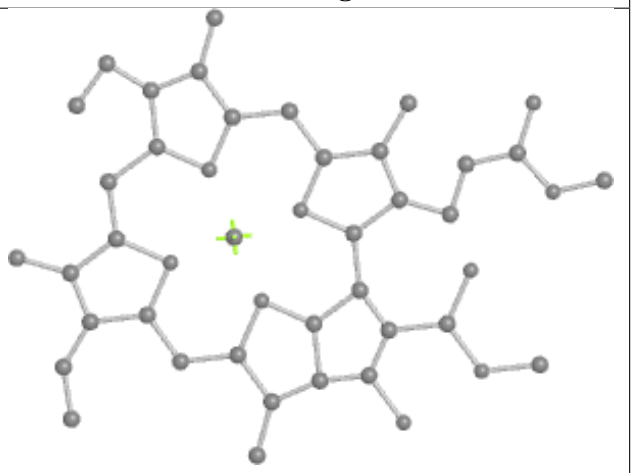
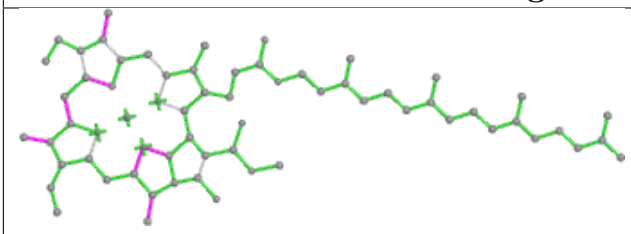


Rings

Ligand CLA b 723



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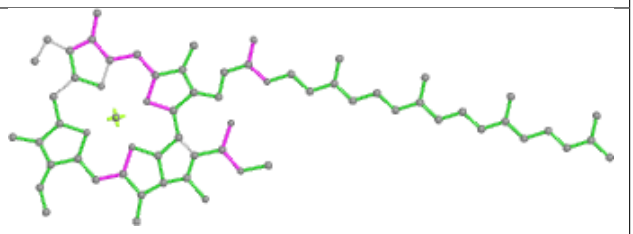
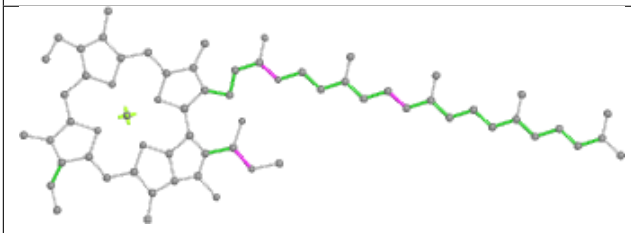


Bond angles



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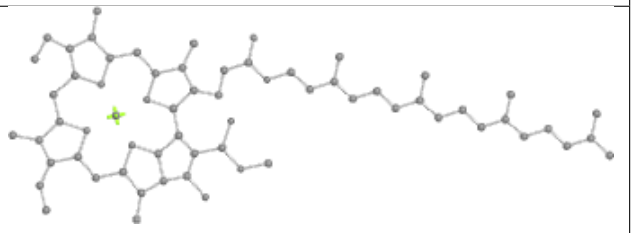
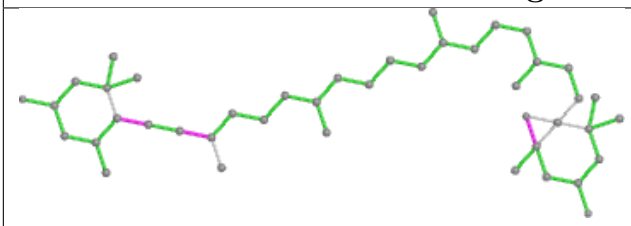


Rings

Ligand DD6 F 303



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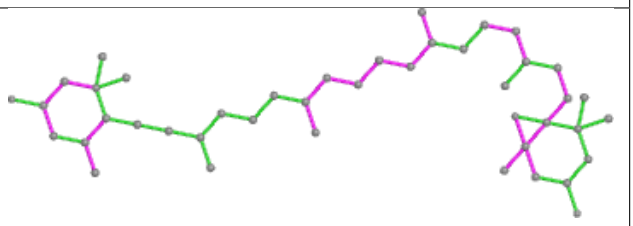
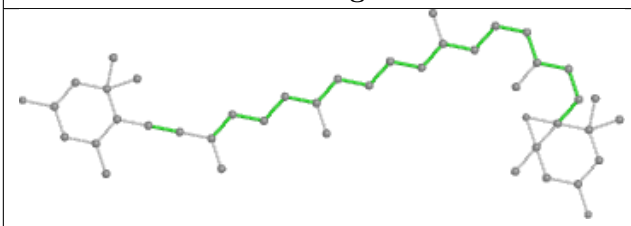


Bond angles



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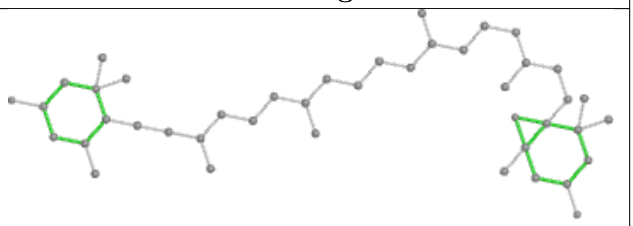
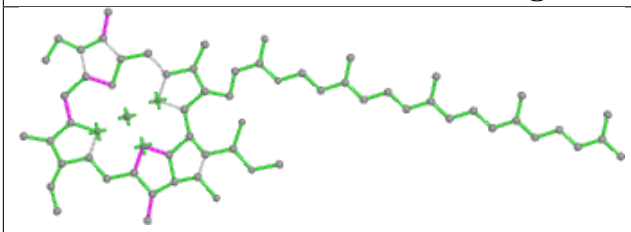


Rings

Ligand CLA a 802



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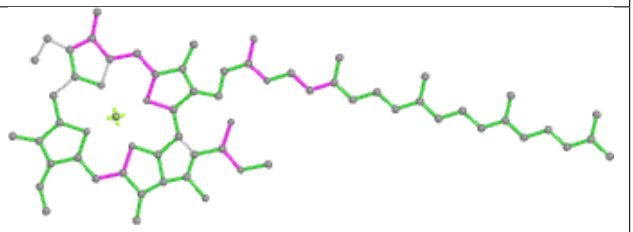
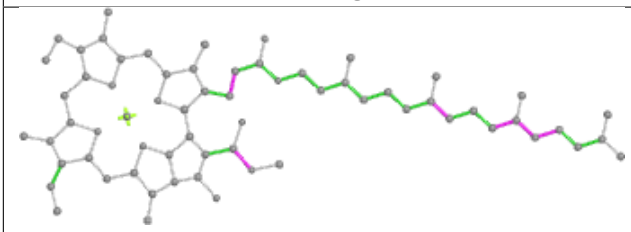


Bond angles



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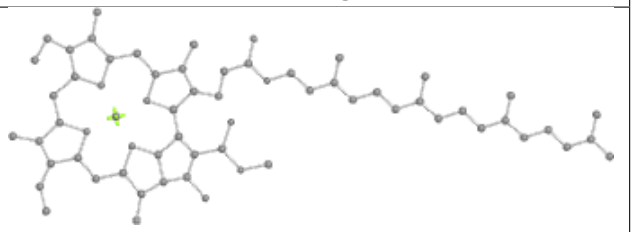
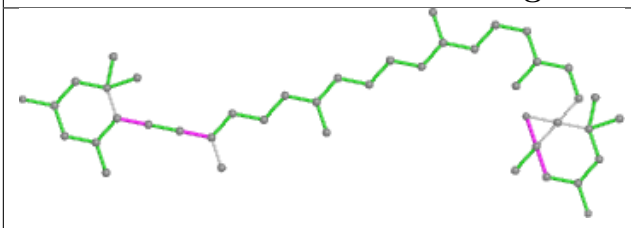


Rings

Ligand DD6 K 221



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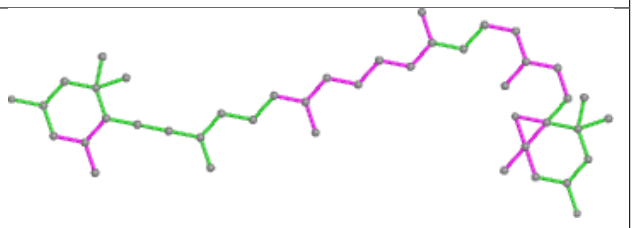
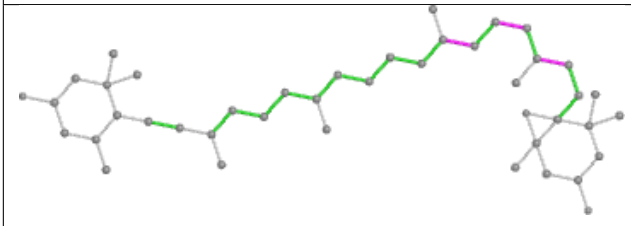


Bond angles



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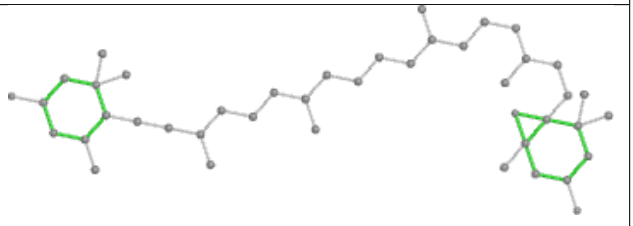
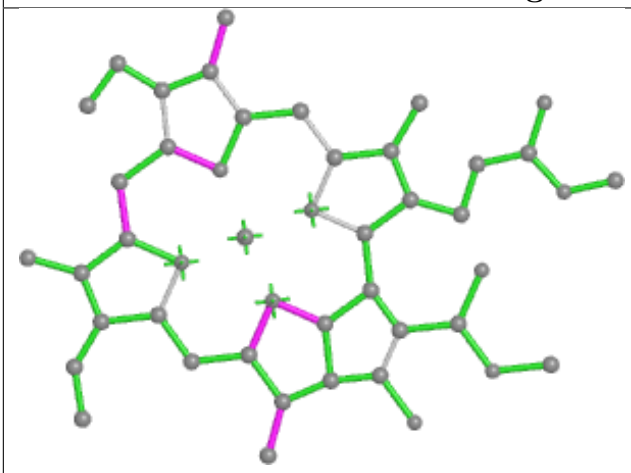


Rings

Ligand CLA F 312



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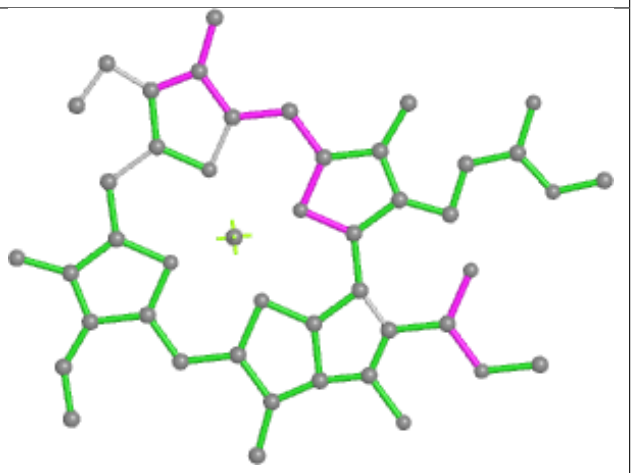
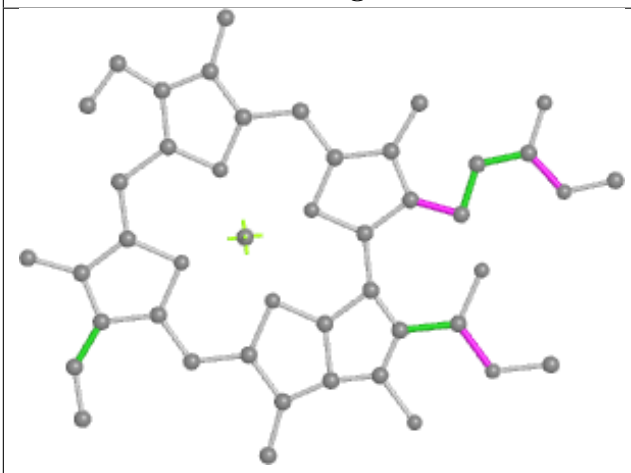


Bond angles



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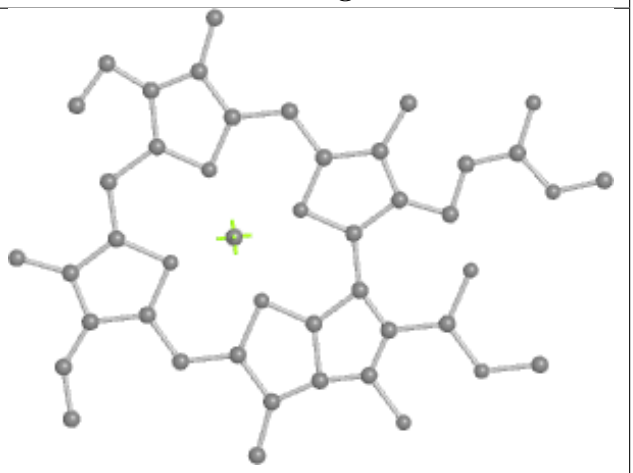
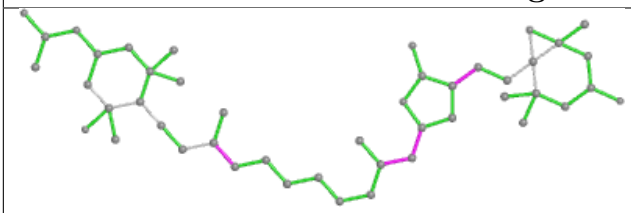
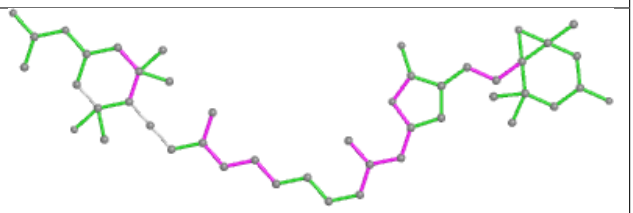


Rings

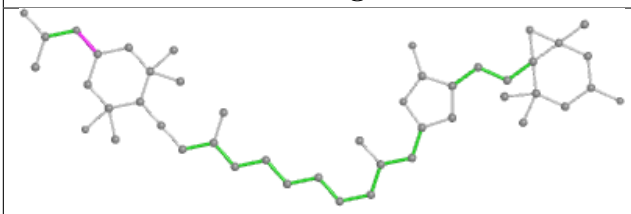
Ligand PID D 303



Bond lengths



Bond angles



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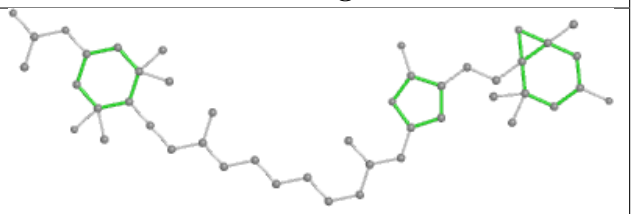
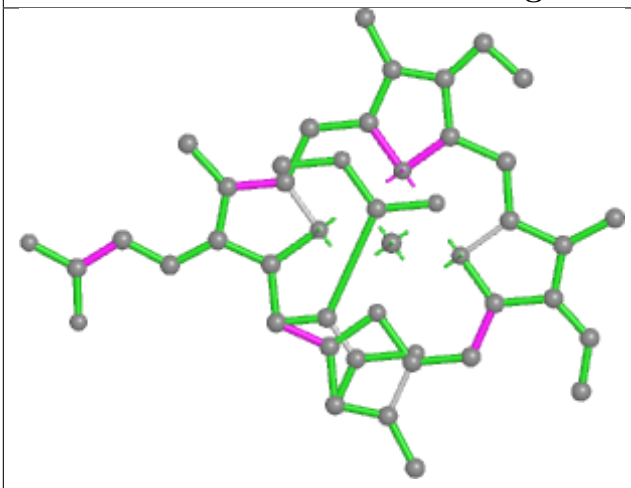
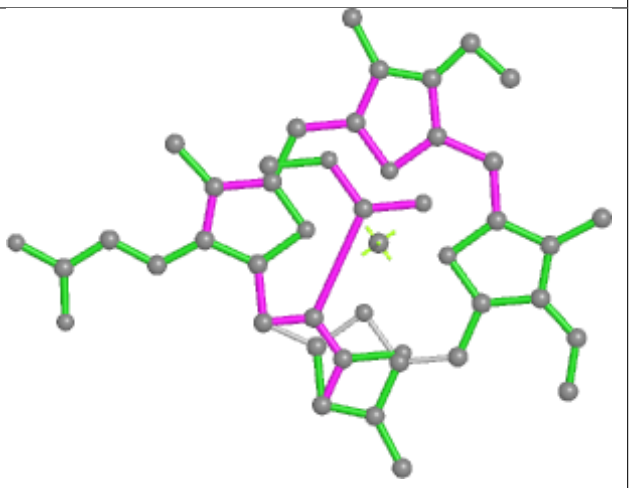


Rings

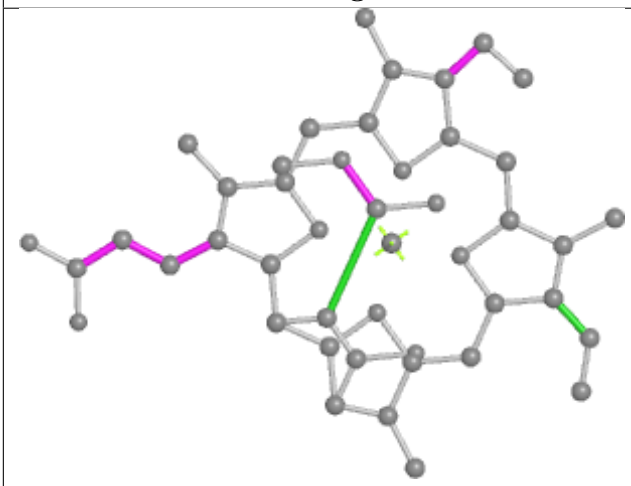
Ligand KC1 H 309



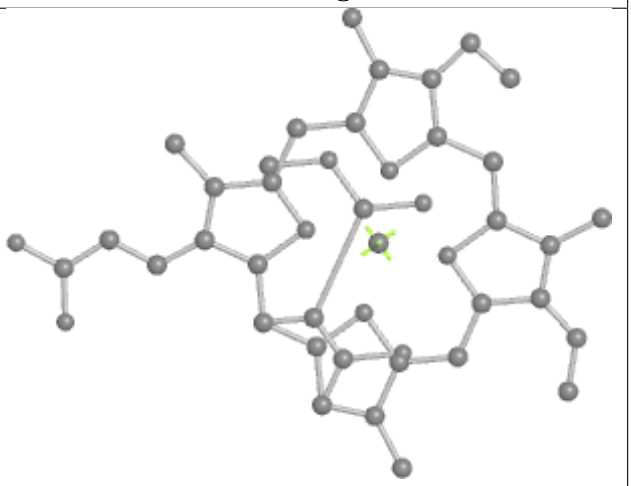
Bond lengths



Bond angles

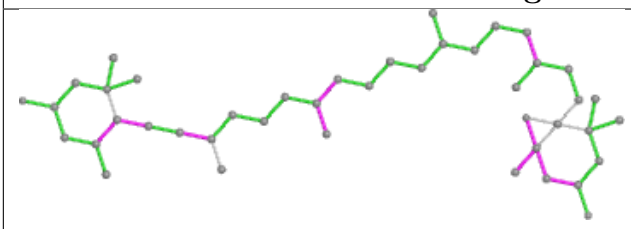


Torsions



Rings

Ligand DD6 G 307



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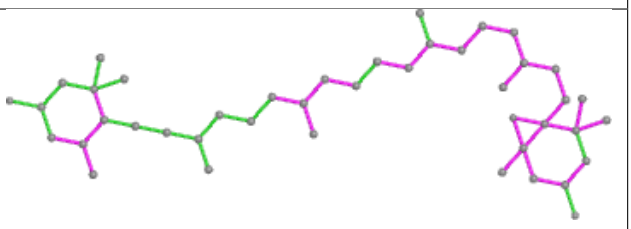

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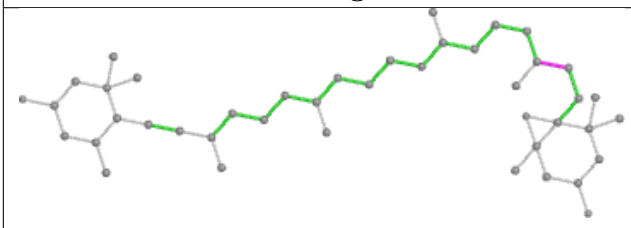

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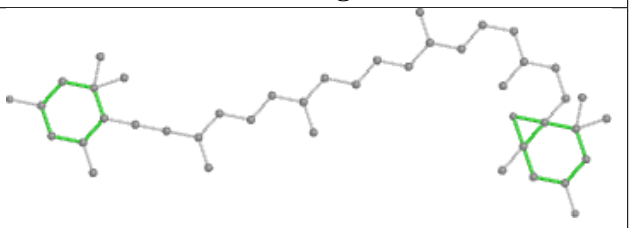
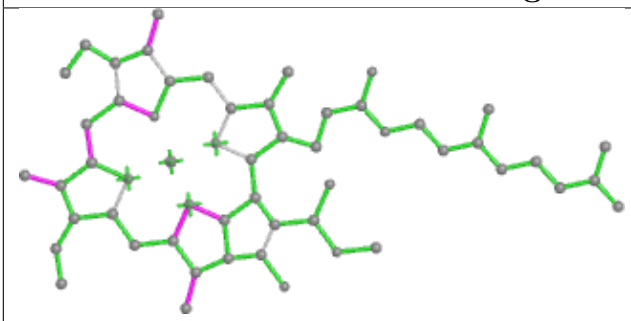


Rings

Ligand CLA A 212



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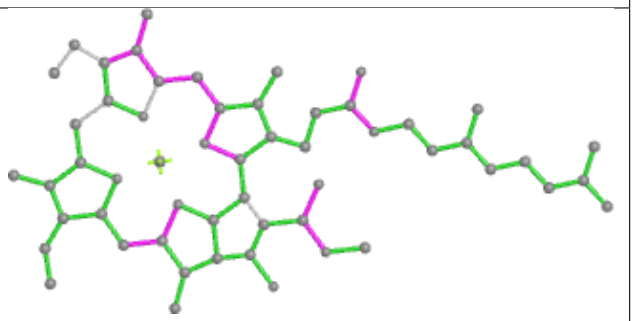
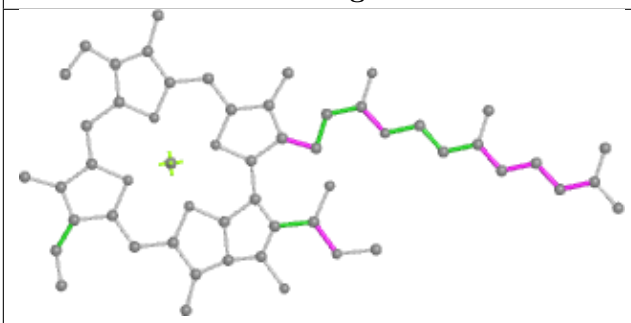


Bond angles



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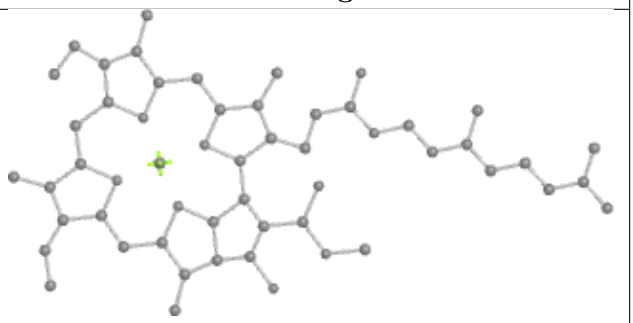
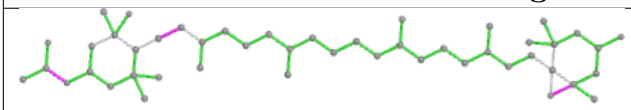


Rings

Ligand UIX L 302



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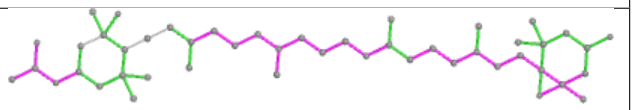

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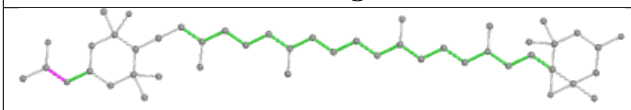

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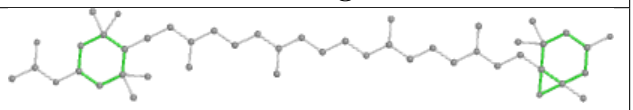
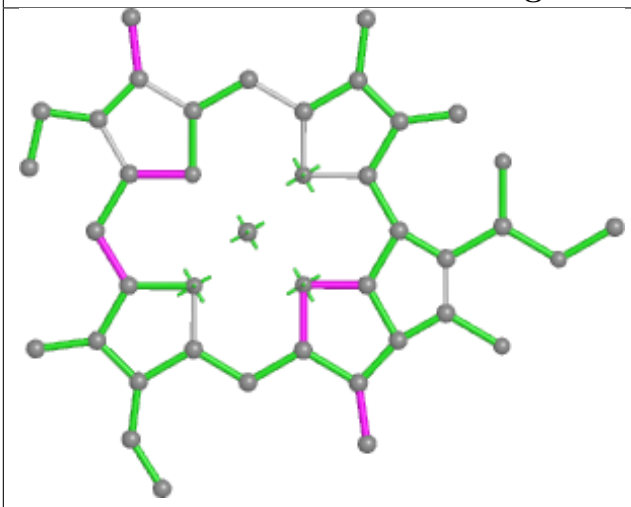


Rings

Ligand CLA T 316



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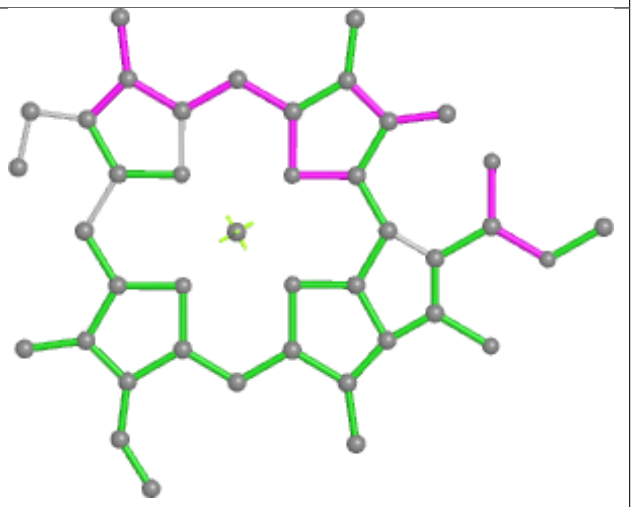
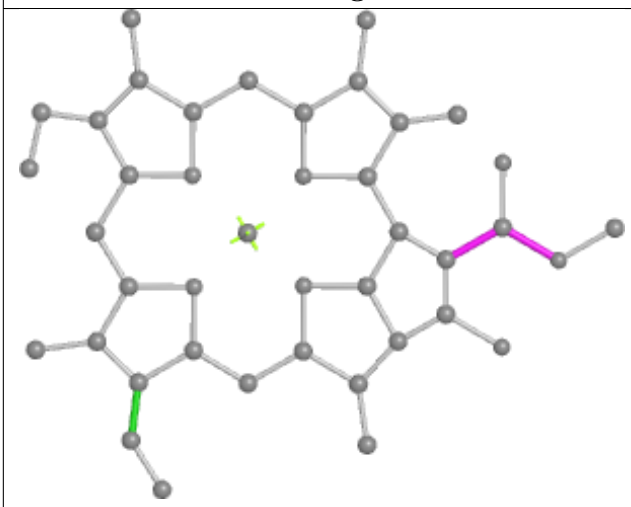


Bond angles



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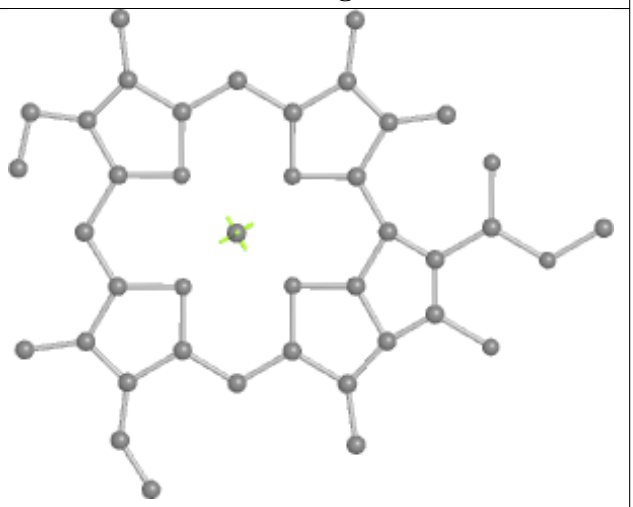
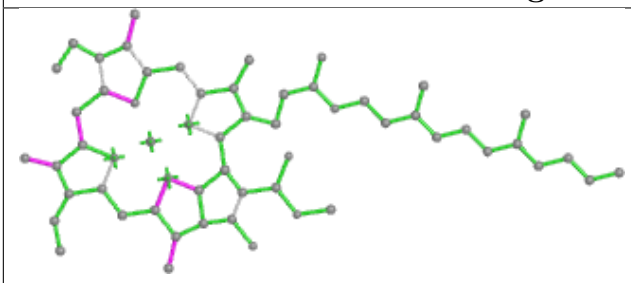
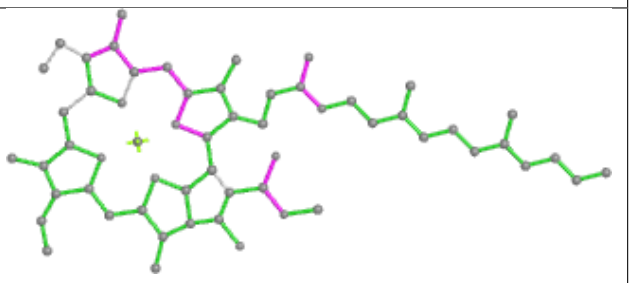
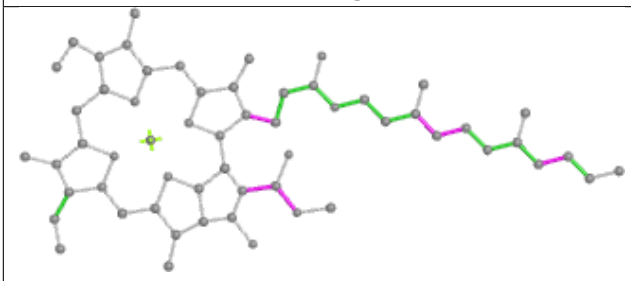
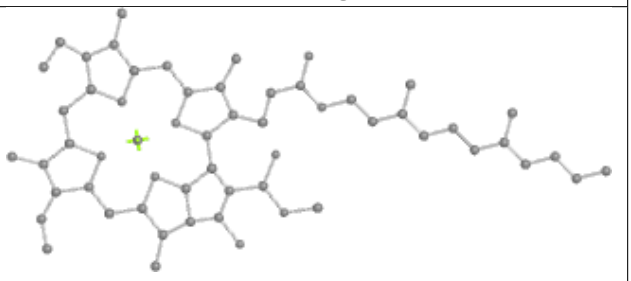


Rings

Ligand CLA b 722	
 Bond lengths	 Bond angles
 Torsions	 Rings

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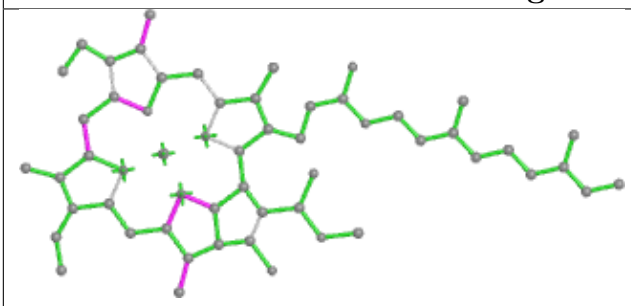
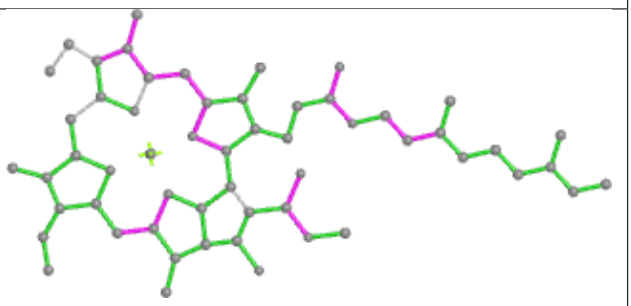
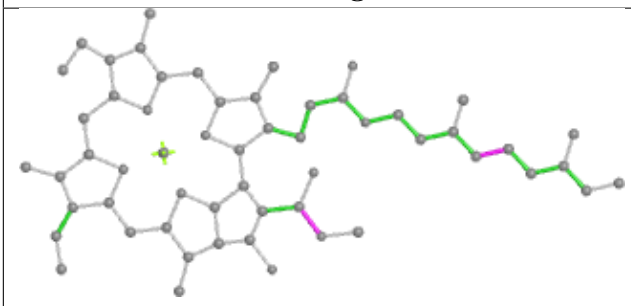
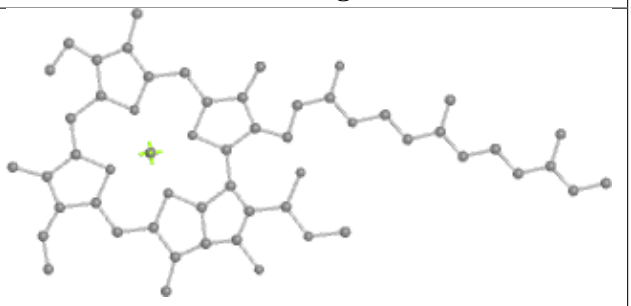
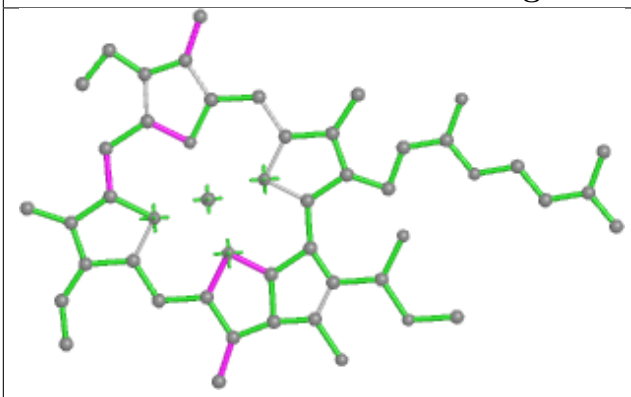
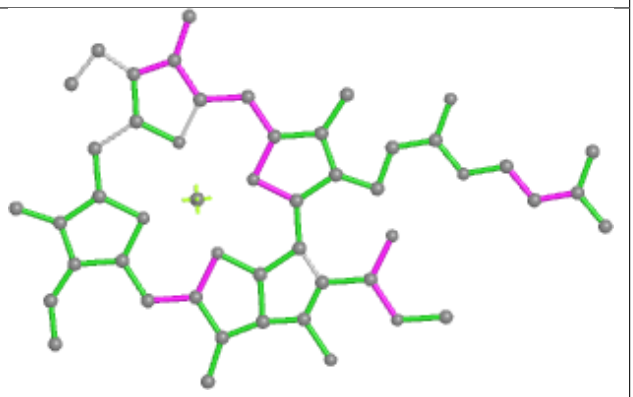
 Bond lengths	 Bond angles
 Torsions	 Rings

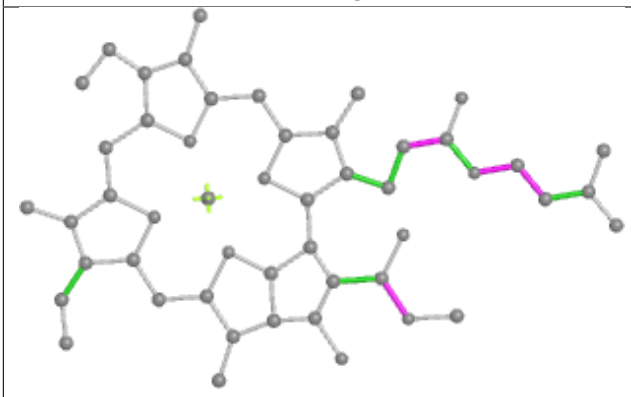
Ligand CLA K 210



Bond lengths



Bond angles



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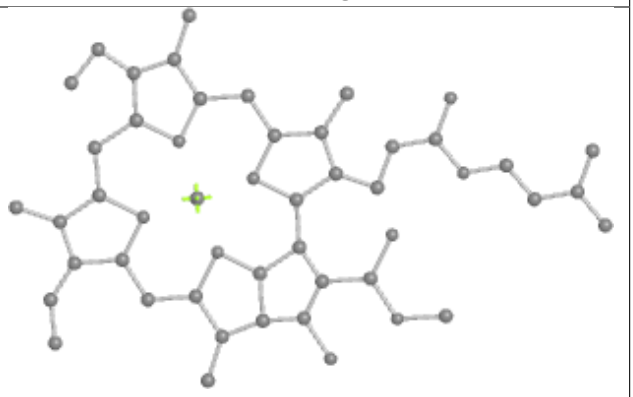
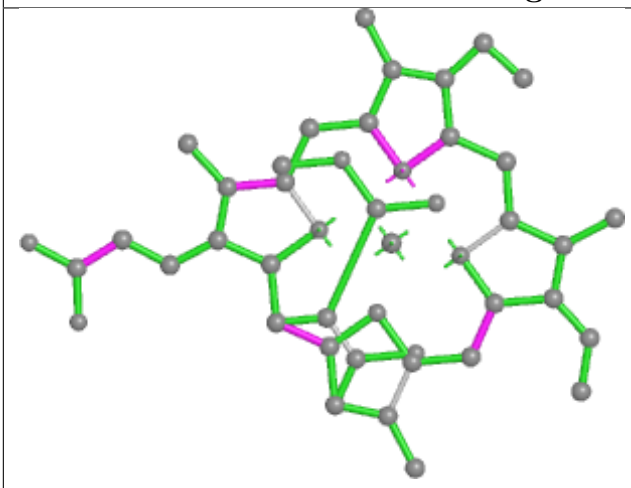
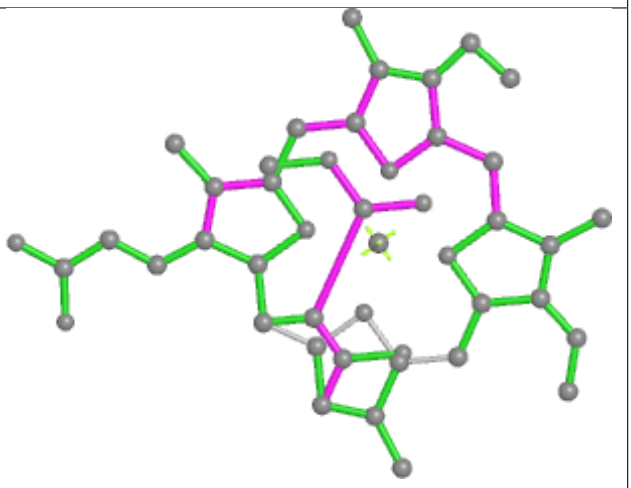


Rings

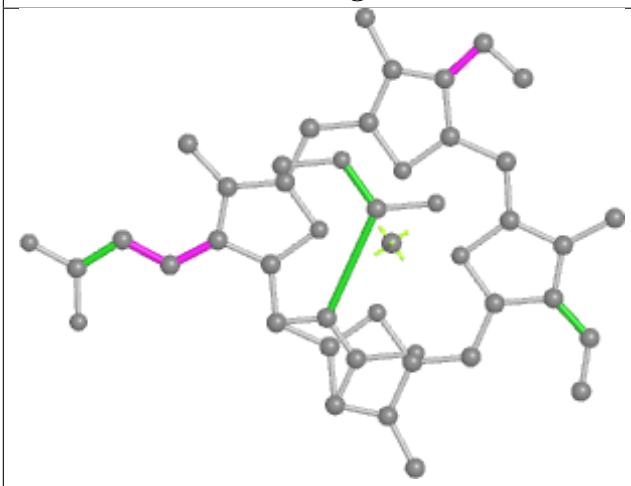
Ligand KC1 D 310



Bond lengths



Bond angles



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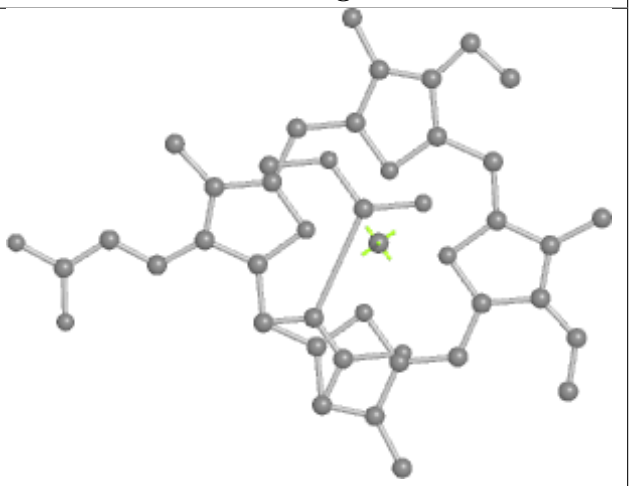
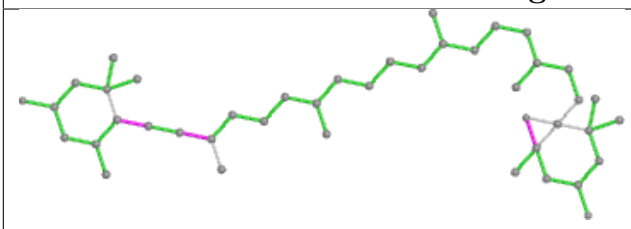


Rings

Ligand DD6 J 301



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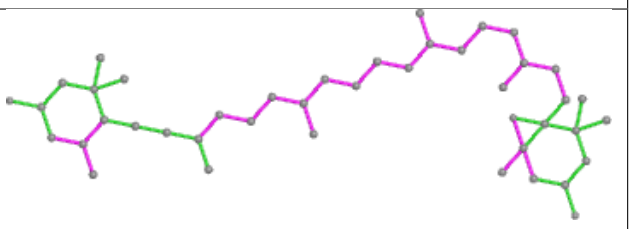

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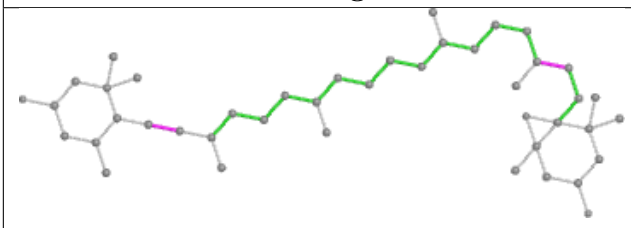

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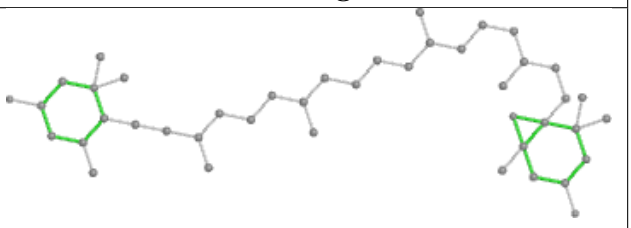
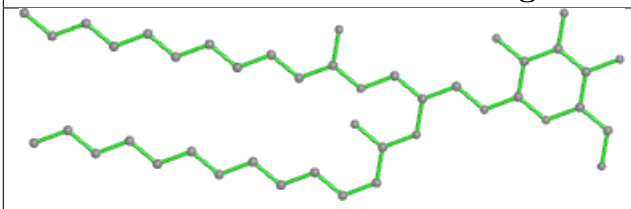


Rings

Ligand LMG K 201



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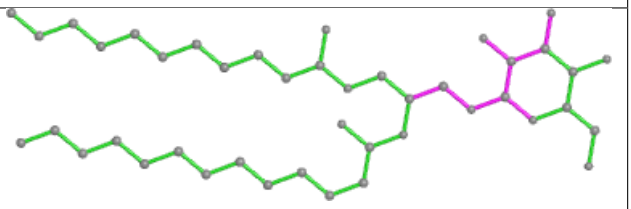
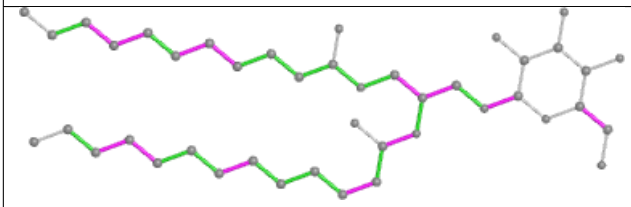


Bond angles



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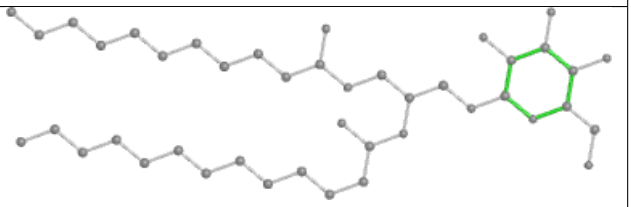
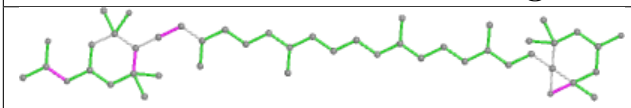


Rings

Ligand UIX N 306



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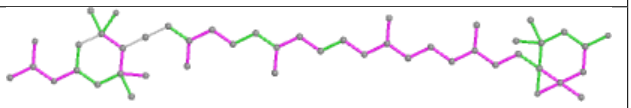
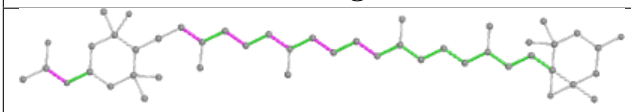


Bond angles



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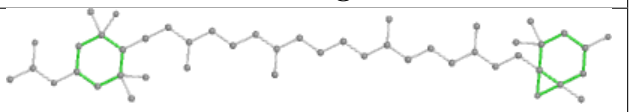
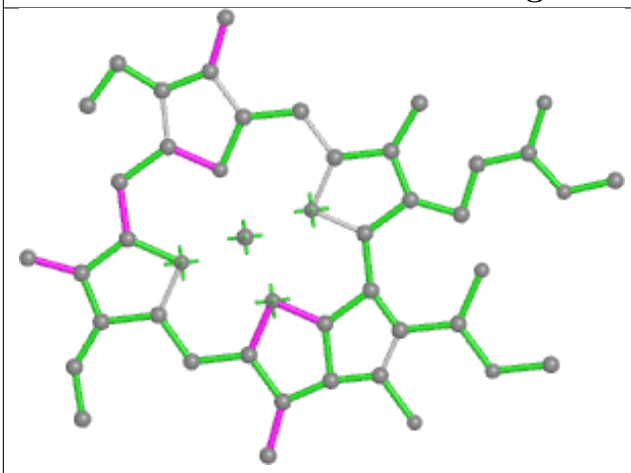


Rings

Ligand CLA F 310



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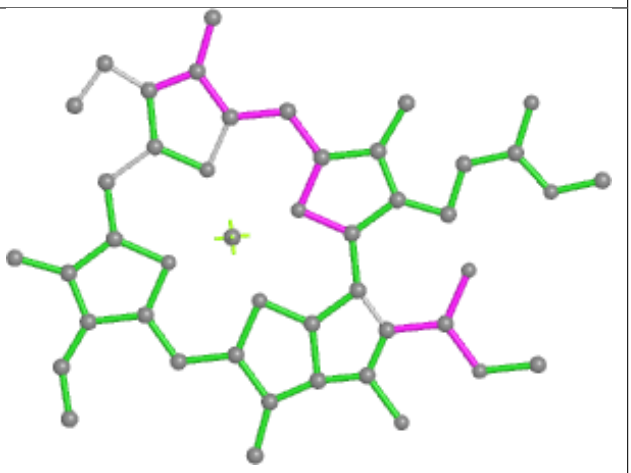
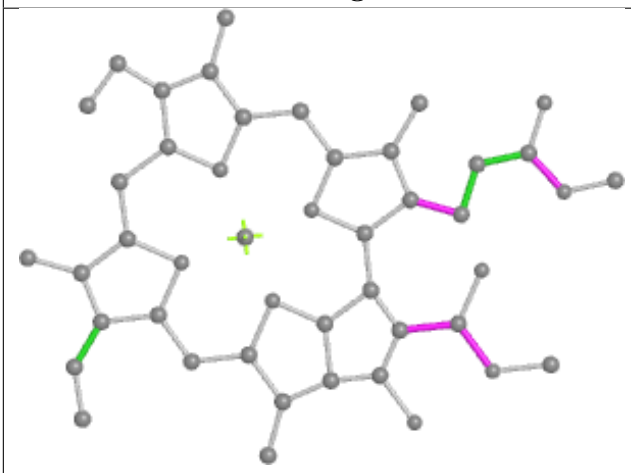


Bond angles



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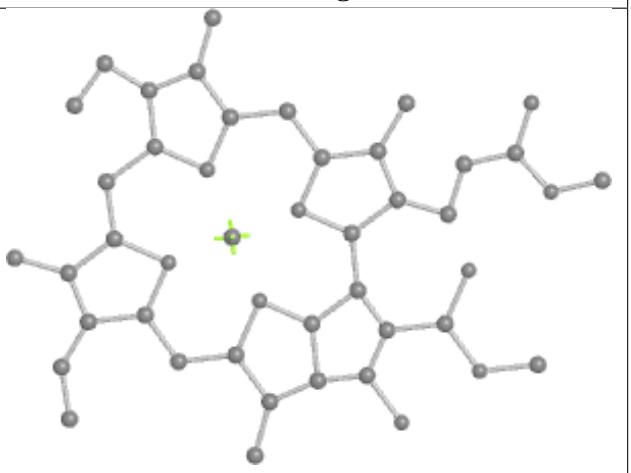
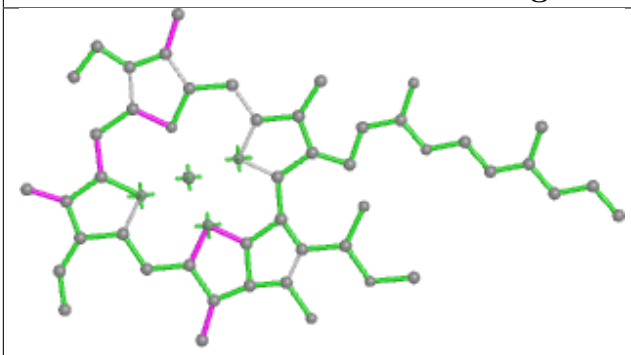
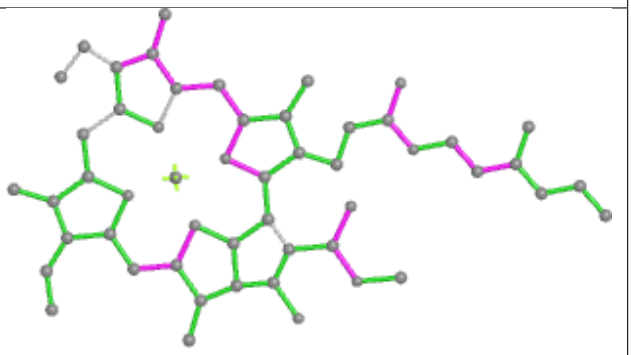
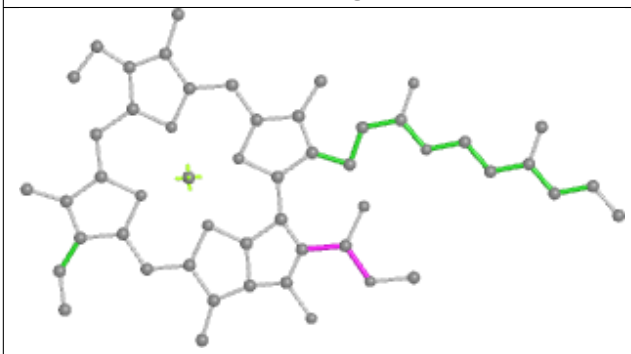
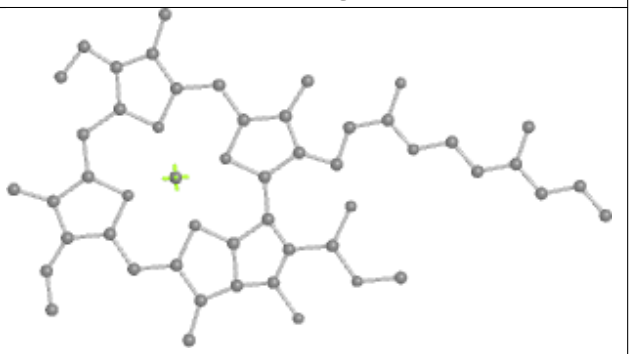
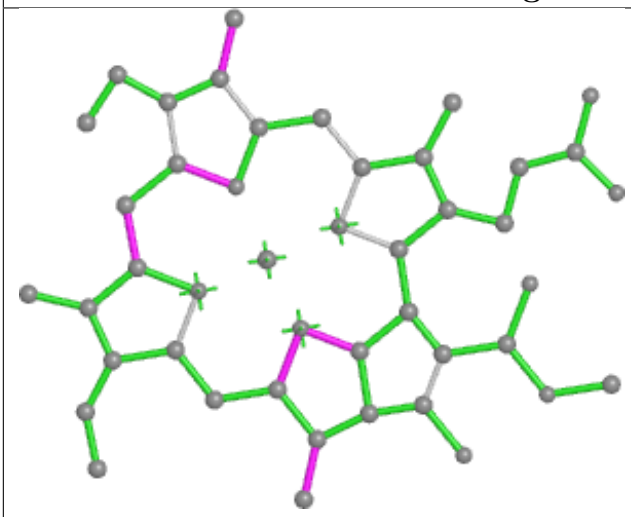


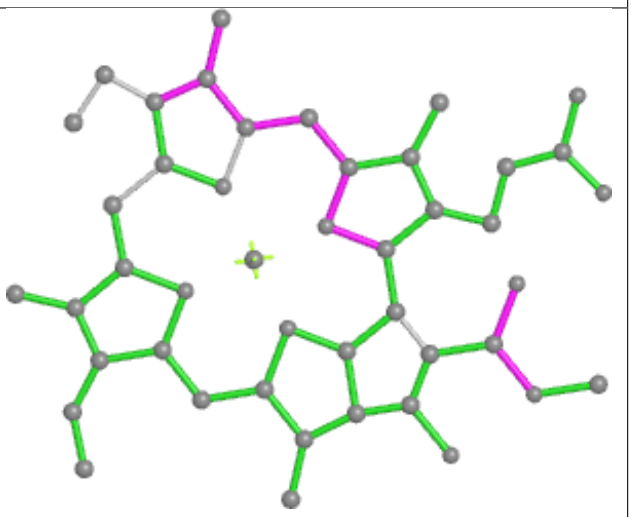
Rings

Ligand CLA I 216	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

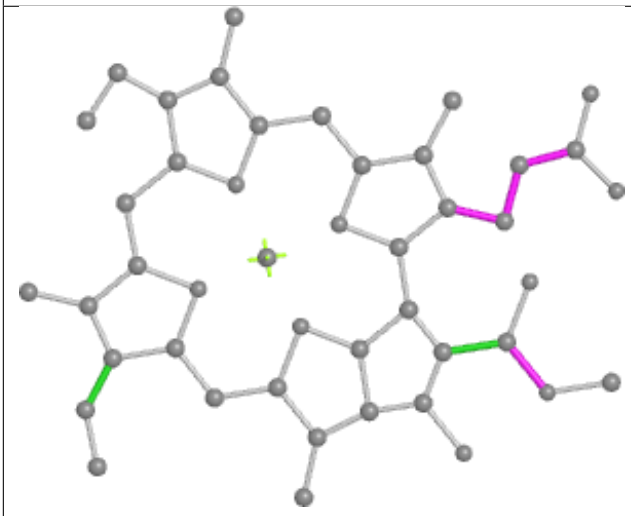
Ligand CLA K 218



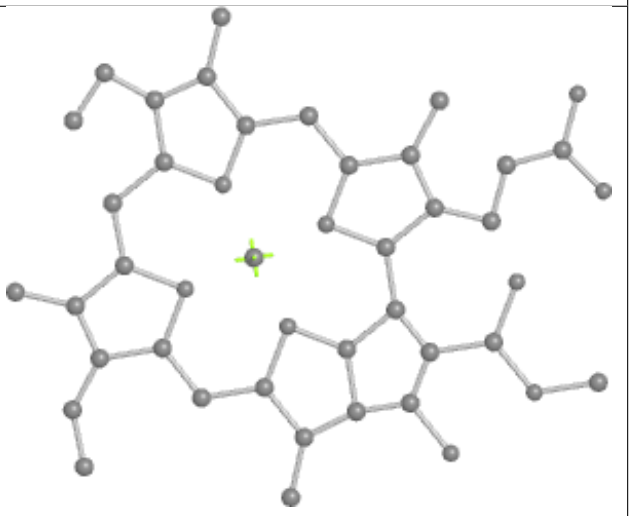
Bond lengths



Bond angles

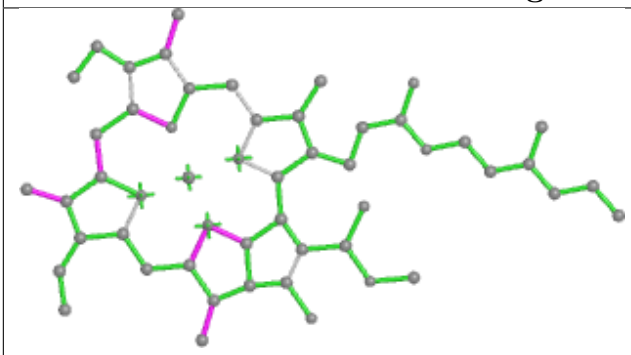


Torsions

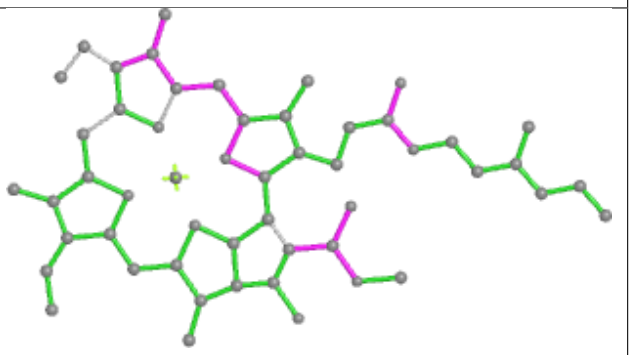


Rings

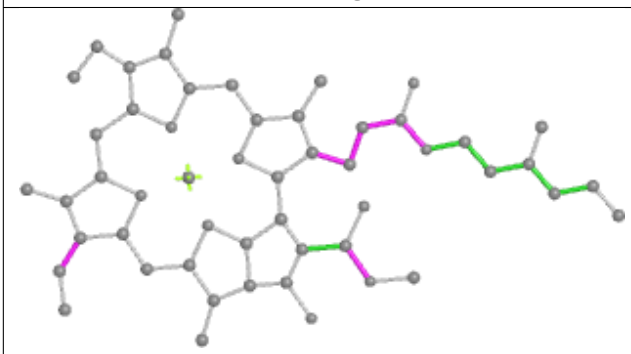
Ligand CLA L 316



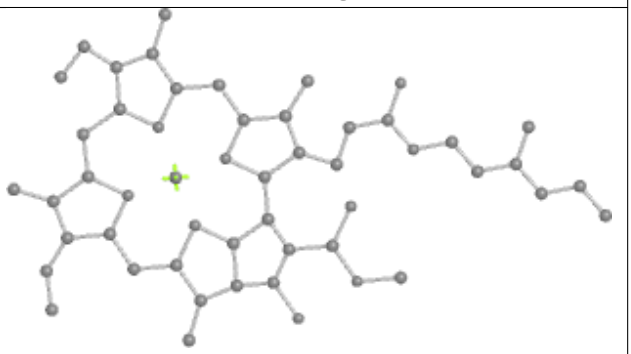
Bond lengths



Bond angles

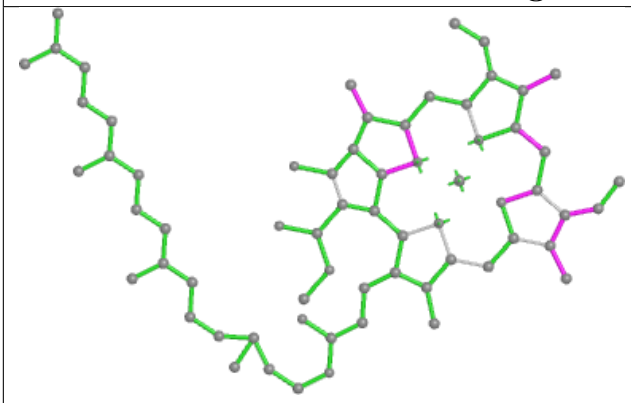


Torsions



Rings

Ligand CLA b 736



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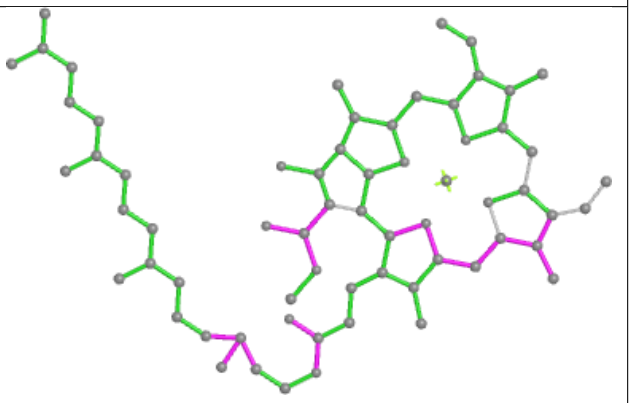
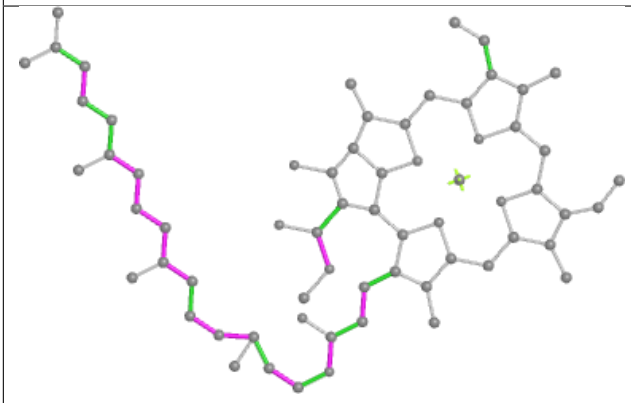


Bond angles



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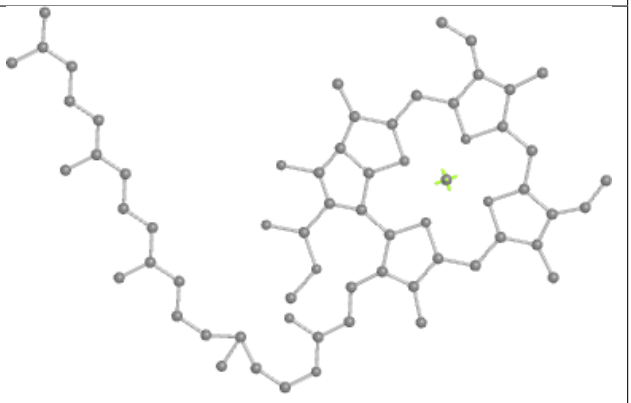
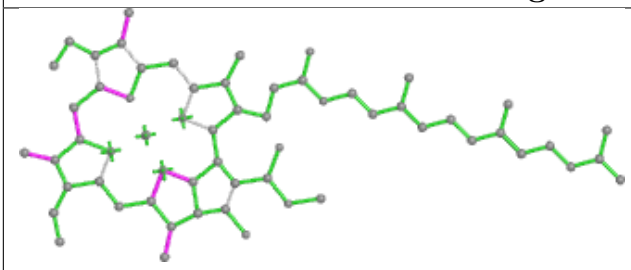


Rings

Ligand CLA a 812



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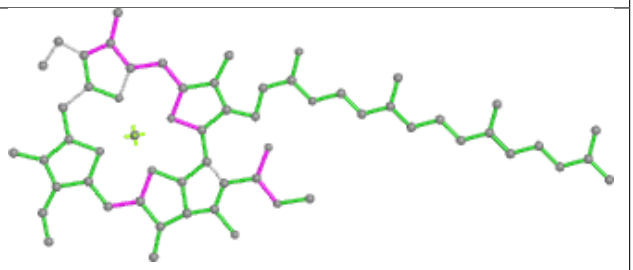

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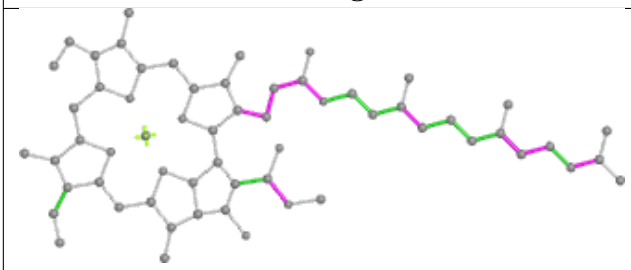

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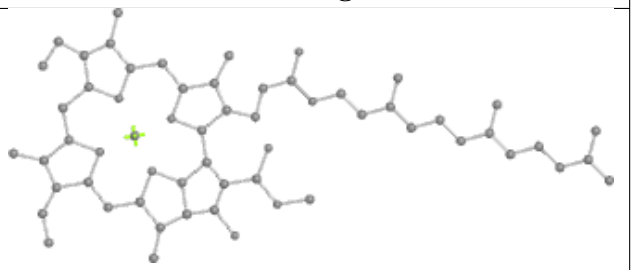
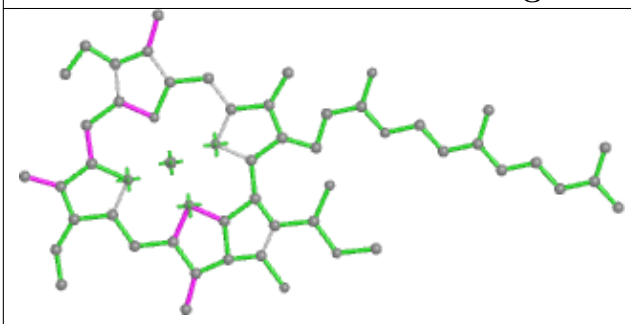


Rings

Ligand CLA A 207



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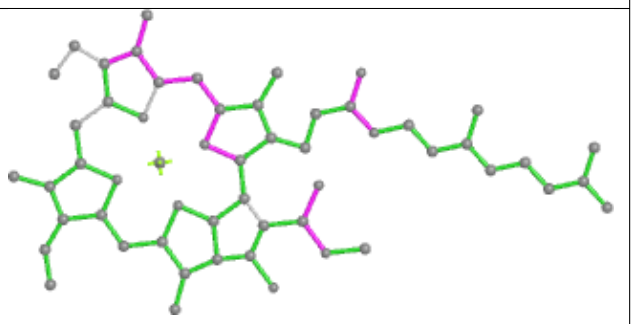
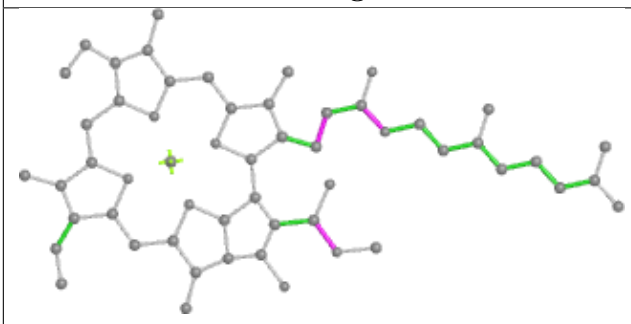
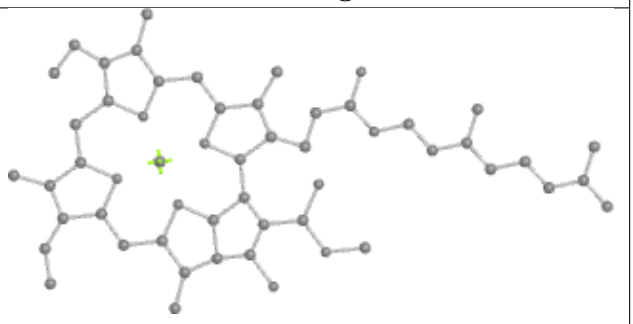


Bond angles

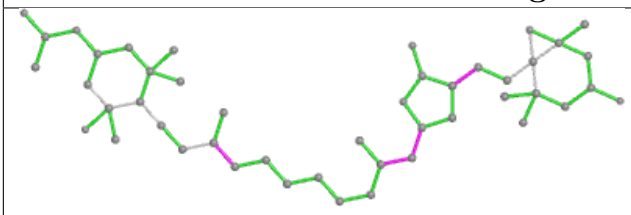


Torsions

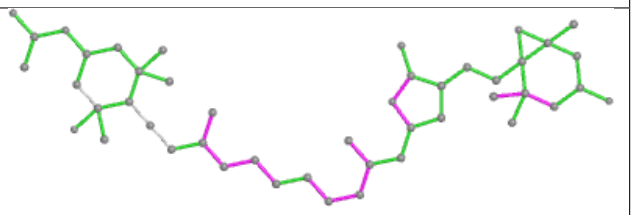


Rings

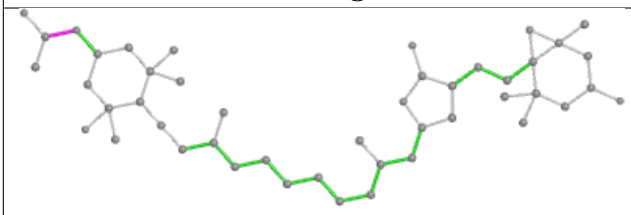
Ligand PID C 307



Bond lengths



Bond angles



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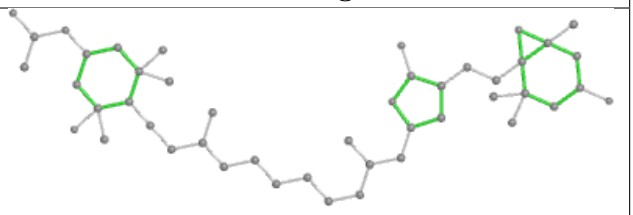
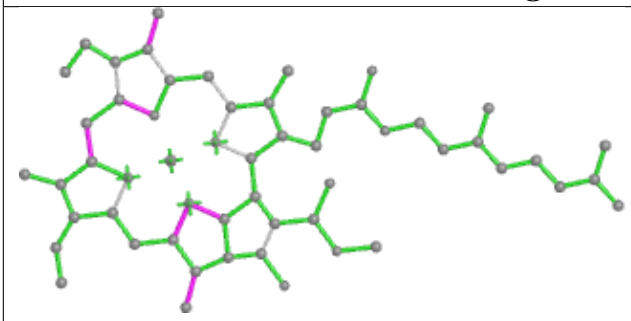
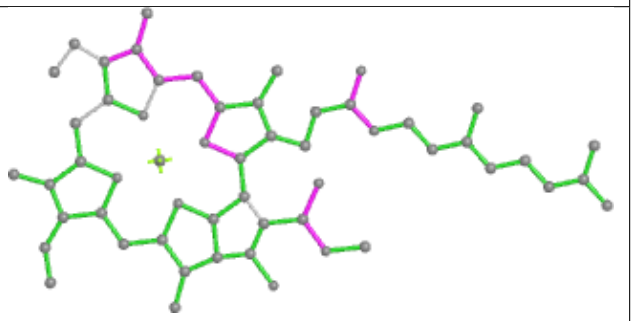


Rings

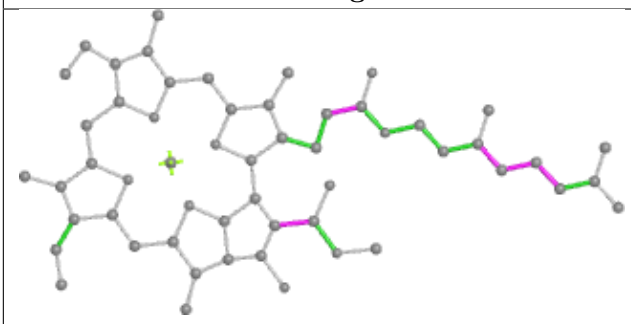
Ligand CLA B 309



Bond lengths



Bond angles



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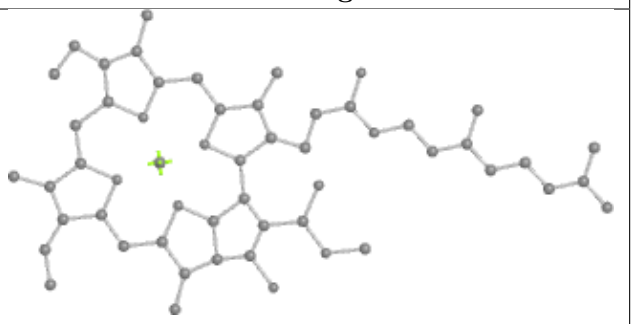
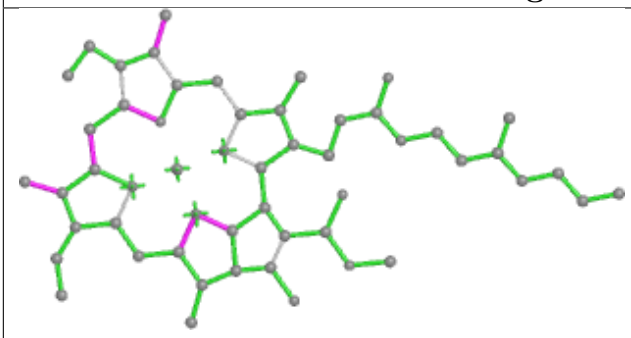
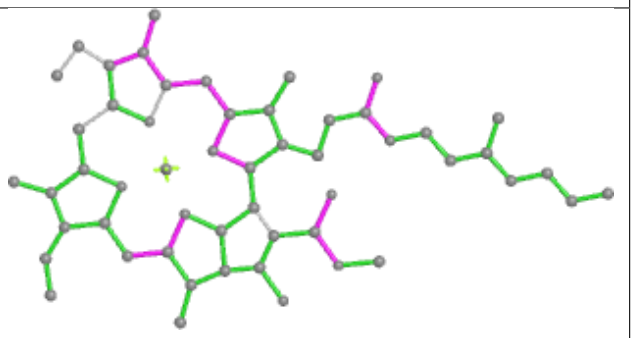
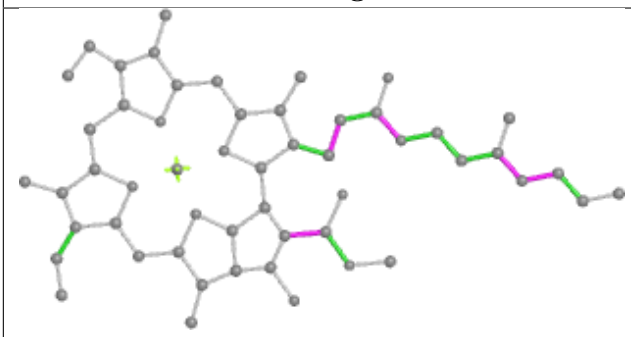
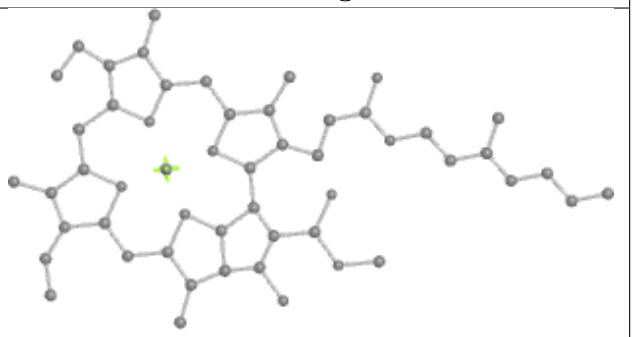
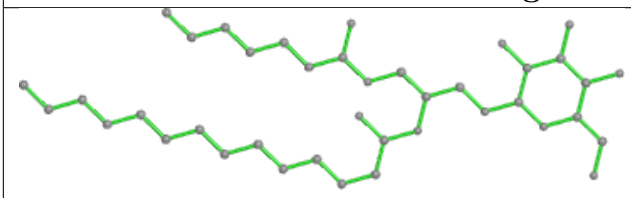
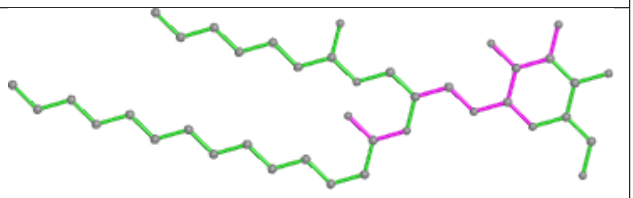
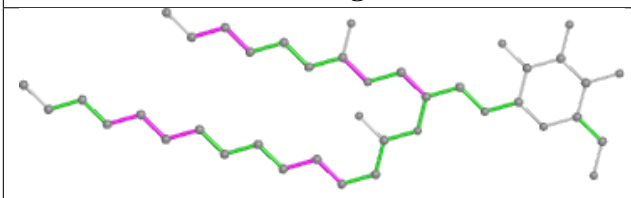
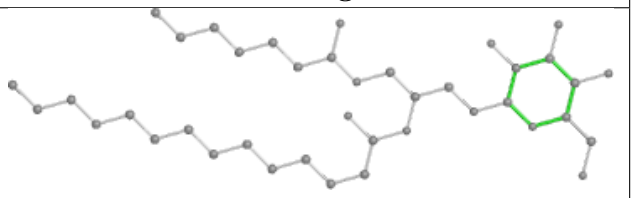
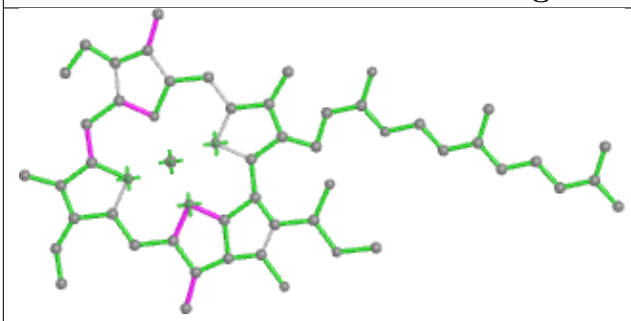


Rings

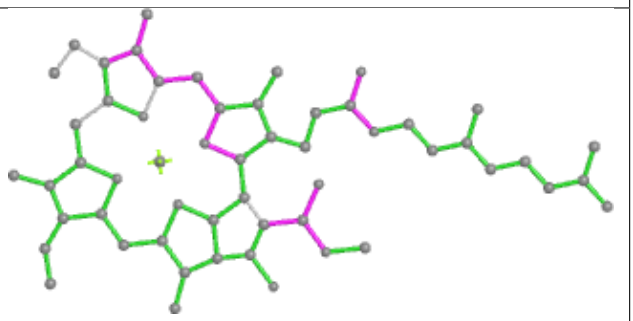
Ligand CLA L 313	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand LMG b 734	
 Bond lengths	 Bond angles
 Torsions	 Rings

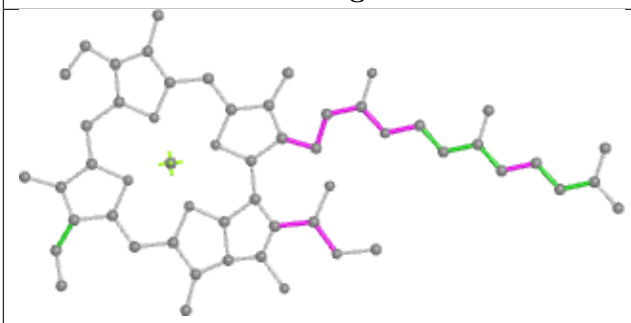
Ligand CLA i 203



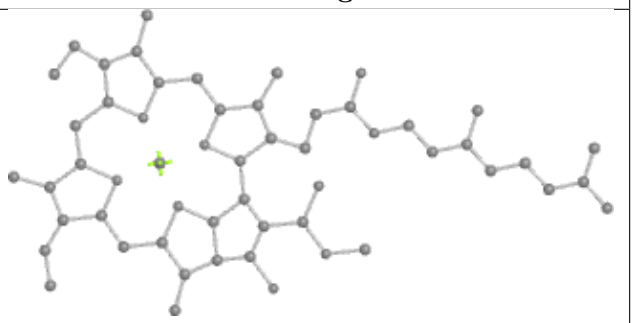
Bond lengths



Bond angles

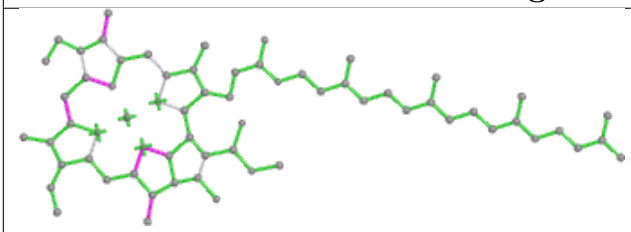


Torsions

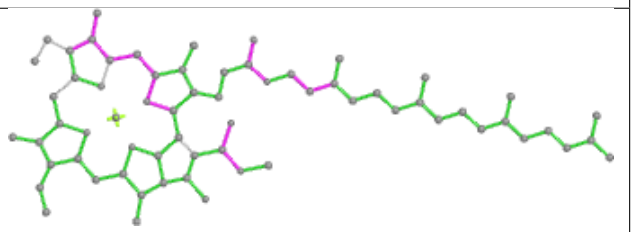


Rings

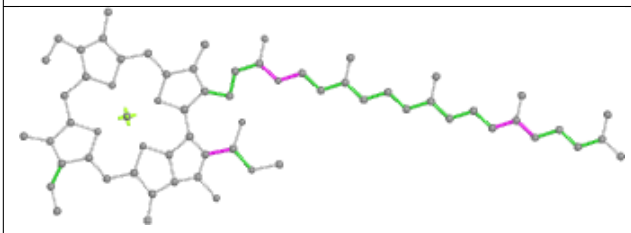
Ligand CLA a 822



Bond lengths



Bond angles



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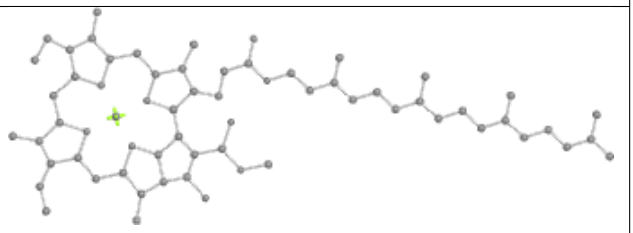
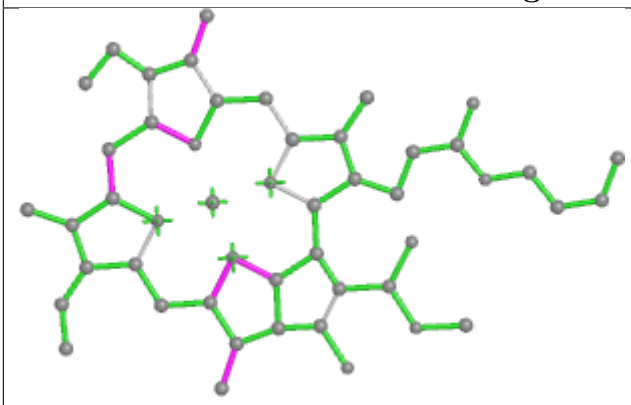


Rings

Ligand CLA K 207



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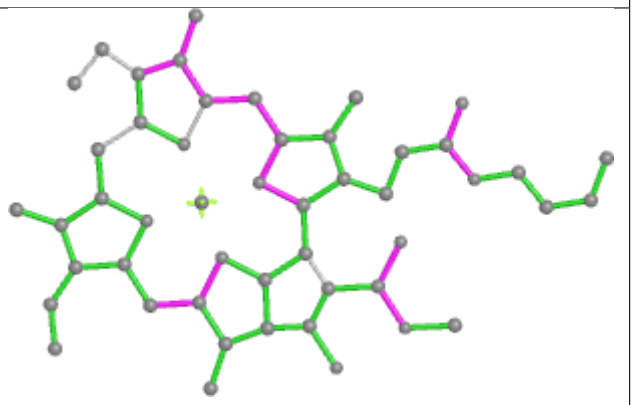
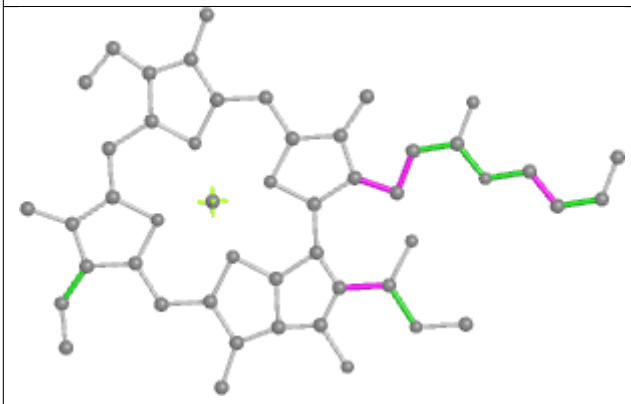


Bond angles



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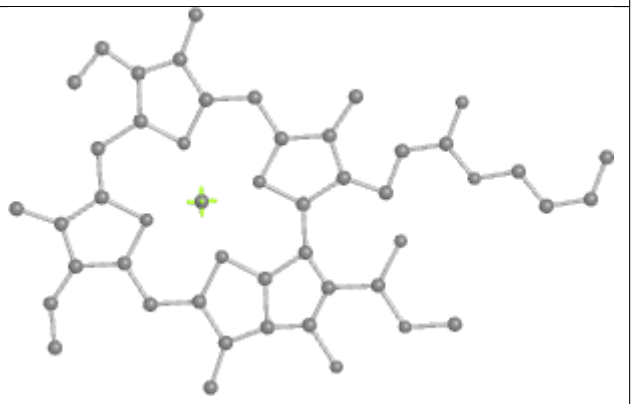
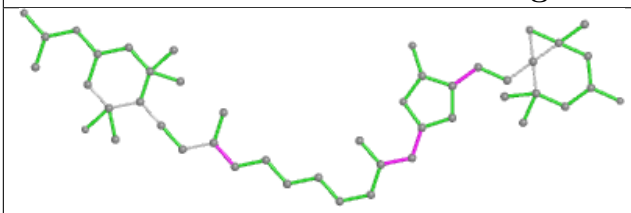
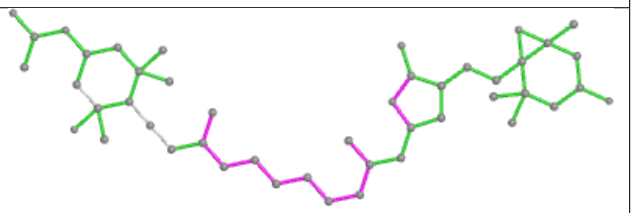


Rings

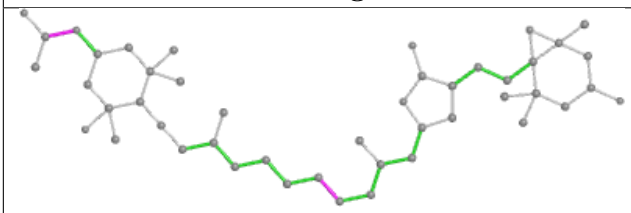
Ligand PID F 302



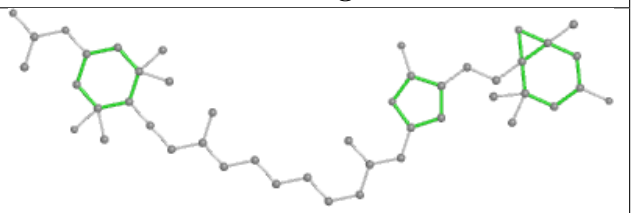
Bond lengths



Bond angles

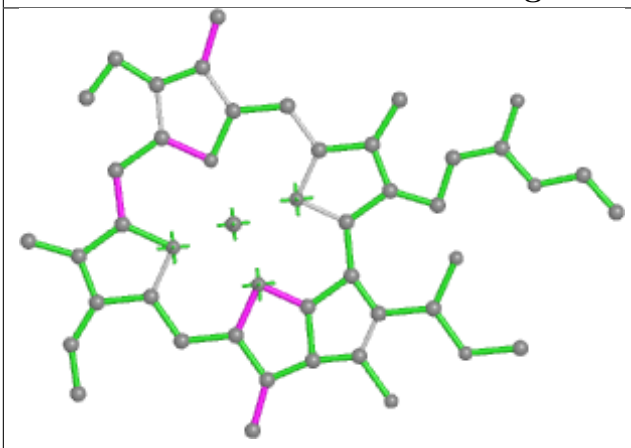


Torsions

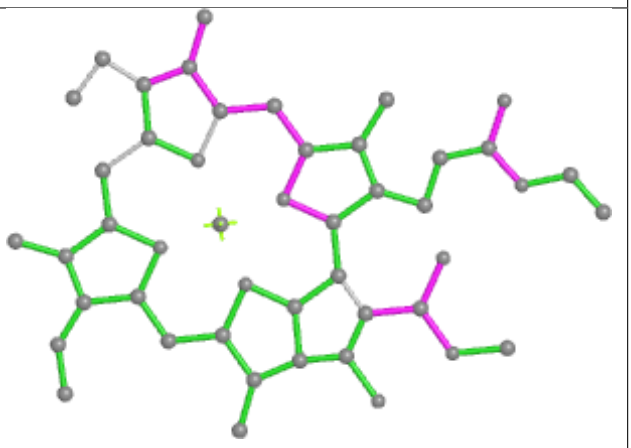


Rings

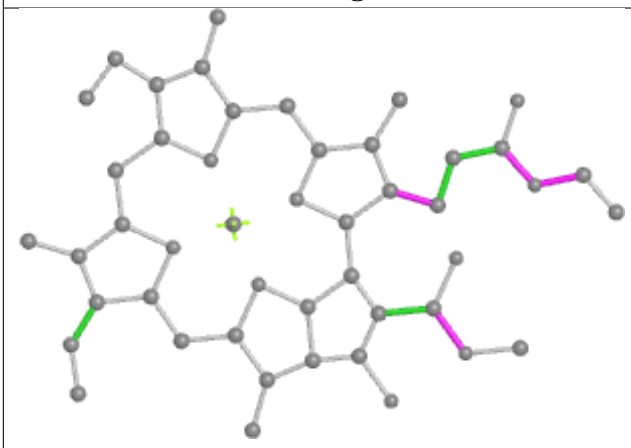
Ligand CLA C 314



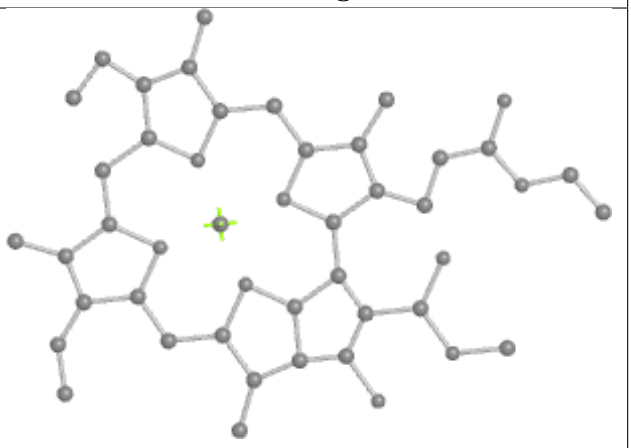
Bond lengths



Bond angles

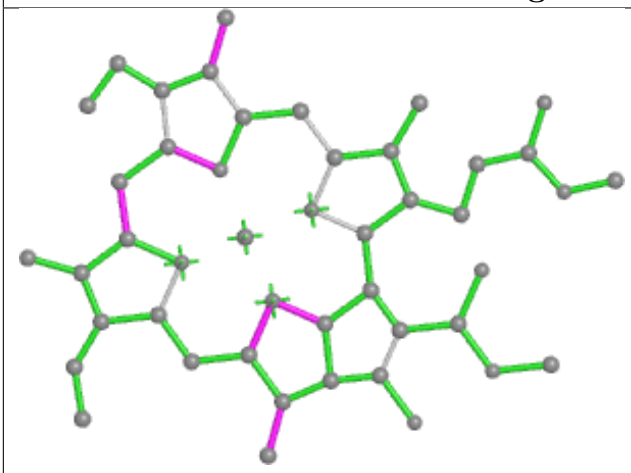


Torsions

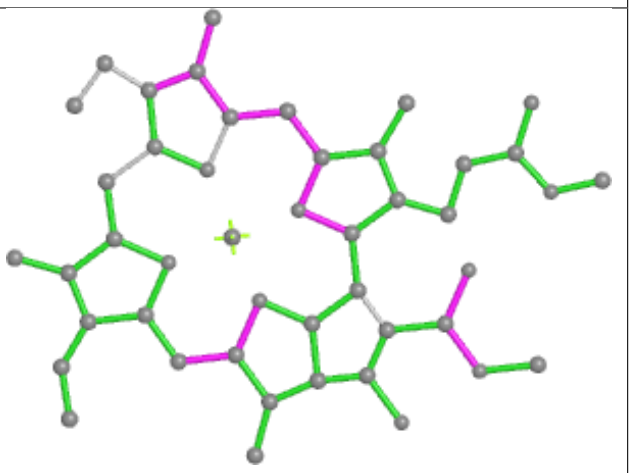


Rings

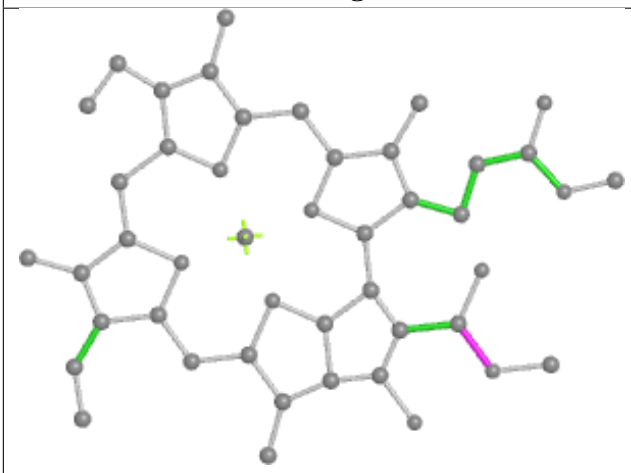
Ligand CLA J 305



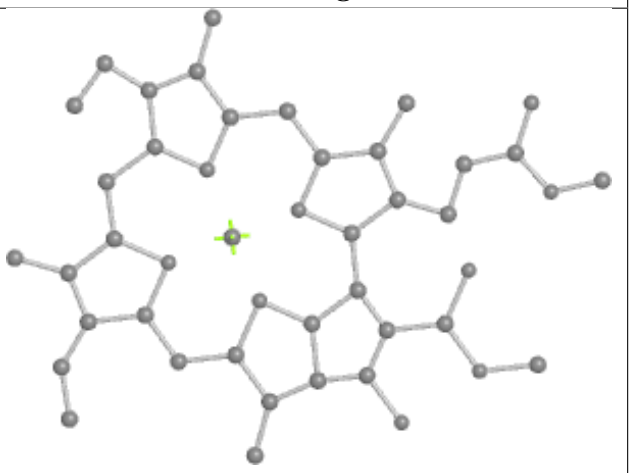
Bond lengths



Bond angles

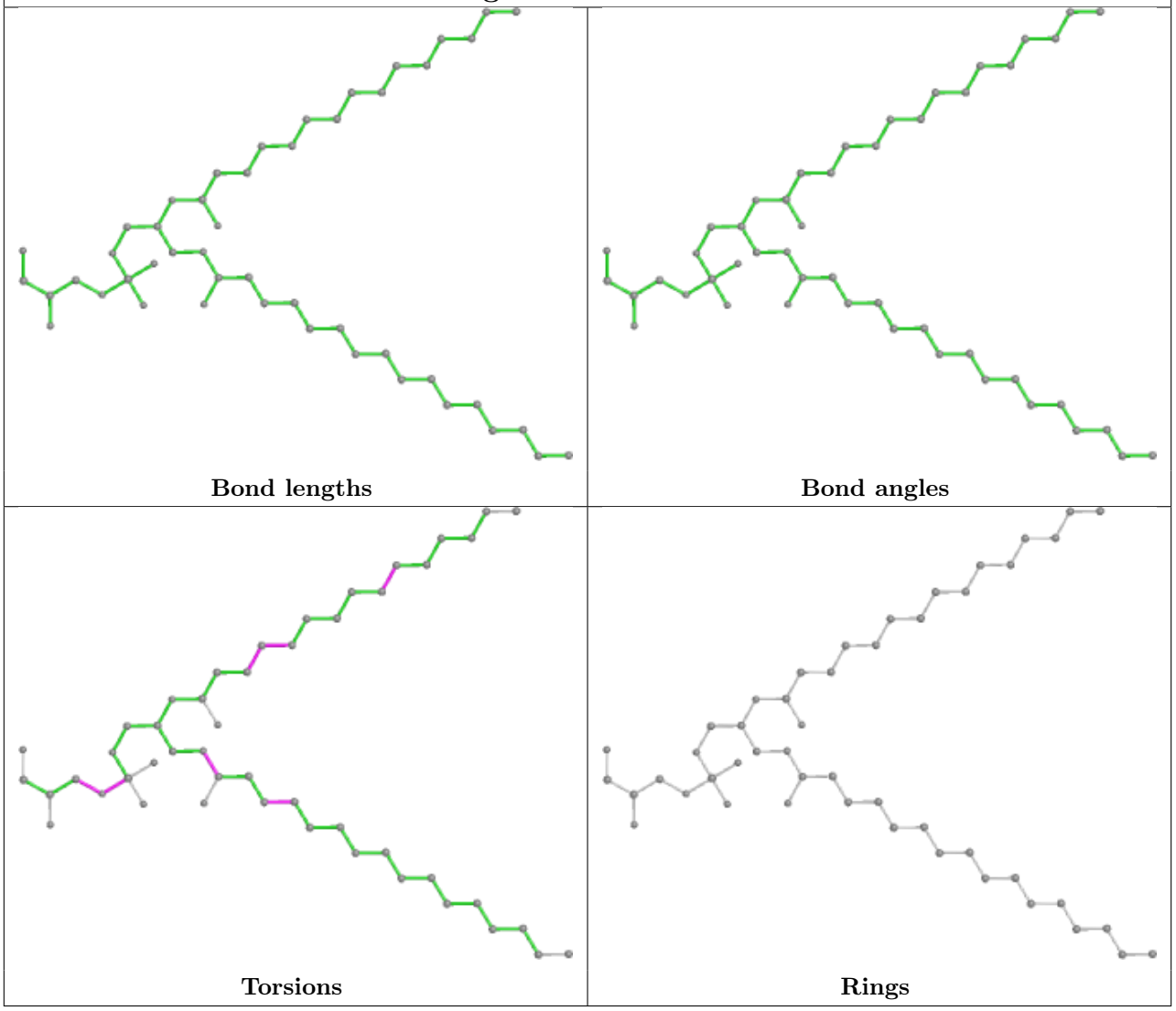


Torsions

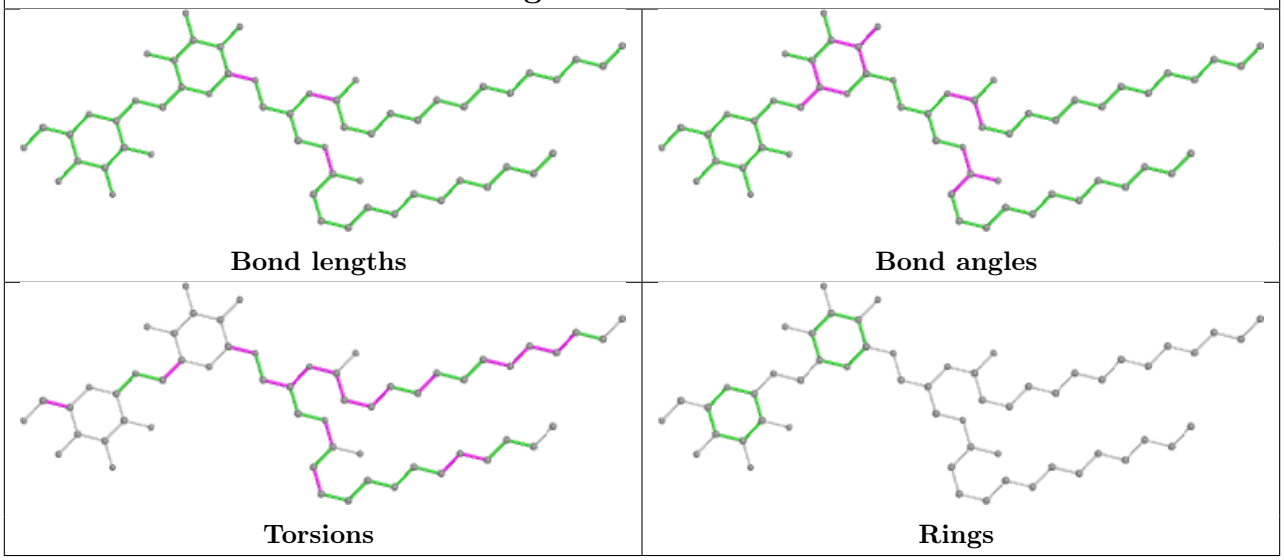


Rings

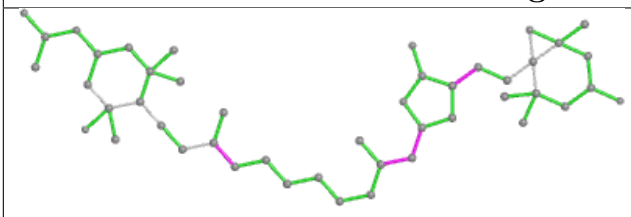
Ligand LHG a 833



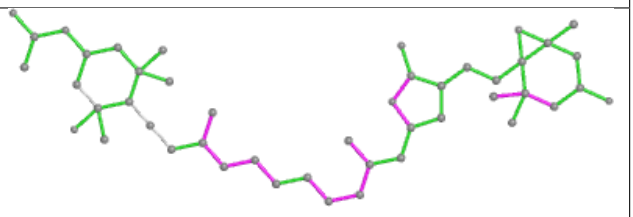
Ligand DGD b 733



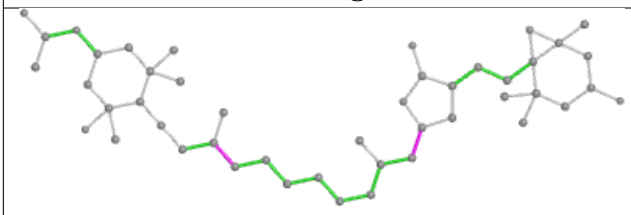
Ligand PID O 304



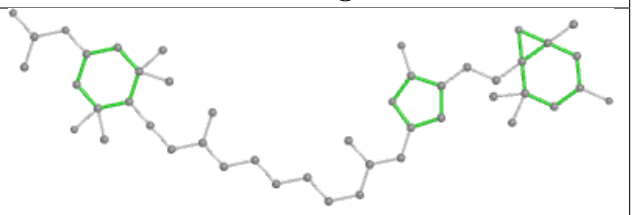
Bond lengths



Bond angles

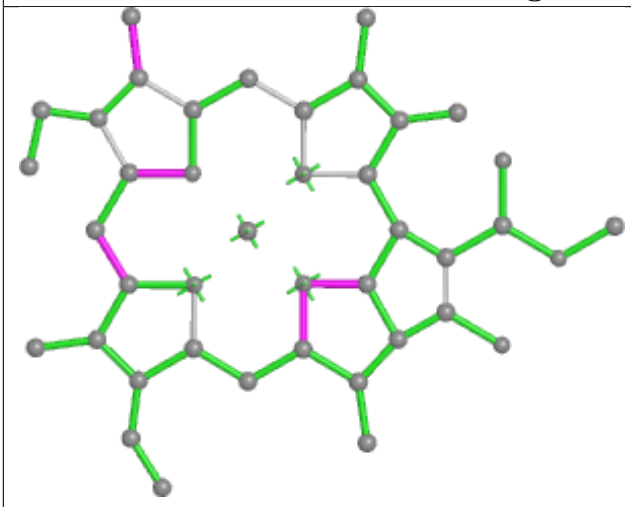


Torsions

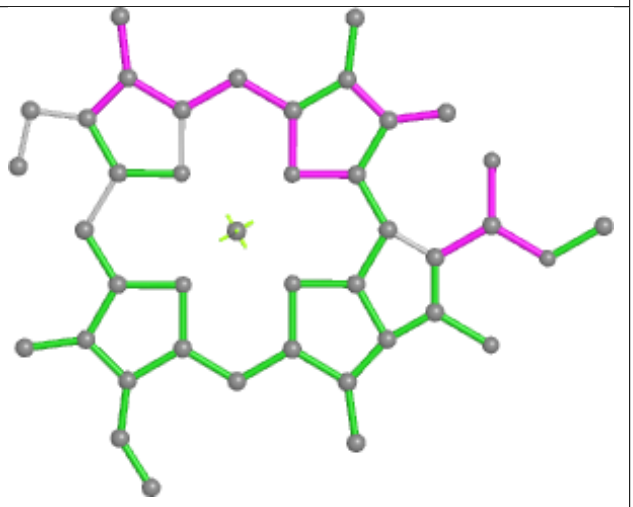


Rings

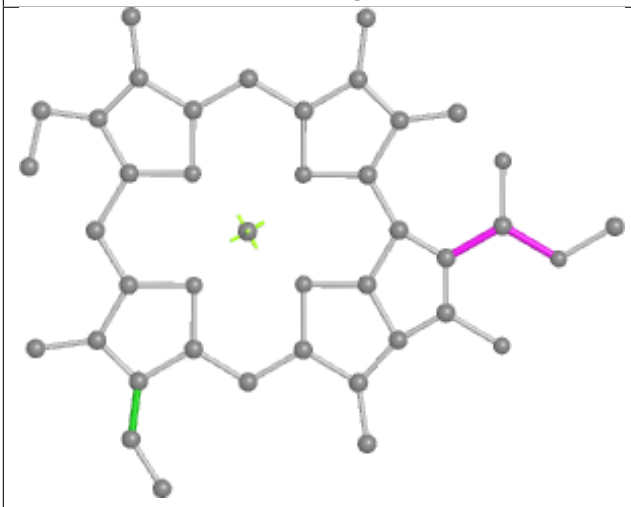
Ligand CLA F 315



Bond lengths



Bond angles



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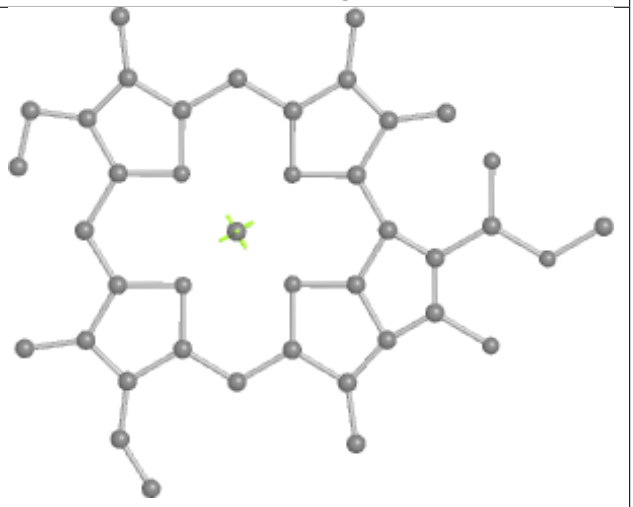
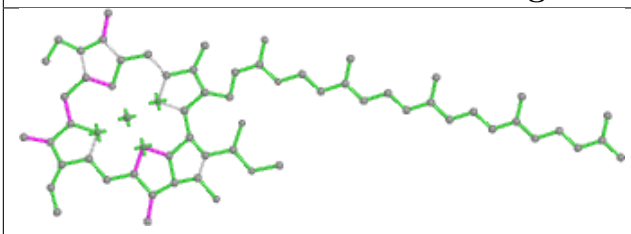
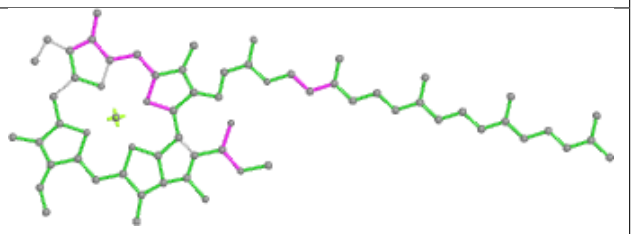


Rings

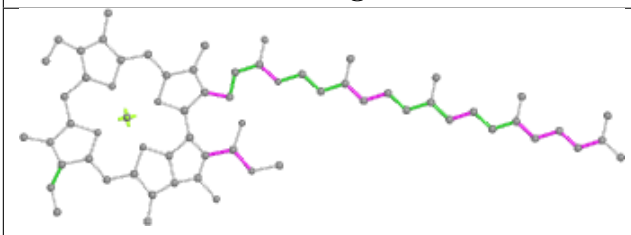
Ligand CLA J 306



Bond lengths



Bond angles



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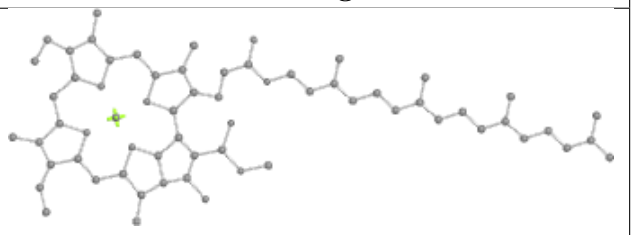
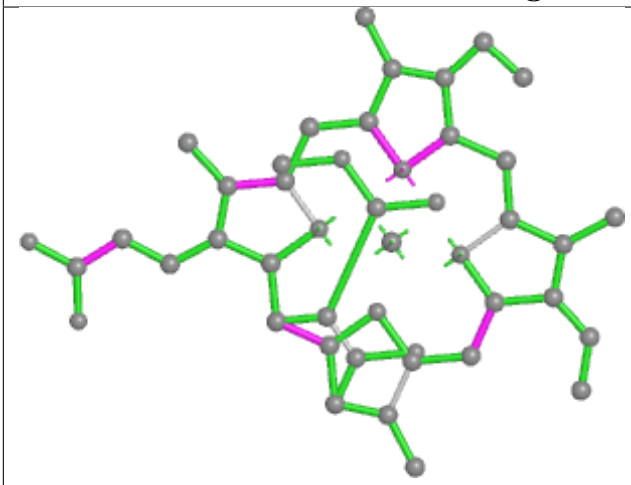


Rings

Ligand KC1 H 311



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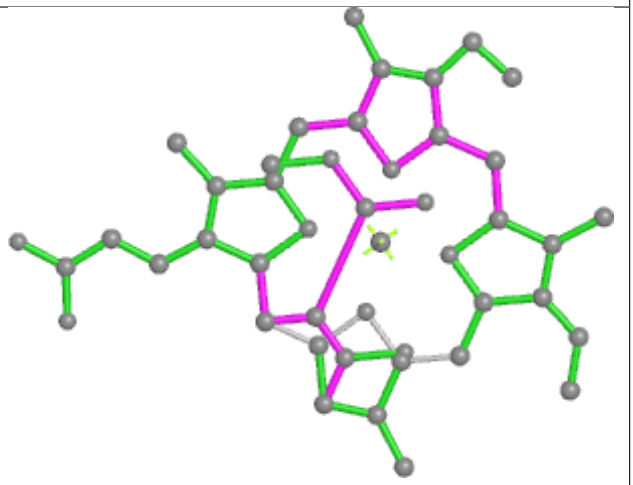
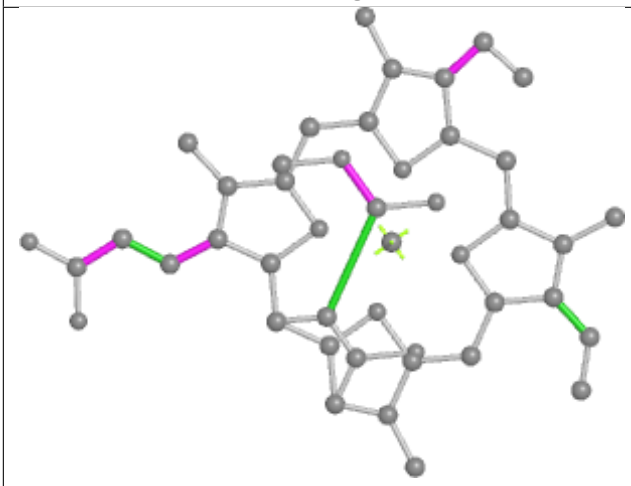
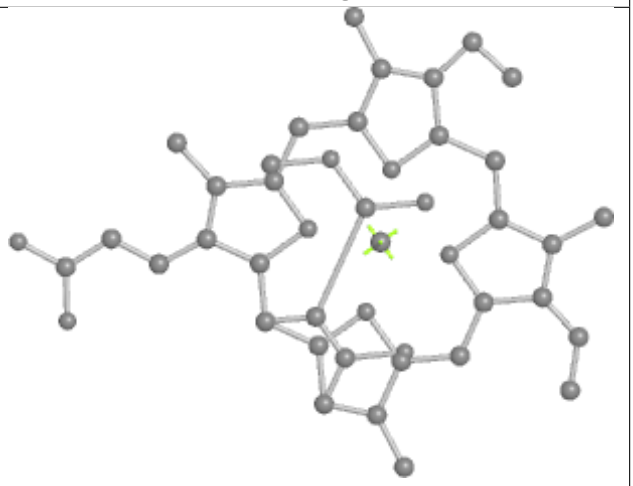


Bond angles

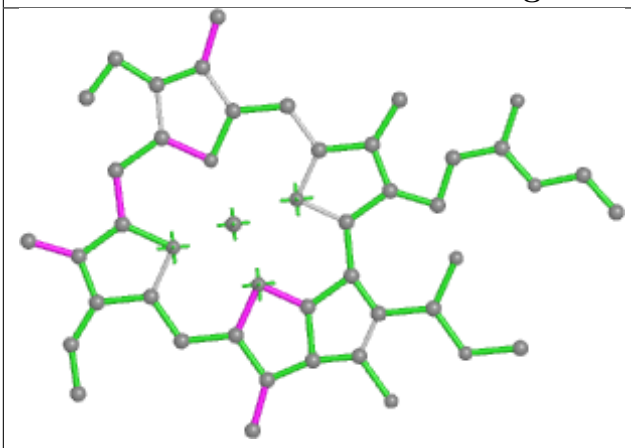


Torsions



Rings

Ligand CLA D 314



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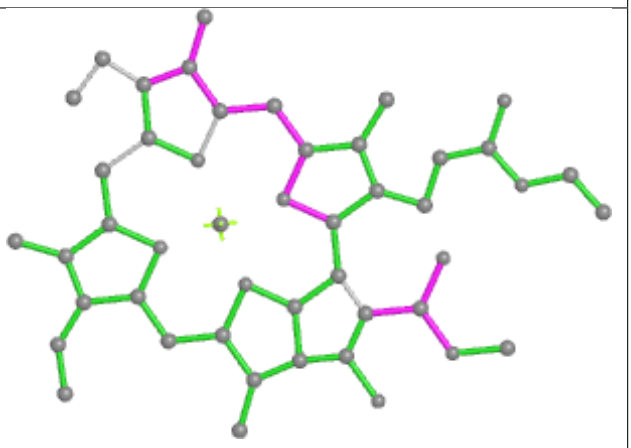
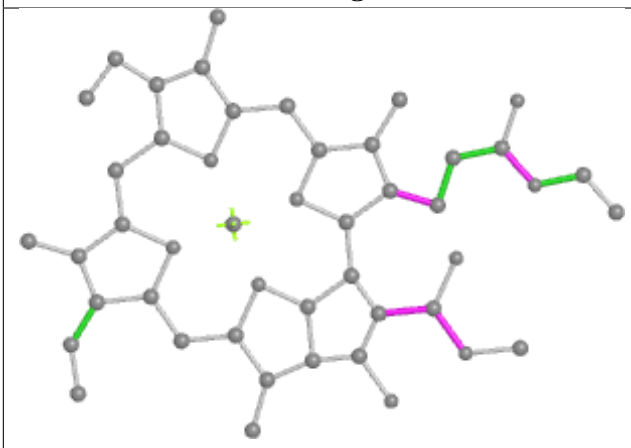


Bond angles



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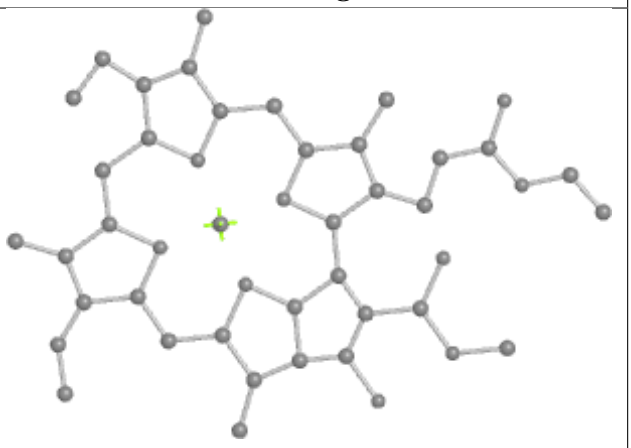
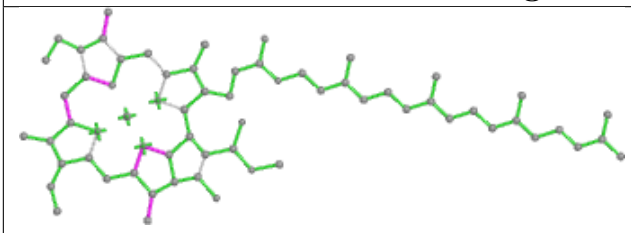


Rings

Ligand CLA N 309



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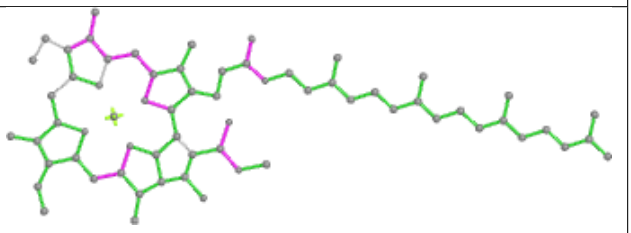

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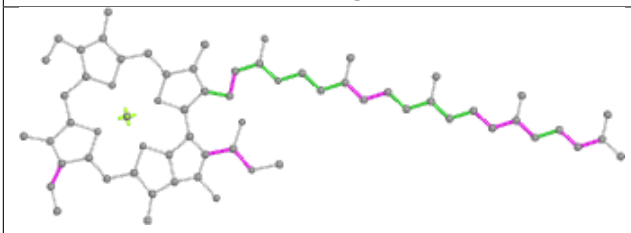

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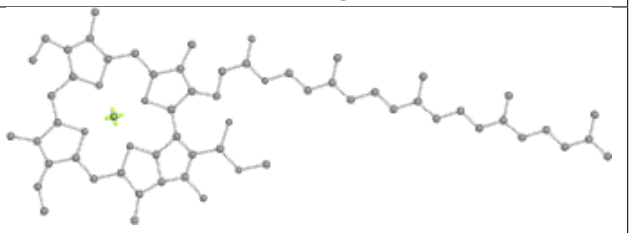
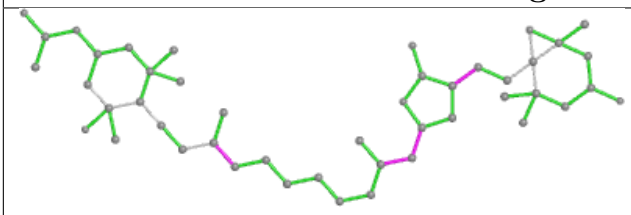
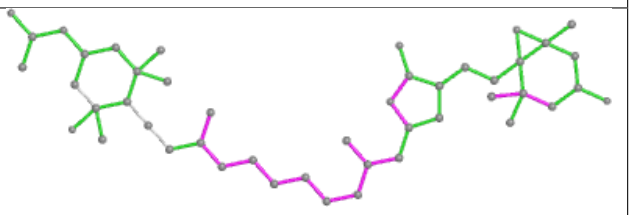
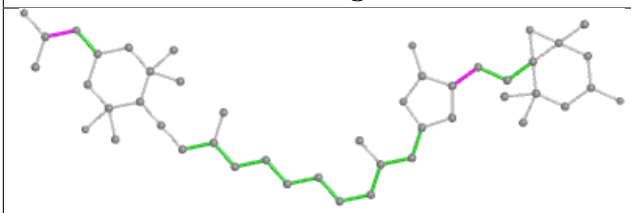
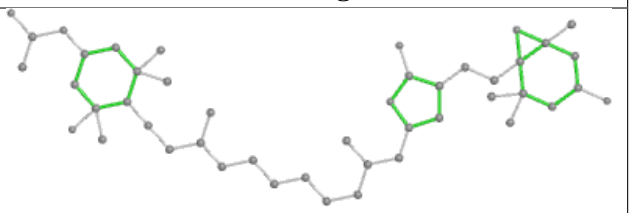
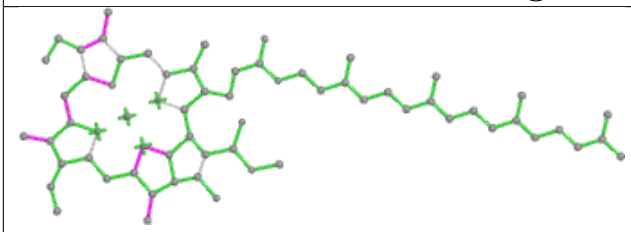
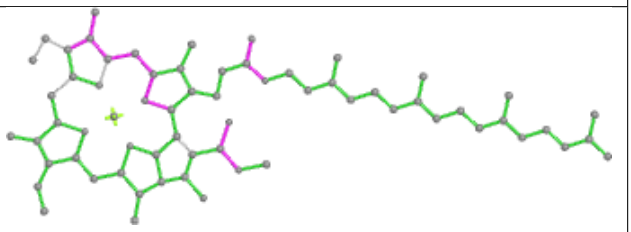
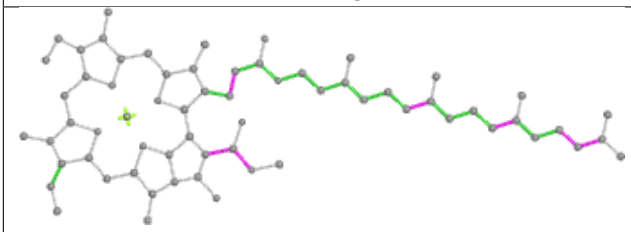
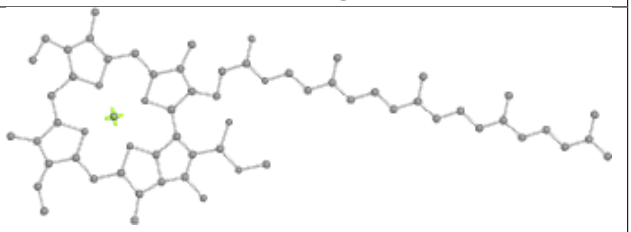
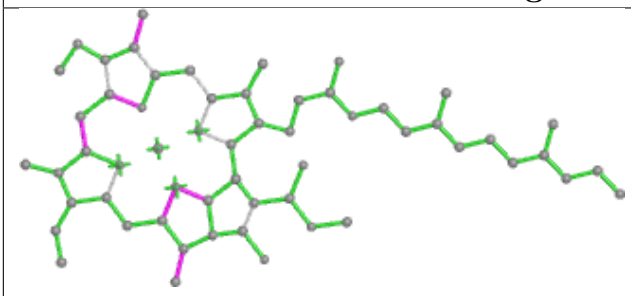


Rings

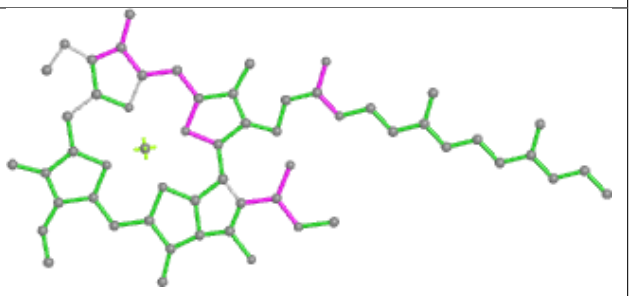
Ligand PID T 307	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA b 725	
 Bond lengths	 Bond angles
 Torsions	 Rings

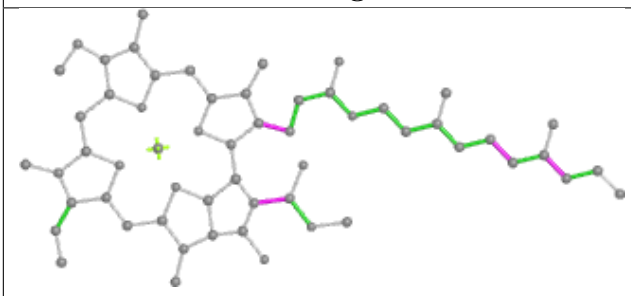
Ligand CLA E 315



Bond lengths



Bond angles



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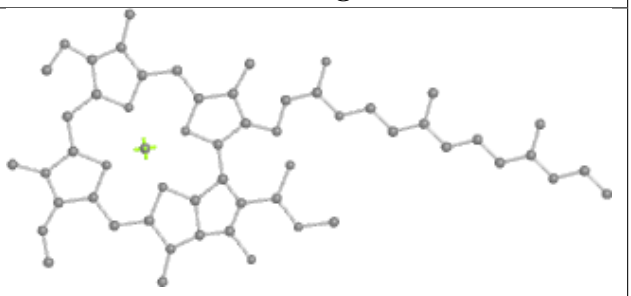
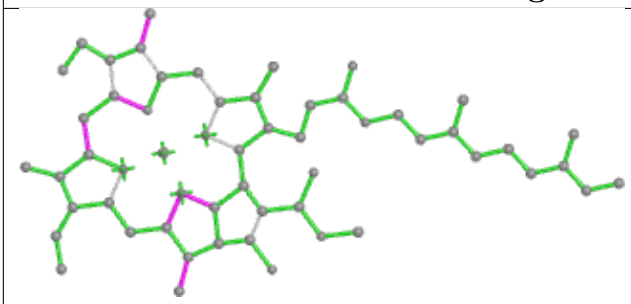


Rings

Ligand CLA J 308



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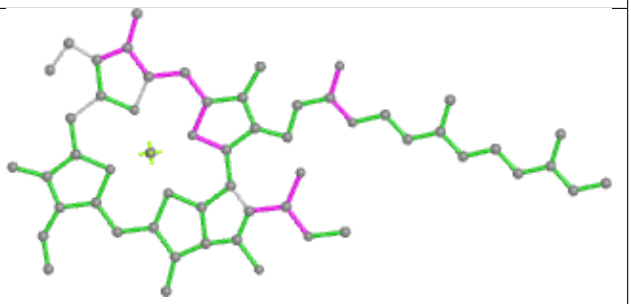
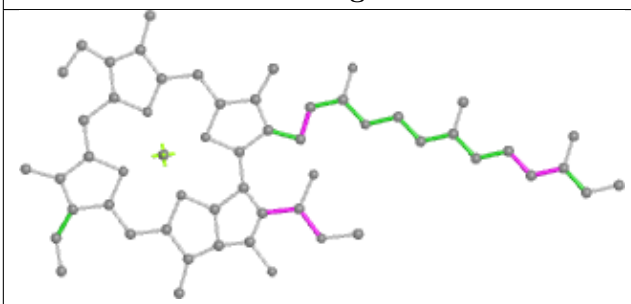


Bond angles



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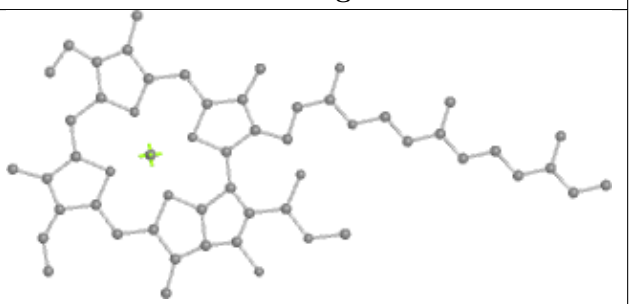
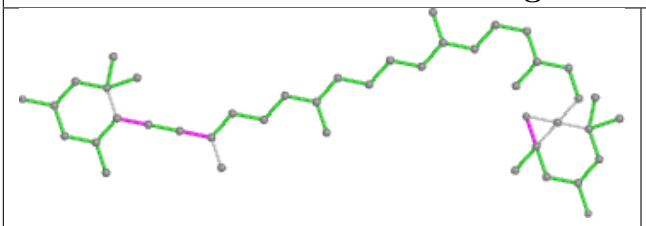


Rings

Ligand DD6 G 306



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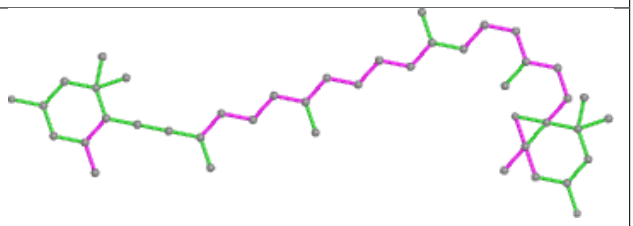
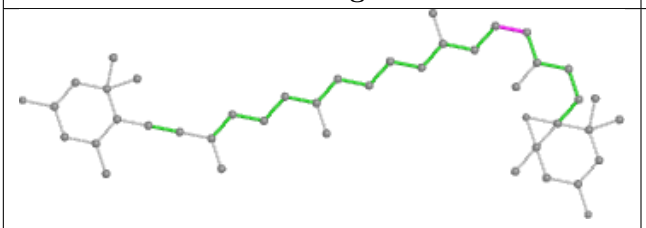
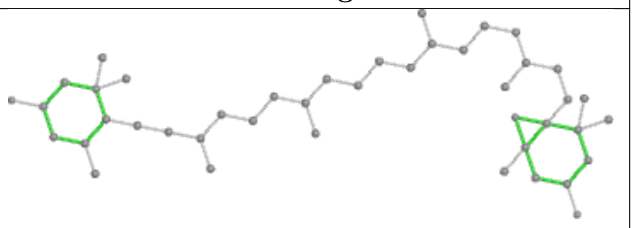


Bond angles

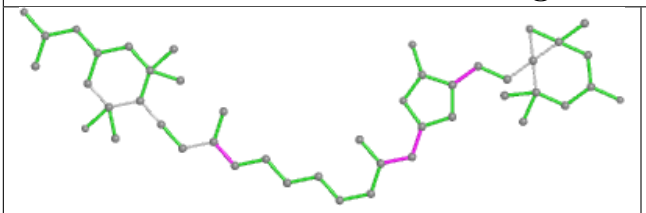


Torsions

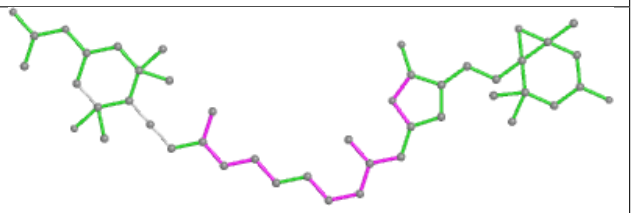


Rings

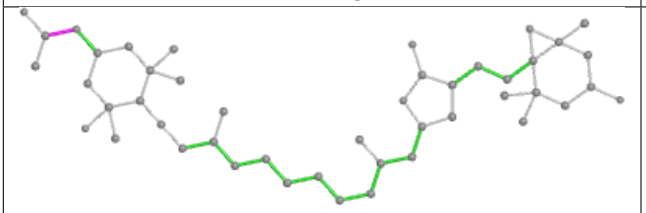
Ligand PID h 204



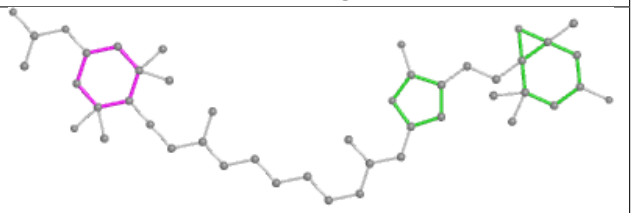
Bond lengths



Bond angles

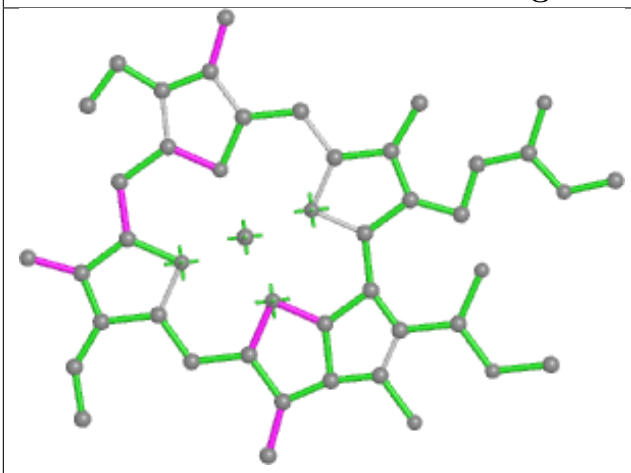


Torsions

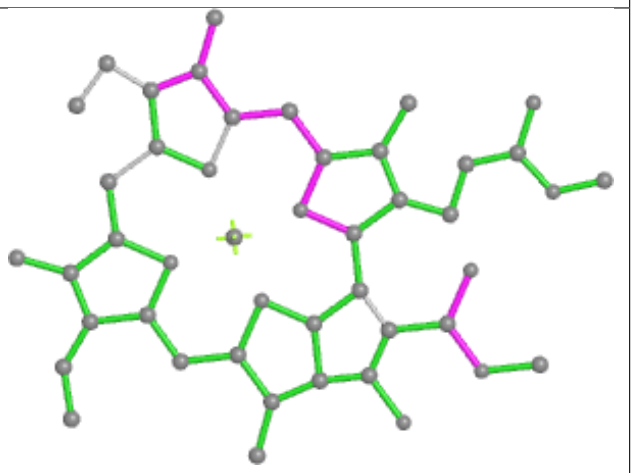


Rings

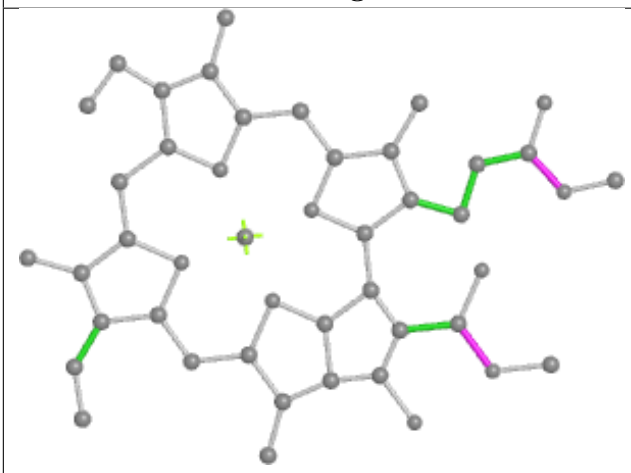
Ligand CLA f 802



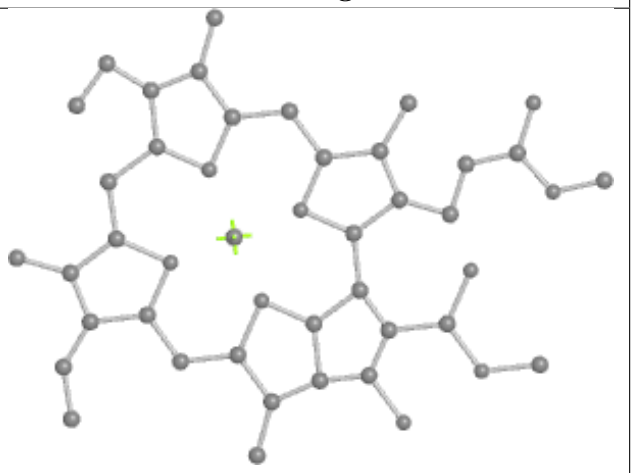
Bond lengths



Bond angles

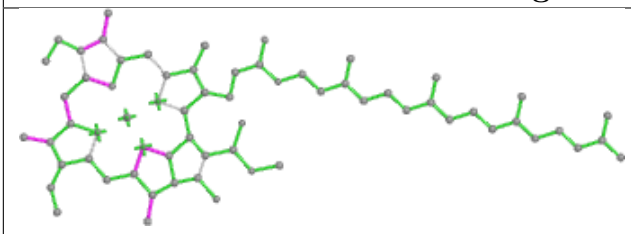


Torsions

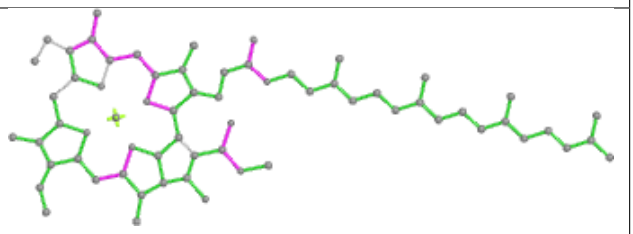


Rings

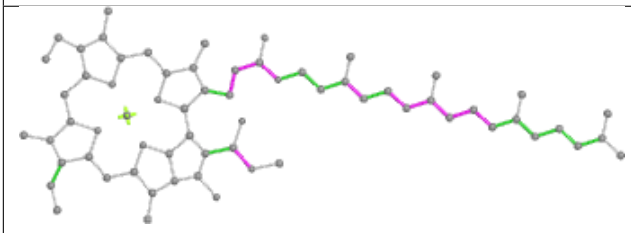
Ligand CLA l 503



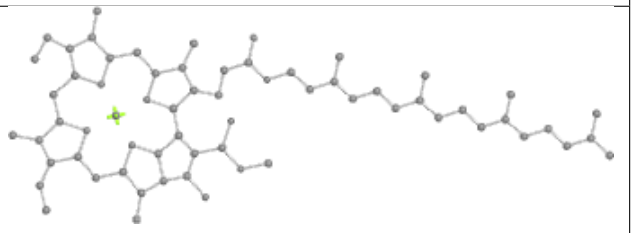
Bond lengths



Bond angles

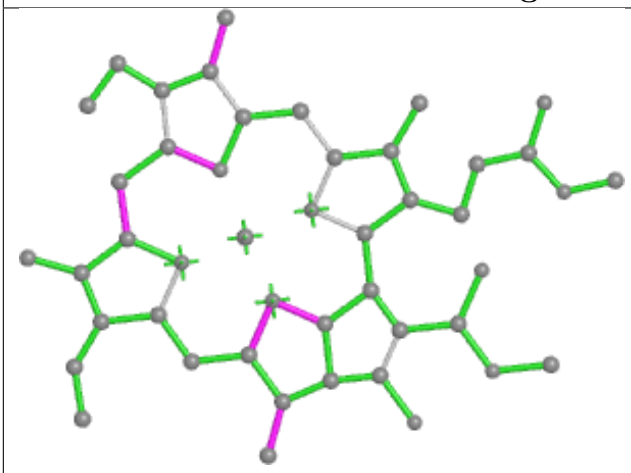


Torsions

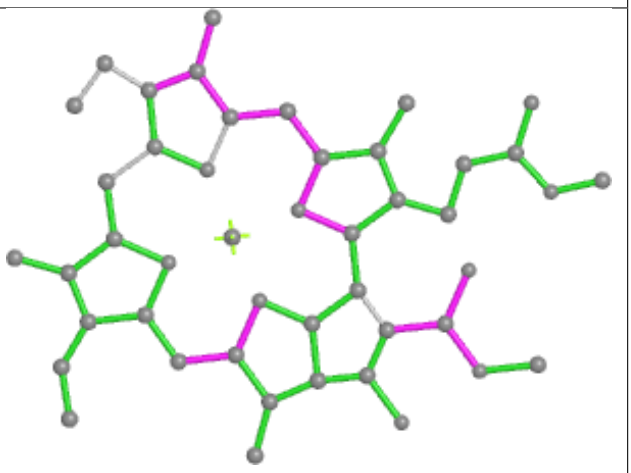


Rings

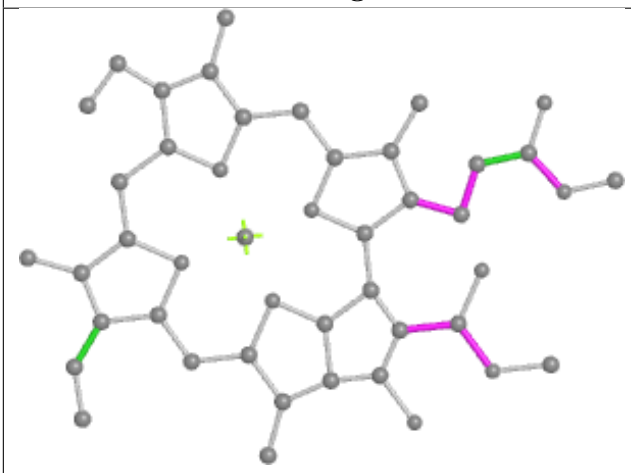
Ligand CLA M 311



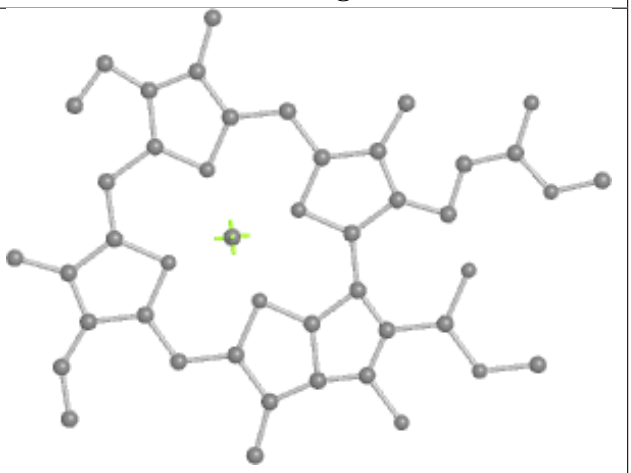
Bond lengths



Bond angles

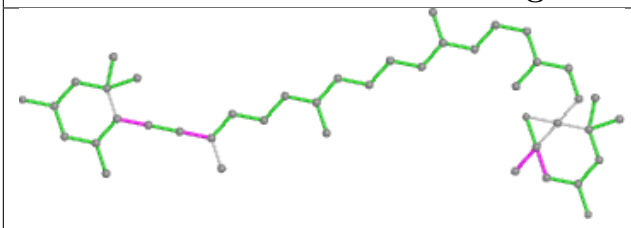


Torsions

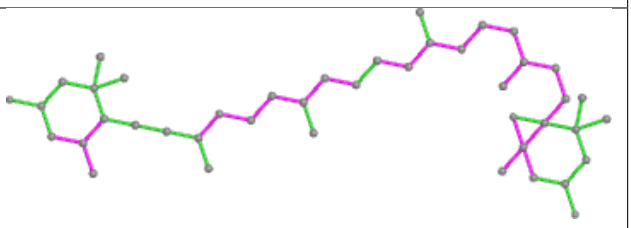


Rings

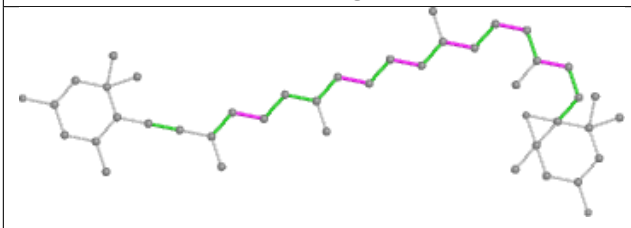
Ligand DD6 F 301



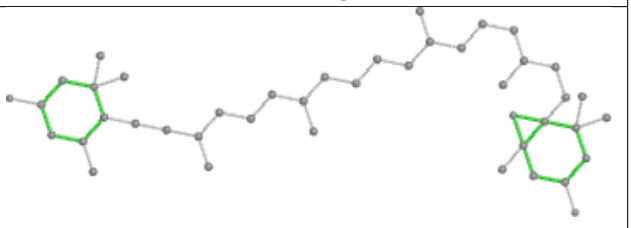
Bond lengths



Bond angles

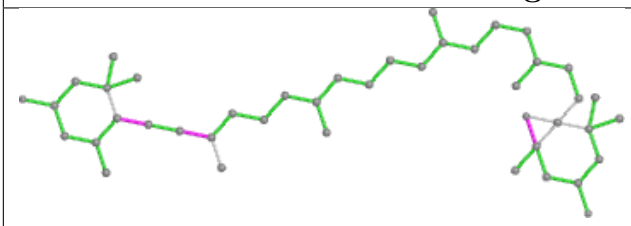


Torsions

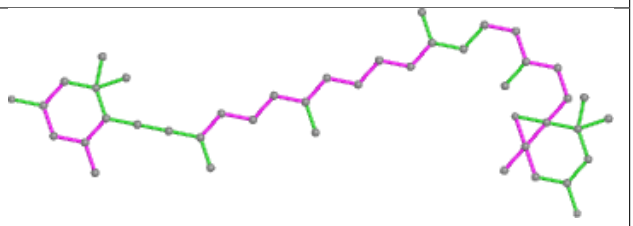


Rings

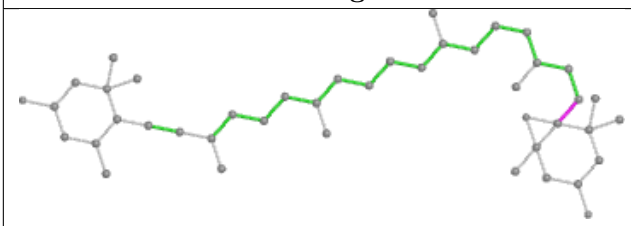
Ligand DD6 K 206



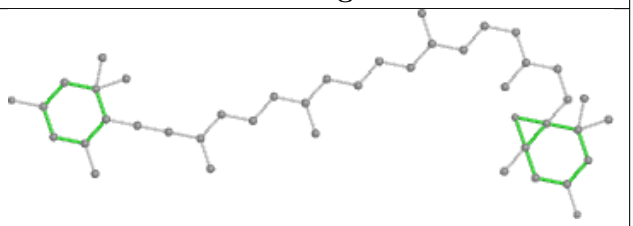
Bond lengths



Bond angles

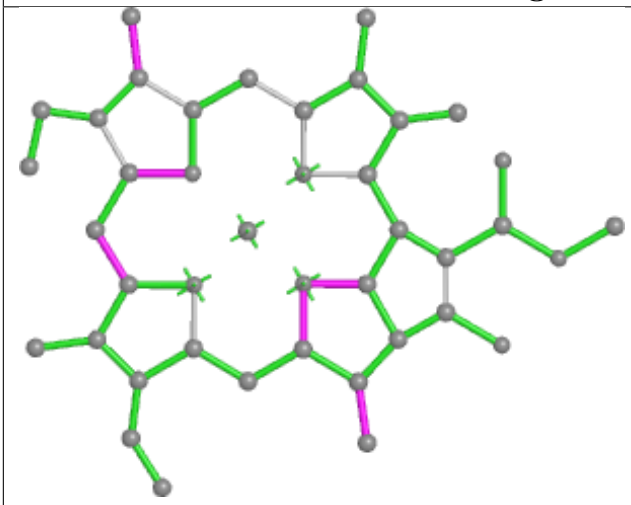


Torsions

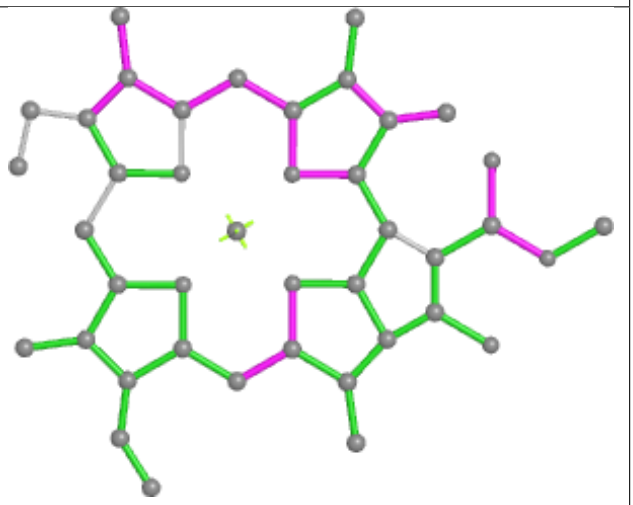


Rings

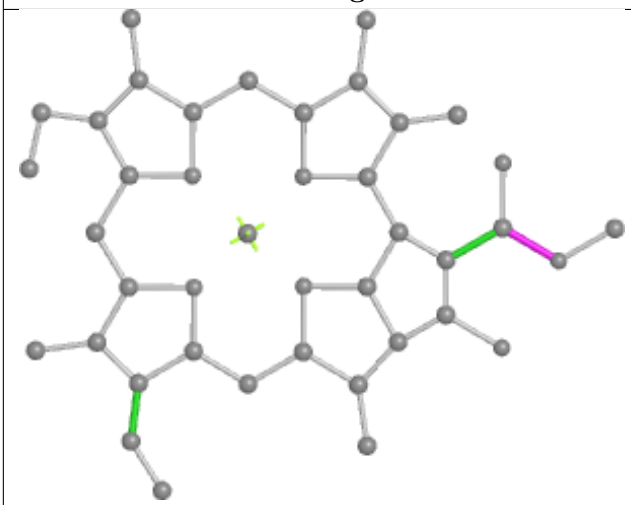
Ligand CLA J 313



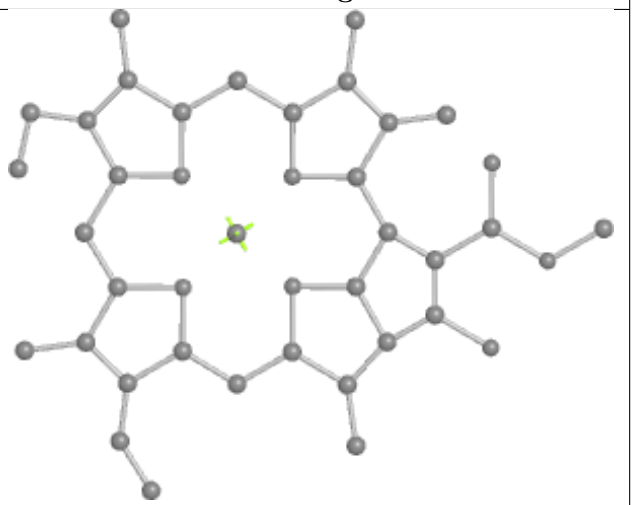
Bond lengths



Bond angles

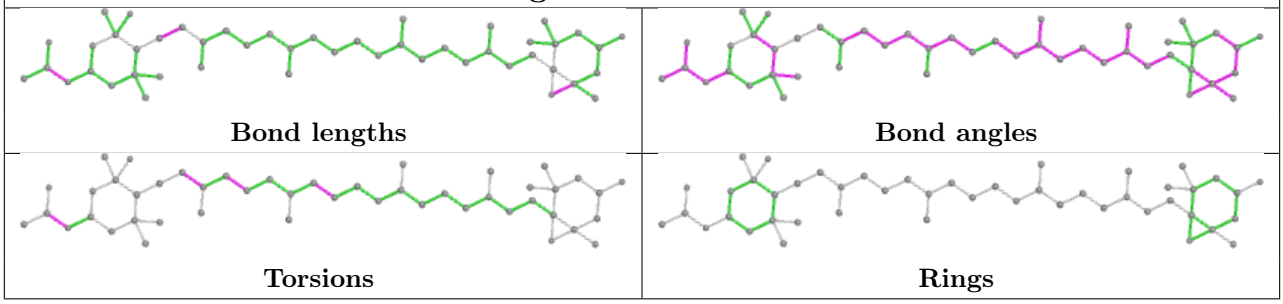


Torsions

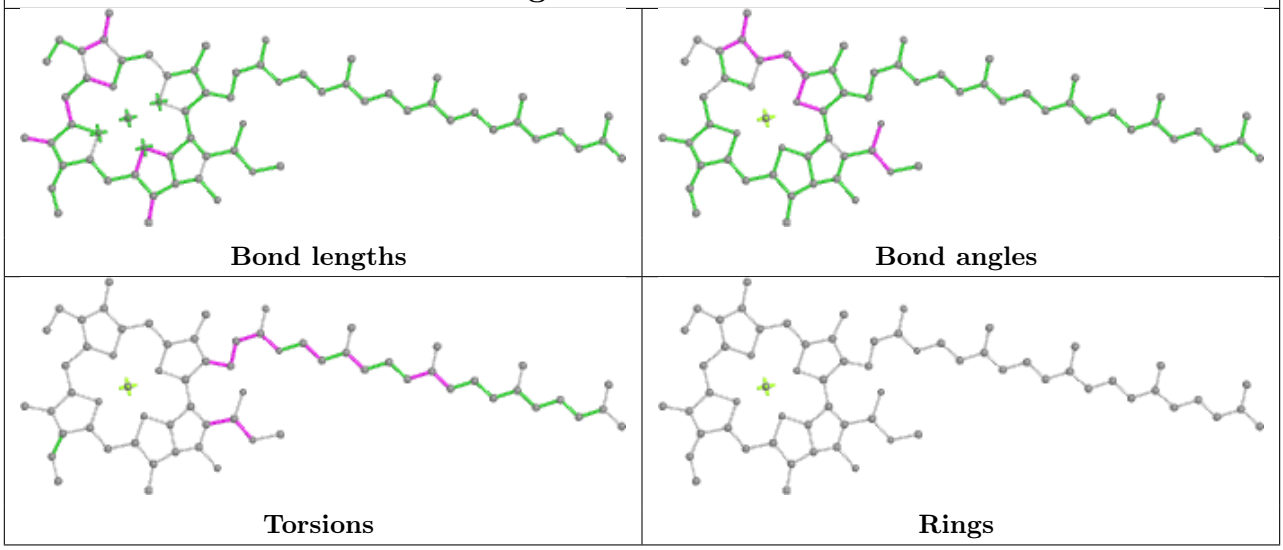


Rings

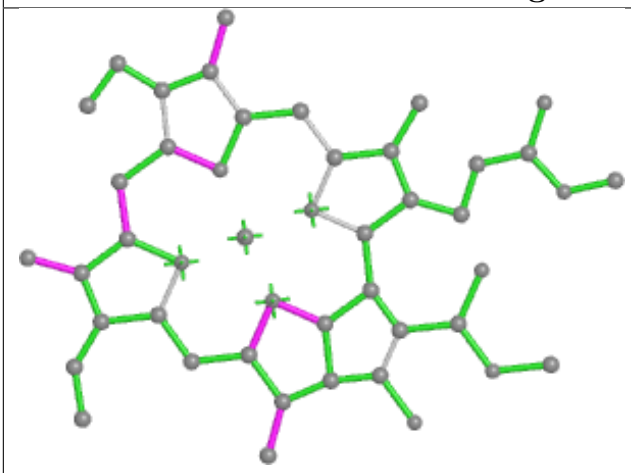
Ligand UIX P 207



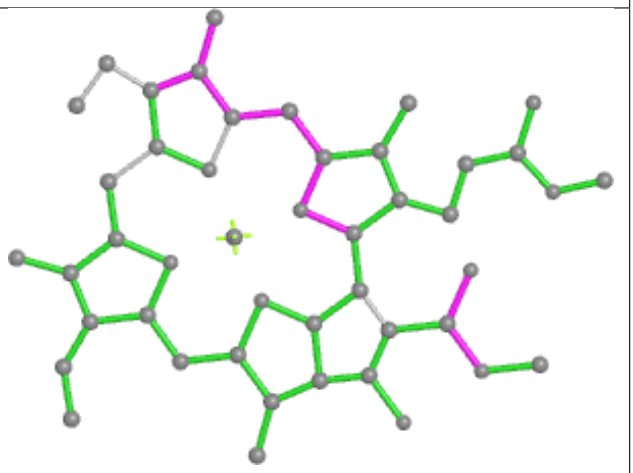
Ligand CLA b 720



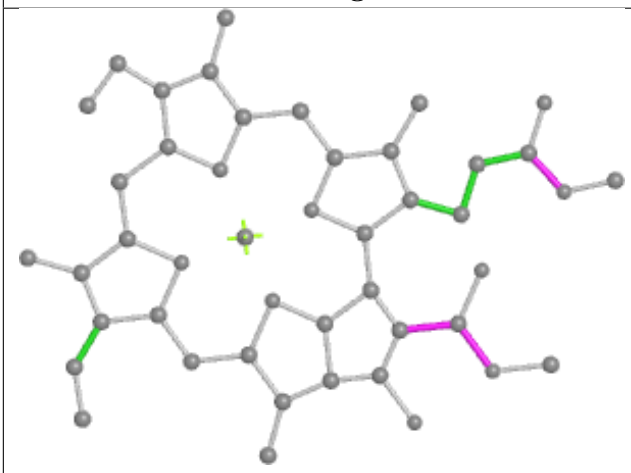
Ligand CLA a 814



Bond lengths



Bond angles



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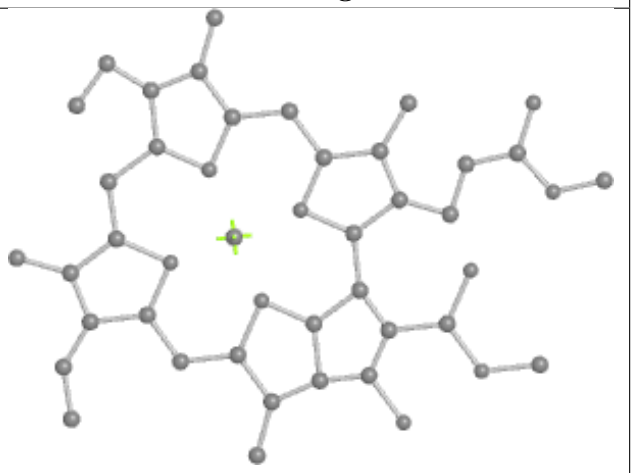
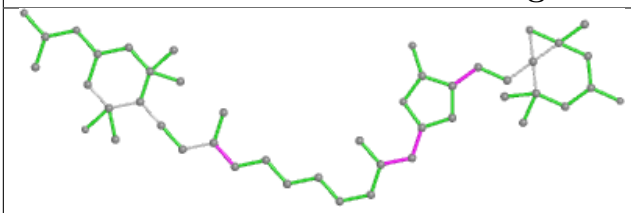


Rings

Ligand PID N 305



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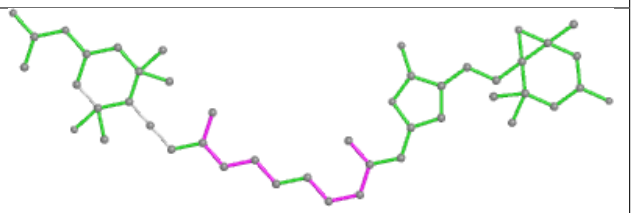
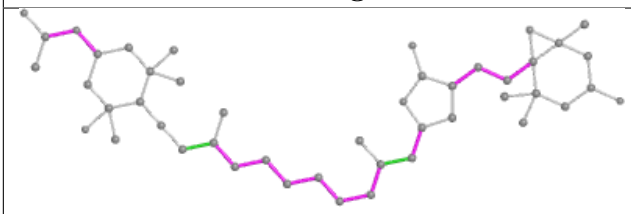


Bond angles



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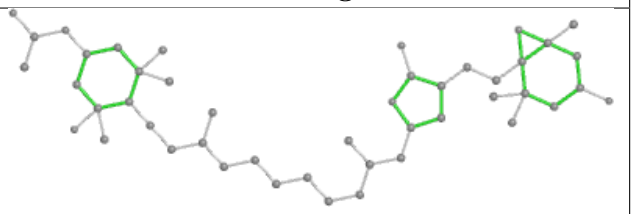
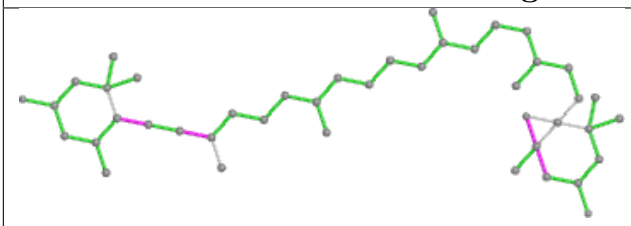


Rings

Ligand DD6 M 303



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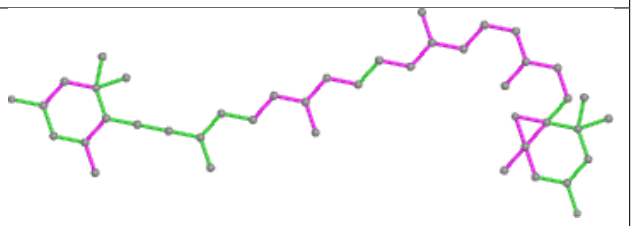
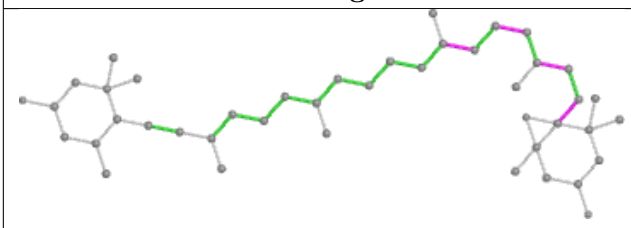


Bond angles



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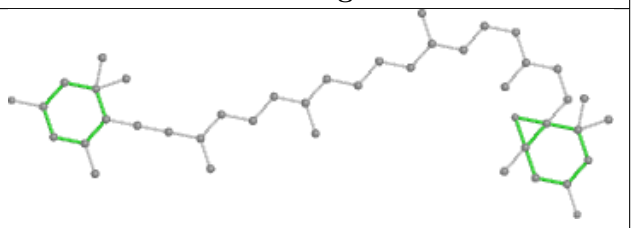
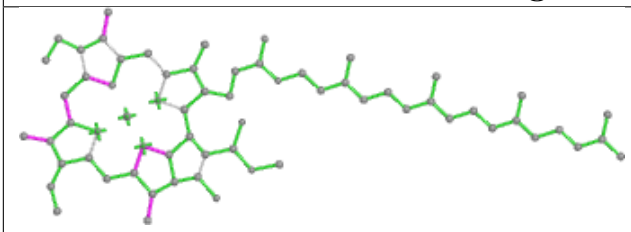
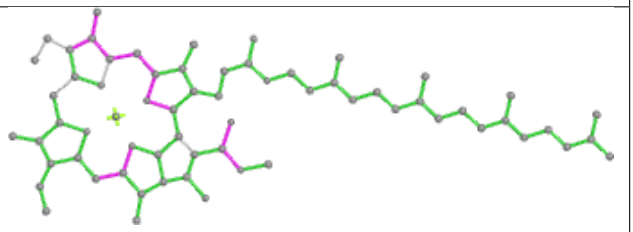


Rings

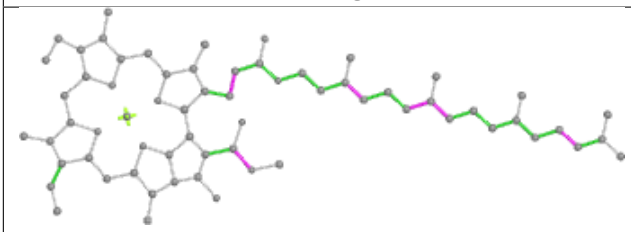
Ligand CLA a 803



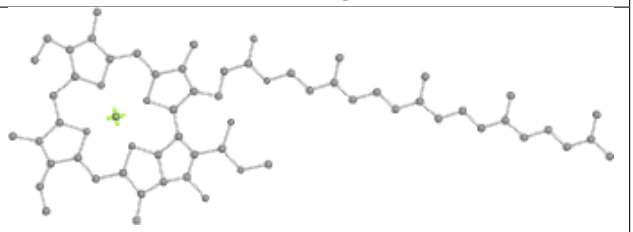
Bond lengths



Bond angles

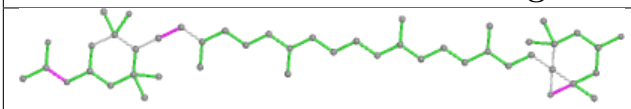


Torsions



Rings

Ligand UIX B 304



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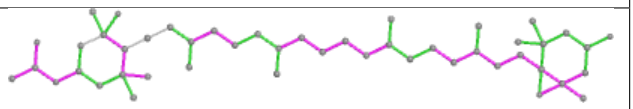
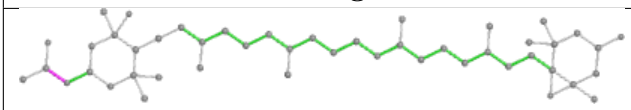


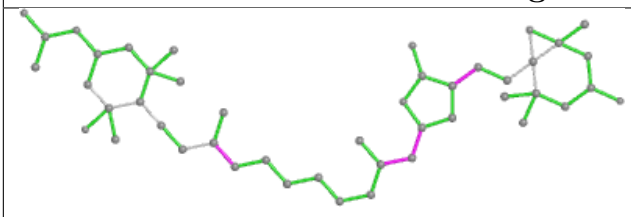
Bond angles



Torsions

Rings

Ligand PID O 302



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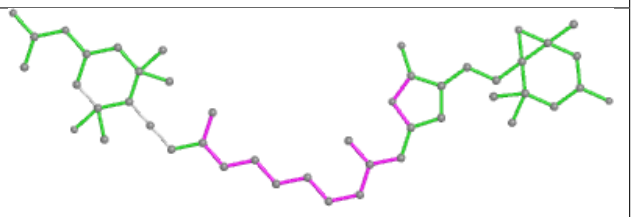
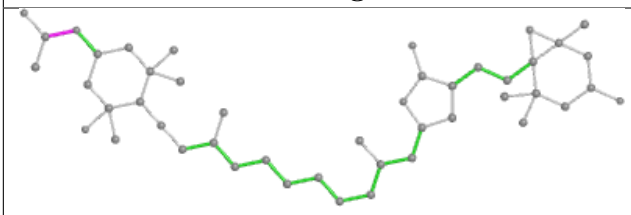


Bond angles



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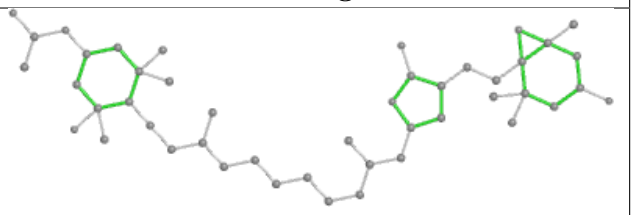
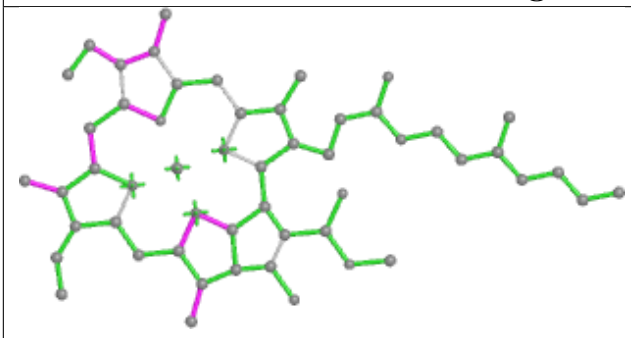


Rings

Ligand CLA J 311



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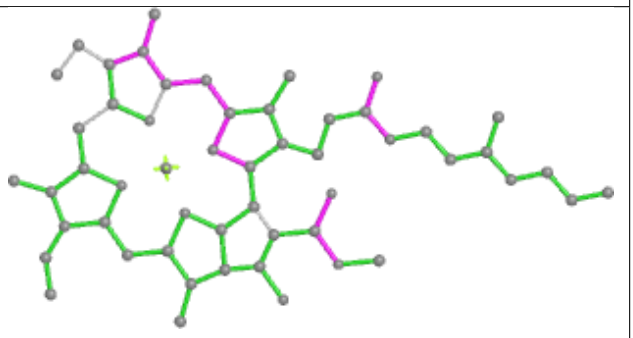
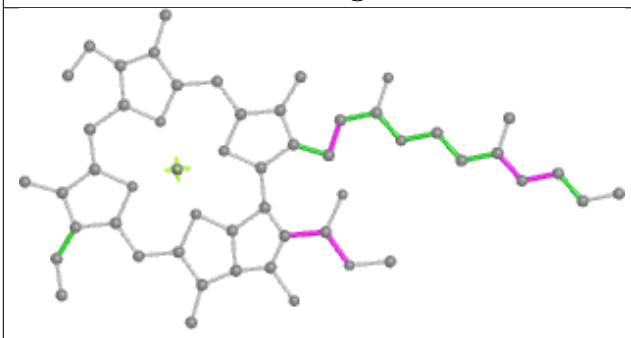


Bond angles



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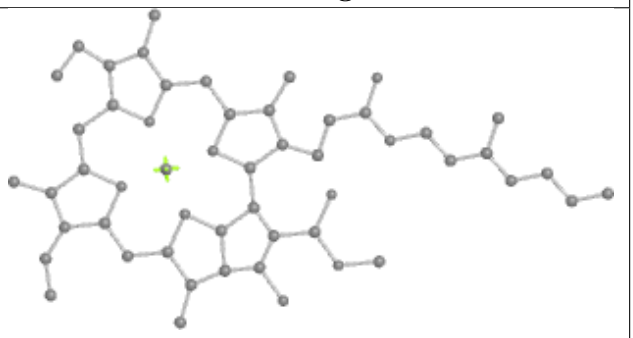
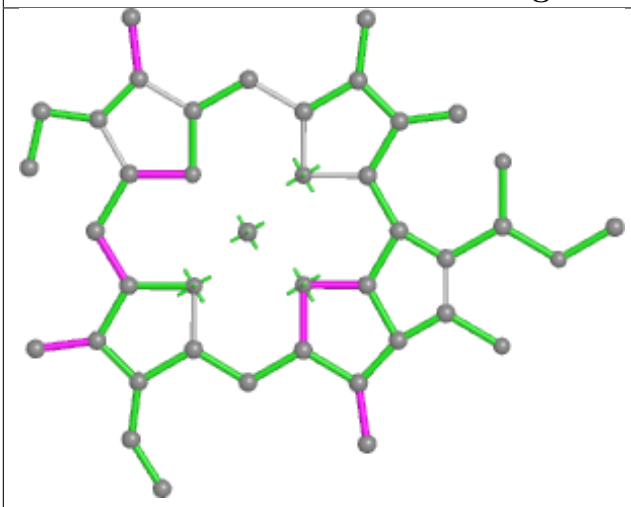


Rings

Ligand CLA l 508



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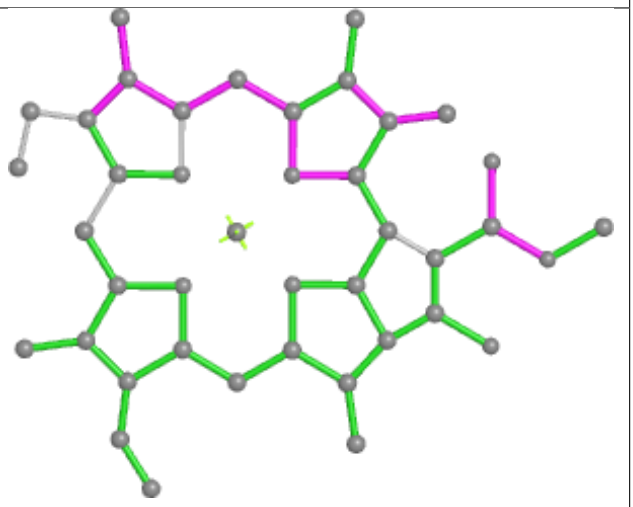
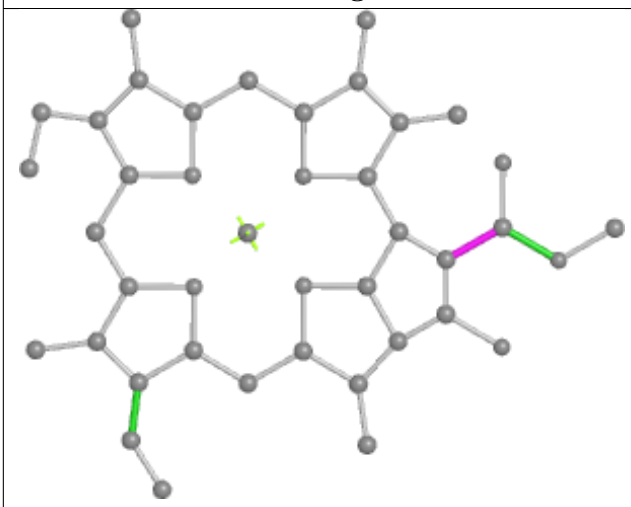
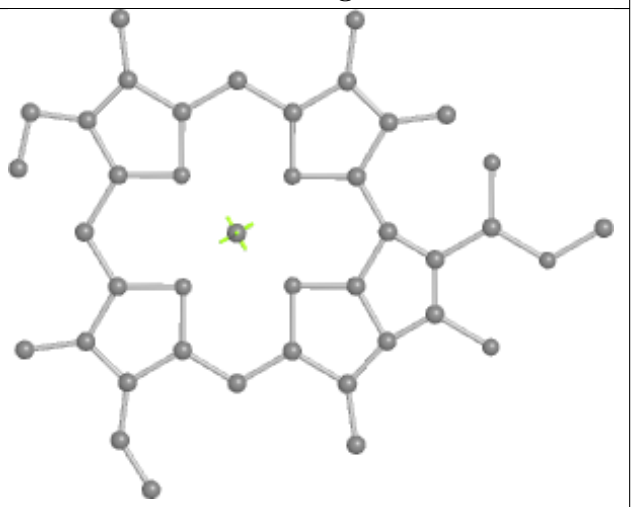


Bond angles

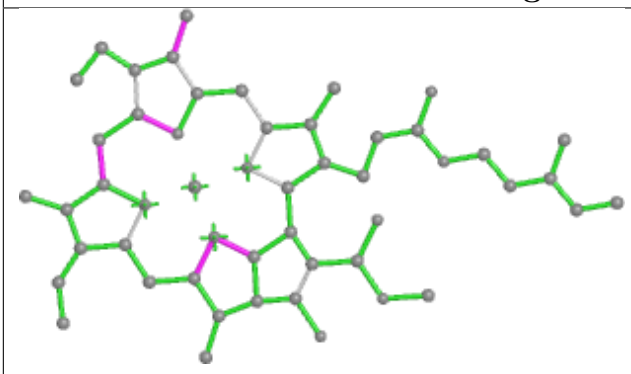


Torsions

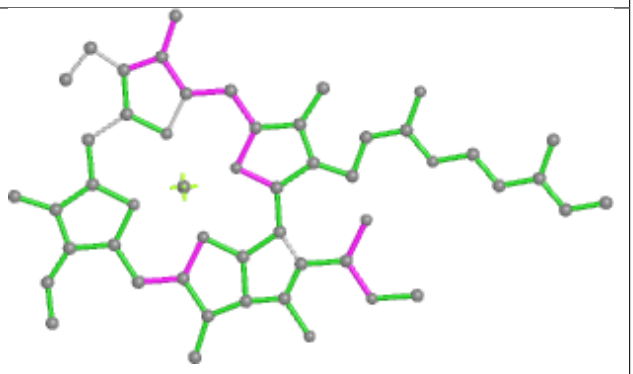


Rings

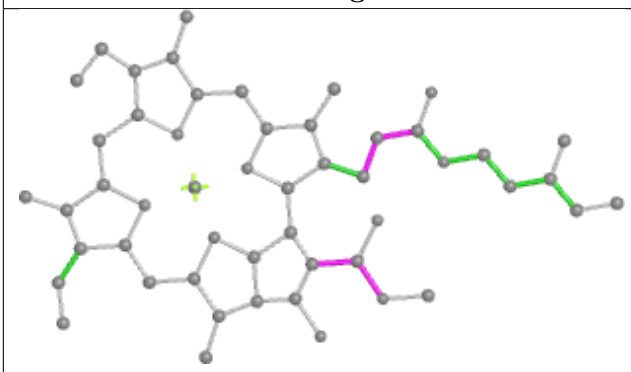
Ligand CLA N 311



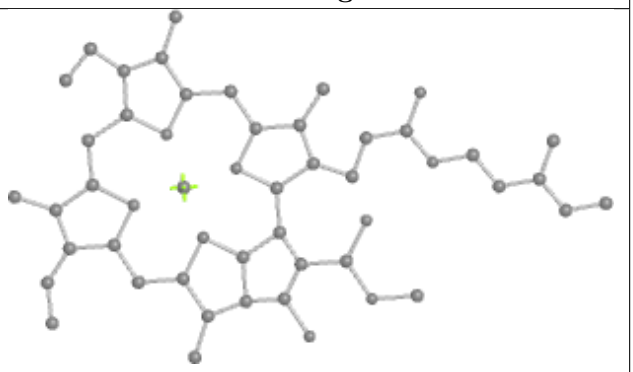
Bond lengths



Bond angles

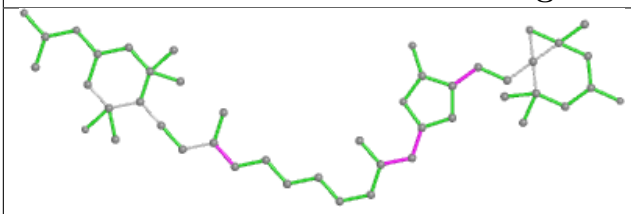


Torsions

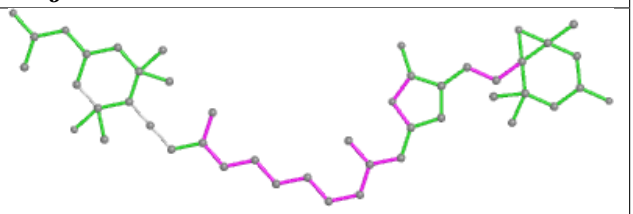


Rings

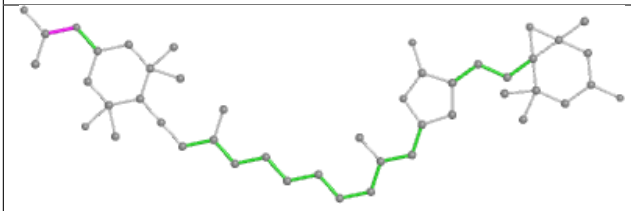
Ligand PID j 101



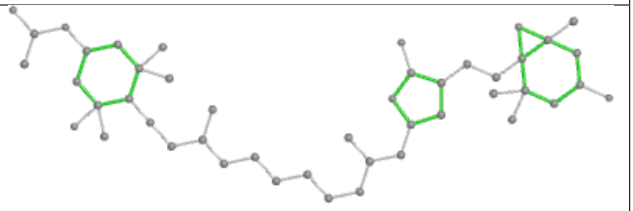
Bond lengths



Bond angles

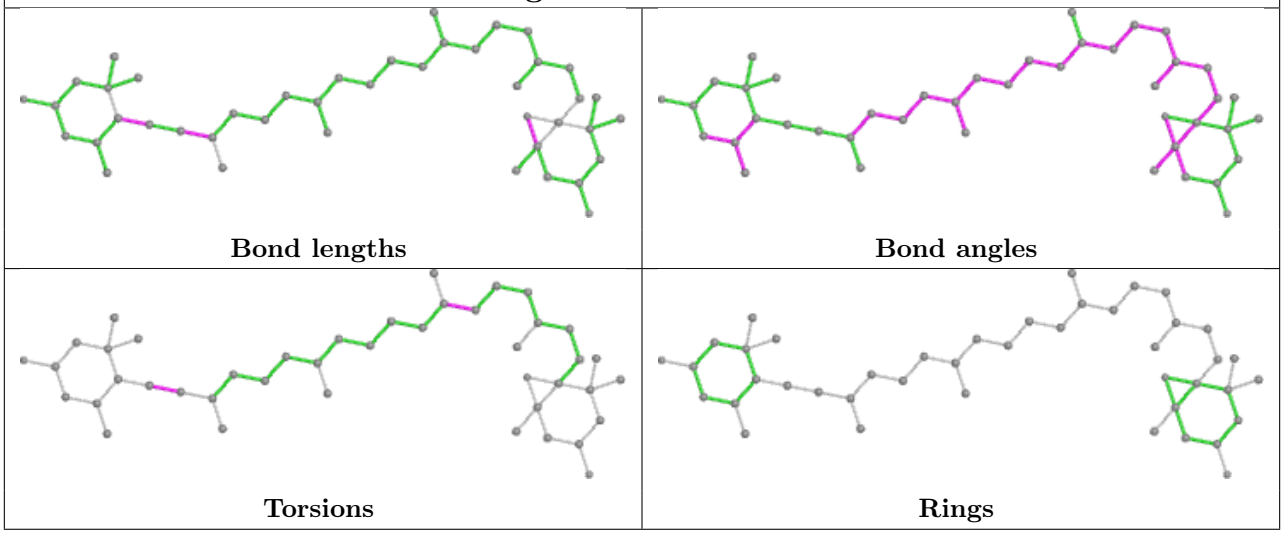


Torsions

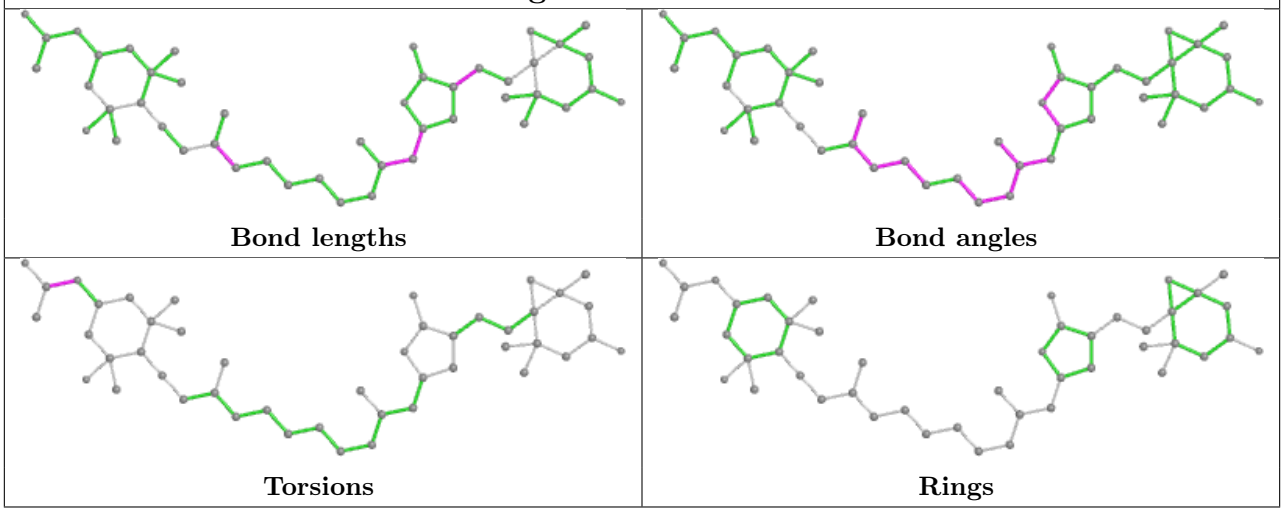


Rings

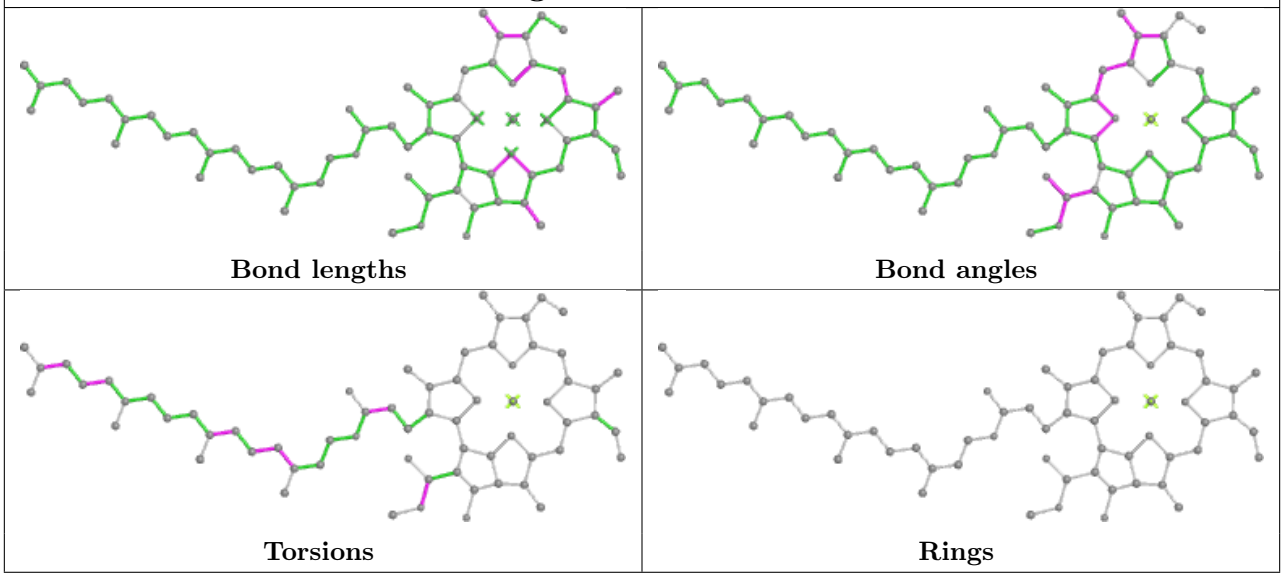
Ligand DD6 A 201



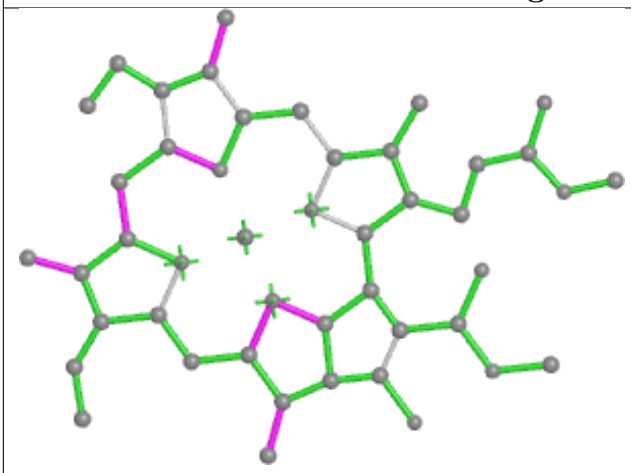
Ligand PID H 302



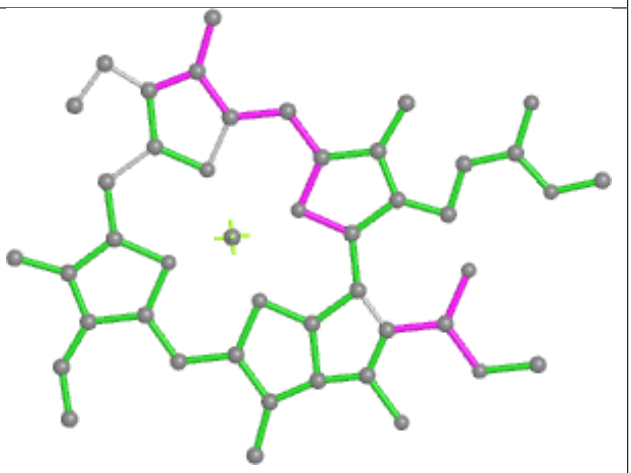
Ligand CLA b 704



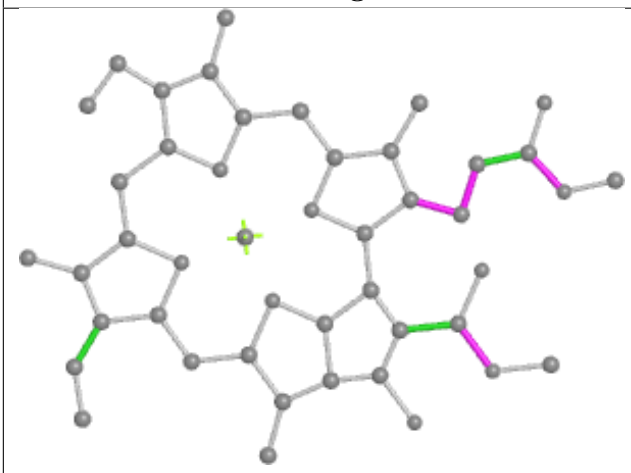
Ligand CLA b 715



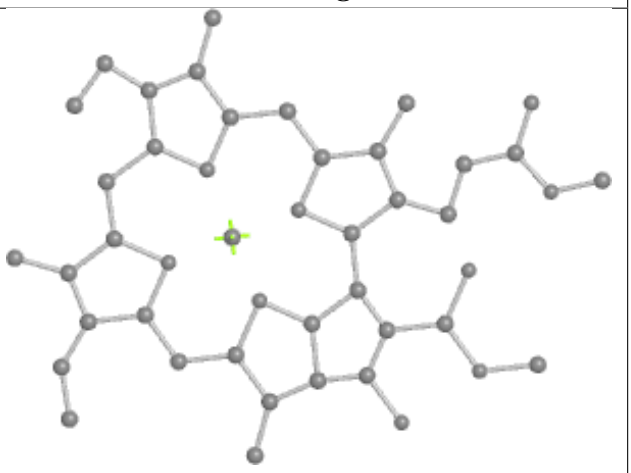
Bond lengths



Bond angles

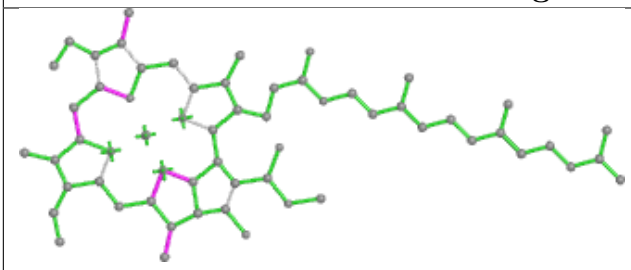


Torsions



Rings

Ligand CLA l 501



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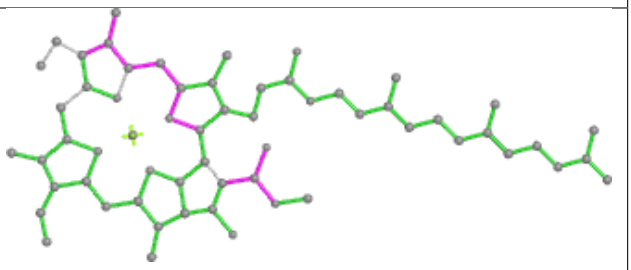
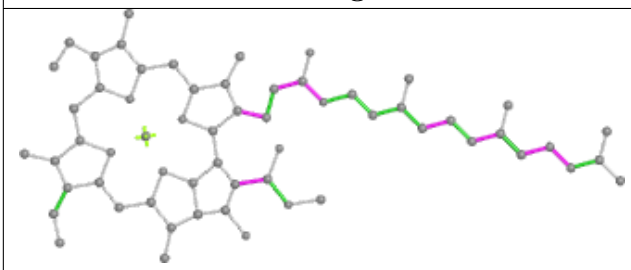


Bond angles



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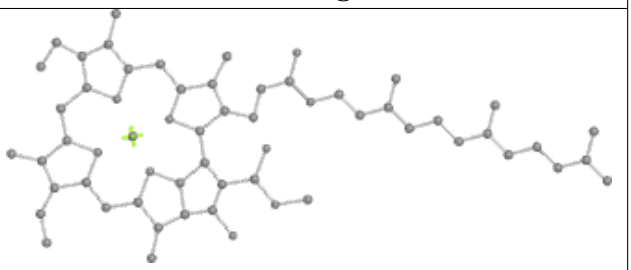
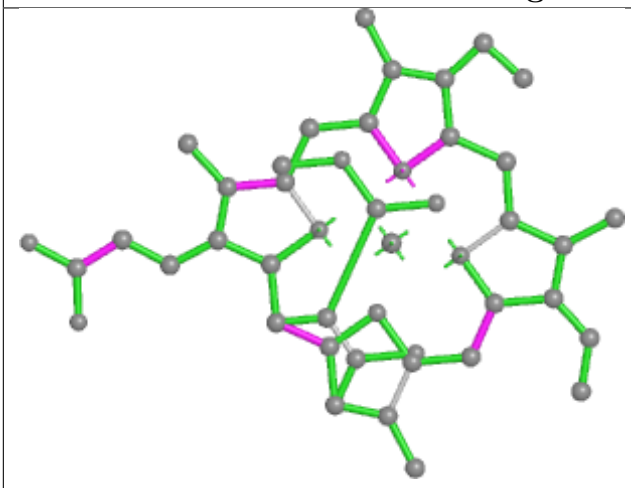


Rings

Ligand KC1 P 211



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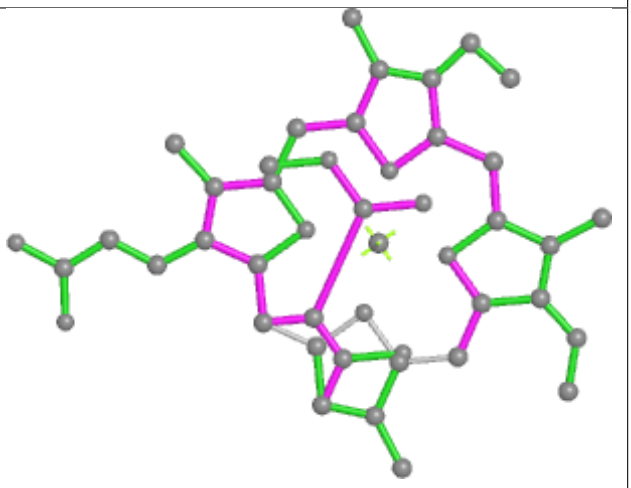
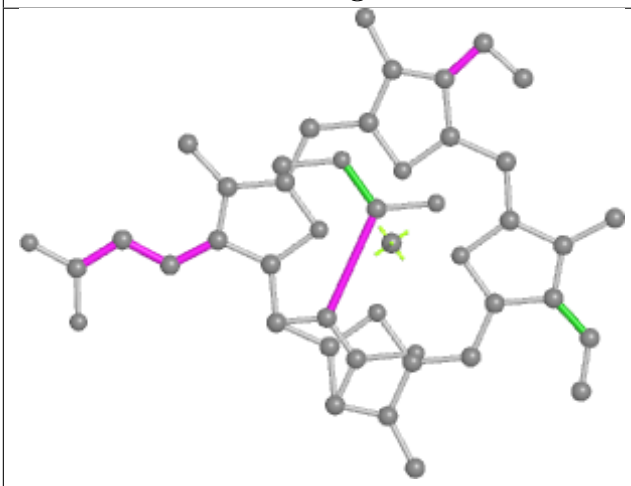


Bond angles



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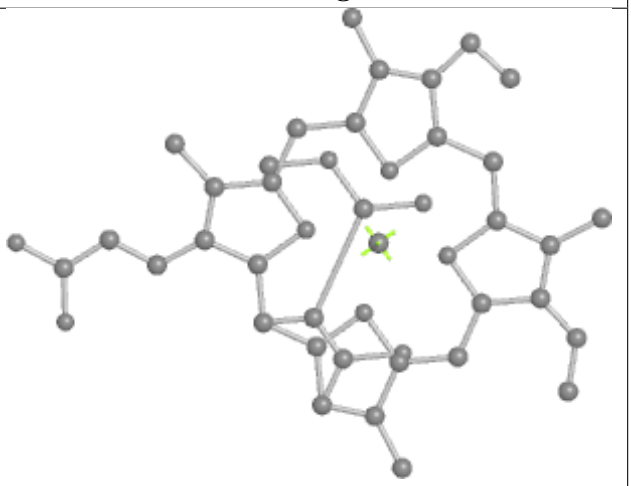
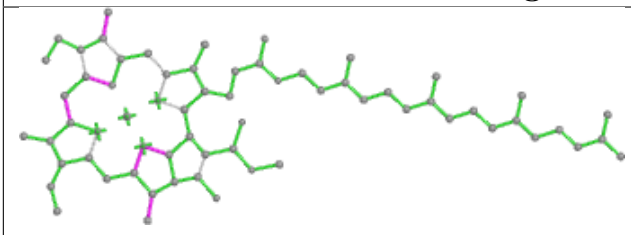


Rings

Ligand CLA H 308



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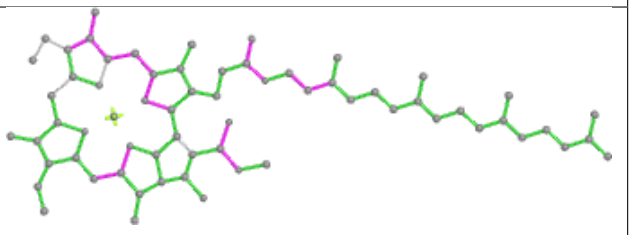
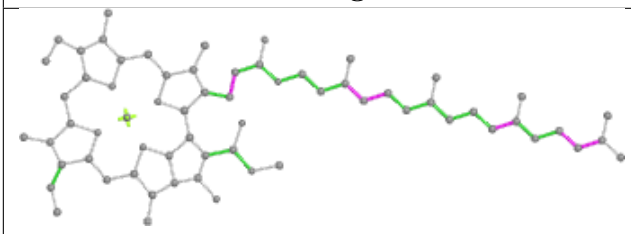


Bond angles



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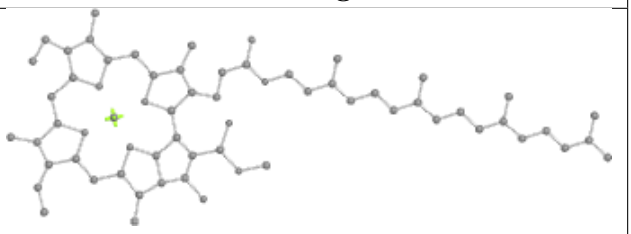
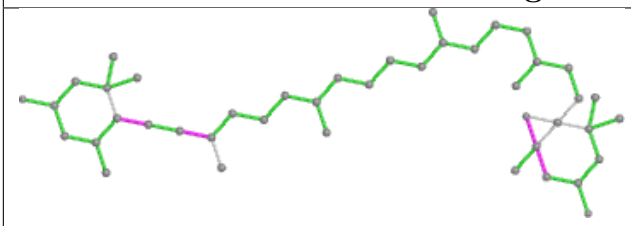
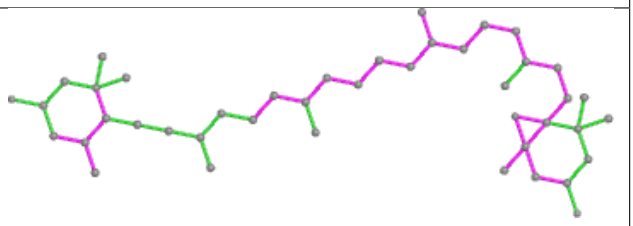


Rings

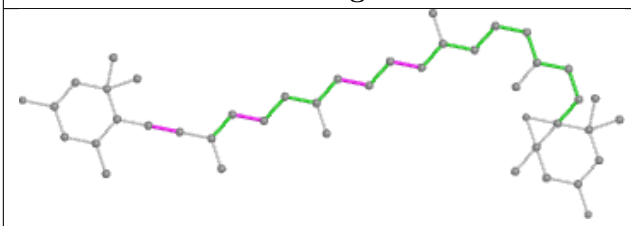
Ligand DD6 O 303



Bond lengths



Bond angles



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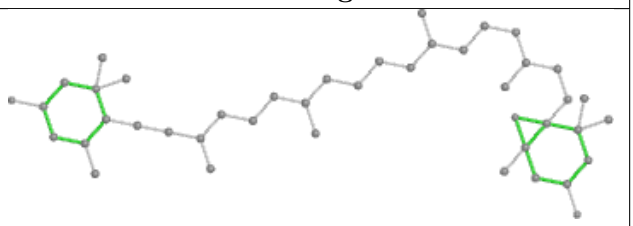
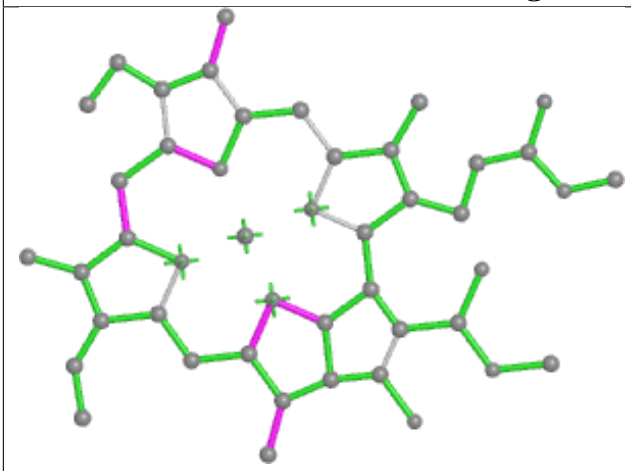


Rings

Ligand CLA E 310



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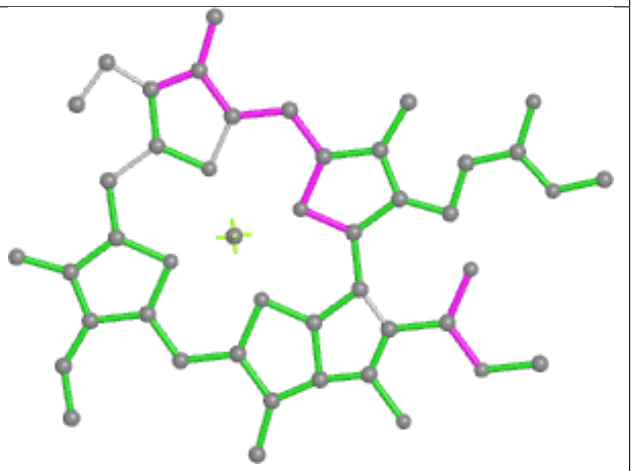
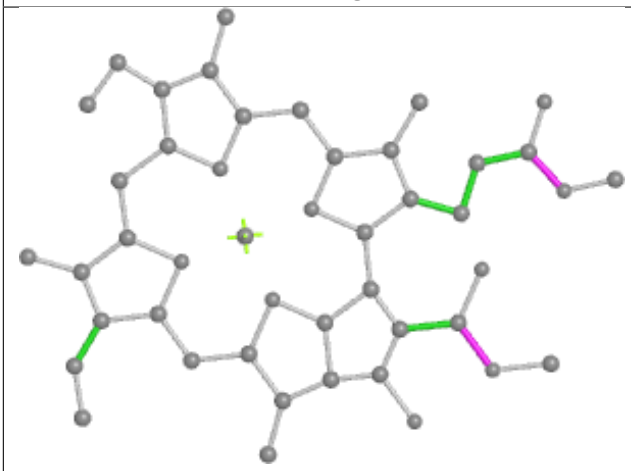


Bond angles



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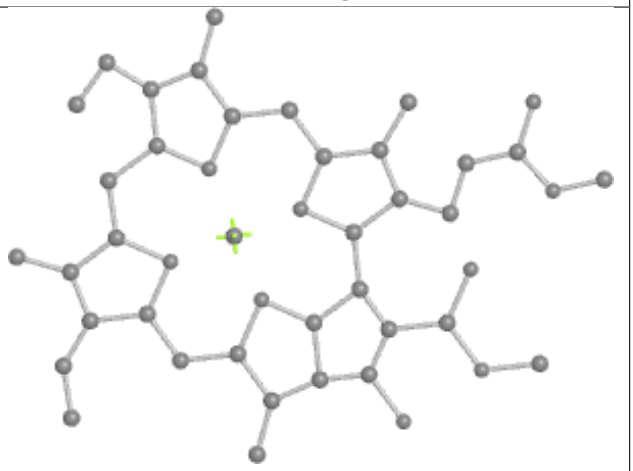
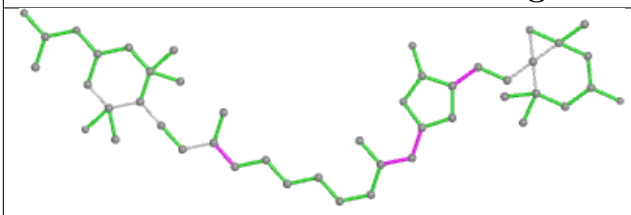


Rings

Ligand PID D 306



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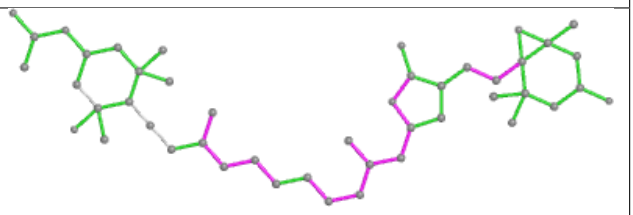
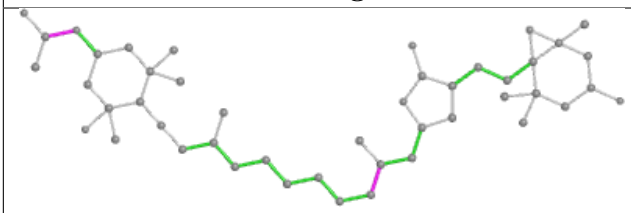


Bond angles



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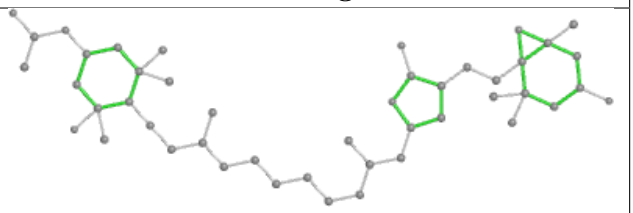
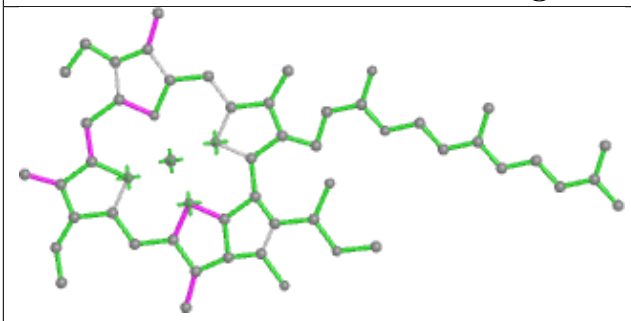


Rings

Ligand CLA I 214



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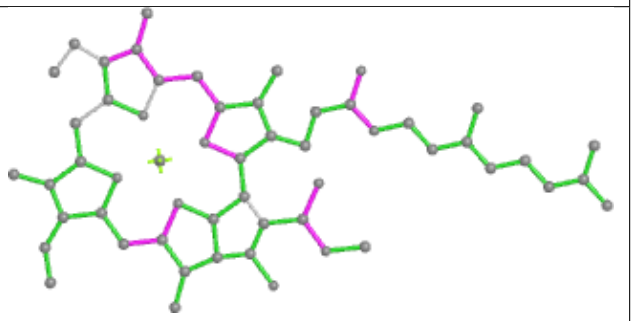
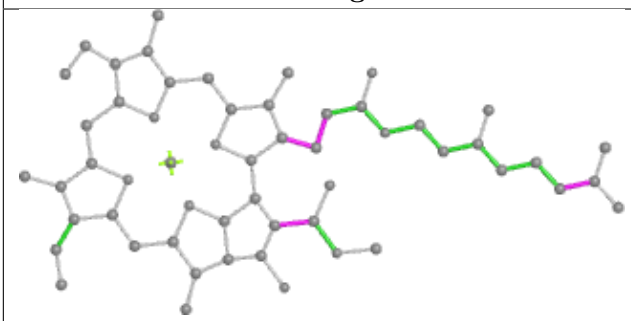


Bond angles



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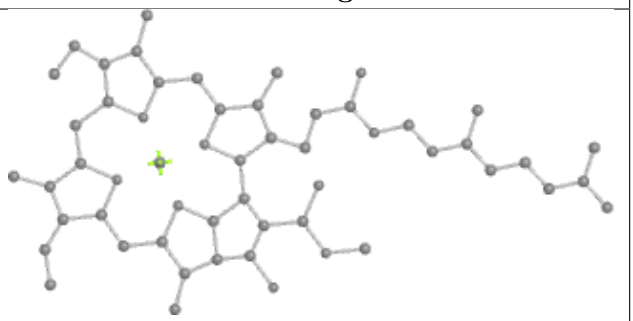
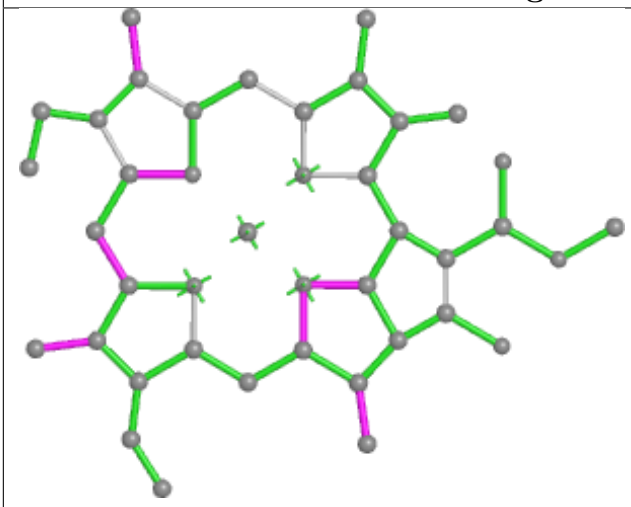
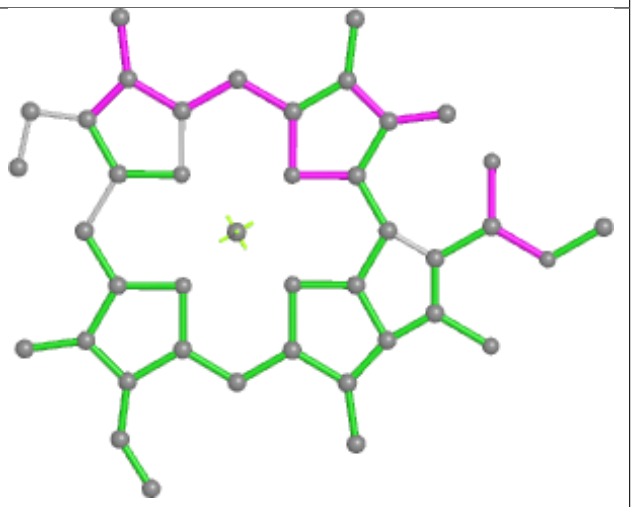


Rings

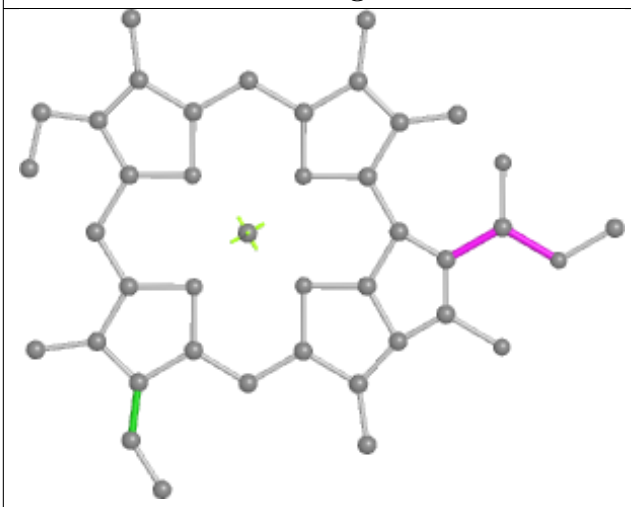
Ligand CLA L 315



Bond lengths



Bond angles



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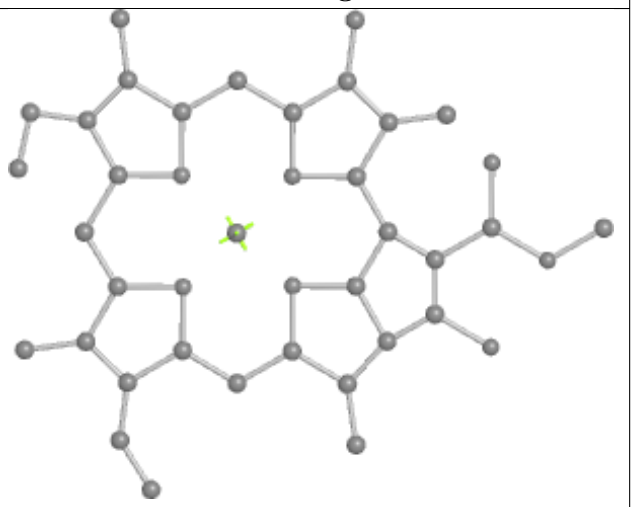
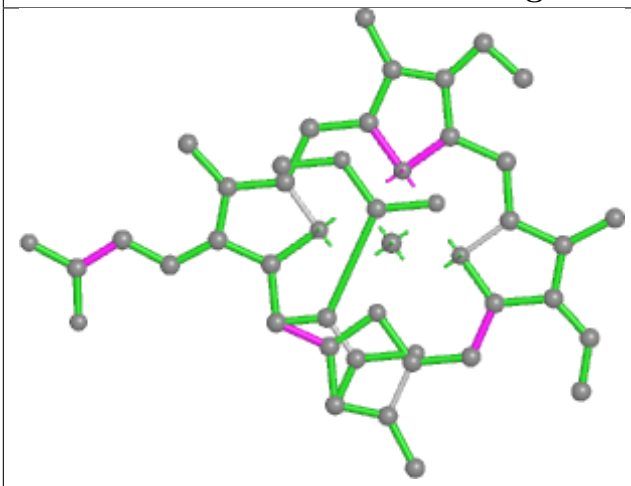
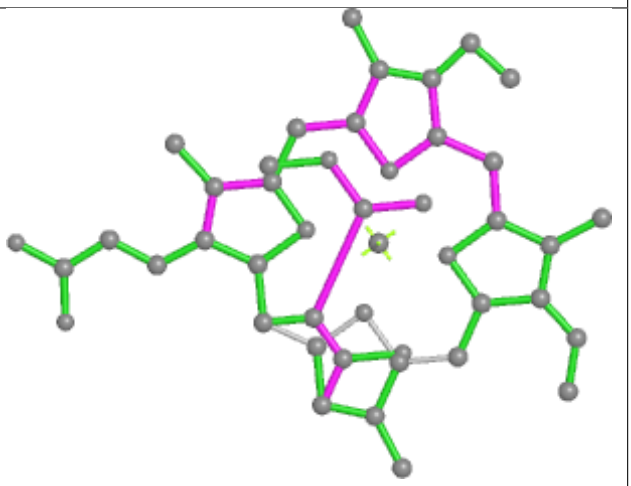


Rings

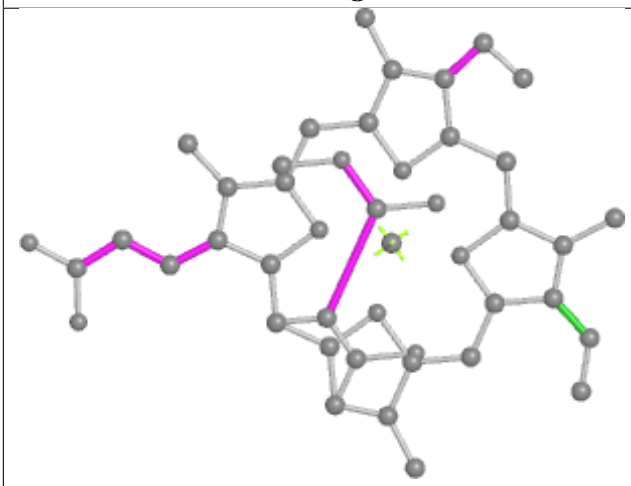
Ligand KC1 O 315



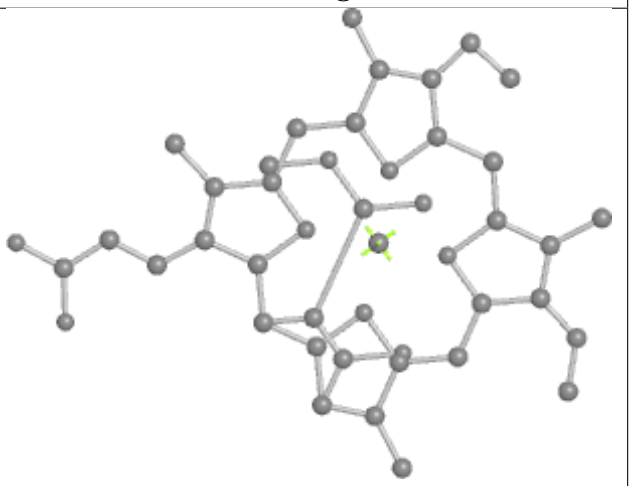
Bond lengths



Bond angles

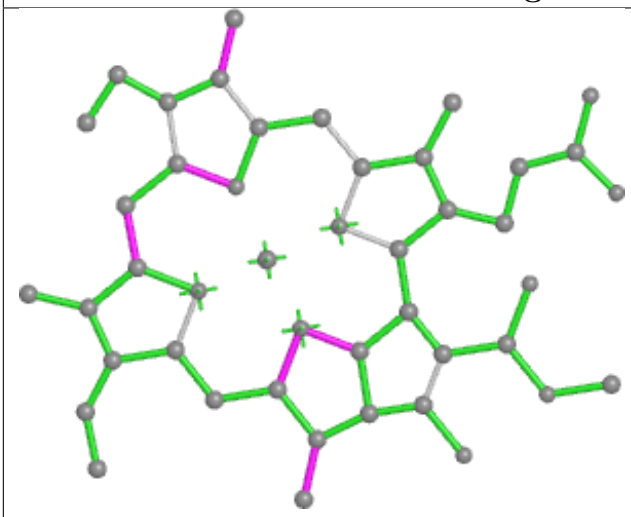


Torsions



Rings

Ligand CLA B 316



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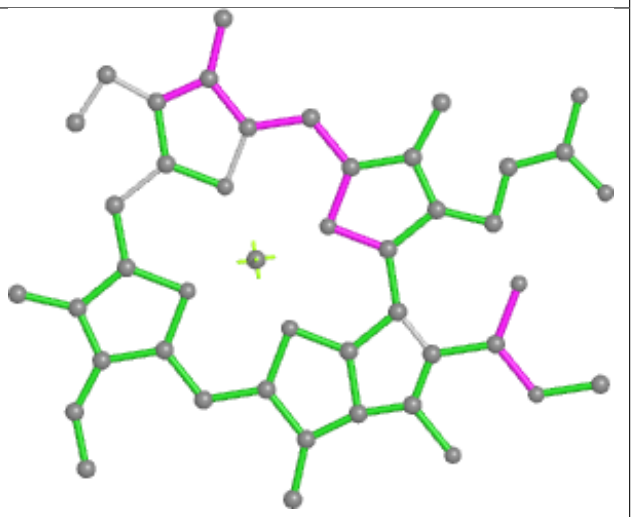
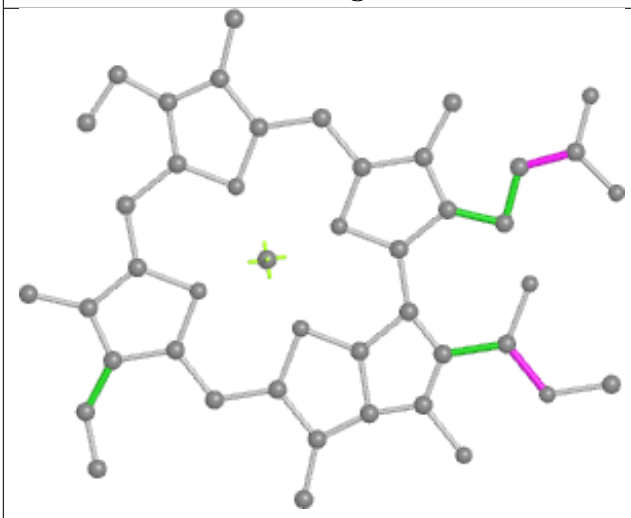


Bond angles



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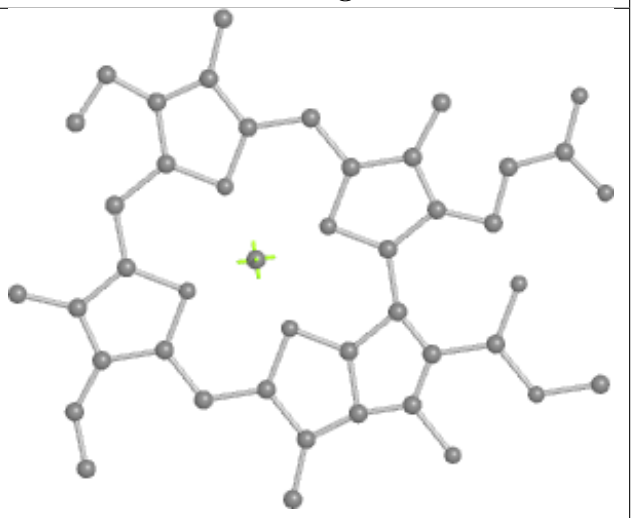
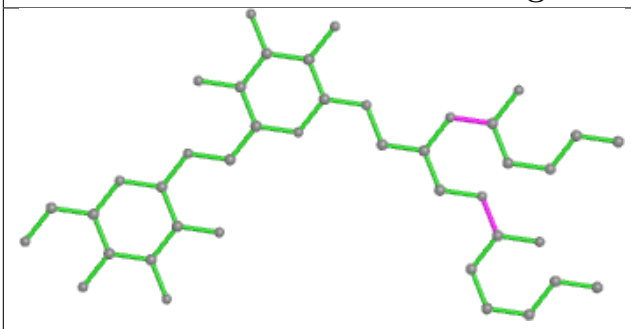


Rings

Ligand DGD j 105



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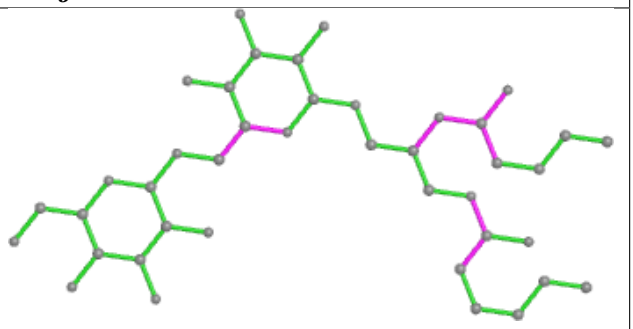
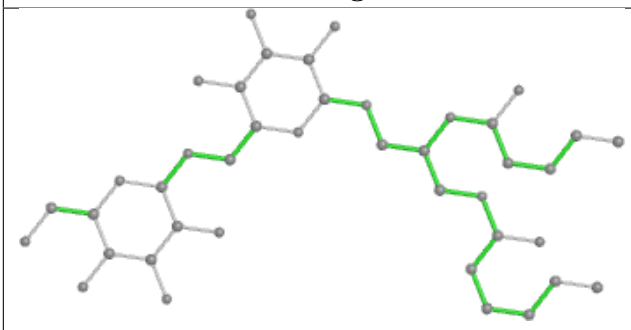


Bond angles



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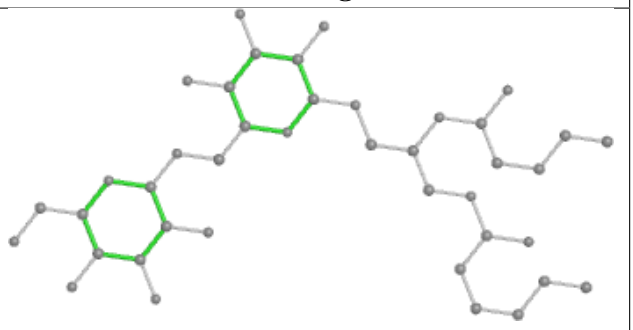
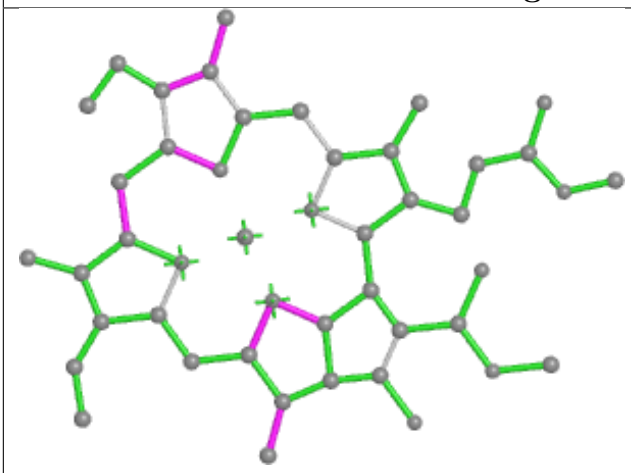
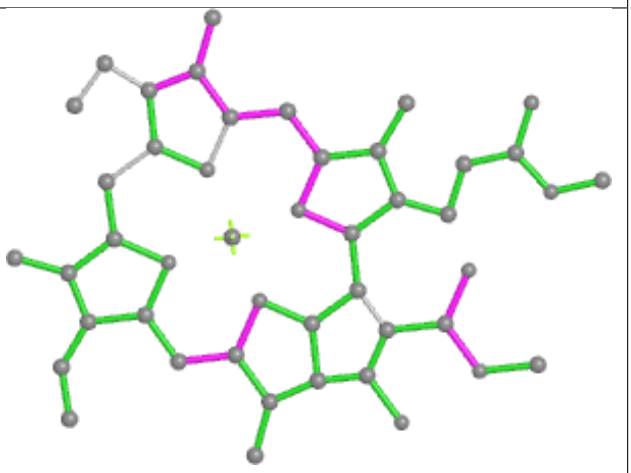


Rings

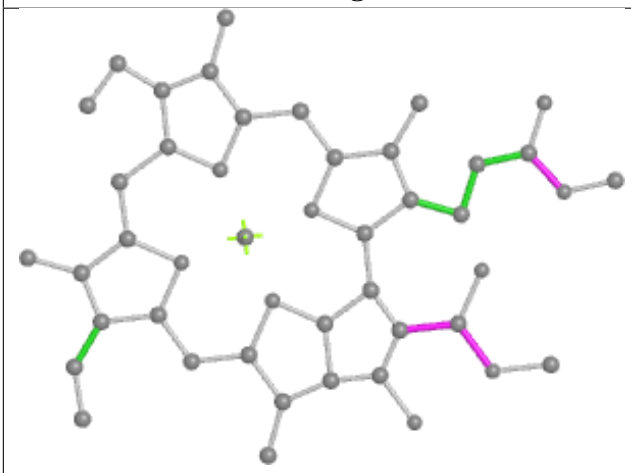
Ligand CLA A 210



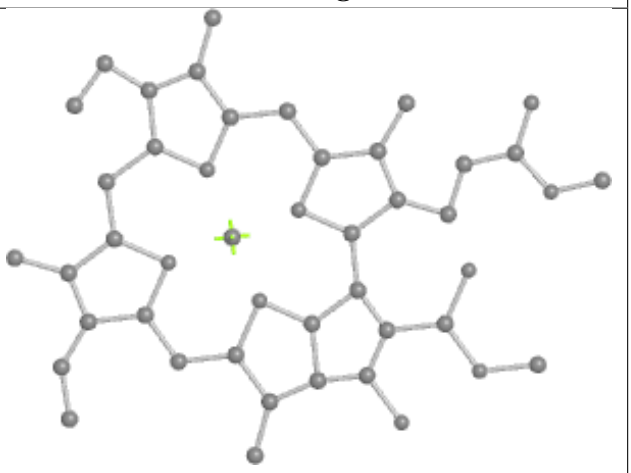
Bond lengths



Bond angles

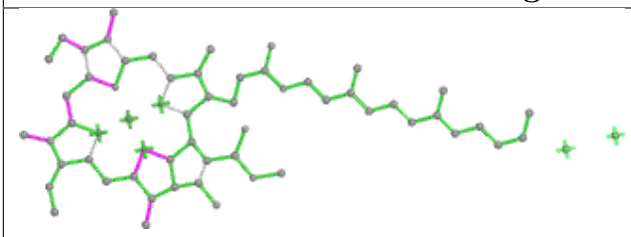


Torsions

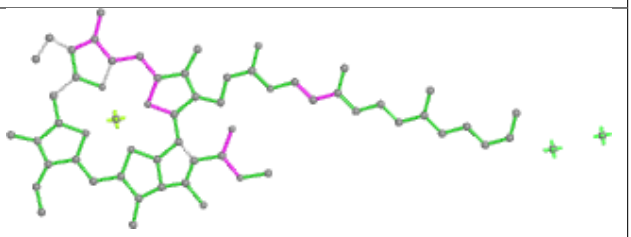


Rings

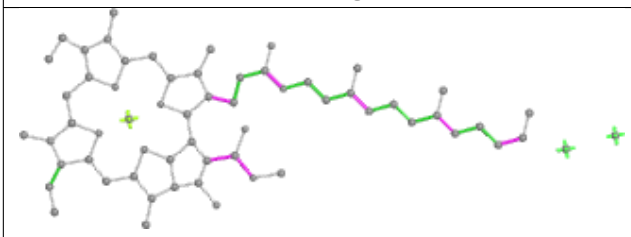
Ligand CLA G 304



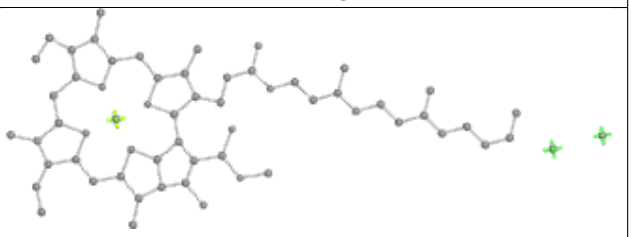
Bond lengths



Bond angles

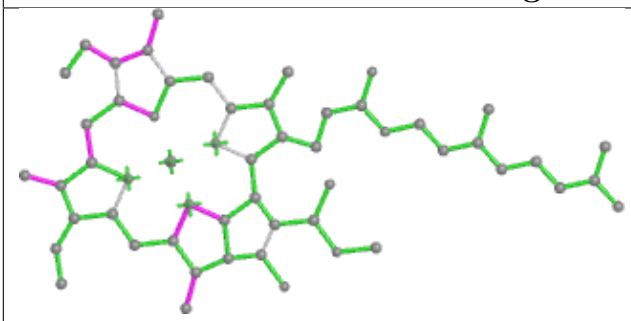


Torsions

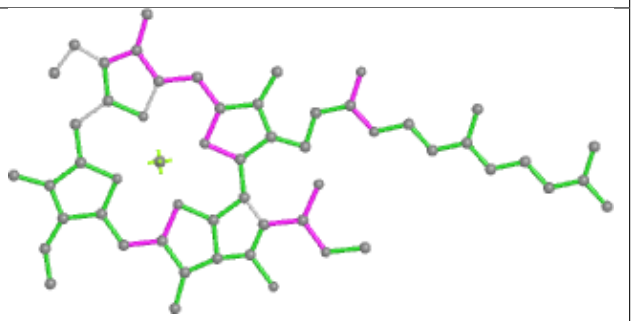


Rings

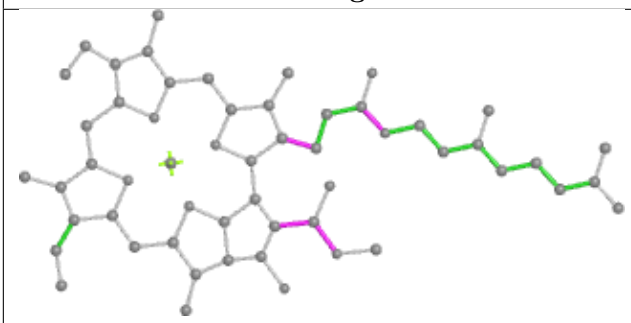
Ligand CLA K 214



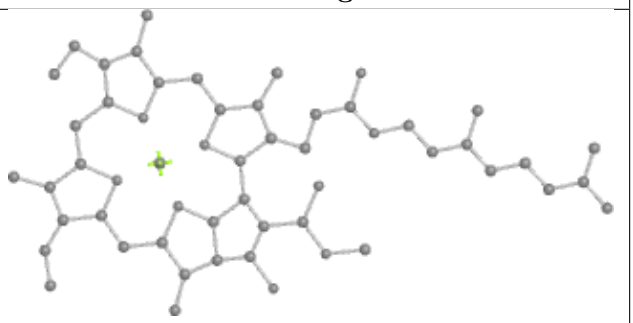
Bond lengths



Bond angles

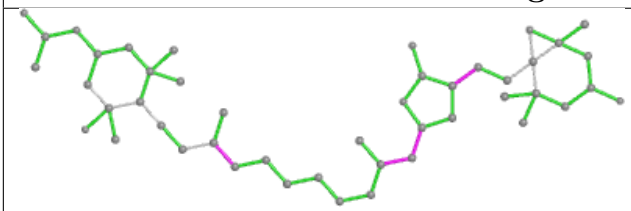


Torsions

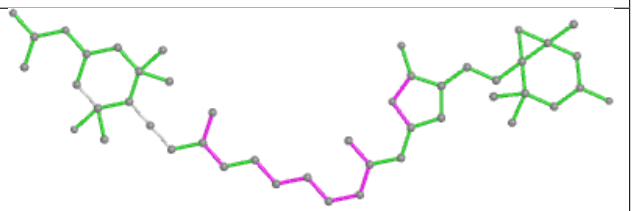


Rings

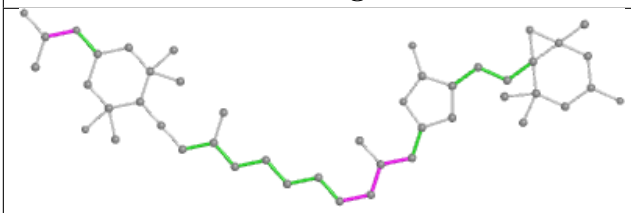
Ligand PID G 303



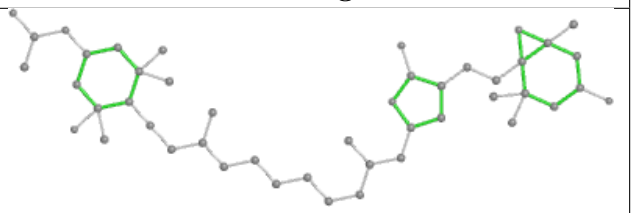
Bond lengths



Bond angles

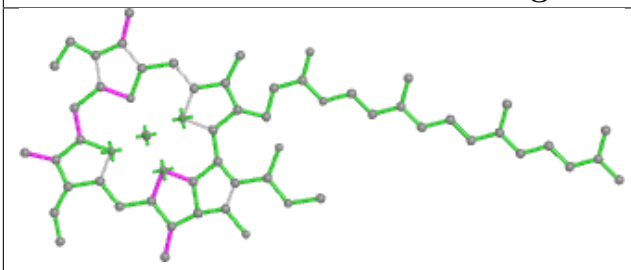


Torsions

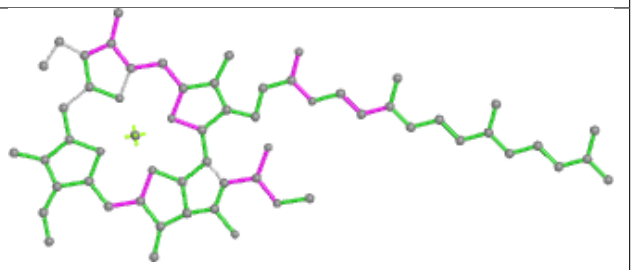


Rings

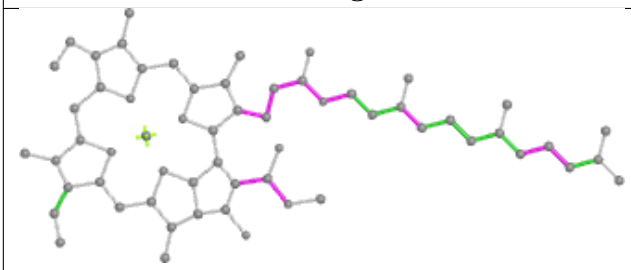
Ligand CLA I 209



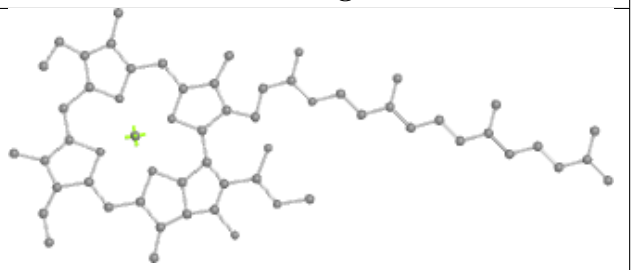
Bond lengths



Bond angles

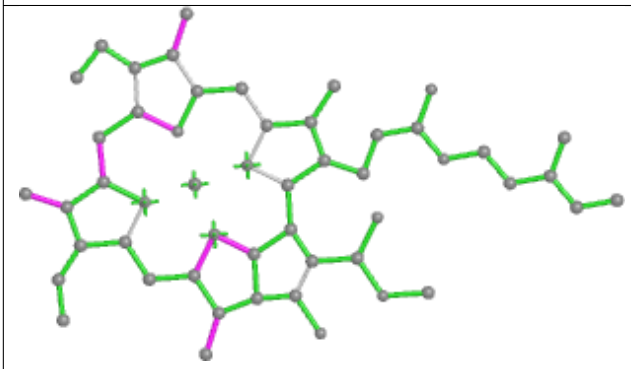


Torsions



Rings

Ligand CLA a 813



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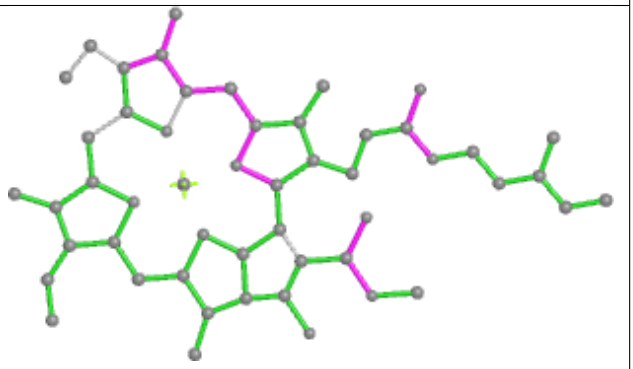
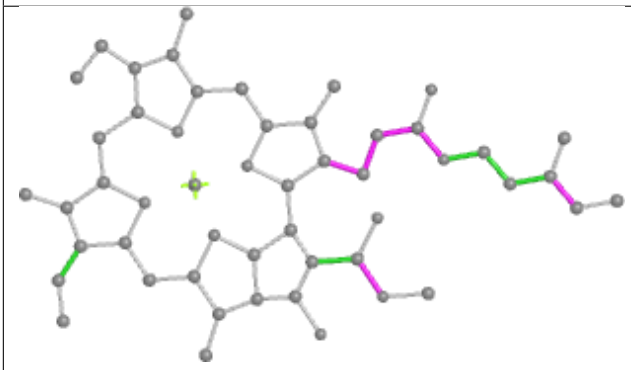
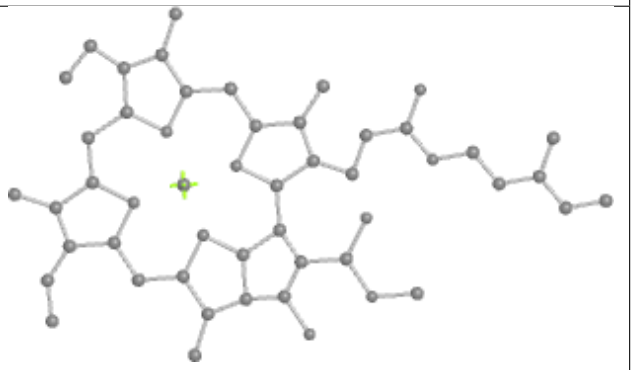


Bond angles

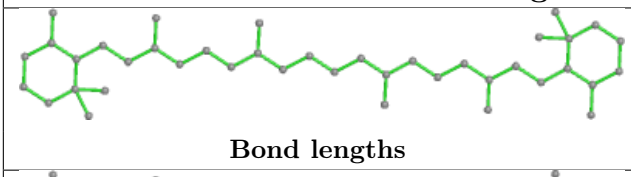


Torsions

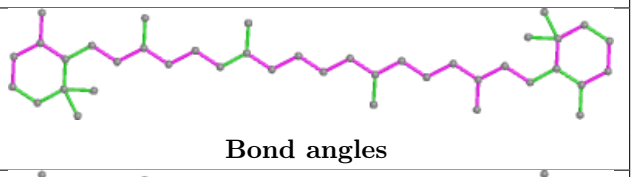


Rings

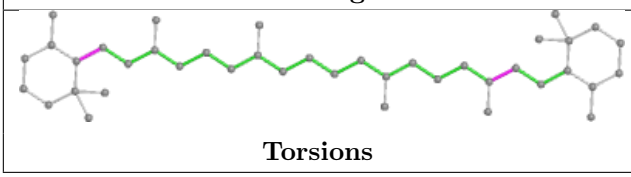
Ligand BCR i 204



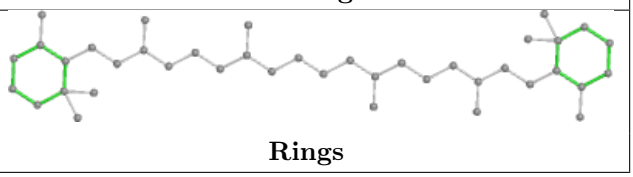
Bond lengths



Bond angles

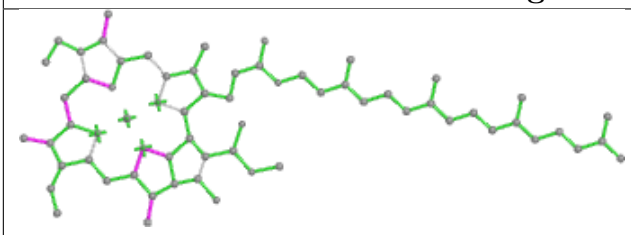


Torsions

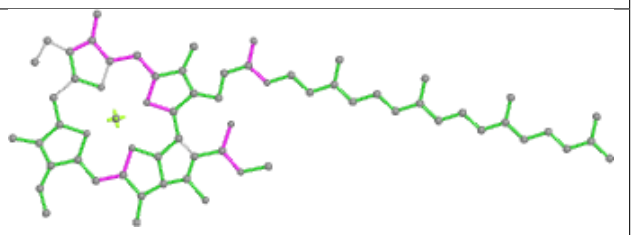


Rings

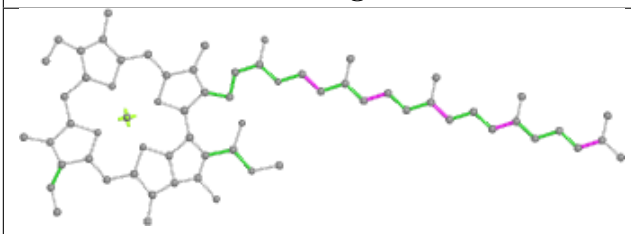
Ligand CLA b 726



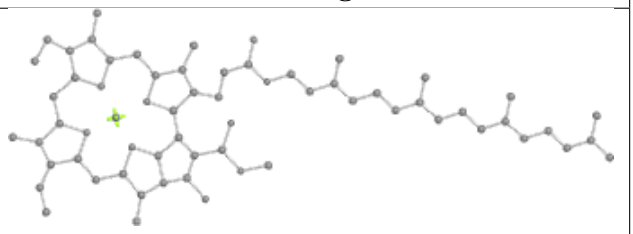
Bond lengths



Bond angles

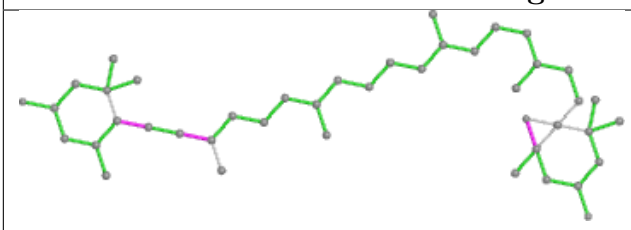


Torsions

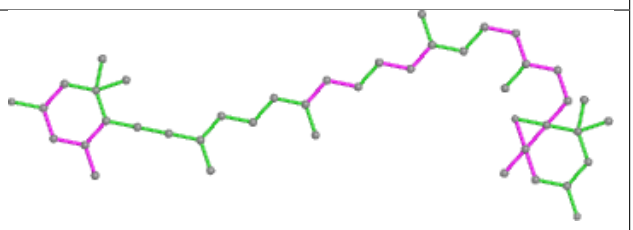


Rings

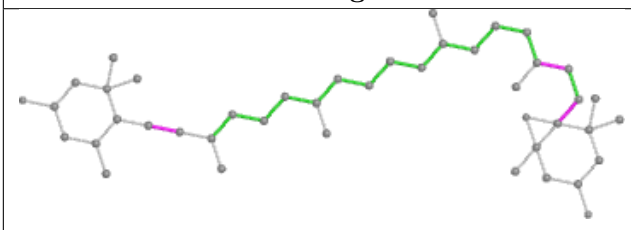
Ligand DD6 L 301



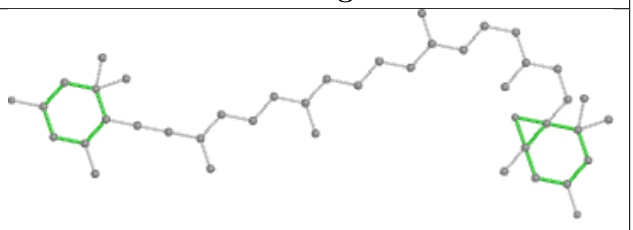
Bond lengths



Bond angles

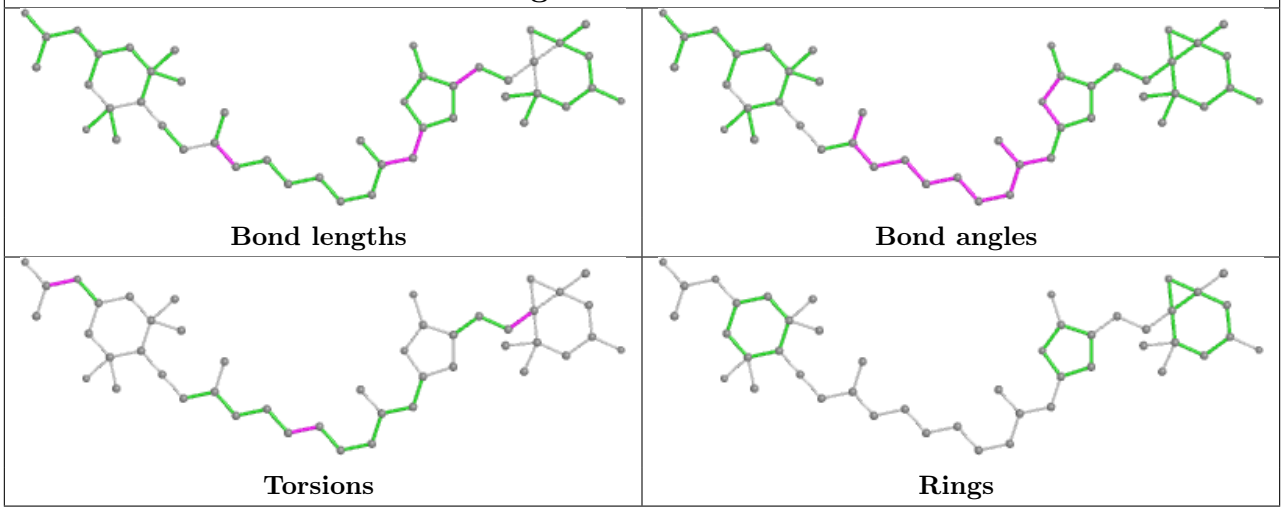


Torsions

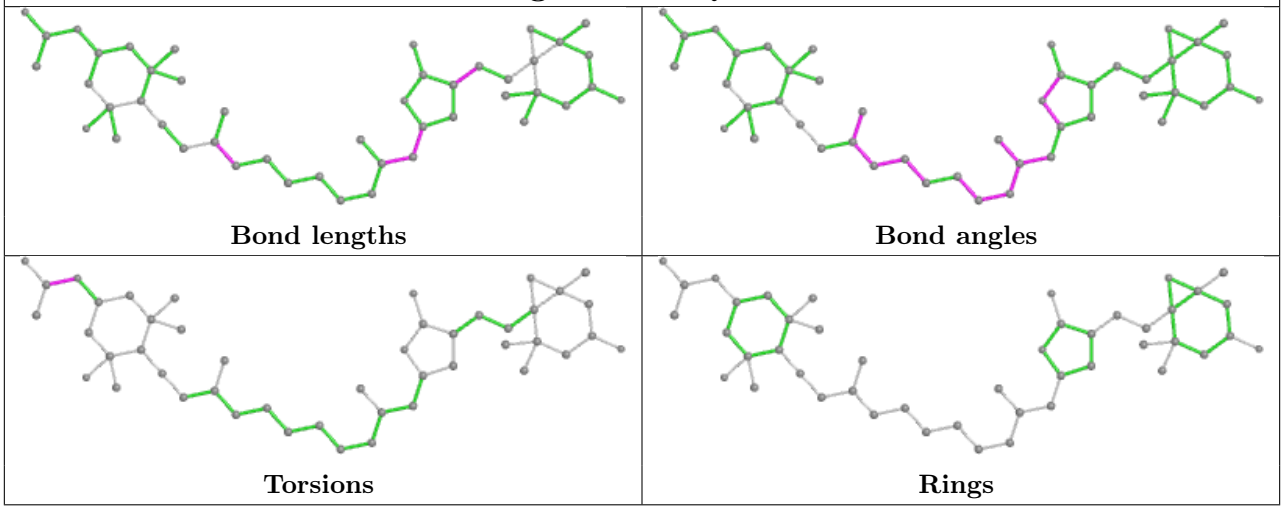


Rings

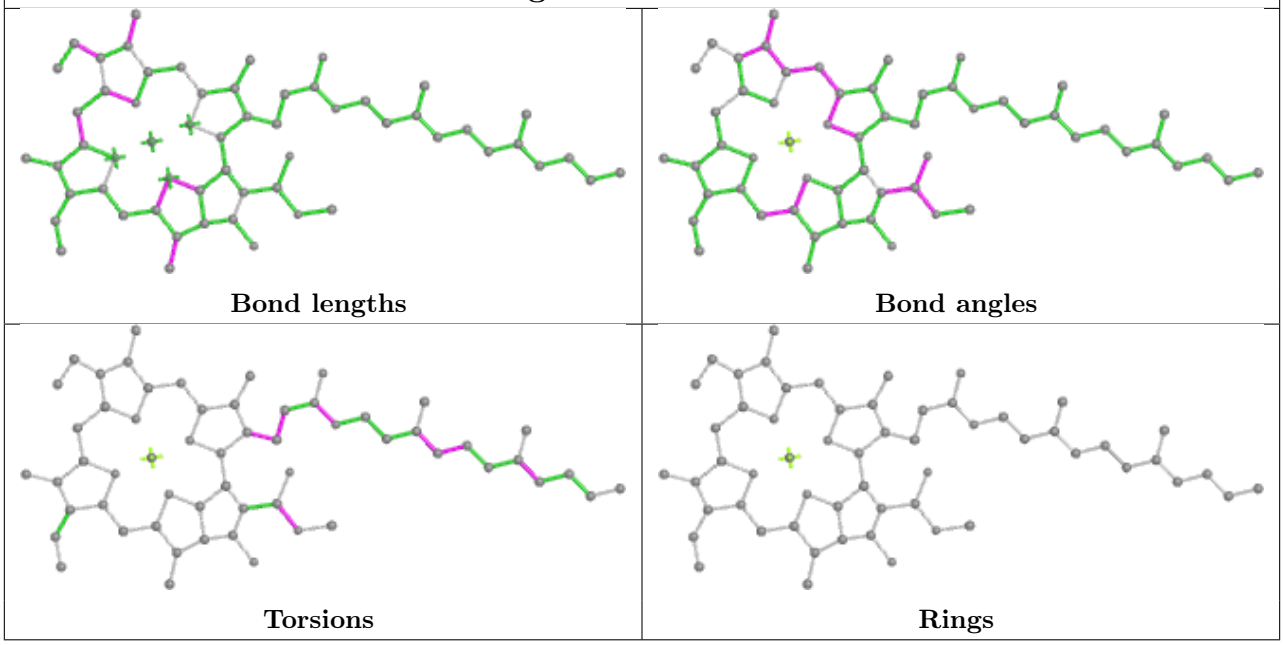
Ligand PID P 202



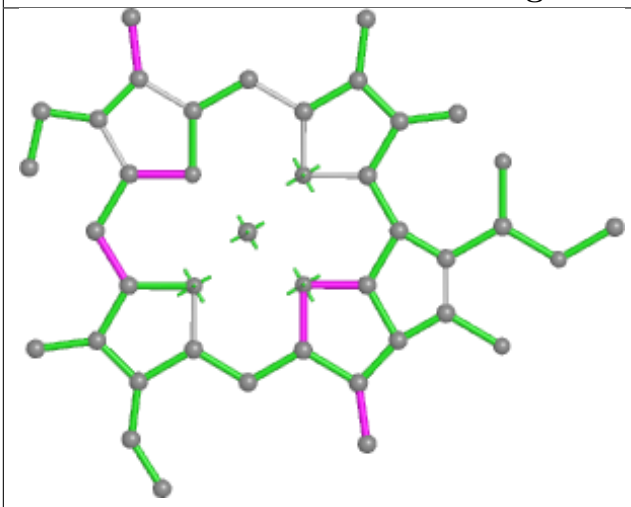
Ligand PID Q 304



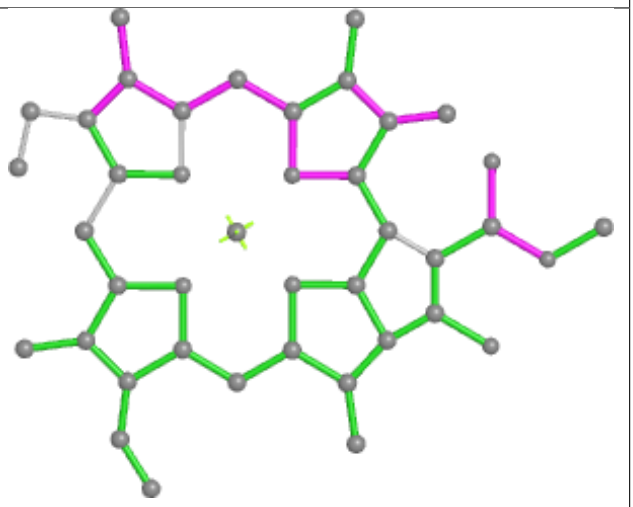
Ligand CLA b 711



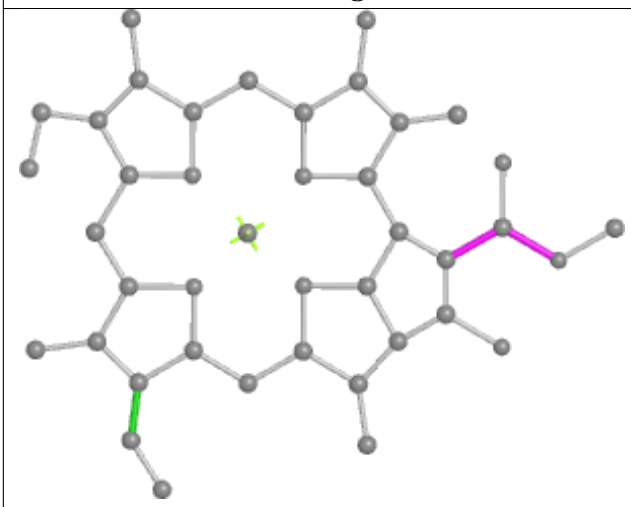
Ligand CLA F 316



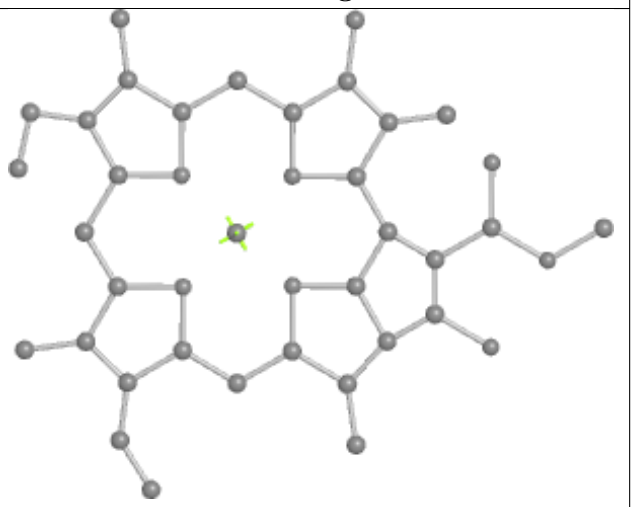
Bond lengths



Bond angles

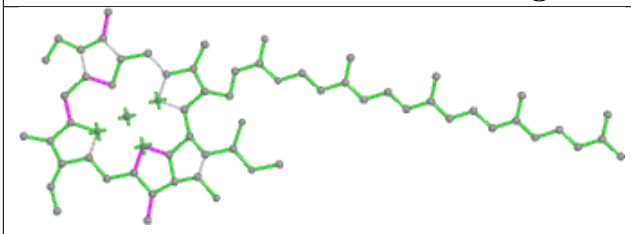


Torsions

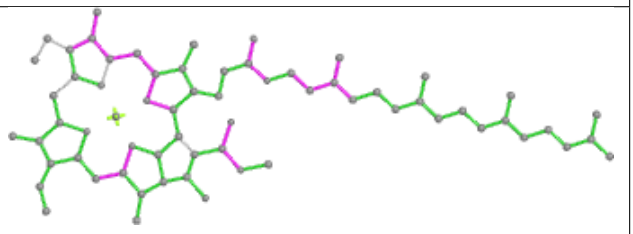


Rings

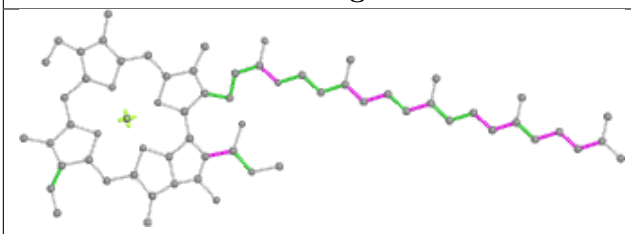
Ligand CLA I 213



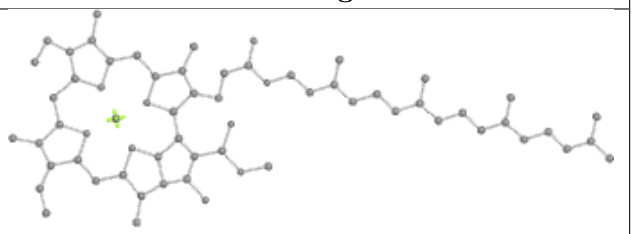
Bond lengths



Bond angles

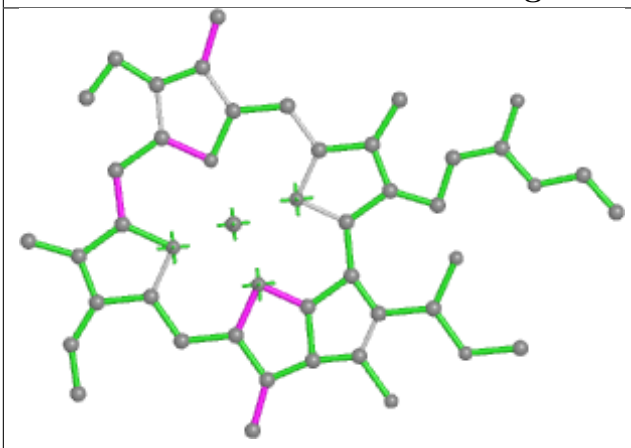


Torsions



Rings

Ligand CLA C 308



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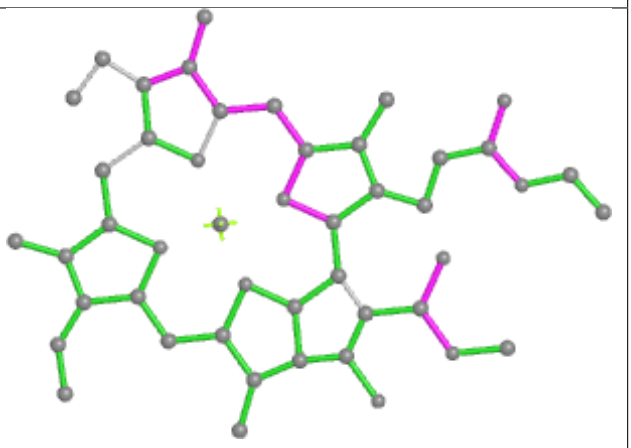
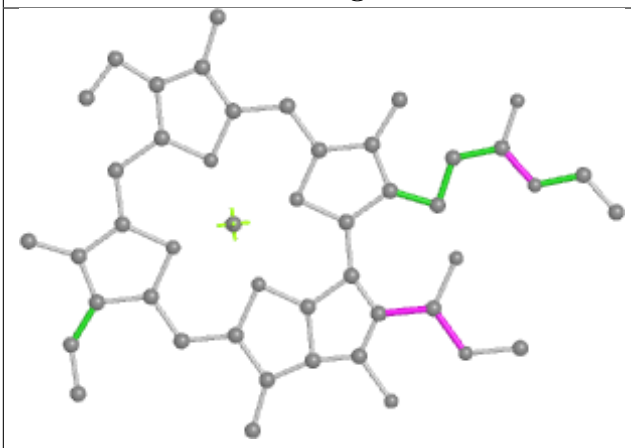
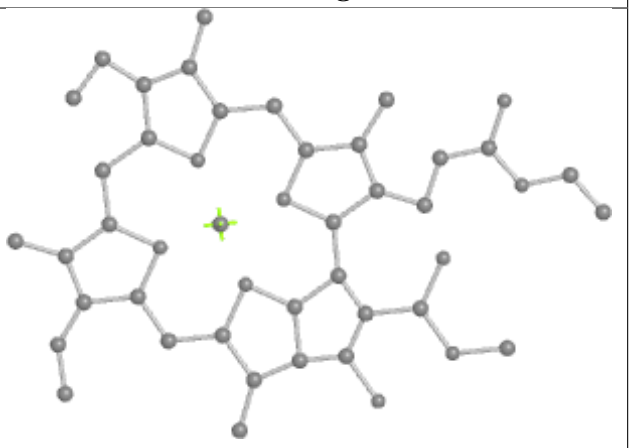


Bond angles

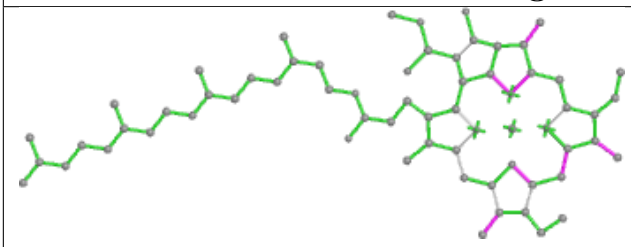


Torsions

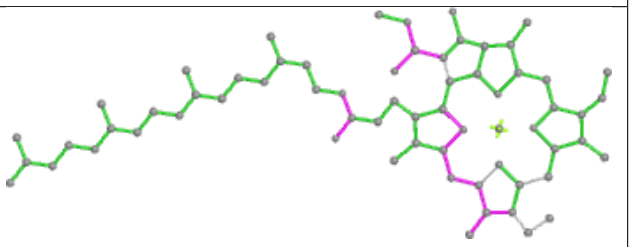


Rings

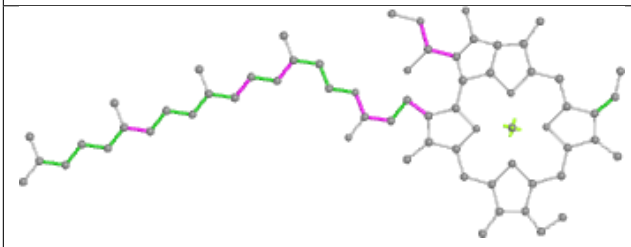
Ligand CLA a 831



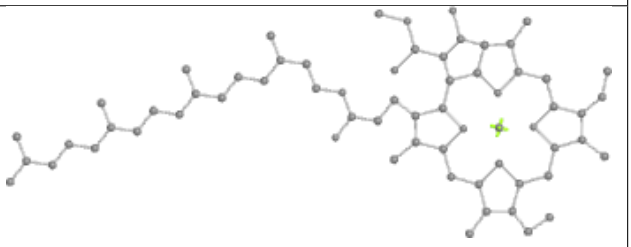
Bond lengths



Bond angles

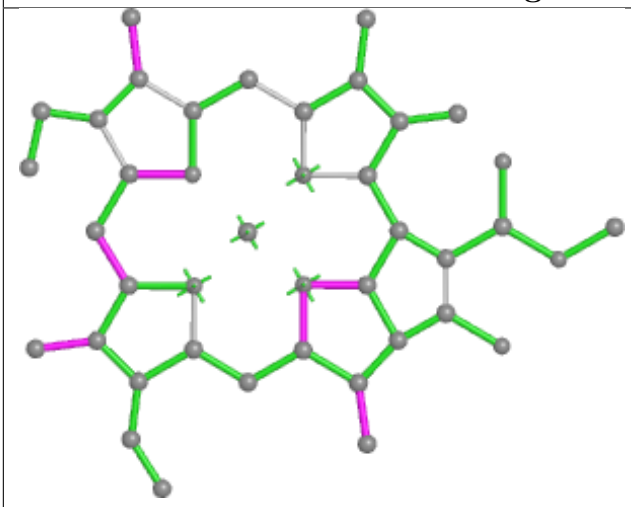


Torsions

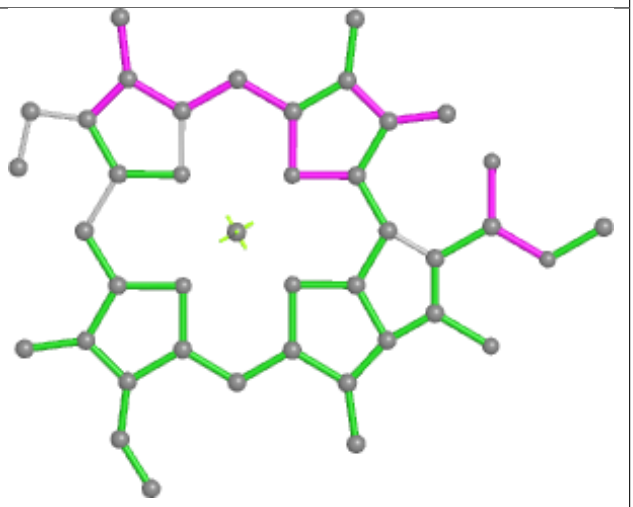


Rings

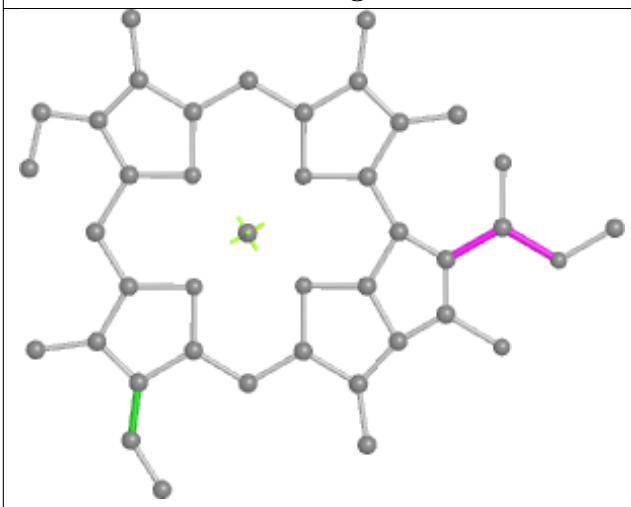
Ligand CLA B 314



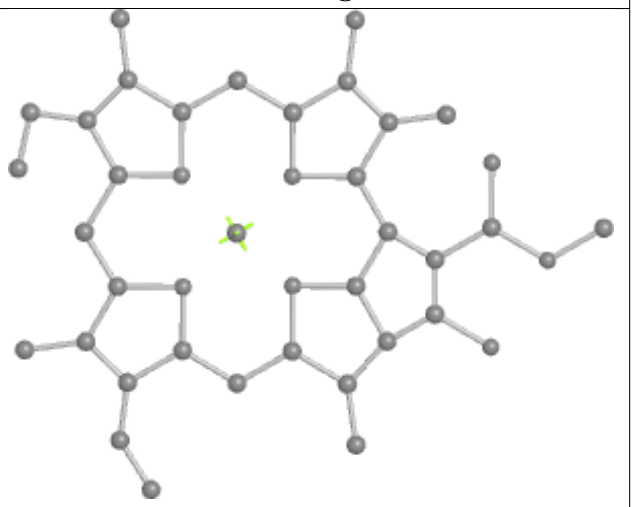
Bond lengths



Bond angles

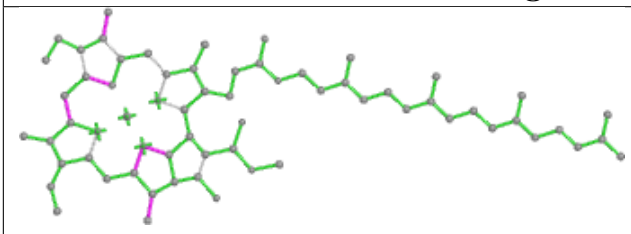


Torsions

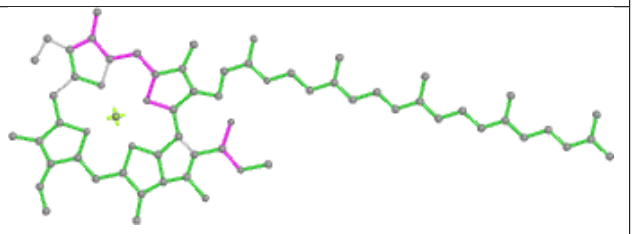


Rings

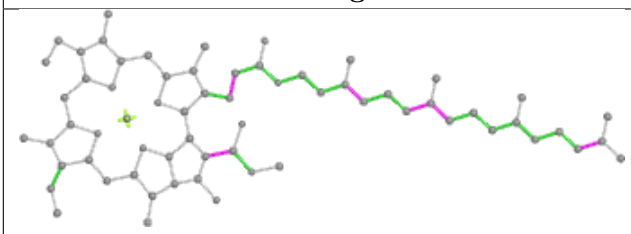
Ligand CLA C 309



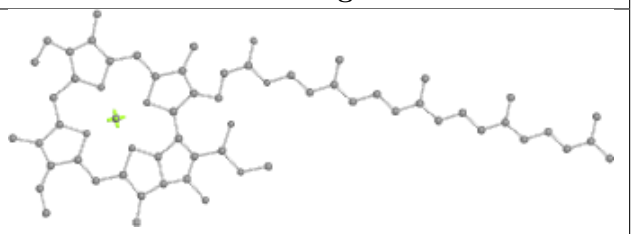
Bond lengths



Bond angles

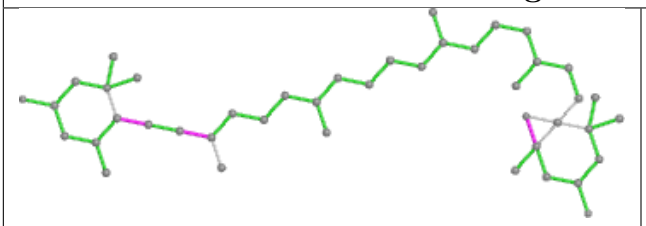


Torsions

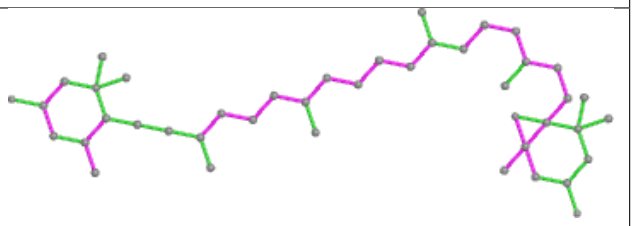


Rings

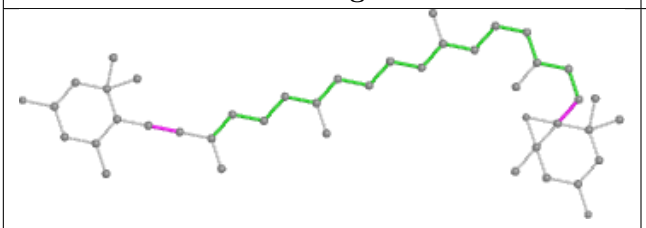
Ligand DD6 A 204



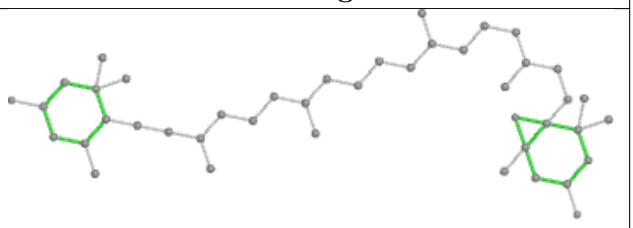
Bond lengths



Bond angles

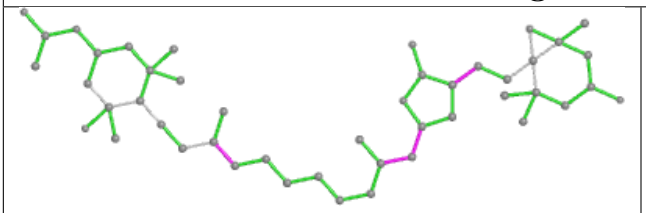


Torsions

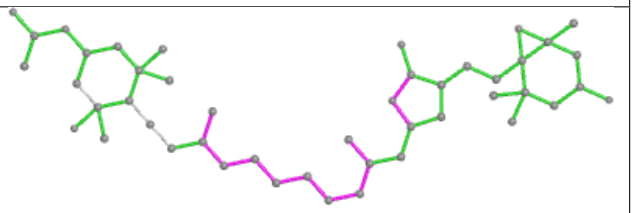


Rings

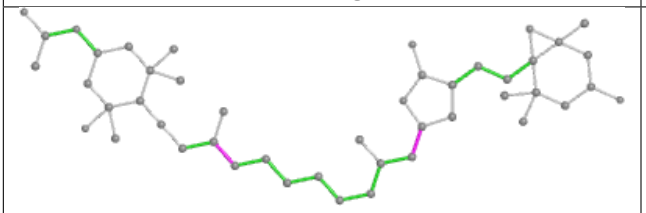
Ligand PID C 304



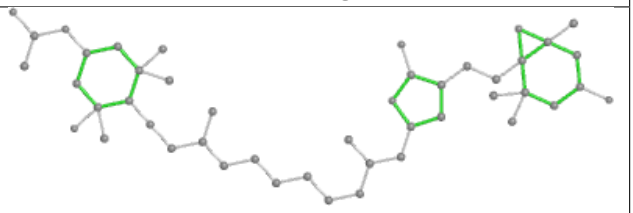
Bond lengths



Bond angles

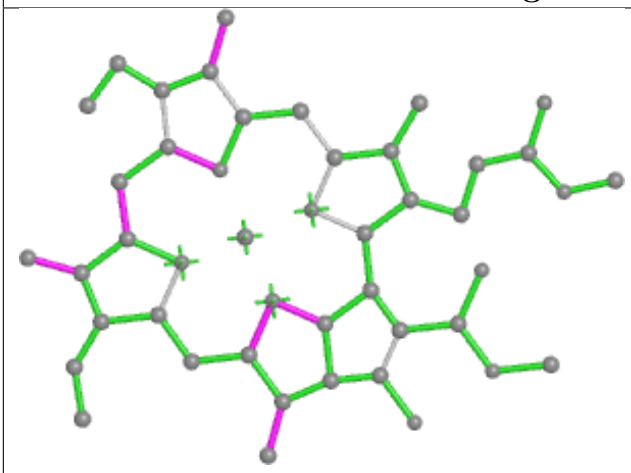


Torsions



Rings

Ligand CLA K 208



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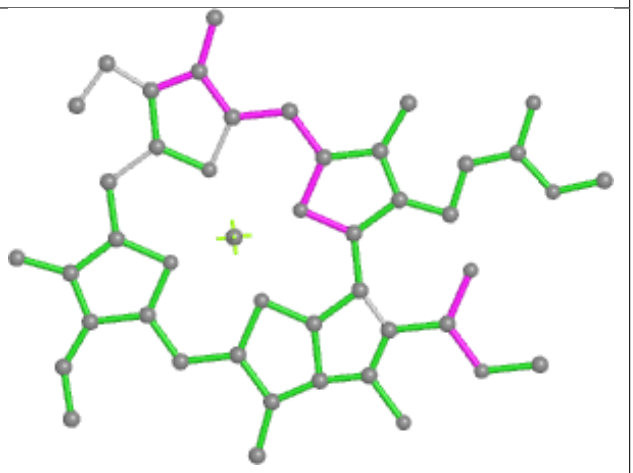
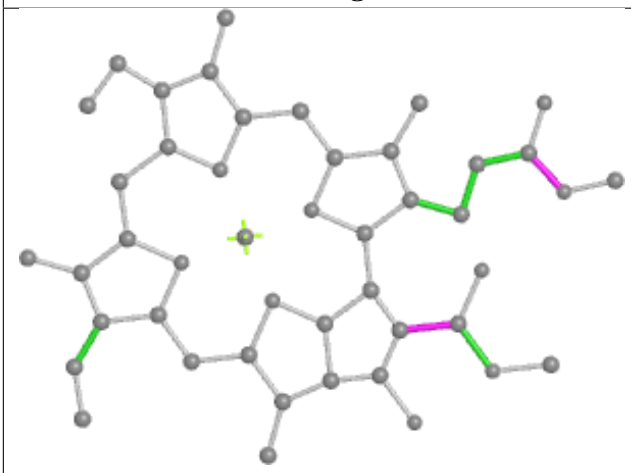
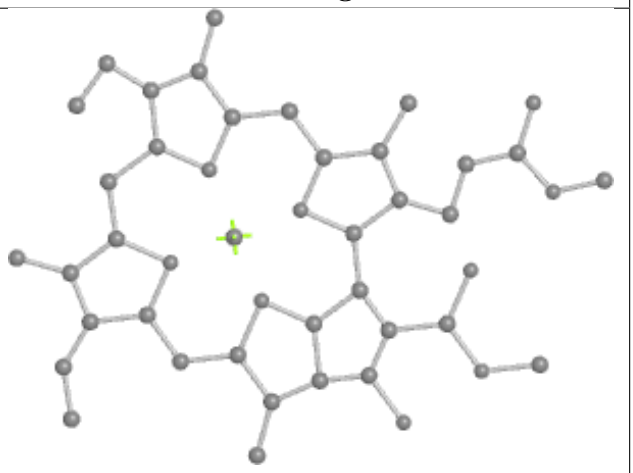


Bond angles

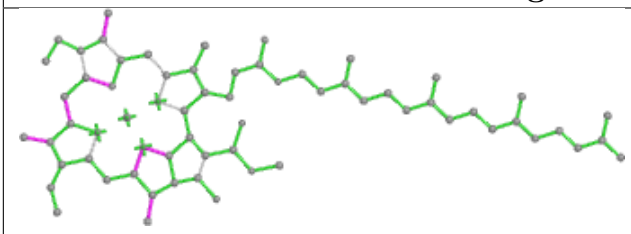


Torsions



Rings

Ligand CLA b 707



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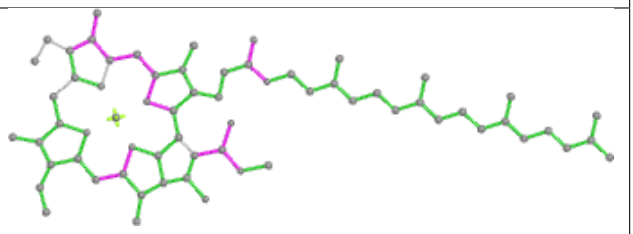
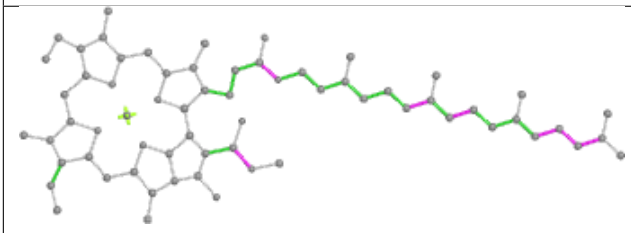
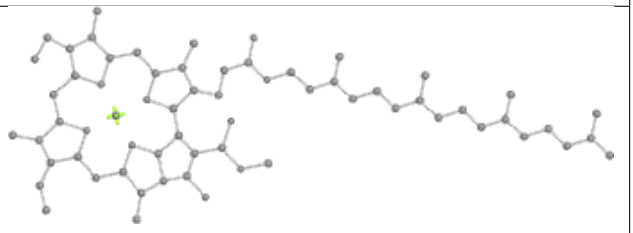


Bond angles

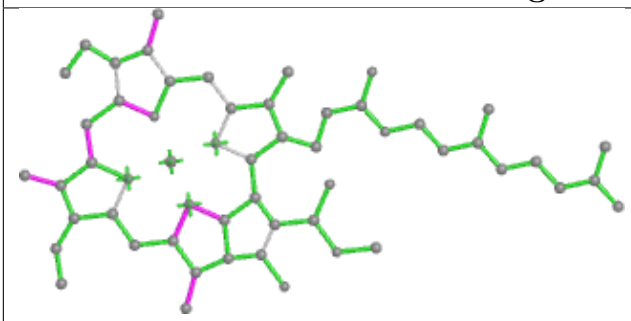


Torsions



Rings

Ligand CLA a 805



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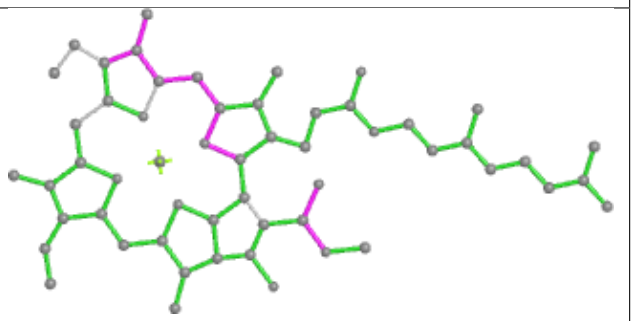
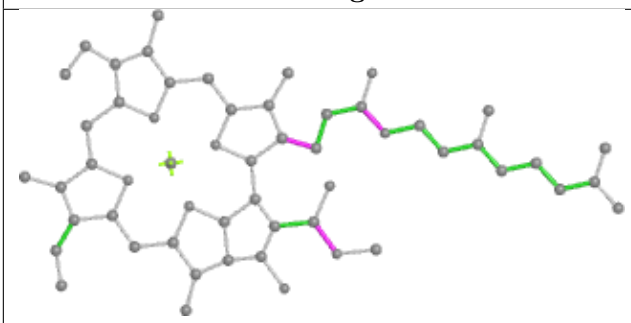


Bond angles



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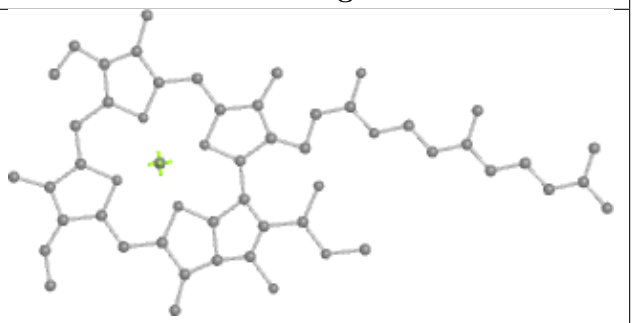
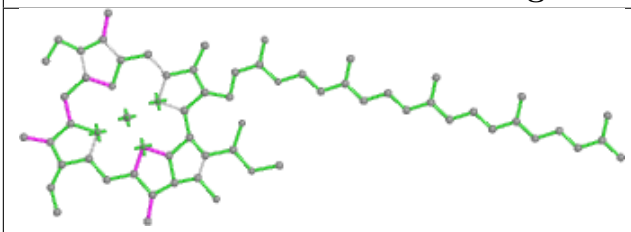


Rings

Ligand CLA b 703



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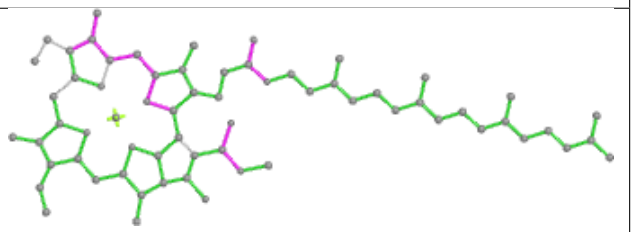
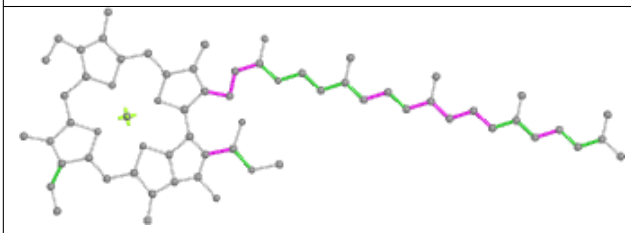


Bond angles



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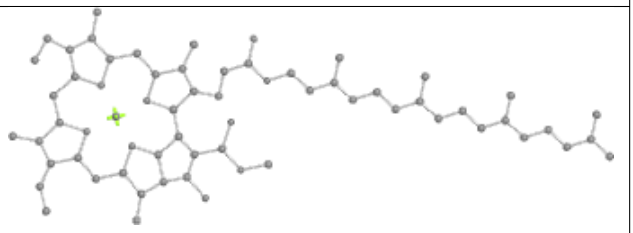
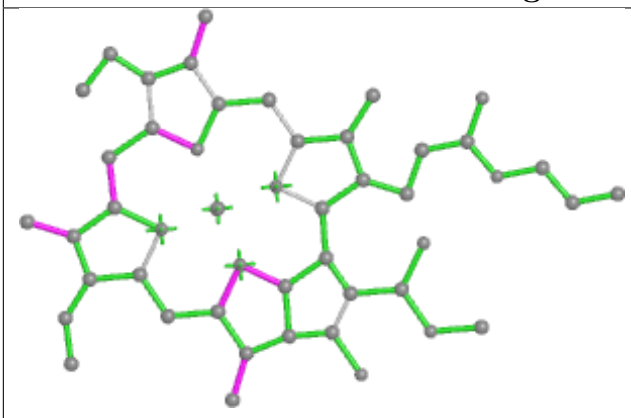


Rings

Ligand CLA K 213



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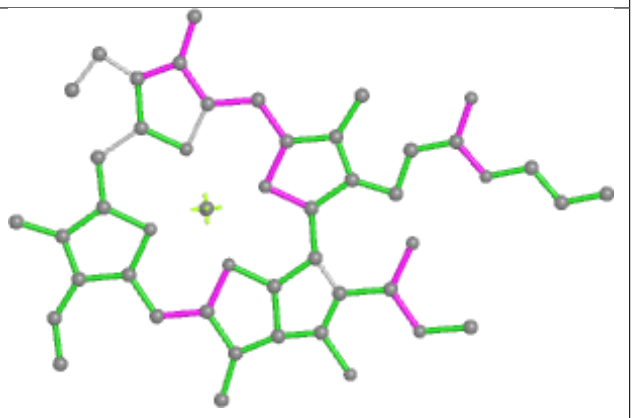
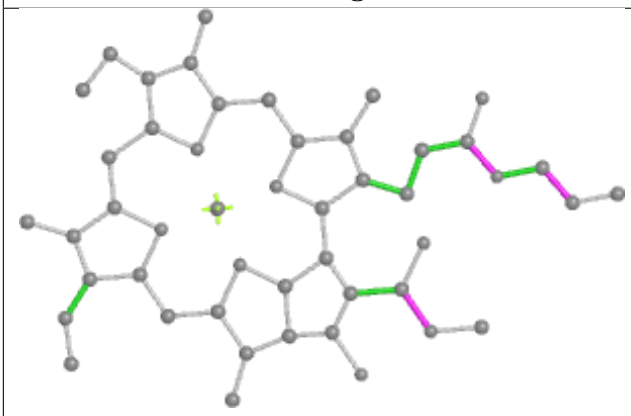


Bond angles



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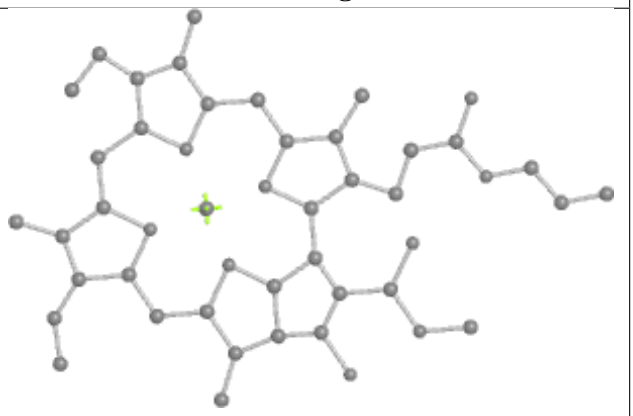
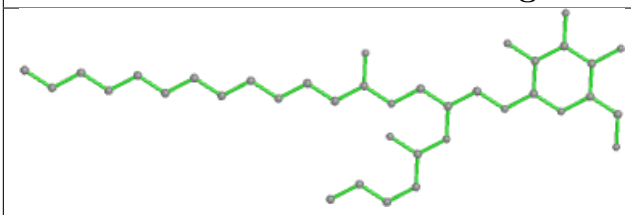


Rings

Ligand LMG A 219



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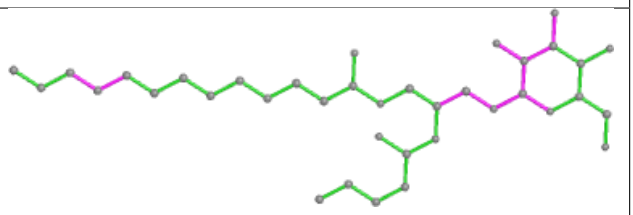
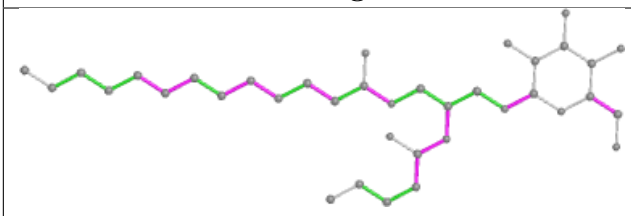


Bond angles



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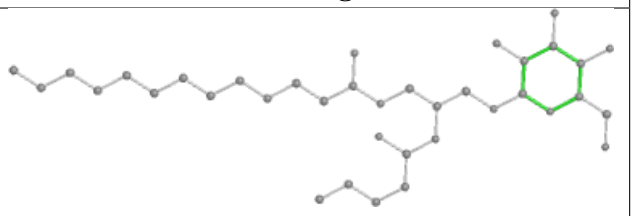
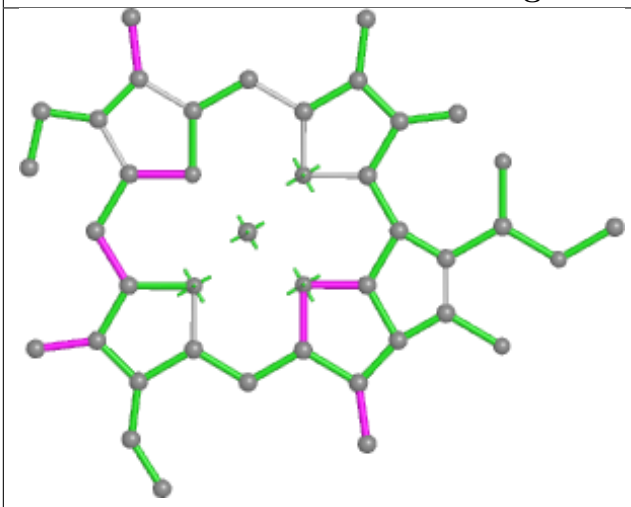
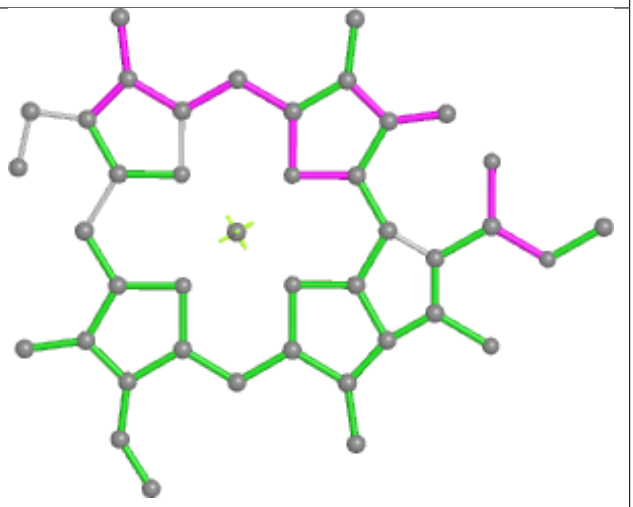


Rings

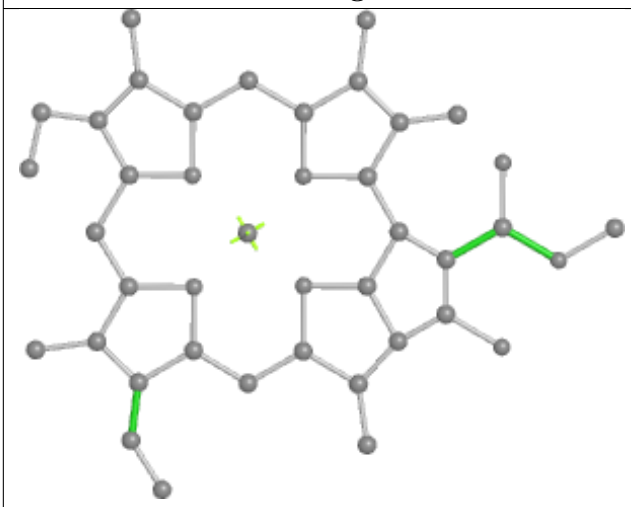
Ligand CLA A 216



Bond lengths



Bond angles



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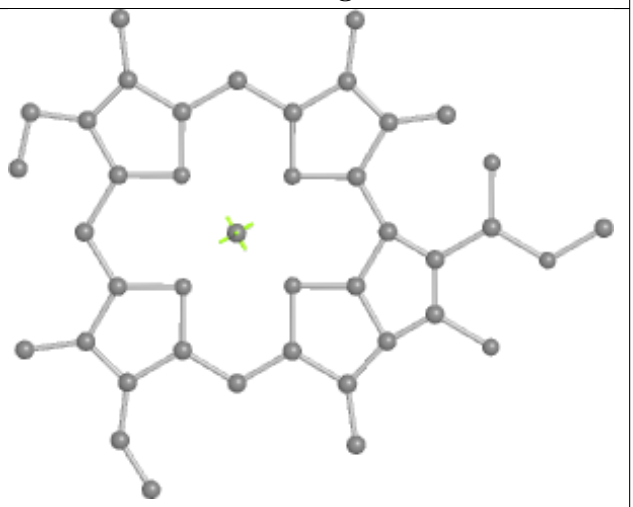
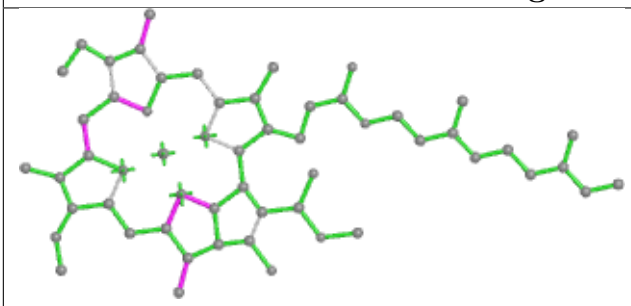


Rings

Ligand CLA a 830



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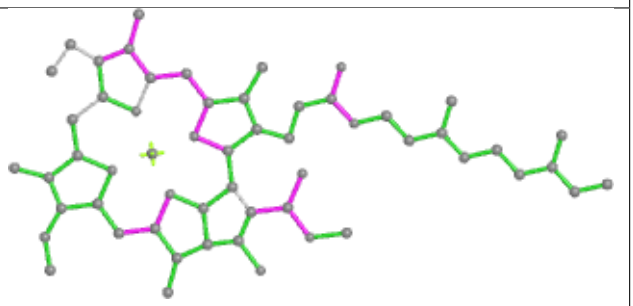
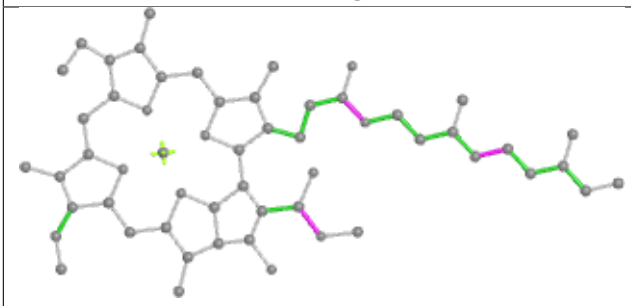


Bond angles



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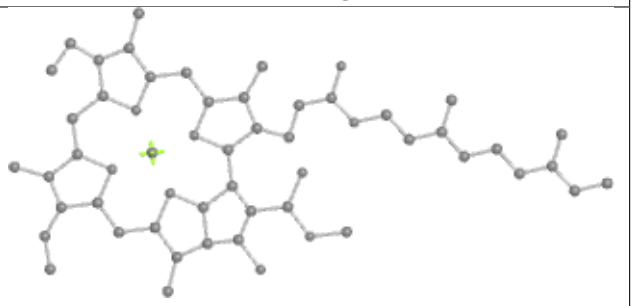
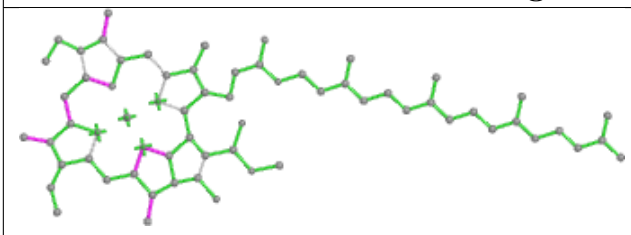


Rings

Ligand CLA b 718



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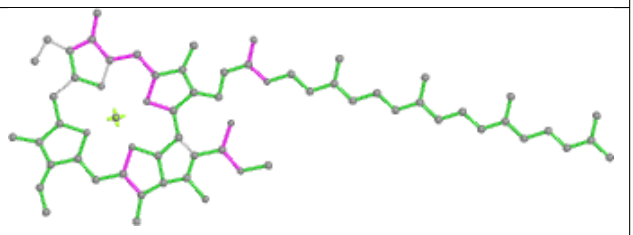
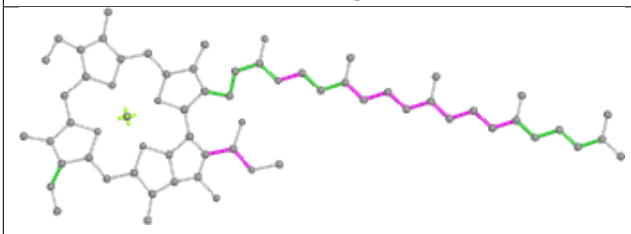
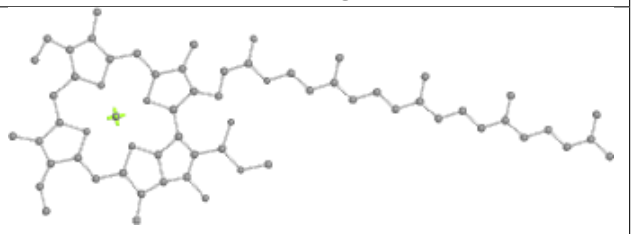


Bond angles

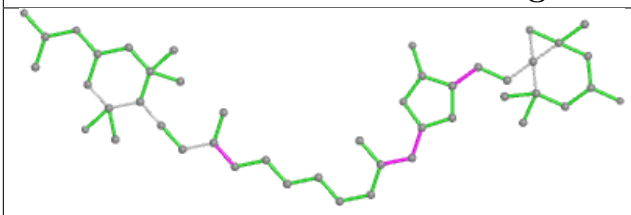


Torsions



Rings

Ligand PID Q 303



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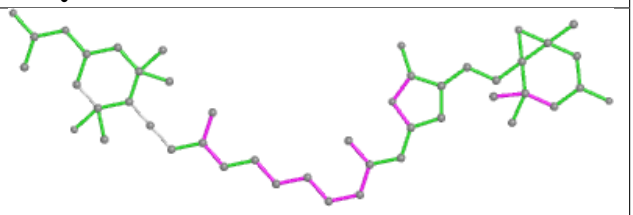
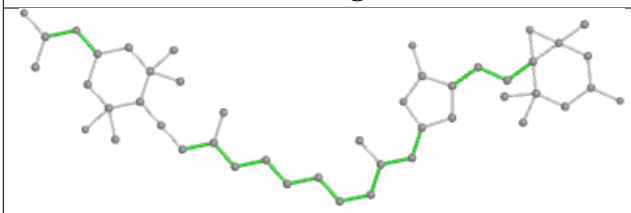
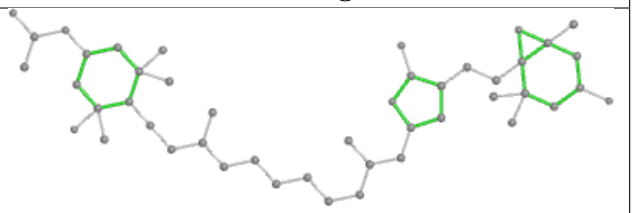


Bond angles

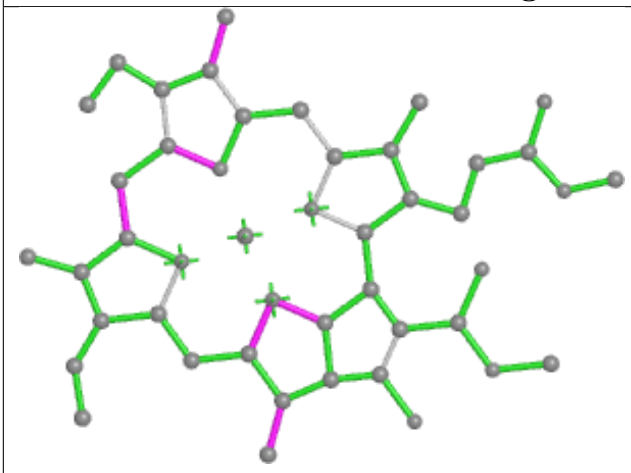


Torsions



Rings

Ligand CLA M 315



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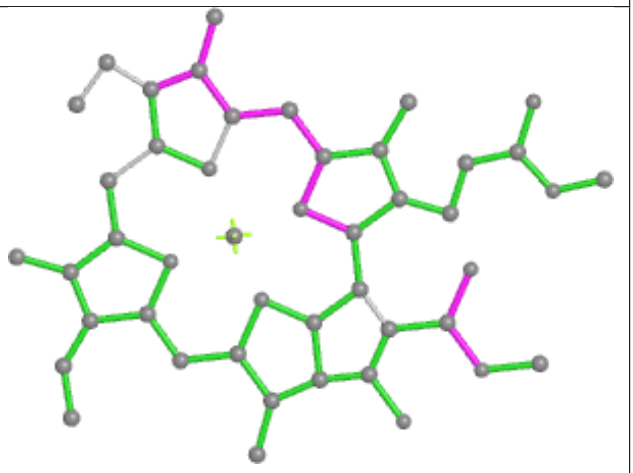
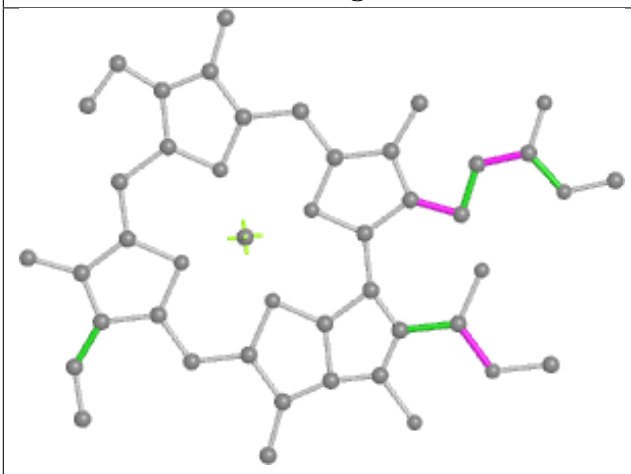


Bond angles



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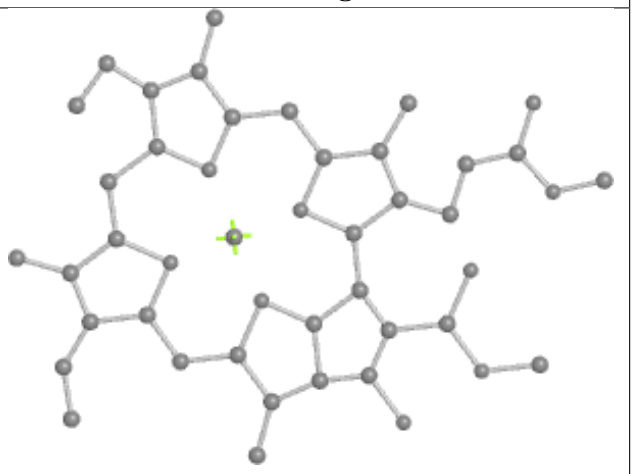
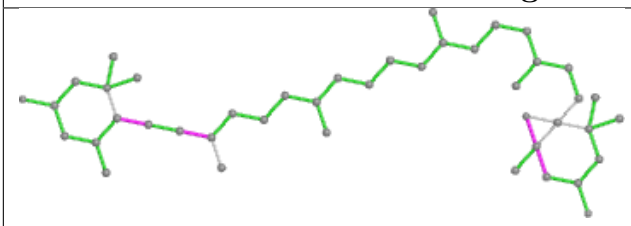
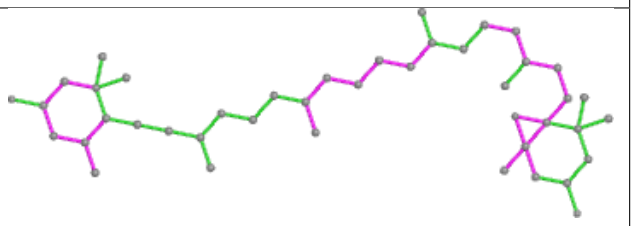


Rings

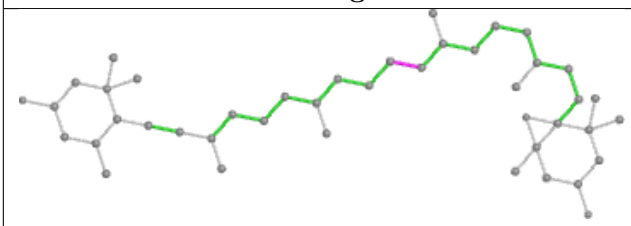
Ligand DD6 M 302



Bond lengths



Bond angles



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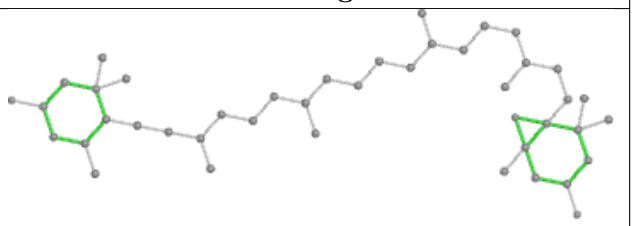
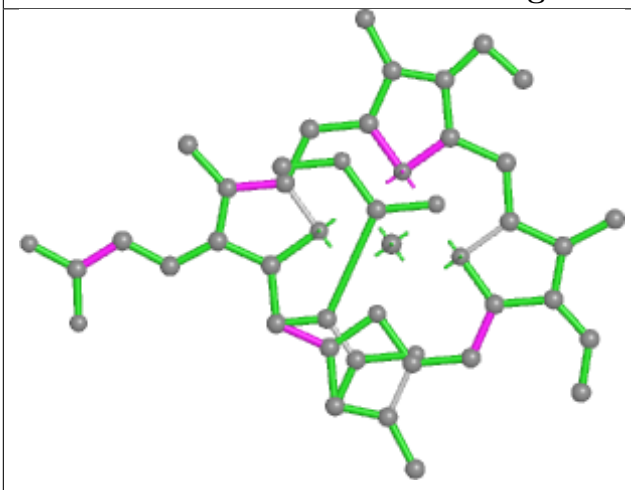


Rings

Ligand KC1 F 309



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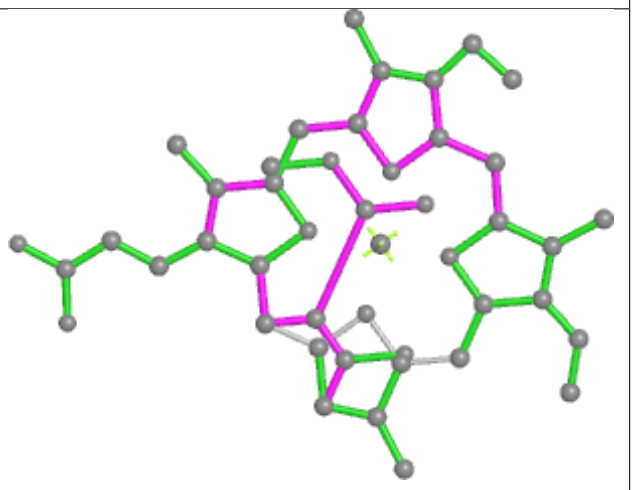
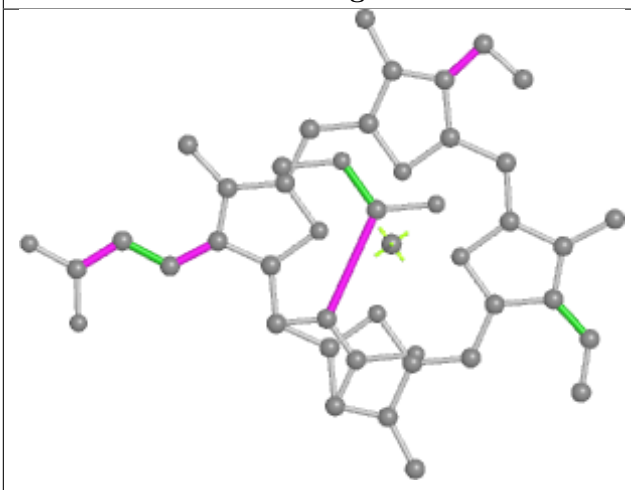
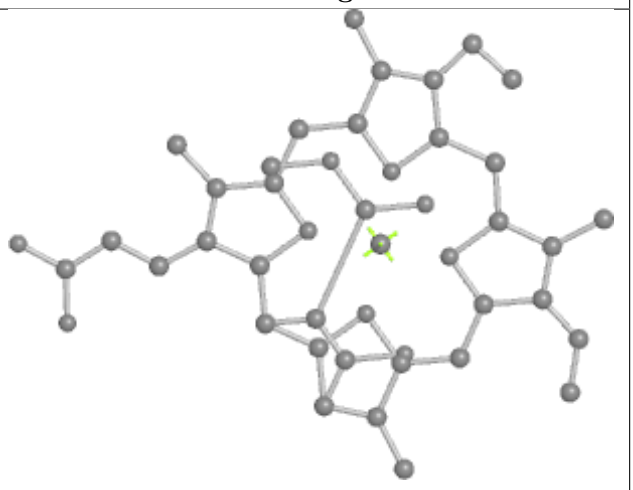


Bond angles

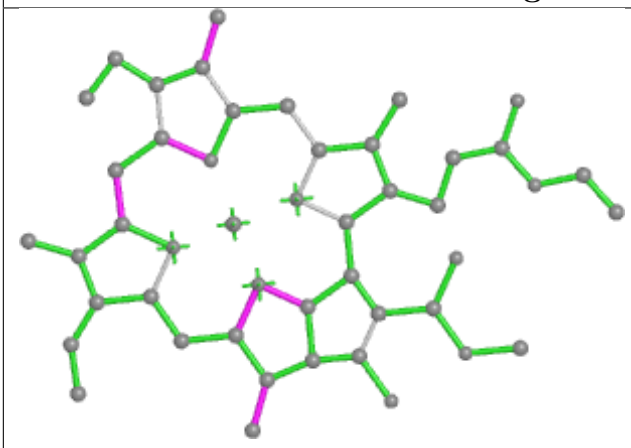


Torsions

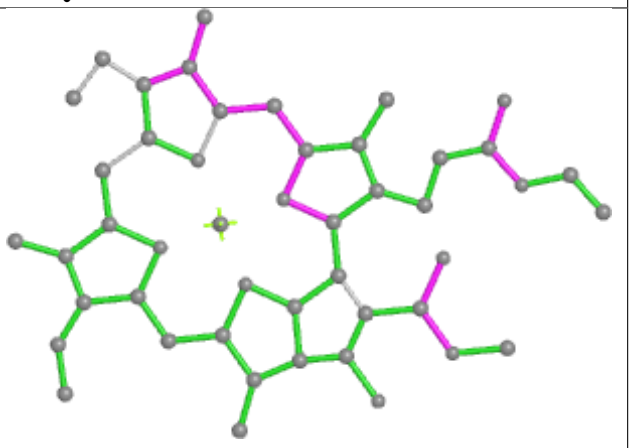


Rings

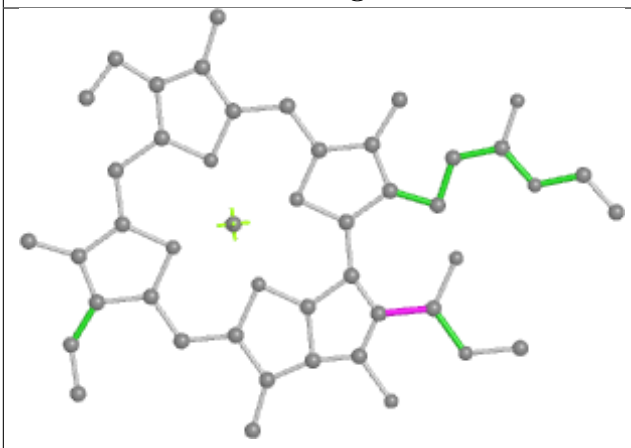
Ligand CLA Q 307



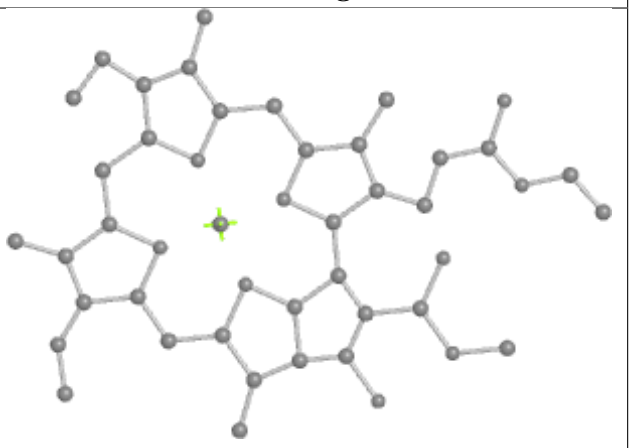
Bond lengths



Bond angles

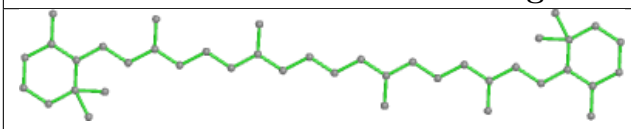


Torsions



Rings

Ligand BCR a 838



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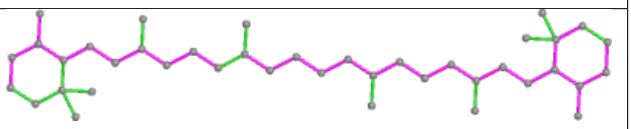

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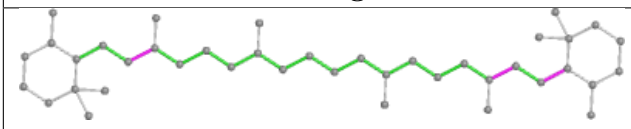

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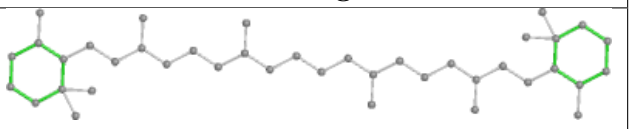
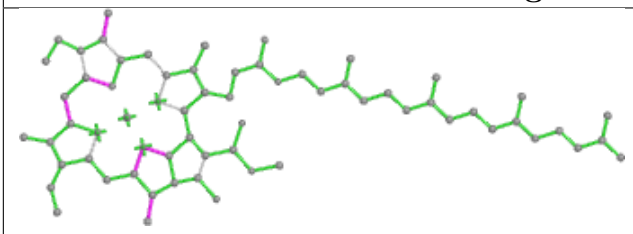


Rings

Ligand CLA P 210



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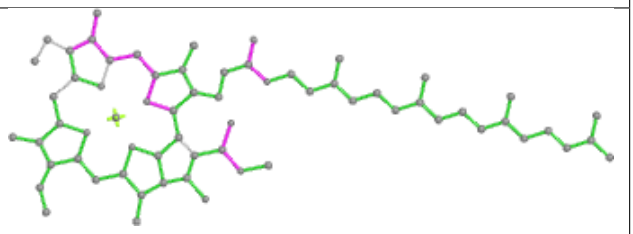
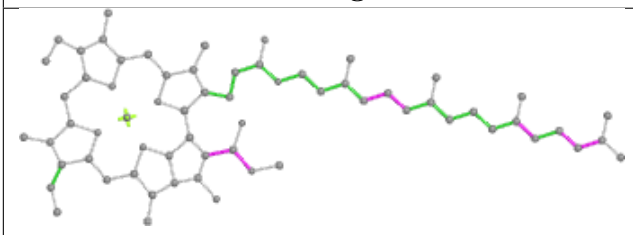


Bond angles



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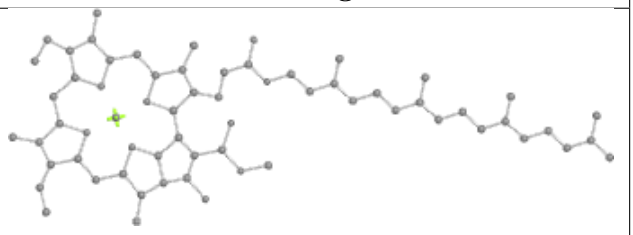
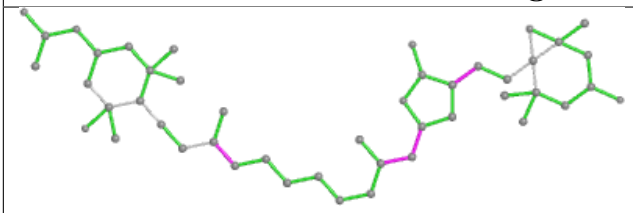


Rings

Ligand PID G 309



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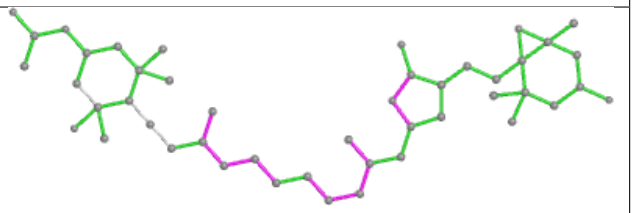
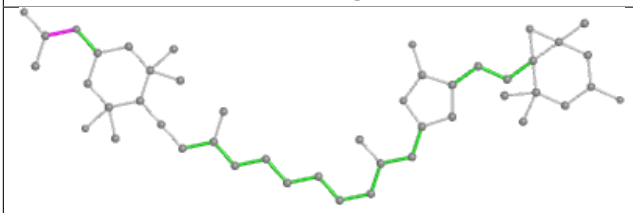


Bond angles



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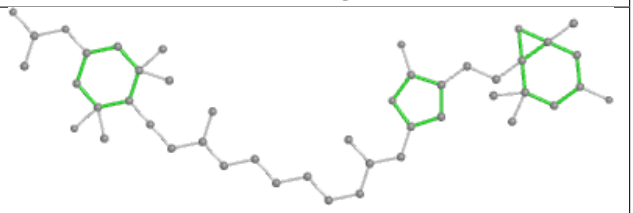
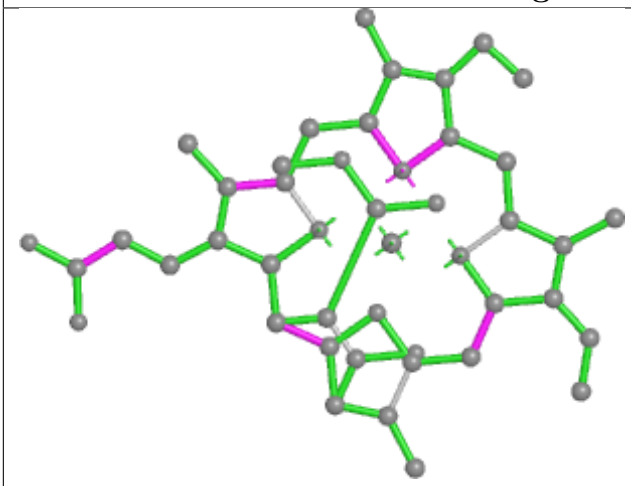


Rings

Ligand KC1 I 215



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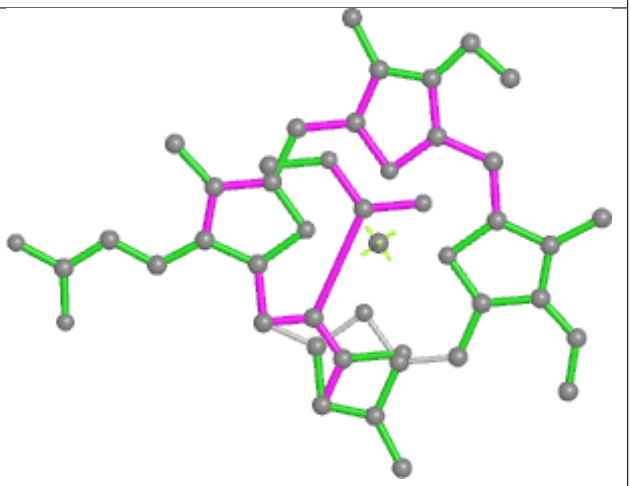

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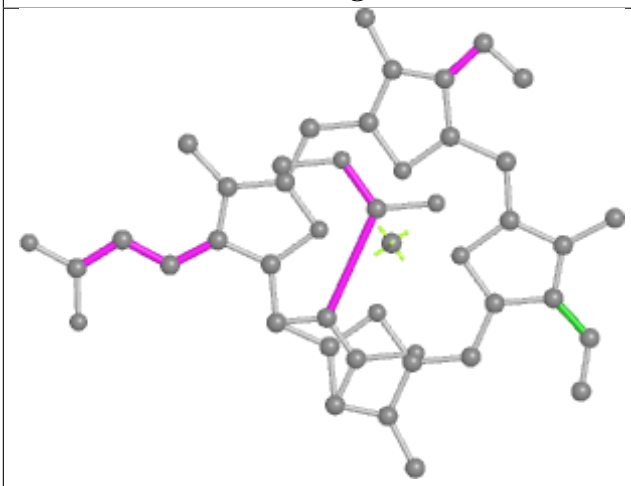

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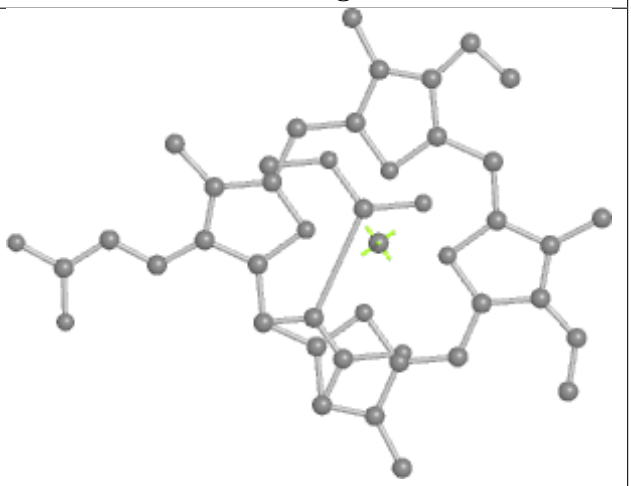
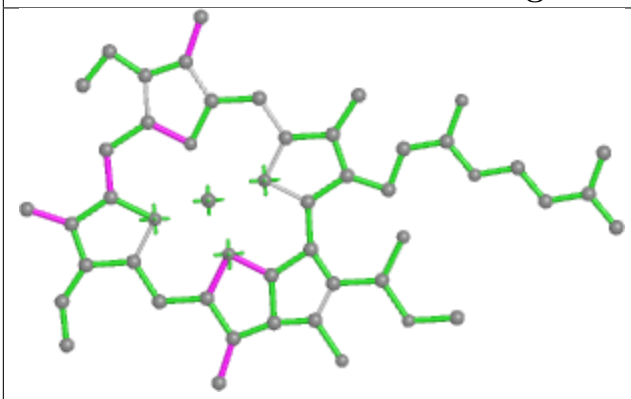


Rings

Ligand CLA L 307



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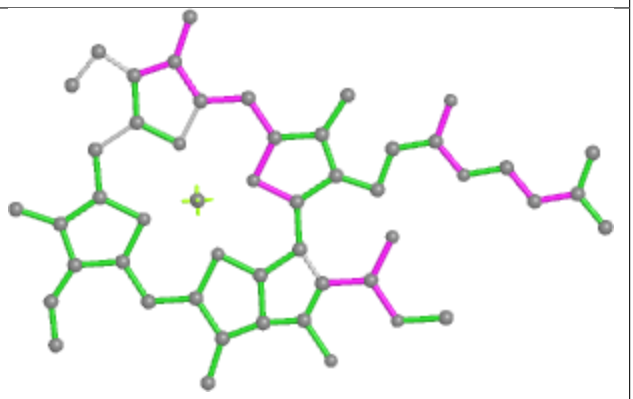
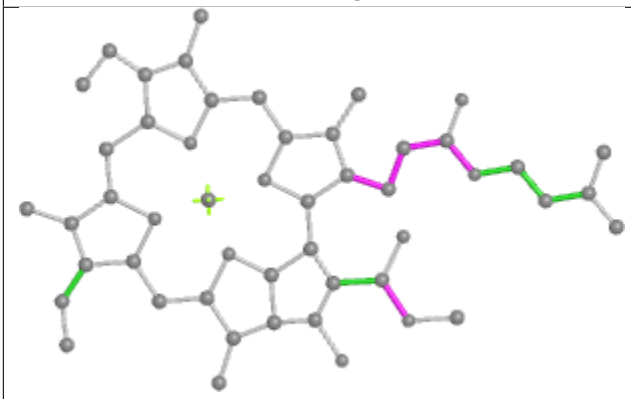


Bond angles



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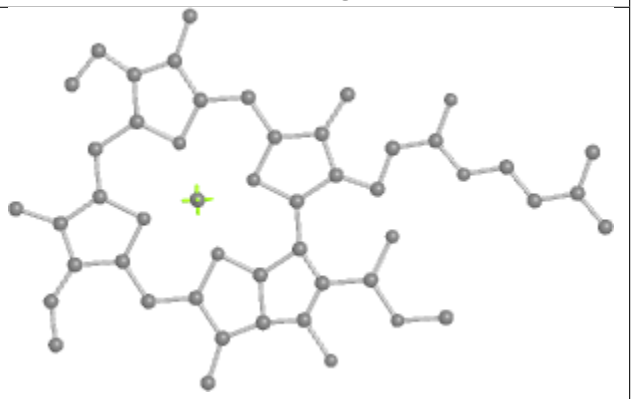
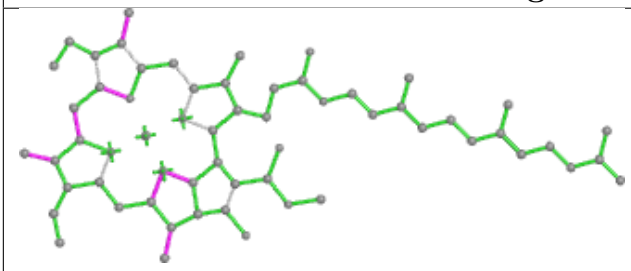


Rings

Ligand CLA b 709



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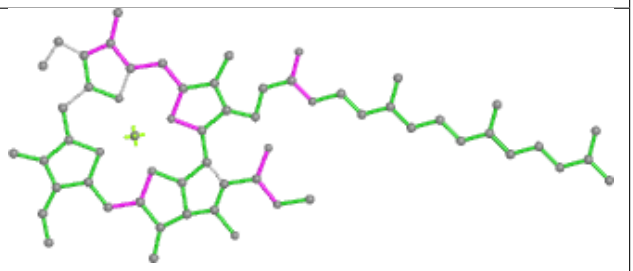
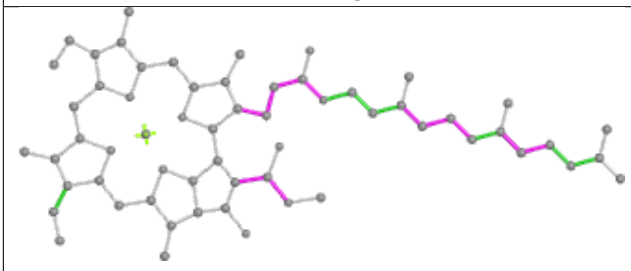


Bond angles



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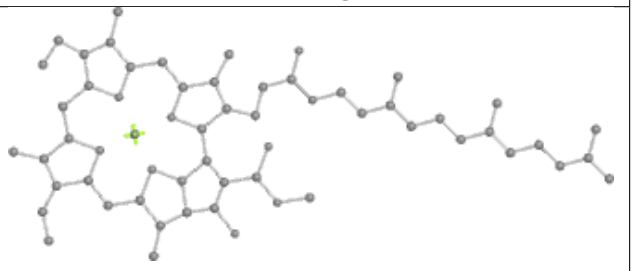
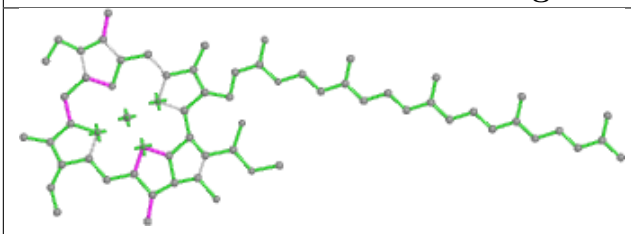


Rings

Ligand CLA l 505



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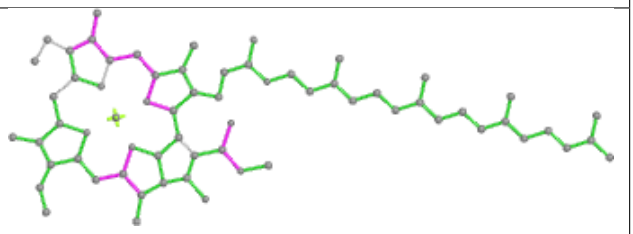
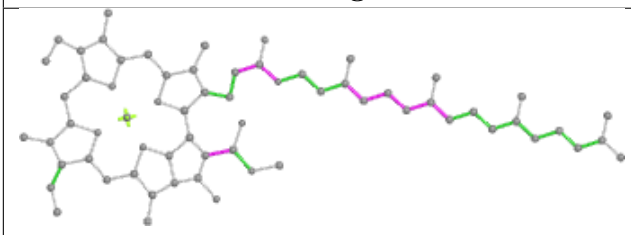


Bond angles



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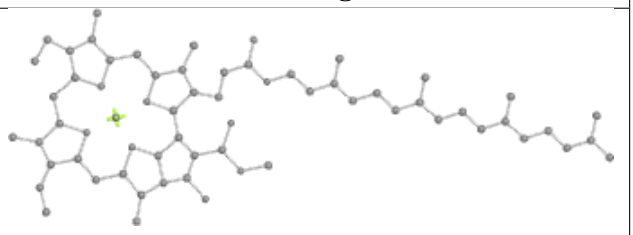
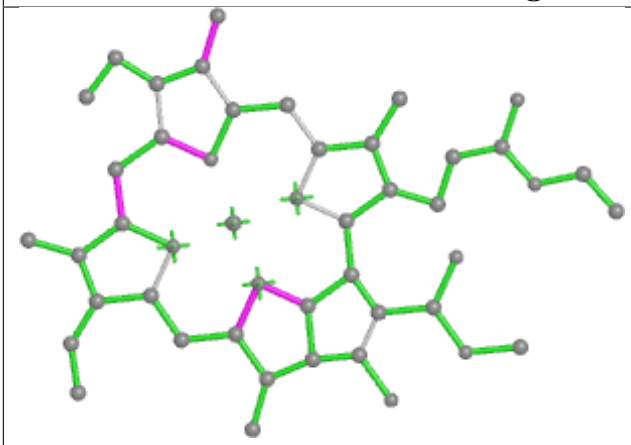
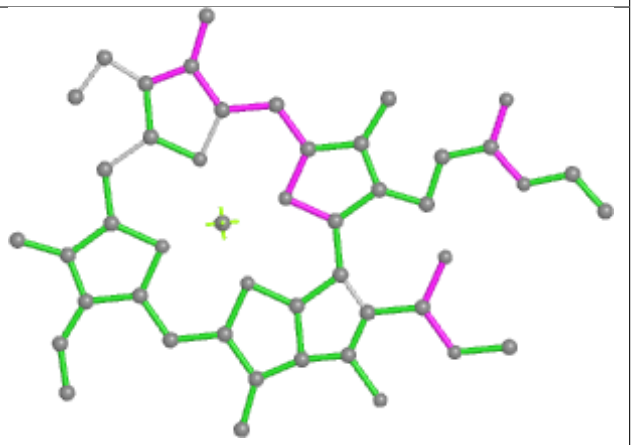


Rings

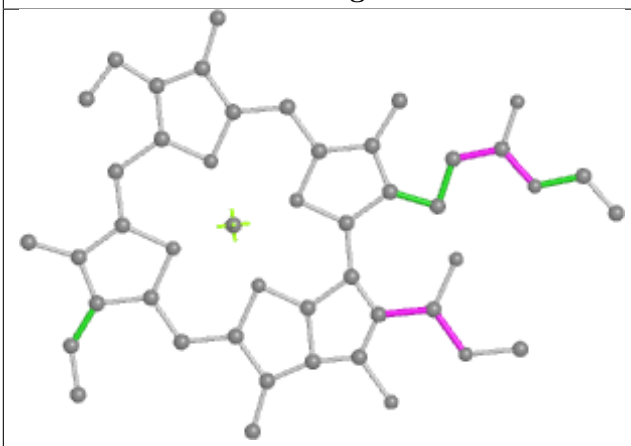
Ligand CLA P 209



Bond lengths



Bond angles



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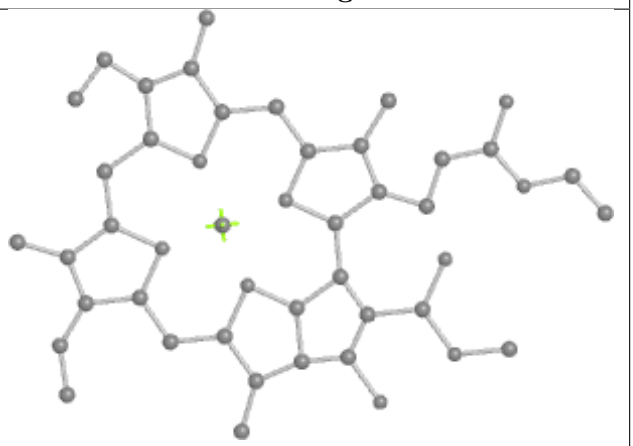
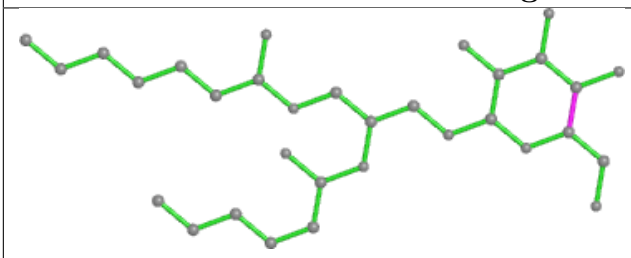


Rings

Ligand LMG E 316



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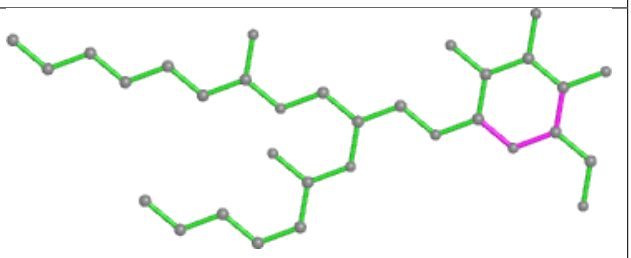
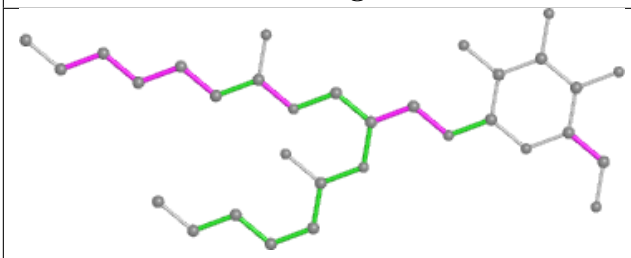


Bond angles



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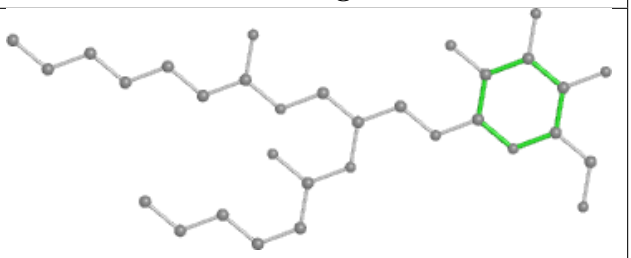
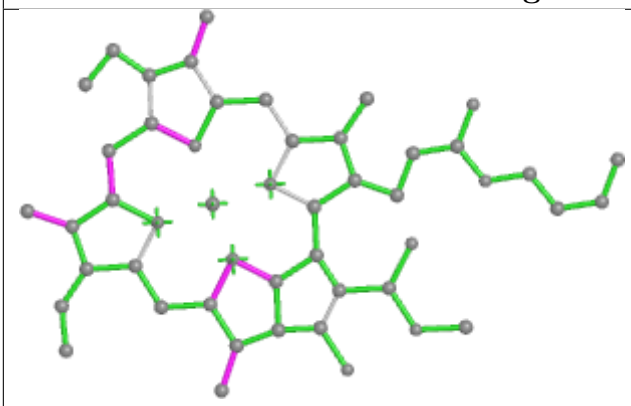


Rings

Ligand CLA G 301



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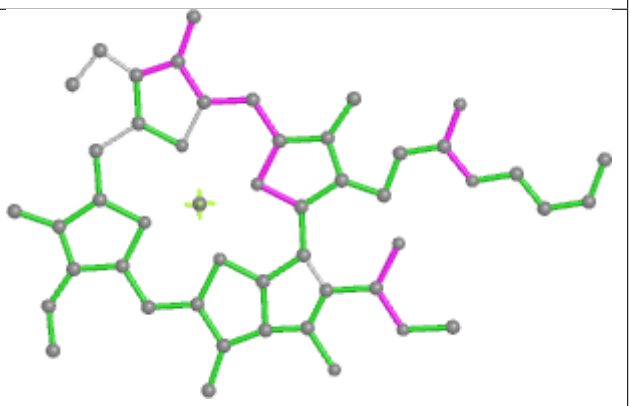

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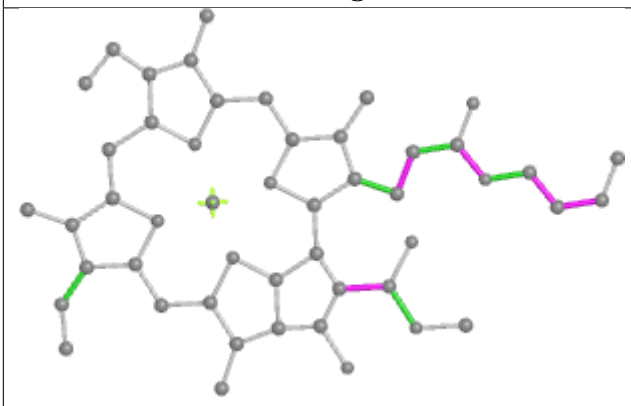

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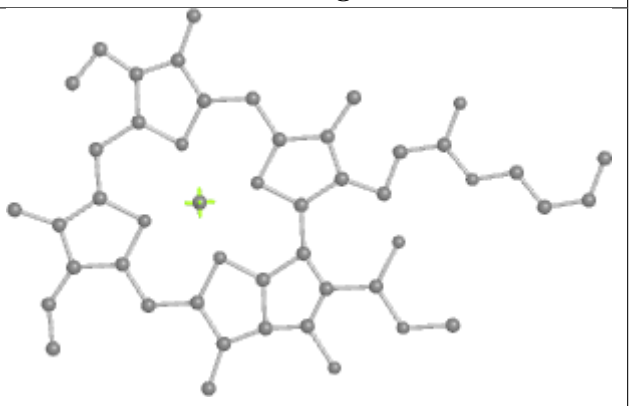
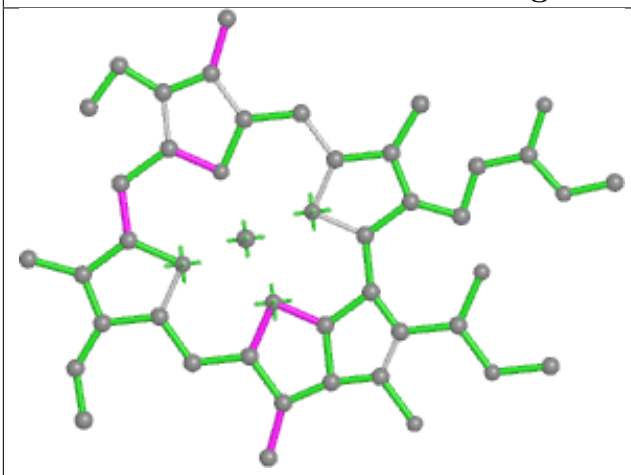


Rings

Ligand CLA I 208



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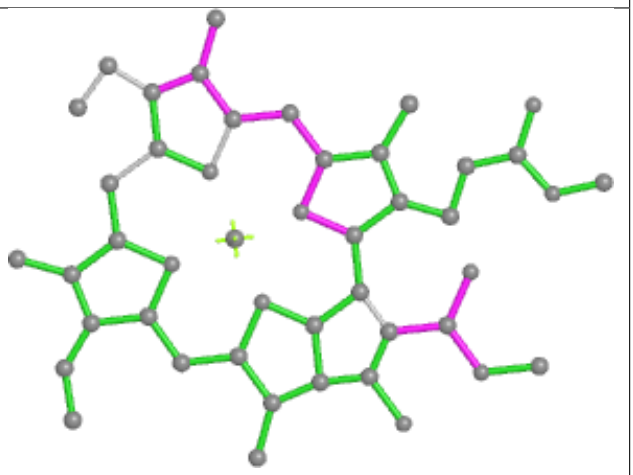
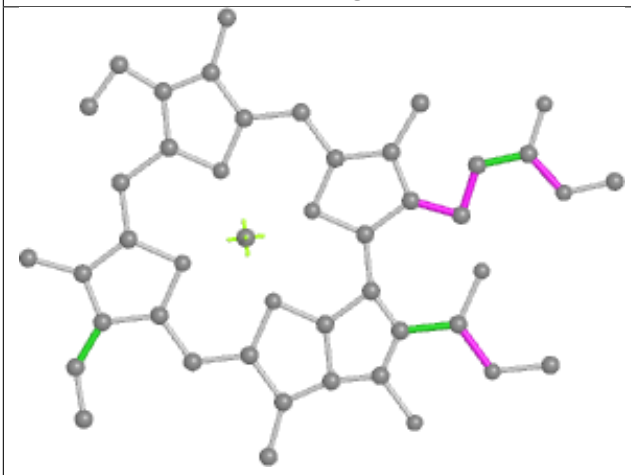


Bond angles



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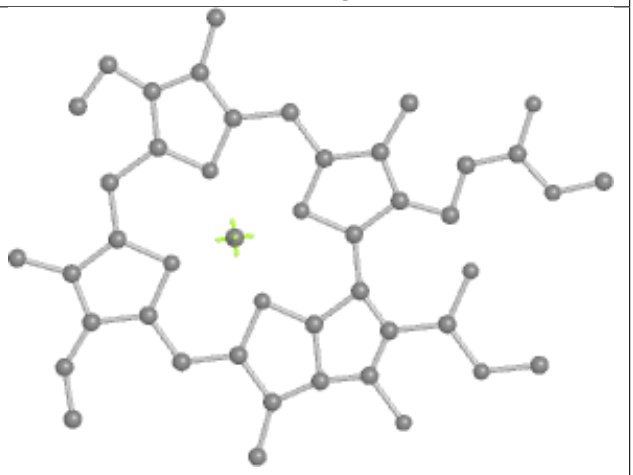
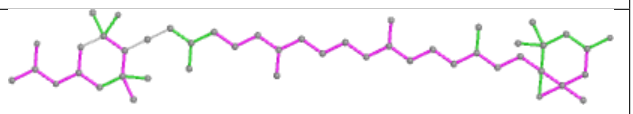


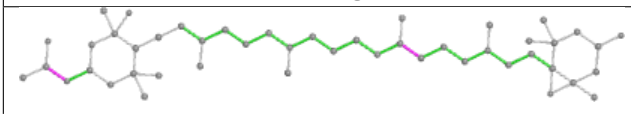
Rings

Ligand UIX A 203

Bond lengths



Bond angles



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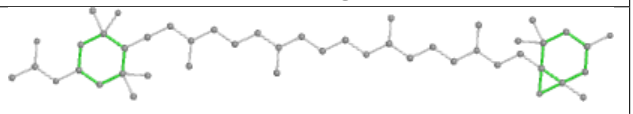
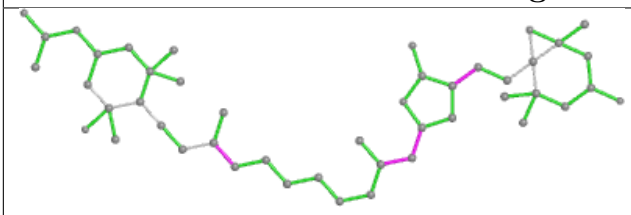
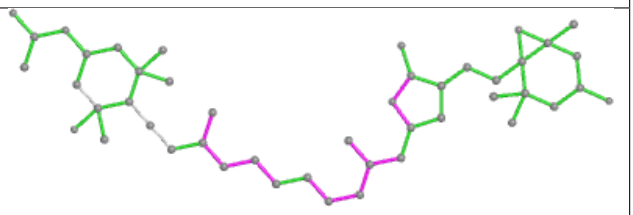


Rings

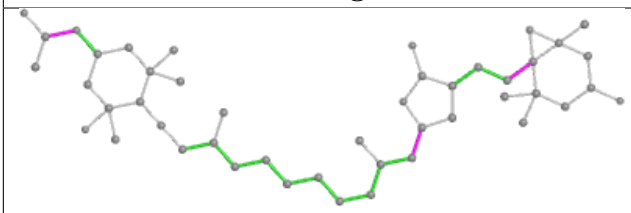
Ligand PID C 301



Bond lengths



Bond angles



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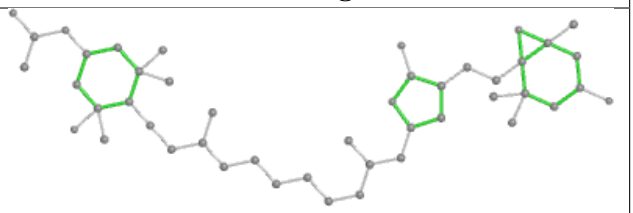
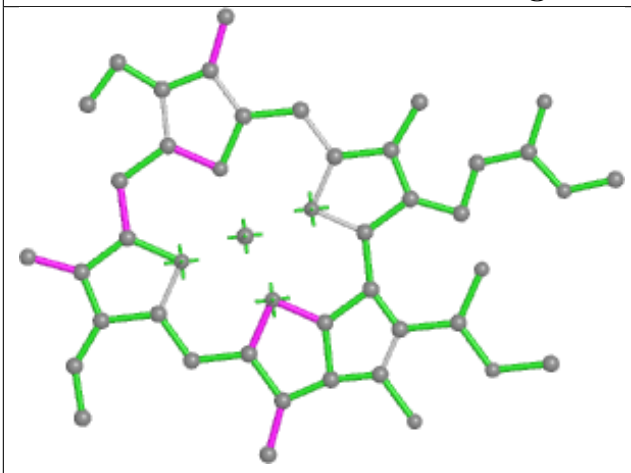
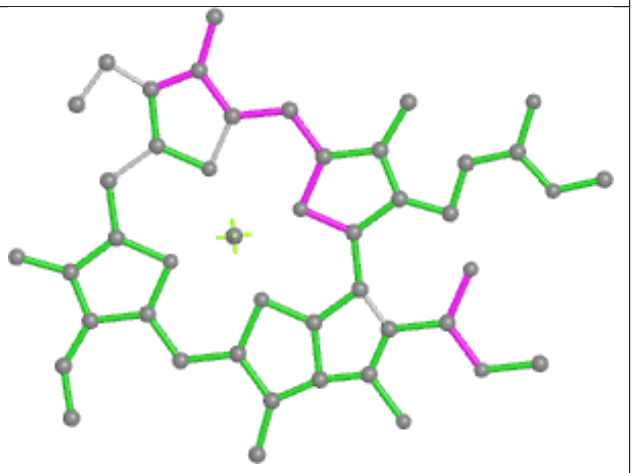


Rings

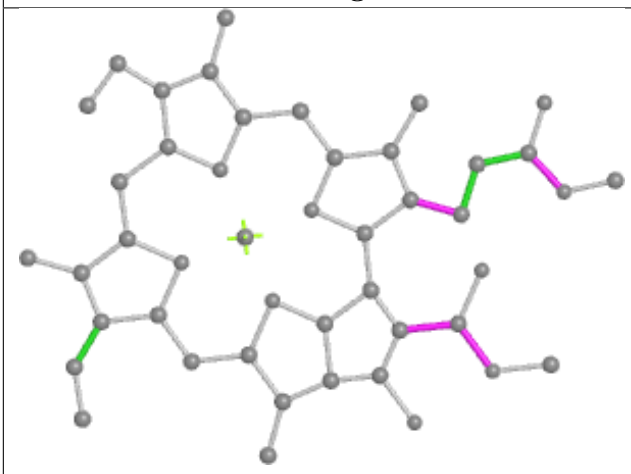
Ligand CLA a 828



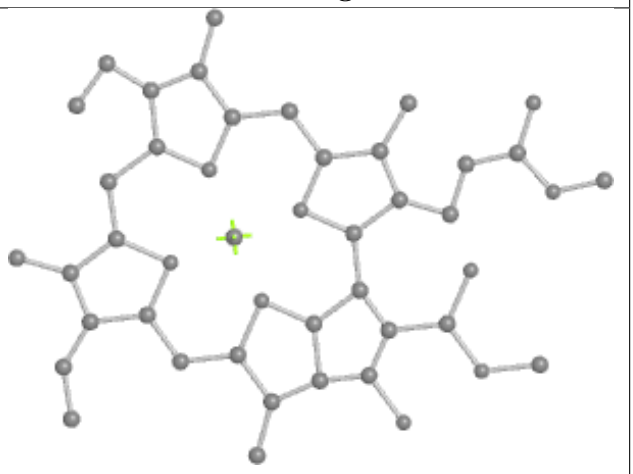
Bond lengths



Bond angles

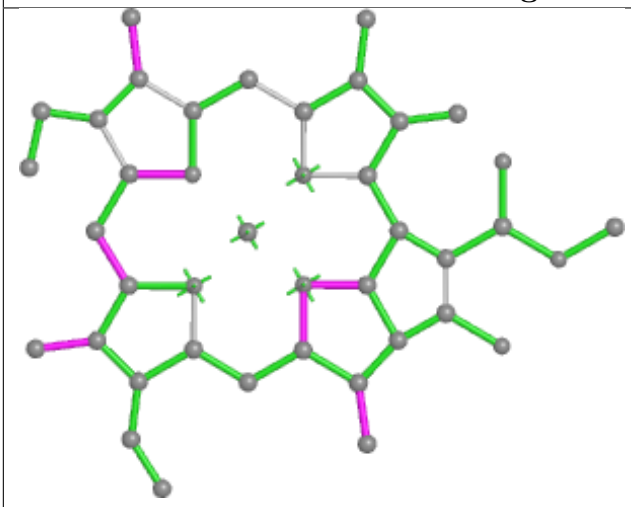


Torsions

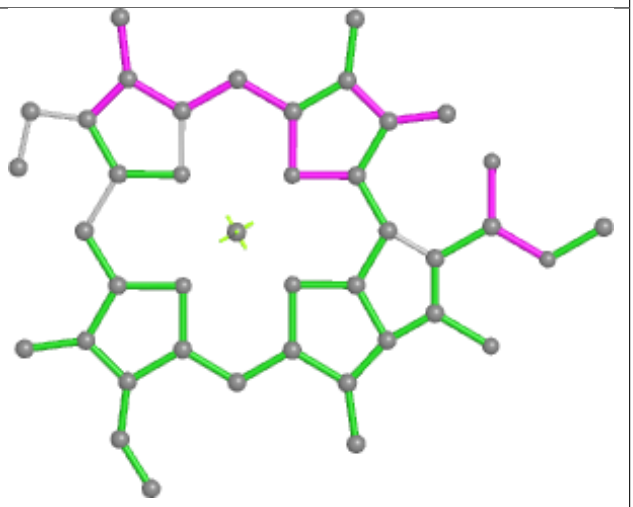


Rings

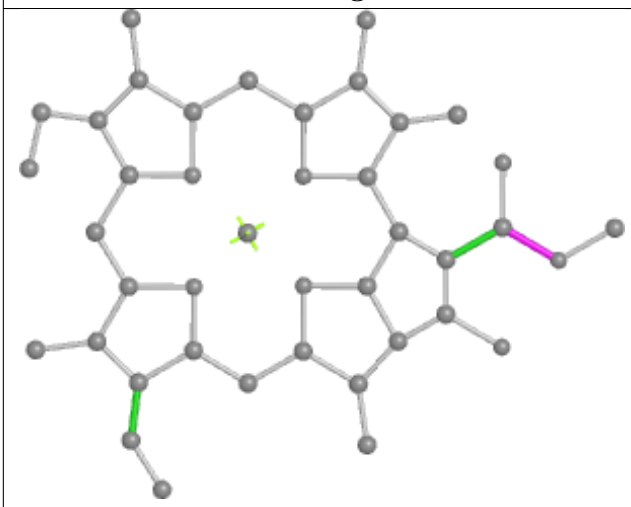
Ligand CLA M 313



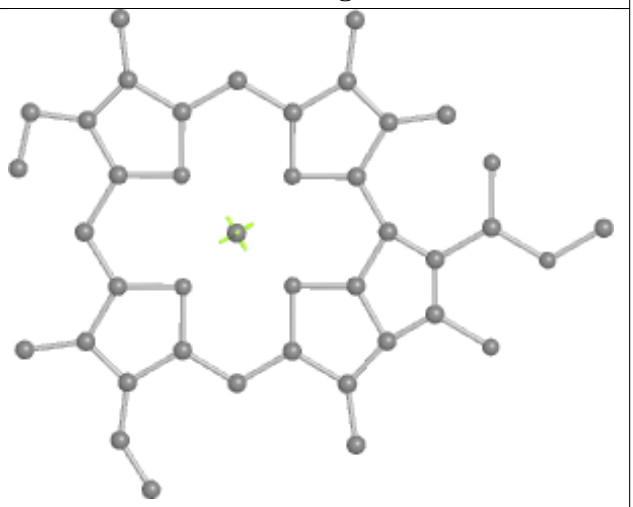
Bond lengths



Bond angles

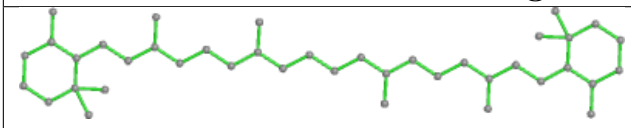


Torsions



Rings

Ligand BCR a 834



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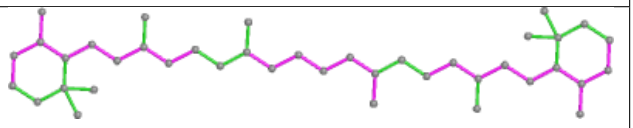
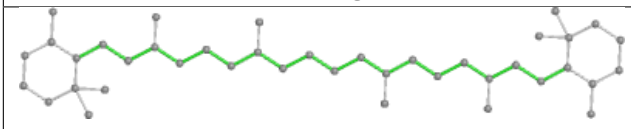


Bond angles



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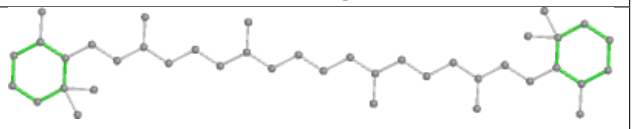
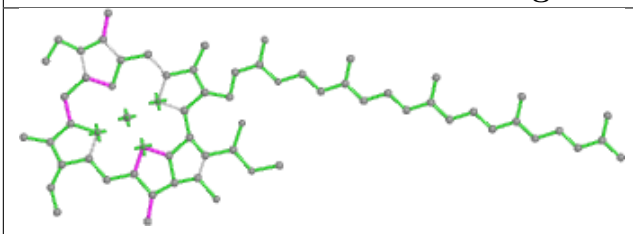


Rings

Ligand CLA i 201



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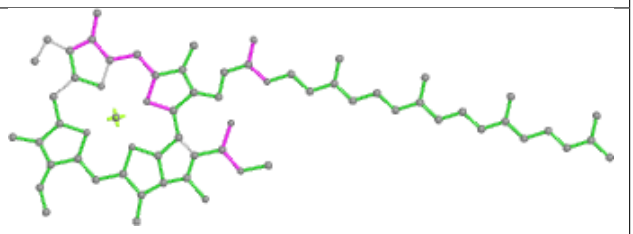
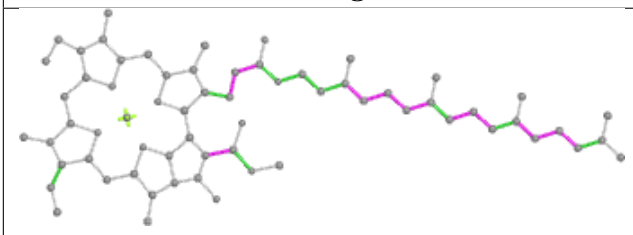


Bond angles



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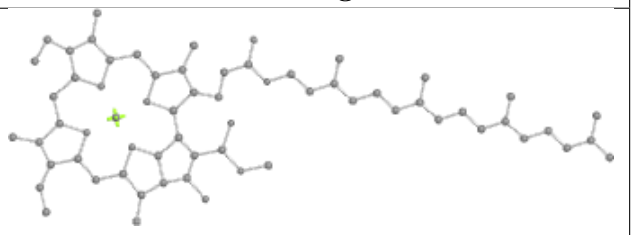
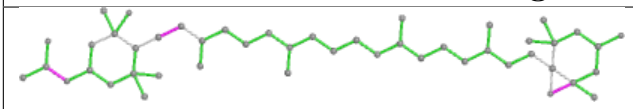


Rings

Ligand UIX F 305



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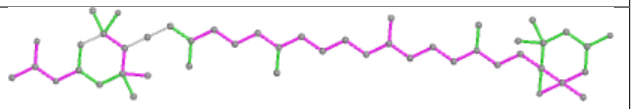
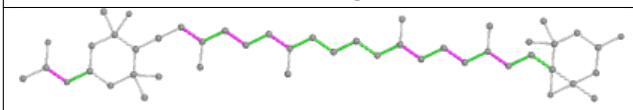


Bond angles



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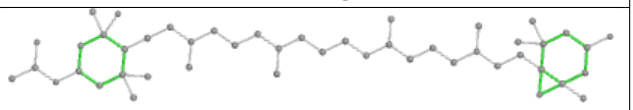
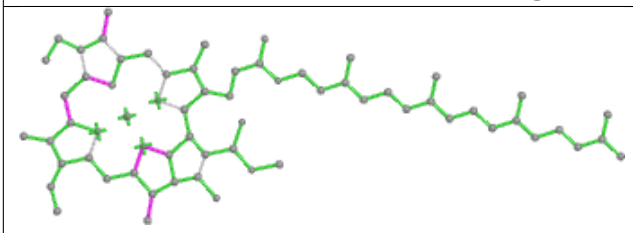


Rings

Ligand CLA a 826



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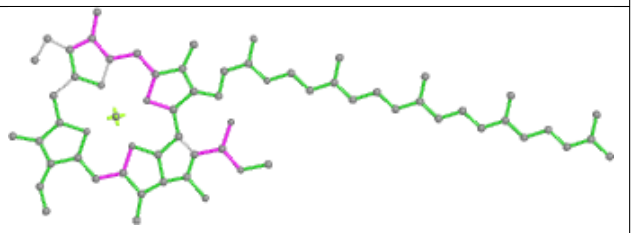
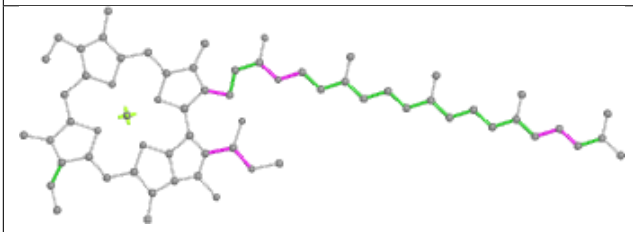


Bond angles



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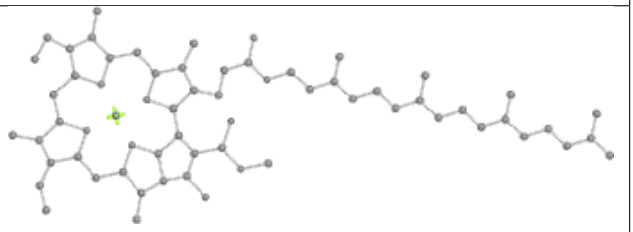
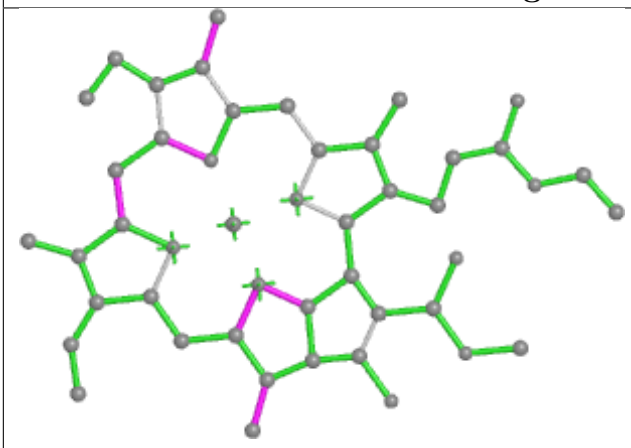


Rings

Ligand CLA N 308



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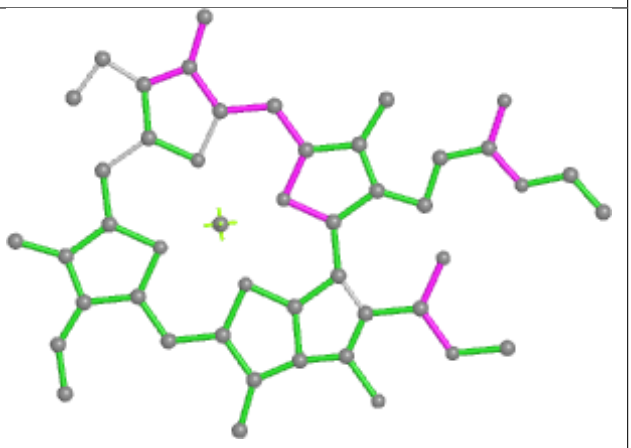
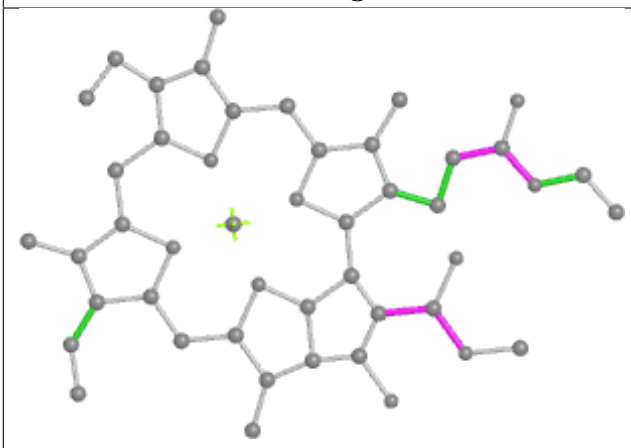


Bond angles



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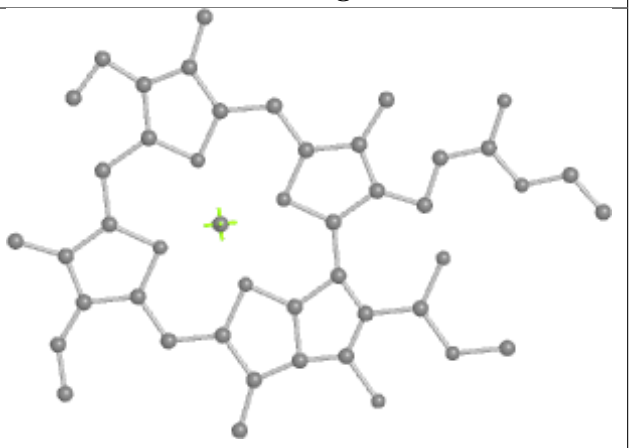
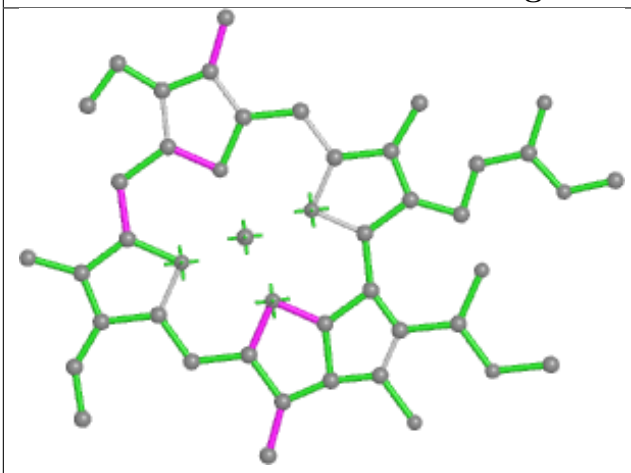


Rings

Ligand CLA T 313



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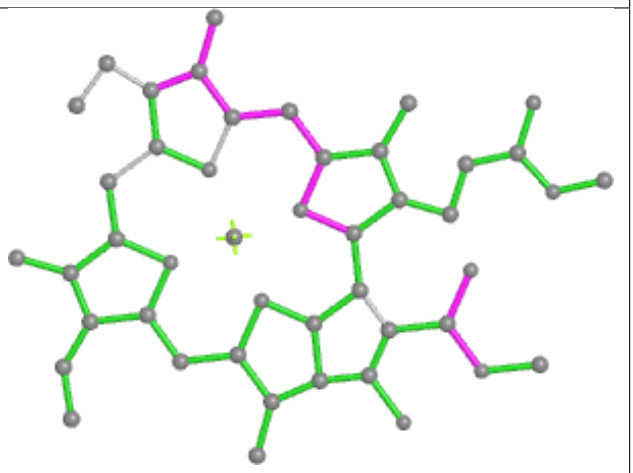
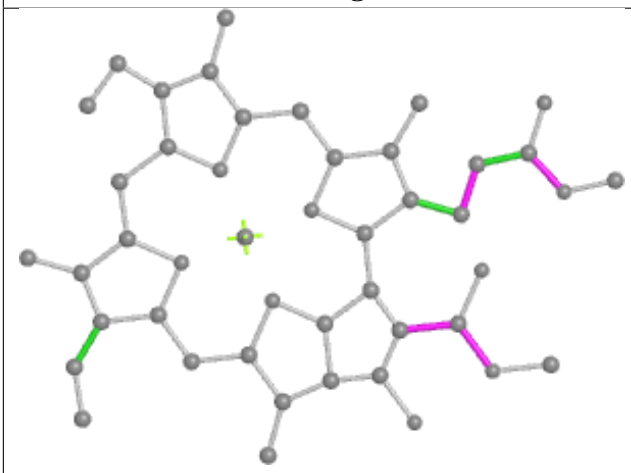


Bond angles



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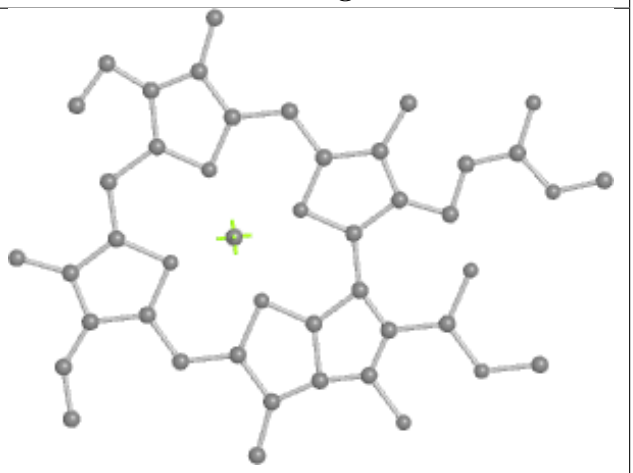
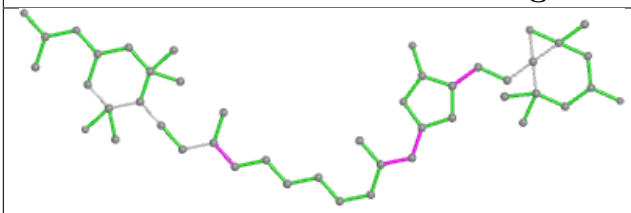


Rings

Ligand PID P 206



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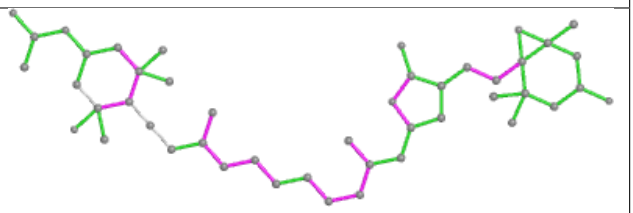
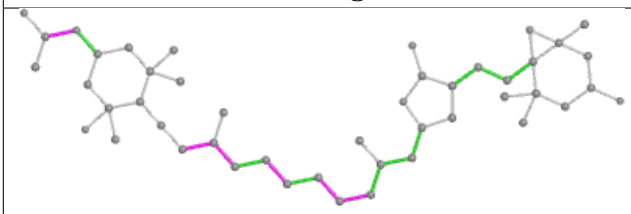


Bond angles



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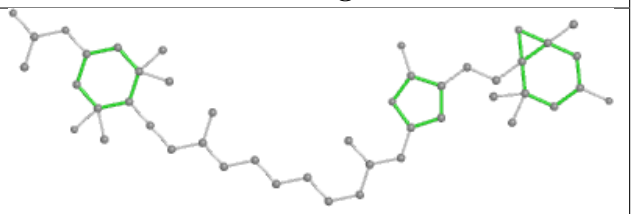
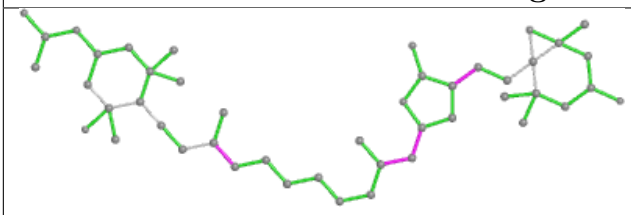


Rings

Ligand PID T 304



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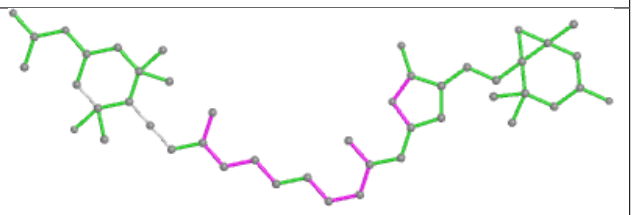
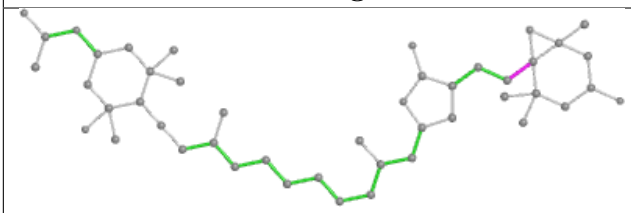


Bond angles



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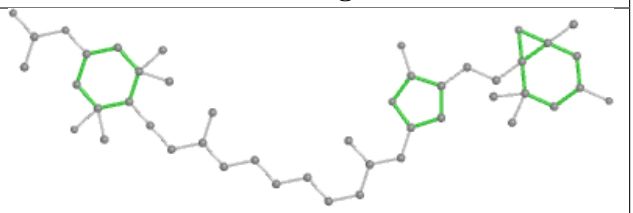
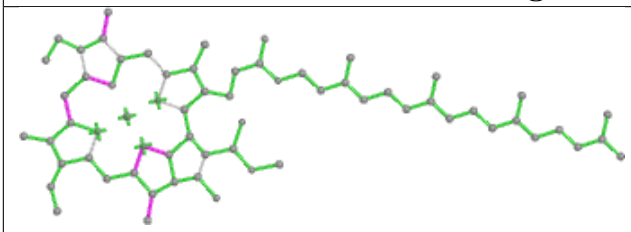


Rings

Ligand CLA b 717



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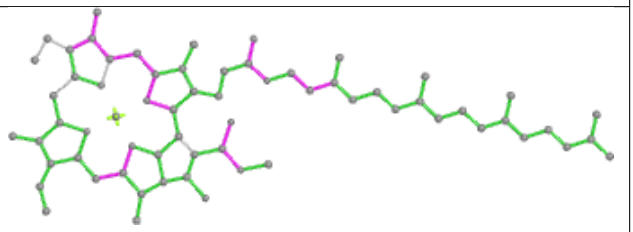
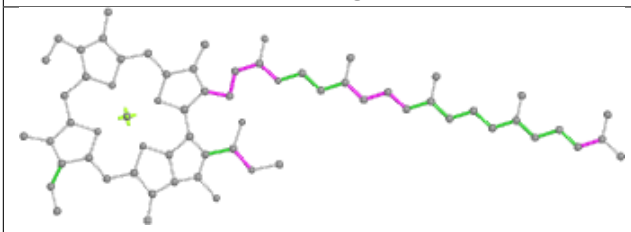
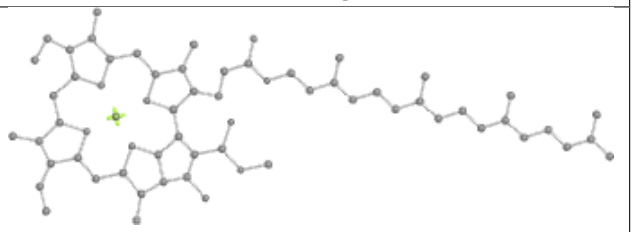


Bond angles

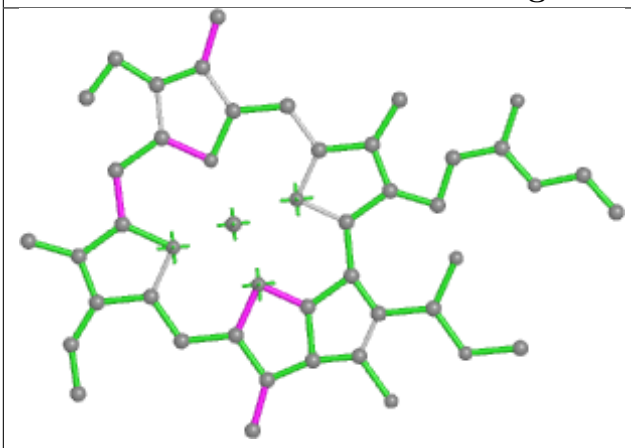


Torsions



Rings

Ligand CLA a 818



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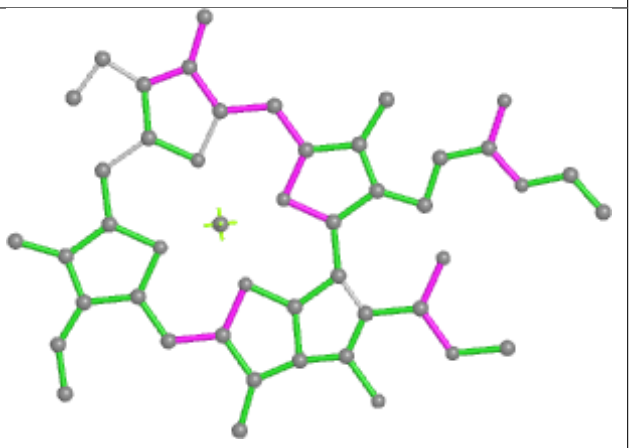
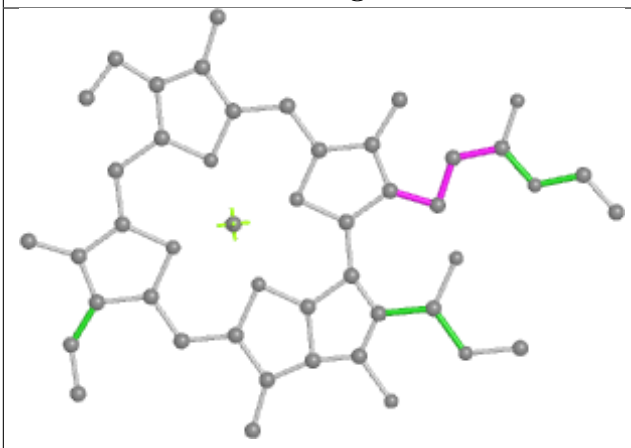


Bond angles



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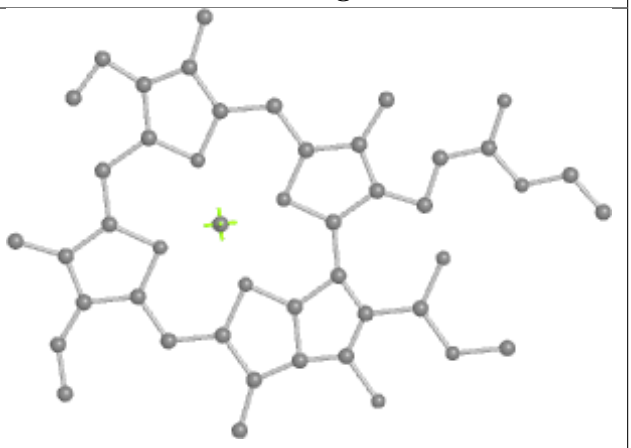
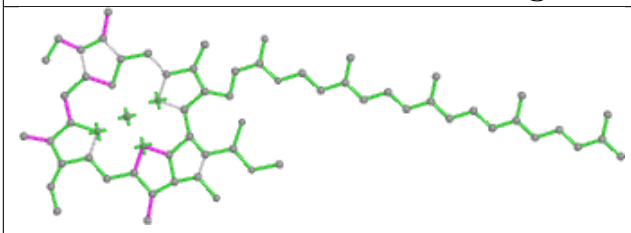


Rings

Ligand CLA a 820



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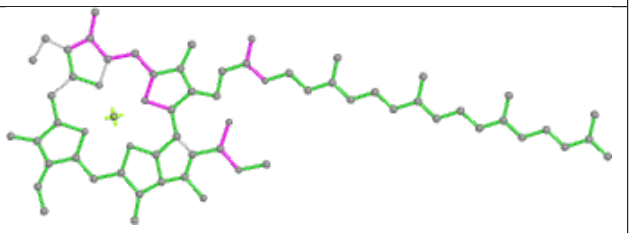
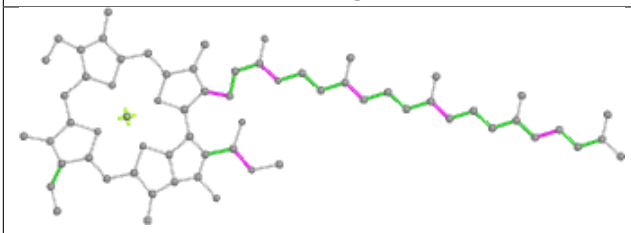


Bond angles



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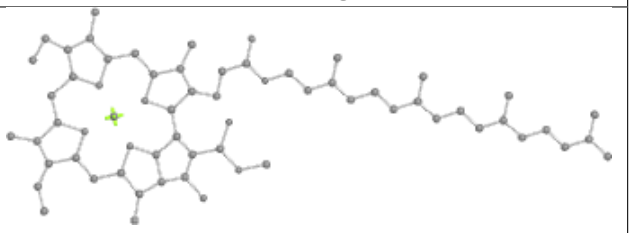
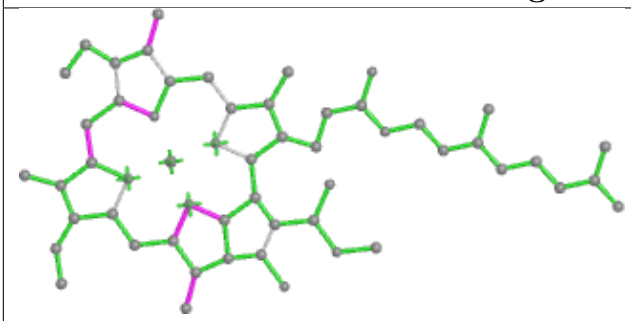


Rings

Ligand CLA a 837



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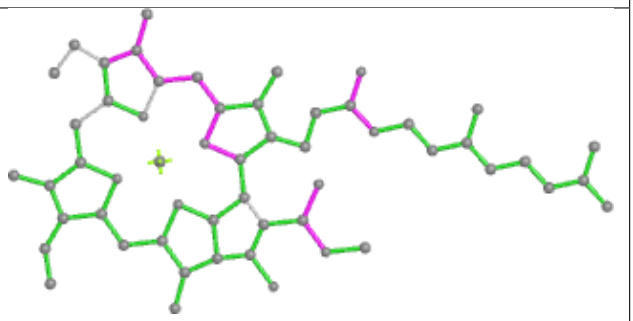
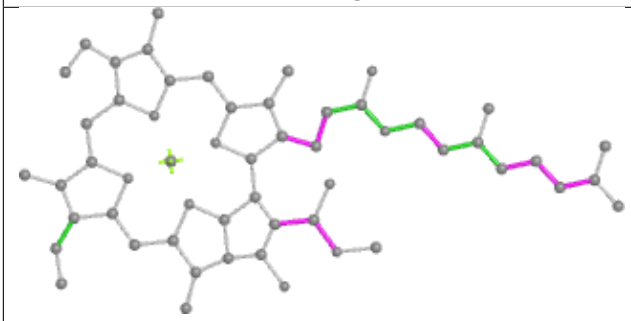


Bond angles



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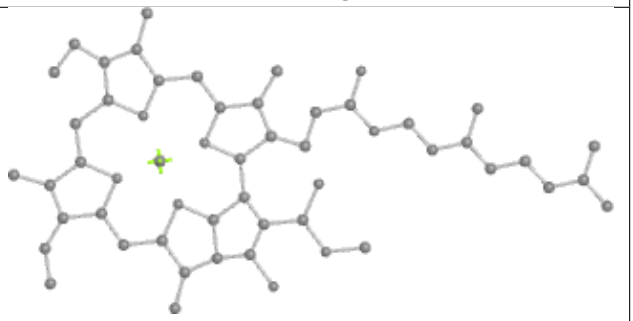
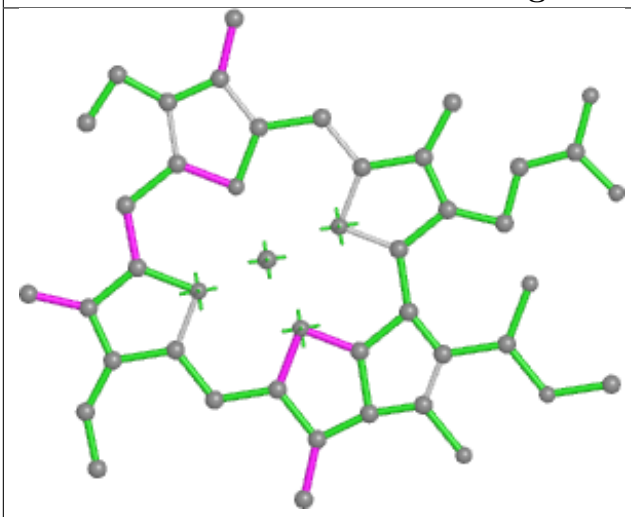
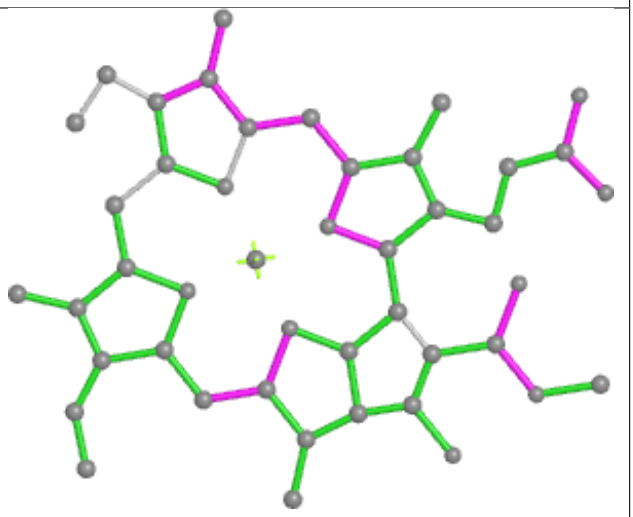


Rings

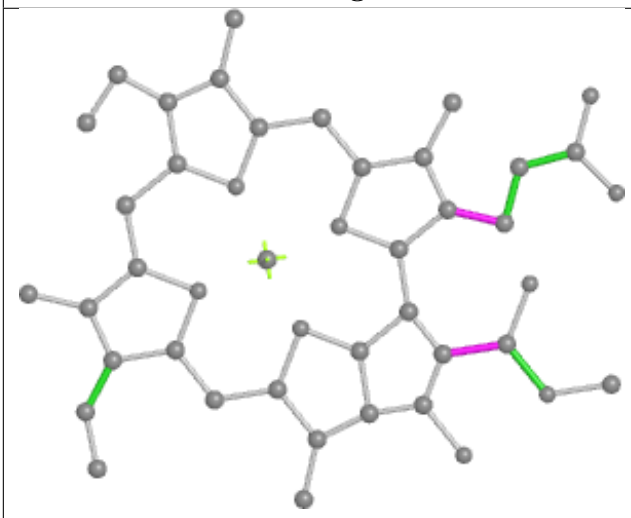
Ligand CLA a 815



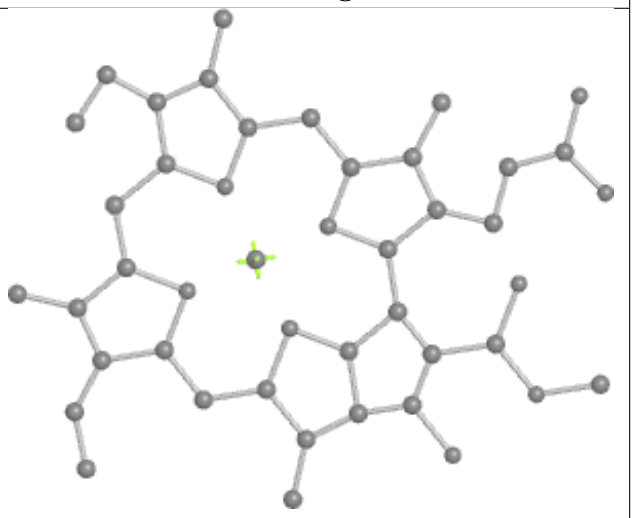
Bond lengths



Bond angles

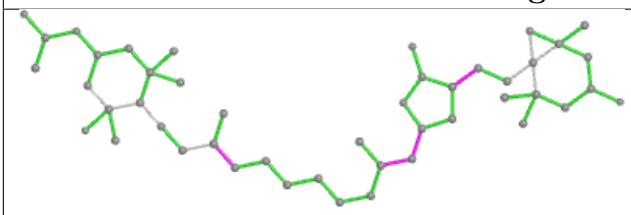


Torsions

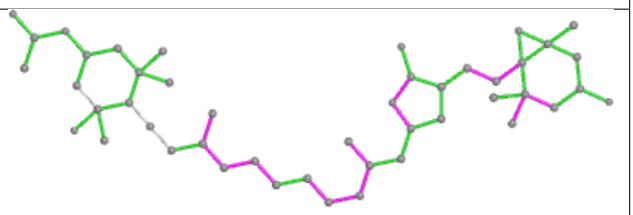


Rings

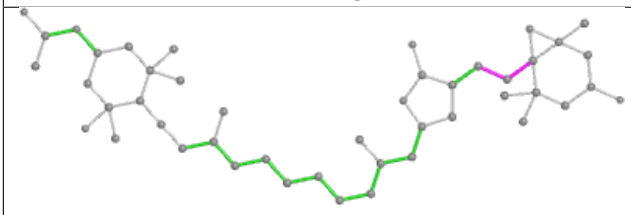
Ligand PID O 307



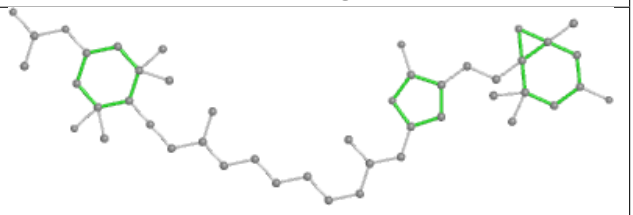
Bond lengths



Bond angles

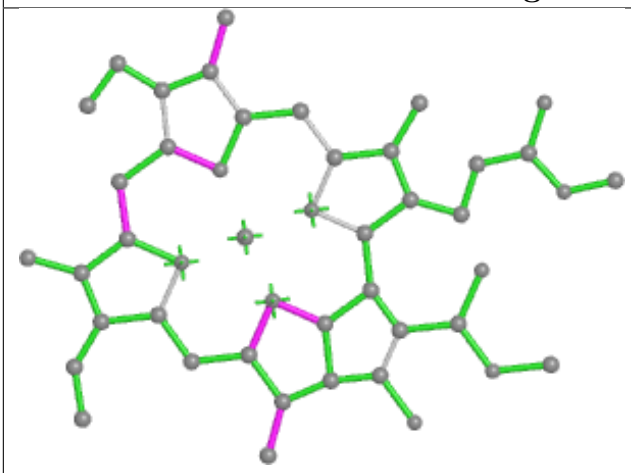


Torsions



Rings

Ligand CLA D 311



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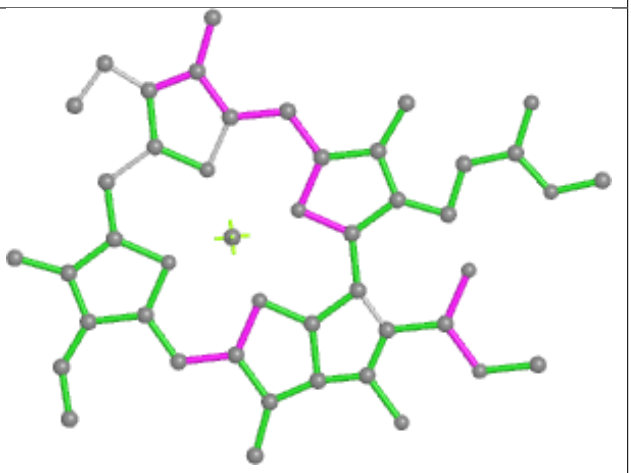

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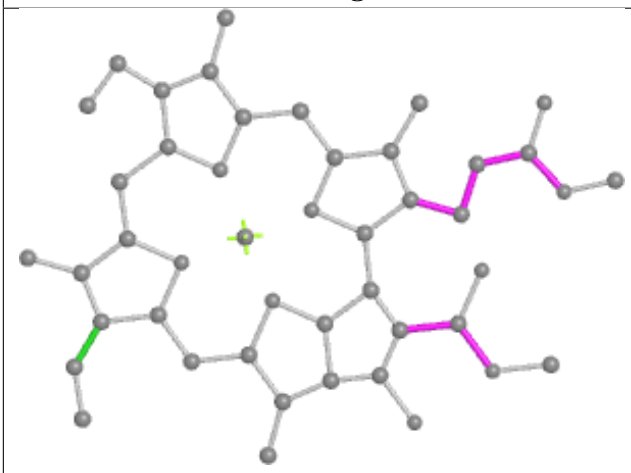

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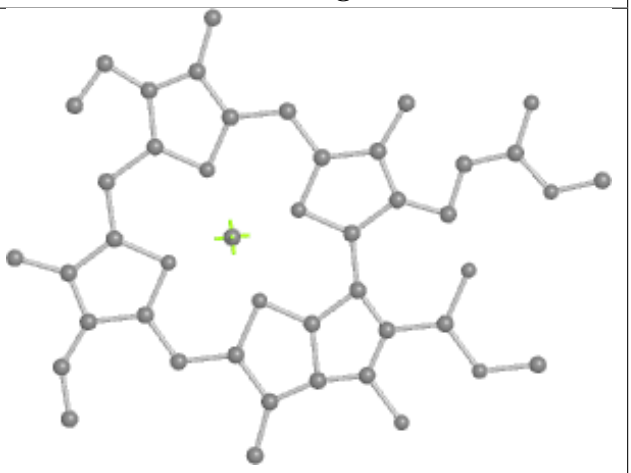
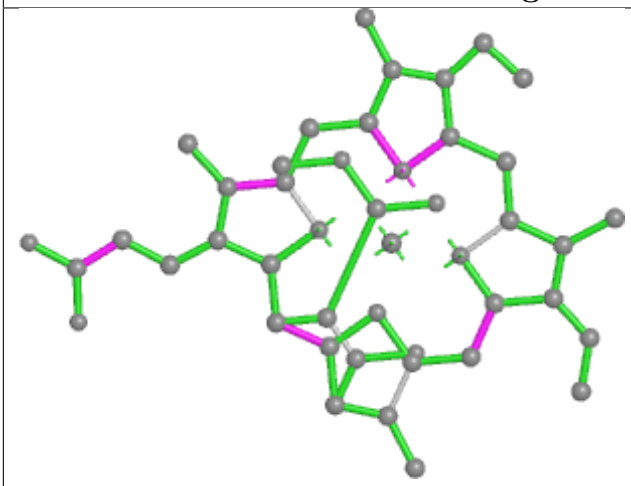


Rings

Ligand KC1 M 305



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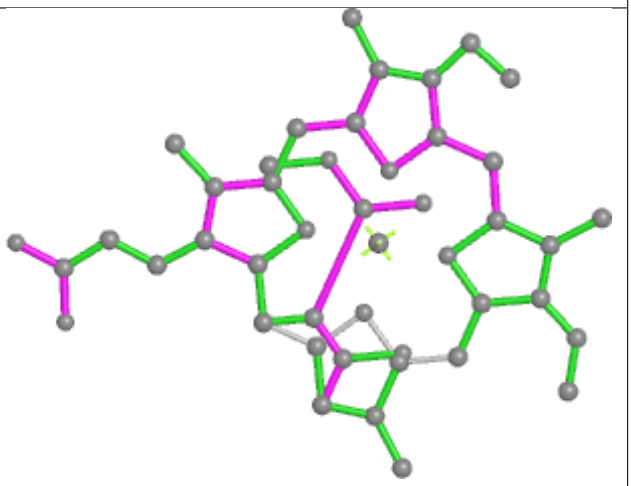

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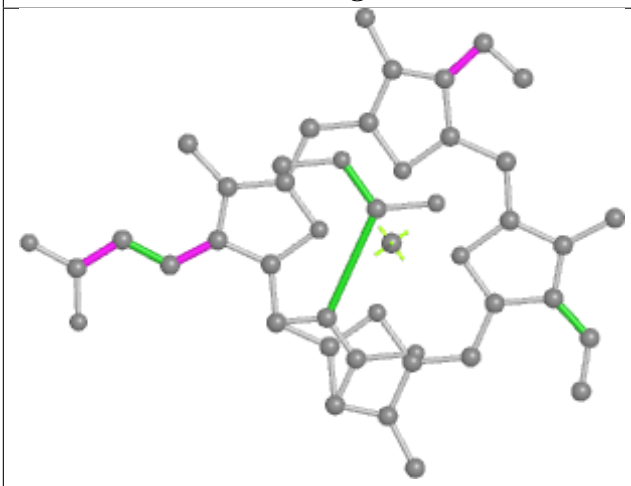

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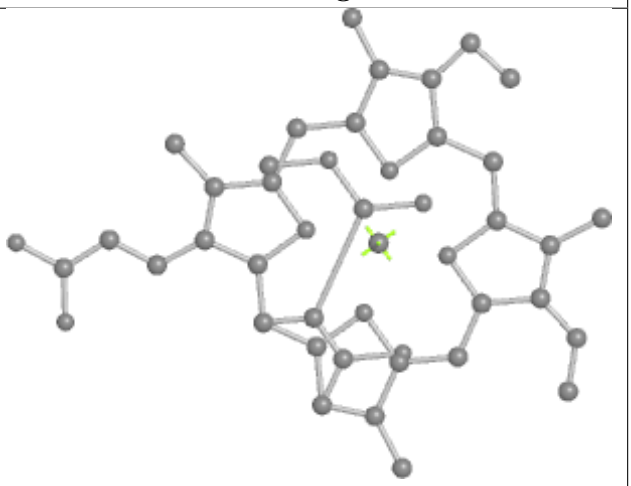
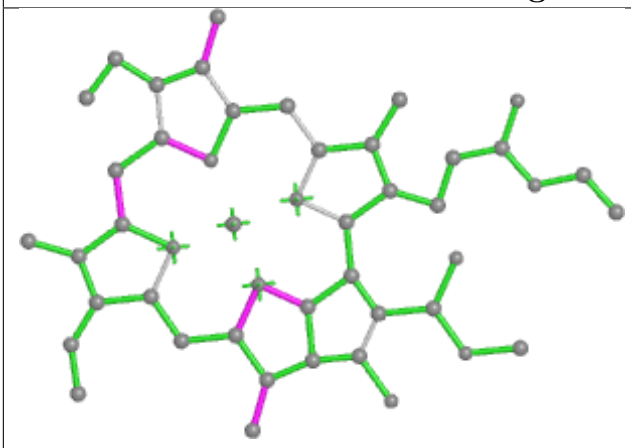


Rings

Ligand CLA a 821



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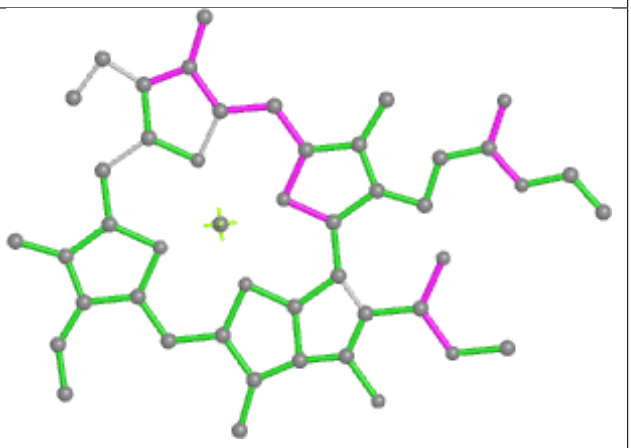

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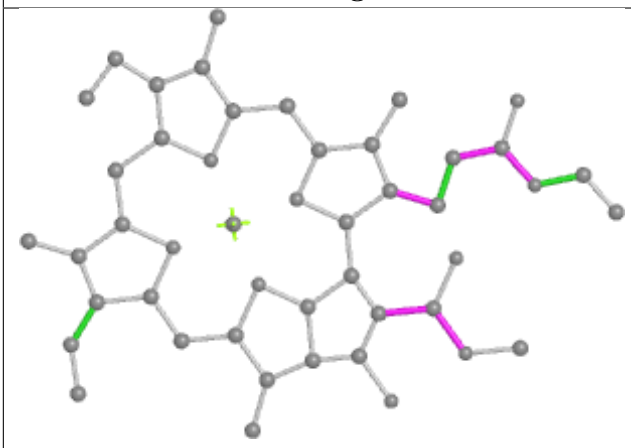

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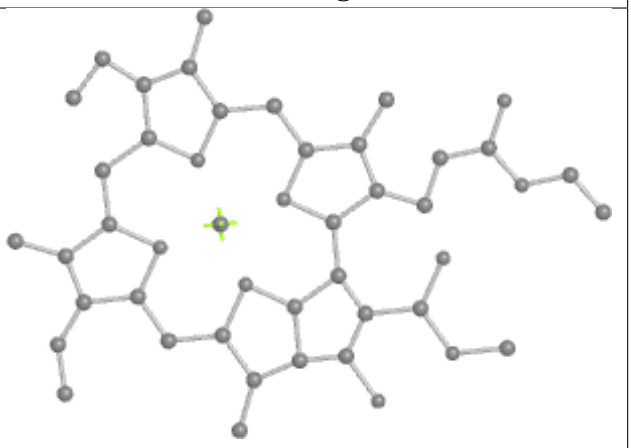
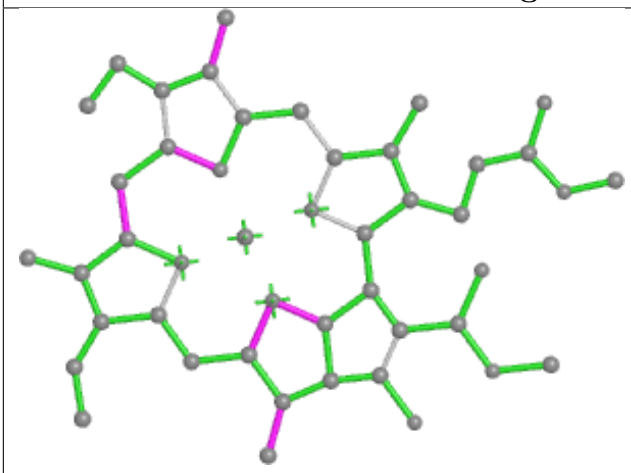


Rings

Ligand CLA M 309



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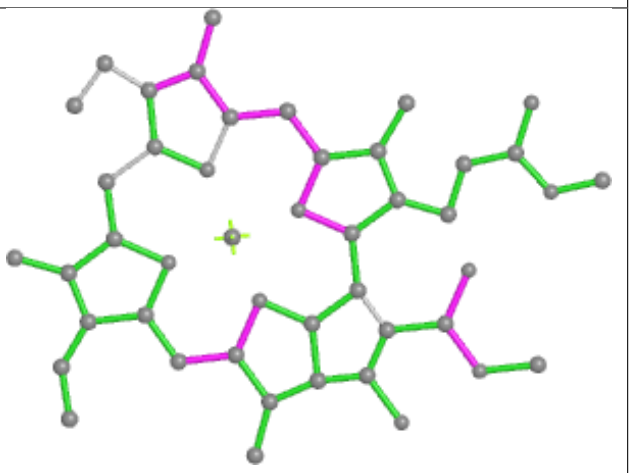

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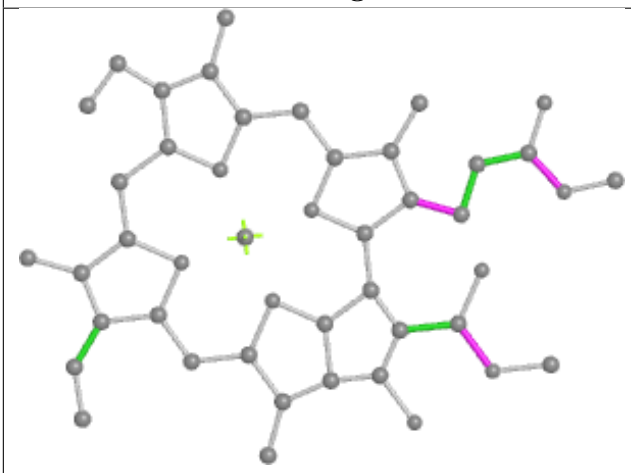

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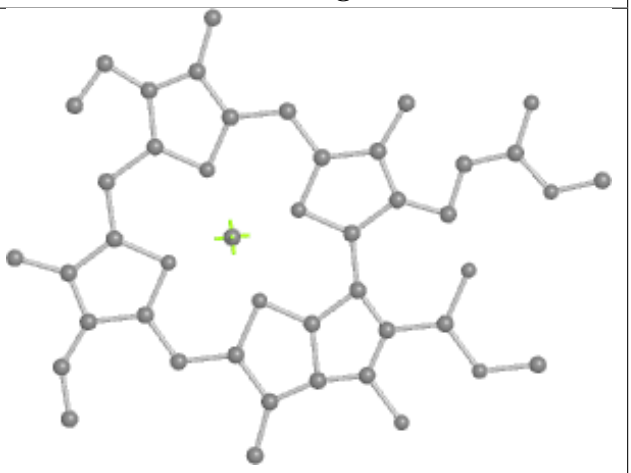
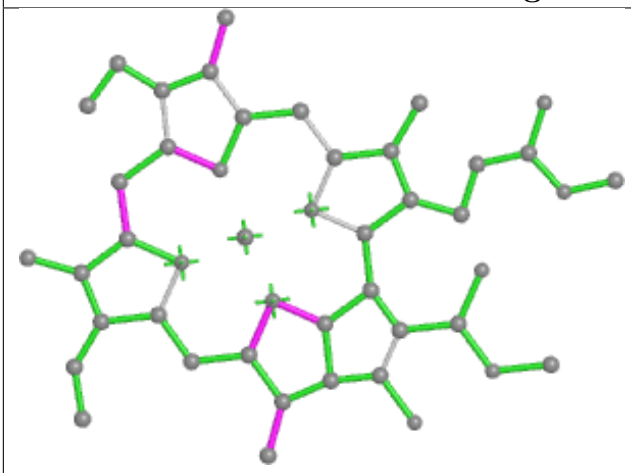


Rings

Ligand CLA Q 312



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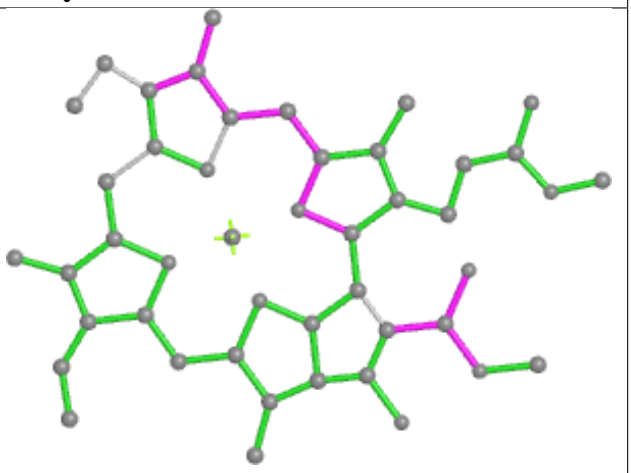
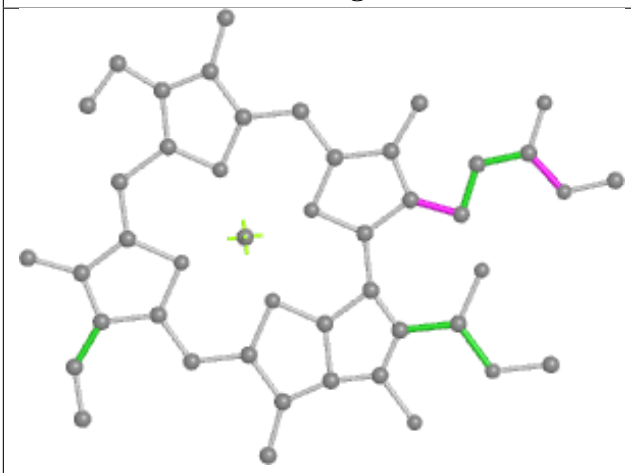


Bond angles



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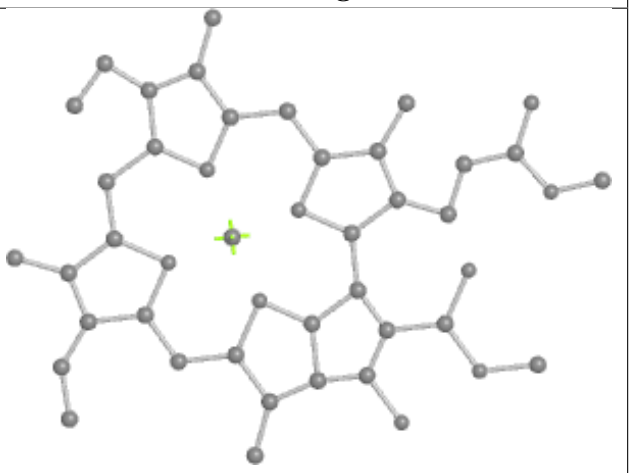
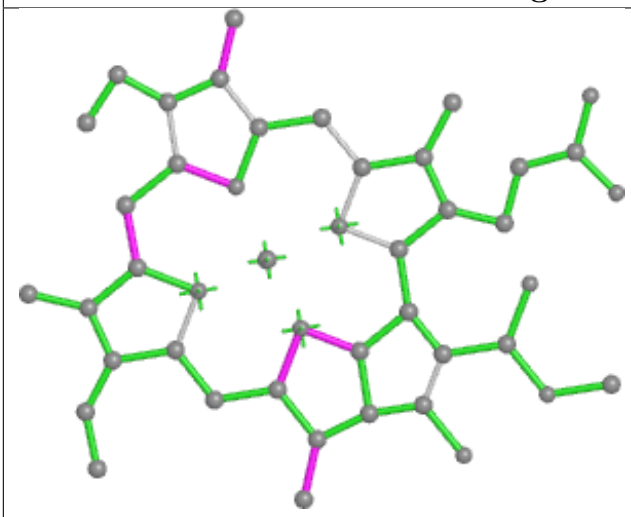


Rings

Ligand CLA I 201



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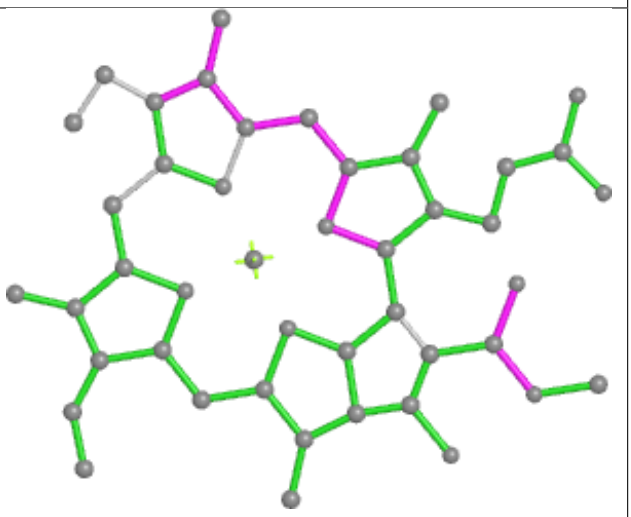
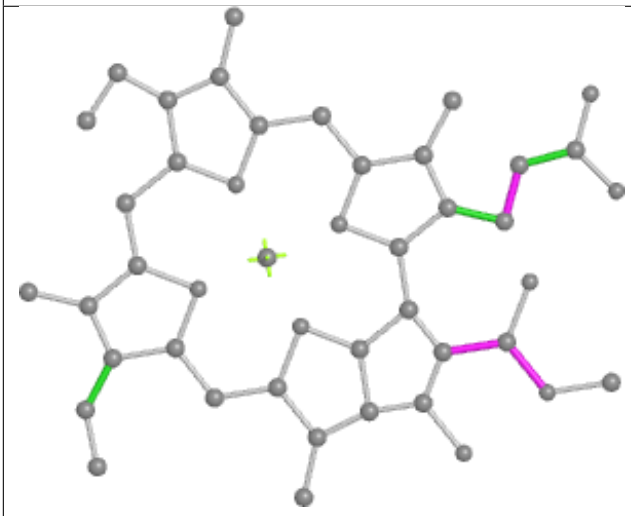


Bond angles



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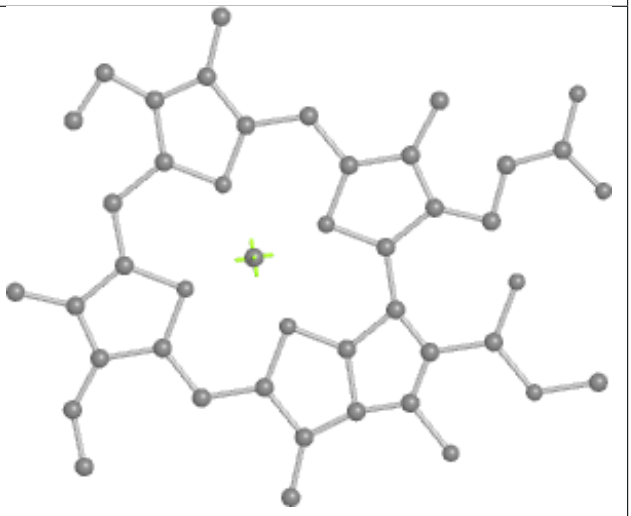
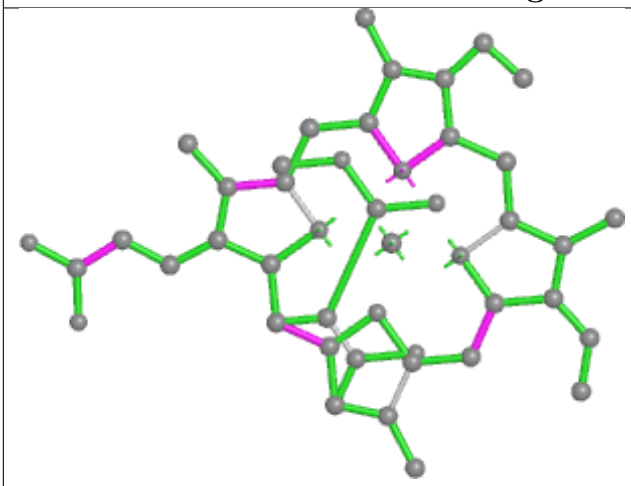


Rings

Ligand KC1 T 310



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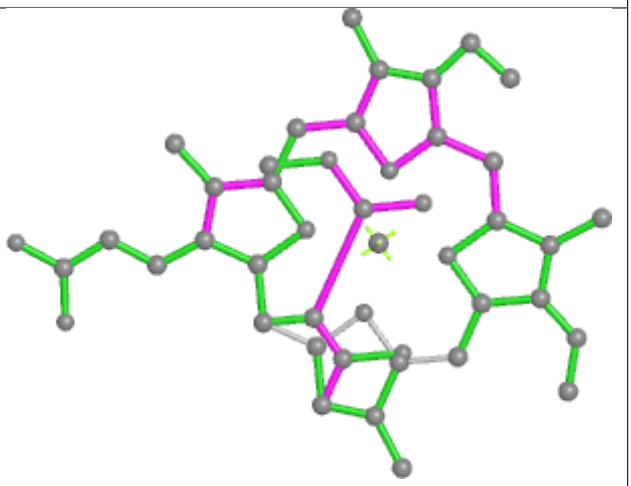
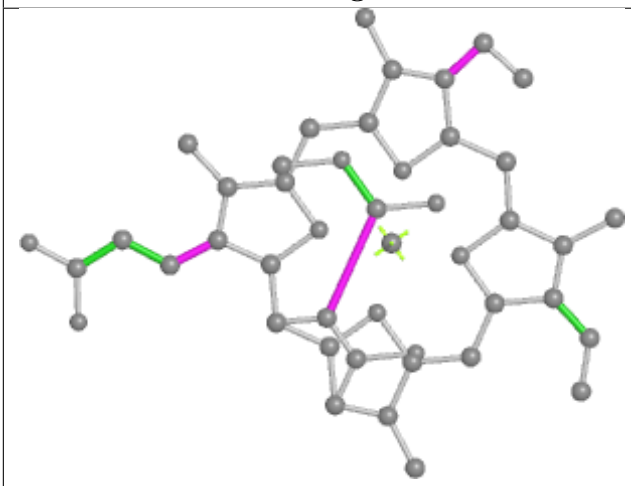


Bond angles



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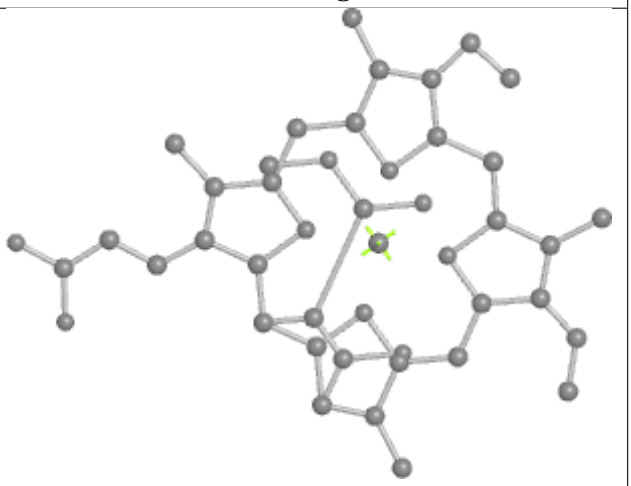
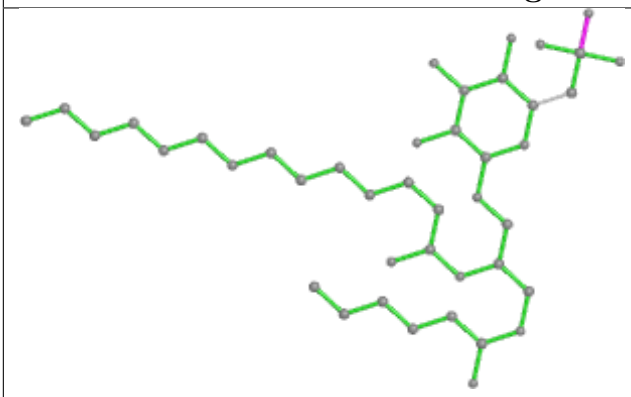


Rings

Ligand SQD B 317



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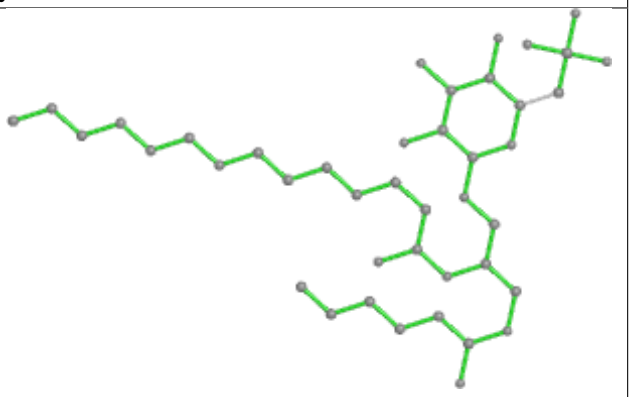
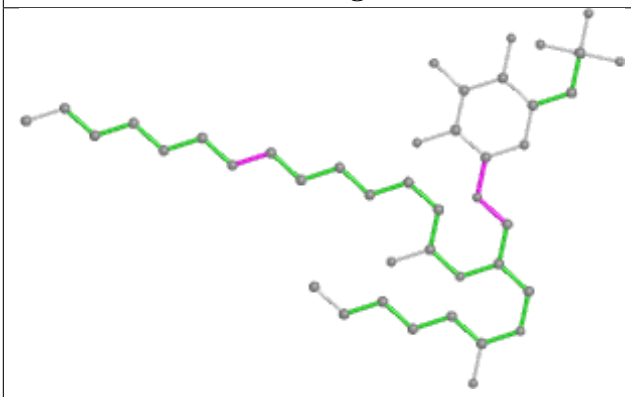


Bond angles



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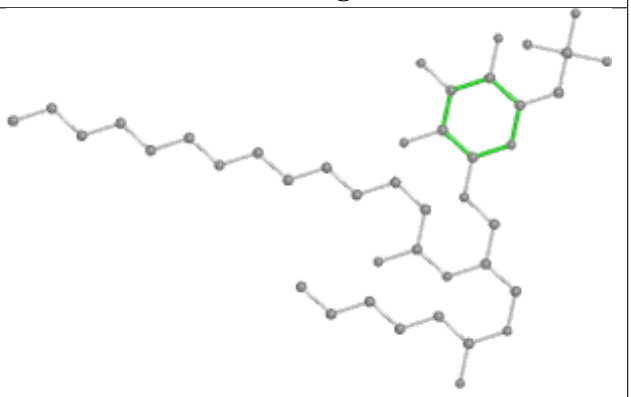
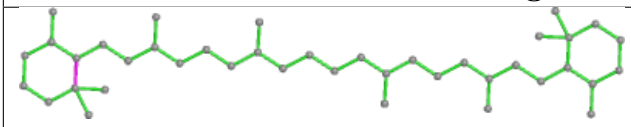


Rings

Ligand BCR b 728



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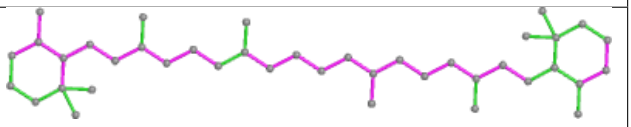

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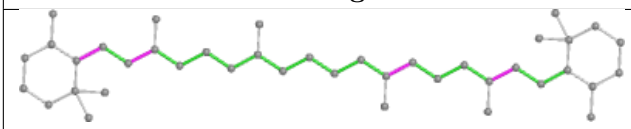
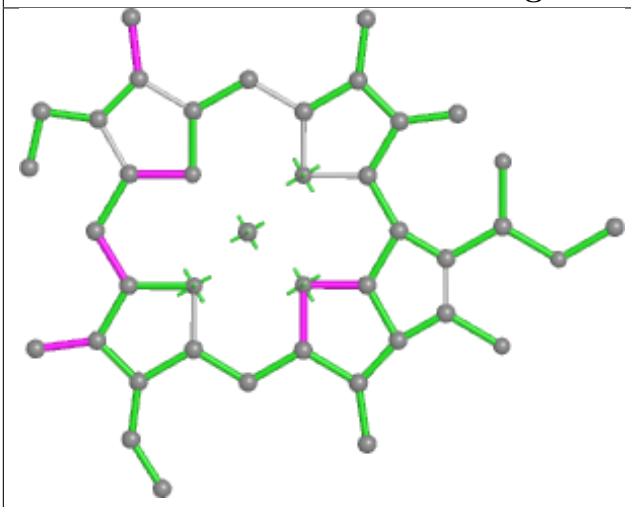


Torsions

Rings

Ligand CLA P 217



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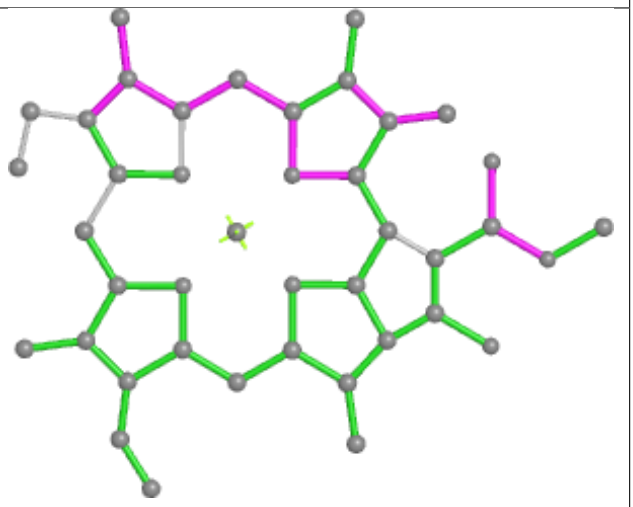
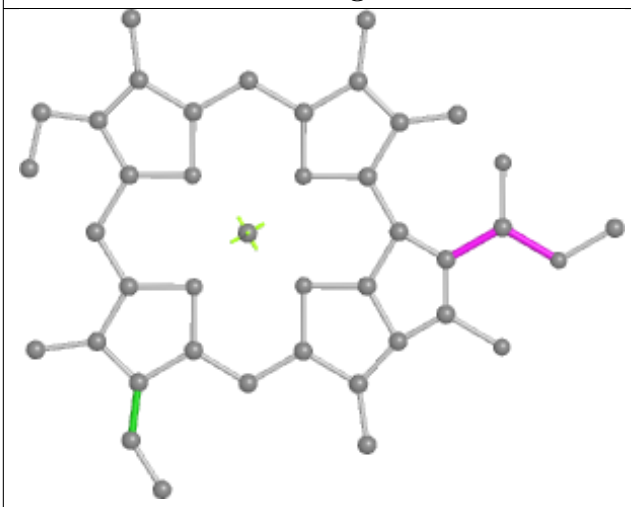


Bond angles



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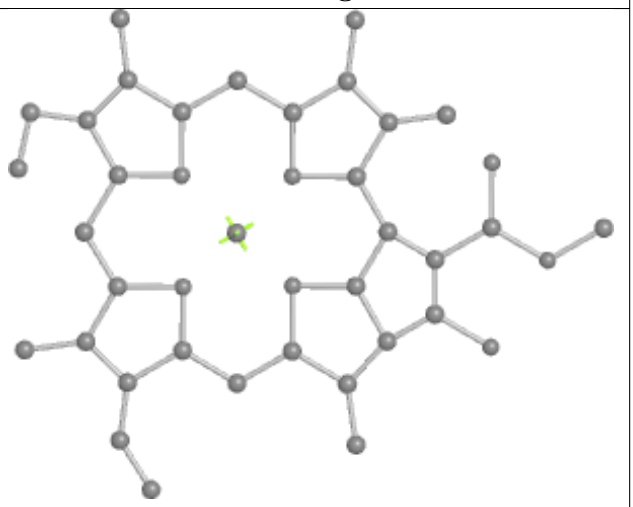
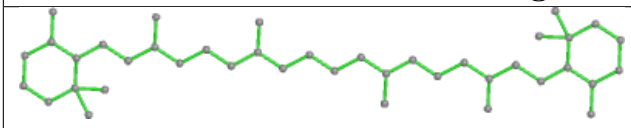


Rings

Ligand BCR f 804



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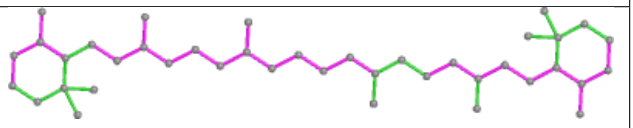

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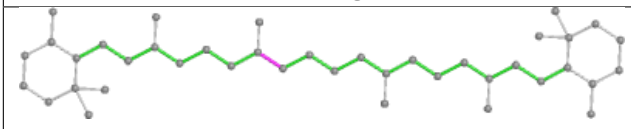

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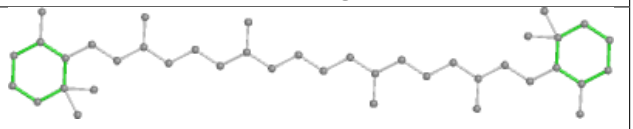
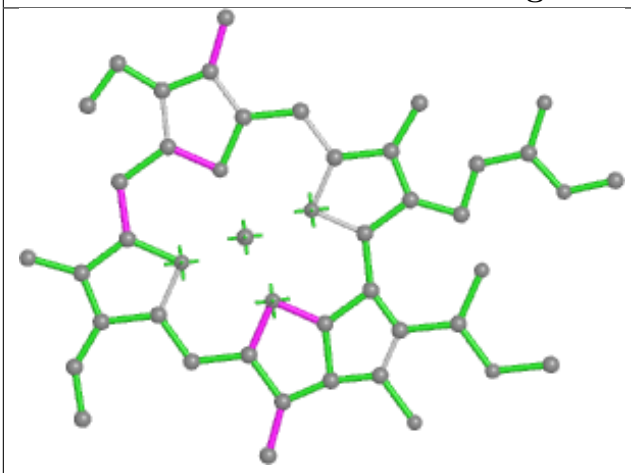


Rings

Ligand CLA L 311



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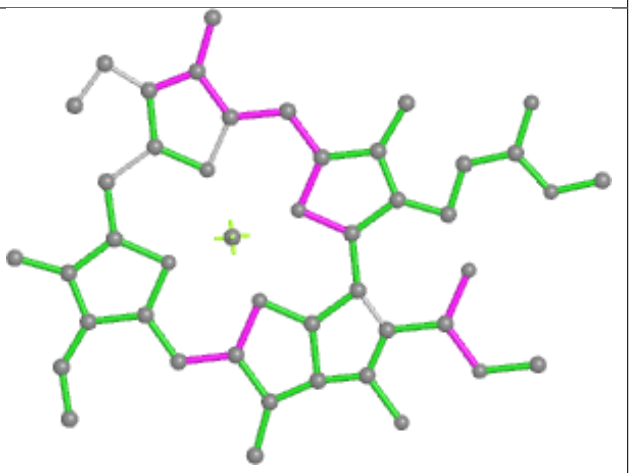
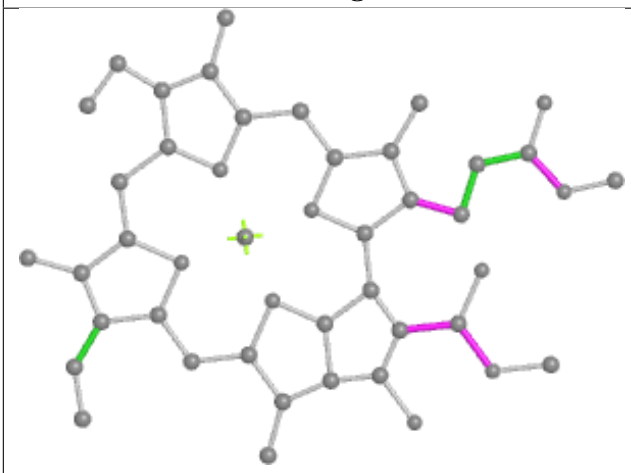


Bond angles



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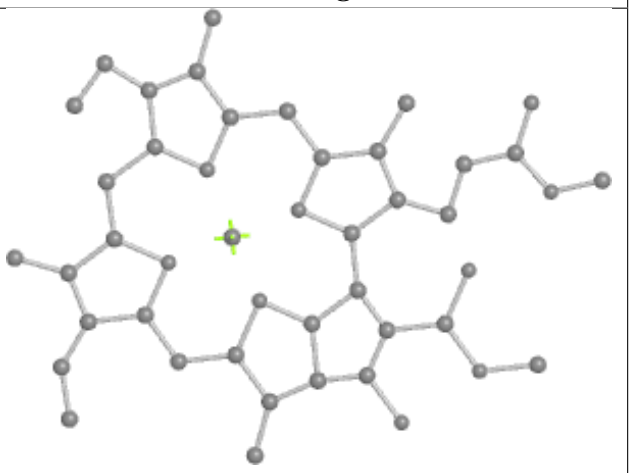
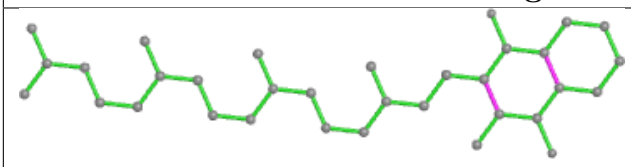
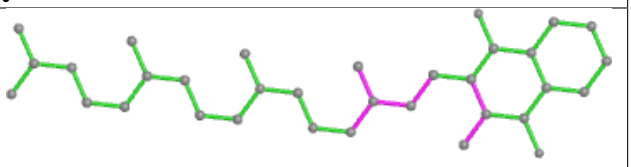


Rings

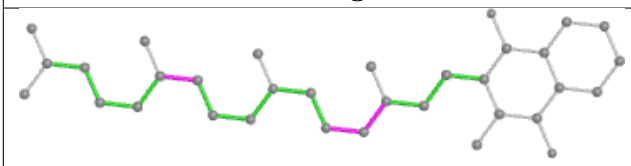
Ligand PQN b 727



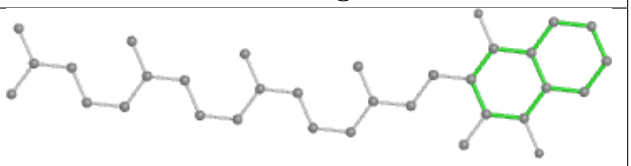
Bond lengths



Bond angles

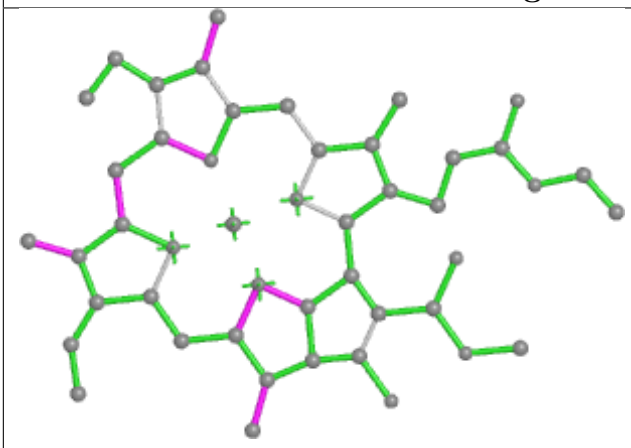


Torsions

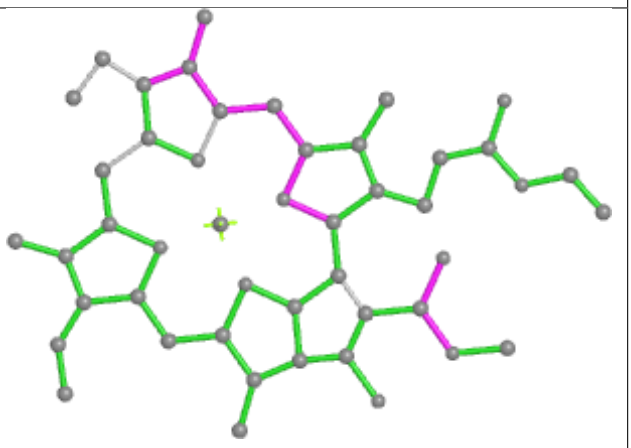


Rings

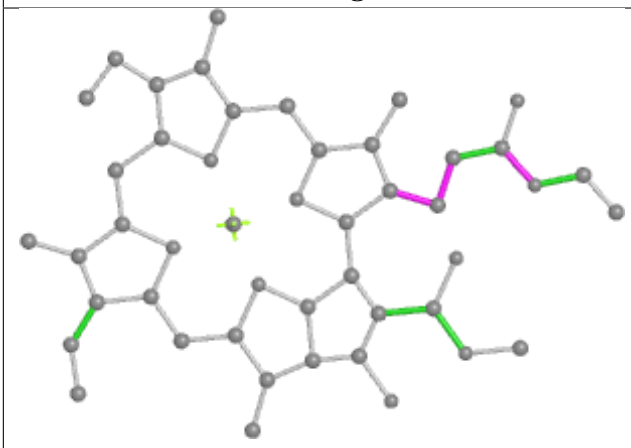
Ligand CLA A 215



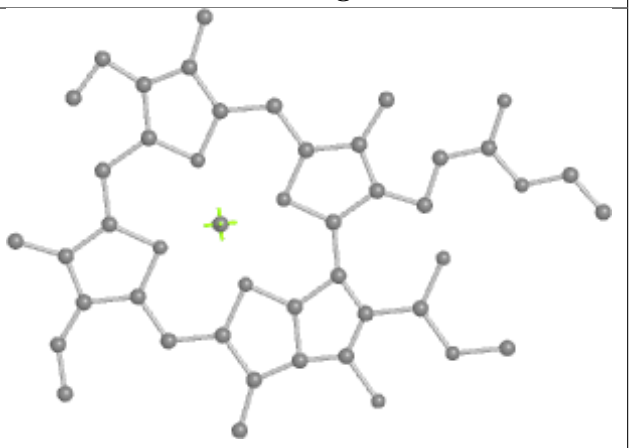
Bond lengths



Bond angles

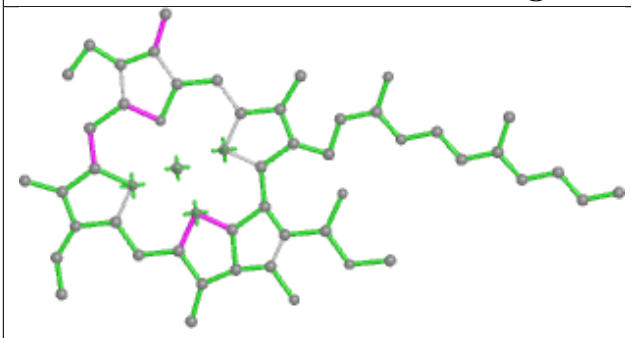


Torsions

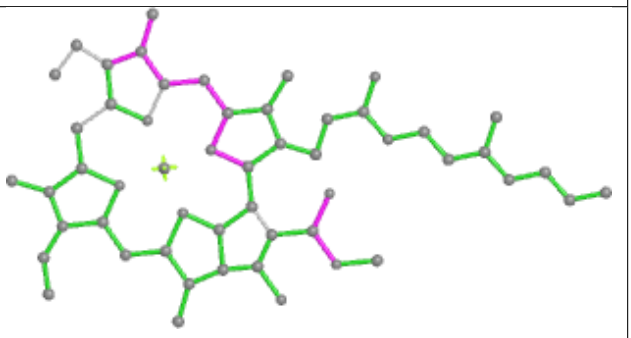


Rings

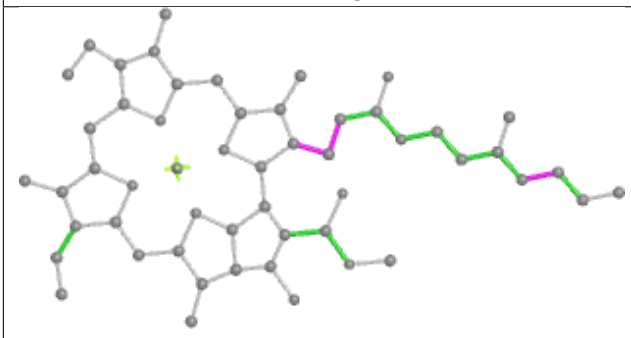
Ligand CLA b 713



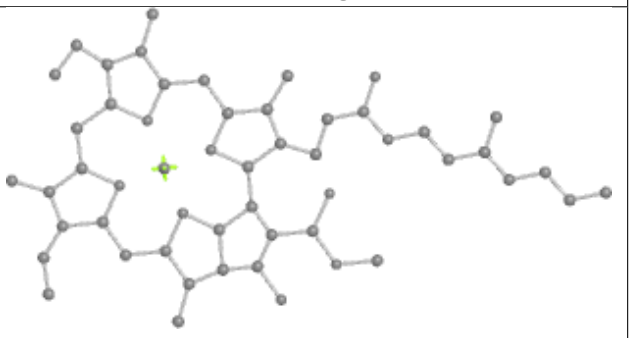
Bond lengths



Bond angles

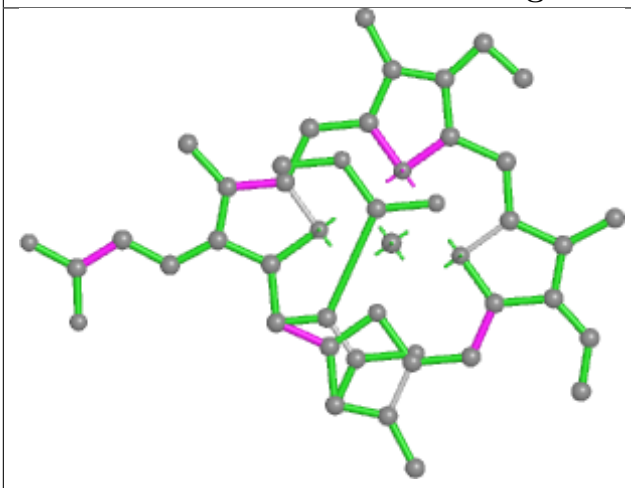


Torsions



Rings

Ligand KC1 T 315



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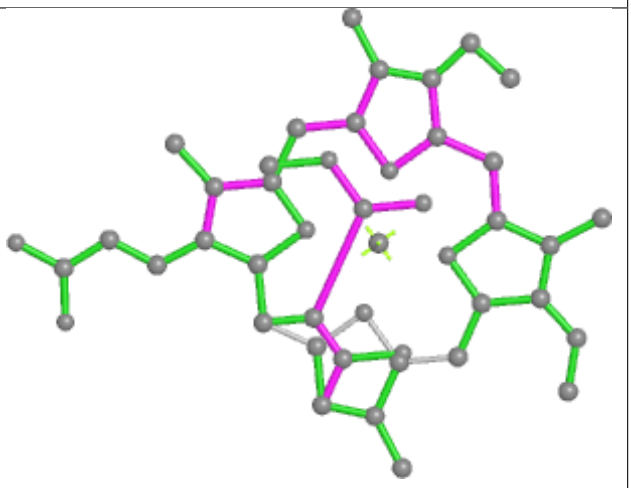
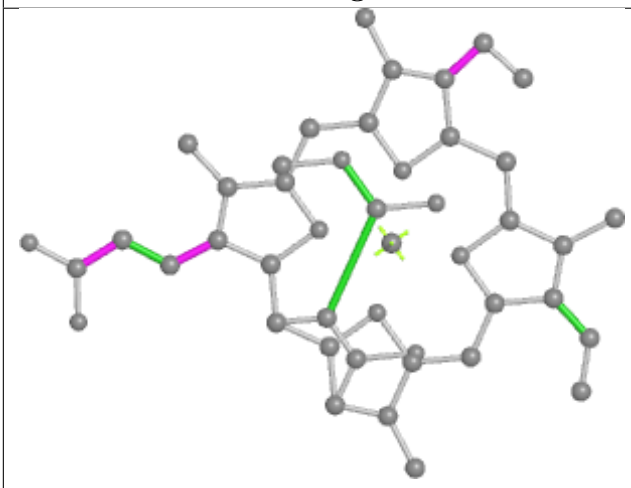
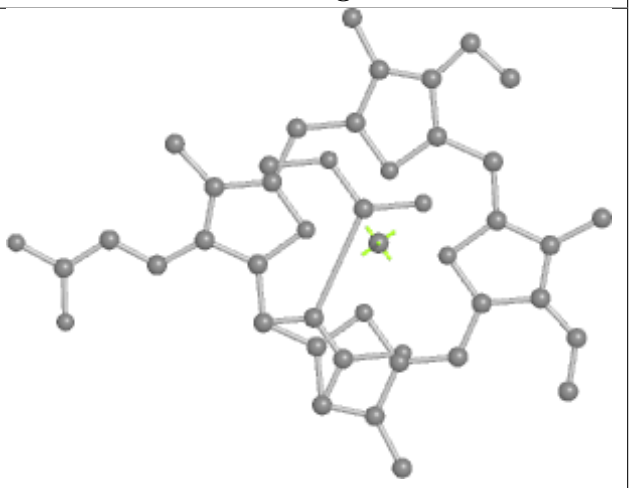


Bond angles

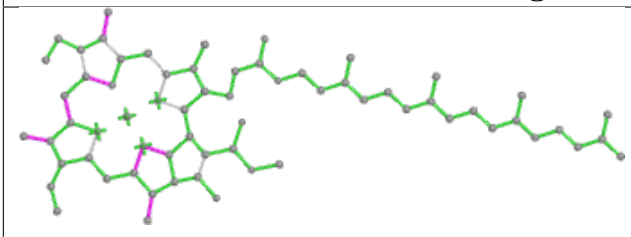


Torsions



Rings

Ligand CLA a 824



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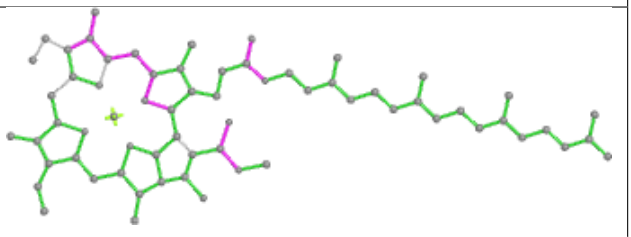
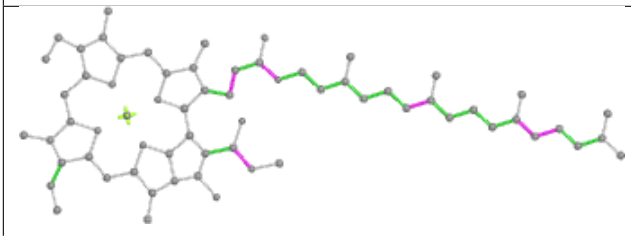


Bond angles



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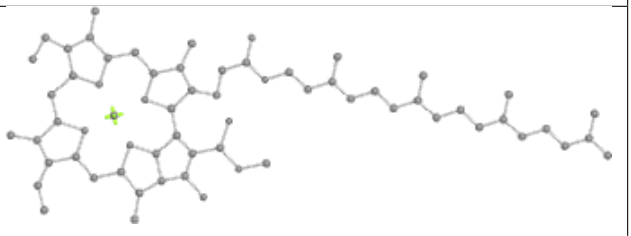
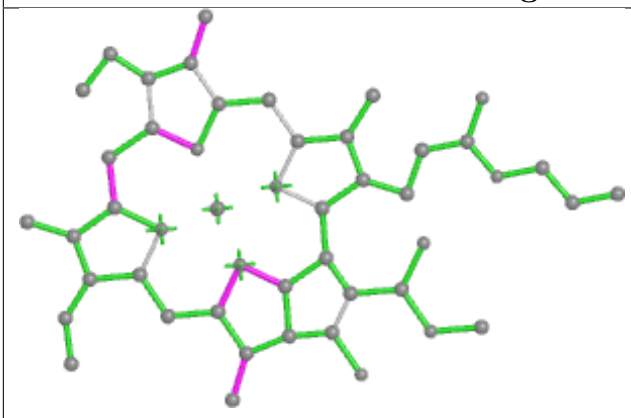


Rings

Ligand CLA M 310



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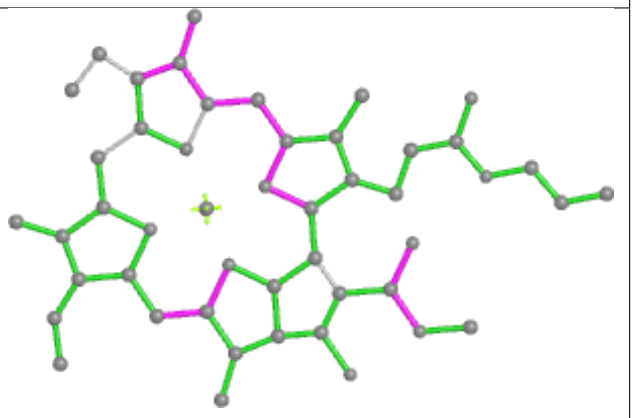
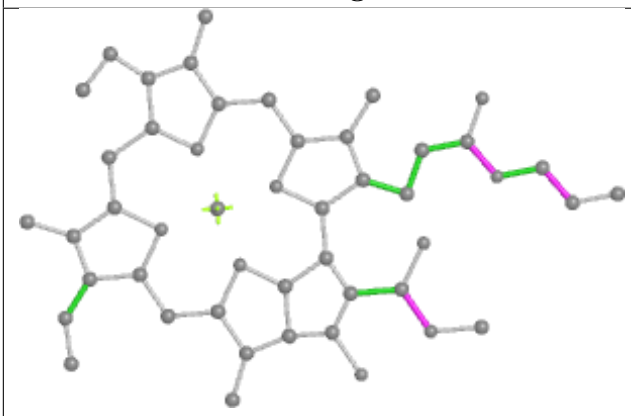


Bond angles



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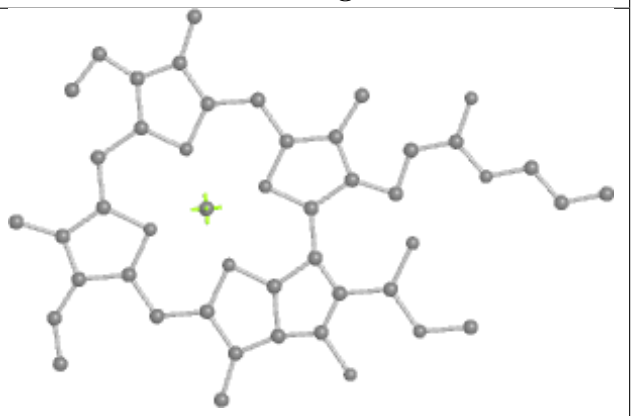
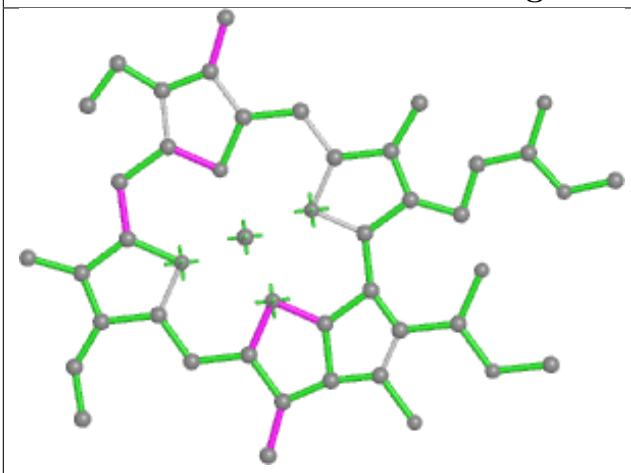


Rings

Ligand CLA F 313



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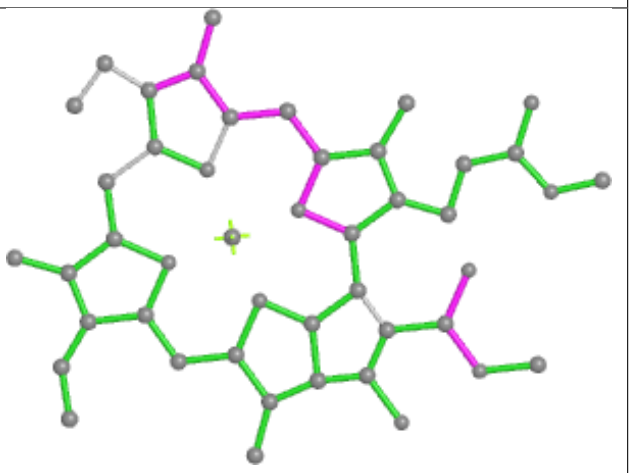
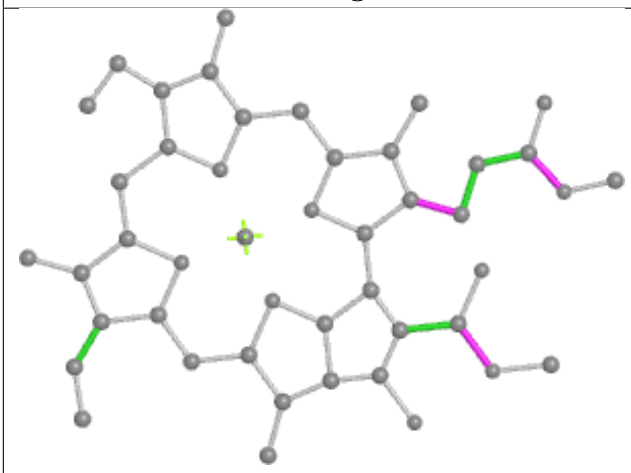


Bond angles



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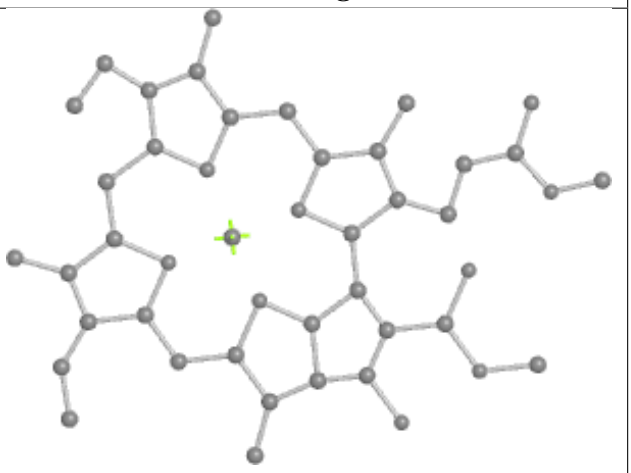
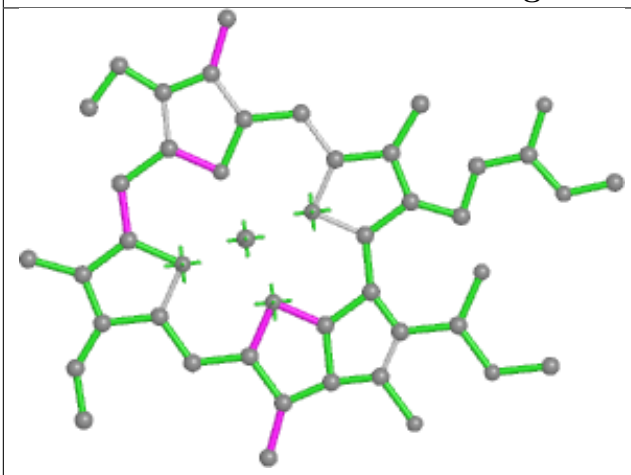


Rings

Ligand CLA N 313



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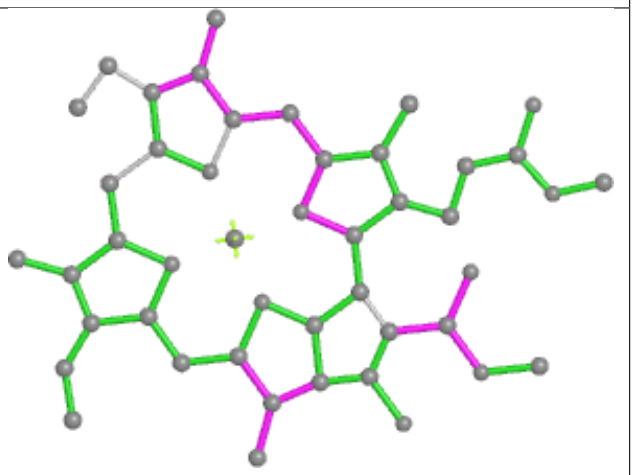
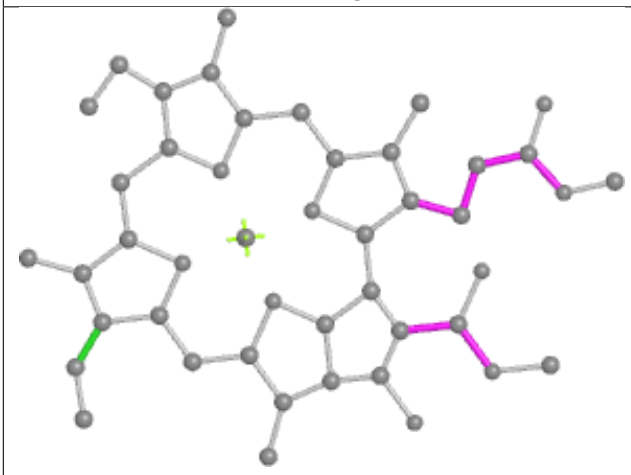


Bond angles



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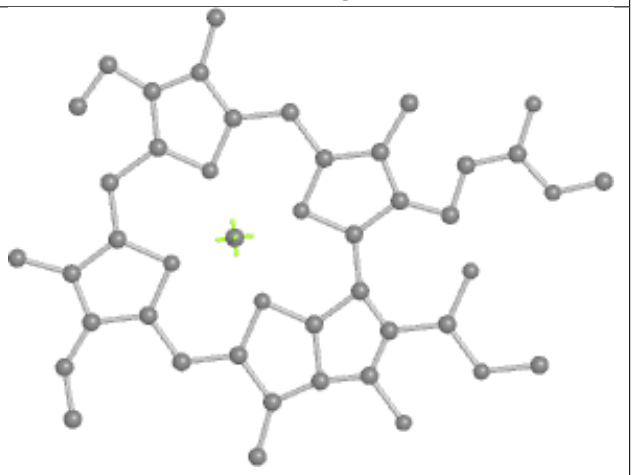
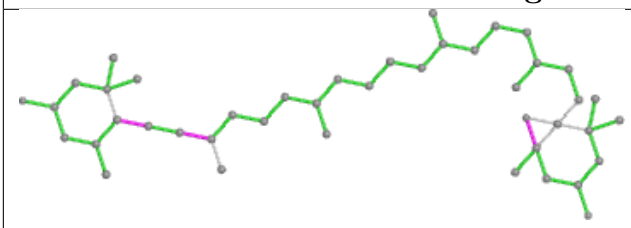


Rings

Ligand DD6 Q 302



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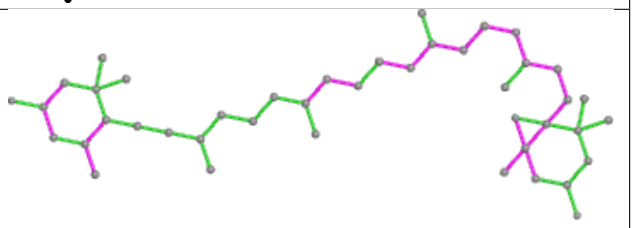

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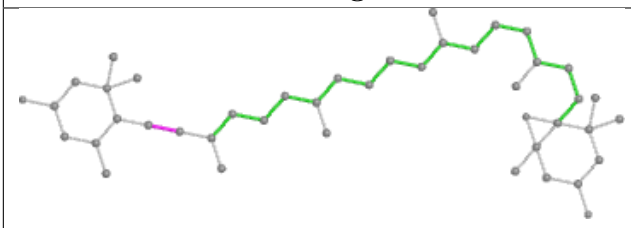

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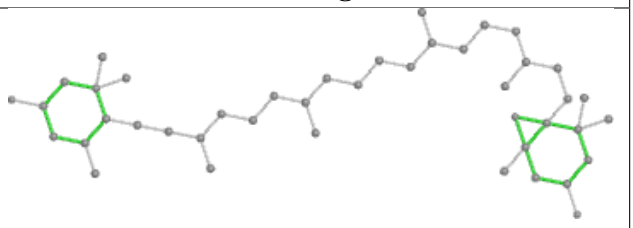
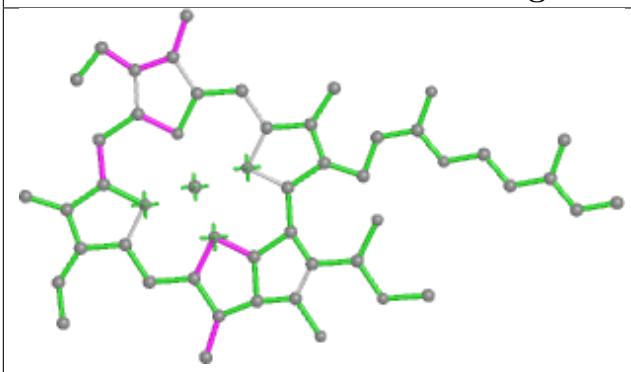


Rings

Ligand CLA a 808



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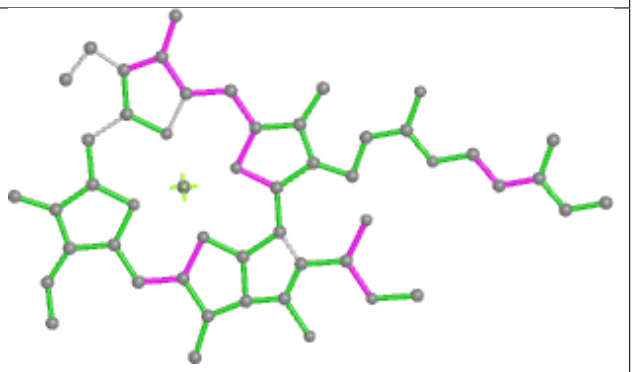
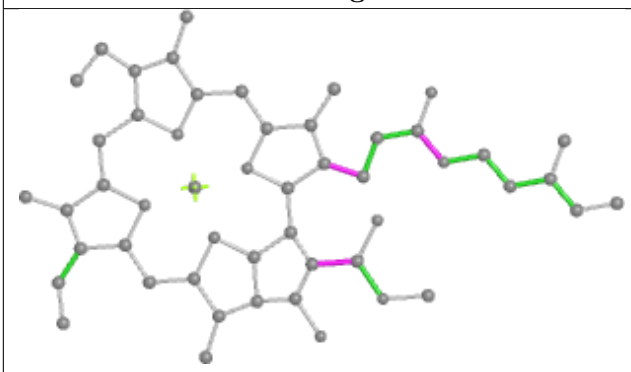


Bond angles



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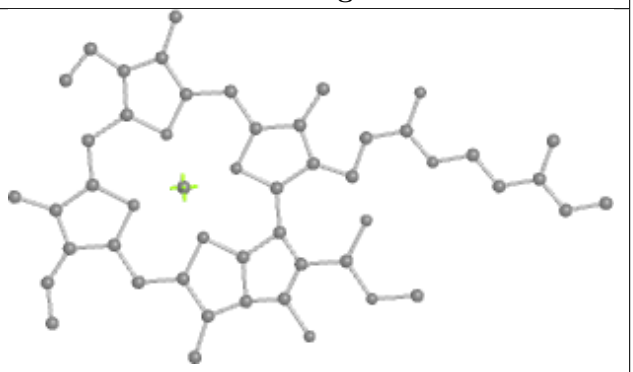
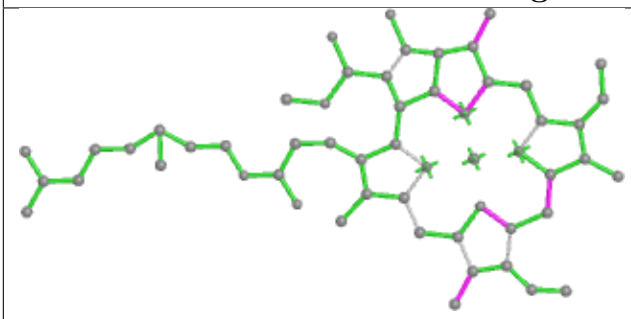


Rings

Ligand CLA I 212



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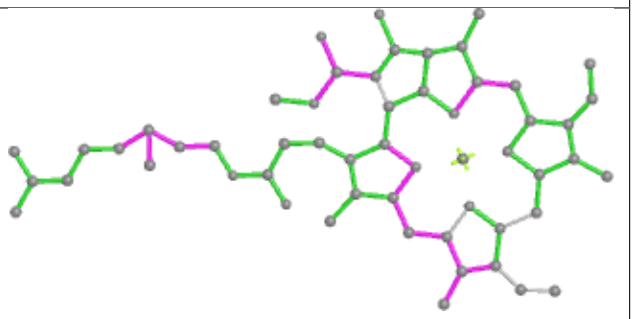
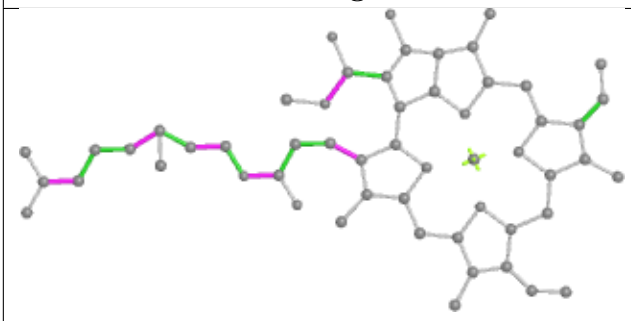


Bond angles



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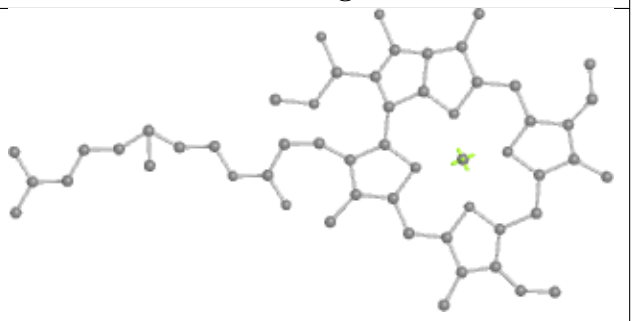
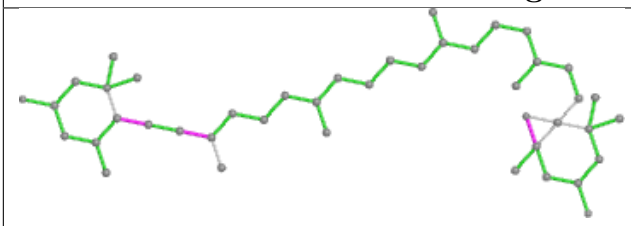


Rings

Ligand DD6 B 302



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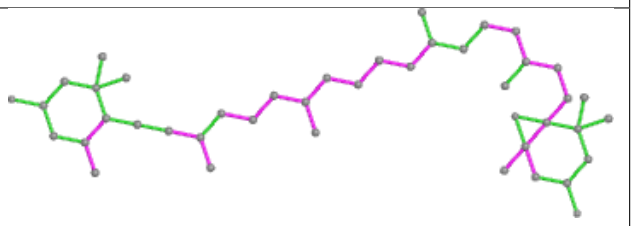
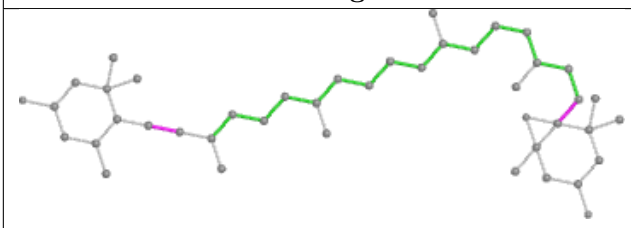


Bond angles



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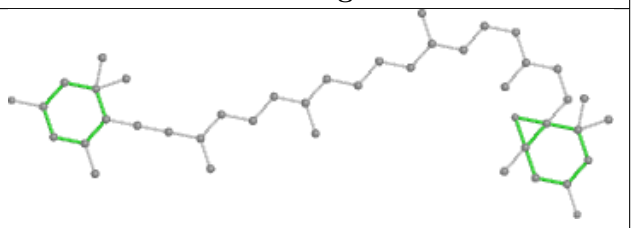
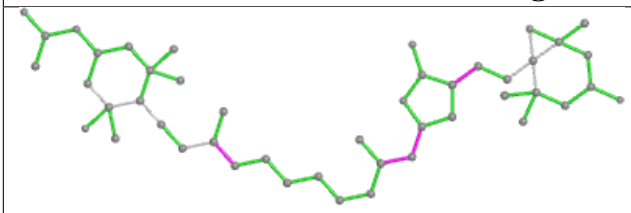


Rings

Ligand PID P 203



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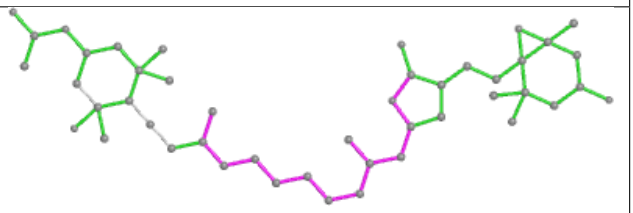
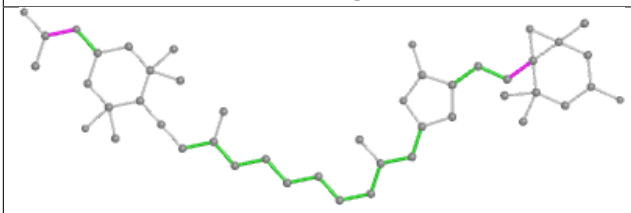


Bond angles



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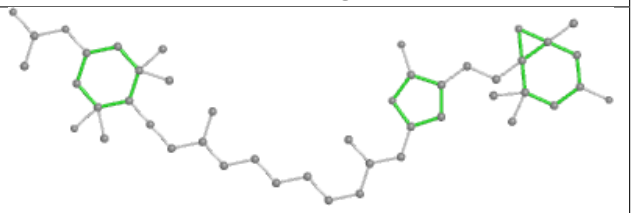
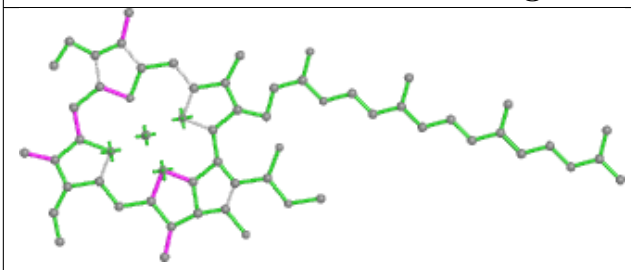


Rings

Ligand CLA A 218



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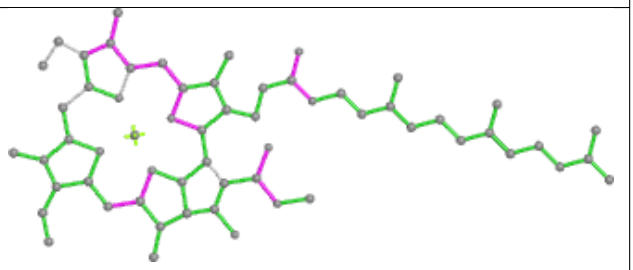
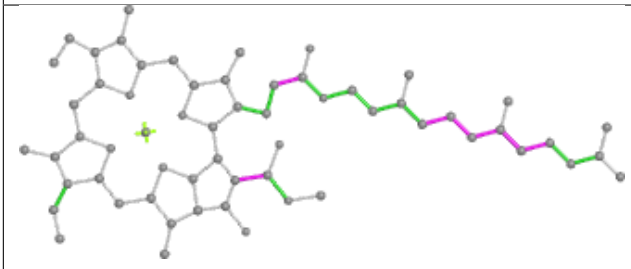


Bond angles



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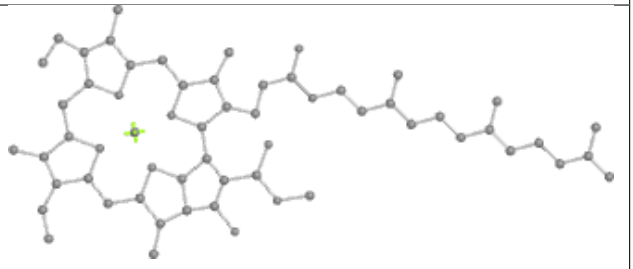
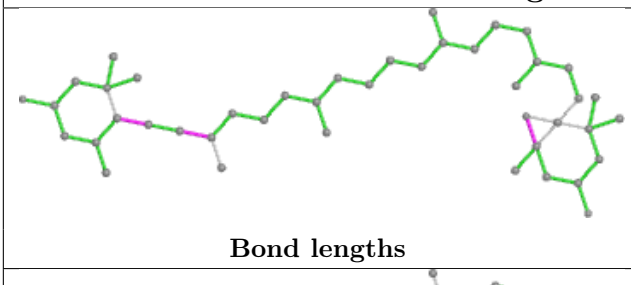
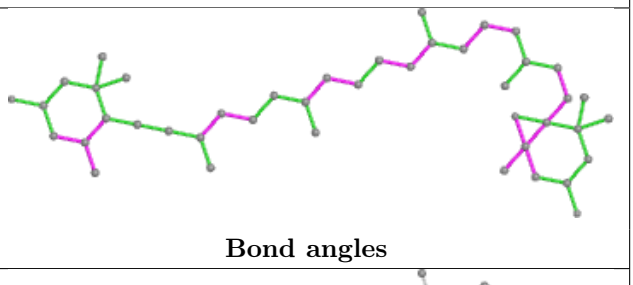


Rings

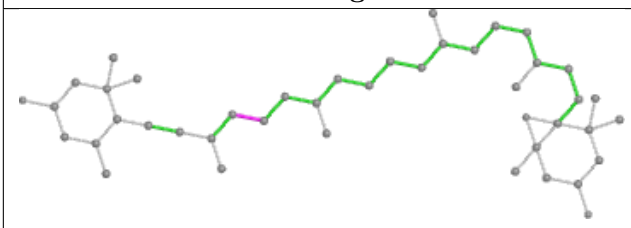
Ligand DD6 E 303



Bond lengths



Bond angles



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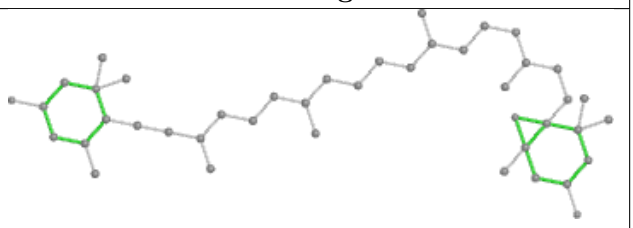
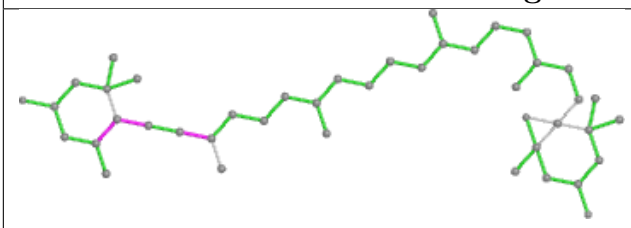


Rings

Ligand DD6 G 305



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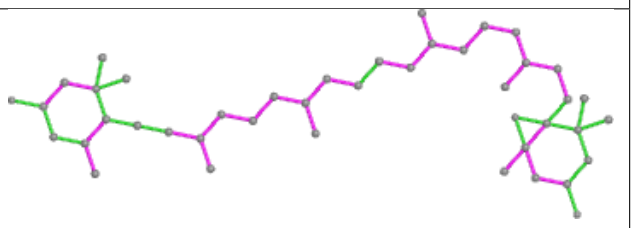
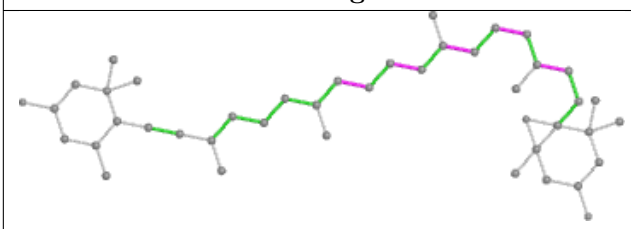
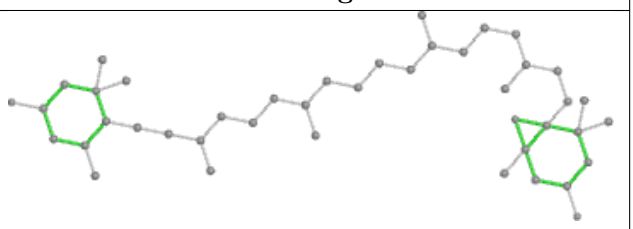


Bond angles

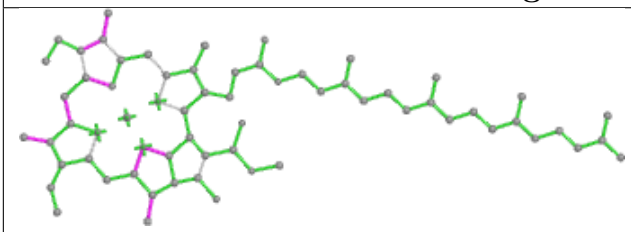


Torsions

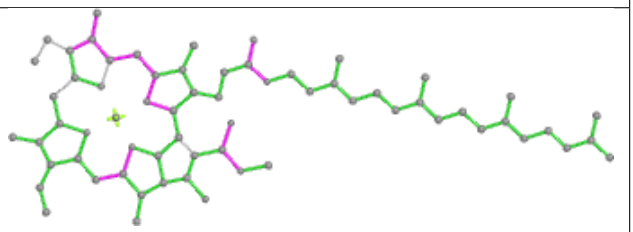


Rings

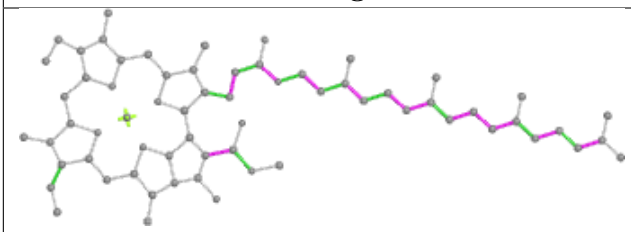
Ligand CLA G 312



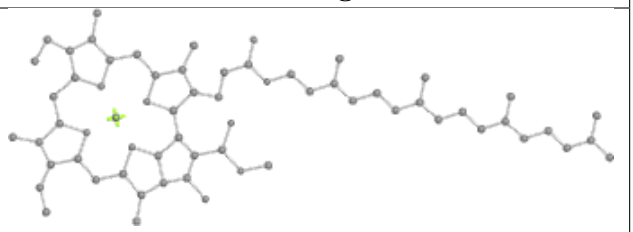
Bond lengths



Bond angles

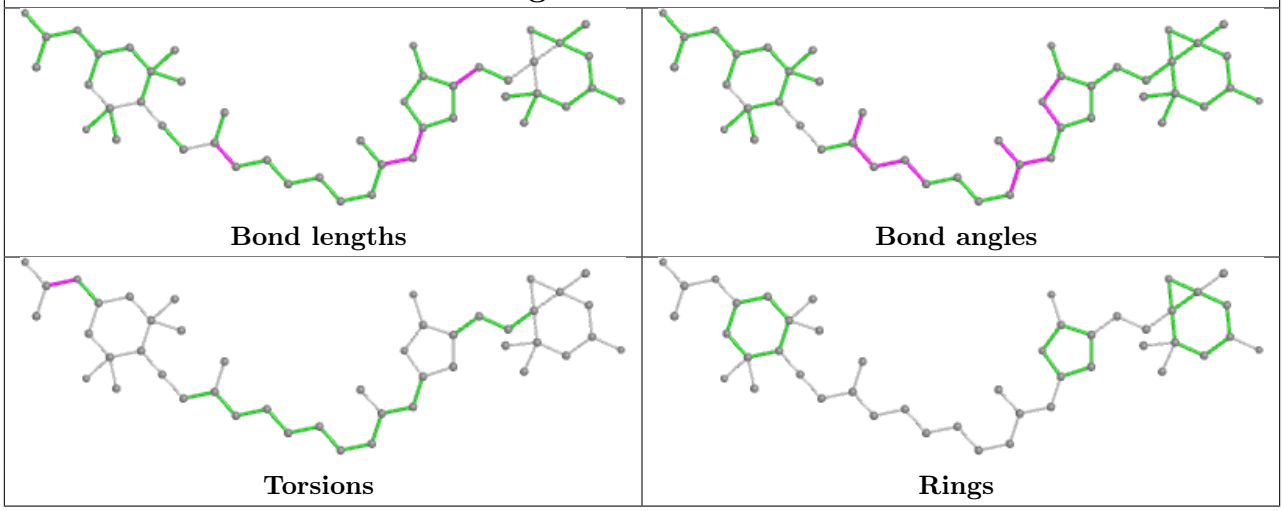


Torsions

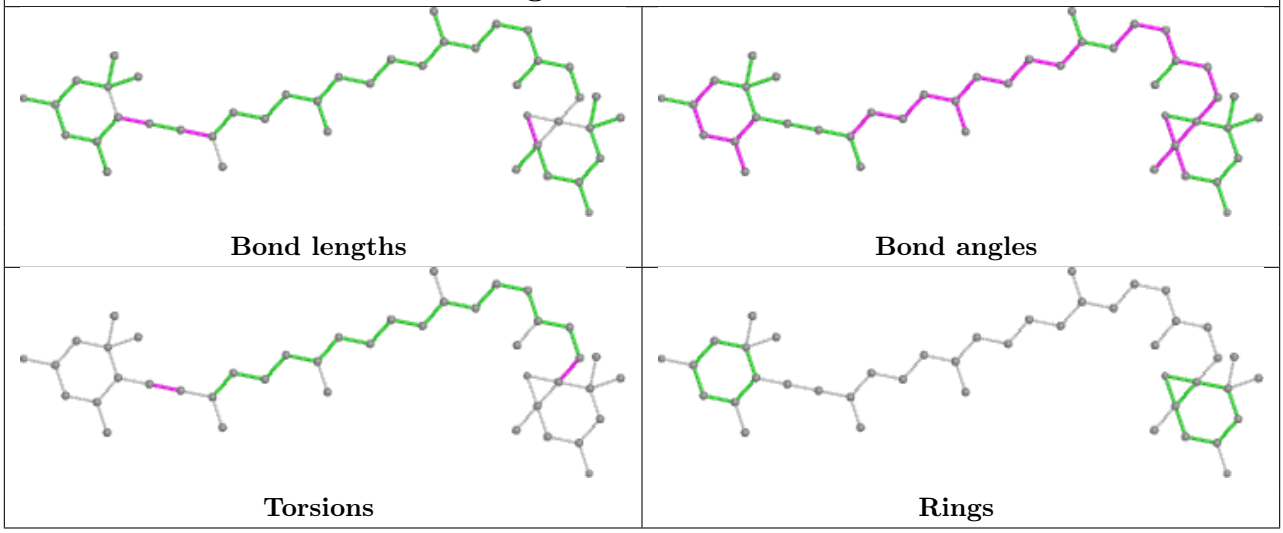


Rings

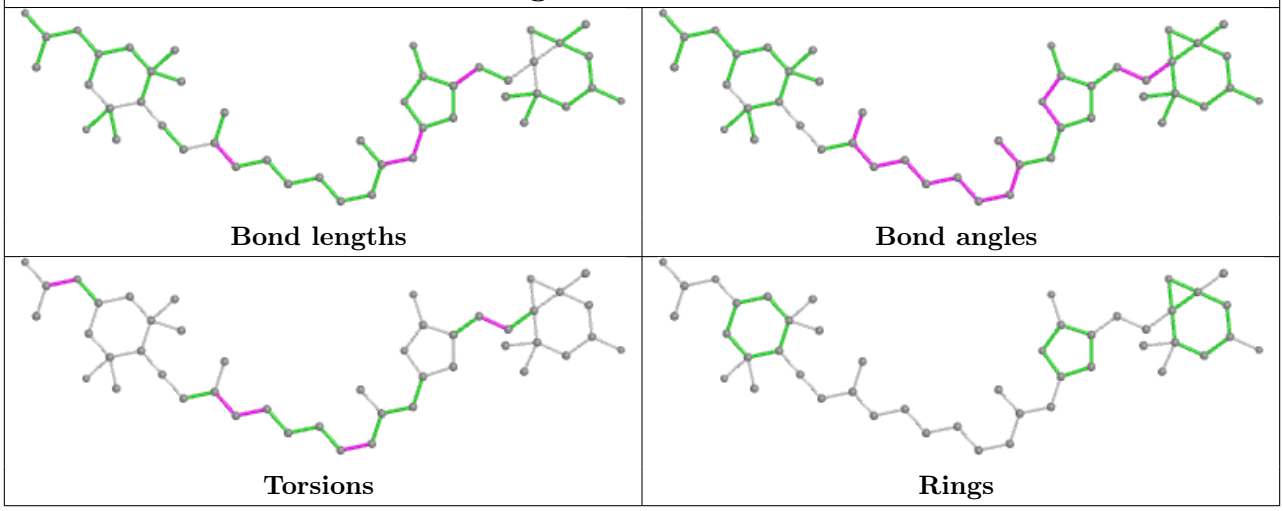
Ligand PID N 302



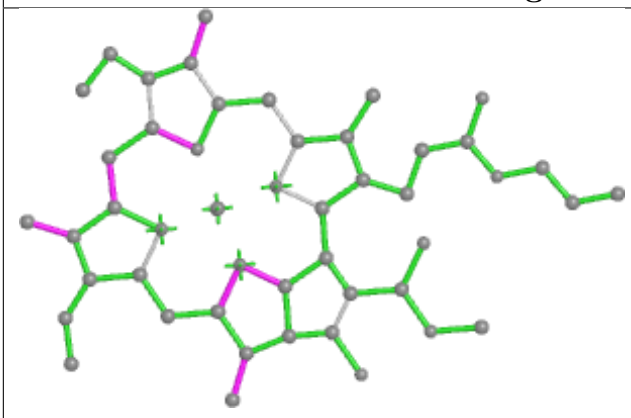
Ligand DD6 B 305



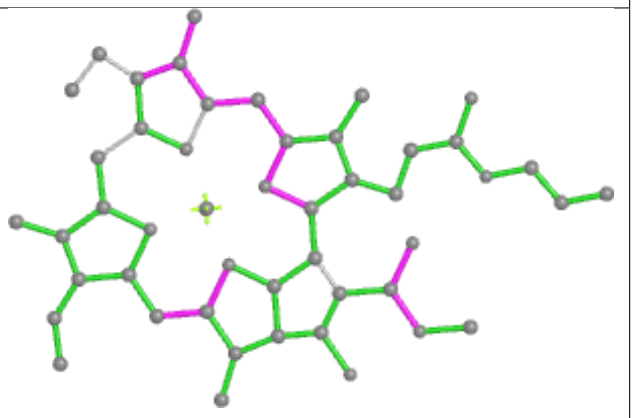
Ligand PID O 305



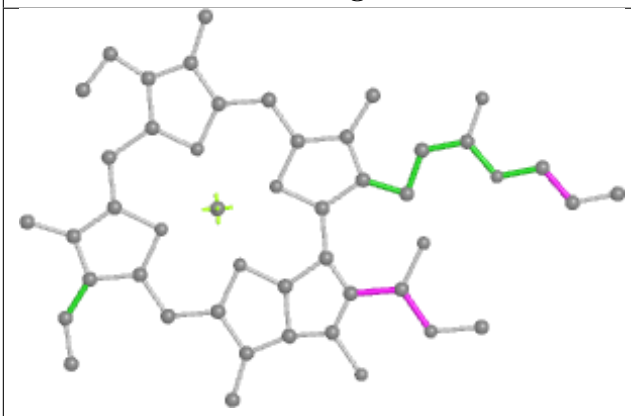
Ligand CLA E 314



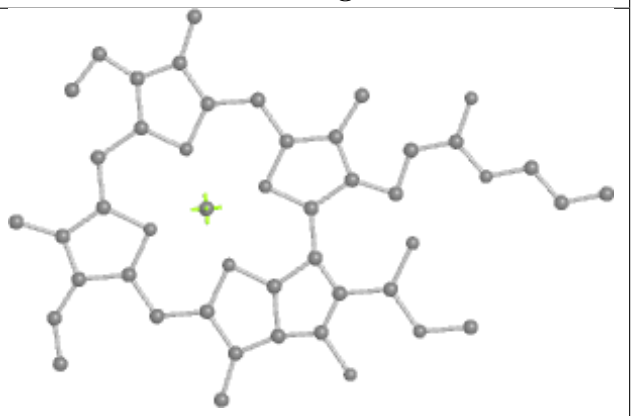
Bond lengths



Bond angles

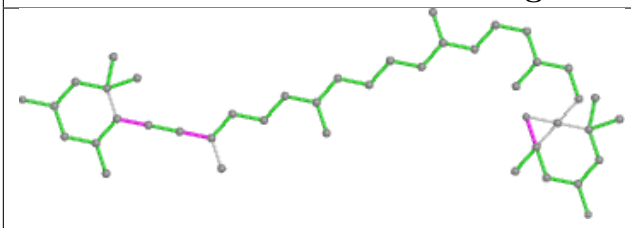


Torsions

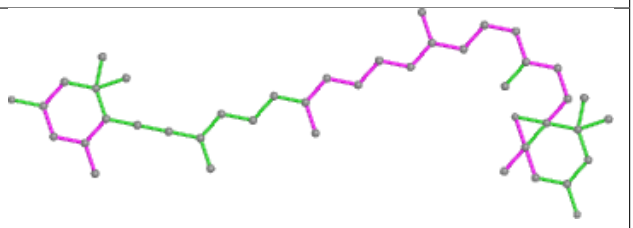


Rings

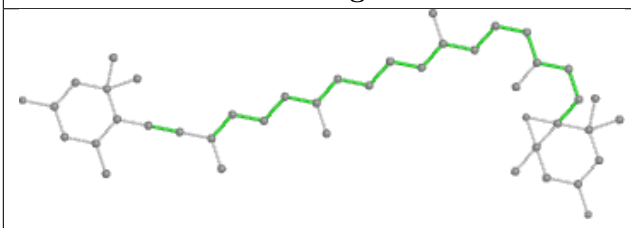
Ligand DD6 C 303



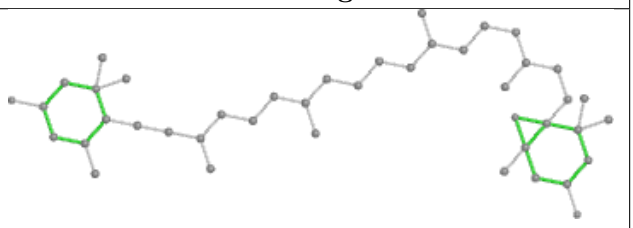
Bond lengths



Bond angles

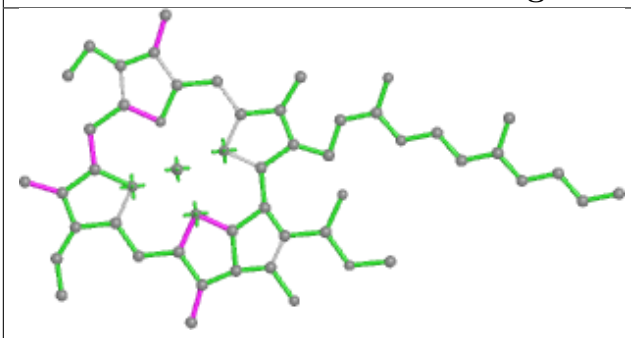


Torsions

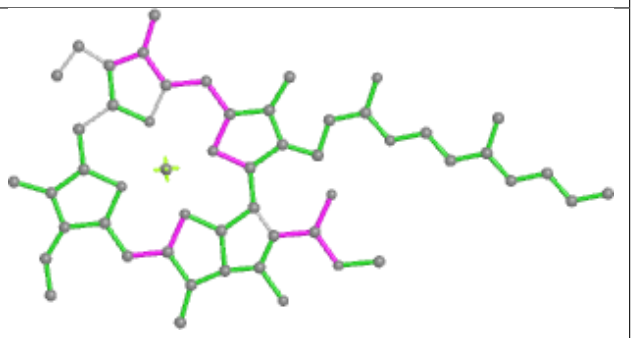


Rings

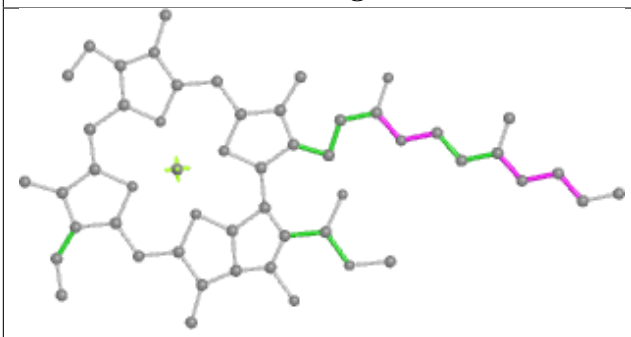
Ligand CLA b 716



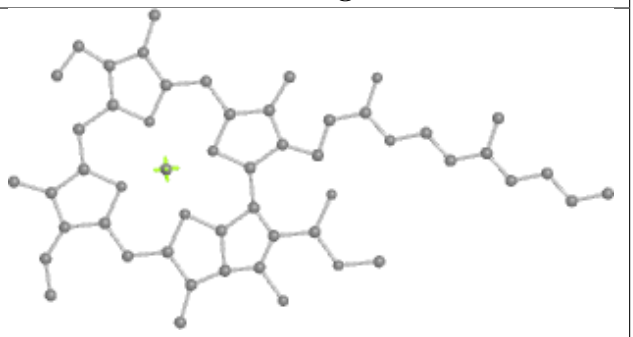
Bond lengths



Bond angles

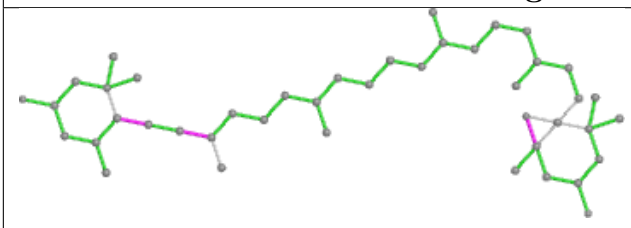


Torsions

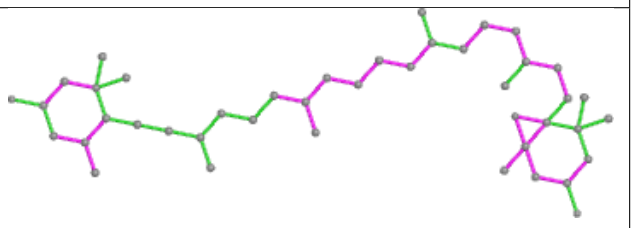


Rings

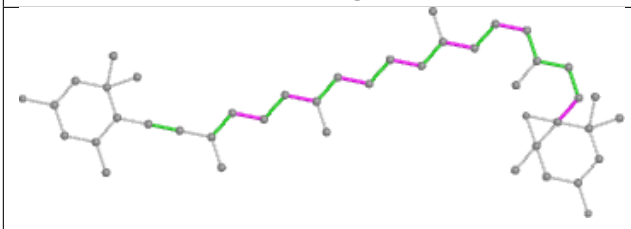
Ligand DD6 B 319



Bond lengths



Bond angles



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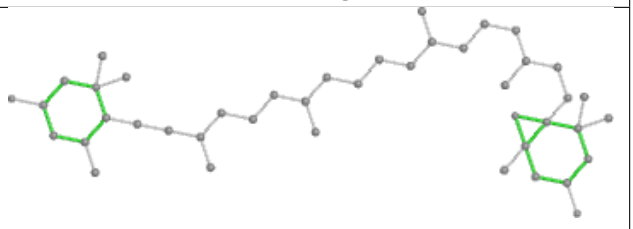
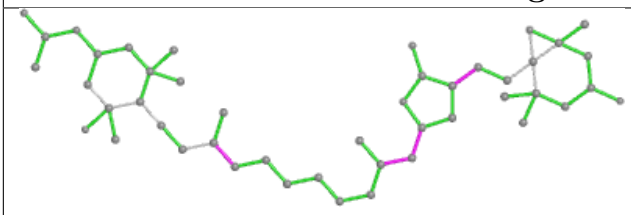
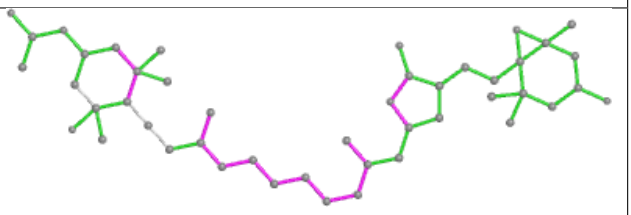
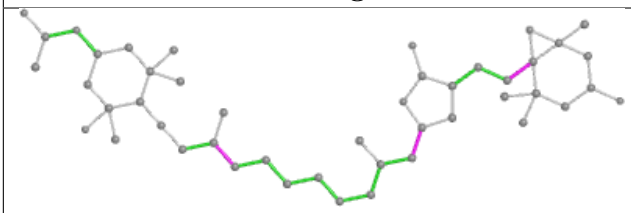
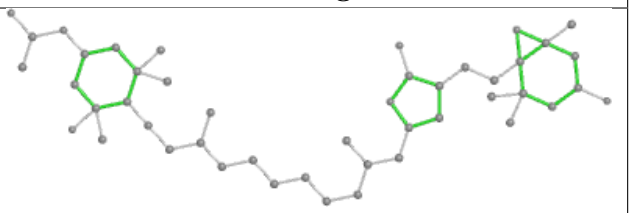
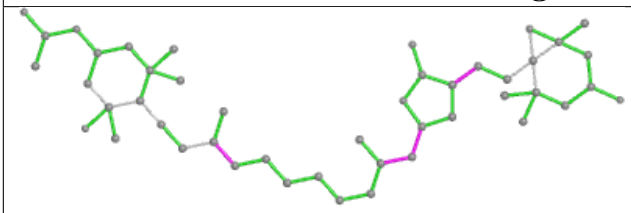
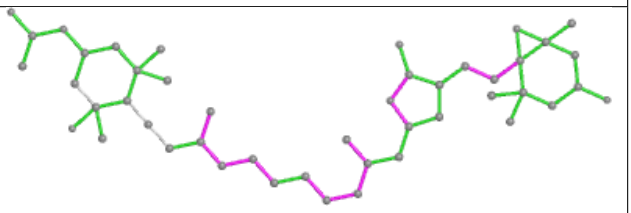
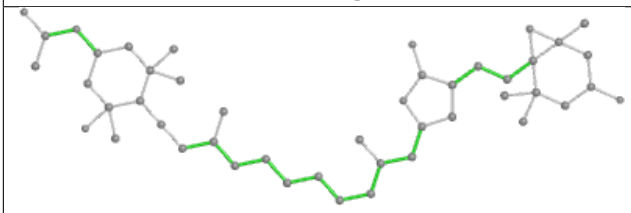
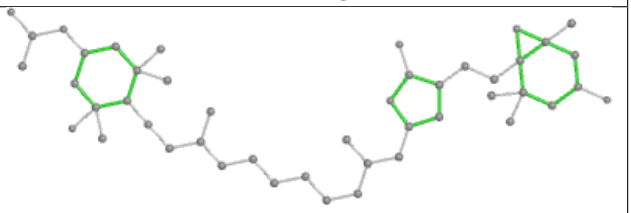
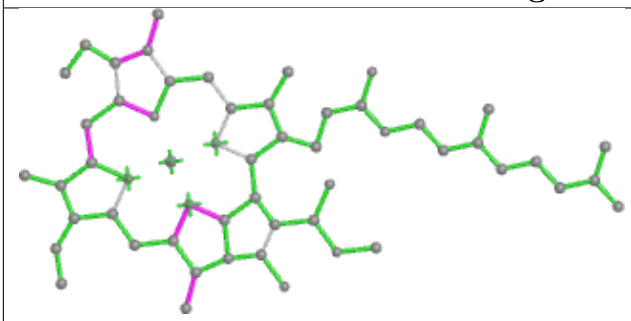


Rings

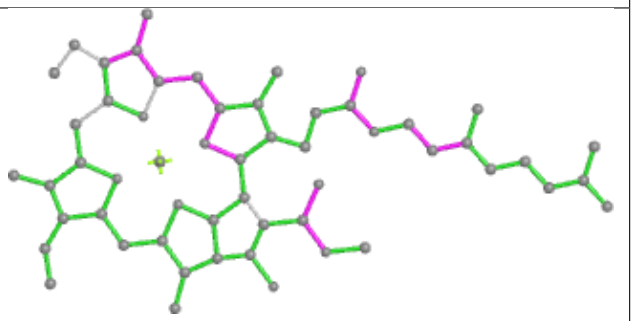
Ligand PID D 307	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand PID F 306	
 Bond lengths	 Bond angles
 Torsions	 Rings

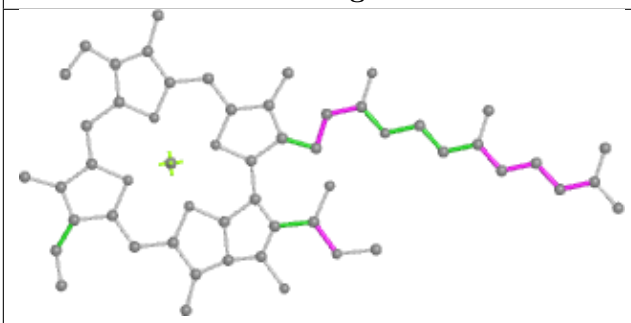
Ligand CLA a 810



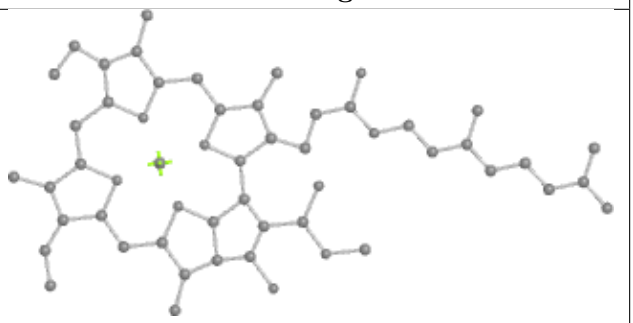
Bond lengths



Bond angles

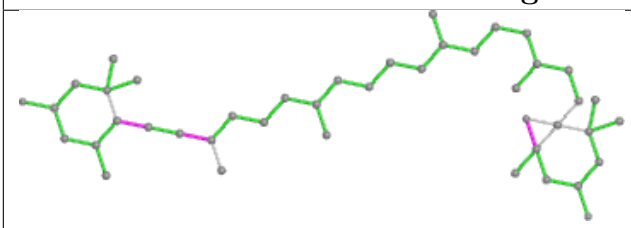


Torsions

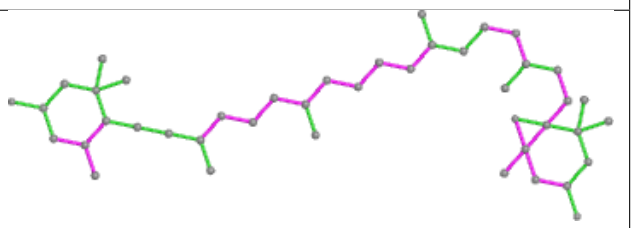


Rings

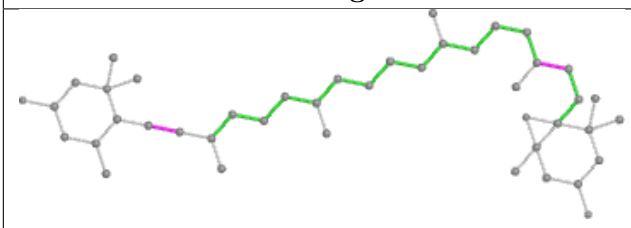
Ligand DD6 M 304



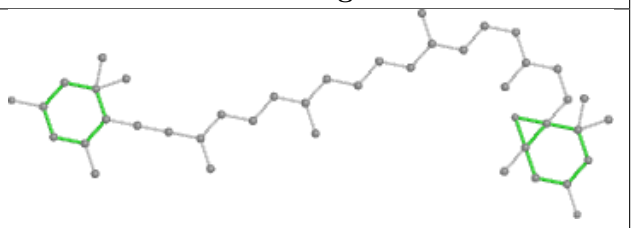
Bond lengths



Bond angles

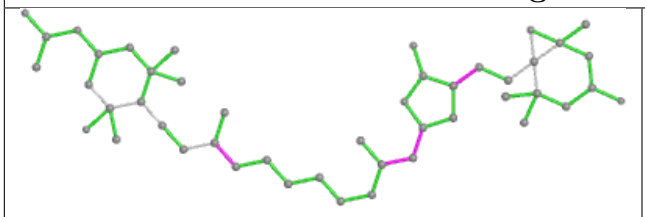


Torsions

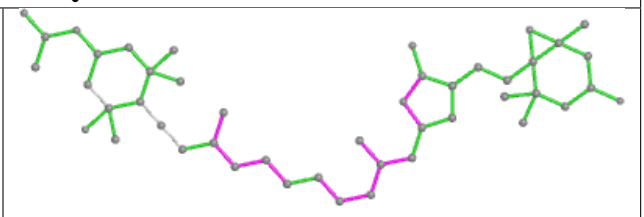


Rings

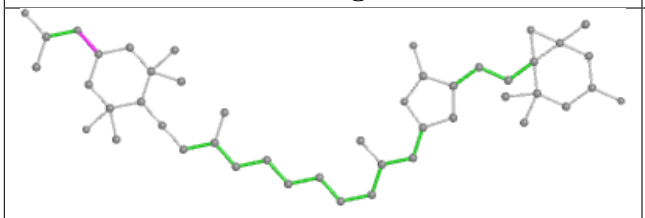
Ligand PID Q 301



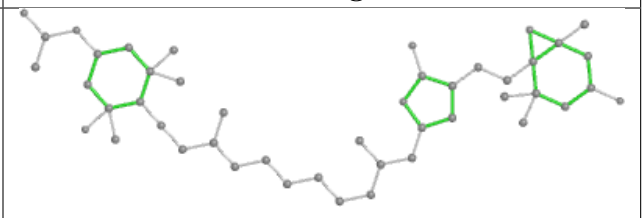
Bond lengths



Bond angles

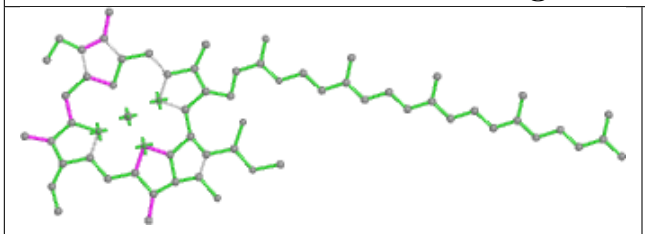


Torsions

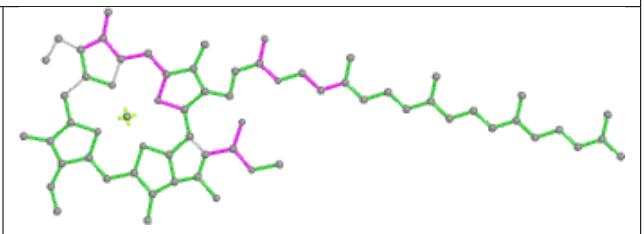


Rings

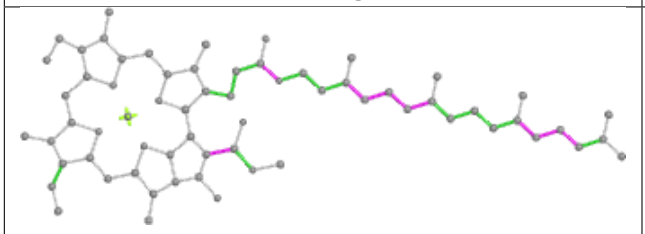
Ligand CLA a 825



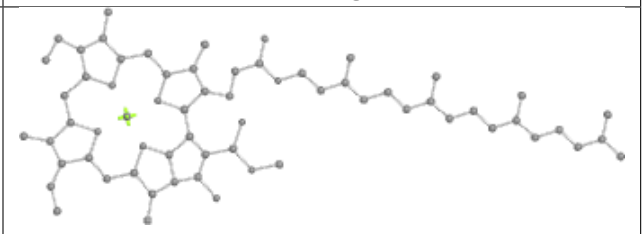
Bond lengths



Bond angles

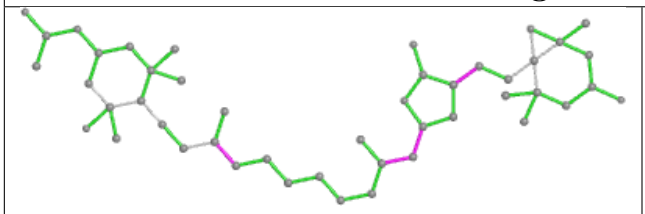


Torsions

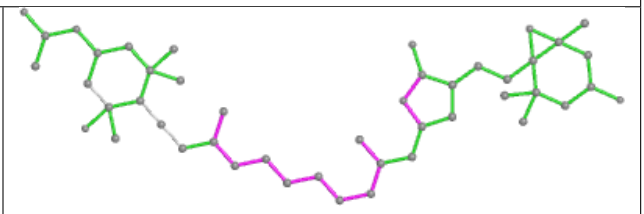


Rings

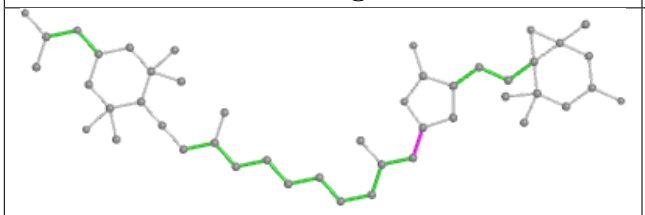
Ligand PID P 205



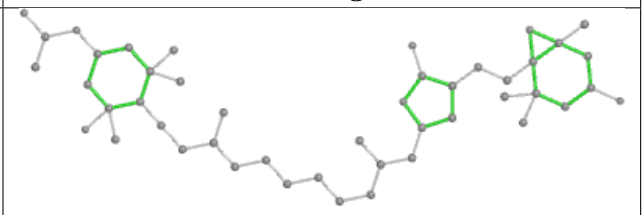
Bond lengths



Bond angles

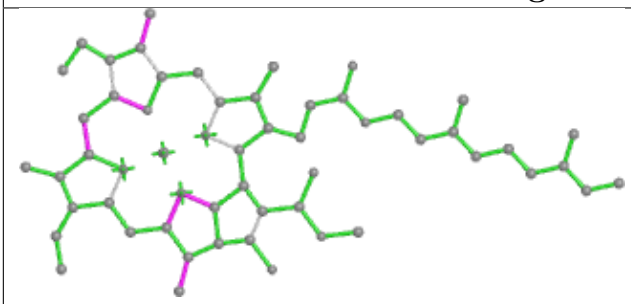


Torsions

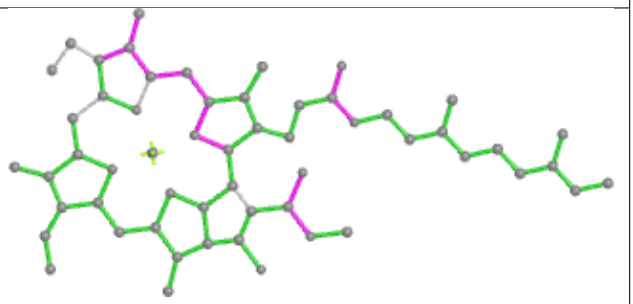


Rings

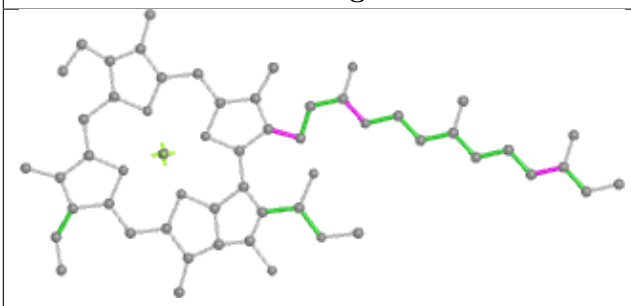
Ligand CLA a 811



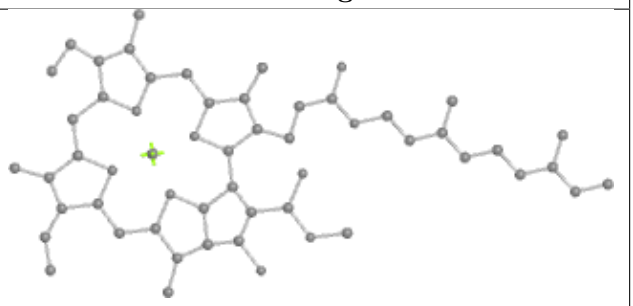
Bond lengths



Bond angles

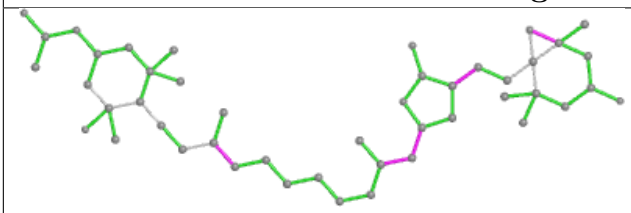


Torsions

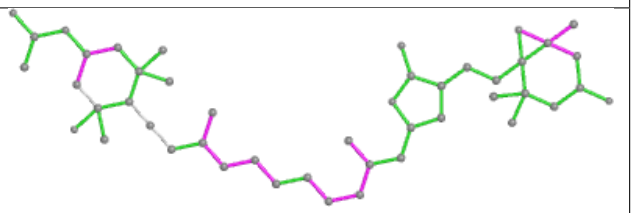


Rings

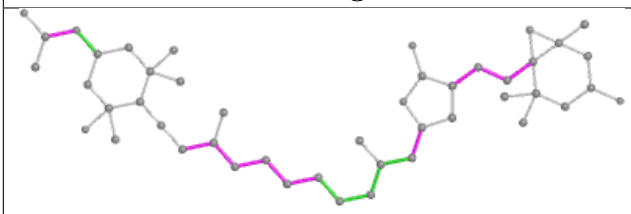
Ligand PID F 304



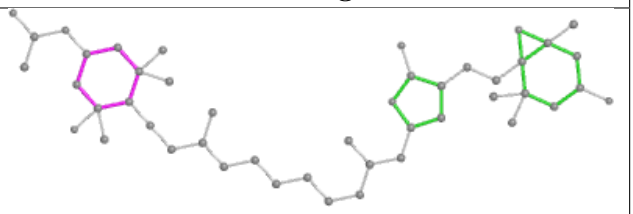
Bond lengths



Bond angles

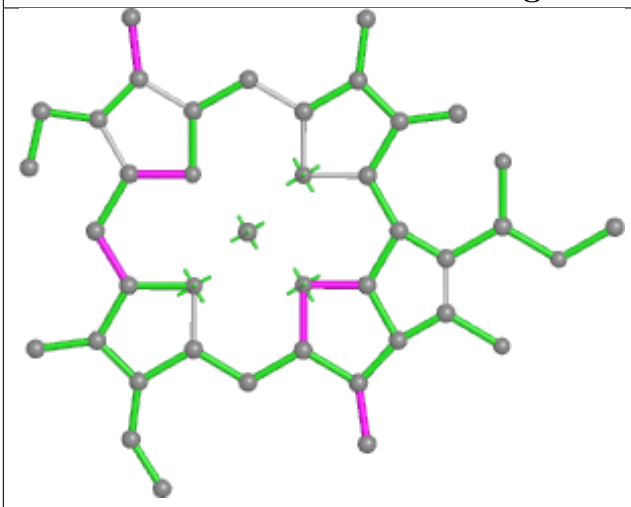


Torsions

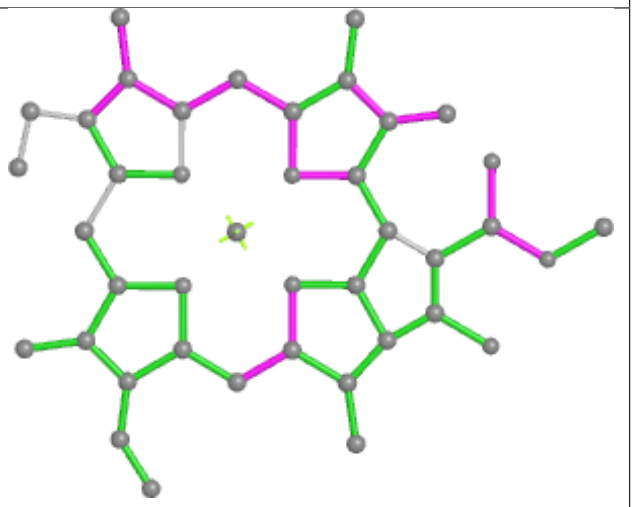


Rings

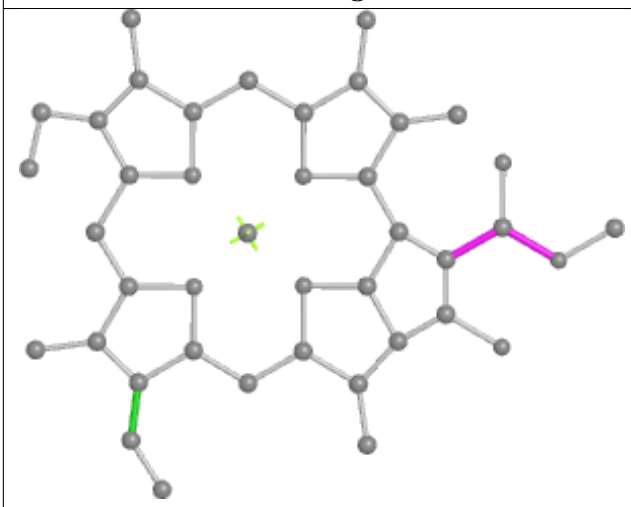
Ligand CLA H 315



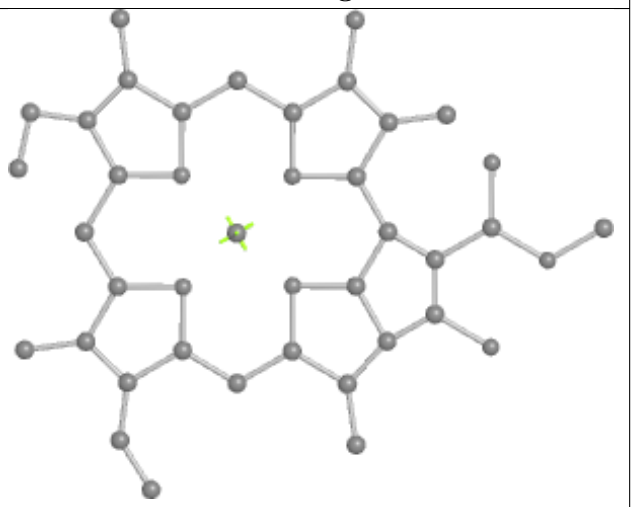
Bond lengths



Bond angles

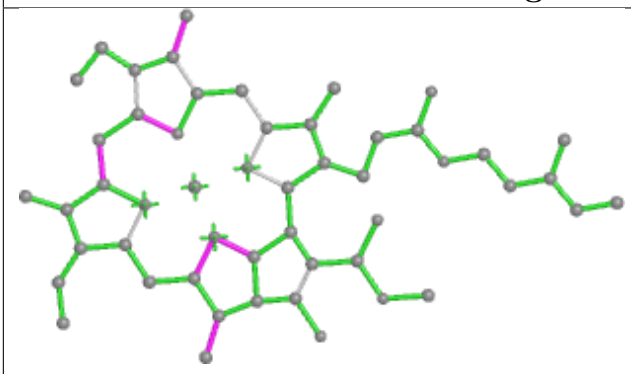


Torsions

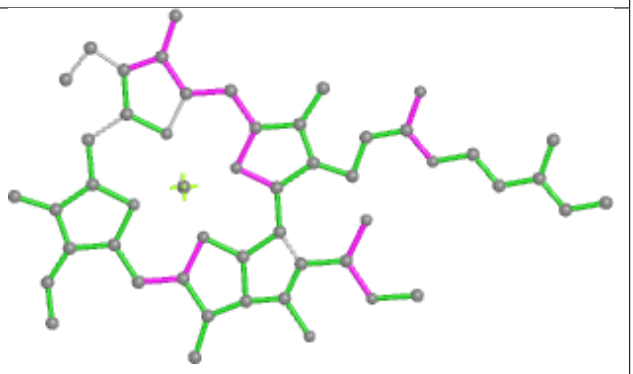


Rings

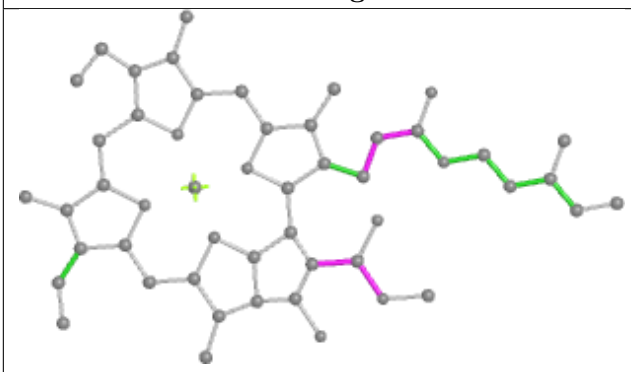
Ligand CLA P 212



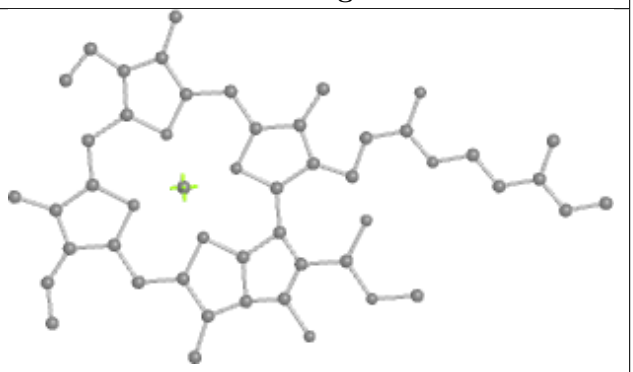
Bond lengths



Bond angles

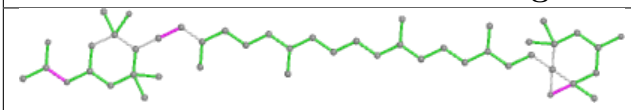


Torsions

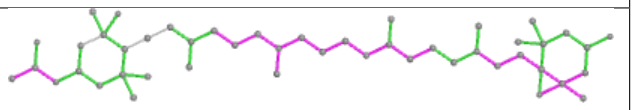


Rings

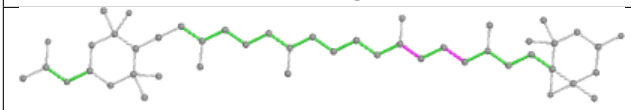
Ligand UIX J 304



Bond lengths



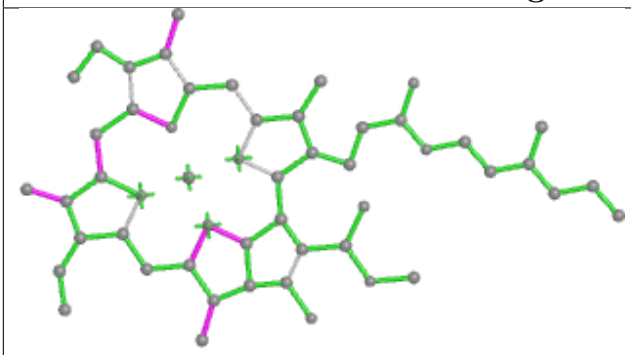
Bond angles



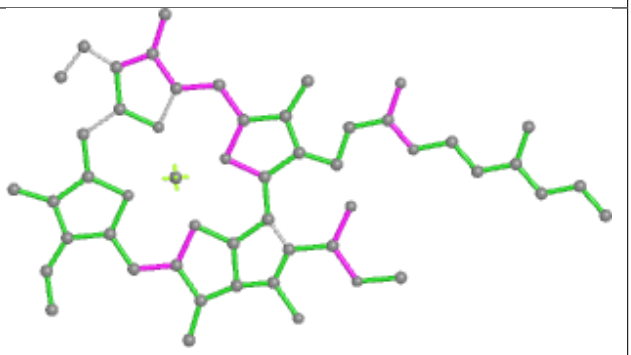
Torsions

Rings

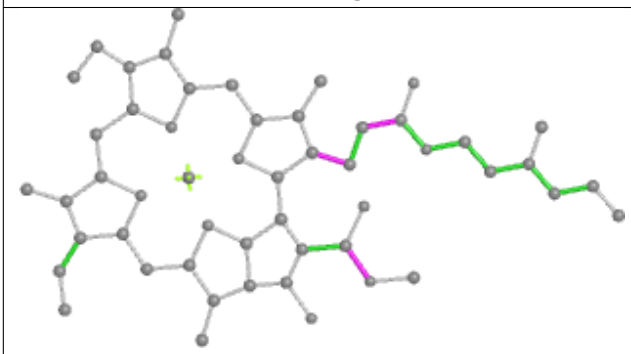
Ligand CLA b 708



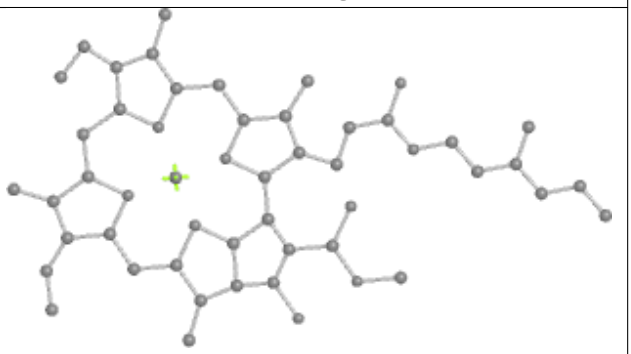
Bond lengths



Bond angles

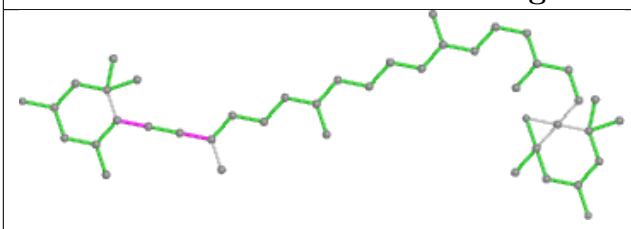


Torsions

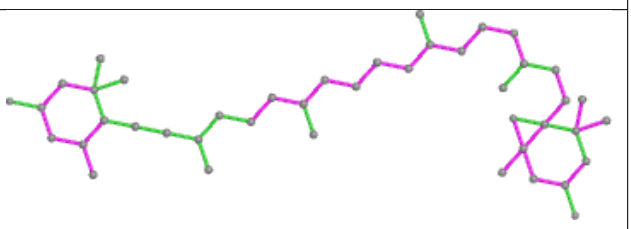


Rings

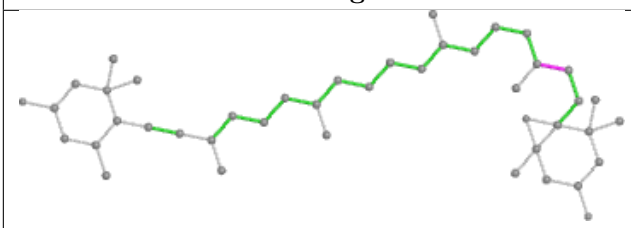
Ligand DD6 J 302



Bond lengths



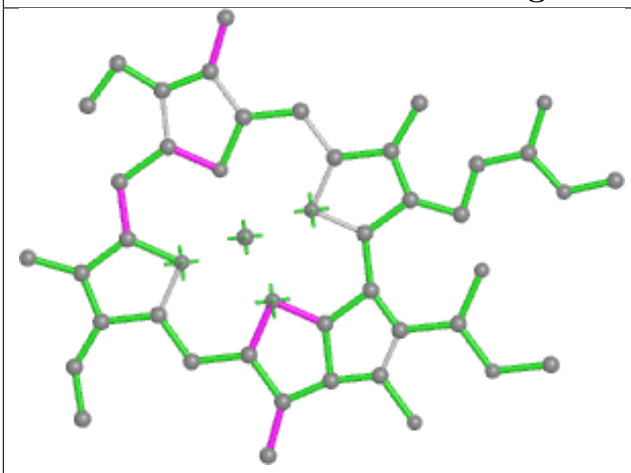
Bond angles



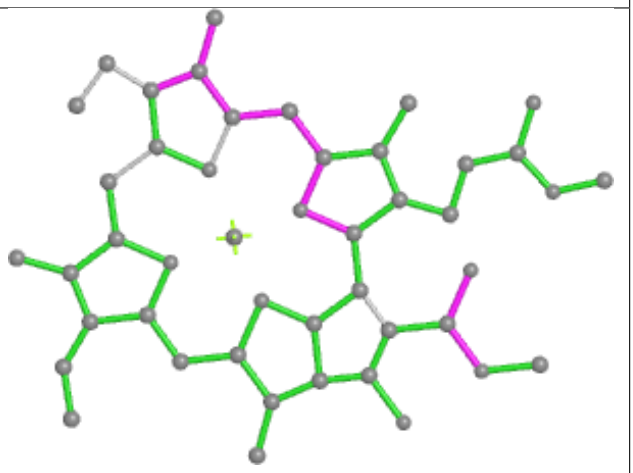
Torsions

Rings

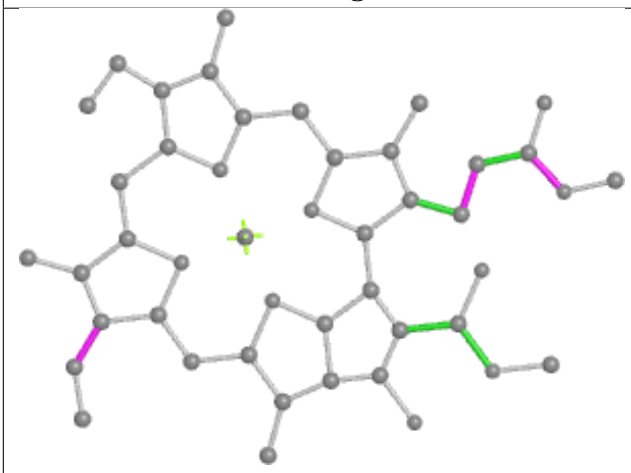
Ligand CLA J 309



Bond lengths



Bond angles



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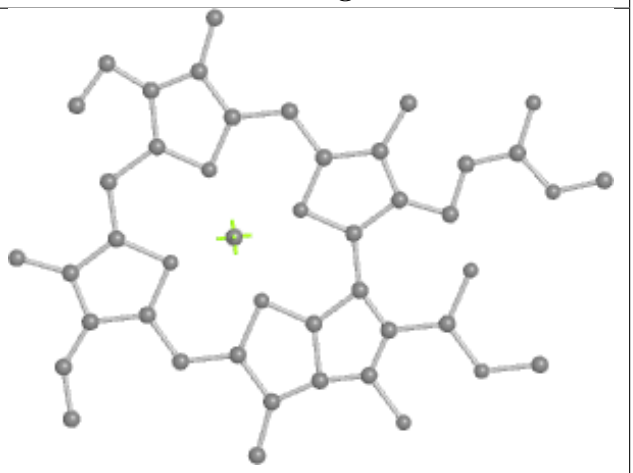
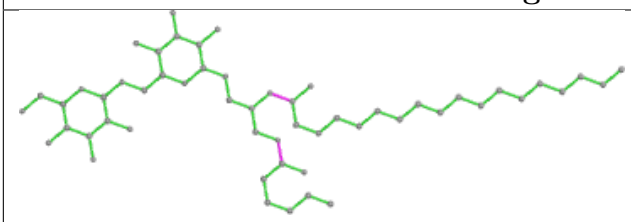
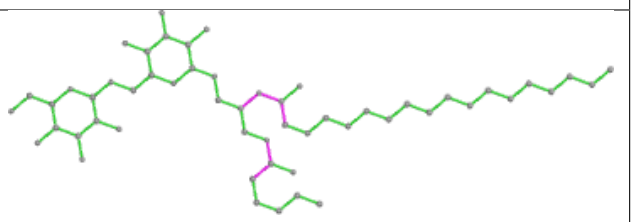


Rings

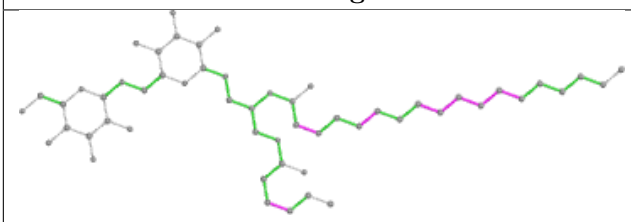
Ligand DGD h 203



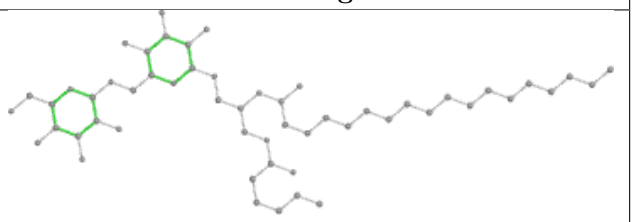
Bond lengths



Bond angles

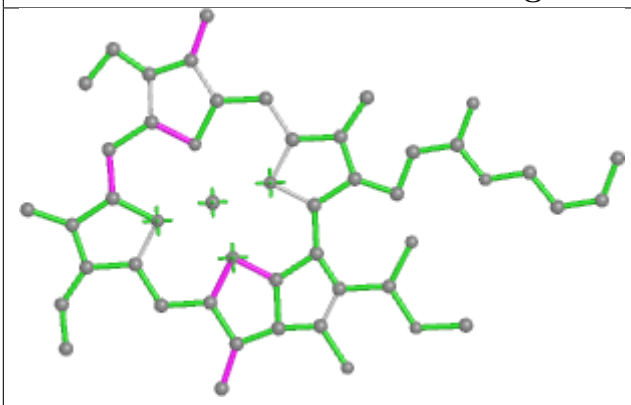


Torsions



Rings

Ligand CLA B 306



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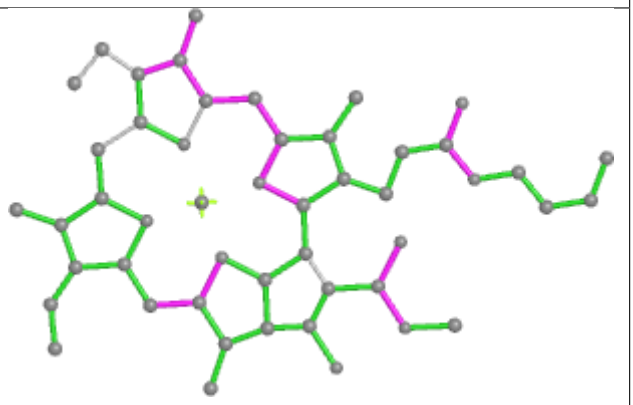
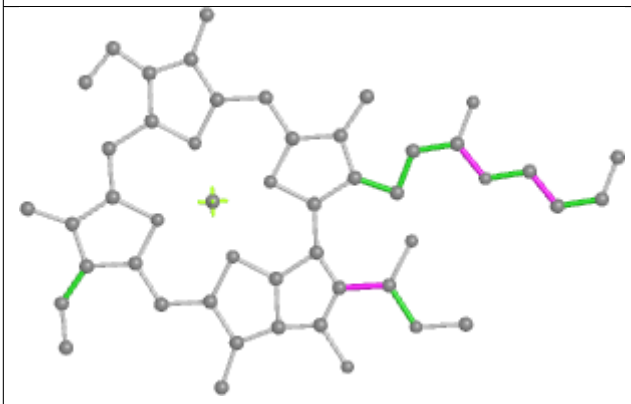
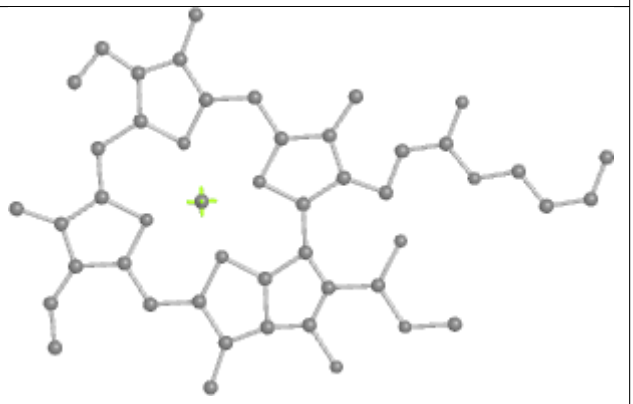


Bond angles

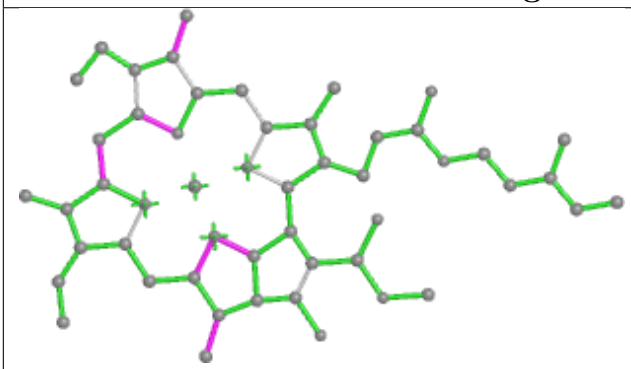


Torsions

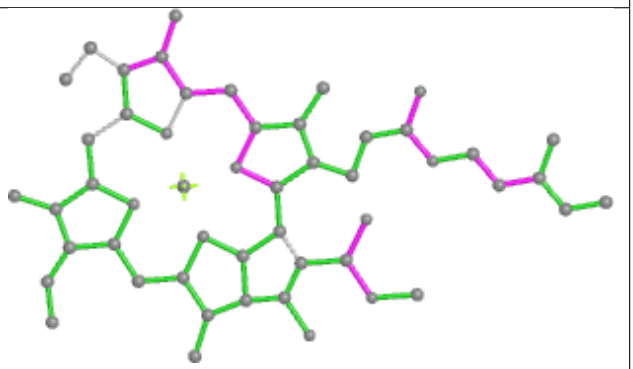


Rings

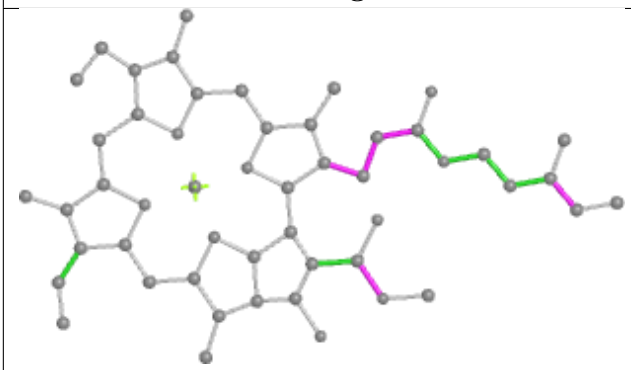
Ligand CLA H 310



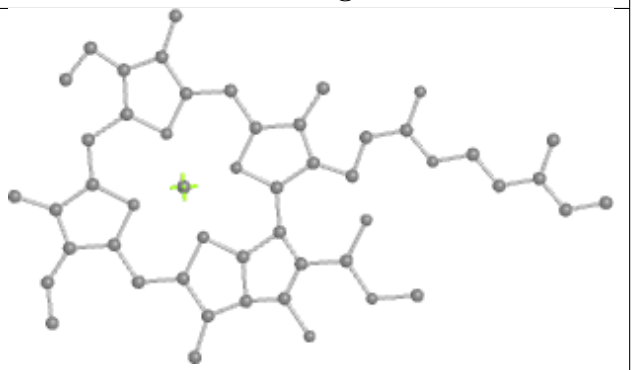
Bond lengths



Bond angles

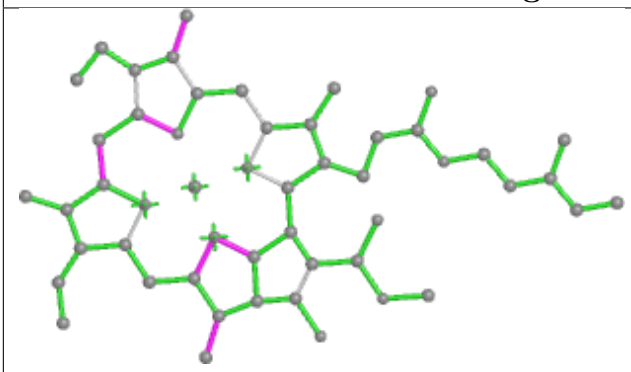


Torsions

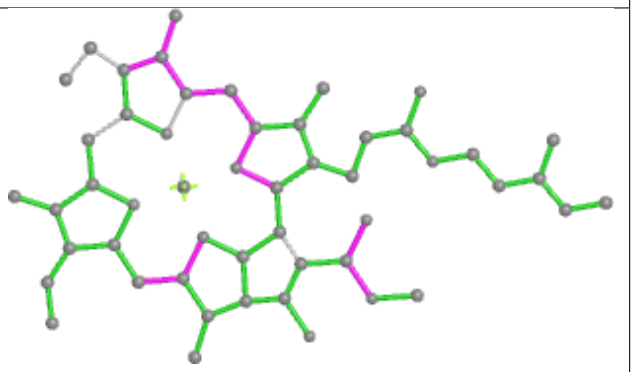


Rings

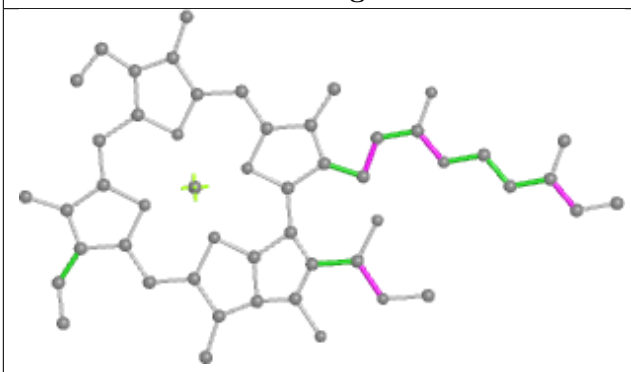
Ligand CLA G 311



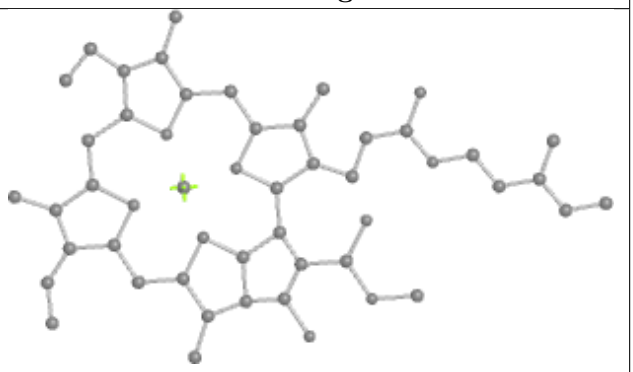
Bond lengths



Bond angles

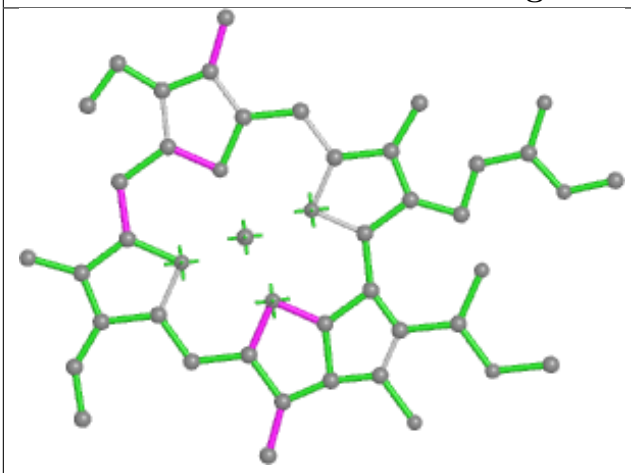


Torsions

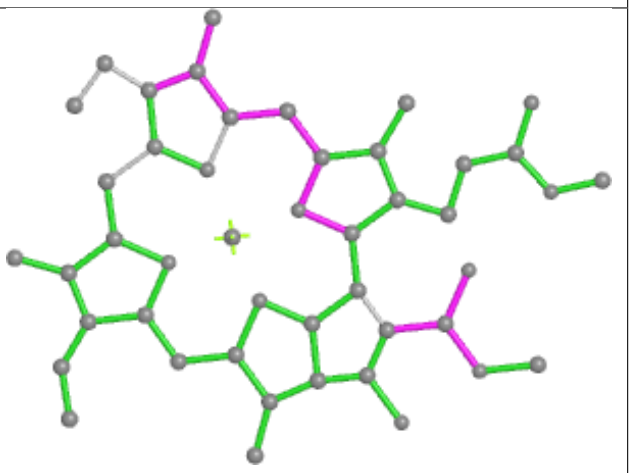


Rings

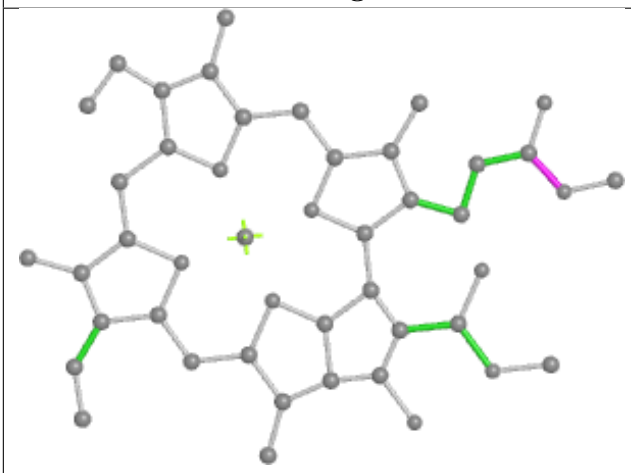
Ligand CLA F 307



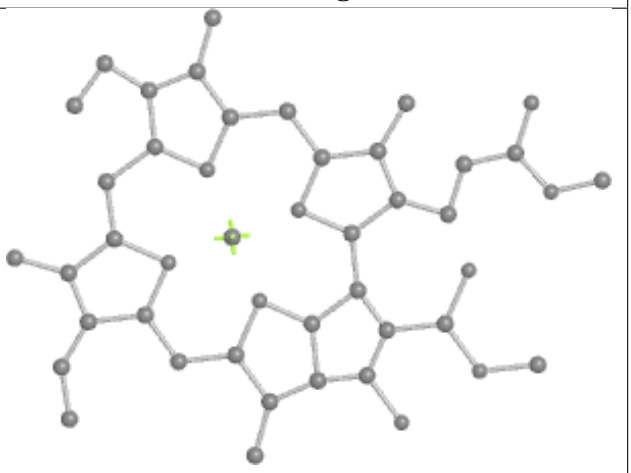
Bond lengths



Bond angles

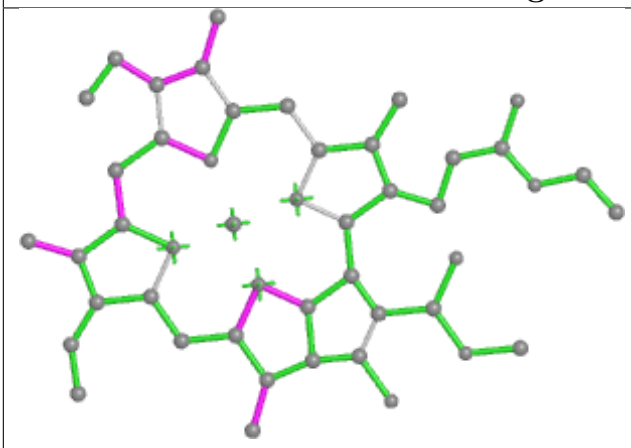


Torsions



Rings

Ligand CLA b 724



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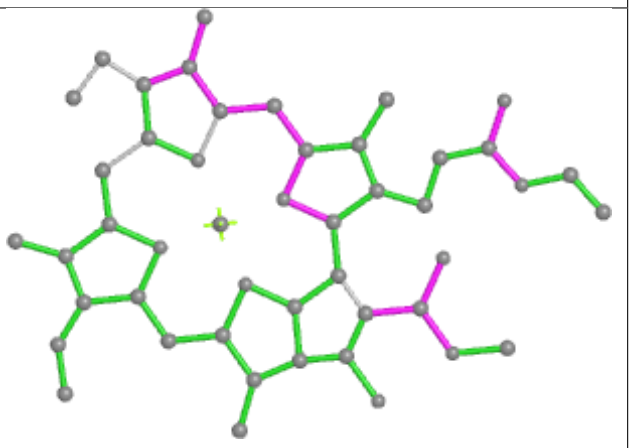
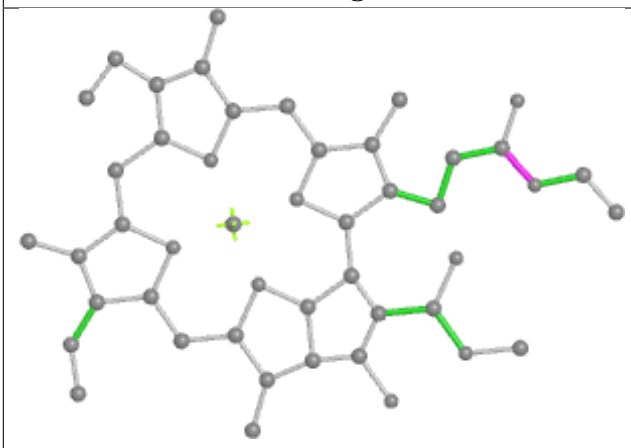
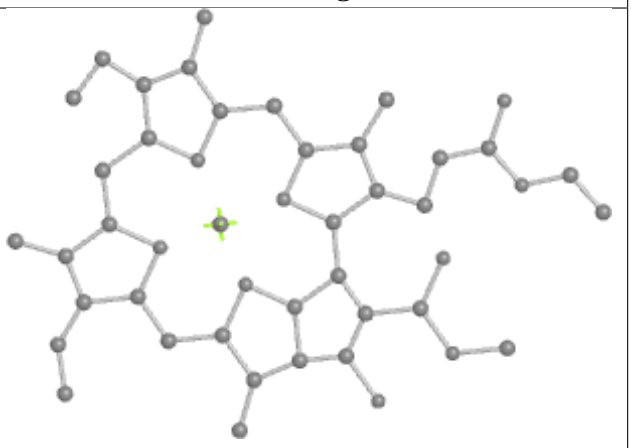


Bond angles

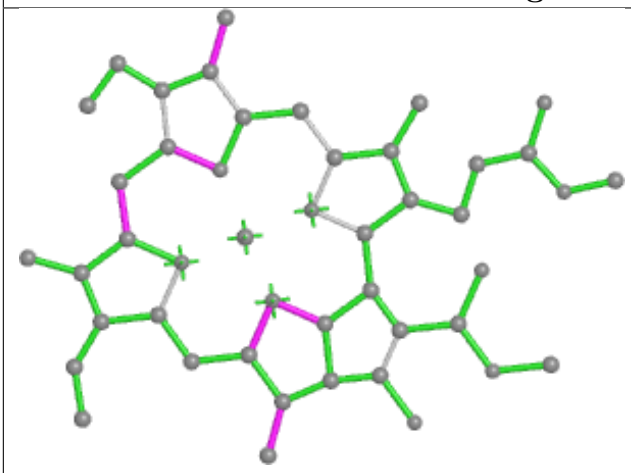


Torsions

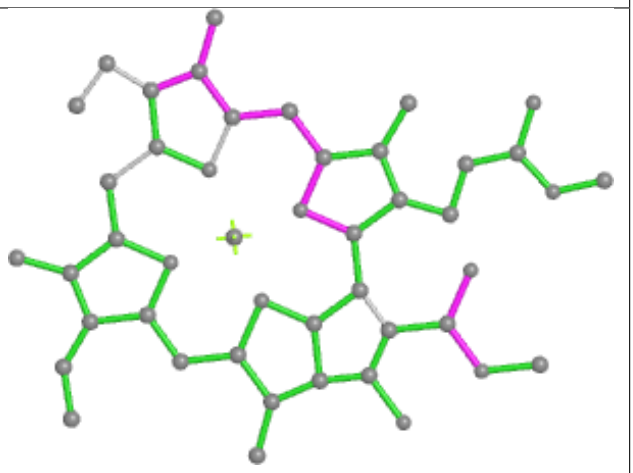


Rings

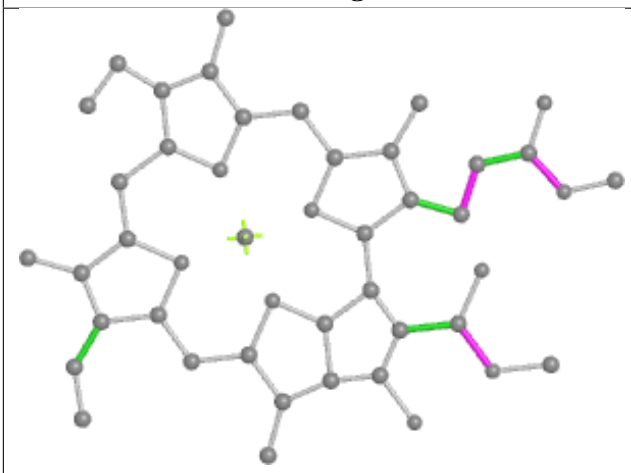
Ligand CLA L 317



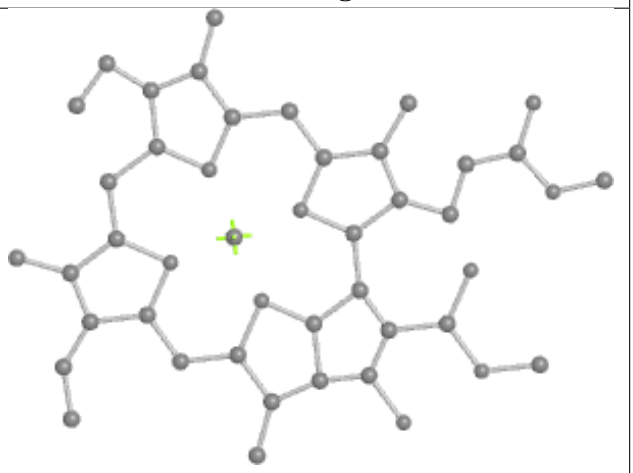
Bond lengths



Bond angles

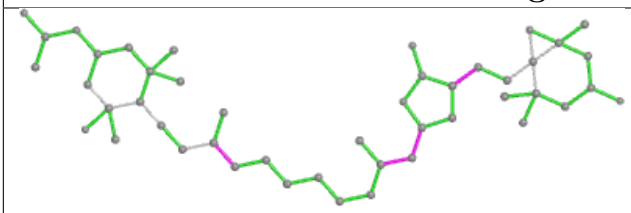


Torsions

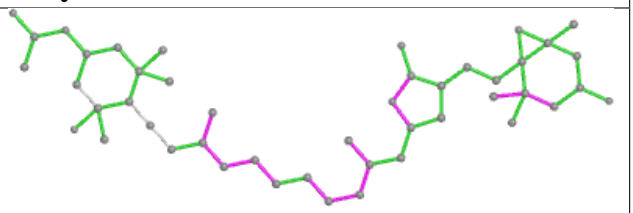


Rings

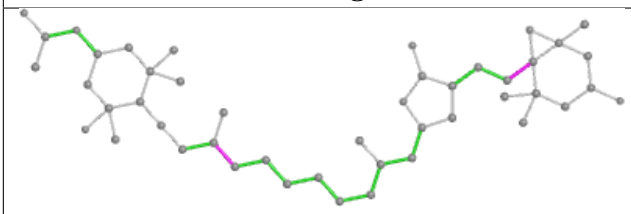
Ligand PID Q 306



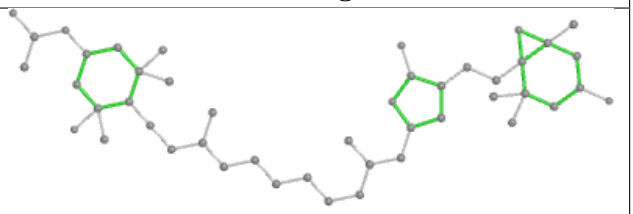
Bond lengths



Bond angles

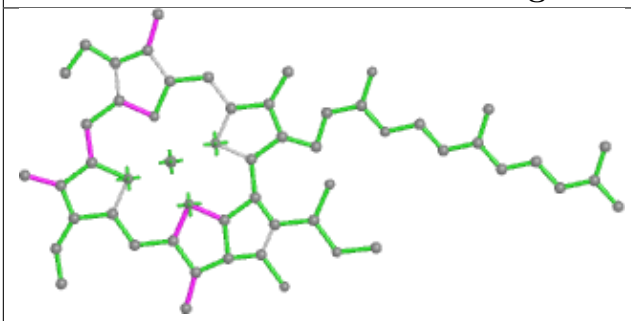


Torsions

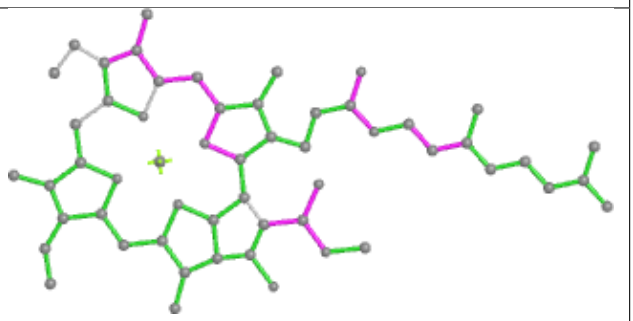


Rings

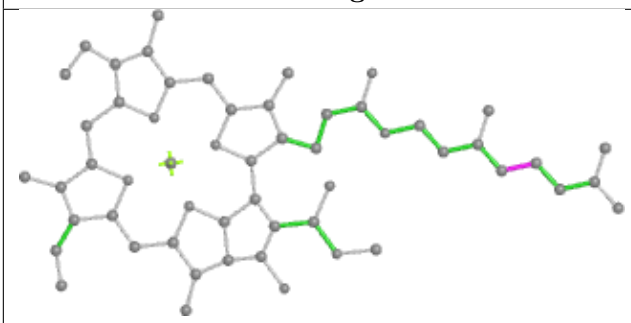
Ligand CLA a 804



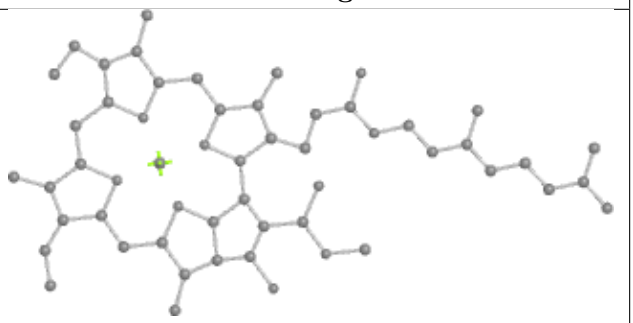
Bond lengths



Bond angles

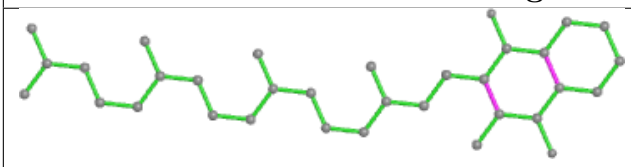


Torsions

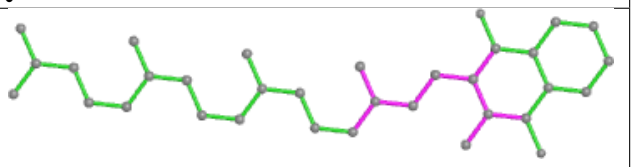


Rings

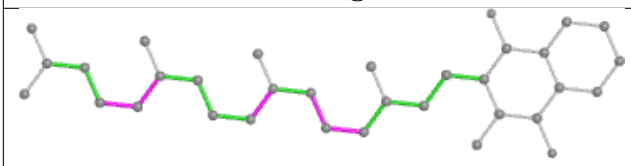
Ligand PQN a 832



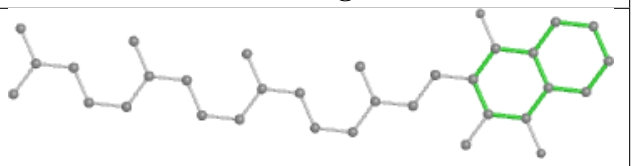
Bond lengths



Bond angles

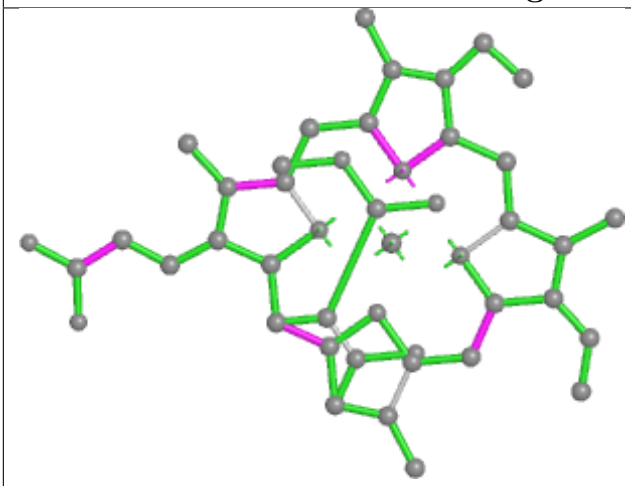


Torsions



Rings

Ligand KC1 B 313



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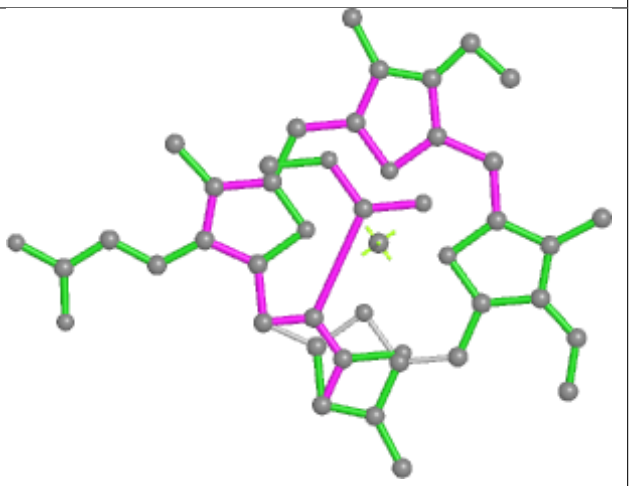

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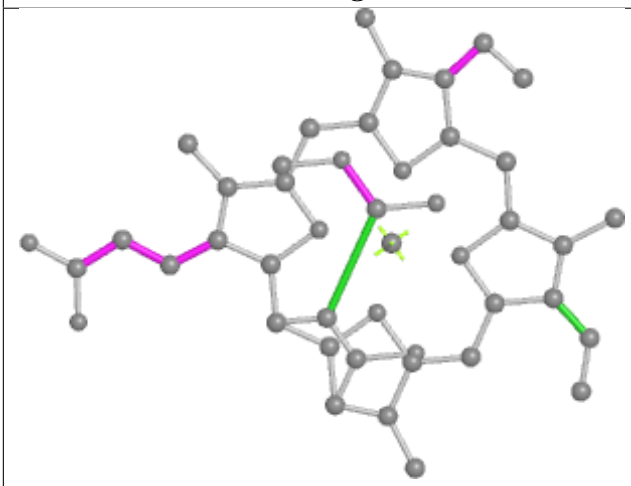

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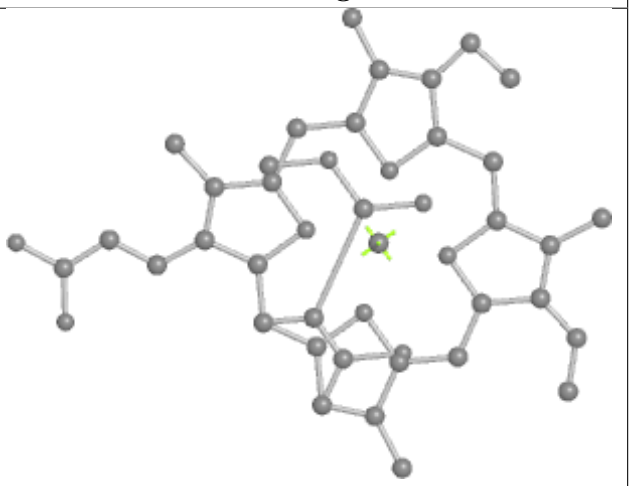
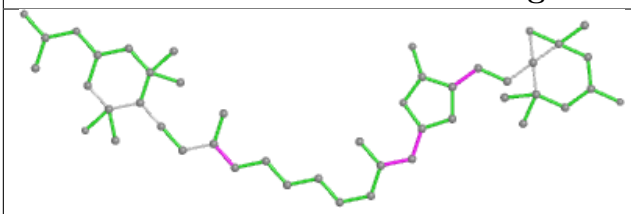


Rings

Ligand PID G 310



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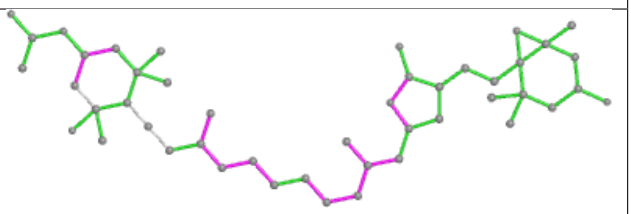

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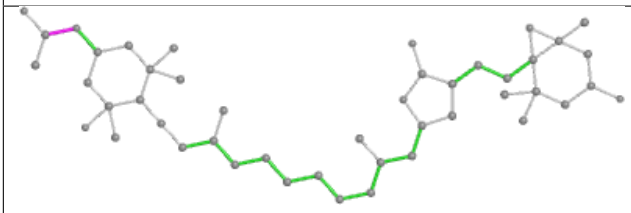

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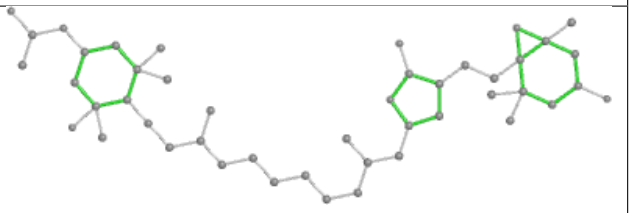
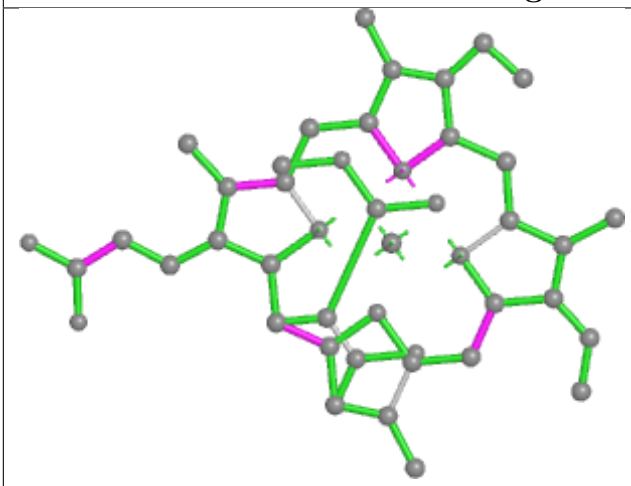


Rings

Ligand KC1 N 310



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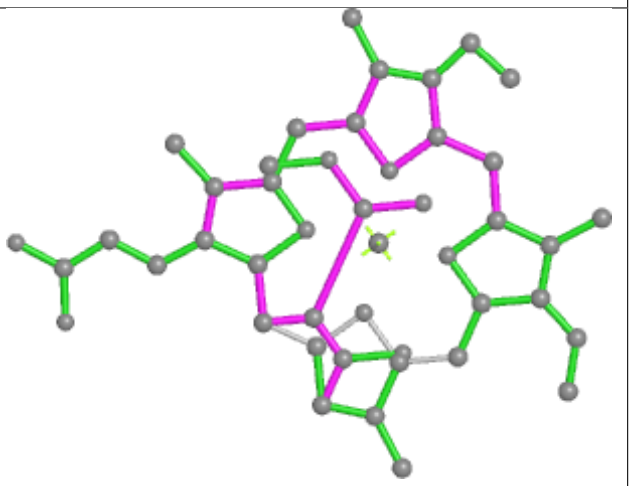

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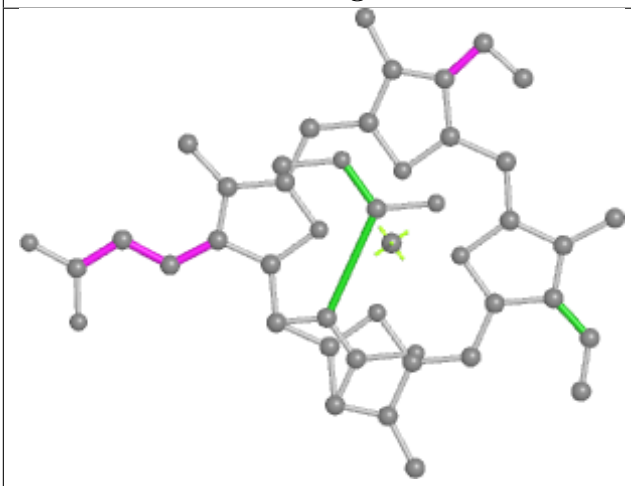

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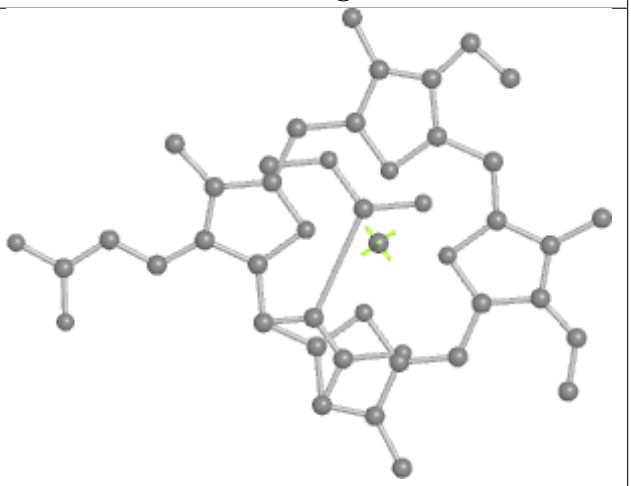
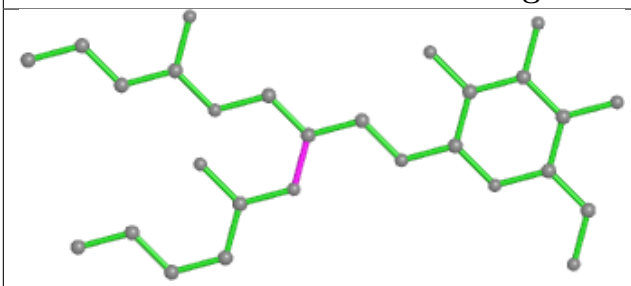
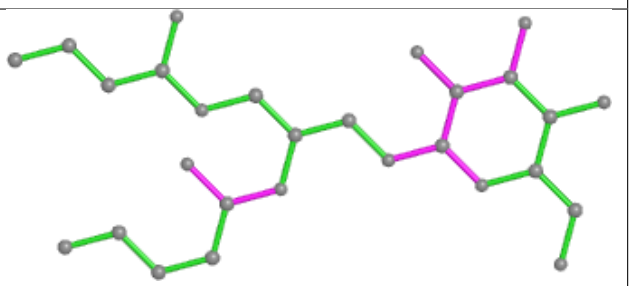


Rings

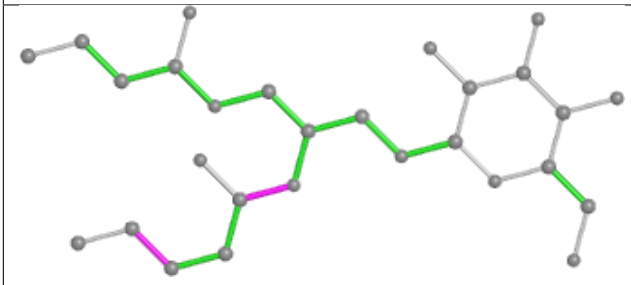
Ligand LMG h 205



Bond lengths



Bond angles



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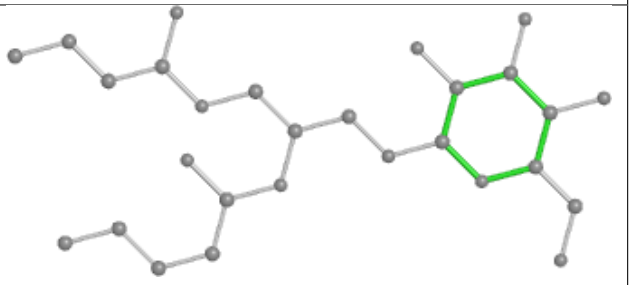
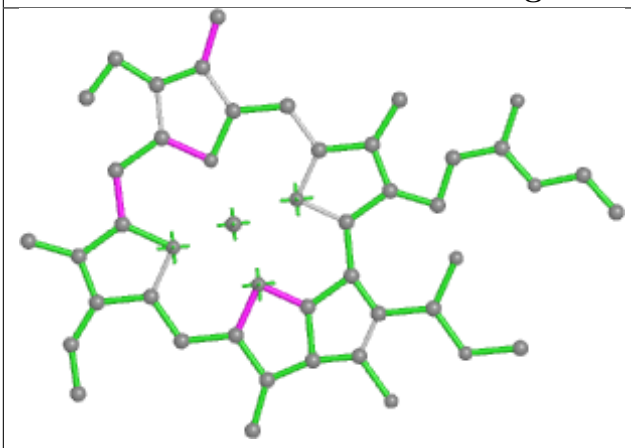


Rings

Ligand CLA T 314



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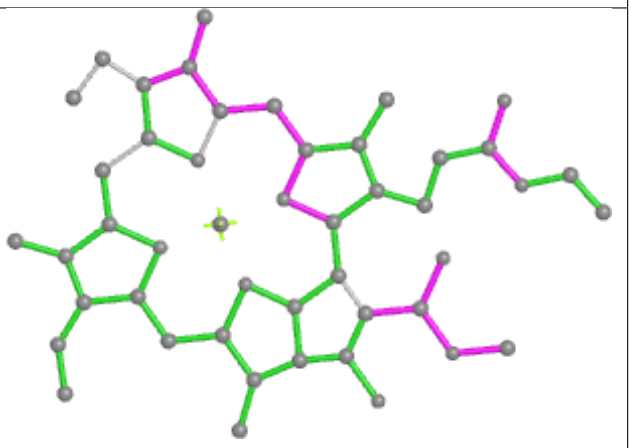

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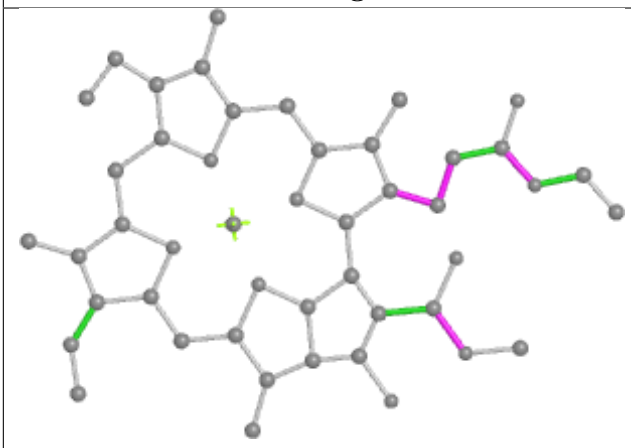

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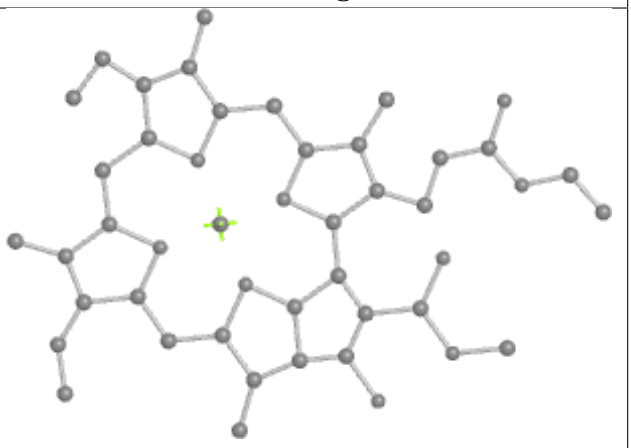
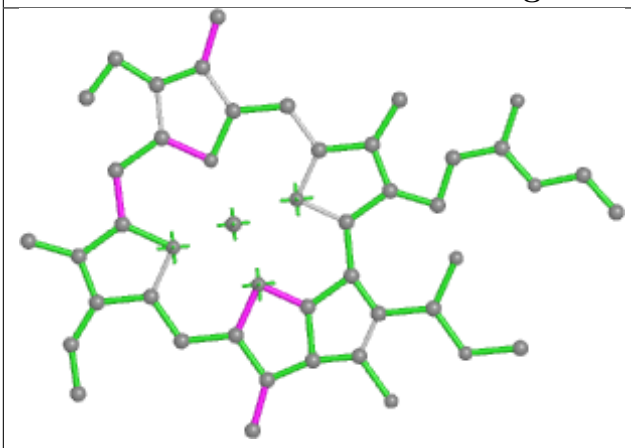


Rings

Ligand CLA D 308



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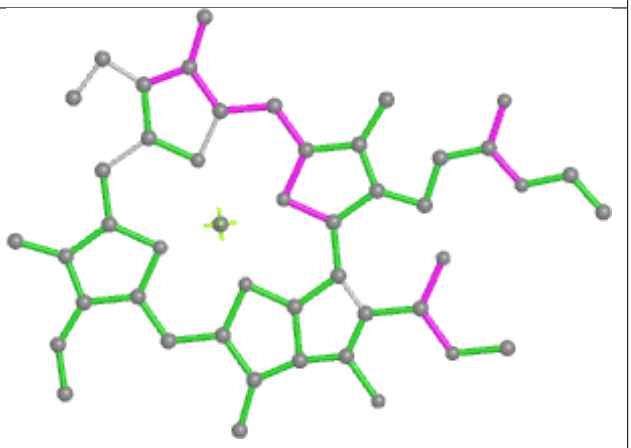

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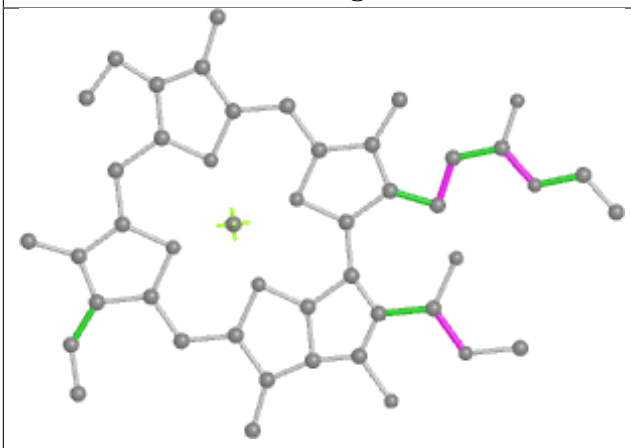

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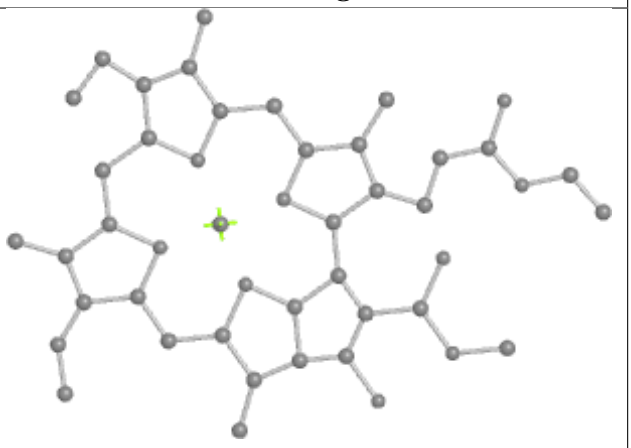
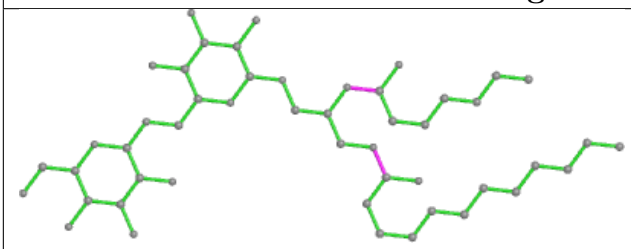


Rings

Ligand DGD j 106



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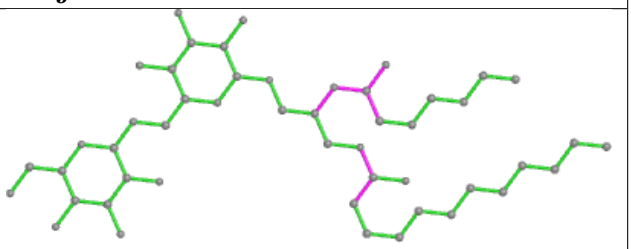
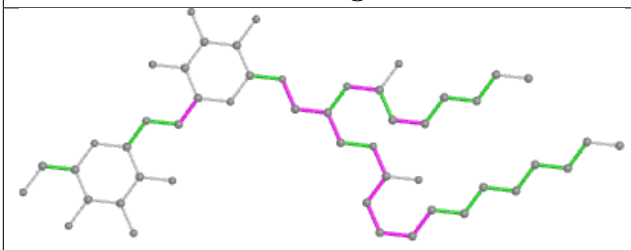


Bond angles



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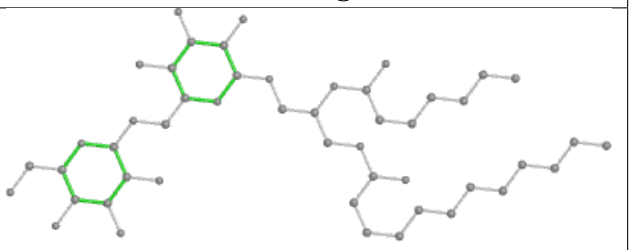
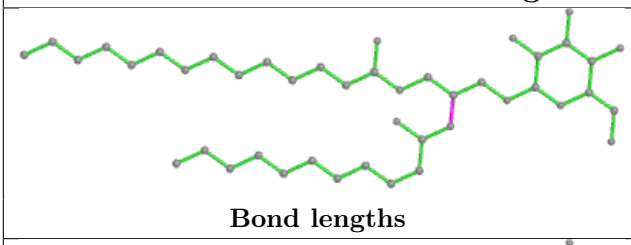


Rings

Ligand LMG b 732



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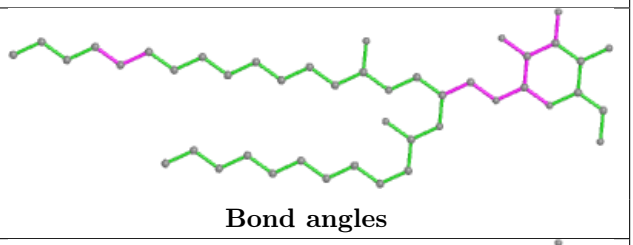
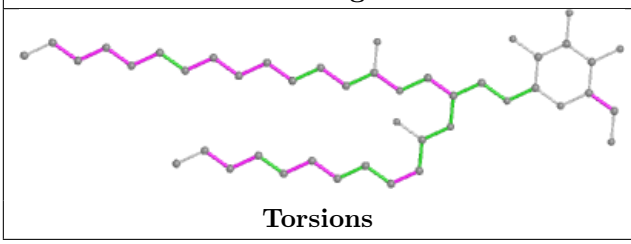


Bond angles



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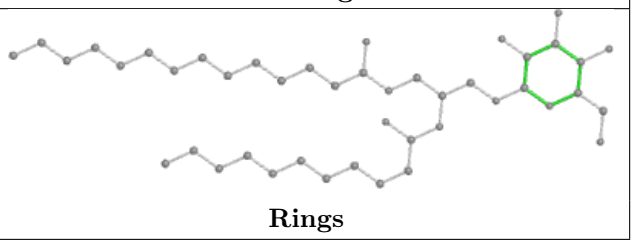
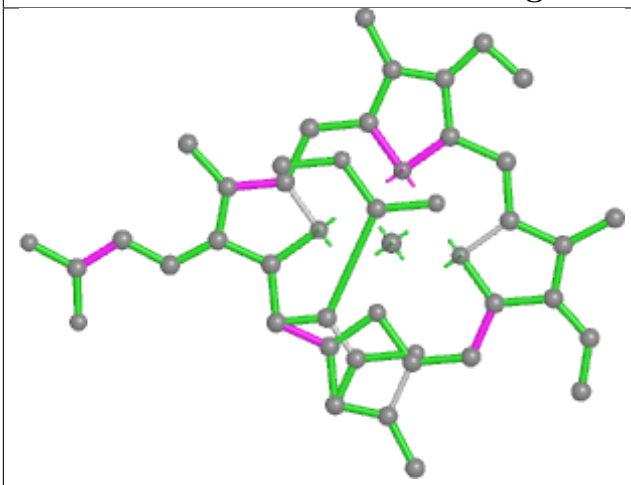


Rings

Ligand KC1 Q 314



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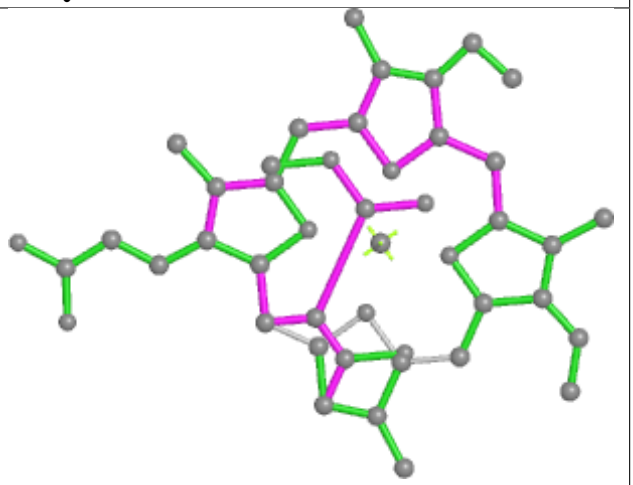
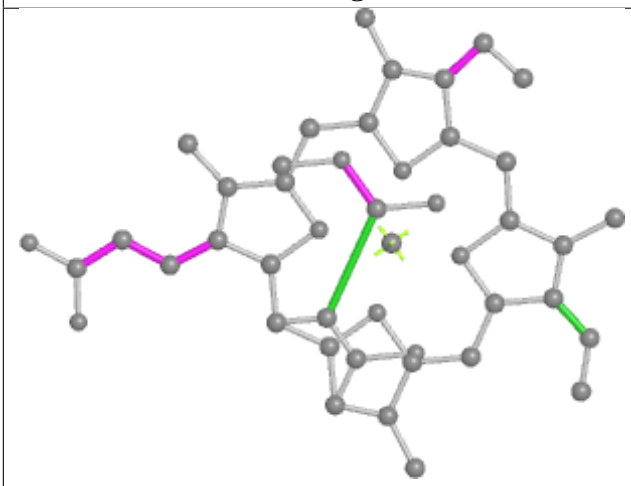


Bond angles



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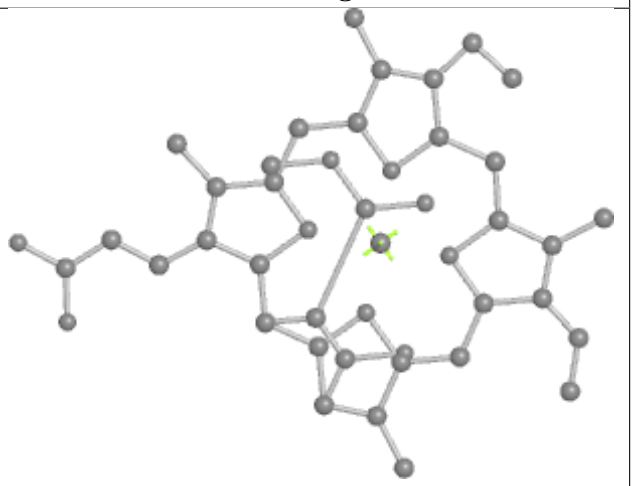
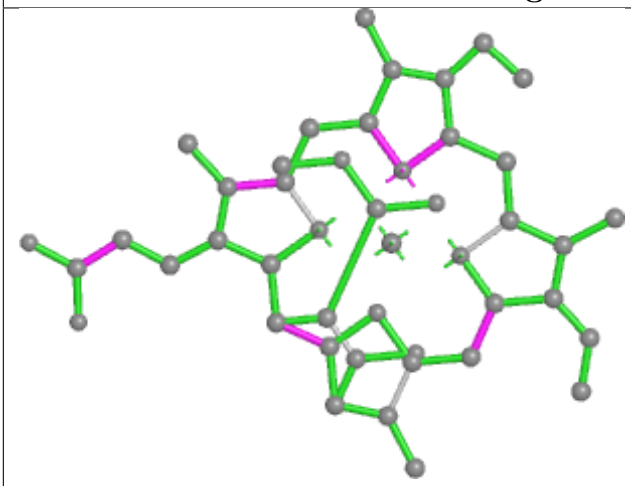


Rings

Ligand KC1 Q 309



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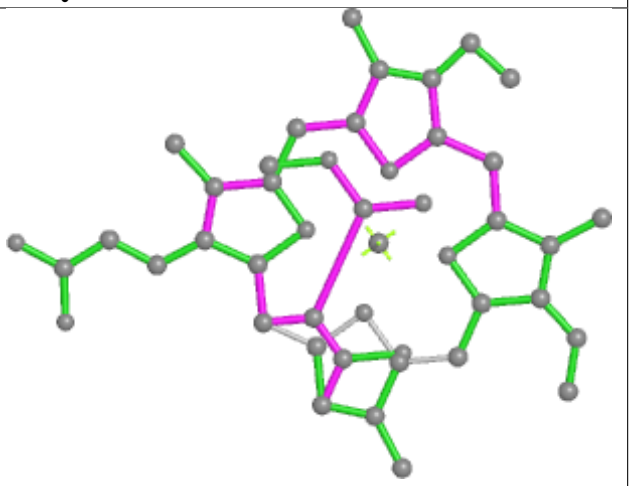
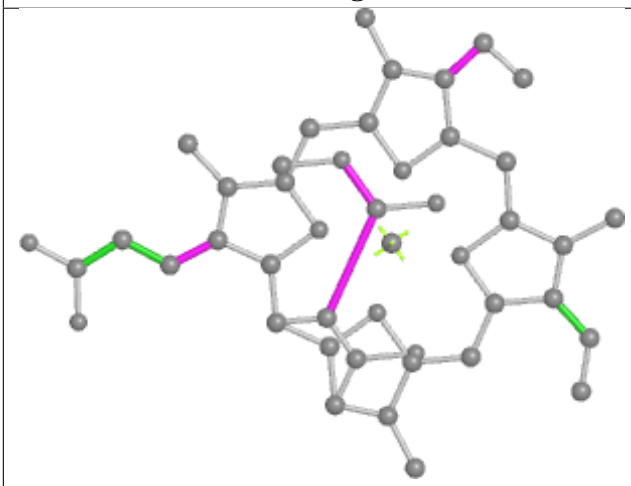


Bond angles



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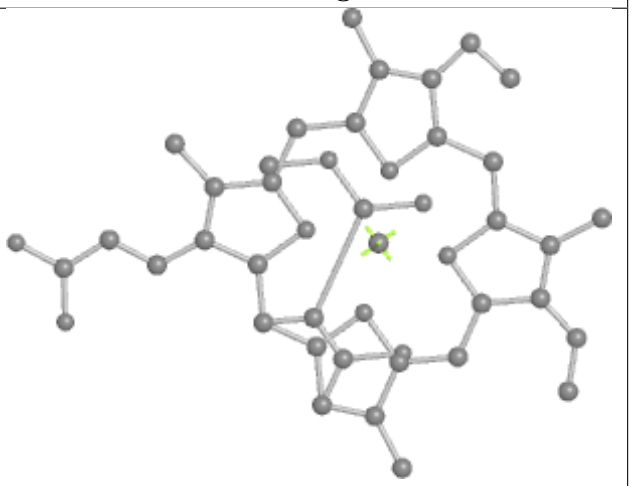
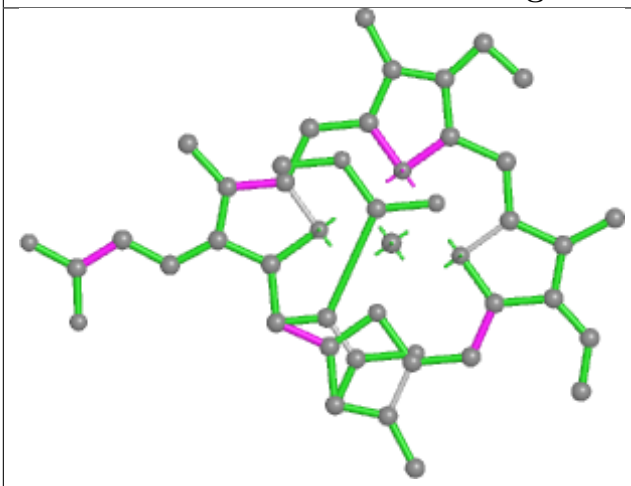


Rings

Ligand KC1 P 216



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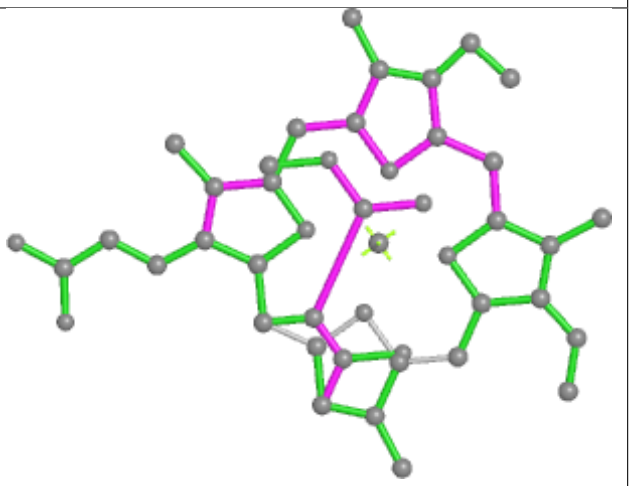
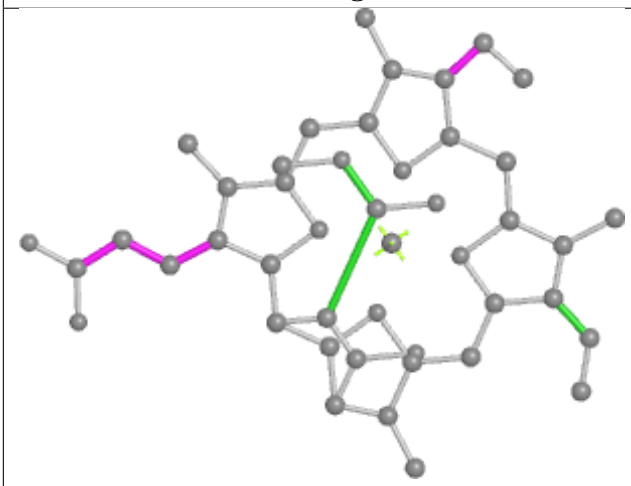


Bond angles



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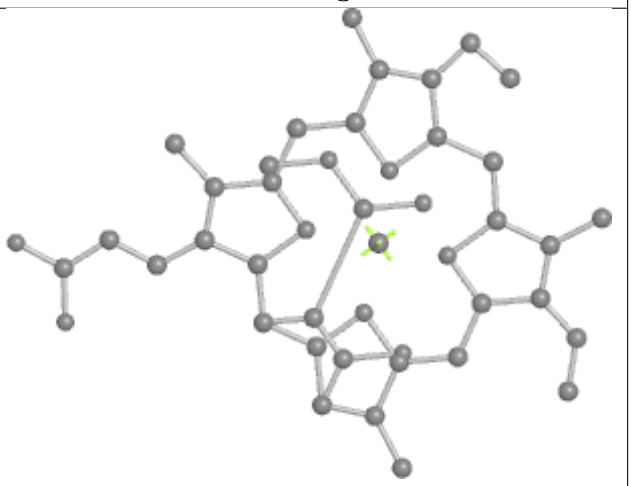
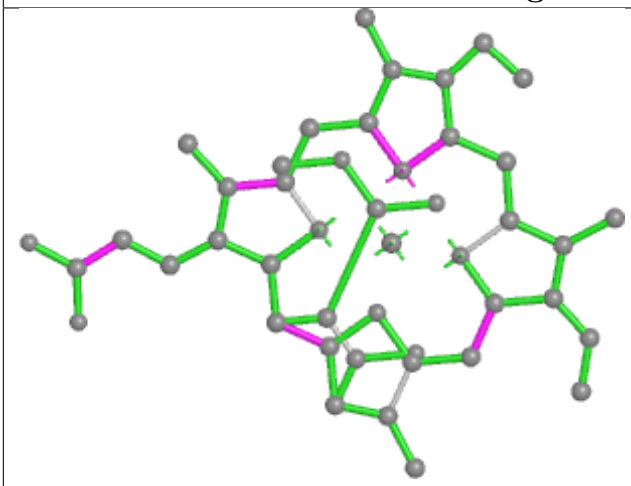


Rings

Ligand KC1 P 213



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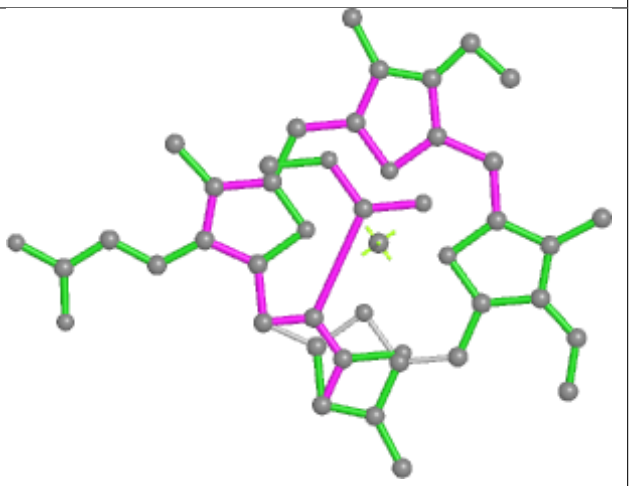
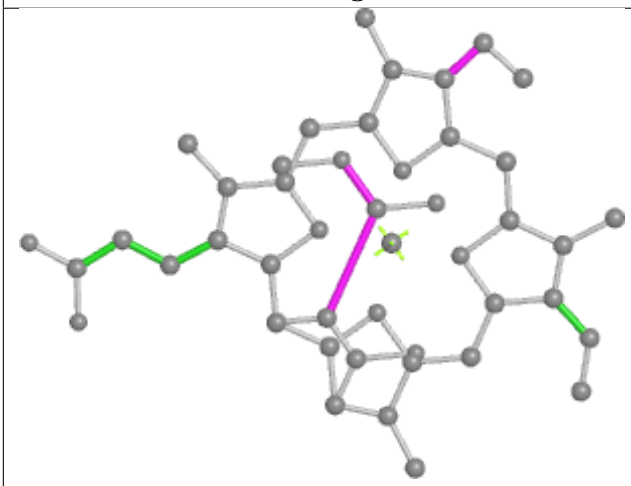


Bond angles



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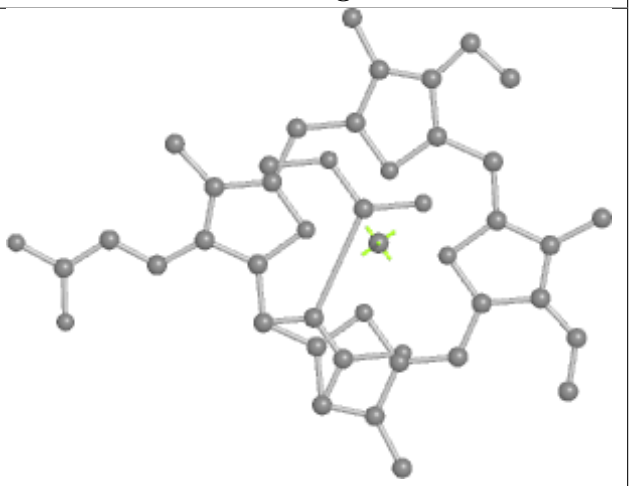
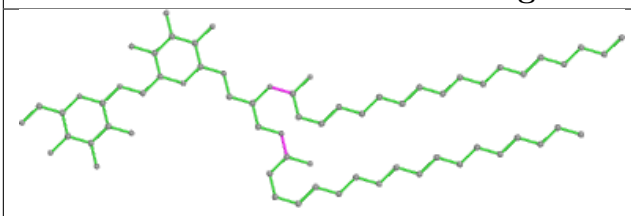


Rings

Ligand DGD m 102



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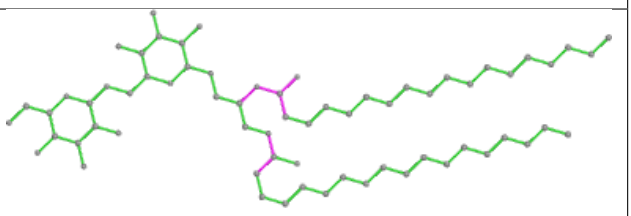
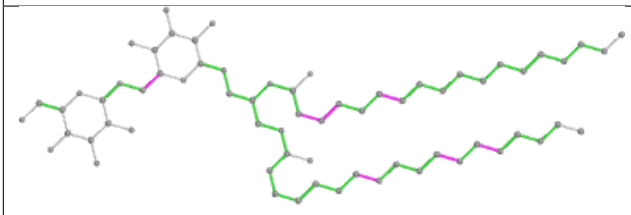


Bond angles



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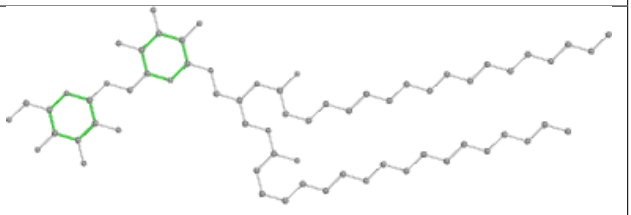
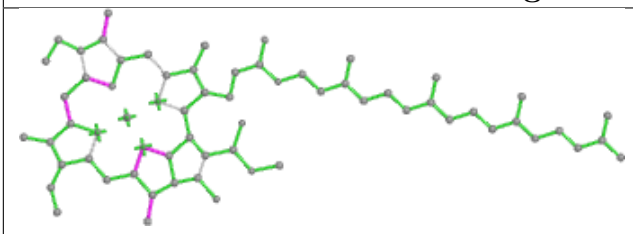
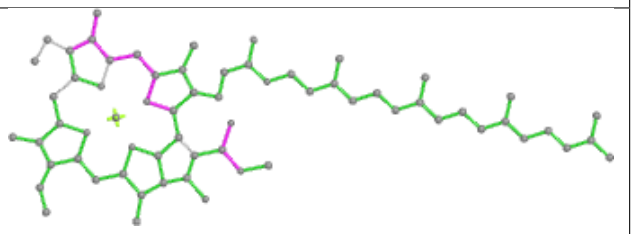


Rings

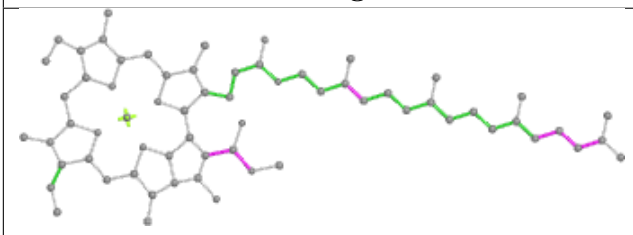
Ligand CLA O 309



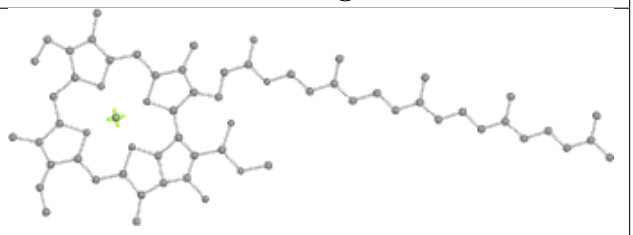
Bond lengths



Bond angles

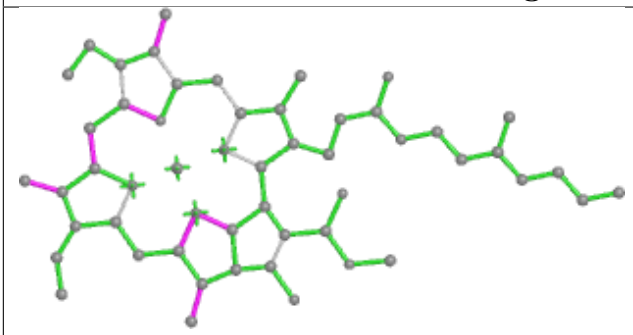


Torsions



Rings

Ligand CLA G 317



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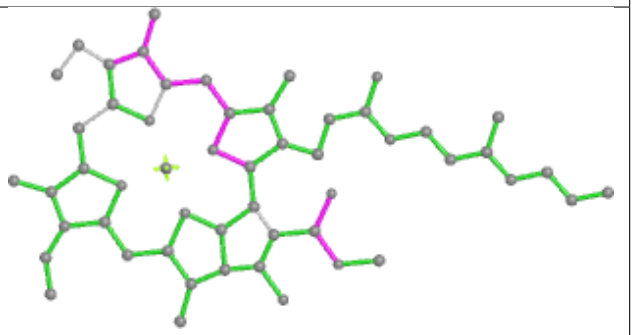

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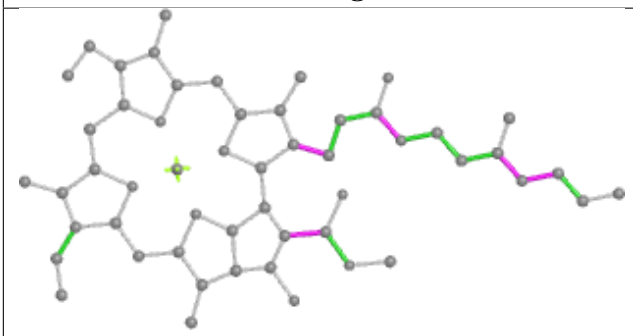

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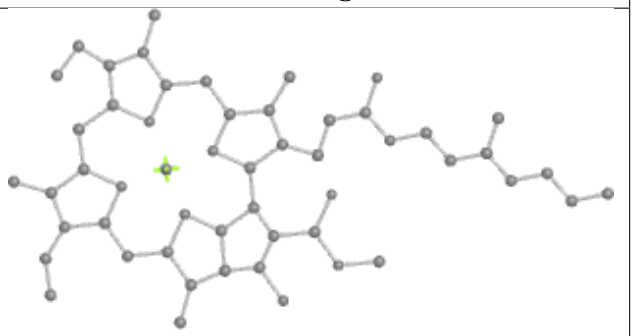
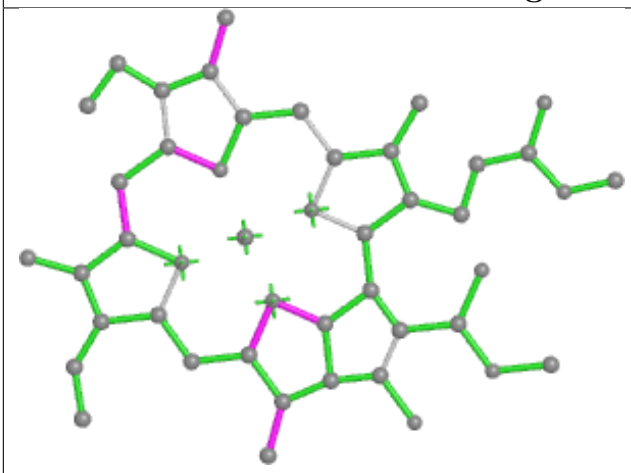


Rings

Ligand CLA E 309



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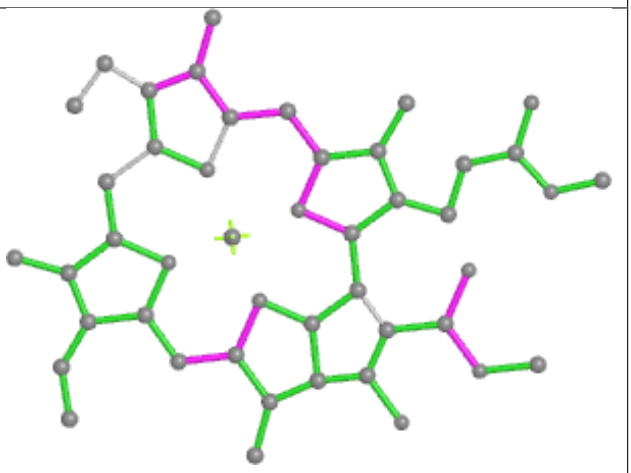
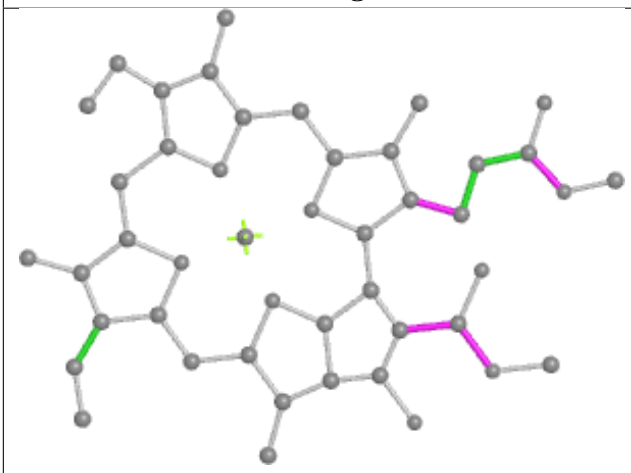
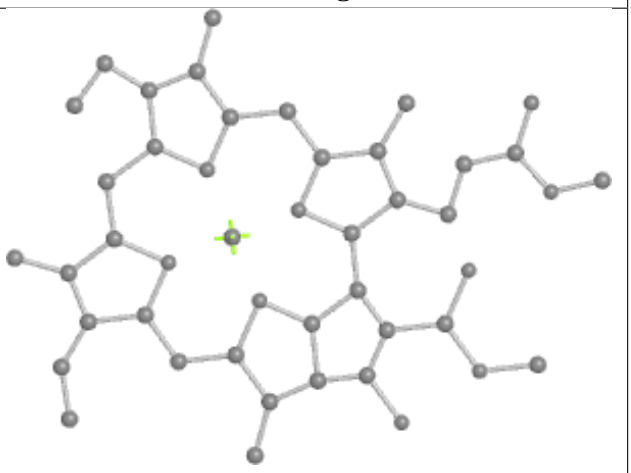


Bond angles

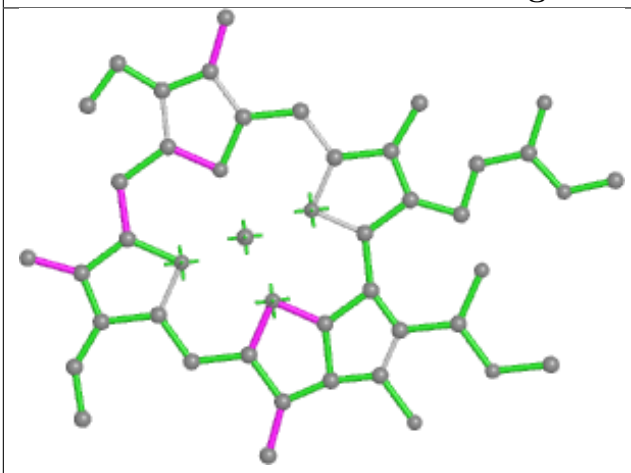


Torsions



Rings

Ligand CLA a 816



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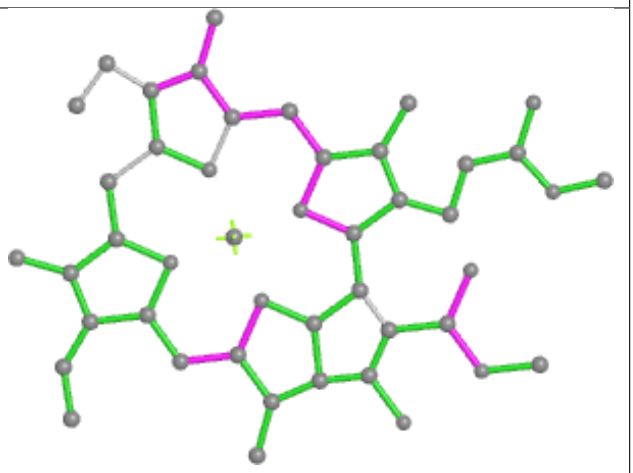
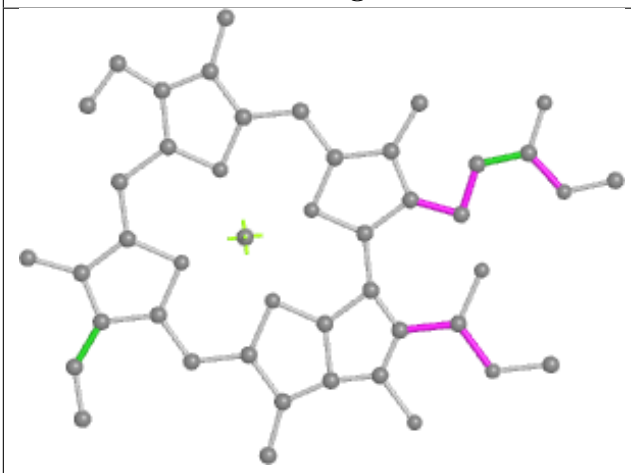
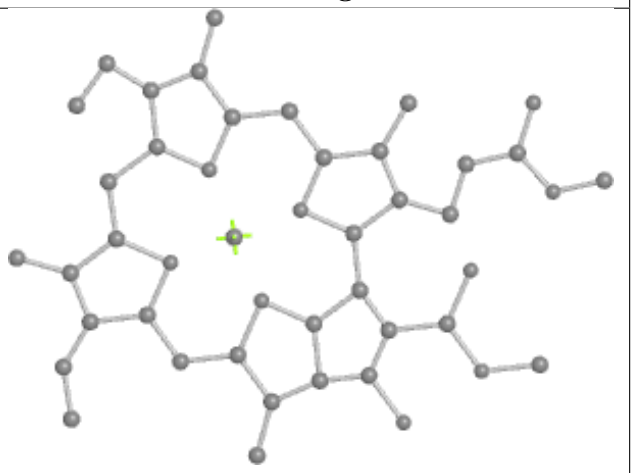


Bond angles

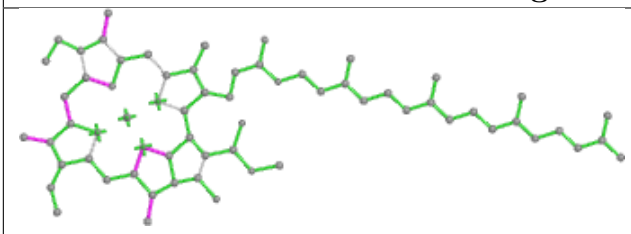


Torsions



Rings

Ligand CLA I 211



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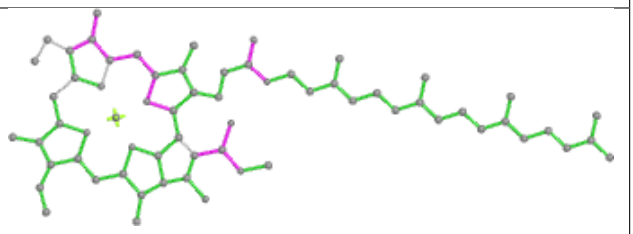
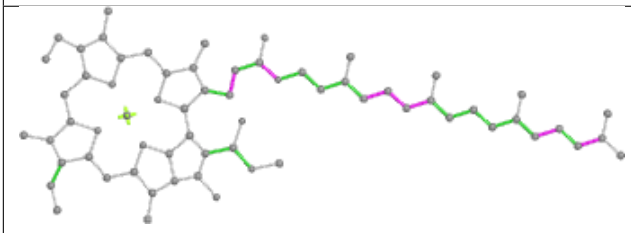


Bond angles



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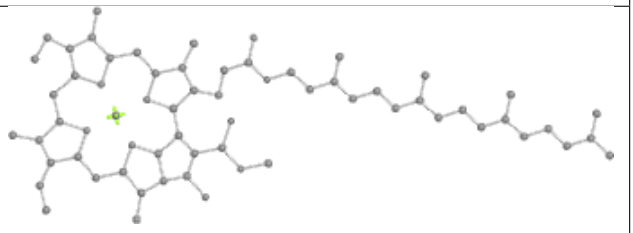
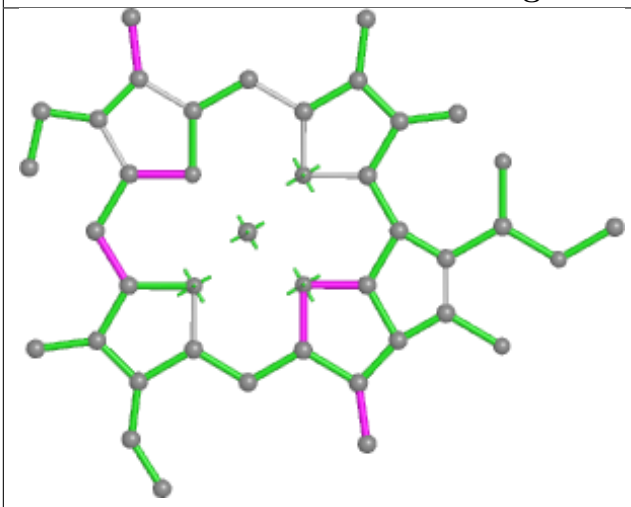


Rings

Ligand CLA G 319



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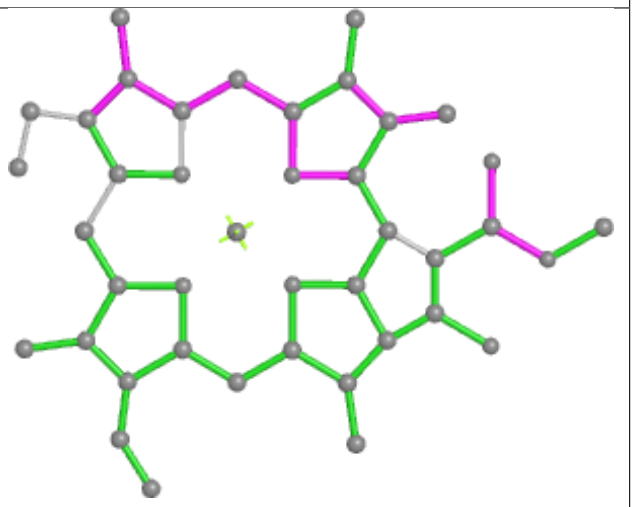
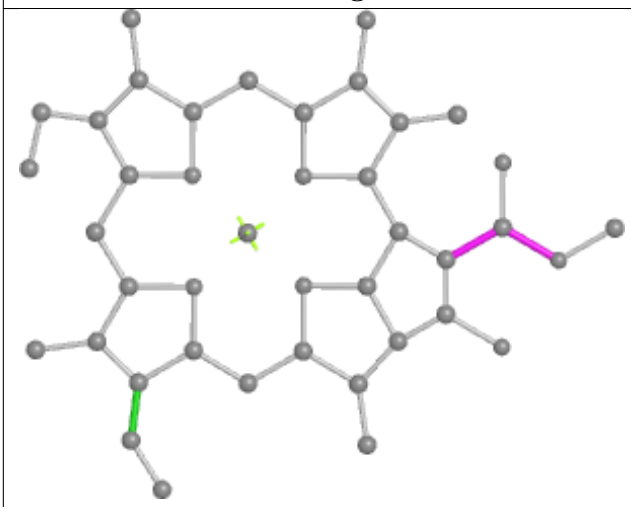


Bond angles



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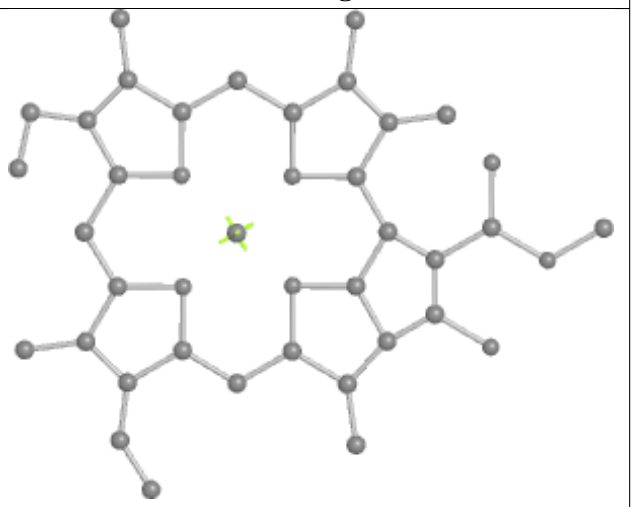
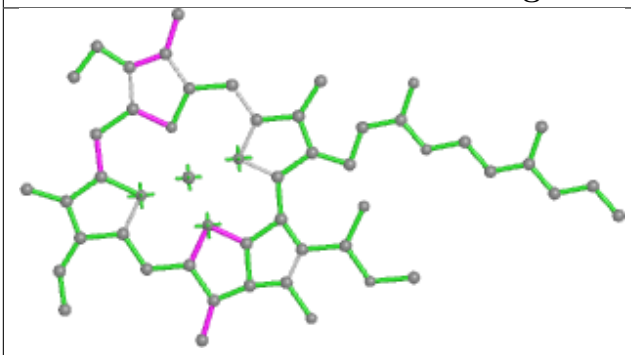


Rings

Ligand CLA K 212



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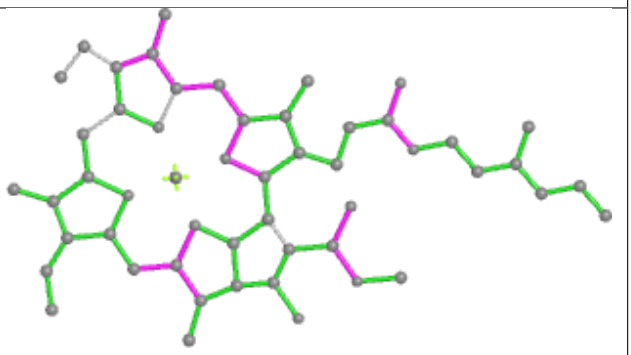
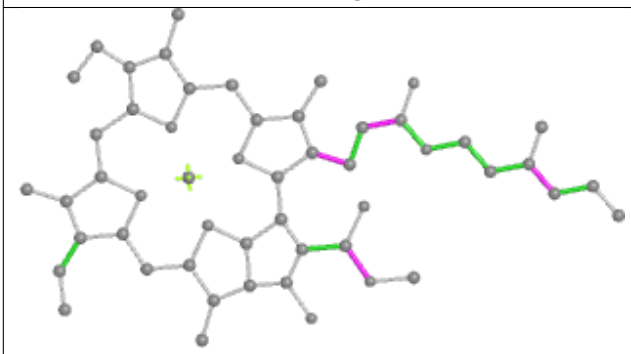


Bond angles



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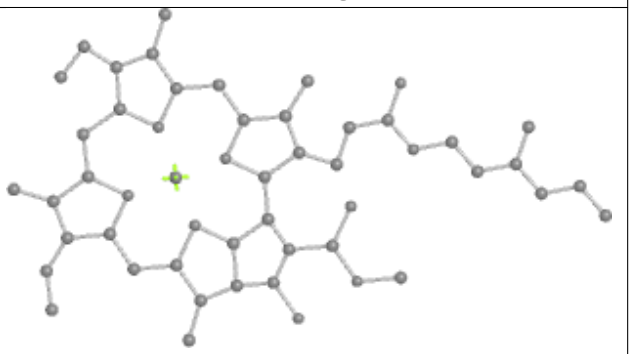
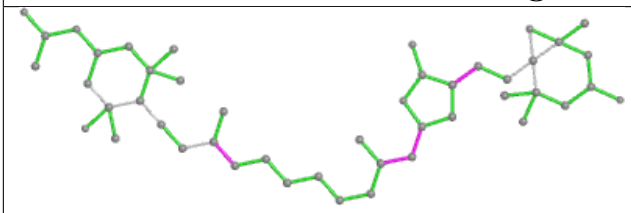


Rings

Ligand PID H 304



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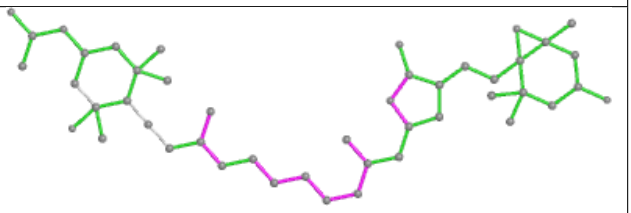
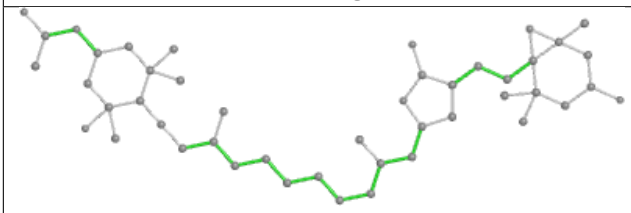


Bond angles



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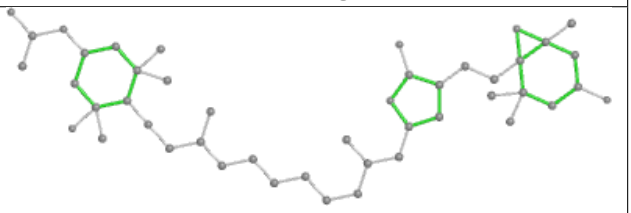
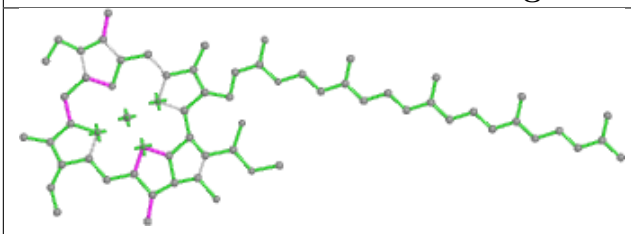


Rings

Ligand CLA Q 310



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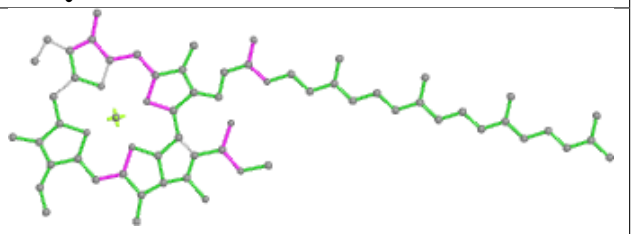
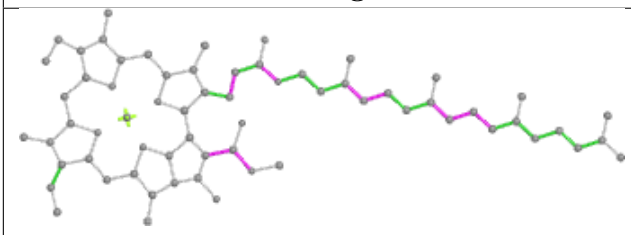


Bond angles



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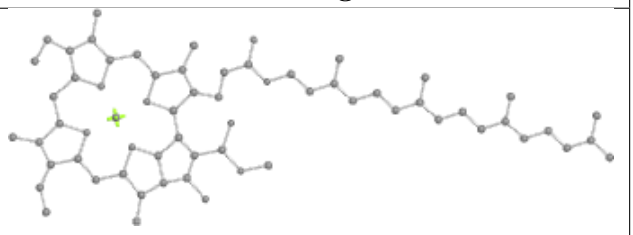
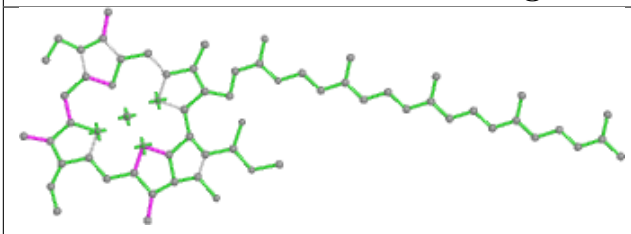


Rings

Ligand CLA Q 308



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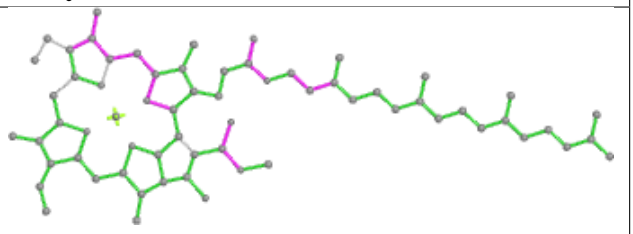
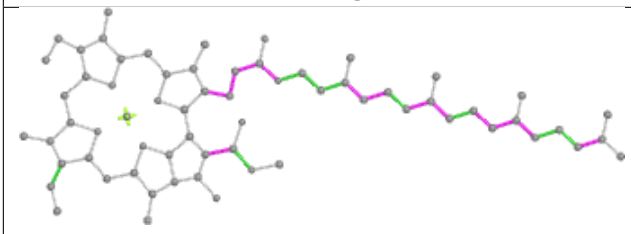


Bond angles



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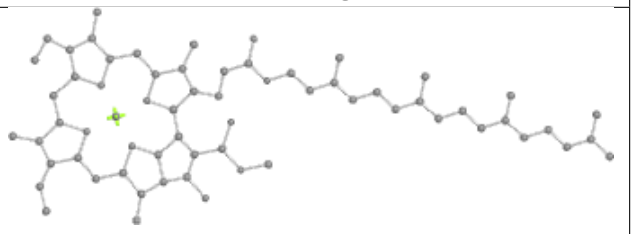
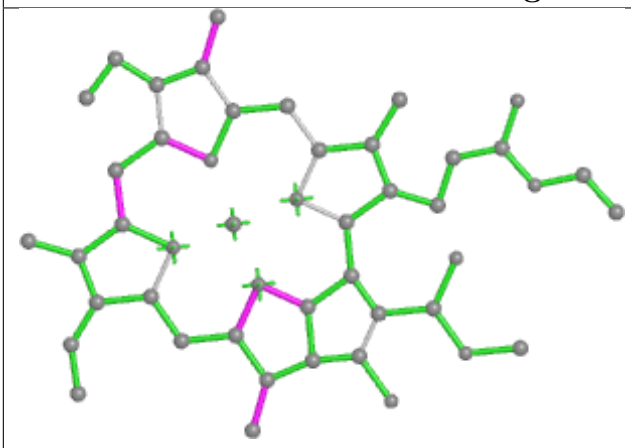


Rings

Ligand CLA Q 313



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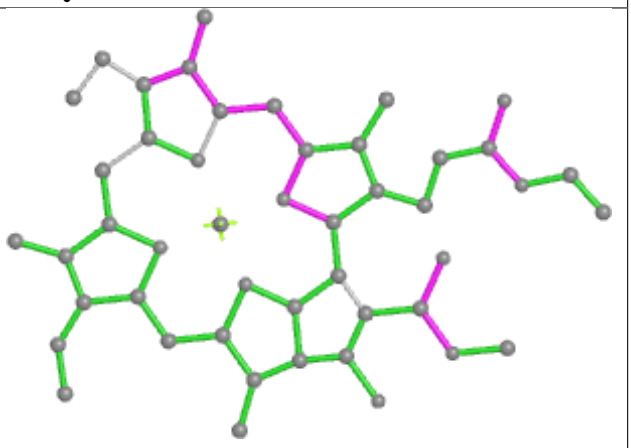
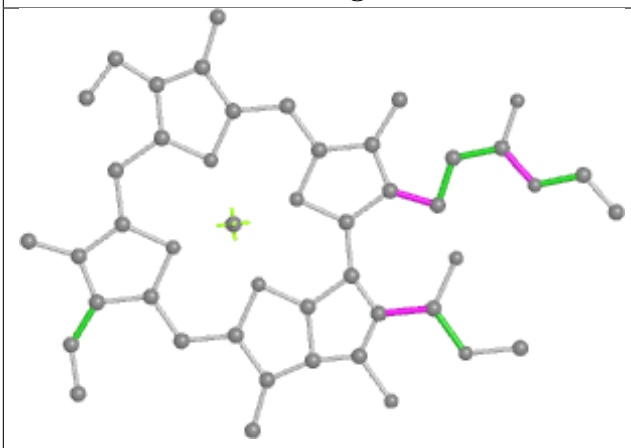


Bond angles



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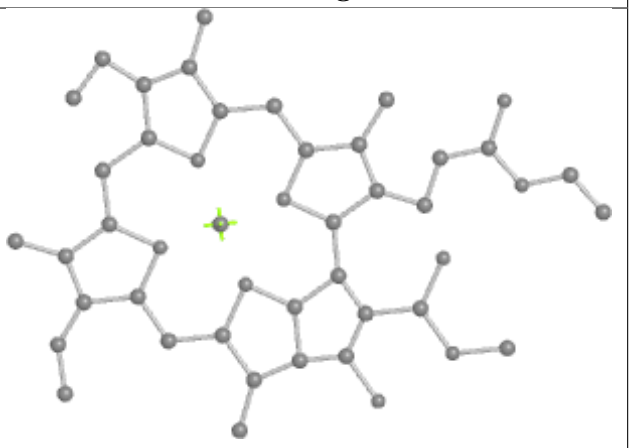
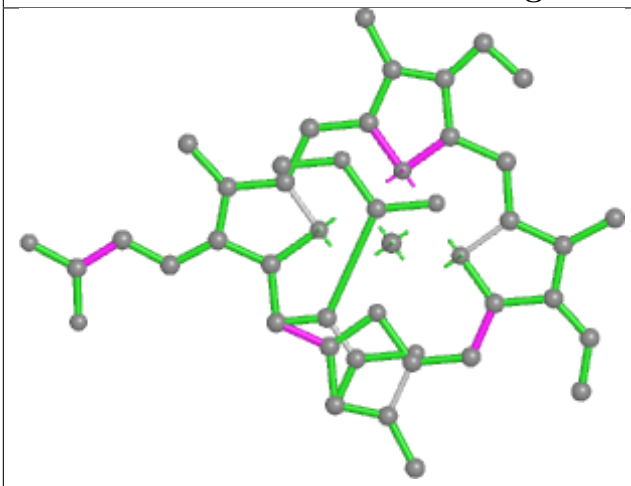


Rings

Ligand KC1 N 315



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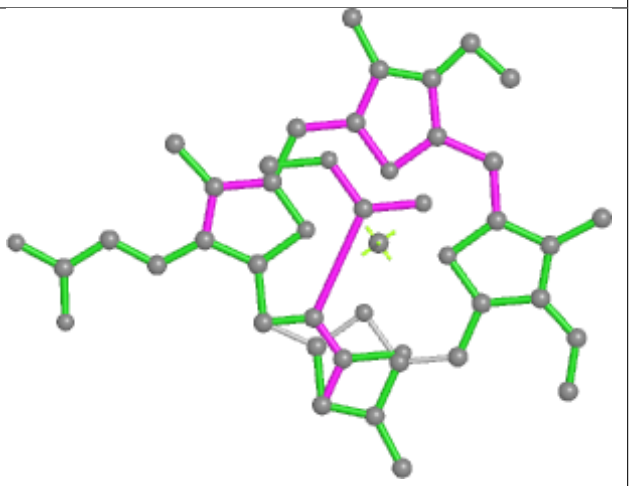
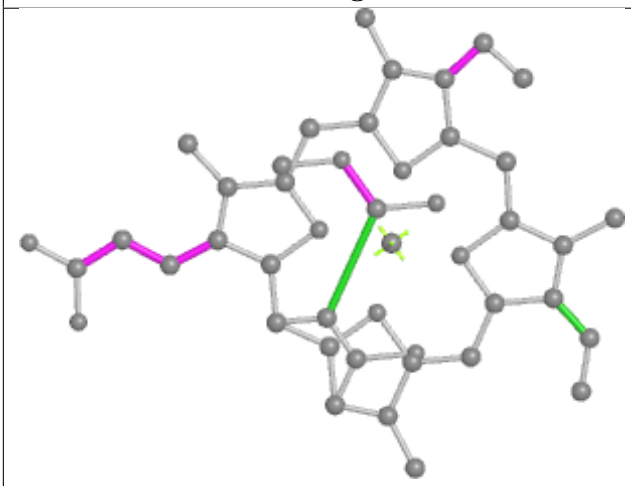


Bond angles



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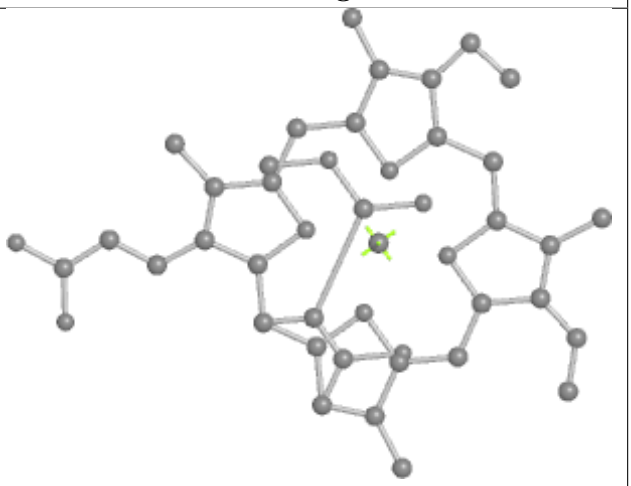
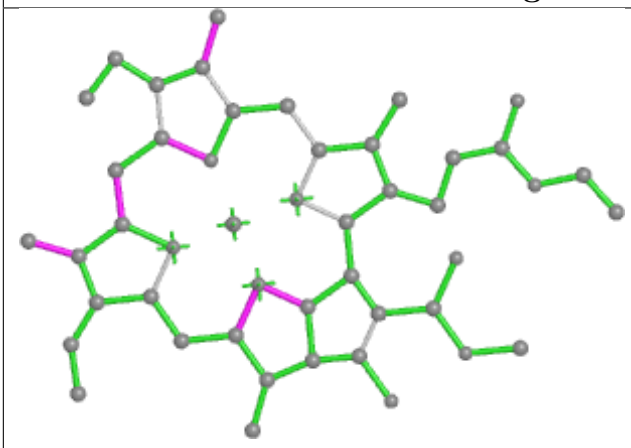


Rings

Ligand CLA H 313



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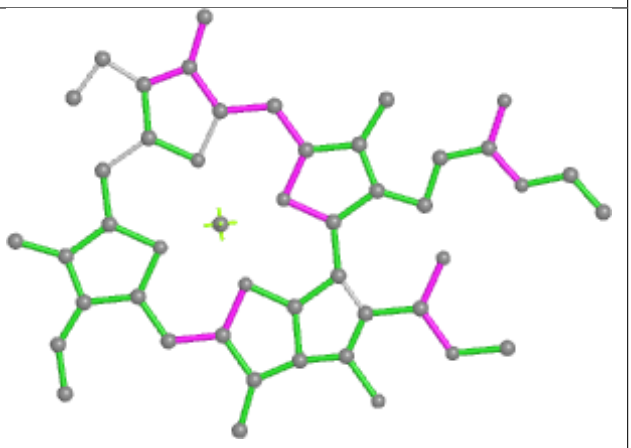
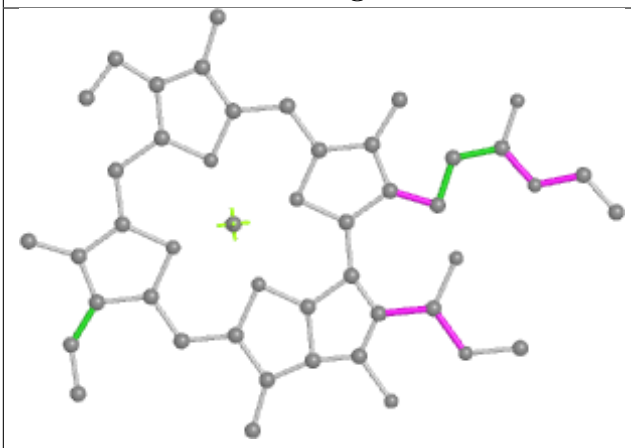


Bond angles



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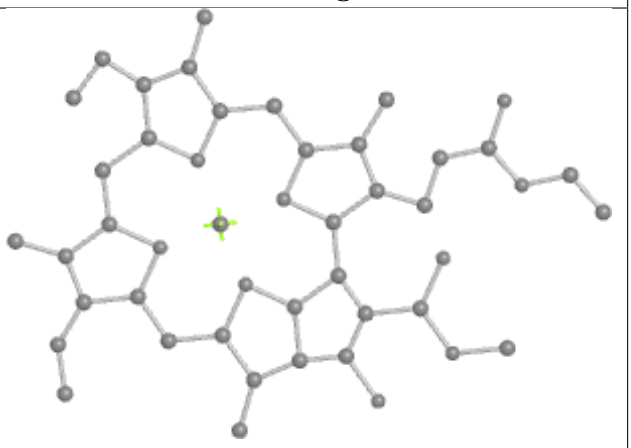
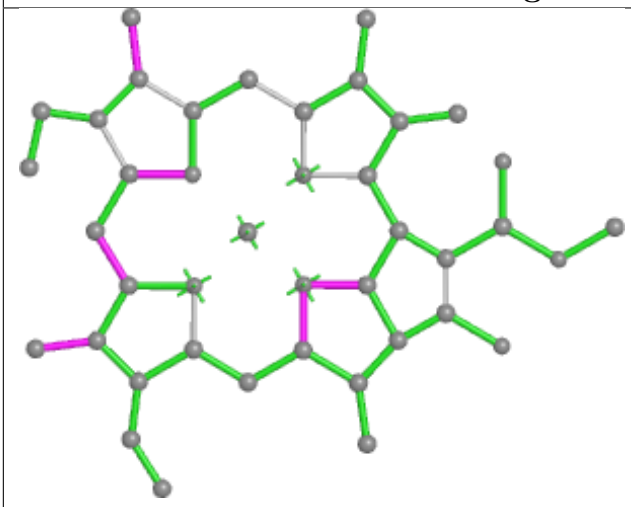
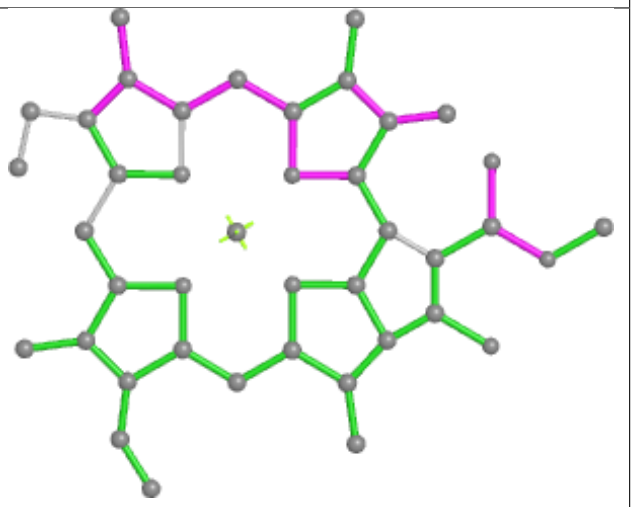


Rings

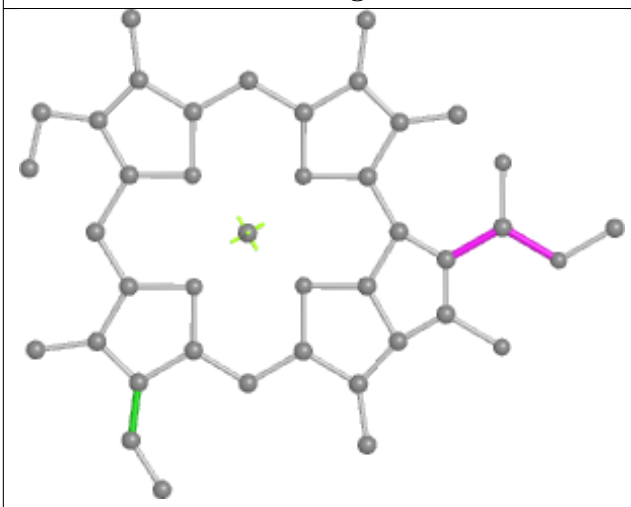
Ligand CLA O 316



Bond lengths



Bond angles



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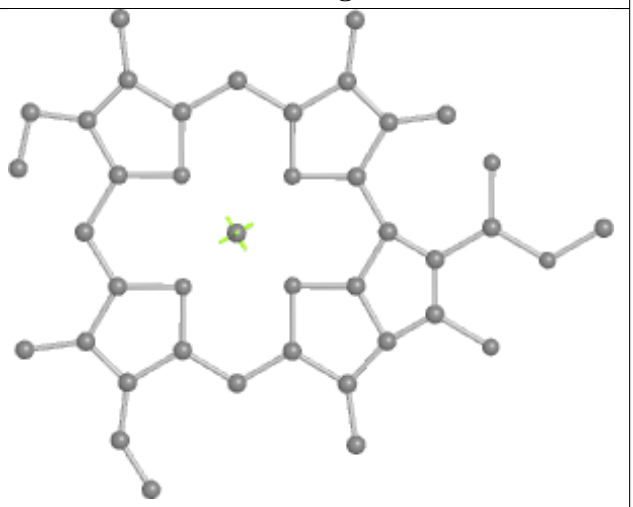
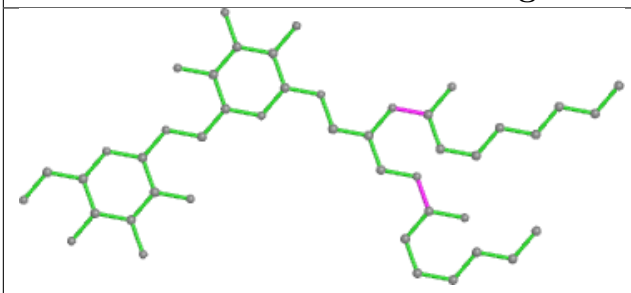
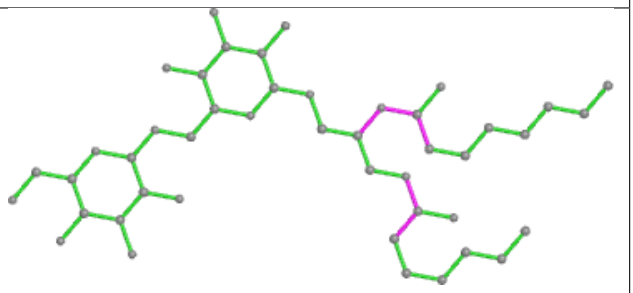


Rings

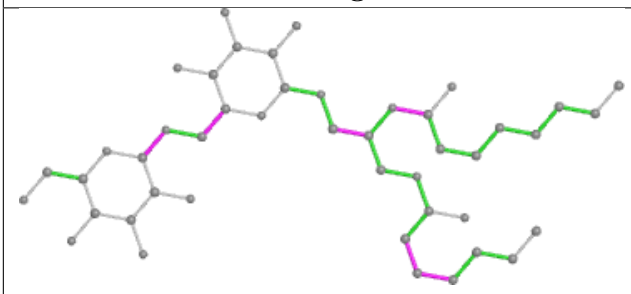
Ligand DGD G 320



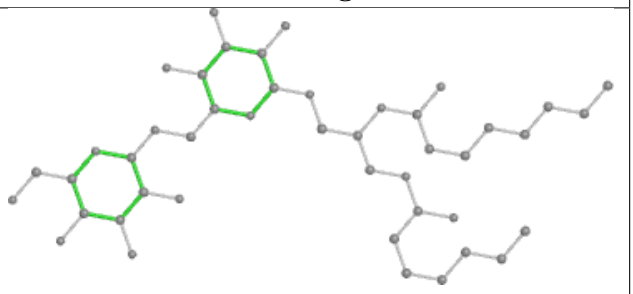
Bond lengths



Bond angles

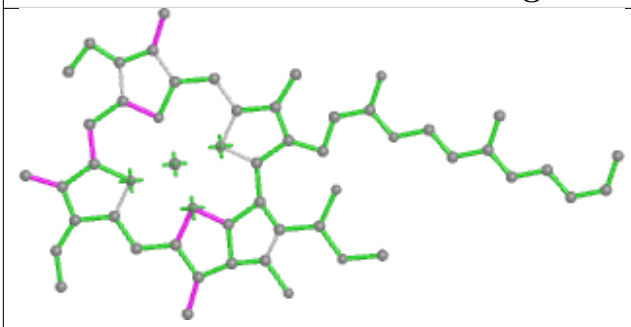


Torsions

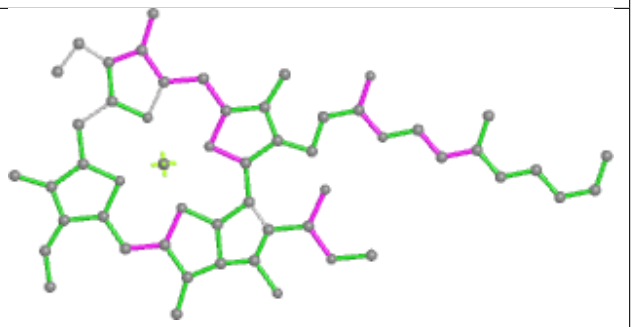


Rings

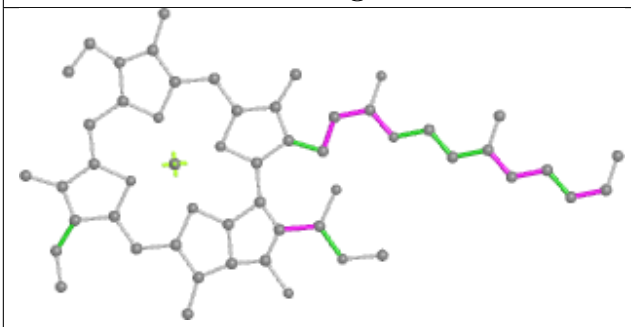
Ligand CLA K 209



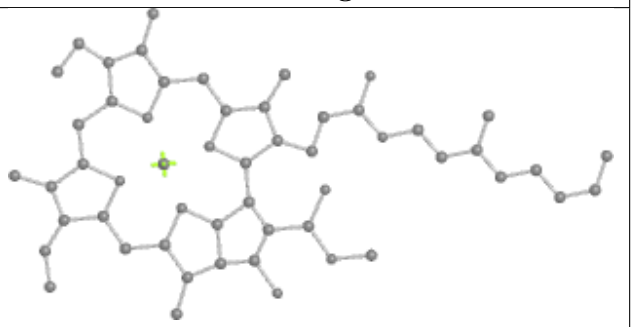
Bond lengths



Bond angles

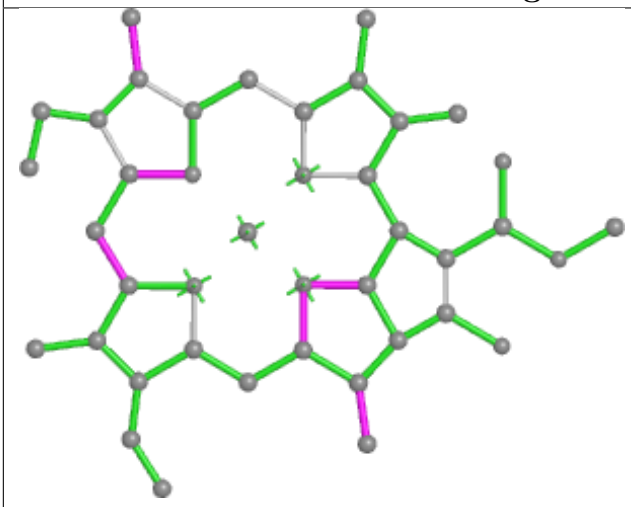


Torsions

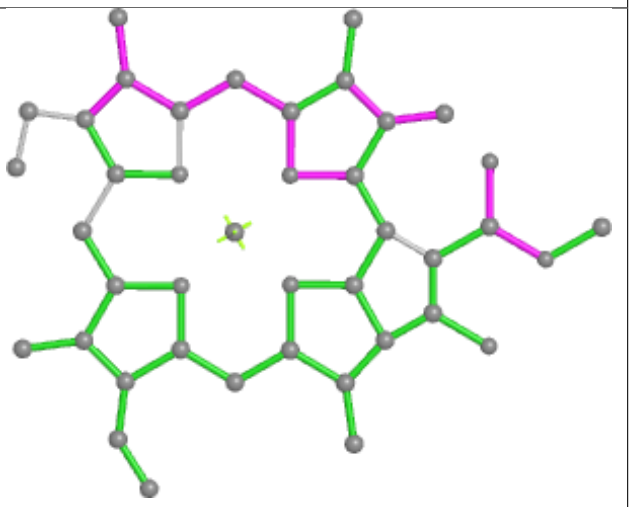


Rings

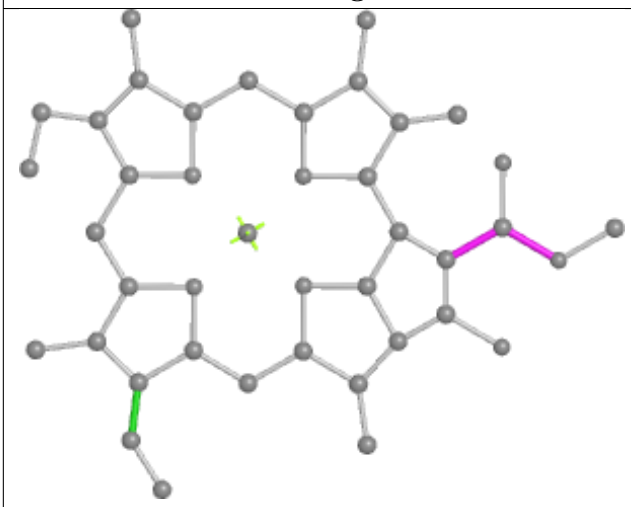
Ligand CLA N 316



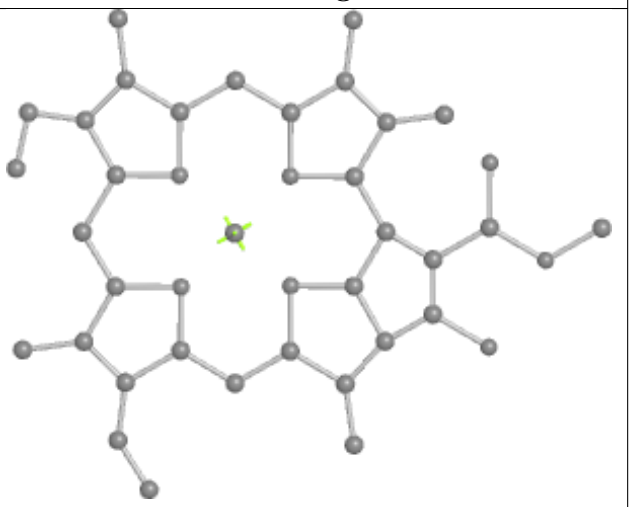
Bond lengths



Bond angles

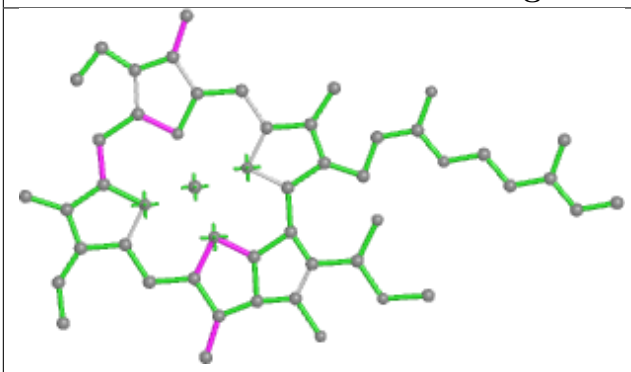


Torsions



Rings

Ligand CLA A 217



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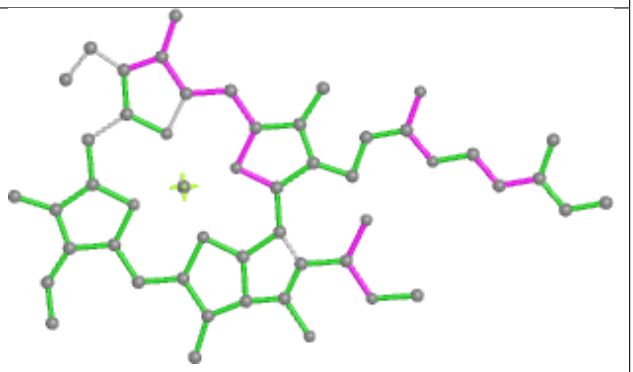
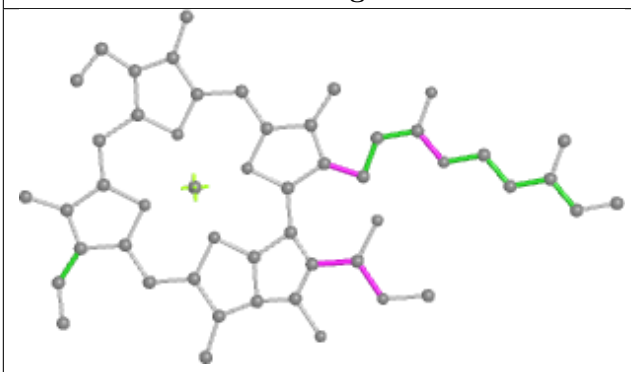
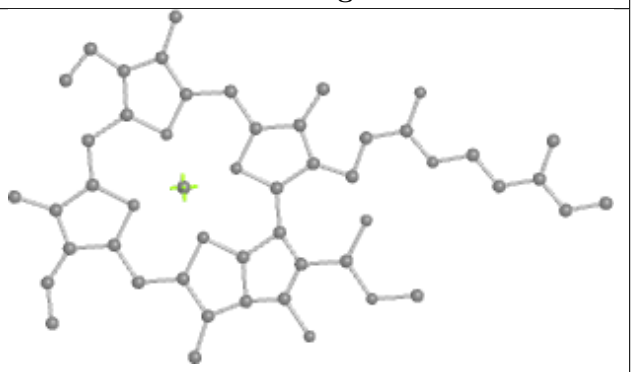


Bond angles

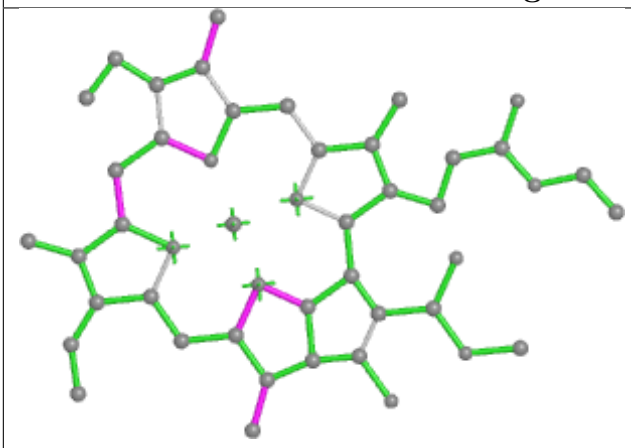


Torsions

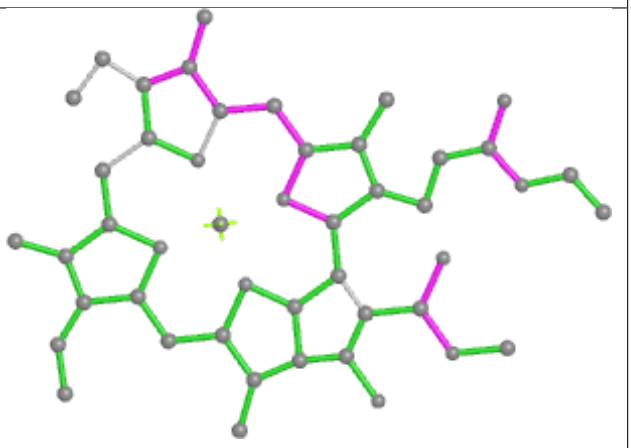


Rings

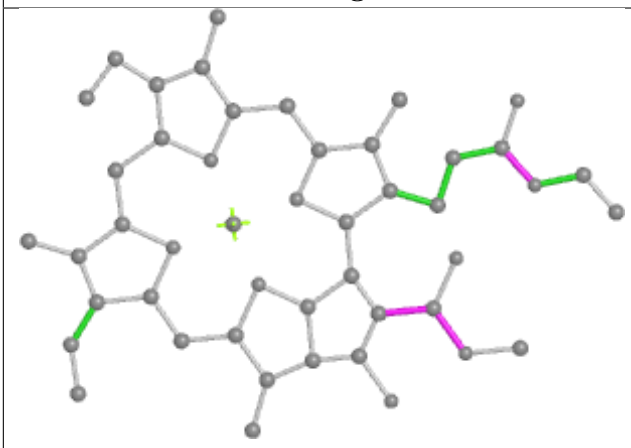
Ligand CLA O 308



Bond lengths



Bond angles



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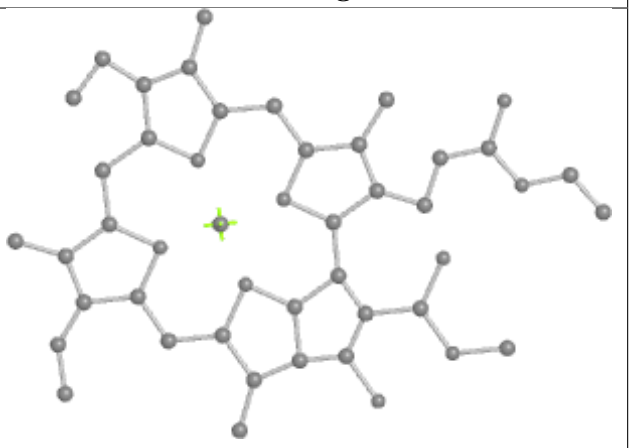
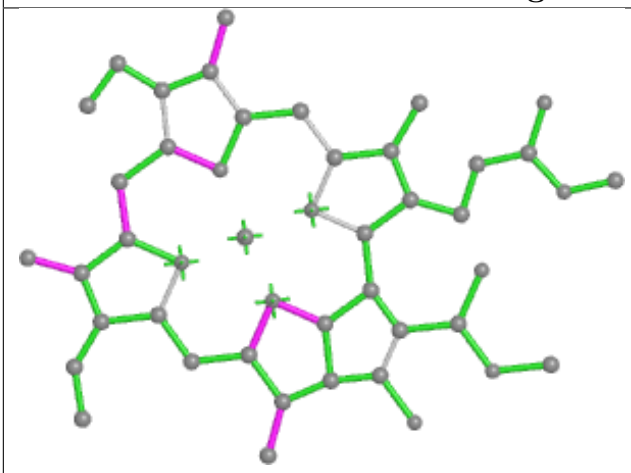
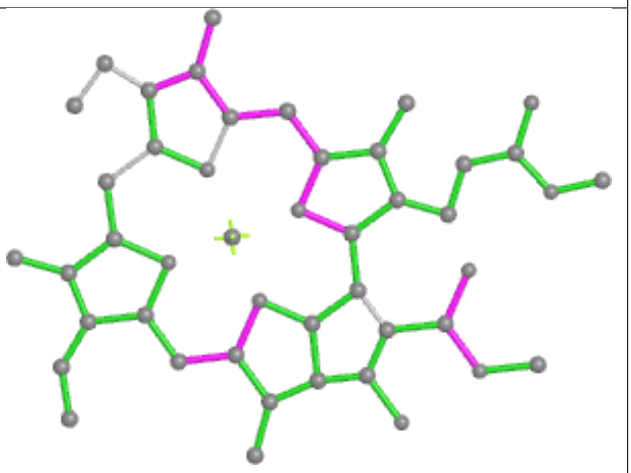


Rings

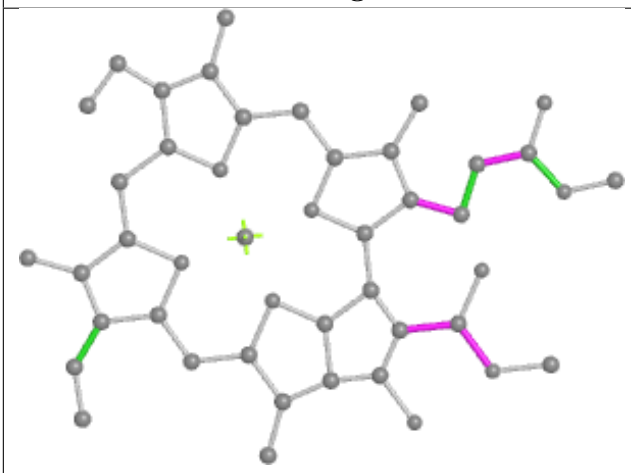
Ligand CLA b 710



Bond lengths



Bond angles



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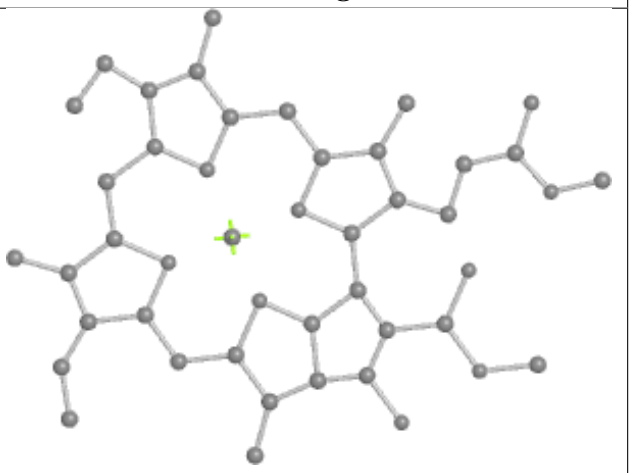
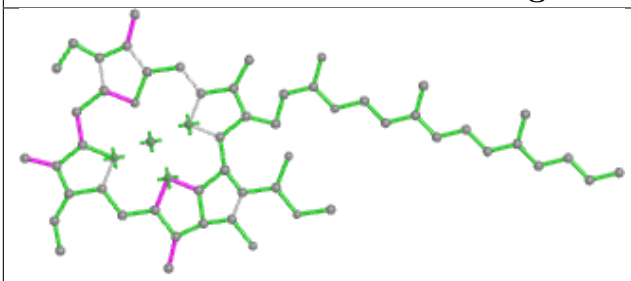
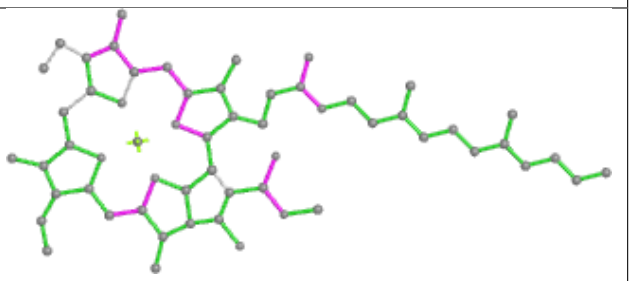


Rings

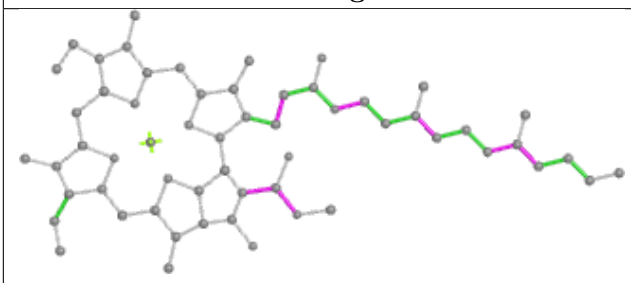
Ligand CLA a 823



Bond lengths



Bond angles



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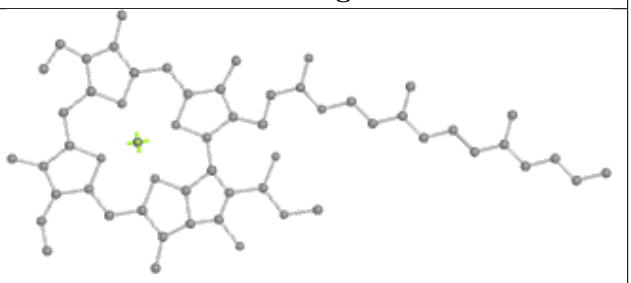
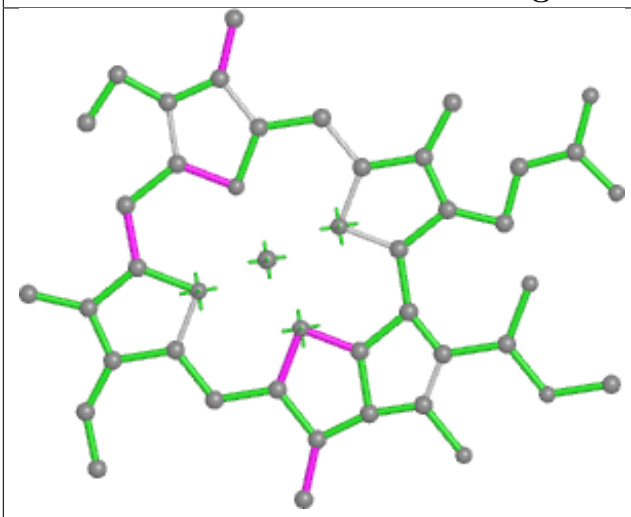
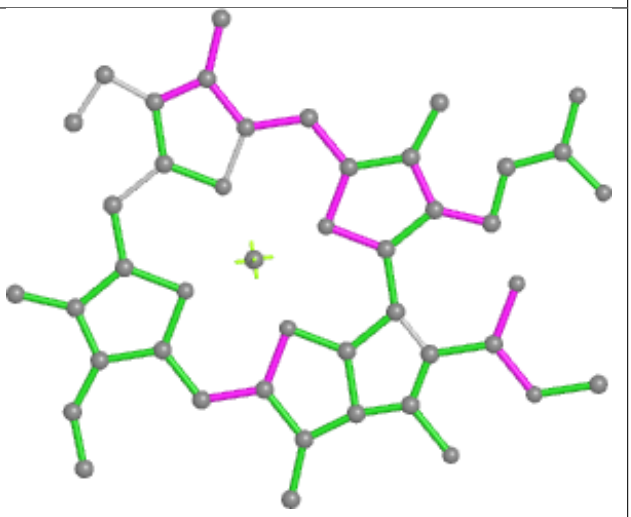


Rings

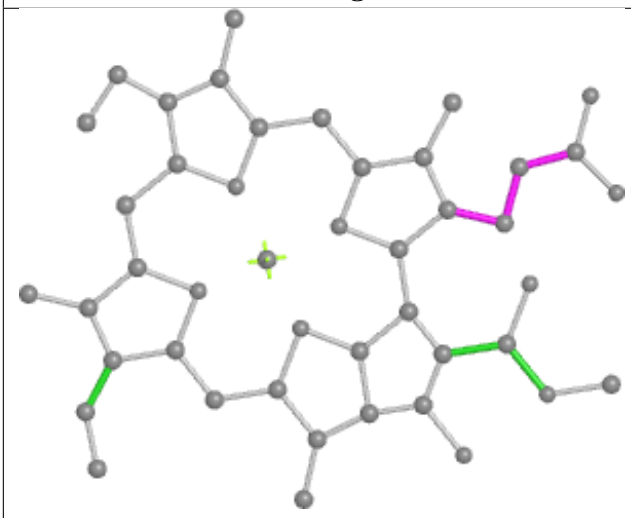
Ligand CLA l 510



Bond lengths



Bond angles



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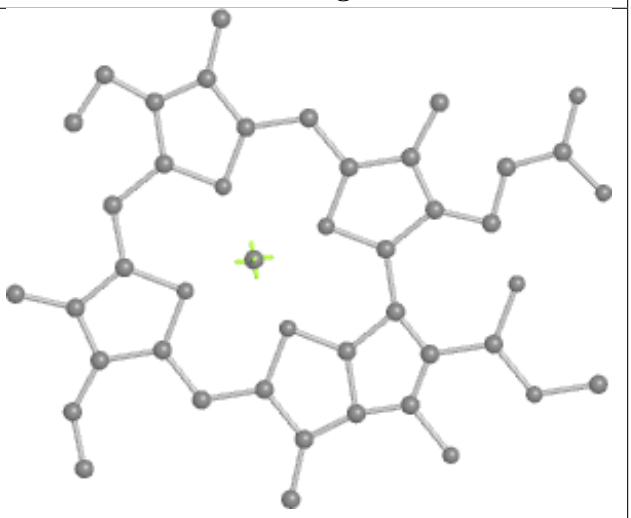
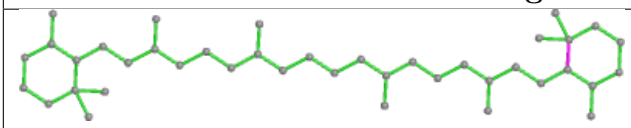
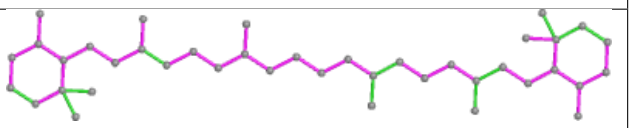


Rings

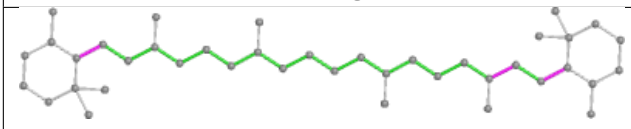
Ligand BCR b 729



Bond lengths



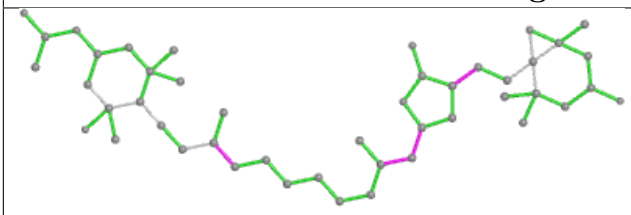
Bond angles



Torsions

Rings

Ligand PID C 302



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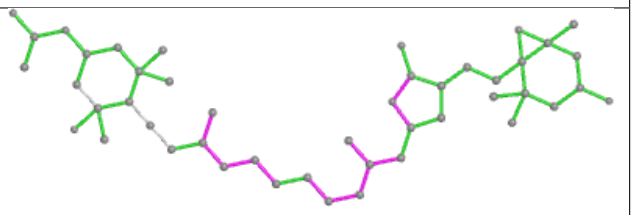
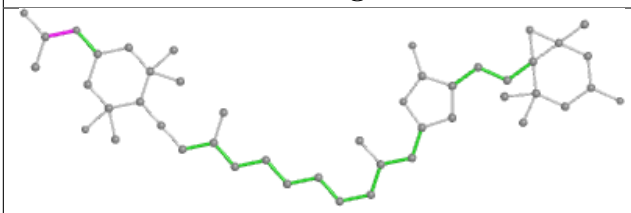
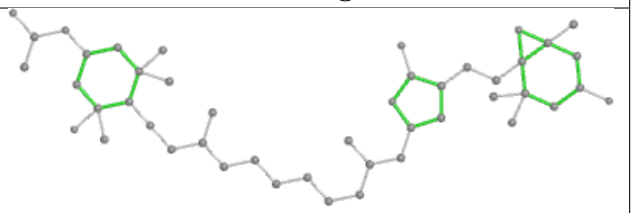


Bond angles

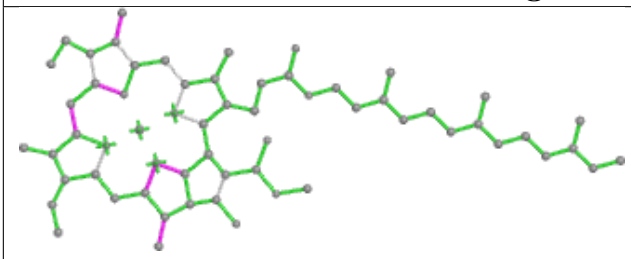


Torsions



Rings

Ligand CLA E 305



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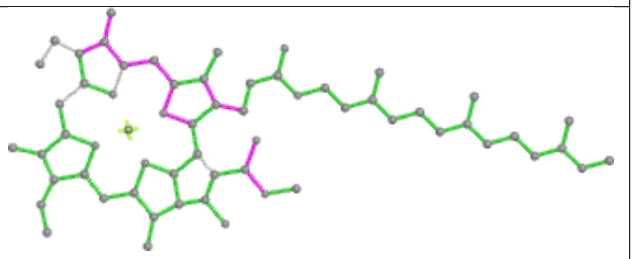
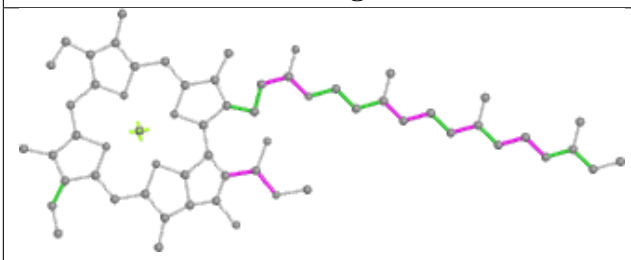


Bond angles



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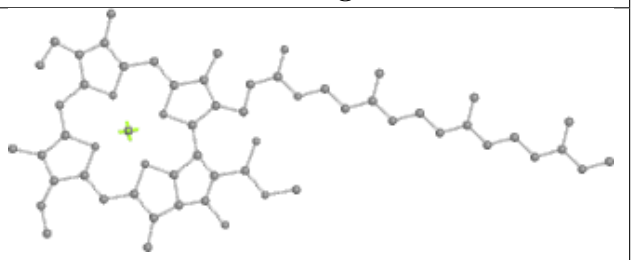
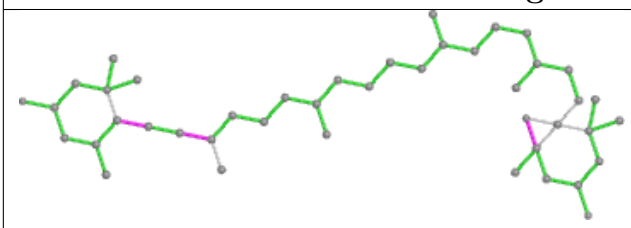


Rings

Ligand DD6 E 302



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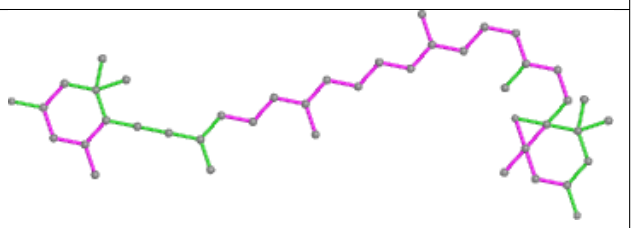

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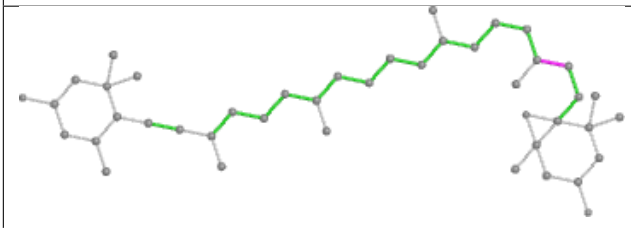

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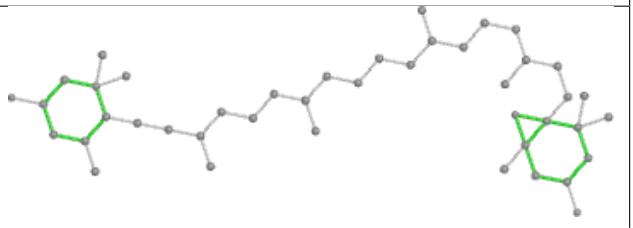
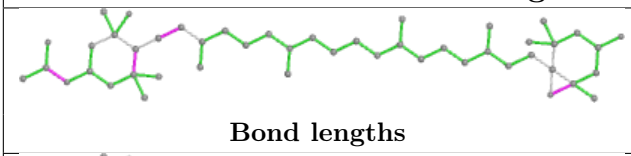
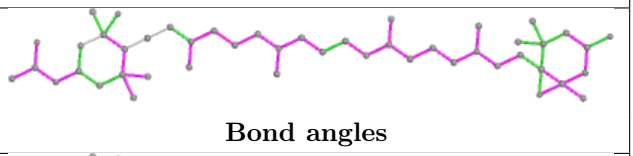


Rings

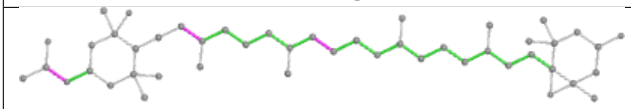
Ligand UIX T 306



Bond lengths



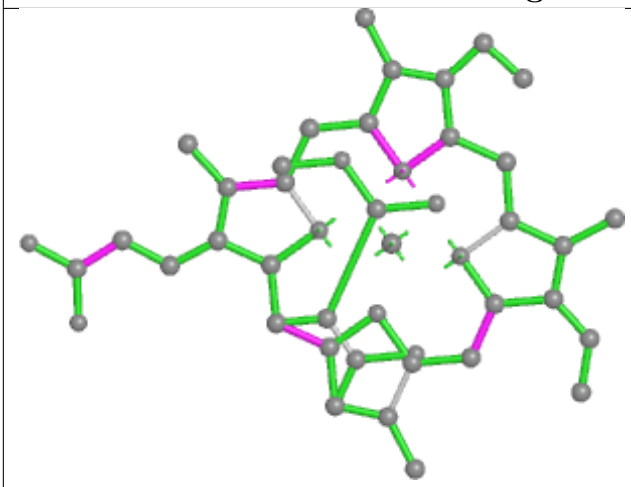
Bond angles



Torsions

Rings

Ligand KC1 C 312



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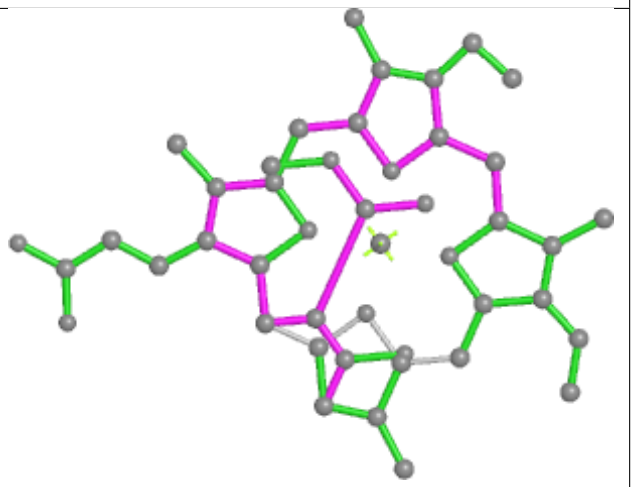
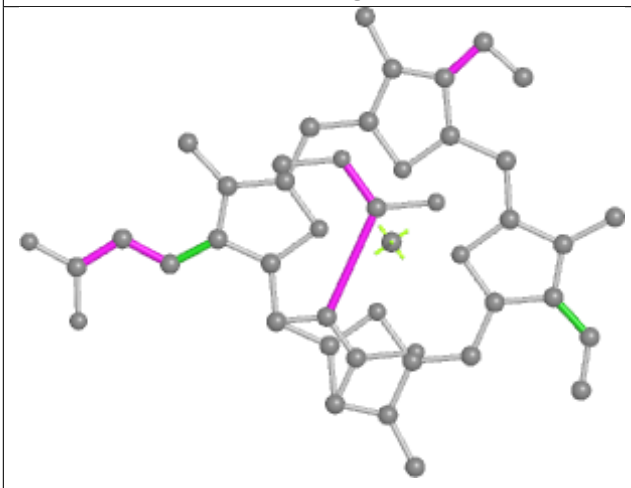


Bond angles



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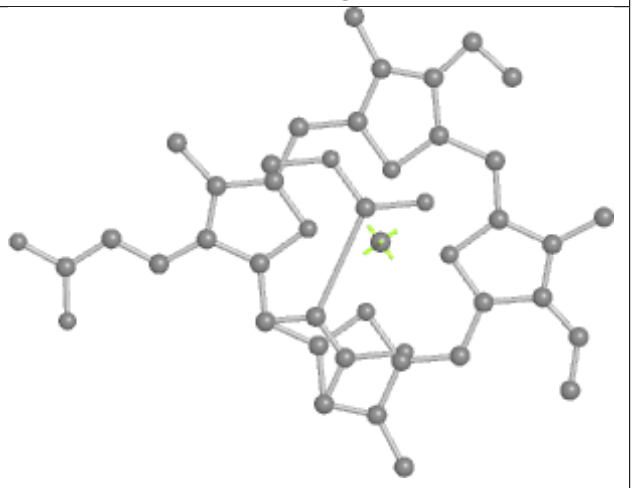
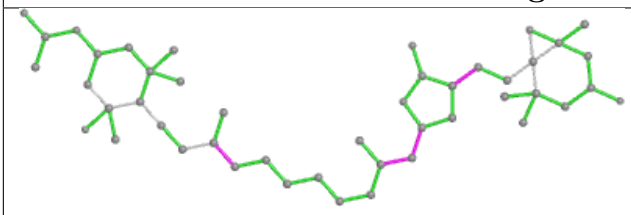
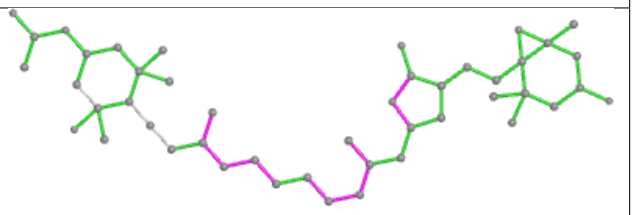


Rings

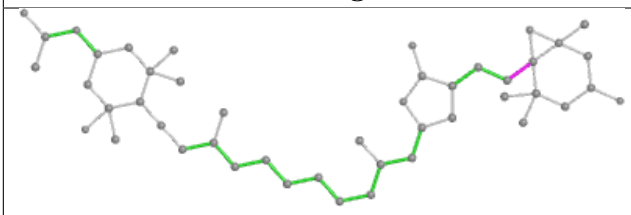
Ligand PID D 302



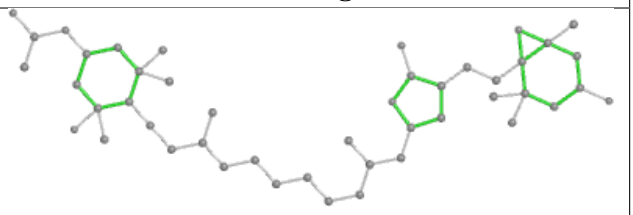
Bond lengths



Bond angles

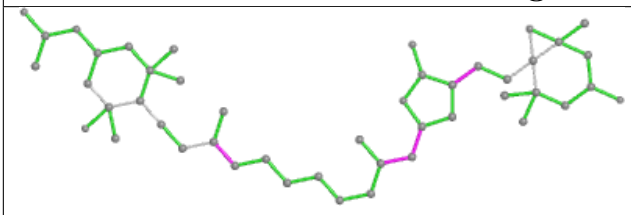


Torsions

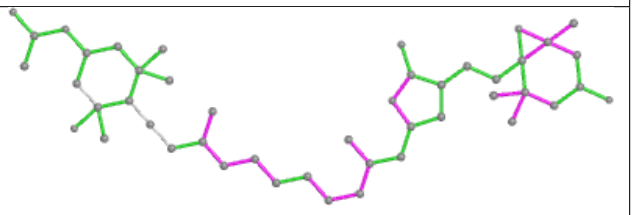


Rings

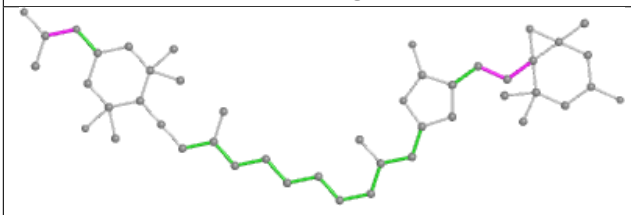
Ligand PID N 307



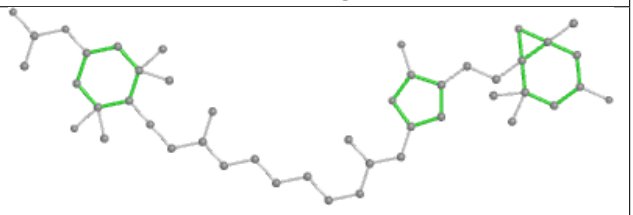
Bond lengths



Bond angles



Torsions

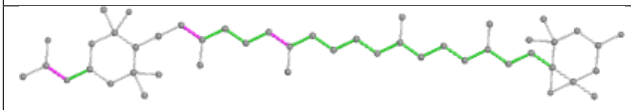


Rings

Ligand UIX C 306

Bond lengths

Bond angles



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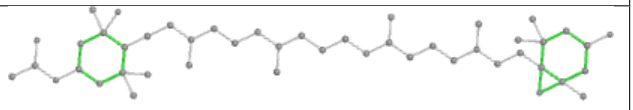
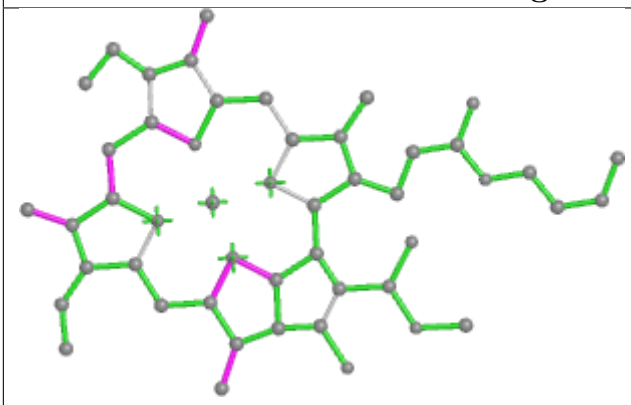


Rings

Ligand CLA I 207



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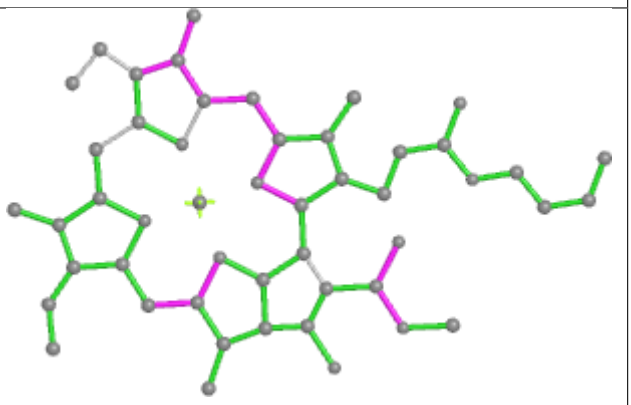
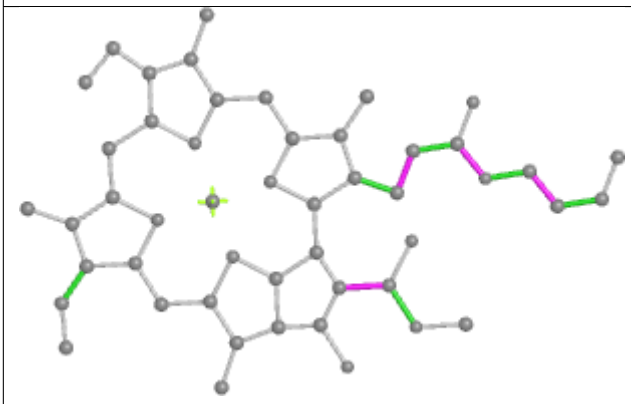


Bond angles



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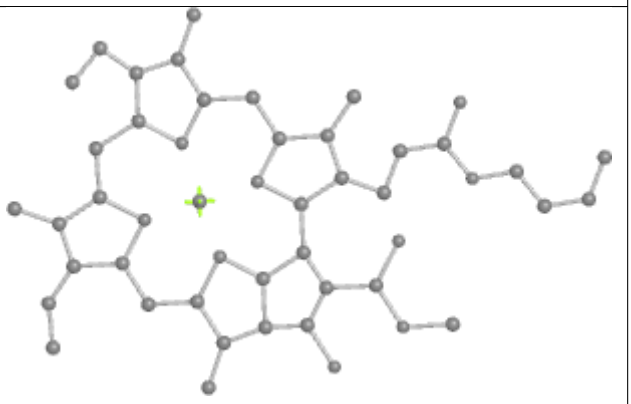
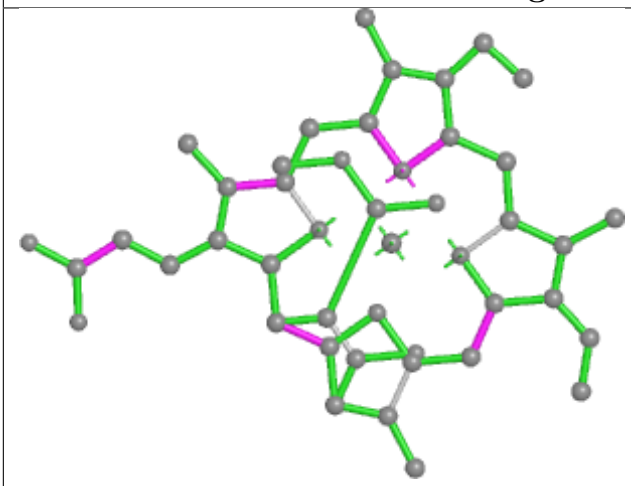


Rings

Ligand KC1 L 314



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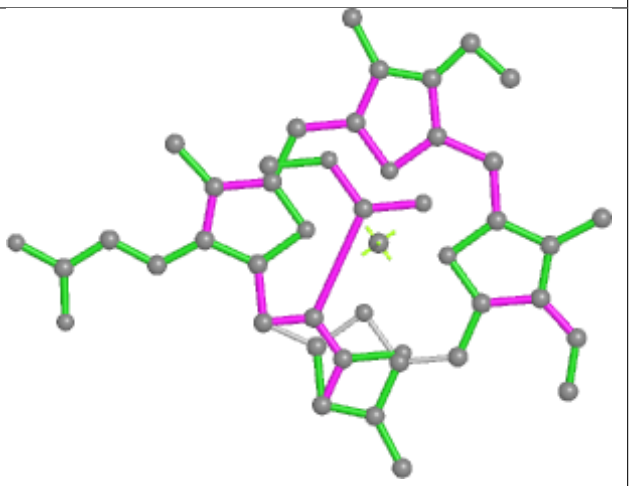
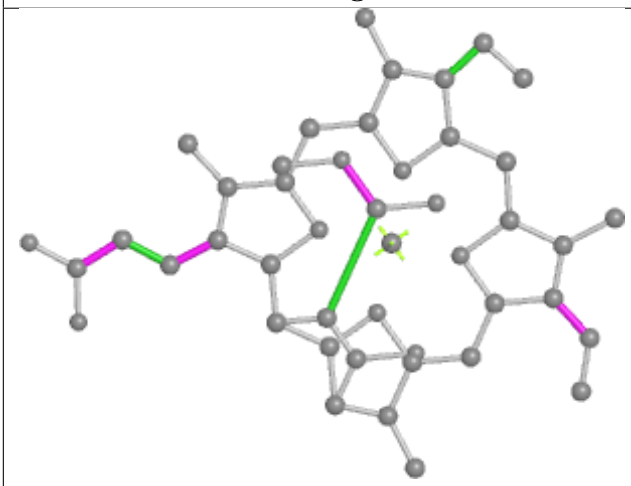


Bond angles



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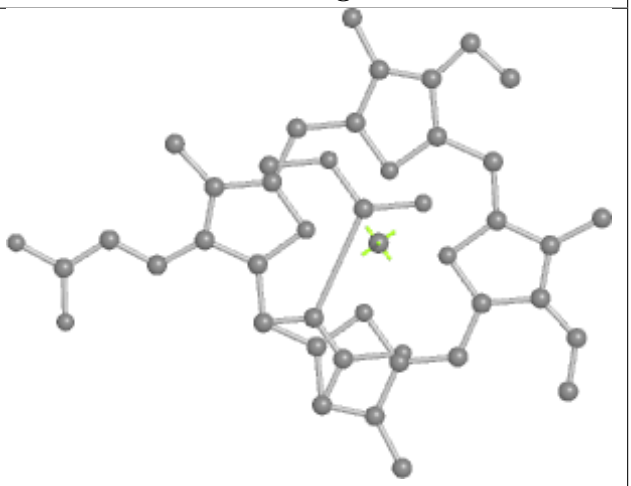
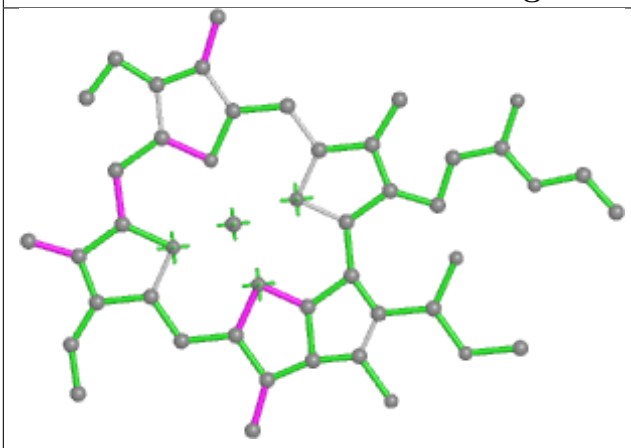


Rings

Ligand CLA N 314



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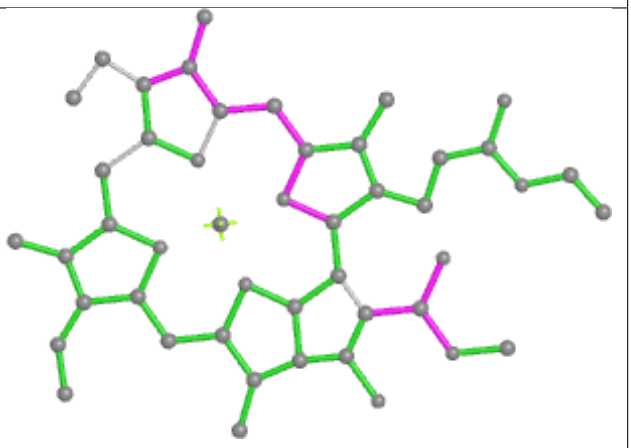
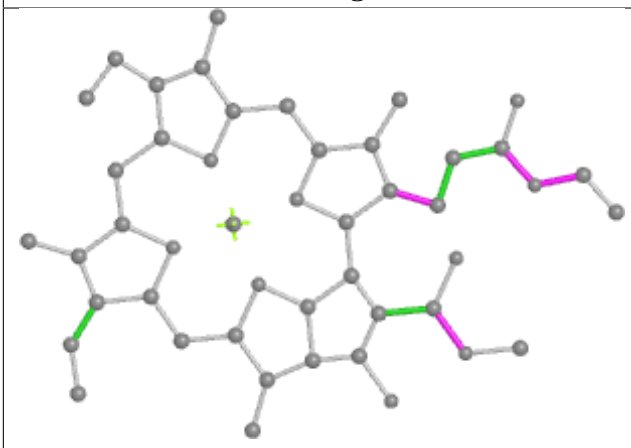


Bond angles



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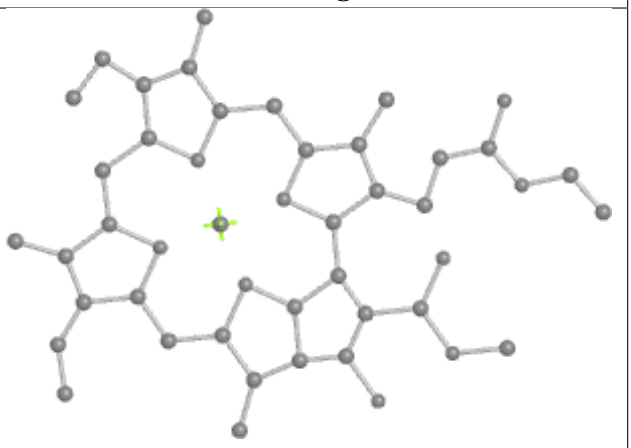
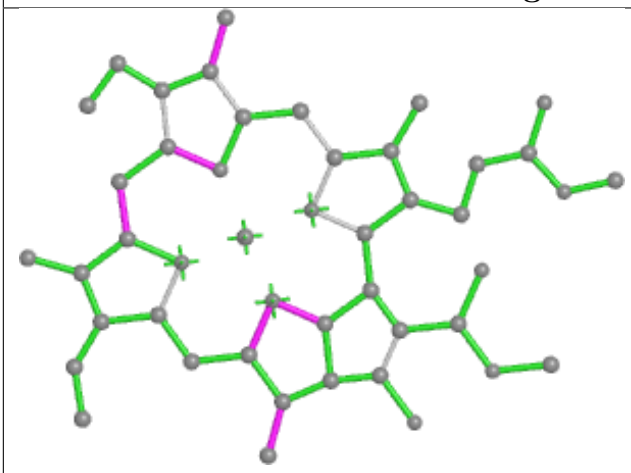


Rings

Ligand CLA D 309



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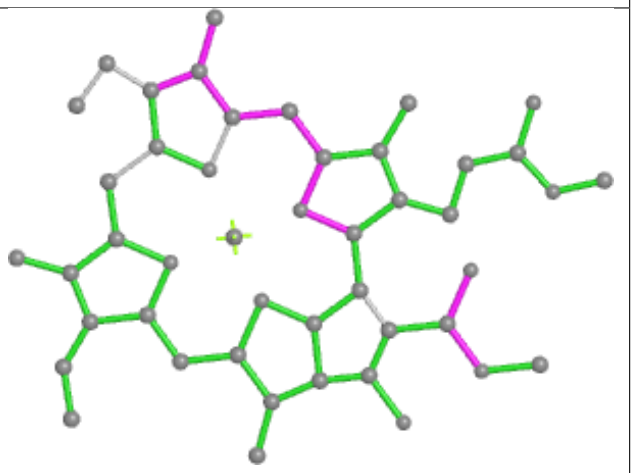
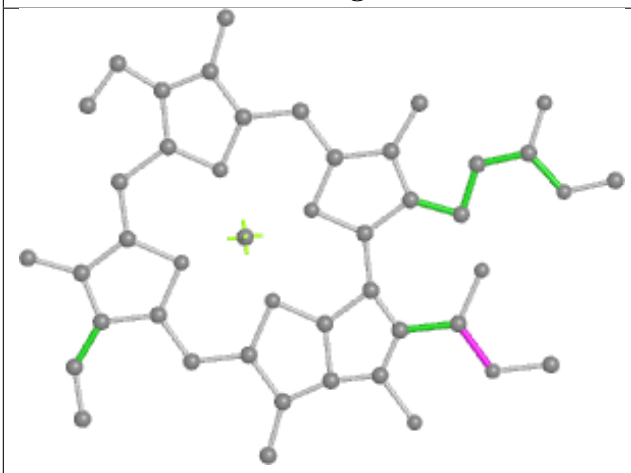


Bond angles



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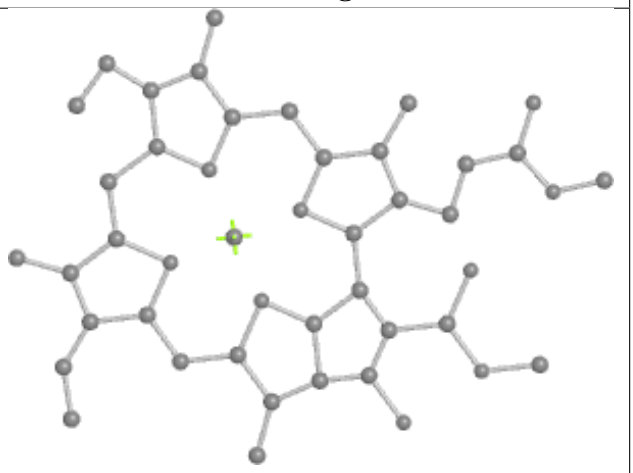
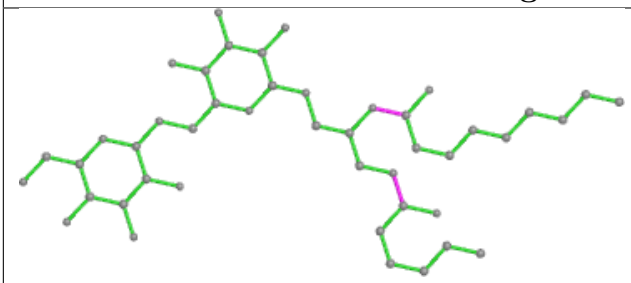


Rings

Ligand DGD B 318



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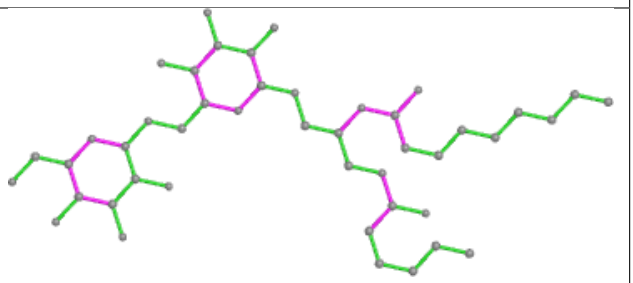
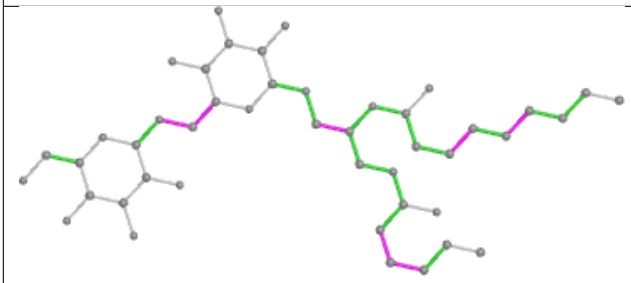


Bond angles



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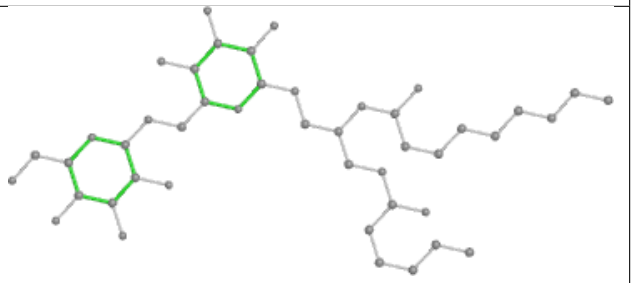
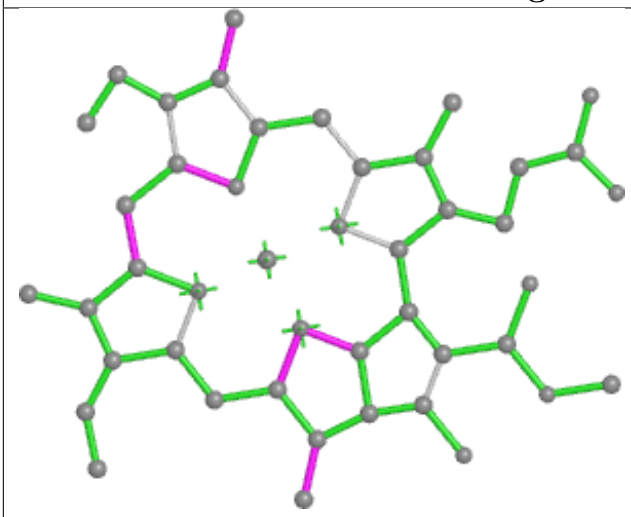


Rings

Ligand CLA a 817



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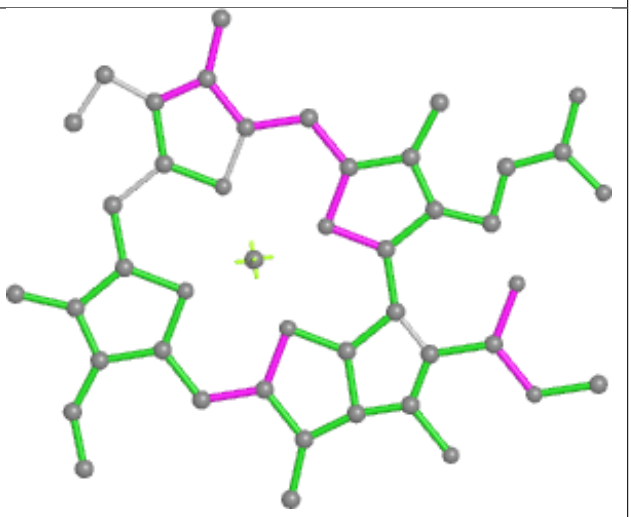
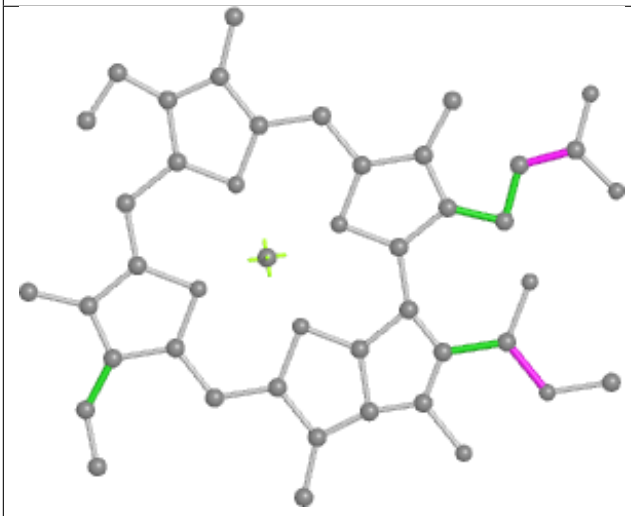


Bond angles



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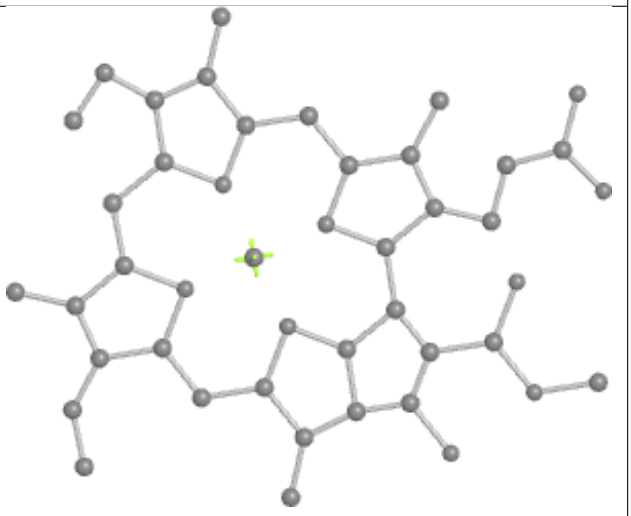
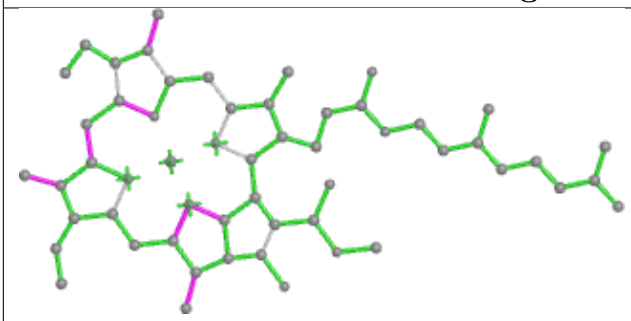


Rings

Ligand CLA M 307



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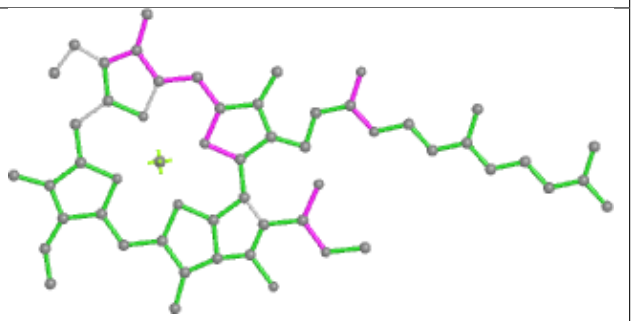
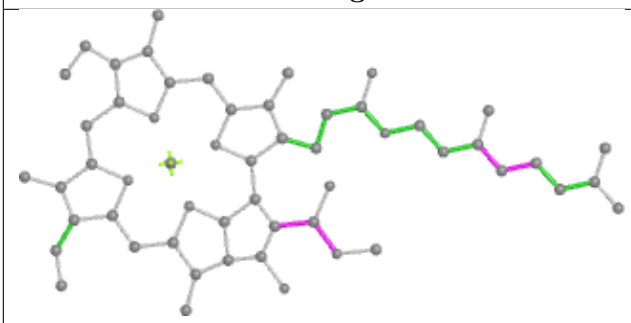


Bond angles



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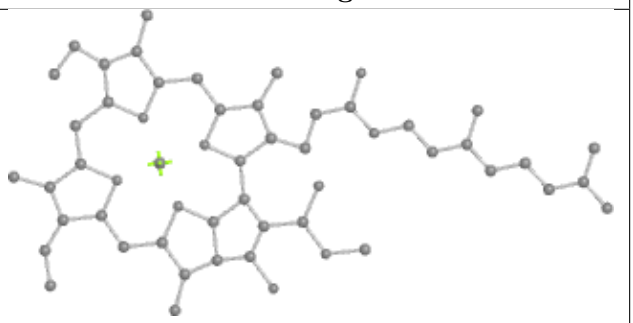
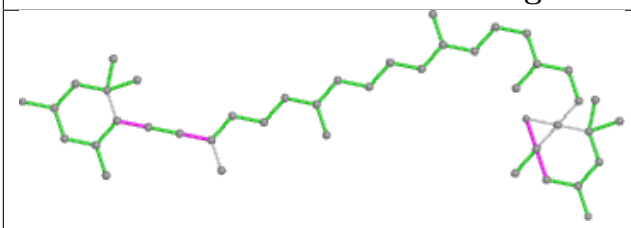


Rings

Ligand DD6 D 304



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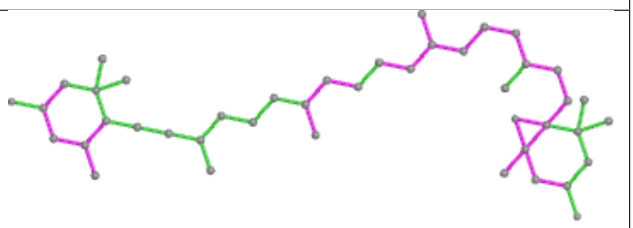
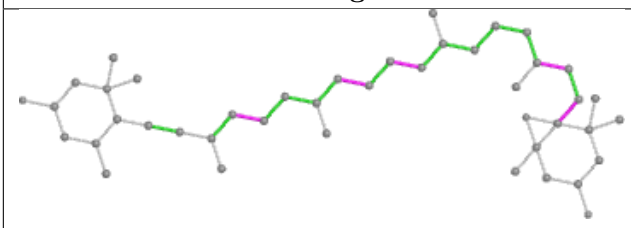


Bond angles



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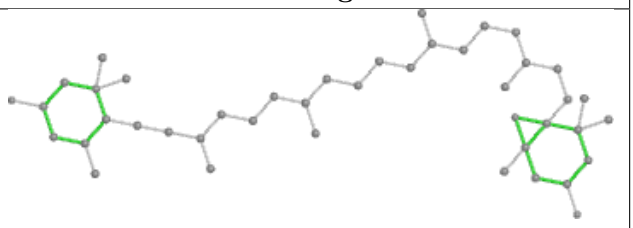
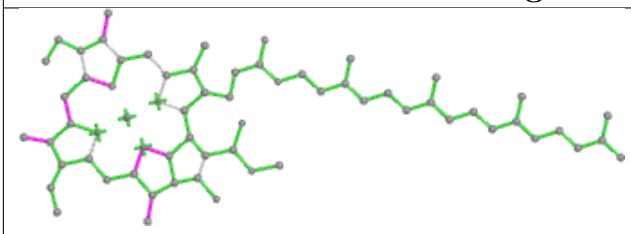


Rings

Ligand CLA E 306



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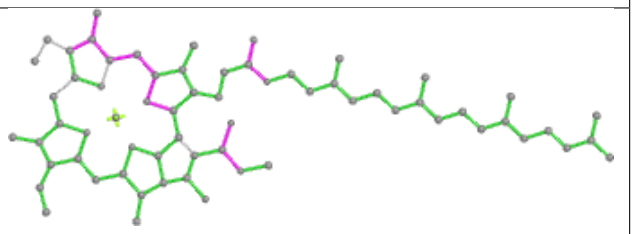
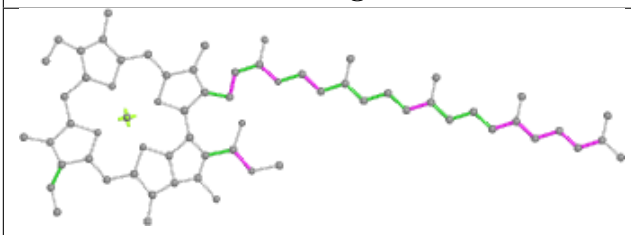


Bond angles



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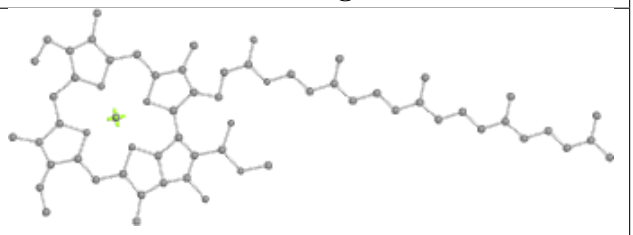
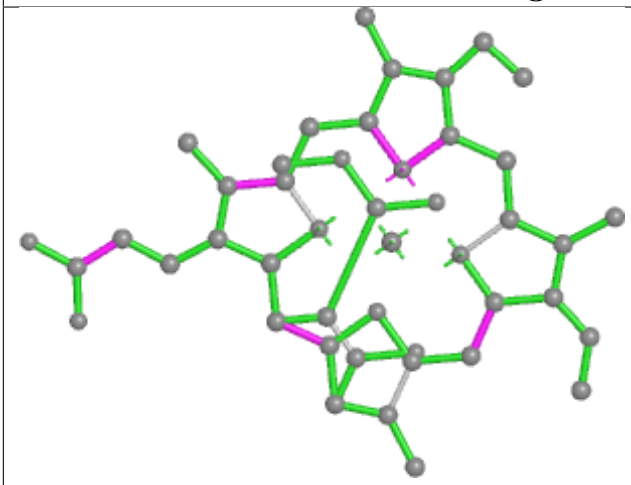


Rings

Ligand KC1 E 307



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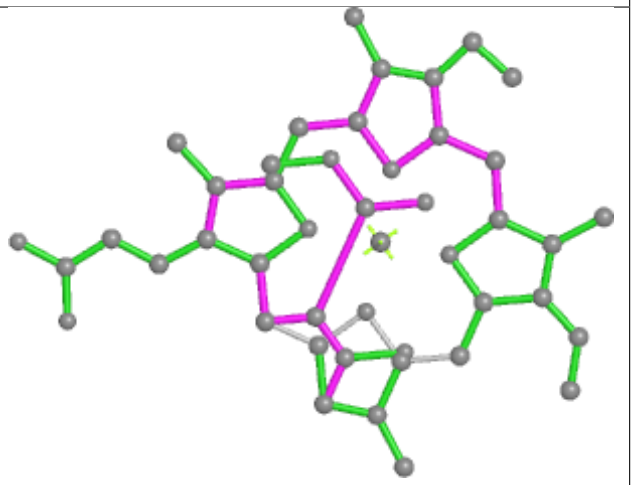
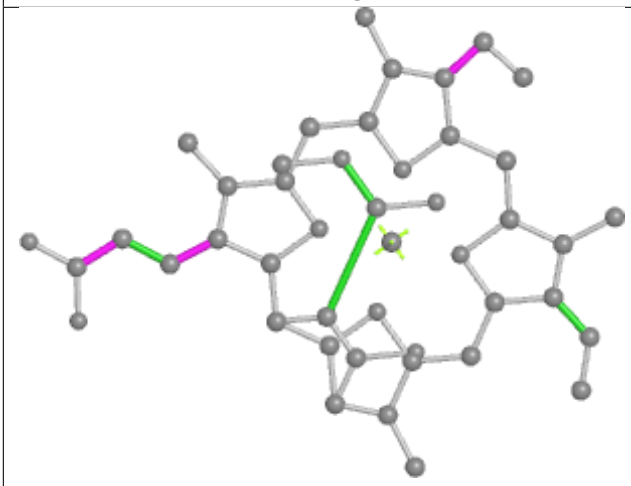


Bond angles



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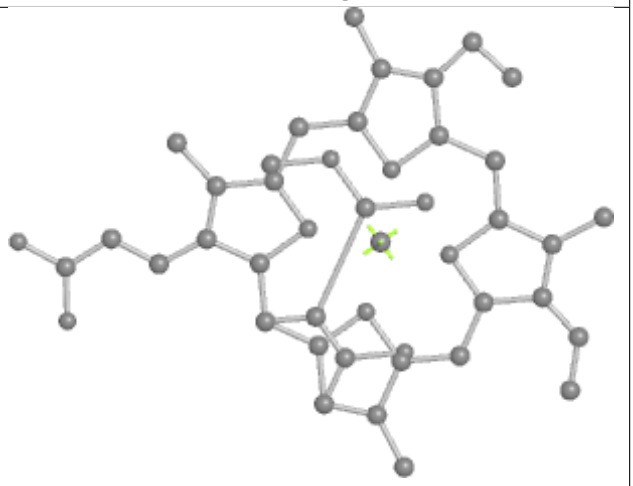
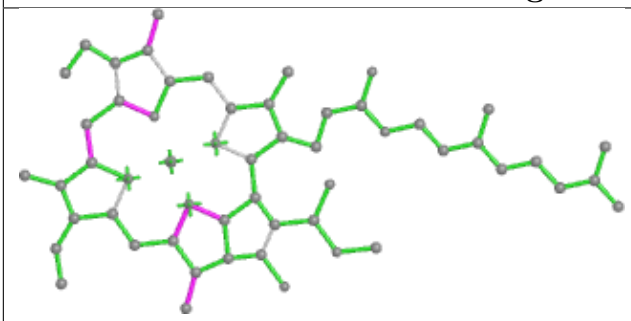


Rings

Ligand CLA L 312



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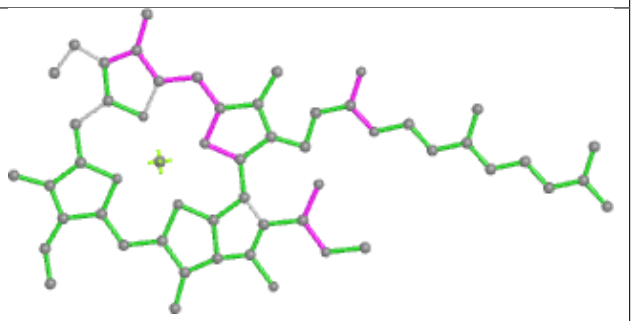
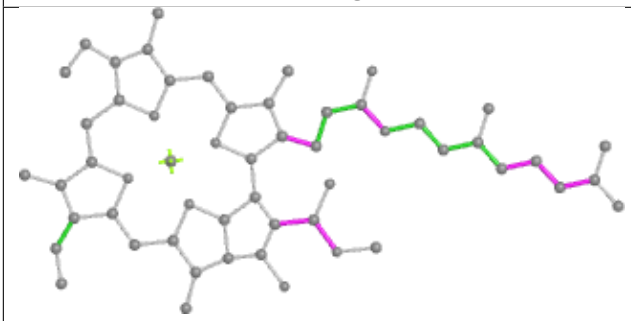


Bond angles



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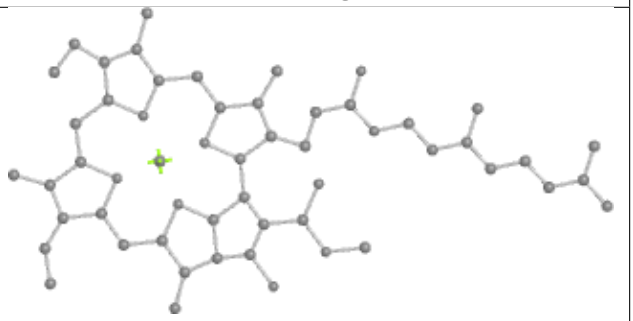
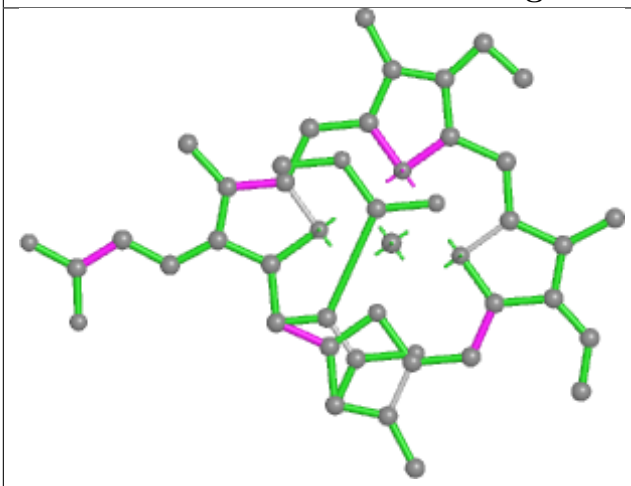
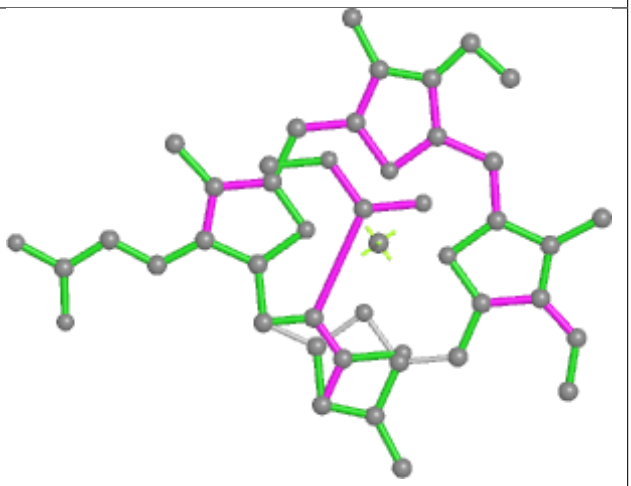


Rings

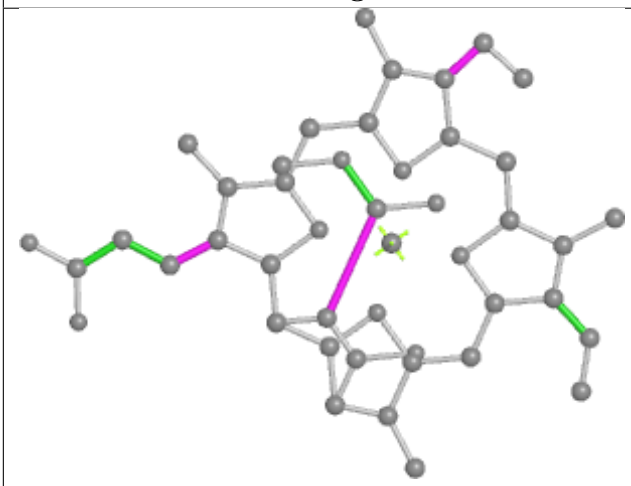
Ligand KC1 O 312



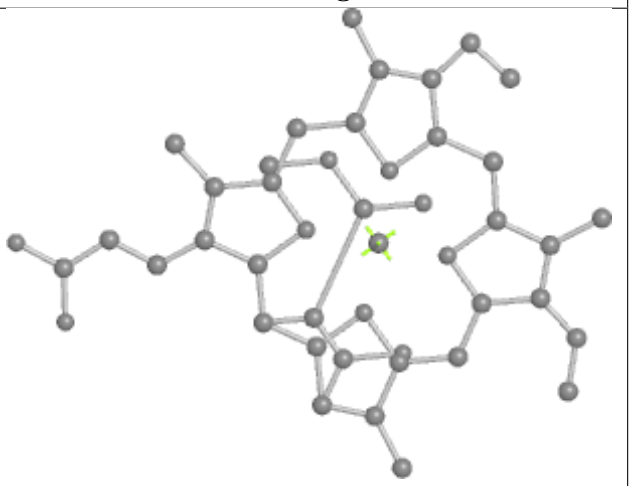
Bond lengths



Bond angles

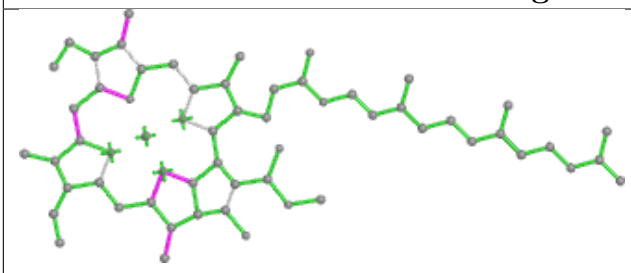


Torsions

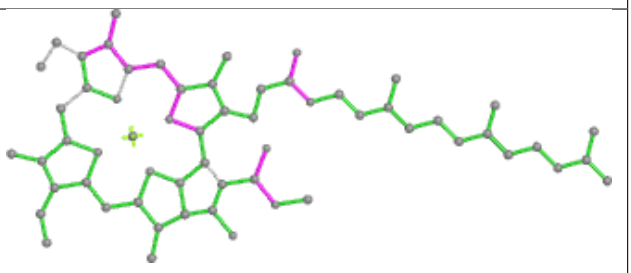


Rings

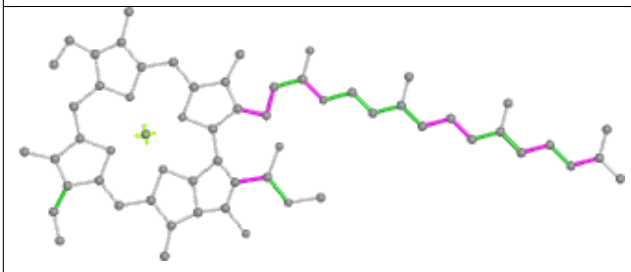
Ligand CLA f 805



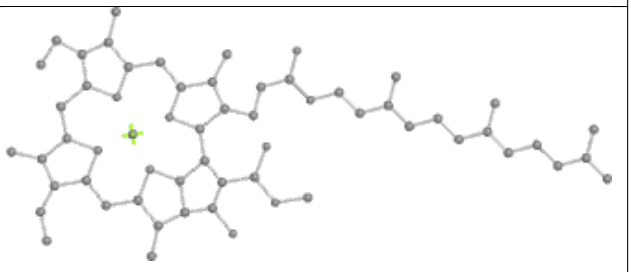
Bond lengths



Bond angles

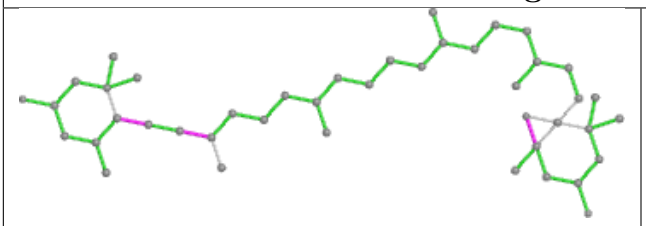


Torsions

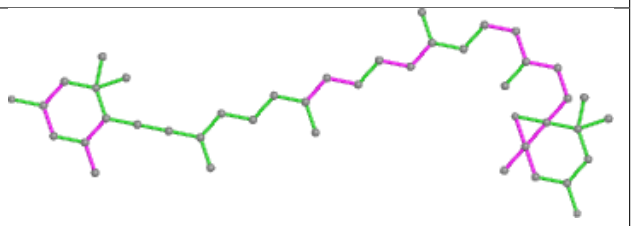


Rings

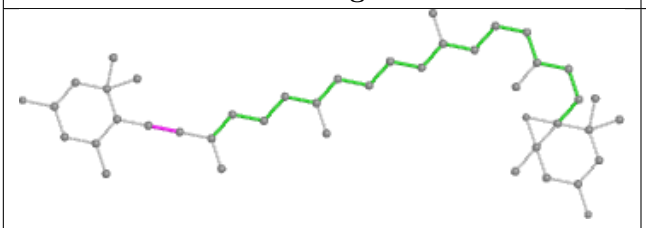
Ligand DD6 A 202



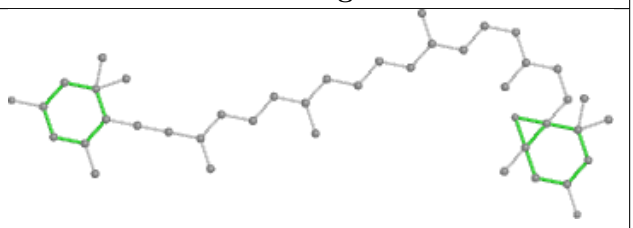
Bond lengths



Bond angles

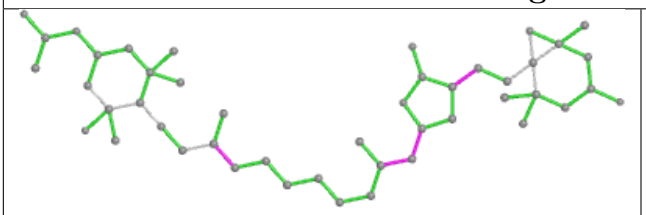


Torsions

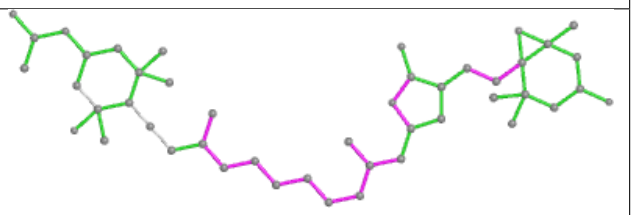


Rings

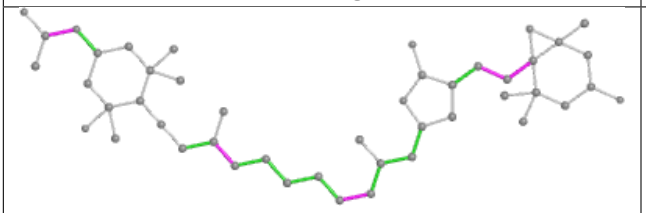
Ligand PID C 305



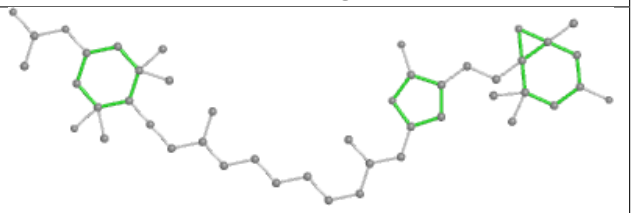
Bond lengths



Bond angles

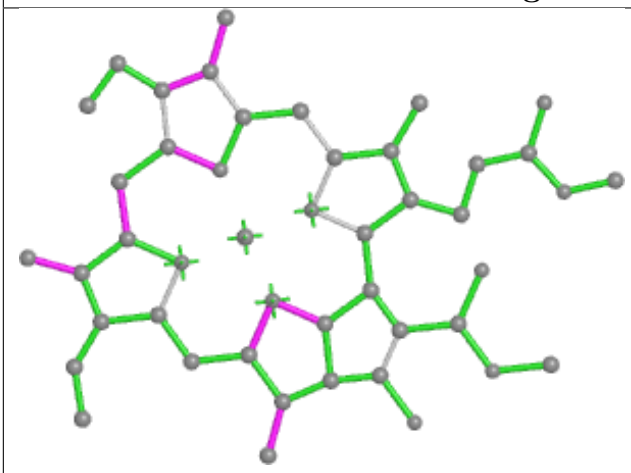


Torsions

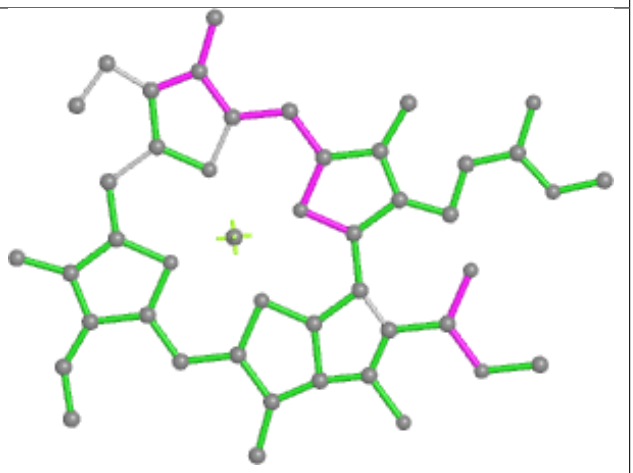


Rings

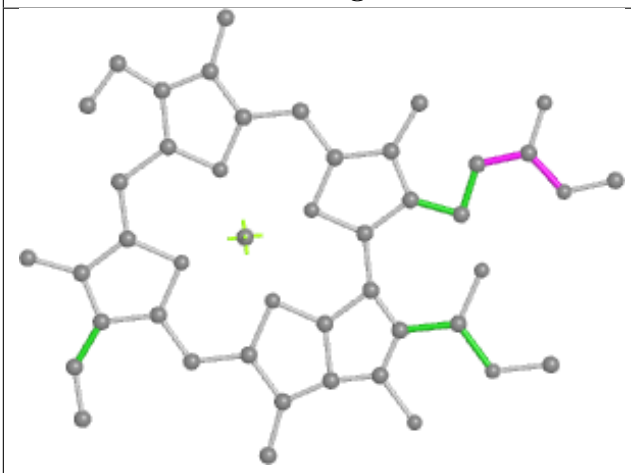
Ligand CLA K 217



Bond lengths



Bond angles



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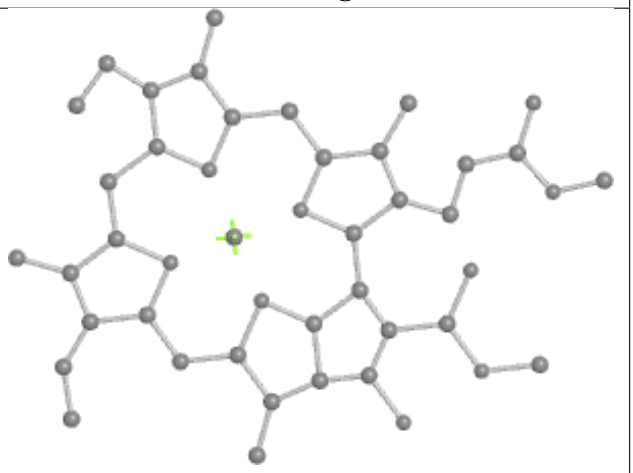
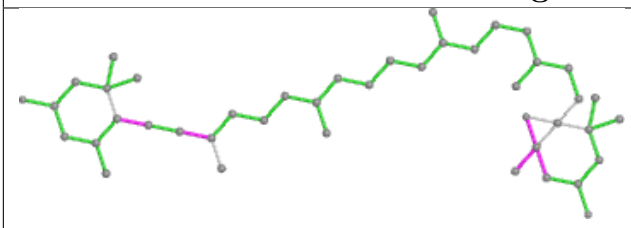


Rings

Ligand DD6 I 204



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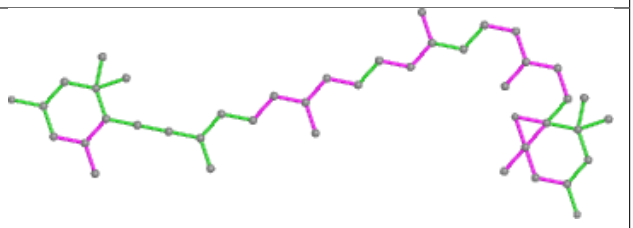
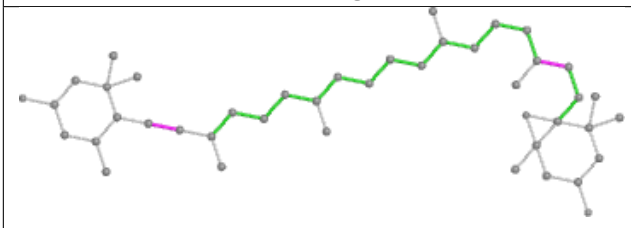
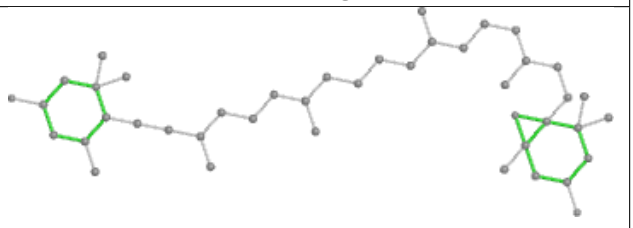


Bond angles

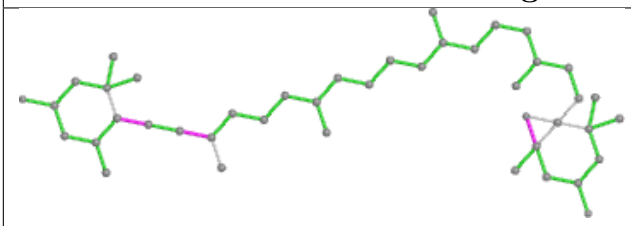


Torsions



Rings

Ligand DD6 M 301



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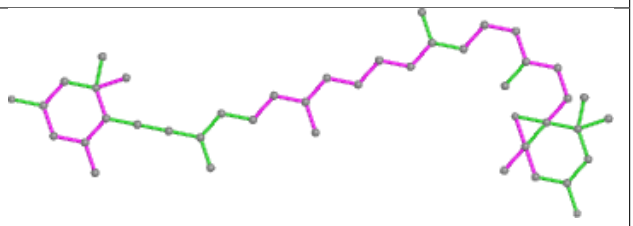
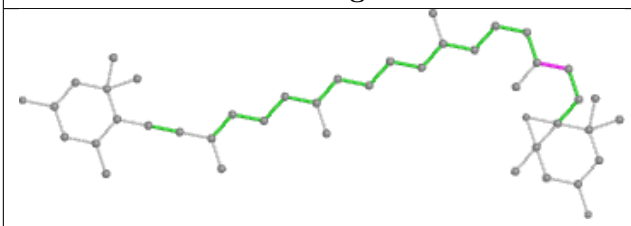


Bond angles



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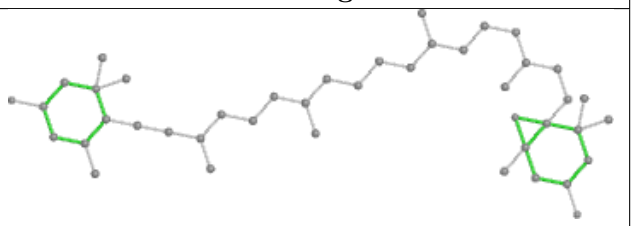
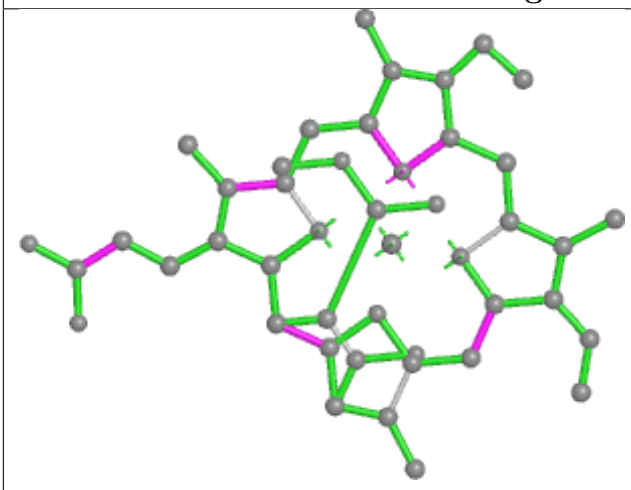
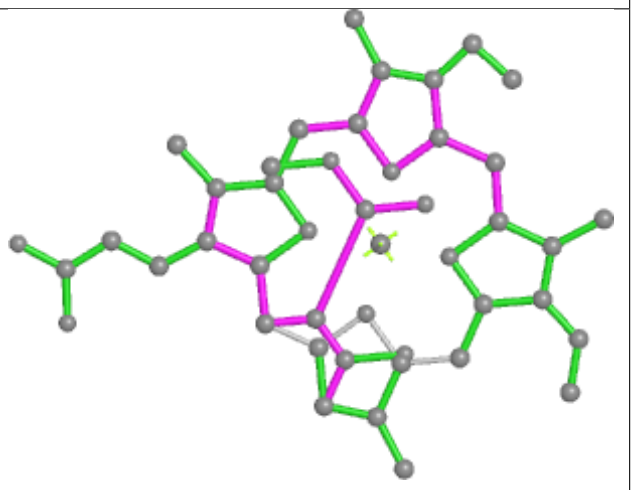


Rings

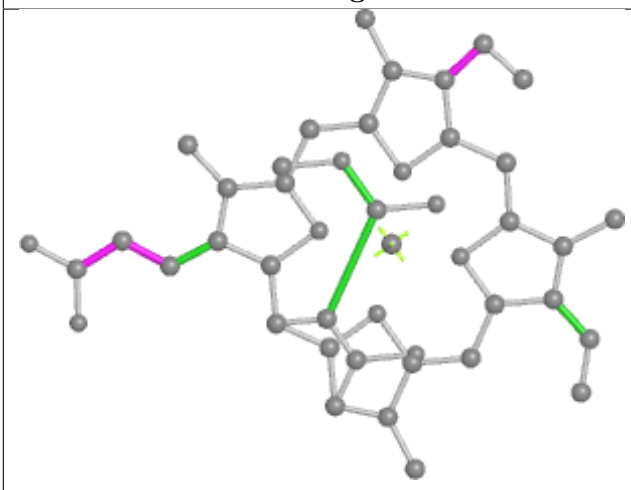
Ligand KC1 G 318



Bond lengths



Bond angles



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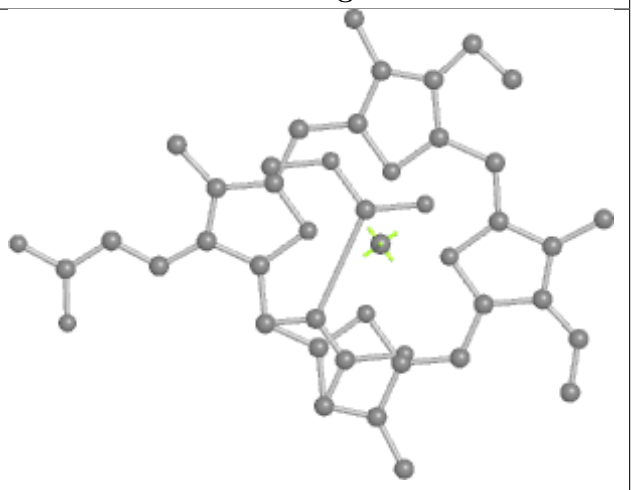
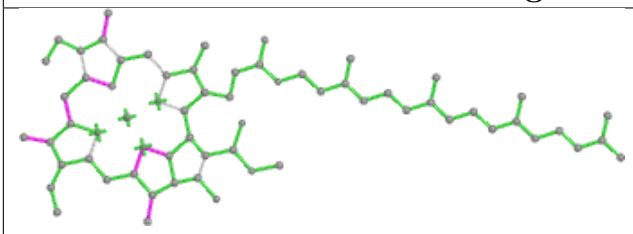


Rings

Ligand CLA E 311



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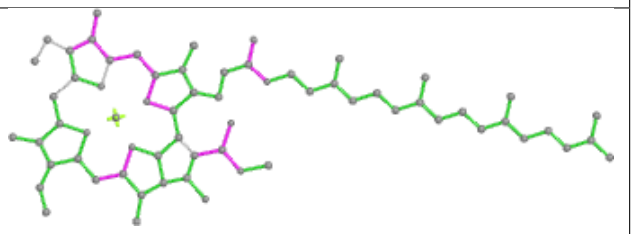
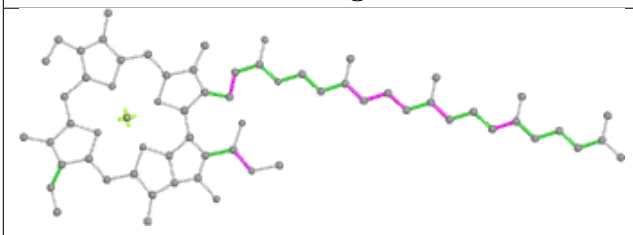


Bond angles



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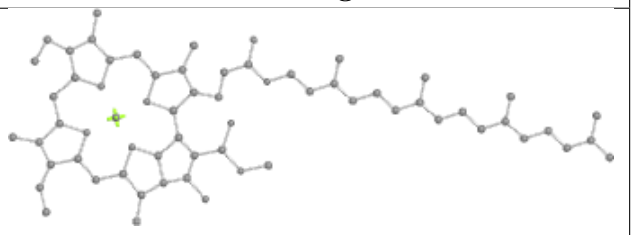
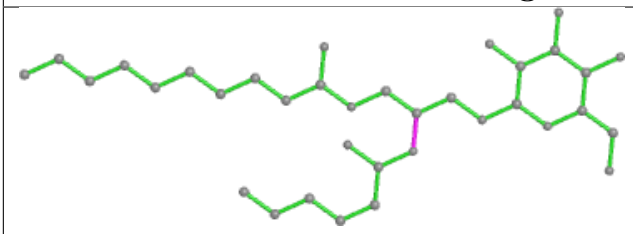
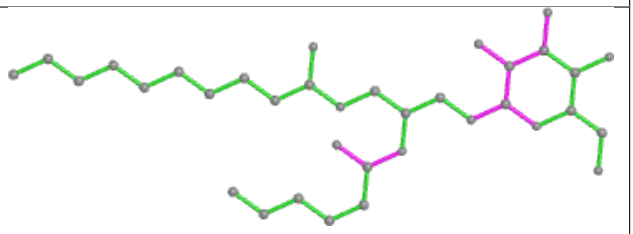


Rings

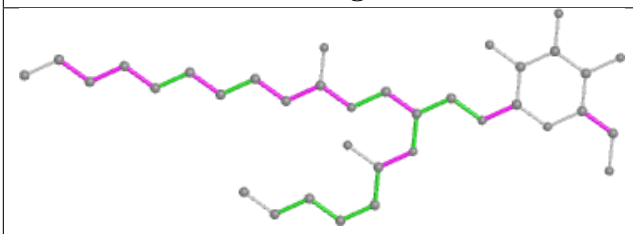
Ligand LMG K 219



Bond lengths



Bond angles



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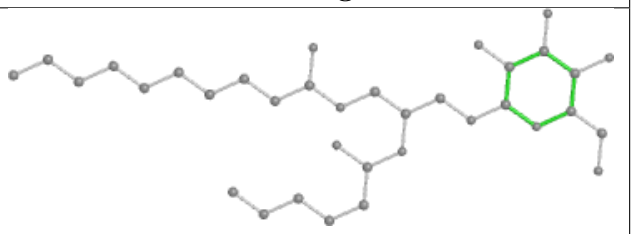
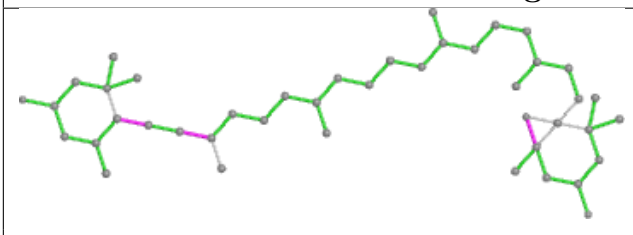


Rings

Ligand DD6 H 303



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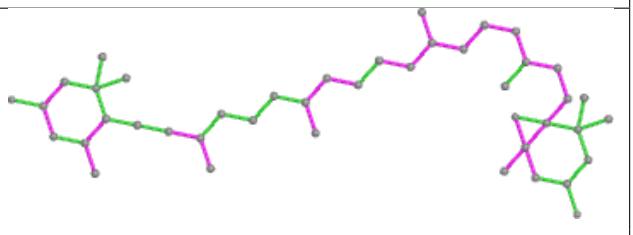
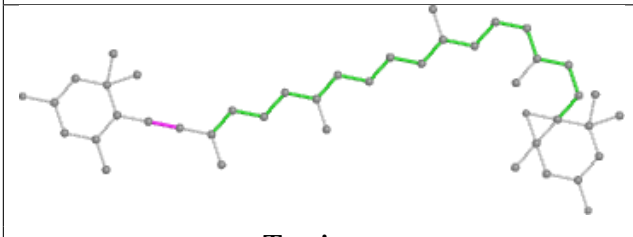


Bond angles



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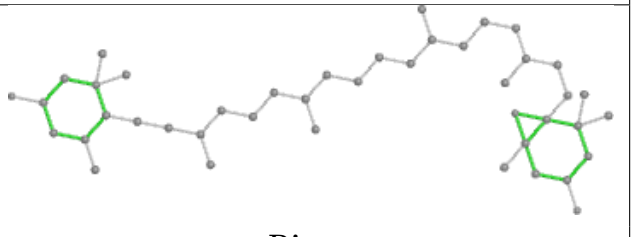
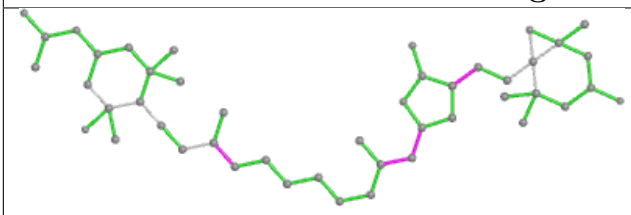


Rings

Ligand PID T 302



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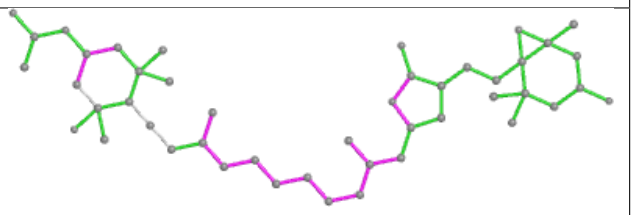
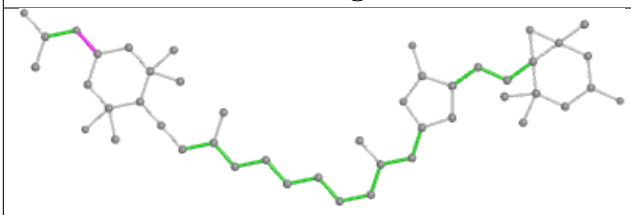


Bond angles



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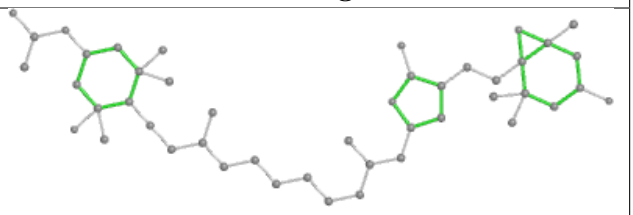
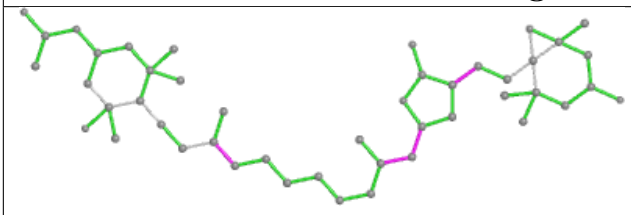


Rings

Ligand PID D 305



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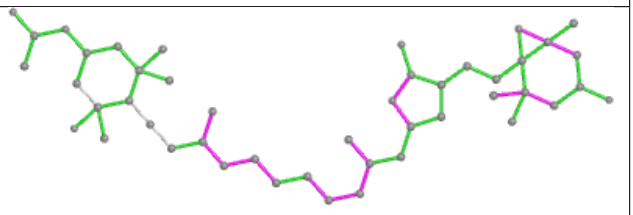
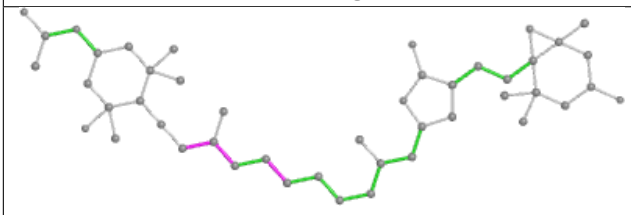


Bond angles



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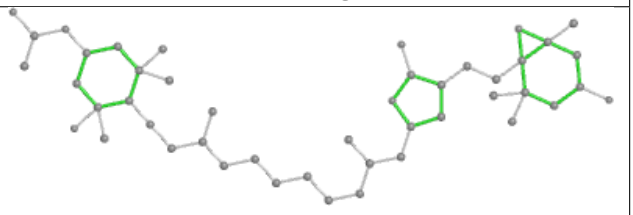
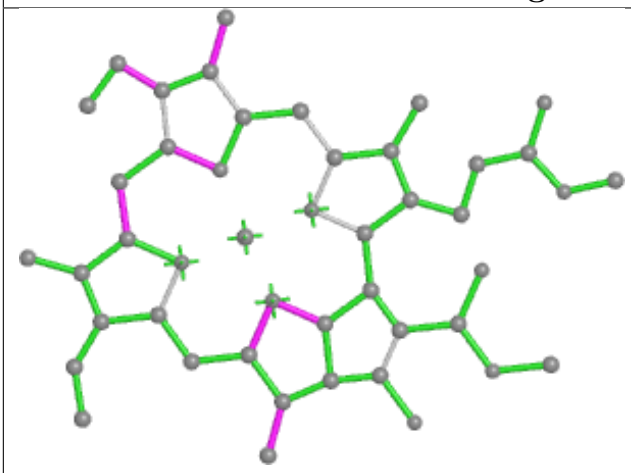


Rings

Ligand CLA J 307



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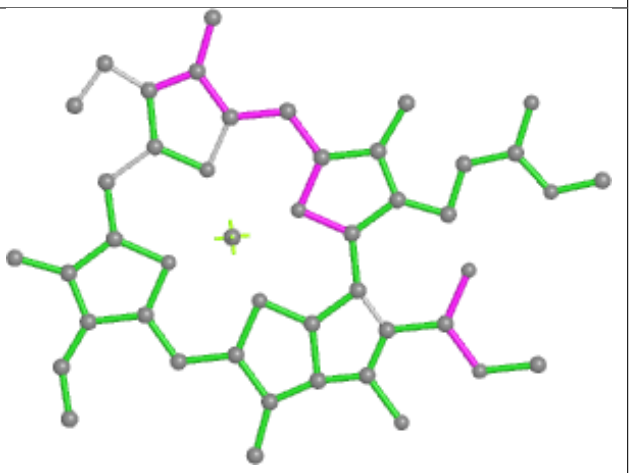
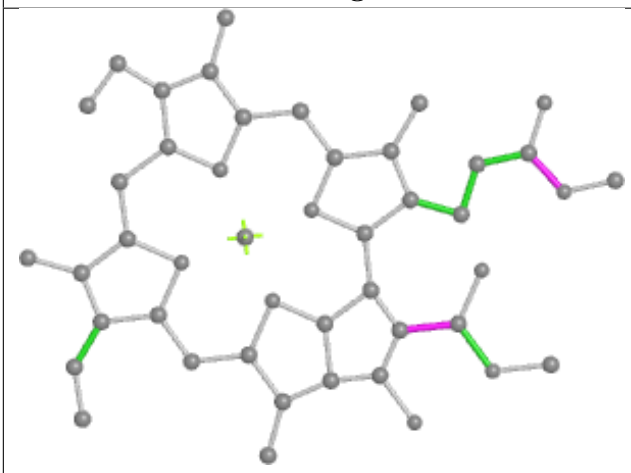


Bond angles



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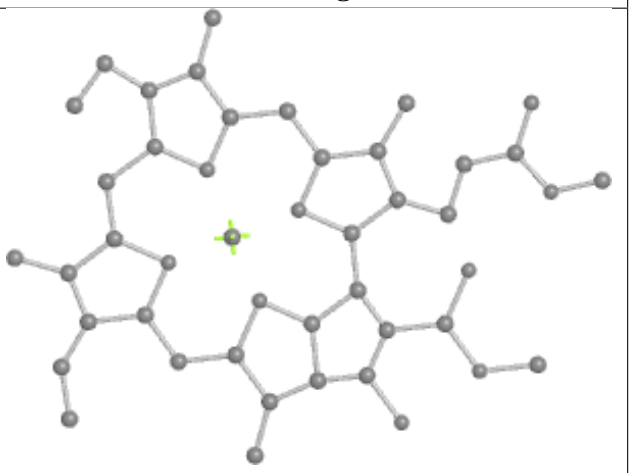
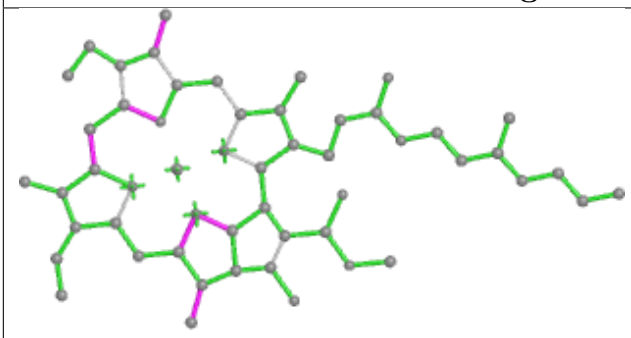


Rings

Ligand CLA M 306



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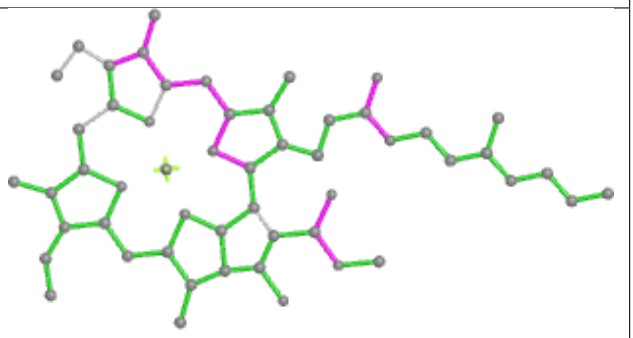
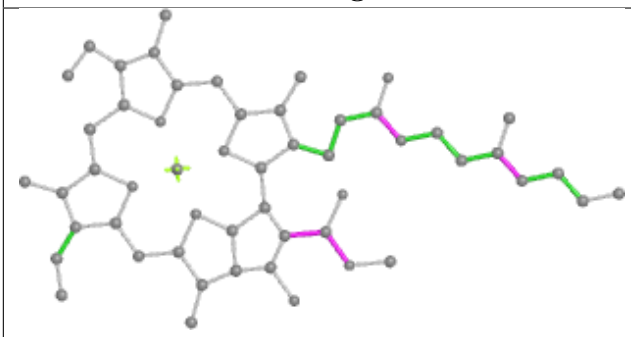
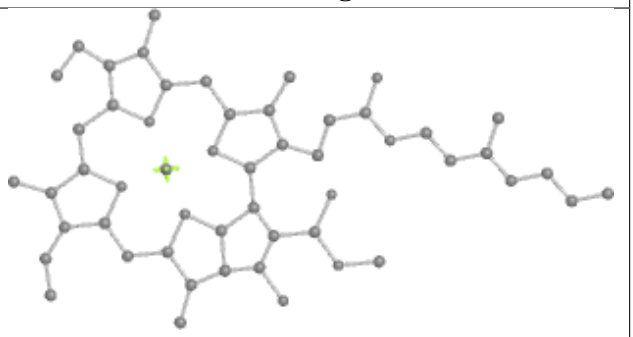


Bond angles

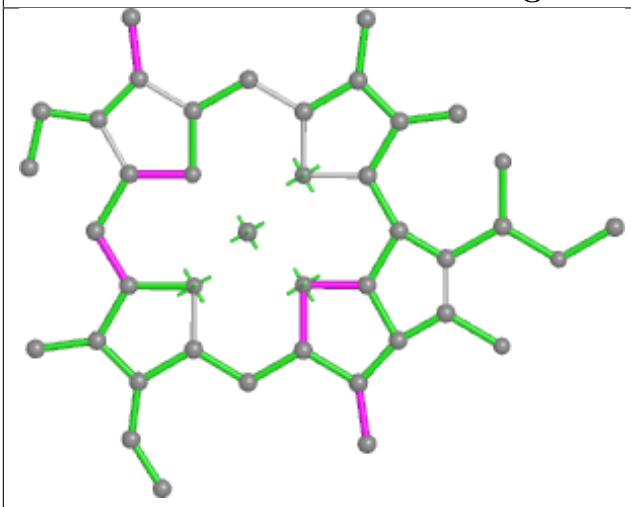


Torsions

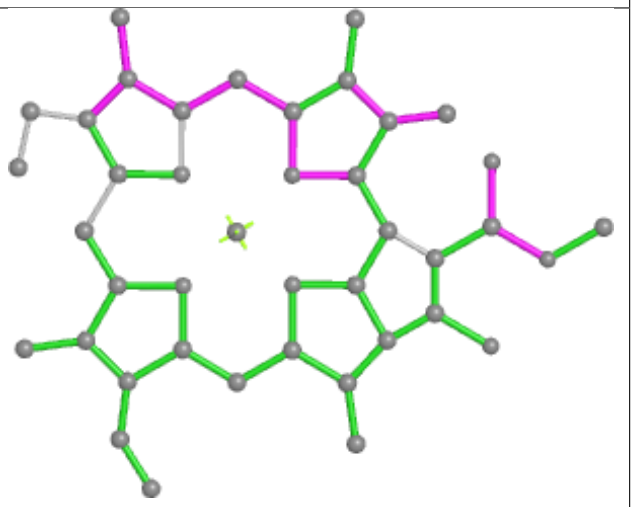


Rings

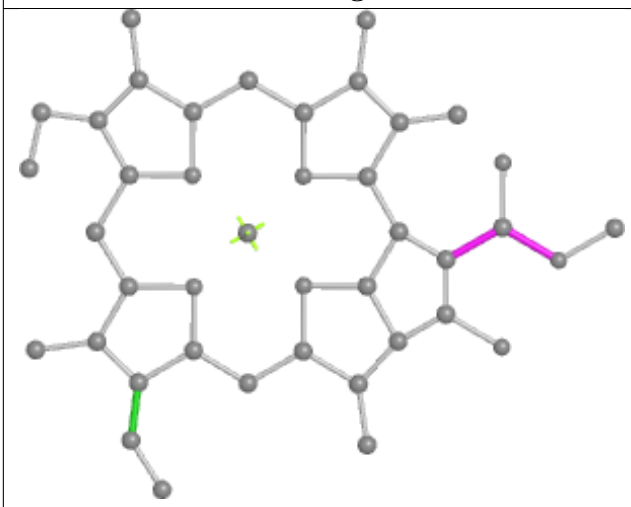
Ligand CLA A 214



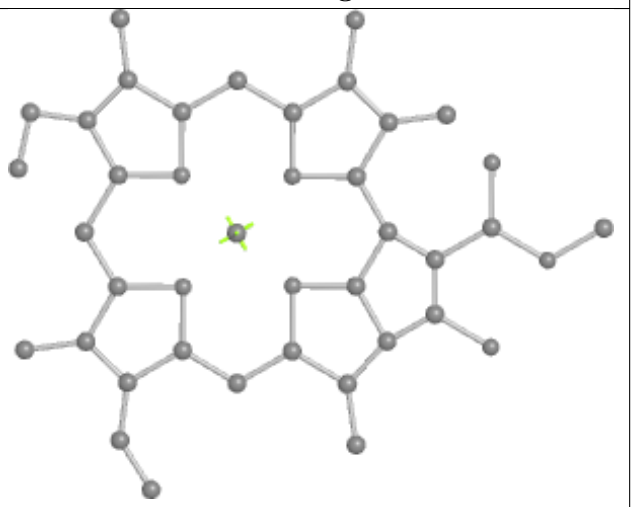
Bond lengths



Bond angles

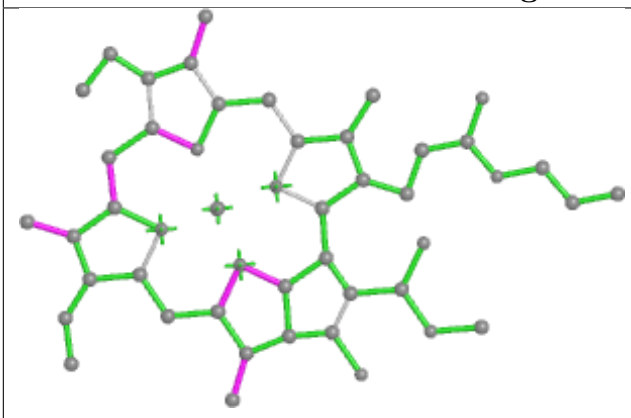


Torsions

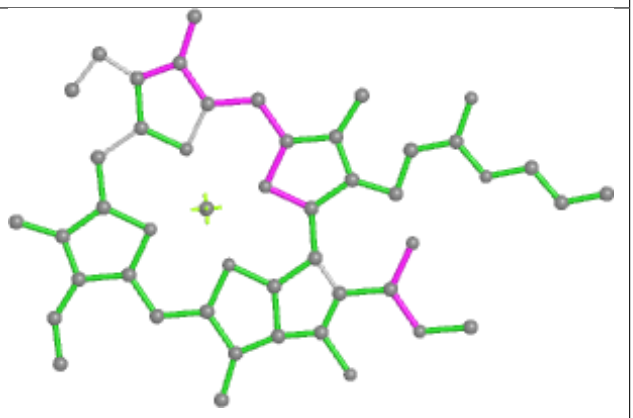


Rings

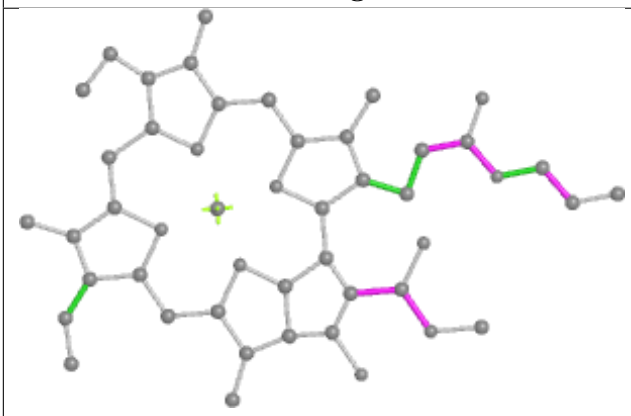
Ligand CLA M 308



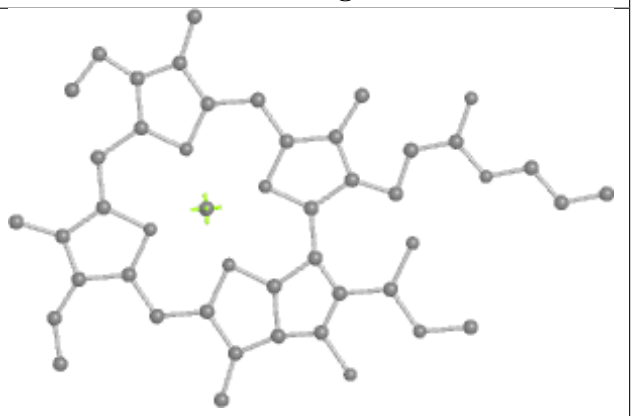
Bond lengths



Bond angles

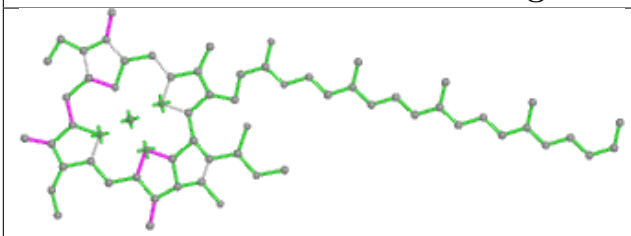


Torsions



Rings

Ligand CLA b 714



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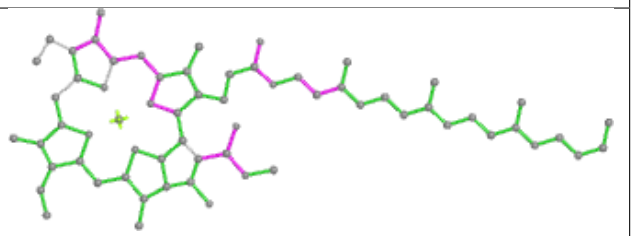
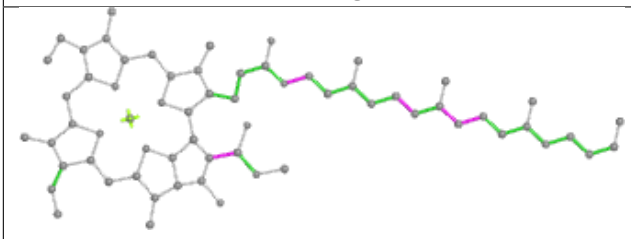


Bond angles



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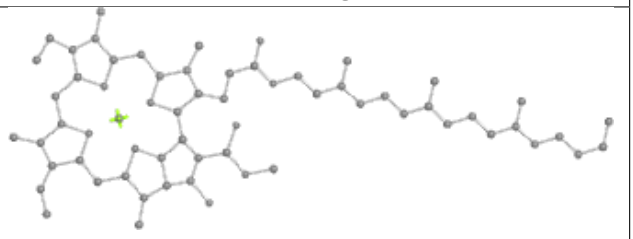
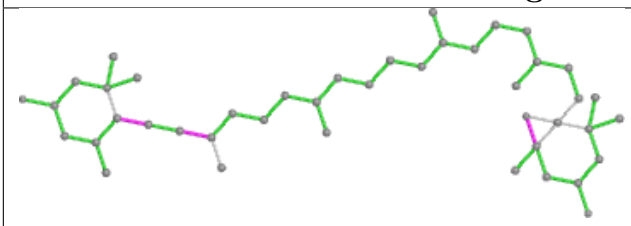


Rings

Ligand DD6 P 204



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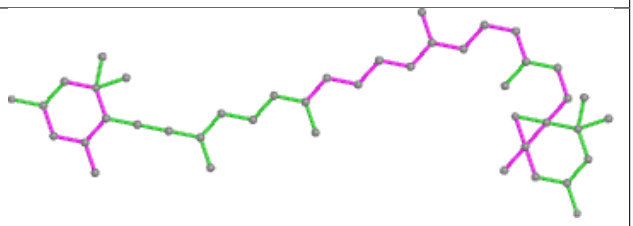

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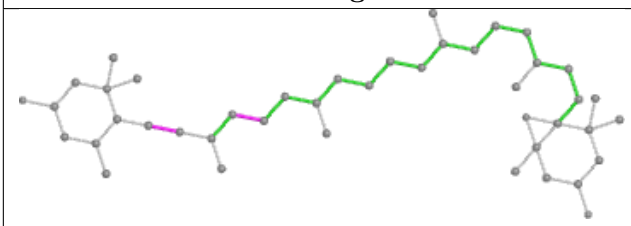

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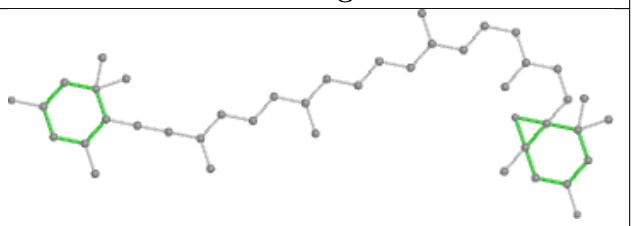
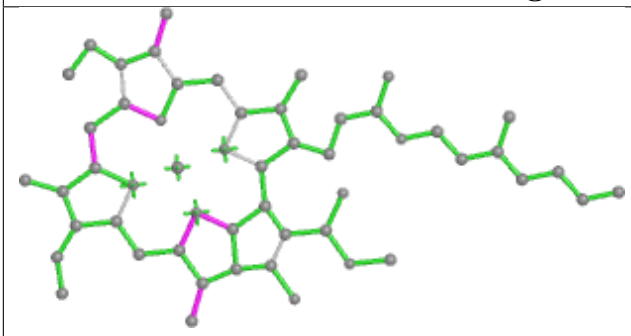


Rings

Ligand CLA L 308



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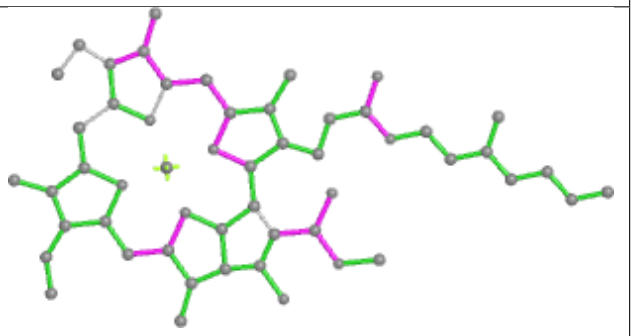

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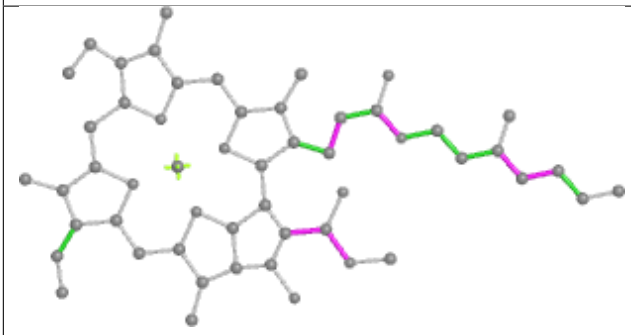

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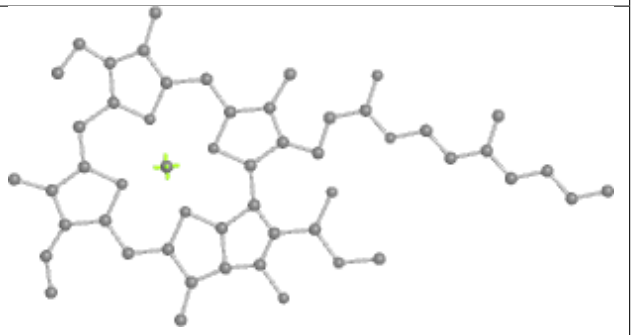
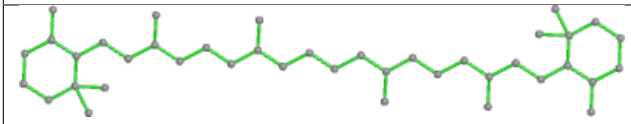


Rings

Ligand BCR f 801



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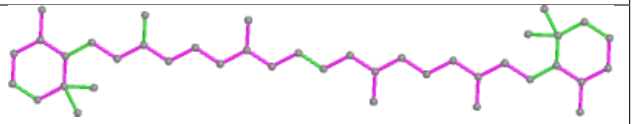

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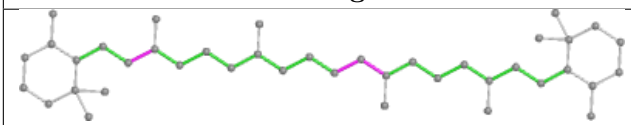

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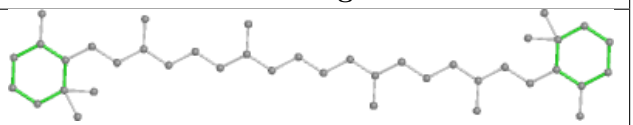
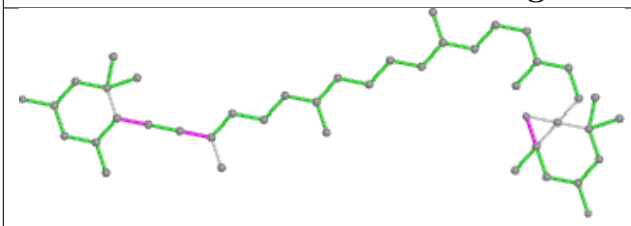


Rings

Ligand DD6 L 304



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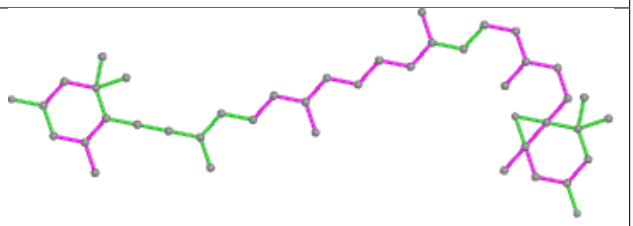

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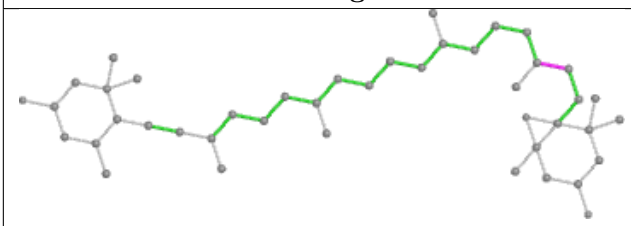

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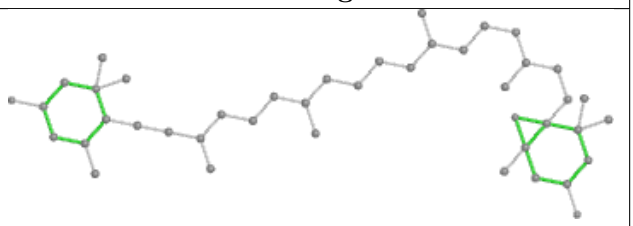
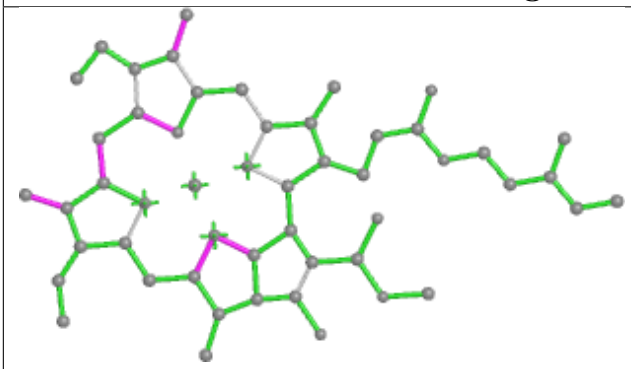


Rings

Ligand CLA O 311



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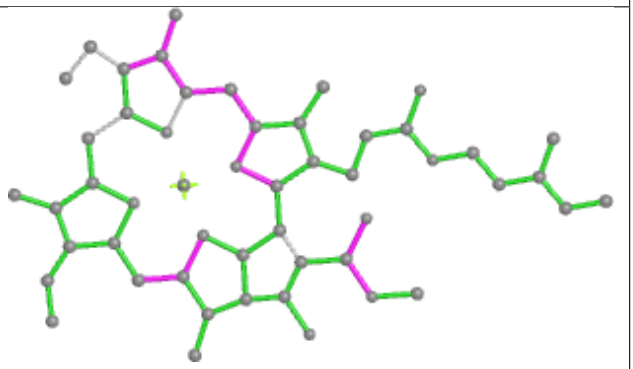

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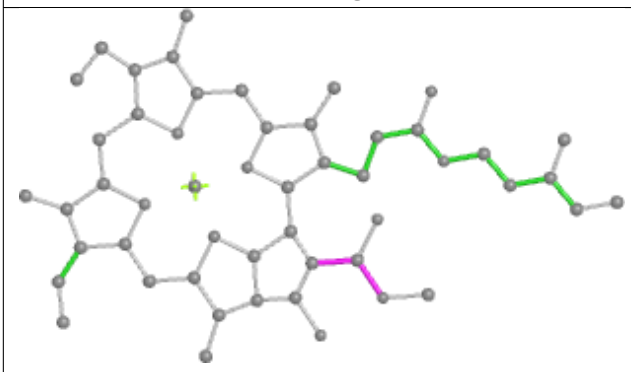

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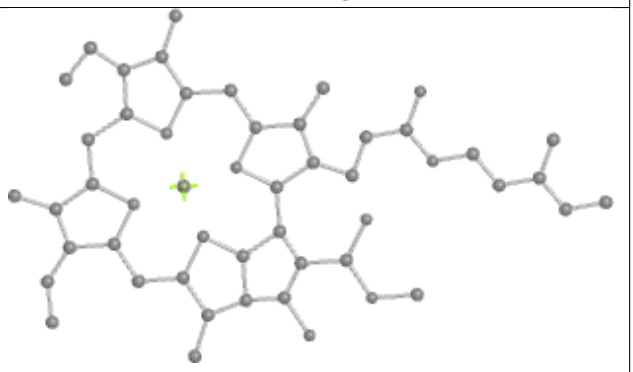
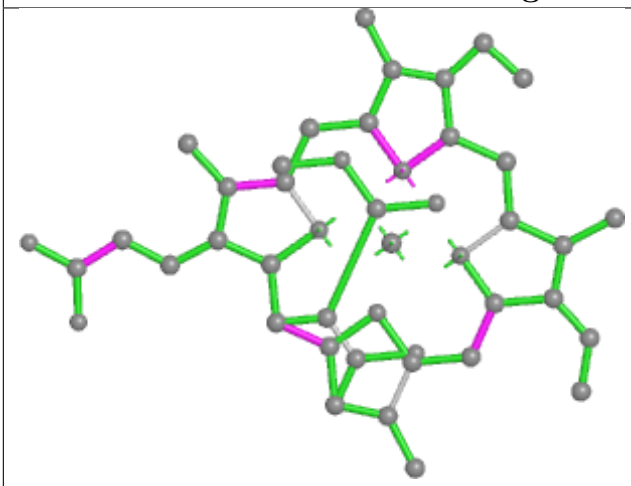


Rings

Ligand KC1 M 312



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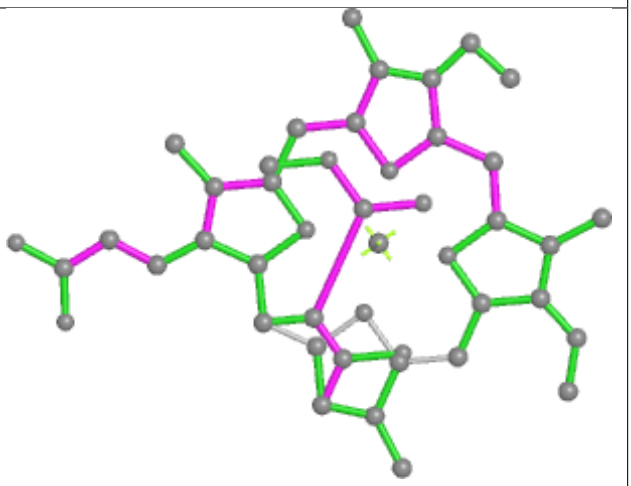

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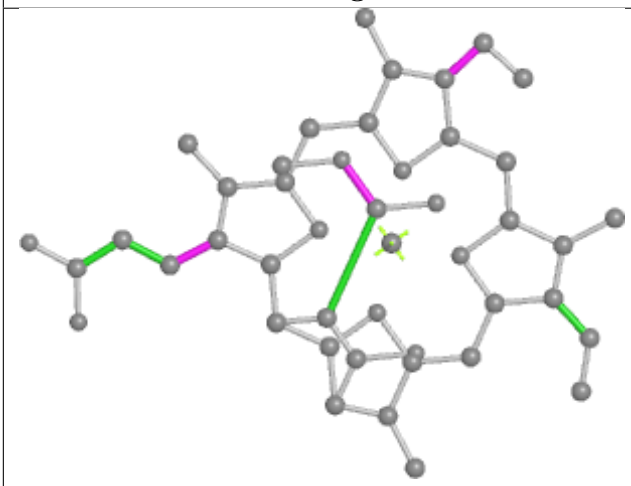

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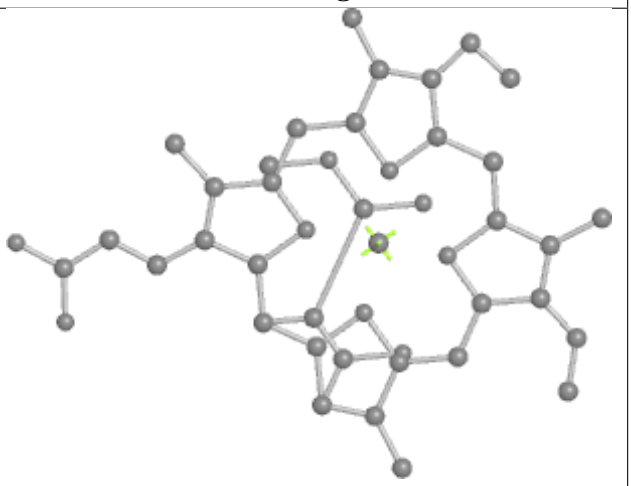
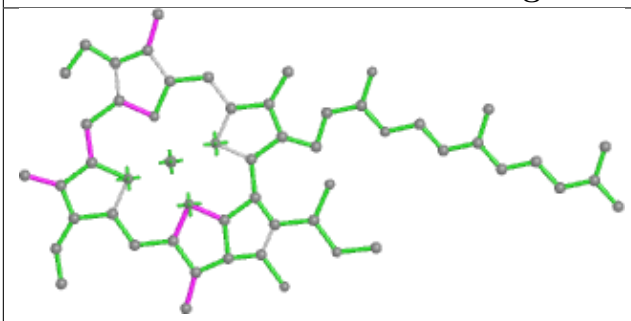


Rings

Ligand CLA K 211



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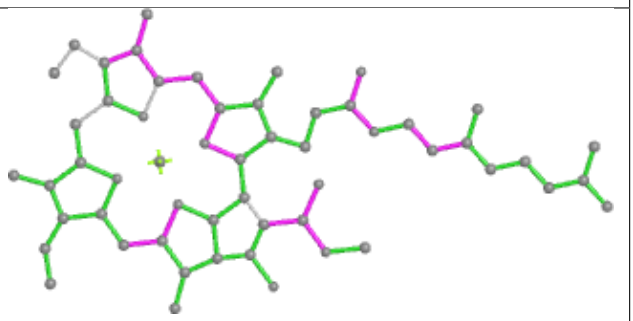

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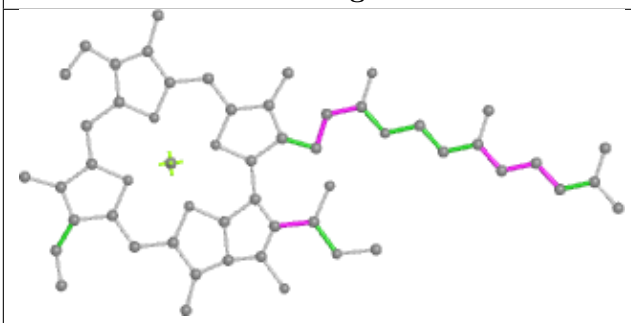

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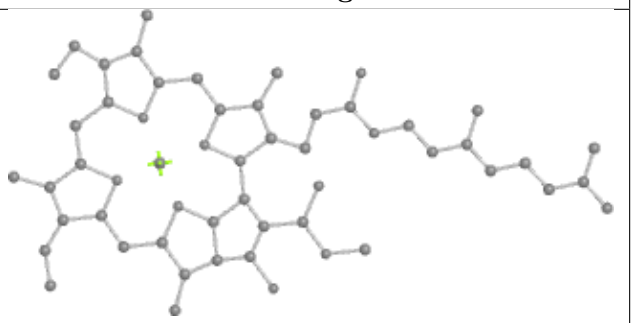
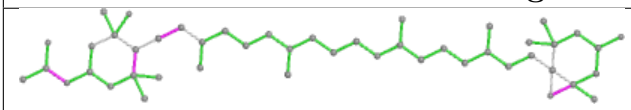


Rings

Ligand UIX Q 305



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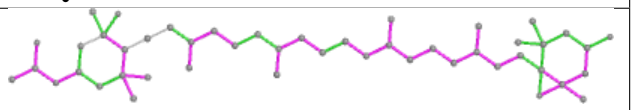

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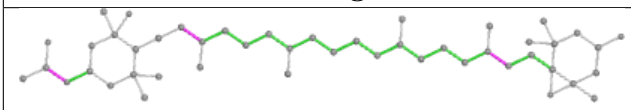

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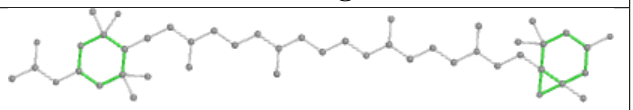
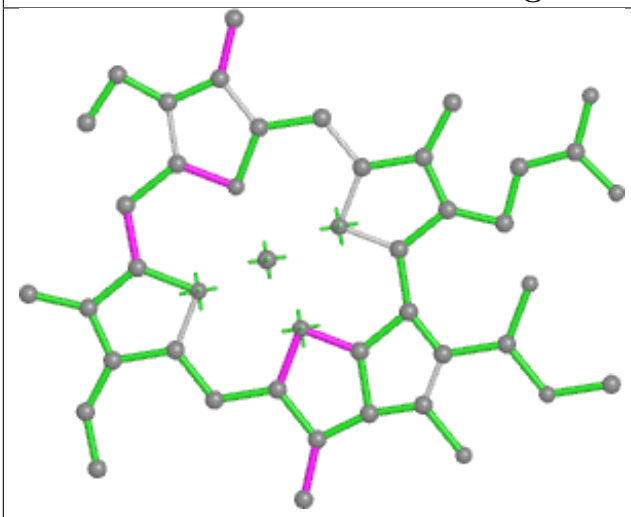


Rings

Ligand CLA B 307



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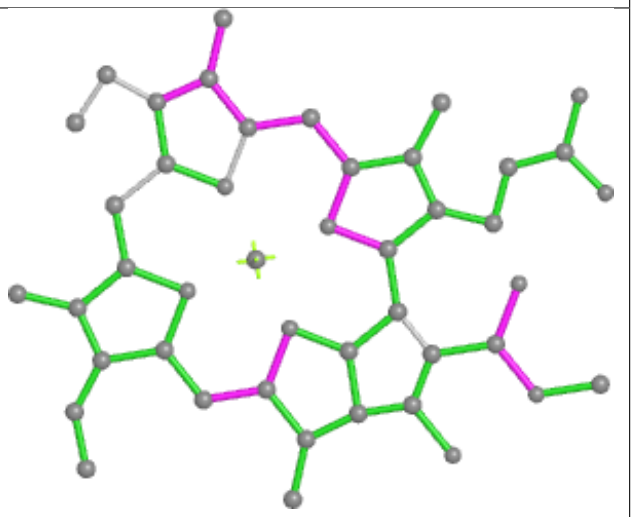

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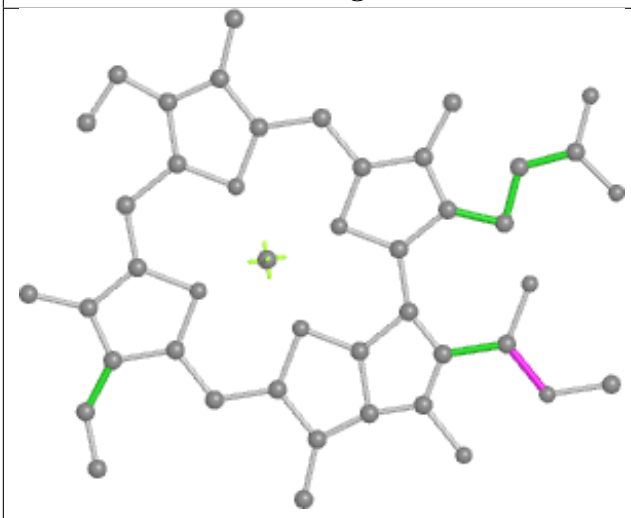

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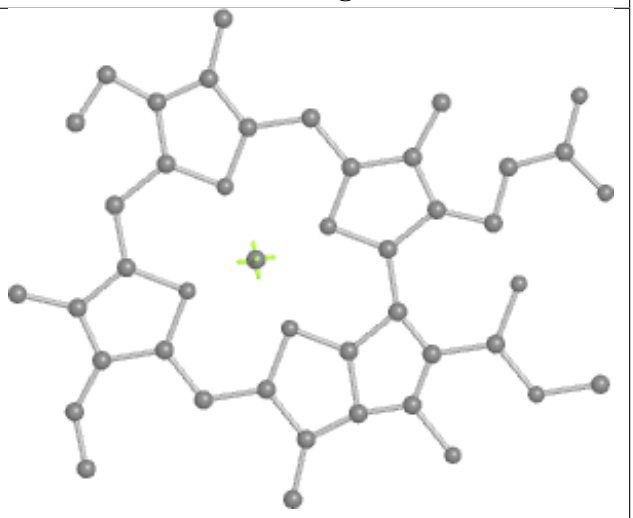
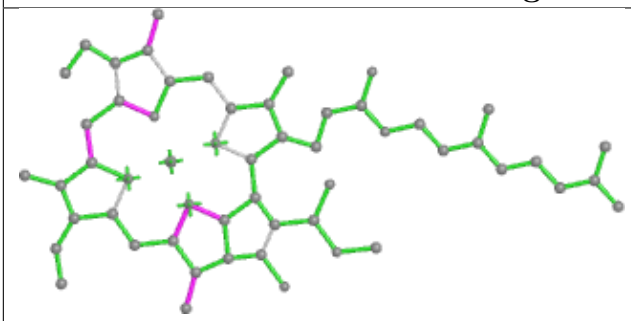


Rings

Ligand CLA G 313



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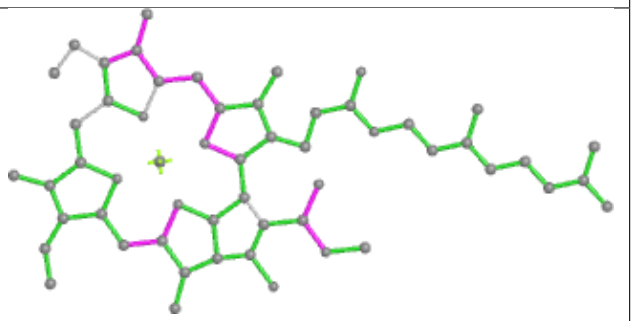

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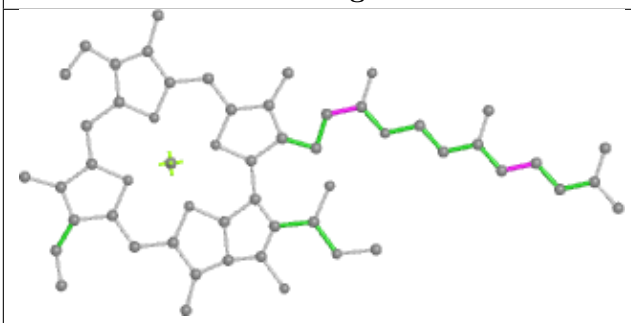

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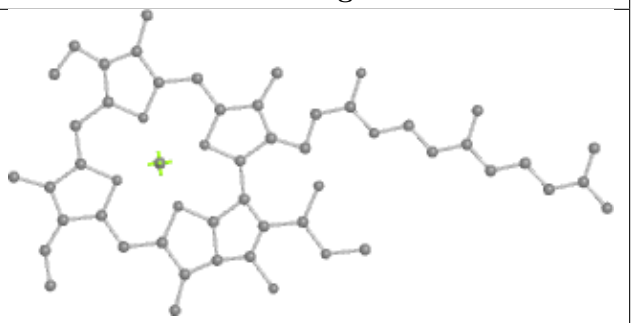
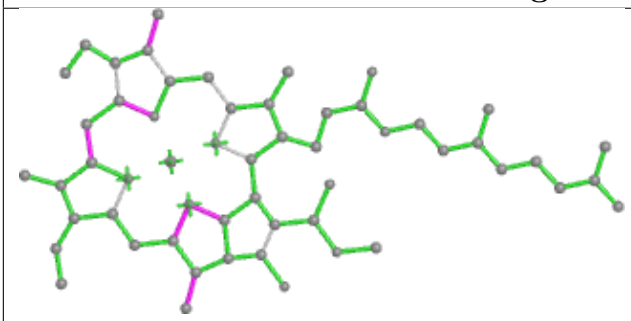


Rings

Ligand CLA I 217



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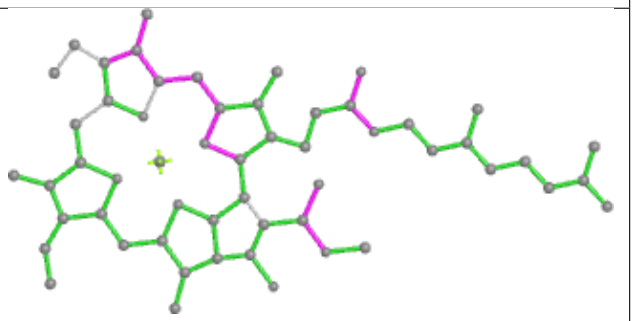
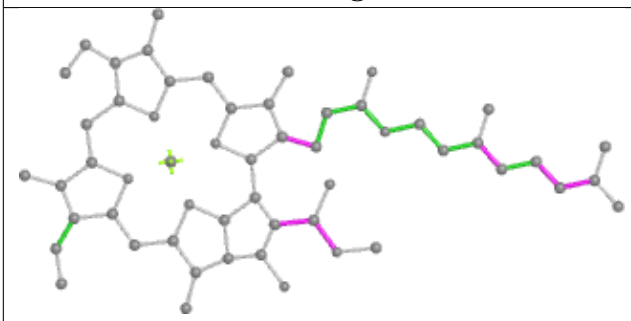


Bond angles



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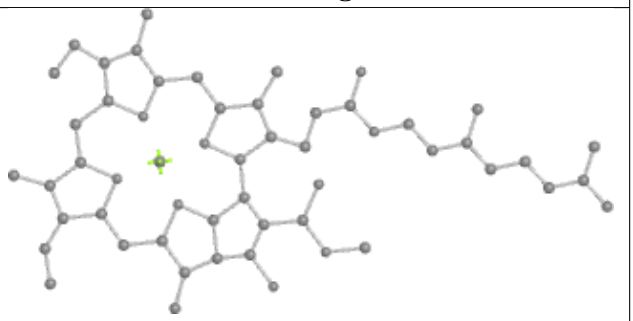
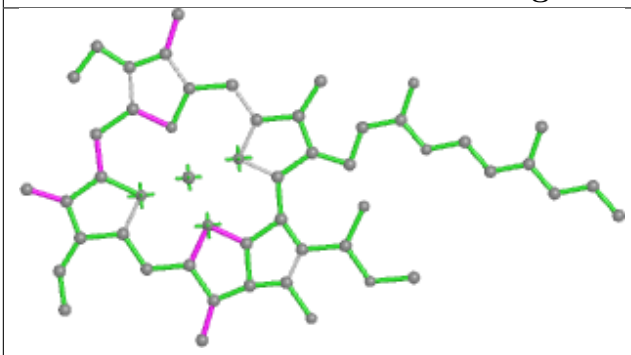
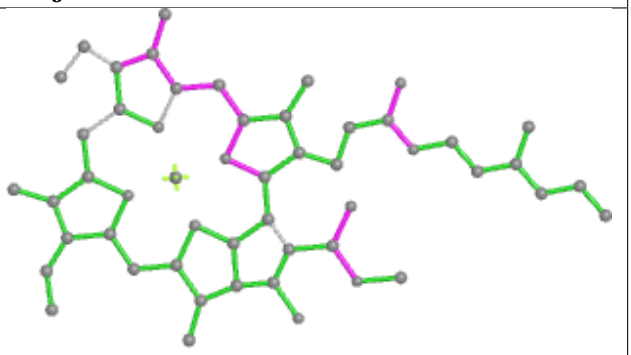


Rings

Ligand CLA j 104	
	
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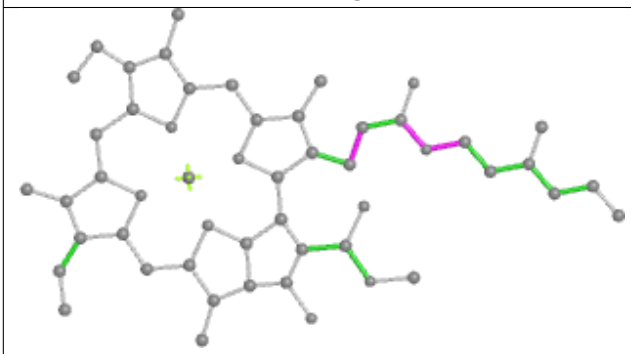
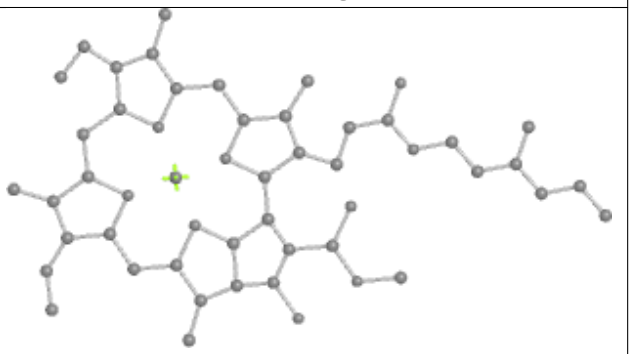
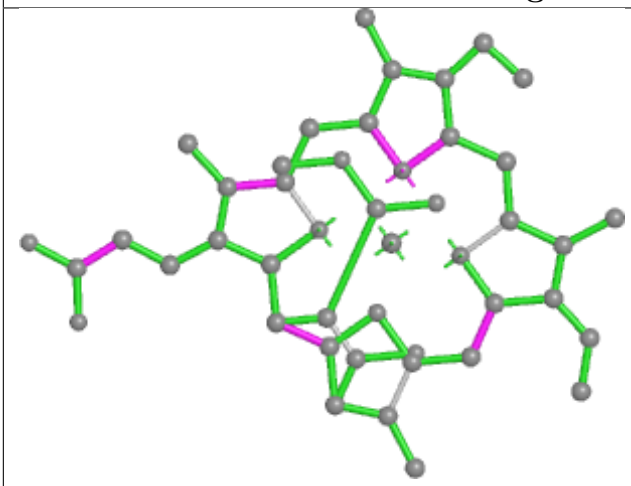
	
Torsions	**Rings**

Ligand KC1 T 312



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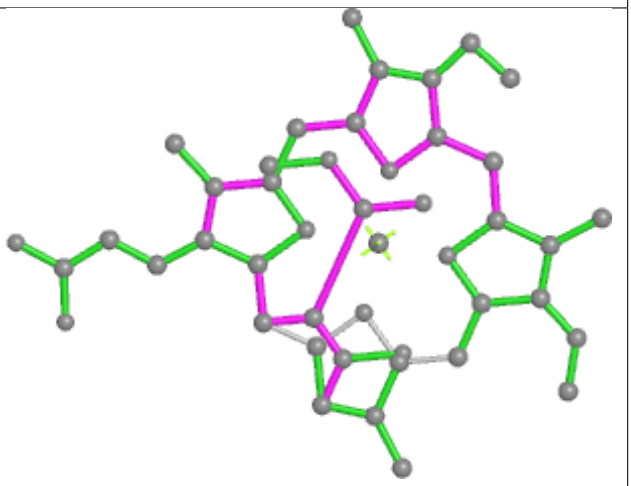
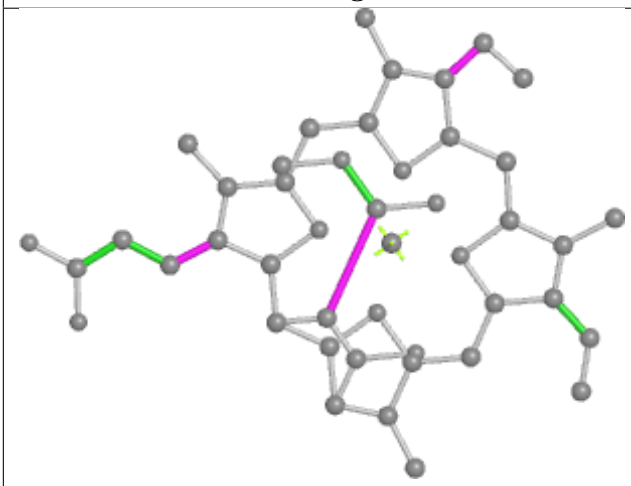


Bond angles



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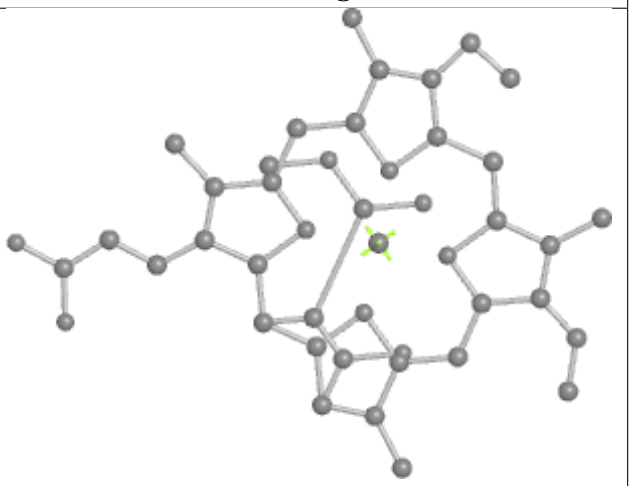
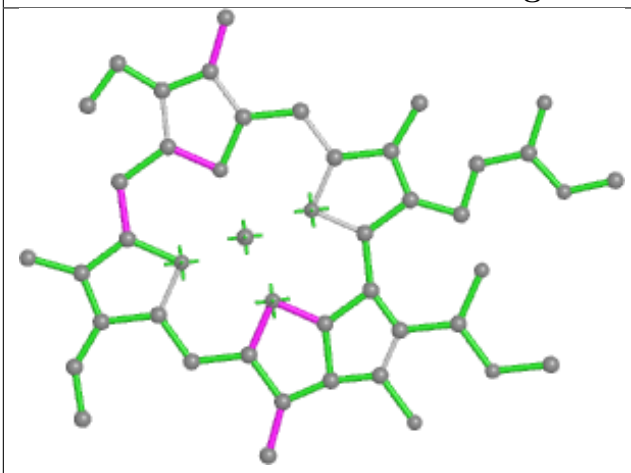
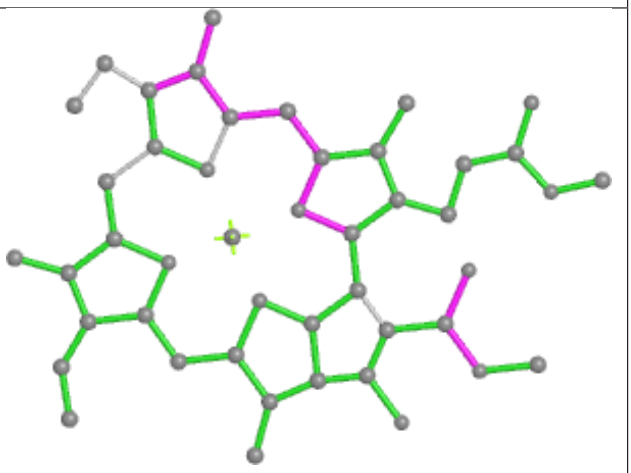


Rings

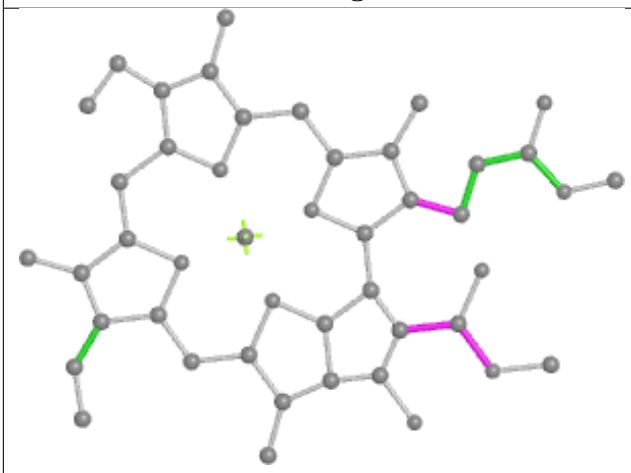
Ligand CLA O 313



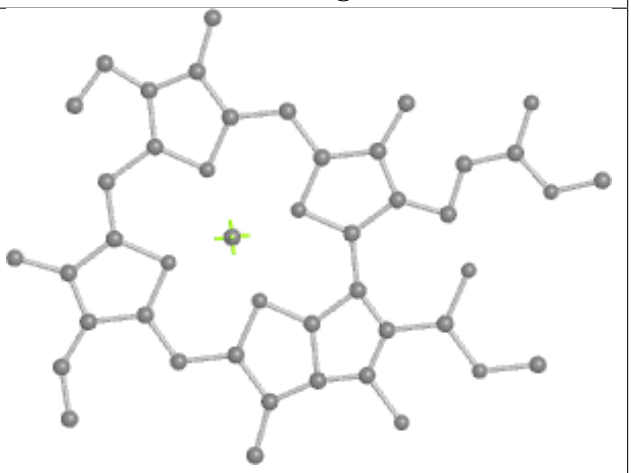
Bond lengths



Bond angles

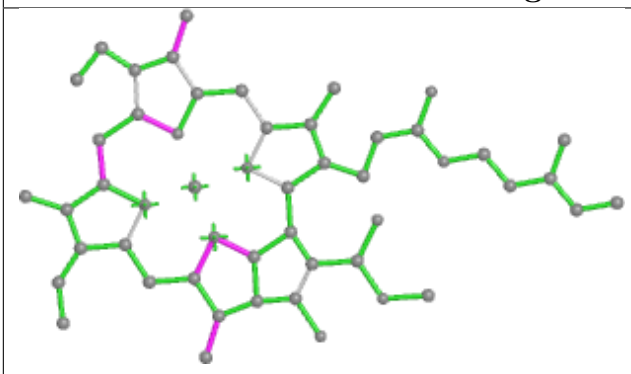


Torsions

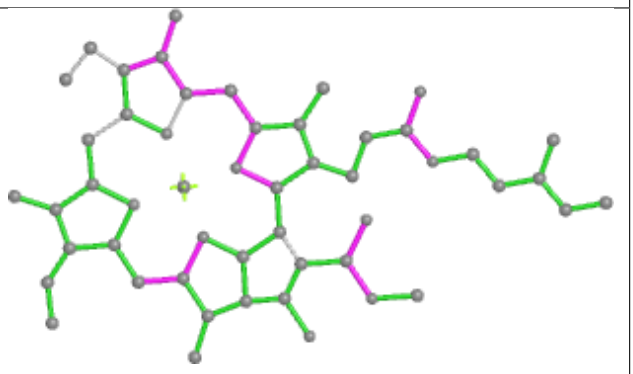


Rings

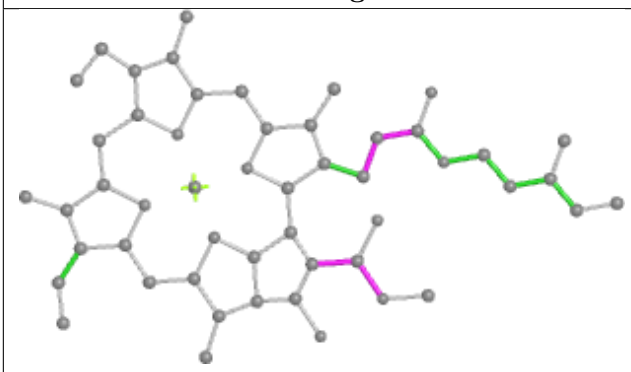
Ligand CLA C 311



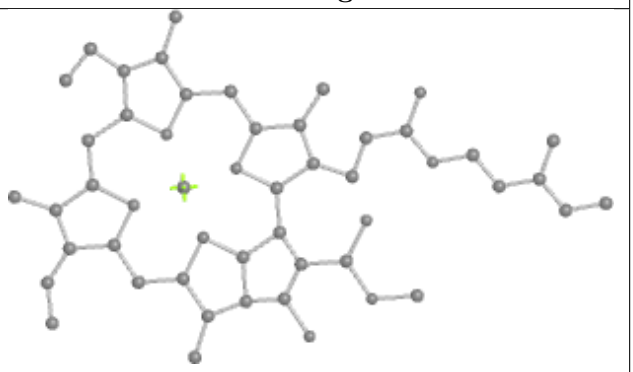
Bond lengths



Bond angles

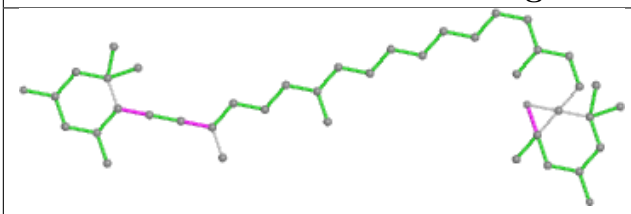


Torsions



Rings

Ligand DD6 B 301



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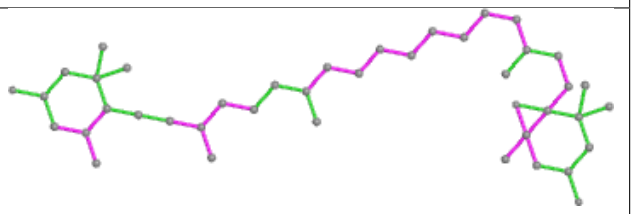
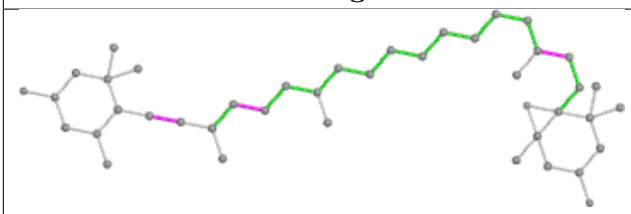
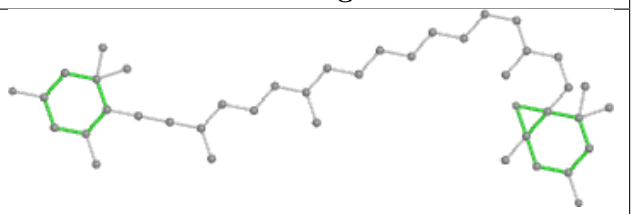


Bond angles

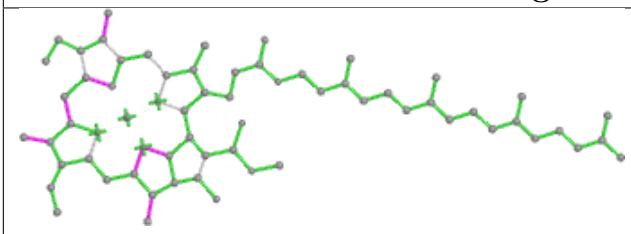


Torsions

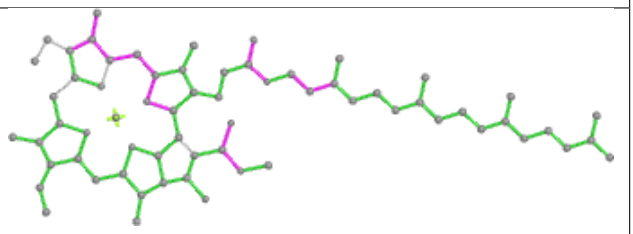


Rings

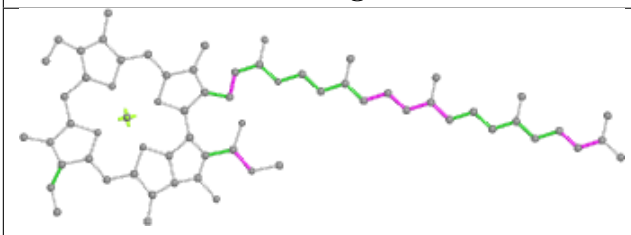
Ligand CLA i 202



Bond lengths



Bond angles



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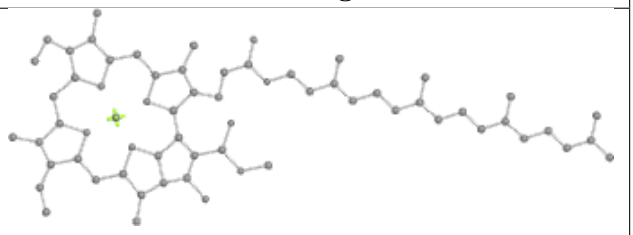
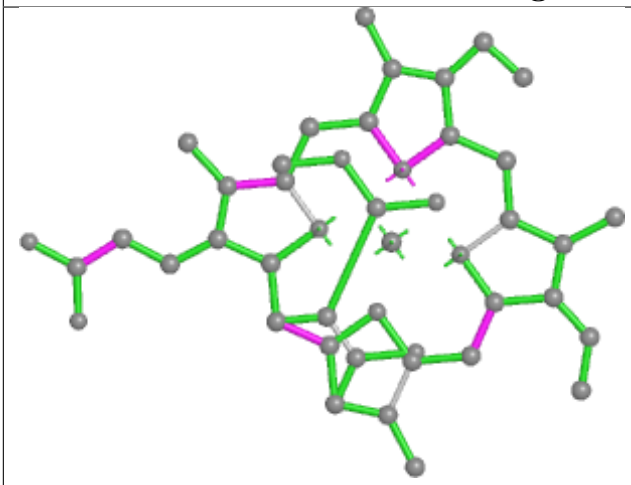


Rings

Ligand KC1 J 312



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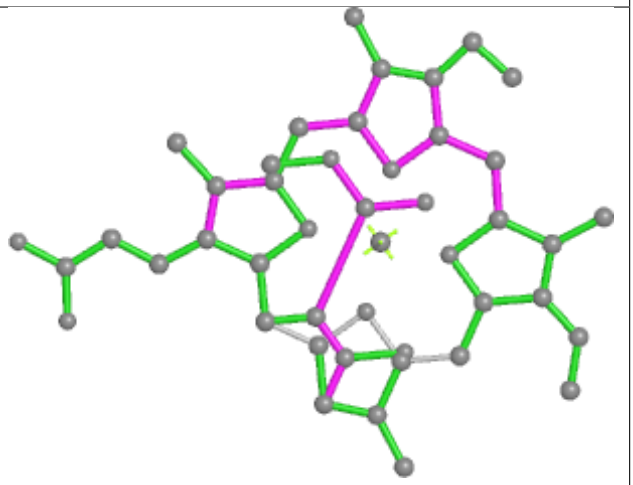
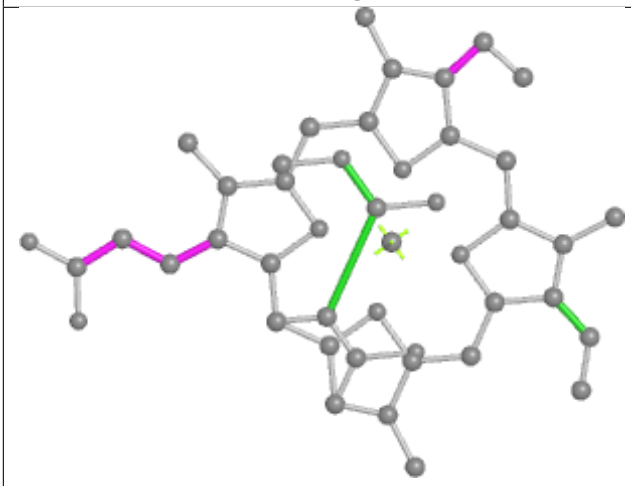


Bond angles



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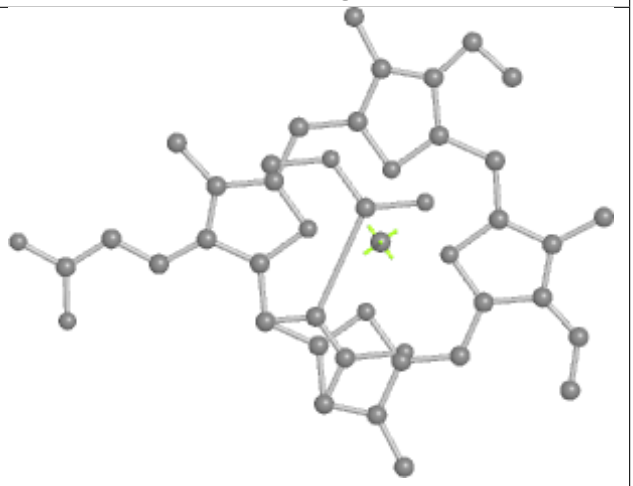
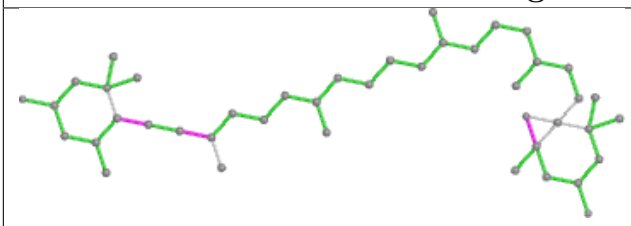
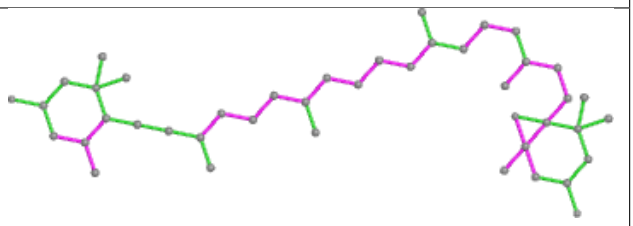


Rings

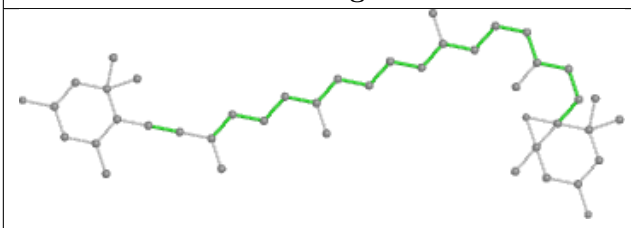
Ligand DD6 L 303



Bond lengths



Bond angles



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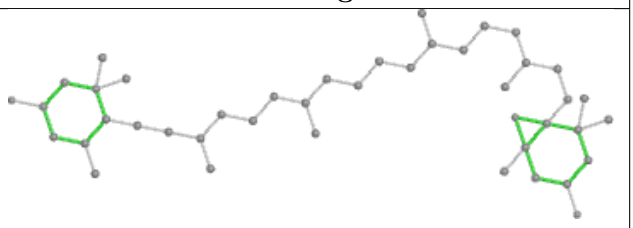
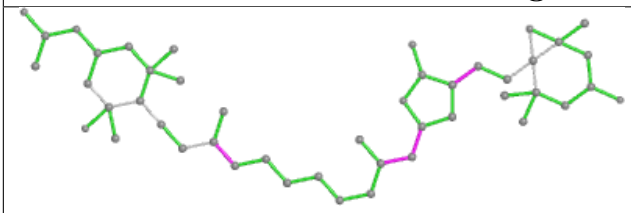


Rings

Ligand PID H 301



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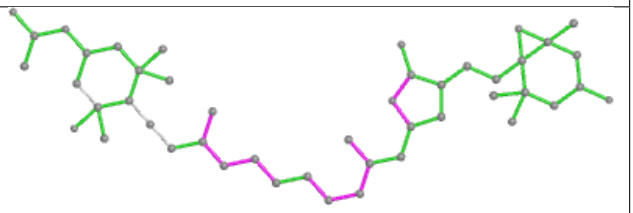

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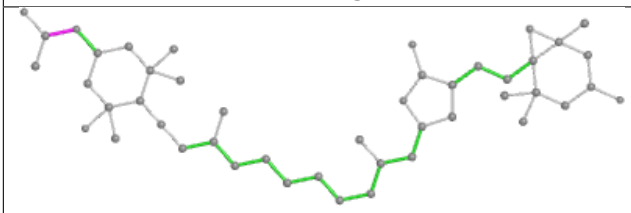

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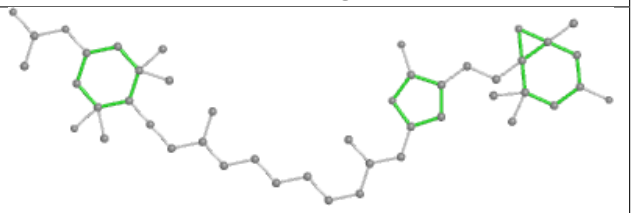
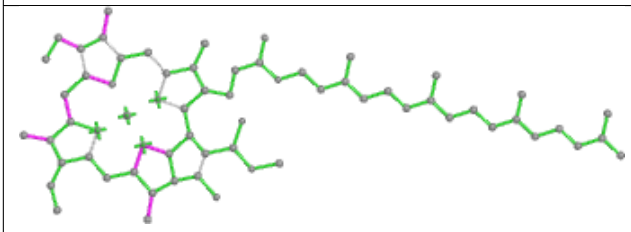
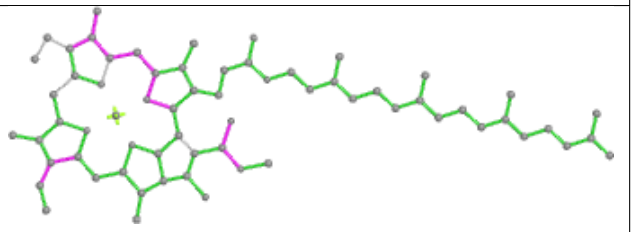


Rings

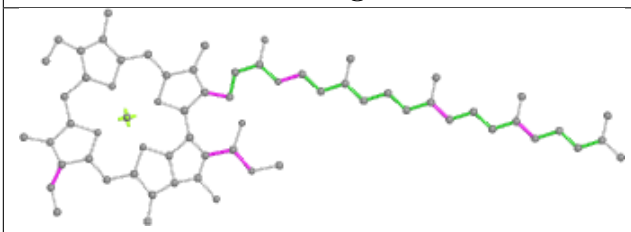
Ligand CLA b 705



Bond lengths



Bond angles



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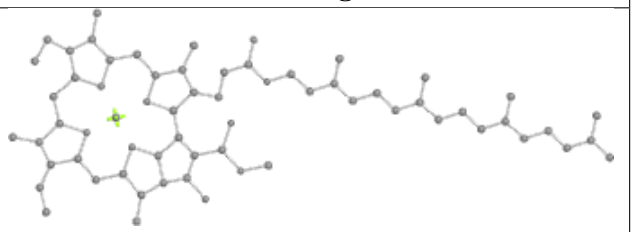
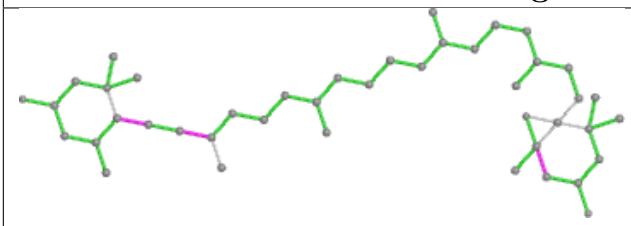


Rings

Ligand DD6 I 203



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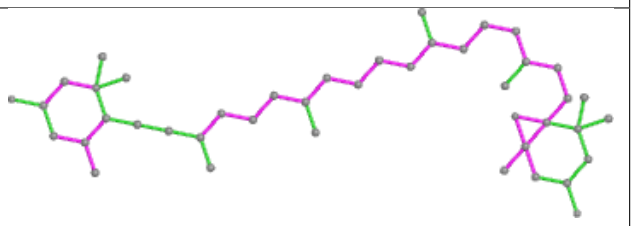
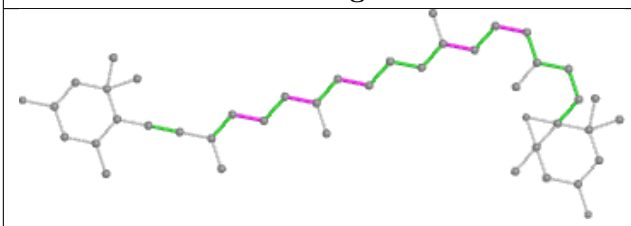
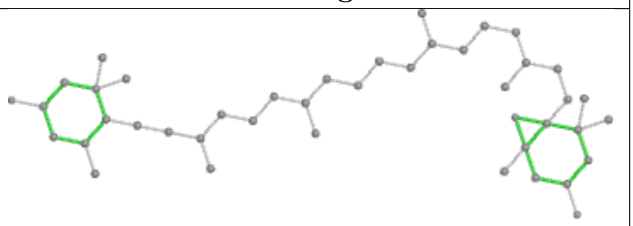


Bond angles

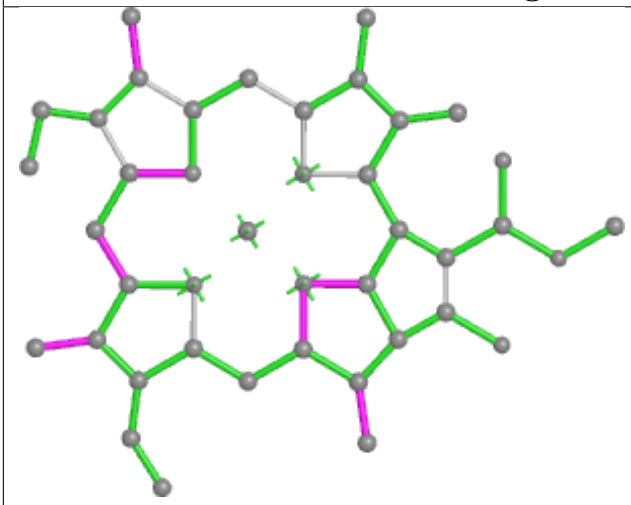


Torsions



Rings

Ligand CLA Q 315



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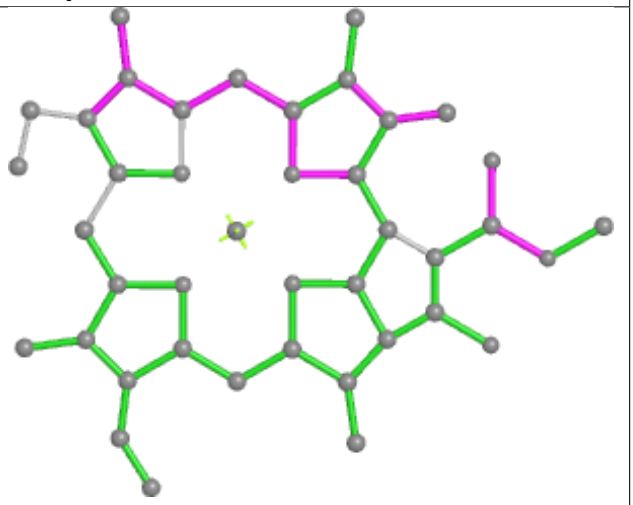
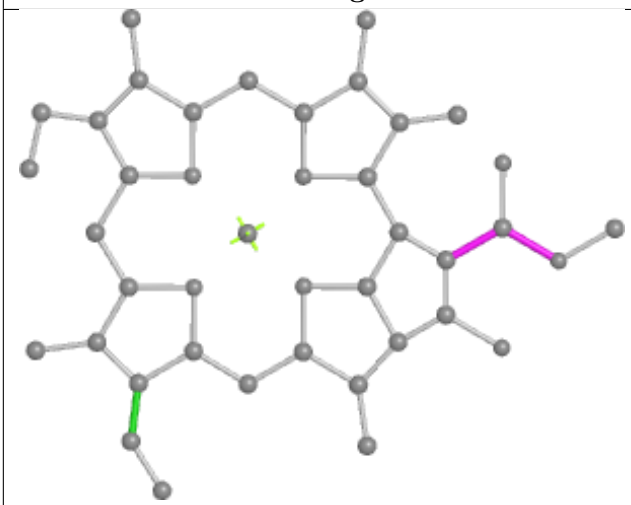


Bond angles



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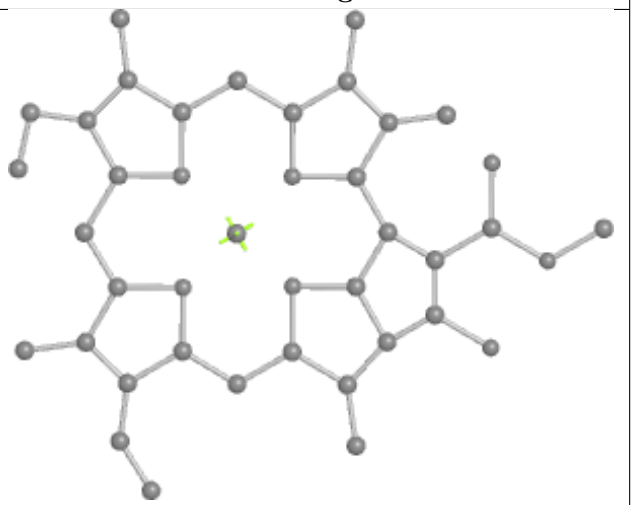
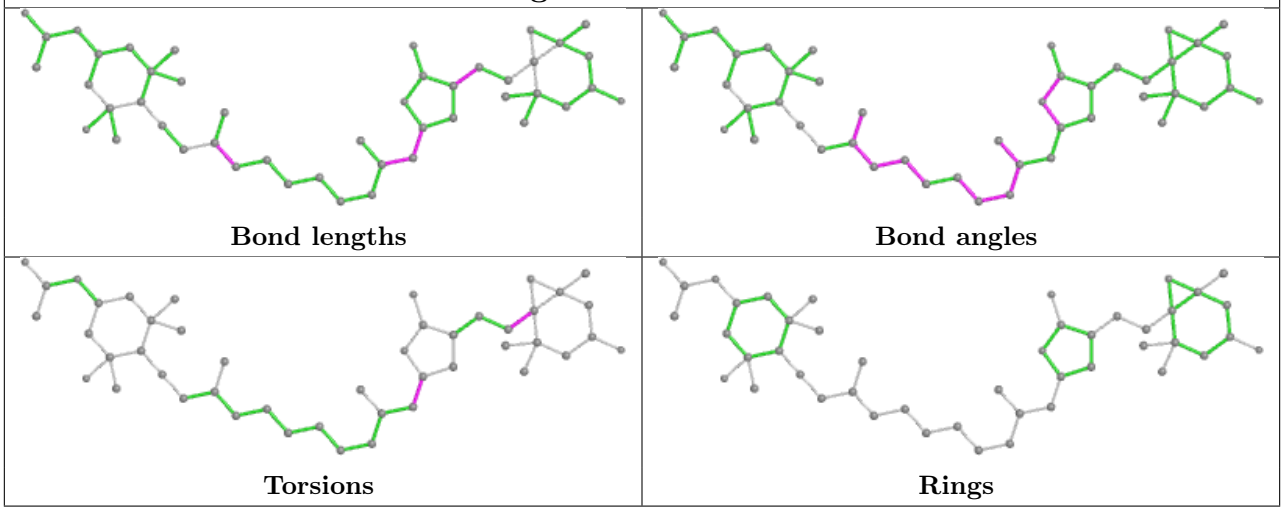
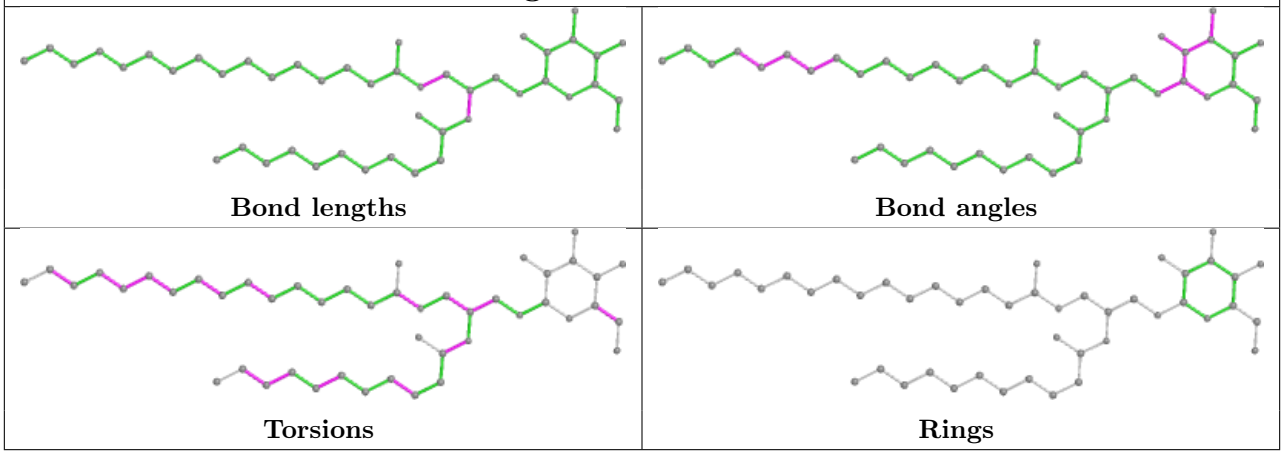


Rings

Ligand PID T 301



Ligand LMG b 730



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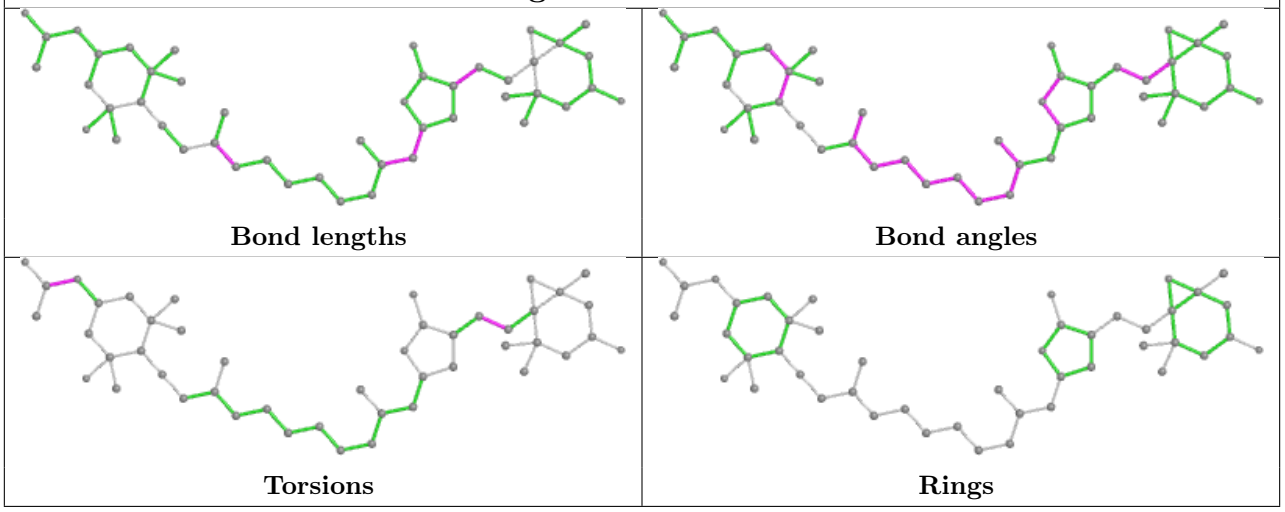

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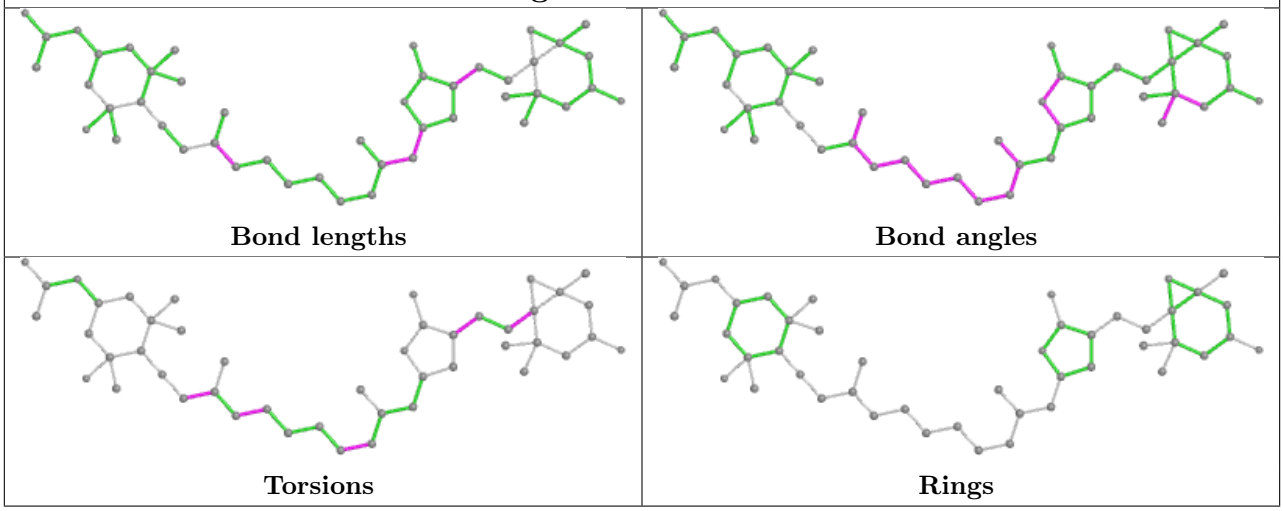
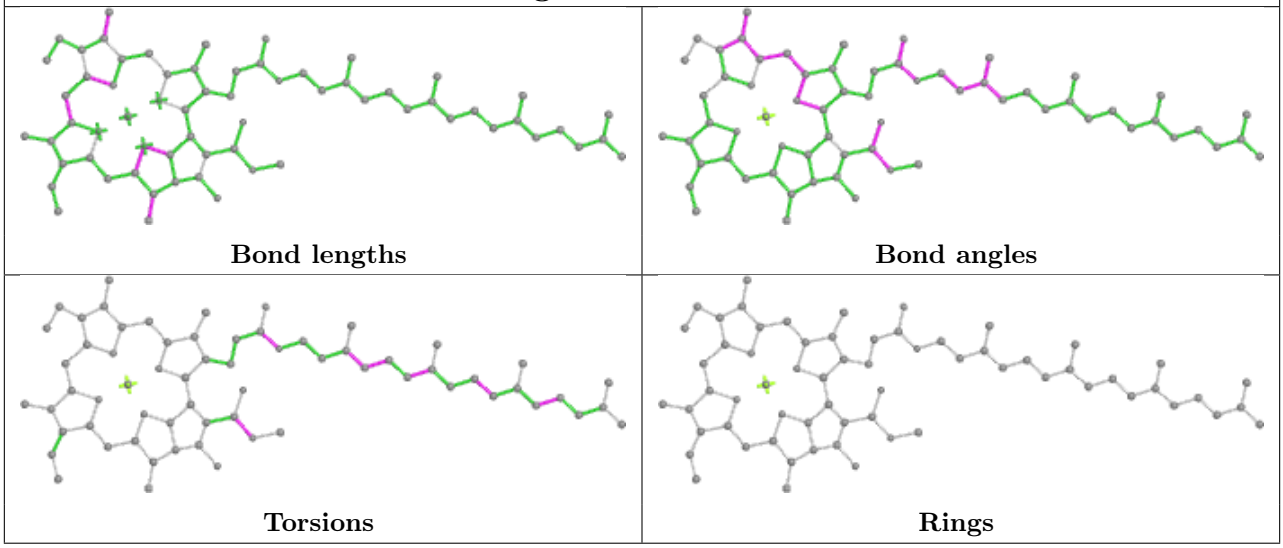


Ligand CLA l 504



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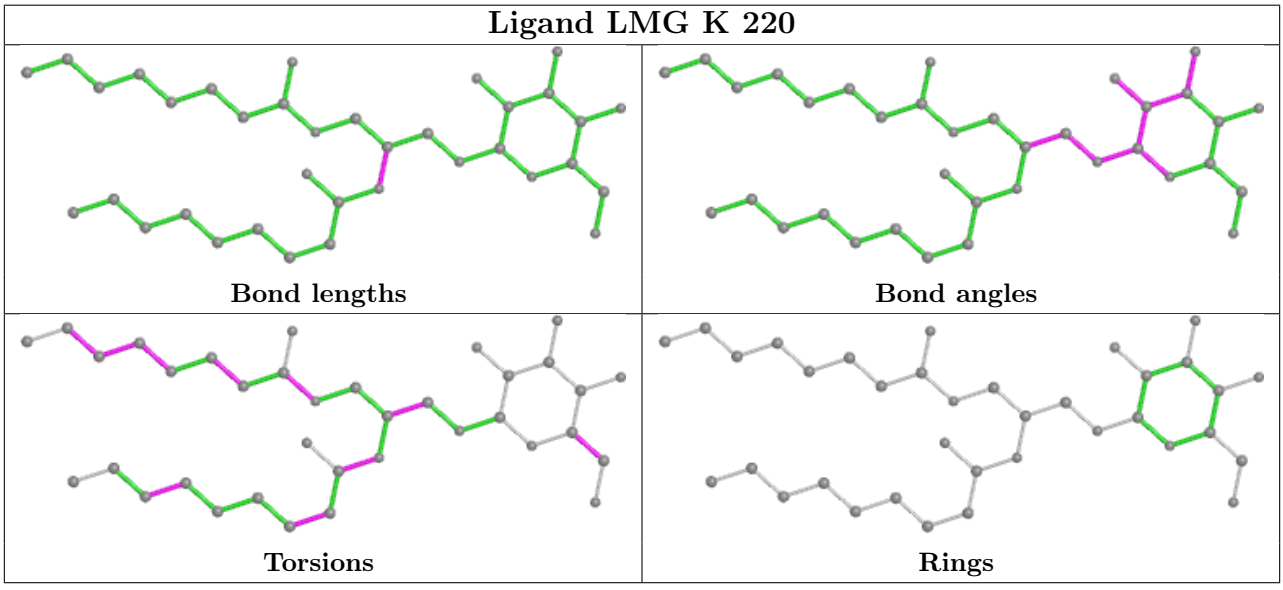
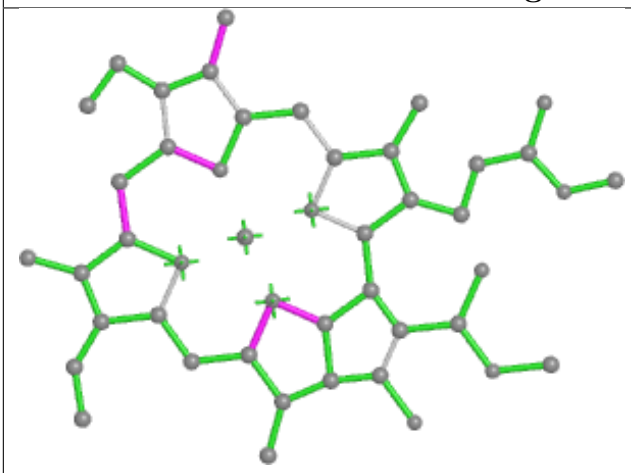
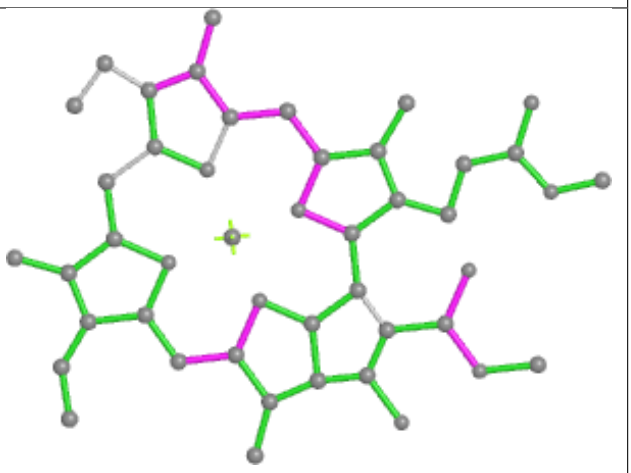


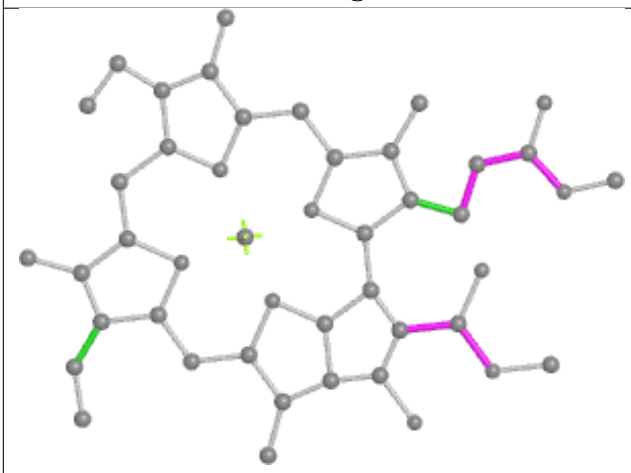
Ligand CLA T 311



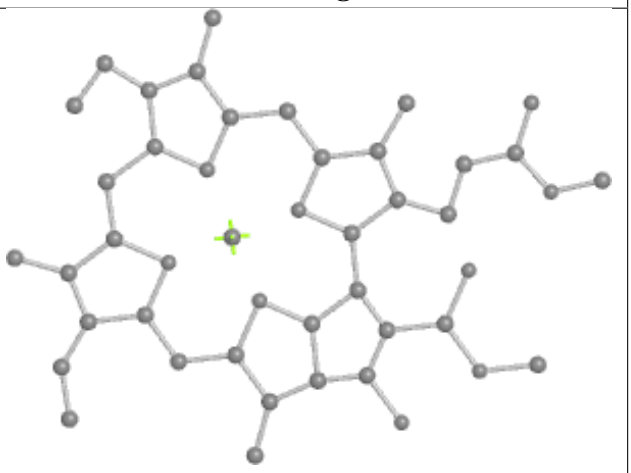
Bond lengths



Bond angles

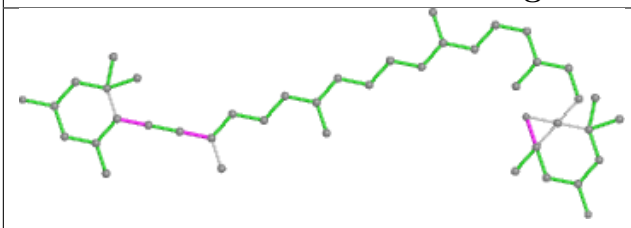


Torsions

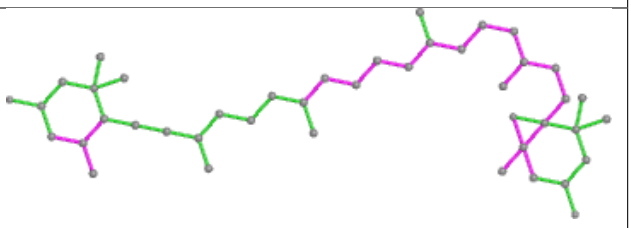


Rings

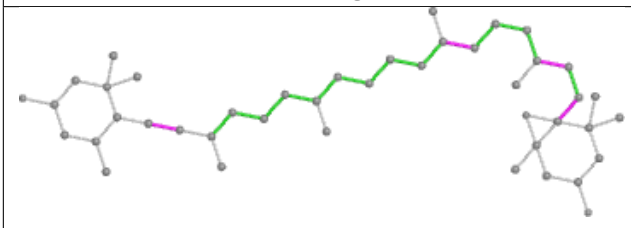
Ligand DD6 K 203



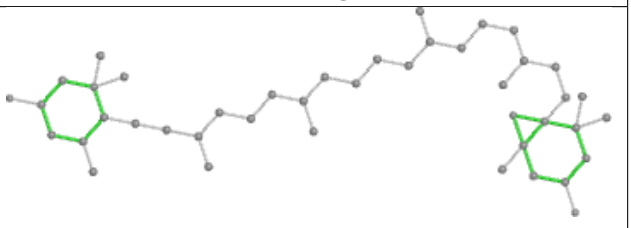
Bond lengths



Bond angles

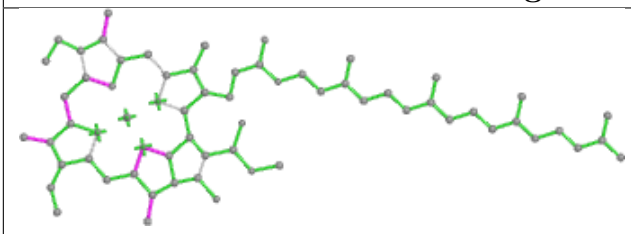


Torsions

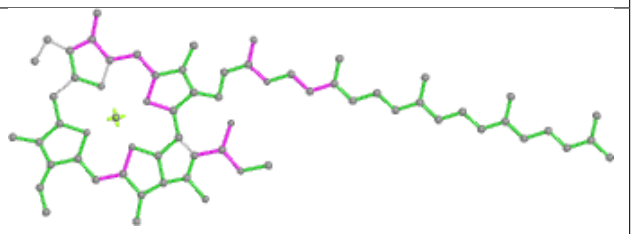


Rings

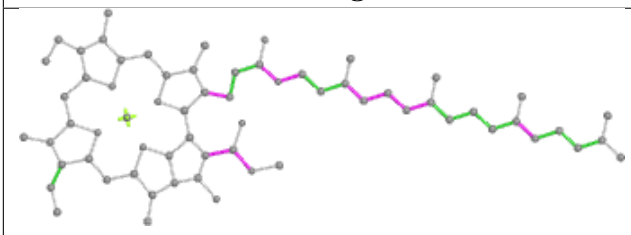
Ligand CLA B 308



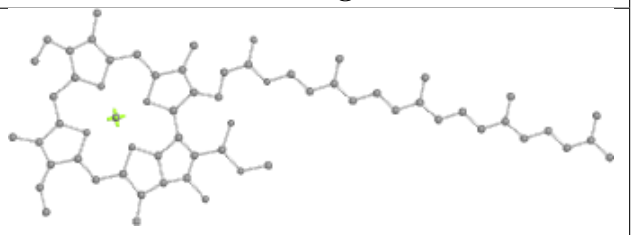
Bond lengths



Bond angles

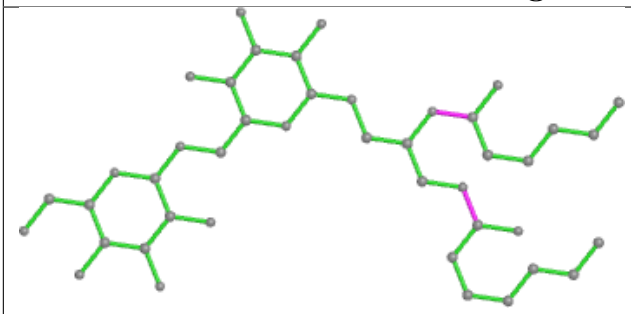


Torsions

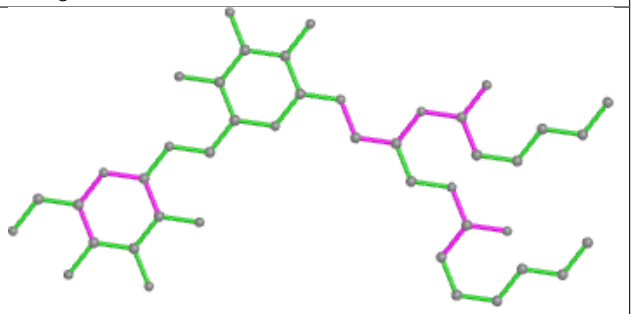


Rings

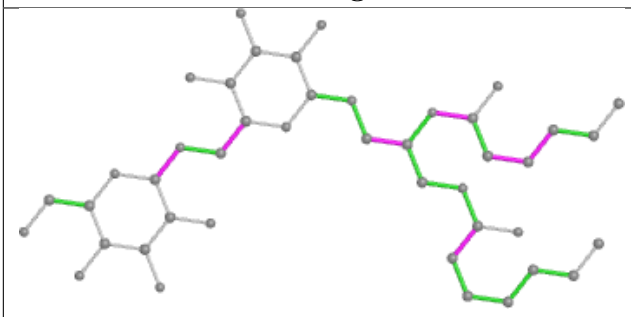
Ligand DGD j 103



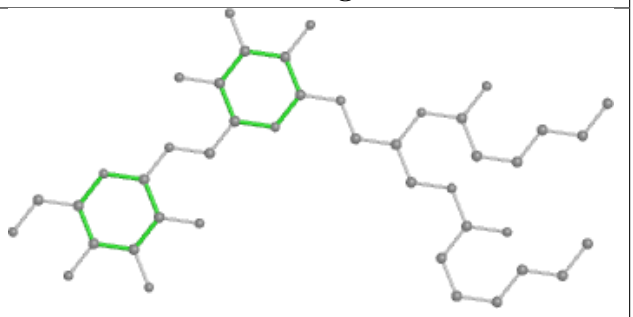
Bond lengths



Bond angles

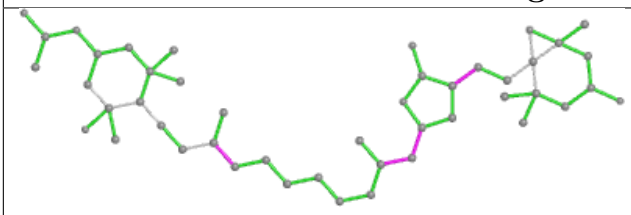


Torsions



Rings

Ligand PID H 306



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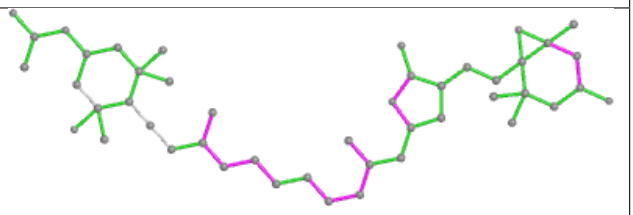

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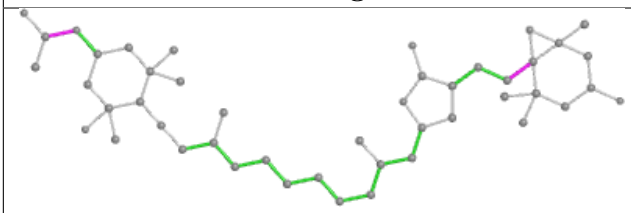

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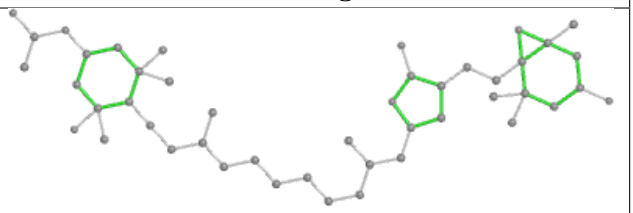
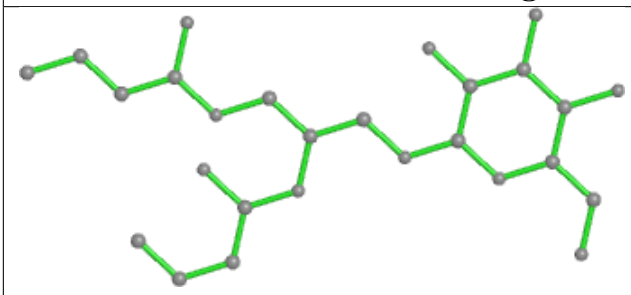


Rings

Ligand LMG P 201



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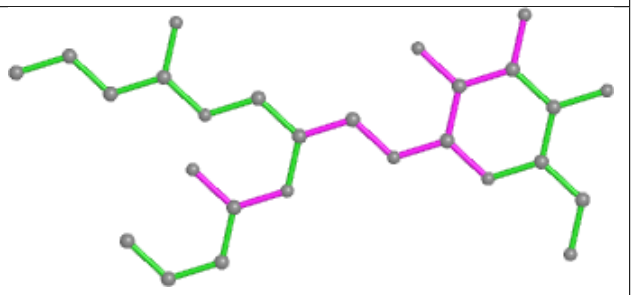

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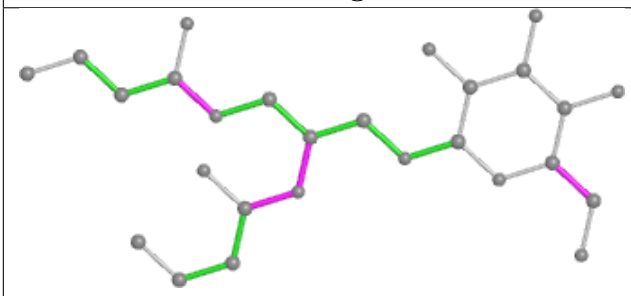

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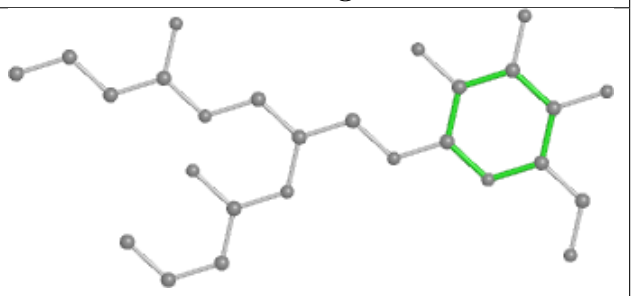
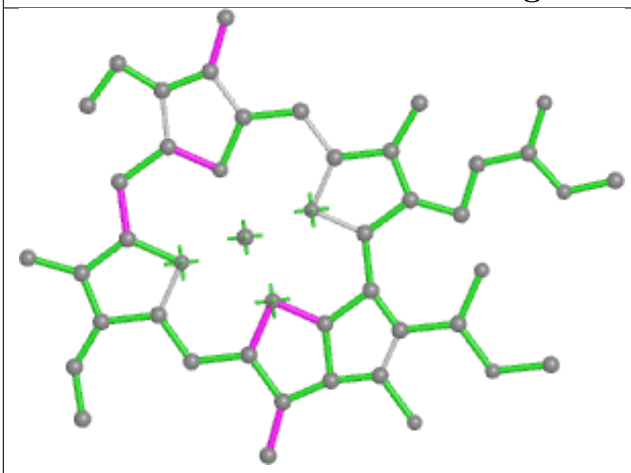


Rings

Ligand CLA D 312



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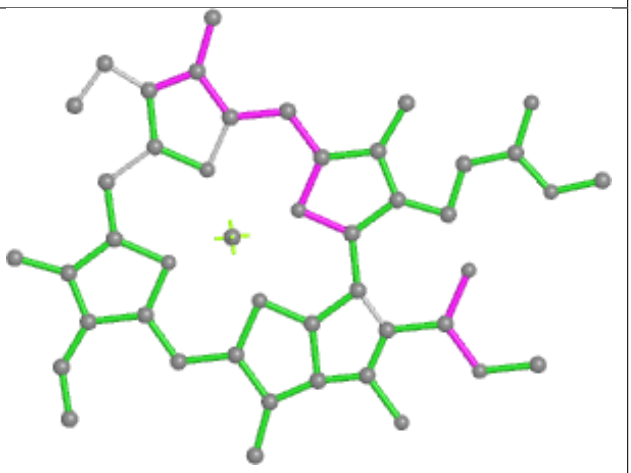

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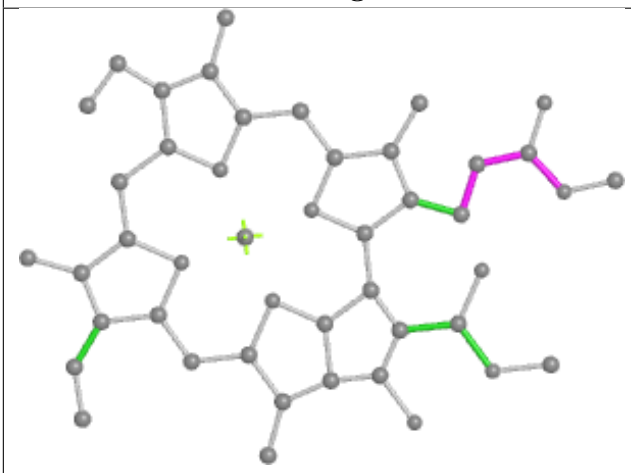

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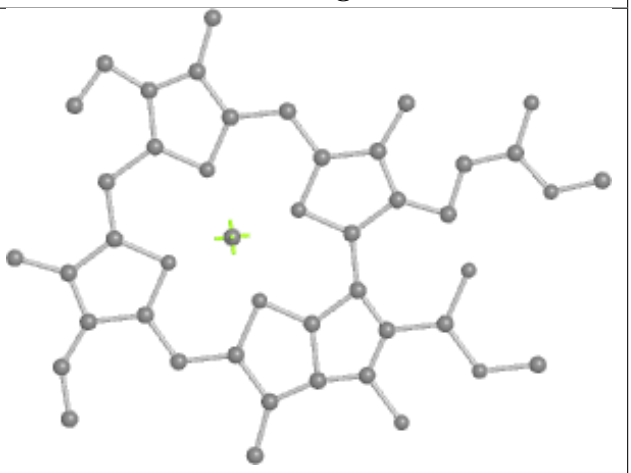
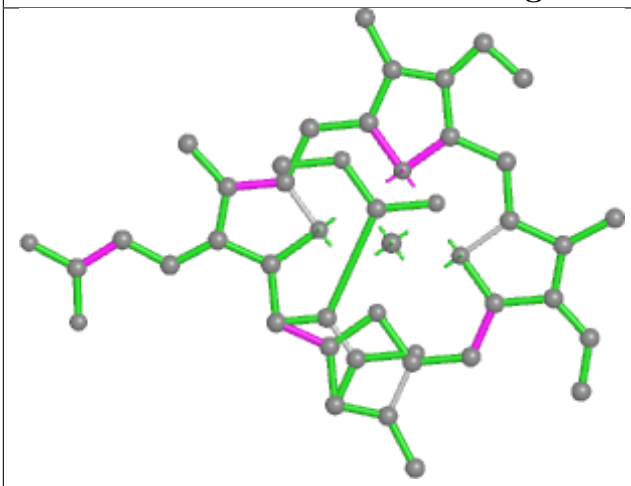


Rings

Ligand KC1 N 312



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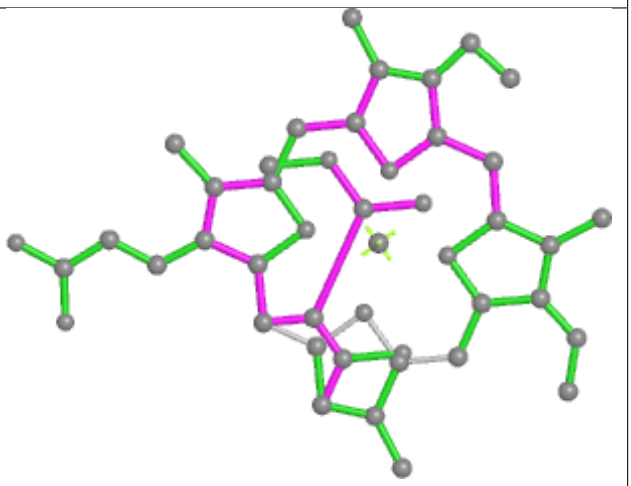

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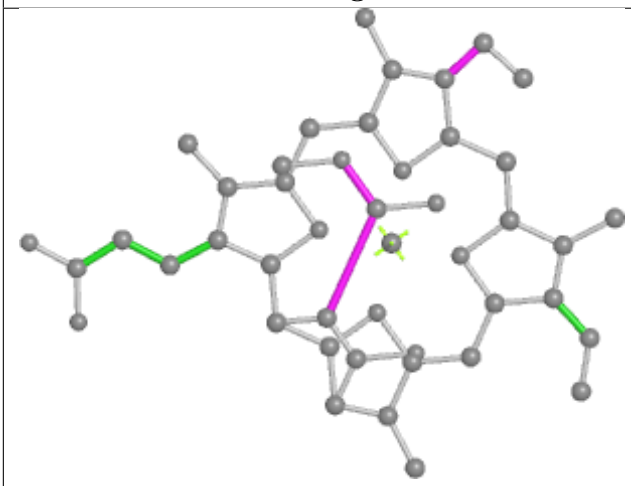

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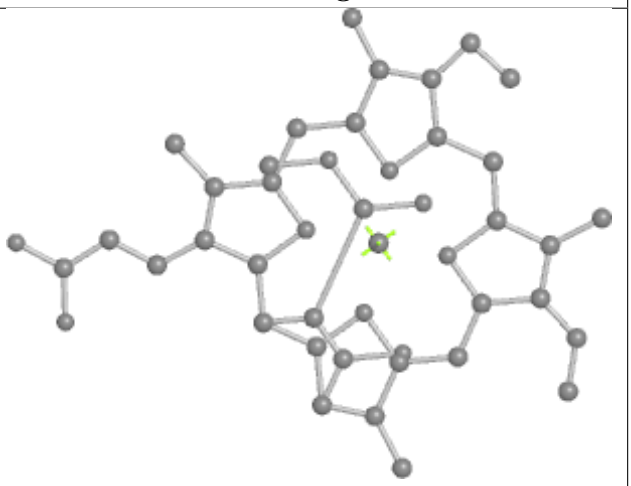
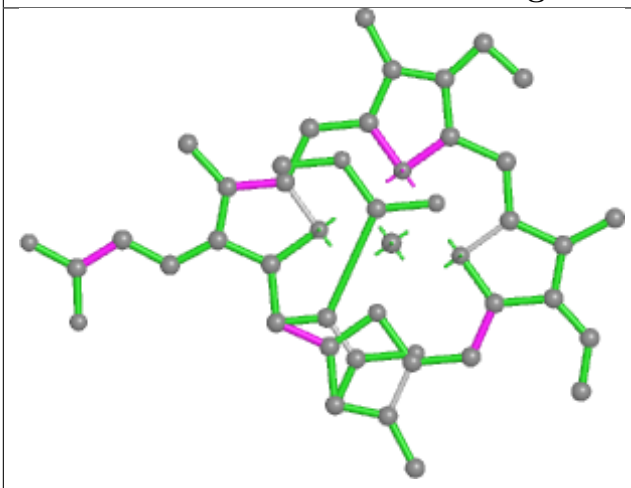


Rings

Ligand KC1 F 314



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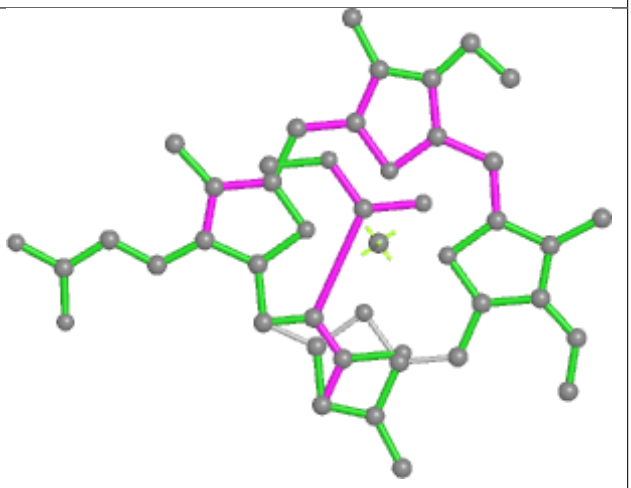

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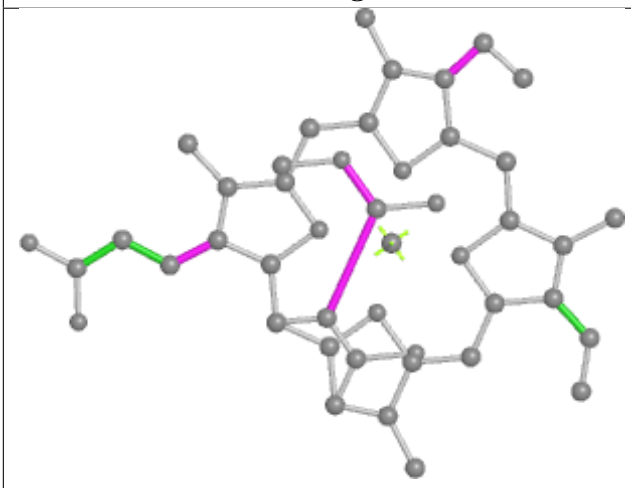

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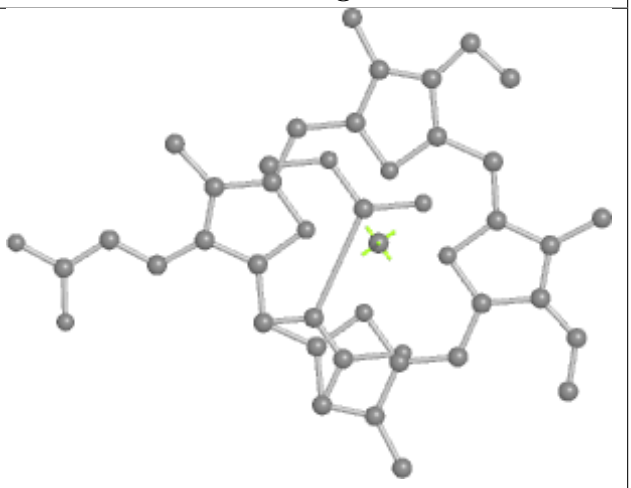
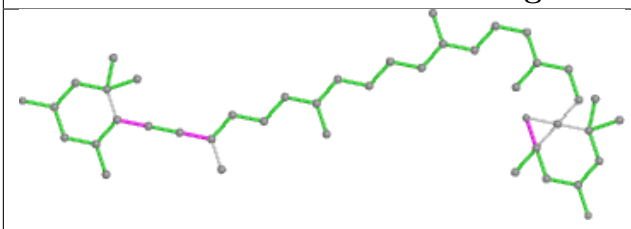


Rings

Ligand DD6 D 301



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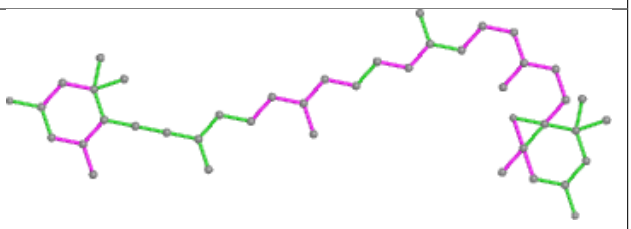

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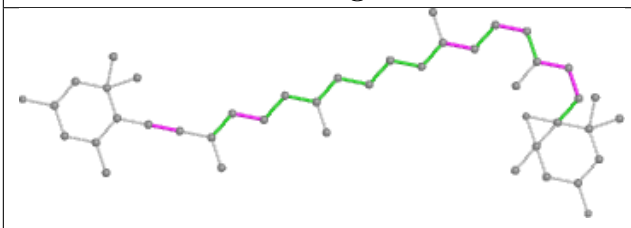

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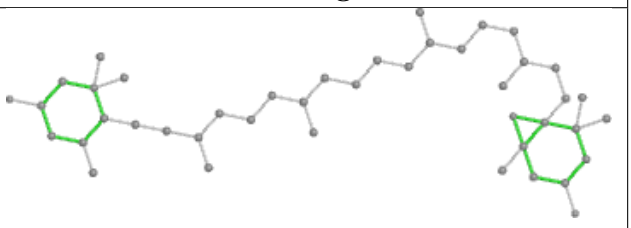
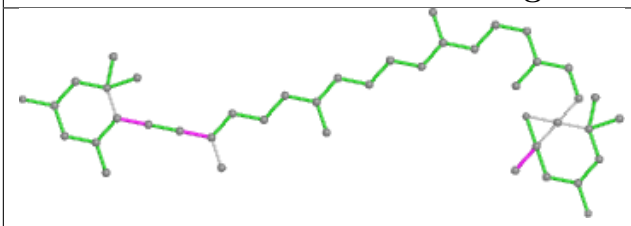


Rings

Ligand DD6 K 202



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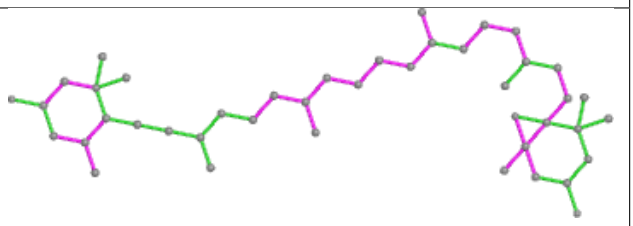
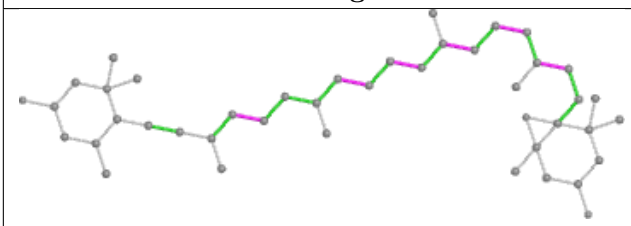


Bond angles



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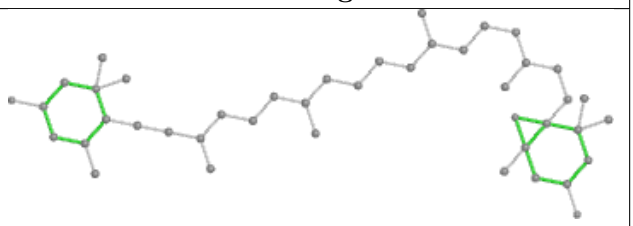
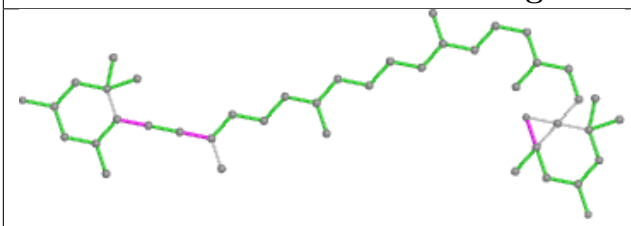


Rings

Ligand DD6 T 303



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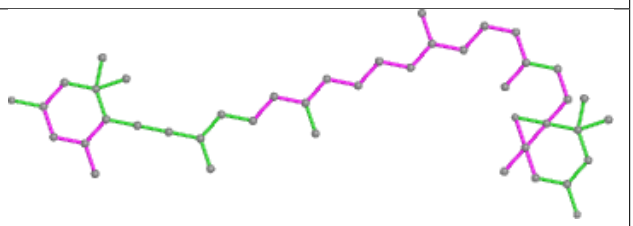

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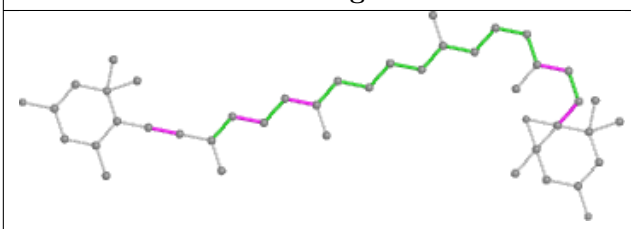

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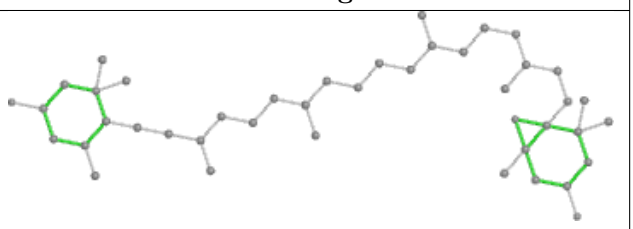
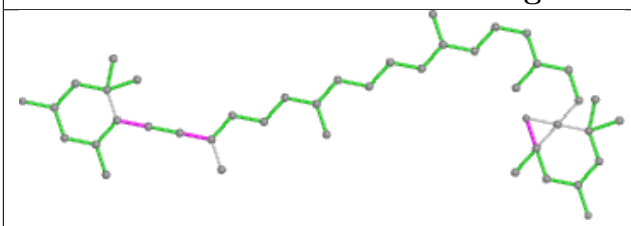


Rings

Ligand DD6 K 205



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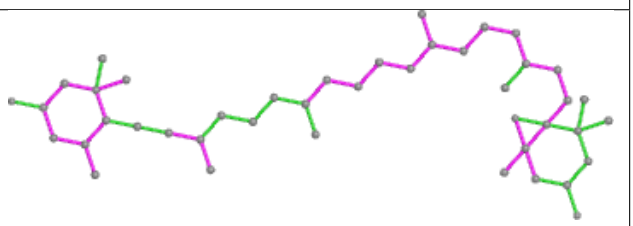

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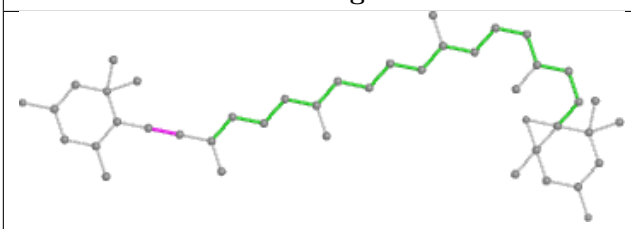
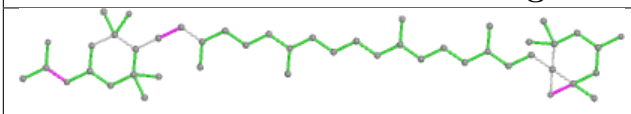


Torsions

Rings

Ligand UIX O 306



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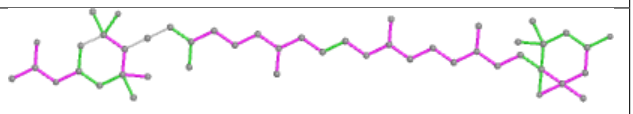

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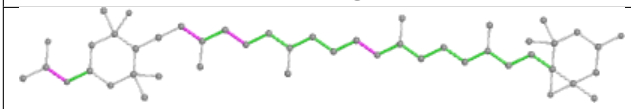
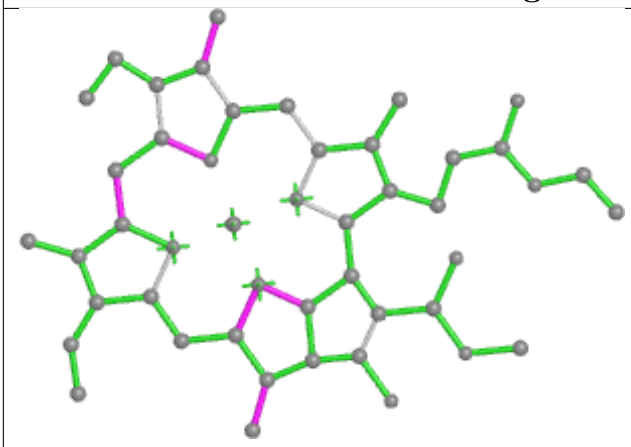


Torsions

Rings

Ligand CLA H 307



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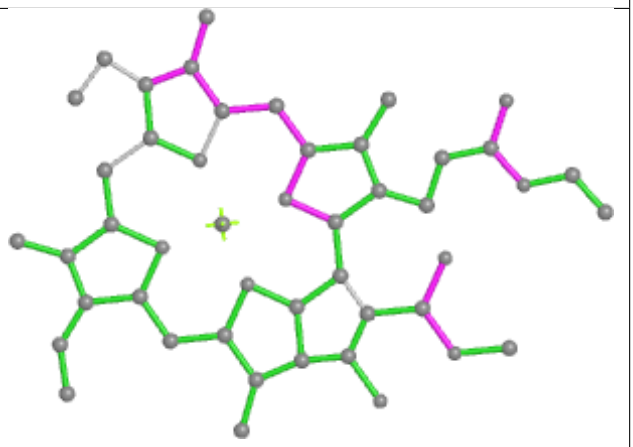
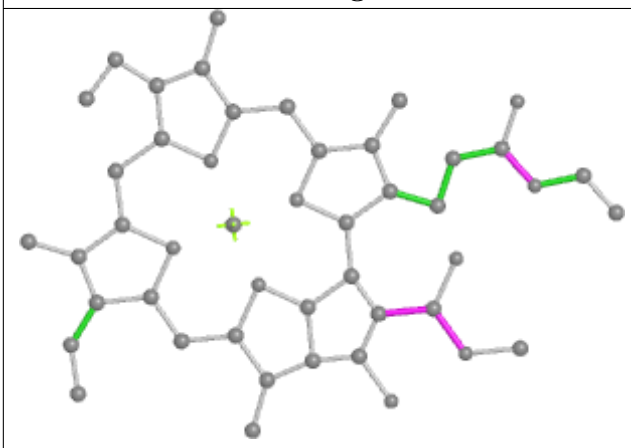


Bond angles



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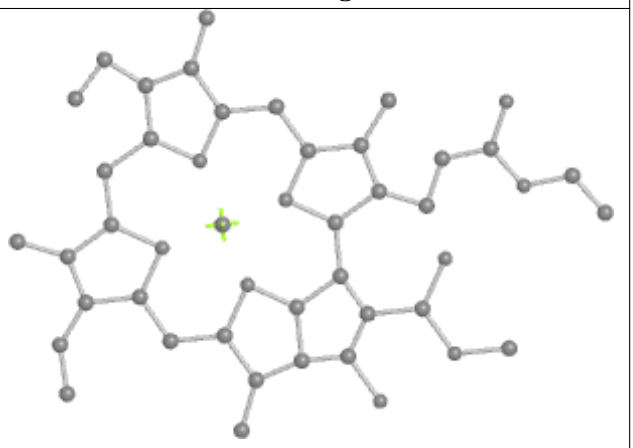
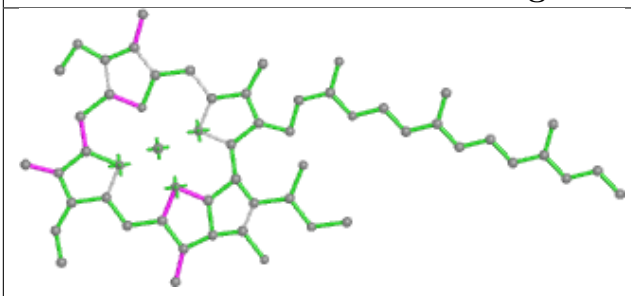


Rings

Ligand CLA a 819



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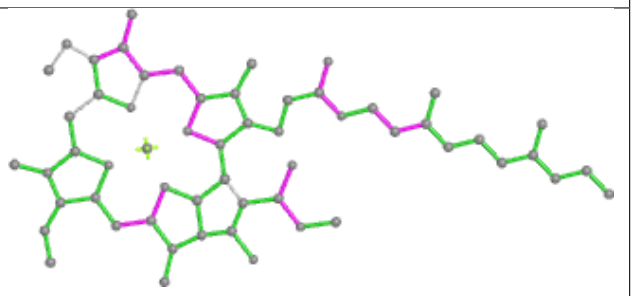
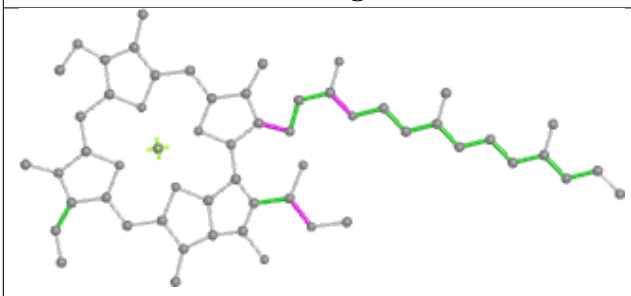


Bond angles



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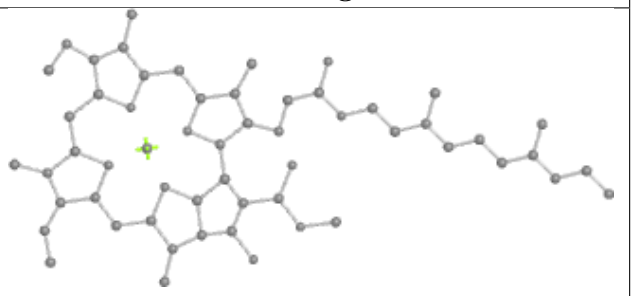
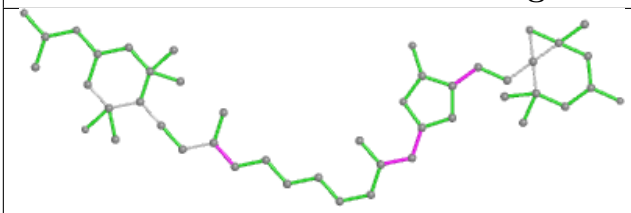


Rings

Ligand PID N 304



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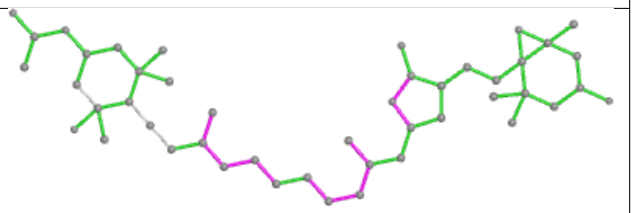
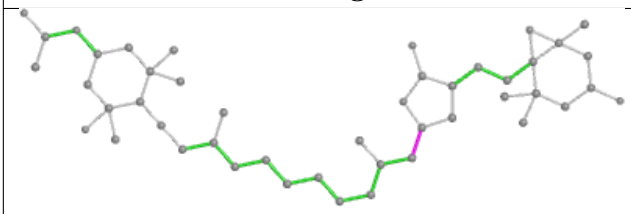


Bond angles



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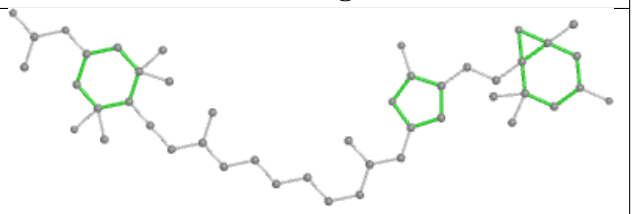
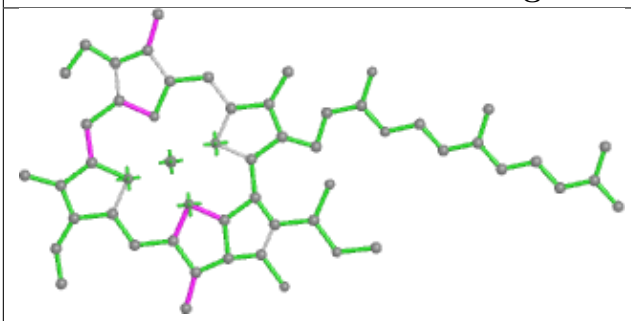


Rings

Ligand CLA A 211



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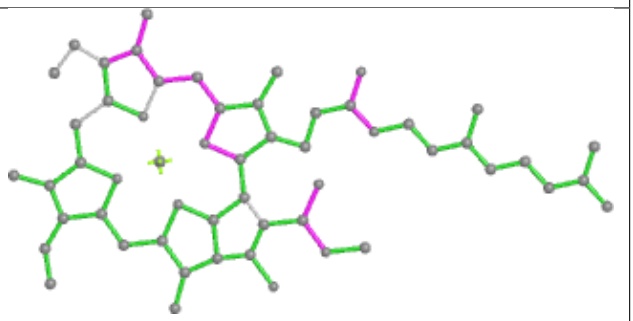
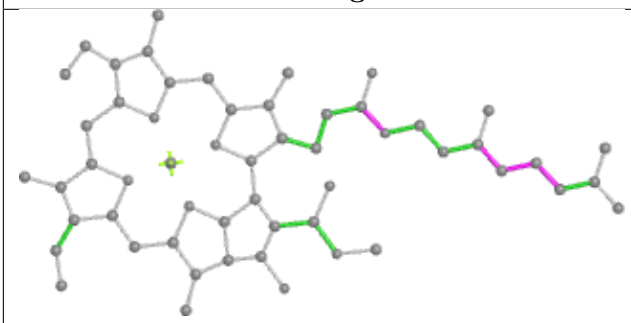


Bond angles



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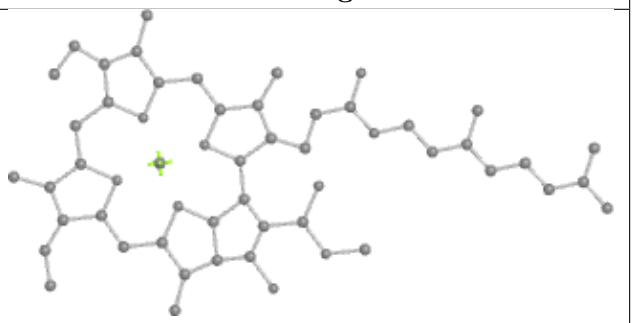
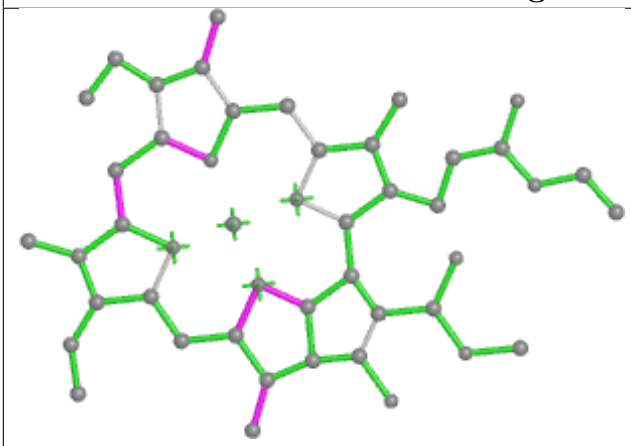
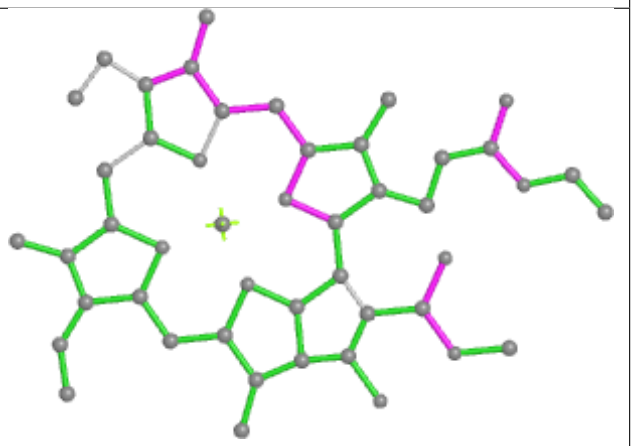


Rings

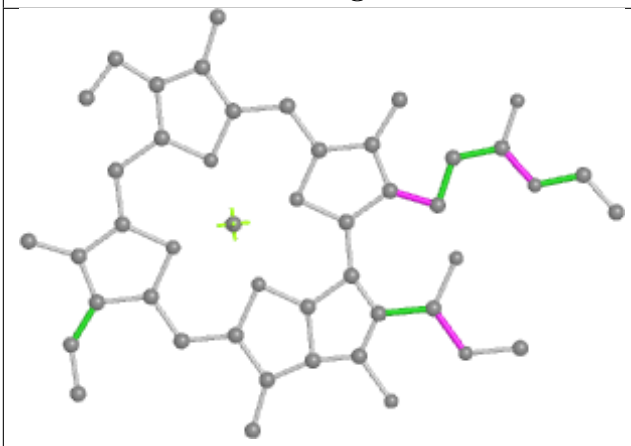
Ligand CLA J 310



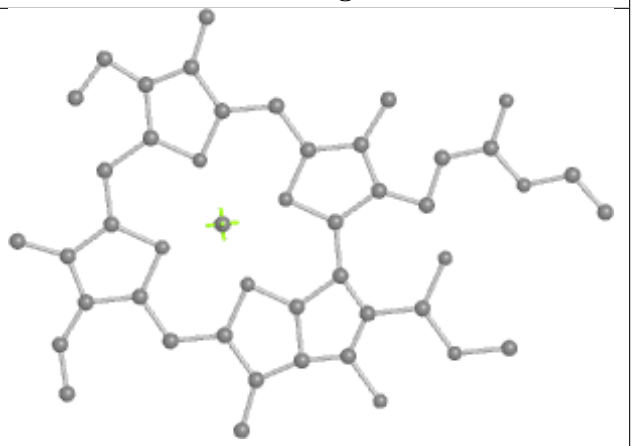
Bond lengths



Bond angles

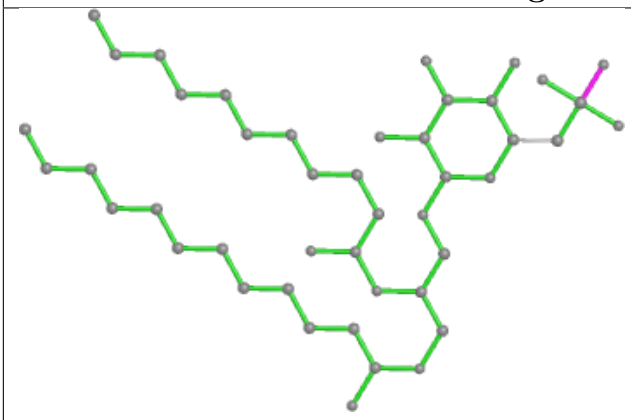


Torsions

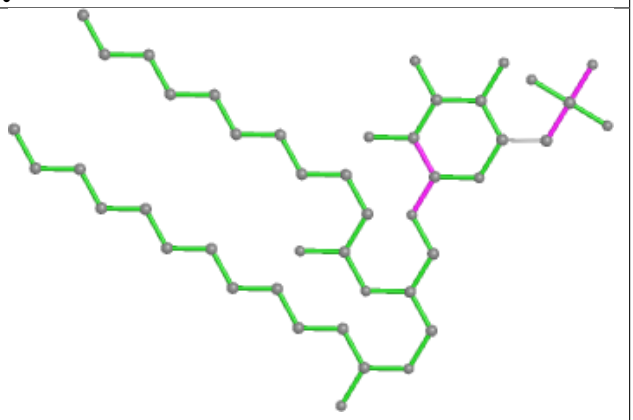


Rings

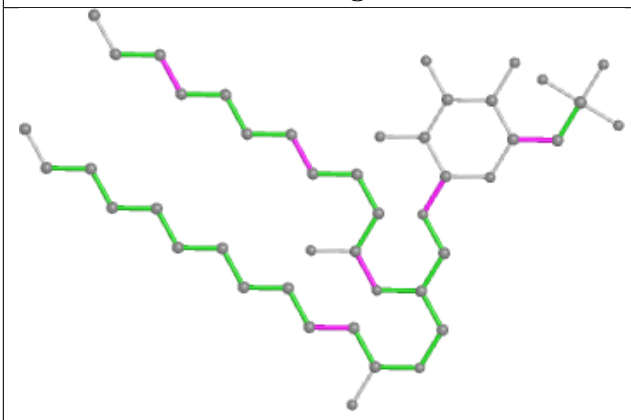
Ligand SQD J 314



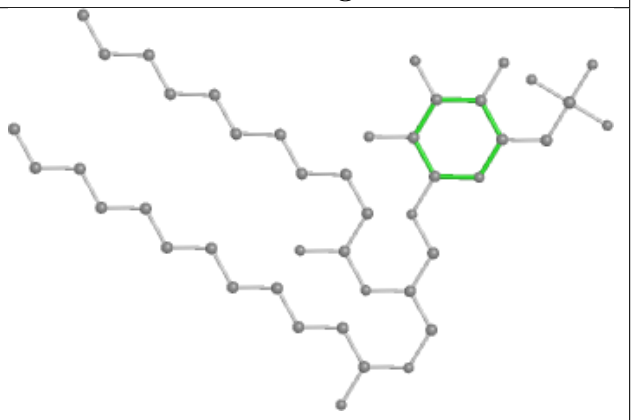
Bond lengths



Bond angles

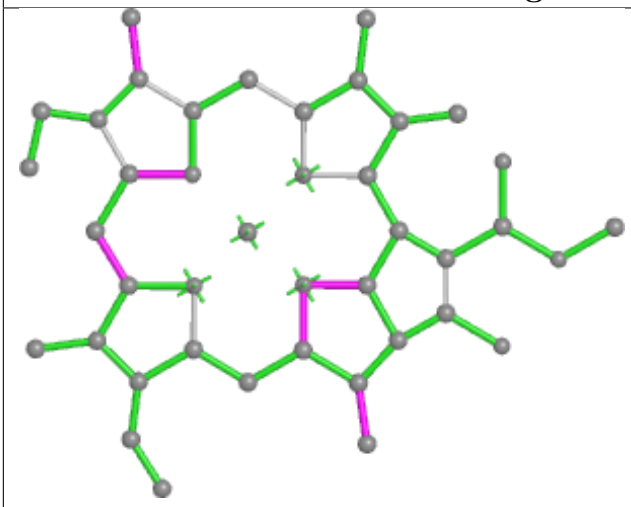


Torsions

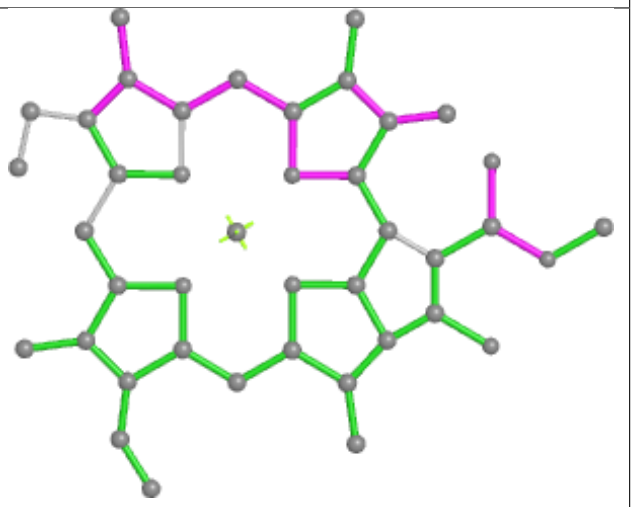


Rings

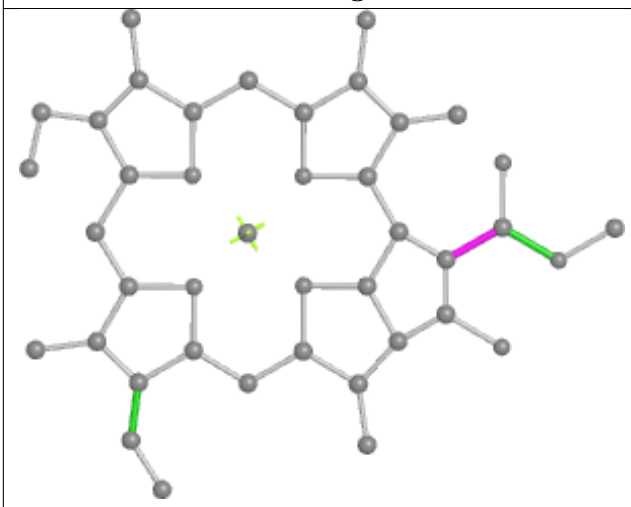
Ligand CLA E 313



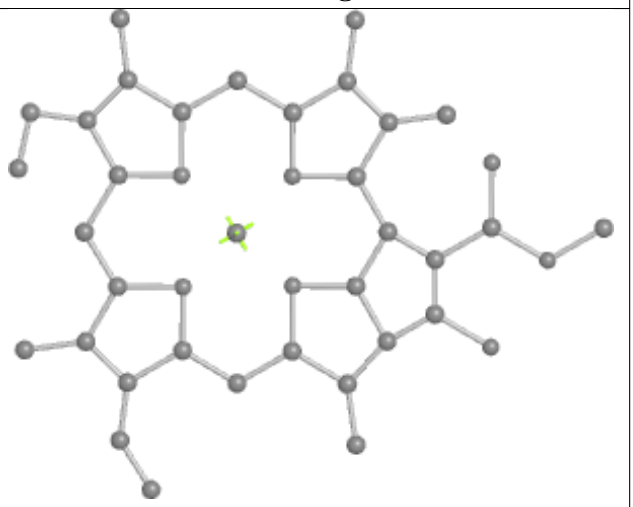
Bond lengths



Bond angles

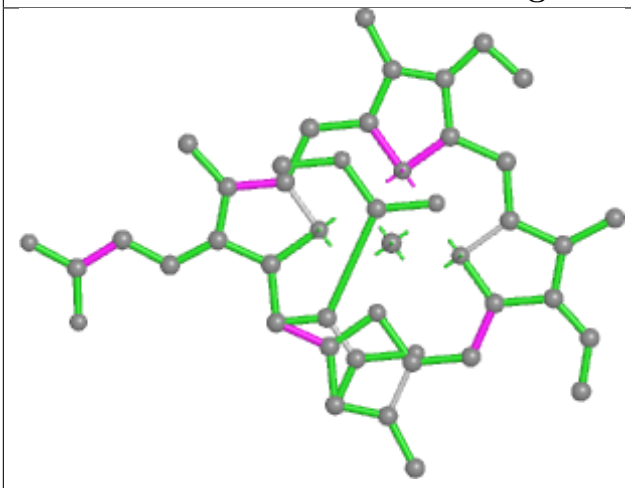


Torsions

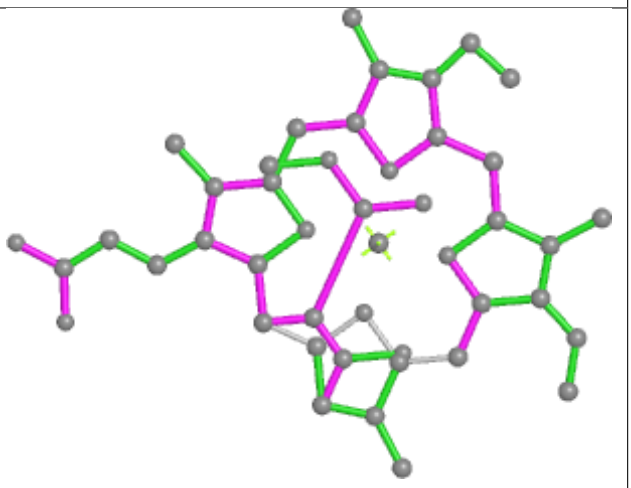


Rings

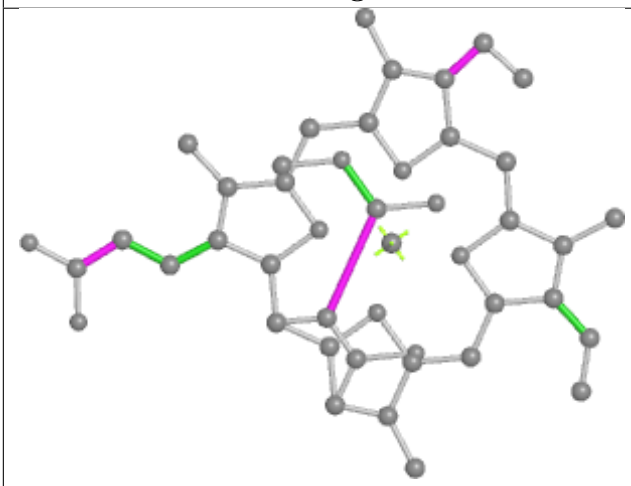
Ligand KC1 L 306



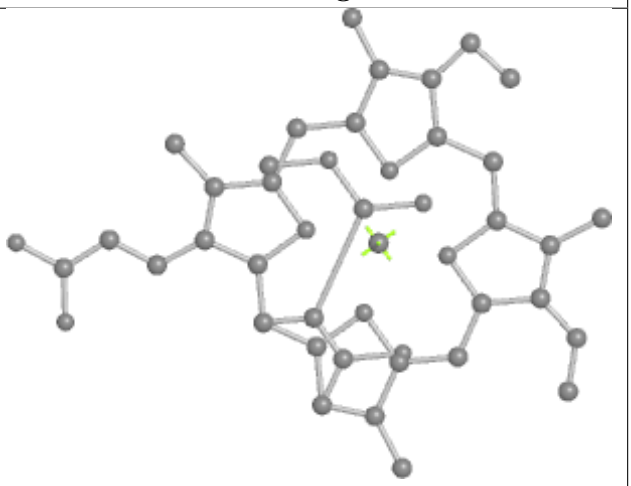
Bond lengths



Bond angles

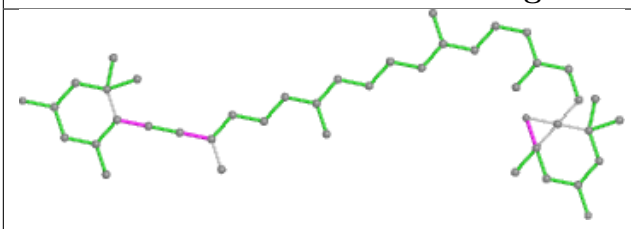


Torsions

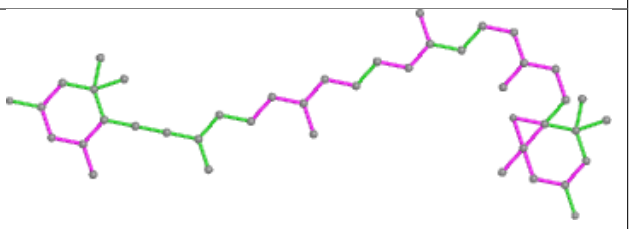


Rings

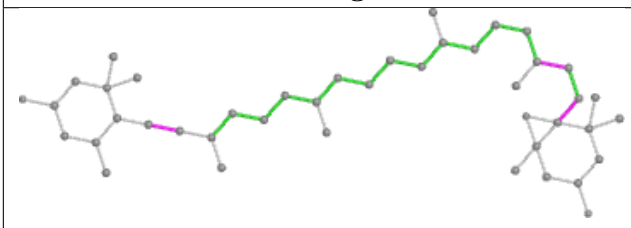
Ligand DD6 K 204



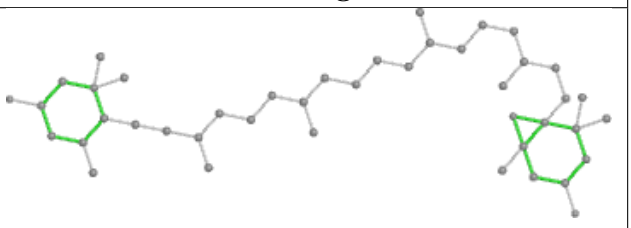
Bond lengths



Bond angles

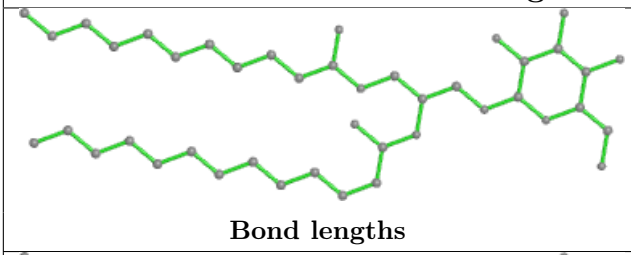


Torsions

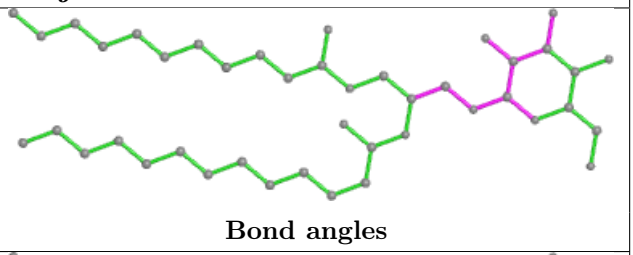


Rings

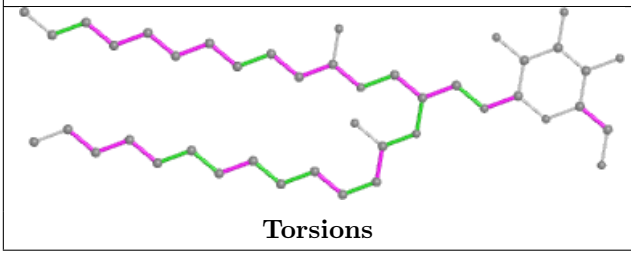
Ligand LMG j 102



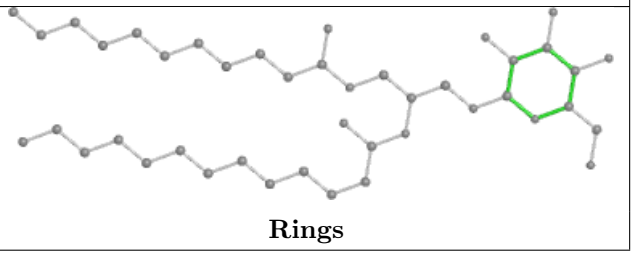
Bond lengths



Bond angles

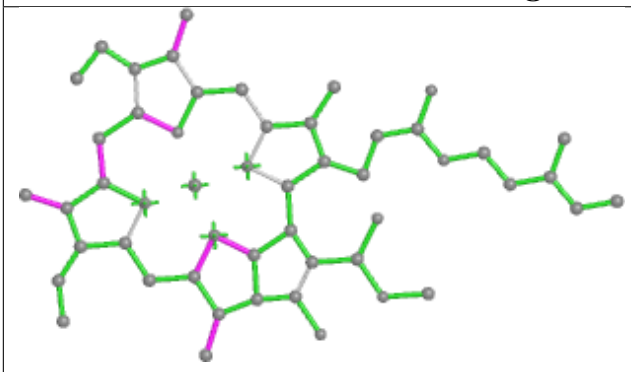


Torsions

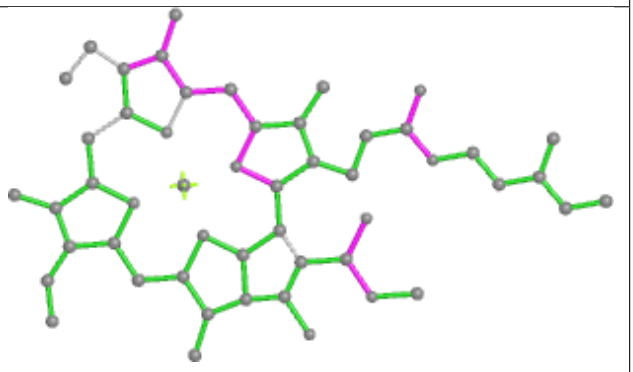


Rings

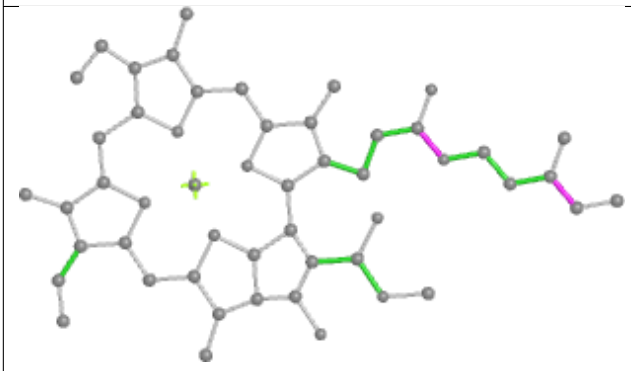
Ligand CLA B 311



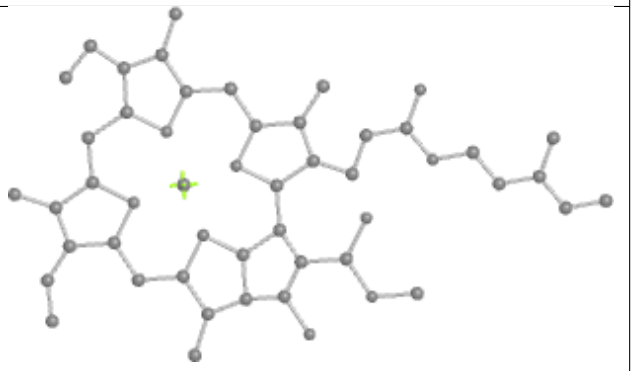
Bond lengths



Bond angles

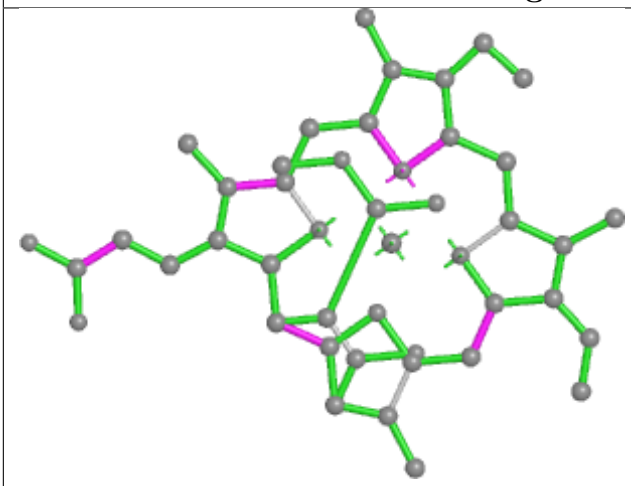


Torsions

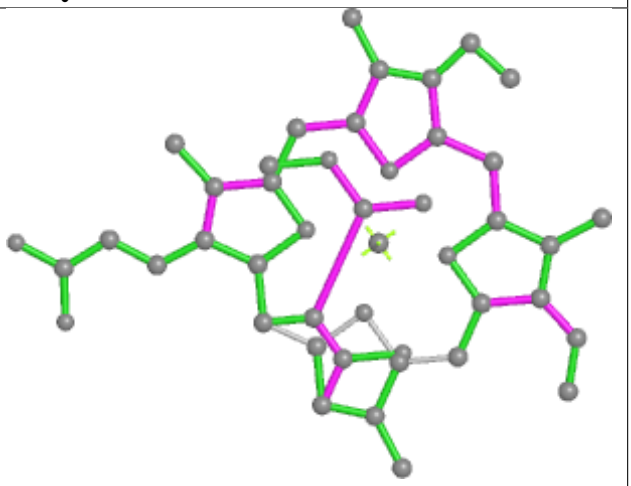


Rings

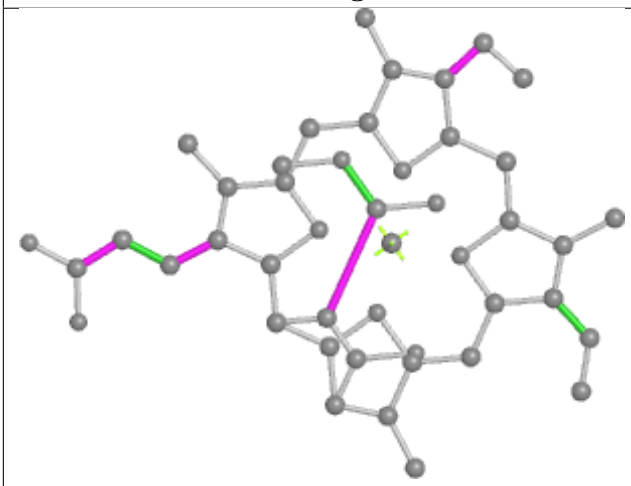
Ligand KC1 Q 311



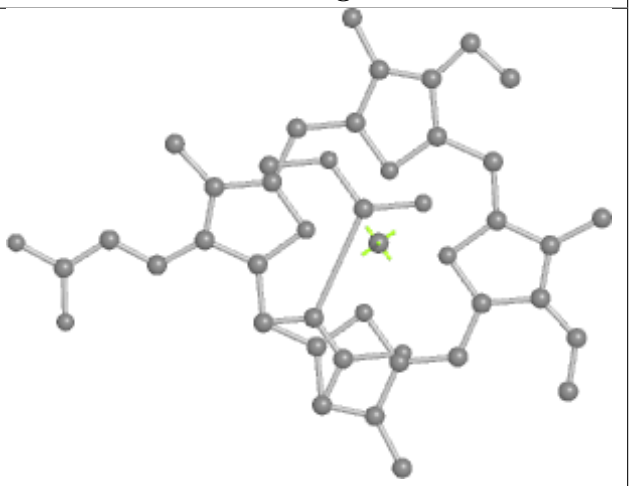
Bond lengths



Bond angles

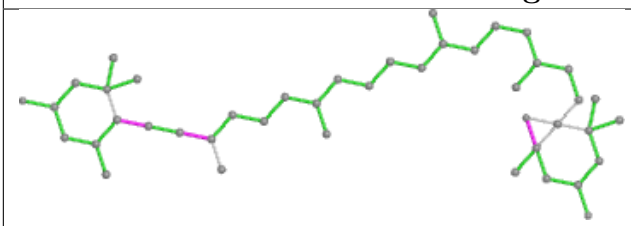


Torsions

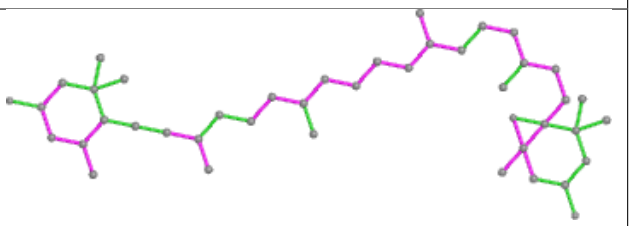


Rings

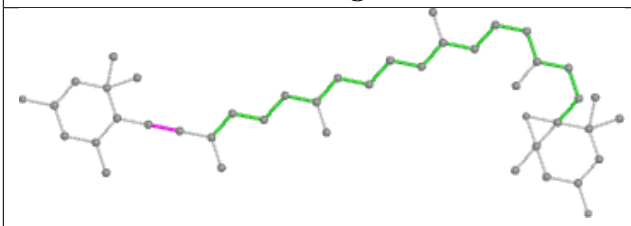
Ligand DD6 m 101



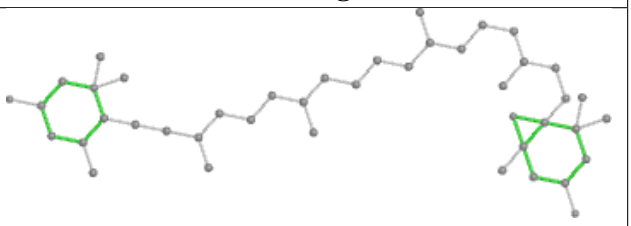
Bond lengths



Bond angles

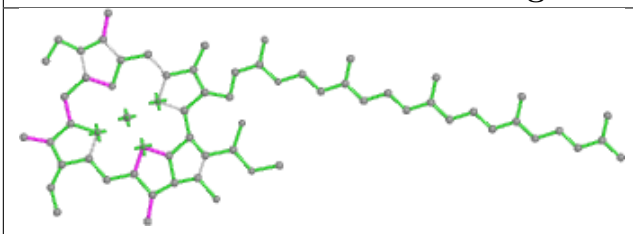


Torsions

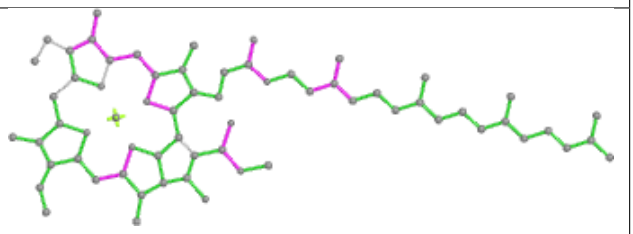


Rings

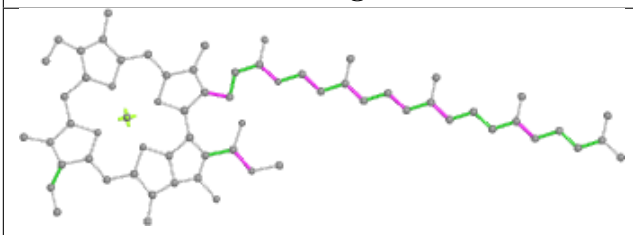
Ligand CLA b 712



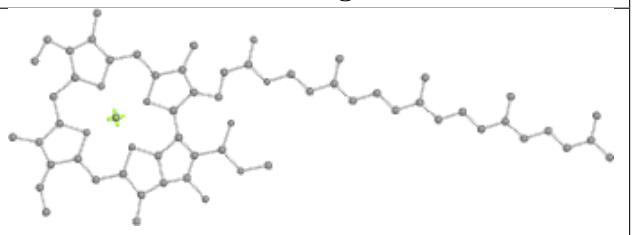
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

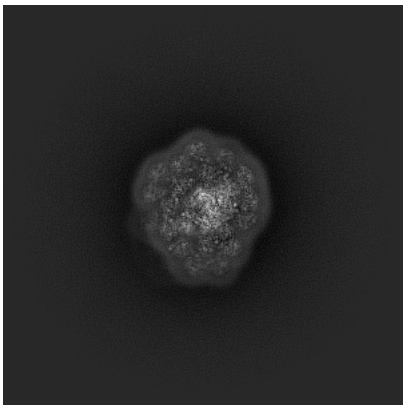
6 Map visualisation

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.

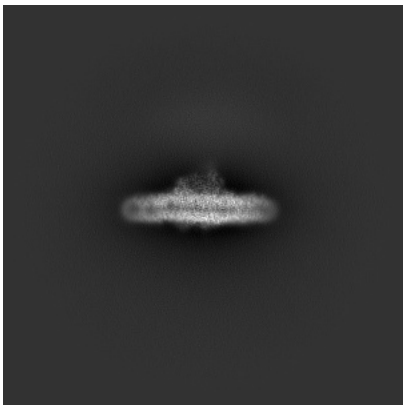
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

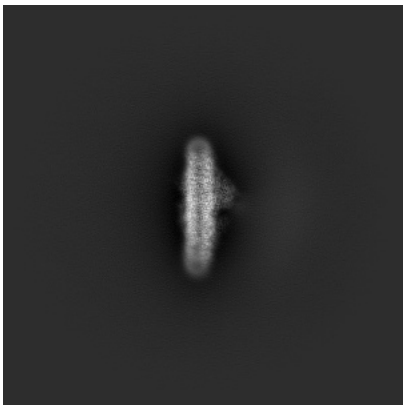
6.1.1 Primary map



X

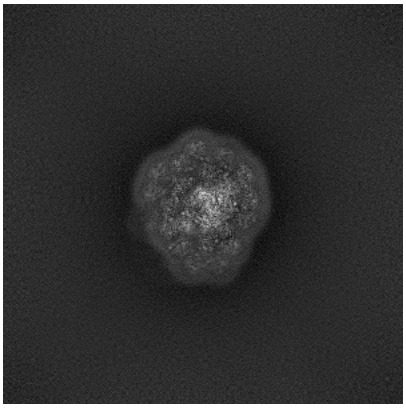


Y

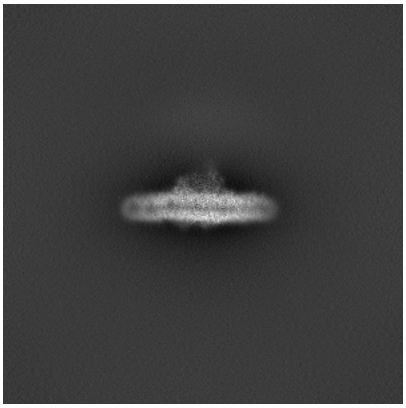


Z

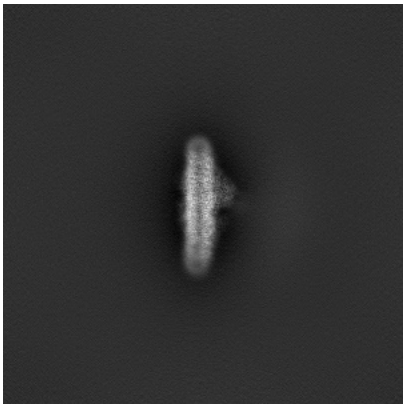
6.1.2 Raw map



X



Y

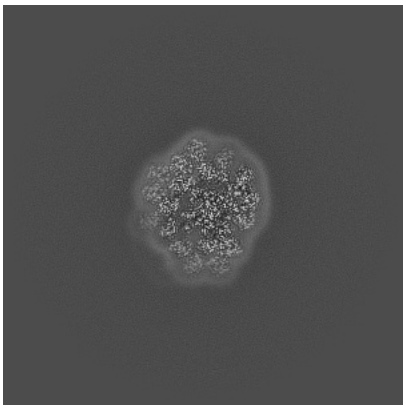


Z

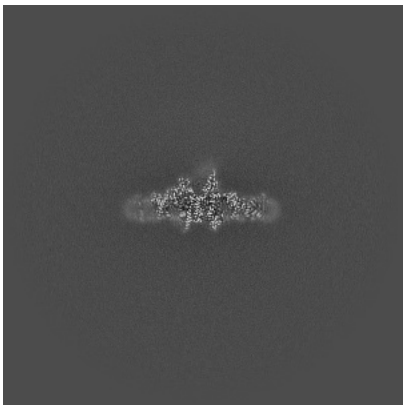
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

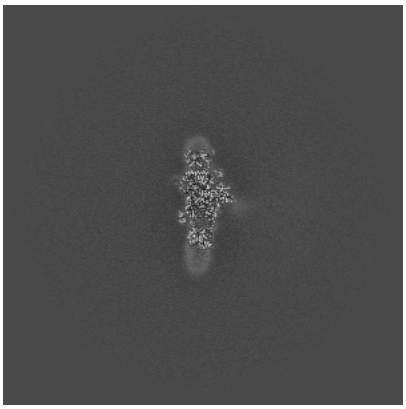
6.2.1 Primary map



X Index: 256

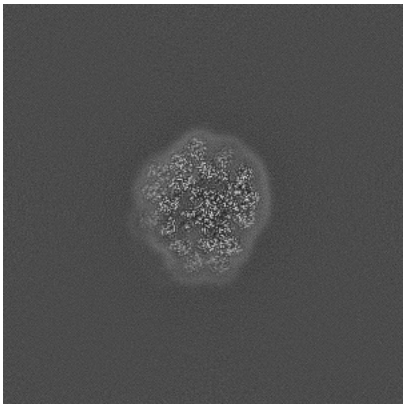


Y Index: 256

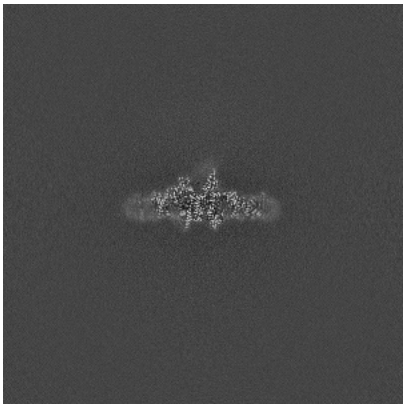


Z Index: 256

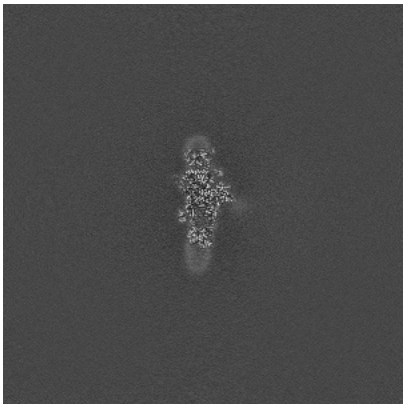
6.2.2 Raw map



X Index: 256



Y Index: 256

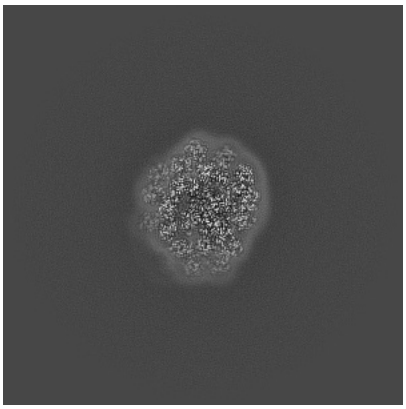


Z Index: 256

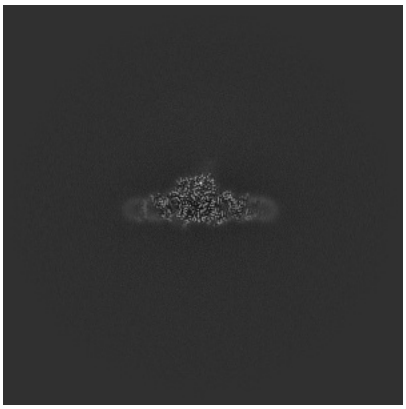
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

6.3.1 Primary map



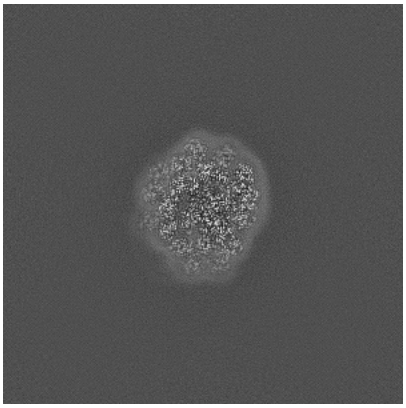
X Index: 259



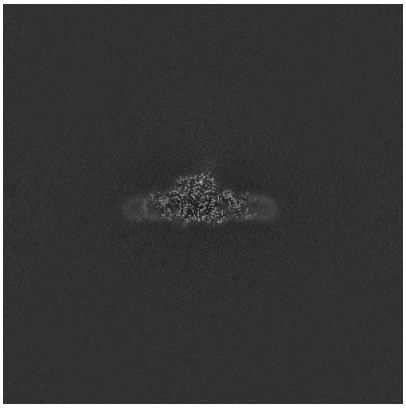
Y Index: 262

Z Index: 262

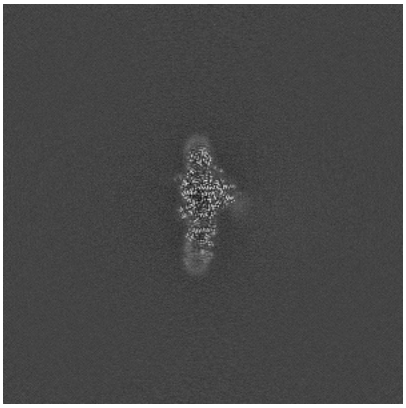
6.3.2 Raw map



X Index: 259



Y Index: 262

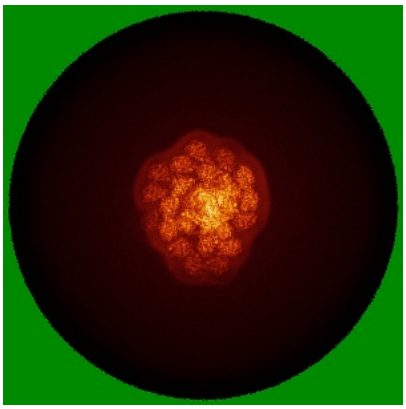


Z Index: 262

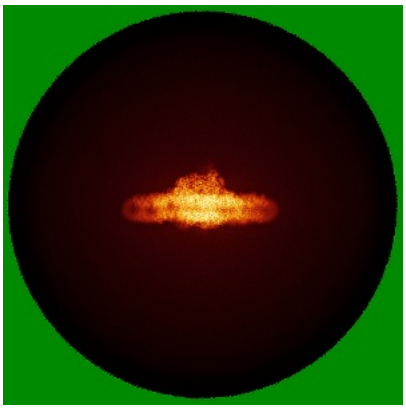
The images above show the largest variance slices of the map in three orthogonal directions.

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

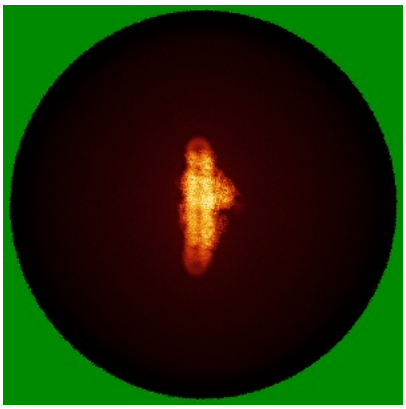
6.4.1 Primary map



X

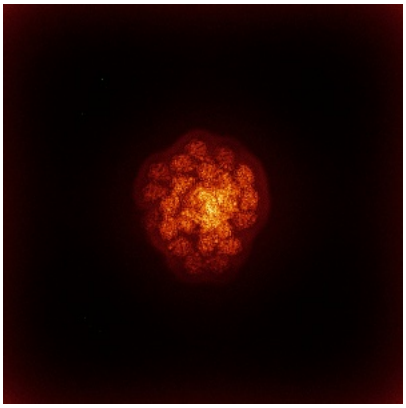


Y

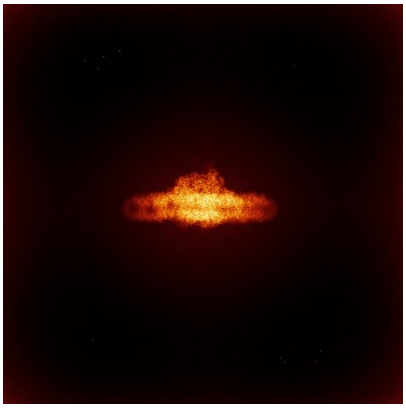


Z

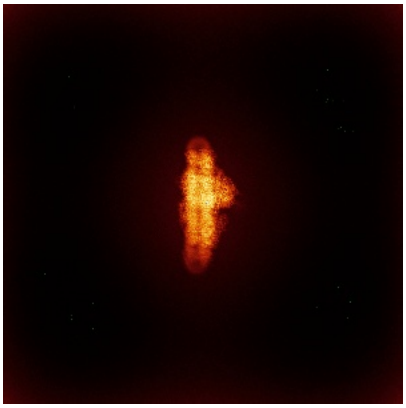
6.4.2 Raw map



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.

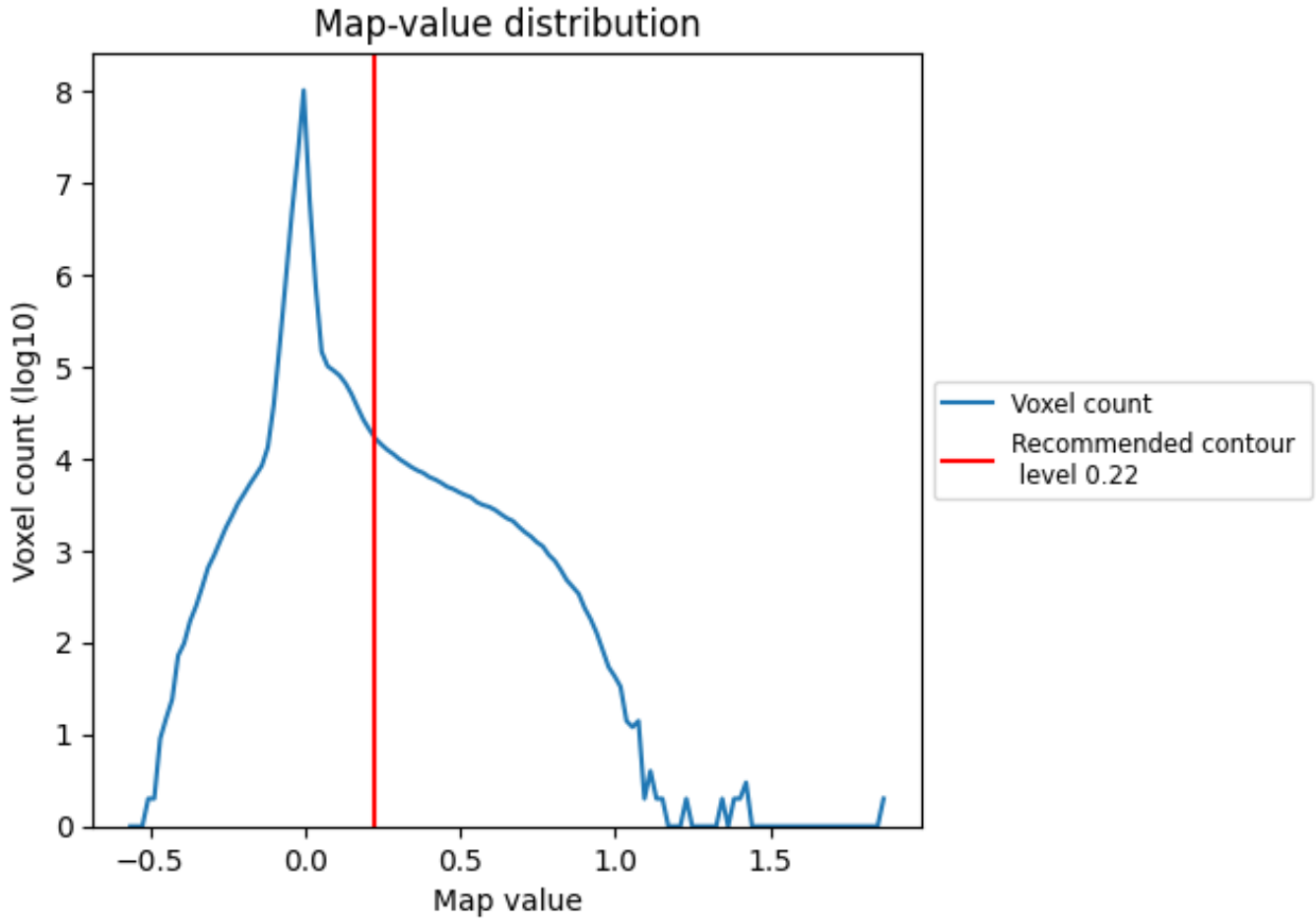
6.6 Mask visualisation (i)

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

7 Map analysis

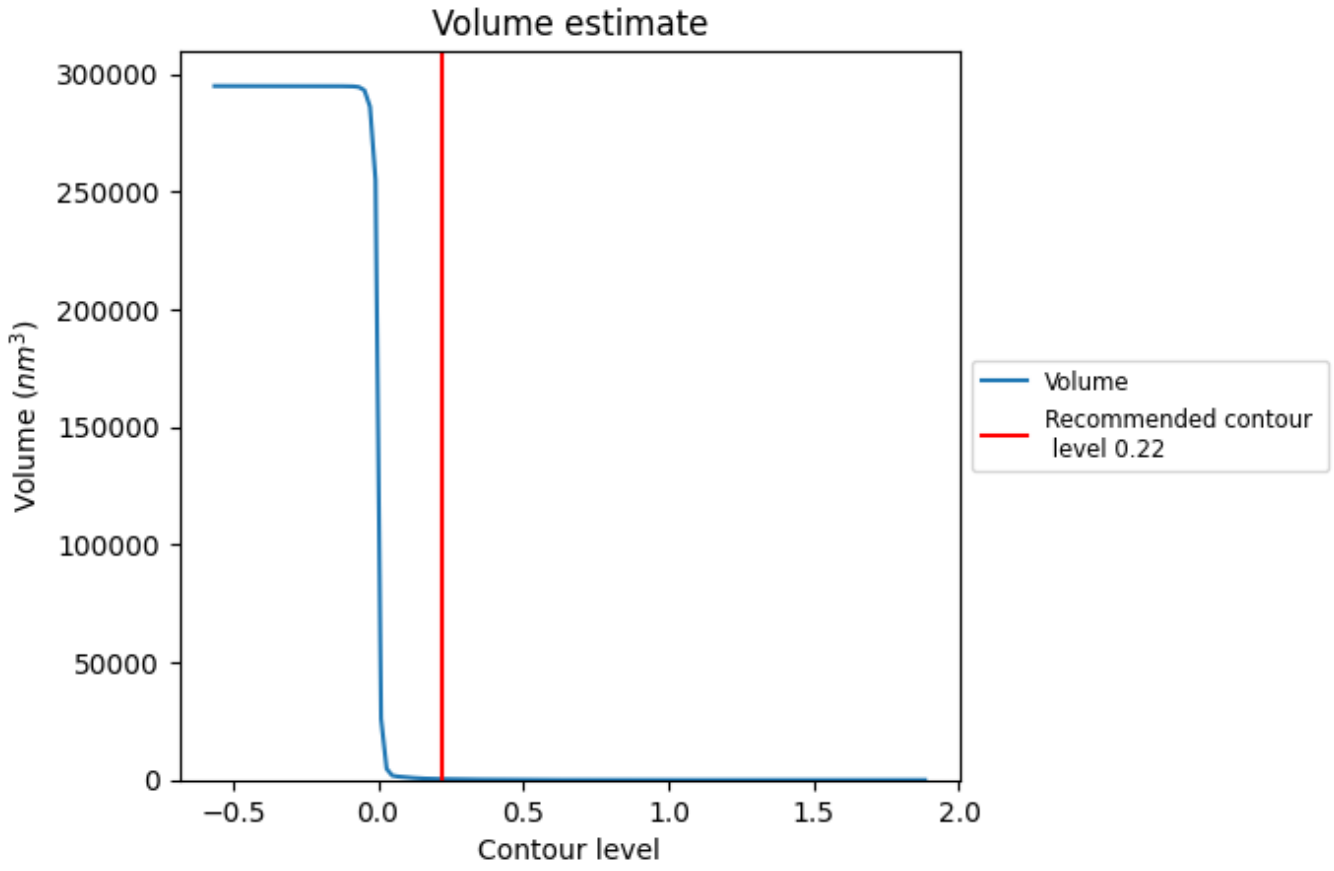
This section contains the results of statistical analysis of the map.

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.

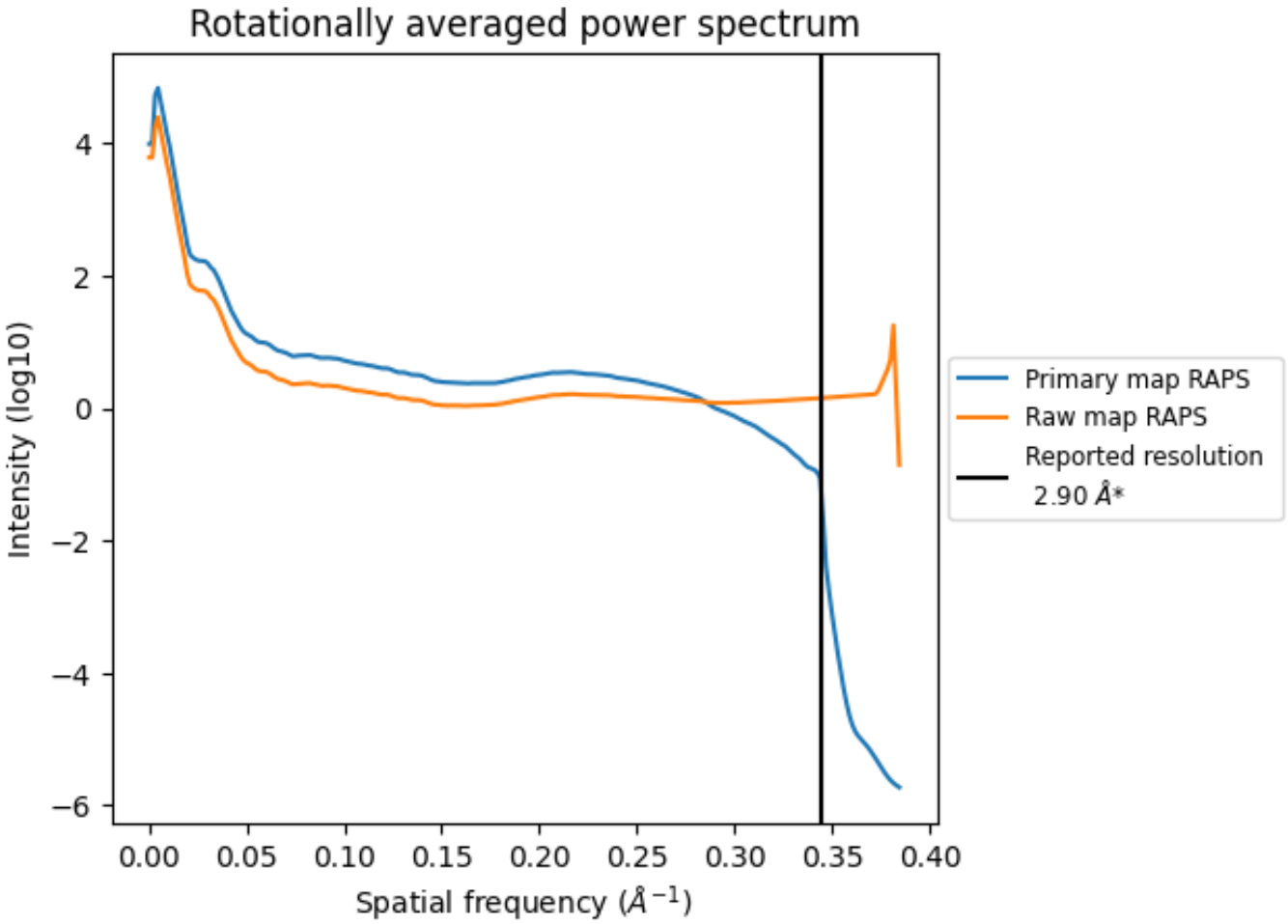
7.2 Volume estimate



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)

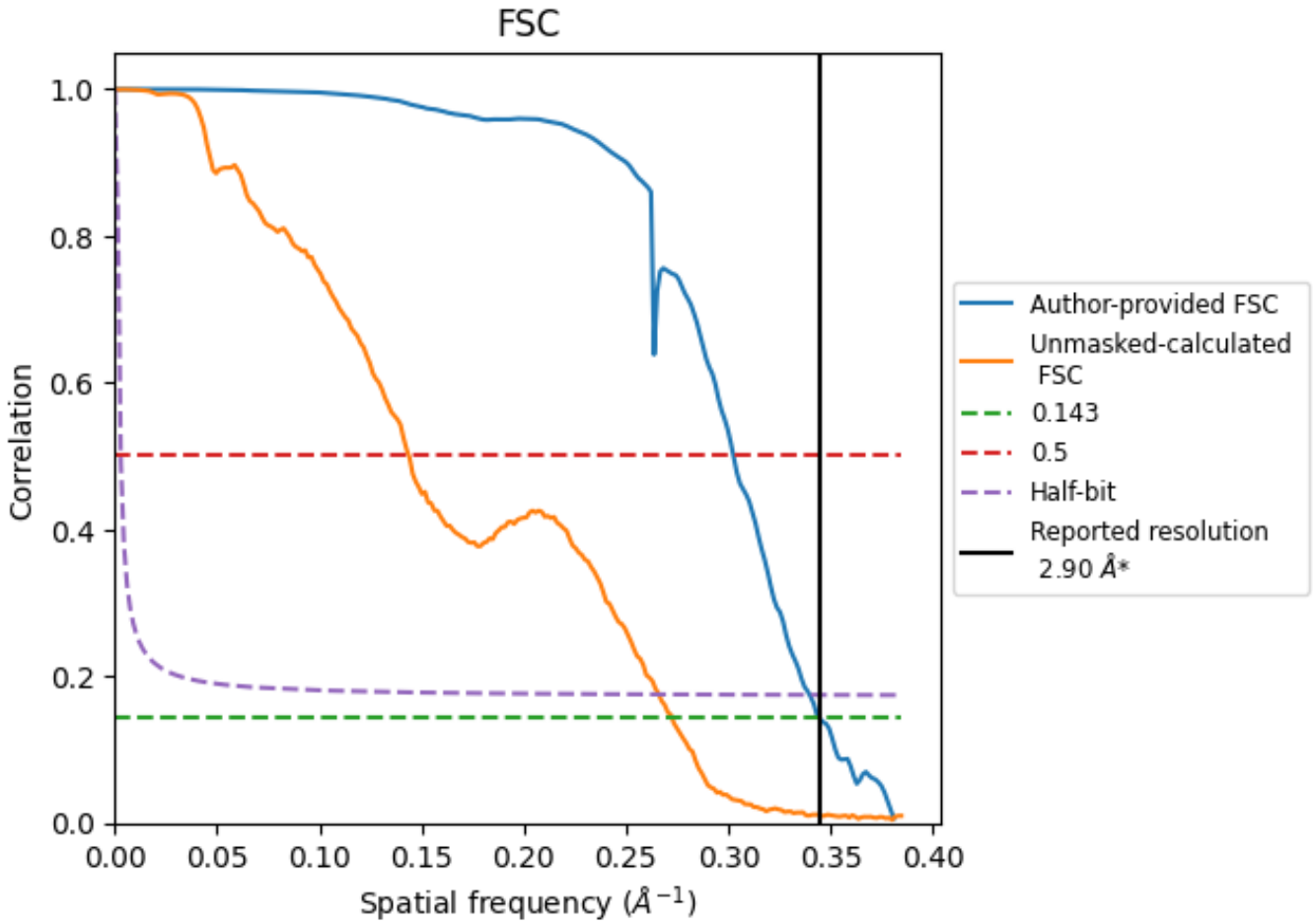


*Reported resolution corresponds to spatial frequency of 0.345 Å^{-1}

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)

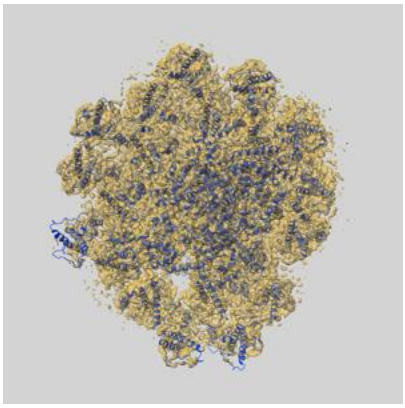
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.90	-	-
Author-provided FSC curve	2.90	3.31	2.94
Unmasked-calculated*	3.67	6.95	3.76

*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 %

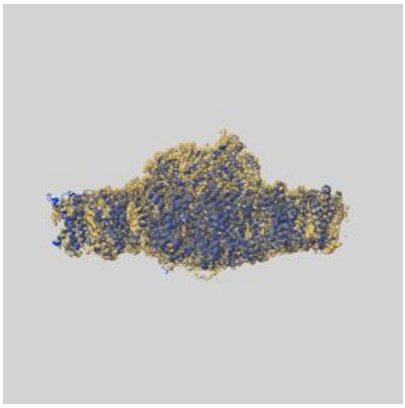
9 Map-model fit

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 40.

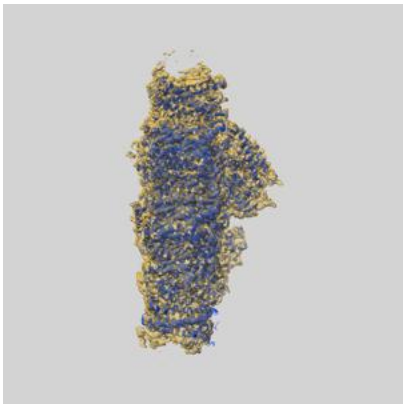
9.1 Map-model overlay



X



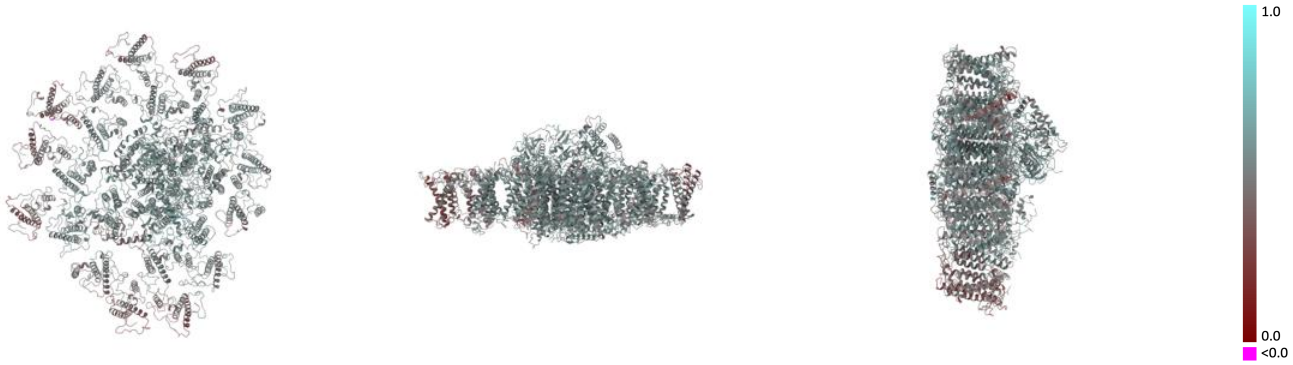
Y



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.

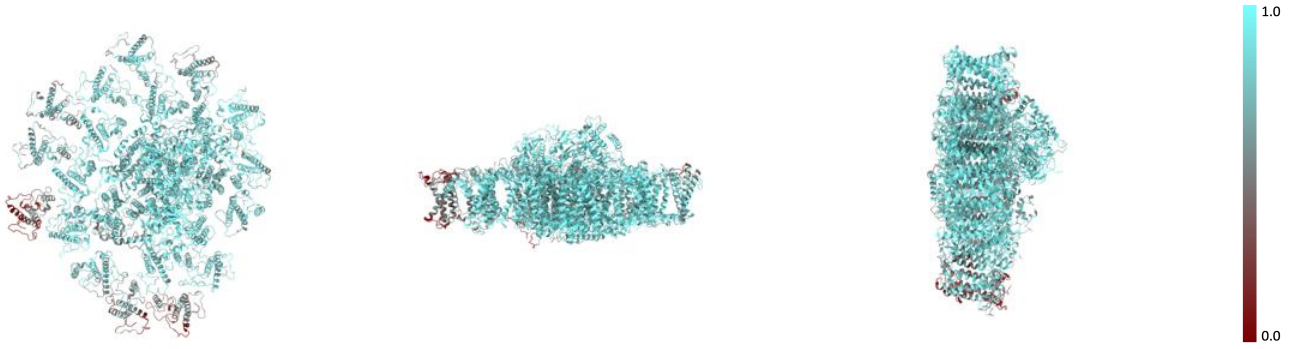
9.2 Q-score mapped to coordinate model



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.

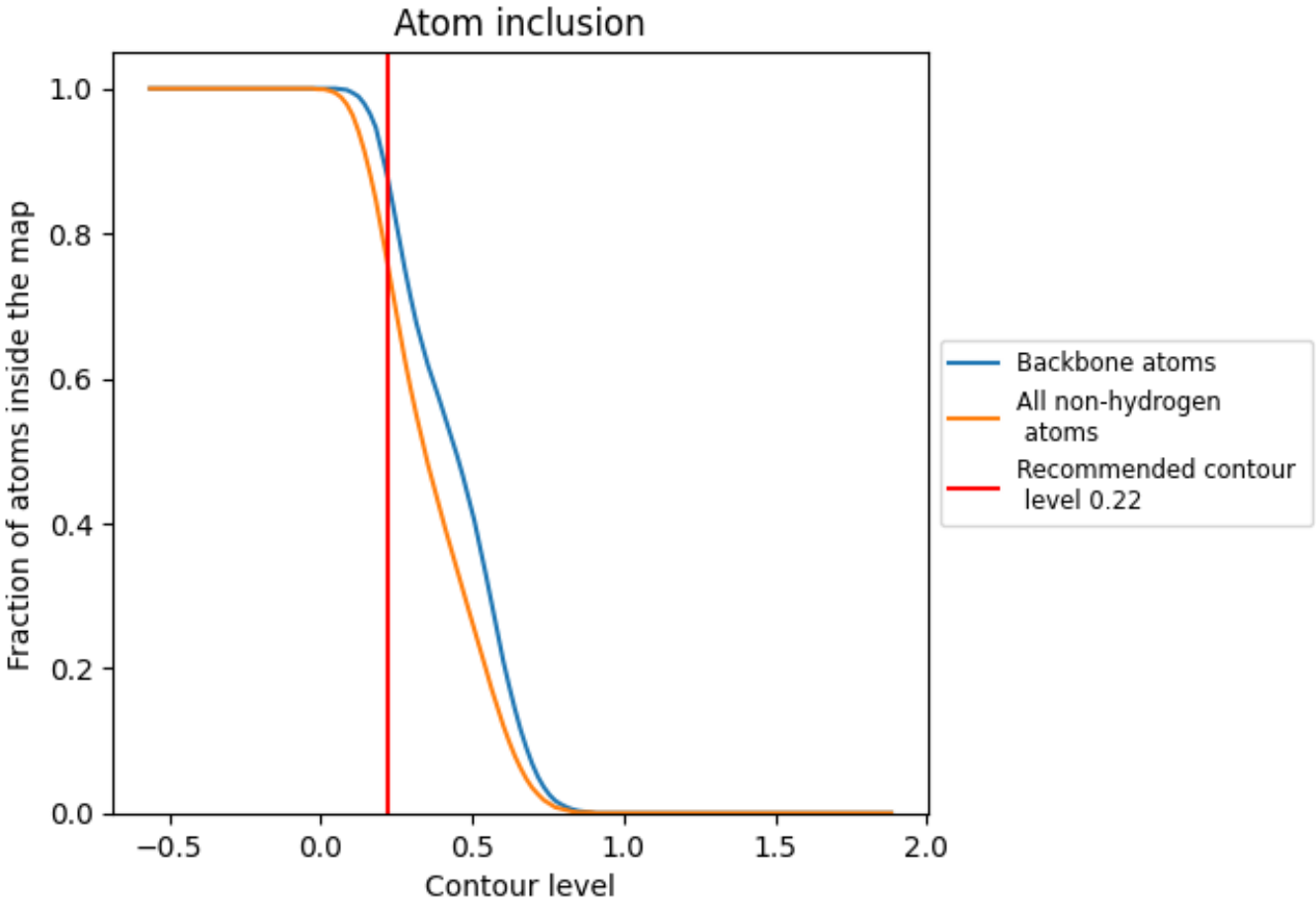
9.3 Atom inclusion mapped to coordinate model



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