wwPDB EM Validation Summary Report (i)

Mar 31, 2025 – 05:32 PM JST

PDB ID	:	6LY5 / pdb_00006ly5
EMDB ID	:	EMD-30012
Title	:	Organization and energy transfer in a huge diatom PSI-FCPI supercomplex
Authors	:	Xiong, P.; Caizhe, X.
Deposited on	:	2020-02-13
Resolution	:	2.38 Å(reported)

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

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

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

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

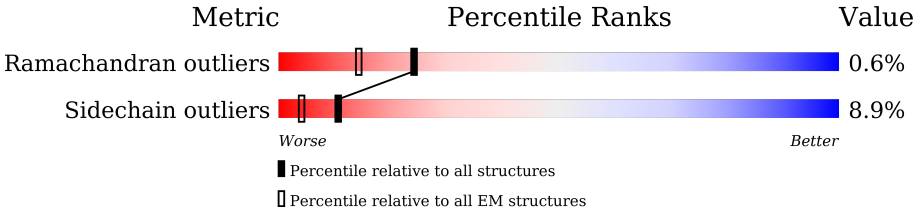
EMDB validation analysis	:	0.0.1.dev117
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.42

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 2.38 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	207382	16835
Sidechain outliers	206894	16415

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	168	95% 5%
2	B	223	54% 5% 41%
3	C	198	76% 7% 18%
4	D	207	74% 9% 17%
5	E	222	82% • 15%
6	F	215	79% 5% 16%
7	G	245	76% 11% 13%
8	H	203	81% • 16%
9	I	195	70% 13% 17%

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Mol	Chain	Length	Quality of chain
10	J	200	77% 6% 16%
11	K	207	80% 18%
12	L	229	6% 83% 14%
13	M	306	58% 39%
14	N	219	71% 90% 10%
15	O	205	13% 80% 16%
15	P	205	75% 9% 16%
15	Q	205	80% 16%
16	R	246	81% 14%
17	S	254	21% 78% 7% 13%
18	T	207	24% 81% 17%
19	W	198	32% 77% 19%
19	X	198	78% 77% 19%
20	a	743	91% 9%
21	b	733	89% 10%
22	c	80	90% 10%
23	d	132	85% 14%
24	e	63	97%
25	f	162	91% 9%
26	i	40	68% 15% 18%
27	j	42	79% 19%
28	l	172	72% 12% 16%
29	m	29	83% 14%
30	g	134	99%
31	h	139	53% 11% 36%

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Mol	Chain	Length	Quality of chain
32	U	160	19% 73% 24%
33	V	179	8% 68% 32%

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
36	CLA	A	305	X	-	-	-
36	CLA	A	306	X	-	-	-
36	CLA	A	307	X	-	-	-
36	CLA	A	308	X	-	-	-
36	CLA	A	309	X	-	-	-
36	CLA	A	310	X	-	-	-
36	CLA	A	311	X	-	-	-
36	CLA	A	313	X	-	-	-
36	CLA	A	314	X	-	-	-
36	CLA	B	305	X	-	-	-
36	CLA	B	306	X	-	-	-
36	CLA	B	307	X	-	-	-
36	CLA	B	308	X	-	-	-
36	CLA	B	309	X	-	-	-
36	CLA	B	311	X	-	-	-
36	CLA	C	205	X	-	-	-
36	CLA	C	206	X	-	-	-
36	CLA	C	207	X	-	-	-
36	CLA	C	208	X	-	-	-
36	CLA	C	209	X	-	-	-
36	CLA	C	210	X	-	-	-
36	CLA	C	211	X	-	-	-
36	CLA	C	212	X	-	-	-
36	CLA	C	214	X	-	-	-
36	CLA	D	306	X	-	-	-
36	CLA	D	307	X	-	-	-
36	CLA	D	308	X	-	-	-
36	CLA	D	309	X	-	-	-
36	CLA	D	310	X	-	-	-
36	CLA	D	312	X	-	-	-
36	CLA	D	313	X	-	-	-
36	CLA	D	315	X	-	-	-
36	CLA	D	316	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
36	CLA	D	317	X	-	-	-
36	CLA	E	308	X	-	-	-
36	CLA	E	311	X	-	-	-
36	CLA	E	312	X	-	-	-
36	CLA	E	313	X	-	-	-
36	CLA	E	314	X	-	-	-
36	CLA	E	315	X	-	-	-
36	CLA	E	316	X	-	-	-
36	CLA	E	317	X	-	-	-
36	CLA	F	309	X	-	-	-
36	CLA	F	310	X	-	-	-
36	CLA	F	311	X	-	-	-
36	CLA	F	312	X	-	-	-
36	CLA	F	313	X	-	-	-
36	CLA	F	314	X	-	-	-
36	CLA	F	316	X	-	-	-
36	CLA	F	317	X	-	-	-
36	CLA	G	309	X	-	-	-
36	CLA	G	310	X	-	-	-
36	CLA	G	311	X	-	-	-
36	CLA	G	312	X	-	-	-
36	CLA	G	313	X	-	-	-
36	CLA	G	314	X	-	-	-
36	CLA	G	315	X	-	-	-
36	CLA	G	316	X	-	-	-
36	CLA	G	319	X	-	-	-
36	CLA	H	305	X	-	-	-
36	CLA	H	306	X	-	-	-
36	CLA	H	307	X	-	-	-
36	CLA	H	308	X	-	-	-
36	CLA	H	309	X	-	-	-
36	CLA	H	310	X	-	-	-
36	CLA	H	311	X	-	-	-
36	CLA	H	312	X	-	-	-
36	CLA	H	314	X	-	-	-
36	CLA	H	315	X	-	-	-
36	CLA	H	316	X	-	-	-
36	CLA	H	317	X	-	-	-
36	CLA	H	318	X	-	-	-
36	CLA	I	305	X	-	-	-
36	CLA	I	306	X	-	-	-
36	CLA	I	307	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
36	CLA	I	308	X	-	-	-
36	CLA	I	309	X	-	-	-
36	CLA	I	310	X	-	-	-
36	CLA	I	311	X	-	-	-
36	CLA	I	312	X	-	-	-
36	CLA	I	313	X	-	-	-
36	CLA	I	314	X	-	-	-
36	CLA	J	307	X	-	-	-
36	CLA	J	309	X	-	-	-
36	CLA	J	310	X	-	-	-
36	CLA	J	311	X	-	-	-
36	CLA	J	312	X	-	-	-
36	CLA	J	313	X	-	-	-
36	CLA	J	315	X	-	-	-
36	CLA	J	316	X	-	-	-
36	CLA	J	317	X	-	-	-
36	CLA	K	307	X	-	-	-
36	CLA	K	308	X	-	-	-
36	CLA	K	309	X	-	-	-
36	CLA	K	310	X	-	-	-
36	CLA	K	311	X	-	-	-
36	CLA	K	312	X	-	-	-
36	CLA	K	313	X	-	-	-
36	CLA	K	315	X	-	-	-
36	CLA	K	316	X	-	-	-
36	CLA	L	308	X	-	-	-
36	CLA	L	309	X	-	-	-
36	CLA	L	310	X	-	-	-
36	CLA	L	311	X	-	-	-
36	CLA	L	313	X	-	-	-
36	CLA	L	314	X	-	-	-
36	CLA	L	316	X	-	-	-
36	CLA	L	320	X	-	-	-
36	CLA	M	306	X	-	-	-
36	CLA	M	307	X	-	-	-
36	CLA	M	308	X	-	-	-
36	CLA	M	309	X	-	-	-
36	CLA	M	310	X	-	-	-
36	CLA	M	311	X	-	-	-
36	CLA	M	312	X	-	-	-
36	CLA	M	314	X	-	-	-
36	CLA	M	316	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
36	CLA	N	307	X	-	-	-
36	CLA	N	308	X	-	-	-
36	CLA	N	309	X	-	-	-
36	CLA	N	310	X	-	-	-
36	CLA	N	311	X	-	-	-
36	CLA	N	312	X	-	-	-
36	CLA	N	313	X	-	-	-
36	CLA	N	316	X	-	-	-
36	CLA	N	317	X	-	-	-
36	CLA	N	318	X	-	-	-
36	CLA	N	319	X	-	-	-
36	CLA	O	306	X	-	-	-
36	CLA	O	307	X	-	-	-
36	CLA	O	308	X	-	-	-
36	CLA	O	309	X	-	-	-
36	CLA	O	310	X	-	-	-
36	CLA	O	311	X	-	-	-
36	CLA	O	314	X	-	-	-
36	CLA	O	316	X	-	-	-
36	CLA	P	301	X	-	-	-
36	CLA	P	308	X	-	-	-
36	CLA	P	309	X	-	-	-
36	CLA	P	310	X	-	-	-
36	CLA	P	311	X	-	-	-
36	CLA	P	312	X	-	-	-
36	CLA	P	313	X	-	-	-
36	CLA	P	316	X	-	-	-
36	CLA	P	318	X	-	-	-
36	CLA	P	319	X	-	-	-
36	CLA	Q	305	X	-	-	-
36	CLA	Q	306	X	-	-	-
36	CLA	Q	307	X	-	-	-
36	CLA	Q	308	X	-	-	-
36	CLA	Q	309	X	-	-	-
36	CLA	Q	312	X	-	-	-
36	CLA	Q	314	X	-	-	-
36	CLA	R	310	X	-	-	-
36	CLA	R	311	X	-	-	-
36	CLA	R	312	X	-	-	-
36	CLA	R	313	X	-	-	-
36	CLA	R	314	X	-	-	-
36	CLA	R	315	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
36	CLA	R	316	X	-	-	-
36	CLA	R	318	X	-	-	-
36	CLA	R	319	X	-	-	-
36	CLA	R	320	X	-	-	-
36	CLA	R	322	X	-	-	-
36	CLA	S	309	X	-	-	-
36	CLA	S	310	X	-	-	-
36	CLA	S	311	X	-	-	-
36	CLA	S	313	X	-	-	-
36	CLA	S	315	X	-	-	-
36	CLA	S	317	X	-	-	-
36	CLA	S	318	X	-	-	-
36	CLA	S	319	X	-	-	-
36	CLA	T	308	X	-	-	-
36	CLA	T	309	X	-	-	-
36	CLA	T	311	X	-	-	-
36	CLA	T	312	X	-	-	-
36	CLA	T	313	X	-	-	-
36	CLA	T	314	X	-	-	-
36	CLA	T	316	X	-	-	-
36	CLA	U	305	X	-	-	-
36	CLA	U	306	X	-	-	-
36	CLA	U	307	X	-	-	-
36	CLA	U	308	X	-	-	-
36	CLA	U	310	X	-	-	-
36	CLA	U	311	X	-	-	-
36	CLA	U	313	X	-	-	-
36	CLA	V	305	X	-	-	-
36	CLA	V	306	X	-	-	-
36	CLA	V	307	X	-	-	-
36	CLA	V	308	X	-	-	-
36	CLA	V	309	X	-	-	-
36	CLA	V	310	X	-	-	-
36	CLA	V	311	X	-	-	-
36	CLA	V	313	X	-	-	-
36	CLA	V	314	X	-	-	-
36	CLA	W	201	X	-	-	-
36	CLA	W	206	X	-	-	-
36	CLA	W	207	X	-	-	-
36	CLA	W	208	X	-	-	-
36	CLA	W	209	X	-	-	-
36	CLA	W	210	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
36	CLA	W	211	X	-	-	-
36	CLA	W	215	X	-	-	-
36	CLA	W	216	X	-	-	-
36	CLA	W	218	X	-	-	-
36	CLA	X	306	X	-	-	-
36	CLA	X	308	X	-	-	-
36	CLA	X	310	X	-	-	-
36	CLA	X	312	X	-	-	-
36	CLA	a	801	X	-	-	-
36	CLA	a	802	X	-	-	-
36	CLA	a	803	X	-	-	-
36	CLA	a	804	X	-	-	-
36	CLA	a	805	X	-	-	-
36	CLA	a	806	X	-	-	-
36	CLA	a	807	X	-	-	-
36	CLA	a	808	X	-	-	-
36	CLA	a	809	X	-	-	-
36	CLA	a	810	X	-	-	-
36	CLA	a	811	X	-	-	-
36	CLA	a	812	X	-	-	-
36	CLA	a	813	X	-	-	-
36	CLA	a	814	X	-	-	-
36	CLA	a	815	X	-	-	-
36	CLA	a	816	X	-	-	-
36	CLA	a	817	X	-	-	-
36	CLA	a	818	X	-	-	-
36	CLA	a	819	X	-	-	-
36	CLA	a	820	X	-	-	-
36	CLA	a	821	X	-	-	-
36	CLA	a	822	X	-	-	-
36	CLA	a	823	X	-	-	-
36	CLA	a	824	X	-	-	-
36	CLA	a	825	X	-	-	-
36	CLA	a	826	X	-	-	-
36	CLA	a	827	X	-	-	-
36	CLA	a	828	X	-	-	-
36	CLA	a	829	X	-	-	-
36	CLA	a	831	X	-	-	-
36	CLA	a	832	X	-	-	-
36	CLA	a	833	X	-	-	-
36	CLA	a	834	X	-	-	-
36	CLA	a	835	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
36	CLA	a	836	X	-	-	-
36	CLA	a	837	X	-	-	-
36	CLA	a	838	X	-	-	-
36	CLA	a	839	X	-	-	-
36	CLA	a	841	X	-	-	-
36	CLA	a	848	X	-	-	-
36	CLA	b	801	X	-	-	-
36	CLA	b	802	X	-	-	-
36	CLA	b	805	X	-	-	-
36	CLA	b	806	X	-	-	-
36	CLA	b	807	X	-	-	-
36	CLA	b	808	X	-	-	-
36	CLA	b	809	X	-	-	-
36	CLA	b	810	X	-	-	-
36	CLA	b	811	X	-	-	-
36	CLA	b	812	X	-	-	-
36	CLA	b	813	X	-	-	-
36	CLA	b	814	X	-	-	-
36	CLA	b	815	X	-	-	-
36	CLA	b	816	X	-	-	-
36	CLA	b	817	X	-	-	-
36	CLA	b	819	X	-	-	-
36	CLA	b	820	X	-	-	-
36	CLA	b	821	X	-	-	-
36	CLA	b	822	X	-	-	-
36	CLA	b	823	X	-	-	-
36	CLA	b	824	X	-	-	-
36	CLA	b	825	X	-	-	-
36	CLA	b	826	X	-	-	-
36	CLA	b	827	X	-	-	-
36	CLA	b	828	X	-	-	-
36	CLA	b	829	X	-	-	-
36	CLA	b	830	X	-	-	-
36	CLA	b	831	X	-	-	-
36	CLA	b	832	X	-	-	-
36	CLA	b	833	X	-	-	-
36	CLA	b	834	X	-	-	-
36	CLA	b	835	X	-	-	-
36	CLA	b	836	X	-	-	-
36	CLA	b	837	X	-	-	-
36	CLA	b	838	X	-	-	-
36	CLA	b	839	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
36	CLA	b	840	X	-	-	-
36	CLA	b	841	X	-	-	-
36	CLA	f	802	X	-	-	-
36	CLA	f	803	X	-	-	-
36	CLA	f	804	X	-	-	-
36	CLA	f	805	X	-	-	-
36	CLA	h	203	X	-	-	-
36	CLA	i	102	X	-	-	-
36	CLA	j	101	X	-	-	-
36	CLA	j	102	X	-	-	-
36	CLA	j	106	X	-	-	-
36	CLA	l	201	X	-	-	-
36	CLA	l	202	X	-	-	-
36	CLA	l	205	X	-	-	-
36	CLA	l	206	X	-	-	-

2 Entry composition (i)

There are 46 unique types of molecules in this entry. The entry contains 81344 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 FCPI-7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	168	1287	825	213	237	12	0	0

- Molecule 2 is a protein called FCPI-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	132	1013	662	166	176	9	0	0

- Molecule 3 is a protein called FCPI-11.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	163	1247	796	210	232	9	0	0

- Molecule 4 is a protein called FCPI-6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	D	172	1337	870	214	245	8	0	0

- Molecule 5 is a protein called FCPI-5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	E	188	1411	891	240	265	15	0	0

- Molecule 6 is a protein called FCPI-8.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	F	180	1375	880	230	253	12	0	0

- Molecule 7 is a protein called FCPI-4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	G	214	1668	1079	276	305	8	0	0

- Molecule 8 is a protein called FCPI-10.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	H	170	1291	832	213	236	10	0	0

- Molecule 9 is a protein called FCPI-3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	I	161	1250	807	208	228	7	0	0

- Molecule 10 is a protein called FCPI-9.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	J	167	1301	843	217	236	5	0	0

- Molecule 11 is a protein called FCPI-13.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	K	169	1304	850	214	232	8	0	0

- Molecule 12 is a protein called FCPI-14.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	L	196	1523	989	250	276	8	0	0

- Molecule 13 is a protein called FCPI-16.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	M	187	1423	914	248	255	6	0	0

- Molecule 14 is a protein called FCPI-21.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	N	219	1716	1119	282	309	6	0	0

- Molecule 15 is a protein called FCPI.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
15	O	173	1302	837	216	241	8	0	0
15	P	173	1296	834	213	241	8	0	0
15	Q	173	1302	837	216	241	8	0	0

- Molecule 16 is a protein called FCPI-24.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
16	R	211	1628	1061	266	294	7	0	0

- Molecule 17 is a protein called FCPI-23.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
17	S	220	1722	1122	283	311	6	0	0

- Molecule 18 is a protein called FCPI-12.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
18	T	172	1326	848	226	247	5	0	0

- Molecule 19 is a protein called FCPI-17.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
19	W	160	1239	799	203	233	4	0	0
19	X	161	1253	808	207	234	4	1	0

- Molecule 20 is a protein called PsaA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
20	a	742	5858	3826	991	1013	28	0	0

- Molecule 21 is a protein called PsaB.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
21	b	732	5820	3828	980	994	18	1	0

- Molecule 22 is a protein called PsaC.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
22	c	80	597	368	104	114	11	0	0

- Molecule 23 is a protein called PsaD.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
23	d	132	1056	681	186	186	3	1	0

- Molecule 24 is a protein called PsaE.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
24	e	63	507	321	90	96	0	0

- Molecule 25 is a protein called PsaF.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
25	f	162	1223	789	211	220	3	0	0

- Molecule 26 is a protein called PsaI.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
26	i	33	256	176	40	38	2	0	0

- Molecule 27 is a protein called PsaJ.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
27	j	41	324	219	50	54	1	0	0

- Molecule 28 is a protein called PsaL.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
28	l	144	1094	726	178	187	3	0	0

- Molecule 29 is a protein called PsaM.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
29	m	28	198	130	32	34	2	0	0

- Molecule 30 is a protein called PsaS.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
30	g	134	670	402	134	134	0	0

- Molecule 31 is a protein called PsaR.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
31	h	89	676	440	110	120	6	0	0

- Molecule 32 is a protein called FCPI-2.

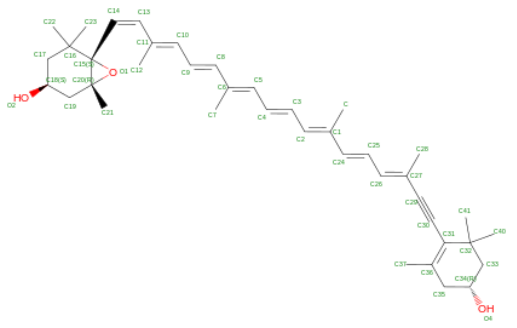
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
32	U	156	1194	766	199	221	8	0	0

- Molecule 33 is a protein called FCPI-19.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
33	V	179	1361	871	234	252	4	0	0

- Molecule 34 is (3S,3'R,5R,6S,7cis)-7',8'-didehydro-5,6-dihydro-5,6-epoxy-beta,beta-carotene -3,3'-diol (CCD ID: DD6) (formula: $C_{40}H_{54}O_3$).

DD6



Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
34	A	1	43	40	3	0
			Total	C	O	
34	A	1	43	40	3	0
			Total	C	O	
34	A	1	43	40	3	0
			Total	C	O	
34	B	1	43	40	3	0
			Total	C	O	
34	B	1	43	40	3	0
			Total	C	O	
34	C	1	43	40	3	0
			Total	C	O	
34	D	1	43	40	3	0
			Total	C	O	
34	D	1	43	40	3	0
			Total	C	O	
34	D	1	43	40	3	0
			Total	C	O	
34	D	1	43	40	3	0
			Total	C	O	
34	E	1	43	40	3	0
			Total	C	O	
34	E	1	43	40	3	0
			Total	C	O	
34	E	1	43	40	3	0
			Total	C	O	
34	E	1	43	40	3	0

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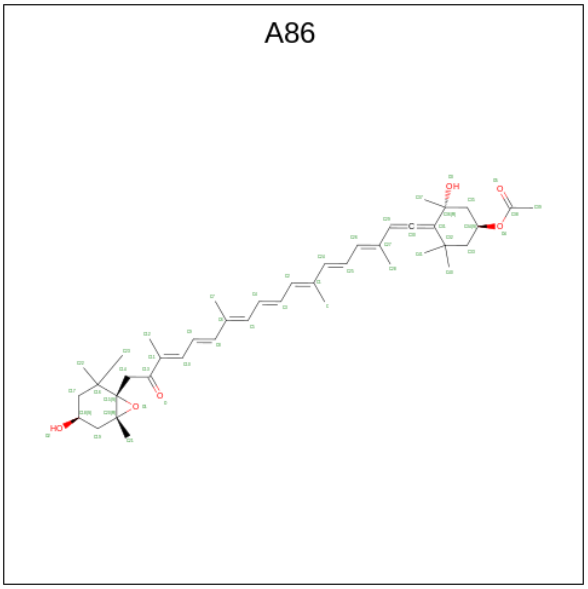
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
34	F	1	43	40	3	0
34	G	1	43	40	3	0
34	H	1	43	40	3	0
34	H	1	43	40	3	0
34	I	1	43	40	3	0
34	J	1	43	40	3	0
34	K	1	43	40	3	0
34	K	1	43	40	3	0
34	L	1	43	40	3	0
34	M	1	43	40	3	0
34	O	1	43	40	3	0
34	P	1	43	40	3	0
34	Q	1	43	40	3	0
34	R	1	43	40	3	0
34	R	1	43	40	3	0
34	S	1	43	40	3	0
34	S	1	43	40	3	0
34	W	1	43	40	3	0
34	W	1	43	40	3	0
34	a	1	43	40	3	0
34	j	1	43	40	3	0

- Molecule 35 is (3S,3'S,5R,5'R,6S,6'R,8'R)-3,5'-dihydroxy-8-oxo-6',7'-didehydro-5,5',6,6',7,8-hexahydro-5,6-epoxy-beta,beta-caroten-3'- yl acetate (CCD ID: A86) (formula: $C_{42}H_{58}O_6$).



Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
35	A	1	48	42	6	0
			Total	C	O	
35	A	1	48	42	6	0
			Total	C	O	
35	B	1	48	42	6	0
			Total	C	O	
35	B	1	48	42	6	0
			Total	C	O	
35	C	1	48	42	6	0
			Total	C	O	
35	C	1	48	42	6	0
			Total	C	O	
35	C	1	48	42	6	0
			Total	C	O	
35	D	1	48	42	6	0
			Total	C	O	
35	E	1	48	42	6	0
			Total	C	O	
35	E	1	48	42	6	0
			Total	C	O	
35	E	1	48	42	6	0
			Total	C	O	
35	F	1	48	42	6	0

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Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
35	F	1	48	42	6	0
35	F	1	48	42	6	0
35	F	1	48	42	6	0
35	F	1	48	42	6	0
35	F	1	48	42	6	0
35	G	1	48	42	6	0
35	G	1	48	42	6	0
35	G	1	48	42	6	0
35	G	1	48	42	6	0
35	H	1	48	42	6	0
35	H	1	48	42	6	0
35	I	1	48	42	6	0
35	I	1	48	42	6	0
35	I	1	48	42	6	0
35	J	1	48	42	6	0
35	J	1	48	42	6	0
35	J	1	48	42	6	0
35	J	1	48	42	6	0
35	J	1	48	42	6	0
35	K	1	48	42	6	0
35	K	1	48	42	6	0

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Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
35	K	1	48	42	6	0
35	K	1	48	42	6	0
35	L	1	48	42	6	0
35	L	1	48	42	6	0
35	L	1	48	42	6	0
35	L	1	48	42	6	0
35	L	1	48	42	6	0
35	M	1	48	42	6	0
35	M	1	48	42	6	0
35	M	1	48	42	6	0
35	M	1	48	42	6	0
35	N	1	48	42	6	0
35	N	1	48	42	6	0
35	N	1	48	42	6	0
35	N	1	48	42	6	0
35	N	1	48	42	6	0
35	N	1	48	42	6	0
35	N	1	48	42	6	0
35	O	1	48	42	6	0
35	O	1	48	42	6	0
35	O	1	48	42	6	0

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Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
35	O	1	48	42	6	0
35	O	1	48	42	6	0
35	P	1	48	42	6	0
35	P	1	48	42	6	0
35	P	1	48	42	6	0
35	P	1	48	42	6	0
35	Q	1	48	42	6	0
35	Q	1	48	42	6	0
35	Q	1	48	42	6	0
35	Q	1	48	42	6	0
35	R	1	48	42	6	0
35	R	1	48	42	6	0
35	R	1	48	42	6	0
35	R	1	48	42	6	0
35	R	1	48	42	6	0
35	R	1	48	42	6	0
35	R	1	48	42	6	0
35	S	1	48	42	6	0
35	S	1	48	42	6	0
35	S	1	48	42	6	0
35	S	1	48	42	6	0

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Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
35	S	1	48	42	6	0
35	S	1	48	42	6	0
35	T	1	48	42	6	0
35	T	1	48	42	6	0
35	T	1	48	42	6	0
35	T	1	48	42	6	0
35	T	1	48	42	6	0
35	T	1	48	42	6	0
35	T	1	48	42	6	0
35	W	1	48	42	6	0
35	W	1	48	42	6	0
35	X	1	48	42	6	0
35	X	1	48	42	6	0
35	X	1	48	42	6	0
35	X	1	48	42	6	0
35	X	1	48	42	6	0
35	X	1	48	42	6	0
35	h	1	48	42	6	0
35	h	1	48	42	6	0
35	U	1	48	42	6	0
35	U	1	48	42	6	0

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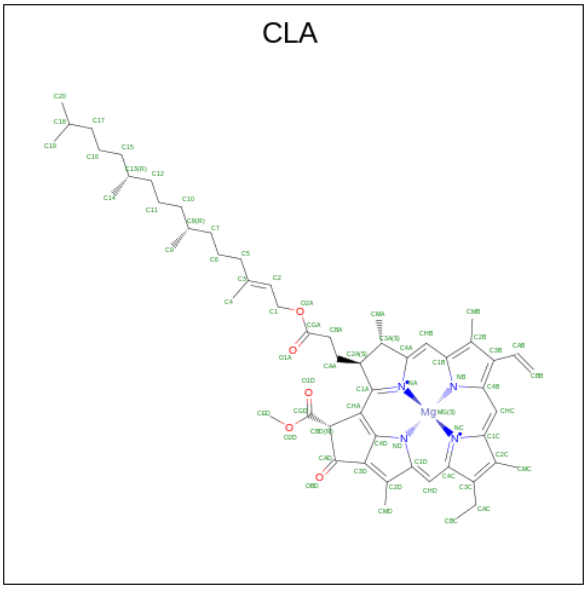
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
35	U	1	48	42	6	0
			Total	C	O	
35	U	1	48	42	6	0
			Total	C	O	
35	V	1	48	42	6	0
			Total	C	O	
35	V	1	48	42	6	0
			Total	C	O	
35	V	1	48	42	6	0
			Total	C	O	
35	V	1	48	42	6	0

- Molecule 36 is CHLOROPHYLL A (CCD ID: CLA) (formula: $C_{55}H_{72}MgN_4O_5$).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
36	A	1	49	39	1	4	5	0
			Total	C	Mg	N	O	
36	A	1	61	51	1	4	5	0
			Total	C	Mg	N	O	
36	A	1	60	50	1	4	5	0
			Total	C	Mg	N	O	
36	A	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
36	A	1	46	36	1	4	5	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
36	A	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
36	A	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
36	A	1	41	33	1	4	3	0
			Total	C	Mg	N	O	
36	A	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
36	B	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
36	B	1	46	36	1	4	5	0
			Total	C	Mg	N	O	
36	B	1	46	36	1	4	5	0
			Total	C	Mg	N	O	
36	B	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
36	B	1	52	42	1	4	5	0
			Total	C	Mg	N	O	
36	B	1	55	45	1	4	5	0
			Total	C	Mg	N	O	
36	C	1	43	35	1	4	3	0
			Total	C	Mg	N	O	
36	C	1	61	51	1	4	5	0
			Total	C	Mg	N	O	
36	C	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
36	C	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
36	C	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
36	C	1	46	36	1	4	5	0
			Total	C	Mg	N	O	
36	C	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
36	C	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
36	C	1	41	33	1	4	3	0
			Total	C	Mg	N	O	
36	D	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
36	D	1	61	51	1	4	5	0

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Mol	Chain	Residues	Atoms					AltConf
36	D	1	Total 65	C 55	Mg 1	N 4	O 5	0
36	D	1	Total 55	C 45	Mg 1	N 4	O 5	0
36	D	1	Total 65	C 55	Mg 1	N 4	O 5	0
36	D	1	Total 46	C 36	Mg 1	N 4	O 5	0
36	D	1	Total 65	C 55	Mg 1	N 4	O 5	0
36	D	1	Total 65	C 55	Mg 1	N 4	O 5	0
36	D	1	Total 41	C 33	Mg 1	N 4	O 3	0
36	D	1	Total 52	C 42	Mg 1	N 4	O 5	0
36	D	1	Total 58	C 48	Mg 1	N 4	O 5	0
36	E	1	Total 49	C 39	Mg 1	N 4	O 5	0
36	E	1	Total 65	C 55	Mg 1	N 4	O 5	0
36	E	1	Total 65	C 55	Mg 1	N 4	O 5	0
36	E	1	Total 65	C 55	Mg 1	N 4	O 5	0
36	E	1	Total 65	C 55	Mg 1	N 4	O 5	0
36	E	1	Total 65	C 55	Mg 1	N 4	O 5	0
36	E	1	Total 65	C 55	Mg 1	N 4	O 5	0
36	E	1	Total 65	C 55	Mg 1	N 4	O 5	0
36	E	1	Total 46	C 36	Mg 1	N 4	O 5	0
36	F	1	Total 65	C 55	Mg 1	N 4	O 5	0
36	F	1	Total 56	C 46	Mg 1	N 4	O 5	0
36	F	1	Total 52	C 42	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
36	F	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
36	F	1	52	42	1	4	5	0
			Total	C	Mg	N	O	
36	F	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
36	F	1	41	33	1	4	3	0
			Total	C	Mg	N	O	
36	F	1	56	46	1	4	5	0
			Total	C	Mg	N	O	
36	G	1	42	34	1	4	3	0
			Total	C	Mg	N	O	
36	G	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
36	G	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
36	G	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
36	G	1	58	48	1	4	5	0
			Total	C	Mg	N	O	
36	G	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
36	G	1	41	33	1	4	3	0
			Total	C	Mg	N	O	
36	G	1	56	46	1	4	5	0
			Total	C	Mg	N	O	
36	G	1	49	39	1	4	5	0
			Total	C	Mg	N	O	
36	G	1	50	40	1	4	5	0
			Total	C	Mg	N	O	
36	H	1	48	38	1	4	5	0
			Total	C	Mg	N	O	
36	H	1	61	51	1	4	5	0
			Total	C	Mg	N	O	
36	H	1	60	50	1	4	5	0
			Total	C	Mg	N	O	
36	H	1	64	54	1	4	5	0
			Total	C	Mg	N	O	
36	H	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
36	H	1	46	36	1	4	5	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
36	H	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
36	H	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
36	H	1	41	33	1	4	3	0
			Total	C	Mg	N	O	
36	H	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
36	H	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
36	H	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
36	H	1	50	40	1	4	5	0
			Total	C	Mg	N	O	
36	I	1	61	51	1	4	5	0
			Total	C	Mg	N	O	
36	I	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
36	I	1	54	44	1	4	5	0
			Total	C	Mg	N	O	
36	I	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
36	I	1	46	36	1	4	5	0
			Total	C	Mg	N	O	
36	I	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
36	I	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
36	I	1	52	42	1	4	5	0
			Total	C	Mg	N	O	
36	I	1	41	33	1	4	3	0
			Total	C	Mg	N	O	
36	I	1	41	33	1	4	3	0
			Total	C	Mg	N	O	
36	J	1	61	51	1	4	5	0
			Total	C	Mg	N	O	
36	J	1	61	51	1	4	5	0
			Total	C	Mg	N	O	
36	J	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
36	J	1	65	55	1	4	5	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
36	J	1	46	36	1	4	5	0
			Total	C	Mg	N	O	
36	J	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
36	J	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
36	J	1	41	33	1	4	3	0
			Total	C	Mg	N	O	
36	J	1	46	36	1	4	5	0
			Total	C	Mg	N	O	
36	J	1	47	37	1	4	5	0
			Total	C	Mg	N	O	
36	K	1	61	51	1	4	5	0
			Total	C	Mg	N	O	
36	K	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
36	K	1	59	49	1	4	5	0
			Total	C	Mg	N	O	
36	K	1	62	52	1	4	5	0
			Total	C	Mg	N	O	
36	K	1	46	36	1	4	5	0
			Total	C	Mg	N	O	
36	K	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
36	K	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
36	K	1	41	33	1	4	3	0
			Total	C	Mg	N	O	
36	K	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
36	L	1	61	51	1	4	5	0
			Total	C	Mg	N	O	
36	L	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
36	L	1	54	44	1	4	5	0
			Total	C	Mg	N	O	
36	L	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
36	L	1	46	36	1	4	5	0
			Total	C	Mg	N	O	
36	L	1	65	55	1	4	5	0

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

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
36	N	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
36	N	1	54	44	1	4	5	0
			Total	C	Mg	N	O	
36	N	1	47	37	1	4	5	0
			Total	C	Mg	N	O	
36	N	1	42	34	1	4	3	0
			Total	C	Mg	N	O	
36	O	1	61	51	1	4	5	0
			Total	C	Mg	N	O	
36	O	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
36	O	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
36	O	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
36	O	1	46	36	1	4	5	0
			Total	C	Mg	N	O	
36	O	1	58	48	1	4	5	0
			Total	C	Mg	N	O	
36	O	1	40	32	1	4	3	0
			Total	C	Mg	N	O	
36	O	1	41	33	1	4	3	0
			Total	C	Mg	N	O	
36	O	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
36	P	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
36	P	1	42	34	1	4	3	0
			Total	C	Mg	N	O	
36	P	1	61	51	1	4	5	0
			Total	C	Mg	N	O	
36	P	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
36	P	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
36	P	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
36	P	1	46	36	1	4	5	0
			Total	C	Mg	N	O	
36	P	1	65	55	1	4	5	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
36	P	1	60	50	1	4	5	0
			Total	C	Mg	N	O	
36	P	1	41	33	1	4	3	0
			Total	C	Mg	N	O	
36	P	1	51	41	1	4	5	0
			Total	C	Mg	N	O	
36	P	1	60	50	1	4	5	0
			Total	C	Mg	N	O	
36	Q	1	61	51	1	4	5	0
			Total	C	Mg	N	O	
36	Q	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
36	Q	1	50	40	1	4	5	0
			Total	C	Mg	N	O	
36	Q	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
36	Q	1	46	36	1	4	5	0
			Total	C	Mg	N	O	
36	Q	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
36	Q	1	41	33	1	4	3	0
			Total	C	Mg	N	O	
36	Q	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
36	R	1	61	51	1	4	5	0
			Total	C	Mg	N	O	
36	R	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
36	R	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
36	R	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
36	R	1	46	36	1	4	5	0
			Total	C	Mg	N	O	
36	R	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
36	R	1	46	36	1	4	5	0
			Total	C	Mg	N	O	
36	R	1	41	33	1	4	3	0
			Total	C	Mg	N	O	
36	R	1	45	35	1	4	5	0

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

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
36	T	1	41	33	1	4	3	0
			Total	C	Mg	N	O	
36	W	1	48	38	1	4	5	0
			Total	C	Mg	N	O	
36	W	1	61	51	1	4	5	0
			Total	C	Mg	N	O	
36	W	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
36	W	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
36	W	1	57	47	1	4	5	0
			Total	C	Mg	N	O	
36	W	1	46	36	1	4	5	0
			Total	C	Mg	N	O	
36	W	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
36	W	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
36	W	1	41	33	1	4	3	0
			Total	C	Mg	N	O	
36	W	1	48	38	1	4	5	0
			Total	C	Mg	N	O	
36	W	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
36	W	1	43	35	1	4	3	0
			Total	C	Mg	N	O	
36	X	1	61	51	1	4	5	0
			Total	C	Mg	N	O	
36	X	1	50	40	1	4	5	0
			Total	C	Mg	N	O	
36	X	1	47	37	1	4	5	0
			Total	C	Mg	N	O	
36	X	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
36	X	1	41	33	1	4	3	0
			Total	C	Mg	N	O	
36	X	1	41	33	1	4	3	0
			Total	C	Mg	N	O	
36	X	1	42	34	1	4	3	0
			Total	C	Mg	N	O	
36	X	1	41	33	1	4	3	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
36	a	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
36	a	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
36	a	1	55	45	1	4	5	0
			Total	C	Mg	N	O	
36	a	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
36	a	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
36	a	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
36	a	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
36	a	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
36	a	1	56	46	1	4	5	0
			Total	C	Mg	N	O	
36	a	1	62	52	1	4	5	0
			Total	C	Mg	N	O	
36	a	1	54	44	1	4	5	0
			Total	C	Mg	N	O	
36	a	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
36	a	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
36	a	1	50	40	1	4	5	0
			Total	C	Mg	N	O	
36	a	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
36	a	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
36	a	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
36	a	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
36	a	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
36	a	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
36	a	1	49	39	1	4	5	0

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

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

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
36	b	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
36	b	1	64	54	1	4	5	0
			Total	C	Mg	N	O	
36	b	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
36	b	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
36	b	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
36	b	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
36	b	1	50	40	1	4	5	0
			Total	C	Mg	N	O	
36	b	1	49	39	1	4	5	0
			Total	C	Mg	N	O	
36	b	1	58	48	1	4	5	0
			Total	C	Mg	N	O	
36	b	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
36	b	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
36	b	1	58	48	1	4	5	0
			Total	C	Mg	N	O	
36	b	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
36	b	1	47	37	1	4	5	0
			Total	C	Mg	N	O	
36	b	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
36	b	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
36	b	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
36	f	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
36	f	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
36	f	1	65	55	1	4	5	0
			Total	C	Mg	N	O	
36	f	1	52	42	1	4	5	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
36	i	1	65	55	1	4	5	0
36	j	1	65	55	1	4	5	0
36	j	1	65	55	1	4	5	0
36	j	1	42	34	1	4	3	0
36	l	1	65	55	1	4	5	0
36	l	1	65	55	1	4	5	0
36	l	1	49	39	1	4	5	0
36	l	1	65	55	1	4	5	0
36	l	1	50	40	1	4	5	0
36	h	1	65	55	1	4	5	0
36	U	1	61	51	1	4	5	0
36	U	1	65	55	1	4	5	0
36	U	1	50	40	1	4	5	0
36	U	1	56	46	1	4	5	0
36	U	1	46	36	1	4	5	0
36	U	1	65	55	1	4	5	0
36	U	1	65	55	1	4	5	0
36	U	1	41	33	1	4	3	0
36	V	1	61	51	1	4	5	0
36	V	1	65	55	1	4	5	0
36	V	1	51	41	1	4	5	0

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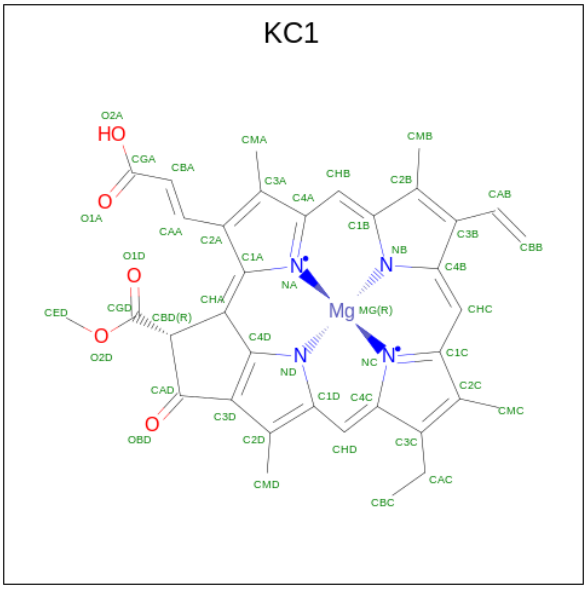
Mol	Chain	Residues	Atoms					AltConf
36	V	1	Total 65	C 55	Mg 1	N 4	O 5	0
36	V	1	Total 43	C 35	Mg 1	N 4	O 3	0
36	V	1	Total 65	C 55	Mg 1	N 4	O 5	0
36	V	1	Total 65	C 55	Mg 1	N 4	O 5	0
36	V	1	Total 65	C 55	Mg 1	N 4	O 5	0
36	V	1	Total 65	C 55	Mg 1	N 4	O 5	0

- Molecule 37 is Chlorophyll c1 (CCD ID: KC1) (formula: $C_{35}H_{30}MgN_4O_5$).



Mol	Chain	Residues	Atoms					AltConf
37	A	1	Total 45	C 35	Mg 1	N 4	O 5	0
37	B	1	Total 45	C 35	Mg 1	N 4	O 5	0
37	C	1	Total 45	C 35	Mg 1	N 4	O 5	0
37	D	1	Total 45	C 35	Mg 1	N 4	O 5	0
37	E	1	Total 45	C 35	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
37	F	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
37	F	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
37	G	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
37	G	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
37	G	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
37	H	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
37	J	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
37	K	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
37	L	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
37	L	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
37	M	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
37	M	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
37	M	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
37	N	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
37	O	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
37	O	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
37	P	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
37	P	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
37	Q	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
37	Q	1	45	35	1	4	5	0
			Total	C	Mg	N	O	
37	R	1	45	35	1	4	5	0

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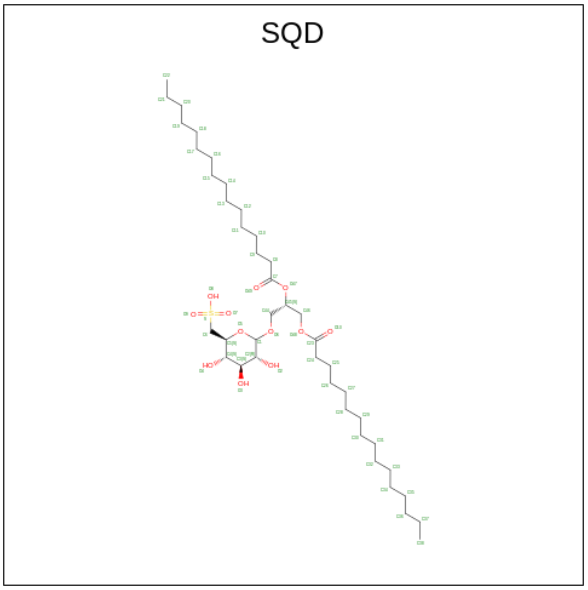
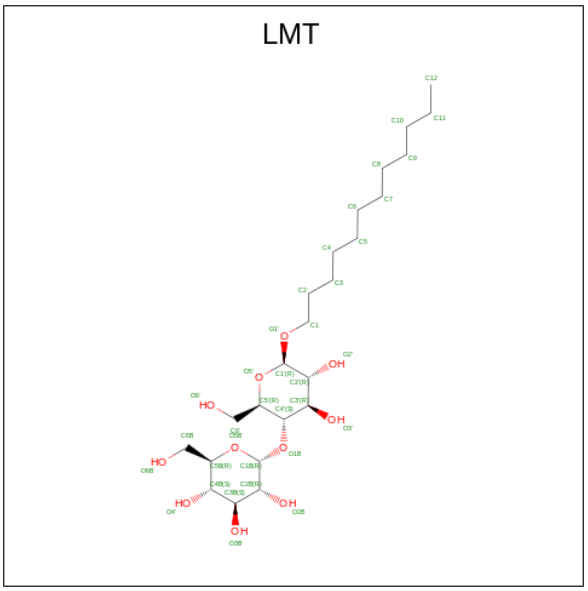
Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
37	S	1	45	35	1	4	5	0
37	T	1	45	35	1	4	5	0
37	T	1	45	35	1	4	5	0
37	W	1	45	35	1	4	5	0
37	W	1	45	35	1	4	5	0
37	X	1	45	35	1	4	5	0
37	U	1	45	35	1	4	5	0
37	V	1	45	35	1	4	5	0

- Molecule 38 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (CCD ID: SQD) (formula: $C_{41}H_{78}O_{12}S$).



Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	S	
38	A	1	28	15	12	1	0
38	b	1	46	33	12	1	0

- Molecule 39 is DODECYL-BETA-D-MALTOSIDE (CCD ID: LMT) (formula: $C_{24}H_{46}O_{11}$).



Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
39	B	1	35	24	11	0
			Total	C	O	
39	B	1	35	24	11	0
			Total	C	O	
39	E	1	35	24	11	0
			Total	C	O	
39	E	1	23	17	6	0
			Total	C	O	
39	E	1	35	24	11	0
			Total	C	O	
39	F	1	35	24	11	0
			Total	C	O	
39	F	1	33	22	11	0
			Total	C	O	
39	G	1	35	24	11	0
			Total	C	O	
39	G	1	35	24	11	0
			Total	C	O	
39	I	1	35	24	11	0
			Total	C	O	
39	I	1	35	24	11	0
			Total	C	O	
39	K	1	31	20	11	0
			Total	C	O	
39	K	1	35	24	11	0
			Total	C	O	
39	L	1	35	24	11	0

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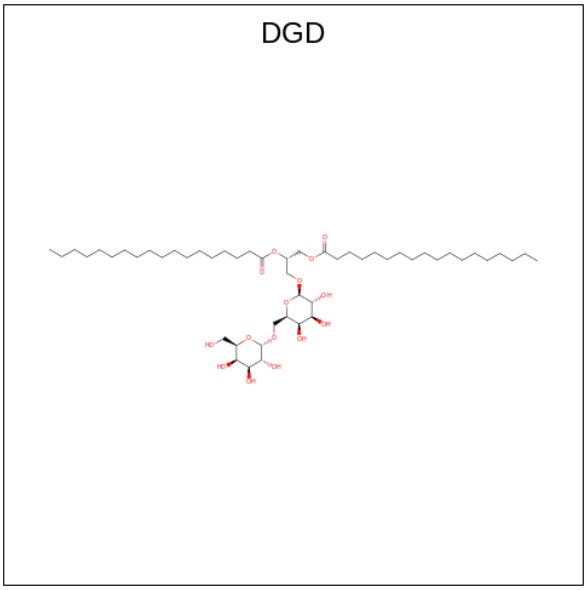
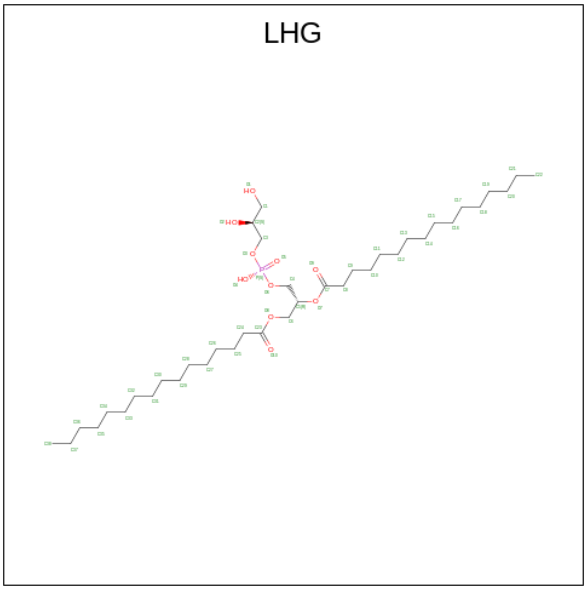
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
39	L	1	31	20	11	0
			Total	C	O	
39	P	1	23	17	6	0
			Total	C	O	
39	P	1	23	17	6	0
			Total	C	O	
39	a	1	35	24	11	0
			Total	C	O	
39	a	1	32	21	11	0
			Total	C	O	
39	a	1	35	24	11	0
			Total	C	O	
39	b	1	35	24	11	0
			Total	C	O	
39	b	1	24	19	5	0
			Total	C	O	
39	f	1	24	18	6	0
			Total	C	O	
39	h	1	35	24	11	0
			Total	C	O	
39	U	1	35	24	11	0
			Total	C	O	
39	U	1	35	24	11	0

- Molecule 40 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: $C_{51}H_{96}O_{15}$).



Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
40	C	1	57	42	15	0
			Total	C	O	
40	L	1	47	32	15	0
			Total	C	O	
40	b	1	60	45	15	0

- Molecule 41 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: $C_{38}H_{75}O_{10}P$).



Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
41	D	1	46	35	10	1	0
			Total	C	O	P	
41	D	1	49	38	10	1	0
			Total	C	O	P	
41	E	1	49	38	10	1	0
			Total	C	O	P	
41	F	1	33	24	8	1	0
			Total	C	O	P	
41	F	1	41	30	10	1	0
			Total	C	O	P	
41	G	1	49	38	10	1	0
			Total	C	O	P	
41	G	1	40	29	10	1	0
			Total	C	O	P	
41	G	1	47	36	10	1	0

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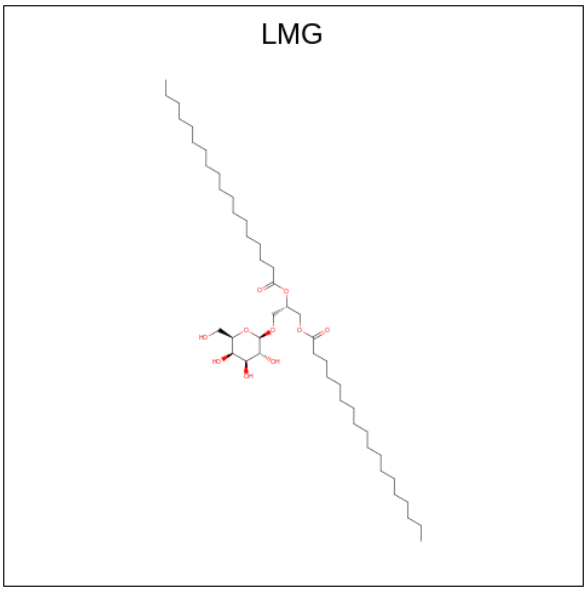
Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
41	I	1	49	38	10	1	0
41	O	1	42	31	10	1	0
41	O	1	49	38	10	1	0
41	Q	1	49	38	10	1	0
41	R	1	49	38	10	1	0
41	a	1	48	37	10	1	0
41	a	1	27	16	10	1	0
41	a	1	47	36	10	1	0
41	b	1	49	38	10	1	0
41	f	1	49	38	10	1	0
41	f	1	42	31	10	1	0
41	i	1	46	35	10	1	0
41	j	1	49	38	10	1	0
41	l	1	48	37	10	1	0

- Molecule 42 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$).



Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
42	D	1	46	36	10	0
			Total	C	O	
42	D	1	37	27	10	0
			Total	C	O	
42	E	1	46	36	10	0
			Total	C	O	
42	E	1	40	30	10	0
			Total	C	O	
42	G	1	55	45	10	0
			Total	C	O	
42	G	1	55	45	10	0
			Total	C	O	
42	I	1	55	45	10	0
			Total	C	O	
42	J	1	55	45	10	0
			Total	C	O	
42	J	1	44	34	10	0
			Total	C	O	
42	L	1	33	23	10	0
			Total	C	O	
42	a	1	54	44	10	0
			Total	C	O	
42	j	1	52	42	10	0
			Total	C	O	
42	m	1	37	27	10	0
			Total	C	O	
42	h	1	45	35	10	0

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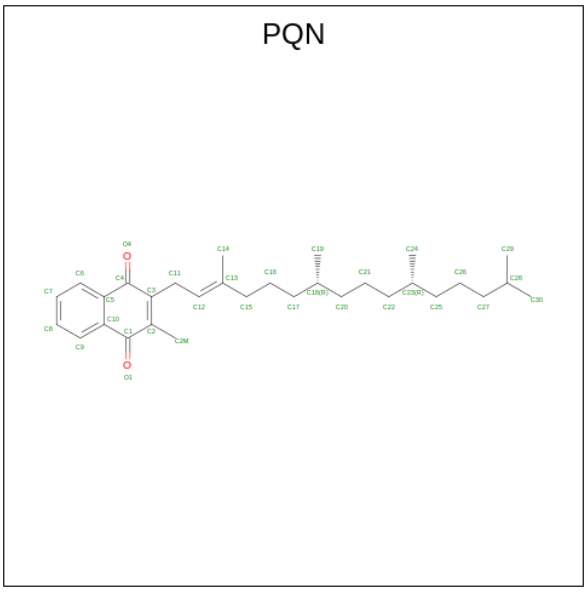
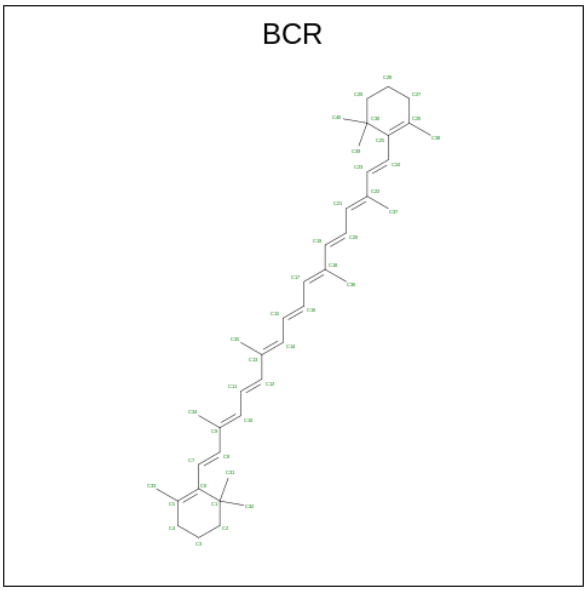
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
42	V	1	46	36	10	0
			Total	C	O	
42	V	1	46	36	10	0

- Molecule 43 is PHYLLOQUINONE (CCD ID: PQN) (formula: $C_{31}H_{46}O_2$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 44 is BETA-CAROTENE (CCD ID: BCR) (formula: $C_{40}H_{56}$).



Mol	Chain	Residues	Atoms		AltConf
			Total	C	
44	a	1	40	40	0
			Total	C	
44	a	1	40	40	0
			Total	C	
44	a	1	40	40	0
			Total	C	
44	a	1	40	40	0
			Total	C	
44	b	1	40	40	0
			Total	C	
44	b	1	40	40	0
			Total	C	
44	b	1	40	40	0
			Total	C	
44	b	1	40	40	0
			Total	C	
44	b	1	40	40	0
			Total	C	
44	f	1	40	40	0
			Total	C	
44	f	1	40	40	0
			Total	C	
44	i	1	40	40	0
			Total	C	
44	i	1	40	40	0
			Total	C	
44	j	1	40	40	0

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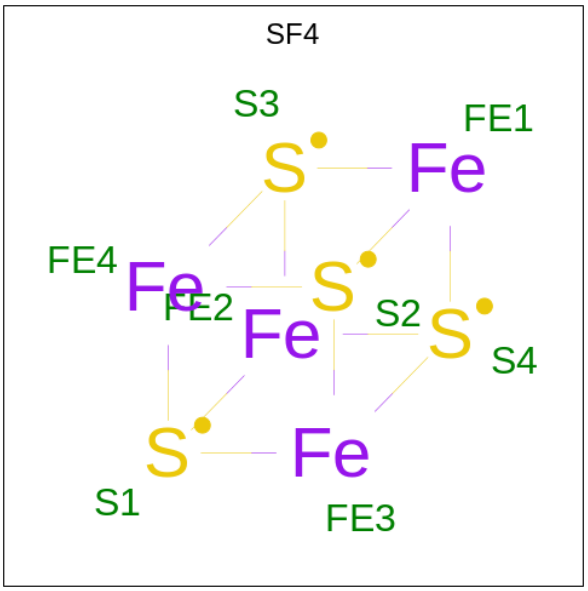
Mol	Chain	Residues	Atoms		AltConf
			Total	C	
44	l	1	40	40	0
			Total	C	
44	l	1	40	40	0
			Total	C	
44	m	1	40	40	0
			Total	C	
44	h	1	40	40	0

- Molecule 45 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
			Total	Fe	S	
45	b	1	8	4	4	0
			Total	Fe	S	
45	c	1	8	4	4	0
			Total	Fe	S	
45	c	1	8	4	4	0

- Molecule 46 is water.

Mol	Chain	Residues	Atoms		AltConf
			Total	O	
46	a	64	64	64	0
			Total	O	
46	b	72	72	72	0

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Mol	Chain	Residues	Atoms		AltConf
			Total	O	
46	c	7	7	7	0
			Total	O	
46	d	4	4	4	0
			Total	O	
46	f	2	2	2	0
			Total	O	
46	j	1	1	1	0
			Total	O	
46	l	3	3	3	0

3 Residue-property plots (i)

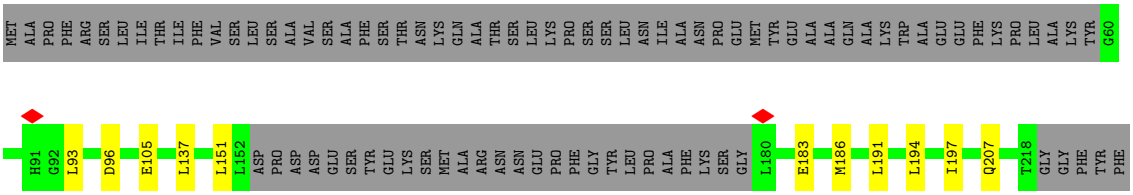
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

- Molecule 1: FCPI-7

Chain A: 95% 5%

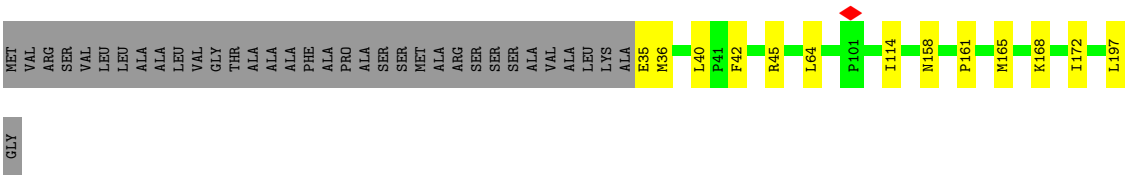
- Molecule 2: FCPI-1

Chain B: 54% 5% 41%



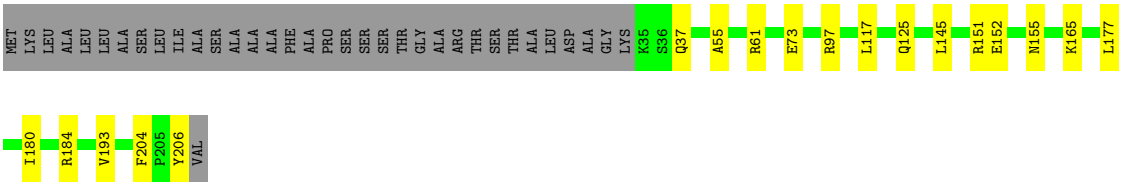
- Molecule 3: FCPI-11

Chain C: 76% 7% 18%



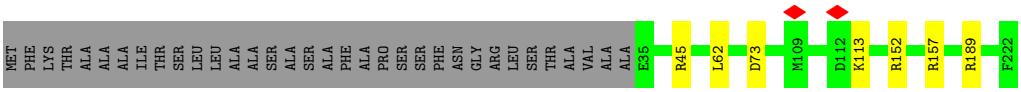
- Molecule 4: FCPI-6

Chain D: 74% 9% 17%



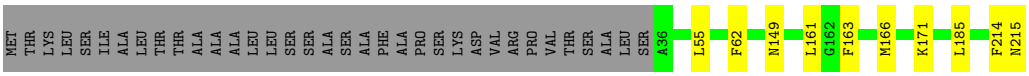
- Molecule 5: FCPI-5

Chain E:



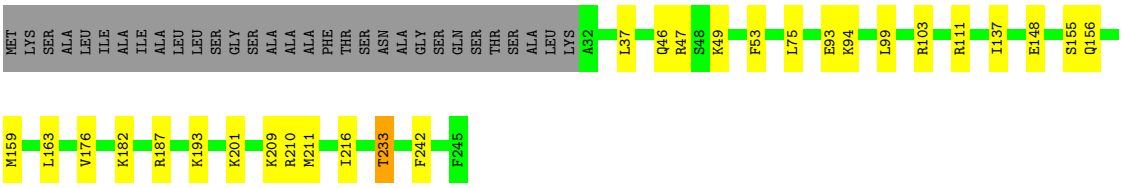
- Molecule 6: FCPI-8

Chain F:



- Molecule 7: FCPI-4

Chain G:

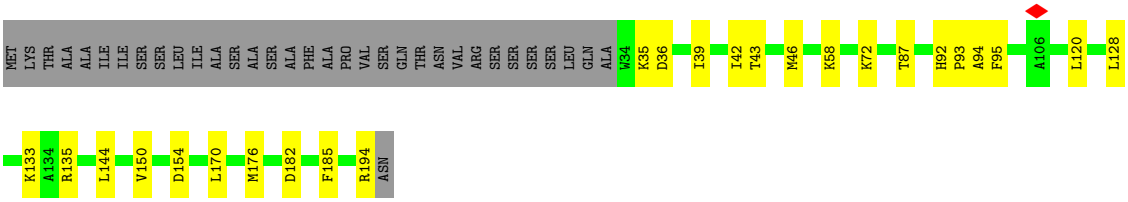


- Molecule 8: FCPI-10

Chain H:

- Molecule 9: FCPI-3

Chain I:

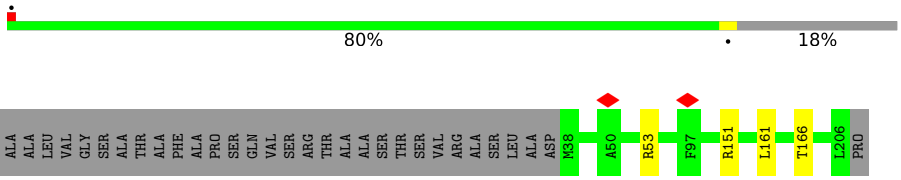


- Molecule 10: FCPI-9

Chain J:

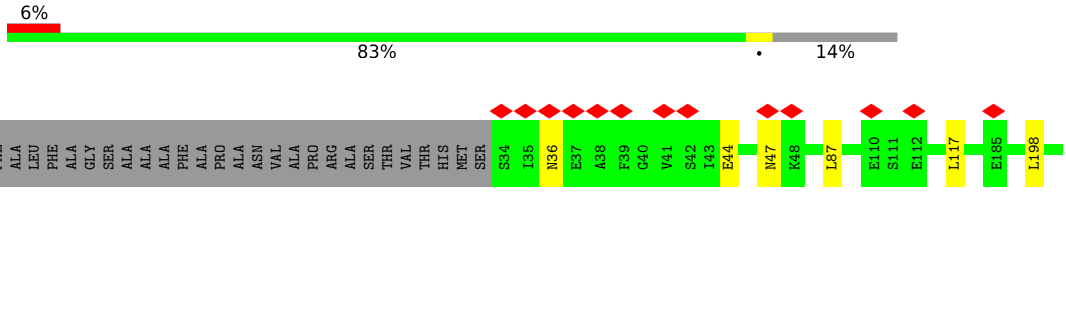
- Molecule 11: FCPI-13

Chain K:



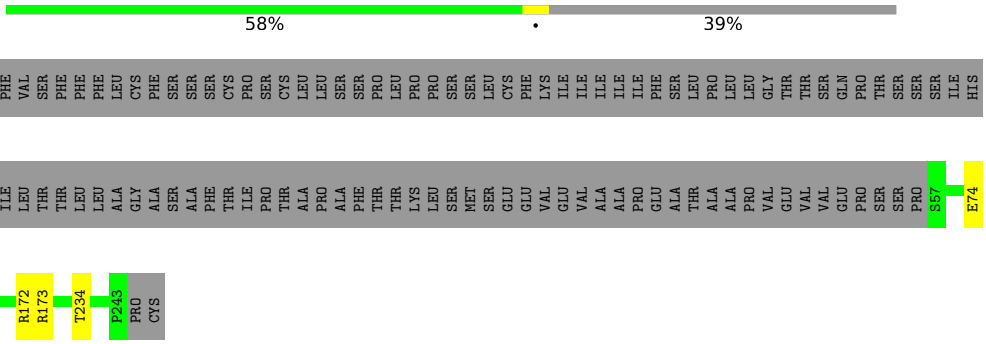
- Molecule 12: FCPI-14

Chain L:



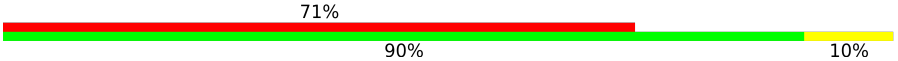
- Molecule 13: FCPI-16

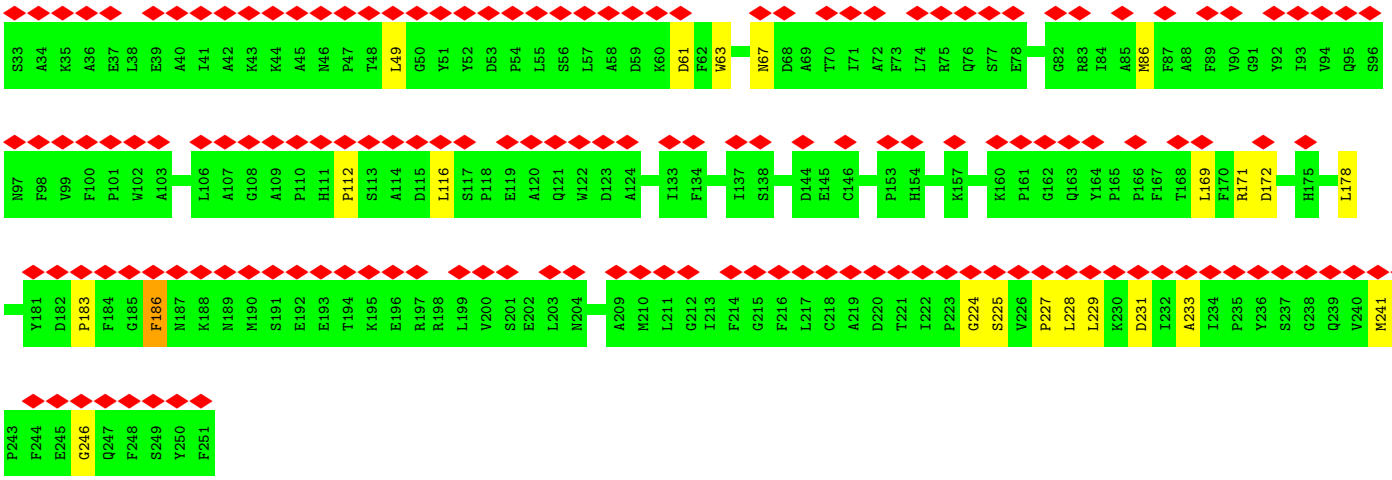
Chain M:



- Molecule 14: FCPI-21

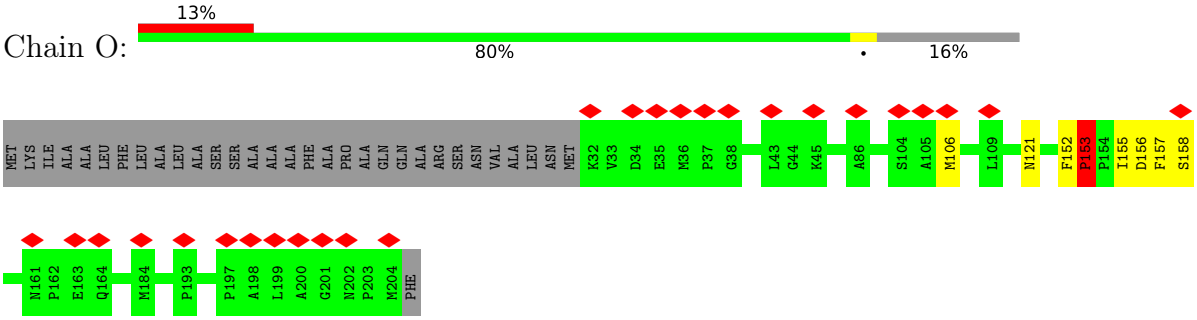
Chain N:





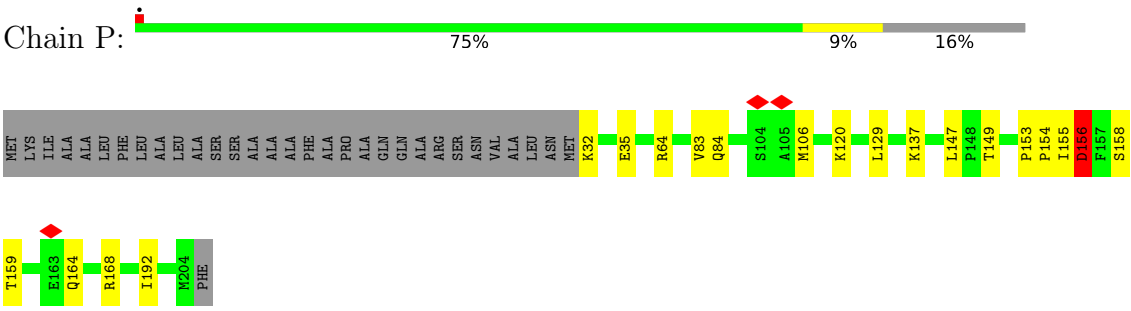
- Molecule 15: FCPI

Chain O:



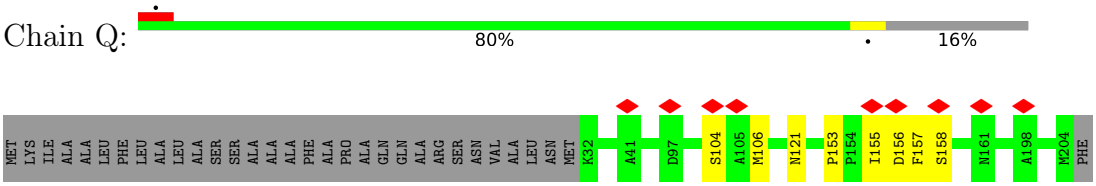
- Molecule 15: FCPI

Chain P:



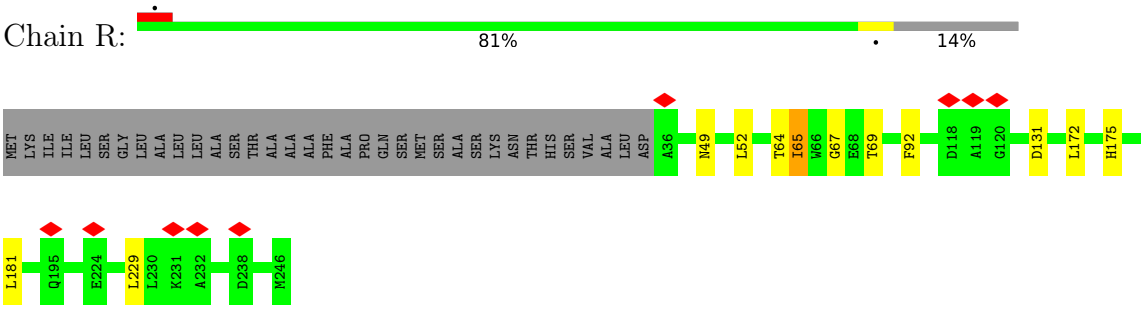
- Molecule 15: FCPI

Chain Q:



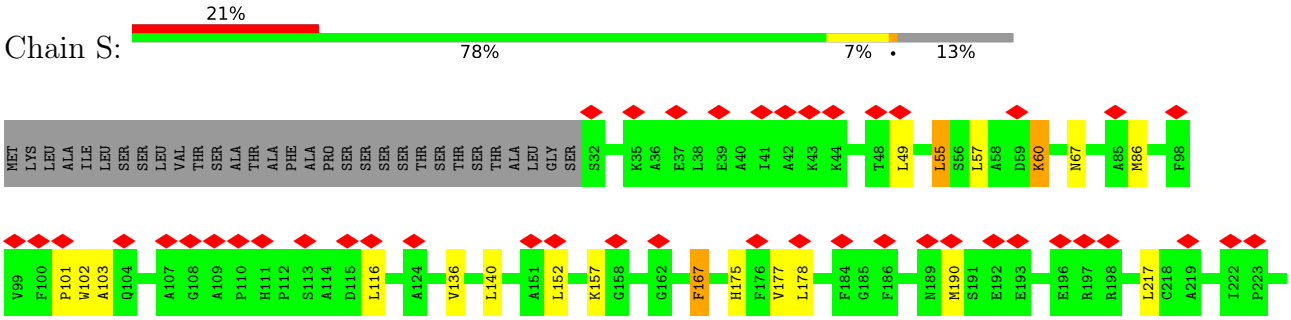
- Molecule 16: FCPI-24

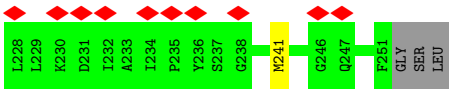
Chain R:



- Molecule 17: FCPI-23

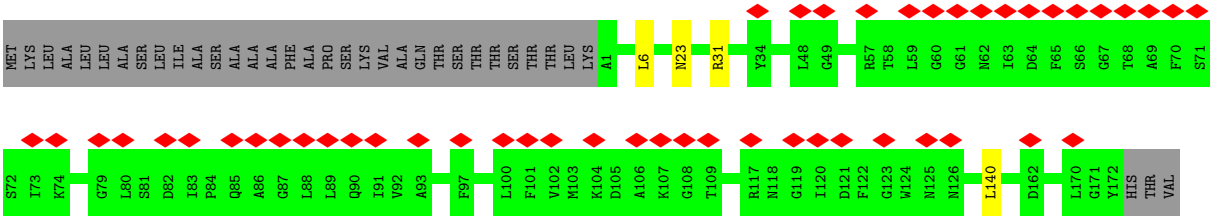
Chain S:





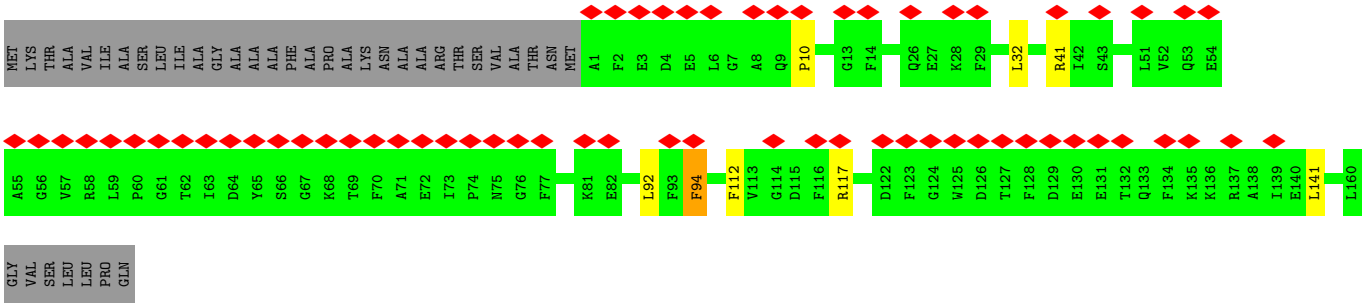
• Molecule 18: FCPI-12

Chain T:



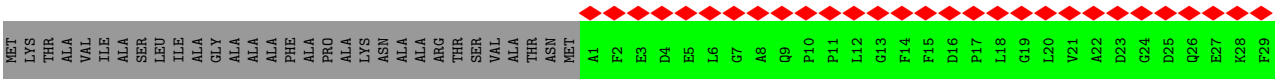
• Molecule 19: FCPI-17

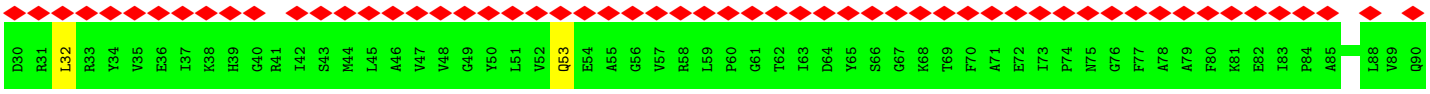
Chain W:

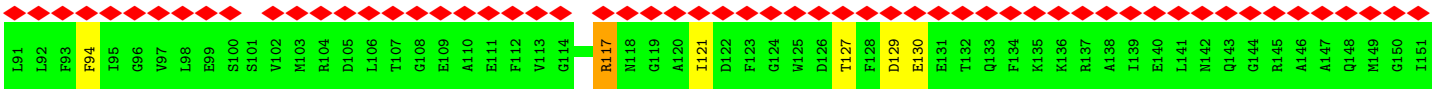


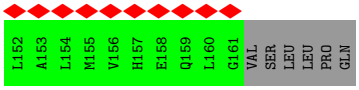
• Molecule 19: FCPI-17

Chain X:







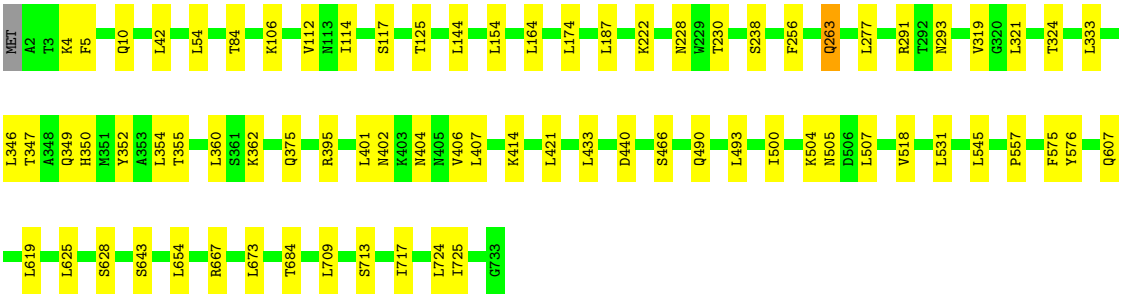


• Molecule 20: PsaA

Chain a:

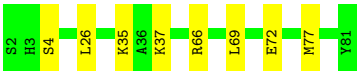
- Molecule 21: PsaB

Chain b:



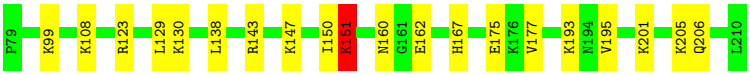
- Molecule 22: PsaC

Chain c:



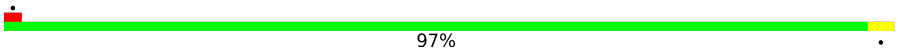
- Molecule 23: PsaD

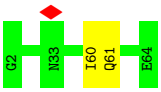
Chain d:



- Molecule 24: PsaE

Chain e:



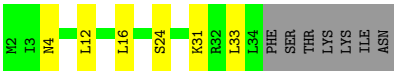


- Molecule 25: PsaF

Chain f:

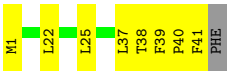
- Molecule 26: PsaI

Chain i:



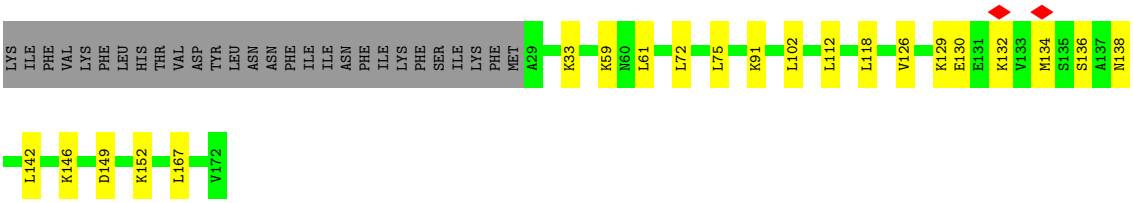
- Molecule 27: PsaJ

Chain j:



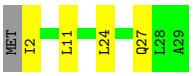
- Molecule 28: PsaL

Chain l:



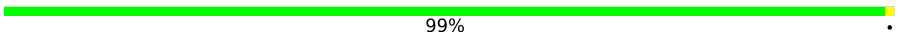
- Molecule 29: PsaM

Chain m:



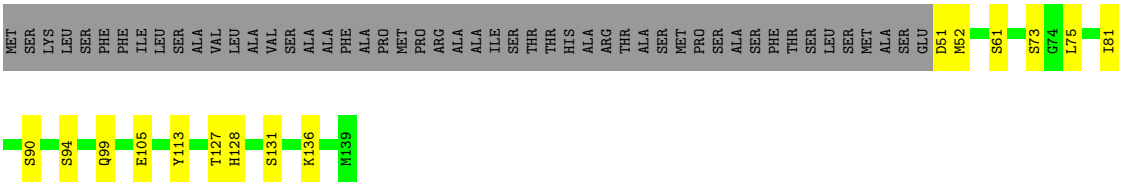
- Molecule 30: PsaS

Chain g:



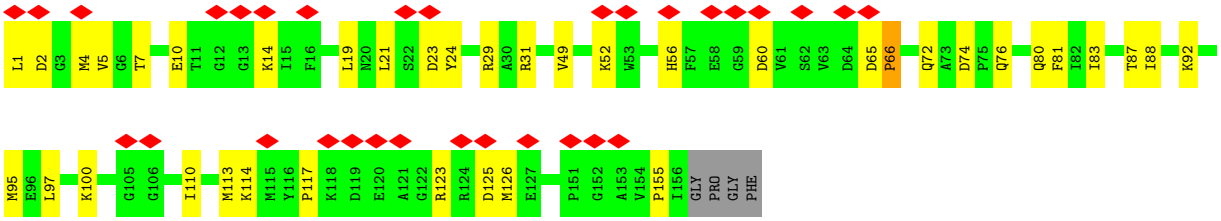
- Molecule 31: PsaR

Chain h:



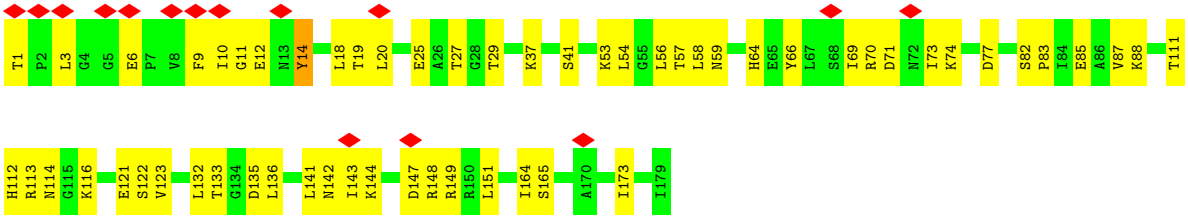
- Molecule 32: FCPI-2

Chain U:



- Molecule 33: FCPI-19

Chain V:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	164480	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)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.163	Depositor
Minimum map value	-0.055	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.016	Depositor
Map size (Å)	567.32, 567.32, 567.32	wwPDB
Map dimensions	520, 520, 520	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.091, 1.091, 1.091	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: SQD, SF4, PQN, LMT, BCR, A86, KC1, CLA, DGD, LMG, LHG, DD6

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	0.47	0/1319	0.67	1/1786 (0.1%)
2	B	0.51	2/1039 (0.2%)	0.98	7/1412 (0.5%)
3	C	0.37	0/1275	0.63	1/1726 (0.1%)
4	D	0.54	3/1373 (0.2%)	0.70	1/1860 (0.1%)
5	E	0.49	0/1439	0.70	2/1944 (0.1%)
6	F	0.47	0/1411	0.68	2/1908 (0.1%)
7	G	0.43	1/1714 (0.1%)	0.59	0/2321
8	H	0.55	1/1326 (0.1%)	0.79	3/1798 (0.2%)
9	I	0.40	0/1285	0.67	5/1746 (0.3%)
10	J	0.46	0/1339	0.73	3/1811 (0.2%)
11	K	0.51	0/1346	0.72	1/1826 (0.1%)
12	L	0.53	1/1571 (0.1%)	0.73	3/2141 (0.1%)
13	M	0.46	1/1464 (0.1%)	0.72	1/1982 (0.1%)
14	N	0.53	0/1770	0.90	6/2405 (0.2%)
15	O	0.55	3/1335 (0.2%)	0.81	4/1817 (0.2%)
15	P	0.40	1/1329 (0.1%)	0.93	4/1810 (0.2%)
15	Q	0.56	3/1335 (0.2%)	0.80	2/1817 (0.1%)
16	R	0.40	0/1680	0.71	5/2282 (0.2%)
17	S	0.44	0/1776	0.84	8/2413 (0.3%)
18	T	0.40	0/1353	0.64	2/1823 (0.1%)
19	W	0.55	1/1265 (0.1%)	0.88	8/1707 (0.5%)
19	X	0.59	3/1282 (0.2%)	0.98	11/1729 (0.6%)
20	a	0.44	3/6053 (0.0%)	0.59	5/8238 (0.1%)
21	b	0.39	0/6031	0.57	8/8231 (0.1%)
22	c	0.46	0/607	0.61	0/822
23	d	1.90	2/1086 (0.2%)	1.23	8/1461 (0.5%)
24	e	0.57	0/517	0.56	0/701
25	f	0.47	1/1248 (0.1%)	0.58	2/1687 (0.1%)
26	i	0.49	0/262	0.75	0/356
27	j	0.46	0/333	0.79	2/455 (0.4%)
28	l	0.47	1/1121 (0.1%)	0.69	6/1520 (0.4%)
29	m	0.44	0/198	0.58	1/269 (0.4%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
31	h	0.33	0/698	0.54	0/951
32	U	0.42	0/1225	0.83	4/1657 (0.2%)
33	V	0.26	0/1393	0.48	0/1894
All	All	0.53	27/51798 (0.1%)	0.72	116/70306 (0.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
10	J	0	1
12	L	0	2
14	N	0	7
15	O	0	1
15	P	0	1
15	Q	0	1
17	S	0	2
19	W	0	3
23	d	0	5
30	g	0	1
33	V	0	1
All	All	0	25

The worst 5 of 27 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	d	151[A]	LYS	CA-C	43.55	2.66	1.52
23	d	151[B]	LYS	CA-C	43.55	2.66	1.52
19	X	94	PHE	CE2-CZ	9.29	1.55	1.37
2	B	186	MET	C-N	8.97	1.54	1.34
4	D	73	GLU	CB-CG	-7.17	1.38	1.52

The worst 5 of 116 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	d	151[A]	LYS	CB-CA-C	-22.80	64.81	110.40
23	d	151[B]	LYS	CB-CA-C	-22.80	64.81	110.40
15	P	156	ASP	O-C-N	-20.21	90.36	122.70
32	U	65	ASP	C-N-CD	-19.93	76.74	120.60
23	d	151[A]	LYS	CA-C-N	-15.35	83.44	117.20

There are no chirality outliers.

5 of 25 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
10	J	91	PHE	Mainchain
12	L	228	HIS	Peptide
12	L	47	ASN	Peptide
14	N	112	PRO	Peptide
14	N	172	ASP	Peptide

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	166/168 (99%)	150 (90%)	14 (8%)	2 (1%)	11 14
2	B	128/223 (57%)	121 (94%)	7 (6%)	0	100 100
3	C	161/198 (81%)	150 (93%)	9 (6%)	2 (1%)	11 14
4	D	170/207 (82%)	160 (94%)	9 (5%)	1 (1%)	22 30
5	E	186/222 (84%)	178 (96%)	8 (4%)	0	100 100
6	F	178/215 (83%)	165 (93%)	13 (7%)	0	100 100
7	G	212/245 (86%)	197 (93%)	14 (7%)	1 (0%)	25 35
8	H	168/203 (83%)	151 (90%)	17 (10%)	0	100 100
9	I	159/195 (82%)	146 (92%)	13 (8%)	0	100 100
10	J	165/200 (82%)	145 (88%)	17 (10%)	3 (2%)	7 8
11	K	167/207 (81%)	152 (91%)	15 (9%)	0	100 100
12	L	194/229 (85%)	176 (91%)	18 (9%)	0	100 100
13	M	185/306 (60%)	169 (91%)	15 (8%)	1 (0%)	25 35

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
14	N	217/219 (99%)	174 (80%)	40 (18%)	3 (1%)	9	12
15	O	171/205 (83%)	147 (86%)	21 (12%)	3 (2%)	7	8
15	P	171/205 (83%)	153 (90%)	16 (9%)	2 (1%)	11	14
15	Q	171/205 (83%)	150 (88%)	19 (11%)	2 (1%)	11	14
16	R	209/246 (85%)	182 (87%)	25 (12%)	2 (1%)	13	18
17	S	218/254 (86%)	184 (84%)	29 (13%)	5 (2%)	5	5
18	T	170/207 (82%)	164 (96%)	6 (4%)	0	100	100
19	W	158/198 (80%)	133 (84%)	25 (16%)	0	100	100
19	X	160/198 (81%)	146 (91%)	13 (8%)	1 (1%)	22	30
20	a	740/743 (100%)	713 (96%)	26 (4%)	1 (0%)	48	63
21	b	731/733 (100%)	699 (96%)	31 (4%)	1 (0%)	48	63
22	c	78/80 (98%)	74 (95%)	4 (5%)	0	100	100
23	d	131/132 (99%)	125 (95%)	6 (5%)	0	100	100
24	e	61/63 (97%)	60 (98%)	1 (2%)	0	100	100
25	f	160/162 (99%)	152 (95%)	8 (5%)	0	100	100
26	i	31/40 (78%)	31 (100%)	0	0	100	100
27	j	39/42 (93%)	37 (95%)	1 (3%)	1 (3%)	4	4
28	l	142/172 (83%)	131 (92%)	11 (8%)	0	100	100
29	m	26/29 (90%)	26 (100%)	0	0	100	100
31	h	87/139 (63%)	87 (100%)	0	0	100	100
32	U	154/160 (96%)	123 (80%)	26 (17%)	5 (3%)	3	2
33	V	177/179 (99%)	152 (86%)	20 (11%)	5 (3%)	4	3
All	All	6441/7429 (87%)	5903 (92%)	497 (8%)	41 (1%)	24	30

5 of 41 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
10	J	87	ILE
15	O	153	PRO
15	O	155	ILE
15	Q	153	PRO
17	S	103	ALA

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	137/137 (100%)	131 (96%)	6 (4%)	24	38
2	B	105/180 (58%)	99 (94%)	6 (6%)	17	27
3	C	131/153 (86%)	121 (92%)	10 (8%)	11	16
4	D	140/163 (86%)	126 (90%)	14 (10%)	6	8
5	E	142/164 (87%)	137 (96%)	5 (4%)	31	48
6	F	142/169 (84%)	134 (94%)	8 (6%)	17	27
7	G	172/193 (89%)	145 (84%)	27 (16%)	2	2
8	H	131/154 (85%)	128 (98%)	3 (2%)	45	64
9	I	124/152 (82%)	104 (84%)	20 (16%)	2	2
10	J	130/154 (84%)	123 (95%)	7 (5%)	18	29
11	K	133/160 (83%)	130 (98%)	3 (2%)	45	64
12	L	159/180 (88%)	158 (99%)	1 (1%)	84	92
13	M	142/247 (58%)	137 (96%)	5 (4%)	31	48
14	N	176/176 (100%)	169 (96%)	7 (4%)	27	42
15	O	138/159 (87%)	135 (98%)	3 (2%)	47	65
15	P	137/159 (86%)	120 (88%)	17 (12%)	4	4
15	Q	138/159 (87%)	135 (98%)	3 (2%)	47	65
16	R	167/193 (86%)	161 (96%)	6 (4%)	30	46
17	S	177/204 (87%)	167 (94%)	10 (6%)	17	27
18	T	136/163 (83%)	134 (98%)	2 (2%)	60	76
19	W	125/151 (83%)	125 (100%)	0	100	100
19	X	127/151 (84%)	124 (98%)	3 (2%)	44	62
20	a	606/606 (100%)	548 (90%)	58 (10%)	7	9
21	b	593/593 (100%)	523 (88%)	70 (12%)	4	5
22	c	67/69 (97%)	59 (88%)	8 (12%)	4	5
23	d	111/111 (100%)	91 (82%)	20 (18%)	1	1

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
24	e	55/55 (100%)	53 (96%)	2 (4%)	30	46
25	f	119/125 (95%)	108 (91%)	11 (9%)	7	10
26	i	29/36 (81%)	23 (79%)	6 (21%)	1	1
27	j	34/35 (97%)	29 (85%)	5 (15%)	2	3
28	l	114/143 (80%)	100 (88%)	14 (12%)	4	4
29	m	20/23 (87%)	17 (85%)	3 (15%)	2	2
31	h	70/109 (64%)	55 (79%)	15 (21%)	1	1
32	U	119/121 (98%)	87 (73%)	32 (27%)	0	0
33	V	137/137 (100%)	84 (61%)	53 (39%)	0	0
All	All	5183/5884 (88%)	4720 (91%)	463 (9%)	10	11

5 of 463 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
21	b	112	VAL
33	V	114	ASN
21	b	643	SER
33	V	85	GLU
32	U	87	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 117 such sidechains are listed below:

Mol	Chain	Res	Type
18	T	23	ASN
32	U	148	HIS
20	a	447	ASN
32	U	80	GLN
21	b	671	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

589 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	$\#\|Z\| > 2$
35	A86	M	304	-	44,50,50	1.23	3 (6%)	51,76,76	2.06	14 (27%)
39	LMT	G	322	-	36,36,36	0.39	0	47,47,47	0.69	0
39	LMT	L	303	-	36,36,36	1.33	6 (16%)	47,47,47	0.96	1 (2%)
36	CLA	W	215	-	48,56,73	1.88	8 (16%)	55,92,113	1.50	8 (14%)
37	KC1	Q	313	-	48,53,53	3.07	20 (41%)	55,89,89	6.90	36 (65%)
35	A86	J	302	-	44,50,50	1.26	4 (9%)	51,76,76	2.08	12 (23%)
36	CLA	F	310	-	56,64,73	1.50	7 (12%)	65,102,113	1.64	12 (18%)
36	CLA	a	829	-	65,73,73	1.45	9 (13%)	76,113,113	1.74	12 (15%)
36	CLA	T	308	18	61,69,73	1.50	5 (8%)	71,108,113	1.53	9 (12%)
36	CLA	b	816	-	60,68,73	1.92	12 (20%)	70,107,113	2.01	18 (25%)
36	CLA	E	310	-	65,73,73	1.47	6 (9%)	76,113,113	1.59	9 (11%)
39	LMT	b	851	-	24,24,36	0.42	0	29,29,47	0.81	0
35	A86	S	305	-	44,50,50	1.27	3 (6%)	51,76,76	2.95	20 (39%)
36	CLA	F	311	-	52,60,73	1.62	9 (17%)	60,97,113	1.62	8 (13%)
36	CLA	M	306	13,37	55,63,73	1.52	10 (18%)	64,101,113	1.57	11 (17%)
36	CLA	A	305	1	49,57,73	1.65	8 (16%)	55,93,113	1.54	7 (12%)
36	CLA	a	801	-	65,73,73	1.44	10 (15%)	76,113,113	1.61	14 (18%)
35	A86	N	303	-	44,50,50	1.31	5 (11%)	51,76,76	3.31	22 (43%)
34	DD6	D	303	-	39,45,45	2.97	8 (20%)	52,67,67	2.65	18 (34%)
36	CLA	D	309	-	55,63,73	2.08	13 (23%)	64,101,113	2.97	25 (39%)
36	CLA	J	307	10	61,69,73	1.46	7 (11%)	71,108,113	1.58	11 (15%)
34	DD6	W	204	36	39,45,45	2.04	3 (7%)	52,67,67	2.01	13 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
36	CLA	J	315	-	41,49,73	1.77	7 (17%)	47,84,113	1.81	8 (17%)
37	KC1	U	312	35,32	48,53,53	3.16	21 (43%)	55,89,89	4.86	31 (56%)
36	CLA	D	306	4	45,53,73	1.81	9 (20%)	52,89,113	1.80	10 (19%)
36	CLA	K	312	-	65,73,73	1.42	7 (10%)	76,113,113	1.45	7 (9%)
36	CLA	H	315	8	65,73,73	1.48	9 (13%)	76,113,113	1.60	14 (18%)
36	CLA	J	317	10	47,55,73	1.70	9 (19%)	54,91,113	1.50	6 (11%)
36	CLA	l	206	46	50,58,73	1.59	7 (14%)	58,95,113	1.63	8 (13%)
36	CLA	a	827	-	62,70,73	1.46	8 (12%)	72,109,113	1.70	10 (13%)
42	LMG	E	318	-	46,46,55	0.98	2 (4%)	54,54,63	1.06	2 (3%)
34	DD6	E	306	-	39,45,45	2.03	3 (7%)	52,67,67	2.04	10 (19%)
36	CLA	A	308	-	65,73,73	1.41	7 (10%)	76,113,113	1.59	9 (11%)
36	CLA	I	307	-	54,62,73	1.51	8 (14%)	62,99,113	1.66	8 (12%)
36	CLA	a	804	-	65,73,73	1.44	10 (15%)	76,113,113	1.42	11 (14%)
36	CLA	C	206	-	61,69,73	1.48	7 (11%)	71,108,113	1.48	7 (9%)
36	CLA	P	314	-	60,68,73	1.66	9 (15%)	70,107,113	1.70	14 (20%)
36	CLA	b	833	-	58,66,73	1.50	8 (13%)	67,104,113	1.63	11 (16%)
36	CLA	a	812	-	65,73,73	1.41	7 (10%)	76,113,113	1.54	8 (10%)
36	CLA	O	306	-	61,69,73	1.49	9 (14%)	71,108,113	1.46	6 (8%)
36	CLA	a	820	-	65,73,73	1.39	8 (12%)	76,113,113	1.54	10 (13%)
34	DD6	P	305	-	39,45,45	2.02	3 (7%)	52,67,67	2.06	16 (30%)
36	CLA	C	208	-	65,73,73	1.45	9 (13%)	76,113,113	1.43	9 (11%)
36	CLA	V	311	33	65,73,73	1.40	8 (12%)	76,113,113	1.76	13 (17%)
41	LHG	i	104	-	45,45,48	0.98	2 (4%)	48,51,54	1.03	2 (4%)
34	DD6	S	306	-	39,45,45	1.96	3 (7%)	52,67,67	2.00	13 (25%)
36	CLA	b	835	-	45,53,73	1.74	9 (20%)	52,89,113	1.74	10 (19%)
35	A86	I	302	-	44,50,50	1.30	4 (9%)	51,76,76	2.66	17 (33%)
41	LHG	I	316	-	48,48,48	0.95	2 (4%)	51,54,54	1.00	2 (3%)
39	LMT	I	317	-	36,36,36	0.41	0	47,47,47	0.75	1 (2%)
34	DD6	K	304	-	39,45,45	2.02	3 (7%)	52,67,67	1.87	13 (25%)
35	A86	O	302	-	44,50,50	1.44	6 (13%)	51,76,76	3.47	23 (45%)
36	CLA	L	314	12	65,73,73	1.41	8 (12%)	76,113,113	1.58	10 (13%)
36	CLA	X	315	-	41,49,73	1.83	5 (12%)	47,84,113	1.78	8 (17%)
36	CLA	G	314	7	41,49,73	1.79	9 (21%)	47,84,113	1.82	9 (19%)
35	A86	E	302	-	44,50,50	1.23	4 (9%)	51,76,76	2.19	13 (25%)
42	LMG	D	320	41	46,46,55	0.98	2 (4%)	54,54,63	1.03	3 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
36	CLA	I	305	-	61,69,73	2.03	11 (18%)	71,108,113	1.76	12 (16%)
36	CLA	b	832	-	49,57,73	1.52	8 (16%)	55,93,113	1.75	8 (14%)
36	CLA	N	311	14	46,54,73	1.72	7 (15%)	53,90,113	1.86	10 (18%)
36	CLA	L	312	12	46,54,73	1.77	8 (17%)	53,90,113	1.91	10 (18%)
36	CLA	O	308	15	65,73,73	1.45	8 (12%)	76,113,113	1.53	9 (11%)
36	CLA	b	807	-	45,53,73	1.66	7 (15%)	52,89,113	1.76	8 (15%)
36	CLA	b	823	-	55,63,73	1.49	7 (12%)	64,101,113	1.61	7 (10%)
35	A86	A	316	-	44,50,50	1.23	4 (9%)	51,76,76	2.16	16 (31%)
37	KC1	T	310	-	48,53,53	4.86	28 (58%)	55,89,89	7.31	33 (60%)
35	A86	T	304	-	44,50,50	1.11	3 (6%)	51,76,76	1.69	11 (21%)
36	CLA	a	806	-	65,73,73	1.72	9 (13%)	76,113,113	1.90	17 (22%)
37	KC1	K	314	11	48,53,53	2.91	19 (39%)	55,89,89	5.96	36 (65%)
36	CLA	L	308	-	61,69,73	1.83	12 (19%)	71,108,113	2.35	17 (23%)
42	LMG	E	319	-	40,40,55	1.04	2 (5%)	48,48,63	1.11	3 (6%)
39	LMT	L	318	-	32,32,36	0.45	0	43,43,47	0.79	1 (2%)
37	KC1	W	217	-	48,53,53	3.14	19 (39%)	55,89,89	4.85	35 (63%)
39	LMT	f	807	-	24,24,36	0.43	0	29,29,47	0.58	0
36	CLA	l	201	-	65,73,73	1.40	8 (12%)	76,113,113	1.55	10 (13%)
44	BCR	a	846	-	41,41,41	1.15	3 (7%)	56,56,56	1.19	3 (5%)
36	CLA	b	837	-	65,73,73	1.40	8 (12%)	76,113,113	1.59	11 (14%)
36	CLA	b	812	21	65,73,73	1.41	9 (13%)	76,113,113	1.61	13 (17%)
36	CLA	P	312	15	46,54,73	1.72	7 (15%)	53,90,113	1.71	10 (18%)
44	BCR	f	806	-	41,41,41	1.18	3 (7%)	56,56,56	1.23	7 (12%)
36	CLA	l	205	-	65,73,73	1.53	10 (15%)	76,113,113	2.19	18 (23%)
39	LMT	a	854	-	36,36,36	0.40	0	47,47,47	0.75	0
35	A86	O	305	-	44,50,50	1.42	4 (9%)	51,76,76	1.95	16 (31%)
36	CLA	C	210	3	46,54,73	1.79	6 (13%)	53,90,113	1.68	9 (16%)
36	CLA	E	315	-	65,73,73	1.96	15 (23%)	76,113,113	2.57	24 (31%)
42	LMG	D	321	-	37,37,55	1.08	2 (5%)	45,45,63	1.02	2 (4%)
45	SF4	b	803	21,20	0,12,12	-	-	-		
37	KC1	G	317	-	48,53,53	2.92	22 (45%)	55,89,89	5.07	35 (63%)
36	CLA	b	802	-	65,73,73	1.45	8 (12%)	76,113,113	1.42	9 (11%)
36	CLA	R	321	16	65,73,73	1.47	7 (10%)	76,113,113	1.58	9 (11%)
36	CLA	E	308	5	49,57,73	1.63	10 (20%)	55,93,113	1.62	9 (16%)
36	CLA	a	836	-	65,73,73	1.34	8 (12%)	76,113,113	1.71	10 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
41	LHG	F	319	-	40,40,48	1.03	2 (5%)	43,46,54	1.10	3 (6%)
44	BCR	f	801	-	41,41,41	1.12	2 (4%)	56,56,56	1.19	5 (8%)
36	CLA	D	308	-	65,73,73	1.43	8 (12%)	76,113,113	1.65	12 (15%)
36	CLA	S	319	17	65,73,73	1.49	8 (12%)	76,113,113	1.57	11 (14%)
38	SQD	b	804	-	45,46,54	1.27	4 (8%)	54,57,65	1.21	4 (7%)
35	A86	P	304	-	44,50,50	1.33	5 (11%)	51,76,76	2.74	17 (33%)
36	CLA	H	317	8	65,73,73	1.46	8 (12%)	76,113,113	1.37	7 (9%)
39	LMT	U	315	-	36,36,36	0.40	0	47,47,47	0.74	1 (2%)
36	CLA	J	316	-	46,54,73	1.72	10 (21%)	53,90,113	1.84	10 (18%)
36	CLA	b	841	41	65,73,73	1.42	12 (18%)	76,113,113	1.99	17 (22%)
36	CLA	A	313	-	41,49,73	1.84	9 (21%)	47,84,113	1.83	7 (14%)
44	BCR	b	847	-	41,41,41	1.18	3 (7%)	56,56,56	1.26	7 (12%)
35	A86	T	302	18	44,50,50	1.24	3 (6%)	51,76,76	2.85	21 (41%)
35	A86	Q	303	-	44,50,50	1.33	5 (11%)	51,76,76	2.05	15 (29%)
36	CLA	U	305	-	61,69,73	1.52	6 (9%)	71,108,113	1.43	7 (9%)
35	A86	L	304	-	44,50,50	1.39	4 (9%)	51,76,76	2.99	15 (29%)
44	BCR	i	103	-	41,41,41	1.19	3 (7%)	56,56,56	1.32	7 (12%)
35	A86	X	303	36	44,50,50	1.47	5 (11%)	51,76,76	3.76	24 (47%)
36	CLA	W	210	-	46,54,73	1.69	6 (13%)	53,90,113	2.10	14 (26%)
36	CLA	H	318	-	50,58,73	1.63	10 (20%)	58,95,113	1.63	10 (17%)
36	CLA	a	825	-	65,73,73	1.53	7 (10%)	76,113,113	1.77	11 (14%)
36	CLA	C	207	-	65,73,73	2.00	14 (21%)	76,113,113	2.81	23 (30%)
36	CLA	T	311	18	65,73,73	1.52	9 (13%)	76,113,113	2.03	16 (21%)
42	LMG	J	318	-	55,55,55	0.89	2 (3%)	63,63,63	1.02	3 (4%)
45	SF4	c	102	-	0,12,12	-	-	-		
36	CLA	U	306	32	65,73,73	2.14	16 (24%)	76,113,113	2.65	23 (30%)
36	CLA	U	311	32	65,73,73	1.46	8 (12%)	76,113,113	1.65	12 (15%)
44	BCR	j	107	-	41,41,41	1.11	2 (4%)	56,56,56	1.22	7 (12%)
36	CLA	L	309	12	65,73,73	1.43	8 (12%)	76,113,113	1.45	8 (10%)
36	CLA	b	829	-	65,73,73	1.44	9 (13%)	76,113,113	1.37	7 (9%)
34	DD6	R	307	-	39,45,45	2.00	2 (5%)	52,67,67	2.11	15 (28%)
35	A86	R	306	-	44,50,50	1.34	4 (9%)	51,76,76	2.91	16 (31%)
36	CLA	D	312	-	65,73,73	1.46	9 (13%)	76,113,113	1.40	9 (11%)
42	LMG	L	321	40	33,33,55	1.13	2 (6%)	41,41,63	1.15	3 (7%)
36	CLA	Q	307	15	50,58,73	1.63	8 (16%)	56,94,113	1.59	7 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
34	DD6	B	304	-	39,45,45	2.01	3 (7%)	52,67,67	2.14	16 (30%)
36	CLA	P	301	15	65,73,73	1.44	8 (12%)	76,113,113	1.56	10 (13%)
36	CLA	a	819	-	45,53,73	1.74	10 (22%)	52,89,113	2.32	10 (19%)
36	CLA	P	319	-	60,68,73	2.34	11 (18%)	70,107,113	2.21	15 (21%)
36	CLA	R	313	-	65,73,73	1.41	8 (12%)	76,113,113	1.37	7 (9%)
36	CLA	Q	309	15	46,54,73	1.73	7 (15%)	53,90,113	1.73	10 (18%)
41	LHG	l	208	-	47,47,48	0.95	2 (4%)	50,53,54	1.02	3 (6%)
36	CLA	N	309	14	51,59,73	1.67	9 (17%)	59,96,113	1.81	8 (13%)
35	A86	V	301	35	44,50,50	1.23	4 (9%)	51,76,76	2.22	16 (31%)
34	DD6	G	303	-	39,45,45	1.99	3 (7%)	52,67,67	1.83	10 (19%)
36	CLA	b	810	-	65,73,73	1.36	9 (13%)	76,113,113	1.42	8 (10%)
41	LHG	G	321	36	46,46,48	0.96	2 (4%)	49,52,54	1.06	2 (4%)
34	DD6	E	304	-	39,45,45	1.99	3 (7%)	52,67,67	1.78	10 (19%)
35	A86	B	303	-	44,50,50	1.30	3 (6%)	51,76,76	4.01	27 (52%)
36	CLA	b	827	-	65,73,73	1.57	8 (12%)	76,113,113	1.44	10 (13%)
36	CLA	P	313	-	65,73,73	1.42	7 (10%)	76,113,113	1.44	6 (7%)
36	CLA	a	848	36	65,73,73	1.72	11 (16%)	76,113,113	1.97	19 (25%)
35	A86	F	306	-	44,50,50	1.26	4 (9%)	51,76,76	2.04	13 (25%)
35	A86	P	303	-	44,50,50	1.44	6 (13%)	51,76,76	3.47	23 (45%)
36	CLA	G	319	7	50,58,73	2.05	14 (28%)	58,95,113	3.97	26 (44%)
36	CLA	a	841	41	52,60,73	1.65	8 (15%)	60,97,113	1.64	9 (15%)
36	CLA	W	218	19	43,51,73	1.75	8 (18%)	49,86,113	1.90	9 (18%)
36	CLA	Q	306	-	65,73,73	1.43	8 (12%)	76,113,113	1.48	6 (7%)
36	CLA	L	313	-	65,73,73	1.39	7 (10%)	76,113,113	1.59	7 (9%)
36	CLA	a	830	-	50,58,73	2.05	12 (24%)	58,95,113	3.35	18 (31%)
36	CLA	f	804	46	65,73,73	2.02	17 (26%)	76,113,113	2.93	29 (38%)
42	LMG	V	315	-	46,46,55	0.98	2 (4%)	54,54,63	4.29	4 (7%)
35	A86	K	306	11	44,50,50	1.22	3 (6%)	51,76,76	3.50	21 (41%)
35	A86	L	307	-	44,50,50	1.24	4 (9%)	51,76,76	1.93	11 (21%)
44	BCR	b	845	-	41,41,41	1.20	3 (7%)	56,56,56	1.37	8 (14%)
36	CLA	b	831	-	50,58,73	1.66	10 (20%)	58,95,113	1.65	8 (13%)
36	CLA	F	316	6	41,49,73	1.78	9 (21%)	47,84,113	1.66	9 (19%)
37	KC1	F	308	6	48,53,53	2.95	21 (43%)	55,89,89	6.07	33 (60%)
36	CLA	b	805	36	65,73,73	1.42	10 (15%)	76,113,113	1.40	14 (18%)
35	A86	E	305	5	44,50,50	1.23	4 (9%)	51,76,76	2.04	14 (27%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
36	CLA	G	313	7	65,73,73	1.49	6 (9%)	76,113,113	1.96	14 (18%)
35	A86	O	301	-	44,50,50	1.25	4 (9%)	51,76,76	2.07	14 (27%)
36	CLA	K	316	-	65,73,73	1.45	9 (13%)	76,113,113	1.32	5 (6%)
36	CLA	b	820	21	60,68,73	1.50	9 (15%)	70,107,113	1.47	8 (11%)
36	CLA	R	316	-	46,54,73	1.73	9 (19%)	53,90,113	2.13	16 (30%)
34	DD6	H	302	-	39,45,45	1.98	3 (7%)	52,67,67	1.92	15 (28%)
36	CLA	a	833	-	50,58,73	1.65	11 (22%)	58,95,113	1.69	7 (12%)
36	CLA	P	316	-	41,49,73	1.84	8 (19%)	47,84,113	1.81	7 (14%)
36	CLA	X	313	19	42,50,73	2.62	8 (19%)	48,85,113	4.07	18 (37%)
37	KC1	M	318	-	48,53,53	5.42	28 (58%)	55,89,89	6.65	32 (58%)
37	KC1	O	313	15	48,53,53	3.07	21 (43%)	55,89,89	6.91	36 (65%)
37	KC1	X	311	-	48,53,53	3.14	19 (39%)	55,89,89	4.85	34 (61%)
39	LMT	E	321	-	23,23,36	0.45	0	28,28,47	0.59	0
36	CLA	f	803	-	65,73,73	1.81	14 (21%)	76,113,113	2.45	24 (31%)
36	CLA	J	313	-	65,73,73	1.44	9 (13%)	76,113,113	1.44	8 (10%)
36	CLA	b	819	-	59,67,73	1.63	9 (15%)	68,105,113	2.04	15 (22%)
36	CLA	H	307	8	60,68,73	1.48	8 (13%)	70,107,113	1.99	18 (25%)
36	CLA	J	309	-	65,73,73	1.45	6 (9%)	76,113,113	1.34	7 (9%)
35	A86	R	303	-	44,50,50	1.36	5 (11%)	51,76,76	3.63	21 (41%)
36	CLA	a	813	-	45,53,73	1.62	10 (22%)	52,89,113	1.89	9 (17%)
36	CLA	a	821	-	49,57,73	1.57	8 (16%)	55,93,113	1.70	6 (10%)
37	KC1	B	310	2	48,53,53	3.13	20 (41%)	55,89,89	5.04	34 (61%)
36	CLA	K	307	-	61,69,73	1.91	13 (21%)	71,108,113	2.94	22 (30%)
37	KC1	E	309	-	48,53,53	2.94	20 (41%)	55,89,89	5.56	37 (67%)
42	LMG	G	324	-	55,55,55	0.90	2 (3%)	63,63,63	1.00	3 (4%)
36	CLA	P	318	-	51,59,73	1.66	7 (13%)	59,96,113	1.56	7 (11%)
35	A86	U	302	-	44,50,50	1.33	4 (9%)	51,76,76	3.12	22 (43%)
35	A86	J	301	-	44,50,50	1.26	4 (9%)	51,76,76	2.23	18 (35%)
35	A86	E	307	36	44,50,50	1.24	4 (9%)	51,76,76	2.07	12 (23%)
35	A86	N	304	-	44,50,50	2.90	7 (15%)	51,76,76	7.45	18 (35%)
36	CLA	a	807	20	65,73,73	1.37	7 (10%)	76,113,113	1.63	12 (15%)
36	CLA	Q	314	-	65,73,73	1.45	6 (9%)	76,113,113	4.16	13 (17%)
36	CLA	W	206	19	61,69,73	1.51	5 (8%)	71,108,113	1.63	7 (9%)
35	A86	O	319	35,36	44,50,50	1.28	5 (11%)	51,76,76	2.93	18 (35%)
39	LMT	U	314	-	36,36,36	0.40	0	47,47,47	0.69	1 (2%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
39	LMT	h	205	-	36,36,36	0.41	0	47,47,47	0.70	1 (2%)
37	KC1	D	314	4	48,53,53	2.90	19 (39%)	55,89,89	5.52	34 (61%)
35	A86	I	301	-	44,50,50	1.23	3 (6%)	51,76,76	2.39	18 (35%)
36	CLA	a	815	46	45,53,73	1.73	8 (17%)	52,89,113	1.63	6 (11%)
36	CLA	G	310	-	65,73,73	1.41	9 (13%)	76,113,113	1.36	6 (7%)
36	CLA	V	313	-	65,73,73	1.46	8 (12%)	76,113,113	1.34	8 (10%)
36	CLA	V	309	33	43,51,73	1.76	8 (18%)	49,86,113	2.05	12 (24%)
35	A86	V	304	-	44,50,50	1.48	6 (13%)	51,76,76	3.49	18 (35%)
34	DD6	a	849	-	39,45,45	2.01	3 (7%)	52,67,67	1.84	13 (25%)
36	CLA	P	302	-	42,50,73	1.72	7 (16%)	48,85,113	1.92	9 (18%)
36	CLA	S	310	17	65,73,73	1.45	7 (10%)	76,113,113	1.70	12 (15%)
41	LHG	O	318	15	48,48,48	0.88	3 (6%)	51,54,54	1.22	4 (7%)
36	CLA	a	828	-	65,73,73	1.36	7 (10%)	76,113,113	1.57	8 (10%)
36	CLA	U	308	35,32	56,64,73	1.59	8 (14%)	65,102,113	1.75	10 (15%)
36	CLA	b	817	-	59,67,73	1.91	11 (18%)	68,105,113	2.25	18 (26%)
36	CLA	V	307	-	51,59,73	1.67	6 (11%)	59,96,113	1.49	6 (10%)
42	LMG	I	315	-	55,55,55	0.89	2 (3%)	63,63,63	1.00	3 (4%)
36	CLA	E	313	-	65,73,73	1.95	13 (20%)	76,113,113	2.19	20 (26%)
36	CLA	a	811	-	54,62,73	1.60	8 (14%)	62,99,113	1.51	7 (11%)
42	LMG	G	325	-	55,55,55	0.89	2 (3%)	63,63,63	1.01	3 (4%)
36	CLA	S	315	17	43,51,73	1.91	9 (20%)	49,86,113	2.11	10 (20%)
35	A86	G	302	-	44,50,50	1.18	3 (6%)	51,76,76	1.92	13 (25%)
36	CLA	a	810	36	62,70,73	1.44	8 (12%)	72,109,113	1.51	8 (11%)
36	CLA	B	309	2	52,60,73	2.05	10 (19%)	60,97,113	2.20	19 (31%)
39	LMT	F	321	-	34,34,36	0.65	0	45,45,47	1.61	6 (13%)
36	CLA	b	821	46	65,73,73	1.43	10 (15%)	76,113,113	1.49	9 (11%)
35	A86	U	301	-	44,50,50	1.37	3 (6%)	51,76,76	3.80	25 (49%)
35	A86	N	320	-	44,50,50	1.38	6 (13%)	51,76,76	3.30	24 (47%)
35	A86	C	203	-	44,50,50	1.24	4 (9%)	51,76,76	2.07	16 (31%)
36	CLA	B	307	-	46,54,73	1.74	8 (17%)	53,90,113	1.65	9 (16%)
36	CLA	F	314	6,35	65,73,73	1.42	7 (10%)	76,113,113	1.56	10 (13%)
36	CLA	S	321	-	52,60,73	1.66	8 (15%)	60,97,113	1.76	10 (16%)
36	CLA	f	805	25	52,60,73	1.55	7 (13%)	60,97,113	1.65	9 (15%)
36	CLA	N	313	14	41,49,73	1.89	8 (19%)	47,84,113	1.90	12 (25%)
37	KC1	L	317	-	48,53,53	2.96	20 (41%)	55,89,89	5.42	36 (65%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
42	LMG	V	316	-	46,46,55	0.98	2 (4%)	54,54,63	1.04	3 (5%)
39	LMT	a	853	-	33,33,36	0.42	0	44,44,47	0.74	1 (2%)
42	LMG	J	319	-	44,44,55	0.99	2 (4%)	52,52,63	1.11	3 (5%)
34	DD6	A	303	-	39,45,45	2.00	3 (7%)	52,67,67	1.86	9 (17%)
35	A86	F	301	-	44,50,50	1.24	4 (9%)	51,76,76	2.32	16 (31%)
36	CLA	Q	312	-	41,49,73	1.85	8 (19%)	47,84,113	1.81	7 (14%)
40	DGD	b	849	-	61,61,67	1.05	7 (11%)	75,75,81	1.49	11 (14%)
36	CLA	D	310	-	65,73,73	1.35	8 (12%)	76,113,113	1.57	8 (10%)
35	A86	N	302	-	44,50,50	1.19	3 (6%)	51,76,76	2.68	15 (29%)
35	A86	K	301	-	44,50,50	1.25	4 (9%)	51,76,76	2.26	13 (25%)
35	A86	C	204	-	44,50,50	1.84	14 (31%)	51,76,76	2.68	16 (31%)
36	CLA	R	314	16	46,54,73	1.74	8 (17%)	53,90,113	1.91	11 (20%)
36	CLA	a	816	-	65,73,73	1.69	9 (13%)	76,113,113	2.11	16 (21%)
35	A86	V	303	35	44,50,50	1.28	4 (9%)	51,76,76	3.25	22 (43%)
36	CLA	R	320	16	45,53,73	1.80	8 (17%)	52,89,113	1.86	14 (26%)
36	CLA	a	831	-	65,73,73	1.42	10 (15%)	76,113,113	1.38	9 (11%)
36	CLA	N	316	14	65,73,73	1.47	7 (10%)	76,113,113	1.40	7 (9%)
36	CLA	b	825	-	65,73,73	1.40	9 (13%)	76,113,113	1.54	10 (13%)
35	A86	P	306	-	44,50,50	1.22	3 (6%)	51,76,76	1.89	13 (25%)
37	KC1	P	317	15	48,53,53	2.81	20 (41%)	55,89,89	5.84	35 (63%)
36	CLA	N	308	14	65,73,73	1.67	7 (10%)	76,113,113	1.84	20 (26%)
41	LHG	D	319	42	48,48,48	0.93	2 (4%)	51,54,54	1.06	3 (5%)
36	CLA	b	811	-	65,73,73	1.43	8 (12%)	76,113,113	1.63	10 (13%)
36	CLA	a	838	-	65,73,73	1.41	10 (15%)	76,113,113	1.44	9 (11%)
36	CLA	b	814	-	55,63,73	1.52	9 (16%)	64,101,113	1.50	7 (10%)
35	A86	U	304	37,32	44,50,50	1.21	3 (6%)	51,76,76	2.34	19 (37%)
36	CLA	b	828	-	65,73,73	1.45	8 (12%)	76,113,113	1.58	14 (18%)
36	CLA	C	214	-	41,49,73	1.77	9 (21%)	47,84,113	1.72	9 (19%)
34	DD6	O	304	-	39,45,45	1.90	3 (7%)	52,67,67	2.00	14 (26%)
36	CLA	H	316	-	65,73,73	1.45	9 (13%)	76,113,113	1.45	7 (9%)
36	CLA	a	809	-	56,64,73	1.49	9 (16%)	65,102,113	1.51	9 (13%)
41	LHG	G	320	-	39,39,48	1.04	2 (5%)	42,45,54	1.11	3 (7%)
36	CLA	A	311	-	65,73,73	1.42	9 (13%)	76,113,113	1.43	7 (9%)
36	CLA	a	839	46	65,73,73	1.38	8 (12%)	76,113,113	1.49	9 (11%)
39	LMT	K	318	-	36,36,36	0.41	0	47,47,47	0.72	1 (2%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
36	CLA	E	312	-	65,73,73	1.42	7 (10%)	76,113,113	1.57	9 (11%)
36	CLA	A	310	-	65,73,73	1.40	8 (12%)	76,113,113	1.49	7 (9%)
36	CLA	S	317	-	41,49,73	1.84	6 (14%)	47,84,113	1.70	8 (17%)
35	A86	G	306	-	44,50,50	1.21	4 (9%)	51,76,76	2.34	18 (35%)
36	CLA	X	308	19	47,55,73	3.10	10 (21%)	54,91,113	2.43	19 (35%)
44	BCR	h	201	-	41,41,41	1.26	5 (12%)	56,56,56	1.42	10 (17%)
34	DD6	D	301	-	39,45,45	2.01	3 (7%)	52,67,67	1.99	13 (25%)
36	CLA	M	312	13,36	47,55,73	1.71	9 (19%)	54,91,113	1.71	9 (16%)
44	BCR	i	101	-	41,41,41	1.09	2 (4%)	56,56,56	1.25	7 (12%)
35	A86	h	202	-	44,50,50	1.24	4 (9%)	51,76,76	1.74	10 (19%)
36	CLA	L	320	12	65,73,73	1.43	7 (10%)	76,113,113	1.44	6 (7%)
36	CLA	N	310	14	41,49,73	1.96	10 (24%)	47,84,113	2.42	15 (31%)
36	CLA	O	316	-	65,73,73	1.83	11 (16%)	76,113,113	2.59	25 (32%)
36	CLA	O	312	-	39,48,73	2.10	10 (25%)	45,82,113	1.56	8 (17%)
36	CLA	M	315	13	47,55,73	1.81	10 (21%)	54,91,113	1.68	8 (14%)
36	CLA	N	312	-	47,55,73	1.62	6 (12%)	54,91,113	1.65	6 (11%)
36	CLA	N	315	-	41,49,73	1.82	6 (14%)	47,84,113	1.98	10 (21%)
34	DD6	j	103	-	39,45,45	1.99	3 (7%)	52,67,67	1.83	12 (23%)
35	A86	K	303	-	44,50,50	1.31	4 (9%)	51,76,76	2.80	17 (33%)
35	A86	Q	301	-	44,50,50	1.33	5 (11%)	51,76,76	2.73	17 (33%)
35	A86	S	301	-	44,50,50	1.46	4 (9%)	51,76,76	3.73	26 (50%)
44	BCR	a	847	-	41,41,41	1.23	4 (9%)	56,56,56	1.25	5 (8%)
35	A86	T	306	-	44,50,50	1.23	4 (9%)	51,76,76	2.88	18 (35%)
36	CLA	b	818	-	55,63,73	1.53	7 (12%)	64,101,113	1.79	11 (17%)
36	CLA	J	308	-	61,69,73	1.47	6 (9%)	71,108,113	1.76	11 (15%)
41	LHG	R	323	-	48,48,48	0.94	2 (4%)	51,54,54	1.04	3 (5%)
35	A86	G	305	-	44,50,50	1.23	3 (6%)	51,76,76	2.23	15 (29%)
36	CLA	K	315	-	41,49,73	1.76	7 (17%)	47,84,113	1.86	7 (14%)
36	CLA	T	313	18	65,73,73	1.46	6 (9%)	76,113,113	1.42	9 (11%)
36	CLA	A	314	-	65,73,73	1.56	9 (13%)	76,113,113	1.92	12 (15%)
36	CLA	R	311	16	65,73,73	1.44	6 (9%)	76,113,113	1.48	8 (10%)
35	A86	X	305	-	44,50,50	1.29	4 (9%)	51,76,76	3.04	18 (35%)
41	LHG	b	850	36	48,48,48	0.92	2 (4%)	51,54,54	1.04	3 (5%)
39	LMT	b	848	-	36,36,36	0.38	0	47,47,47	0.67	1 (2%)
36	CLA	U	309	32	46,54,73	1.84	7 (15%)	53,90,113	1.84	11 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
35	A86	J	305	-	44,50,50	1.24	3 (6%)	51,76,76	2.08	15 (29%)
36	CLA	a	835	-	51,59,73	1.65	10 (19%)	59,96,113	1.49	9 (15%)
35	A86	Q	304	-	44,50,50	1.39	6 (13%)	51,76,76	3.30	24 (47%)
41	LHG	j	104	-	48,48,48	0.93	2 (4%)	51,54,54	1.04	3 (5%)
36	CLA	a	824	-	65,73,73	1.45	8 (12%)	76,113,113	1.94	18 (23%)
36	CLA	L	311	-	65,73,73	1.42	8 (12%)	76,113,113	1.48	9 (11%)
34	DD6	D	304	-	39,45,45	1.97	3 (7%)	52,67,67	1.91	12 (23%)
36	CLA	b	808	-	65,73,73	1.42	8 (12%)	76,113,113	1.49	10 (13%)
44	BCR	l	207	-	41,41,41	1.08	2 (4%)	56,56,56	1.35	8 (14%)
35	A86	A	302	-	44,50,50	1.61	6 (13%)	51,76,76	4.76	25 (49%)
36	CLA	V	314	-	65,73,73	1.98	14 (21%)	76,113,113	2.97	22 (28%)
36	CLA	b	809	-	65,73,73	1.40	8 (12%)	76,113,113	1.39	7 (9%)
36	CLA	b	813	-	54,62,73	1.58	9 (16%)	67,100,113	1.47	11 (16%)
36	CLA	H	310	8	46,54,73	2.01	10 (21%)	53,90,113	2.83	19 (35%)
36	CLA	O	309	-	65,73,73	1.46	8 (12%)	76,113,113	1.53	10 (13%)
36	CLA	J	312	10	65,73,73	1.43	7 (10%)	76,113,113	1.57	8 (10%)
36	CLA	M	311	13,35	65,73,73	1.47	7 (10%)	76,113,113	1.41	6 (7%)
36	CLA	R	322	16	52,60,73	1.66	7 (13%)	60,97,113	1.77	11 (18%)
36	CLA	H	312	8	65,73,73	1.41	10 (15%)	76,113,113	1.57	13 (17%)
34	DD6	B	302	-	39,45,45	2.01	3 (7%)	52,67,67	2.07	16 (30%)
34	DD6	I	303	-	39,45,45	2.03	3 (7%)	52,67,67	1.95	15 (28%)
35	A86	B	301	-	44,50,50	1.23	4 (9%)	51,76,76	1.98	13 (25%)
36	CLA	a	837	-	65,73,73	1.38	7 (10%)	76,113,113	1.53	8 (10%)
35	A86	X	304	19	44,50,50	1.34	4 (9%)	51,76,76	3.26	20 (39%)
39	LMT	G	323	-	36,36,36	0.39	0	47,47,47	0.82	0
41	LHG	G	301	-	48,48,48	0.77	2 (4%)	51,54,54	1.28	6 (11%)
41	LHG	D	318	36	45,45,48	0.30	0	48,51,54	0.39	0
41	LHG	E	322	-	48,48,48	0.93	2 (4%)	51,54,54	0.99	2 (3%)
36	CLA	A	309	1	46,54,73	1.73	9 (19%)	53,90,113	1.61	6 (11%)
36	CLA	K	311	-	46,54,73	1.75	7 (15%)	53,90,113	1.63	10 (18%)
36	CLA	W	207	34	65,73,73	1.47	6 (9%)	76,113,113	1.52	9 (11%)
36	CLA	l	204	28	49,57,73	2.30	14 (28%)	55,93,113	2.26	17 (30%)
36	CLA	T	316	-	41,49,73	1.82	7 (17%)	47,84,113	1.71	7 (14%)
36	CLA	A	307	-	60,68,73	1.46	7 (11%)	70,107,113	1.50	10 (14%)
36	CLA	a	832	-	65,73,73	1.40	9 (13%)	76,113,113	1.59	13 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
36	CLA	B	311	2	55,63,73	1.63	6 (10%)	64,101,113	1.79	13 (20%)
39	LMT	F	320	-	36,36,36	0.38	0	47,47,47	0.67	1 (2%)
36	CLA	F	317	6	56,64,73	1.95	13 (23%)	65,102,113	2.70	23 (35%)
36	CLA	X	306	-	61,69,73	1.54	5 (8%)	71,108,113	1.46	8 (11%)
36	CLA	D	313	-	65,73,73	1.36	7 (10%)	76,113,113	1.66	11 (14%)
35	A86	X	301	-	44,50,50	1.55	5 (11%)	51,76,76	3.61	28 (54%)
36	CLA	C	205	-	43,51,73	1.69	7 (16%)	49,86,113	1.74	9 (18%)
36	CLA	C	211	-	65,73,73	1.44	10 (15%)	76,113,113	1.46	8 (10%)
42	LMG	m	102	-	37,37,55	1.08	2 (5%)	45,45,63	1.08	3 (6%)
36	CLA	S	314	17	65,73,73	1.57	9 (13%)	76,113,113	1.56	13 (17%)
39	LMT	B	312	-	36,36,36	0.42	0	47,47,47	0.66	1 (2%)
42	LMG	j	105	-	52,52,55	0.91	2 (3%)	60,60,63	1.00	3 (5%)
44	BCR	b	843	-	41,41,41	1.18	3 (7%)	56,56,56	1.18	5 (8%)
35	A86	H	301	-	44,50,50	1.29	3 (6%)	51,76,76	4.88	20 (39%)
36	CLA	O	310	15	46,54,73	1.72	8 (17%)	53,90,113	1.73	10 (18%)
36	CLA	Q	310	15	65,73,73	2.92	15 (23%)	76,113,113	2.92	21 (27%)
36	CLA	a	817	-	65,73,73	1.38	8 (12%)	76,113,113	1.84	13 (17%)
36	CLA	O	307	-	65,73,73	1.43	8 (12%)	76,113,113	1.48	6 (7%)
37	KC1	M	317	-	48,53,53	2.95	21 (43%)	55,89,89	5.39	34 (61%)
36	CLA	R	319	16	45,53,73	1.75	9 (20%)	52,89,113	2.00	14 (26%)
37	KC1	H	313	-	48,53,53	2.88	21 (43%)	55,89,89	5.03	32 (58%)
36	CLA	b	826	21,46	64,72,73	1.48	10 (15%)	74,111,113	2.11	17 (22%)
36	CLA	T	312	18	46,54,73	1.74	6 (13%)	53,90,113	1.79	11 (20%)
36	CLA	J	311	-	46,54,73	1.74	10 (21%)	53,90,113	1.59	9 (16%)
36	CLA	N	318	-	47,55,73	1.74	6 (12%)	54,91,113	1.84	10 (18%)
44	BCR	a	844	-	41,41,41	1.07	2 (4%)	56,56,56	1.29	5 (8%)
39	LMT	P	321	-	23,23,36	0.43	0	28,28,47	0.61	0
36	CLA	W	216	35,19	45,53,73	2.27	10 (22%)	52,89,113	2.80	14 (26%)
36	CLA	H	309	8	65,73,73	1.44	8 (12%)	76,113,113	1.44	7 (9%)
36	CLA	H	311	-	65,73,73	1.36	7 (10%)	76,113,113	1.59	9 (11%)
36	CLA	B	306	-	46,54,73	1.71	8 (17%)	53,90,113	1.76	8 (15%)
36	CLA	I	309	9	46,54,73	1.74	7 (15%)	53,90,113	2.08	10 (18%)
36	CLA	V	310	33	65,73,73	1.44	7 (10%)	76,113,113	1.43	7 (9%)
36	CLA	E	317	-	46,54,73	1.76	7 (15%)	53,90,113	1.54	7 (13%)
36	CLA	K	309	-	59,67,73	1.53	9 (15%)	68,105,113	1.41	8 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
44	BCR	m	101	-	41,41,41	1.15	4 (9%)	56,56,56	1.34	7 (12%)
36	CLA	V	306	33	65,73,73	1.50	6 (9%)	76,113,113	1.62	11 (14%)
34	DD6	L	305	-	39,45,45	2.04	3 (7%)	52,67,67	2.00	15 (28%)
35	A86	P	307	-	44,50,50	1.22	3 (6%)	51,76,76	2.05	13 (25%)
36	CLA	a	814	-	50,58,73	1.62	9 (18%)	58,95,113	1.87	10 (17%)
35	A86	S	308	37	44,50,50	1.23	4 (9%)	51,76,76	2.12	16 (31%)
35	A86	X	302	35	44,50,50	1.22	4 (9%)	51,76,76	2.97	18 (35%)
36	CLA	a	802	-	65,73,73	1.45	7 (10%)	76,113,113	1.83	12 (15%)
37	KC1	C	213	-	48,53,53	2.99	19 (39%)	55,89,89	4.91	31 (56%)
36	CLA	b	801	46	65,73,73	1.46	8 (12%)	76,113,113	1.57	11 (14%)
36	CLA	l	202	28	65,73,73	1.44	9 (13%)	76,113,113	1.40	10 (13%)
36	CLA	I	306	9	65,73,73	1.65	13 (20%)	76,113,113	2.44	22 (28%)
34	DD6	E	301	-	39,45,45	1.98	3 (7%)	52,67,67	1.93	10 (19%)
35	A86	M	302	-	44,50,50	1.29	4 (9%)	51,76,76	2.78	16 (31%)
41	LHG	a	842	-	47,47,48	0.76	1 (2%)	50,53,54	1.27	4 (8%)
34	DD6	A	304	-	39,45,45	2.00	3 (7%)	52,67,67	1.90	12 (23%)
35	A86	O	303	-	44,50,50	1.34	5 (11%)	51,76,76	2.73	17 (33%)
36	CLA	a	808	20	65,73,73	1.44	10 (15%)	76,113,113	1.50	10 (13%)
34	DD6	C	201	-	39,45,45	2.03	3 (7%)	52,67,67	1.92	13 (25%)
34	DD6	D	305	-	39,45,45	2.00	3 (7%)	52,67,67	1.63	9 (17%)
35	A86	D	302	-	44,50,50	1.23	4 (9%)	51,76,76	2.08	11 (21%)
35	A86	J	303	-	44,50,50	1.41	4 (9%)	51,76,76	2.80	20 (39%)
36	CLA	D	311	-	46,54,73	1.71	9 (19%)	53,90,113	1.63	7 (13%)
36	CLA	i	102	26	65,73,73	1.44	7 (10%)	76,113,113	1.59	8 (10%)
36	CLA	W	214	19	41,49,73	2.04	7 (17%)	47,84,113	2.00	14 (29%)
36	CLA	Q	305	-	61,69,73	1.50	8 (13%)	71,108,113	1.46	6 (8%)
43	PQN	a	840	-	34,34,34	1.58	2 (5%)	42,45,45	1.15	4 (9%)
35	A86	F	304	36	44,50,50	1.25	4 (9%)	51,76,76	2.03	13 (25%)
36	CLA	Q	308	-	65,73,73	1.45	7 (10%)	76,113,113	1.54	10 (13%)
36	CLA	S	320	-	65,73,73	1.49	6 (9%)	76,113,113	1.38	8 (10%)
38	SQD	A	315	-	27,28,54	1.50	4 (14%)	36,39,65	1.29	5 (13%)
40	DGD	L	302	42	48,48,67	0.98	2 (4%)	62,62,81	1.05	4 (6%)
36	CLA	b	839	-	65,73,73	1.42	8 (12%)	76,113,113	1.52	9 (11%)
34	DD6	F	303	-	39,45,45	2.00	3 (7%)	52,67,67	1.91	14 (26%)
34	DD6	R	308	-	39,45,45	2.02	3 (7%)	52,67,67	2.12	13 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
36	CLA	F	309	-	65,73,73	1.42	6 (9%)	76,113,113	1.57	11 (14%)
37	KC1	A	312	1	48,53,53	2.88	19 (39%)	55,89,89	6.87	40 (72%)
36	CLA	b	830	-	65,73,73	1.49	10 (15%)	76,113,113	1.82	13 (17%)
35	A86	R	302	16	44,50,50	1.38	5 (11%)	51,76,76	2.80	15 (29%)
36	CLA	R	318	35	41,49,73	1.83	7 (17%)	47,84,113	1.76	9 (19%)
35	A86	L	319	-	44,50,50	1.43	6 (13%)	51,76,76	3.47	24 (47%)
36	CLA	a	822	-	51,59,73	1.89	8 (15%)	59,96,113	2.05	14 (23%)
35	A86	I	304	-	44,50,50	1.47	4 (9%)	51,76,76	3.38	21 (41%)
41	LHG	f	808	25	48,48,48	0.95	2 (4%)	51,54,54	1.02	3 (5%)
36	CLA	V	305	35	61,69,73	1.66	7 (11%)	71,108,113	1.57	9 (12%)
35	A86	L	306	37	44,50,50	1.24	3 (6%)	51,76,76	2.98	19 (37%)
36	CLA	T	314	-	65,73,73	1.44	7 (10%)	76,113,113	1.68	12 (15%)
37	KC1	G	318	-	48,53,53	2.98	21 (43%)	55,89,89	4.77	36 (65%)
36	CLA	M	314	-	41,49,73	1.81	7 (17%)	47,84,113	1.71	7 (14%)
36	CLA	I	313	-	41,49,73	1.79	7 (17%)	47,84,113	1.73	7 (14%)
36	CLA	F	313	-	52,60,73	1.60	9 (17%)	60,97,113	1.55	8 (13%)
36	CLA	b	836	-	58,66,73	2.01	13 (22%)	67,104,113	3.05	24 (35%)
36	CLA	M	316	36	42,50,73	1.78	8 (19%)	48,85,113	1.61	6 (12%)
35	A86	N	306	-	44,50,50	1.22	3 (6%)	51,76,76	2.83	16 (31%)
36	CLA	a	805	20	65,73,73	1.40	10 (15%)	76,113,113	1.43	9 (11%)
36	CLA	O	311	-	58,66,73	1.51	7 (12%)	67,104,113	1.51	6 (8%)
36	CLA	P	311	-	65,73,73	1.45	7 (10%)	76,113,113	1.54	10 (13%)
36	CLA	D	316	-	52,60,73	1.61	10 (19%)	60,97,113	1.82	13 (21%)
35	A86	Q	316	15,36	44,50,50	1.65	8 (18%)	51,76,76	2.29	17 (33%)
36	CLA	E	311	-	65,73,73	1.40	7 (10%)	76,113,113	1.47	6 (7%)
36	CLA	P	308	-	61,69,73	1.50	9 (14%)	71,108,113	1.46	6 (8%)
36	CLA	H	306	-	61,69,73	1.48	9 (14%)	71,108,113	1.42	6 (8%)
39	LMT	a	851	-	36,36,36	0.43	0	47,47,47	0.74	1 (2%)
36	CLA	D	307	41	61,69,73	1.45	8 (13%)	71,108,113	1.73	16 (22%)
36	CLA	D	315	-	41,49,73	1.70	7 (17%)	47,84,113	2.05	9 (19%)
39	LMT	E	320	-	36,36,36	0.37	0	47,47,47	0.67	0
36	CLA	M	307	-	65,73,73	1.46	9 (13%)	76,113,113	1.56	9 (11%)
36	CLA	H	305	8	48,56,73	1.71	7 (14%)	55,92,113	1.59	8 (14%)
36	CLA	R	312	-	65,73,73	1.49	9 (13%)	76,113,113	1.59	11 (14%)
40	DGD	C	215	-	58,58,67	0.90	2 (3%)	72,72,81	0.96	3 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
36	CLA	b	815	-	65,73,73	1.43	8 (12%)	76,113,113	1.48	7 (9%)
36	CLA	W	211	19	65,73,73	1.45	7 (10%)	76,113,113	1.60	11 (14%)
36	CLA	M	309	-	65,73,73	1.46	7 (10%)	76,113,113	1.40	7 (9%)
36	CLA	W	208	-	45,53,73	1.75	7 (15%)	52,89,113	1.60	6 (11%)
36	CLA	I	308	9	65,73,73	2.07	15 (23%)	76,113,113	2.55	21 (27%)
37	KC1	R	317	-	48,53,53	2.91	20 (41%)	55,89,89	6.06	36 (65%)
36	CLA	G	311	-	65,73,73	1.40	9 (13%)	76,113,113	1.40	8 (10%)
36	CLA	E	316	-	65,73,73	1.45	6 (9%)	76,113,113	1.63	11 (14%)
36	CLA	K	308	-	65,73,73	1.45	6 (9%)	76,113,113	1.50	8 (10%)
37	KC1	O	315	15	48,53,53	3.07	20 (41%)	55,89,89	6.90	36 (65%)
36	CLA	O	314	-	41,49,73	1.83	8 (19%)	47,84,113	1.80	7 (14%)
39	LMT	I	318	-	36,36,36	0.39	0	47,47,47	0.75	1 (2%)
36	CLA	b	824	-	53,61,73	2.22	14 (26%)	61,98,113	2.40	22 (36%)
42	LMG	a	852	-	54,54,55	0.90	2 (3%)	62,62,63	1.03	3 (4%)
36	CLA	H	308	8	63,72,73	1.45	8 (12%)	73,112,113	1.44	10 (13%)
36	CLA	R	315	-	65,73,73	1.44	7 (10%)	76,113,113	1.47	7 (9%)
36	CLA	L	316	-	41,49,73	1.81	6 (14%)	47,84,113	1.75	8 (17%)
37	KC1	J	314	-	48,53,53	2.92	19 (39%)	55,89,89	6.21	35 (63%)
36	CLA	b	822	-	46,54,73	1.66	8 (17%)	53,90,113	1.62	9 (16%)
36	CLA	G	316	-	49,57,73	1.66	9 (18%)	55,93,113	1.61	7 (12%)
36	CLA	j	106	27	42,50,73	1.75	9 (21%)	48,85,113	1.74	8 (16%)
37	KC1	F	315	-	48,53,53	2.84	18 (37%)	55,89,89	6.66	33 (60%)
35	A86	R	305	-	44,50,50	1.22	4 (9%)	51,76,76	1.81	11 (21%)
36	CLA	G	315	-	56,64,73	1.92	12 (21%)	65,102,113	2.50	19 (29%)
35	A86	T	303	-	44,50,50	1.22	4 (9%)	51,76,76	3.14	21 (41%)
36	CLA	L	310	-	54,62,73	1.61	7 (12%)	62,99,113	1.41	6 (9%)
41	LHG	O	317	-	41,41,48	1.00	2 (4%)	44,47,54	1.08	3 (6%)
36	CLA	j	101	27	65,73,73	1.40	8 (12%)	76,113,113	1.37	7 (9%)
41	LHG	Q	315	36	48,48,48	0.93	2 (4%)	51,54,54	1.04	3 (5%)
36	CLA	S	313	-	46,54,73	1.74	6 (13%)	53,90,113	1.99	12 (22%)
36	CLA	P	310	15,41	65,73,73	1.45	7 (10%)	76,113,113	1.44	8 (10%)
36	CLA	S	318	-	42,50,73	1.83	6 (14%)	48,85,113	1.77	9 (18%)
34	DD6	W	205	-	39,45,45	1.99	3 (7%)	52,67,67	2.03	15 (28%)
34	DD6	J	304	-	39,45,45	2.00	3 (7%)	52,67,67	1.87	12 (23%)
35	A86	F	307	-	44,50,50	1.31	3 (6%)	51,76,76	3.94	22 (43%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
44	BCR	l	203	-	41,41,41	1.23	4 (9%)	56,56,56	1.21	5 (8%)
36	CLA	N	307	-	61,69,73	1.53	6 (9%)	71,108,113	1.45	6 (8%)
35	A86	R	304	16,36	44,50,50	1.30	3 (6%)	51,76,76	2.95	17 (33%)
44	BCR	b	846	-	41,41,41	1.15	4 (9%)	56,56,56	1.44	10 (17%)
36	CLA	b	840	-	65,73,73	1.40	9 (13%)	76,113,113	1.56	13 (17%)
36	CLA	A	306	-	61,69,73	1.93	13 (21%)	71,108,113	2.41	25 (35%)
35	A86	X	314	19	44,50,50	1.26	4 (9%)	51,76,76	2.07	13 (25%)
37	KC1	S	316	-	48,53,53	3.10	20 (41%)	55,89,89	6.04	36 (65%)
35	A86	F	302	-	44,50,50	1.24	4 (9%)	51,76,76	1.92	11 (21%)
36	CLA	I	312	9	52,60,73	1.67	8 (15%)	60,97,113	1.50	7 (11%)
35	A86	M	305	-	44,50,50	1.34	4 (9%)	51,76,76	2.88	15 (29%)
37	KC1	G	308	-	48,53,53	2.94	21 (43%)	55,89,89	5.62	35 (63%)
44	BCR	a	845	-	41,41,41	1.18	2 (4%)	56,56,56	1.19	5 (8%)
37	KC1	P	315	35	48,53,53	3.07	21 (43%)	55,89,89	6.91	36 (65%)
39	LMT	P	320	-	23,23,36	0.43	0	28,28,47	0.62	0
35	A86	V	302	-	44,50,50	1.32	4 (9%)	51,76,76	2.92	21 (41%)
42	LMG	h	206	-	45,45,55	0.99	2 (4%)	53,53,63	1.03	3 (5%)
36	CLA	U	313	-	41,49,73	1.87	7 (17%)	47,84,113	1.92	11 (23%)
36	CLA	S	312	17	65,73,73	1.46	7 (10%)	76,113,113	1.50	9 (11%)
36	CLA	K	310	-	62,70,73	1.98	16 (25%)	72,109,113	2.51	26 (36%)
36	CLA	j	102	-	65,73,73	1.77	10 (15%)	76,113,113	2.26	18 (23%)
36	CLA	R	310	-	61,69,73	1.51	8 (13%)	71,108,113	1.51	6 (8%)
36	CLA	G	312	7	58,66,73	1.48	10 (17%)	67,104,113	1.57	8 (11%)
36	CLA	N	319	14	42,50,73	3.74	14 (33%)	48,85,113	6.10	30 (62%)
37	KC1	L	315	12,35	48,53,53	3.06	19 (39%)	55,89,89	6.27	36 (65%)
44	BCR	b	844	-	41,41,41	1.11	3 (7%)	56,56,56	1.31	5 (8%)
36	CLA	V	308	-	65,73,73	1.43	7 (10%)	76,113,113	1.50	9 (11%)
36	CLA	D	317	-	58,66,73	1.52	8 (13%)	67,104,113	1.50	8 (11%)
39	LMT	E	323	-	36,36,36	0.35	0	47,47,47	0.82	1 (2%)
36	CLA	X	312	-	41,49,73	1.81	7 (17%)	47,84,113	1.95	8 (17%)
35	A86	J	306	-	44,50,50	1.25	3 (6%)	51,76,76	1.96	11 (21%)
35	A86	S	302	-	44,50,50	1.20	3 (6%)	51,76,76	2.68	15 (29%)
36	CLA	b	806	-	65,73,73	1.42	9 (13%)	76,113,113	1.76	12 (15%)
36	CLA	a	823	-	55,63,73	1.95	11 (20%)	64,101,113	2.18	18 (28%)
36	CLA	h	203	-	65,73,73	1.40	8 (12%)	76,113,113	1.59	10 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
36	CLA	W	201	19	48,56,73	1.72	7 (14%)	55,92,113	1.57	7 (12%)
36	CLA	M	310	13,35	46,54,73	2.28	10 (21%)	53,90,113	1.84	13 (24%)
35	A86	H	304	-	44,50,50	1.24	4 (9%)	51,76,76	2.31	17 (33%)
36	CLA	T	309	18	65,73,73	1.45	7 (10%)	76,113,113	1.51	9 (11%)
34	DD6	Q	302	-	39,45,45	2.04	3 (7%)	52,67,67	2.04	16 (30%)
35	A86	M	301	-	44,50,50	1.36	4 (9%)	51,76,76	3.39	22 (43%)
35	A86	N	305	-	44,50,50	1.65	8 (18%)	51,76,76	2.29	17 (33%)
37	KC1	N	314	14	48,53,53	3.16	22 (45%)	55,89,89	4.92	33 (60%)
37	KC1	W	213	-	48,53,53	3.12	20 (41%)	55,89,89	5.79	34 (61%)
34	DD6	S	307	-	39,45,45	2.03	3 (7%)	52,67,67	2.07	15 (28%)
36	CLA	f	802	-	65,73,73	1.51	8 (12%)	76,113,113	1.43	10 (13%)
35	A86	W	203	36	44,50,50	1.37	4 (9%)	51,76,76	2.83	20 (39%)
34	DD6	E	303	-	39,45,45	2.00	3 (7%)	52,67,67	2.00	10 (19%)
34	DD6	H	303	-	39,45,45	1.99	3 (7%)	52,67,67	1.97	12 (23%)
36	CLA	F	312	-	65,73,73	1.43	7 (10%)	76,113,113	1.44	8 (10%)
45	SF4	c	101	22	0,12,12	-	-	-		
34	DD6	K	305	-	39,45,45	2.00	3 (7%)	52,67,67	2.00	14 (26%)
36	CLA	a	818	-	65,73,73	1.40	10 (15%)	76,113,113	1.71	10 (13%)
34	DD6	M	303	-	39,45,45	2.03	3 (7%)	52,67,67	1.96	11 (21%)
35	A86	G	304	-	44,50,50	1.43	5 (11%)	51,76,76	3.69	25 (49%)
36	CLA	a	803	36	55,63,73	1.53	8 (14%)	64,101,113	1.72	12 (18%)
36	CLA	C	212	35	65,73,73	1.38	8 (12%)	76,113,113	1.68	12 (15%)
35	A86	K	302	-	44,50,50	1.38	4 (9%)	51,76,76	3.29	20 (39%)
36	CLA	C	209	-	65,73,73	1.48	9 (13%)	76,113,113	1.44	9 (11%)
36	CLA	B	305	2	65,73,73	1.44	7 (10%)	76,113,113	1.50	9 (11%)
36	CLA	a	834	20	45,53,73	1.75	7 (15%)	52,89,113	1.70	8 (15%)
36	CLA	B	308	-	65,73,73	1.41	7 (10%)	76,113,113	1.64	12 (15%)
36	CLA	I	314	-	41,49,73	1.84	7 (17%)	47,84,113	1.68	6 (12%)
39	LMT	K	317	-	32,32,36	0.43	0	43,43,47	0.70	0
36	CLA	M	308	-	52,60,73	1.65	10 (19%)	60,97,113	1.71	9 (15%)
36	CLA	N	317	14	54,62,73	1.64	6 (11%)	62,99,113	1.66	9 (14%)
35	A86	T	307	-	44,50,50	1.24	3 (6%)	51,76,76	3.14	21 (41%)
35	A86	R	301	-	44,50,50	1.47	4 (9%)	51,76,76	3.48	24 (47%)
36	CLA	E	314	-	65,73,73	1.36	8 (12%)	76,113,113	1.66	13 (17%)
36	CLA	J	310	-	65,73,73	1.39	7 (10%)	76,113,113	1.50	7 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
36	CLA	U	310	-	65,73,73	1.48	7 (10%)	76,113,113	1.62	13 (17%)
36	CLA	a	826	-	65,73,73	1.40	7 (10%)	76,113,113	1.65	9 (11%)
35	A86	F	305	-	44,50,50	1.35	6 (13%)	51,76,76	2.84	20 (39%)
36	CLA	H	314	-	41,49,73	1.74	8 (19%)	47,84,113	1.95	7 (14%)
35	A86	L	301	-	44,50,50	1.25	4 (9%)	51,76,76	2.01	14 (27%)
35	A86	T	305	18	44,50,50	1.48	5 (11%)	51,76,76	3.68	22 (43%)
37	KC1	T	315	-	48,53,53	3.05	19 (39%)	55,89,89	5.84	34 (61%)
35	A86	U	303	36	44,50,50	1.23	4 (9%)	51,76,76	2.00	14 (27%)
37	KC1	V	312	33	48,53,53	3.13	21 (43%)	55,89,89	5.51	34 (61%)
36	CLA	K	313	-	65,73,73	1.44	9 (13%)	76,113,113	1.62	10 (13%)
36	CLA	I	310	35	65,73,73	1.39	7 (10%)	76,113,113	1.55	7 (9%)
36	CLA	X	310	19	41,49,73	1.88	7 (17%)	47,84,113	2.18	11 (23%)
36	CLA	U	307	-	50,58,73	1.68	8 (16%)	58,95,113	1.51	6 (10%)
37	KC1	M	313	13,36	48,53,53	2.95	20 (41%)	55,89,89	6.15	36 (65%)
36	CLA	P	309	41	65,73,73	1.44	8 (12%)	76,113,113	1.48	6 (7%)
35	A86	N	301	-	44,50,50	1.46	4 (9%)	51,76,76	3.73	26 (50%)
35	A86	S	304	-	44,50,50	1.24	4 (9%)	51,76,76	2.13	16 (31%)
36	CLA	I	311	9	65,73,73	1.36	7 (10%)	76,113,113	1.64	9 (11%)
36	CLA	W	212	19	65,73,73	1.48	6 (9%)	76,113,113	1.75	10 (13%)
36	CLA	W	209	19	57,65,73	1.59	7 (12%)	66,103,113	1.55	10 (15%)
34	DD6	A	301	-	39,45,45	2.04	3 (7%)	52,67,67	2.08	15 (28%)
35	A86	C	202	3,36	44,50,50	1.40	5 (11%)	51,76,76	3.09	17 (33%)
41	LHG	a	850	-	46,46,48	0.96	2 (4%)	49,52,54	1.04	3 (6%)
37	KC1	Q	311	15	48,53,53	3.07	20 (41%)	55,89,89	6.90	36 (65%)
43	PQN	b	842	-	34,34,34	1.56	2 (5%)	42,45,45	1.19	4 (9%)
36	CLA	S	309	-	61,69,73	1.53	8 (13%)	71,108,113	1.41	8 (11%)
36	CLA	S	311	35	46,54,73	1.81	9 (19%)	53,90,113	1.64	10 (18%)
35	A86	R	309	-	44,50,50	1.23	4 (9%)	51,76,76	2.84	16 (31%)
35	A86	S	303	17	44,50,50	1.32	5 (11%)	51,76,76	3.30	22 (43%)
36	CLA	G	309	7	65,73,73	1.38	8 (12%)	76,113,113	1.95	14 (18%)
41	LHG	a	843	36	26,26,48	1.24	2 (7%)	29,32,54	1.31	2 (6%)
41	LHG	F	318	-	32,32,48	0.88	1 (3%)	36,37,54	1.72	6 (16%)
36	CLA	X	309	19	44,53,73	1.82	6 (13%)	50,89,113	1.83	12 (24%)
35	A86	T	301	36	44,50,50	1.25	4 (9%)	51,76,76	2.07	16 (31%)
36	CLA	G	307	-	41,50,73	2.21	12 (29%)	46,85,113	3.26	17 (36%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
36	CLA	b	834	-	65,73,73	1.47	8 (12%)	76,113,113	1.41	8 (10%)
39	LMT	B	313	-	36,36,36	0.43	0	47,47,47	0.73	1 (2%)
35	A86	h	204	-	44,50,50	1.23	4 (9%)	51,76,76	2.14	11 (21%)
36	CLA	X	307	35,19	50,58,73	1.76	7 (14%)	58,95,113	1.94	13 (22%)
41	LHG	f	809	-	41,41,48	1.01	2 (4%)	44,47,54	1.09	3 (6%)
36	CLA	b	838	-	47,55,73	1.59	7 (14%)	54,91,113	1.66	8 (14%)
35	A86	W	202	19,36	44,50,50	1.50	6 (13%)	51,76,76	3.63	29 (56%)

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
35	A86	M	304	-	-	14/34/90/90	0/3/3/3
39	LMT	G	322	-	-	17/21/61/61	0/2/2/2
39	LMT	L	303	-	-	10/21/61/61	0/2/2/2
36	CLA	W	215	-	1/1/11/20	4/17/95/115	-
37	KC1	Q	313	-	-	2/15/71/71	-
35	A86	J	302	-	-	5/34/90/90	1/3/3/3
36	CLA	F	310	-	1/1/13/20	10/27/105/115	-
36	CLA	a	829	-	1/1/15/20	13/37/115/115	-
36	CLA	T	308	18	1/1/14/20	8/33/111/115	-
36	CLA	b	816	-	2/2/14/20	17/31/109/115	-
36	CLA	E	310	-	-	7/37/115/115	-
39	LMT	b	851	-	-	7/15/35/61	0/1/1/2
36	CLA	F	311	-	1/1/12/20	8/22/100/115	-
35	A86	S	305	-	-	9/34/90/90	0/3/3/3
36	CLA	M	306	13,37	1/1/13/20	8/25/103/115	-
36	CLA	A	305	1	1/1/11/20	4/18/96/115	-
36	CLA	a	801	-	1/1/15/20	10/37/115/115	-
35	A86	N	303	-	-	4/34/90/90	0/3/3/3
34	DD6	D	303	-	-	9/26/80/80	0/3/3/3
36	CLA	D	309	-	2/2/13/20	6/25/103/115	-
36	CLA	J	307	10	1/1/14/20	9/33/111/115	-
36	CLA	J	315	-	1/1/10/20	2/8/86/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
34	DD6	W	204	36	-	7/26/80/80	0/3/3/3
37	KC1	U	312	35,32	-	4/15/71/71	-
36	CLA	D	306	4	1/1/11/20	4/13/91/115	-
36	CLA	K	312	-	1/1/15/20	6/37/115/115	-
36	CLA	H	315	8	1/1/15/20	14/37/115/115	-
36	CLA	J	317	10	1/1/11/20	3/16/94/115	-
36	CLA	l	206	46	1/1/12/20	6/19/97/115	-
36	CLA	a	827	-	1/1/14/20	14/34/112/115	-
42	LMG	E	318	-	-	24/41/61/70	0/1/1/1
34	DD6	E	306	-	-	4/26/80/80	0/3/3/3
36	CLA	A	308	-	1/1/15/20	13/37/115/115	-
36	CLA	I	307	-	1/1/12/20	4/24/102/115	-
36	CLA	a	804	-	1/1/15/20	16/37/115/115	-
36	CLA	C	206	-	1/1/14/20	15/33/111/115	-
36	CLA	P	314	-	-	21/31/109/115	-
36	CLA	b	833	-	1/1/13/20	9/29/107/115	-
36	CLA	a	812	-	1/1/15/20	14/37/115/115	-
36	CLA	O	306	-	1/1/14/20	9/33/111/115	-
36	CLA	a	820	-	1/1/15/20	11/37/115/115	-
34	DD6	P	305	-	-	2/26/80/80	0/3/3/3
36	CLA	C	208	-	1/1/15/20	17/37/115/115	-
36	CLA	V	311	33	1/1/15/20	13/37/115/115	-
41	LHG	i	104	-	-	29/50/50/53	-
34	DD6	S	306	-	-	5/26/80/80	0/3/3/3
36	CLA	b	835	-	1/1/11/20	3/13/91/115	-
35	A86	I	302	-	-	7/34/90/90	0/3/3/3
41	LHG	I	316	-	-	30/53/53/53	-
39	LMT	I	317	-	-	13/21/61/61	0/2/2/2
34	DD6	K	304	-	-	2/26/80/80	0/3/3/3
35	A86	O	302	-	-	9/34/90/90	0/3/3/3
36	CLA	L	314	12	1/1/15/20	19/37/115/115	-
36	CLA	X	315	-	-	3/8/86/115	-
36	CLA	G	314	7	1/1/10/20	2/8/86/115	-
35	A86	E	302	-	-	4/34/90/90	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
42	LMG	D	320	41	-	24/41/61/70	0/1/1/1
36	CLA	I	305	-	2/2/14/20	10/33/111/115	-
36	CLA	b	832	-	1/1/11/20	4/18/96/115	-
36	CLA	N	311	14	1/1/11/20	4/15/93/115	-
36	CLA	O	308	15	1/1/15/20	13/37/115/115	-
36	CLA	L	312	12	-	6/15/93/115	-
36	CLA	b	807	-	1/1/11/20	3/13/91/115	-
36	CLA	b	823	-	1/1/13/20	4/25/103/115	-
35	A86	A	316	-	-	9/34/90/90	0/3/3/3
37	KC1	T	310	-	-	11/15/71/71	-
36	CLA	a	806	-	2/2/15/20	10/37/115/115	-
35	A86	T	304	-	-	0/34/90/90	0/3/3/3
37	KC1	K	314	11	-	5/15/71/71	-
36	CLA	L	308	-	2/2/14/20	20/33/111/115	-
42	LMG	E	319	-	-	23/35/55/70	0/1/1/1
39	LMT	L	318	-	-	13/17/57/61	0/2/2/2
37	KC1	W	217	-	-	4/15/71/71	-
39	LMT	f	807	-	-	7/15/35/61	0/1/1/2
36	CLA	l	201	-	1/1/15/20	16/37/115/115	-
44	BCR	a	846	-	-	7/29/63/63	0/2/2/2
36	CLA	b	837	-	1/1/15/20	8/37/115/115	-
36	CLA	b	812	21	1/1/15/20	6/37/115/115	-
36	CLA	P	312	15	1/1/11/20	7/15/93/115	-
44	BCR	f	806	-	-	9/29/63/63	0/2/2/2
36	CLA	l	205	-	2/2/15/20	14/37/115/115	-
39	LMT	a	854	-	-	16/21/61/61	0/2/2/2
35	A86	O	305	-	-	14/34/90/90	0/3/3/3
36	CLA	C	210	3	1/1/11/20	4/15/93/115	-
36	CLA	E	315	-	2/2/15/20	16/37/115/115	-
42	LMG	D	321	-	-	21/32/52/70	0/1/1/1
45	SF4	b	803	21,20	-	-	0/6/5/5
37	KC1	G	317	-	-	6/15/71/71	-
36	CLA	b	802	-	1/1/15/20	10/37/115/115	-
36	CLA	R	321	16	-	9/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
36	CLA	E	308	5	1/1/11/20	8/18/96/115	-
36	CLA	a	836	-	1/1/15/20	11/37/115/115	-
41	LHG	F	319	-	-	33/45/45/53	-
44	BCR	f	801	-	-	9/29/63/63	0/2/2/2
36	CLA	D	308	-	1/1/15/20	16/37/115/115	-
36	CLA	S	319	17	1/1/15/20	6/37/115/115	-
38	SQD	b	804	-	-	23/41/61/69	0/1/1/1
35	A86	P	304	-	-	6/34/90/90	0/3/3/3
36	CLA	H	317	8	1/1/15/20	8/37/115/115	-
39	LMT	U	315	-	-	17/21/61/61	0/2/2/2
36	CLA	J	316	-	1/1/11/20	6/15/93/115	-
36	CLA	b	841	41	1/1/15/20	9/37/115/115	-
36	CLA	A	313	-	1/1/10/20	2/8/86/115	-
44	BCR	b	847	-	-	8/29/63/63	0/2/2/2
35	A86	T	302	18	-	7/34/90/90	0/3/3/3
35	A86	Q	303	-	-	8/34/90/90	0/3/3/3
36	CLA	U	305	-	1/1/14/20	11/33/111/115	-
35	A86	L	304	-	-	6/34/90/90	0/3/3/3
44	BCR	i	103	-	-	11/29/63/63	0/2/2/2
35	A86	X	303	36	-	9/34/90/90	0/3/3/3
36	CLA	W	210	-	1/1/11/20	7/15/93/115	-
36	CLA	H	318	-	1/1/12/20	8/19/97/115	-
36	CLA	a	825	-	2/2/15/20	15/37/115/115	-
36	CLA	C	207	-	1/1/15/20	16/37/115/115	-
36	CLA	T	311	18	1/1/15/20	11/37/115/115	-
42	LMG	J	318	-	-	28/50/70/70	0/1/1/1
45	SF4	c	102	-	-	-	0/6/5/5
36	CLA	U	306	32	1/1/15/20	20/37/115/115	-
36	CLA	U	311	32	1/1/15/20	21/37/115/115	-
44	BCR	j	107	-	-	5/29/63/63	0/2/2/2
36	CLA	L	309	12	1/1/15/20	12/37/115/115	-
36	CLA	b	829	-	1/1/15/20	9/37/115/115	-
36	CLA	D	312	-	1/1/15/20	11/37/115/115	-
34	DD6	R	307	-	-	11/26/80/80	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
35	A86	R	306	-	-	8/34/90/90	0/3/3/3
42	LMG	L	321	40	-	15/28/48/70	0/1/1/1
36	CLA	Q	307	15	1/1/11/20	4/19/97/115	-
36	CLA	P	301	15	1/1/15/20	16/37/115/115	-
36	CLA	a	819	-	1/1/11/20	3/13/91/115	-
34	DD6	B	304	-	-	2/26/80/80	0/3/3/3
36	CLA	P	319	-	1/1/14/20	14/31/109/115	-
36	CLA	R	313	-	1/1/15/20	13/37/115/115	-
36	CLA	Q	309	15	1/1/11/20	7/15/93/115	-
41	LHG	l	208	-	-	34/52/52/53	-
36	CLA	N	309	14	1/1/12/20	7/21/99/115	-
35	A86	V	301	35	-	10/34/90/90	1/3/3/3
34	DD6	G	303	-	-	4/26/80/80	0/3/3/3
36	CLA	b	810	-	1/1/15/20	8/37/115/115	-
41	LHG	G	321	36	-	27/51/51/53	-
36	CLA	b	827	-	1/1/15/20	10/37/115/115	-
34	DD6	E	304	-	-	4/26/80/80	0/3/3/3
35	A86	B	303	-	-	13/34/90/90	0/3/3/3
36	CLA	P	313	-	1/1/15/20	12/37/115/115	-
36	CLA	a	848	36	2/2/15/20	12/37/115/115	-
35	A86	F	306	-	-	0/34/90/90	1/3/3/3
36	CLA	G	319	7	1/1/12/20	8/19/97/115	-
36	CLA	a	841	41	1/1/12/20	7/22/100/115	-
35	A86	P	303	-	-	9/34/90/90	0/3/3/3
36	CLA	W	218	19	1/1/10/20	9/11/89/115	-
36	CLA	Q	306	-	1/1/15/20	14/37/115/115	-
36	CLA	L	313	-	1/1/15/20	8/37/115/115	-
36	CLA	f	804	46	2/2/15/20	10/37/115/115	-
36	CLA	a	830	-	-	10/19/97/115	-
42	LMG	V	315	-	-	24/41/61/70	0/1/1/1
35	A86	K	306	11	-	8/34/90/90	0/3/3/3
35	A86	L	307	-	-	8/34/90/90	1/3/3/3
44	BCR	b	845	-	-	7/29/63/63	0/2/2/2
36	CLA	b	831	-	1/1/12/20	7/19/97/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
36	CLA	F	316	6	1/1/10/20	1/8/86/115	-
37	KC1	F	308	6	-	7/15/71/71	-
36	CLA	b	805	36	1/1/15/20	16/37/115/115	-
36	CLA	G	313	7	1/1/15/20	16/37/115/115	-
35	A86	E	305	5	-	5/34/90/90	0/3/3/3
35	A86	O	301	-	-	4/34/90/90	0/3/3/3
36	CLA	K	316	-	1/1/15/20	10/37/115/115	-
36	CLA	b	820	21	1/1/14/20	15/31/109/115	-
36	CLA	R	316	-	1/1/11/20	8/15/93/115	-
34	DD6	H	302	-	-	2/26/80/80	0/3/3/3
36	CLA	a	833	-	1/1/12/20	2/19/97/115	-
36	CLA	P	316	-	1/1/10/20	3/8/86/115	-
36	CLA	X	313	19	-	5/10/88/115	-
37	KC1	M	318	-	-	10/15/71/71	-
37	KC1	O	313	15	-	2/15/71/71	-
37	KC1	X	311	-	-	3/15/71/71	-
39	LMT	E	321	-	-	9/15/35/61	0/1/1/2
36	CLA	f	803	-	2/2/15/20	13/37/115/115	-
36	CLA	J	313	-	1/1/15/20	13/37/115/115	-
36	CLA	b	819	-	1/1/13/20	5/30/108/115	-
36	CLA	H	307	8	1/1/14/20	5/31/109/115	-
36	CLA	J	309	-	1/1/15/20	8/37/115/115	-
36	CLA	a	813	-	1/1/11/20	2/13/91/115	-
36	CLA	a	821	-	1/1/11/20	4/18/96/115	-
35	A86	R	303	-	-	7/34/90/90	0/3/3/3
37	KC1	B	310	2	-	3/15/71/71	-
36	CLA	K	307	-	2/2/14/20	21/33/111/115	-
37	KC1	E	309	-	-	5/15/71/71	-
42	LMG	G	324	-	-	31/50/70/70	0/1/1/1
36	CLA	P	318	-	1/1/12/20	7/21/99/115	-
35	A86	U	302	-	-	9/34/90/90	0/3/3/3
35	A86	J	301	-	-	11/34/90/90	0/3/3/3
35	A86	E	307	36	-	3/34/90/90	0/3/3/3
35	A86	N	304	-	-	8/34/90/90	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
36	CLA	a	807	20	1/1/15/20	13/37/115/115	-
36	CLA	Q	314	-	1/1/15/20	22/37/115/115	-
36	CLA	W	206	19	1/1/14/20	10/33/111/115	-
35	A86	O	319	35,36	-	8/34/90/90	0/3/3/3
39	LMT	U	314	-	-	14/21/61/61	0/2/2/2
39	LMT	h	205	-	-	10/21/61/61	0/2/2/2
37	KC1	D	314	4	-	5/15/71/71	-
35	A86	I	301	-	-	10/34/90/90	0/3/3/3
36	CLA	a	815	46	1/1/11/20	5/13/91/115	-
36	CLA	G	310	-	1/1/15/20	5/37/115/115	-
36	CLA	V	313	-	1/1/15/20	13/37/115/115	-
36	CLA	V	309	33	1/1/10/20	2/11/89/115	-
35	A86	V	304	-	-	9/34/90/90	0/3/3/3
34	DD6	a	849	-	-	6/26/80/80	0/3/3/3
36	CLA	S	310	17	1/1/15/20	14/37/115/115	-
36	CLA	P	302	-	-	5/10/88/115	-
41	LHG	O	318	15	-	30/53/53/53	-
36	CLA	a	828	-	1/1/15/20	20/37/115/115	-
36	CLA	U	308	35,32	1/1/13/20	10/27/105/115	-
36	CLA	b	817	-	2/2/13/20	9/30/108/115	-
36	CLA	V	307	-	1/1/12/20	5/21/99/115	-
42	LMG	I	315	-	-	32/50/70/70	0/1/1/1
36	CLA	E	313	-	2/2/15/20	8/37/115/115	-
36	CLA	a	811	-	1/1/12/20	6/24/102/115	-
42	LMG	G	325	-	-	27/50/70/70	0/1/1/1
36	CLA	S	315	17	1/1/10/20	3/11/89/115	-
35	A86	G	302	-	-	7/34/90/90	0/3/3/3
36	CLA	a	810	36	1/1/14/20	15/34/112/115	-
36	CLA	B	309	2	1/1/12/20	6/22/100/115	-
39	LMT	F	321	-	-	11/19/59/61	0/2/2/2
36	CLA	b	821	46	1/1/15/20	11/37/115/115	-
35	A86	U	301	-	-	8/34/90/90	0/3/3/3
35	A86	N	320	-	-	10/34/90/90	0/3/3/3
36	CLA	B	307	-	1/1/11/20	5/15/93/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
35	A86	C	203	-	-	8/34/90/90	1/3/3/3
36	CLA	F	314	6,35	1/1/15/20	14/37/115/115	-
36	CLA	S	321	-	-	10/22/100/115	-
36	CLA	f	805	25	1/1/12/20	9/22/100/115	-
36	CLA	N	313	14	1/1/10/20	2/8/86/115	-
37	KC1	L	317	-	-	3/15/71/71	-
42	LMG	V	316	-	-	24/41/61/70	0/1/1/1
39	LMT	a	853	-	-	10/18/58/61	0/2/2/2
42	LMG	J	319	-	-	23/39/59/70	0/1/1/1
34	DD6	A	303	-	-	5/26/80/80	0/3/3/3
35	A86	F	301	-	-	4/34/90/90	0/3/3/3
36	CLA	Q	312	-	1/1/10/20	3/8/86/115	-
40	DGD	b	849	-	-	21/49/89/95	0/2/2/2
36	CLA	D	310	-	1/1/15/20	9/37/115/115	-
35	A86	N	302	-	-	6/34/90/90	0/3/3/3
35	A86	K	301	-	-	6/34/90/90	1/3/3/3
35	A86	C	204	-	-	12/34/90/90	0/3/3/3
36	CLA	R	314	16	1/1/11/20	9/15/93/115	-
36	CLA	a	816	-	1/1/15/20	20/37/115/115	-
35	A86	V	303	35	-	8/34/90/90	0/3/3/3
36	CLA	R	320	16	1/1/11/20	3/13/91/115	-
36	CLA	a	831	-	1/1/15/20	14/37/115/115	-
36	CLA	N	316	14	1/1/15/20	11/37/115/115	-
36	CLA	b	825	-	1/1/15/20	13/37/115/115	-
35	A86	P	306	-	-	3/34/90/90	0/3/3/3
37	KC1	P	317	15	-	4/15/71/71	-
36	CLA	N	308	14	1/1/15/20	15/37/115/115	-
41	LHG	D	319	42	-	30/53/53/53	-
36	CLA	b	811	-	1/1/15/20	10/37/115/115	-
36	CLA	a	838	-	1/1/15/20	6/37/115/115	-
36	CLA	b	814	-	1/1/13/20	3/25/103/115	-
35	A86	U	304	37,32	-	11/34/90/90	0/3/3/3
36	CLA	b	828	-	1/1/15/20	14/37/115/115	-
36	CLA	C	214	-	1/1/10/20	2/8/86/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
34	DD6	O	304	-	-	5/26/80/80	0/3/3/3
36	CLA	H	316	-	1/1/15/20	16/37/115/115	-
36	CLA	a	809	-	1/1/13/20	9/27/105/115	-
41	LHG	G	320	-	-	18/44/44/53	-
36	CLA	A	311	-	1/1/15/20	18/37/115/115	-
36	CLA	a	839	46	1/1/15/20	15/37/115/115	-
39	LMT	K	318	-	-	12/21/61/61	0/2/2/2
36	CLA	E	312	-	1/1/15/20	15/37/115/115	-
36	CLA	A	310	-	1/1/15/20	11/37/115/115	-
36	CLA	S	317	-	1/1/10/20	3/8/86/115	-
36	CLA	X	308	19	1/1/11/20	10/16/94/115	-
35	A86	G	306	-	-	6/34/90/90	1/3/3/3
44	BCR	h	201	-	-	9/29/63/63	0/2/2/2
34	DD6	D	301	-	-	11/26/80/80	0/3/3/3
36	CLA	M	312	13,36	1/1/11/20	10/16/94/115	-
44	BCR	i	101	-	-	2/29/63/63	0/2/2/2
35	A86	h	202	-	-	3/34/90/90	1/3/3/3
36	CLA	L	320	12	1/1/15/20	11/37/115/115	-
36	CLA	N	310	14	1/1/10/20	1/8/86/115	-
36	CLA	O	316	-	1/1/15/20	26/37/115/115	-
36	CLA	O	312	-	-	4/8/82/115	-
36	CLA	M	315	13	-	6/16/94/115	-
36	CLA	N	312	-	1/1/11/20	7/16/94/115	-
36	CLA	N	315	-	-	0/8/86/115	-
34	DD6	j	103	-	-	9/26/80/80	0/3/3/3
35	A86	K	303	-	-	5/34/90/90	0/3/3/3
35	A86	Q	301	-	-	6/34/90/90	0/3/3/3
35	A86	S	301	-	-	8/34/90/90	0/3/3/3
44	BCR	a	847	-	-	6/29/63/63	0/2/2/2
35	A86	T	306	-	-	6/34/90/90	0/3/3/3
36	CLA	b	818	-	-	4/25/103/115	-
36	CLA	J	308	-	-	12/33/111/115	-
41	LHG	R	323	-	-	29/53/53/53	-
35	A86	G	305	-	-	4/34/90/90	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
36	CLA	K	315	-	1/1/10/20	3/8/86/115	-
36	CLA	T	313	18	1/1/15/20	8/37/115/115	-
36	CLA	A	314	-	1/1/15/20	20/37/115/115	-
36	CLA	R	311	16	1/1/15/20	13/37/115/115	-
35	A86	X	305	-	-	8/34/90/90	0/3/3/3
41	LHG	b	850	36	-	27/53/53/53	-
39	LMT	b	848	-	-	12/21/61/61	0/2/2/2
36	CLA	U	309	32	-	4/15/93/115	-
36	CLA	a	835	-	1/1/12/20	1/21/99/115	-
35	A86	J	305	-	-	6/34/90/90	0/3/3/3
35	A86	Q	304	-	-	10/34/90/90	0/3/3/3
41	LHG	j	104	-	-	32/53/53/53	-
36	CLA	a	824	-	1/1/15/20	11/37/115/115	-
36	CLA	L	311	-	1/1/15/20	14/37/115/115	-
34	DD6	D	304	-	-	8/26/80/80	0/3/3/3
36	CLA	b	808	-	1/1/15/20	12/37/115/115	-
44	BCR	l	207	-	-	7/29/63/63	0/2/2/2
35	A86	A	302	-	-	9/34/90/90	0/3/3/3
36	CLA	V	314	-	1/1/15/20	17/37/115/115	-
36	CLA	b	809	-	1/1/15/20	16/37/115/115	-
36	CLA	b	813	-	1/1/13/20	3/25/101/115	-
36	CLA	H	310	8	1/1/11/20	5/15/93/115	-
36	CLA	O	309	-	1/1/15/20	17/37/115/115	-
36	CLA	J	312	10	1/1/15/20	10/37/115/115	-
36	CLA	M	311	13,35	1/1/15/20	10/37/115/115	-
36	CLA	R	322	16	1/1/12/20	11/22/100/115	-
36	CLA	H	312	8	1/1/15/20	17/37/115/115	-
34	DD6	B	302	-	-	4/26/80/80	0/3/3/3
34	DD6	I	303	-	-	4/26/80/80	0/3/3/3
35	A86	B	301	-	-	10/34/90/90	0/3/3/3
36	CLA	a	837	-	1/1/15/20	10/37/115/115	-
35	A86	X	304	19	-	7/34/90/90	0/3/3/3
39	LMT	G	323	-	-	16/21/61/61	0/2/2/2
41	LHG	G	301	-	-	24/53/53/53	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
41	LHG	D	318	36	-	30/50/50/53	-
41	LHG	E	322	-	-	28/53/53/53	-
36	CLA	A	309	1	1/1/11/20	7/15/93/115	-
36	CLA	K	311	-	1/1/11/20	6/15/93/115	-
36	CLA	W	207	34	1/1/15/20	15/37/115/115	-
36	CLA	l	204	28	-	8/18/96/115	-
36	CLA	T	316	-	1/1/10/20	0/8/86/115	-
36	CLA	A	307	-	1/1/14/20	10/31/109/115	-
36	CLA	a	832	-	1/1/15/20	14/37/115/115	-
36	CLA	B	311	2	1/1/13/20	13/25/103/115	-
39	LMT	F	320	-	-	12/21/61/61	0/2/2/2
36	CLA	F	317	6	2/2/13/20	10/27/105/115	-
36	CLA	X	306	-	1/1/14/20	9/33/111/115	-
36	CLA	D	313	-	1/1/15/20	8/37/115/115	-
35	A86	X	301	-	-	8/34/90/90	0/3/3/3
36	CLA	C	205	-	1/1/10/20	2/11/89/115	-
36	CLA	C	211	-	1/1/15/20	11/37/115/115	-
42	LMG	m	102	-	-	14/32/52/70	0/1/1/1
36	CLA	S	314	17	-	9/37/115/115	-
39	LMT	B	312	-	-	14/21/61/61	0/2/2/2
42	LMG	j	105	-	-	31/47/67/70	0/1/1/1
44	BCR	b	843	-	-	9/29/63/63	0/2/2/2
36	CLA	O	310	15	1/1/11/20	7/15/93/115	-
35	A86	H	301	-	-	5/34/90/90	0/3/3/3
36	CLA	Q	310	15	-	20/37/115/115	-
36	CLA	a	817	-	1/1/15/20	15/37/115/115	-
36	CLA	O	307	-	1/1/15/20	14/37/115/115	-
37	KC1	M	317	-	-	3/15/71/71	-
36	CLA	R	319	16	1/1/11/20	5/13/91/115	-
37	KC1	H	313	-	-	6/15/71/71	-
36	CLA	b	826	21,46	1/1/14/20	10/36/114/115	-
36	CLA	T	312	18	1/1/11/20	5/15/93/115	-
36	CLA	J	311	-	1/1/11/20	3/15/93/115	-
36	CLA	N	318	-	1/1/11/20	5/16/94/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
44	BCR	a	844	-	-	6/29/63/63	0/2/2/2
39	LMT	P	321	-	-	10/14/34/61	0/1/1/2
36	CLA	W	216	35,19	1/1/11/20	3/13/91/115	-
36	CLA	H	309	8	1/1/15/20	15/37/115/115	-
36	CLA	H	311	-	1/1/15/20	9/37/115/115	-
36	CLA	B	306	-	1/1/11/20	4/15/93/115	-
36	CLA	I	309	9	1/1/11/20	6/15/93/115	-
36	CLA	V	310	33	1/1/15/20	8/37/115/115	-
36	CLA	E	317	-	1/1/11/20	5/15/93/115	-
36	CLA	K	309	-	1/1/13/20	12/30/108/115	-
44	BCR	m	101	-	-	9/29/63/63	0/2/2/2
36	CLA	V	306	33	1/1/15/20	19/37/115/115	-
34	DD6	L	305	-	-	7/26/80/80	0/3/3/3
36	CLA	a	814	-	1/1/12/20	2/19/97/115	-
35	A86	P	307	-	-	2/34/90/90	0/3/3/3
35	A86	S	308	37	-	12/34/90/90	0/3/3/3
35	A86	X	302	35	-	6/34/90/90	0/3/3/3
36	CLA	a	802	-	2/2/15/20	11/37/115/115	-
37	KC1	C	213	-	-	6/15/71/71	-
36	CLA	b	801	46	1/1/15/20	8/37/115/115	-
36	CLA	l	202	28	1/1/15/20	11/37/115/115	-
36	CLA	I	306	9	2/2/15/20	15/37/115/115	-
34	DD6	E	301	-	-	4/26/80/80	0/3/3/3
35	A86	M	302	-	-	7/34/90/90	0/3/3/3
41	LHG	a	842	-	-	24/52/52/53	-
34	DD6	A	304	-	-	4/26/80/80	0/3/3/3
35	A86	O	303	-	-	6/34/90/90	0/3/3/3
36	CLA	a	808	20	1/1/15/20	9/37/115/115	-
34	DD6	C	201	-	-	7/26/80/80	0/3/3/3
34	DD6	D	305	-	-	3/26/80/80	0/3/3/3
35	A86	D	302	-	-	7/34/90/90	0/3/3/3
36	CLA	i	102	26	1/1/15/20	20/37/115/115	-
35	A86	J	303	-	-	7/34/90/90	0/3/3/3
36	CLA	D	311	-	-	5/15/93/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
36	CLA	W	214	19	-	3/8/86/115	-
36	CLA	Q	305	-	1/1/14/20	9/33/111/115	-
43	PQN	a	840	-	-	7/23/43/43	0/2/2/2
35	A86	F	304	36	-	4/34/90/90	0/3/3/3
36	CLA	Q	308	-	1/1/15/20	18/37/115/115	-
36	CLA	S	320	-	-	16/37/115/115	-
38	SQD	A	315	-	-	11/22/42/69	0/1/1/1
40	DGD	L	302	42	-	21/36/76/95	0/2/2/2
36	CLA	b	839	-	1/1/15/20	4/37/115/115	-
34	DD6	F	303	-	-	8/26/80/80	0/3/3/3
34	DD6	R	308	-	-	10/26/80/80	0/3/3/3
36	CLA	F	309	-	1/1/15/20	13/37/115/115	-
37	KC1	A	312	1	-	2/15/71/71	-
36	CLA	b	830	-	1/1/15/20	5/37/115/115	-
36	CLA	R	318	35	1/1/10/20	2/8/86/115	-
35	A86	R	302	16	-	6/34/90/90	0/3/3/3
35	A86	L	319	-	-	9/34/90/90	0/3/3/3
36	CLA	a	822	-	1/1/12/20	4/21/99/115	-
35	A86	I	304	-	-	9/34/90/90	0/3/3/3
41	LHG	f	808	25	-	29/53/53/53	-
36	CLA	V	305	35	1/1/14/20	11/33/111/115	-
35	A86	L	306	37	-	10/34/90/90	0/3/3/3
36	CLA	T	314	-	1/1/15/20	15/37/115/115	-
37	KC1	G	318	-	-	5/15/71/71	-
36	CLA	M	314	-	1/1/10/20	2/8/86/115	-
36	CLA	I	313	-	1/1/10/20	3/8/86/115	-
36	CLA	F	313	-	1/1/12/20	6/22/100/115	-
36	CLA	b	836	-	1/1/13/20	8/29/107/115	-
36	CLA	M	316	36	1/1/10/20	4/10/88/115	-
35	A86	N	306	-	-	8/34/90/90	0/3/3/3
36	CLA	a	805	20	1/1/15/20	16/37/115/115	-
36	CLA	O	311	-	1/1/13/20	9/29/107/115	-
36	CLA	P	311	-	1/1/15/20	17/37/115/115	-
36	CLA	D	316	-	1/1/12/20	9/22/100/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
35	A86	Q	316	15,36	-	2/34/90/90	0/3/3/3
36	CLA	E	311	-	1/1/15/20	16/37/115/115	-
36	CLA	P	308	-	1/1/14/20	9/33/111/115	-
36	CLA	H	306	-	1/1/14/20	6/33/111/115	-
39	LMT	a	851	-	-	15/21/61/61	0/2/2/2
36	CLA	D	307	41	1/1/14/20	17/33/111/115	-
36	CLA	D	315	-	1/1/10/20	2/8/86/115	-
39	LMT	E	320	-	-	13/21/61/61	0/2/2/2
36	CLA	M	307	-	1/1/15/20	12/37/115/115	-
36	CLA	H	305	8	1/1/11/20	8/17/95/115	-
36	CLA	R	312	-	1/1/15/20	12/37/115/115	-
40	DGD	C	215	-	-	31/46/86/95	0/2/2/2
36	CLA	b	815	-	1/1/15/20	19/37/115/115	-
36	CLA	W	211	19	1/1/15/20	8/37/115/115	-
36	CLA	M	309	-	1/1/15/20	13/37/115/115	-
36	CLA	W	208	-	1/1/11/20	5/13/91/115	-
36	CLA	I	308	9	1/1/15/20	19/37/115/115	-
37	KC1	R	317	-	-	3/15/71/71	-
36	CLA	G	311	-	1/1/15/20	17/37/115/115	-
36	CLA	E	316	-	1/1/15/20	17/37/115/115	-
36	CLA	K	308	-	1/1/15/20	11/37/115/115	-
37	KC1	O	315	15	-	2/15/71/71	-
36	CLA	O	314	-	1/1/10/20	3/8/86/115	-
39	LMT	I	318	-	-	17/21/61/61	0/2/2/2
36	CLA	b	824	-	1/1/12/20	12/23/101/115	-
42	LMG	a	852	-	-	26/49/69/70	0/1/1/1
36	CLA	H	308	8	1/1/15/20	15/35/113/115	-
36	CLA	R	315	-	1/1/15/20	11/37/115/115	-
36	CLA	L	316	-	1/1/10/20	1/8/86/115	-
37	KC1	J	314	-	-	4/15/71/71	-
36	CLA	b	822	-	1/1/11/20	5/15/93/115	-
36	CLA	G	316	-	1/1/11/20	8/18/96/115	-
36	CLA	j	106	27	1/1/10/20	6/10/88/115	-
37	KC1	F	315	-	-	3/15/71/71	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
35	A86	R	305	-	-	5/34/90/90	0/3/3/3
36	CLA	G	315	-	2/2/13/20	11/27/105/115	-
35	A86	T	303	-	-	6/34/90/90	0/3/3/3
36	CLA	L	310	-	1/1/12/20	2/24/102/115	-
41	LHG	O	317	-	-	33/46/46/53	-
36	CLA	j	101	27	1/1/15/20	17/37/115/115	-
41	LHG	Q	315	36	-	33/53/53/53	-
36	CLA	S	313	-	1/1/11/20	6/15/93/115	-
36	CLA	P	310	15,41	1/1/15/20	11/37/115/115	-
36	CLA	S	318	-	1/1/10/20	7/10/88/115	-
34	DD6	J	304	-	-	5/26/80/80	0/3/3/3
34	DD6	W	205	-	-	8/26/80/80	0/3/3/3
35	A86	F	307	-	-	6/34/90/90	0/3/3/3
44	BCR	l	203	-	-	10/29/63/63	0/2/2/2
36	CLA	N	307	-	1/1/14/20	7/33/111/115	-
35	A86	R	304	16,36	-	8/34/90/90	0/3/3/3
44	BCR	b	846	-	-	8/29/63/63	0/2/2/2
36	CLA	b	840	-	1/1/15/20	12/37/115/115	-
36	CLA	A	306	-	2/2/14/20	19/33/111/115	-
35	A86	X	314	19	-	3/34/90/90	1/3/3/3
37	KC1	S	316	-	-	6/15/71/71	-
35	A86	F	302	-	-	8/34/90/90	0/3/3/3
36	CLA	I	312	9	1/1/12/20	4/22/100/115	-
35	A86	M	305	-	-	8/34/90/90	0/3/3/3
37	KC1	G	308	-	-	5/15/71/71	-
44	BCR	a	845	-	-	9/29/63/63	0/2/2/2
37	KC1	P	315	35	-	2/15/71/71	-
39	LMT	P	320	-	-	8/14/34/61	0/1/1/2
35	A86	V	302	-	-	5/34/90/90	0/3/3/3
42	LMG	h	206	-	-	24/40/60/70	0/1/1/1
36	CLA	U	313	-	1/1/10/20	2/8/86/115	-
36	CLA	S	312	17	-	17/37/115/115	-
36	CLA	K	310	-	2/2/14/20	14/34/112/115	-
36	CLA	j	102	-	1/1/15/20	13/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
36	CLA	R	310	-	1/1/14/20	16/33/111/115	-
36	CLA	G	312	7	1/1/13/20	4/29/107/115	-
36	CLA	N	319	14	1/1/10/20	3/10/88/115	-
37	KC1	L	315	12,35	-	6/15/71/71	-
44	BCR	b	844	-	-	6/29/63/63	0/2/2/2
36	CLA	V	308	-	1/1/15/20	18/37/115/115	-
36	CLA	D	317	-	1/1/13/20	10/29/107/115	-
39	LMT	E	323	-	-	11/21/61/61	0/2/2/2
36	CLA	X	312	-	1/1/10/20	3/8/86/115	-
35	A86	J	306	-	-	10/34/90/90	0/3/3/3
35	A86	S	302	-	-	6/34/90/90	0/3/3/3
36	CLA	b	806	-	1/1/15/20	14/37/115/115	-
36	CLA	a	823	-	2/2/13/20	10/25/103/115	-
36	CLA	h	203	-	1/1/15/20	20/37/115/115	-
36	CLA	W	201	19	1/1/11/20	2/17/95/115	-
36	CLA	M	310	13,35	1/1/11/20	5/15/93/115	-
36	CLA	T	309	18	1/1/15/20	18/37/115/115	-
35	A86	H	304	-	-	8/34/90/90	0/3/3/3
34	DD6	Q	302	-	-	8/26/80/80	0/3/3/3
35	A86	M	301	-	-	8/34/90/90	0/3/3/3
35	A86	N	305	-	-	2/34/90/90	0/3/3/3
37	KC1	N	314	14	-	7/15/71/71	-
37	KC1	W	213	-	-	5/15/71/71	-
34	DD6	S	307	-	-	6/26/80/80	0/3/3/3
36	CLA	f	802	-	1/1/15/20	16/37/115/115	-
35	A86	W	203	36	-	6/34/90/90	0/3/3/3
34	DD6	E	303	-	-	7/26/80/80	0/3/3/3
34	DD6	H	303	-	-	6/26/80/80	0/3/3/3
36	CLA	F	312	-	1/1/15/20	20/37/115/115	-
45	SF4	c	101	22	-	-	0/6/5/5
36	CLA	a	818	-	1/1/15/20	14/37/115/115	-
34	DD6	K	305	-	-	0/26/80/80	0/3/3/3
34	DD6	M	303	-	-	3/26/80/80	0/3/3/3
35	A86	G	304	-	-	8/34/90/90	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
36	CLA	a	803	36	1/1/13/20	5/25/103/115	-
36	CLA	C	212	35	1/1/15/20	23/37/115/115	-
35	A86	K	302	-	-	8/34/90/90	0/3/3/3
36	CLA	C	209	-	1/1/15/20	10/37/115/115	-
36	CLA	B	305	2	1/1/15/20	24/37/115/115	-
36	CLA	a	834	20	1/1/11/20	5/13/91/115	-
36	CLA	B	308	-	1/1/15/20	14/37/115/115	-
36	CLA	I	314	-	1/1/10/20	0/8/86/115	-
39	LMT	K	317	-	-	14/17/57/61	0/2/2/2
36	CLA	M	308	-	1/1/12/20	5/22/100/115	-
36	CLA	N	317	14	1/1/12/20	8/24/102/115	-
35	A86	T	307	-	-	9/34/90/90	0/3/3/3
35	A86	R	301	-	-	9/34/90/90	0/3/3/3
36	CLA	E	314	-	1/1/15/20	8/37/115/115	-
36	CLA	J	310	-	1/1/15/20	11/37/115/115	-
36	CLA	U	310	-	1/1/15/20	17/37/115/115	-
36	CLA	a	826	-	1/1/15/20	12/37/115/115	-
36	CLA	H	314	-	1/1/10/20	3/8/86/115	-
35	A86	F	305	-	-	8/34/90/90	0/3/3/3
35	A86	L	301	-	-	5/34/90/90	1/3/3/3
35	A86	T	305	18	-	7/34/90/90	0/3/3/3
37	KC1	T	315	-	-	7/15/71/71	-
35	A86	U	303	36	-	17/34/90/90	0/3/3/3
37	KC1	V	312	33	-	7/15/71/71	-
36	CLA	K	313	-	1/1/15/20	13/37/115/115	-
36	CLA	U	307	-	1/1/12/20	1/19/97/115	-
36	CLA	I	310	35	1/1/15/20	10/37/115/115	-
36	CLA	X	310	19	1/1/10/20	2/8/86/115	-
37	KC1	M	313	13,36	-	5/15/71/71	-
36	CLA	P	309	41	1/1/15/20	14/37/115/115	-
35	A86	N	301	-	-	8/34/90/90	0/3/3/3
35	A86	S	304	-	-	9/34/90/90	0/3/3/3
36	CLA	I	311	9	1/1/15/20	17/37/115/115	-
36	CLA	W	212	19	-	15/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
36	CLA	W	209	19	1/1/13/20	13/28/106/115	-
34	DD6	A	301	-	-	7/26/80/80	0/3/3/3
35	A86	C	202	3,36	-	8/34/90/90	0/3/3/3
41	LHG	a	850	-	-	36/51/51/53	-
37	KC1	Q	311	15	-	2/15/71/71	-
43	PQN	b	842	-	-	11/23/43/43	0/2/2/2
36	CLA	S	309	-	1/1/14/20	8/33/111/115	-
36	CLA	S	311	35	1/1/11/20	2/15/93/115	-
35	A86	R	309	-	-	8/34/90/90	0/3/3/3
35	A86	S	303	17	-	4/34/90/90	0/3/3/3
36	CLA	G	309	7	1/1/15/20	13/37/115/115	-
41	LHG	a	843	36	-	10/31/31/53	-
41	LHG	F	318	-	-	15/34/34/53	-
36	CLA	X	309	19	-	6/13/91/115	-
35	A86	T	301	36	-	4/34/90/90	1/3/3/3
36	CLA	G	307	-	-	2/9/87/115	-
36	CLA	b	834	-	1/1/15/20	10/37/115/115	-
39	LMT	B	313	-	-	16/21/61/61	0/2/2/2
35	A86	h	204	-	-	1/34/90/90	0/3/3/3
36	CLA	X	307	35,19	-	6/19/97/115	-
41	LHG	f	809	-	-	28/46/46/53	-
36	CLA	b	838	-	1/1/11/20	3/16/94/115	-
35	A86	W	202	19,36	-	8/34/90/90	0/3/3/3

The worst 5 of 4148 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	M	318	KC1	C4C-NC	17.10	1.63	1.37
36	Q	310	CLA	CAA-C2A	15.78	1.83	1.54
37	M	318	KC1	C1A-NA	15.77	1.68	1.38
37	T	310	KC1	C1A-NA	14.39	1.66	1.38
36	X	308	CLA	C4B-NB	13.90	1.47	1.35

The worst 5 of 7259 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	N	304	A86	O1-C20-C21	-47.08	58.64	115.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	Q	314	CLA	C4-C3-C5	-24.40	74.22	115.27
42	V	315	LMG	O7-C10-C11	22.29	159.53	111.50
35	A	302	A86	C33-C32-C31	-21.39	88.43	109.21
36	N	319	CLA	CHD-C1D-ND	-21.33	104.86	124.45

5 of 321 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
36	A	305	CLA	ND
36	A	306	CLA	C8
36	A	306	CLA	ND
36	A	307	CLA	ND
36	A	308	CLA	ND

5 of 5822 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
34	A	301	DD6	C10-C11-C13-C14
34	A	301	DD6	C12-C11-C13-C14
34	A	301	DD6	C13-C14-C15-C20
34	A	301	DD6	C13-C14-C15-O1
34	A	303	DD6	C10-C11-C13-C14

5 of 11 ring outliers are listed below:

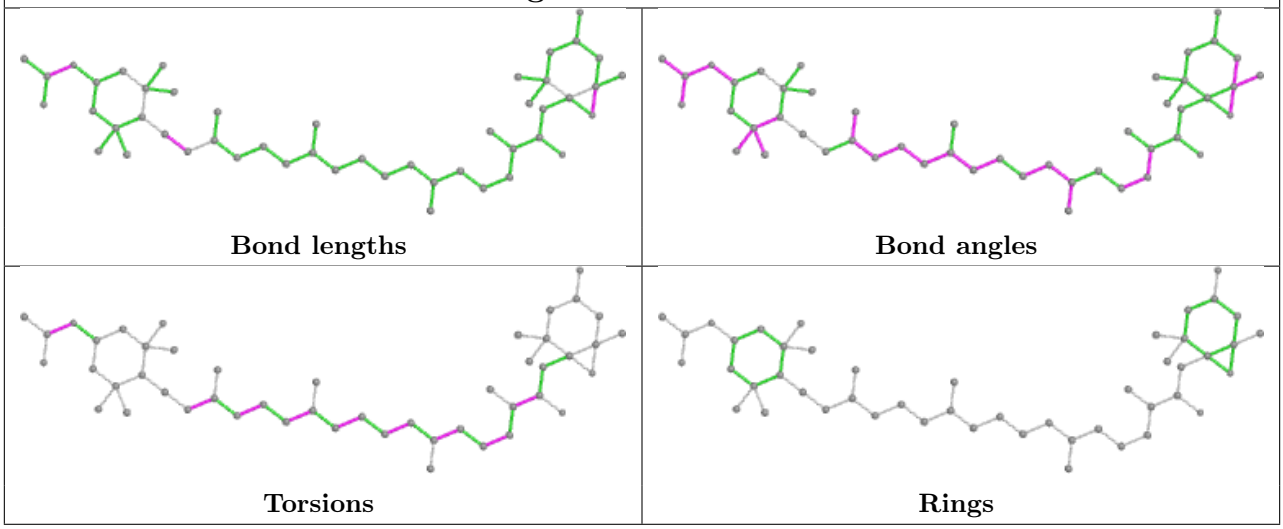
Mol	Chain	Res	Type	Atoms
35	V	301	A86	C31-C32-C33-C34-C35-C36
35	J	302	A86	C31-C32-C33-C34-C35-C36
35	K	301	A86	C31-C32-C33-C34-C35-C36
35	G	306	A86	C31-C32-C33-C34-C35-C36
35	T	301	A86	C31-C32-C33-C34-C35-C36

No monomer is involved in short contacts.

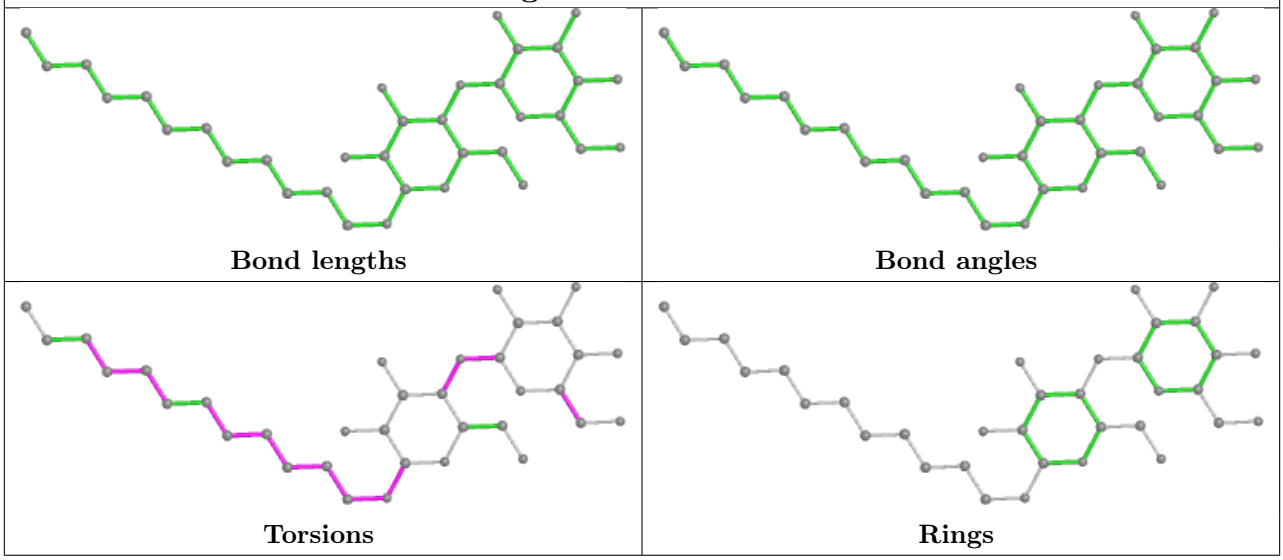
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

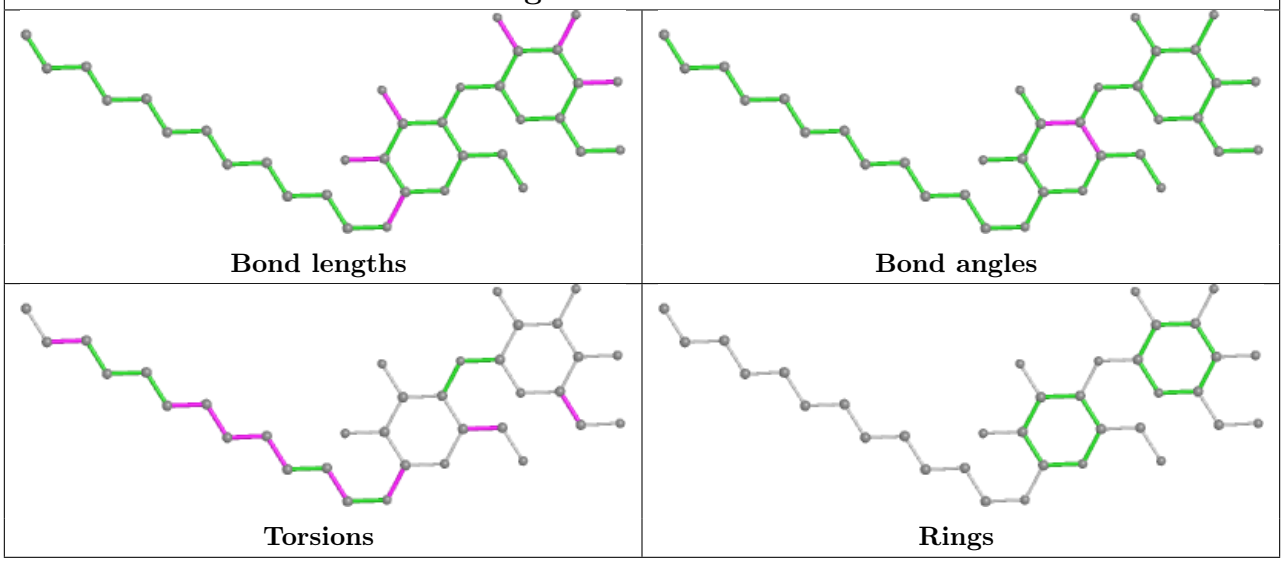
Ligand A86 M 304



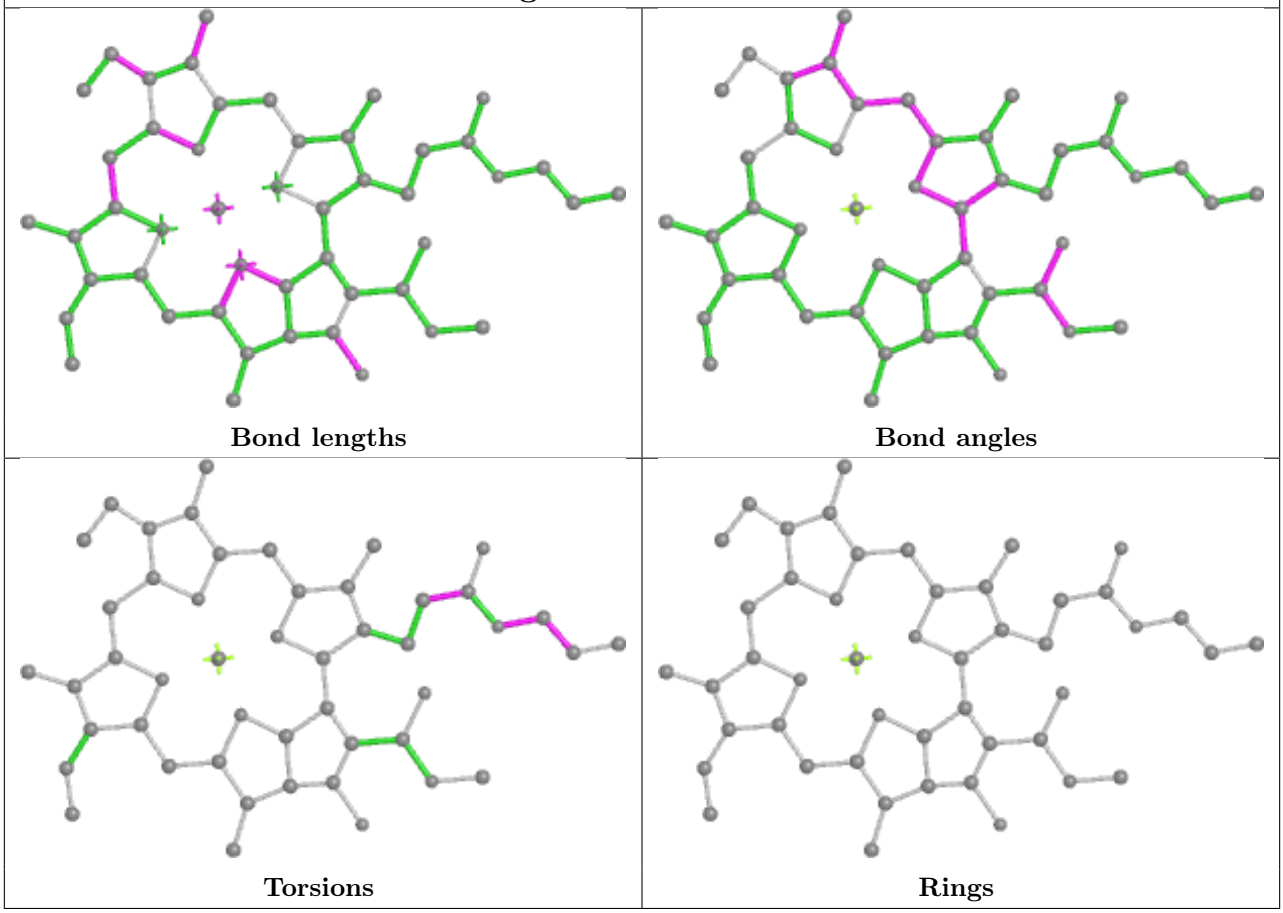
Ligand LMT G 322



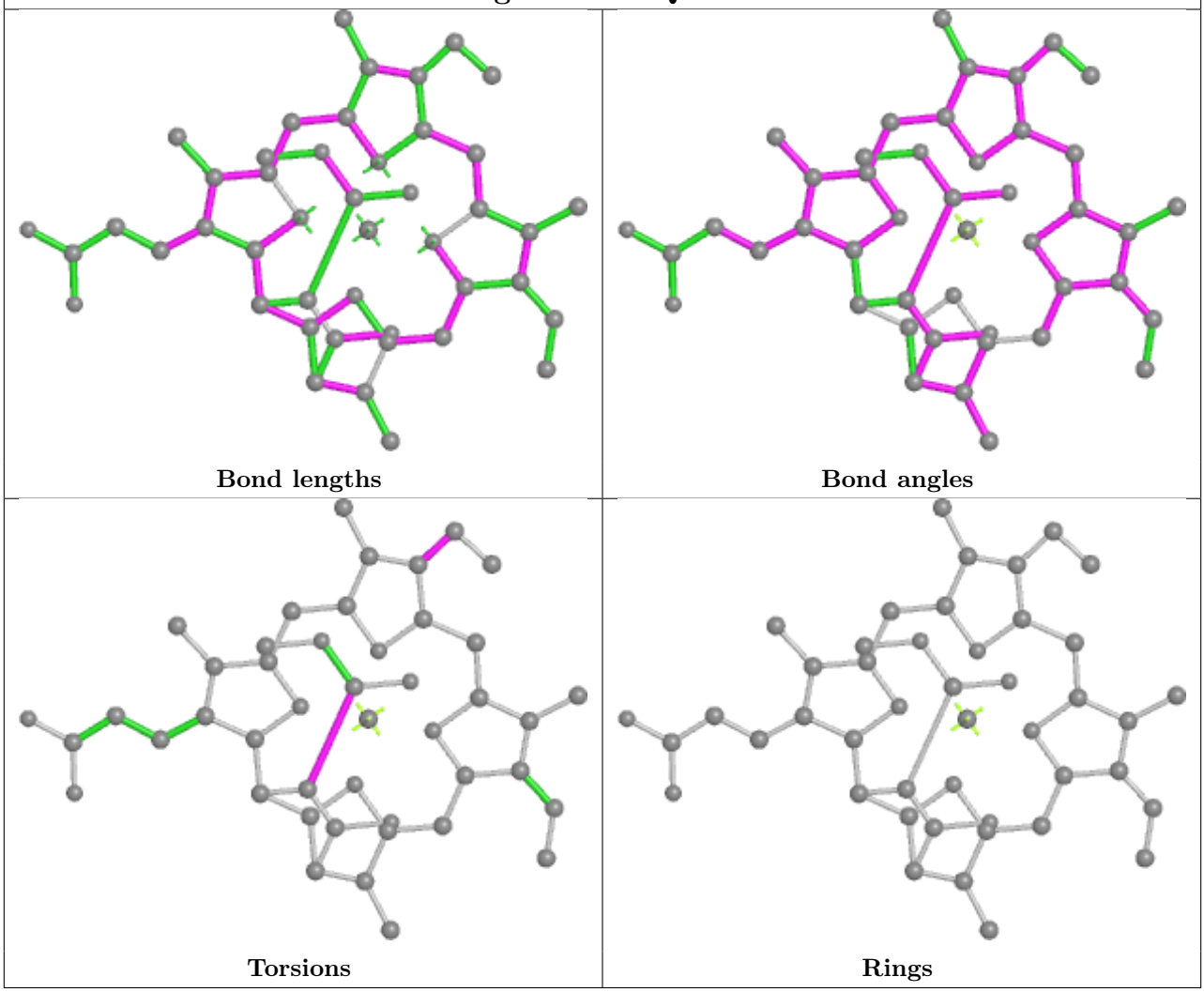
Ligand LMT L 303



Ligand CLA W 215



Ligand KC1 Q 313



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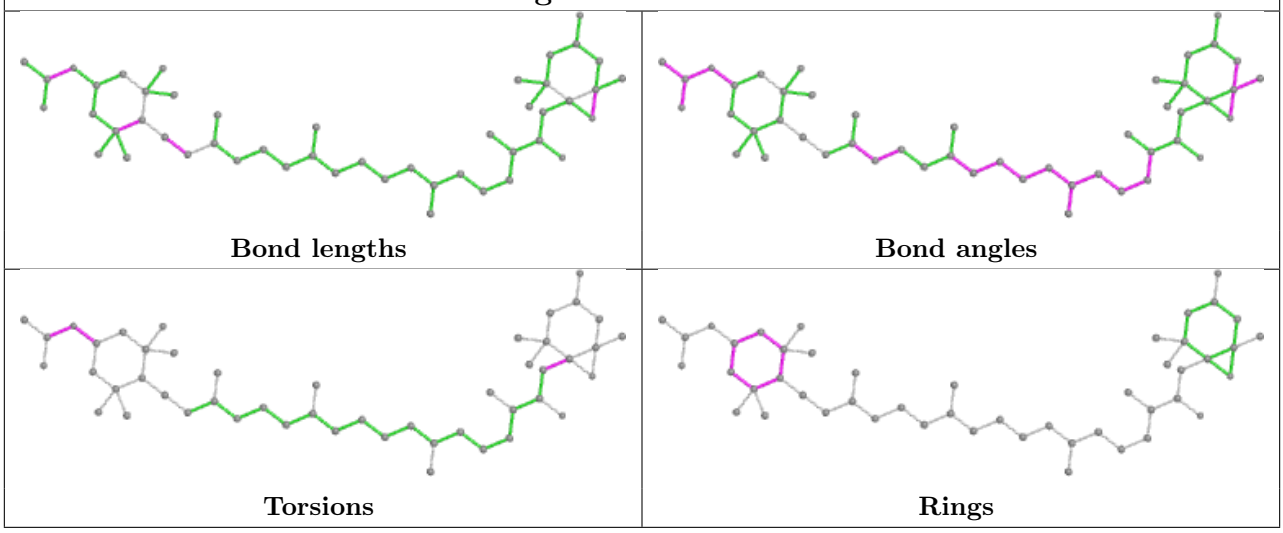

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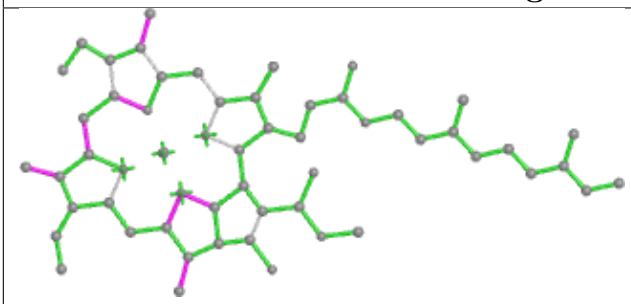
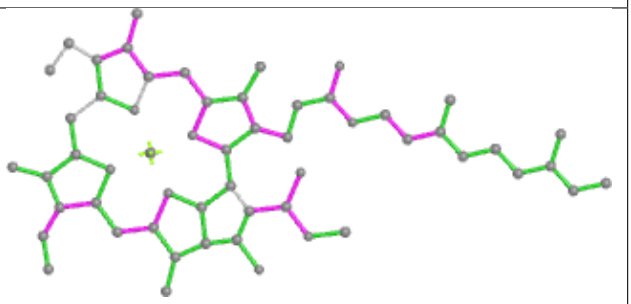
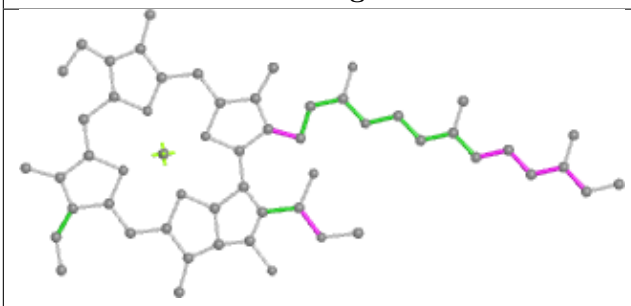
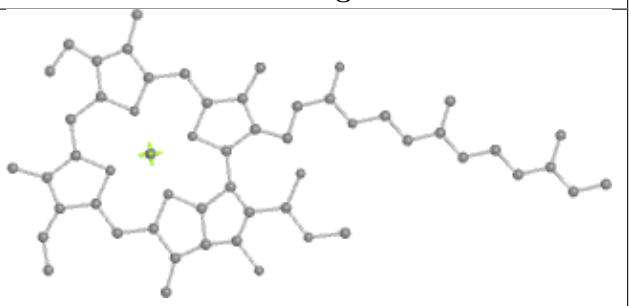
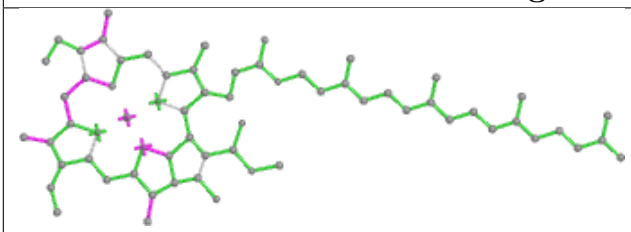
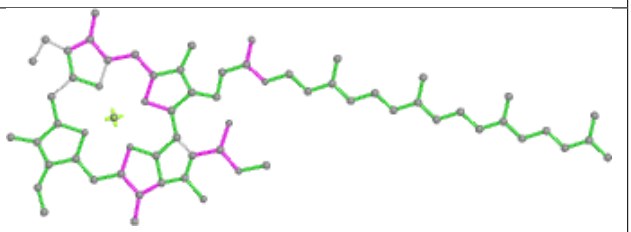
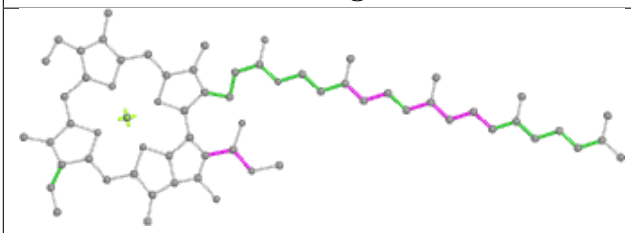
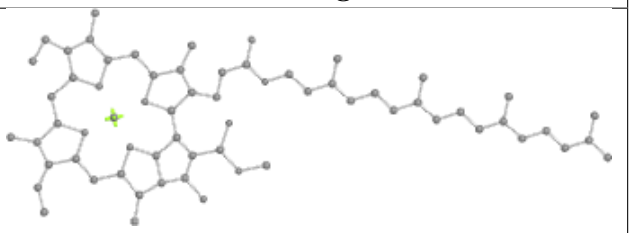
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA a 829	
 Bond lengths	 Bond angles
 Torsions	 Rings

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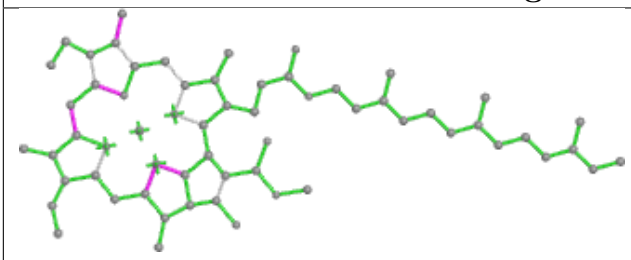
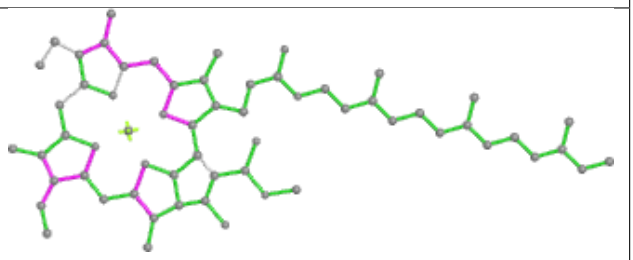
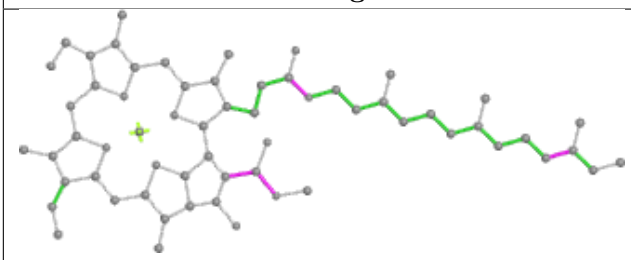
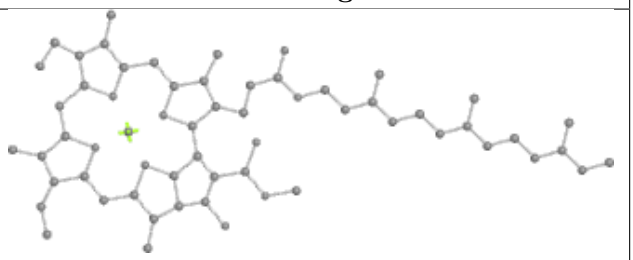
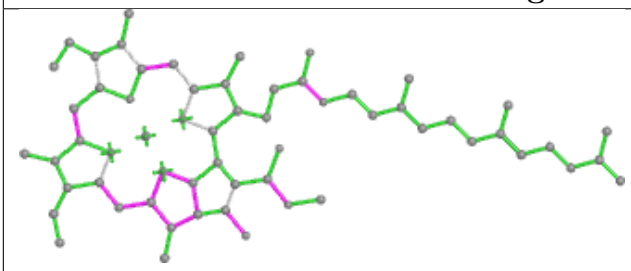
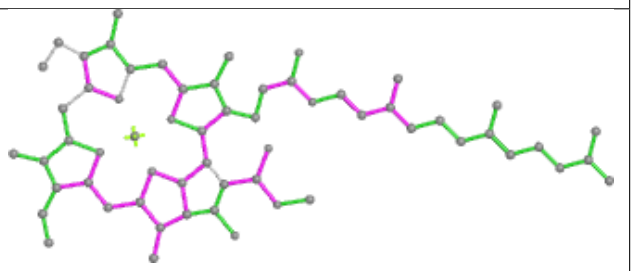
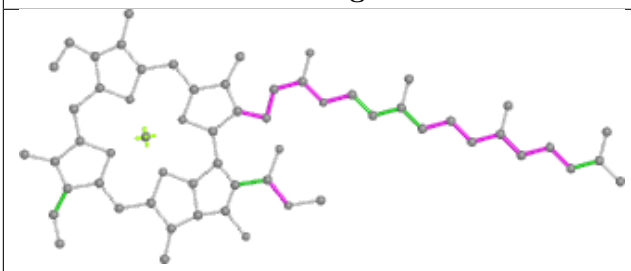
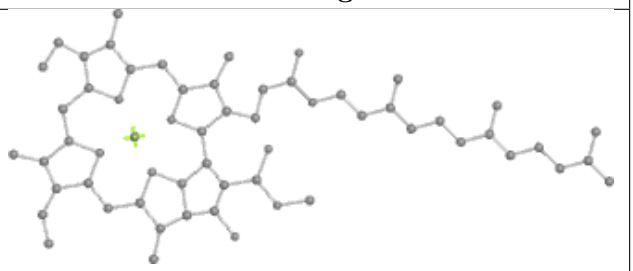
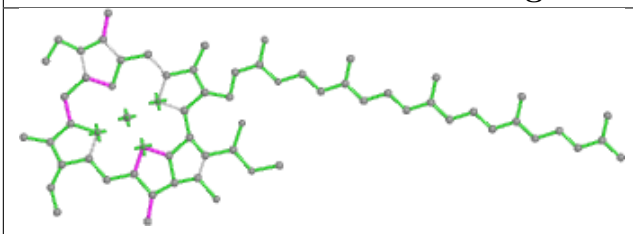
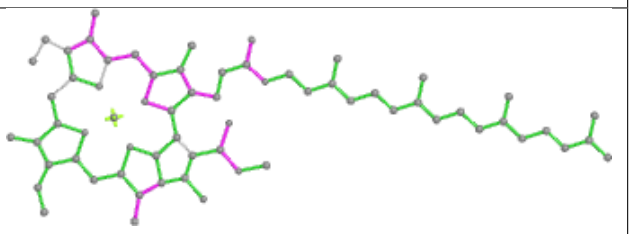
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA b 816	
 Bond lengths	 Bond angles
 Torsions	 Rings

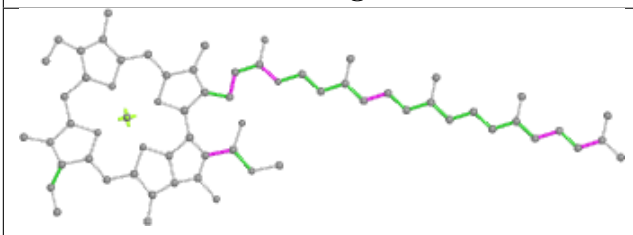
Ligand CLA E 310



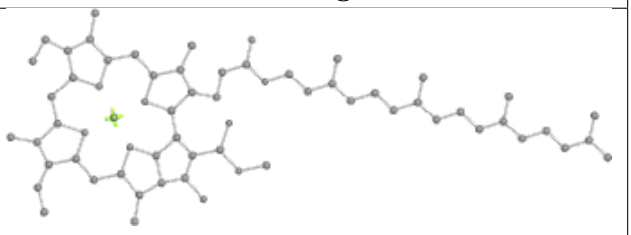
Bond lengths



Bond angles

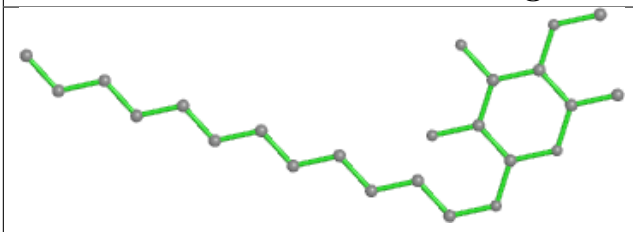


Torsions

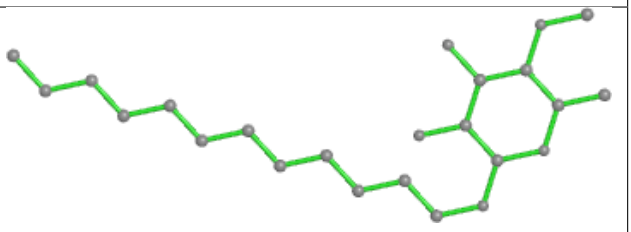


Rings

Ligand LMT b 851



Bond lengths



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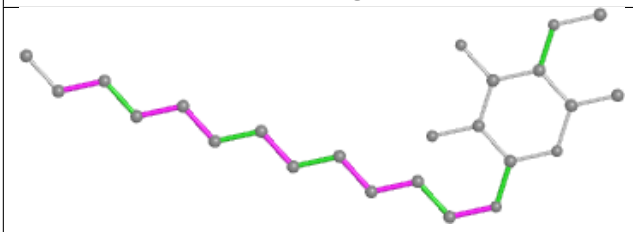
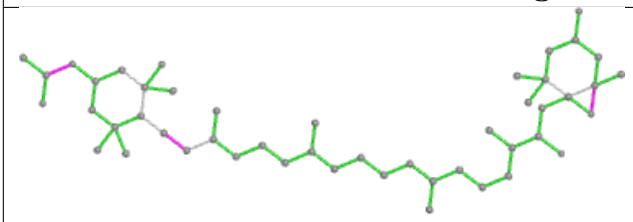


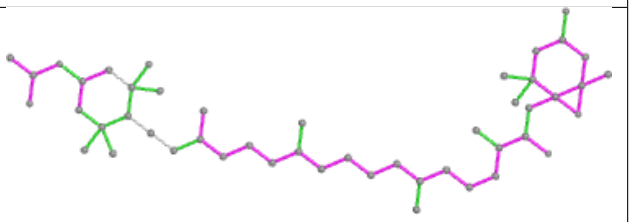
Torsions

Rings

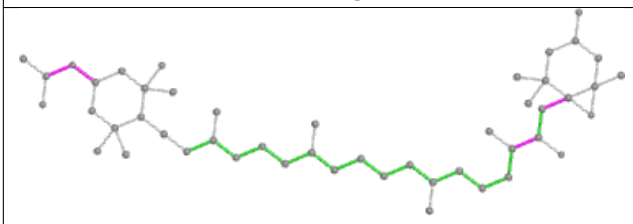
Ligand A86 S 305



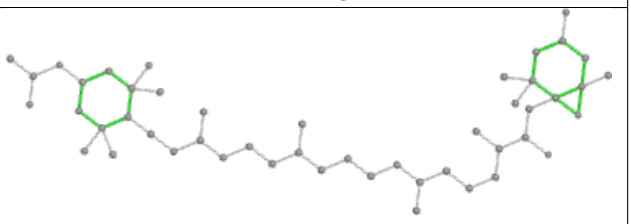
Bond lengths



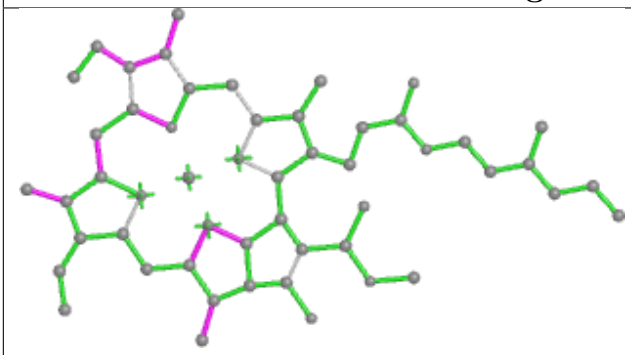
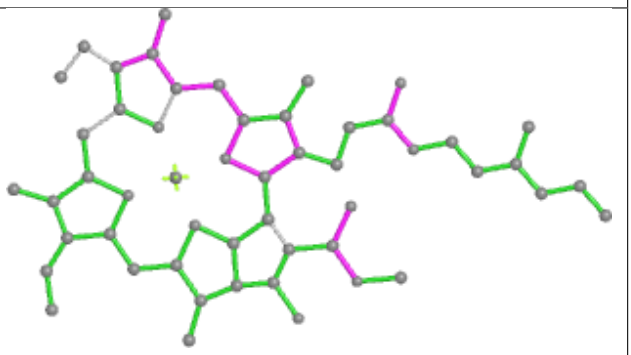
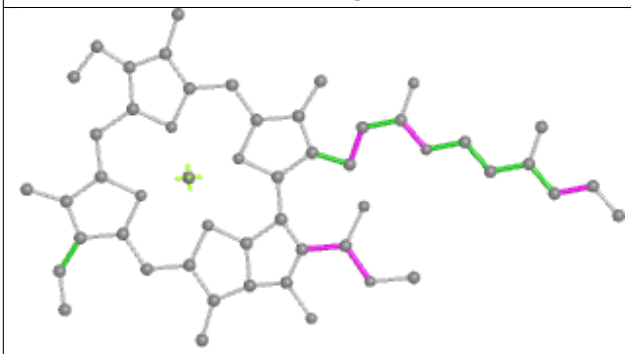
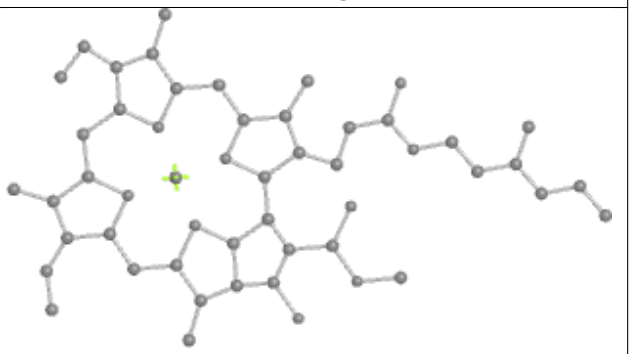
Bond angles



Torsions



Rings

Ligand CLA F 311	
 Bond lengths	 Bond angles
 Torsions	 Rings

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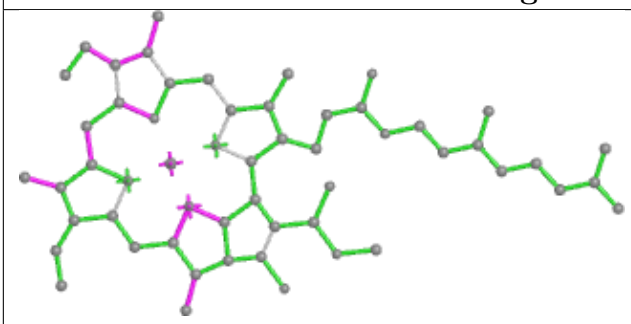
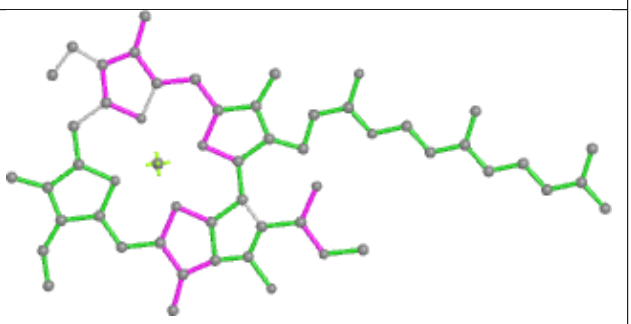
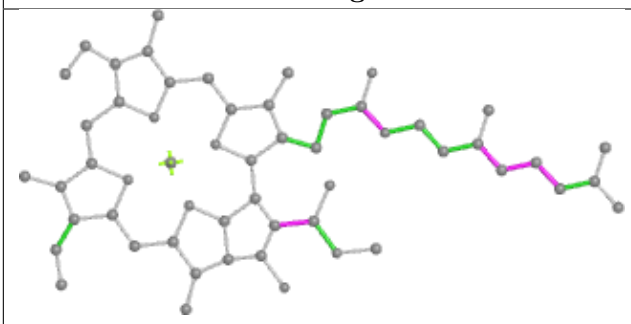
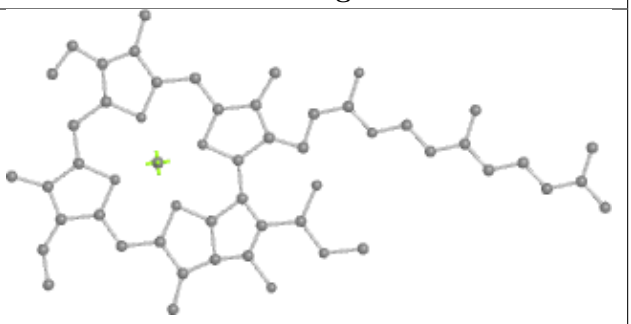
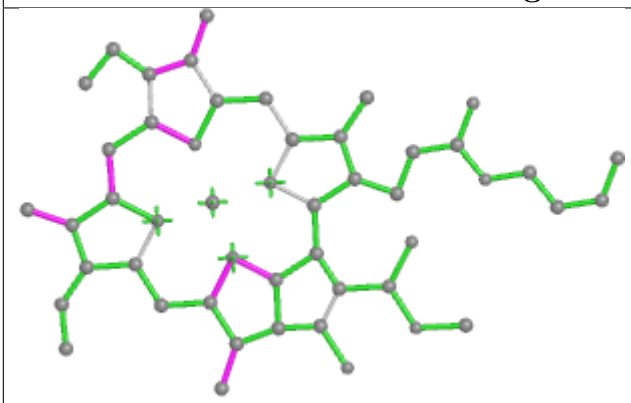
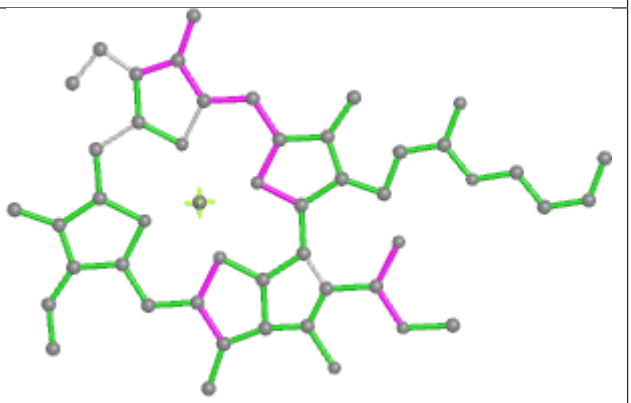
 Bond lengths	 Bond angles
 Torsions	 Rings

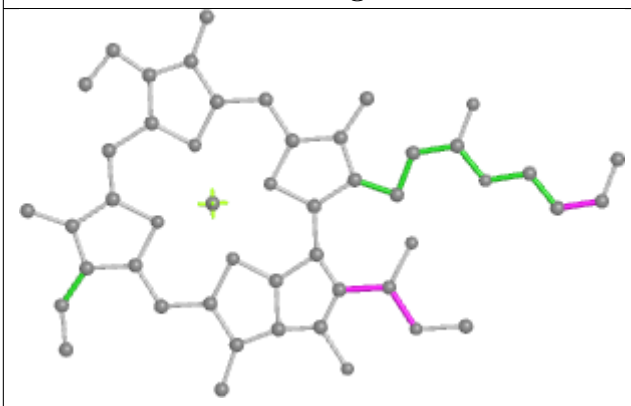
Ligand CLA A 305



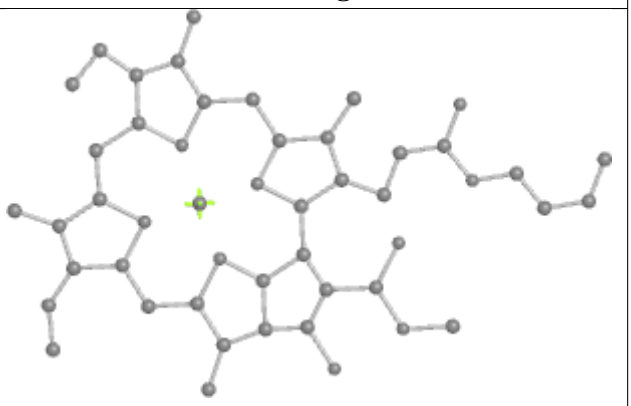
Bond lengths



Bond angles

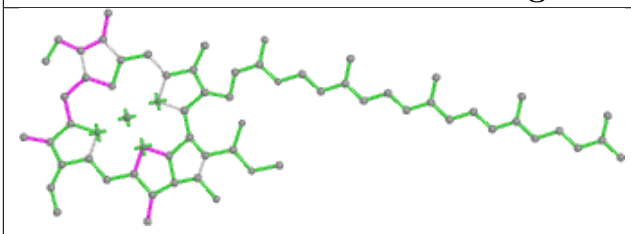


Torsions

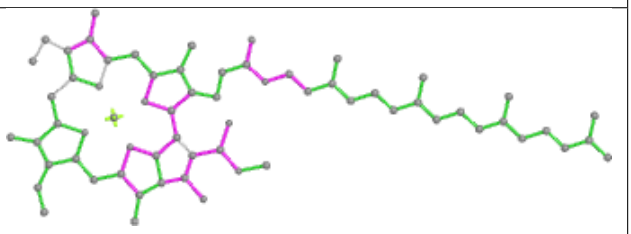


Rings

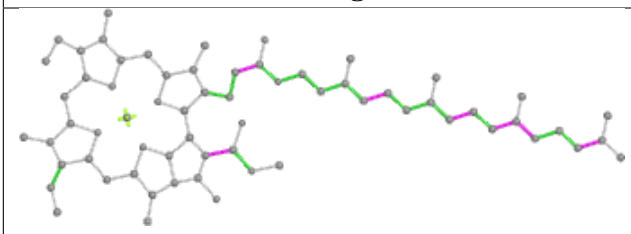
Ligand CLA a 801



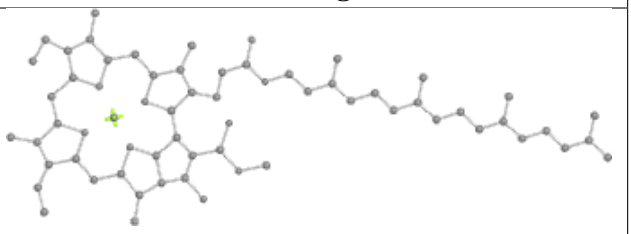
Bond lengths



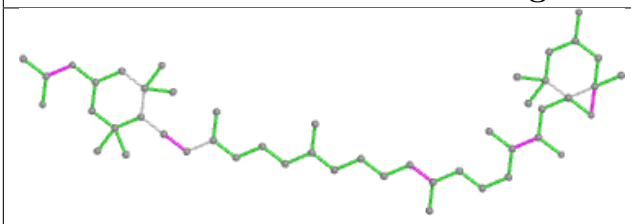
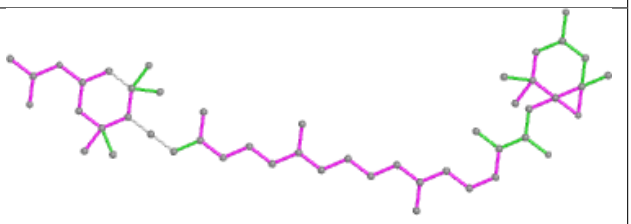
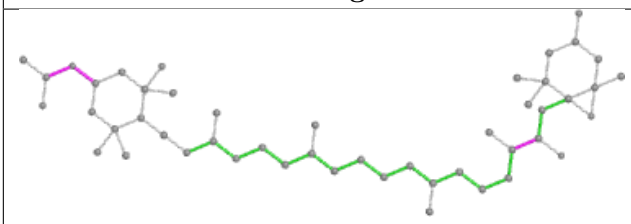
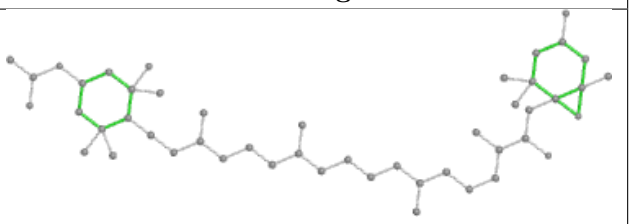
Bond angles

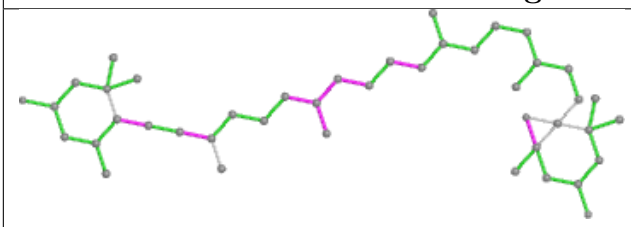
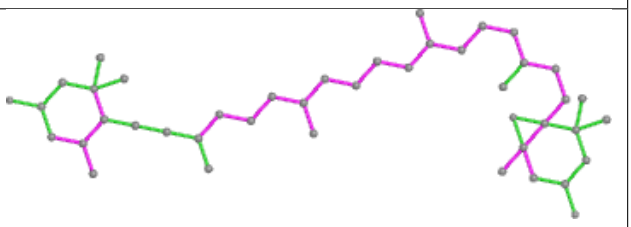
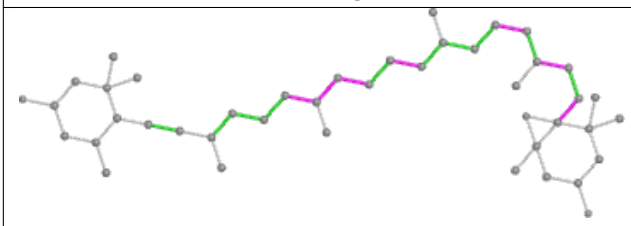
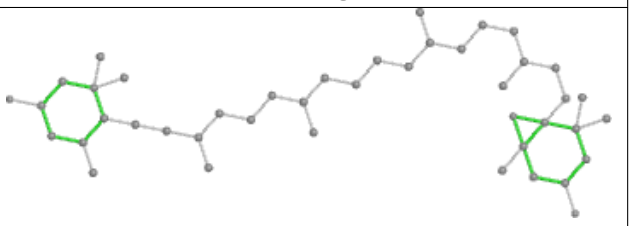


Torsions

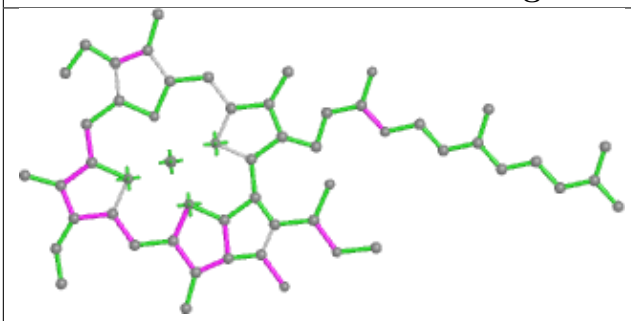


Rings

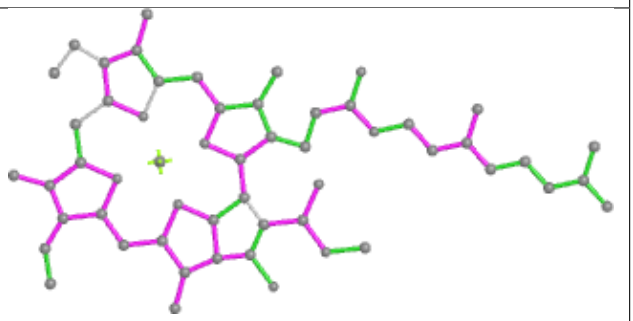
Ligand A86 N 303	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand DD6 D 303	
 Bond lengths	 Bond angles
 Torsions	 Rings

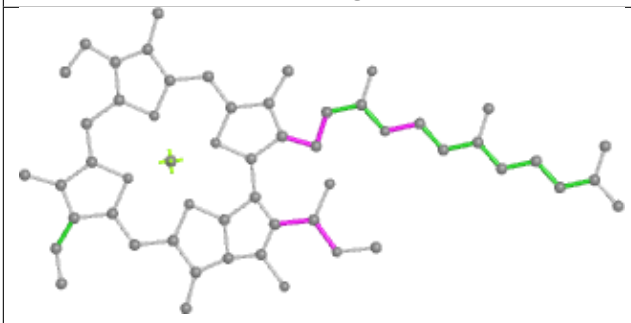
Ligand CLA D 309



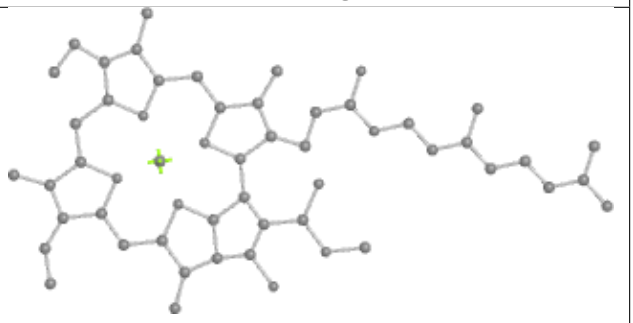
Bond lengths



Bond angles

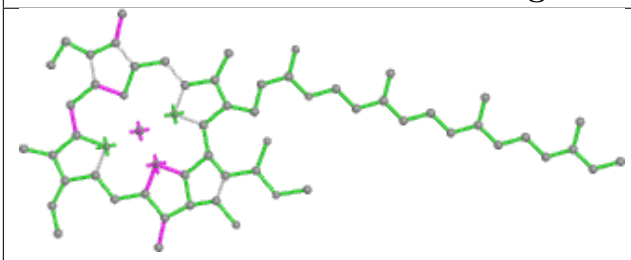


Torsions

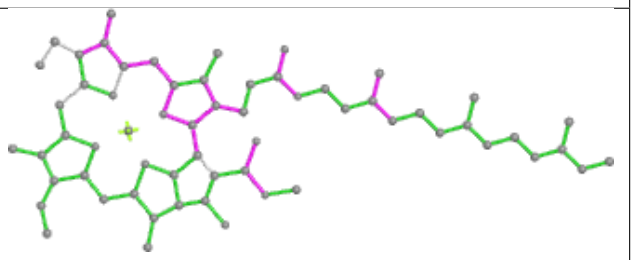


Rings

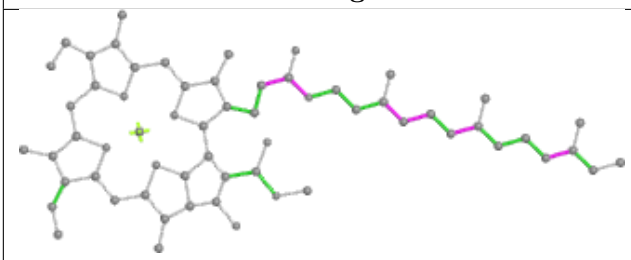
Ligand CLA J 307



Bond lengths



Bond angles



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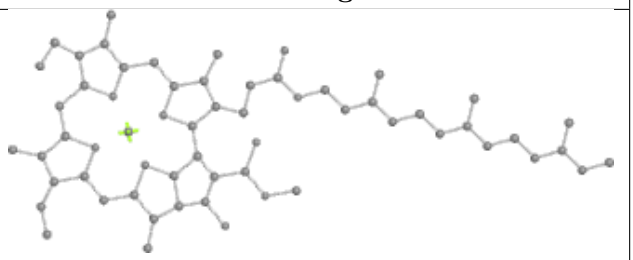
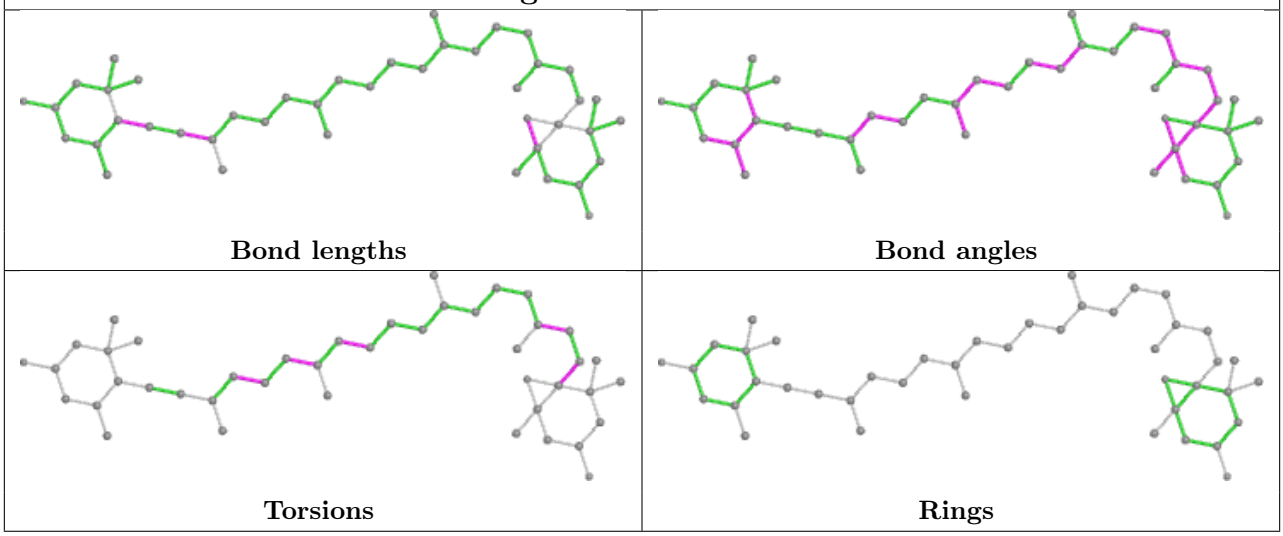
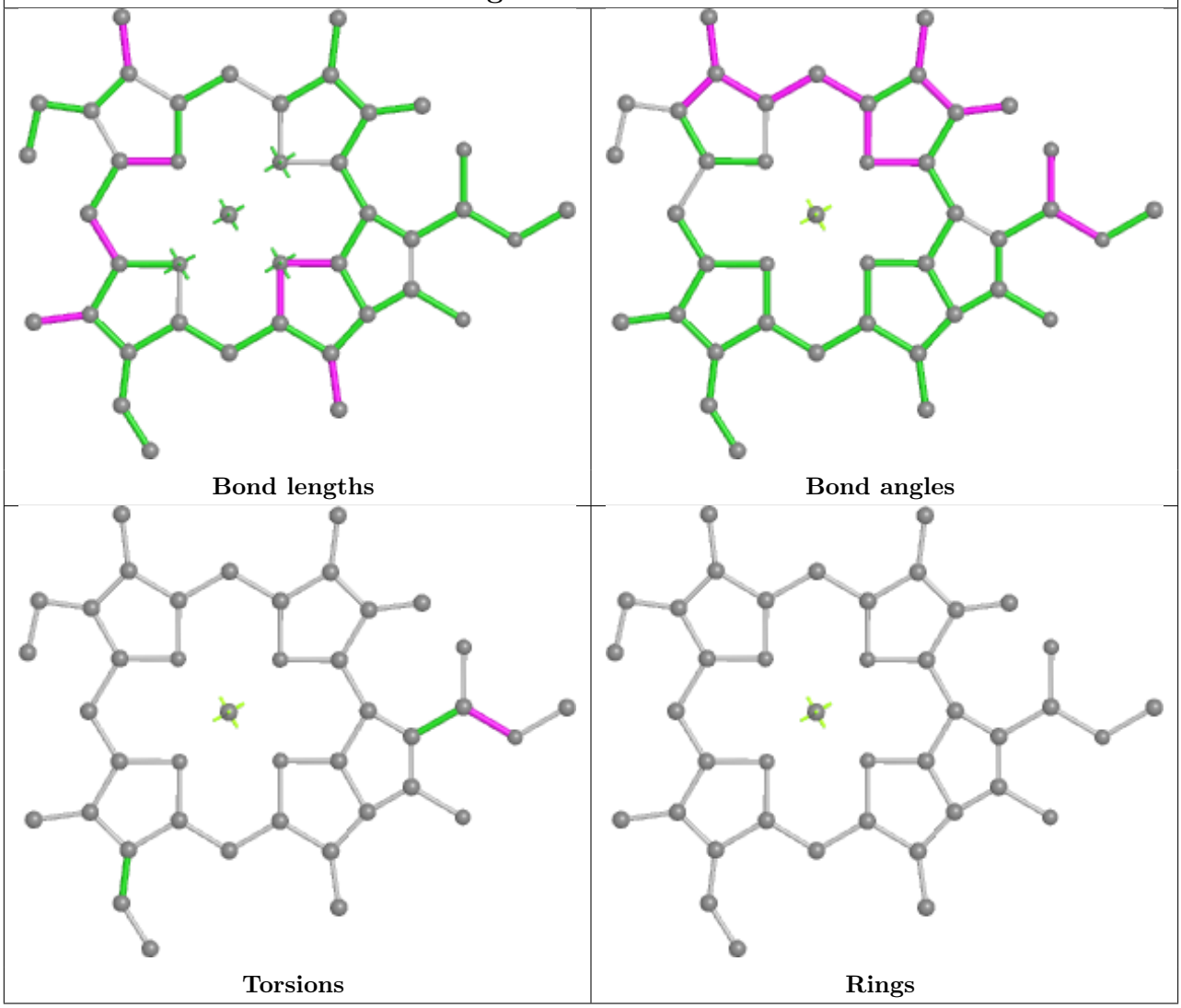


Rings

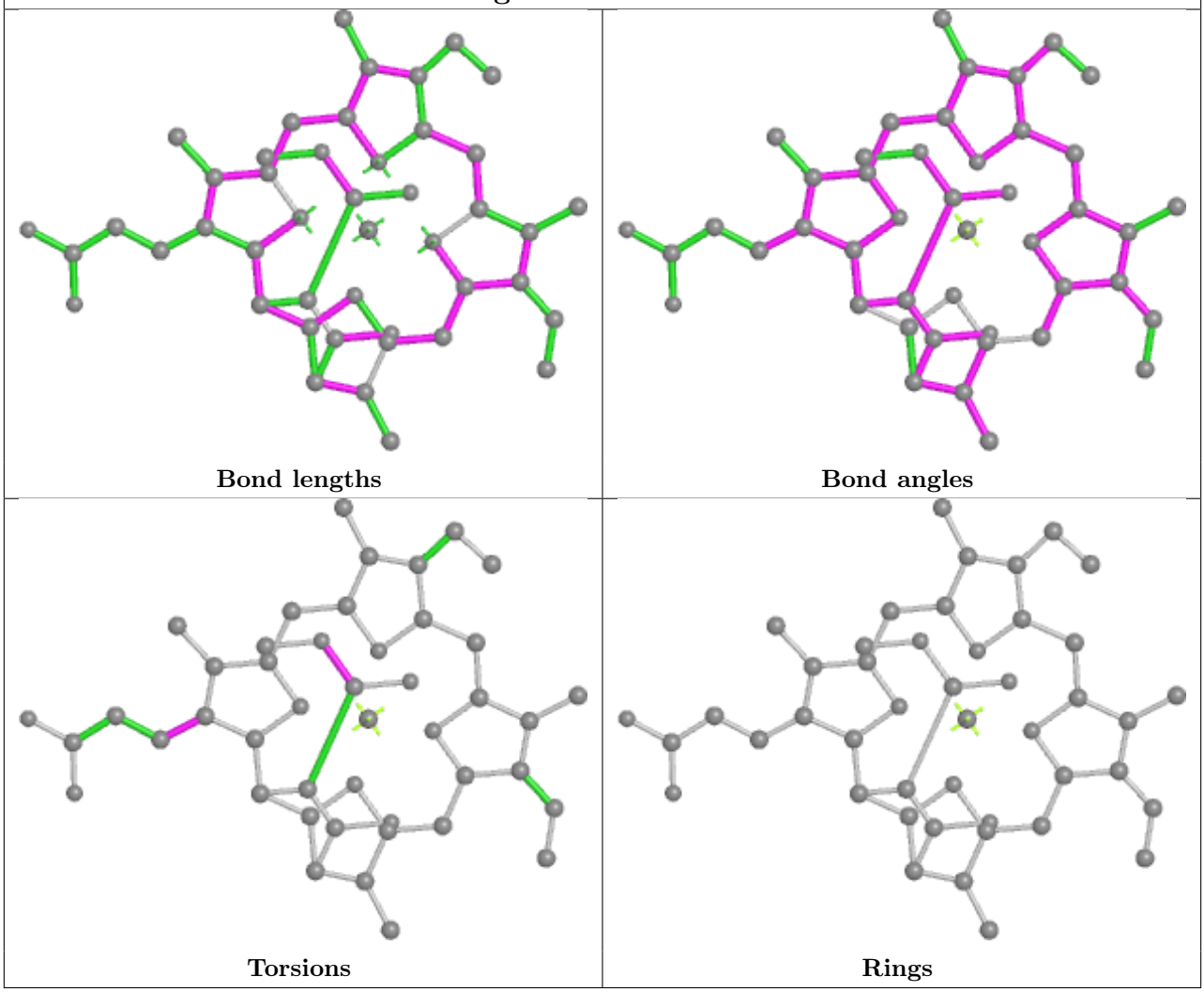
Ligand DD6 W 204



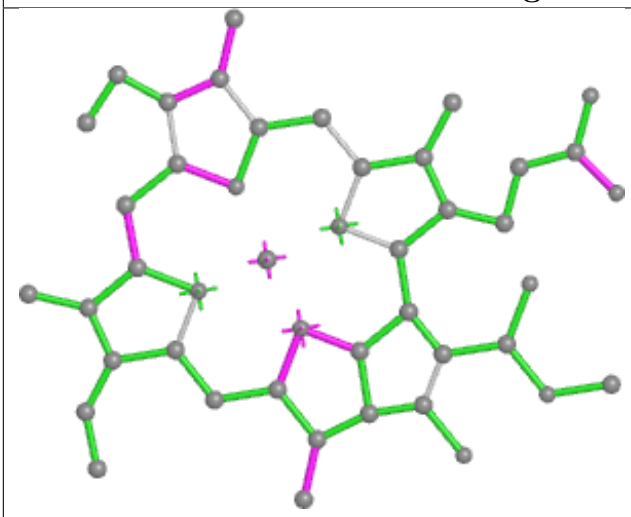
Ligand CLA J 315



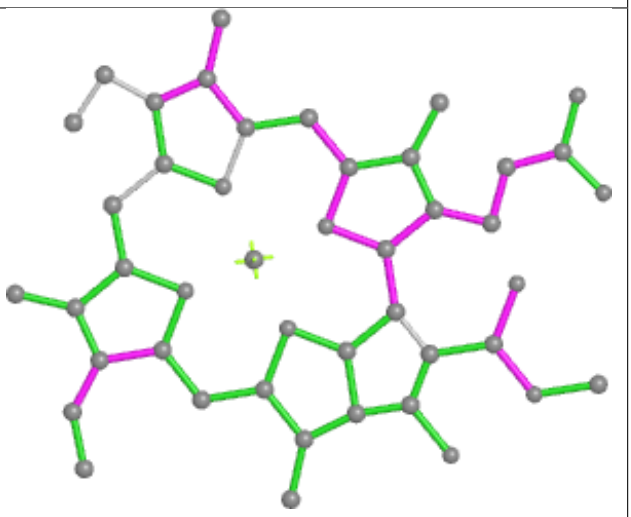
Ligand KC1 U 312



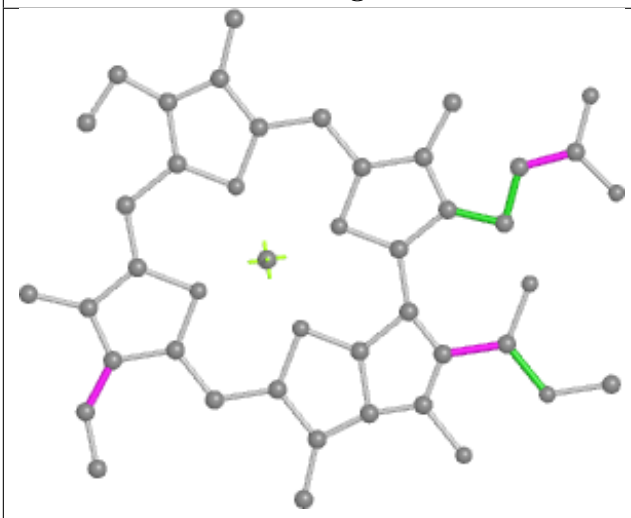
Ligand CLA D 306



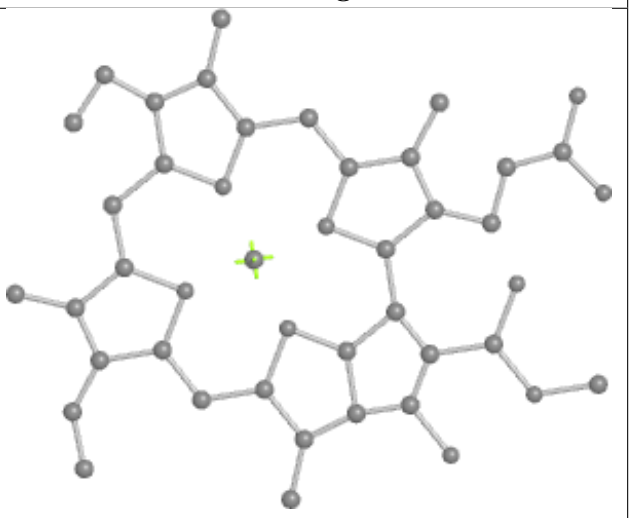
Bond lengths



Bond angles

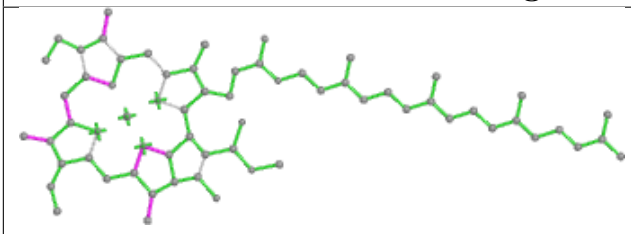


Torsions

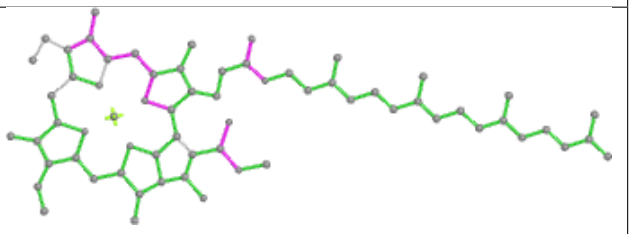


Rings

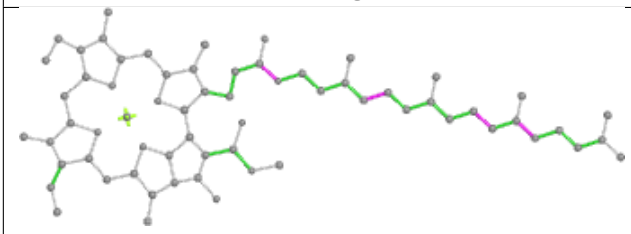
Ligand CLA K 312



Bond lengths



Bond angles



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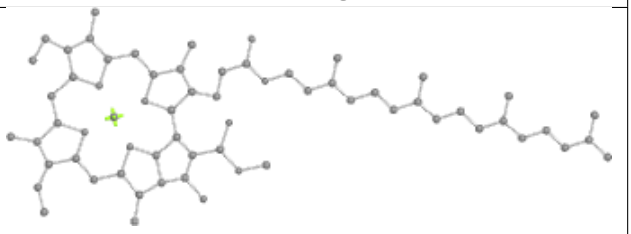
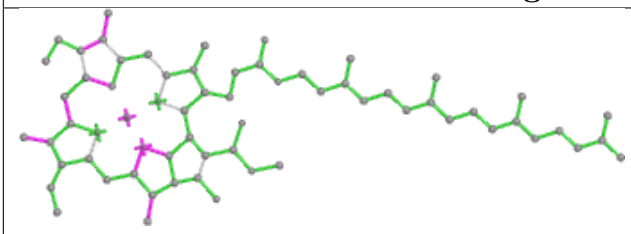
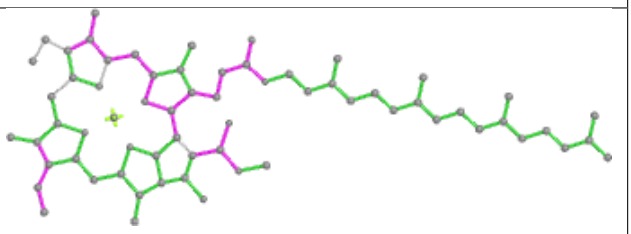


Rings

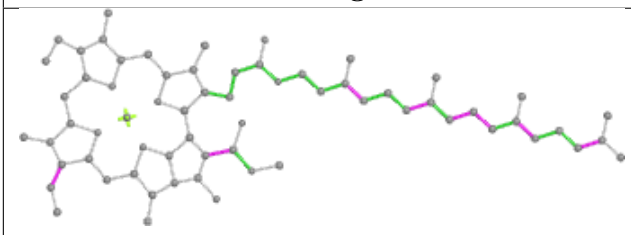
Ligand CLA H 315



Bond lengths



Bond angles



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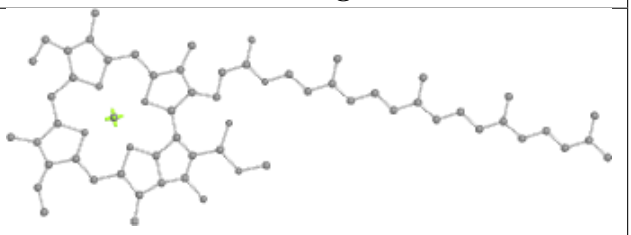
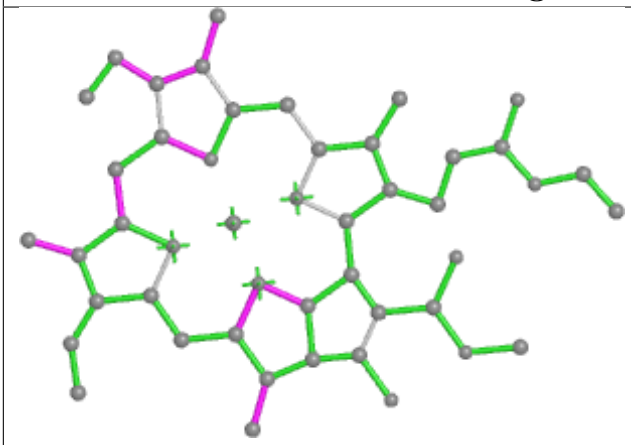
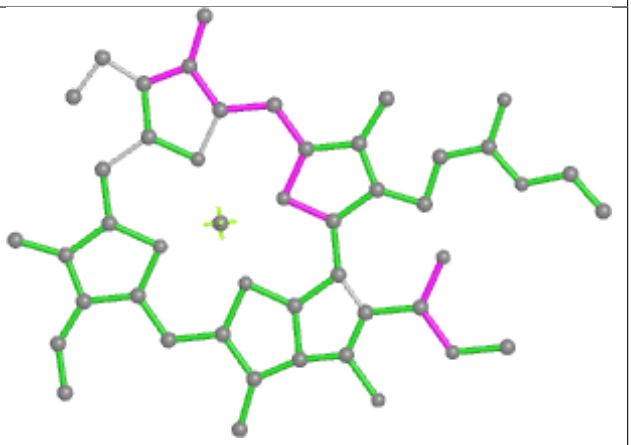


Rings

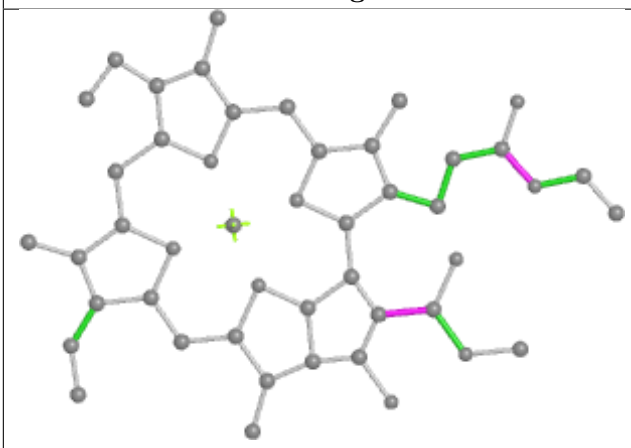
Ligand CLA J 317



Bond lengths



Bond angles



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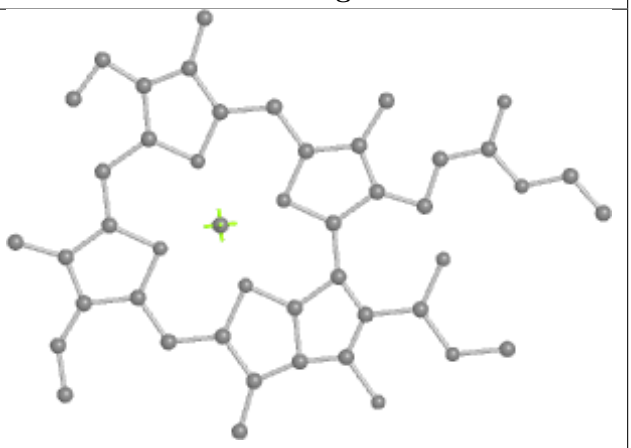
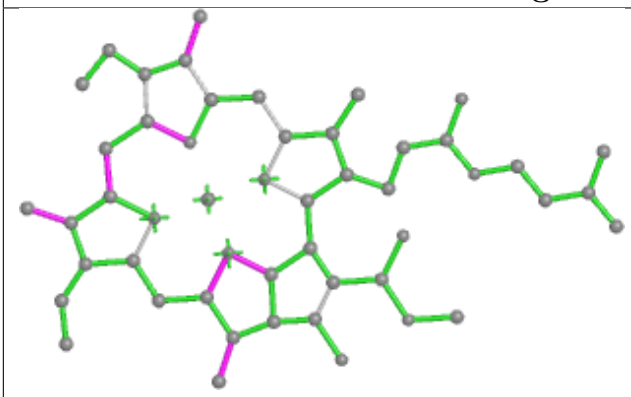
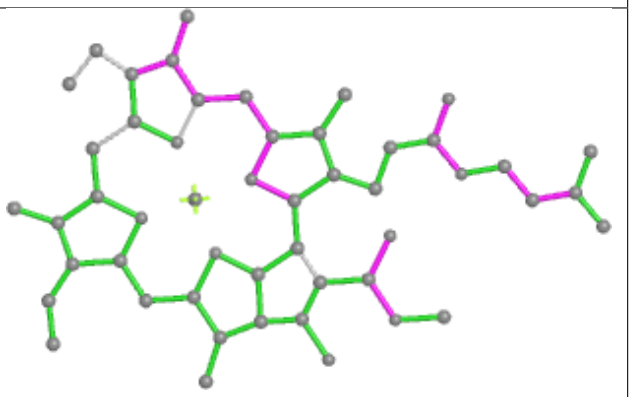


Rings

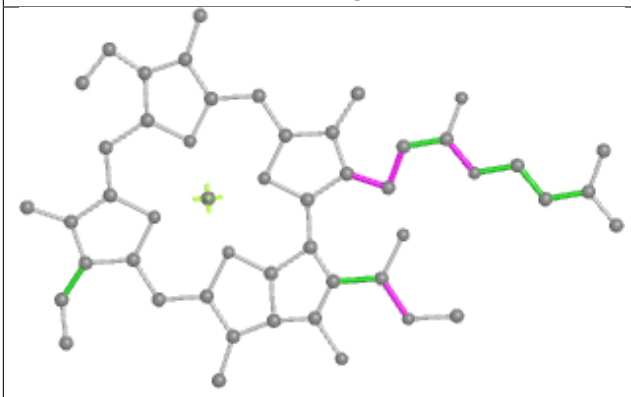
Ligand CLA l 206



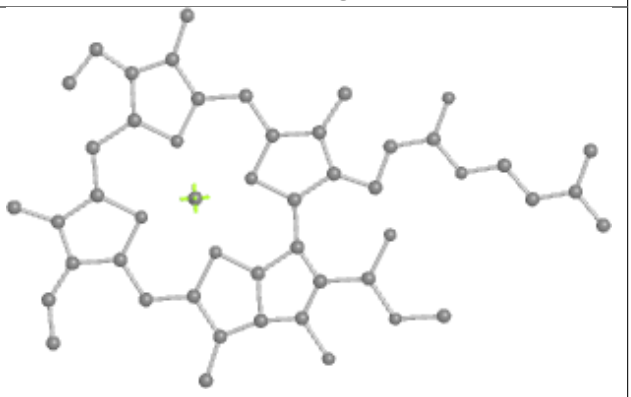
Bond lengths



Bond angles

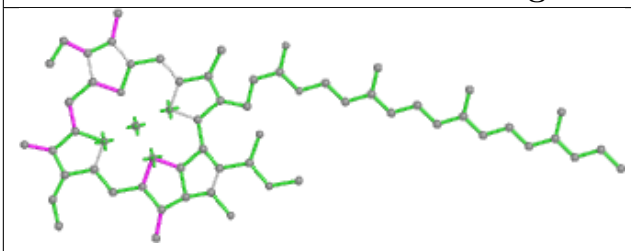


Torsions

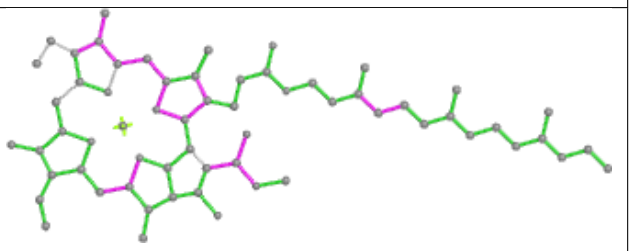


Rings

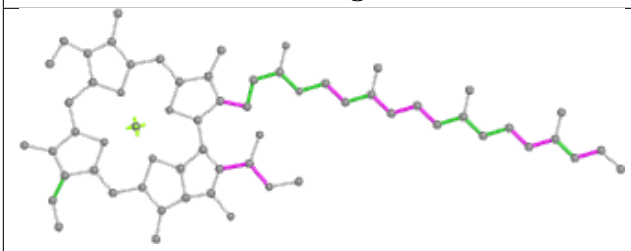
Ligand CLA a 827



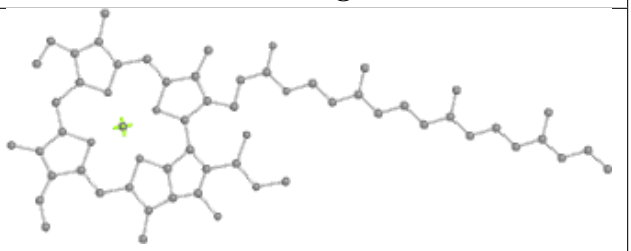
Bond lengths



Bond angles

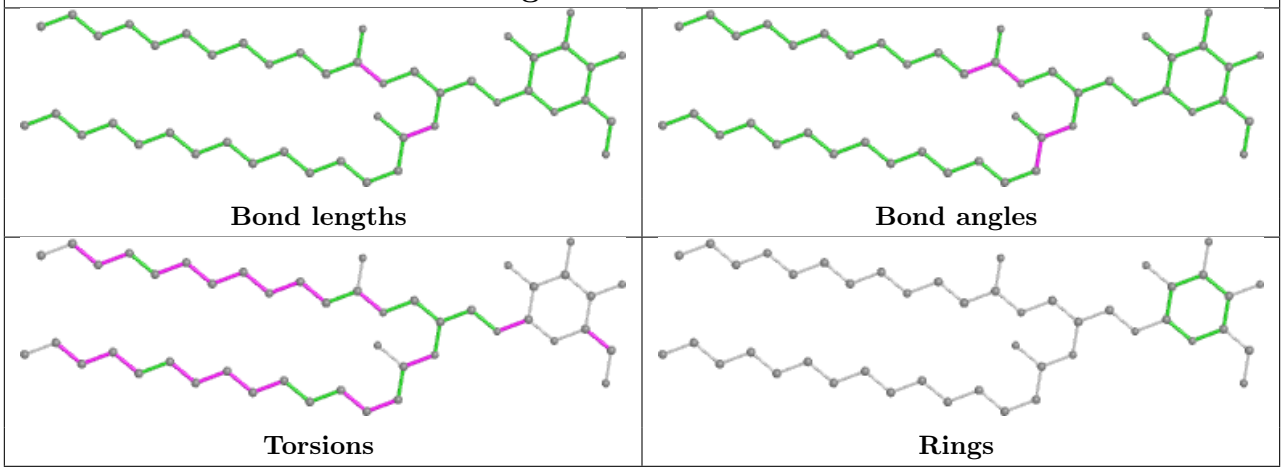


Torsions

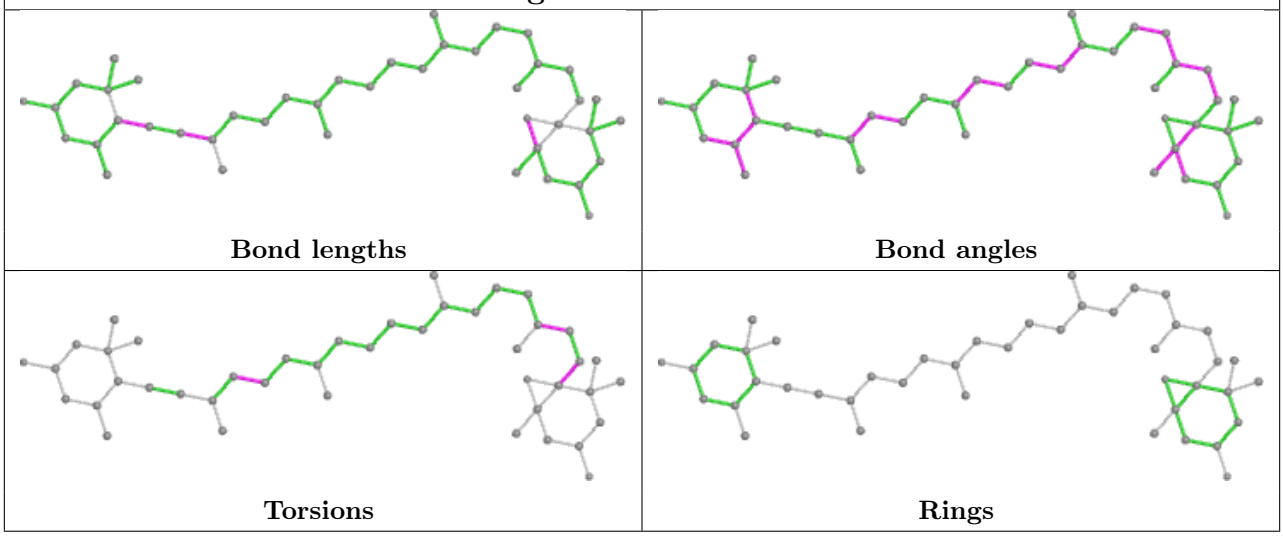


Rings

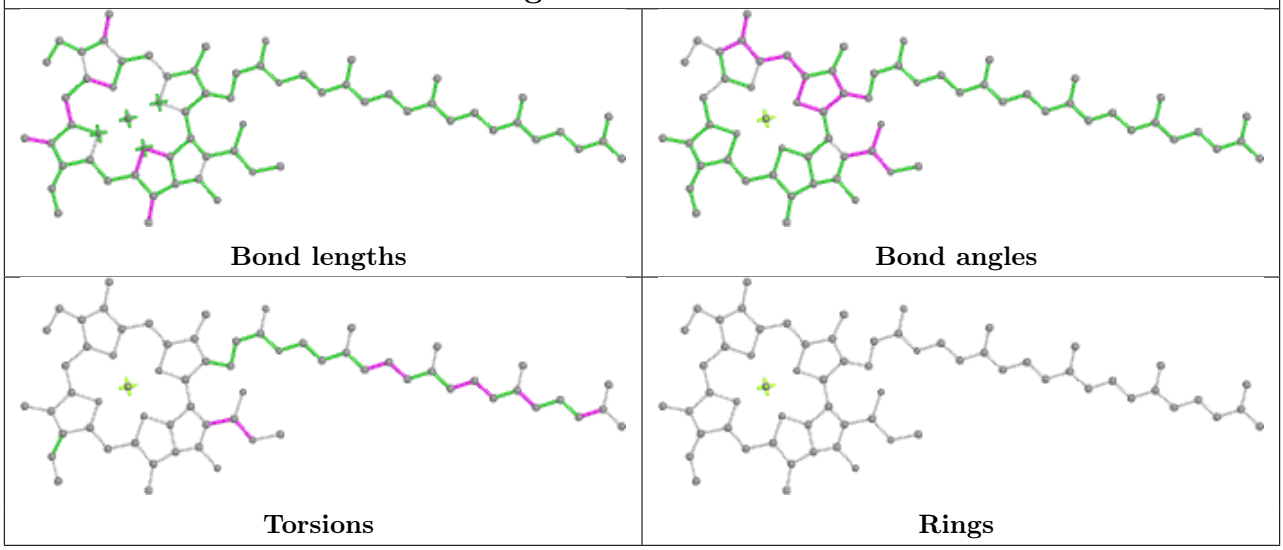
Ligand LMG E 318

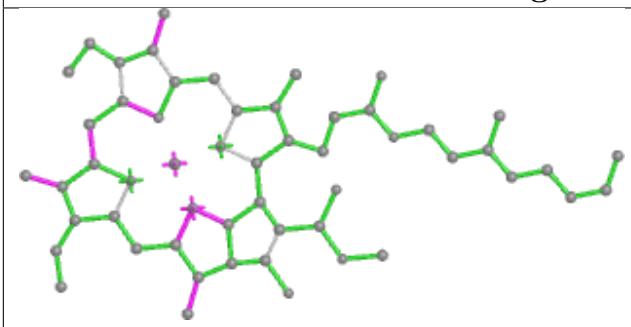
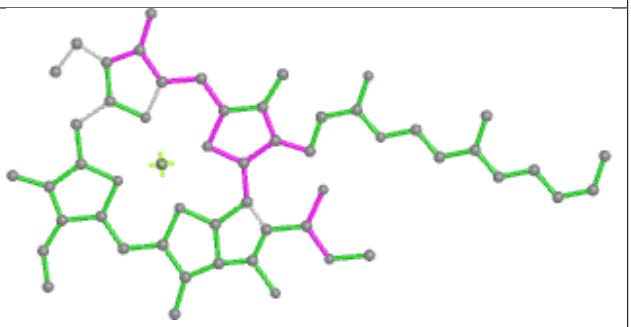
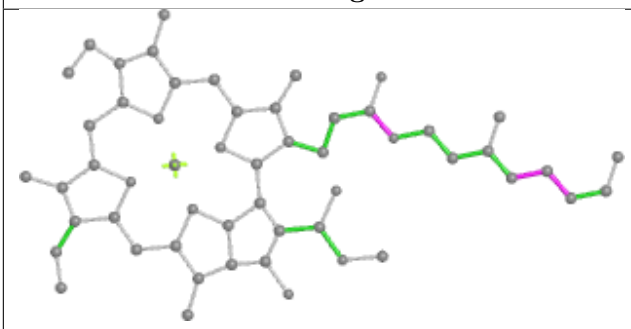
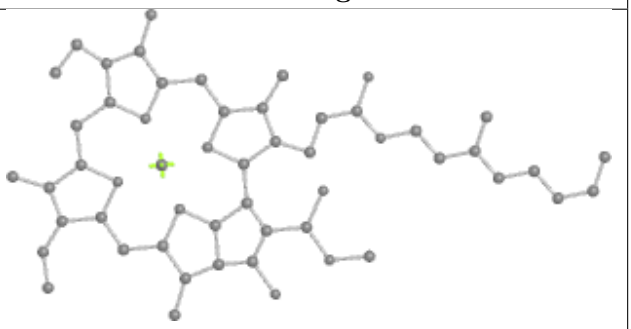


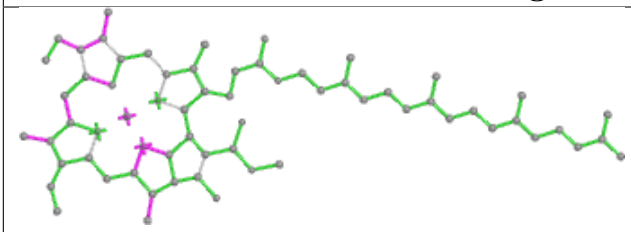
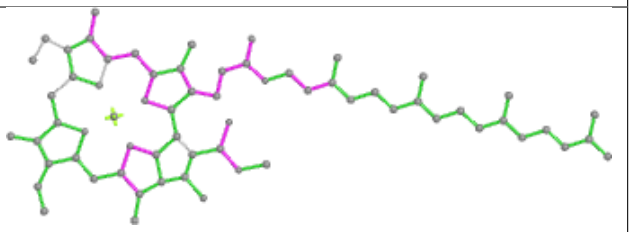
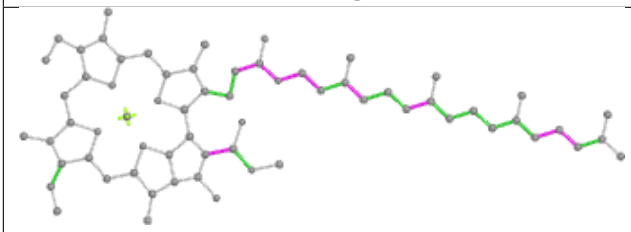
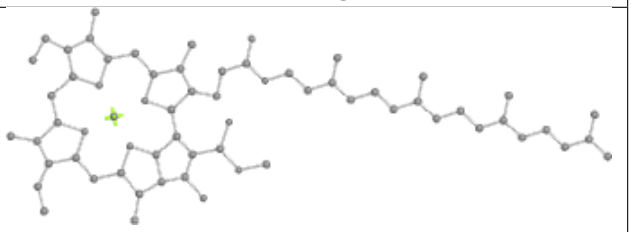
Ligand DD6 E 306

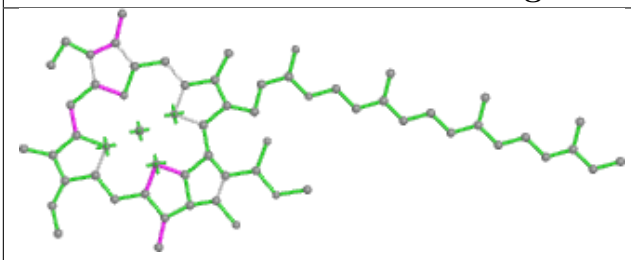
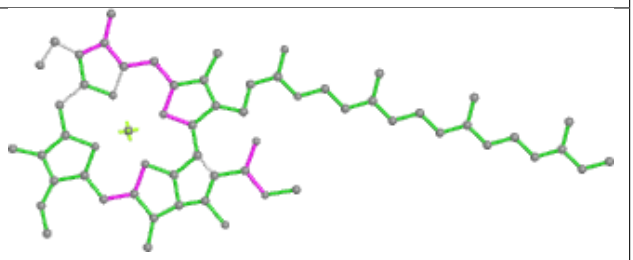
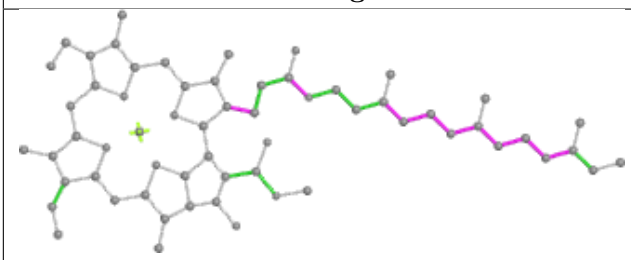
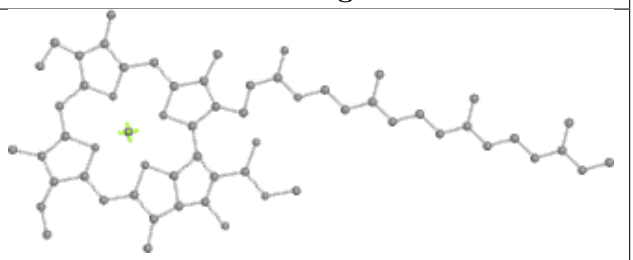


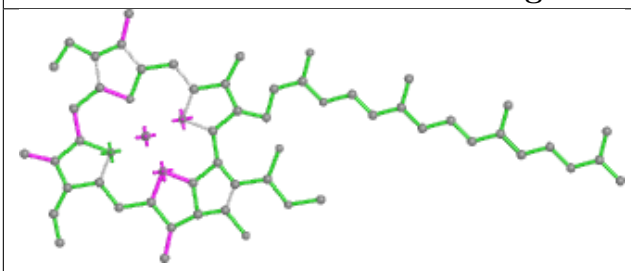
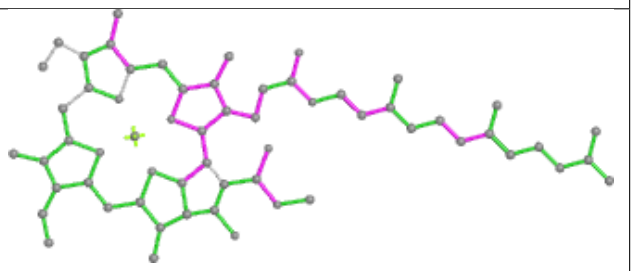
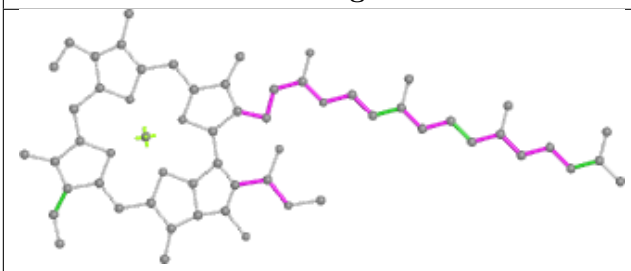
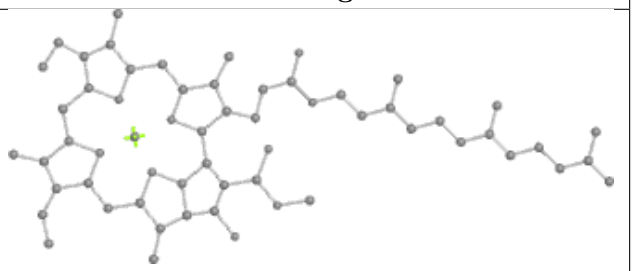
Ligand CLA A 308

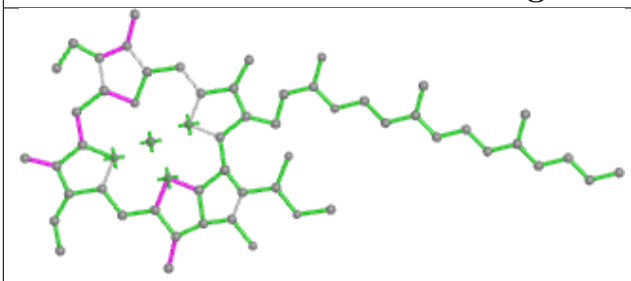
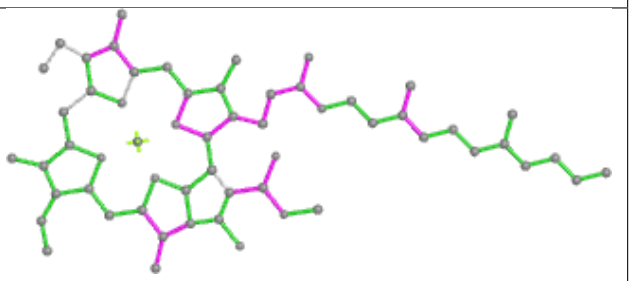
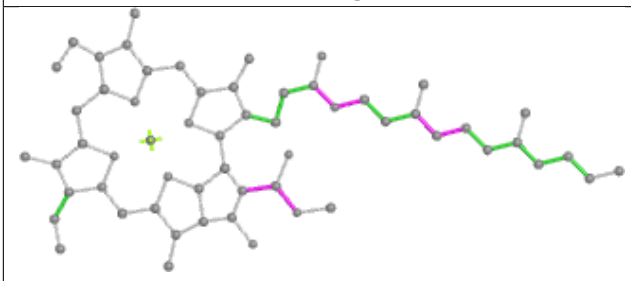
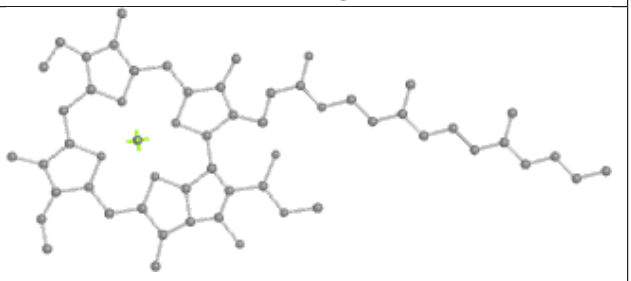


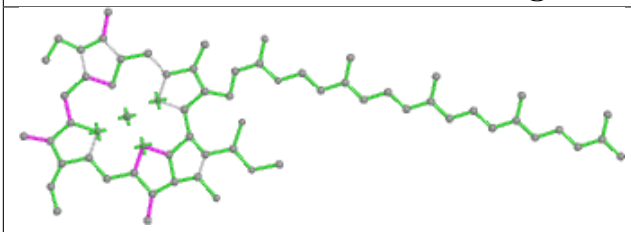
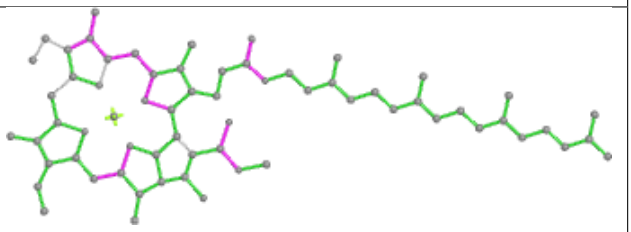
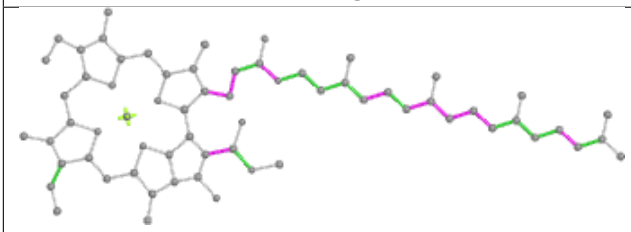
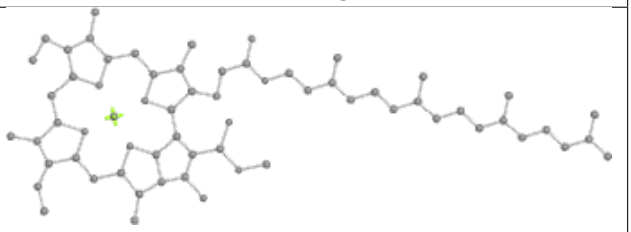
Ligand CLA I 307	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA a 804	
 Bond lengths	 Bond angles
 Torsions	 Rings

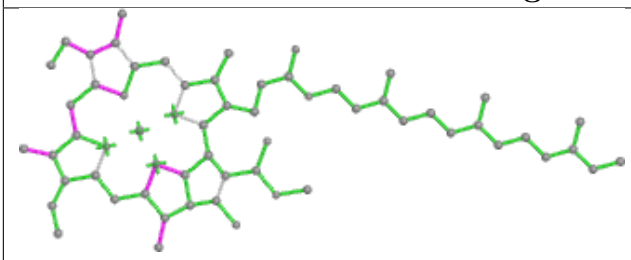
Ligand CLA C 206	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA P 314	
 Bond lengths	 Bond angles
 Torsions	 Rings

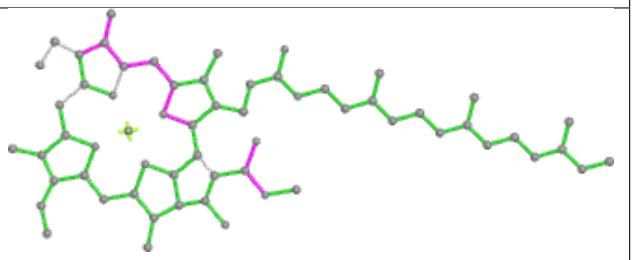
Ligand CLA b 833	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA a 812	
 Bond lengths	 Bond angles
 Torsions	 Rings

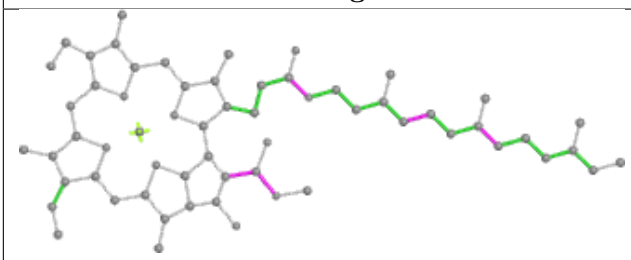
Ligand CLA O 306



Bond lengths



Bond angles



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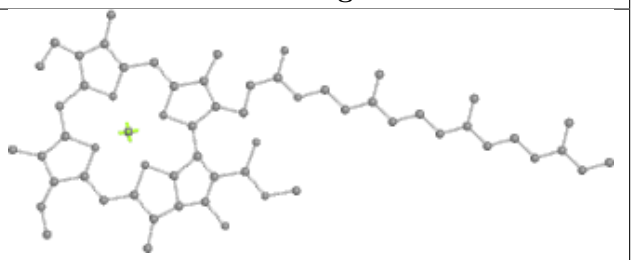
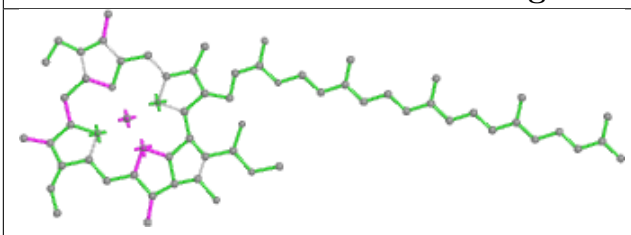


Rings

Ligand CLA a 820



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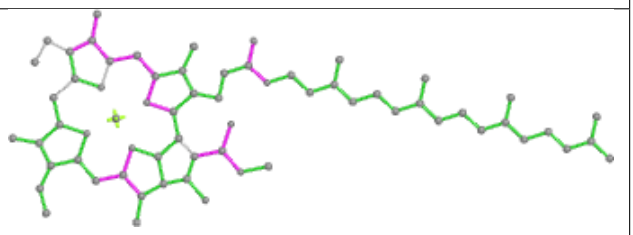
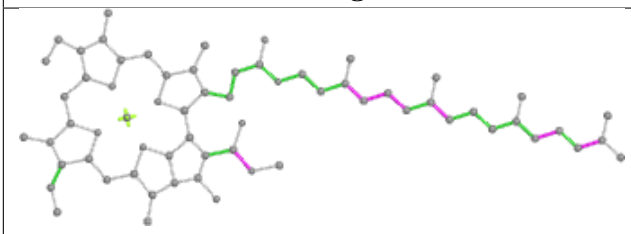


Bond angles



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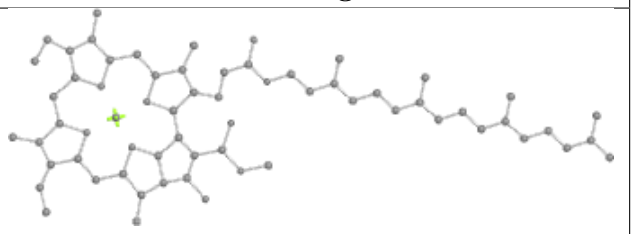
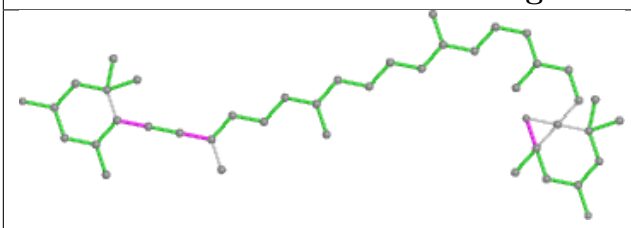
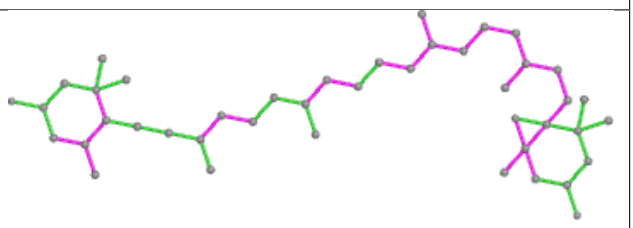


Rings

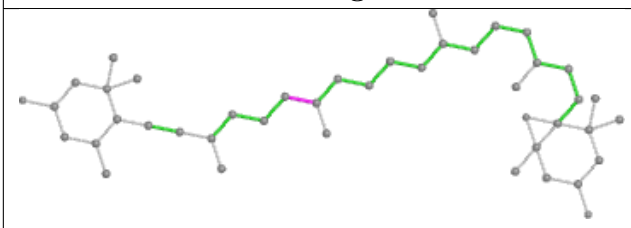
Ligand DD6 P 305



Bond lengths



Bond angles



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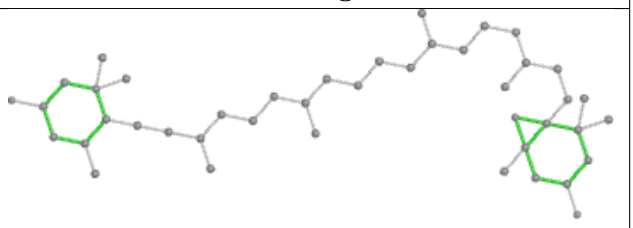
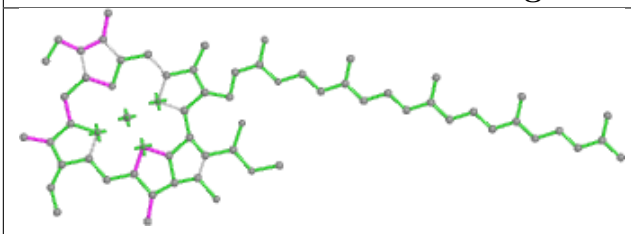
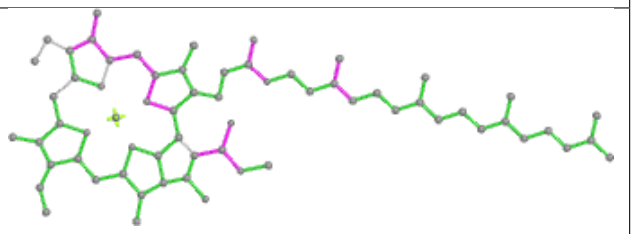
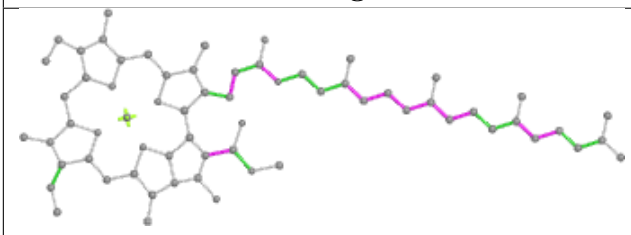
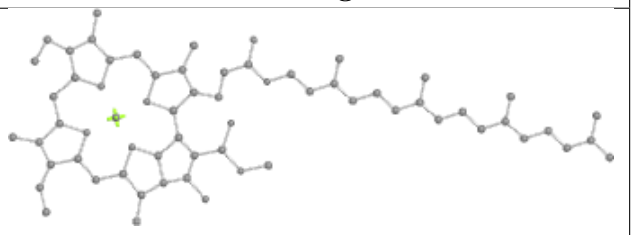
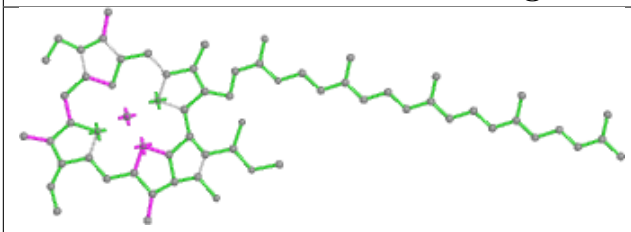
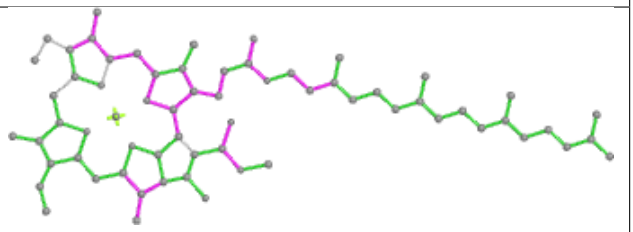
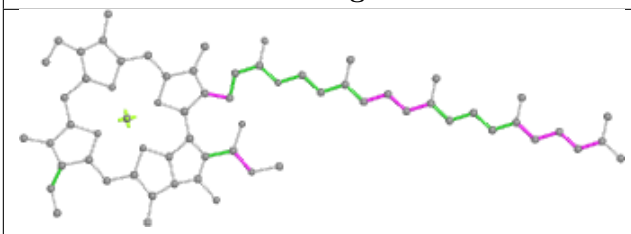
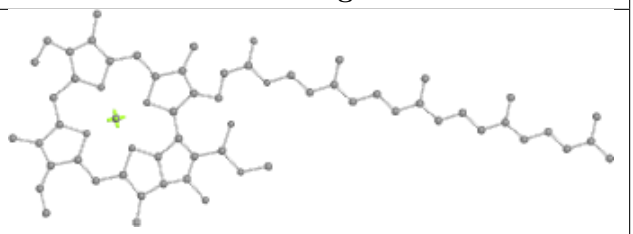
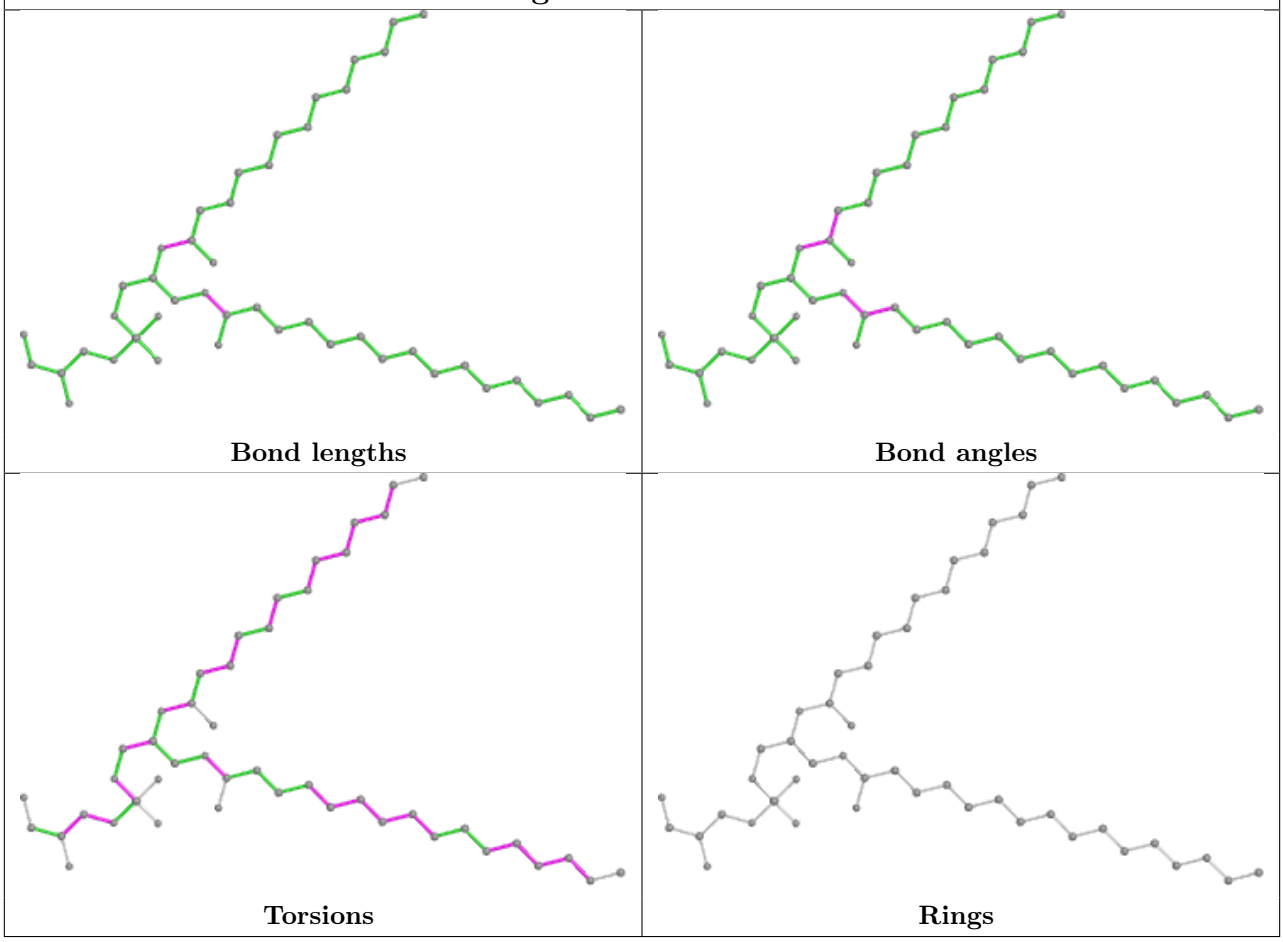


Rings

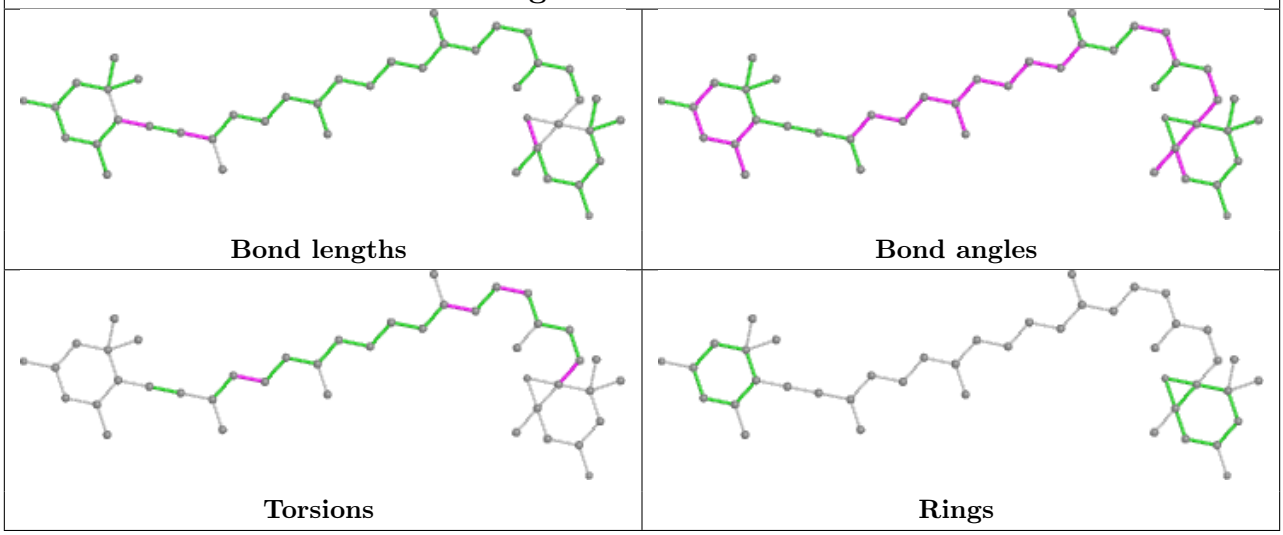
Ligand CLA C 208	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA V 311	
 Bond lengths	 Bond angles
 Torsions	 Rings

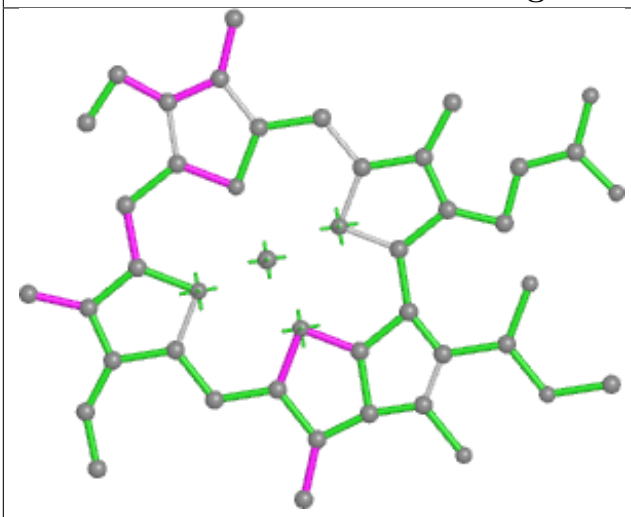
Ligand LHG i 104



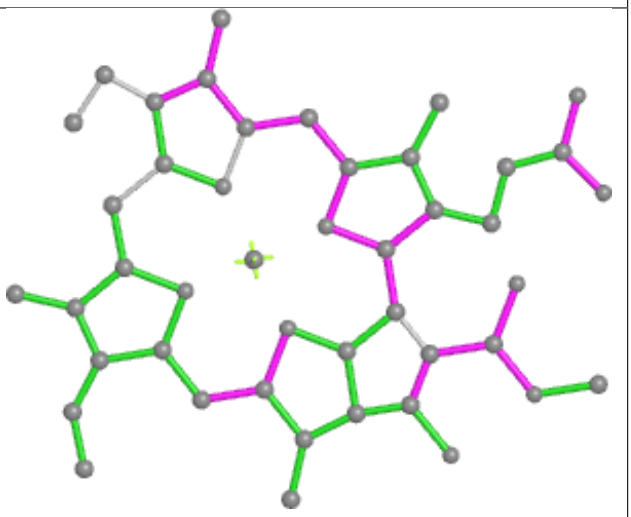
Ligand DD6 S 306



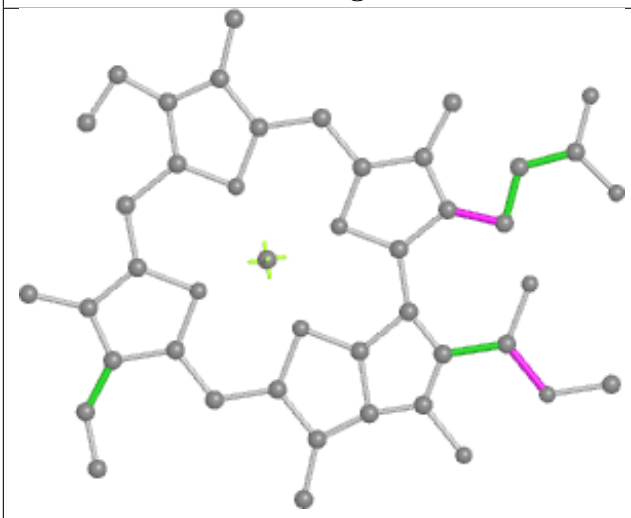
Ligand CLA b 835



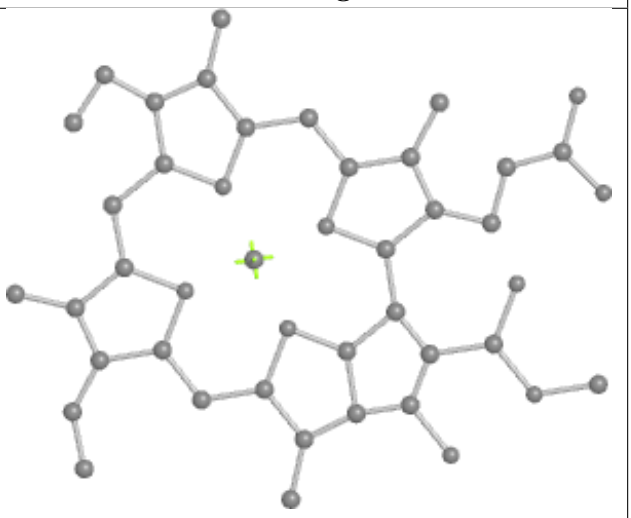
Bond lengths



Bond angles

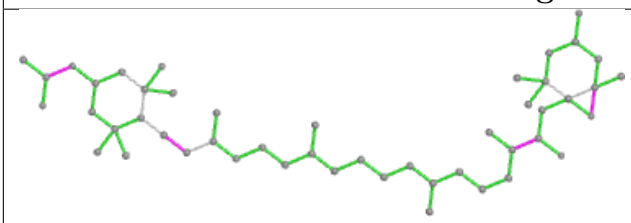


Torsions



Rings

Ligand A86 I 302



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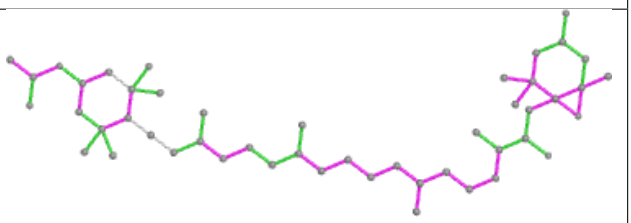
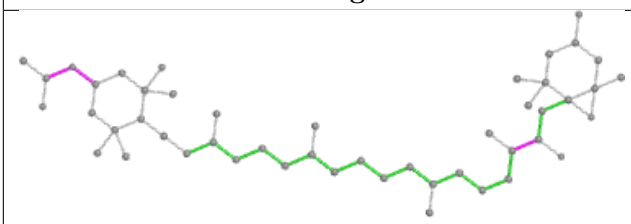
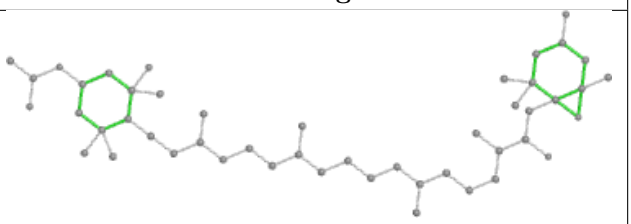


Bond angles

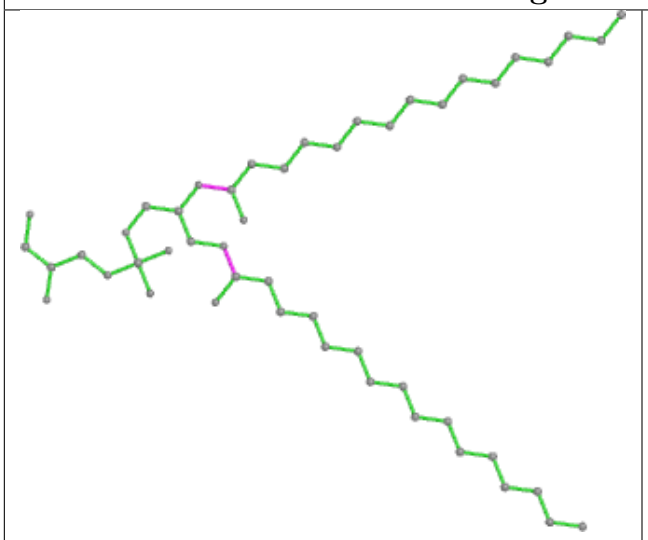


Torsions

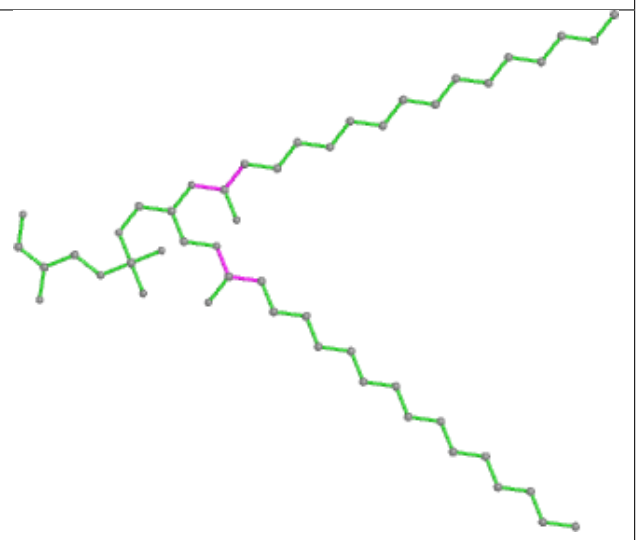


Rings

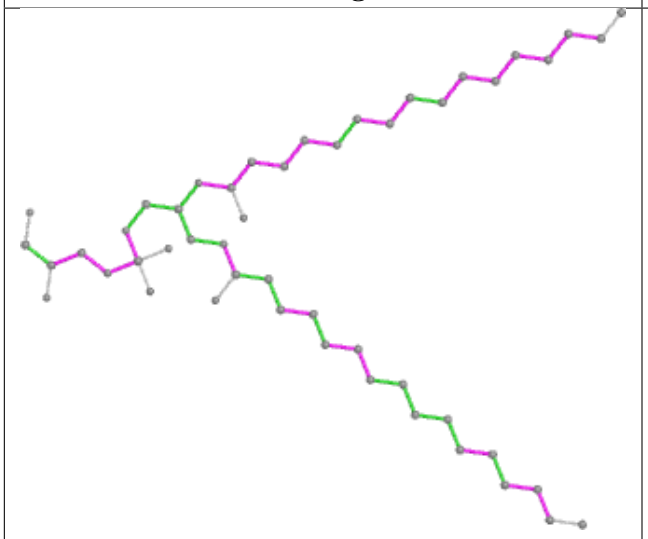
Ligand LHG I 316



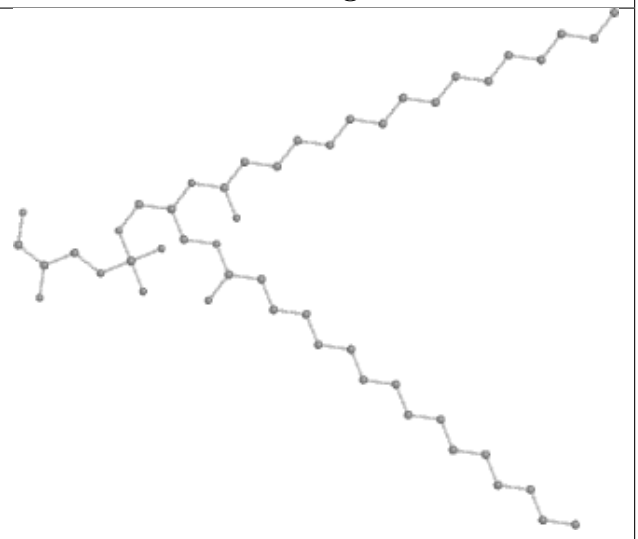
Bond lengths



Bond angles

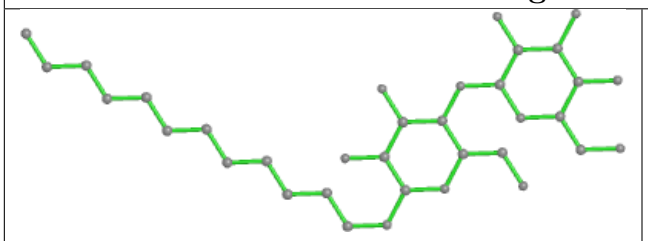


Torsions

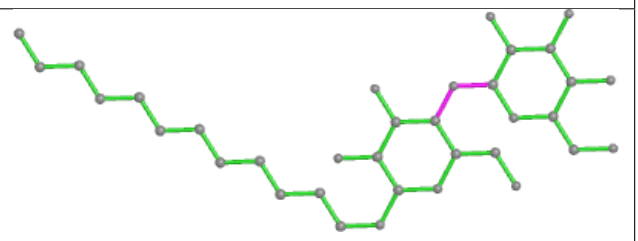


Rings

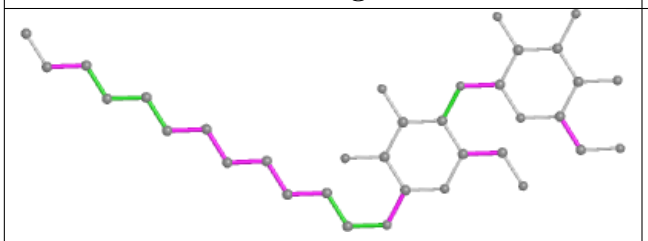
Ligand LMT I 317



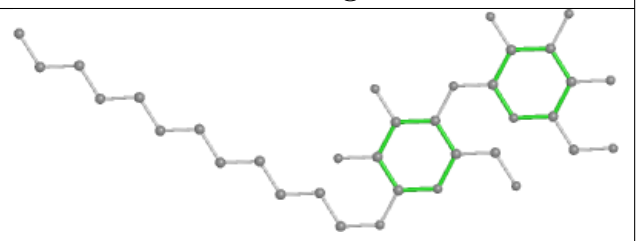
Bond lengths



Bond angles

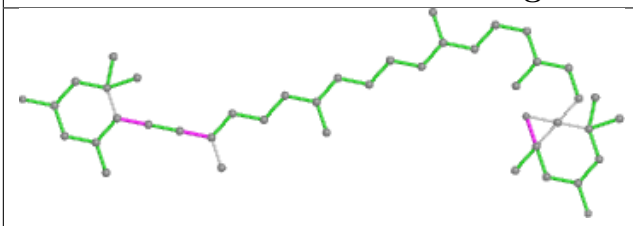


Torsions

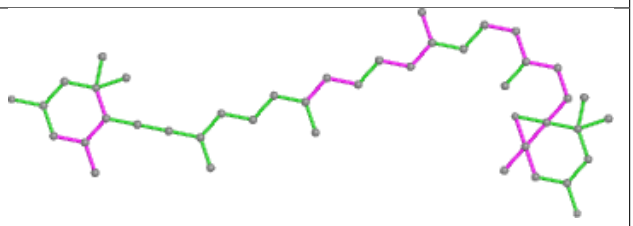


Rings

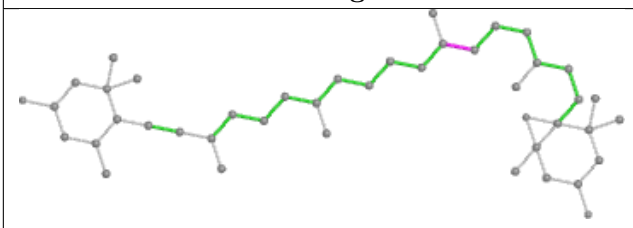
Ligand DD6 K 304



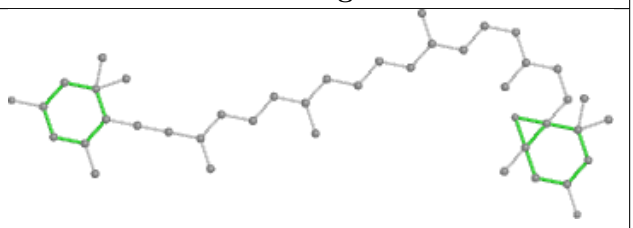
Bond lengths



Bond angles

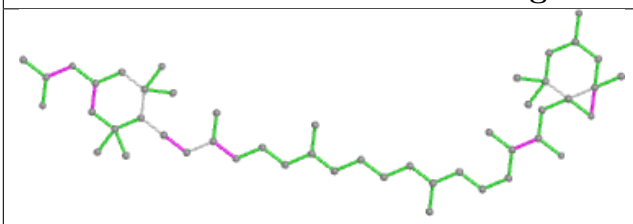


Torsions

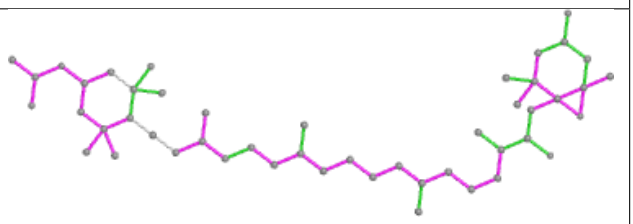


Rings

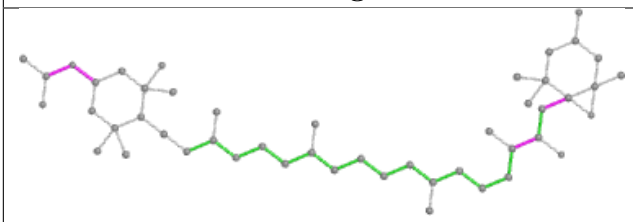
Ligand A86 O 302



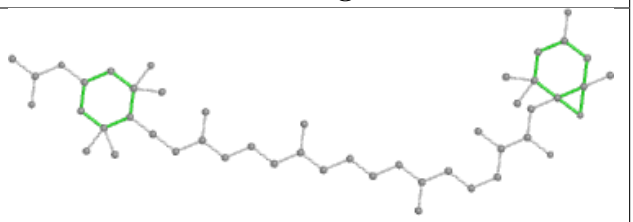
Bond lengths



Bond angles

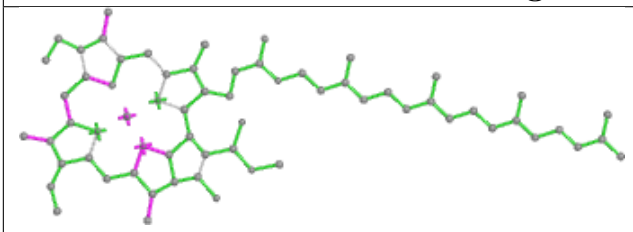


Torsions

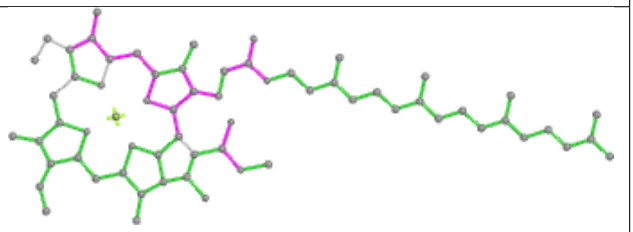


Rings

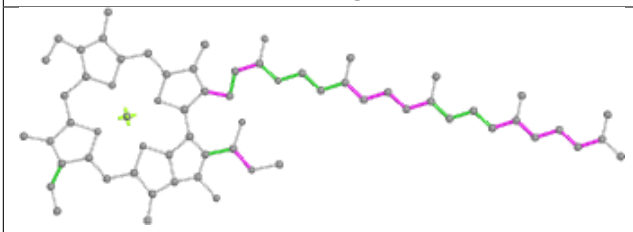
Ligand CLA L 314



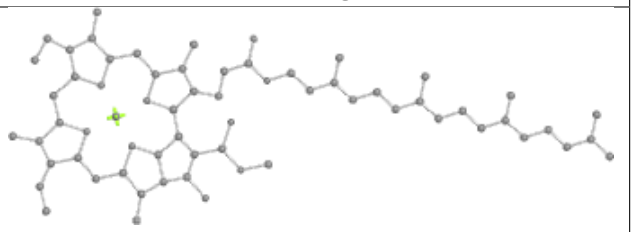
Bond lengths



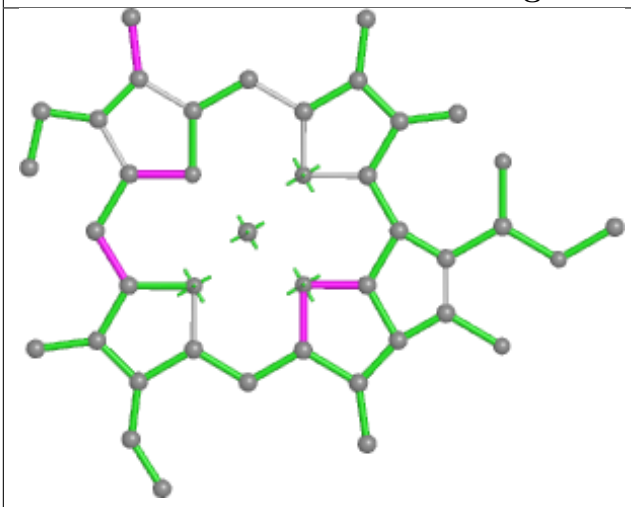
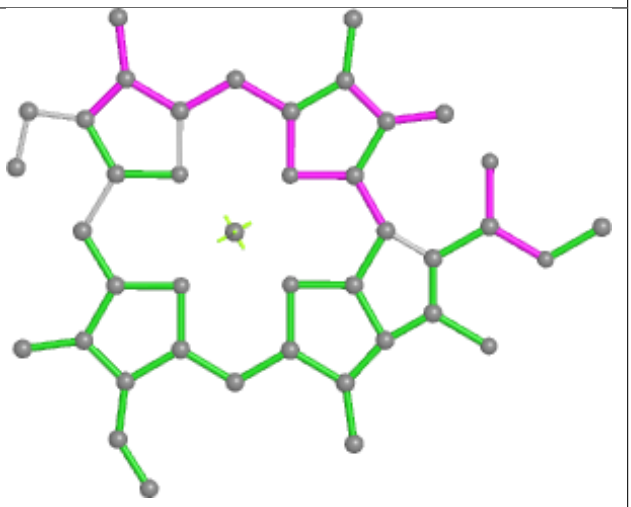
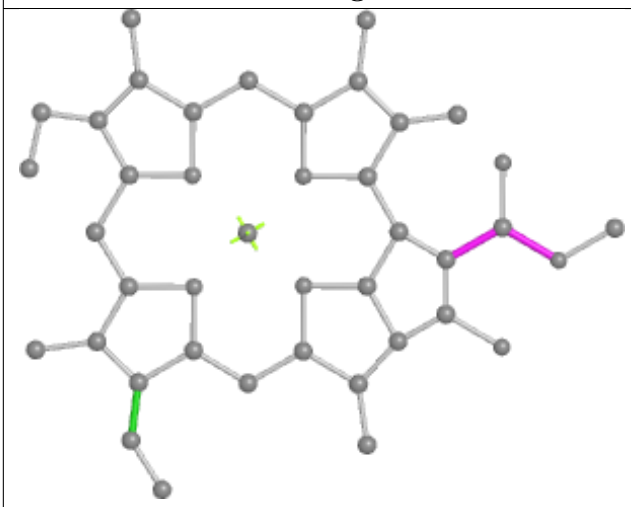
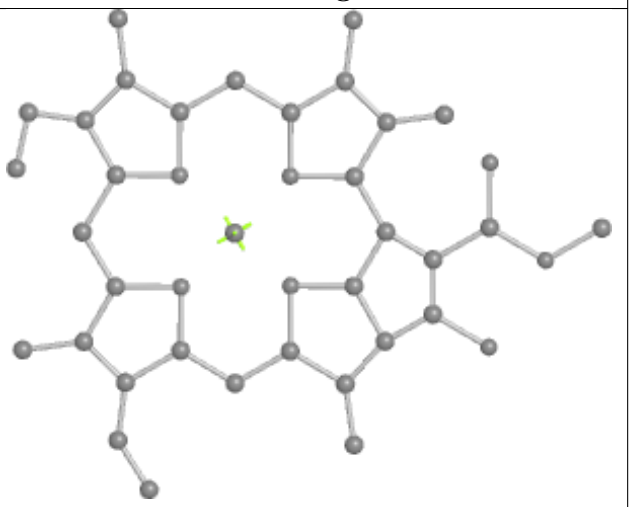
Bond angles



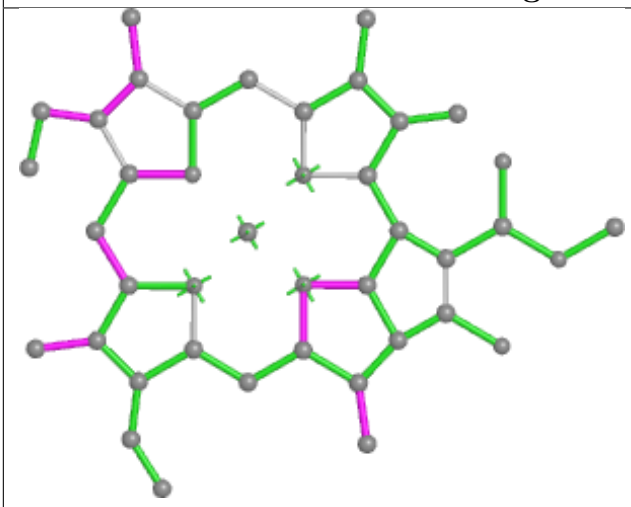
Torsions



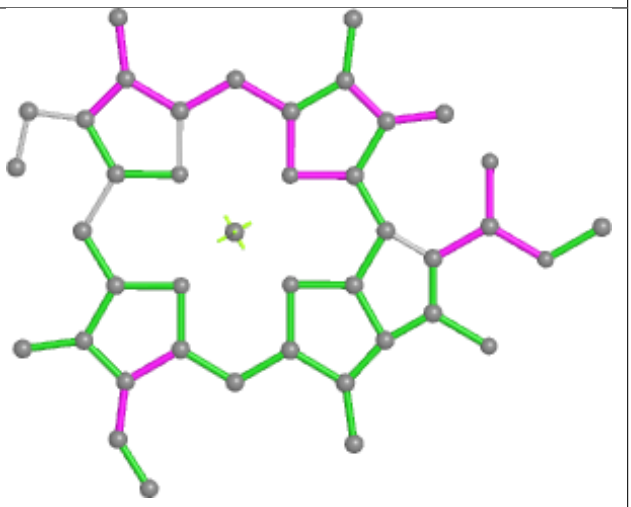
Rings

Ligand CLA X 315	
 Bond lengths	 Bond angles
 Torsions	 Rings

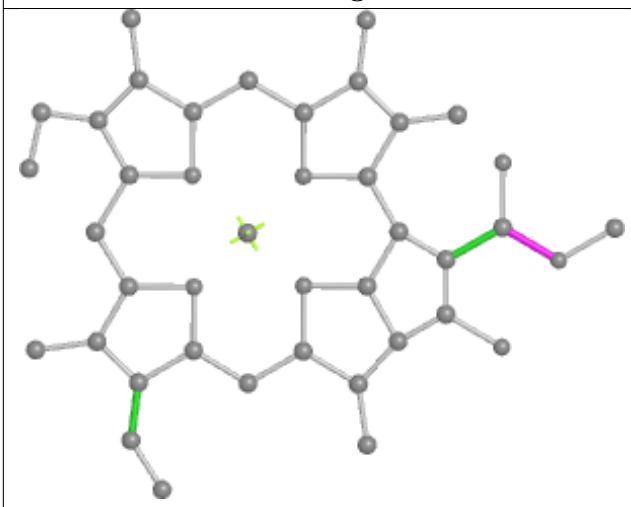
Ligand CLA G 314



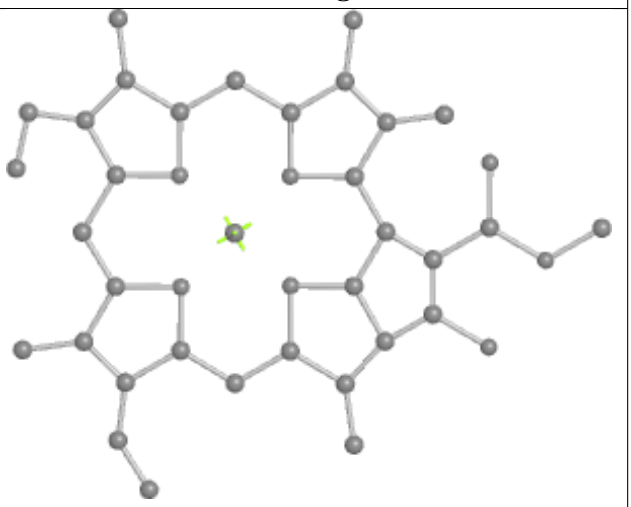
Bond lengths



Bond angles

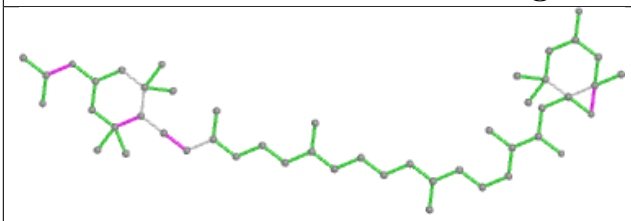


Torsions

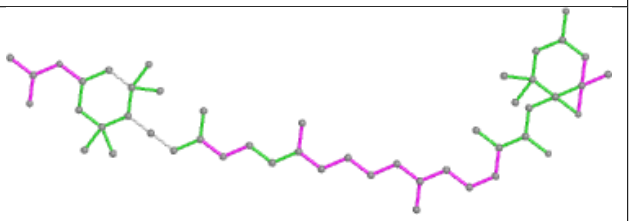


Rings

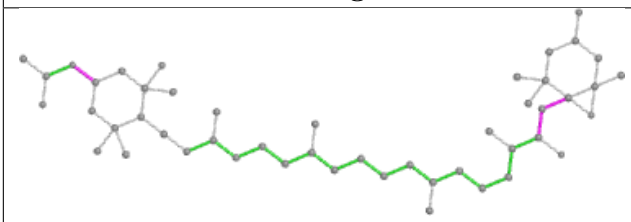
Ligand A86 E 302



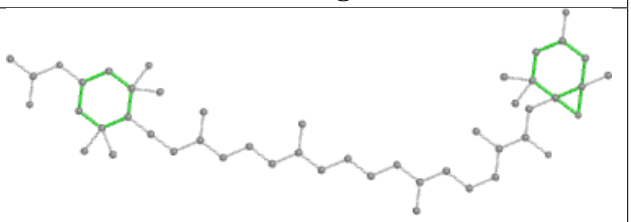
Bond lengths



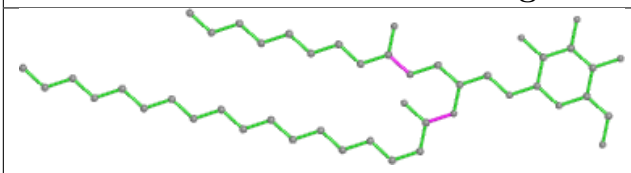
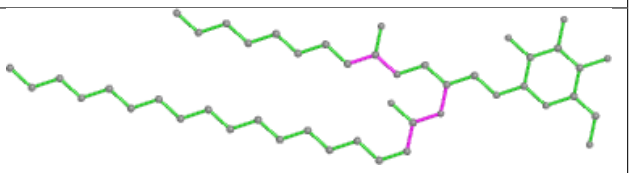
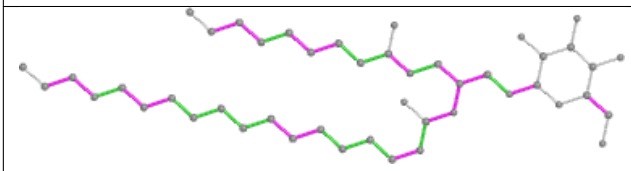
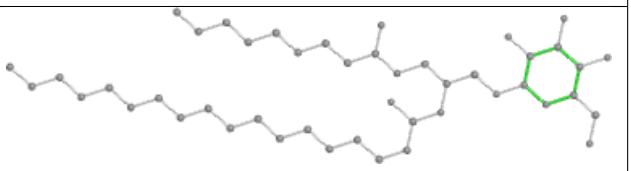
Bond angles

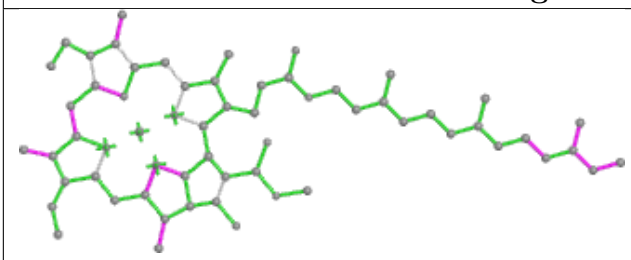
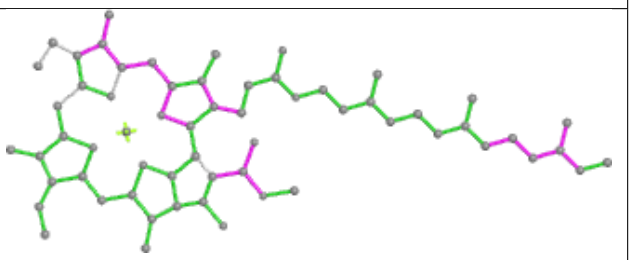
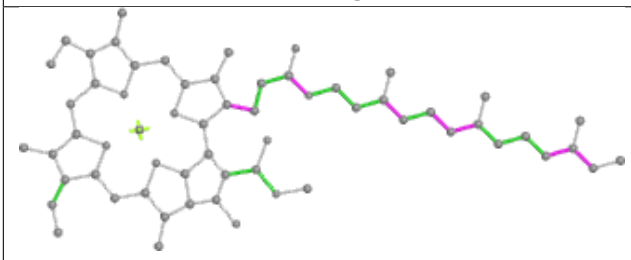
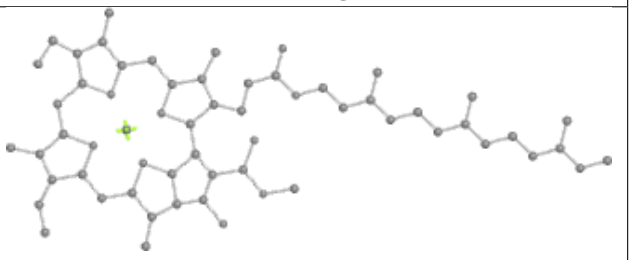


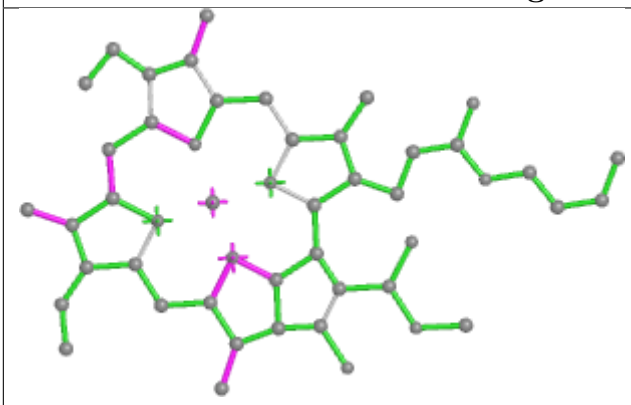
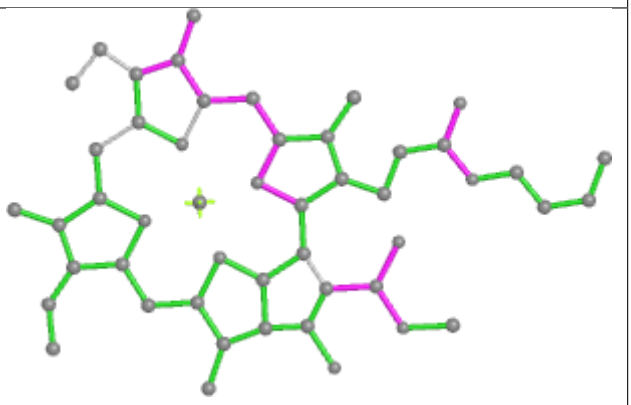
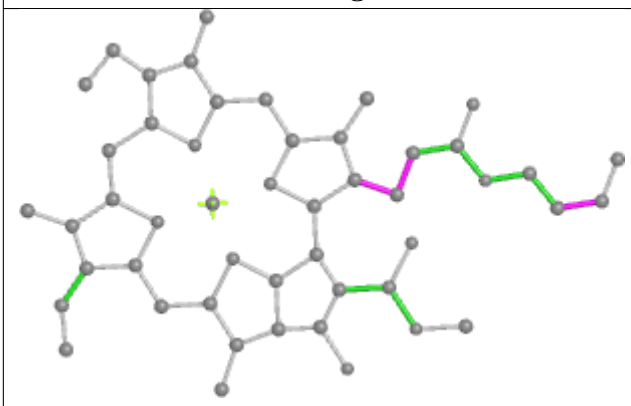
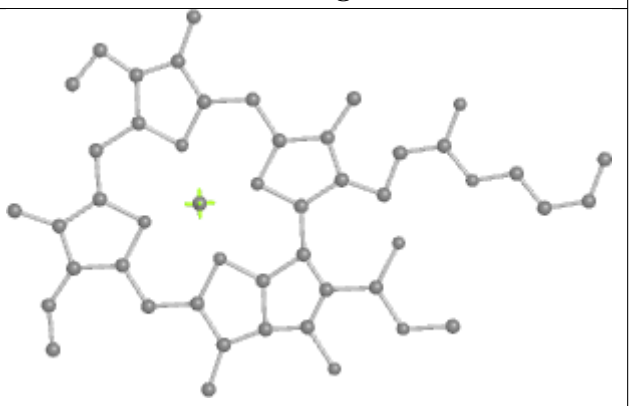
Torsions

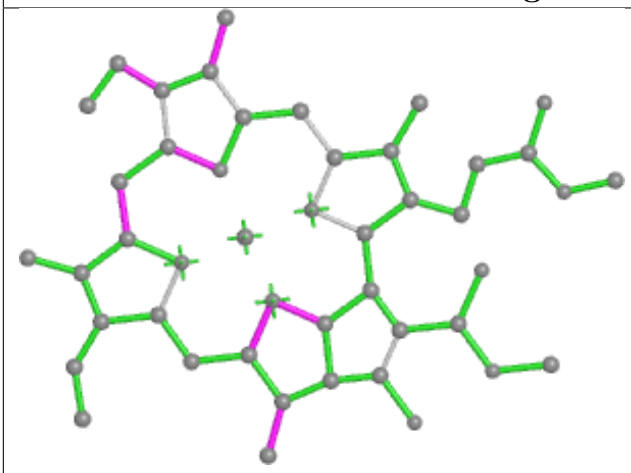
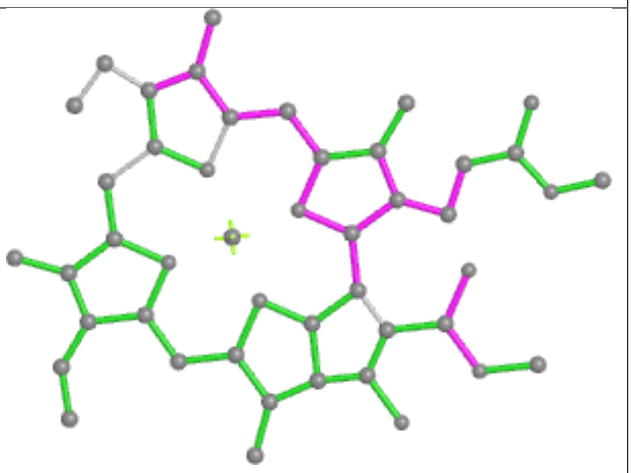
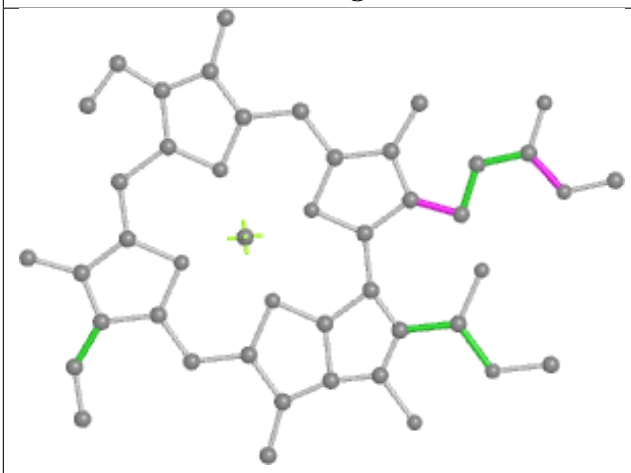
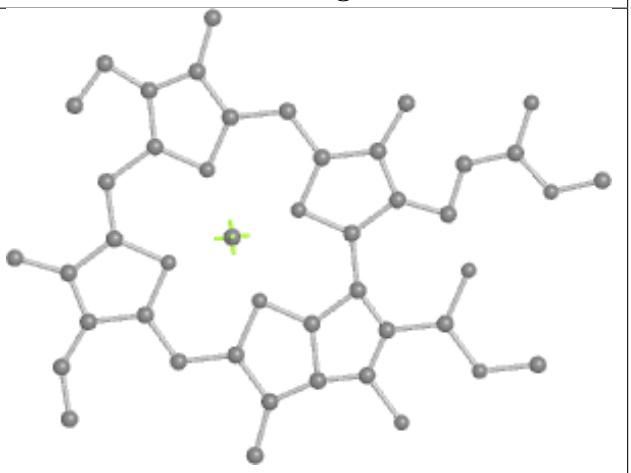


Rings

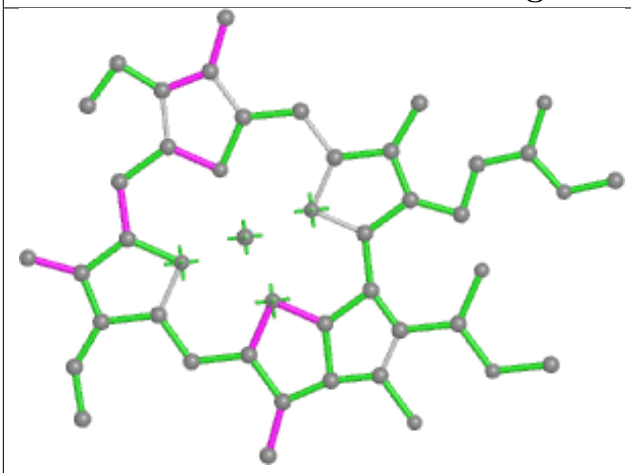
Ligand LMG D 320	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA I 305	
 Bond lengths	 Bond angles
 Torsions	 Rings

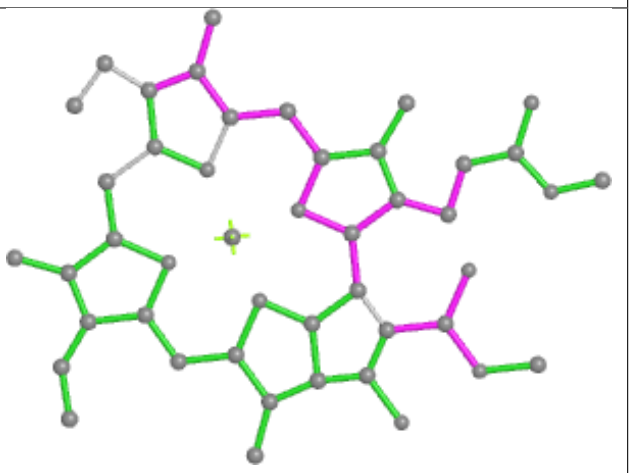
Ligand CLA b 832	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA N 311	
 Bond lengths	 Bond angles
 Torsions	 Rings

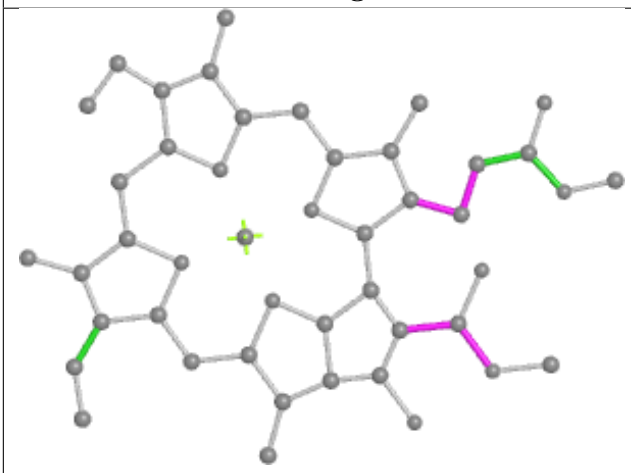
Ligand CLA L 312



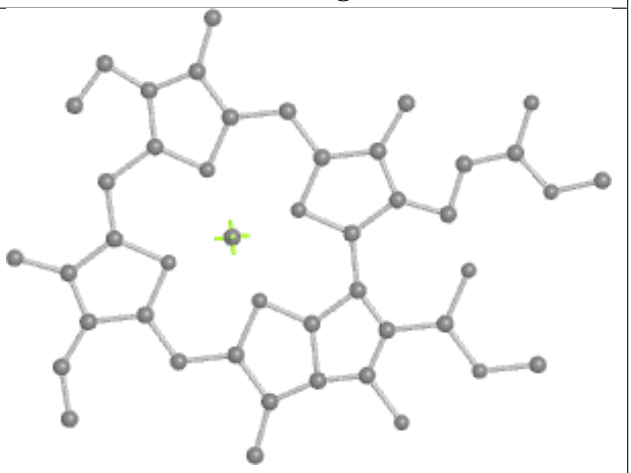
Bond lengths



Bond angles

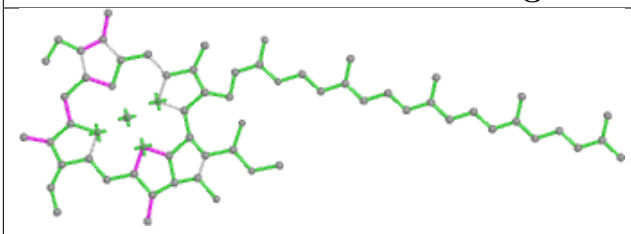


Torsions

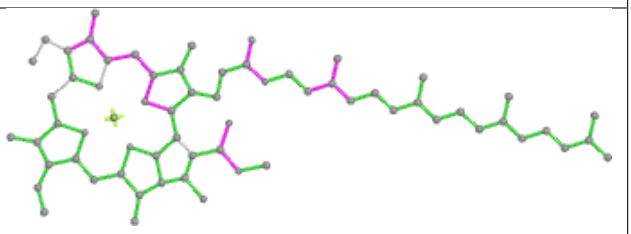


Rings

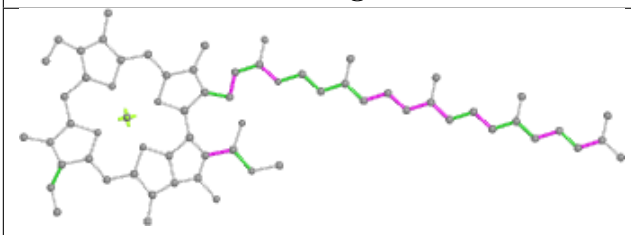
Ligand CLA O 308



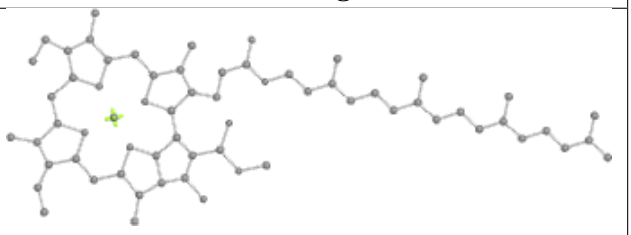
Bond lengths



Bond angles

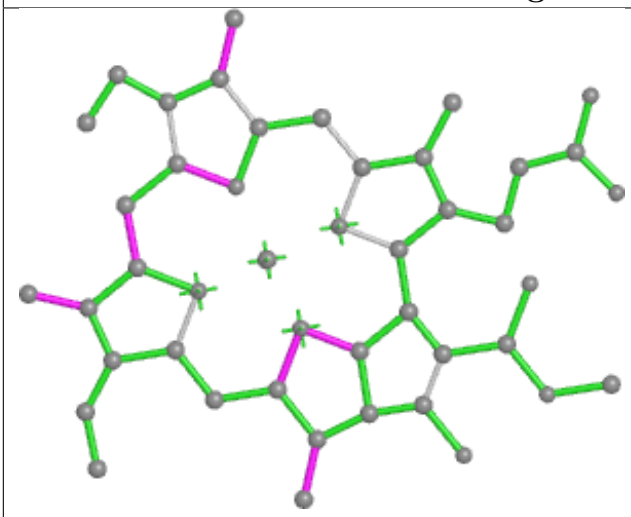


Torsions

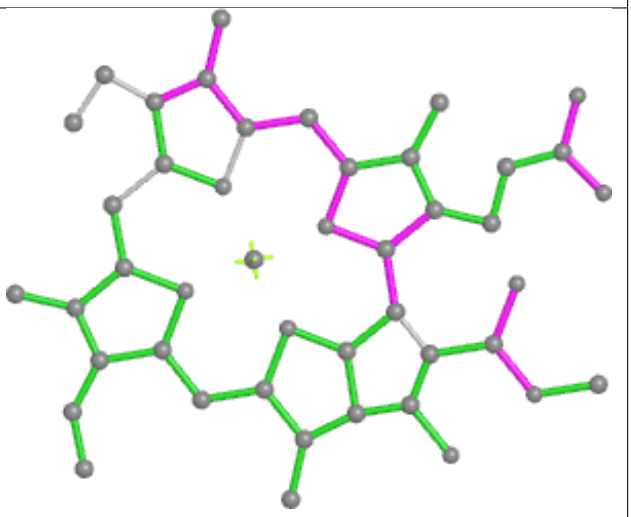


Rings

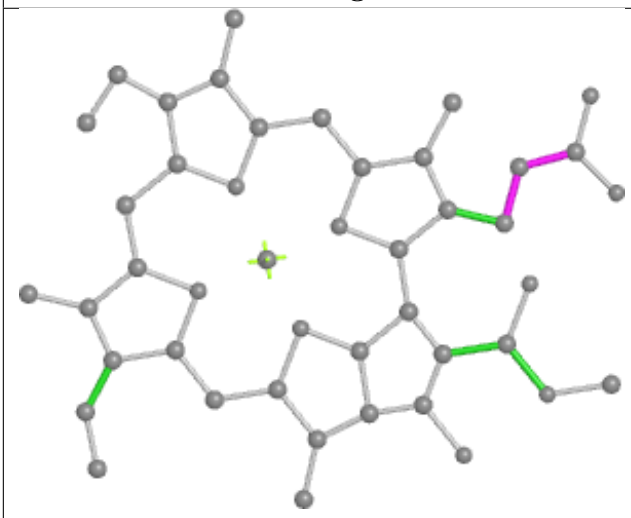
Ligand CLA b 807



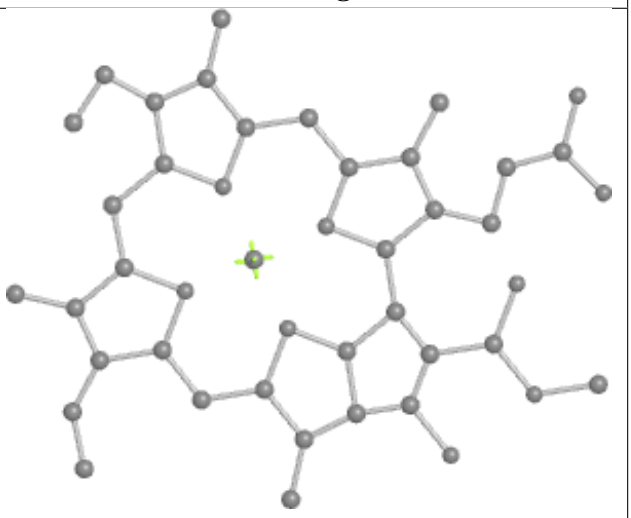
Bond lengths



Bond angles

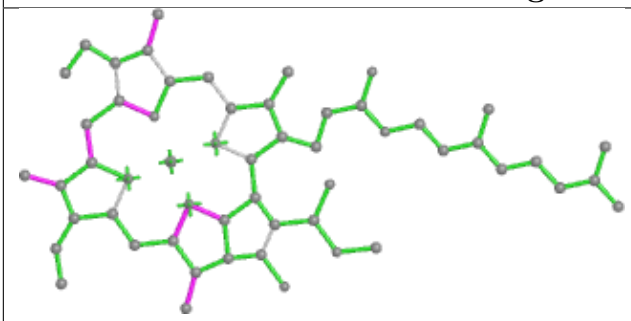


Torsions

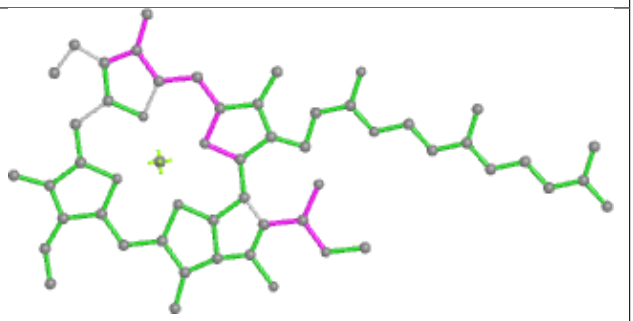


Rings

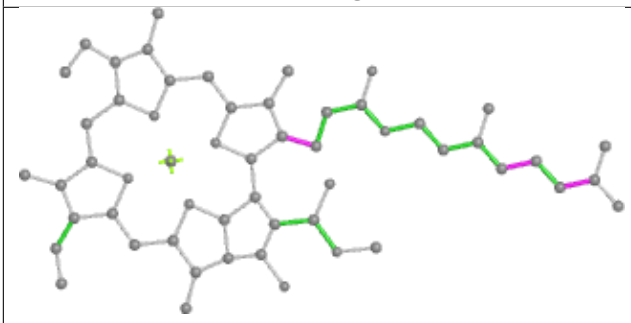
Ligand CLA b 823



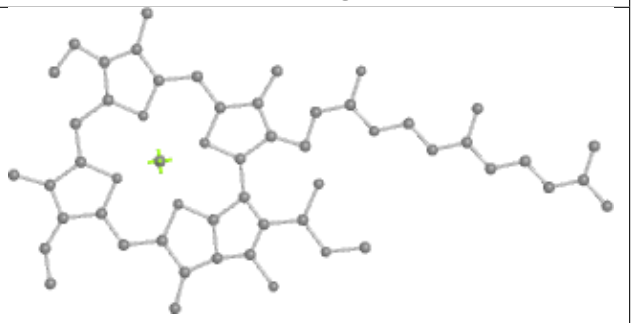
Bond lengths



Bond angles

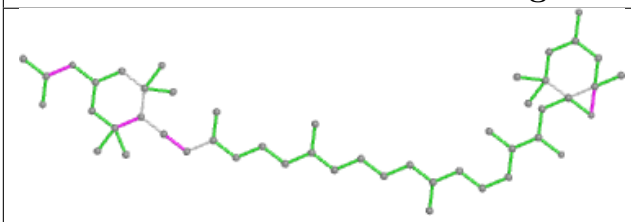


Torsions

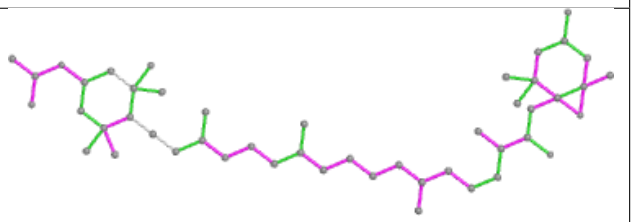


Rings

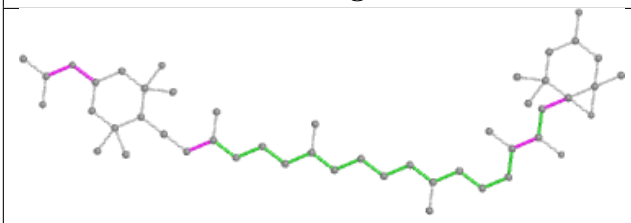
Ligand A86 A 316



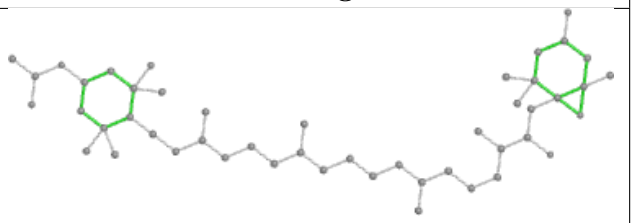
Bond lengths



Bond angles

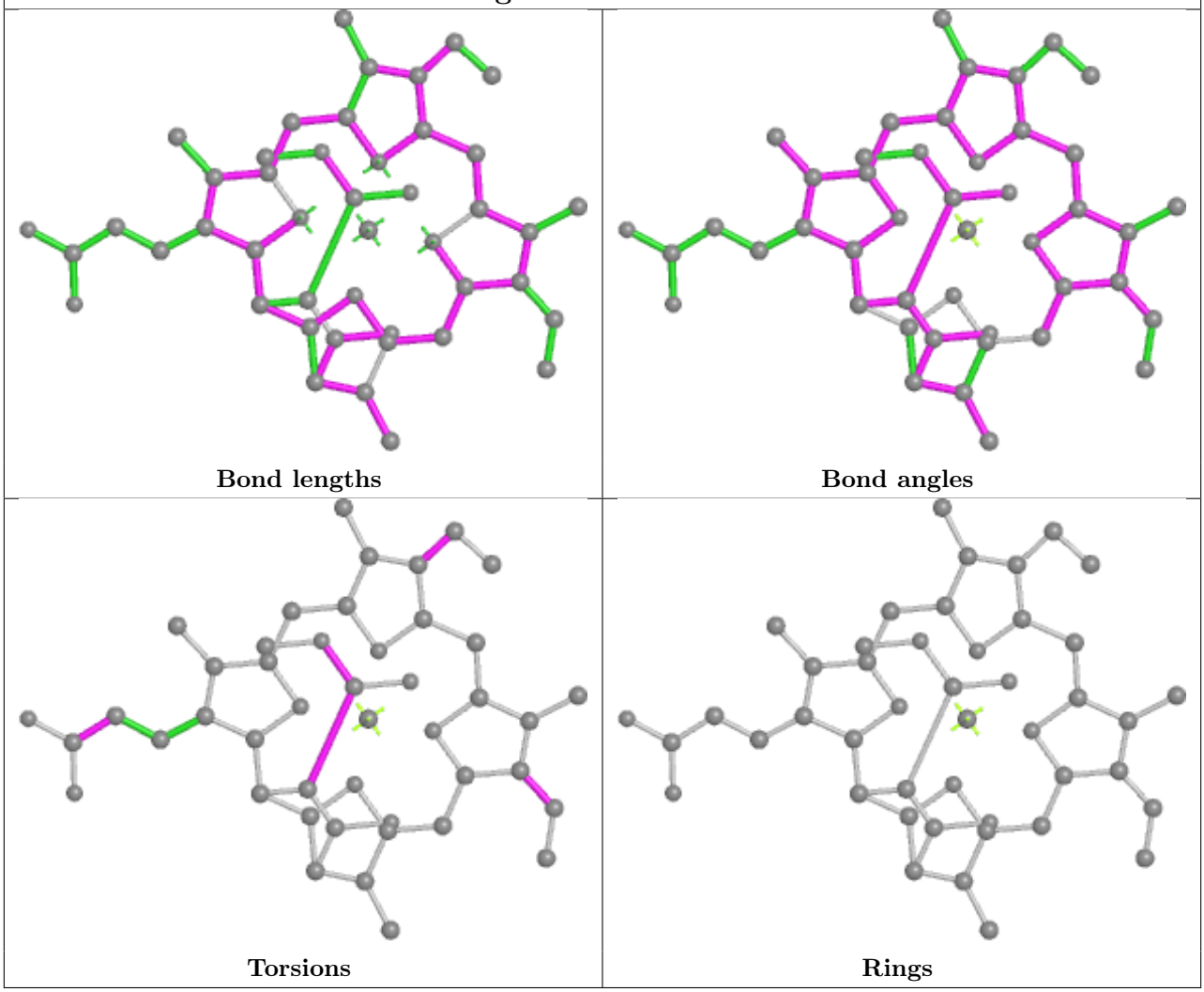


Torsions

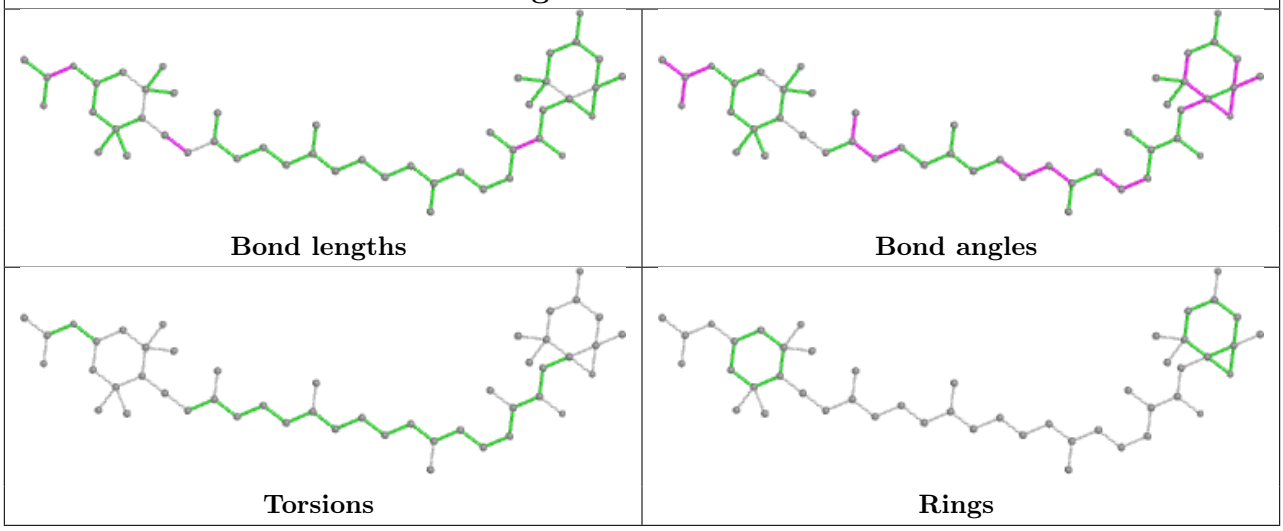


Rings

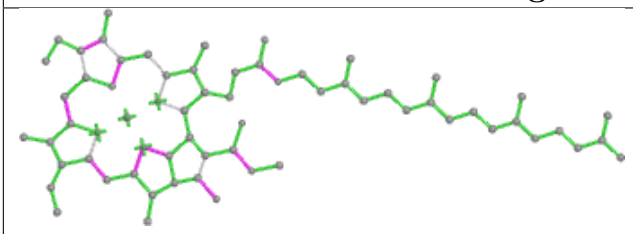
Ligand KC1 T 310



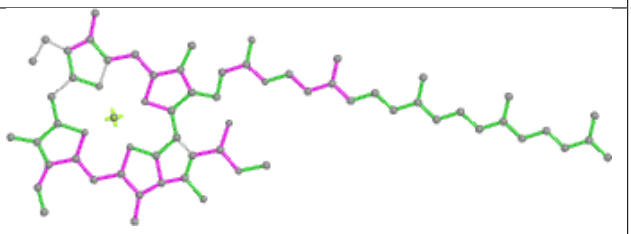
Ligand A86 T 304



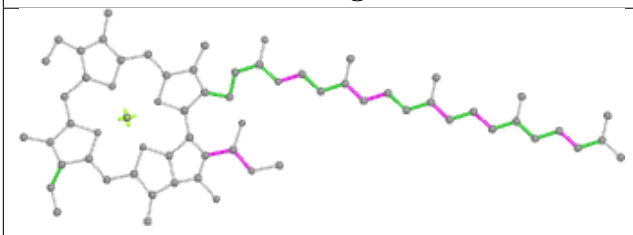
Ligand CLA a 806



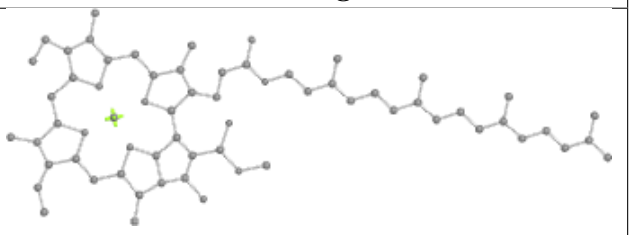
Bond lengths



Bond angles

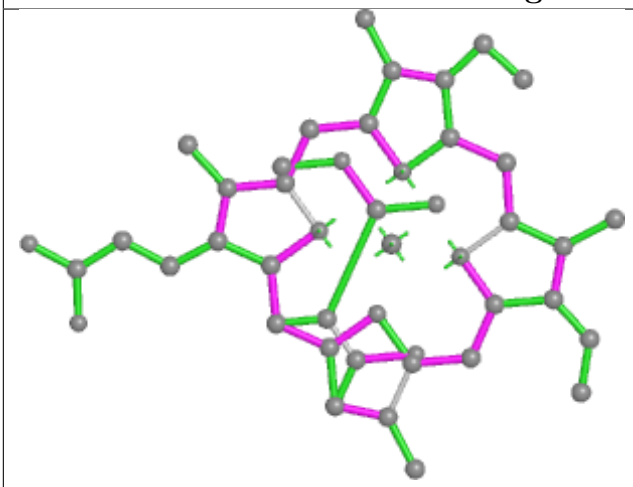


Torsions

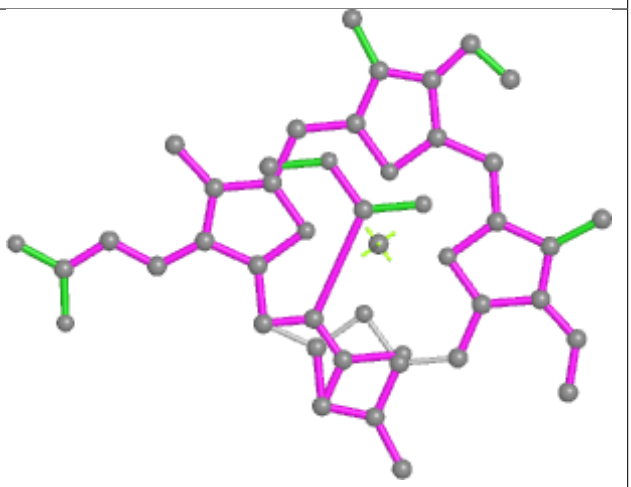


Rings

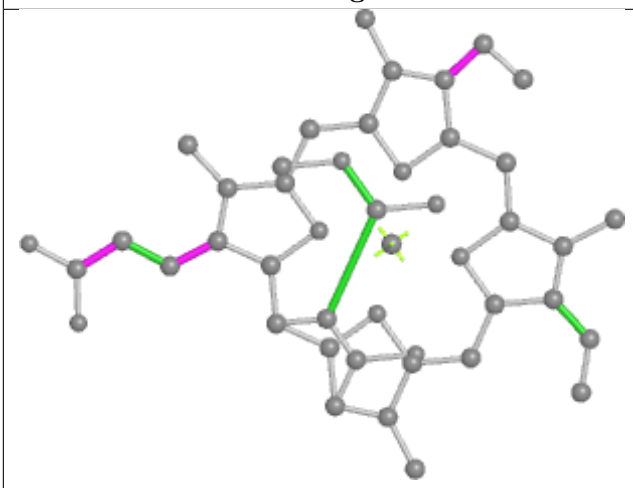
Ligand KC1 K 314



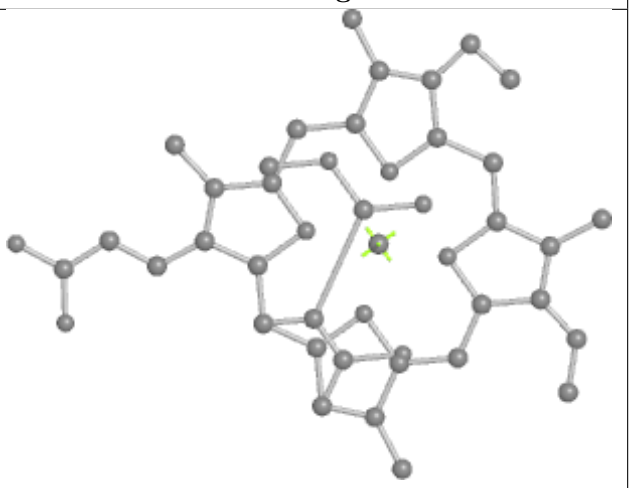
Bond lengths



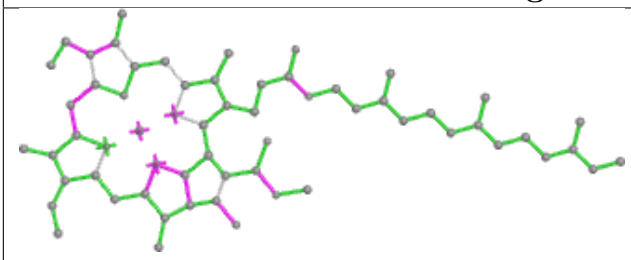
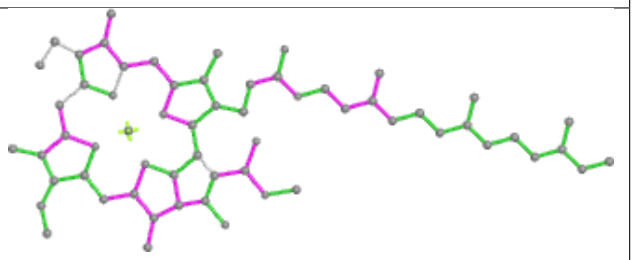
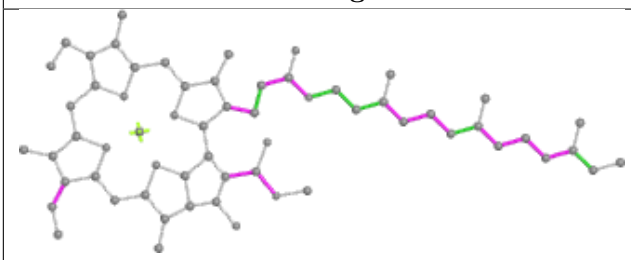
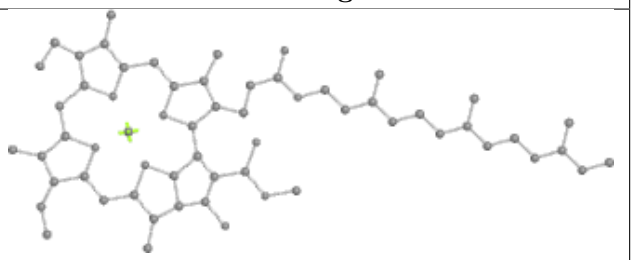
Bond angles

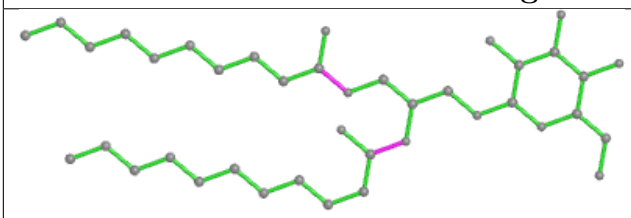
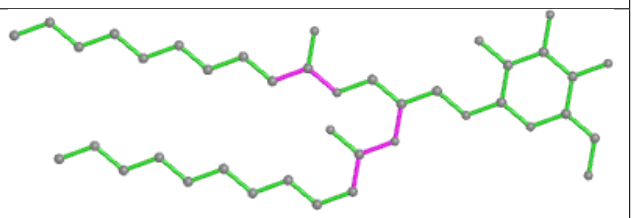
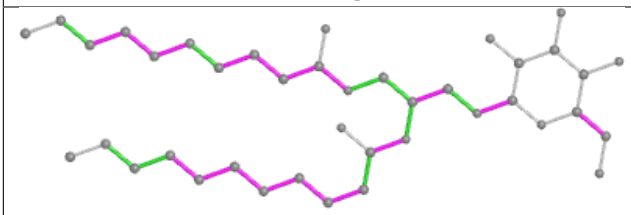
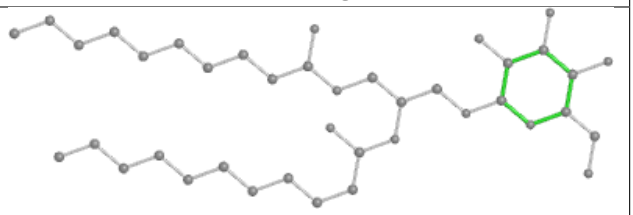


Torsions

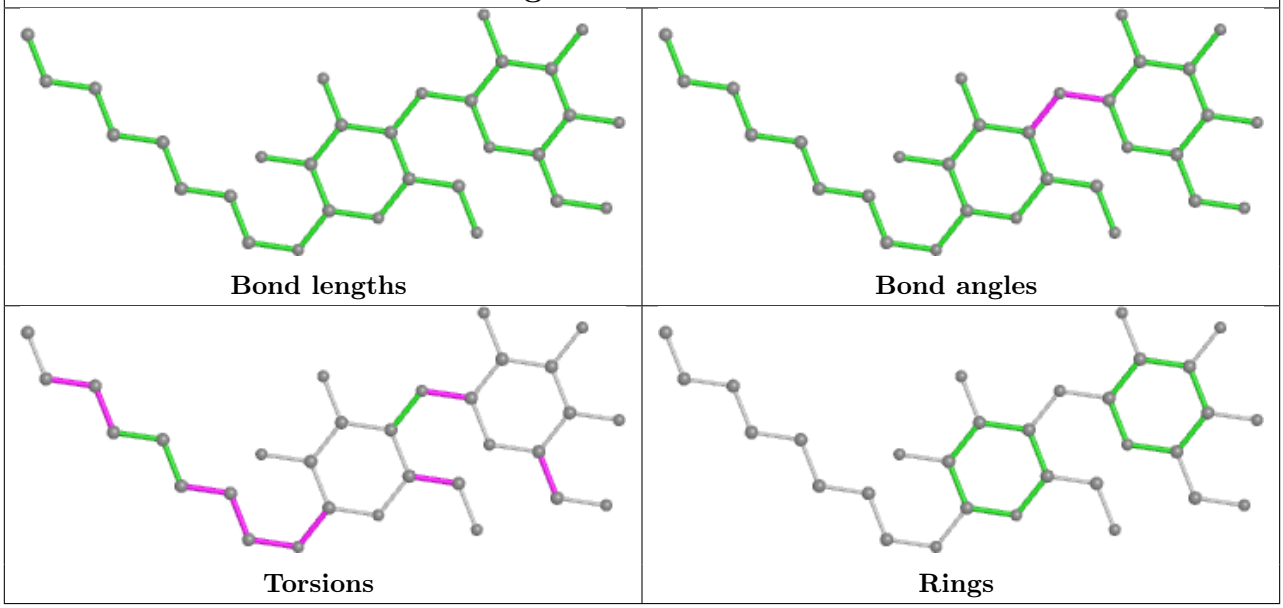


Rings

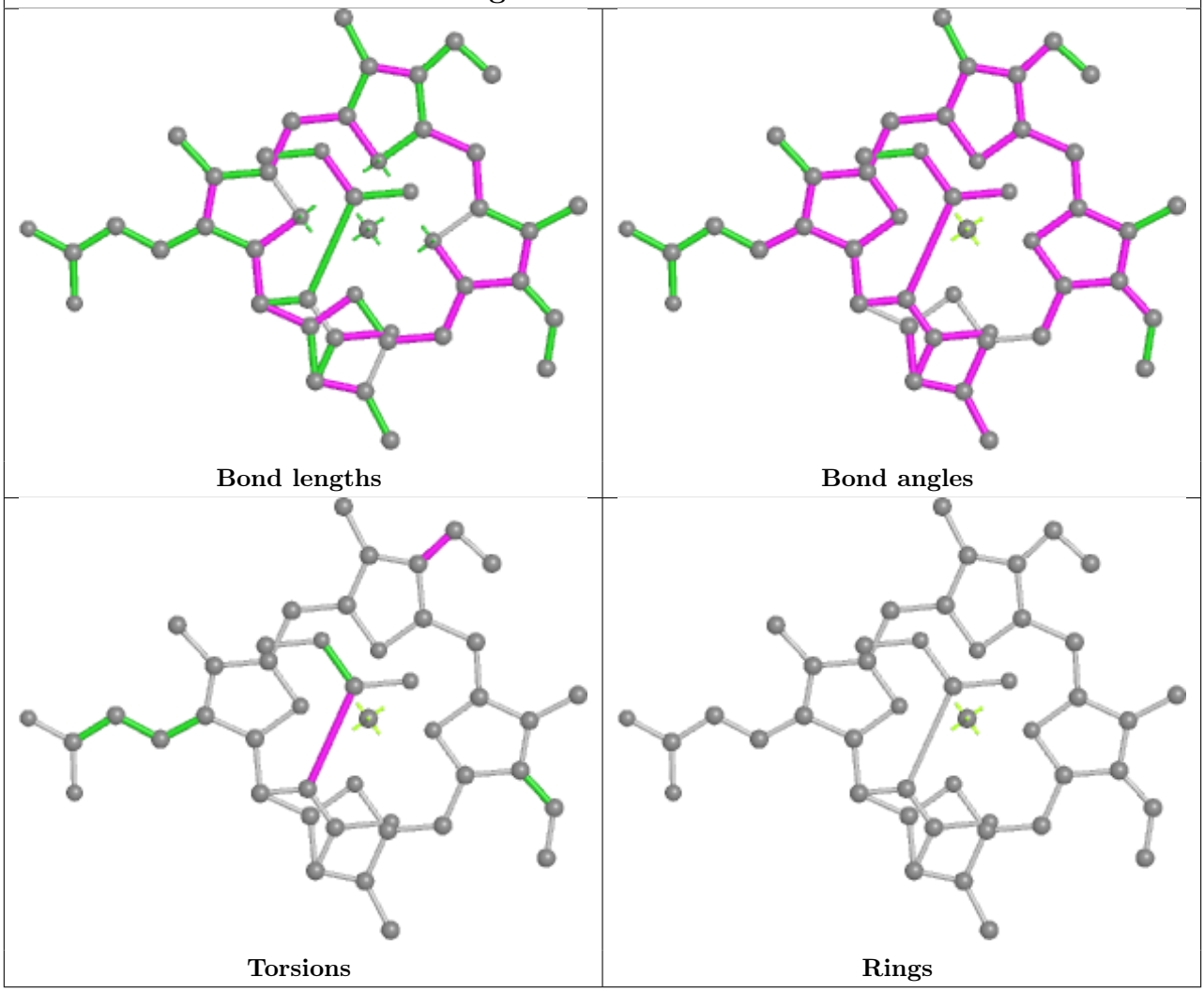
Ligand CLA L 308	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand LMG E 319	
 Bond lengths	 Bond angles
 Torsions	 Rings

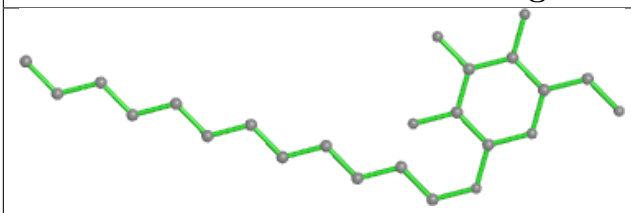
Ligand LMT L 318



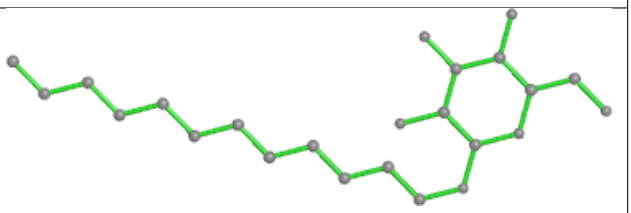
Ligand KC1 W 217



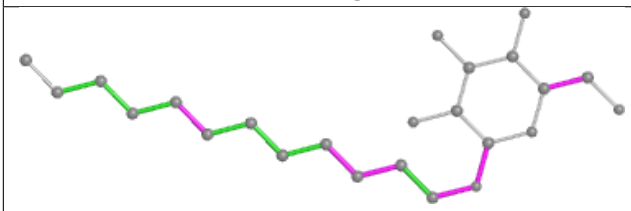
Ligand LMT f 807



Bond lengths



Bond angles



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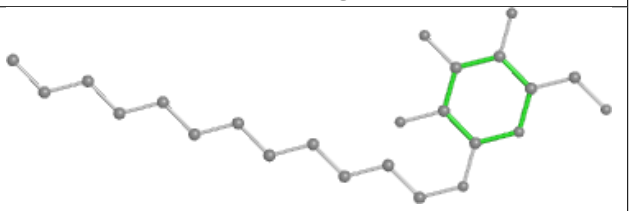
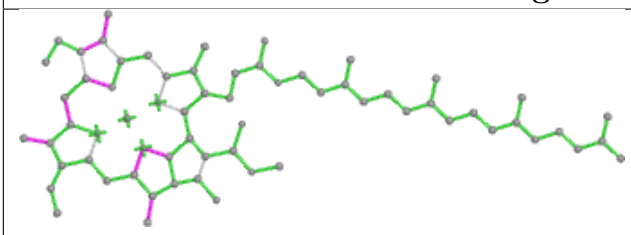
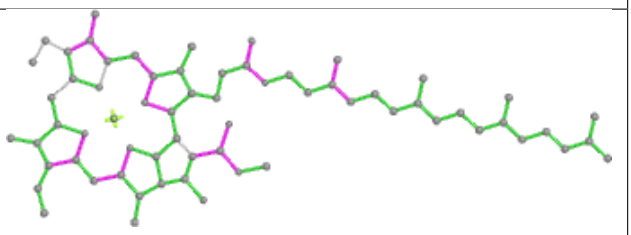


Rings

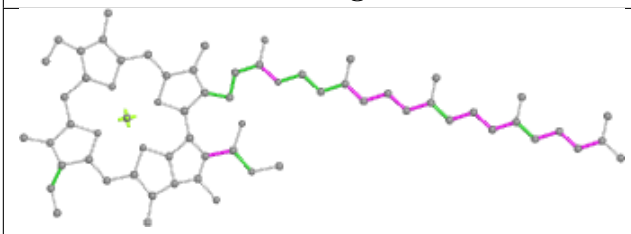
Ligand CLA l 201



Bond lengths



Bond angles



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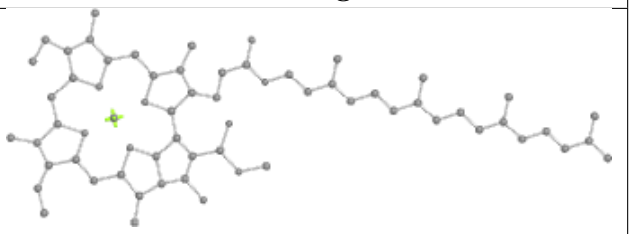
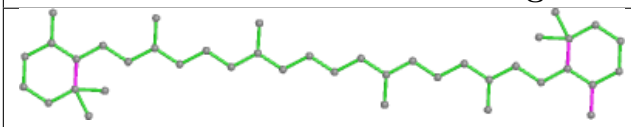
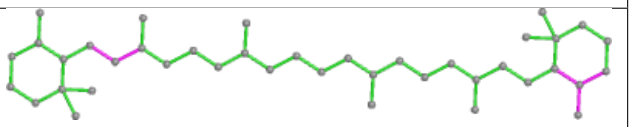


Rings

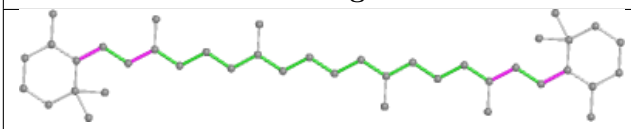
Ligand BCR a 846



Bond lengths

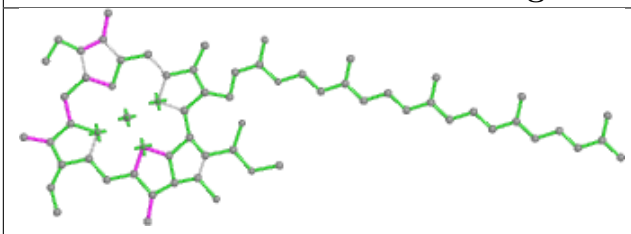
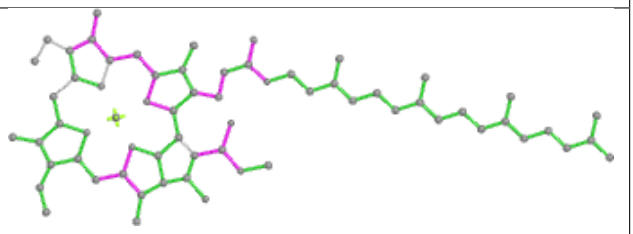
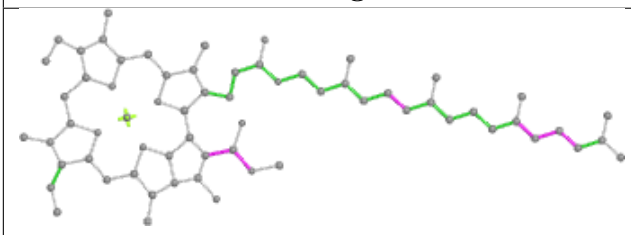
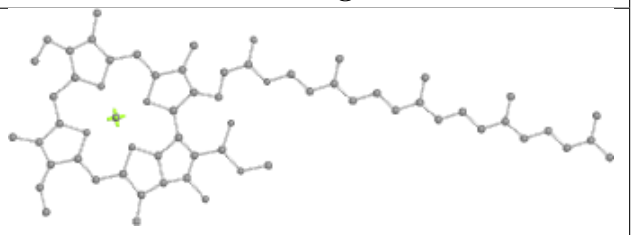


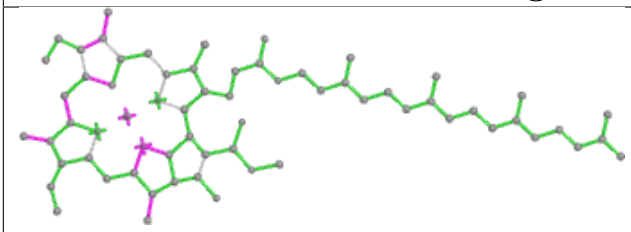
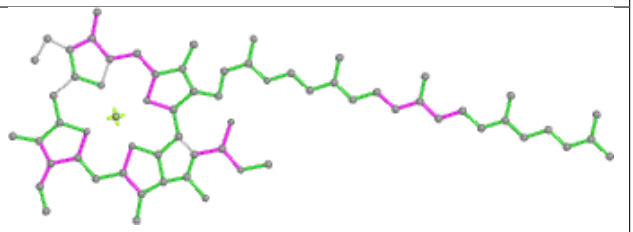
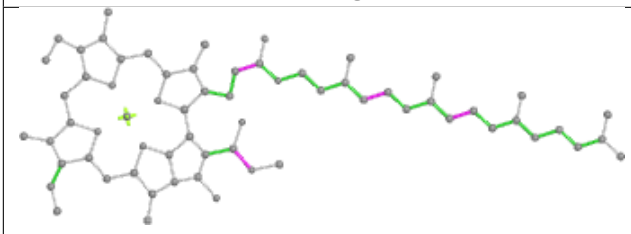
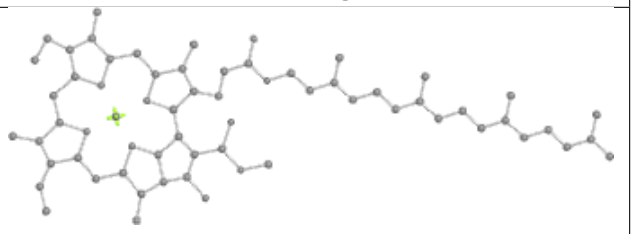
Bond angles



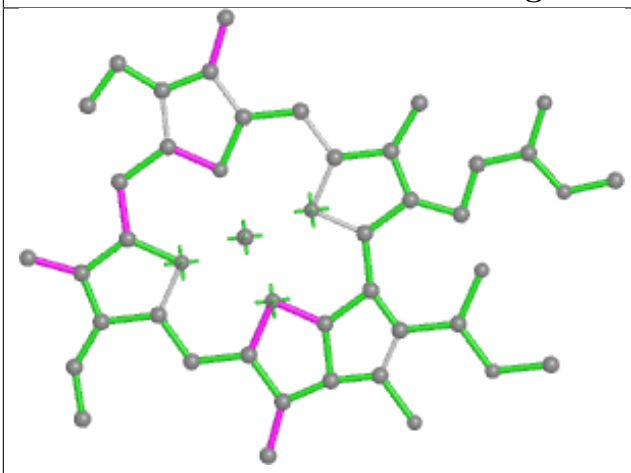
Torsions

Rings

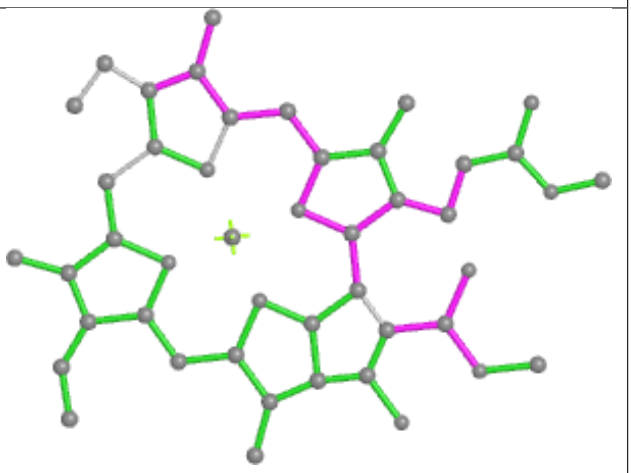
Ligand CLA b 837	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA b 812	
 Bond lengths	 Bond angles
 Torsions	 Rings

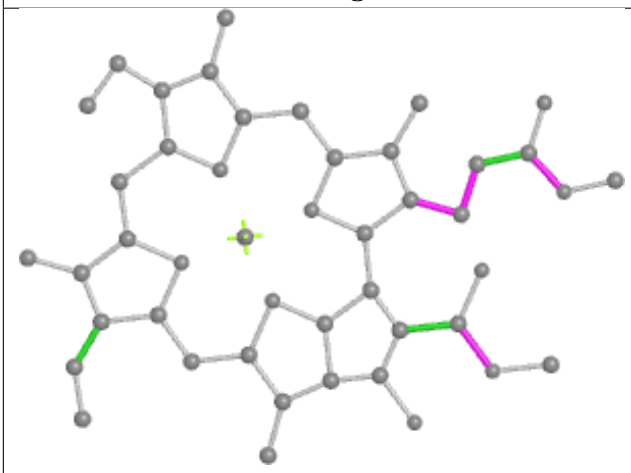
Ligand CLA P 312



Bond lengths



Bond angles



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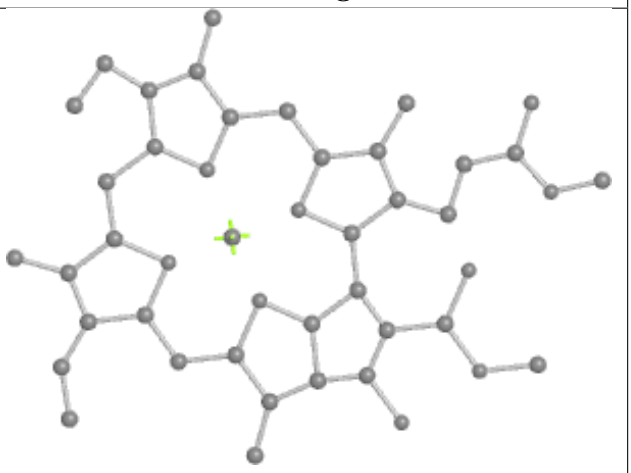
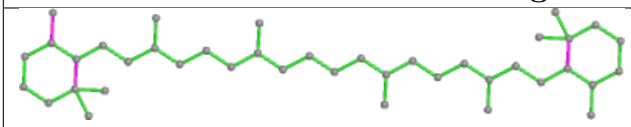


Rings

Ligand BCR f 806



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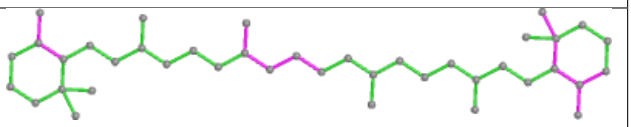
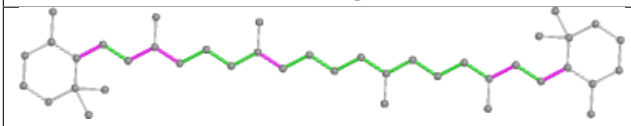


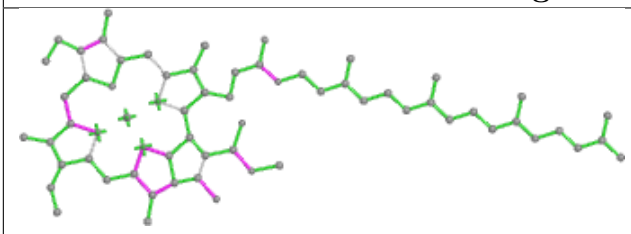
Bond angles



Torsions

Rings

Ligand CLA l 205



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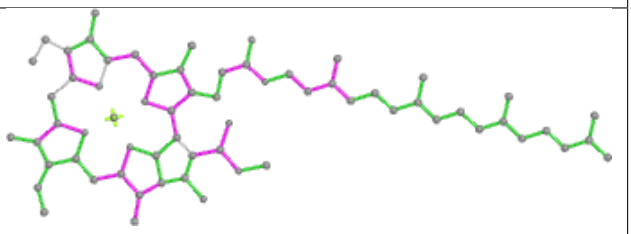
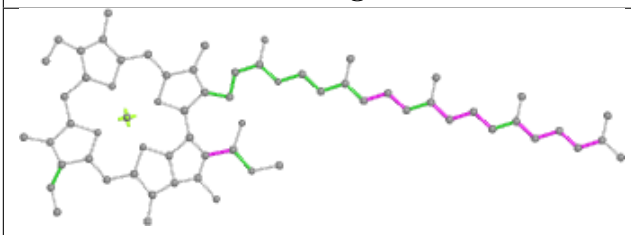
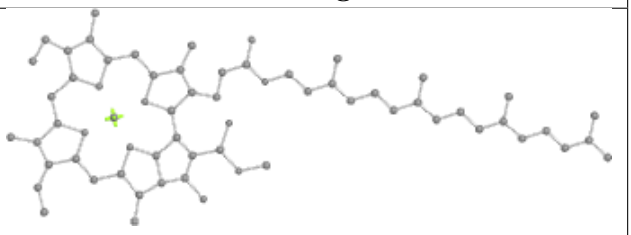


Bond angles

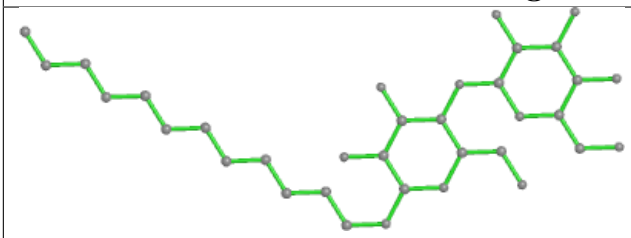


Torsions



Rings

Ligand LMT a 854



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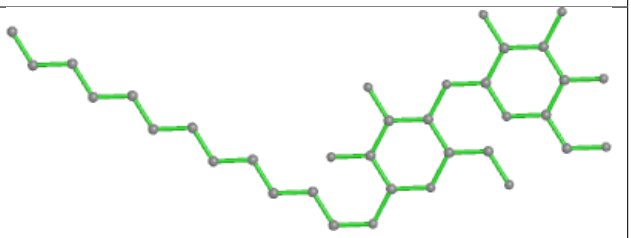
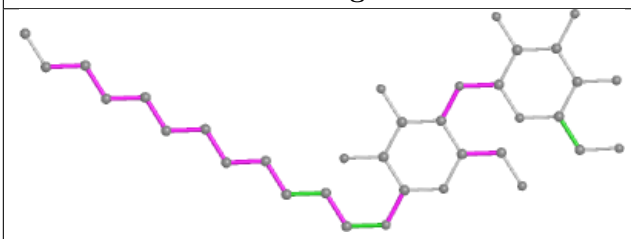
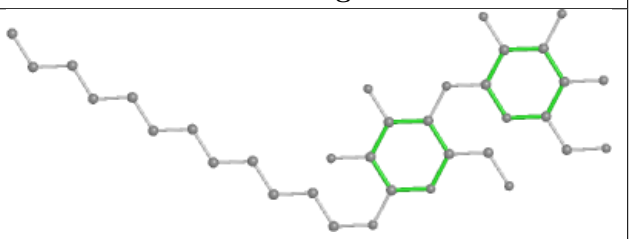


Bond angles

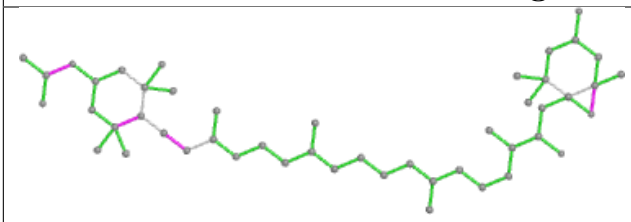


Torsions

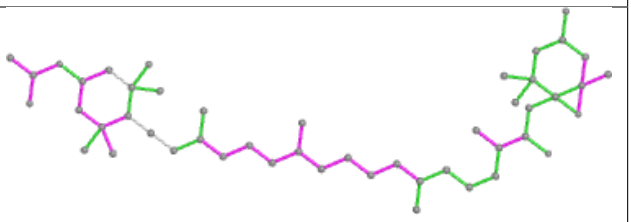


Rings

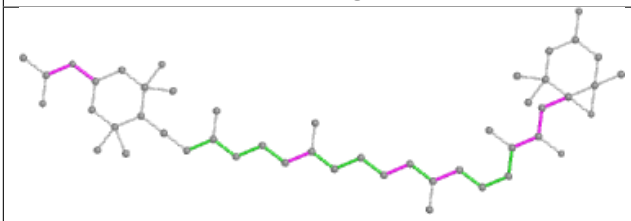
Ligand A86 O 305



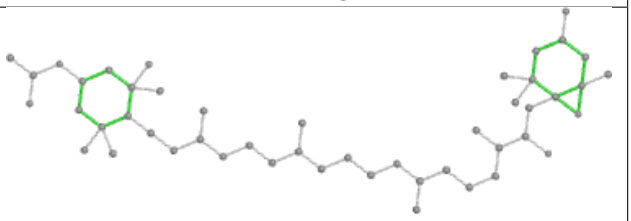
Bond lengths



Bond angles

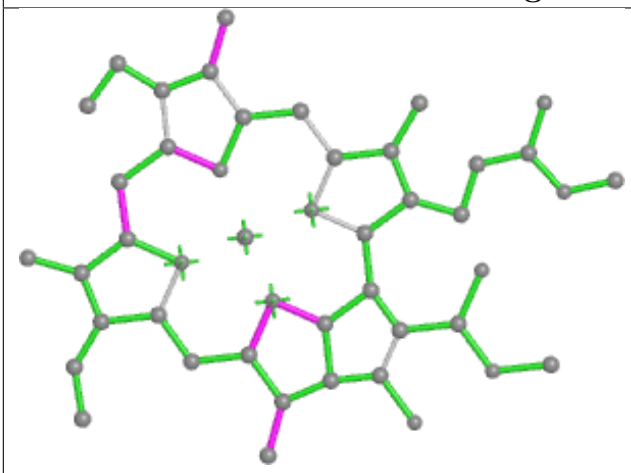


Torsions

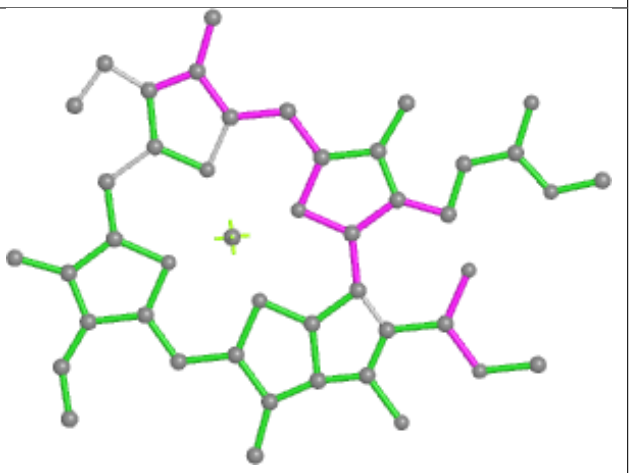


Rings

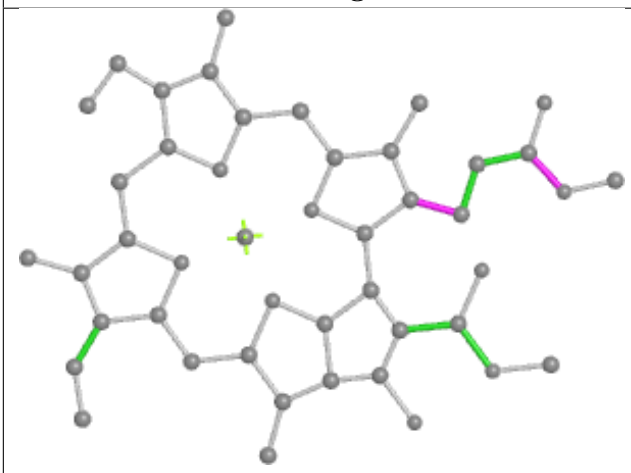
Ligand CLA C 210



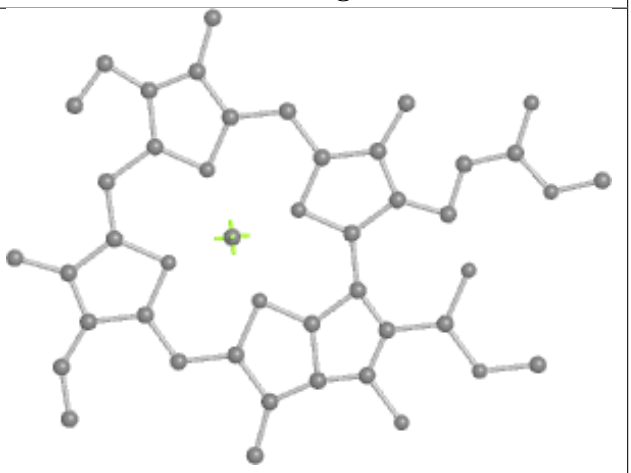
Bond lengths



Bond angles

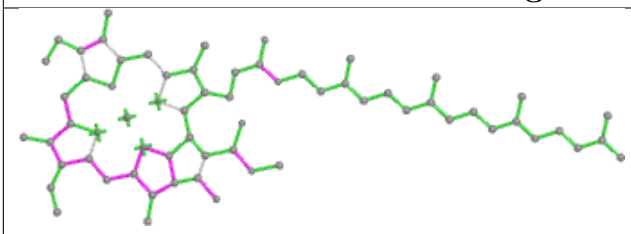


Torsions

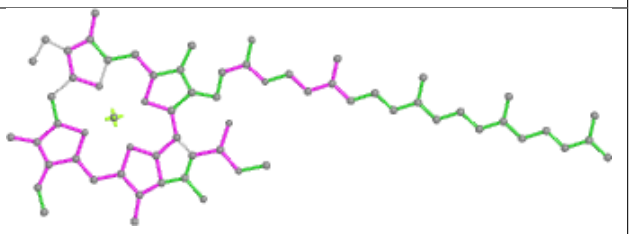


Rings

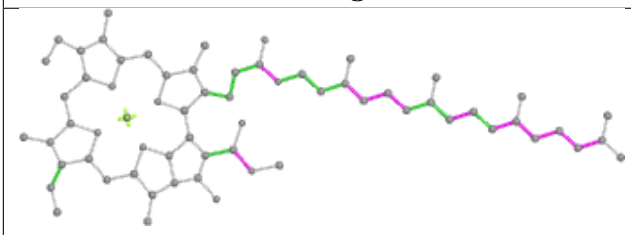
Ligand CLA E 315



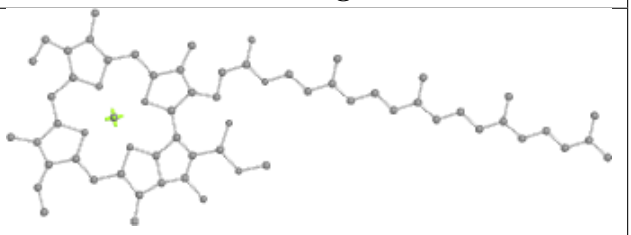
Bond lengths



Bond angles

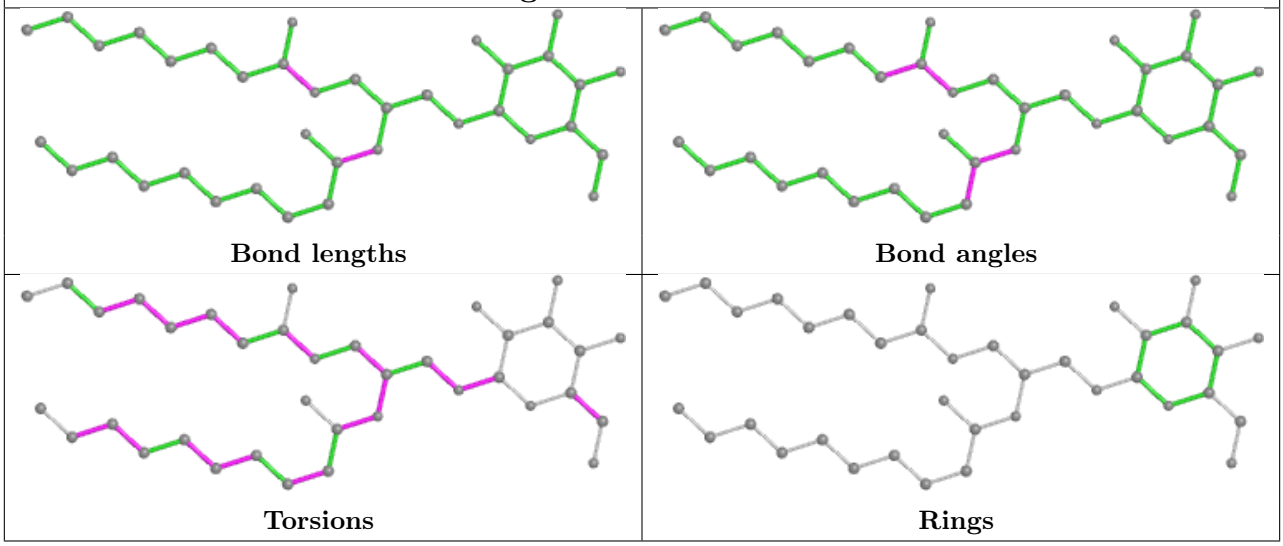


Torsions

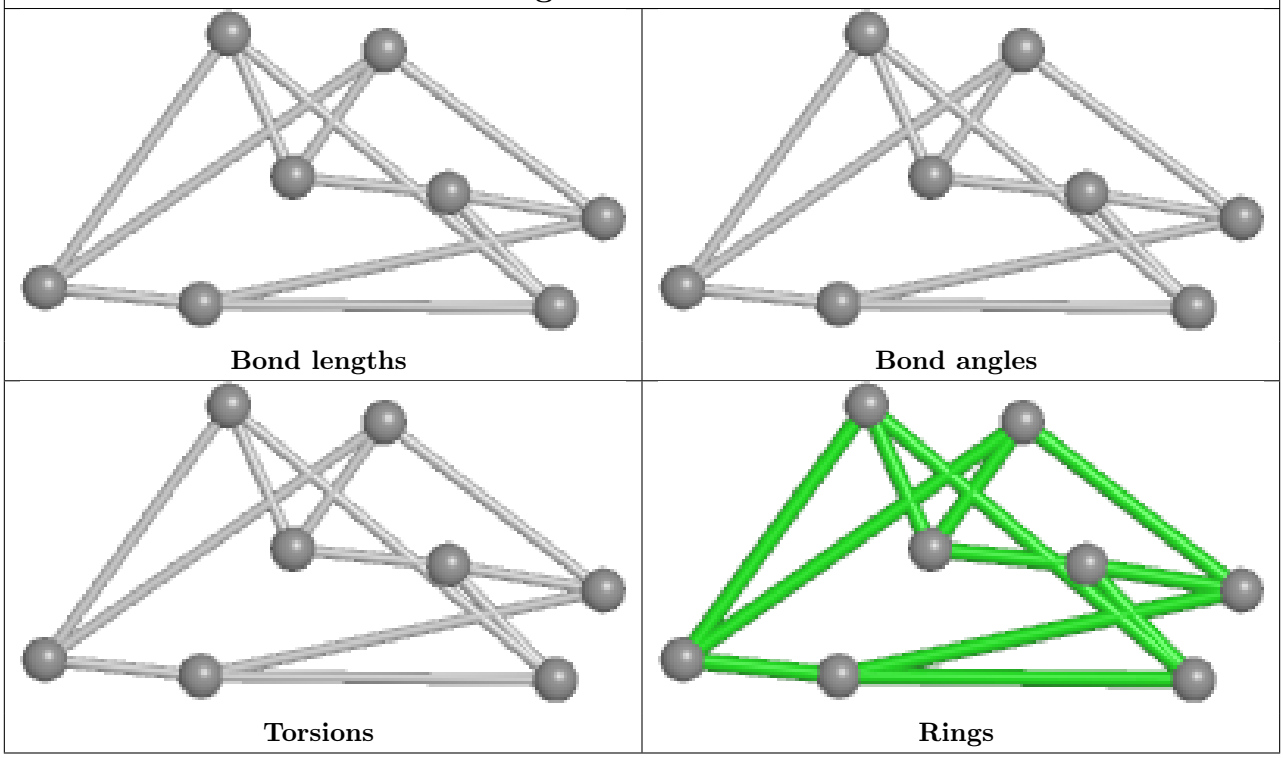


Rings

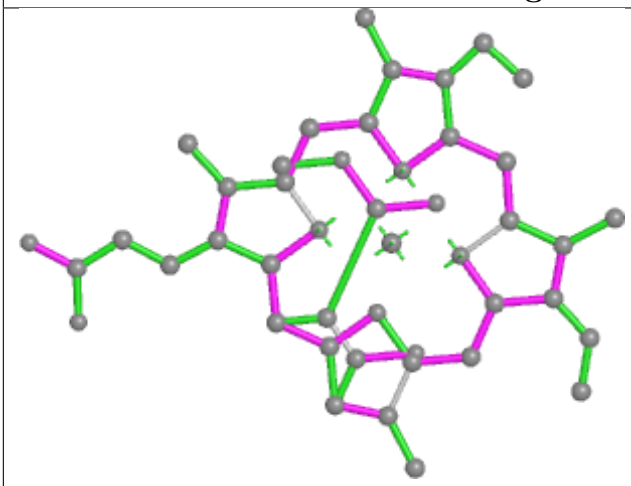
Ligand LMG D 321



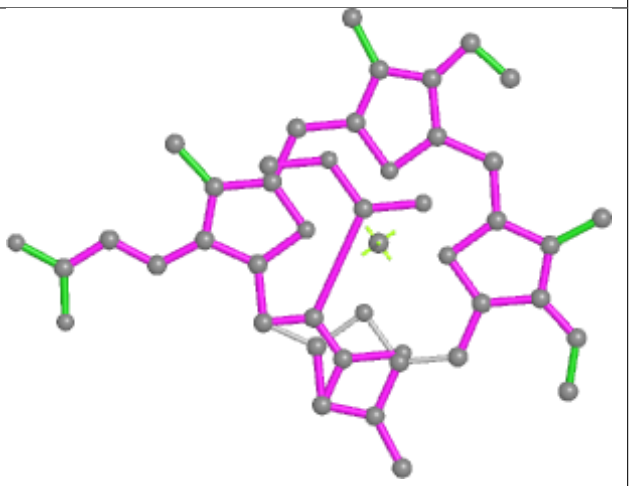
Ligand SF4 b 803



Ligand KC1 G 317



Bond lengths



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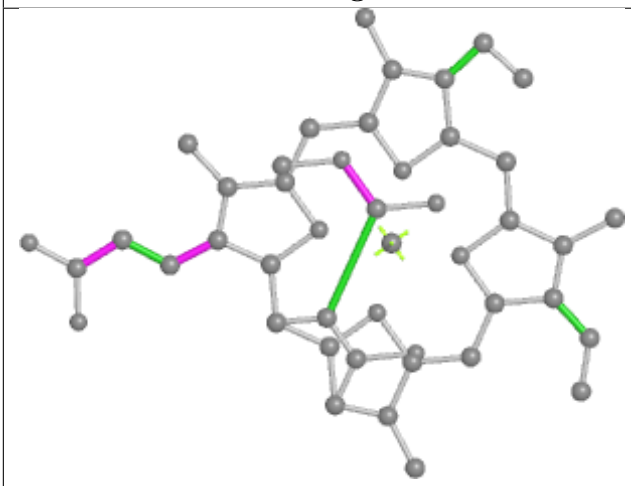

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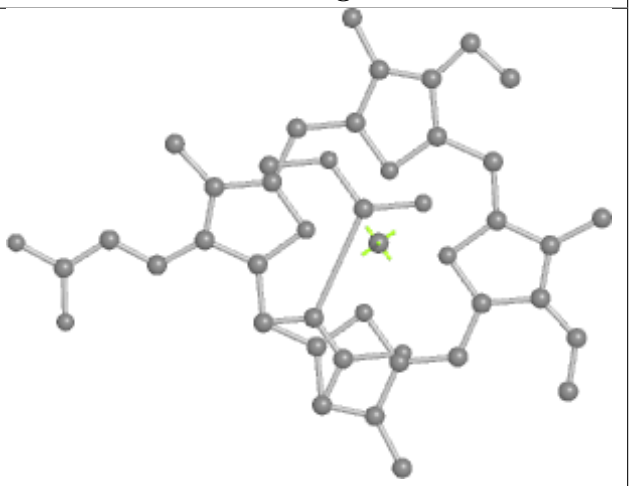
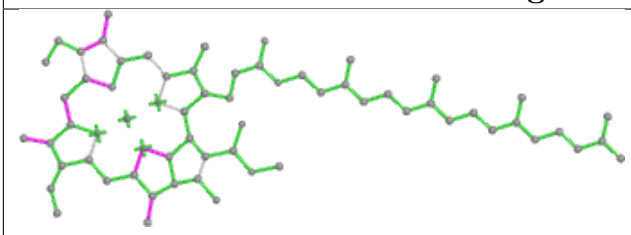


Rings

Ligand CLA b 802



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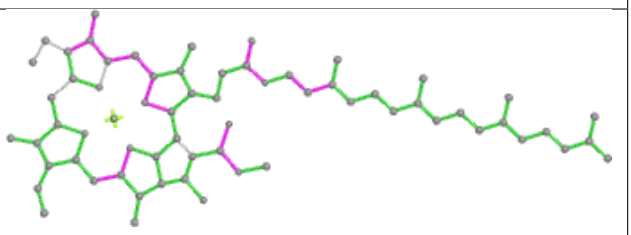
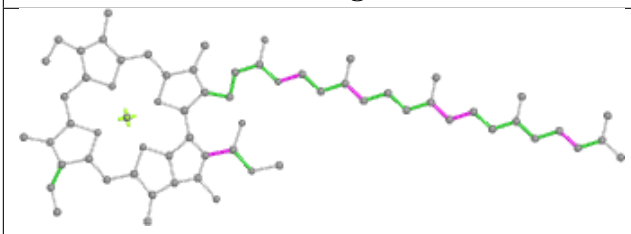


Bond angles



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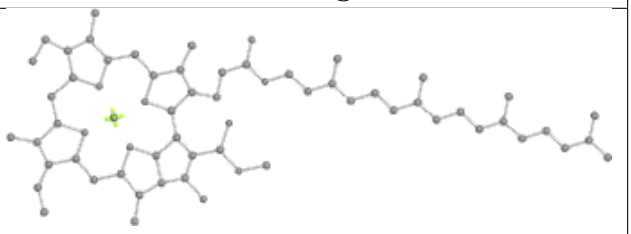
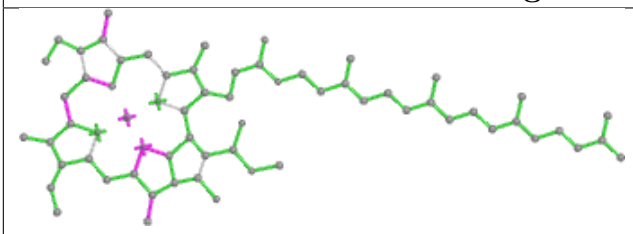


Rings

Ligand CLA R 321



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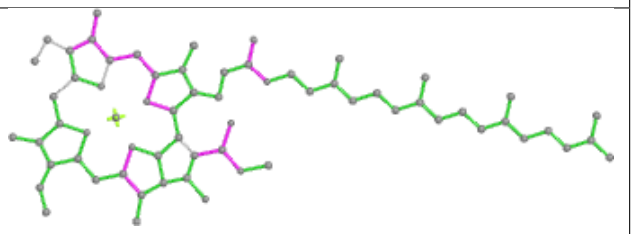
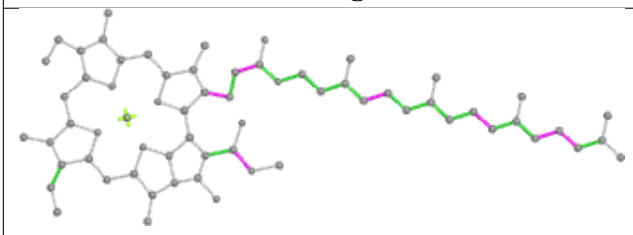


Bond angles



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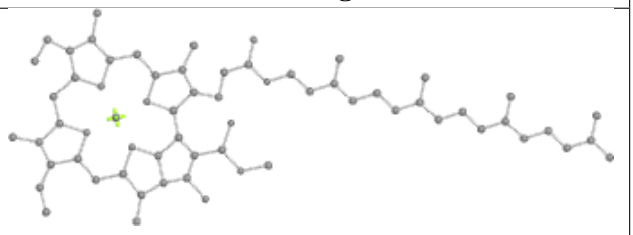
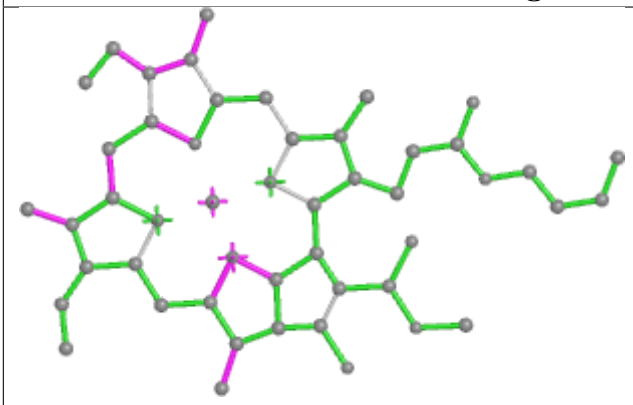


Rings

Ligand CLA E 308



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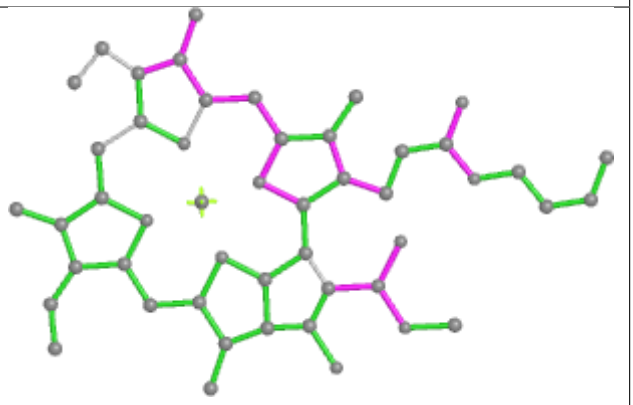
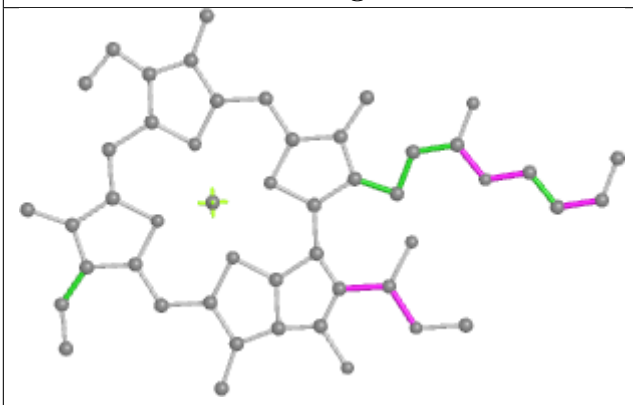


Bond angles



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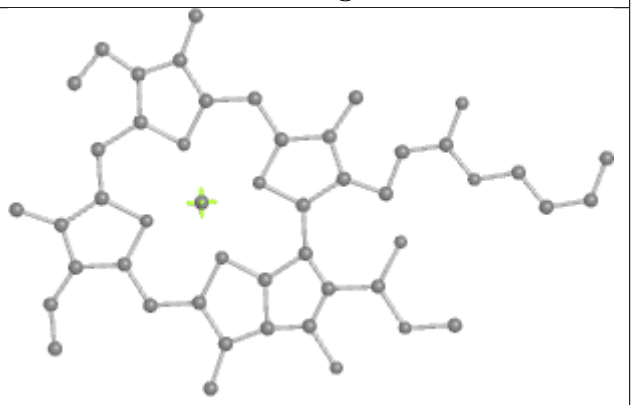
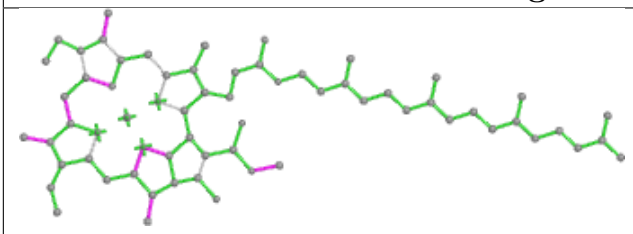


Rings

Ligand CLA a 836



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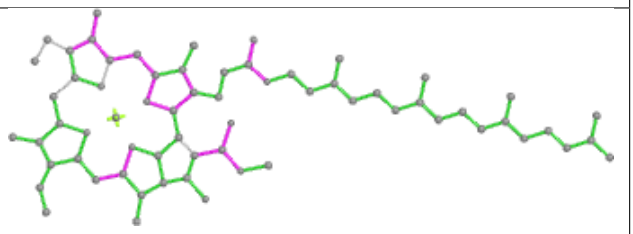
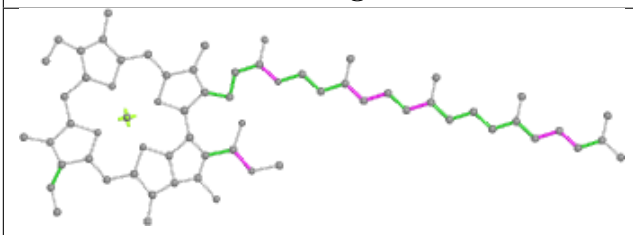


Bond angles



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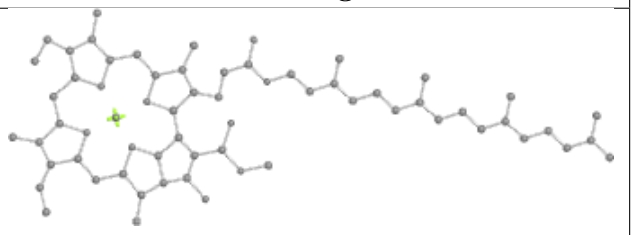
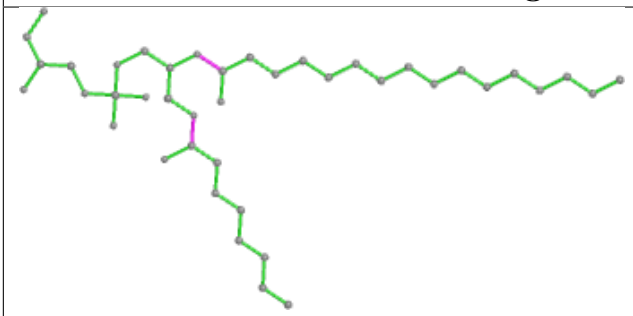


Rings

Ligand LHG F 319



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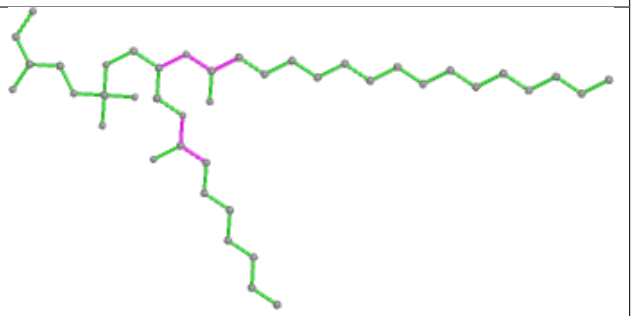
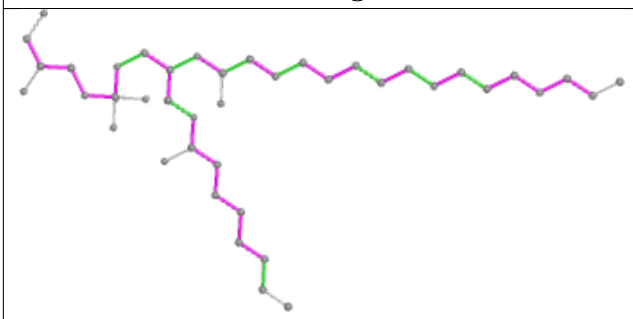


Bond angles



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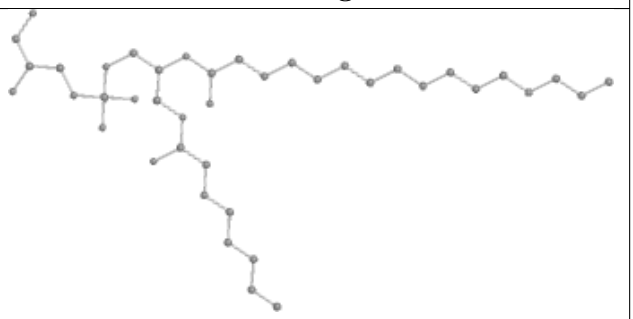
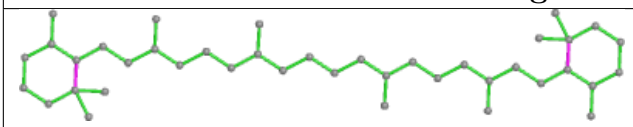


Rings

Ligand BCR f 801



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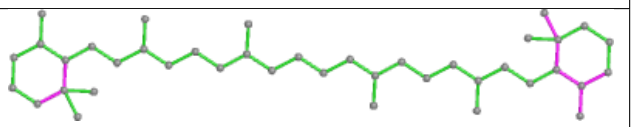
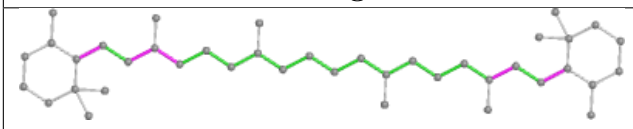


Bond angles



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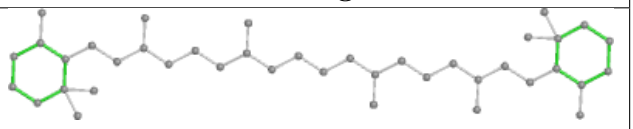
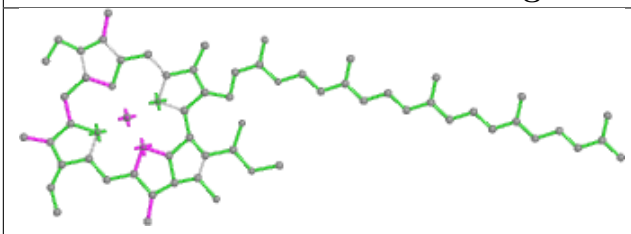
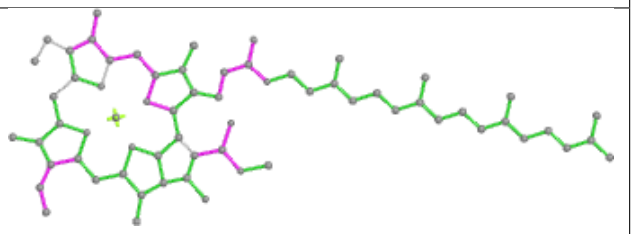
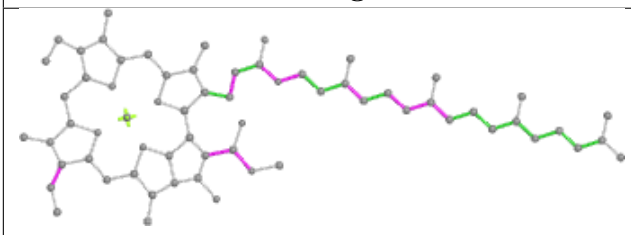
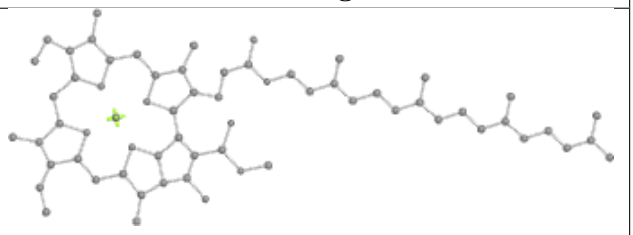
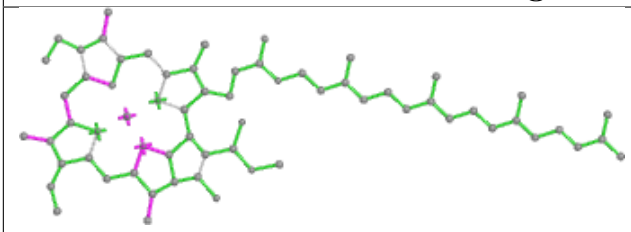
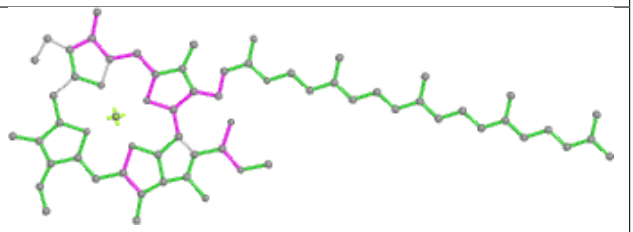
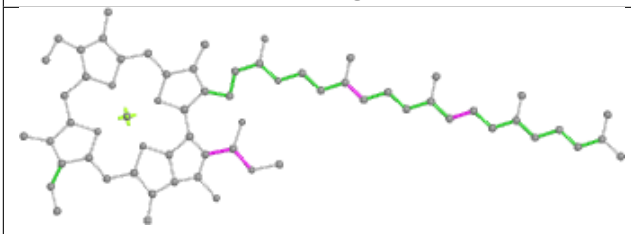
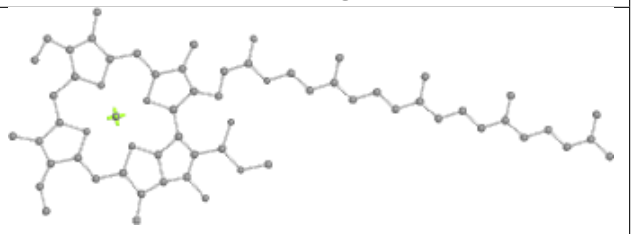
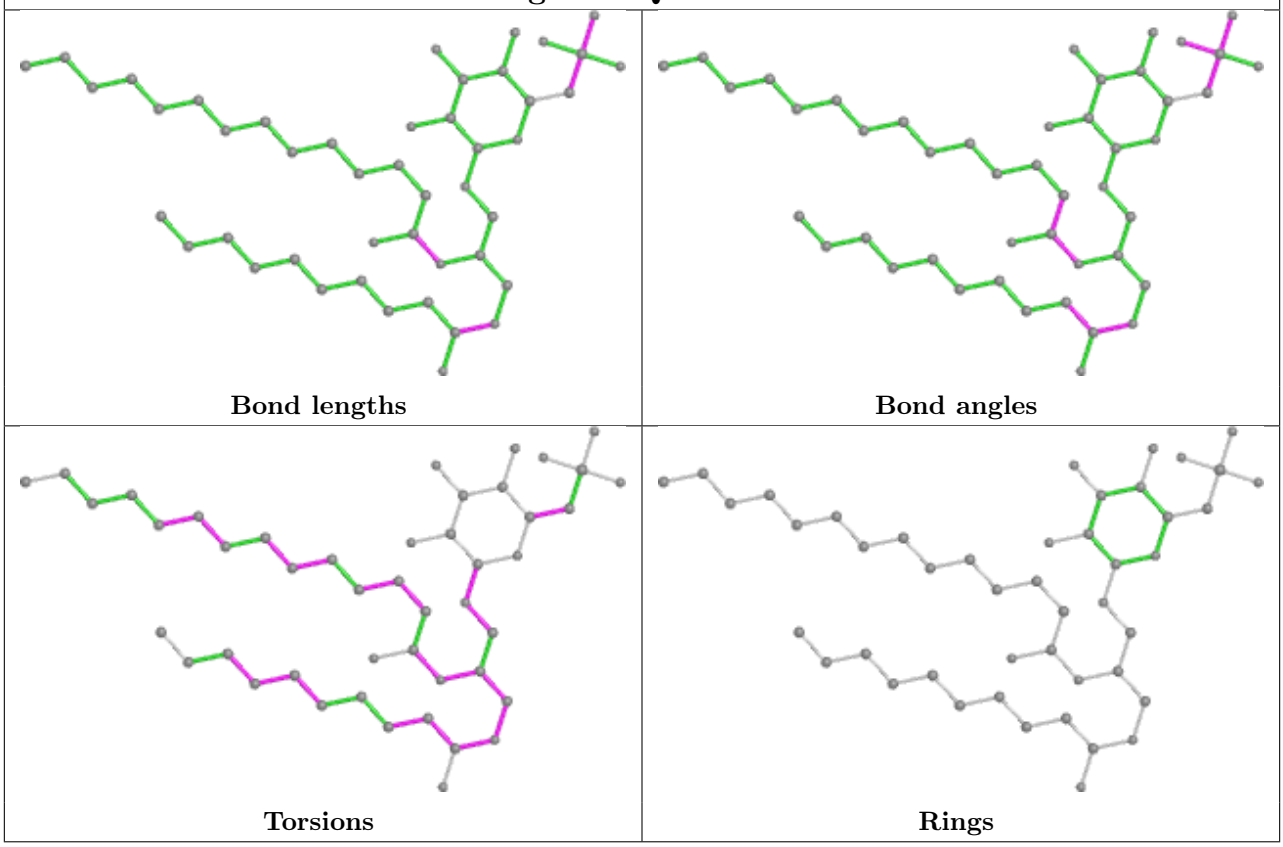


Rings

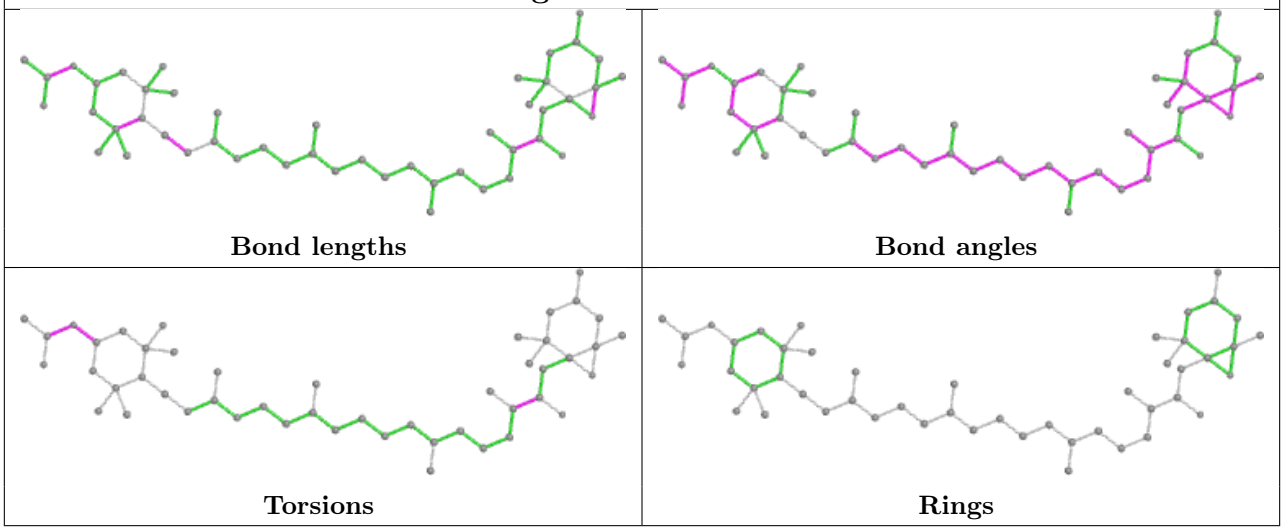
Ligand CLA D 308	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA S 319	
 Bond lengths	 Bond angles
 Torsions	 Rings

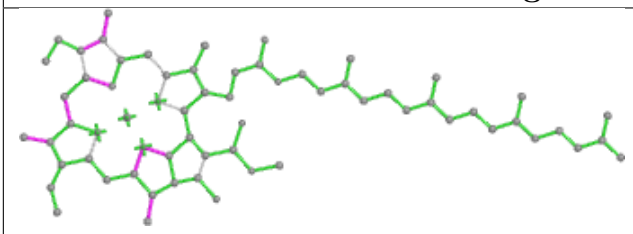
Ligand SQD b 804



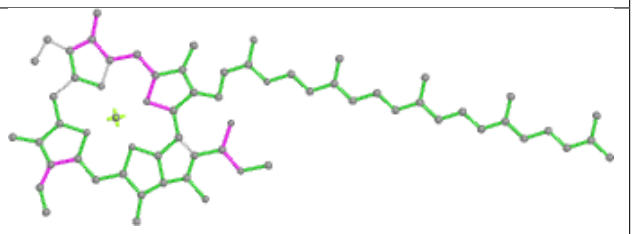
Ligand A86 P 304



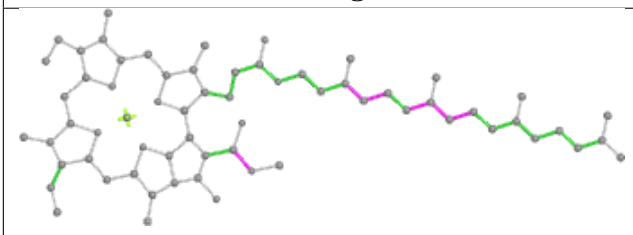
Ligand CLA H 317



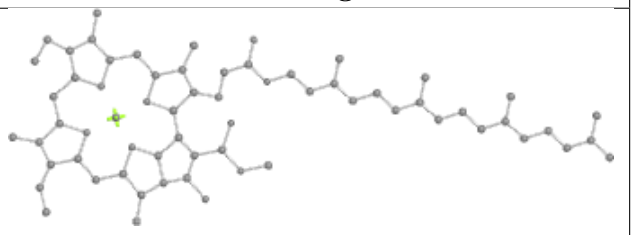
Bond lengths



Bond angles

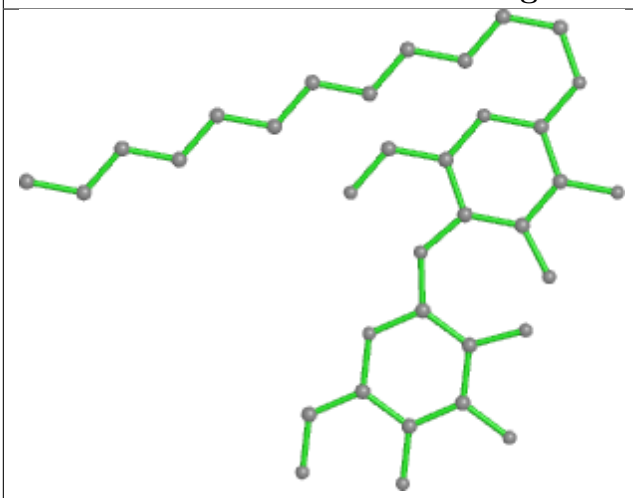


Torsions

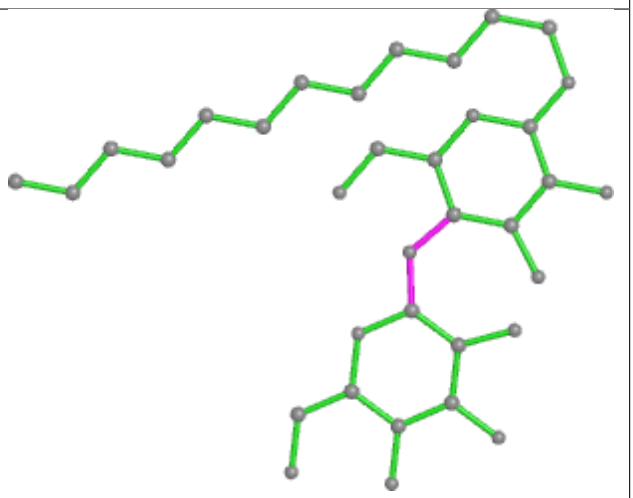


Rings

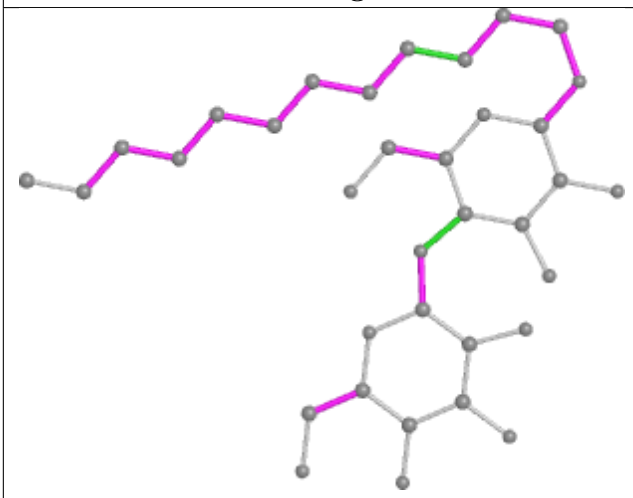
Ligand LMT U 315



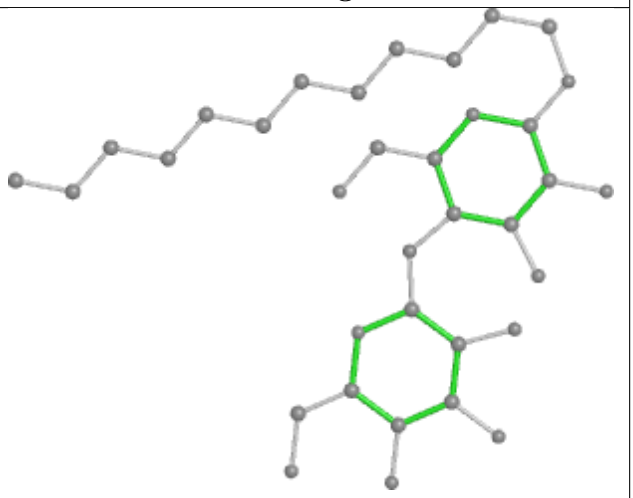
Bond lengths



Bond angles

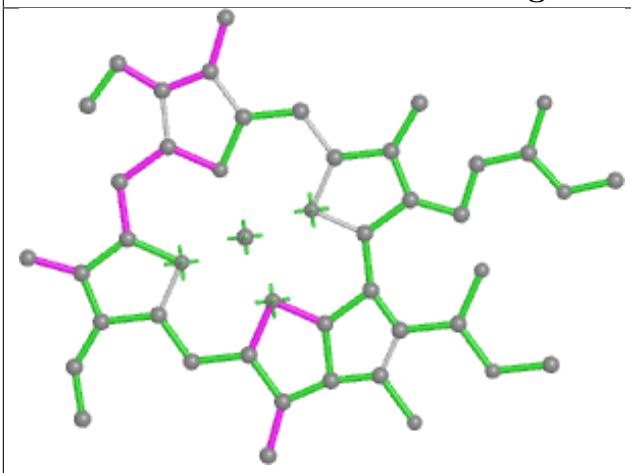


Torsions

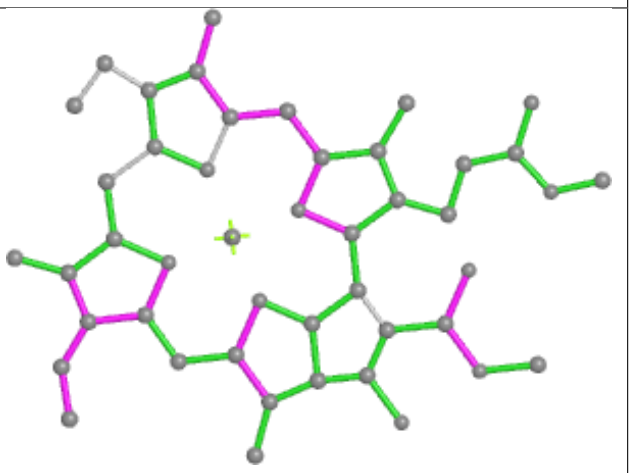


Rings

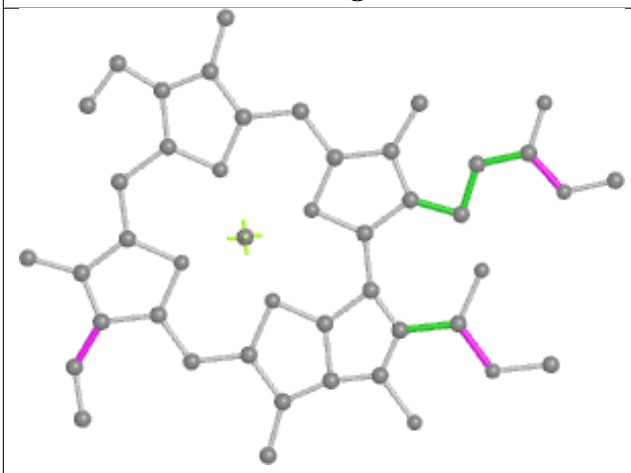
Ligand CLA J 316



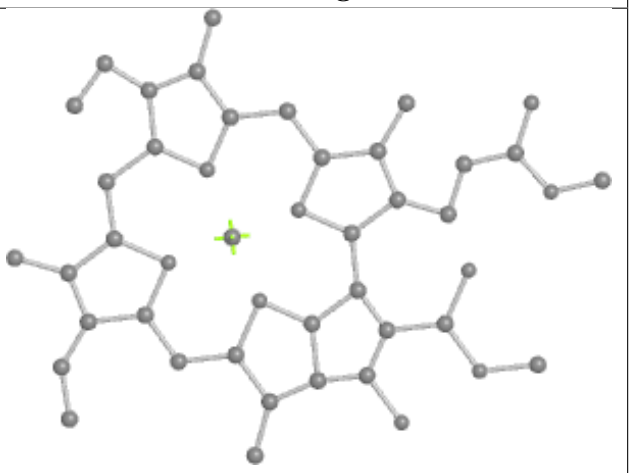
Bond lengths



Bond angles

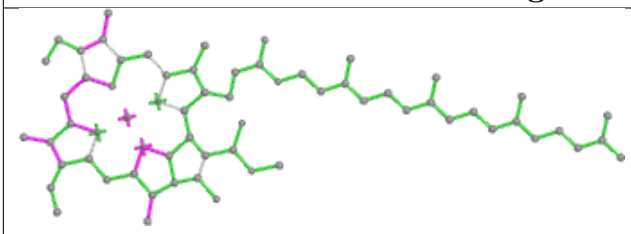


Torsions

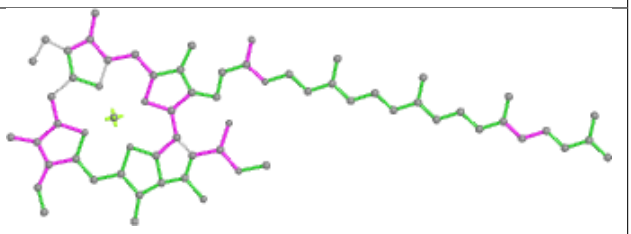


Rings

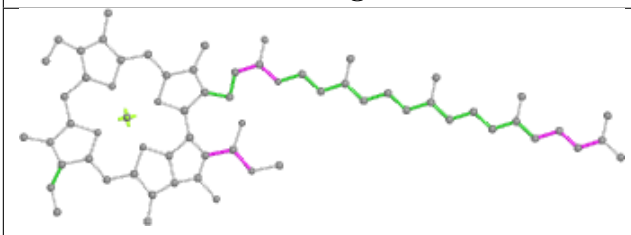
Ligand CLA b 841



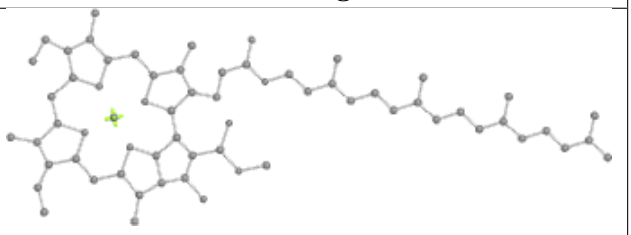
Bond lengths



Bond angles

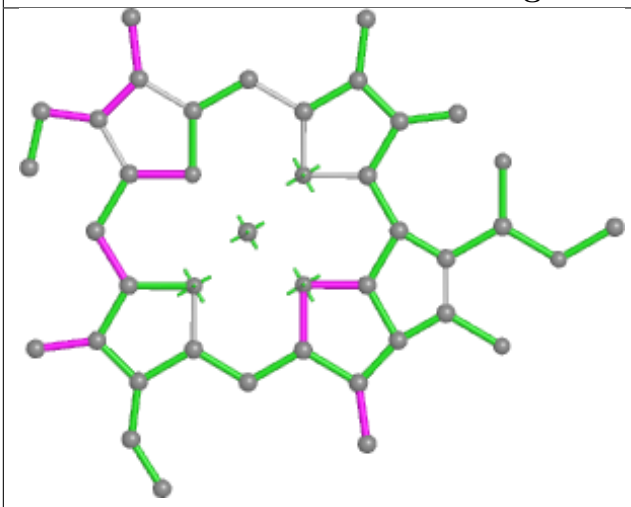


Torsions



Rings

Ligand CLA A 313



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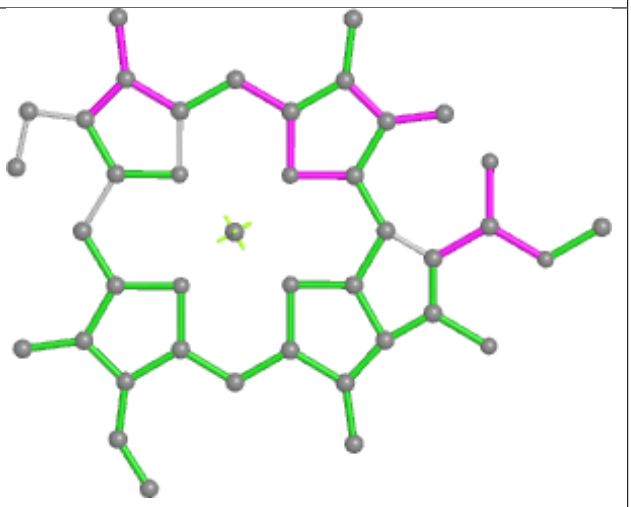
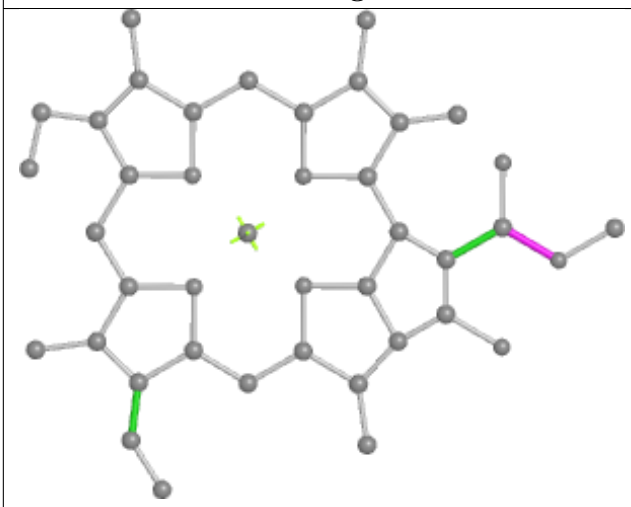
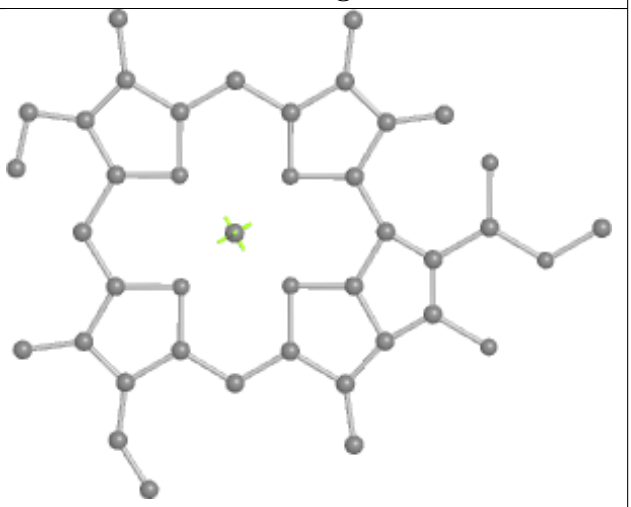


Bond angles

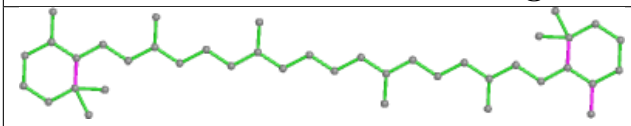


Torsions

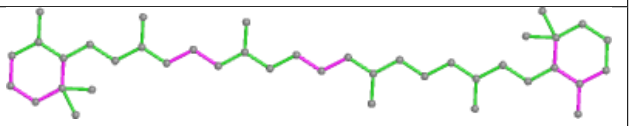


Rings

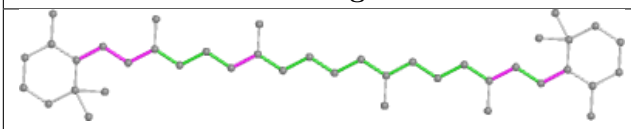
Ligand BCR b 847



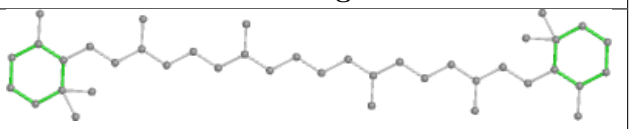
Bond lengths



Bond angles

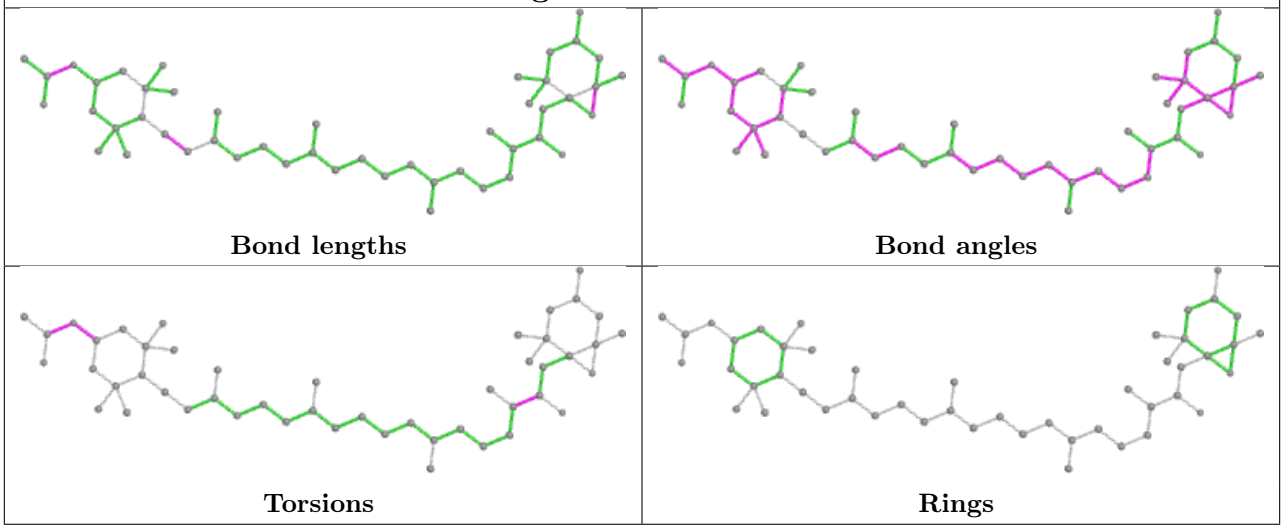


Torsions

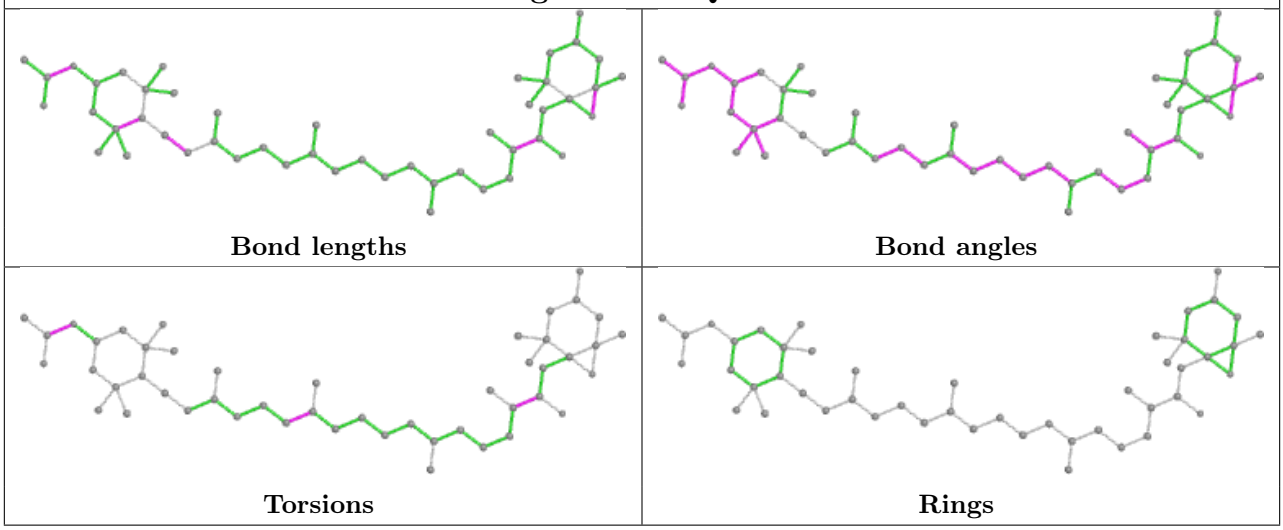


Rings

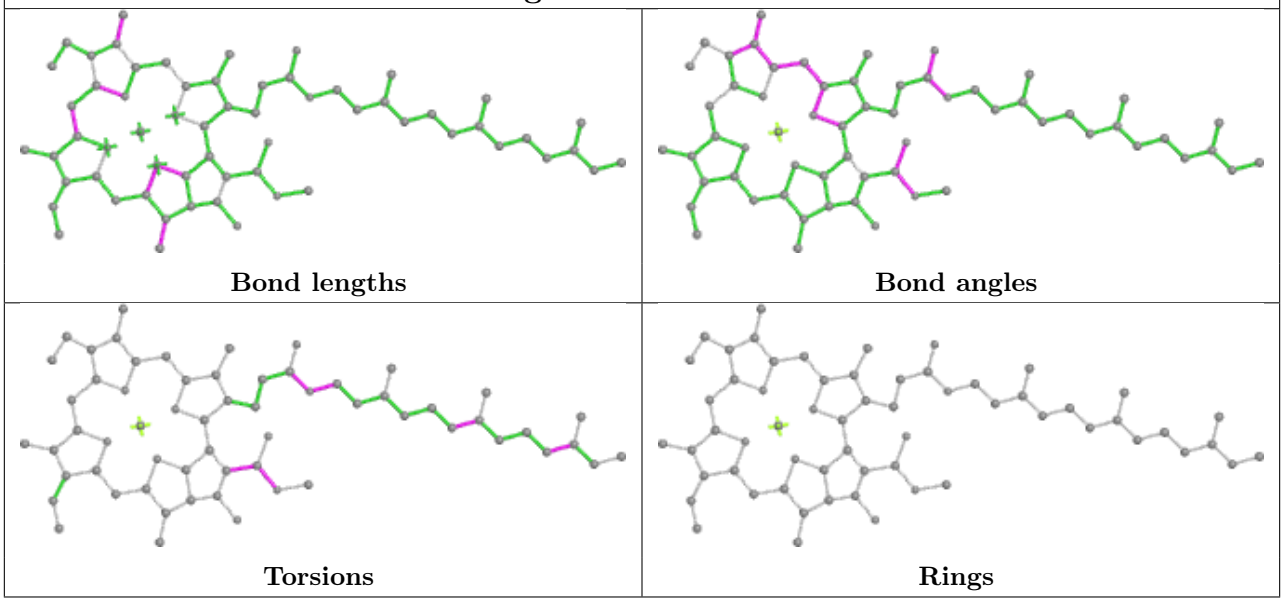
Ligand A86 T 302



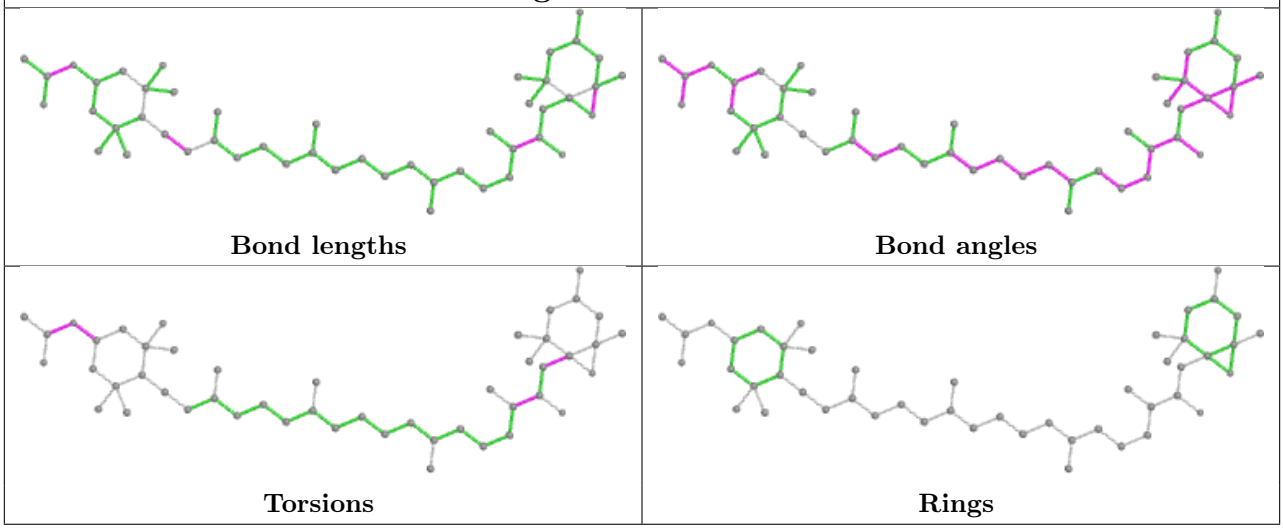
Ligand A86 Q 303



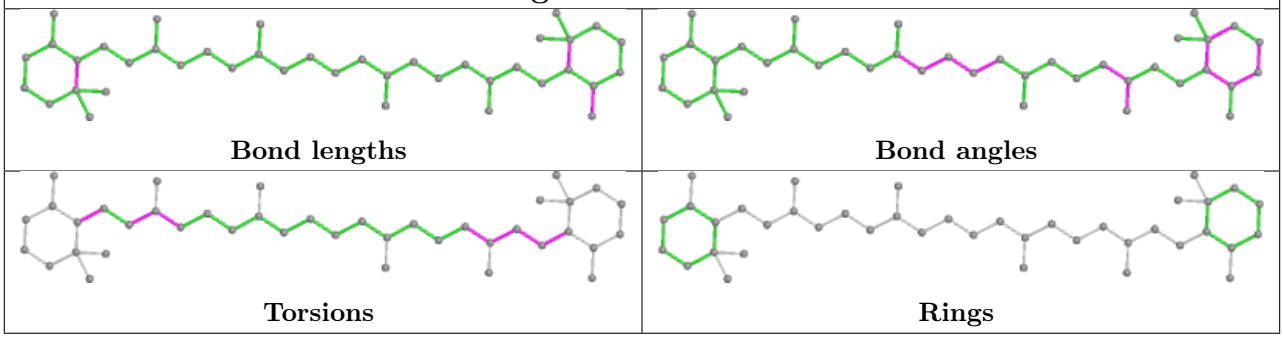
Ligand CLA U 305



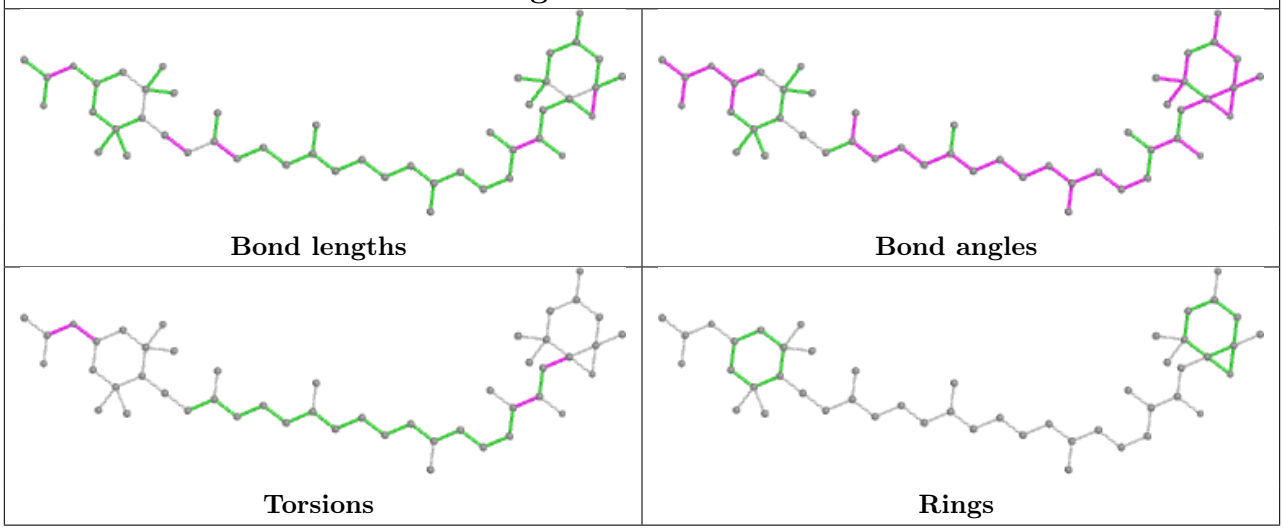
Ligand A86 L 304



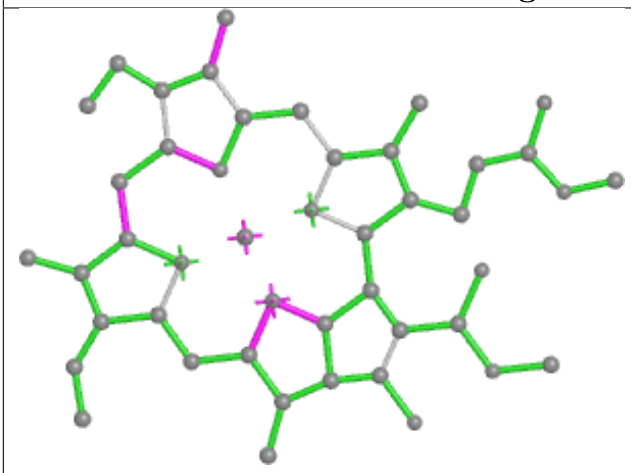
Ligand BCR i 103



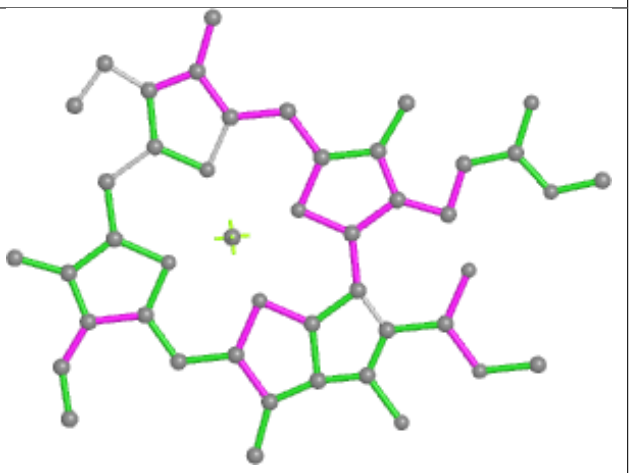
Ligand A86 X 303



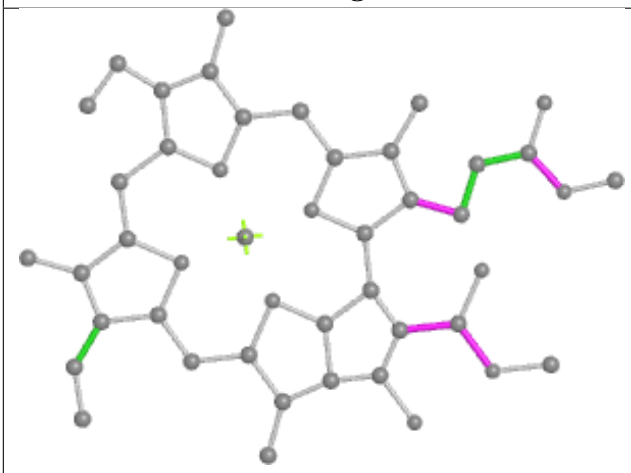
Ligand CLA W 210



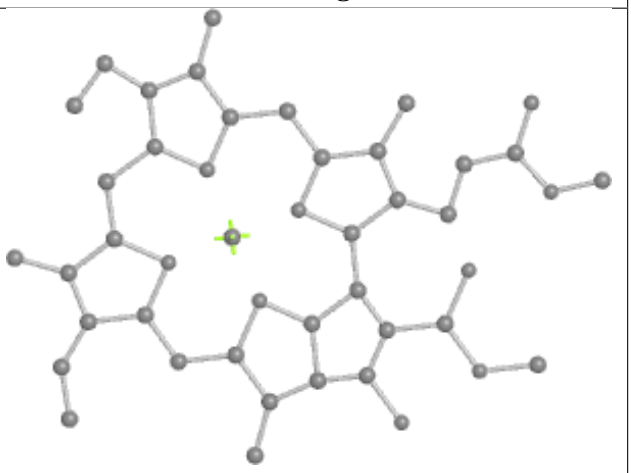
Bond lengths



Bond angles

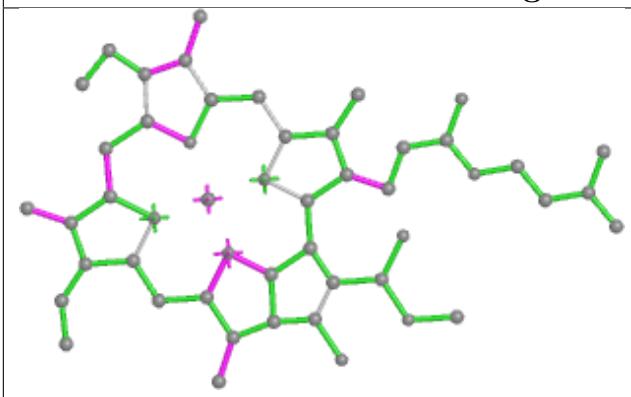


Torsions

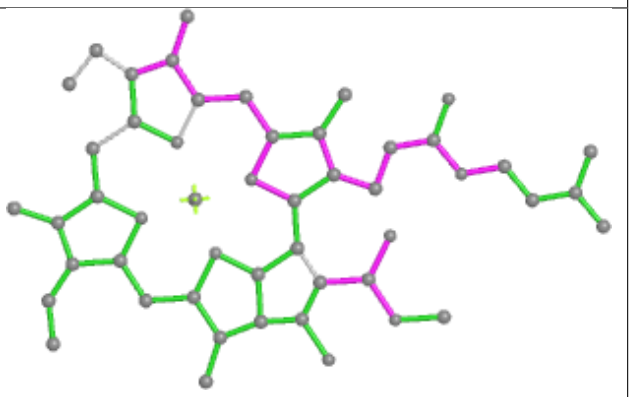


Rings

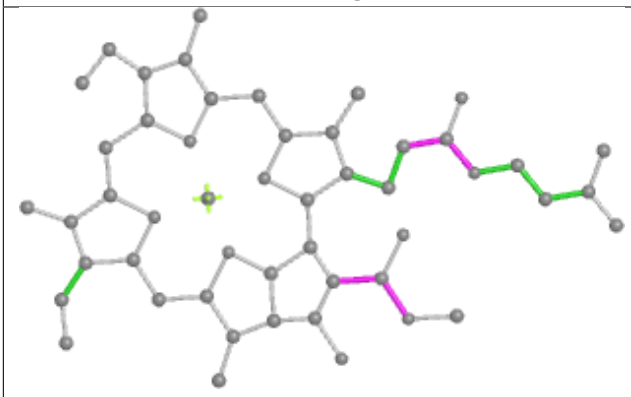
Ligand CLA H 318



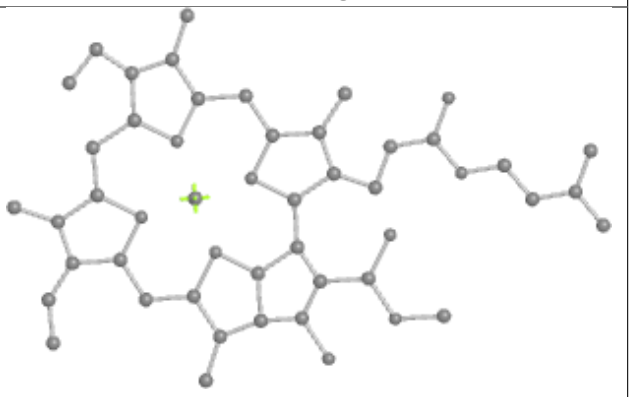
Bond lengths



Bond angles

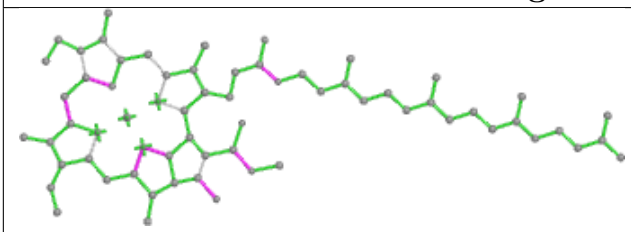


Torsions

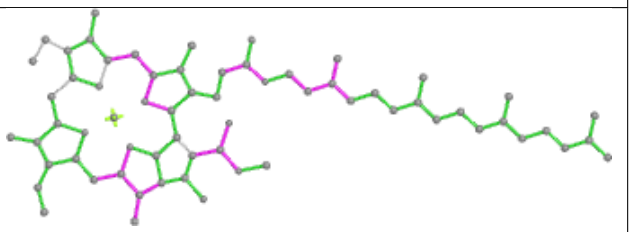


Rings

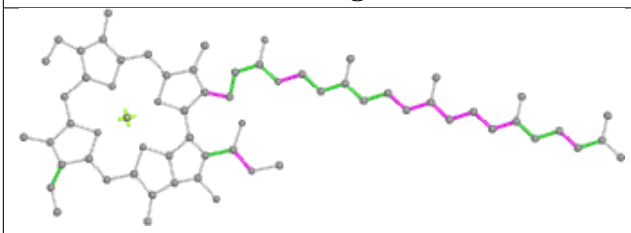
Ligand CLA a 825



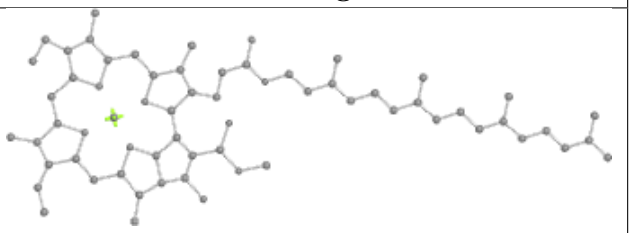
Bond lengths



Bond angles

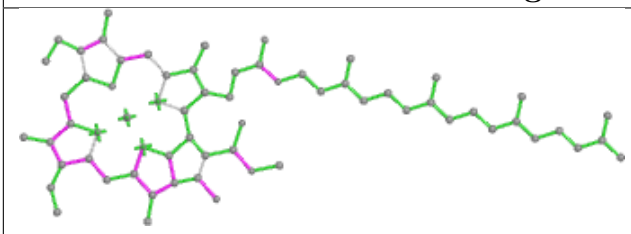


Torsions

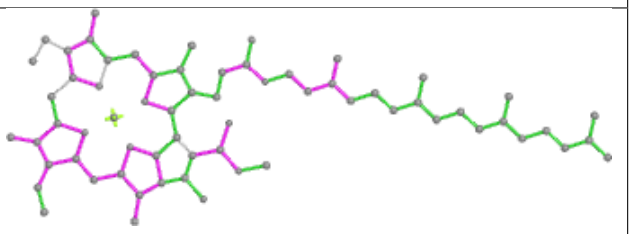


Rings

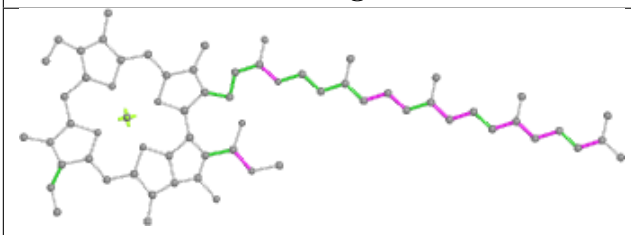
Ligand CLA C 207



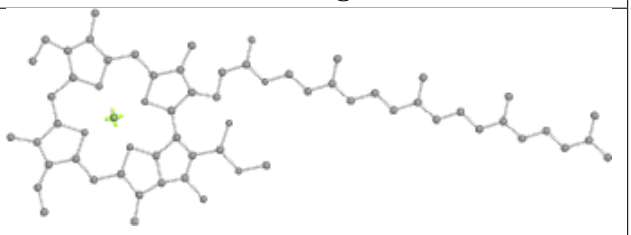
Bond lengths



Bond angles

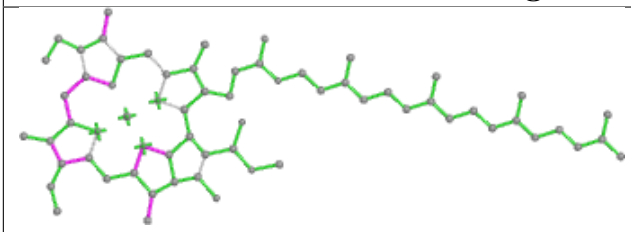


Torsions

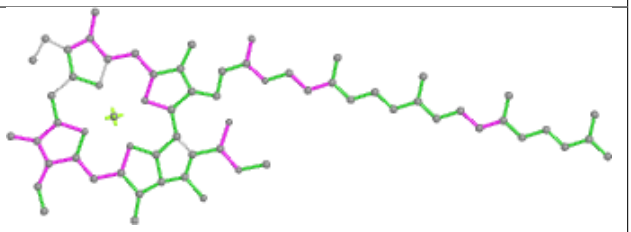


Rings

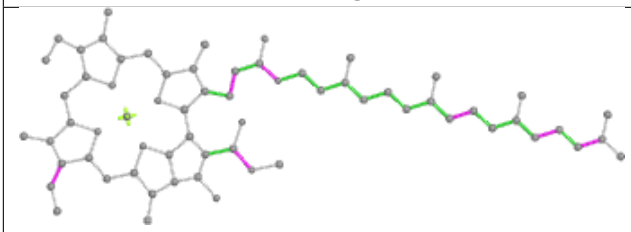
Ligand CLA T 311



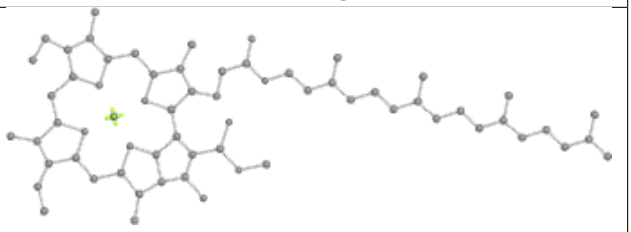
Bond lengths



Bond angles

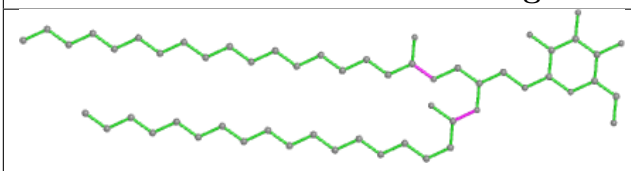


Torsions

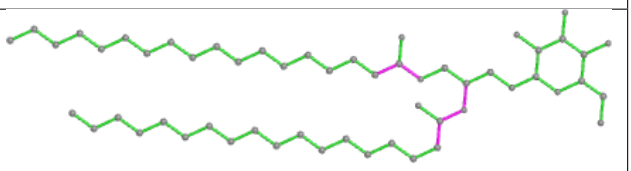


Rings

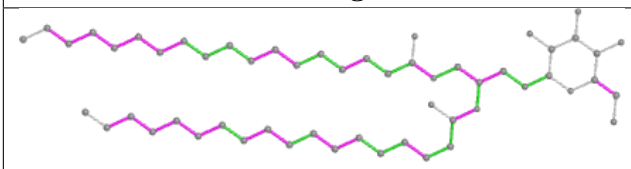
Ligand LMG J 318



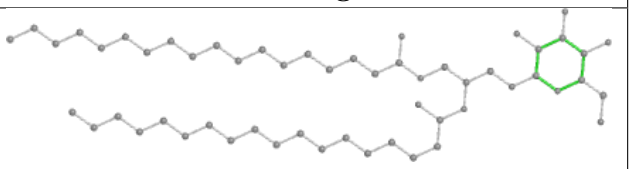
Bond lengths



Bond angles

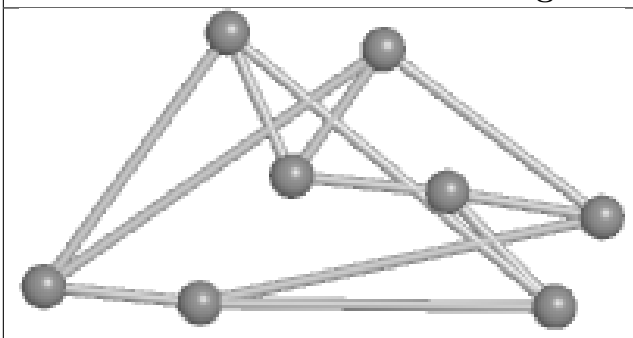


Torsions

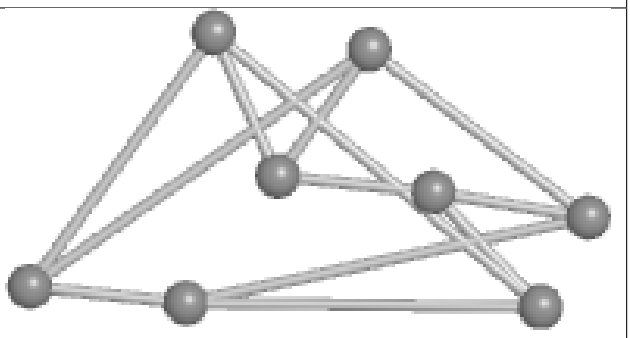


Rings

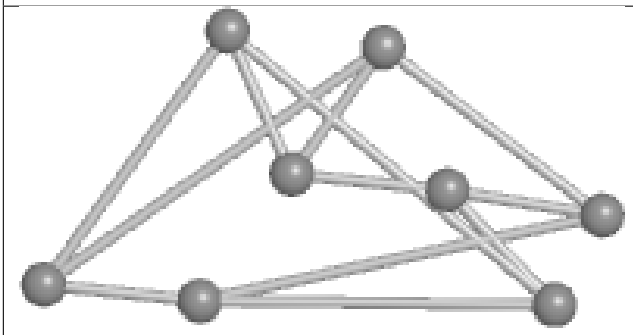
Ligand SF4 c 102



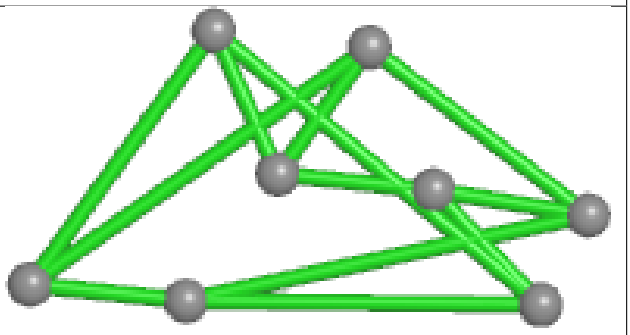
Bond lengths



Bond angles

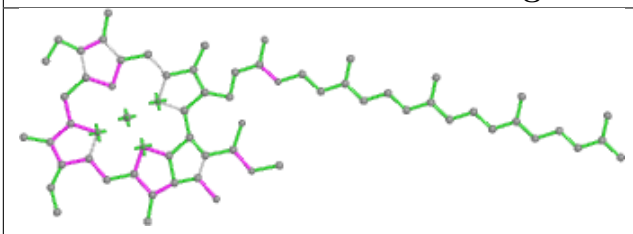


Torsions

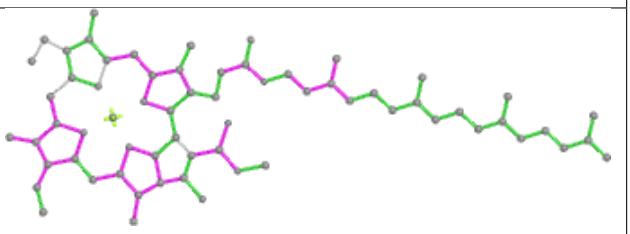


Rings

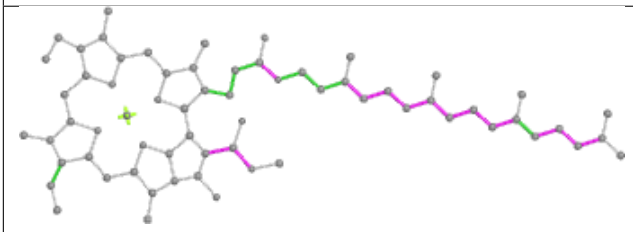
Ligand CLA U 306



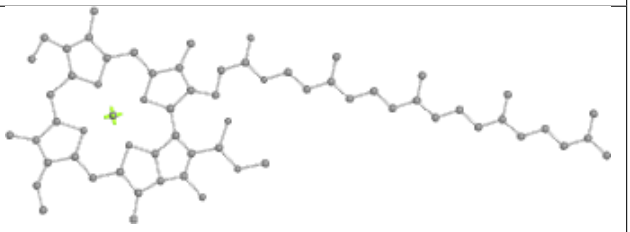
Bond lengths



Bond angles

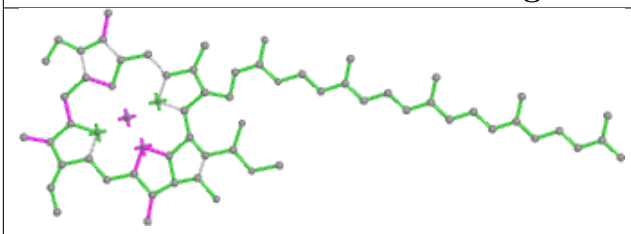


Torsions

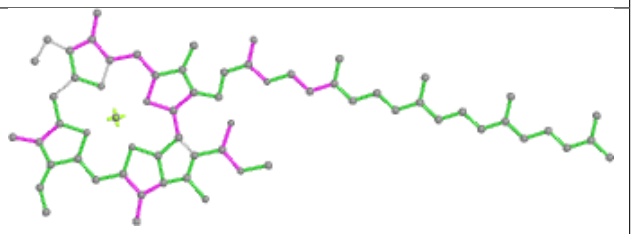


Rings

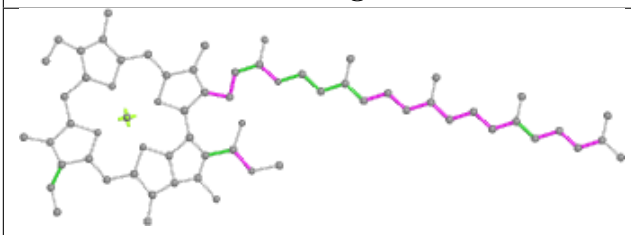
Ligand CLA U 311



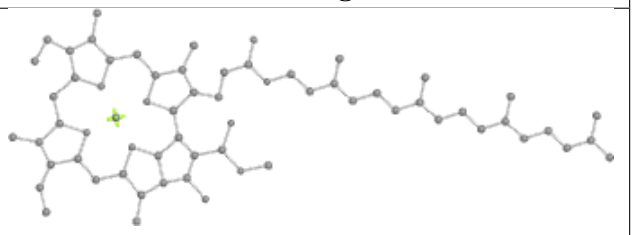
Bond lengths



Bond angles

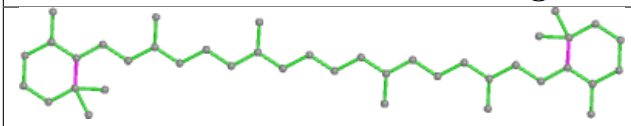


Torsions

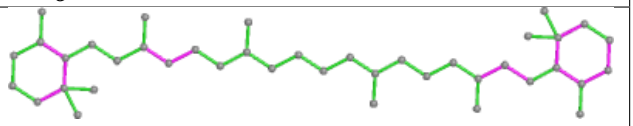


Rings

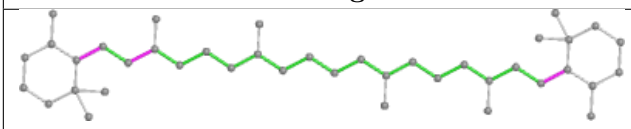
Ligand BCR j 107



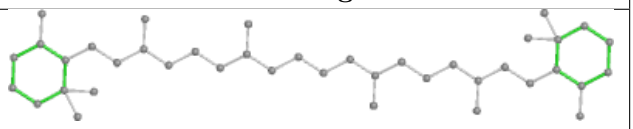
Bond lengths



Bond angles

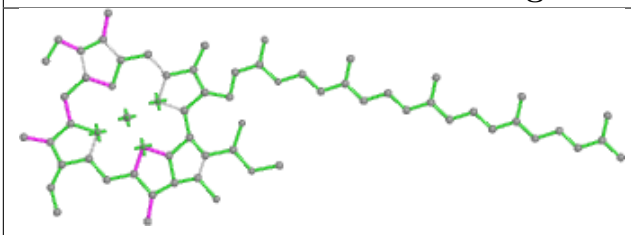


Torsions

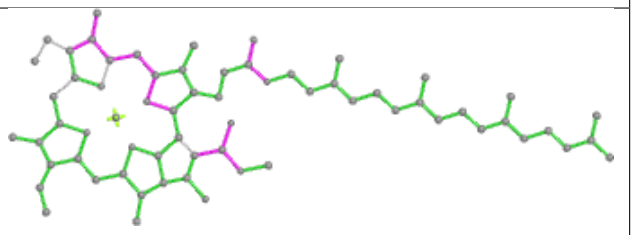


Rings

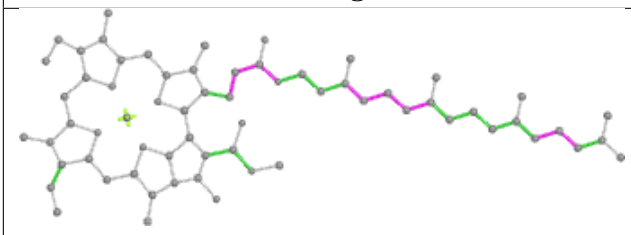
Ligand CLA L 309



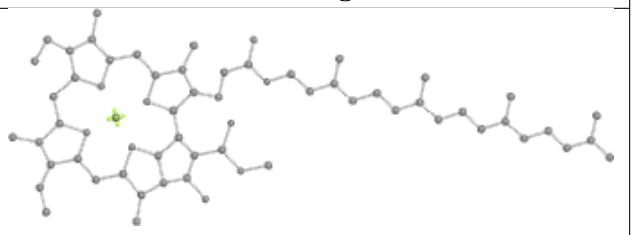
Bond lengths



Bond angles

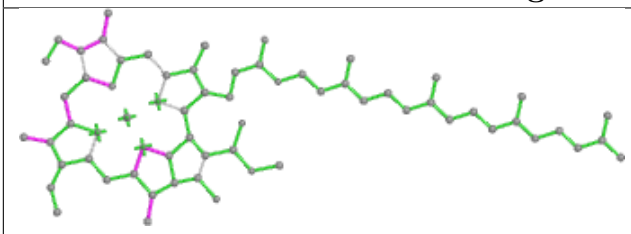


Torsions

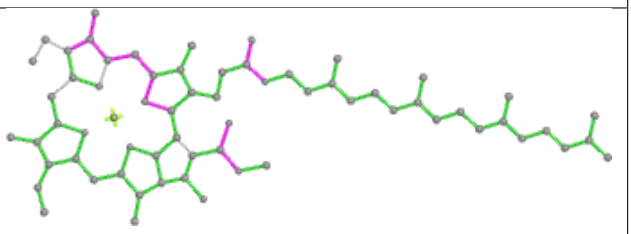


Rings

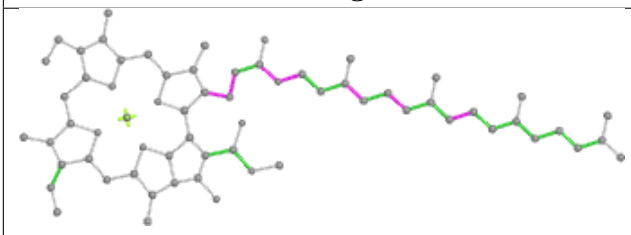
Ligand CLA b 829



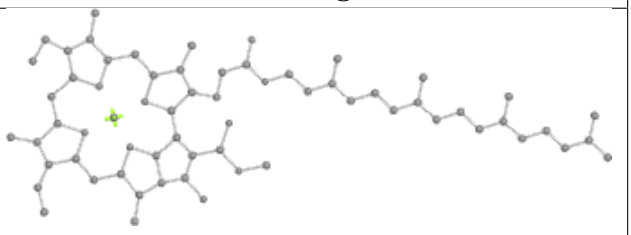
Bond lengths



Bond angles

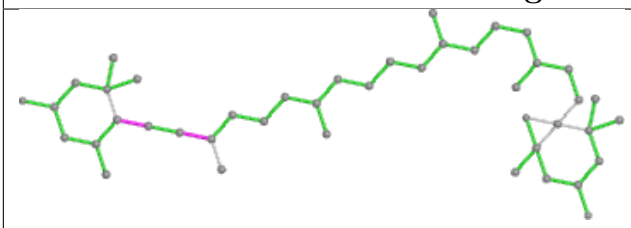


Torsions

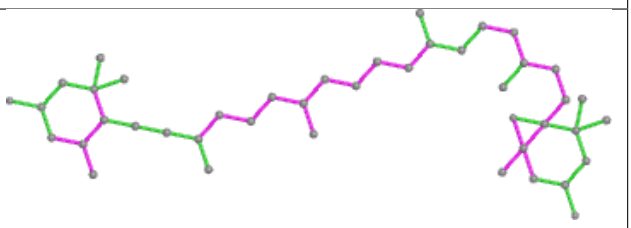


Rings

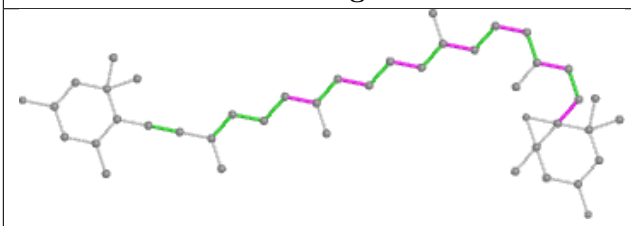
Ligand DD6 R 307



Bond lengths



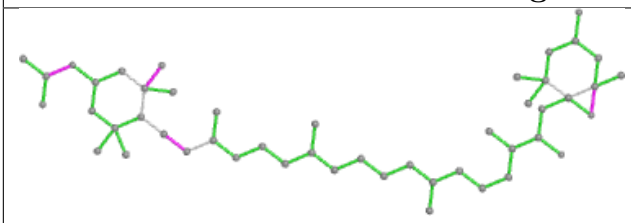
Bond angles



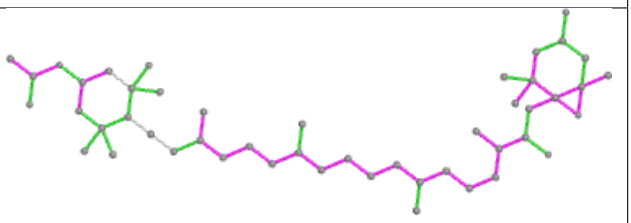
Torsions

Rings

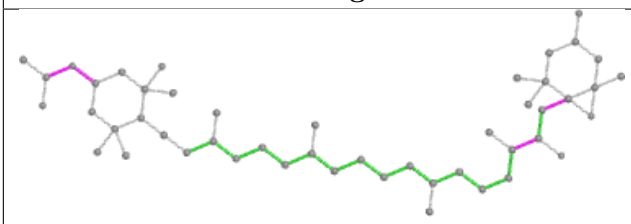
Ligand A86 R 306



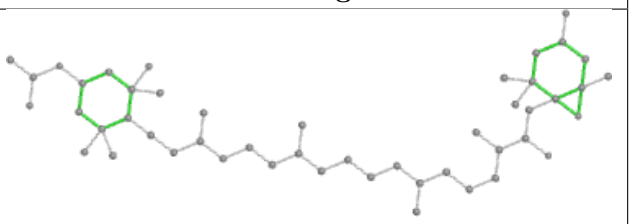
Bond lengths



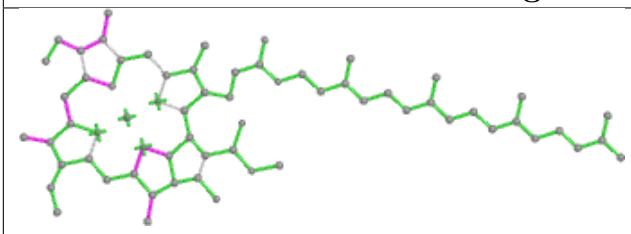
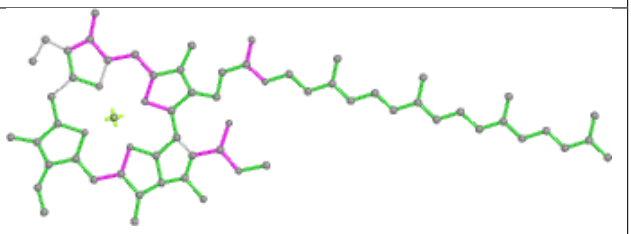
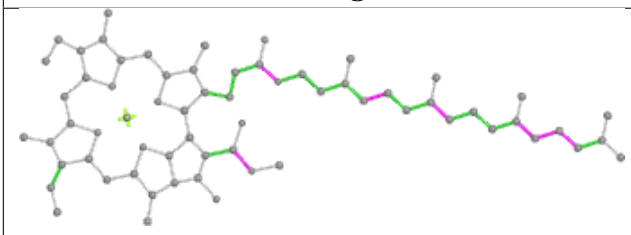
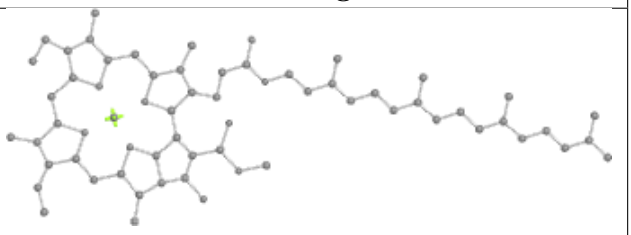
Bond angles

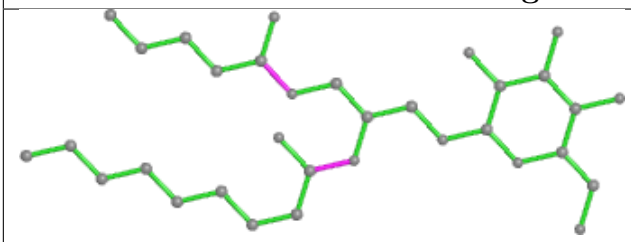
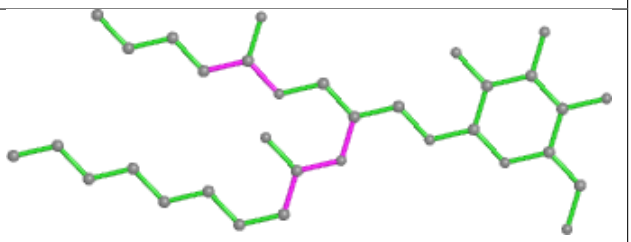
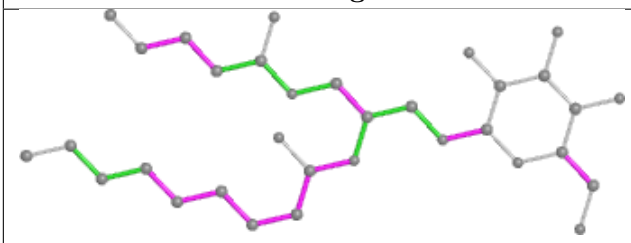
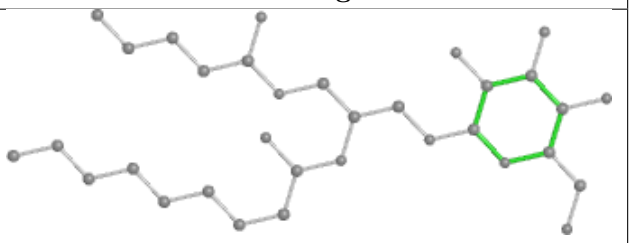


Torsions

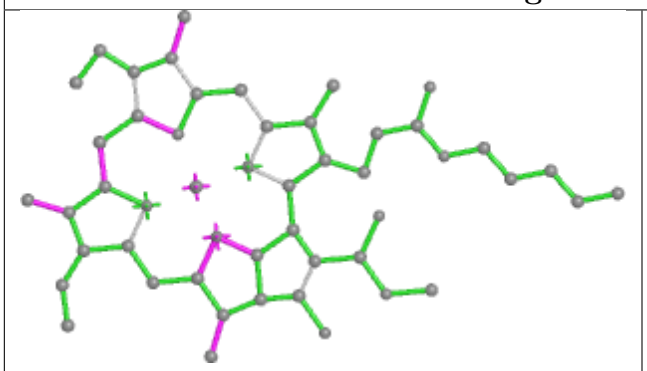


Rings

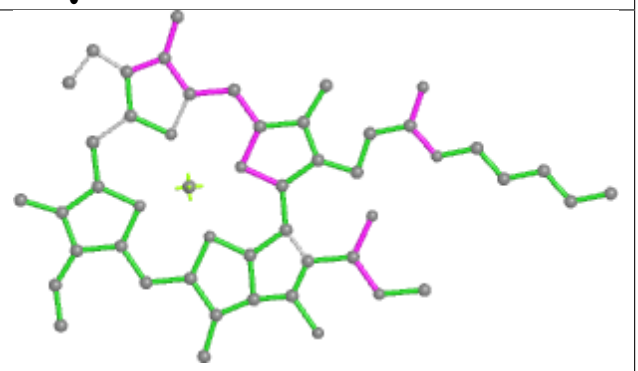
Ligand CLA D 312	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand LMG L 321	
 Bond lengths	 Bond angles
 Torsions	 Rings

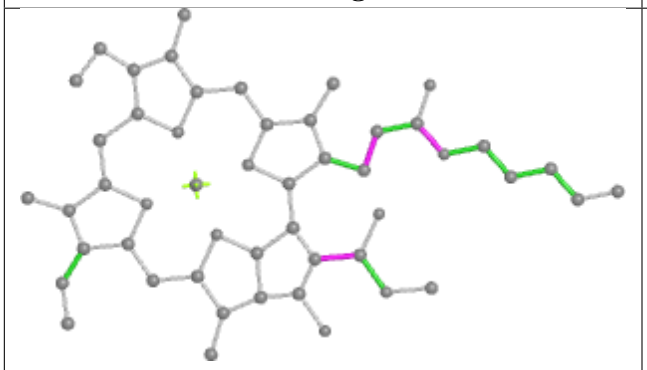
Ligand CLA Q 307



Bond lengths



Bond angles



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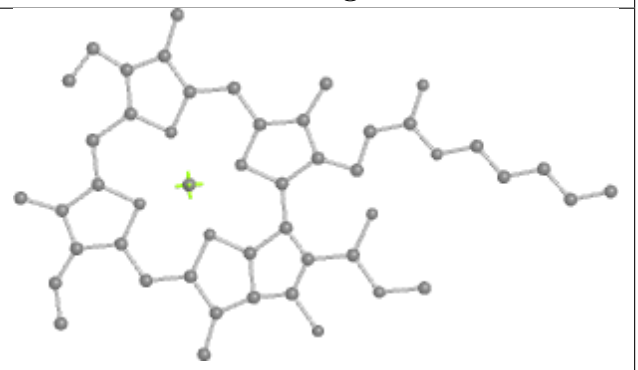
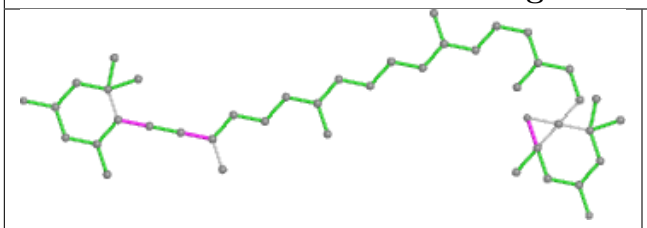
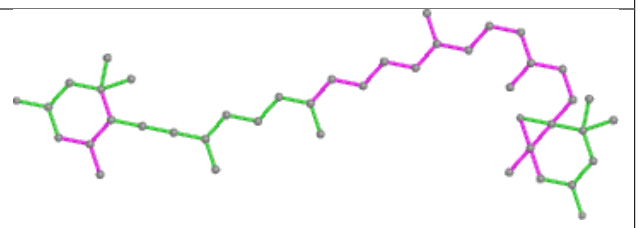


Rings

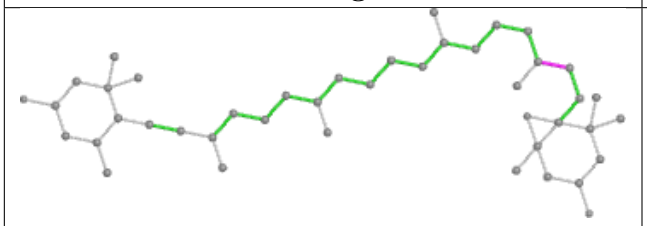
Ligand DD6 B 304



Bond lengths



Bond angles



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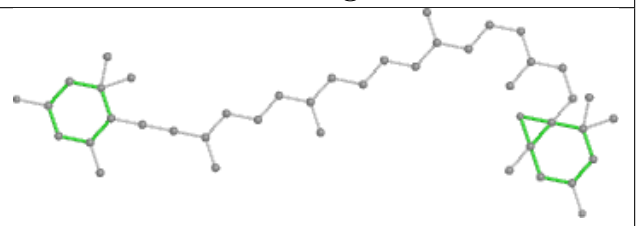
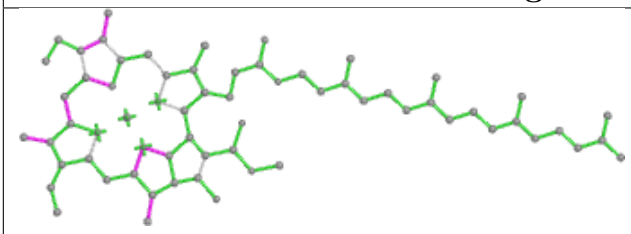


Rings

Ligand CLA P 301



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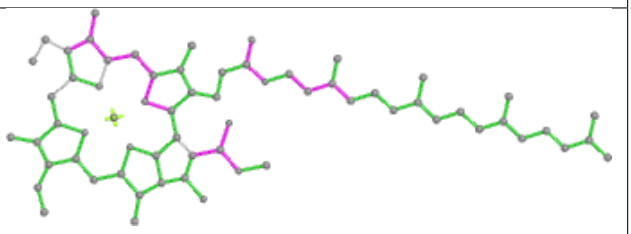
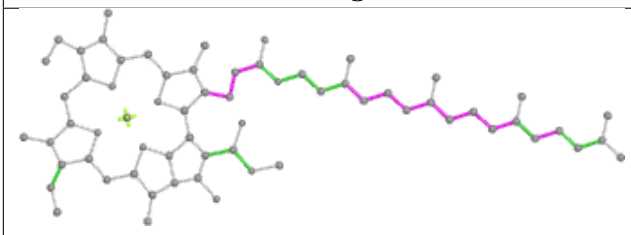


Bond angles



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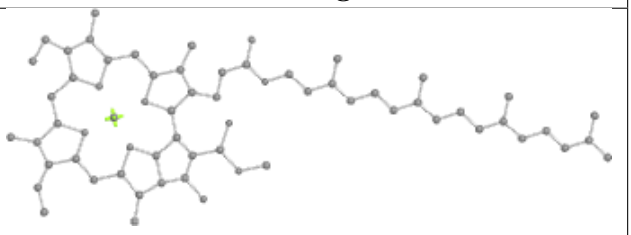
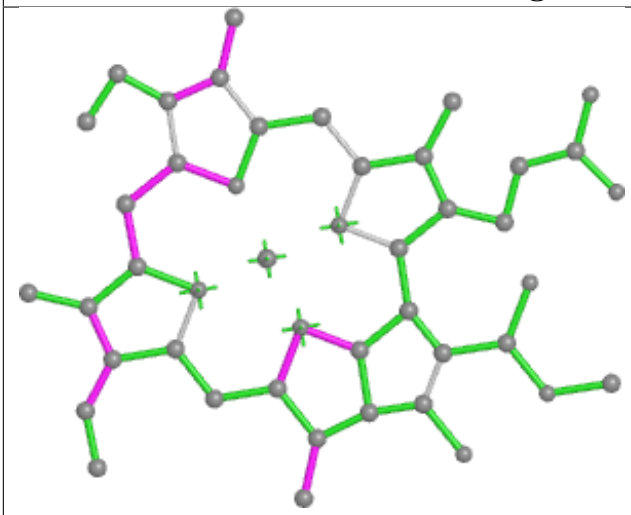
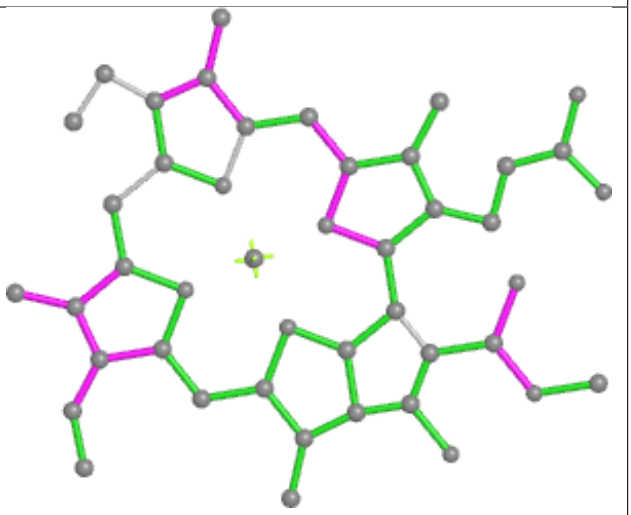


Rings

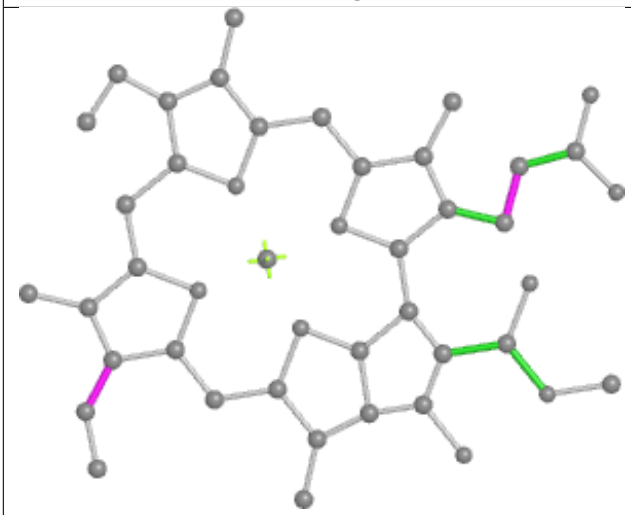
Ligand CLA a 819



Bond lengths



Bond angles



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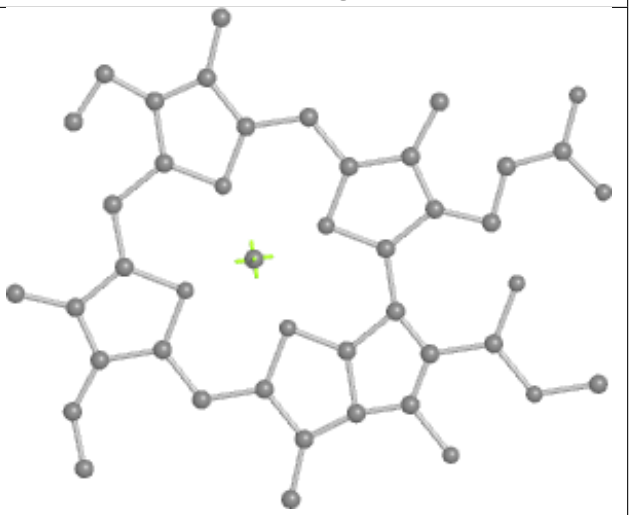
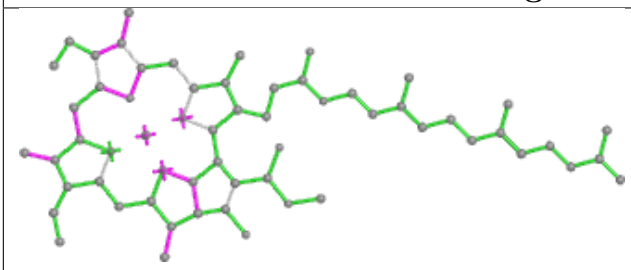
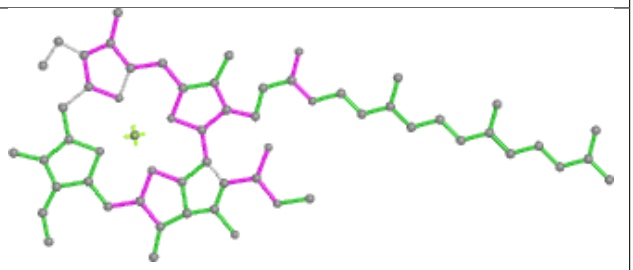
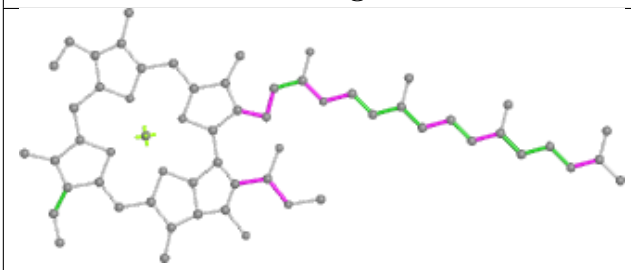
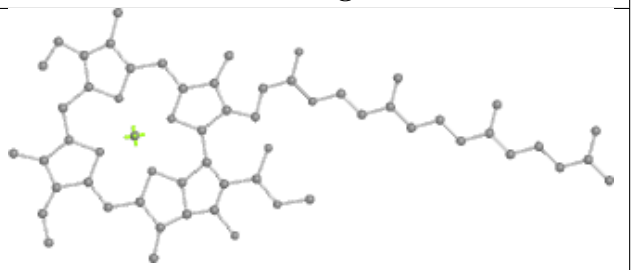
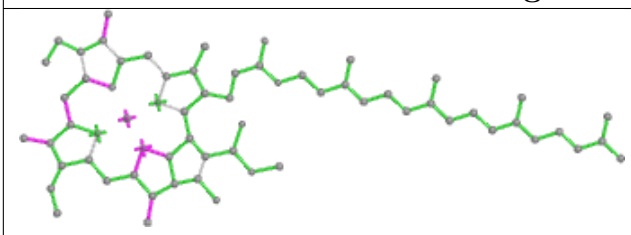
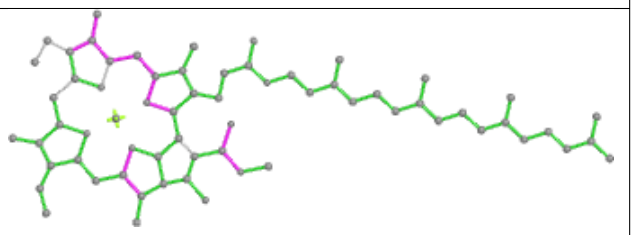
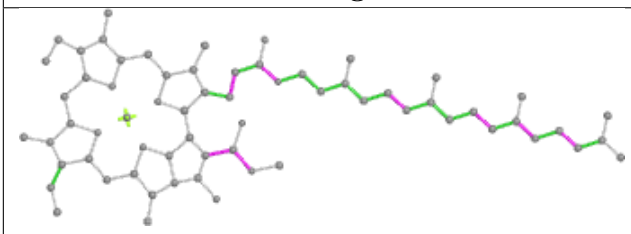
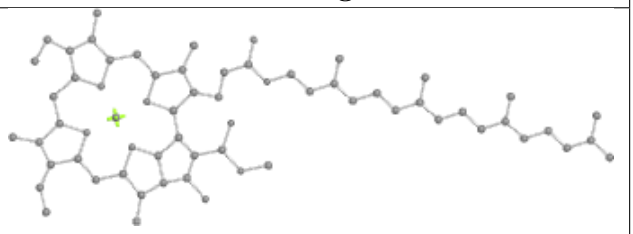
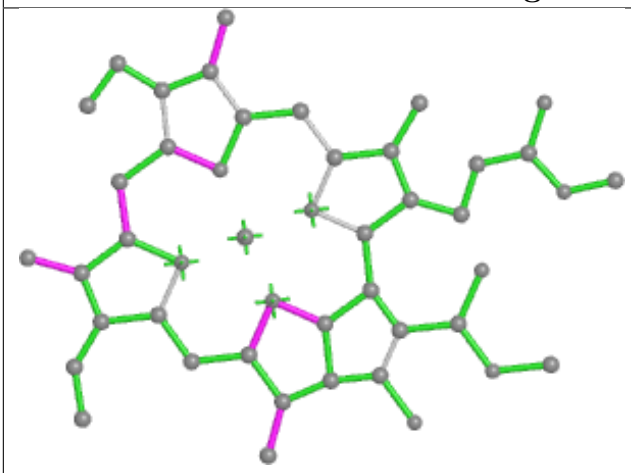
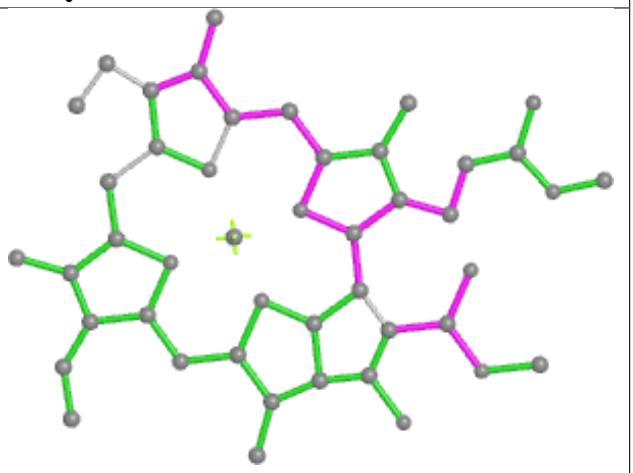
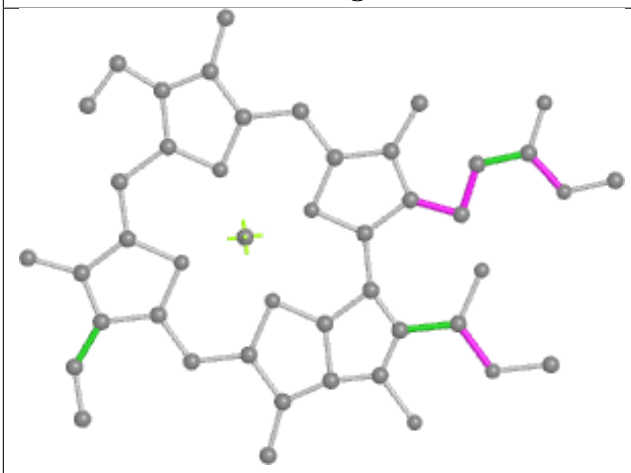
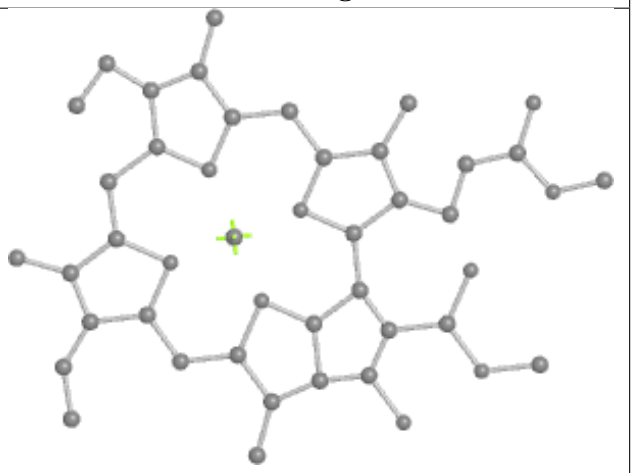


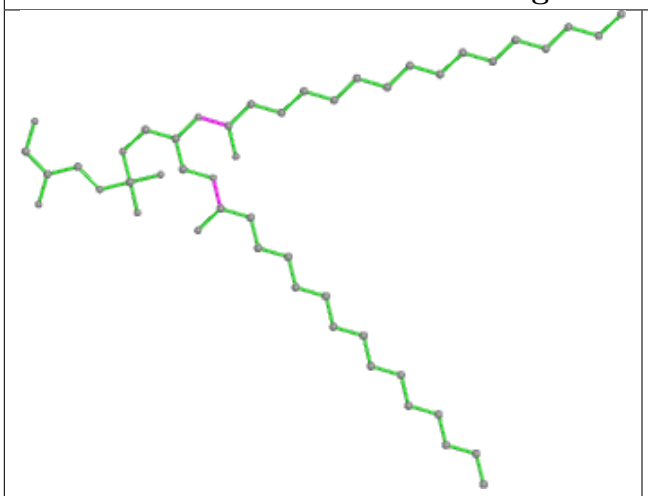
Rings

Ligand CLA P 319	
 Bond lengths	 Bond angles
 Torsions	 Rings

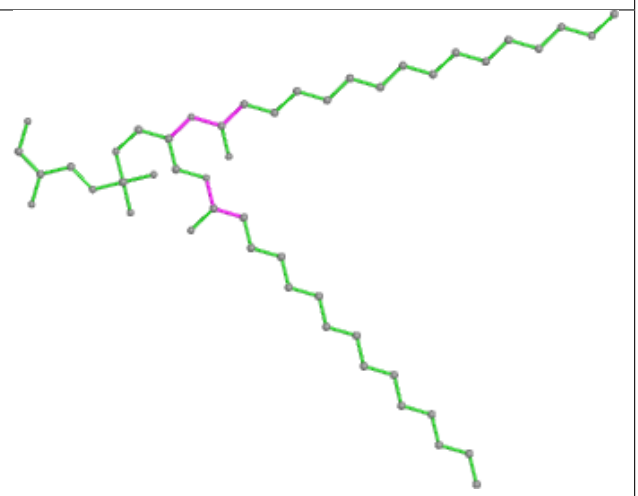
Ligand CLA R 313	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA Q 309	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

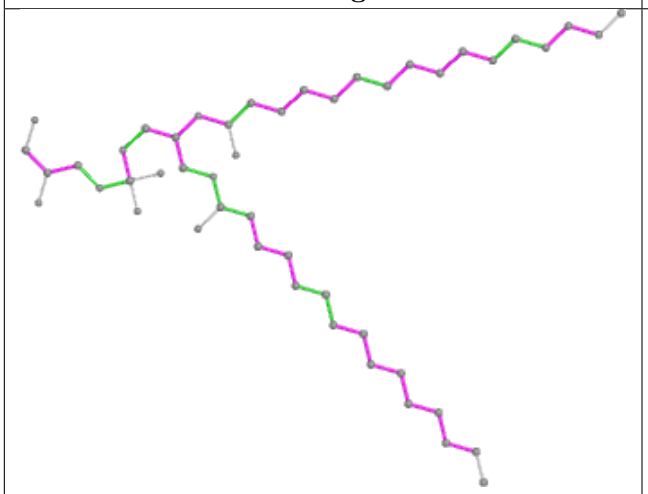
Ligand LHG l 208



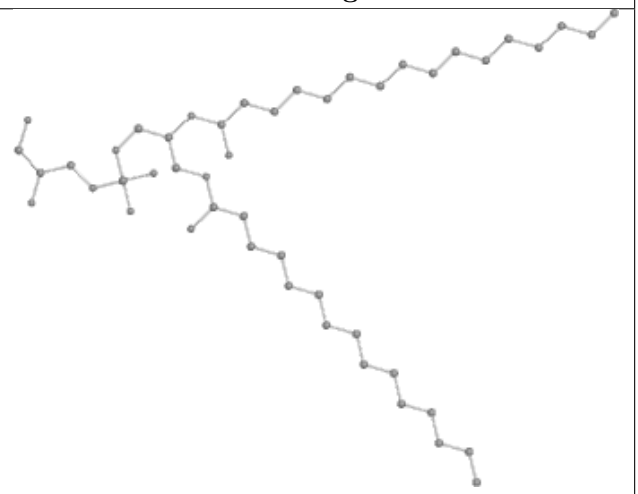
Bond lengths



Bond angles

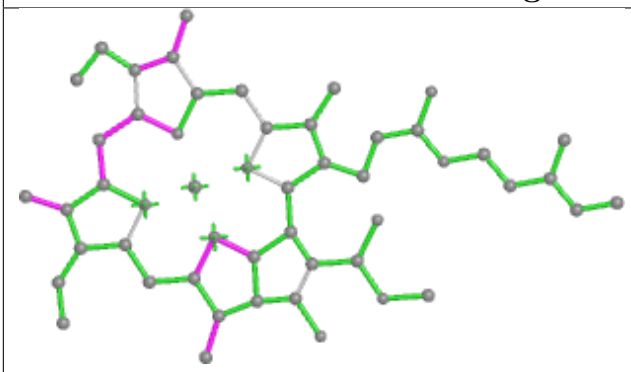


Torsions

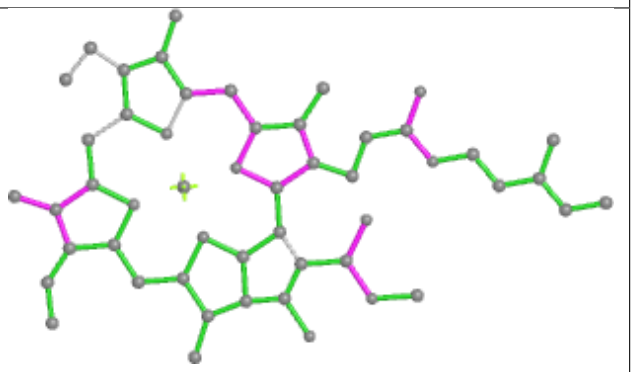


Rings

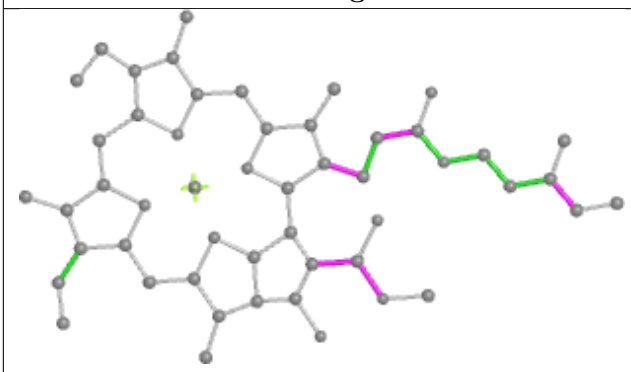
Ligand CLA N 309



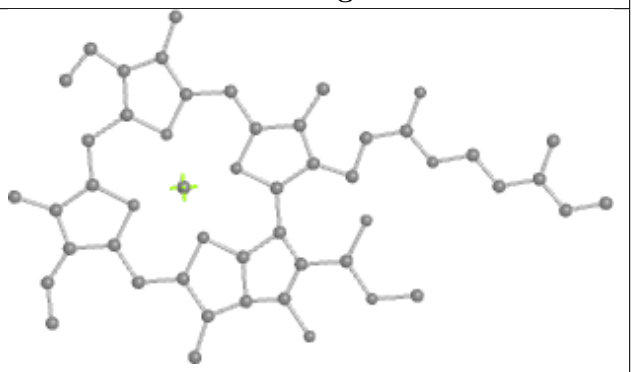
Bond lengths



Bond angles

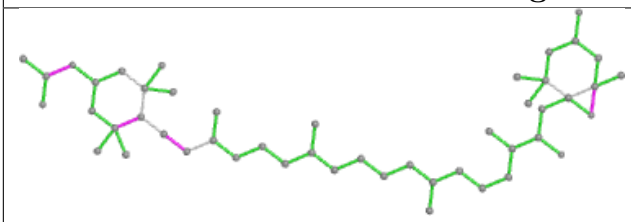


Torsions

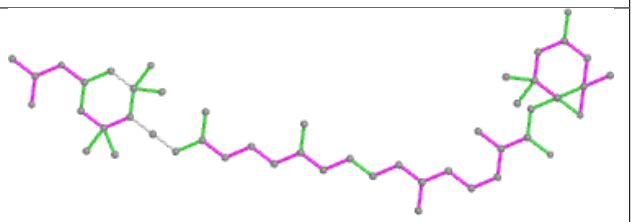


Rings

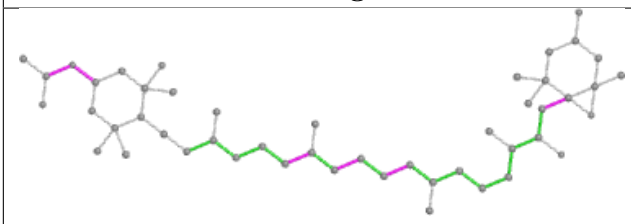
Ligand A86 V 301



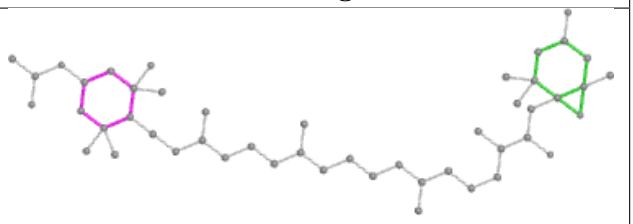
Bond lengths



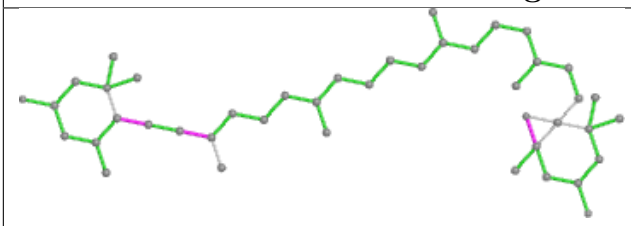
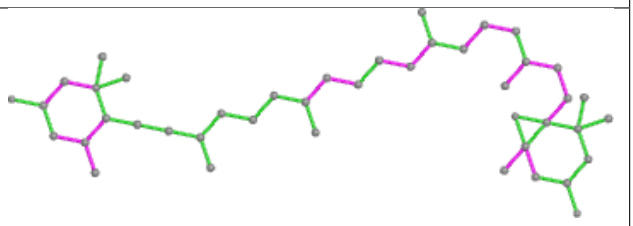
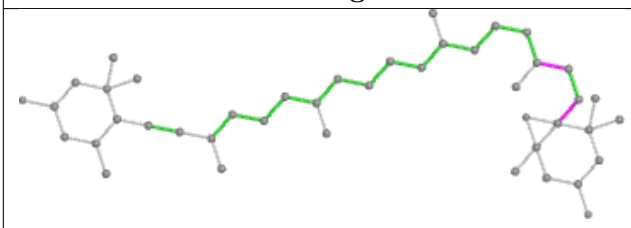
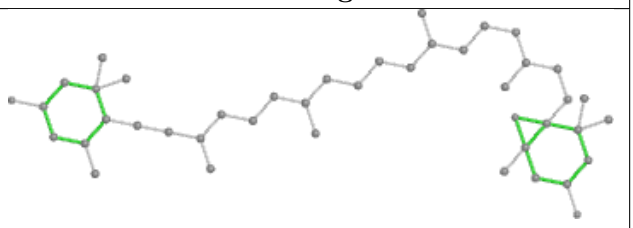
Bond angles

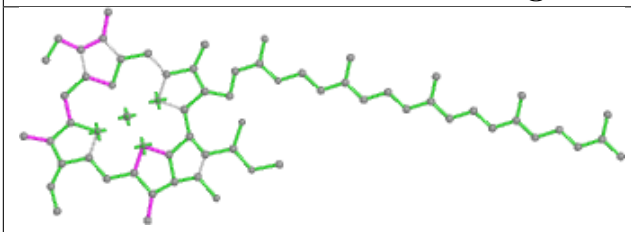
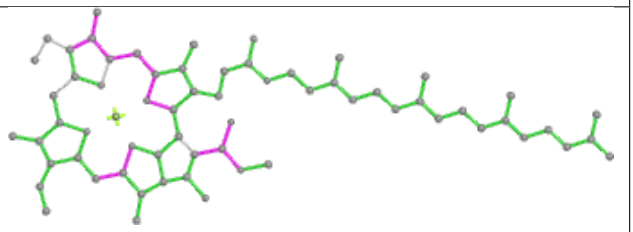
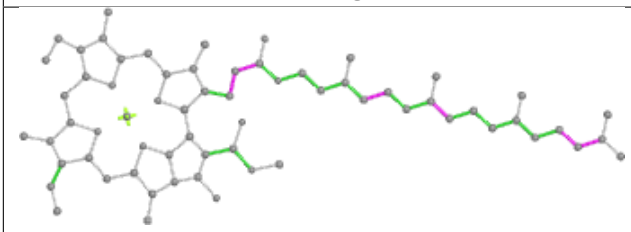
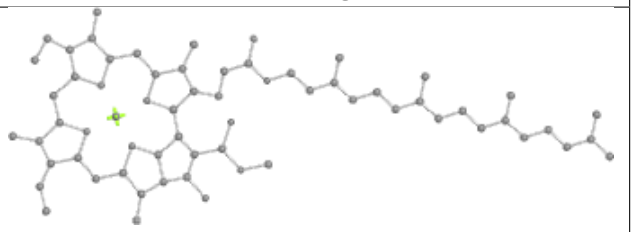


Torsions

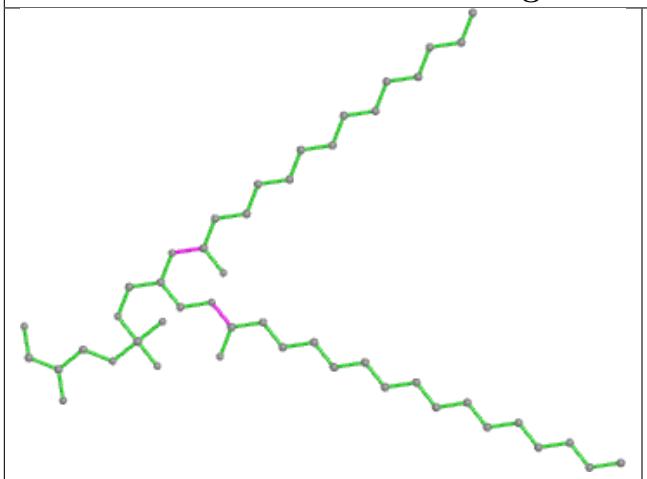


Rings

Ligand DD6 G 303	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA b 810	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand LHG G 321



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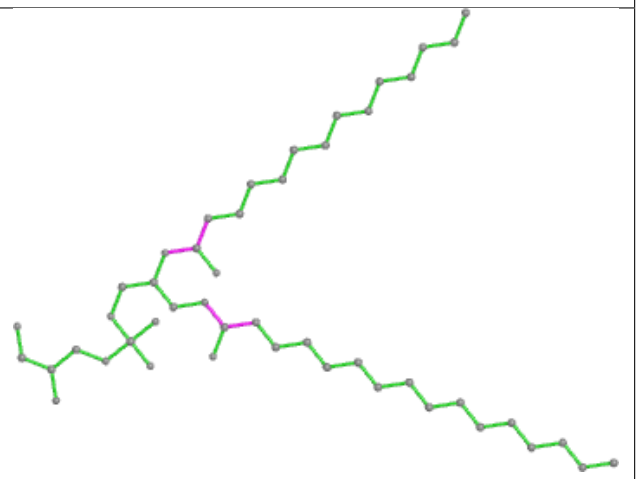

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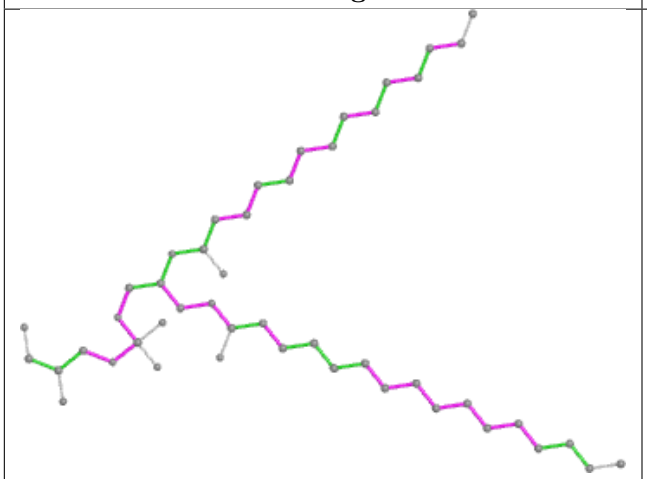

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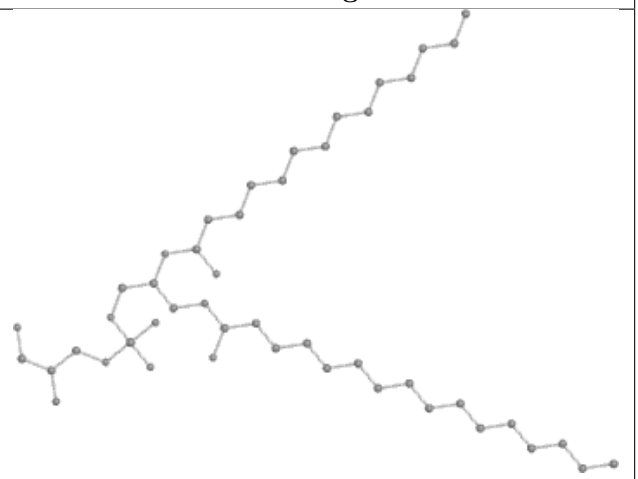
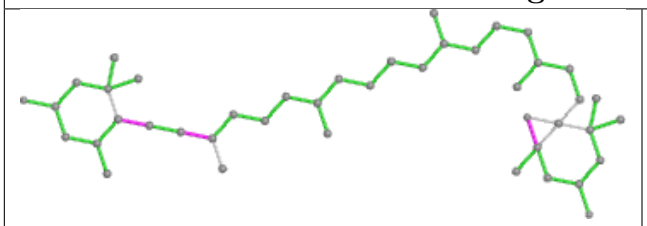


Rings

Ligand DD6 E 304



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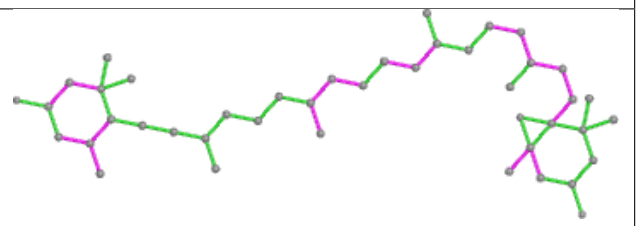
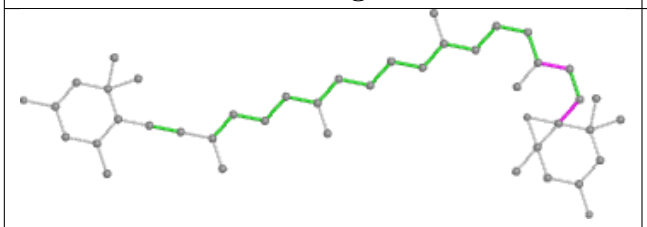


Bond angles



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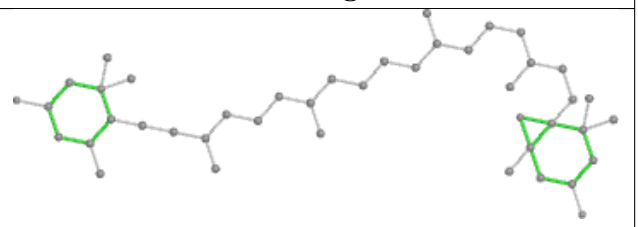
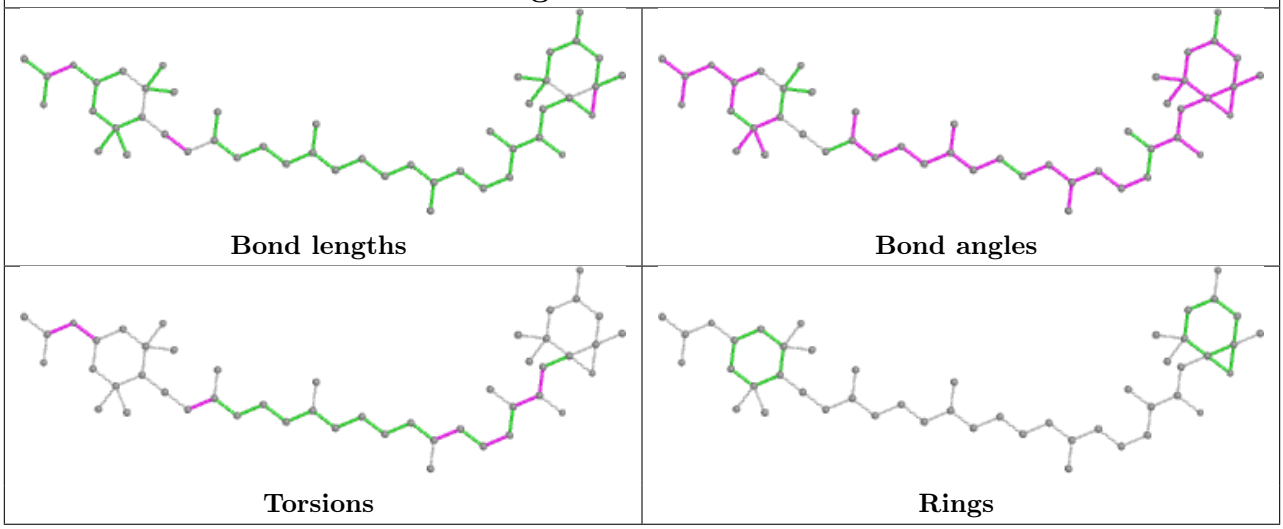
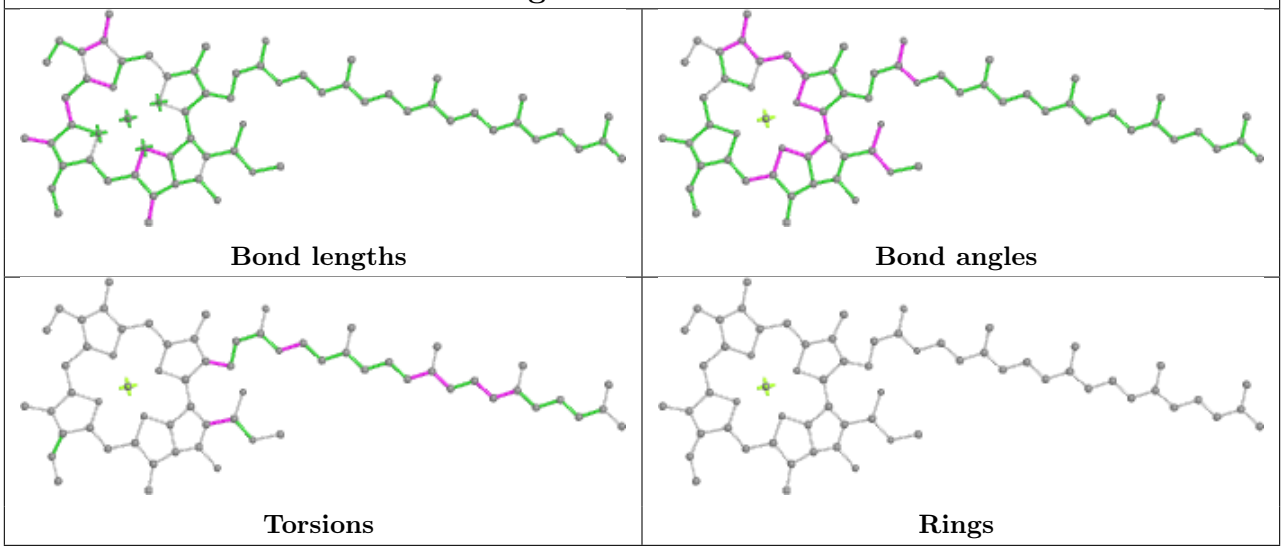


Rings

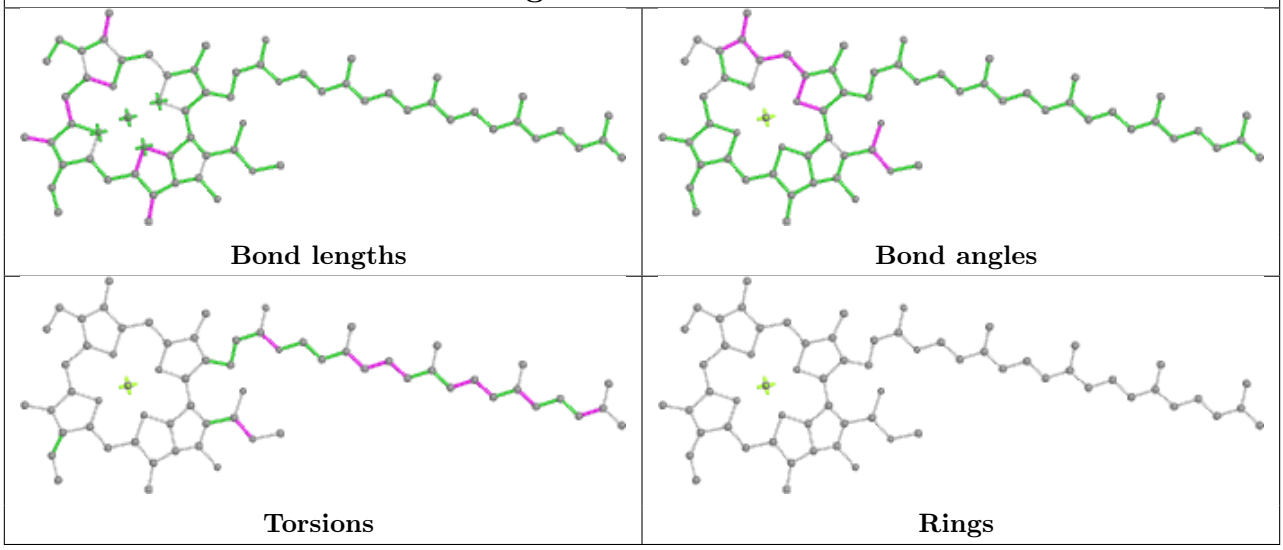
Ligand A86 B 303



Ligand CLA b 827



Ligand CLA P 313



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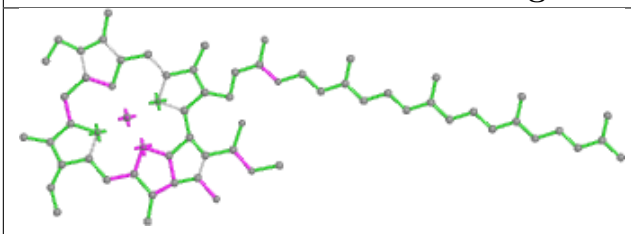

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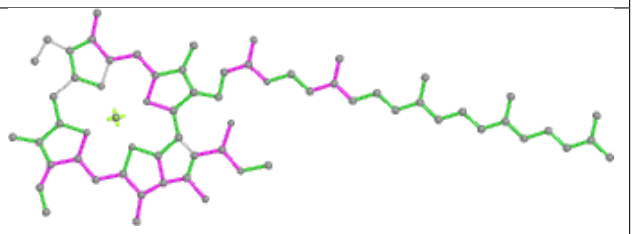

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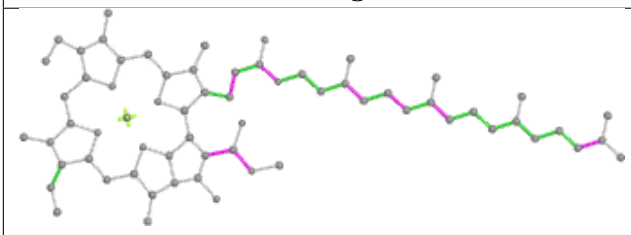

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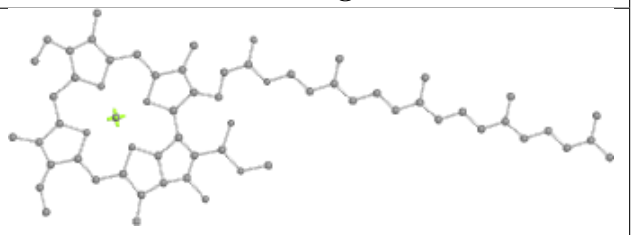
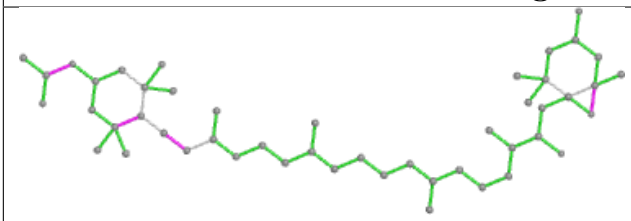


Rings

Ligand A86 F 306



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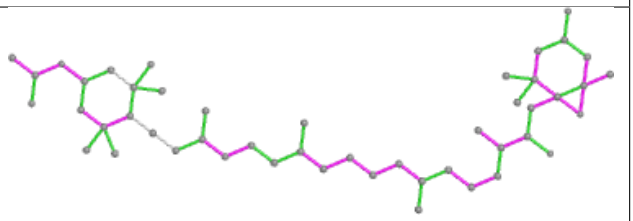

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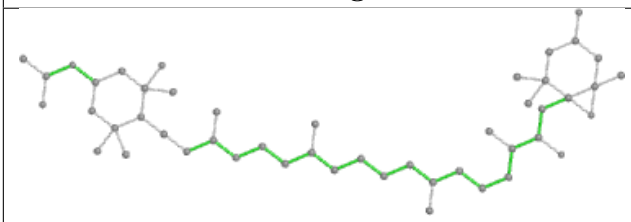

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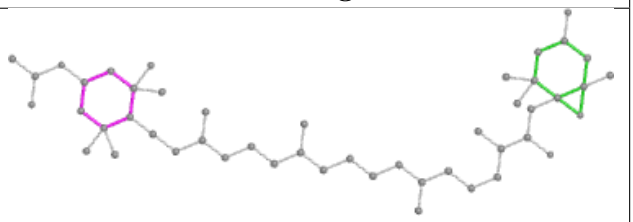
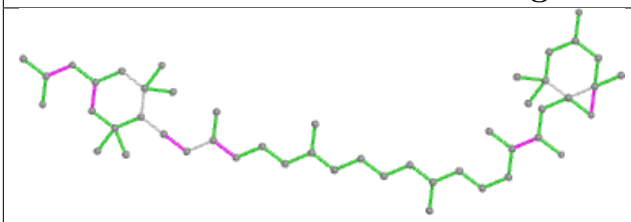


Rings

Ligand A86 P 303



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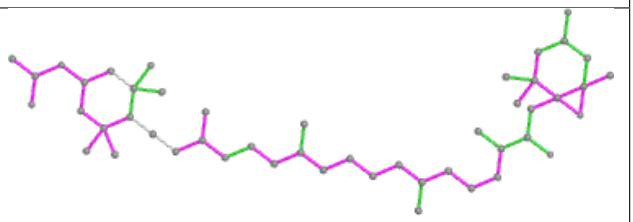
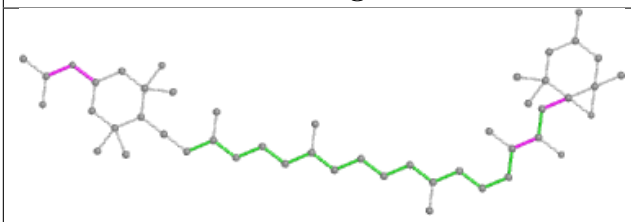


Bond angles



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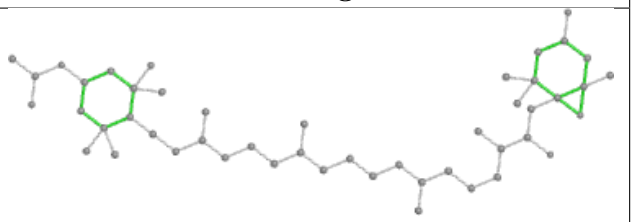
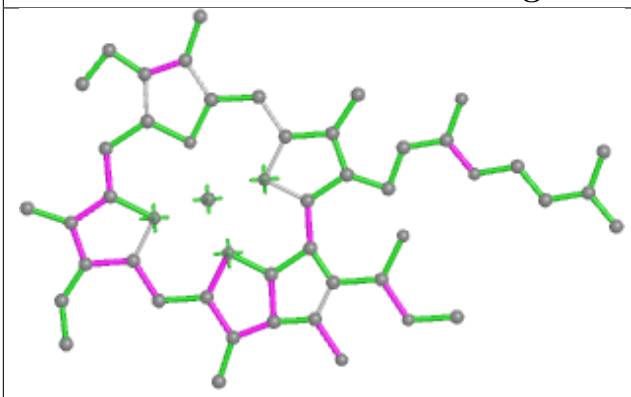


Rings

Ligand CLA G 319



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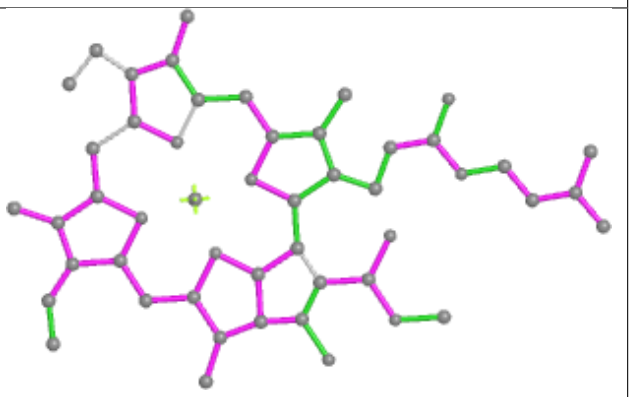

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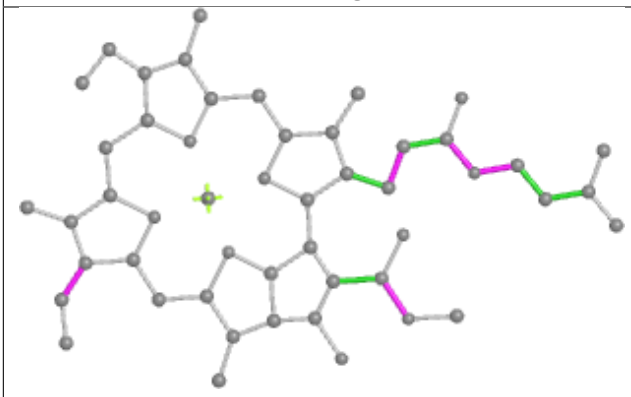

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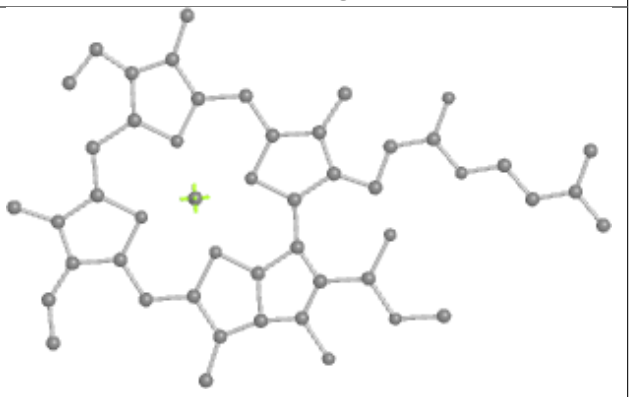
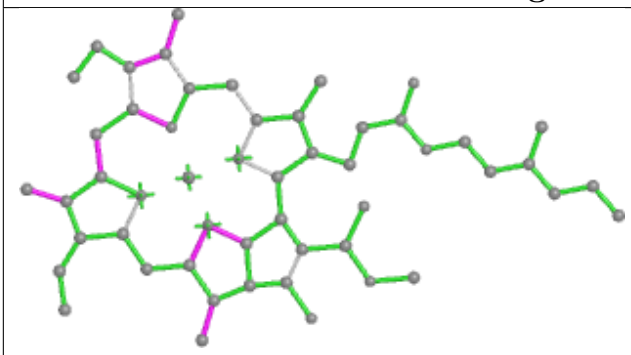


Rings

Ligand CLA a 841



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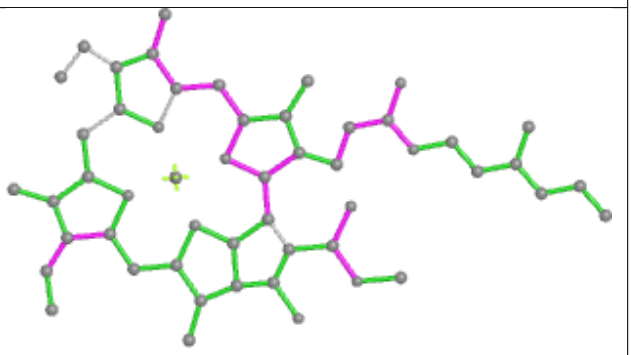

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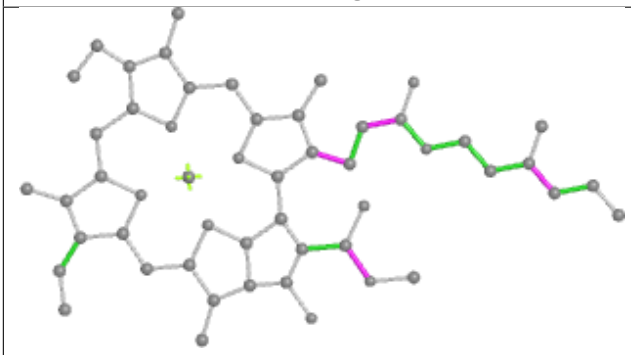

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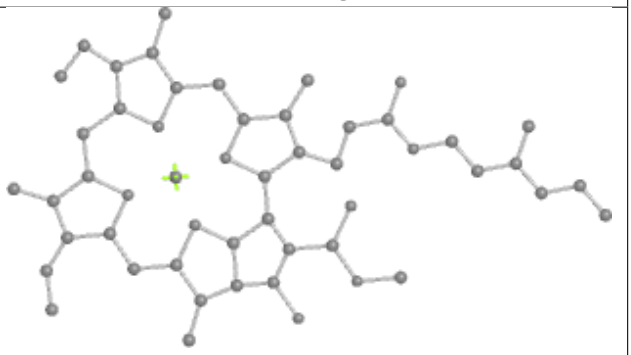
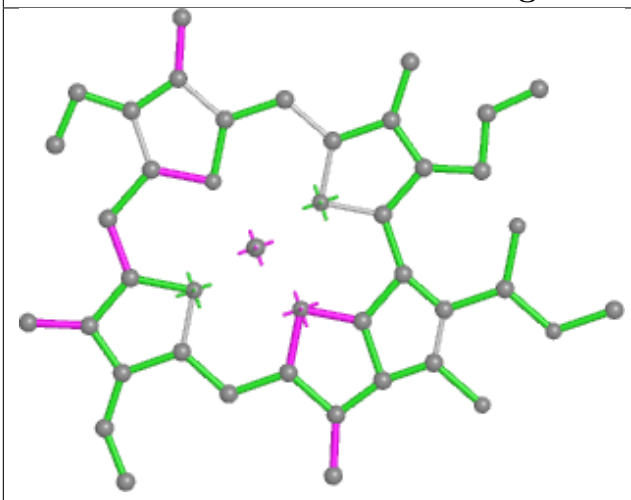


Rings

Ligand CLA W 218



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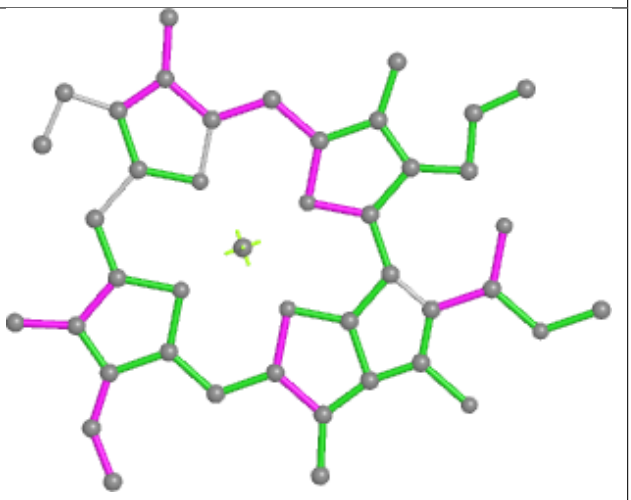
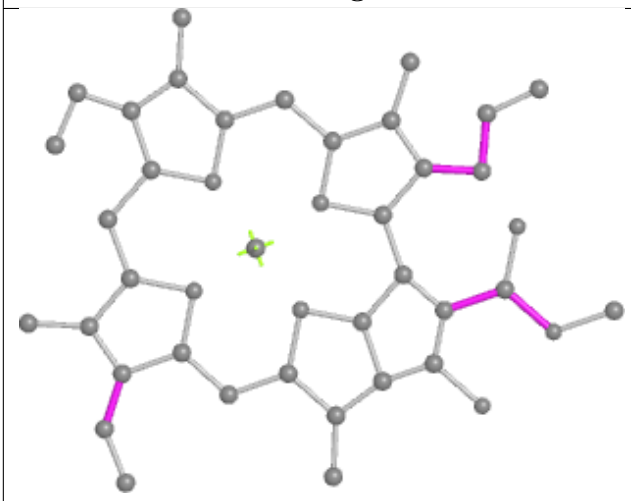


Bond angles



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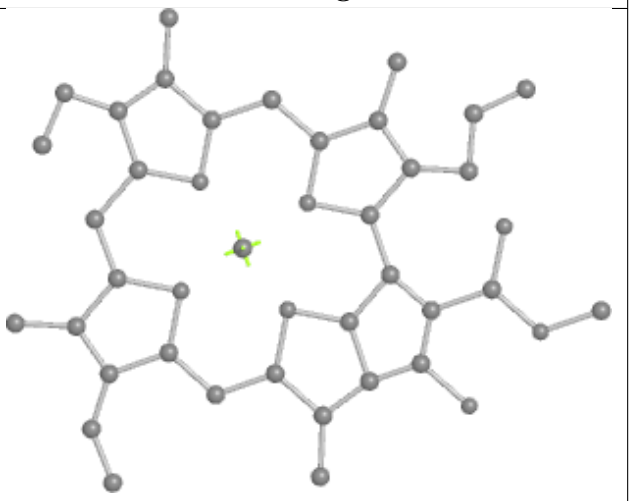
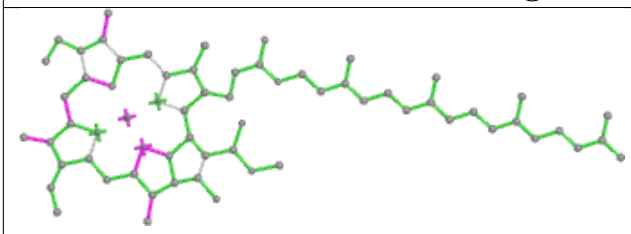


Rings

Ligand CLA Q 306



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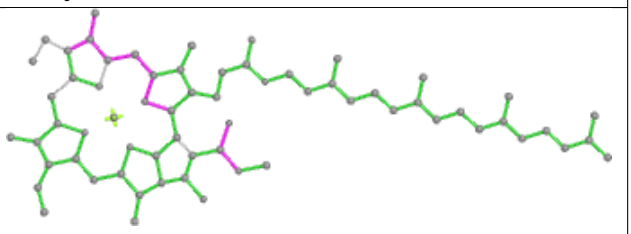
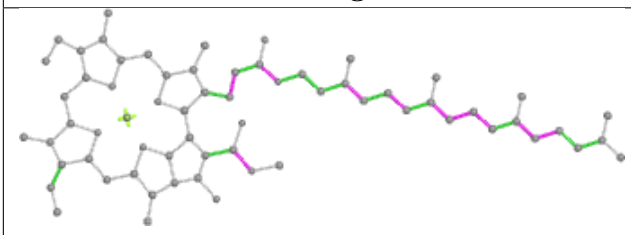


Bond angles



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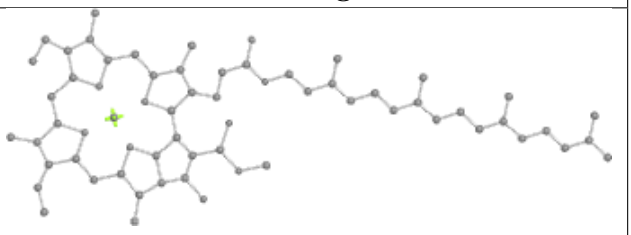
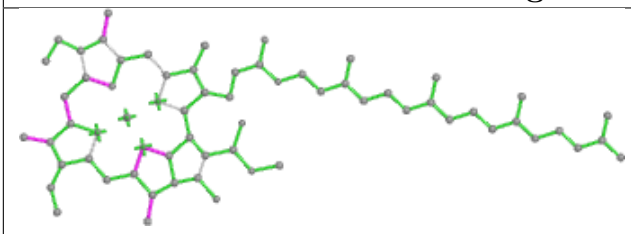
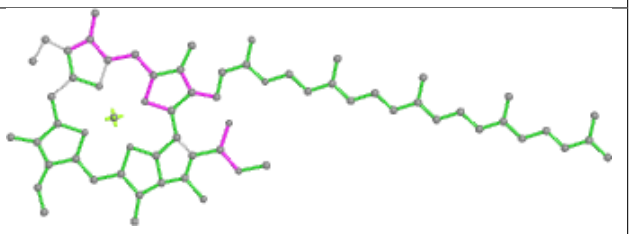
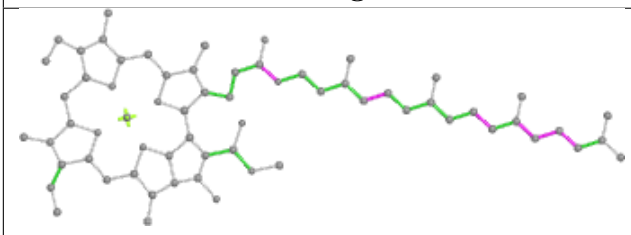
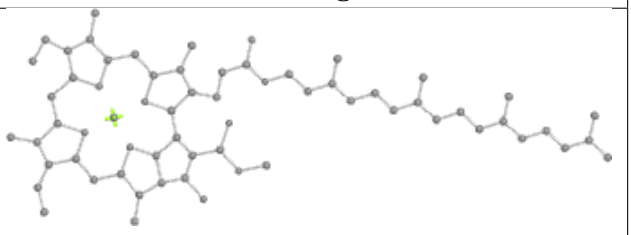


Rings

Ligand CLA L 313	
 Bond lengths	 Bond angles
 Torsions	 Rings

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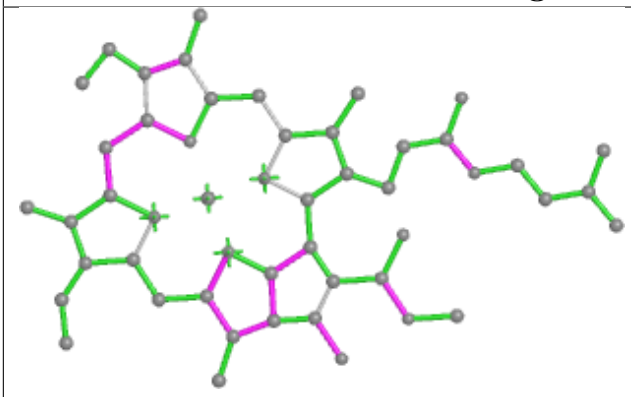
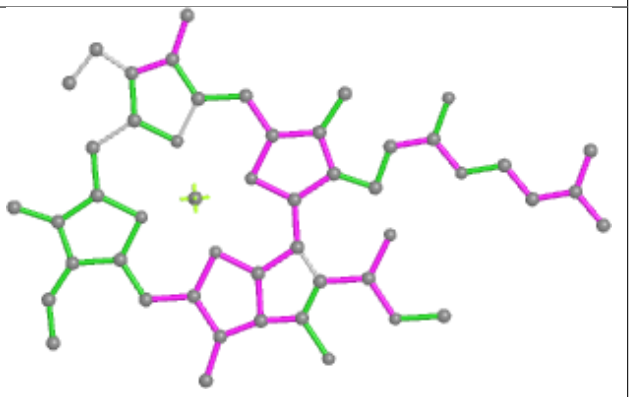
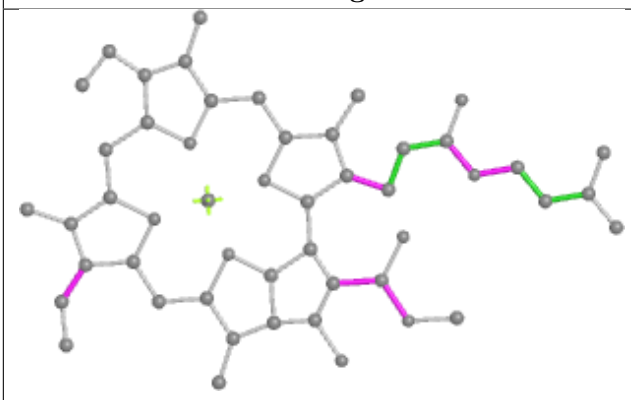
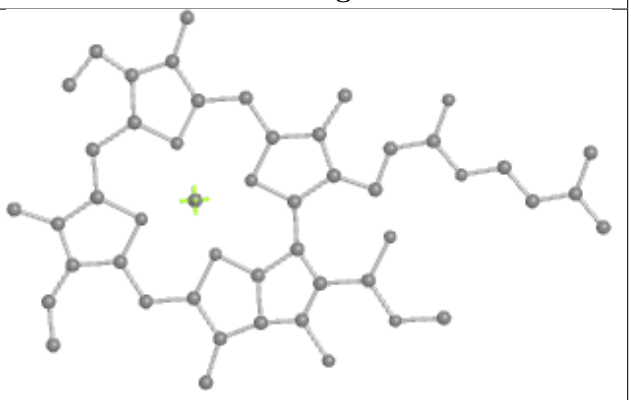
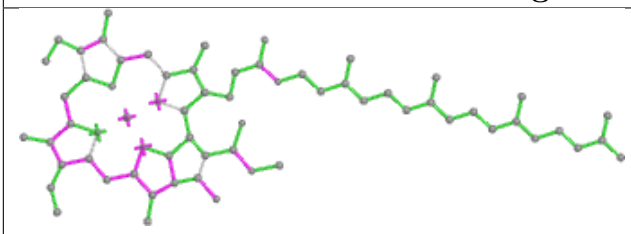
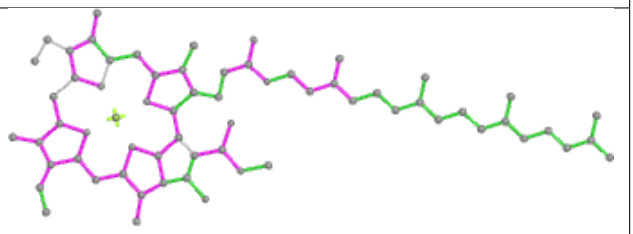
 Bond lengths	 Bond angles
 Torsions	 Rings

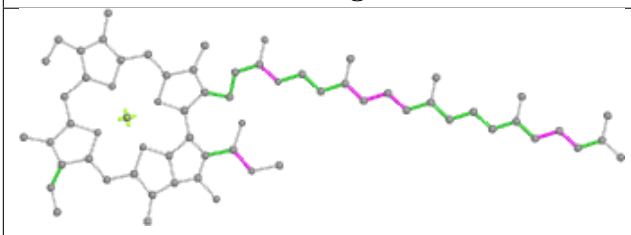
Ligand CLA f 804



Bond lengths



Bond angles



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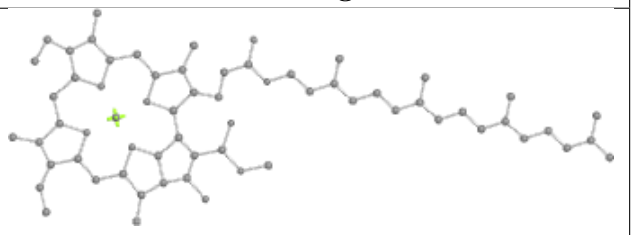
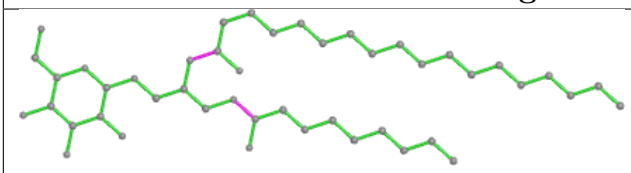


Rings

Ligand LMG V 315



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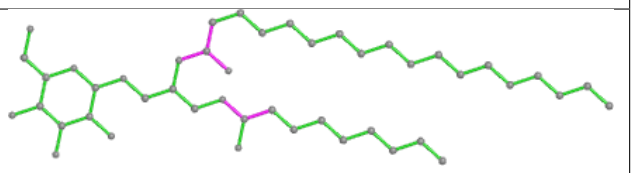
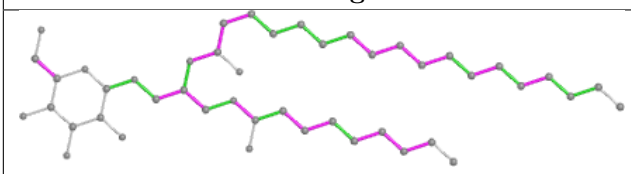


Bond angles



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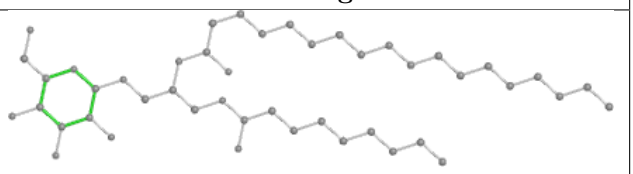
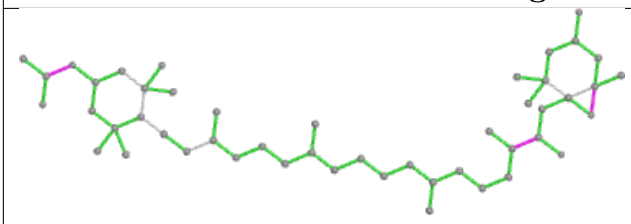
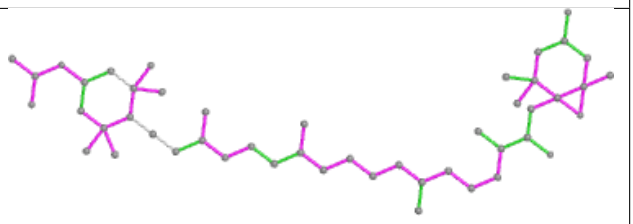


Rings

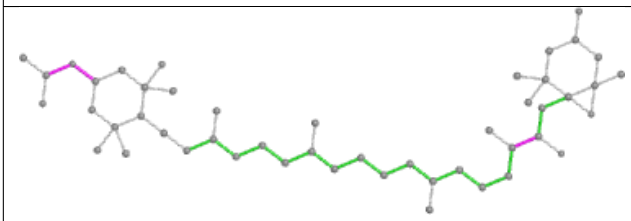
Ligand A86 K 306



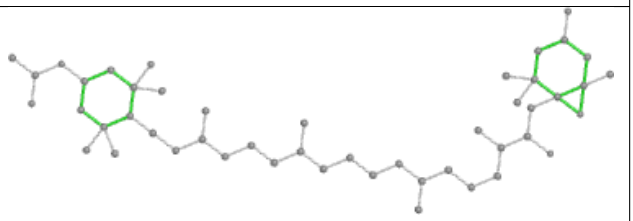
Bond lengths



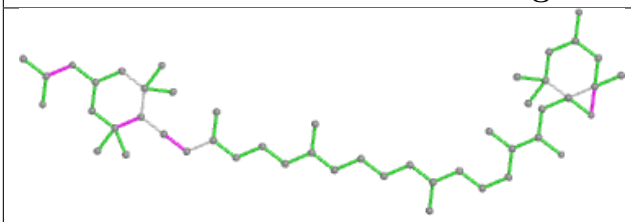
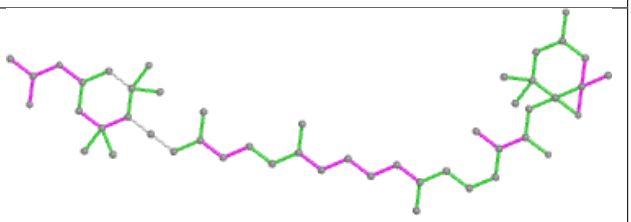
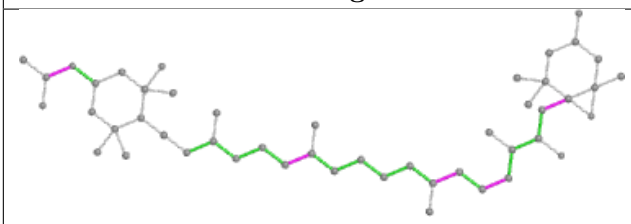
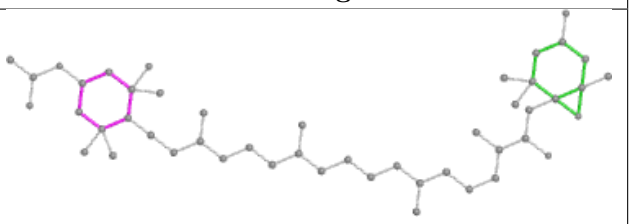
Bond angles

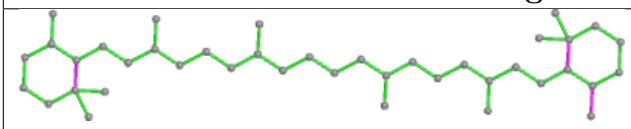
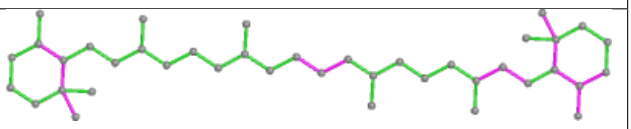
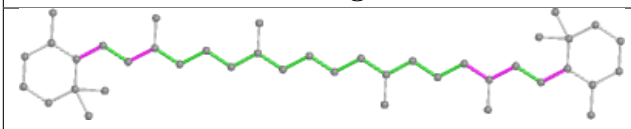
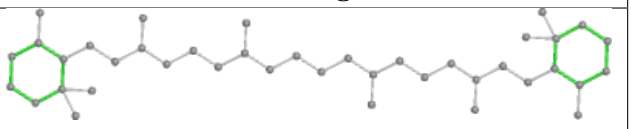


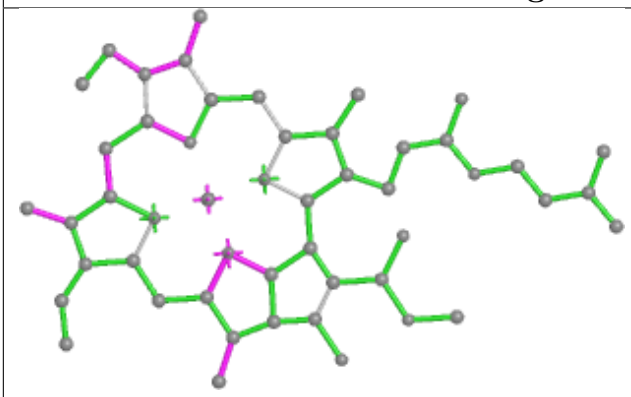
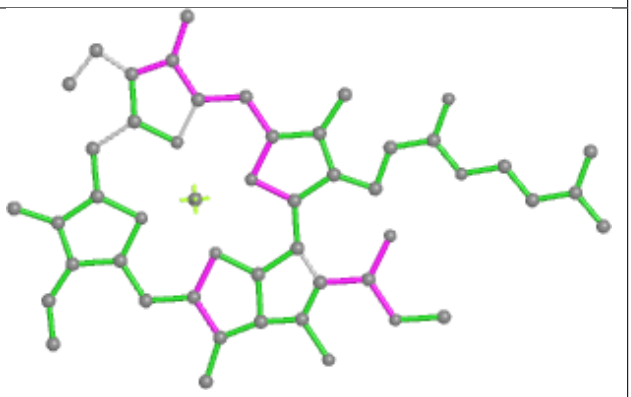
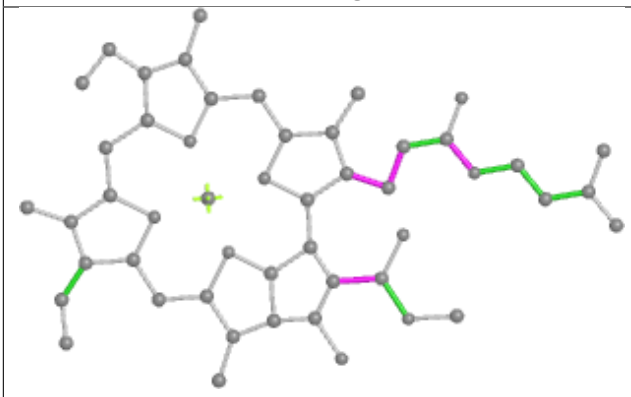
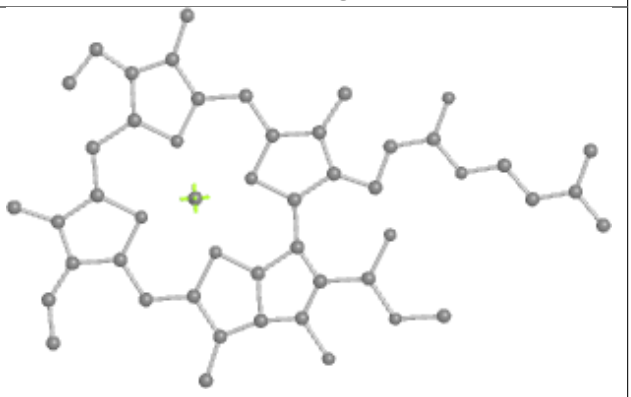
Torsions

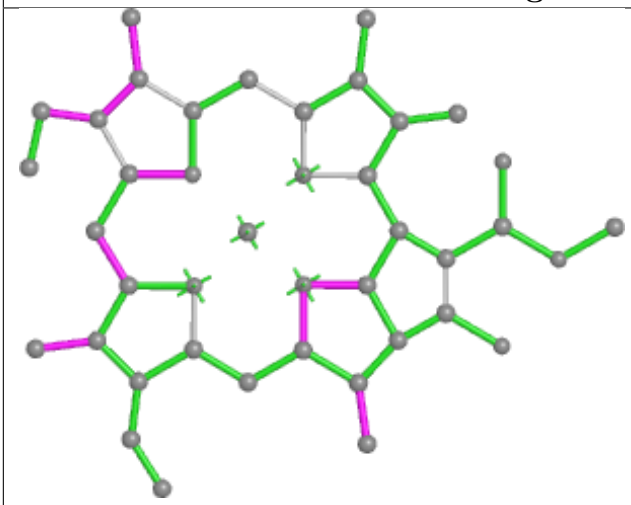
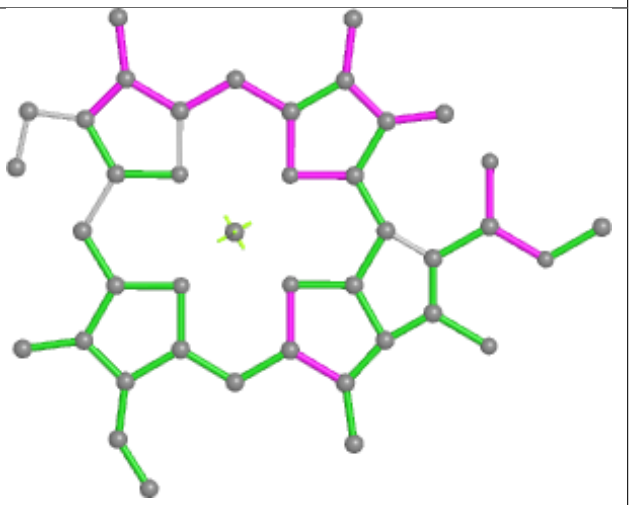
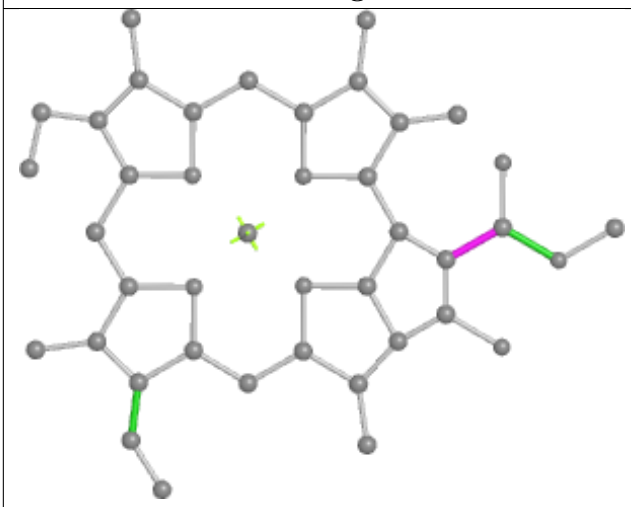
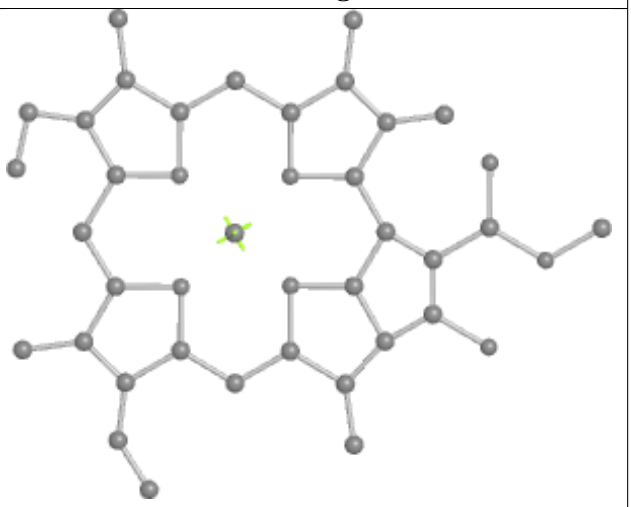


Rings

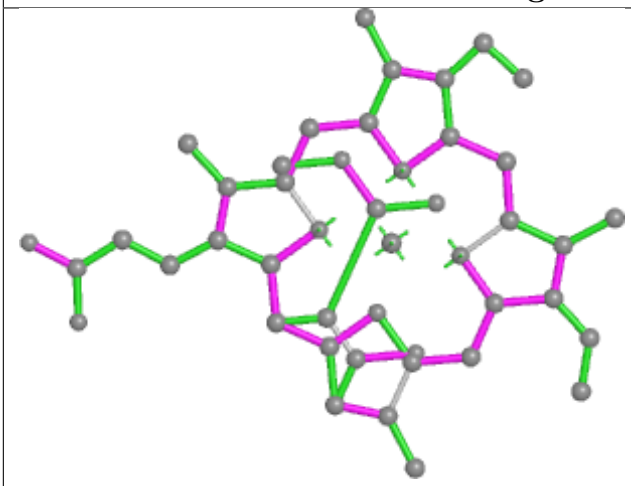
Ligand A86 L 307	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand BCR b 845	
 Bond lengths	 Bond angles
 Torsions	 Rings

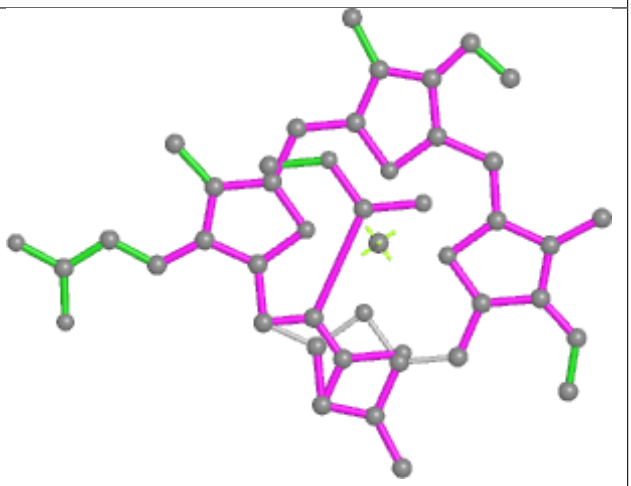
Ligand CLA b 831	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA F 316	
 Bond lengths	 Bond angles
 Torsions	 Rings

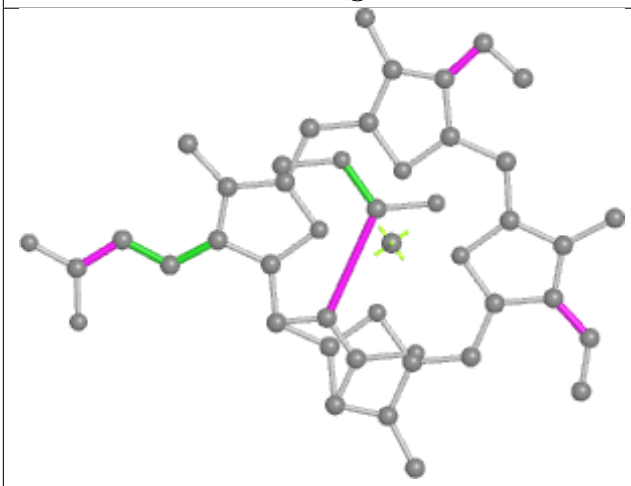
Ligand KC1 F 308



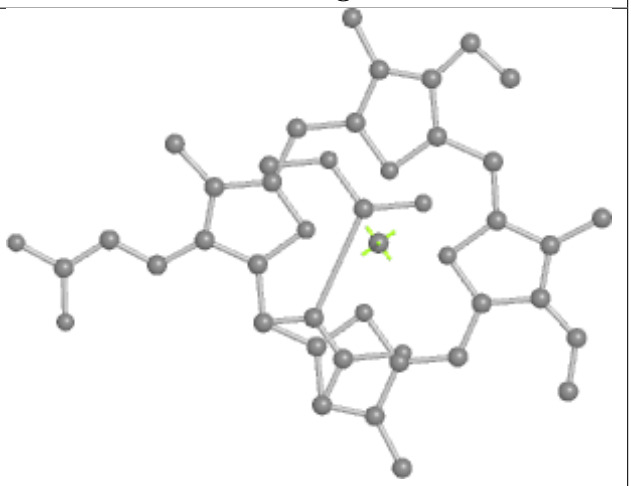
Bond lengths



Bond angles

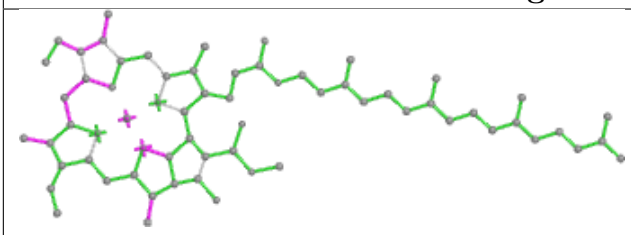


Torsions

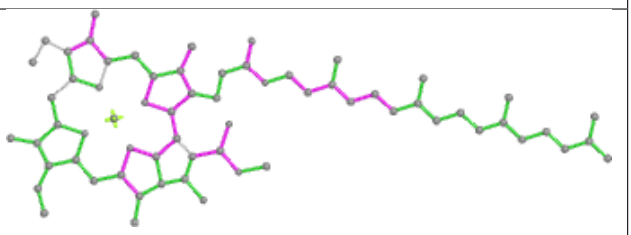


Rings

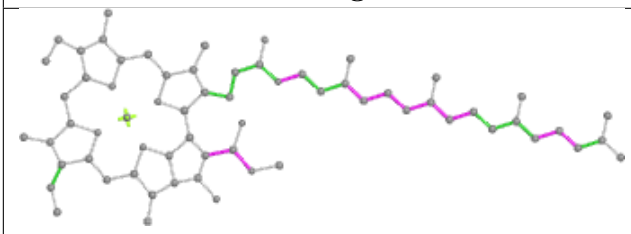
Ligand CLA b 805



Bond lengths



Bond angles



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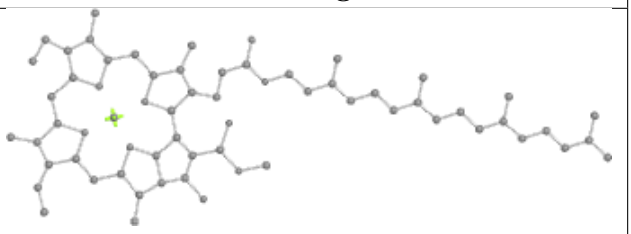
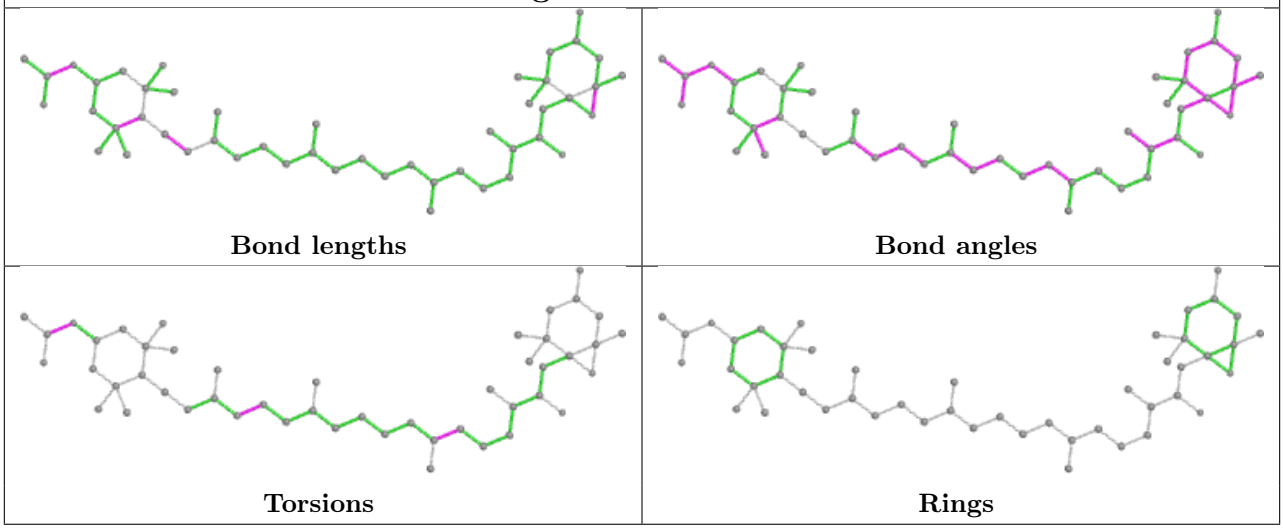
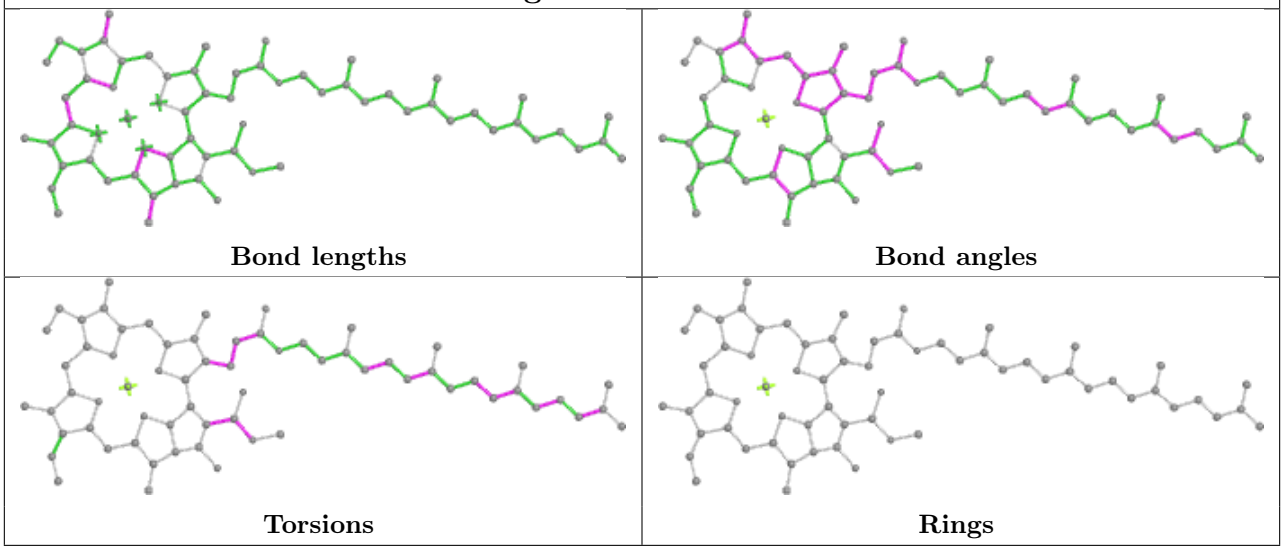


Rings

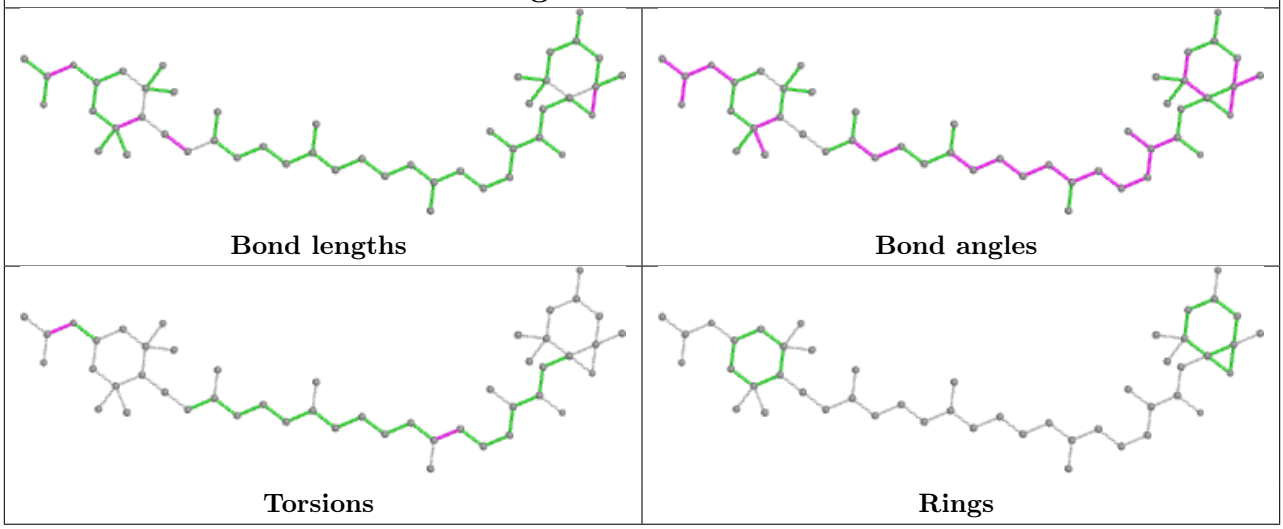
Ligand A86 E 305

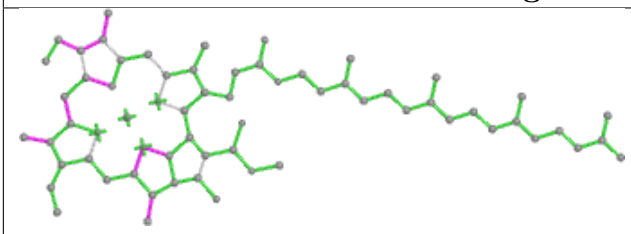
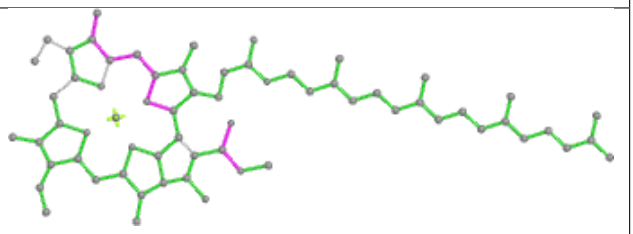
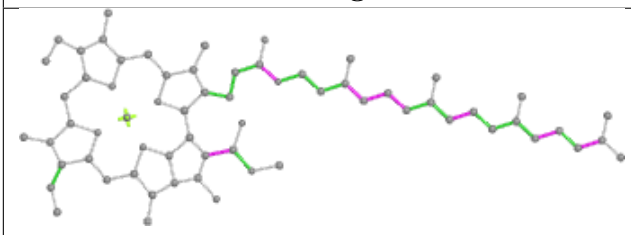
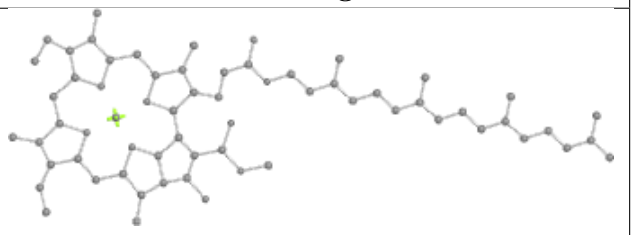


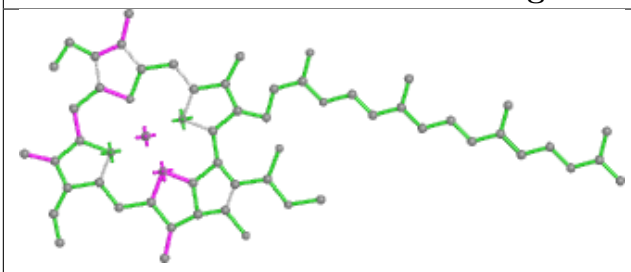
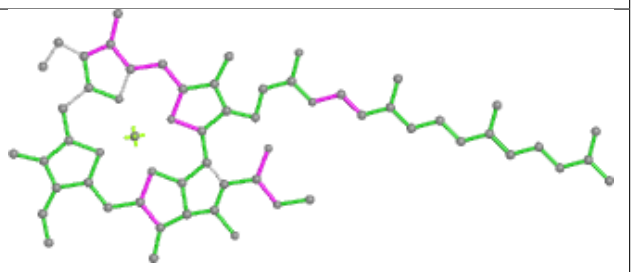
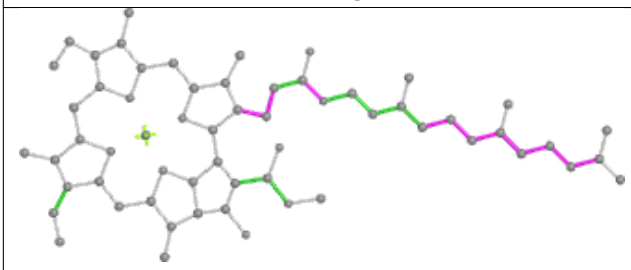
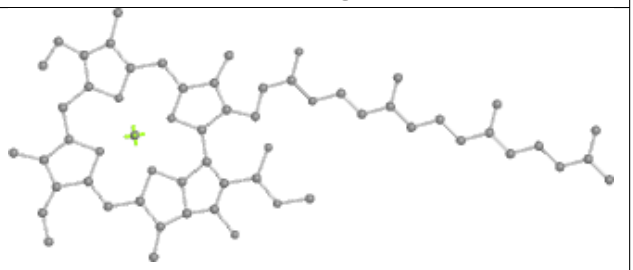
Ligand CLA G 313



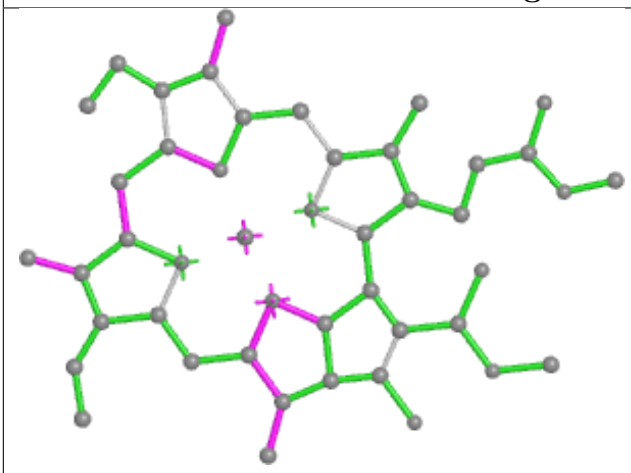
Ligand A86 O 301



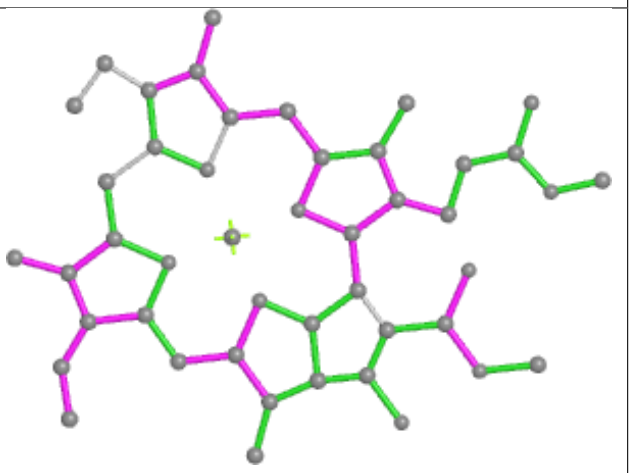
Ligand CLA K 316	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA b 820	
 Bond lengths	 Bond angles
 Torsions	 Rings

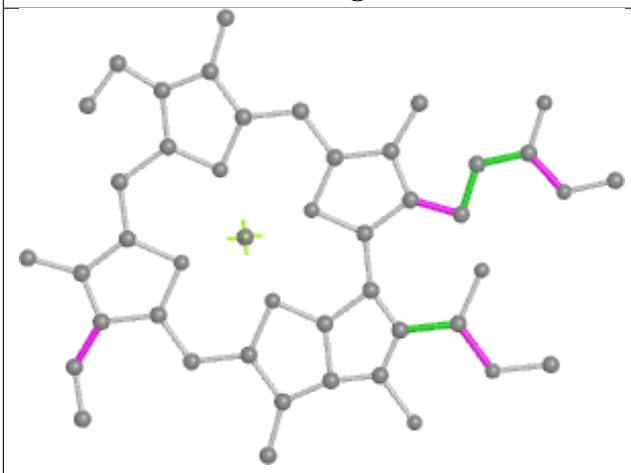
Ligand CLA R 316



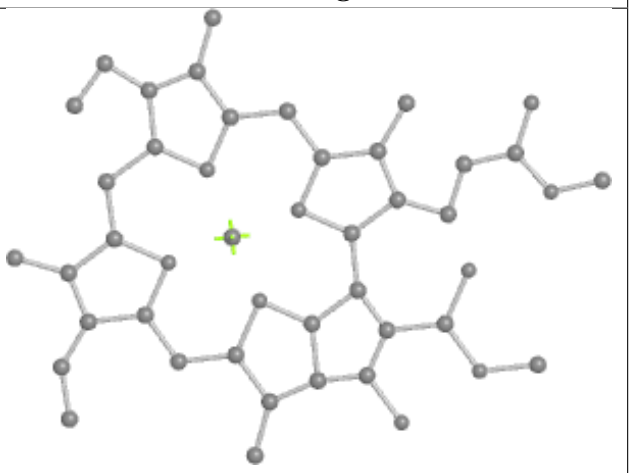
Bond lengths



Bond angles

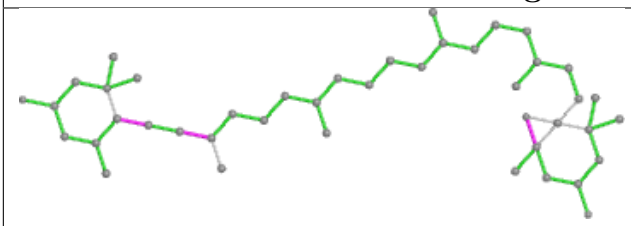


Torsions

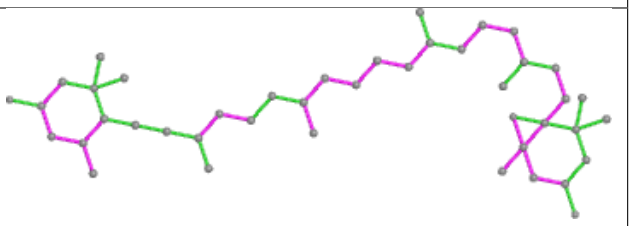


Rings

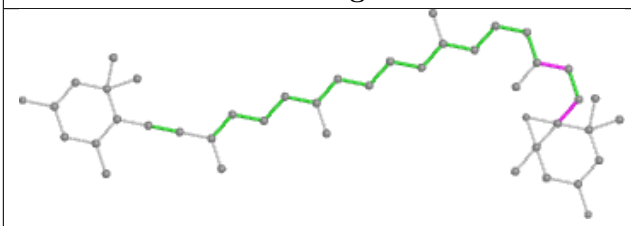
Ligand DD6 H 302



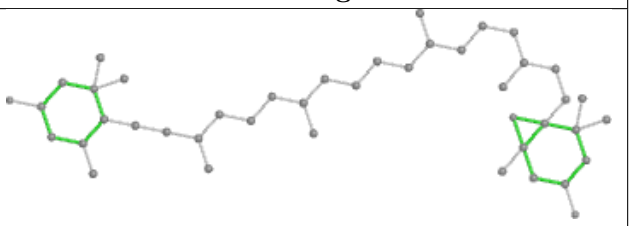
Bond lengths



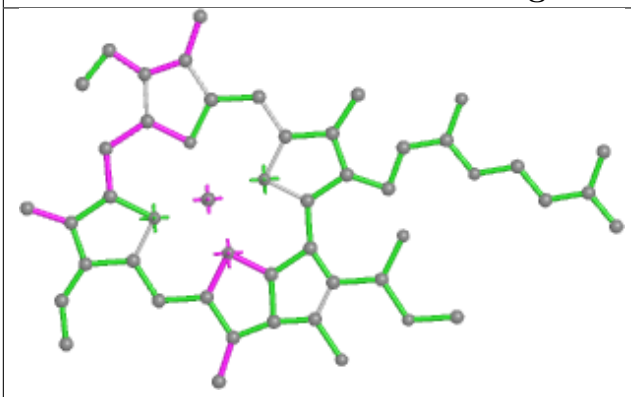
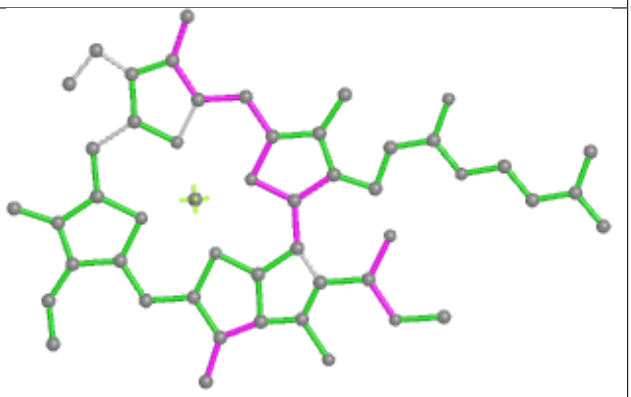
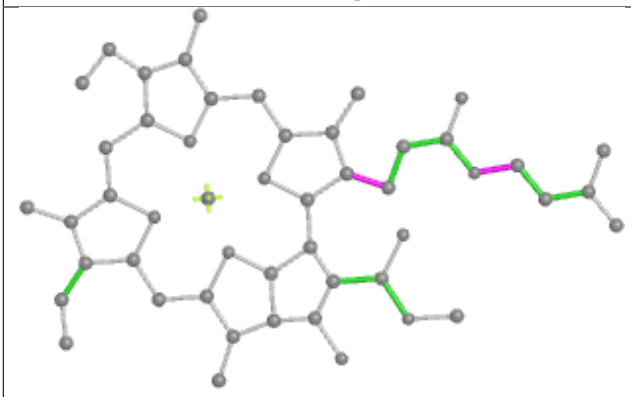
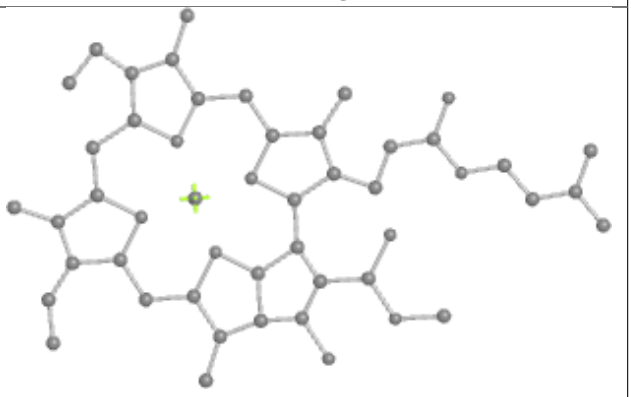
Bond angles



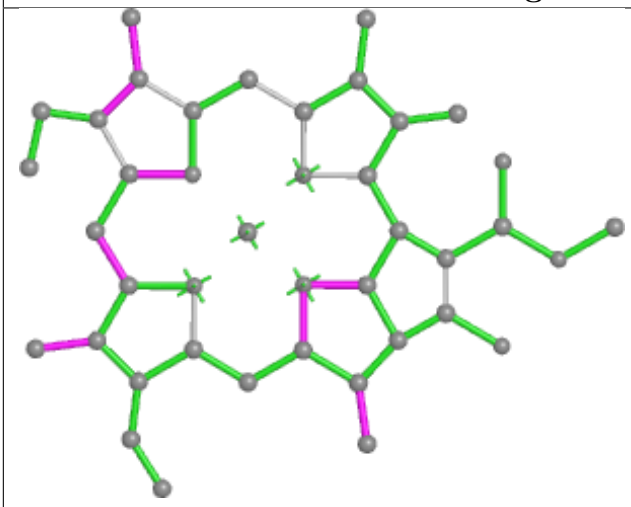
Torsions



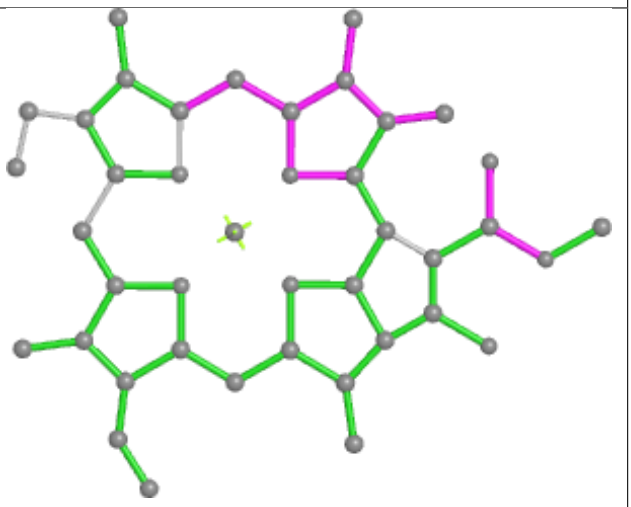
Rings

Ligand CLA a 833	
 Bond lengths	 Bond angles
 Torsions	 Rings

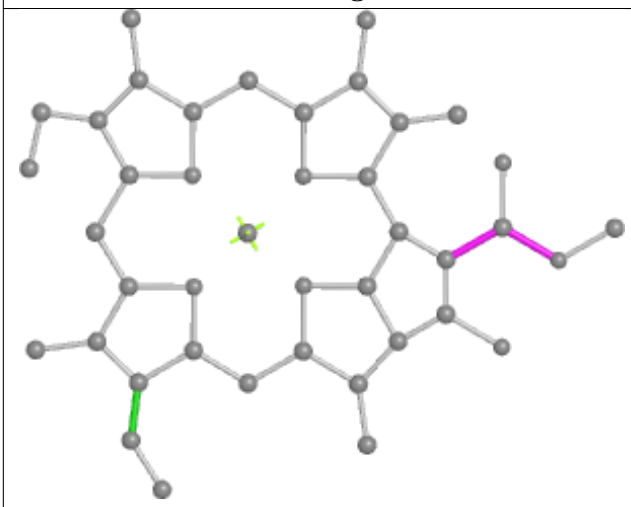
Ligand CLA P 316



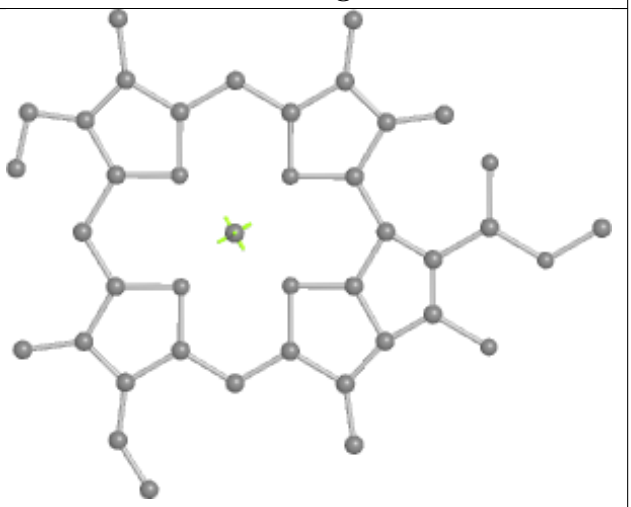
Bond lengths



Bond angles

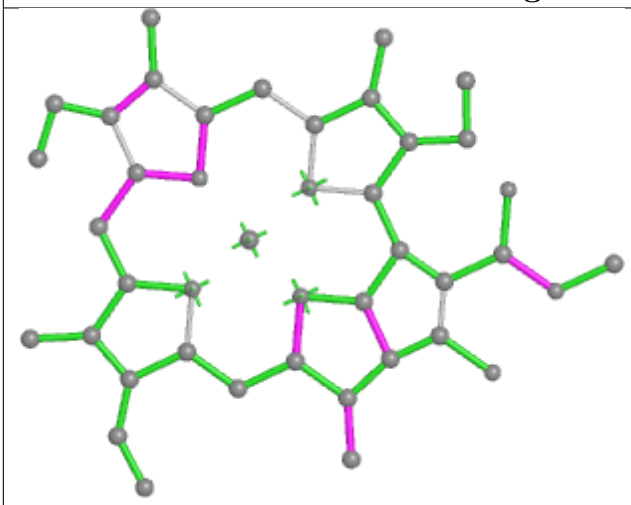


Torsions

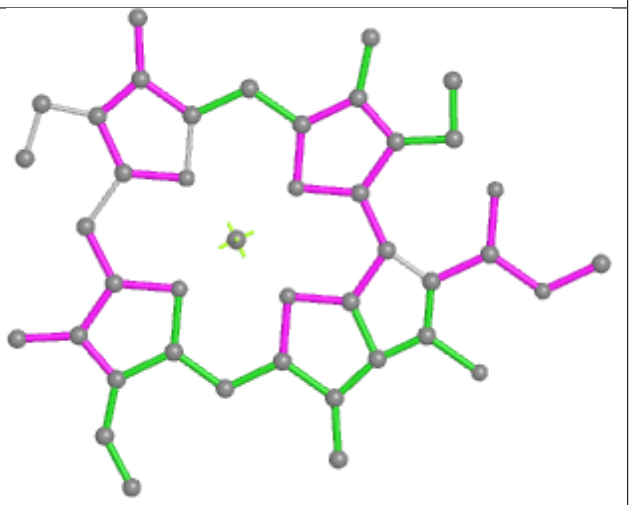


Rings

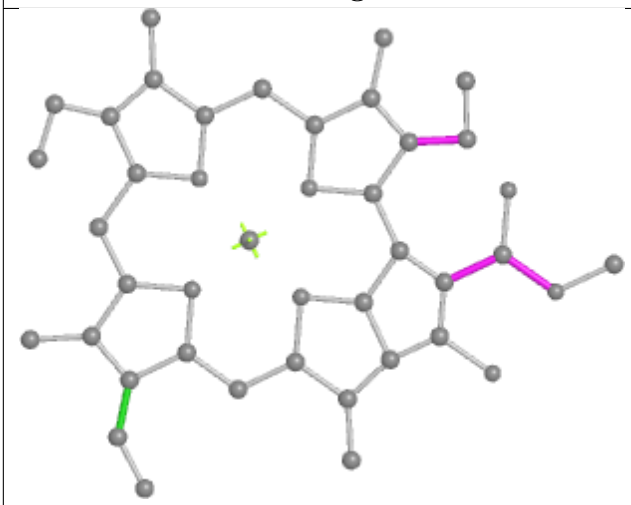
Ligand CLA X 313



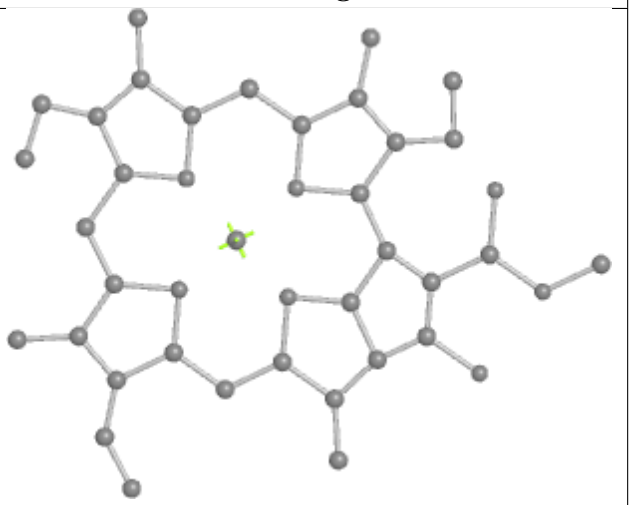
Bond lengths



Bond angles

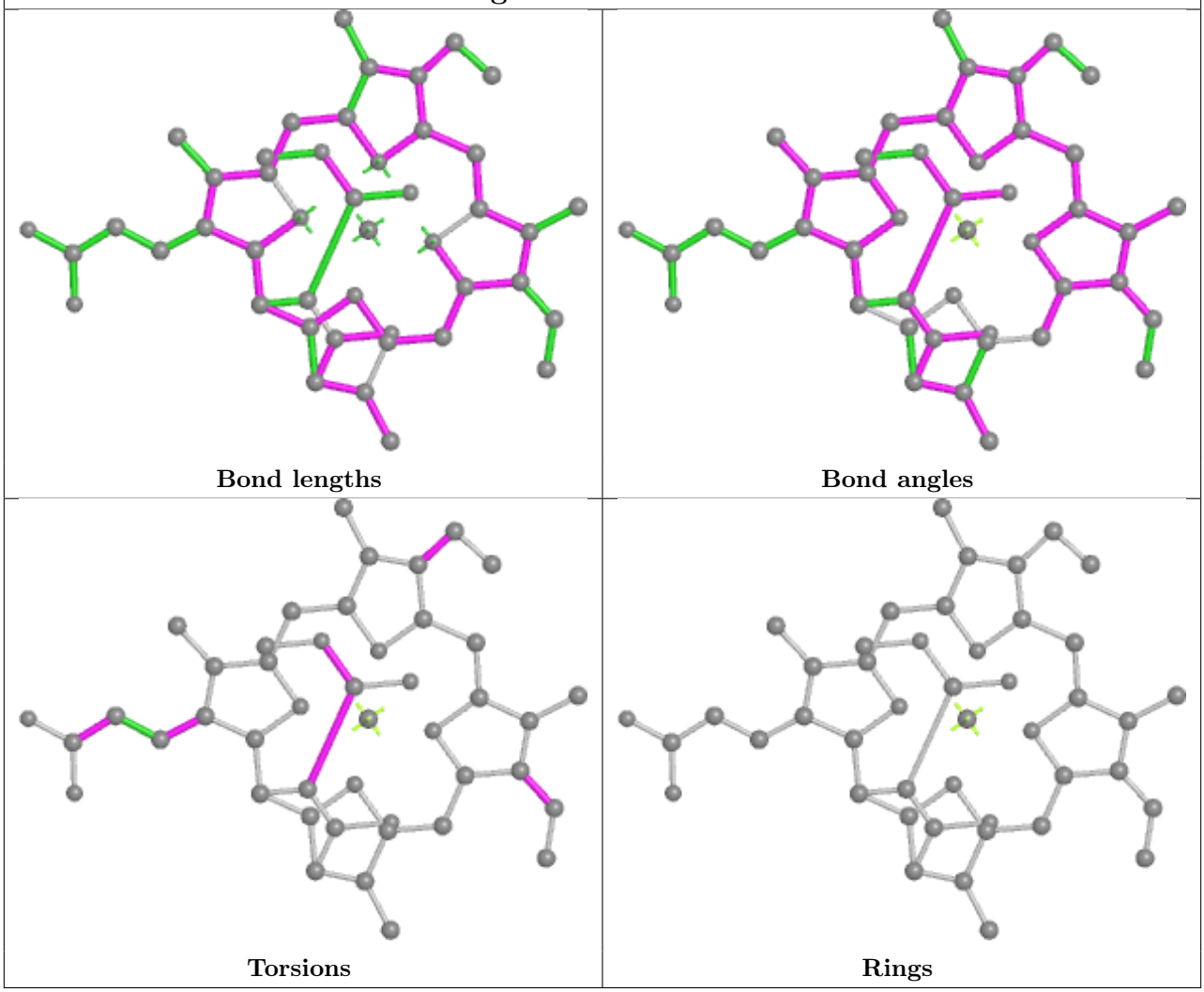


Torsions

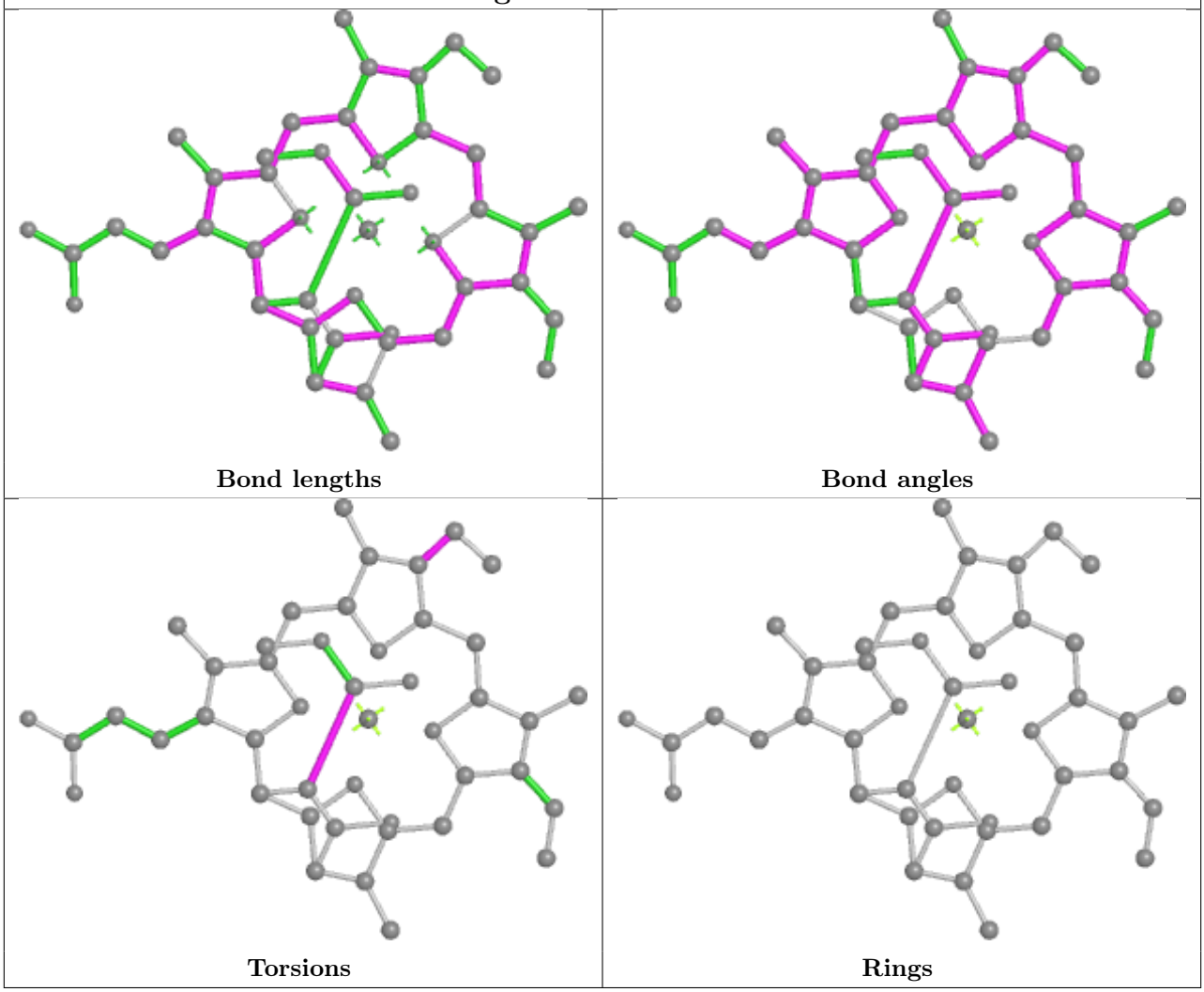


Rings

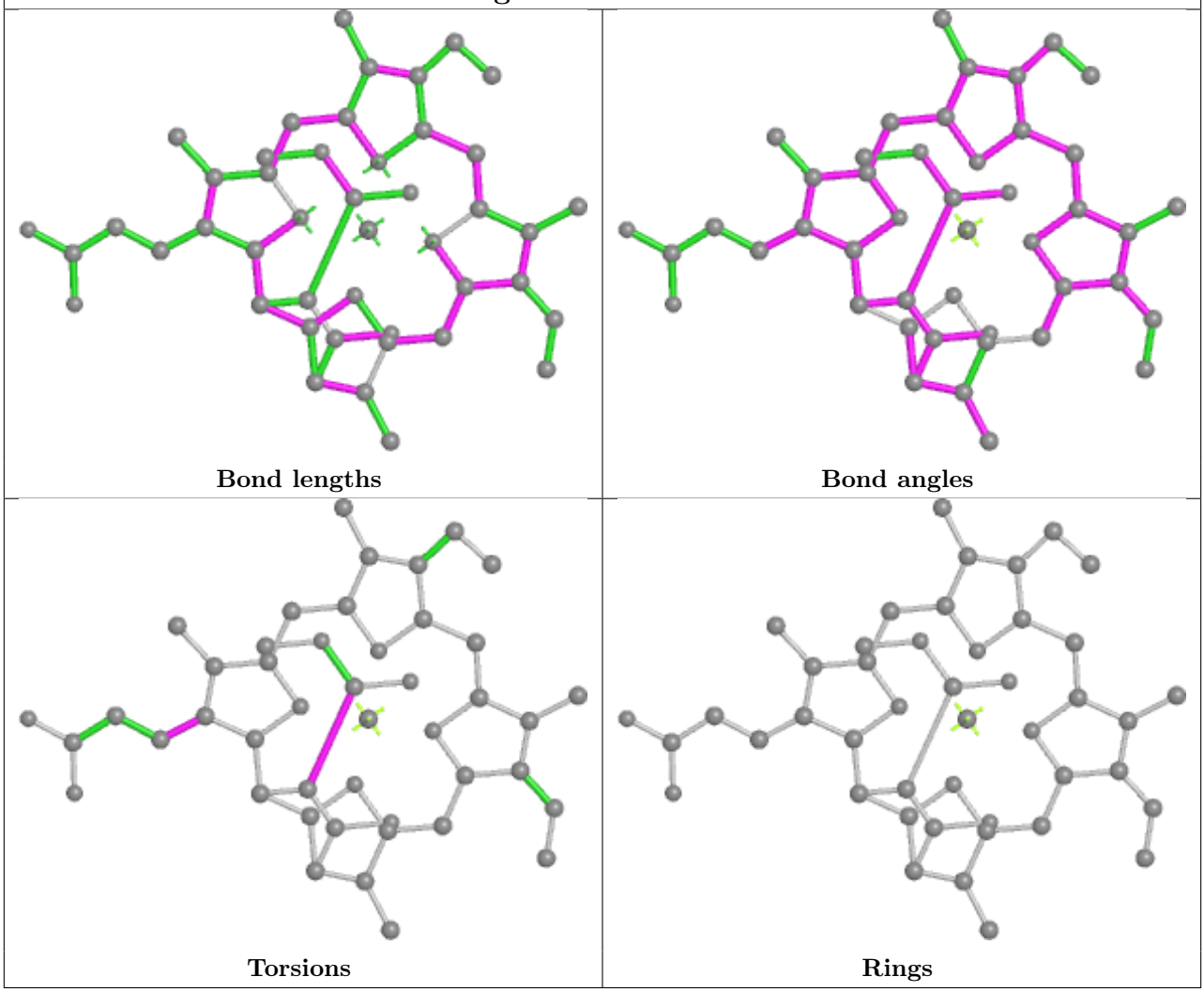
Ligand KC1 M 318



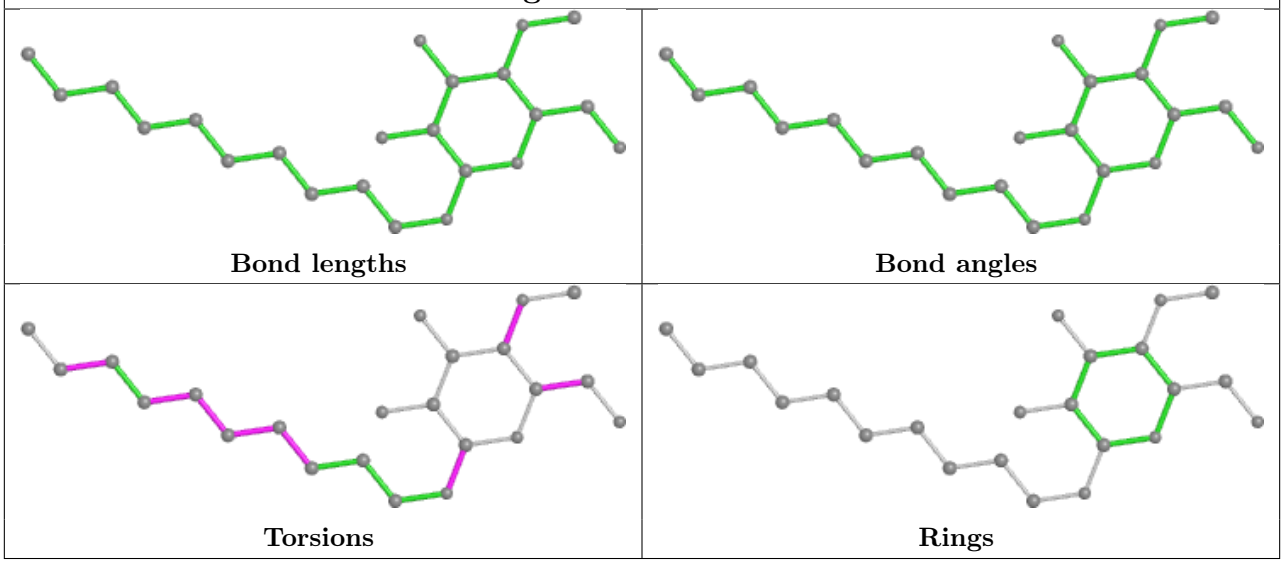
Ligand KC1 O 313

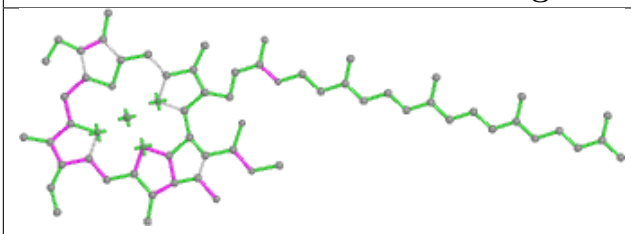
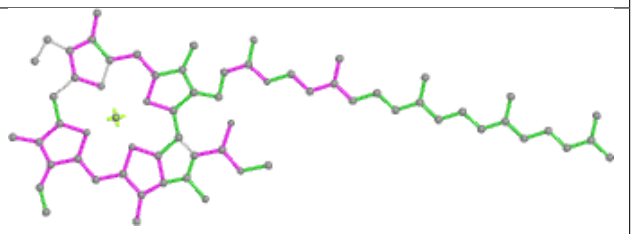
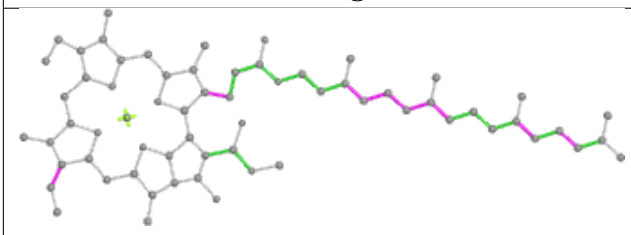
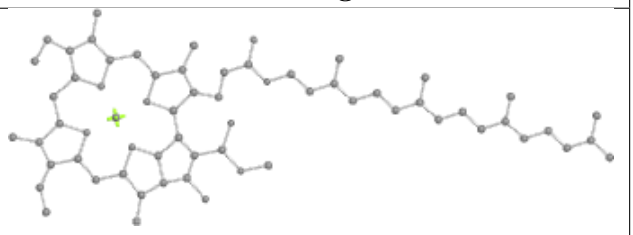


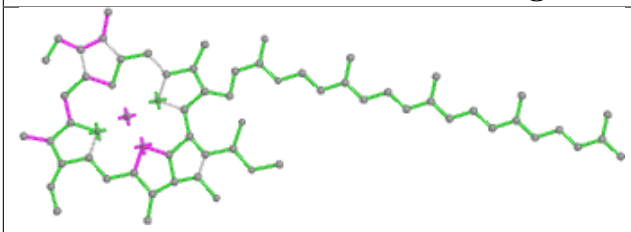
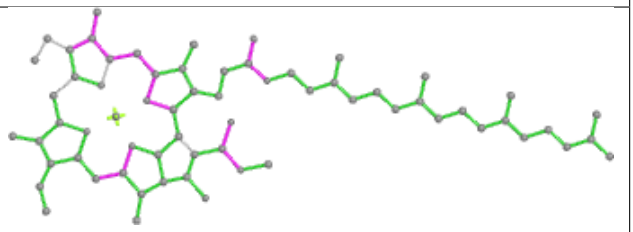
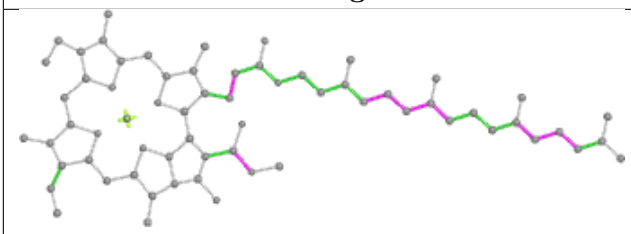
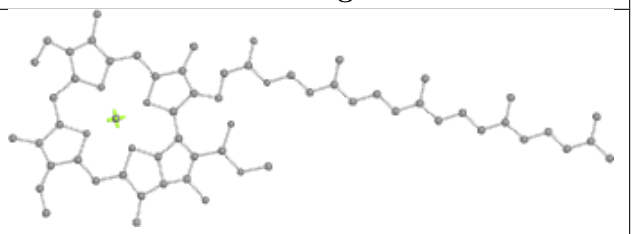
Ligand KC1 X 311

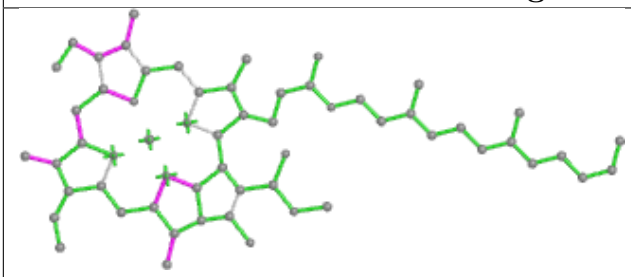
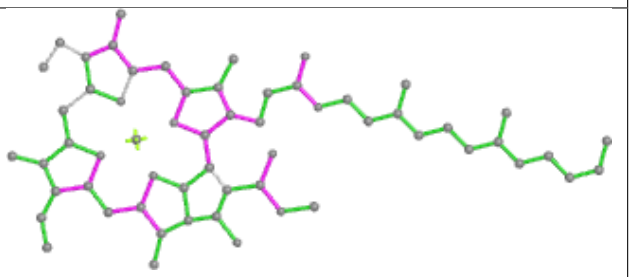
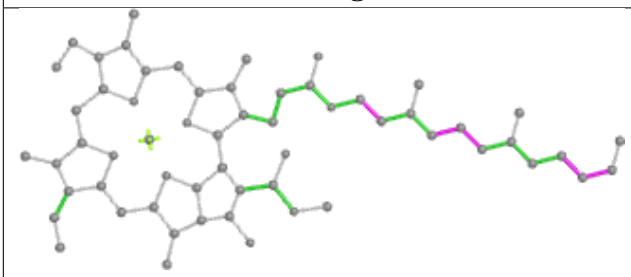
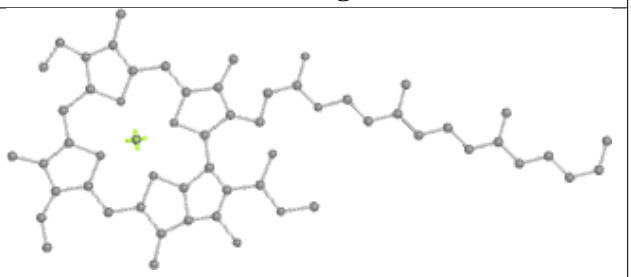


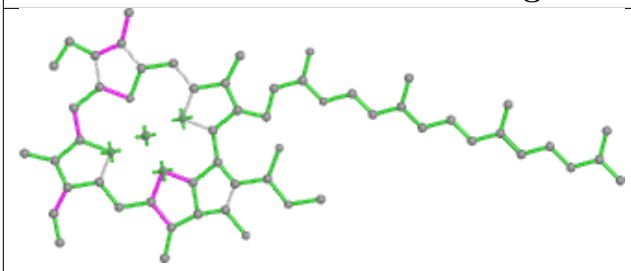
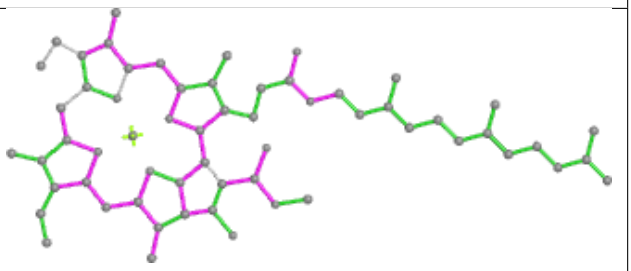
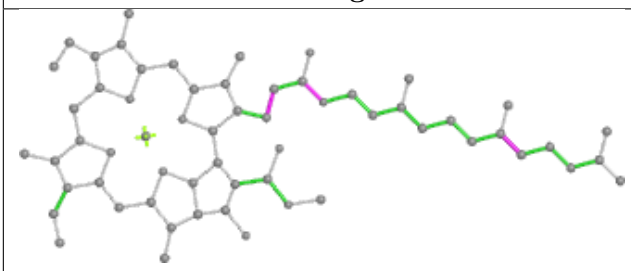
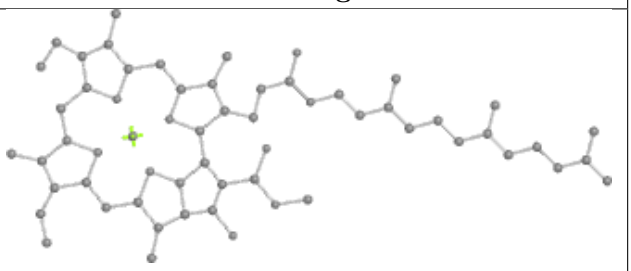
Ligand LMT E 321

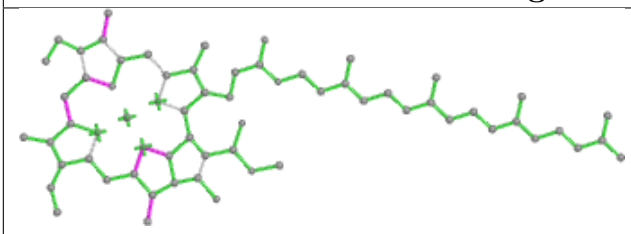
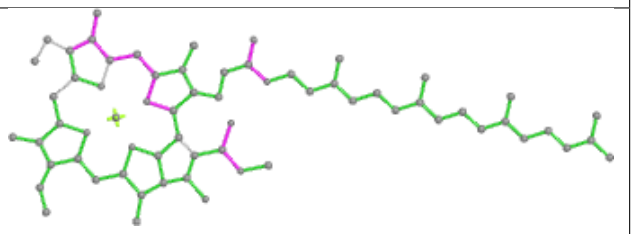
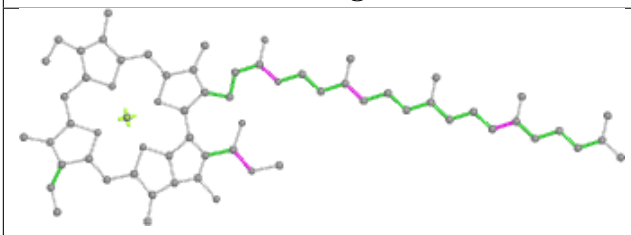
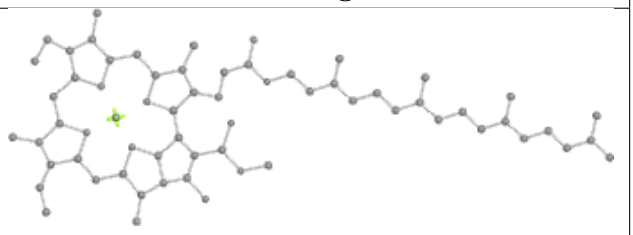


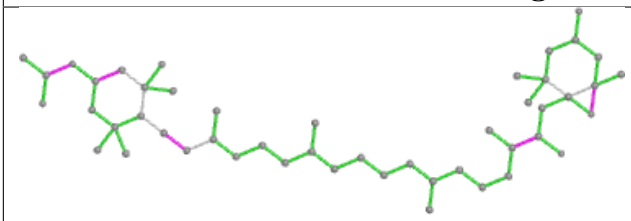
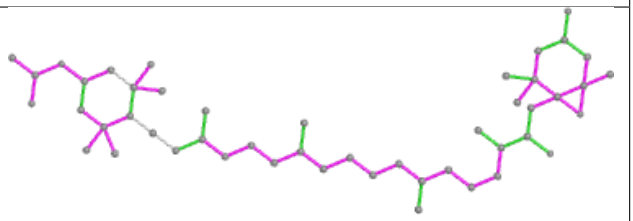
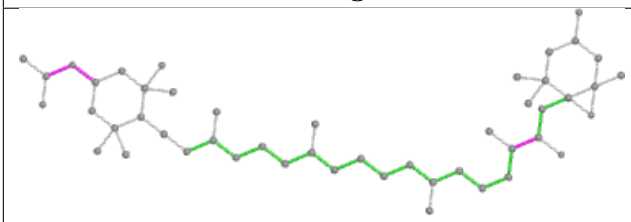
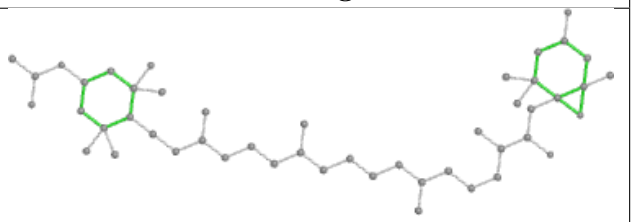
Ligand CLA f 803	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA J 313	
 Bond lengths	 Bond angles
 Torsions	 Rings

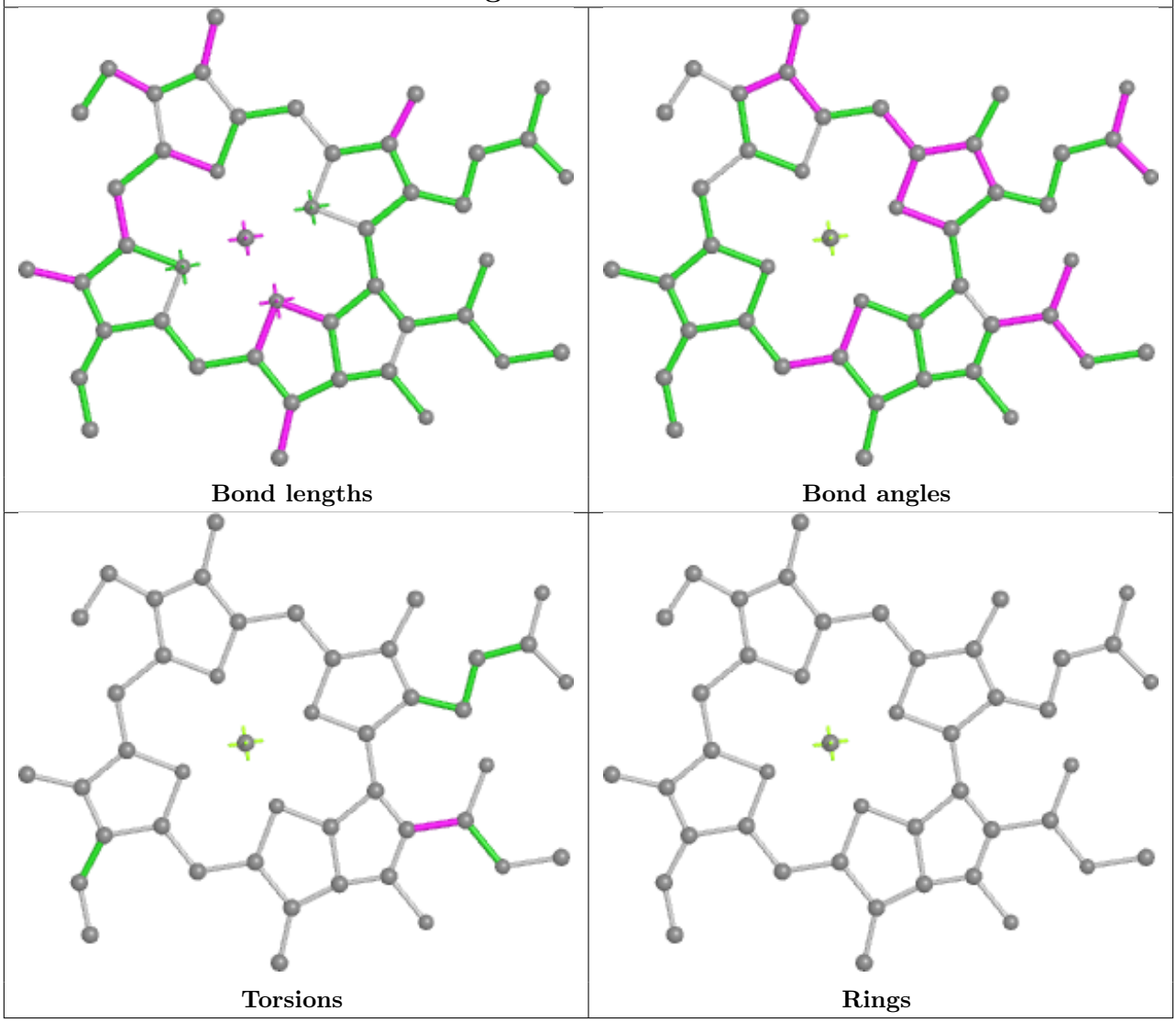
Ligand CLA b 819	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA H 307	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA J 309	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand A86 R 303	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA a 813



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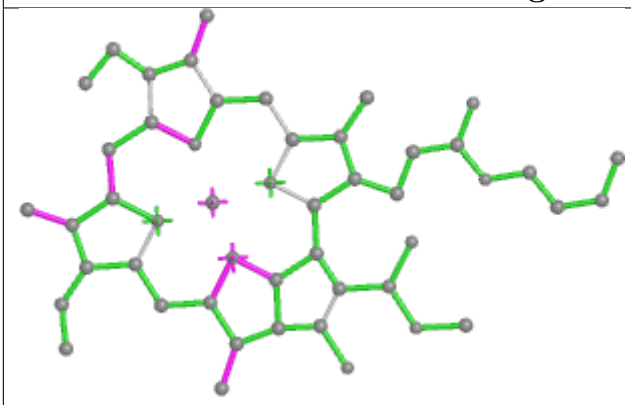
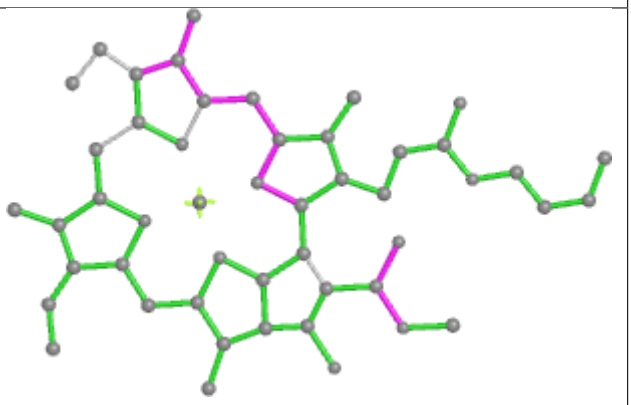
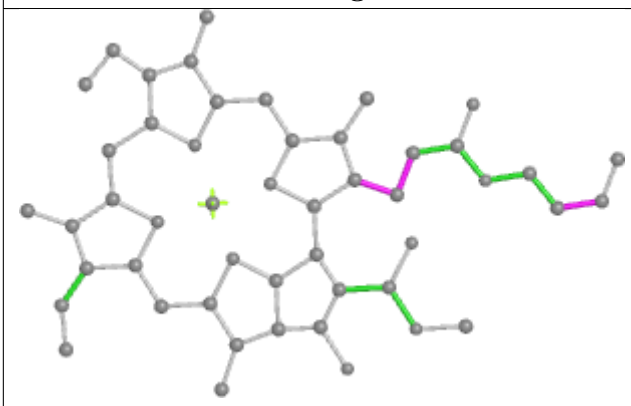
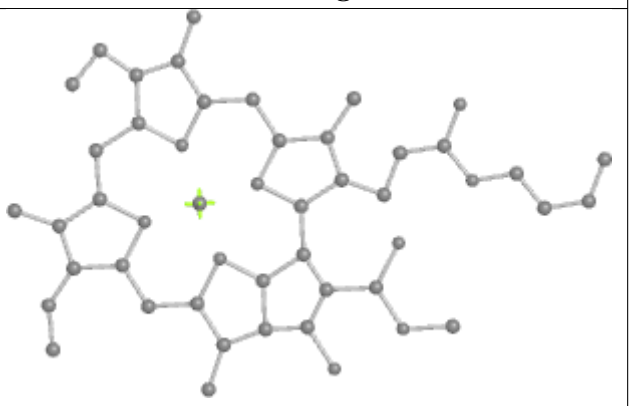
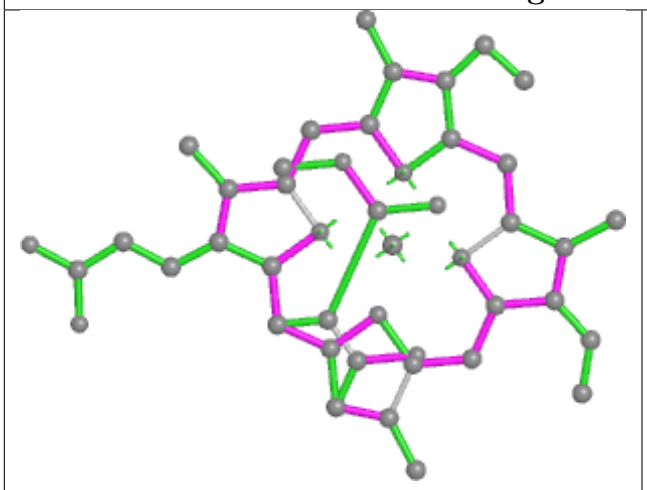
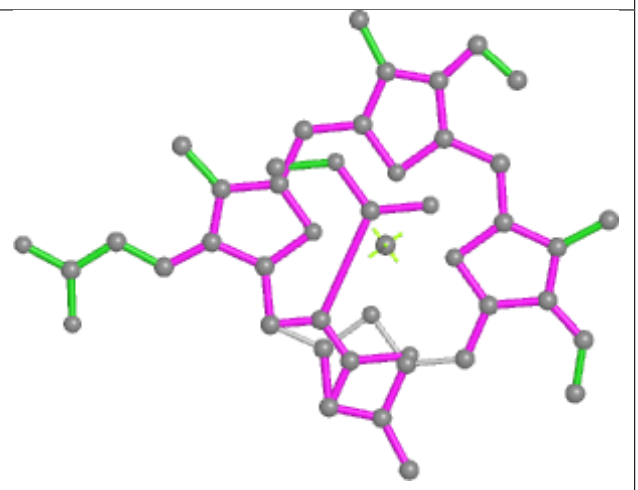
 Bond lengths	 Bond angles
 Torsions	 Rings

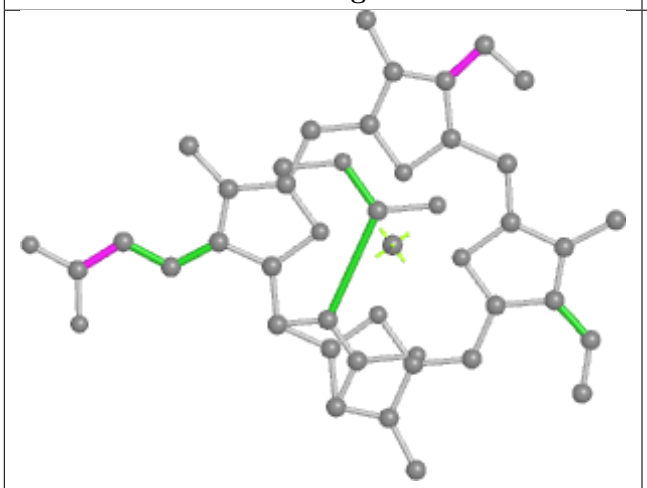
Ligand KC1 B 310



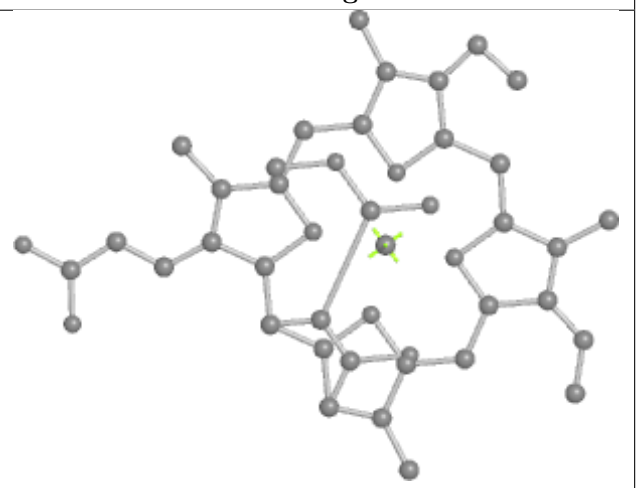
Bond lengths



Bond angles

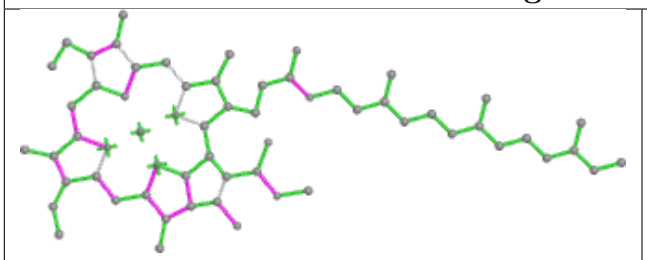


Torsions

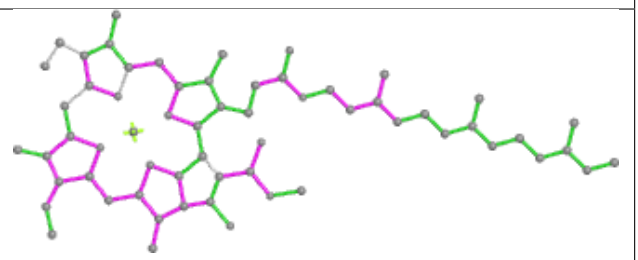


Rings

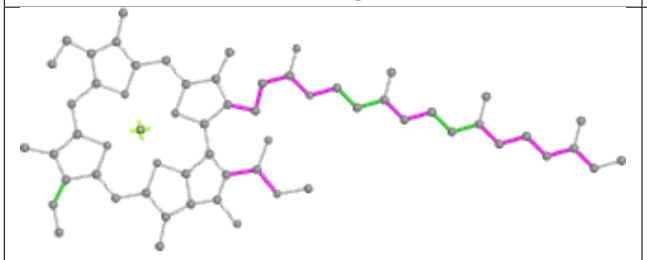
Ligand CLA K 307



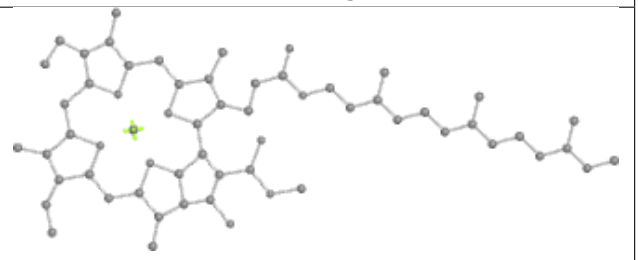
Bond lengths



Bond angles

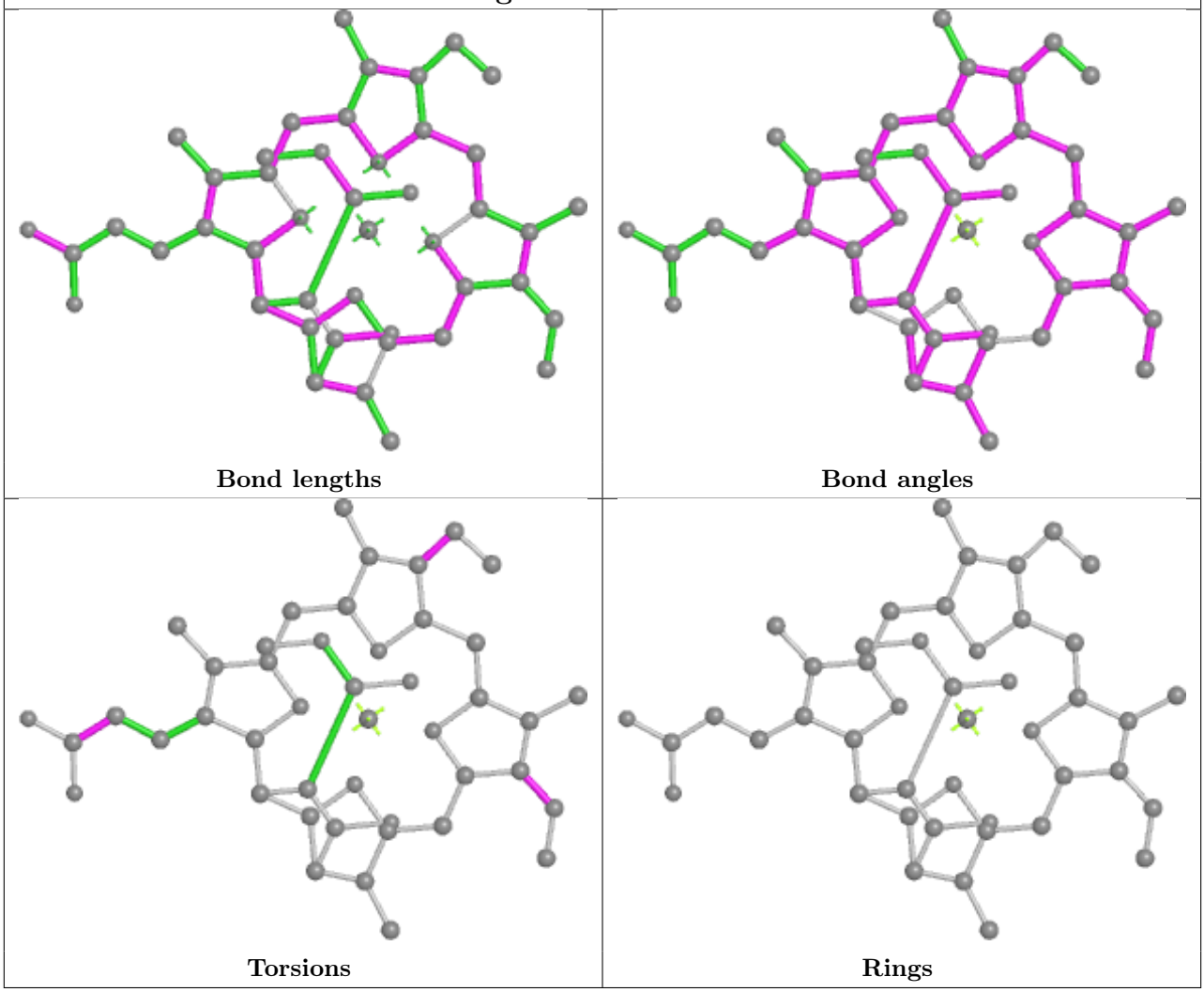


Torsions

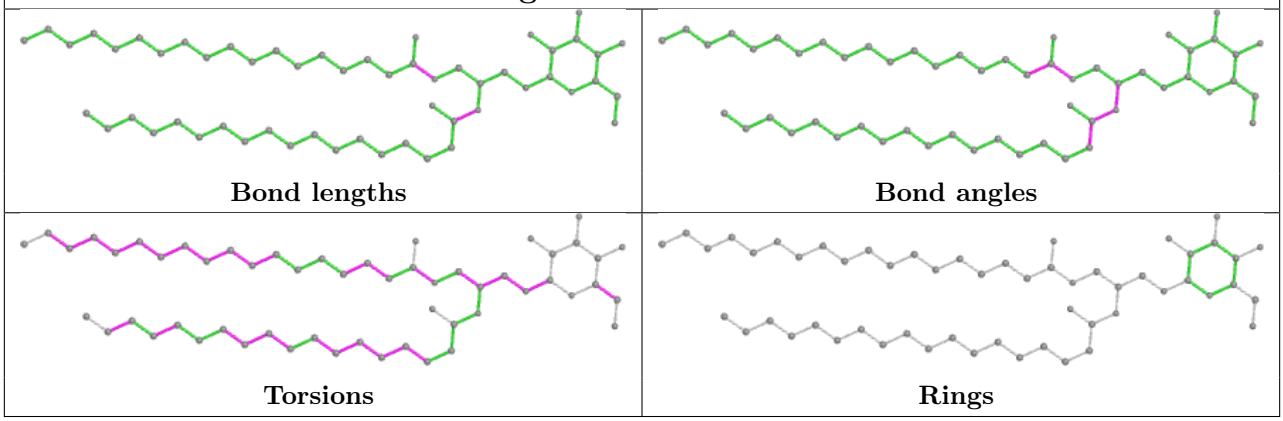


Rings

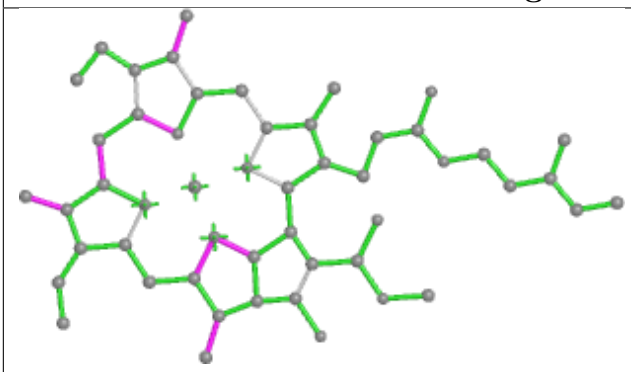
Ligand KC1 E 309



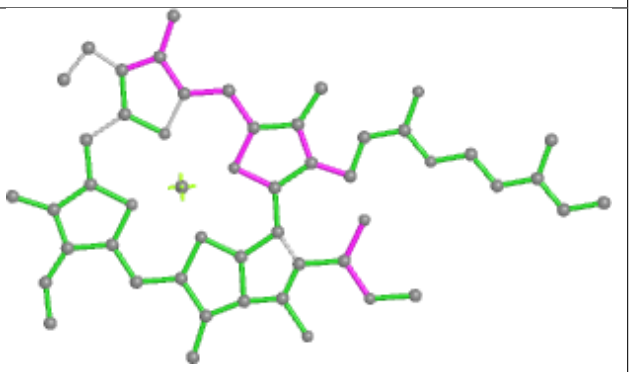
Ligand LMG G 324



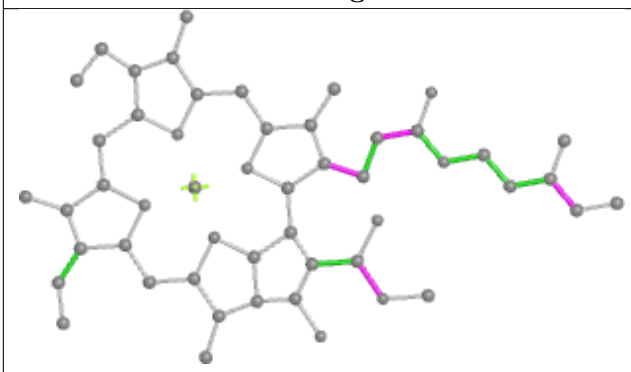
Ligand CLA P 318



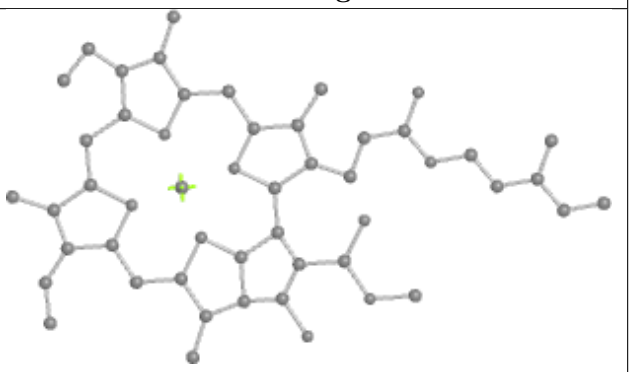
Bond lengths



Bond angles

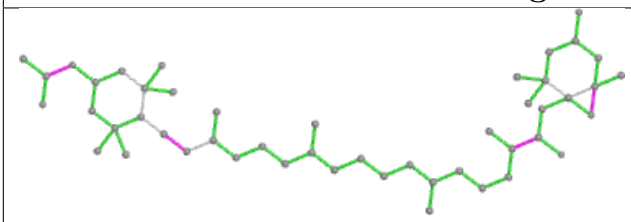


Torsions

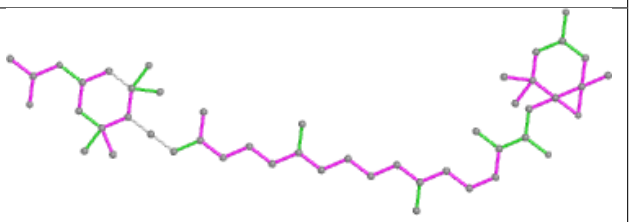


Rings

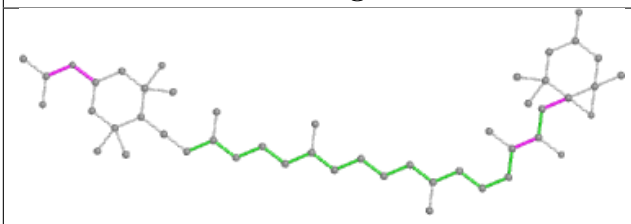
Ligand A86 U 302



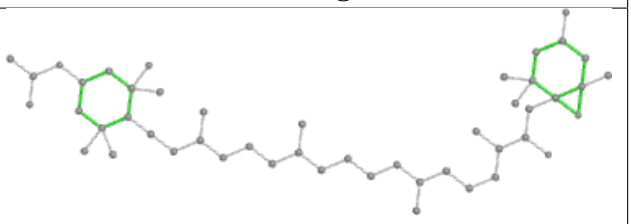
Bond lengths



Bond angles

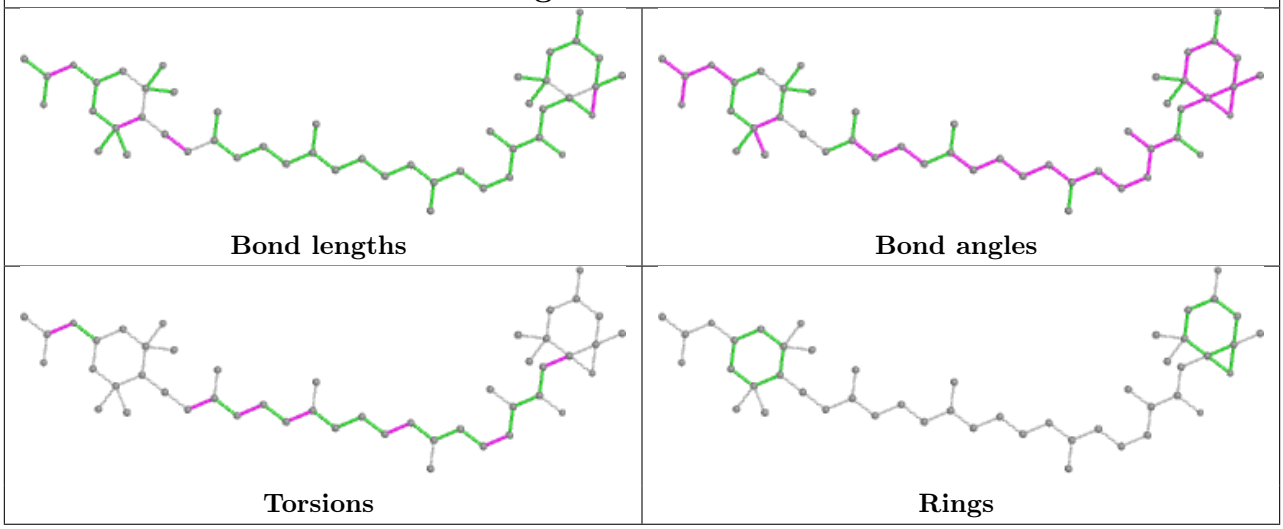


Torsions

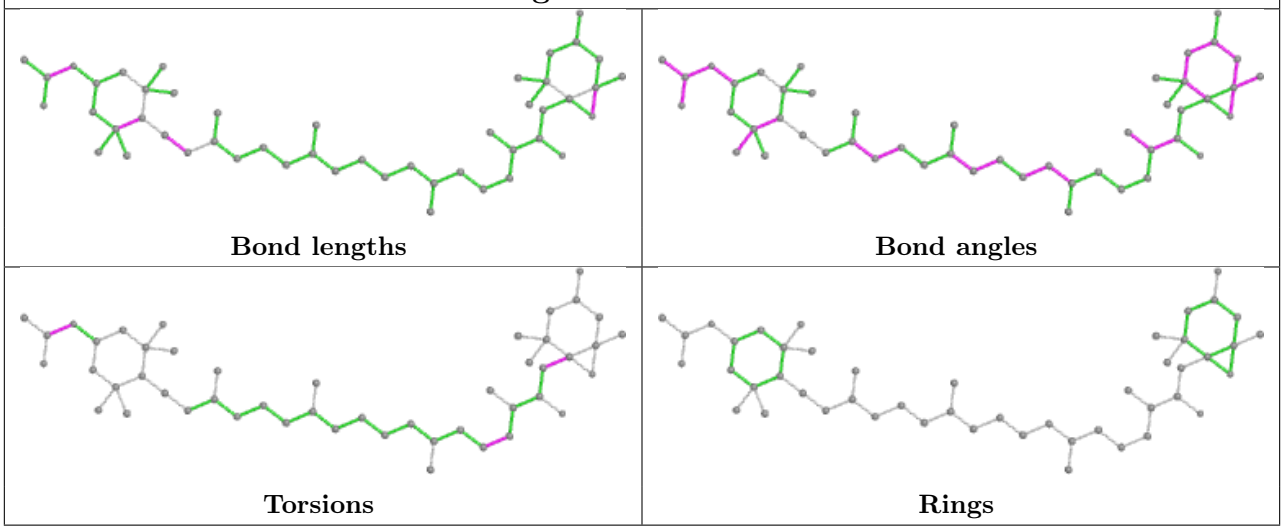


Rings

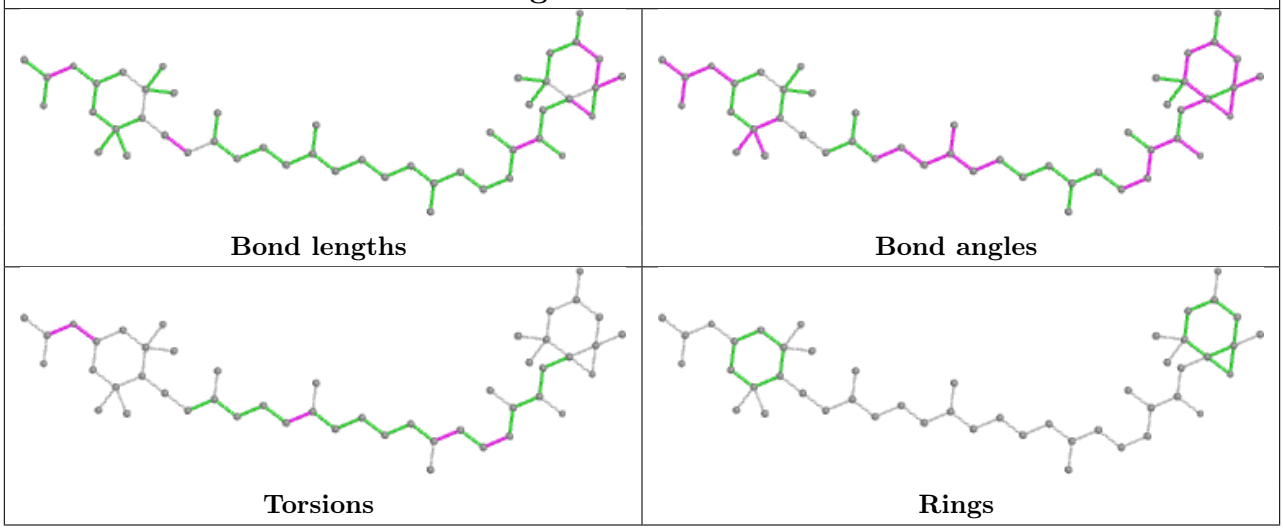
Ligand A86 J 301



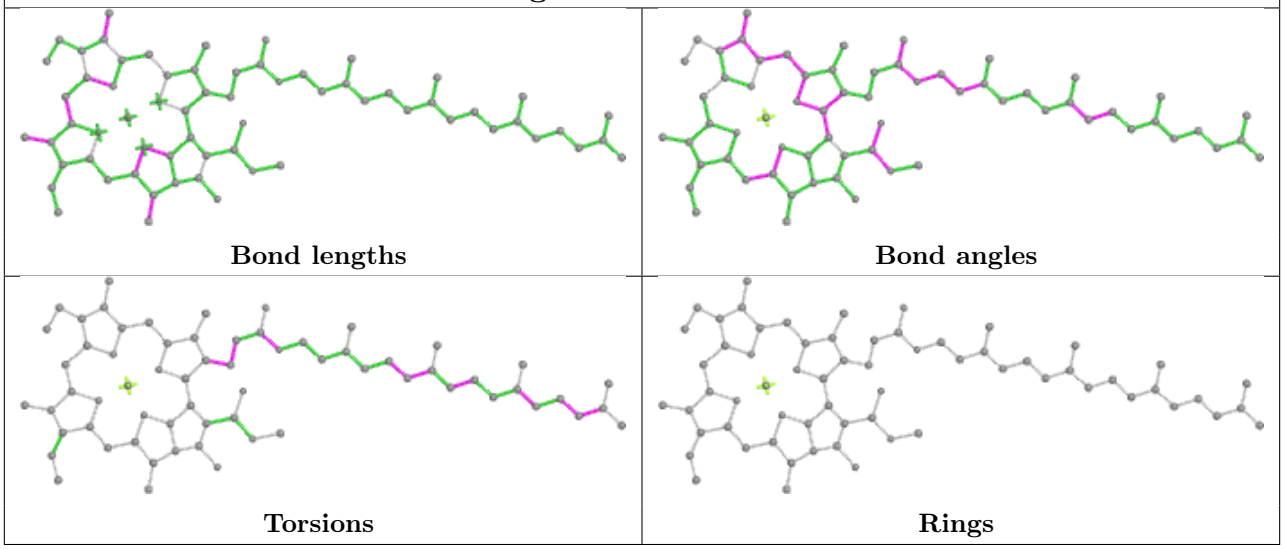
Ligand A86 E 307



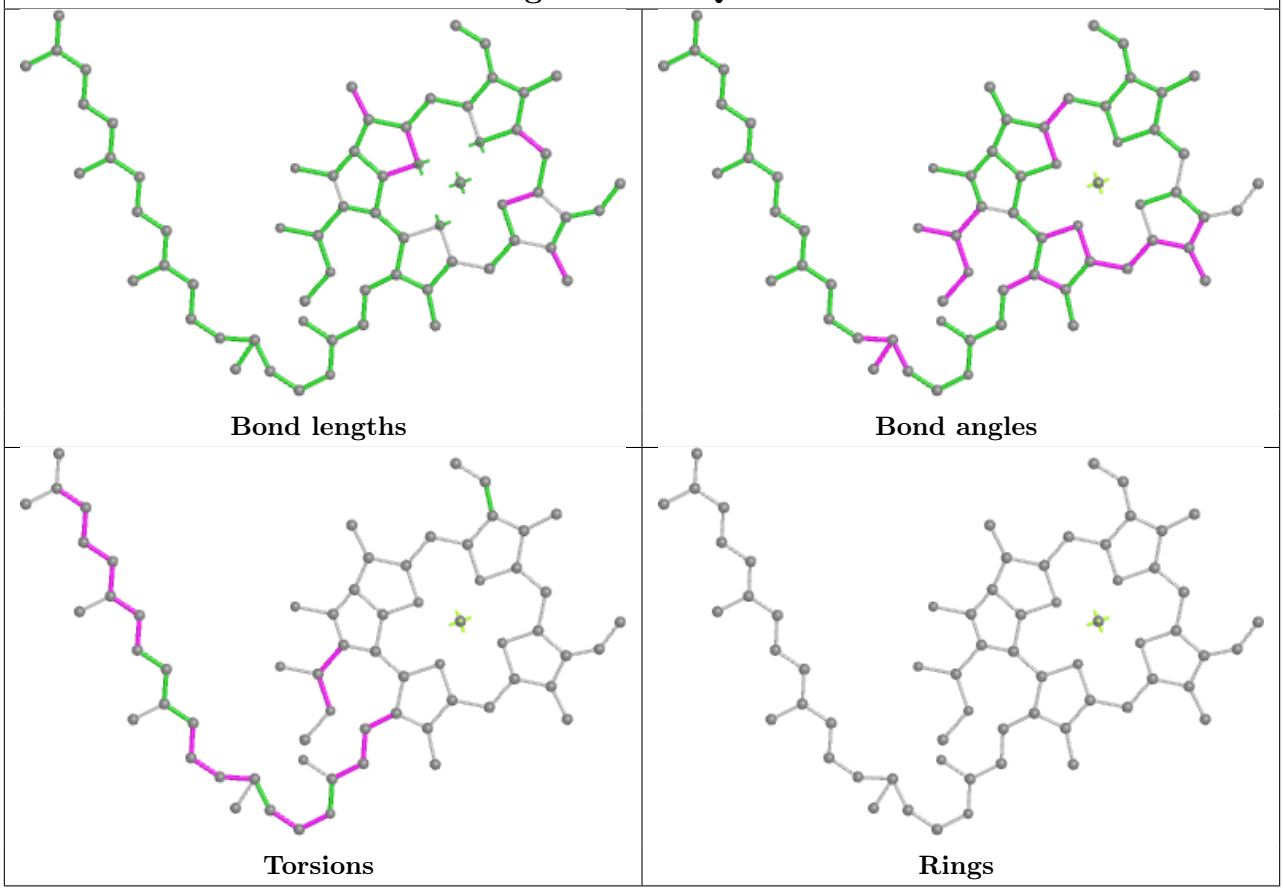
Ligand A86 N 304

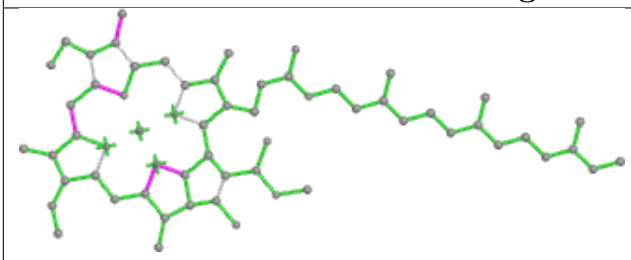
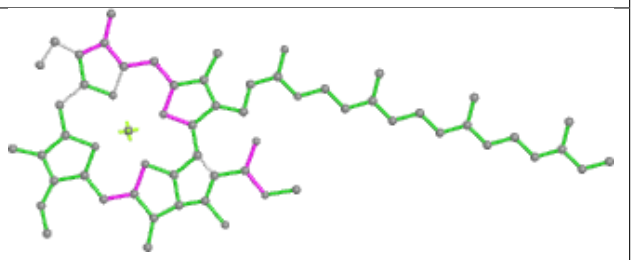
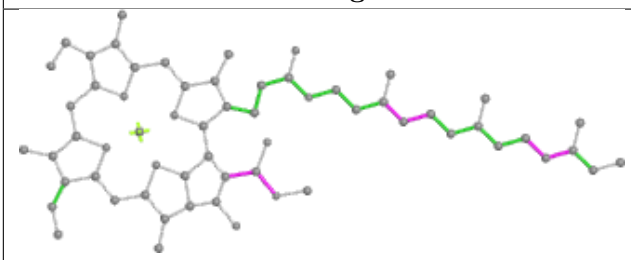
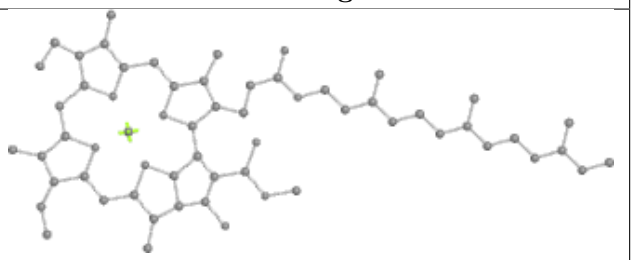


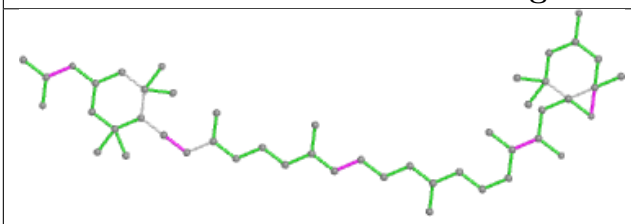
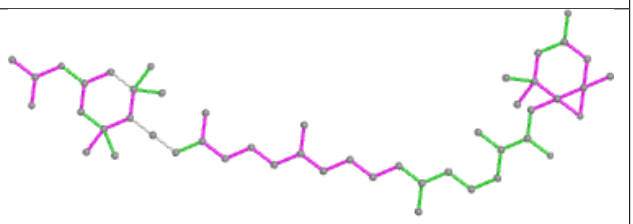
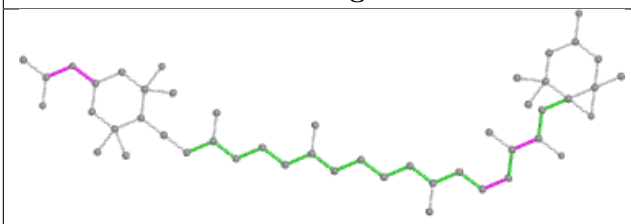
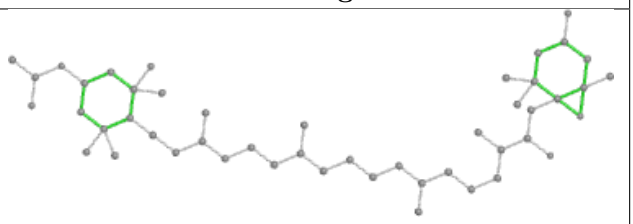
Ligand CLA a 807

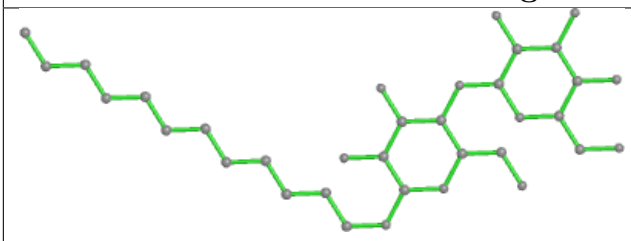
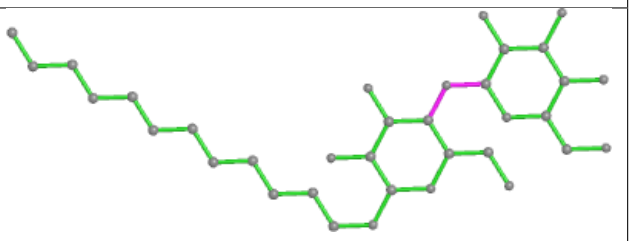
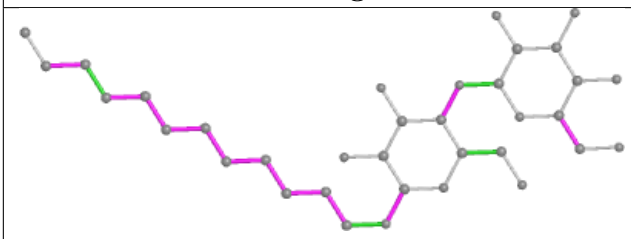
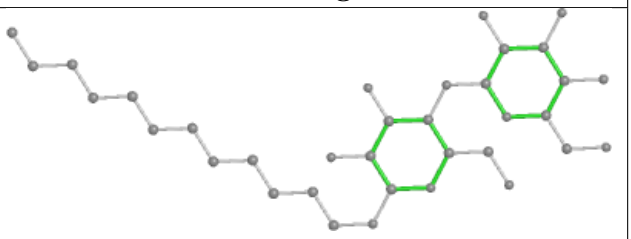


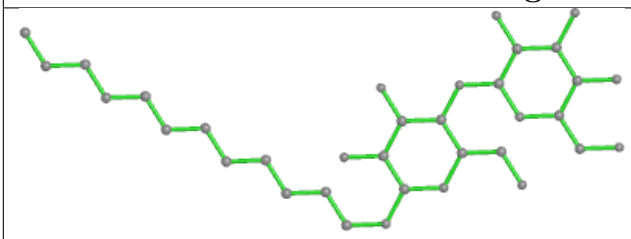
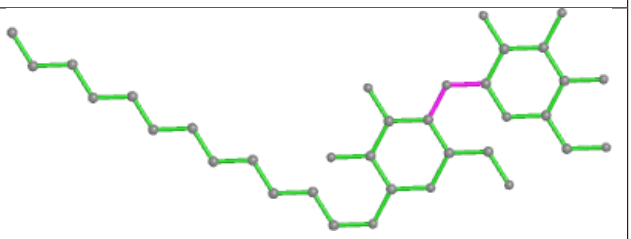
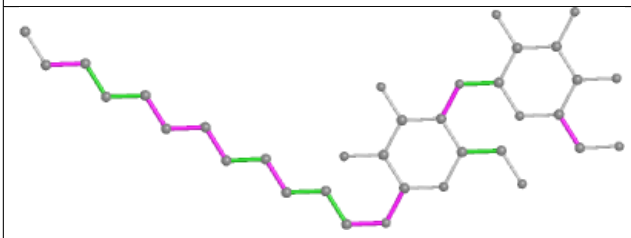
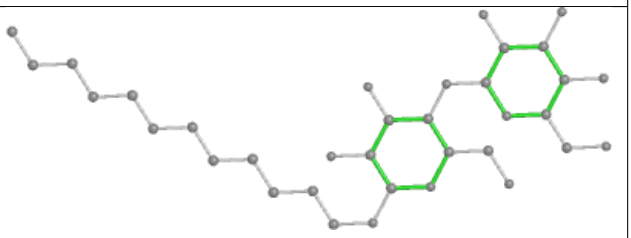
Ligand CLA Q 314



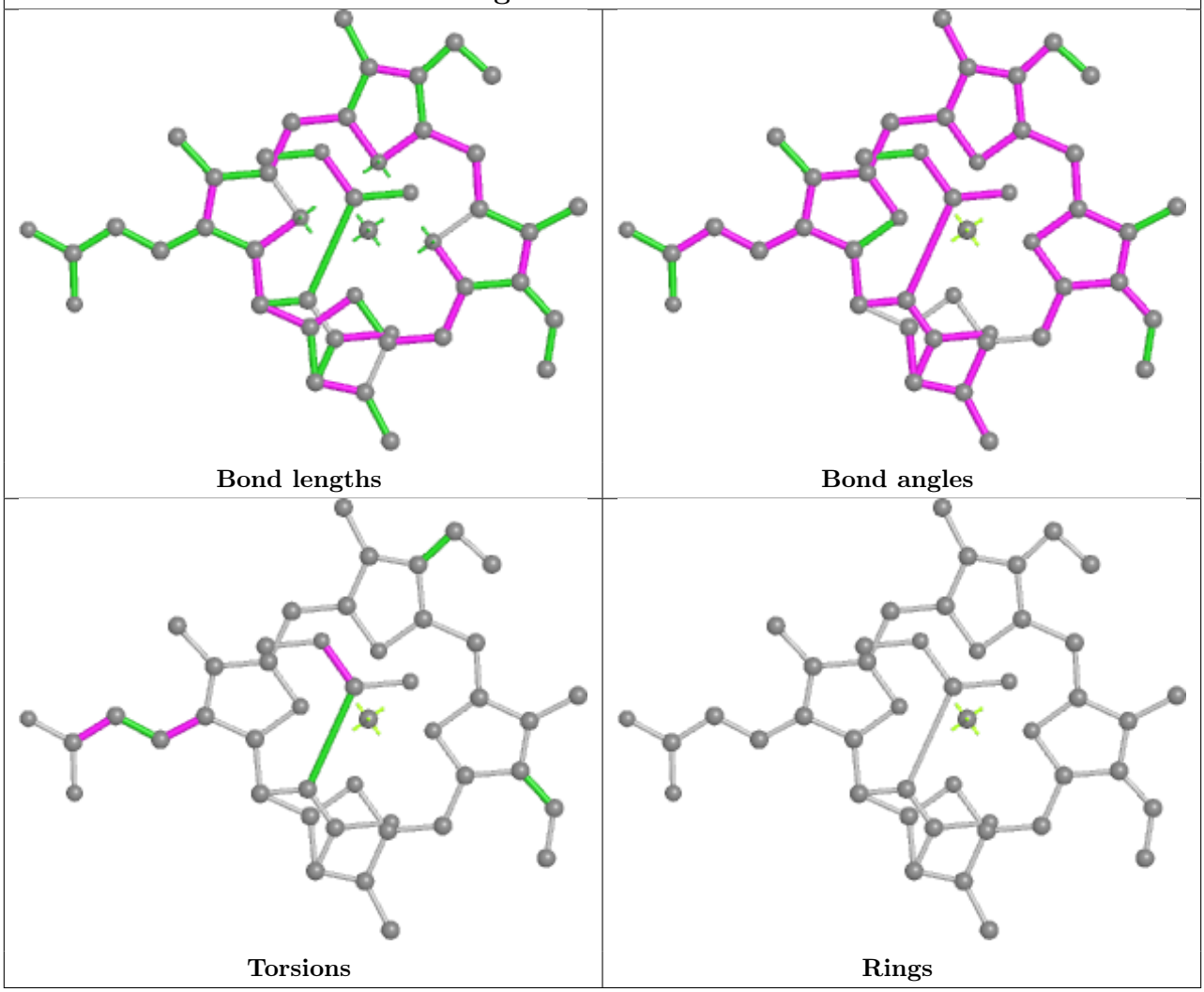
Ligand CLA W 206	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand A86 O 319	
 Bond lengths	 Bond angles
 Torsions	 Rings

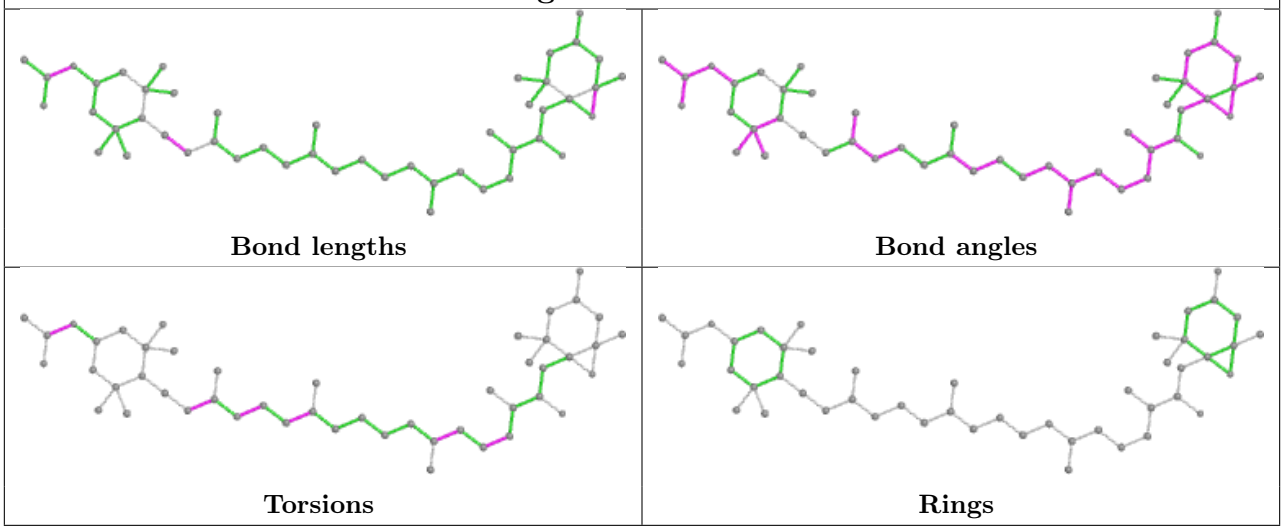
Ligand LMT U 314	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand LMT h 205	
 Bond lengths	 Bond angles
 Torsions	 Rings

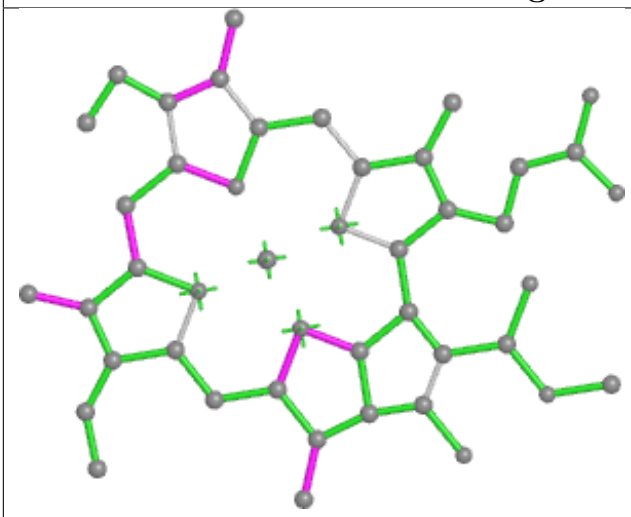
Ligand KC1 D 314



Ligand A86 I 301



Ligand CLA a 815



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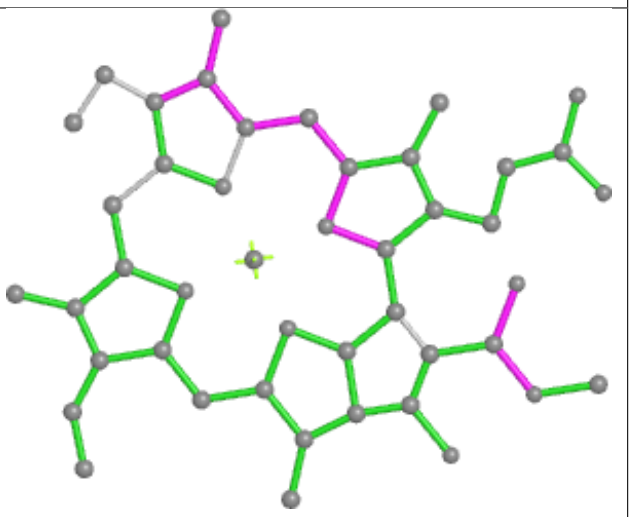
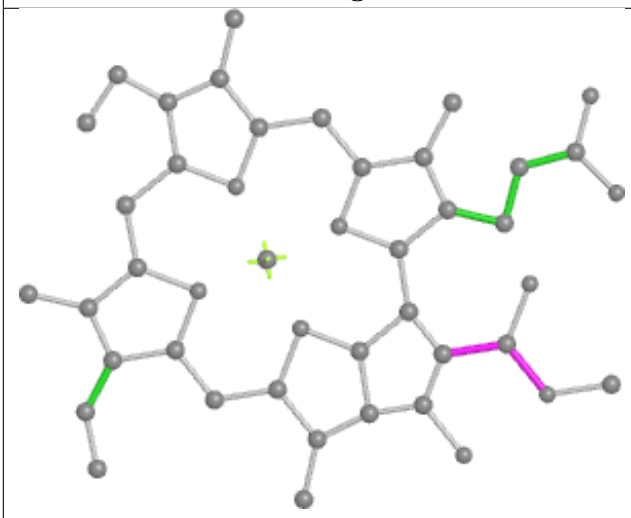


Bond angles



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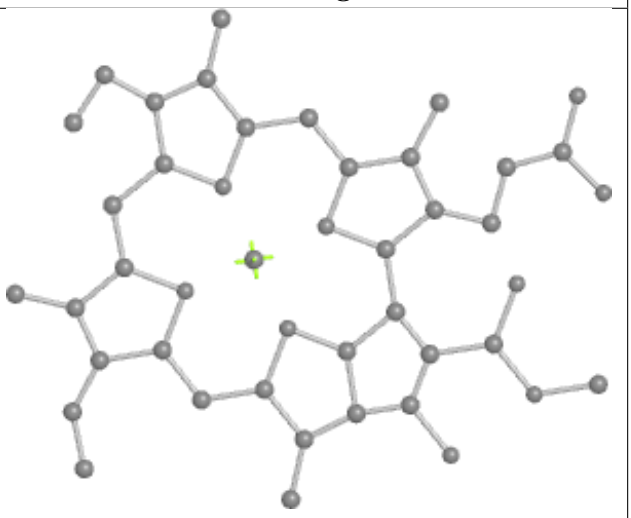
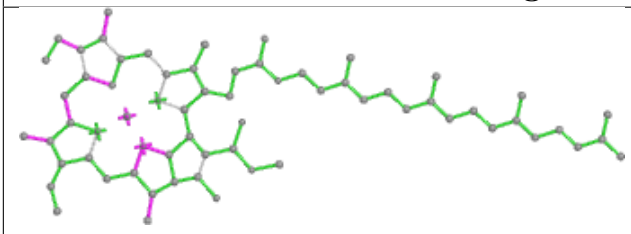


Rings

Ligand CLA G 310



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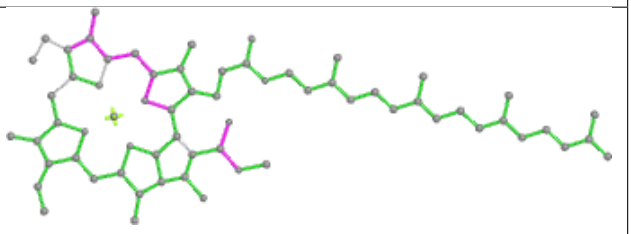

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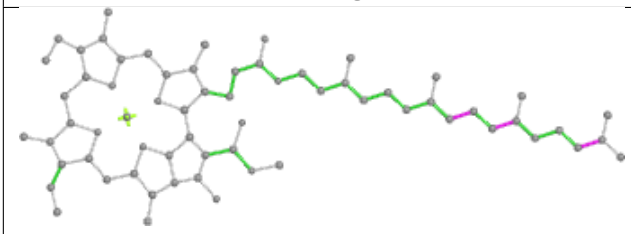

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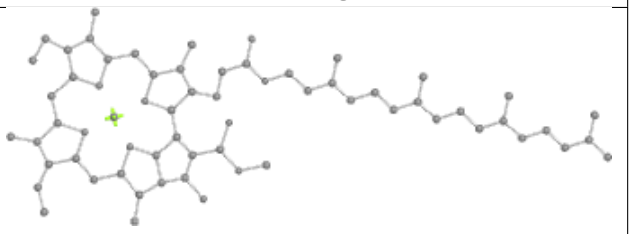
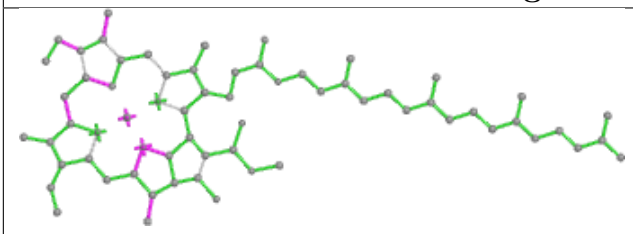


Rings

Ligand CLA V 313



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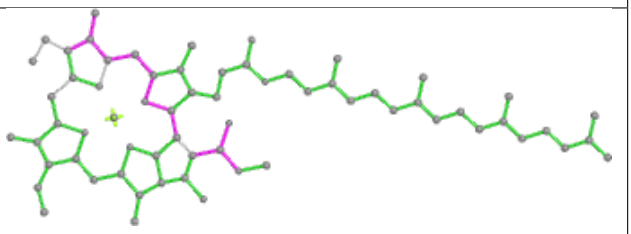
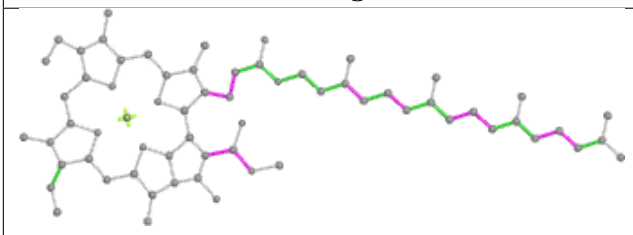


Bond angles



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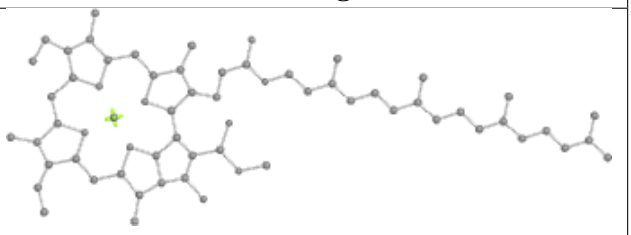

Rings

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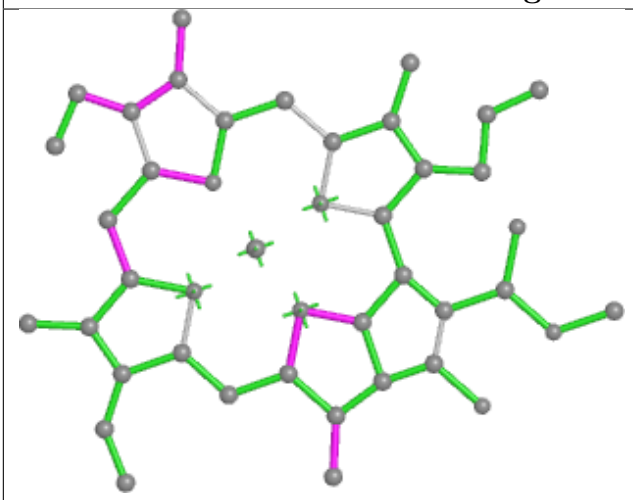

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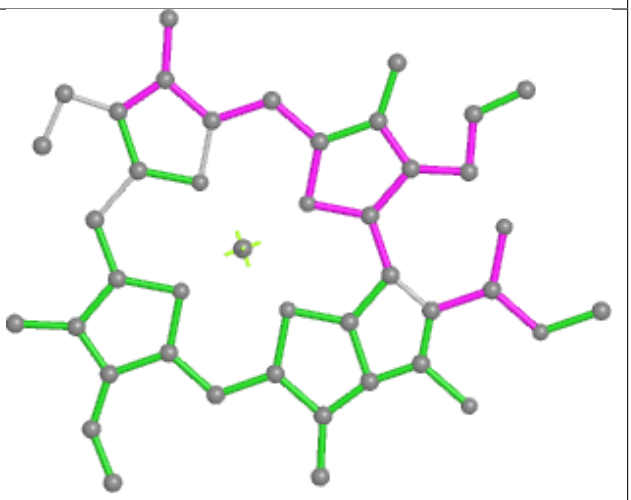

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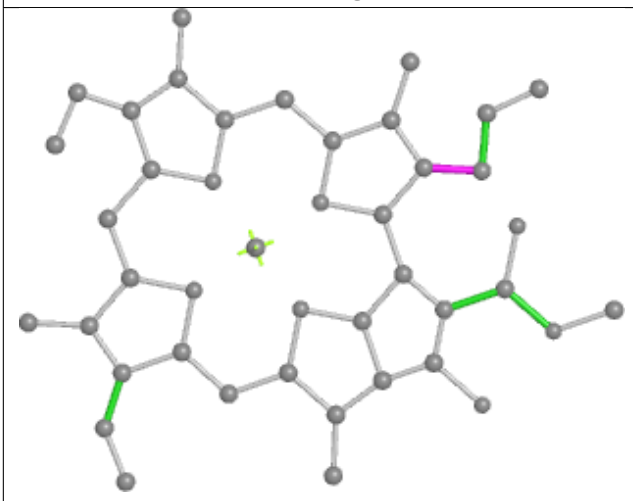

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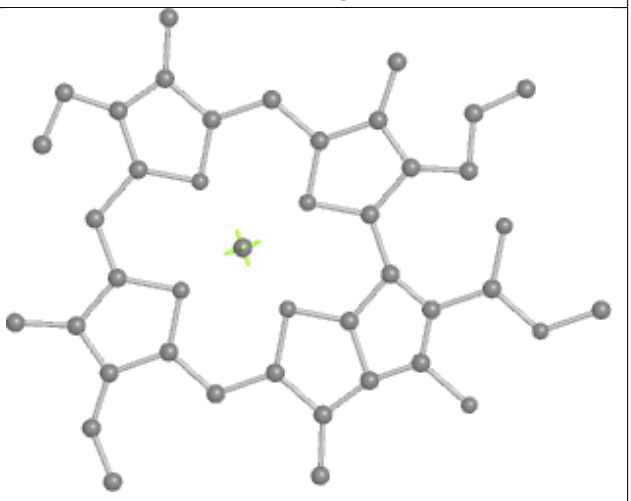
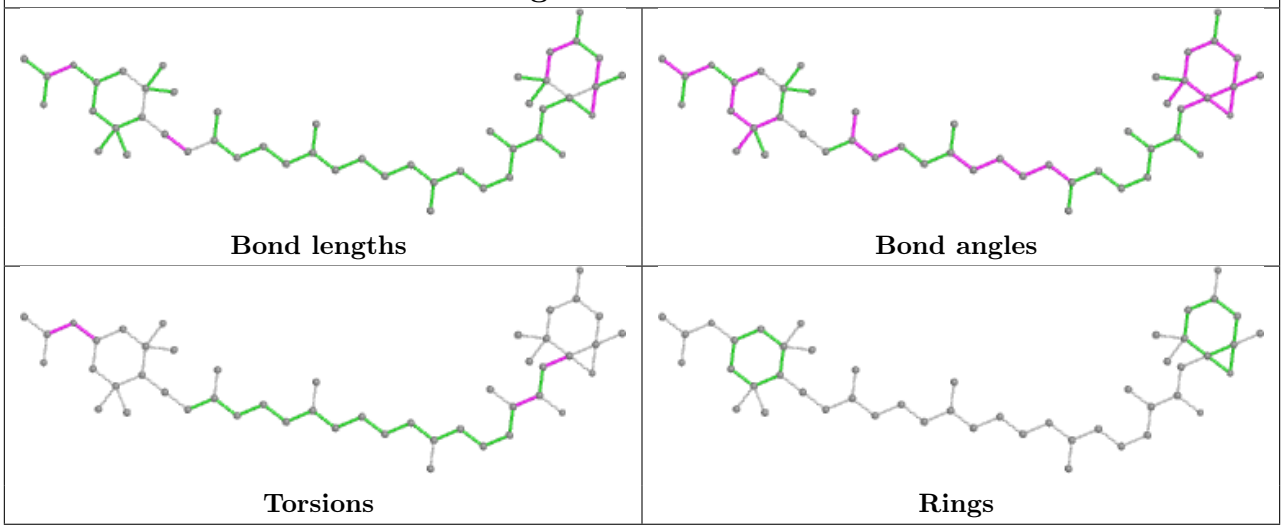
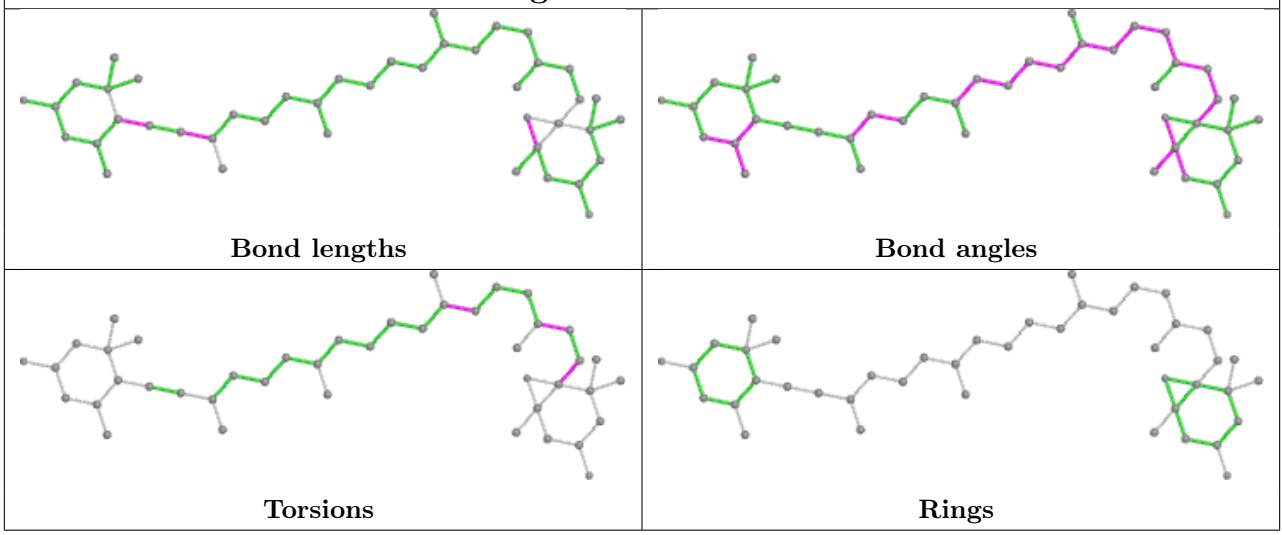


Rings

Ligand A86 V 304



Ligand DD6 a 849



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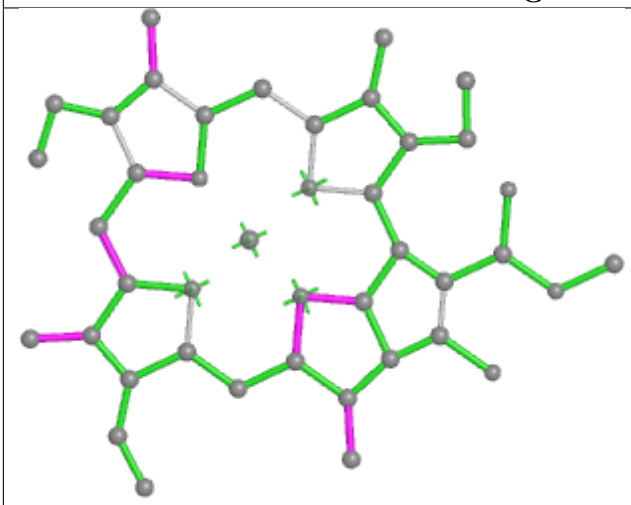

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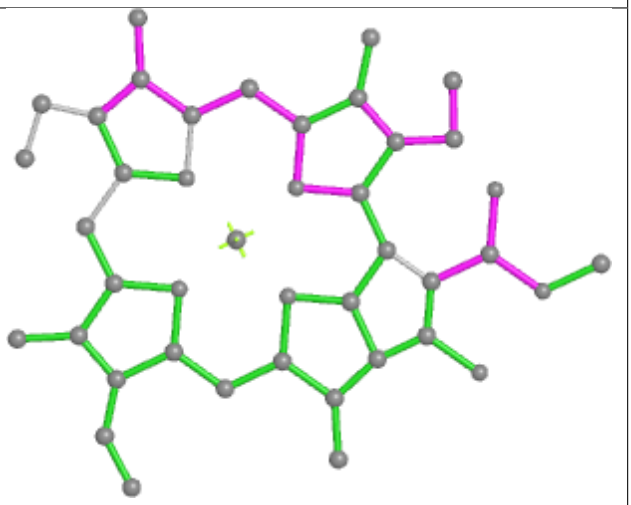

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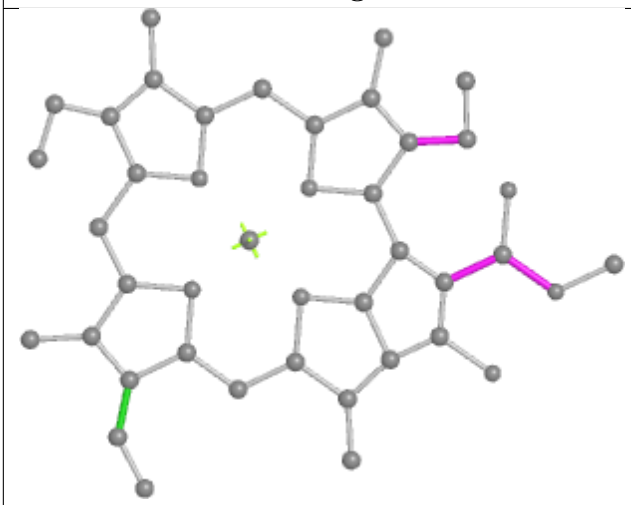

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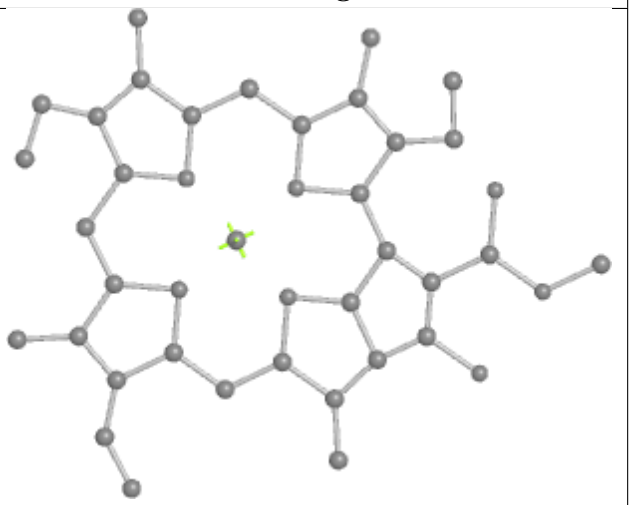
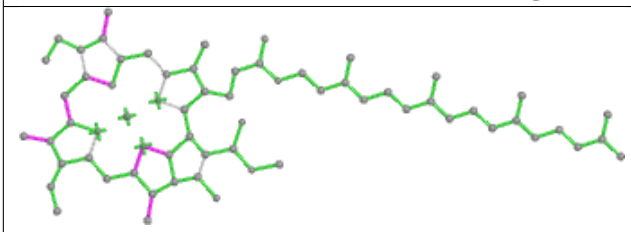


Rings

Ligand CLA S 310



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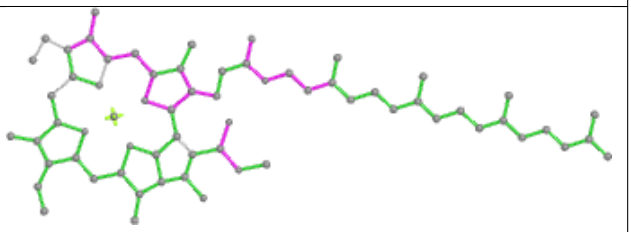

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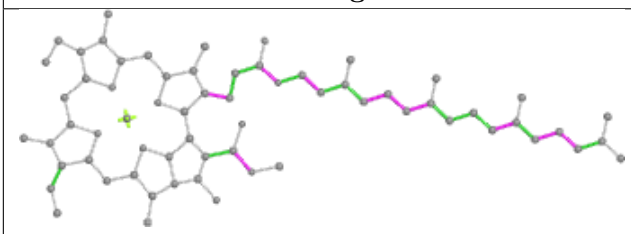

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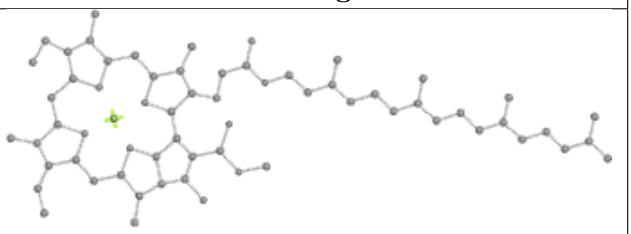
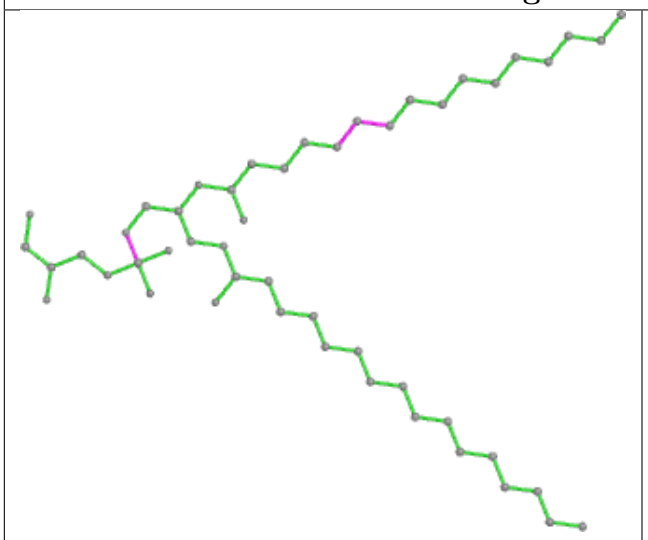


Rings

Ligand LHG O 318



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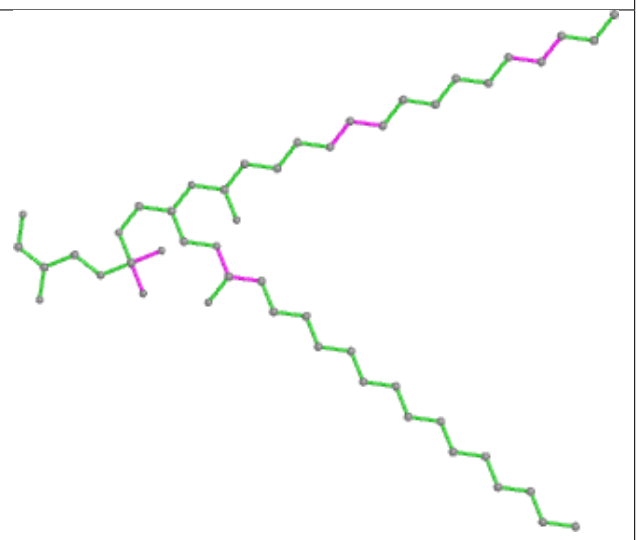
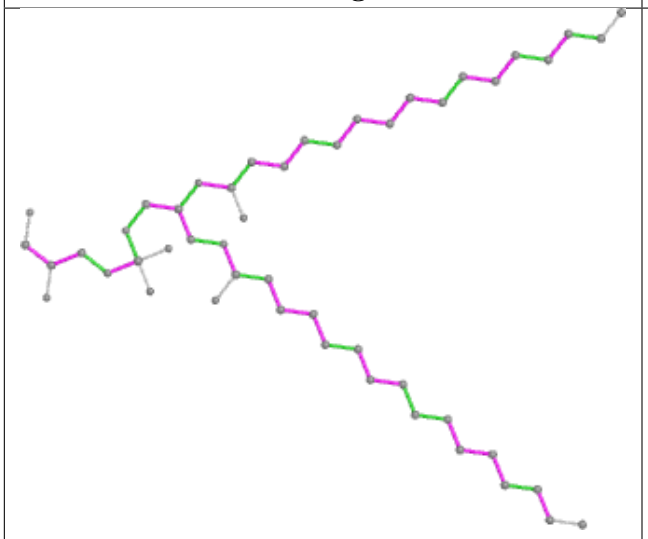


Bond angles



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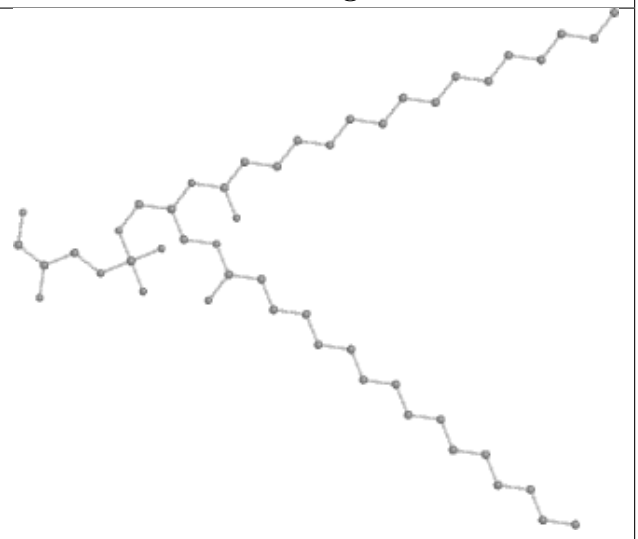
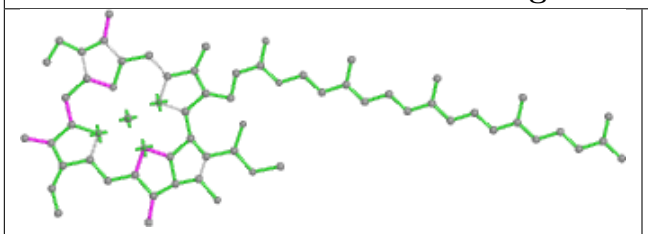


Rings

Ligand CLA a 828



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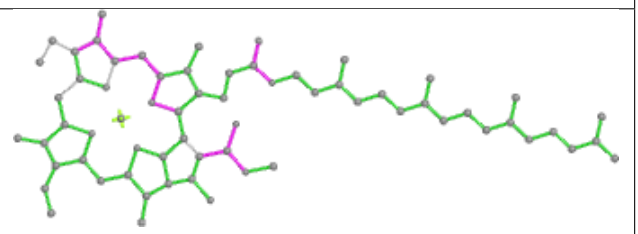

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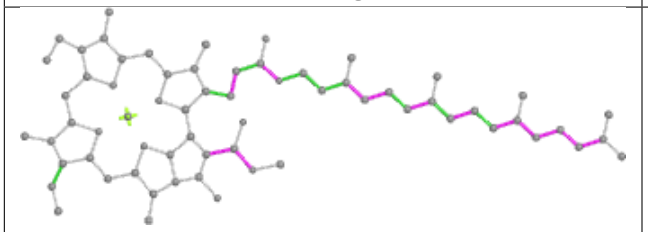
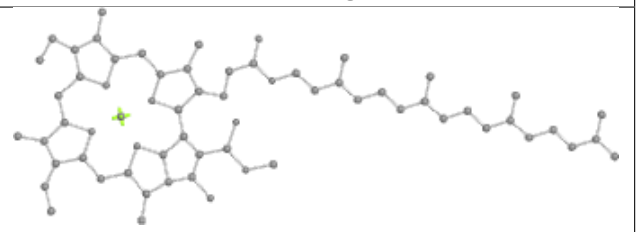
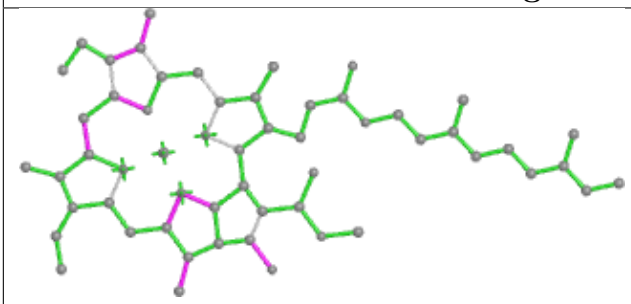
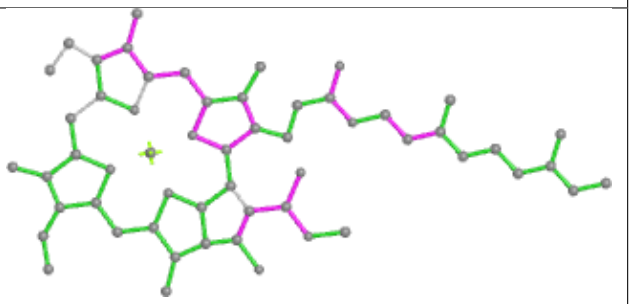
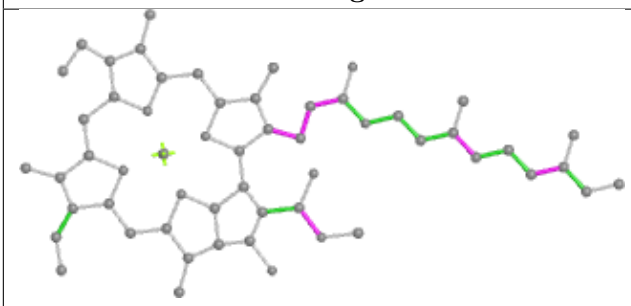
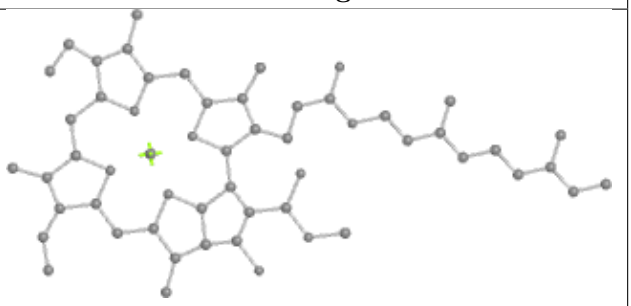
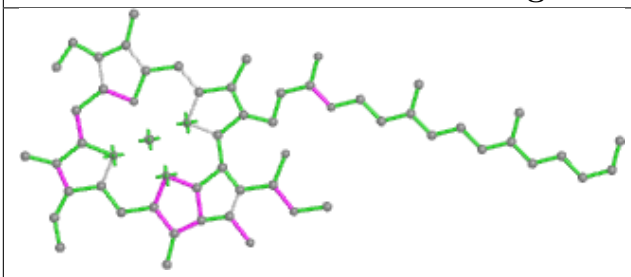
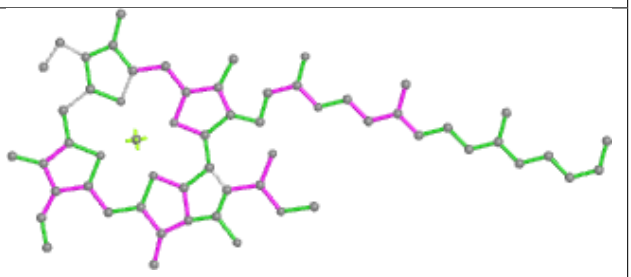
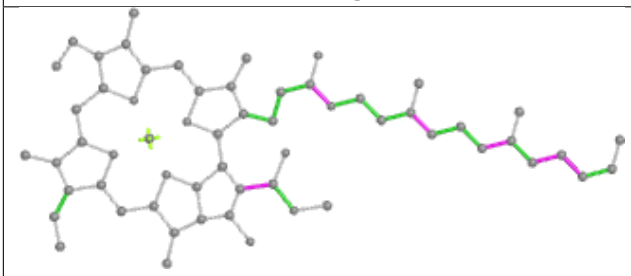
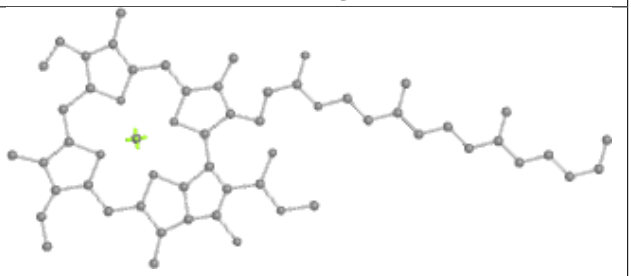


Torsions

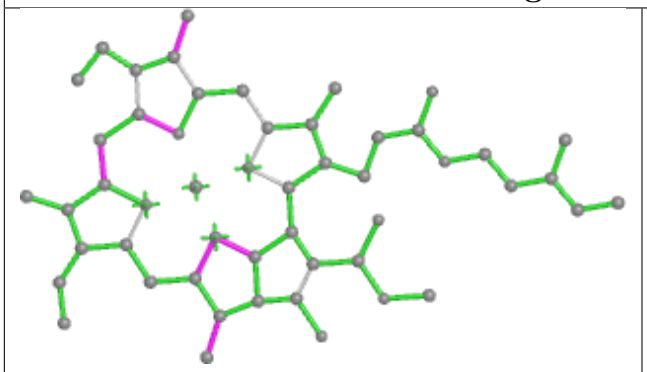


Rings

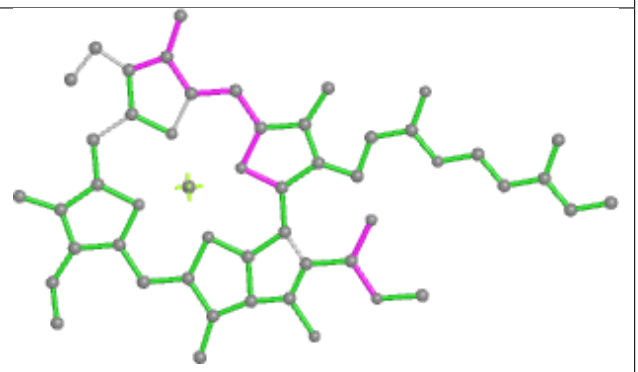
Ligand CLA U 308	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA b 817	
 Bond lengths	 Bond angles
 Torsions	 Rings

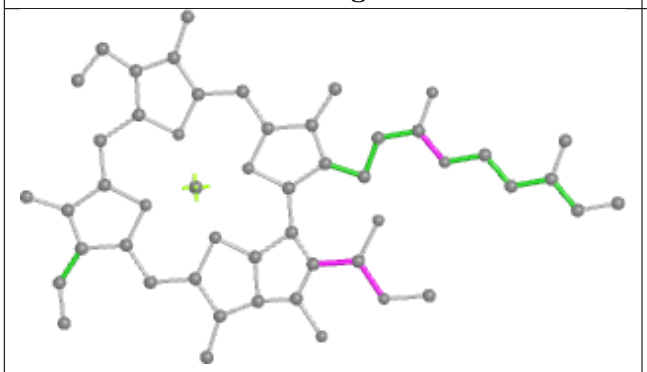
Ligand CLA V 307



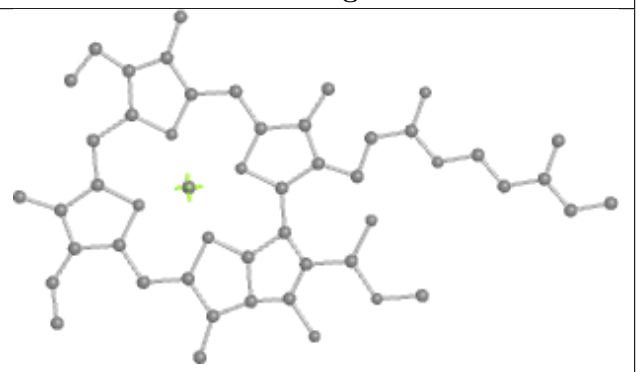
Bond lengths



Bond angles

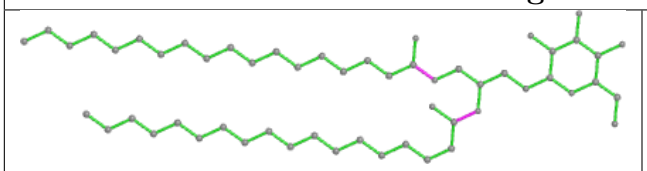


Torsions

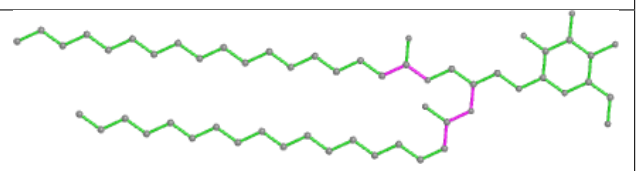


Rings

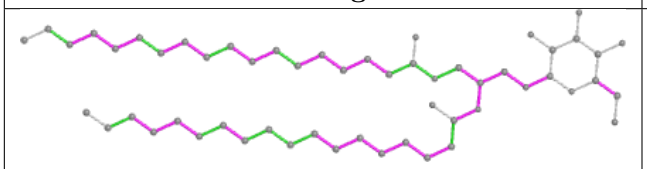
Ligand LMG I 315



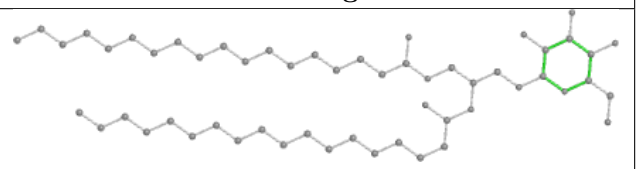
Bond lengths



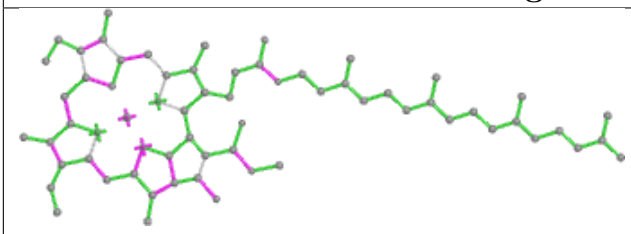
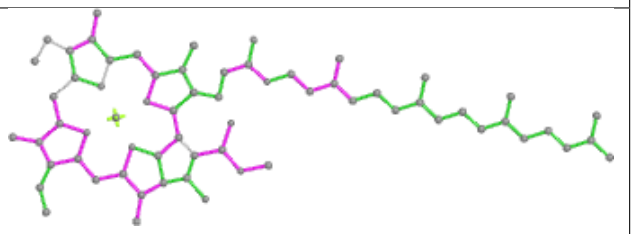
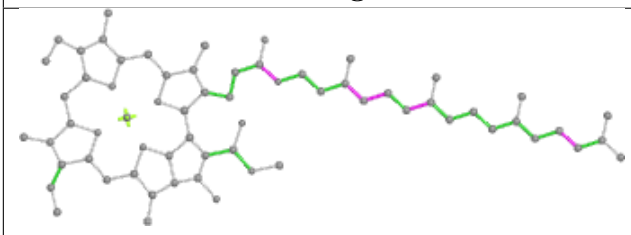
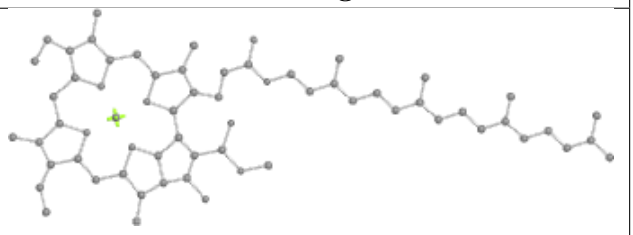
Bond angles

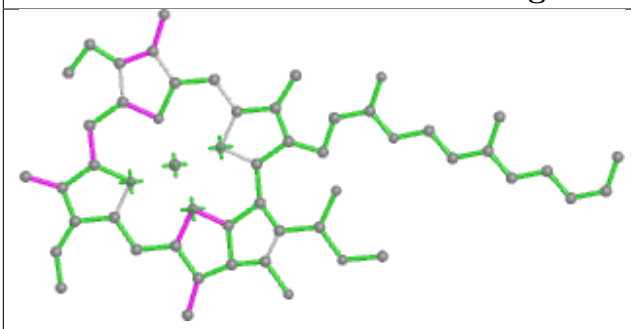
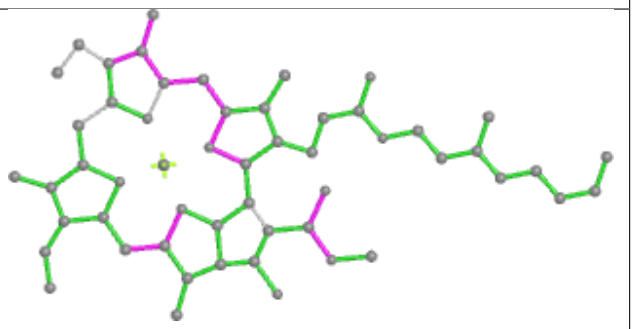
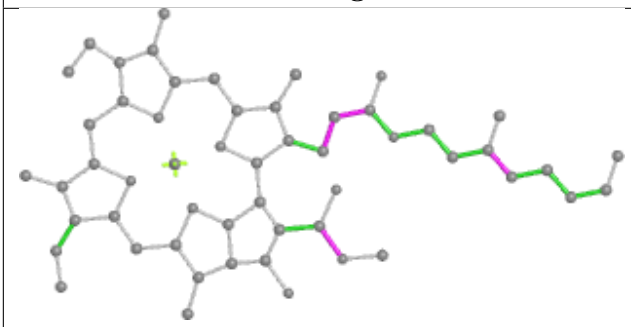
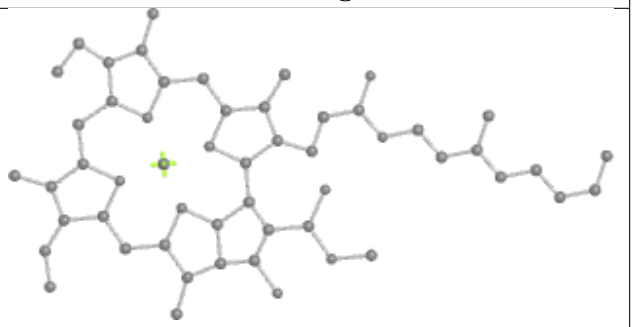


Torsions

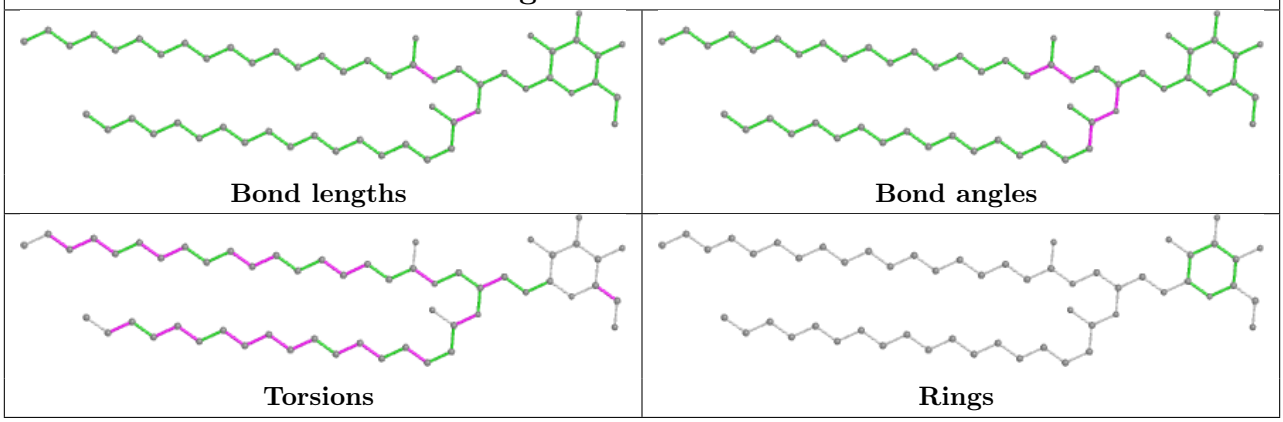


Rings

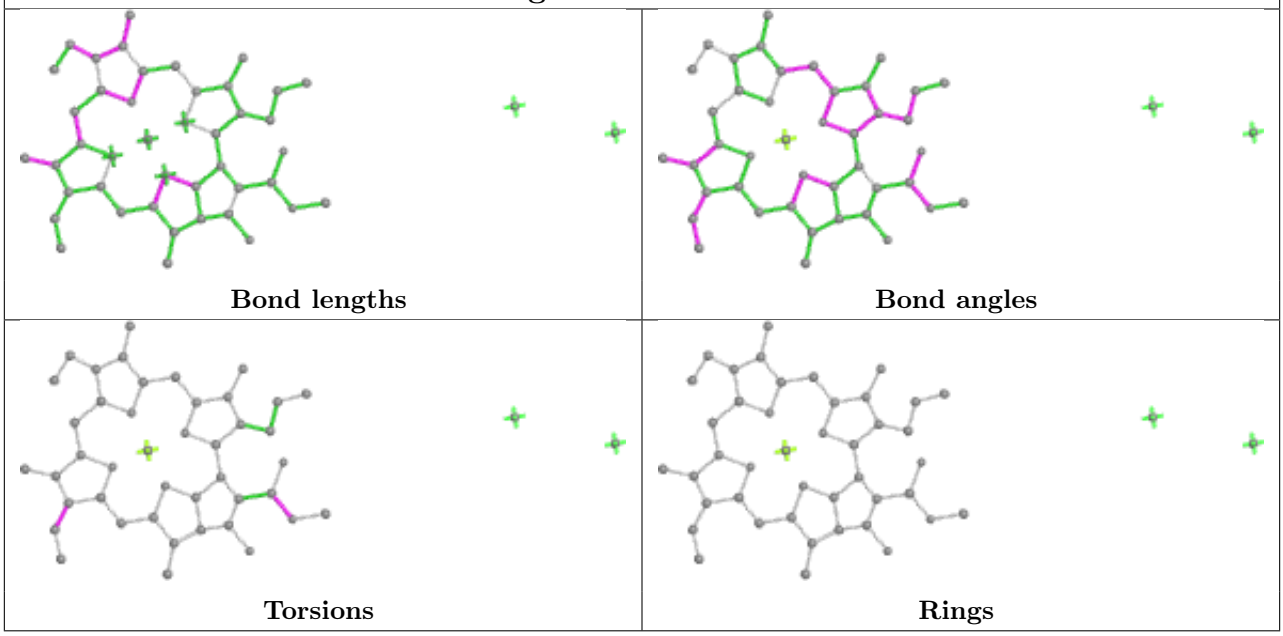
Ligand CLA E 313	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA a 811	
 Bond lengths	 Bond angles
 Torsions	 Rings

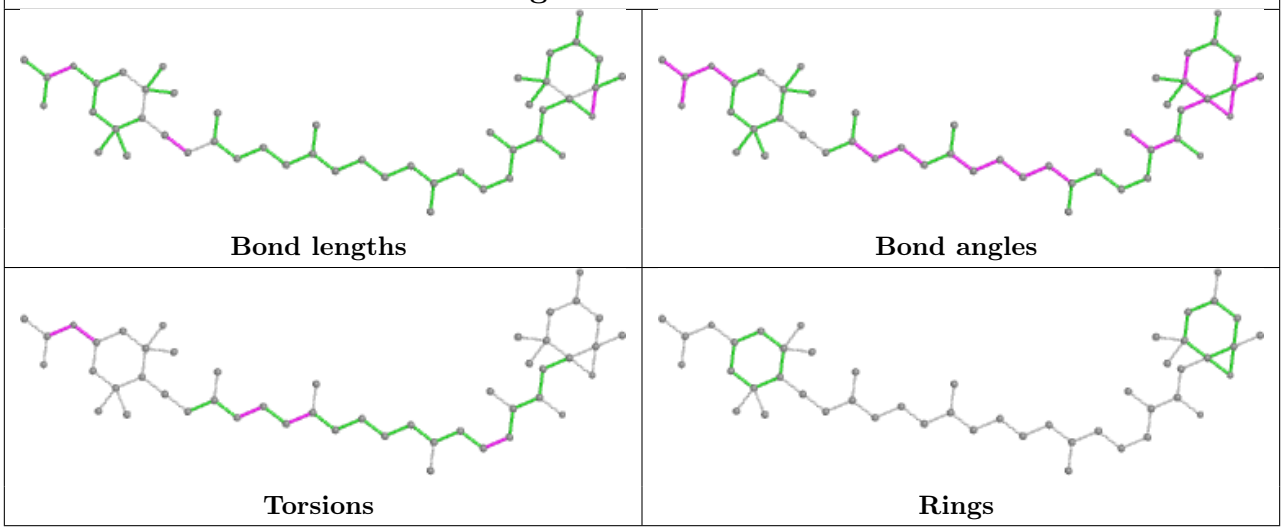
Ligand LMG G 325

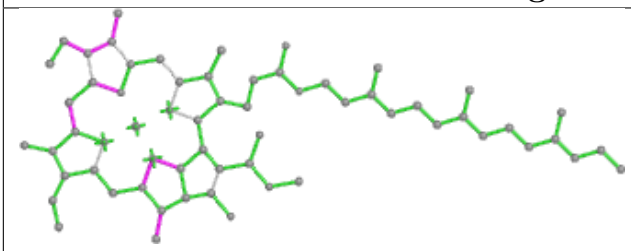
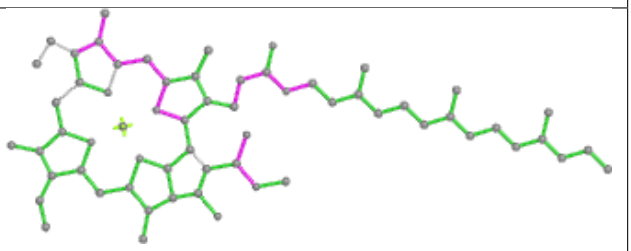
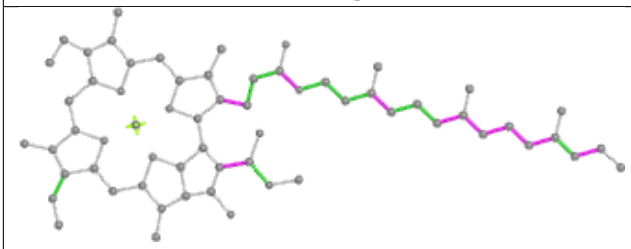
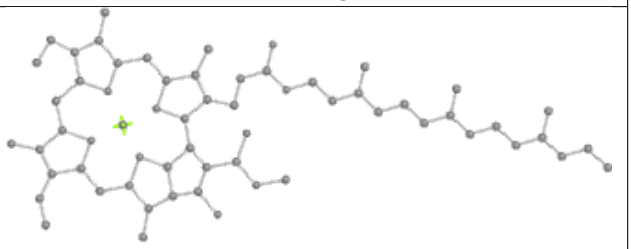


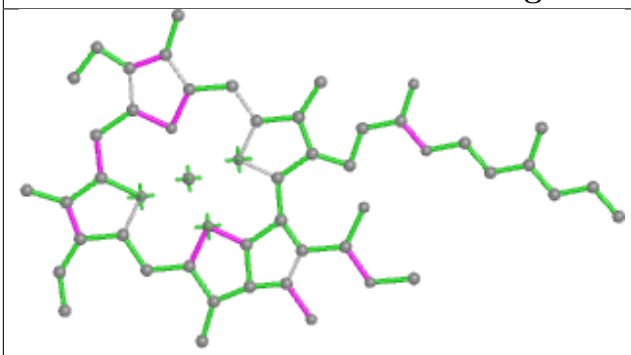
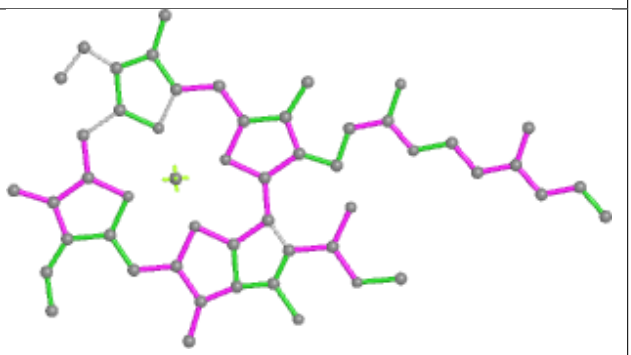
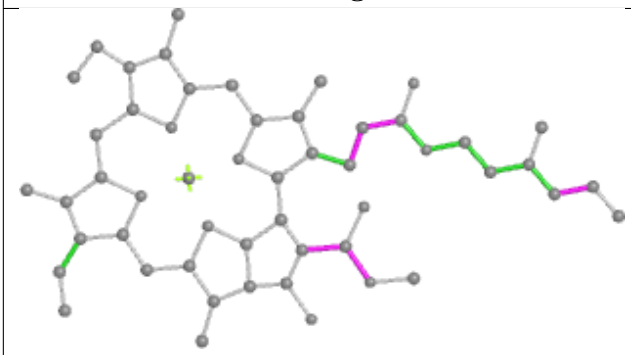
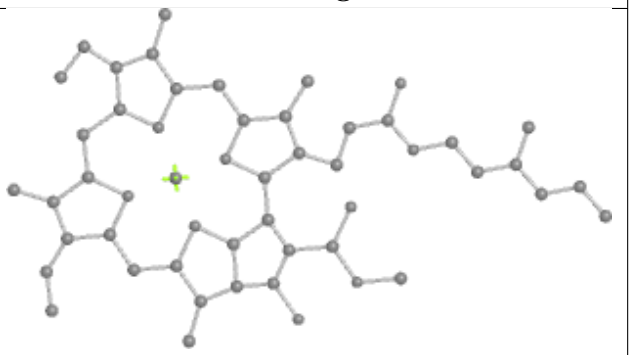
Ligand CLA S 315



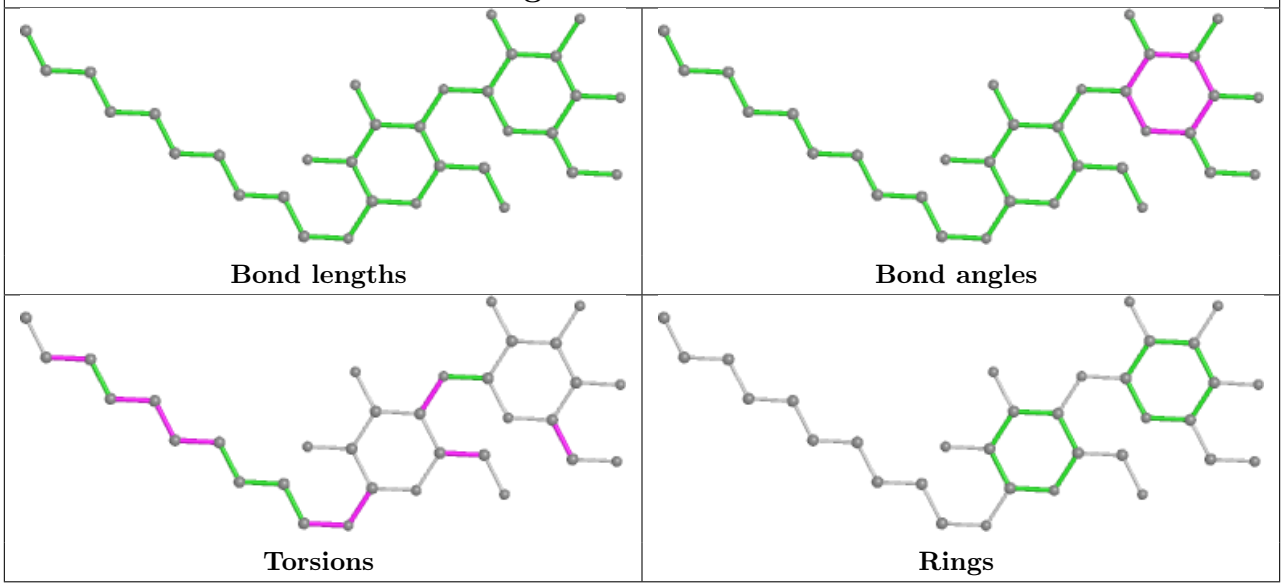
Ligand A86 G 302



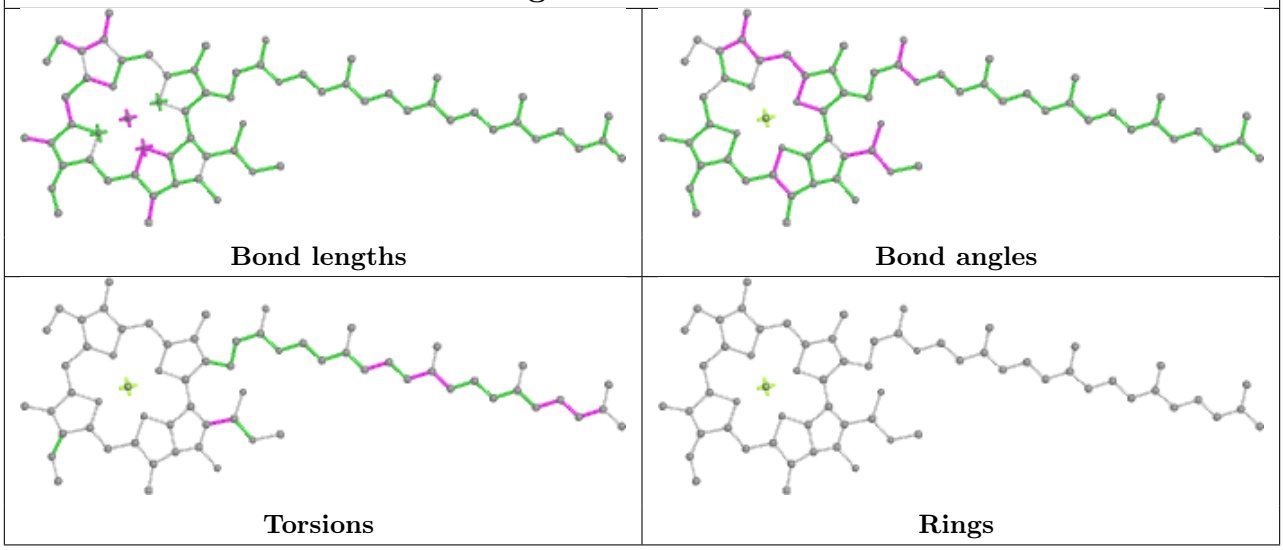
Ligand CLA a 810	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA B 309	
 Bond lengths	 Bond angles
 Torsions	 Rings

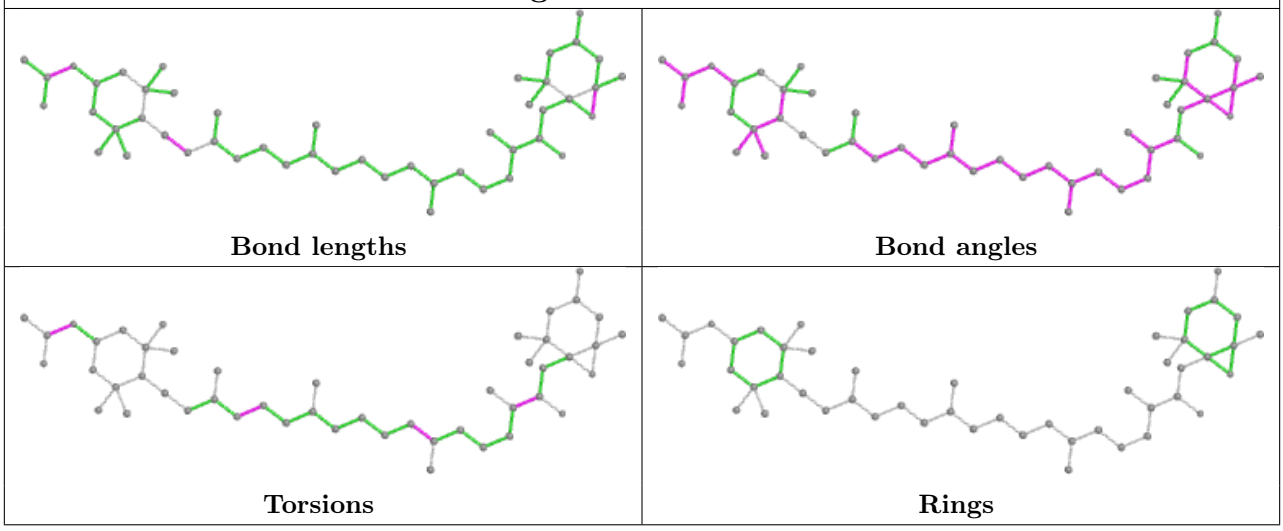
Ligand LMT F 321

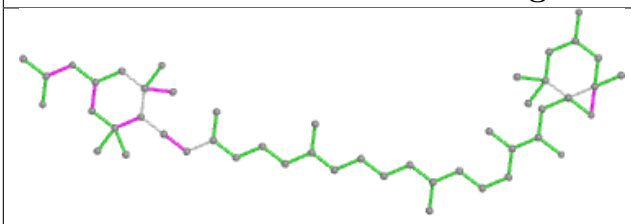
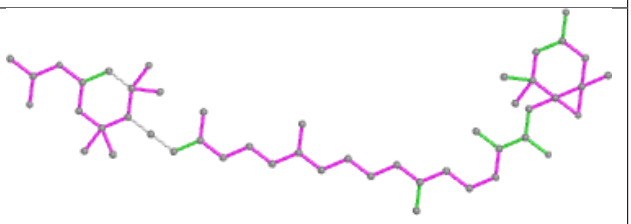
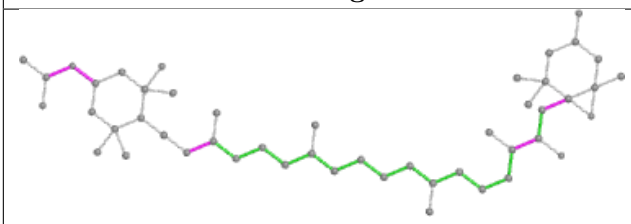
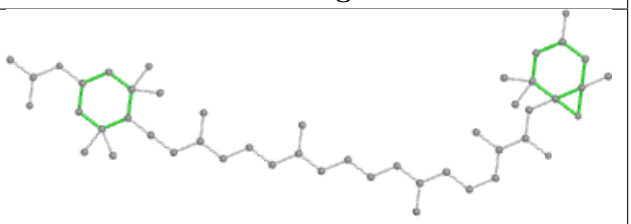


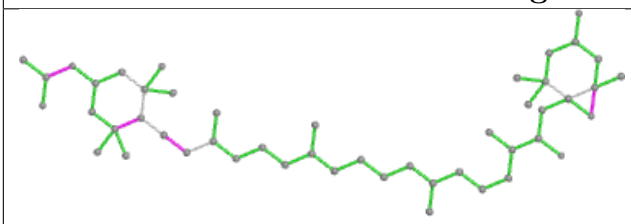
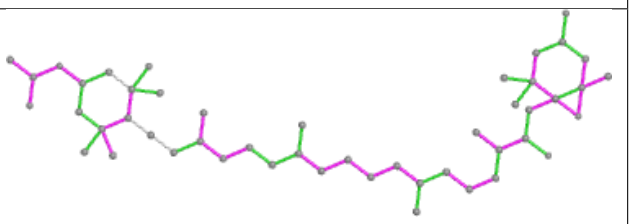
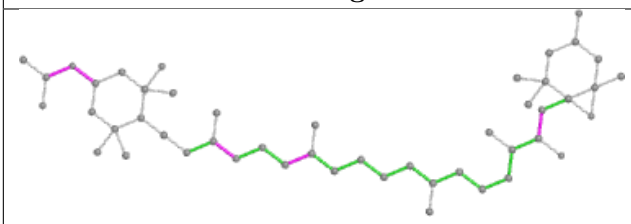
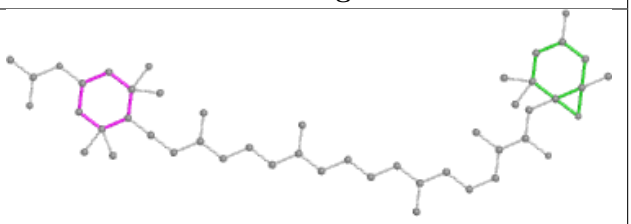
Ligand CLA b 821



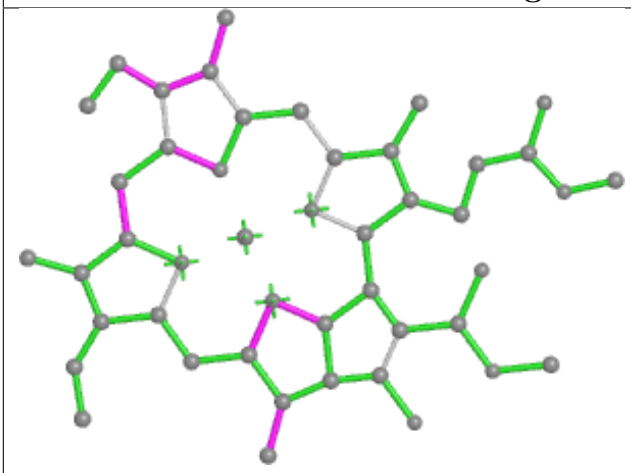
Ligand A86 U 301



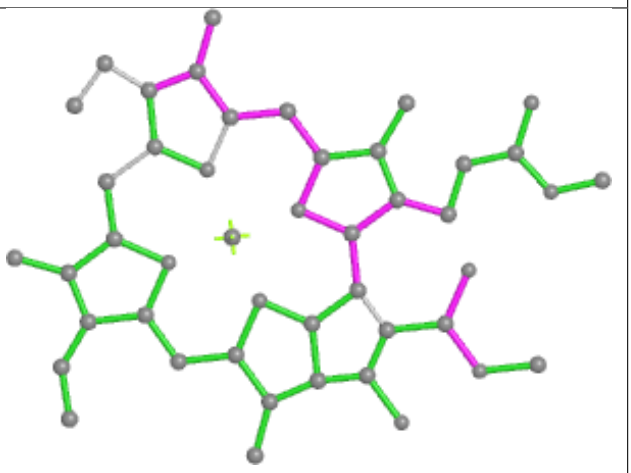
Ligand A86 N 320	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand A86 C 203	
 Bond lengths	 Bond angles
 Torsions	 Rings

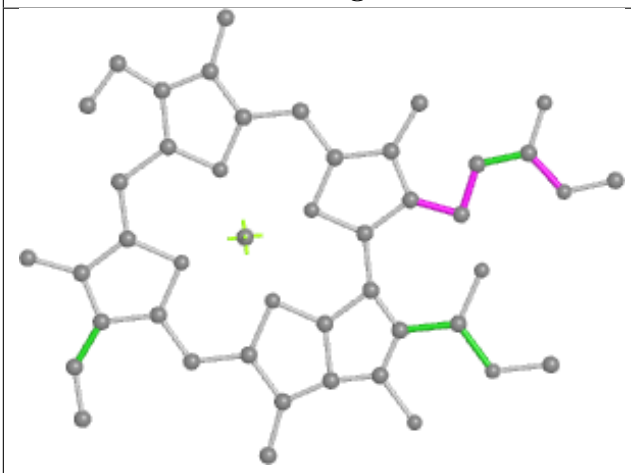
Ligand CLA B 307



Bond lengths



Bond angles



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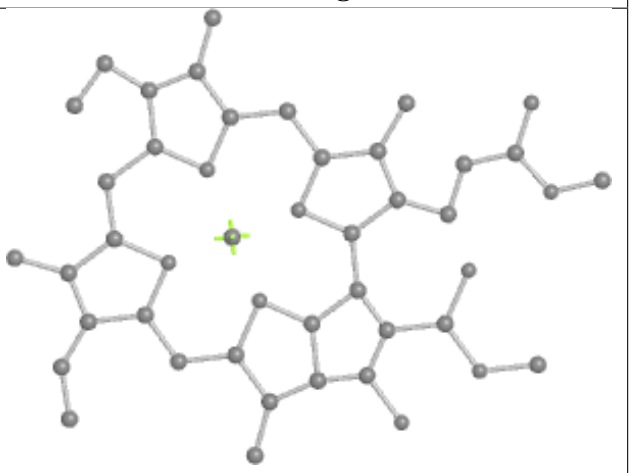
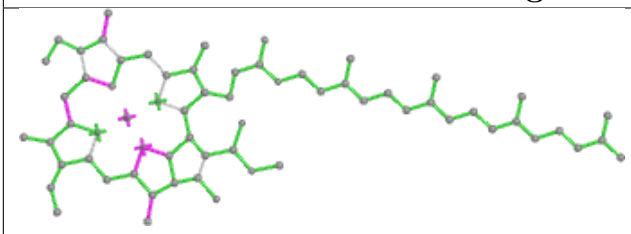
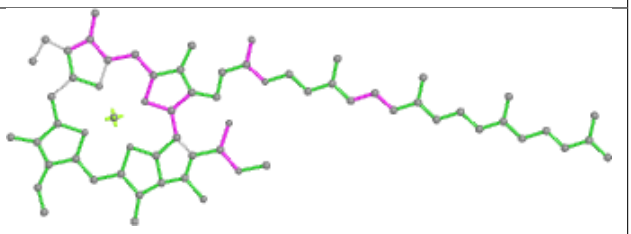


Rings

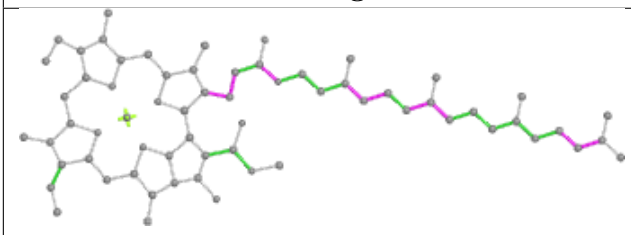
Ligand CLA F 314



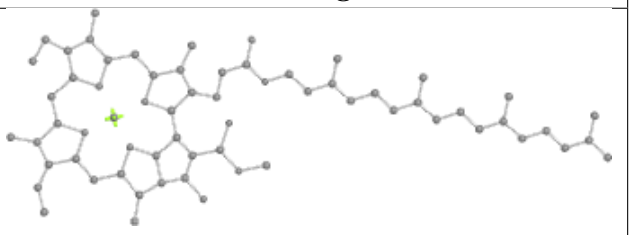
Bond lengths



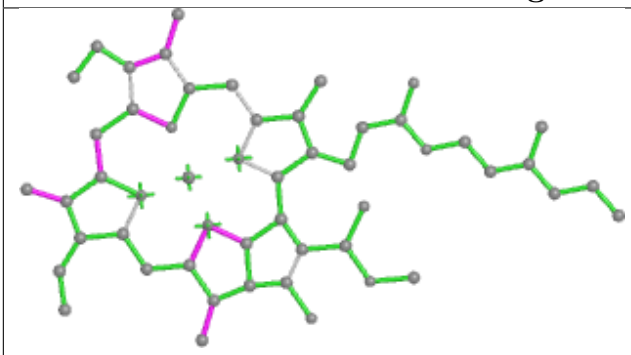
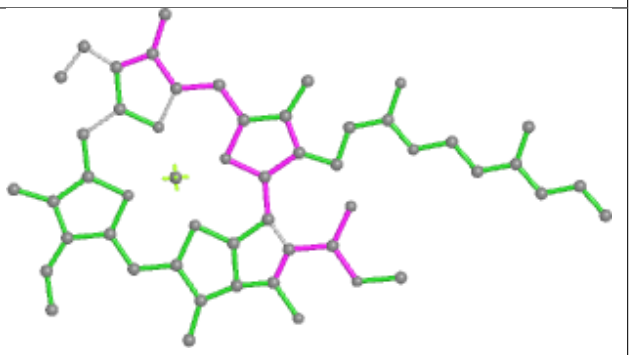
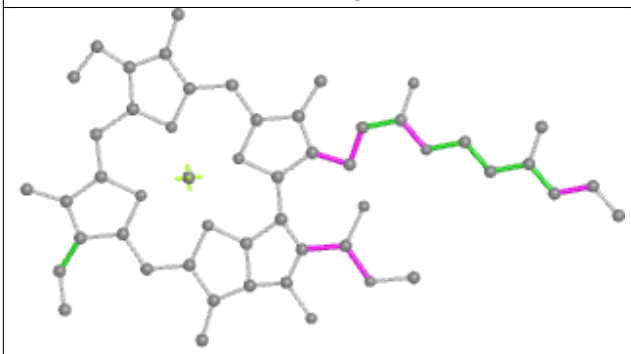
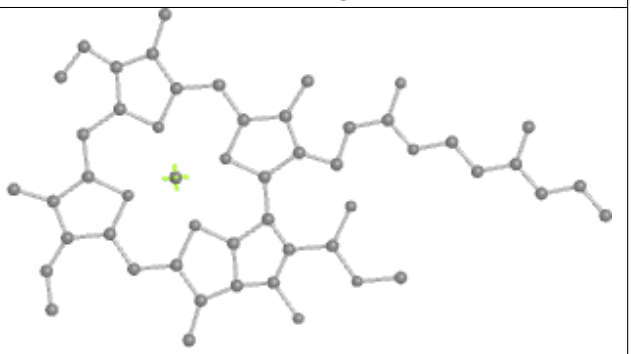
Bond angles

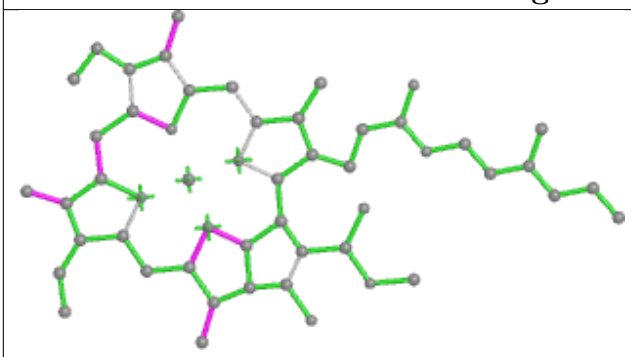
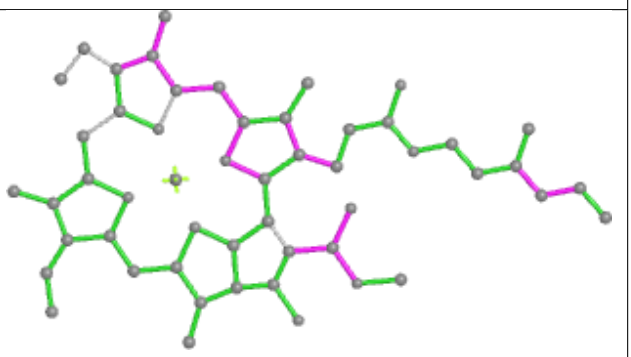
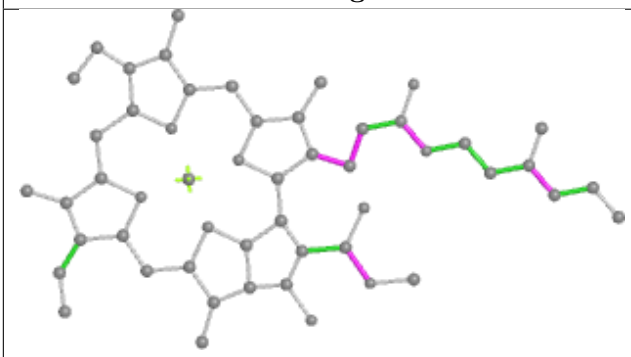
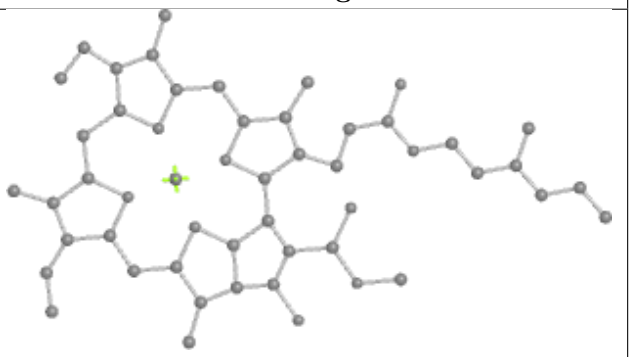


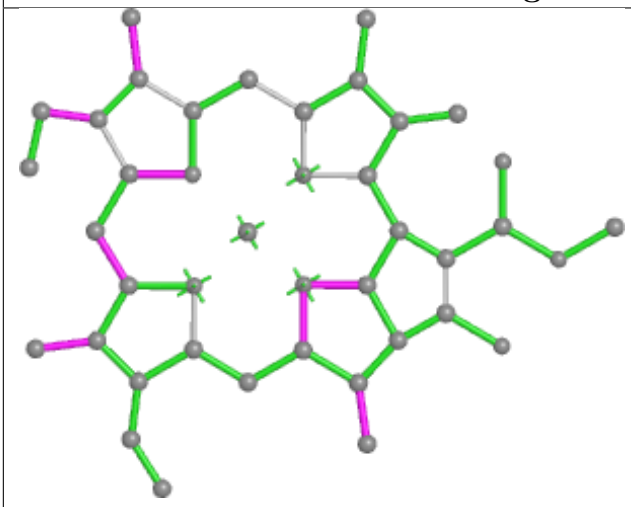
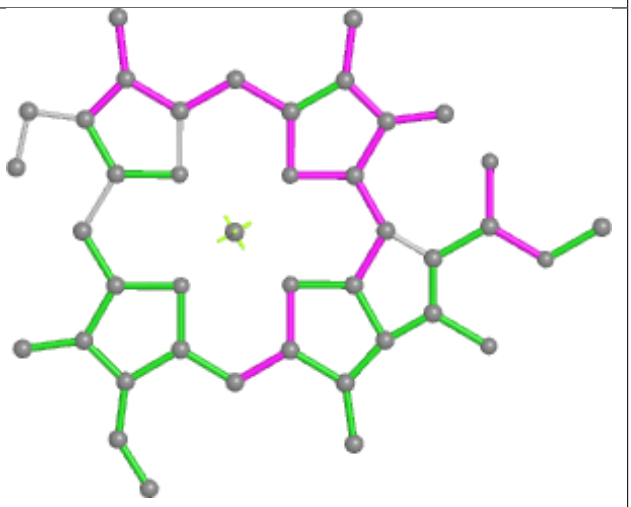
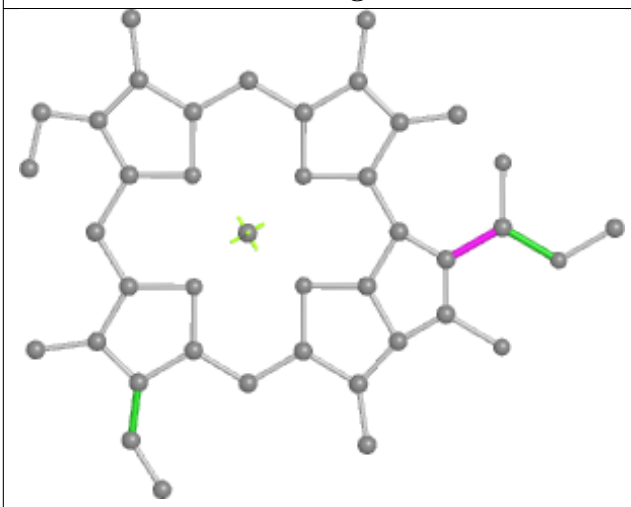
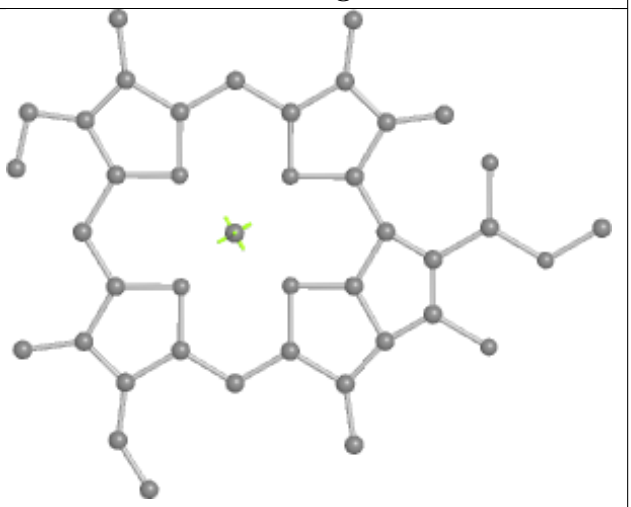
Torsions



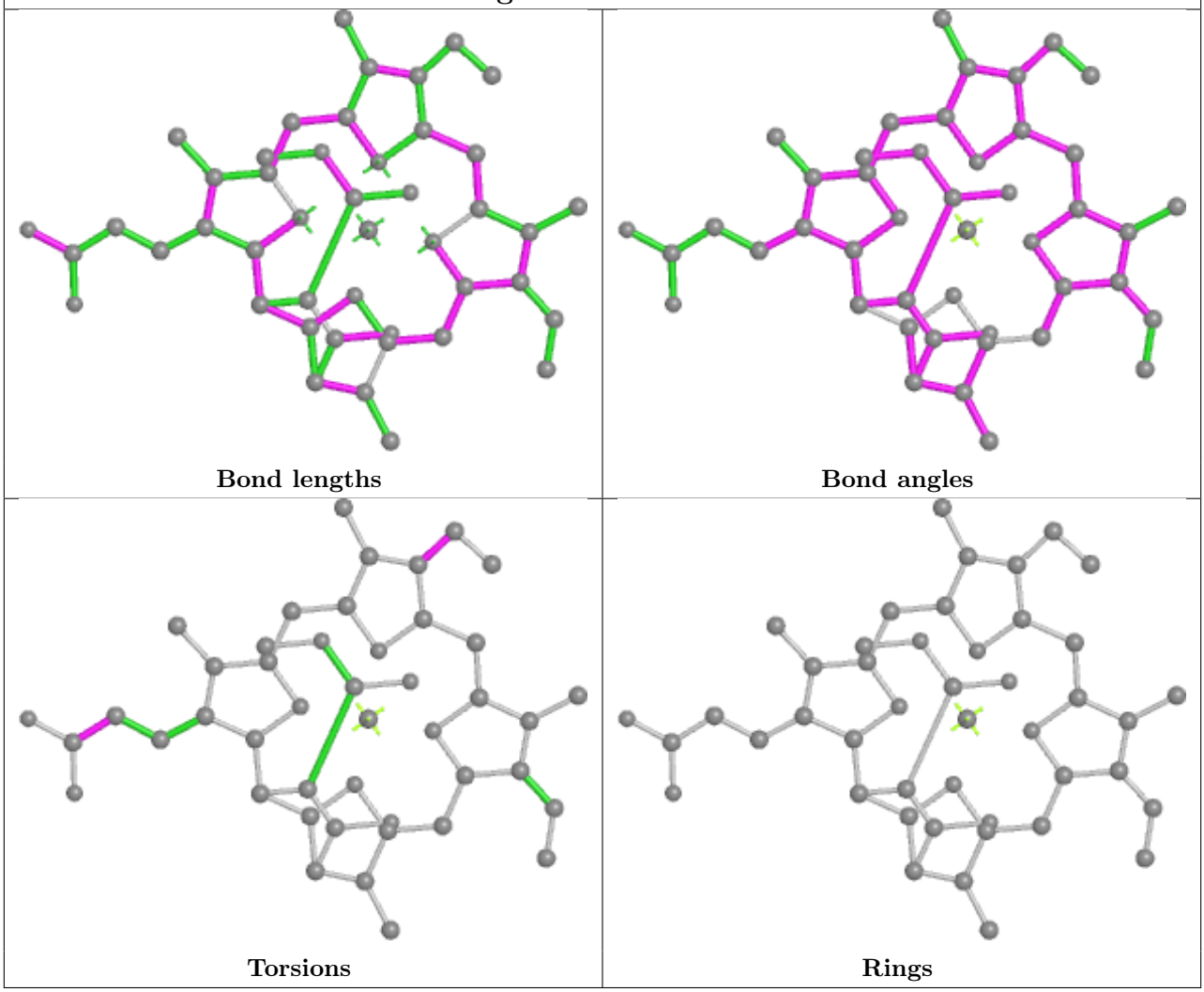
Rings

Ligand CLA S 321	
 Bond lengths	 Bond angles
 Torsions	 Rings

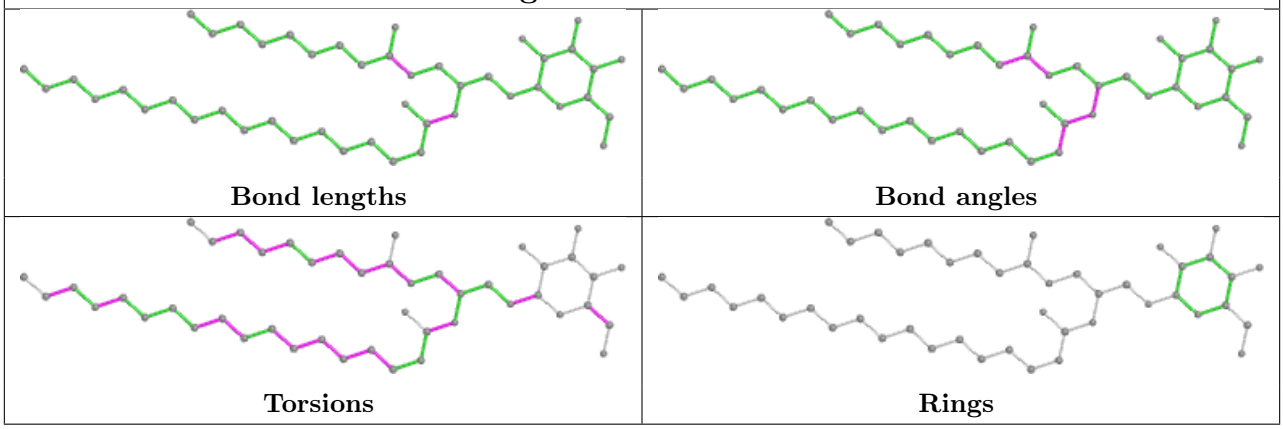
Ligand CLA f 805	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA N 313	
 Bond lengths	 Bond angles
 Torsions	 Rings

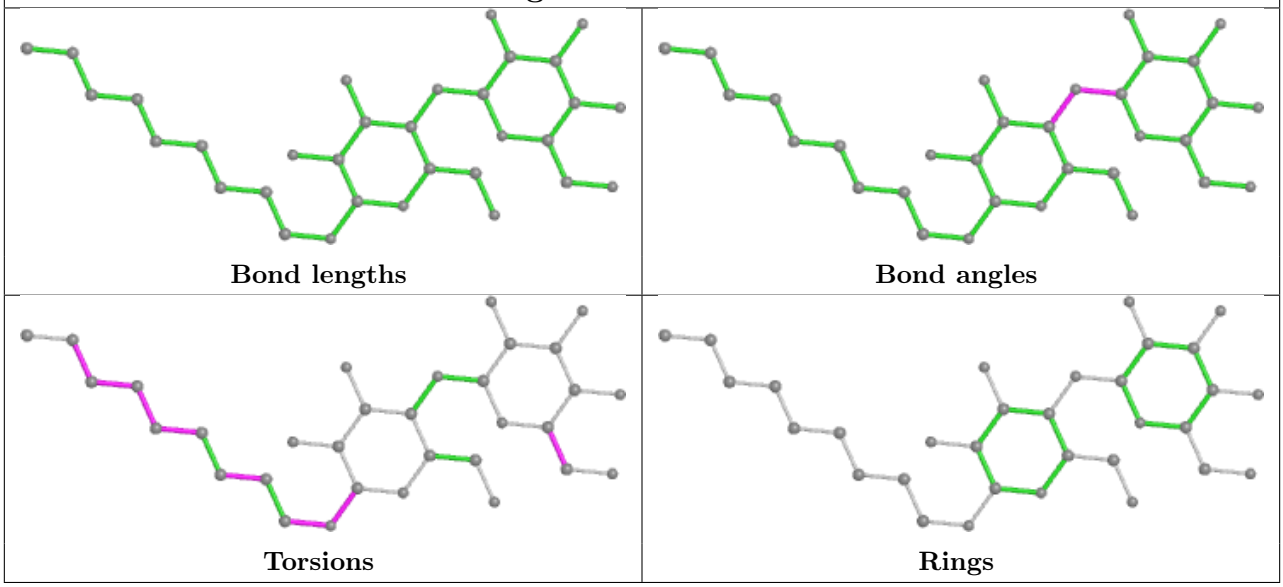
Ligand KC1 L 317



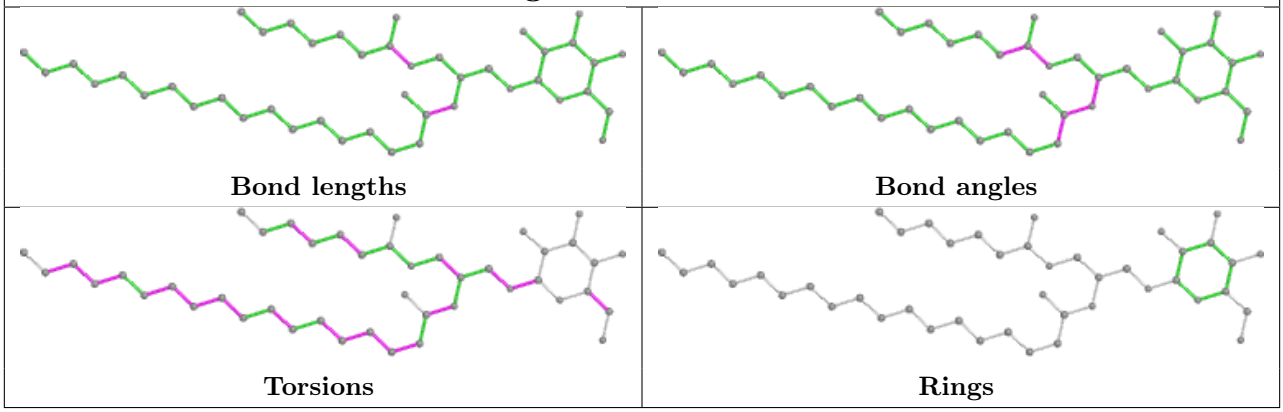
Ligand LMG V 316



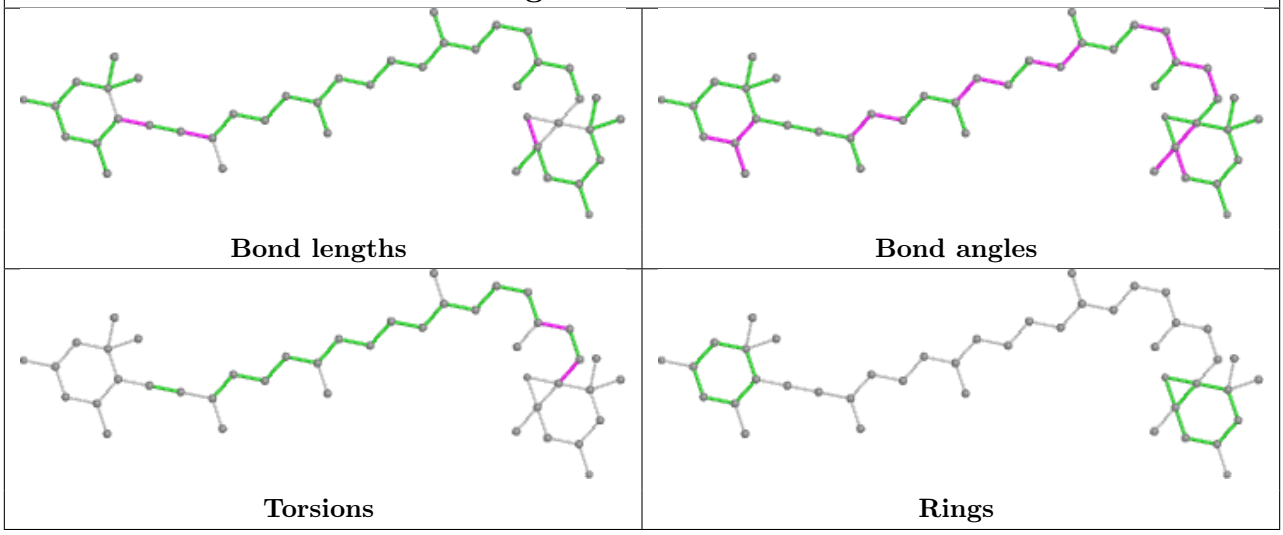
Ligand LMT a 853



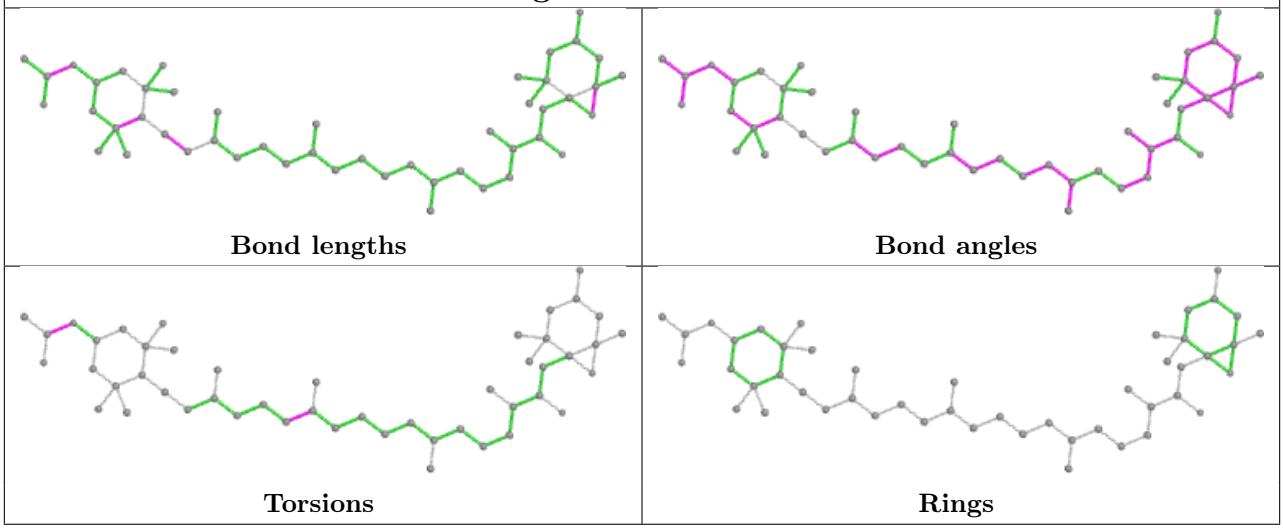
Ligand LMG J 319



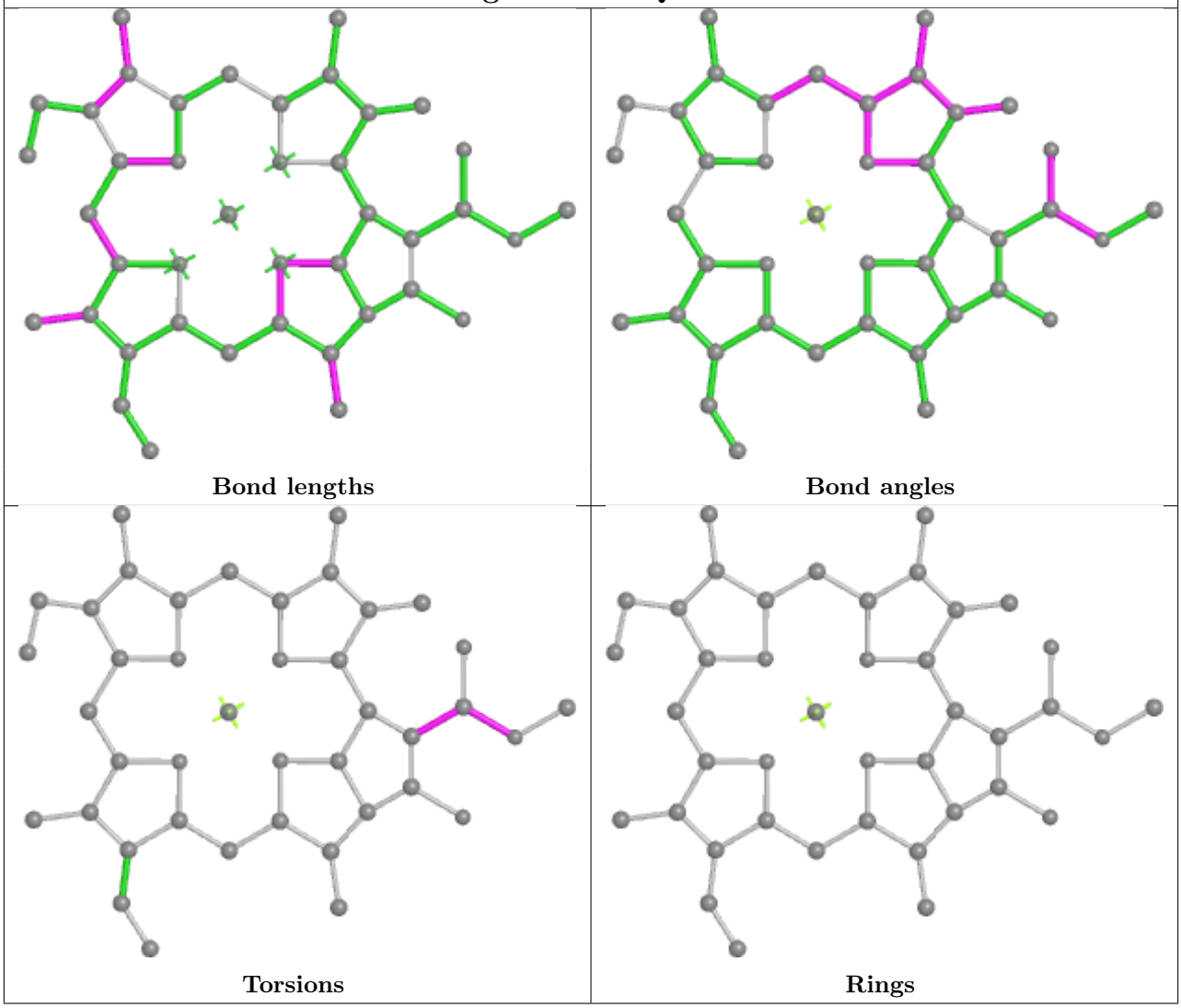
Ligand DD6 A 303



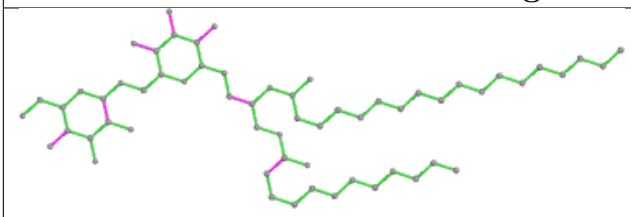
Ligand A86 F 301



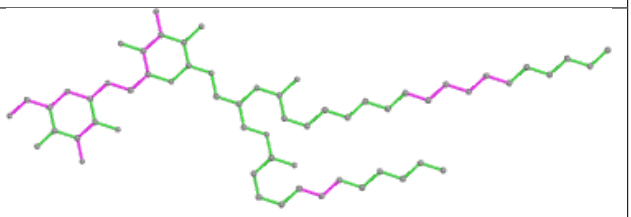
Ligand CLA Q 312



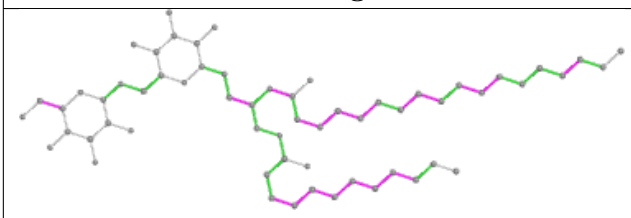
Ligand DGD b 849



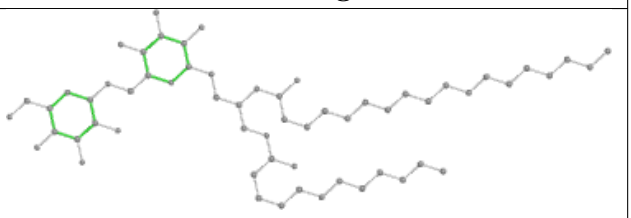
Bond lengths



Bond angles

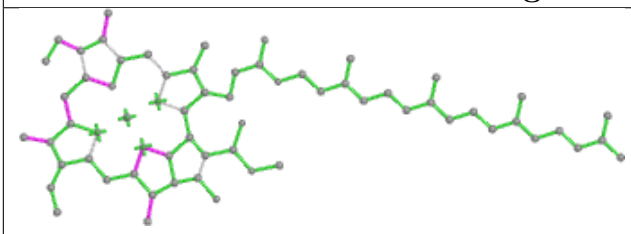


Torsions

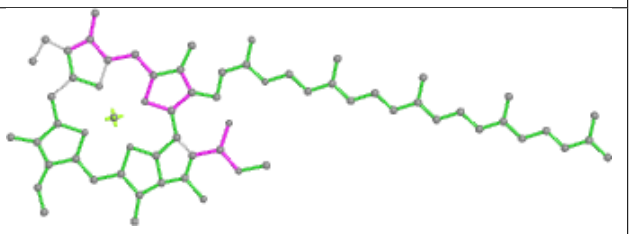


Rings

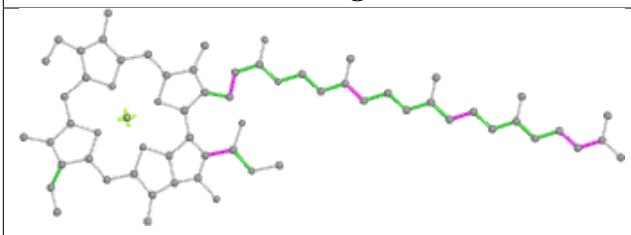
Ligand CLA D 310



Bond lengths



Bond angles



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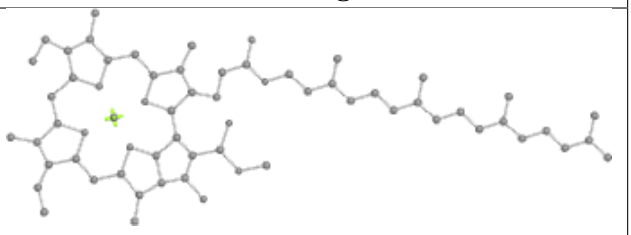
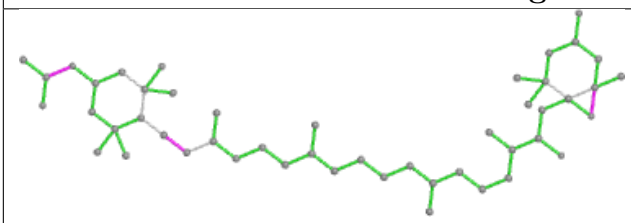
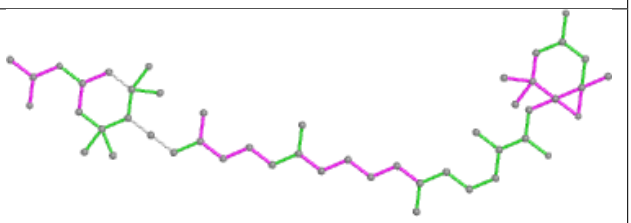


Rings

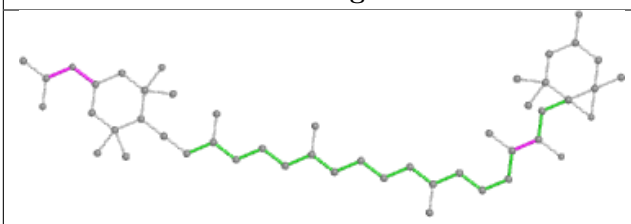
Ligand A86 N 302



Bond lengths



Bond angles



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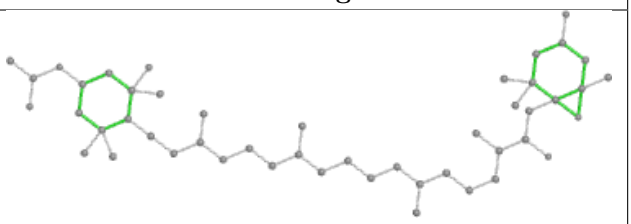
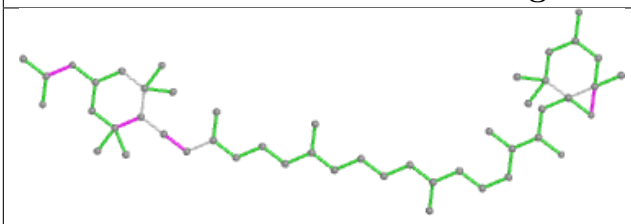
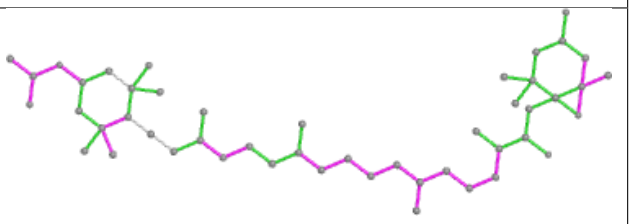
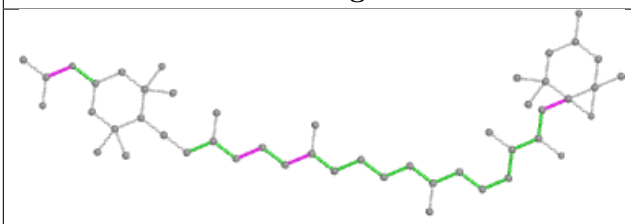
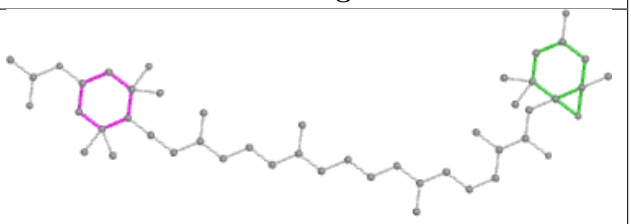
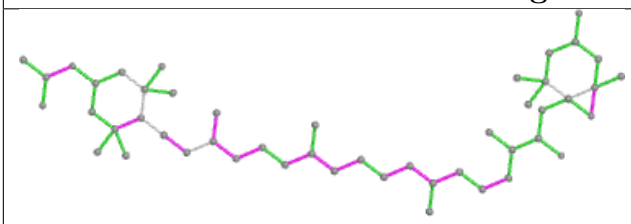
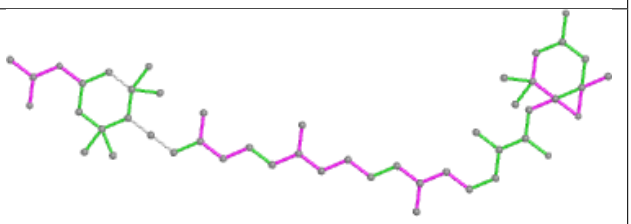
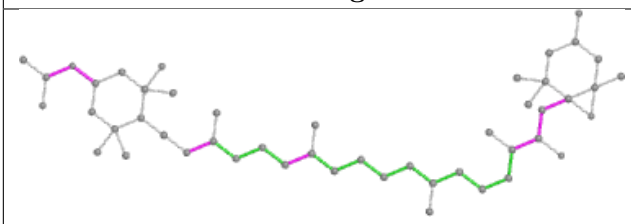
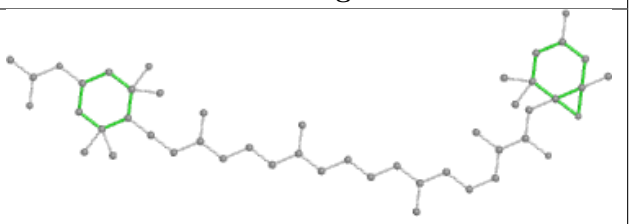
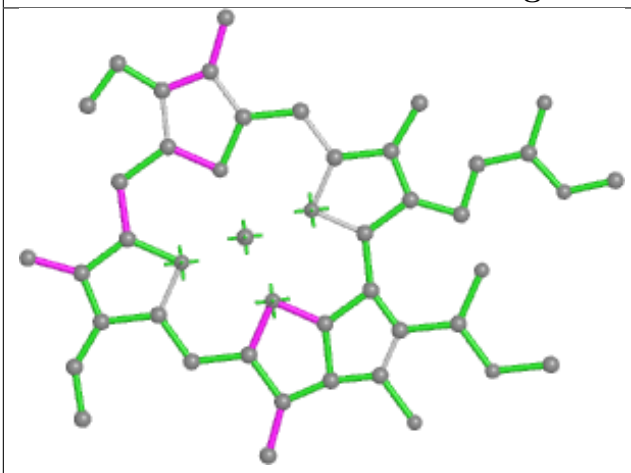


Rings

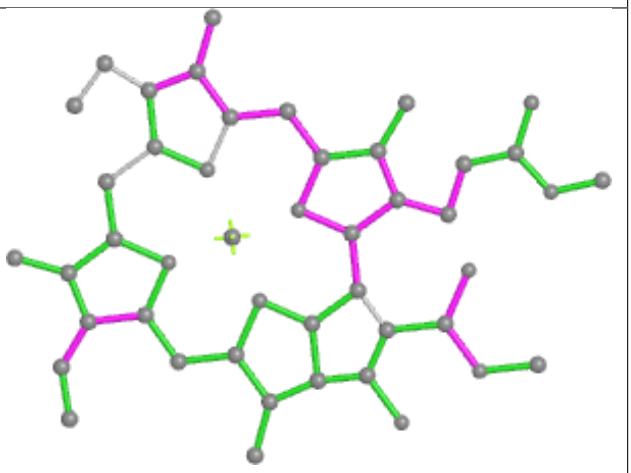
Ligand A86 K 301	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand A86 C 204	
 Bond lengths	 Bond angles
 Torsions	 Rings

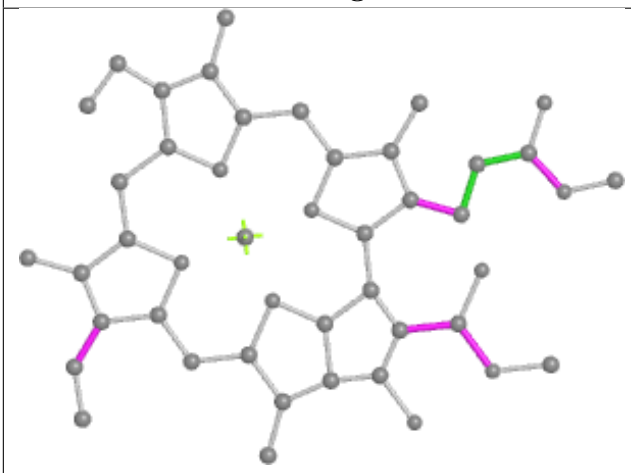
Ligand CLA R 314



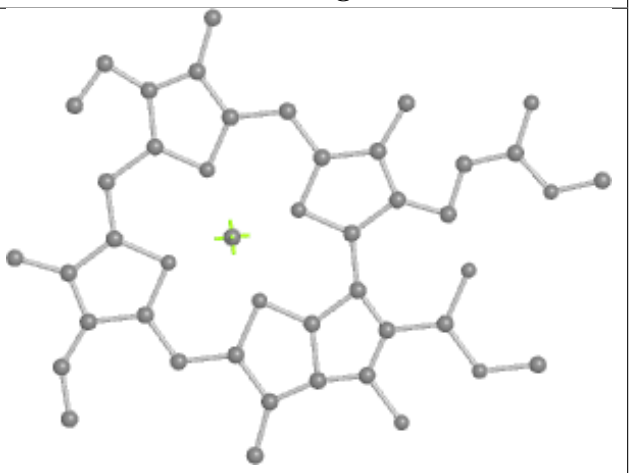
Bond lengths



Bond angles

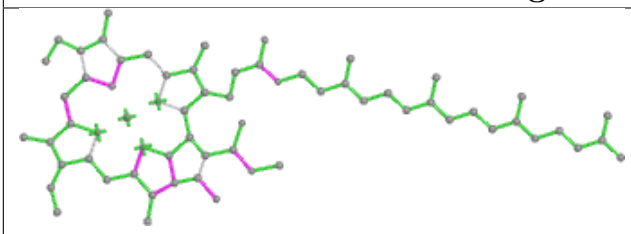


Torsions



Rings

Ligand CLA a 816



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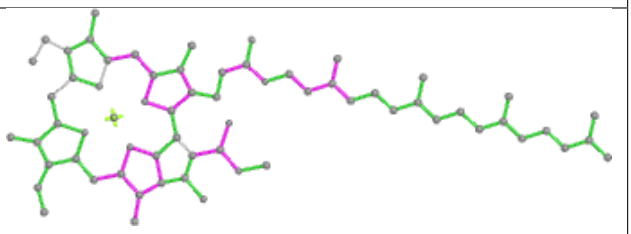
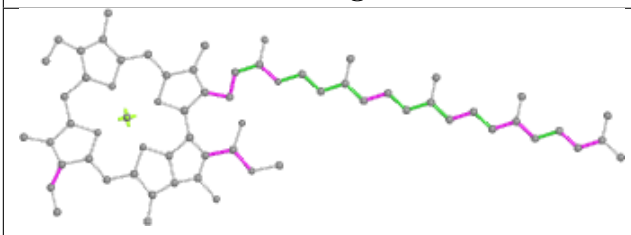
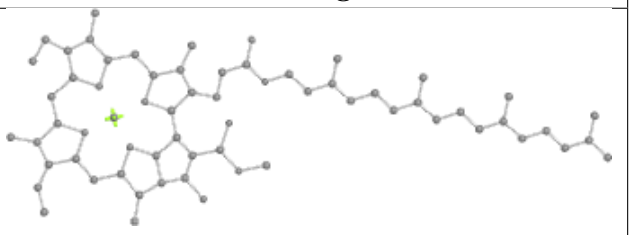


Bond angles

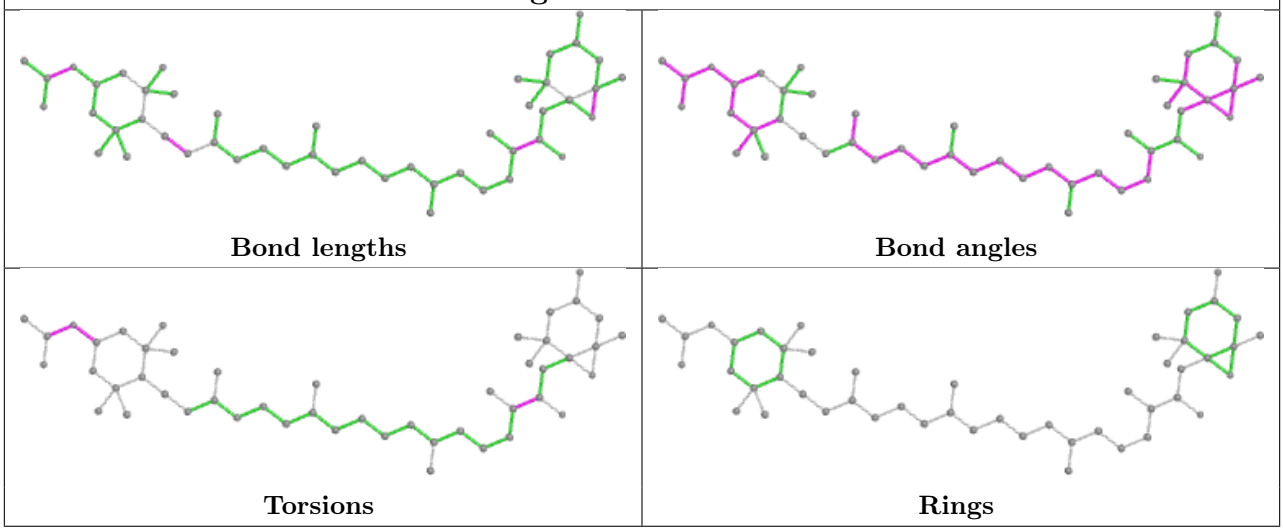


Torsions

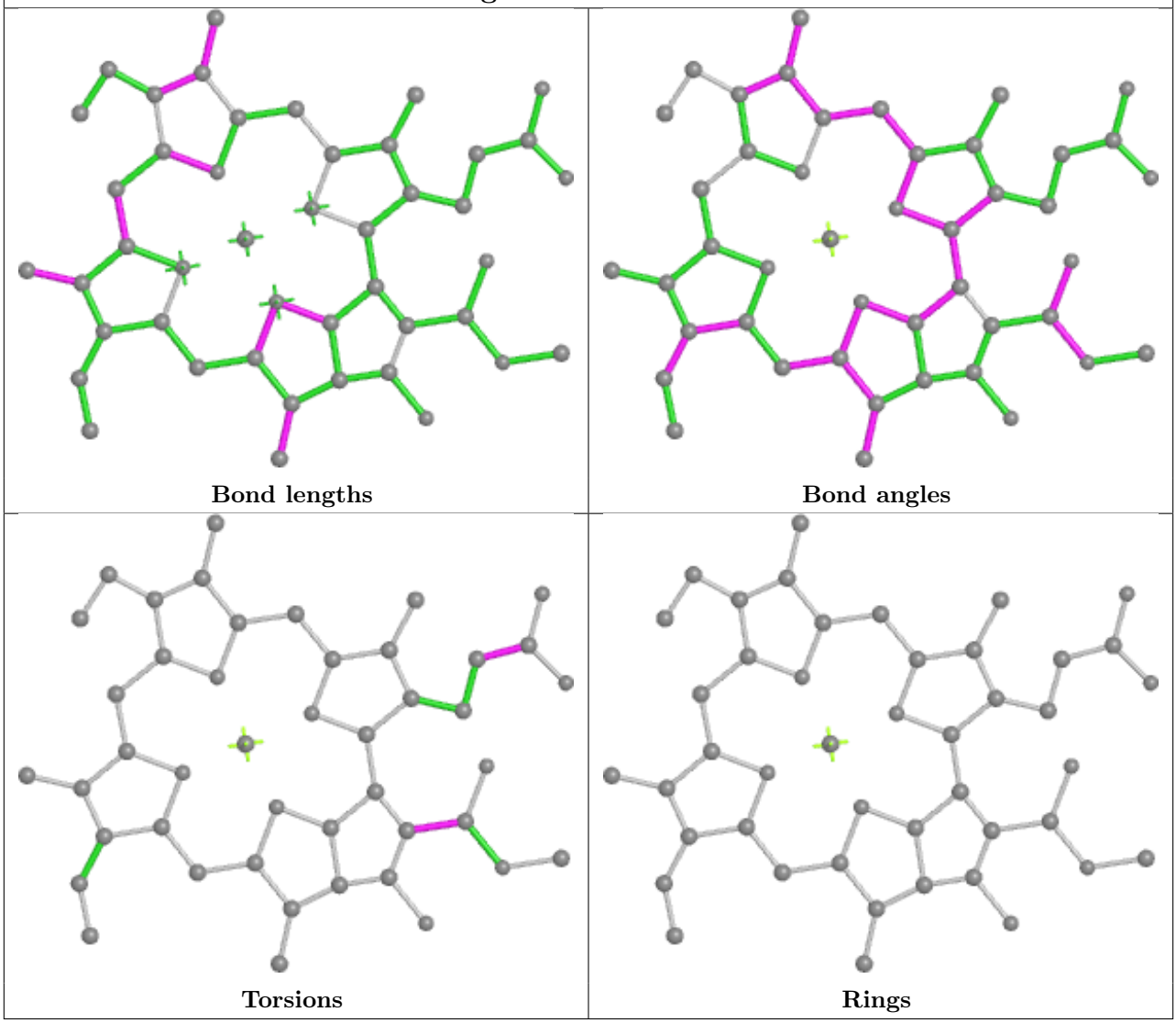


Rings

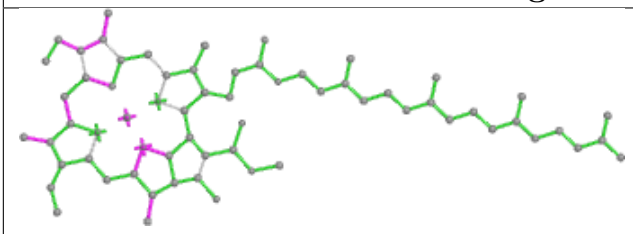
Ligand A86 V 303



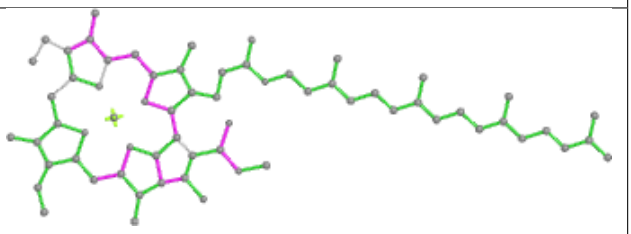
Ligand CLA R 320



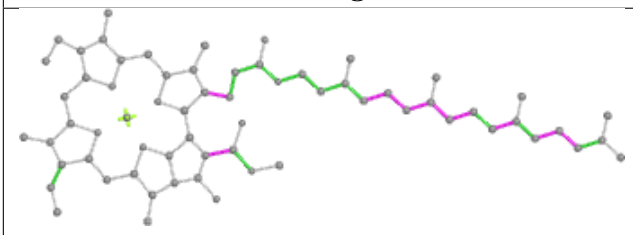
Ligand CLA a 831



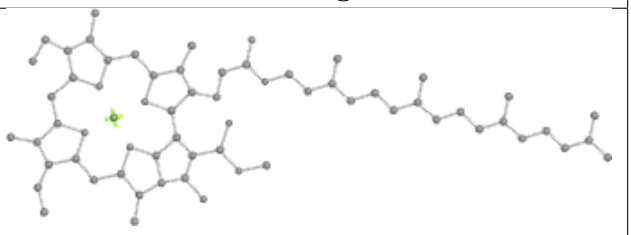
Bond lengths



Bond angles

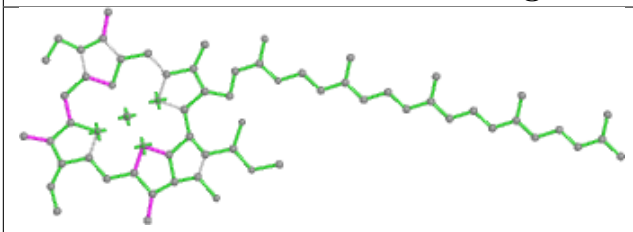


Torsions

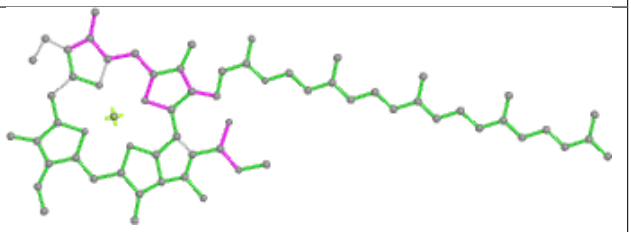


Rings

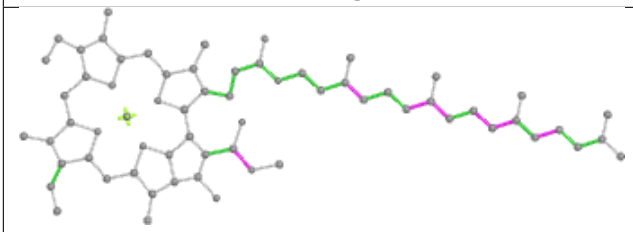
Ligand CLA N 316



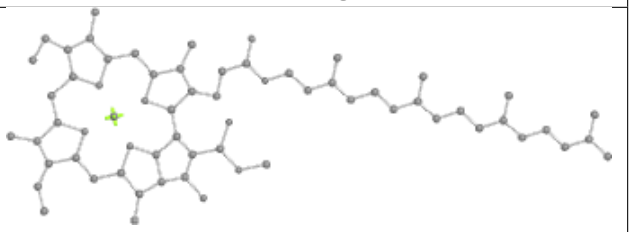
Bond lengths



Bond angles

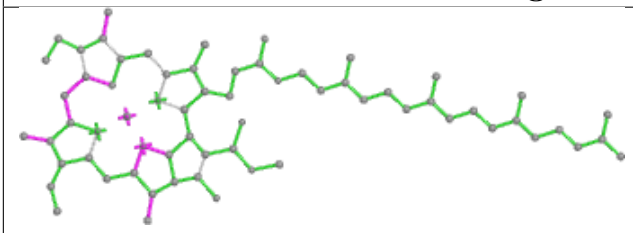


Torsions

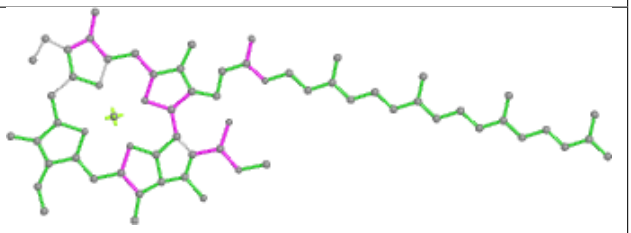


Rings

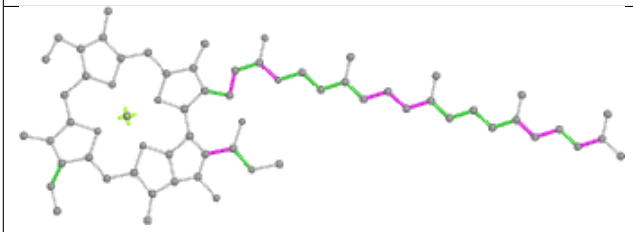
Ligand CLA b 825



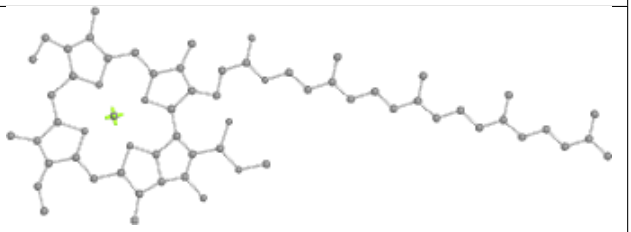
Bond lengths



Bond angles

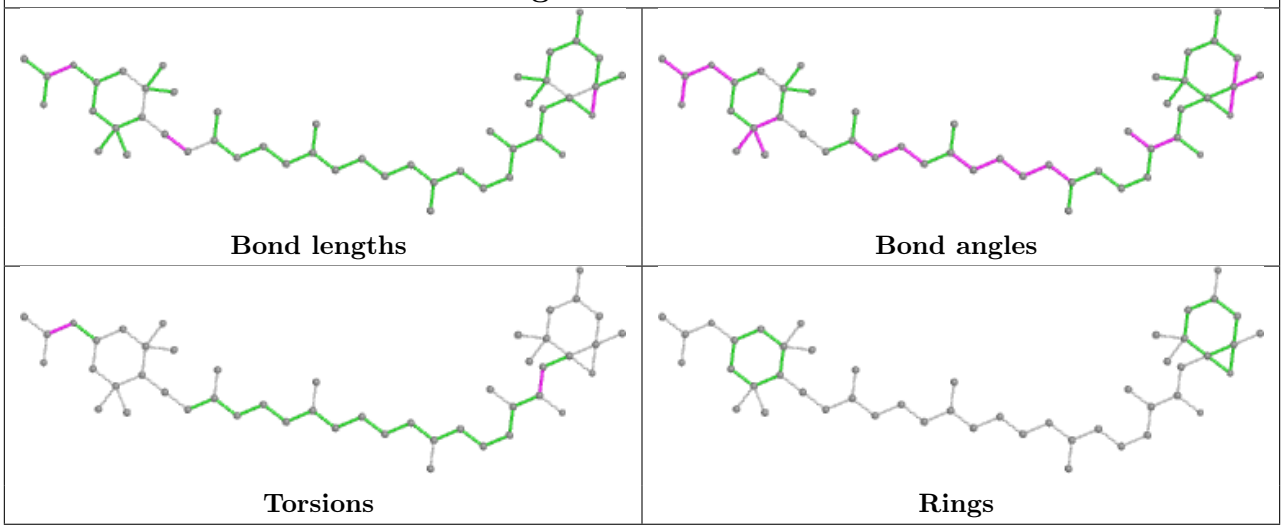


Torsions

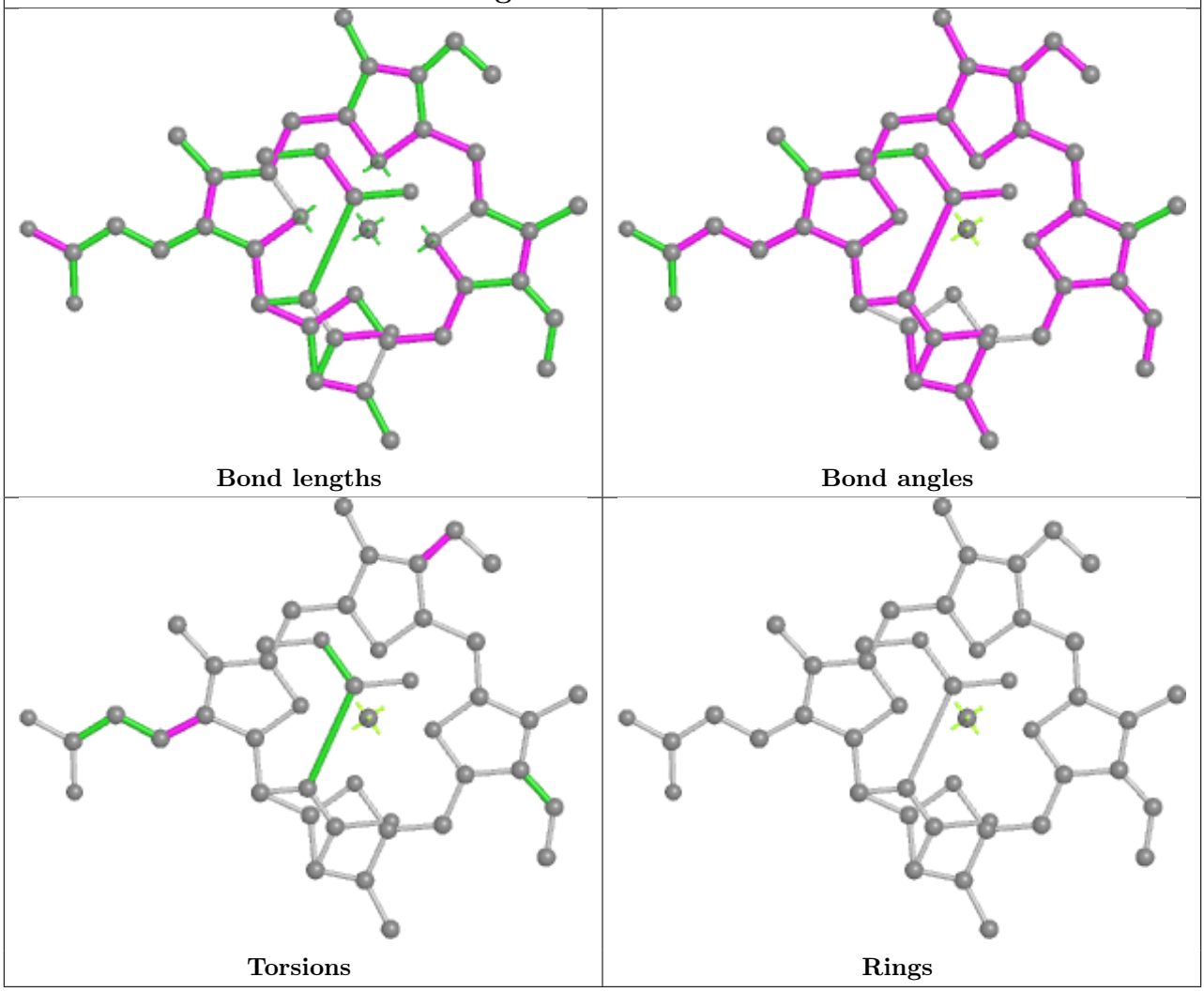


Rings

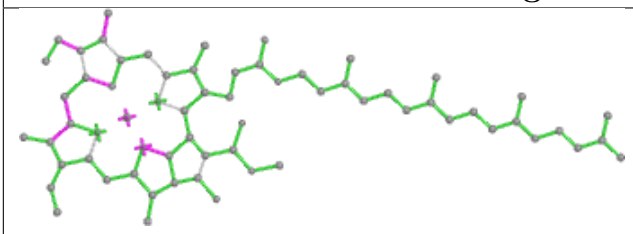
Ligand A86 P 306



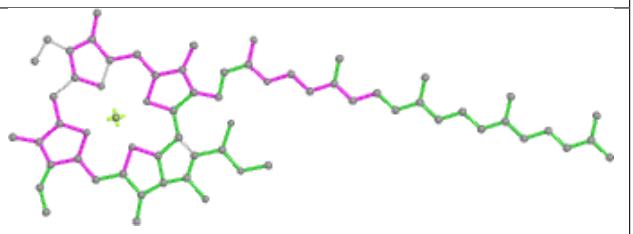
Ligand KC1 P 317



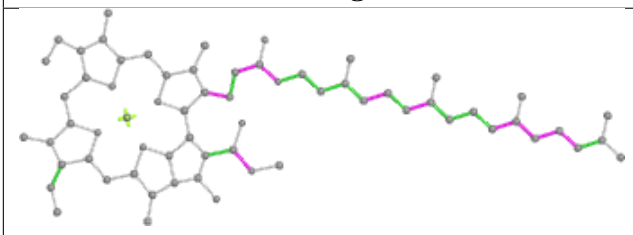
Ligand CLA N 308



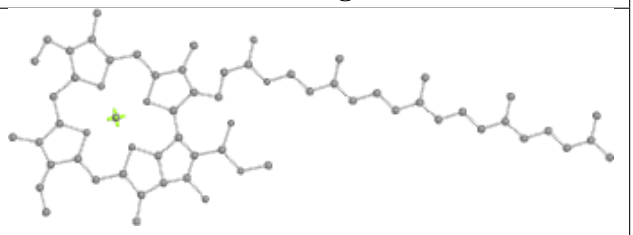
Bond lengths



Bond angles

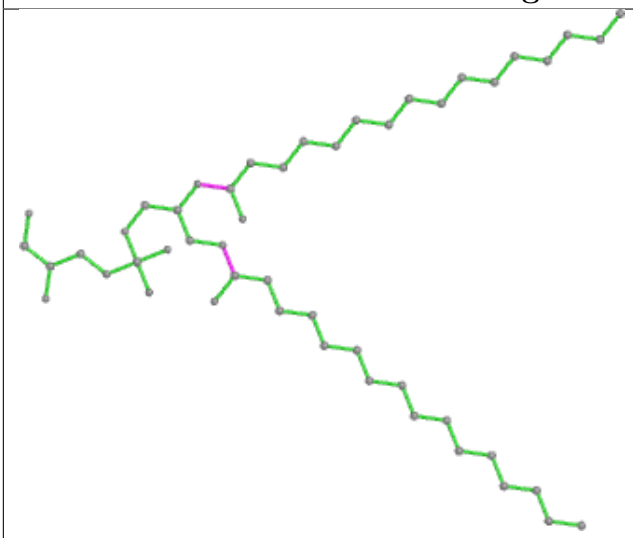


Torsions

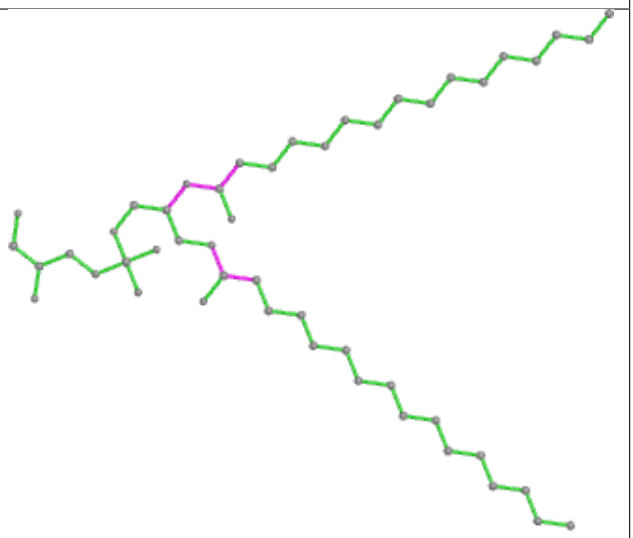


Rings

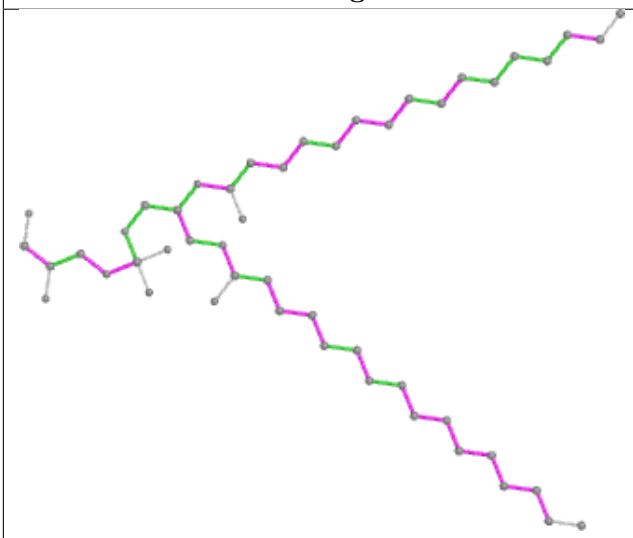
Ligand LHG D 319



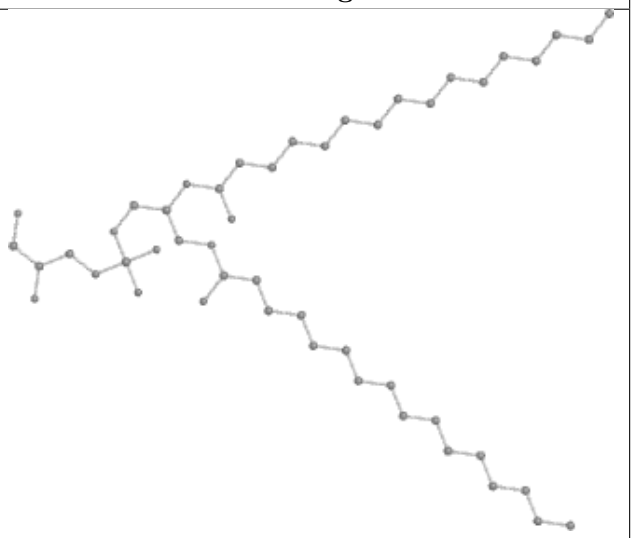
Bond lengths



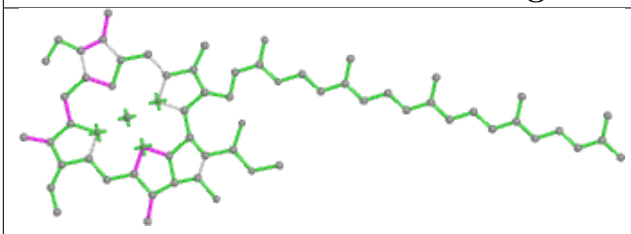
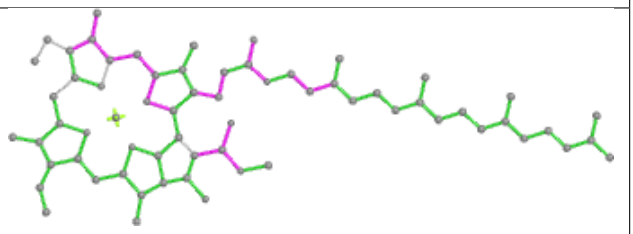
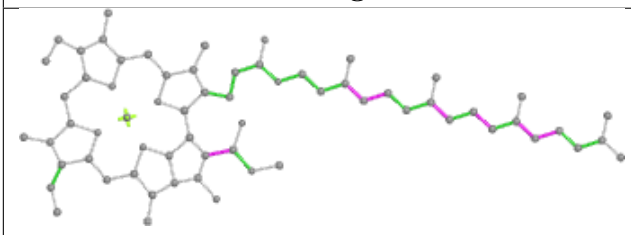
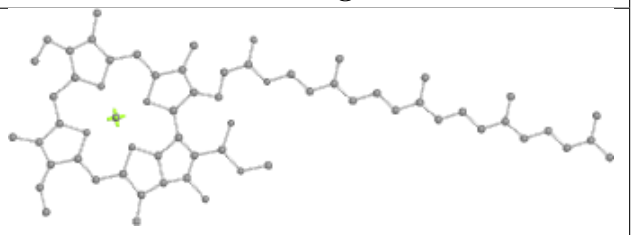
Bond angles

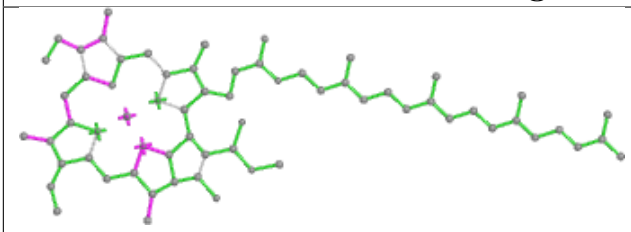
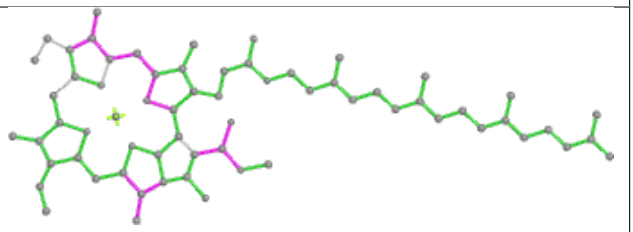
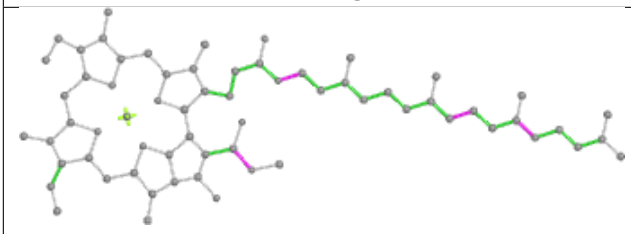
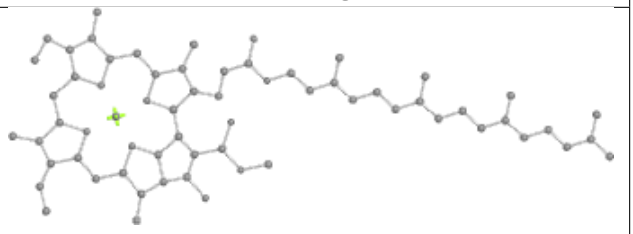


Torsions

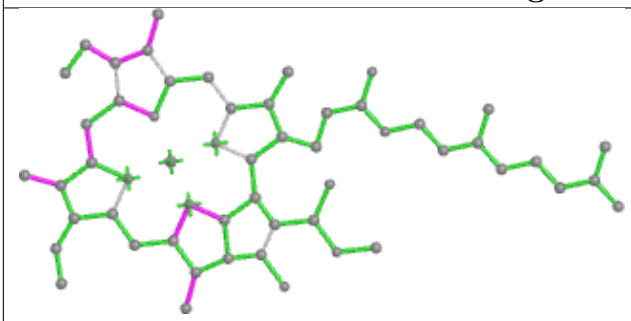


Rings

Ligand CLA b 811	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA a 838	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA b 814



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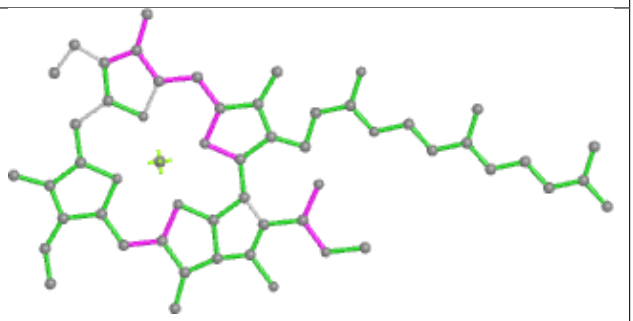
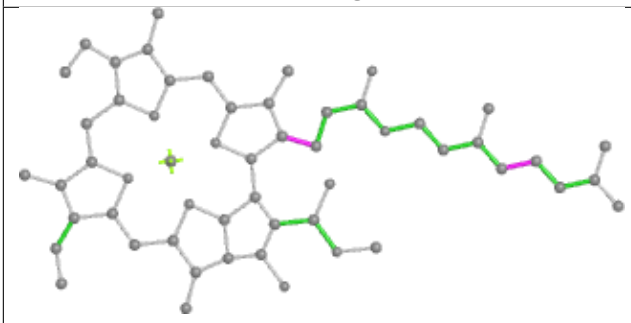


Bond angles



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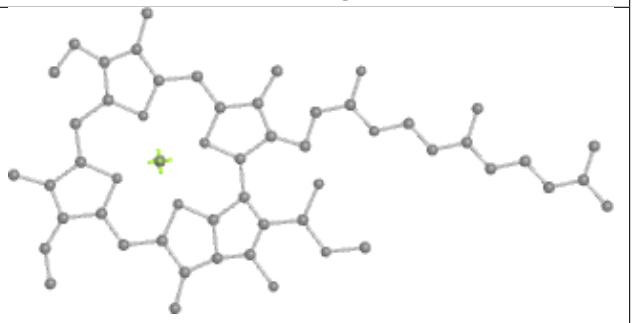
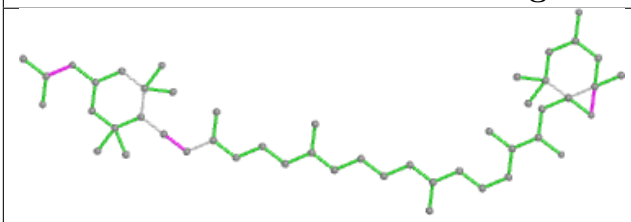


Rings

Ligand A86 U 304



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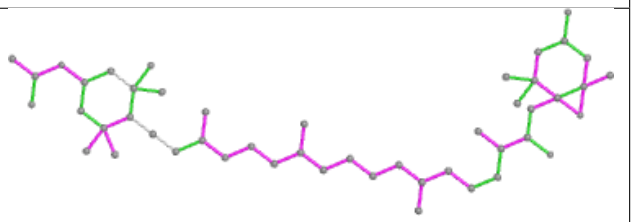

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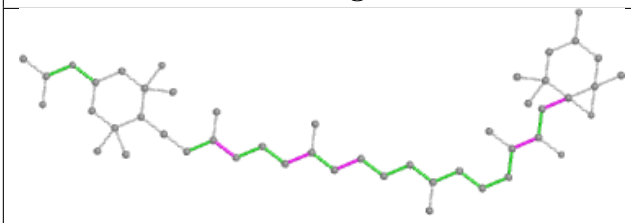

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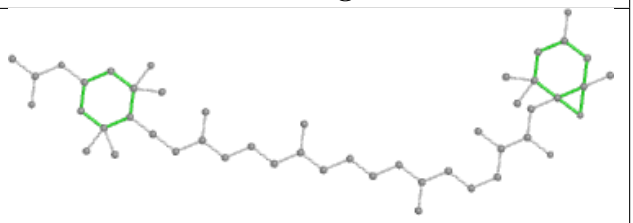
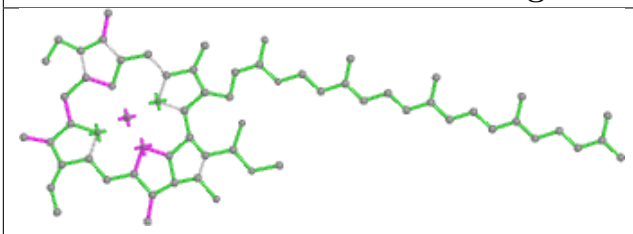


Rings

Ligand CLA b 828



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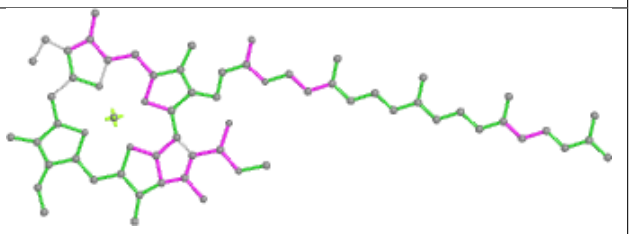

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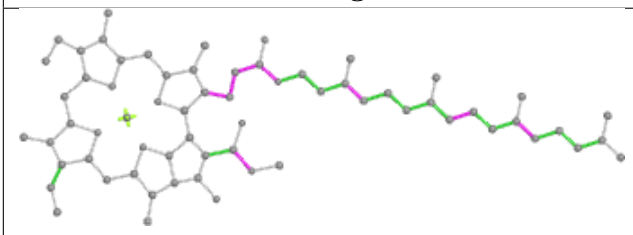

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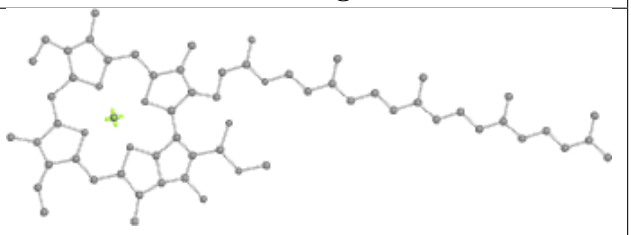
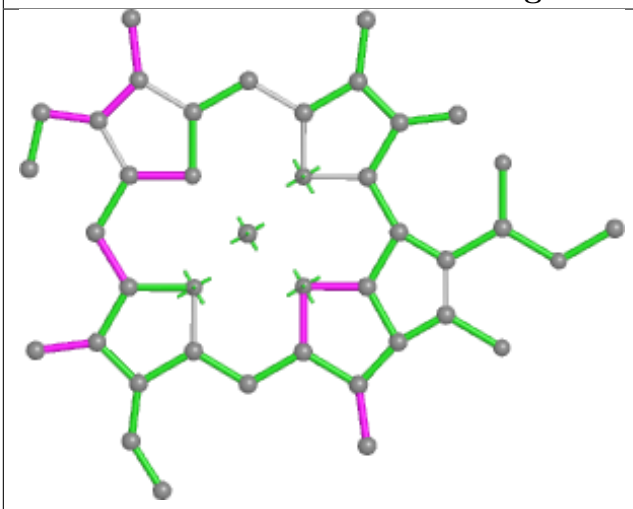


Rings

Ligand CLA C 214



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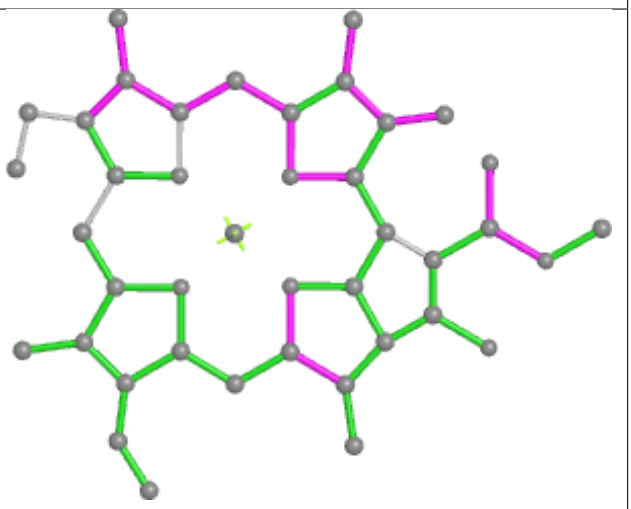
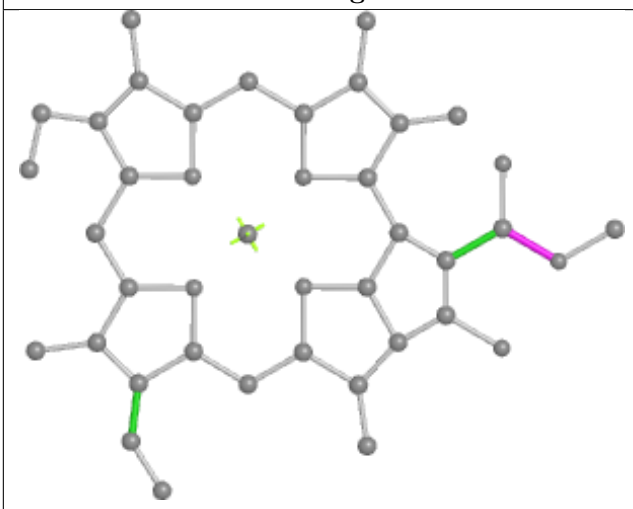


Bond angles



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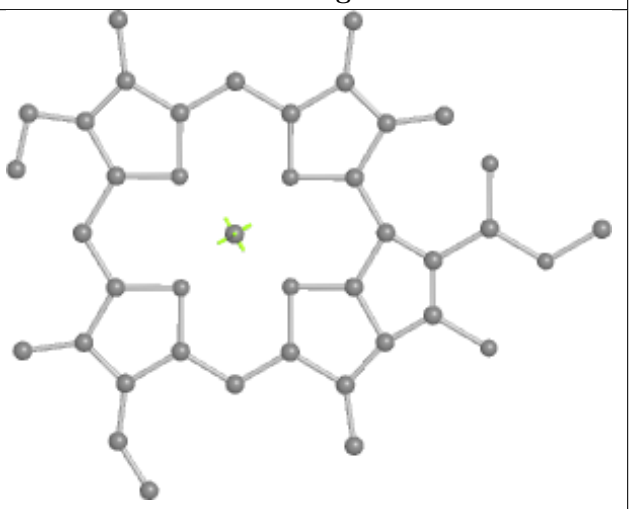
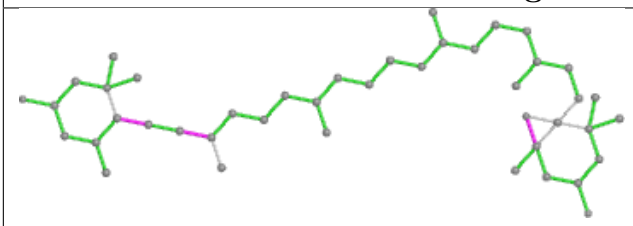


Rings

Ligand DD6 O 304



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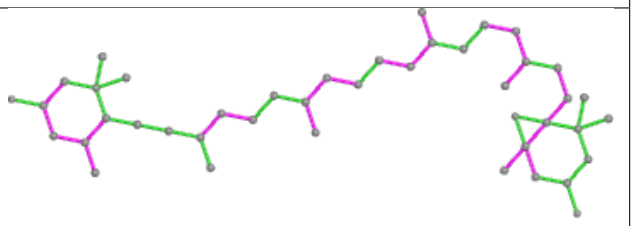

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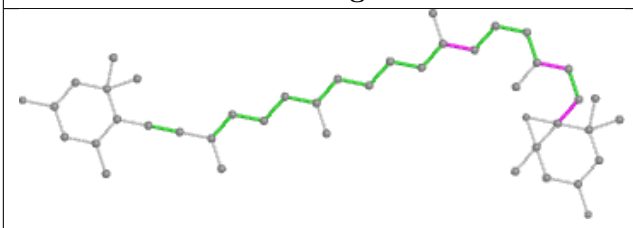

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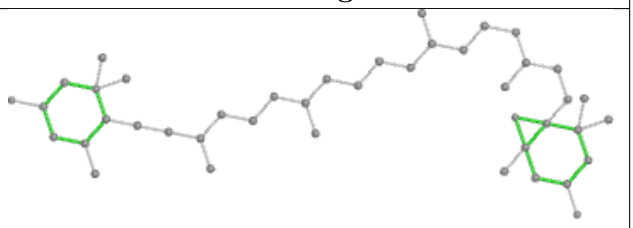
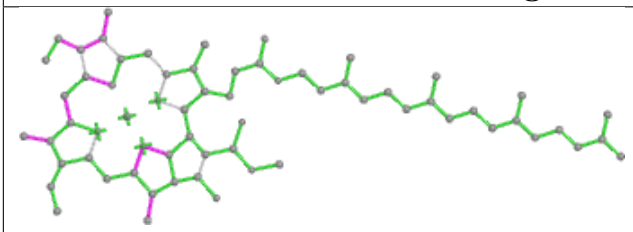


Rings

Ligand CLA H 316



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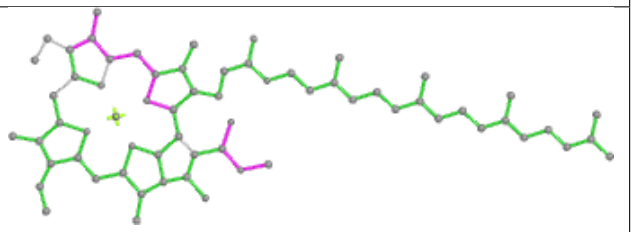

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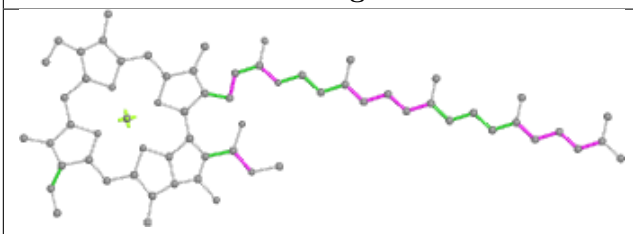

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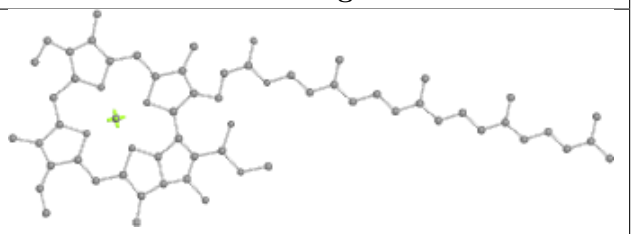
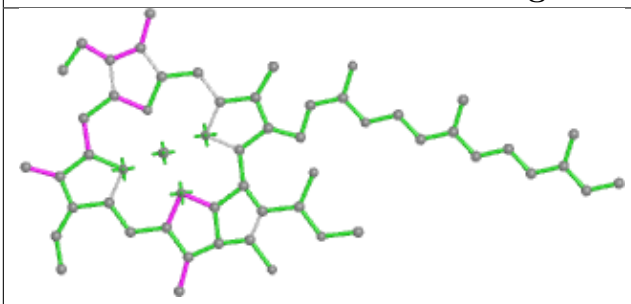


Rings

Ligand CLA a 809



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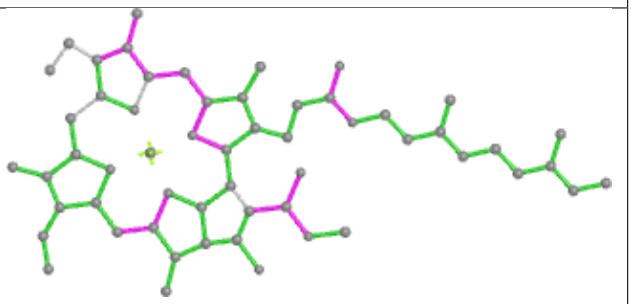

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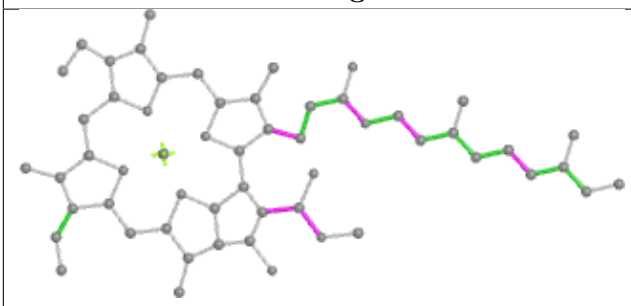

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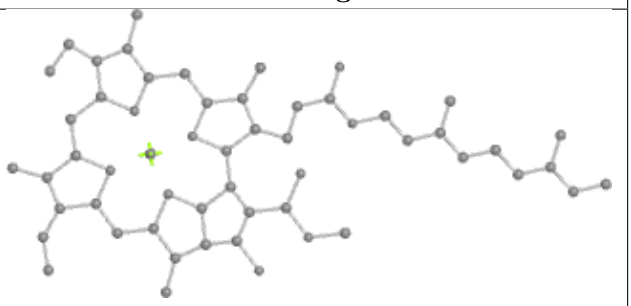
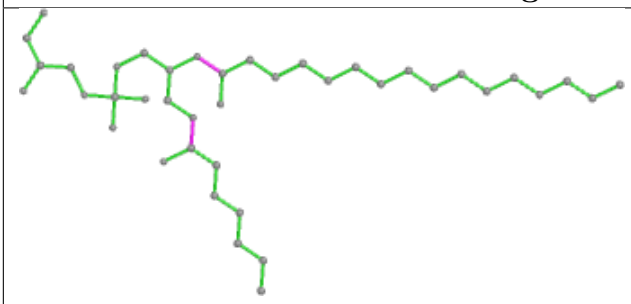


Rings

Ligand LHG G 320



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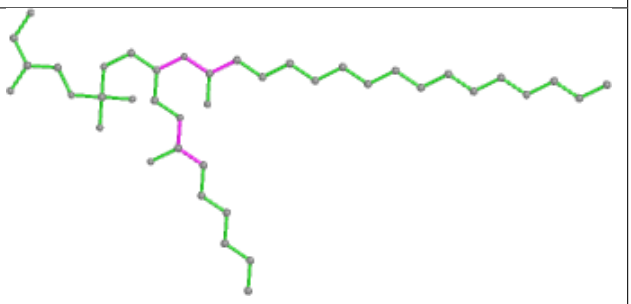
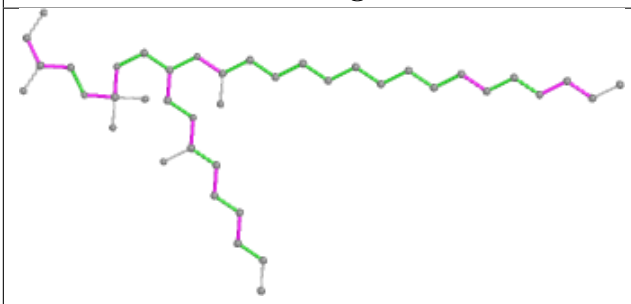
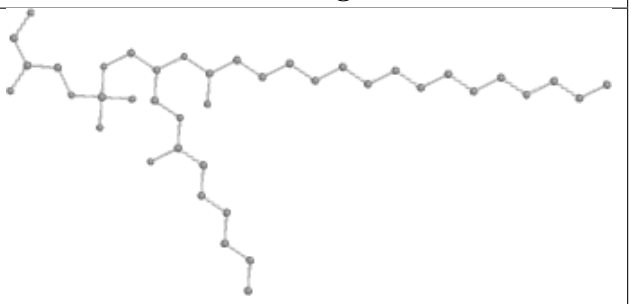


Bond angles

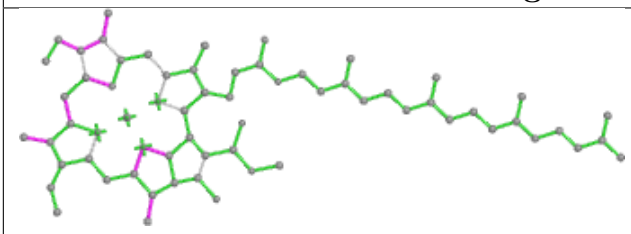


Torsions



Rings

Ligand CLA A 311



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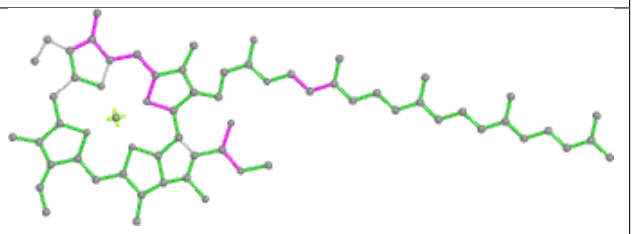
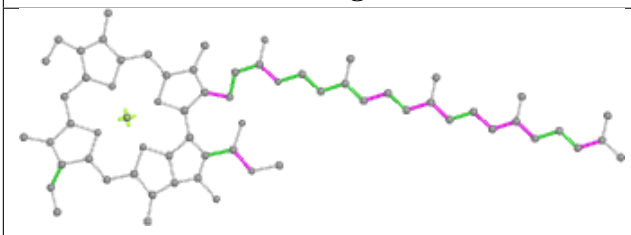


Bond angles



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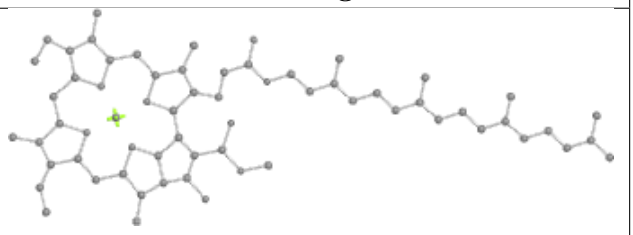
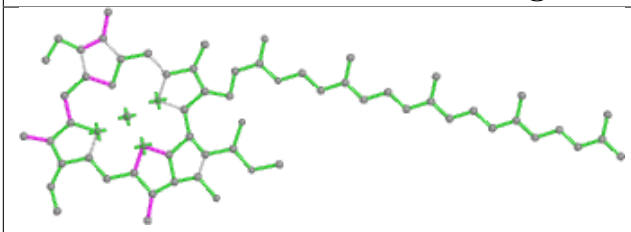
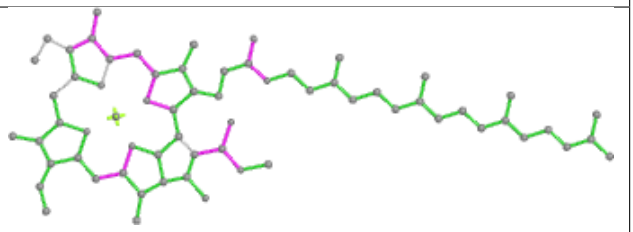


Rings

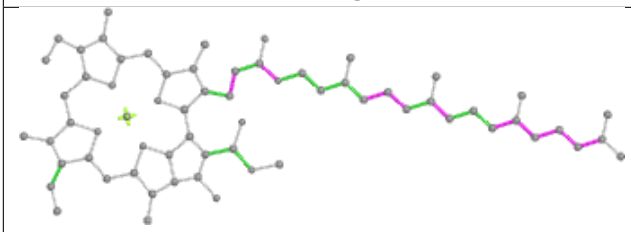
Ligand CLA a 839



Bond lengths



Bond angles



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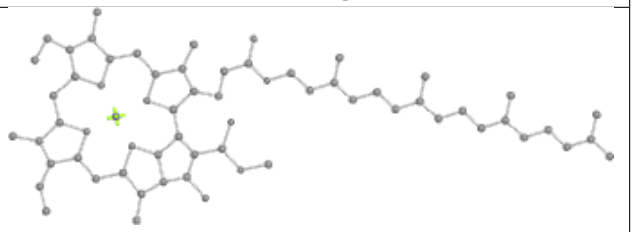
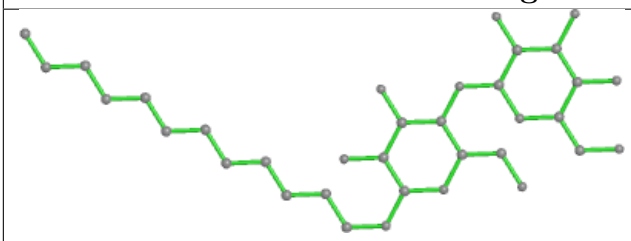


Rings

Ligand LMT K 318



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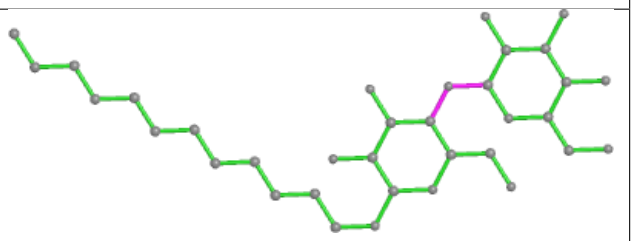
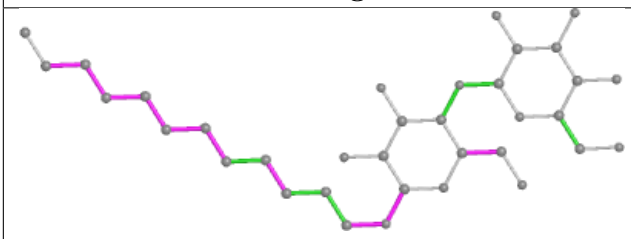


Bond angles



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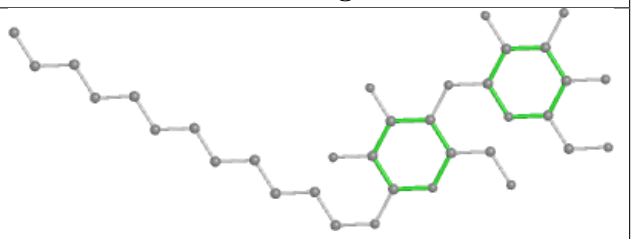
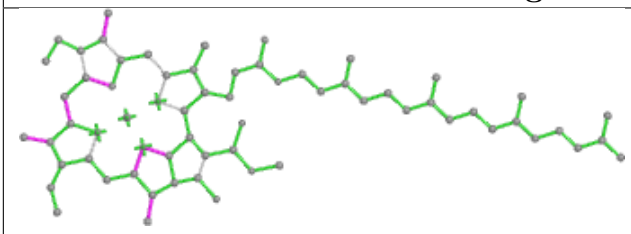
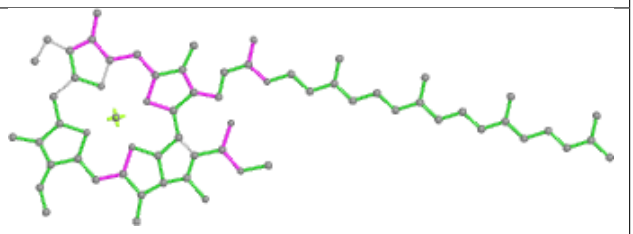
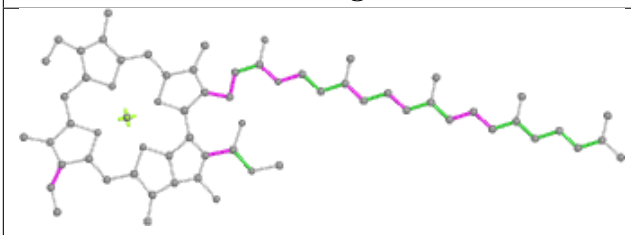
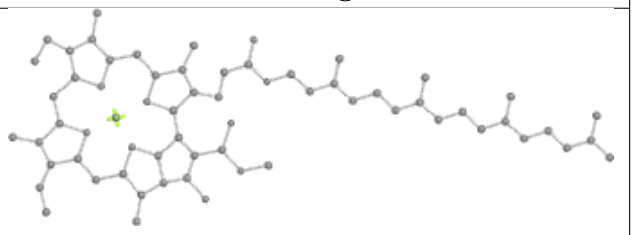
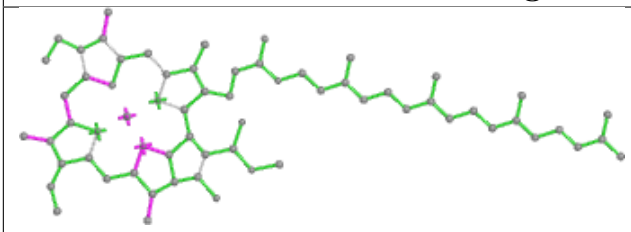
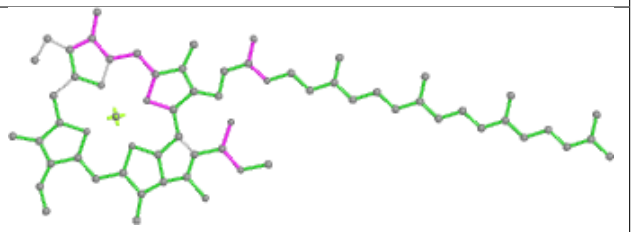
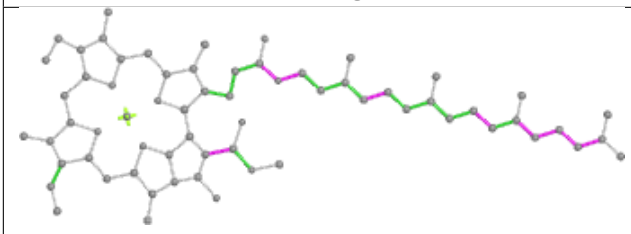
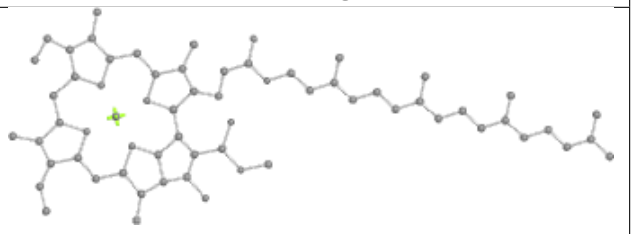
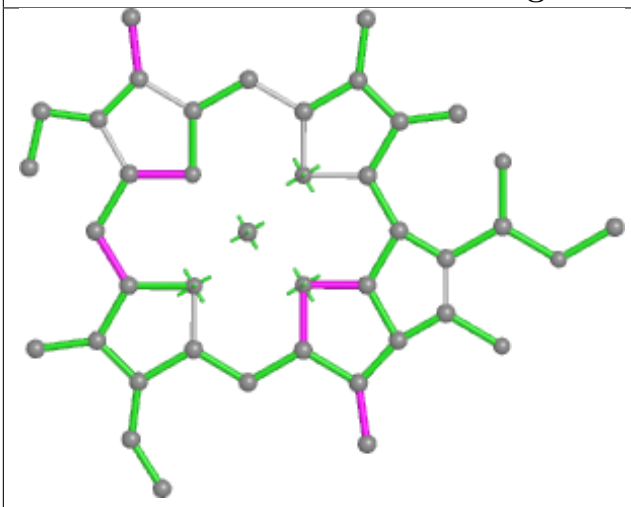


Rings

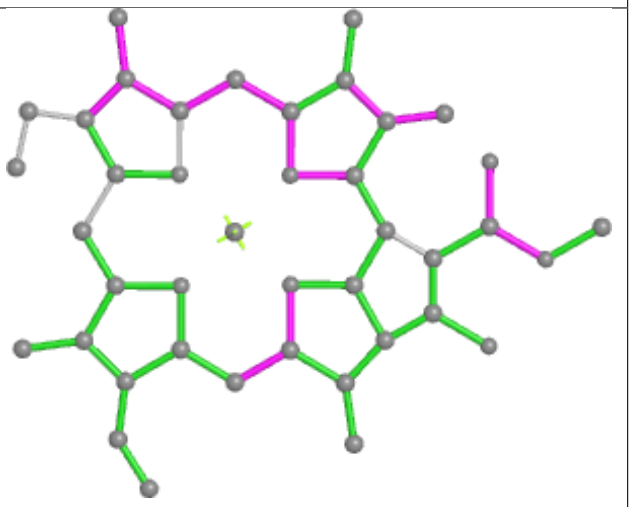
Ligand CLA E 312	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA A 310	
 Bond lengths	 Bond angles
 Torsions	 Rings

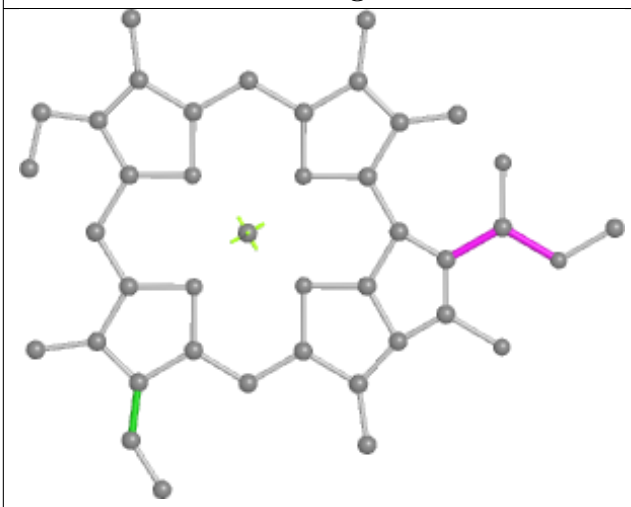
Ligand CLA S 317



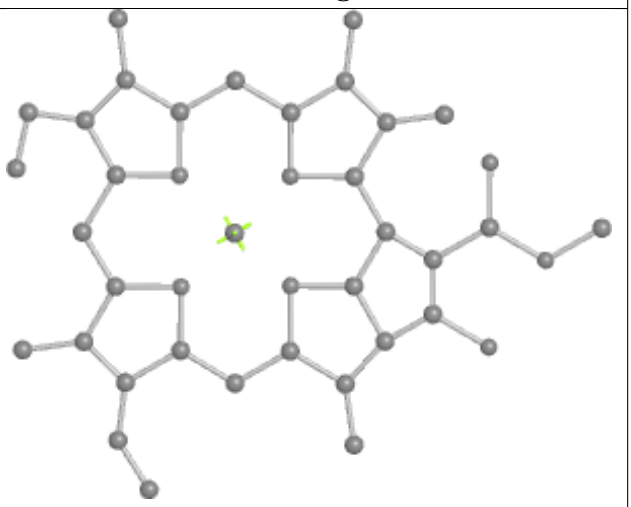
Bond lengths



Bond angles

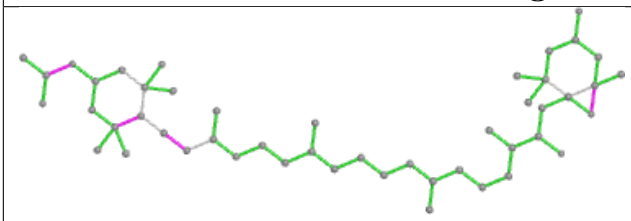


Torsions

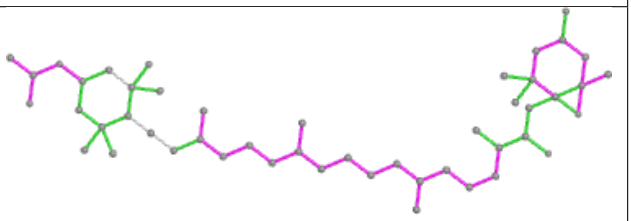


Rings

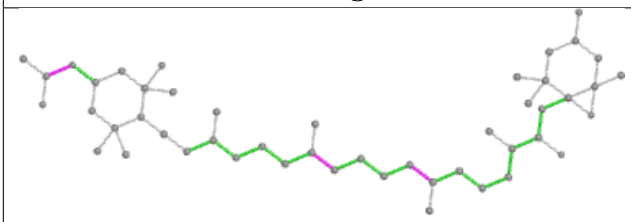
Ligand A86 G 306



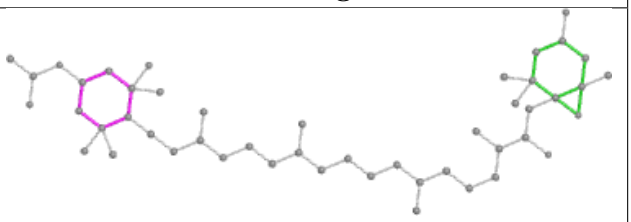
Bond lengths



Bond angles

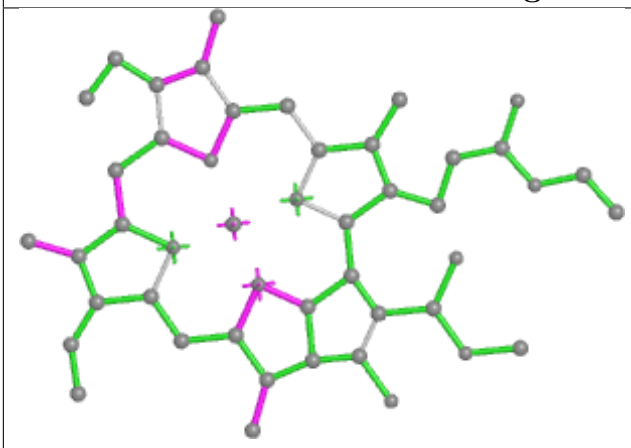


Torsions



Rings

Ligand CLA X 308



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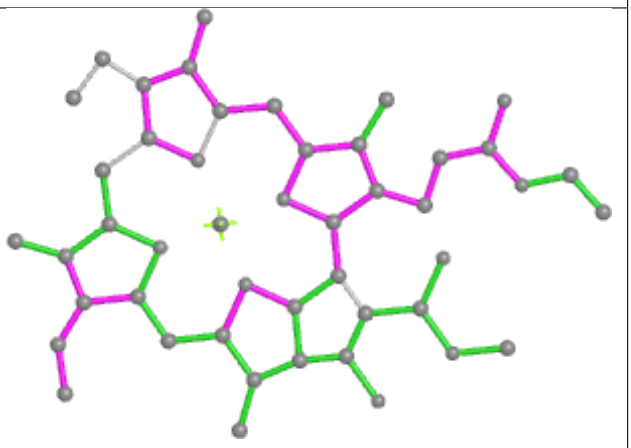
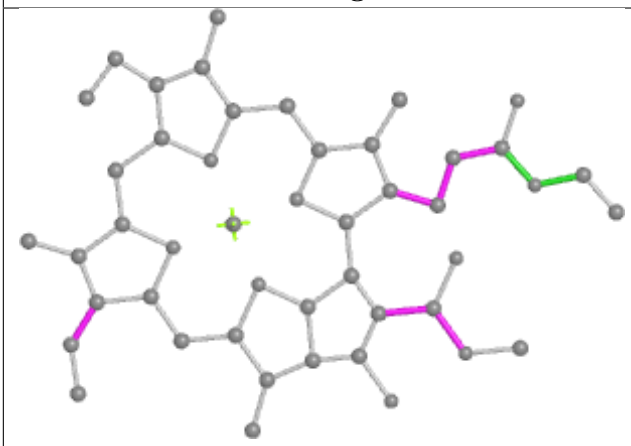


Bond angles



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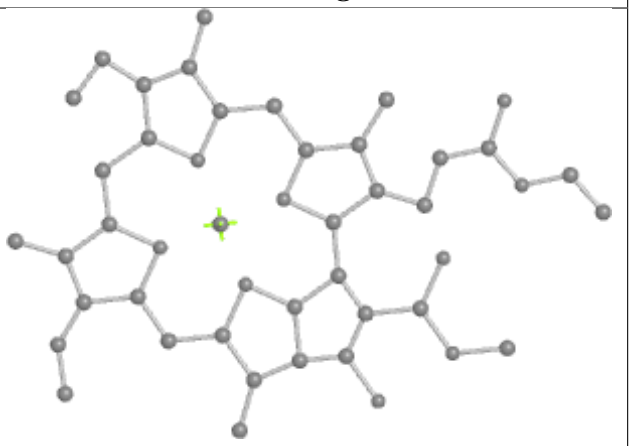
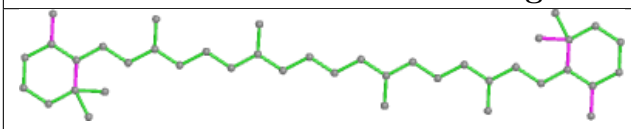


Rings

Ligand BCR h 201



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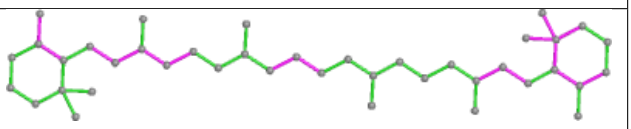
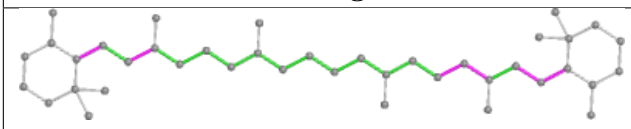
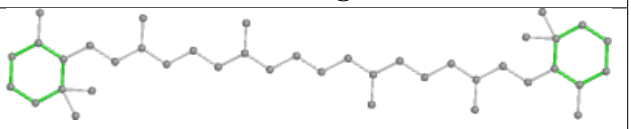


Bond angles

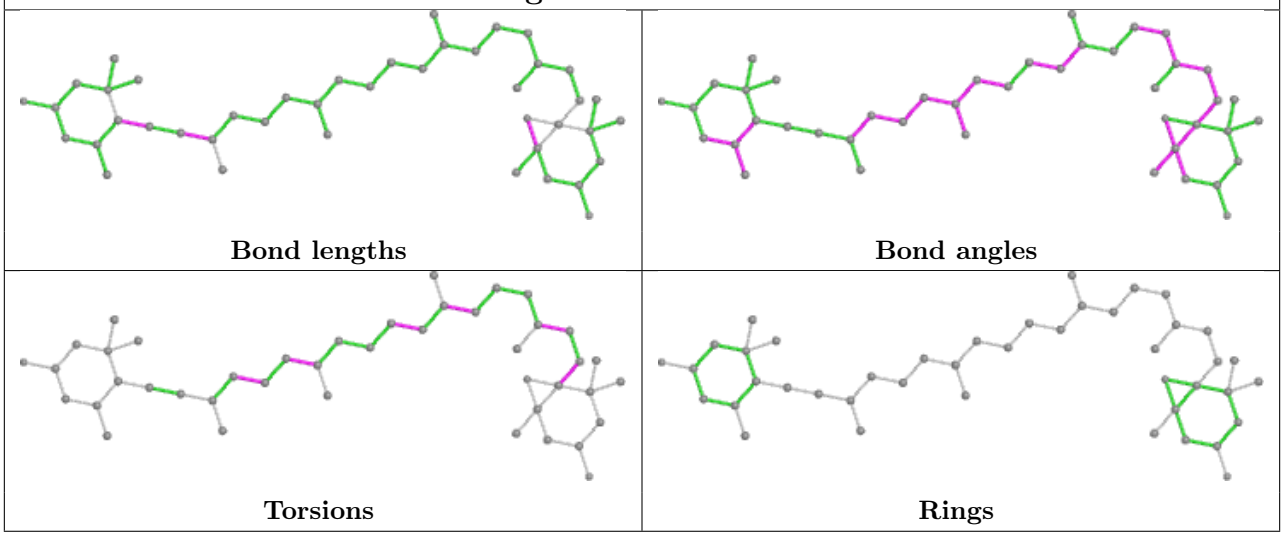


Torsions

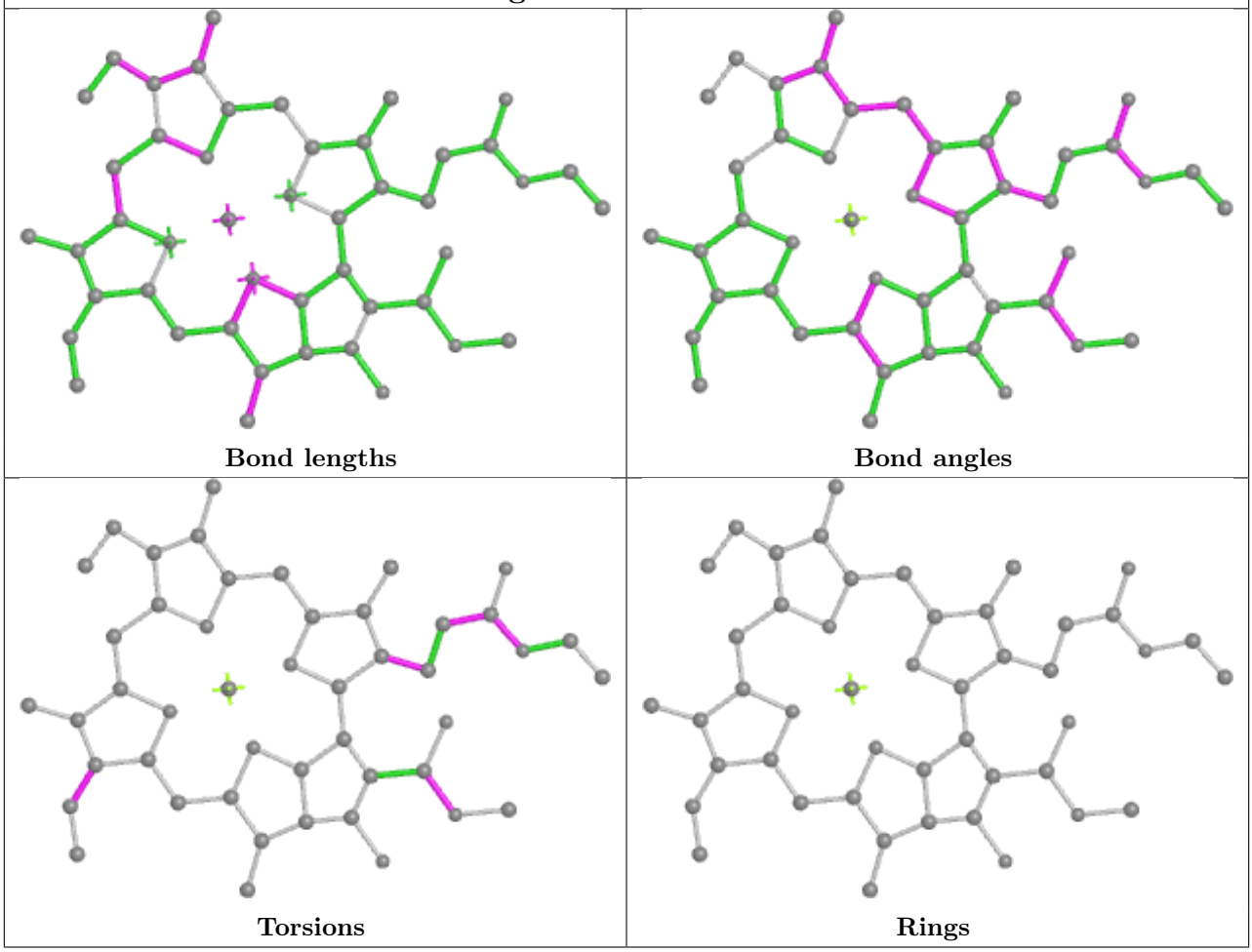


Rings

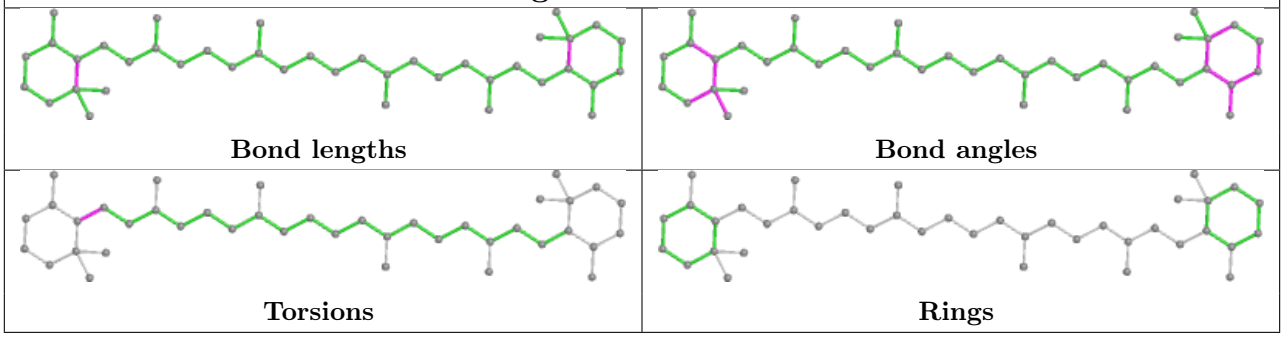
Ligand DD6 D 301



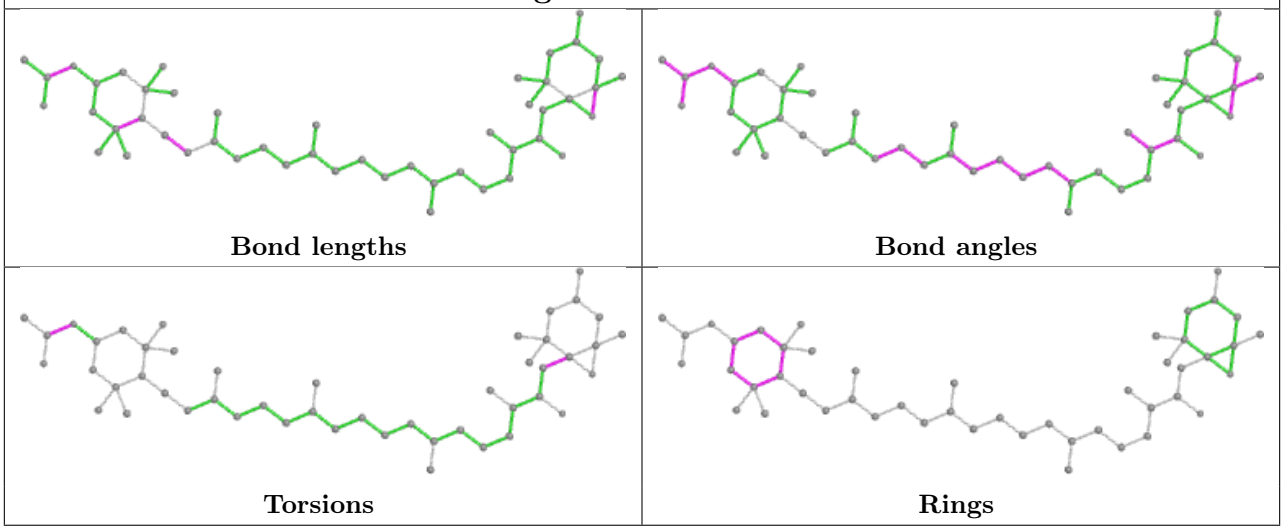
Ligand CLA M 312



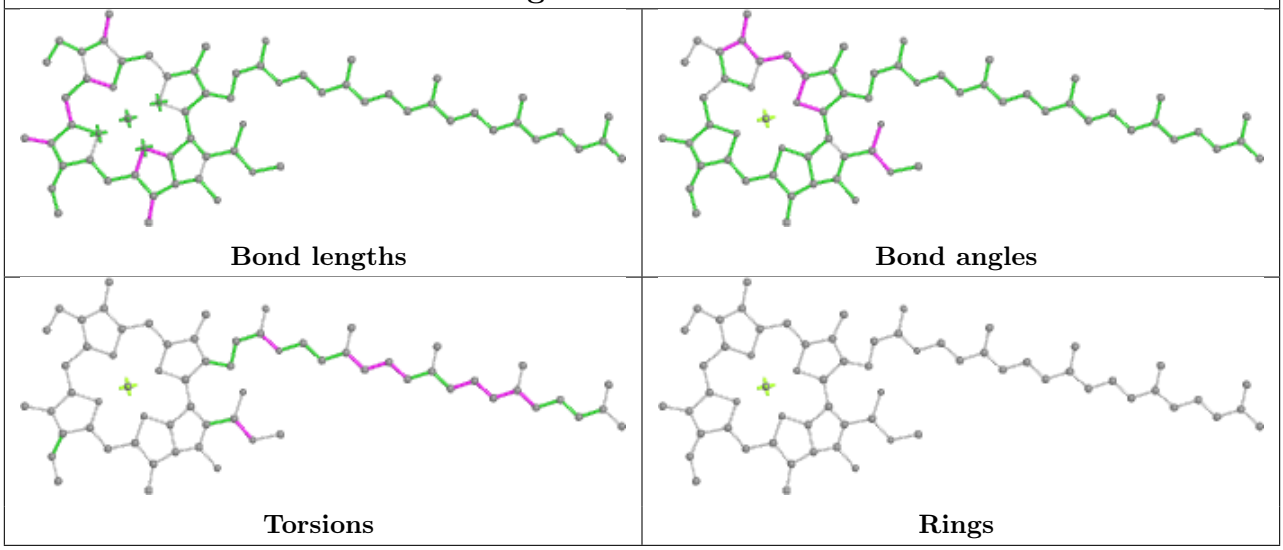
Ligand BCR i 101



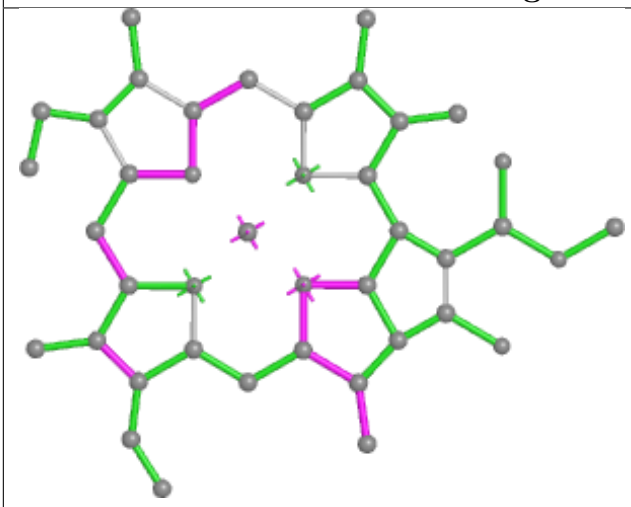
Ligand A86 h 202



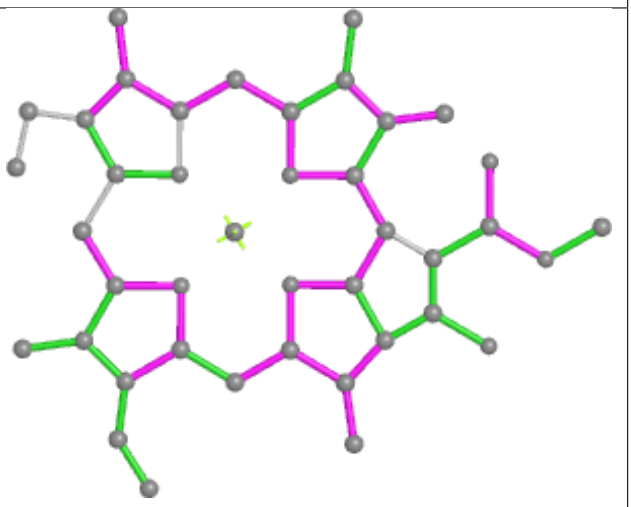
Ligand CLA L 320



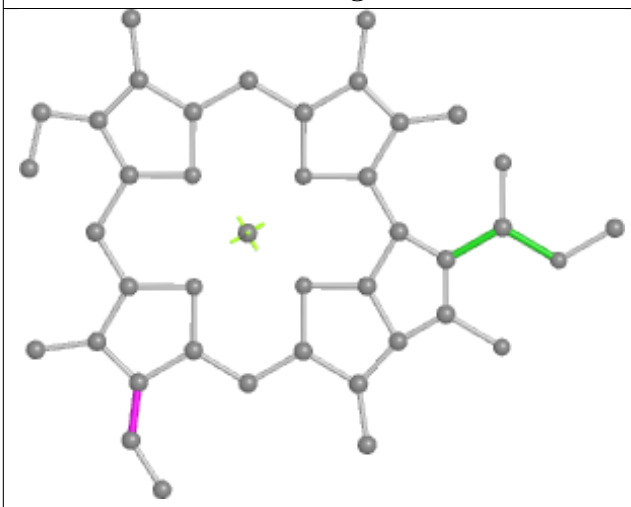
Ligand CLA N 310



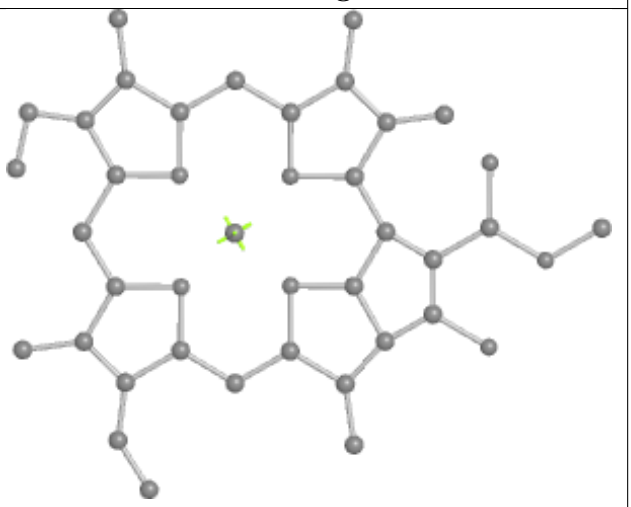
Bond lengths



Bond angles

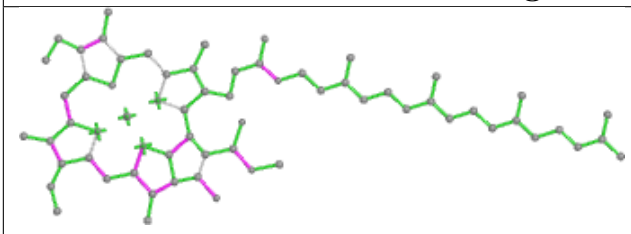


Torsions



Rings

Ligand CLA O 316



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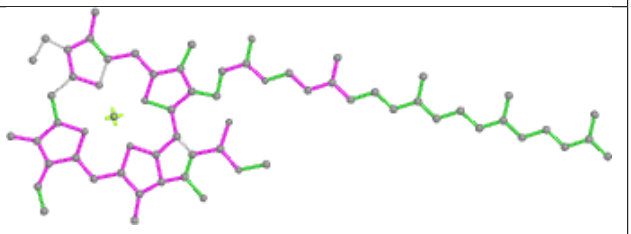
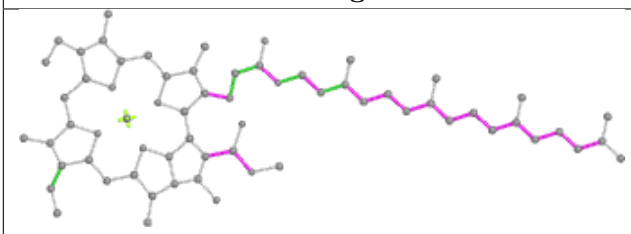


Bond angles



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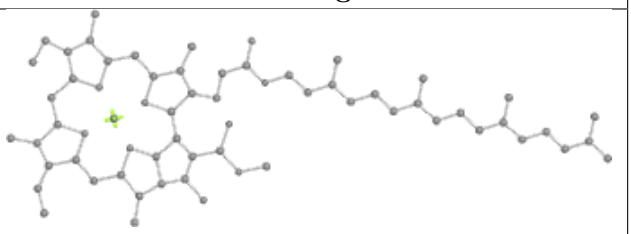
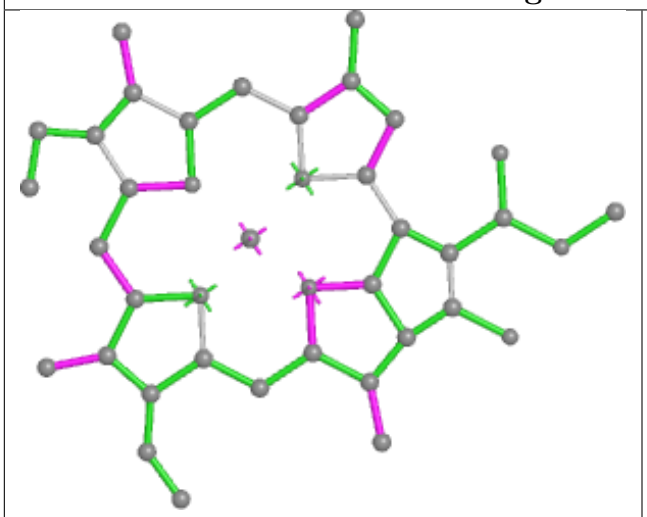


Rings

Ligand CLA O 312



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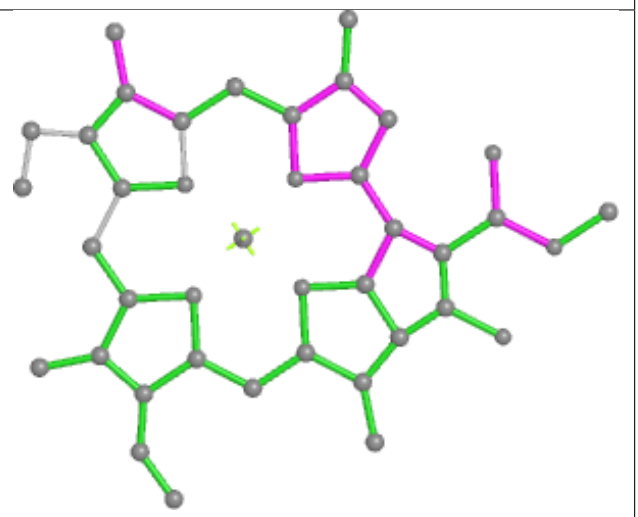
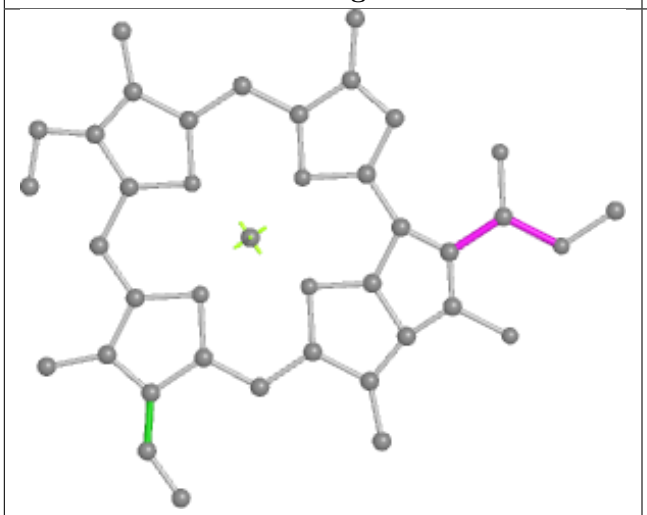


Bond angles



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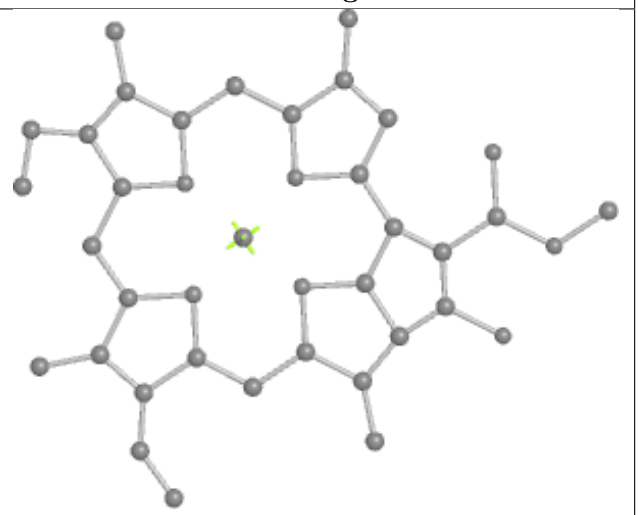
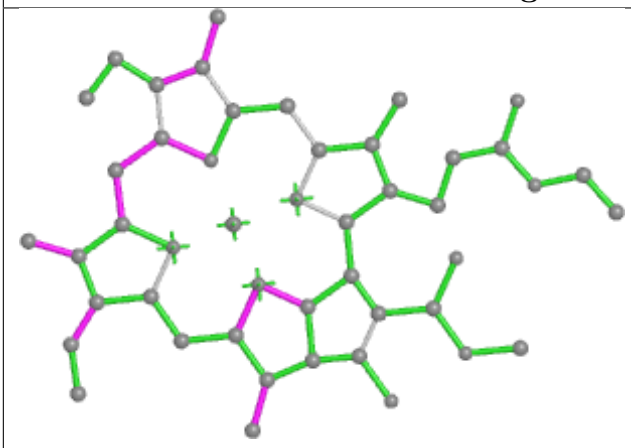
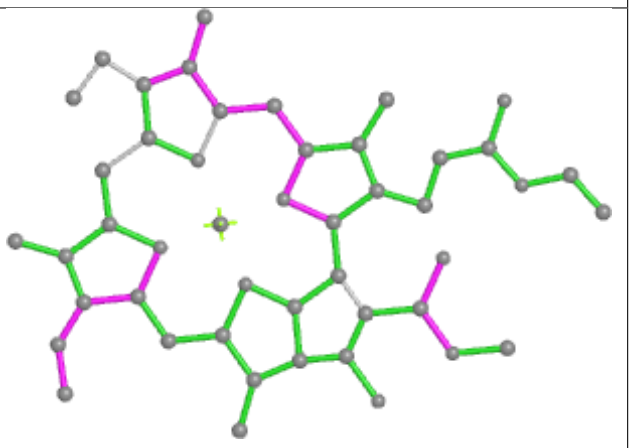
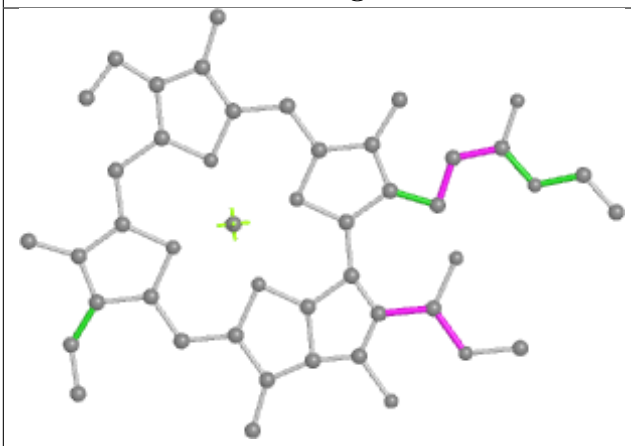
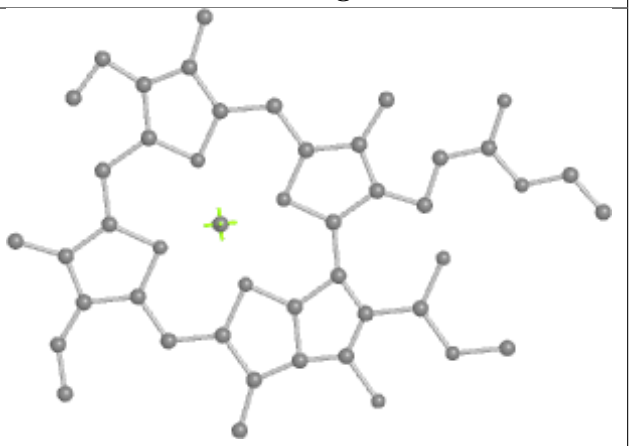
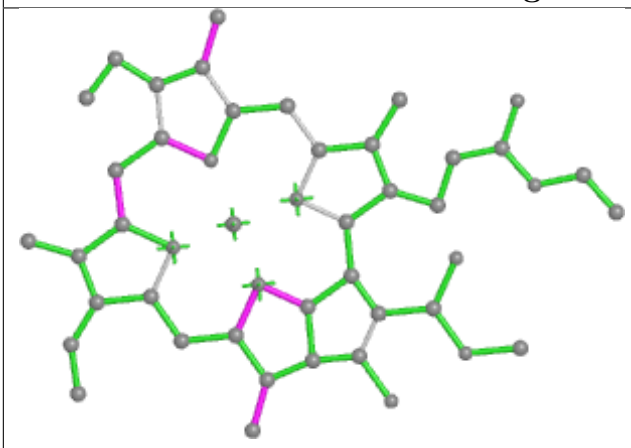
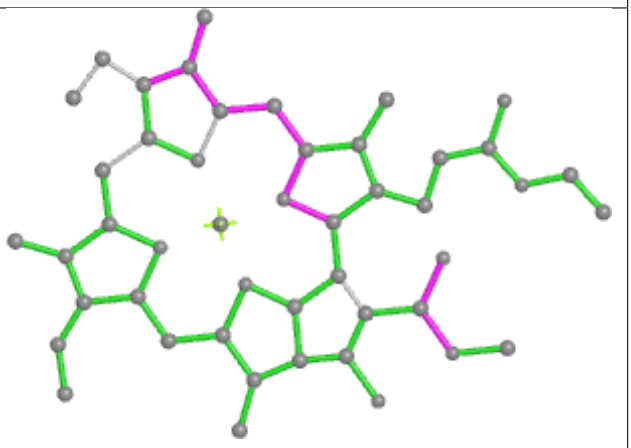
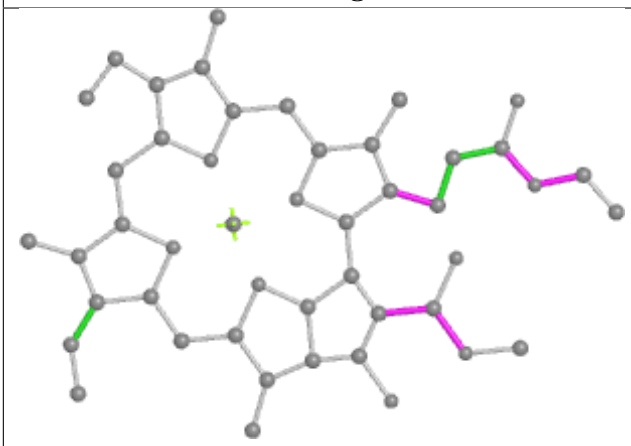
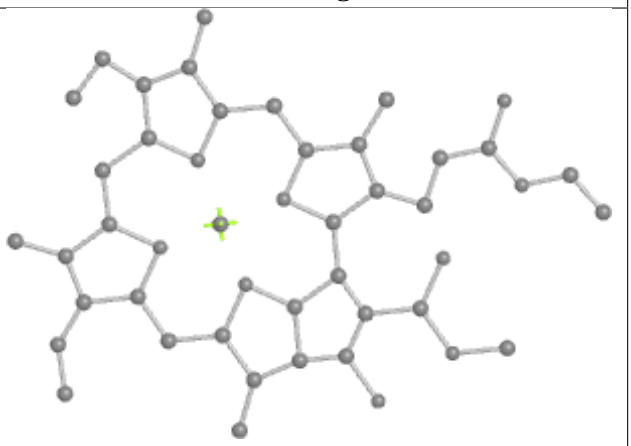
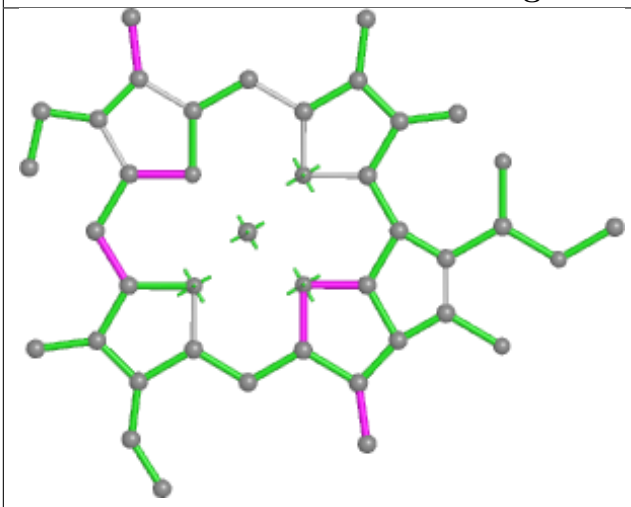


Rings

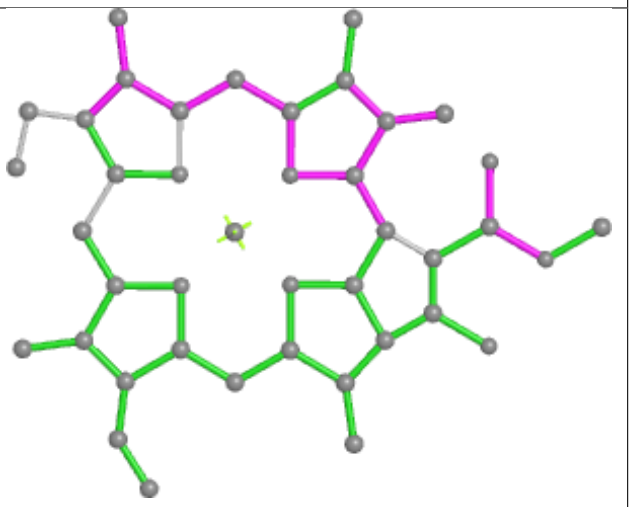
Ligand CLA M 315	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA N 312	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

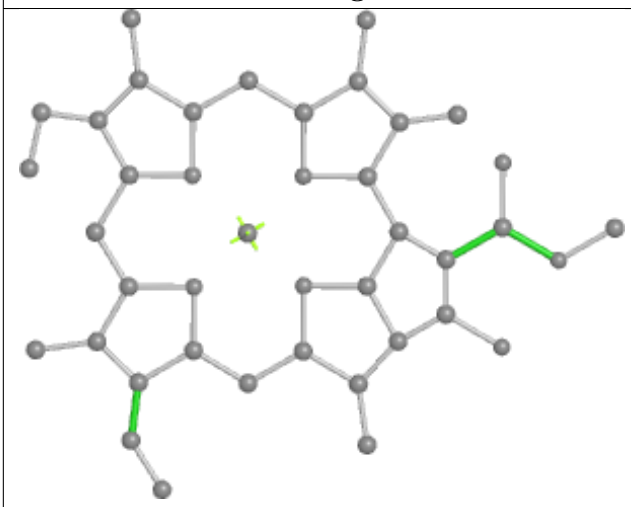
Ligand CLA N 315



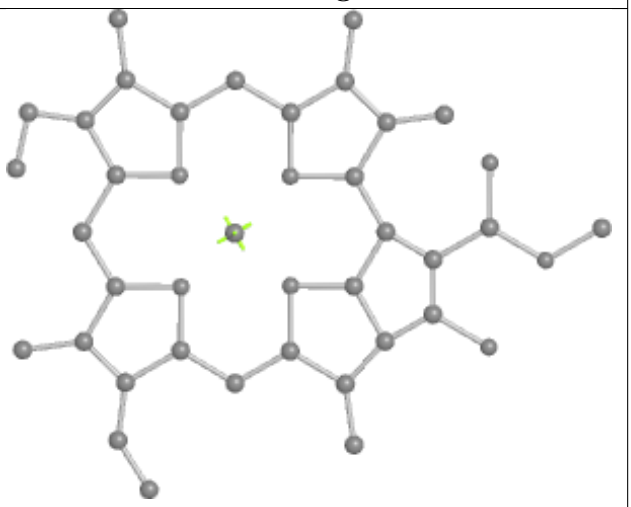
Bond lengths



Bond angles

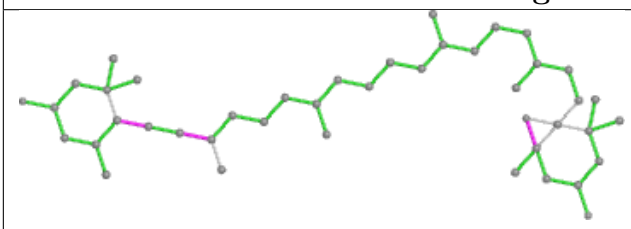


Torsions

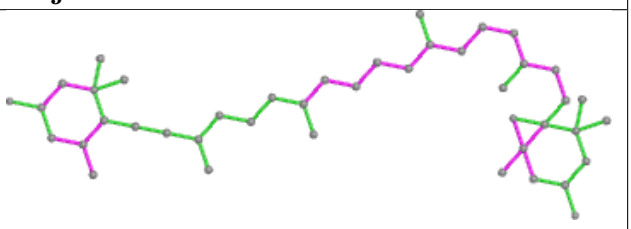


Rings

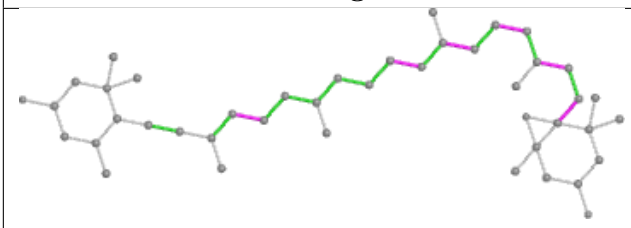
Ligand DD6 j 103



Bond lengths



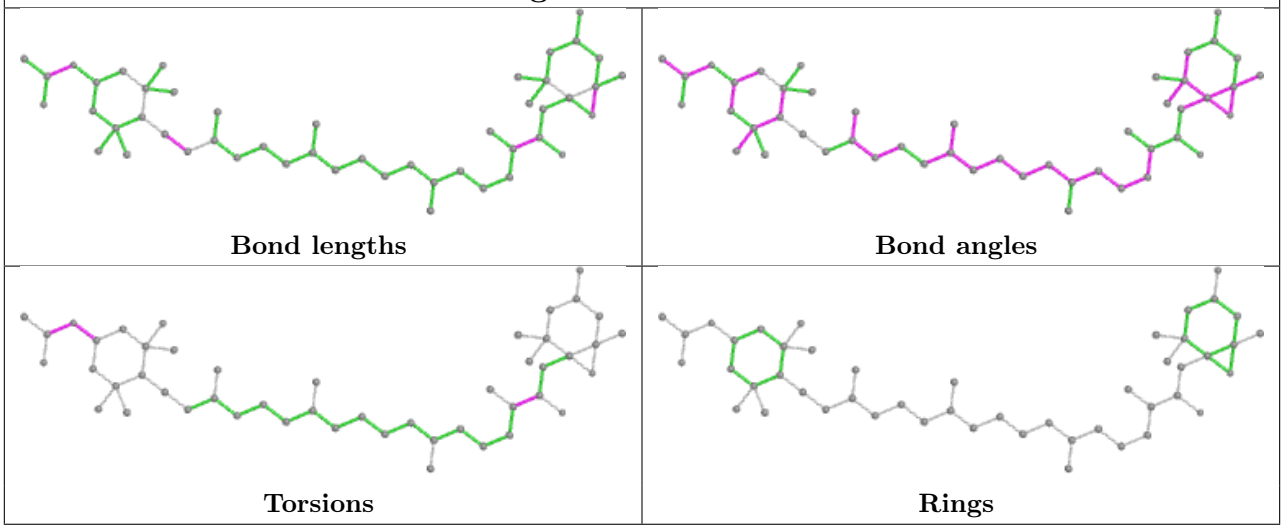
Bond angles



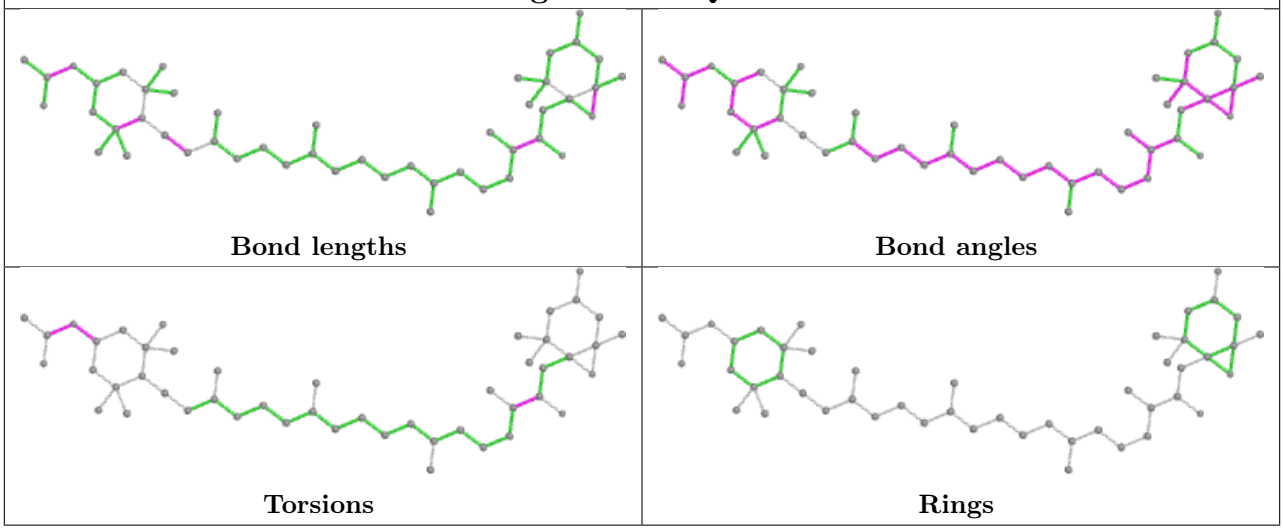
Torsions

Rings

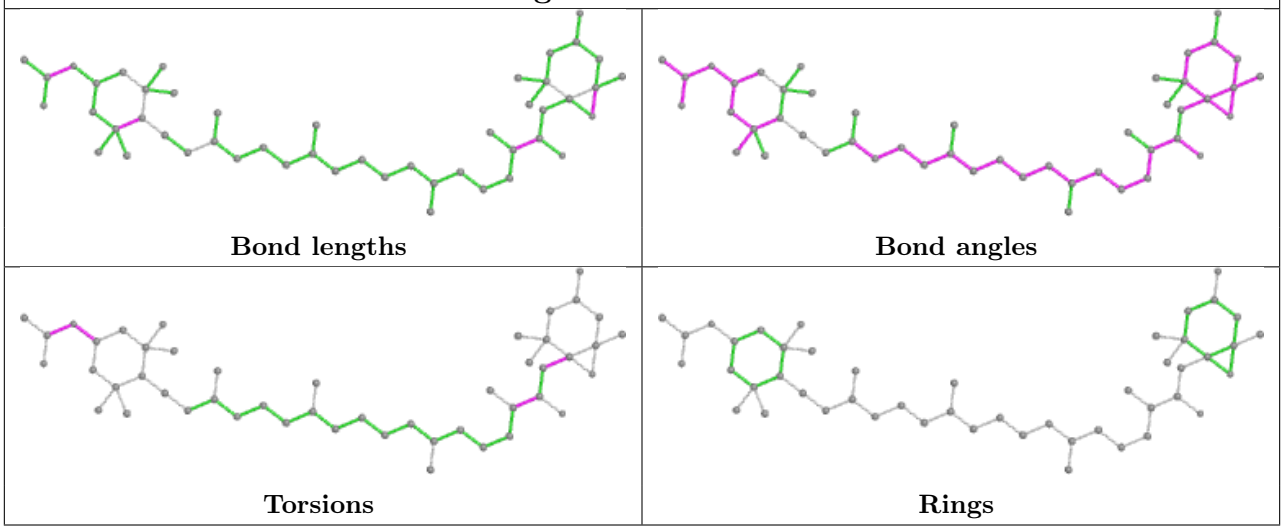
Ligand A86 K 303



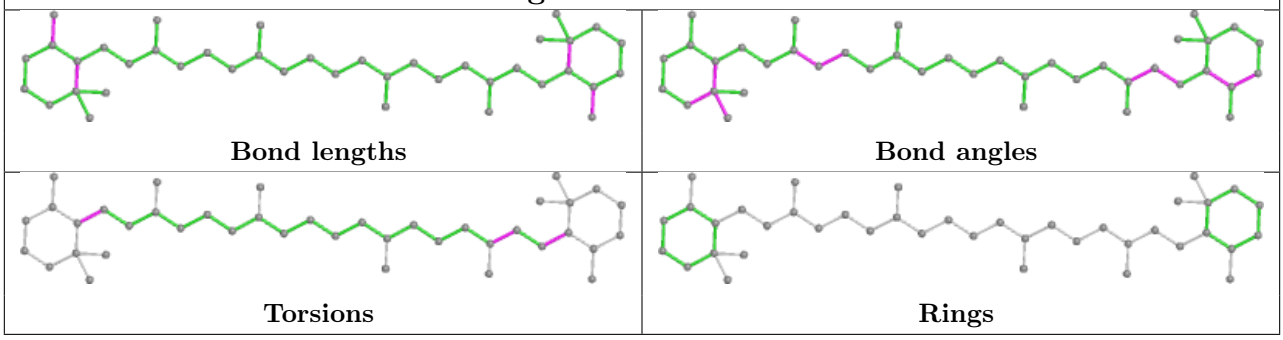
Ligand A86 Q 301



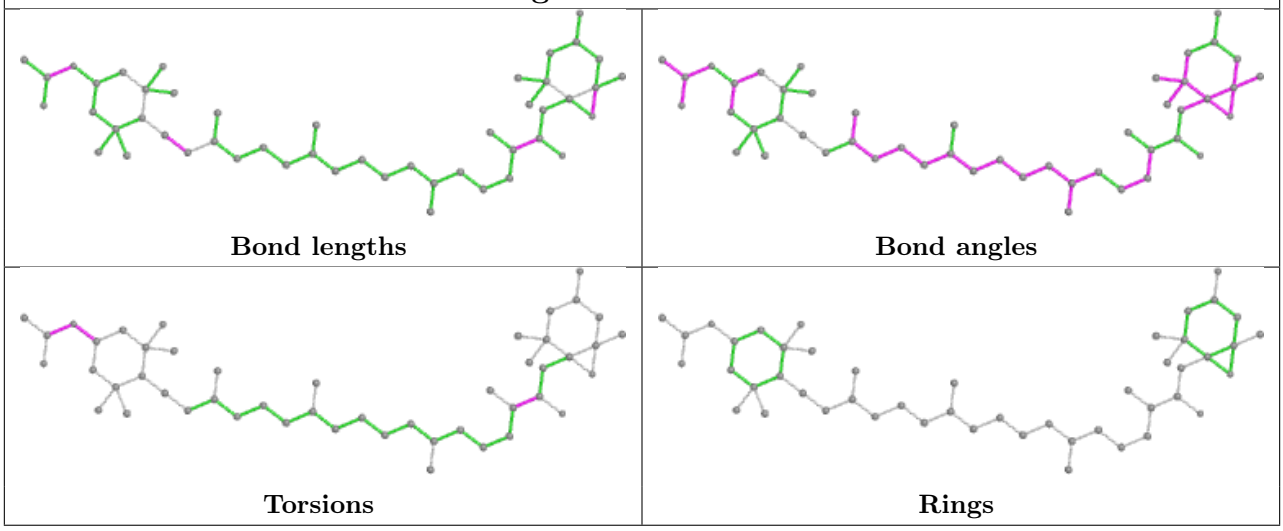
Ligand A86 S 301



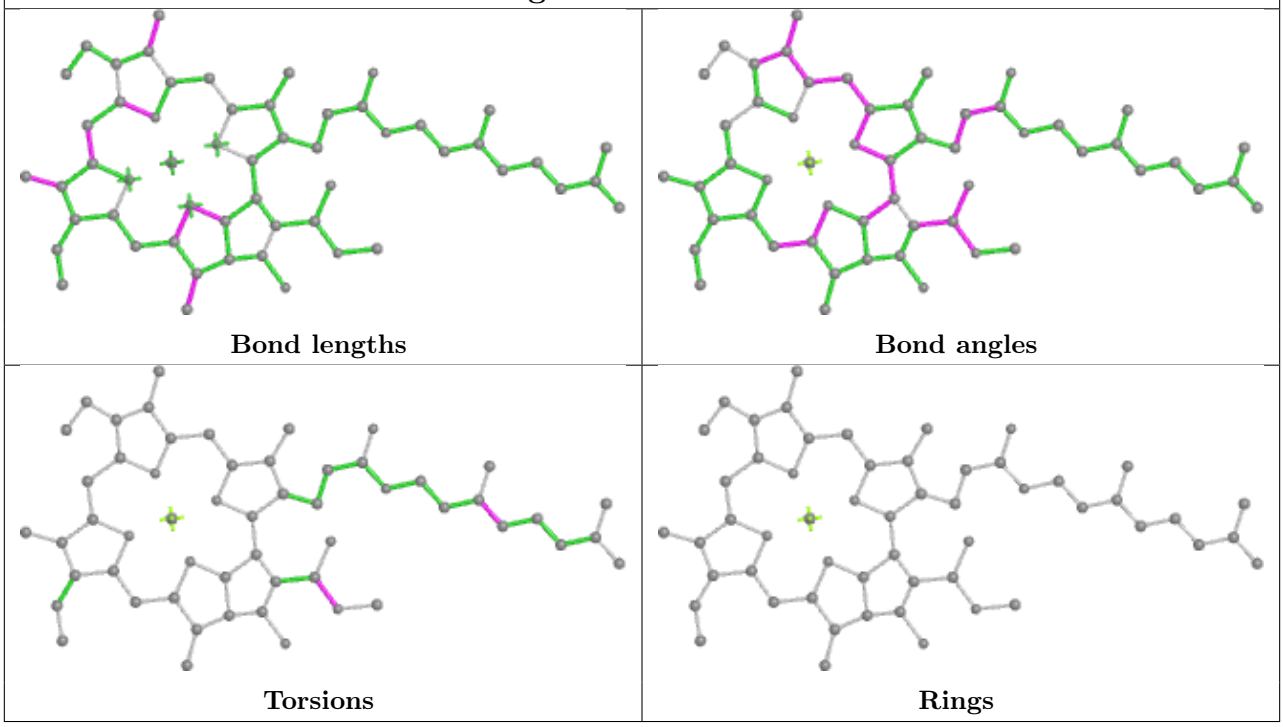
Ligand BCR a 847

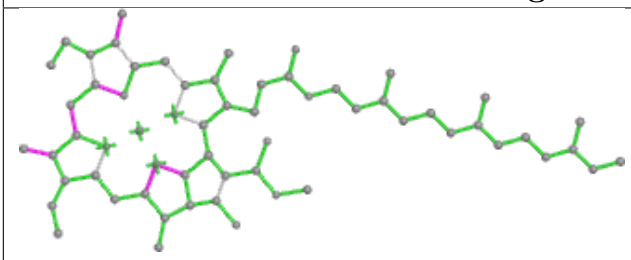
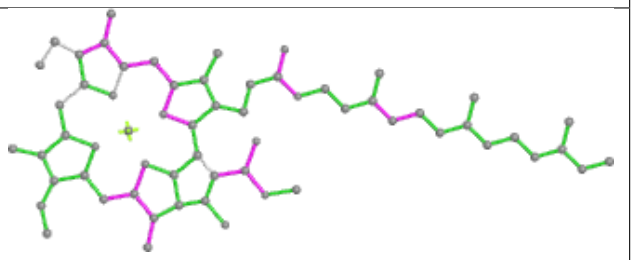
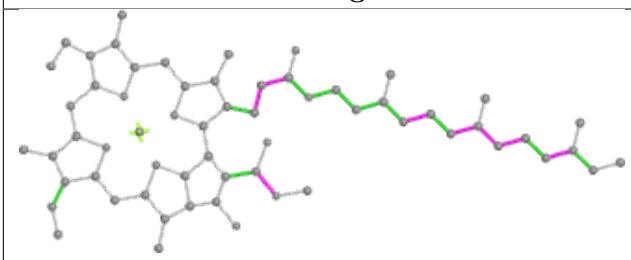
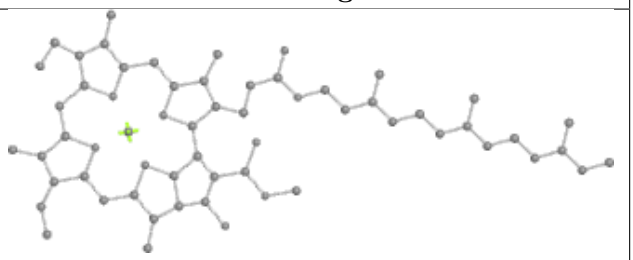


Ligand A86 T 306

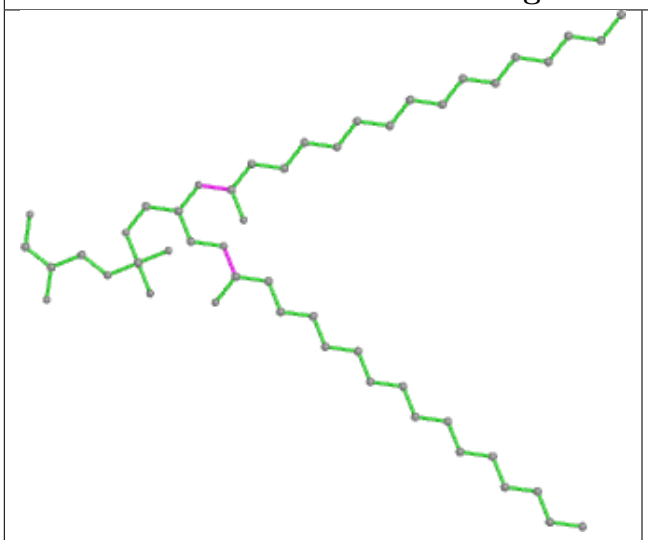


Ligand CLA b 818

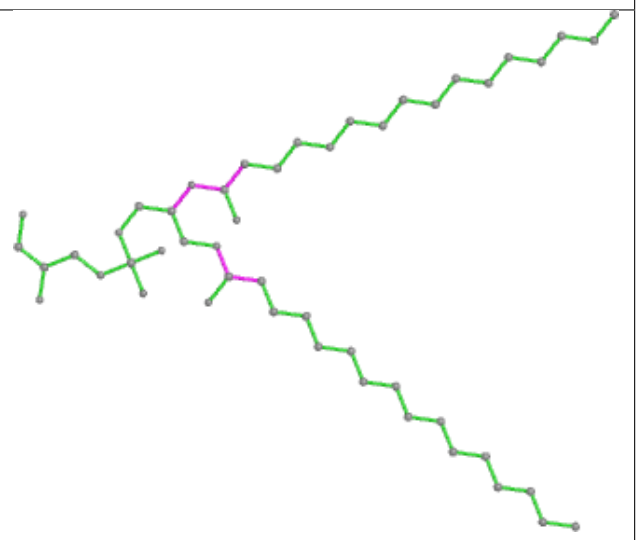


Ligand CLA J 308	
 Bond lengths	 Bond angles
 Torsions	 Rings

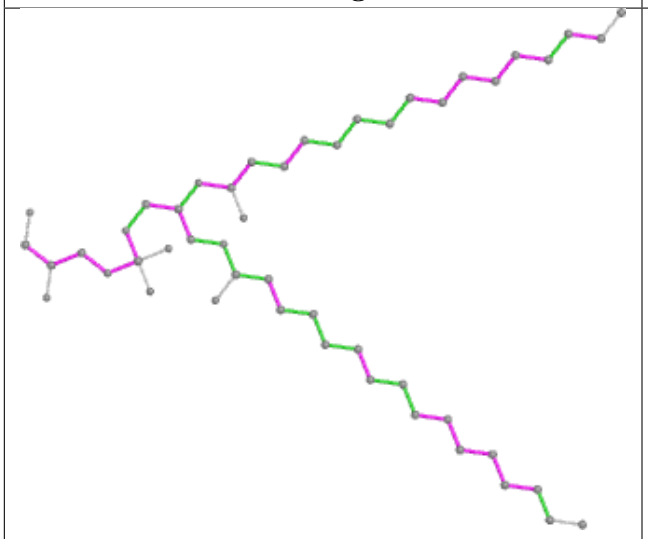
Ligand LHG R 323



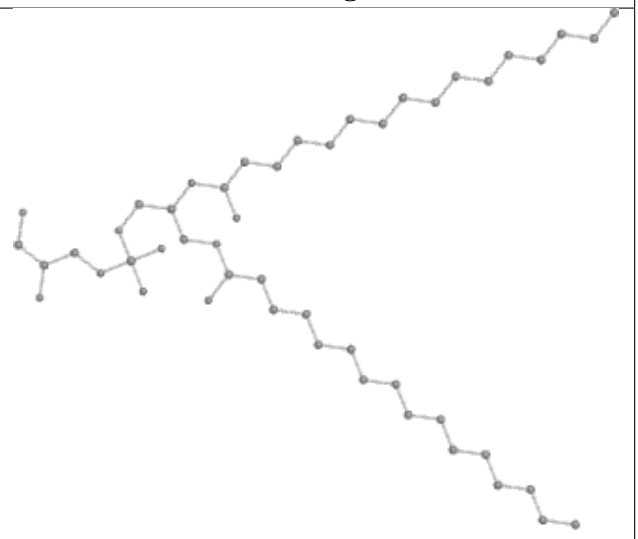
Bond lengths



Bond angles

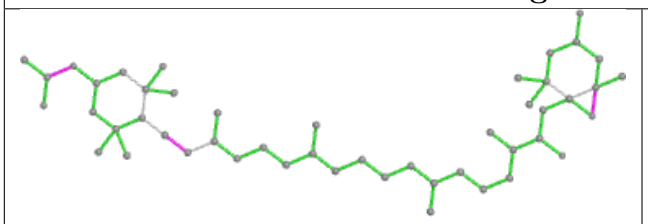


Torsions

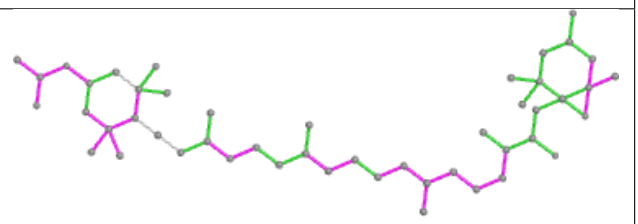


Rings

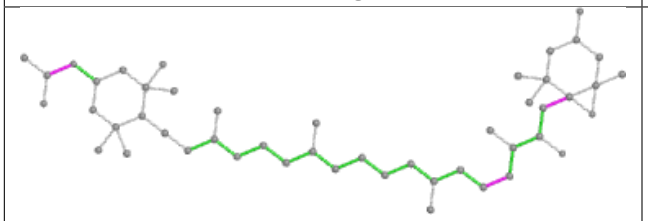
Ligand A86 G 305



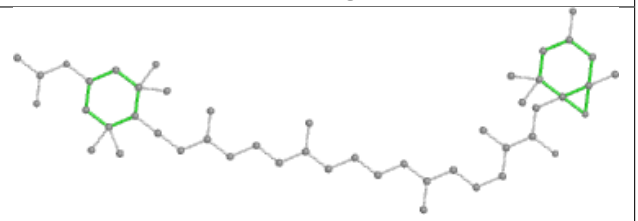
Bond lengths



Bond angles

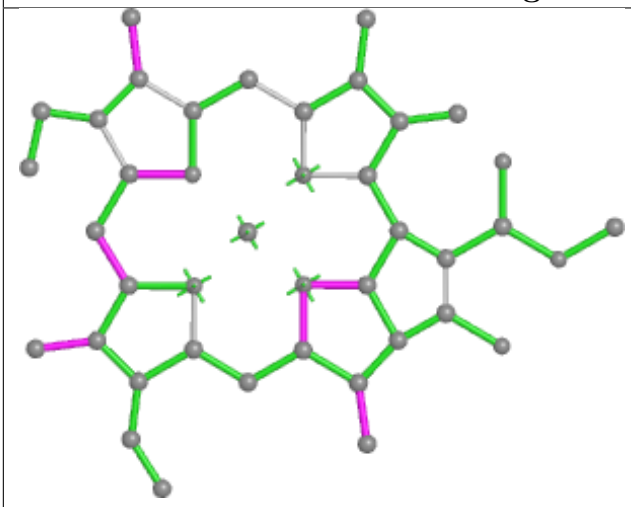


Torsions



Rings

Ligand CLA K 315



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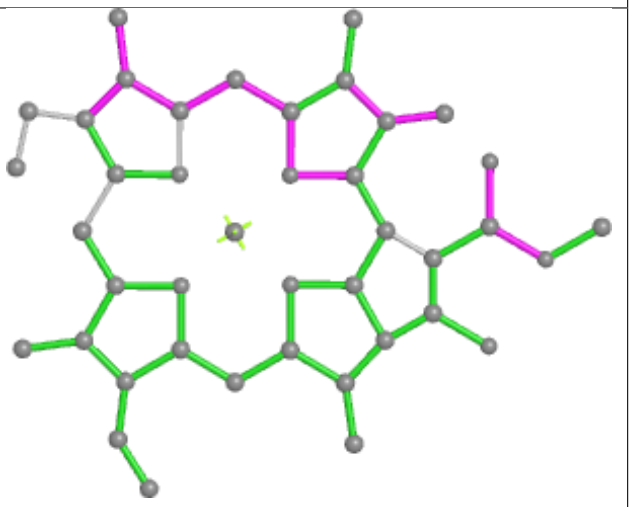

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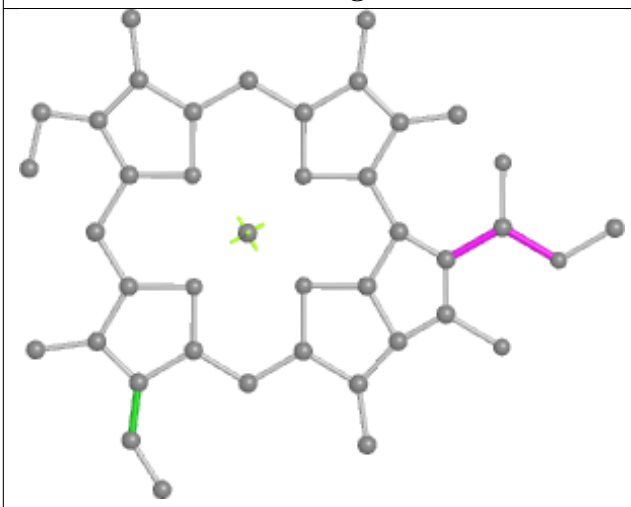

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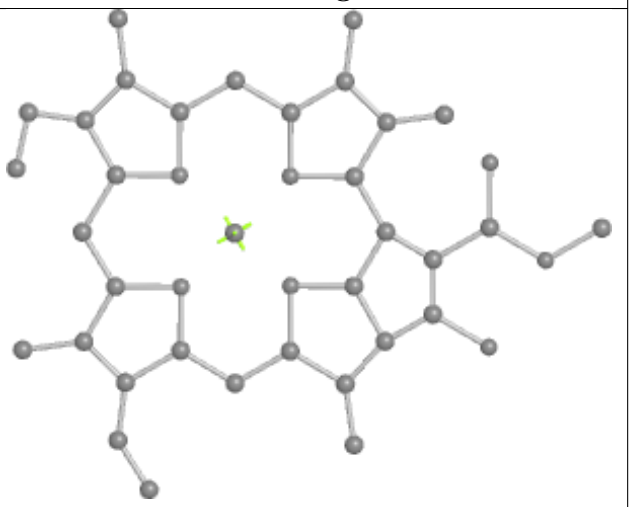
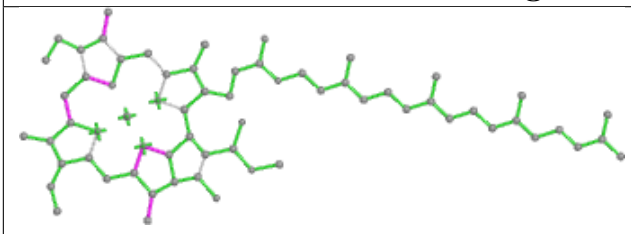


Rings

Ligand CLA T 313



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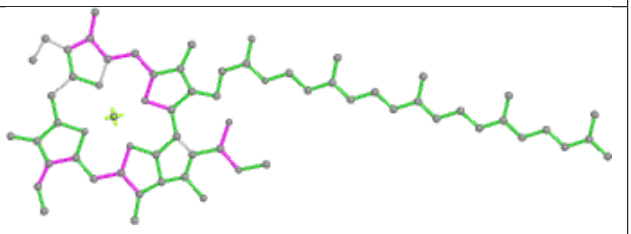

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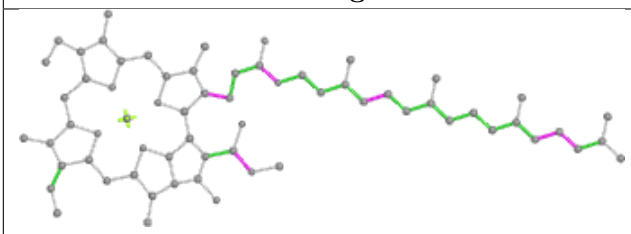

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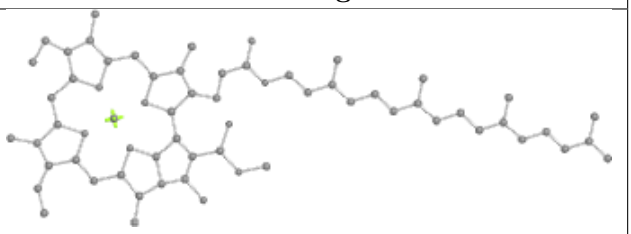
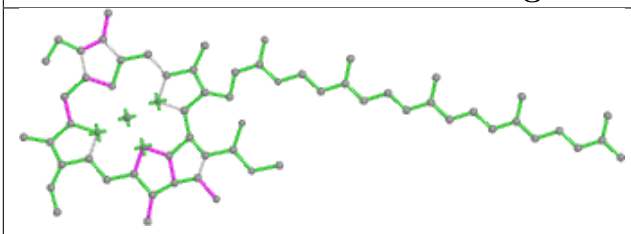


Rings

Ligand CLA A 314



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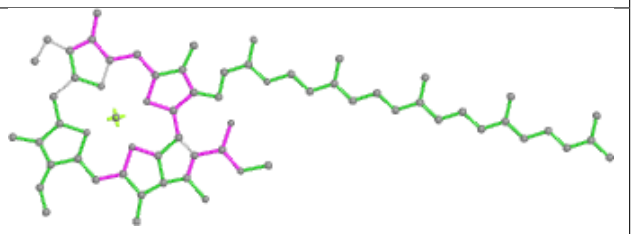
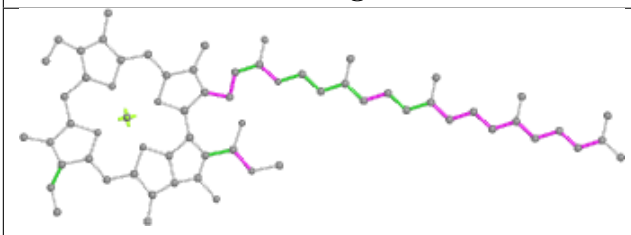


Bond angles



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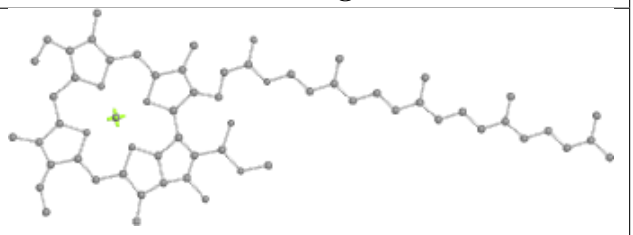
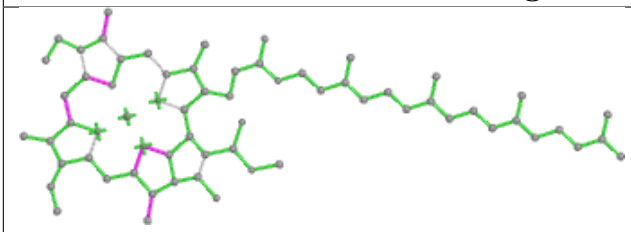


Rings

Ligand CLA R 311



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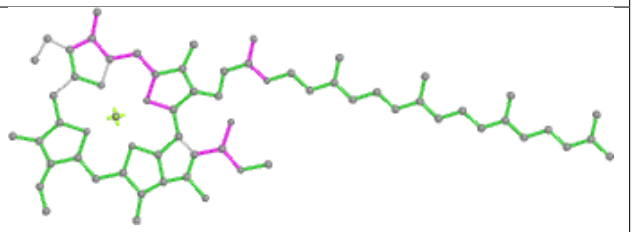
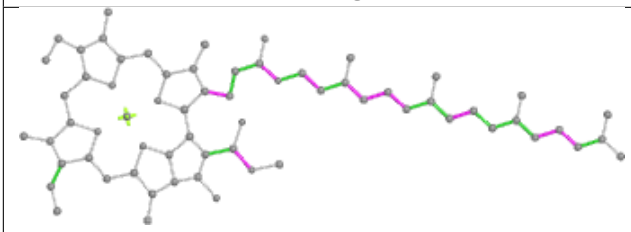


Bond angles



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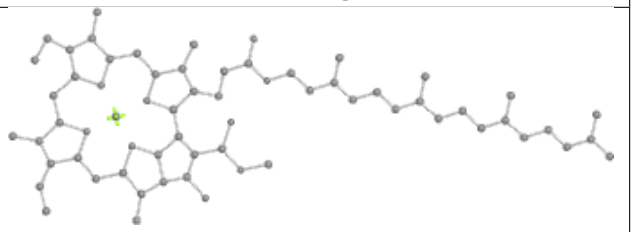
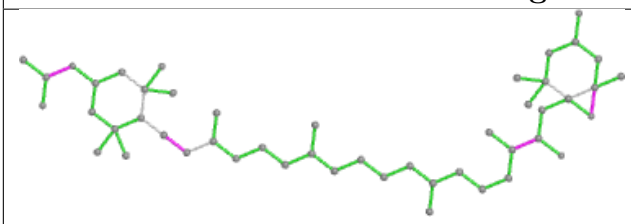


Rings

Ligand A86 X 305



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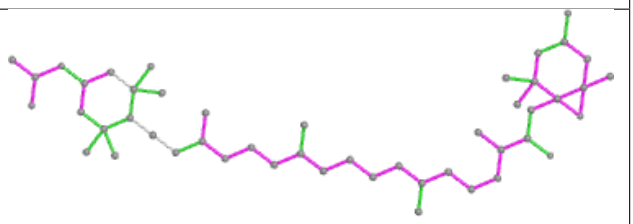
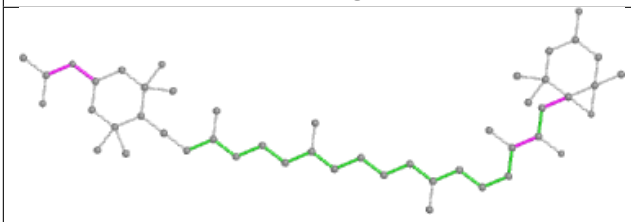


Bond angles



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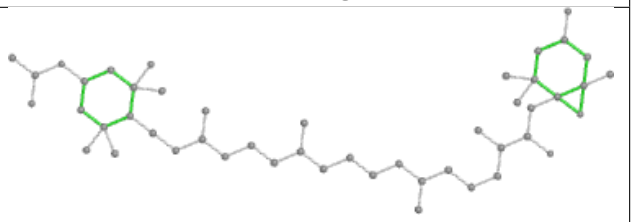
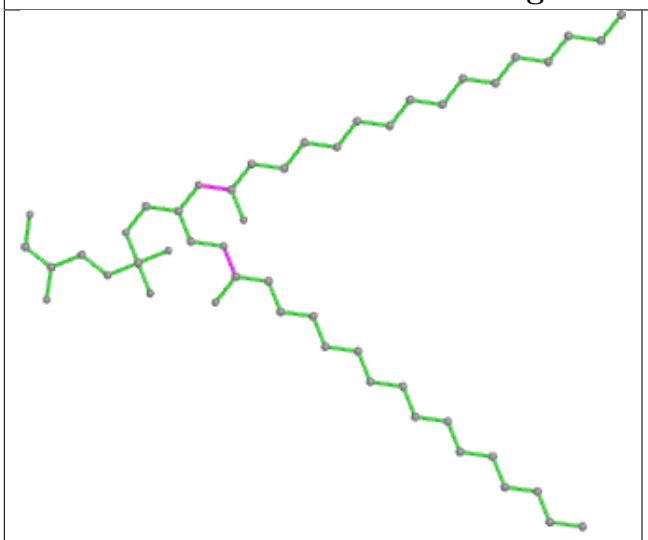


Rings

Ligand LHG b 850



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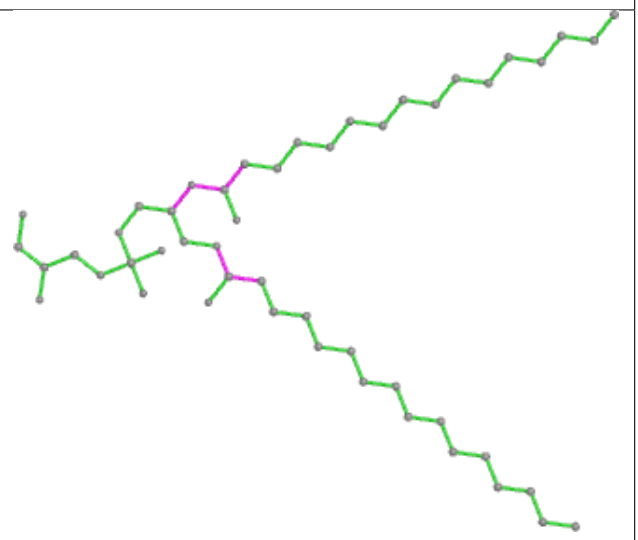
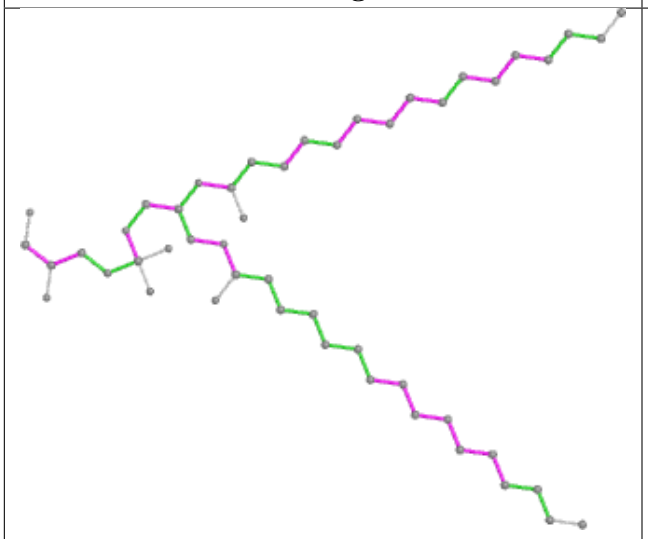


Bond angles



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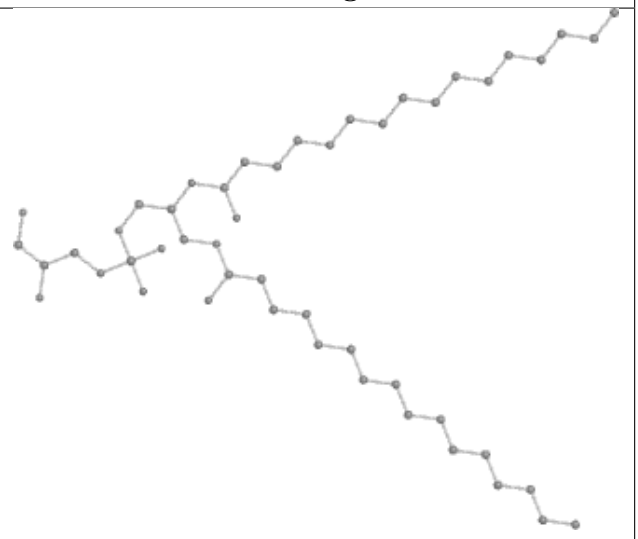
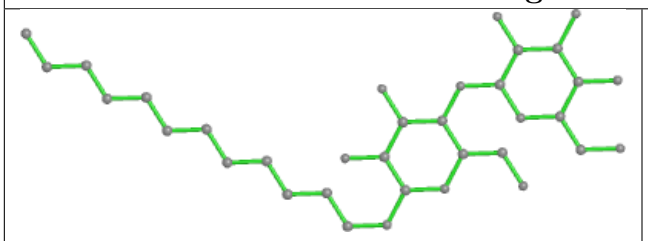


Rings

Ligand LMT b 848



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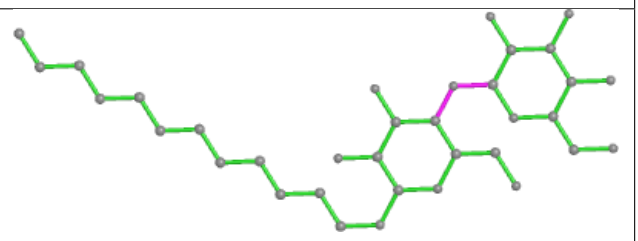
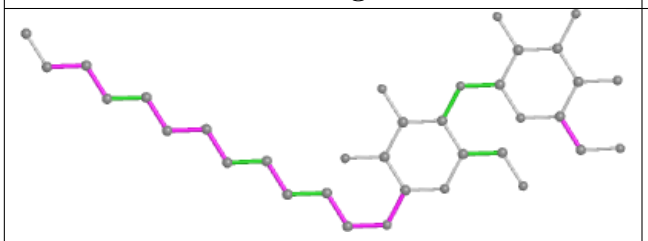


Bond angles



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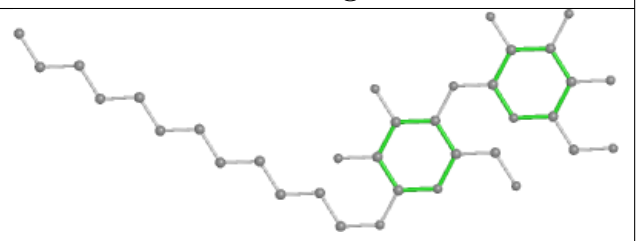
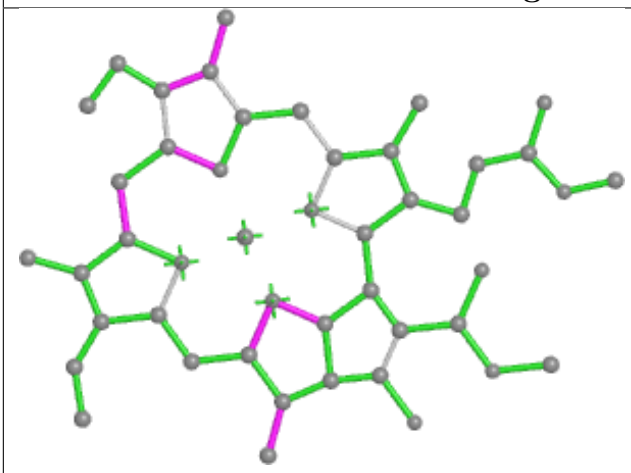


Rings

Ligand CLA U 309



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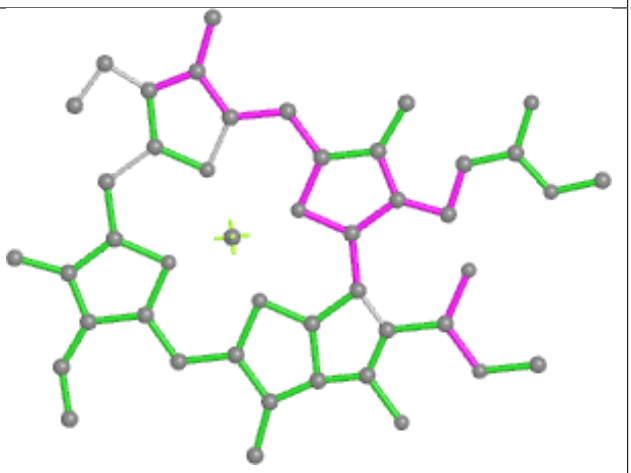
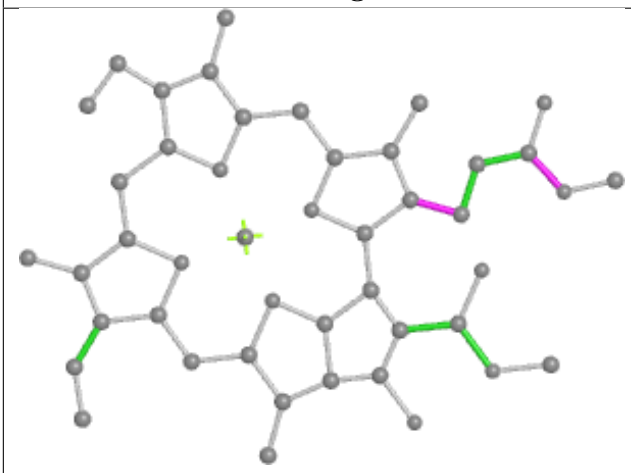


Bond angles



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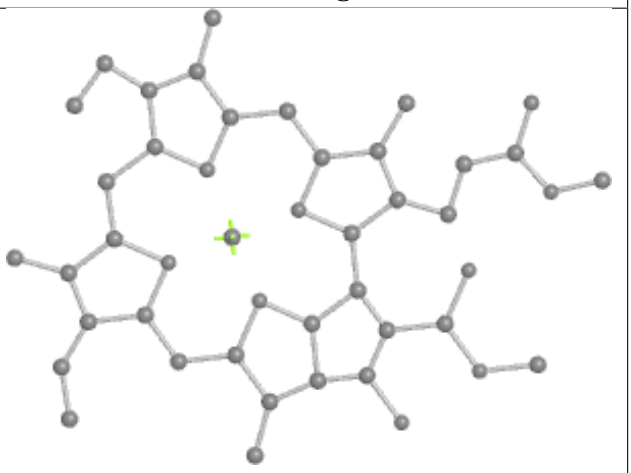
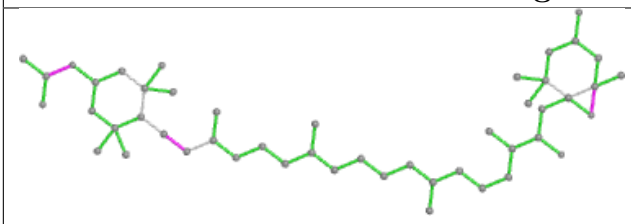


Rings

Ligand A86 J 305



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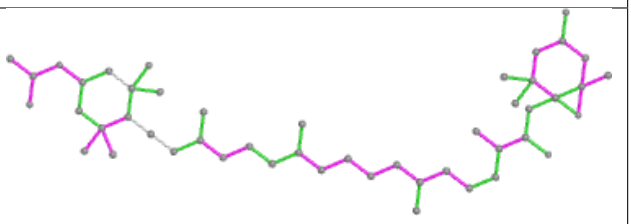
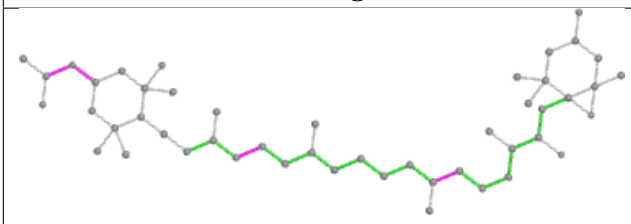


Bond angles



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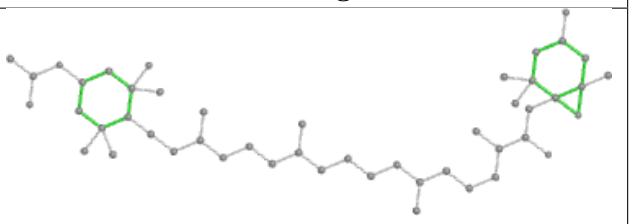
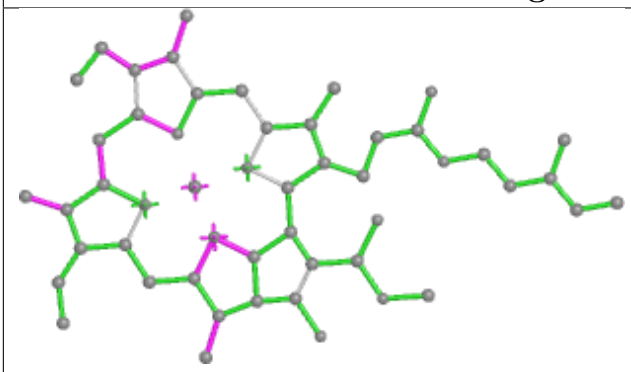


Rings

Ligand CLA a 835



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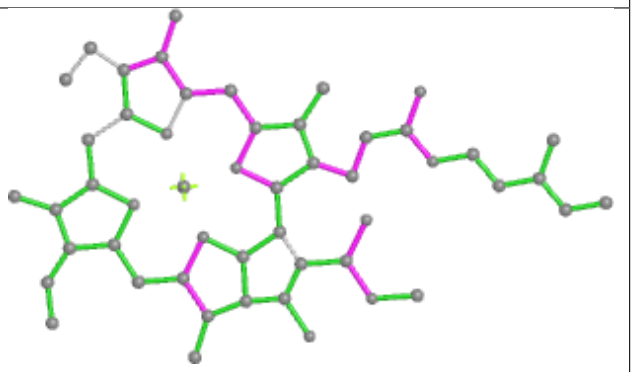
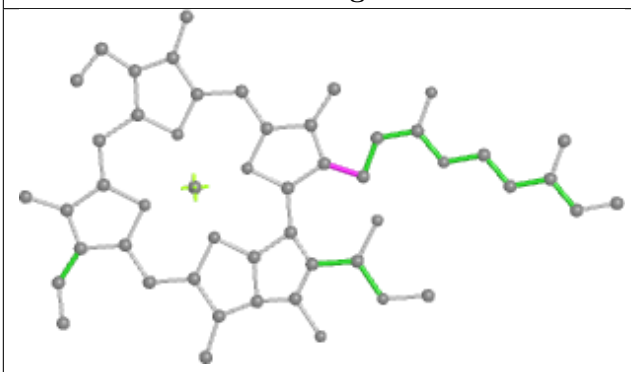


Bond angles



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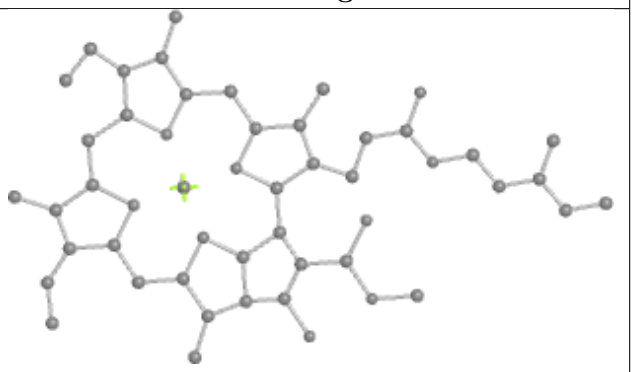
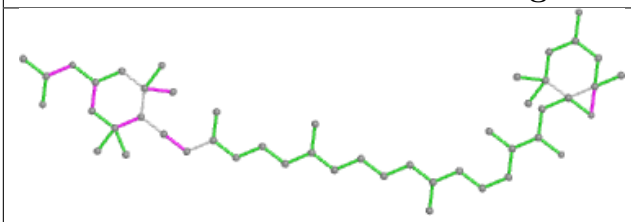


Rings

Ligand A86 Q 304



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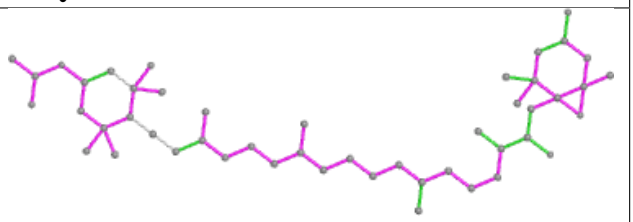
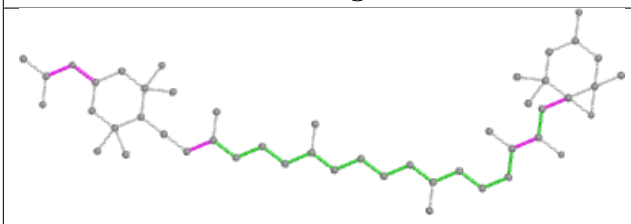
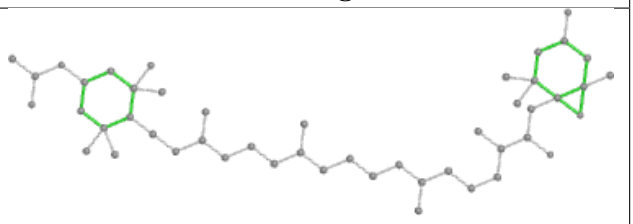


Bond angles

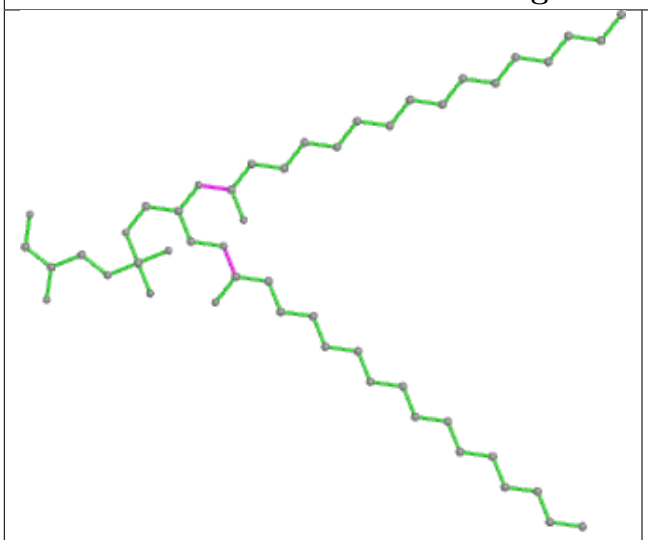


Torsions

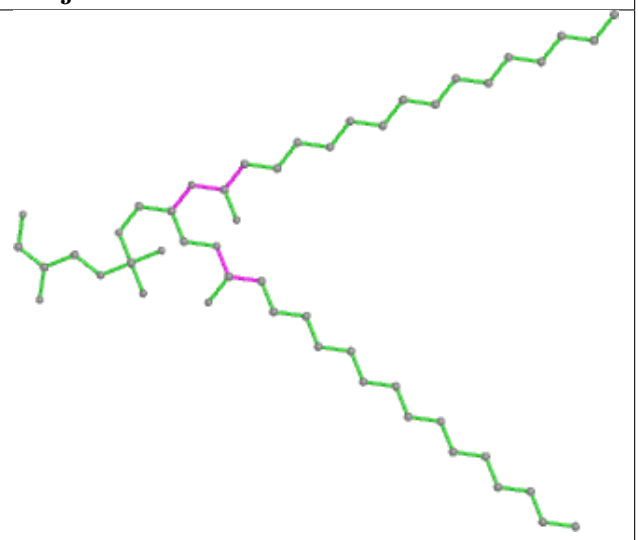


Rings

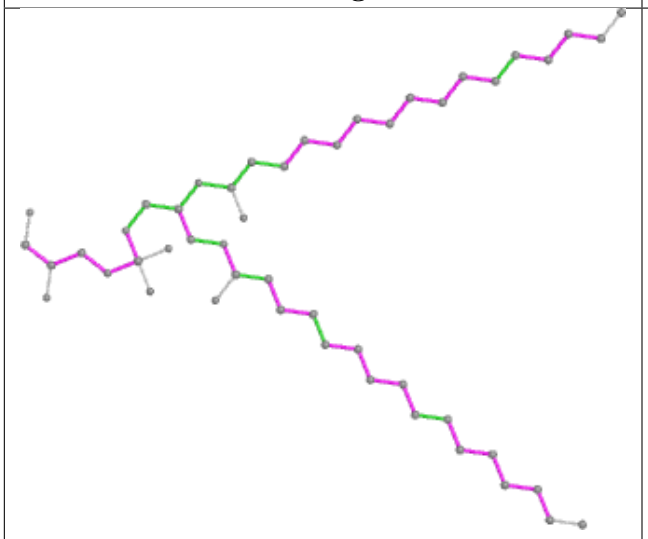
Ligand LHG j 104



Bond lengths



Bond angles



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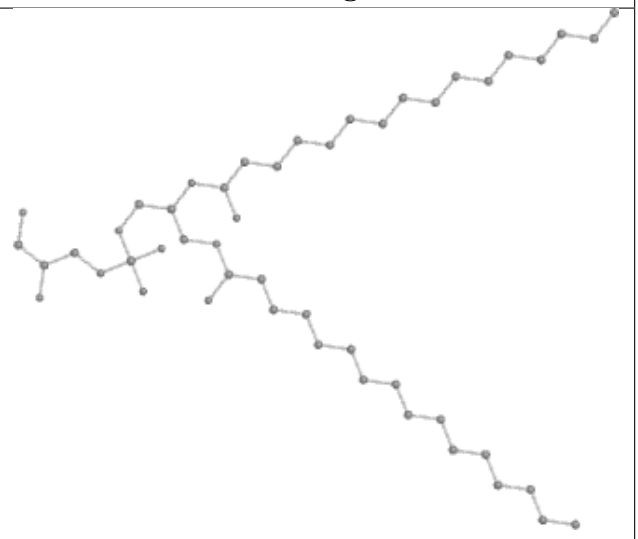
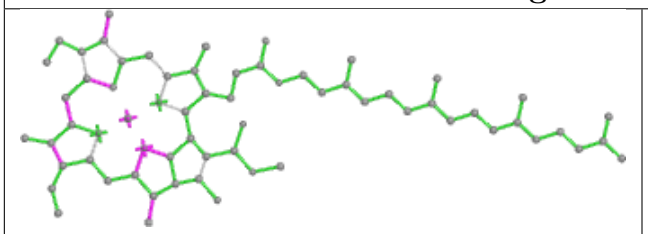


Rings

Ligand CLA a 824



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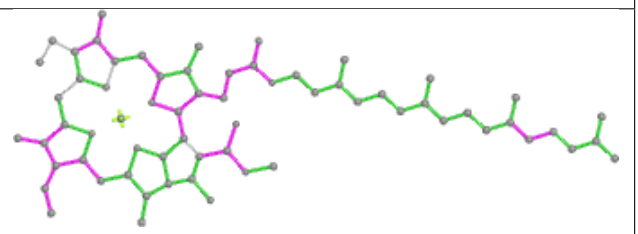
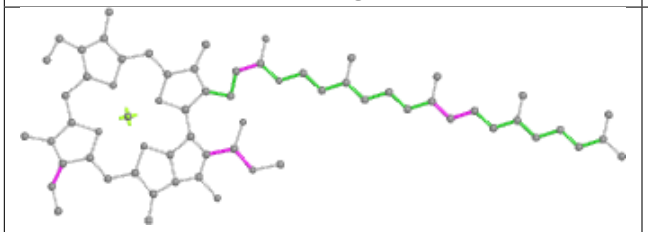


Bond angles



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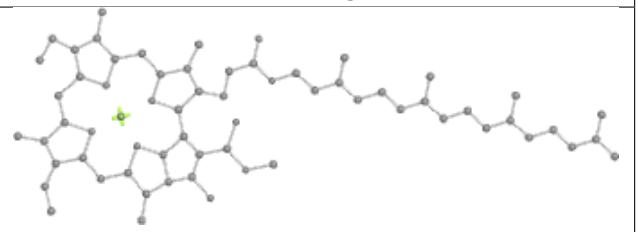
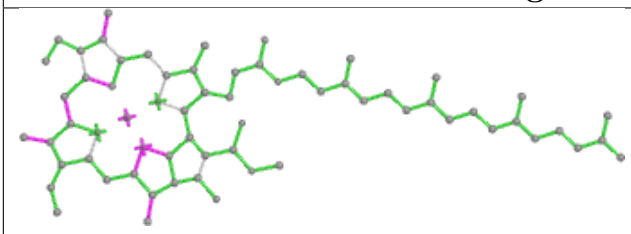
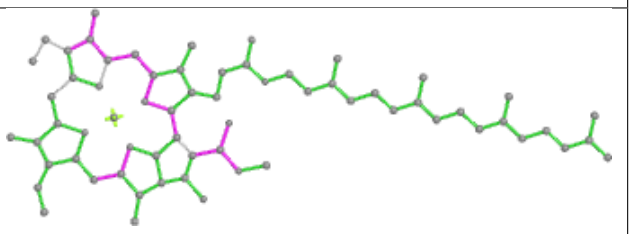


Rings

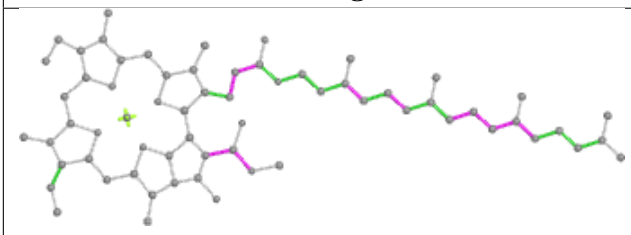
Ligand CLA L 311



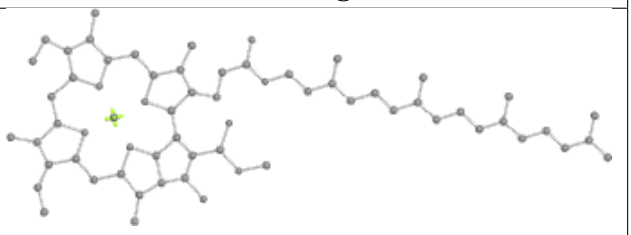
Bond lengths



Bond angles

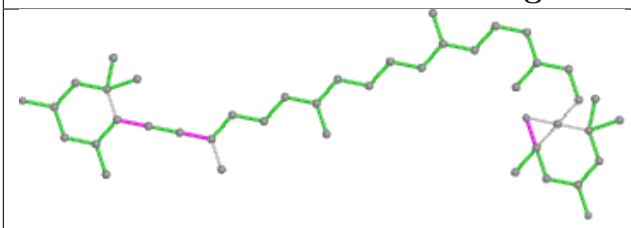


Torsions

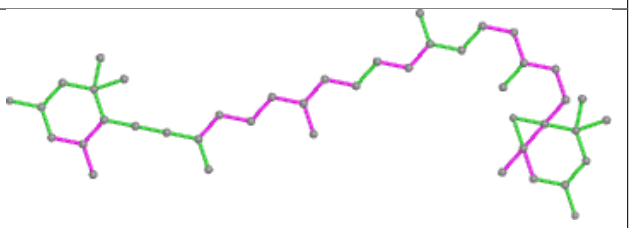


Rings

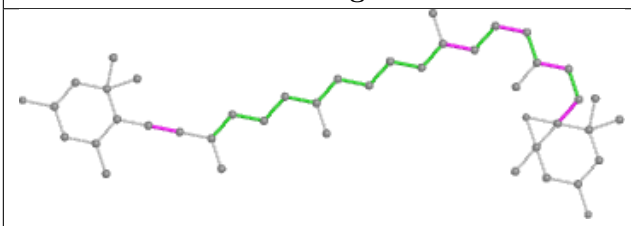
Ligand DD6 D 304



Bond lengths



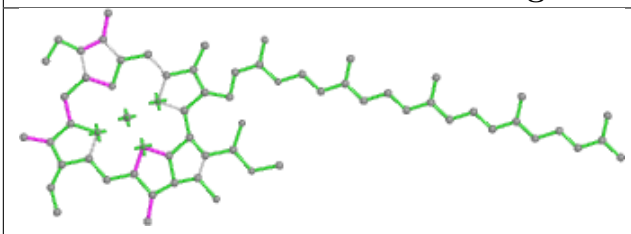
Bond angles



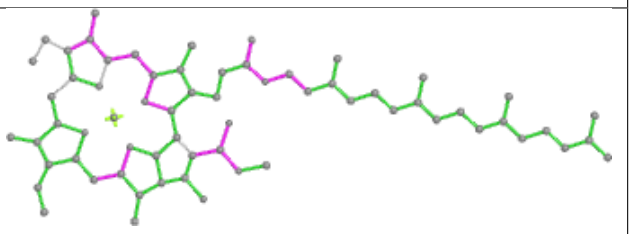
Torsions

Rings

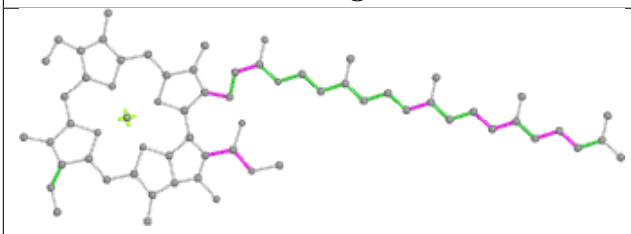
Ligand CLA b 808



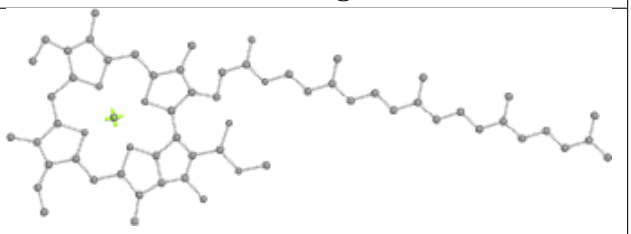
Bond lengths



Bond angles

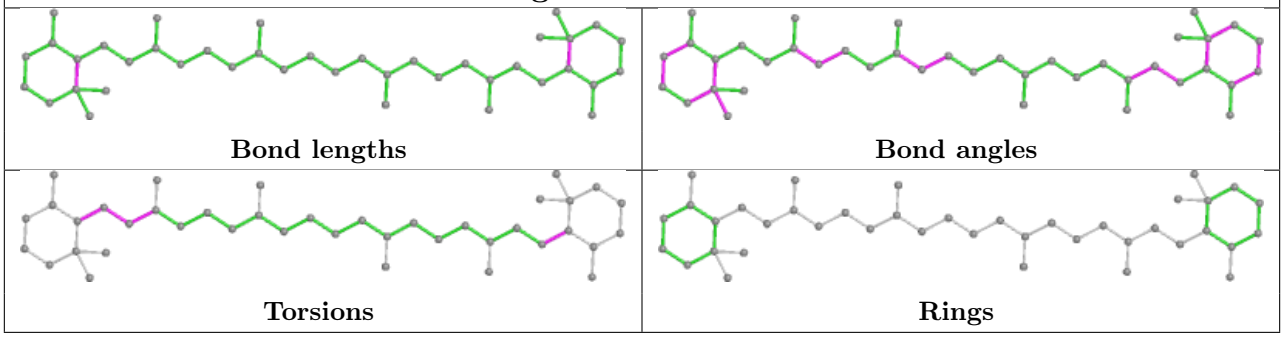


Torsions

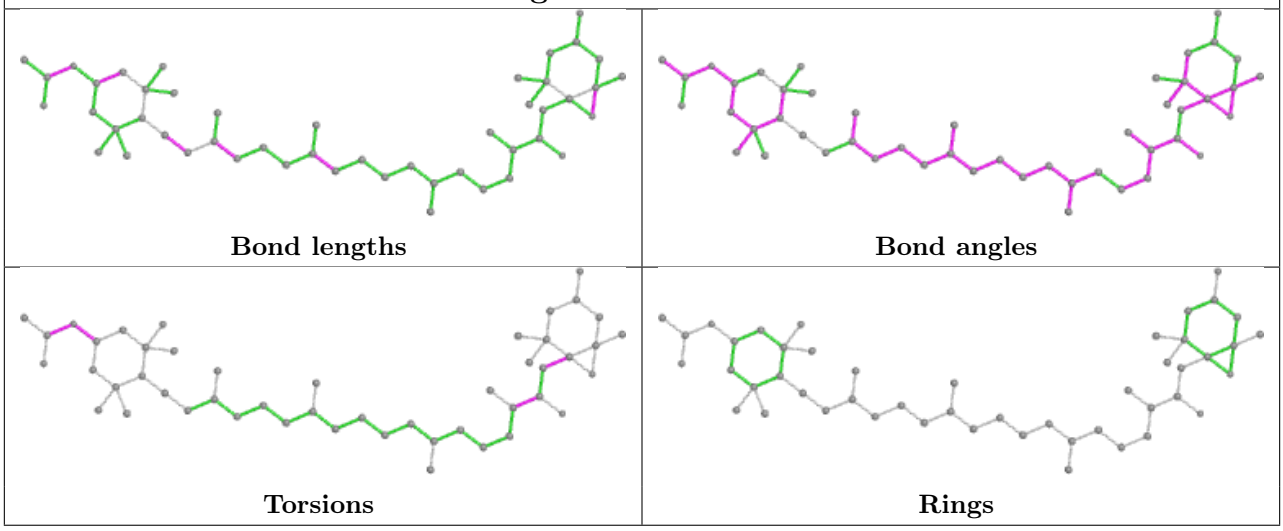


Rings

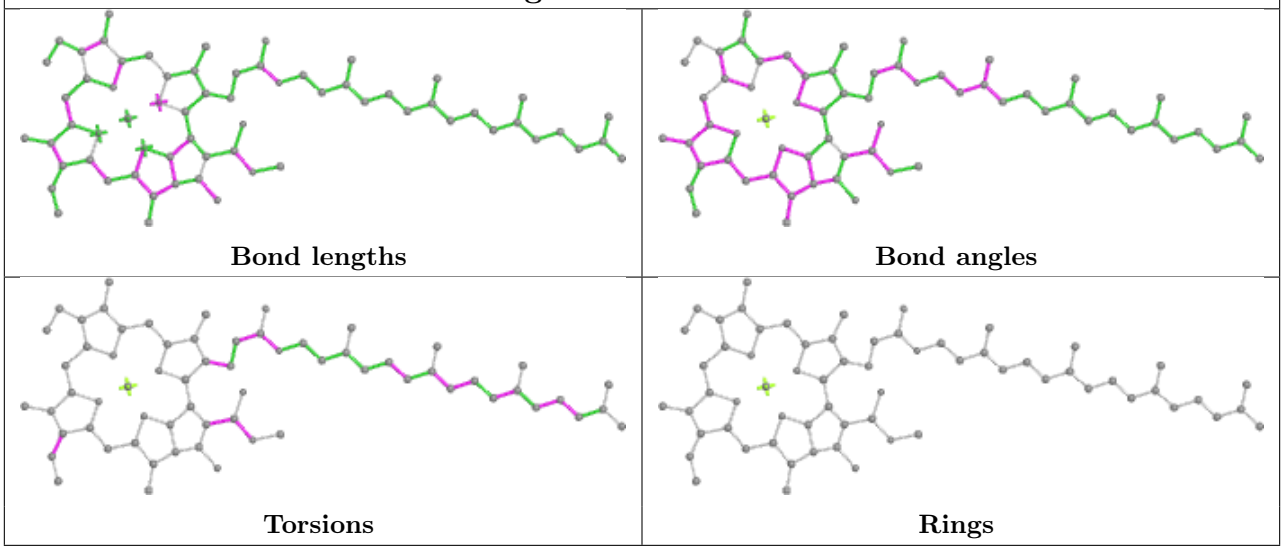
Ligand BCR l 207



Ligand A86 A 302



Ligand CLA V 314



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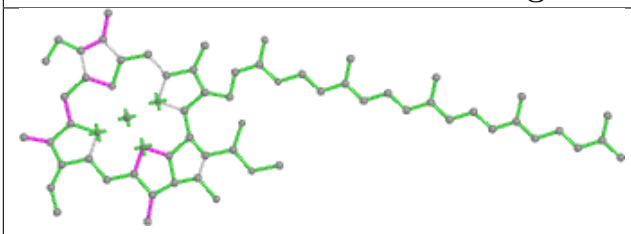
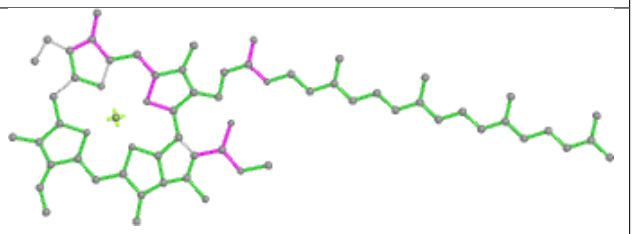
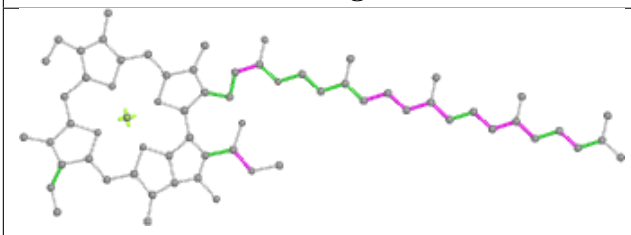
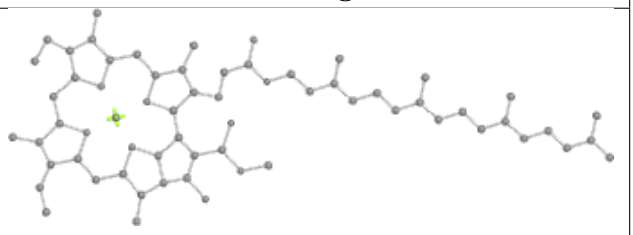
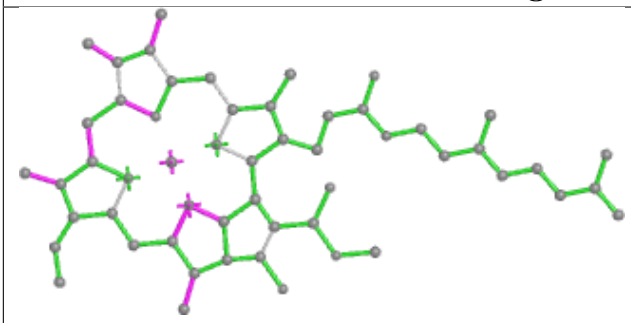
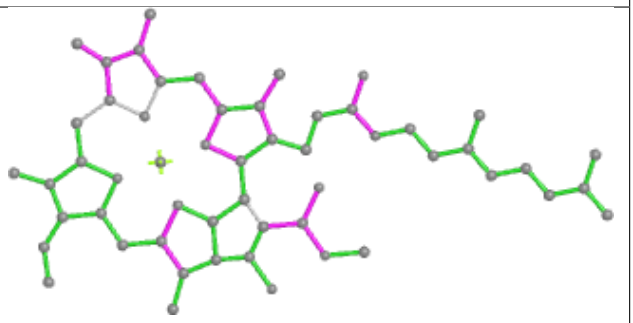
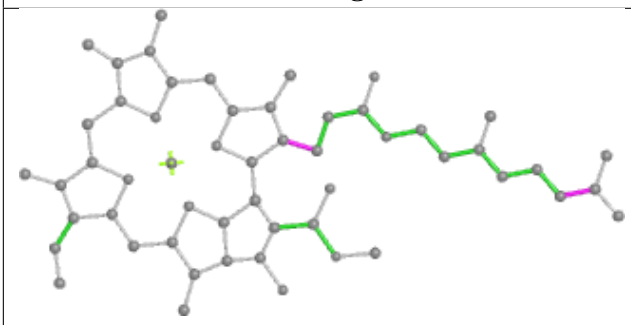
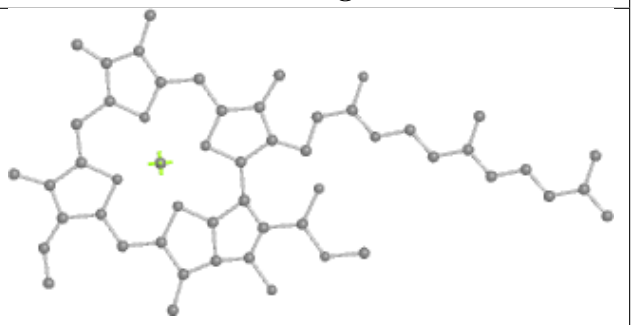
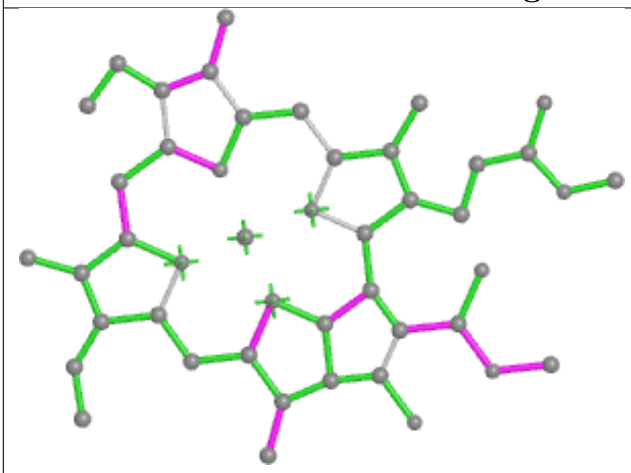
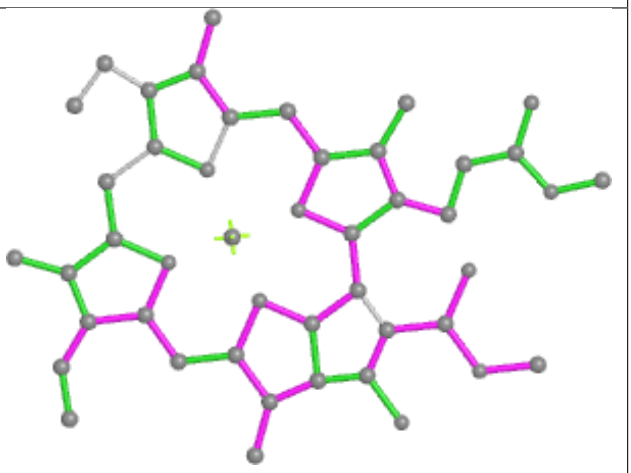
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA b 813	
 Bond lengths	 Bond angles
 Torsions	 Rings

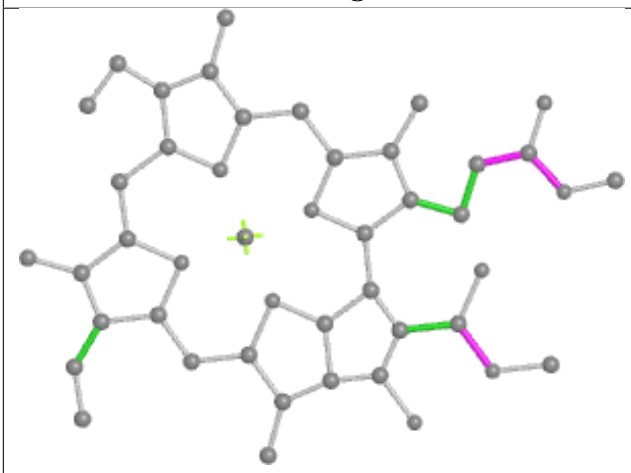
Ligand CLA H 310



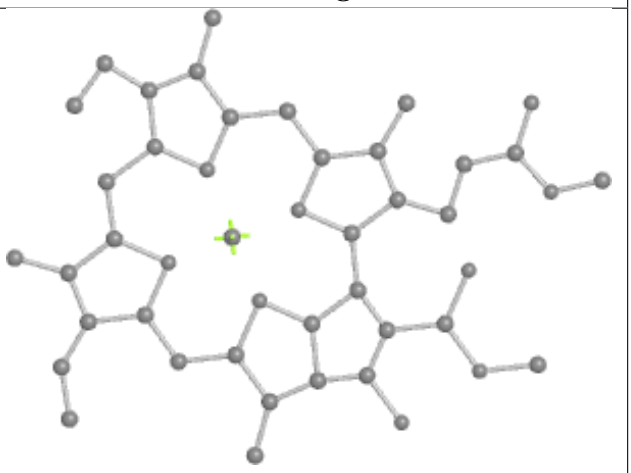
Bond lengths



Bond angles

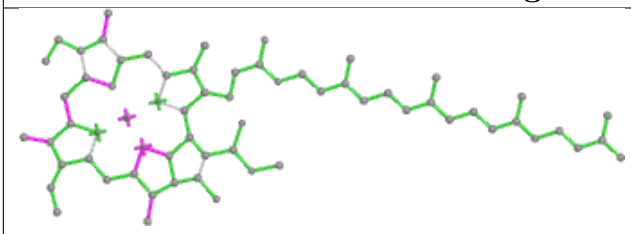


Torsions

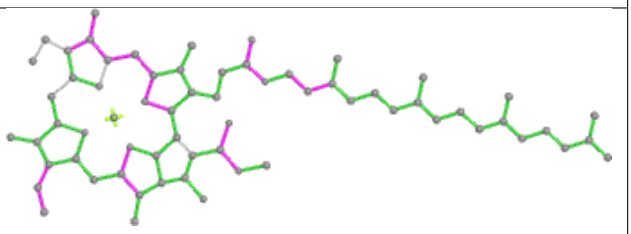


Rings

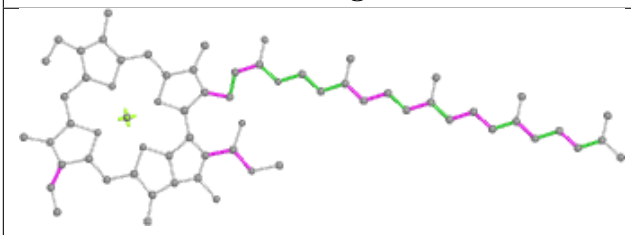
Ligand CLA O 309



Bond lengths



Bond angles



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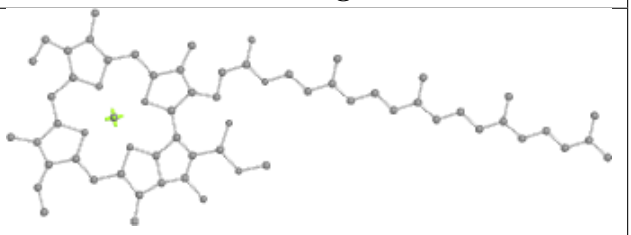
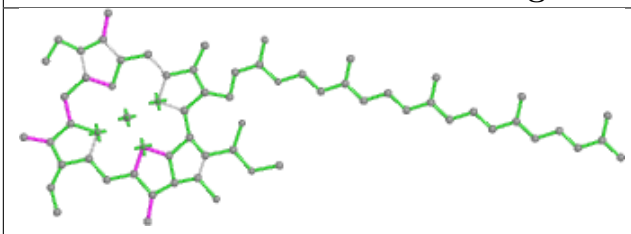
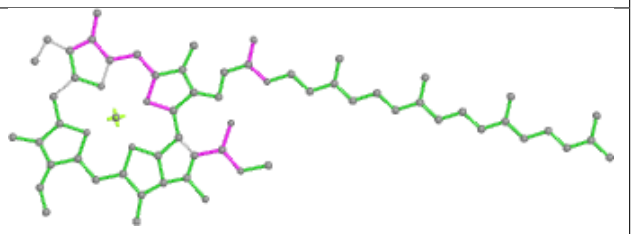
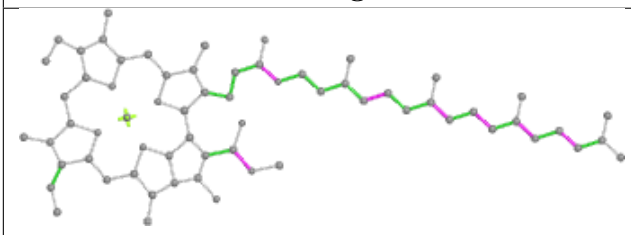
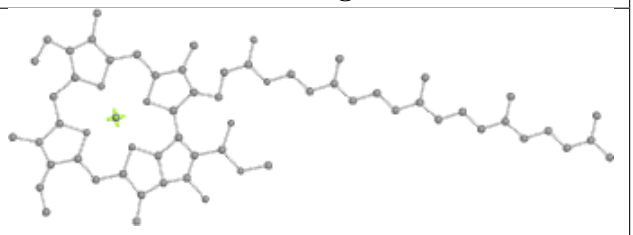


Rings

Ligand CLA J 312	
 Bond lengths	 Bond angles
 Torsions	 Rings

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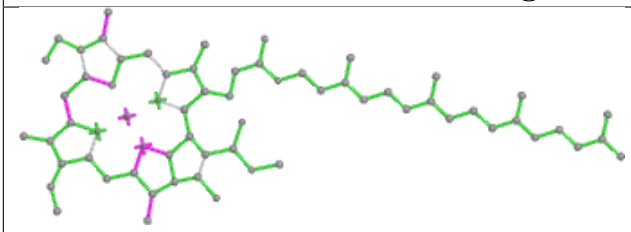
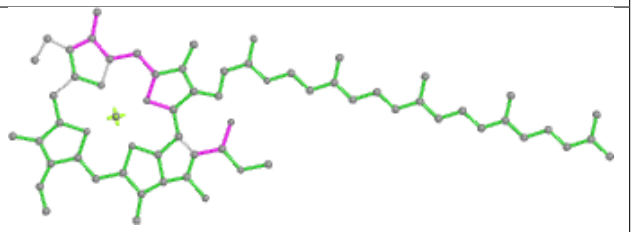
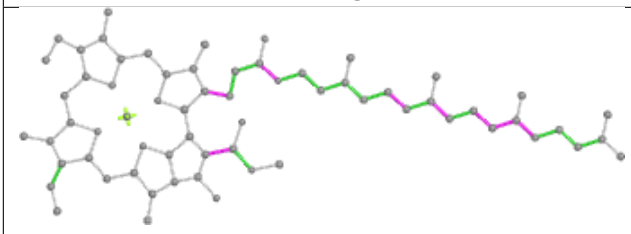
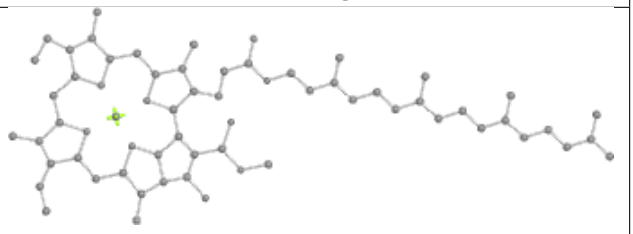
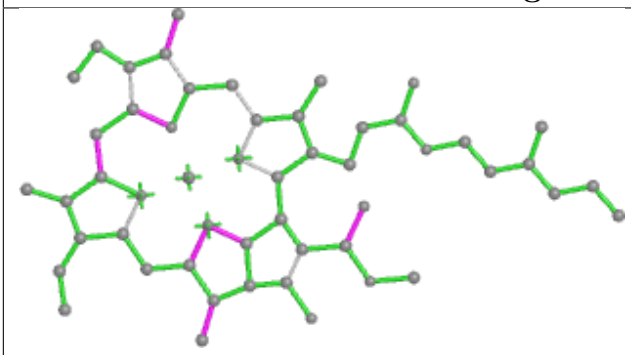
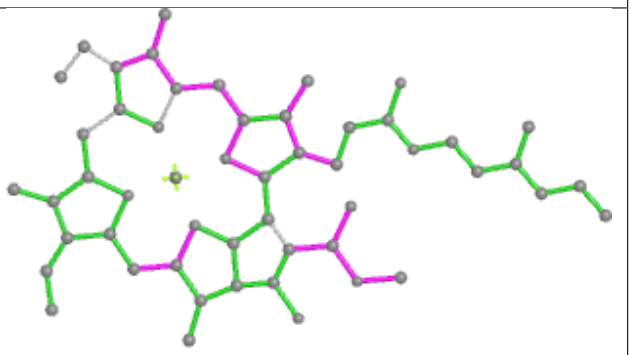
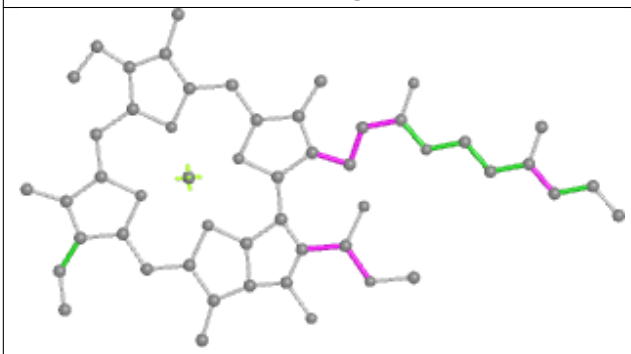
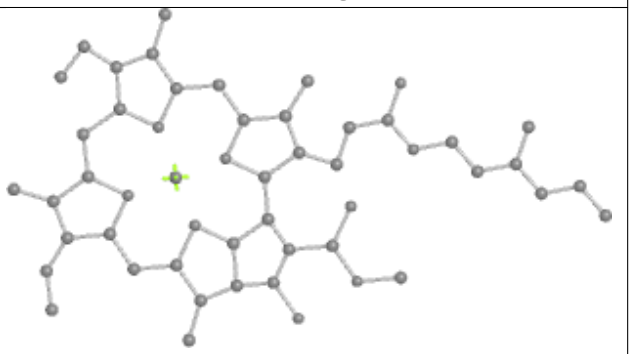
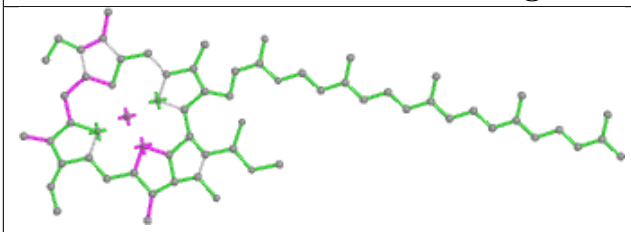
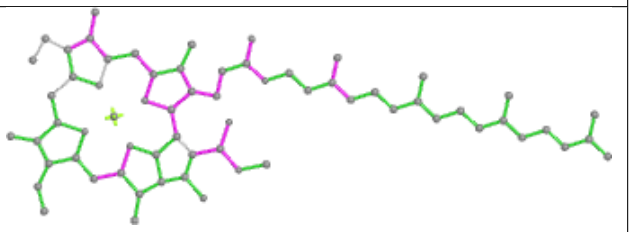
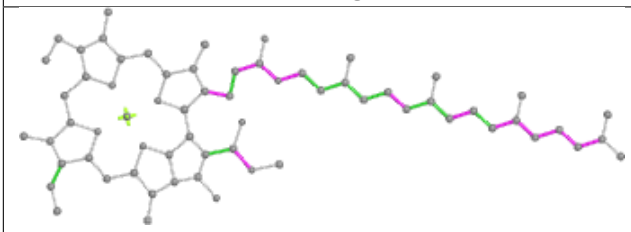
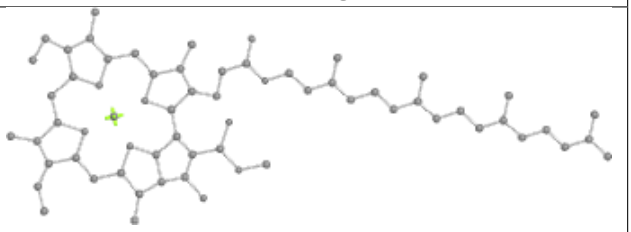
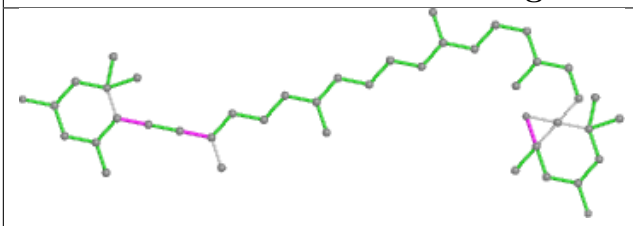
 Bond lengths	 Bond angles
 Torsions	 Rings

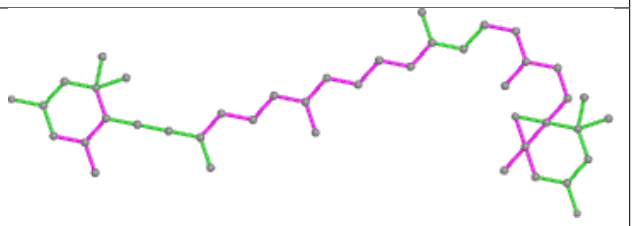
Ligand CLA R 322	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA H 312	
 Bond lengths	 Bond angles
 Torsions	 Rings

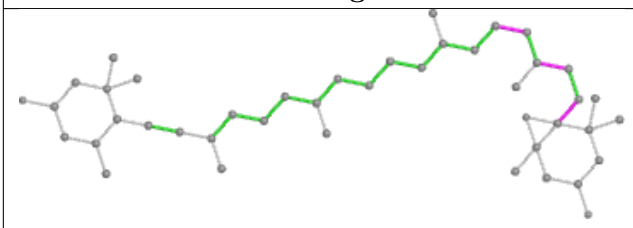
Ligand DD6 B 302



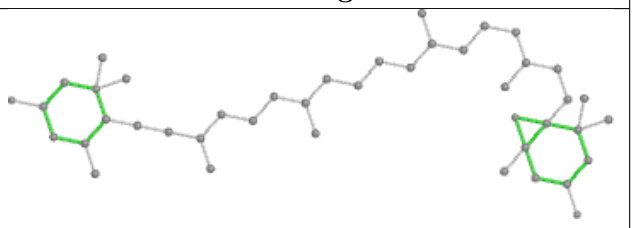
Bond lengths



Bond angles

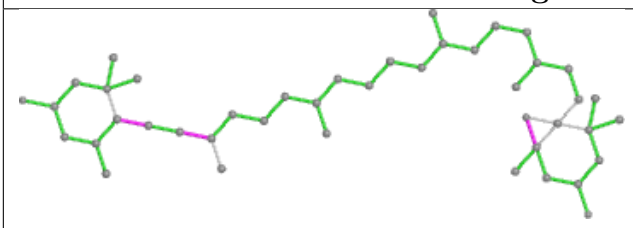


Torsions



Rings

Ligand DD6 I 303



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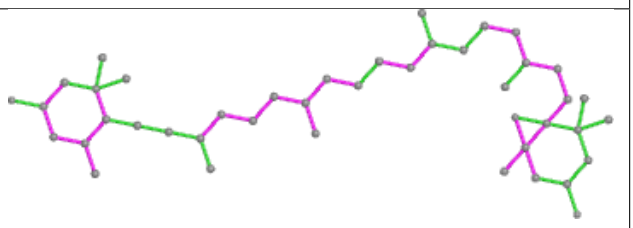
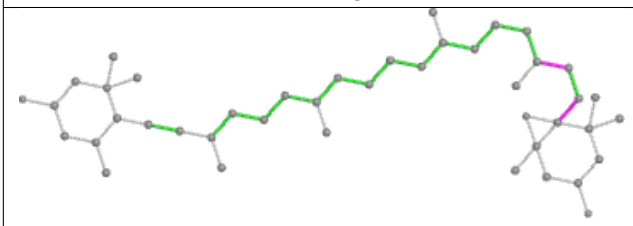
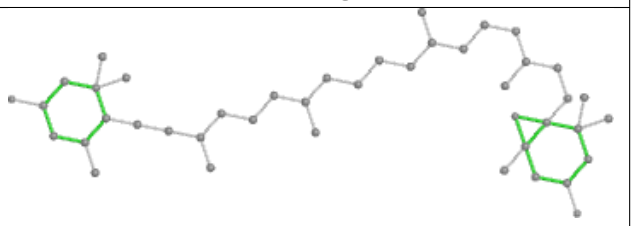


Bond angles

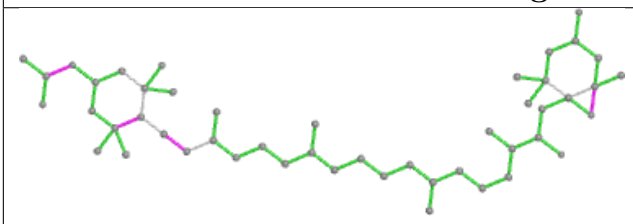


Torsions

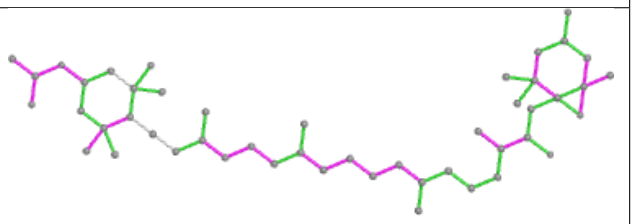


Rings

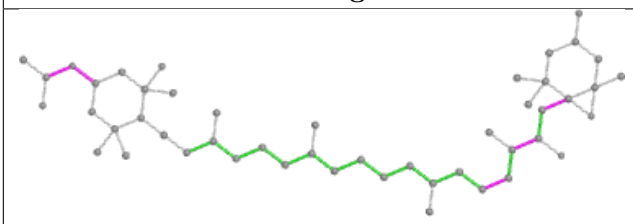
Ligand A86 B 301



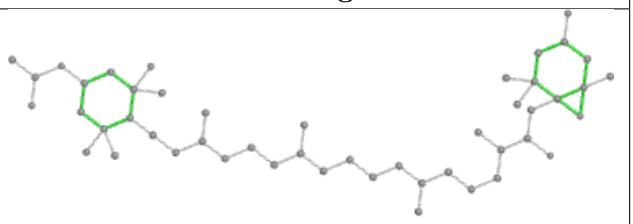
Bond lengths



Bond angles

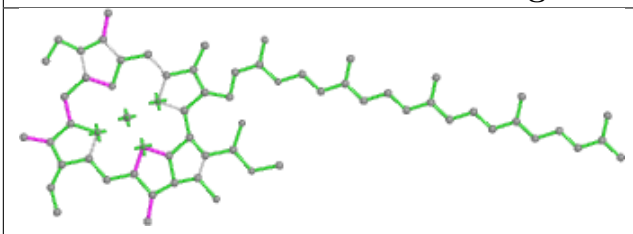


Torsions

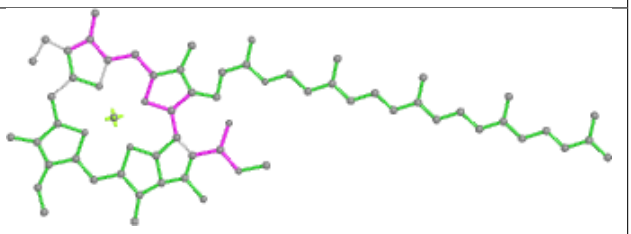


Rings

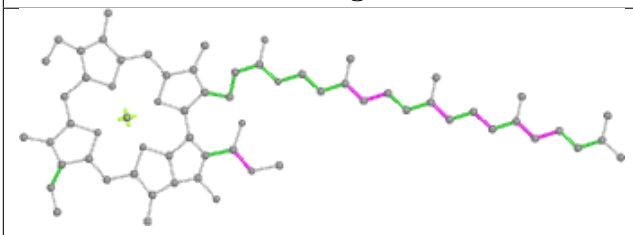
Ligand CLA a 837



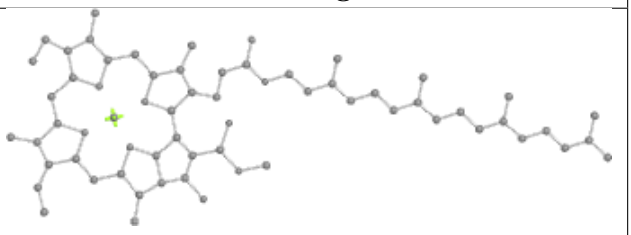
Bond lengths



Bond angles

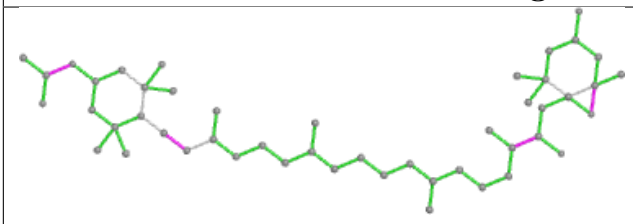


Torsions

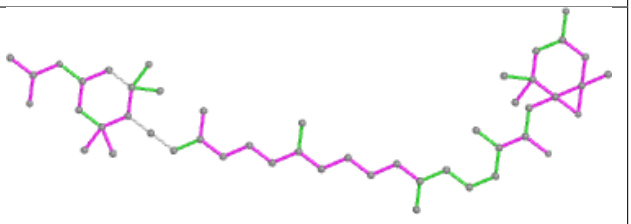


Rings

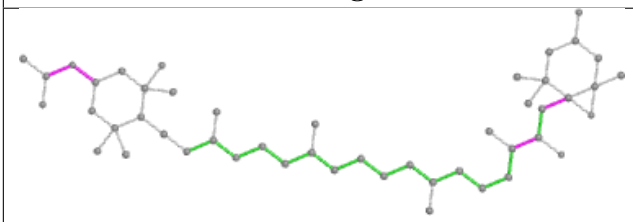
Ligand A86 X 304



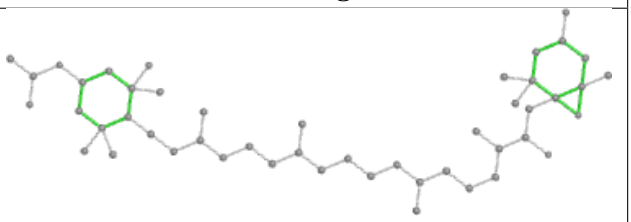
Bond lengths



Bond angles

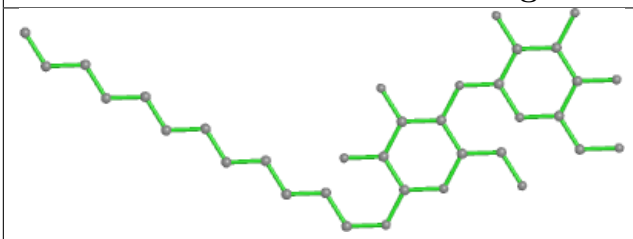


Torsions

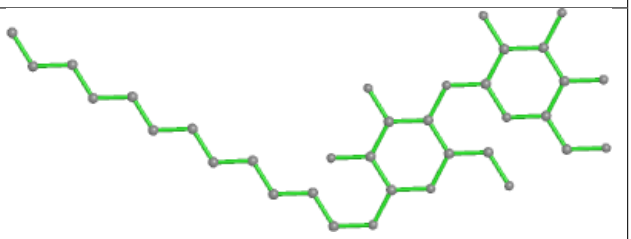


Rings

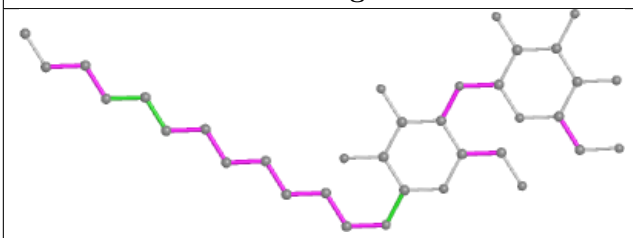
Ligand LMT G 323



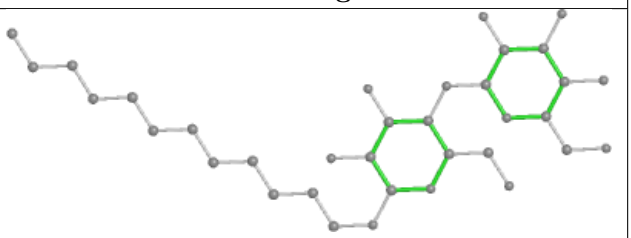
Bond lengths



Bond angles

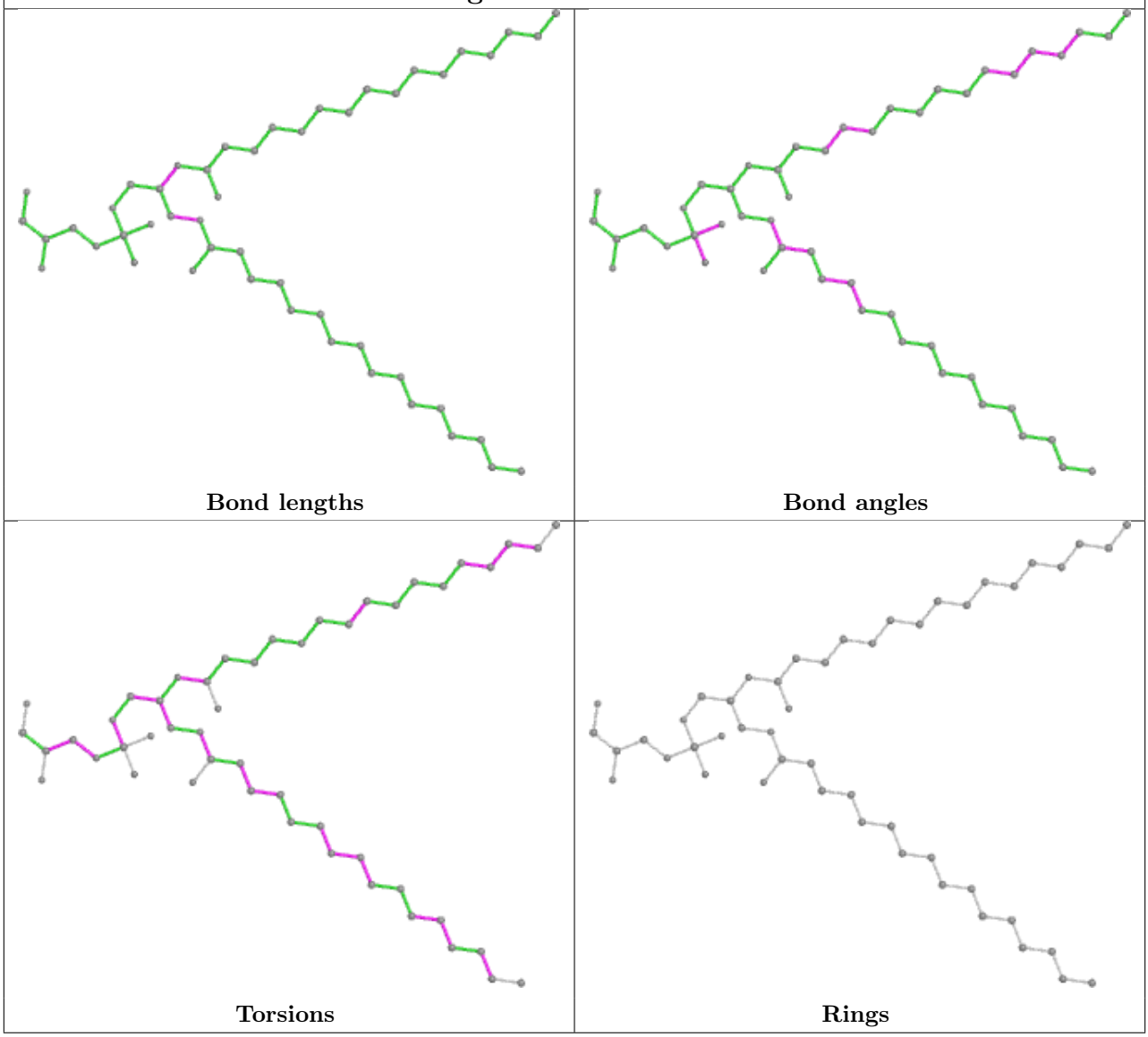


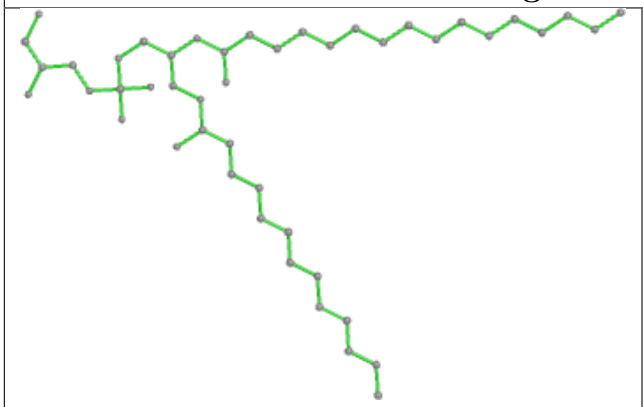
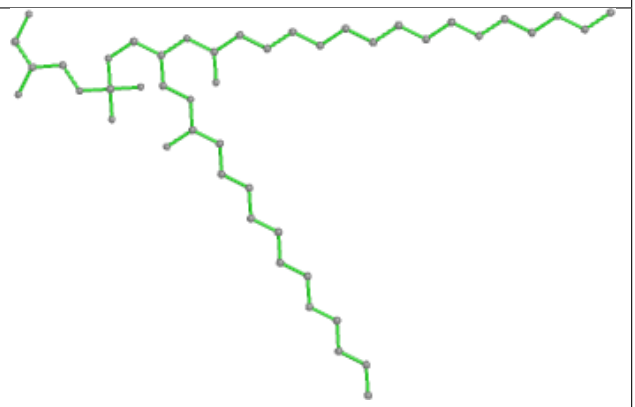
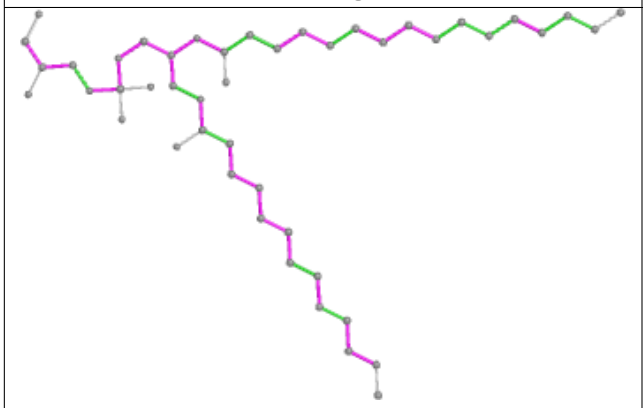
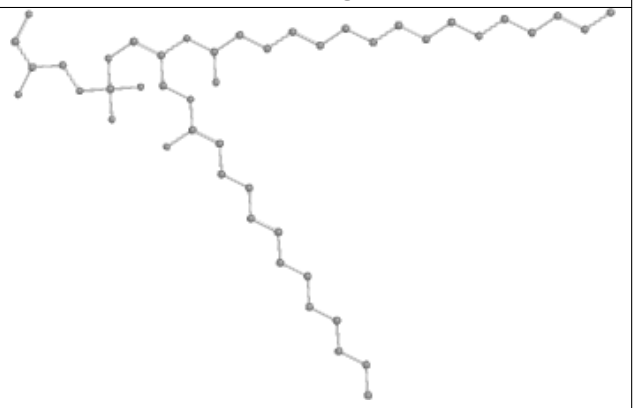
Torsions



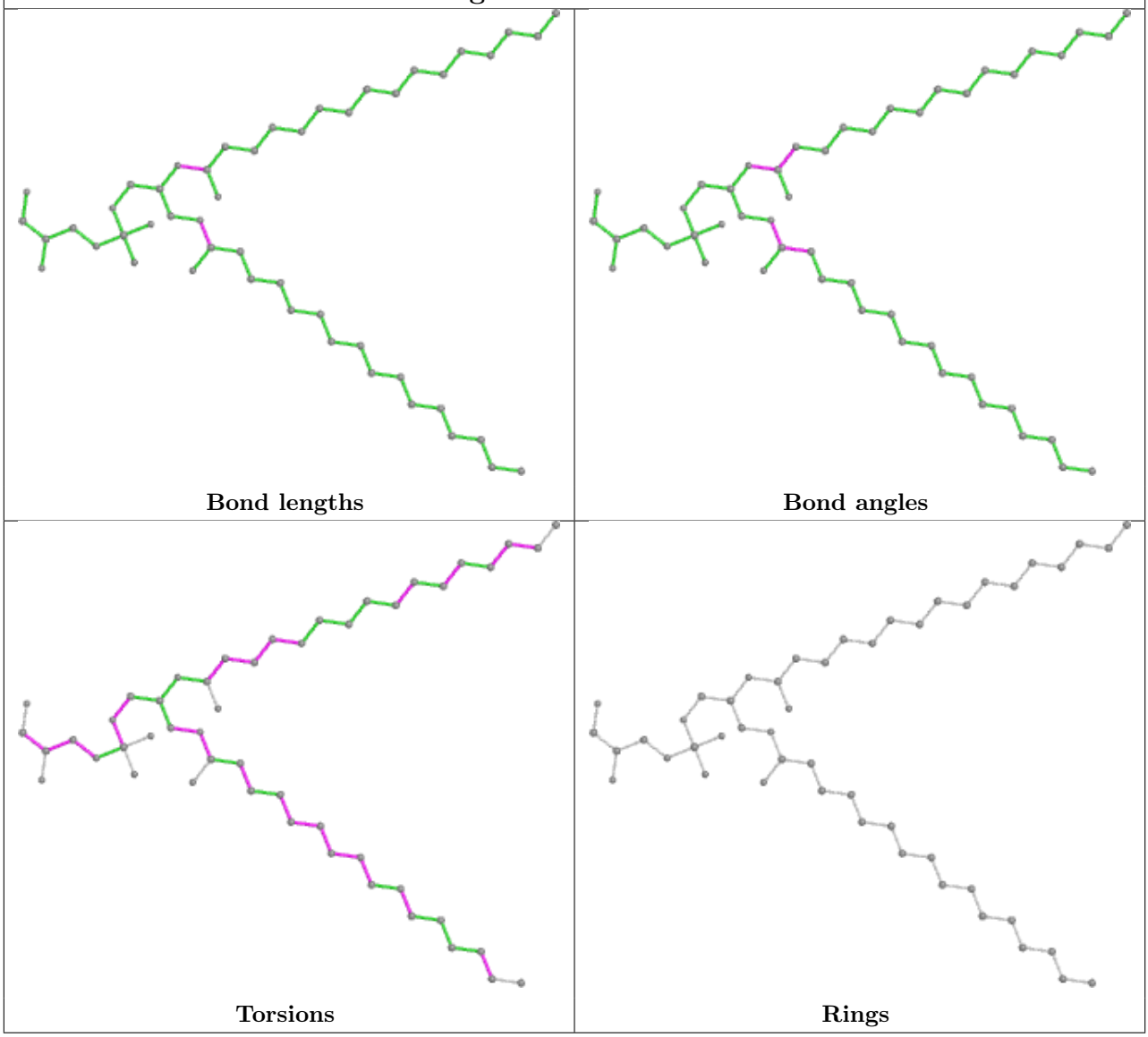
Rings

Ligand LHG G 301

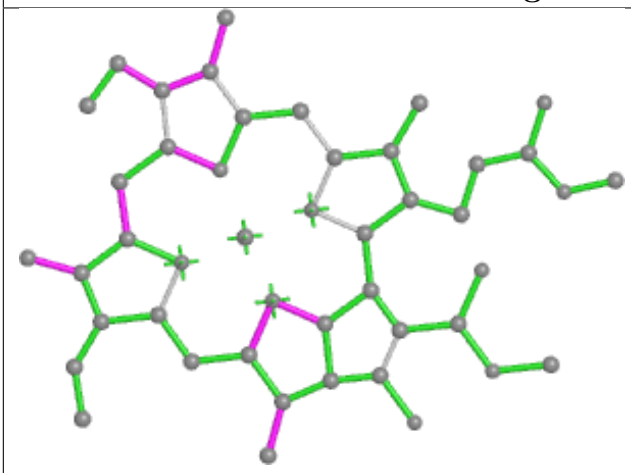


Ligand LHG D 318	
 Bond lengths	 Bond angles
 Torsions	 Rings

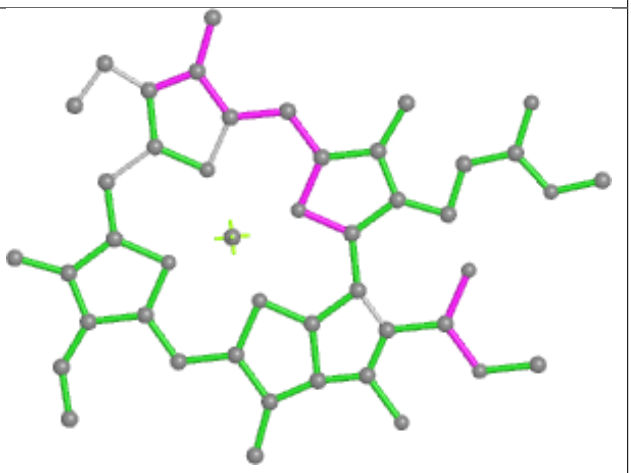
Ligand LHG E 322



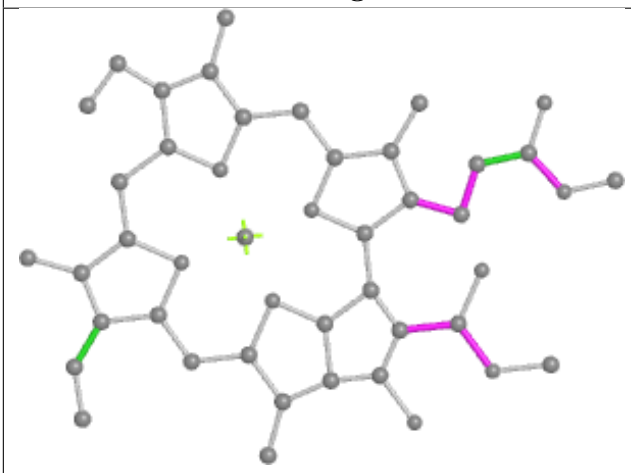
Ligand CLA A 309



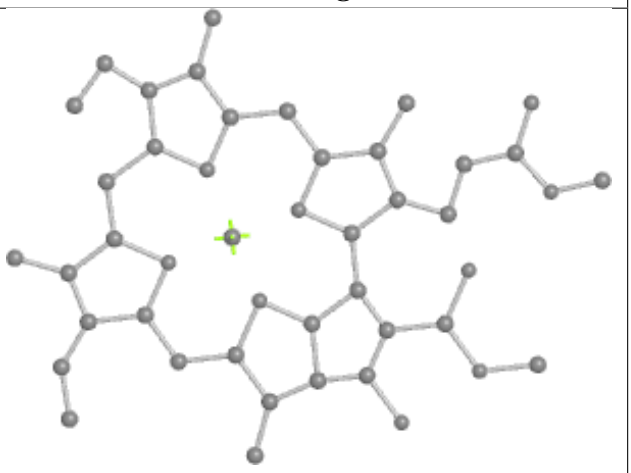
Bond lengths



Bond angles

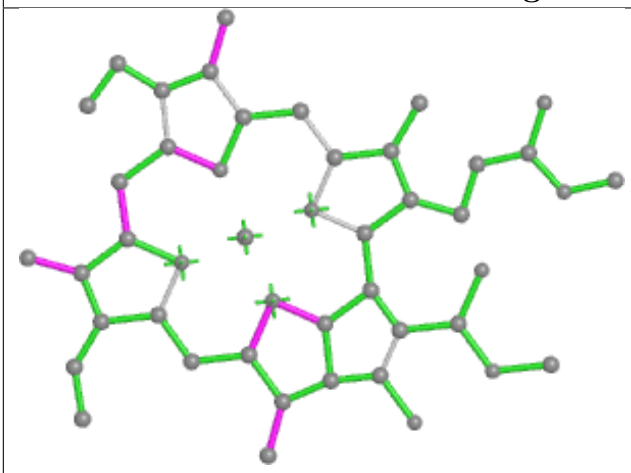


Torsions

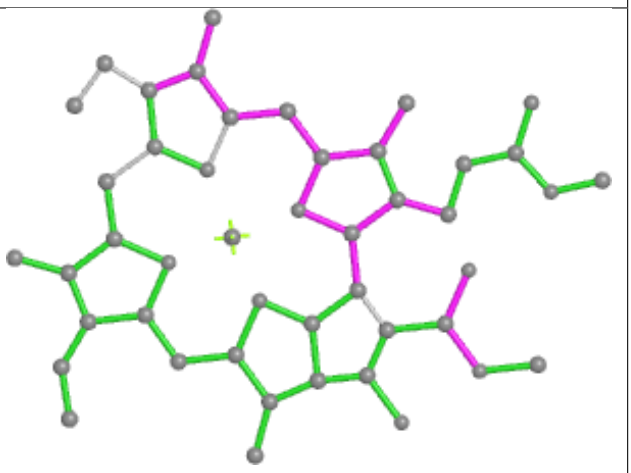


Rings

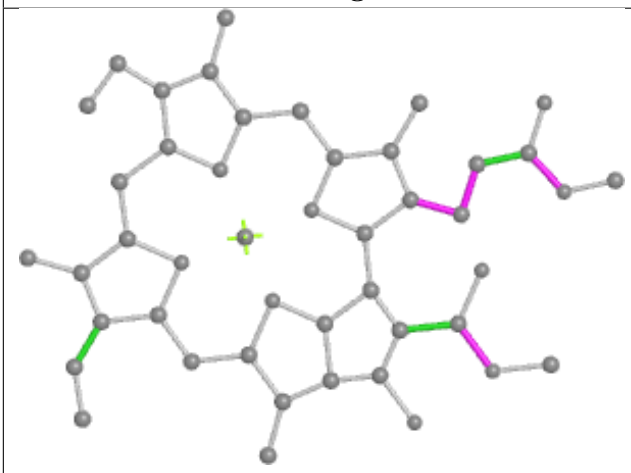
Ligand CLA K 311



Bond lengths



Bond angles



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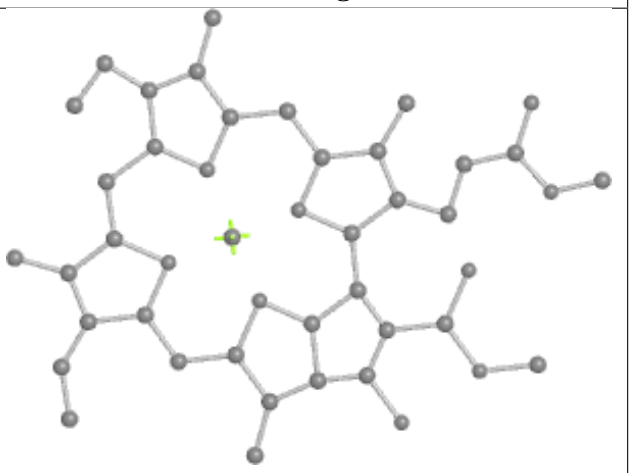
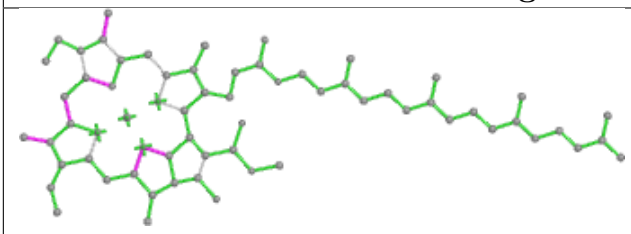
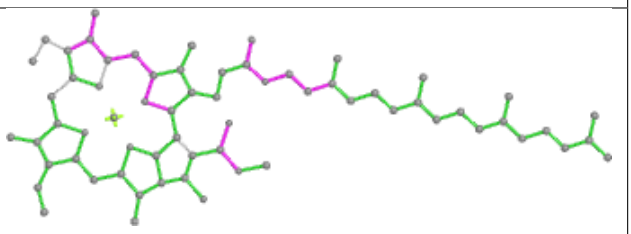


Rings

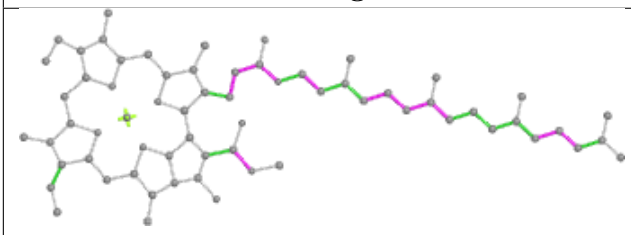
Ligand CLA W 207



Bond lengths



Bond angles



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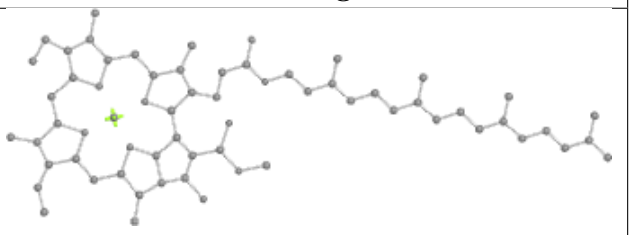
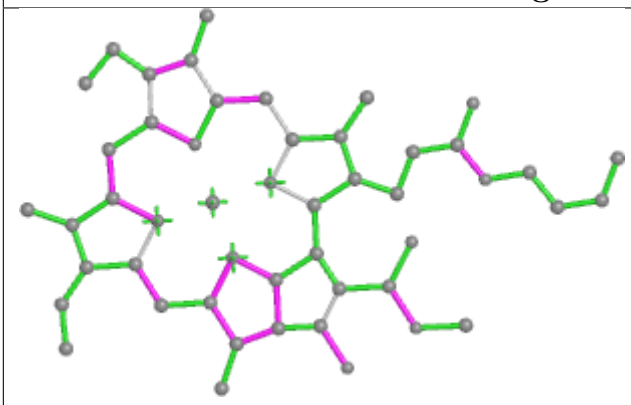
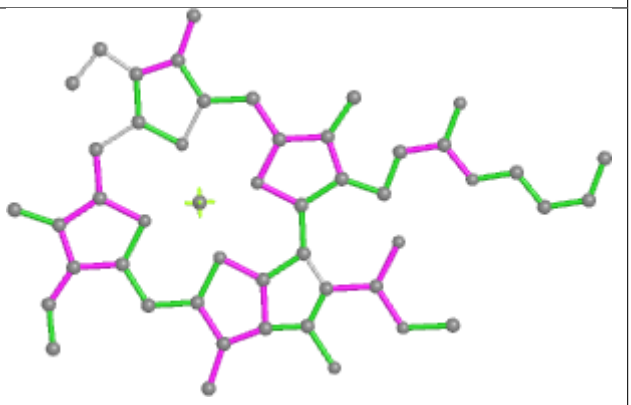
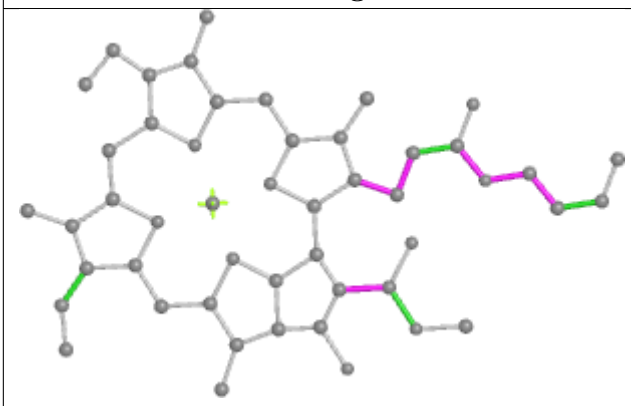
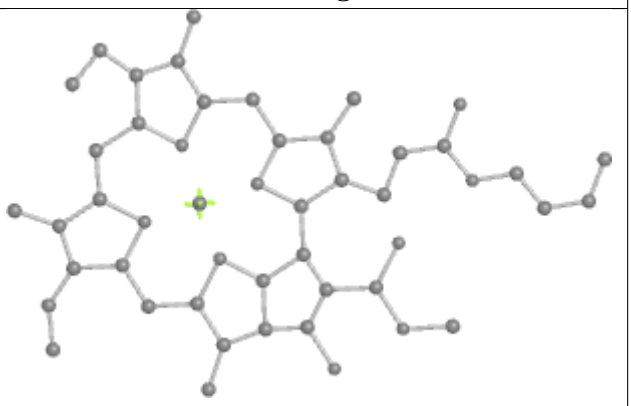
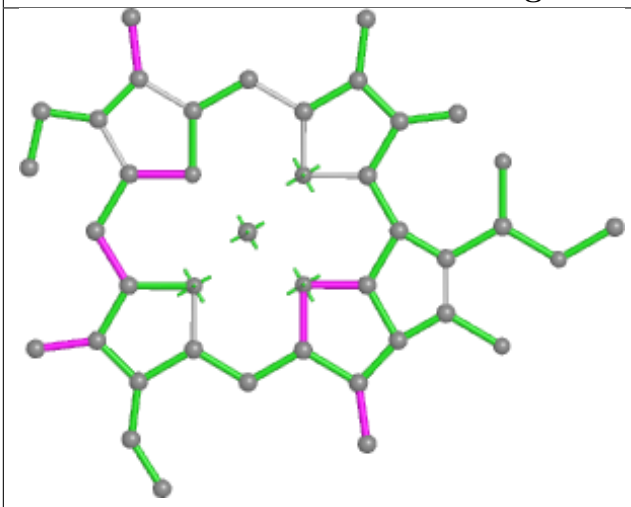


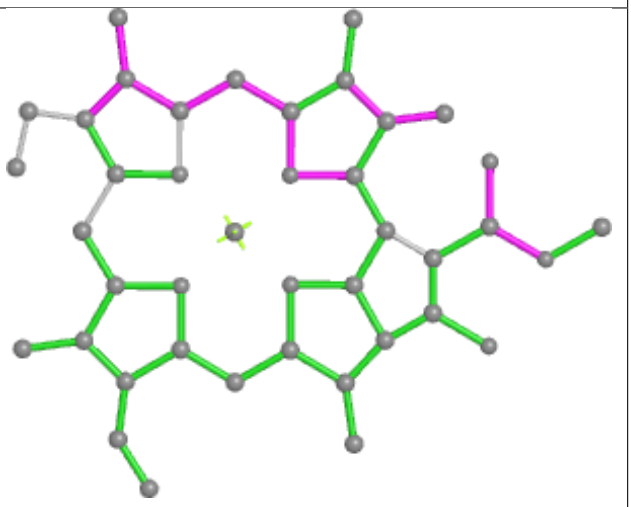
Rings

Ligand CLA l 204	
 Bond lengths	 Bond angles
 Torsions	 Rings

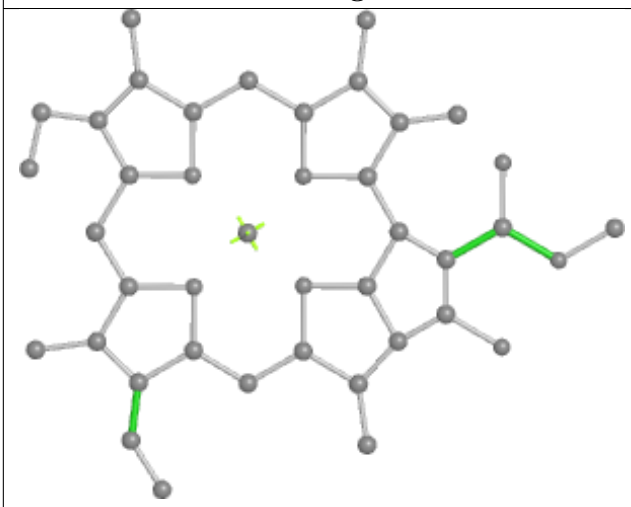
Ligand CLA T 316



Bond lengths



Bond angles



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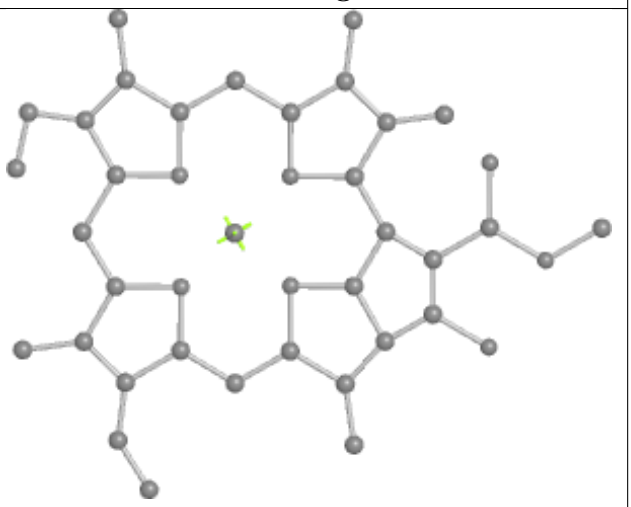
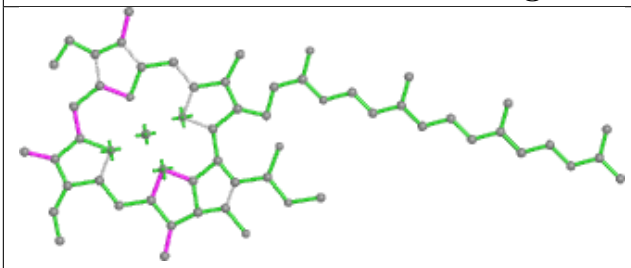
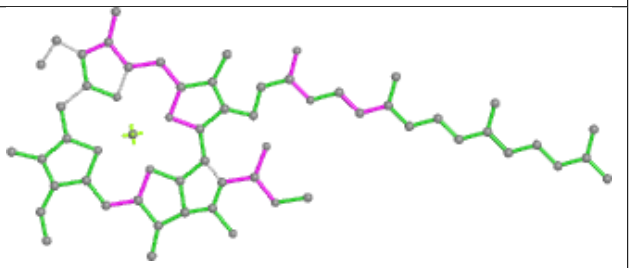


Rings

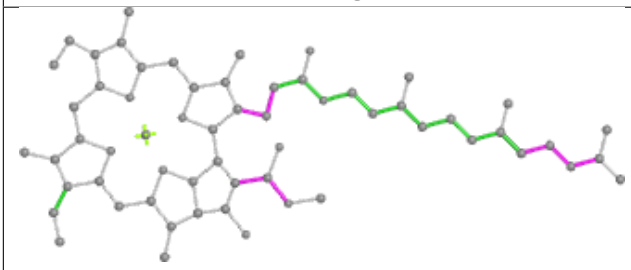
Ligand CLA A 307



Bond lengths



Bond angles



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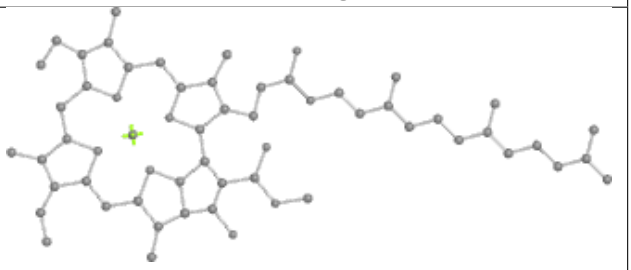
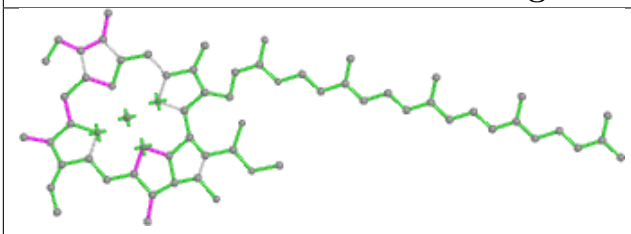
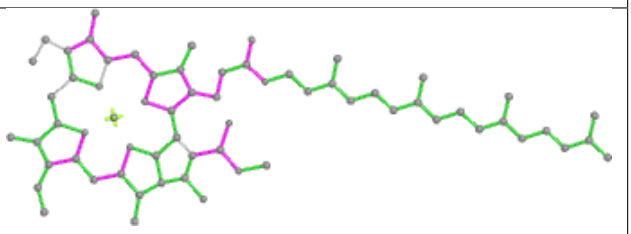
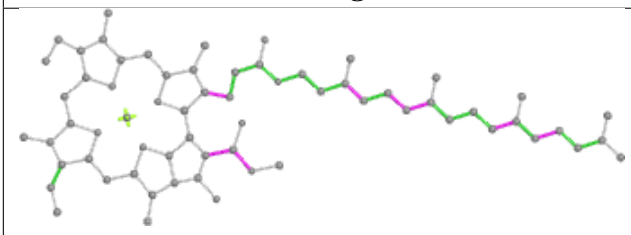
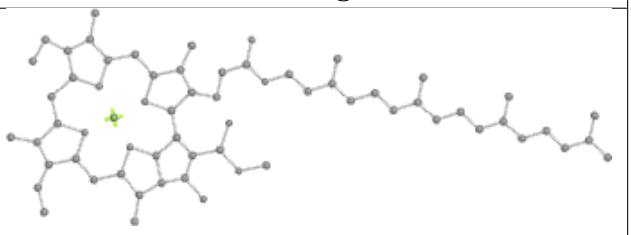
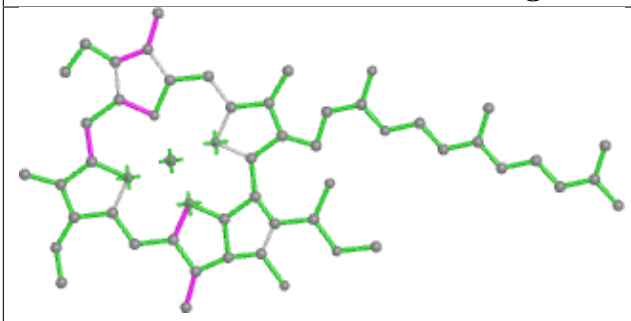
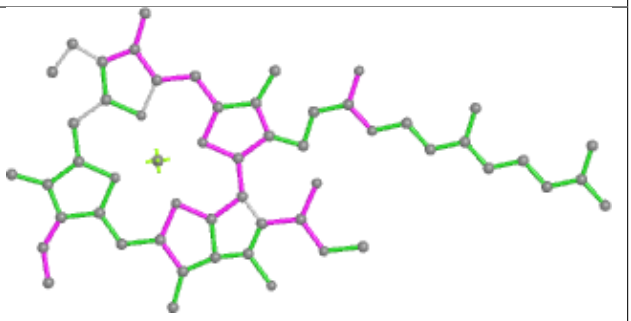
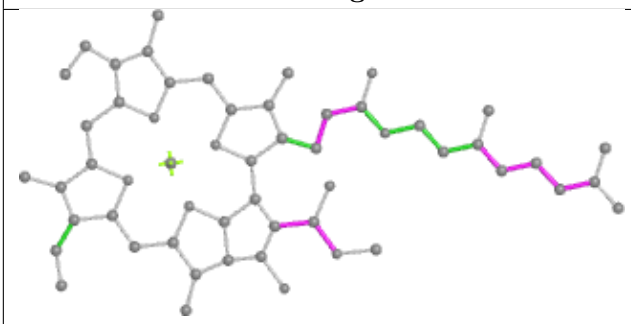
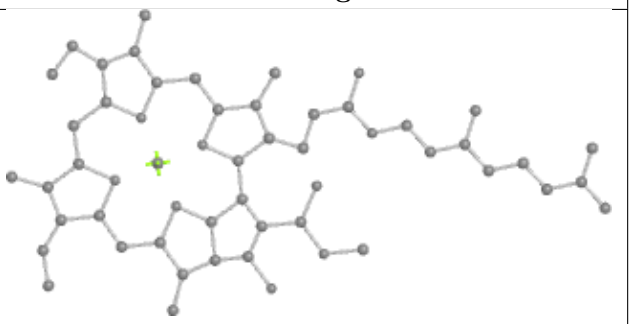
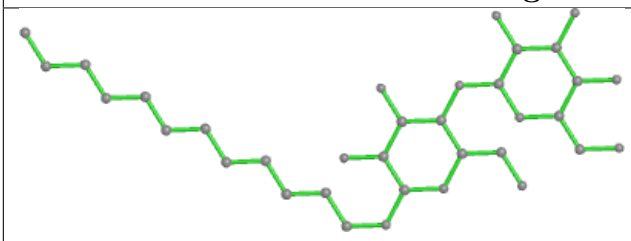
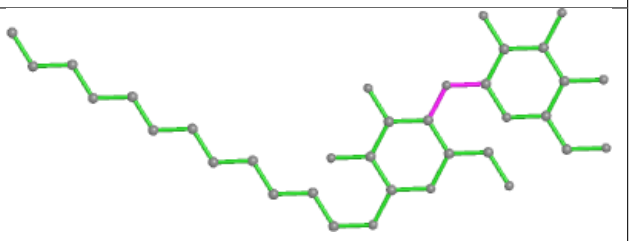
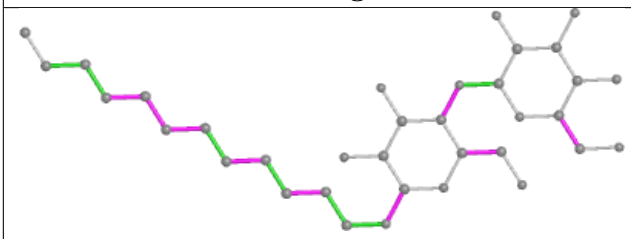
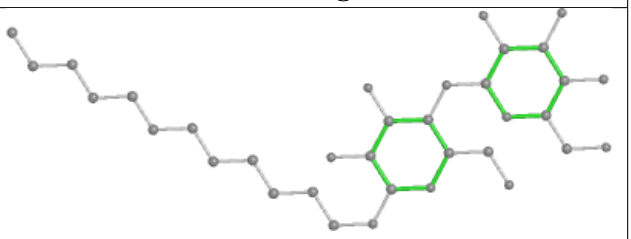
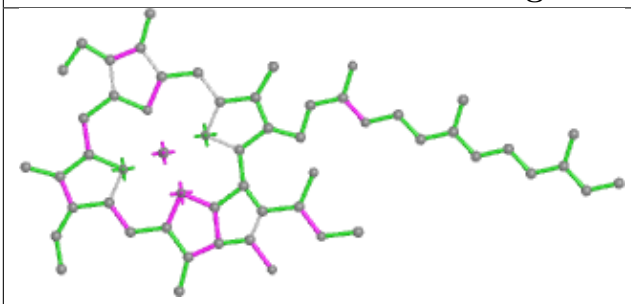
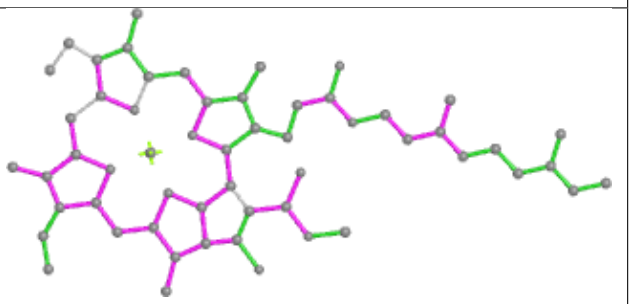
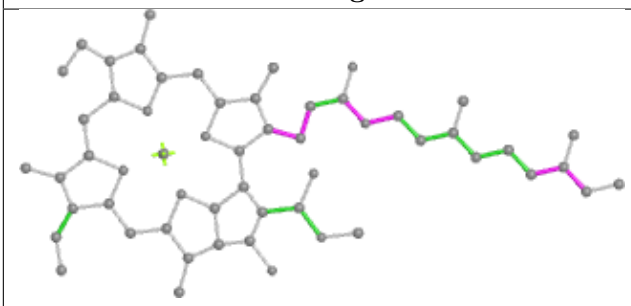
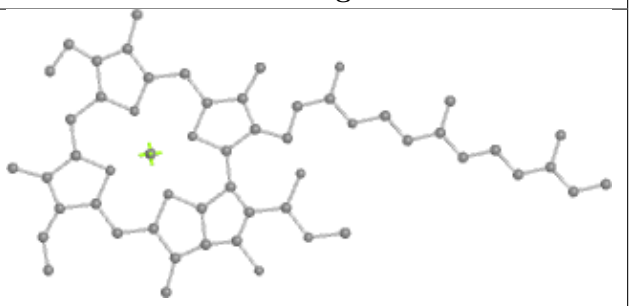


Rings

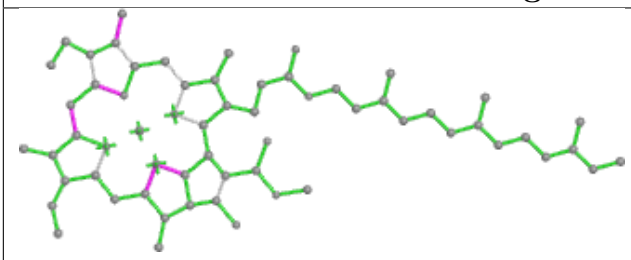
Ligand CLA a 832	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA B 311	
 Bond lengths	 Bond angles
 Torsions	 Rings

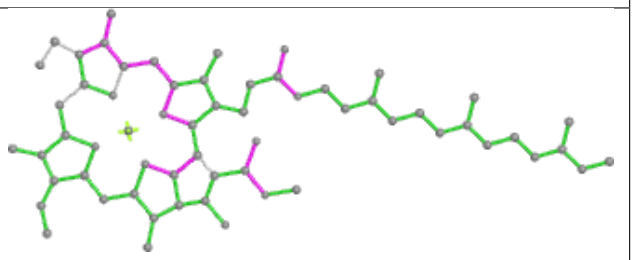
Ligand LMT F 320	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA F 317	
 Bond lengths	 Bond angles
 Torsions	 Rings

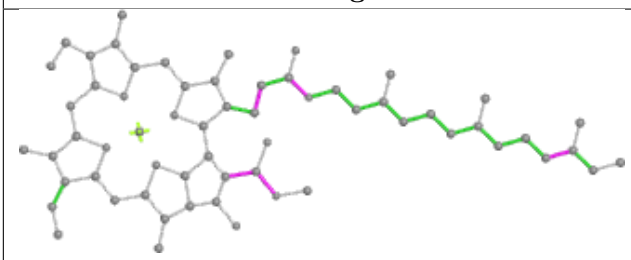
Ligand CLA X 306



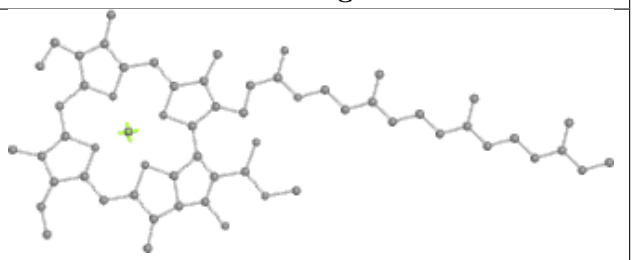
Bond lengths



Bond angles

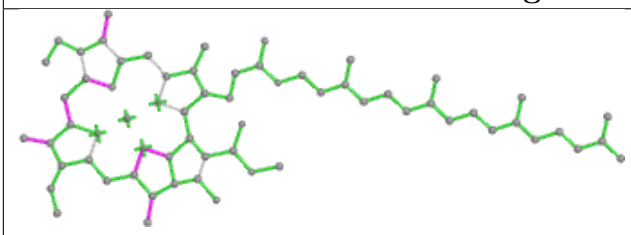


Torsions

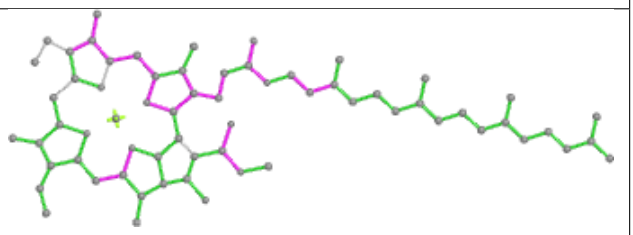


Rings

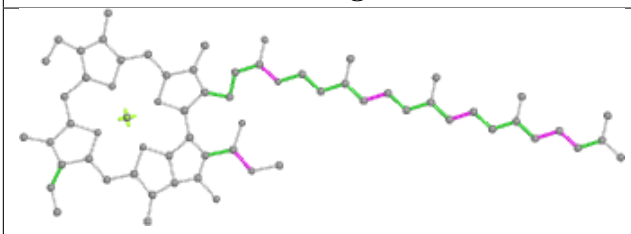
Ligand CLA D 313



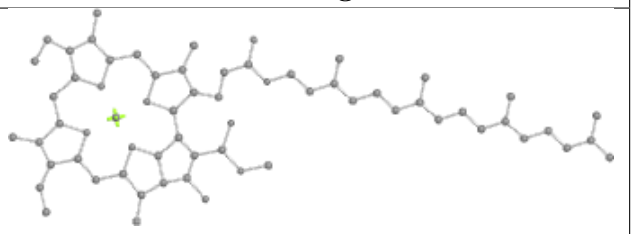
Bond lengths



Bond angles

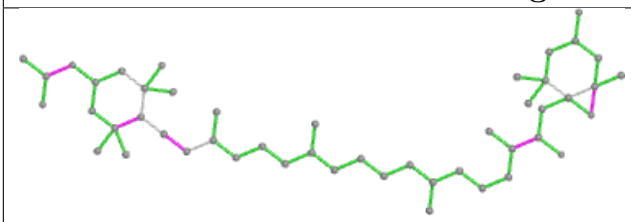


Torsions

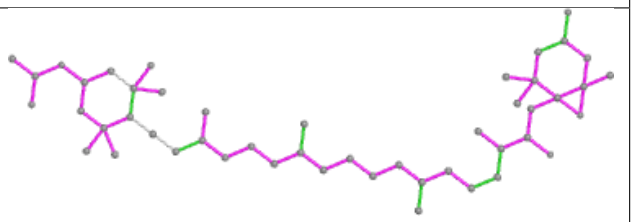


Rings

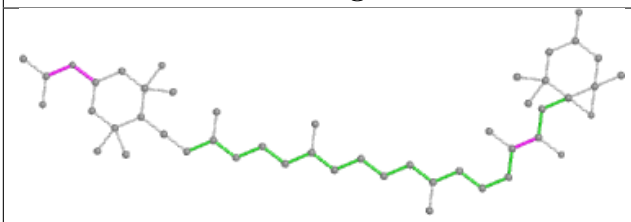
Ligand A86 X 301



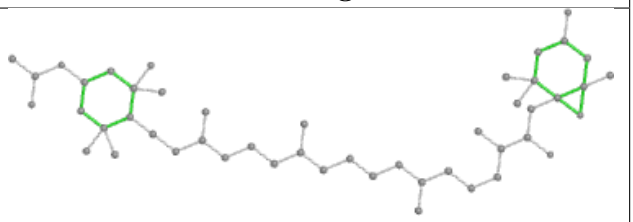
Bond lengths



Bond angles

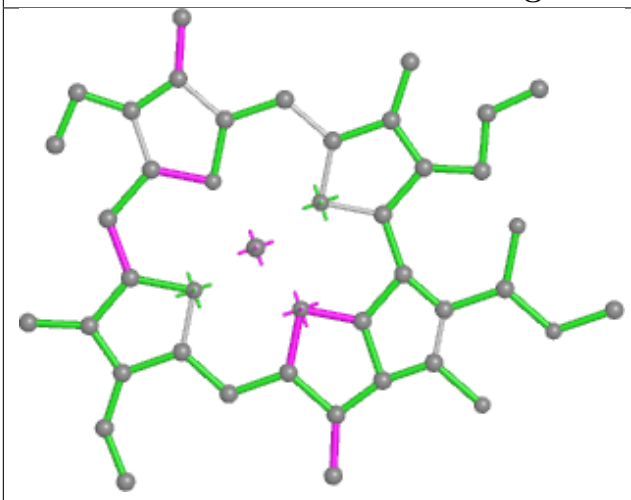


Torsions

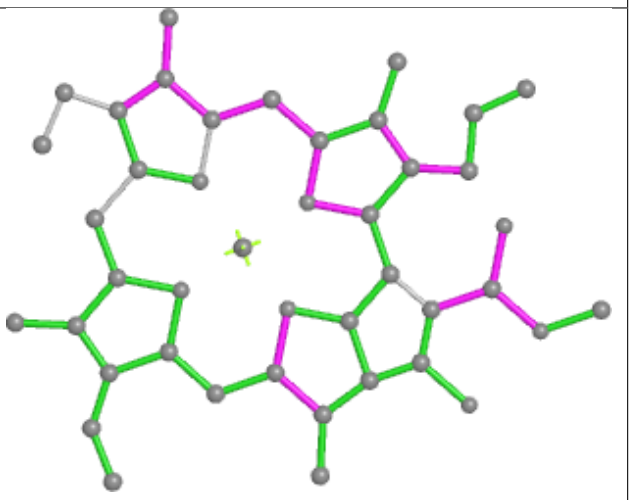


Rings

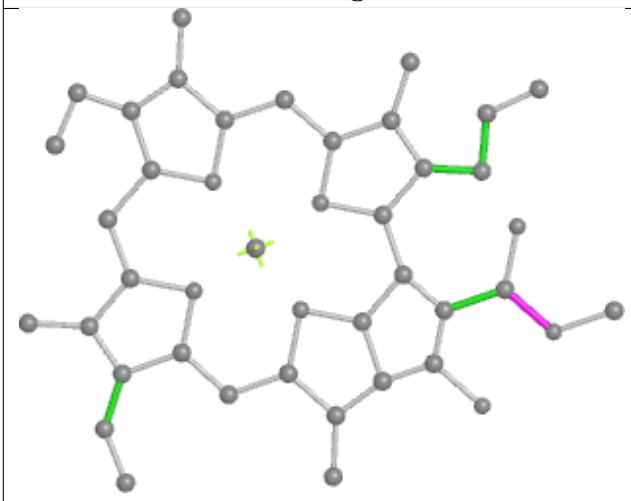
Ligand CLA C 205



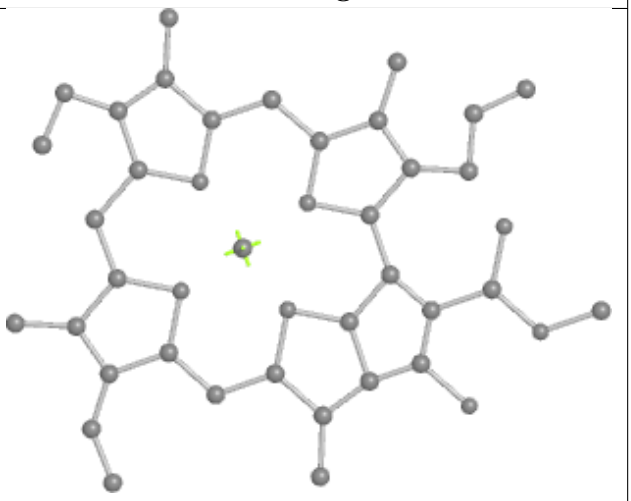
Bond lengths



Bond angles

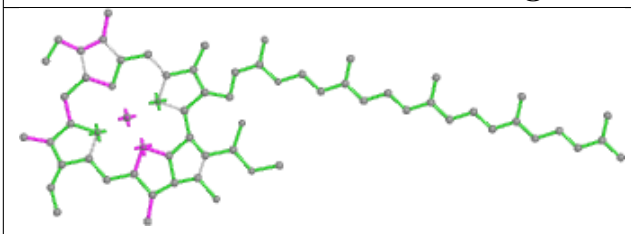


Torsions

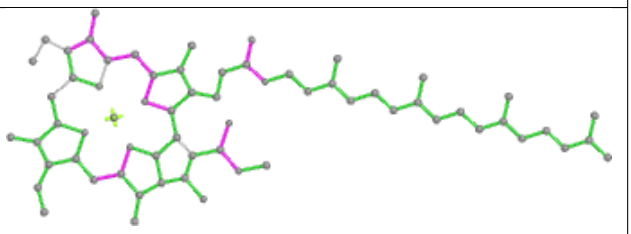


Rings

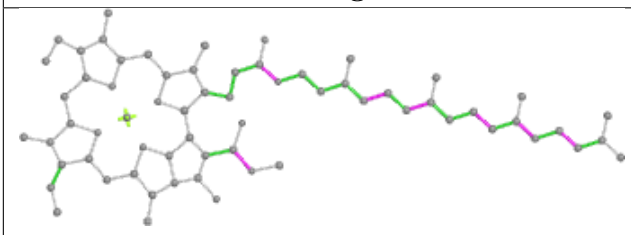
Ligand CLA C 211



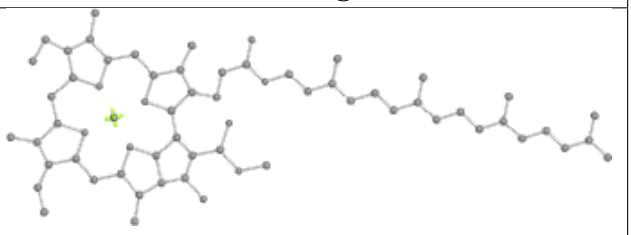
Bond lengths



Bond angles

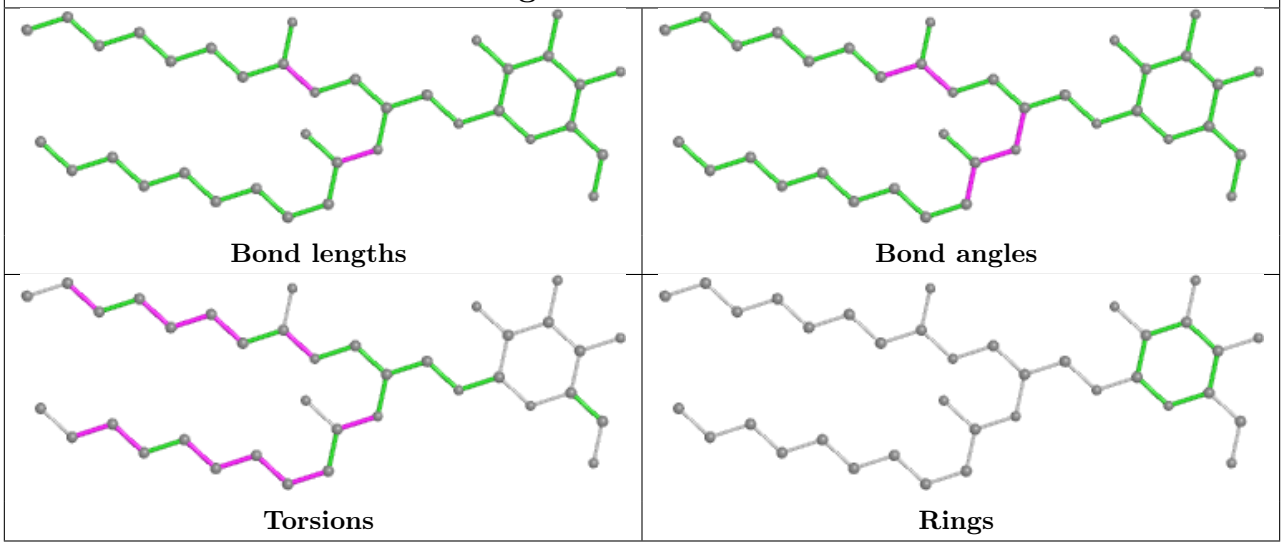


Torsions

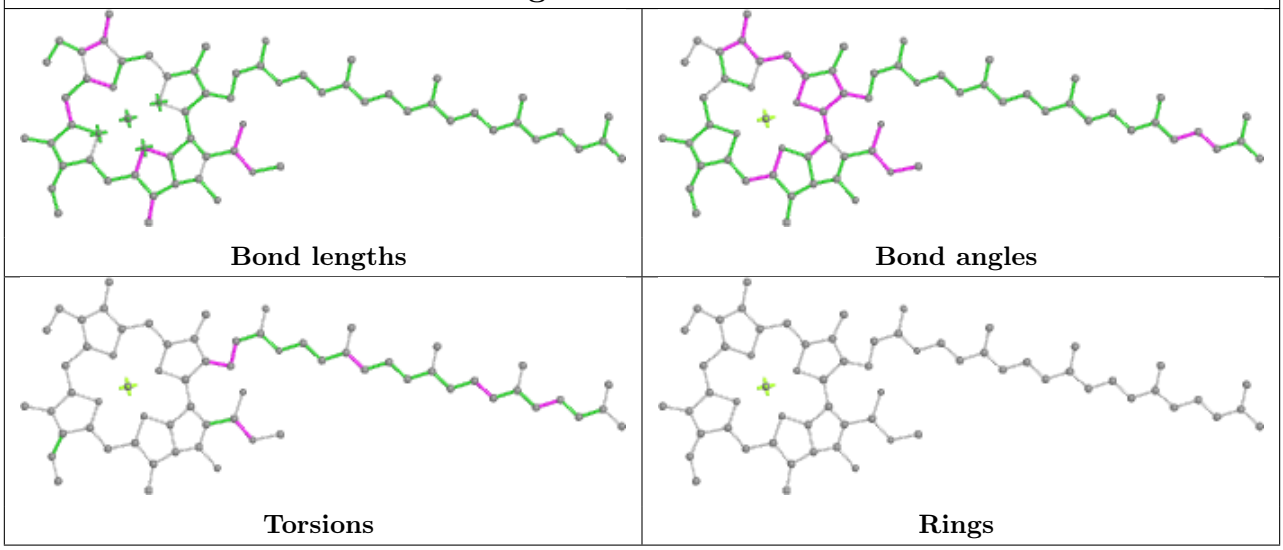


Rings

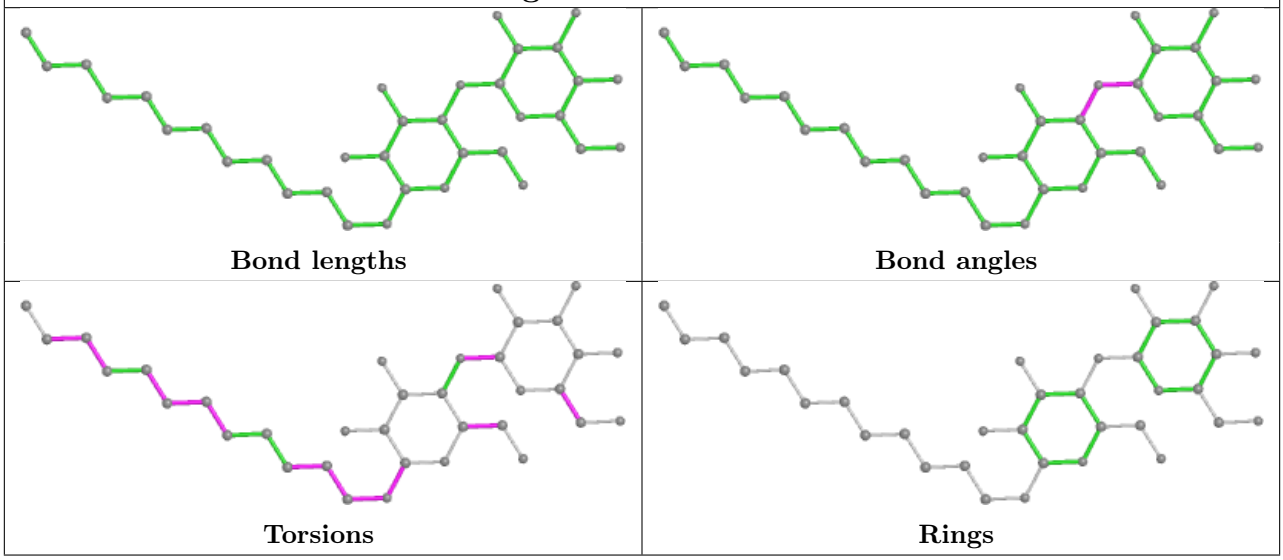
Ligand LMG m 102



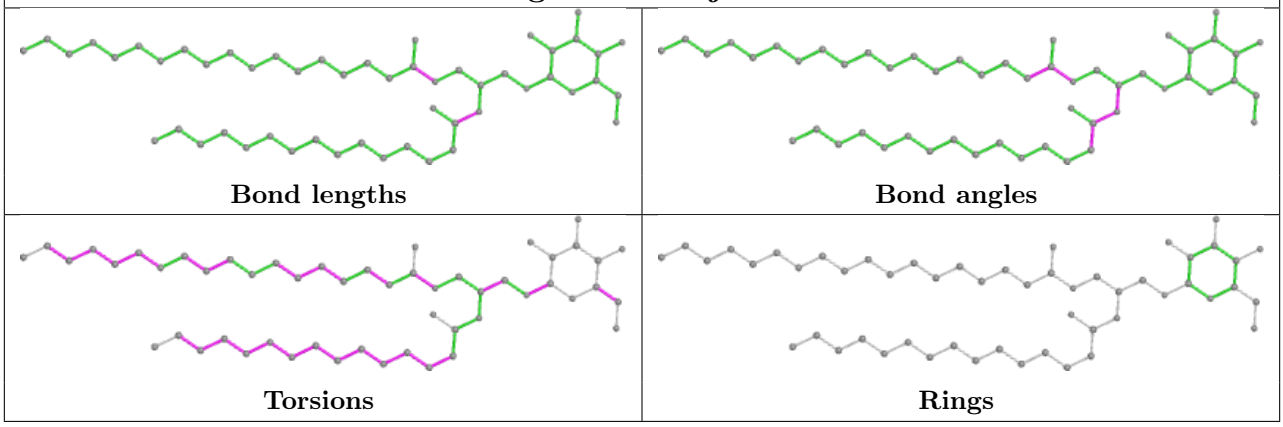
Ligand CLA S 314



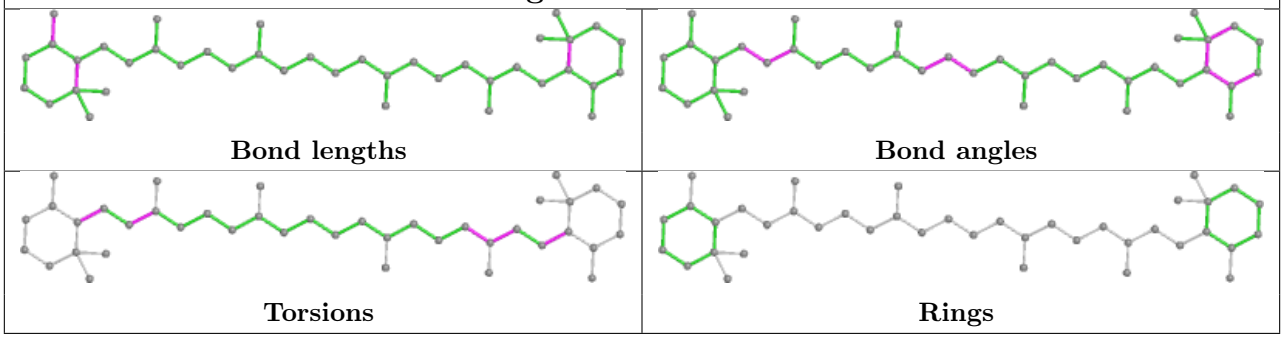
Ligand LMT B 312



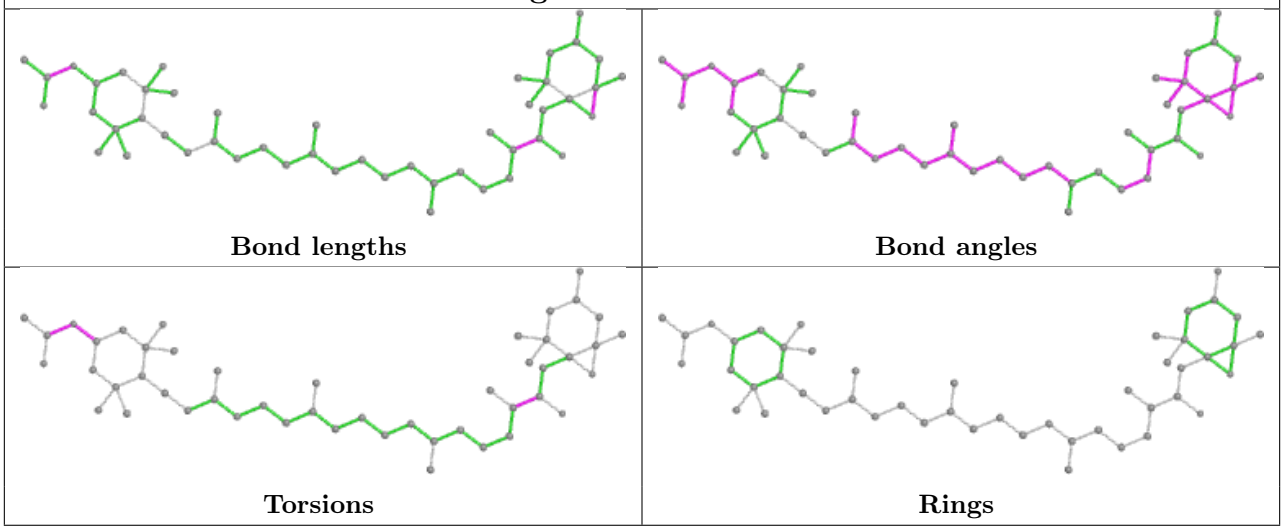
Ligand LMG j 105



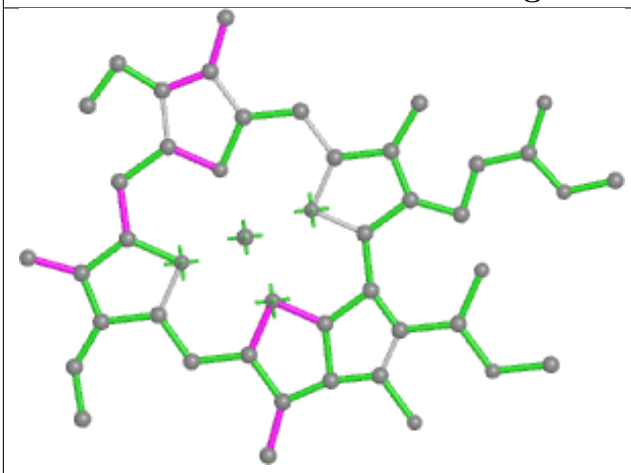
Ligand BCR b 843



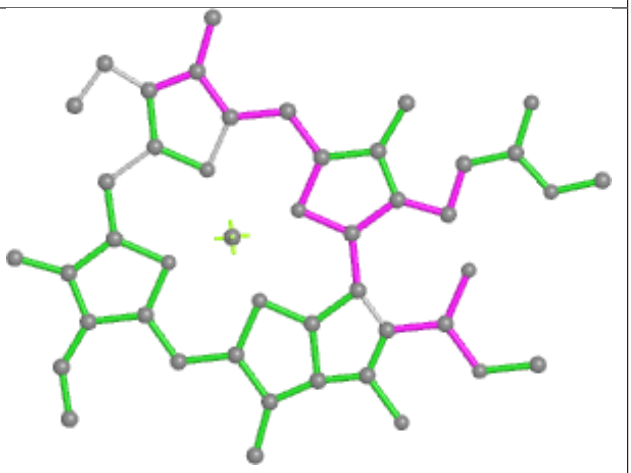
Ligand A86 H 301



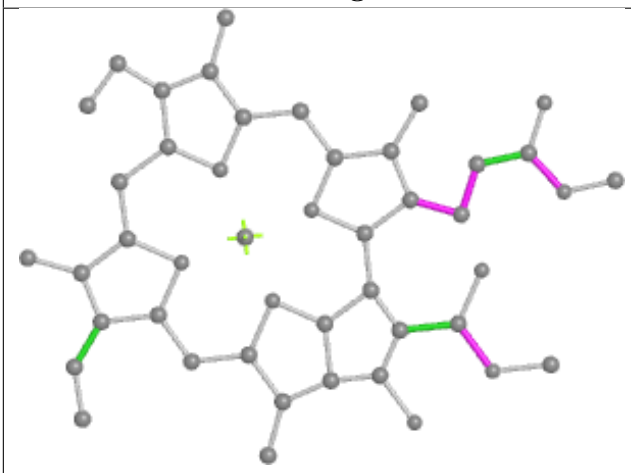
Ligand CLA O 310



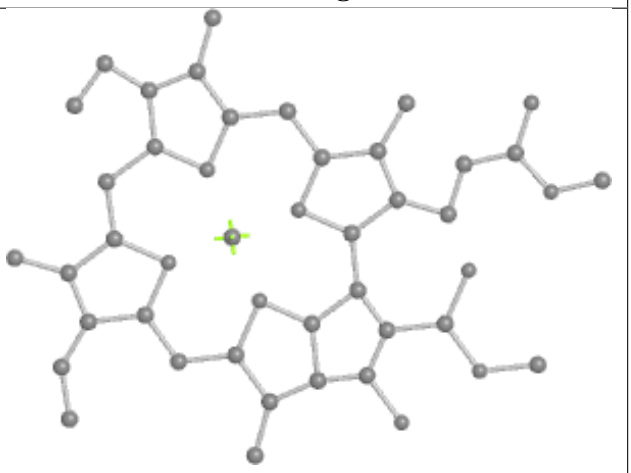
Bond lengths



Bond angles

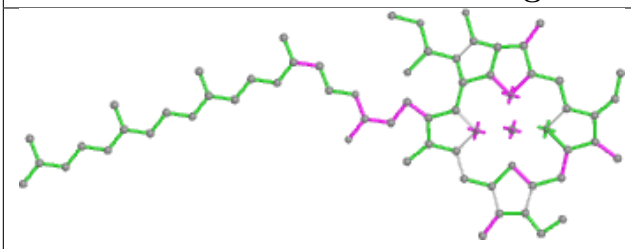


Torsions

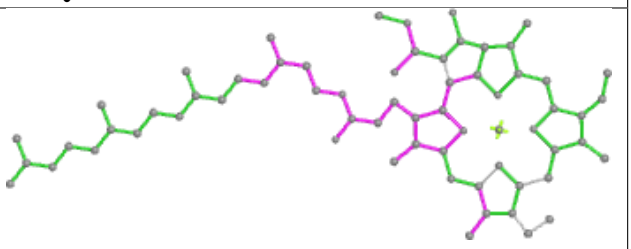


Rings

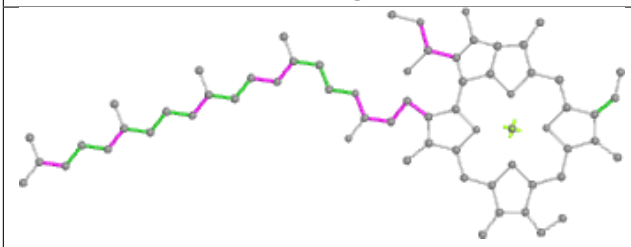
Ligand CLA Q 310



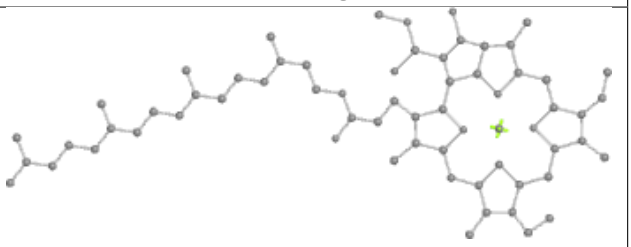
Bond lengths



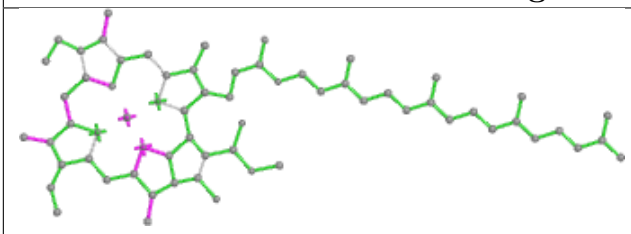
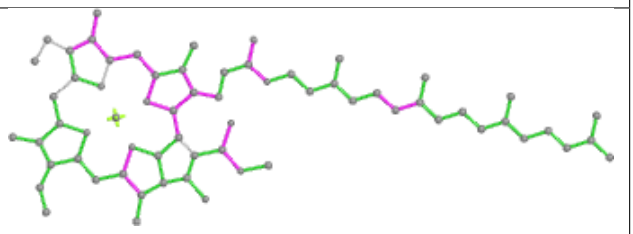
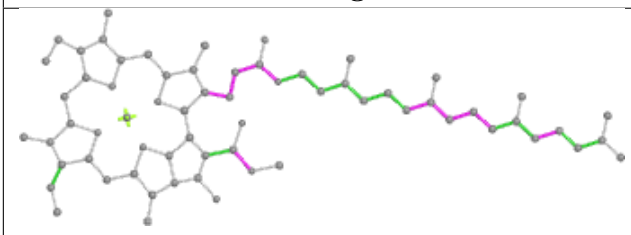
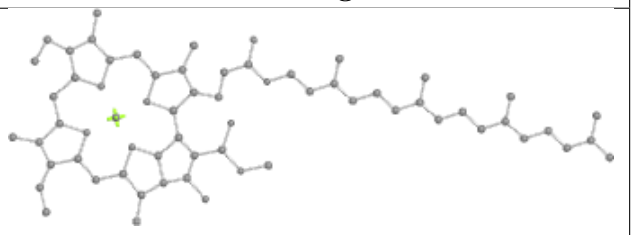
Bond angles

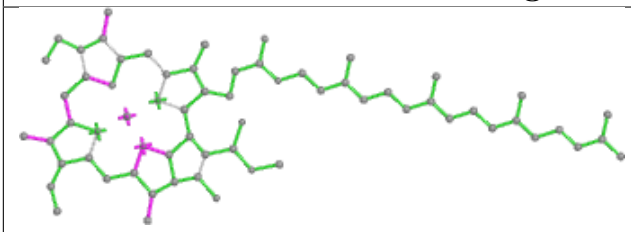
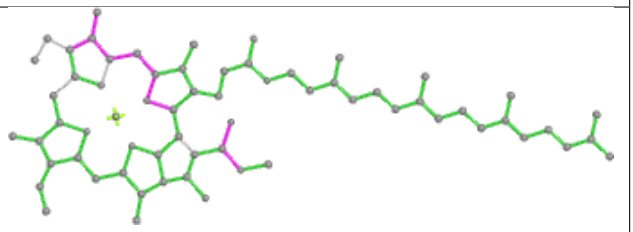
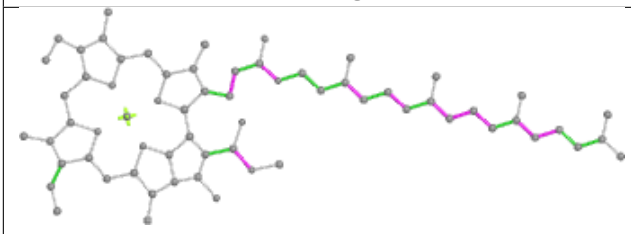
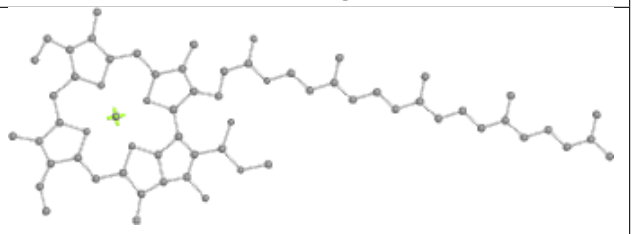


Torsions

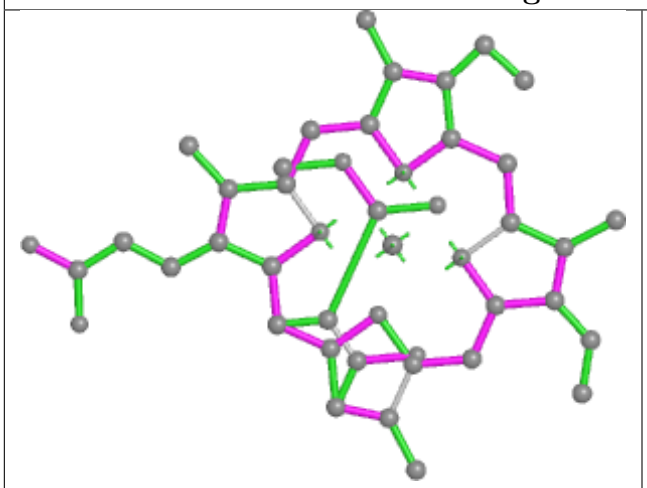


Rings

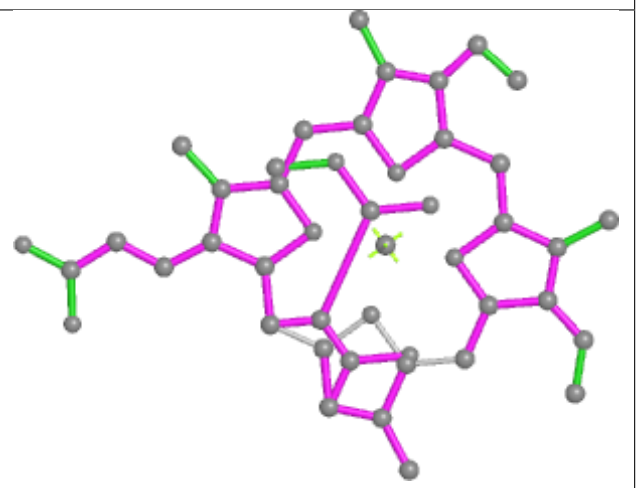
Ligand CLA a 817	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA O 307	
 Bond lengths	 Bond angles
 Torsions	 Rings

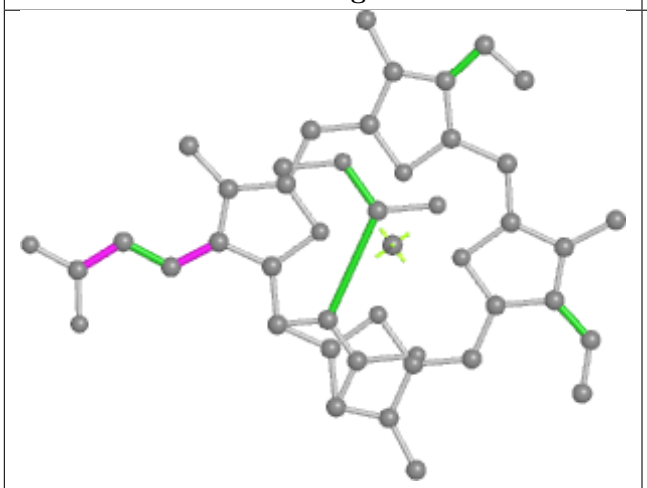
Ligand KC1 M 317



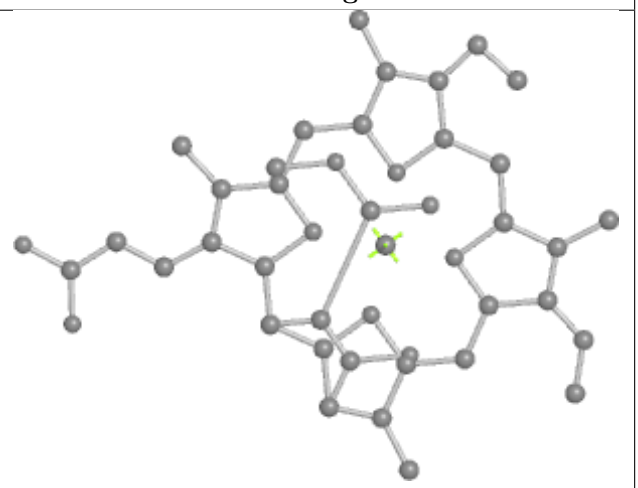
Bond lengths



Bond angles

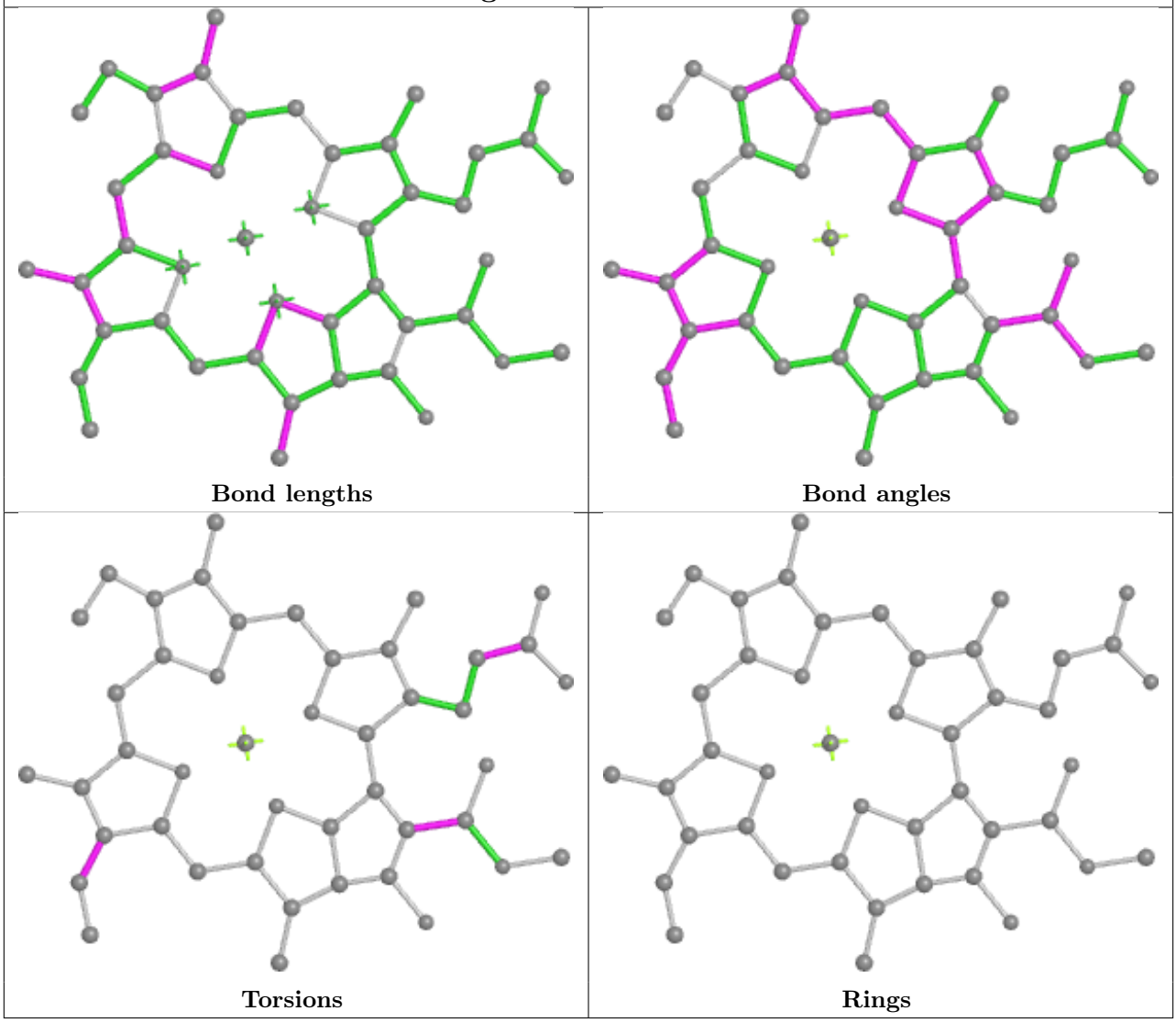


Torsions

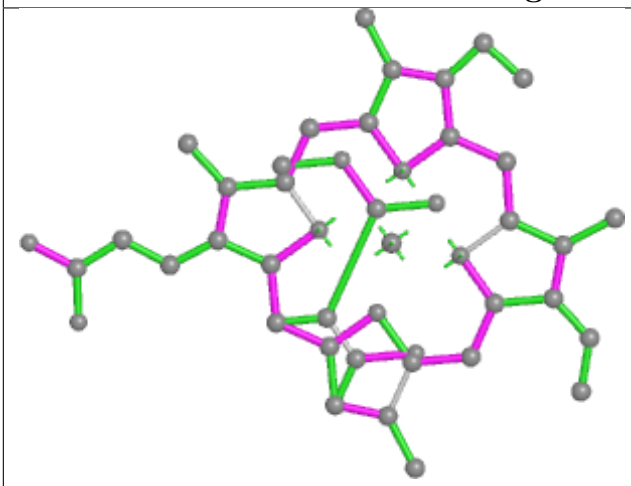


Rings

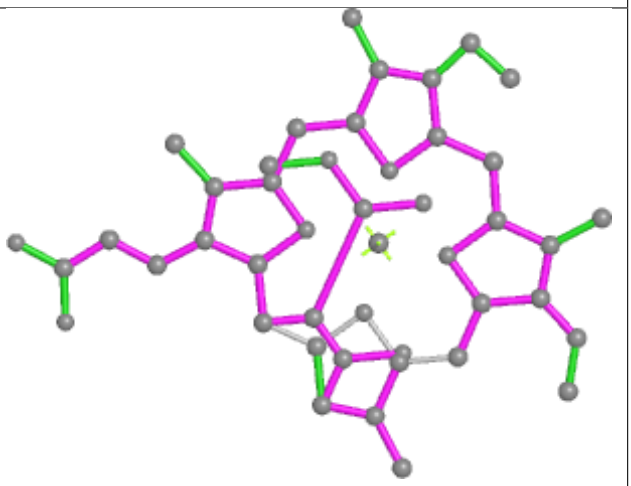
Ligand CLA R 319



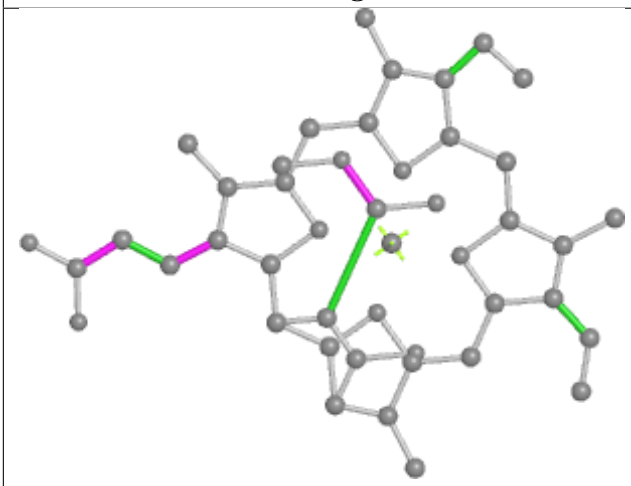
Ligand KC1 H 313



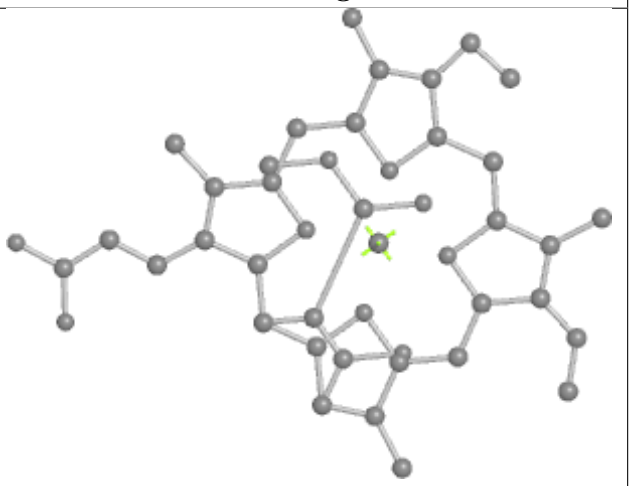
Bond lengths



Bond angles

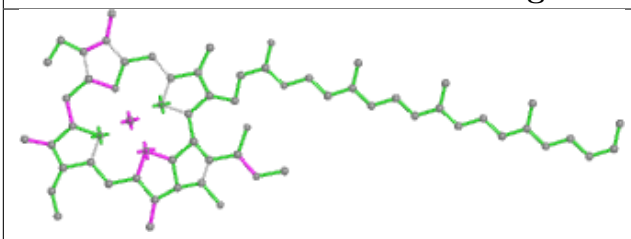


Torsions

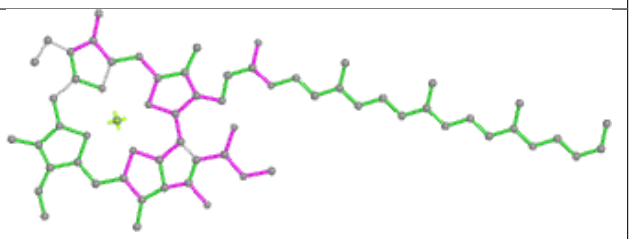


Rings

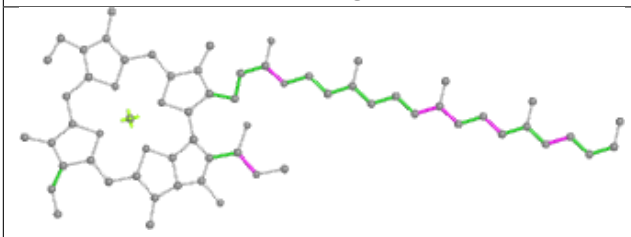
Ligand CLA b 826



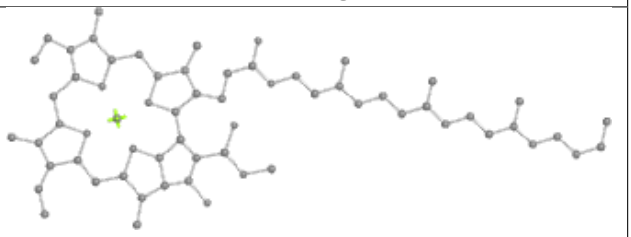
Bond lengths



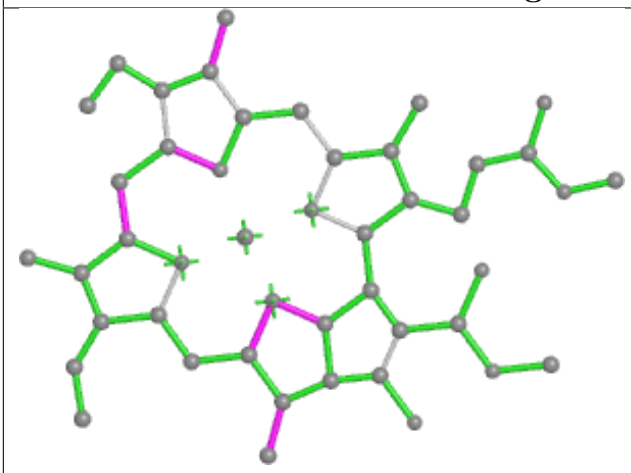
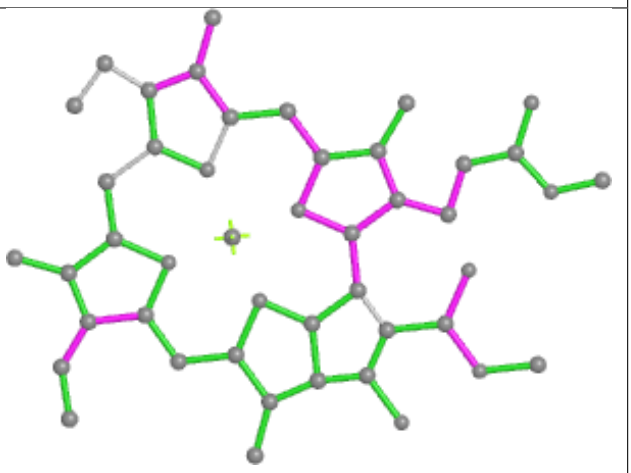
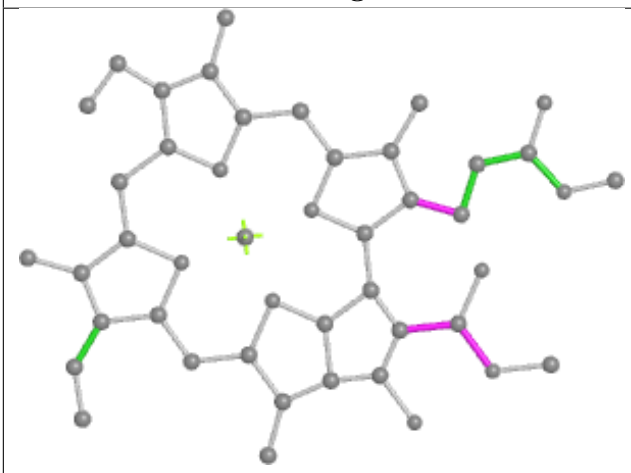
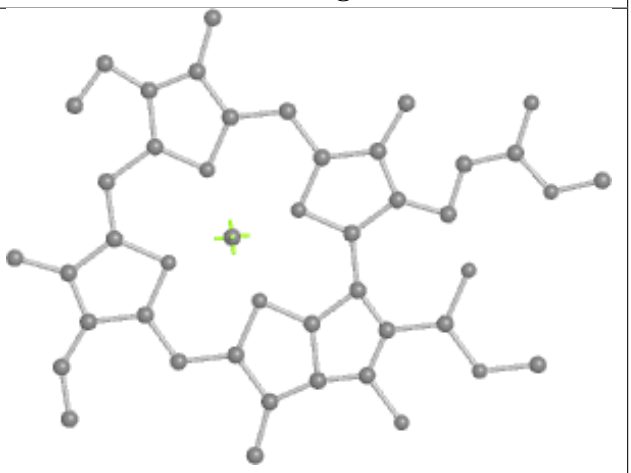
Bond angles



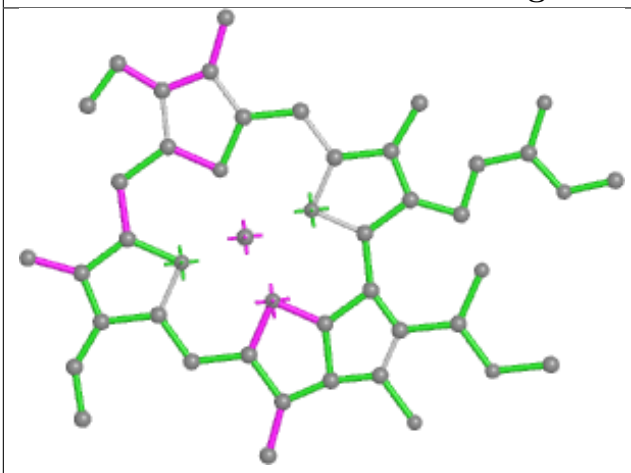
Torsions



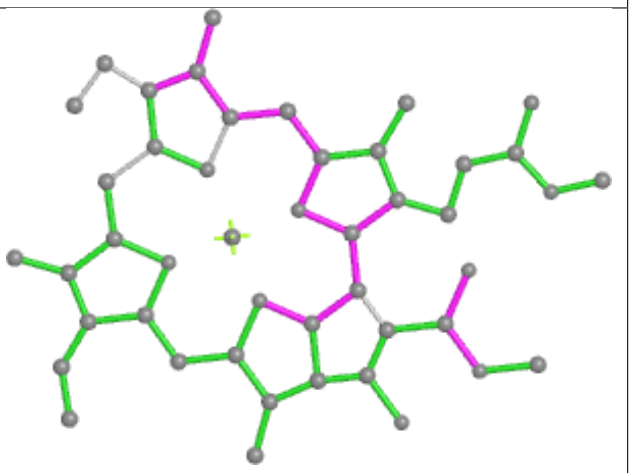
Rings

Ligand CLA T 312	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

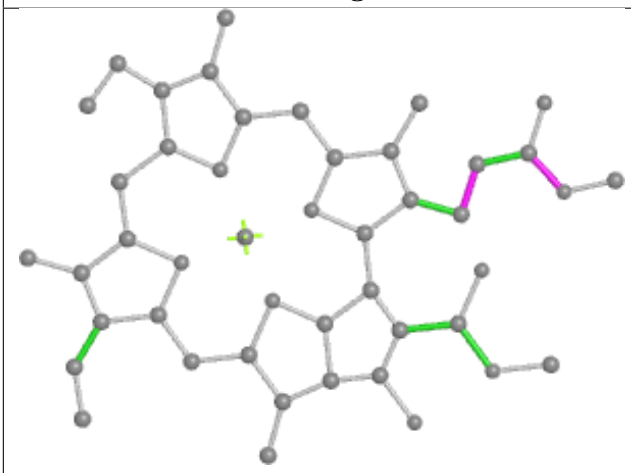
Ligand CLA J 311



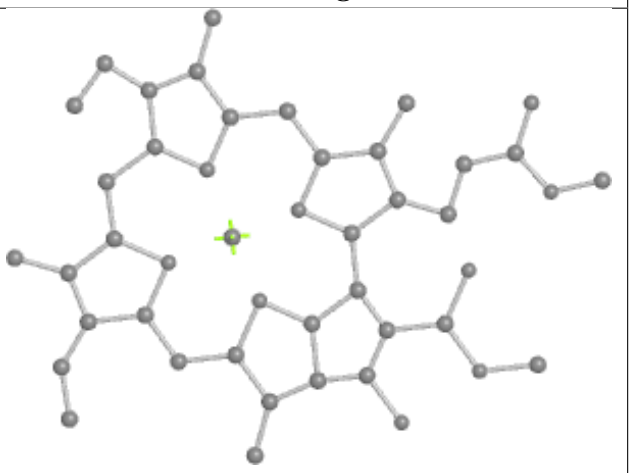
Bond lengths



Bond angles

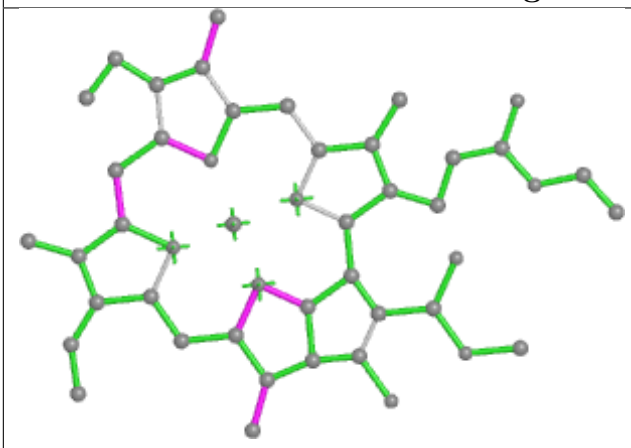


Torsions

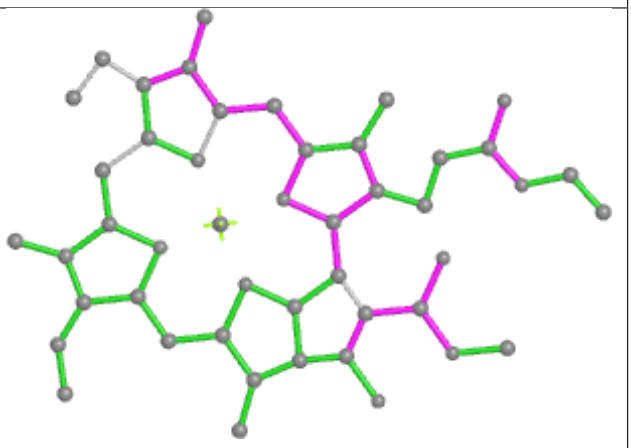


Rings

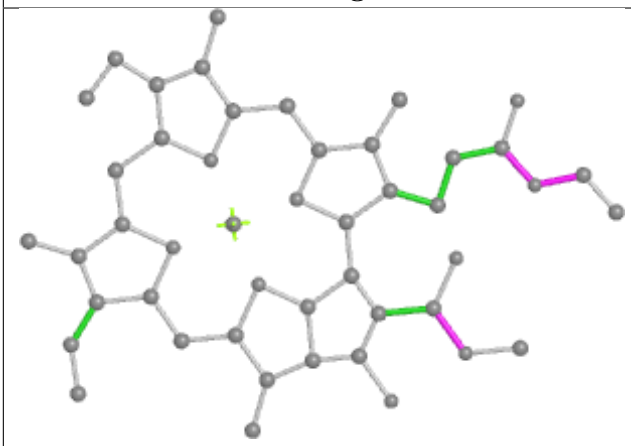
Ligand CLA N 318



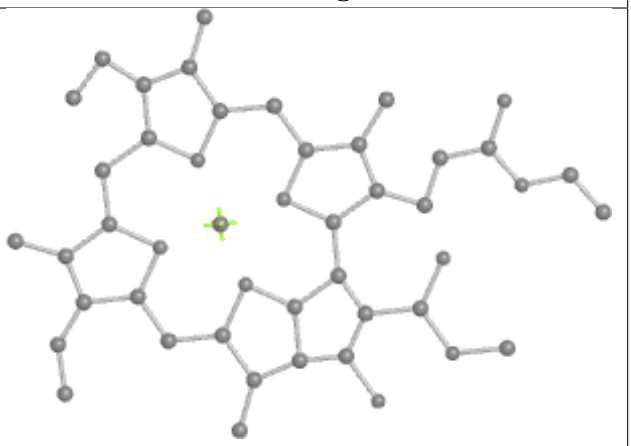
Bond lengths



Bond angles

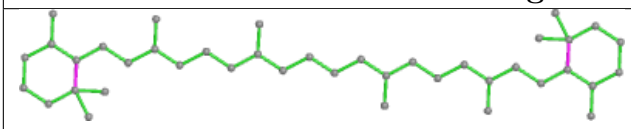


Torsions

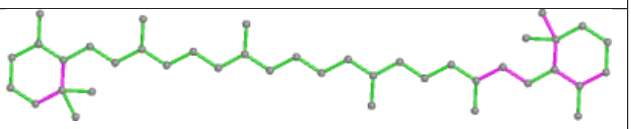


Rings

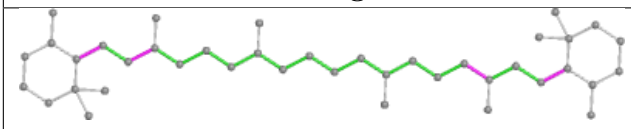
Ligand BCR a 844



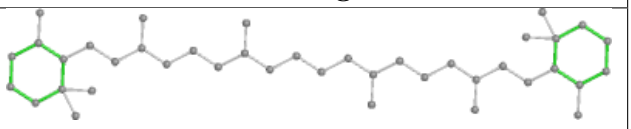
Bond lengths



Bond angles

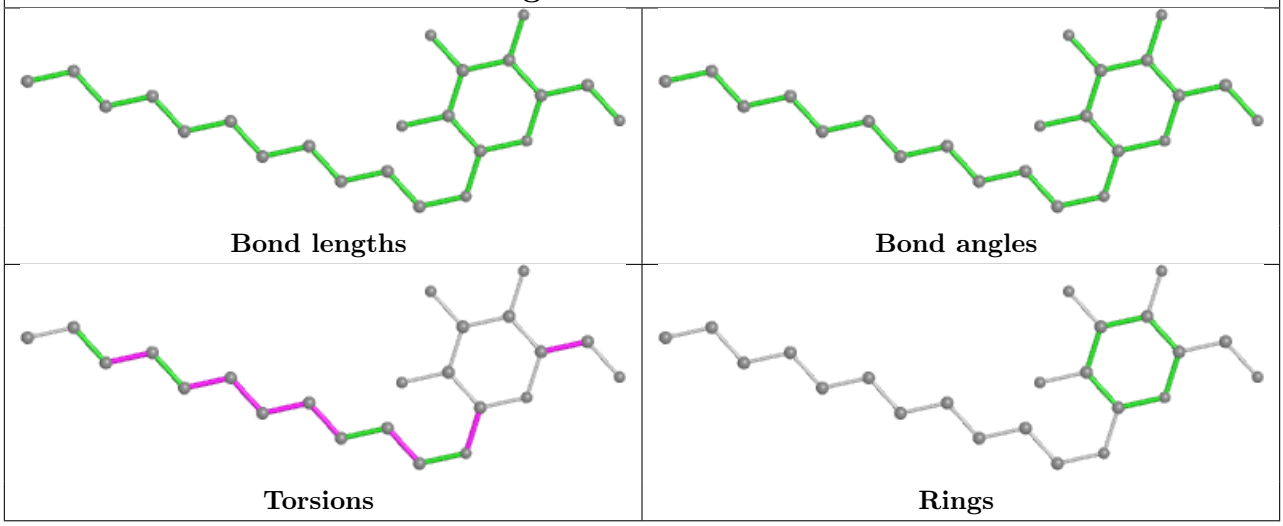


Torsions

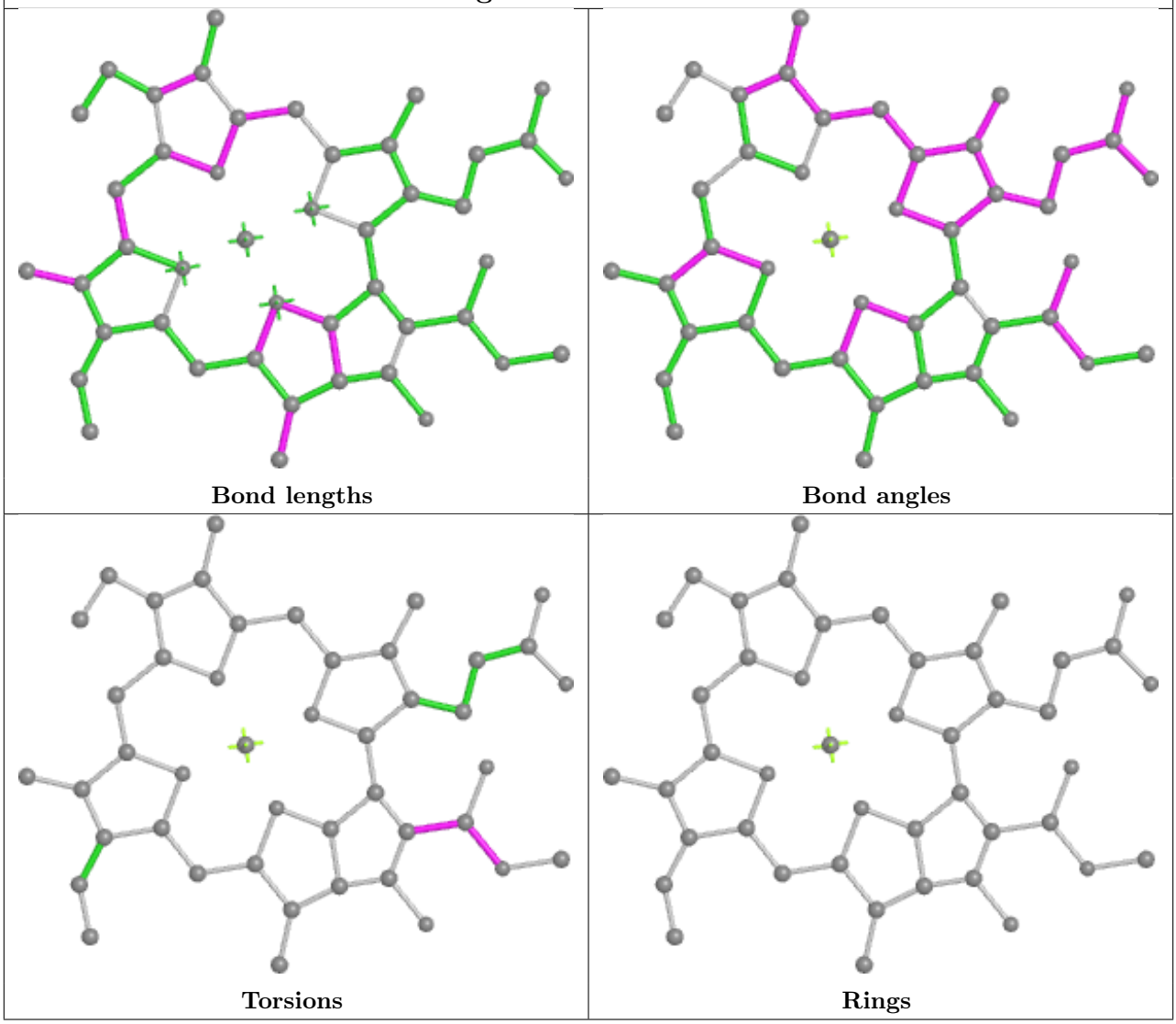


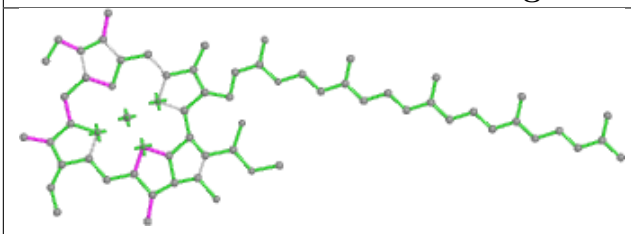
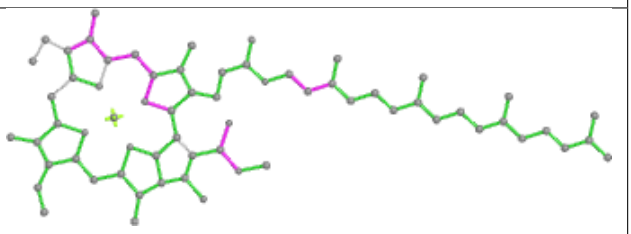
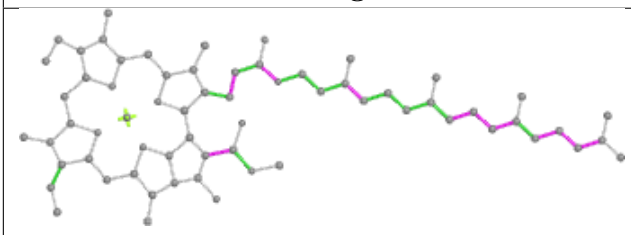
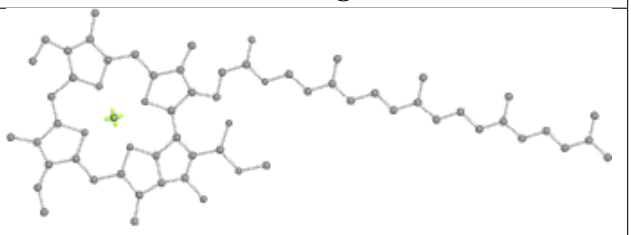
Rings

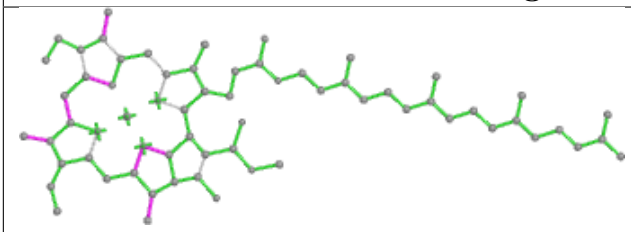
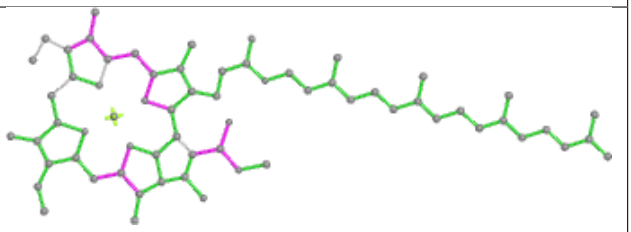
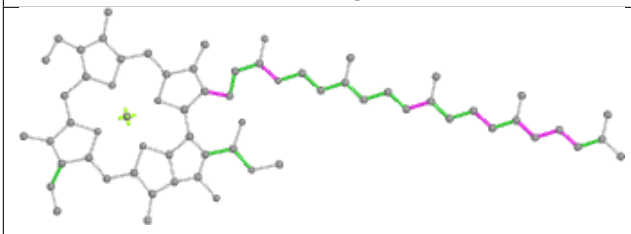
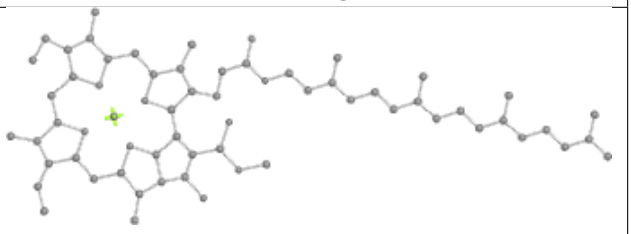
Ligand LMT P 321



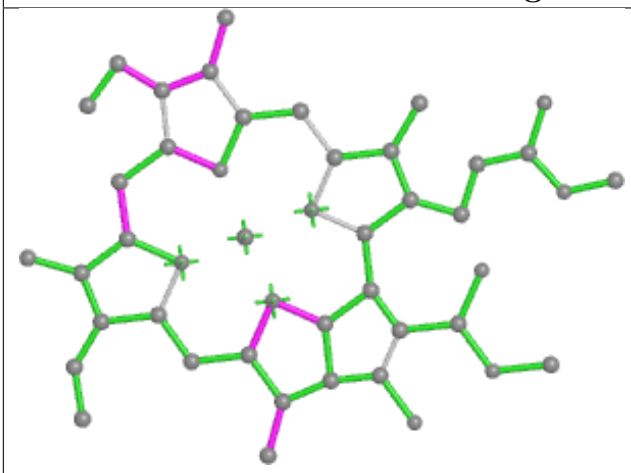
Ligand CLA W 216



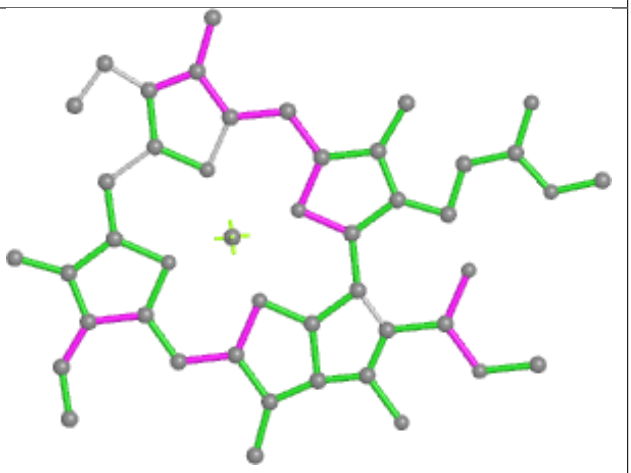
Ligand CLA H 309	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA H 311	
 Bond lengths	 Bond angles
 Torsions	 Rings

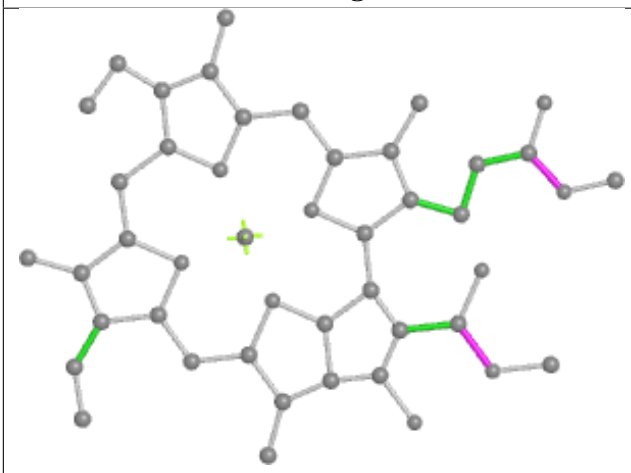
Ligand CLA B 306



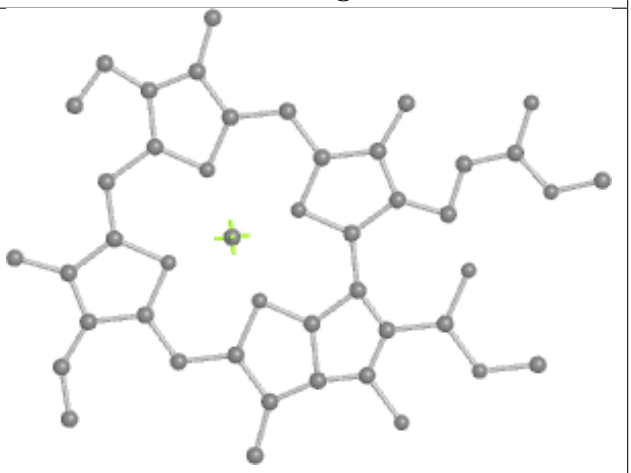
Bond lengths



Bond angles

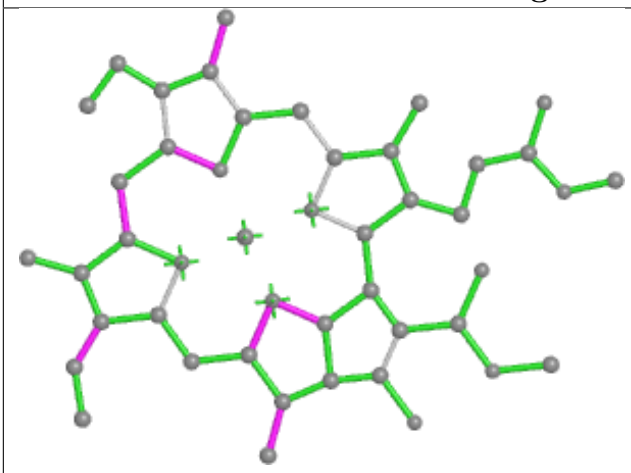


Torsions

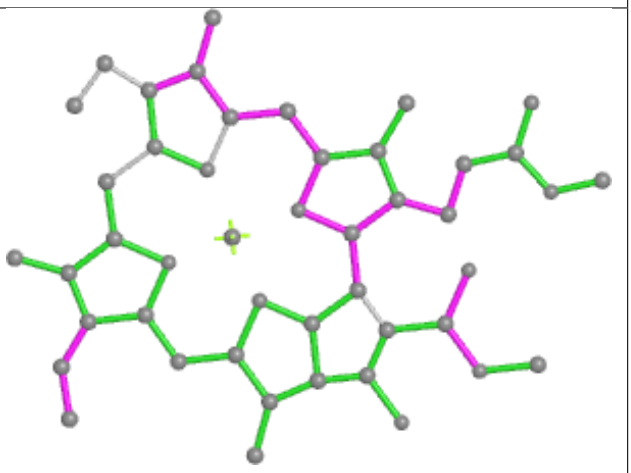


Rings

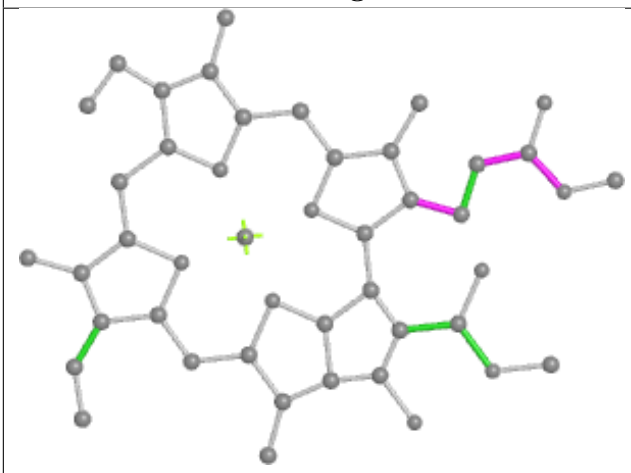
Ligand CLA I 309



Bond lengths



Bond angles



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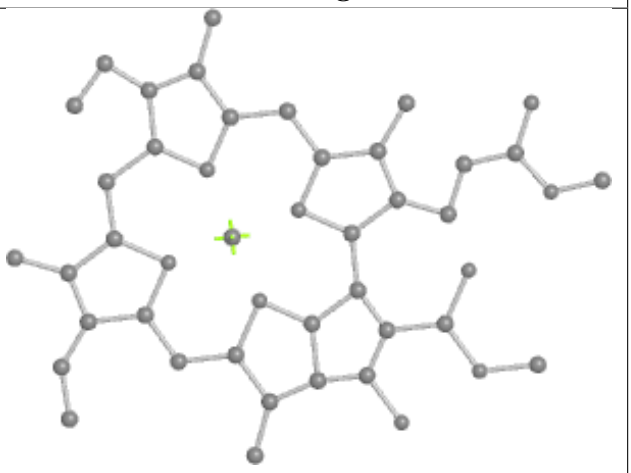
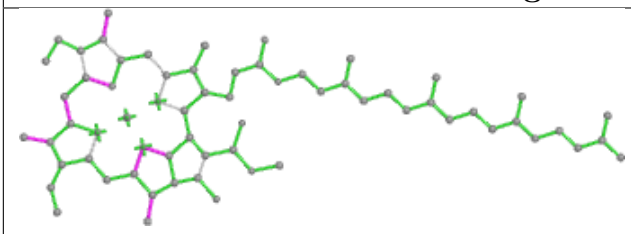
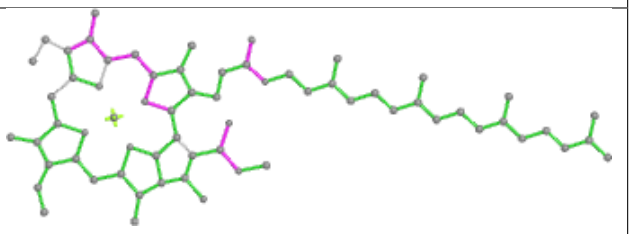


Rings

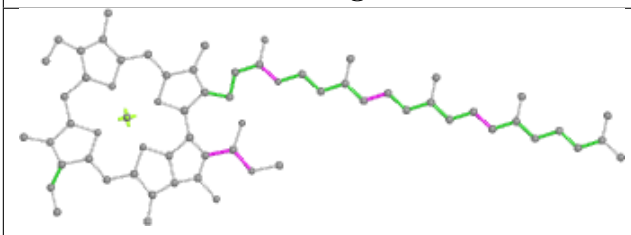
Ligand CLA V 310



Bond lengths



Bond angles



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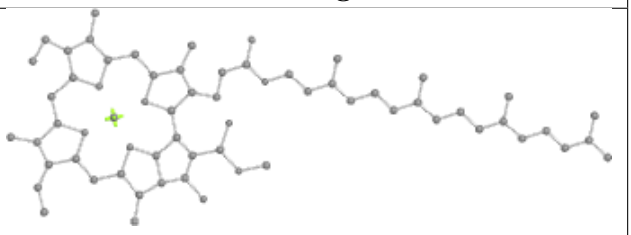
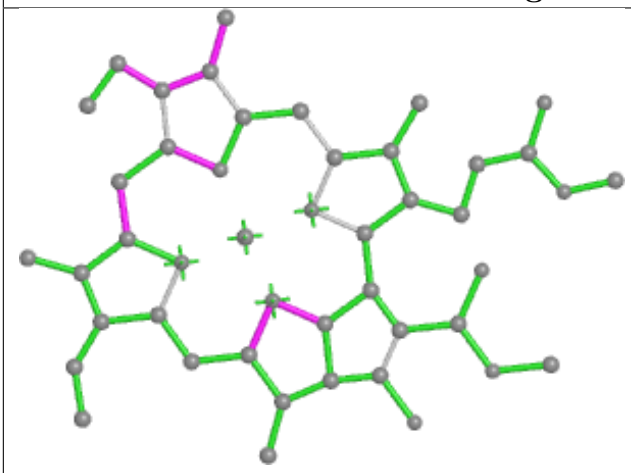
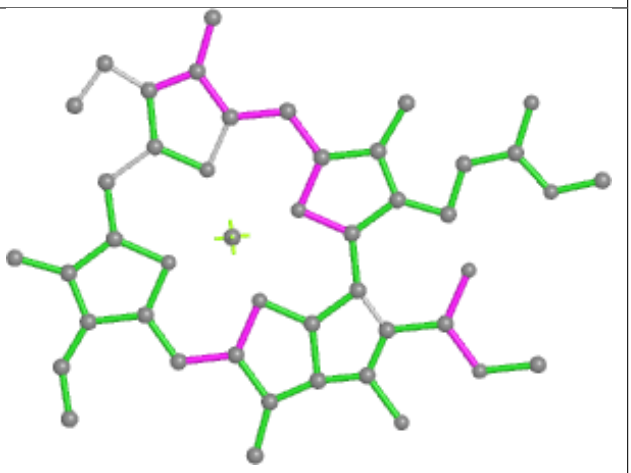


Rings

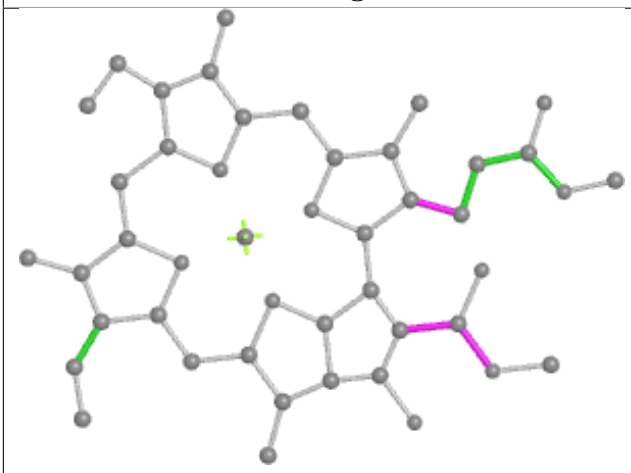
Ligand CLA E 317



Bond lengths



Bond angles



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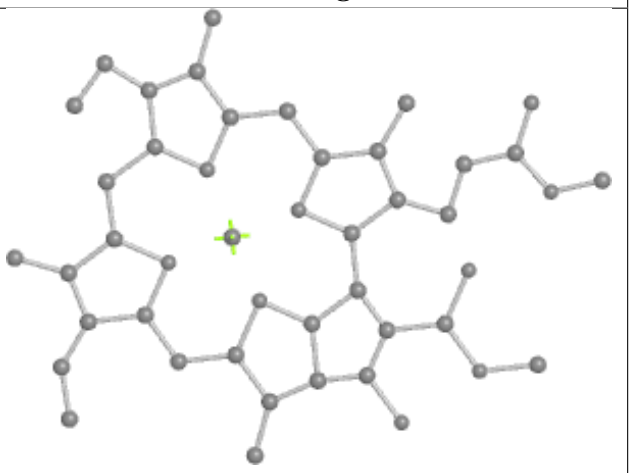
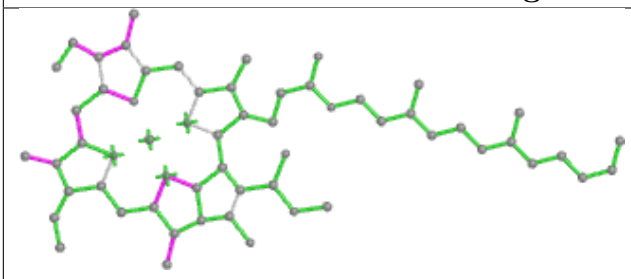
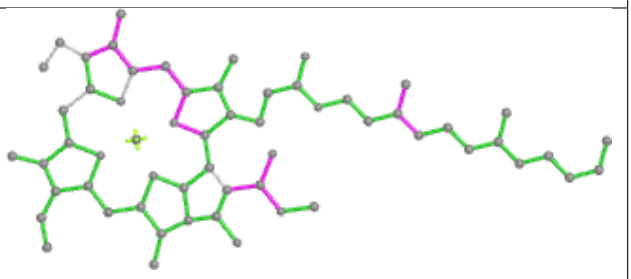


Rings

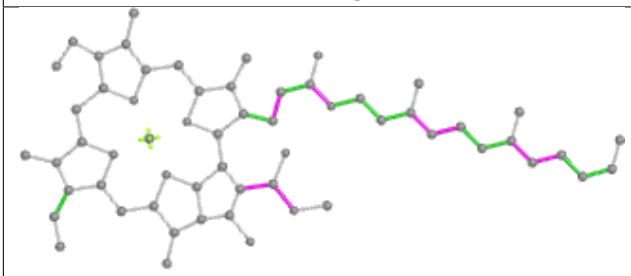
Ligand CLA K 309



Bond lengths



Bond angles



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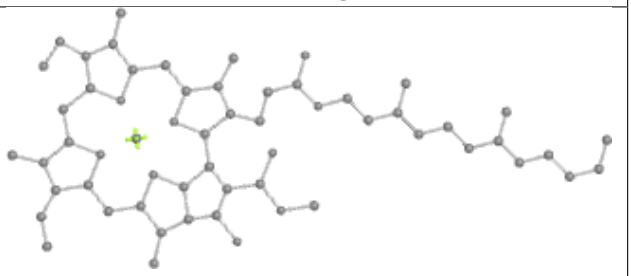
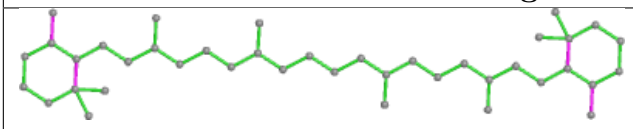
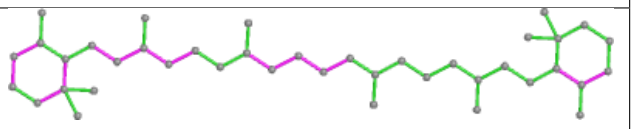


Rings

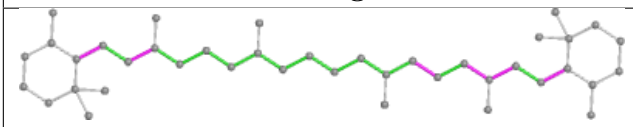
Ligand BCR m 101



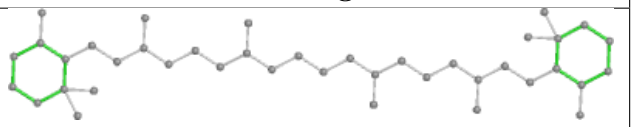
Bond lengths



Bond angles

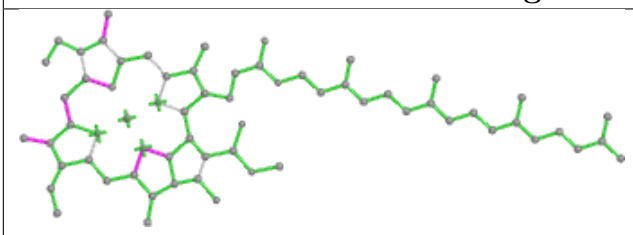


Torsions

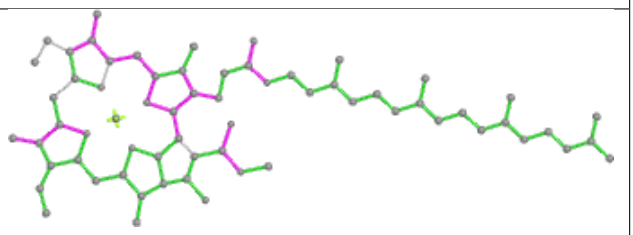


Rings

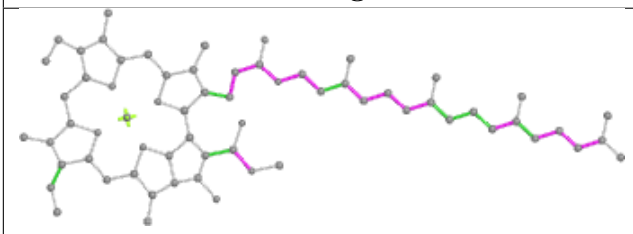
Ligand CLA V 306



Bond lengths



Bond angles



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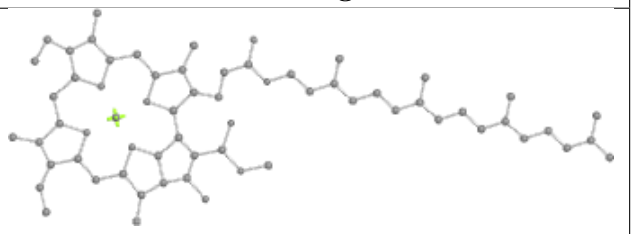
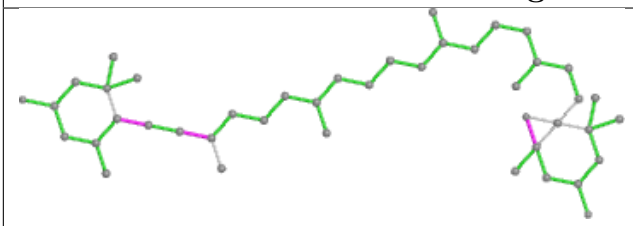
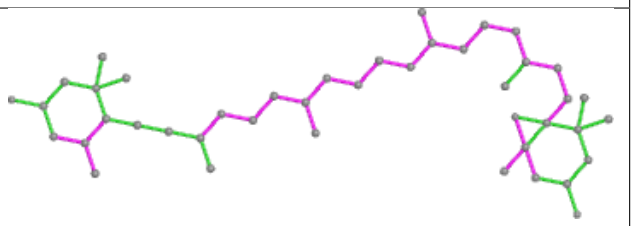


Rings

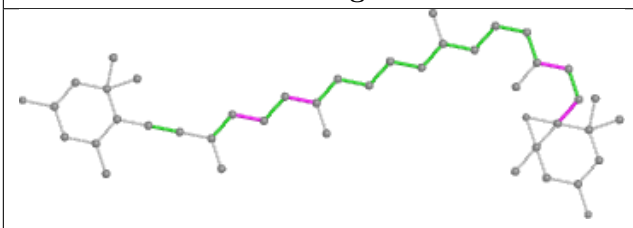
Ligand DD6 L 305



Bond lengths



Bond angles



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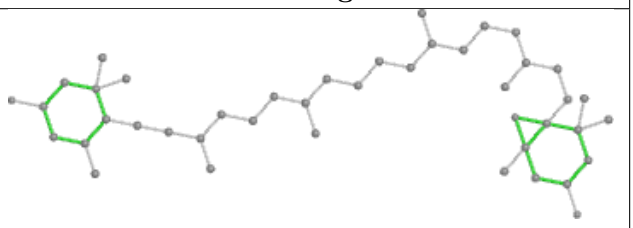
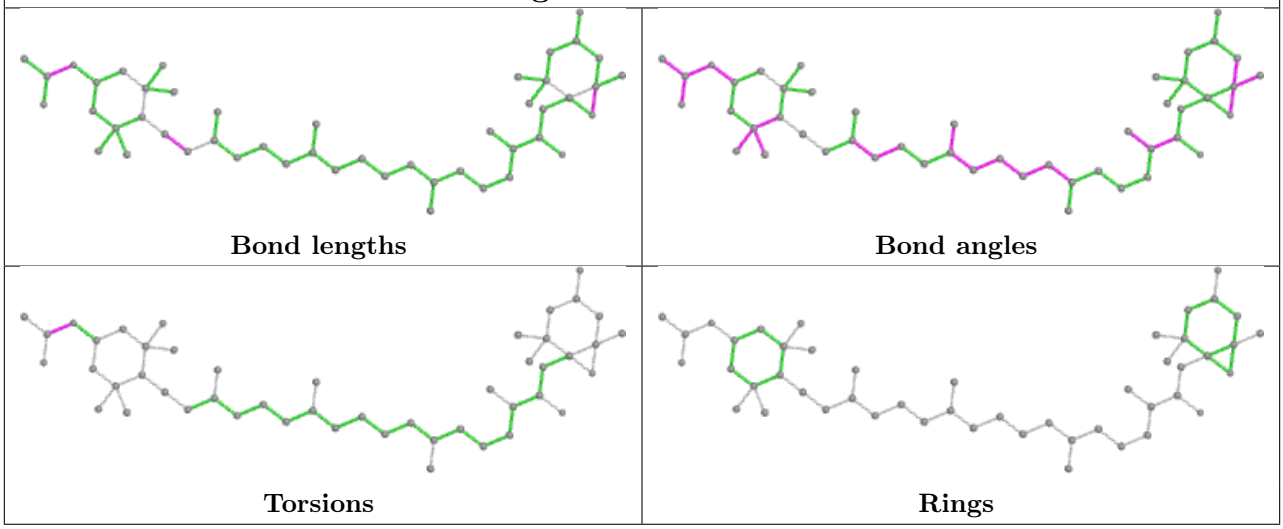
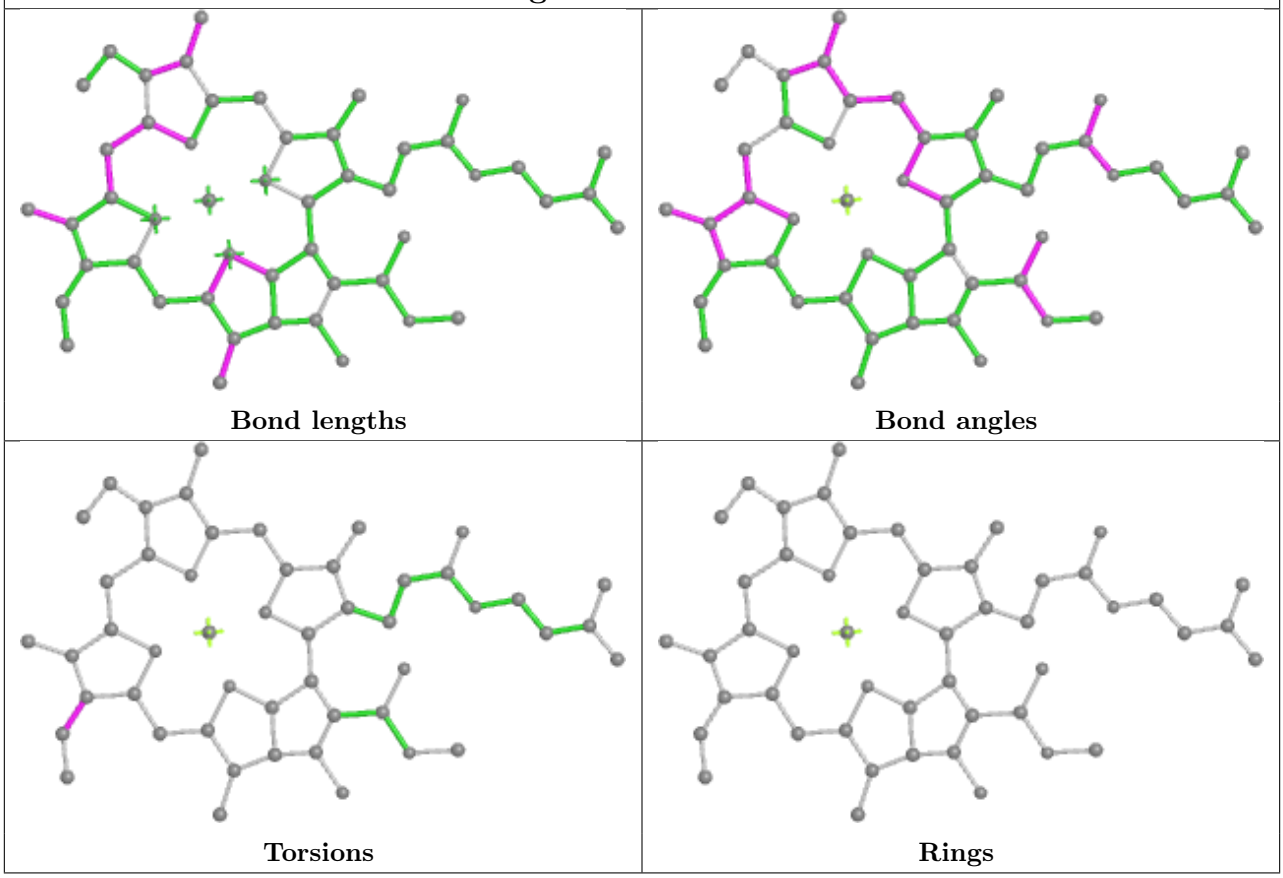


Rings

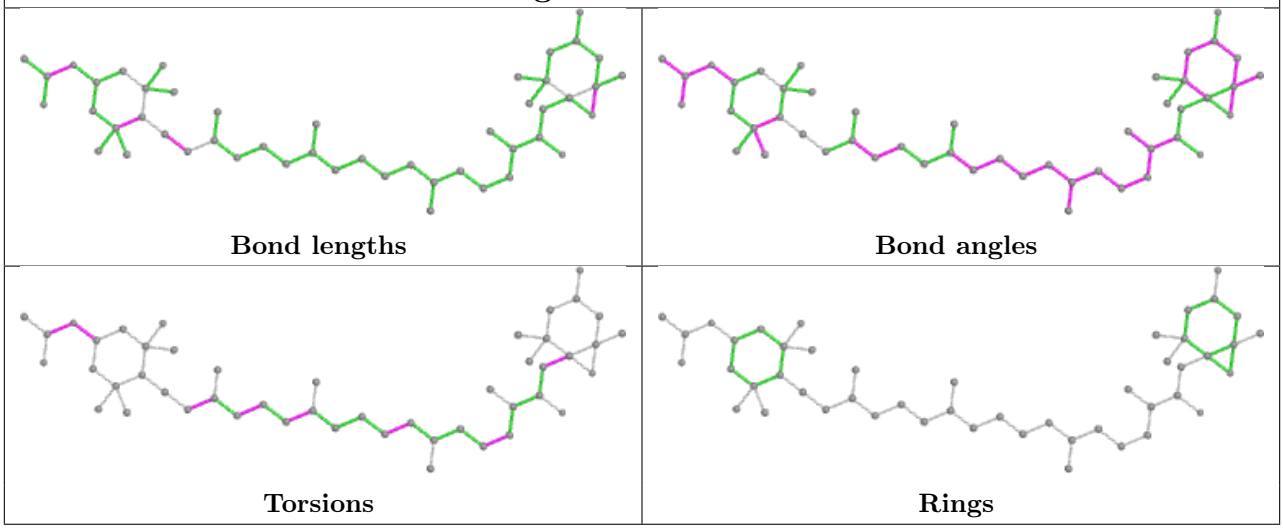
Ligand A86 P 307



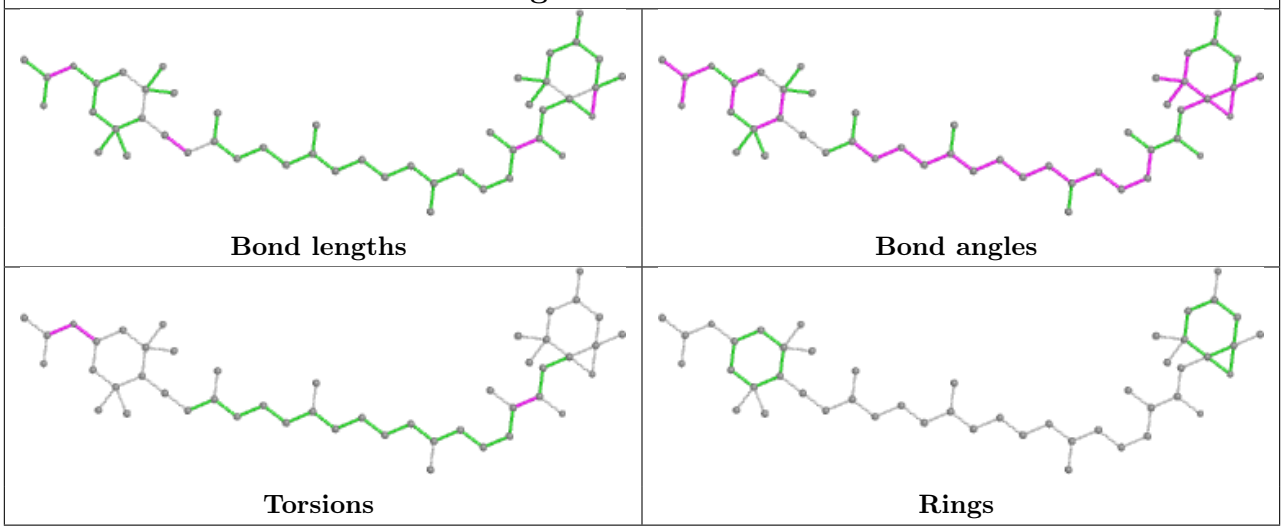
Ligand CLA a 814



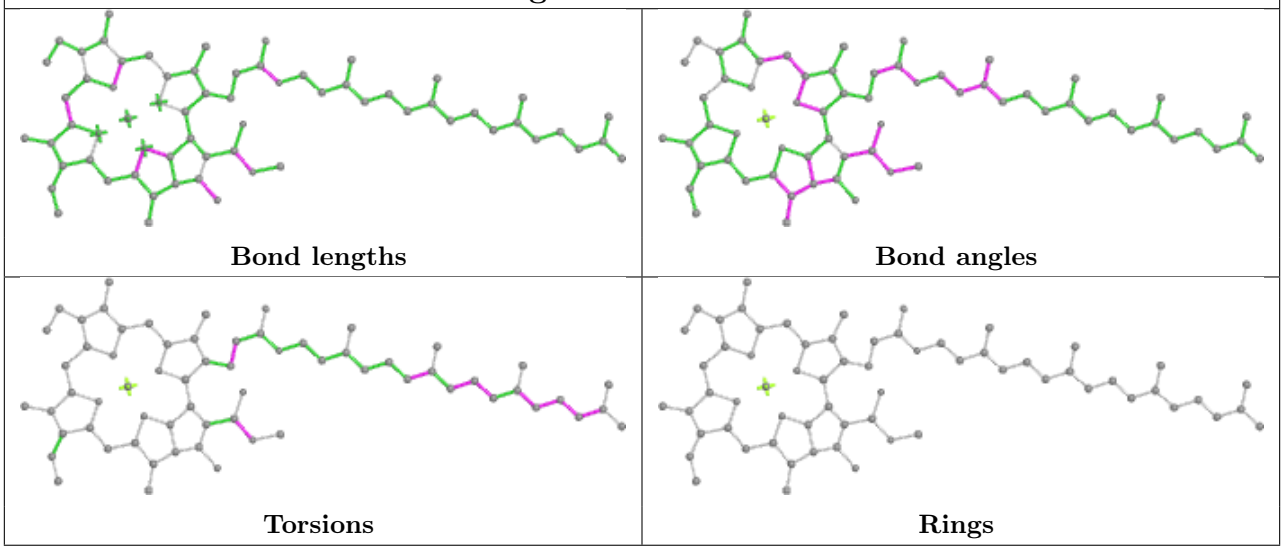
Ligand A86 S 308



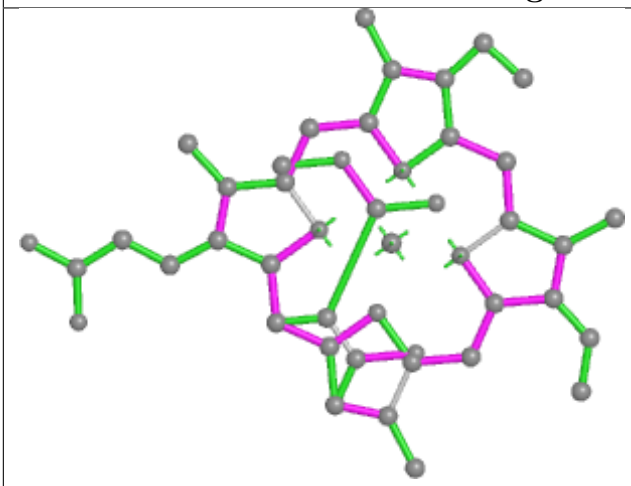
Ligand A86 X 302



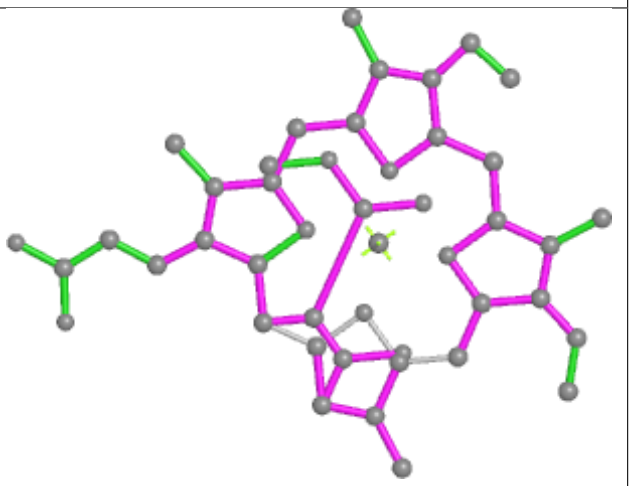
Ligand CLA a 802



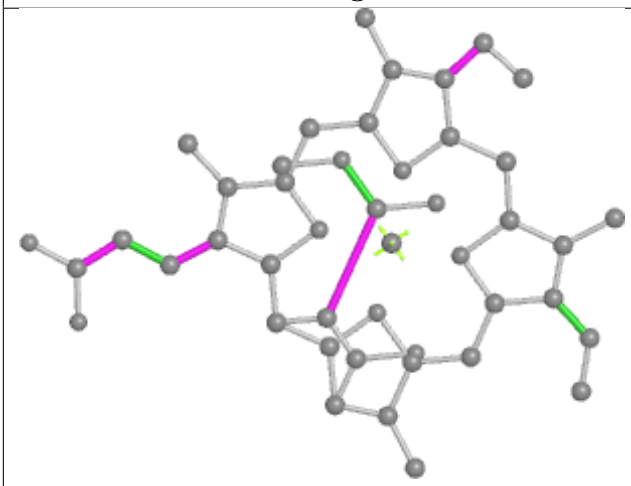
Ligand KC1 C 213



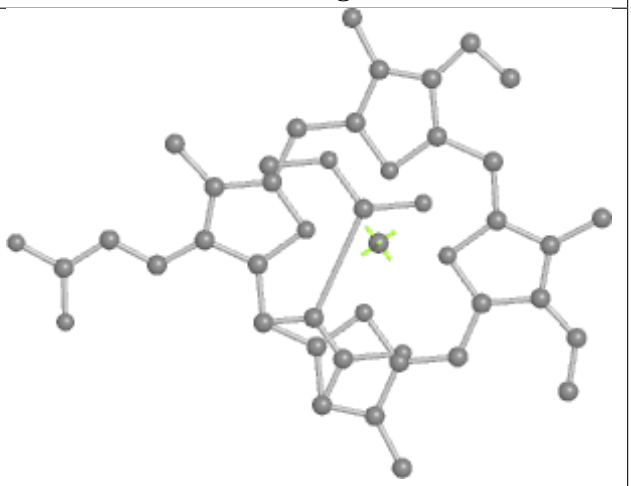
Bond lengths



Bond angles

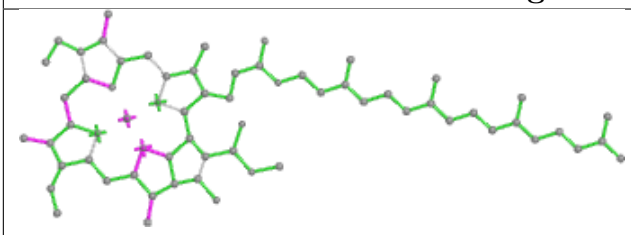


Torsions

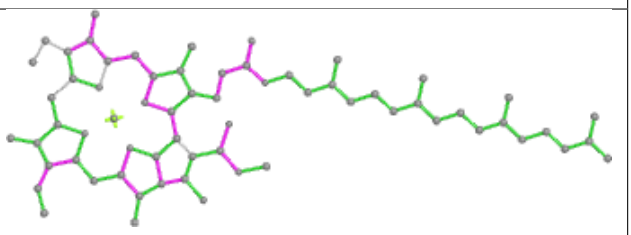


Rings

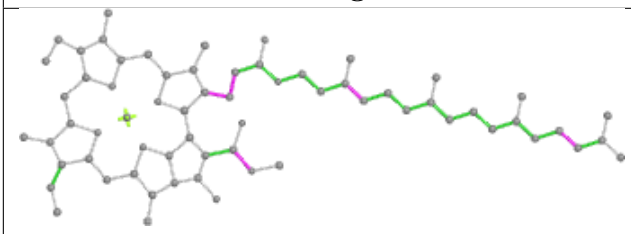
Ligand CLA b 801



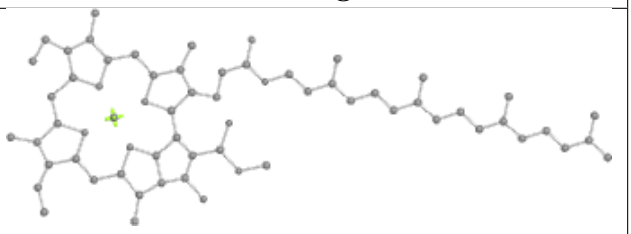
Bond lengths



Bond angles

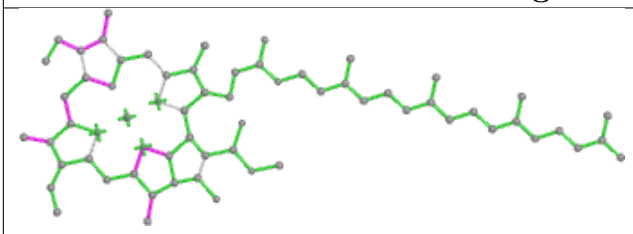


Torsions

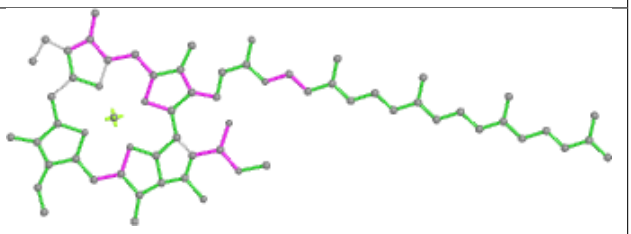


Rings

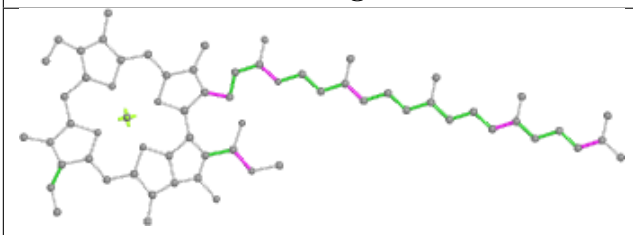
Ligand CLA l 202



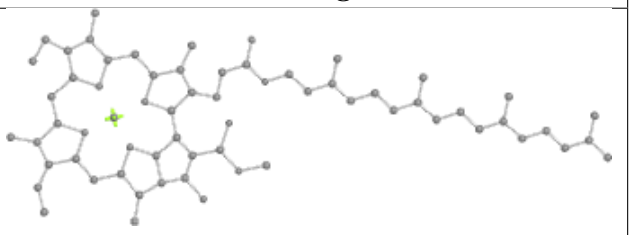
Bond lengths



Bond angles

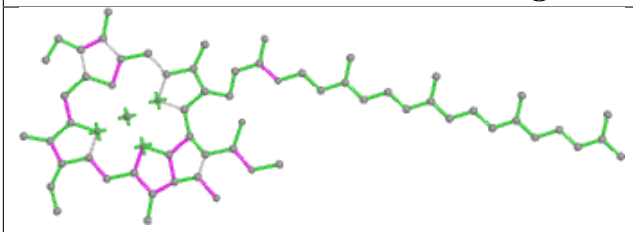


Torsions

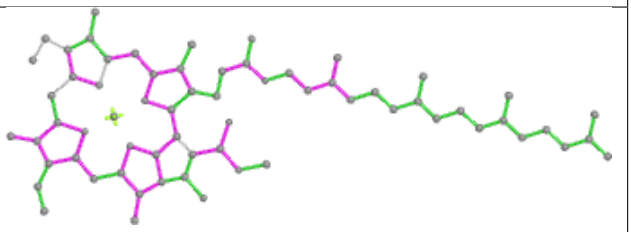


Rings

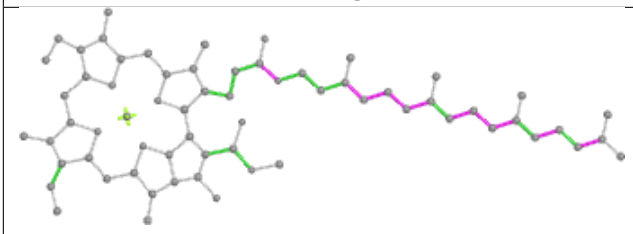
Ligand CLA I 306



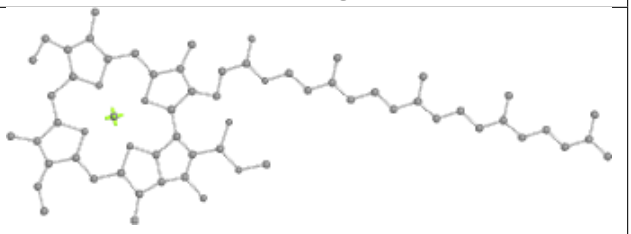
Bond lengths



Bond angles

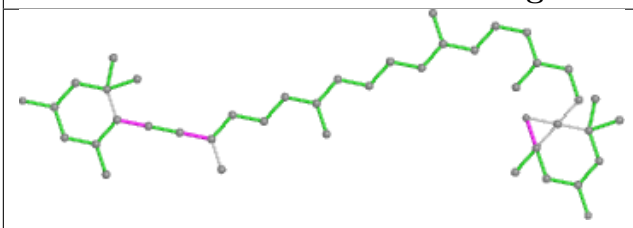


Torsions

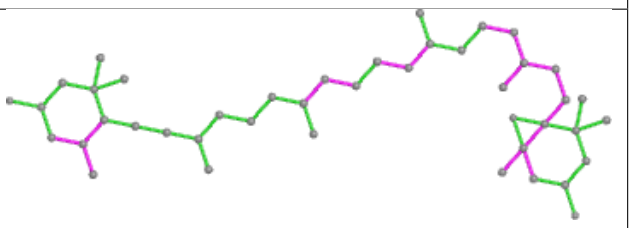


Rings

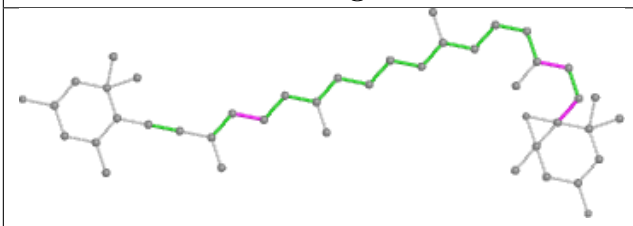
Ligand DD6 E 301



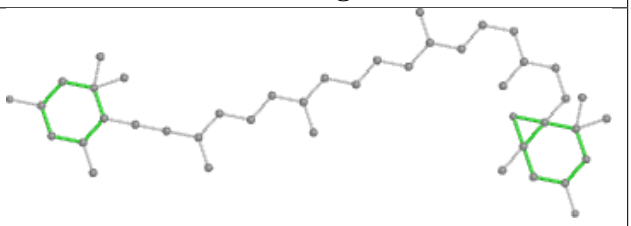
Bond lengths



Bond angles

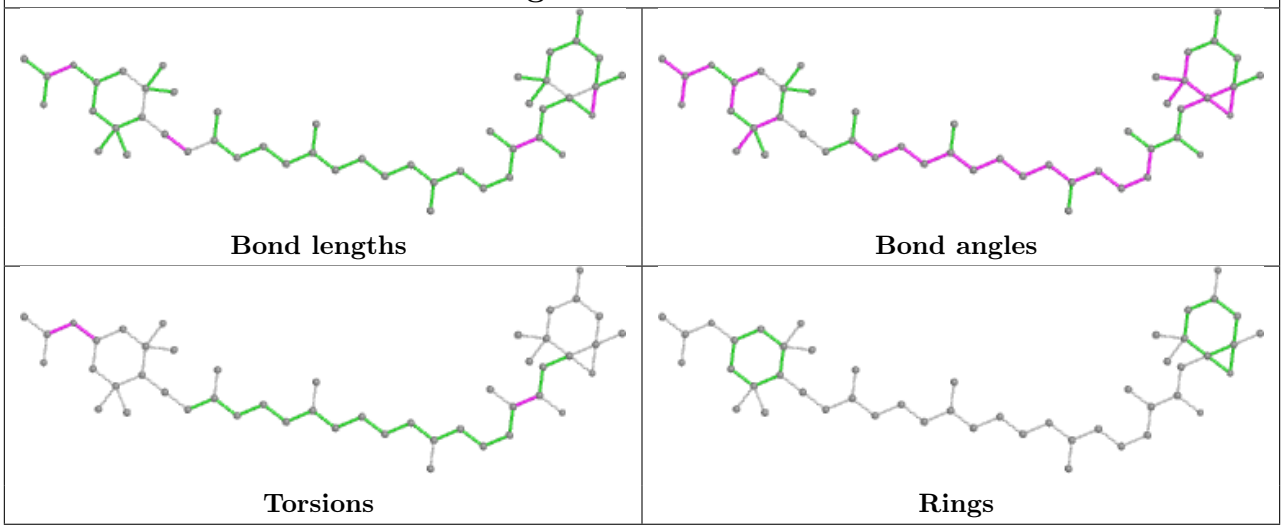


Torsions

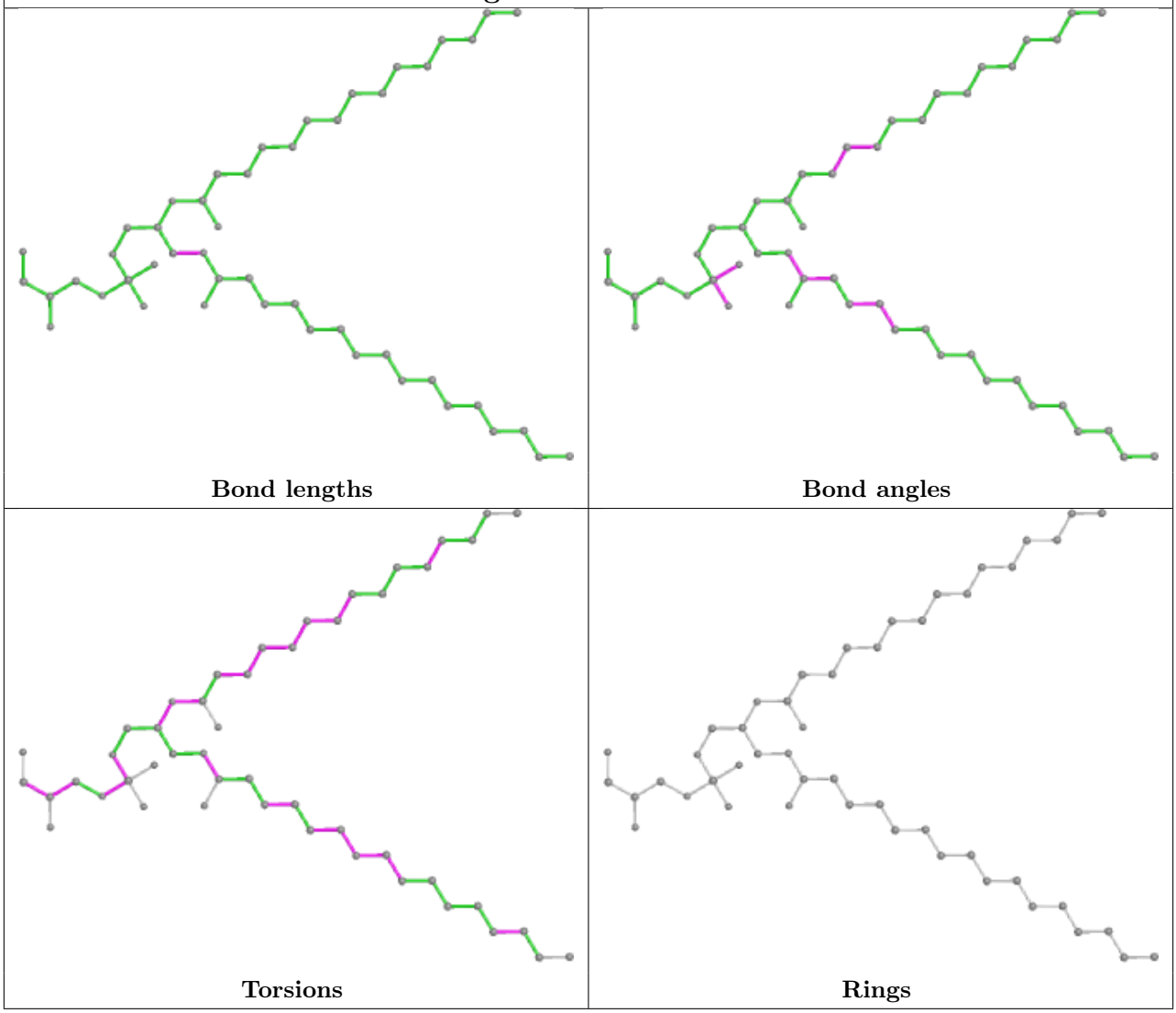


Rings

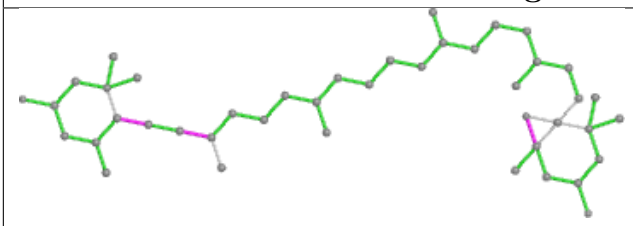
Ligand A86 M 302



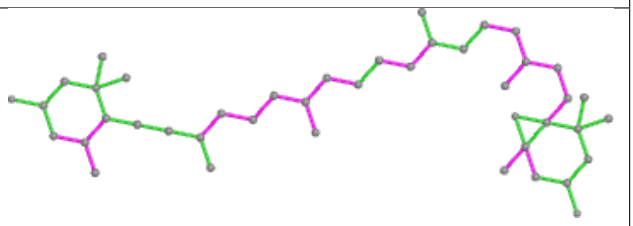
Ligand LHG a 842



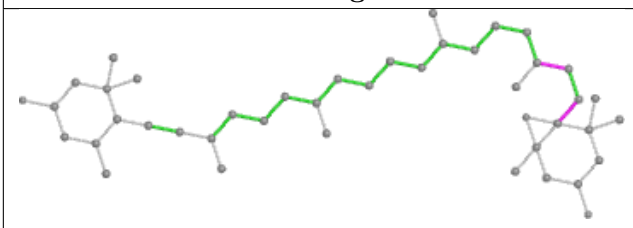
Ligand DD6 A 304



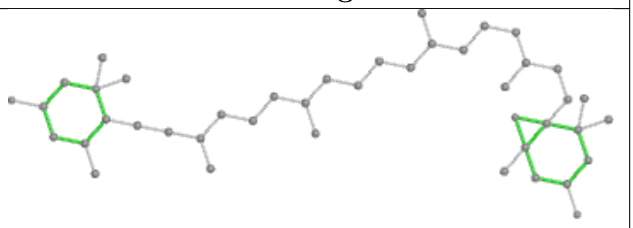
Bond lengths



Bond angles

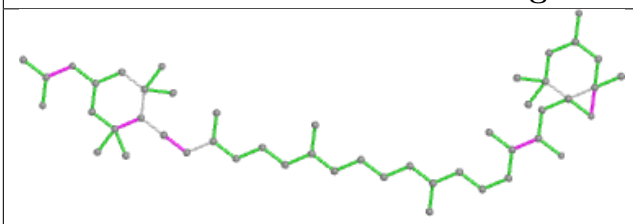


Torsions



Rings

Ligand A86 O 303



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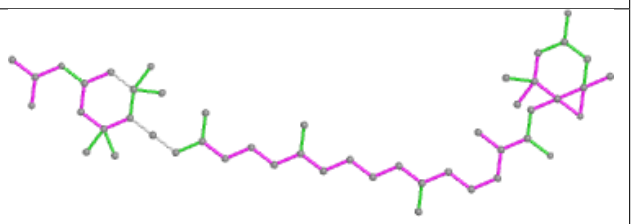
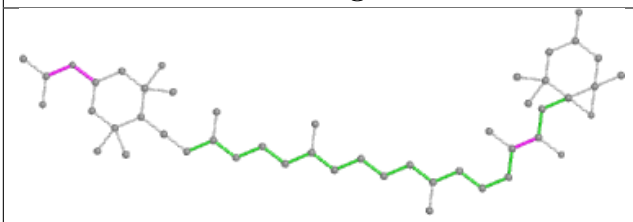


Bond angles



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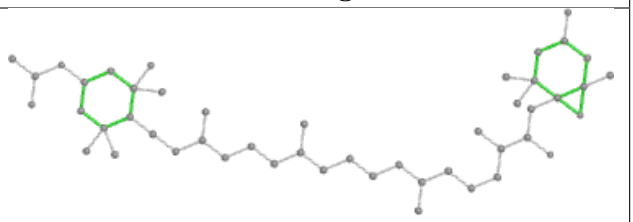
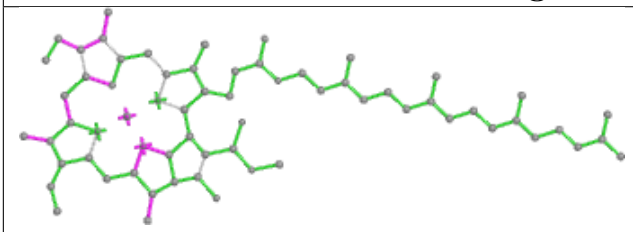
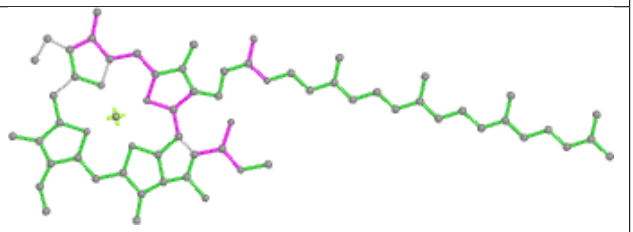


Rings

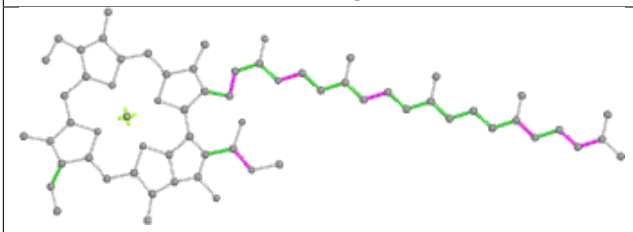
Ligand CLA a 808



Bond lengths



Bond angles



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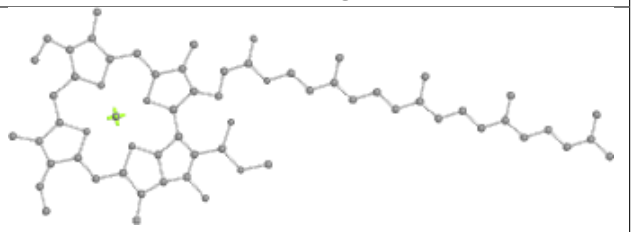
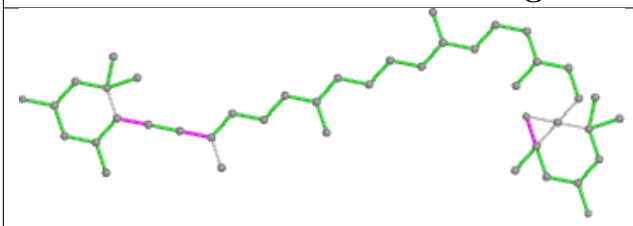
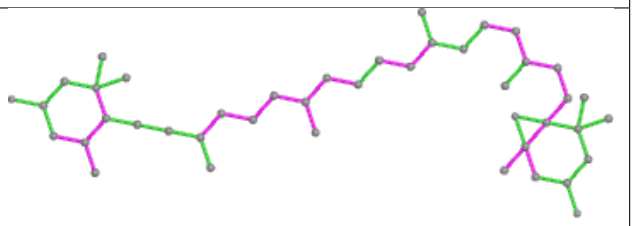


Rings

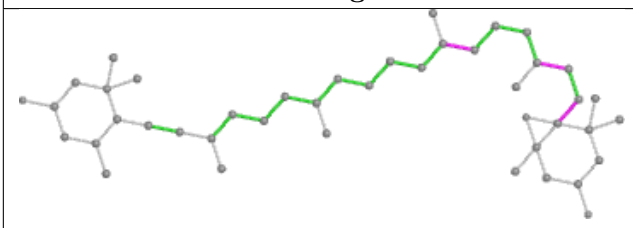
Ligand DD6 C 201



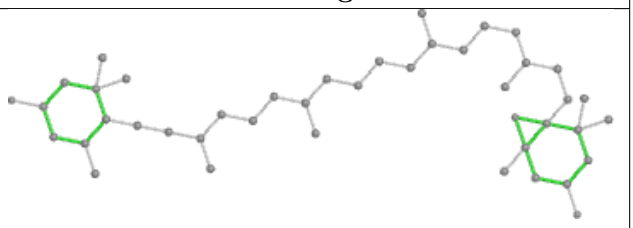
Bond lengths



Bond angles

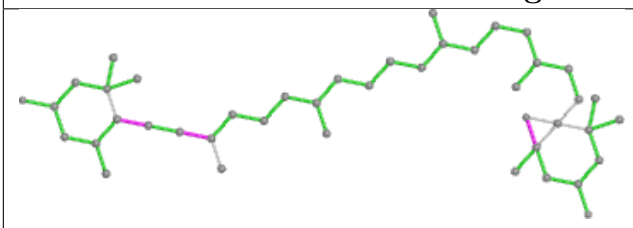


Torsions



Rings

Ligand DD6 D 305



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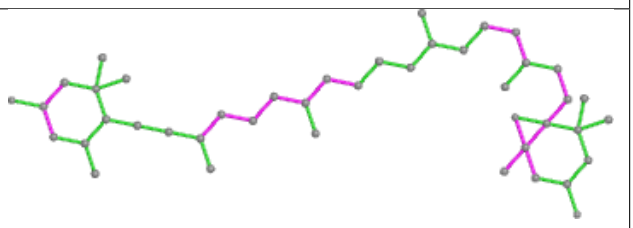
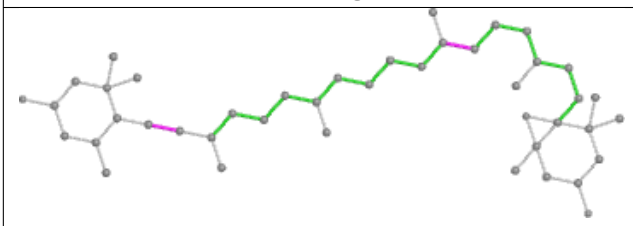
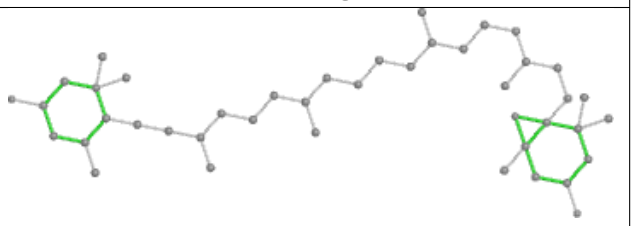


Bond angles

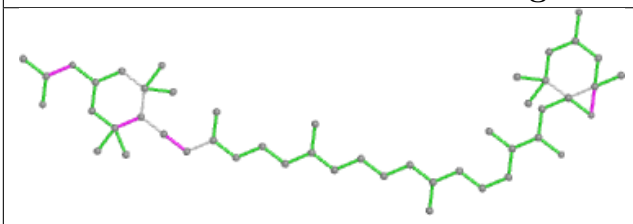


Torsions



Rings

Ligand A86 D 302



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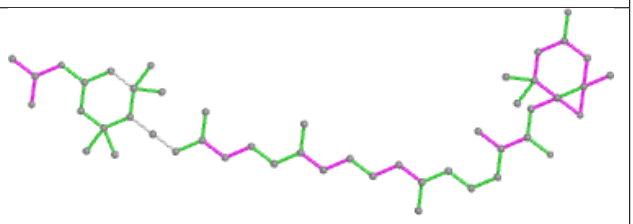
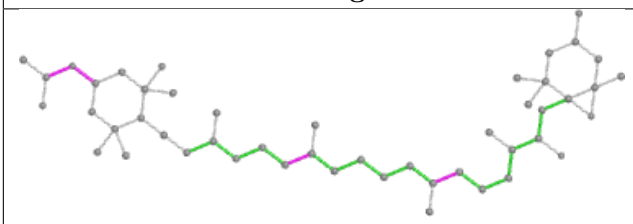
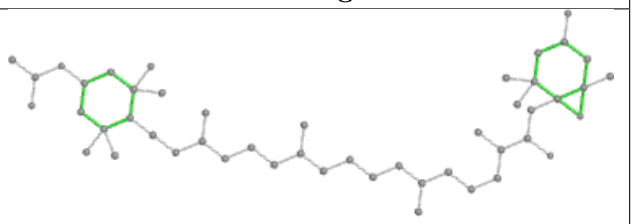


Bond angles

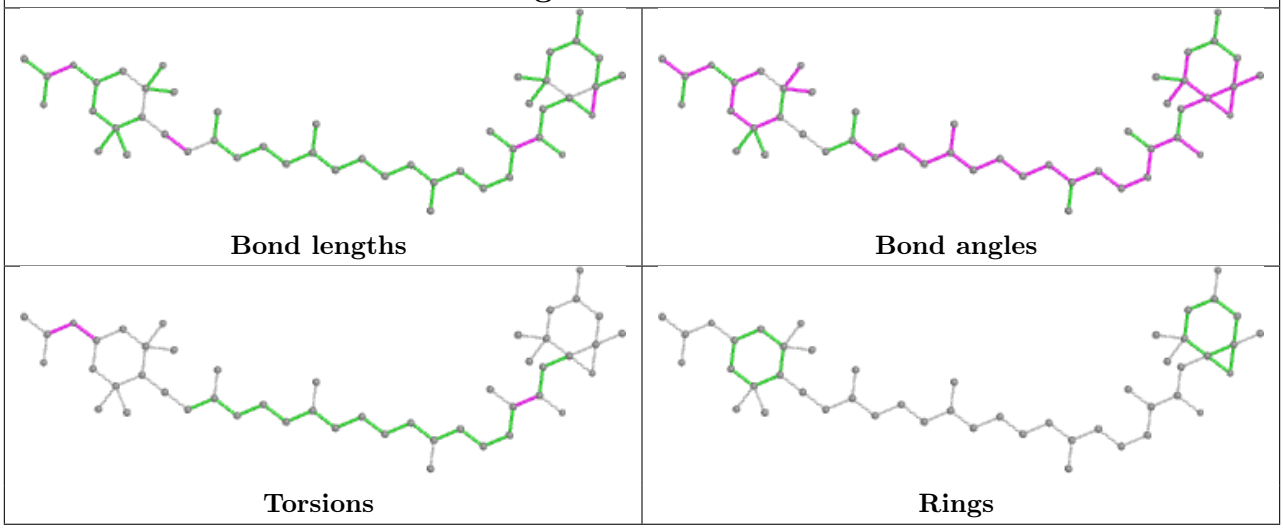


Torsions

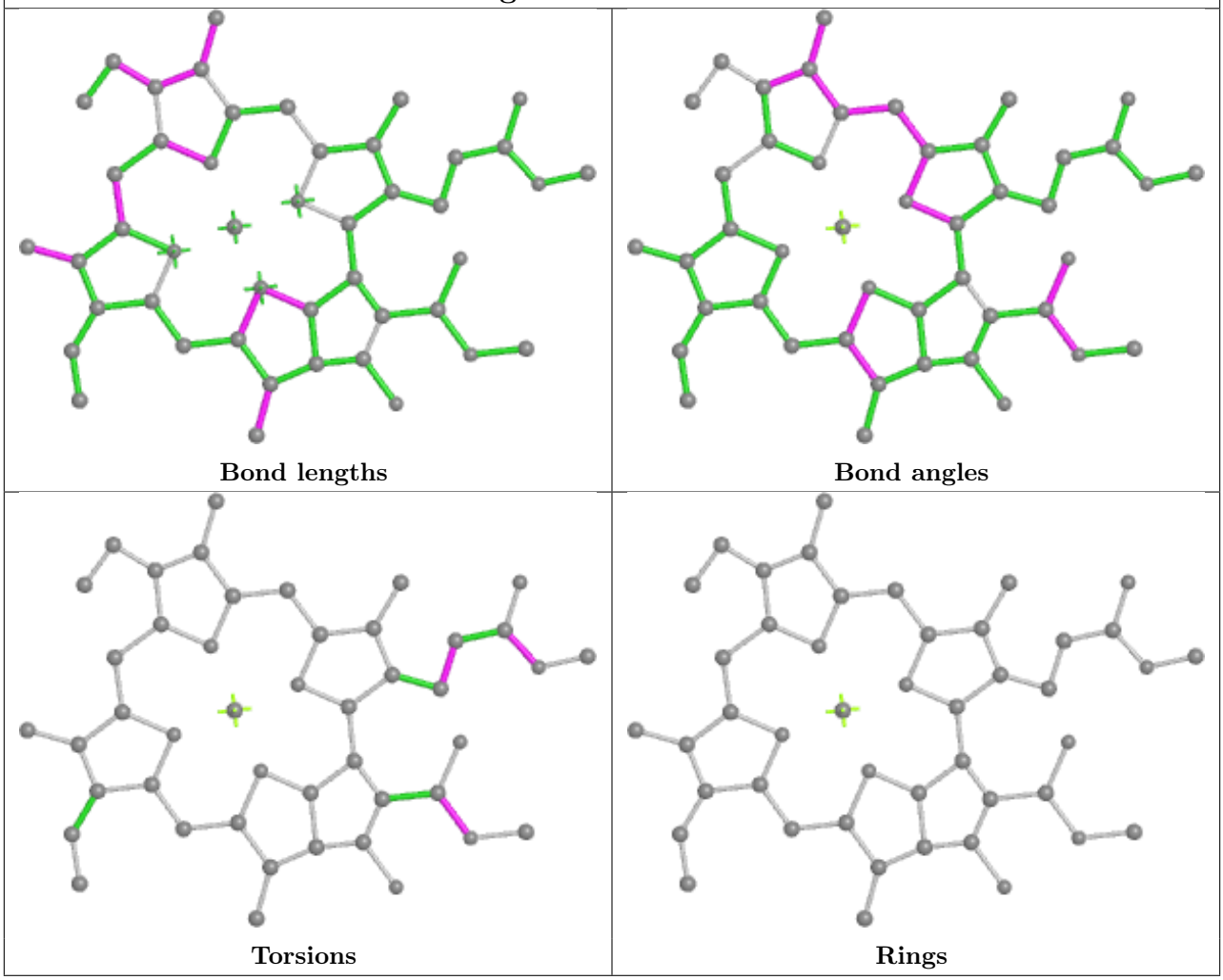


Rings

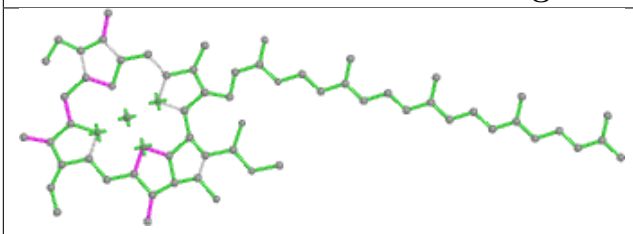
Ligand A86 J 303



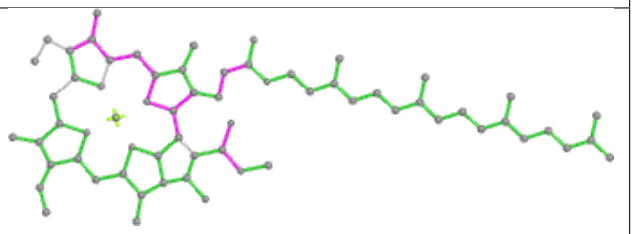
Ligand CLA D 311



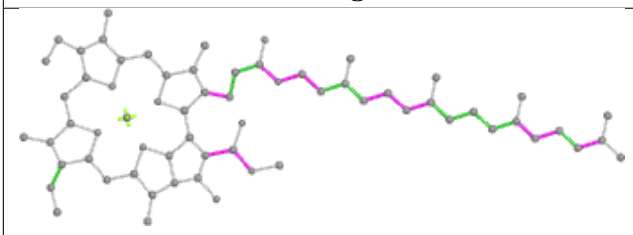
Ligand CLA i 102



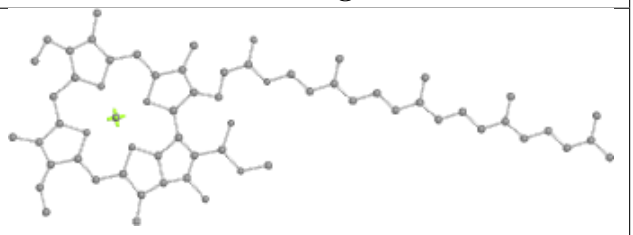
Bond lengths



Bond angles

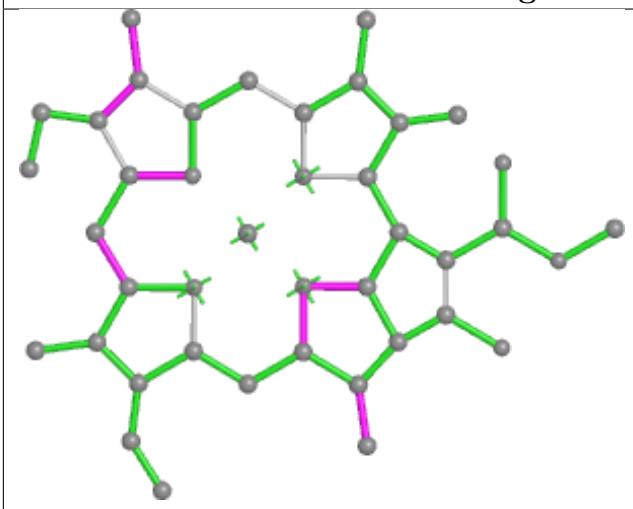


Torsions

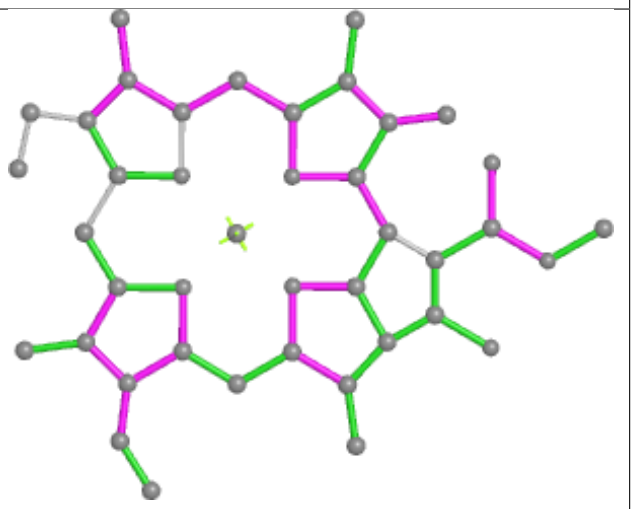


Rings

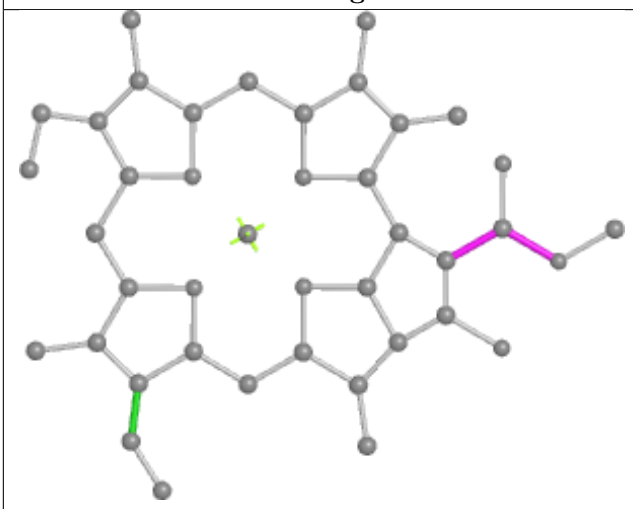
Ligand CLA W 214



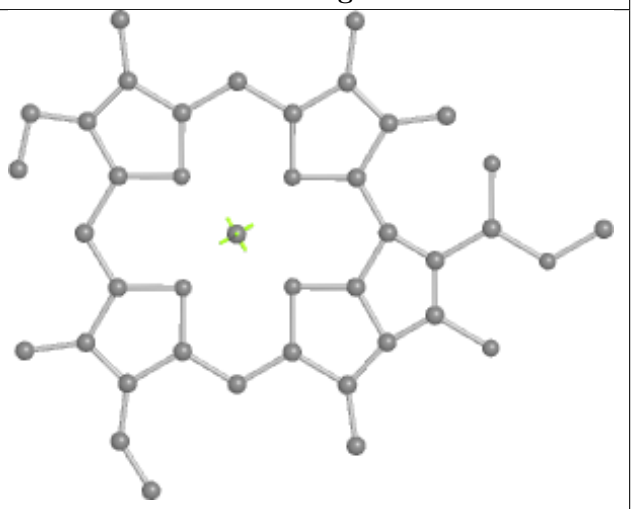
Bond lengths



Bond angles

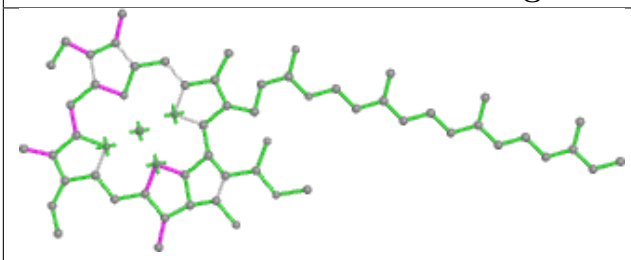


Torsions

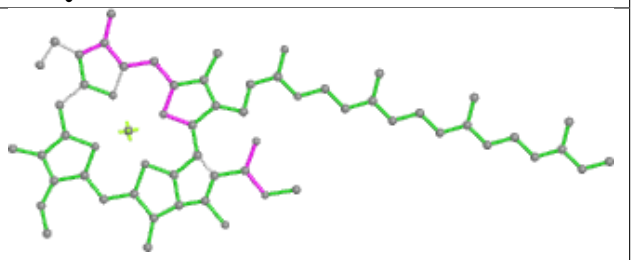


Rings

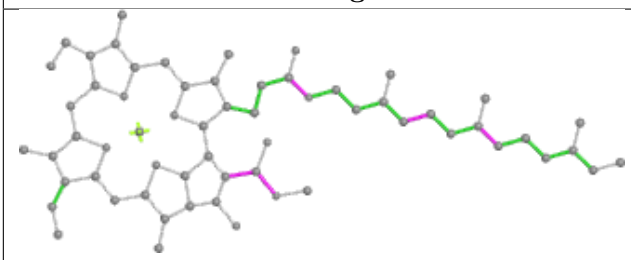
Ligand CLA Q 305



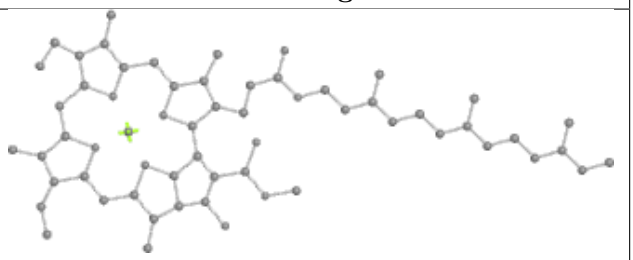
Bond lengths



Bond angles

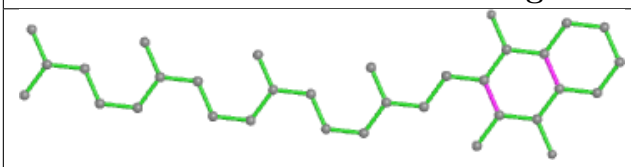


Torsions

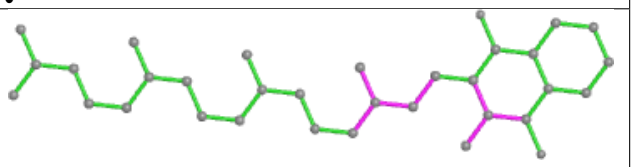


Rings

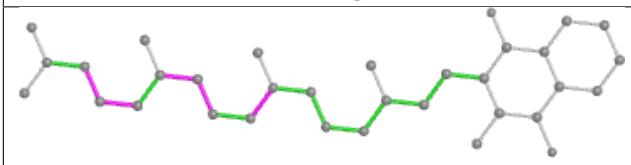
Ligand PQN a 840



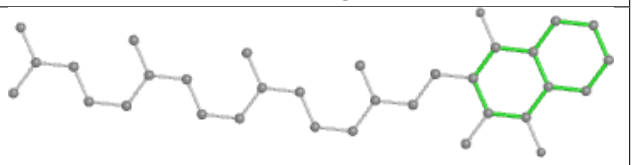
Bond lengths



Bond angles

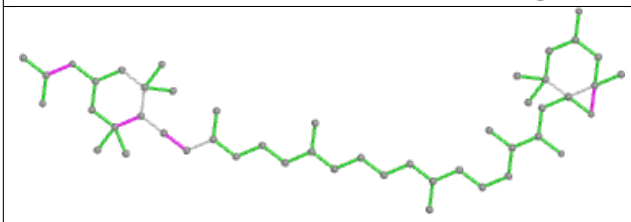


Torsions

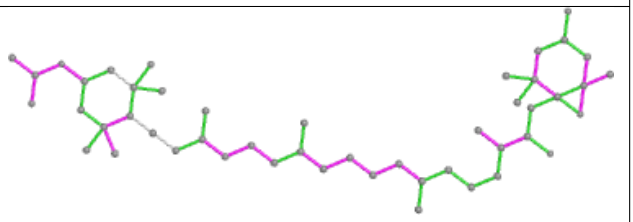


Rings

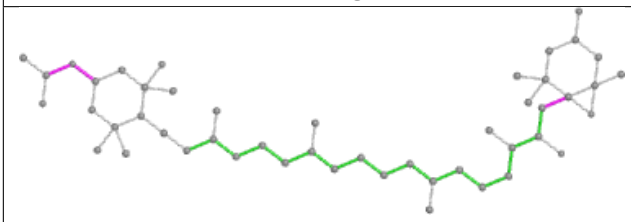
Ligand A86 F 304



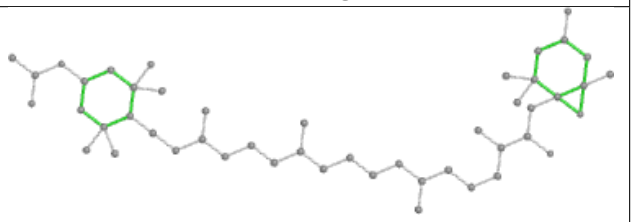
Bond lengths



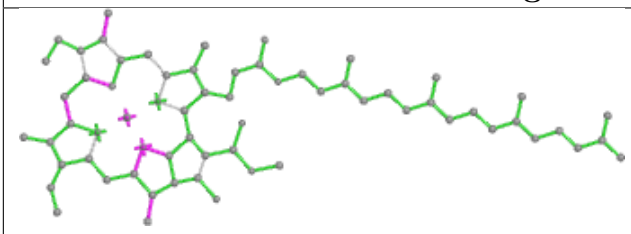
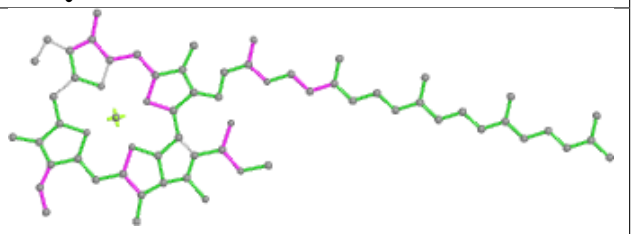
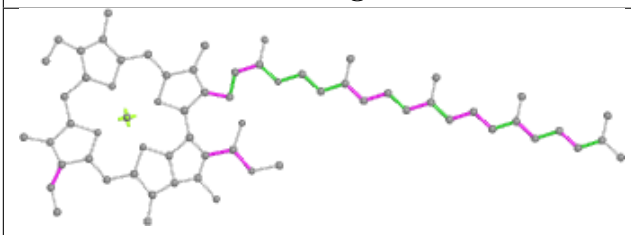
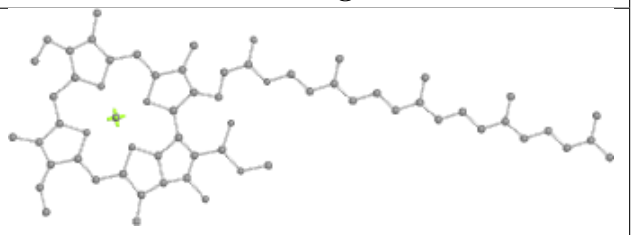
Bond angles

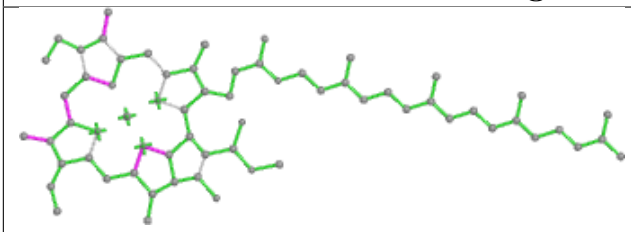
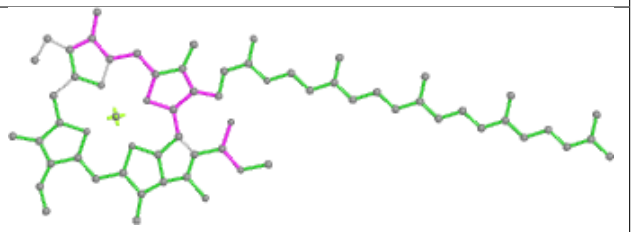
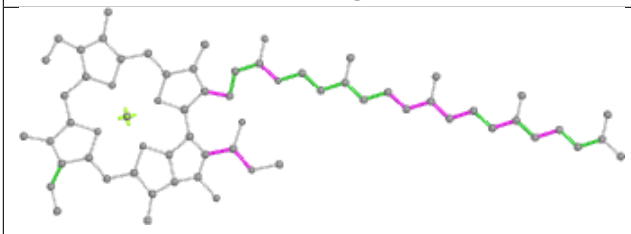
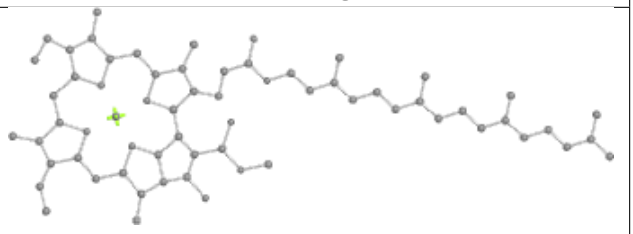


Torsions

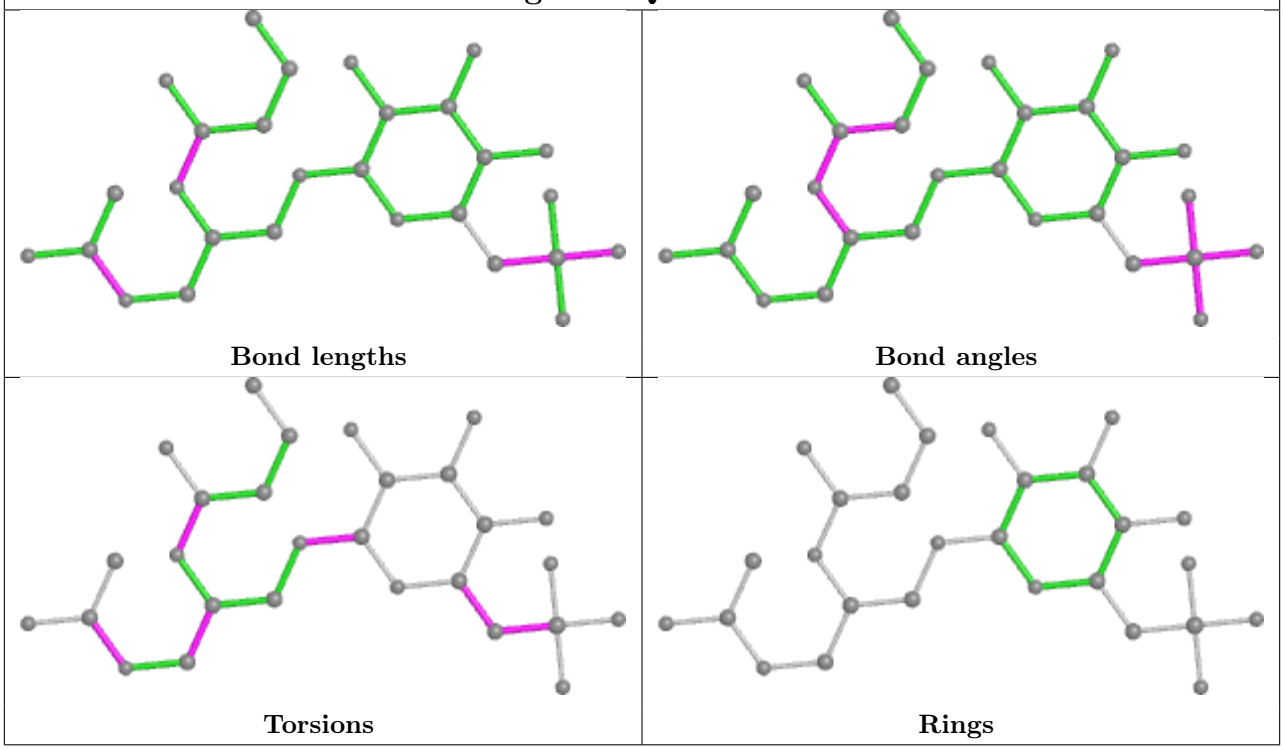


Rings

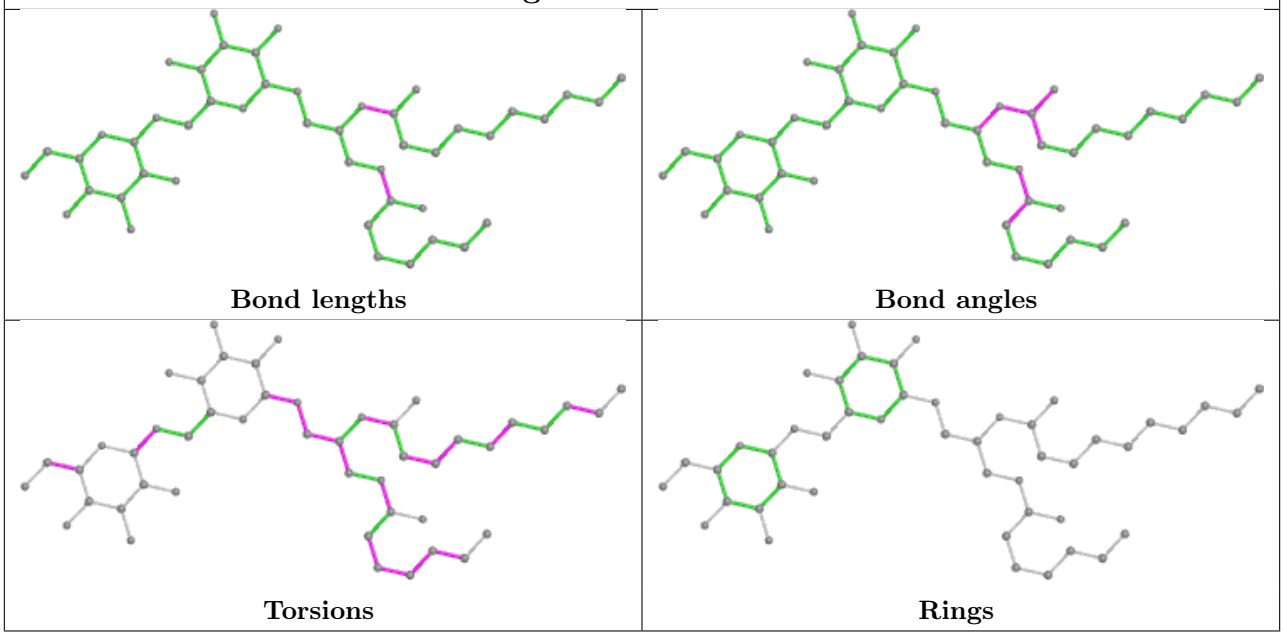
Ligand CLA Q 308	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA S 320	
 Bond lengths	 Bond angles
 Torsions	 Rings

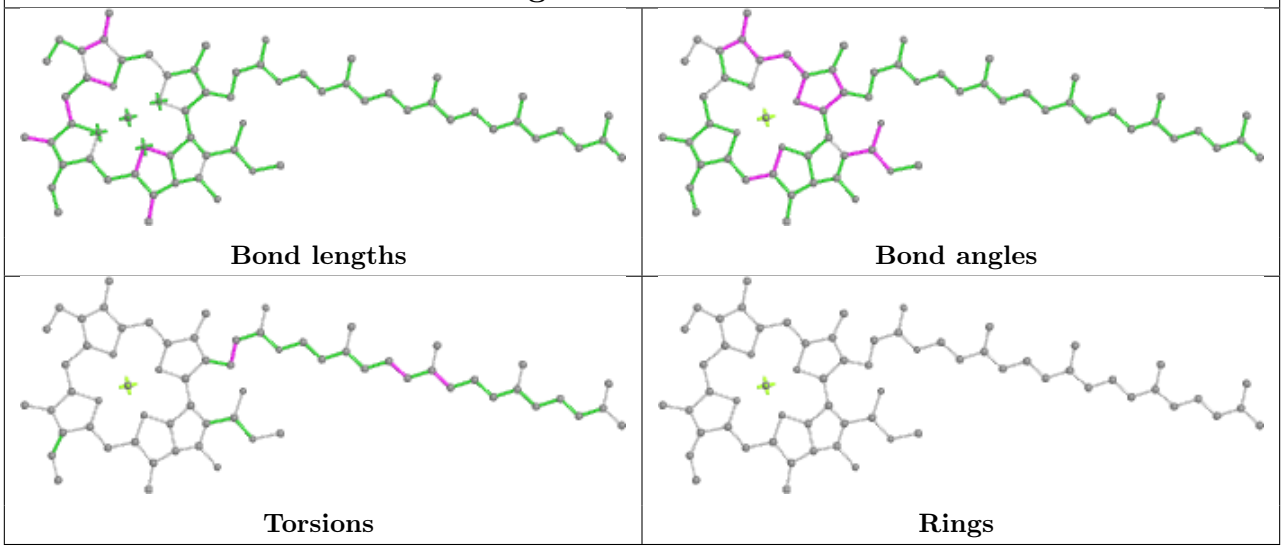
Ligand SQD A 315



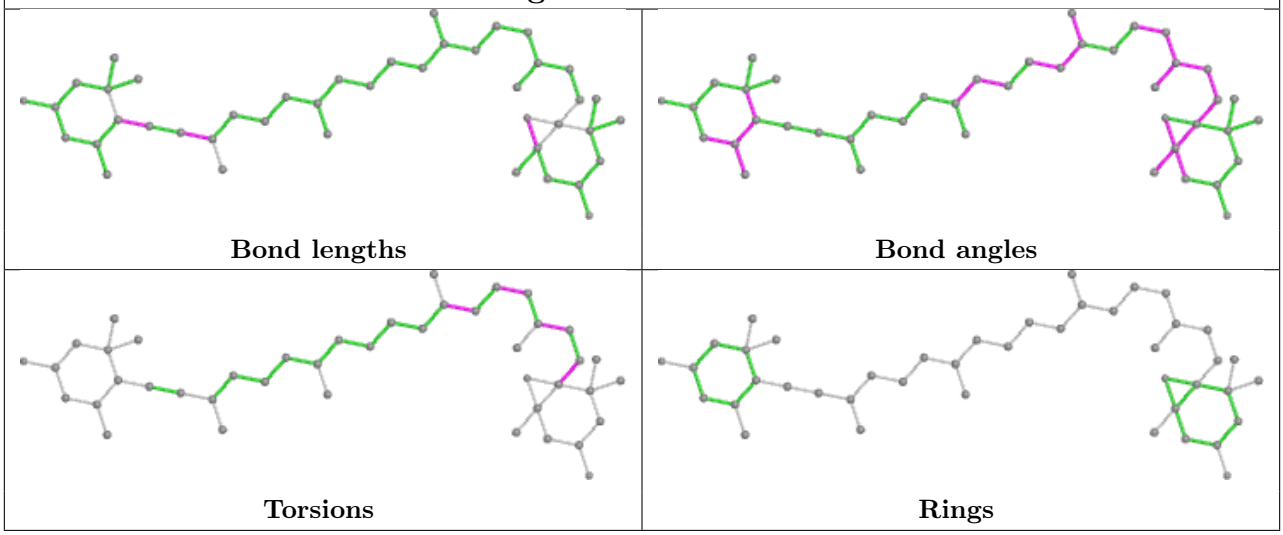
Ligand DGD L 302



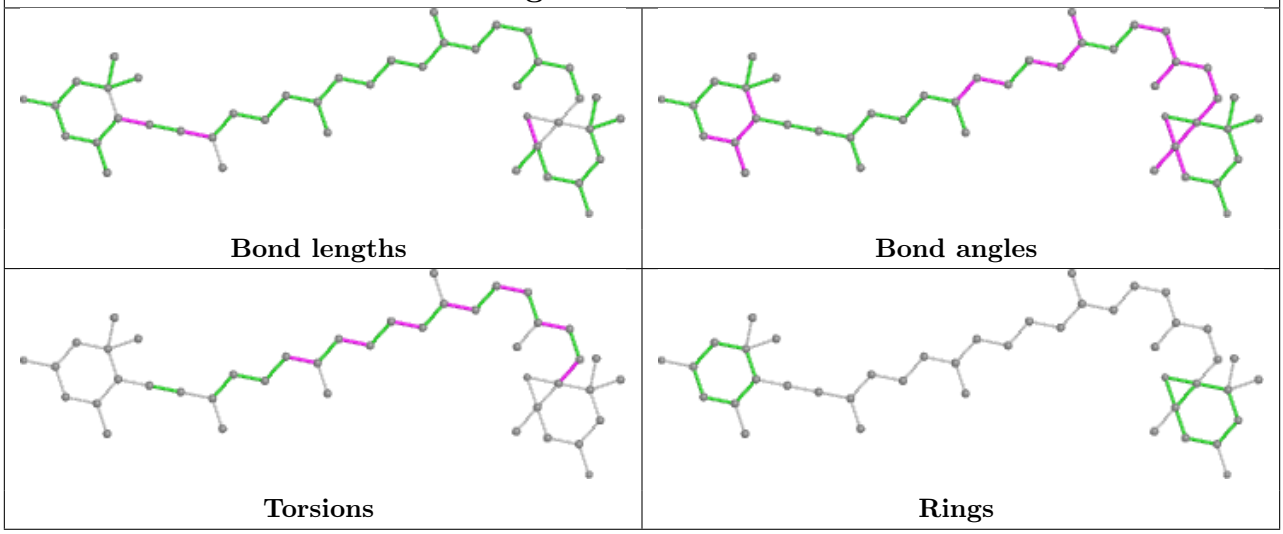
Ligand CLA b 839



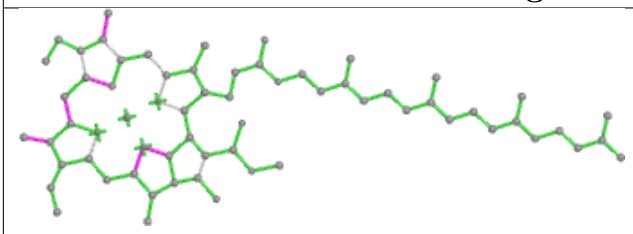
Ligand DD6 F 303



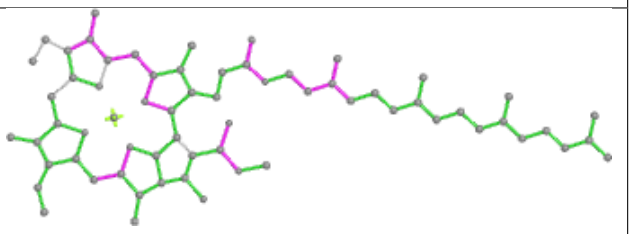
Ligand DD6 R 308



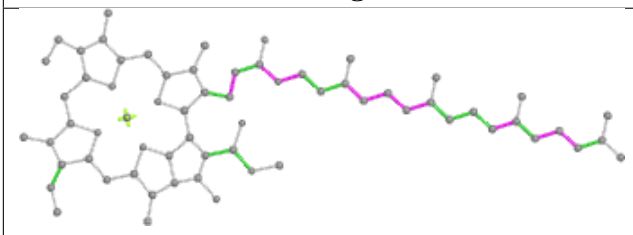
Ligand CLA F 309



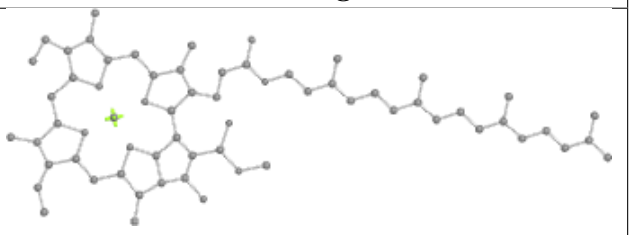
Bond lengths



Bond angles

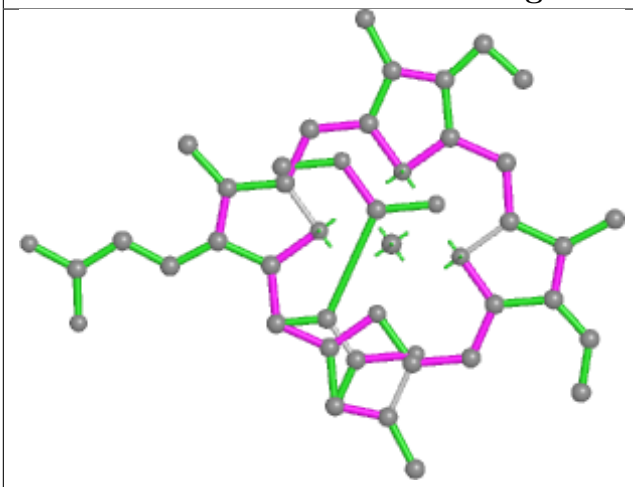


Torsions

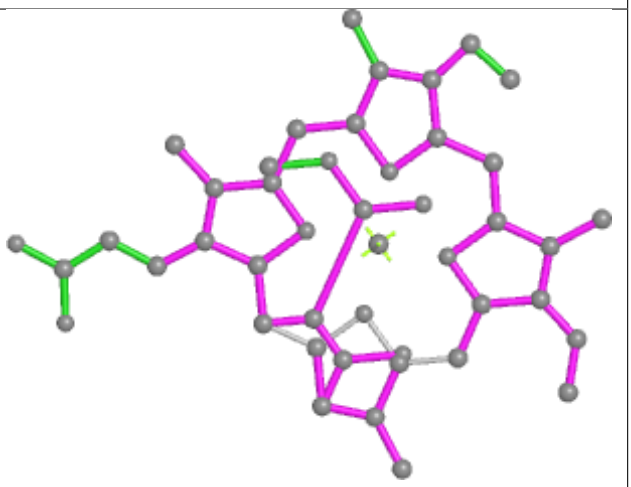


Rings

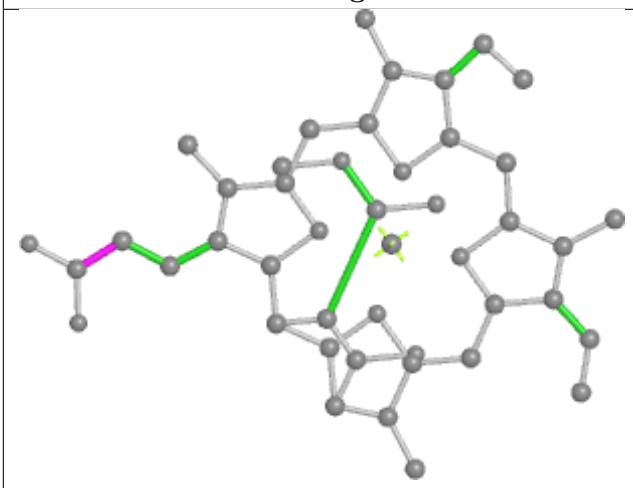
Ligand KC1 A 312



Bond lengths



Bond angles



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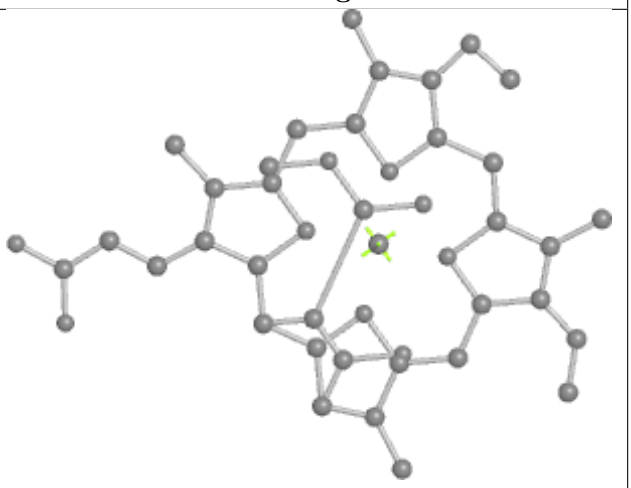
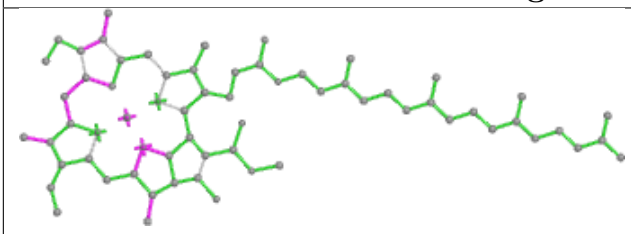
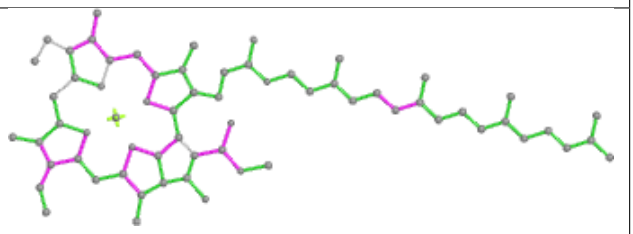
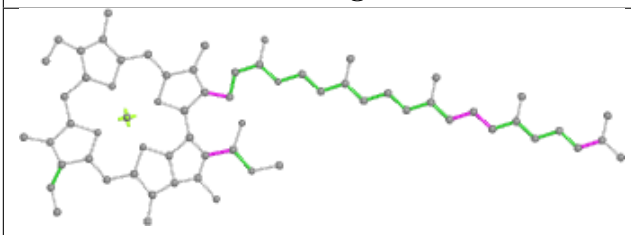
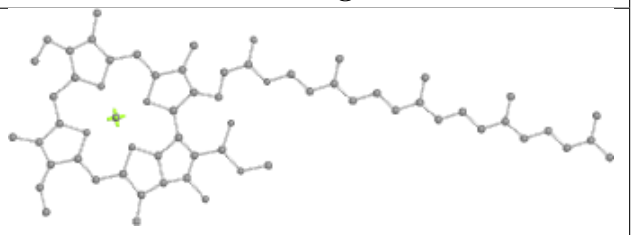
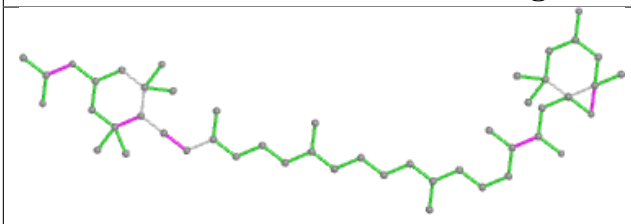
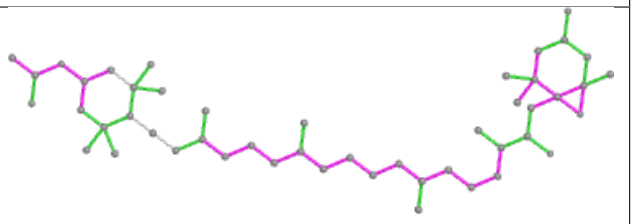
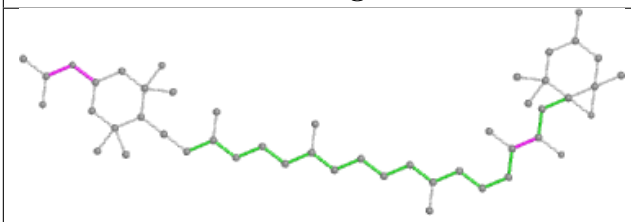
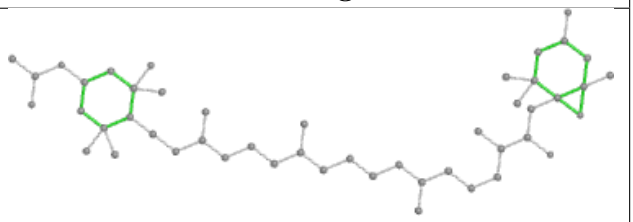
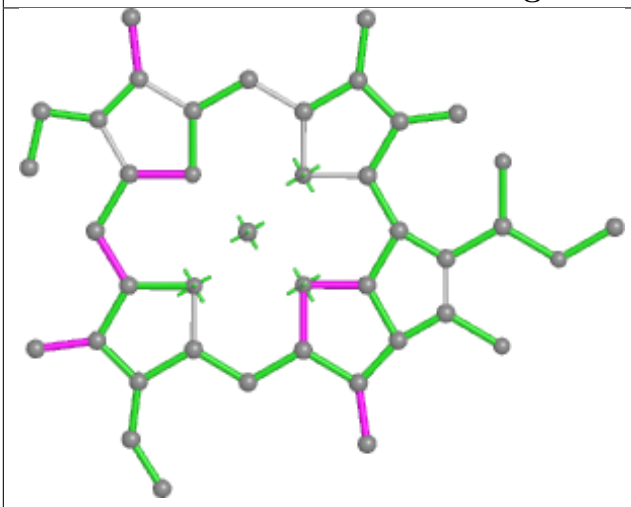


Rings

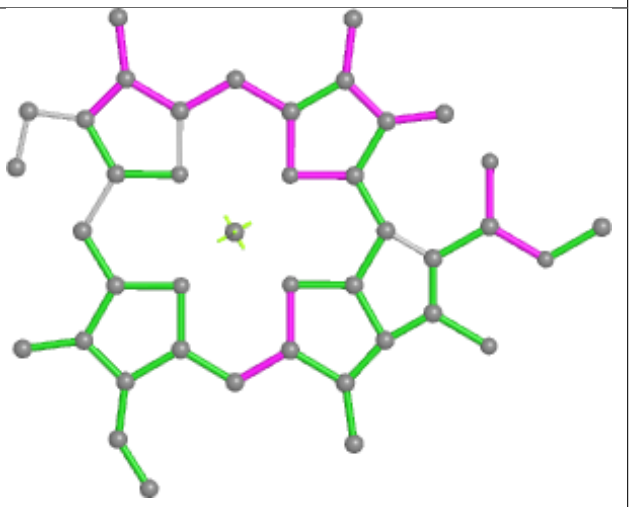
Ligand CLA b 830	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand A86 R 302	
 Bond lengths	 Bond angles
 Torsions	 Rings

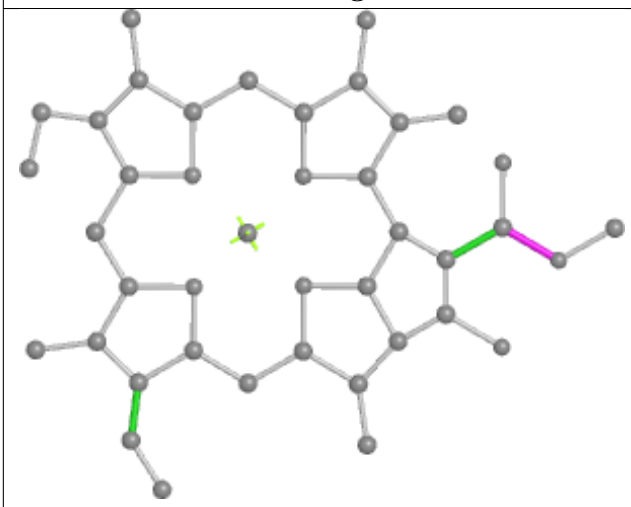
Ligand CLA R 318



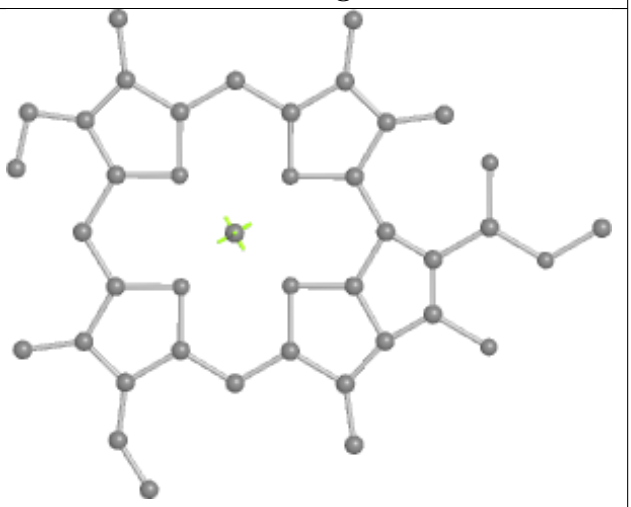
Bond lengths



Bond angles

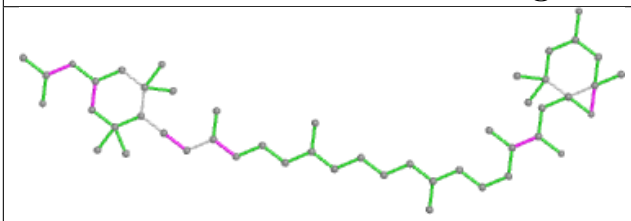


Torsions



Rings

Ligand A86 L 319



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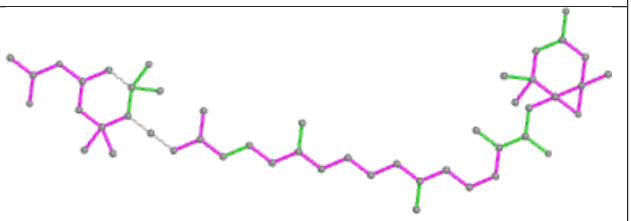
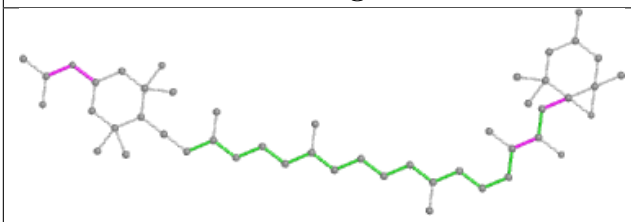
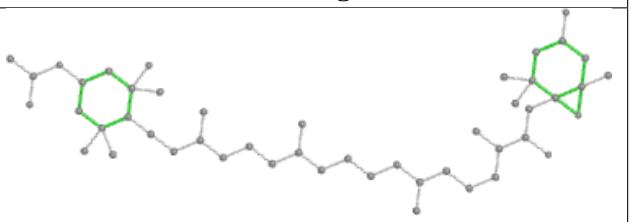


Bond angles

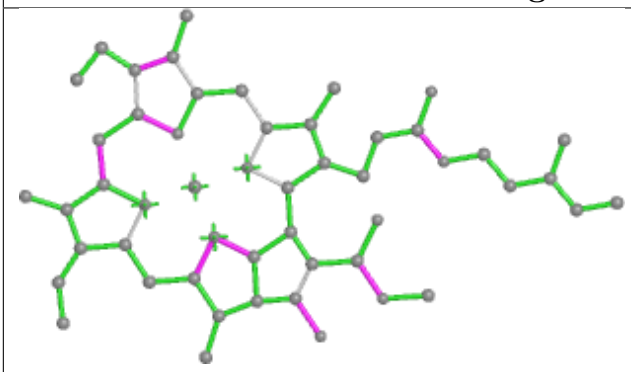


Torsions



Rings

Ligand CLA a 822



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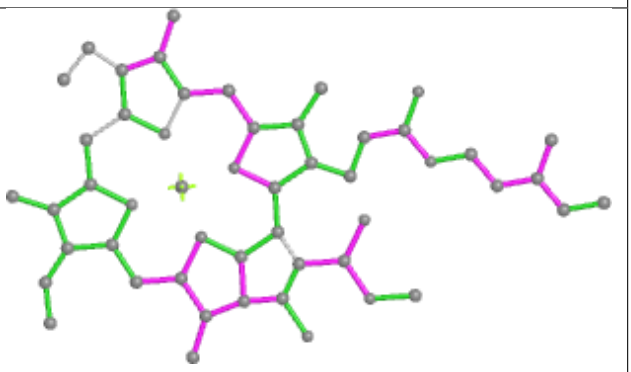
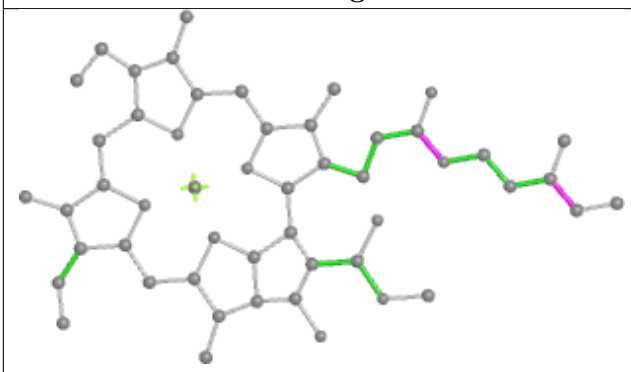
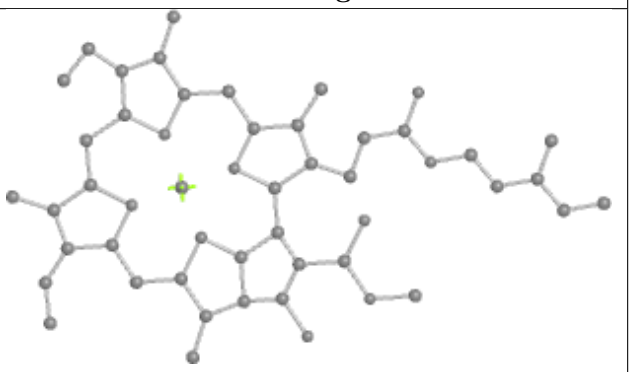


Bond angles

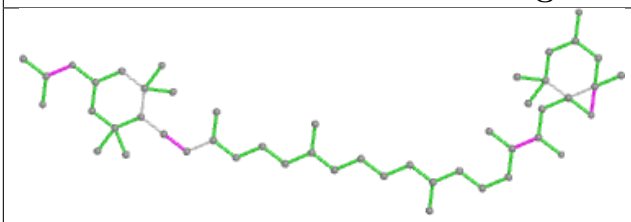


Torsions



Rings

Ligand A86 I 304



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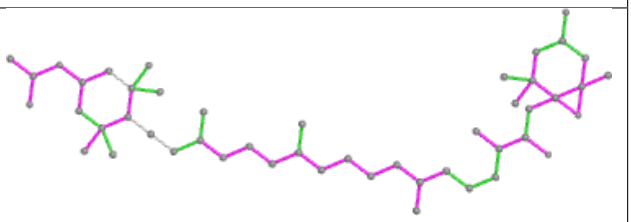
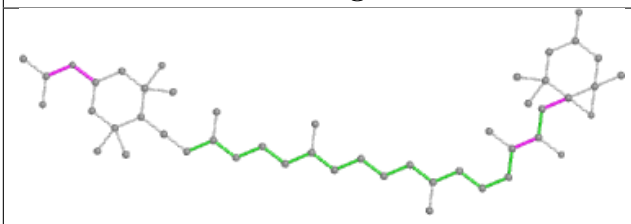


Bond angles



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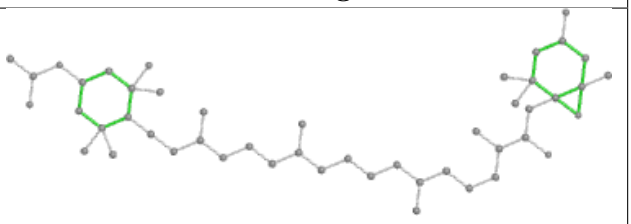
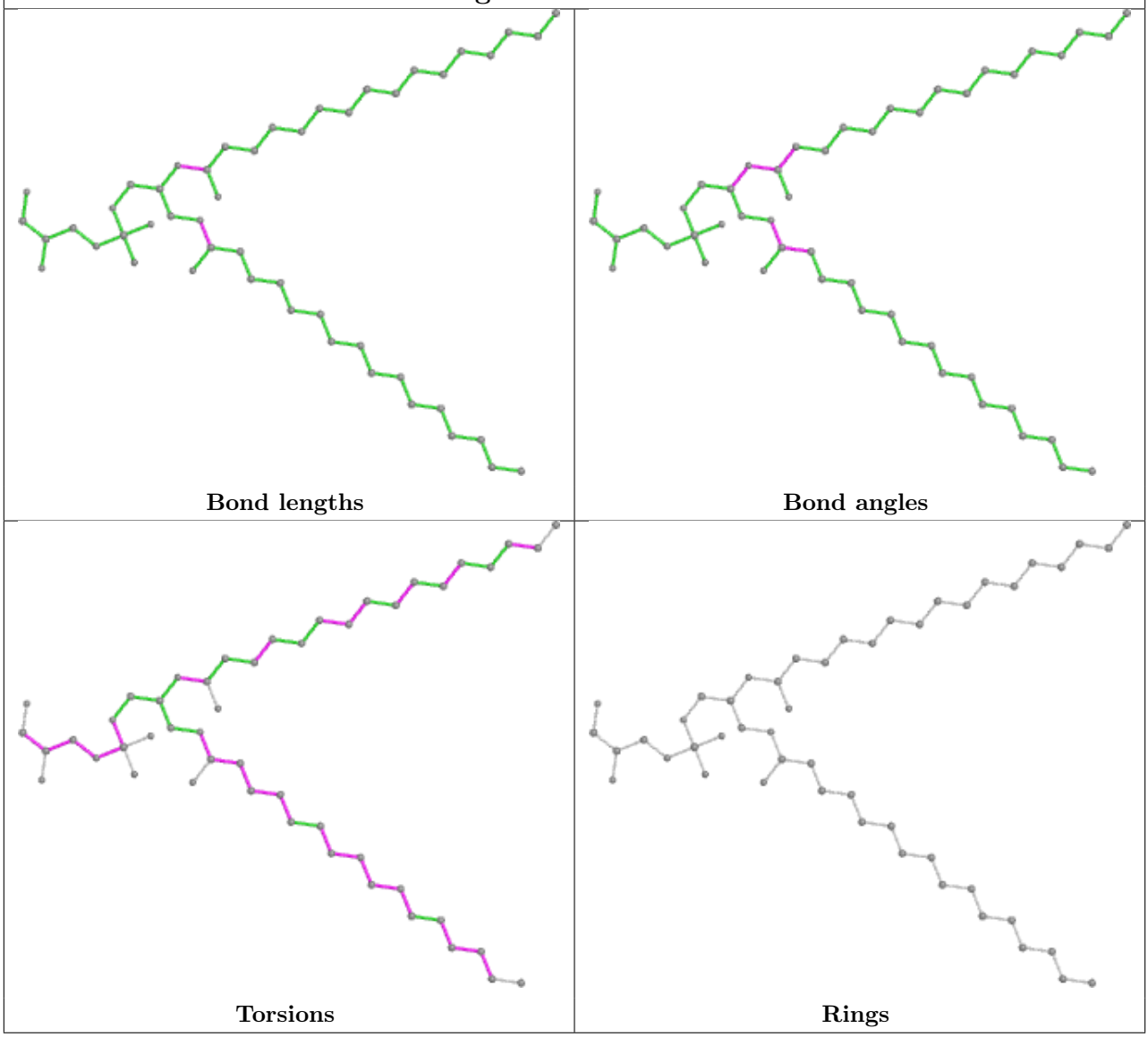
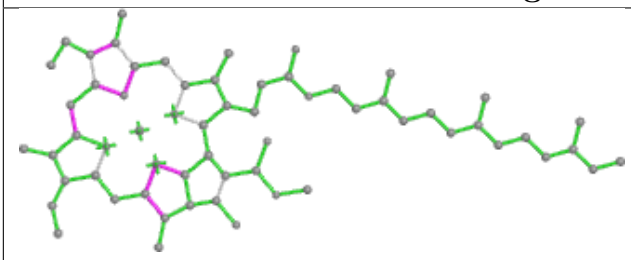


Rings

Ligand LHG f 808



Ligand CLA V 305



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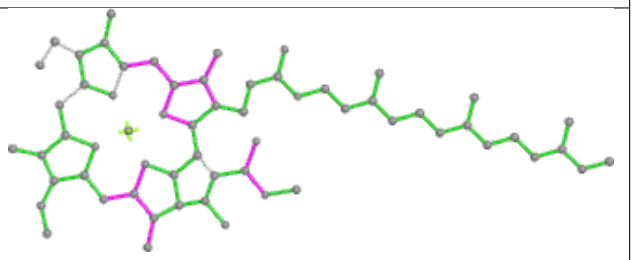
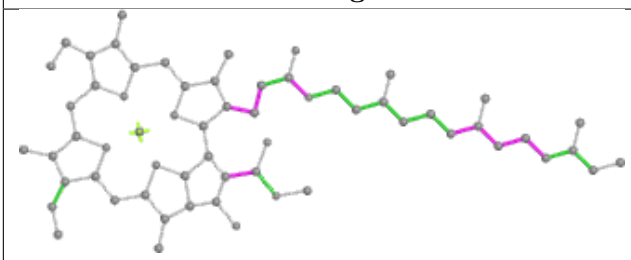


Bond angles



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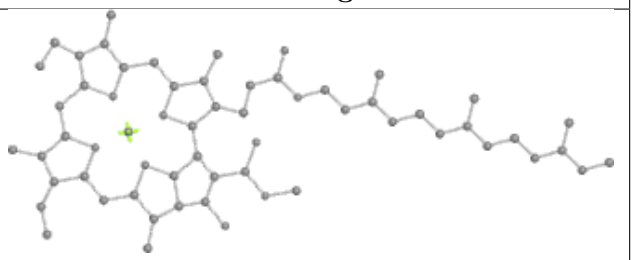
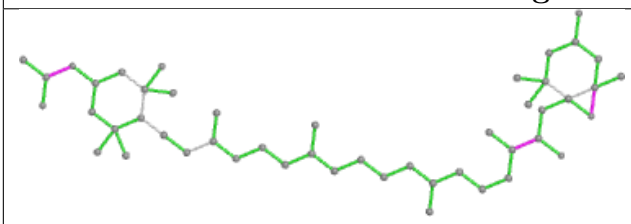


Rings

Ligand A86 L 306



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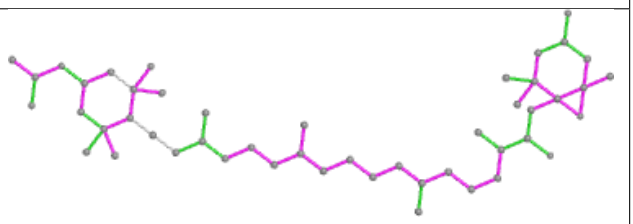
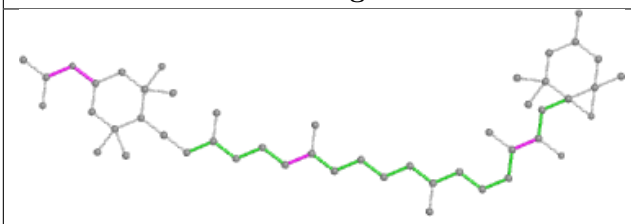
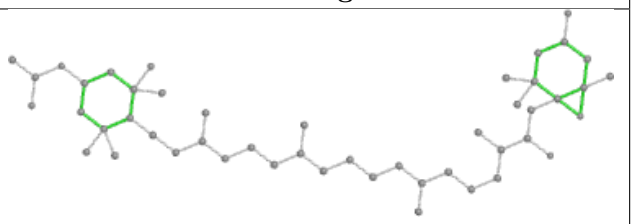


Bond angles

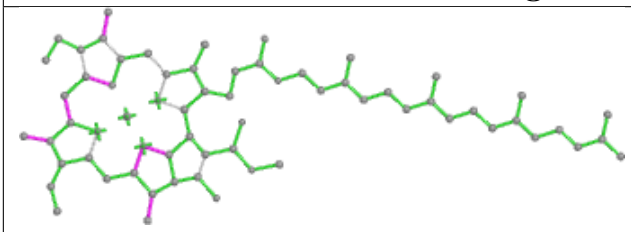


Torsions

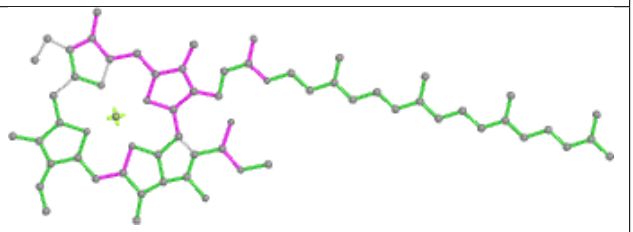


Rings

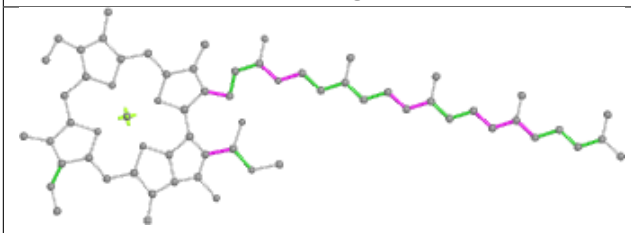
Ligand CLA T 314



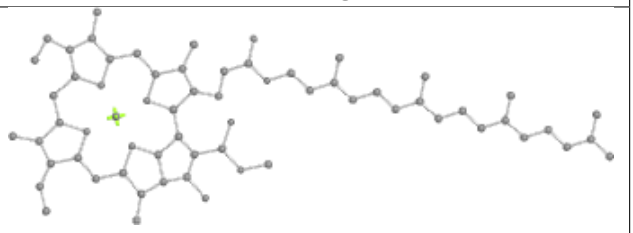
Bond lengths



Bond angles

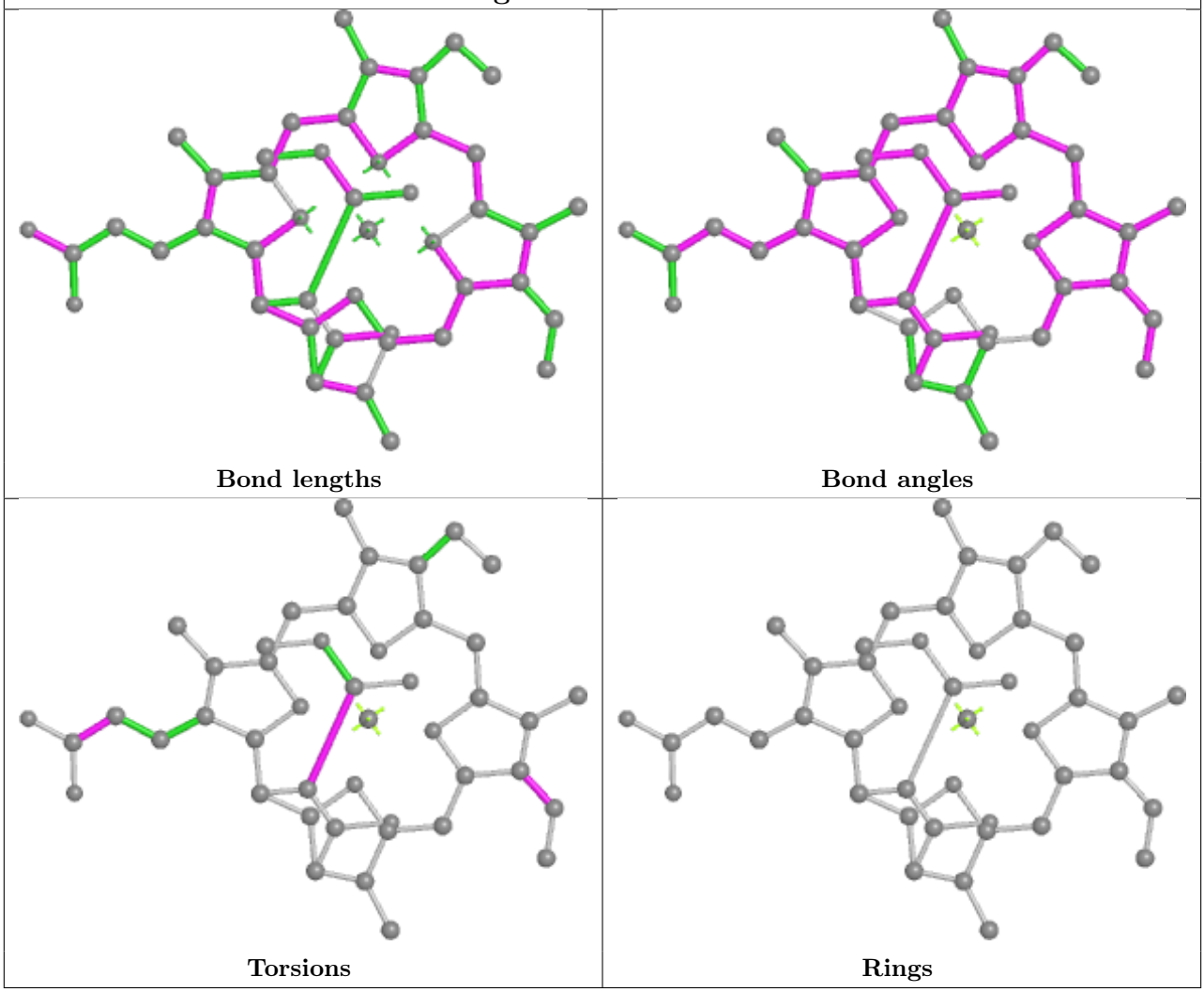


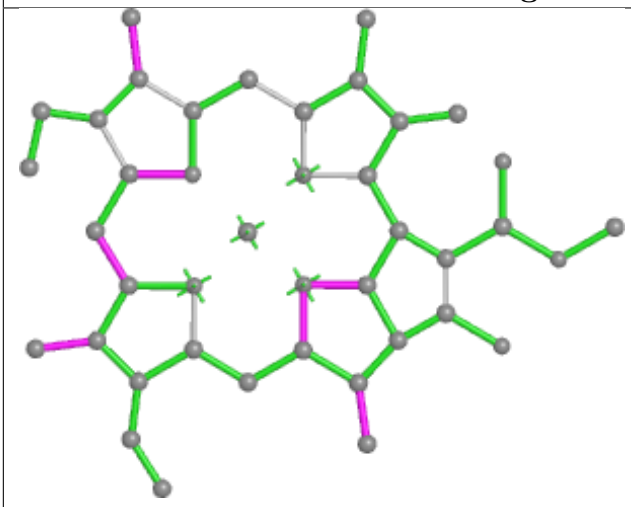
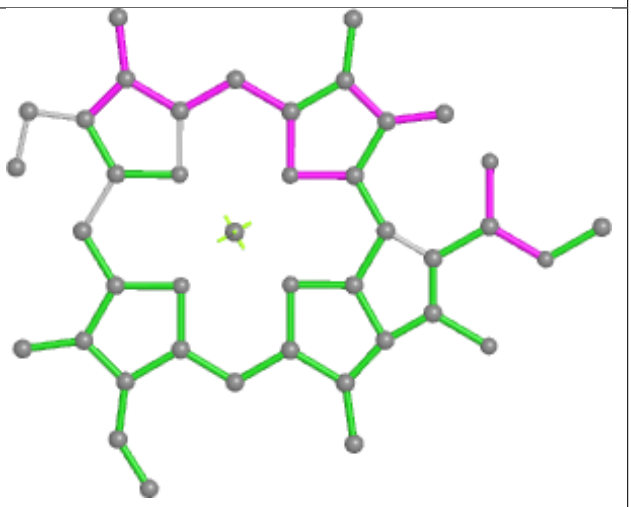
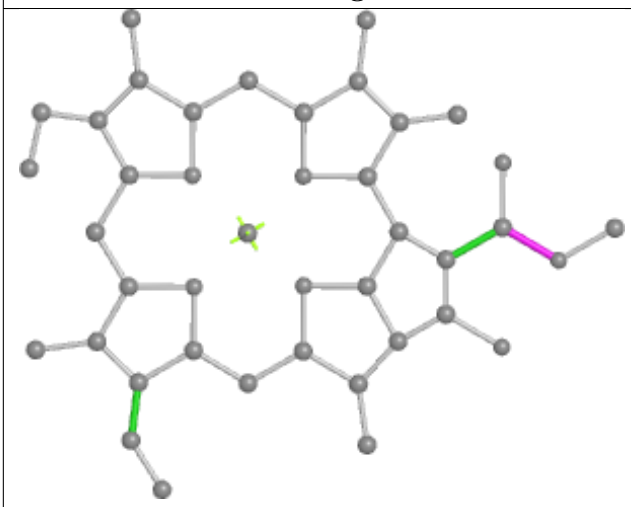
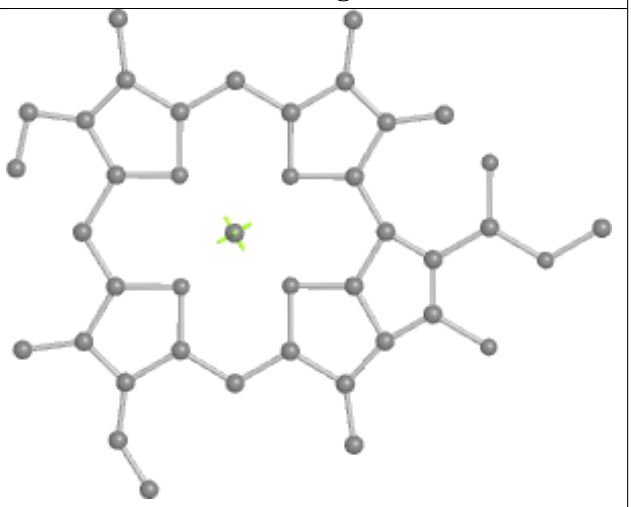
Torsions



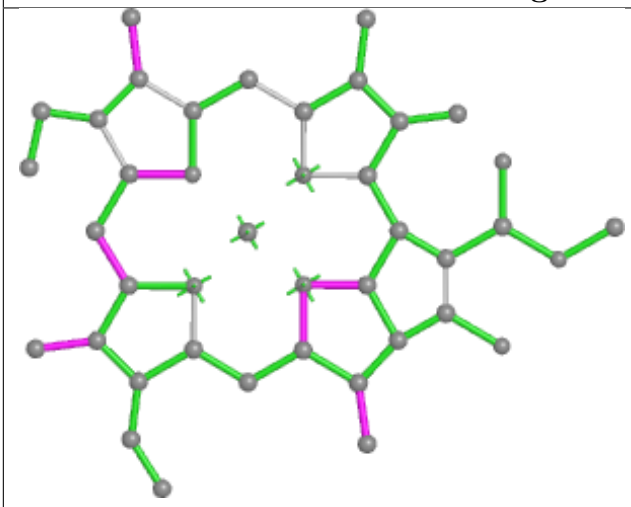
Rings

Ligand KC1 G 318

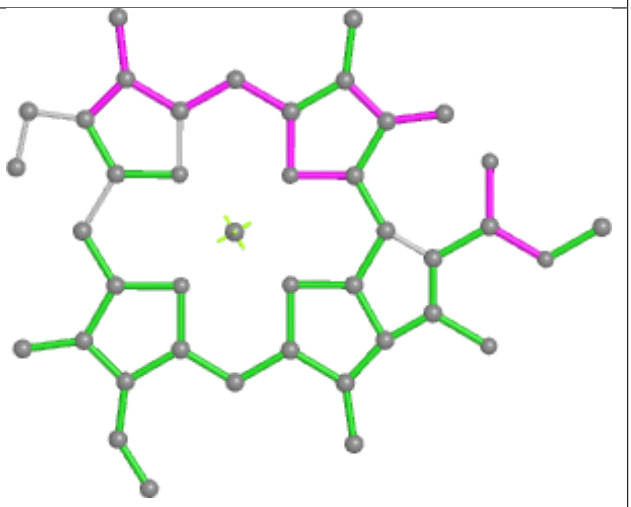


Ligand CLA M 314	
 Bond lengths	 Bond angles
 Torsions	 Rings

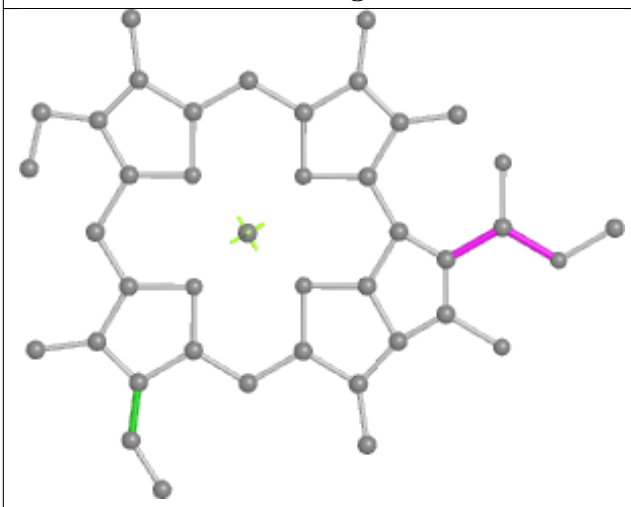
Ligand CLA I 313



Bond lengths



Bond angles



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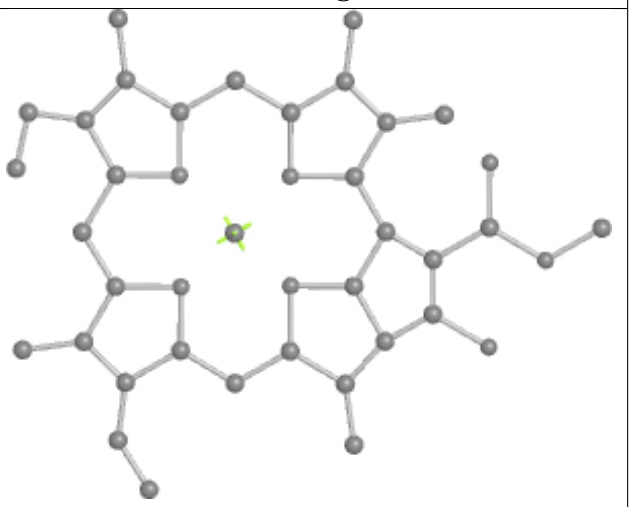
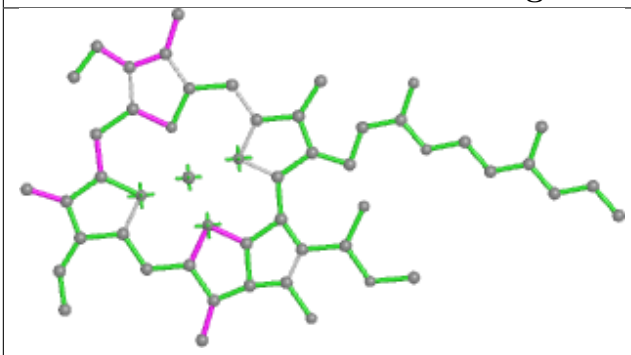
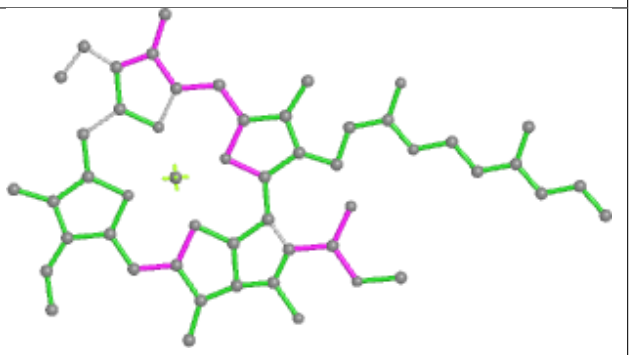
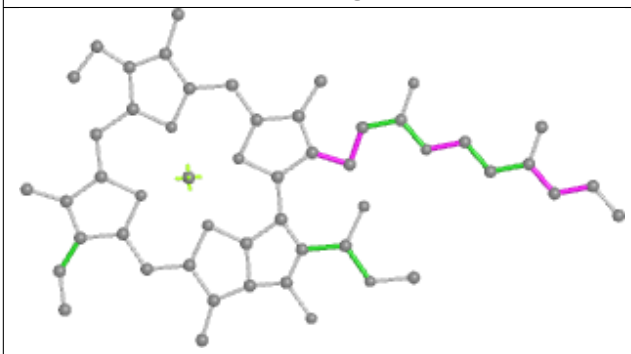
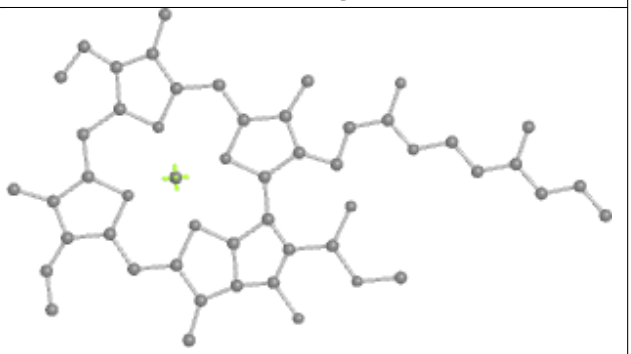
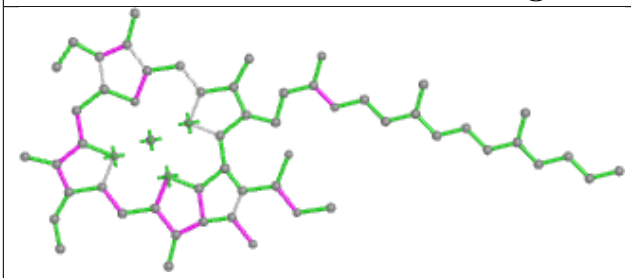
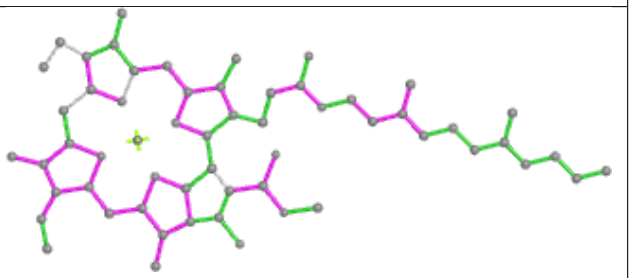
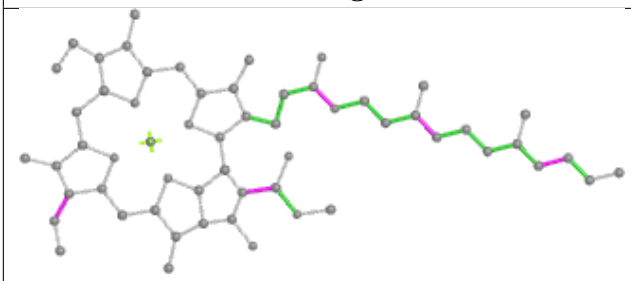
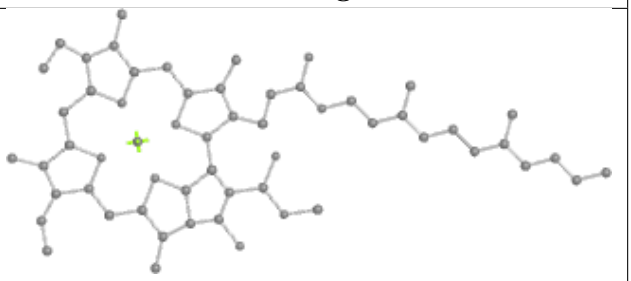
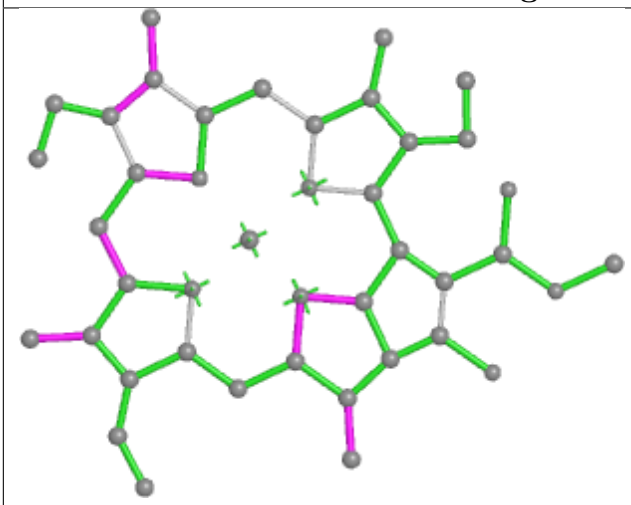


Rings

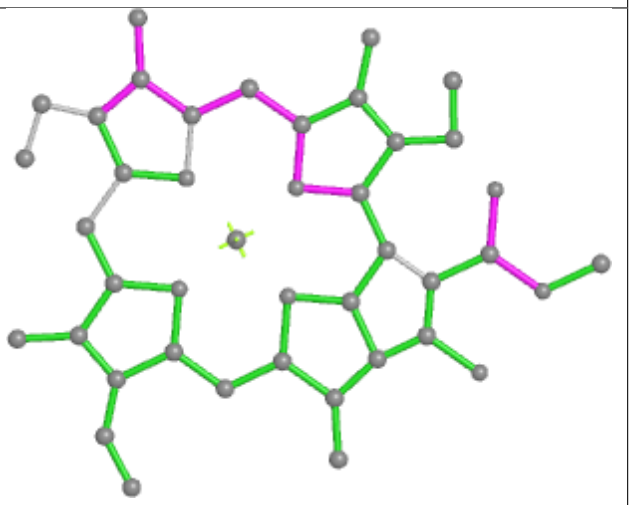
Ligand CLA F 313	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA b 836	
 Bond lengths	 Bond angles
 Torsions	 Rings

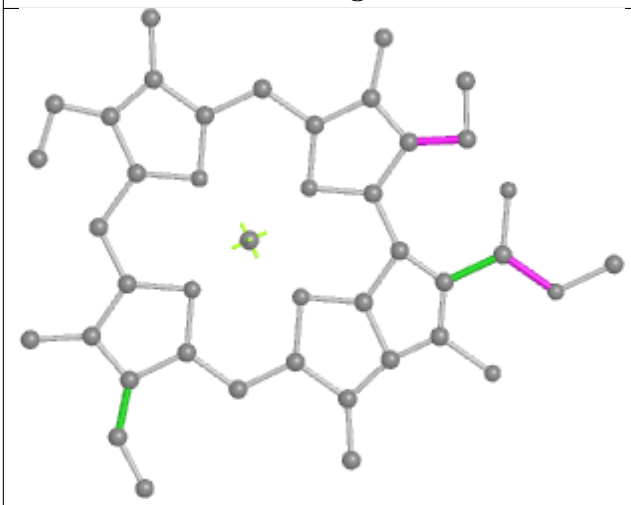
Ligand CLA M 316



Bond lengths



Bond angles



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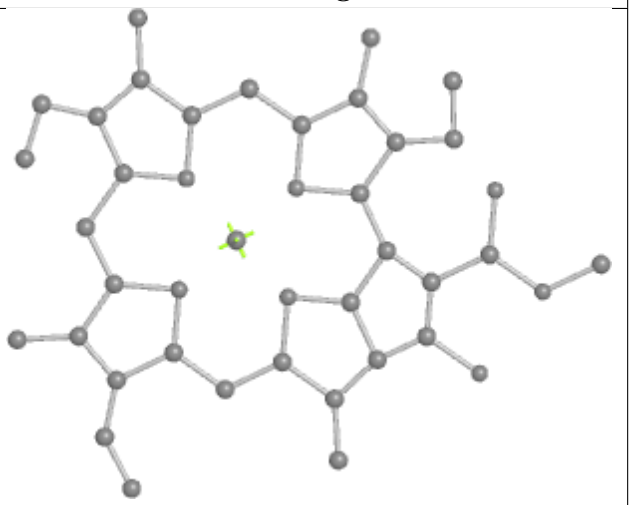
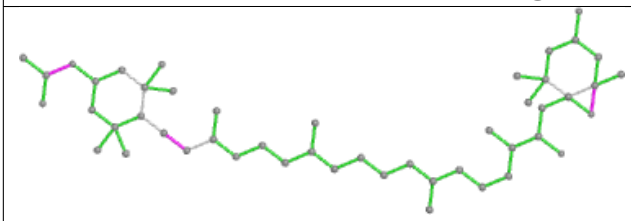


Rings

Ligand A86 N 306



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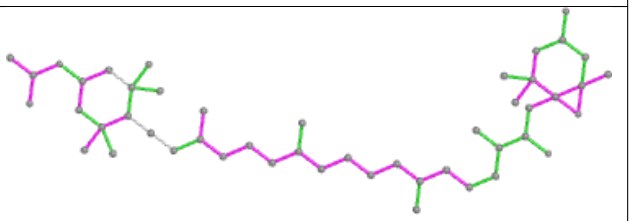
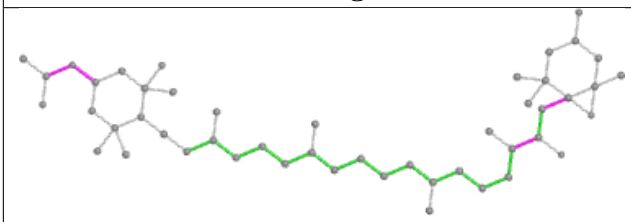


Bond angles



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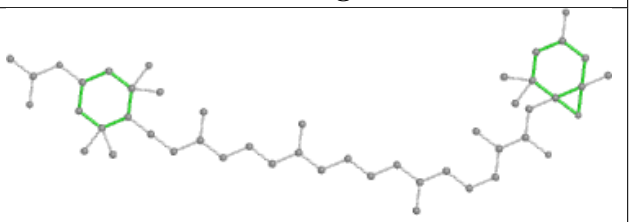
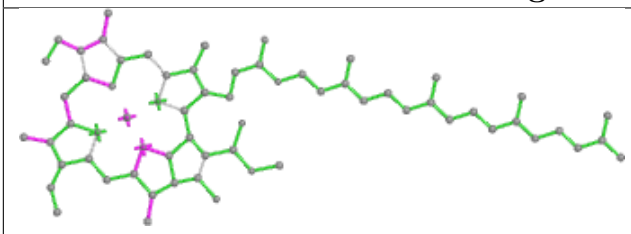
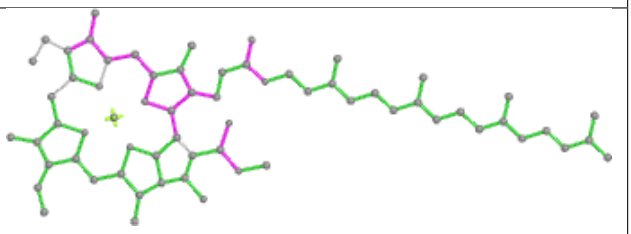
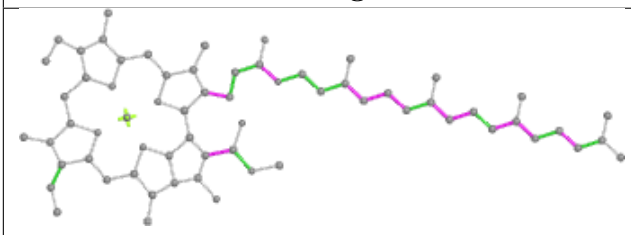
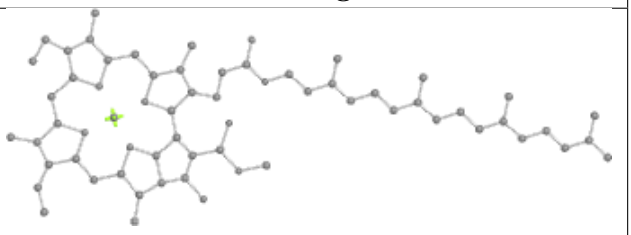
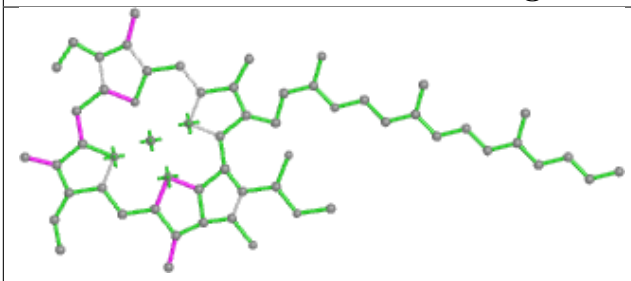
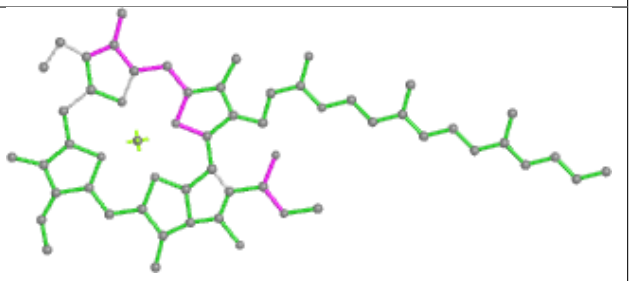
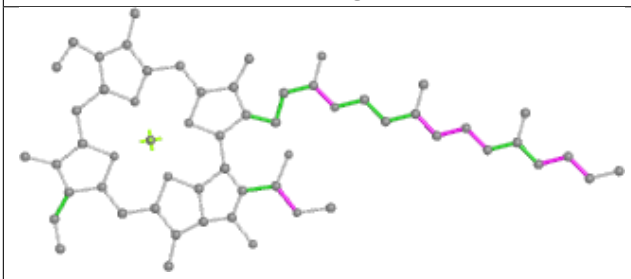
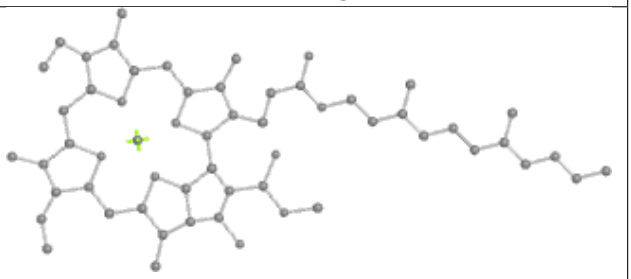
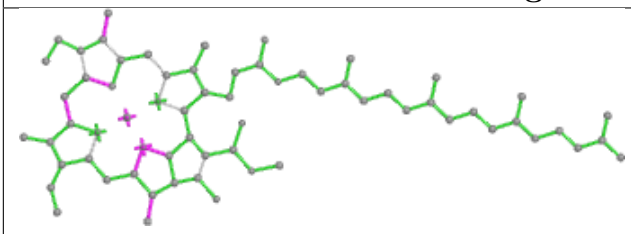
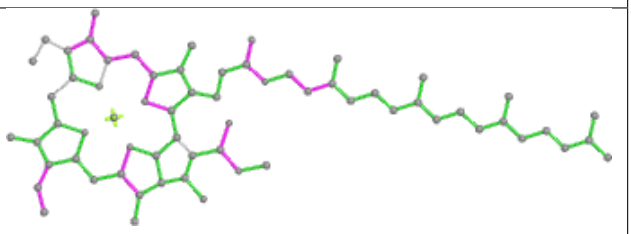
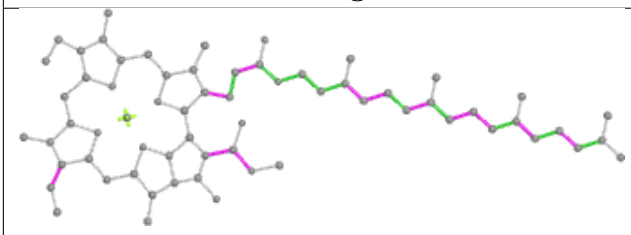
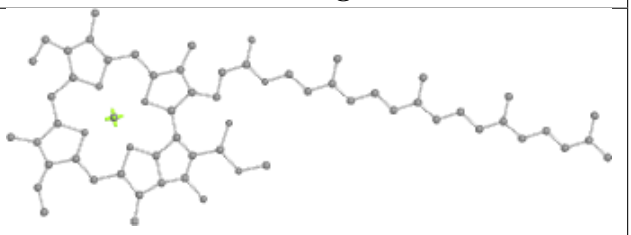


Rings

Ligand CLA a 805	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA O 311	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA P 311	
 Bond lengths	 Bond angles
 Torsions	 Rings

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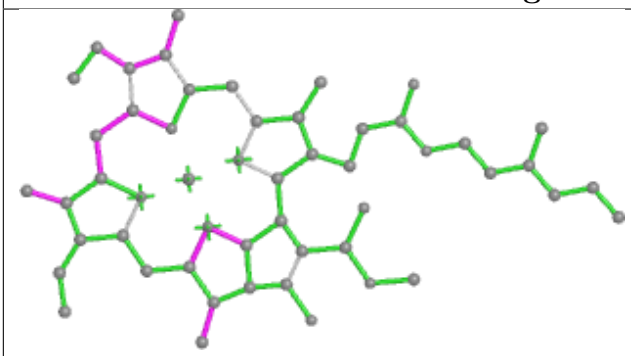
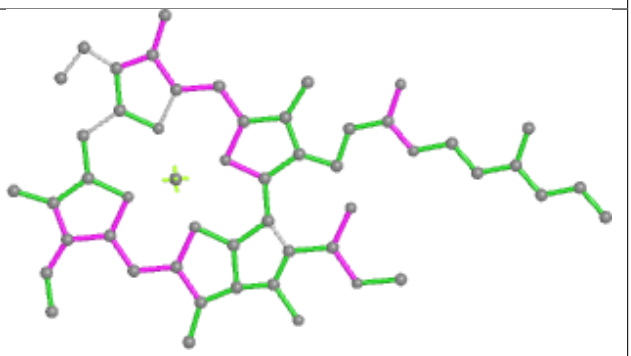
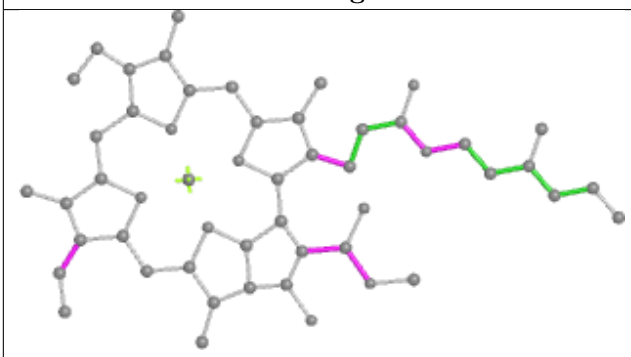
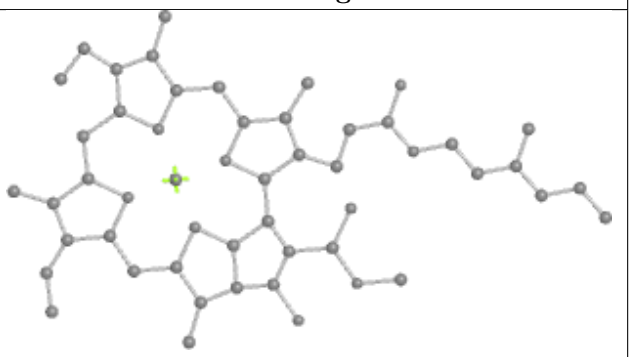
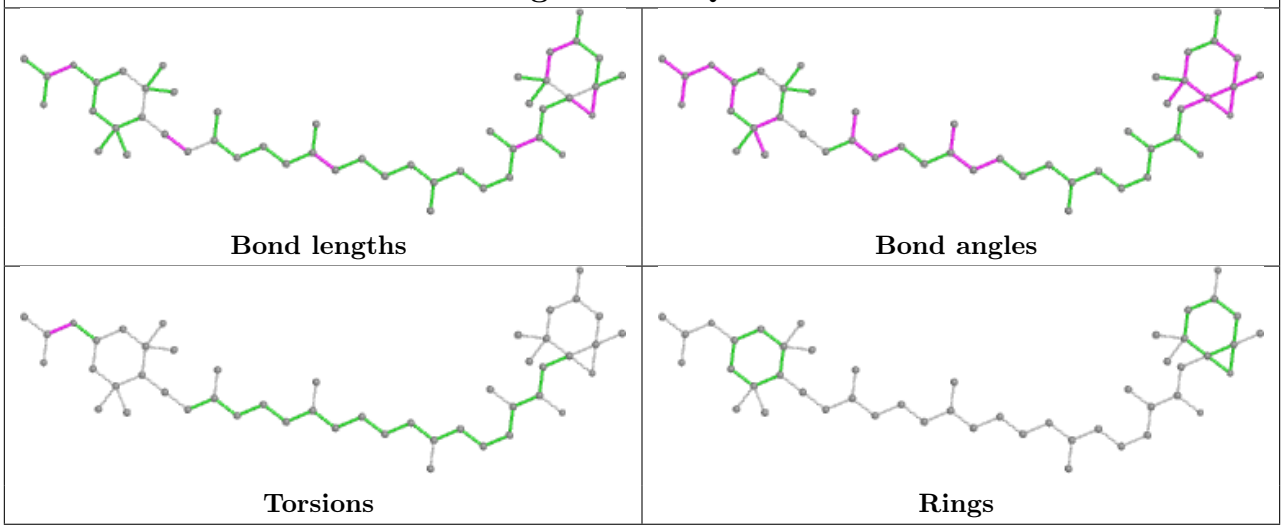
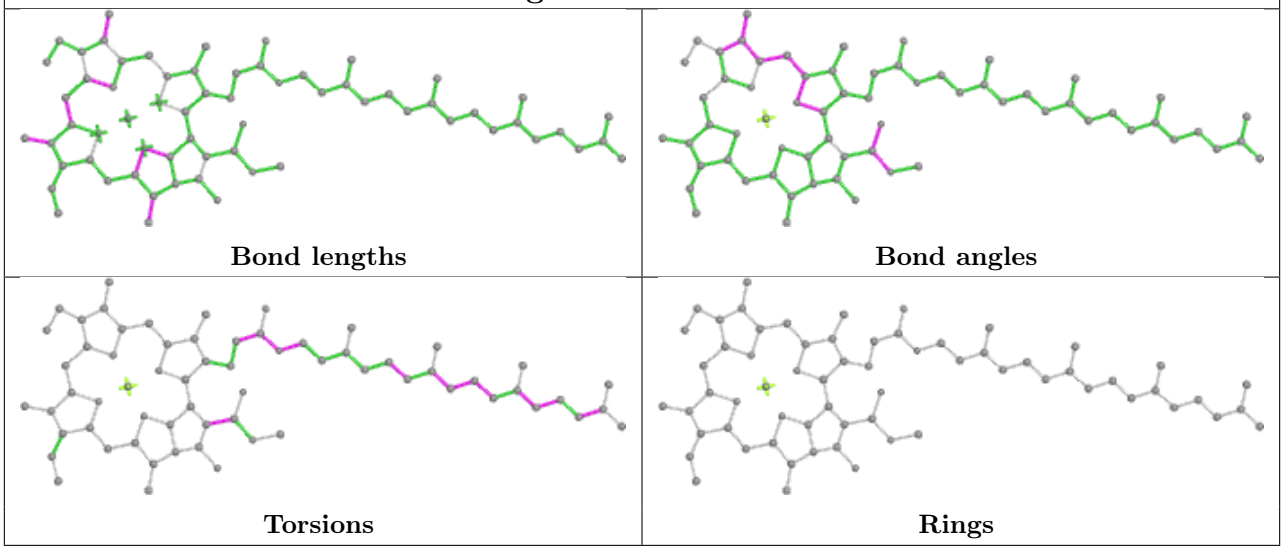
 Bond lengths	 Bond angles
 Torsions	 Rings

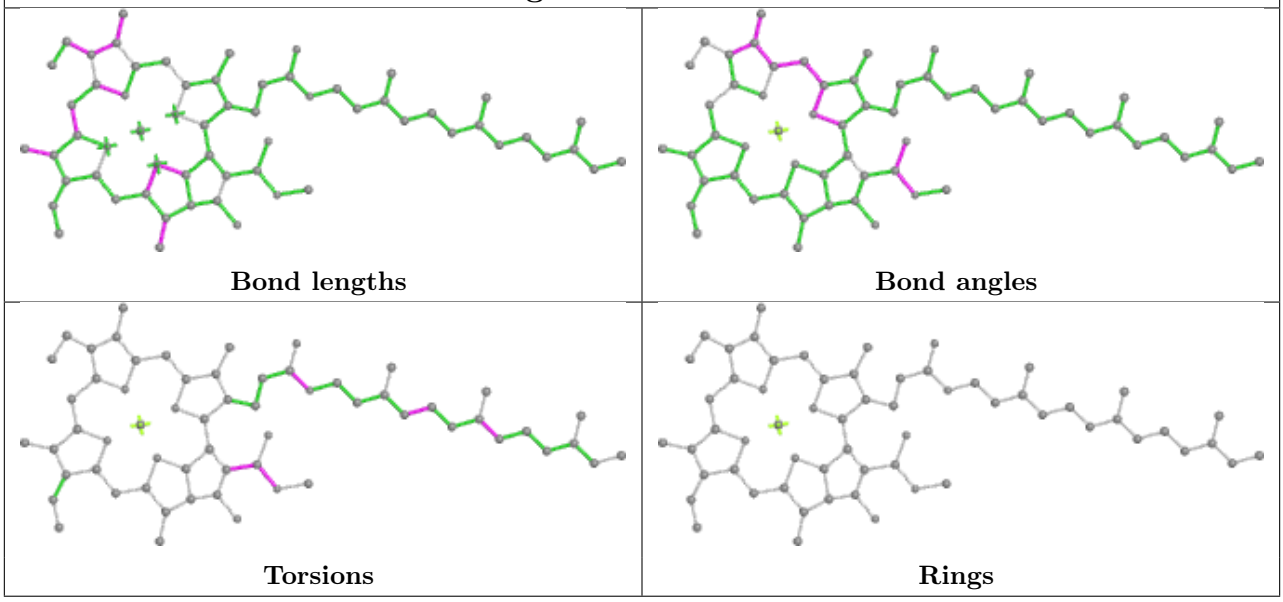
Ligand A86 Q 316

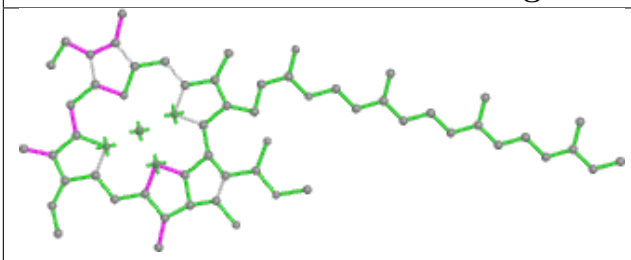
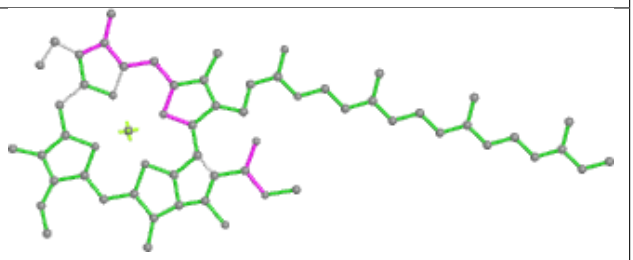
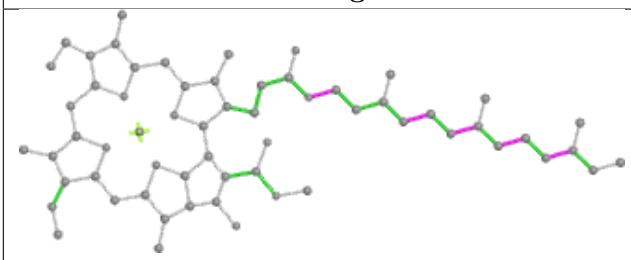
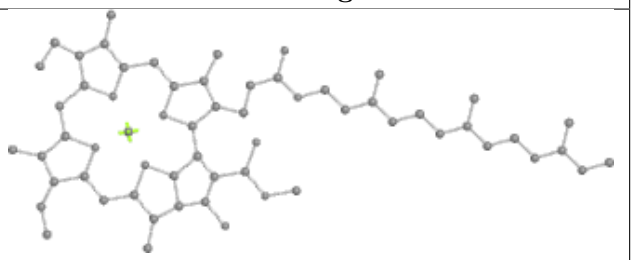


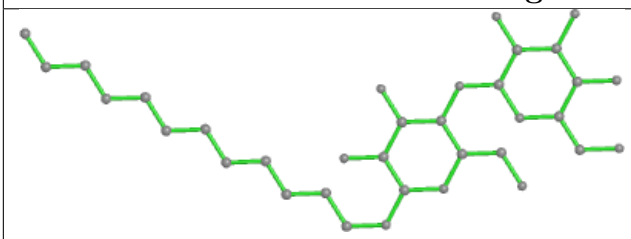
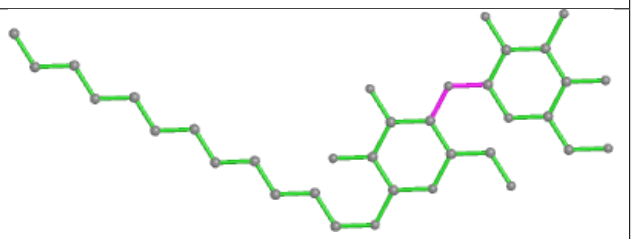
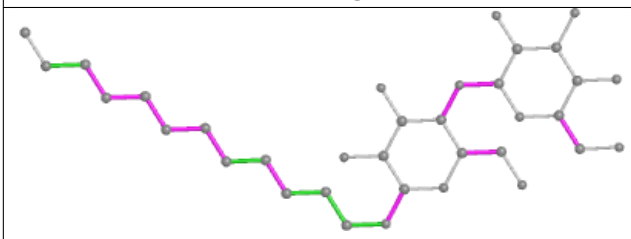
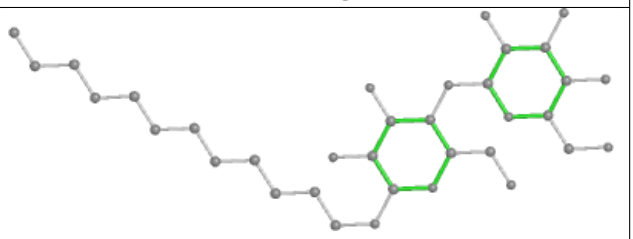
Ligand CLA E 311



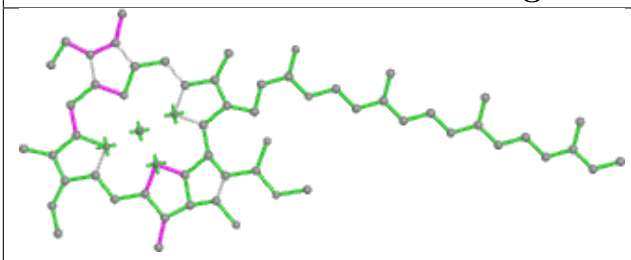
Ligand CLA P 308



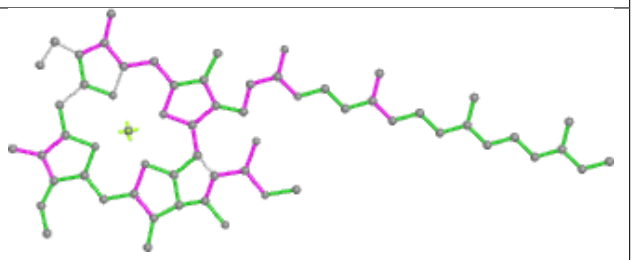
Ligand CLA H 306	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand LMT a 851	
 Bond lengths	 Bond angles
 Torsions	 Rings

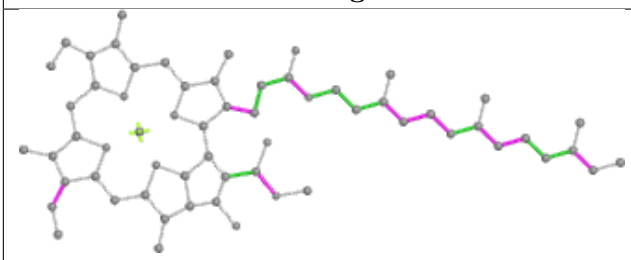
Ligand CLA D 307



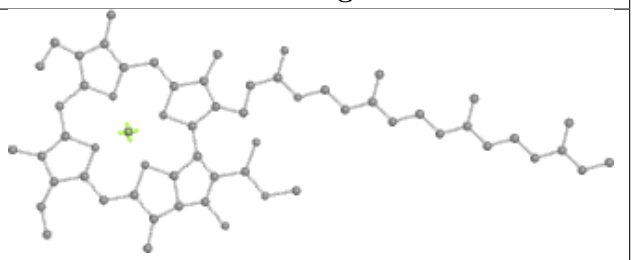
Bond lengths



Bond angles

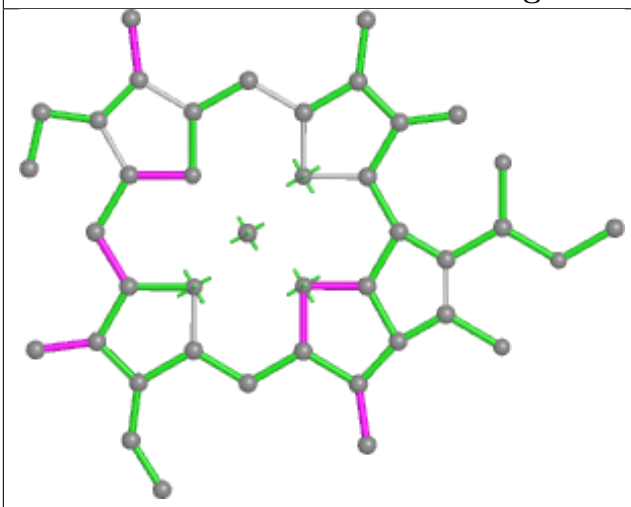


Torsions

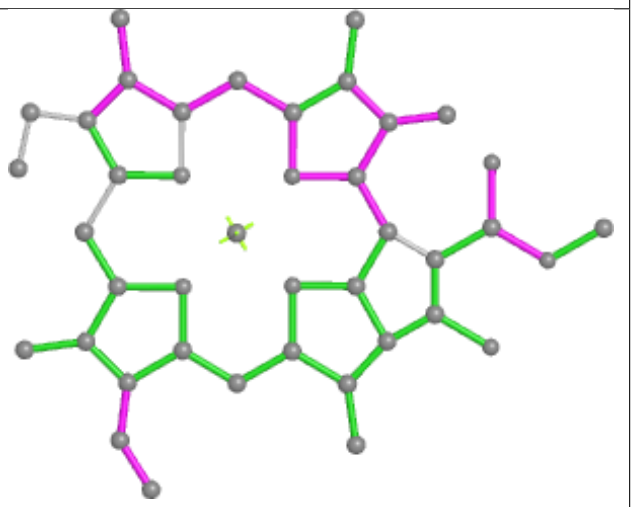


Rings

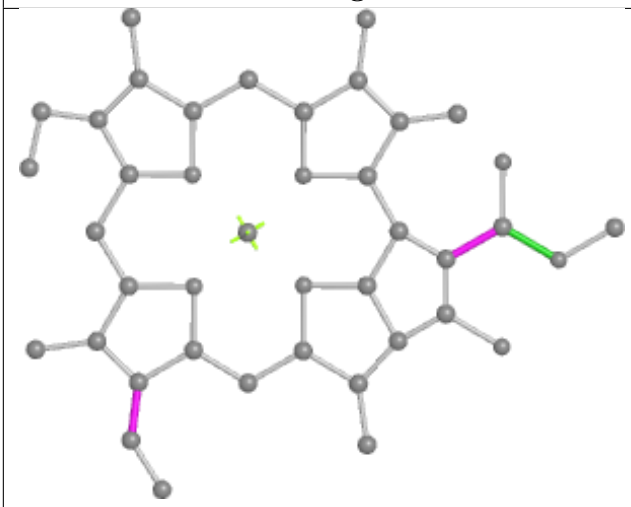
Ligand CLA D 315



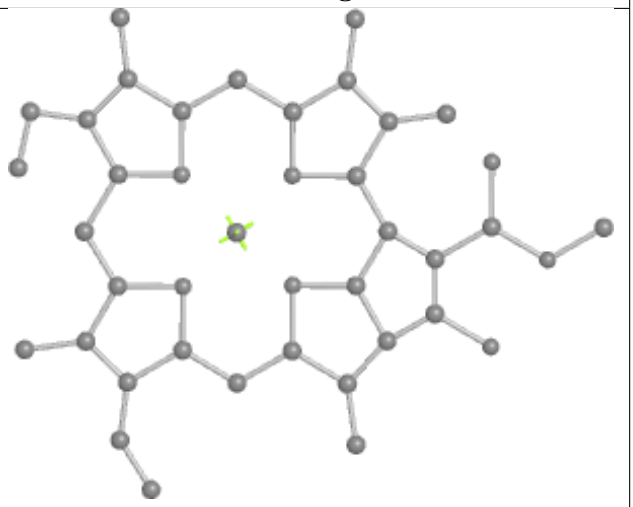
Bond lengths



Bond angles

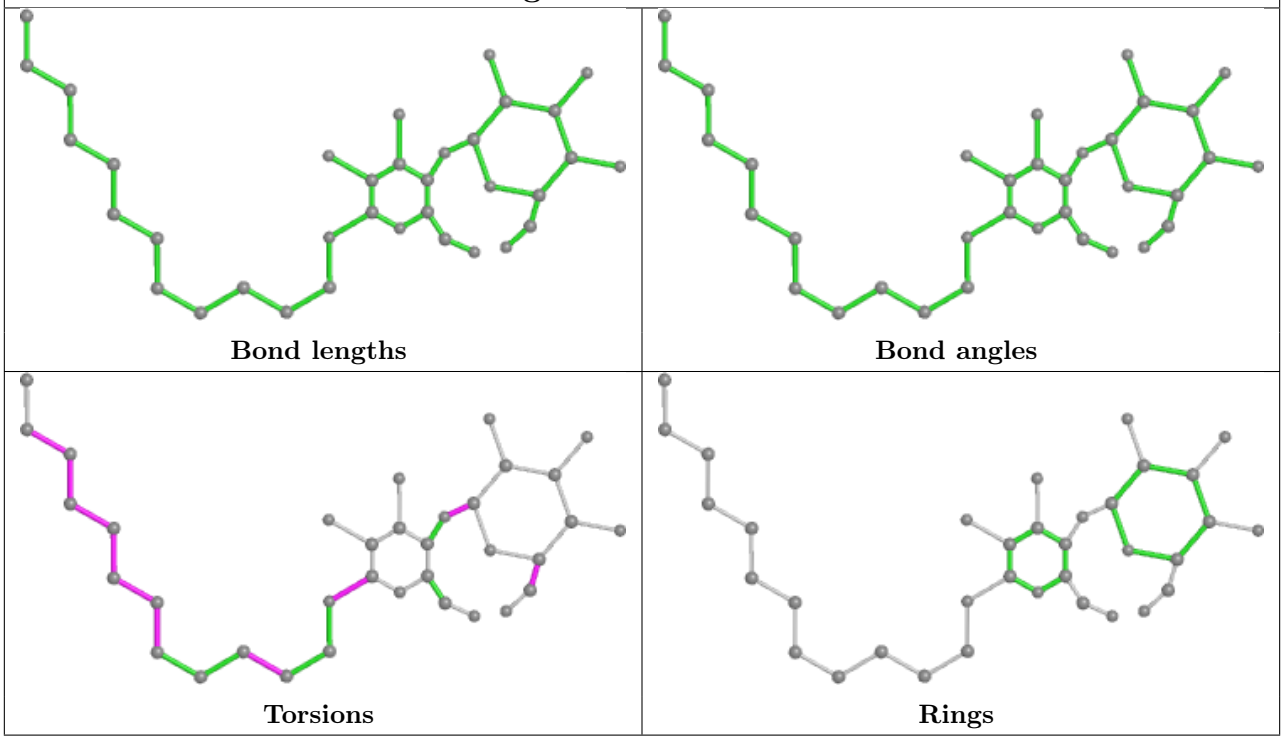


Torsions

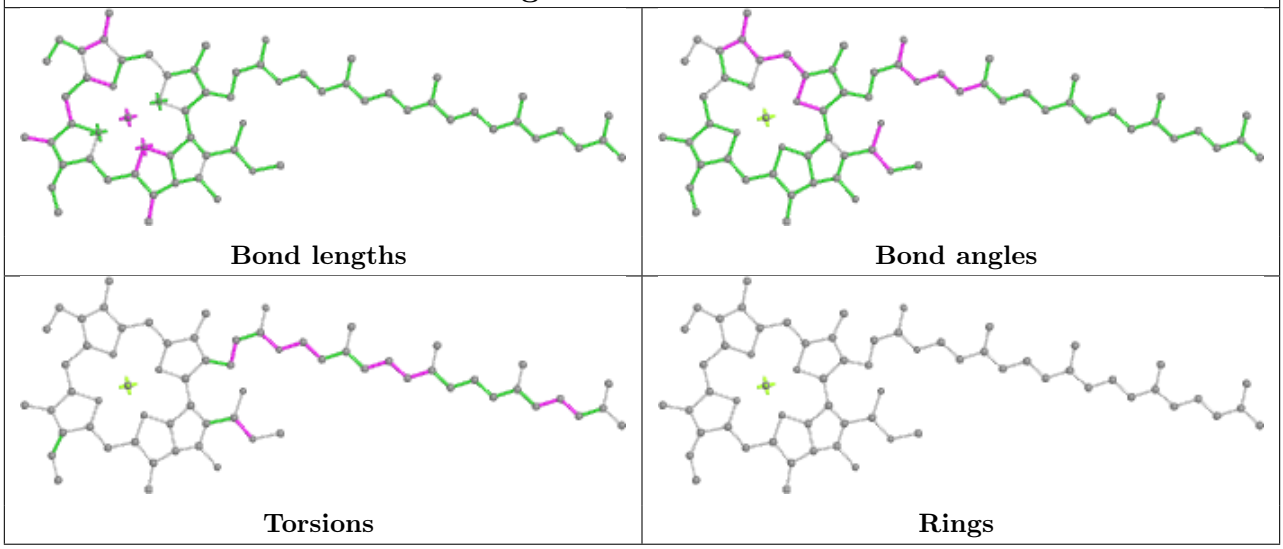


Rings

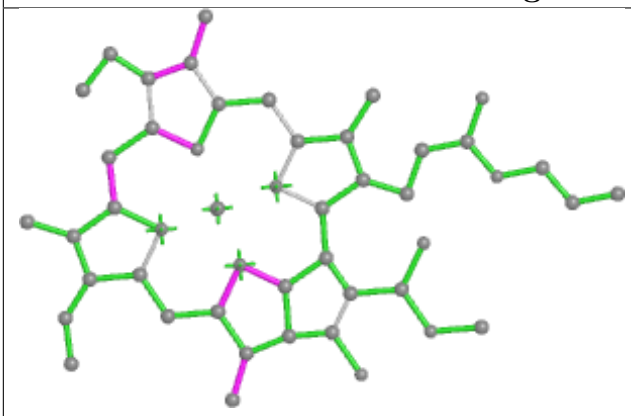
Ligand LMT E 320



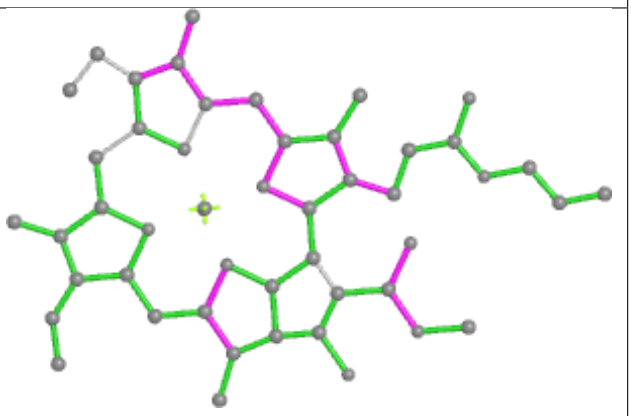
Ligand CLA M 307



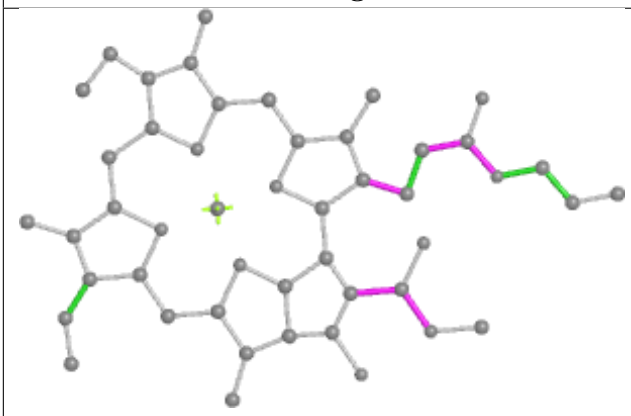
Ligand CLA H 305



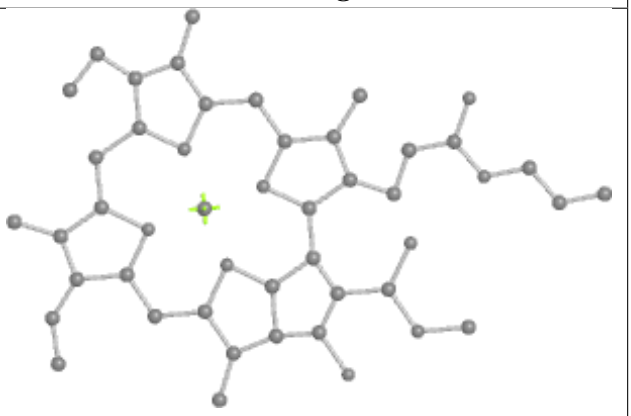
Bond lengths



Bond angles

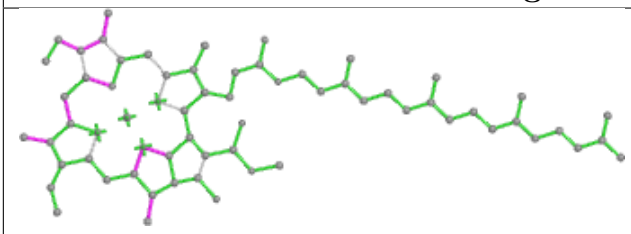


Torsions

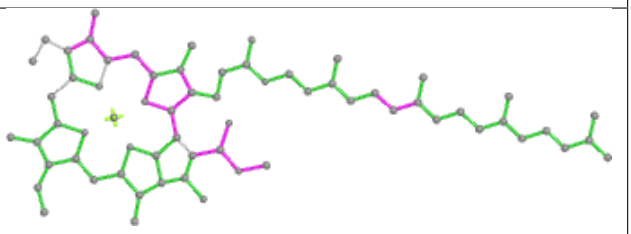


Rings

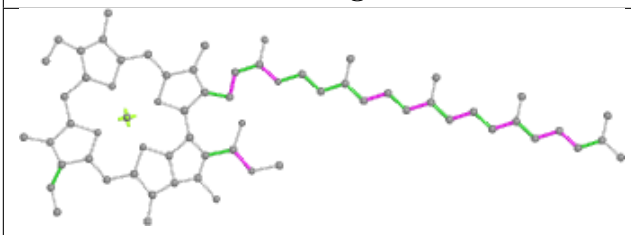
Ligand CLA R 312



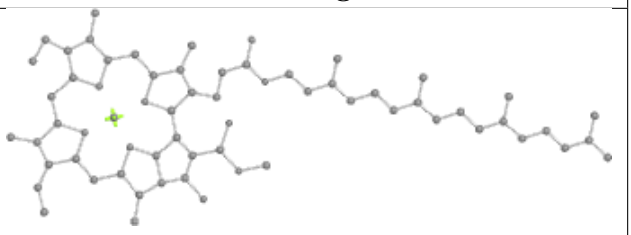
Bond lengths



Bond angles

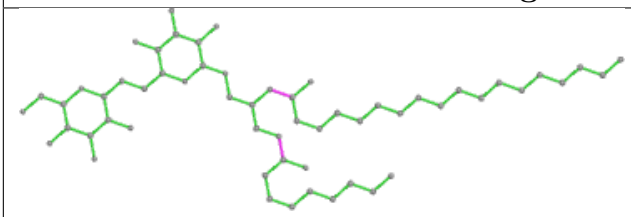


Torsions

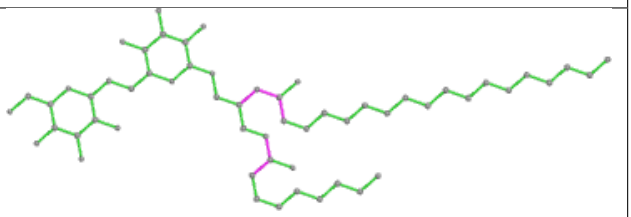


Rings

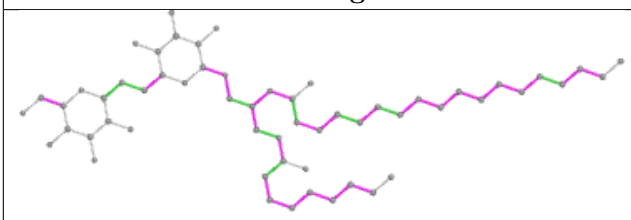
Ligand DGD C 215



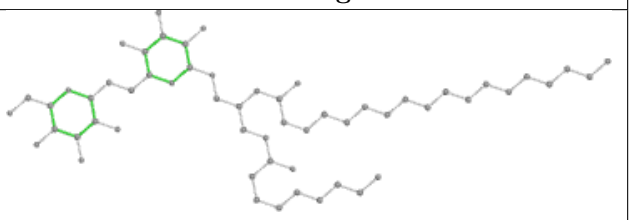
Bond lengths



Bond angles

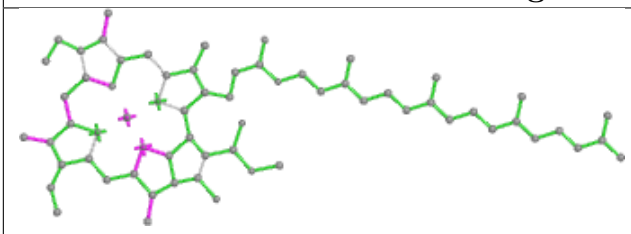


Torsions

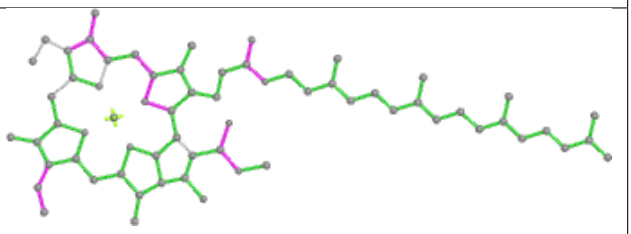


Rings

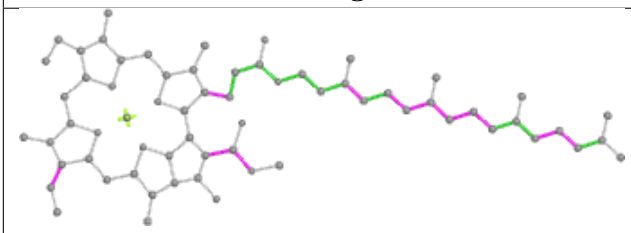
Ligand CLA b 815



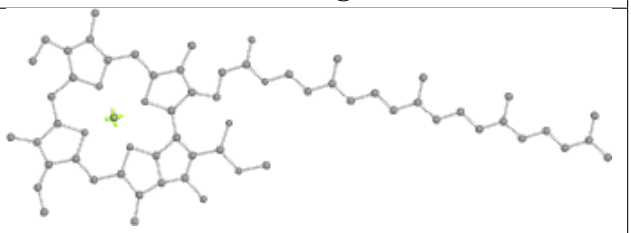
Bond lengths



Bond angles

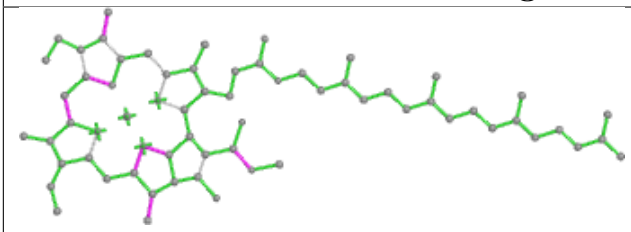


Torsions

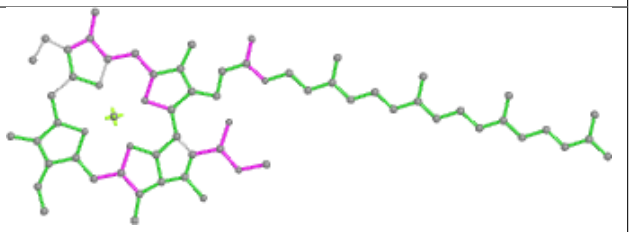


Rings

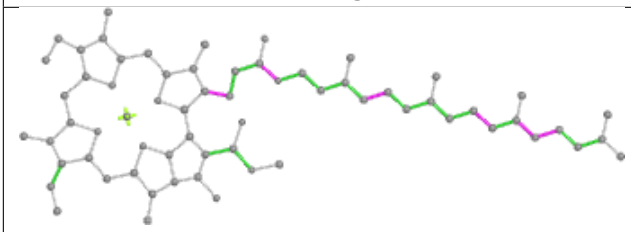
Ligand CLA W 211



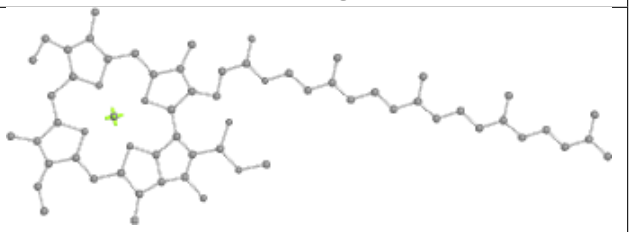
Bond lengths



Bond angles

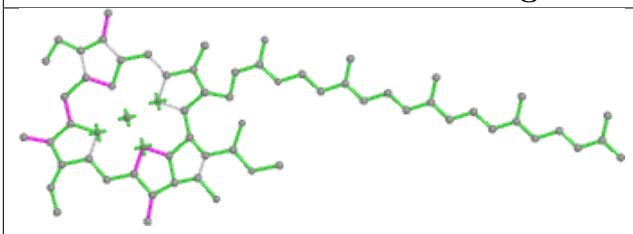


Torsions



Rings

Ligand CLA M 309



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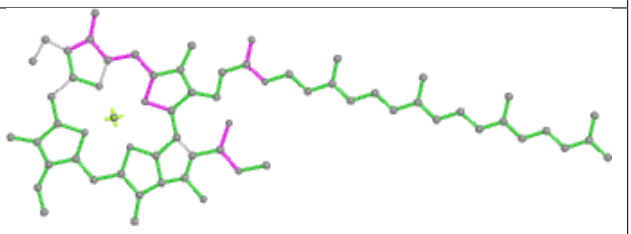
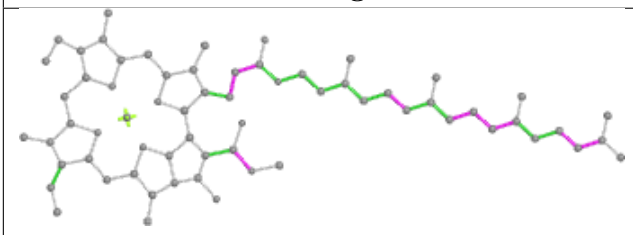
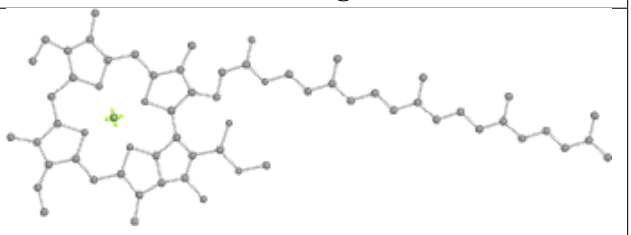


Bond angles

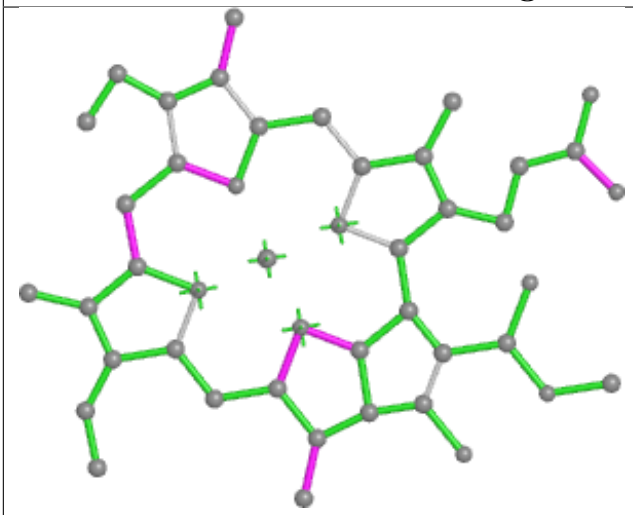


Torsions

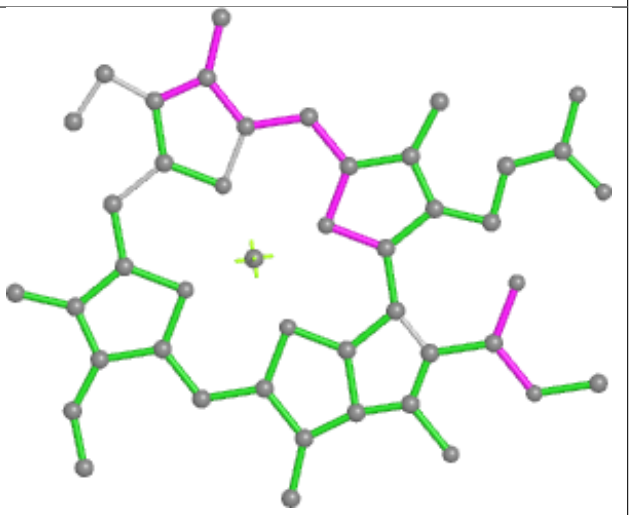


Rings

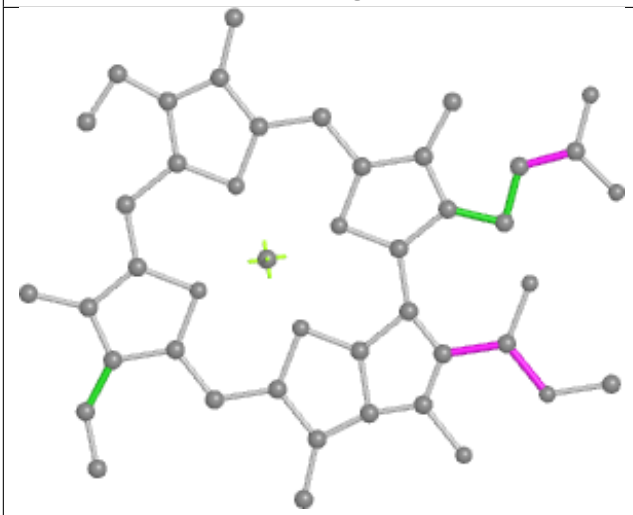
Ligand CLA W 208



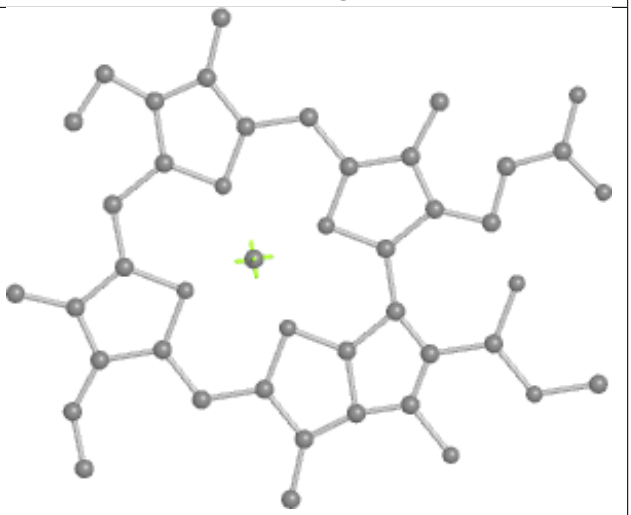
Bond lengths



Bond angles

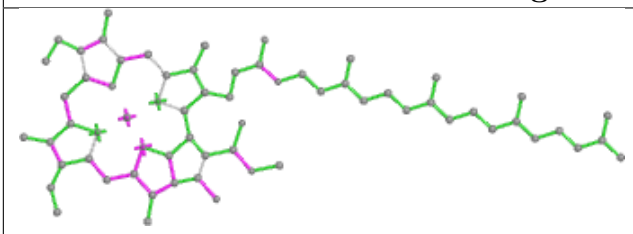


Torsions

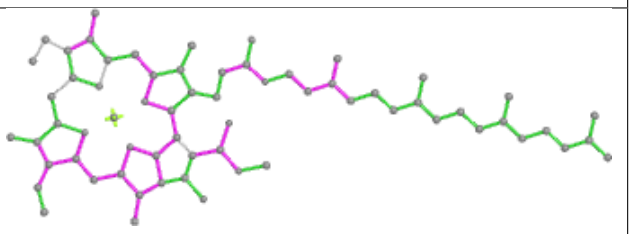


Rings

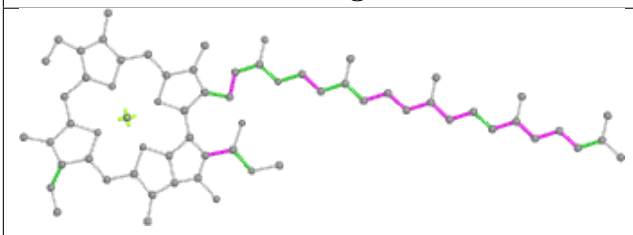
Ligand CLA I 308



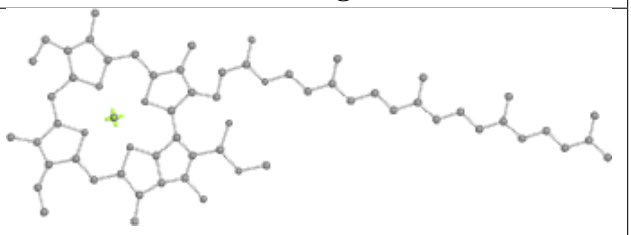
Bond lengths



Bond angles

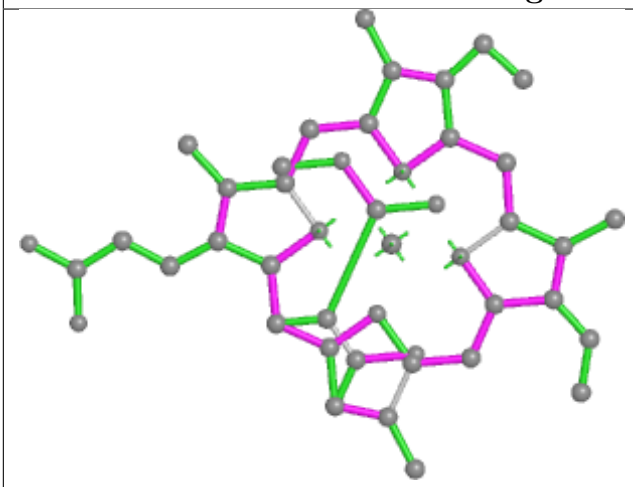


Torsions

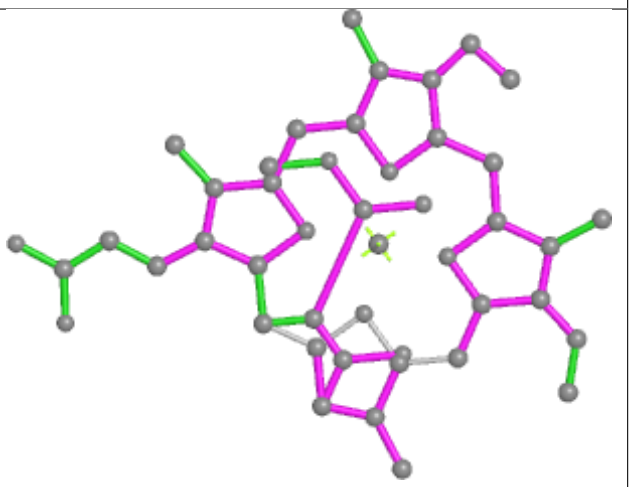


Rings

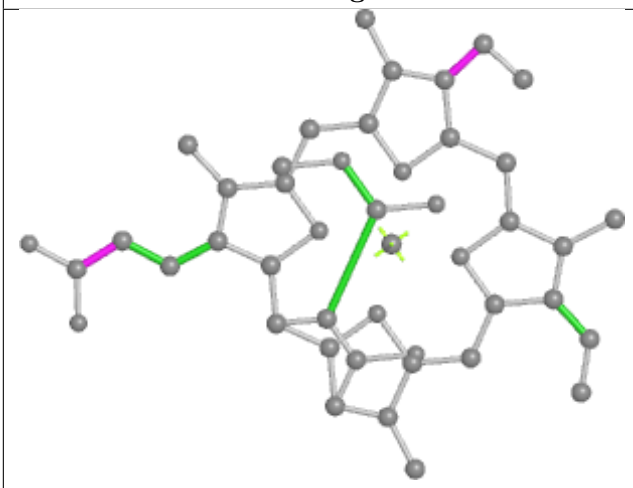
Ligand KC1 R 317



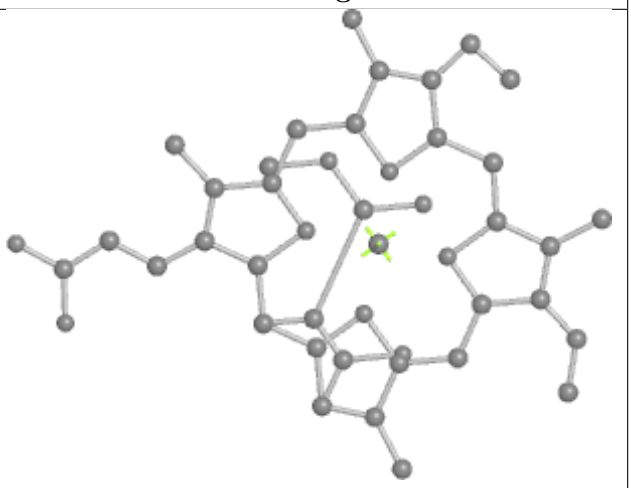
Bond lengths



Bond angles

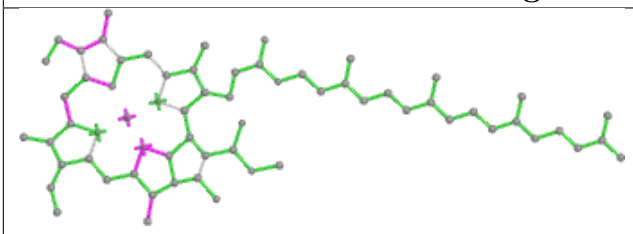


Torsions

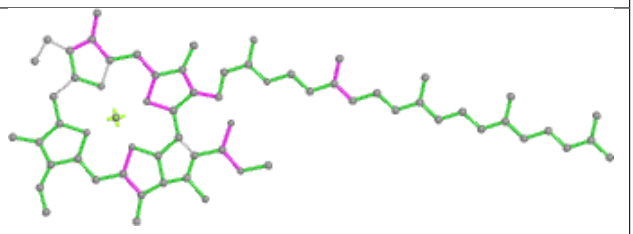


Rings

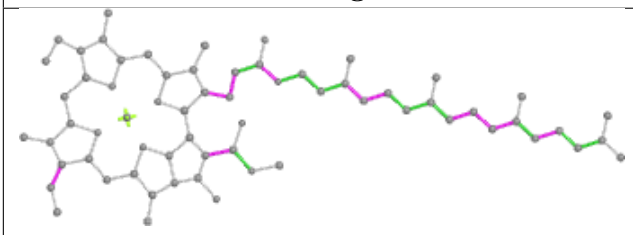
Ligand CLA G 311



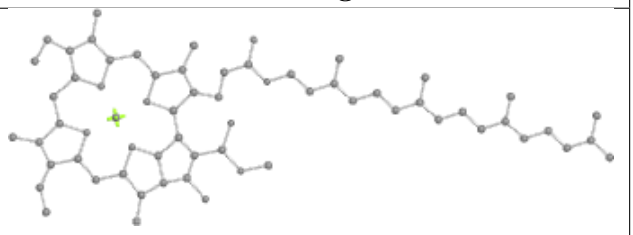
Bond lengths



Bond angles

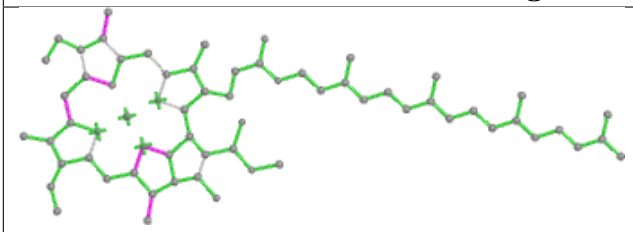


Torsions

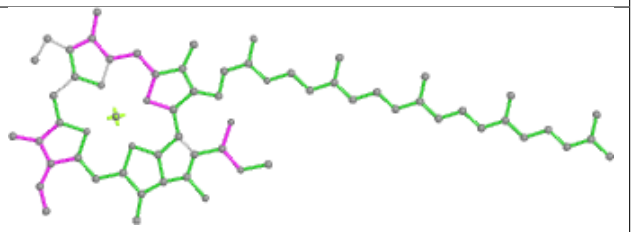


Rings

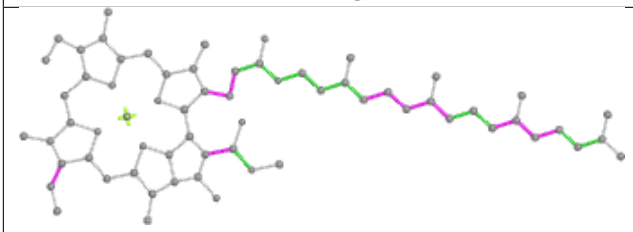
Ligand CLA E 316



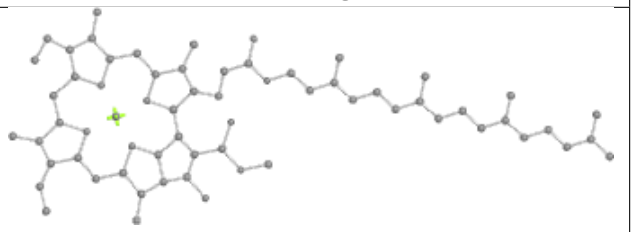
Bond lengths



Bond angles

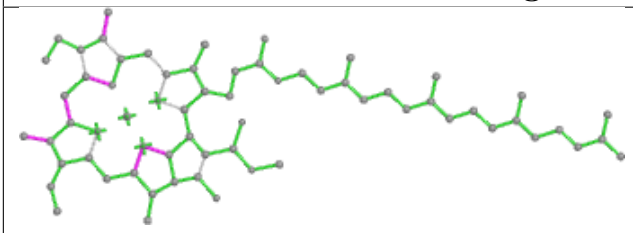


Torsions

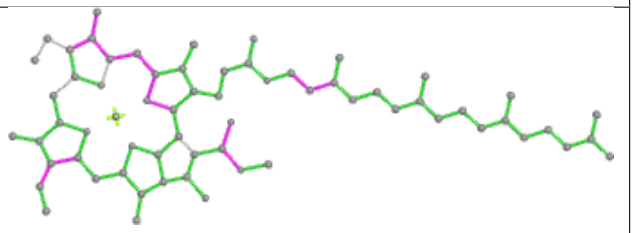


Rings

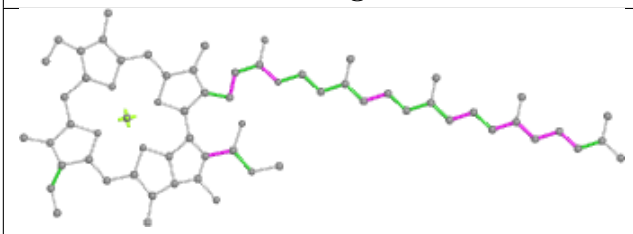
Ligand CLA K 308



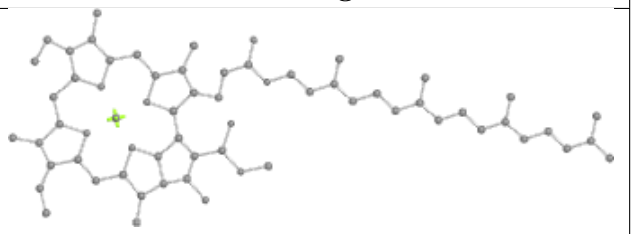
Bond lengths



Bond angles

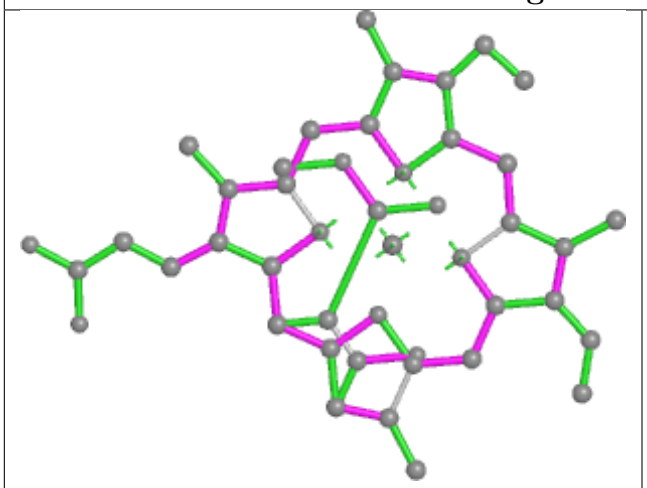


Torsions

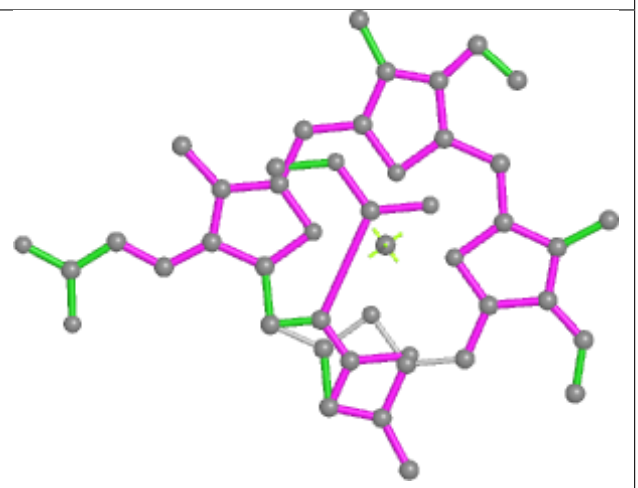


Rings

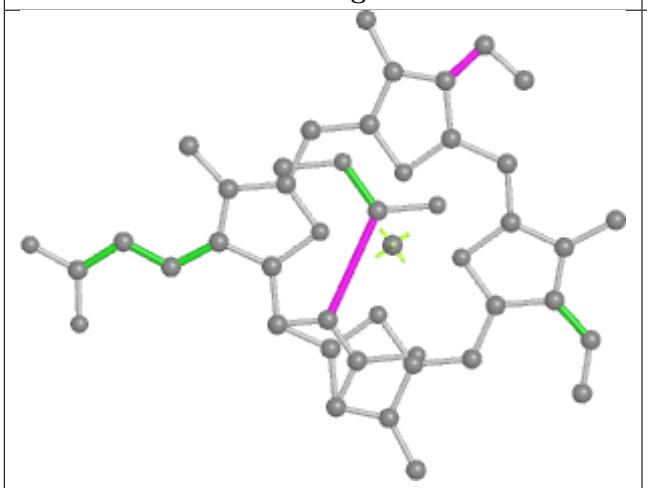
Ligand KC1 O 315



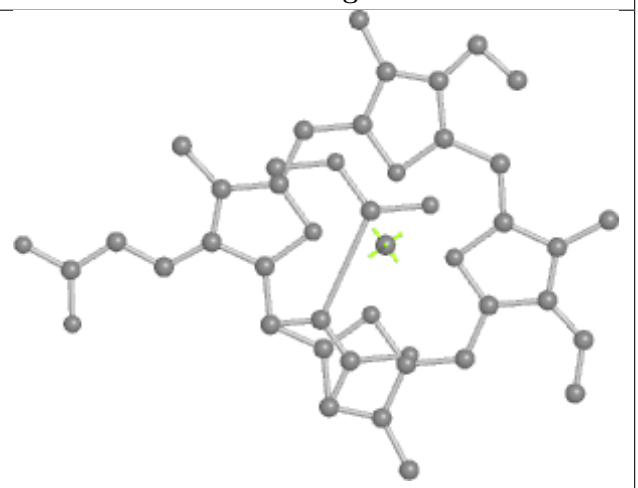
Bond lengths



Bond angles

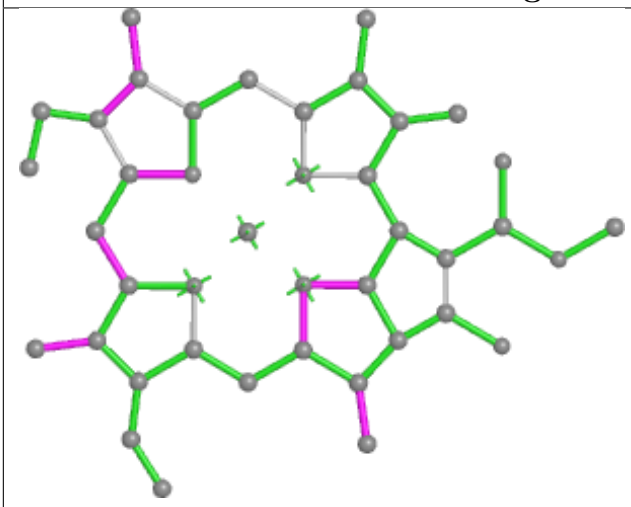


Torsions

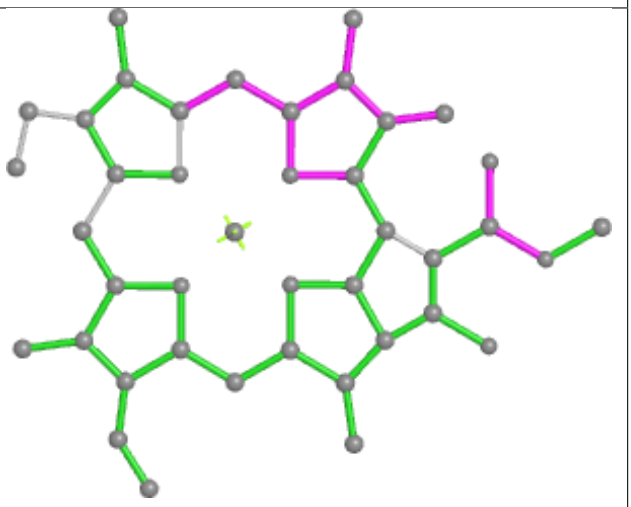


Rings

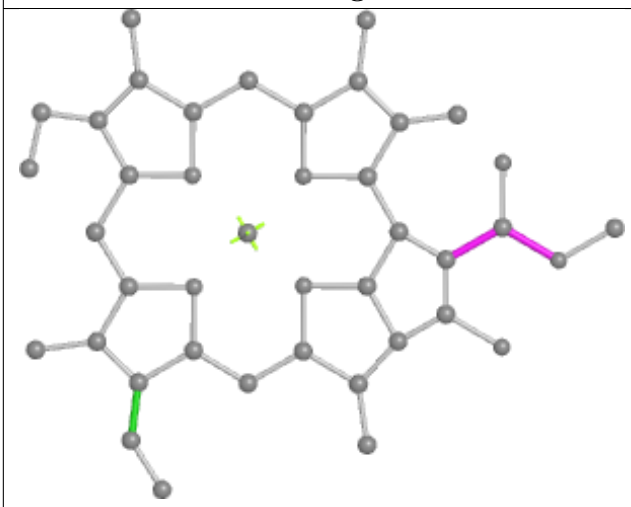
Ligand CLA O 314



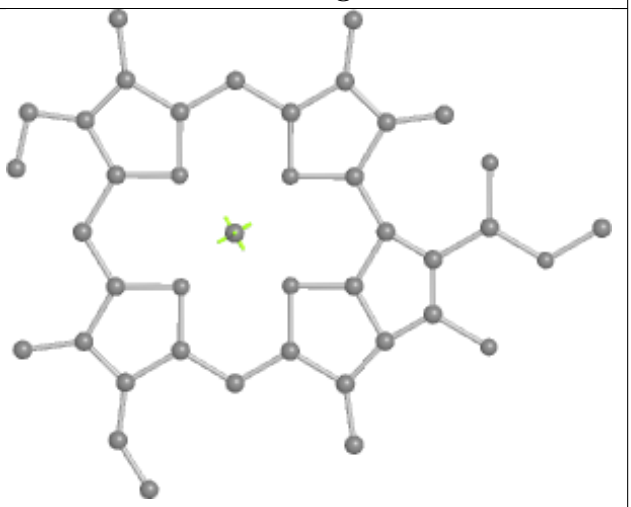
Bond lengths



Bond angles

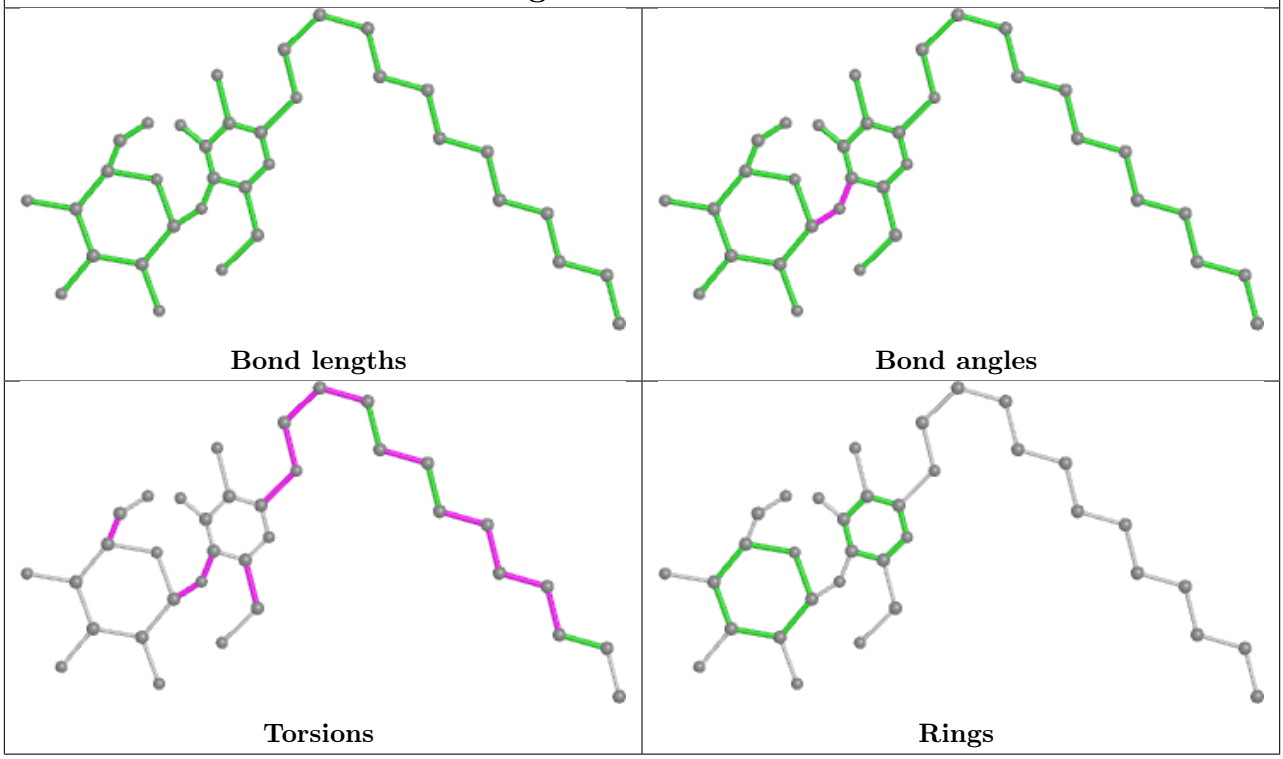


Torsions

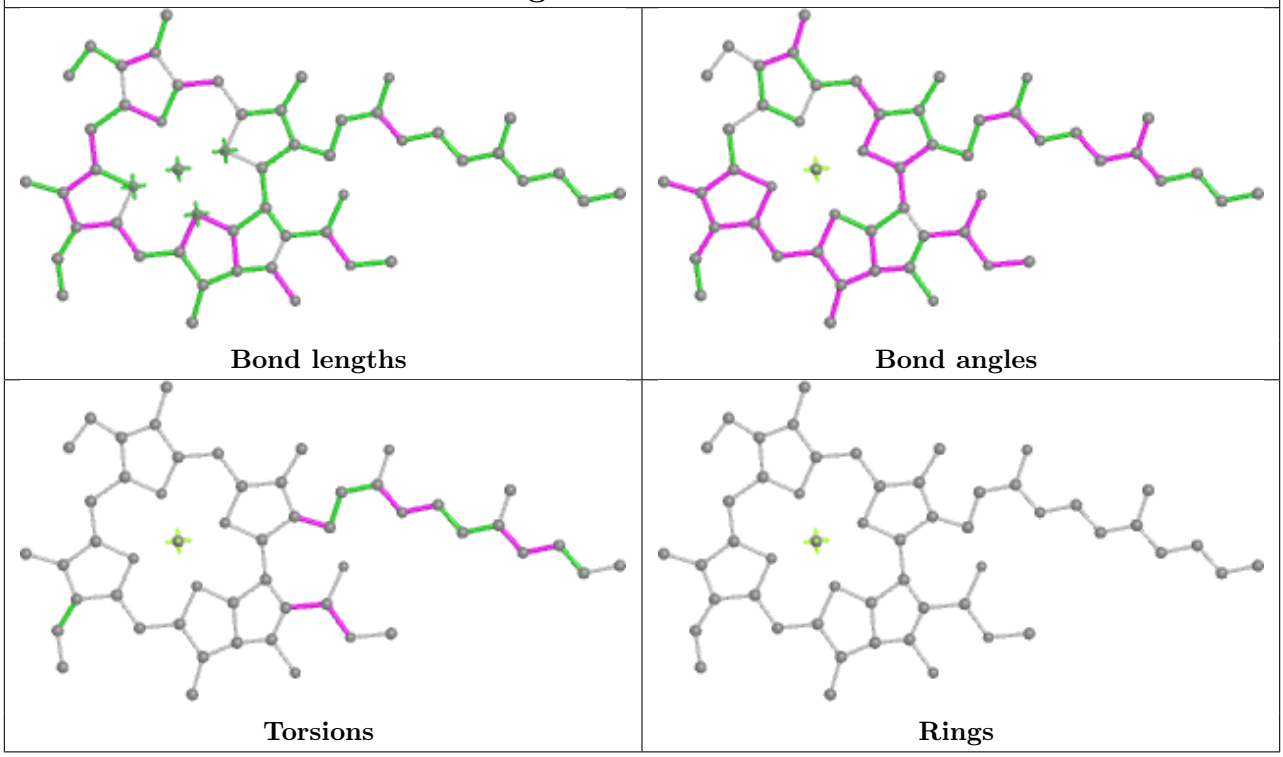


Rings

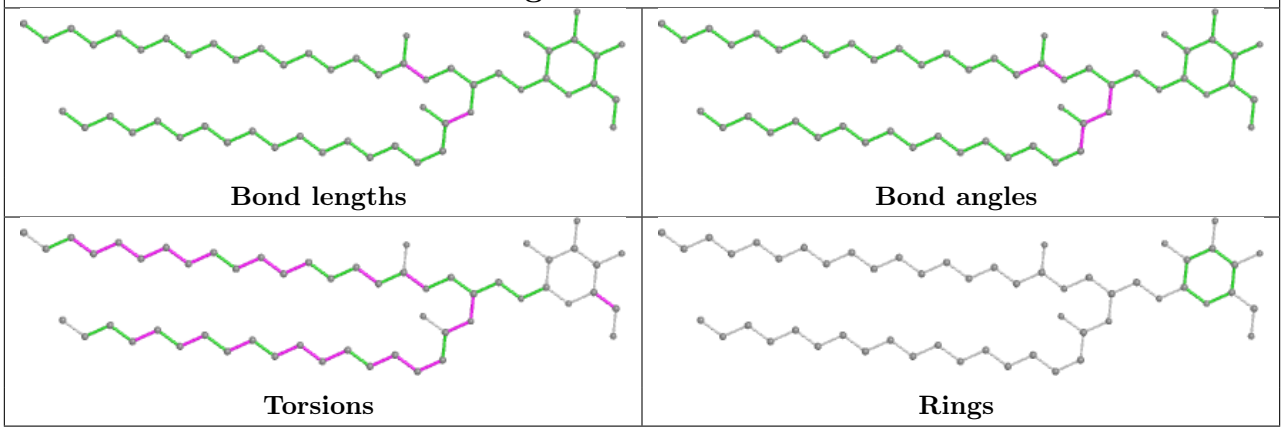
Ligand LMT I 318



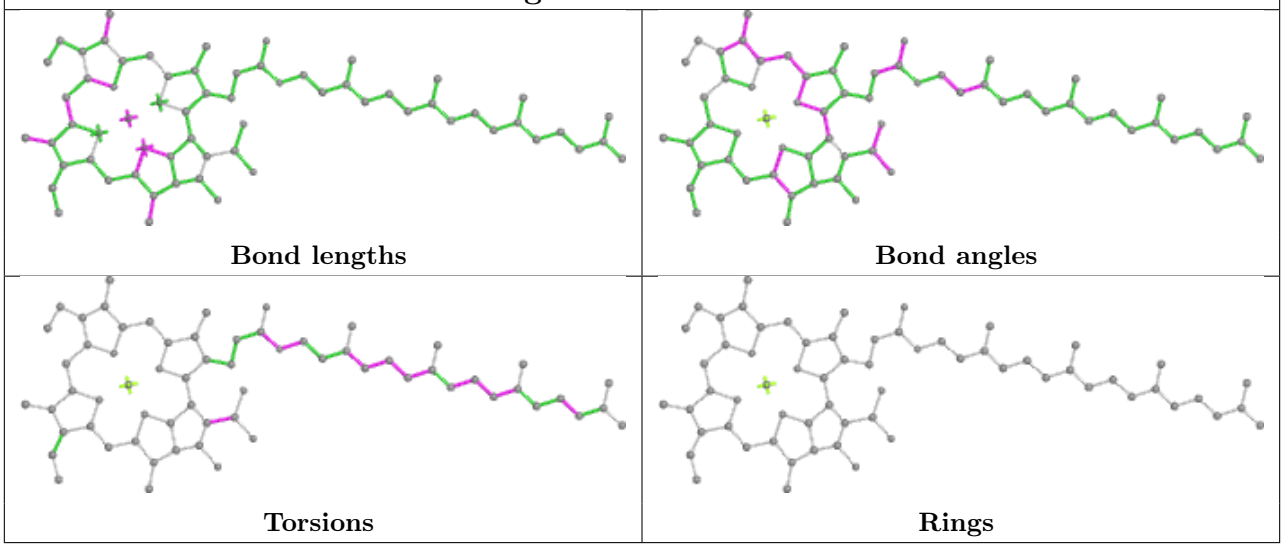
Ligand CLA b 824



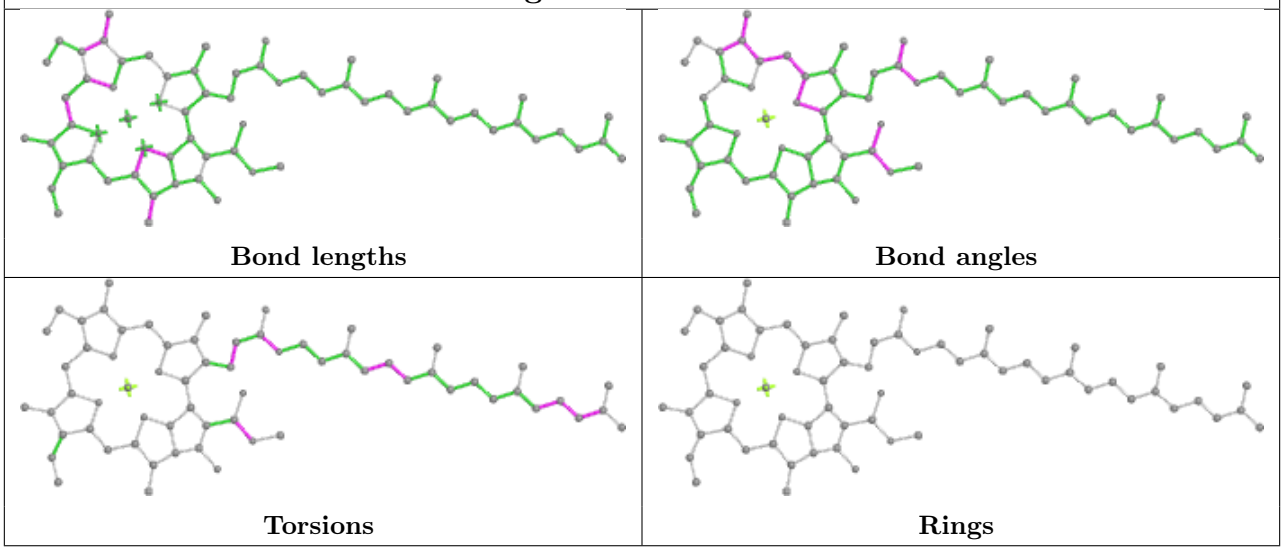
Ligand LMG a 852

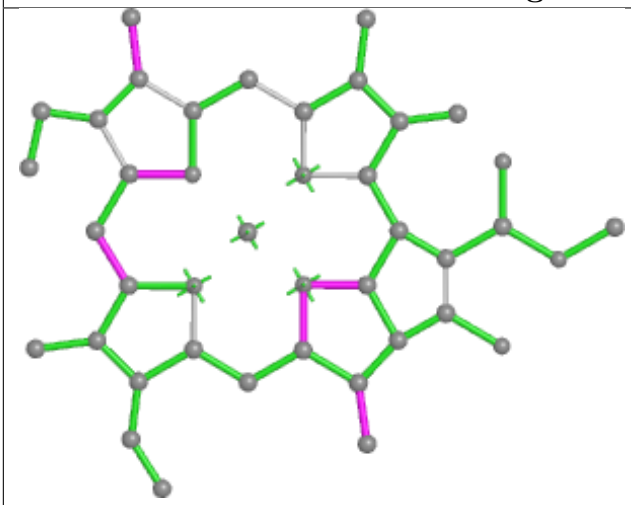
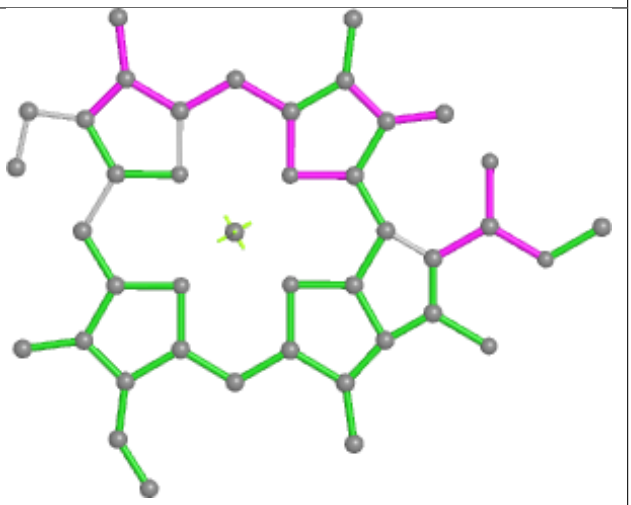
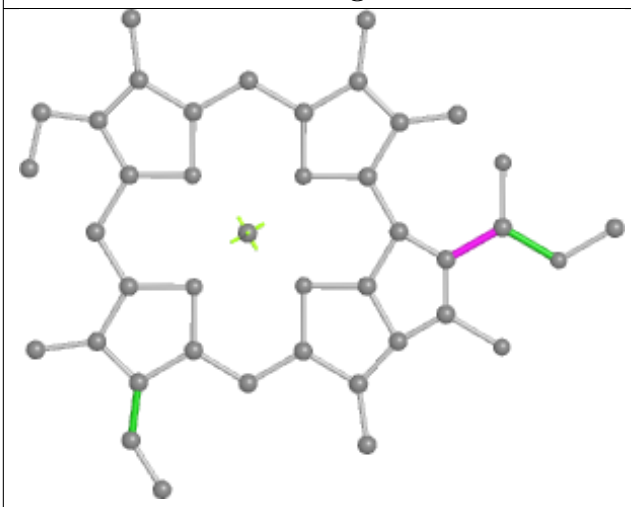
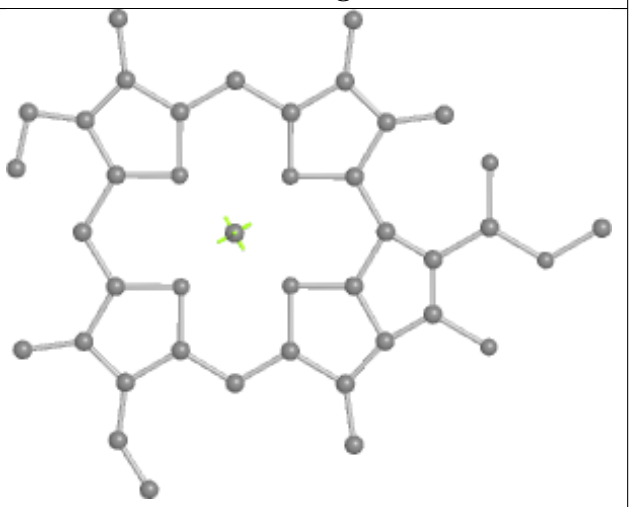


Ligand CLA H 308

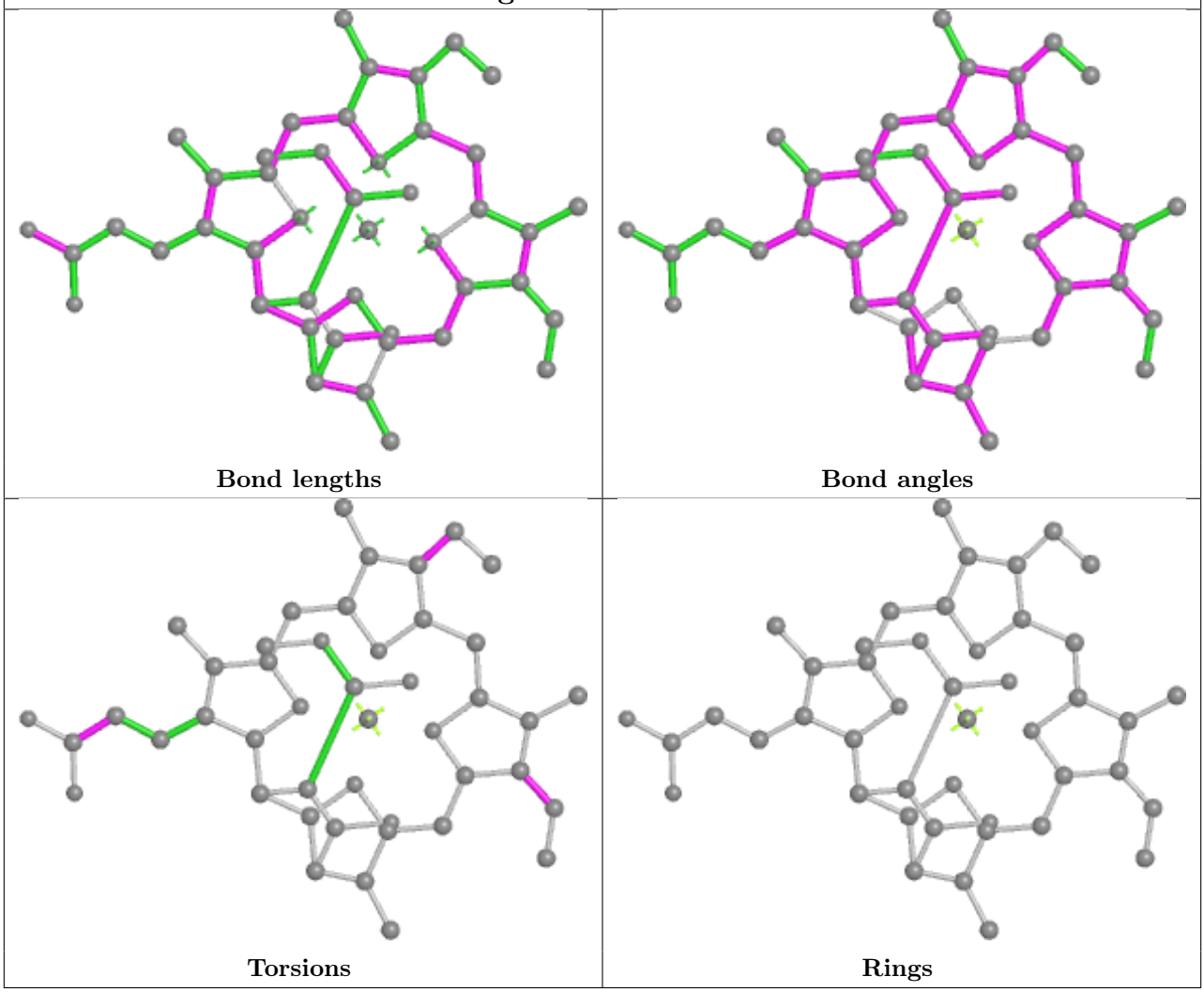


Ligand CLA R 315

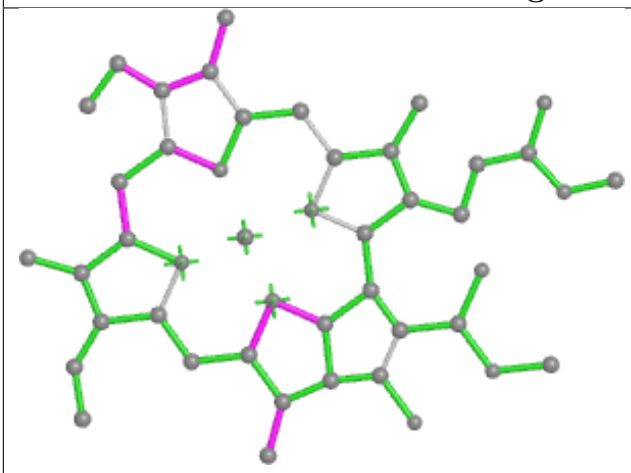


Ligand CLA L 316	
 Bond lengths	 Bond angles
 Torsions	 Rings

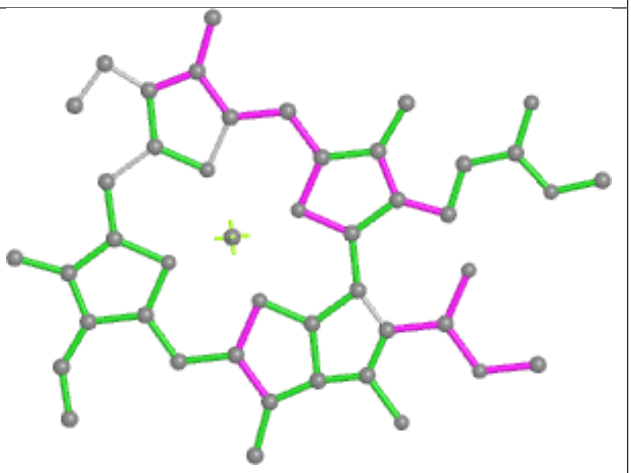
Ligand KC1 J 314



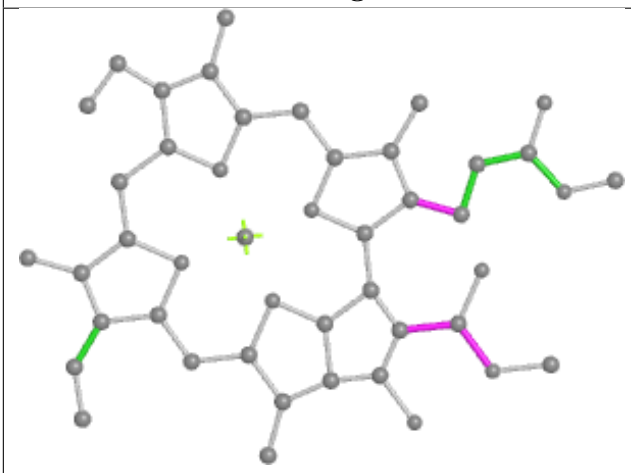
Ligand CLA b 822



Bond lengths



Bond angles



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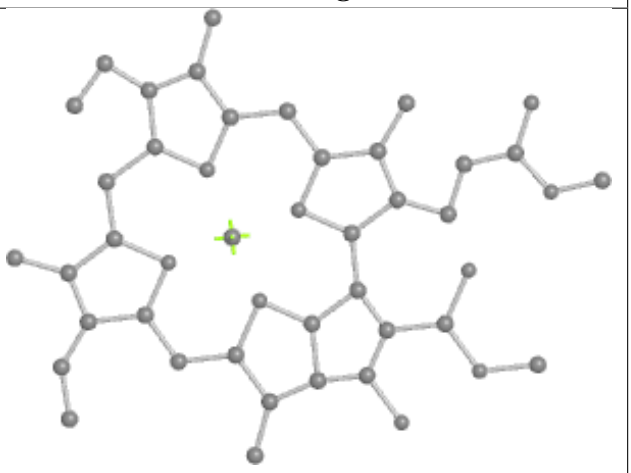
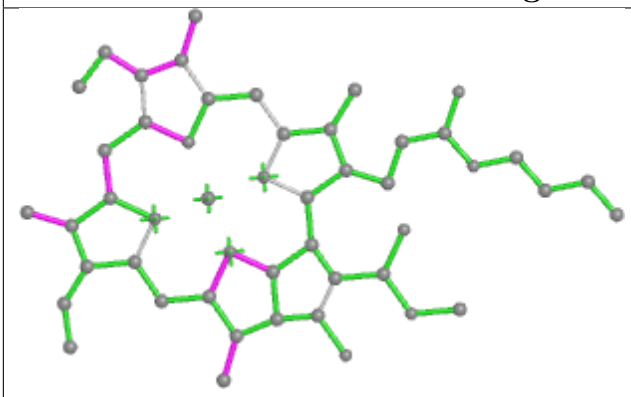
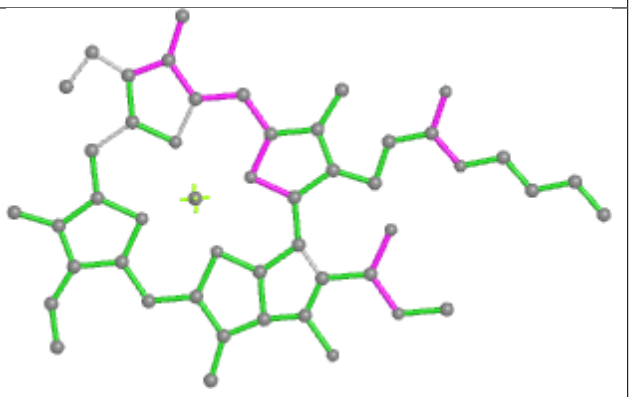
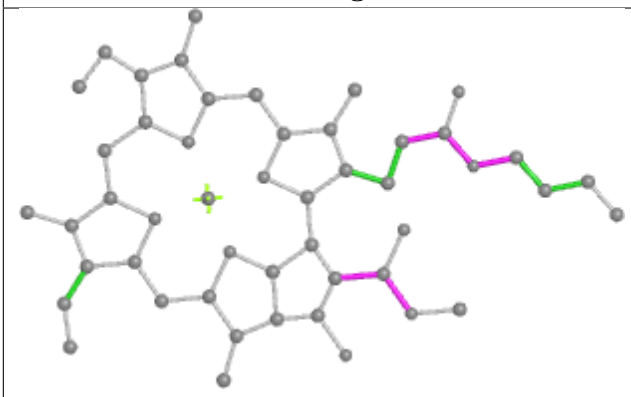
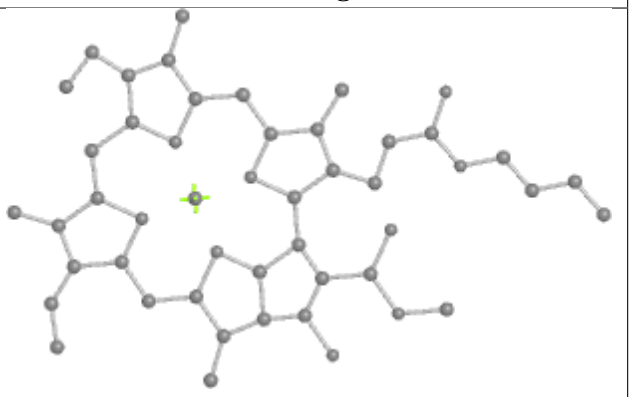
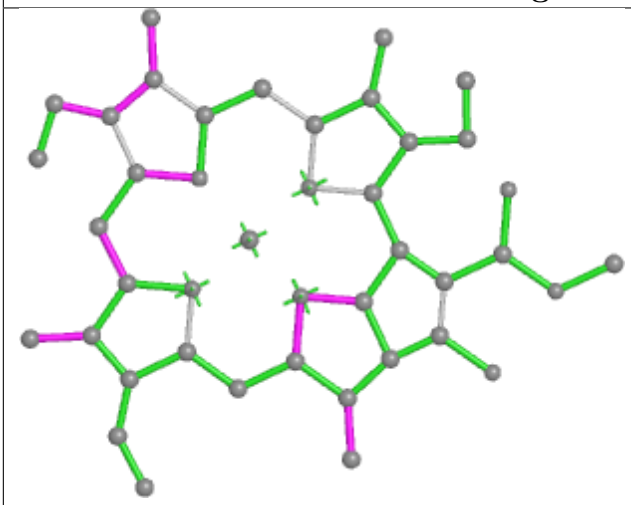


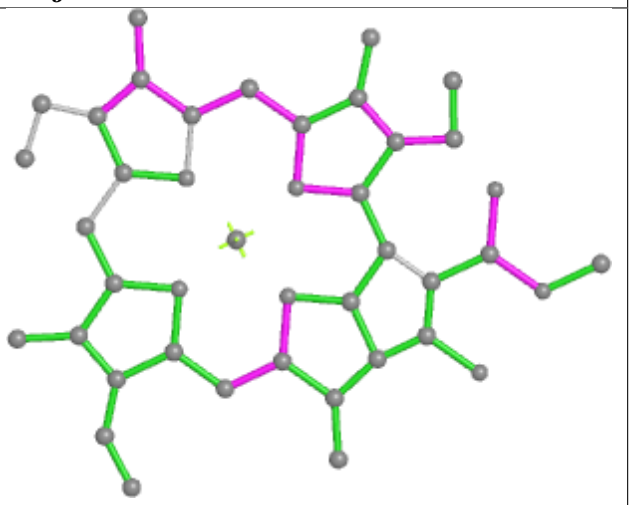
Rings

Ligand CLA G 316	
 Bond lengths	 Bond angles
 Torsions	 Rings

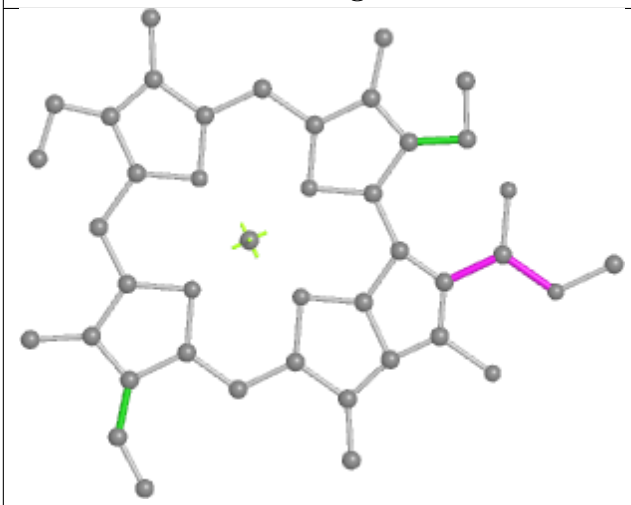
Ligand CLA j 106



Bond lengths



Bond angles



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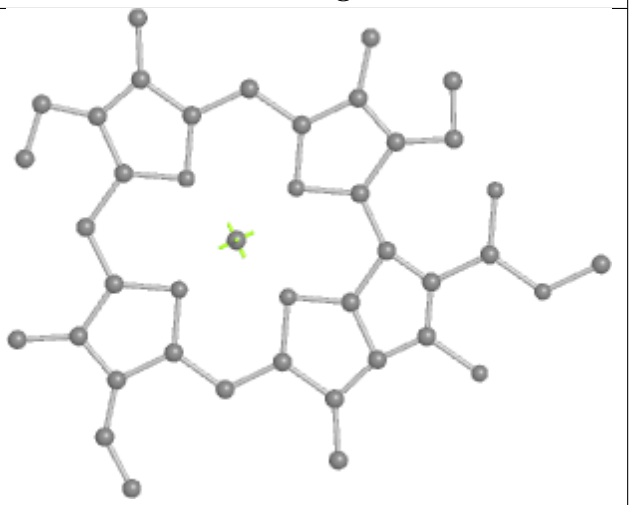
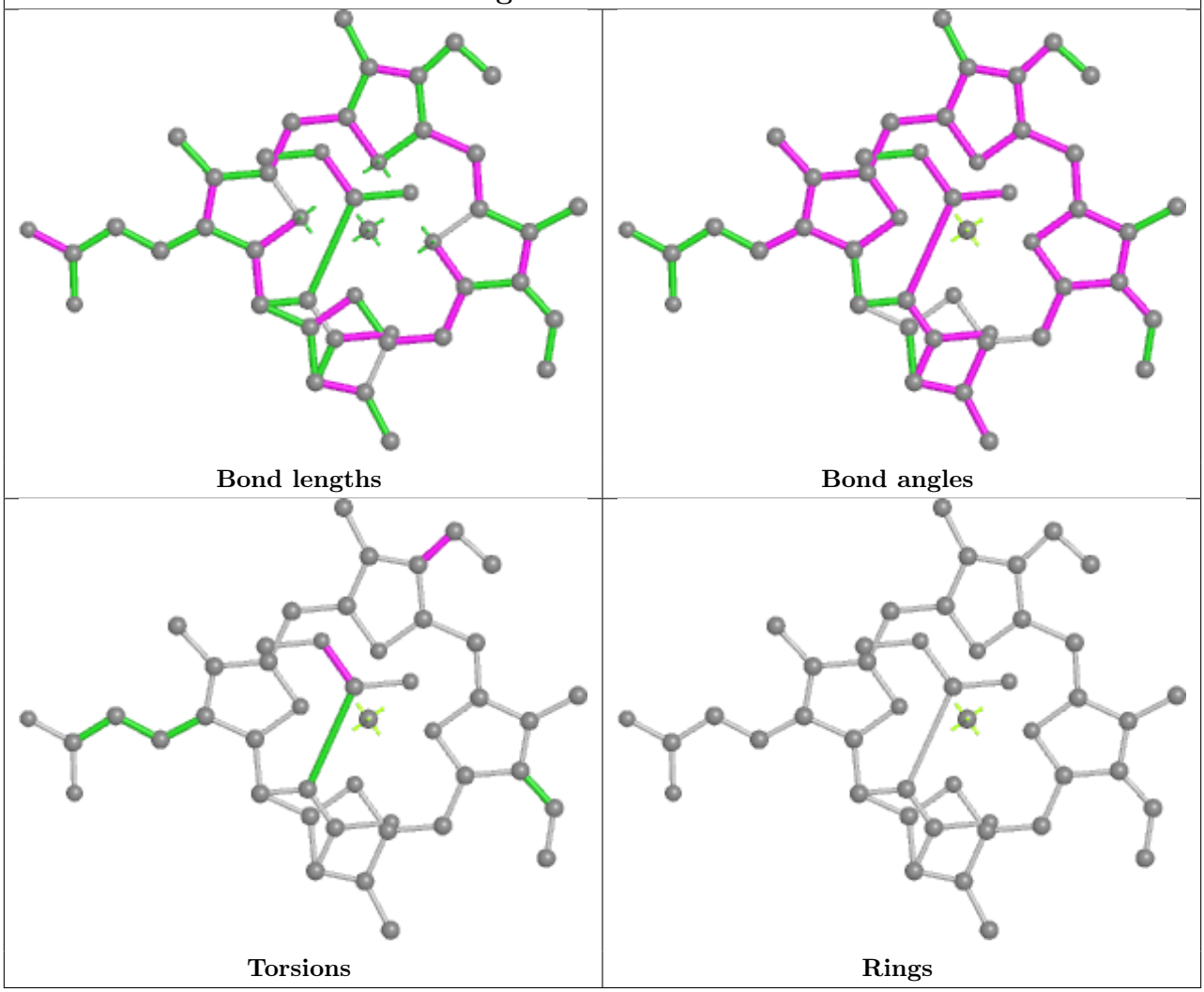
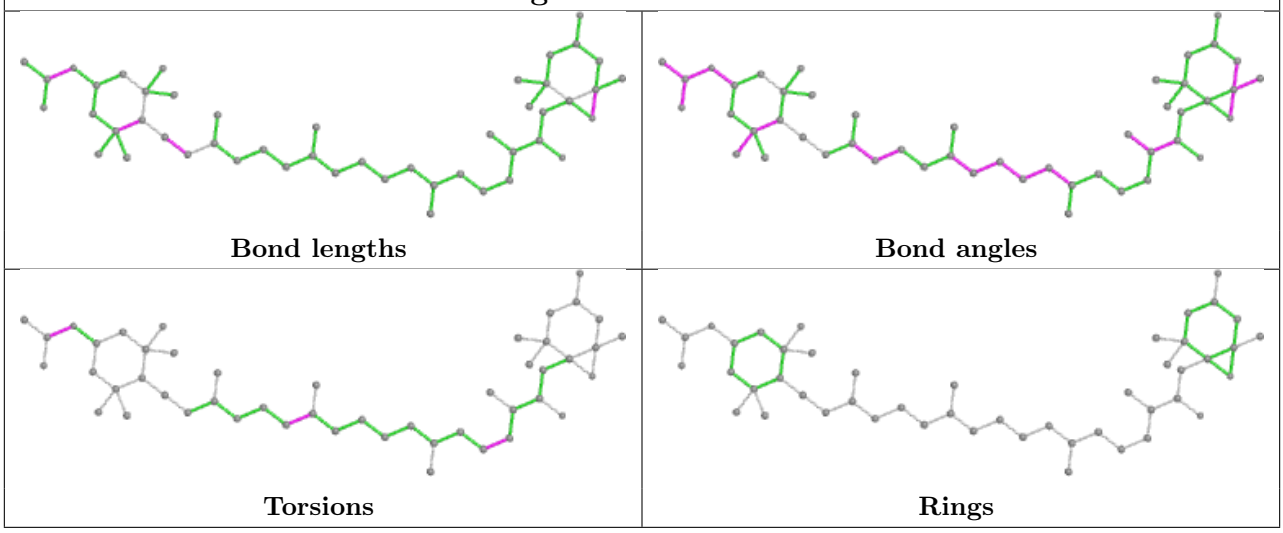


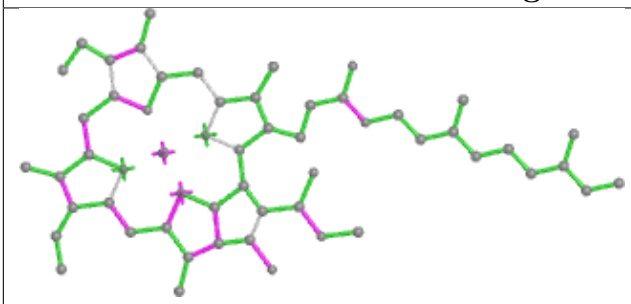
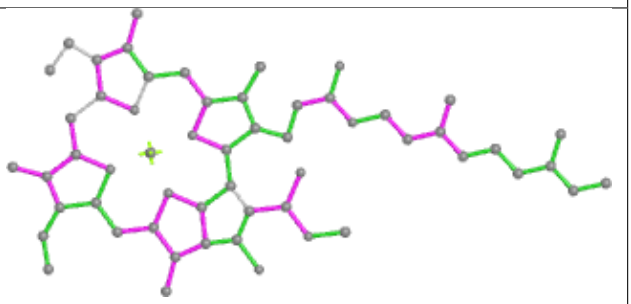
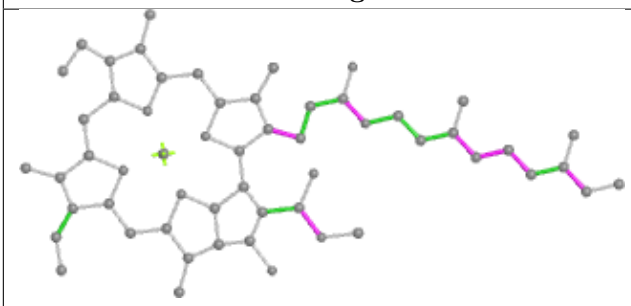
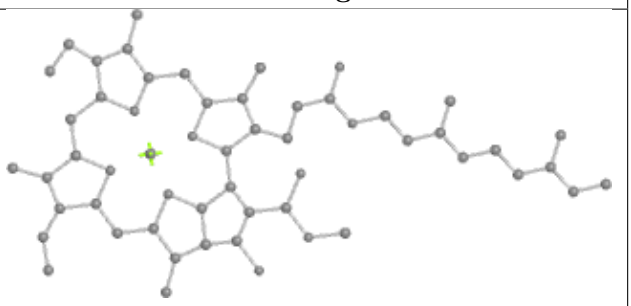
Rings

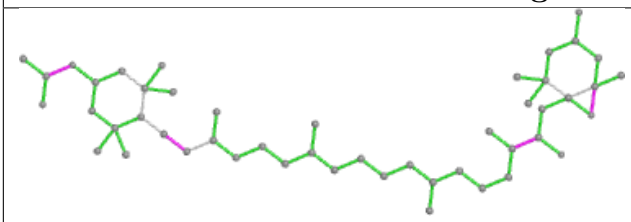
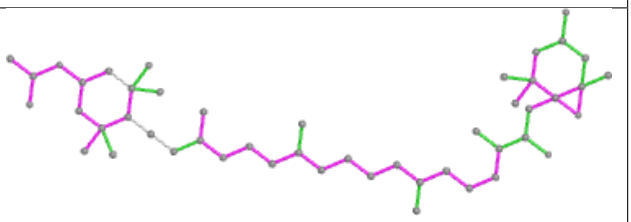
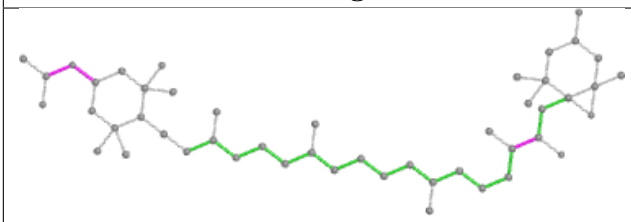
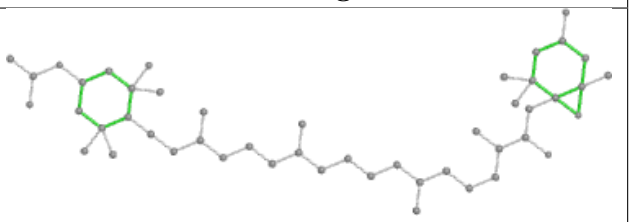
Ligand KC1 F 315



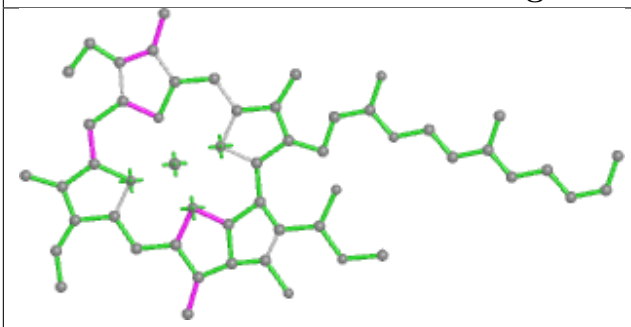
Ligand A86 R 305



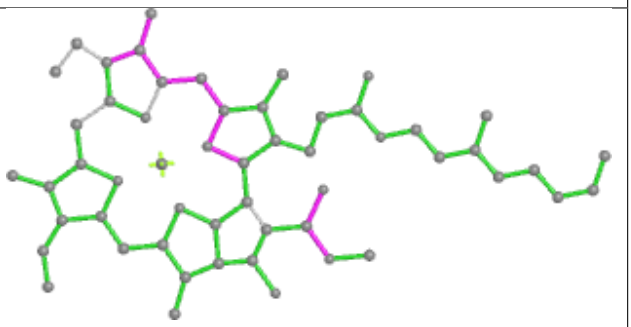
Ligand CLA G 315	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand A86 T 303	
 Bond lengths	 Bond angles
 Torsions	 Rings

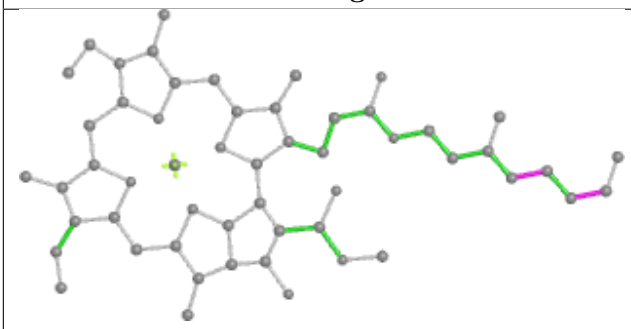
Ligand CLA L 310



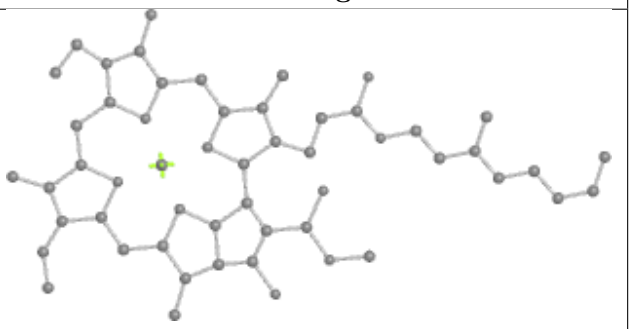
Bond lengths



Bond angles

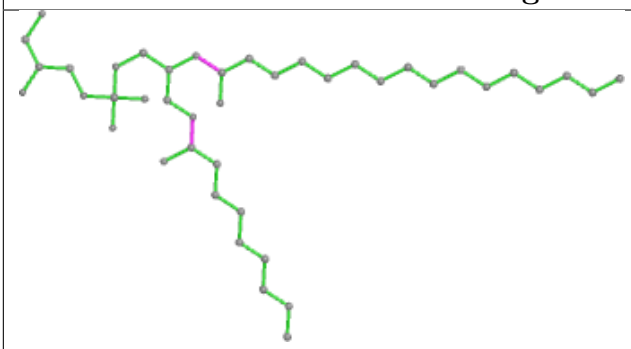


Torsions



Rings

Ligand LHG O 317



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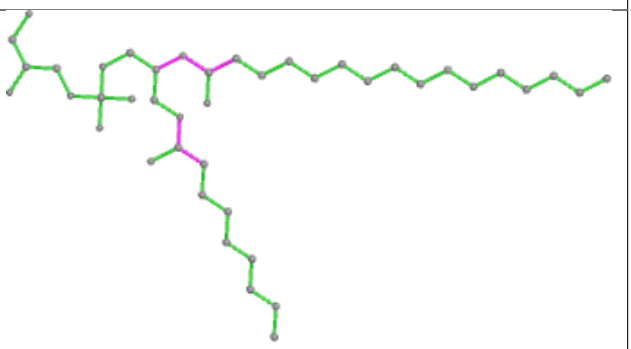
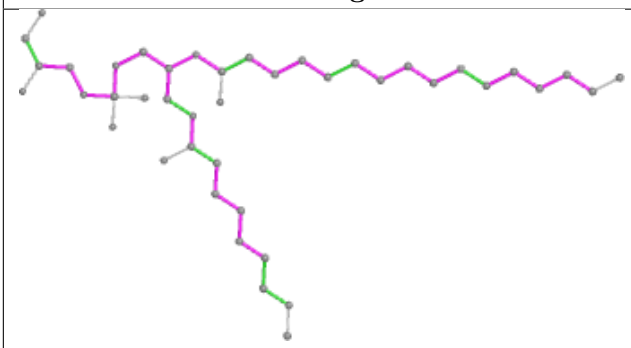


Bond angles



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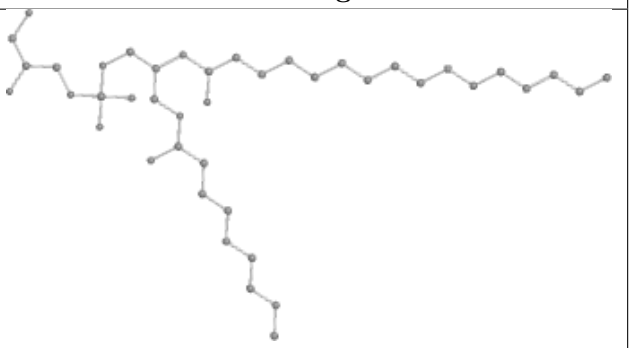
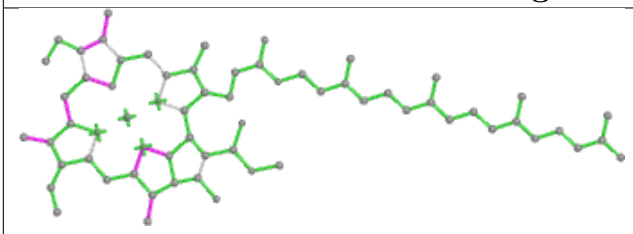


Rings

Ligand CLA j 101



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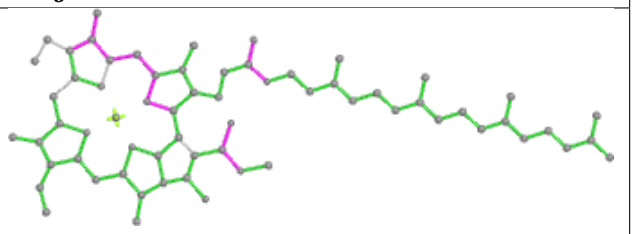
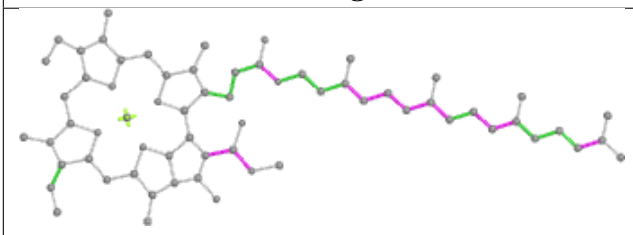
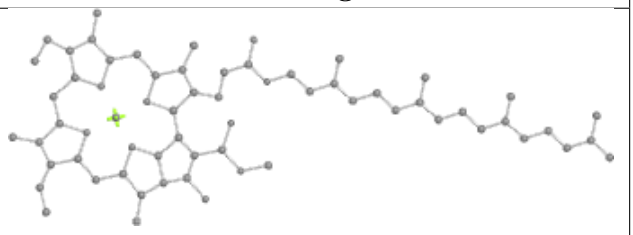


Bond angles

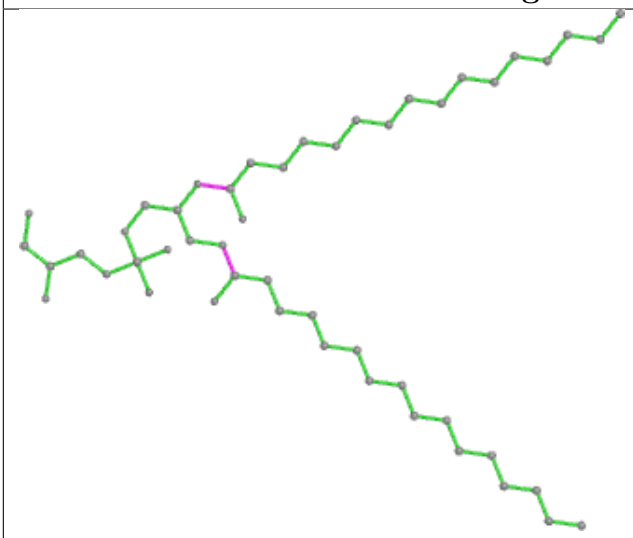


Torsions



Rings

Ligand LHG Q 315



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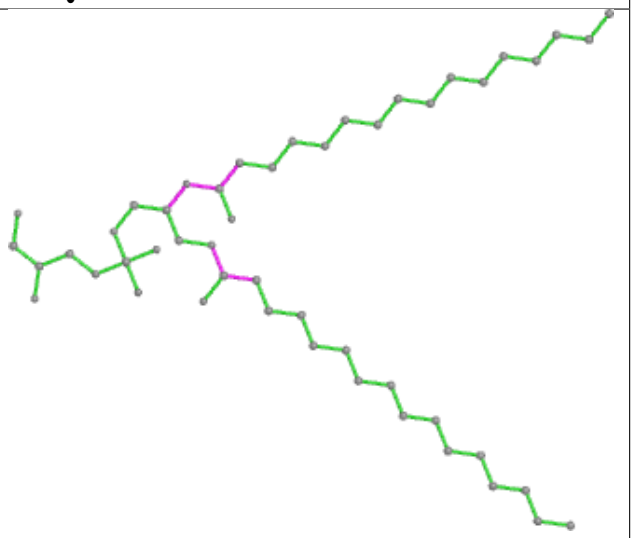
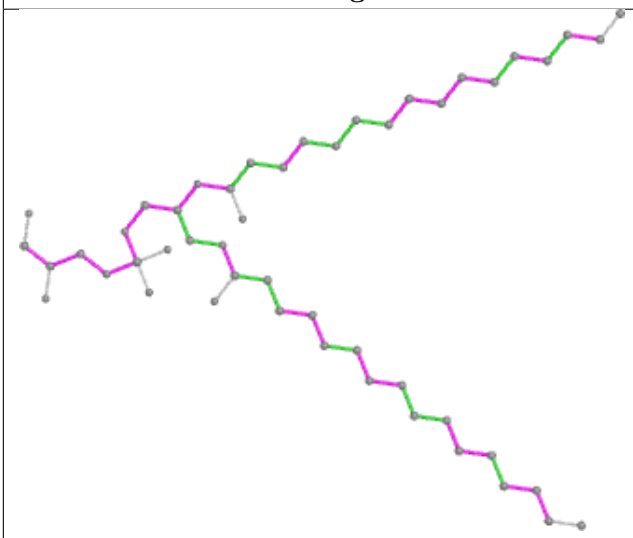
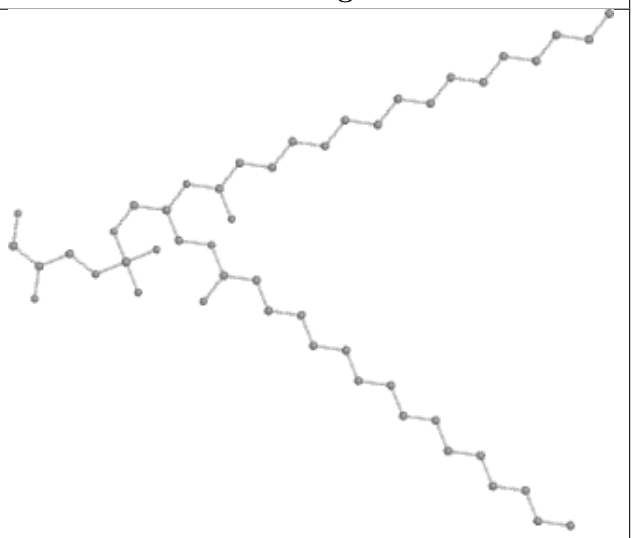


Bond angles

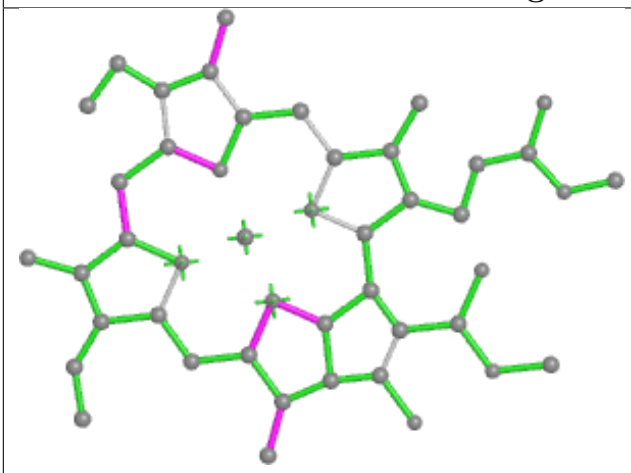


Torsions



Rings

Ligand CLA S 313



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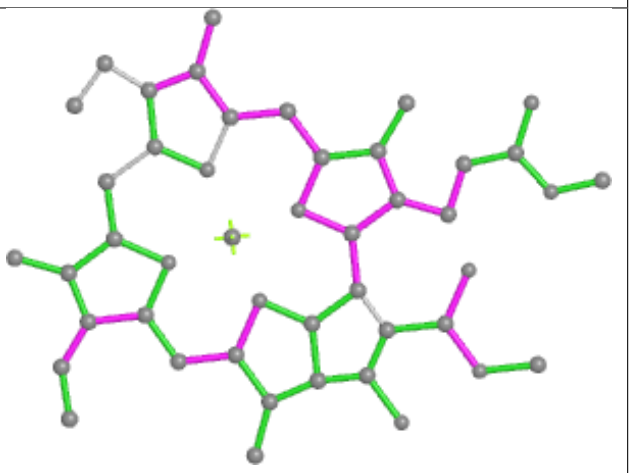
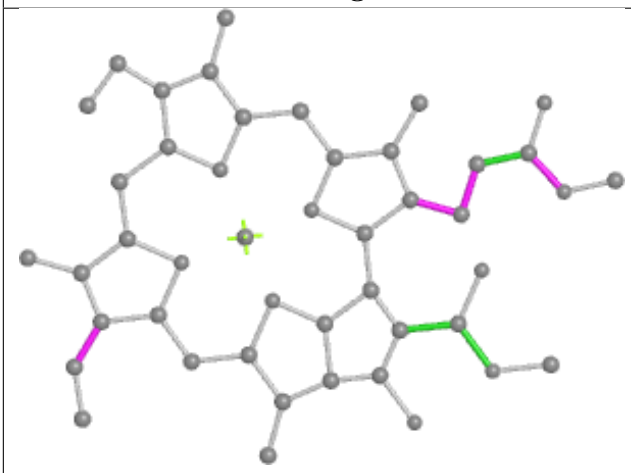


Bond angles



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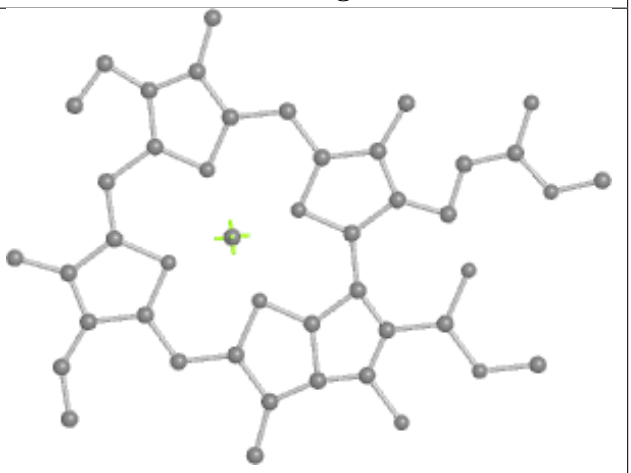
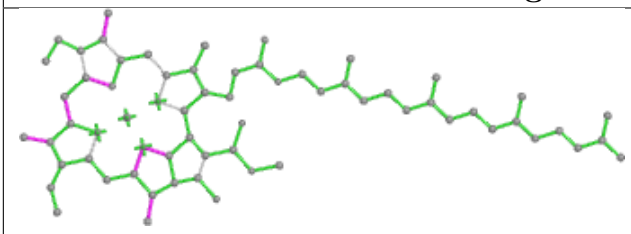


Rings

Ligand CLA P 310



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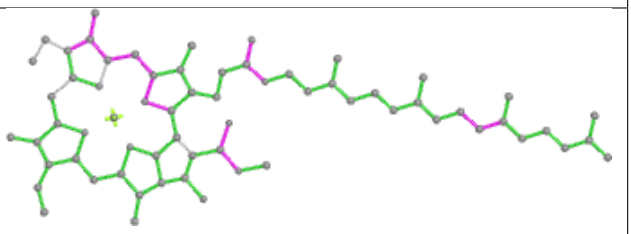
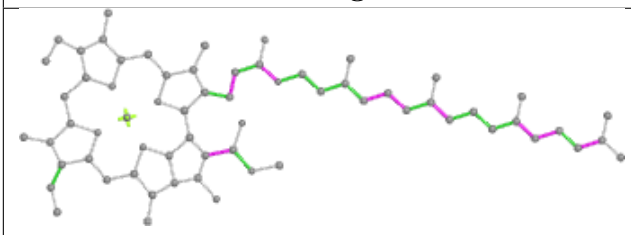
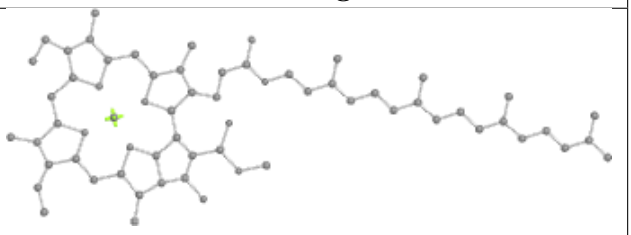


Bond angles

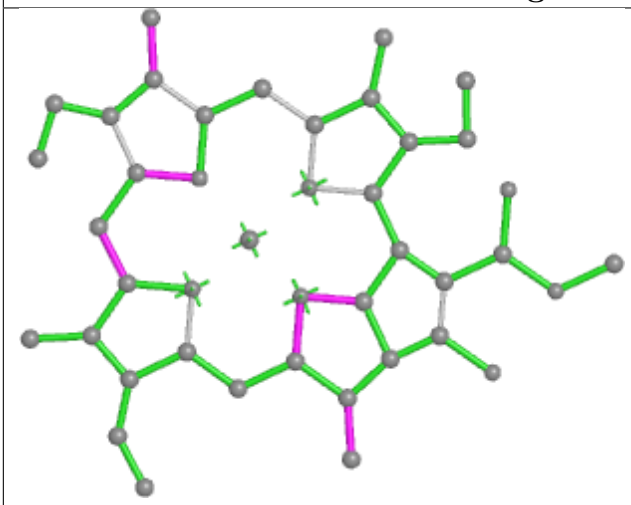


Torsions

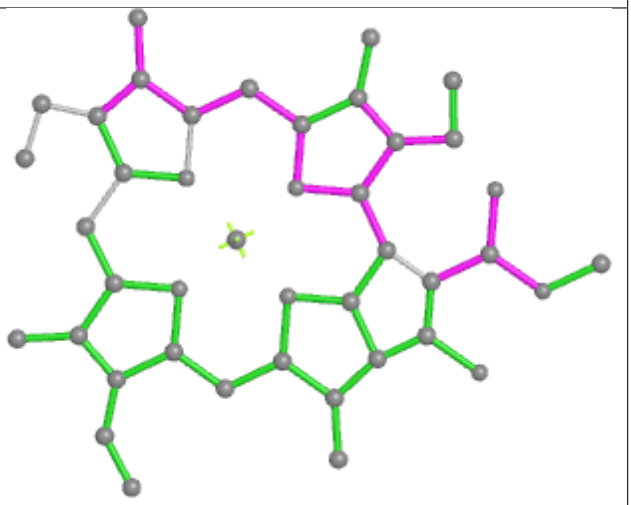


Rings

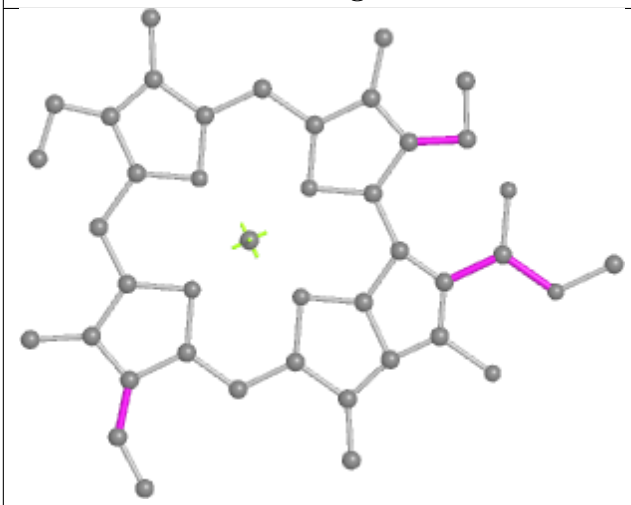
Ligand CLA S 318



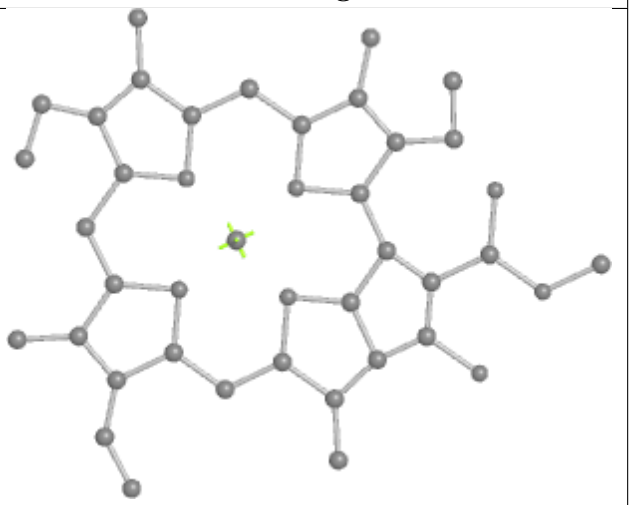
Bond lengths



Bond angles

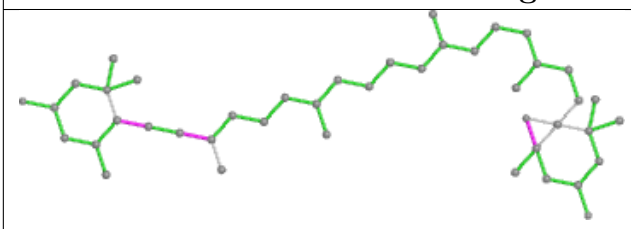


Torsions

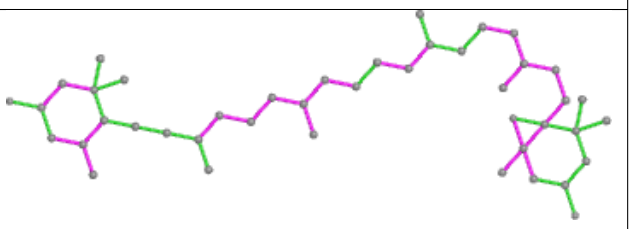


Rings

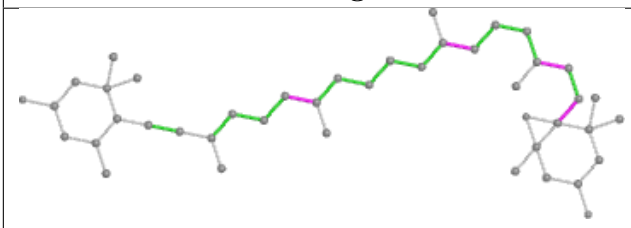
Ligand DD6 W 205



Bond lengths



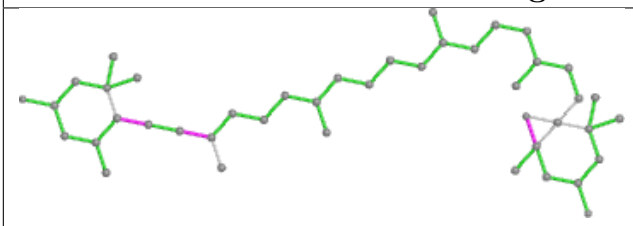
Bond angles



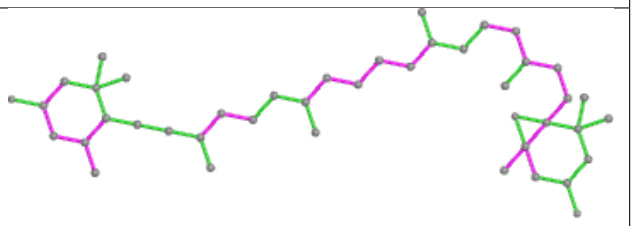
Torsions

Rings

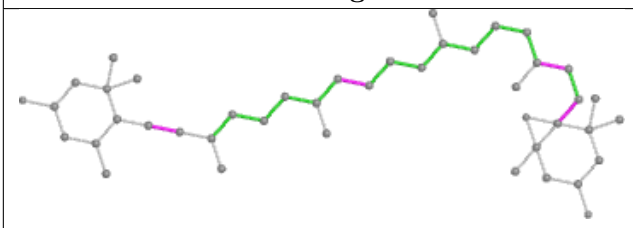
Ligand DD6 J 304



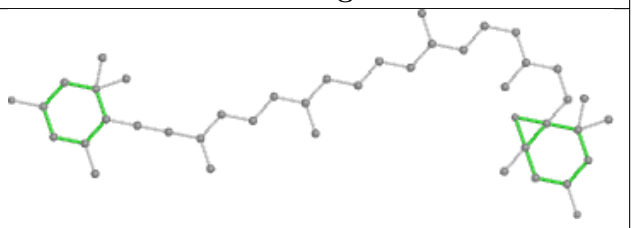
Bond lengths



Bond angles

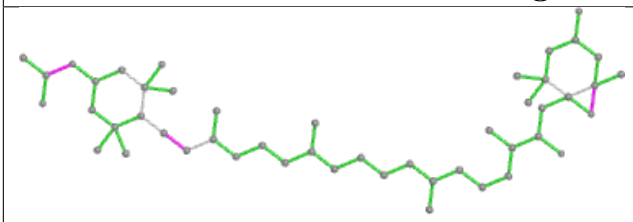


Torsions



Rings

Ligand A86 F 307



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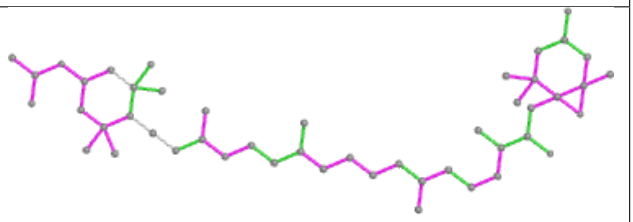
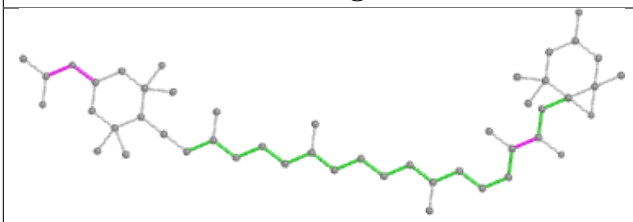


Bond angles



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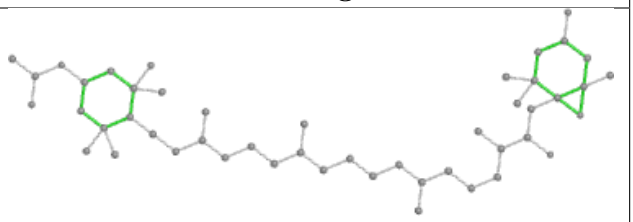
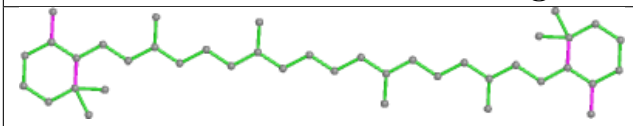
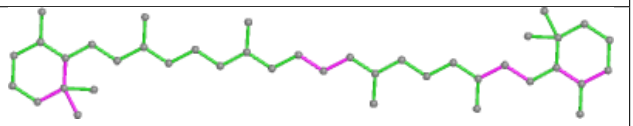


Rings

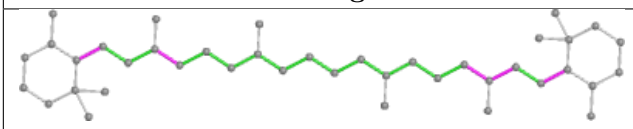
Ligand BCR l 203



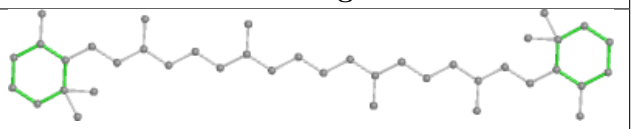
Bond lengths



Bond angles

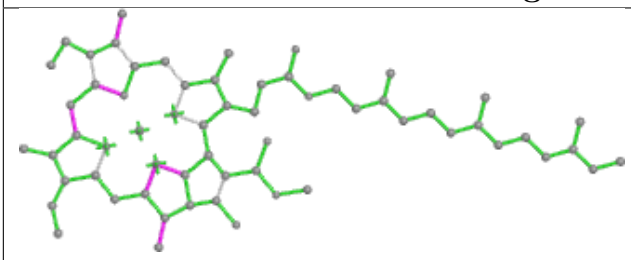


Torsions



Rings

Ligand CLA N 307



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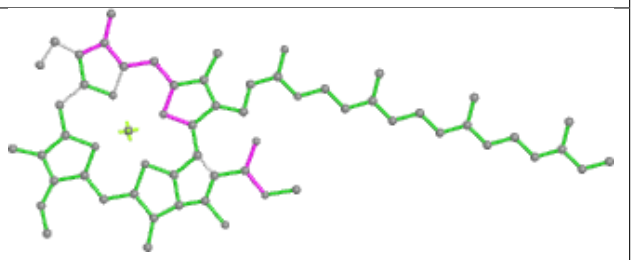
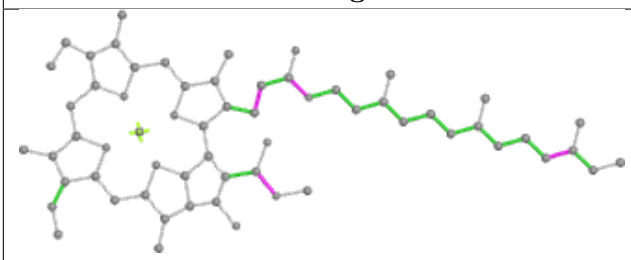
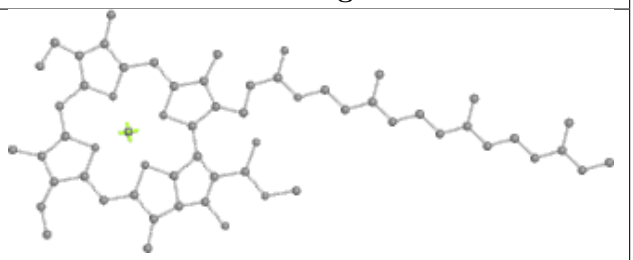


Bond angles

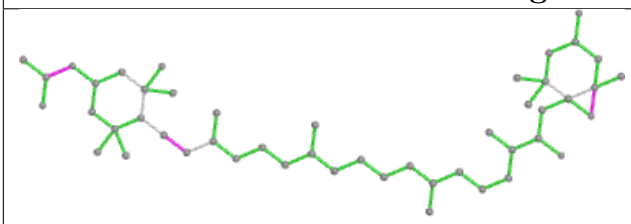


Torsions



Rings

Ligand A86 R 304



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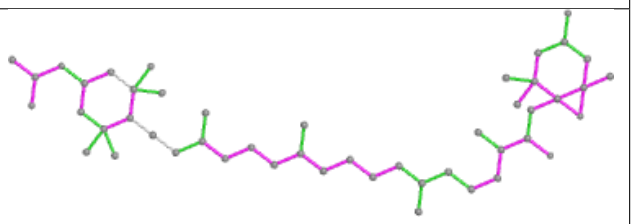
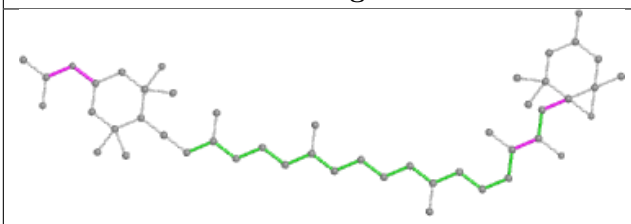


Bond angles



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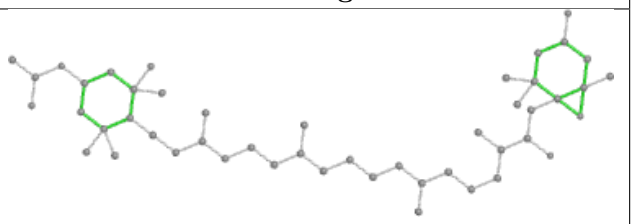
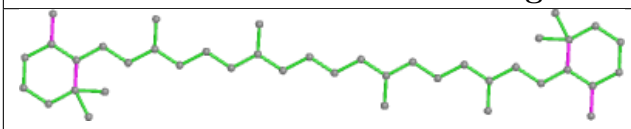


Rings

Ligand BCR b 846



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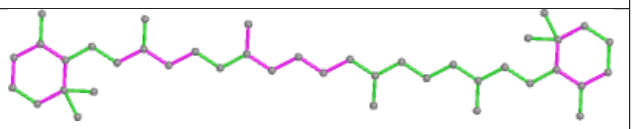
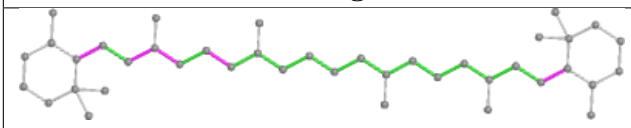


Bond angles



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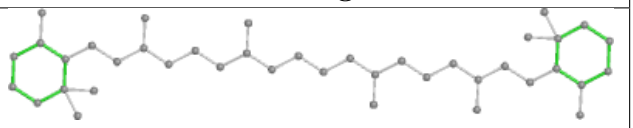
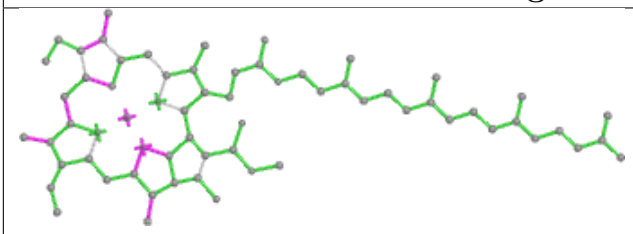


Rings

Ligand CLA b 840



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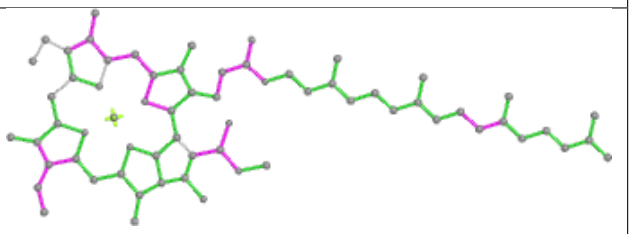
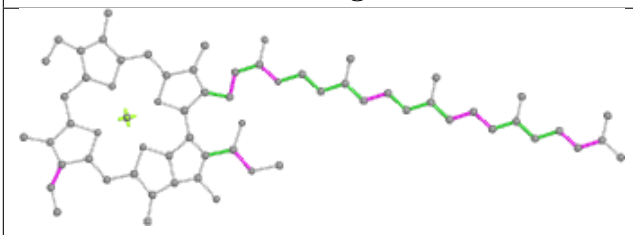
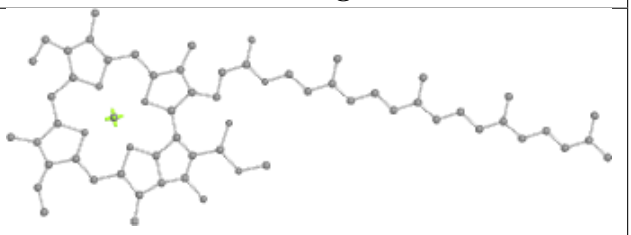


Bond angles

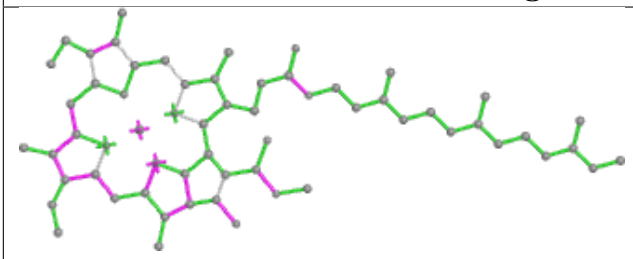


Torsions

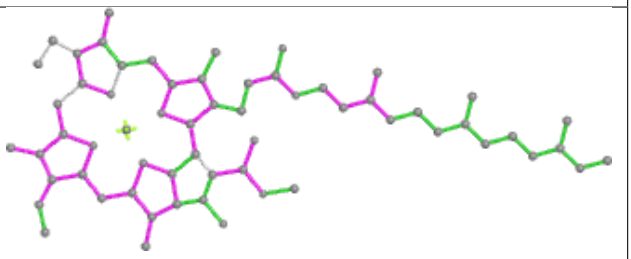


Rings

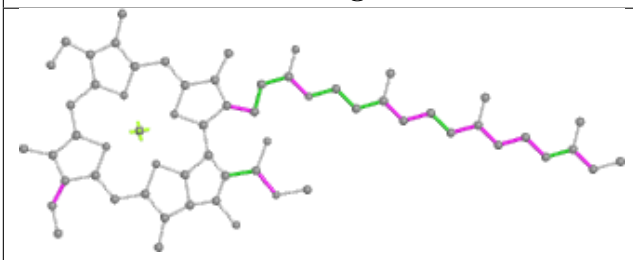
Ligand CLA A 306



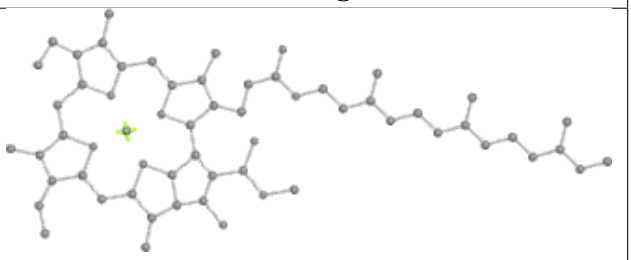
Bond lengths



Bond angles

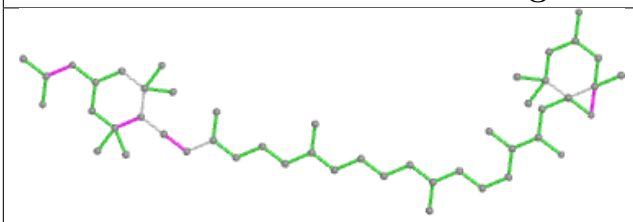


Torsions

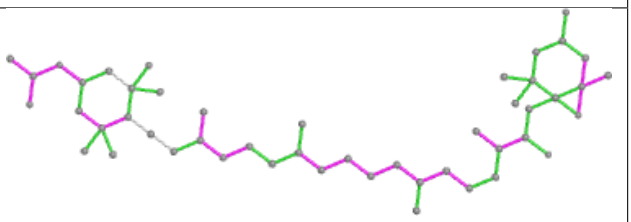


Rings

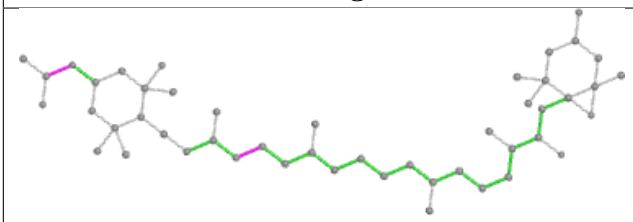
Ligand A86 X 314



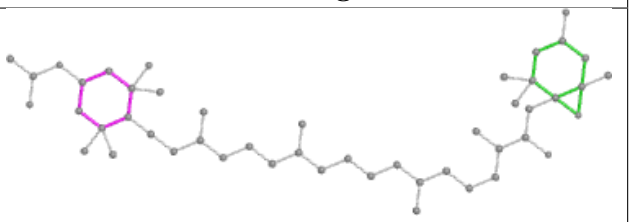
Bond lengths



Bond angles

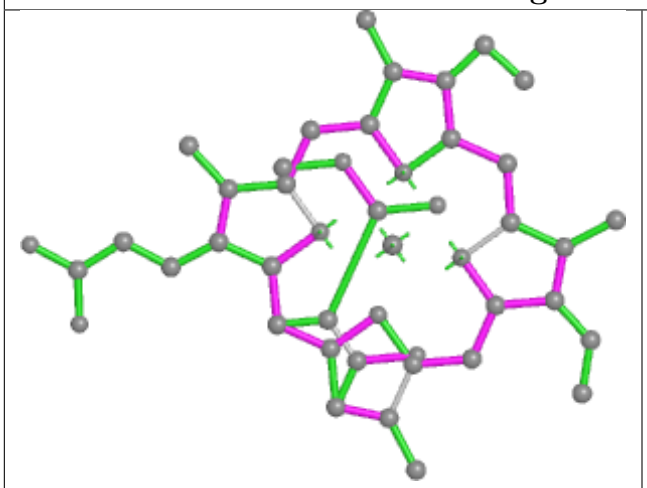


Torsions



Rings

Ligand KC1 S 316



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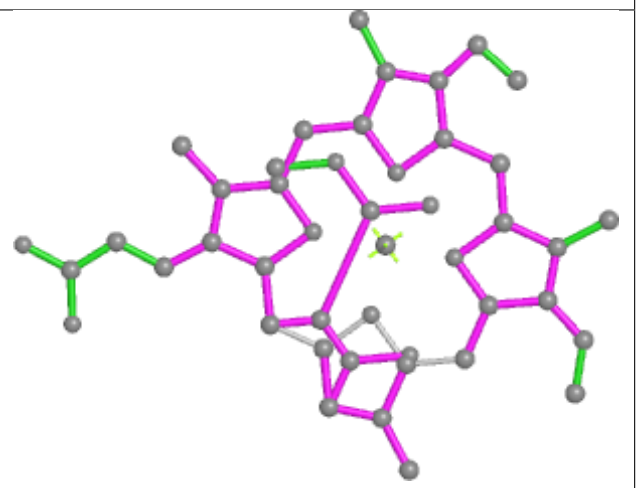
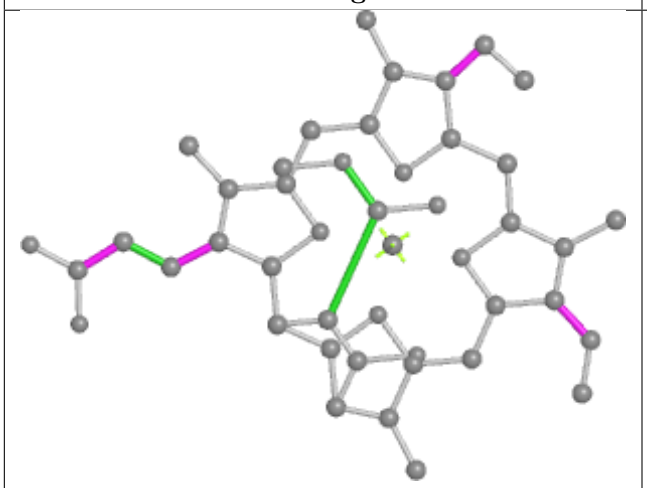
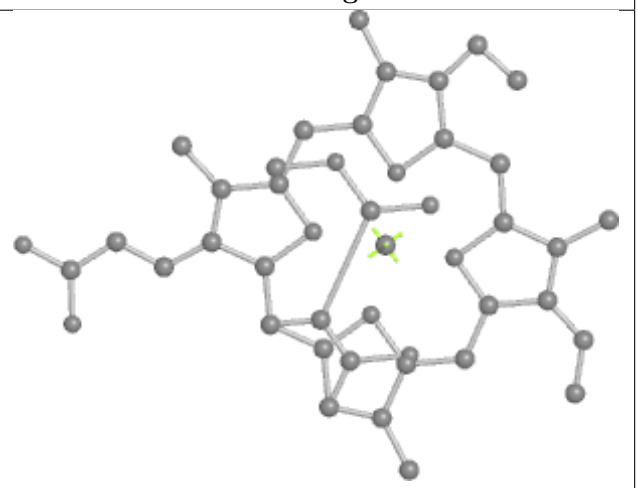


Bond angles

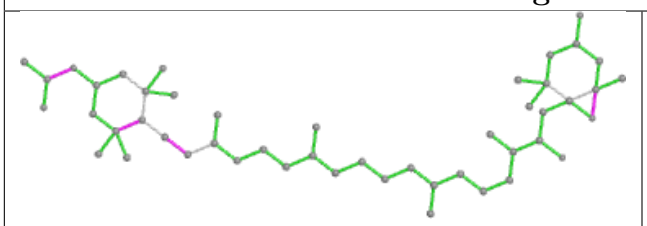


Torsions



Rings

Ligand A86 F 302



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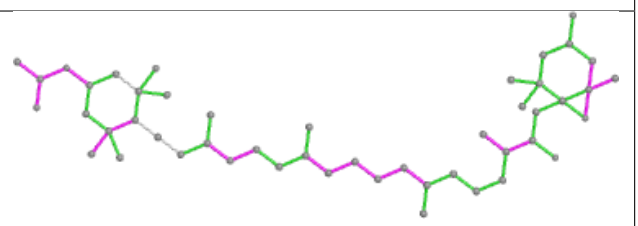
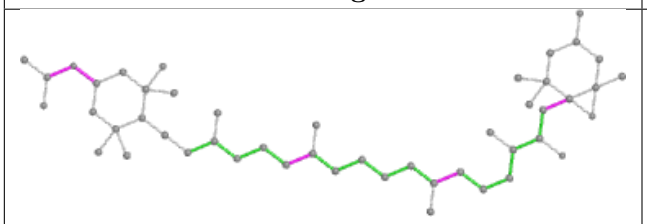
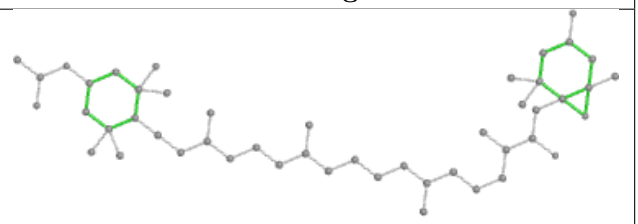


Bond angles

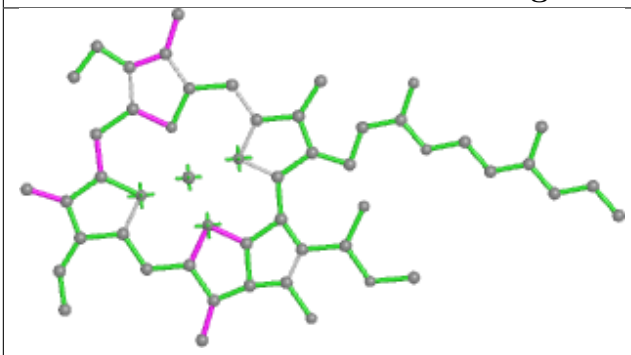


Torsions



Rings

Ligand CLA I 312



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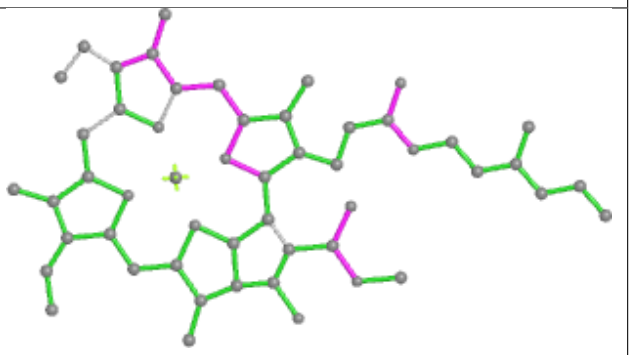
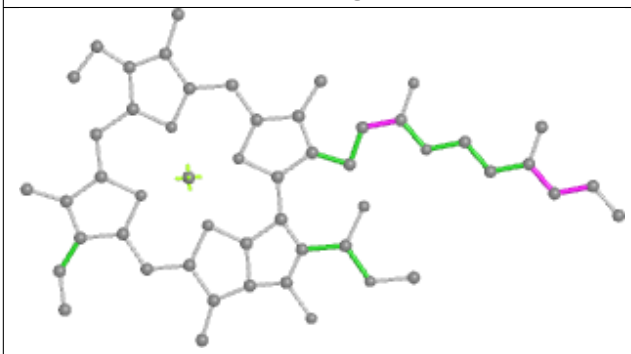
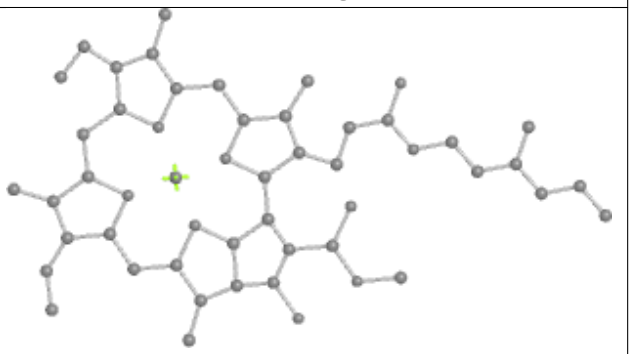


Bond angles

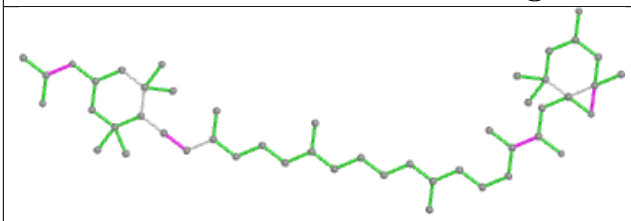


Torsions

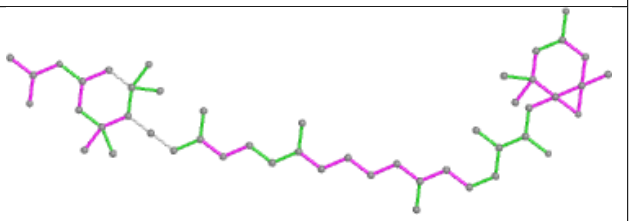


Rings

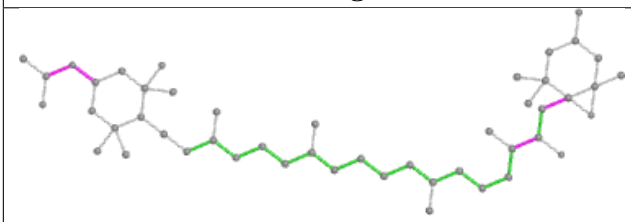
Ligand A86 M 305



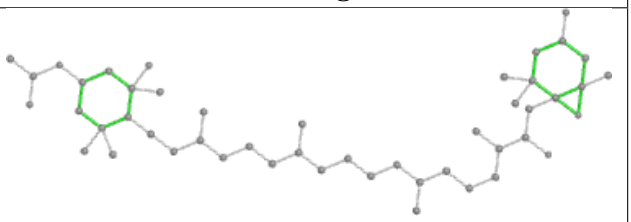
Bond lengths



Bond angles

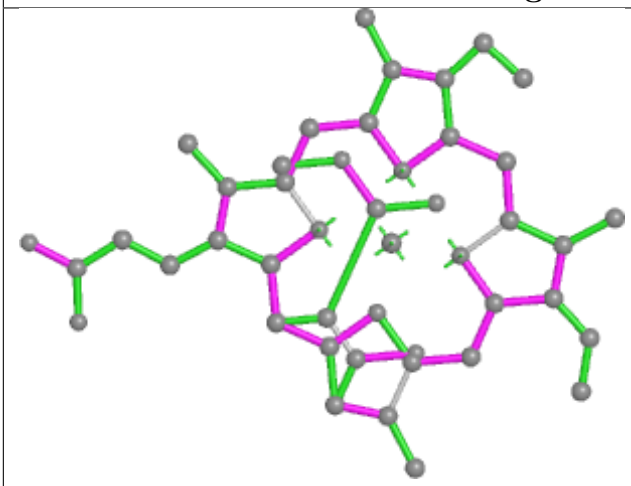


Torsions

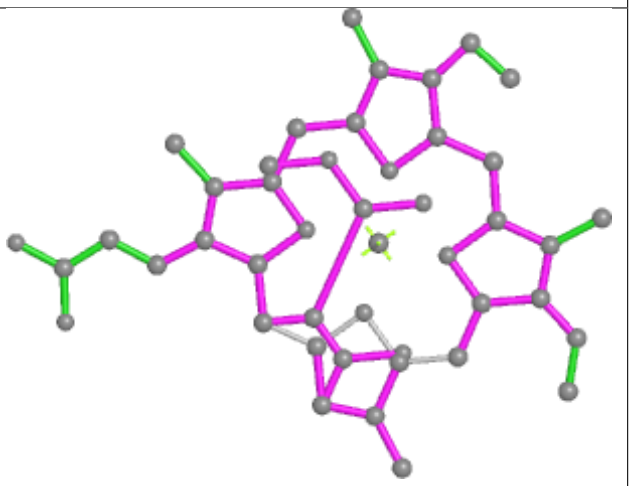


Rings

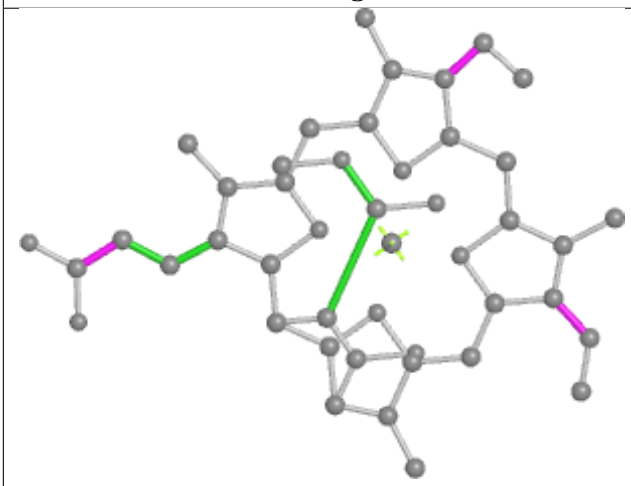
Ligand KC1 G 308



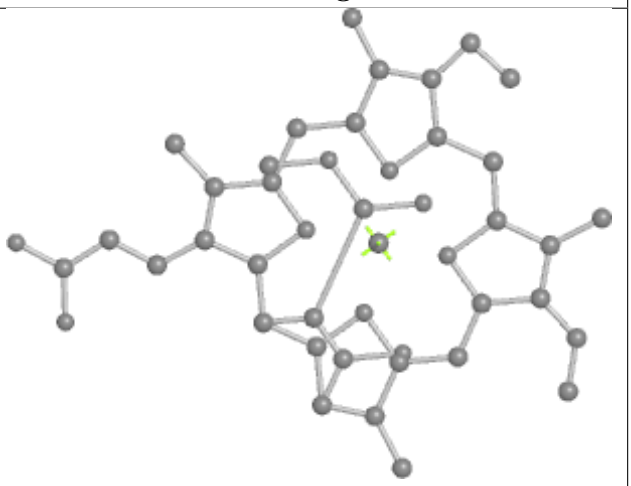
Bond lengths



Bond angles

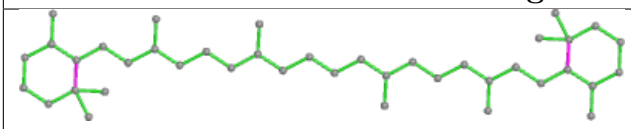


Torsions

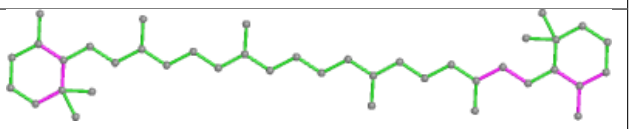


Rings

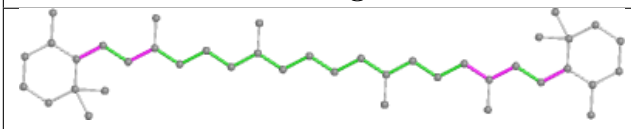
Ligand BCR a 845



Bond lengths



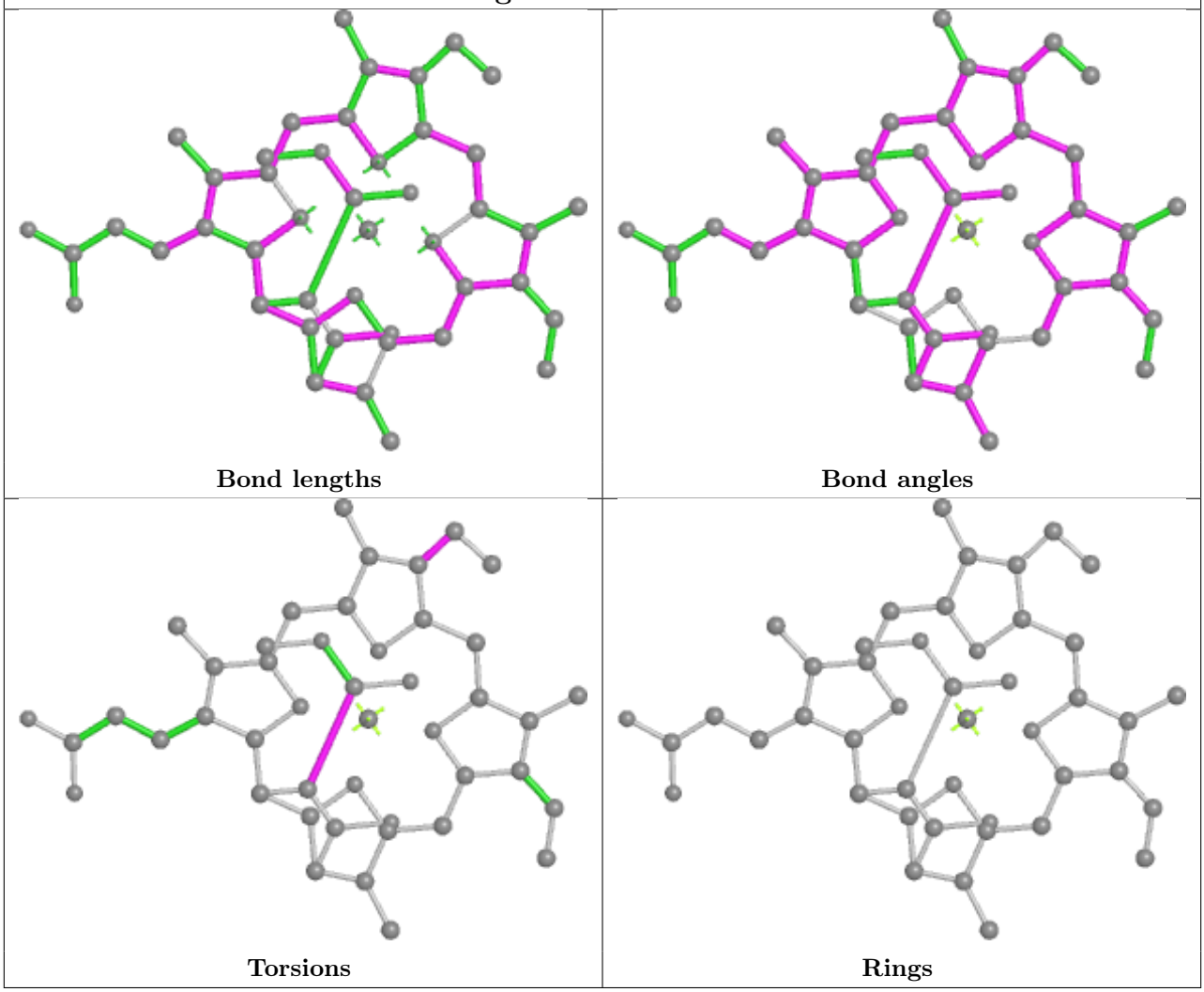
Bond angles



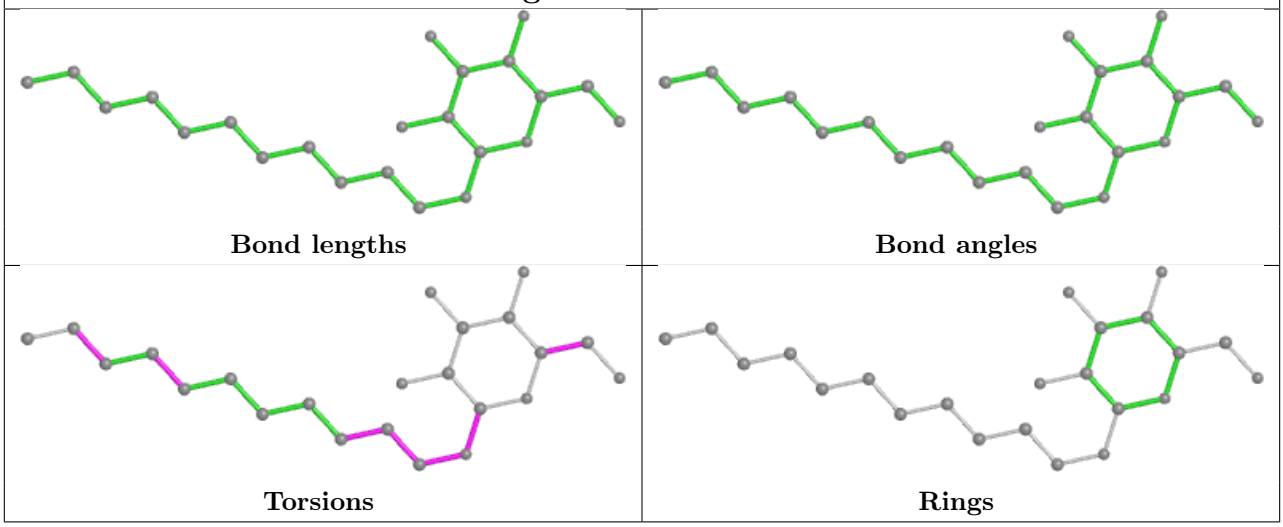
Torsions

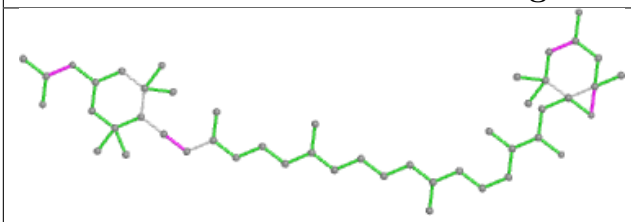
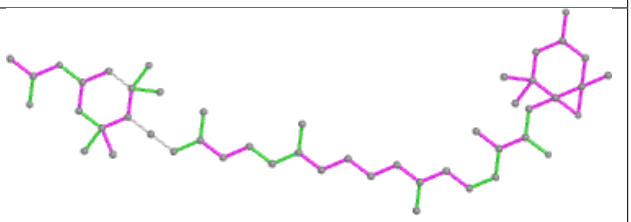
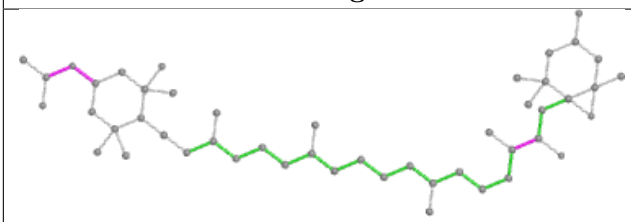
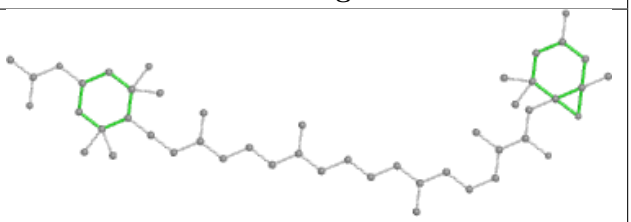
Rings

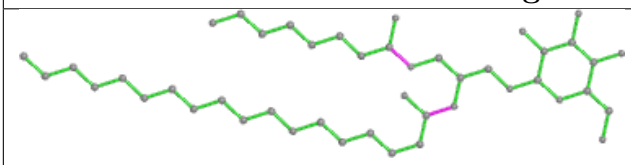
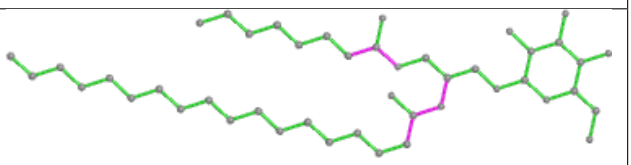
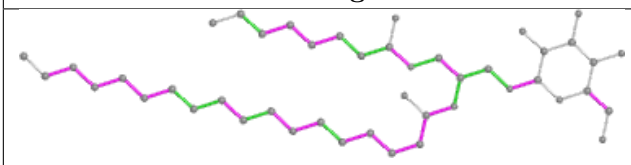
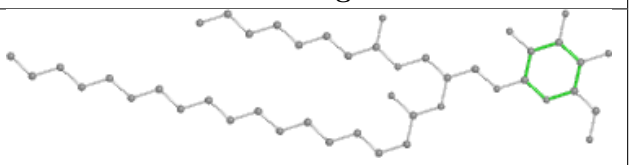
Ligand KC1 P 315



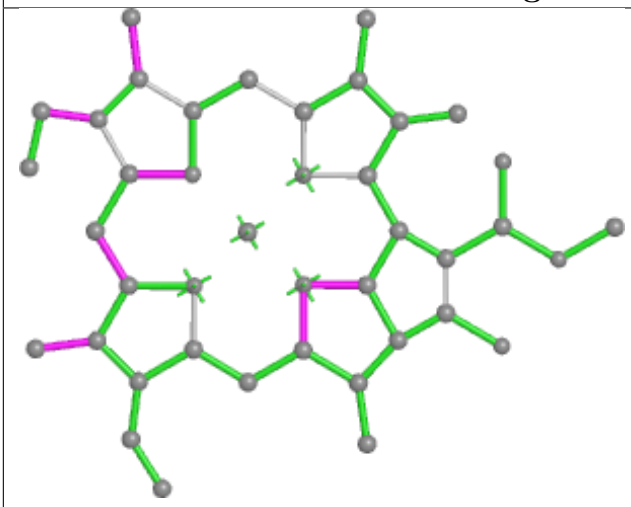
Ligand LMT P 320



Ligand A86 V 302	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand LMG h 206	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA U 313



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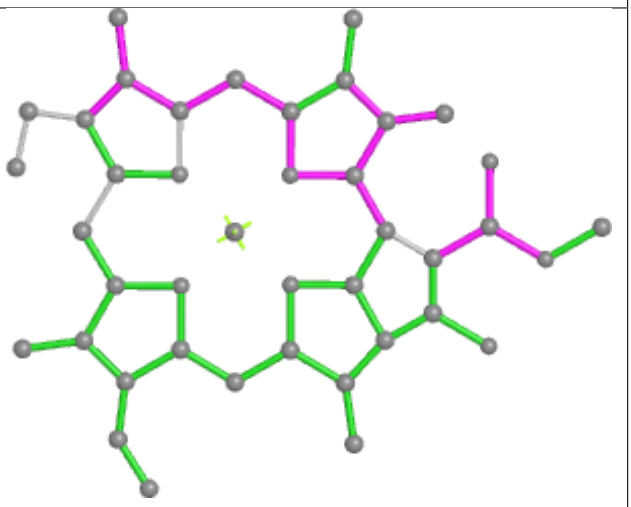
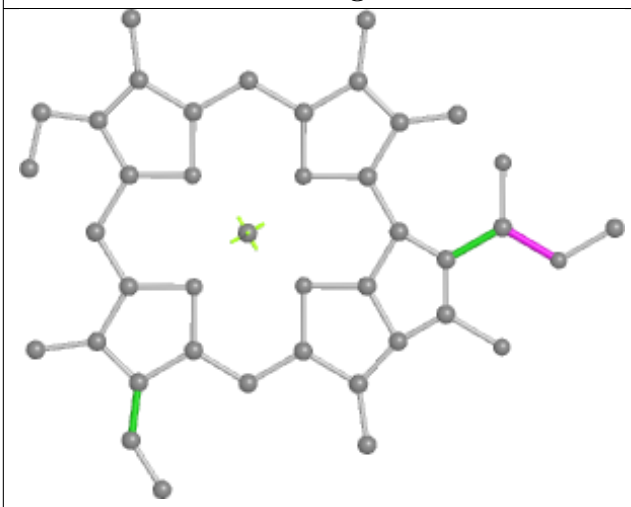


Bond angles



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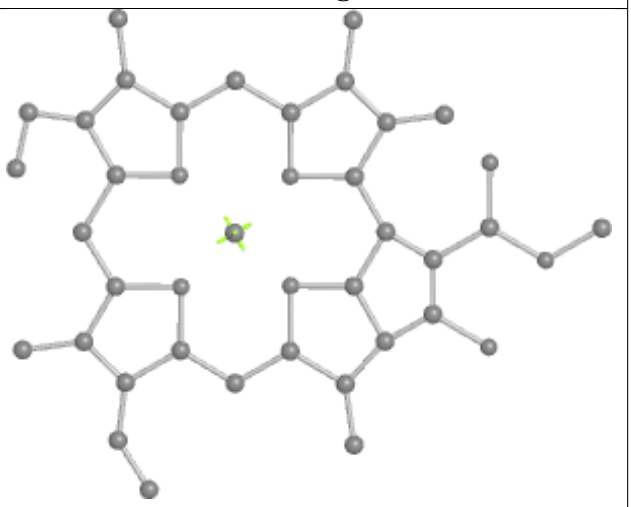
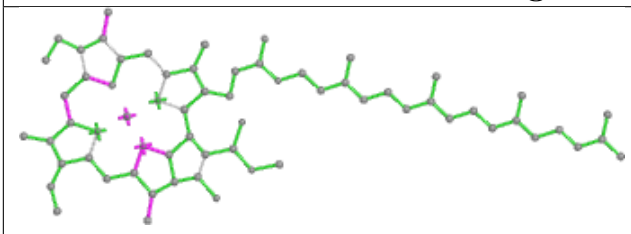


Rings

Ligand CLA S 312



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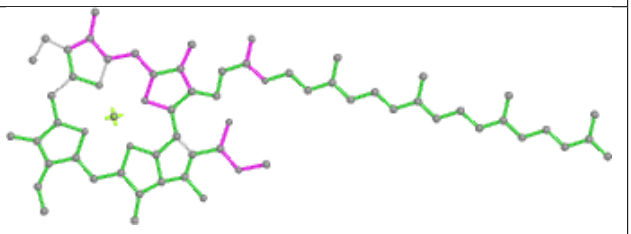
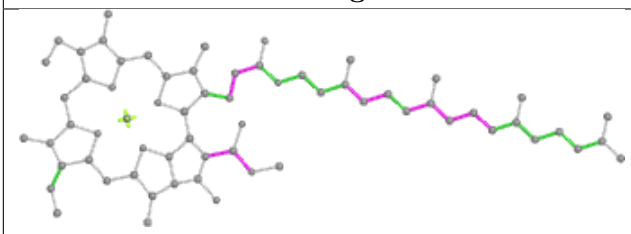


Bond angles



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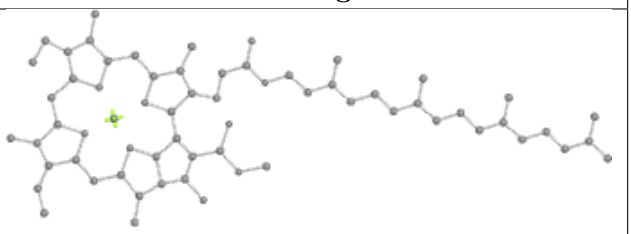
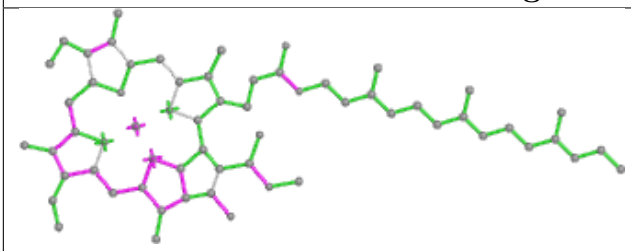
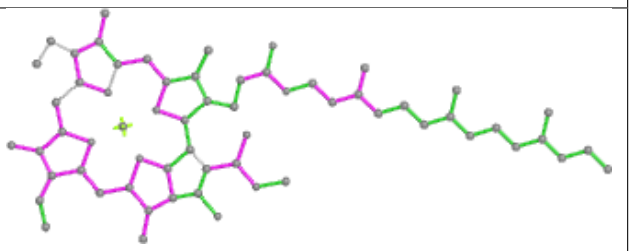
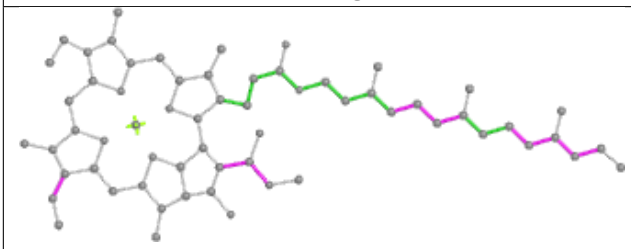
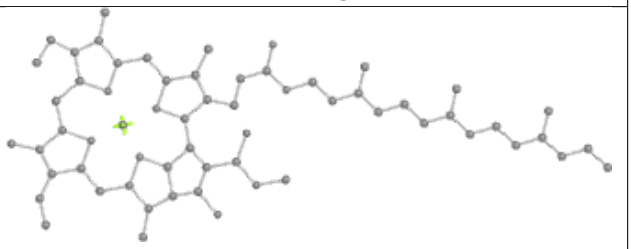


Rings

Ligand CLA K 310	
 Bond lengths	 Bond angles
 Torsions	 Rings

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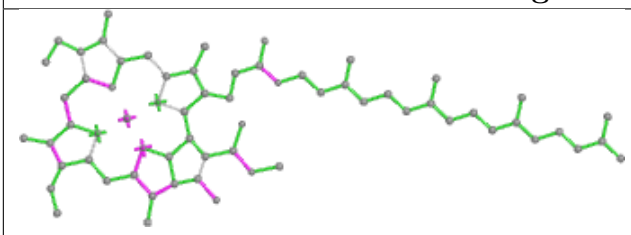
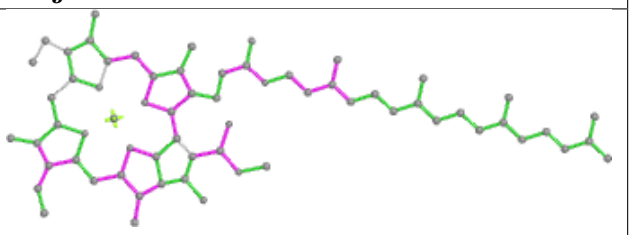
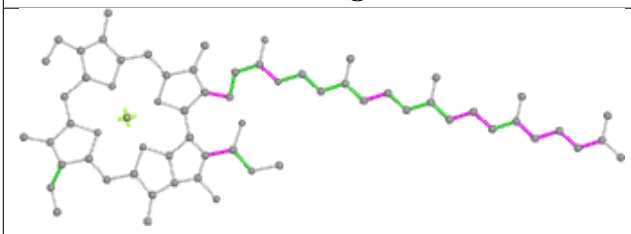
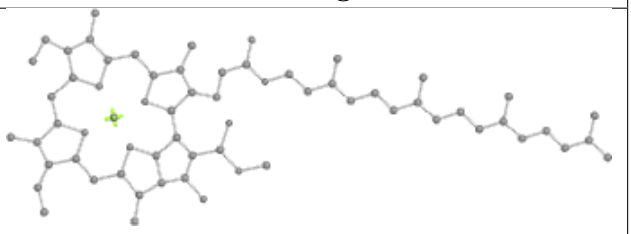
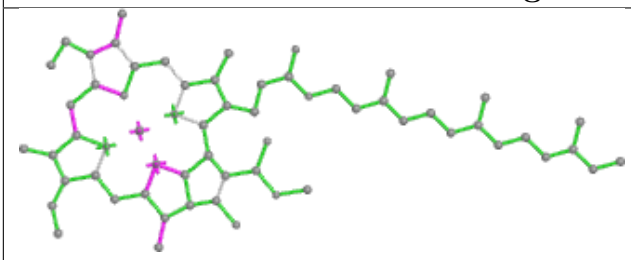
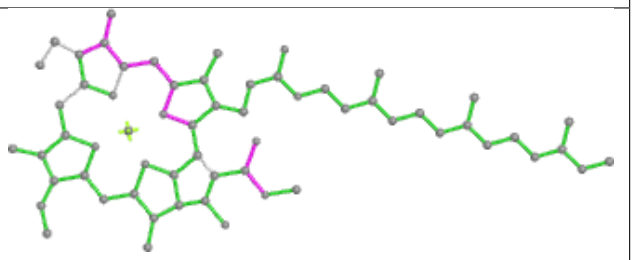
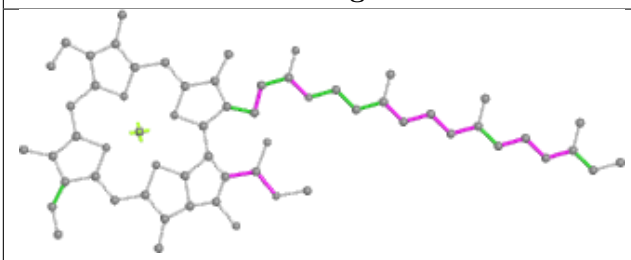
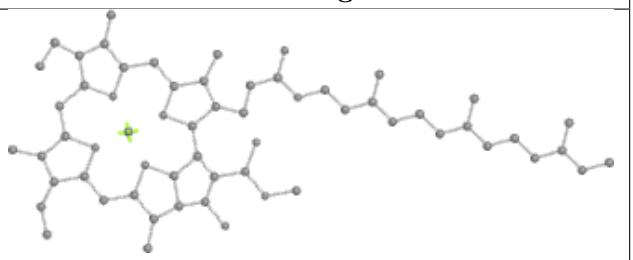
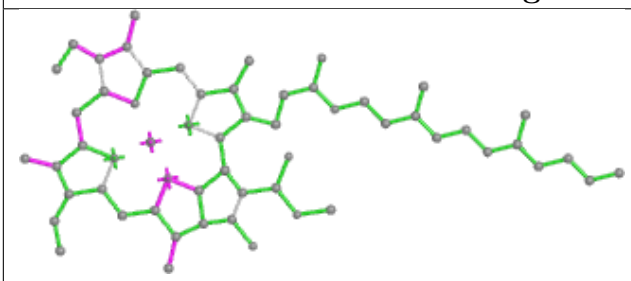
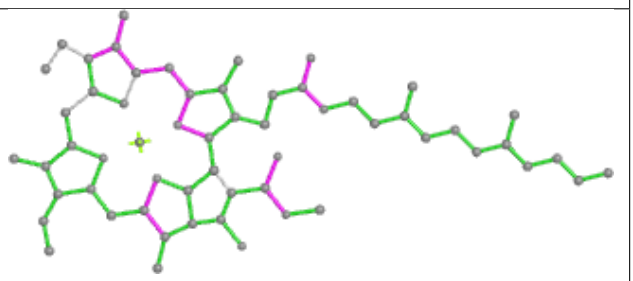
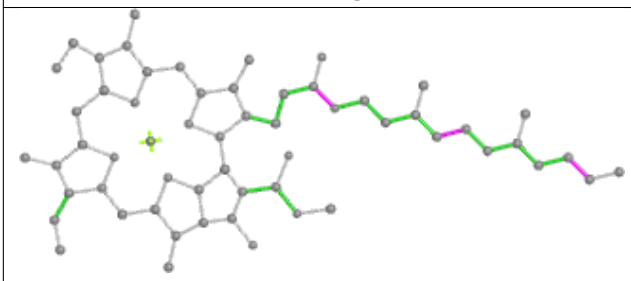
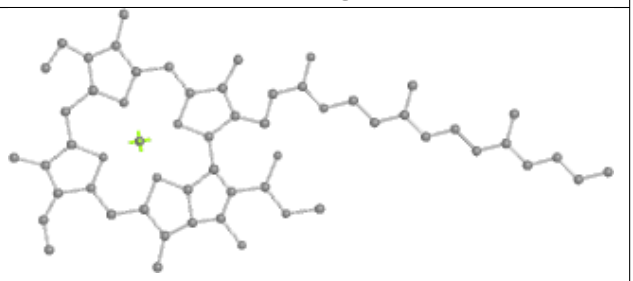
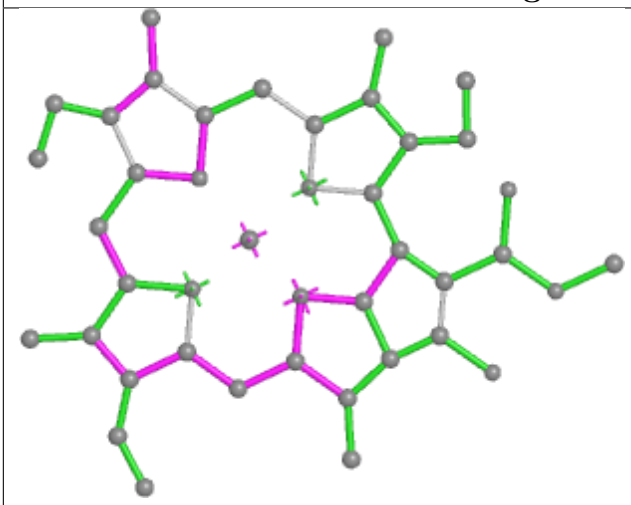
 Bond lengths	 Bond angles
 Torsions	 Rings

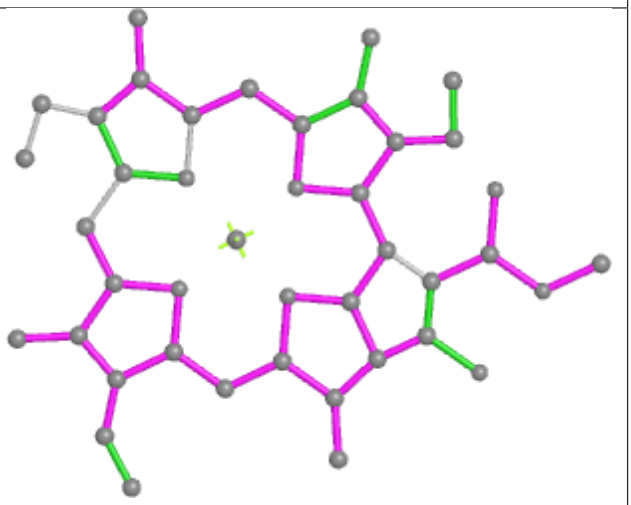
Ligand CLA R 310	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA G 312	
 Bond lengths	 Bond angles
 Torsions	 Rings

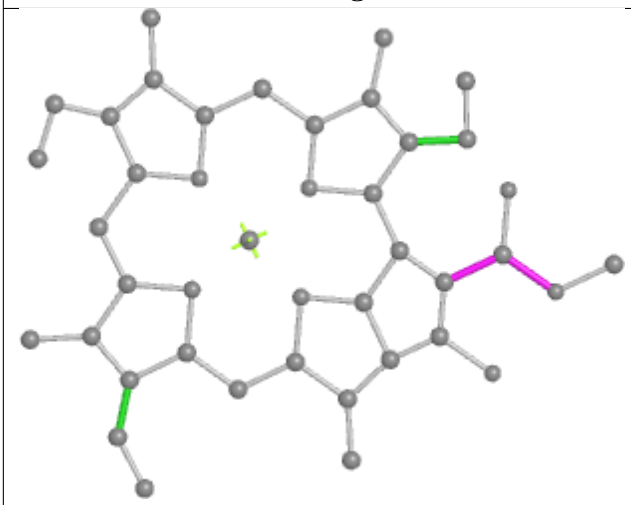
Ligand CLA N 319



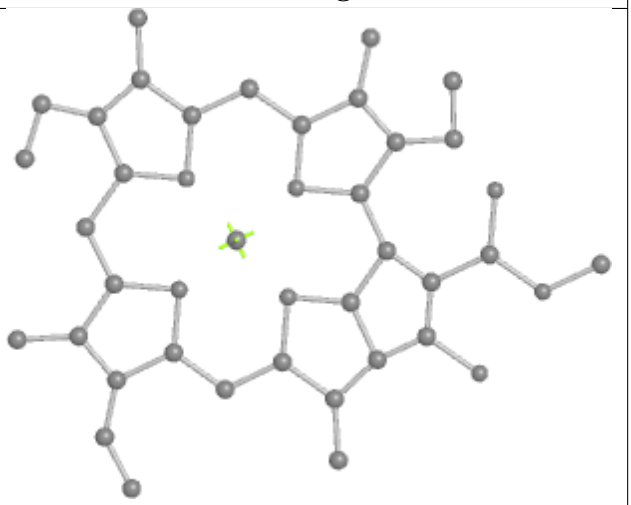
Bond lengths



Bond angles

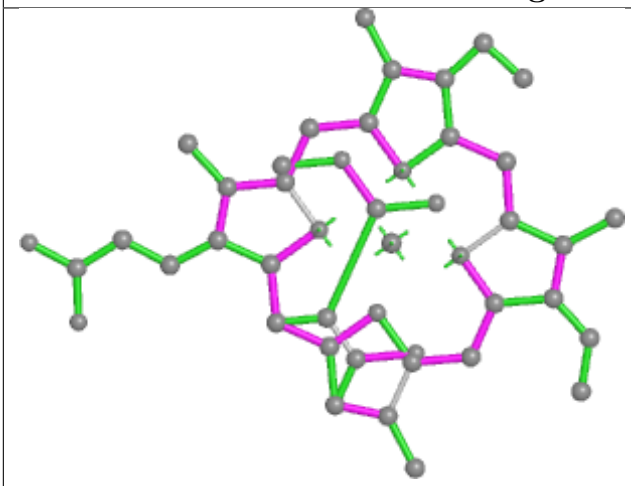


Torsions



Rings

Ligand KC1 L 315



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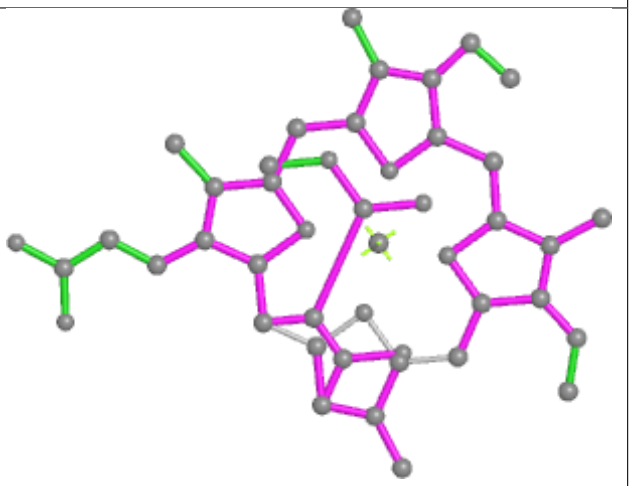
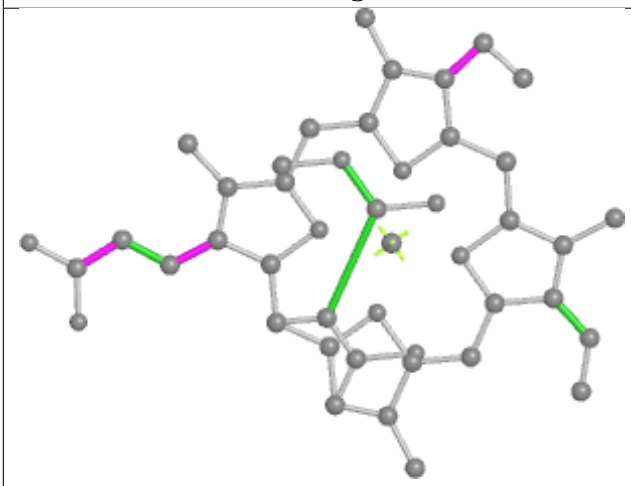


Bond angles



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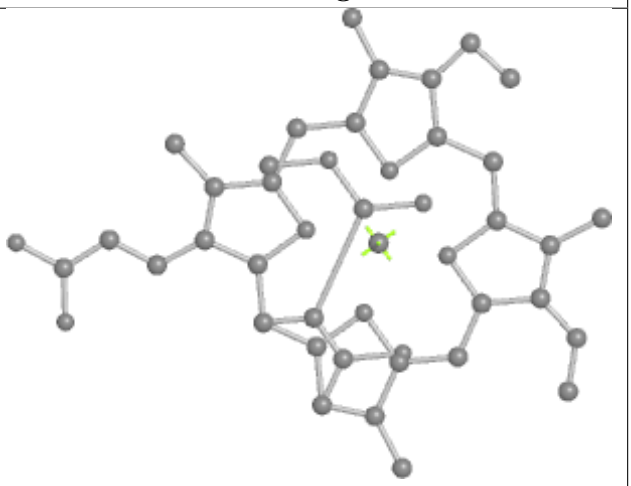
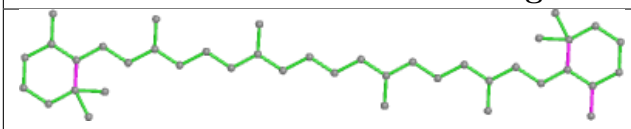
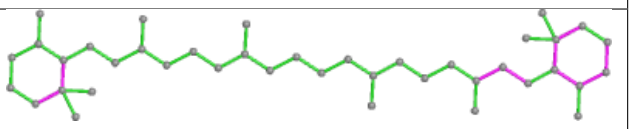


Rings

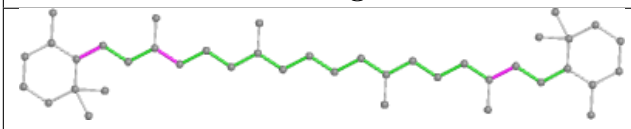
Ligand BCR b 844



Bond lengths

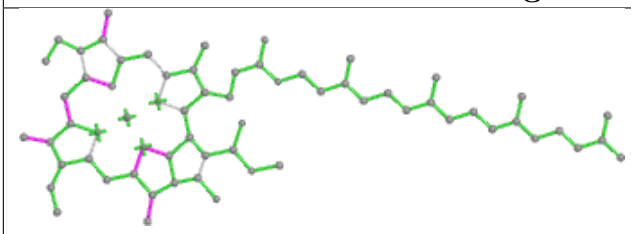
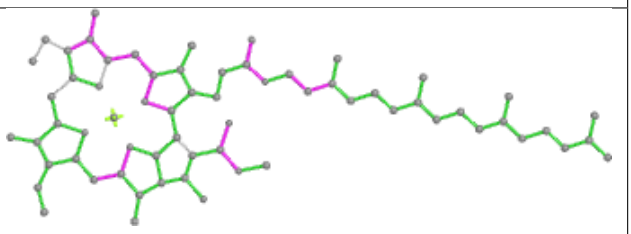
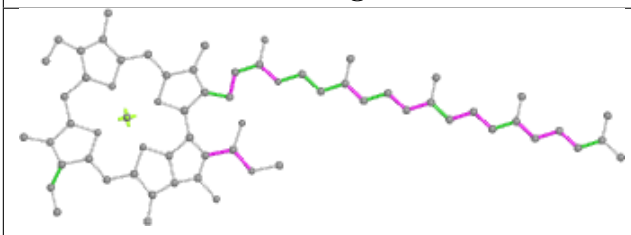
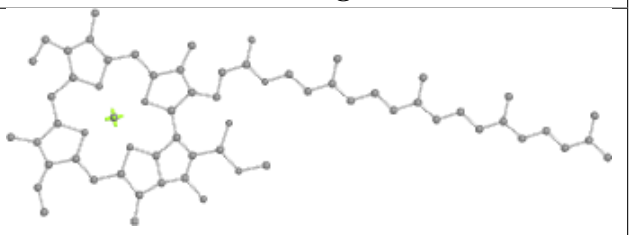


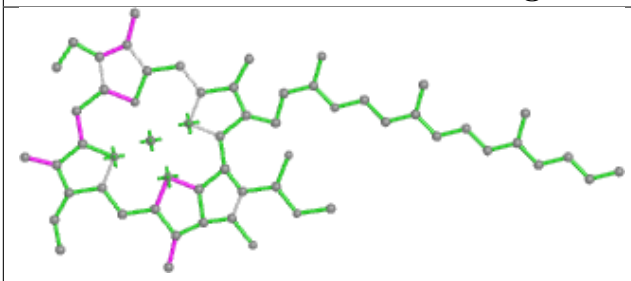
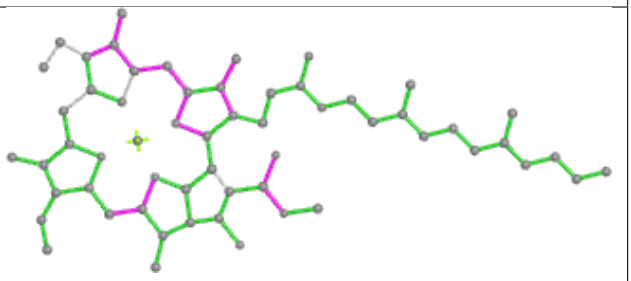
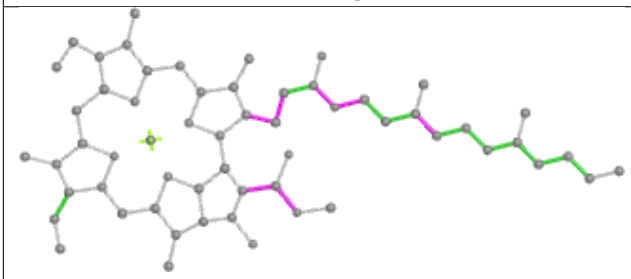
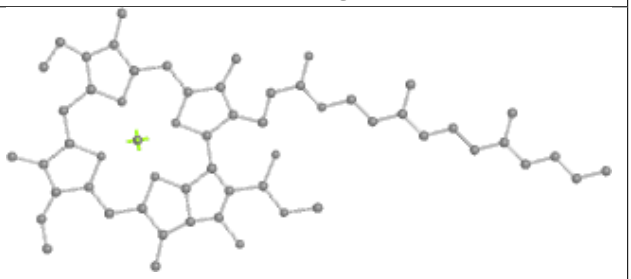
Bond angles



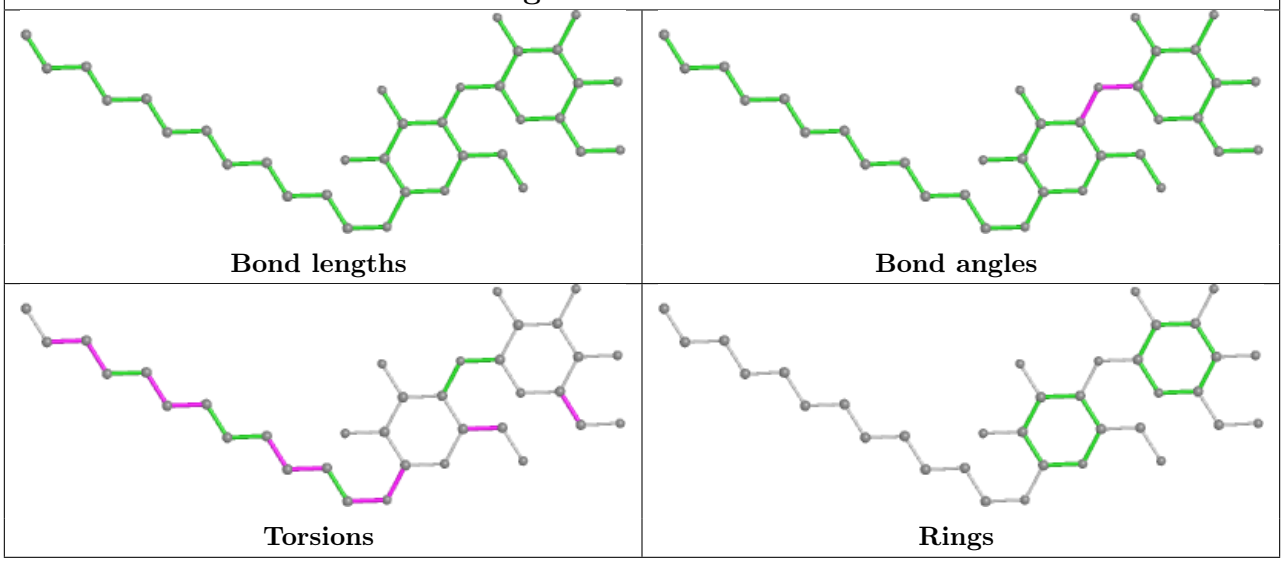
Torsions

Rings

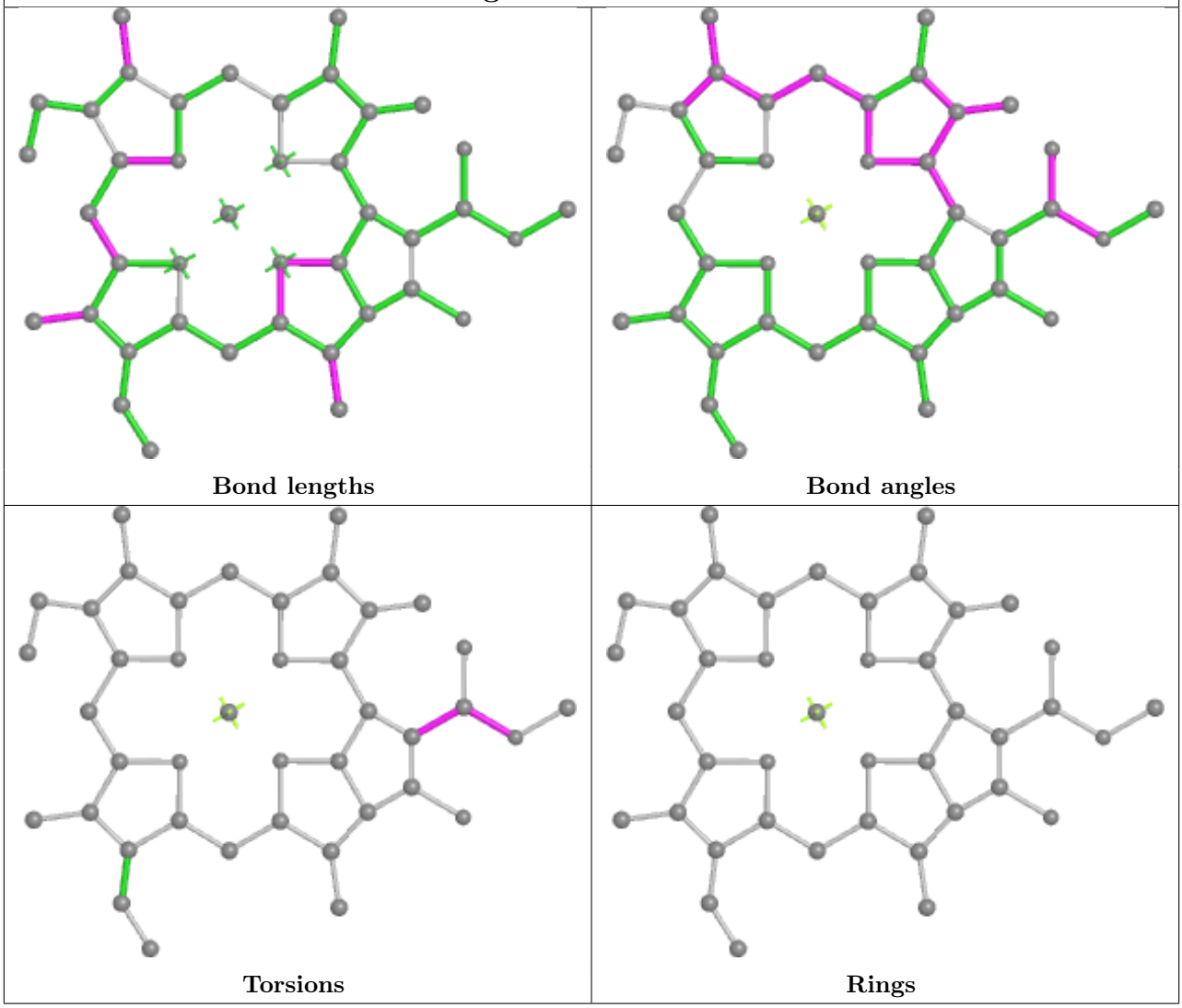
Ligand CLA V 308	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA D 317	
 Bond lengths	 Bond angles
 Torsions	 Rings

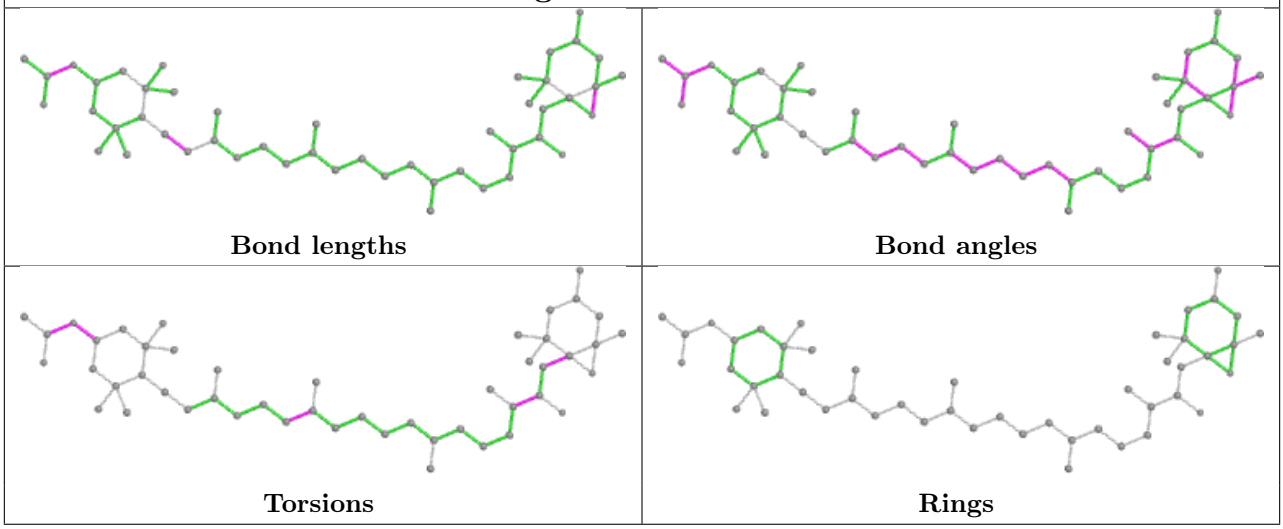
Ligand LMT E 323



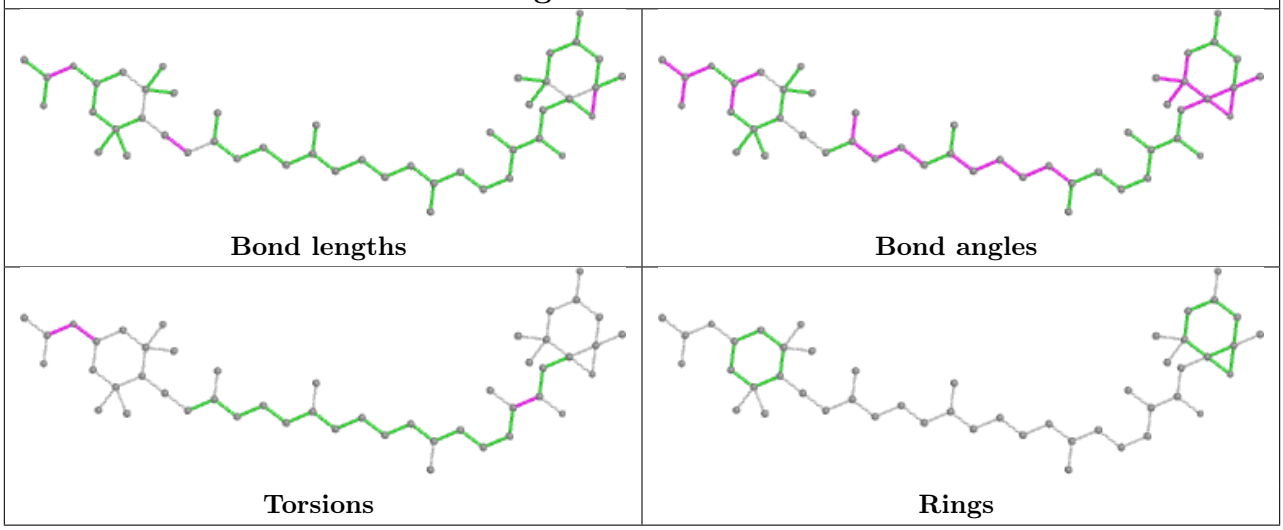
Ligand CLA X 312



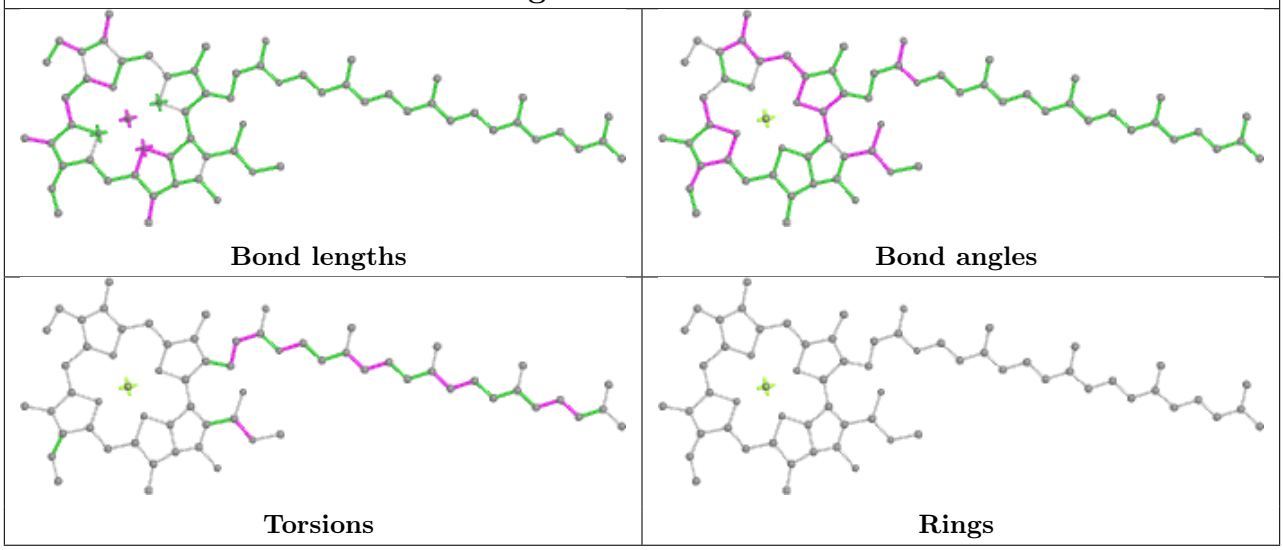
Ligand A86 J 306



Ligand A86 S 302



Ligand CLA b 806



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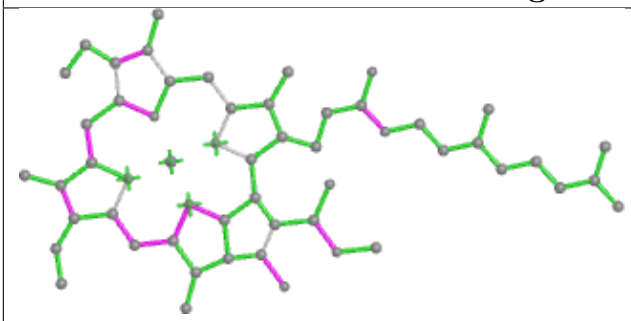
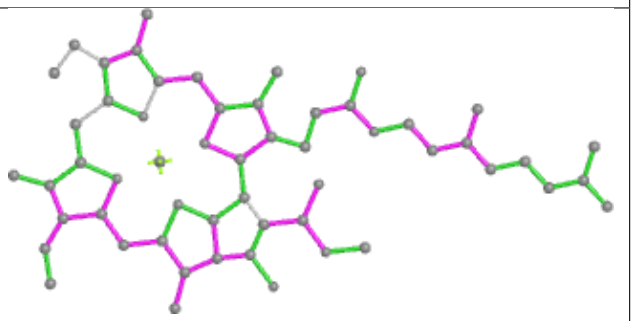
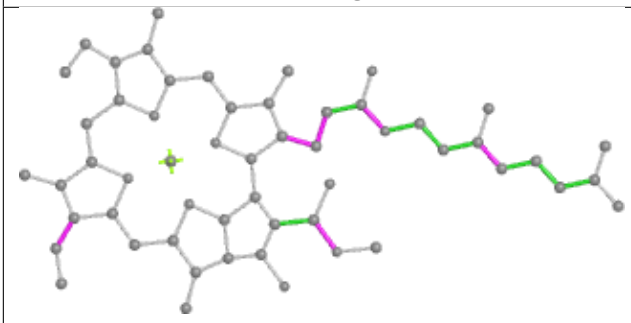
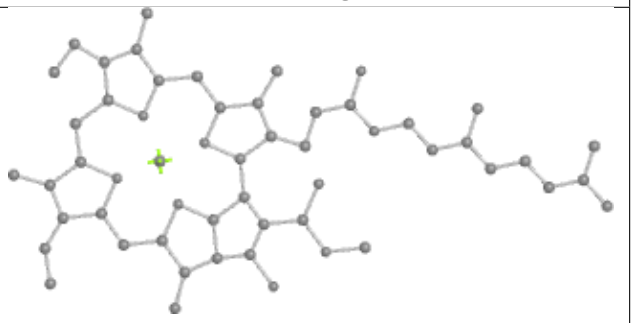
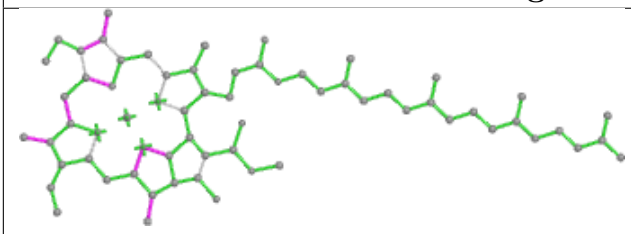
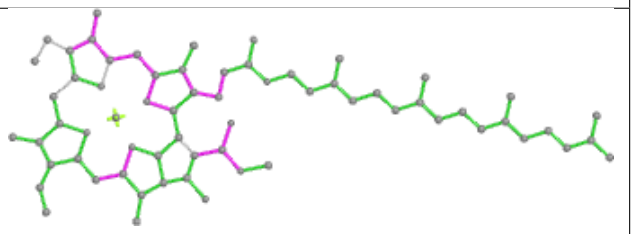
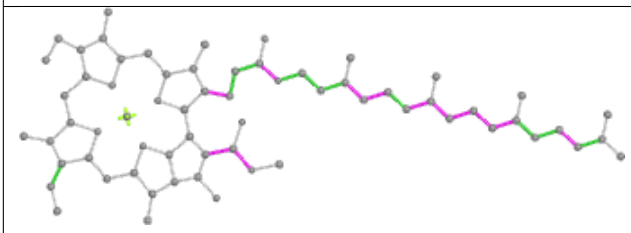
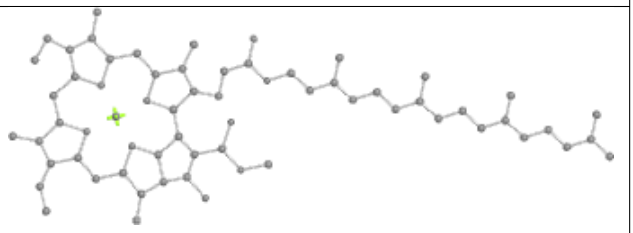
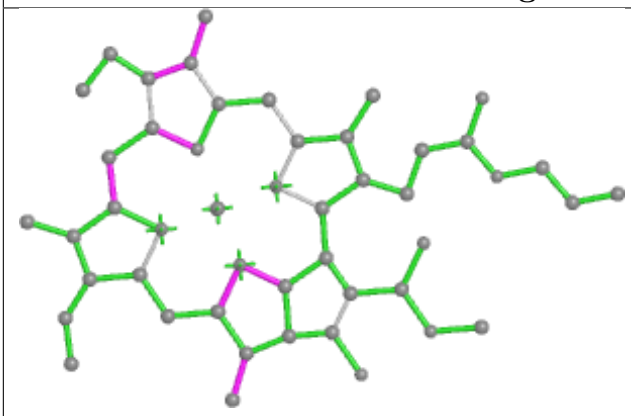
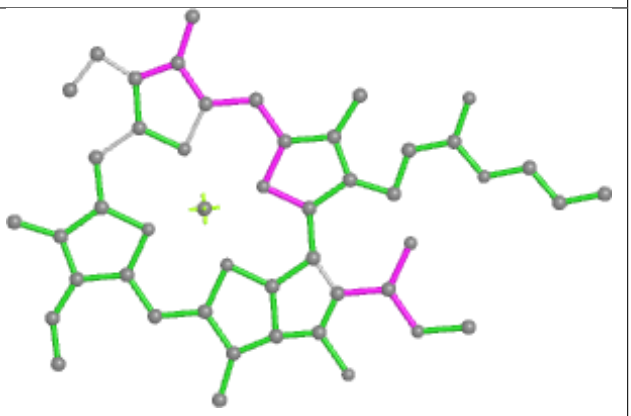
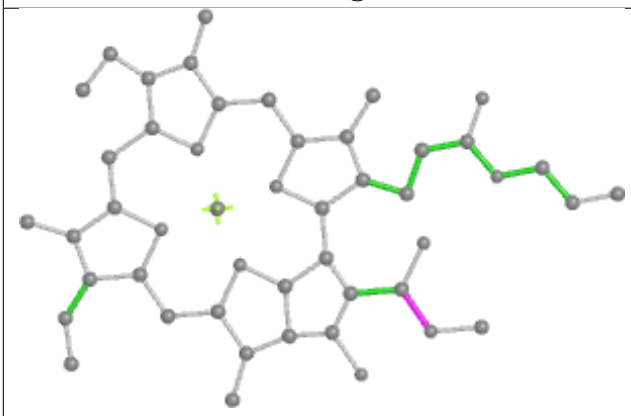
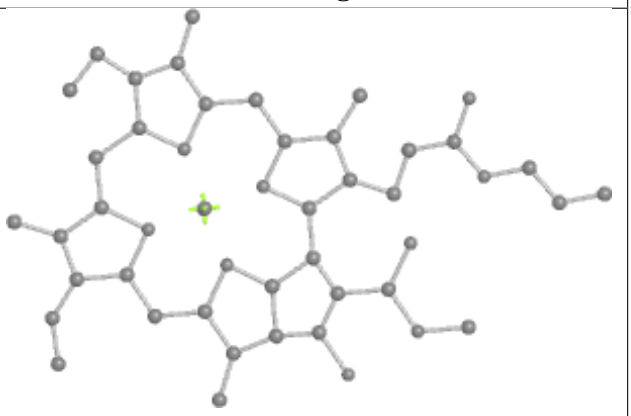
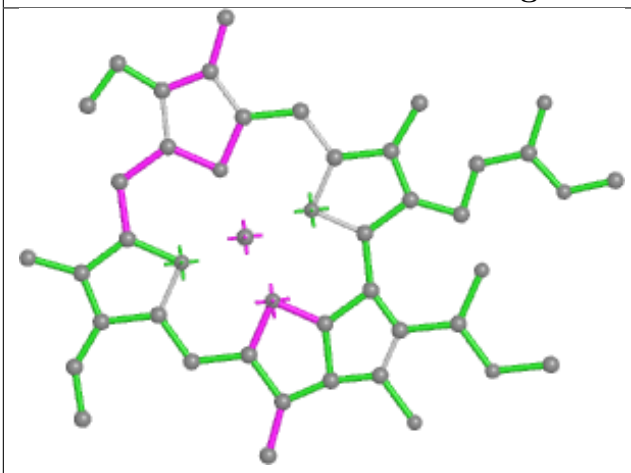
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA h 203	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA W 201	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA M 310



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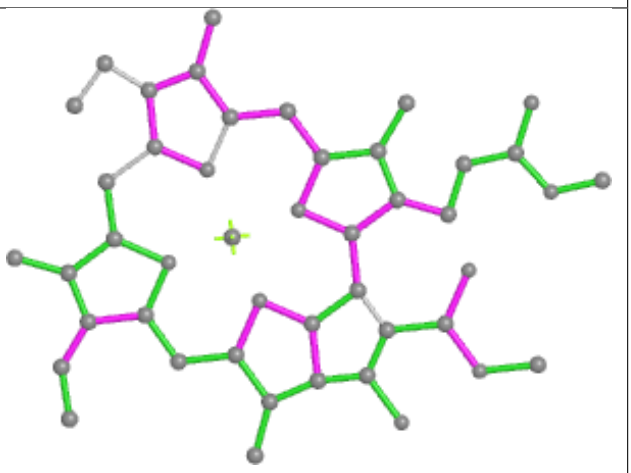
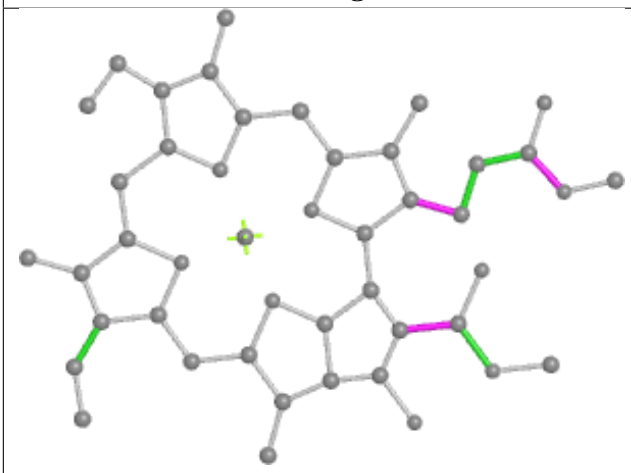
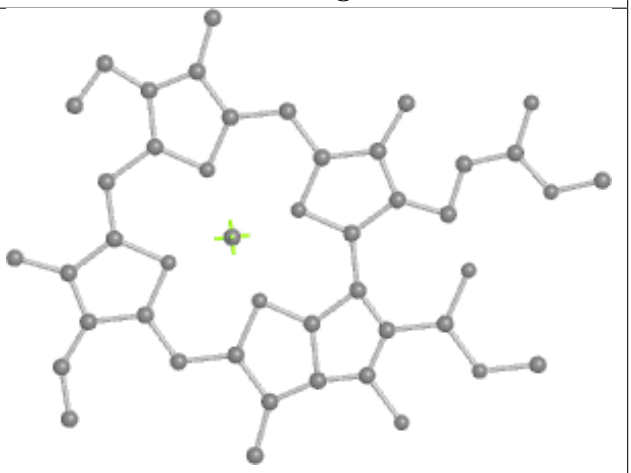


Bond angles

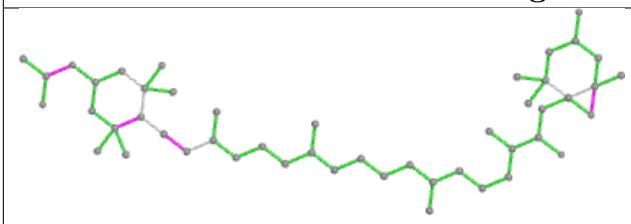


Torsions



Rings

Ligand A86 H 304



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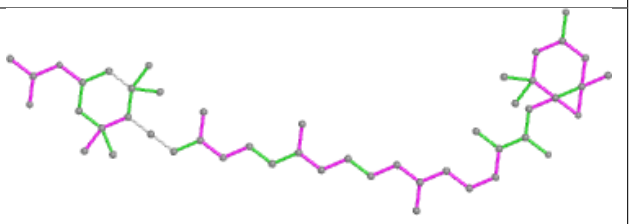
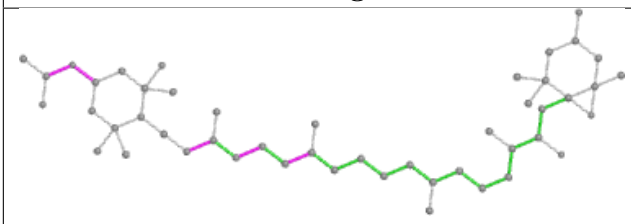


Bond angles



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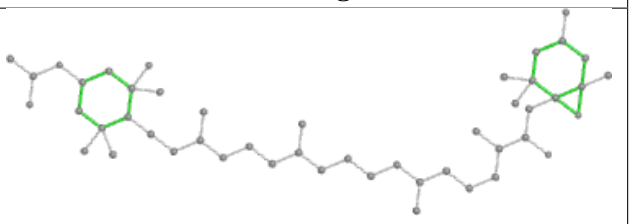
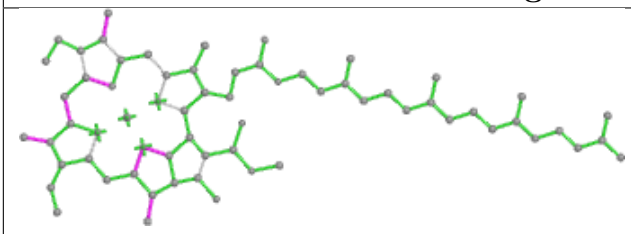


Rings

Ligand CLA T 309



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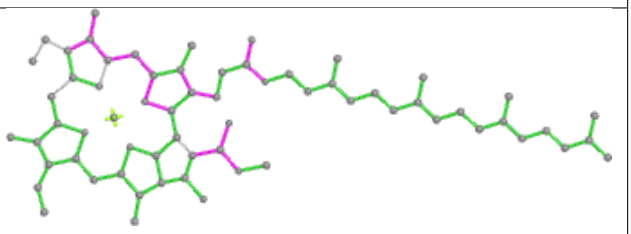
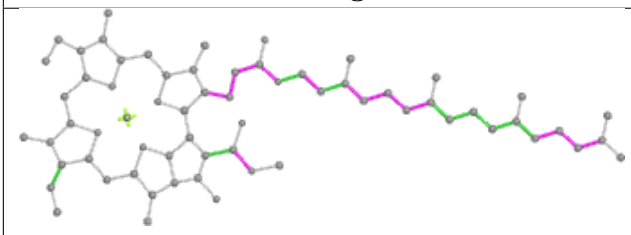


Bond angles



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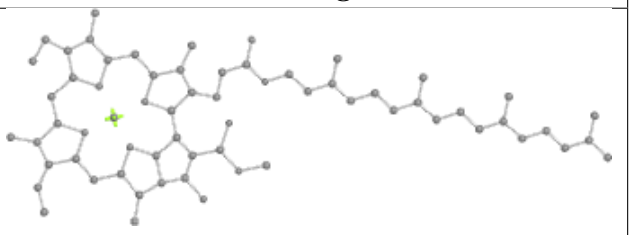
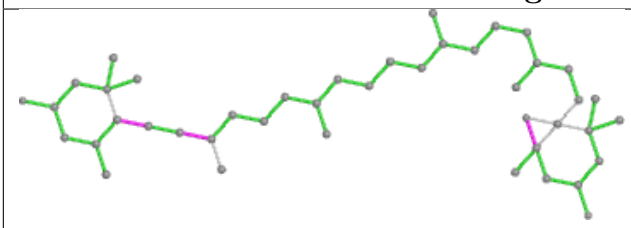
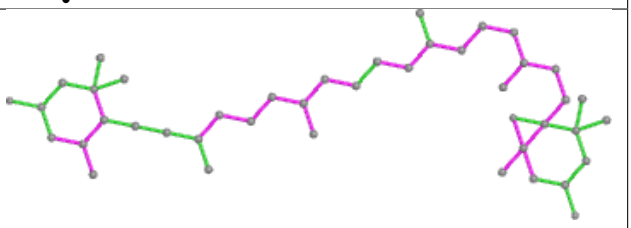


Rings

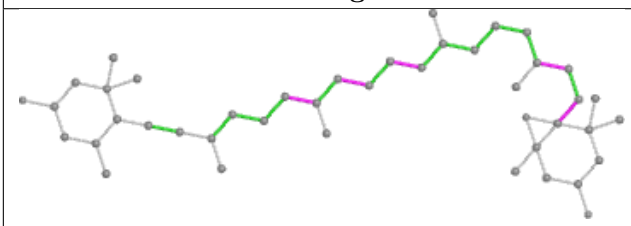
Ligand DD6 Q 302



Bond lengths



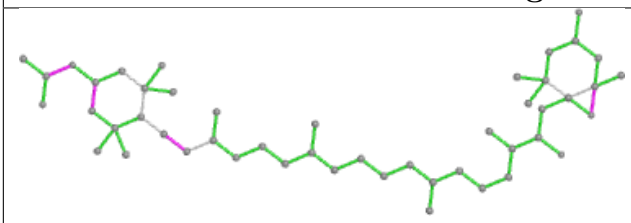
Bond angles



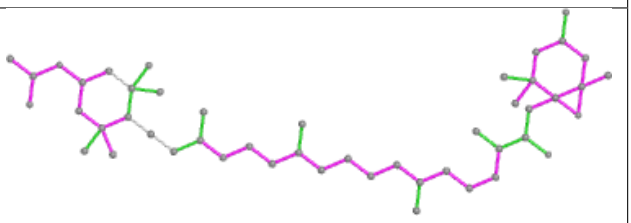
Torsions

Rings

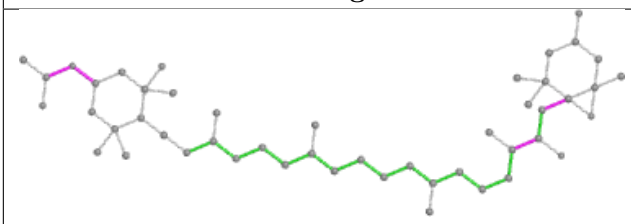
Ligand A86 M 301



Bond lengths



Bond angles



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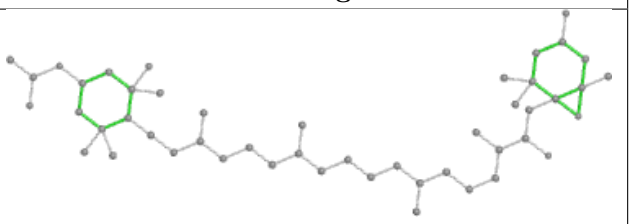
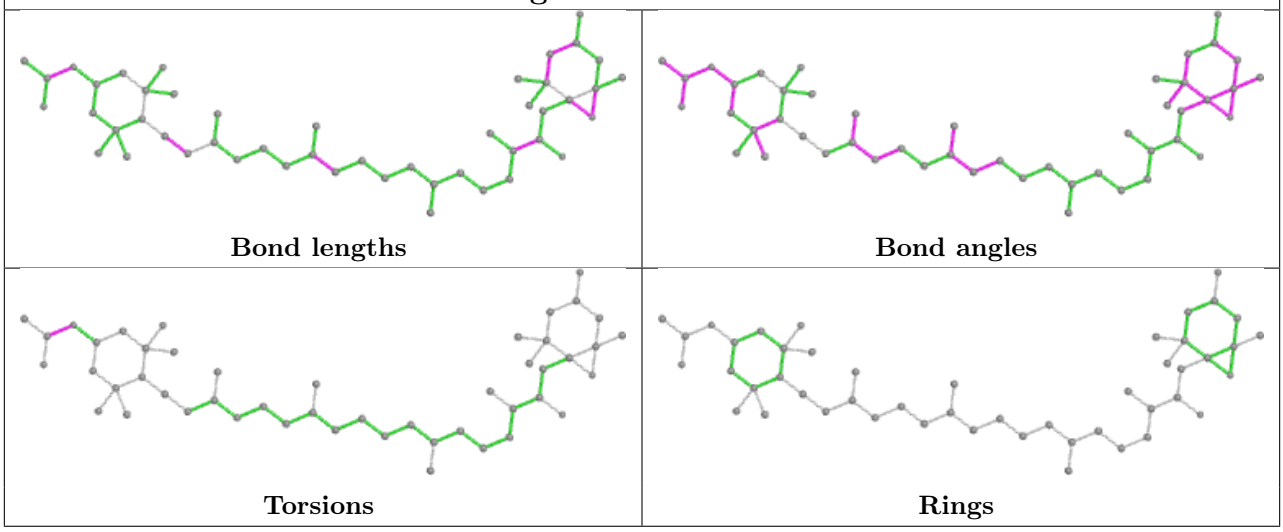
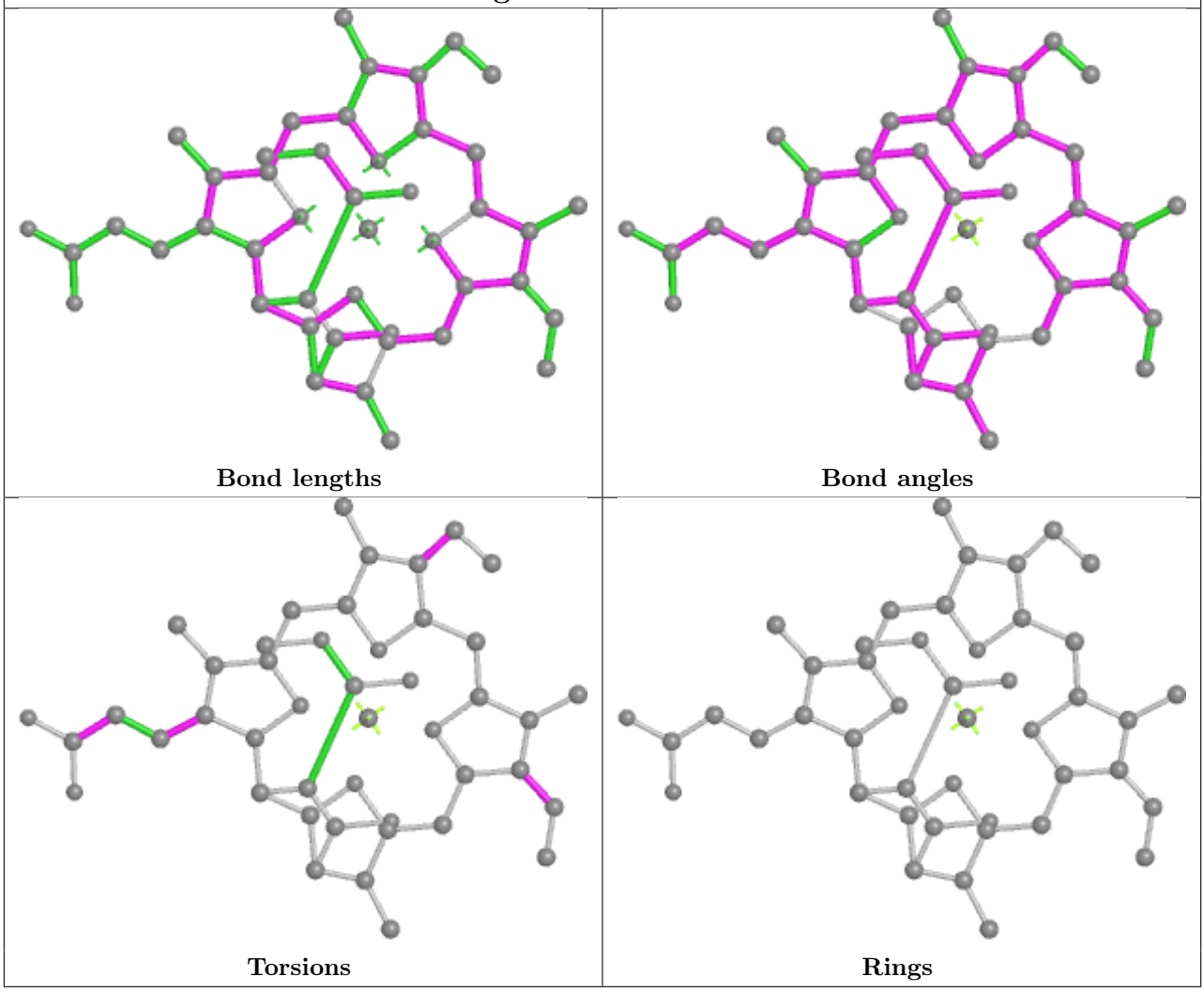


Rings

Ligand A86 N 305



Ligand KC1 N 314



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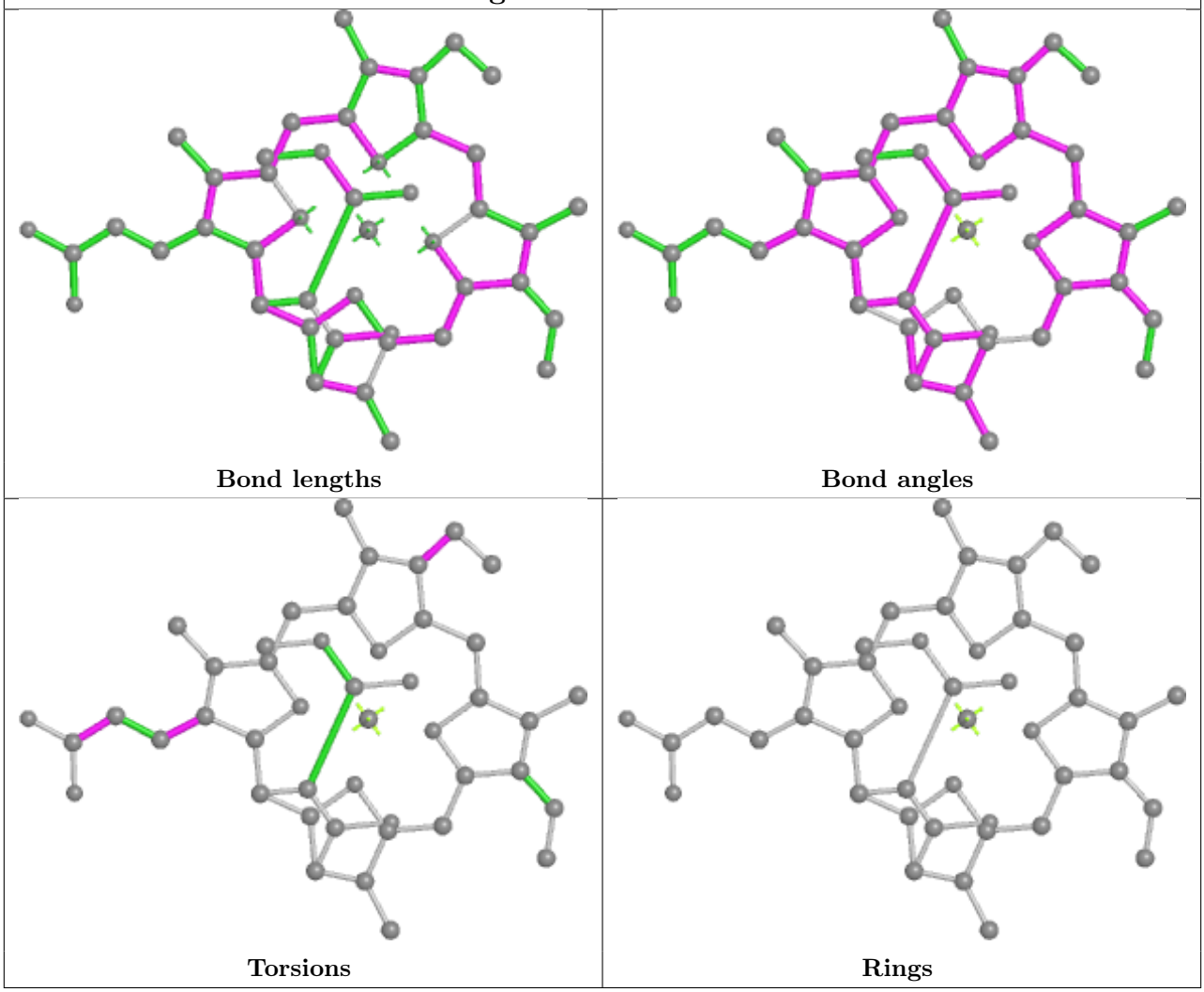
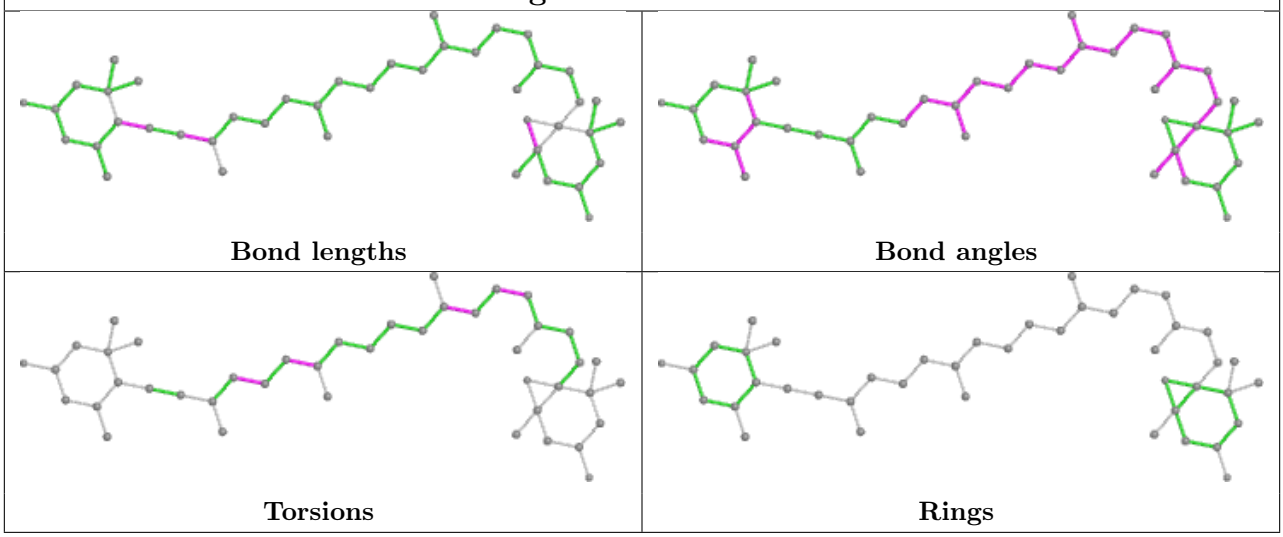
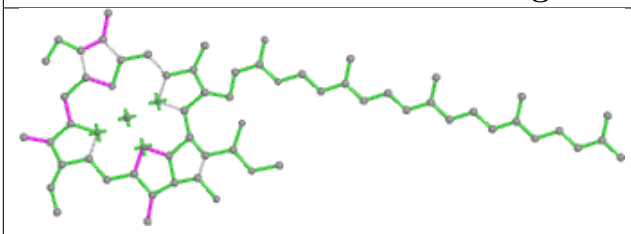


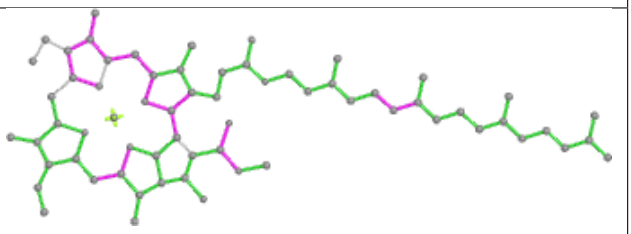
Ligand DD6 S 307



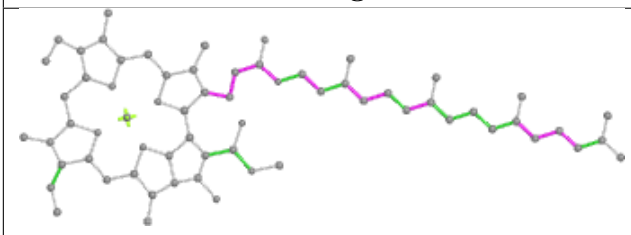
Ligand CLA f 802



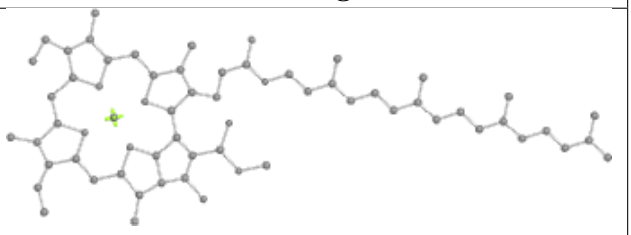
Bond lengths



Bond angles

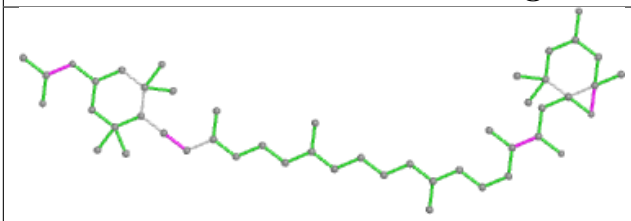


Torsions



Rings

Ligand A86 W 203



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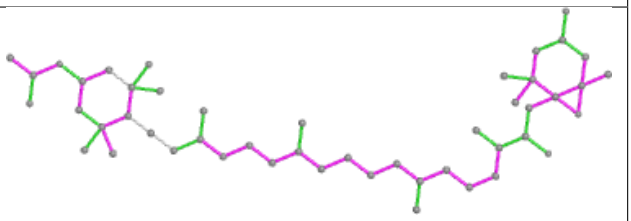
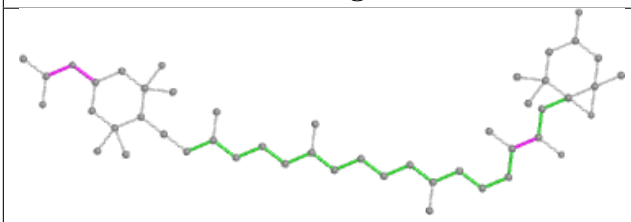


Bond angles



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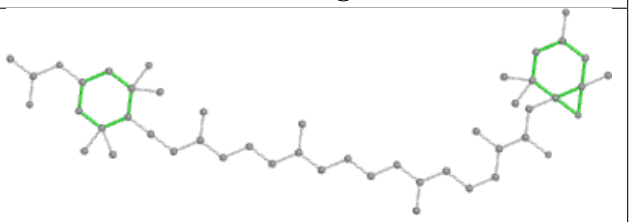
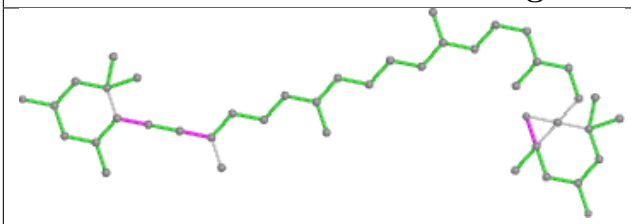
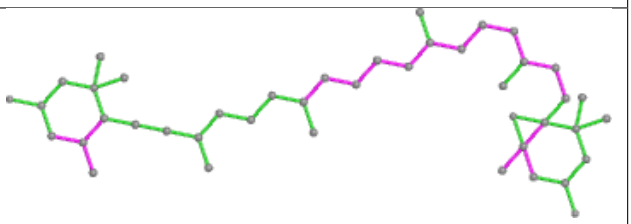


Rings

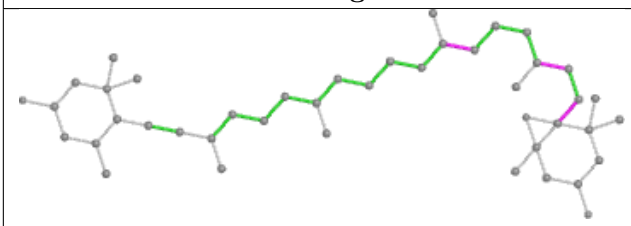
Ligand DD6 E 303



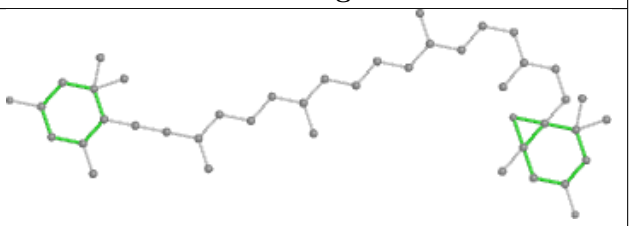
Bond lengths



Bond angles

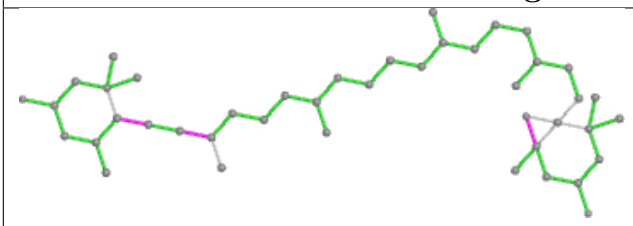


Torsions



Rings

Ligand DD6 H 303



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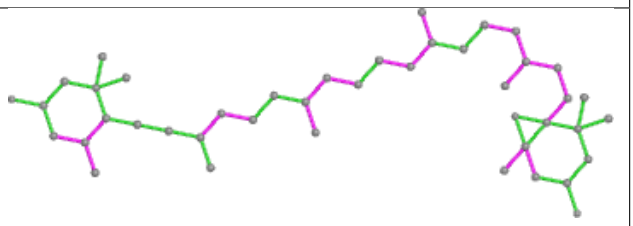
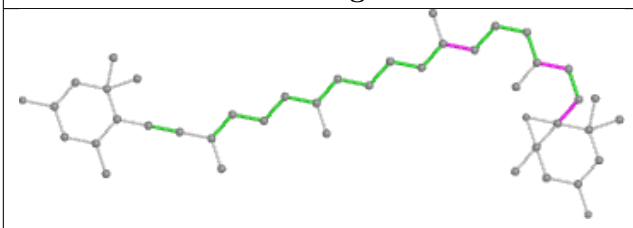


Bond angles



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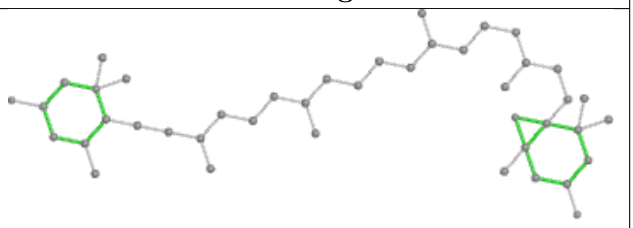
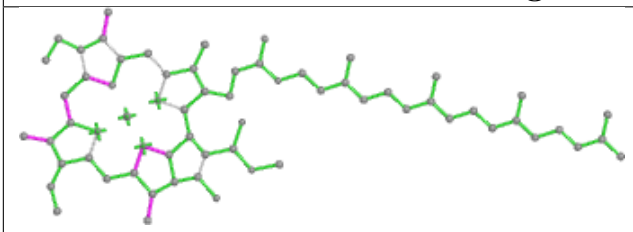


Rings

Ligand CLA F 312



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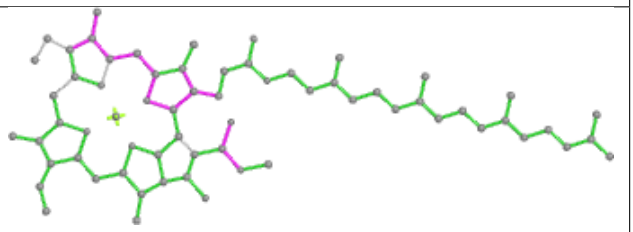
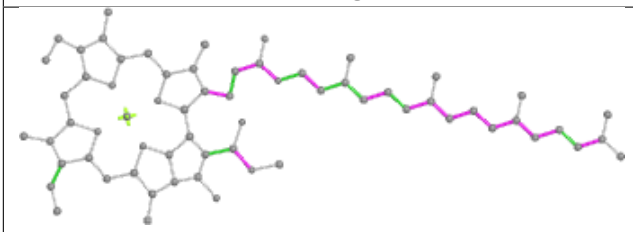


Bond angles



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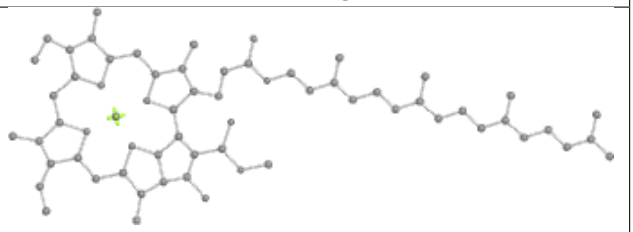
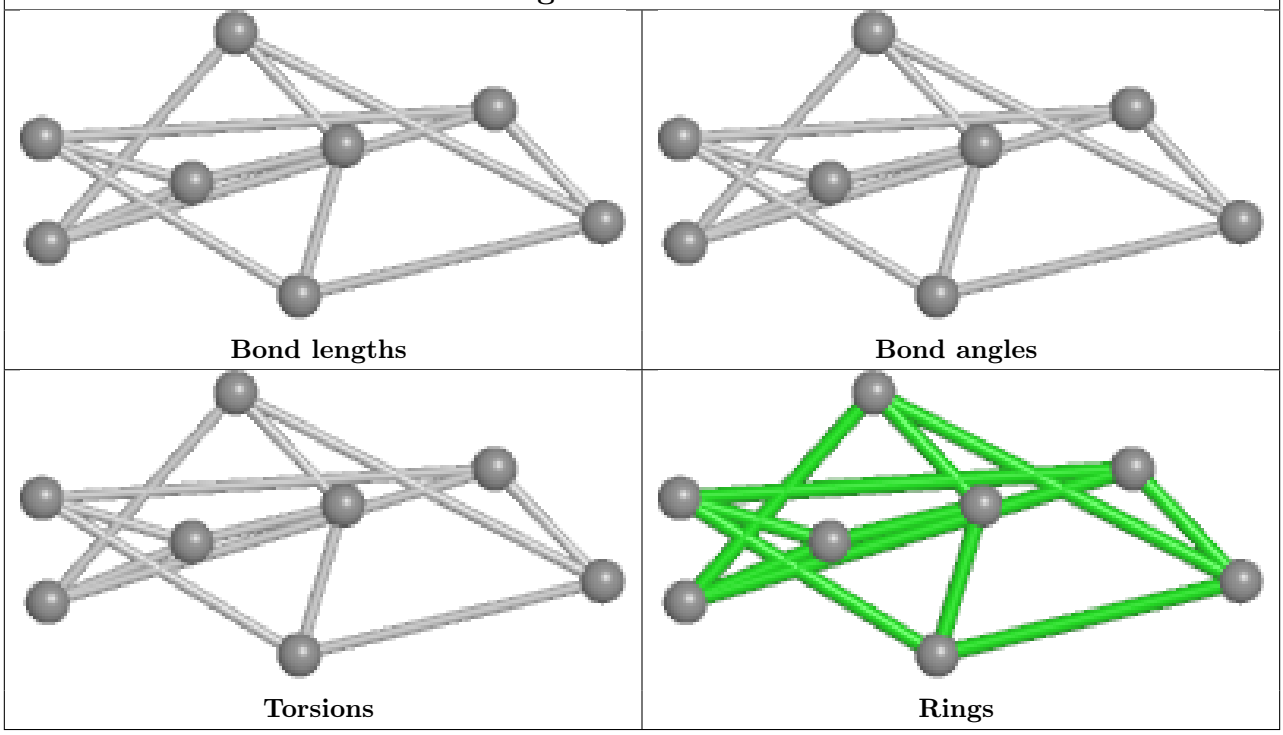
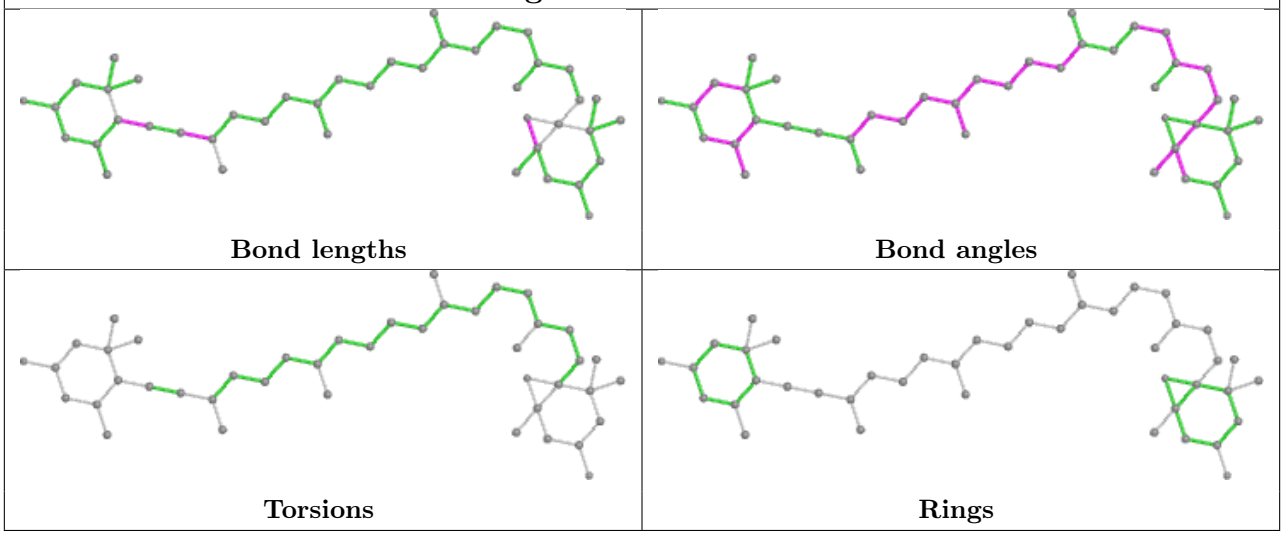


Rings

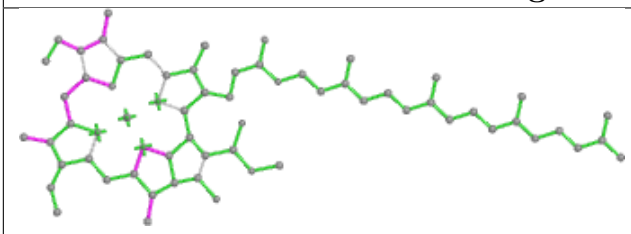
Ligand SF4 c 101



Ligand DD6 K 305



Ligand CLA a 818



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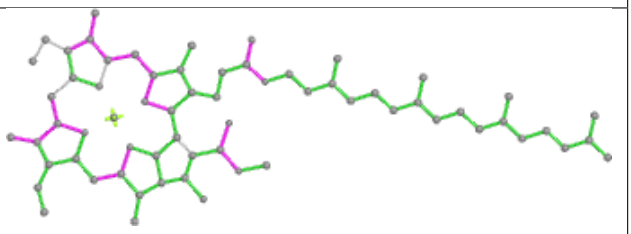
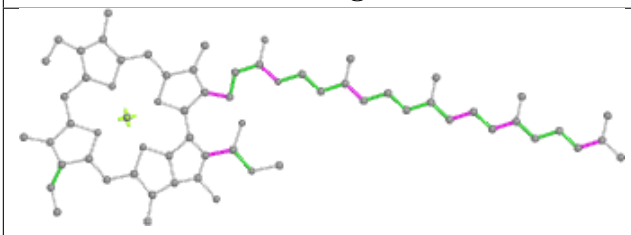
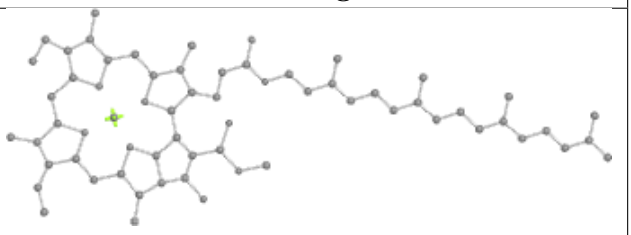


Bond angles

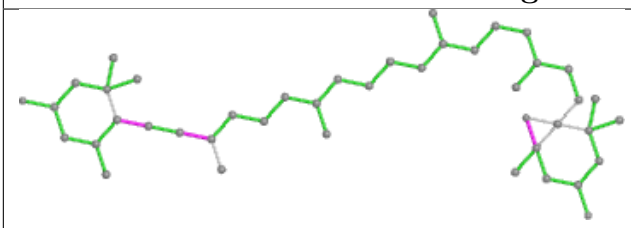


Torsions

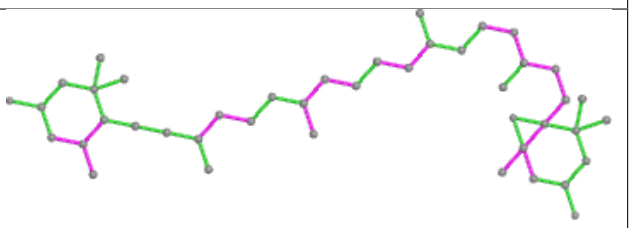


Rings

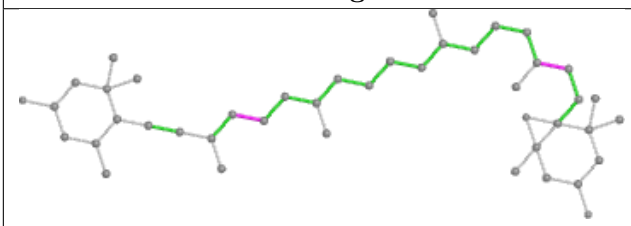
Ligand DD6 M 303



Bond lengths



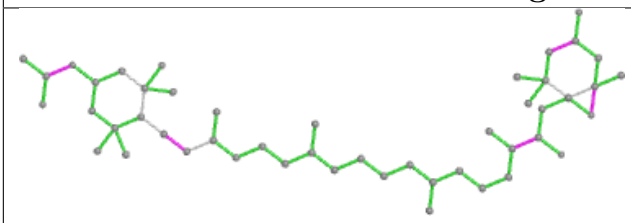
Bond angles



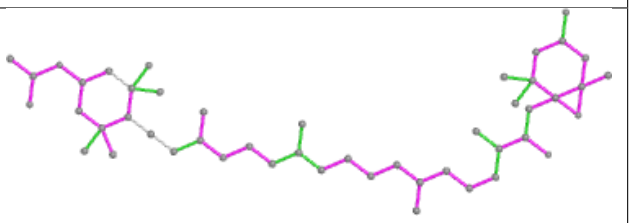
Torsions

Rings

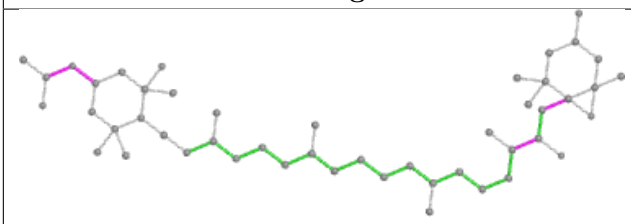
Ligand A86 G 304



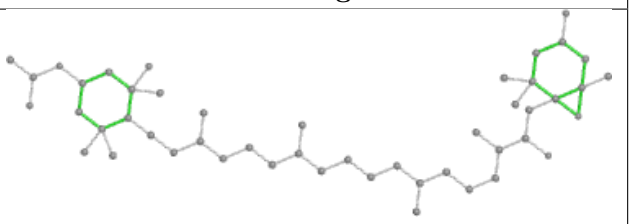
Bond lengths



Bond angles

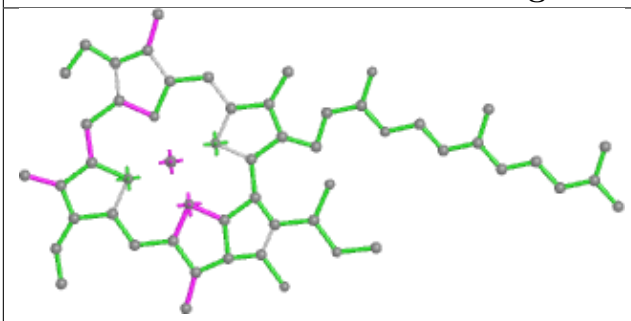


Torsions

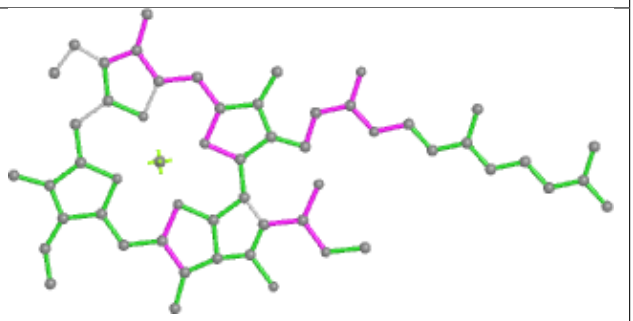


Rings

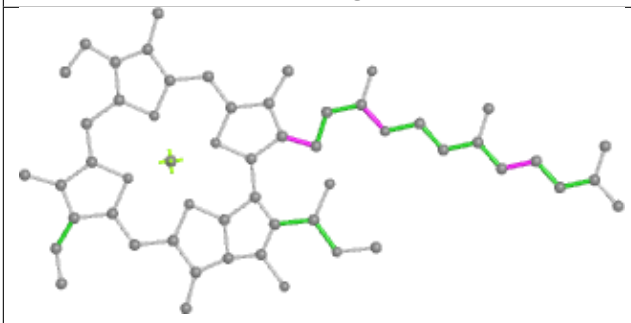
Ligand CLA a 803



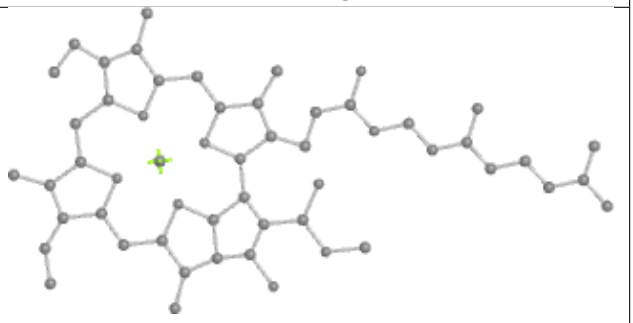
Bond lengths



Bond angles

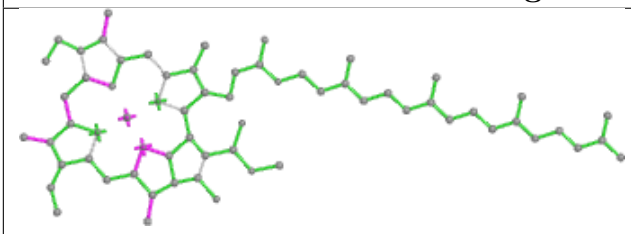


Torsions

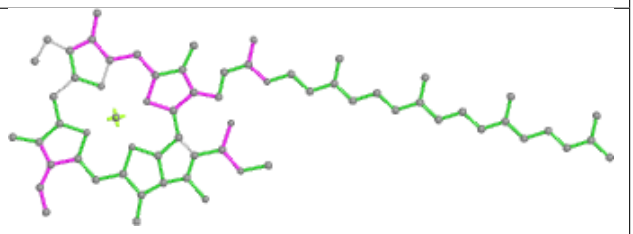


Rings

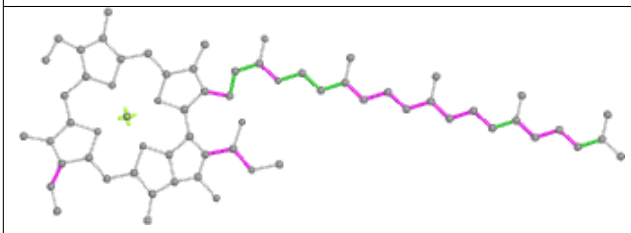
Ligand CLA C 212



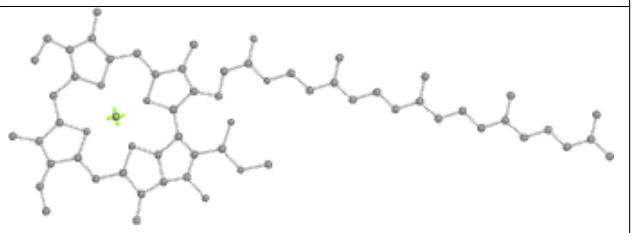
Bond lengths



Bond angles

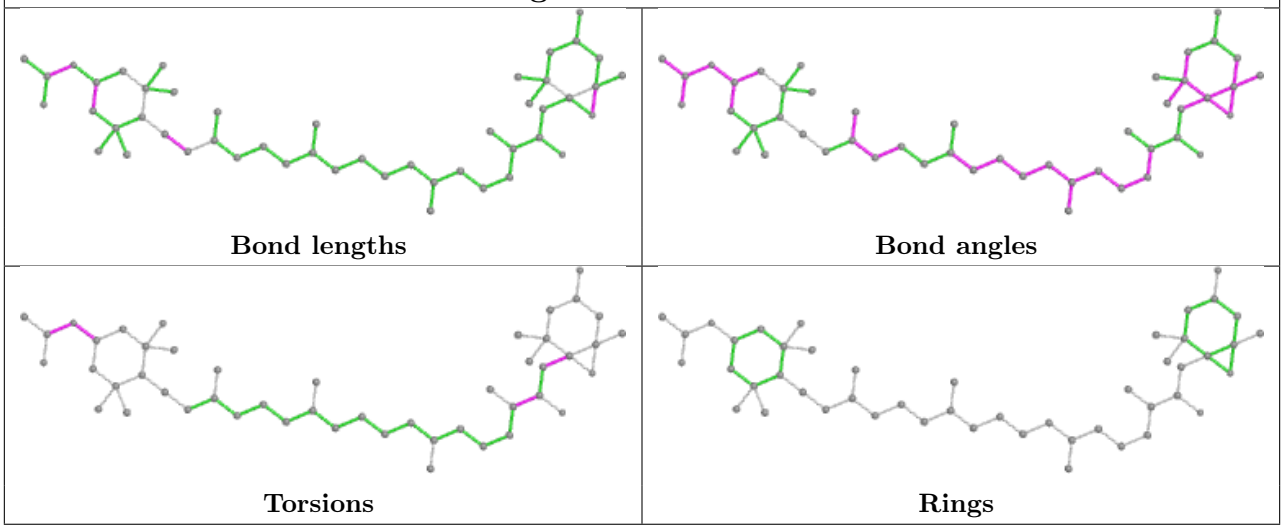


Torsions

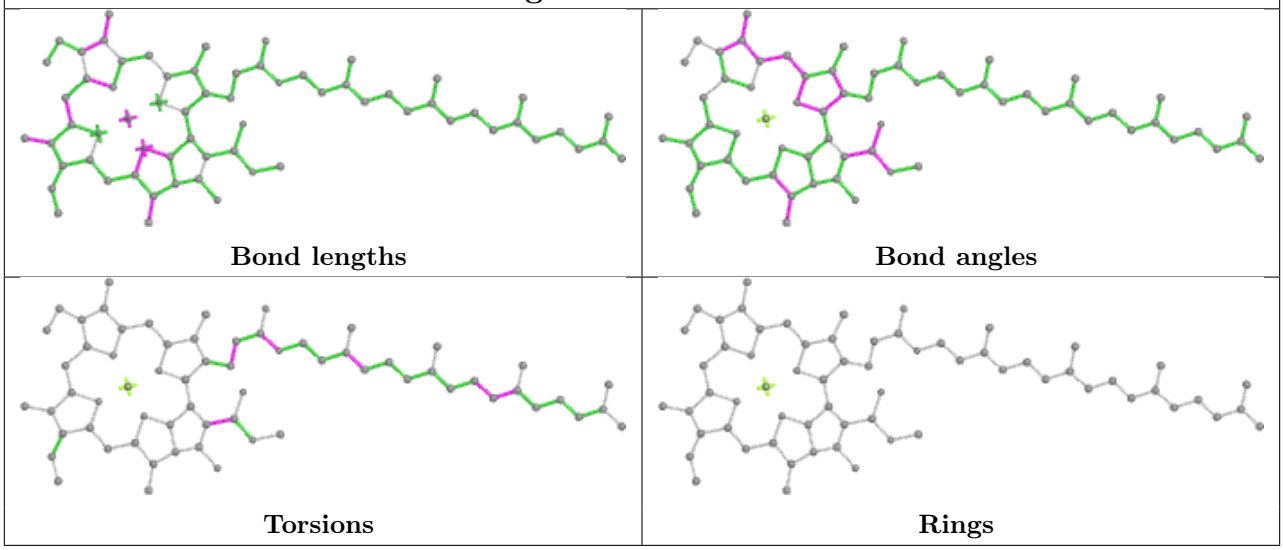


Rings

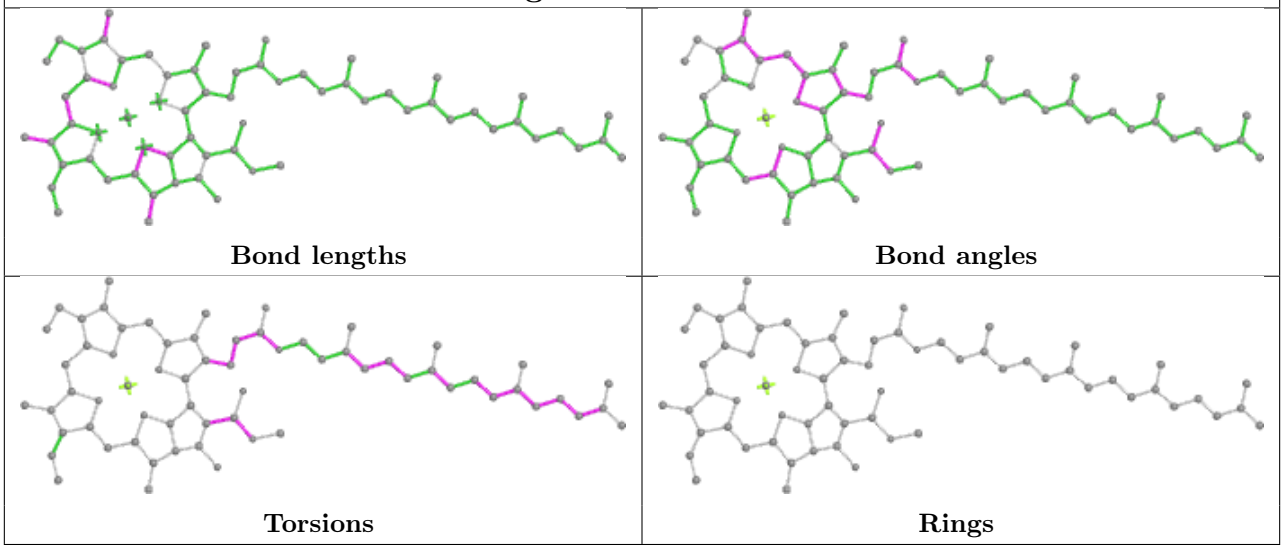
Ligand A86 K 302



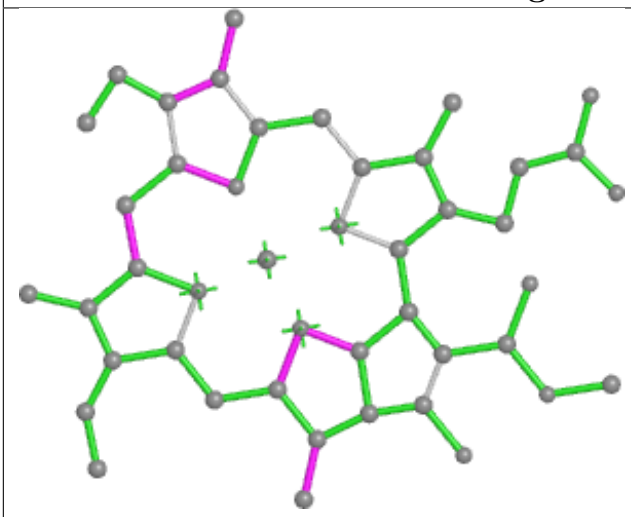
Ligand CLA C 209



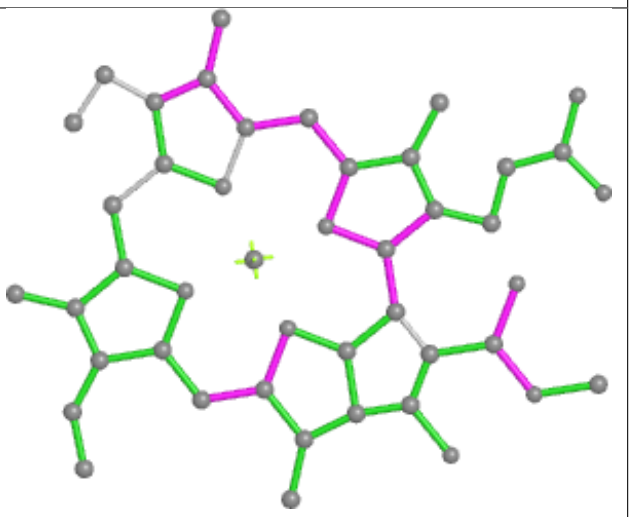
Ligand CLA B 305



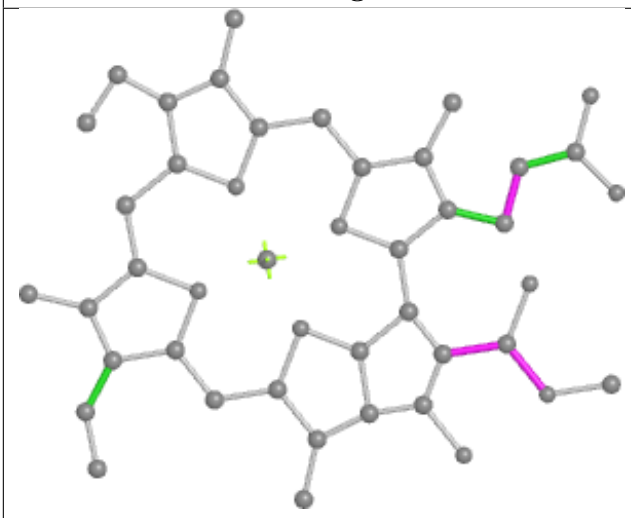
Ligand CLA a 834



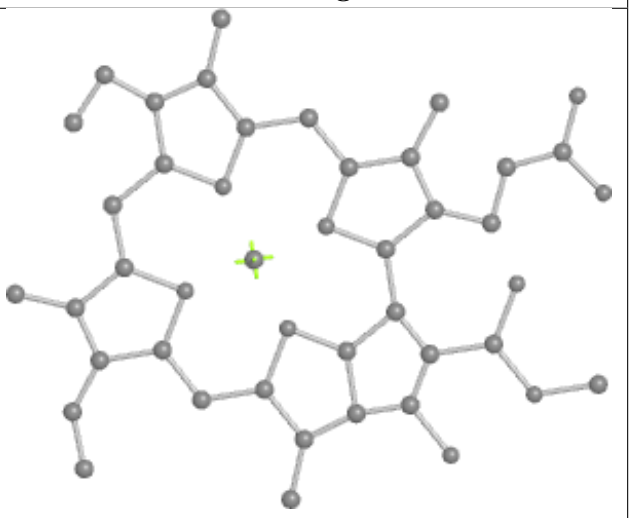
Bond lengths



Bond angles

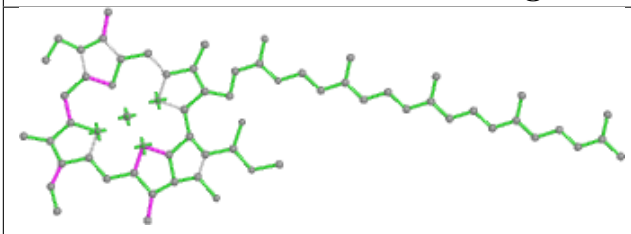


Torsions

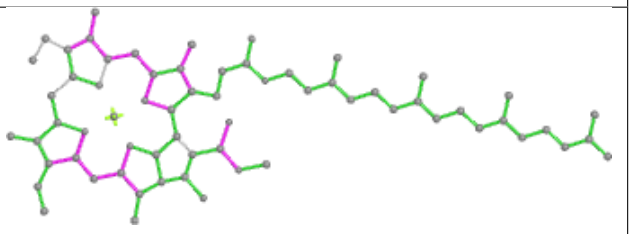


Rings

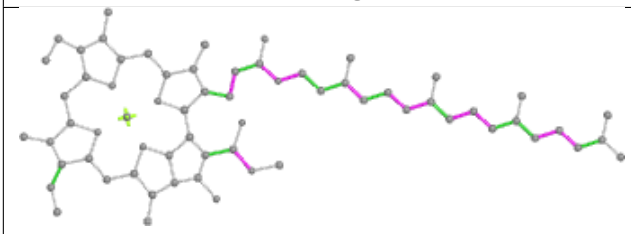
Ligand CLA B 308



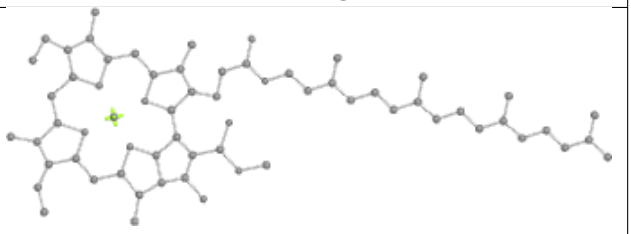
Bond lengths



Bond angles

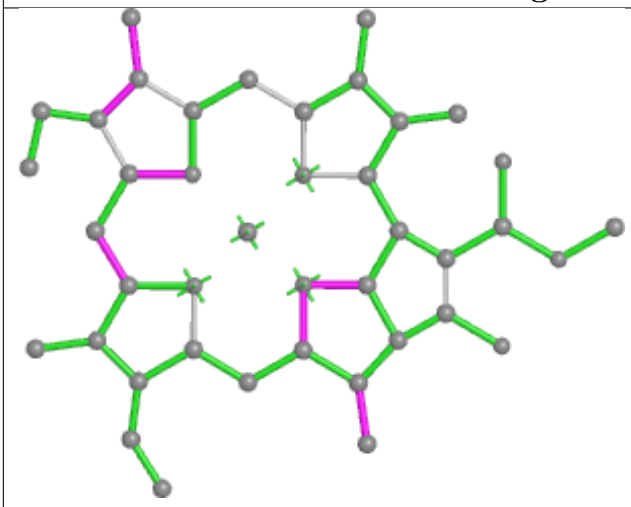


Torsions

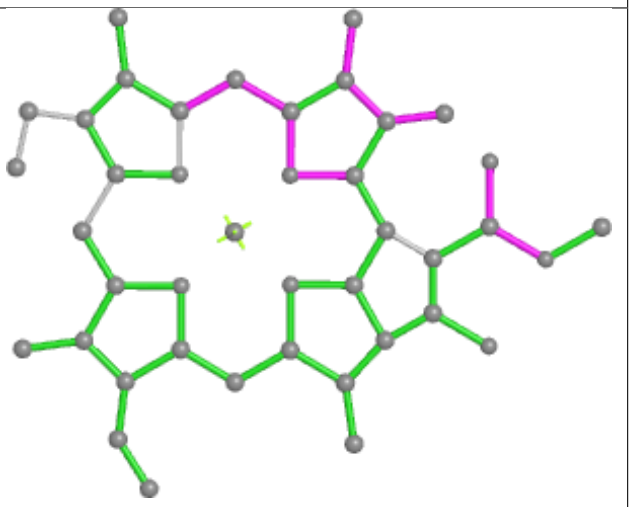


Rings

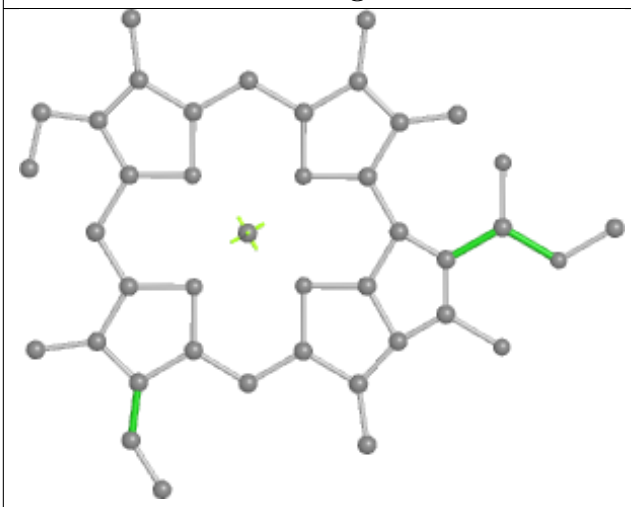
Ligand CLA I 314



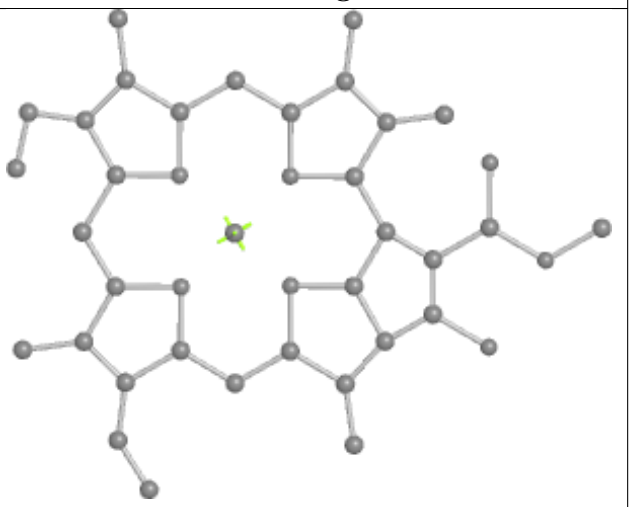
Bond lengths



Bond angles

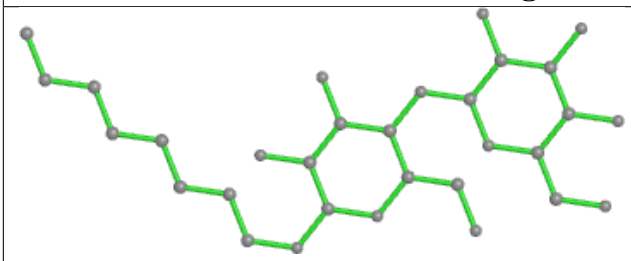


Torsions

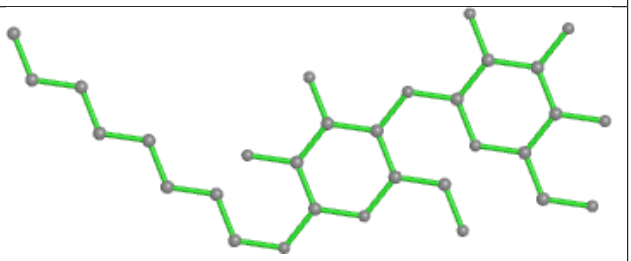


Rings

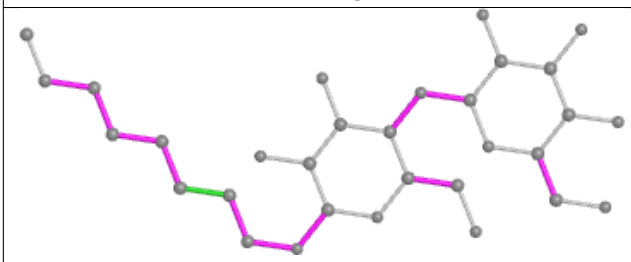
Ligand LMT K 317



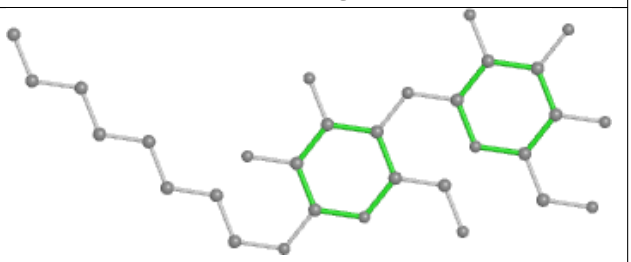
Bond lengths



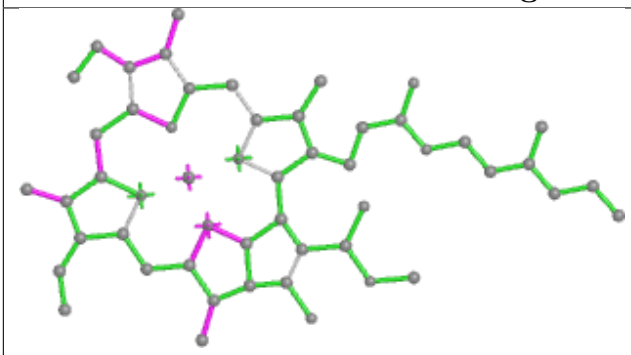
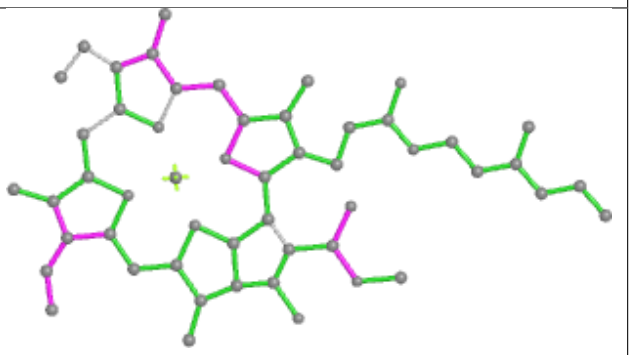
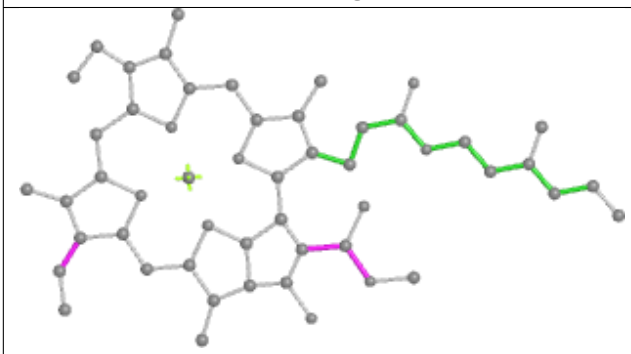
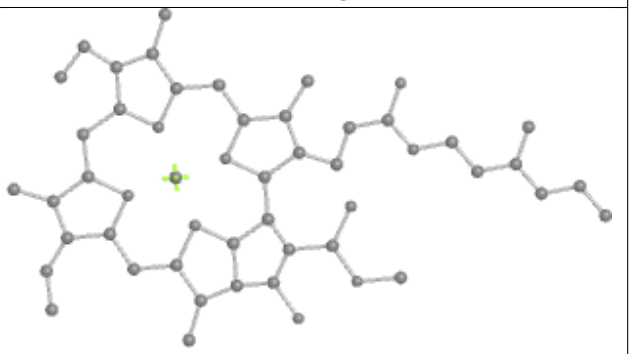
Bond angles

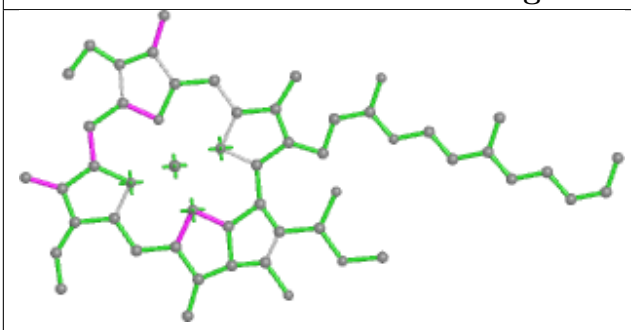
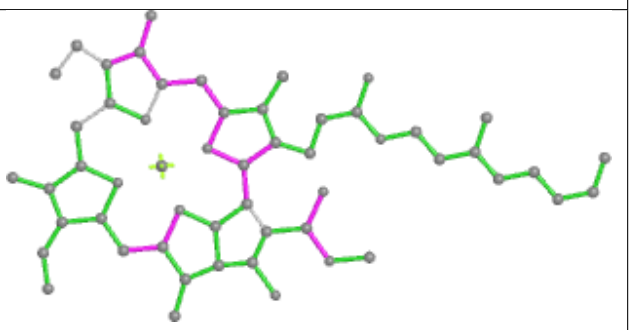
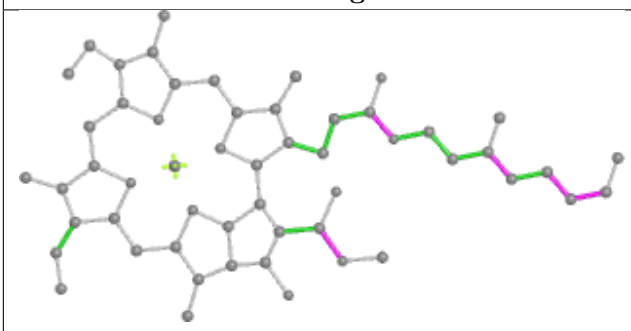
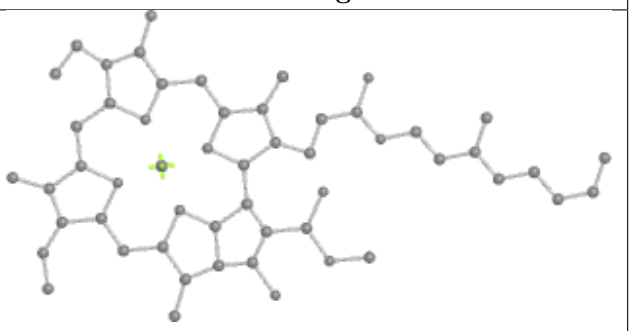


Torsions

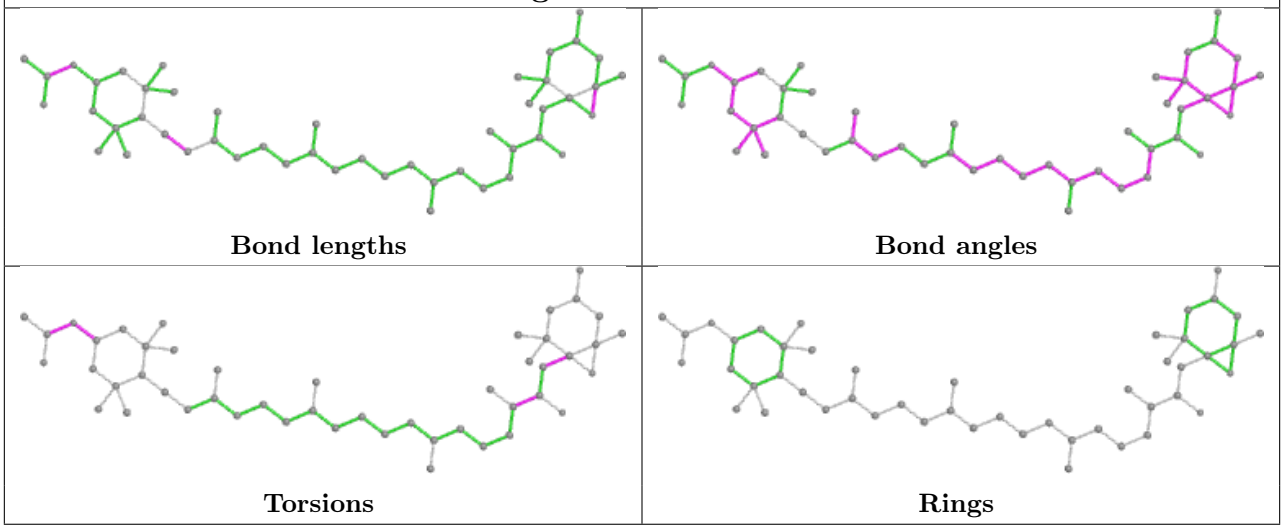


Rings

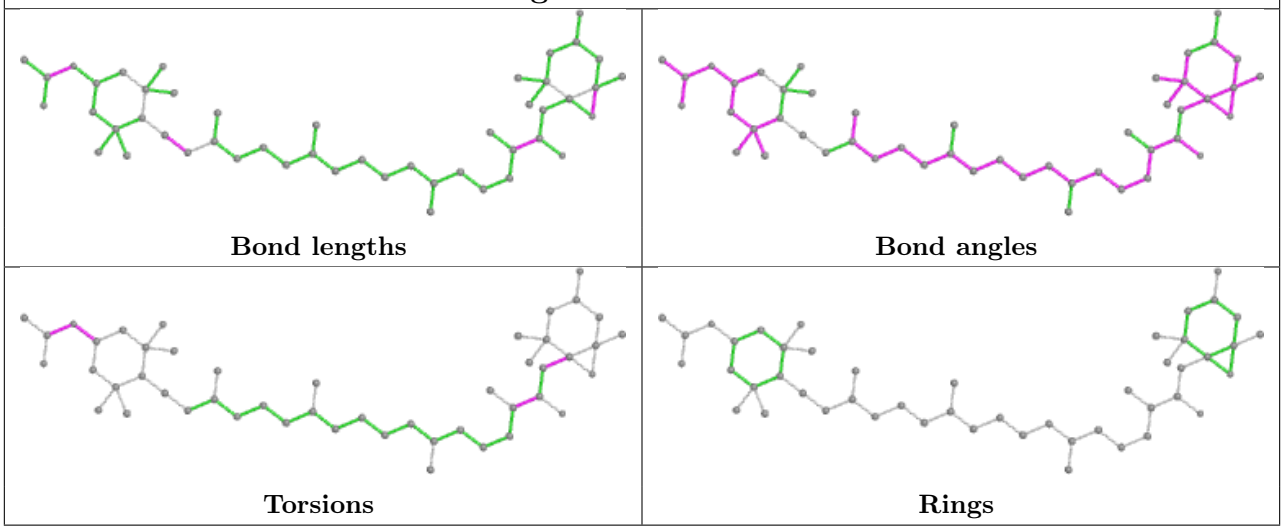
Ligand CLA M 308	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA N 317	
 Bond lengths	 Bond angles
 Torsions	 Rings

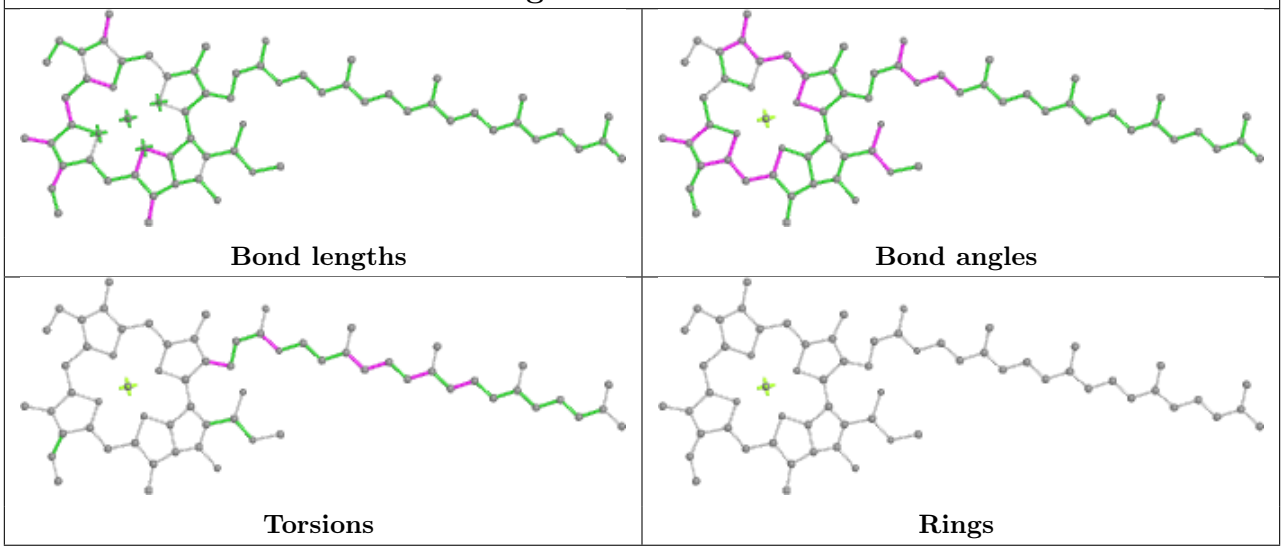
Ligand A86 T 307



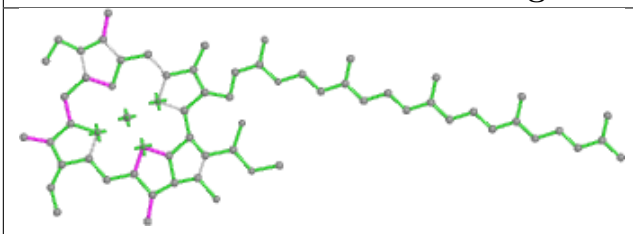
Ligand A86 R 301



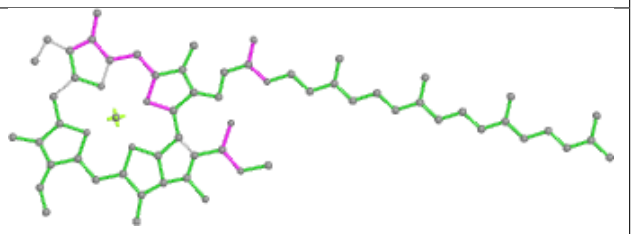
Ligand CLA E 314



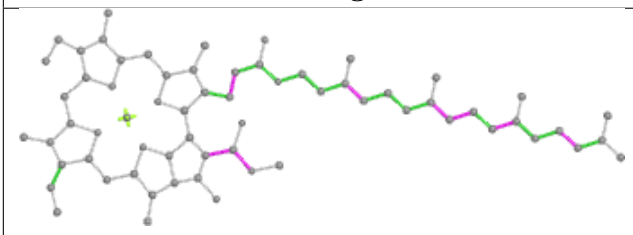
Ligand CLA J 310



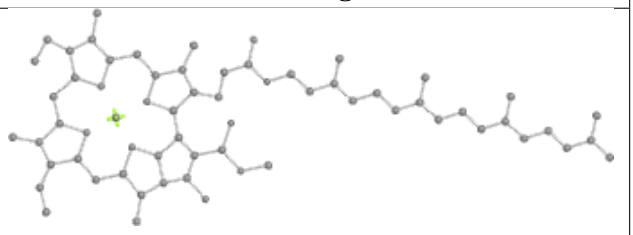
Bond lengths



Bond angles

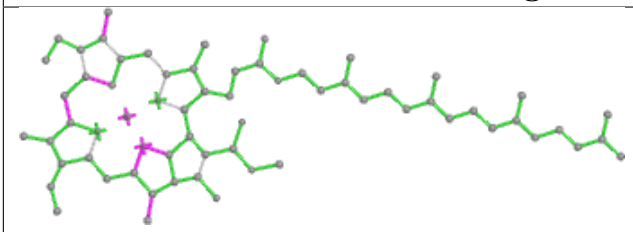


Torsions

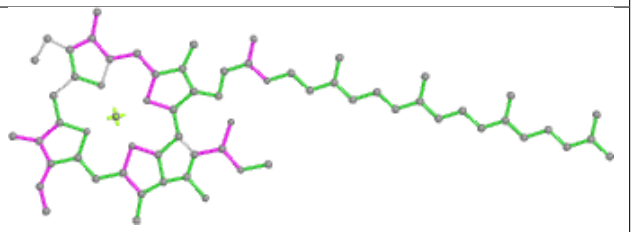


Rings

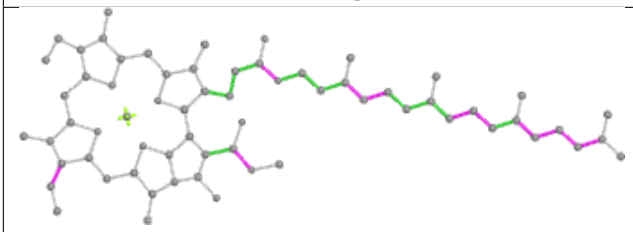
Ligand CLA U 310



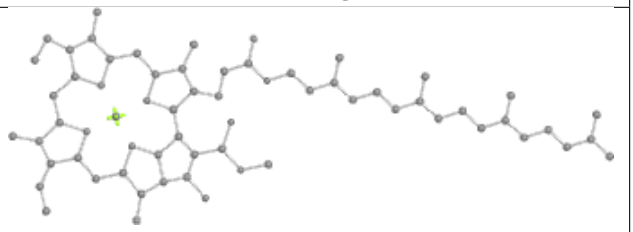
Bond lengths



Bond angles

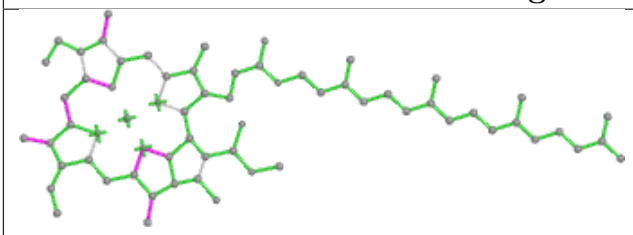


Torsions

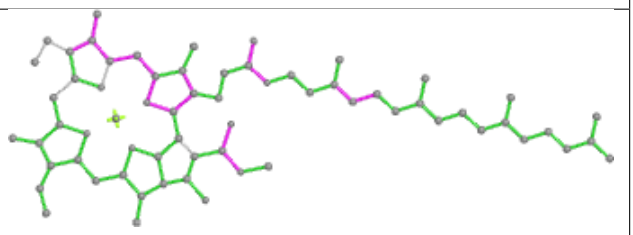


Rings

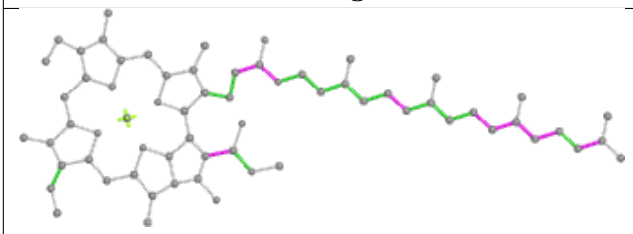
Ligand CLA a 826



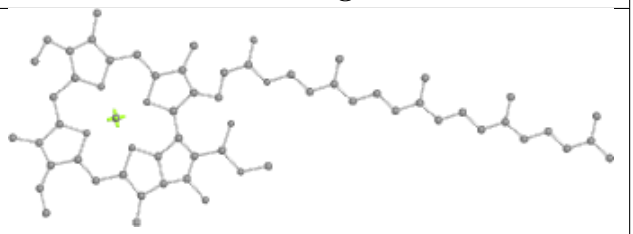
Bond lengths



Bond angles

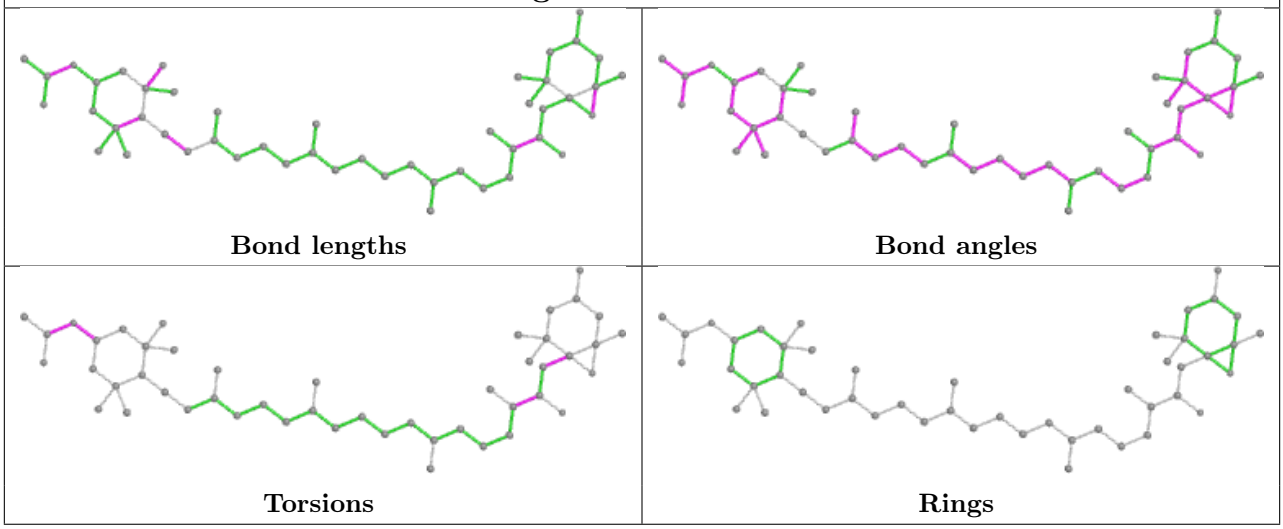


Torsions

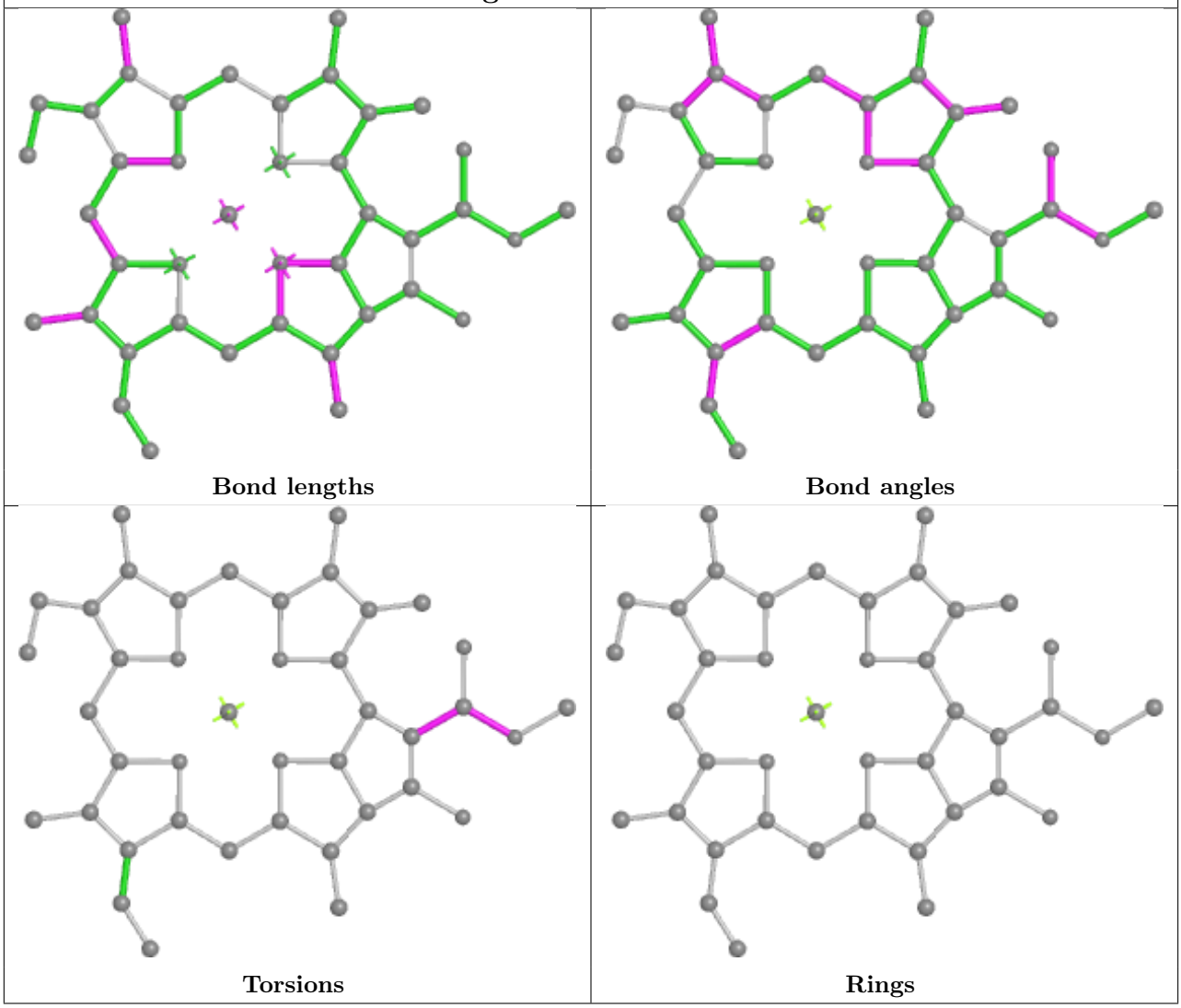


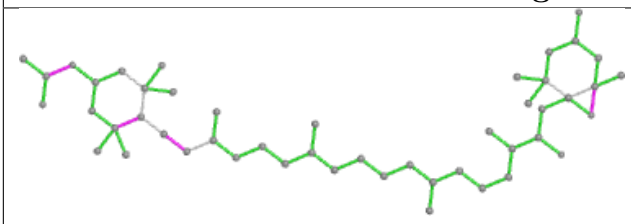
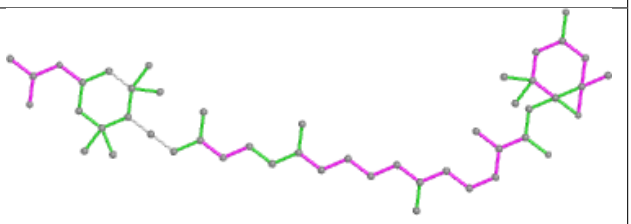
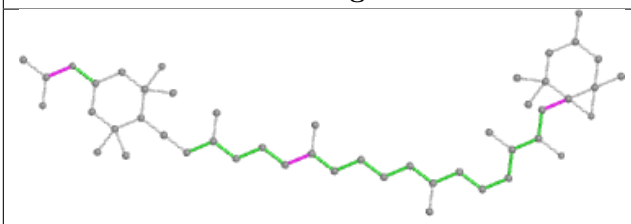
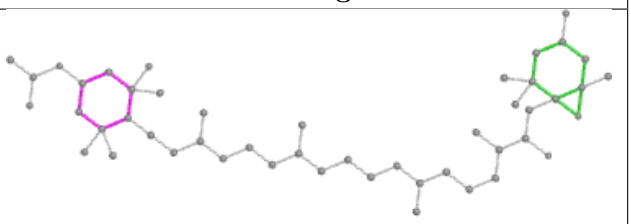
Rings

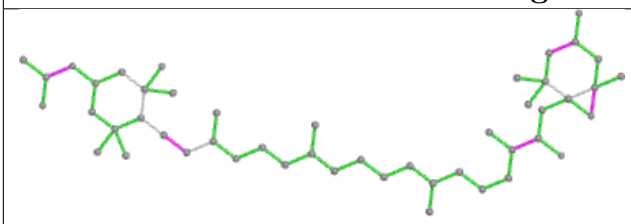
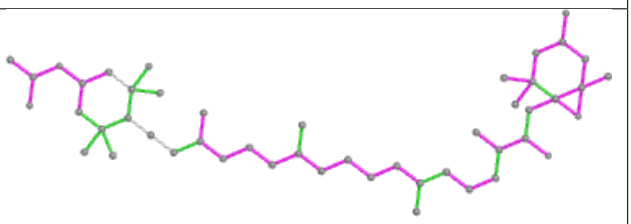
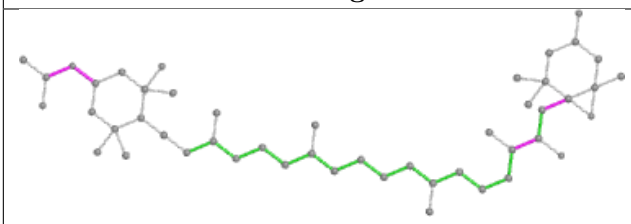
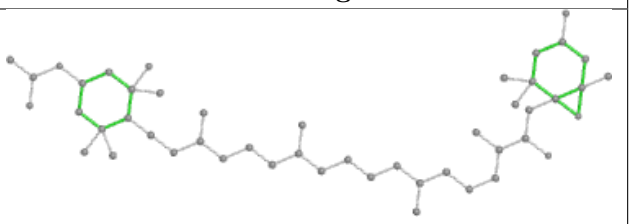
Ligand A86 F 305



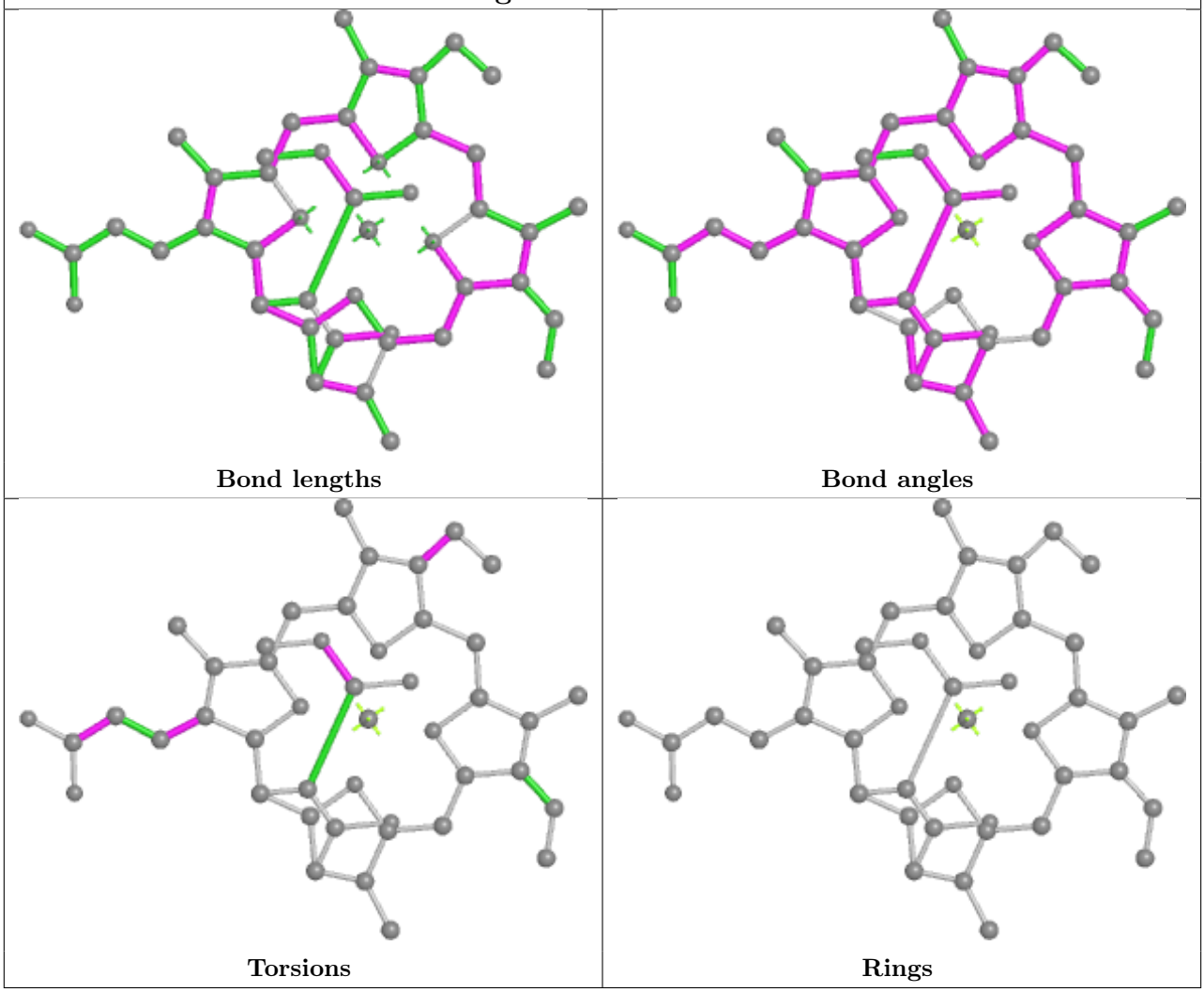
Ligand CLA H 314



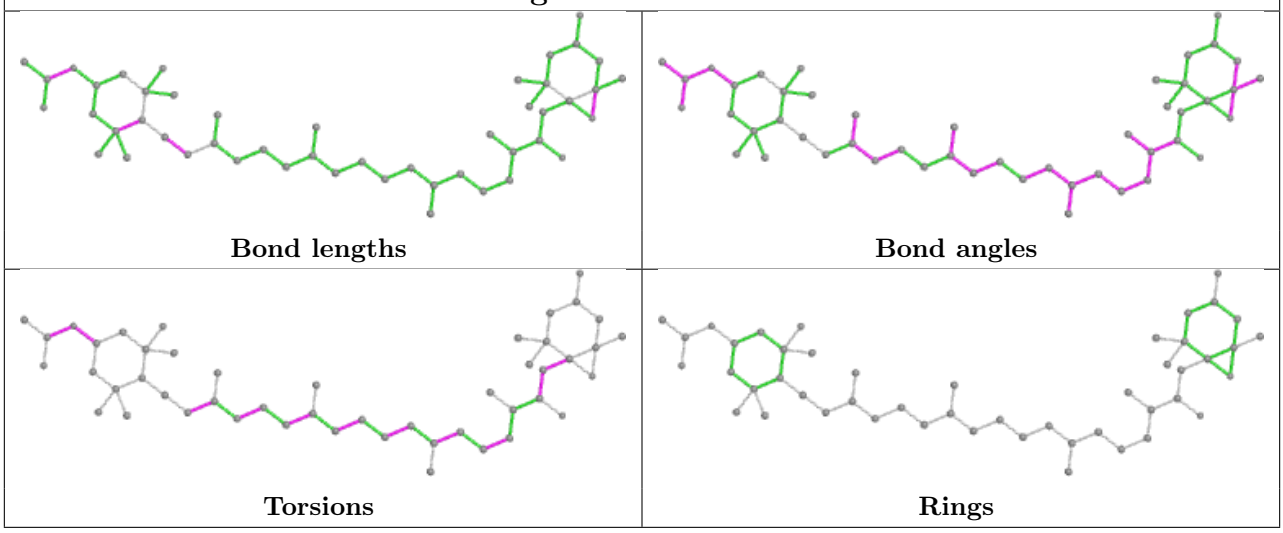
Ligand A86 L 301	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand A86 T 305	
 Bond lengths	 Bond angles
 Torsions	 Rings

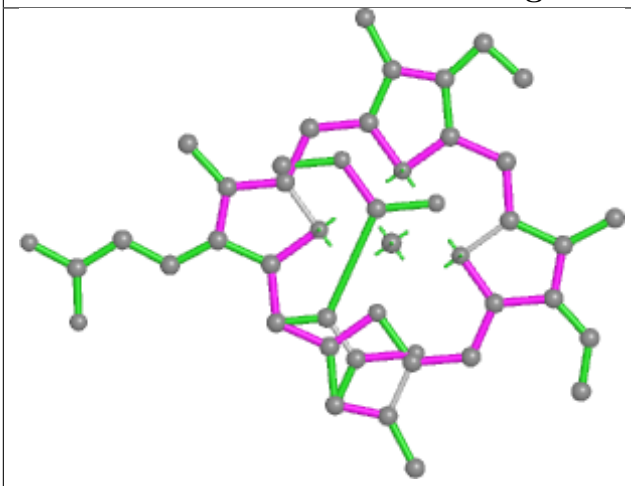
Ligand KC1 T 315



Ligand A86 U 303



Ligand KC1 V 312



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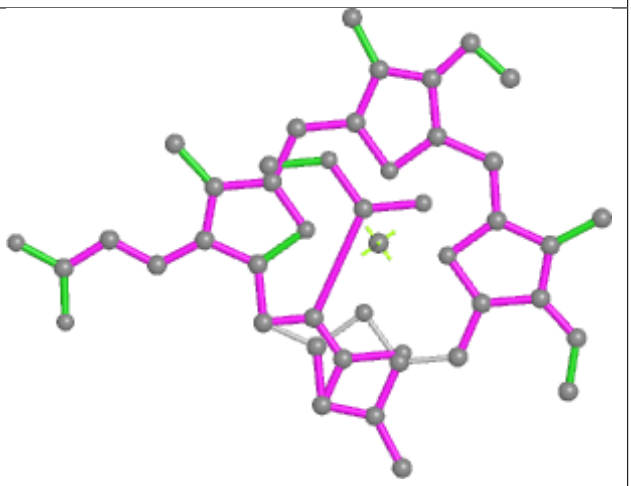
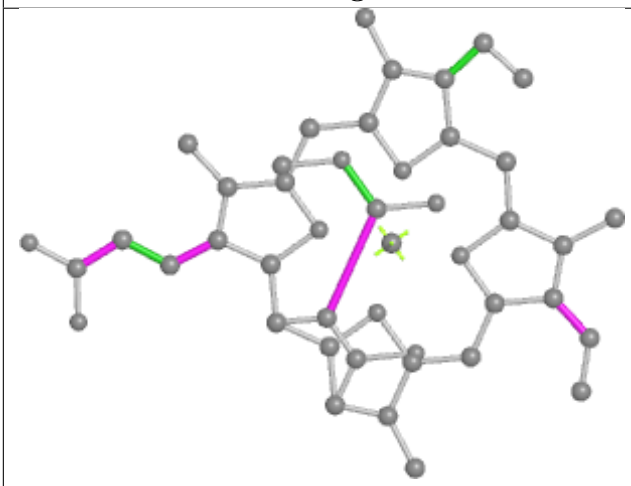


Bond angles



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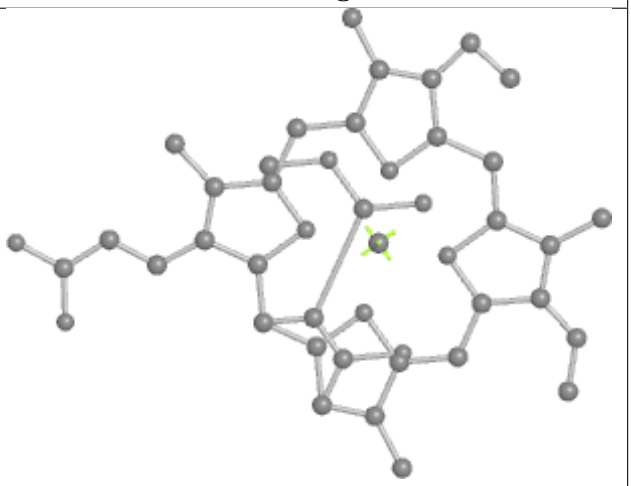
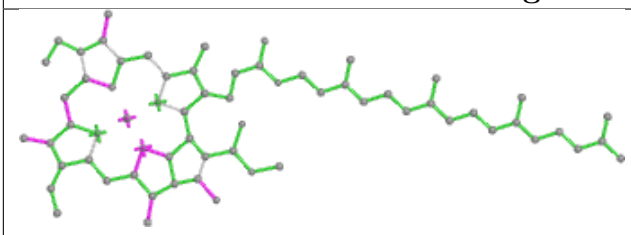


Rings

Ligand CLA K 313



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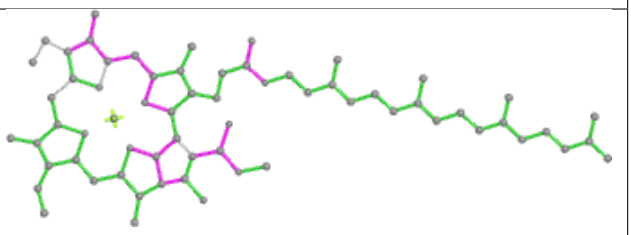
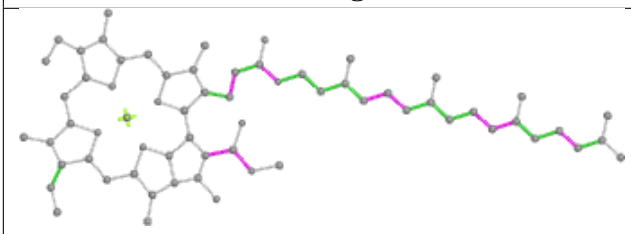


Bond angles



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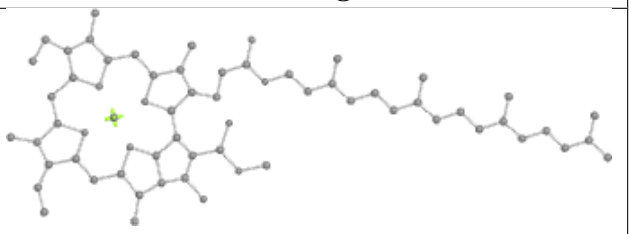
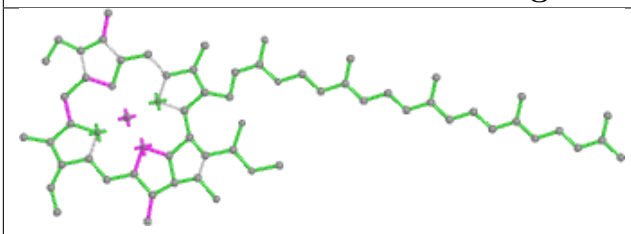


Rings

Ligand CLA I 310



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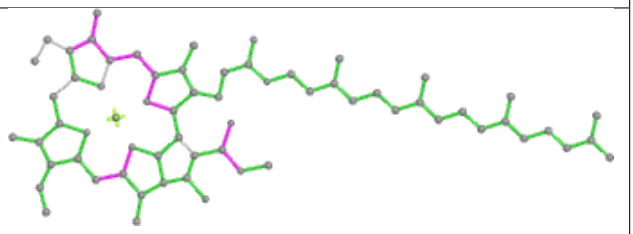
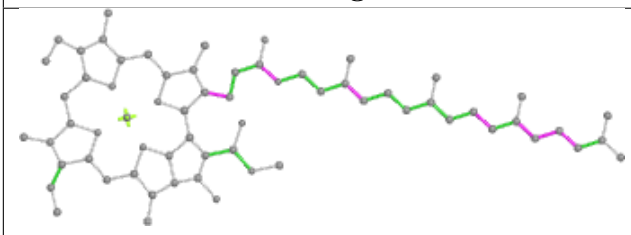


Bond angles



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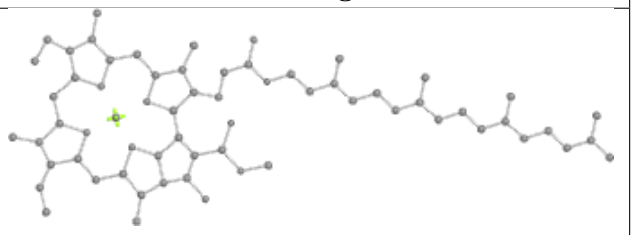
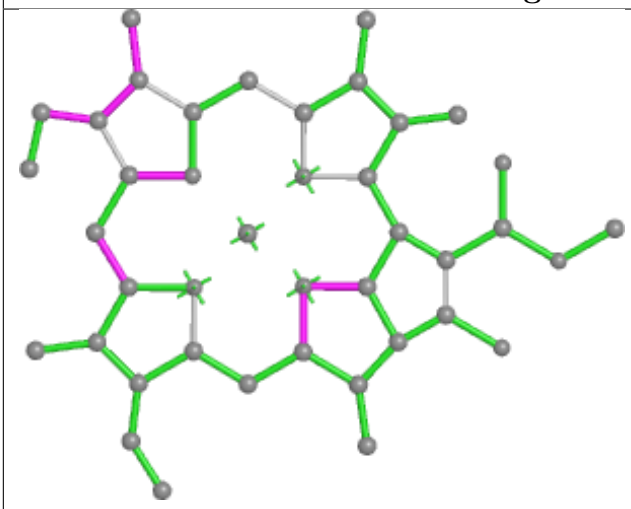


Rings

Ligand CLA X 310



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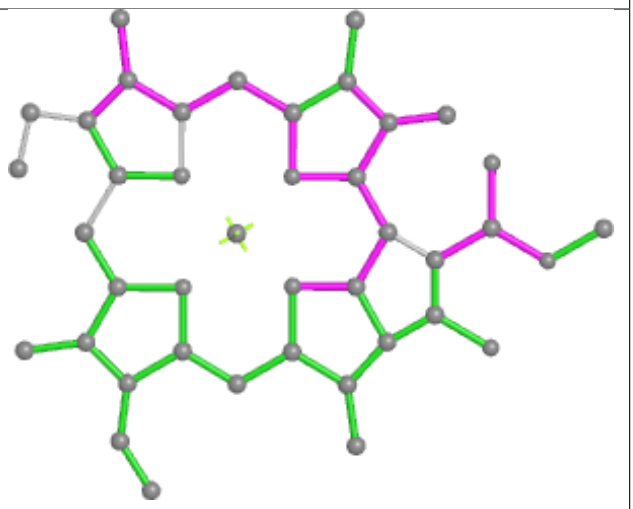
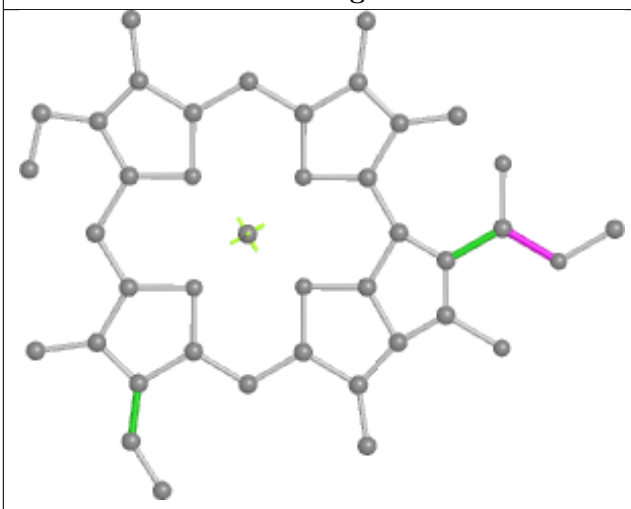


Bond angles



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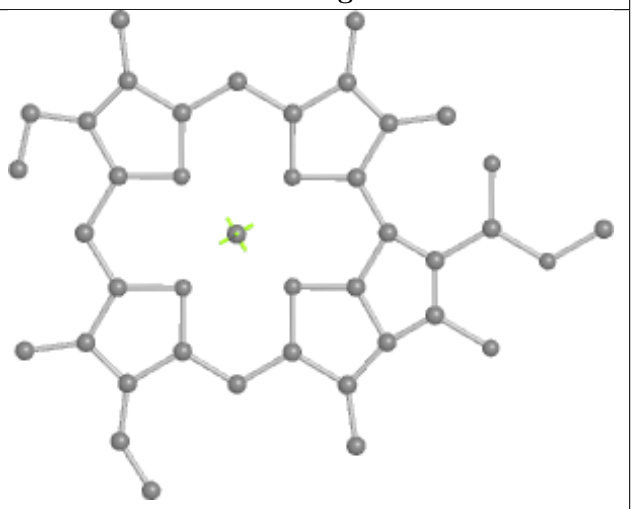
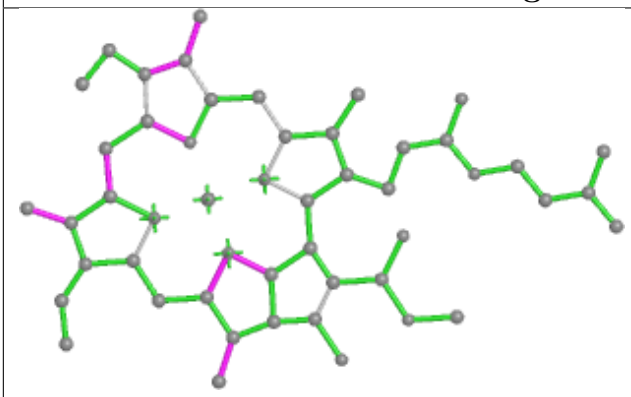
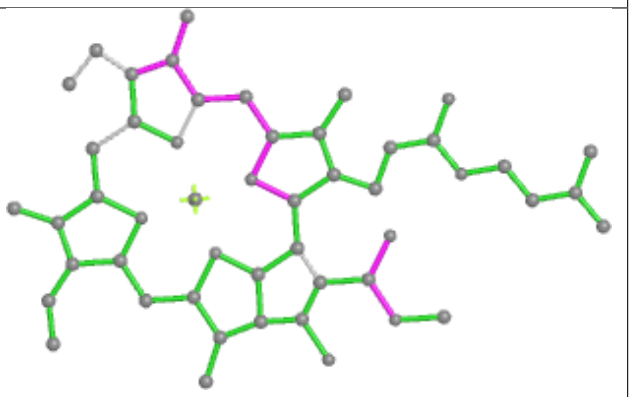
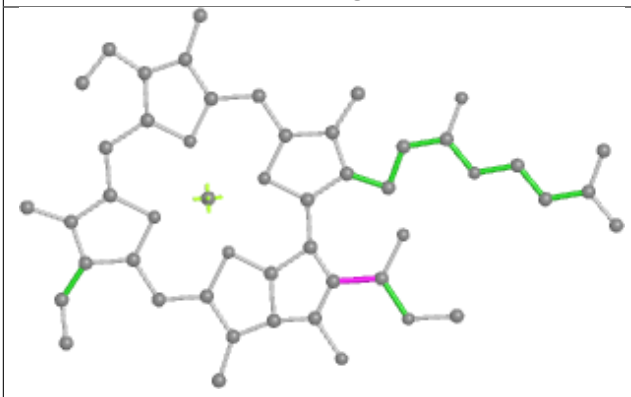
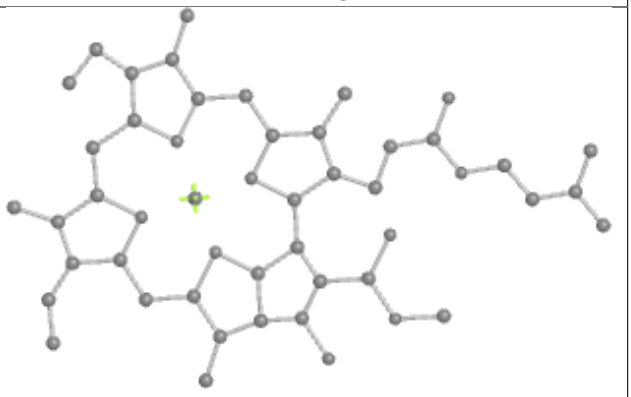
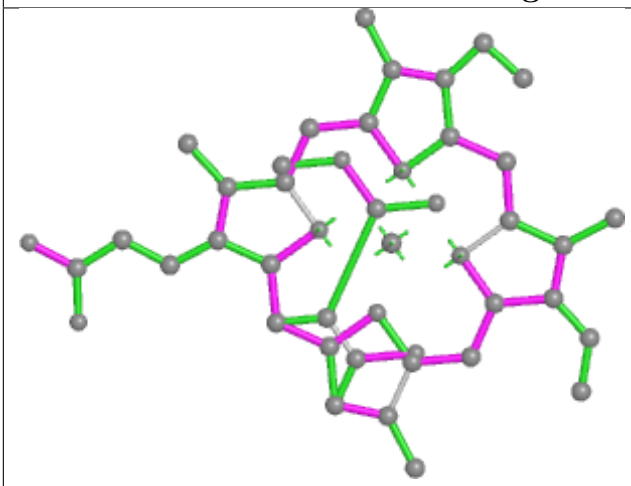


Rings

Ligand CLA U 307	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand KC1 M 313



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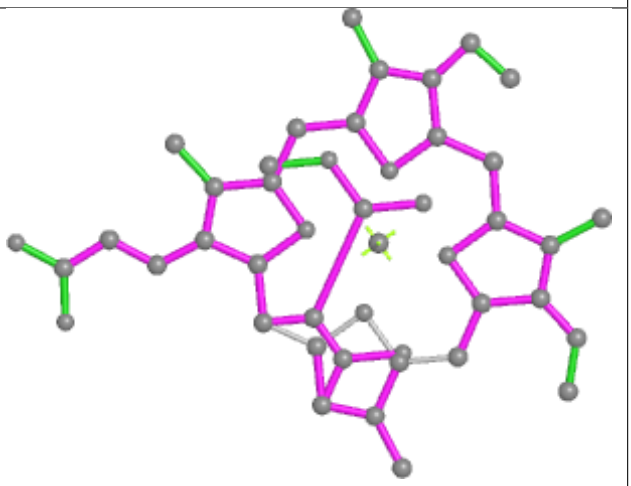
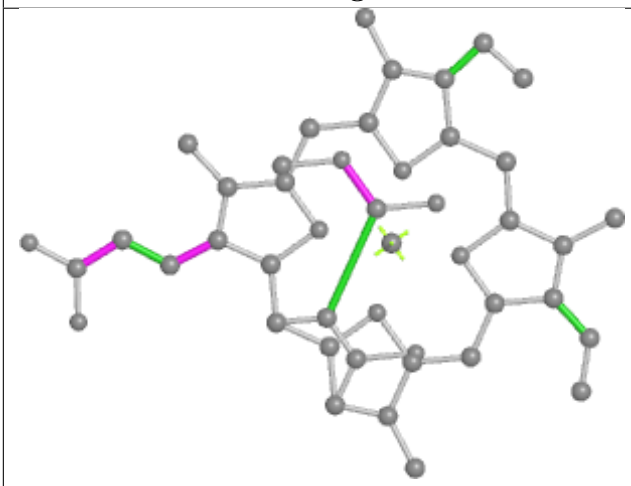


Bond angles



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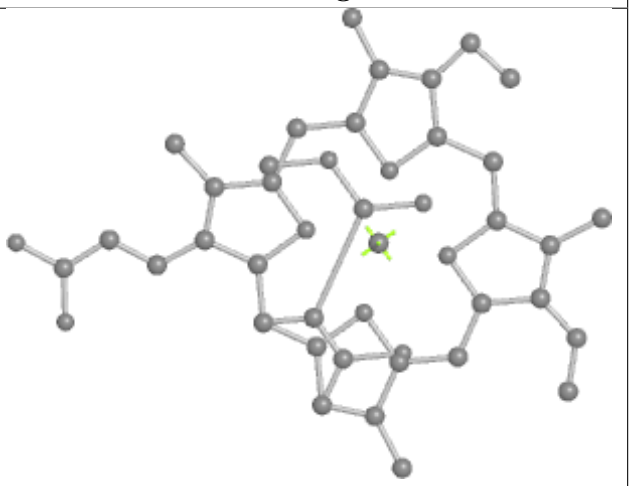
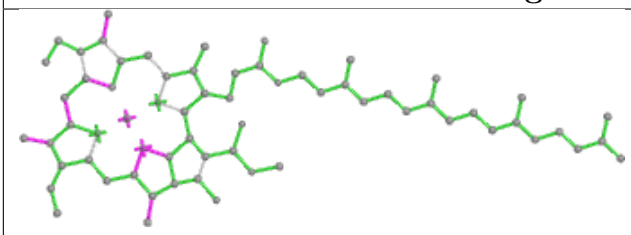


Rings

Ligand CLA P 309



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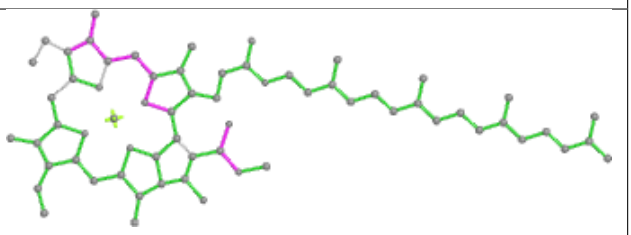
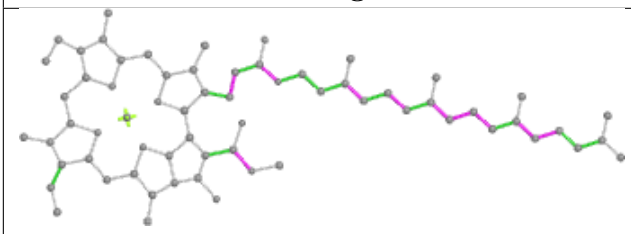


Bond angles



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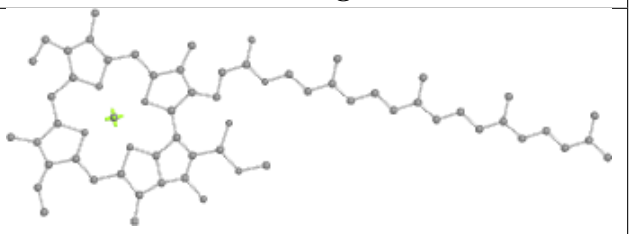
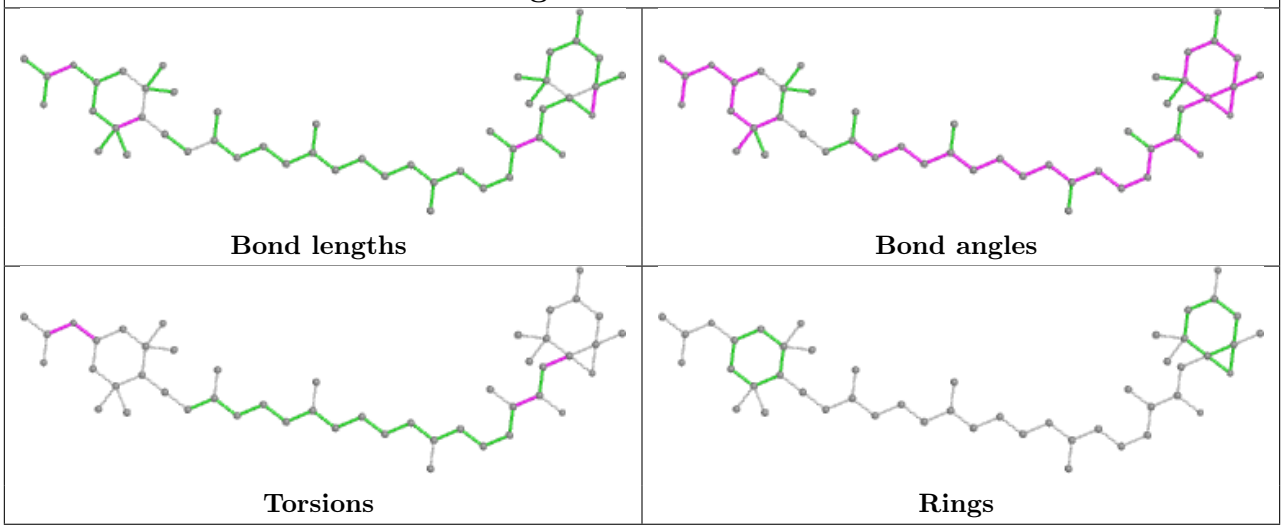
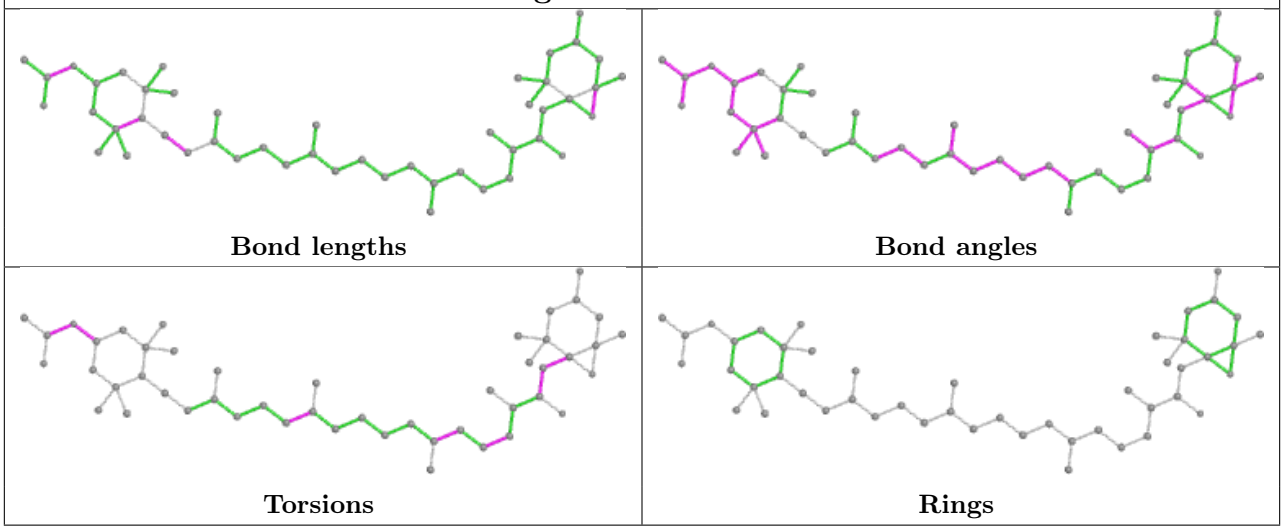


Rings

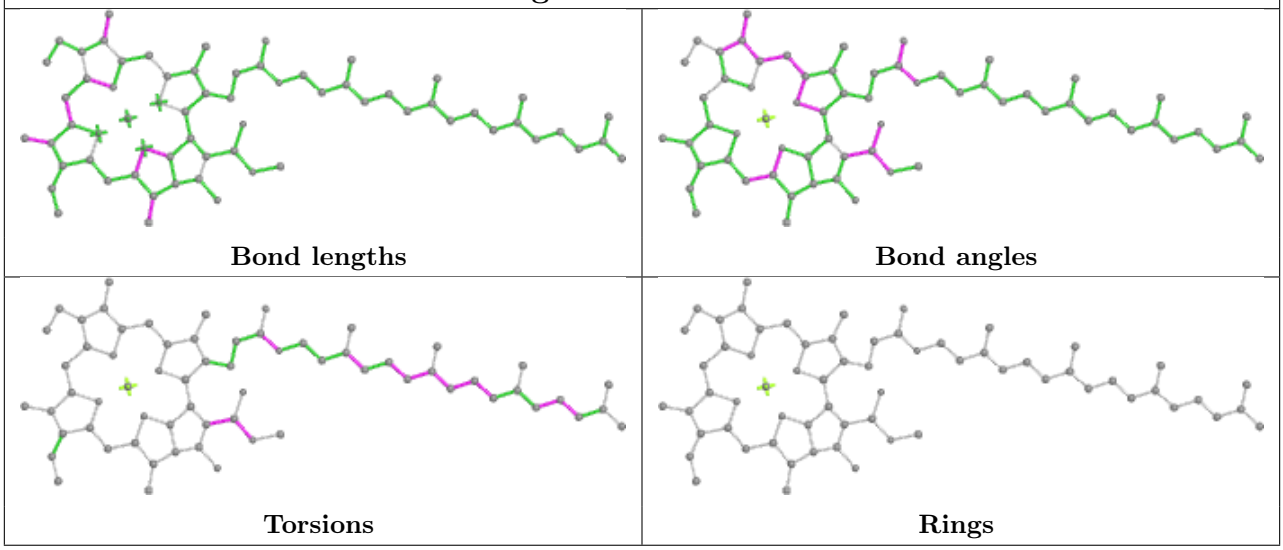
Ligand A86 N 301

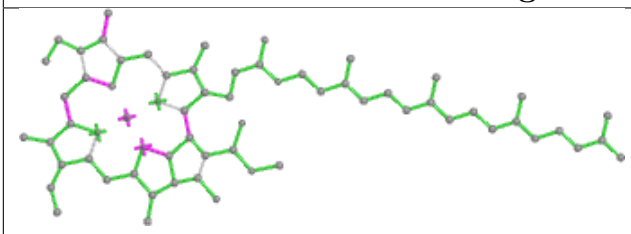
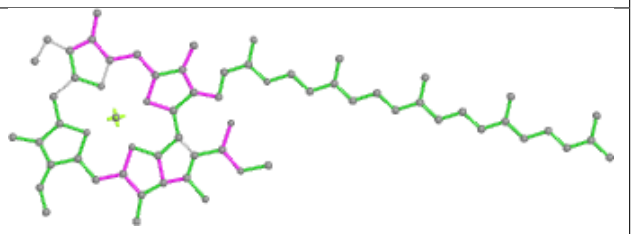
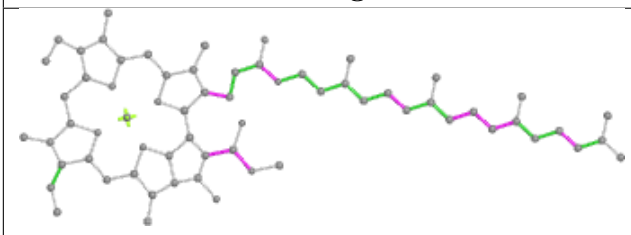
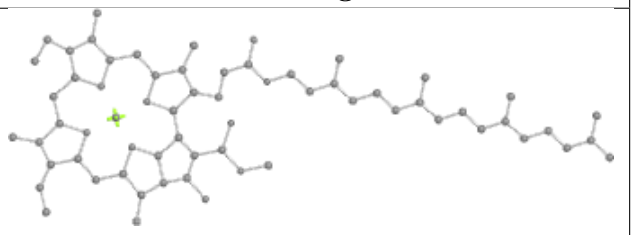


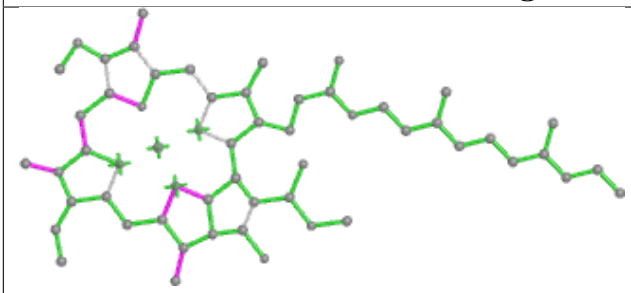
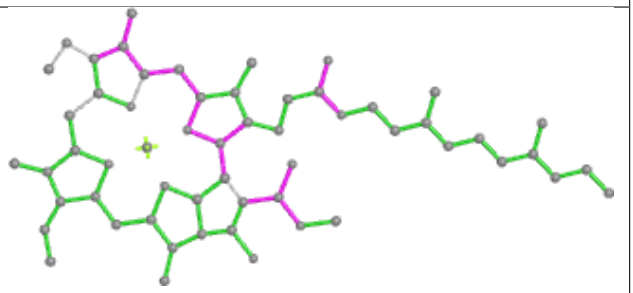
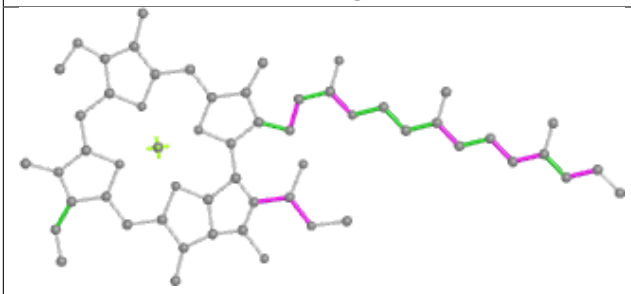
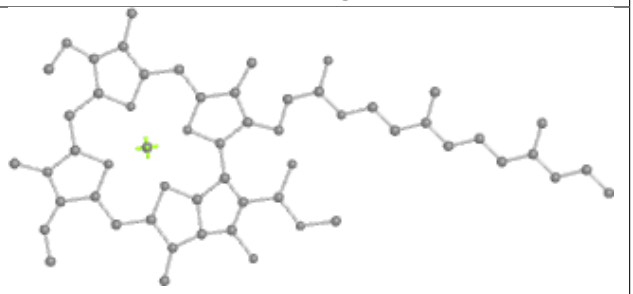
Ligand A86 S 304

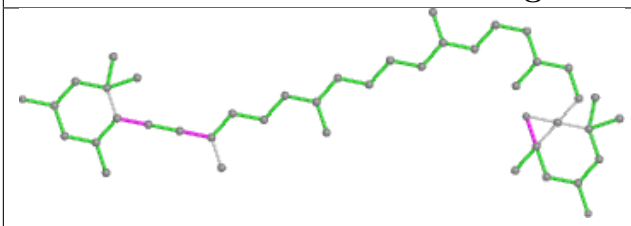
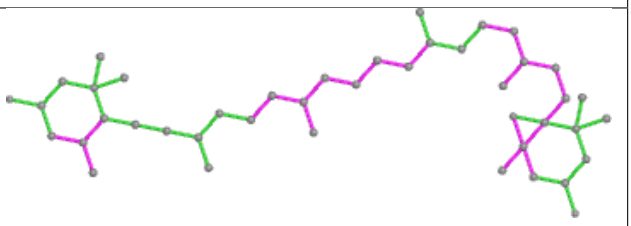
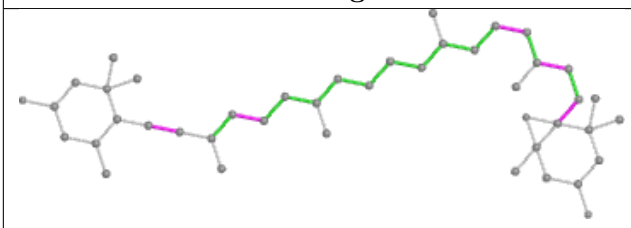
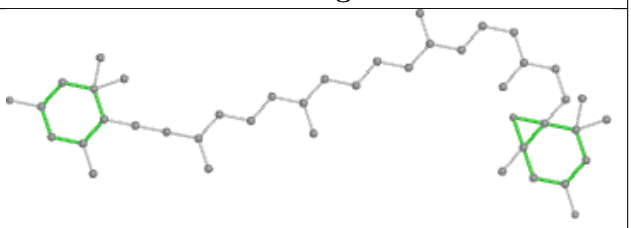


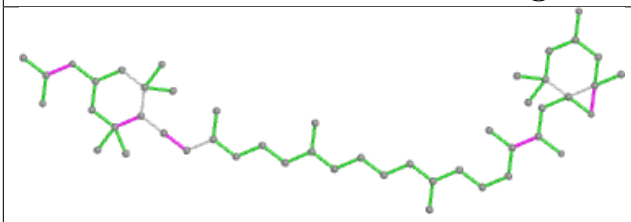
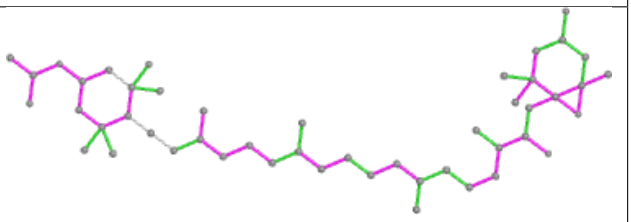
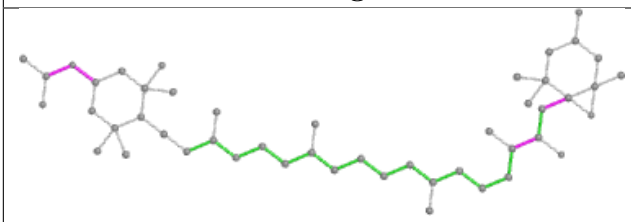
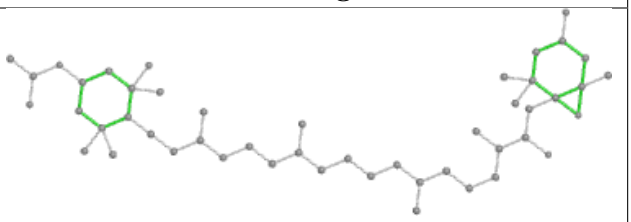
Ligand CLA I 311

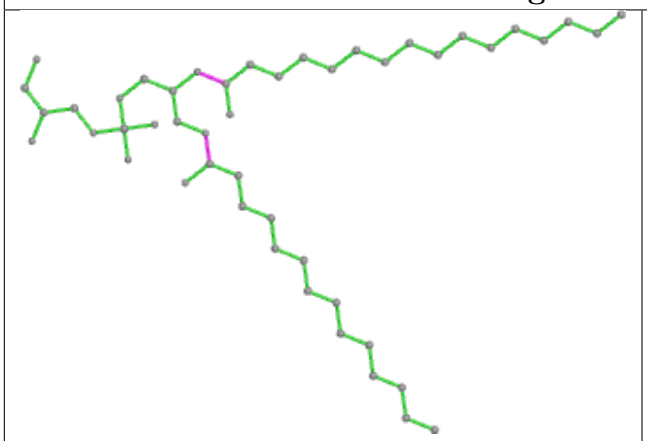
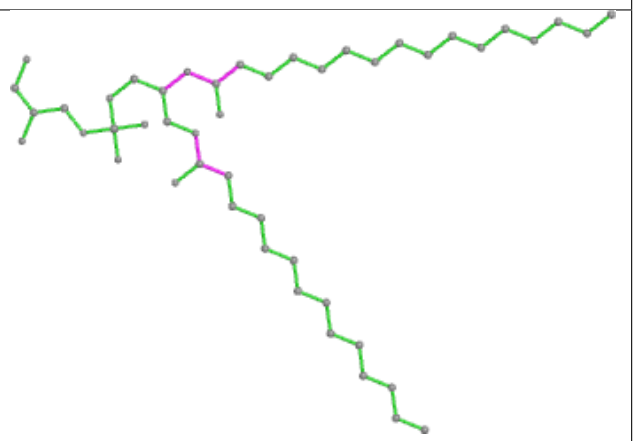
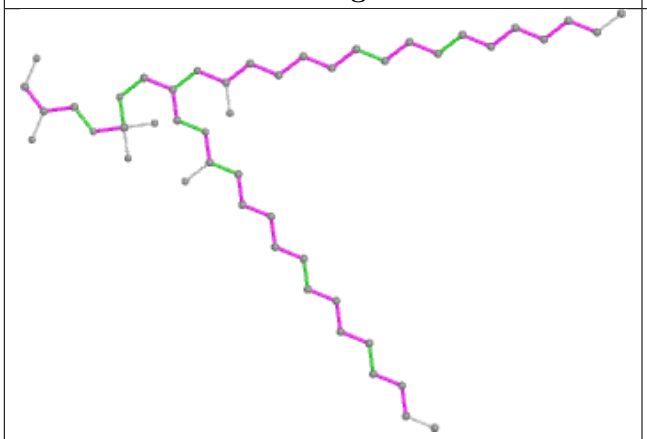
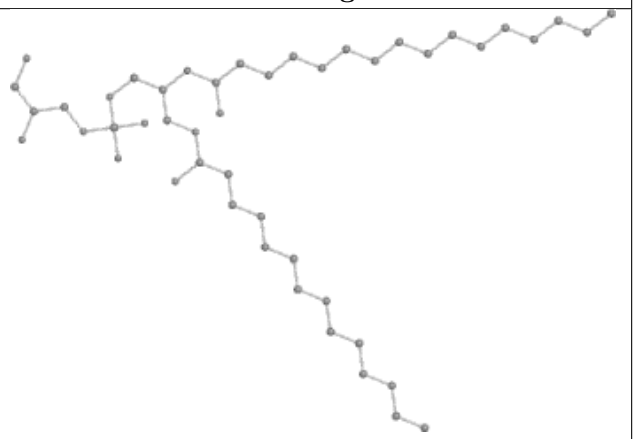


Ligand CLA W 212	
 Bond lengths	 Bond angles
 Torsions	 Rings

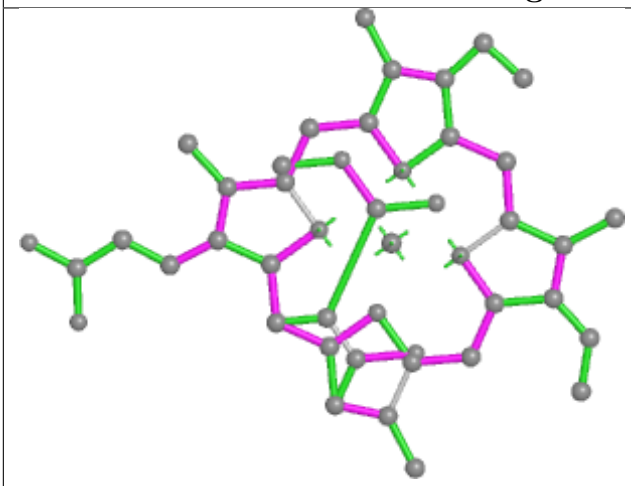
Ligand CLA W 209	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand DD6 A 301	
 Bond lengths	 Bond angles
 Torsions	 Rings

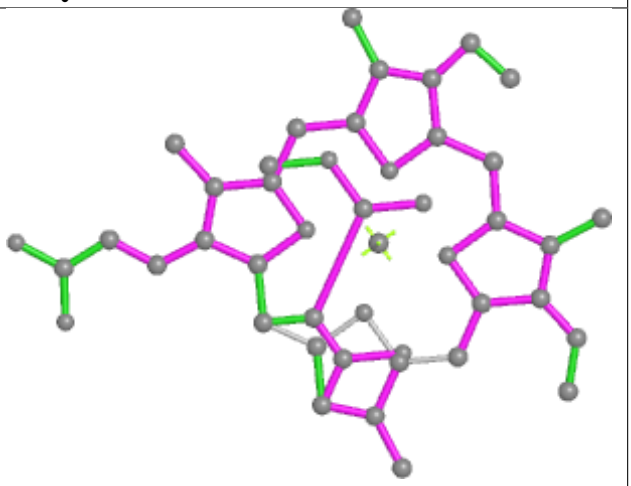
Ligand A86 C 202	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand LHG a 850	
 Bond lengths	 Bond angles
 Torsions	 Rings

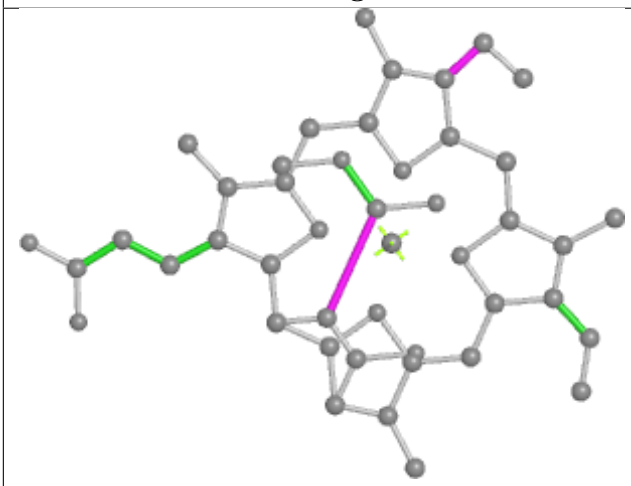
Ligand KC1 Q 311



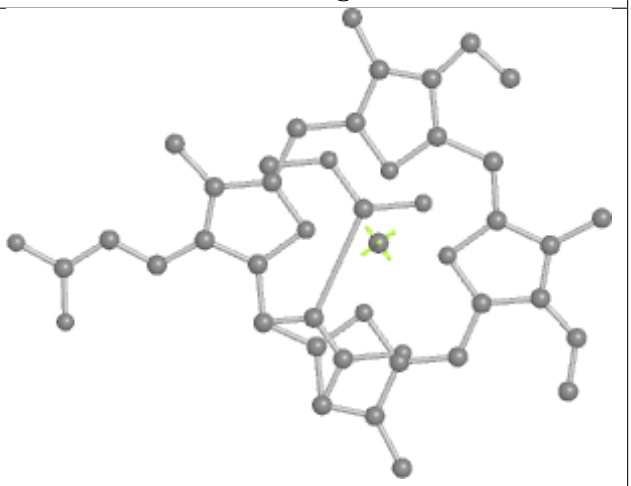
Bond lengths



Bond angles

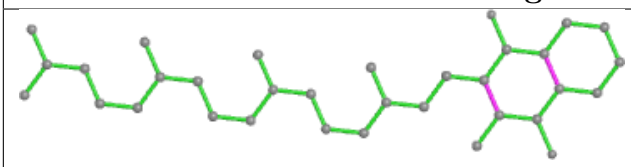


Torsions

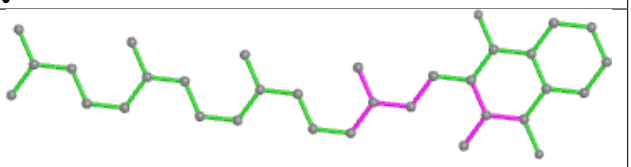


Rings

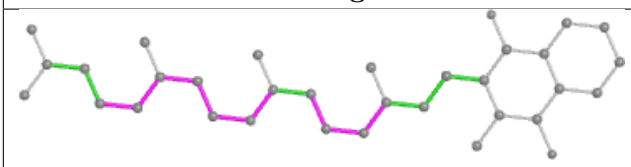
Ligand PQN b 842



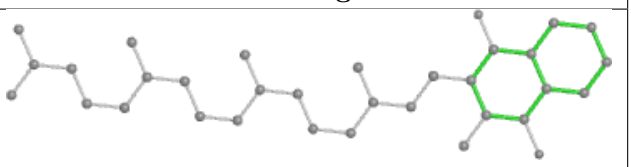
Bond lengths



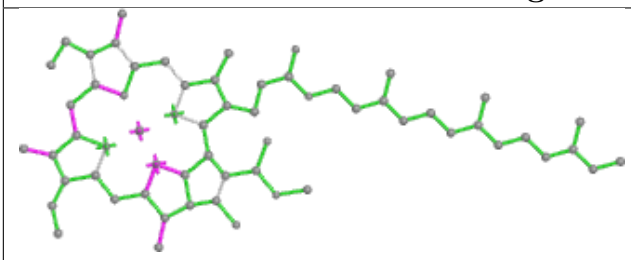
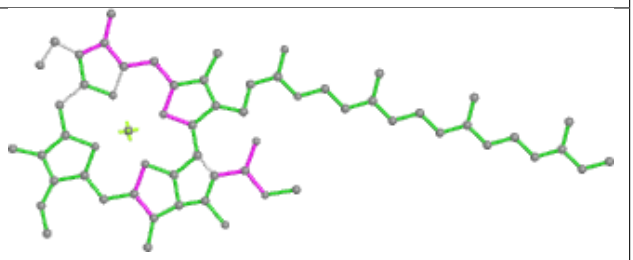
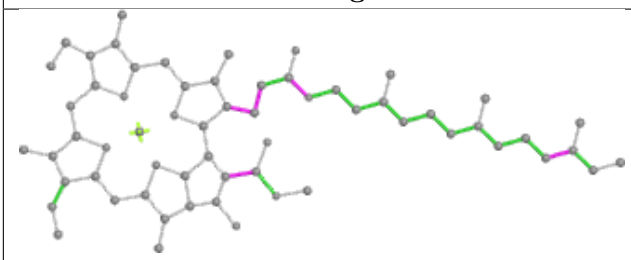
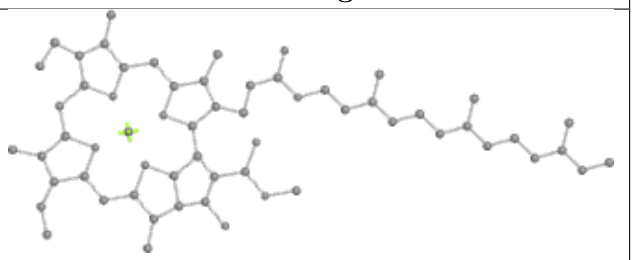
Bond angles

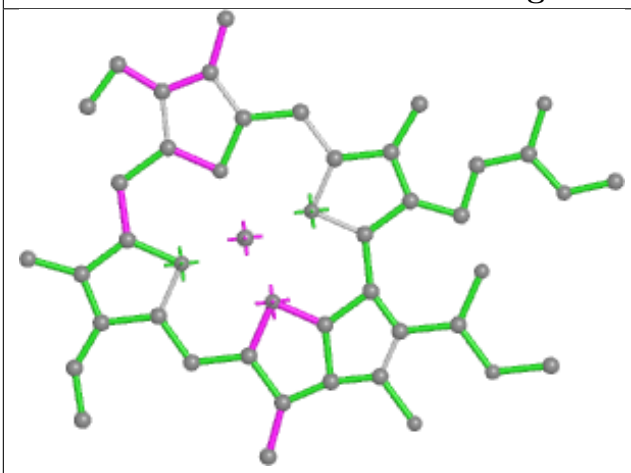
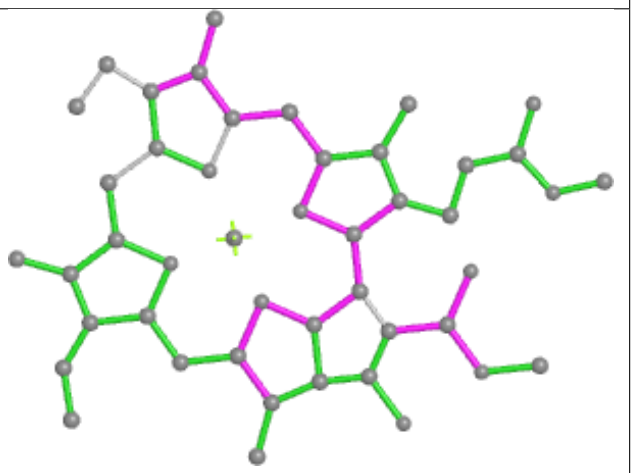
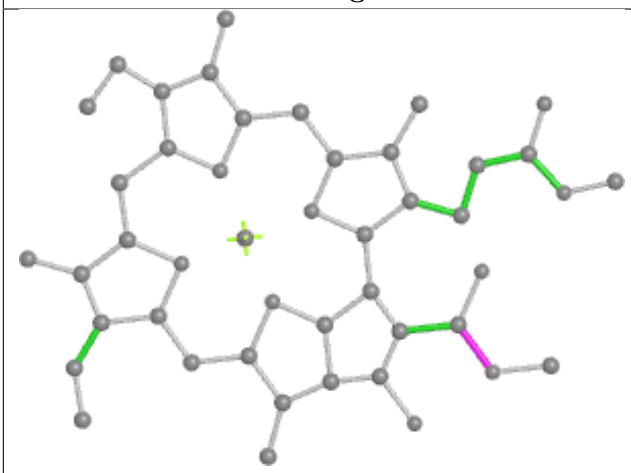
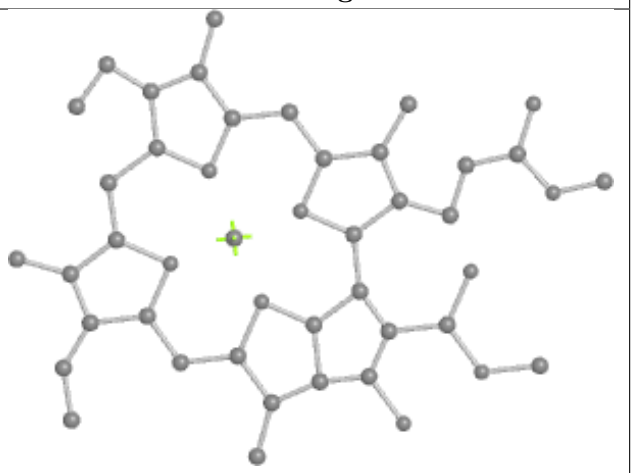


Torsions

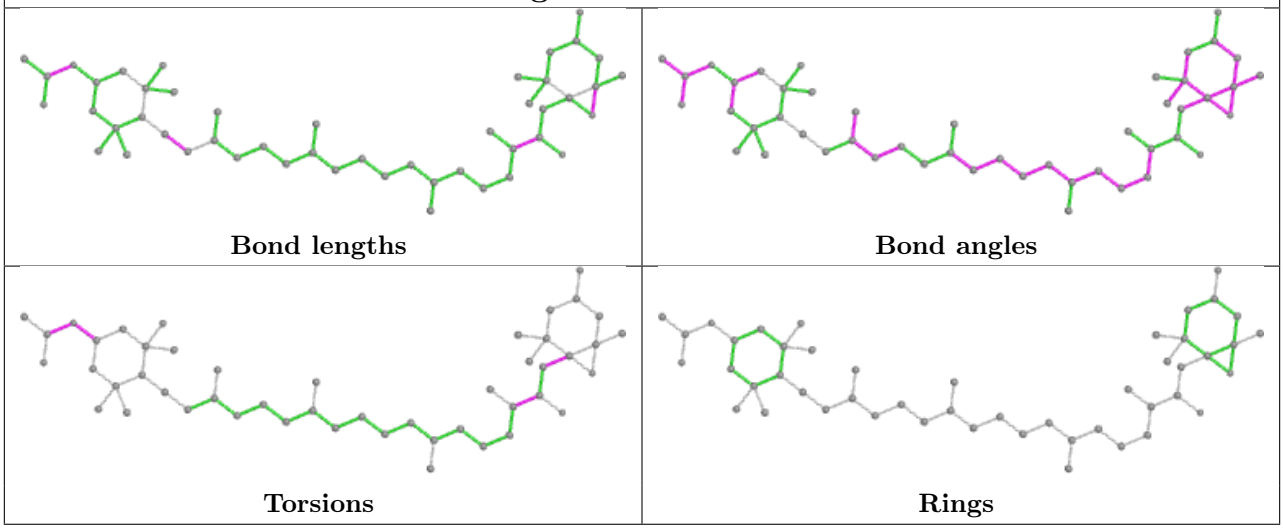


Rings

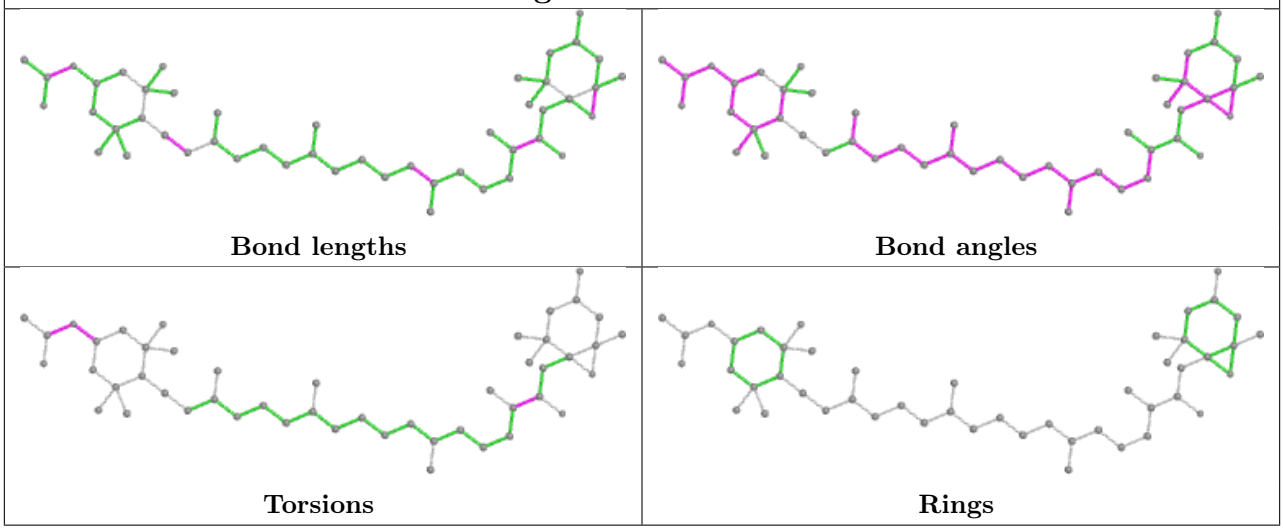
Ligand CLA S 309	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA S 311	
 Bond lengths	 Bond angles
 Torsions	 Rings

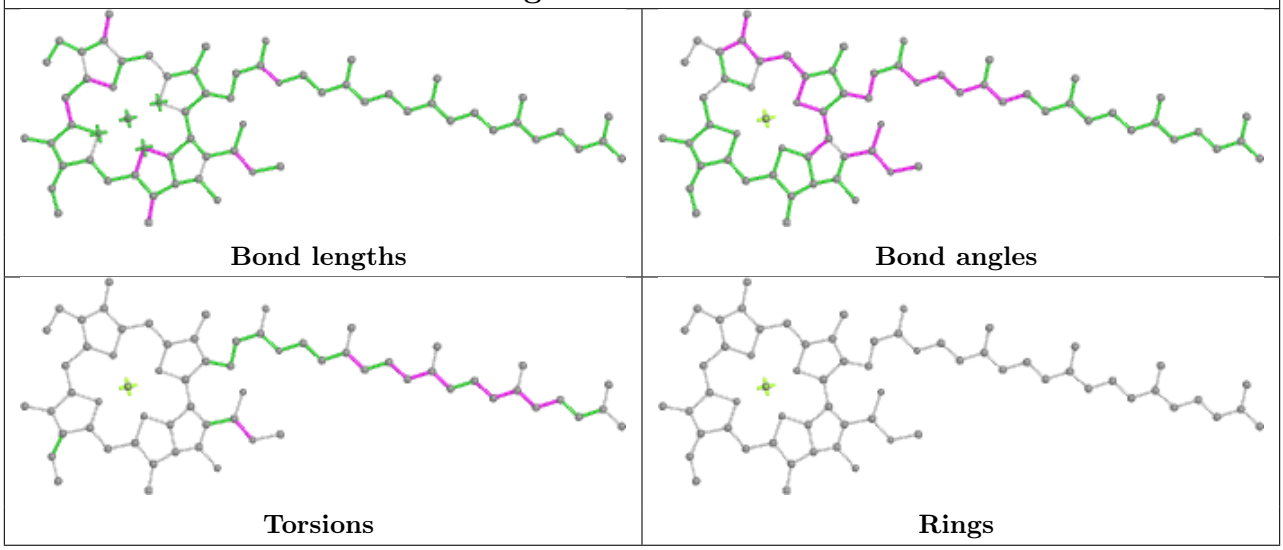
Ligand A86 R 309



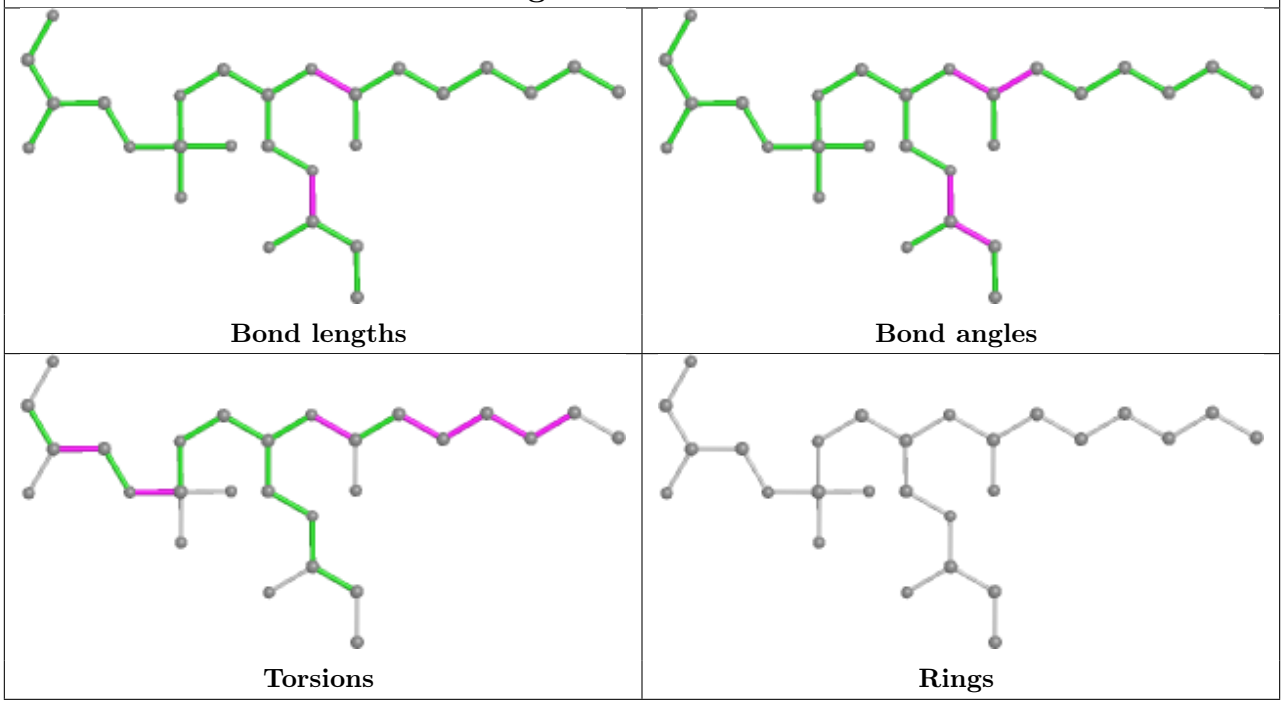
Ligand A86 S 303



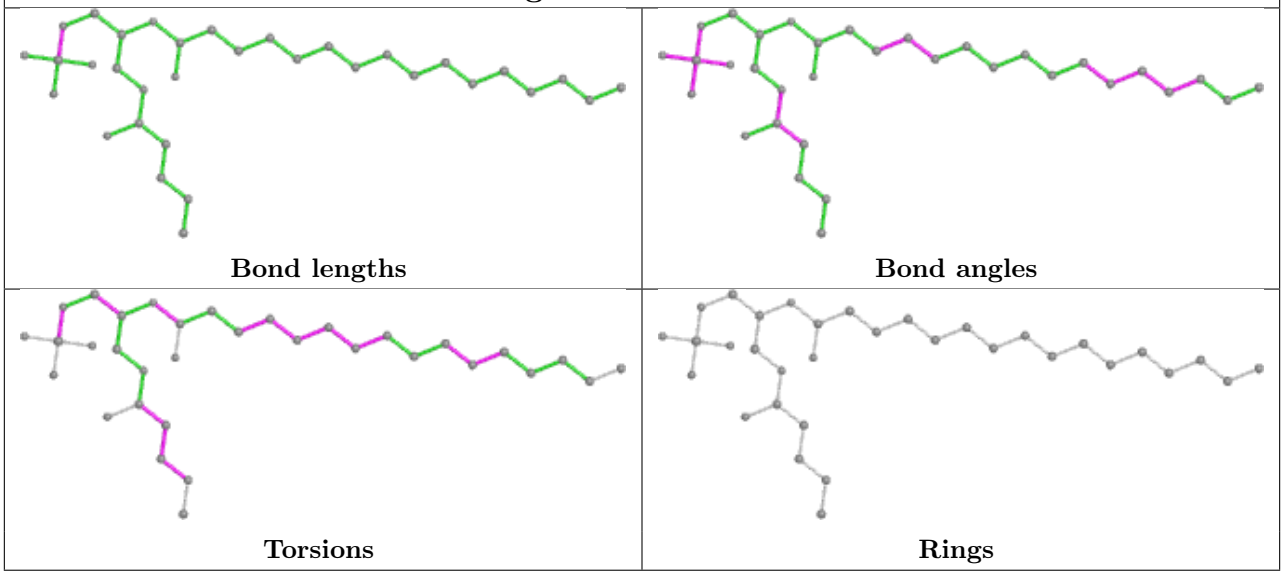
Ligand CLA G 309



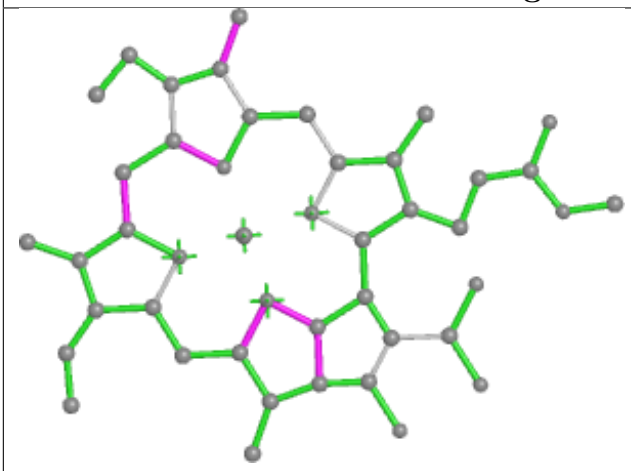
Ligand LHG a 843



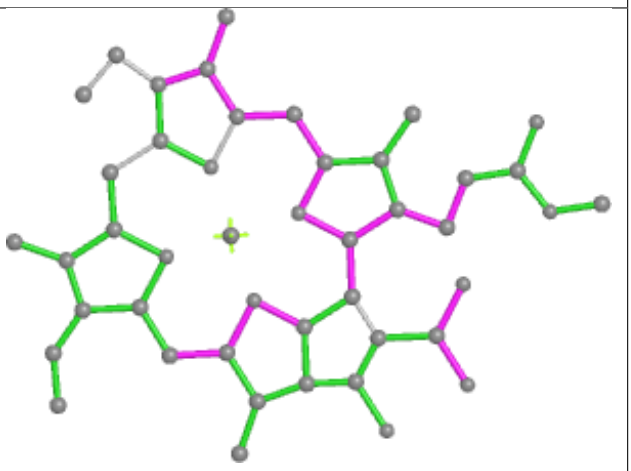
Ligand LHG F 318



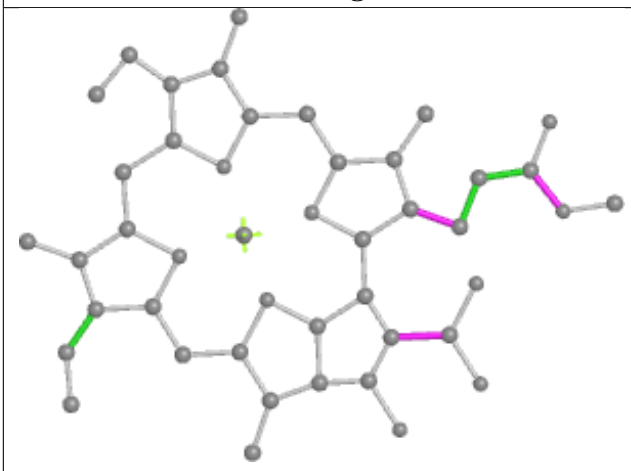
Ligand CLA X 309



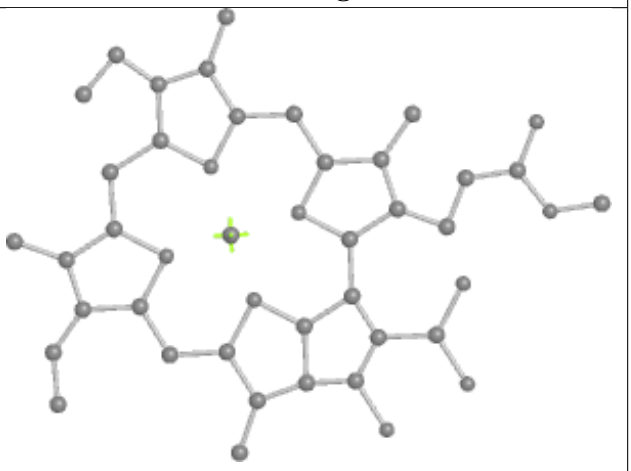
Bond lengths



Bond angles

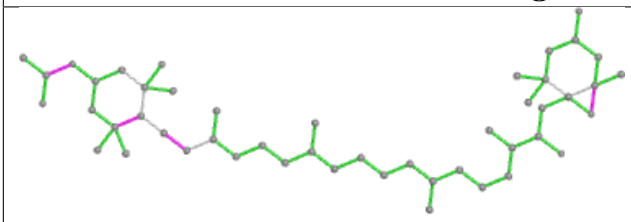


Torsions

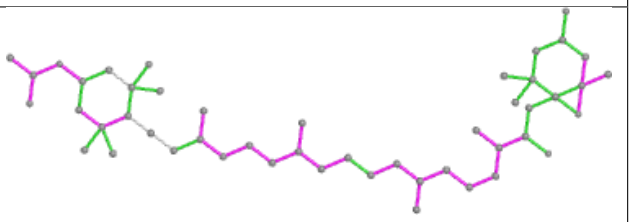


Rings

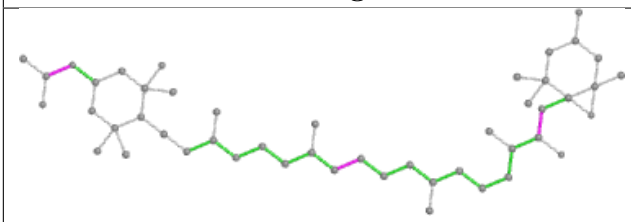
Ligand A86 T 301



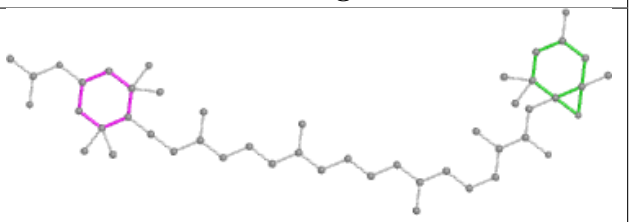
Bond lengths



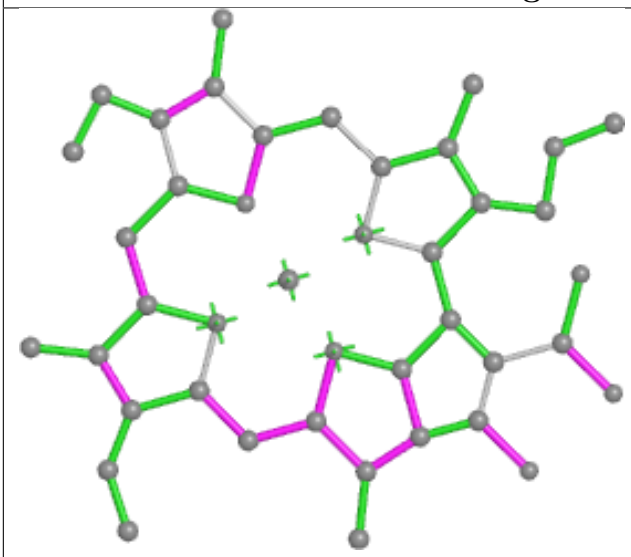
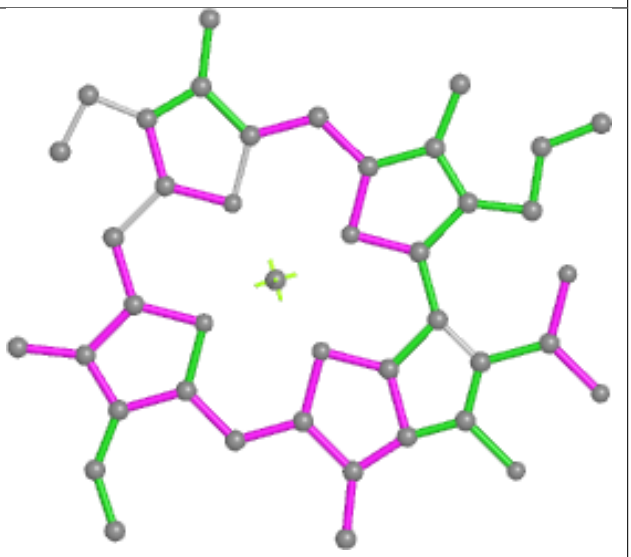
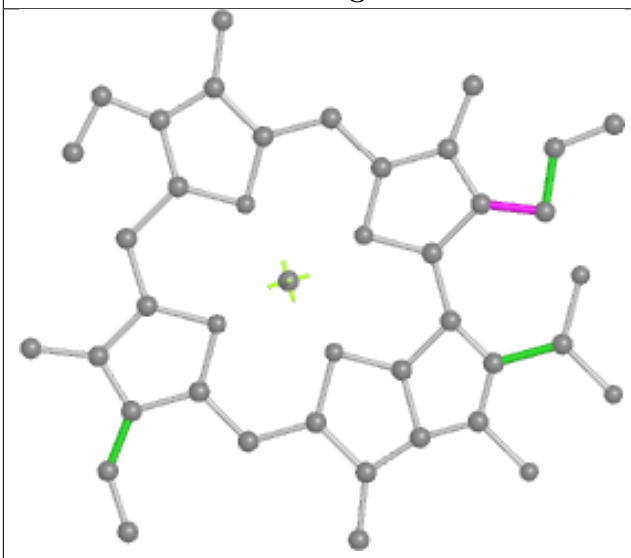
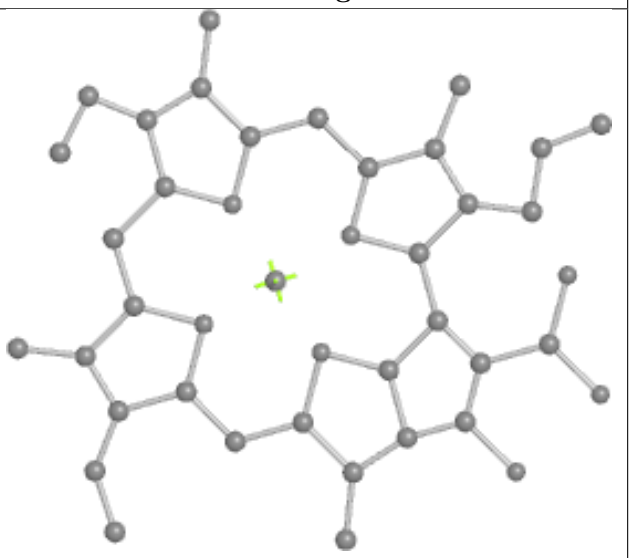
Bond angles



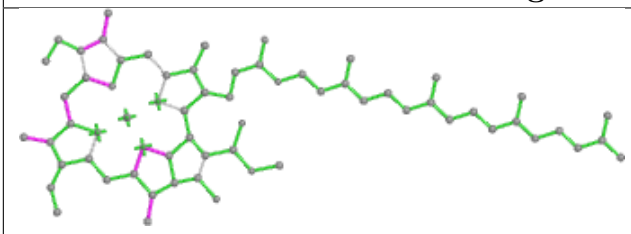
Torsions



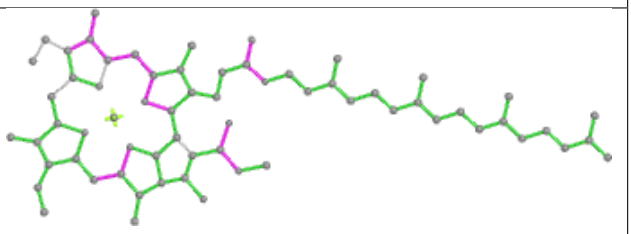
Rings

Ligand CLA G 307	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

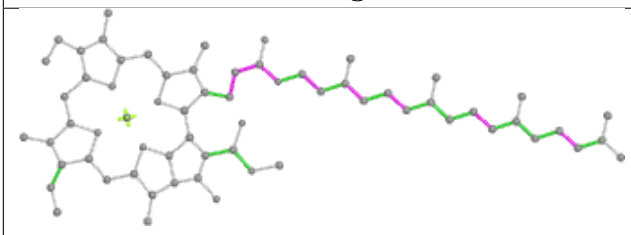
Ligand CLA b 834



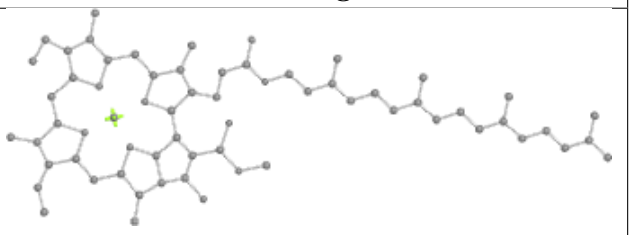
Bond lengths



Bond angles

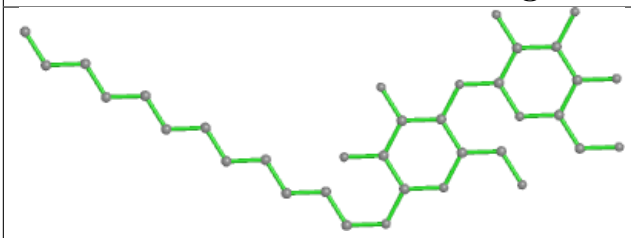


Torsions

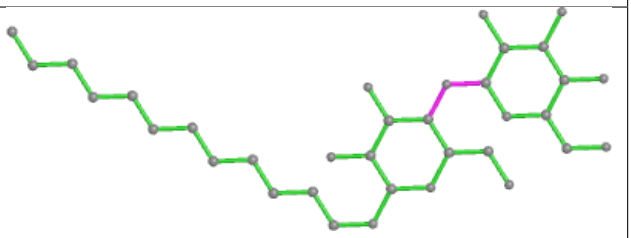


Rings

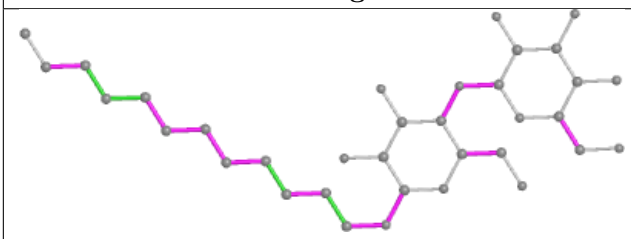
Ligand LMT B 313



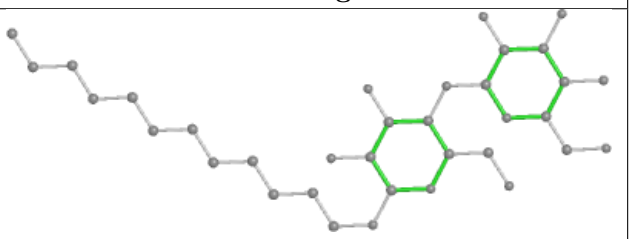
Bond lengths



Bond angles

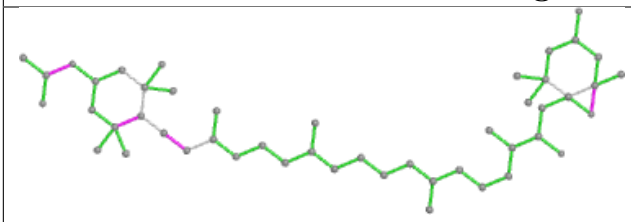


Torsions

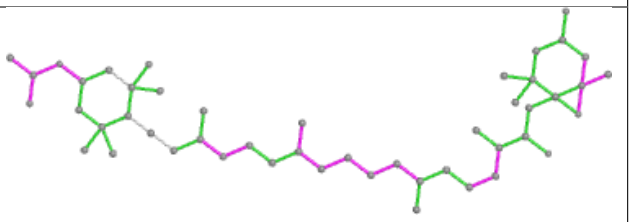


Rings

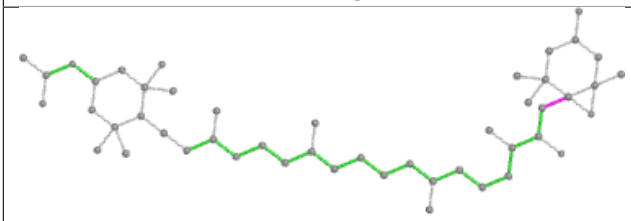
Ligand A86 h 204



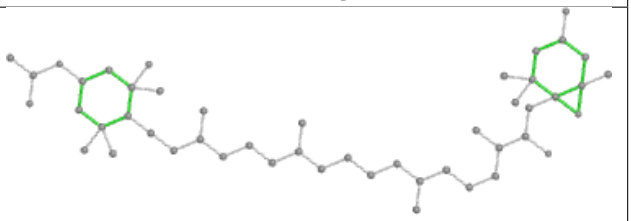
Bond lengths



Bond angles

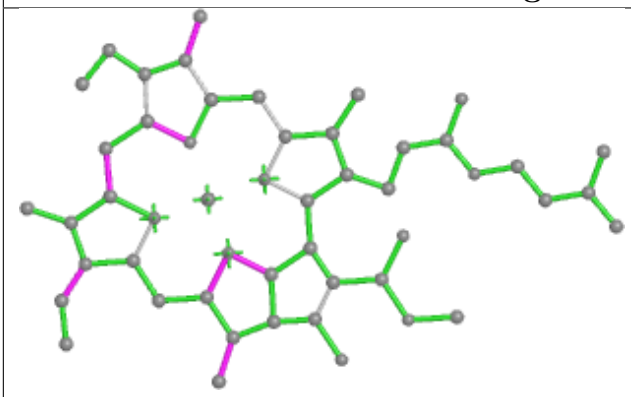


Torsions

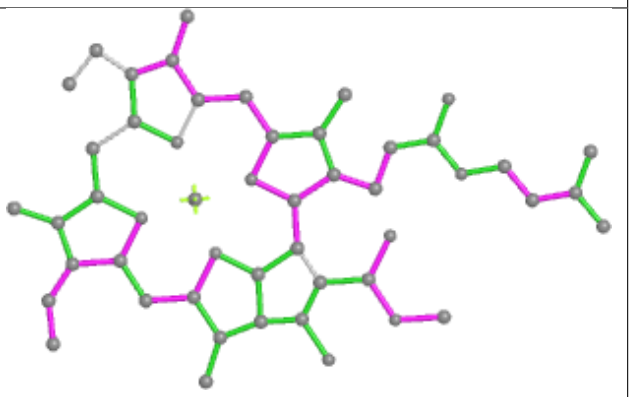


Rings

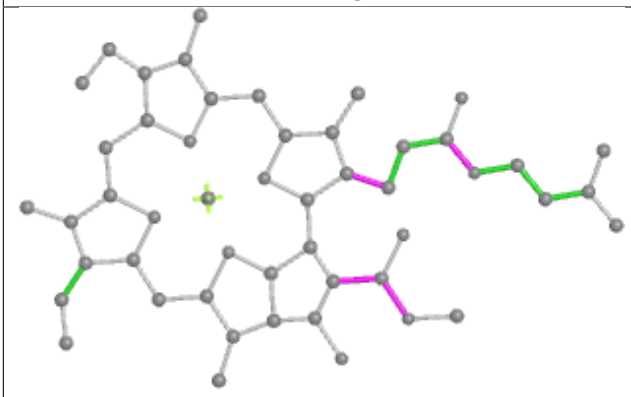
Ligand CLA X 307



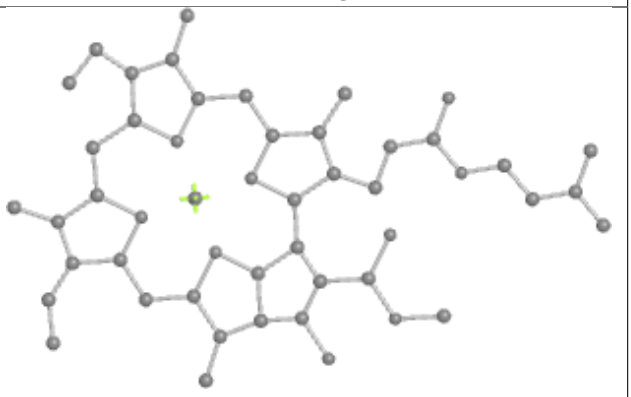
Bond lengths



Bond angles

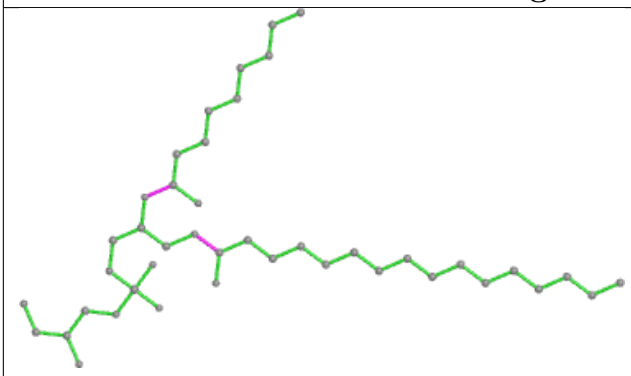


Torsions

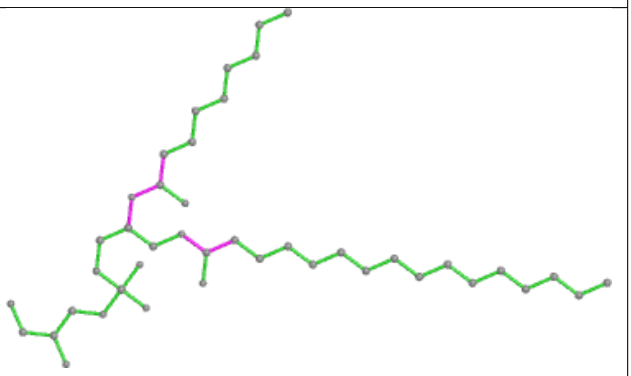


Rings

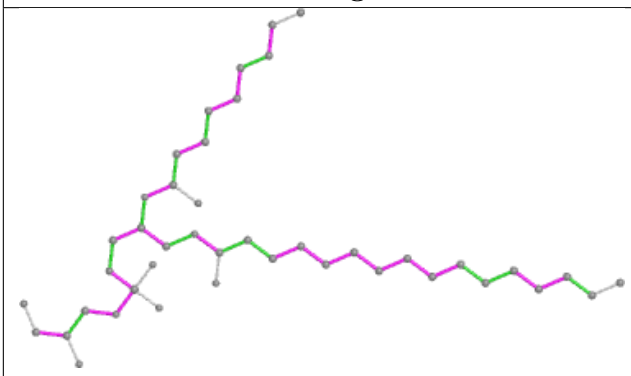
Ligand LHG f 809



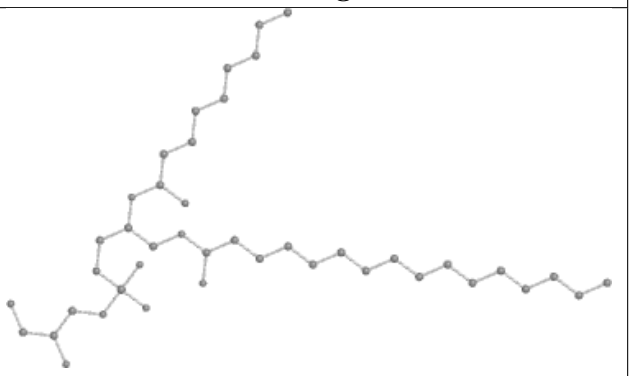
Bond lengths



Bond angles

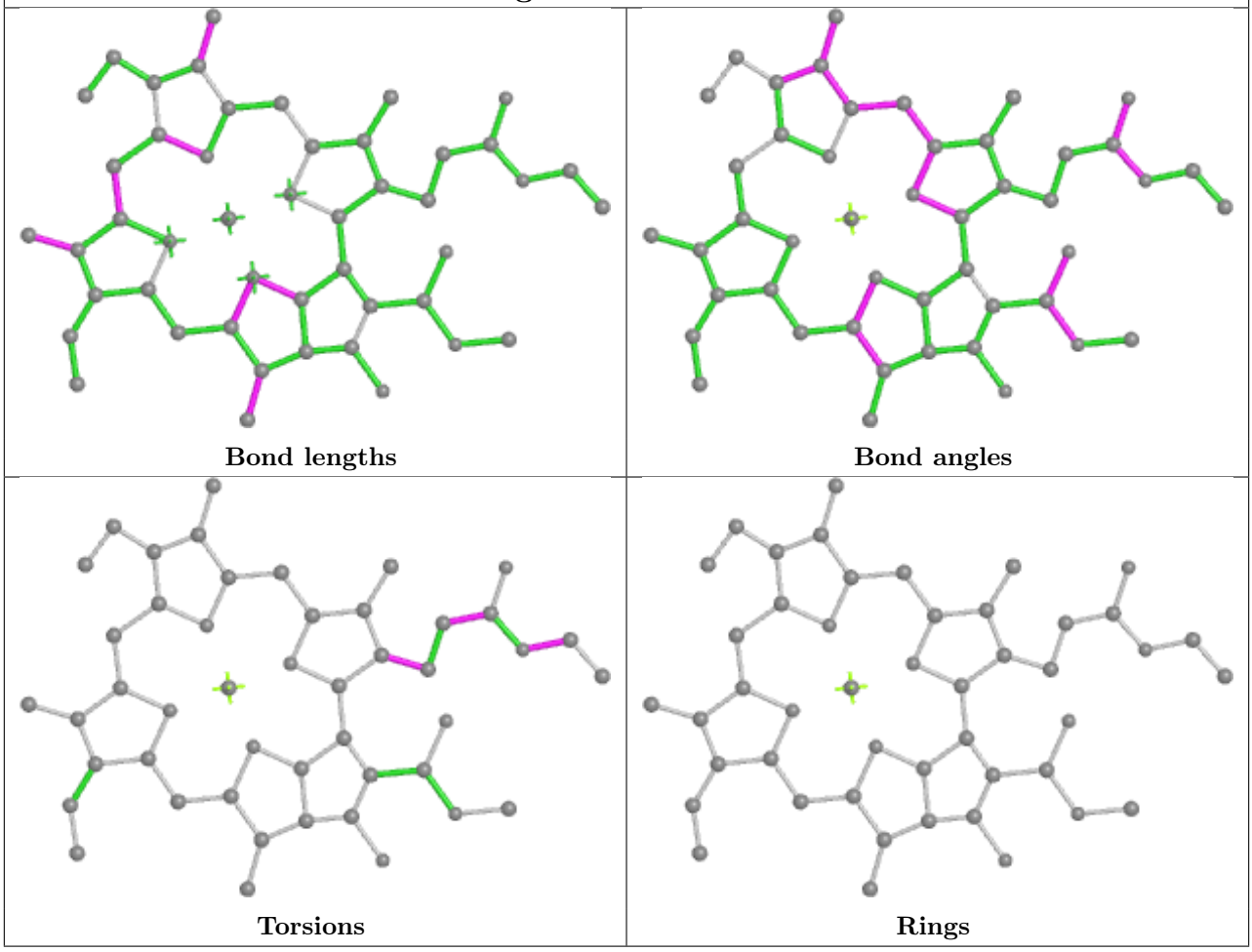


Torsions

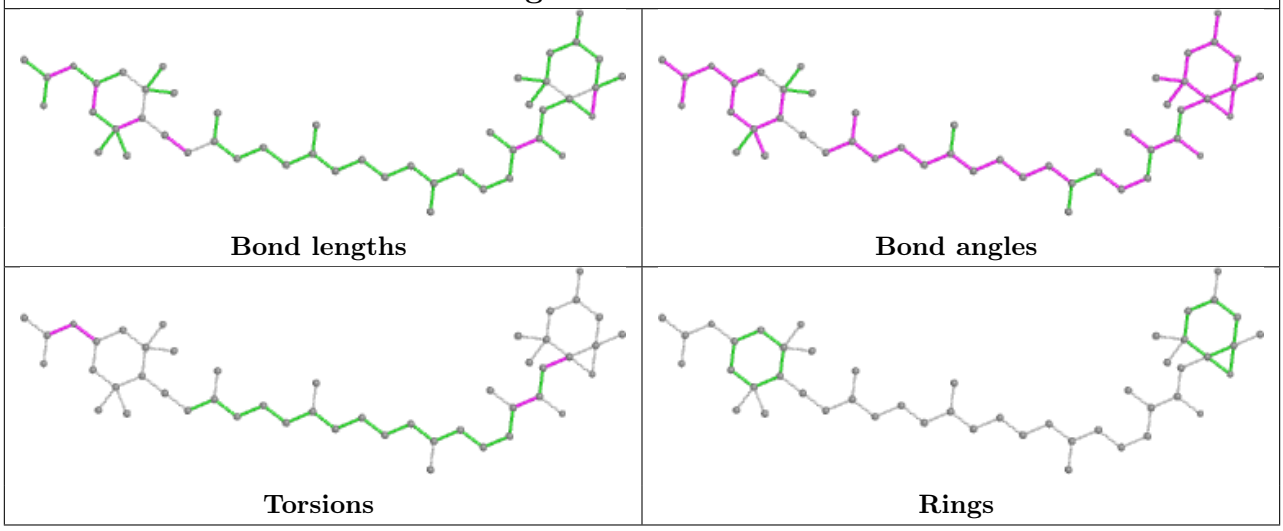


Rings

Ligand CLA b 838



Ligand A86 W 202



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Map visualisation (i)

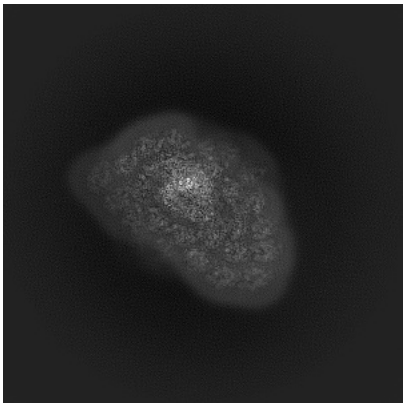
This section contains visualisations of the EMDB entry EMD-30012. These allow visual inspection of the internal detail of the map and identification of artifacts.

No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

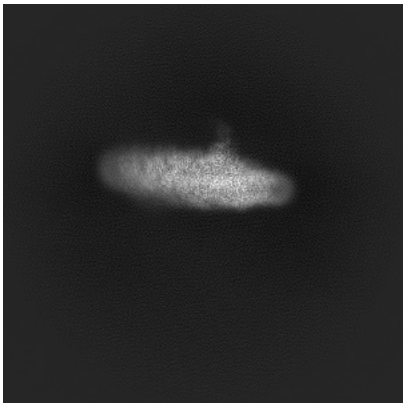
6.1 Orthogonal projections (i)

6.1.1 Primary map

X



Y

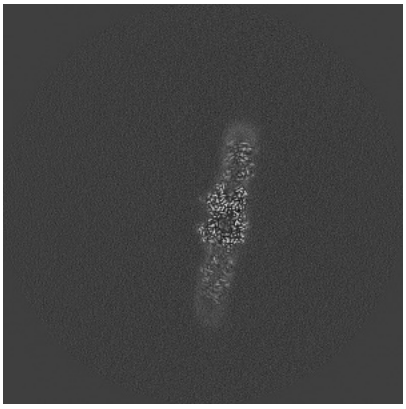


Z

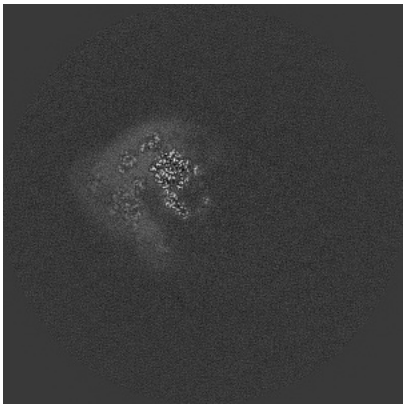
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

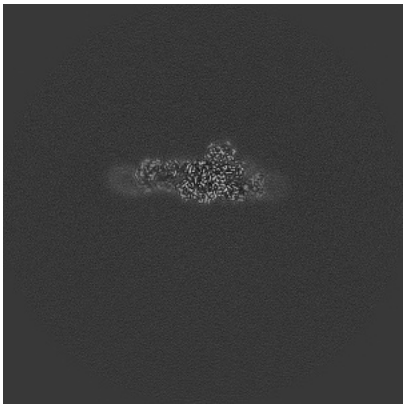
6.2.1 Primary map



X Index: 260



Y Index: 260

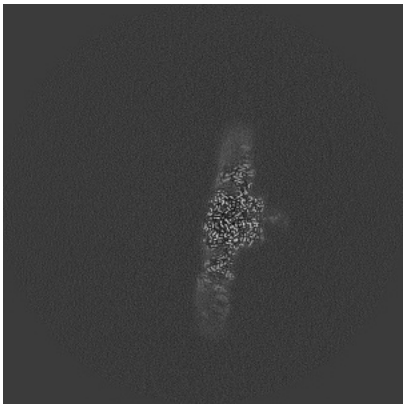


Z Index: 260

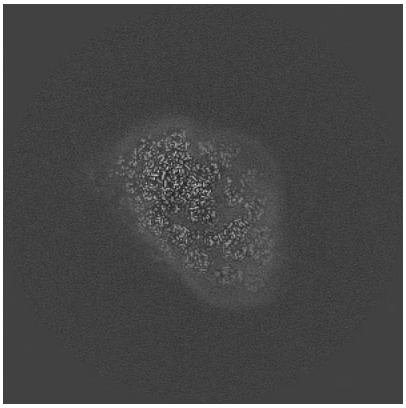
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

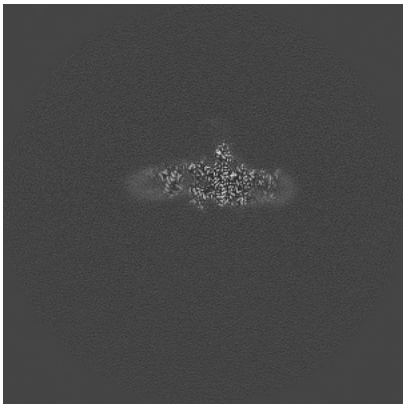
6.3.1 Primary map



X Index: 278



Y Index: 294

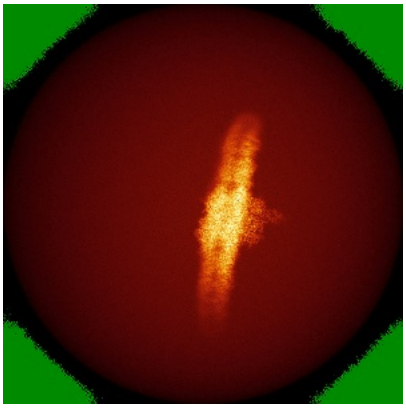


Z Index: 231

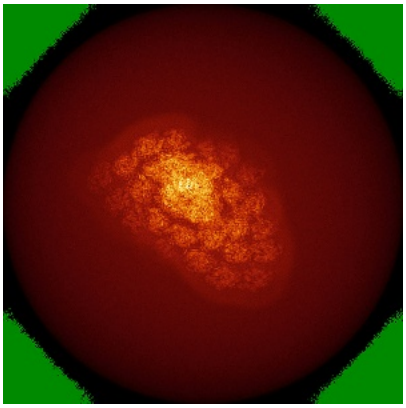
The images above show the largest variance slices of the map in three orthogonal directions.

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

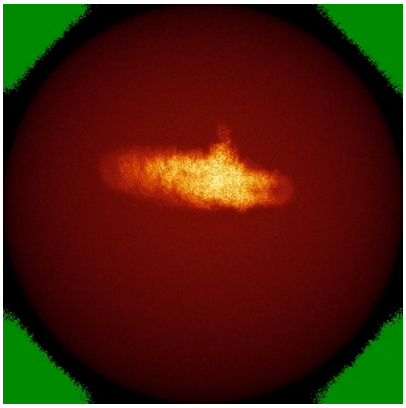
6.4.1 Primary map



X



Y



Z

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

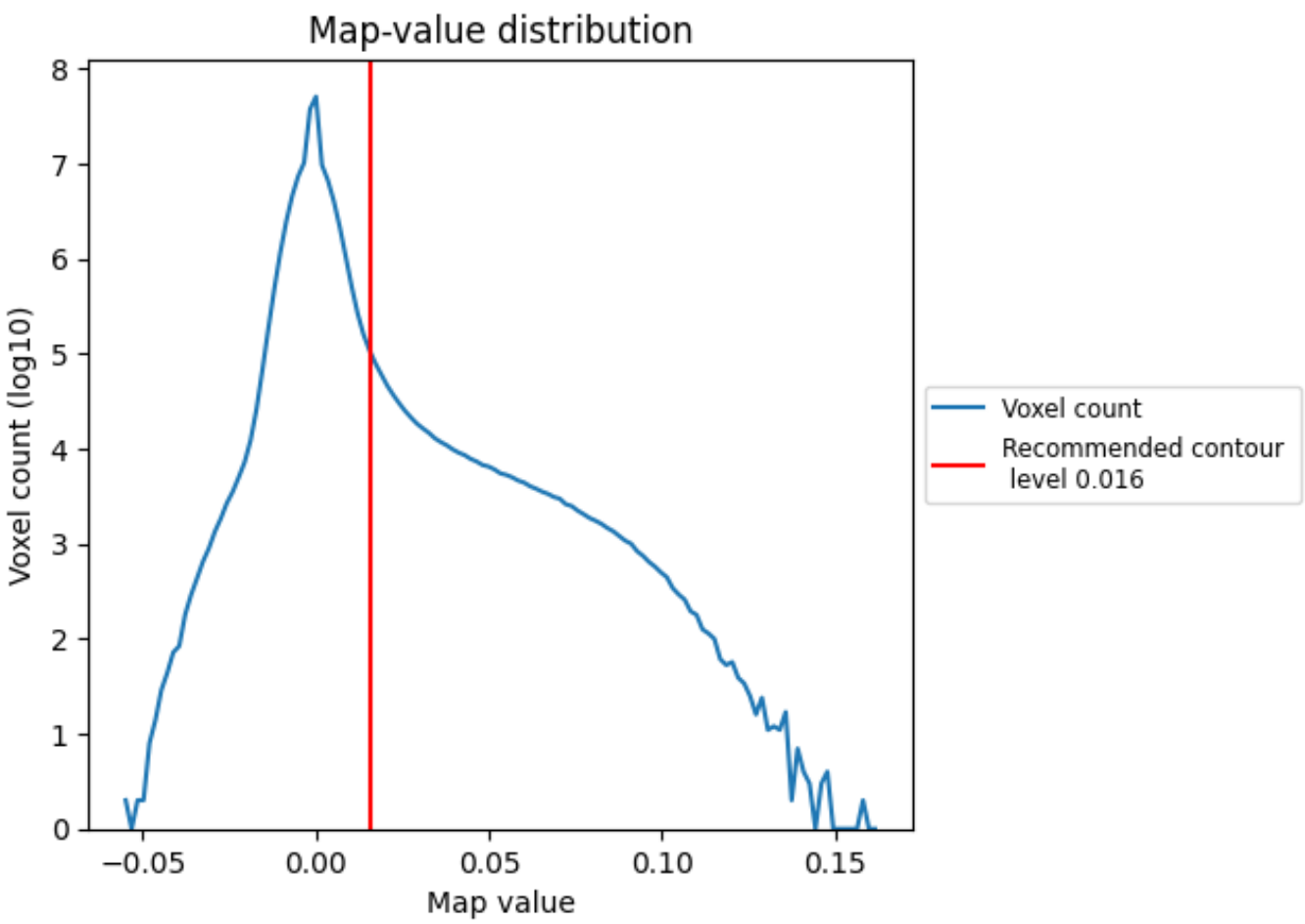
6.6 Mask visualisation (i)

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

7 Map analysis (i)

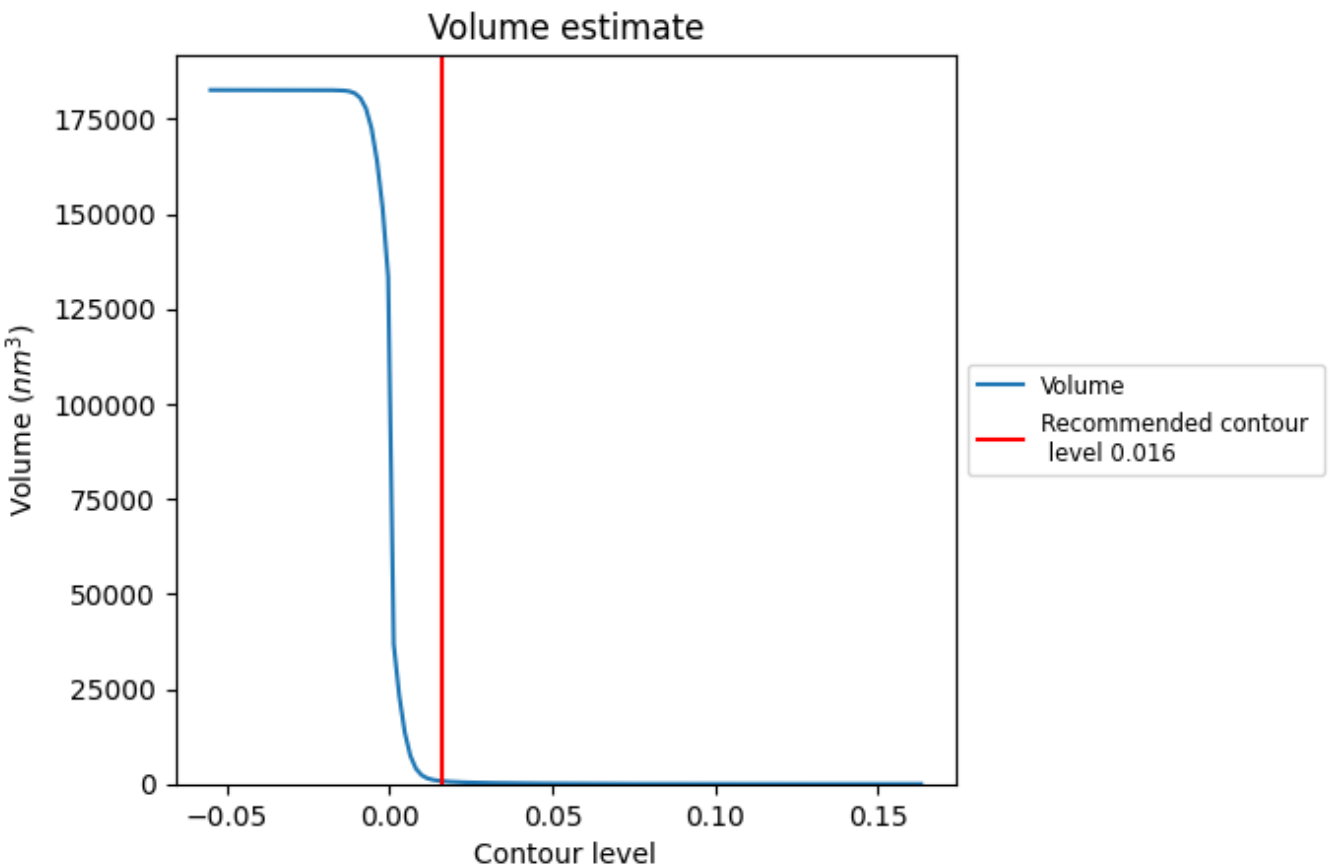
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)



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

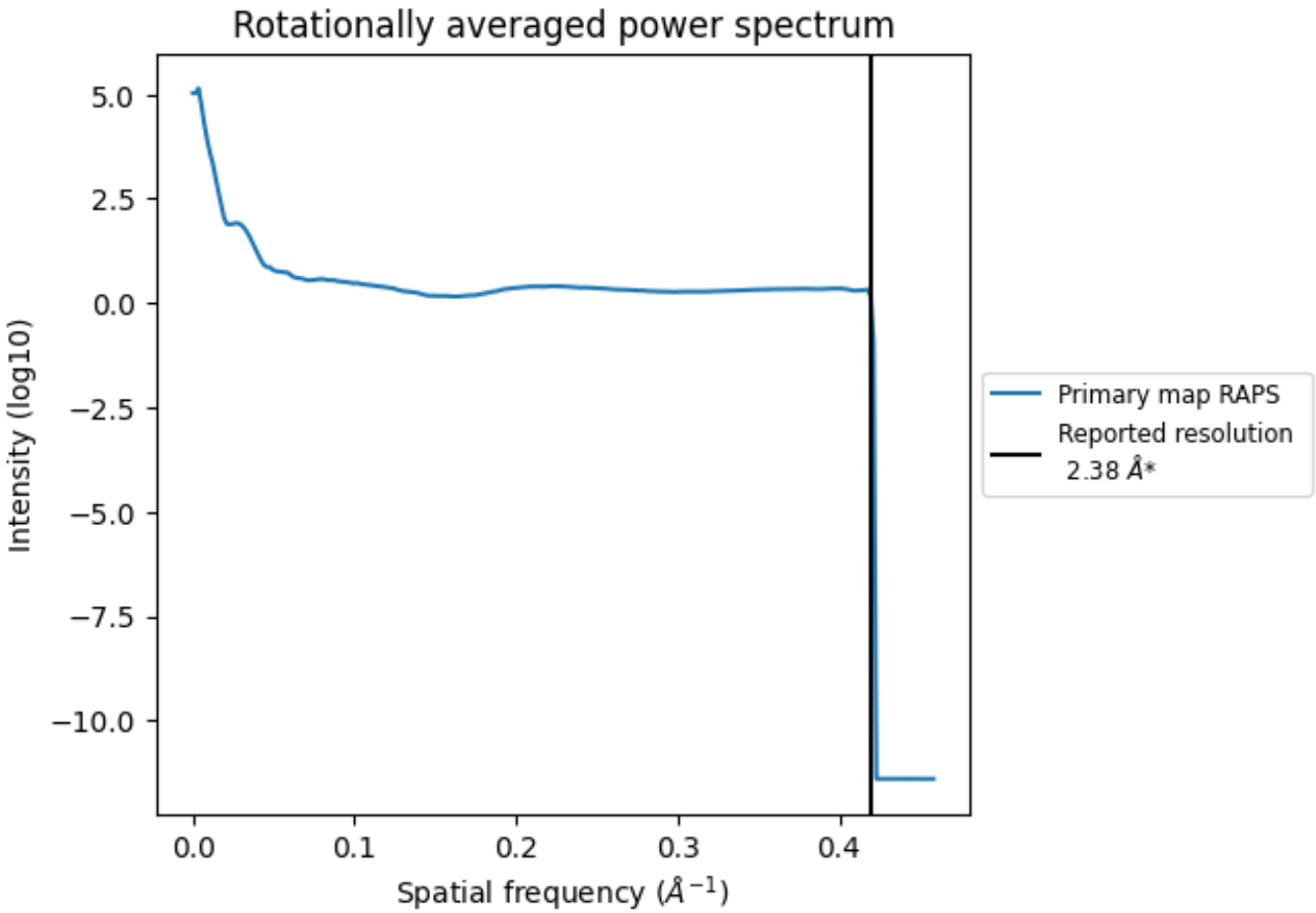
7.2 Volume estimate (i)



The volume at the recommended contour level is 778 nm^3; this corresponds to an approximate mass of 703 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 0.420 Å^{-1}

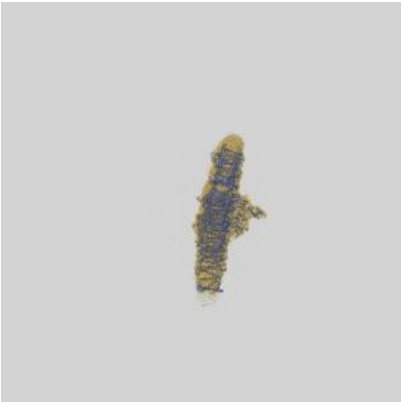
8 Fourier-Shell correlation (i)

This section was not generated. No FSC curve or half-maps provided.

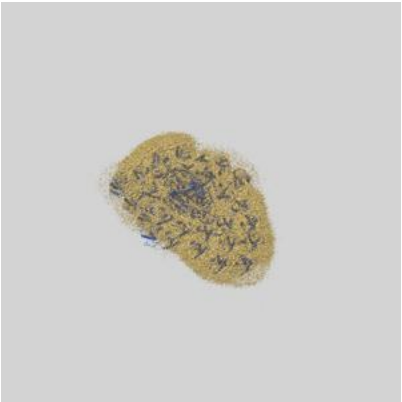
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-30012 and PDB model 6LY5. Per-residue inclusion information can be found in section 3 on page 52.

9.1 Map-model overlay (i)



X

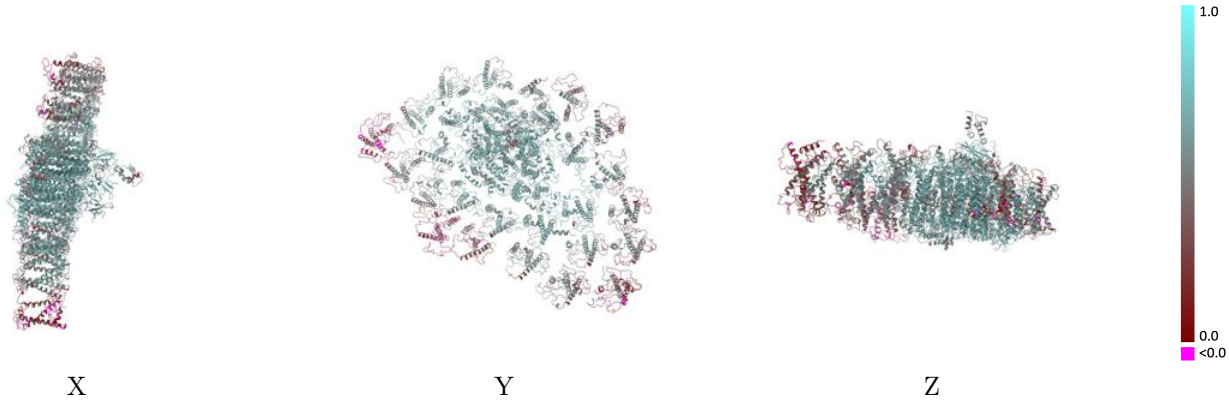


Y

Z

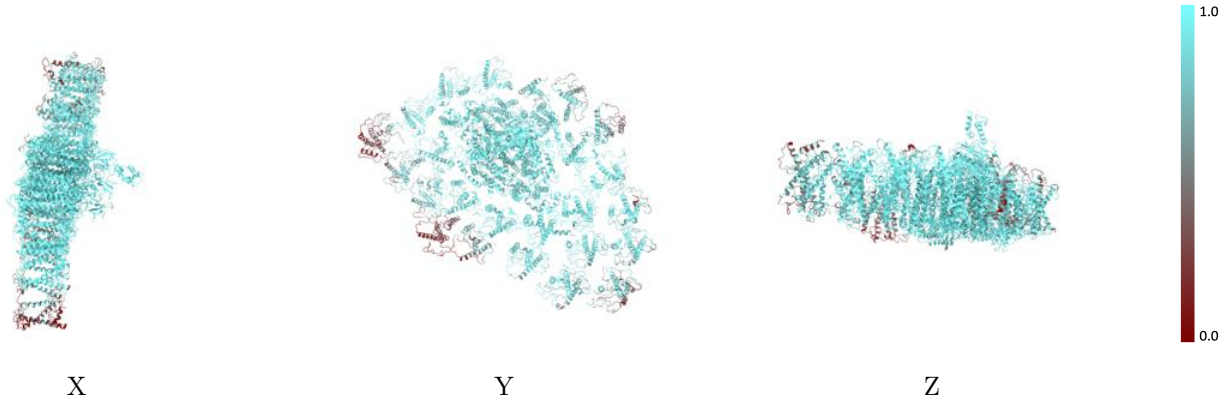
The images above show the 3D surface view of the map at the recommended contour level 0.016 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model (i)



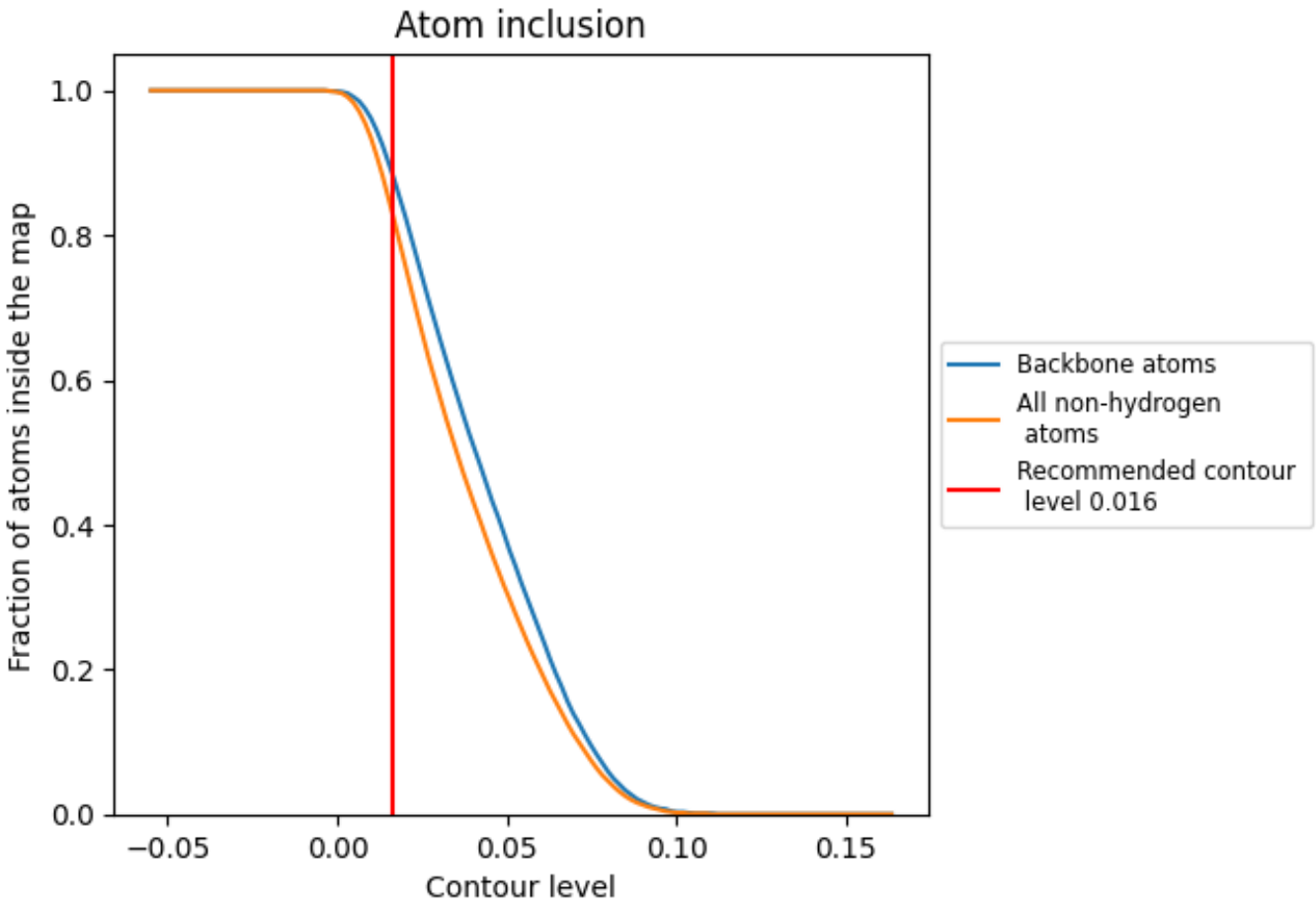
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

9.3 Atom inclusion mapped to coordinate model (i)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.016).

9.4 Atom inclusion (i)



At the recommended contour level, 89% of all backbone atoms, 84% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.016) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8350	0.5170
A	0.9410	0.5810
B	0.8370	0.4930
C	0.8980	0.5340
D	0.9340	0.5870
E	0.9530	0.6050
F	0.9430	0.5960
G	0.9570	0.6150
H	0.8900	0.5450
I	0.9240	0.5640
J	0.9060	0.5400
K	0.8890	0.5170
L	0.8050	0.4220
M	0.8700	0.4820
N	0.3040	0.1740
O	0.6670	0.4100
P	0.8980	0.5260
Q	0.7760	0.3880
R	0.7930	0.4220
S	0.5670	0.2610
T	0.6280	0.3920
U	0.6600	0.3880
V	0.7550	0.4470
W	0.4970	0.2640
X	0.1530	0.1400
a	0.9830	0.6690
b	0.9910	0.6730
c	0.9770	0.6620
d	0.9460	0.6200
e	0.9210	0.5940
f	0.9320	0.6150
g	0.8870	0.4480
h	0.9690	0.6040
i	0.9430	0.6250
j	0.9380	0.6250

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Chain	Atom inclusion	Q-score
l	0.9580	0.6310
m	0.9420	0.6140