



wwPDB EM Validation Summary Report ⓘ

Oct 16, 2024 – 12:53 AM JST

PDB ID : 8JW0
EMDB ID : EMD-36678
Title : PSI-AcpPCI supercomplex from *Amphidinium carterae*
Authors : Li, Z.H.; Li, X.Y.; Wang, W.D.
Deposited on : 2023-06-28
Resolution : 2.90 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

EMDB validation analysis	: FAILED
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	: FAILED
Ideal geometry (proteins)	: Engh & Huber (2001)
Ideal geometry (DNA, RNA)	: Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	: 2.39

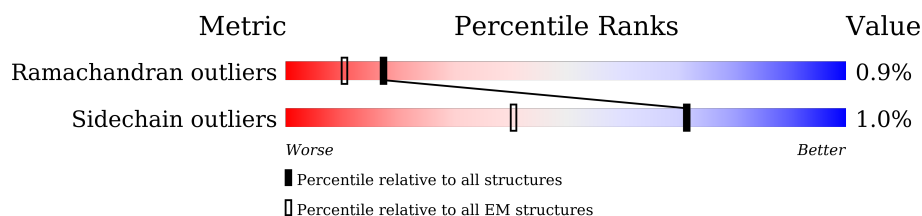
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.90 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



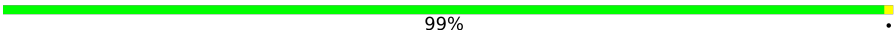
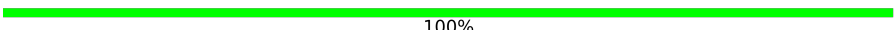
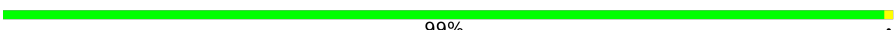
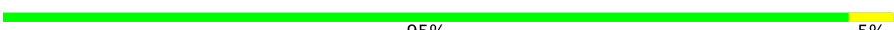
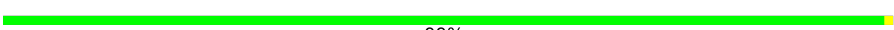





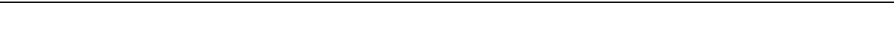

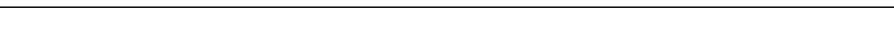

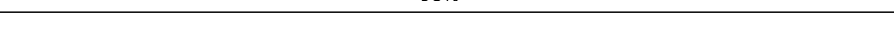
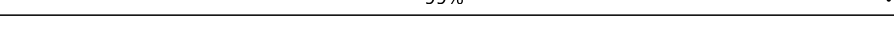
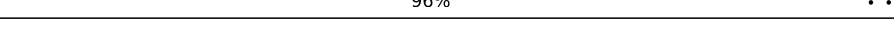
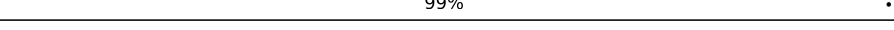
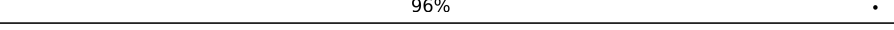
Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	a	645	 99% .
2	b	617	 99% .
3	c	86	 100%
4	d	257	 99% .
5	e	74	 100%
6	f	185	 100%
7	h	132	 95% 5%
8	i	126	 98% .
9	j	70	 97% .
10	l	253	 100%

Continued on next page...

Continued from previous page...

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

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
29	CLA	A	206	X	-	-	-
29	CLA	A	207	X	-	-	-
29	CLA	A	208	X	-	-	-
29	CLA	A	209	X	-	-	-
29	CLA	A	210	X	-	-	-

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
29	CLA	K	210	X	-	-	-
29	CLA	K	211	X	-	-	-
29	CLA	K	212	X	-	-	-
29	CLA	K	213	X	-	-	-
29	CLA	K	214	X	-	-	-
29	CLA	K	216	X	-	-	-
29	CLA	K	217	X	-	-	-
29	CLA	K	218	X	-	-	-
29	CLA	L	307	X	-	-	-
29	CLA	L	308	X	-	-	-
29	CLA	L	309	X	-	-	-
29	CLA	L	310	X	-	-	-
29	CLA	L	311	X	-	-	-
29	CLA	L	312	X	-	-	-
29	CLA	L	313	X	-	-	-
29	CLA	L	315	X	-	-	-
29	CLA	L	316	X	-	-	-
29	CLA	L	317	X	-	-	-
29	CLA	M	306	X	-	-	-
29	CLA	M	307	X	-	-	-
29	CLA	M	308	X	-	-	-
29	CLA	M	309	X	-	-	-
29	CLA	M	310	X	-	-	-
29	CLA	M	311	X	-	-	-
29	CLA	M	313	X	-	-	-
29	CLA	M	314	X	-	-	-
29	CLA	M	315	X	-	-	-
29	CLA	N	308	X	-	-	-
29	CLA	N	309	X	-	-	-
29	CLA	N	311	X	-	-	-
29	CLA	N	313	X	-	-	-
29	CLA	N	314	X	-	-	-
29	CLA	N	316	X	-	-	-
29	CLA	O	308	X	-	-	-
29	CLA	O	311	X	-	-	-
29	CLA	O	313	X	-	-	-
29	CLA	O	316	X	-	-	-
29	CLA	P	209	X	-	-	-
29	CLA	P	210	X	-	-	-
29	CLA	P	212	X	-	-	-
29	CLA	P	214	X	-	-	-
29	CLA	P	215	X	-	-	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
29	CLA	P	217	X	-	-	-
29	CLA	Q	307	X	-	-	-
29	CLA	Q	308	X	-	-	-
29	CLA	Q	310	X	-	-	-
29	CLA	Q	312	X	-	-	-
29	CLA	Q	313	X	-	-	-
29	CLA	Q	315	X	-	-	-
29	CLA	T	308	X	-	-	-
29	CLA	T	309	X	-	-	-
29	CLA	T	311	X	-	-	-
29	CLA	T	313	X	-	-	-
29	CLA	T	314	X	-	-	-
29	CLA	T	316	X	-	-	-
29	CLA	a	801	X	-	-	-
29	CLA	a	802	X	-	-	-
29	CLA	a	803	X	-	-	-
29	CLA	a	804	X	-	-	-
29	CLA	a	805	X	-	-	-
29	CLA	a	806	X	-	-	-
29	CLA	a	807	X	-	-	-
29	CLA	a	808	X	-	-	-
29	CLA	a	809	X	-	-	-
29	CLA	a	810	X	-	-	-
29	CLA	a	811	X	-	-	-
29	CLA	a	812	X	-	-	-
29	CLA	a	813	X	-	-	-
29	CLA	a	814	X	-	-	-
29	CLA	a	815	X	-	-	-
29	CLA	a	816	X	-	-	-
29	CLA	a	817	X	-	-	-
29	CLA	a	818	X	-	-	-
29	CLA	a	819	X	-	-	-
29	CLA	a	820	X	-	-	-
29	CLA	a	821	X	-	-	-
29	CLA	a	822	X	-	-	-
29	CLA	a	823	X	-	-	-
29	CLA	a	824	X	-	-	-
29	CLA	a	825	X	-	-	-
29	CLA	a	826	X	-	-	-
29	CLA	a	827	X	-	-	-
29	CLA	a	828	X	-	-	-
29	CLA	a	829	X	-	-	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
29	CLA	a	830	X	-	-	-
29	CLA	a	831	X	-	-	-
29	CLA	a	837	X	-	-	-
29	CLA	b	701	X	-	-	-
29	CLA	b	702	X	-	-	-
29	CLA	b	703	X	-	-	-
29	CLA	b	704	X	-	-	-
29	CLA	b	705	X	-	-	-
29	CLA	b	706	X	-	-	-
29	CLA	b	707	X	-	-	-
29	CLA	b	708	X	-	-	-
29	CLA	b	709	X	-	-	-
29	CLA	b	710	X	-	-	-
29	CLA	b	711	X	-	-	-
29	CLA	b	712	X	-	-	-
29	CLA	b	713	X	-	-	-
29	CLA	b	714	X	-	-	-
29	CLA	b	715	X	-	-	-
29	CLA	b	716	X	-	-	-
29	CLA	b	717	X	-	-	-
29	CLA	b	718	X	-	-	-
29	CLA	b	719	X	-	-	-
29	CLA	b	720	X	-	-	-
29	CLA	b	721	X	-	-	-
29	CLA	b	722	X	-	-	-
29	CLA	b	723	X	-	-	-
29	CLA	b	724	X	-	-	-
29	CLA	b	725	X	-	-	-
29	CLA	b	726	X	-	-	-
29	CLA	b	731	X	-	-	-
29	CLA	b	736	X	-	-	-
29	CLA	f	802	X	-	-	-
29	CLA	f	803	X	-	-	-
29	CLA	f	805	X	-	-	-
29	CLA	h	201	X	-	-	-
29	CLA	i	201	X	-	-	-
29	CLA	i	202	X	-	-	-
29	CLA	i	203	X	-	-	-
29	CLA	j	104	X	-	-	-
29	CLA	l	501	X	-	-	-
29	CLA	l	502	X	-	-	-
29	CLA	l	503	X	-	-	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
29	CLA	1	504	X	-	-	-
29	CLA	1	505	X	-	-	-
29	CLA	1	508	X	-	-	-
29	CLA	1	509	X	-	-	-
29	CLA	1	510	X	-	-	-

2 Entry composition [i](#)

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

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

- Molecule 1 is a protein called Photosystem I PsaA.

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

- Molecule 2 is a protein called Photosystem I PsaB.

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

- Molecule 3 is a protein called Photosystem I PsaC.

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

- Molecule 4 is a protein called Photosystem I PsaD.

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

- Molecule 5 is a protein called Photosystem I PsaE.

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

- Molecule 6 is a protein called Photosystem I PsaF.

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

- Molecule 7 is a protein called Photosystem I PsaR.

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

- Molecule 8 is a protein called Photosystem I Psal.

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

- Molecule 9 is a protein called Photosystem I Psaj.

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

- Molecule 10 is a protein called Photosystem I Psal.

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

- Molecule 11 is a protein called Photosystem I Psam.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

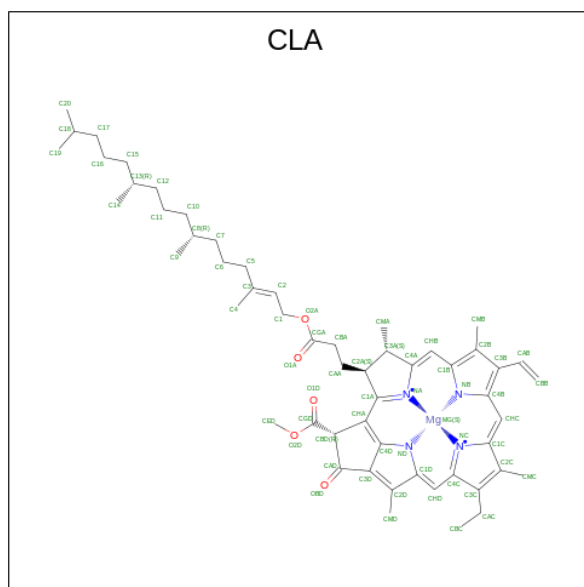
- Molecule 27 is a protein called Chlorophyll a-chlorophyll c-peridinin-protein-complex I-14, acpPCI-14.

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

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

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

- Molecule 29 is CHLOROPHYLL A (three-letter code: CLA) (formula: $C_{55}H_{72}MgN_4O_5$) (labeled as "Ligand of Interest" by depositor).



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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

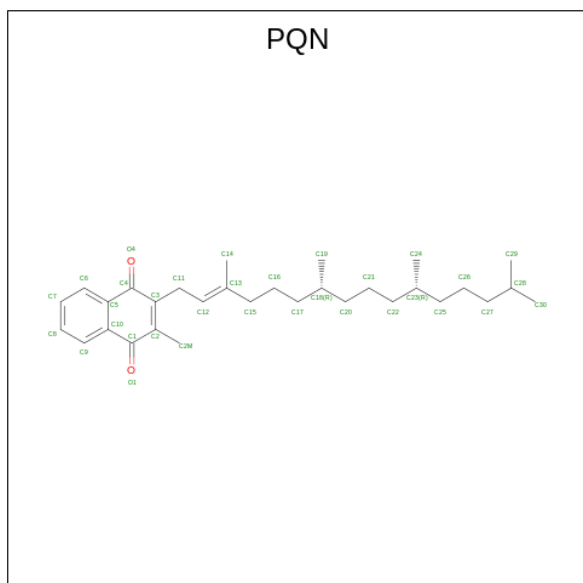
Mol	Chain	Residues	Atoms					AltConf
29	T	1	Total 46	C 36	Mg 1	N 4	O 5	0
29	T	1	Total 46	C 36	Mg 1	N 4	O 5	0
29	T	1	Total 47	C 37	Mg 1	N 4	O 5	0
29	T	1	Total 41	C 33	Mg 1	N 4	O 3	0
29	Q	1	Total 47	C 37	Mg 1	N 4	O 5	0
29	Q	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	Q	1	Total 65	C 55	Mg 1	N 4	O 5	0
29	Q	1	Total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

Continued on next page...

Continued from previous page...

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

- Molecule 30 is PHYLLOQUINONE (three-letter code: PQN) (formula: C₃₁H₄₆O₂).



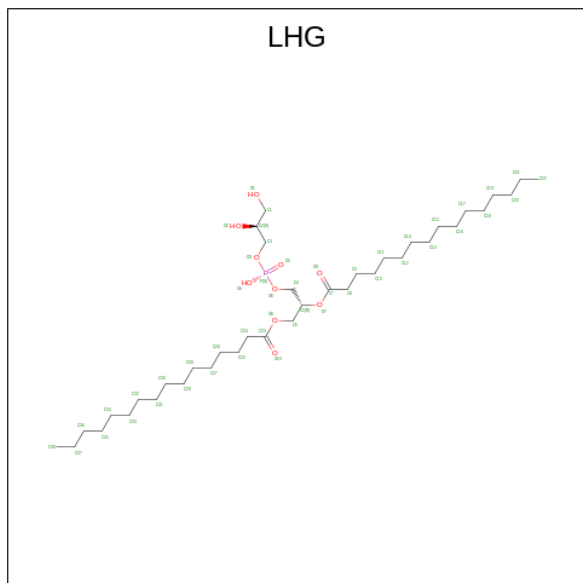
Mol	Chain	Residues	Atoms			AltConf
30	a	1	Total	C	O	0
			33	31	2	

Continued on next page...

Continued from previous page...

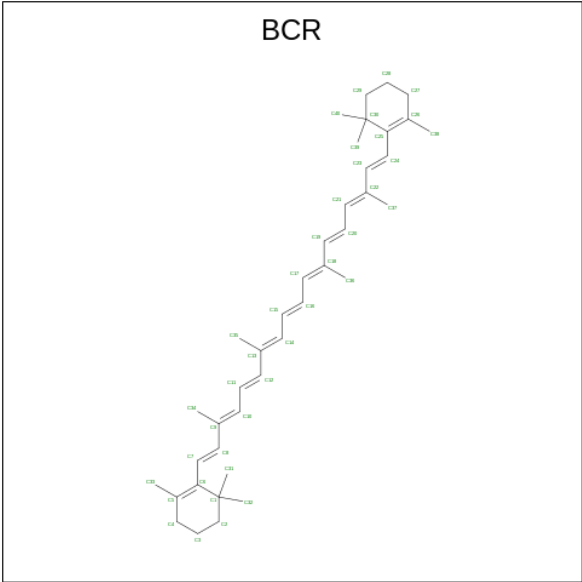
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
30	b	1	33	31	2	0

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



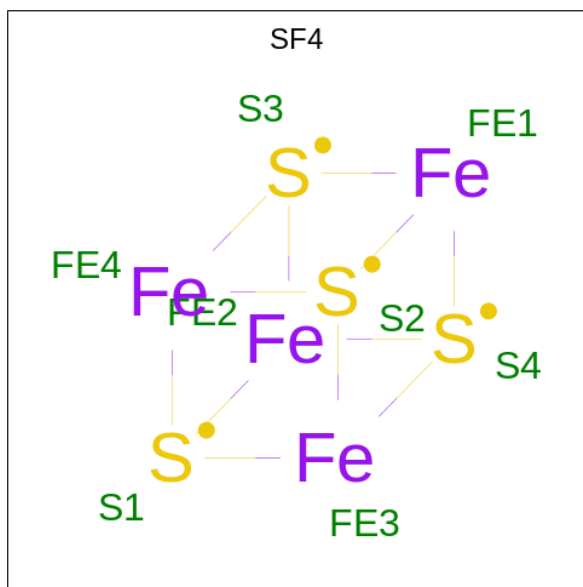
Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
31	a	1	48	37	10	1	0

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



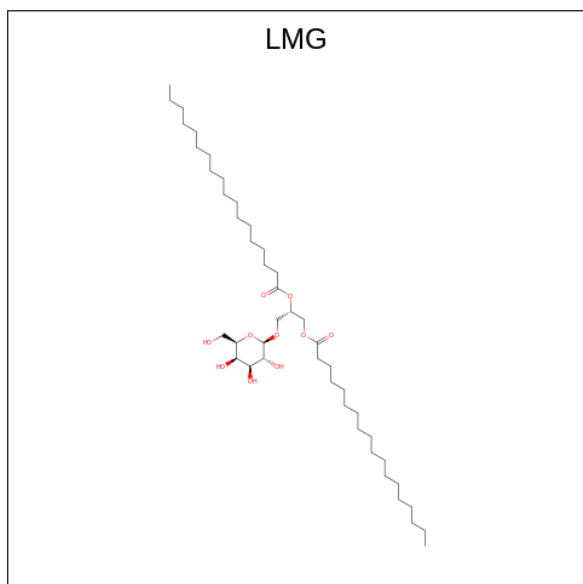
Mol	Chain	Residues	Atoms	AltConf
32	a	1	Total C 40 40	0
32	a	1	Total C 40 40	0
32	a	1	Total C 40 40	0
32	b	1	Total C 40 40	0
32	b	1	Total C 40 40	0
32	b	1	Total C 40 40	0
32	f	1	Total C 40 40	0
32	f	1	Total C 40 40	0
32	i	1	Total C 40 40	0
32	l	1	Total C 40 40	0
32	l	1	Total C 40 40	0
32	m	1	Total C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

- Molecule 33 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe₄S₄).



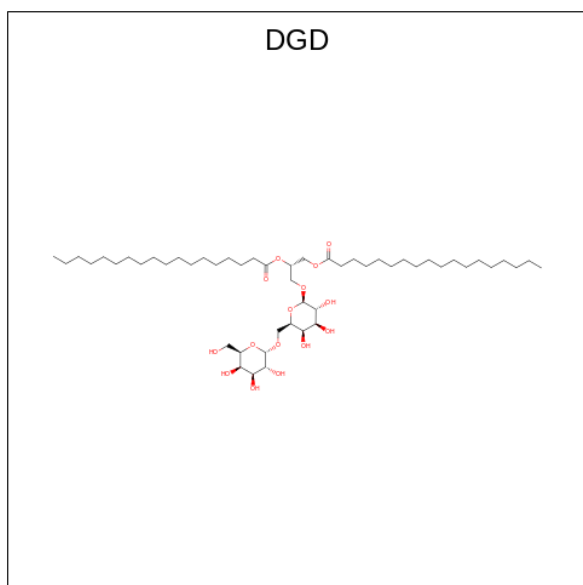
Mol	Chain	Residues	Atoms			AltConf
33	a	1	Total	Fe	S	0
			8	4	4	
33	c	1	Total	Fe	S	0
			8	4	4	
33	c	1	Total	Fe	S	0
			8	4	4	

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



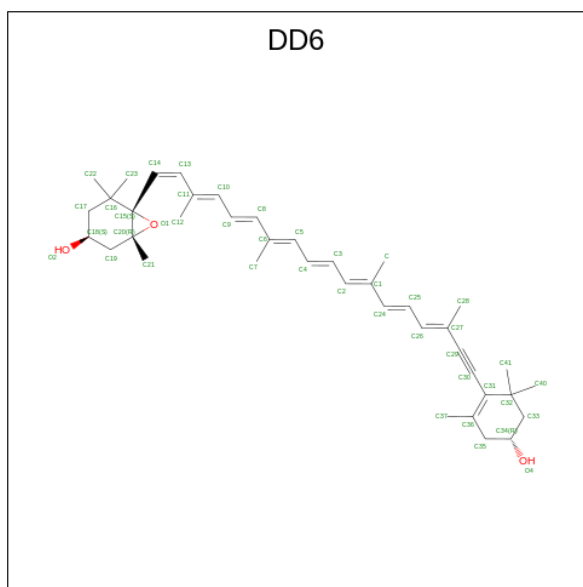
Mol	Chain	Residues	Atoms			AltConf
34	b	1	Total	C	O	0
			46	36	10	
34	b	1	Total	C	O	0
			44	34	10	
34	b	1	Total	C	O	0
			40	30	10	
34	h	1	Total	C	O	0
			28	18	10	
34	j	1	Total	C	O	0
			43	33	10	
34	A	1	Total	C	O	0
			37	27	10	
34	K	1	Total	C	O	0
			43	33	10	
34	K	1	Total	C	O	0
			35	25	10	
34	K	1	Total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

- Molecule 35 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (three-letter code: DGD) (formula: $C_{51}H_{96}O_{15}$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
35	b	1	Total	C	O	0
			57	42	15	
35	h	1	Total	C	O	0
			54	39	15	
35	j	1	Total	C	O	0
			43	28	15	
35	j	1	Total	C	O	0
			41	26	15	
35	j	1	Total	C	O	0
			49	34	15	
35	m	1	Total	C	O	0
			66	51	15	
35	G	1	Total	C	O	0
			45	30	15	
35	B	1	Total	C	O	0
			45	30	15	

- Molecule 36 is (3S,3'R,5R,6S,7cis)-7',8'-didehydro-5,6-dihydro-5,6-epoxy-beta,beta-carotene -3,3'-diol (three-letter code: DD6) (formula: C₄₀H₅₄O₃) (labeled as "Ligand of Interest" by depositor).



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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

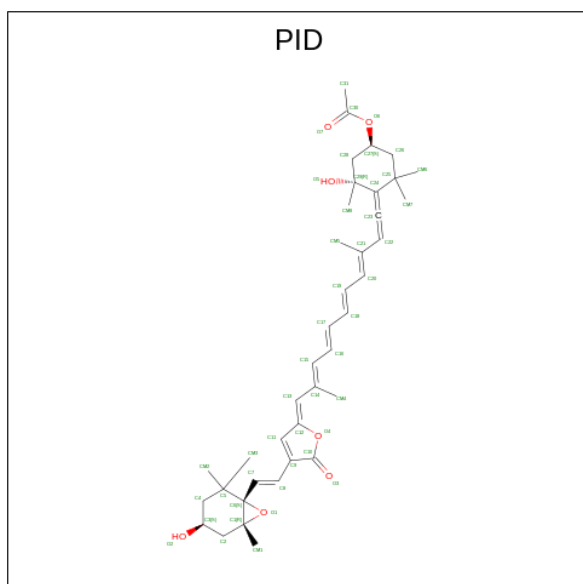
Mol	Chain	Residues	Atoms			AltConf
36	J	1	Total 43	C 40	O 3	0
36	M	1	Total 43	C 40	O 3	0
36	M	1	Total 43	C 40	O 3	0
36	M	1	Total 43	C 40	O 3	0
36	M	1	Total 43	C 40	O 3	0
36	L	1	Total 43	C 40	O 3	0
36	L	1	Total 43	C 40	O 3	0
36	L	1	Total 43	C 40	O 3	0
36	L	1	Total 43	C 40	O 3	0
36	D	1	Total 43	C 40	O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

Continued on next page...

Continued from previous page...

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

- Molecule 37 is PERIDININ (three-letter code: PID) (formula: C₃₉H₅₀O₇) (labeled as "Ligand of Interest" by depositor).



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

Continued on next page...

Continued from previous page...

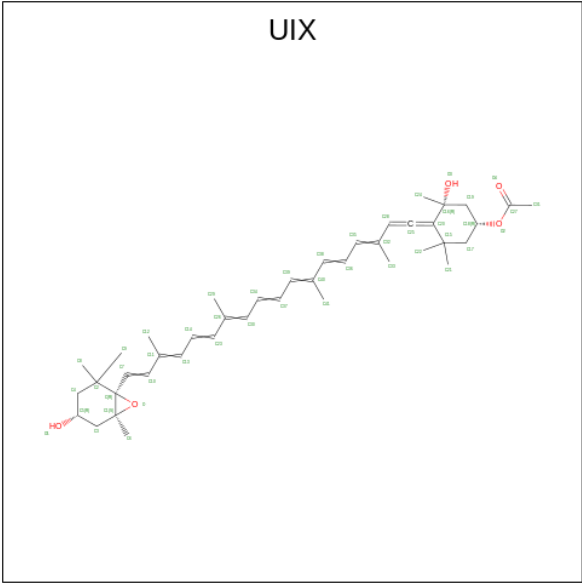
Mol	Chain	Residues	Atoms			AltConf
37	F	1	Total 46	C 39	O 7	0
37	D	1	Total 46	C 39	O 7	0
37	D	1	Total 46	C 39	O 7	0
37	D	1	Total 46	C 39	O 7	0
37	D	1	Total 46	C 39	O 7	0
37	D	1	Total 46	C 39	O 7	0
37	H	1	Total 46	C 39	O 7	0
37	H	1	Total 46	C 39	O 7	0
37	H	1	Total 46	C 39	O 7	0
37	H	1	Total 46	C 39	O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

Continued on next page...

Continued from previous page...

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

- Molecule 38 is [(1 {S},5 {R})-3,3,5-trimethyl-5-oxidanyl-4-[(3 {E},5 {E},7 {E},9 {E},11 {E},13 {E},15 {E},17 {E})-3,7,12,16-tetramethyl-18-[(1 {S},4 {S},6 {R})-2,2,6-trimethyl-4-oxidanyl-7-oxabicyclo[4.1.0]heptan-1-yl]octadeca-1,3,5,7,9,11,13,15,17-nonaenylidene]cyclohexyl] ethanoate (three-letter code: UIX) (formula: C₄₂H₅₈O₅) (labeled as "Ligand of Interest" by depositor).



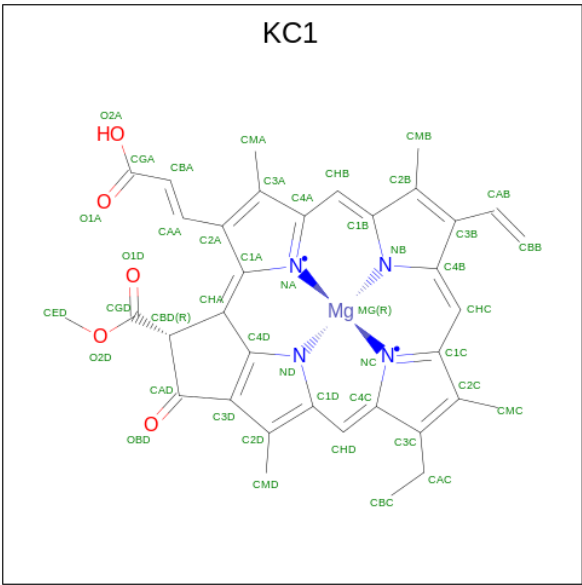
Mol	Chain	Residues	Atoms			AltConf
38	A	1	Total	C	O	0
			47	42	5	
38	F	1	Total	C	O	0
			47	42	5	
38	J	1	Total	C	O	0
			47	42	5	
38	L	1	Total	C	O	0
			47	42	5	
38	B	1	Total	C	O	0
			47	42	5	
38	N	1	Total	C	O	0
			47	42	5	
38	O	1	Total	C	O	0
			47	42	5	
38	T	1	Total	C	O	0
			47	42	5	
38	Q	1	Total	C	O	0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

Continued on next page...

Continued from previous page...

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

- Molecule 39 is Chlorophyll c1 (three-letter code: KC1) (formula: C₃₅H₃₀MgN₄O₅) (labeled as "Ligand of Interest" by depositor).



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

Continued on next page...

Continued from previous page...

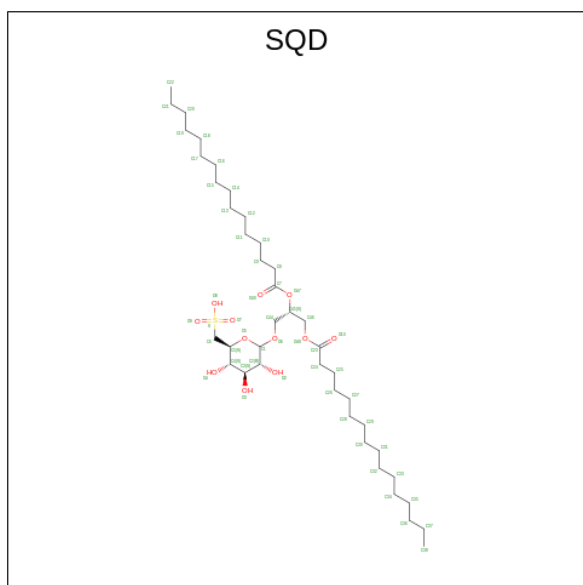
Mol	Chain	Residues	Atoms					AltConf
39	M	1	Total 45	C 35	Mg 1	N 4	O 5	0
39	L	1	Total 45	C 35	Mg 1	N 4	O 5	0
39	L	1	Total 45	C 35	Mg 1	N 4	O 5	0
39	D	1	Total 45	C 35	Mg 1	N 4	O 5	0
39	D	1	Total 45	C 35	Mg 1	N 4	O 5	0
39	B	1	Total 45	C 35	Mg 1	N 4	O 5	0
39	H	1	Total 45	C 35	Mg 1	N 4	O 5	0
39	H	1	Total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

Continued on next page...

Continued from previous page...

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

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



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

3 Residue-property plots

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. 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. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Photosystem I PsaA

Chain a:  99%



- Molecule 2: Photosystem I PsaB

Chain b:  99%



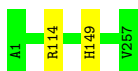
- Molecule 3: Photosystem I PsaC

Chain c:  100%

There are no outlier residues recorded for this chain.

- Molecule 4: Photosystem I PsaD

Chain d:  99%



- Molecule 5: Photosystem I PsaE

Chain e:  100%

There are no outlier residues recorded for this chain.

- Molecule 6: Photosystem I PsaF

Chain f:  100%

There are no outlier residues recorded for this chain.

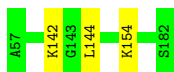
- Molecule 7: Photosystem I PsaR

Chain h:  95% 5%



- Molecule 8: Photosystem I PsaI

Chain i:  98% .



- Molecule 9: Photosystem I PsaJ

Chain j:  97% .



- Molecule 10: Photosystem I PsaL

Chain l:  100%

There are no outlier residues recorded for this chain.

- Molecule 11: Photosystem I PsaM

Chain m:  99% .



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

Chain A:  100%

There are no outlier residues recorded for this chain.

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

Chain G:  99% .



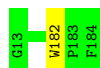
- Molecule 14: Chlorophyll a-chlorophyll c-peridinin-protein-complex I-7, acpPCI-7

Chain I:  95% 5%



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

Chain K: 99% .



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

Chain F: 99% .



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

Chain J: 99% .



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

Chain M: 95% 5% .



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

Chain L: 97% .



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

Chain D: 98% .



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

Chain B: 99% .



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

Chain H: 97%



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

Chain N: 96%



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

Chain O: 98%



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

Chain T: 96%



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

Chain C: 99%



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

Chain Q: 99%



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

Chain P: 96%



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

Chain E:  97% .



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	356838	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	
Image detector	GATAN K2 BASE (4k x 4k)	Depositor

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

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

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	a	643/645 (100%)	594 (92%)	47 (7%)	2 (0%)	37	66
2	b	615/617 (100%)	581 (94%)	34 (6%)	0	100	100
3	c	84/86 (98%)	81 (96%)	3 (4%)	0	100	100
4	d	255/257 (99%)	239 (94%)	15 (6%)	1 (0%)	30	60
5	e	72/74 (97%)	68 (94%)	4 (6%)	0	100	100
6	f	183/185 (99%)	177 (97%)	6 (3%)	0	100	100
7	h	130/132 (98%)	121 (93%)	6 (5%)	3 (2%)	5	20
8	i	124/126 (98%)	116 (94%)	8 (6%)	0	100	100
9	j	68/70 (97%)	60 (88%)	8 (12%)	0	100	100
10	l	251/253 (99%)	231 (92%)	20 (8%)	0	100	100
11	m	87/89 (98%)	79 (91%)	8 (9%)	0	100	100
12	A	178/180 (99%)	163 (92%)	15 (8%)	0	100	100
13	G	213/215 (99%)	189 (89%)	23 (11%)	1 (0%)	25	56
14	I	192/194 (99%)	165 (86%)	21 (11%)	6 (3%)	3	14
15	K	170/172 (99%)	153 (90%)	16 (9%)	1 (1%)	22	52
16	F	174/176 (99%)	154 (88%)	19 (11%)	1 (1%)	22	52

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
17	J	163/165 (99%)	144 (88%)	18 (11%)	1 (1%)	22	52
18	M	166/168 (99%)	134 (81%)	26 (16%)	6 (4%)	3	12
19	L	183/185 (99%)	152 (83%)	26 (14%)	5 (3%)	4	17
20	D	158/160 (99%)	142 (90%)	15 (10%)	1 (1%)	22	52
21	B	170/172 (99%)	153 (90%)	17 (10%)	0	100	100
22	H	158/160 (99%)	135 (85%)	19 (12%)	4 (2%)	4	18
23	N	158/160 (99%)	126 (80%)	31 (20%)	1 (1%)	22	52
24	O	159/161 (99%)	144 (91%)	12 (8%)	3 (2%)	6	24
25	C	158/160 (99%)	146 (92%)	11 (7%)	1 (1%)	22	52
25	T	157/160 (98%)	142 (90%)	11 (7%)	4 (2%)	4	18
26	Q	160/162 (99%)	138 (86%)	20 (12%)	2 (1%)	10	33
27	P	158/160 (99%)	139 (88%)	16 (10%)	3 (2%)	6	24
28	E	140/142 (99%)	120 (86%)	17 (12%)	3 (2%)	5	22
All	All	5527/5586 (99%)	4986 (90%)	492 (9%)	49 (1%)	17	43

5 of 49 Ramachandran outliers are listed below:

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

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	a	531/535 (99%)	527 (99%)	4 (1%)	79	93
2	b	502/504 (100%)	498 (99%)	4 (1%)	79	93
3	c	73/74 (99%)	73 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	d	213/222 (96%)	212 (100%)	1 (0%)	86	96
5	e	65/66 (98%)	65 (100%)	0	100	100
6	f	151/151 (100%)	151 (100%)	0	100	100
7	h	109/109 (100%)	106 (97%)	3 (3%)	38	73
8	i	106/106 (100%)	103 (97%)	3 (3%)	38	73
9	j	60/60 (100%)	58 (97%)	2 (3%)	33	68
10	l	200/203 (98%)	200 (100%)	0	100	100
11	m	72/72 (100%)	71 (99%)	1 (1%)	62	86
12	A	136/141 (96%)	136 (100%)	0	100	100
13	G	171/171 (100%)	170 (99%)	1 (1%)	84	95
14	I	141/156 (90%)	138 (98%)	3 (2%)	48	78
15	K	133/138 (96%)	133 (100%)	0	100	100
16	F	140/140 (100%)	139 (99%)	1 (1%)	81	94
17	J	136/136 (100%)	135 (99%)	1 (1%)	81	94
18	M	128/128 (100%)	126 (98%)	2 (2%)	58	84
19	L	145/145 (100%)	144 (99%)	1 (1%)	81	94
20	D	123/123 (100%)	120 (98%)	3 (2%)	44	76
21	B	146/146 (100%)	145 (99%)	1 (1%)	81	94
22	H	123/123 (100%)	122 (99%)	1 (1%)	79	93
23	N	124/124 (100%)	119 (96%)	5 (4%)	27	61
24	O	124/124 (100%)	123 (99%)	1 (1%)	79	93
25	C	121/121 (100%)	120 (99%)	1 (1%)	79	93
25	T	120/121 (99%)	119 (99%)	1 (1%)	79	93
26	Q	120/120 (100%)	120 (100%)	0	100	100
27	P	123/123 (100%)	120 (98%)	3 (2%)	44	76
28	E	108/108 (100%)	107 (99%)	1 (1%)	75	92
All	All	4444/4490 (99%)	4400 (99%)	44 (1%)	71	91

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

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

Continued on next page...

Continued from previous page...

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

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

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

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

411 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
29	CLA	B	308	-	65,73,73	1.47	7 (10%)	76,113,113	1.40	10 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
29	CLA	D	312	20	46,54,73	1.76	6 (13%)	53,90,113	1.53	6 (11%)
29	CLA	J	305	-	46,54,73	1.76	6 (13%)	53,90,113	1.53	7 (13%)
38	UIX	B	304	-	41,49,49	1.27	3 (7%)	52,74,74	2.45	16 (30%)
29	CLA	b	707	-	65,73,73	1.48	7 (10%)	76,113,113	1.42	9 (11%)
36	DD6	A	202	-	39,45,45	1.97	3 (7%)	52,67,67	1.81	10 (19%)
29	CLA	C	311	-	51,59,73	1.65	6 (11%)	59,96,113	1.54	8 (13%)
29	CLA	M	306	-	53,61,73	1.62	6 (11%)	61,98,113	1.51	7 (11%)
37	PID	T	302	-	41,49,49	1.38	4 (9%)	49,76,76	1.51	8 (16%)
29	CLA	A	208	-	55,63,73	1.58	7 (12%)	64,101,113	1.50	7 (10%)
37	PID	Q	303	-	41,49,49	1.34	4 (9%)	49,76,76	1.48	6 (12%)
29	CLA	F	311	-	46,54,73	1.73	6 (13%)	53,90,113	1.59	6 (11%)
29	CLA	J	309	17	46,54,73	1.72	6 (13%)	53,90,113	1.61	6 (11%)
33	SF4	a	836	1,2	0,12,12	-	-	-	-	-
29	CLA	A	212	-	55,63,73	1.56	7 (12%)	64,101,113	1.47	8 (12%)
37	PID	G	303	-	41,49,49	1.37	4 (9%)	49,76,76	1.33	5 (10%)
36	DD6	T	303	-	39,45,45	1.98	3 (7%)	52,67,67	1.97	15 (28%)
29	CLA	C	314	-	47,55,73	1.74	6 (12%)	54,91,113	1.64	8 (14%)
29	CLA	a	809	1	65,73,73	1.46	7 (10%)	76,113,113	1.41	8 (10%)
29	CLA	M	309	-	46,54,73	1.76	6 (13%)	53,90,113	1.53	7 (13%)
29	CLA	D	316	-	41,49,73	1.84	6 (14%)	47,84,113	1.71	7 (14%)
38	UIX	P	207	-	41,49,49	1.27	3 (7%)	52,74,74	2.56	19 (36%)
29	CLA	l	501	-	60,68,73	1.54	6 (10%)	70,107,113	1.48	7 (10%)
36	DD6	K	206	-	39,45,45	2.05	3 (7%)	52,67,67	2.01	14 (26%)
39	KC1	I	215	14	48,53,53	1.54	7 (14%)	55,89,89	1.87	11 (20%)
37	PID	G	309	-	41,49,49	1.33	4 (9%)	49,76,76	1.45	5 (10%)
33	SF4	c	101	3	0,12,12	-	-	-	-	-
39	KC1	D	315	-	48,53,53	1.52	7 (14%)	55,89,89	1.84	8 (14%)
36	DD6	h	202	-	39,45,45	2.19	5 (12%)	52,67,67	2.33	19 (36%)
29	CLA	I	210	-	55,63,73	1.58	6 (10%)	64,101,113	1.47	7 (10%)
29	CLA	E	313	-	41,49,73	1.85	6 (14%)	47,84,113	1.67	7 (14%)
29	CLA	F	313	16	46,54,73	1.75	6 (13%)	53,90,113	1.59	6 (11%)
38	UIX	J	304	-	41,49,49	1.26	3 (7%)	52,74,74	2.40	13 (25%)
37	PID	Q	301	-	41,49,49	1.34	4 (9%)	49,76,76	1.47	6 (12%)
37	PID	C	307	-	41,49,49	1.34	4 (9%)	49,76,76	1.52	6 (12%)
29	CLA	L	309	-	55,63,73	1.59	6 (10%)	64,101,113	1.48	7 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
29	CLA	E	310	28	46,54,73	1.72	6 (13%)	53,90,113	1.57	6 (11%)
29	CLA	G	301	-	49,57,73	1.69	7 (14%)	55,93,113	1.57	7 (12%)
35	DGD	B	318	-	46,46,67	1.00	2 (4%)	60,60,81	1.32	10 (16%)
29	CLA	i	202	-	65,73,73	1.45	7 (10%)	76,113,113	1.38	8 (10%)
29	CLA	C	308	-	47,55,73	1.73	6 (12%)	54,91,113	1.52	7 (12%)
29	CLA	P	212	-	51,59,73	1.68	6 (11%)	59,96,113	1.50	8 (13%)
29	CLA	N	313	23	46,54,73	1.72	6 (13%)	53,90,113	4.81	10 (18%)
35	DGD	h	203	-	55,55,67	0.90	2 (3%)	69,69,81	0.98	3 (4%)
29	CLA	a	830	-	56,64,73	1.56	6 (10%)	65,102,113	5.34	10 (15%)
29	CLA	b	731	-	56,64,73	1.57	6 (10%)	65,102,113	1.47	9 (13%)
29	CLA	L	311	19	46,54,73	1.75	6 (13%)	53,90,113	1.49	7 (13%)
32	BCR	l	507	-	41,41,41	0.75	0	56,56,56	1.99	16 (28%)
29	CLA	N	311	-	51,59,73	1.67	5 (9%)	59,96,113	1.53	7 (11%)
29	CLA	a	837	-	55,63,73	1.60	6 (10%)	64,101,113	1.40	7 (10%)
29	CLA	M	307	-	55,63,73	1.60	7 (12%)	64,101,113	1.44	7 (10%)
29	CLA	T	308	-	47,55,73	1.75	6 (12%)	54,91,113	1.52	7 (12%)
29	CLA	N	316	-	41,49,73	1.85	6 (14%)	47,84,113	1.66	7 (14%)
36	DD6	K	205	-	39,45,45	2.05	3 (7%)	52,67,67	1.91	17 (32%)
29	CLA	B	312	-	65,73,73	1.45	7 (10%)	76,113,113	1.41	7 (9%)
37	PID	E	301	-	41,49,49	1.39	4 (9%)	49,76,76	1.95	9 (18%)
29	CLA	D	311	-	46,54,73	1.72	6 (13%)	53,90,113	1.58	7 (13%)
29	CLA	a	816	-	46,54,73	1.73	7 (15%)	53,90,113	1.56	7 (13%)
29	CLA	a	802	-	65,73,73	1.47	6 (9%)	76,113,113	1.47	9 (11%)
29	CLA	E	315	-	57,65,73	1.60	6 (10%)	66,103,113	1.45	8 (12%)
37	PID	N	305	-	41,49,49	1.37	4 (9%)	49,76,76	1.36	4 (8%)
29	CLA	a	813	-	51,59,73	1.69	7 (13%)	59,96,113	1.50	7 (11%)
29	CLA	G	316	-	65,73,73	1.50	8 (12%)	76,113,113	4.94	11 (14%)
29	CLA	Q	308	-	65,73,73	1.48	7 (10%)	76,113,113	1.41	8 (10%)
29	CLA	D	308	-	47,55,73	1.73	6 (12%)	54,91,113	1.55	7 (12%)
32	BCR	b	728	-	41,41,41	0.78	1 (2%)	56,56,56	2.04	15 (26%)
38	UIX	Q	305	-	41,49,49	1.26	4 (9%)	52,74,74	2.78	22 (42%)
37	PID	O	305	-	41,49,49	1.35	4 (9%)	49,76,76	1.59	7 (14%)
39	KC1	H	309	-	48,53,53	1.53	7 (14%)	55,89,89	1.87	11 (20%)
29	CLA	a	826	-	65,73,73	1.48	6 (9%)	76,113,113	1.40	8 (10%)
39	KC1	T	310	-	48,53,53	1.53	7 (14%)	55,89,89	1.79	10 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
36	DD6	H	303	-	39,45,45	1.94	3 (7%)	52,67,67	1.98	14 (26%)
37	PID	O	301	-	41,49,49	1.32	4 (9%)	49,76,76	1.62	6 (12%)
29	CLA	a	821	-	47,55,73	1.73	6 (12%)	54,91,113	1.53	7 (12%)
36	DD6	K	204	-	39,45,45	2.08	3 (7%)	52,67,67	1.95	18 (34%)
35	DGD	j	106	-	50,50,67	0.97	2 (4%)	64,64,81	1.04	4 (6%)
39	KC1	H	314	-	48,53,53	1.51	7 (14%)	55,89,89	1.86	10 (18%)
29	CLA	b	720	-	65,73,73	1.49	8 (12%)	76,113,113	1.36	6 (7%)
29	CLA	I	214	-	55,63,73	1.57	7 (12%)	64,101,113	1.48	8 (12%)
29	CLA	G	312	13	65,73,73	1.47	8 (12%)	76,113,113	1.39	8 (10%)
37	PID	P	202	-	41,49,49	1.32	4 (9%)	49,76,76	1.37	8 (16%)
37	PID	F	304	-	41,49,49	1.61	5 (12%)	49,76,76	1.57	7 (14%)
29	CLA	H	315	-	41,49,73	1.84	6 (14%)	47,84,113	1.66	8 (17%)
34	LMG	h	205	-	28,28,55	1.02	1 (3%)	36,36,63	1.27	4 (11%)
29	CLA	I	209	-	60,68,73	1.52	7 (11%)	70,107,113	5.16	11 (15%)
36	DD6	I	204	-	39,45,45	2.19	5 (12%)	52,67,67	2.08	16 (30%)
29	CLA	A	211	-	55,63,73	1.57	6 (10%)	64,101,113	1.45	7 (10%)
39	KC1	C	310	-	48,53,53	1.54	7 (14%)	55,89,89	1.89	10 (18%)
29	CLA	b	709	-	60,68,73	1.52	7 (11%)	70,107,113	1.43	8 (11%)
29	CLA	B	314	21	41,49,73	1.80	7 (17%)	47,84,113	1.72	7 (14%)
29	CLA	L	310	-	55,63,73	1.60	6 (10%)	64,101,113	1.48	7 (10%)
29	CLA	E	308	-	65,73,73	1.47	6 (9%)	76,113,113	1.39	8 (10%)
37	PID	P	205	-	41,49,49	1.34	4 (9%)	49,76,76	1.54	6 (12%)
29	CLA	E	305	-	61,69,73	1.54	6 (9%)	71,108,113	1.45	7 (9%)
29	CLA	K	212	-	52,60,73	1.69	7 (13%)	60,97,113	1.50	9 (15%)
38	UIX	F	305	-	41,49,49	1.27	3 (7%)	52,74,74	2.89	19 (36%)
39	KC1	M	305	-	48,53,53	1.52	7 (14%)	55,89,89	1.89	12 (21%)
37	PID	C	302	-	41,49,49	1.34	4 (9%)	49,76,76	1.44	6 (12%)
29	CLA	a	805	-	55,63,73	1.59	7 (12%)	64,101,113	1.50	6 (9%)
29	CLA	H	313	-	47,55,73	1.74	6 (12%)	54,91,113	1.64	8 (14%)
36	DD6	J	303	-	39,45,45	2.10	3 (7%)	52,67,67	2.11	18 (34%)
29	CLA	b	721	-	58,66,73	1.56	8 (13%)	67,104,113	1.48	9 (13%)
29	CLA	G	317	-	53,61,73	1.62	7 (13%)	61,98,113	1.47	6 (9%)
29	CLA	O	316	-	41,49,73	1.85	6 (14%)	47,84,113	1.68	7 (14%)
29	CLA	b	701	-	65,73,73	1.45	7 (10%)	76,113,113	1.44	9 (11%)
29	CLA	O	308	-	47,55,73	1.76	6 (12%)	54,91,113	1.55	7 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
29	CLA	b	715	-	46,54,73	1.75	7 (15%)	53,90,113	1.55	7 (13%)
39	KC1	C	315	25	48,53,53	1.52	7 (14%)	55,89,89	1.82	10 (18%)
29	CLA	F	308	-	46,54,73	1.74	7 (15%)	53,90,113	1.52	6 (11%)
29	CLA	G	314	-	60,68,73	1.52	7 (11%)	70,107,113	1.49	8 (11%)
29	CLA	a	801	-	65,73,73	1.44	10 (15%)	76,113,113	1.40	7 (9%)
29	CLA	b	702	-	65,73,73	1.47	6 (9%)	76,113,113	1.40	6 (7%)
39	KC1	N	312	23	48,53,53	1.52	7 (14%)	55,89,89	1.86	12 (21%)
29	CLA	E	306	28	65,73,73	1.47	7 (10%)	76,113,113	1.38	7 (9%)
29	CLA	b	724	-	47,55,73	1.73	9 (19%)	54,91,113	1.54	8 (14%)
38	UIX	N	306	-	41,49,49	1.26	4 (9%)	52,74,74	2.60	20 (38%)
34	LMG	b	734	-	40,40,55	0.81	0	48,48,63	1.29	6 (12%)
34	LMG	A	219	-	37,37,55	0.85	0	45,45,63	1.31	5 (11%)
29	CLA	B	310	-	65,73,73	1.45	7 (10%)	76,113,113	1.38	7 (9%)
29	CLA	a	812	-	60,68,73	1.51	7 (11%)	70,107,113	1.50	7 (10%)
29	CLA	N	308	-	47,55,73	1.75	6 (12%)	54,91,113	1.53	7 (12%)
29	CLA	b	706	-	65,73,73	1.48	7 (10%)	76,113,113	1.41	7 (9%)
37	PID	C	301	-	41,49,49	1.34	4 (9%)	49,76,76	1.59	6 (12%)
37	PID	P	203	-	41,49,49	1.36	4 (9%)	49,76,76	1.45	8 (16%)
29	CLA	l	503	10	65,73,73	1.48	8 (12%)	76,113,113	1.40	8 (10%)
29	CLA	B	311	21	51,59,73	1.66	7 (13%)	59,96,113	1.52	7 (11%)
29	CLA	b	716	-	53,61,73	1.62	7 (13%)	61,98,113	1.53	8 (13%)
36	DD6	B	301	-	38,44,45	2.03	3 (7%)	50,65,67	2.00	14 (28%)
36	DD6	I	203	-	39,45,45	2.29	3 (7%)	52,67,67	2.41	17 (32%)
29	CLA	J	313	-	41,49,73	1.83	6 (14%)	47,84,113	1.67	8 (17%)
37	PID	N	304	-	41,49,49	1.34	4 (9%)	49,76,76	1.48	5 (10%)
29	CLA	E	314	28	48,56,73	1.72	7 (14%)	55,92,113	1.54	7 (12%)
36	DD6	L	303	-	39,45,45	2.06	3 (7%)	52,67,67	1.73	13 (25%)
36	DD6	I	206	-	39,45,45	2.03	3 (7%)	52,67,67	1.90	12 (23%)
29	CLA	L	317	-	46,54,73	1.75	6 (13%)	53,90,113	1.55	6 (11%)
29	CLA	b	704	-	65,73,73	1.47	8 (12%)	76,113,113	3.99	8 (10%)
29	CLA	D	309	-	46,54,73	1.74	6 (13%)	53,90,113	1.57	6 (11%)
34	LMG	E	316	-	32,32,55	0.99	1 (3%)	40,40,63	1.27	2 (5%)
37	PID	T	301	-	41,49,49	1.34	4 (9%)	49,76,76	1.49	5 (10%)
32	BCR	f	801	-	41,41,41	0.71	0	56,56,56	2.03	17 (30%)
35	DGD	b	733	-	58,58,67	0.94	3 (5%)	72,72,81	1.25	7 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
29	CLA	T	316	-	41,49,73	1.84	6 (14%)	47,84,113	1.67	7 (14%)
34	LMG	K	219	-	35,35,55	0.92	1 (2%)	43,43,63	1.19	4 (9%)
29	CLA	A	214	12	41,49,73	1.83	6 (14%)	47,84,113	1.62	7 (14%)
29	CLA	a	806	1	65,73,73	1.45	7 (10%)	76,113,113	1.44	7 (9%)
37	PID	D	306	-	41,49,49	1.36	4 (9%)	49,76,76	1.42	8 (16%)
29	CLA	N	314	-	47,55,73	1.72	7 (14%)	54,91,113	1.61	7 (12%)
37	PID	H	304	-	41,49,49	1.34	4 (9%)	49,76,76	1.63	5 (10%)
38	UIX	O	306	-	41,49,49	1.25	3 (7%)	52,74,74	2.70	21 (40%)
32	BCR	a	834	-	41,41,41	0.74	0	56,56,56	2.05	16 (28%)
29	CLA	i	203	-	55,63,73	1.56	6 (10%)	64,101,113	1.51	8 (12%)
37	PID	P	206	-	41,49,49	1.36	4 (9%)	49,76,76	1.79	8 (16%)
29	CLA	T	314	-	47,55,73	1.73	5 (10%)	54,91,113	1.66	9 (16%)
37	PID	N	307	-	41,49,49	1.36	4 (9%)	49,76,76	1.59	9 (18%)
29	CLA	b	710	-	46,54,73	1.74	7 (15%)	53,90,113	1.53	7 (13%)
29	CLA	G	311	13	51,59,73	1.64	6 (11%)	59,96,113	1.50	7 (11%)
39	KC1	L	314	-	48,53,53	1.55	7 (14%)	55,89,89	1.86	11 (20%)
36	DD6	K	221	-	39,45,45	2.14	4 (10%)	52,67,67	2.24	15 (28%)
39	KC1	J	312	17	48,53,53	1.52	7 (14%)	55,89,89	1.84	10 (18%)
29	CLA	C	309	-	65,73,73	1.47	6 (9%)	76,113,113	1.37	6 (7%)
37	PID	O	304	-	41,49,49	1.34	4 (9%)	49,76,76	1.50	6 (12%)
29	CLA	B	307	-	45,53,73	1.78	6 (13%)	52,89,113	1.58	7 (13%)
32	BCR	f	804	-	41,41,41	0.74	0	56,56,56	1.98	16 (28%)
32	BCR	a	835	-	41,41,41	0.79	0	56,56,56	2.12	16 (28%)
29	CLA	L	316	-	52,60,73	1.68	7 (13%)	60,97,113	1.48	8 (13%)
29	CLA	J	310	-	47,55,73	1.71	6 (12%)	54,91,113	1.59	7 (12%)
29	CLA	H	307	-	47,55,73	1.74	6 (12%)	54,91,113	1.52	7 (12%)
35	DGD	j	103	-	44,44,67	0.99	2 (4%)	58,58,81	1.32	9 (15%)
39	KC1	D	310	-	48,53,53	1.51	7 (14%)	55,89,89	1.84	9 (16%)
29	CLA	K	211	-	55,63,73	1.58	7 (12%)	64,101,113	1.51	10 (15%)
37	PID	H	302	-	41,49,49	1.36	4 (9%)	49,76,76	1.40	6 (12%)
29	CLA	I	201	29	45,53,73	1.77	6 (13%)	52,89,113	1.62	6 (11%)
29	CLA	Q	312	-	46,54,73	1.74	6 (13%)	53,90,113	1.54	7 (13%)
29	CLA	b	717	-	65,73,73	1.48	6 (9%)	76,113,113	1.37	9 (11%)
29	CLA	A	216	-	41,49,73	1.83	7 (17%)	47,84,113	1.66	7 (14%)
30	PQN	b	727	-	34,34,34	1.54	2 (5%)	42,45,45	1.19	3 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
29	CLA	O	313	24	46,54,73	1.73	6 (13%)	53,90,113	1.59	6 (11%)
29	CLA	l	509	-	41,49,73	1.83	7 (17%)	47,84,113	1.65	8 (17%)
29	CLA	H	310	-	51,59,73	1.69	6 (11%)	59,96,113	1.54	8 (13%)
36	DD6	J	301	-	39,45,45	2.06	3 (7%)	52,67,67	2.26	17 (32%)
36	DD6	B	319	-	39,45,45	2.09	3 (7%)	52,67,67	2.26	16 (30%)
29	CLA	E	311	-	65,73,73	1.46	7 (10%)	76,113,113	1.43	9 (11%)
29	CLA	P	209	-	47,55,73	1.75	5 (10%)	54,91,113	1.53	7 (12%)
29	CLA	I	211	-	65,73,73	1.44	7 (10%)	76,113,113	1.43	8 (10%)
29	CLA	L	313	-	53,61,73	1.61	6 (11%)	61,98,113	1.52	8 (13%)
29	CLA	j	104	29	52,60,73	1.64	7 (13%)	60,97,113	1.57	7 (11%)
36	DD6	I	205	-	39,45,45	2.45	5 (12%)	52,67,67	2.18	17 (32%)
29	CLA	I	217	-	55,63,73	1.61	6 (10%)	64,101,113	1.45	7 (10%)
39	KC1	Q	311	-	48,53,53	1.53	7 (14%)	55,89,89	1.85	11 (20%)
36	DD6	B	305	-	39,45,45	2.02	3 (7%)	52,67,67	1.91	16 (30%)
29	CLA	I	207	14	49,57,73	1.68	7 (14%)	55,93,113	1.59	7 (12%)
29	CLA	l	505	-	65,73,73	1.48	6 (9%)	76,113,113	1.37	8 (10%)
37	PID	Q	306	-	41,49,49	1.33	4 (9%)	49,76,76	1.52	6 (12%)
29	CLA	a	827	-	65,73,73	1.48	9 (13%)	76,113,113	1.37	8 (10%)
36	DD6	P	204	-	39,45,45	1.99	3 (7%)	52,67,67	2.19	15 (28%)
38	UIX	L	302	-	41,49,49	1.26	3 (7%)	52,74,74	2.41	17 (32%)
29	CLA	l	510	-	45,53,73	1.80	6 (13%)	52,89,113	1.54	8 (15%)
37	PID	H	306	-	41,49,49	1.31	4 (9%)	49,76,76	1.46	6 (12%)
29	CLA	K	207	15	49,57,73	1.70	6 (12%)	55,93,113	1.54	8 (14%)
31	LHG	a	833	-	47,47,48	0.28	0	50,53,54	0.31	0
29	CLA	O	314	-	47,55,73	1.78	7 (14%)	54,91,113	1.58	8 (14%)
36	DD6	L	304	-	39,45,45	2.02	3 (7%)	52,67,67	1.98	17 (32%)
35	DGD	j	105	-	42,42,67	1.03	2 (4%)	56,56,81	1.07	5 (8%)
29	CLA	K	209	-	54,62,73	1.61	7 (12%)	62,99,113	1.50	9 (14%)
29	CLA	I	208	-	46,54,73	1.74	6 (13%)	53,90,113	5.89	8 (15%)
29	CLA	T	311	-	46,54,73	1.74	5 (10%)	53,90,113	1.56	7 (13%)
36	DD6	L	301	-	39,45,45	2.00	3 (7%)	52,67,67	1.97	11 (21%)
29	CLA	L	308	-	53,61,73	1.62	6 (11%)	61,98,113	5.52	10 (16%)
37	PID	T	317	-	41,49,49	1.33	4 (9%)	49,76,76	1.70	9 (18%)
39	KC1	M	312	-	48,53,53	1.53	7 (14%)	55,89,89	1.89	11 (20%)
29	CLA	a	823	-	58,66,73	1.54	7 (12%)	67,104,113	1.48	8 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
34	LMG	K	220	-	36,36,55	0.86	1 (2%)	44,44,63	1.23	4 (9%)
39	KC1	E	307	-	48,53,53	1.52	7 (14%)	55,89,89	1.87	11 (20%)
40	SQD	J	314	-	44,45,54	0.42	1 (2%)	53,56,65	0.61	2 (3%)
29	CLA	M	310	18	48,56,73	1.71	6 (12%)	55,92,113	1.55	7 (12%)
36	DD6	B	302	-	39,45,45	2.06	3 (7%)	52,67,67	1.92	13 (25%)
29	CLA	a	817	-	45,53,73	1.80	6 (13%)	52,89,113	1.55	7 (13%)
39	KC1	P	213	27	48,53,53	1.52	7 (14%)	55,89,89	1.78	12 (21%)
29	CLA	f	805	-	60,68,73	1.53	6 (10%)	70,107,113	1.40	7 (10%)
36	DD6	E	302	-	39,45,45	2.11	3 (7%)	52,67,67	2.26	18 (34%)
29	CLA	a	811	-	56,64,73	1.62	6 (10%)	65,102,113	1.43	7 (10%)
29	CLA	l	508	-	41,49,73	1.82	7 (17%)	47,84,113	1.66	7 (14%)
29	CLA	J	307	-	46,54,73	1.73	7 (15%)	53,90,113	1.52	6 (11%)
29	CLA	O	309	-	65,73,73	1.51	6 (9%)	76,113,113	1.34	6 (7%)
29	CLA	J	308	-	56,64,73	1.57	6 (10%)	65,102,113	1.49	8 (12%)
29	CLA	i	201	-	65,73,73	1.43	6 (9%)	76,113,113	1.42	7 (9%)
36	DD6	K	202	-	39,45,45	2.15	3 (7%)	52,67,67	3.00	16 (30%)
36	DD6	M	304	-	39,45,45	2.05	3 (7%)	52,67,67	1.76	13 (25%)
39	KC1	B	313	21	48,53,53	1.53	7 (14%)	55,89,89	1.86	12 (21%)
37	PID	h	204	-	41,49,49	1.35	4 (9%)	49,76,76	1.40	6 (12%)
36	DD6	C	303	-	39,45,45	2.07	3 (7%)	52,67,67	2.04	15 (28%)
29	CLA	b	736	-	65,73,73	1.48	9 (13%)	76,113,113	6.29	12 (15%)
29	CLA	A	210	12	46,54,73	1.77	7 (15%)	53,90,113	1.51	7 (13%)
36	DD6	D	304	-	39,45,45	2.09	4 (10%)	52,67,67	2.14	15 (28%)
29	CLA	a	810	1	55,63,73	1.61	7 (12%)	64,101,113	1.46	8 (12%)
32	BCR	m	103	-	41,41,41	0.82	1 (2%)	56,56,56	2.35	18 (32%)
36	DD6	A	201	-	39,45,45	2.02	3 (7%)	52,67,67	2.02	16 (30%)
39	KC1	A	213	-	48,53,53	1.53	7 (14%)	55,89,89	1.84	11 (20%)
29	CLA	Q	315	-	41,49,73	1.84	7 (17%)	47,84,113	1.69	7 (14%)
29	CLA	K	208	-	46,54,73	1.74	7 (15%)	53,90,113	1.52	6 (11%)
29	CLA	l	504	-	65,73,73	1.46	6 (9%)	76,113,113	4.11	11 (14%)
29	CLA	M	308	-	48,56,73	1.71	7 (14%)	55,92,113	1.52	6 (10%)
29	CLA	O	311	-	51,59,73	1.67	6 (11%)	59,96,113	1.52	7 (11%)
29	CLA	I	212	-	55,63,73	1.61	6 (10%)	64,101,113	6.83	13 (20%)
37	PID	D	307	-	41,49,49	1.35	4 (9%)	49,76,76	1.59	7 (14%)
36	DD6	G	308	-	39,45,45	2.01	2 (5%)	52,67,67	2.12	15 (28%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
38	UIX	E	304	-	41,49,49	1.30	4 (9%)	52,74,74	2.43	18 (34%)
29	CLA	A	217	-	51,59,73	1.66	6 (11%)	59,96,113	1.49	8 (13%)
37	PID	N	301	-	41,49,49	1.34	4 (9%)	49,76,76	1.49	5 (10%)
29	CLA	b	725	-	65,73,73	1.47	8 (12%)	76,113,113	1.35	7 (9%)
37	PID	D	302	-	41,49,49	1.34	4 (9%)	49,76,76	1.45	5 (10%)
37	PID	P	208	-	41,49,49	1.37	4 (9%)	49,76,76	2.42	7 (14%)
36	DD6	M	302	-	39,45,45	2.11	4 (10%)	52,67,67	2.09	14 (26%)
38	UIX	A	203	-	41,49,49	1.27	4 (9%)	52,74,74	2.39	21 (40%)
38	UIX	T	306	-	41,49,49	1.29	4 (9%)	52,74,74	2.77	24 (46%)
39	KC1	G	315	-	48,53,53	1.54	7 (14%)	55,89,89	1.90	11 (20%)
29	CLA	a	822	-	65,73,73	1.46	6 (9%)	76,113,113	1.38	8 (10%)
29	CLA	M	315	-	46,54,73	1.73	6 (13%)	53,90,113	1.53	6 (11%)
29	CLA	a	814	-	46,54,73	1.74	7 (15%)	53,90,113	1.53	6 (11%)
29	CLA	b	719	-	50,58,73	1.69	6 (12%)	58,95,113	1.60	10 (17%)
29	CLA	F	312	16	46,54,73	1.73	6 (13%)	53,90,113	1.53	6 (11%)
29	CLA	B	309	-	55,63,73	1.58	6 (10%)	64,101,113	1.49	7 (10%)
32	BCR	a	838	-	41,41,41	0.76	0	56,56,56	2.12	18 (32%)
29	CLA	A	207	-	55,63,73	1.60	7 (12%)	64,101,113	1.48	7 (10%)
29	CLA	a	818	-	47,55,73	1.74	6 (12%)	54,91,113	1.53	8 (14%)
36	DD6	F	303	-	39,45,45	2.11	3 (7%)	52,67,67	2.09	13 (25%)
29	CLA	A	215	-	47,55,73	1.72	7 (14%)	54,91,113	1.55	6 (11%)
29	CLA	M	314	-	52,60,73	1.65	5 (9%)	60,97,113	1.49	7 (11%)
33	SF4	c	102	3	0,12,12	-	-	-	-	-
29	CLA	L	315	-	41,49,73	1.87	7 (17%)	47,84,113	1.63	7 (14%)
39	KC1	F	314	-	48,53,53	1.50	7 (14%)	55,89,89	1.87	10 (18%)
29	CLA	P	210	-	65,73,73	1.47	6 (9%)	76,113,113	1.36	7 (9%)
29	CLA	P	215	-	47,55,73	1.77	5 (10%)	54,91,113	1.70	9 (16%)
29	CLA	f	803	6	46,54,73	1.73	6 (13%)	53,90,113	1.56	6 (11%)
29	CLA	E	309	-	46,54,73	1.76	6 (13%)	53,90,113	1.56	7 (13%)
32	BCR	b	729	-	41,41,41	0.79	1 (2%)	56,56,56	1.88	20 (35%)
36	DD6	A	204	-	39,45,45	2.02	3 (7%)	52,67,67	1.87	15 (28%)
36	DD6	D	301	-	39,45,45	2.08	3 (7%)	52,67,67	2.07	15 (28%)
29	CLA	b	705	-	65,73,73	1.45	8 (12%)	76,113,113	1.45	7 (9%)
36	DD6	K	203	-	39,45,45	2.04	3 (7%)	52,67,67	1.90	13 (25%)
29	CLA	M	313	-	41,49,73	1.85	7 (17%)	47,84,113	1.69	7 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
37	PID	O	302	-	41,49,49	1.36	4 (9%)	49,76,76	1.42	7 (14%)
37	PID	T	304	-	41,49,49	1.33	4 (9%)	49,76,76	1.45	5 (10%)
39	KC1	N	310	-	48,53,53	1.52	7 (14%)	55,89,89	1.86	10 (18%)
34	LMG	b	732	-	44,44,55	0.80	1 (2%)	52,52,63	1.32	6 (11%)
37	PID	F	302	-	41,49,49	1.34	4 (9%)	49,76,76	1.67	6 (12%)
29	CLA	A	218	12	60,68,73	1.52	7 (11%)	70,107,113	1.46	8 (11%)
29	CLA	B	306	21	49,57,73	1.70	6 (12%)	55,93,113	1.55	8 (14%)
36	DD6	M	301	-	39,45,45	2.00	3 (7%)	52,67,67	1.85	15 (28%)
36	DD6	G	305	-	39,45,45	2.20	3 (7%)	52,67,67	2.96	17 (32%)
29	CLA	G	313	-	55,63,73	1.57	6 (10%)	64,101,113	1.50	7 (10%)
29	CLA	b	723	-	65,73,73	1.45	7 (10%)	76,113,113	1.41	8 (10%)
37	PID	N	302	-	41,49,49	1.36	4 (9%)	49,76,76	1.41	5 (10%)
39	KC1	L	306	29	48,53,53	1.55	7 (14%)	55,89,89	1.90	14 (25%)
37	PID	H	305	-	41,49,49	1.33	4 (9%)	49,76,76	1.75	8 (16%)
39	KC1	P	211	-	48,53,53	1.54	7 (14%)	55,89,89	1.86	13 (23%)
29	CLA	a	808	-	51,59,73	1.67	8 (15%)	59,96,113	1.50	8 (13%)
39	KC1	Q	314	26	48,53,53	1.54	7 (14%)	55,89,89	1.87	10 (18%)
29	CLA	h	201	-	60,68,73	1.51	7 (11%)	70,107,113	1.46	8 (11%)
35	DGD	G	320	-	46,46,67	1.01	2 (4%)	60,60,81	0.98	3 (5%)
29	CLA	K	213	-	48,56,73	1.71	7 (14%)	55,92,113	1.51	8 (14%)
37	PID	O	307	-	41,49,49	1.33	4 (9%)	49,76,76	1.45	7 (14%)
39	KC1	O	315	-	48,53,53	1.51	6 (12%)	55,89,89	1.87	10 (18%)
29	CLA	F	316	16	41,49,73	1.82	6 (14%)	47,84,113	1.68	7 (14%)
37	PID	C	305	-	41,49,49	1.36	4 (9%)	49,76,76	1.95	9 (18%)
32	BCR	i	204	-	41,41,41	0.76	0	56,56,56	2.35	15 (26%)
29	CLA	P	217	-	41,49,73	1.84	6 (14%)	47,84,113	1.74	7 (14%)
29	CLA	M	311	-	46,54,73	1.76	6 (13%)	53,90,113	1.55	8 (15%)
36	DD6	O	303	-	39,45,45	2.10	4 (10%)	52,67,67	2.19	17 (32%)
29	CLA	a	828	-	46,54,73	1.75	7 (15%)	53,90,113	1.54	6 (11%)
29	CLA	K	210	-	50,58,73	1.65	6 (12%)	58,95,113	1.58	8 (13%)
29	CLA	A	206	39	45,53,73	1.76	6 (13%)	52,89,113	1.63	7 (13%)
37	PID	H	301	-	41,49,49	1.34	4 (9%)	49,76,76	1.48	5 (10%)
39	KC1	Q	309	-	48,53,53	1.54	7 (14%)	55,89,89	1.88	11 (20%)
29	CLA	a	803	-	65,73,73	1.49	7 (10%)	76,113,113	1.38	6 (7%)
29	CLA	J	306	-	65,73,73	1.44	7 (10%)	76,113,113	1.42	7 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
37	PID	T	305	-	41,49,49	1.32	4 (9%)	49,76,76	1.52	7 (14%)
29	CLA	C	313	25	46,54,73	1.73	6 (13%)	53,90,113	1.53	6 (11%)
39	KC1	E	312	28	48,53,53	1.56	7 (14%)	55,89,89	1.84	12 (21%)
29	CLA	C	316	-	41,49,73	1.82	6 (14%)	47,84,113	1.73	7 (14%)
37	PID	j	101	-	41,49,49	1.37	4 (9%)	49,76,76	1.46	9 (18%)
29	CLA	G	319	13	41,49,73	1.81	6 (14%)	47,84,113	1.69	7 (14%)
29	CLA	N	309	-	65,73,73	1.48	6 (9%)	76,113,113	1.36	8 (10%)
29	CLA	Q	307	-	47,55,73	1.74	6 (12%)	54,91,113	1.52	7 (12%)
36	DD6	B	303	-	39,45,45	2.04	3 (7%)	52,67,67	1.80	14 (26%)
29	CLA	H	308	-	65,73,73	1.48	6 (9%)	76,113,113	1.41	9 (11%)
29	CLA	b	722	-	58,66,73	1.53	7 (12%)	67,104,113	1.50	7 (10%)
29	CLA	K	217	-	46,54,73	1.76	8 (17%)	53,90,113	1.55	6 (11%)
29	CLA	H	312	22	46,54,73	1.73	6 (13%)	53,90,113	1.59	6 (11%)
29	CLA	K	216	-	41,49,73	1.81	7 (17%)	47,84,113	1.74	7 (14%)
39	KC1	N	315	-	48,53,53	1.50	6 (12%)	55,89,89	1.81	10 (18%)
29	CLA	G	304	-	59,67,73	1.54	8 (13%)	68,105,113	1.51	7 (10%)
36	DD6	F	301	-	39,45,45	2.11	4 (10%)	52,67,67	1.99	14 (26%)
29	CLA	T	313	-	46,54,73	1.76	6 (13%)	53,90,113	1.55	6 (11%)
29	CLA	b	711	-	58,66,73	1.56	7 (12%)	67,104,113	1.44	8 (11%)
35	DGD	m	102	-	67,67,67	0.83	2 (2%)	81,81,81	0.91	4 (4%)
29	CLA	B	315	-	46,54,73	1.73	6 (13%)	53,90,113	1.59	6 (11%)
29	CLA	F	310	-	46,54,73	1.70	7 (15%)	53,90,113	1.63	7 (13%)
29	CLA	L	307	39	50,58,73	1.68	7 (14%)	58,95,113	5.67	10 (17%)
34	LMG	b	730	-	46,46,55	0.81	2 (4%)	54,54,63	1.32	5 (9%)
36	DD6	G	306	-	39,45,45	2.12	3 (7%)	52,67,67	2.19	13 (25%)
29	CLA	a	824	-	65,73,73	1.46	7 (10%)	76,113,113	1.37	7 (9%)
39	KC1	O	310	-	48,53,53	1.53	7 (14%)	55,89,89	1.86	12 (21%)
39	KC1	P	216	-	48,53,53	1.51	7 (14%)	55,89,89	1.84	9 (16%)
29	CLA	a	815	-	45,53,73	1.75	7 (15%)	52,89,113	1.63	8 (15%)
29	CLA	I	216	-	52,60,73	1.64	7 (13%)	60,97,113	1.58	9 (15%)
37	PID	G	310	-	41,49,49	1.33	4 (9%)	49,76,76	1.45	7 (14%)
29	CLA	T	309	25	46,54,73	1.74	7 (15%)	53,90,113	1.58	7 (13%)
40	SQD	B	317	-	41,42,54	0.44	1 (2%)	50,53,65	0.50	0
29	CLA	b	718	-	65,73,73	1.47	7 (10%)	76,113,113	1.48	8 (10%)
29	CLA	G	302	-	65,73,73	1.47	6 (9%)	76,113,113	1.40	7 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
29	CLA	F	315	-	41,49,73	1.84	5 (12%)	47,84,113	1.71	8 (17%)
39	KC1	C	312	-	48,53,53	1.54	7 (14%)	55,89,89	1.87	12 (21%)
29	CLA	L	312	-	55,63,73	1.58	6 (10%)	64,101,113	1.45	7 (10%)
29	CLA	f	802	-	46,54,73	1.73	7 (15%)	53,90,113	1.54	6 (11%)
39	KC1	K	215	-	48,53,53	1.56	7 (14%)	55,89,89	1.89	13 (23%)
29	CLA	b	712	-	65,73,73	1.47	7 (10%)	76,113,113	4.09	11 (14%)
29	CLA	Q	310	-	65,73,73	1.48	6 (9%)	76,113,113	1.39	8 (10%)
30	PQN	a	832	-	34,34,34	1.52	2 (5%)	42,45,45	1.23	5 (11%)
29	CLA	b	726	-	65,73,73	1.48	7 (10%)	76,113,113	1.37	8 (10%)
29	CLA	K	218	-	45,53,73	1.79	6 (13%)	52,89,113	1.56	6 (11%)
36	DD6	I	202	-	39,45,45	2.03	3 (7%)	52,67,67	1.92	14 (26%)
36	DD6	Q	302	-	39,45,45	1.99	3 (7%)	52,67,67	1.86	12 (23%)
29	CLA	J	311	-	53,61,73	1.64	9 (16%)	61,98,113	1.48	7 (11%)
37	PID	Q	304	-	41,49,49	1.33	4 (9%)	49,76,76	1.54	6 (12%)
39	KC1	T	312	-	48,53,53	1.50	7 (14%)	55,89,89	1.84	10 (18%)
29	CLA	K	214	-	55,63,73	1.62	9 (16%)	64,101,113	1.45	9 (14%)
29	CLA	a	831	-	65,73,73	1.46	7 (10%)	76,113,113	4.96	9 (11%)
39	KC1	H	311	-	48,53,53	1.52	7 (14%)	55,89,89	1.82	10 (18%)
29	CLA	a	825	-	65,73,73	1.49	8 (12%)	76,113,113	1.48	9 (11%)
29	CLA	b	713	-	53,61,73	1.65	5 (9%)	61,98,113	1.45	6 (9%)
29	CLA	a	829	-	65,73,73	1.46	7 (10%)	76,113,113	1.40	7 (9%)
29	CLA	F	307	-	46,54,73	1.74	6 (13%)	53,90,113	1.56	7 (13%)
34	LMG	P	201	-	27,27,55	0.98	0	35,35,63	1.29	5 (14%)
38	UIX	C	306	-	41,49,49	1.27	4 (9%)	52,74,74	2.55	22 (42%)
39	KC1	O	312	-	48,53,53	1.48	7 (14%)	55,89,89	1.98	11 (20%)
29	CLA	a	807	-	65,73,73	1.48	7 (10%)	76,113,113	1.42	9 (11%)
39	KC1	G	318	-	48,53,53	1.56	7 (14%)	55,89,89	1.83	10 (18%)
37	PID	F	306	-	41,49,49	1.35	4 (9%)	49,76,76	1.47	6 (12%)
29	CLA	I	213	14	65,73,73	1.48	6 (9%)	76,113,113	4.10	12 (15%)
36	DD6	G	307	-	39,45,45	2.71	10 (25%)	52,67,67	2.55	19 (36%)
37	PID	D	303	-	41,49,49	1.37	4 (9%)	49,76,76	1.51	8 (16%)
32	BCR	l	506	-	41,41,41	0.75	0	56,56,56	1.93	14 (25%)
29	CLA	b	708	2	52,60,73	1.66	7 (13%)	60,97,113	1.55	8 (13%)
29	CLA	D	314	-	47,55,73	1.72	7 (14%)	54,91,113	1.65	7 (12%)
37	PID	C	304	-	41,49,49	1.34	4 (9%)	49,76,76	1.44	6 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
37	PID	D	305	-	41,49,49	1.32	4 (9%)	49,76,76	1.48	7 (14%)
29	CLA	b	703	-	65,73,73	1.48	7 (10%)	76,113,113	1.34	6 (7%)
36	DD6	E	303	-	39,45,45	2.02	3 (7%)	52,67,67	1.74	10 (19%)
29	CLA	A	209	-	65,73,73	1.47	6 (9%)	76,113,113	1.39	9 (11%)
32	BCR	b	735	-	41,41,41	0.77	0	56,56,56	2.04	17 (30%)
36	DD6	m	101	-	39,45,45	2.04	3 (7%)	52,67,67	2.04	16 (30%)
29	CLA	a	819	-	57,65,73	1.58	7 (12%)	66,103,113	1.44	9 (13%)
34	LMG	K	201	-	43,43,55	0.79	0	51,51,63	1.32	5 (9%)
39	KC1	A	205	29	48,53,53	1.53	7 (14%)	55,89,89	1.87	13 (23%)
34	LMG	j	102	-	43,43,55	0.78	0	51,51,63	1.29	5 (9%)
29	CLA	Q	313	-	47,55,73	1.73	6 (12%)	54,91,113	1.53	7 (12%)
29	CLA	D	313	20	45,53,73	1.76	6 (13%)	52,89,113	1.55	6 (11%)
29	CLA	a	804	-	55,63,73	1.62	7 (12%)	64,101,113	1.54	9 (14%)
39	KC1	F	309	-	48,53,53	1.53	7 (14%)	55,89,89	1.88	11 (20%)
29	CLA	P	214	27	46,54,73	1.77	6 (13%)	53,90,113	1.55	6 (11%)
37	PID	T	307	-	41,49,49	1.33	4 (9%)	49,76,76	1.58	8 (16%)
39	KC1	T	315	25	48,53,53	1.51	7 (14%)	55,89,89	1.83	10 (18%)
36	DD6	M	303	-	39,45,45	2.11	4 (10%)	52,67,67	2.03	14 (26%)
36	DD6	N	303	-	39,45,45	1.96	3 (7%)	52,67,67	1.76	12 (23%)
36	DD6	J	302	-	39,45,45	2.08	2 (5%)	52,67,67	2.19	17 (32%)
29	CLA	b	714	-	64,72,73	1.47	7 (10%)	74,111,113	1.40	9 (12%)
29	CLA	l	502	10	65,73,73	1.49	9 (13%)	76,113,113	1.39	9 (11%)
36	DD6	L	305	-	39,45,45	2.05	3 (7%)	52,67,67	1.95	14 (26%)
29	CLA	a	820	-	65,73,73	1.47	8 (12%)	76,113,113	1.36	7 (9%)
29	CLA	B	316	-	45,53,73	1.78	6 (13%)	52,89,113	1.57	6 (11%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	CLA	B	308	-	1/1/15/20	13/37/115/115	-
29	CLA	D	312	20	1/1/11/20	5/15/93/115	-
29	CLA	J	305	-	1/1/11/20	2/15/93/115	-
38	UIX	B	304	-	-	2/31/87/87	0/3/3/3

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	CLA	b	707	-	1/1/15/20	11/37/115/115	-
36	DD6	A	202	-	-	1/26/80/80	0/3/3/3
29	CLA	C	311	-	1/1/12/20	7/21/99/115	-
29	CLA	M	306	-	1/1/12/20	6/23/101/115	-
37	PID	T	302	-	-	1/24/93/93	0/4/4/4
29	CLA	A	208	-	1/1/13/20	3/25/103/115	-
37	PID	Q	303	-	-	0/24/93/93	0/4/4/4
29	CLA	F	311	-	1/1/11/20	3/15/93/115	-
29	CLA	J	309	17	1/1/11/20	5/15/93/115	-
33	SF4	a	836	1,2	-	-	0/6/5/5
29	CLA	A	212	-	1/1/13/20	10/25/103/115	-
37	PID	G	303	-	-	6/24/93/93	0/4/4/4
36	DD6	T	303	-	-	7/26/80/80	0/3/3/3
29	CLA	C	314	-	1/1/11/20	7/16/94/115	-
29	CLA	a	809	1	1/1/15/20	17/37/115/115	-
29	CLA	M	309	-	1/1/11/20	6/15/93/115	-
29	CLA	D	316	-	1/1/10/20	5/8/86/115	-
38	UIX	P	207	-	-	6/31/87/87	0/3/3/3
29	CLA	l	501	-	1/1/14/20	13/31/109/115	-
36	DD6	K	206	-	-	1/26/80/80	0/3/3/3
39	KC1	I	215	14	-	10/15/71/71	-
37	PID	G	309	-	-	2/24/93/93	0/4/4/4
33	SF4	c	101	3	-	-	0/6/5/5
39	KC1	D	315	-	-	6/15/71/71	-
36	DD6	h	202	-	-	2/26/80/80	0/3/3/3
29	CLA	I	210	-	1/1/13/20	6/25/103/115	-
29	CLA	E	313	-	1/1/10/20	2/8/86/115	-
29	CLA	F	313	16	1/1/11/20	6/15/93/115	-
38	UIX	J	304	-	-	3/31/87/87	0/3/3/3
37	PID	Q	301	-	-	2/24/93/93	0/4/4/4
37	PID	C	307	-	-	2/24/93/93	0/4/4/4
29	CLA	L	309	-	1/1/13/20	2/25/103/115	-
29	CLA	E	310	28	1/1/11/20	4/15/93/115	-
29	CLA	G	301	-	1/1/11/20	6/18/96/115	-
35	DGD	B	318	-	-	9/34/74/95	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	CLA	i	202	-	1/1/15/20	12/37/115/115	-
29	CLA	C	308	-	1/1/11/20	7/16/94/115	-
29	CLA	P	212	-	1/1/12/20	8/21/99/115	-
29	CLA	N	313	23	1/1/11/20	9/15/93/115	-
35	DGD	h	203	-	-	8/43/83/95	0/2/2/2
29	CLA	a	830	-	1/1/13/20	5/27/105/115	-
29	CLA	b	731	-	1/1/13/20	3/27/105/115	-
29	CLA	L	311	19	1/1/11/20	7/15/93/115	-
32	BCR	l	507	-	-	5/29/63/63	0/2/2/2
29	CLA	N	311	-	1/1/12/20	6/21/99/115	-
29	CLA	a	837	-	1/1/13/20	12/25/103/115	-
29	CLA	M	307	-	1/1/13/20	6/25/103/115	-
29	CLA	T	308	-	1/1/11/20	2/16/94/115	-
29	CLA	N	316	-	1/1/10/20	5/8/86/115	-
36	DD6	K	205	-	-	1/26/80/80	0/3/3/3
29	CLA	B	312	-	1/1/15/20	10/37/115/115	-
37	PID	E	301	-	-	6/24/93/93	0/4/4/4
29	CLA	D	311	-	1/1/11/20	12/15/93/115	-
29	CLA	a	816	-	1/1/11/20	8/15/93/115	-
29	CLA	a	802	-	1/1/15/20	10/37/115/115	-
29	CLA	E	315	-	1/1/13/20	6/28/106/115	-
37	PID	N	305	-	-	19/24/93/93	0/4/4/4
29	CLA	a	813	-	1/1/12/20	10/21/99/115	-
29	CLA	G	316	-	1/1/15/20	12/37/115/115	-
29	CLA	Q	308	-	1/1/15/20	21/37/115/115	-
29	CLA	D	308	-	1/1/11/20	5/16/94/115	-
32	BCR	b	728	-	-	7/29/63/63	0/2/2/2
38	UIX	Q	305	-	-	5/31/87/87	0/3/3/3
37	PID	O	305	-	-	7/24/93/93	0/4/4/4
39	KC1	H	309	-	-	8/15/71/71	-
29	CLA	a	826	-	1/1/15/20	10/37/115/115	-
39	KC1	T	310	-	-	5/15/71/71	-
36	DD6	H	303	-	-	1/26/80/80	0/3/3/3
37	PID	O	301	-	-	3/24/93/93	0/4/4/4

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	CLA	a	821	-	1/1/11/20	9/16/94/115	-
36	DD6	K	204	-	-	5/26/80/80	0/3/3/3
35	DGD	j	106	-	-	16/38/78/95	0/2/2/2
39	KC1	H	314	-	-	6/15/71/71	-
29	CLA	b	720	-	1/1/15/20	15/37/115/115	-
29	CLA	I	214	-	1/1/13/20	5/25/103/115	-
29	CLA	G	312	13	1/1/15/20	16/37/115/115	-
37	PID	P	202	-	-	4/24/93/93	0/4/4/4
37	PID	F	304	-	-	15/24/93/93	1/4/4/4
29	CLA	H	315	-	1/1/10/20	3/8/86/115	-
34	LMG	h	205	-	-	3/23/43/70	0/1/1/1
29	CLA	I	209	-	1/1/14/20	14/31/109/115	-
36	DD6	I	204	-	-	3/26/80/80	0/3/3/3
29	CLA	A	211	-	1/1/13/20	5/25/103/115	-
39	KC1	C	310	-	-	9/15/71/71	-
29	CLA	b	709	-	1/1/14/20	17/31/109/115	-
29	CLA	B	314	21	1/1/10/20	6/8/86/115	-
29	CLA	L	310	-	1/1/13/20	9/25/103/115	-
29	CLA	E	308	-	1/1/15/20	10/37/115/115	-
37	PID	P	205	-	-	1/24/93/93	0/4/4/4
29	CLA	E	305	-	1/1/14/20	14/33/111/115	-
29	CLA	K	212	-	1/1/12/20	5/22/100/115	-
38	UIX	F	305	-	-	12/31/87/87	0/3/3/3
39	KC1	M	305	-	-	5/15/71/71	-
37	PID	C	302	-	-	2/24/93/93	0/4/4/4
29	CLA	a	805	-	1/1/13/20	6/25/103/115	-
29	CLA	H	313	-	1/1/11/20	8/16/94/115	-
36	DD6	J	303	-	-	2/26/80/80	0/3/3/3
29	CLA	b	721	-	1/1/13/20	10/29/107/115	-
29	CLA	G	317	-	1/1/12/20	8/23/101/115	-
29	CLA	O	316	-	1/1/10/20	5/8/86/115	-
29	CLA	b	701	-	1/1/15/20	13/37/115/115	-
29	CLA	O	308	-	1/1/11/20	6/16/94/115	-
29	CLA	b	715	-	1/1/11/20	7/15/93/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
39	KC1	C	315	25	-	8/15/71/71	-
29	CLA	F	308	-	1/1/11/20	3/15/93/115	-
29	CLA	G	314	-	1/1/14/20	8/31/109/115	-
29	CLA	a	801	-	1/1/15/20	10/37/115/115	-
29	CLA	b	702	-	1/1/15/20	17/37/115/115	-
39	KC1	N	312	23	-	6/15/71/71	-
29	CLA	E	306	28	1/1/15/20	14/37/115/115	-
29	CLA	b	724	-	1/1/11/20	2/16/94/115	-
38	UIX	N	306	-	-	9/31/87/87	0/3/3/3
34	LMG	b	734	-	-	10/35/55/70	0/1/1/1
34	LMG	A	219	-	-	17/32/52/70	0/1/1/1
29	CLA	B	310	-	1/1/15/20	16/37/115/115	-
29	CLA	a	812	-	1/1/14/20	15/31/109/115	-
29	CLA	N	308	-	1/1/11/20	7/16/94/115	-
29	CLA	b	706	-	1/1/15/20	11/37/115/115	-
37	PID	C	301	-	-	4/24/93/93	0/4/4/4
37	PID	P	203	-	-	3/24/93/93	0/4/4/4
29	CLA	l	503	10	1/1/15/20	15/37/115/115	-
29	CLA	B	311	21	1/1/12/20	4/21/99/115	-
29	CLA	b	716	-	1/1/12/20	7/23/101/115	-
36	DD6	B	301	-	-	4/24/78/80	0/3/3/3
36	DD6	I	203	-	-	7/26/80/80	0/3/3/3
29	CLA	J	313	-	1/1/10/20	2/8/86/115	-
37	PID	N	304	-	-	1/24/93/93	0/4/4/4
29	CLA	E	314	28	-	5/17/95/115	-
36	DD6	L	303	-	-	0/26/80/80	0/3/3/3
36	DD6	I	206	-	-	2/26/80/80	0/3/3/3
29	CLA	L	317	-	1/1/11/20	5/15/93/115	-
29	CLA	b	704	-	1/1/15/20	10/37/115/115	-
29	CLA	D	309	-	1/1/11/20	2/15/93/115	-
34	LMG	E	316	-	-	10/27/47/70	0/1/1/1
37	PID	T	301	-	-	2/24/93/93	0/4/4/4
32	BCR	f	801	-	-	5/29/63/63	0/2/2/2
35	DGD	b	733	-	-	24/46/86/95	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	CLA	T	316	-	1/1/10/20	6/8/86/115	-
34	LMG	K	219	-	-	16/30/50/70	0/1/1/1
29	CLA	A	214	12	1/1/10/20	4/8/86/115	-
29	CLA	a	806	1	1/1/15/20	16/37/115/115	-
37	PID	D	306	-	-	3/24/93/93	0/4/4/4
29	CLA	N	314	-	1/1/11/20	7/16/94/115	-
37	PID	H	304	-	-	0/24/93/93	0/4/4/4
38	UIX	O	306	-	-	6/31/87/87	0/3/3/3
32	BCR	a	834	-	-	0/29/63/63	0/2/2/2
29	CLA	i	203	-	1/1/13/20	12/25/103/115	-
37	PID	P	206	-	-	8/24/93/93	0/4/4/4
29	CLA	T	314	-	1/1/11/20	7/16/94/115	-
37	PID	N	307	-	-	6/24/93/93	0/4/4/4
29	CLA	b	710	-	1/1/11/20	7/15/93/115	-
29	CLA	G	311	13	1/1/12/20	7/21/99/115	-
39	KC1	L	314	-	-	7/15/71/71	-
36	DD6	K	221	-	-	5/26/80/80	0/3/3/3
39	KC1	J	312	17	-	5/15/71/71	-
29	CLA	C	309	-	1/1/15/20	10/37/115/115	-
37	PID	O	304	-	-	3/24/93/93	0/4/4/4
29	CLA	B	307	-	1/1/11/20	2/13/91/115	-
32	BCR	f	804	-	-	2/29/63/63	0/2/2/2
32	BCR	a	835	-	-	2/29/63/63	0/2/2/2
29	CLA	L	316	-	1/1/12/20	11/22/100/115	-
29	CLA	J	310	-	1/1/11/20	6/16/94/115	-
29	CLA	H	307	-	1/1/11/20	5/16/94/115	-
35	DGD	j	103	-	-	10/32/72/95	0/2/2/2
39	KC1	D	310	-	-	5/15/71/71	-
29	CLA	K	211	-	1/1/13/20	7/25/103/115	-
37	PID	H	302	-	-	2/24/93/93	0/4/4/4
29	CLA	I	201	29	1/1/11/20	4/13/91/115	-
29	CLA	Q	312	-	1/1/11/20	3/15/93/115	-
29	CLA	b	717	-	1/1/15/20	14/37/115/115	-
29	CLA	A	216	-	1/1/10/20	0/8/86/115	-
30	PQN	b	727	-	-	4/23/43/43	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	CLA	O	313	24	1/1/11/20	5/15/93/115	-
29	CLA	l	509	-	1/1/10/20	2/8/86/115	-
29	CLA	H	310	-	1/1/12/20	9/21/99/115	-
36	DD6	J	301	-	-	3/26/80/80	0/3/3/3
36	DD6	B	319	-	-	9/26/80/80	0/3/3/3
29	CLA	E	311	-	1/1/15/20	11/37/115/115	-
29	CLA	P	209	-	1/1/11/20	8/16/94/115	-
29	CLA	I	211	-	1/1/15/20	8/37/115/115	-
29	CLA	L	313	-	1/1/12/20	8/23/101/115	-
29	CLA	j	104	29	1/1/12/20	4/22/100/115	-
36	DD6	I	205	-	-	6/26/80/80	0/3/3/3
29	CLA	I	217	-	1/1/13/20	9/25/103/115	-
39	KC1	Q	311	-	-	6/15/71/71	-
36	DD6	B	305	-	-	2/26/80/80	0/3/3/3
29	CLA	I	207	14	1/1/11/20	6/18/96/115	-
29	CLA	l	505	-	1/1/15/20	12/37/115/115	-
37	PID	Q	306	-	-	3/24/93/93	0/4/4/4
29	CLA	a	827	-	1/1/15/20	12/37/115/115	-
36	DD6	P	204	-	-	2/26/80/80	0/3/3/3
38	UIX	L	302	-	-	2/31/87/87	0/3/3/3
29	CLA	l	510	-	1/1/11/20	5/13/91/115	-
37	PID	H	306	-	-	4/24/93/93	0/4/4/4
29	CLA	K	207	15	1/1/11/20	6/18/96/115	-
31	LHG	a	833	-	-	8/52/52/53	-
29	CLA	O	314	-	-	6/16/94/115	-
36	DD6	L	304	-	-	2/26/80/80	0/3/3/3
35	DGD	j	105	-	-	0/30/70/95	0/2/2/2
29	CLA	K	209	-	1/1/12/20	10/24/102/115	-
29	CLA	I	208	-	1/1/11/20	7/15/93/115	-
29	CLA	T	311	-	1/1/11/20	10/15/93/115	-
36	DD6	L	301	-	-	4/26/80/80	0/3/3/3
29	CLA	L	308	-	1/1/12/20	10/23/101/115	-
37	PID	T	317	-	-	10/24/93/93	1/4/4/4
39	KC1	M	312	-	-	6/15/71/71	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	CLA	a	823	-	1/1/13/20	11/29/107/115	-
34	LMG	K	220	-	-	13/31/51/70	0/1/1/1
39	KC1	E	307	-	-	6/15/71/71	-
40	SQD	J	314	-	-	9/40/60/69	0/1/1/1
29	CLA	M	310	18	1/1/11/20	5/17/95/115	-
36	DD6	B	302	-	-	2/26/80/80	0/3/3/3
29	CLA	a	817	-	1/1/11/20	4/13/91/115	-
39	KC1	P	213	27	-	5/15/71/71	-
29	CLA	f	805	-	1/1/14/20	10/31/109/115	-
36	DD6	E	302	-	-	2/26/80/80	0/3/3/3
29	CLA	a	811	-	1/1/13/20	6/27/105/115	-
29	CLA	l	508	-	1/1/10/20	2/8/86/115	-
29	CLA	J	307	-	1/1/11/20	3/15/93/115	-
29	CLA	O	309	-	-	10/37/115/115	-
29	CLA	J	308	-	1/1/13/20	8/27/105/115	-
29	CLA	i	201	-	1/1/15/20	16/37/115/115	-
36	DD6	K	202	-	-	8/26/80/80	0/3/3/3
36	DD6	M	304	-	-	3/26/80/80	0/3/3/3
39	KC1	B	313	21	-	8/15/71/71	-
37	PID	h	204	-	-	2/24/93/93	1/4/4/4
36	DD6	C	303	-	-	0/26/80/80	0/3/3/3
29	CLA	b	736	-	1/1/15/20	16/37/115/115	-
29	CLA	A	210	12	1/1/11/20	6/15/93/115	-
36	DD6	D	304	-	-	6/26/80/80	0/3/3/3
29	CLA	a	810	1	1/1/13/20	10/25/103/115	-
32	BCR	m	103	-	-	5/29/63/63	0/2/2/2
36	DD6	A	201	-	-	3/26/80/80	0/3/3/3
39	KC1	A	213	-	-	7/15/71/71	-
29	CLA	Q	315	-	1/1/10/20	6/8/86/115	-
29	CLA	K	208	-	1/1/11/20	5/15/93/115	-
29	CLA	l	504	-	1/1/15/20	10/37/115/115	-
29	CLA	M	308	-	1/1/11/20	9/17/95/115	-
29	CLA	O	311	-	1/1/12/20	3/21/99/115	-
29	CLA	I	212	-	1/1/13/20	10/25/103/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
37	PID	D	307	-	-	4/24/93/93	0/4/4/4
36	DD6	G	308	-	-	1/26/80/80	0/3/3/3
38	UIX	E	304	-	-	2/31/87/87	0/3/3/3
29	CLA	A	217	-	1/1/12/20	7/21/99/115	-
37	PID	N	301	-	-	4/24/93/93	0/4/4/4
29	CLA	b	725	-	1/1/15/20	9/37/115/115	-
37	PID	D	302	-	-	1/24/93/93	0/4/4/4
37	PID	P	208	-	-	4/24/93/93	0/4/4/4
36	DD6	M	302	-	-	1/26/80/80	0/3/3/3
38	UIX	A	203	-	-	4/31/87/87	0/3/3/3
38	UIX	T	306	-	-	4/31/87/87	0/3/3/3
39	KC1	G	315	-	-	6/15/71/71	-
29	CLA	a	822	-	1/1/15/20	8/37/115/115	-
29	CLA	M	315	-	1/1/11/20	5/15/93/115	-
29	CLA	a	814	-	1/1/11/20	6/15/93/115	-
29	CLA	b	719	-	1/1/12/20	10/19/97/115	-
29	CLA	F	312	16	1/1/11/20	5/15/93/115	-
29	CLA	B	309	-	1/1/13/20	6/25/103/115	-
32	BCR	a	838	-	-	6/29/63/63	0/2/2/2
29	CLA	A	207	-	1/1/13/20	5/25/103/115	-
29	CLA	a	818	-	1/1/11/20	4/16/94/115	-
36	DD6	F	303	-	-	0/26/80/80	0/3/3/3
29	CLA	A	215	-	1/1/11/20	4/16/94/115	-
29	CLA	M	314	-	1/1/12/20	7/22/100/115	-
33	SF4	c	102	3	-	-	0/6/5/5
29	CLA	L	315	-	1/1/10/20	4/8/86/115	-
39	KC1	F	314	-	-	6/15/71/71	-
29	CLA	P	210	-	1/1/15/20	10/37/115/115	-
29	CLA	P	215	-	1/1/11/20	7/16/94/115	-
29	CLA	f	803	6	1/1/11/20	8/15/93/115	-
29	CLA	E	309	-	1/1/11/20	8/15/93/115	-
32	BCR	b	729	-	-	6/29/63/63	0/2/2/2
36	DD6	A	204	-	-	2/26/80/80	0/3/3/3
36	DD6	D	301	-	-	8/26/80/80	0/3/3/3
29	CLA	b	705	-	1/1/15/20	12/37/115/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
36	DD6	K	203	-	-	6/26/80/80	0/3/3/3
29	CLA	M	313	-	1/1/10/20	2/8/86/115	-
37	PID	O	302	-	-	2/24/93/93	0/4/4/4
37	PID	T	304	-	-	1/24/93/93	0/4/4/4
39	KC1	N	310	-	-	6/15/71/71	-
34	LMG	b	732	-	-	20/39/59/70	0/1/1/1
37	PID	F	302	-	-	3/24/93/93	0/4/4/4
29	CLA	A	218	12	1/1/14/20	10/31/109/115	-
29	CLA	B	306	21	1/1/11/20	5/18/96/115	-
36	DD6	M	301	-	-	2/26/80/80	0/3/3/3
36	DD6	G	305	-	-	7/26/80/80	0/3/3/3
29	CLA	G	313	-	1/1/13/20	3/25/103/115	-
29	CLA	b	723	-	1/1/15/20	5/37/115/115	-
37	PID	N	302	-	-	2/24/93/93	0/4/4/4
39	KC1	L	306	29	-	5/15/71/71	-
37	PID	H	305	-	-	3/24/93/93	0/4/4/4
39	KC1	P	211	-	-	7/15/71/71	-
29	CLA	a	808	-	1/1/12/20	4/21/99/115	-
39	KC1	Q	314	26	-	8/15/71/71	-
29	CLA	h	201	-	1/1/14/20	7/31/109/115	-
35	DGD	G	320	-	-	9/34/74/95	0/2/2/2
29	CLA	K	213	-	1/1/11/20	5/17/95/115	-
37	PID	O	307	-	-	4/24/93/93	0/4/4/4
39	KC1	O	315	-	-	9/15/71/71	-
29	CLA	F	316	16	1/1/10/20	4/8/86/115	-
37	PID	C	305	-	-	9/24/93/93	0/4/4/4
32	BCR	i	204	-	-	4/29/63/63	0/2/2/2
29	CLA	P	217	-	1/1/10/20	3/8/86/115	-
29	CLA	M	311	-	1/1/11/20	8/15/93/115	-
36	DD6	O	303	-	-	4/26/80/80	0/3/3/3
29	CLA	a	828	-	1/1/11/20	8/15/93/115	-
29	CLA	K	210	-	1/1/12/20	6/19/97/115	-
29	CLA	A	206	39	1/1/11/20	3/13/91/115	-
37	PID	H	301	-	-	2/24/93/93	0/4/4/4

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
39	KC1	Q	309	-	-	7/15/71/71	-
29	CLA	a	803	-	1/1/15/20	8/37/115/115	-
29	CLA	J	306	-	1/1/15/20	17/37/115/115	-
37	PID	T	305	-	-	0/24/93/93	0/4/4/4
29	CLA	C	313	25	1/1/11/20	5/15/93/115	-
39	KC1	E	312	28	-	7/15/71/71	-
29	CLA	C	316	-	1/1/10/20	6/8/86/115	-
37	PID	j	101	-	-	2/24/93/93	0/4/4/4
29	CLA	G	319	13	1/1/10/20	3/8/86/115	-
29	CLA	N	309	-	1/1/15/20	15/37/115/115	-
29	CLA	Q	307	-	1/1/11/20	1/16/94/115	-
36	DD6	B	303	-	-	0/26/80/80	0/3/3/3
29	CLA	H	308	-	1/1/15/20	9/37/115/115	-
29	CLA	b	722	-	1/1/13/20	8/29/107/115	-
29	CLA	K	217	-	1/1/11/20	4/15/93/115	-
29	CLA	H	312	22	1/1/11/20	7/15/93/115	-
29	CLA	K	216	-	1/1/10/20	3/8/86/115	-
39	KC1	N	315	-	-	9/15/71/71	-
29	CLA	G	304	-	1/1/13/20	12/30/108/115	-
36	DD6	F	301	-	-	8/26/80/80	0/3/3/3
29	CLA	T	313	-	1/1/11/20	7/15/93/115	-
29	CLA	b	711	-	1/1/13/20	11/29/107/115	-
35	DGD	m	102	-	-	8/55/95/95	0/2/2/2
29	CLA	B	315	-	1/1/11/20	3/15/93/115	-
29	CLA	F	310	-	1/1/11/20	8/15/93/115	-
29	CLA	L	307	39	1/1/12/20	9/19/97/115	-
34	LMG	b	730	-	-	19/41/61/70	0/1/1/1
36	DD6	G	306	-	-	1/26/80/80	0/3/3/3
29	CLA	a	824	-	1/1/15/20	9/37/115/115	-
39	KC1	O	310	-	-	6/15/71/71	-
39	KC1	P	216	-	-	6/15/71/71	-
29	CLA	a	815	-	1/1/11/20	4/13/91/115	-
29	CLA	I	216	-	1/1/12/20	4/22/100/115	-
37	PID	G	310	-	-	2/24/93/93	0/4/4/4
29	CLA	T	309	25	1/1/11/20	4/15/93/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
40	SQD	B	317	-	-	4/37/57/69	0/1/1/1
29	CLA	b	718	-	1/1/15/20	14/37/115/115	-
29	CLA	G	302	-	1/1/15/20	15/37/115/115	-
29	CLA	F	315	-	1/1/10/20	3/8/86/115	-
39	KC1	C	312	-	-	8/15/71/71	-
29	CLA	L	312	-	1/1/13/20	11/25/103/115	-
29	CLA	f	802	-	1/1/11/20	4/15/93/115	-
39	KC1	K	215	-	-	6/15/71/71	-
29	CLA	b	712	-	1/1/15/20	12/37/115/115	-
29	CLA	Q	310	-	1/1/15/20	13/37/115/115	-
30	PQN	a	832	-	-	6/23/43/43	0/2/2/2
29	CLA	b	726	-	1/1/15/20	6/37/115/115	-
29	CLA	K	218	-	1/1/11/20	7/13/91/115	-
36	DD6	I	202	-	-	5/26/80/80	0/3/3/3
36	DD6	Q	302	-	-	1/26/80/80	0/3/3/3
29	CLA	J	311	-	1/1/12/20	8/23/101/115	-
37	PID	Q	304	-	-	2/24/93/93	0/4/4/4
39	KC1	T	312	-	-	5/15/71/71	-
29	CLA	K	214	-	1/1/13/20	8/25/103/115	-
29	CLA	a	831	-	1/1/15/20	14/37/115/115	-
39	KC1	H	311	-	-	6/15/71/71	-
29	CLA	a	825	-	1/1/15/20	13/37/115/115	-
29	CLA	b	713	-	1/1/12/20	4/23/101/115	-
29	CLA	a	829	-	1/1/15/20	16/37/115/115	-
29	CLA	F	307	-	1/1/11/20	2/15/93/115	-
34	LMG	P	201	-	-	6/22/42/70	0/1/1/1
38	UIX	C	306	-	-	6/31/87/87	0/3/3/3
39	KC1	O	312	-	-	4/15/71/71	-
29	CLA	a	807	-	1/1/15/20	16/37/115/115	-
39	KC1	G	318	-	-	5/15/71/71	-
37	PID	F	306	-	-	0/24/93/93	0/4/4/4
29	CLA	I	213	14	1/1/15/20	13/37/115/115	-
36	DD6	G	307	-	-	2/26/80/80	0/3/3/3
37	PID	D	303	-	-	1/24/93/93	0/4/4/4
32	BCR	l	506	-	-	9/29/63/63	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	CLA	b	708	2	1/1/12/20	5/22/100/115	-
29	CLA	D	314	-	1/1/11/20	7/16/94/115	-
37	PID	C	304	-	-	3/24/93/93	0/4/4/4
37	PID	D	305	-	-	5/24/93/93	0/4/4/4
29	CLA	b	703	-	1/1/15/20	13/37/115/115	-
36	DD6	E	303	-	-	1/26/80/80	0/3/3/3
29	CLA	A	209	-	1/1/15/20	20/37/115/115	-
32	BCR	b	735	-	-	4/29/63/63	0/2/2/2
36	DD6	m	101	-	-	1/26/80/80	0/3/3/3
29	CLA	a	819	-	1/1/13/20	6/28/106/115	-
34	LMG	K	201	-	-	17/38/58/70	0/1/1/1
39	KC1	A	205	29	-	6/15/71/71	-
34	LMG	j	102	-	-	24/38/58/70	0/1/1/1
29	CLA	Q	313	-	1/1/11/20	6/16/94/115	-
29	CLA	D	313	20	1/1/11/20	4/13/91/115	-
29	CLA	a	804	-	1/1/13/20	1/25/103/115	-
39	KC1	F	309	-	-	7/15/71/71	-
29	CLA	P	214	27	1/1/11/20	7/15/93/115	-
37	PID	T	307	-	-	4/24/93/93	0/4/4/4
39	KC1	T	315	25	-	5/15/71/71	-
36	DD6	M	303	-	-	6/26/80/80	0/3/3/3
36	DD6	N	303	-	-	1/26/80/80	0/3/3/3
36	DD6	J	302	-	-	2/26/80/80	0/3/3/3
29	CLA	b	714	-	1/1/14/20	6/36/114/115	-
29	CLA	l	502	10	1/1/15/20	13/37/115/115	-
36	DD6	L	305	-	-	4/26/80/80	0/3/3/3
29	CLA	a	820	-	1/1/15/20	10/37/115/115	-
29	CLA	B	316	-	1/1/11/20	4/13/91/115	-

The worst 5 of 2170 bond length outliers are listed below:

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

The worst 5 of 3687 bond angle outliers are listed below:

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

5 of 220 chirality outliers are listed below:

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

5 of 2704 torsion outliers are listed below:

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

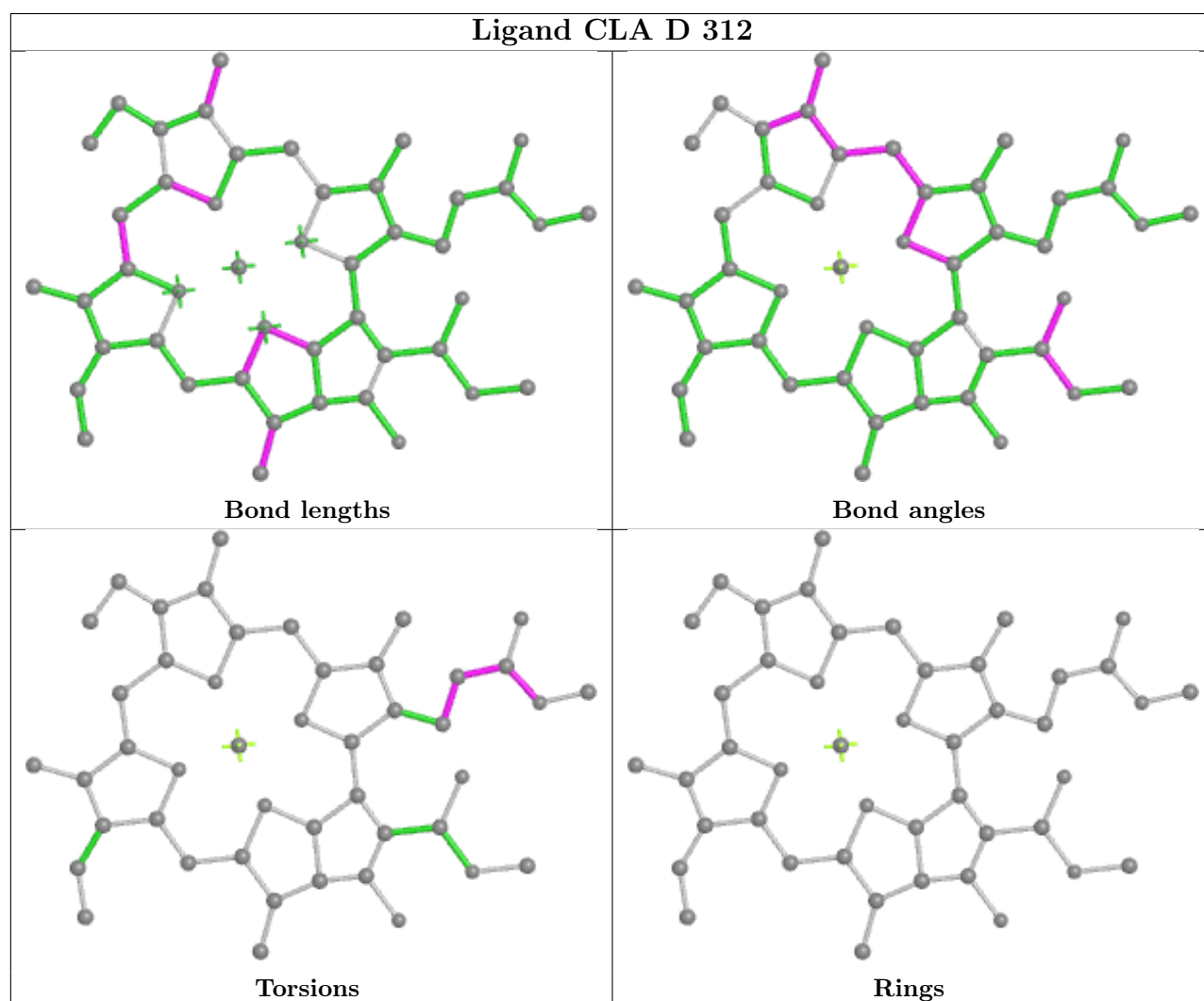
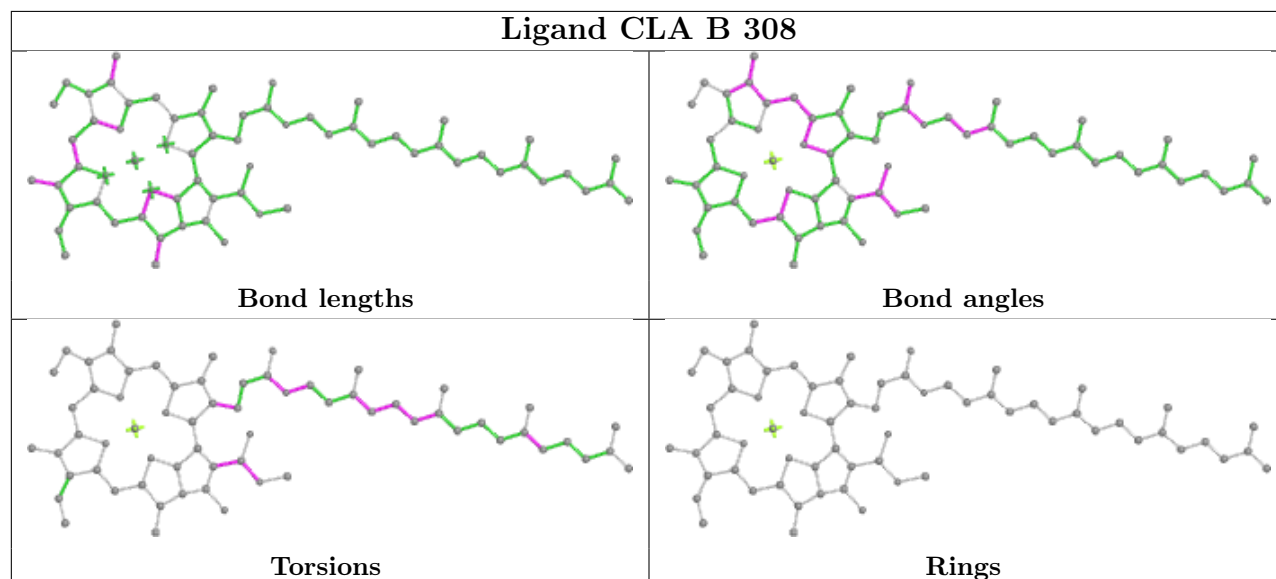
All (3) ring outliers are listed below:

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

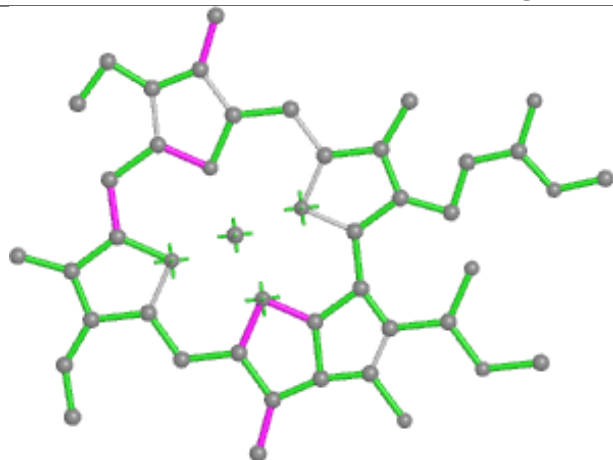
No monomer is involved in short contacts.

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

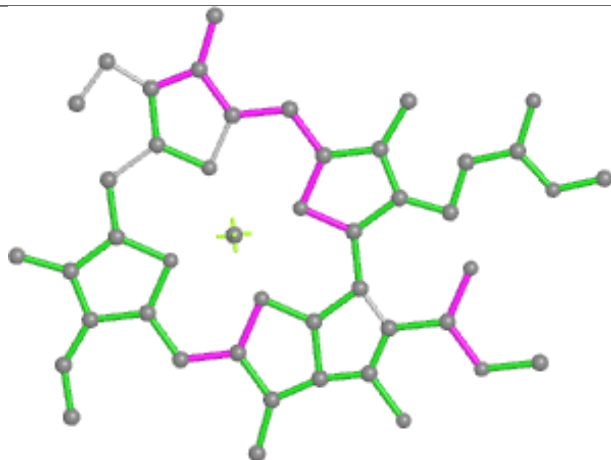
any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



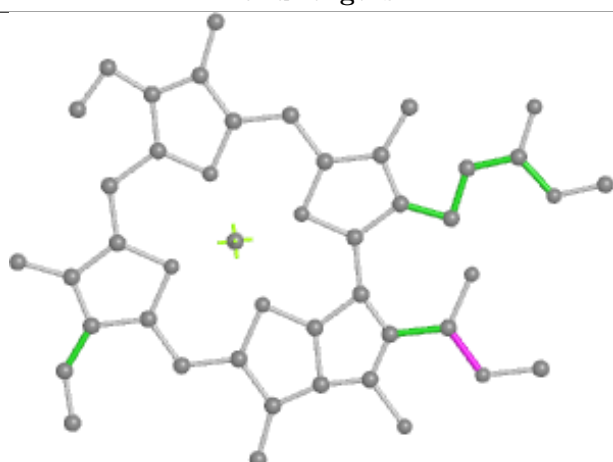
Ligand CLA J 305



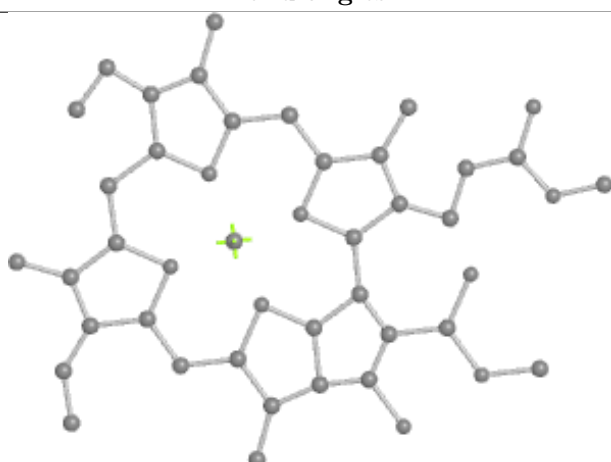
Bond lengths



Bond angles

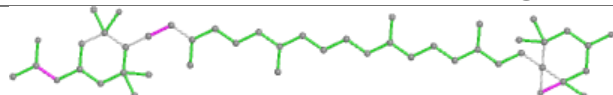


Torsions

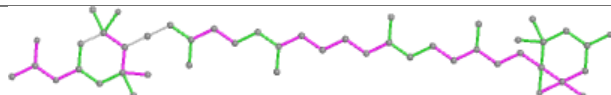


Rings

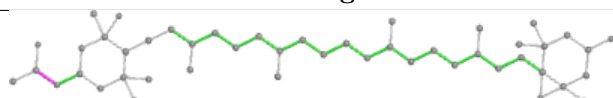
Ligand UIX B 304



Bond lengths



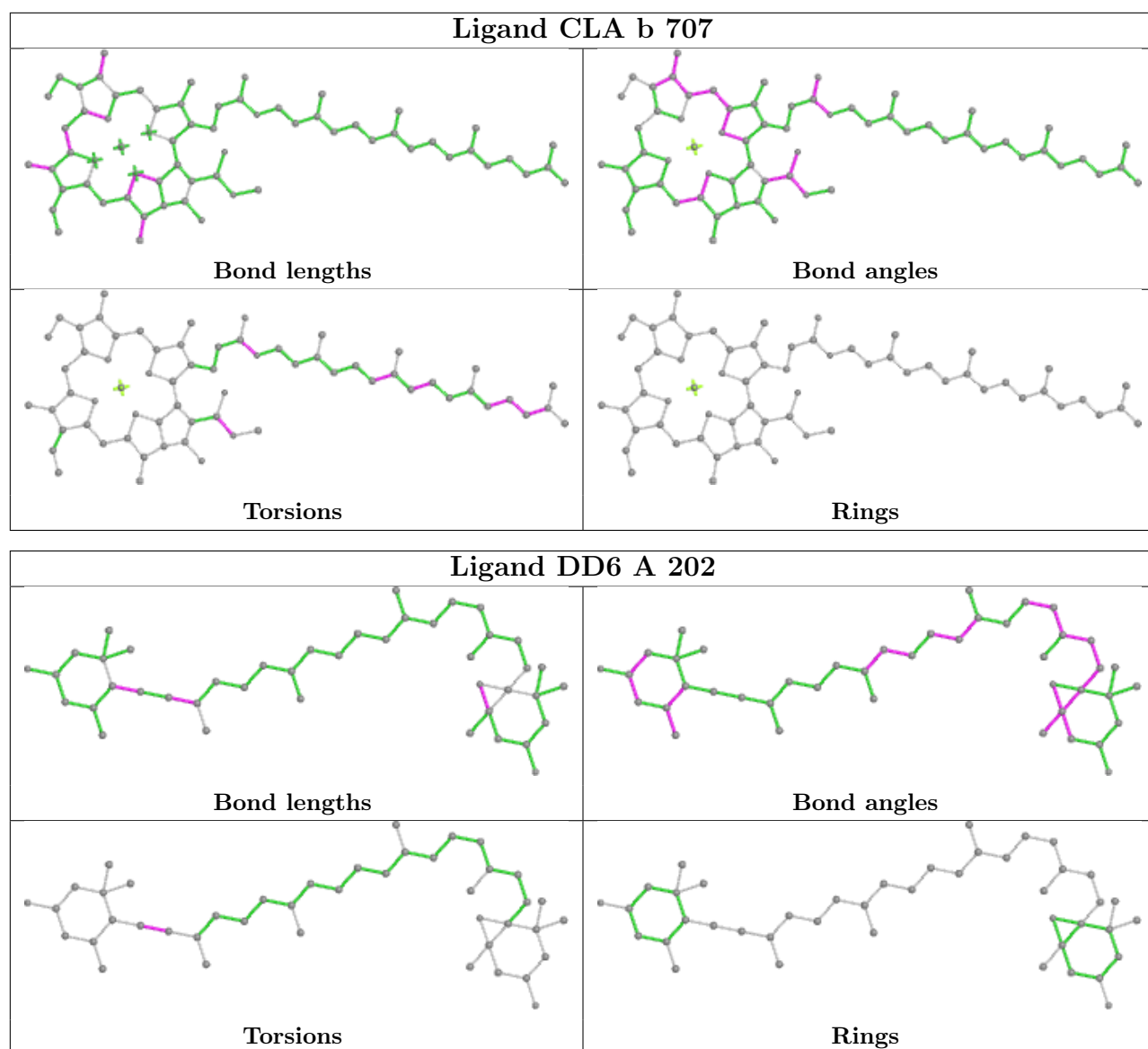
Bond angles



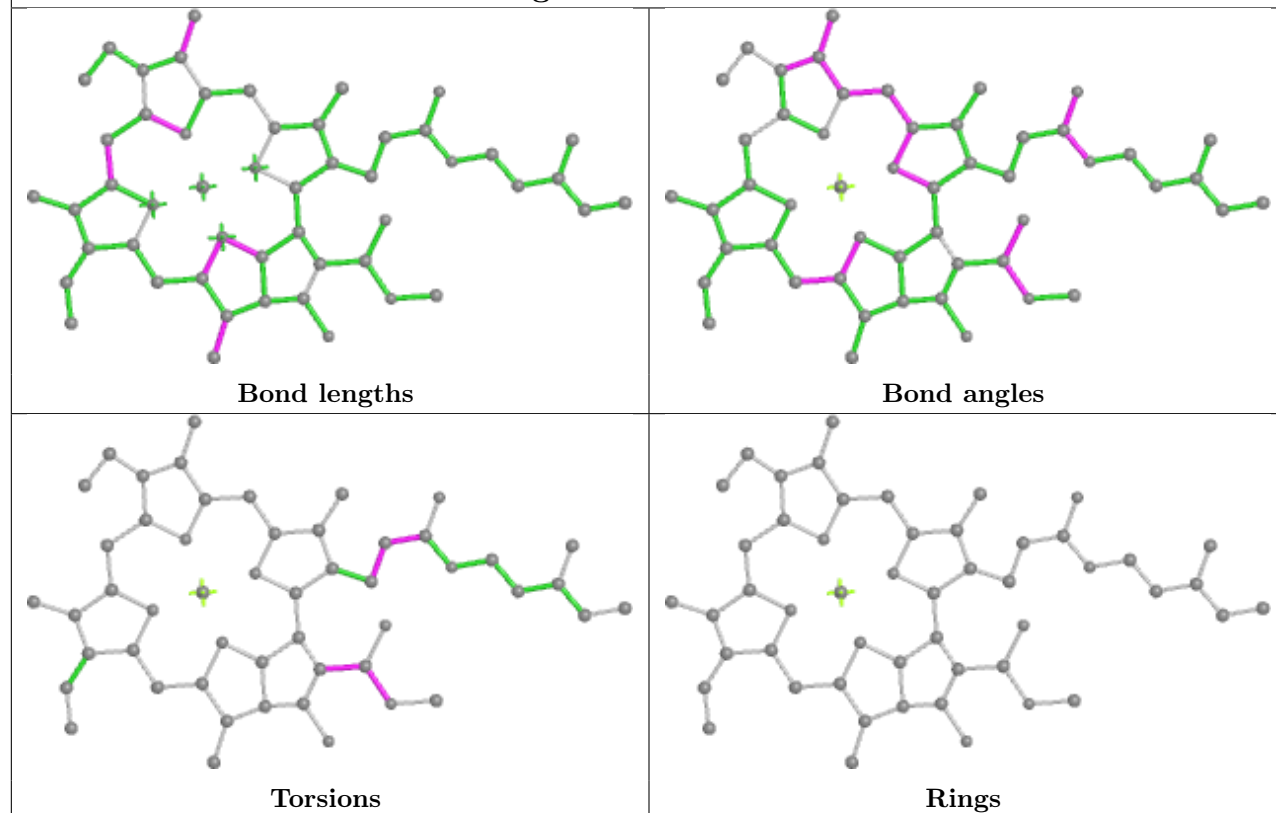
Torsions



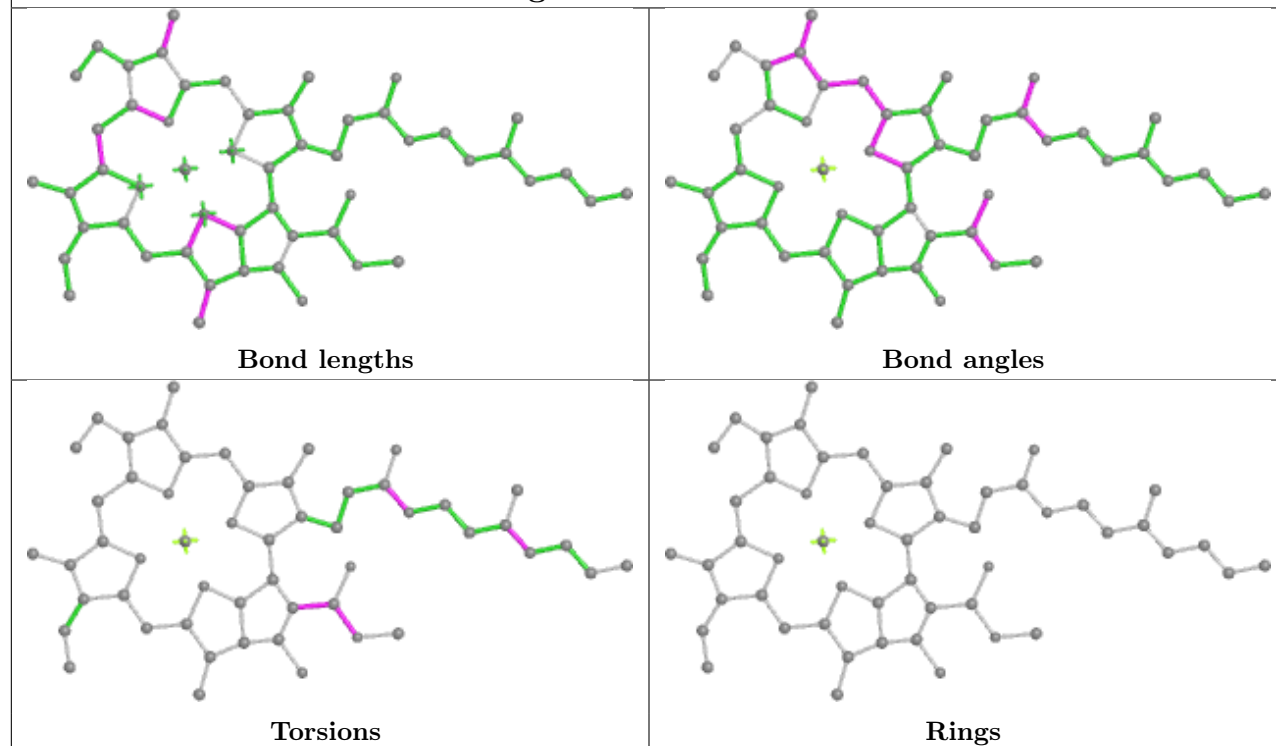
Rings

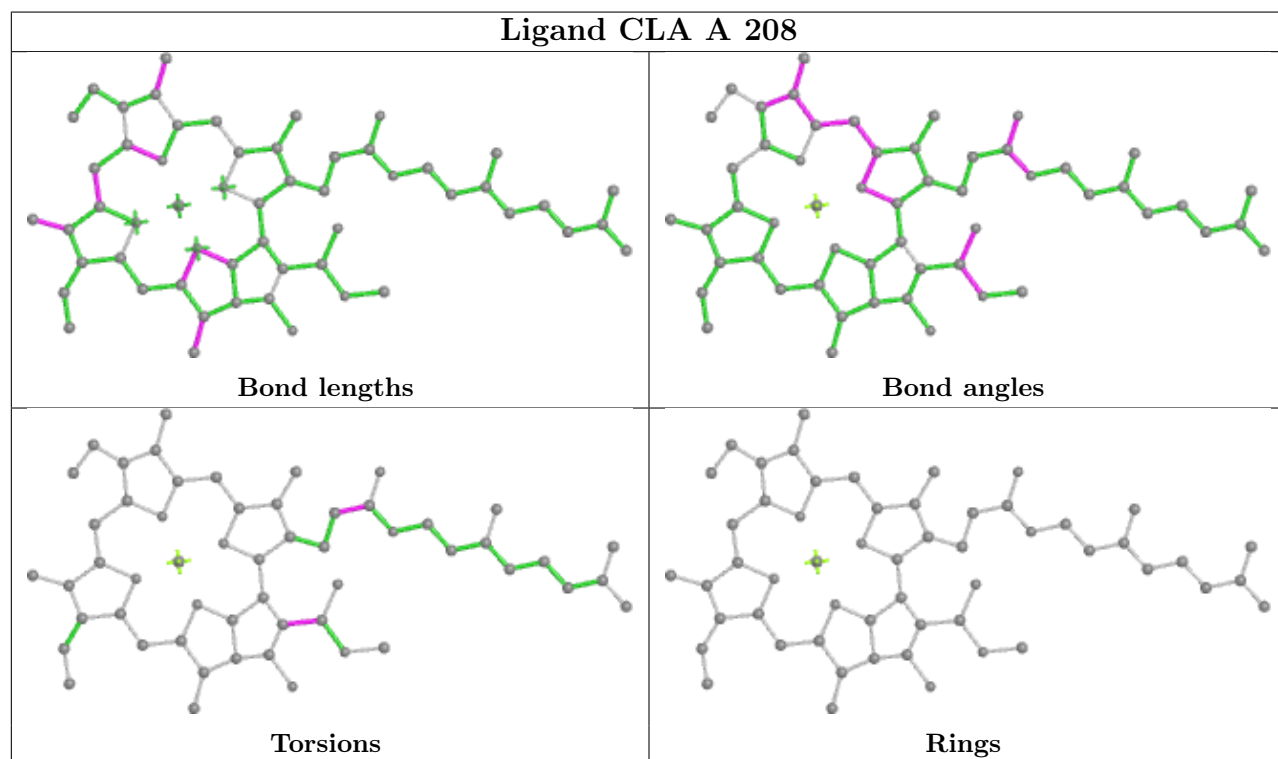
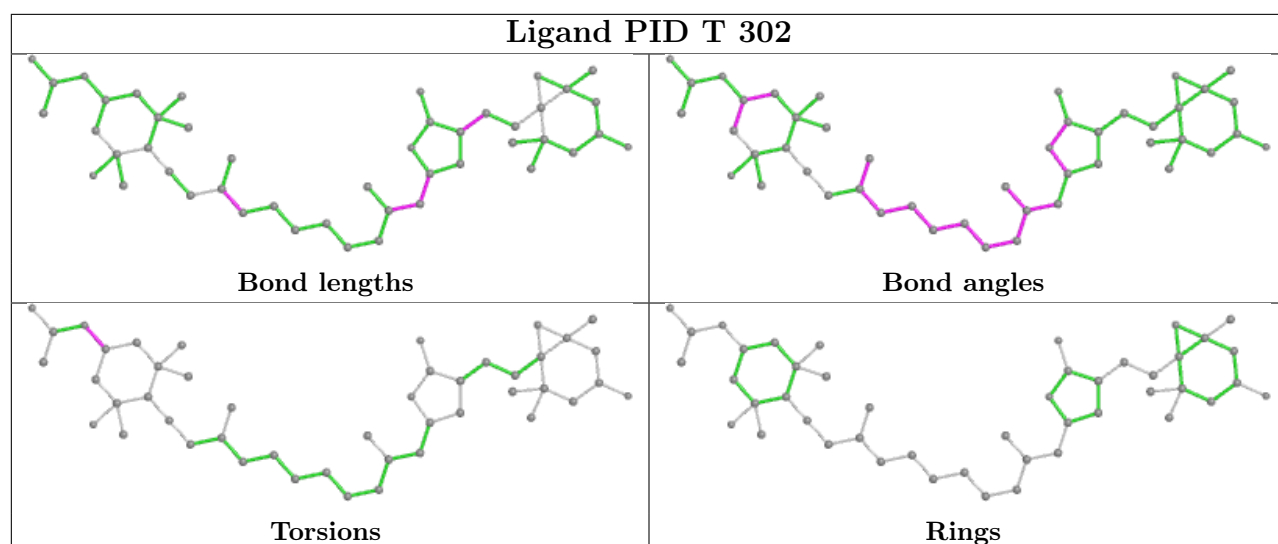


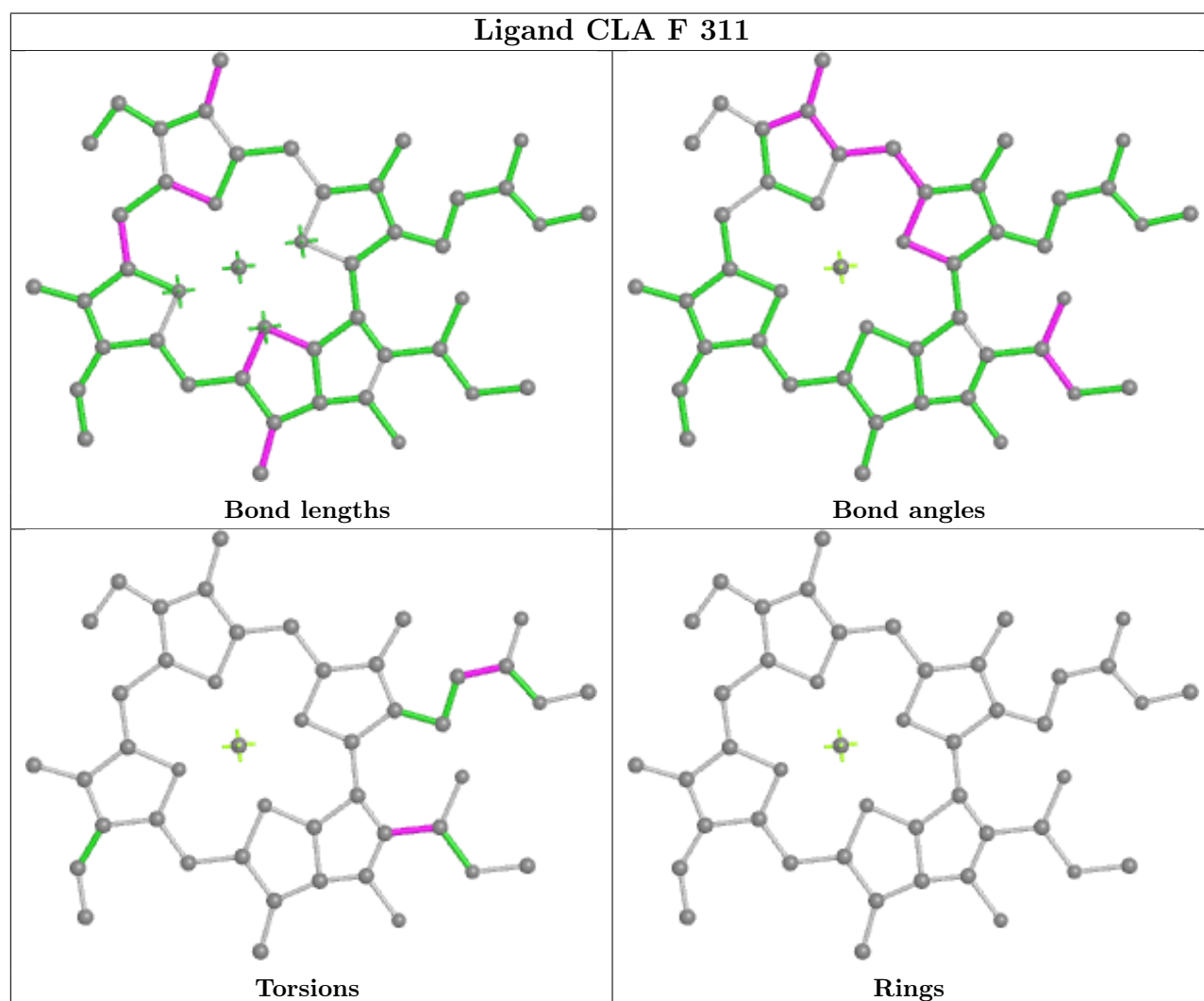
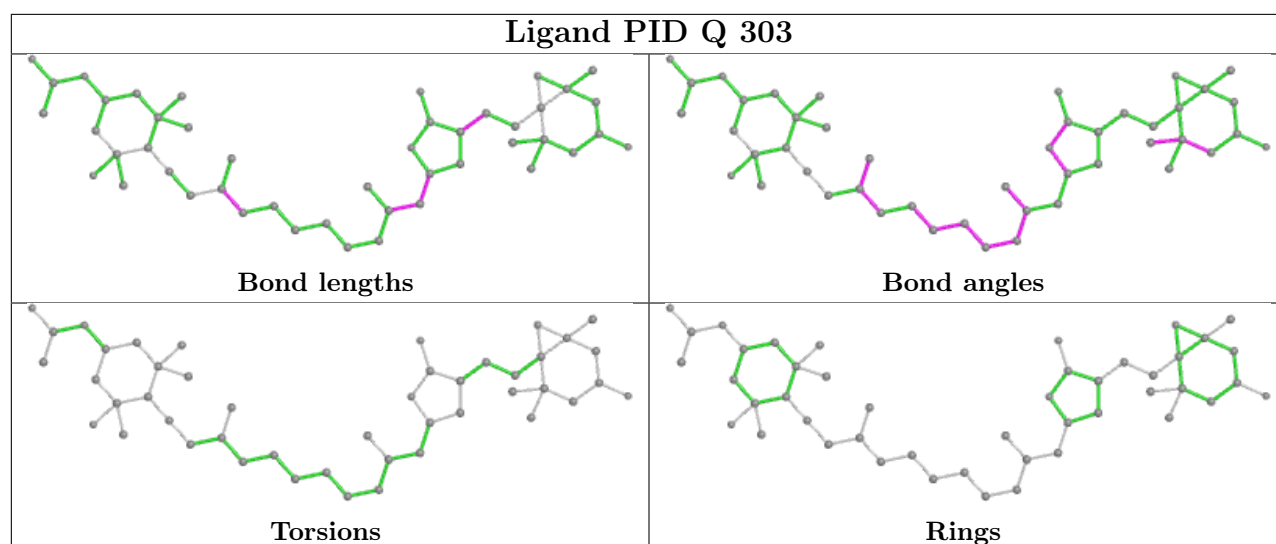
Ligand CLA C 311



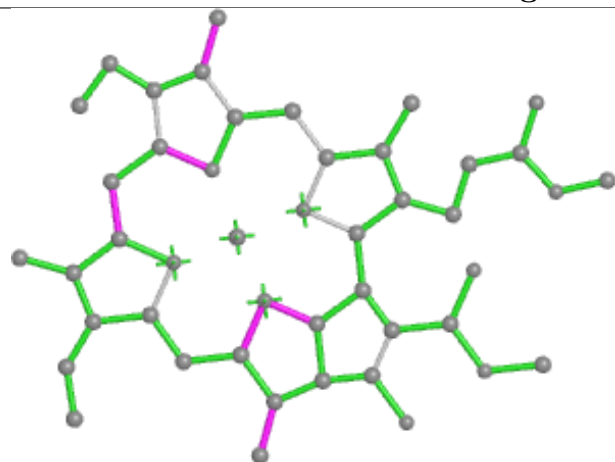
Ligand CLA M 306



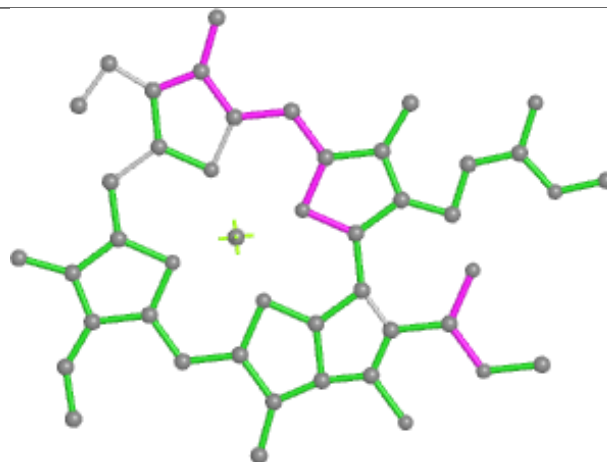




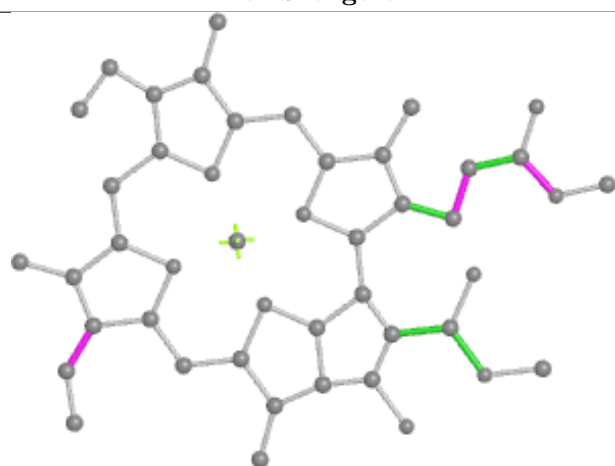
Ligand CLA J 309



Bond lengths



Bond angles

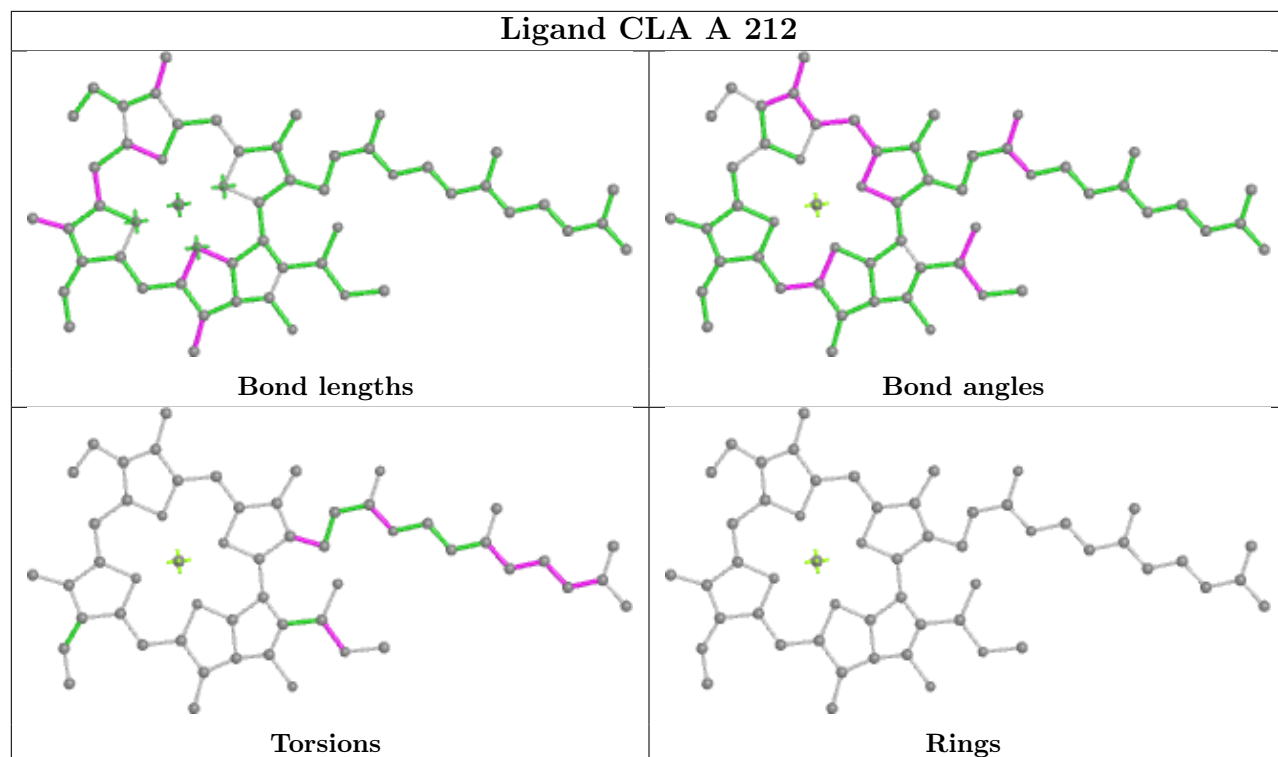


Torsions

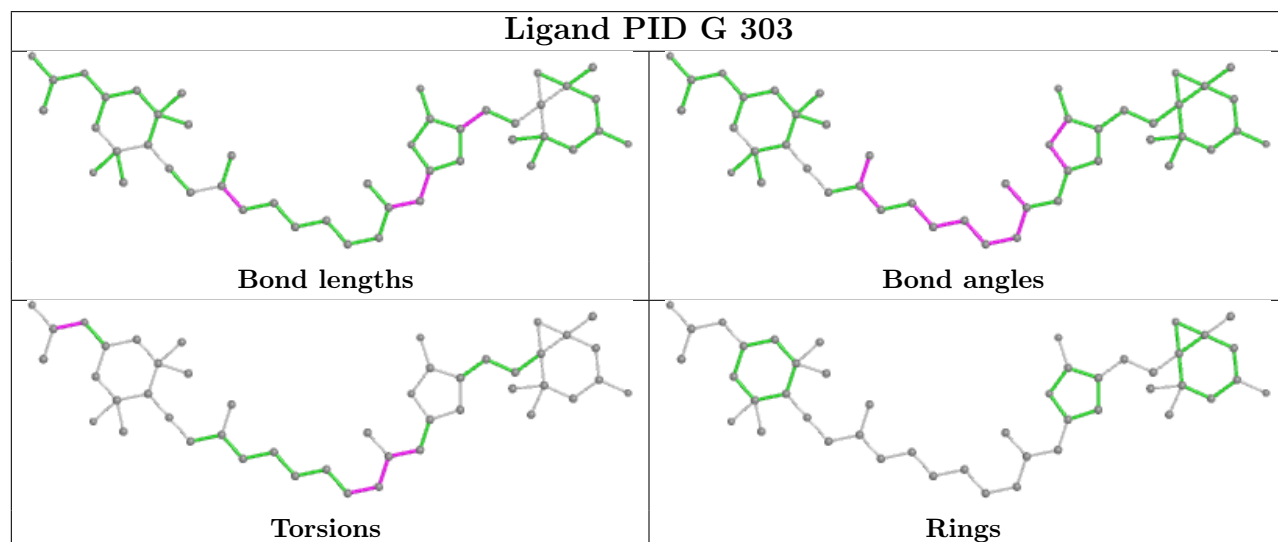


Rings

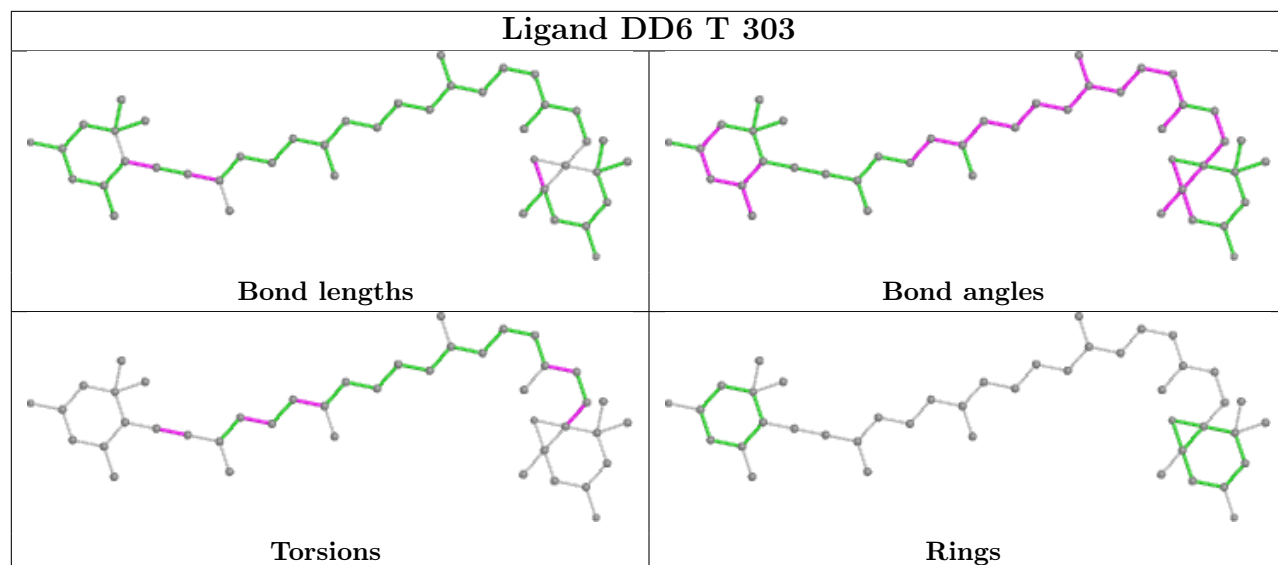
Ligand CLA A 212



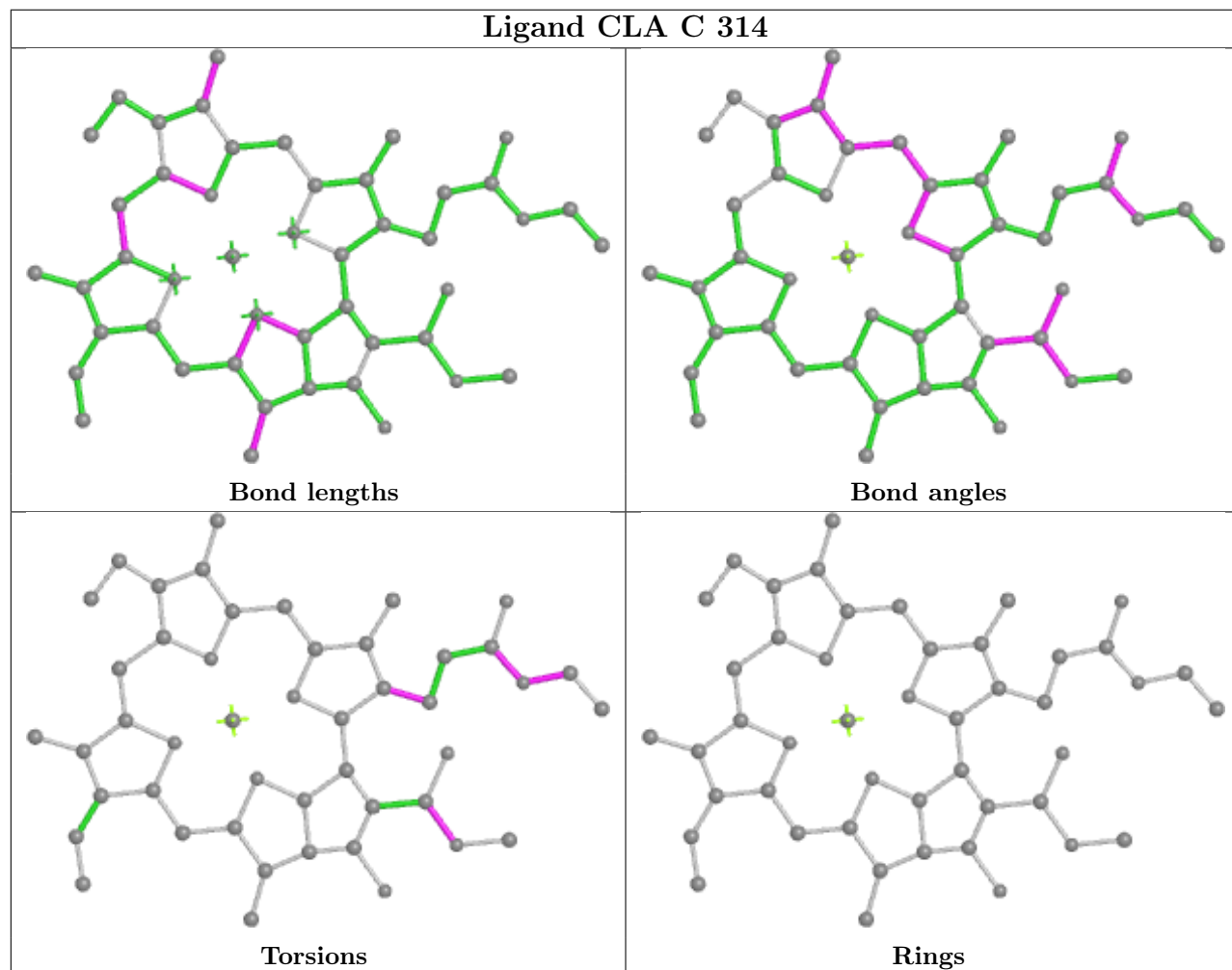
Ligand PID G 303



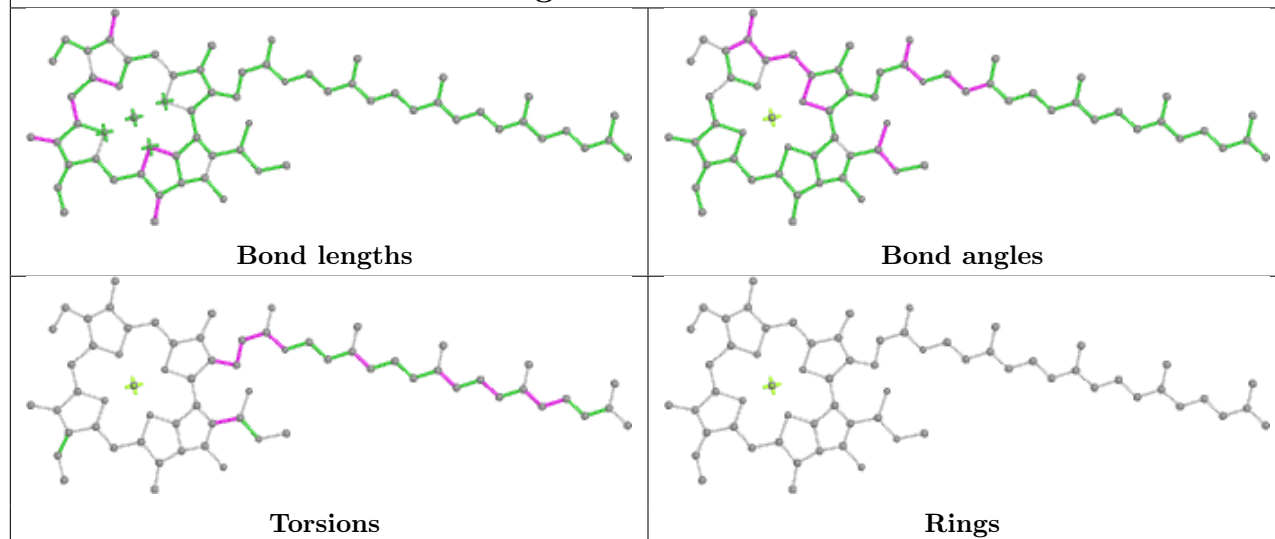
Ligand DD6 T 303



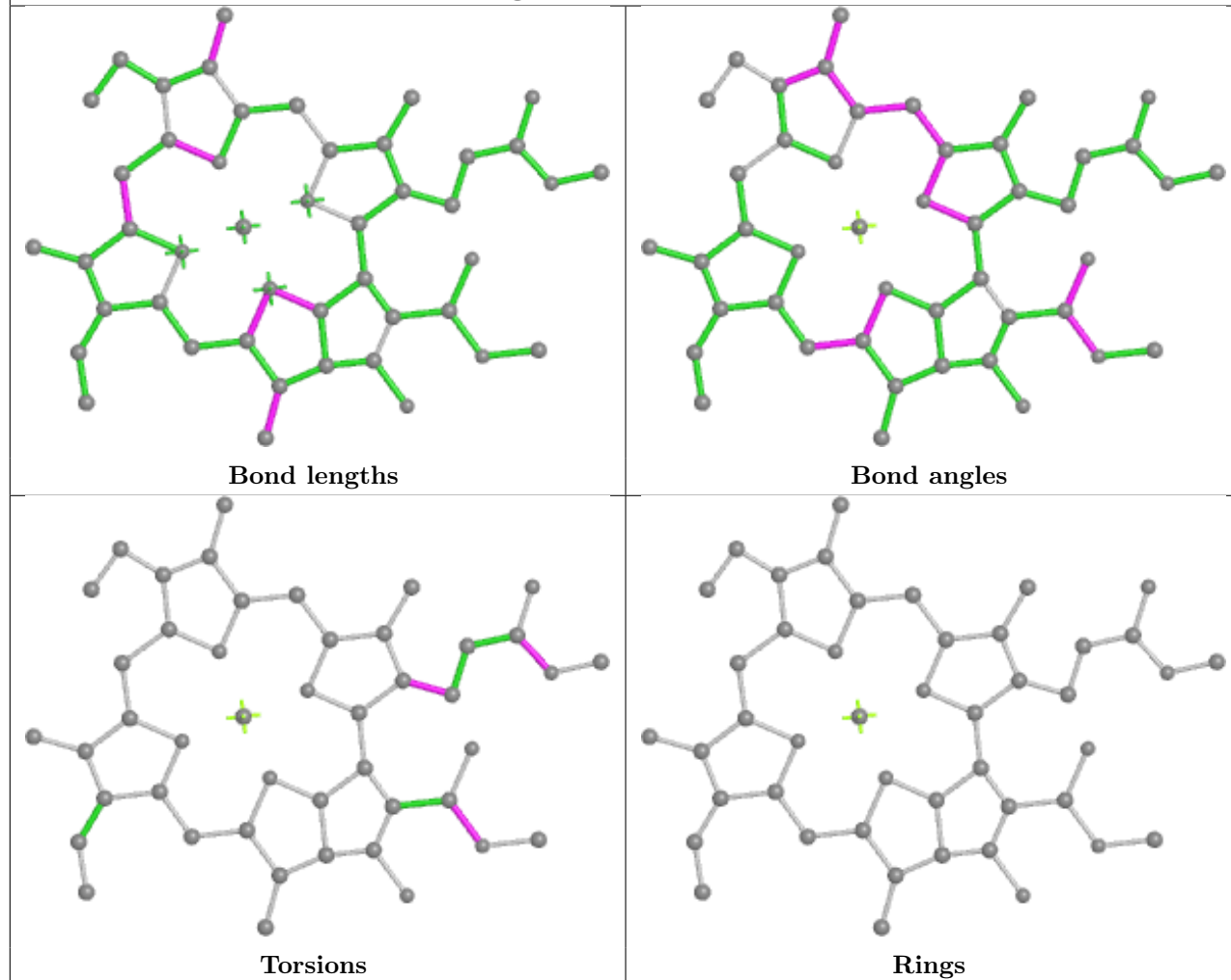
Ligand CLA C 314



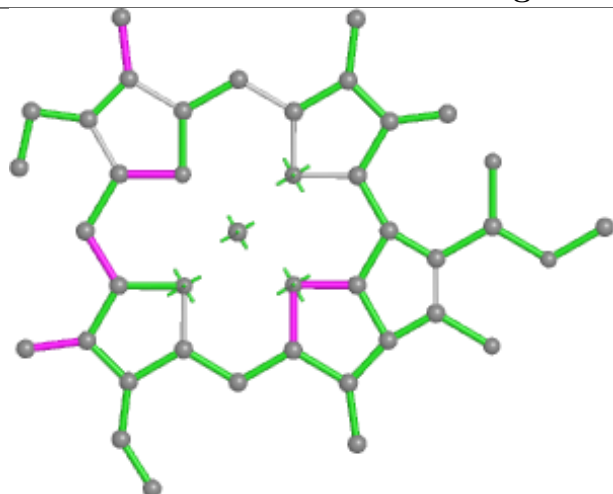
Ligand CLA a 809



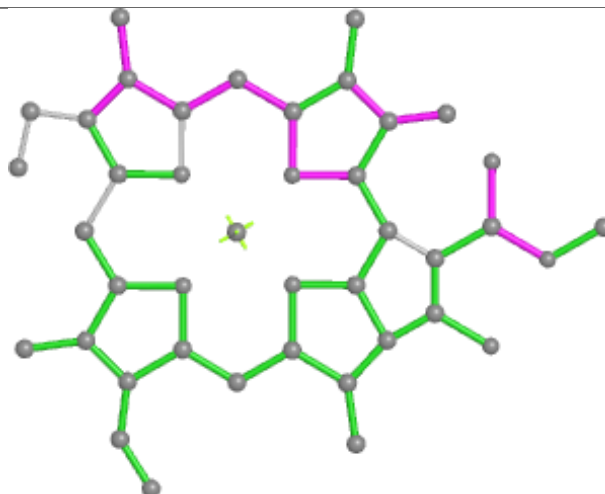
Ligand CLA M 309



Ligand CLA D 316



Bond lengths



Bond angles

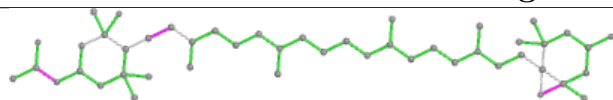


Torsions

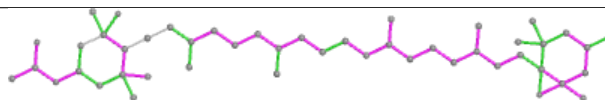


Rings

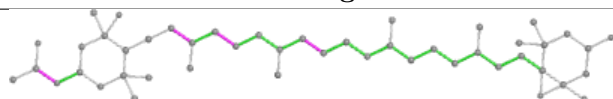
Ligand UIX P 207



Bond lengths



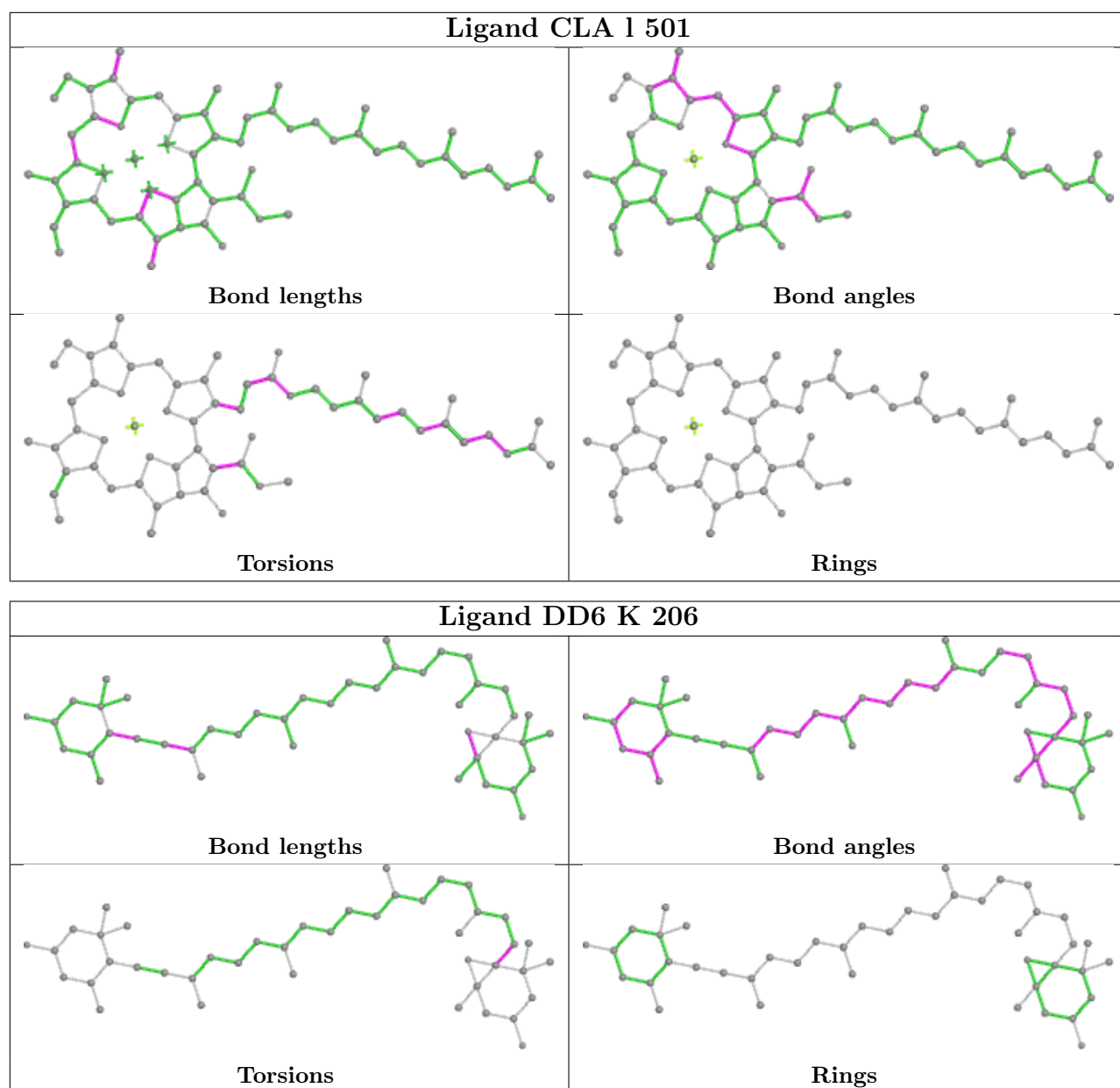
Bond angles



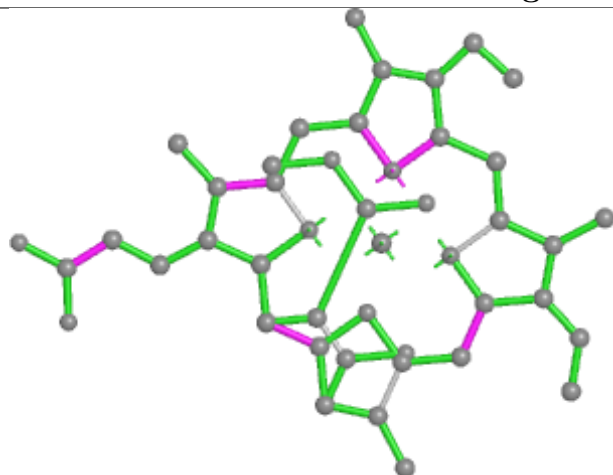
Torsions



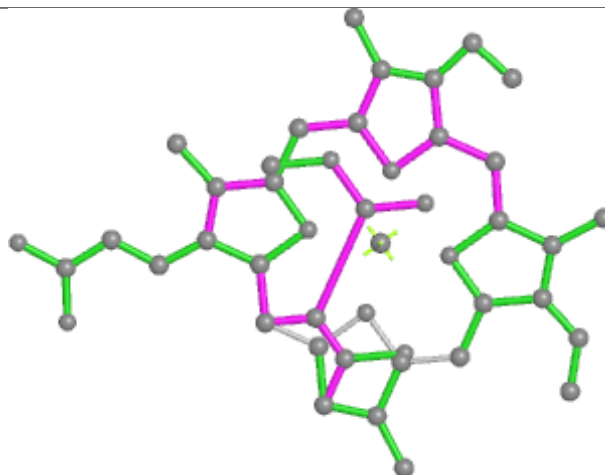
Rings



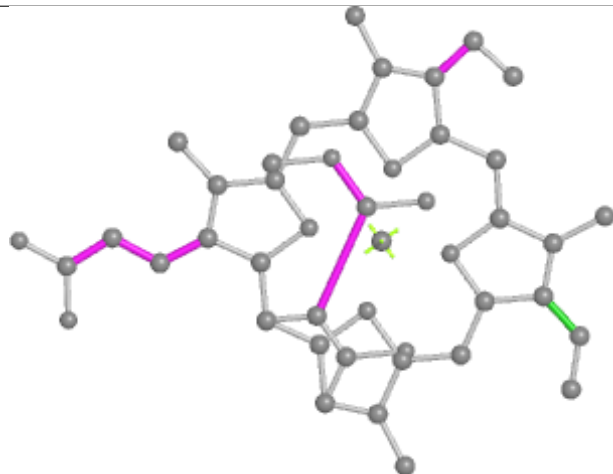
Ligand KC1 I 215



Bond lengths



Bond angles

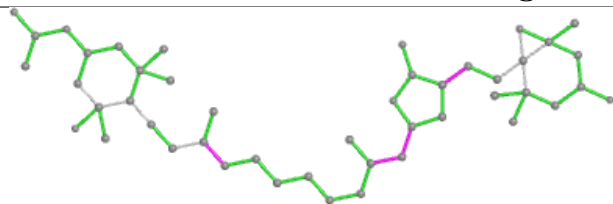


Torsions

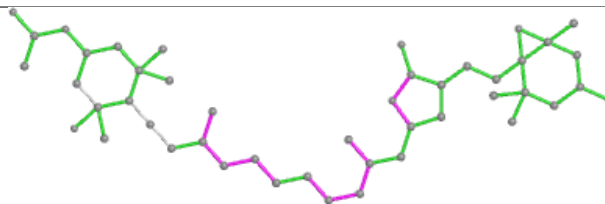


Rings

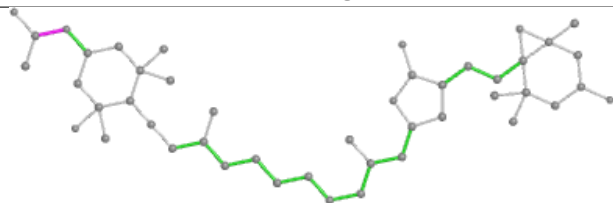
Ligand PID G 309



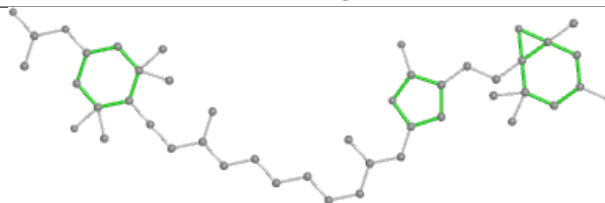
Bond lengths



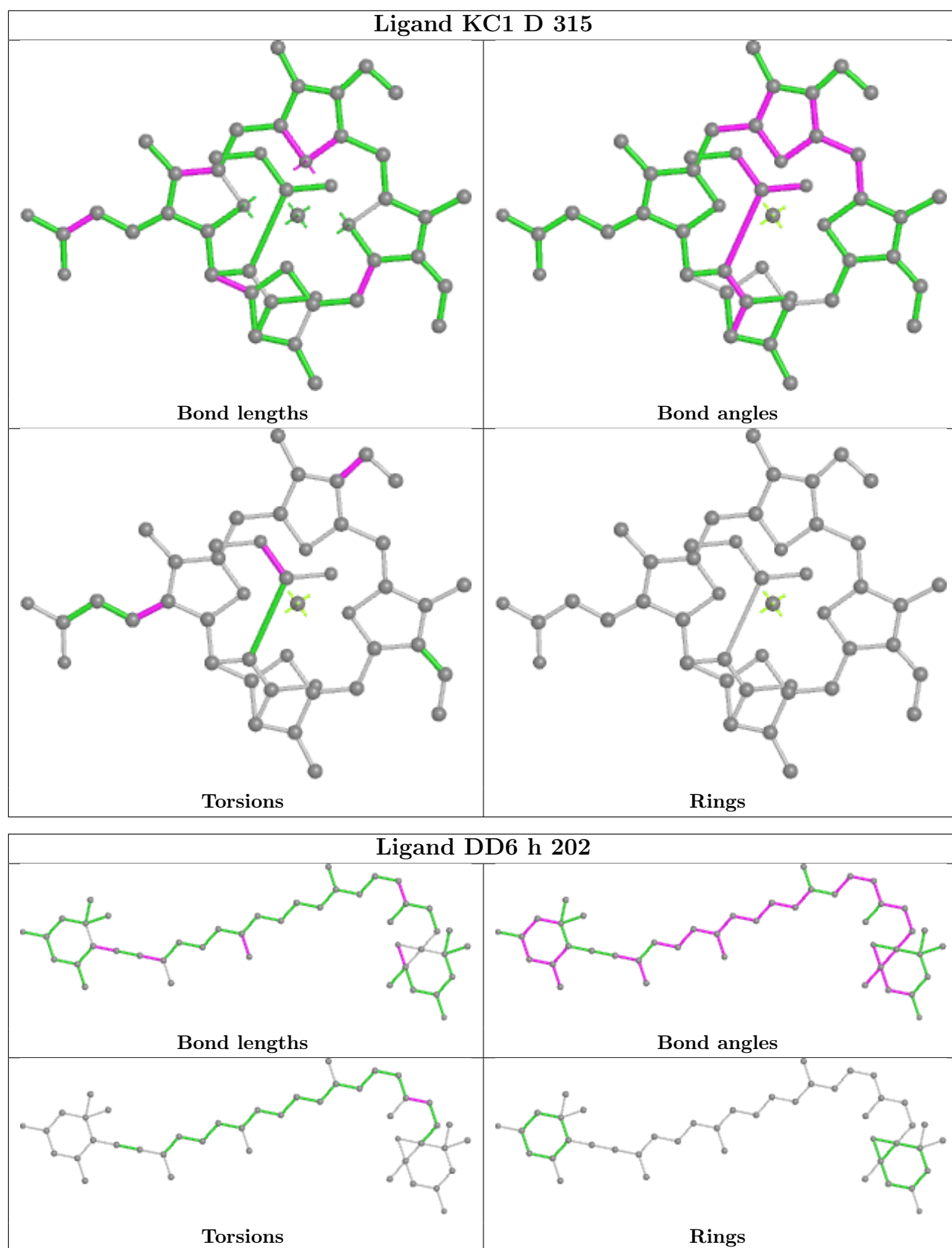
Bond angles

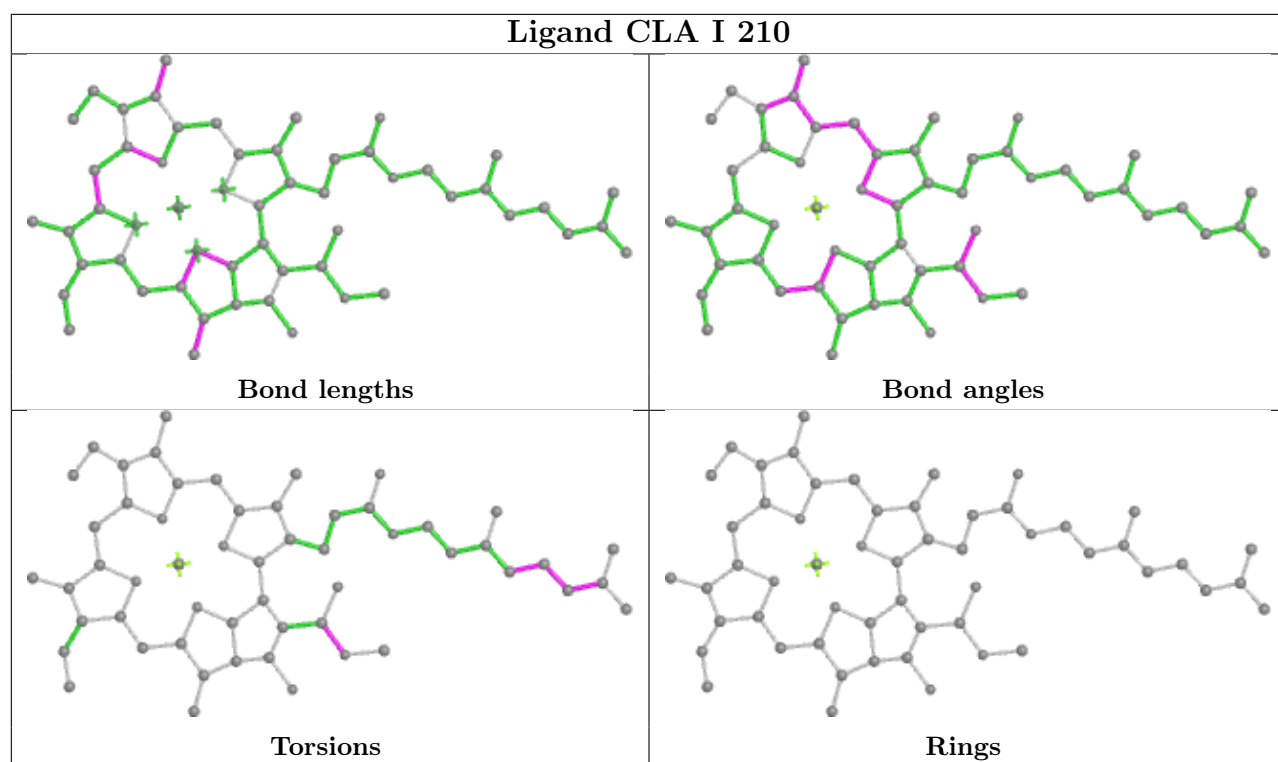


Torsions

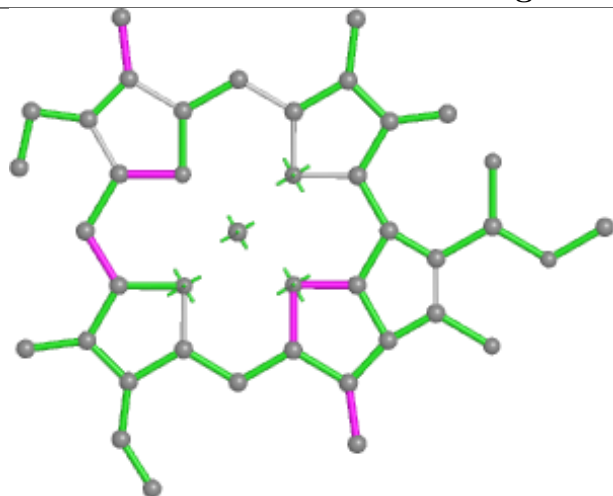


Rings

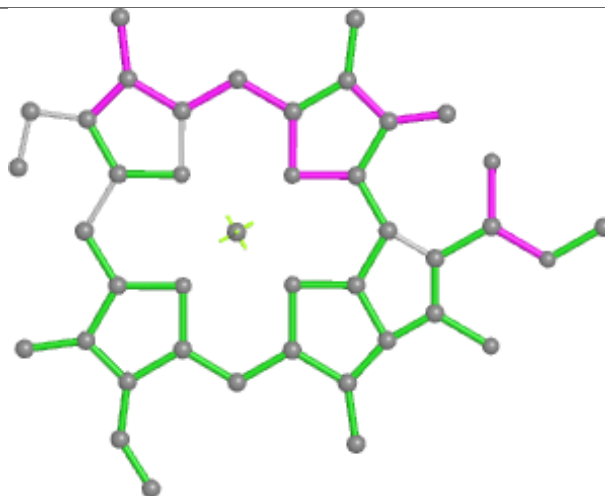




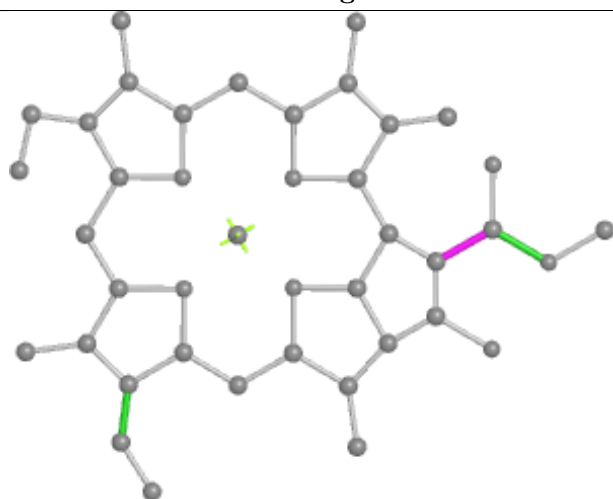
Ligand CLA E 313



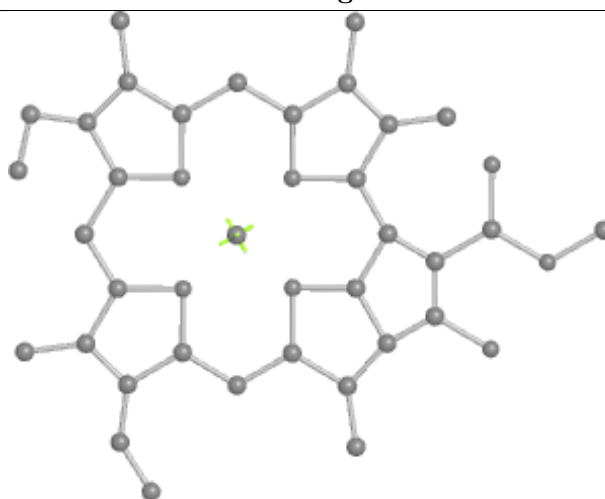
Bond lengths



Bond angles

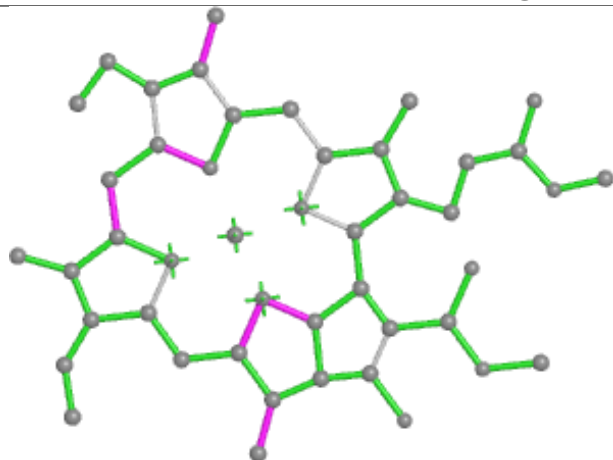


Torsions

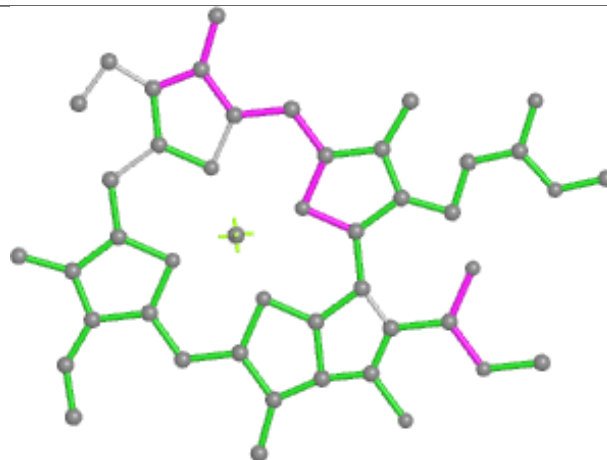


Rings

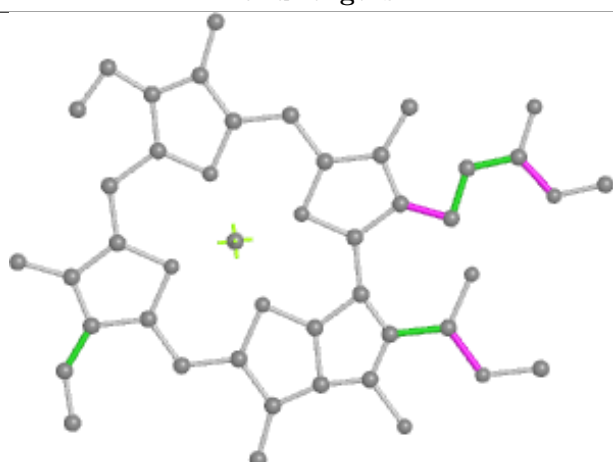
Ligand CLA F 313



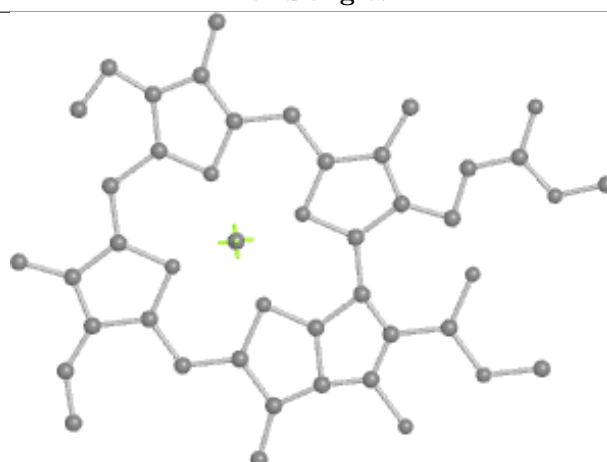
Bond lengths



Bond angles

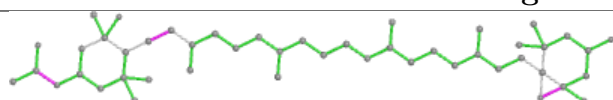


Torsions

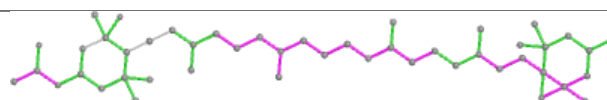


Rings

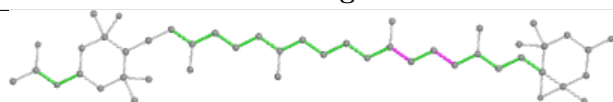
Ligand UIX J 304



Bond lengths



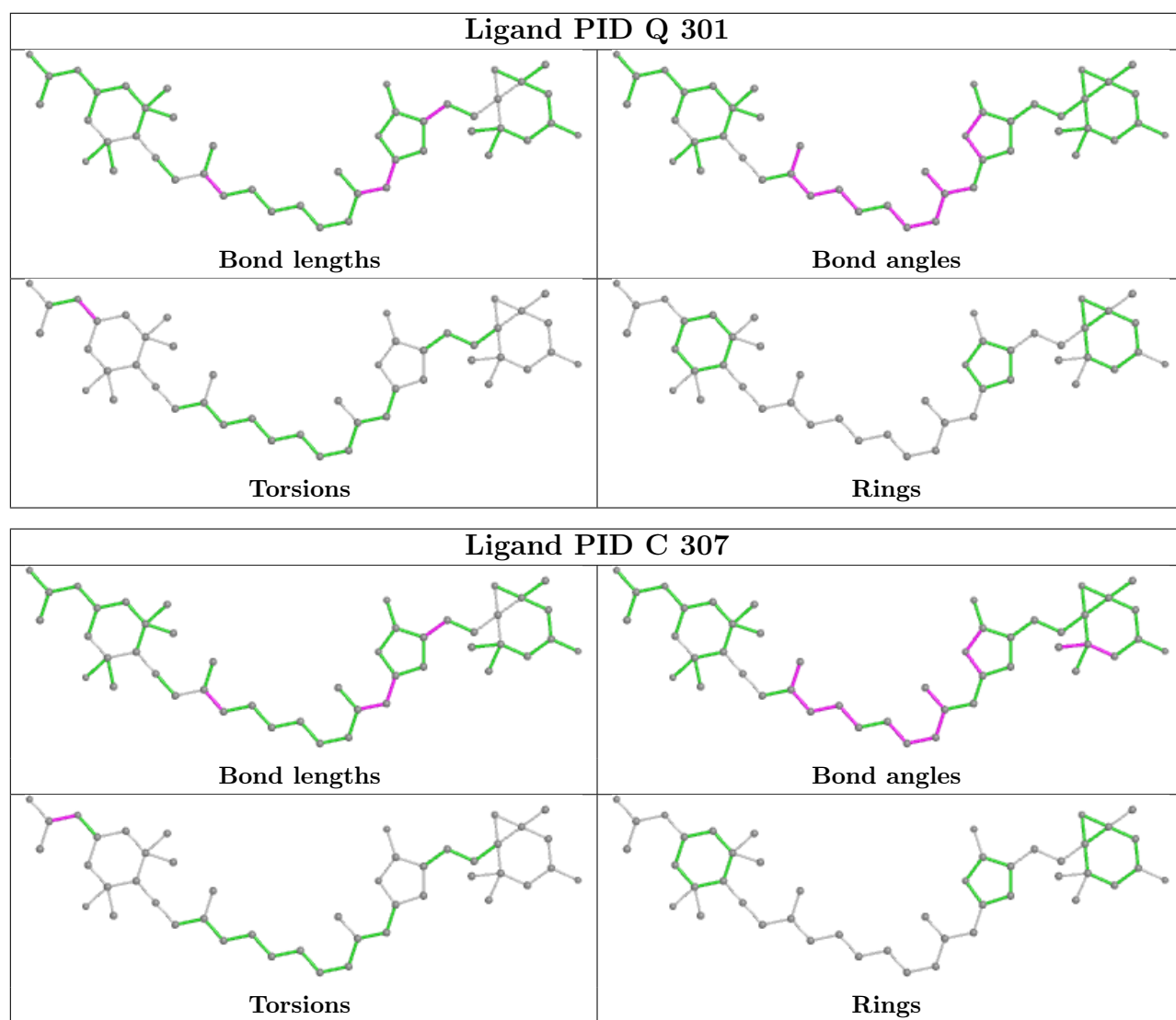
Bond angles

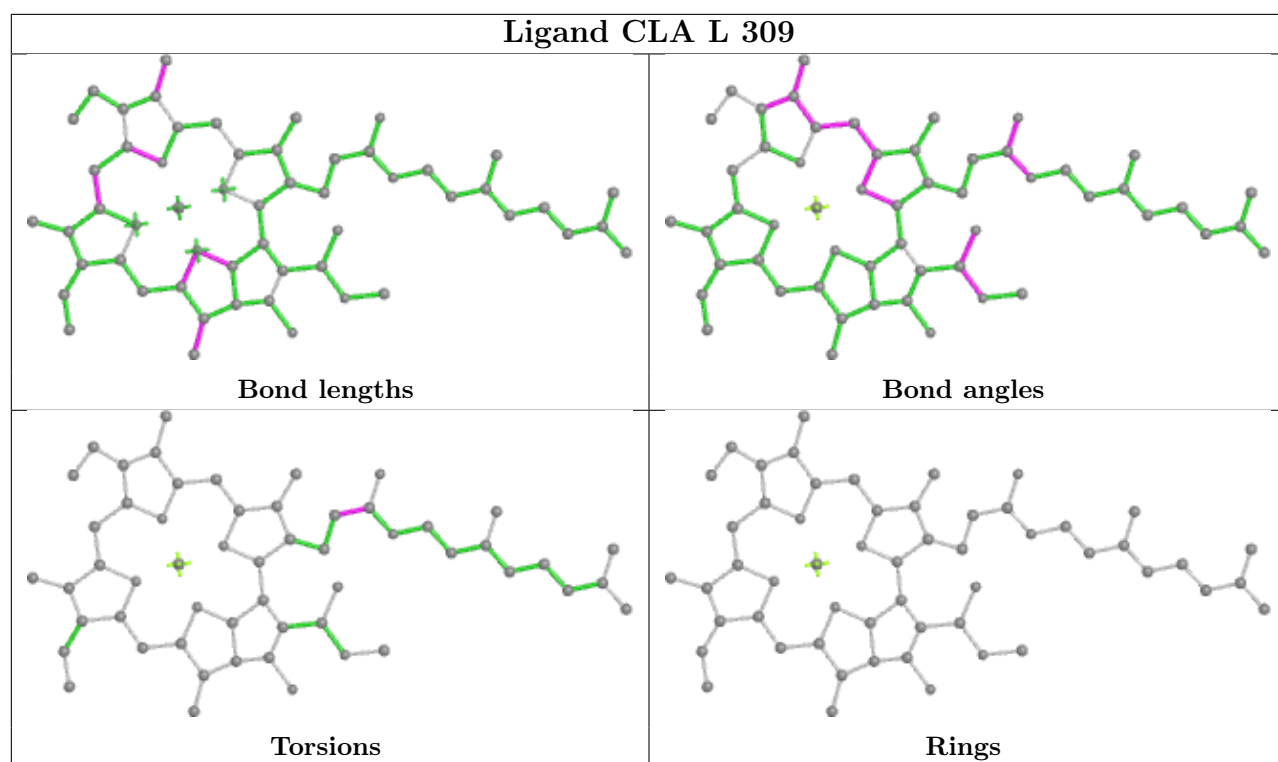


Torsions

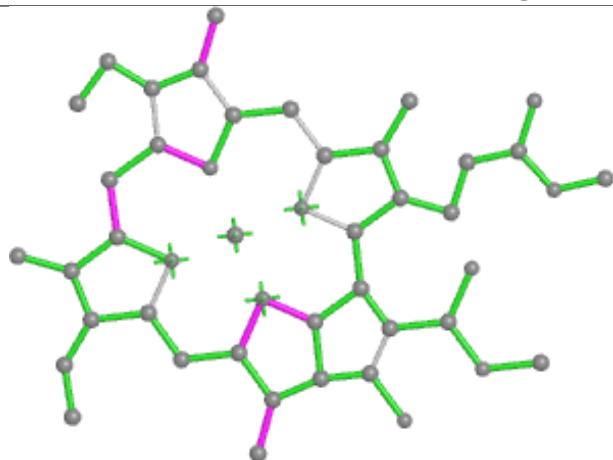


Rings

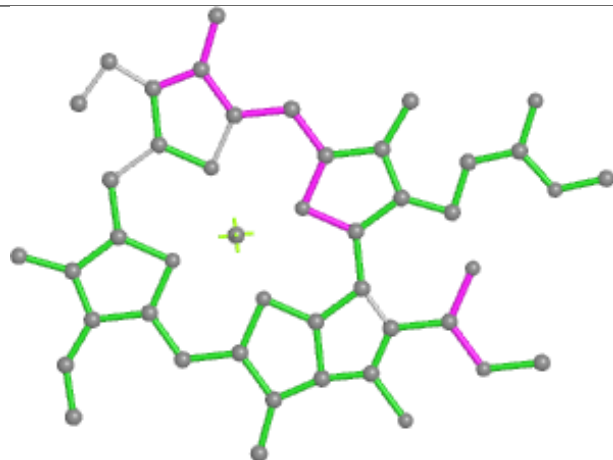




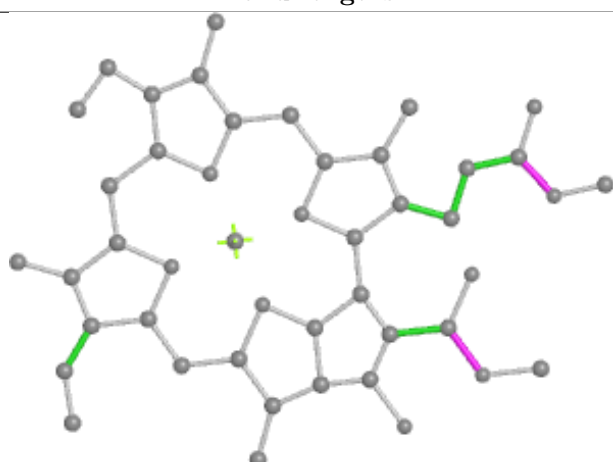
Ligand CLA E 310



Bond lengths



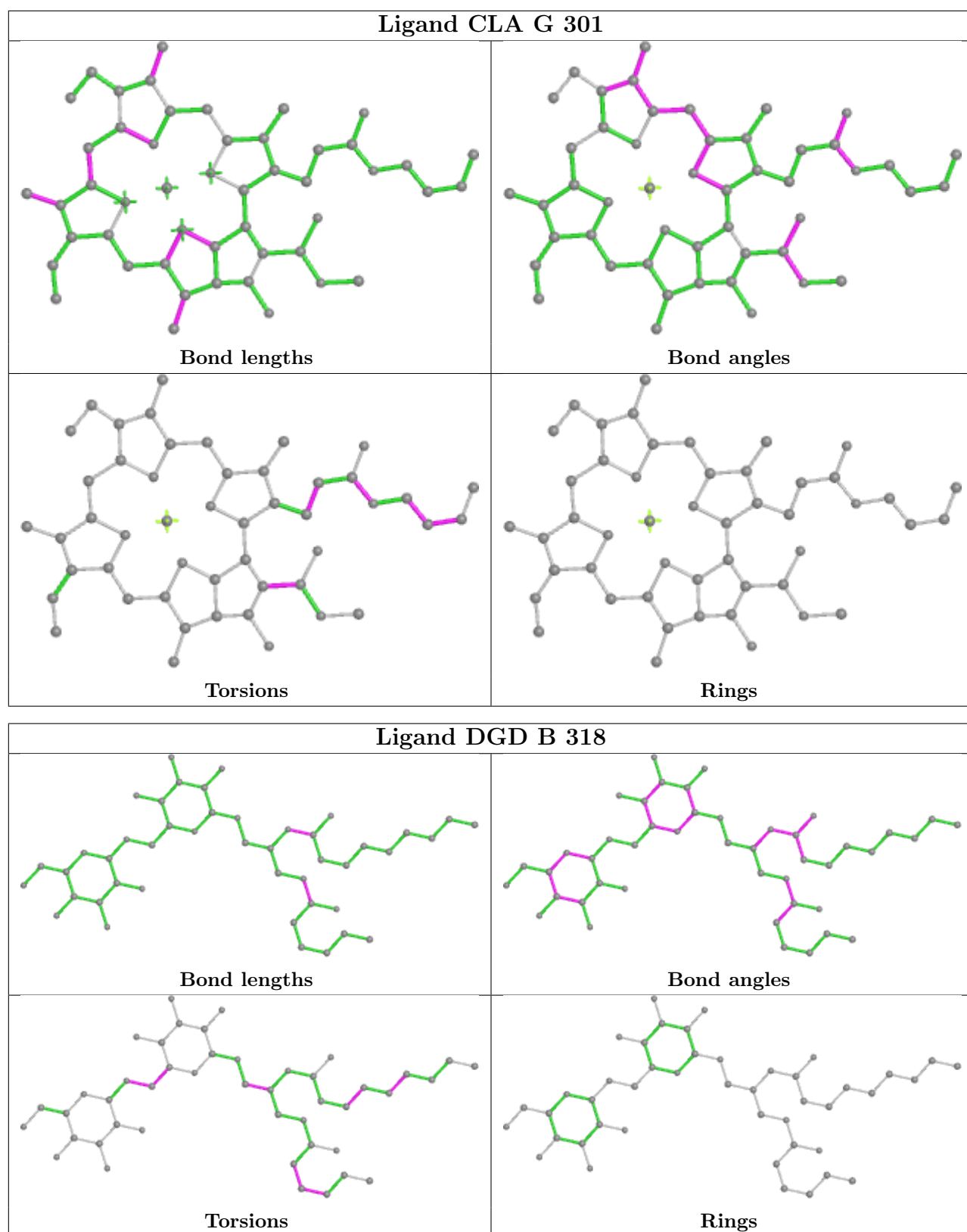
Bond angles



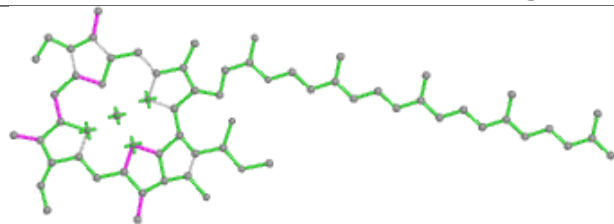
Torsions



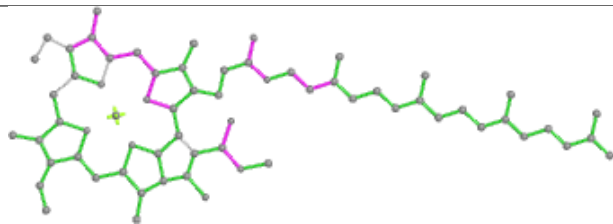
Rings



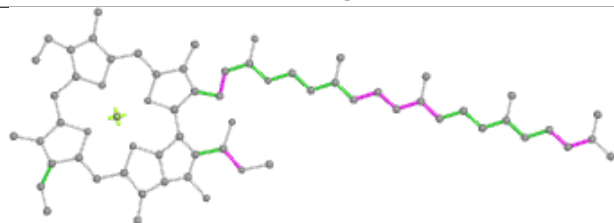
Ligand CLA i 202



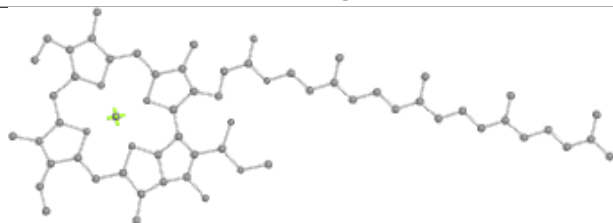
Bond lengths



Bond angles

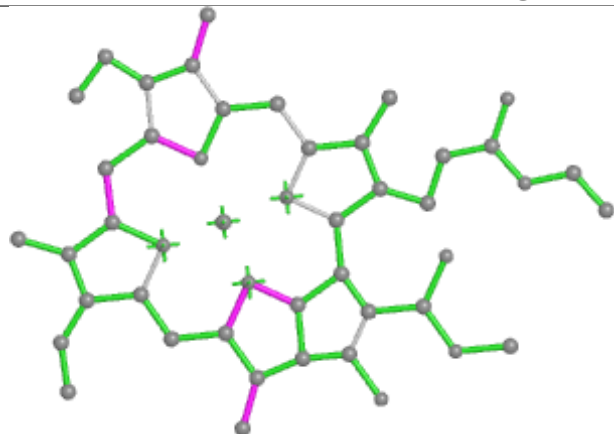


Torsions

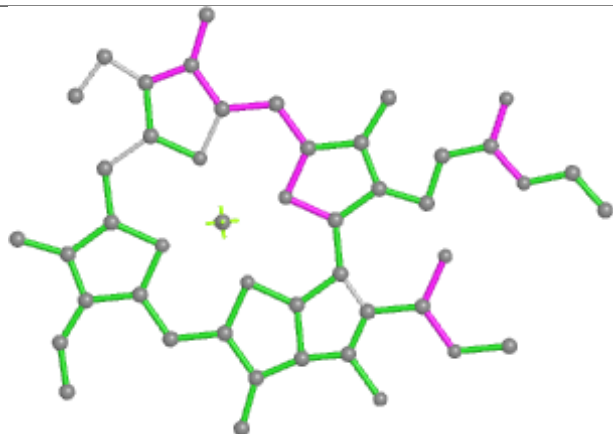


Rings

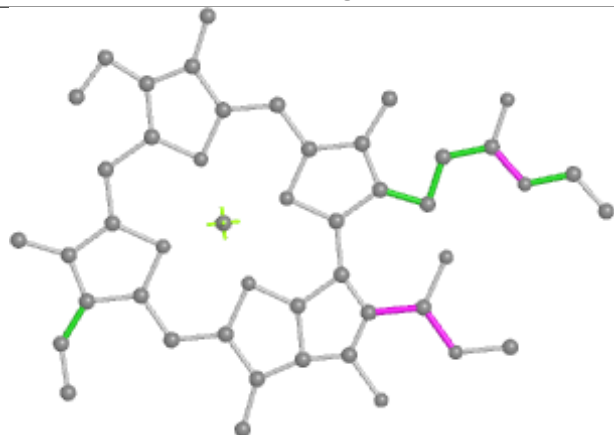
Ligand CLA C 308



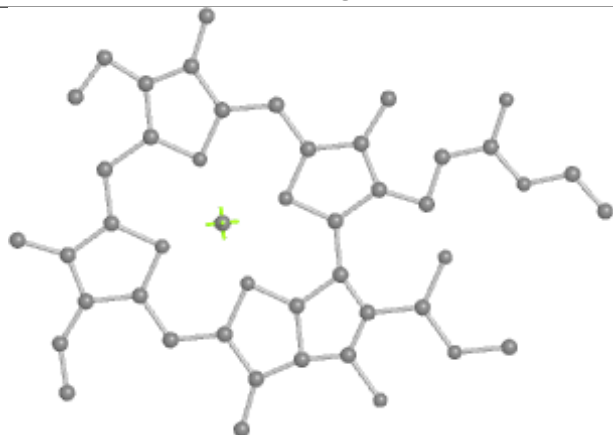
Bond lengths



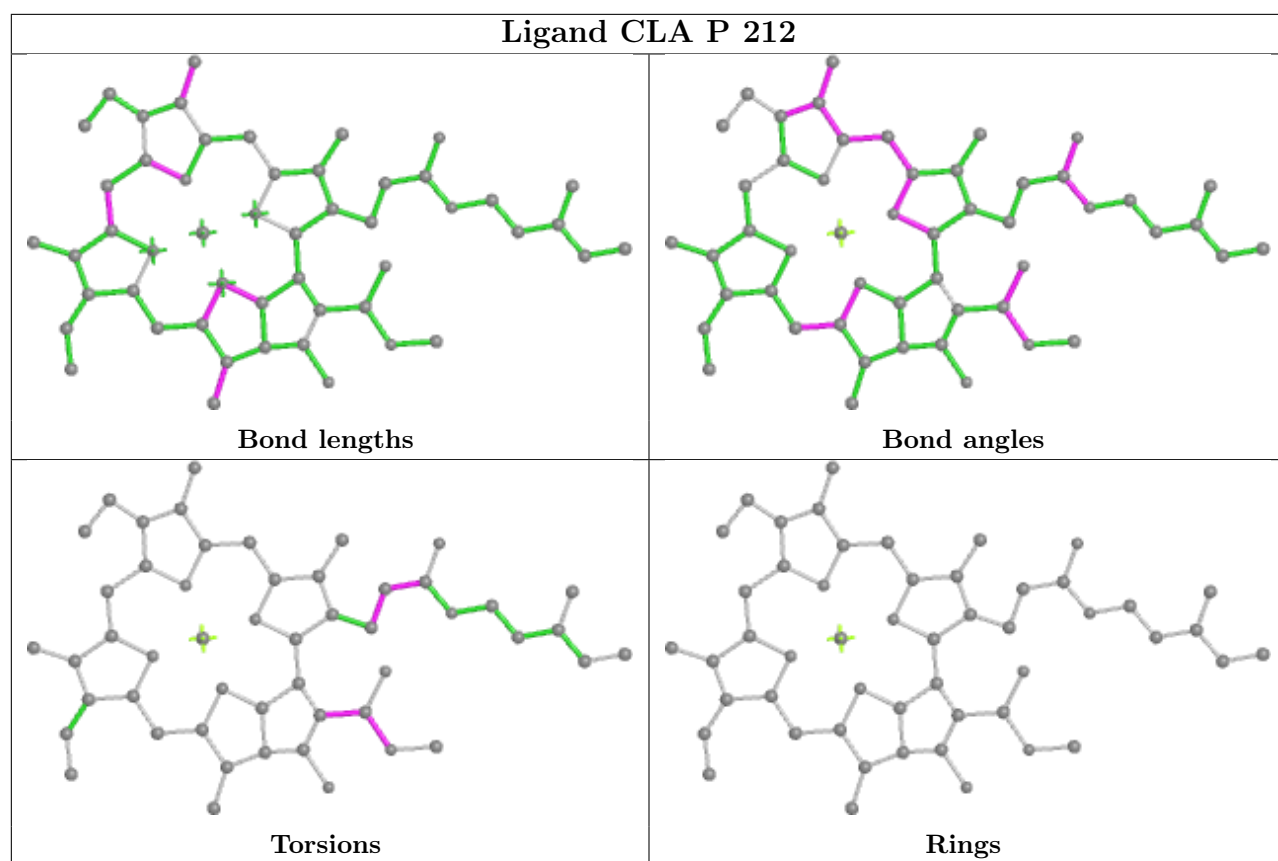
Bond angles



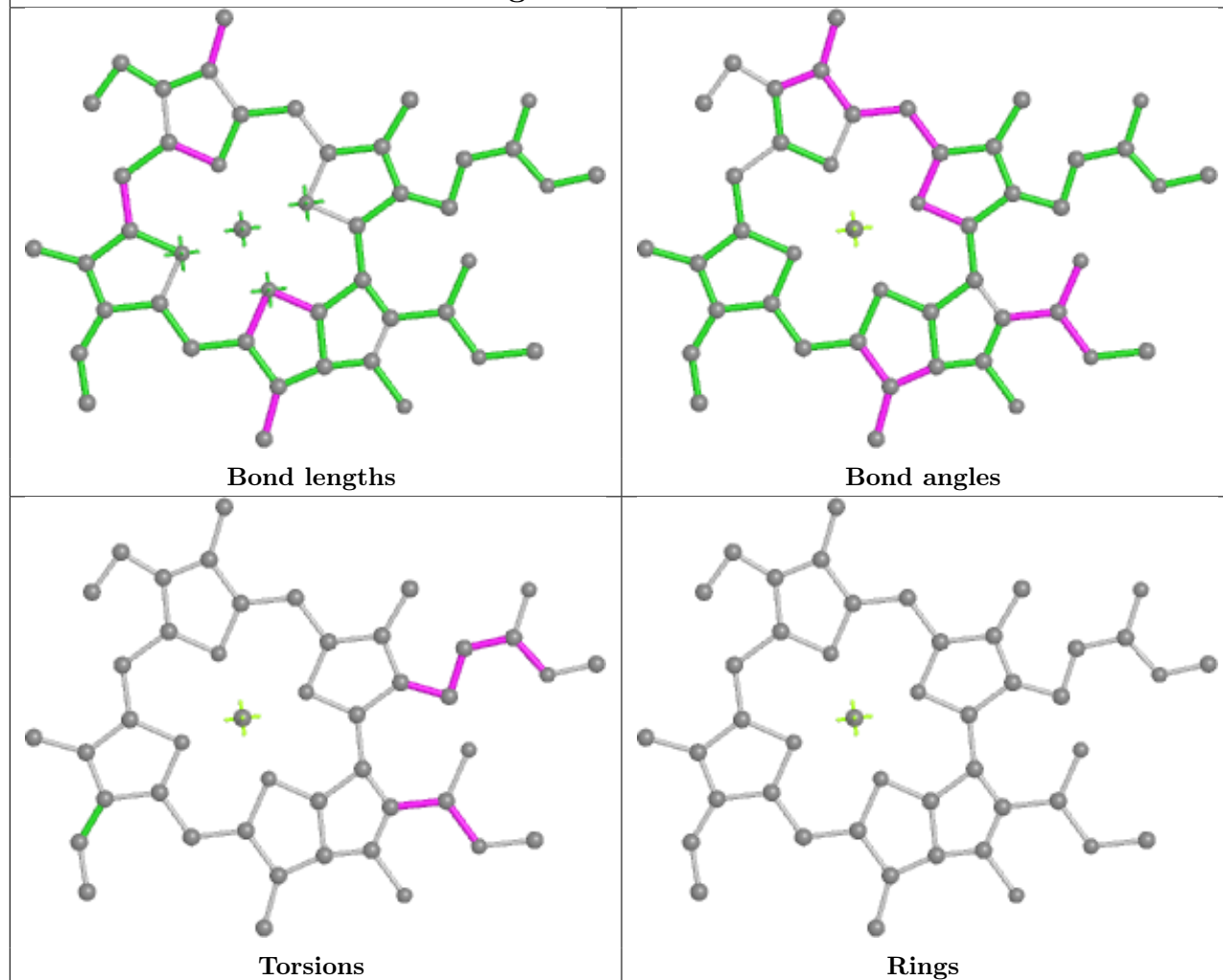
Torsions



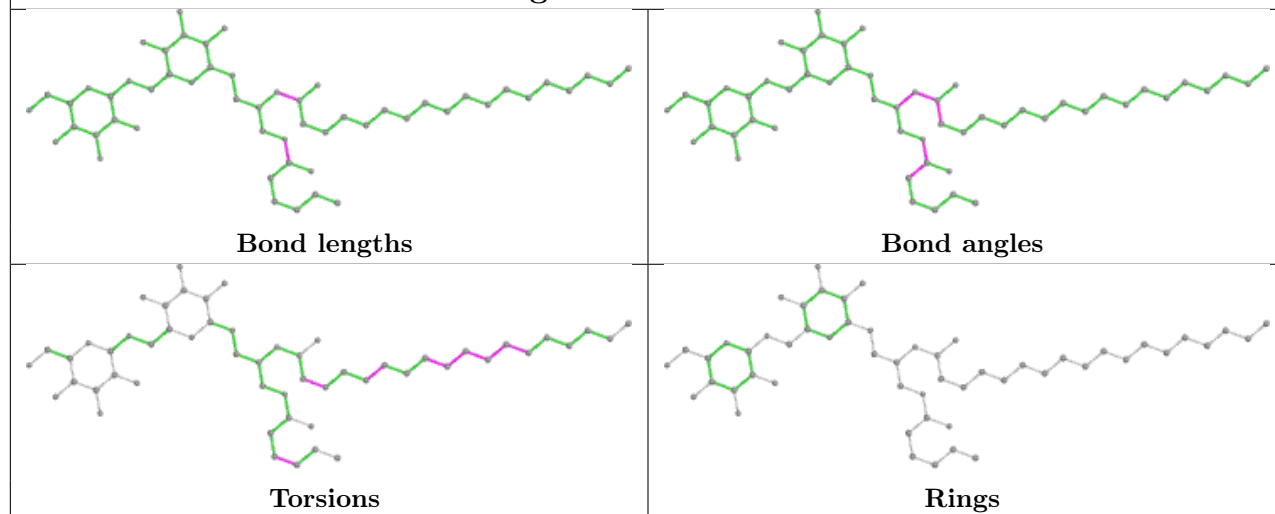
Rings

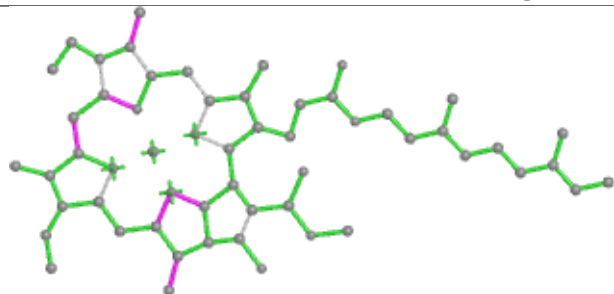
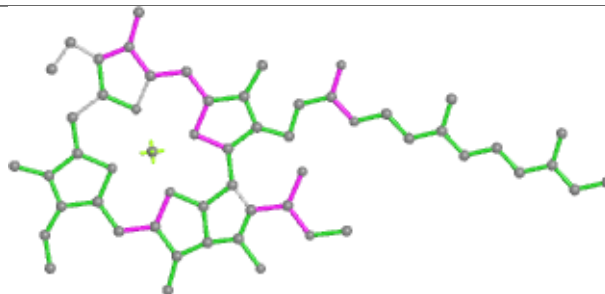
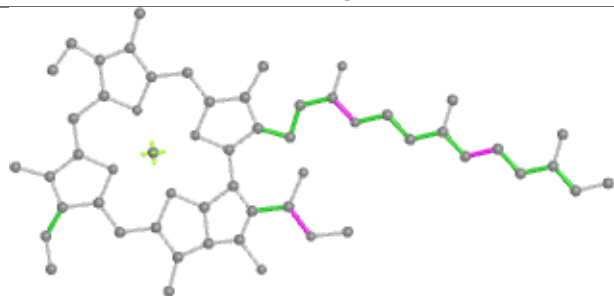
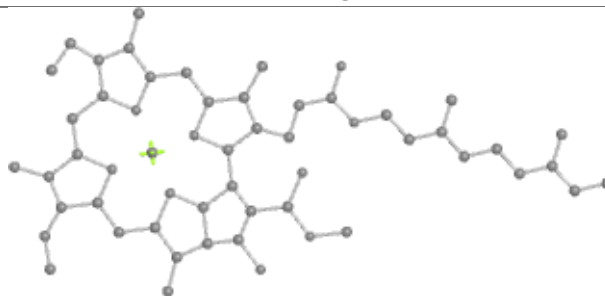
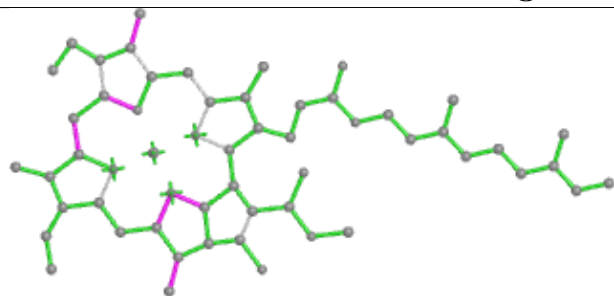
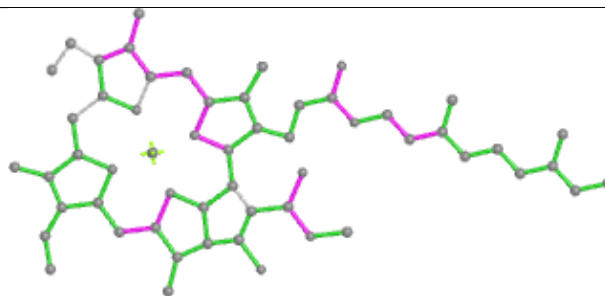
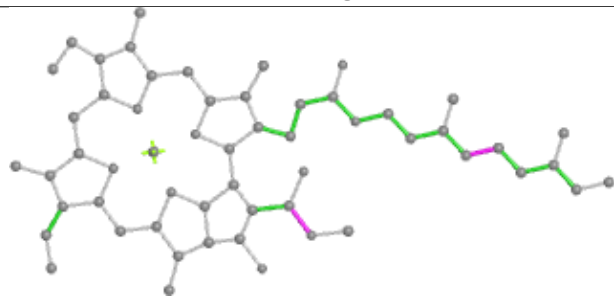
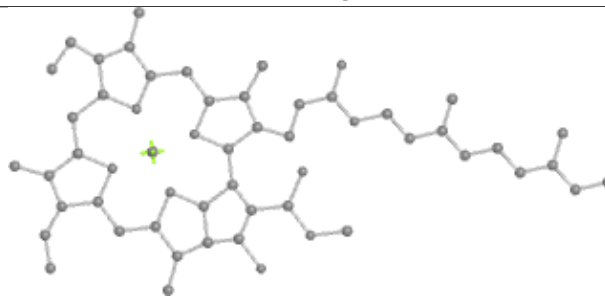


Ligand CLA N 313

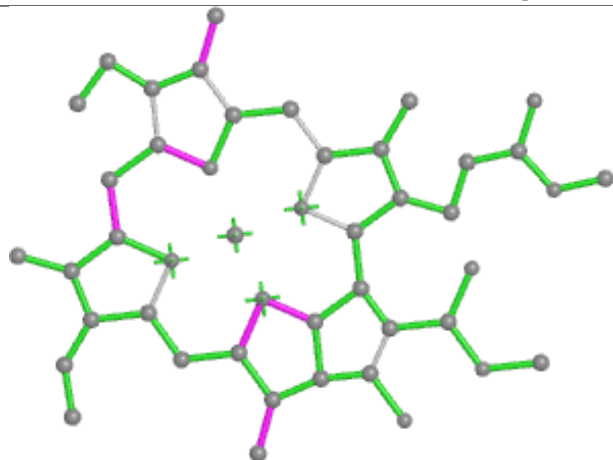


Ligand DGD h 203

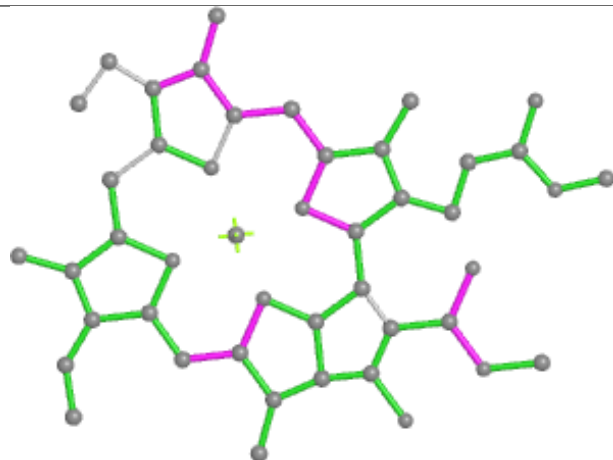


Ligand CLA a 830**Bond lengths****Bond angles****Torsions****Rings****Ligand CLA b 731****Bond lengths****Bond angles****Torsions****Rings**

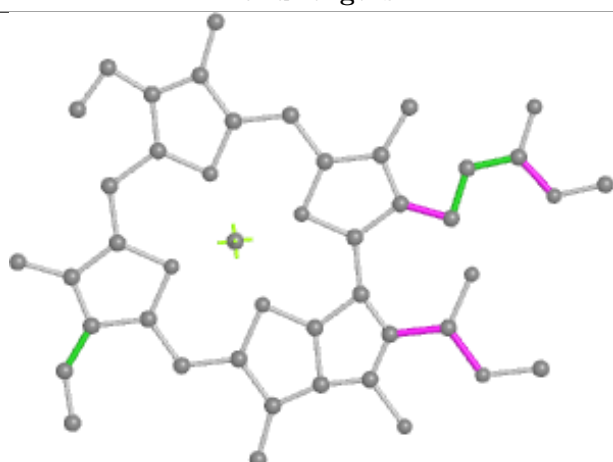
Ligand CLA L 311



Bond lengths



Bond angles

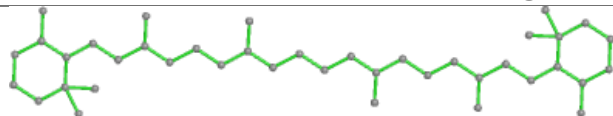


Torsions

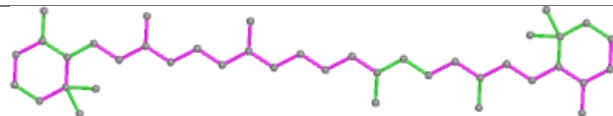


Rings

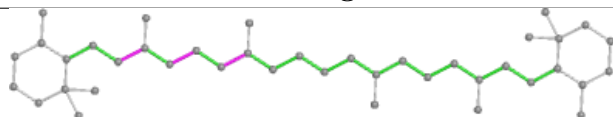
Ligand BCR 1 507



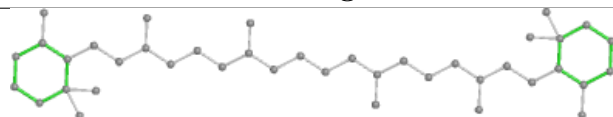
Bond lengths



Bond angles

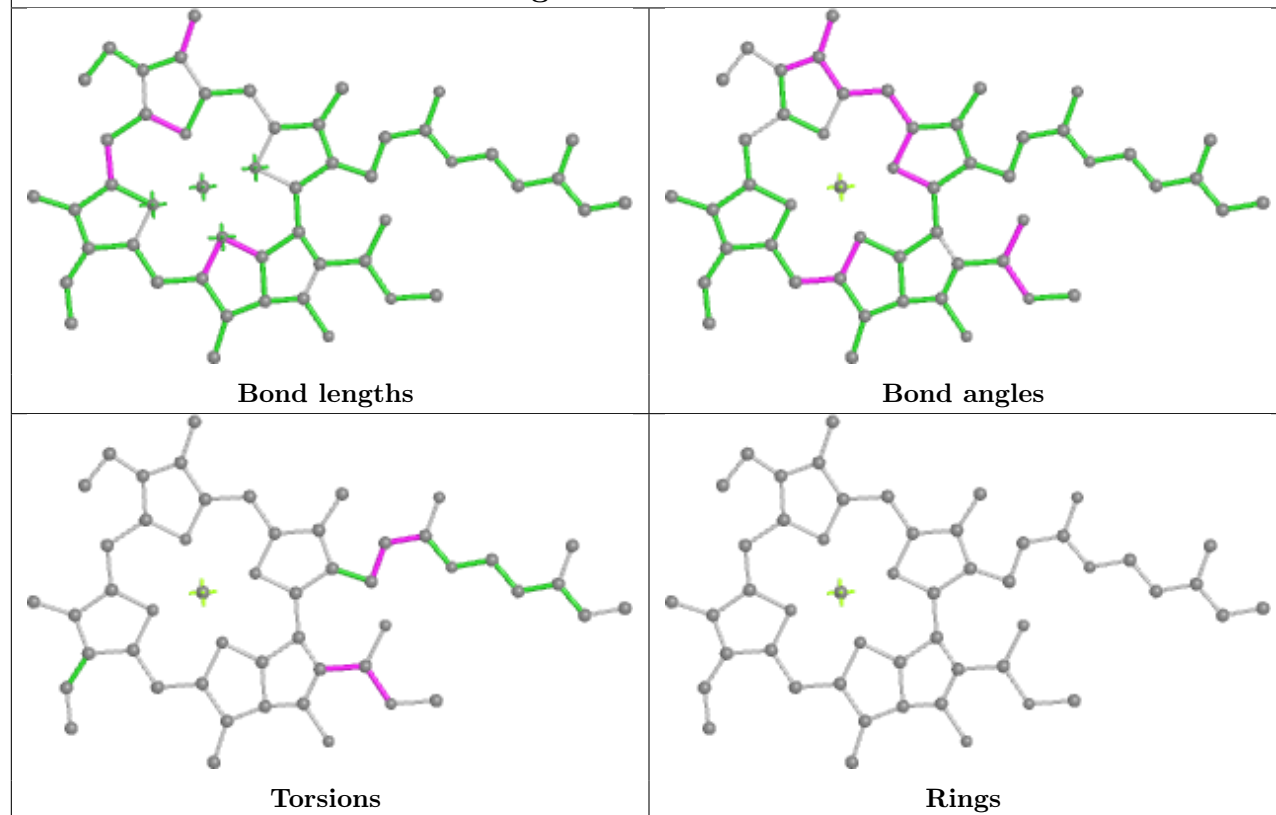


Torsions

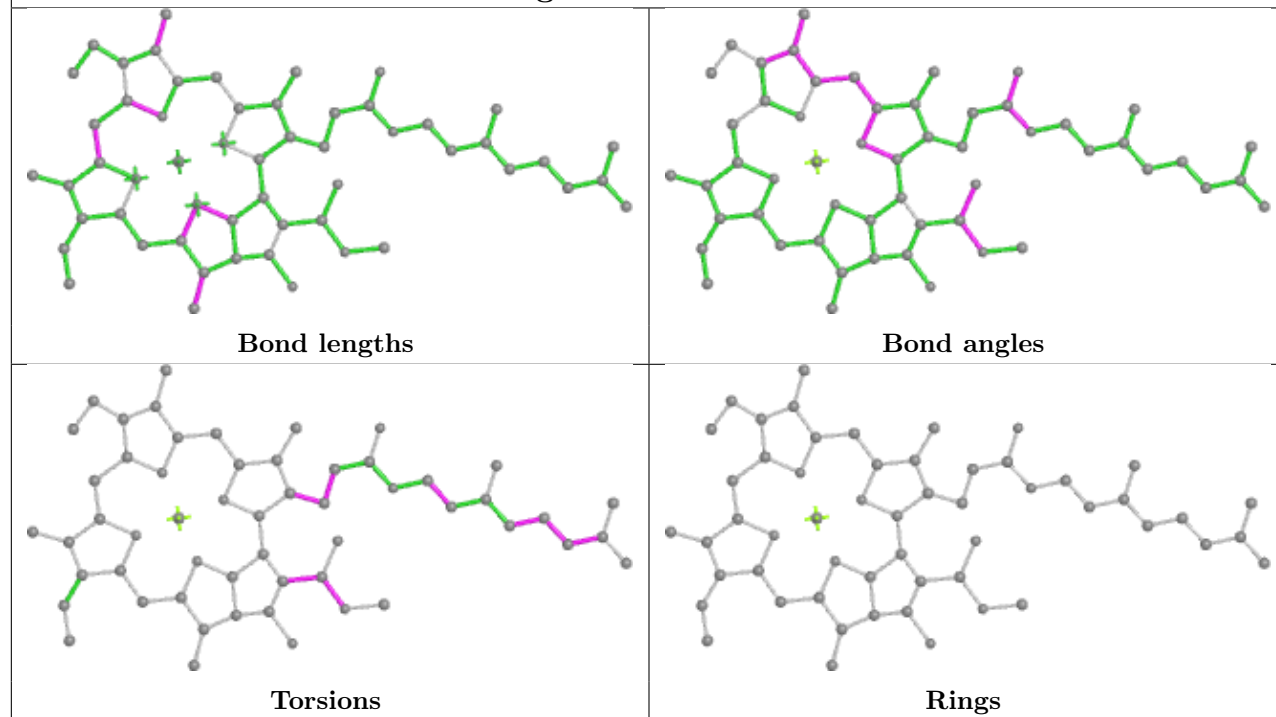


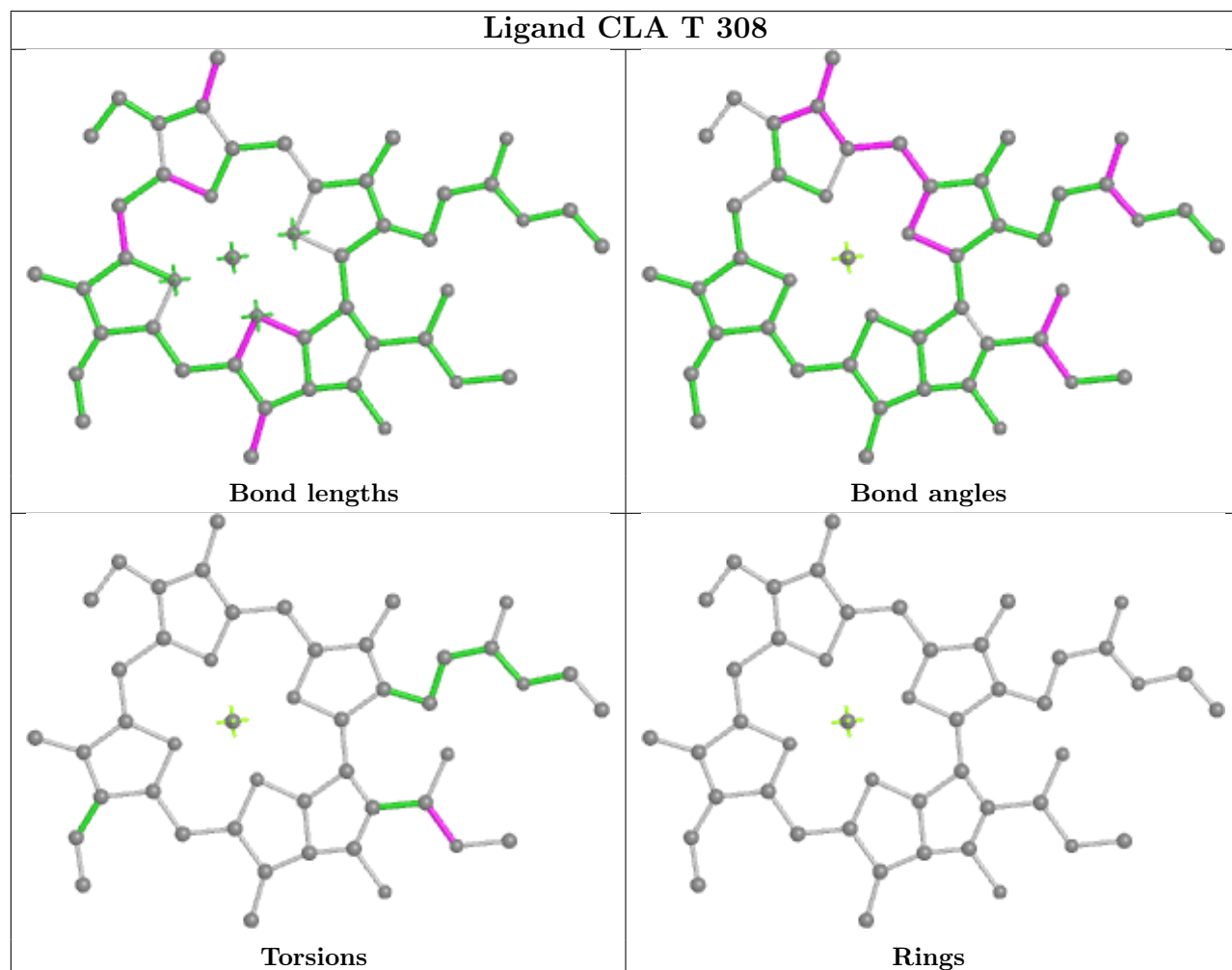
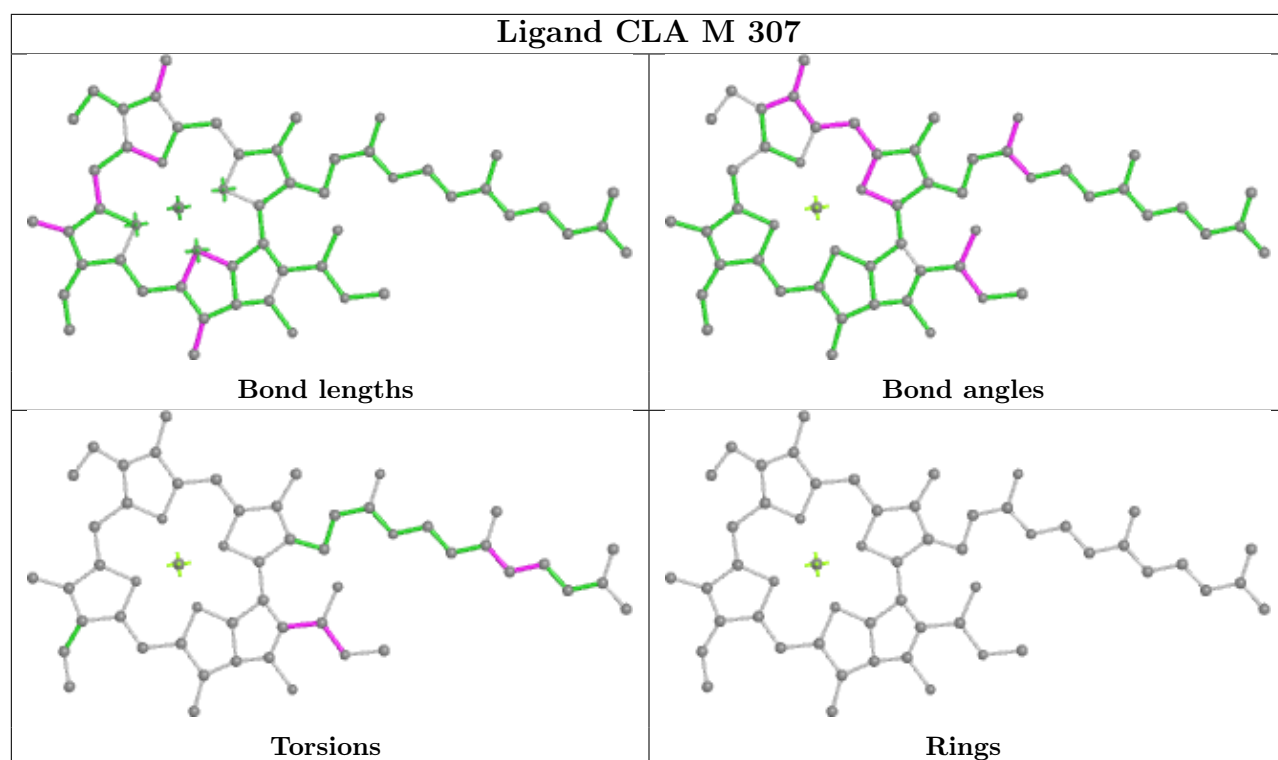
Rings

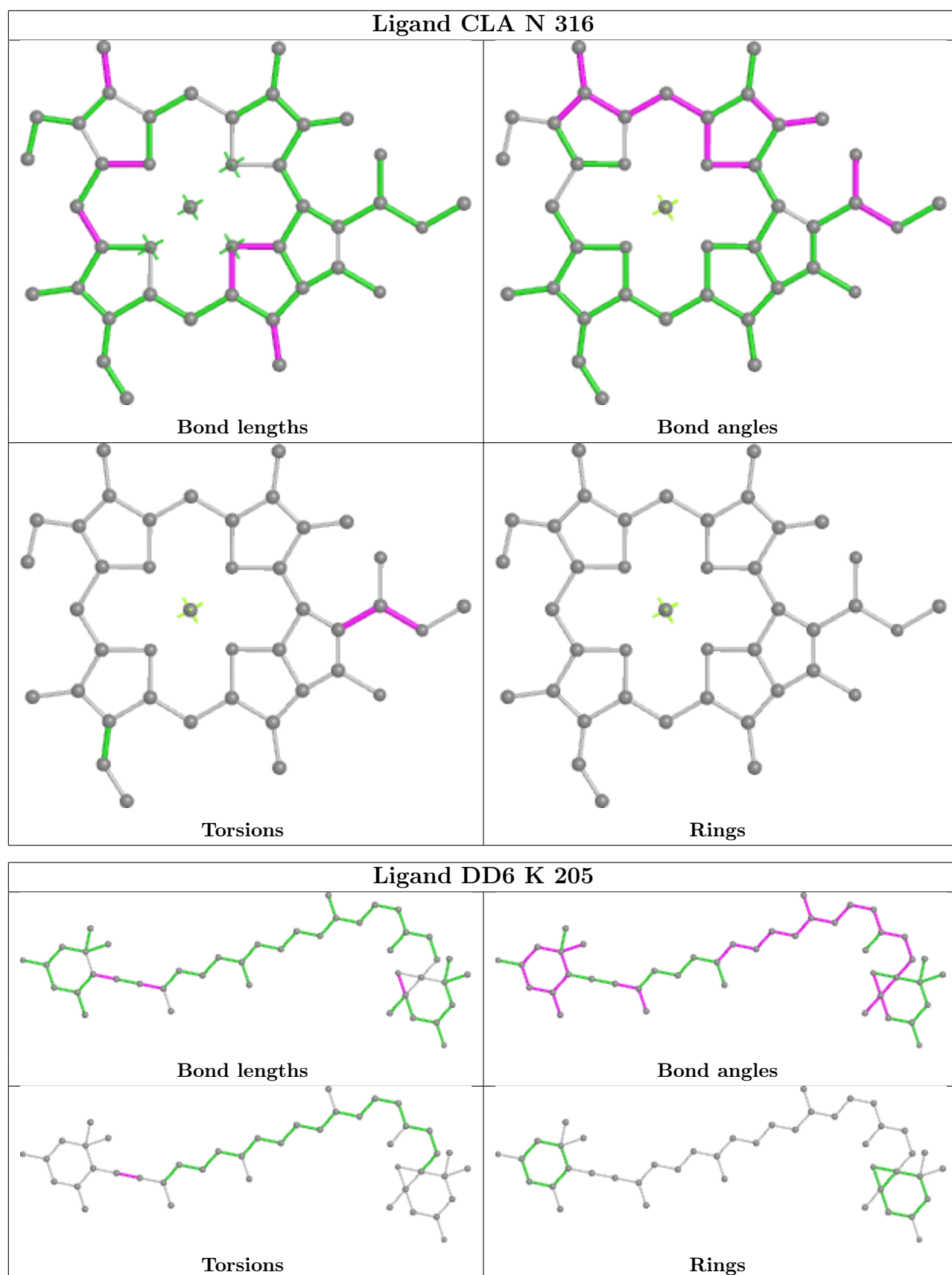
Ligand CLA N 311

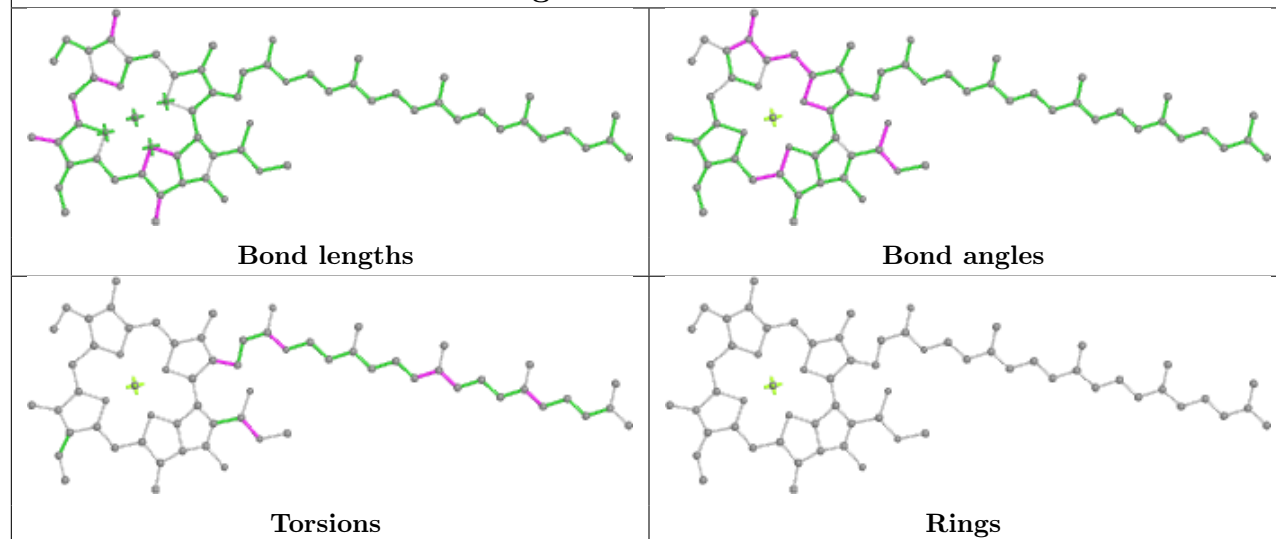
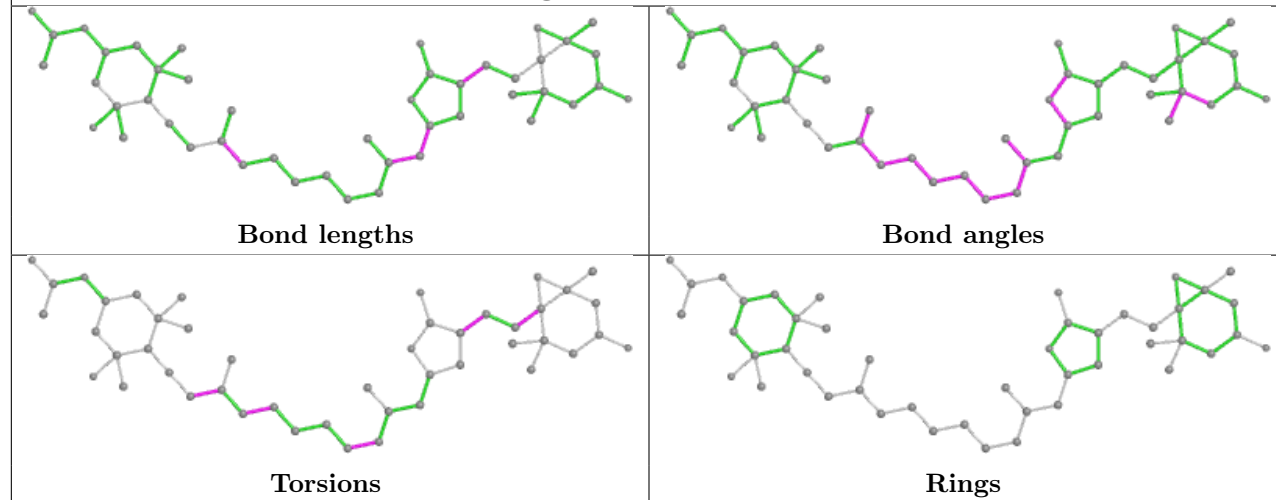


Ligand CLA a 837

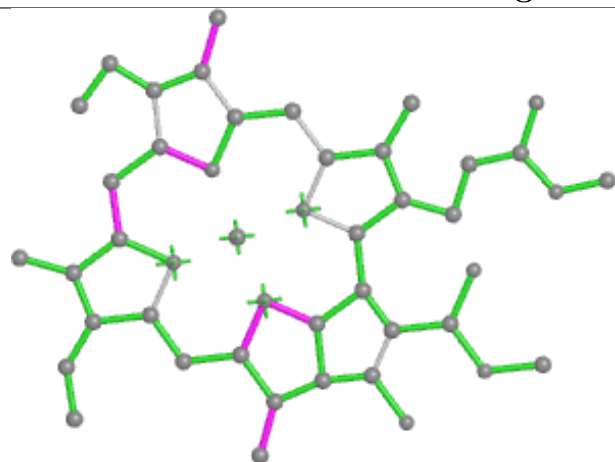




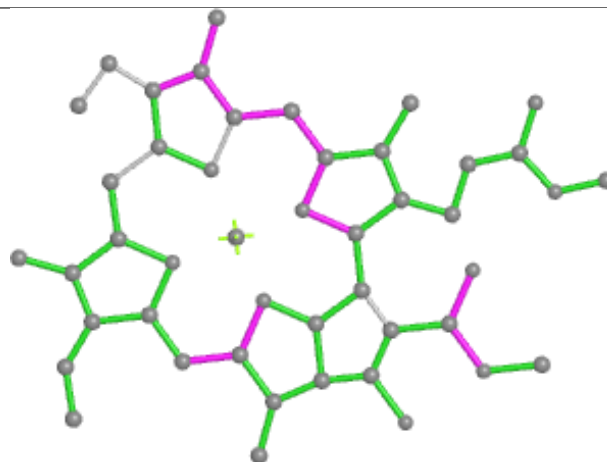


Ligand CLA B 312**Ligand PID E 301**

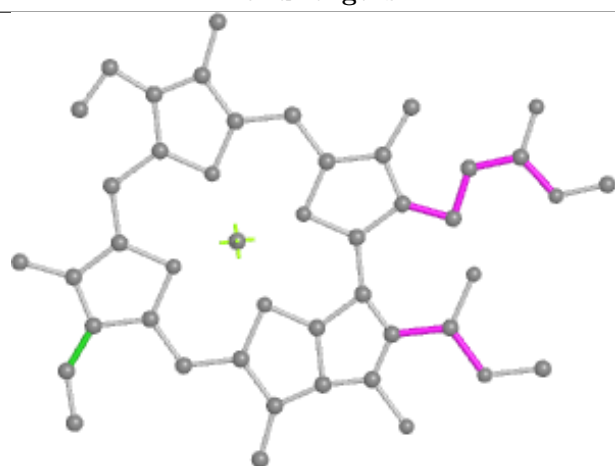
Ligand CLA D 311



Bond lengths



Bond angles

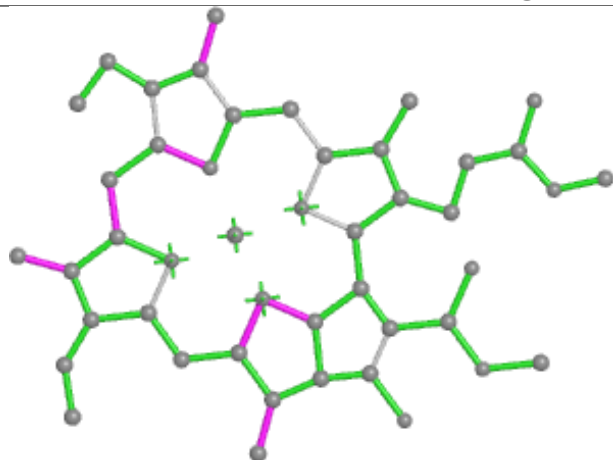


Torsions

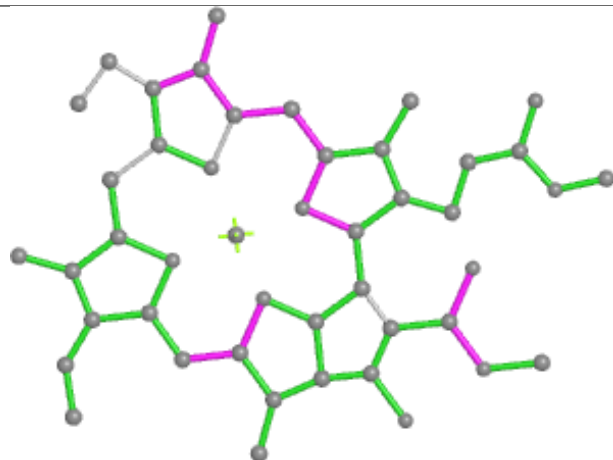


Rings

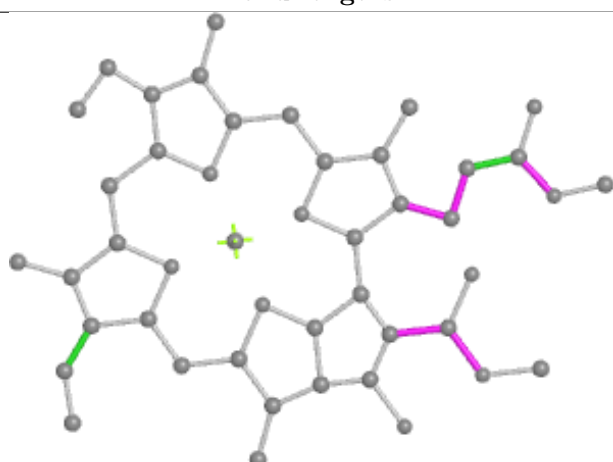
Ligand CLA a 816



Bond lengths



Bond angles

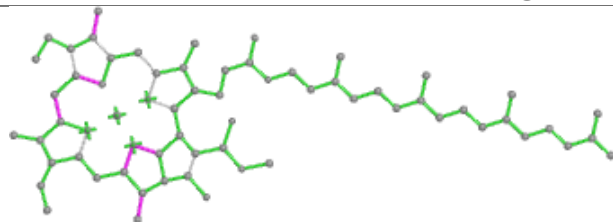


Torsions

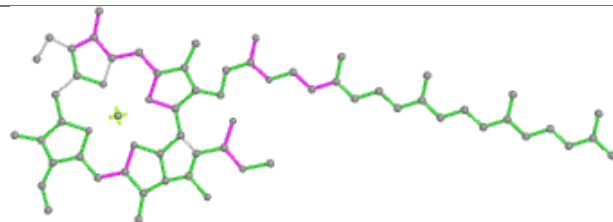


Rings

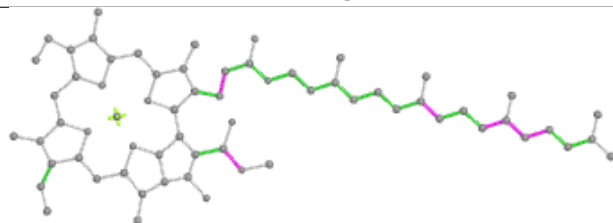
Ligand CLA a 802



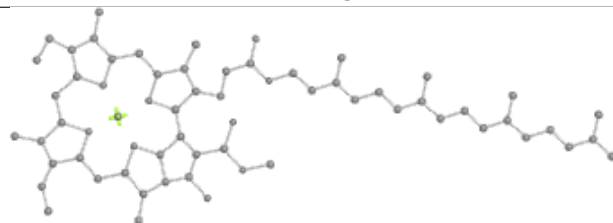
Bond lengths



Bond angles

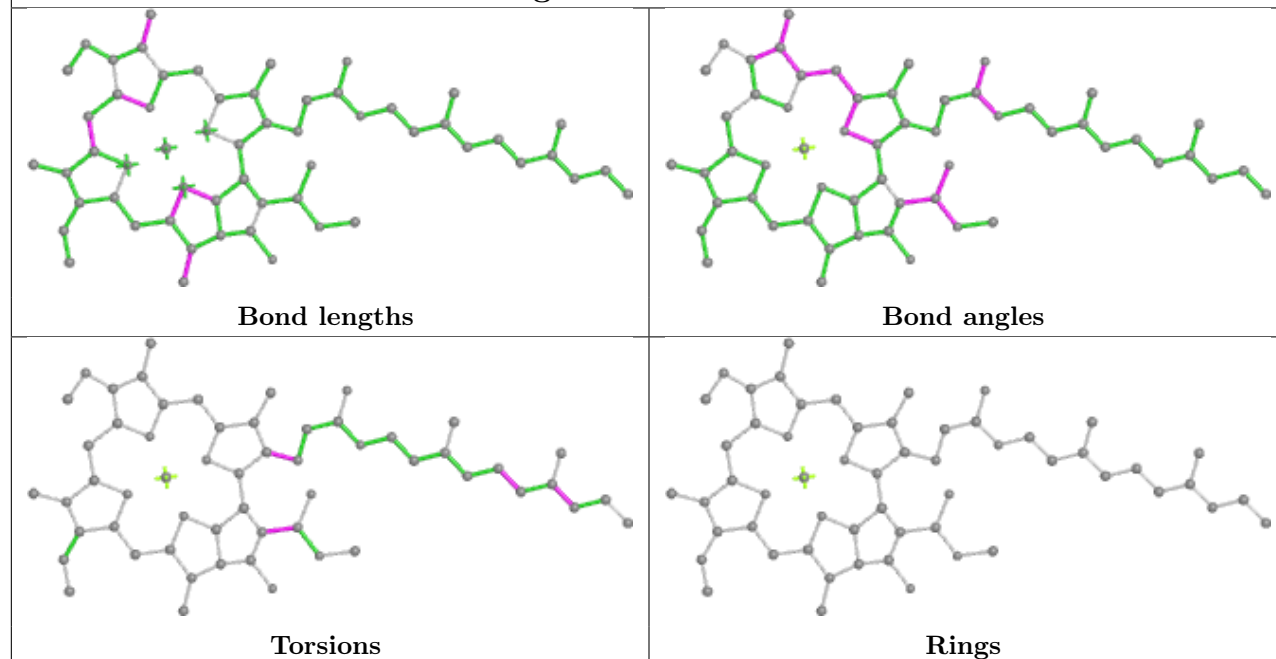


Torsions

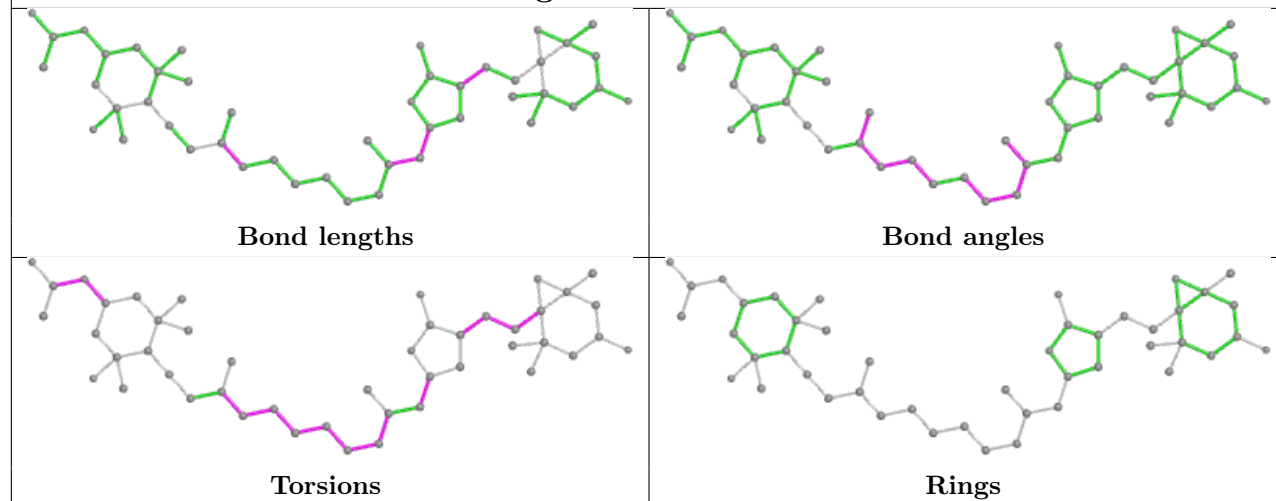


Rings

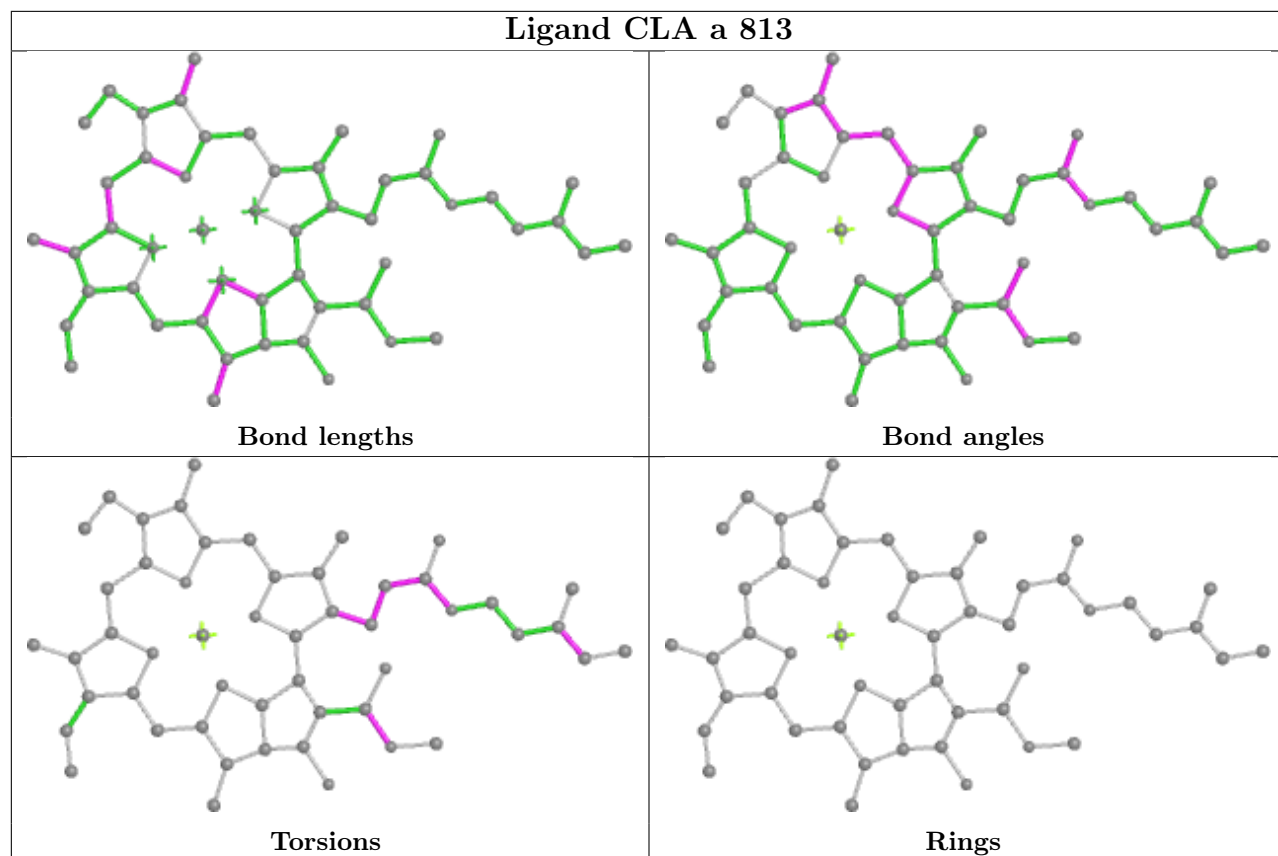
Ligand CLA E 315



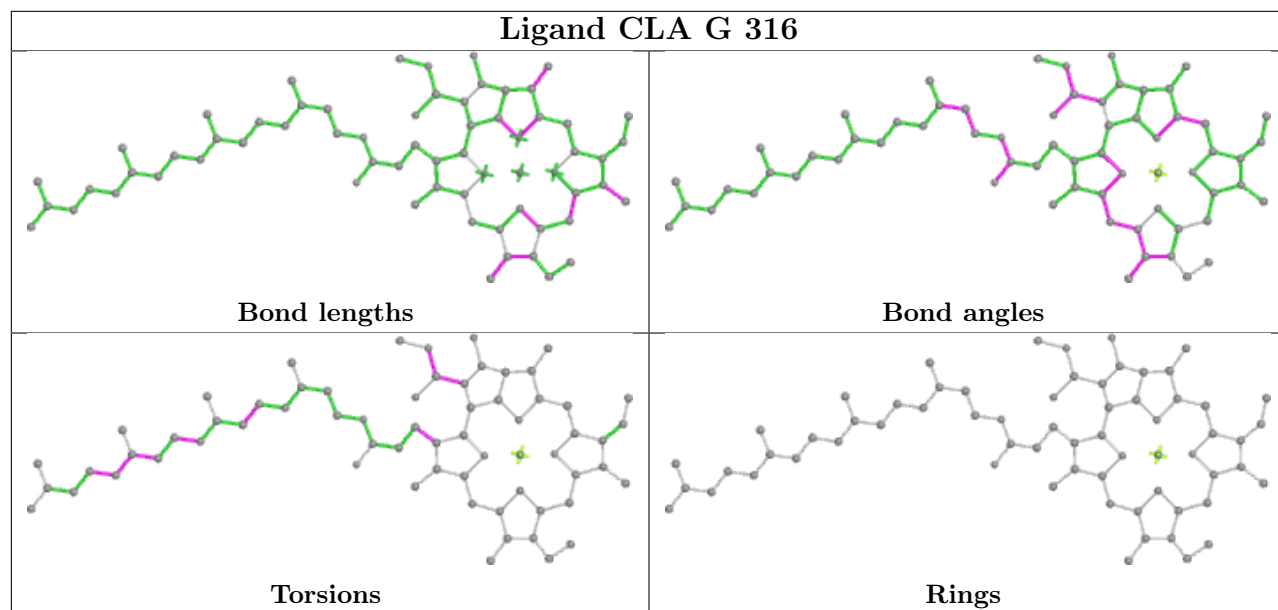
Ligand PID N 305



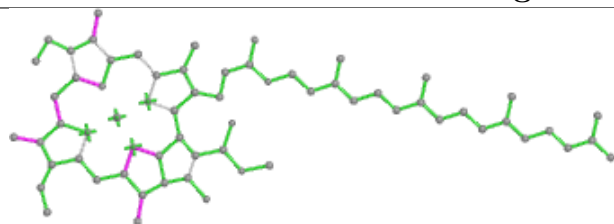
Ligand CLA a 813



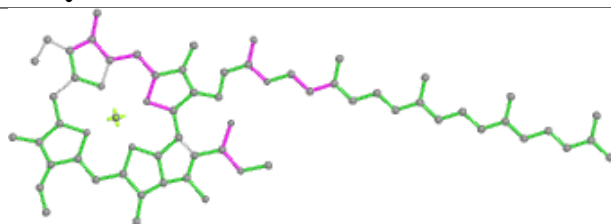
Ligand CLA G 316



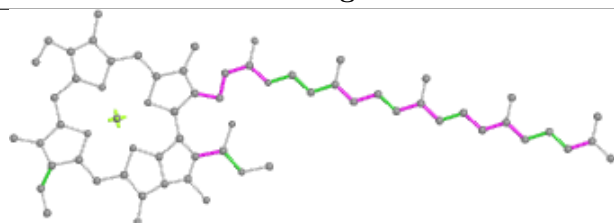
Ligand CLA Q 308



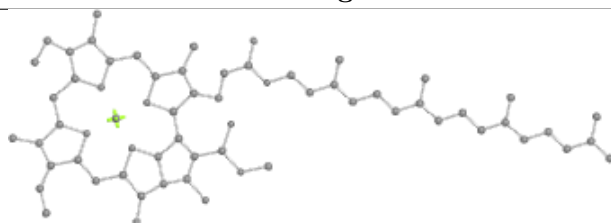
Bond lengths



Bond angles

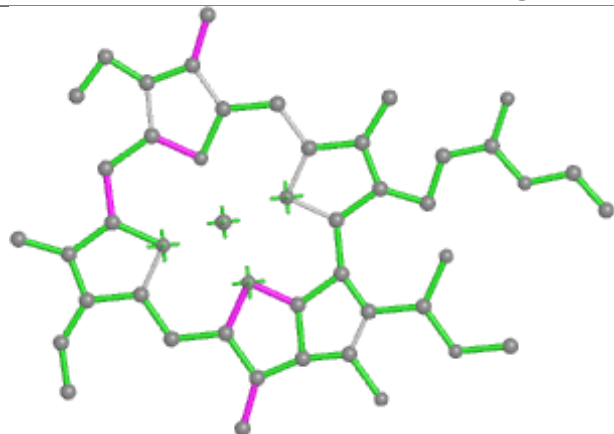


Torsions

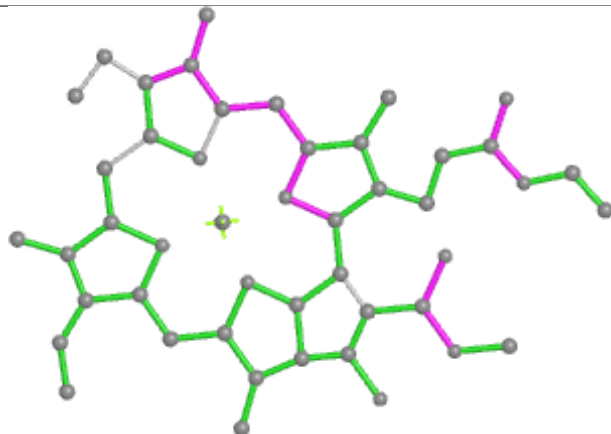


Rings

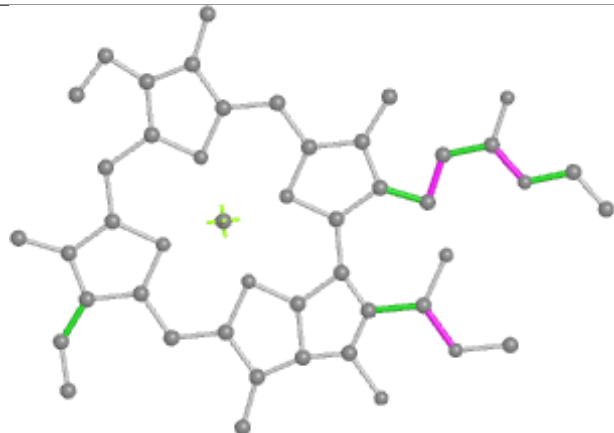
Ligand CLA D 308



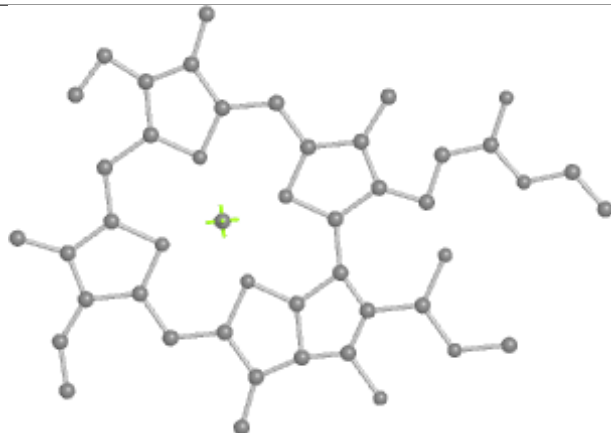
Bond lengths



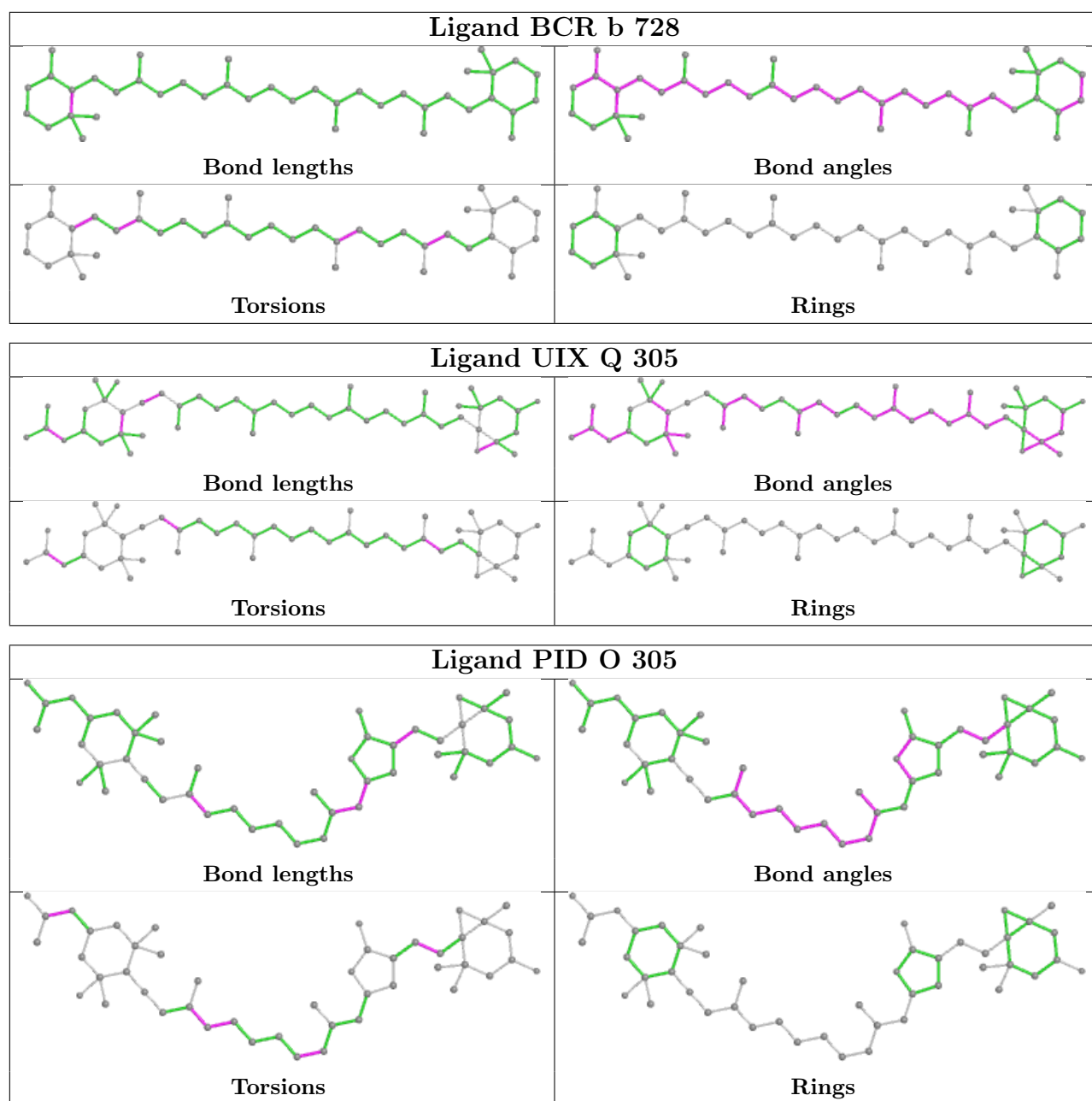
Bond angles



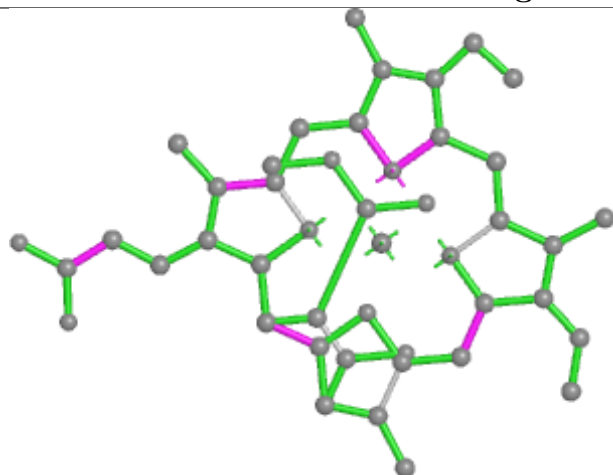
Torsions



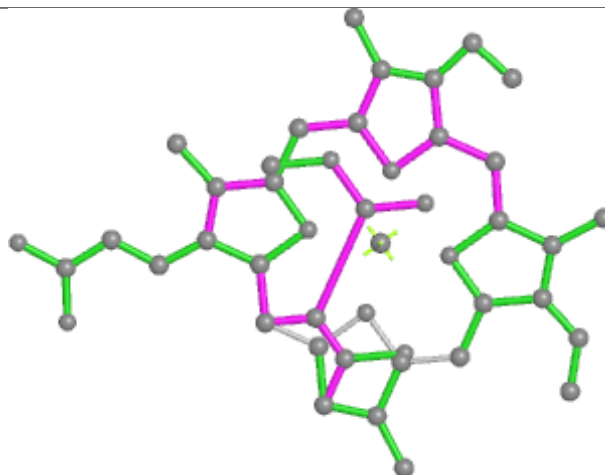
Rings



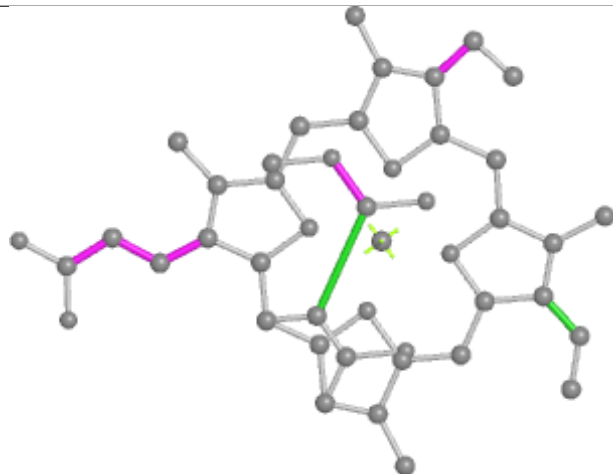
Ligand KC1 H 309



Bond lengths



Bond angles

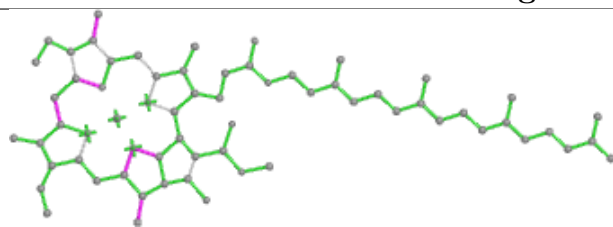


Torsions

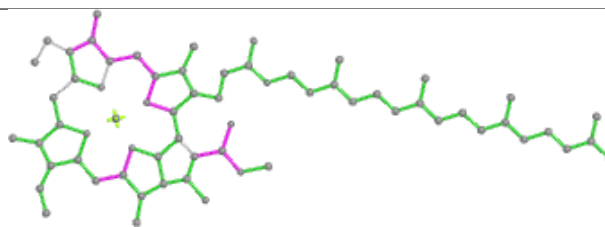


Rings

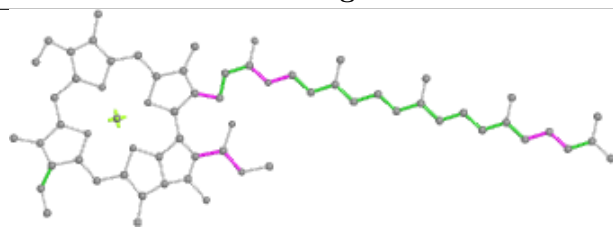
Ligand CLA a 826



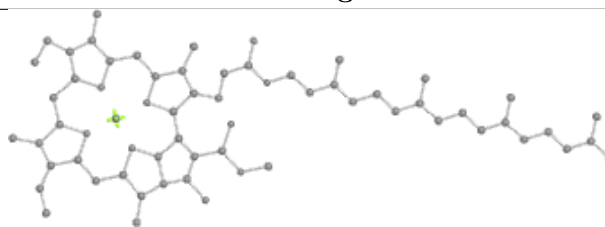
Bond lengths



Bond angles

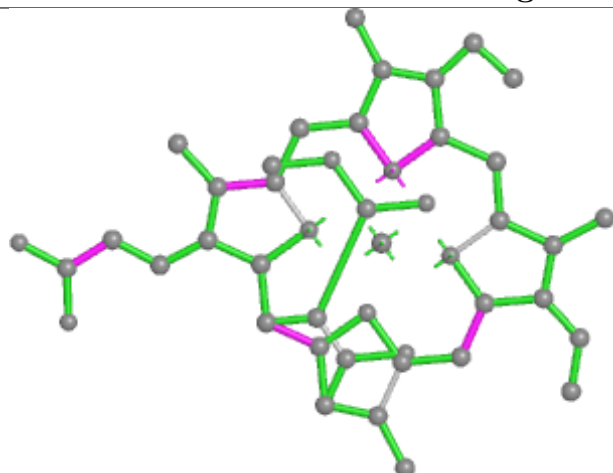


Torsions

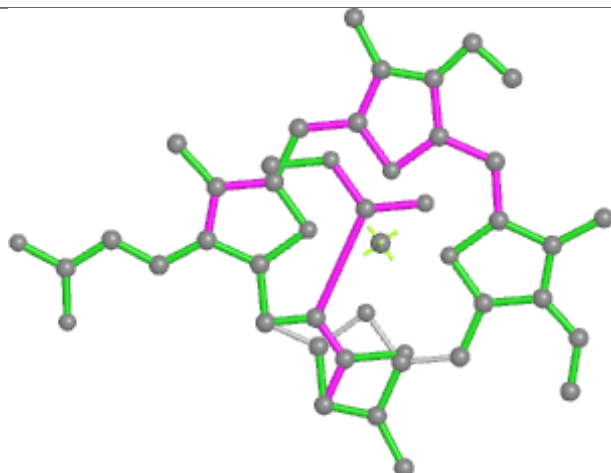


Rings

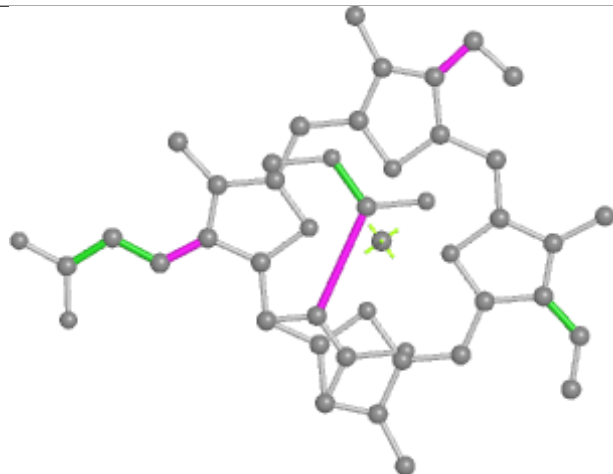
Ligand KC1 T 310



Bond lengths



Bond angles

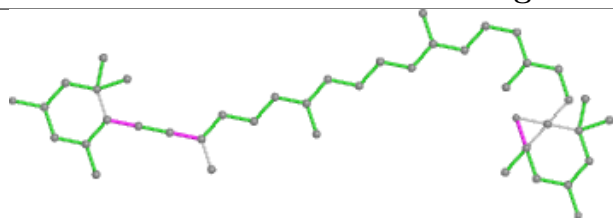


Torsions

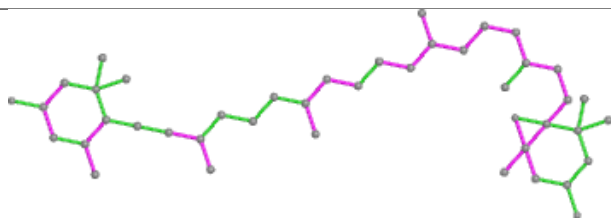


Rings

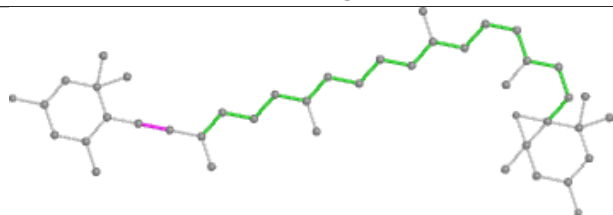
Ligand DD6 H 303



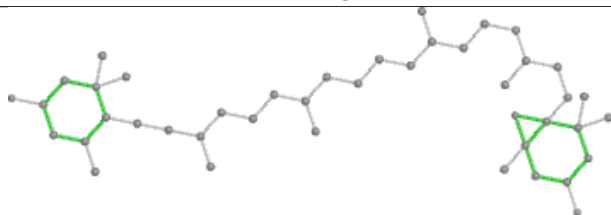
Bond lengths



Bond angles

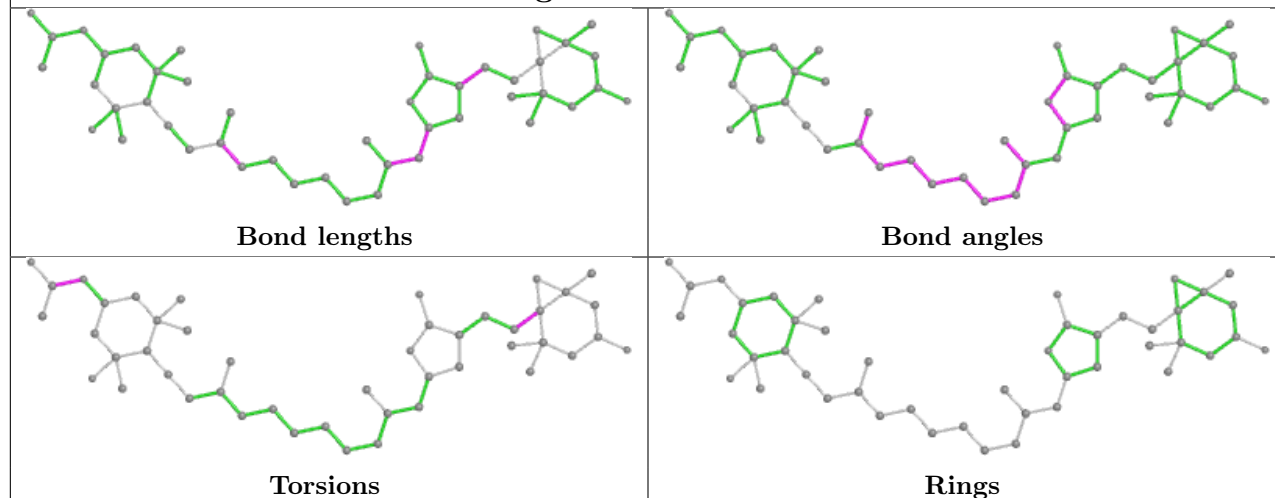


Torsions

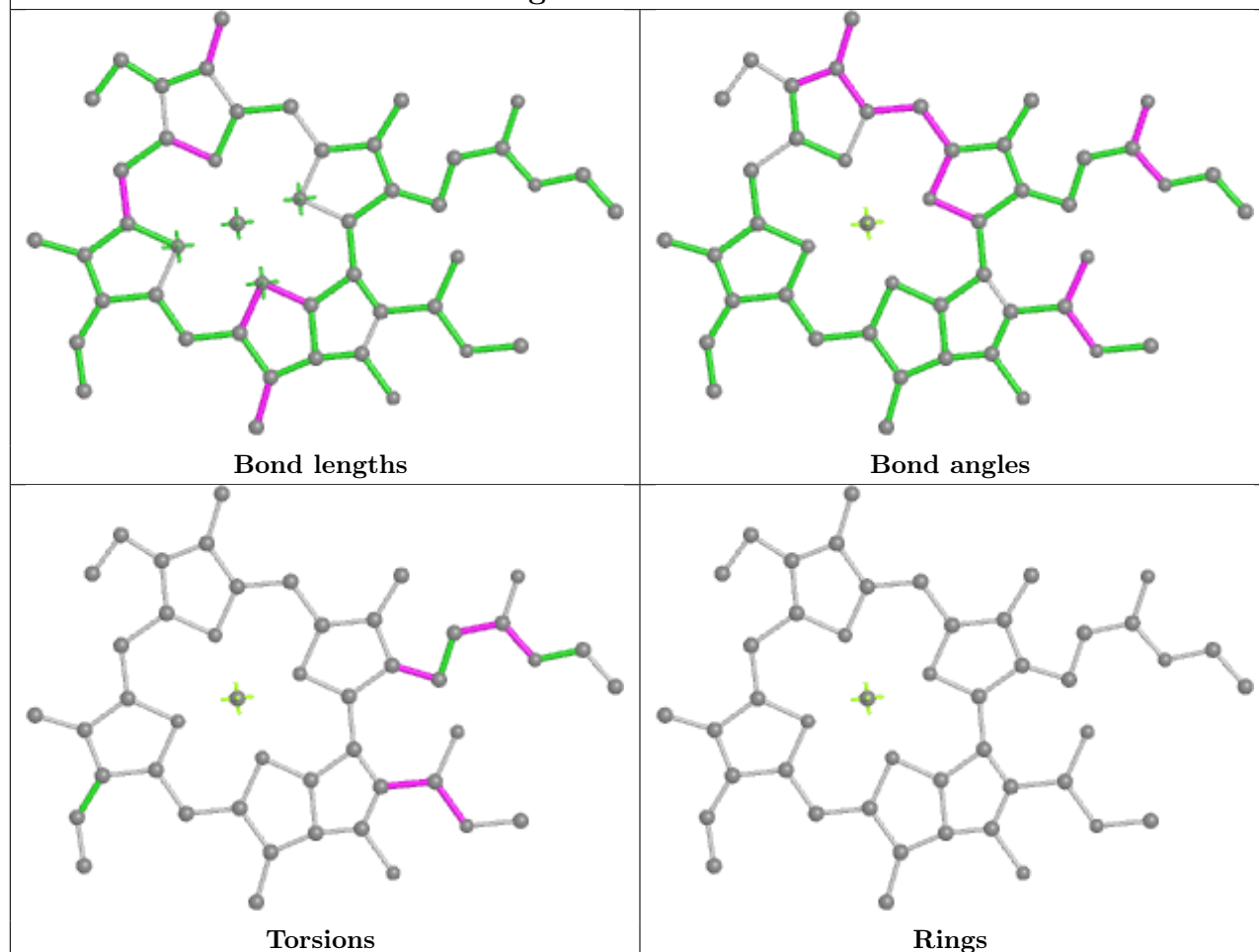


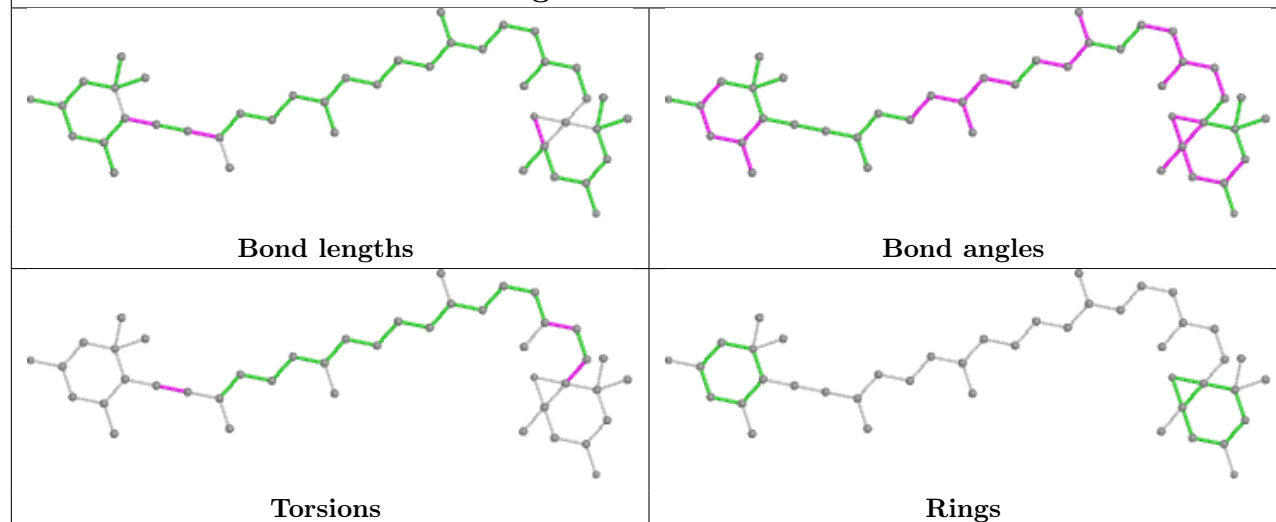
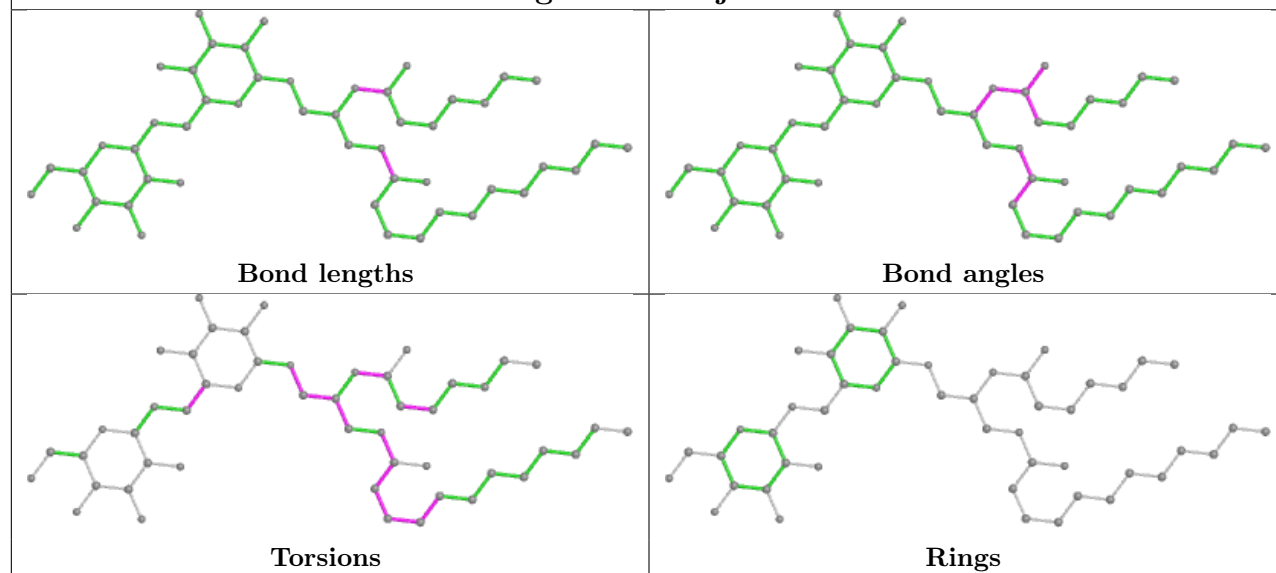
Rings

Ligand PID O 301

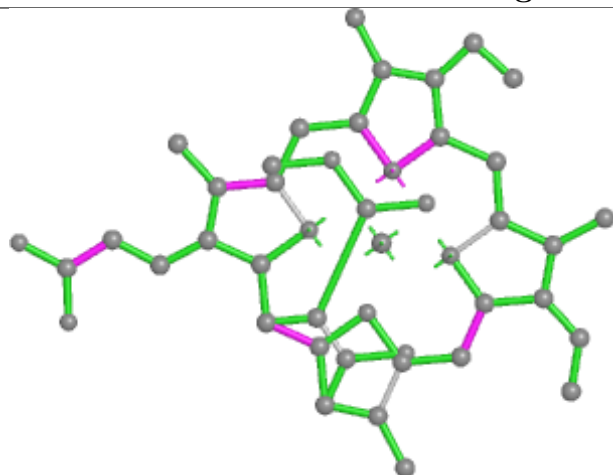


Ligand CLA a 821

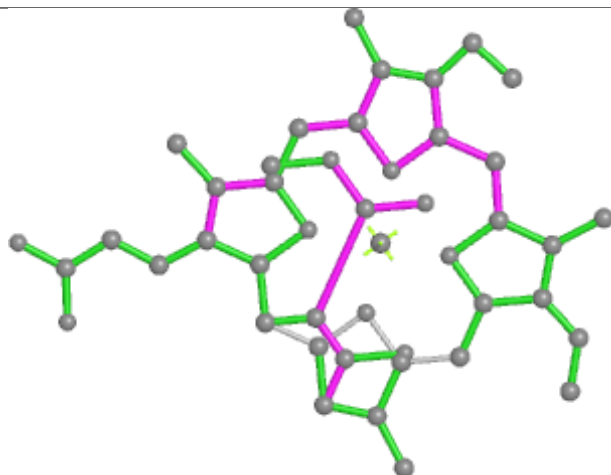


Ligand DD6 K 204**Ligand DGD j 106**

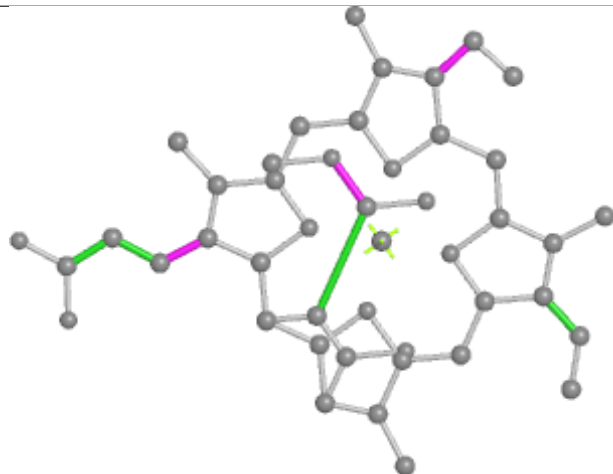
Ligand KC1 H 314



Bond lengths



Bond angles

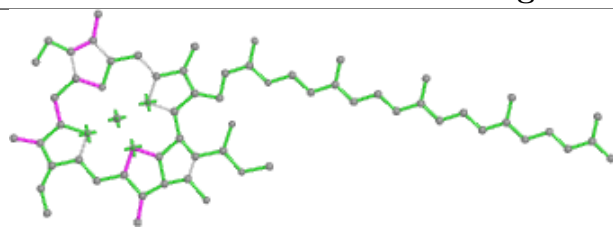


Torsions

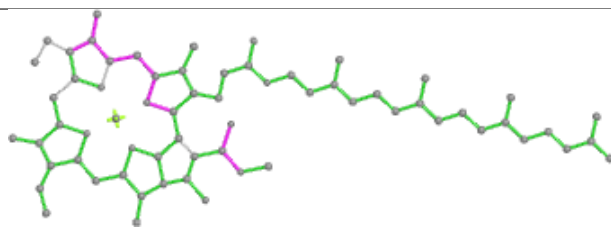


Rings

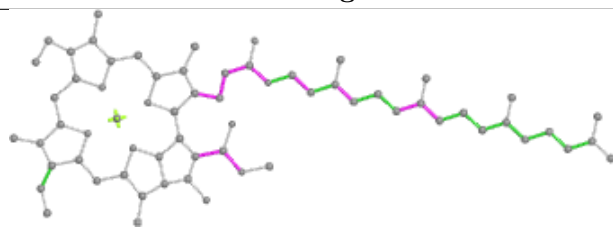
Ligand CLA b 720



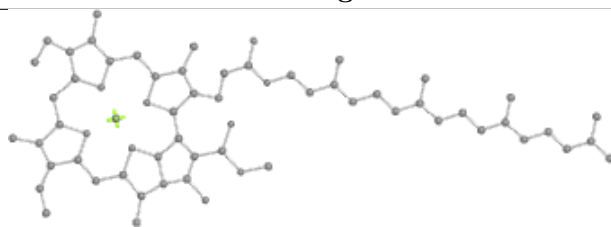
Bond lengths



Bond angles

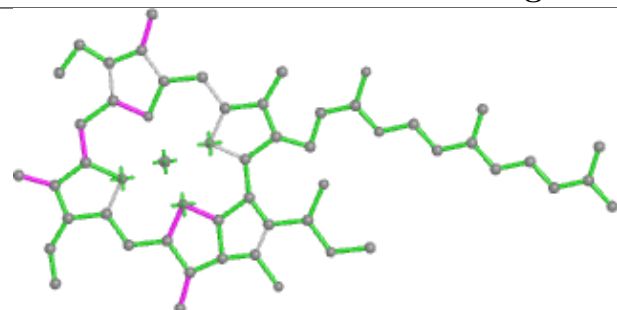


Torsions

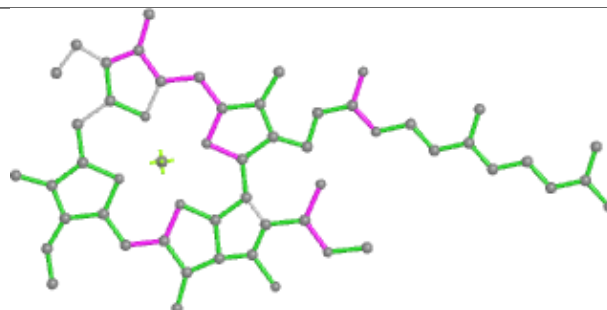


Rings

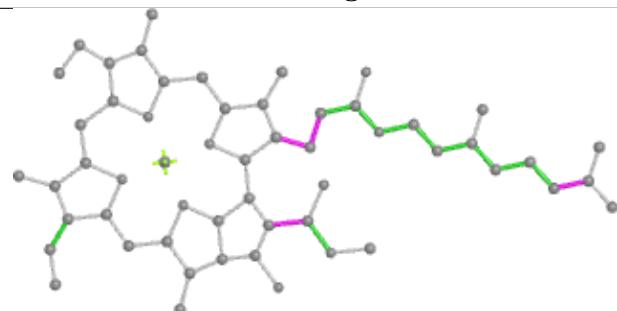
Ligand CLA I 214



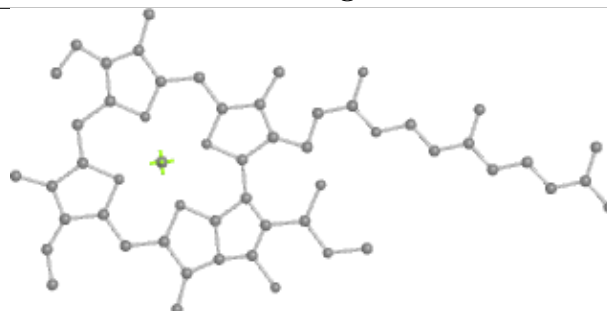
Bond lengths



Bond angles

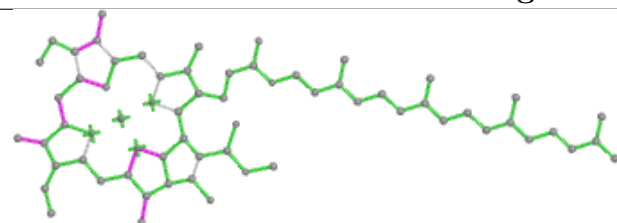


Torsions

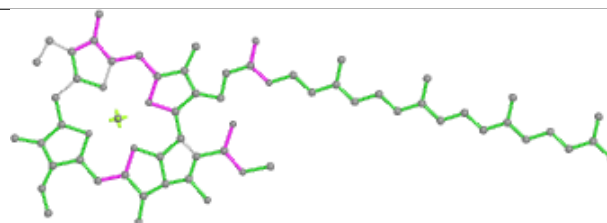


Rings

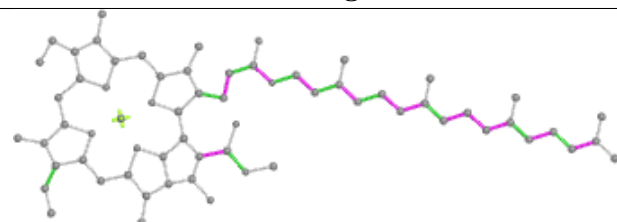
Ligand CLA G 312



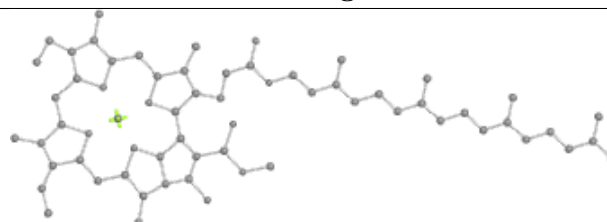
Bond lengths



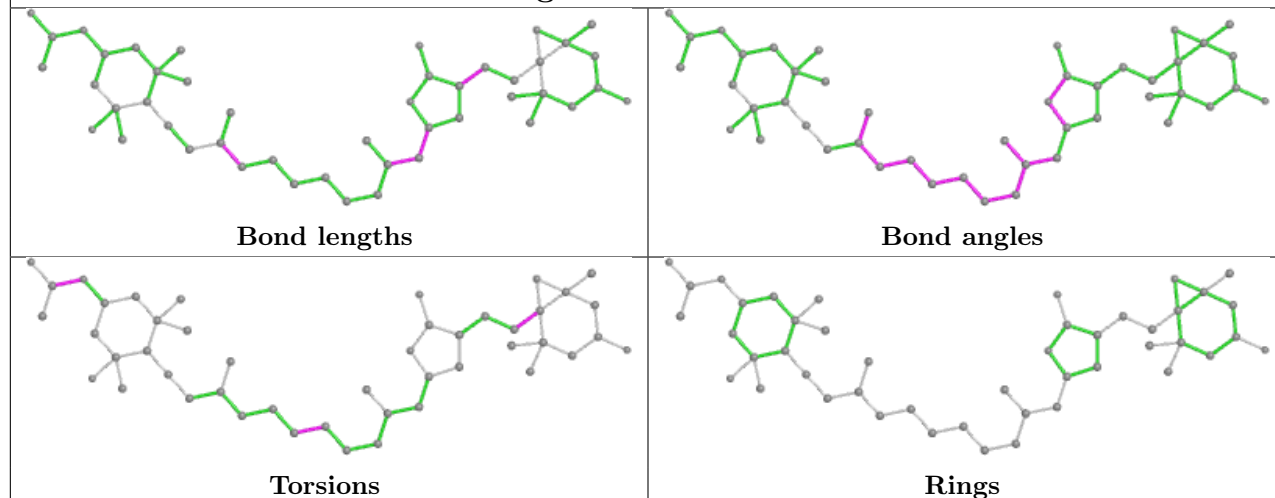
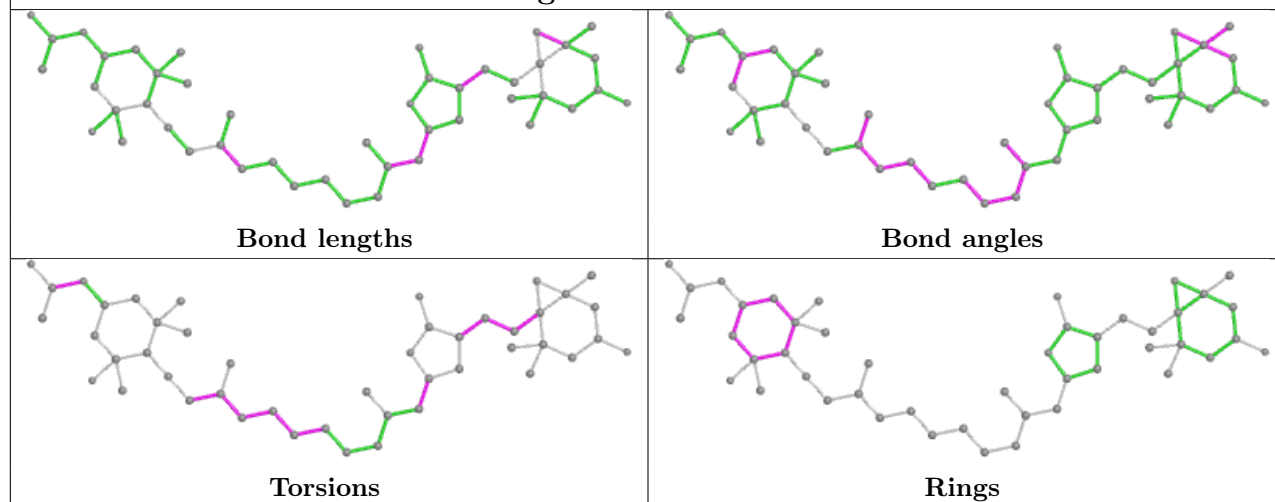
Bond angles



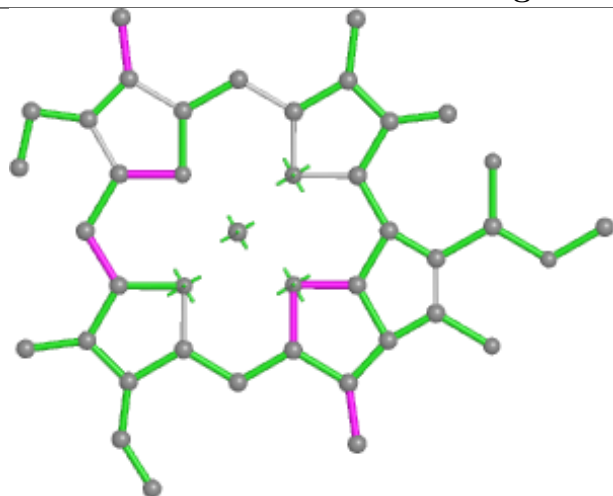
Torsions



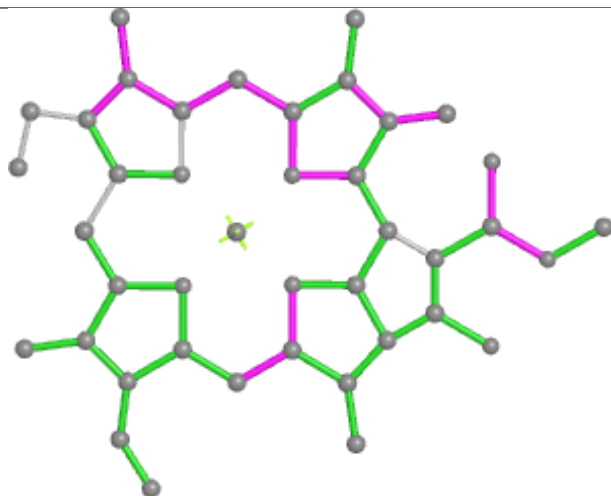
Rings

Ligand PID P 202**Ligand PID F 304**

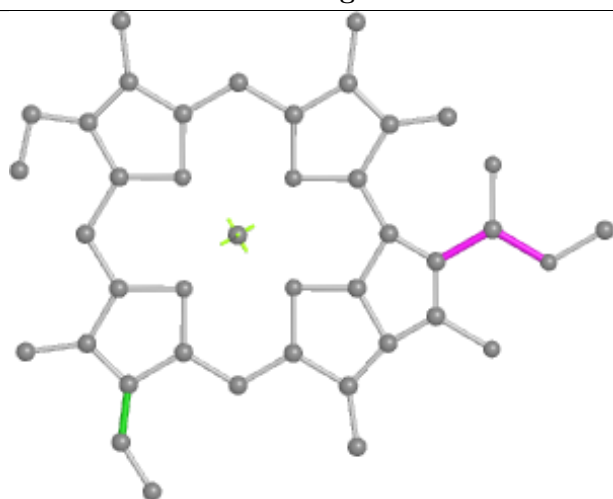
Ligand CLA H 315



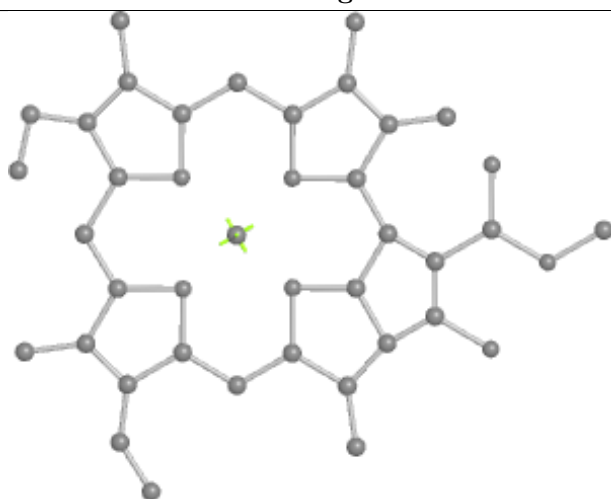
Bond lengths



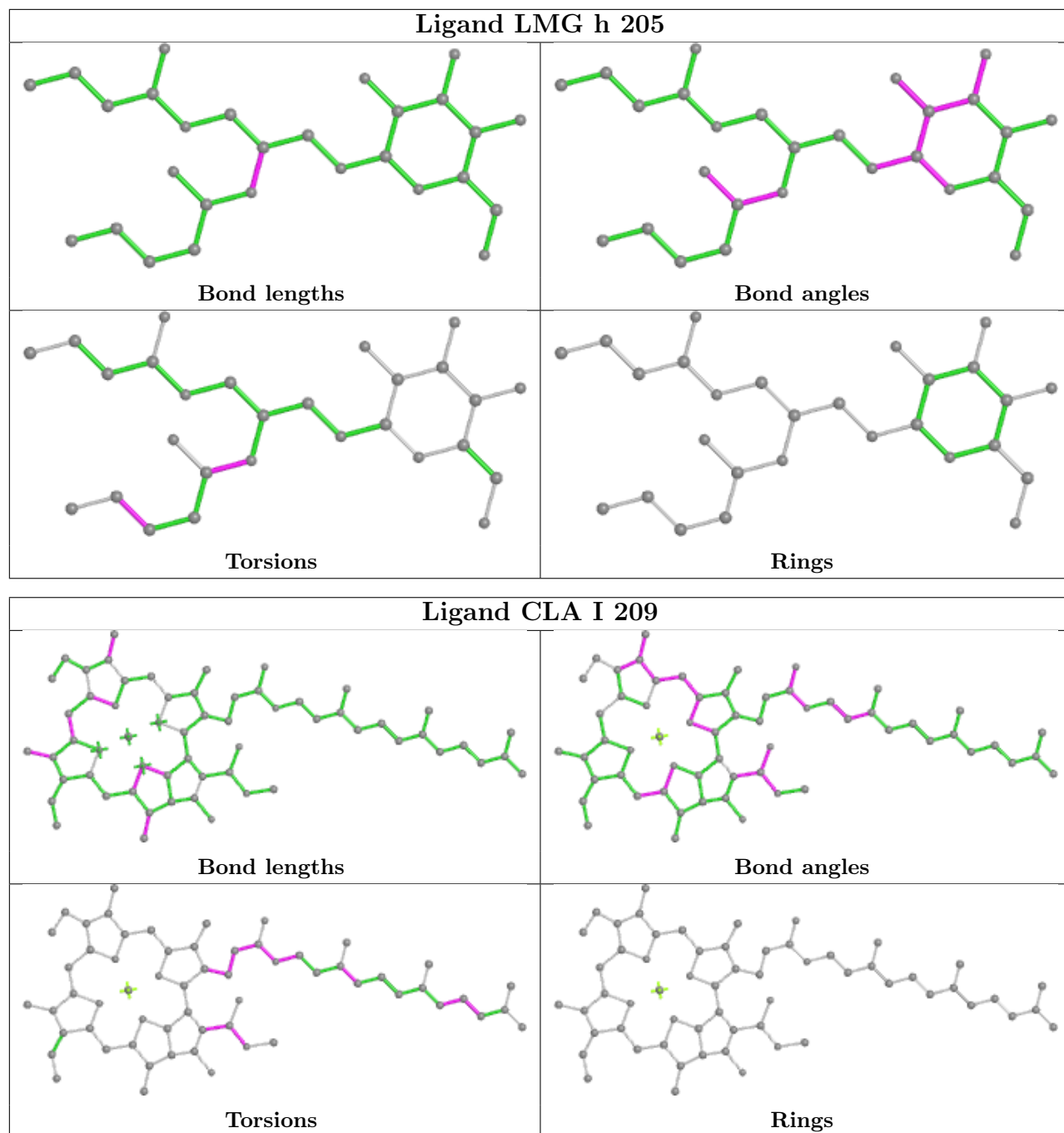
Bond angles

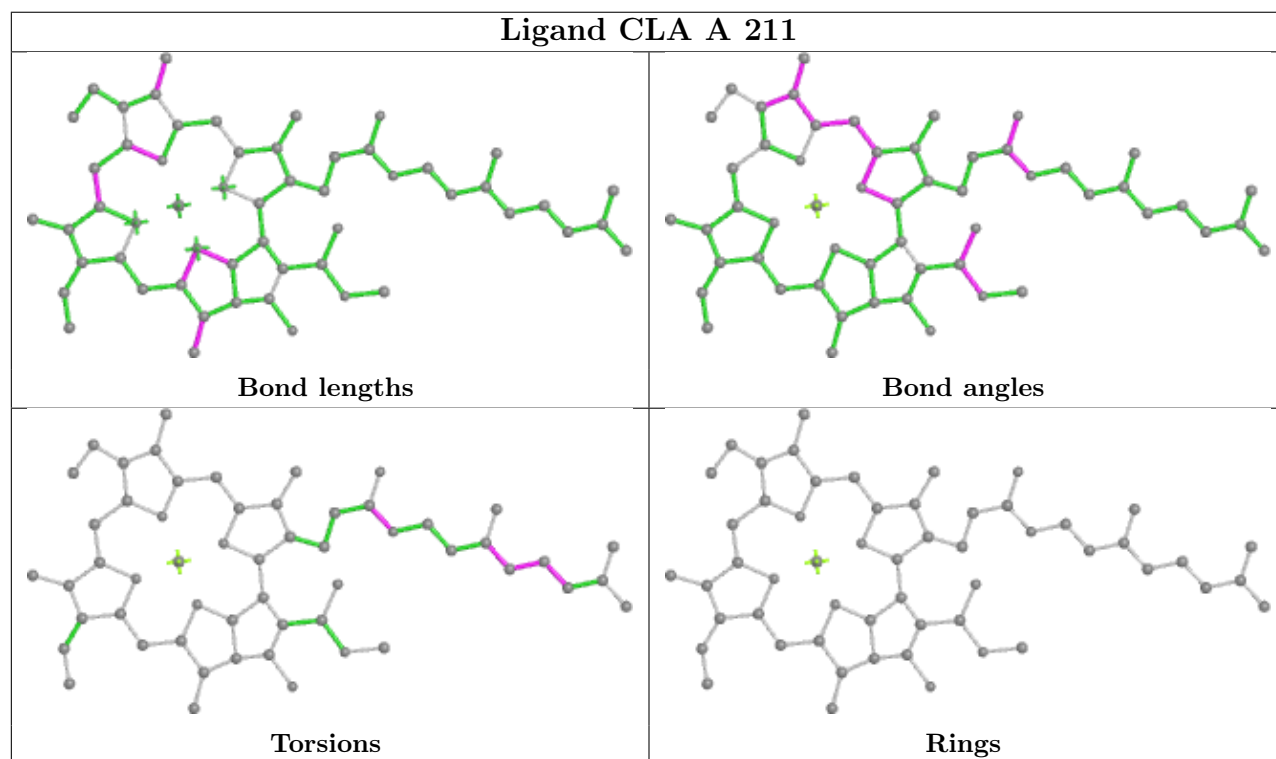
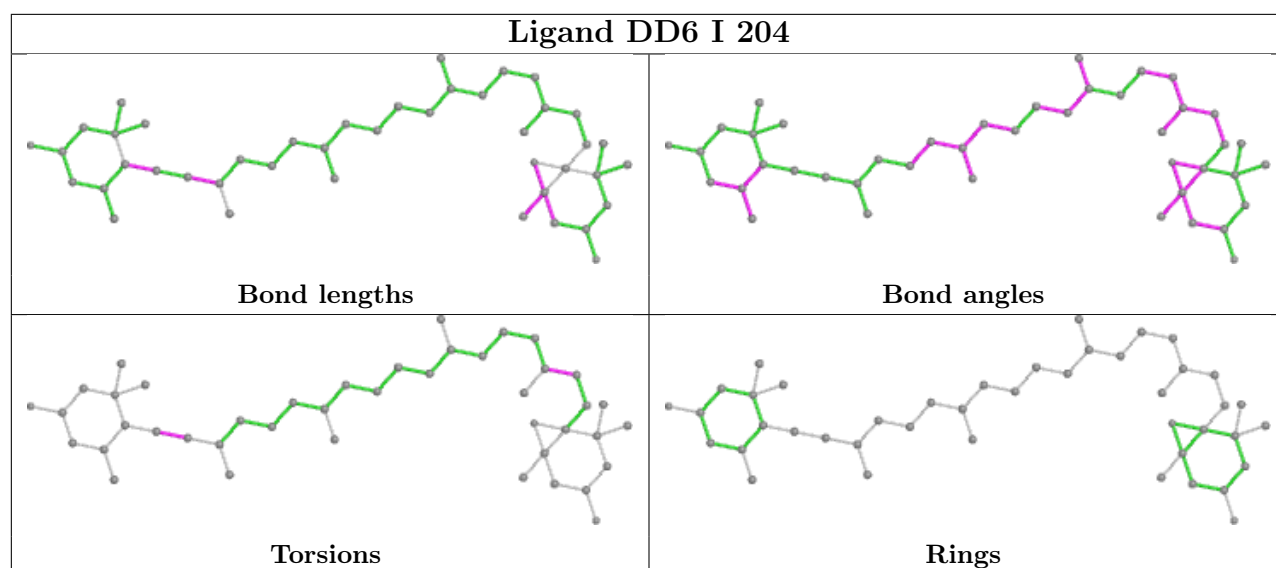


Torsions

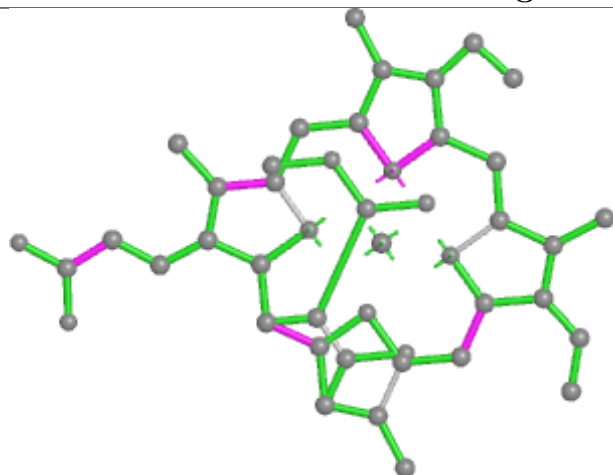


Rings

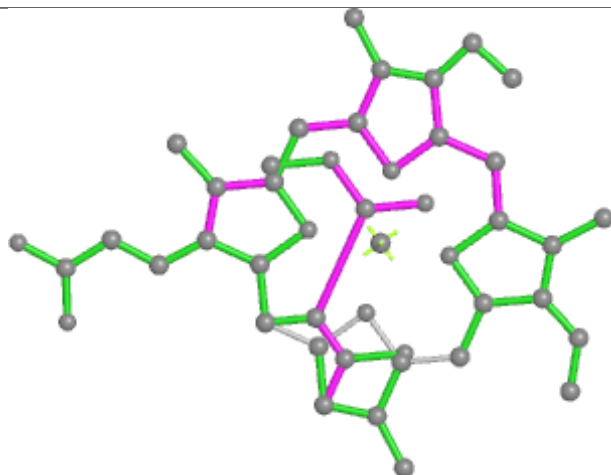




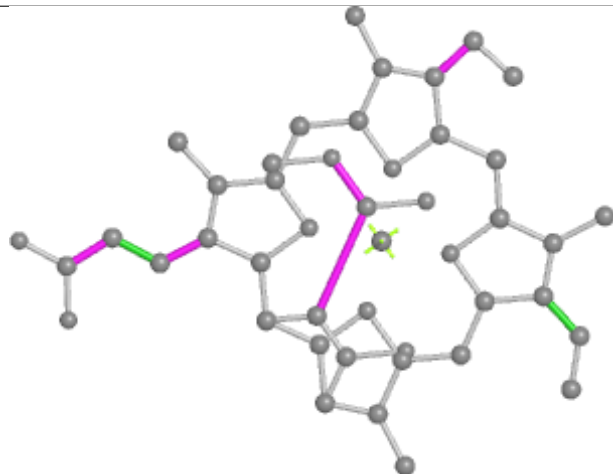
Ligand KC1 C 310



Bond lengths



Bond angles

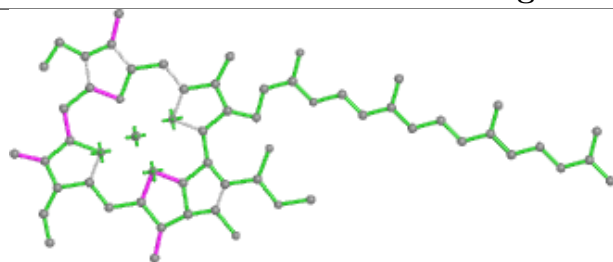


Torsions

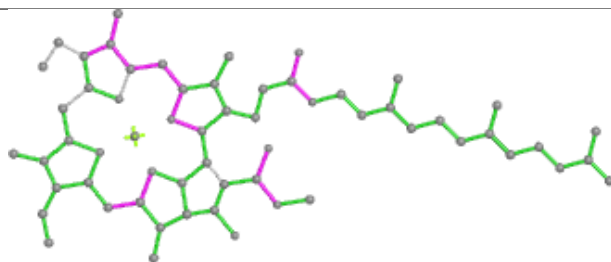


Rings

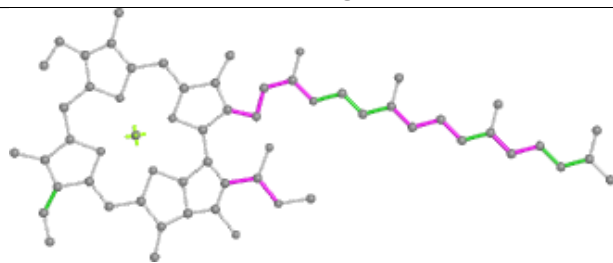
Ligand CLA b 709



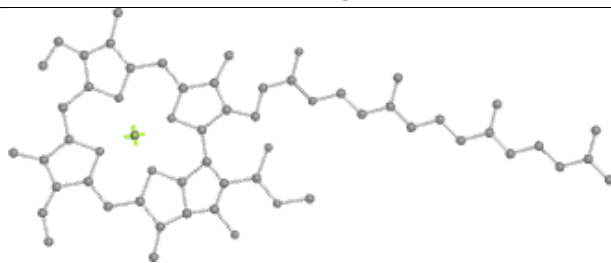
Bond lengths



Bond angles

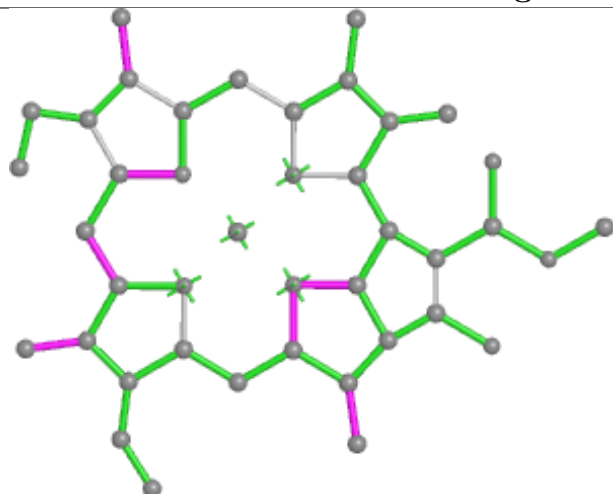


Torsions

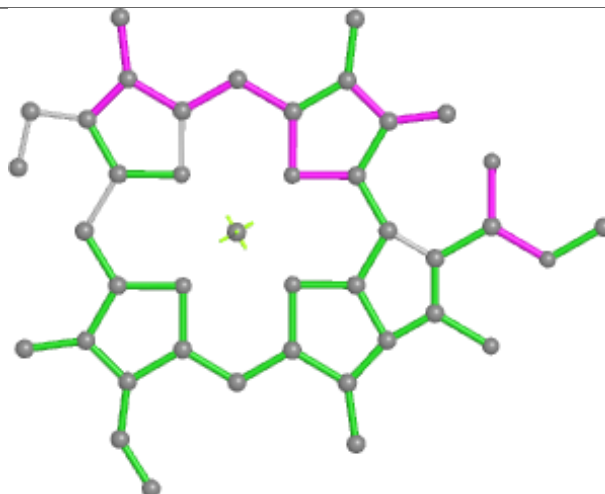


Rings

Ligand CLA B 314



Bond lengths



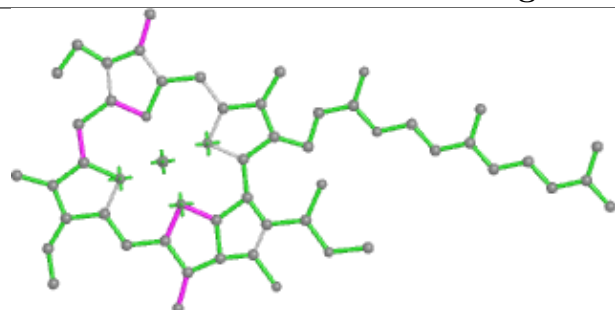
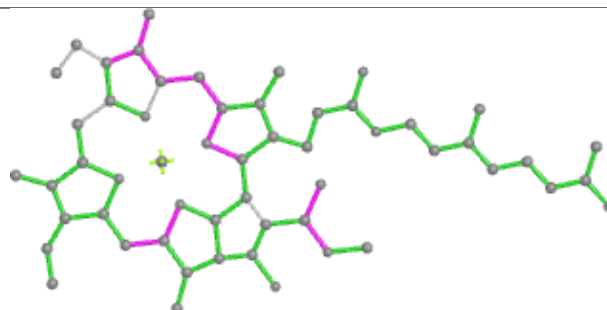
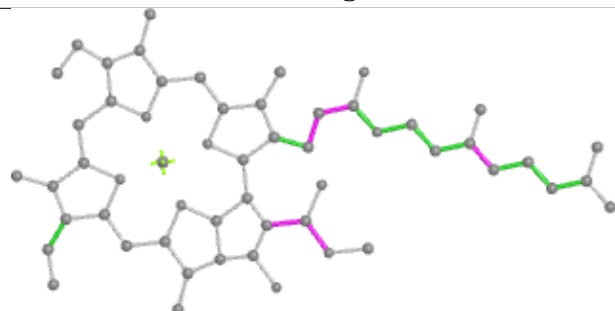
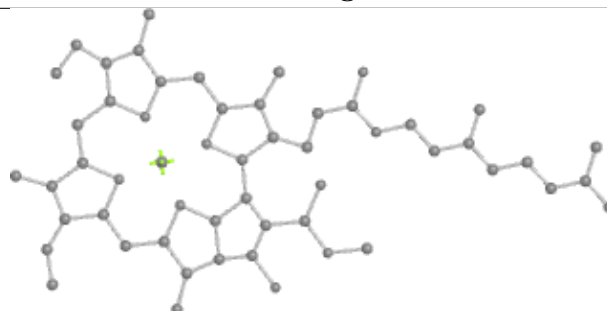
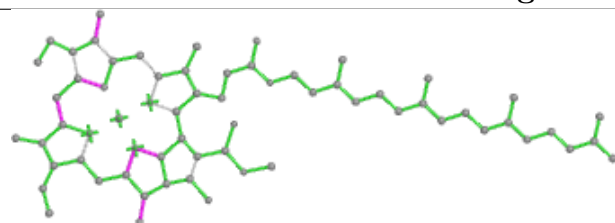
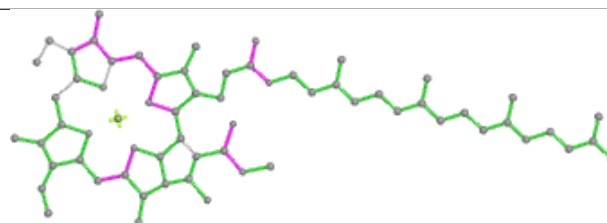
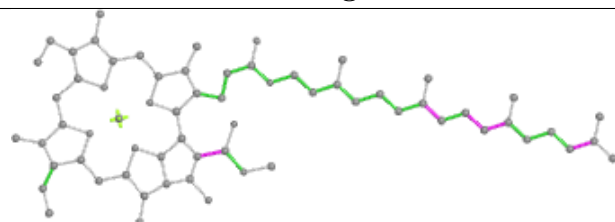
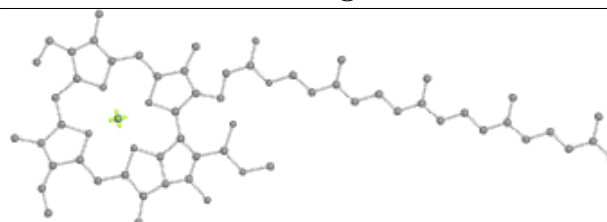
Bond angles

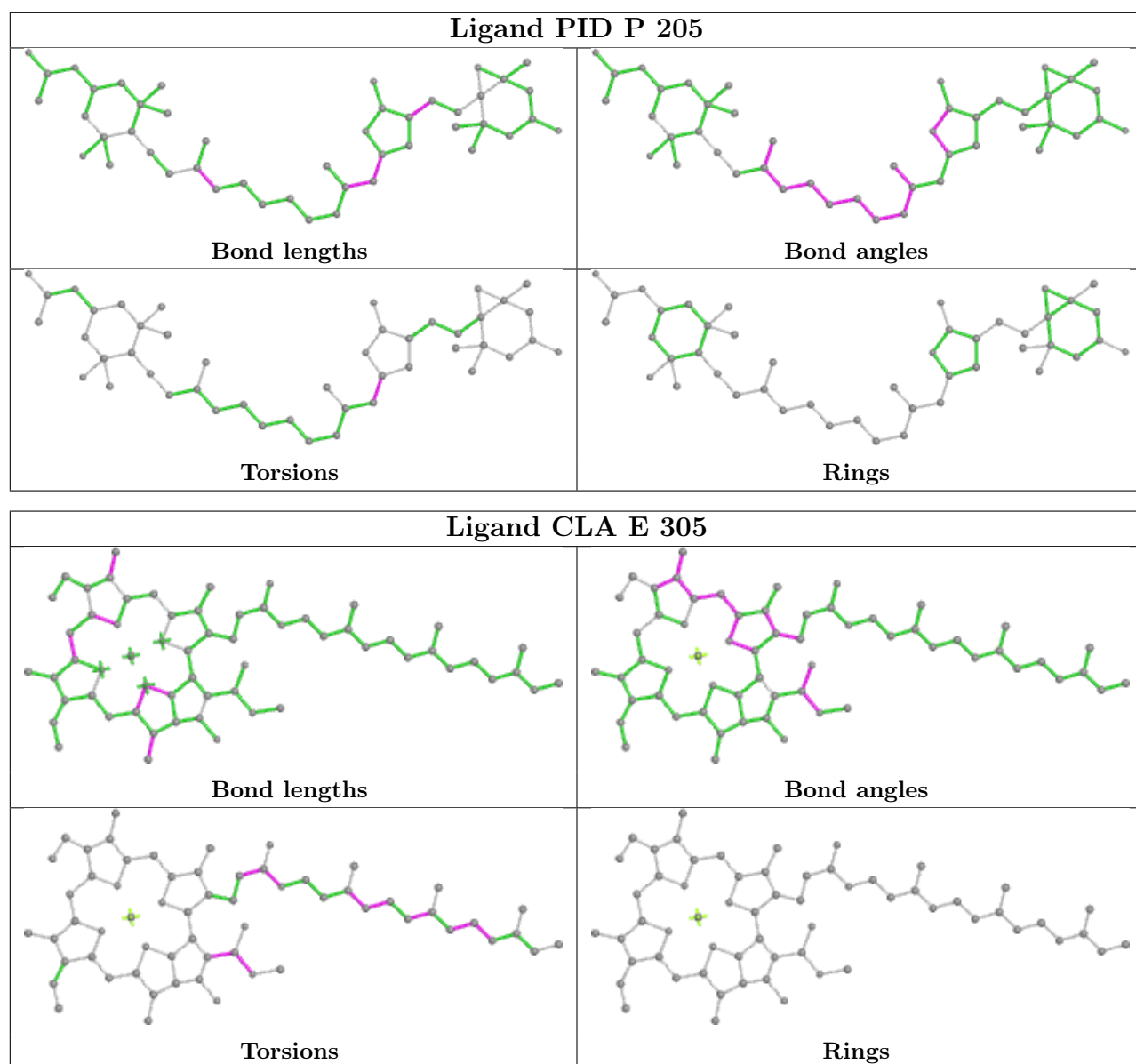


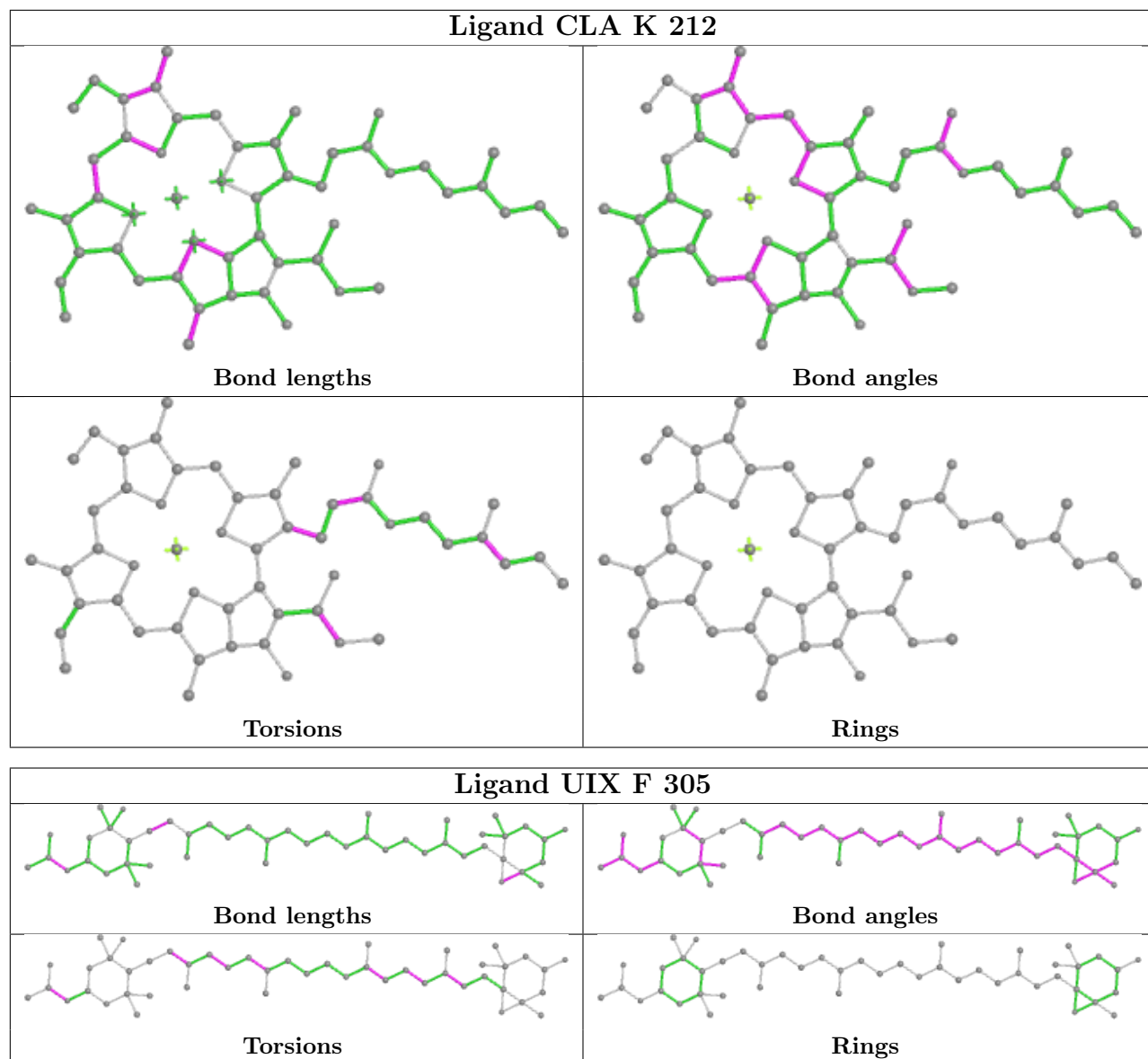
Torsions

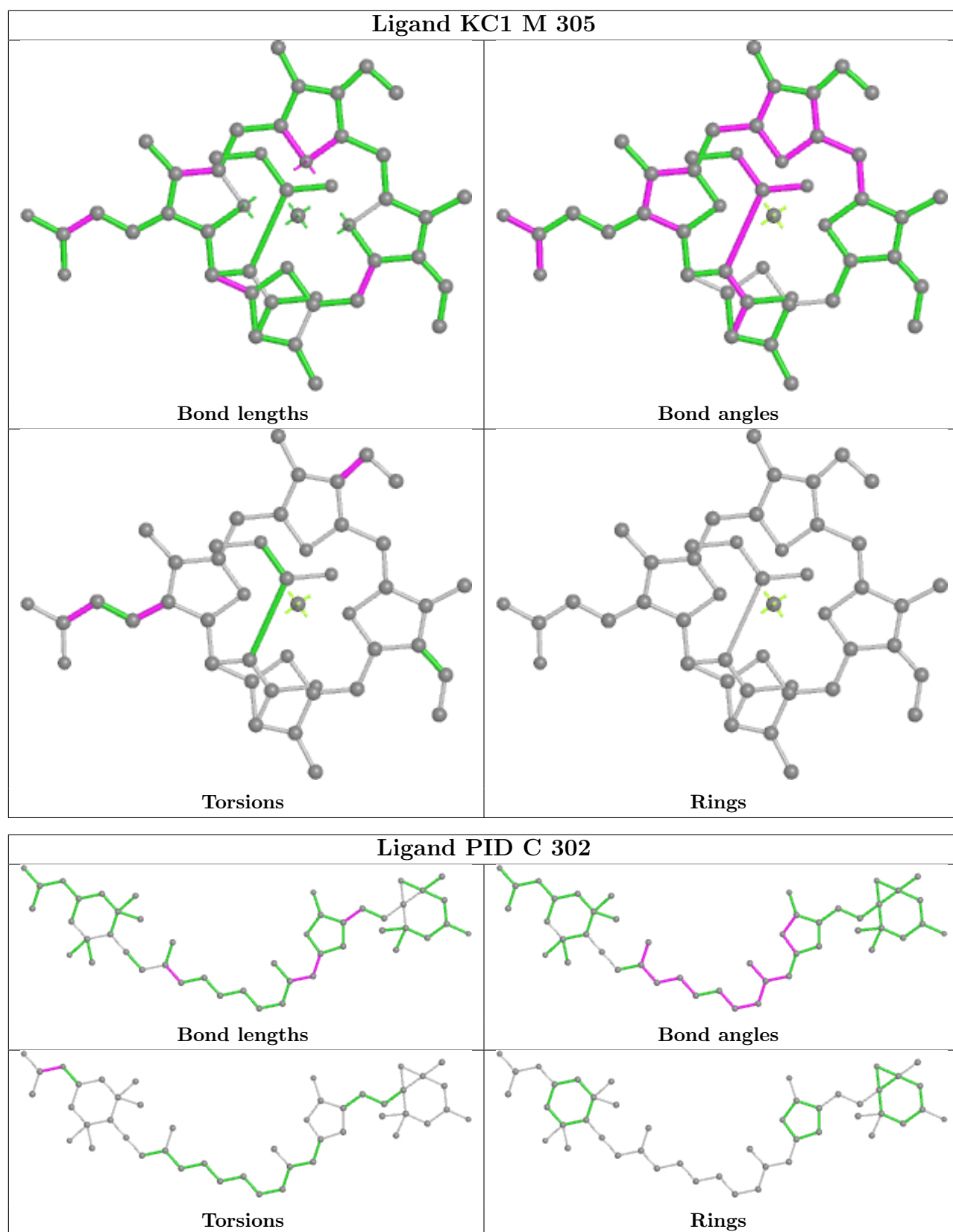


Rings

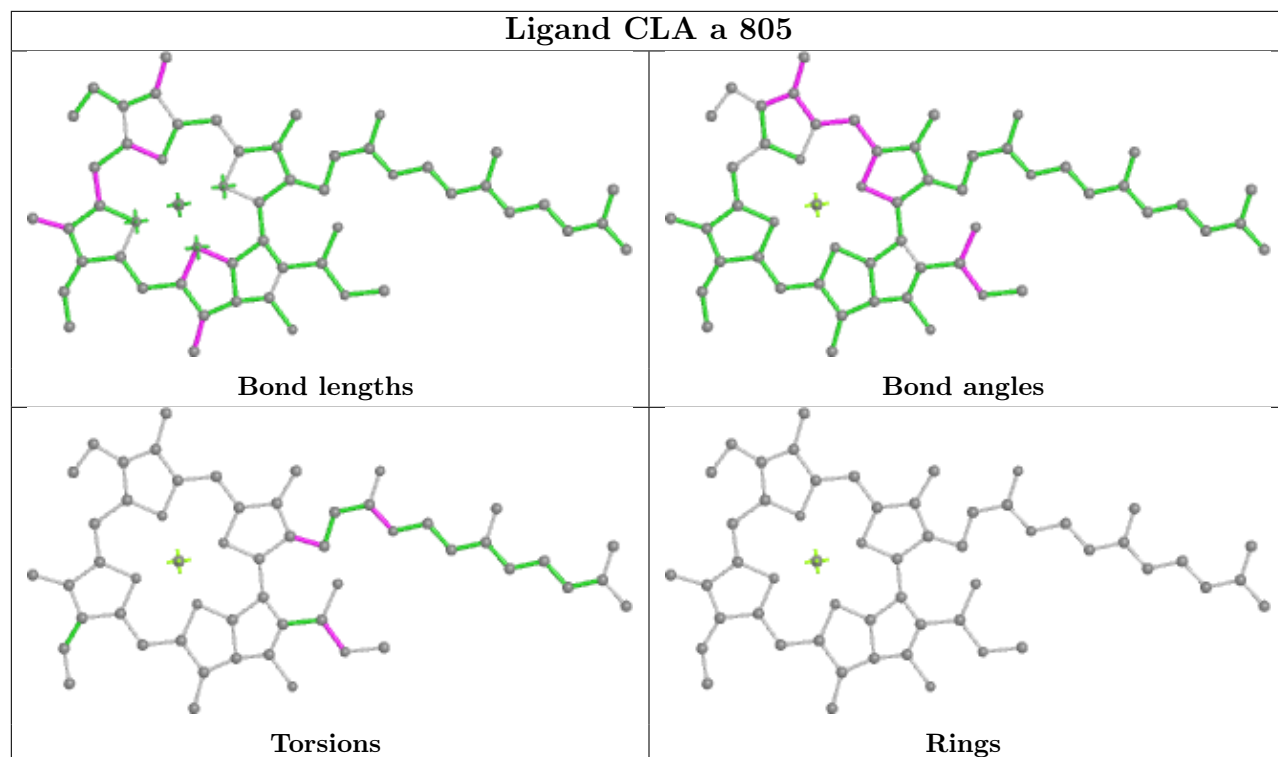
Ligand CLA L 310**Bond lengths****Bond angles****Torsions****Rings****Ligand CLA E 308****Bond lengths****Bond angles****Torsions****Rings**



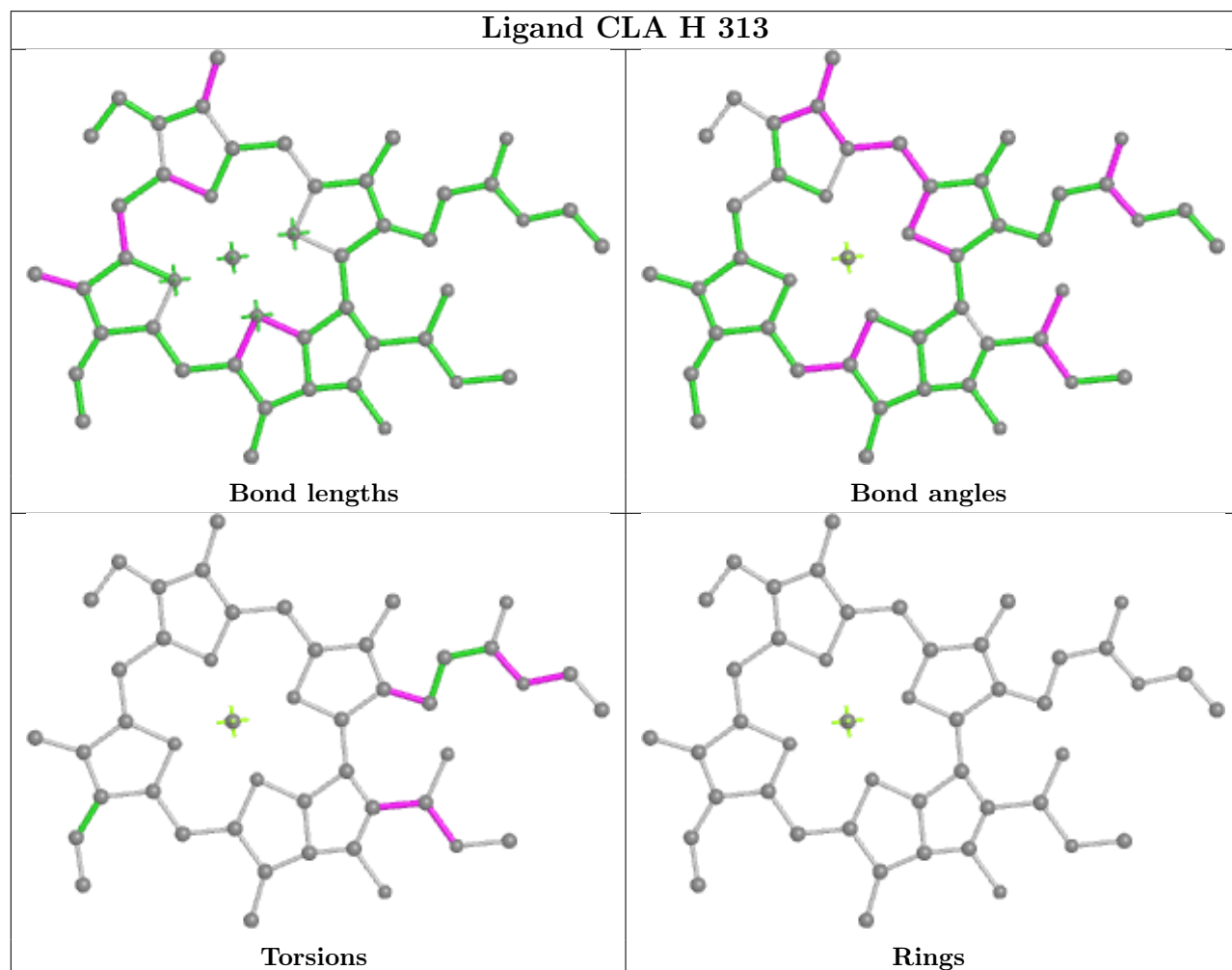


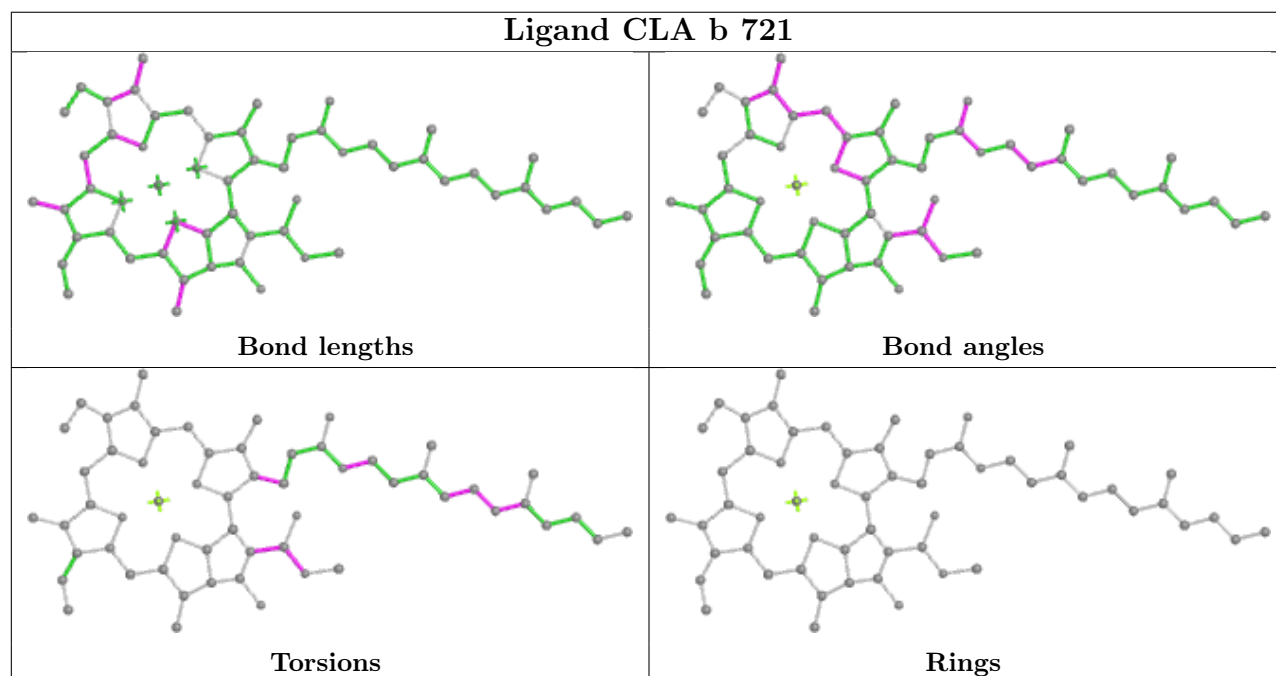
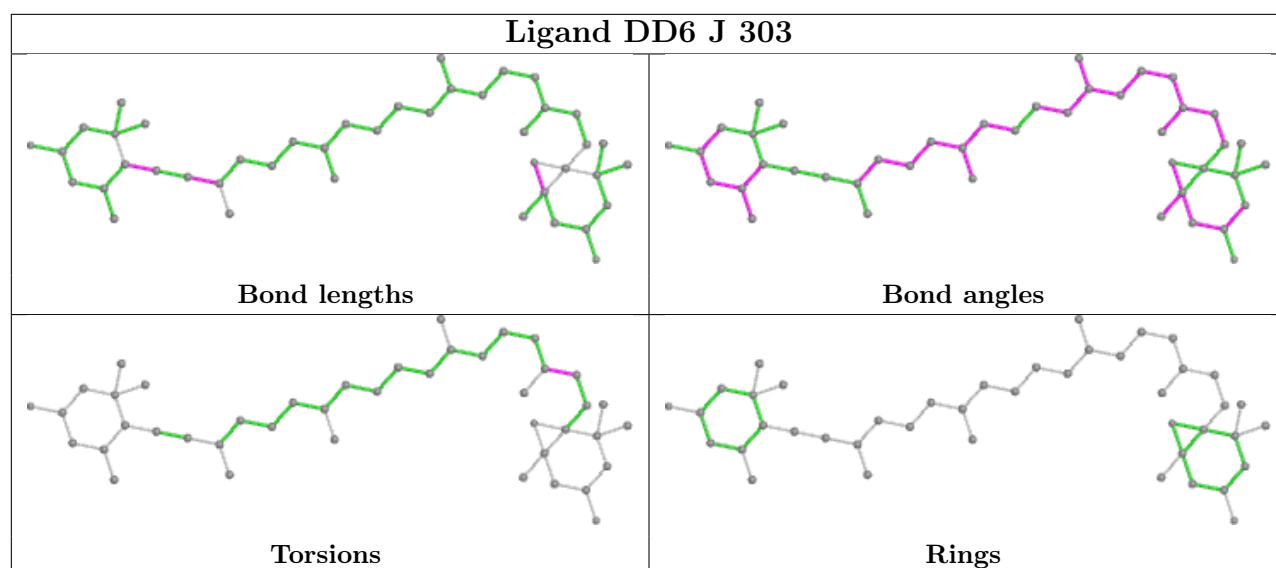


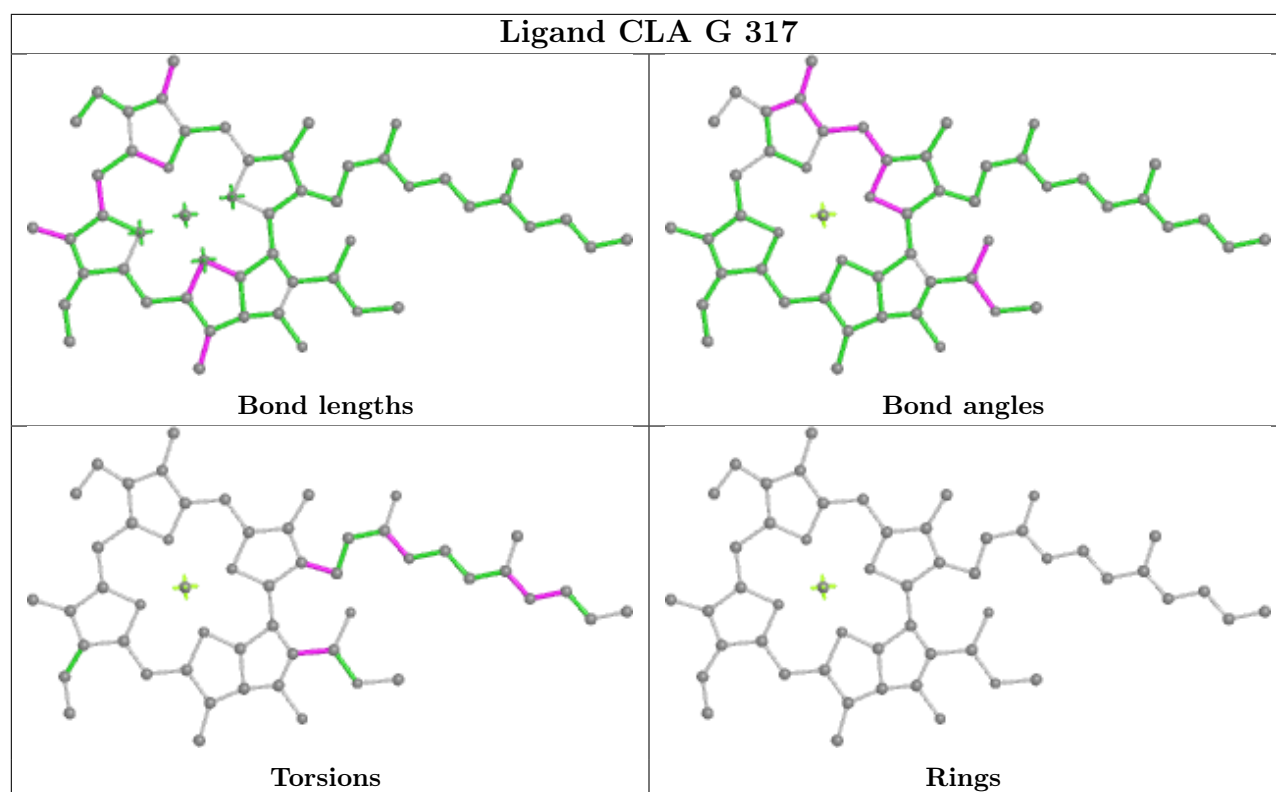
Ligand CLA a 805



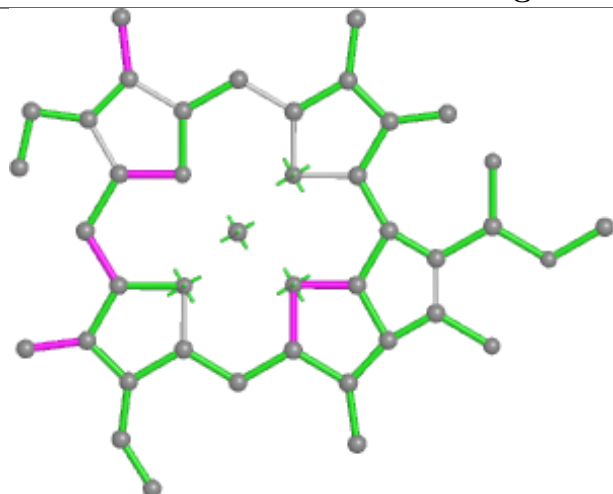
Ligand CLA H 313



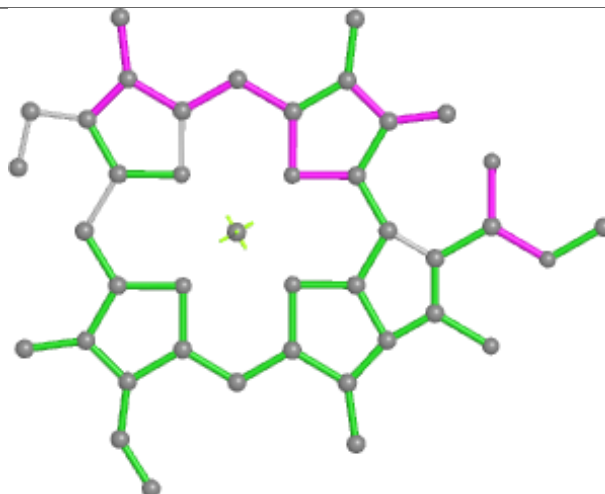




Ligand CLA O 316



Bond lengths



Bond angles

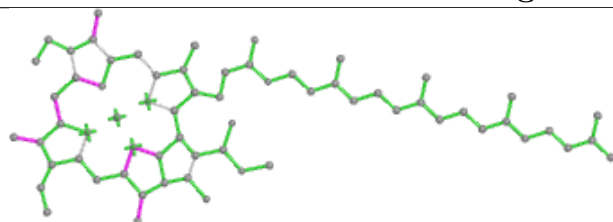


Torsions

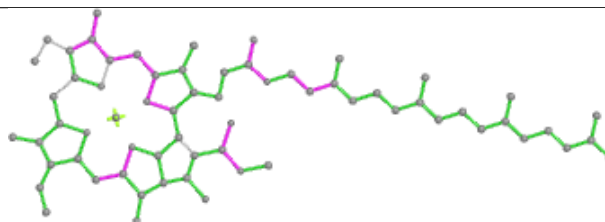


Rings

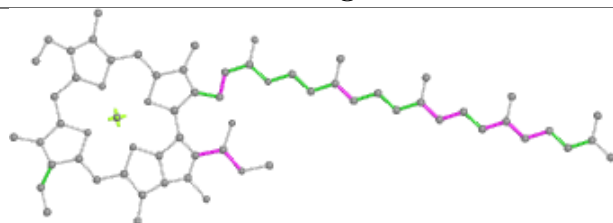
Ligand CLA b 701



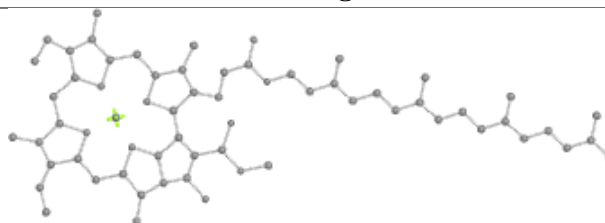
Bond lengths



Bond angles

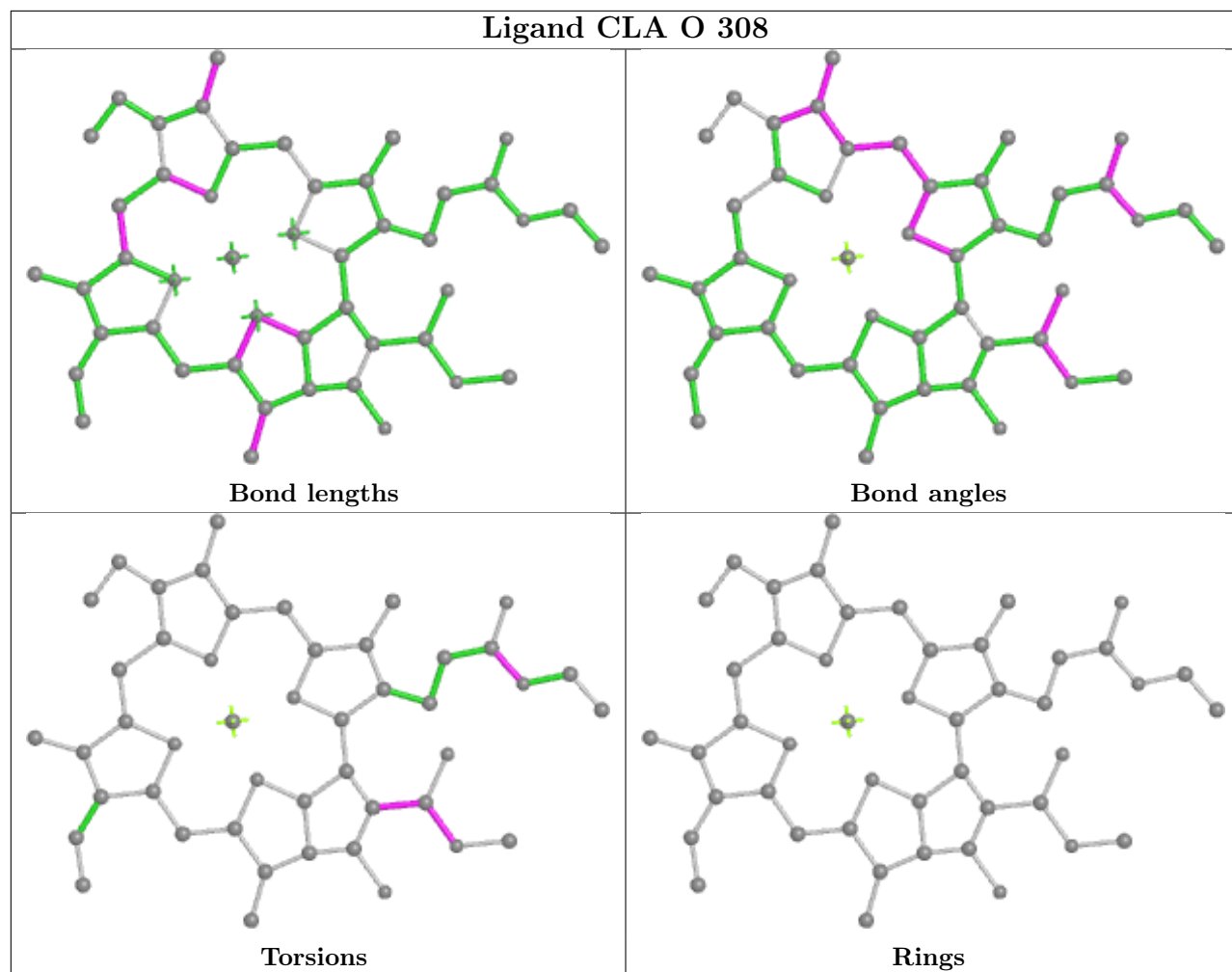


Torsions

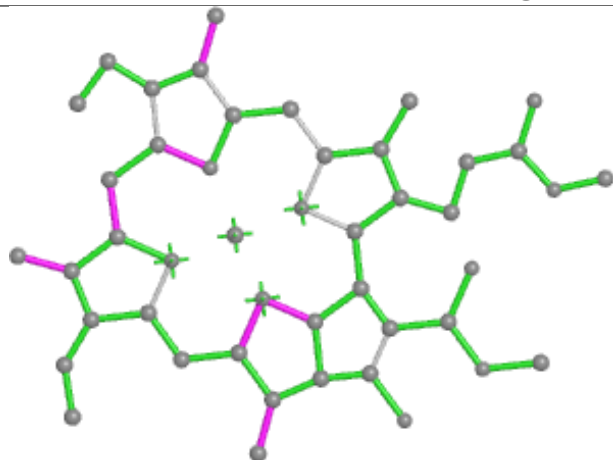


Rings

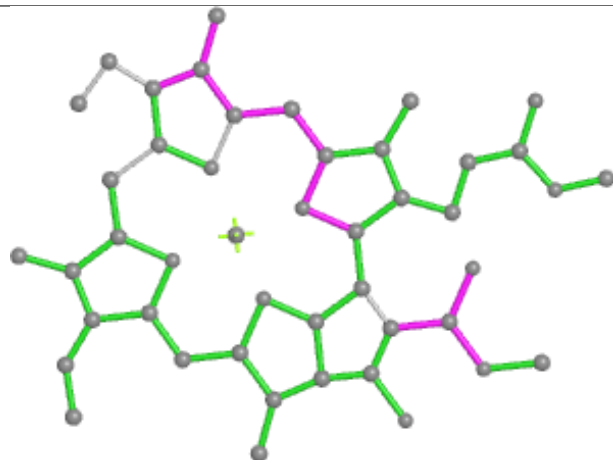
Ligand CLA O 308



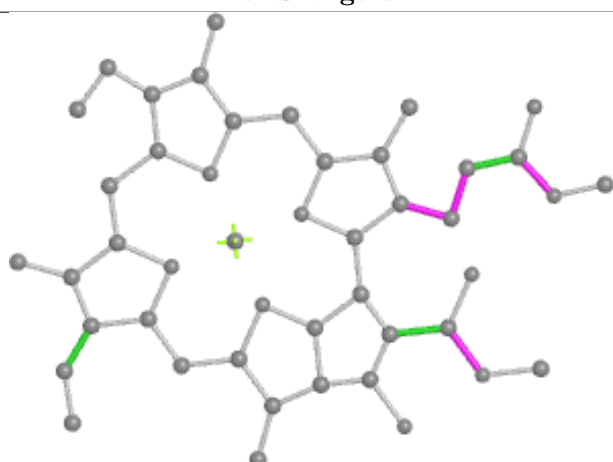
Ligand CLA b 715



Bond lengths



Bond angles

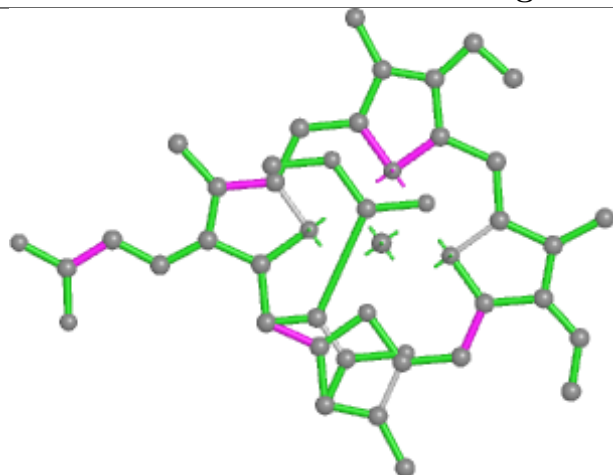


Torsions

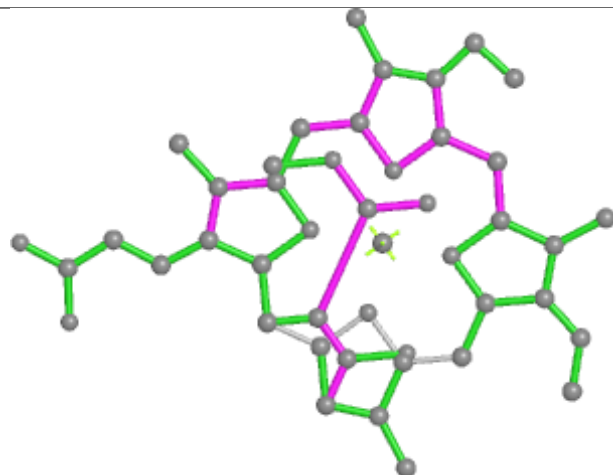


Rings

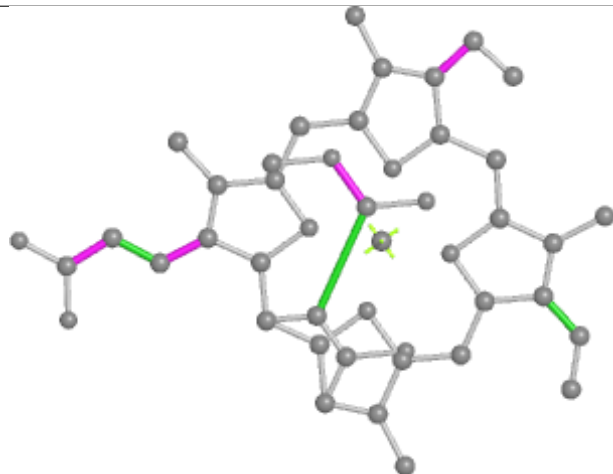
Ligand KC1 C 315



Bond lengths



Bond angles

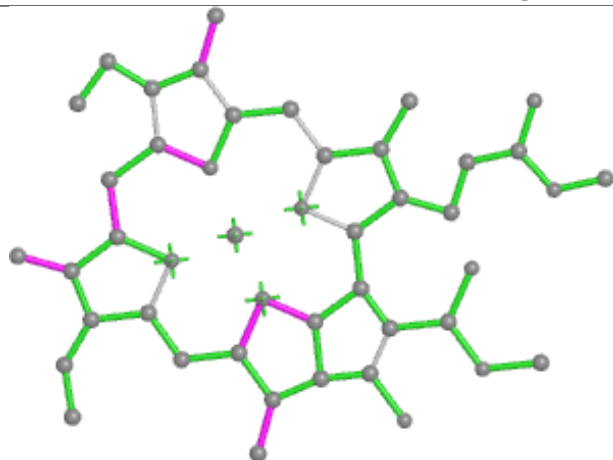


Torsions

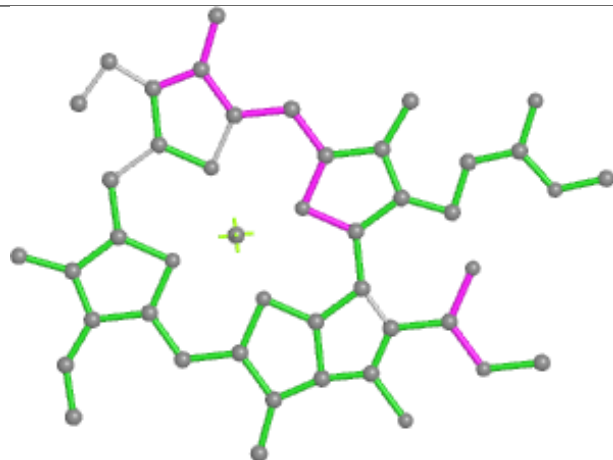


Rings

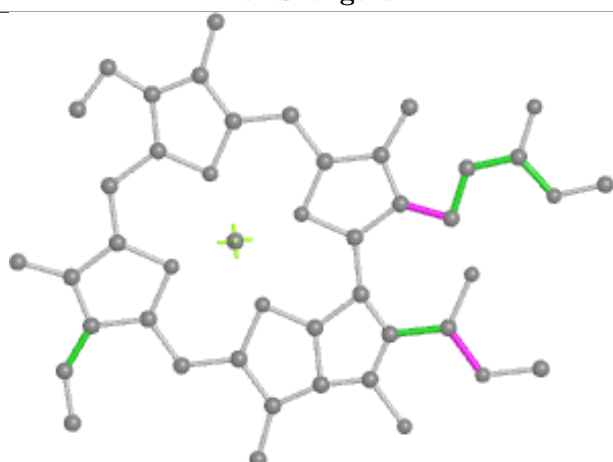
Ligand CLA F 308



Bond lengths



Bond angles

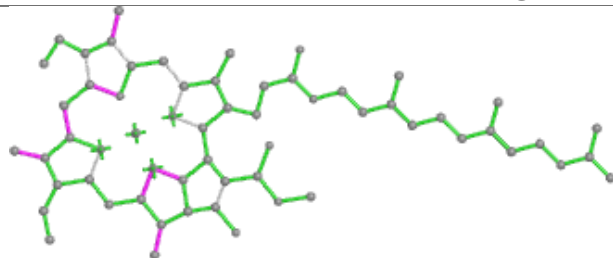


Torsions

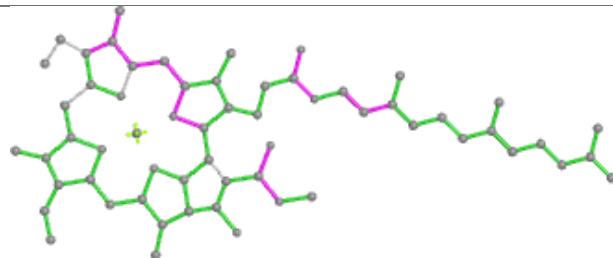


Rings

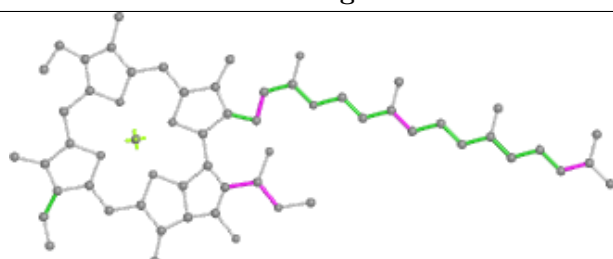
Ligand CLA G 314



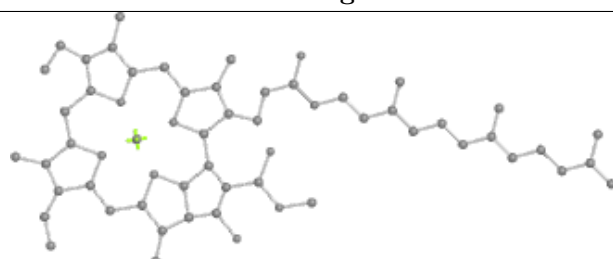
Bond lengths



Bond angles

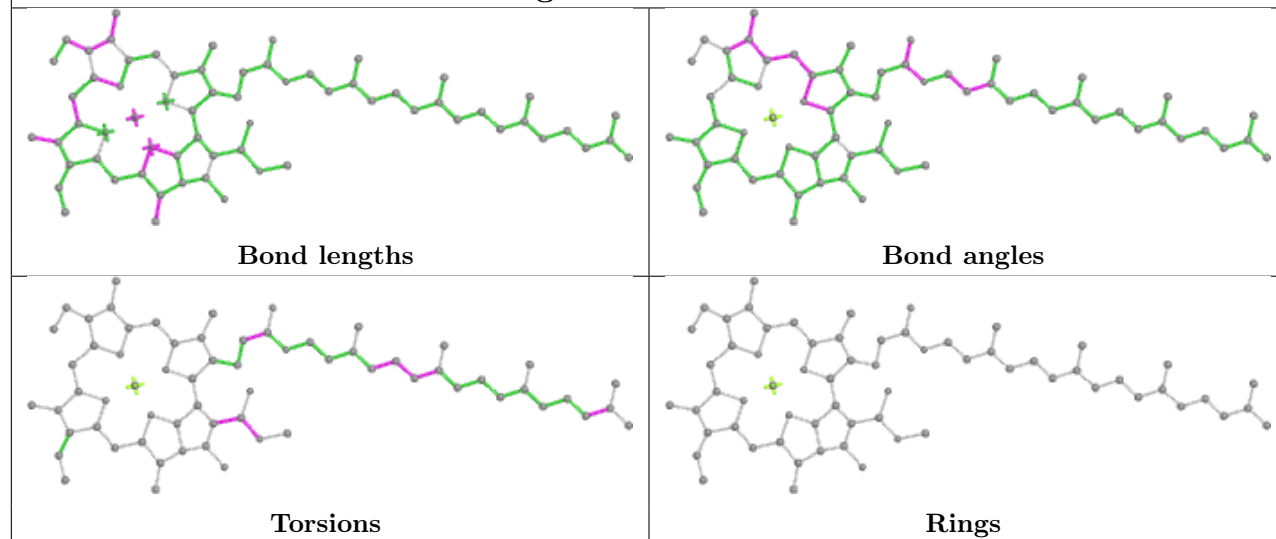


Torsions

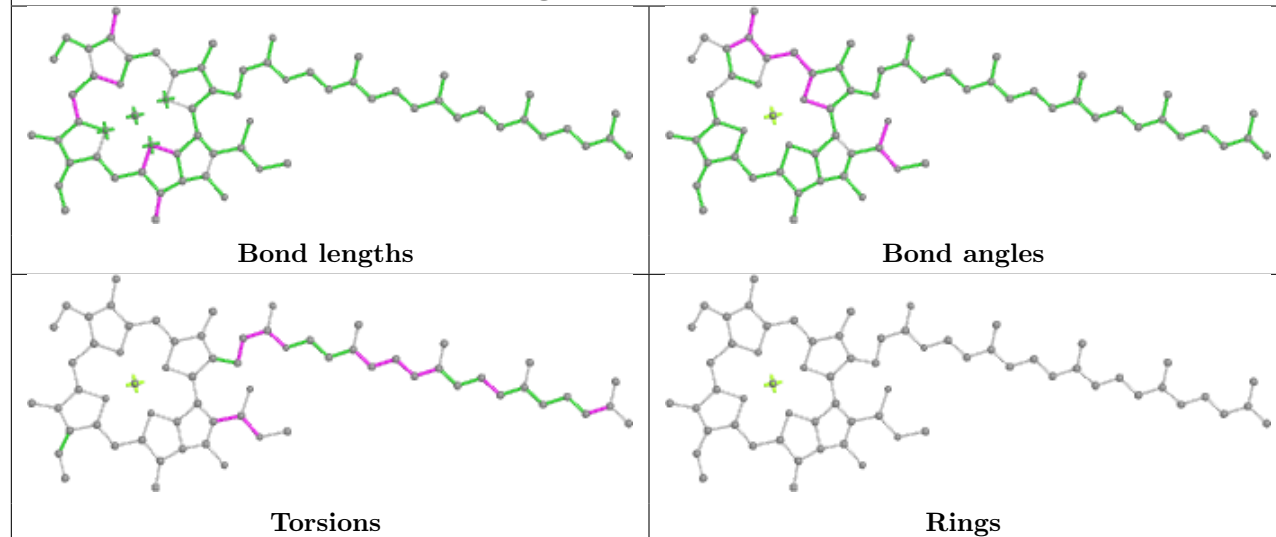


Rings

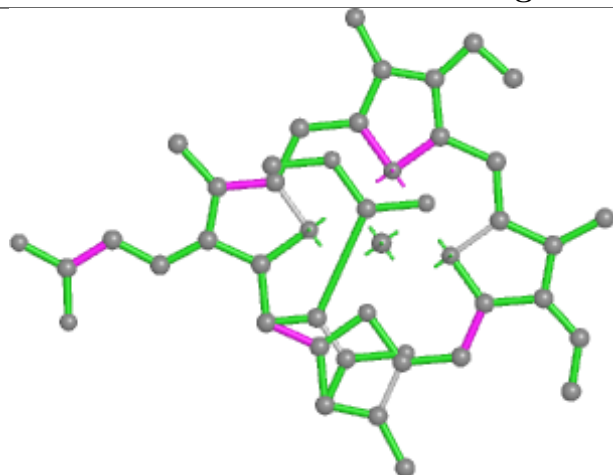
Ligand CLA a 801



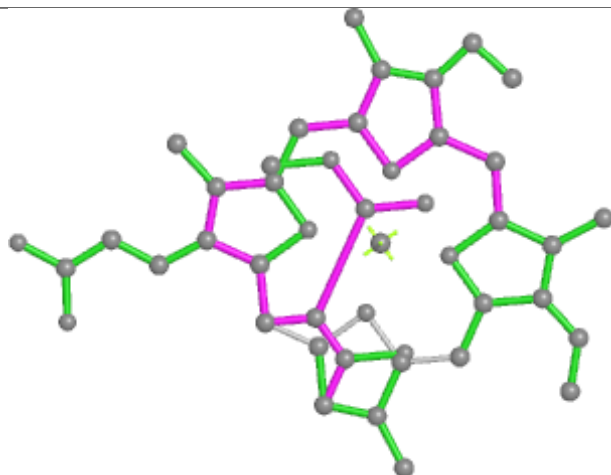
Ligand CLA b 702



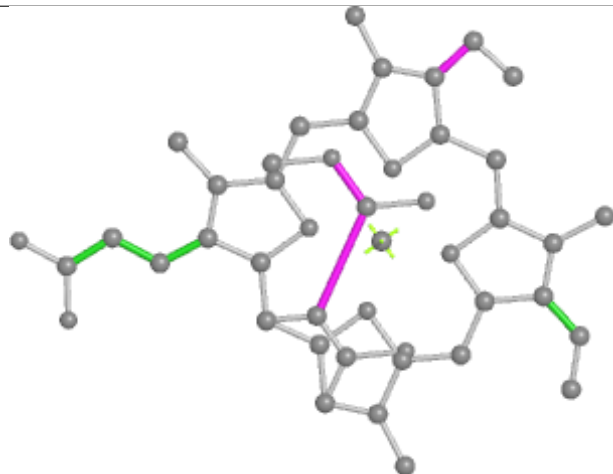
Ligand KC1 N 312



Bond lengths



Bond angles

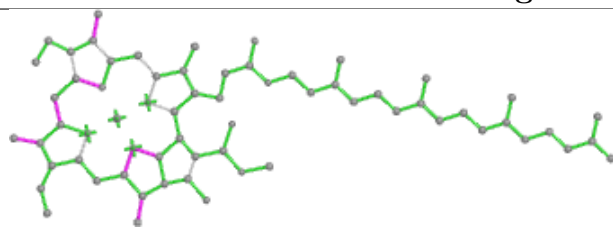


Torsions

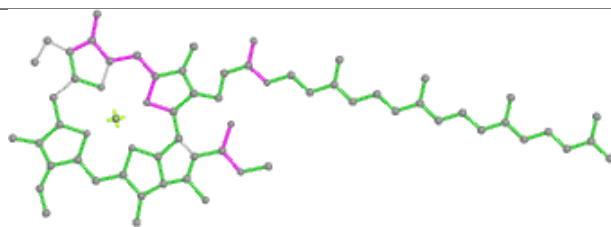


Rings

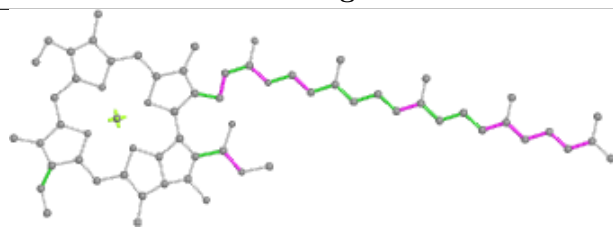
Ligand CLA E 306



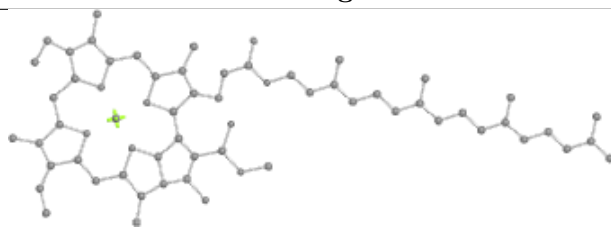
Bond lengths



Bond angles

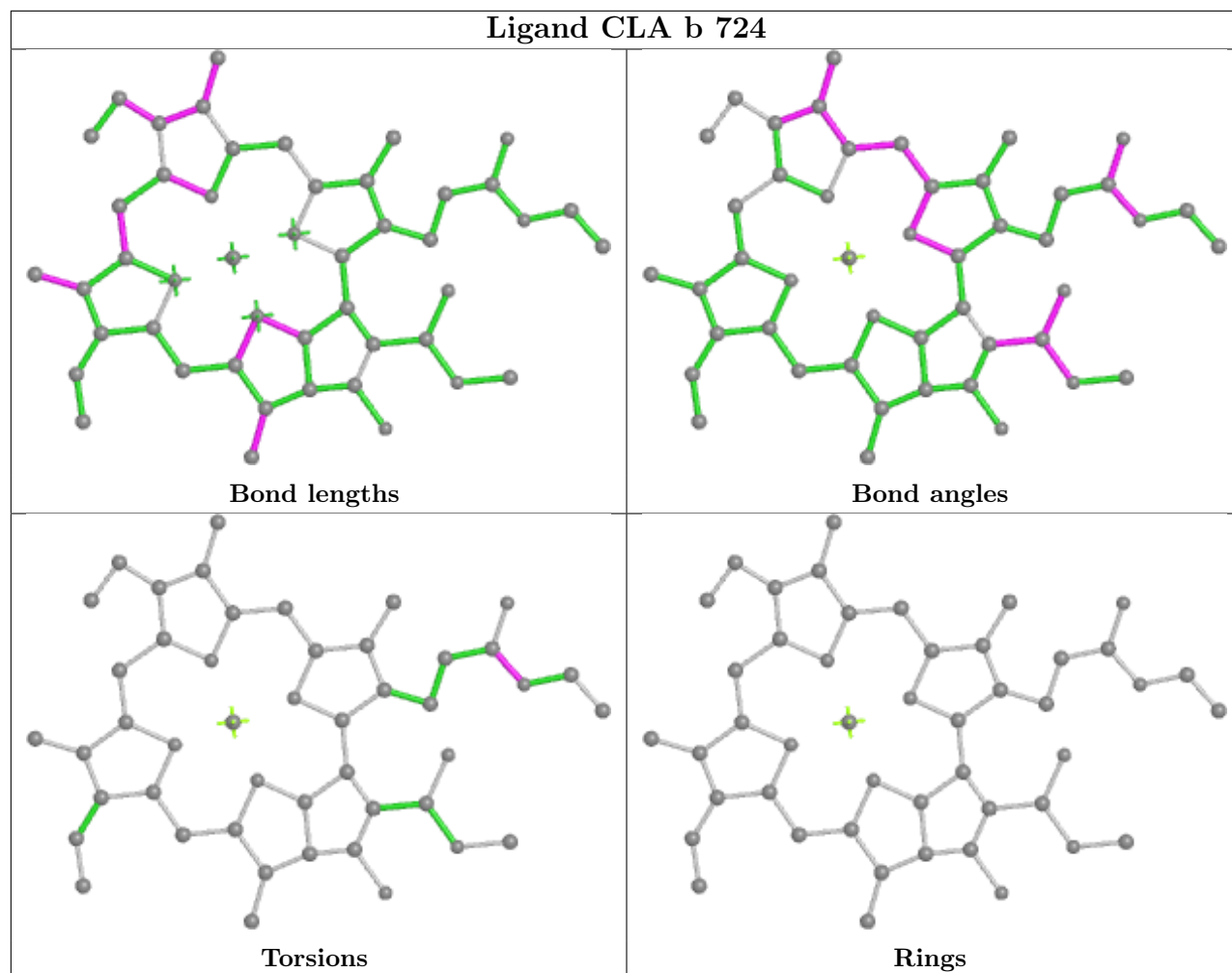


Torsions

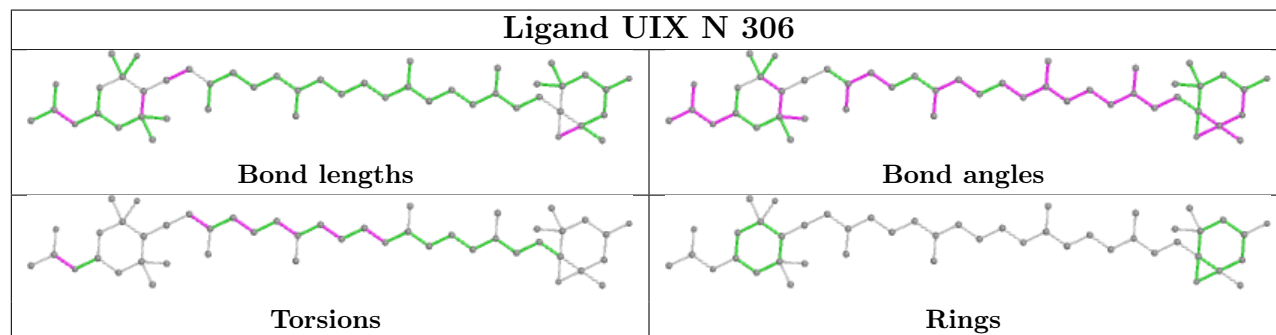


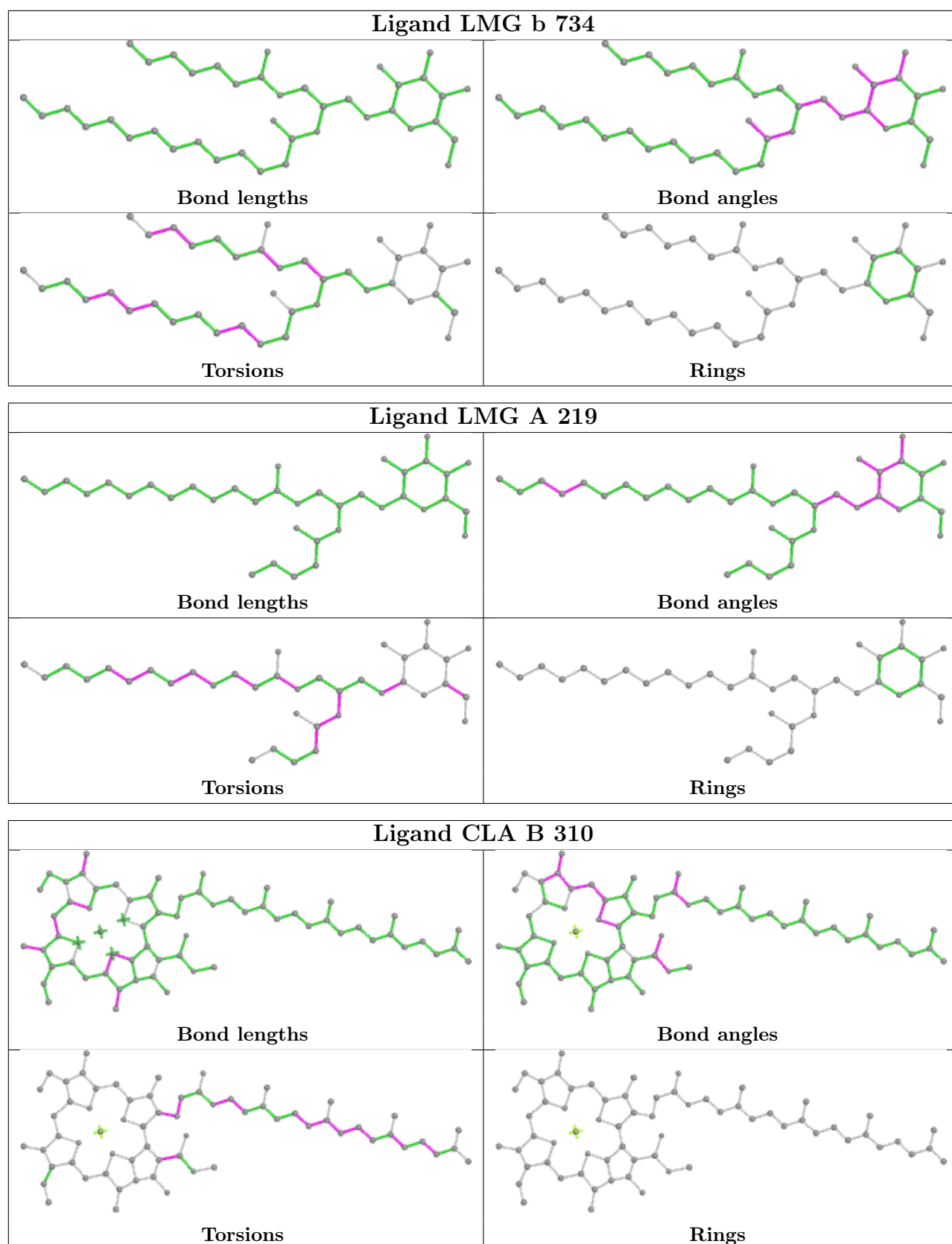
Rings

Ligand CLA b 724

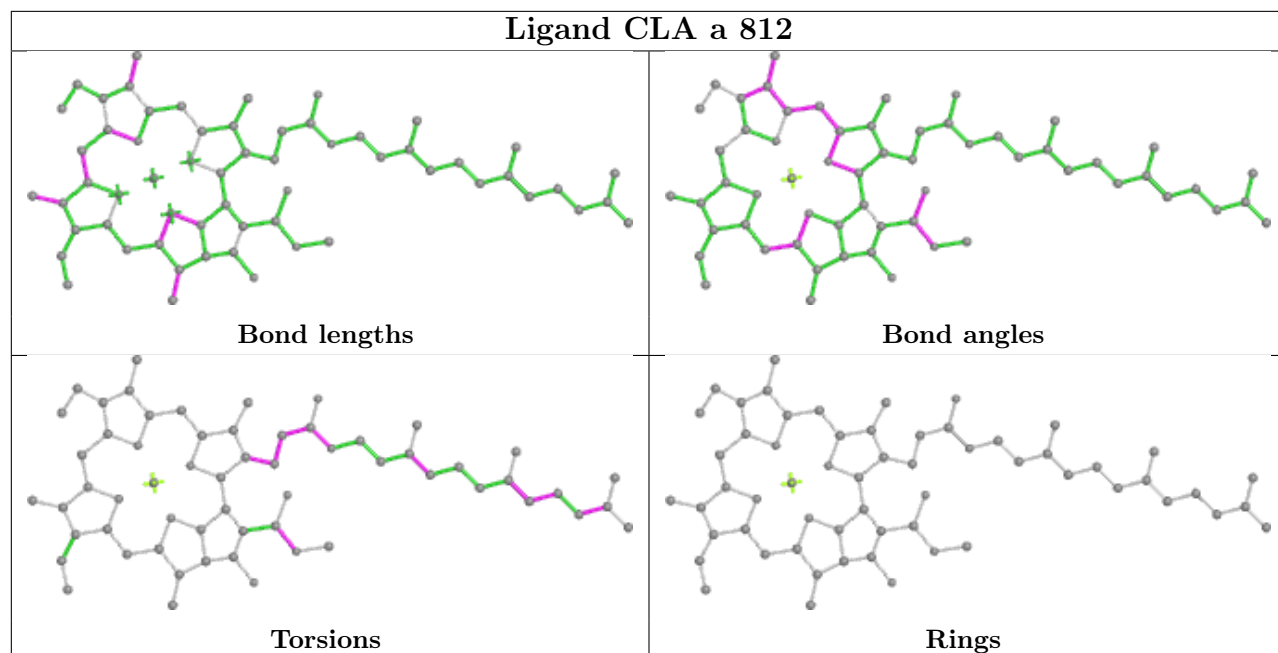


Ligand UIX N 306

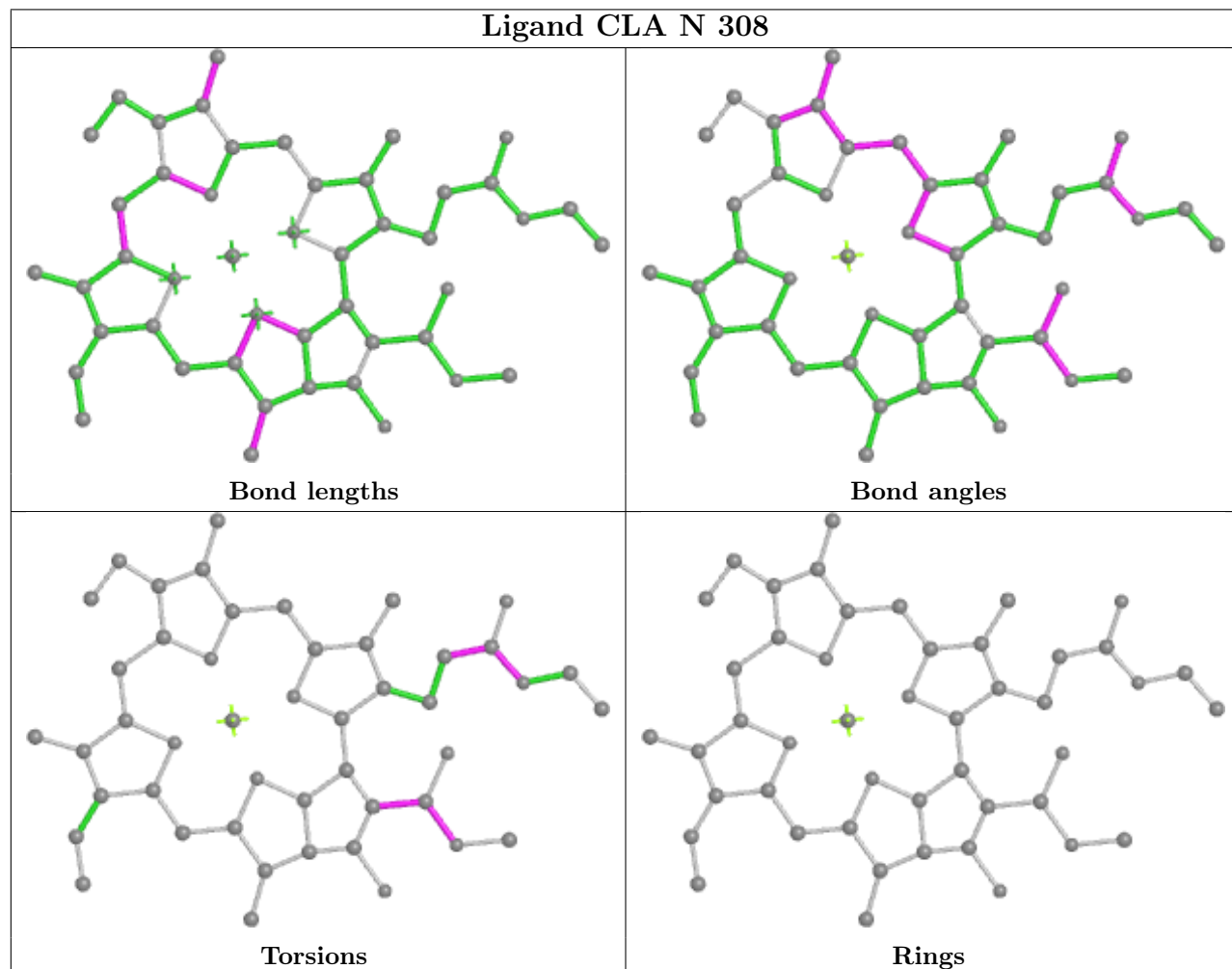




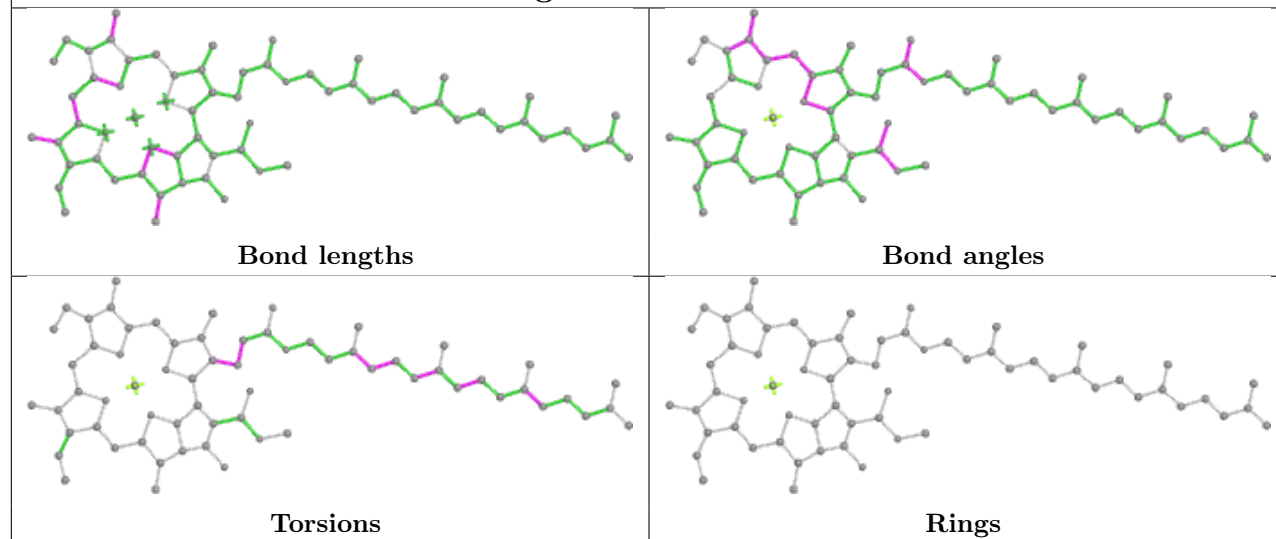
Ligand CLA a 812



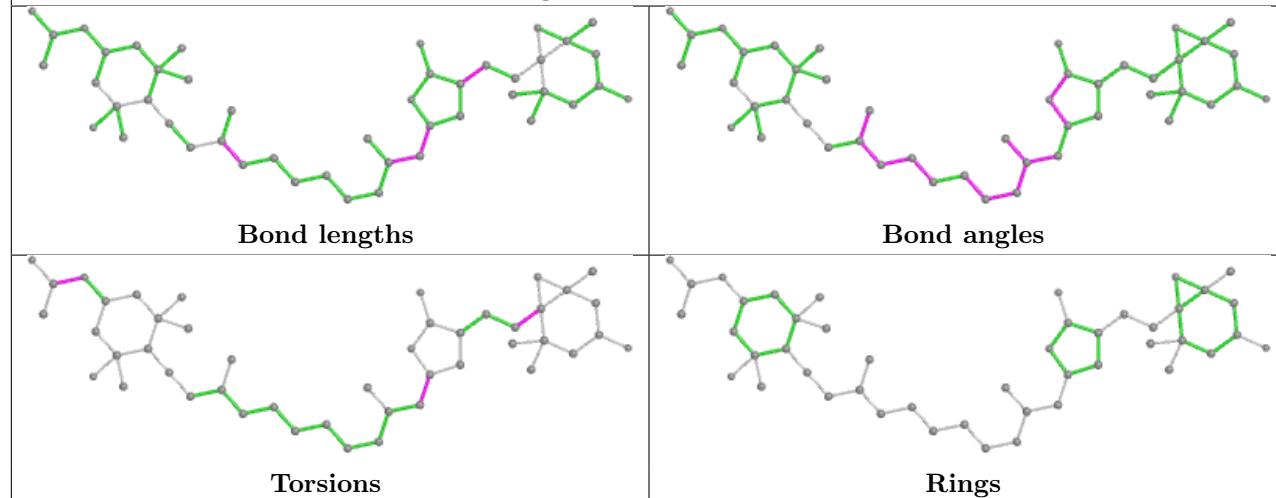
Ligand CLA N 308



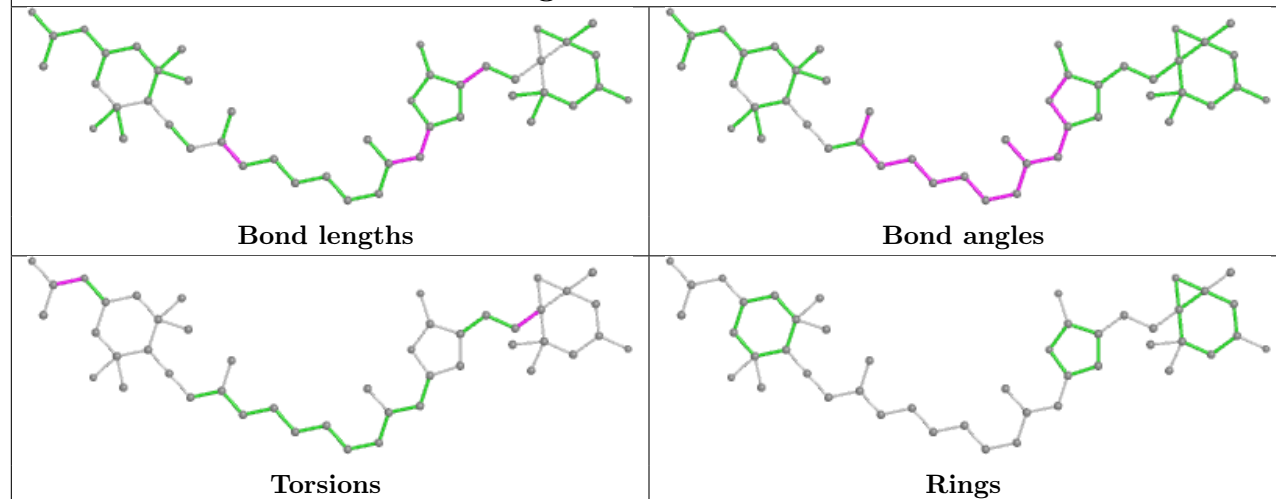
Ligand CLA b 706



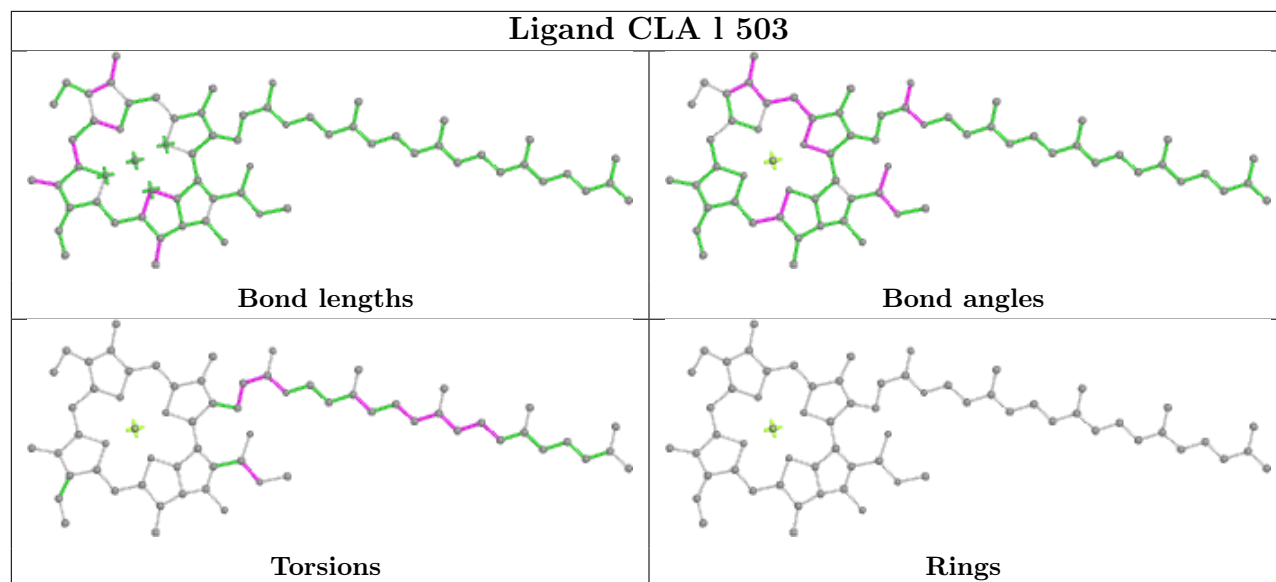
Ligand PID C 301



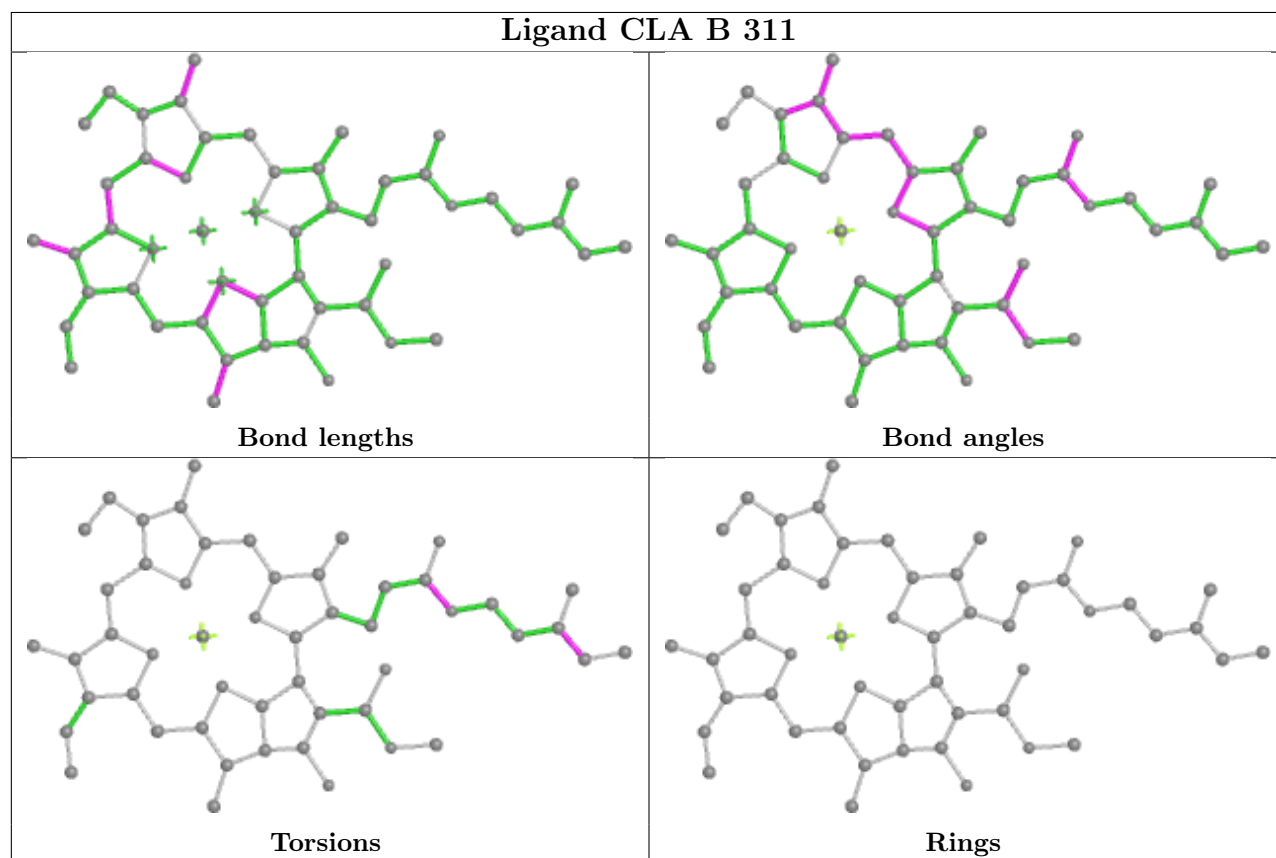
Ligand PID P 203

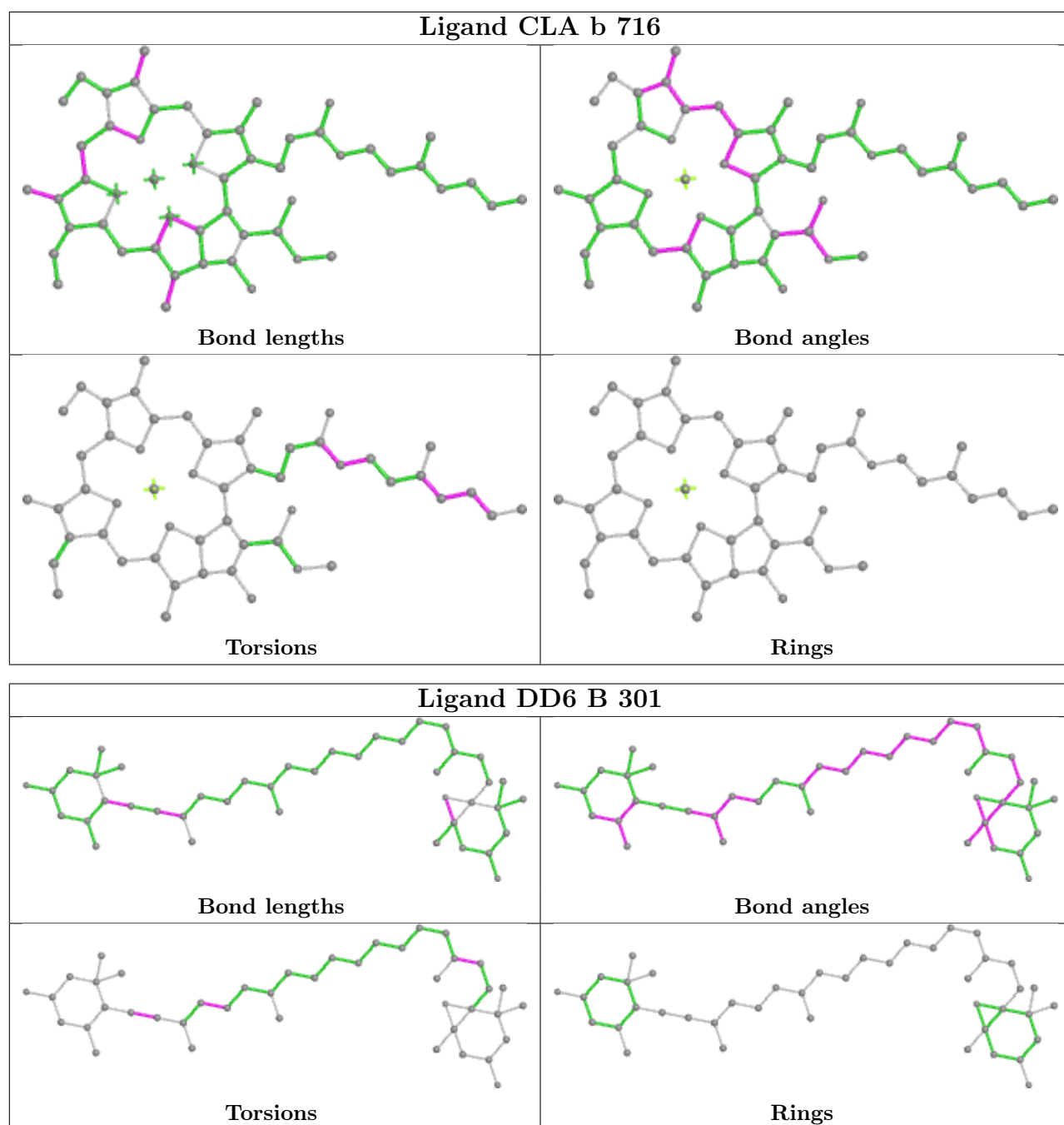


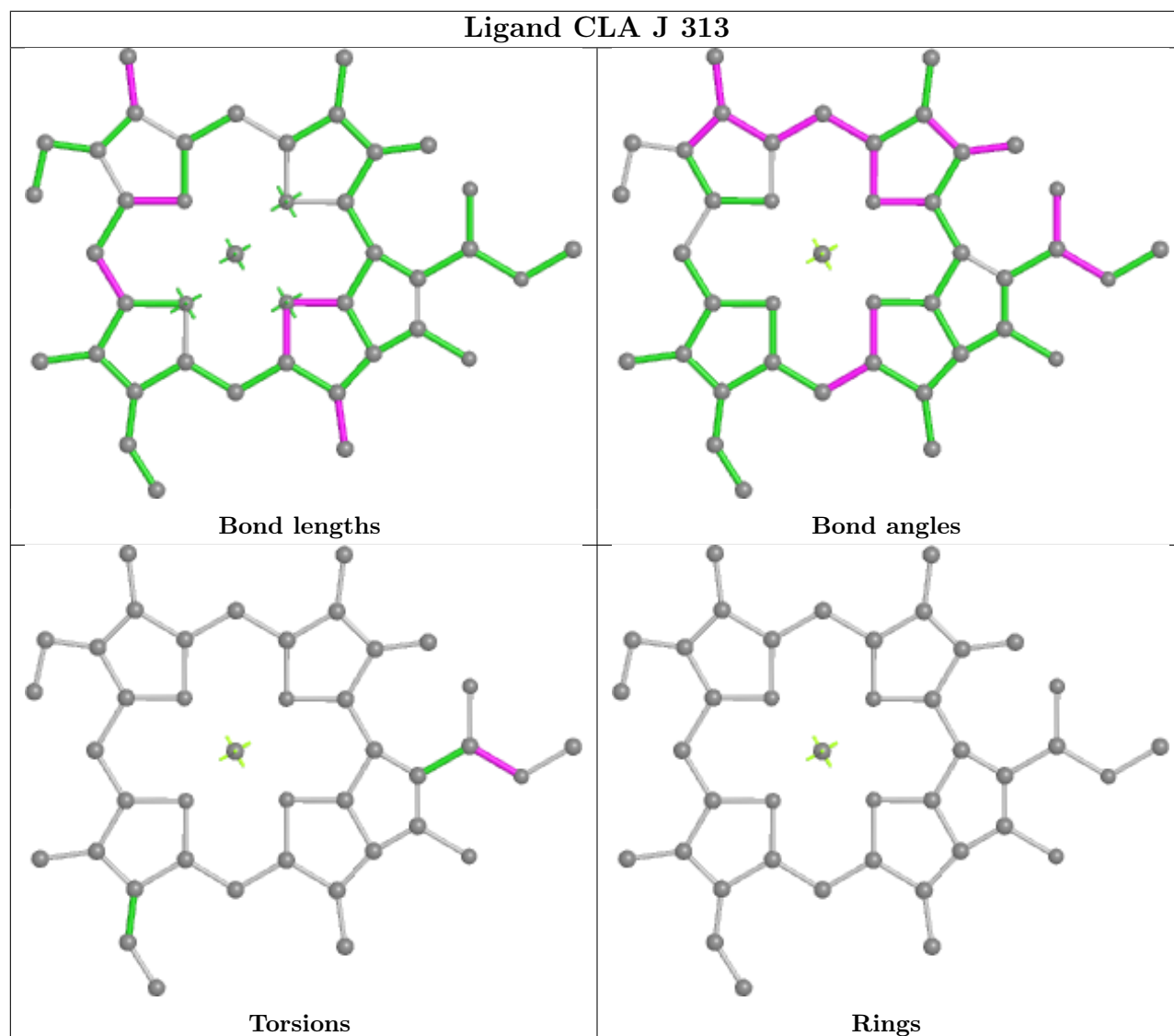
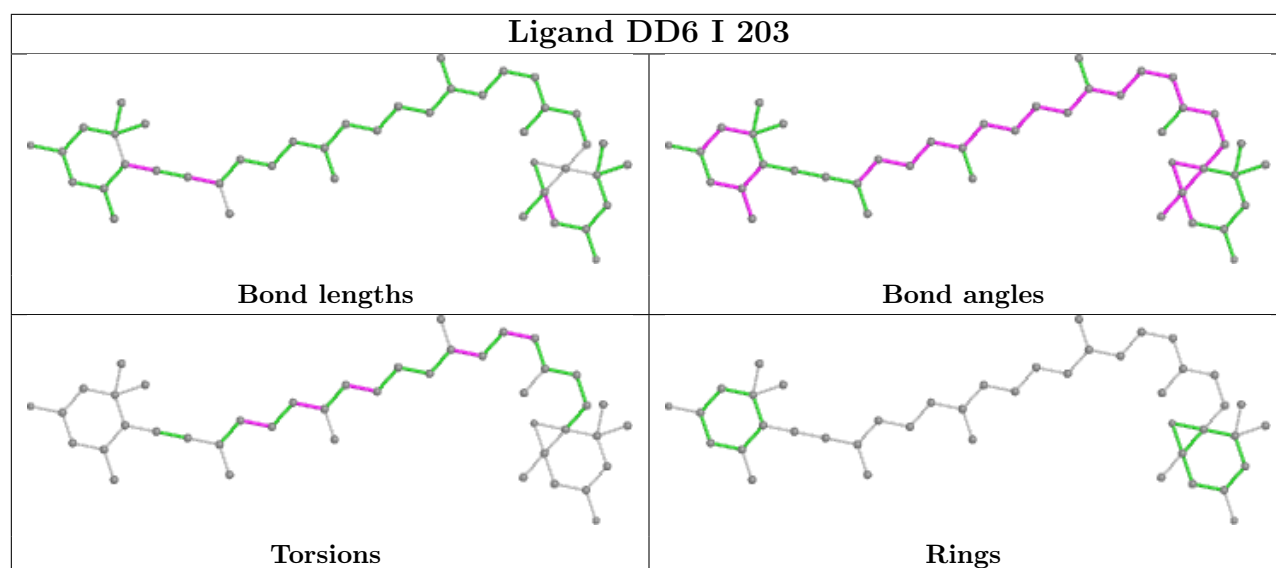
Ligand CLA I 503



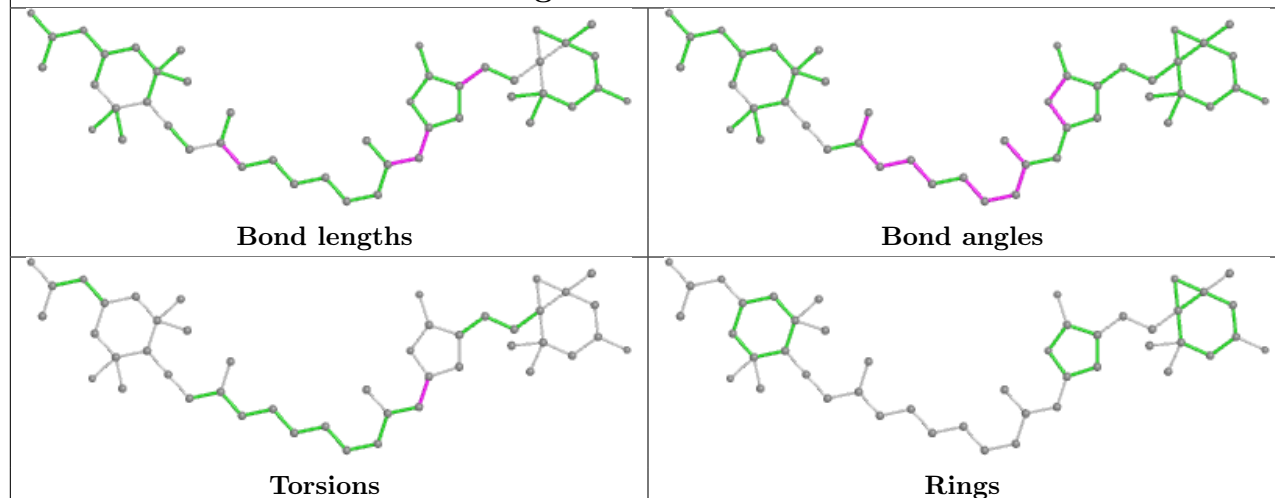
Ligand CLA B 311



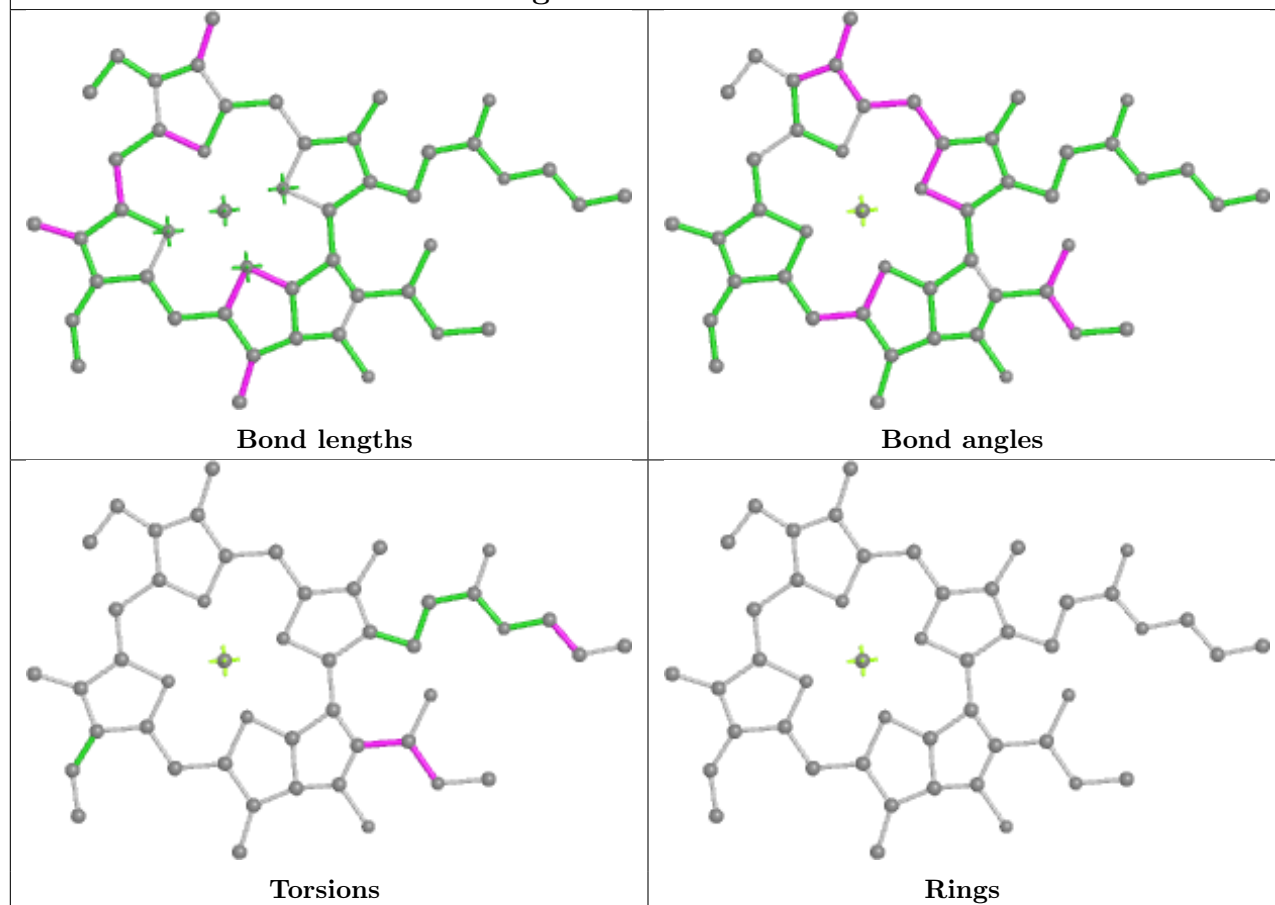


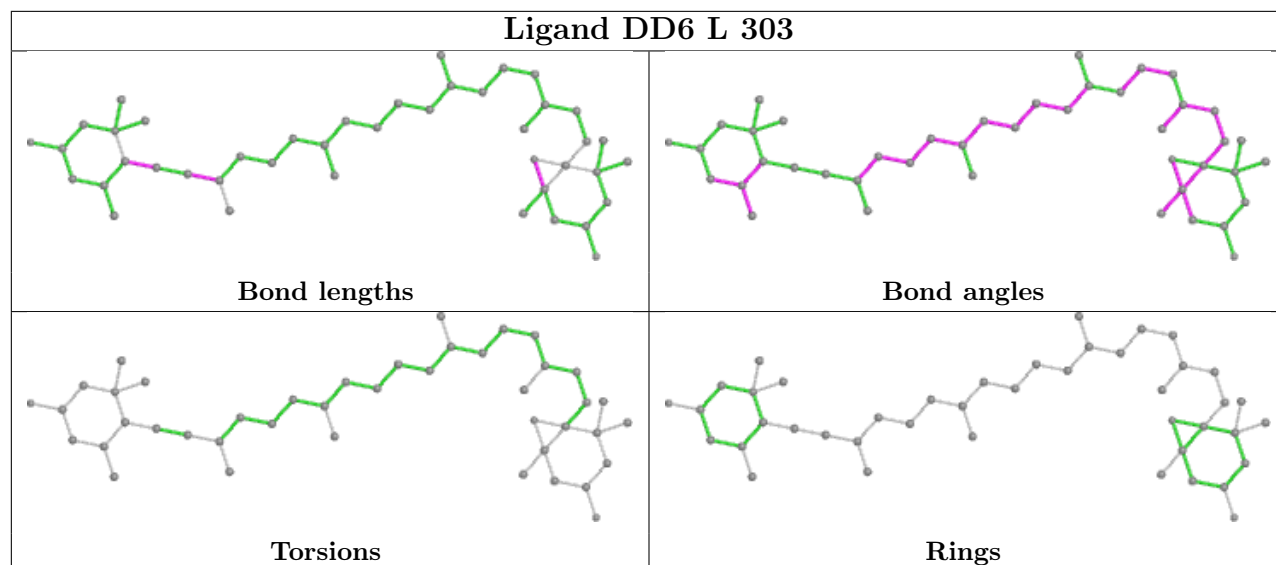
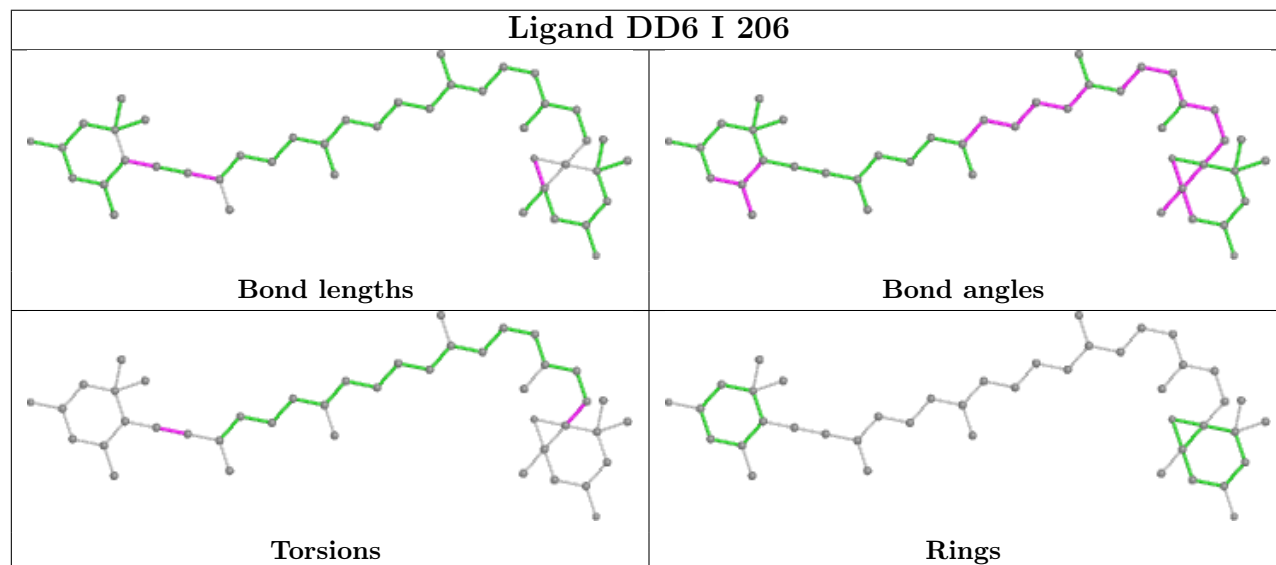


Ligand PID N 304

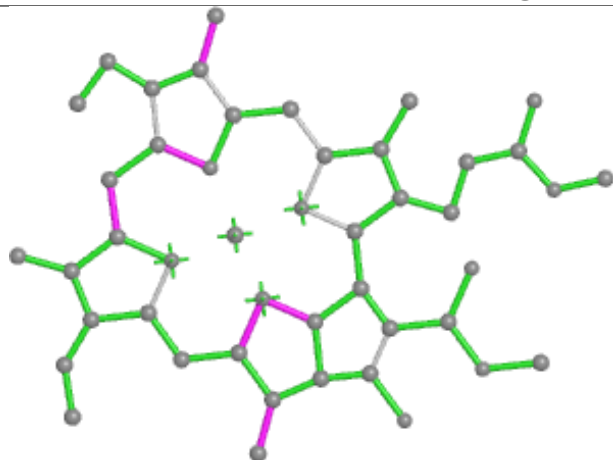


Ligand CLA E 314

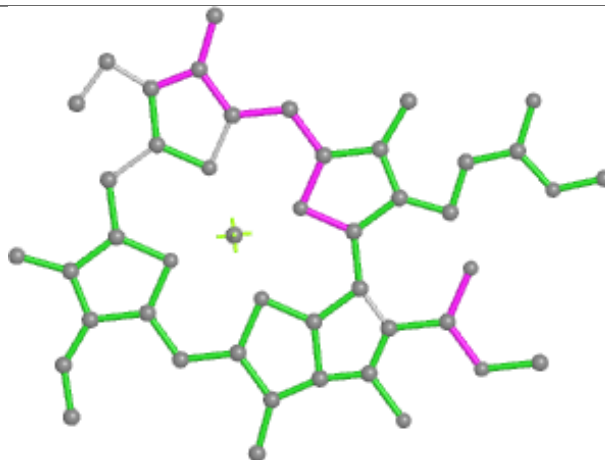


Ligand DD6 L 303**Ligand DD6 I 206**

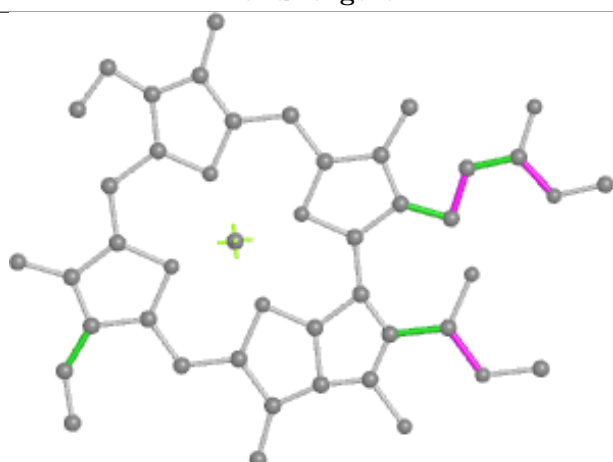
Ligand CLA L 317



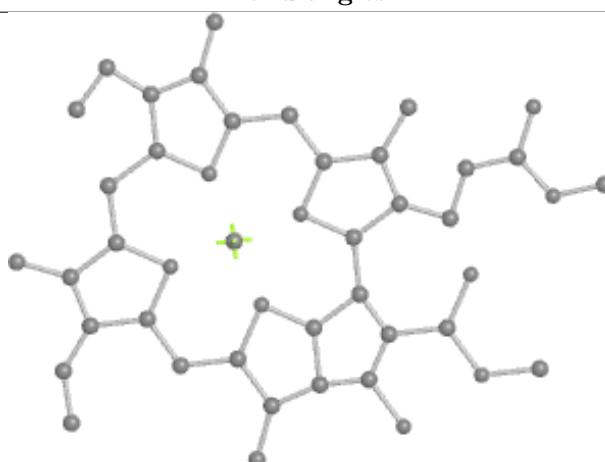
Bond lengths



Bond angles

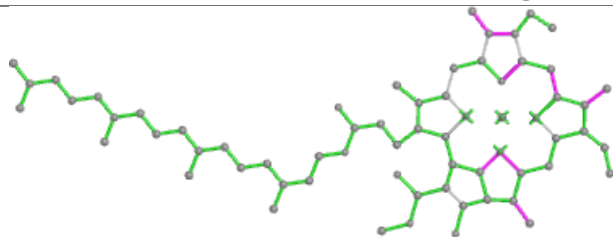


Torsions

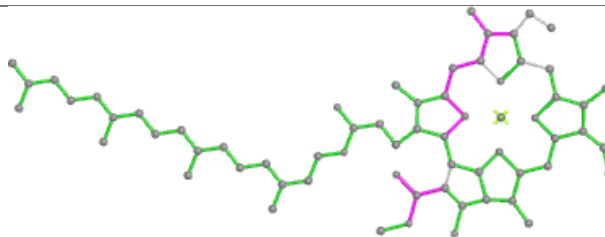


Rings

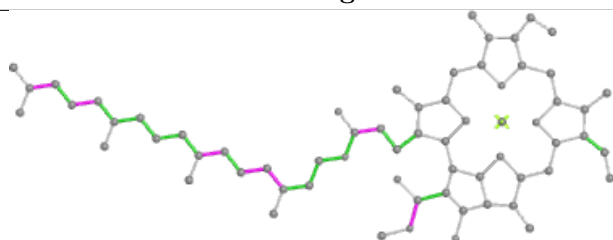
Ligand CLA b 704



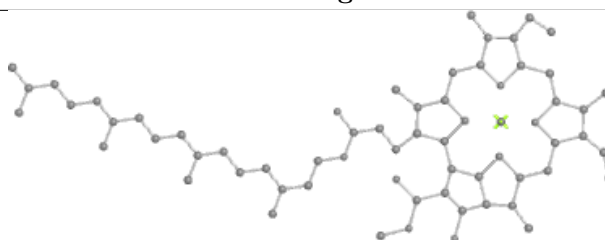
Bond lengths



Bond angles

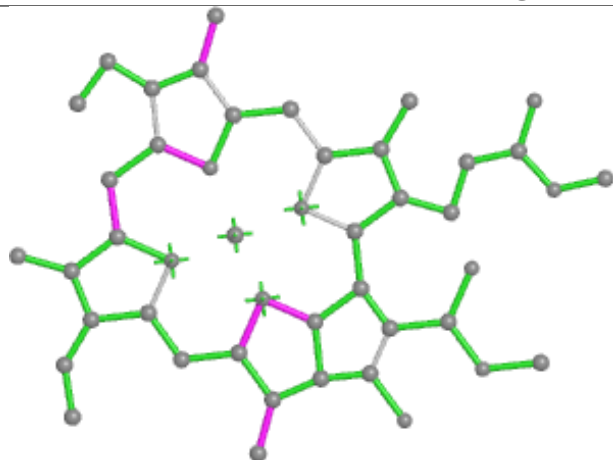


Torsions

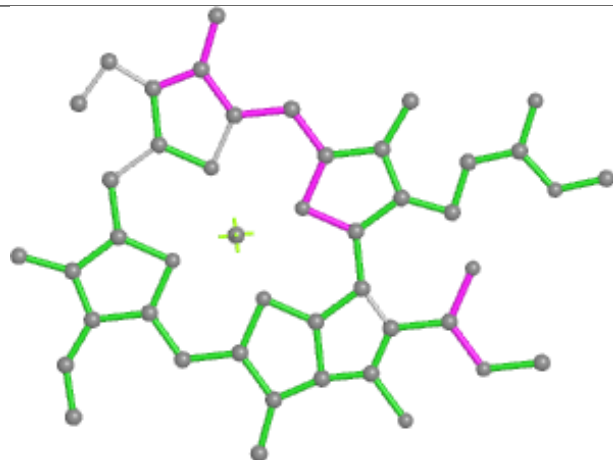


Rings

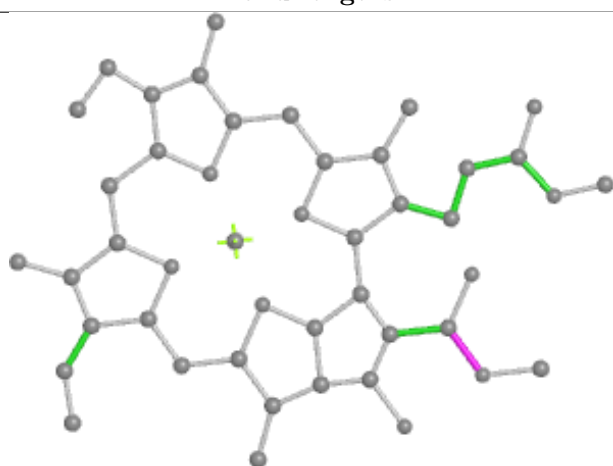
Ligand CLA D 309



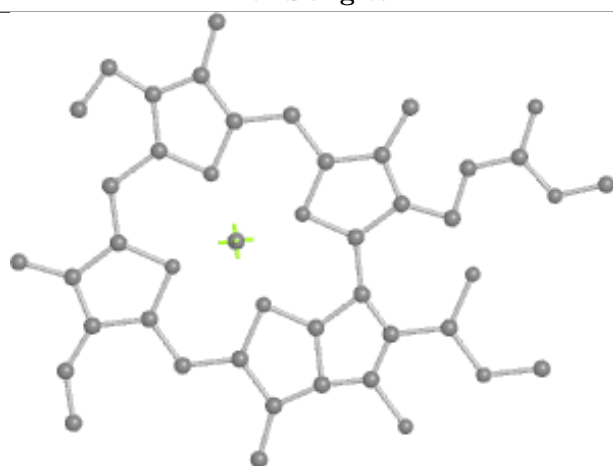
Bond lengths



Bond angles

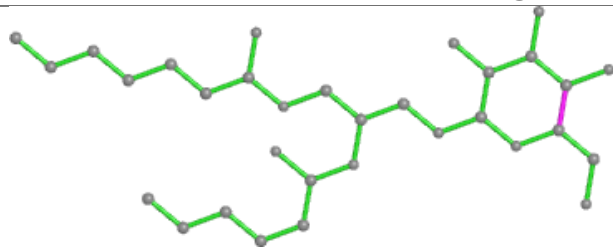


Torsions

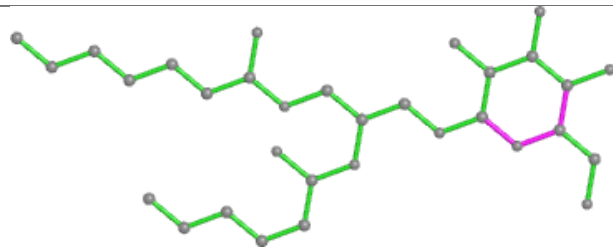


Rings

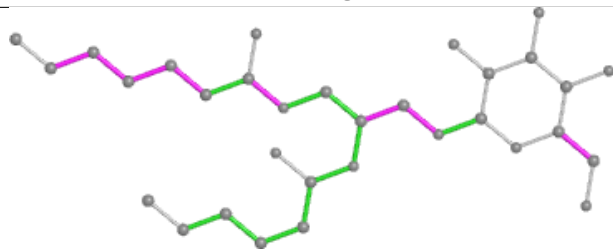
Ligand LMG E 316



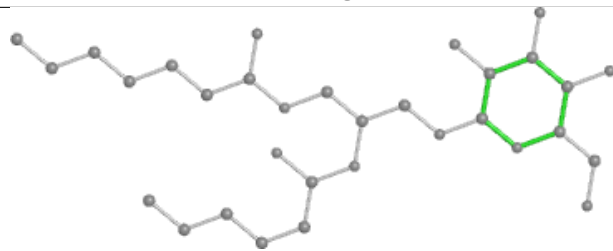
Bond lengths



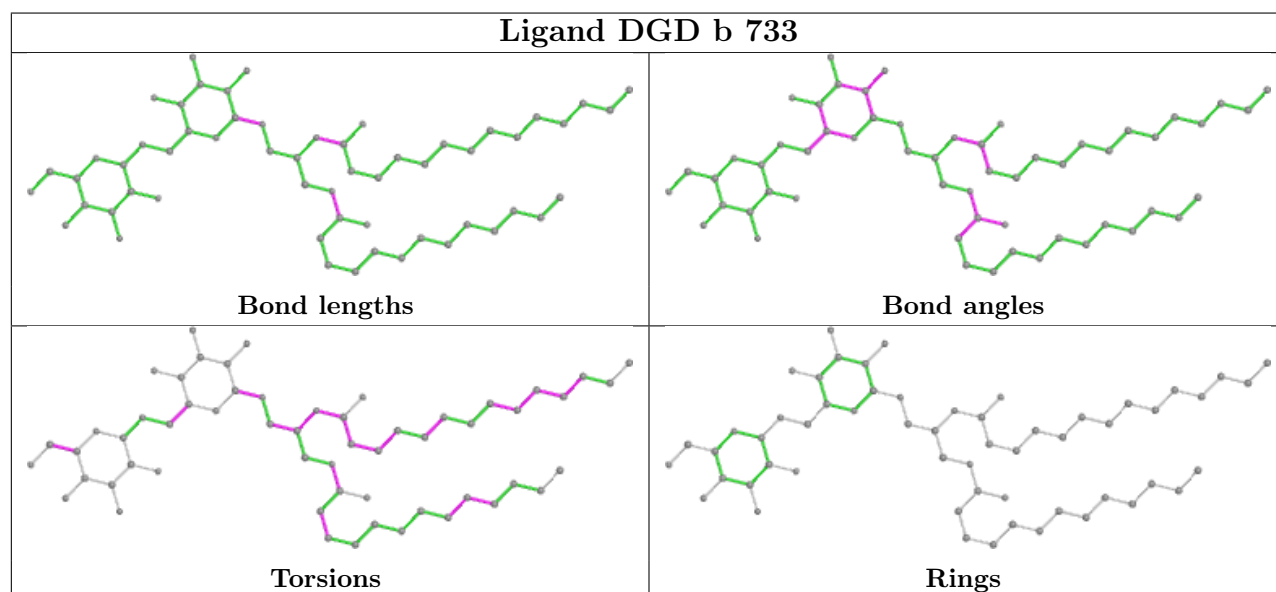
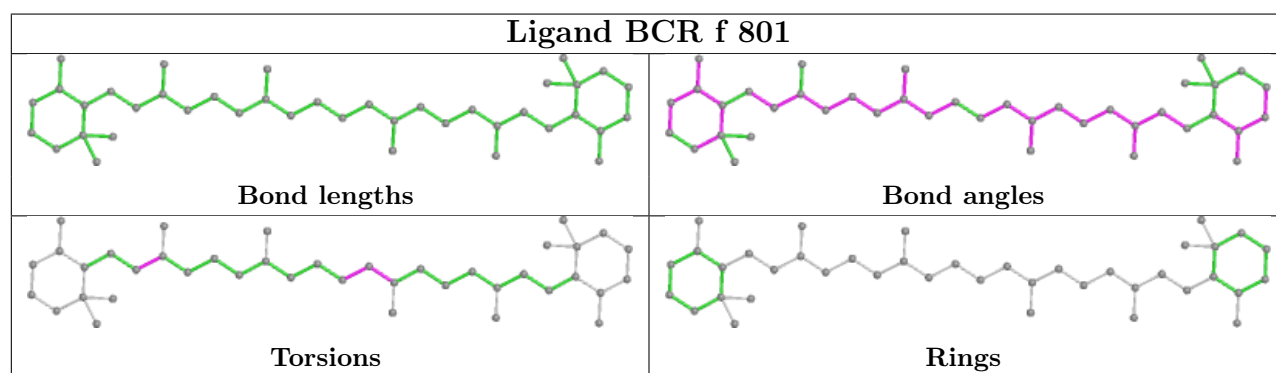
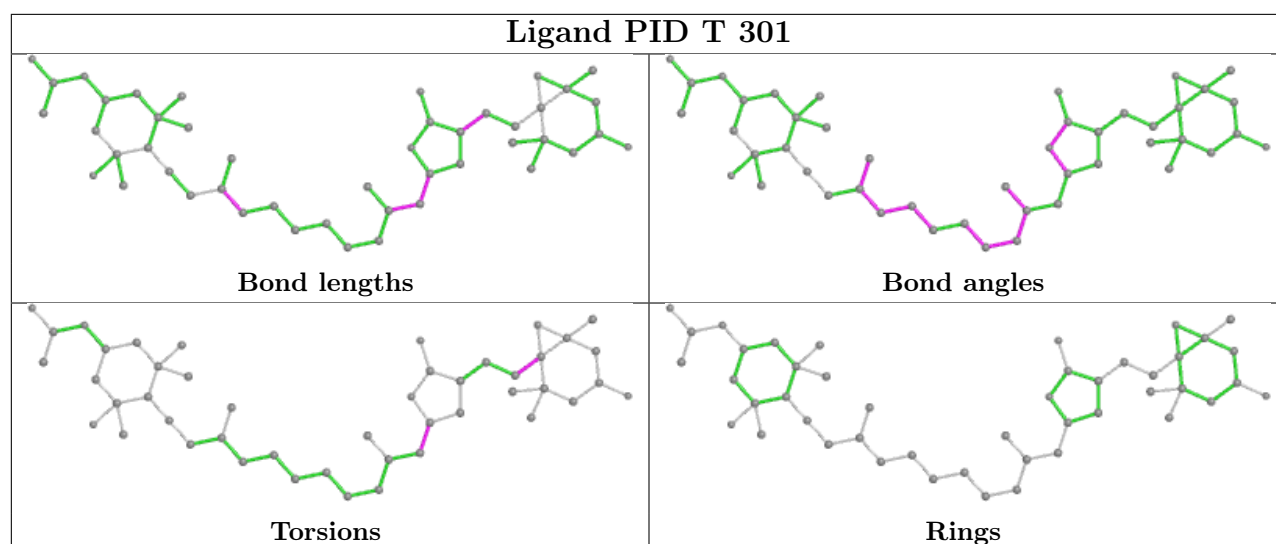
Bond angles



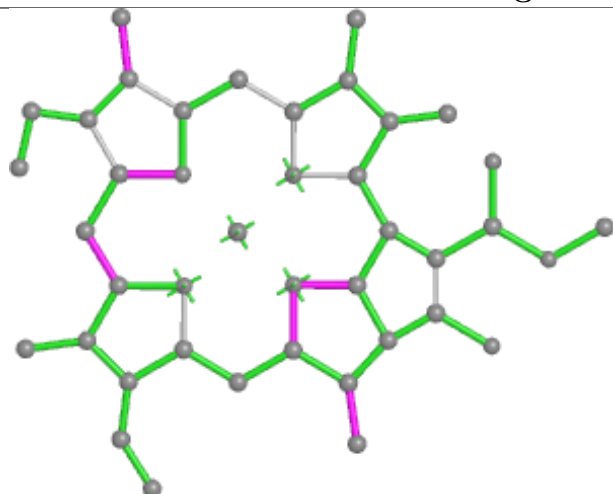
Torsions



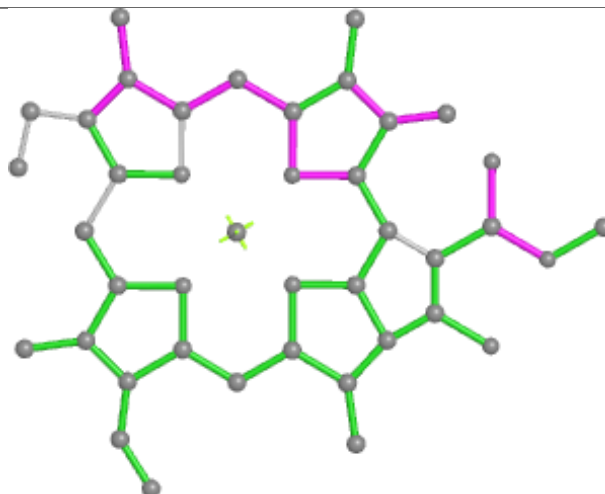
Rings



Ligand CLA T 316



Bond lengths



Bond angles

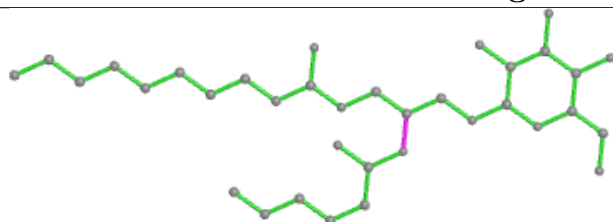


Torsions

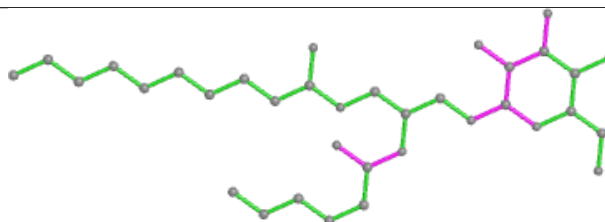


Rings

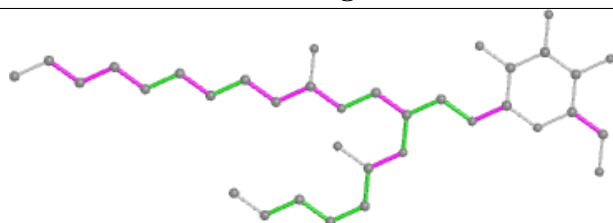
Ligand LMG K 219



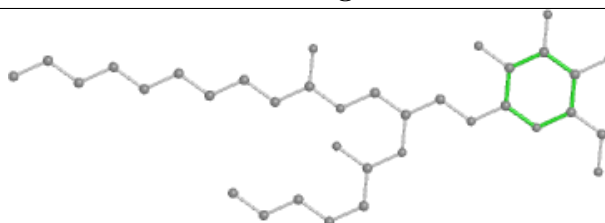
Bond lengths



Bond angles

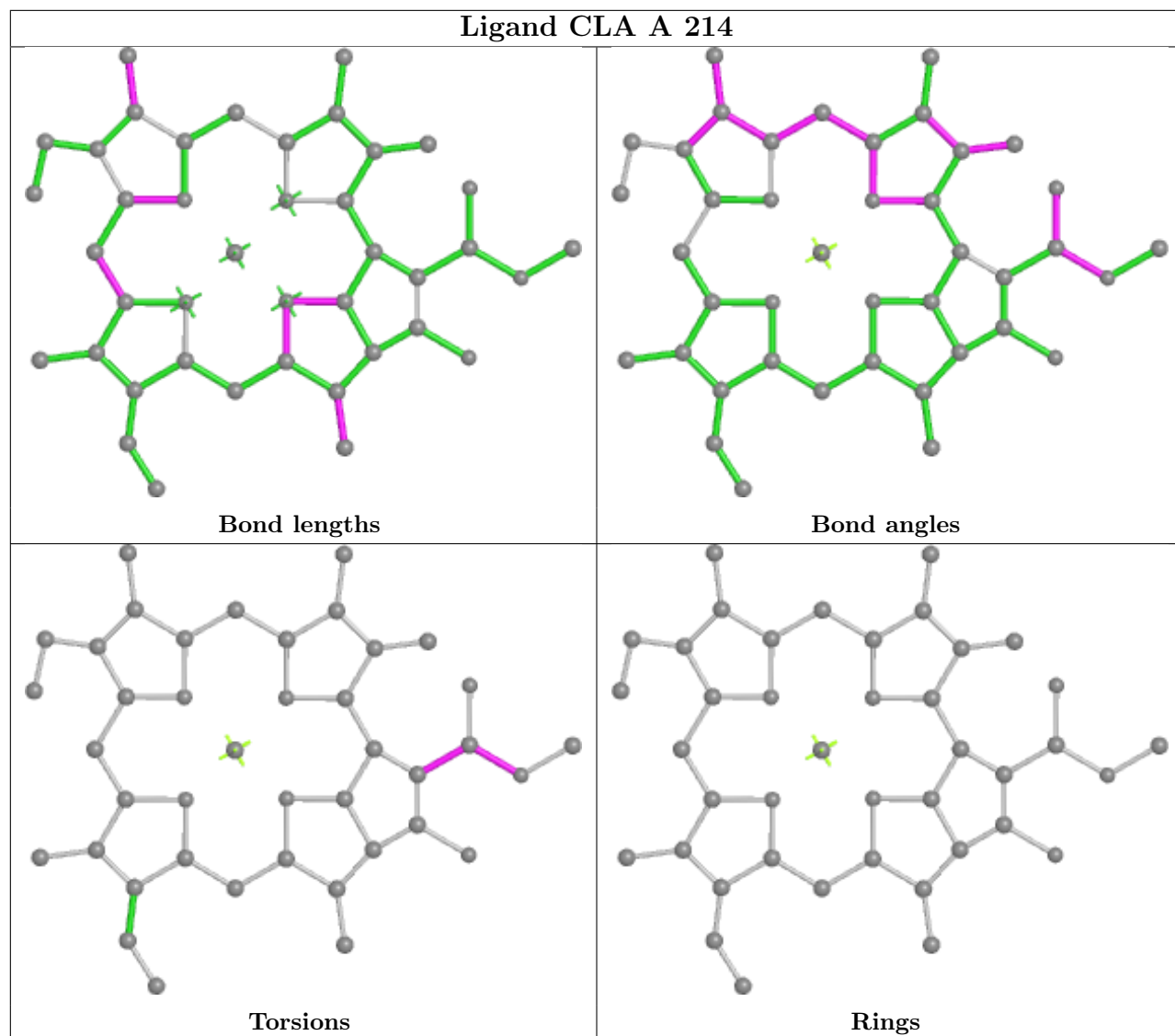


Torsions

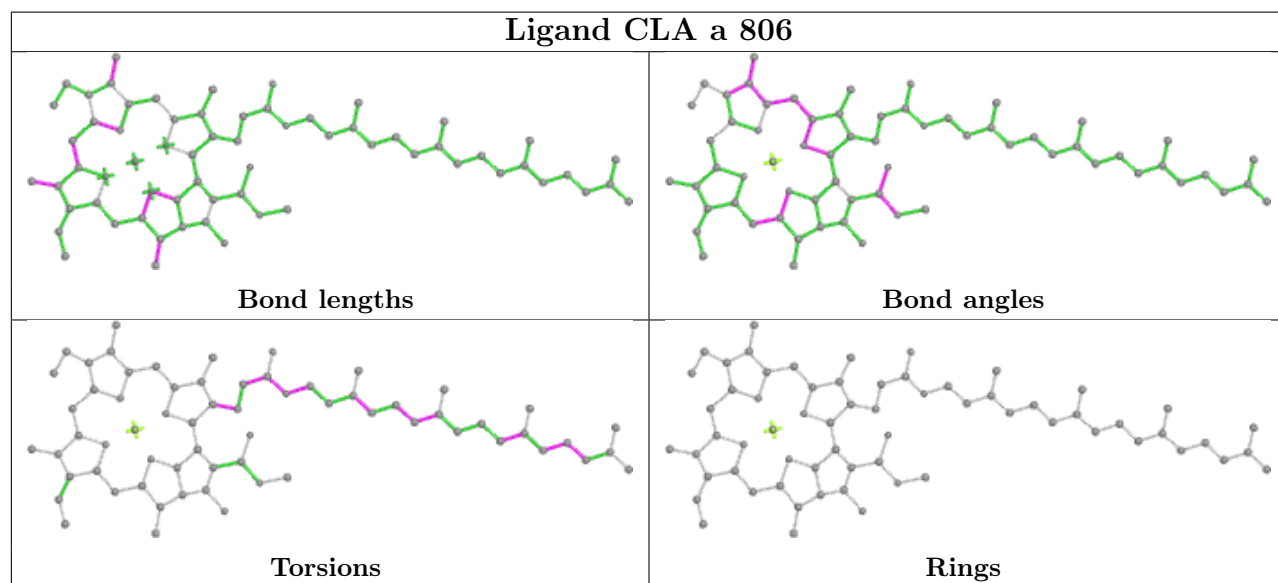


Rings

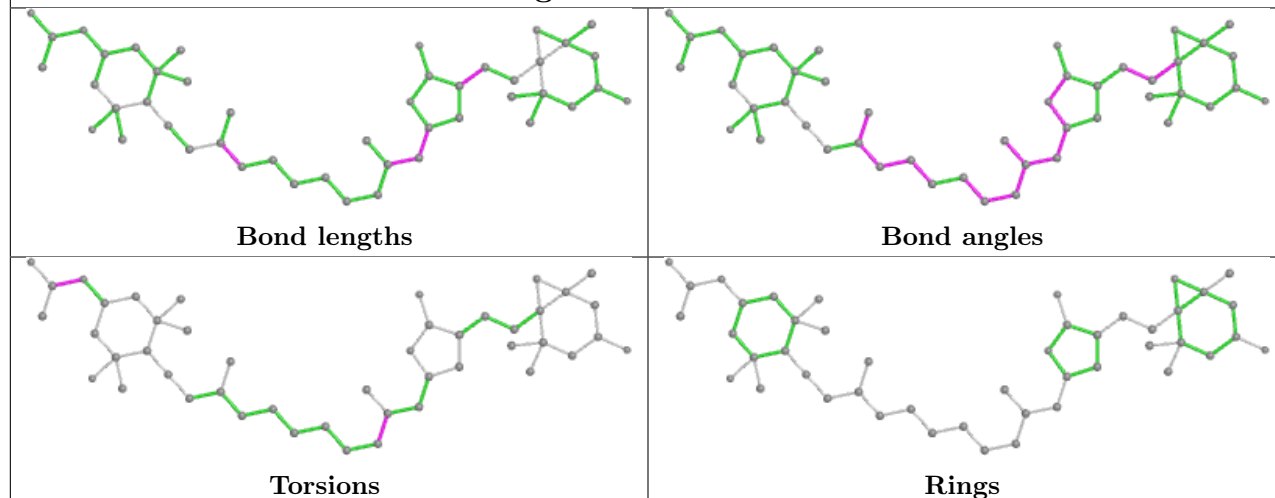
Ligand CLA A 214



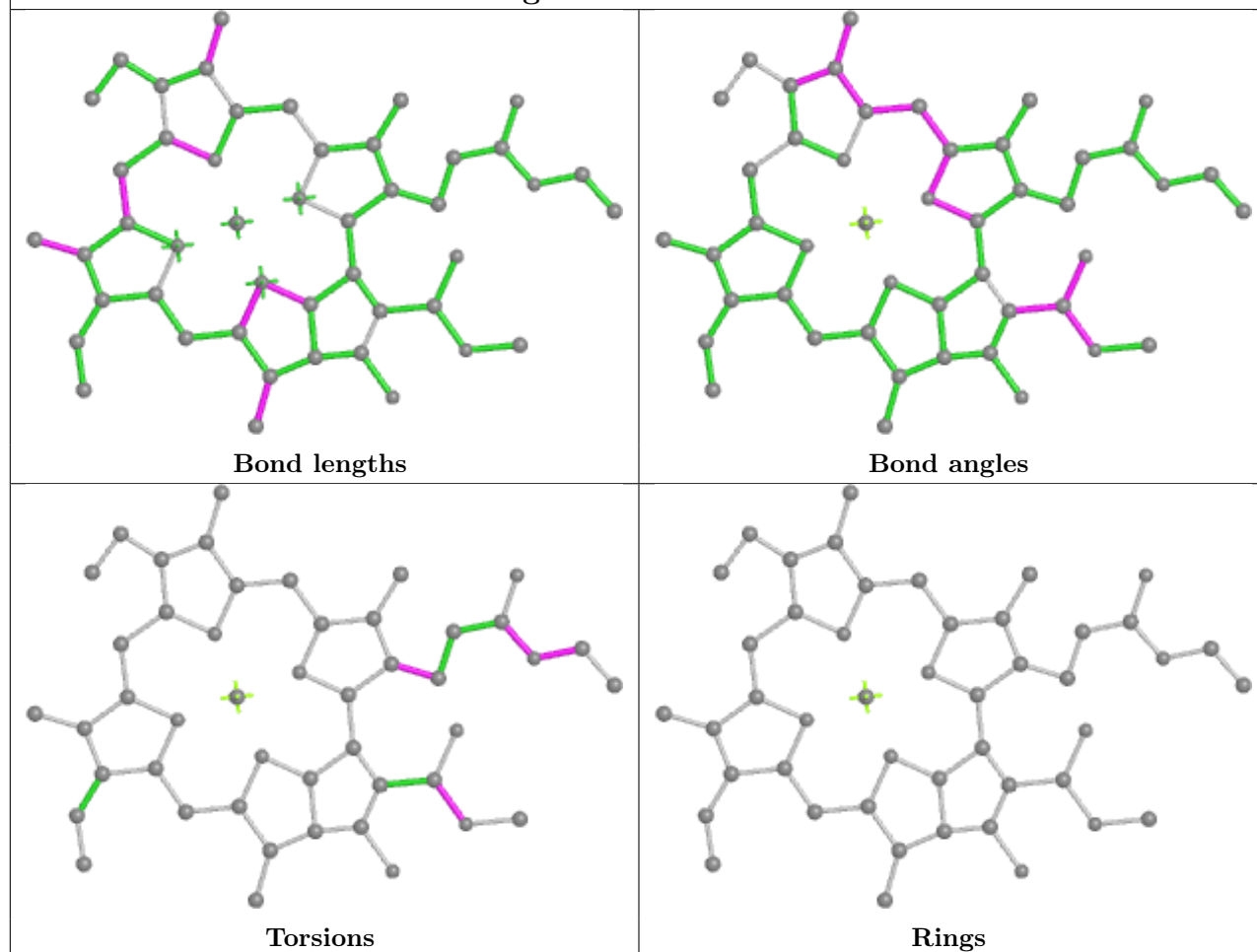
Ligand CLA a 806

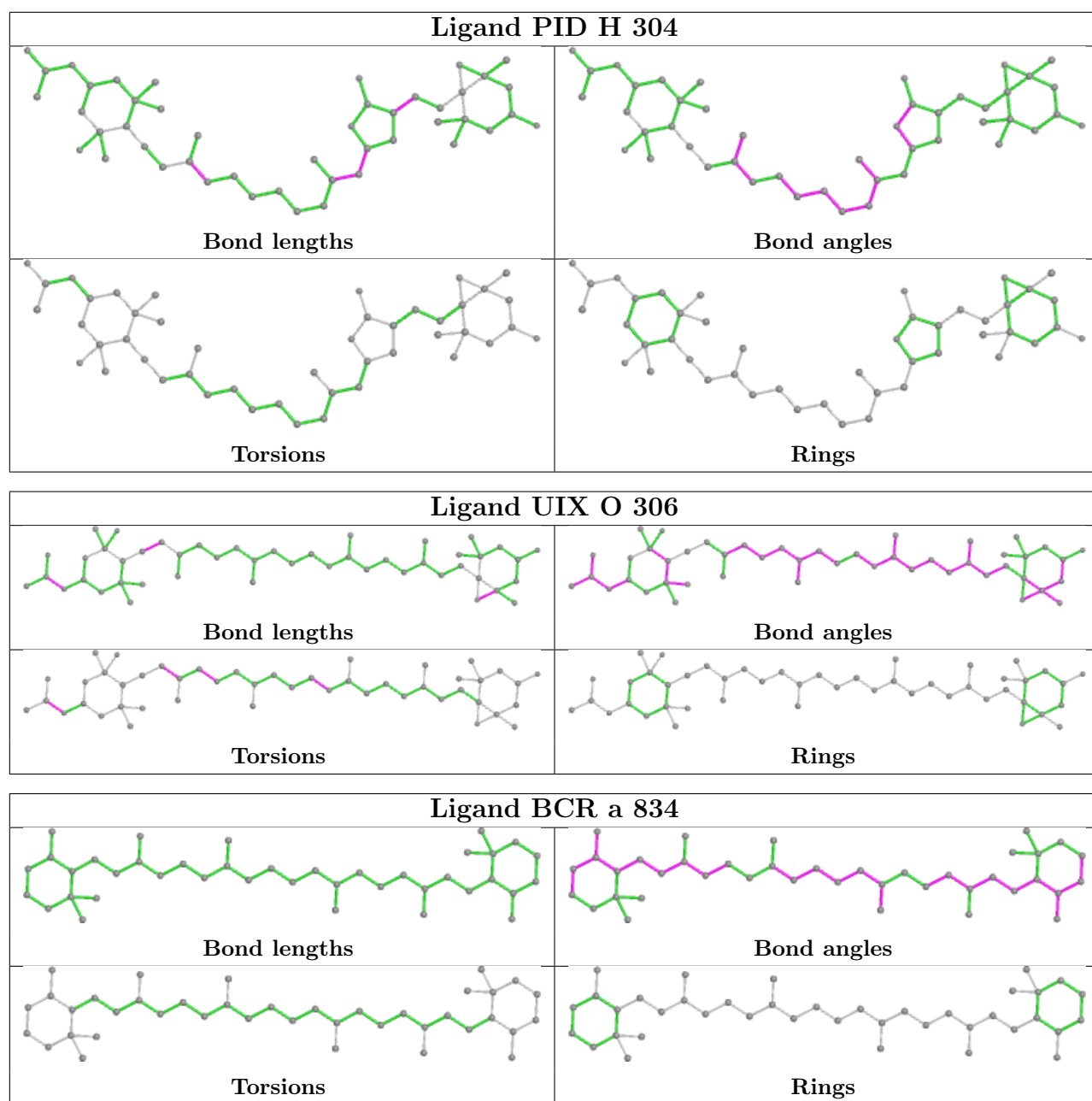


Ligand PID D 306

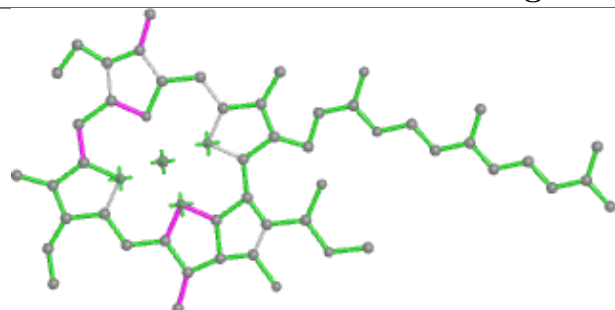


Ligand CLA N 314

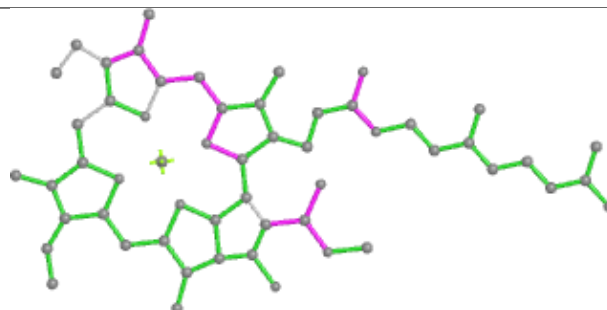




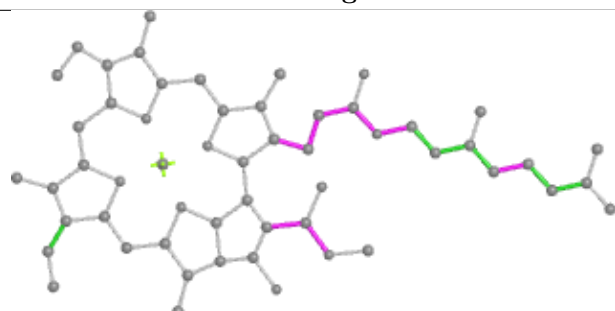
Ligand CLA i 203



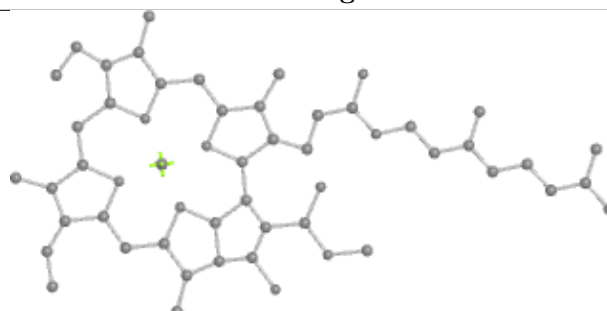
Bond lengths



Bond angles

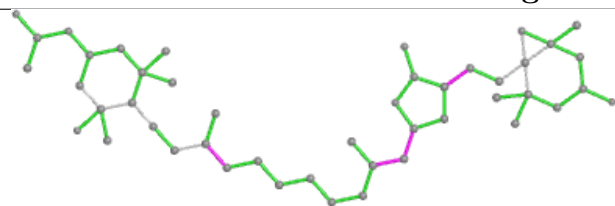


Torsions

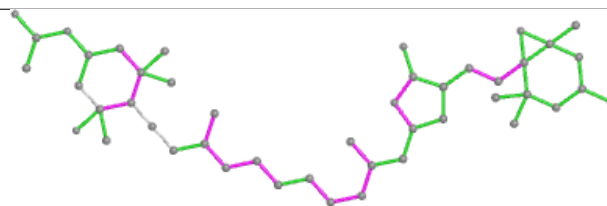


Rings

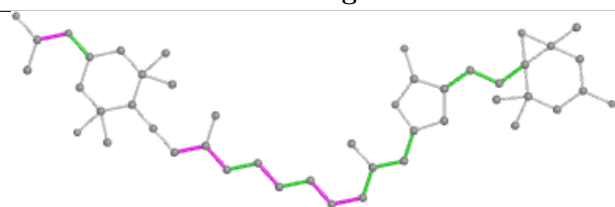
Ligand PID P 206



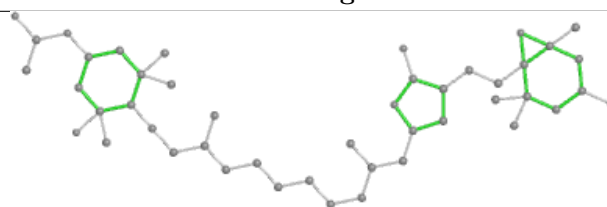
Bond lengths



Bond angles

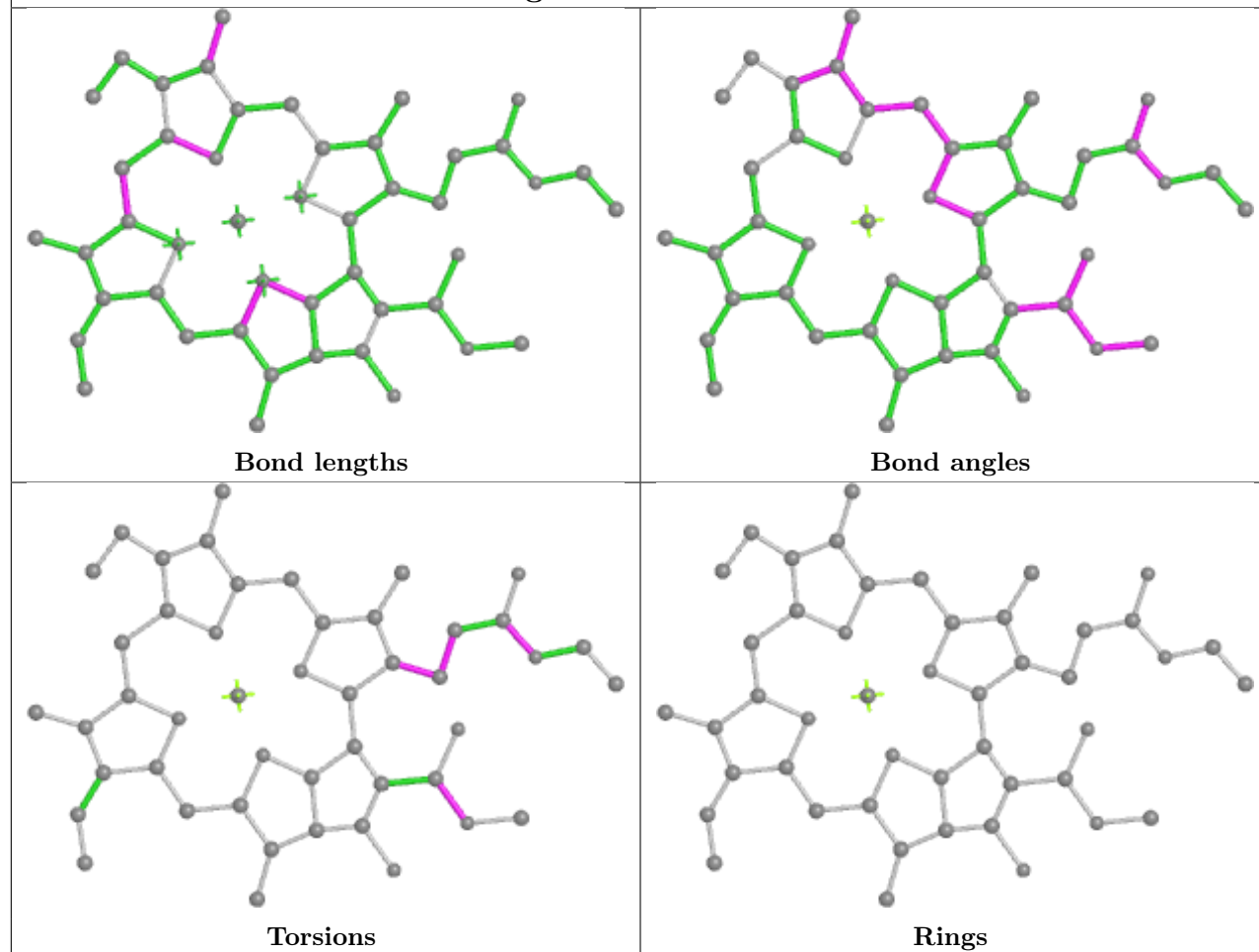


Torsions

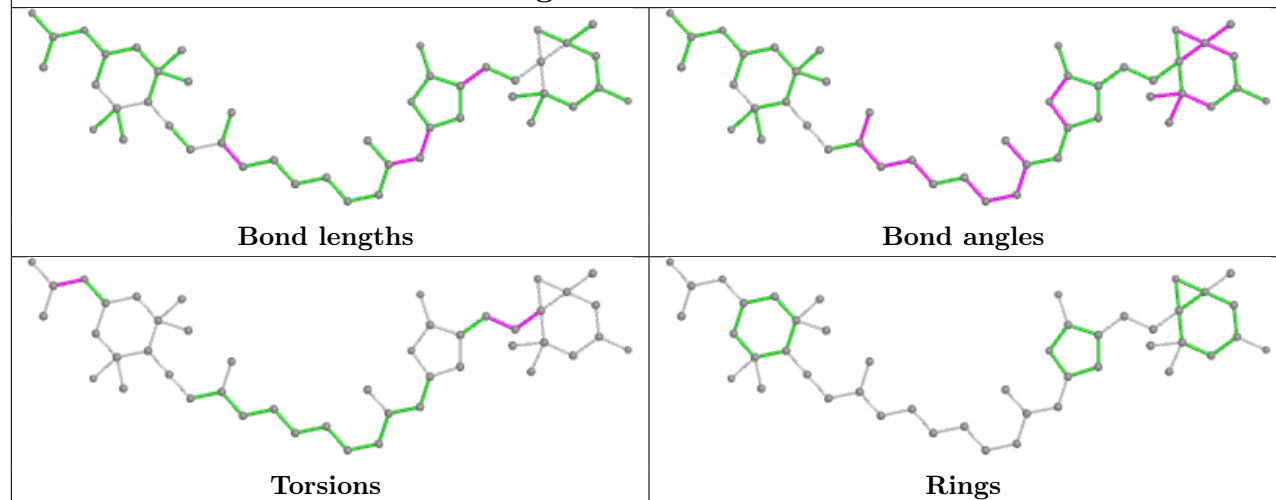


Rings

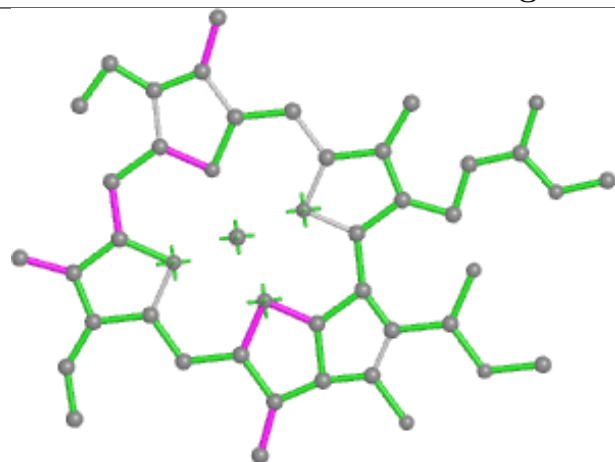
Ligand CLA T 314



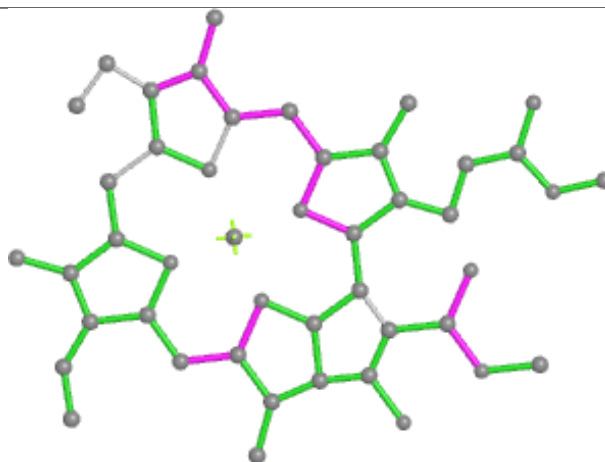
Ligand PID N 307



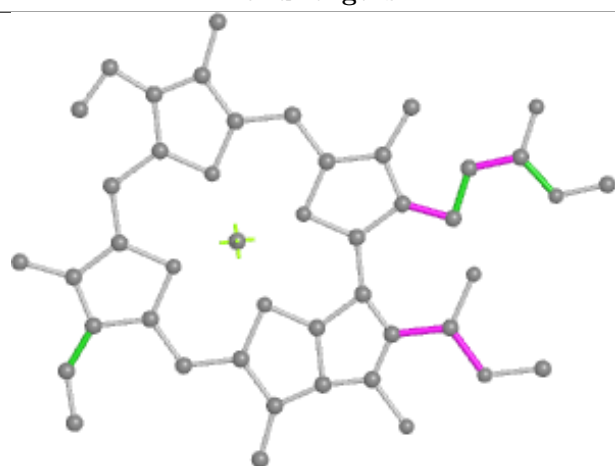
Ligand CLA b 710



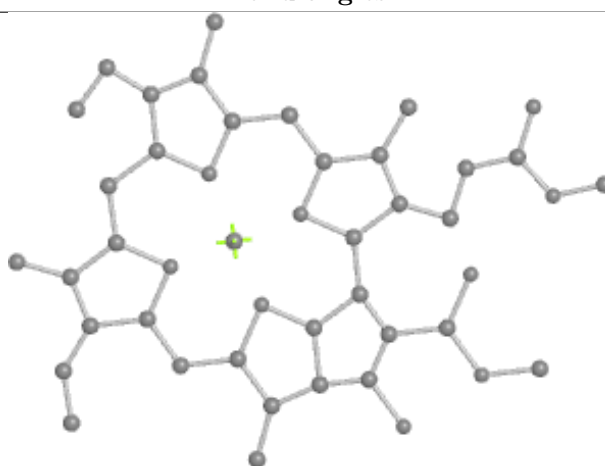
Bond lengths



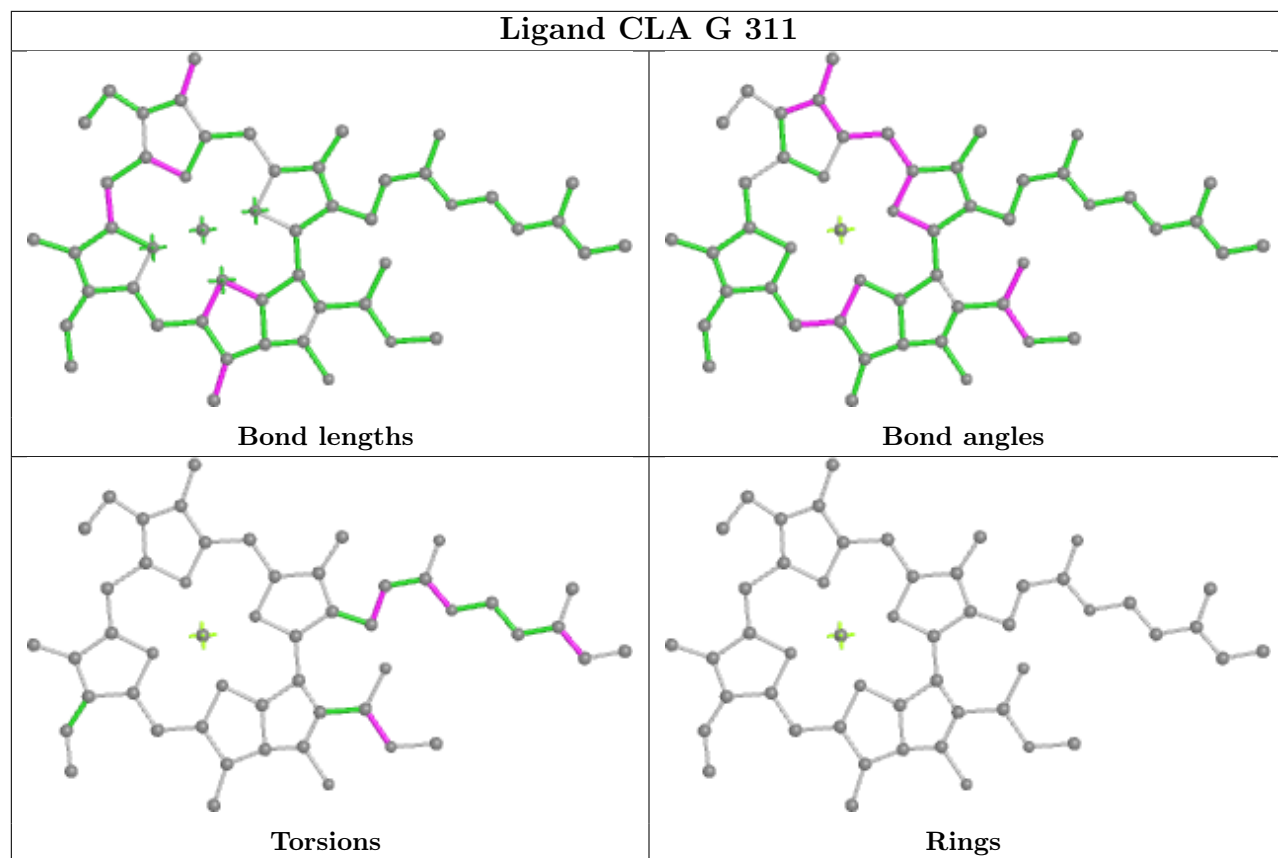
Bond angles



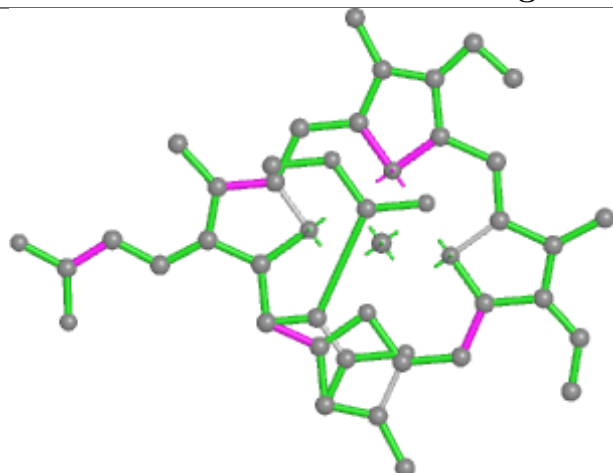
Torsions



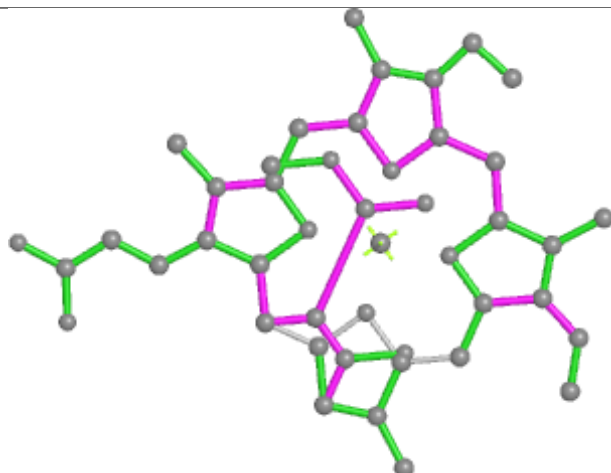
Rings



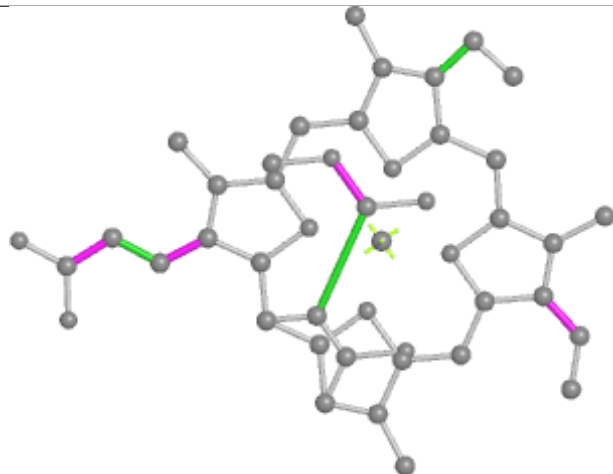
Ligand KC1 L 314



Bond lengths



Bond angles

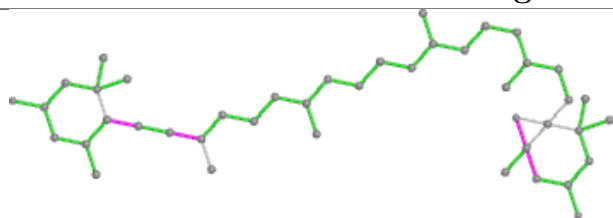


Torsions

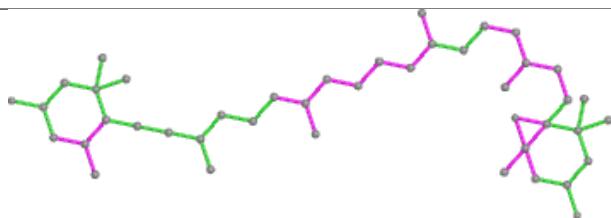


Rings

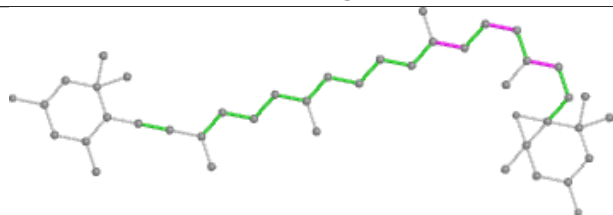
Ligand DD6 K 221



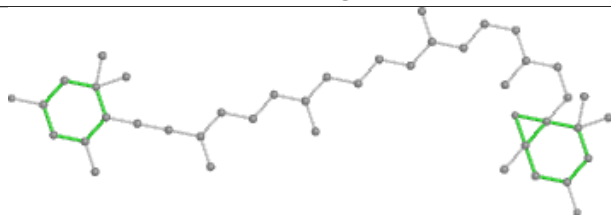
Bond lengths



Bond angles

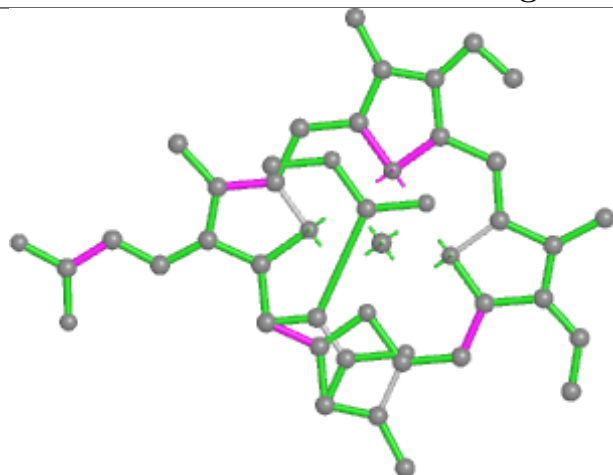


Torsions

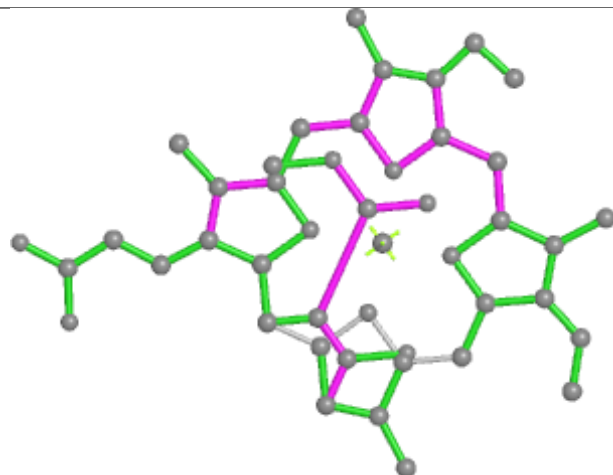


Rings

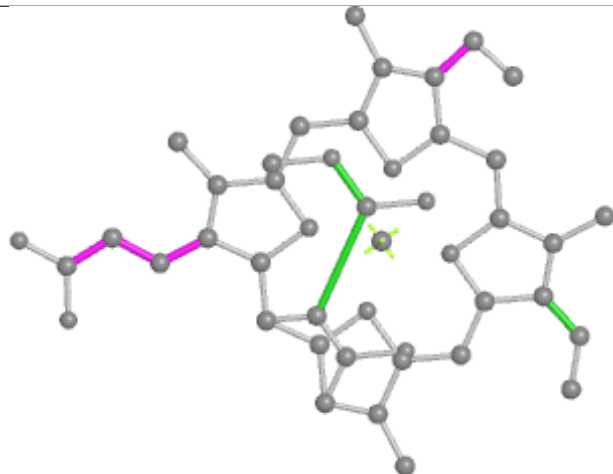
Ligand KC1 J 312



Bond lengths



Bond angles

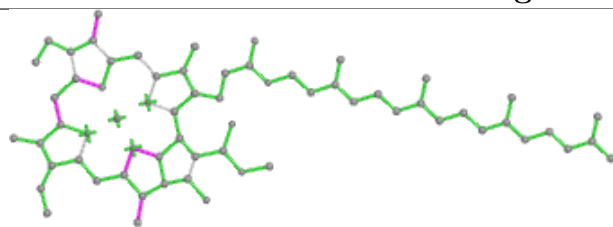


Torsions

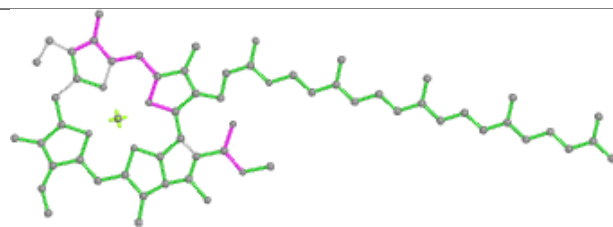


Rings

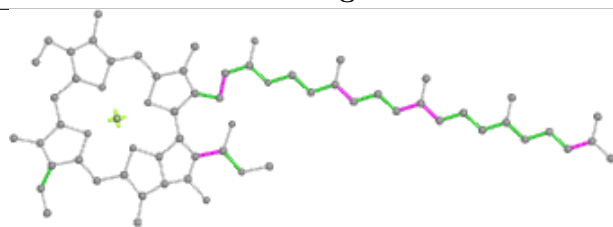
Ligand CLA C 309



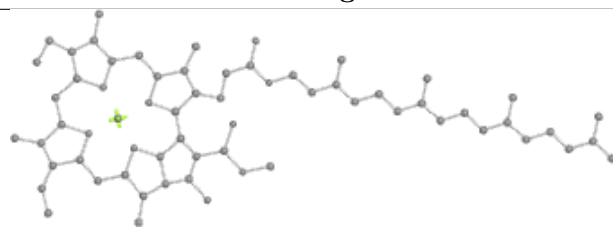
Bond lengths



Bond angles

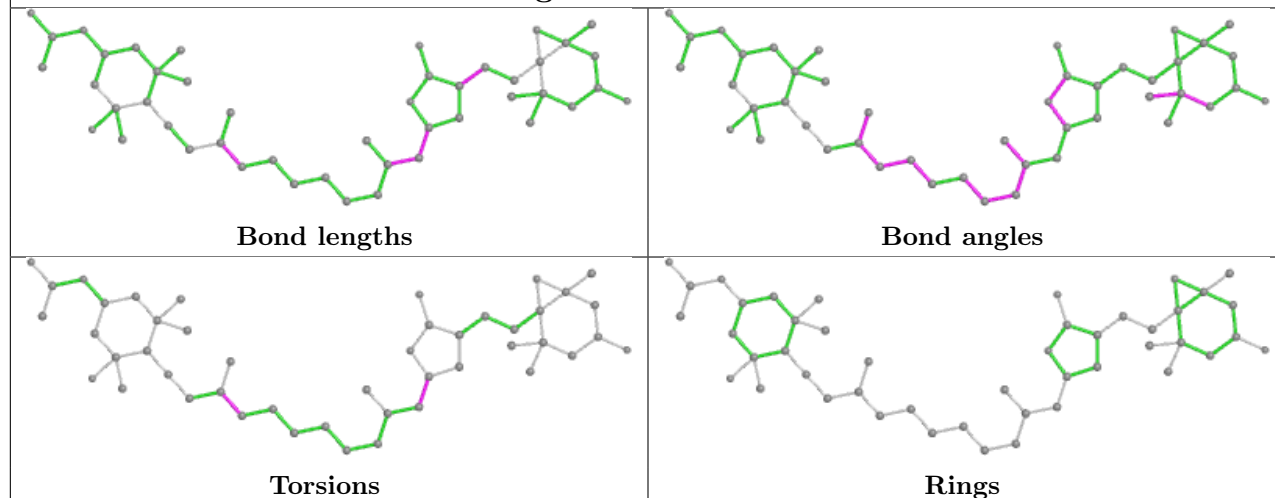


Torsions

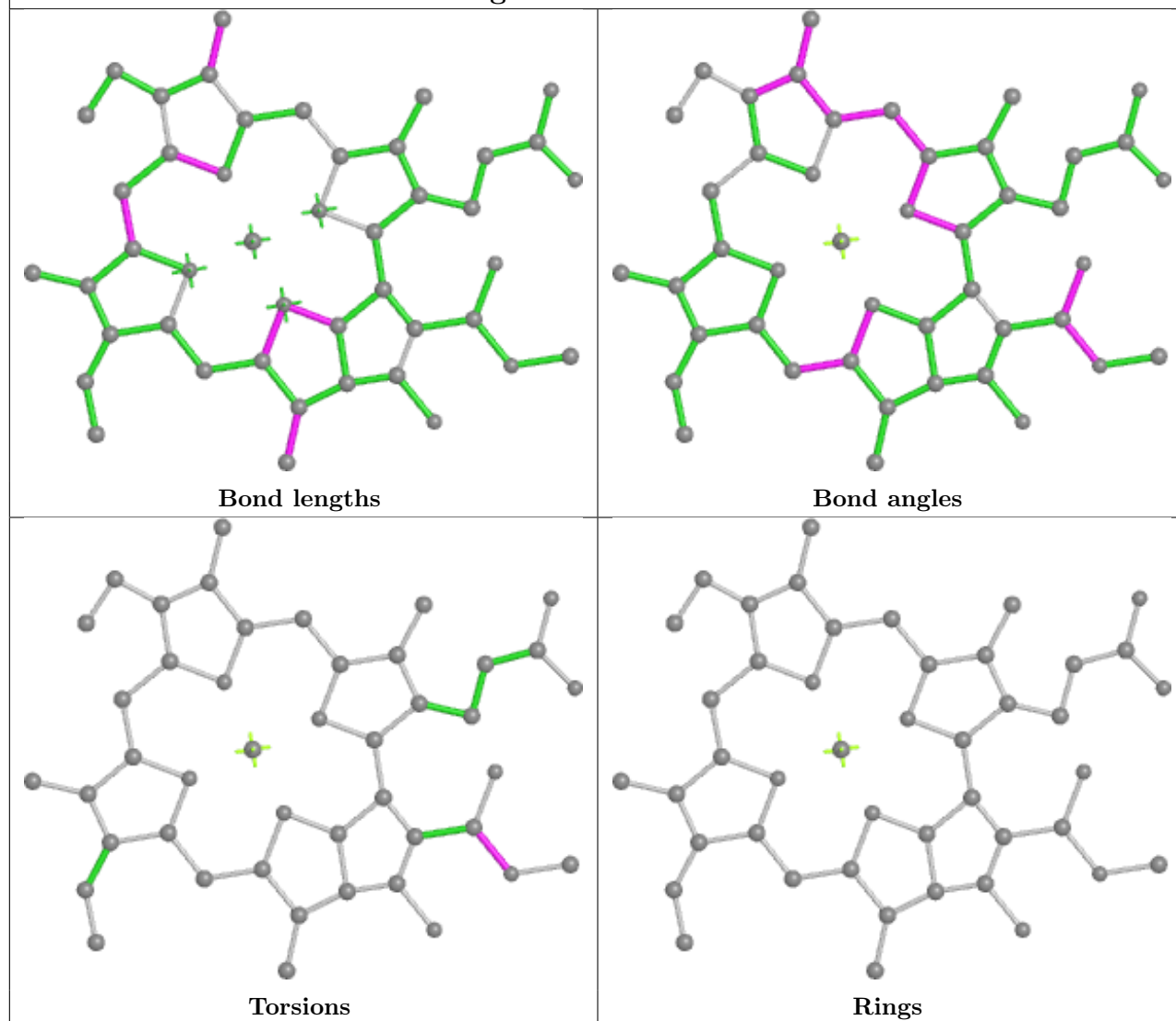


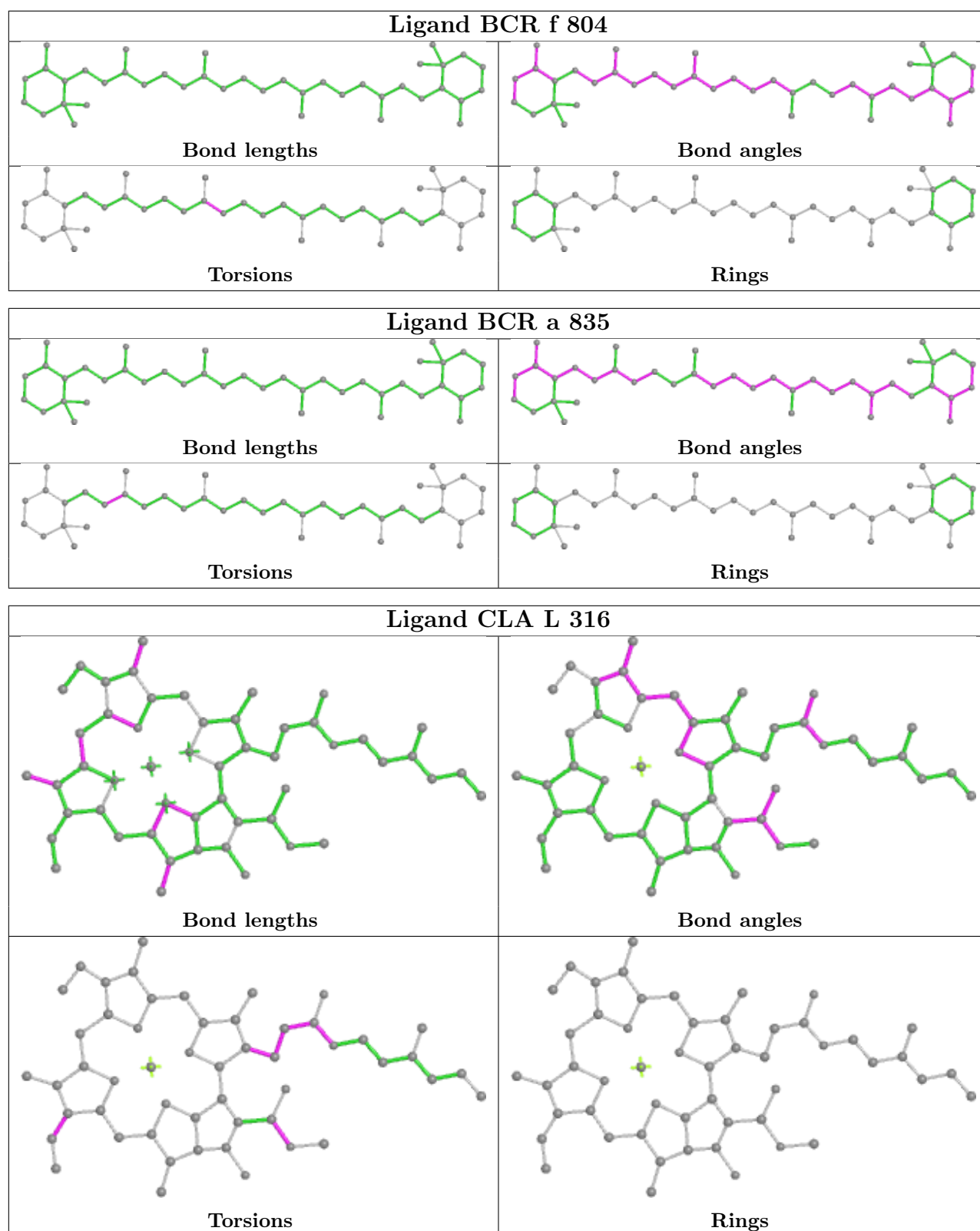
Rings

Ligand PID O 304

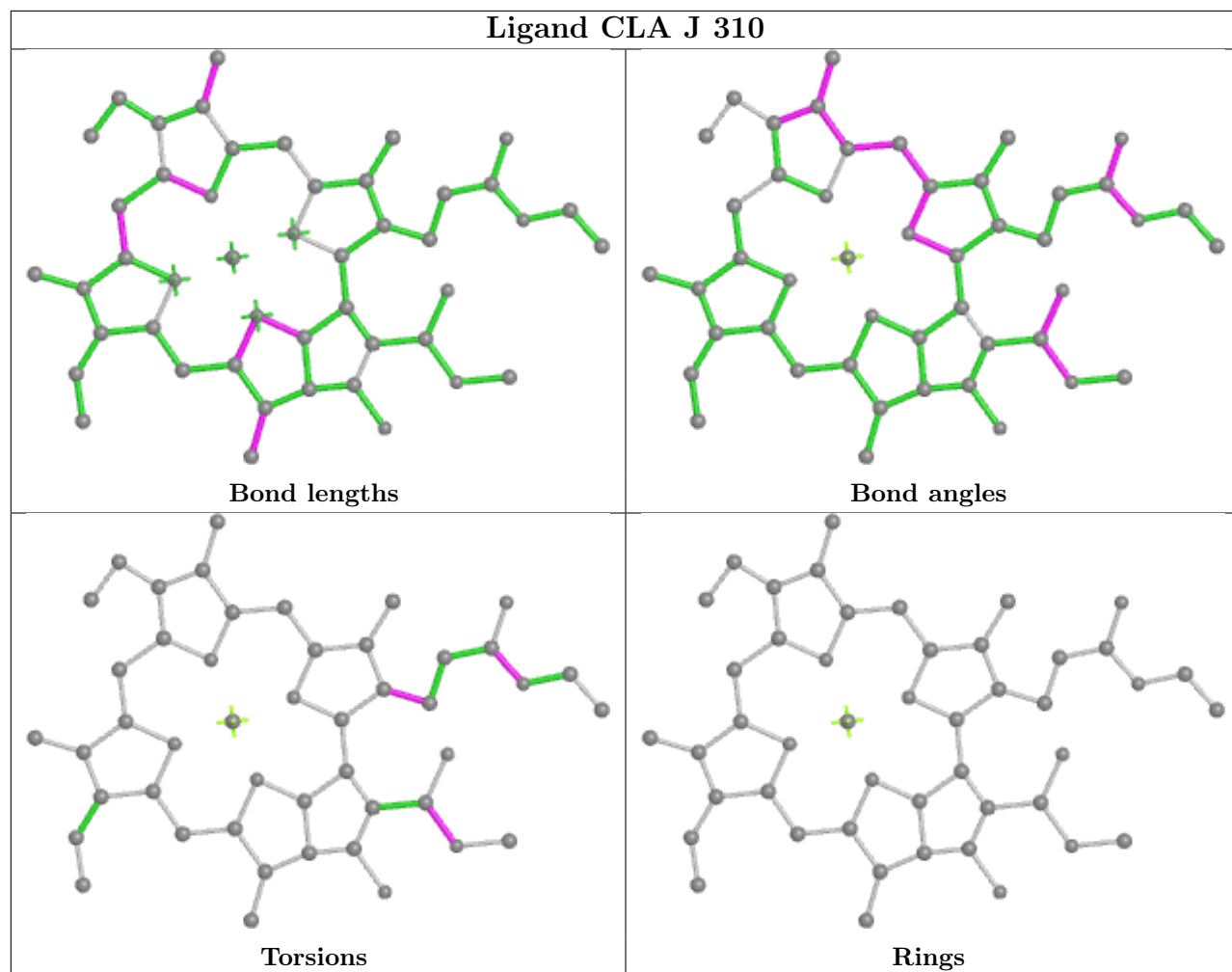


Ligand CLA B 307

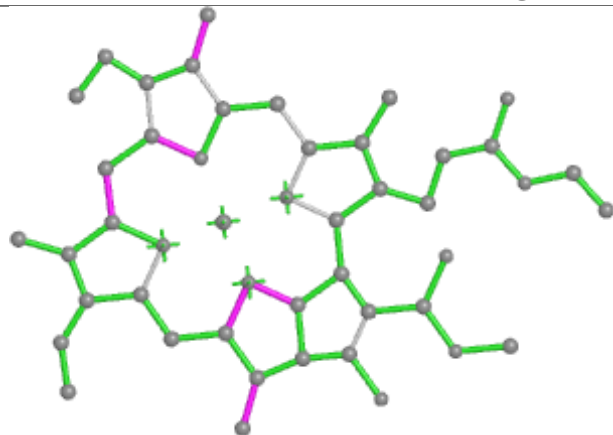




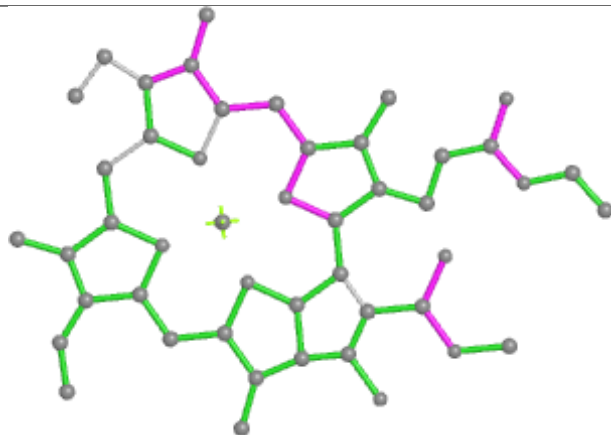
Ligand CLA J 310



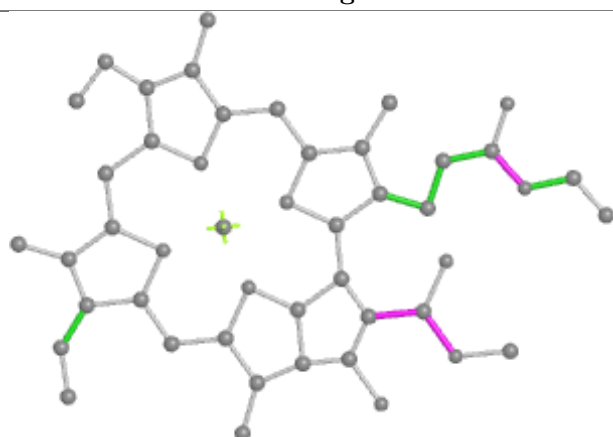
Ligand CLA H 307



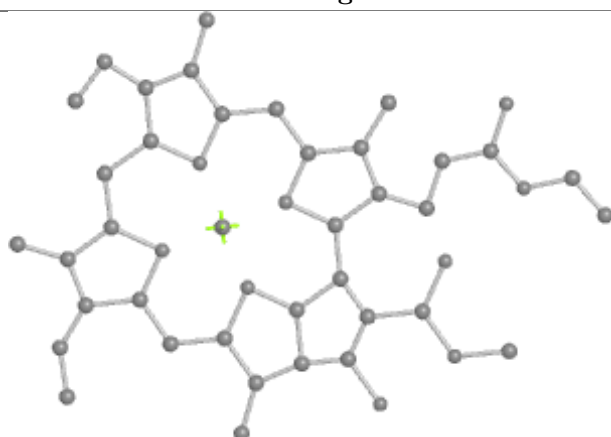
Bond lengths



Bond angles

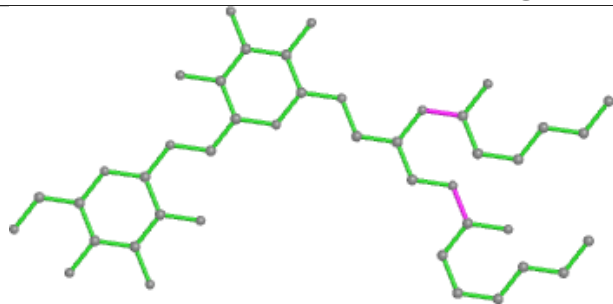


Torsions

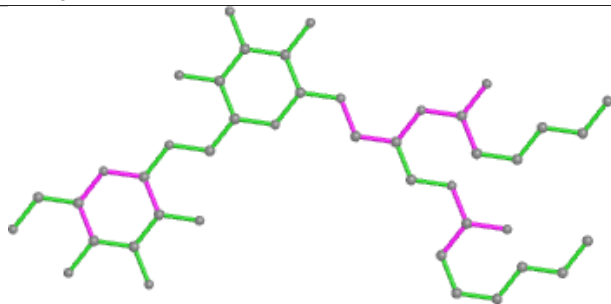


Rings

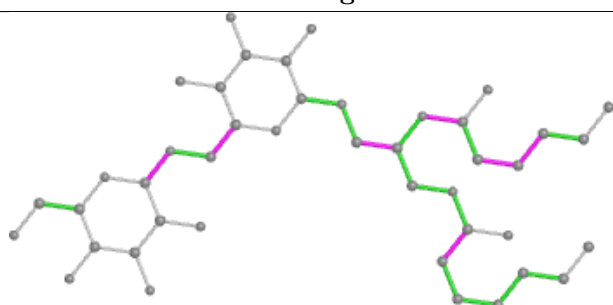
Ligand DGD j 103



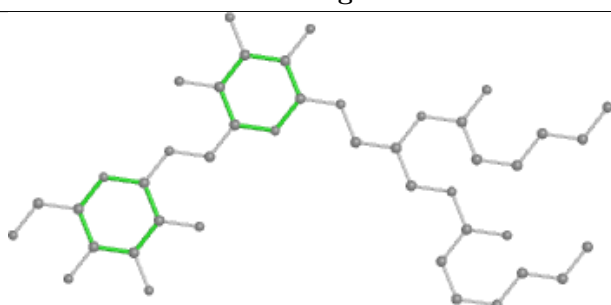
Bond lengths



Bond angles

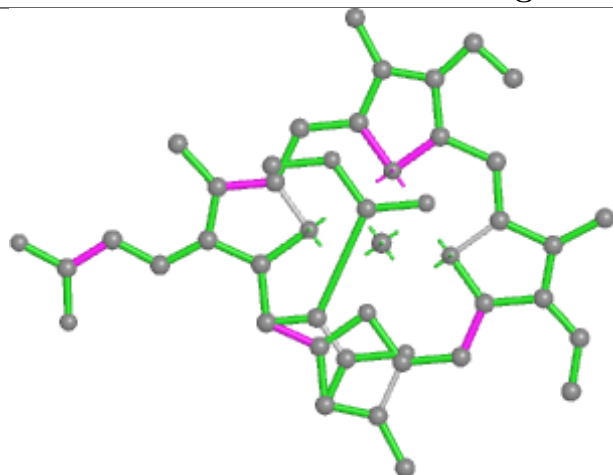


Torsions

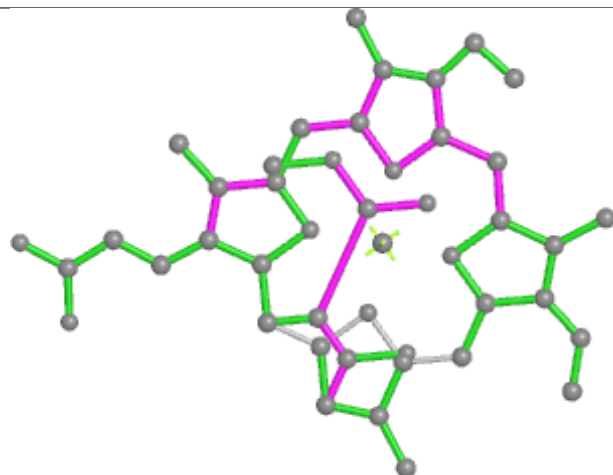


Rings

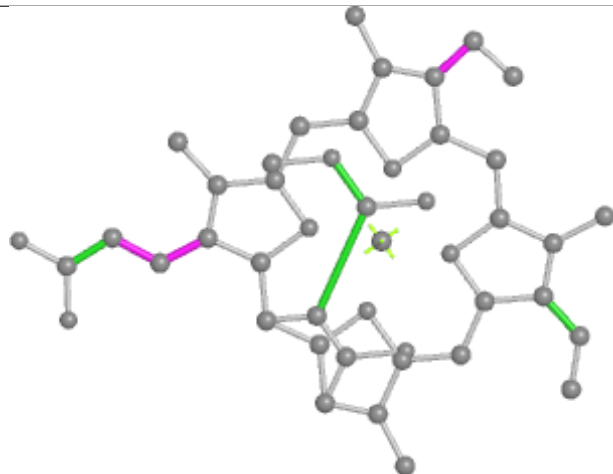
Ligand KC1 D 310



Bond lengths



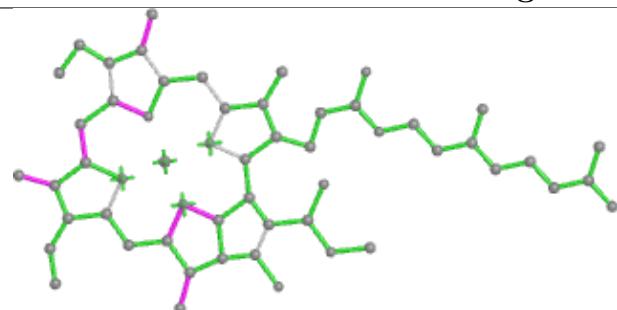
Bond angles



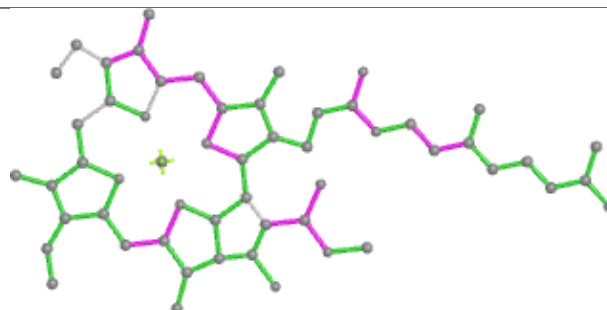
Torsions



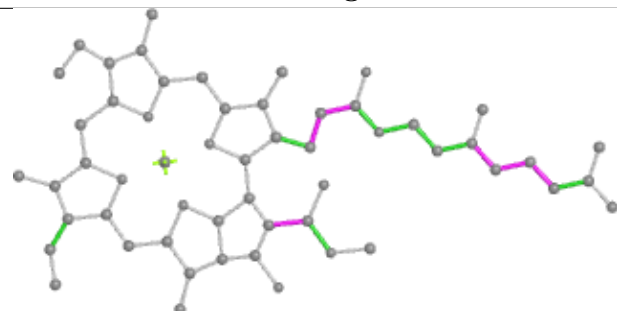
Rings

Ligand CLA K 211

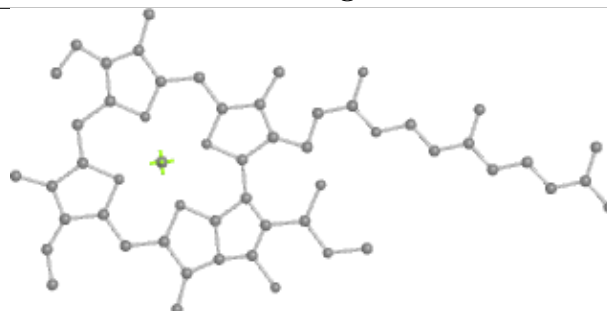
Bond lengths



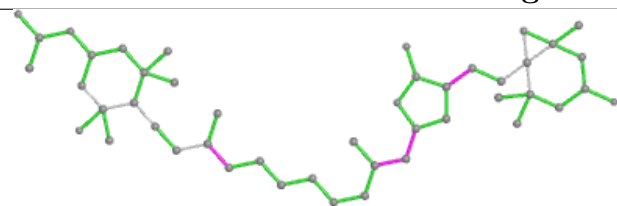
Bond angles



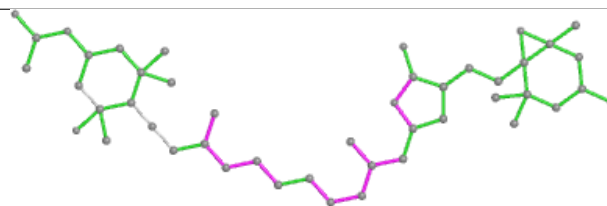
Torsions



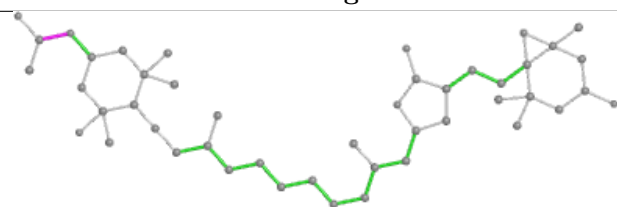
Rings

Ligand PID H 302

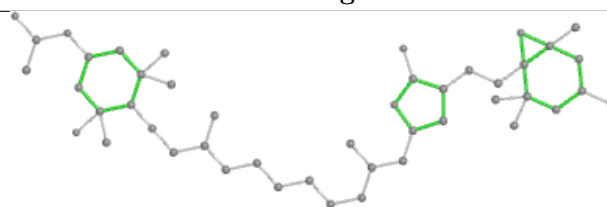
Bond lengths



Bond angles

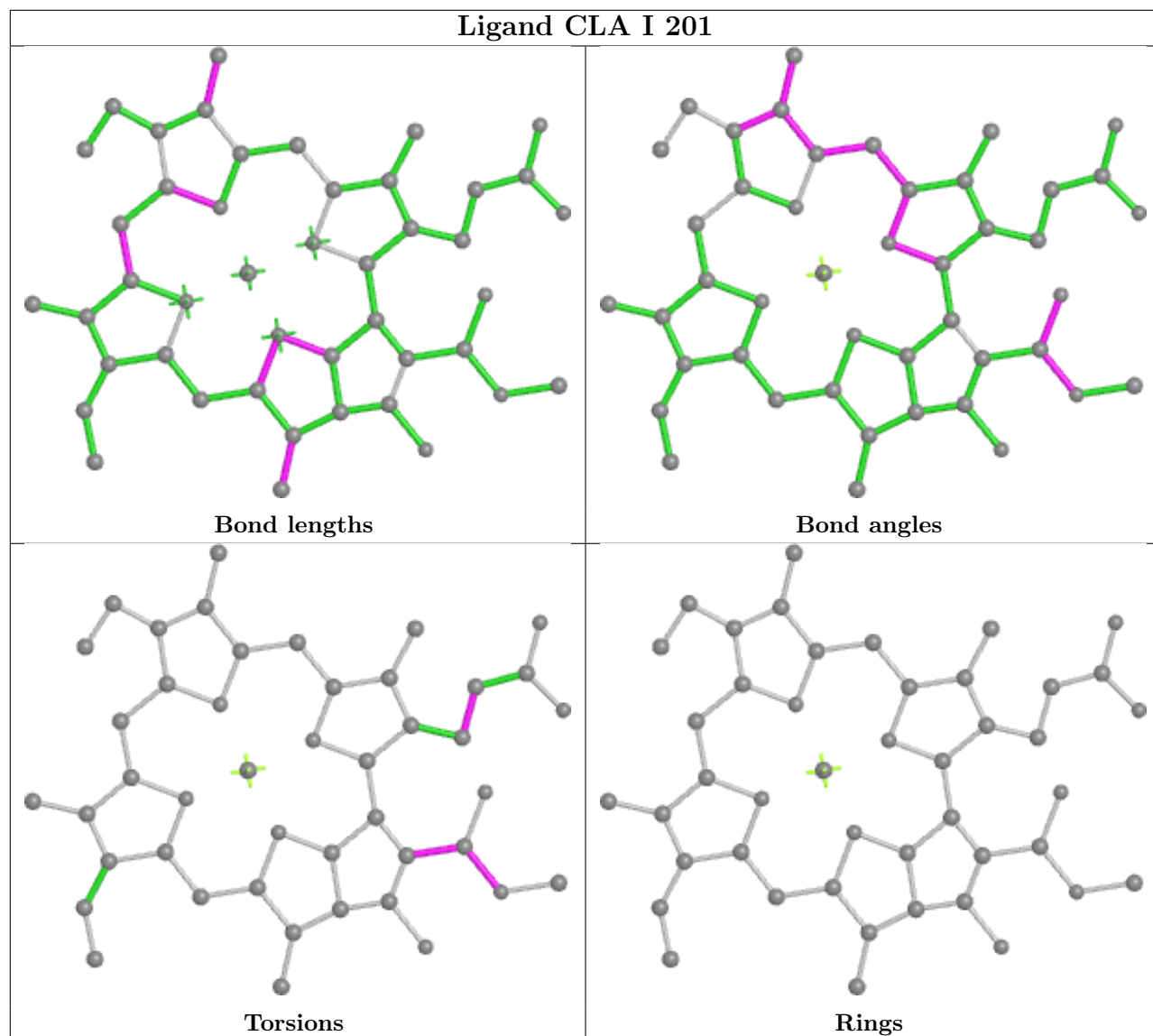


Torsions

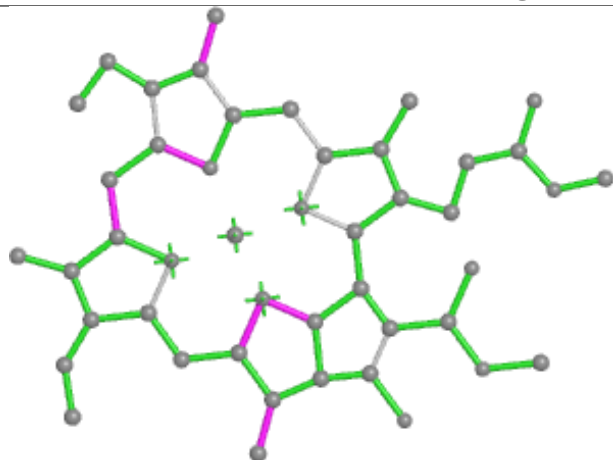


Rings

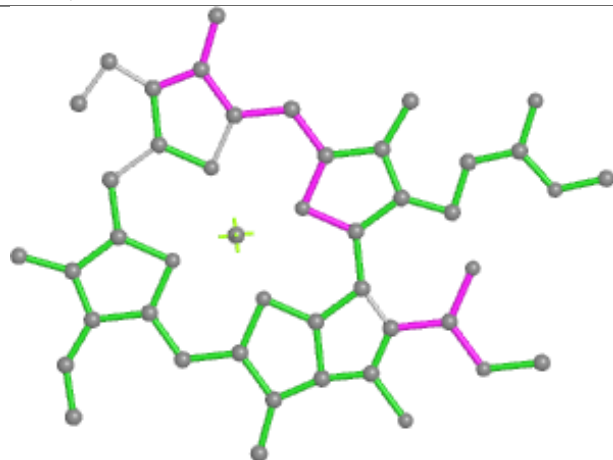
Ligand CLA I 201



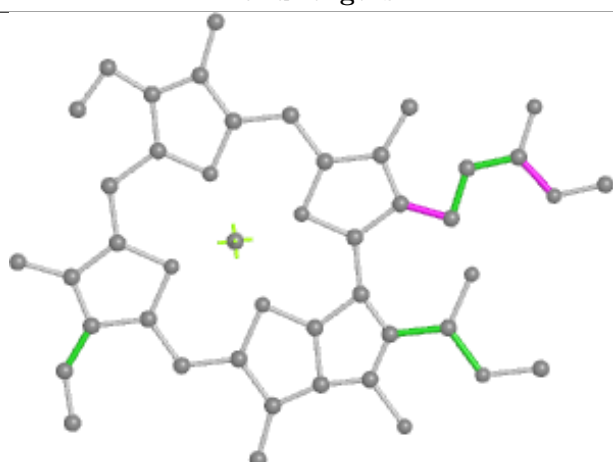
Ligand CLA Q 312



Bond lengths



Bond angles

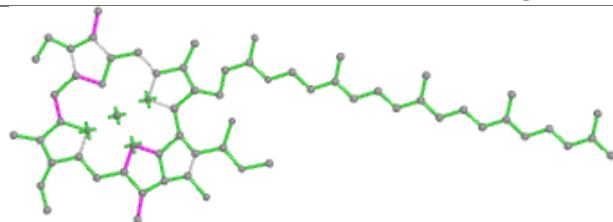


Torsions

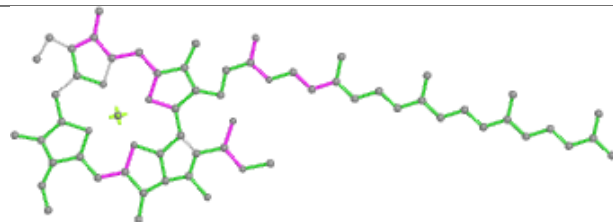


Rings

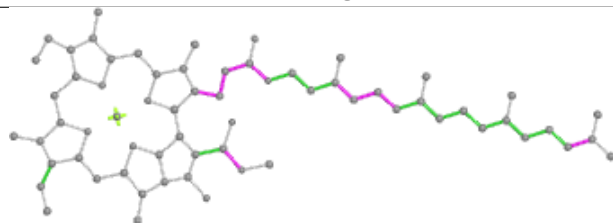
Ligand CLA b 717



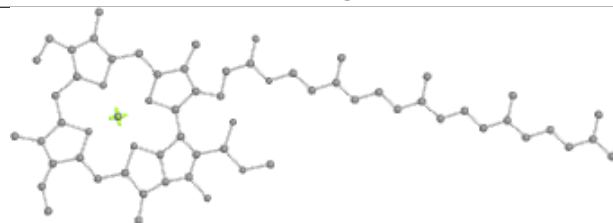
Bond lengths



Bond angles

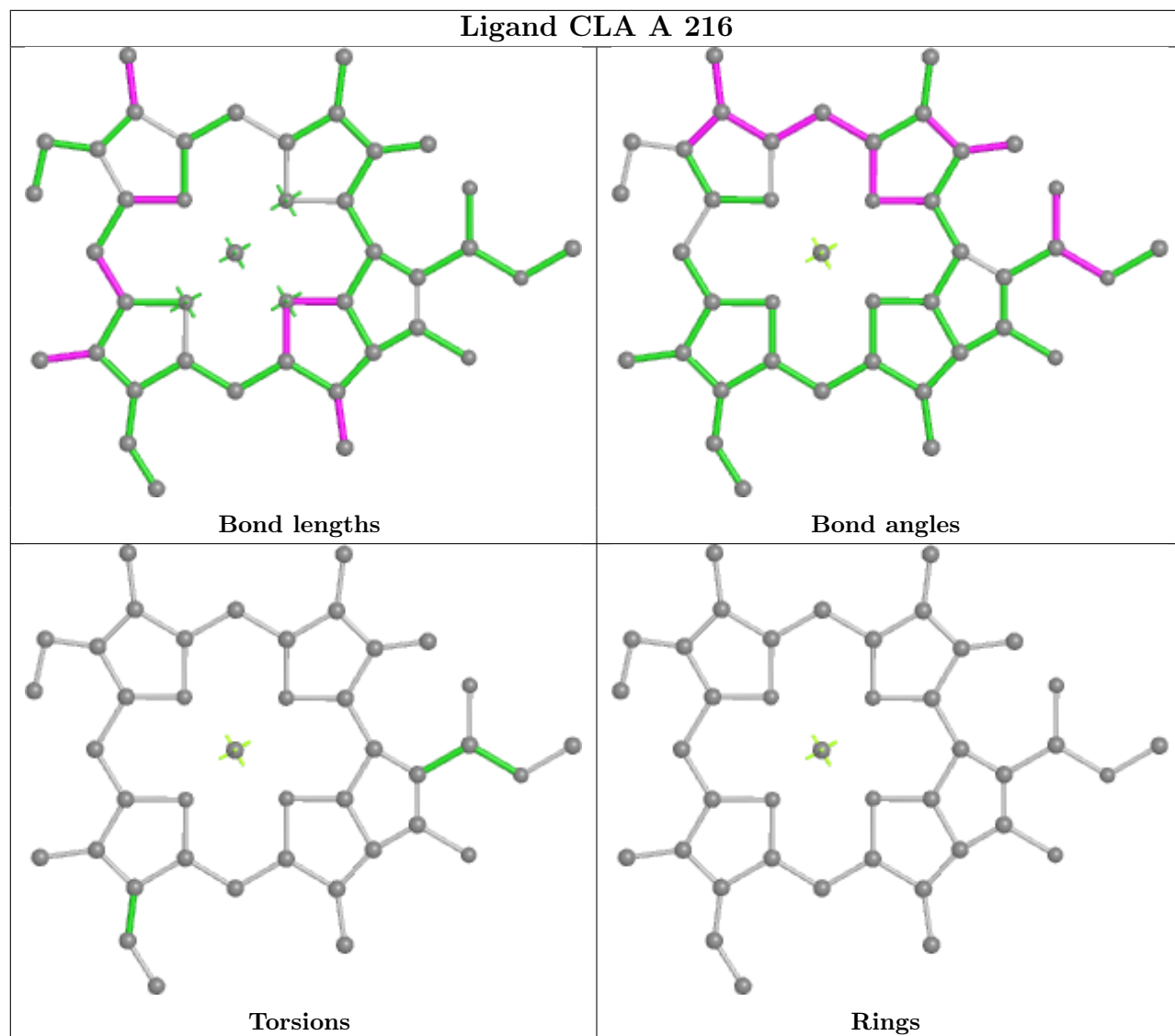


Torsions

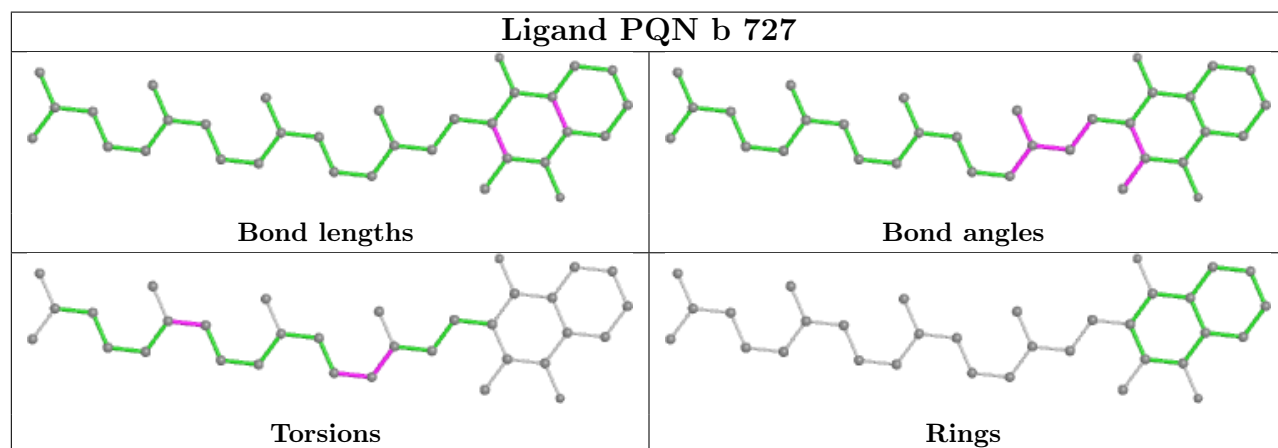


Rings

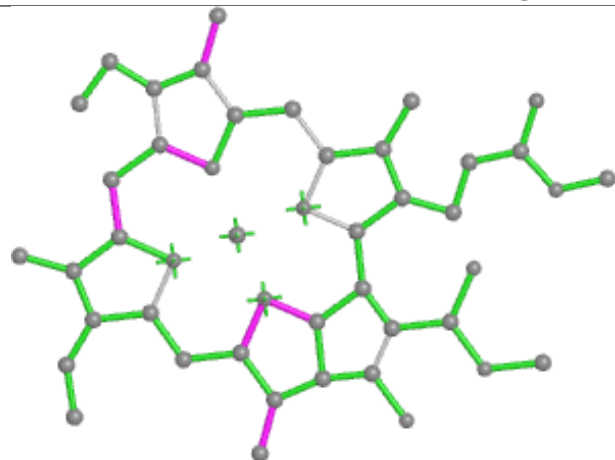
Ligand CLA A 216



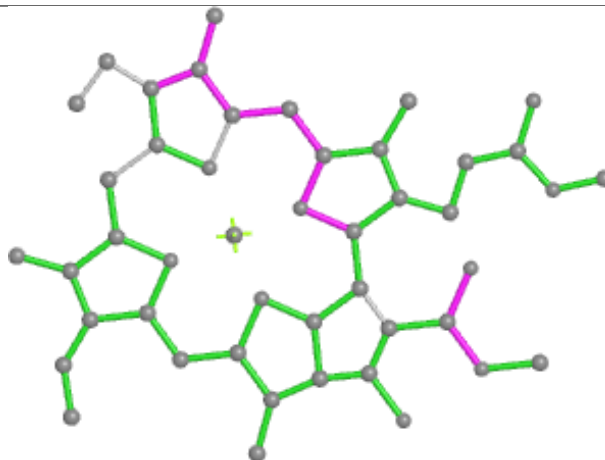
Ligand PQN b 727



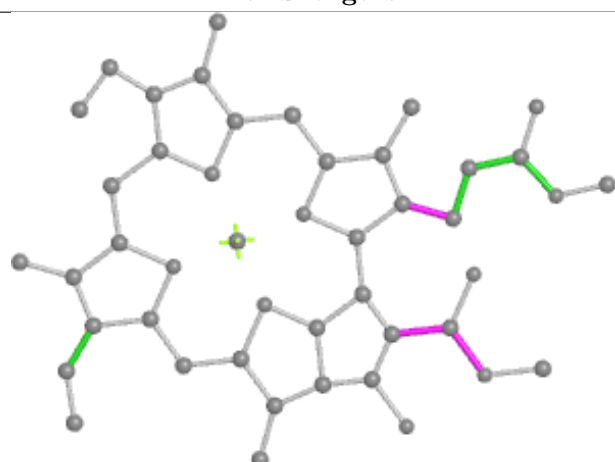
Ligand CLA O 313



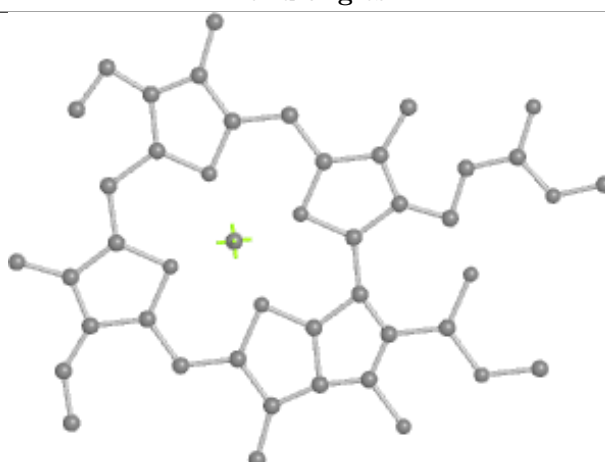
Bond lengths



Bond angles

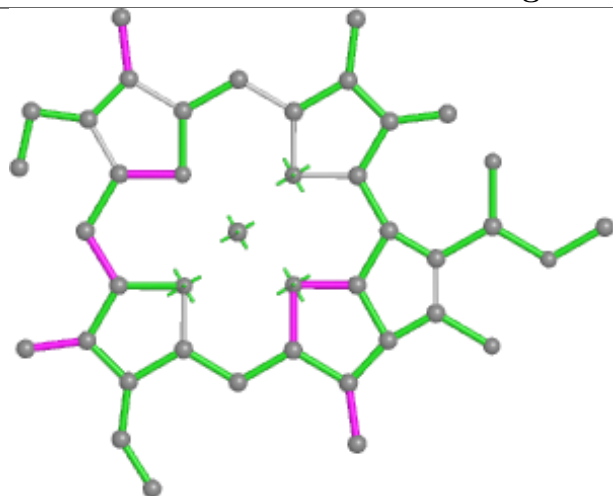


Torsions

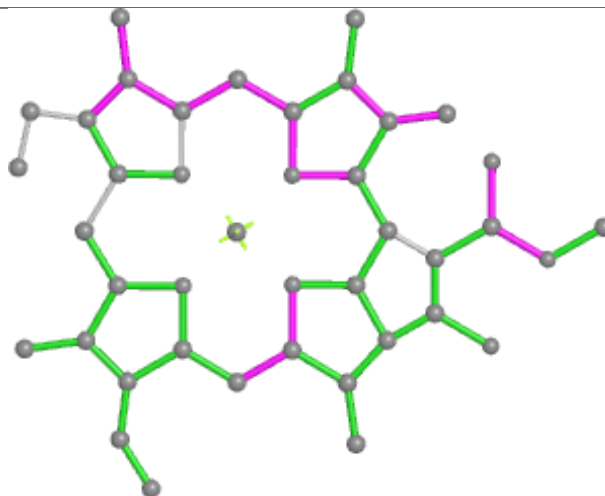


Rings

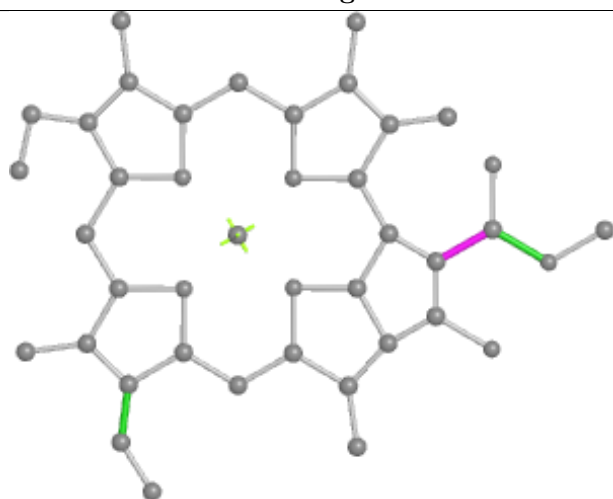
Ligand CLA 1 509



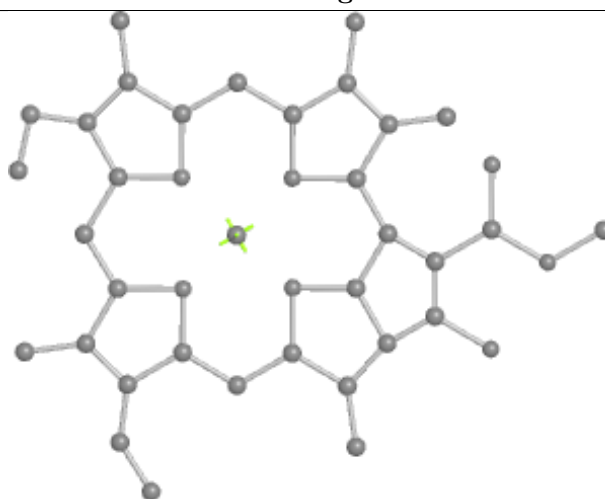
Bond lengths



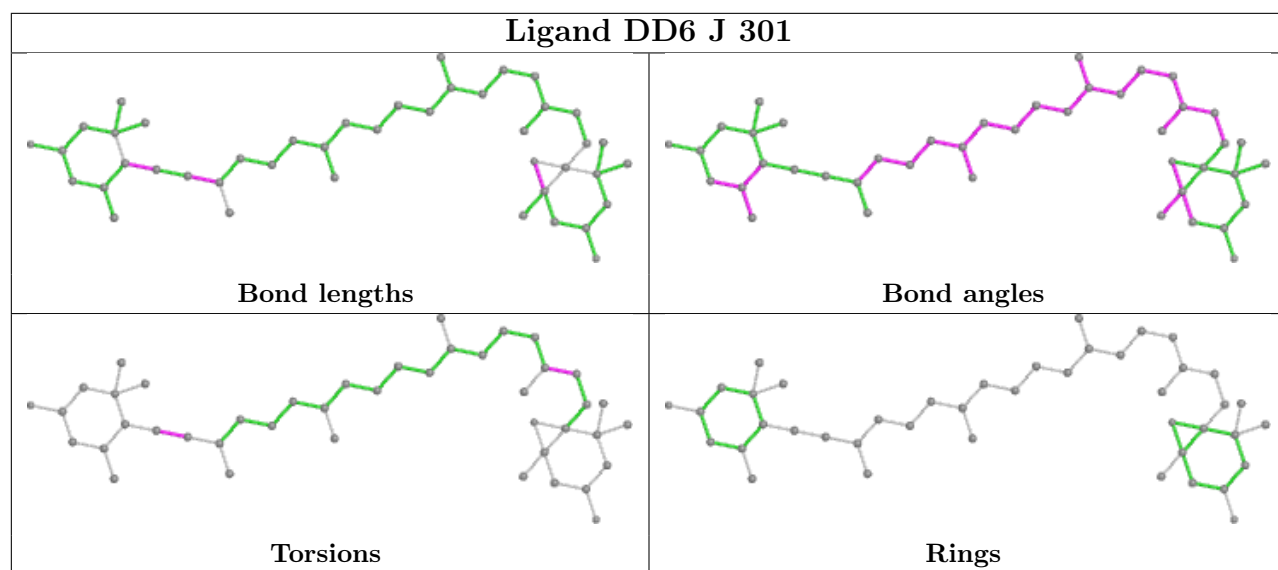
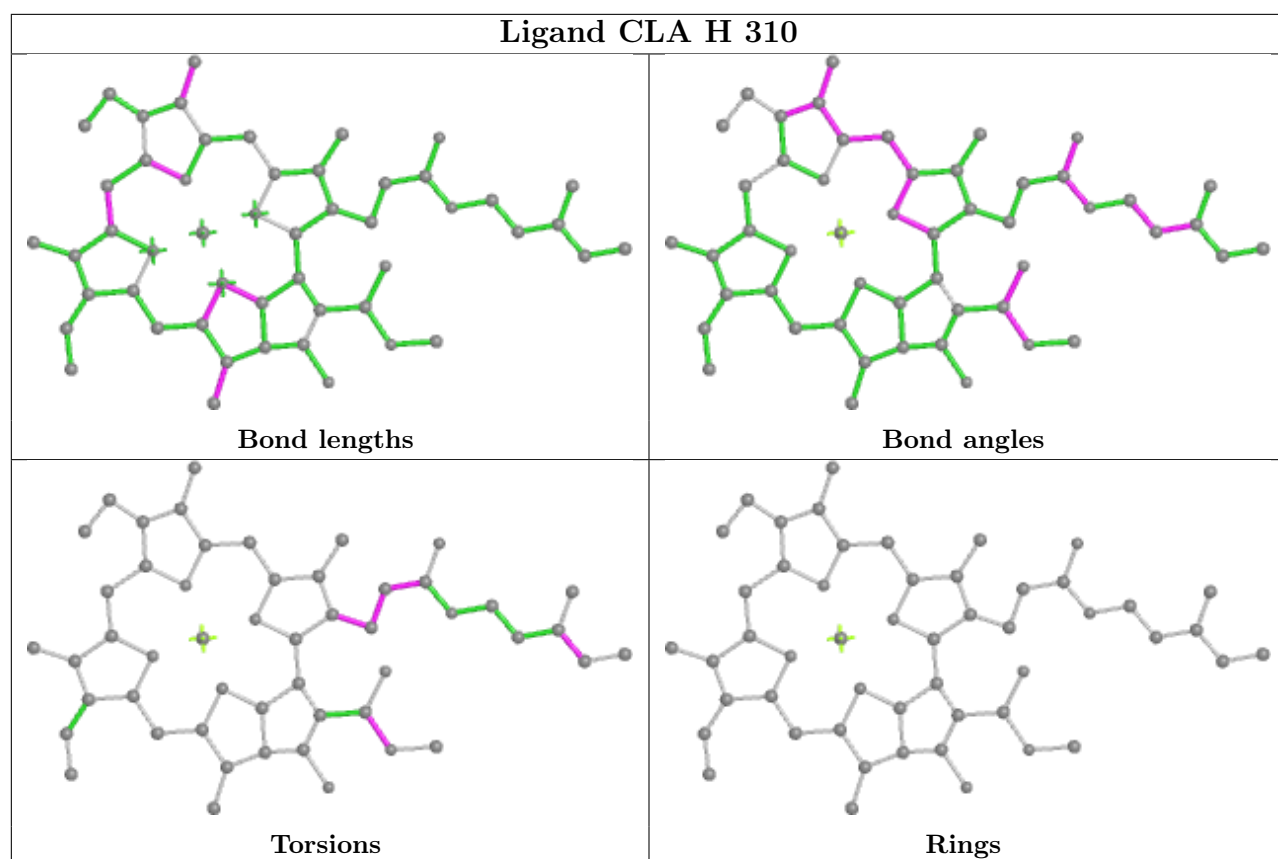
Bond angles

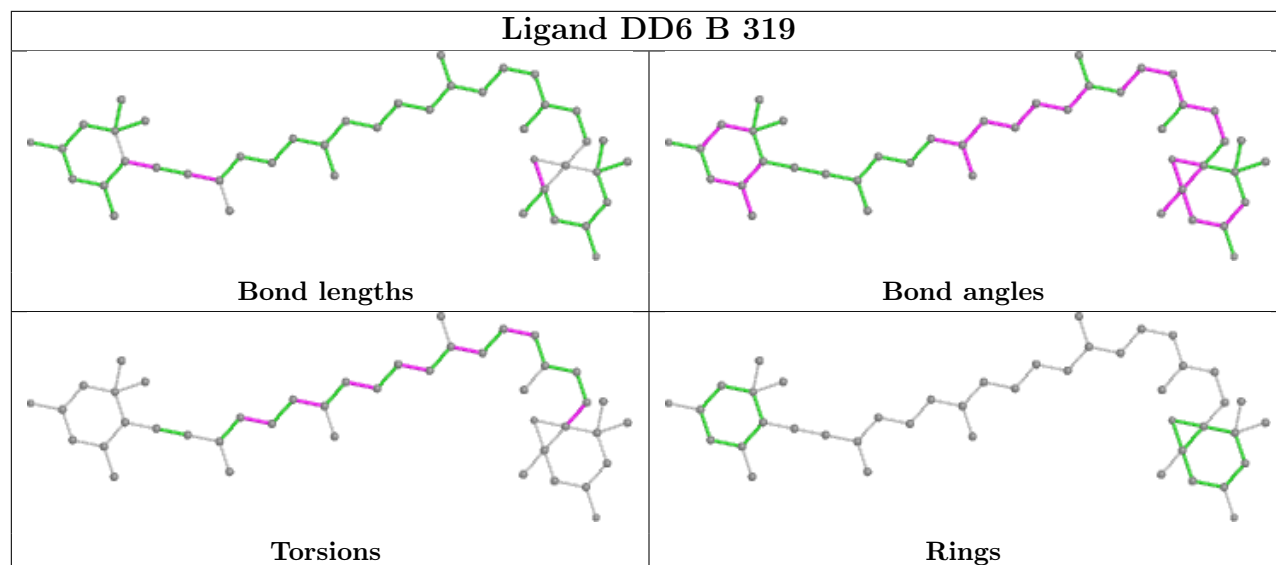
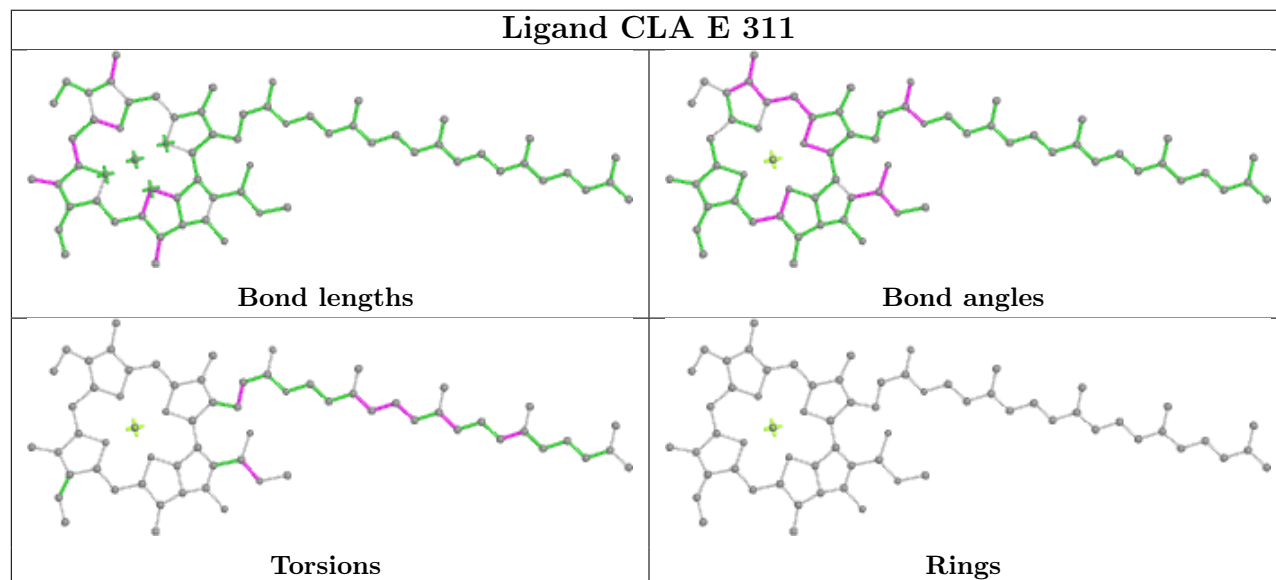


Torsions

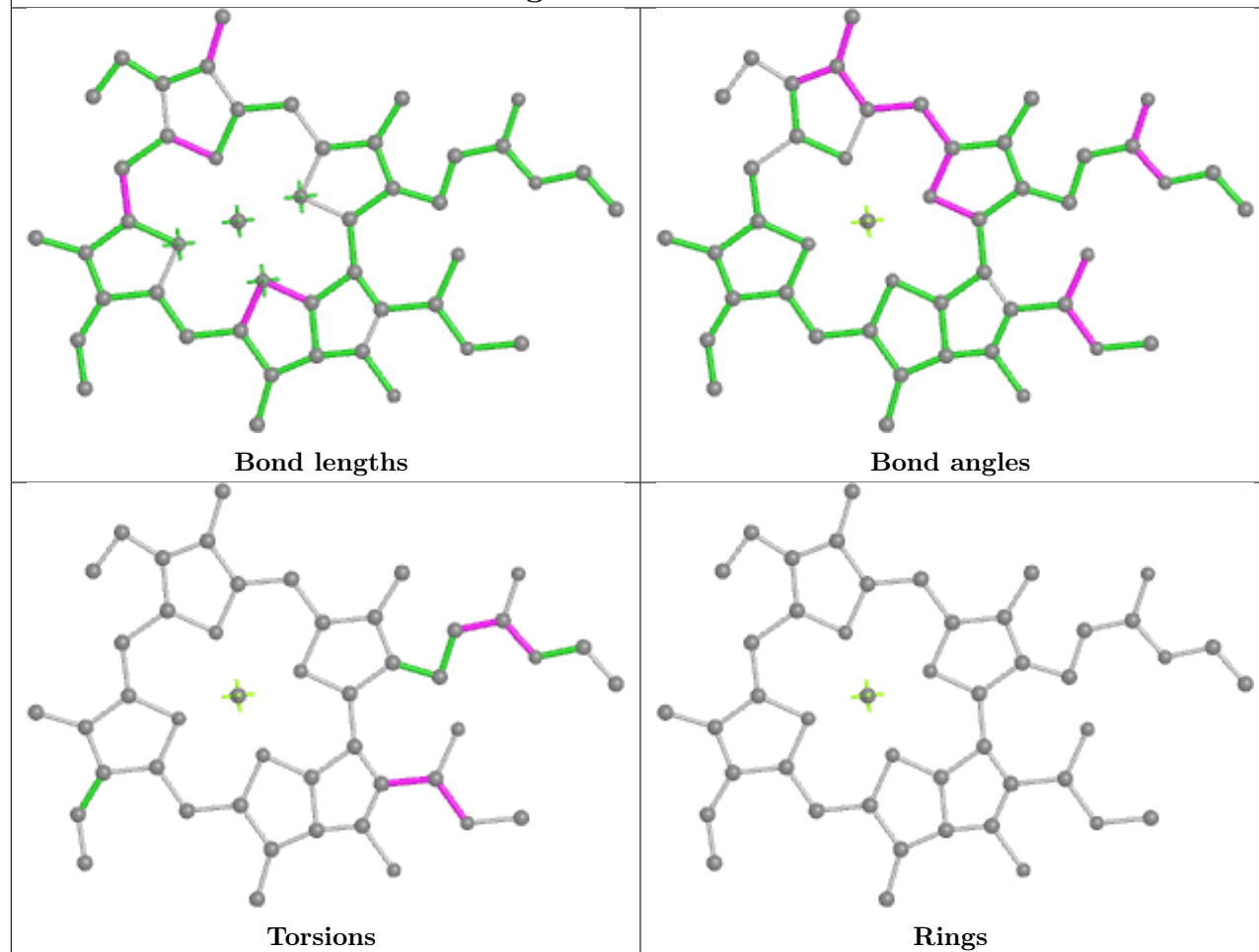


Rings

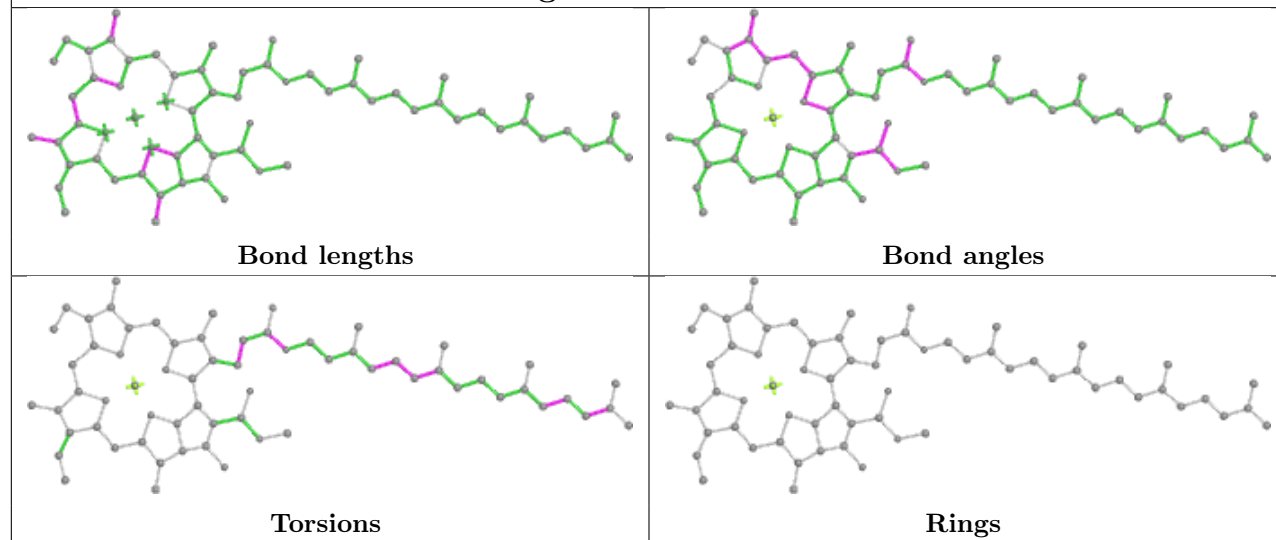


Ligand DD6 B 319**Ligand CLA E 311**

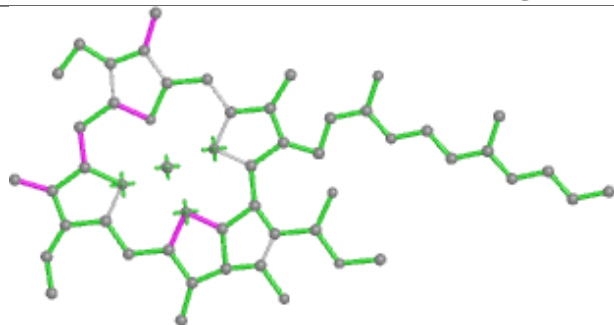
Ligand CLA P 209



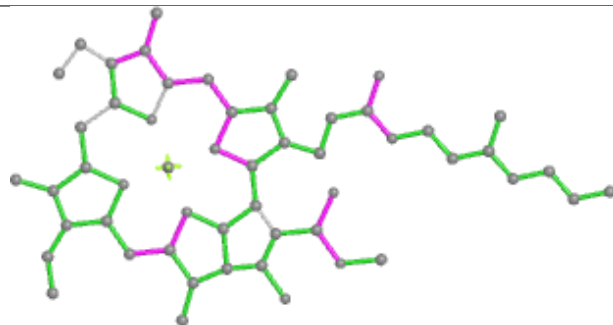
Ligand CLA I 211



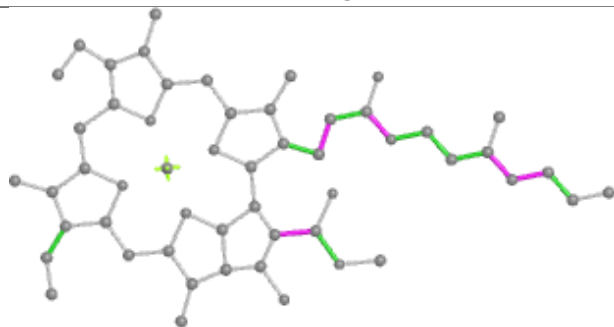
Ligand CLA L 313



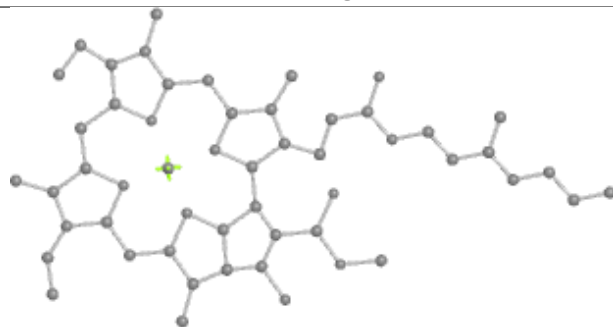
Bond lengths



Bond angles

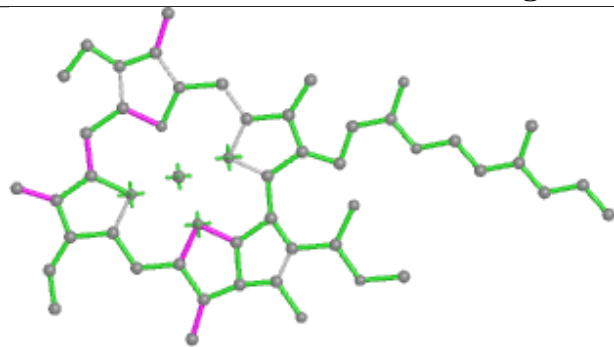


Torsions

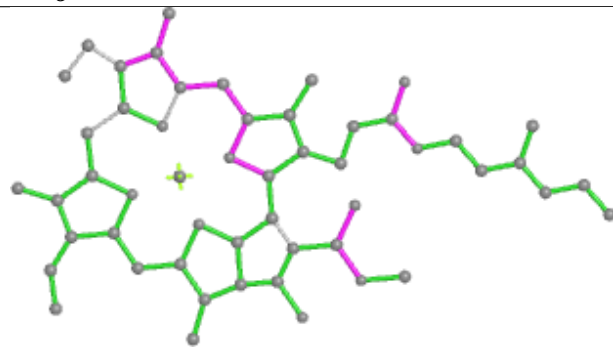


Rings

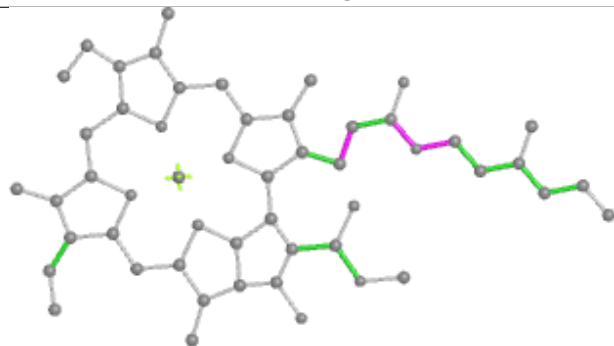
Ligand CLA j 104



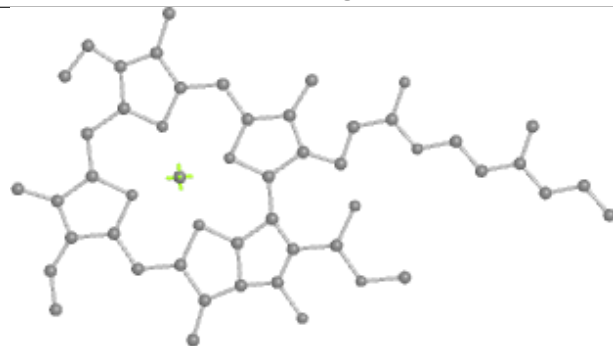
Bond lengths



Bond angles

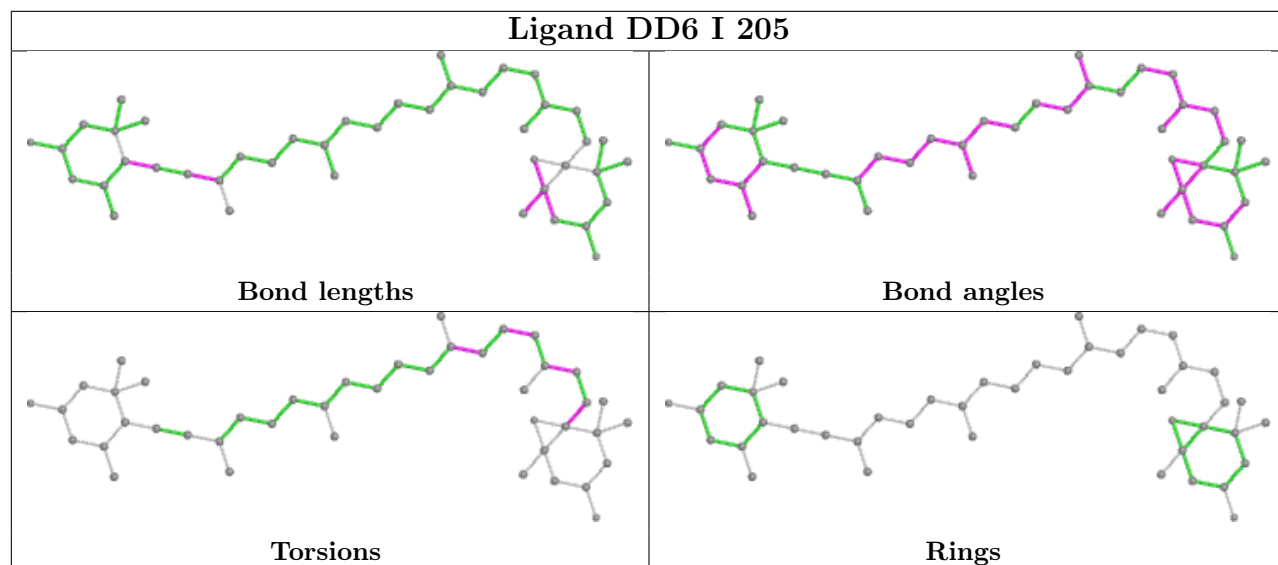


Torsions

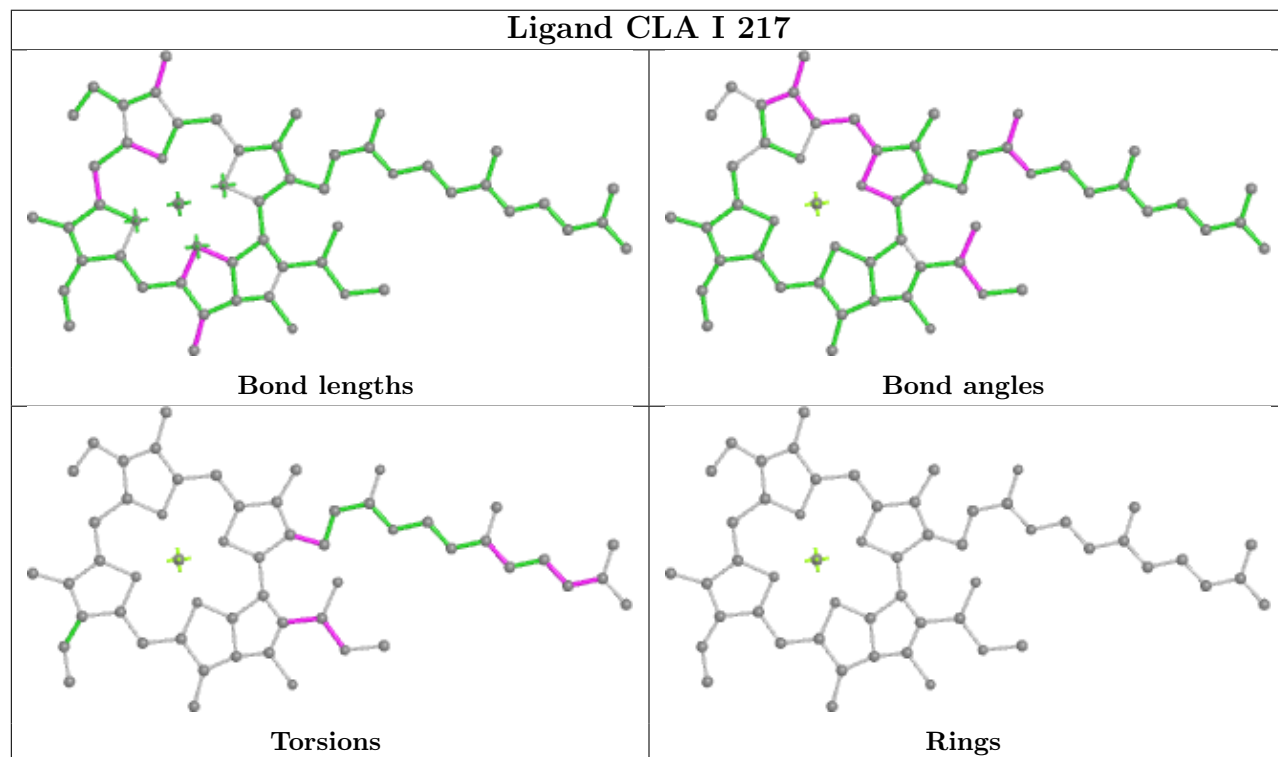


Rings

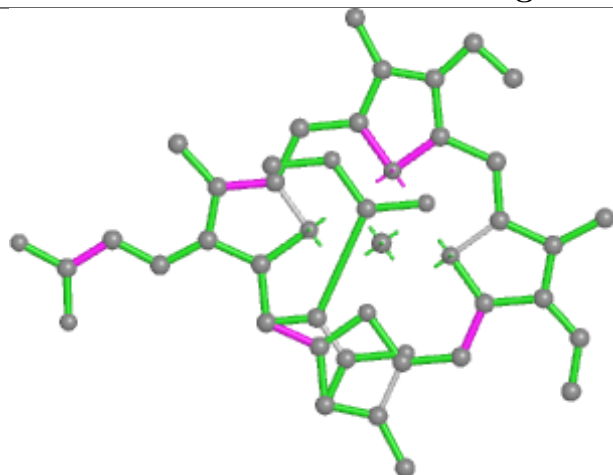
Ligand DD6 I 205



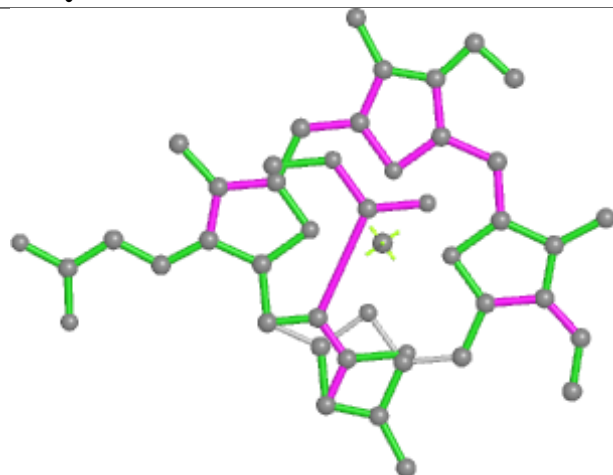
Ligand CLA I 217



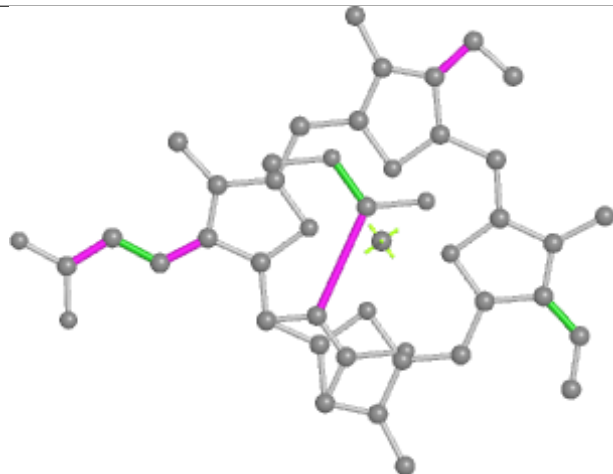
Ligand KC1 Q 311



Bond lengths



Bond angles

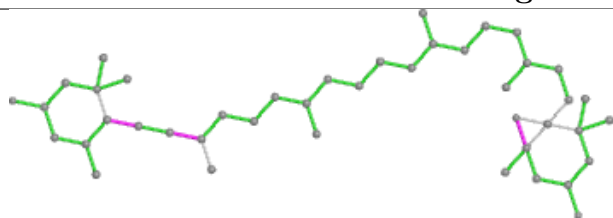


Torsions

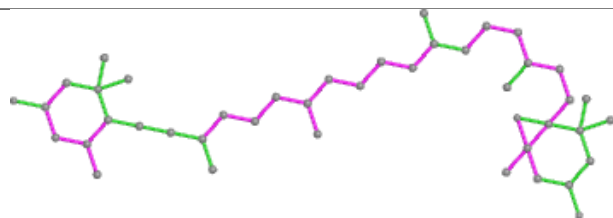


Rings

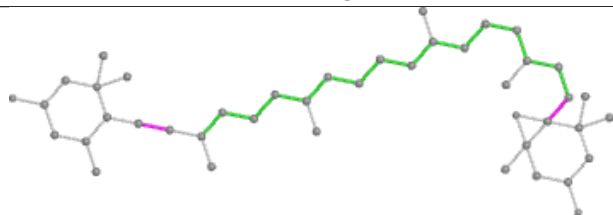
Ligand DD6 B 305



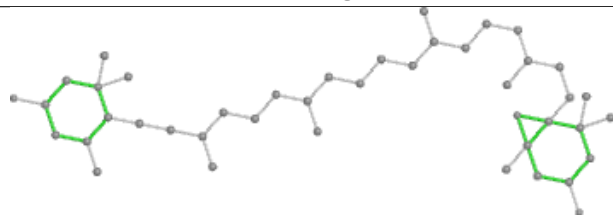
Bond lengths



Bond angles

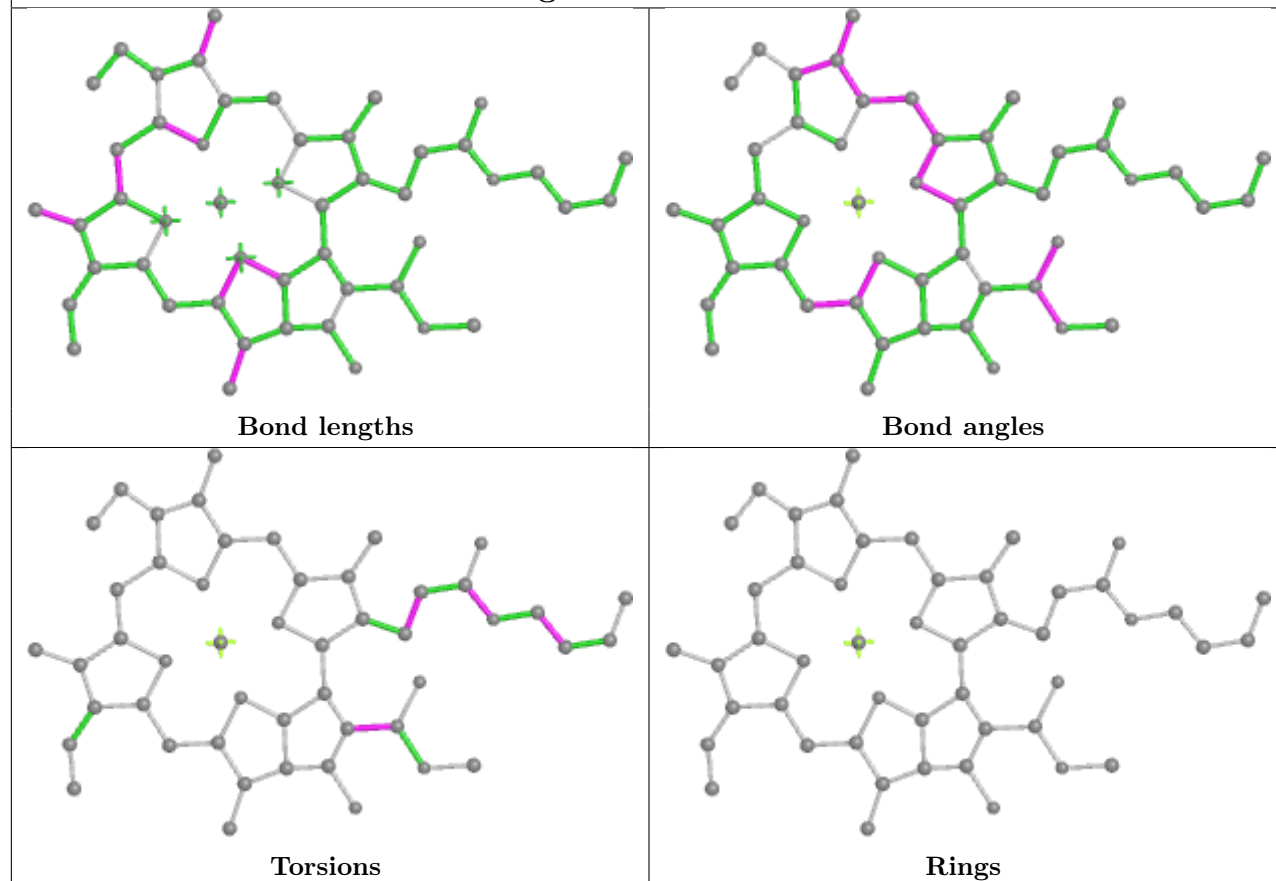


Torsions

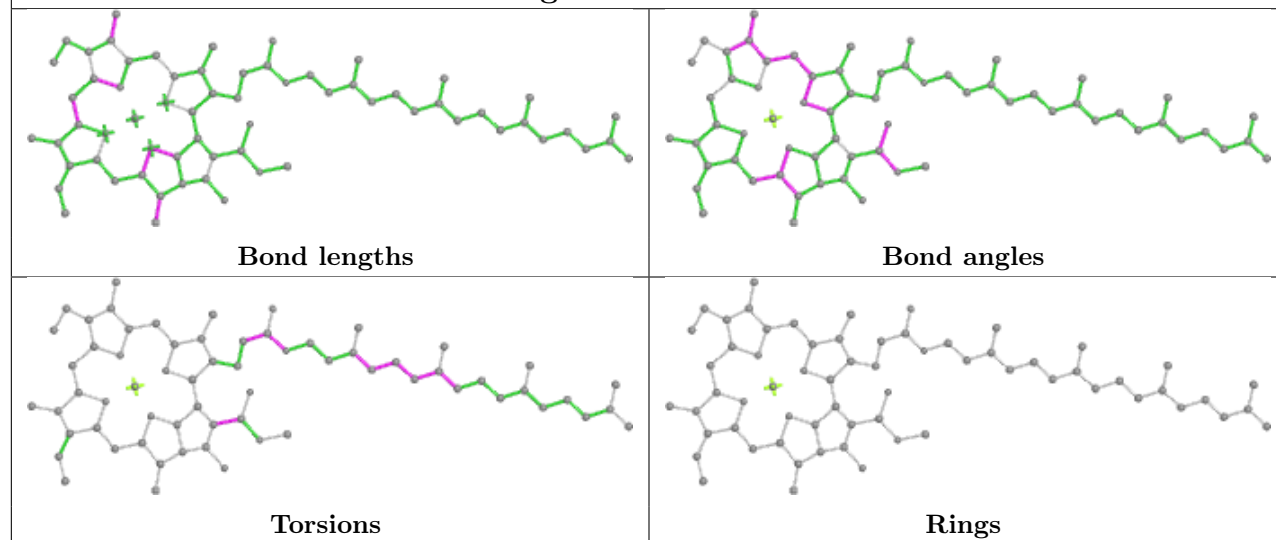


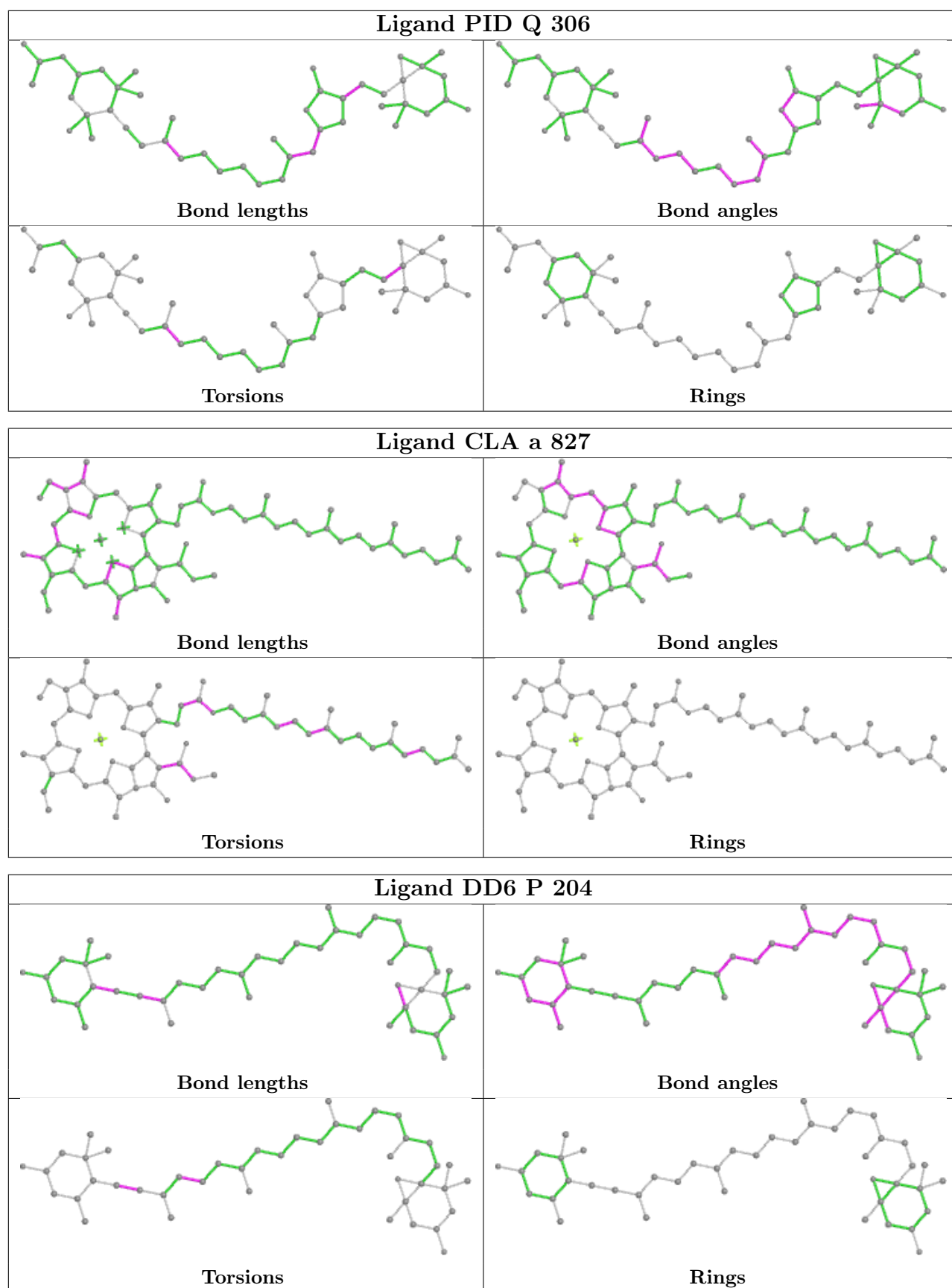
Rings

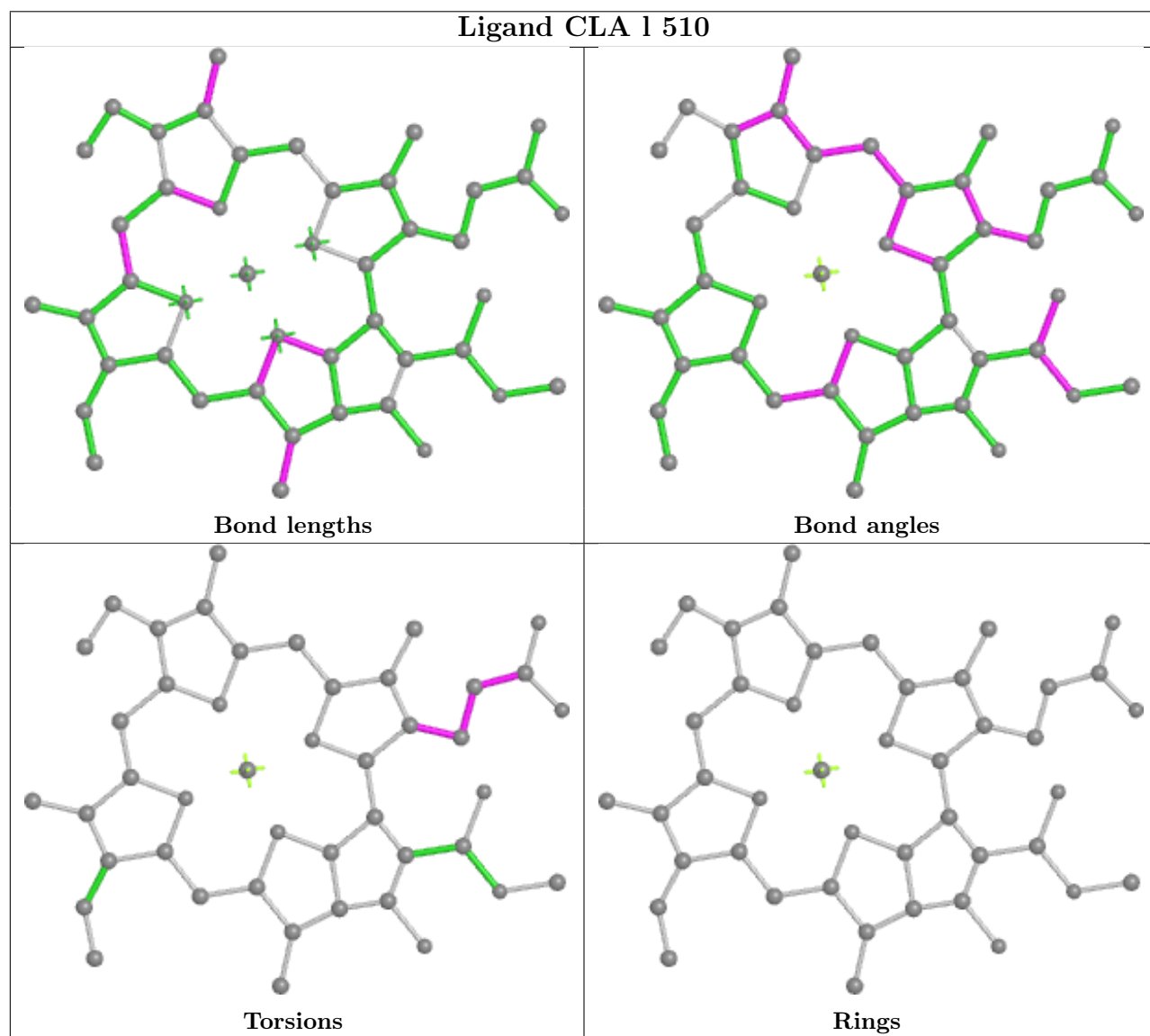
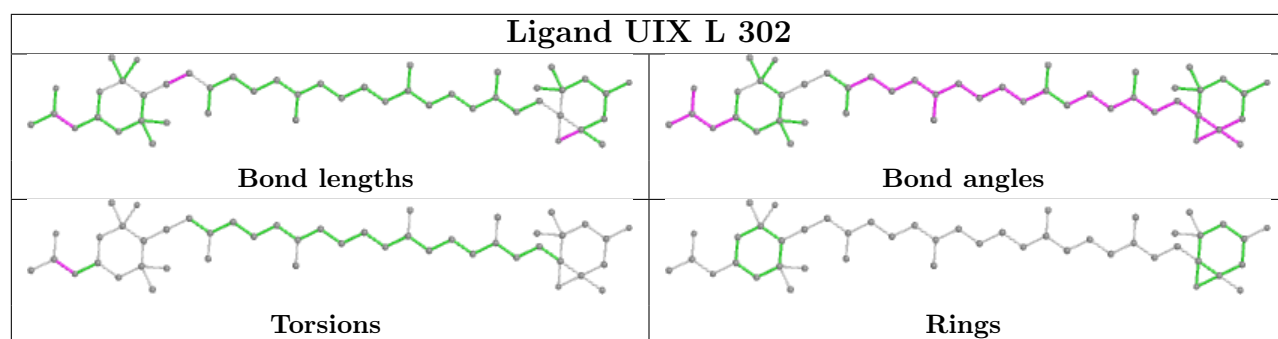
Ligand CLA I 207



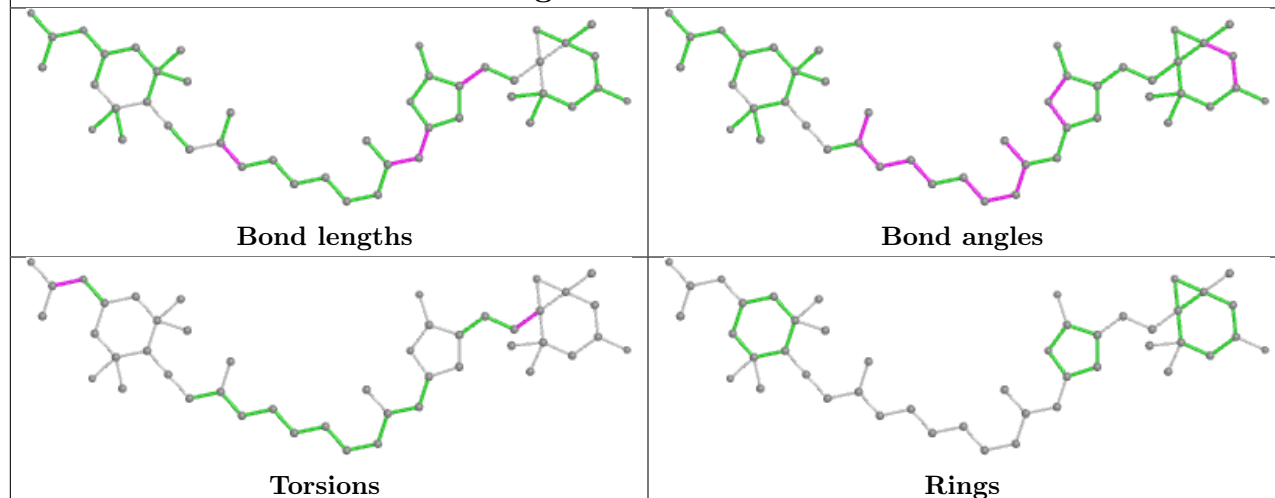
Ligand CLA I 505



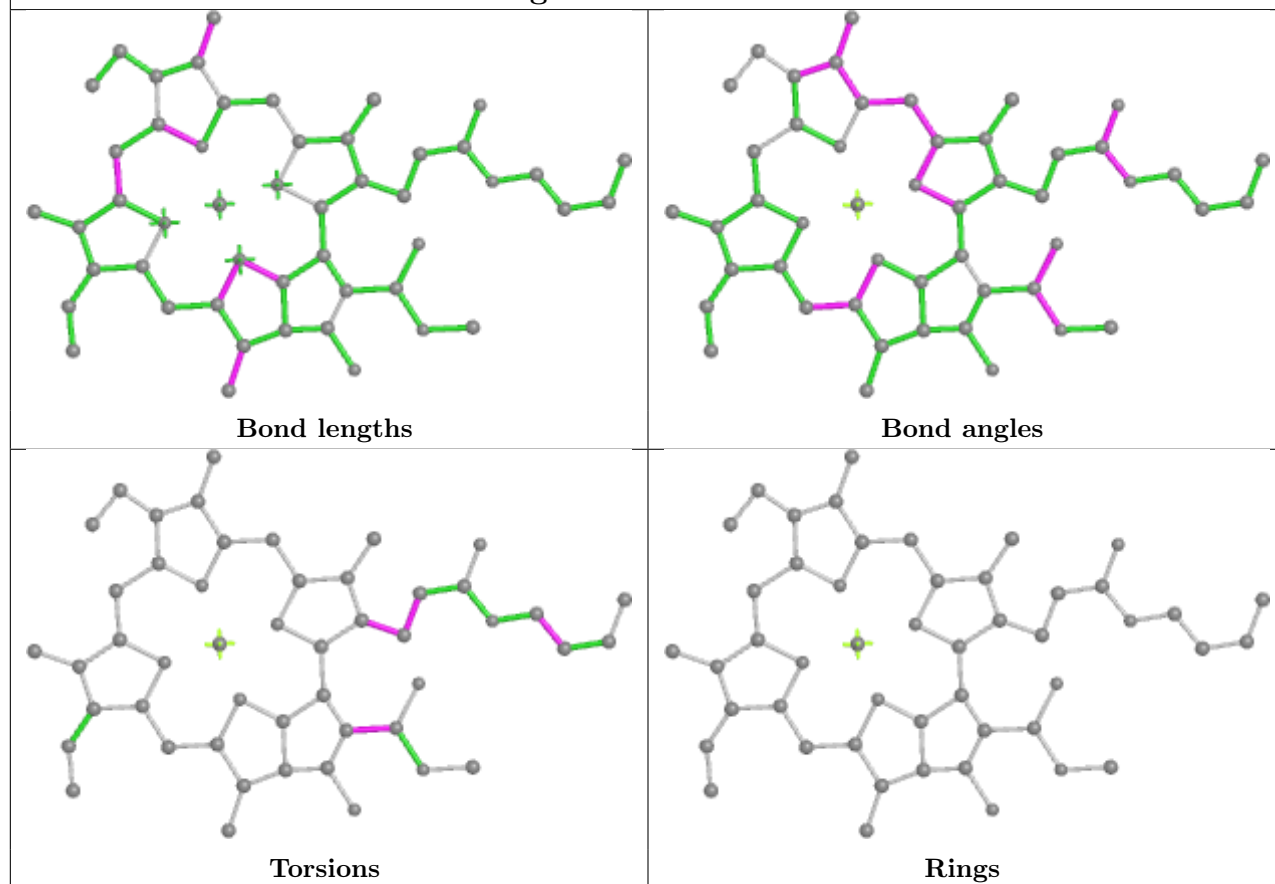


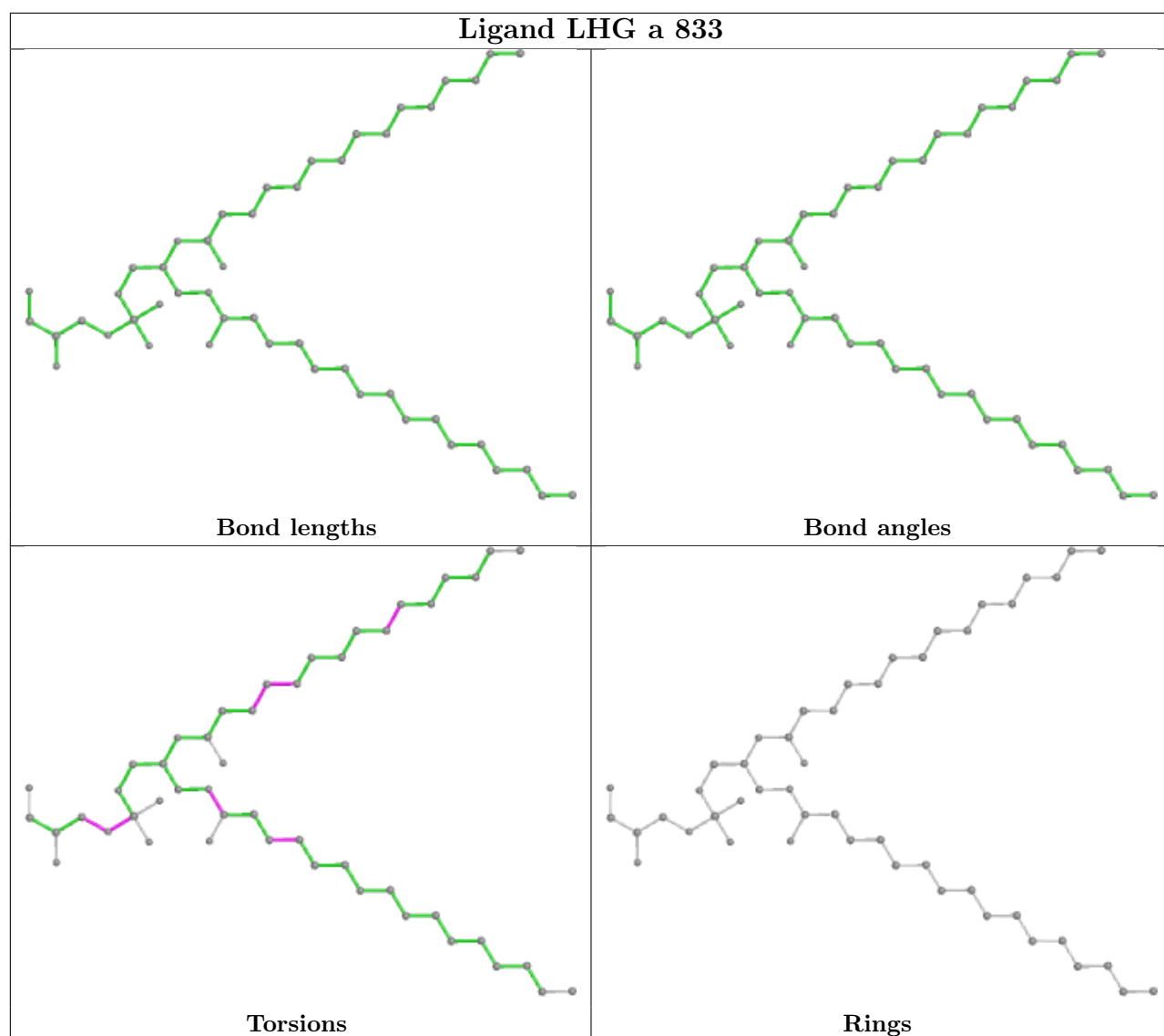


Ligand PID H 306

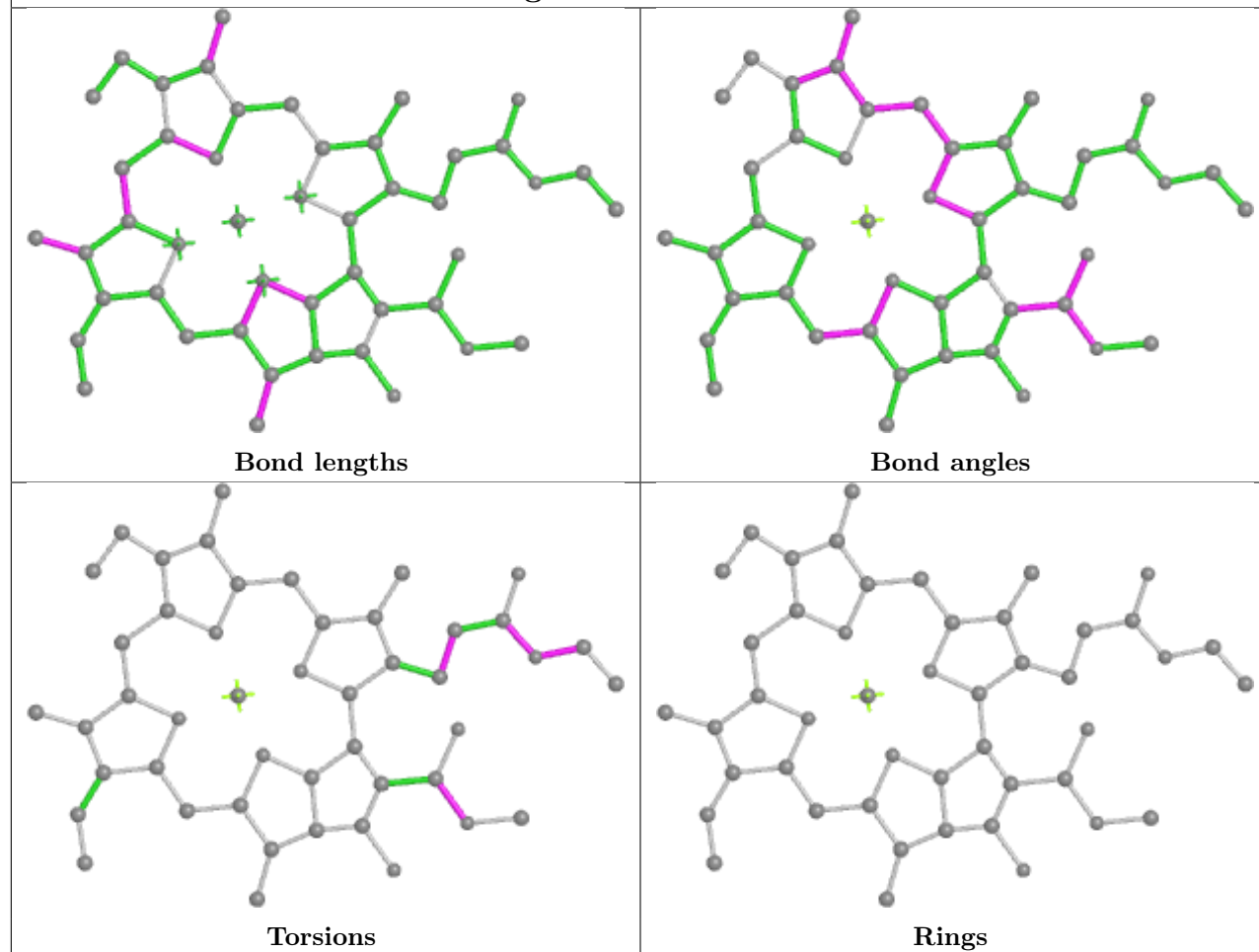


Ligand CLA K 207

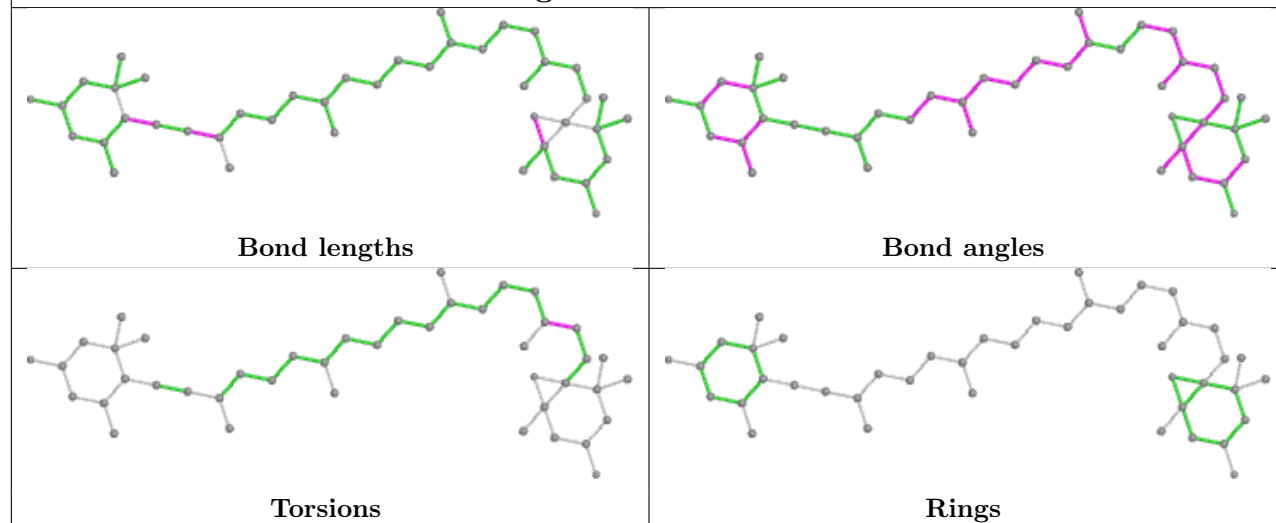




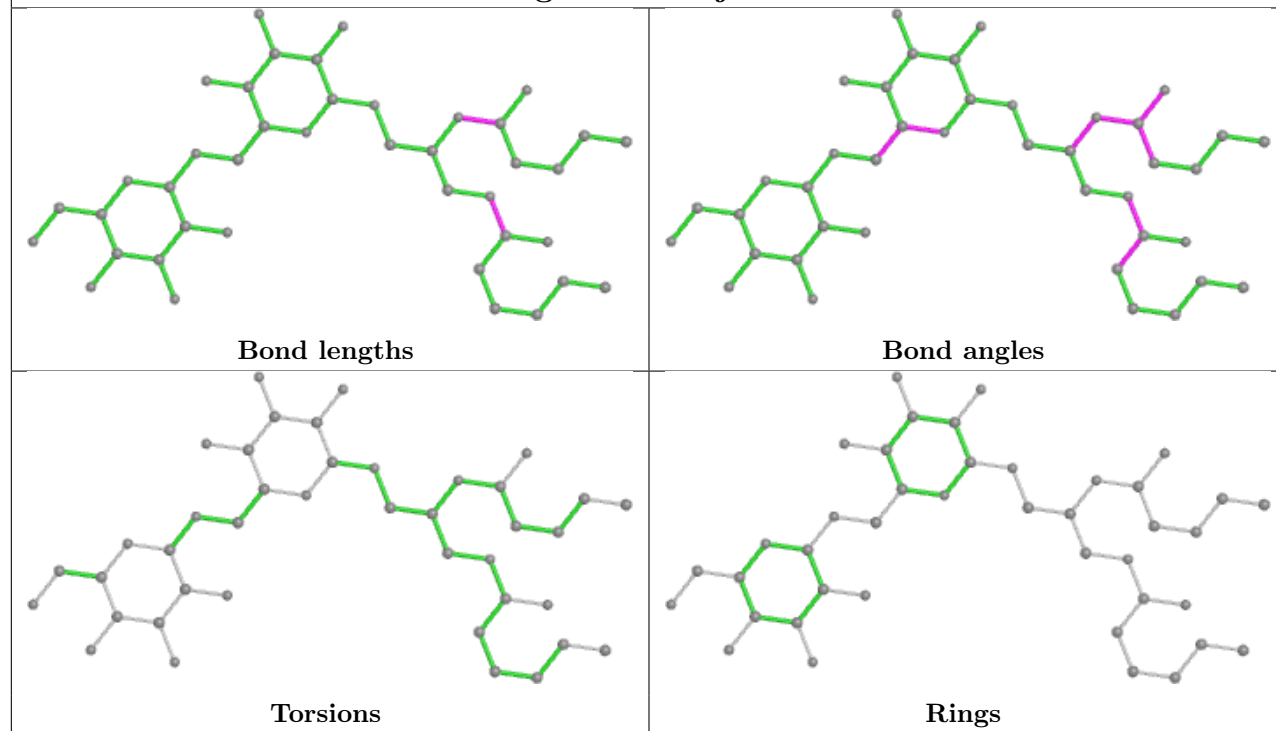
Ligand CLA O 314



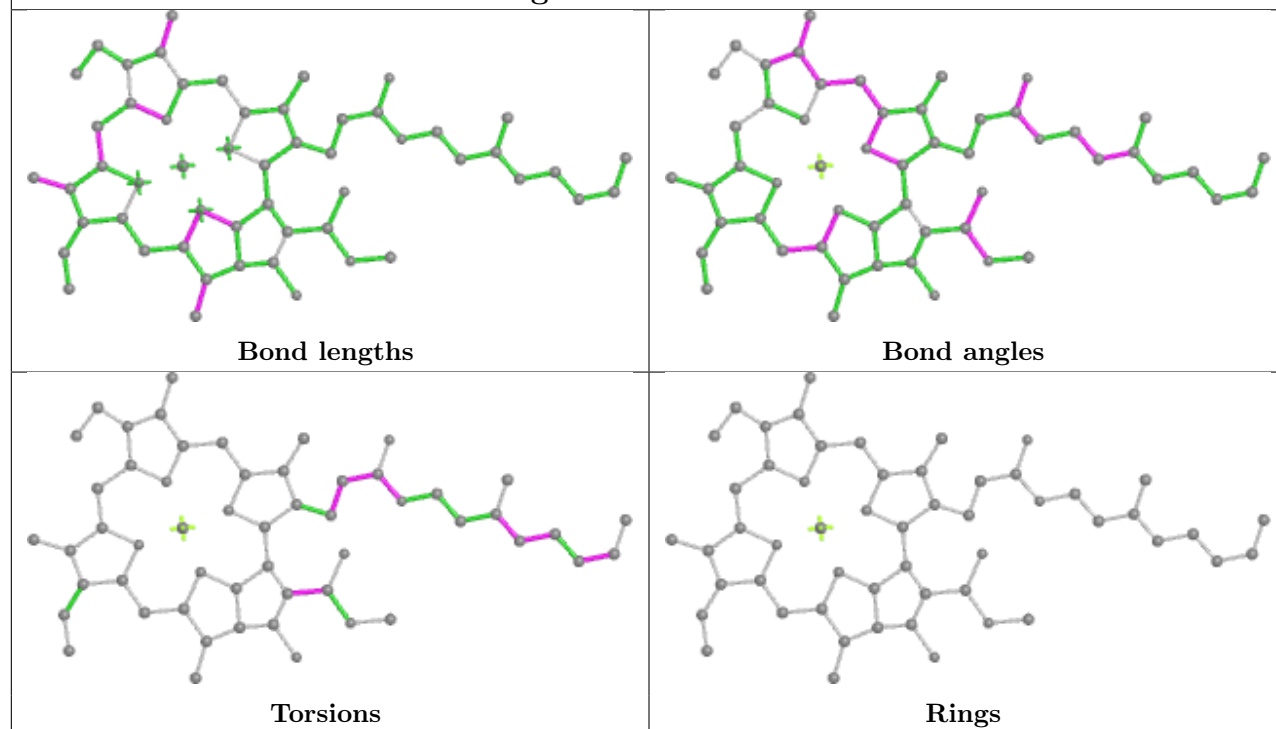
Ligand DD6 L 304



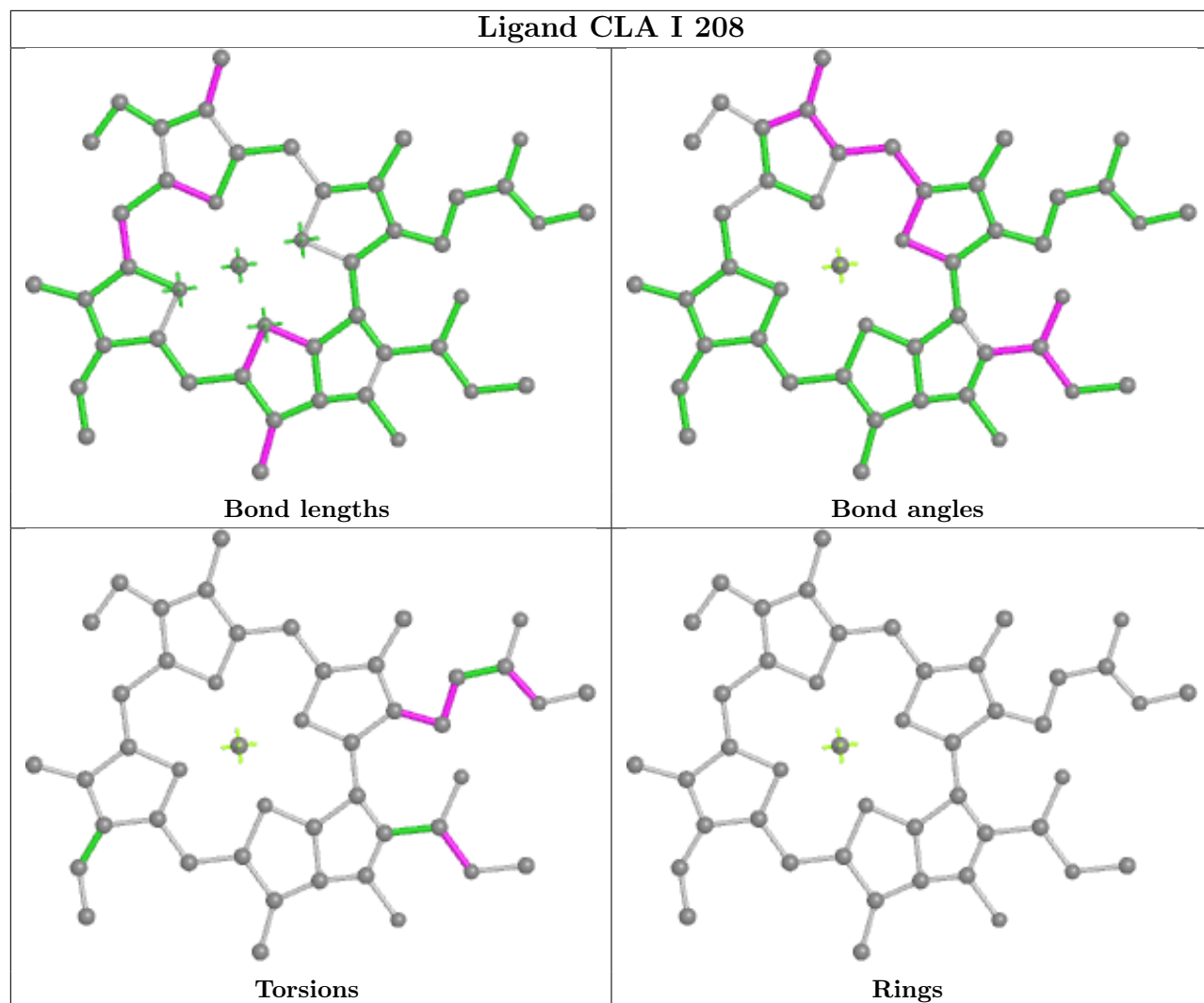
Ligand DGD j 105



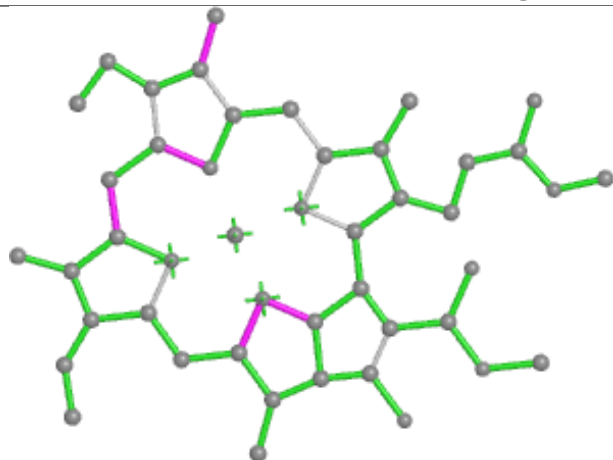
Ligand CLA K 209



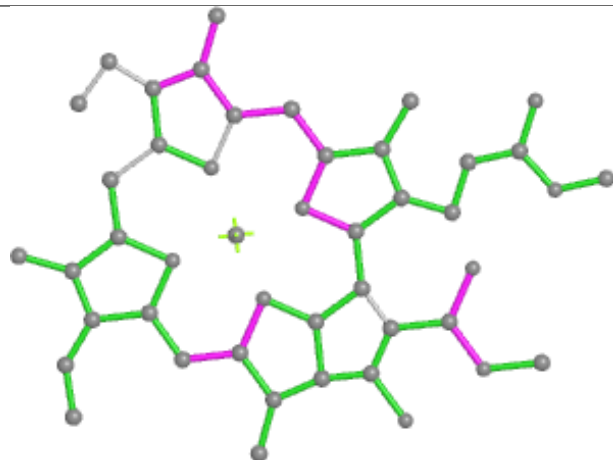
Ligand CLA I 208



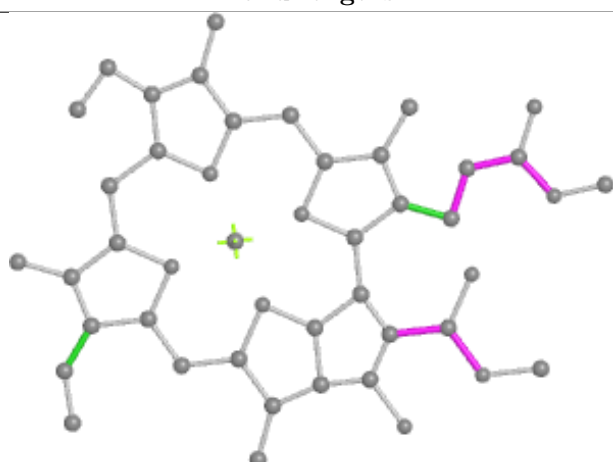
Ligand CLA T 311



Bond lengths



Bond angles

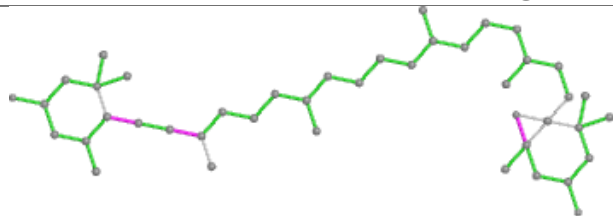


Torsions

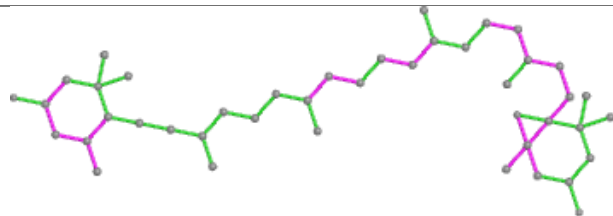


Rings

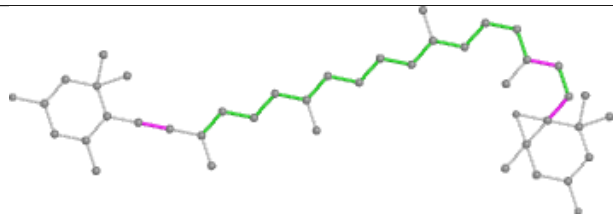
Ligand DD6 L 301



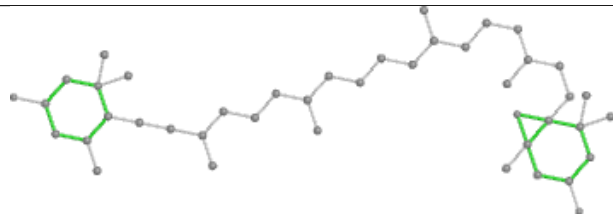
Bond lengths



Bond angles

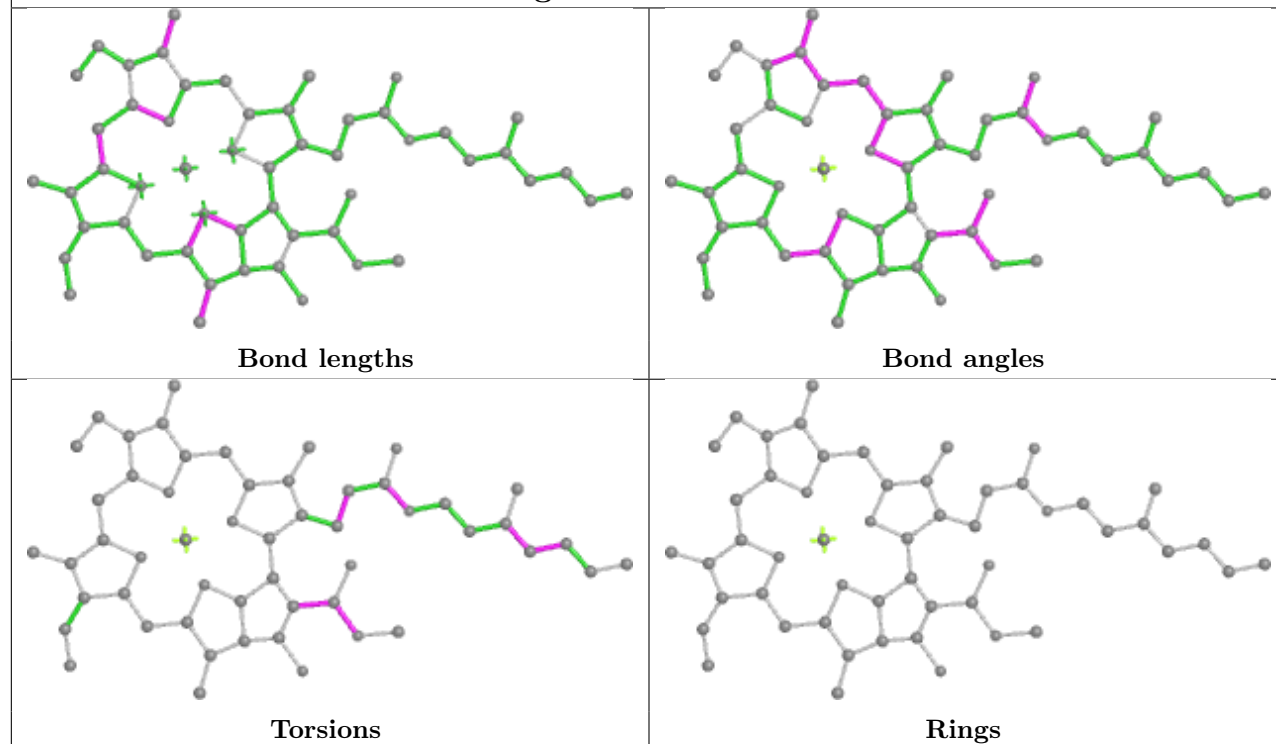


Torsions

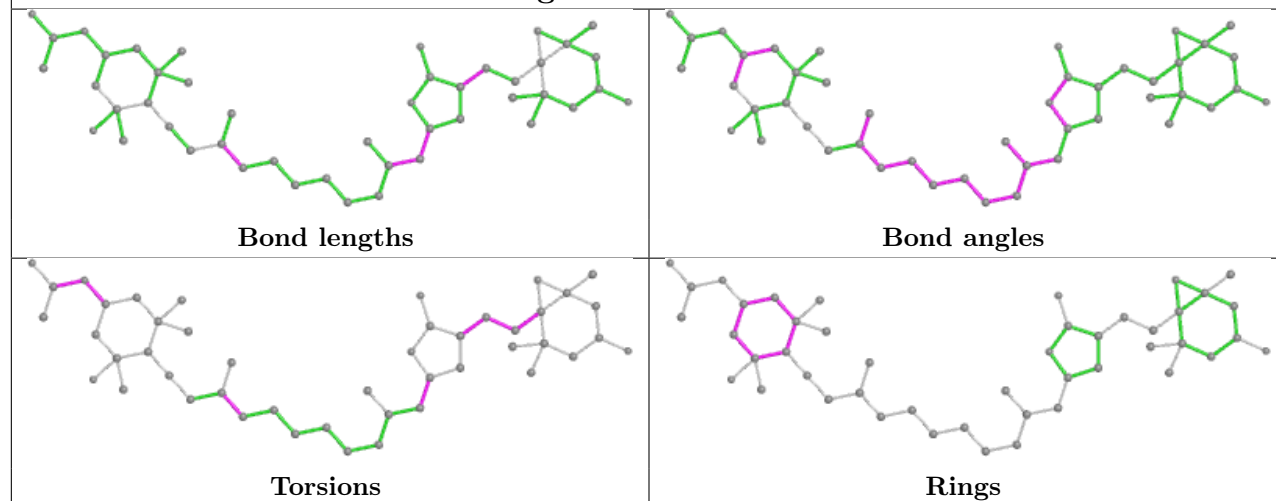


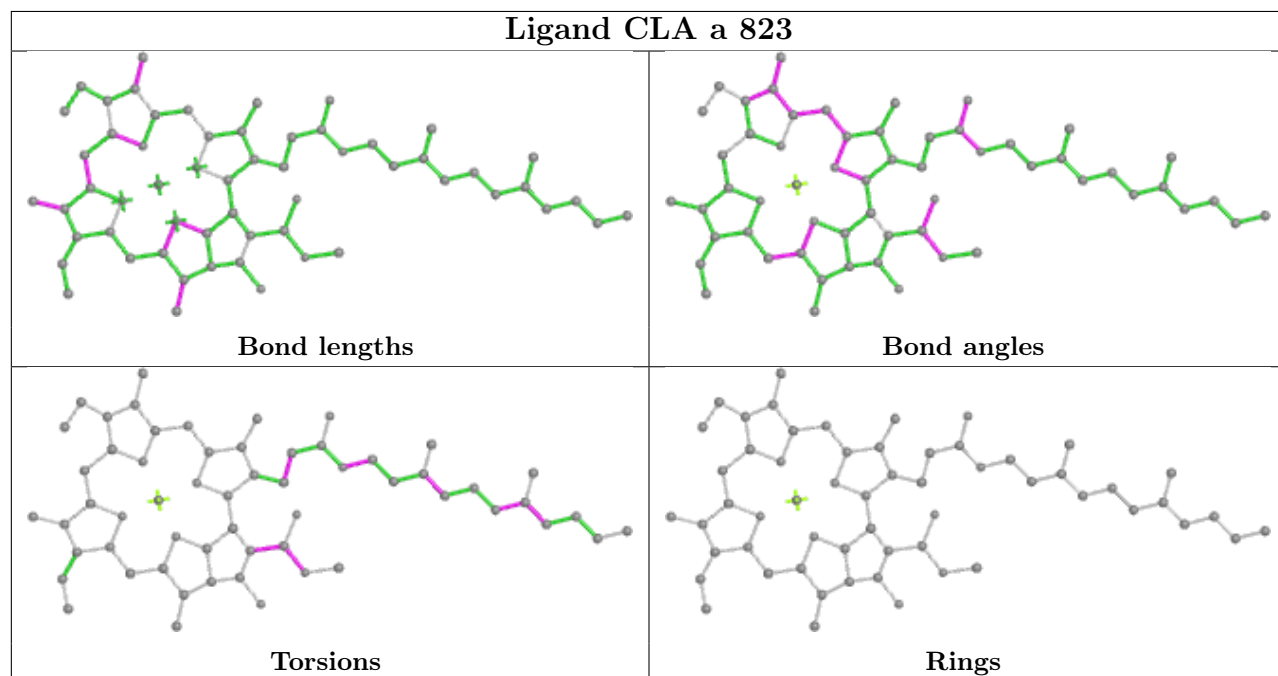
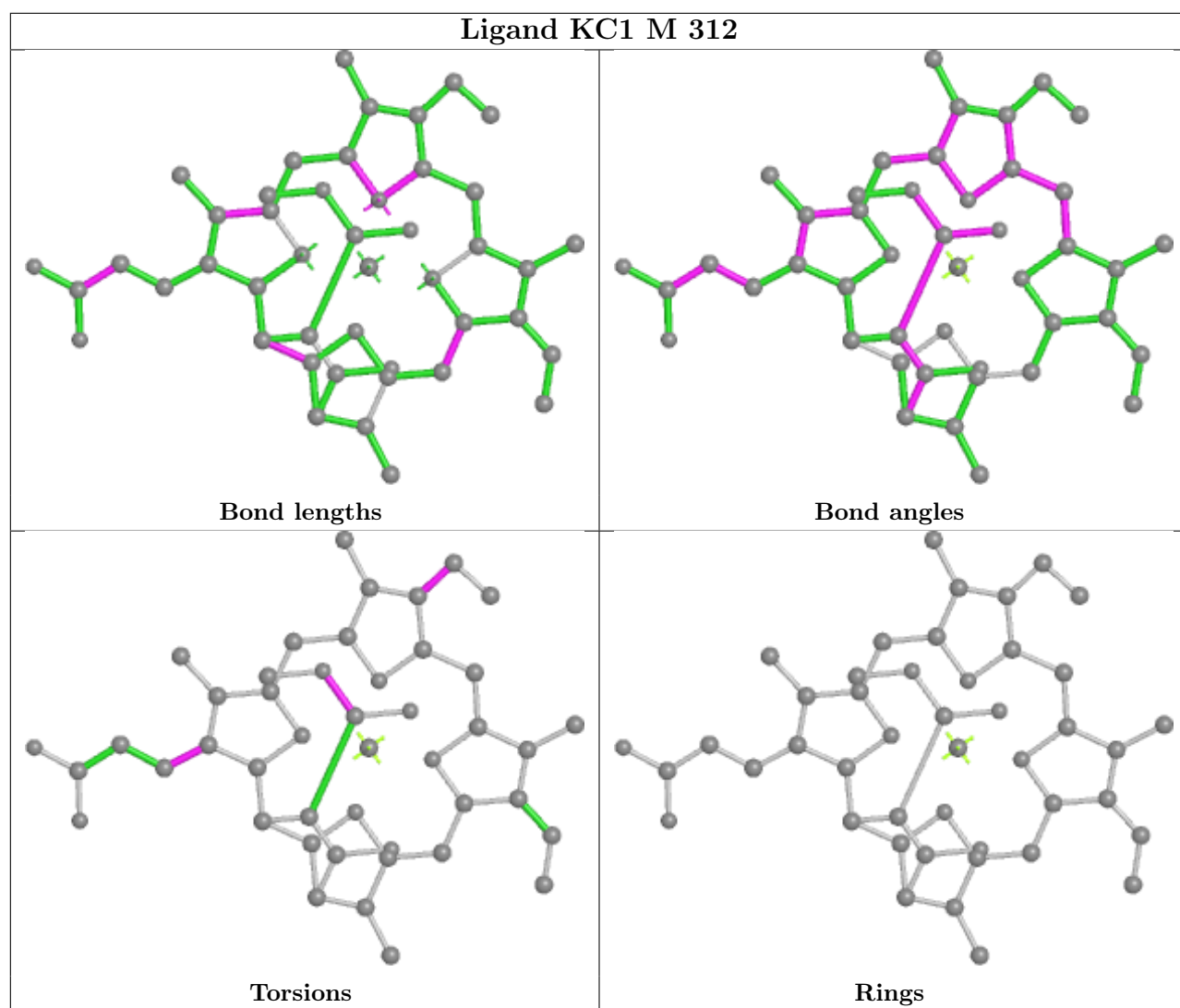
Rings

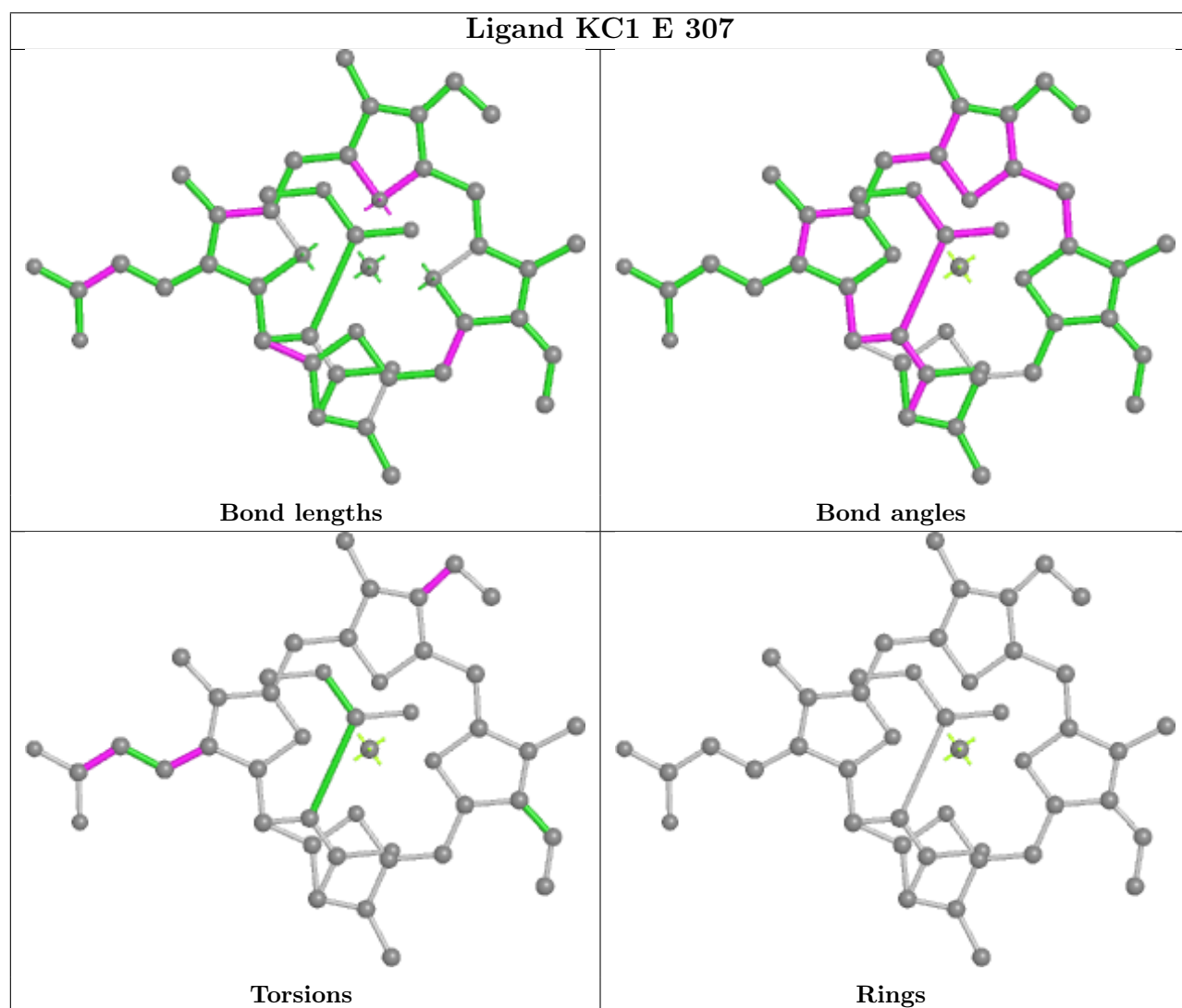
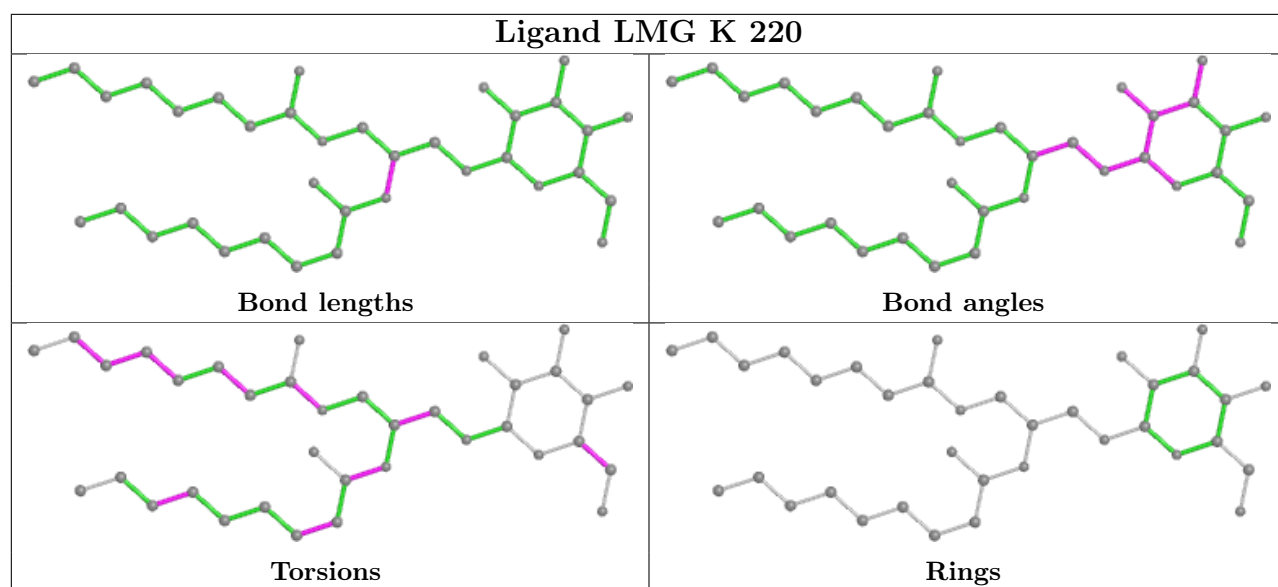
Ligand CLA L 308

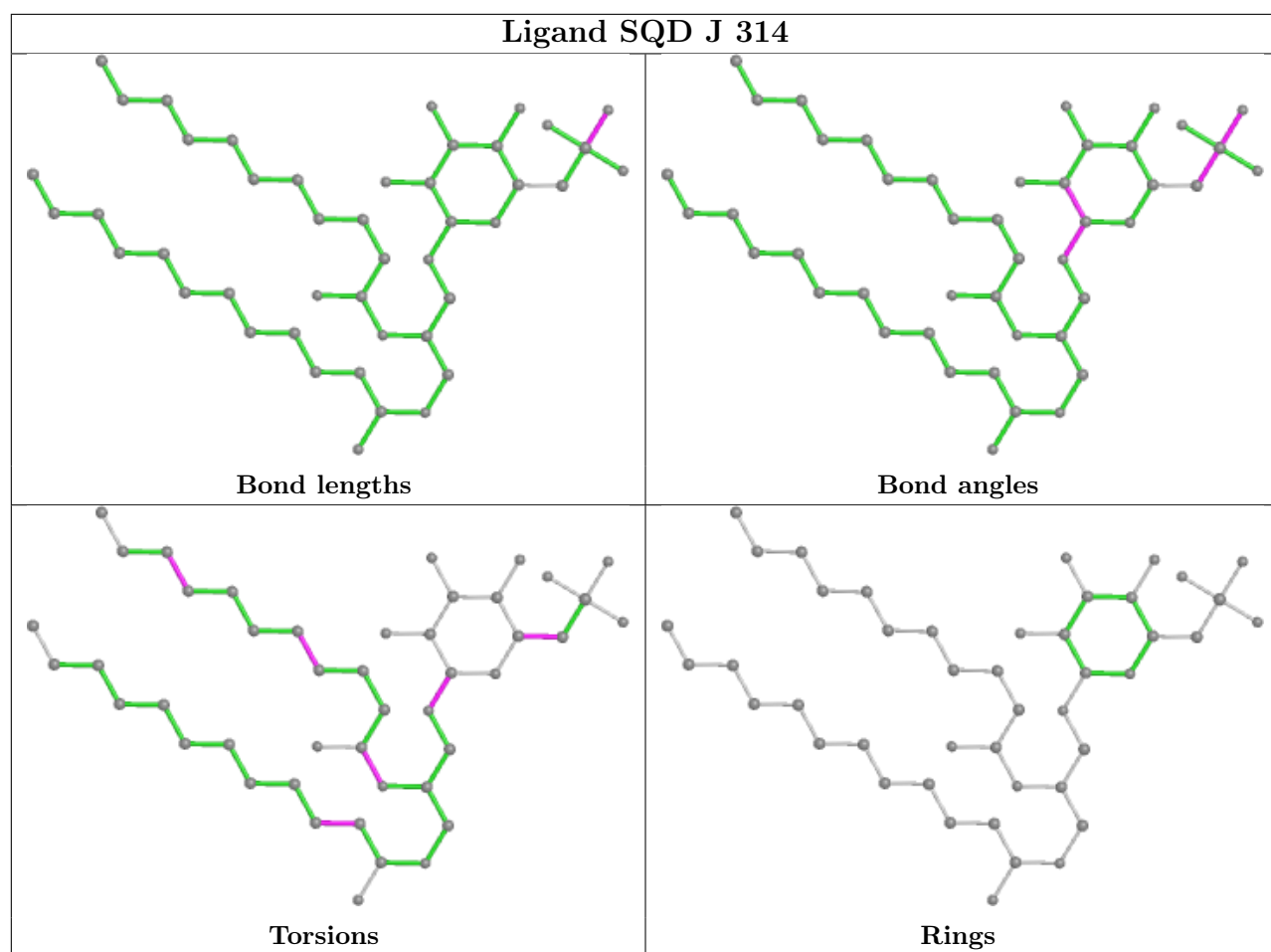


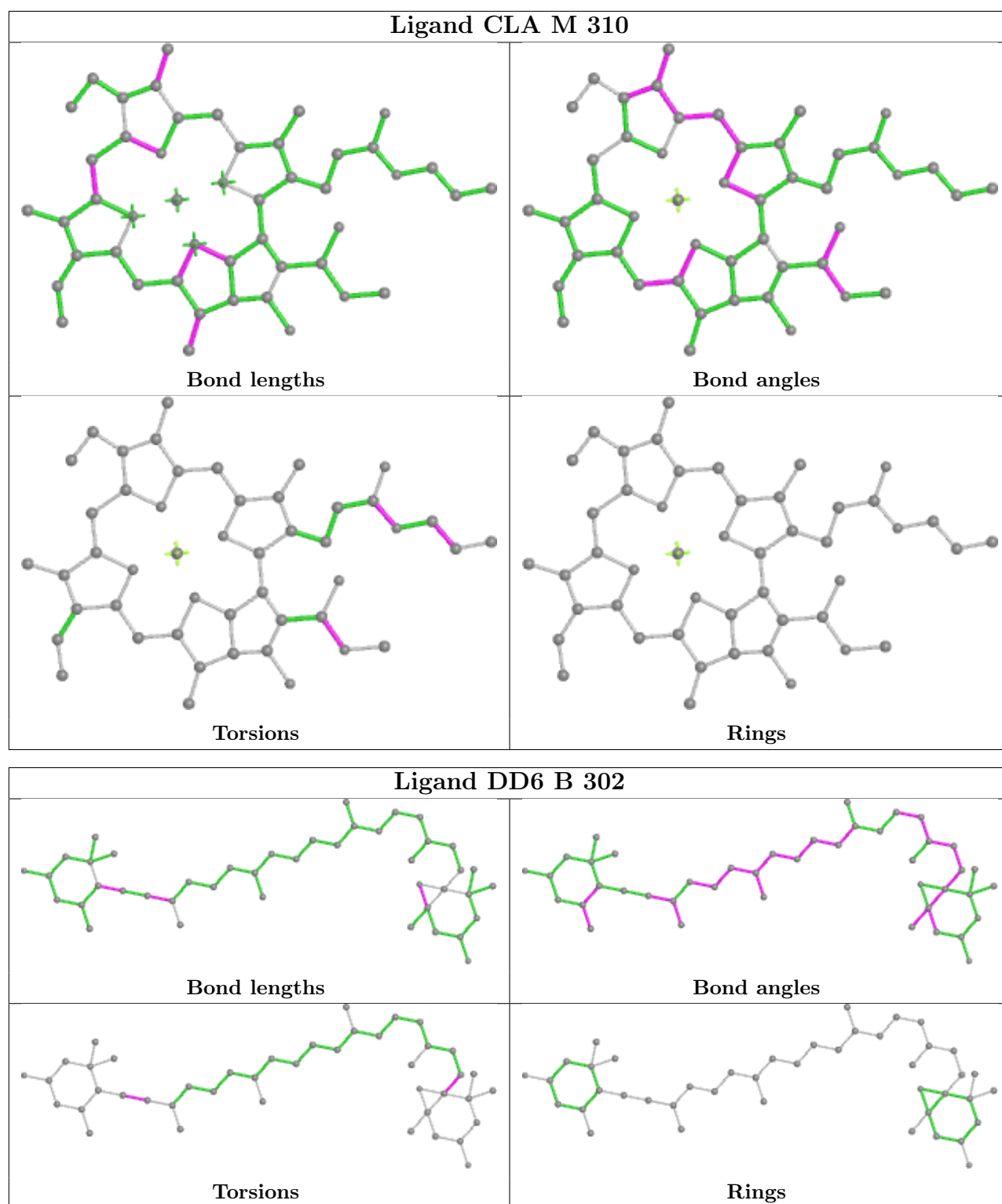
Ligand PID T 317



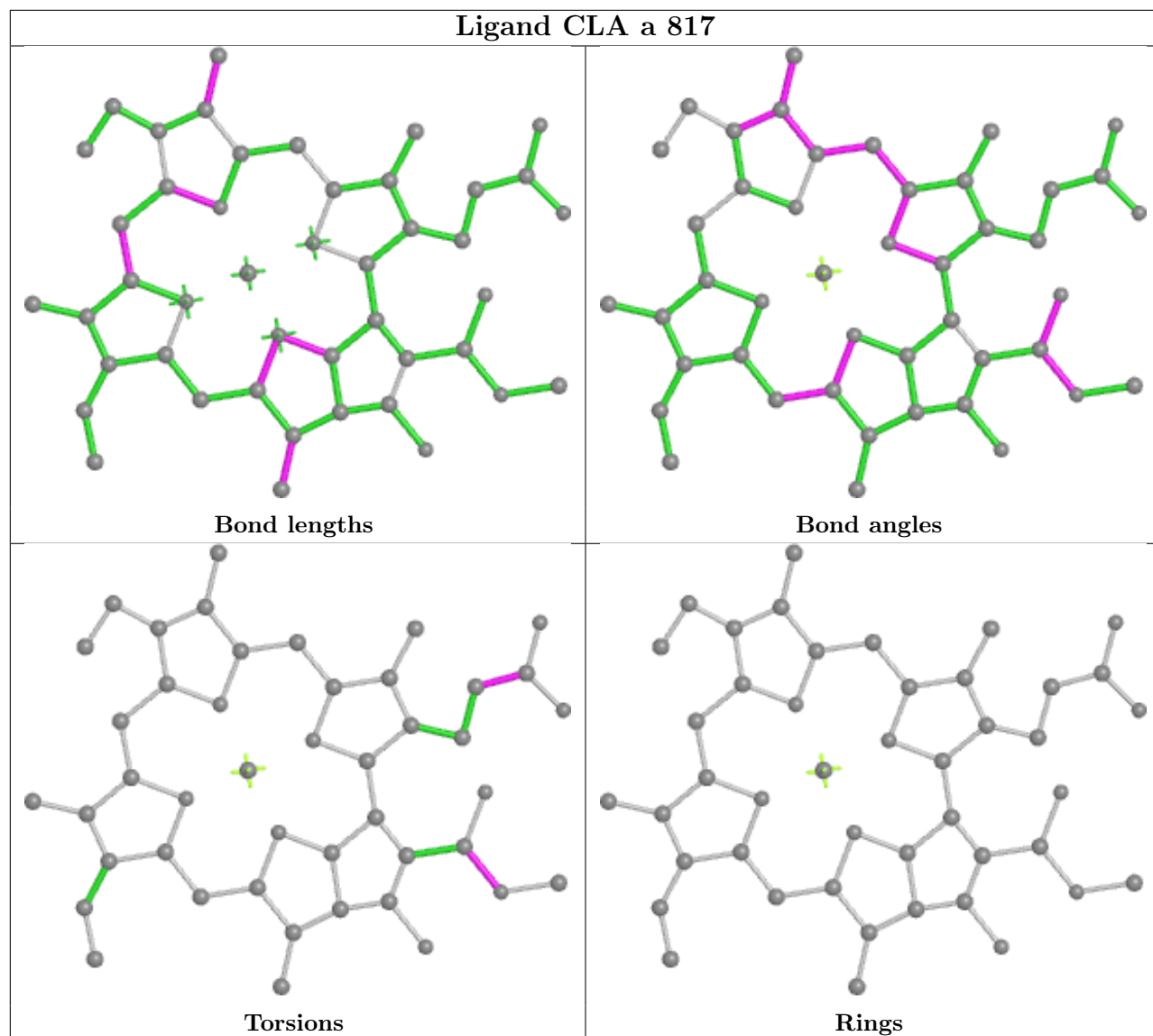




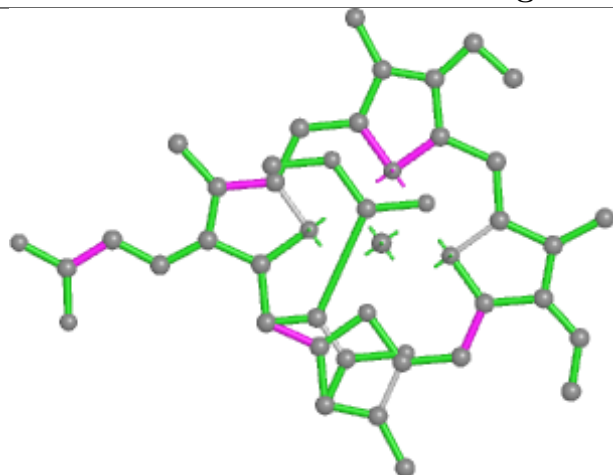




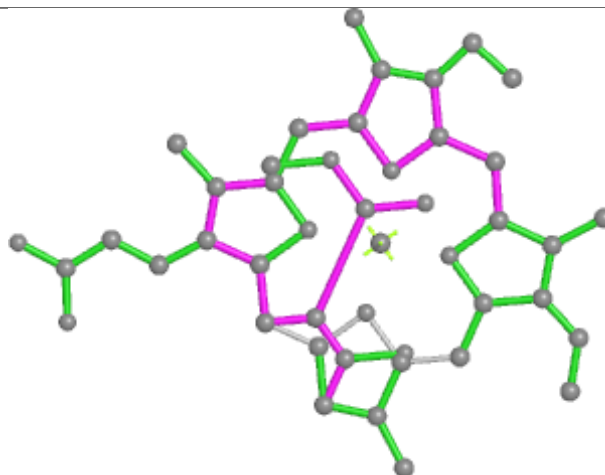
Ligand CLA a 817



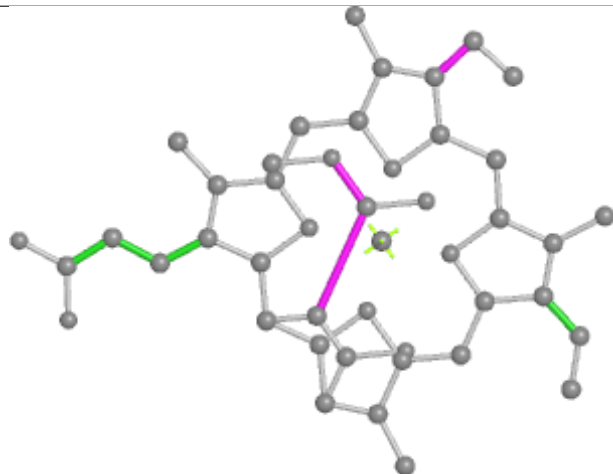
Ligand KC1 P 213



Bond lengths



Bond angles

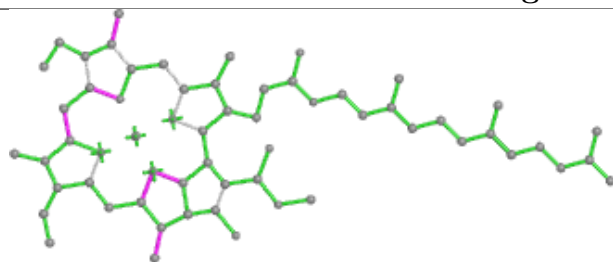


Torsions

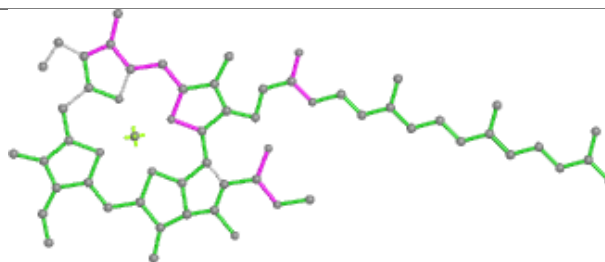


Rings

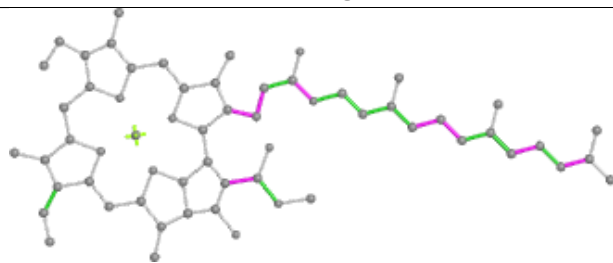
Ligand CLA f 805



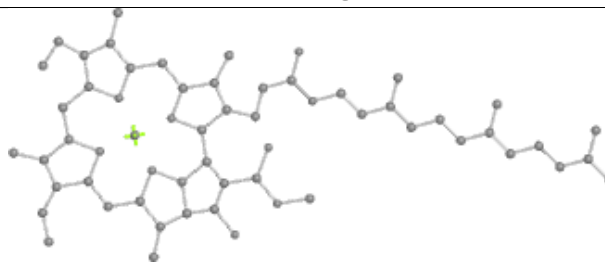
Bond lengths



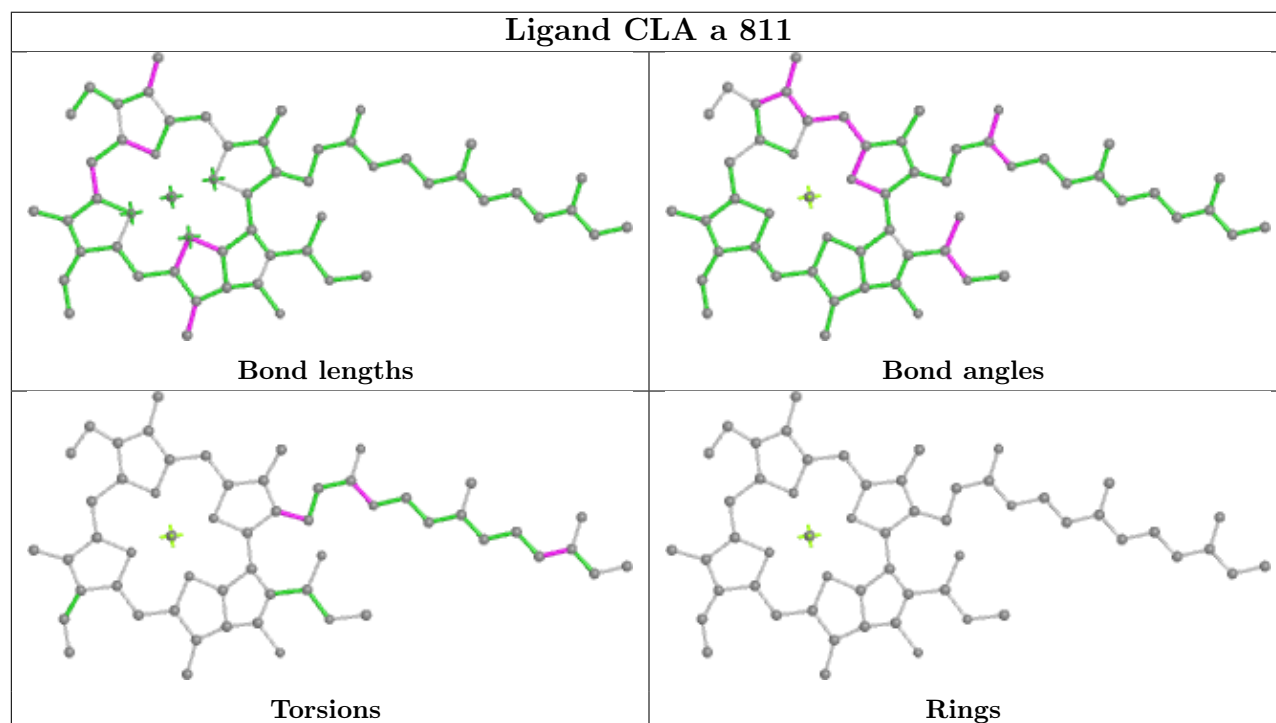
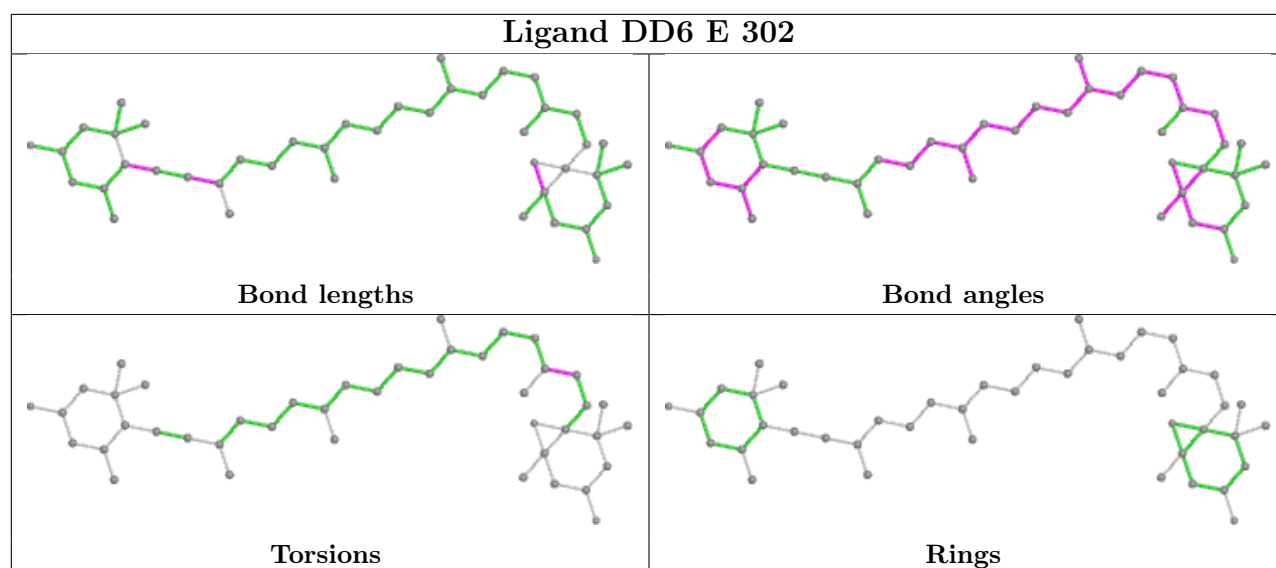
Bond angles



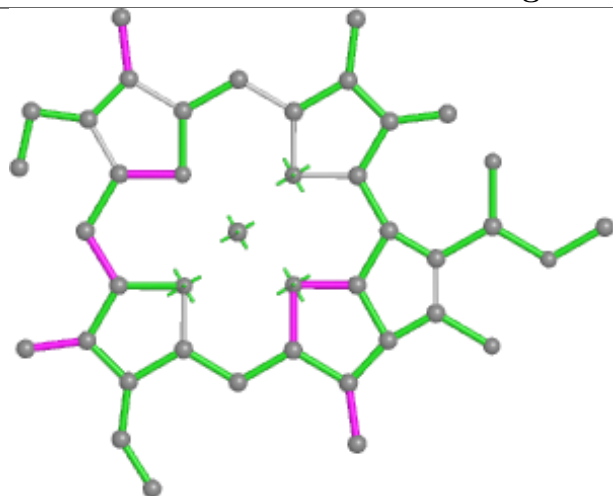
Torsions



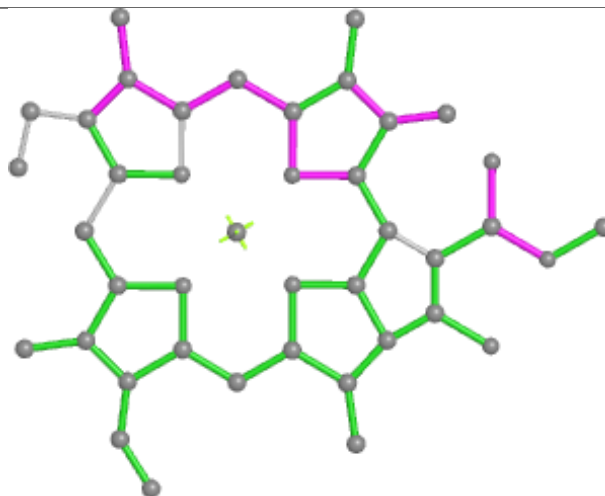
Rings



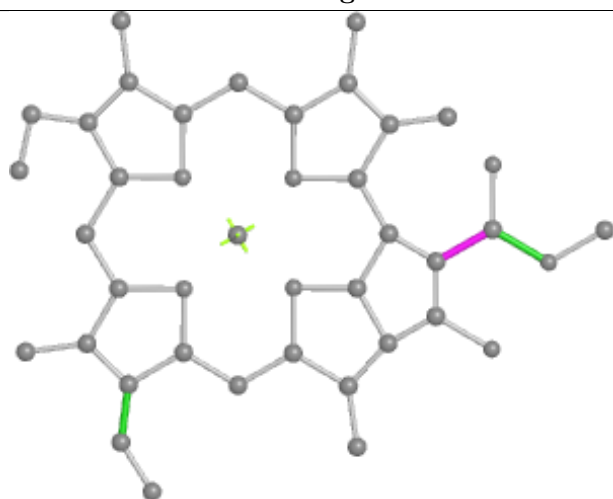
Ligand CLA 1 508



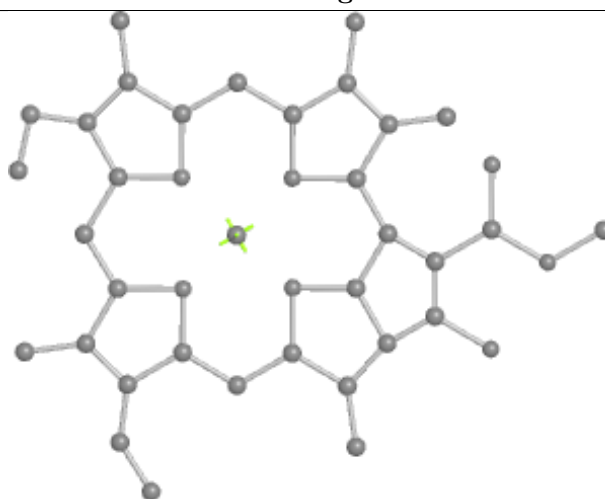
Bond lengths



Bond angles

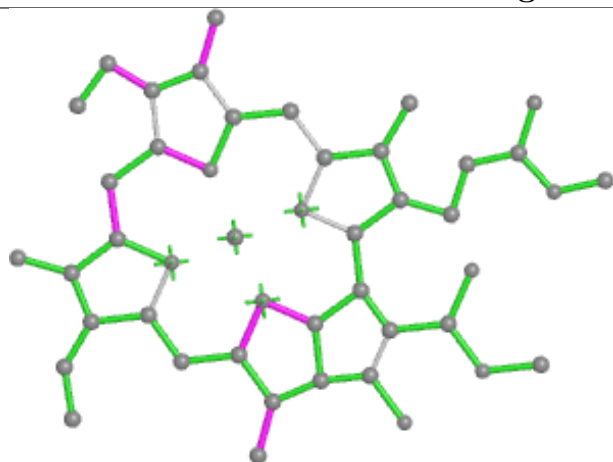


Torsions

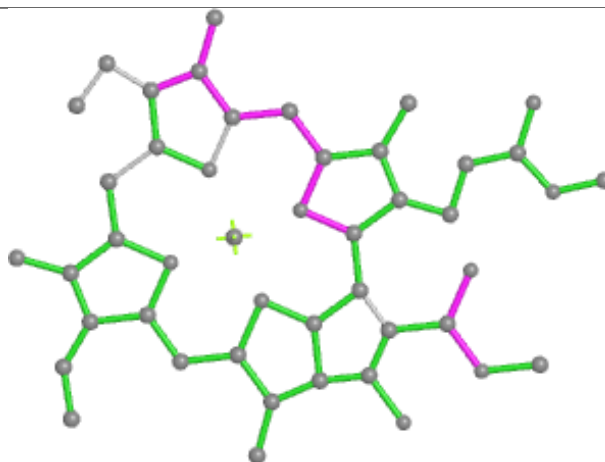


Rings

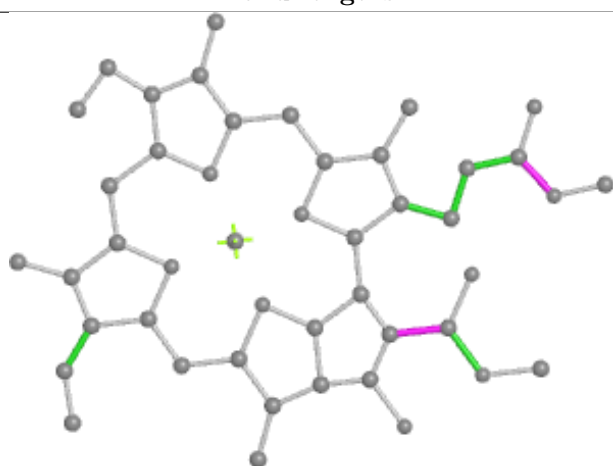
Ligand CLA J 307



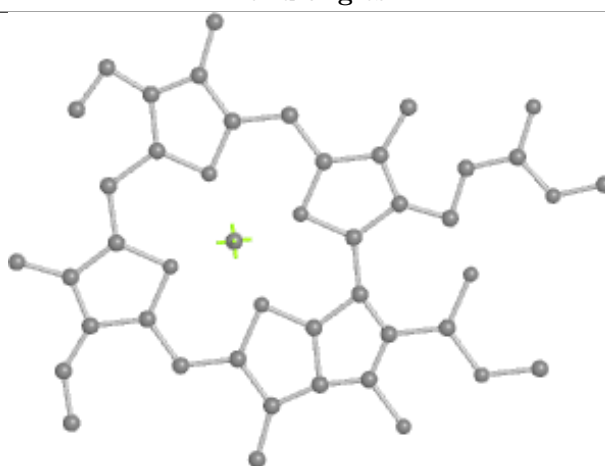
Bond lengths



Bond angles

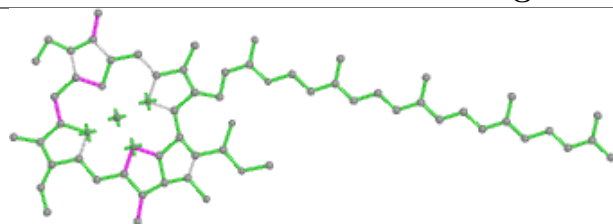


Torsions

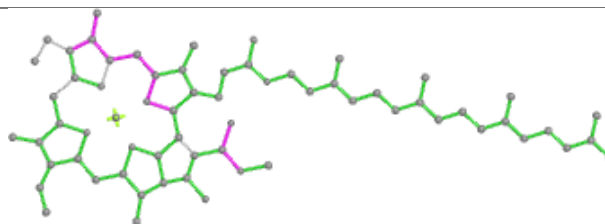


Rings

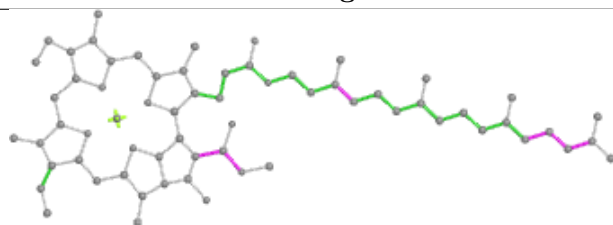
Ligand CLA O 309



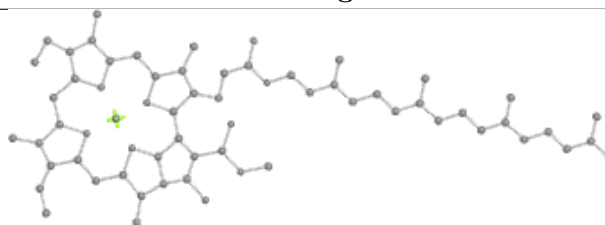
Bond lengths



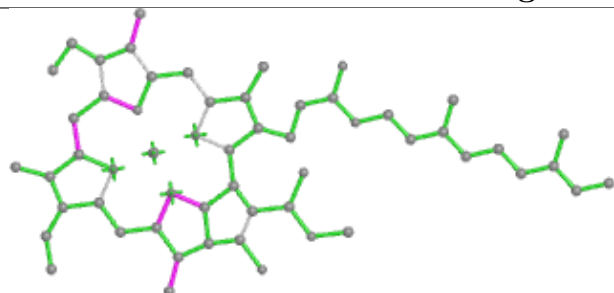
Bond angles



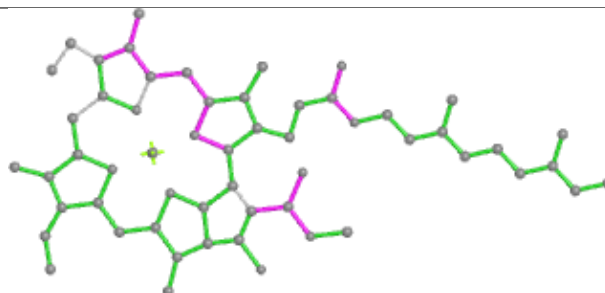
Torsions



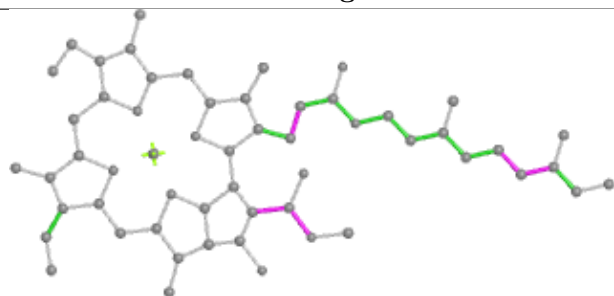
Rings

Ligand CLA J 308

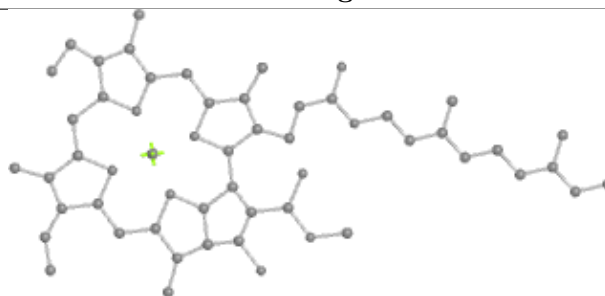
Bond lengths



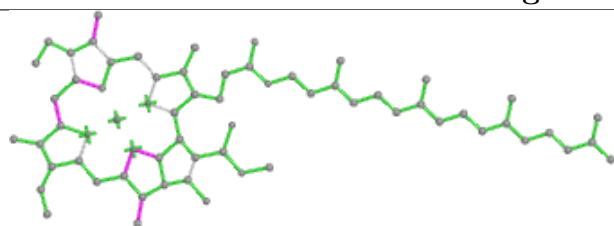
Bond angles



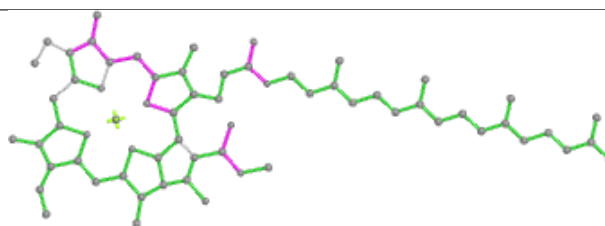
Torsions



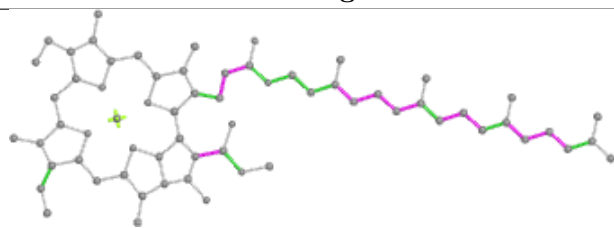
Rings

Ligand CLA i 201

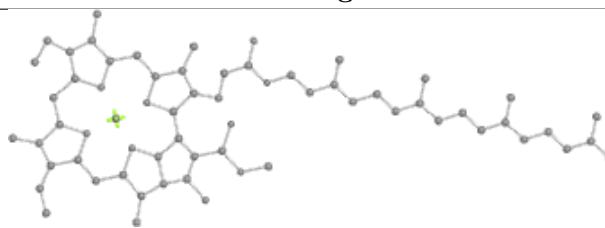
Bond lengths



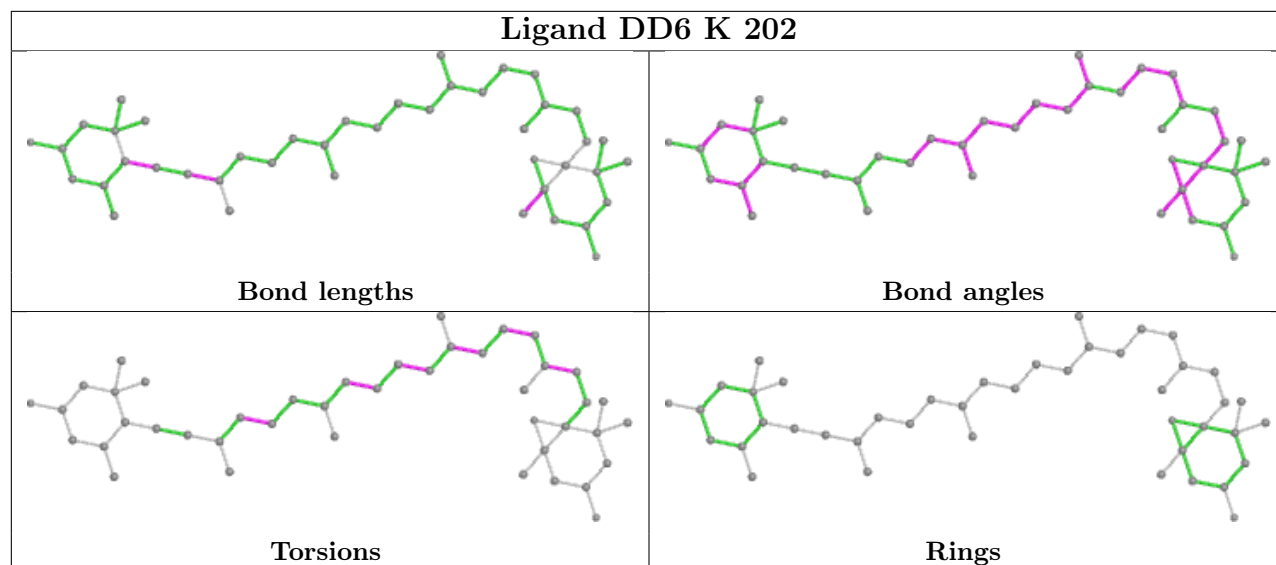
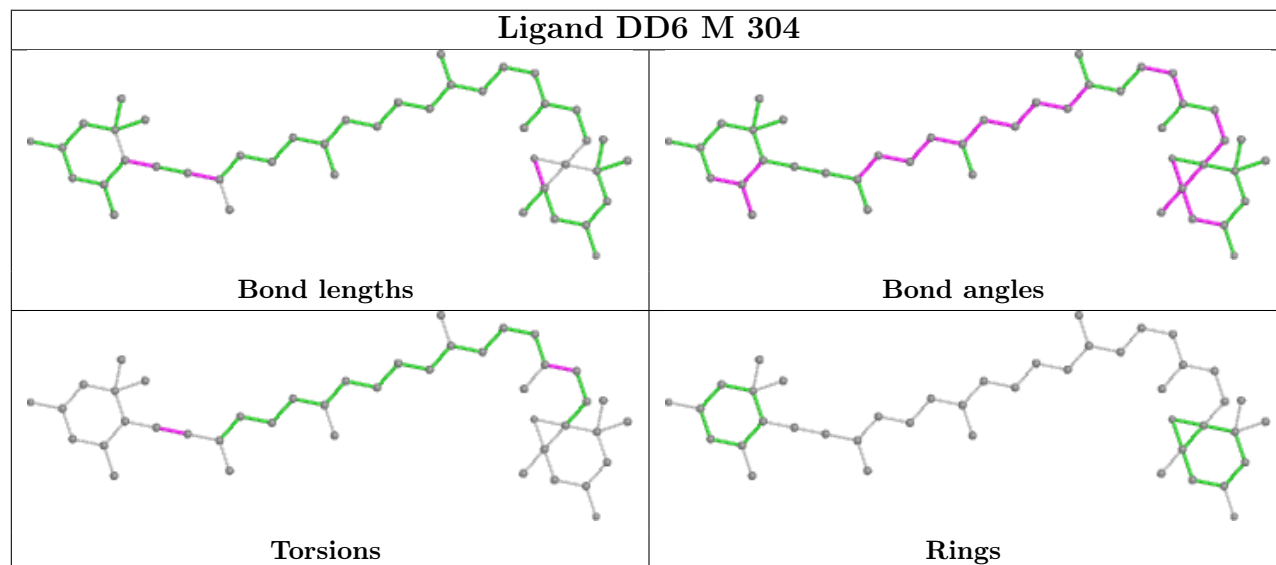
Bond angles



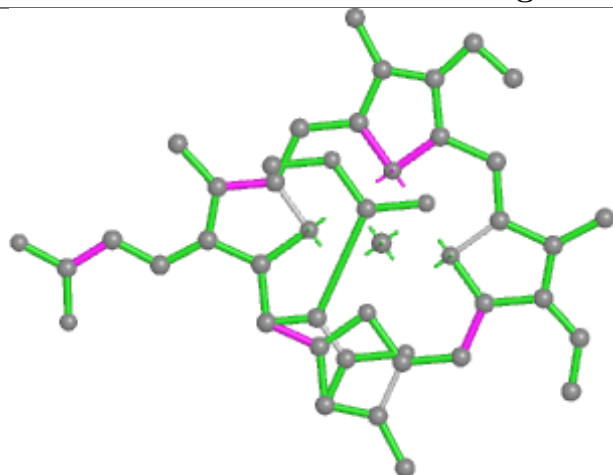
Torsions



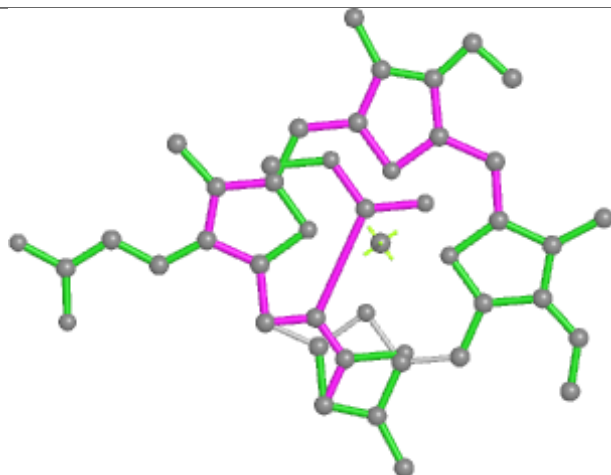
Rings

Ligand DD6 K 202**Ligand DD6 M 304**

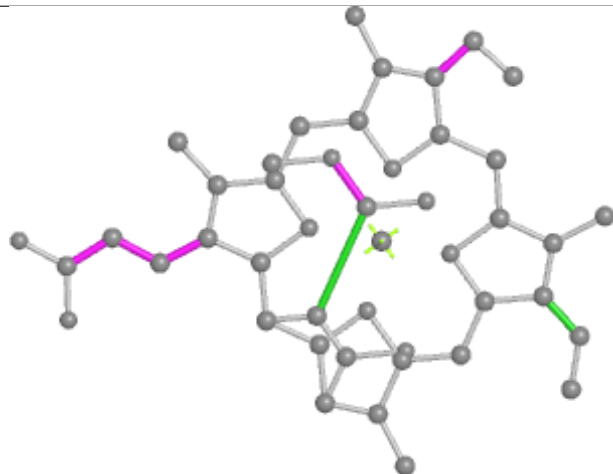
Ligand KC1 B 313



Bond lengths



Bond angles

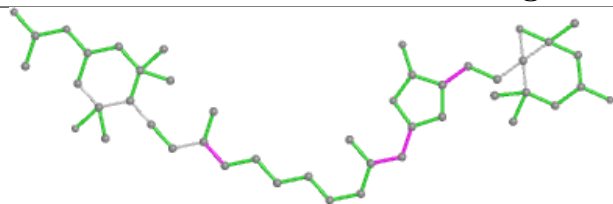


Torsions

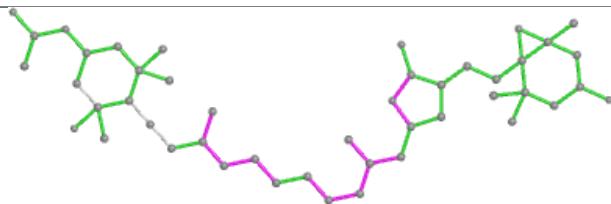


Rings

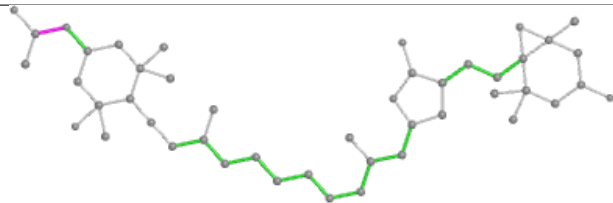
Ligand PID h 204



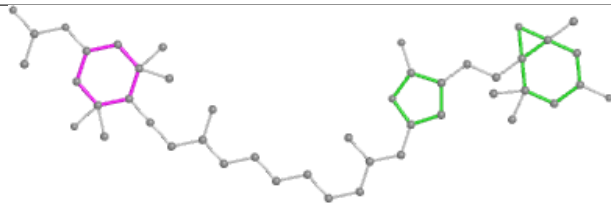
Bond lengths



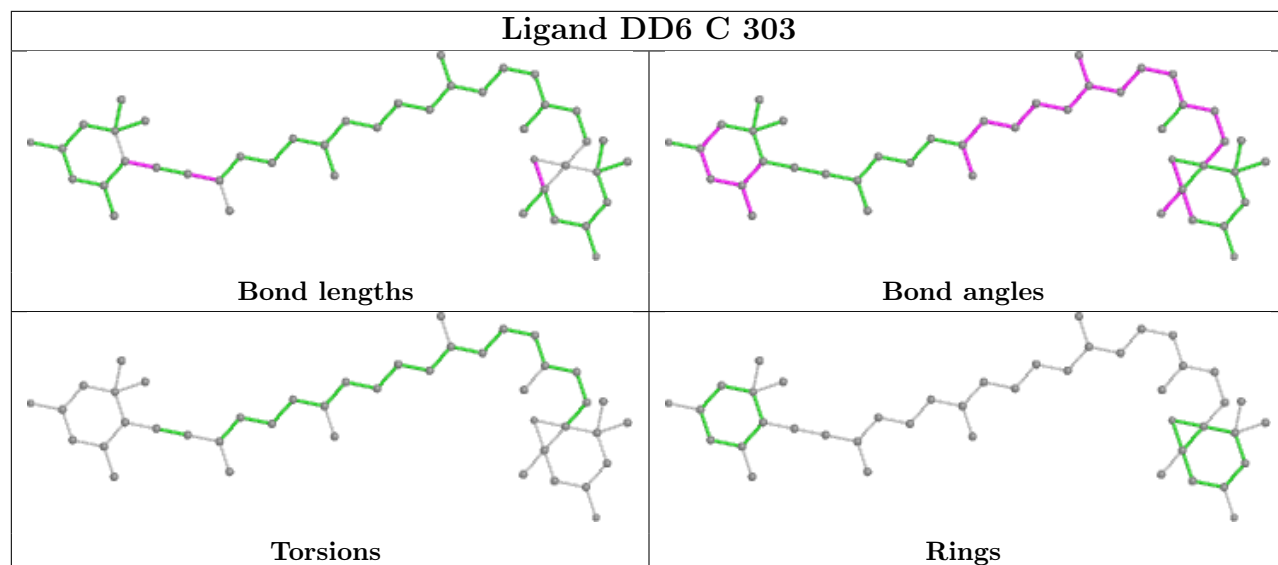
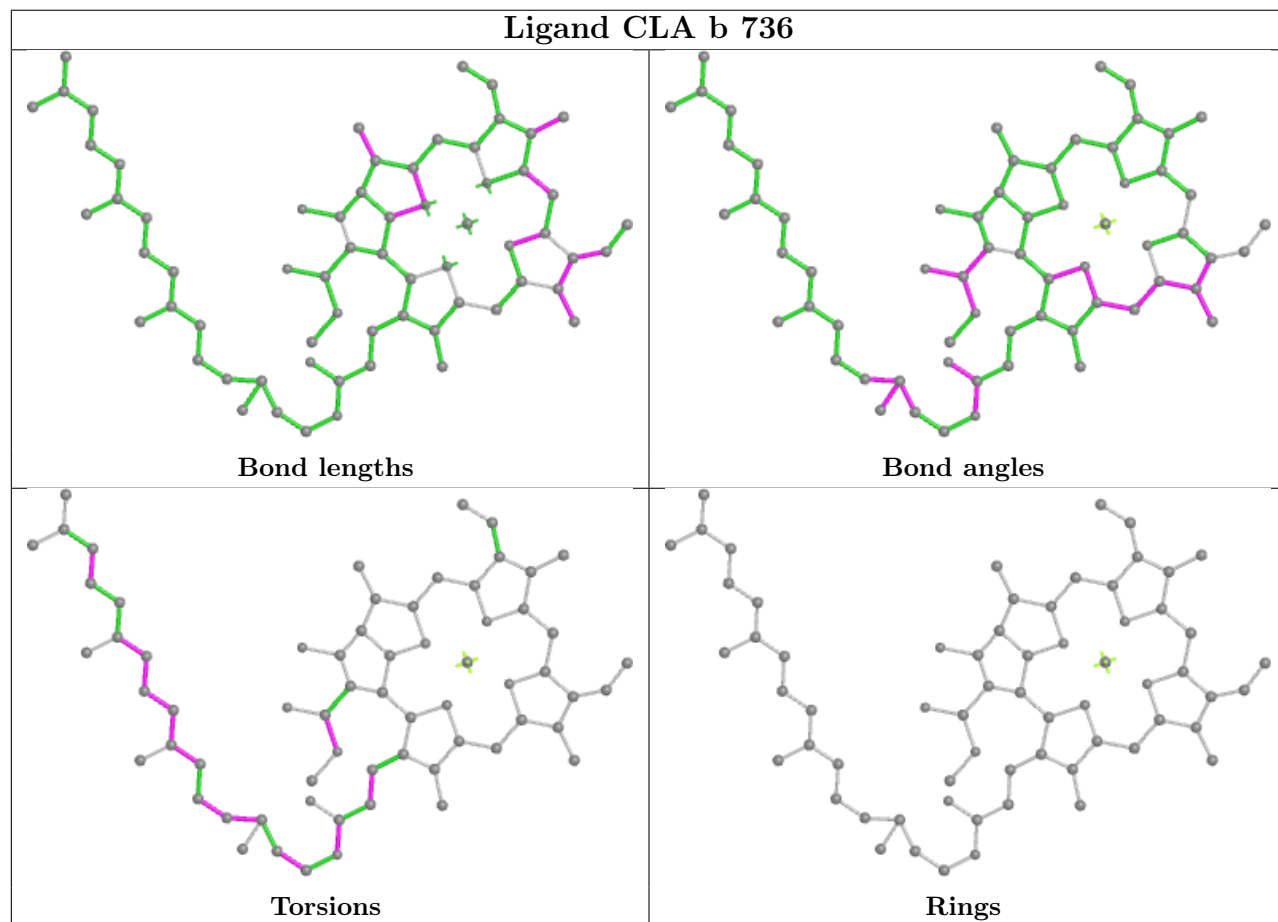
Bond angles



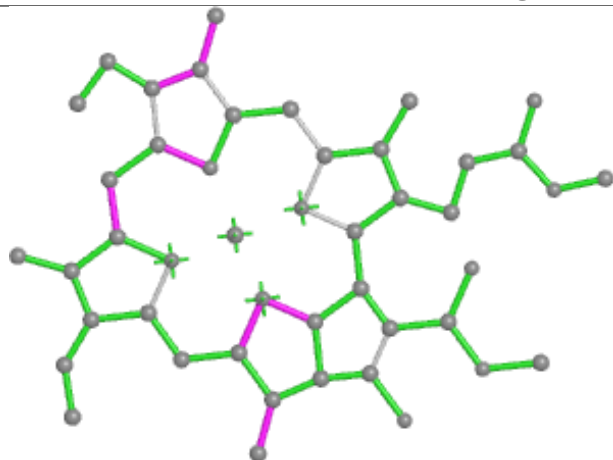
Torsions



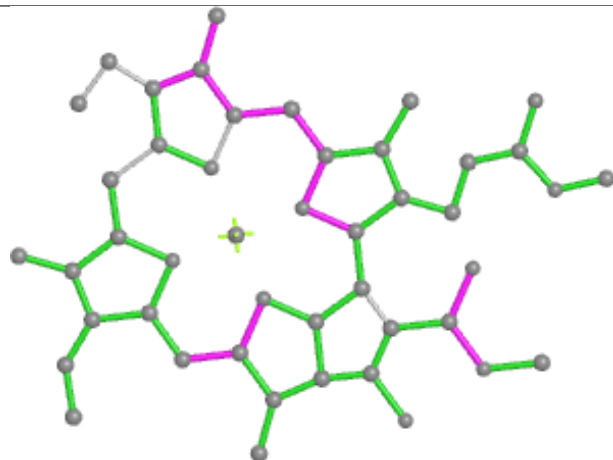
Rings

Ligand DD6 C 303**Ligand CLA b 736**

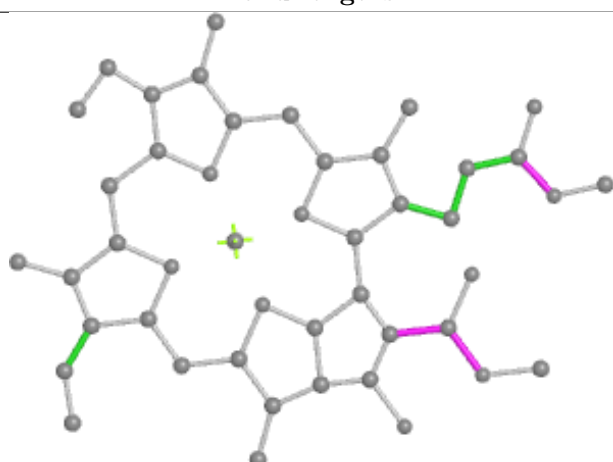
Ligand CLA A 210



Bond lengths



Bond angles

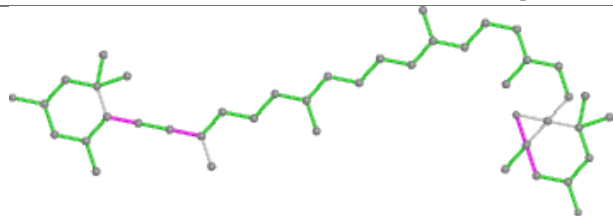


Torsions

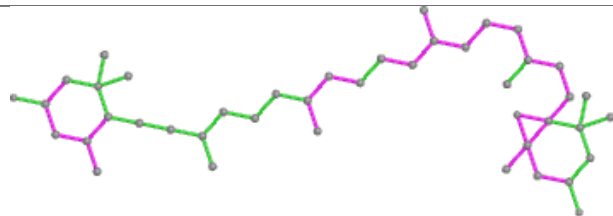


Rings

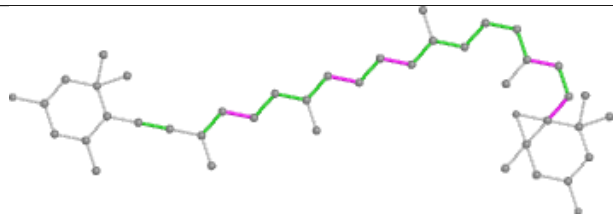
Ligand DD6 D 304



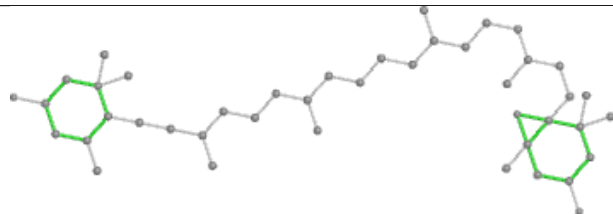
Bond lengths



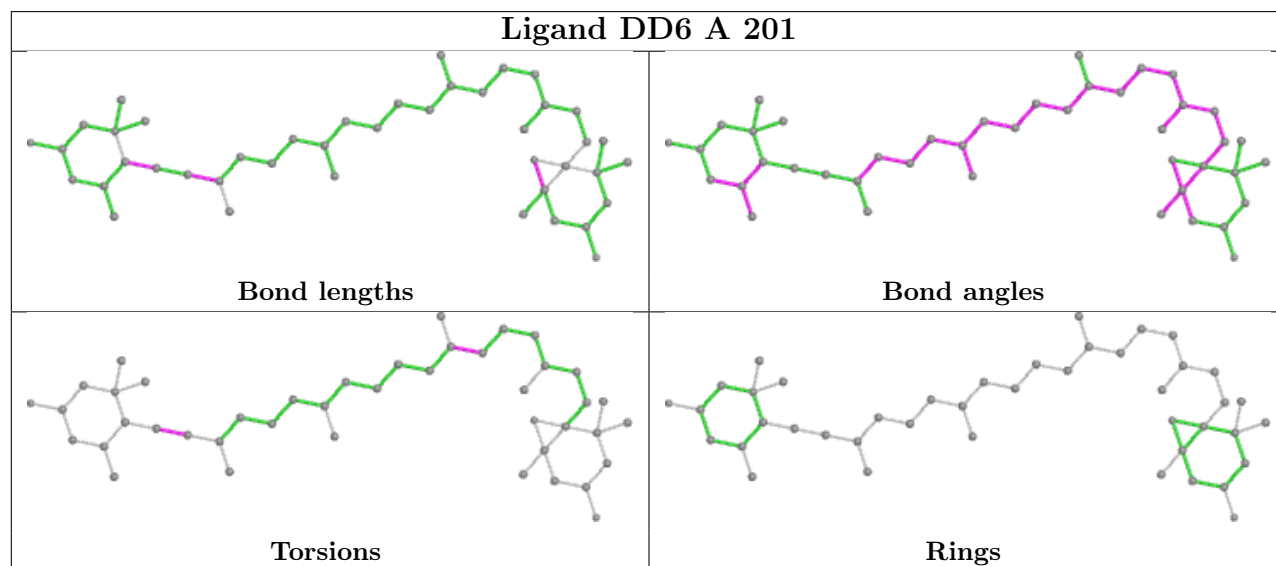
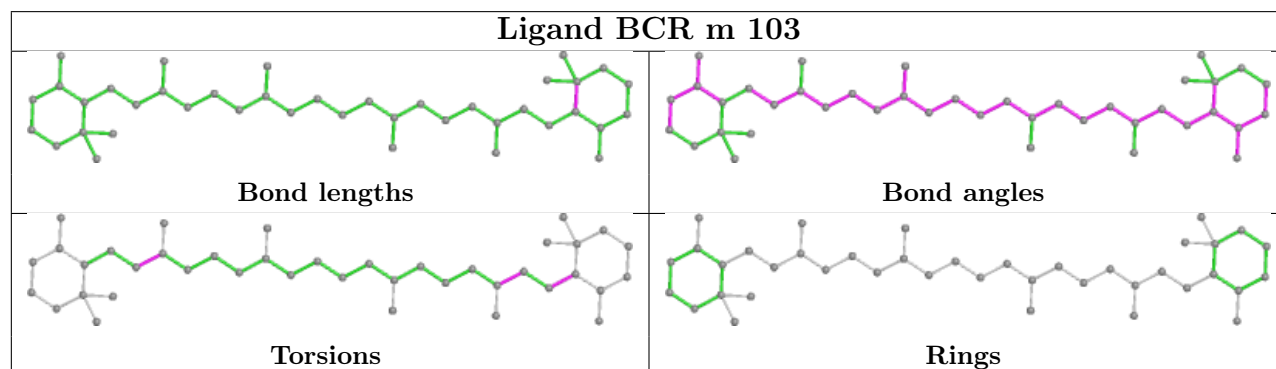
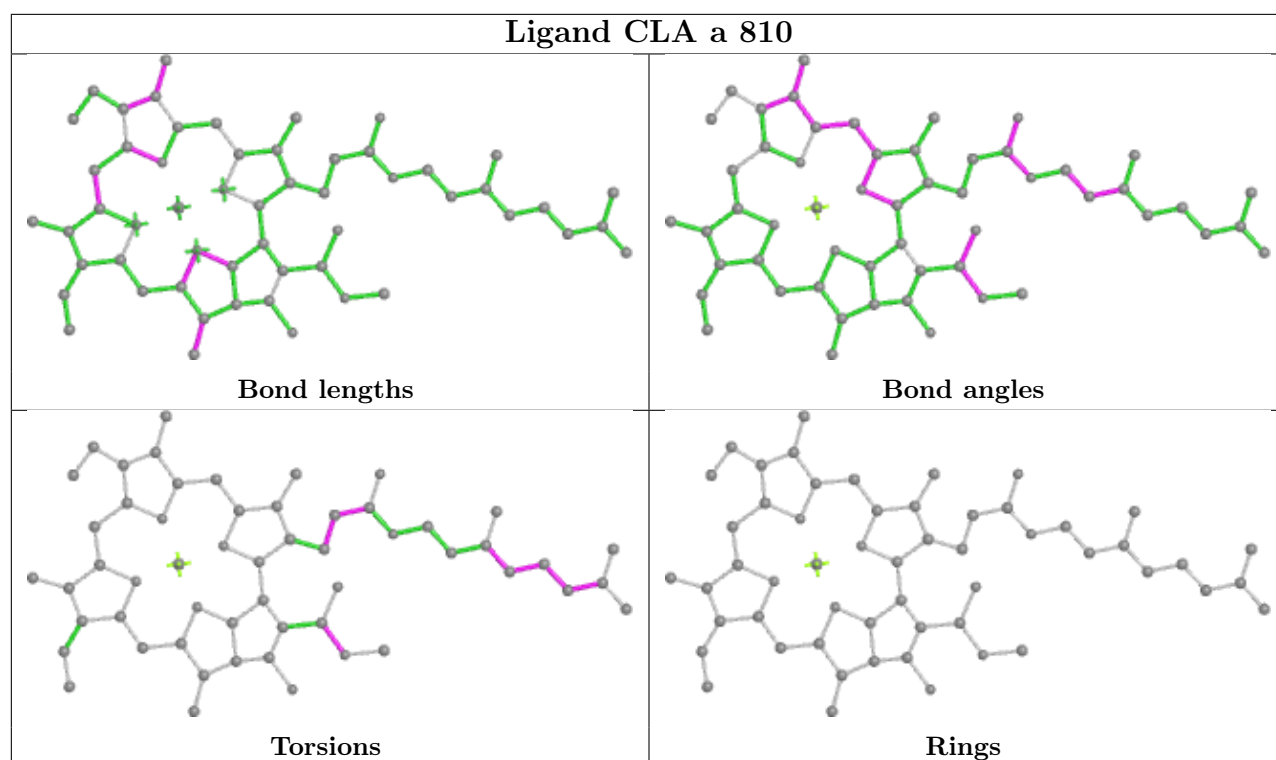
Bond angles



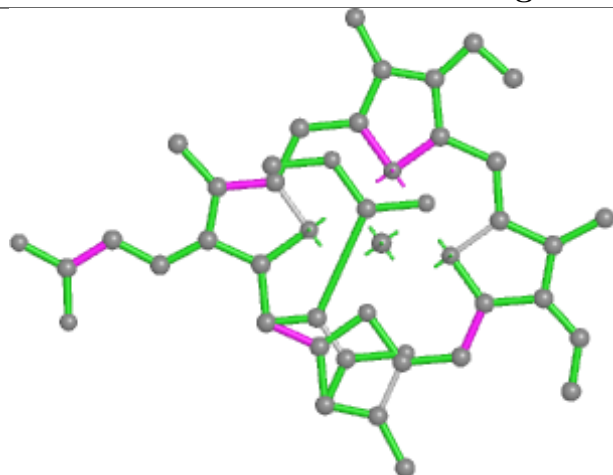
Torsions



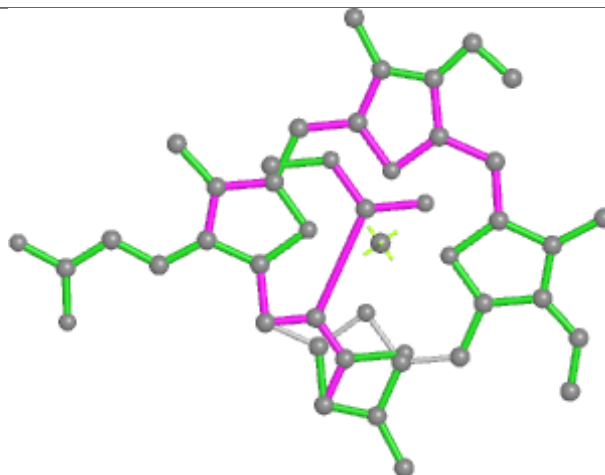
Rings



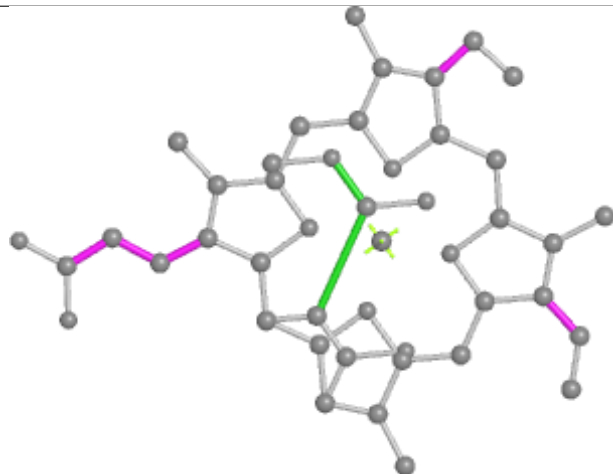
Ligand KC1 A 213



Bond lengths



Bond angles

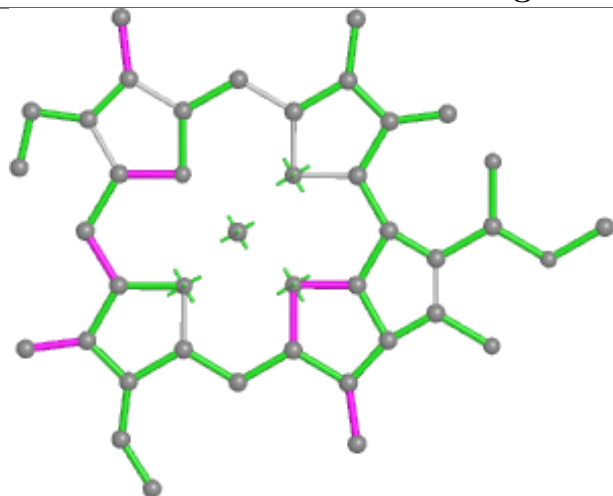


Torsions

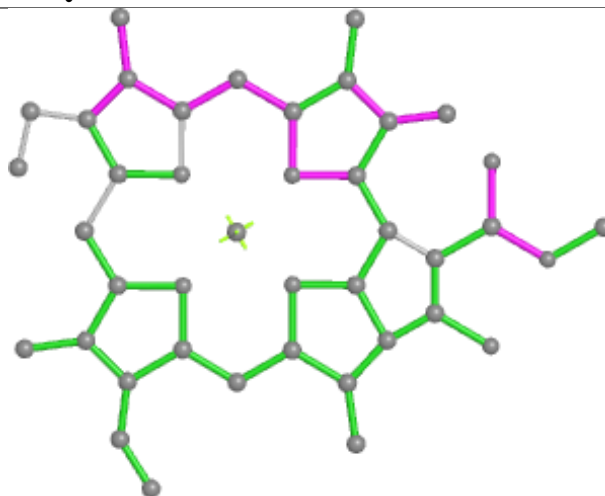


Rings

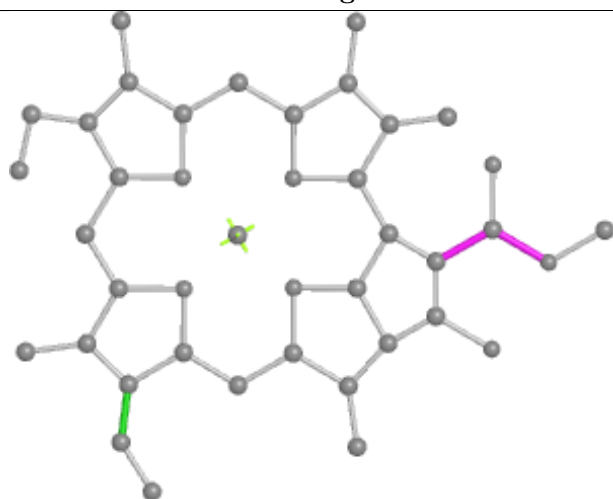
Ligand CLA Q 315



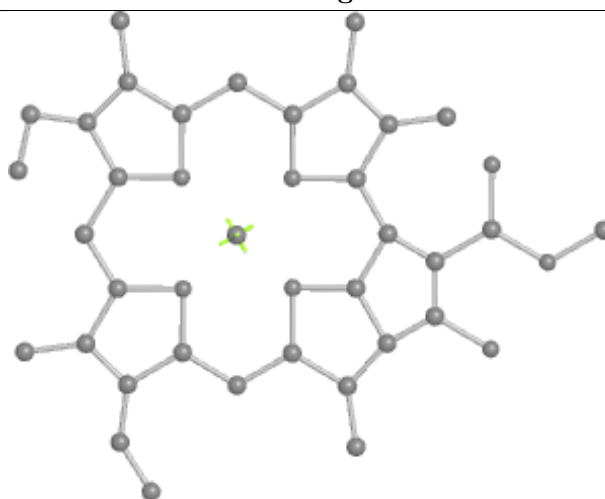
Bond lengths



Bond angles

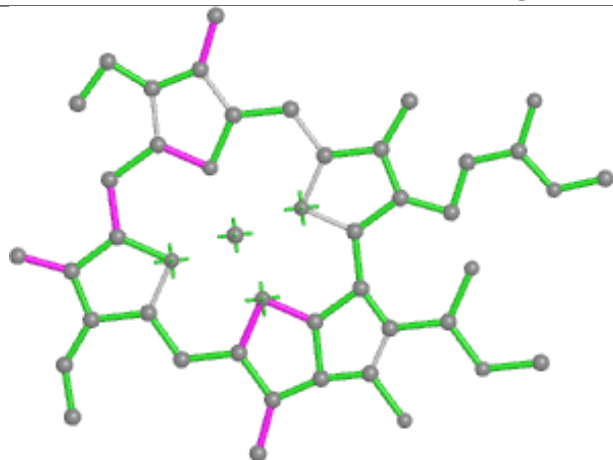


Torsions

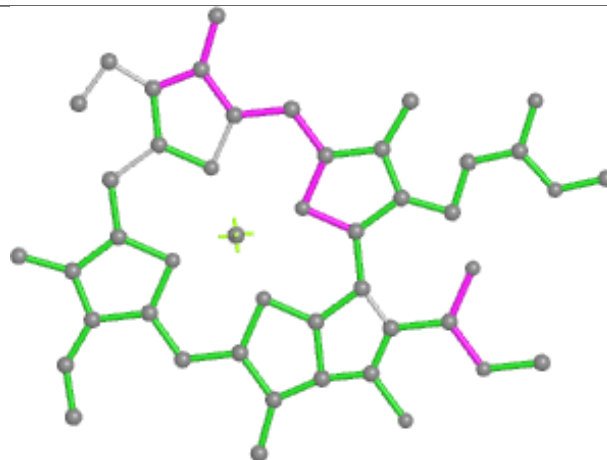


Rings

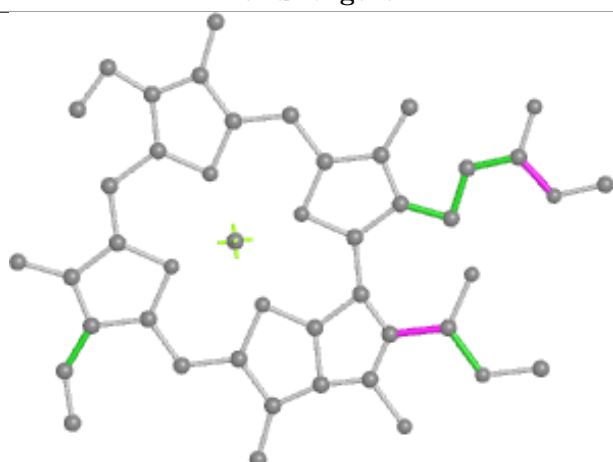
Ligand CLA K 208



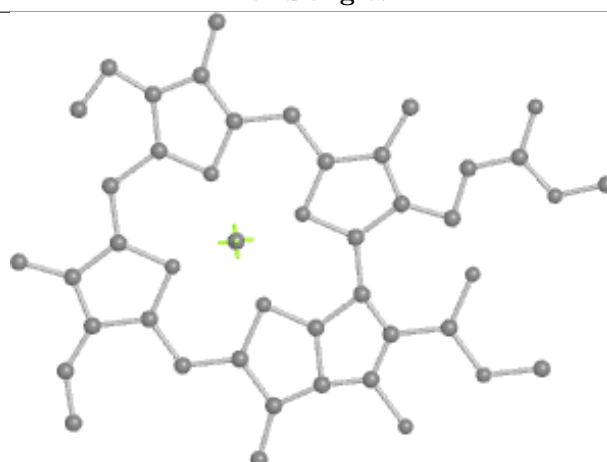
Bond lengths



Bond angles

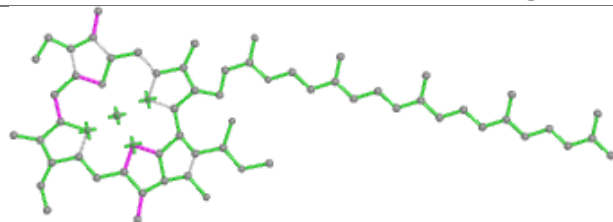


Torsions

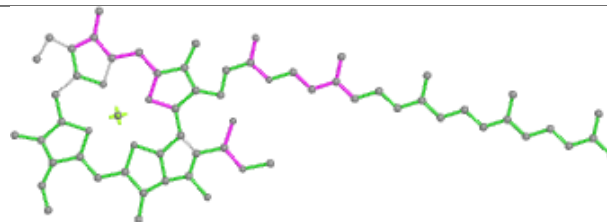


Rings

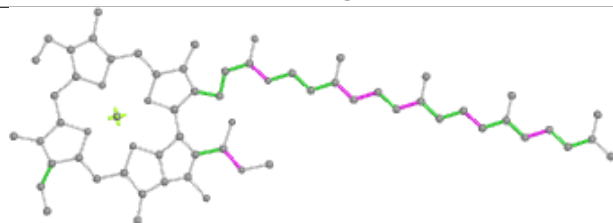
Ligand CLA I 504



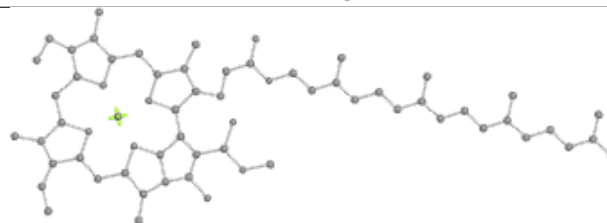
Bond lengths



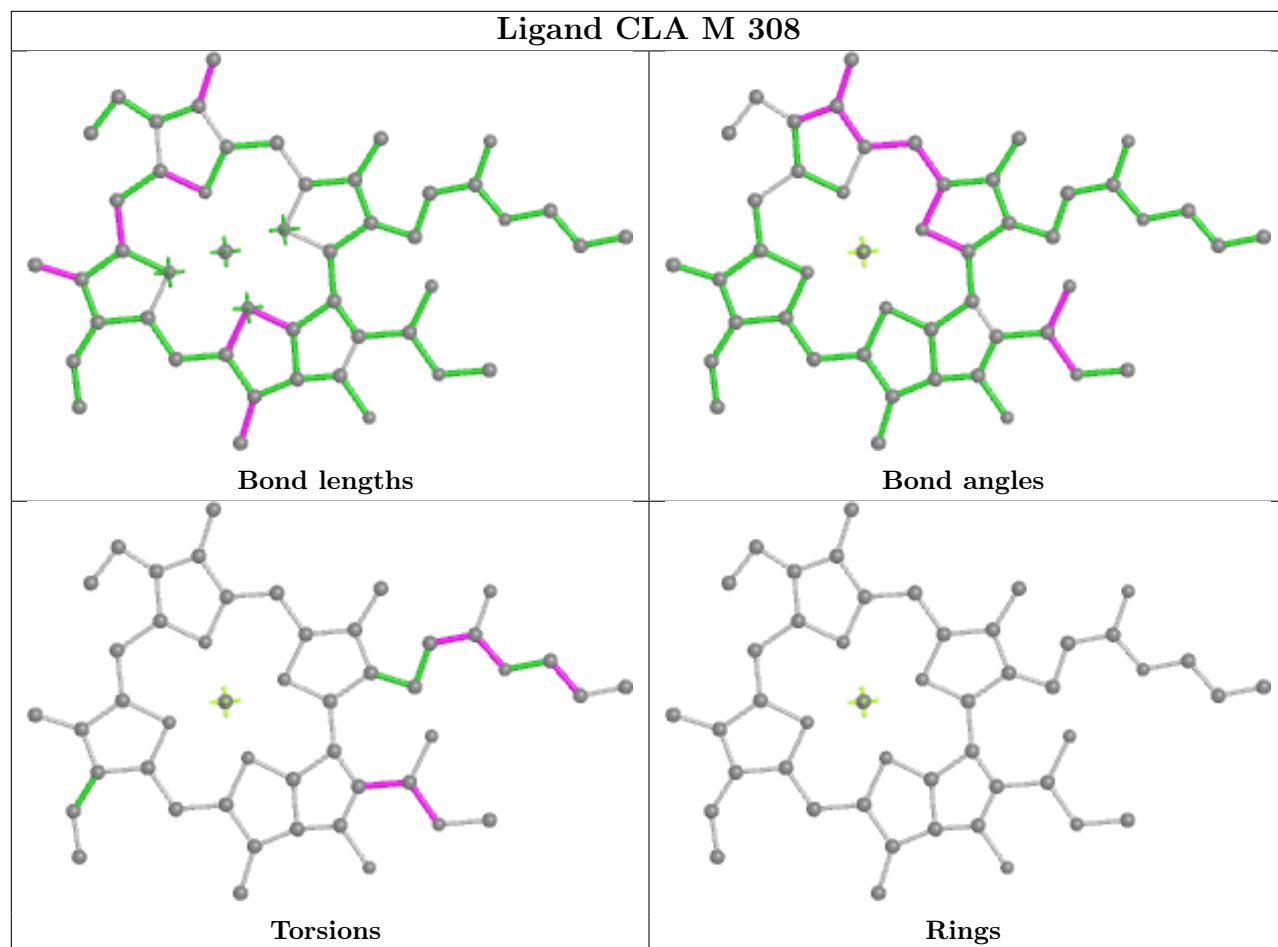
Bond angles



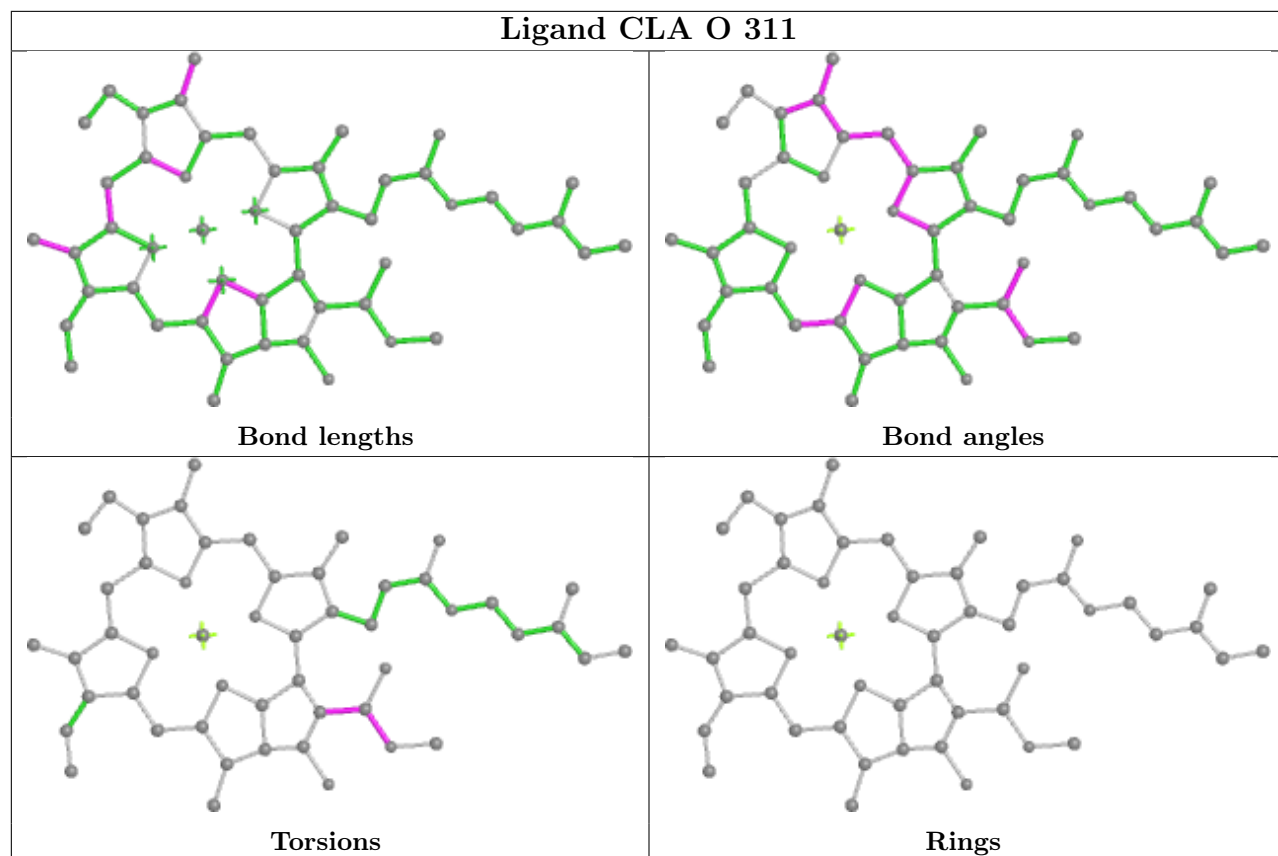
Torsions



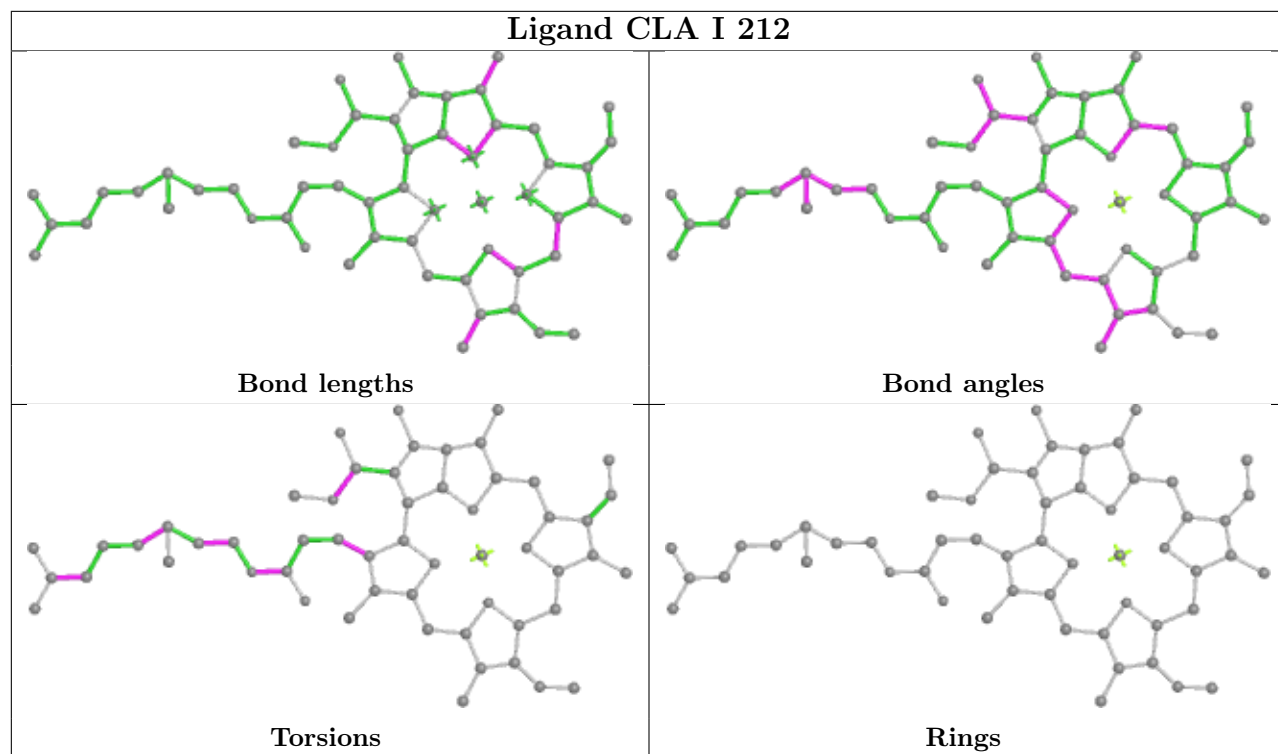
Rings



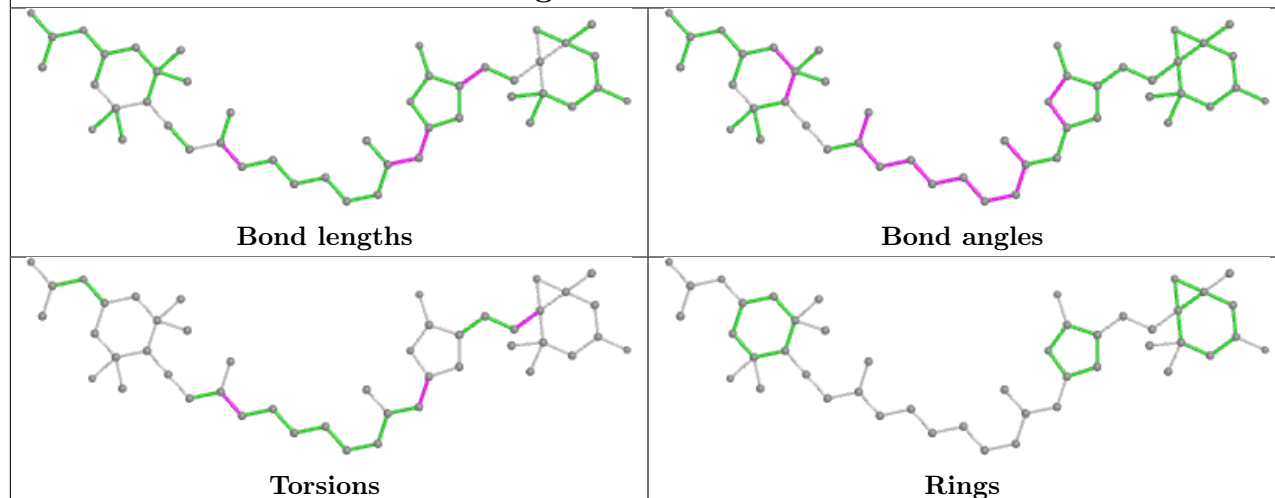
Ligand CLA O 311



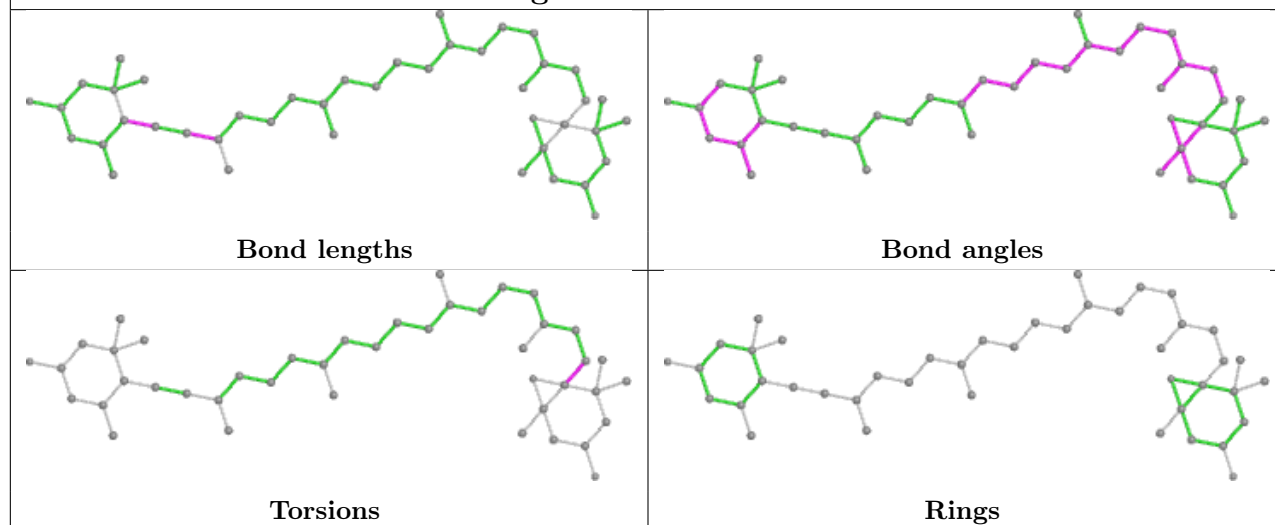
Ligand CLA I 212



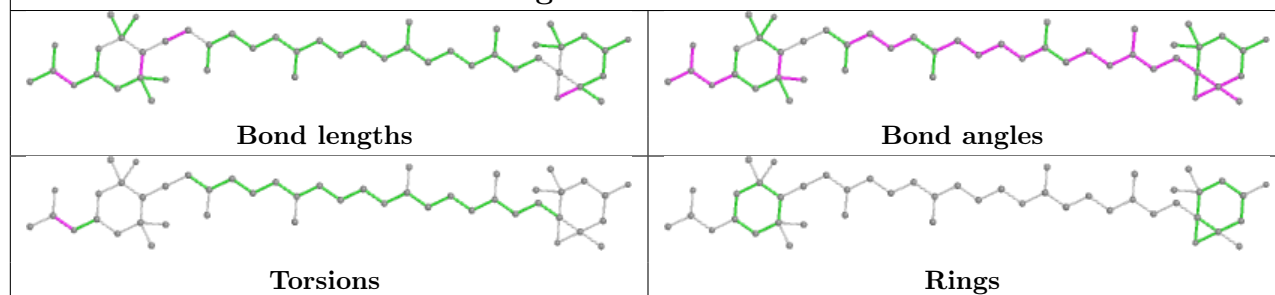
Ligand PID D 307



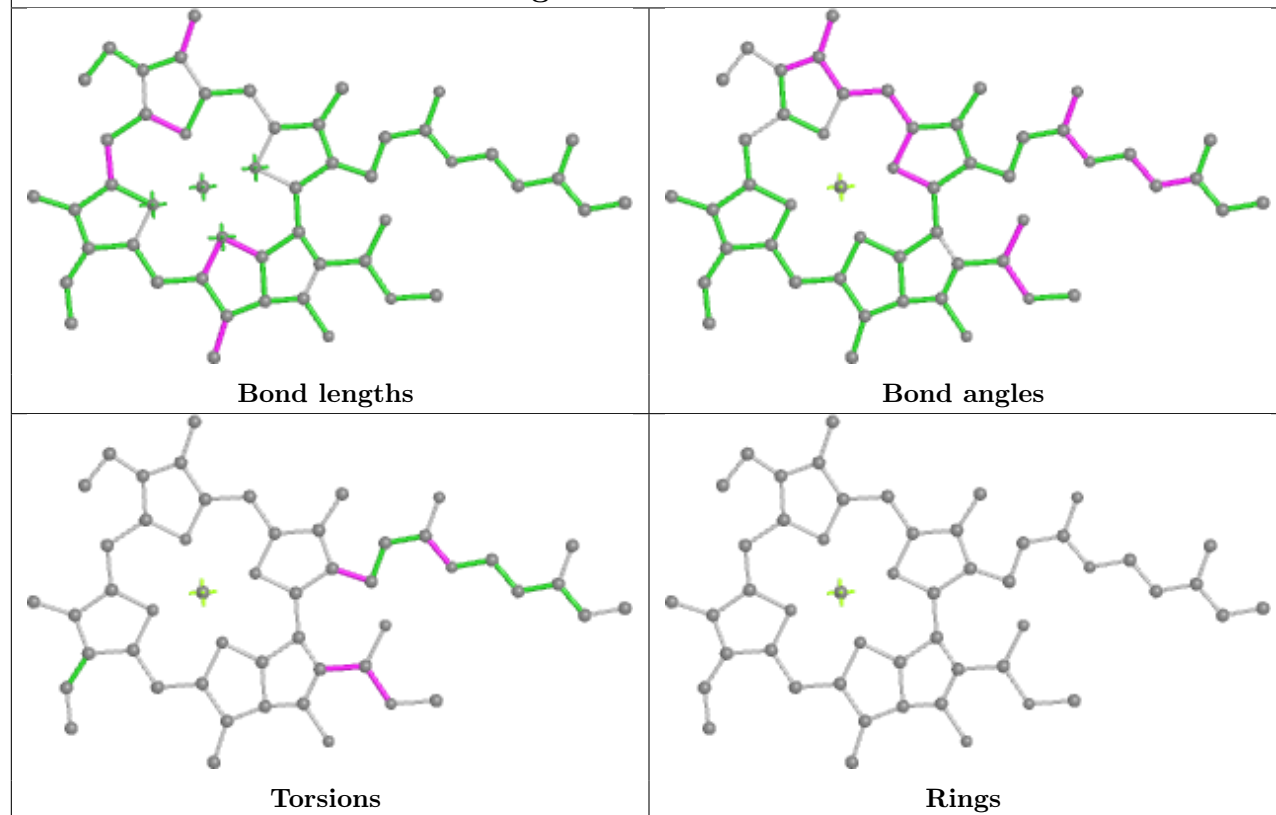
Ligand DD6 G 308



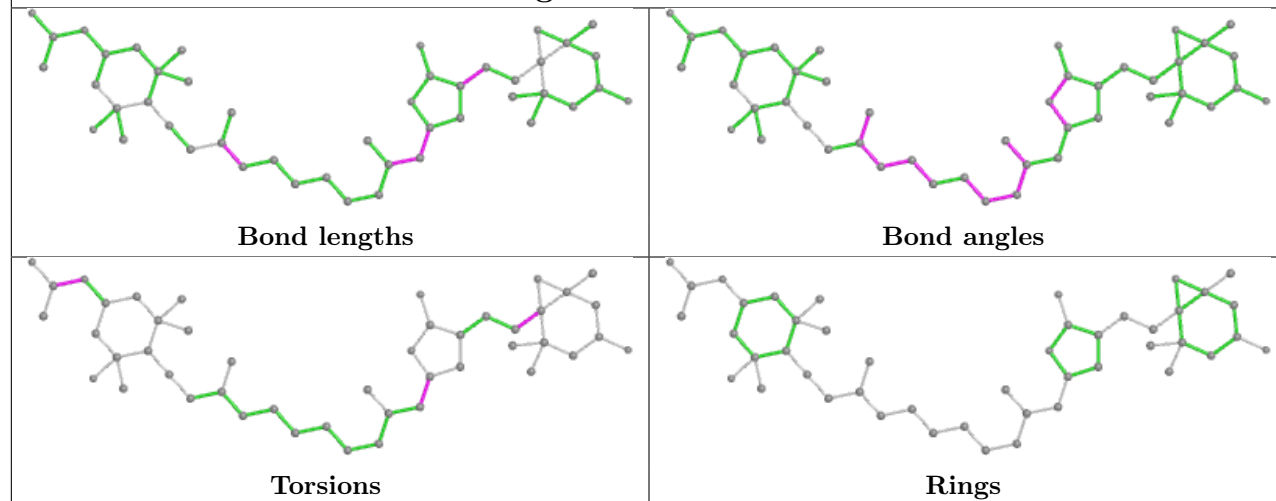
Ligand UIX E 304



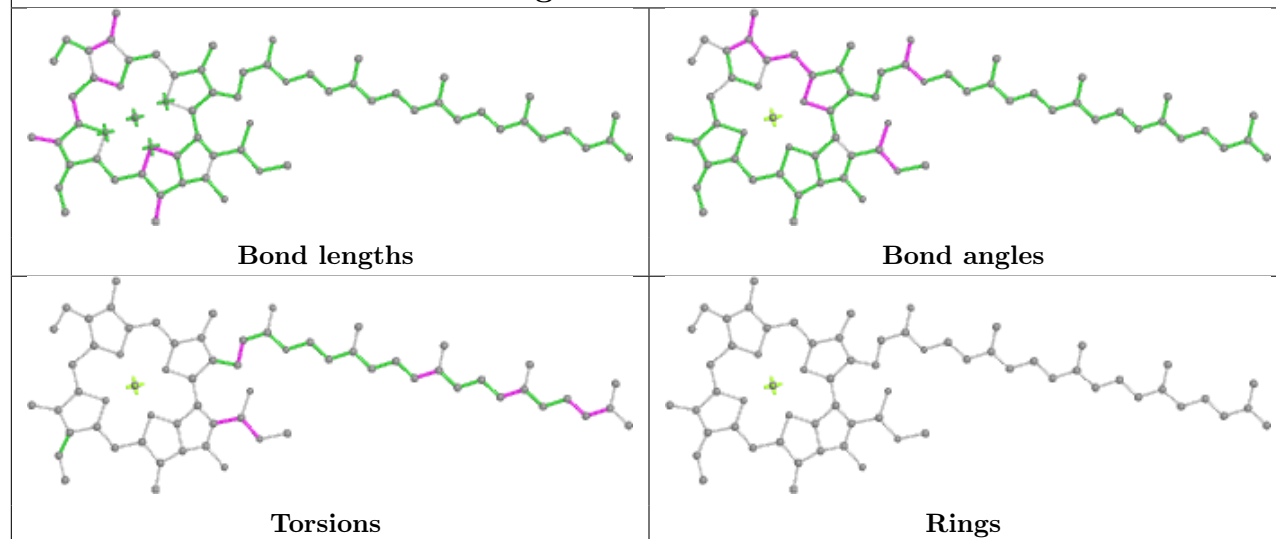
Ligand CLA A 217



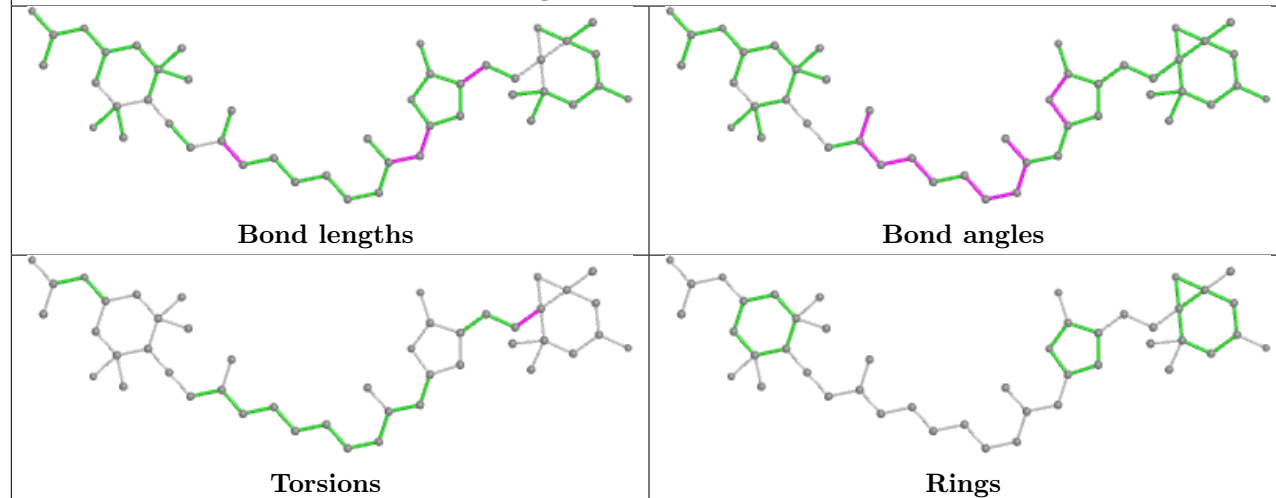
Ligand PID N 301



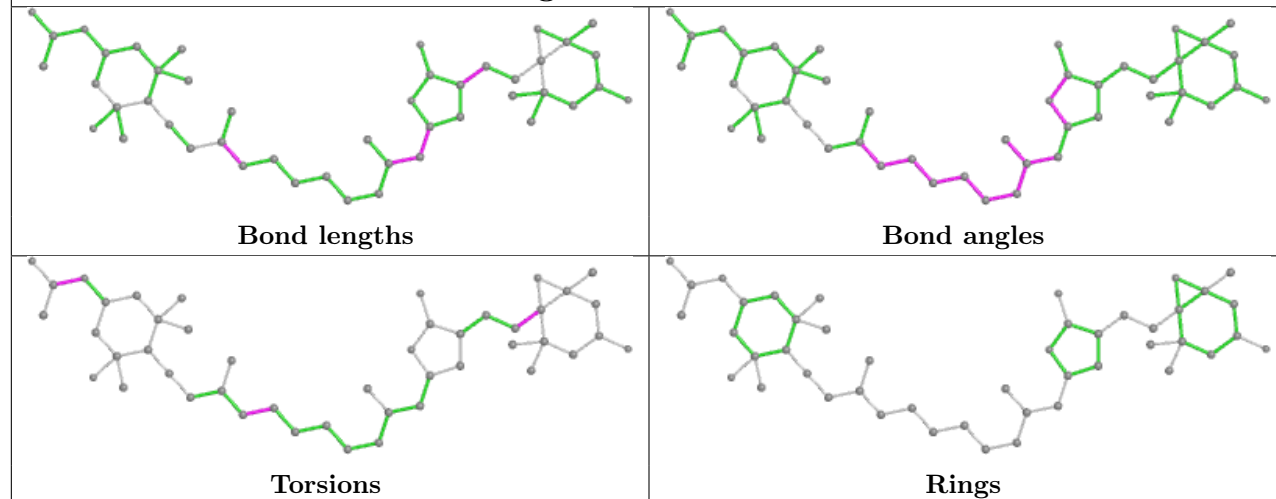
Ligand CLA b 725

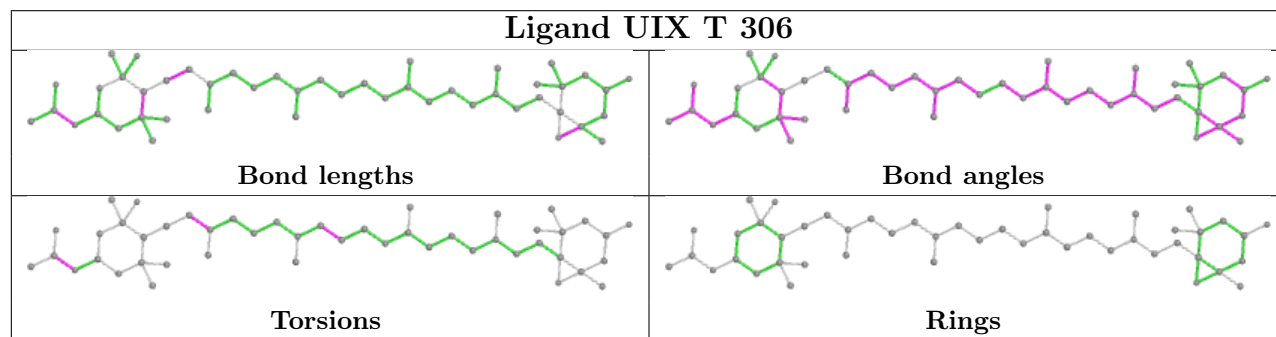
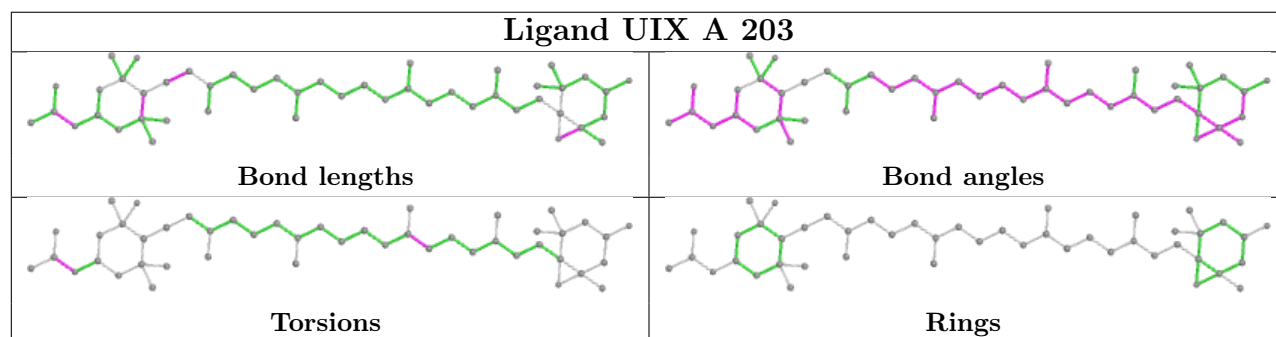
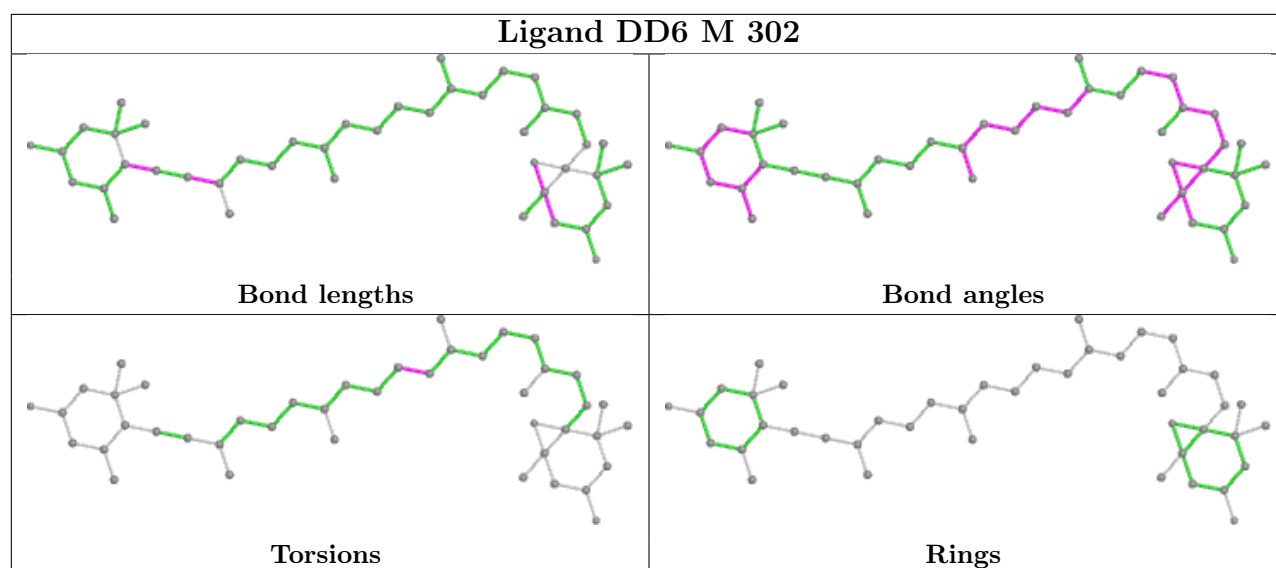


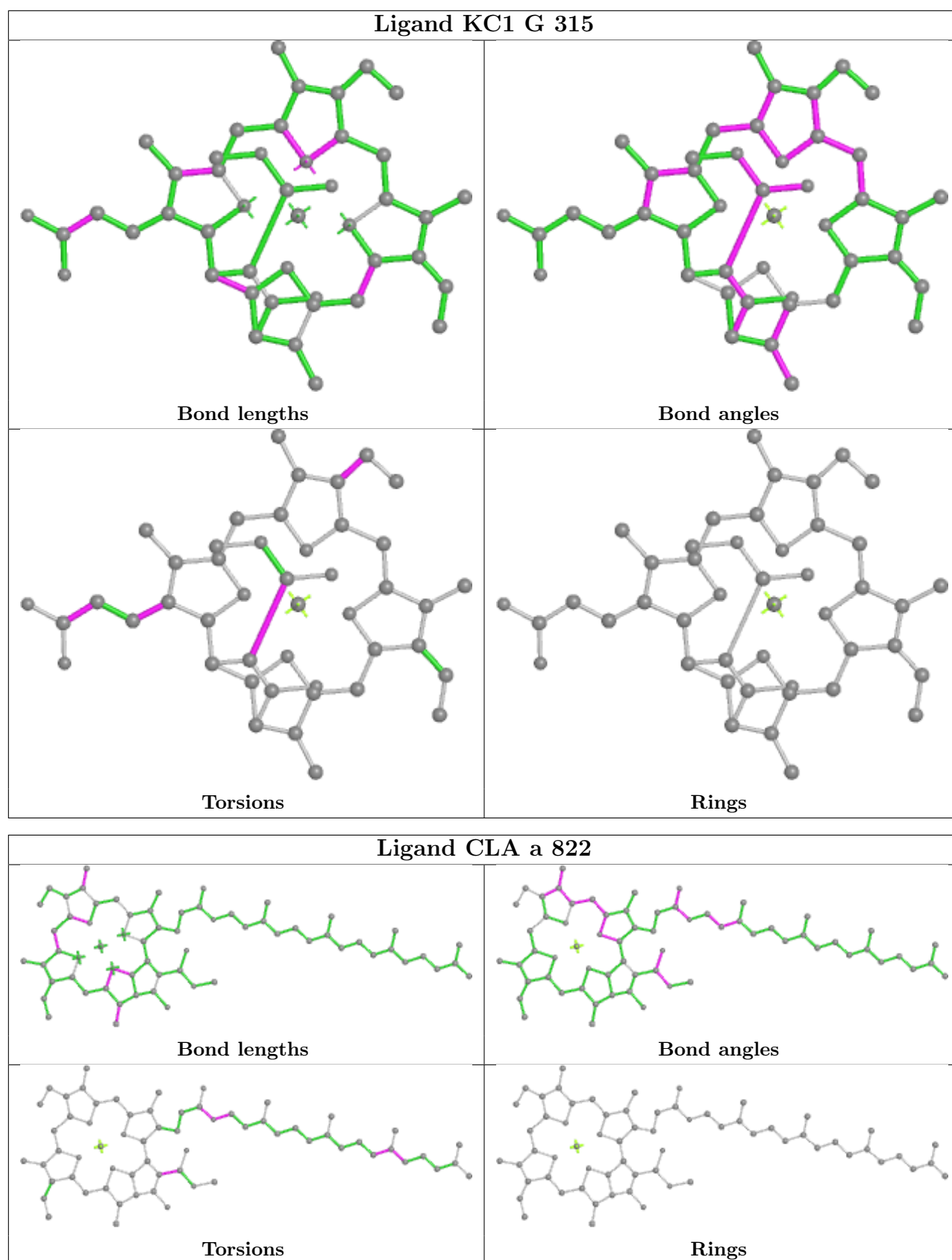
Ligand PID D 302

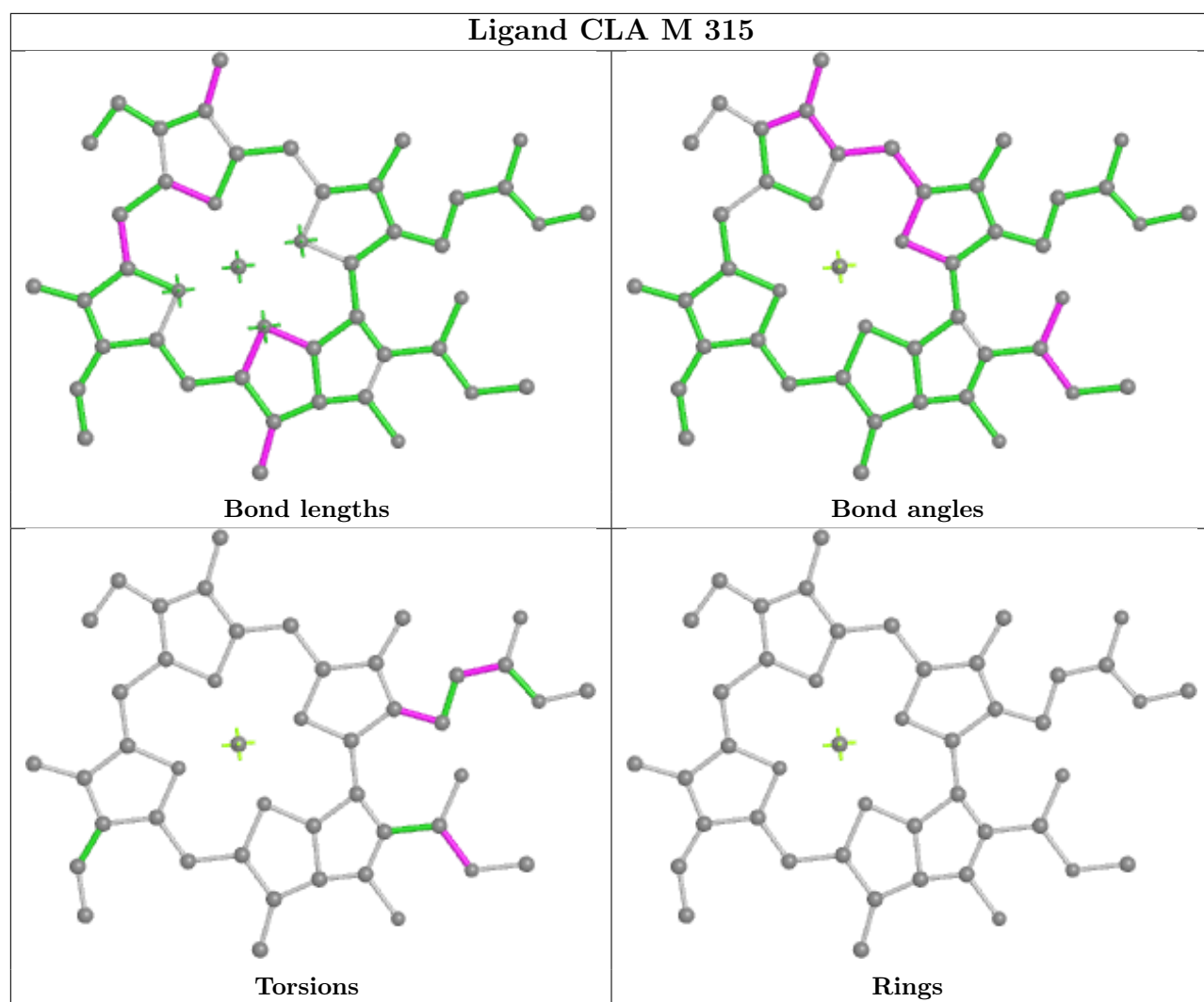


Ligand PID P 208

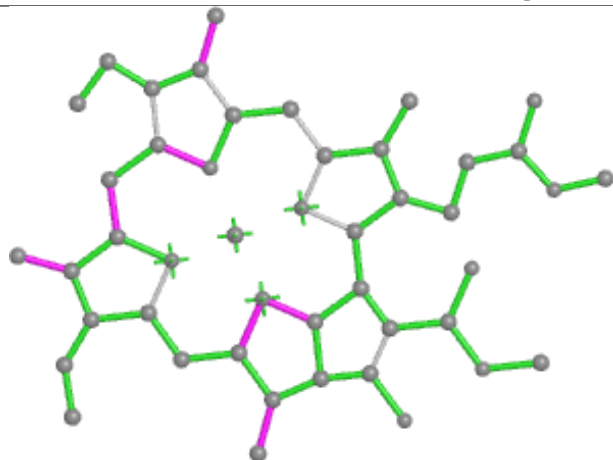




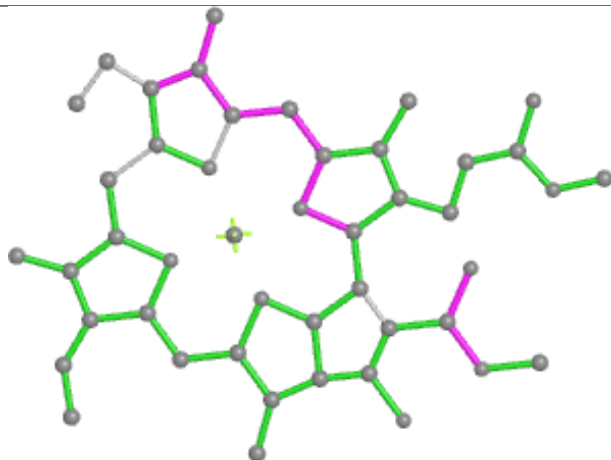




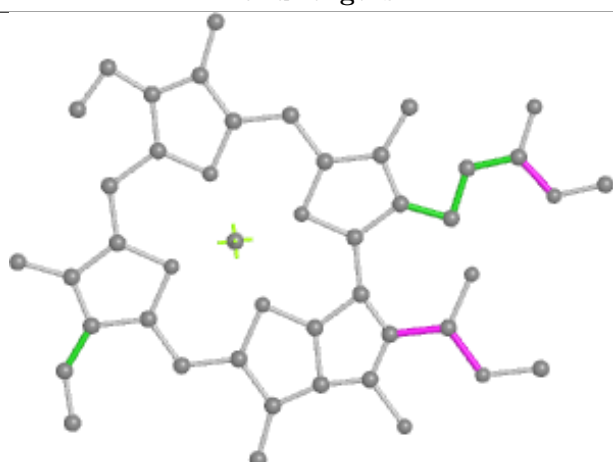
Ligand CLA a 814



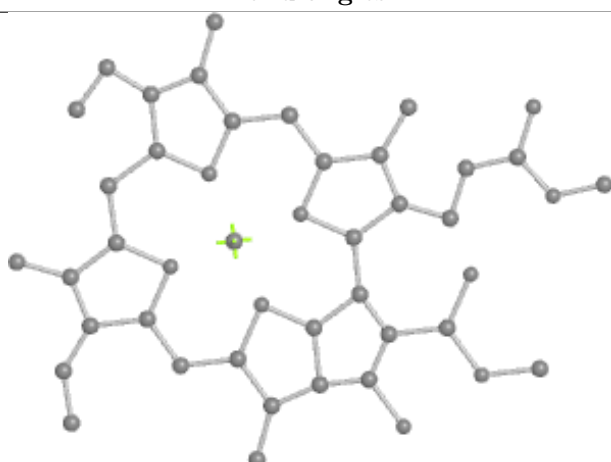
Bond lengths



Bond angles

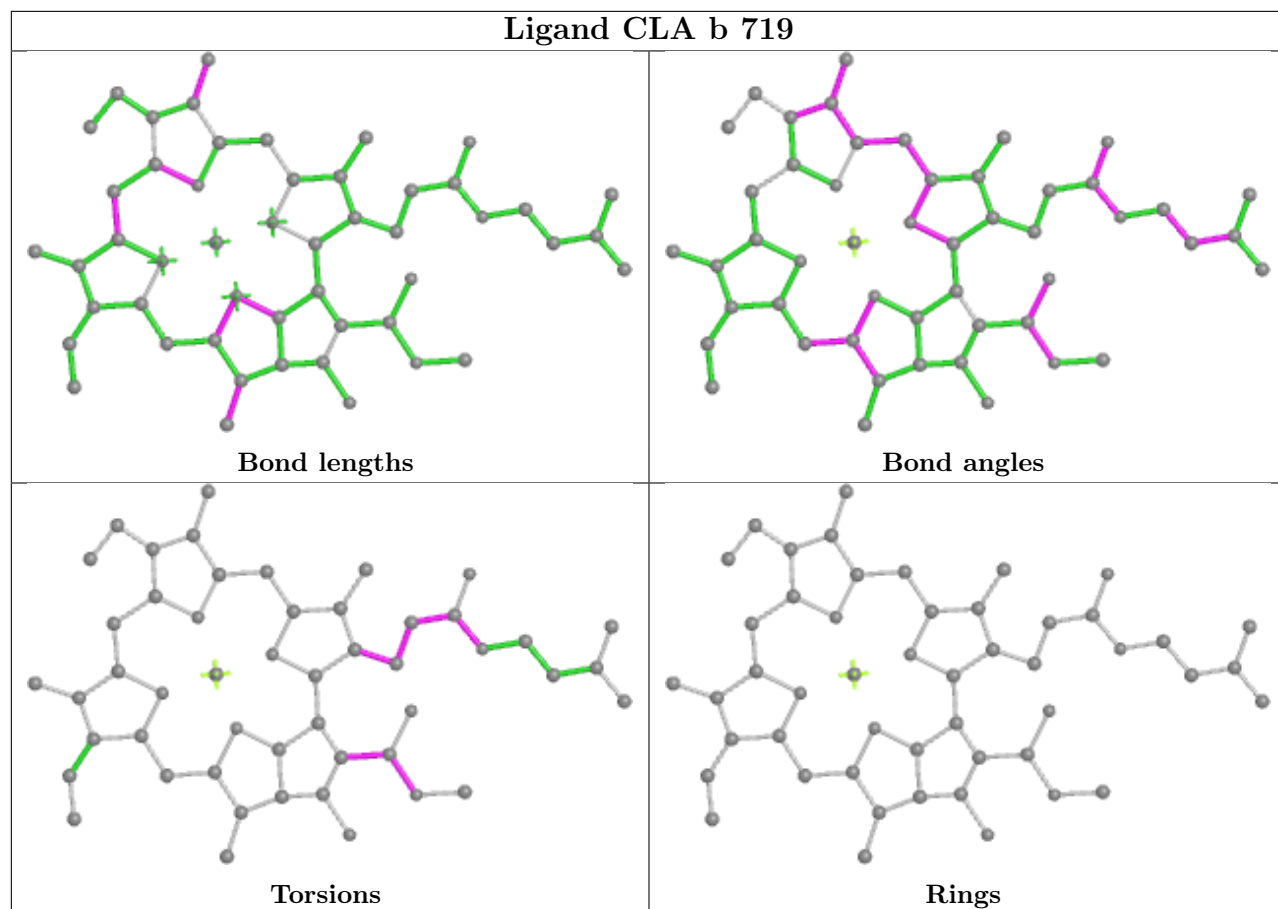


Torsions

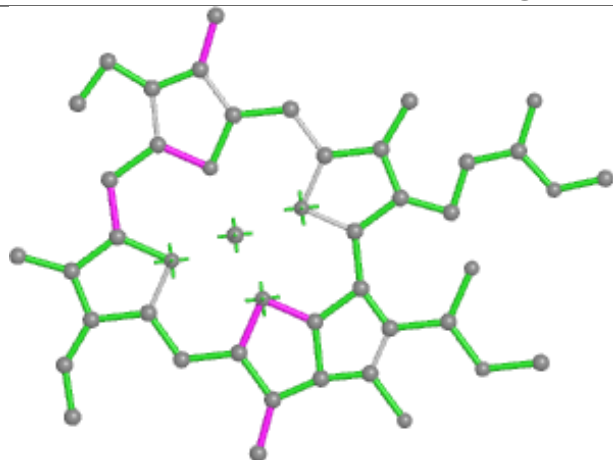


Rings

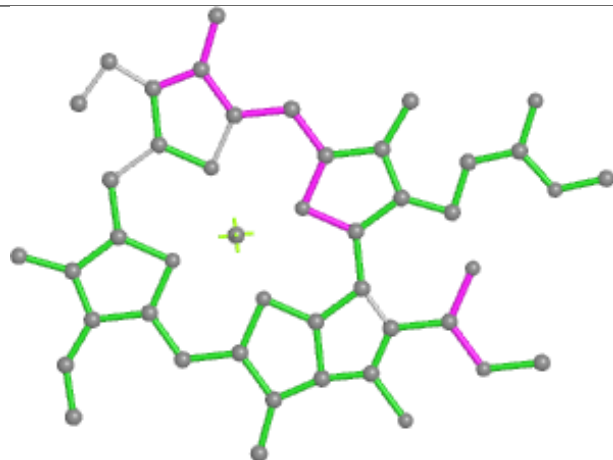
Ligand CLA b 719



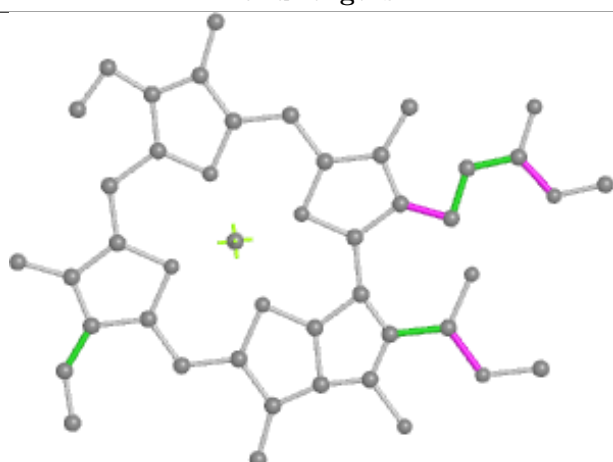
Ligand CLA F 312



Bond lengths



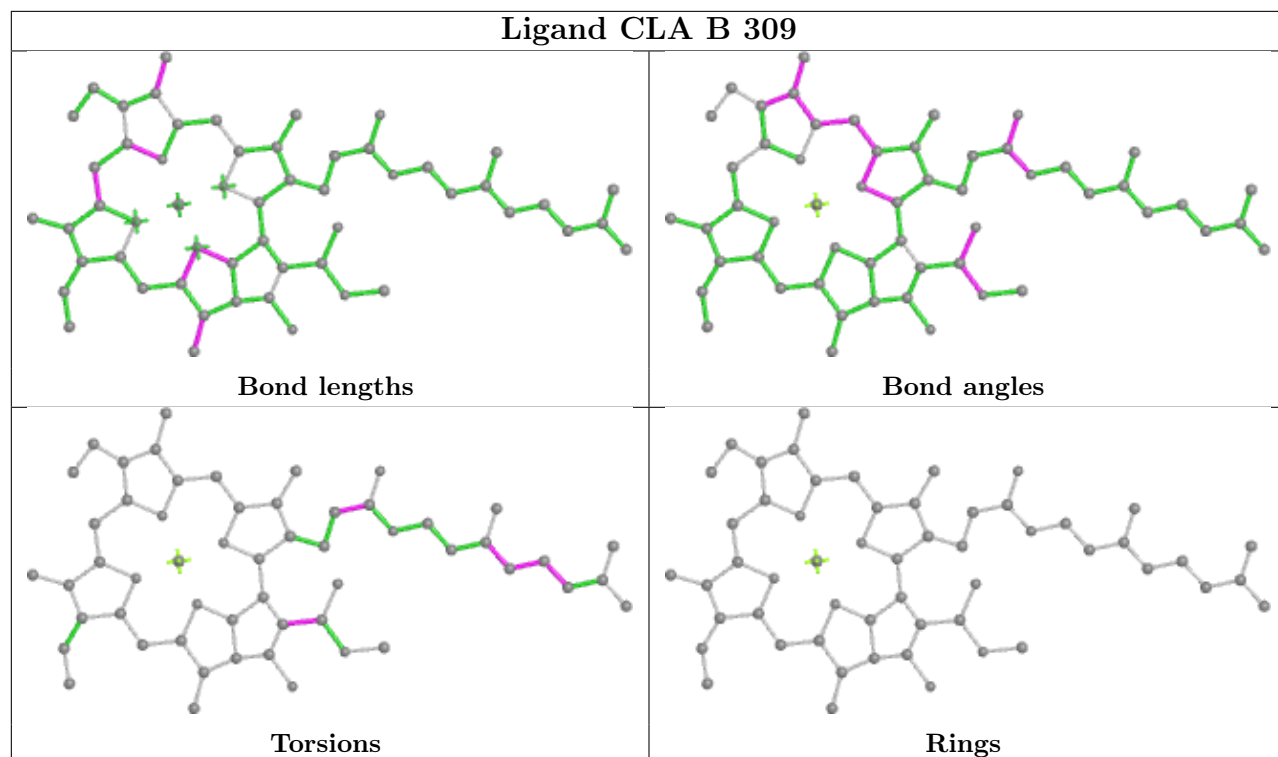
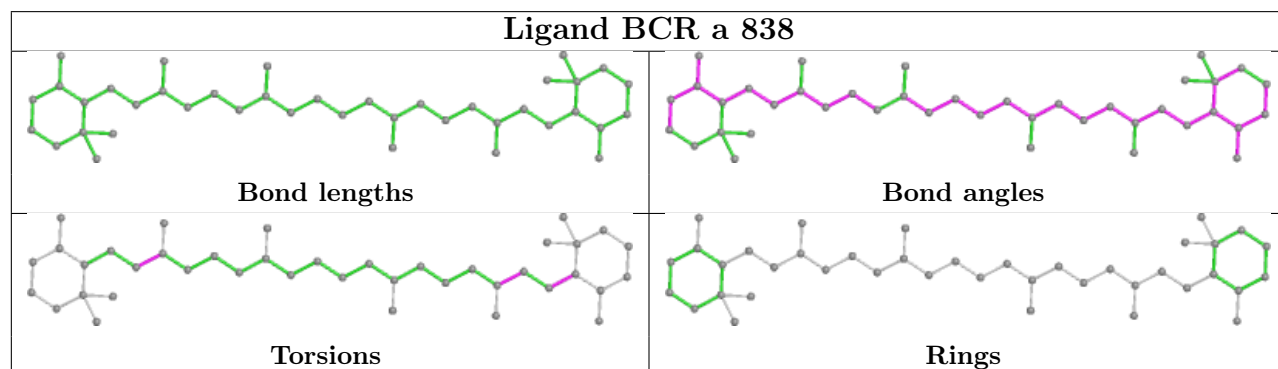
Bond angles



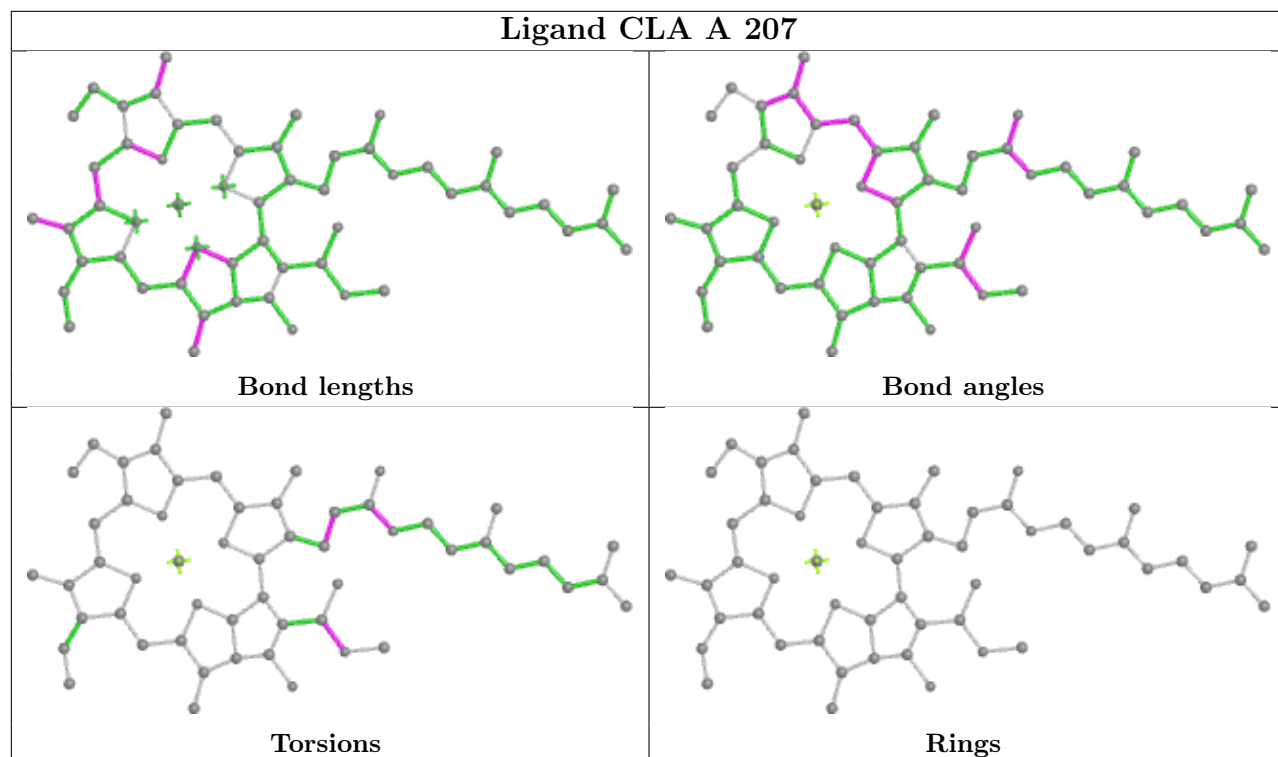
Torsions



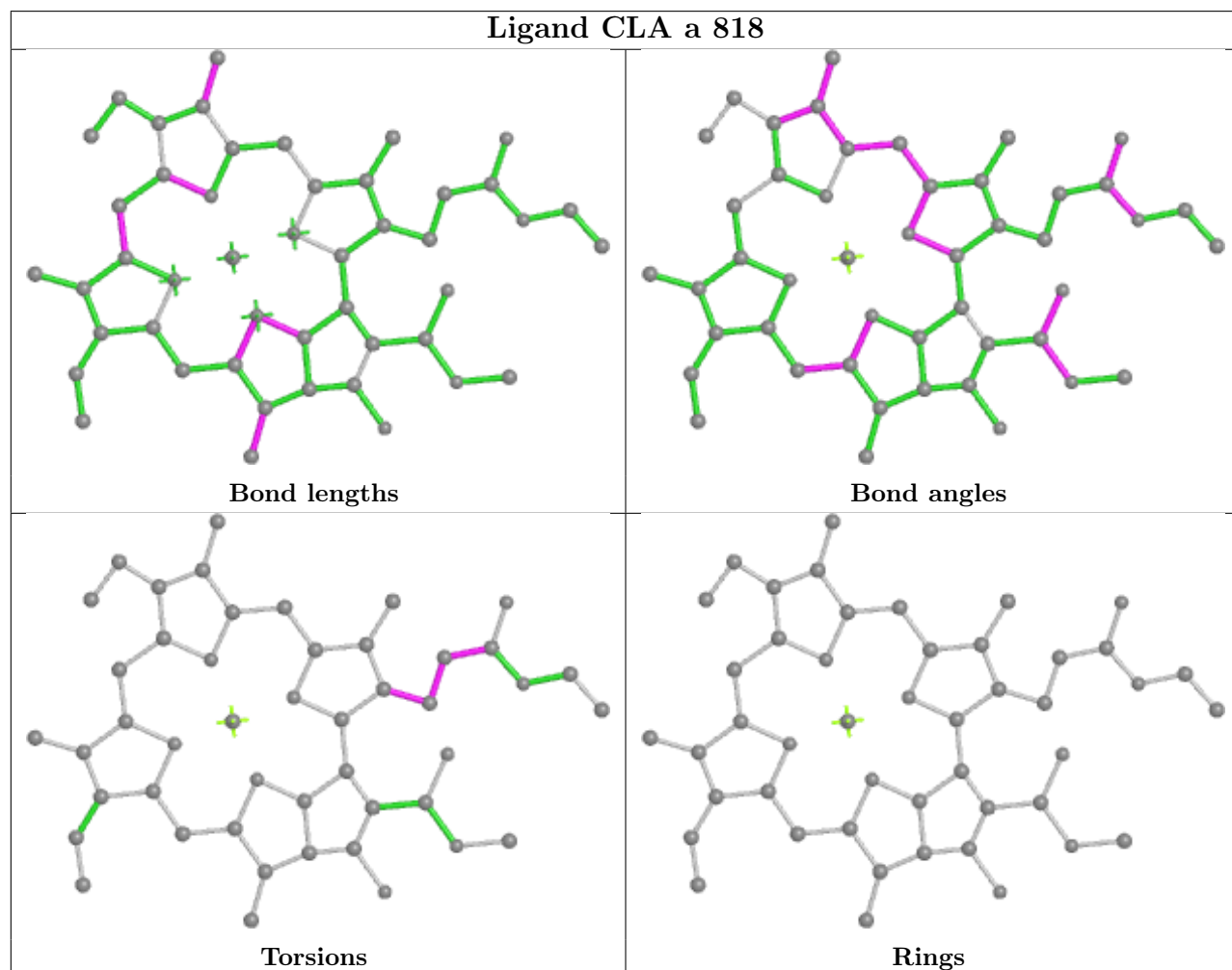
Rings

Ligand CLA B 309**Ligand BCR a 838**

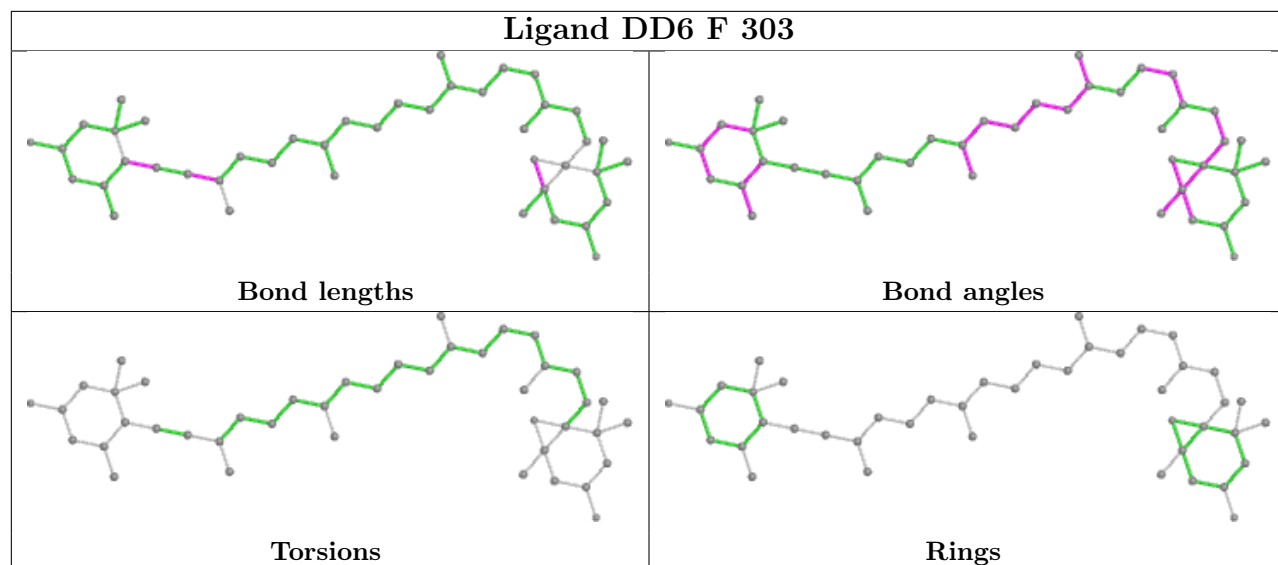
Ligand CLA A 207



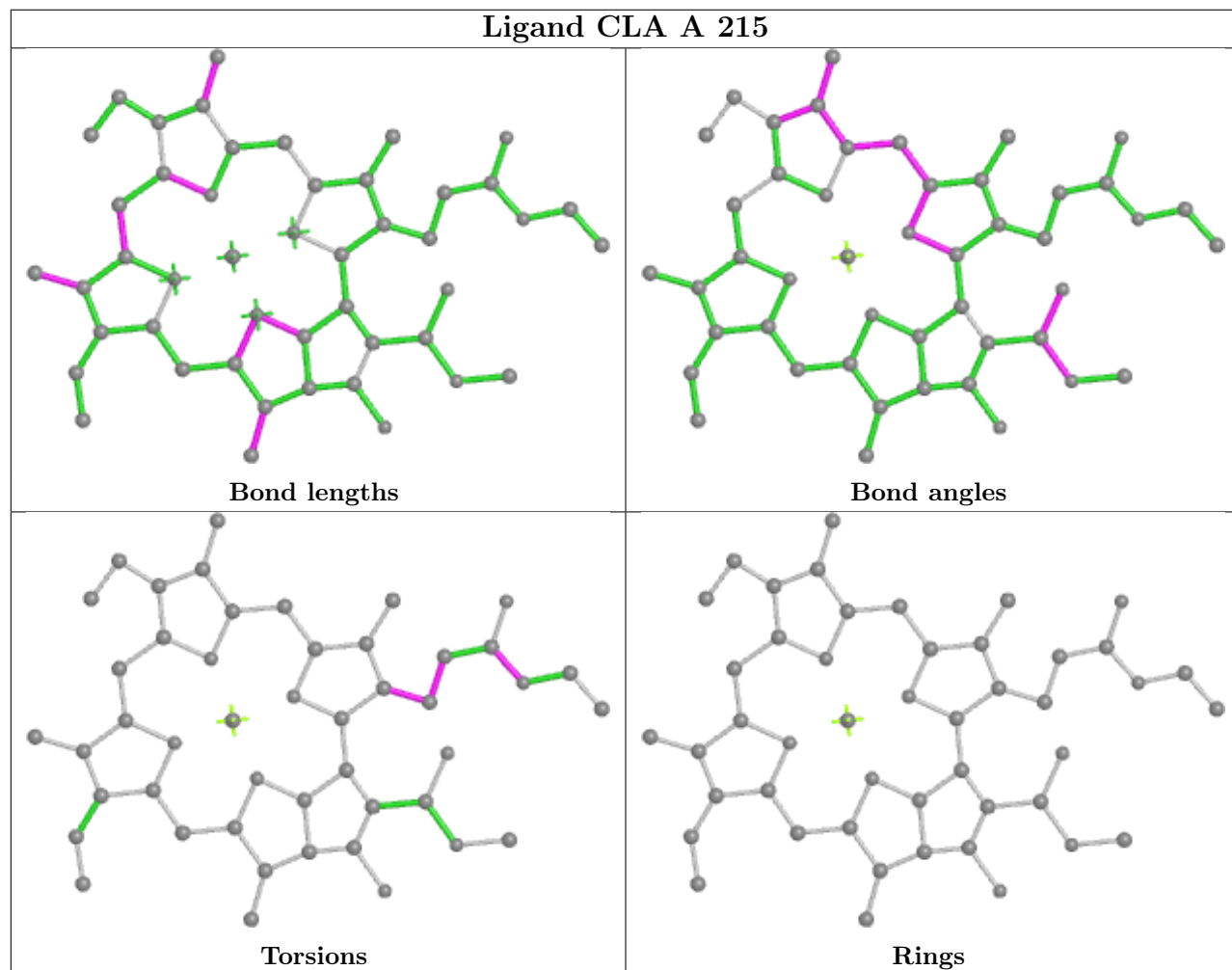
Ligand CLA a 818

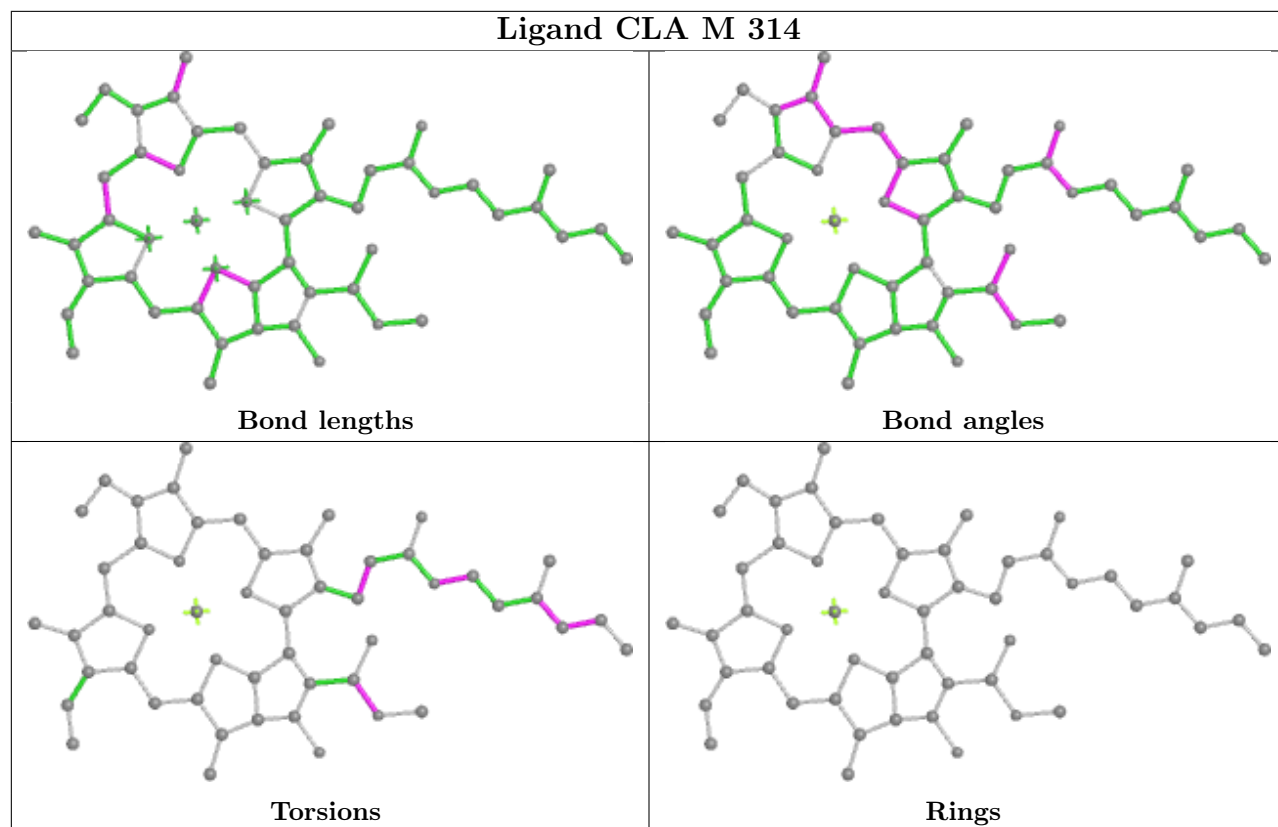


Ligand DD6 F 303

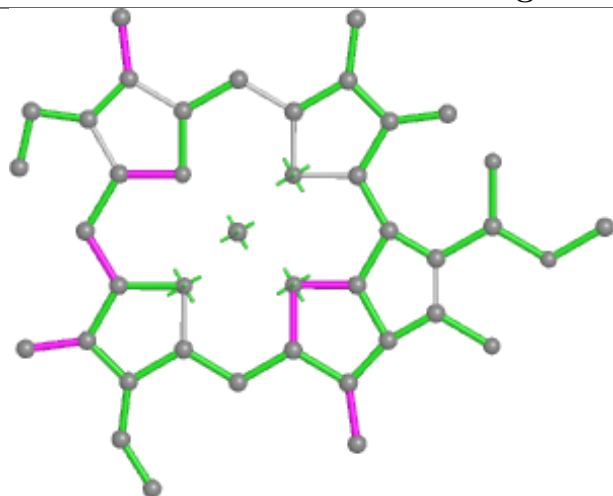


Ligand CLA A 215

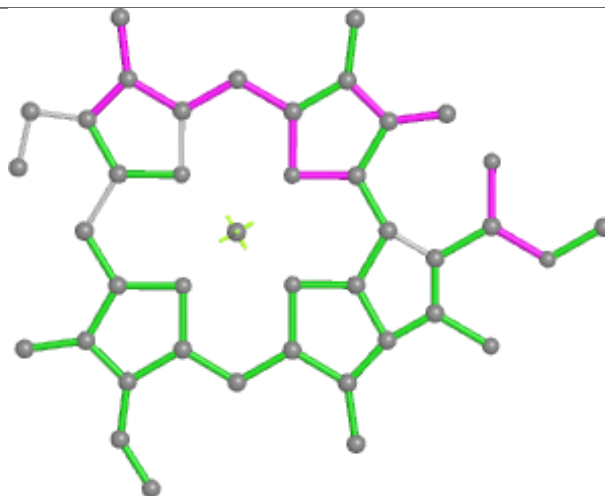




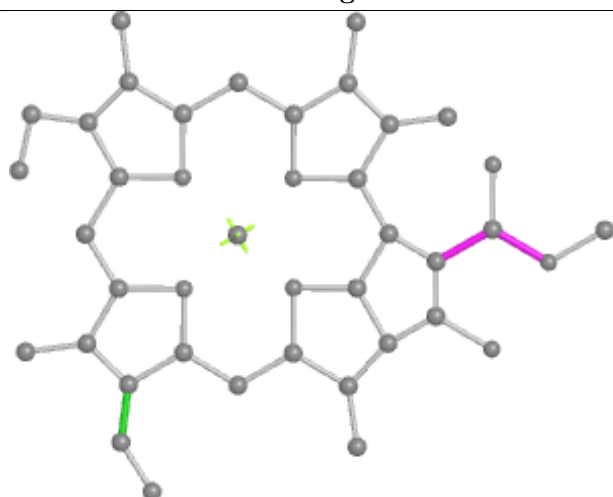
Ligand CLA L 315



Bond lengths



Bond angles

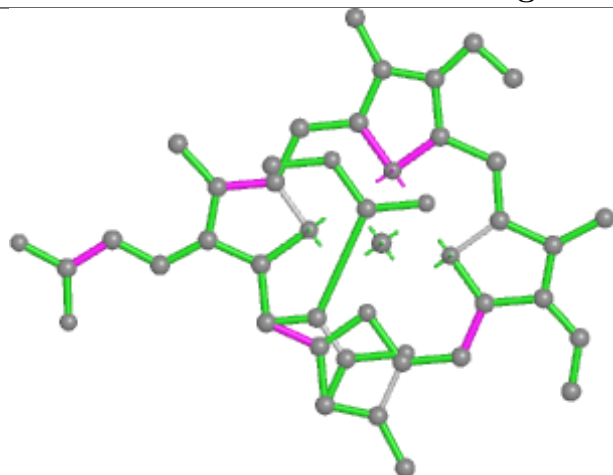


Torsions

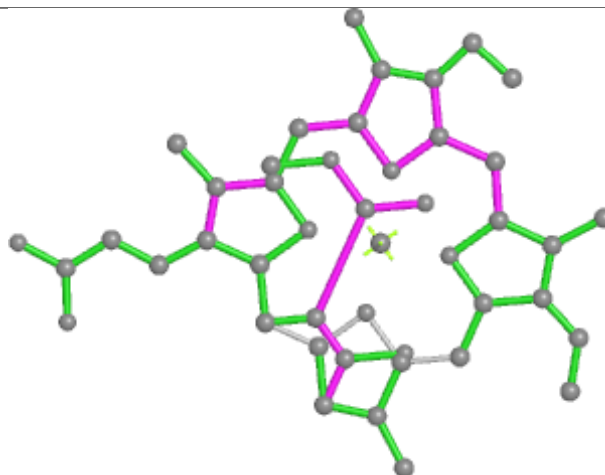


Rings

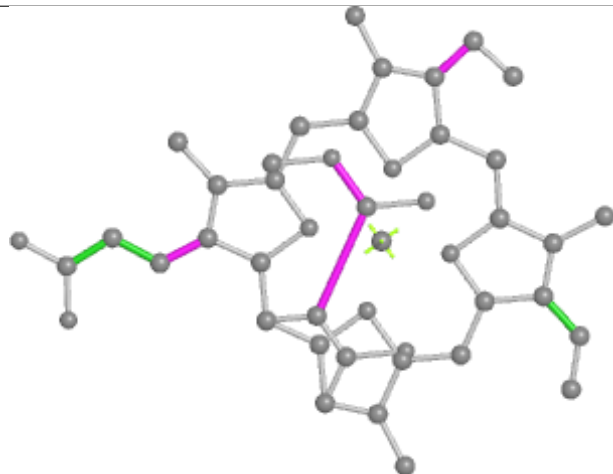
Ligand KC1 F 314



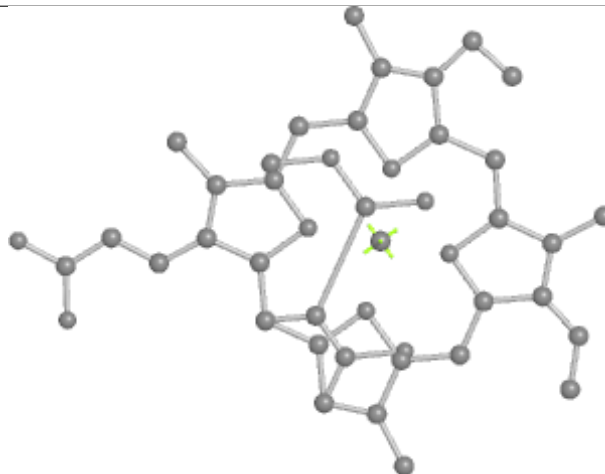
Bond lengths



Bond angles

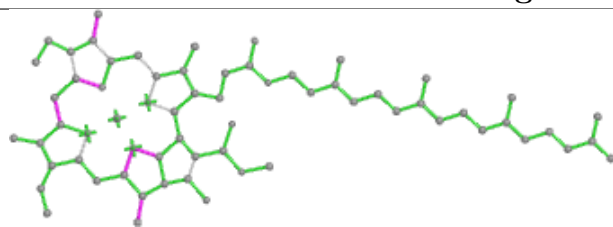


Torsions

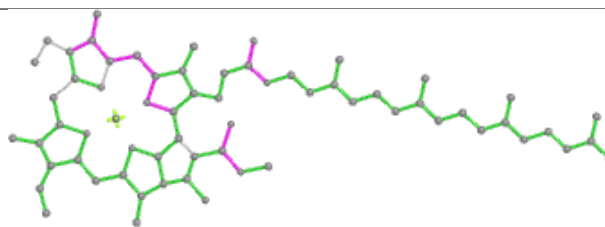


Rings

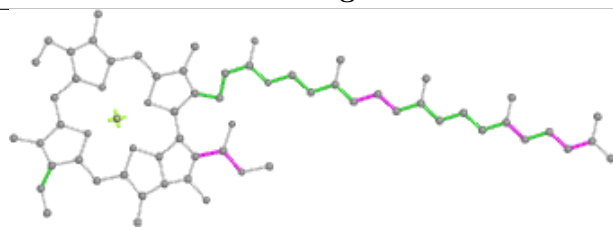
Ligand CLA P 210



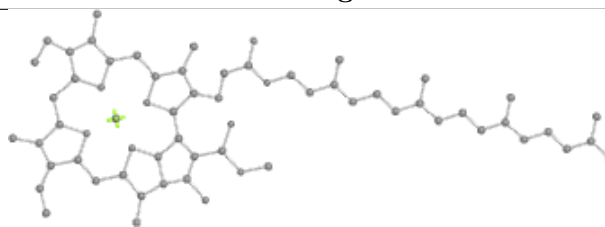
Bond lengths



Bond angles

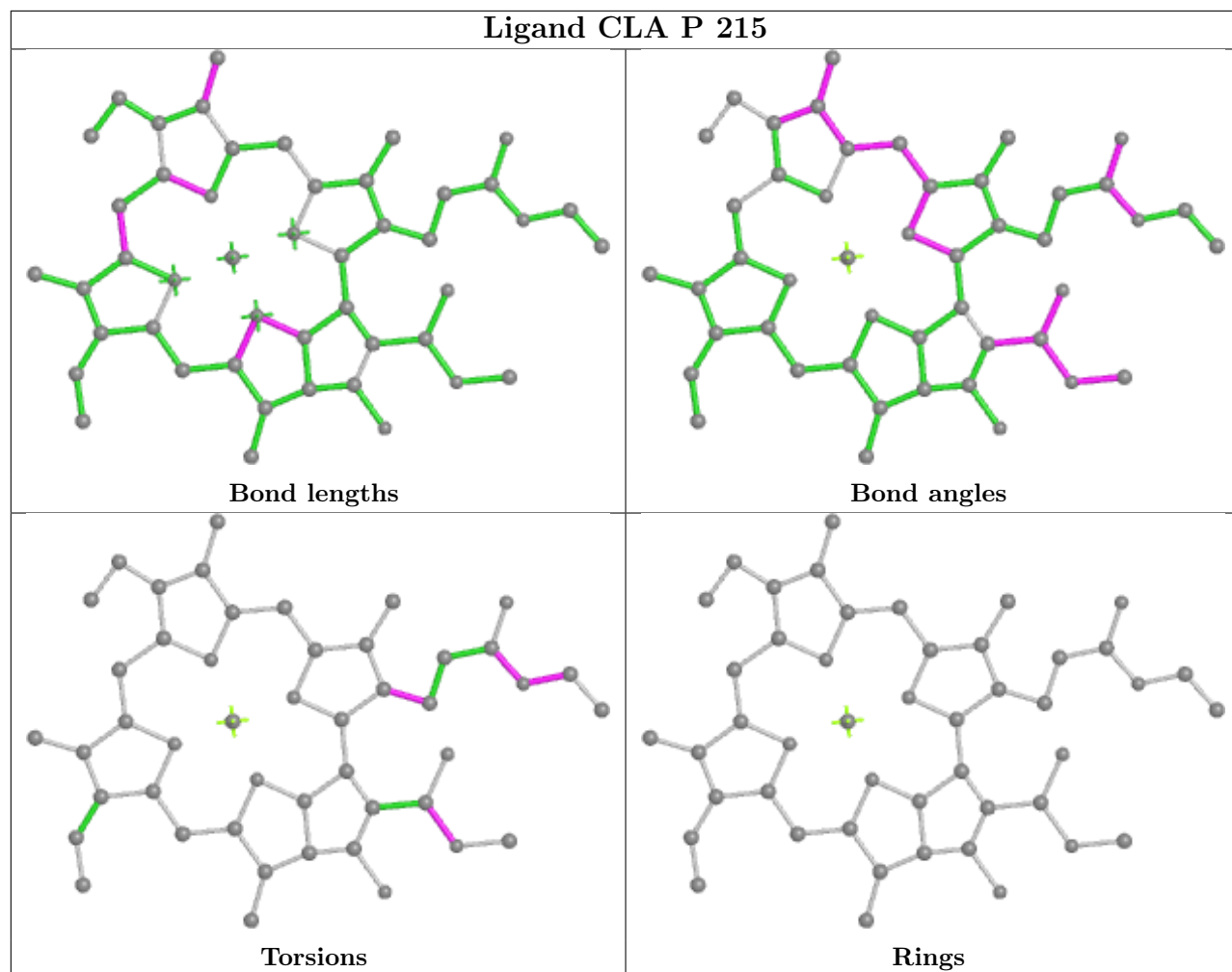


Torsions

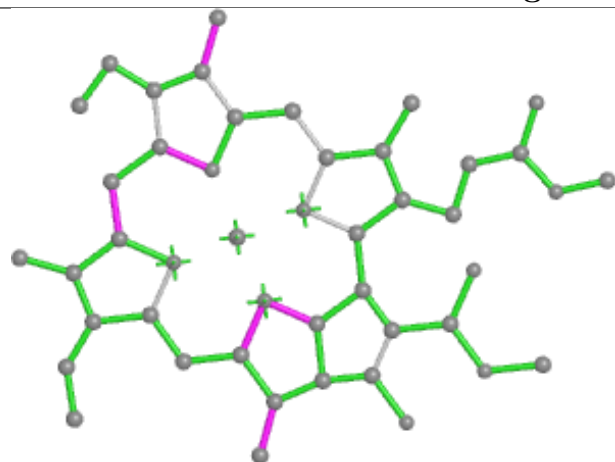


Rings

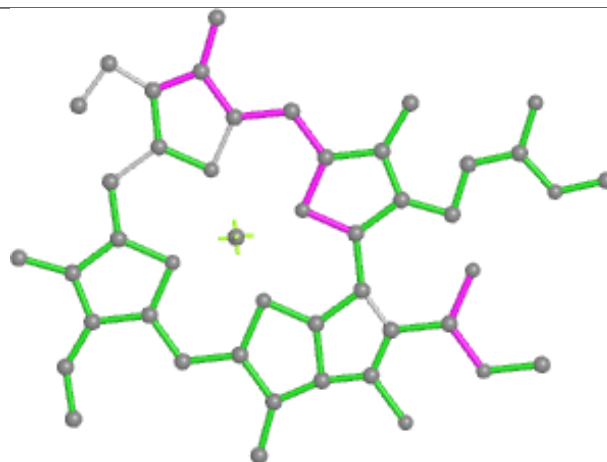
Ligand CLA P 215



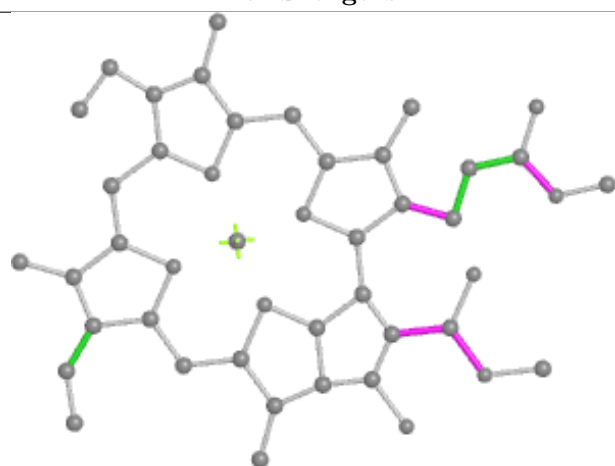
Ligand CLA f 803



Bond lengths



Bond angles

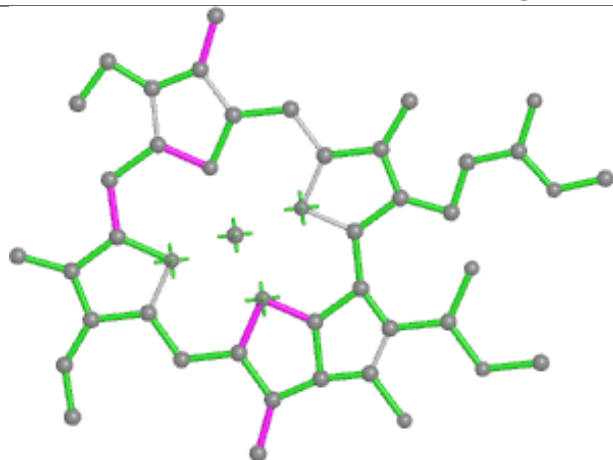


Torsions

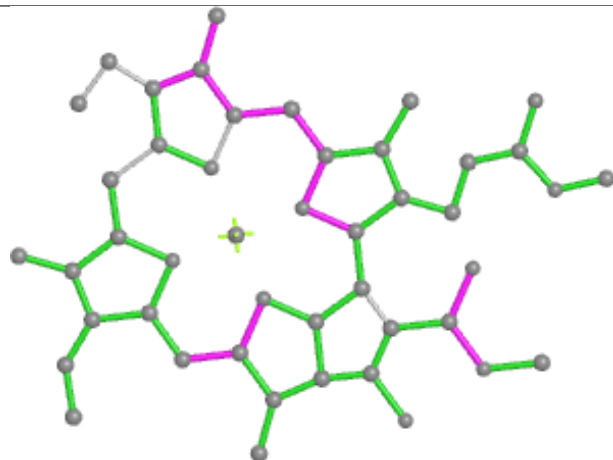


Rings

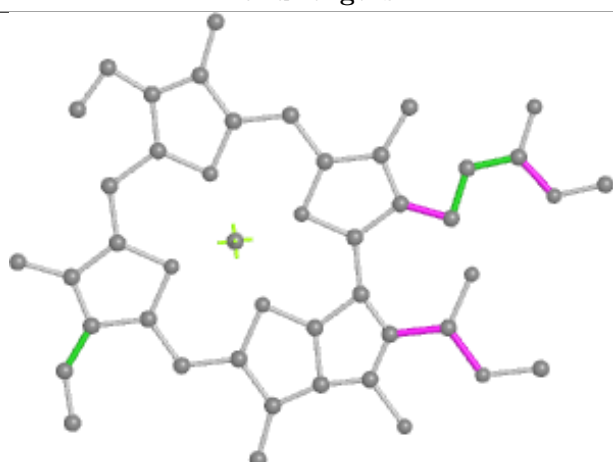
Ligand CLA E 309



Bond lengths



Bond angles

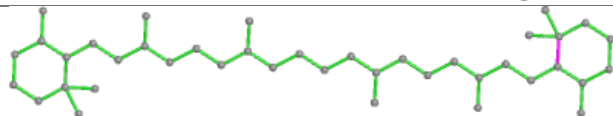


Torsions

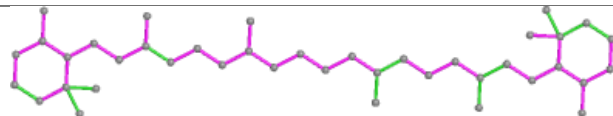


Rings

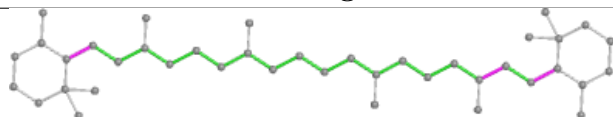
Ligand BCR b 729



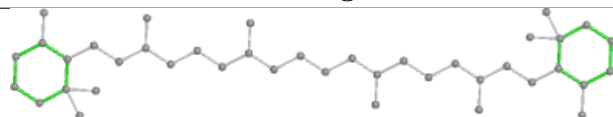
Bond lengths



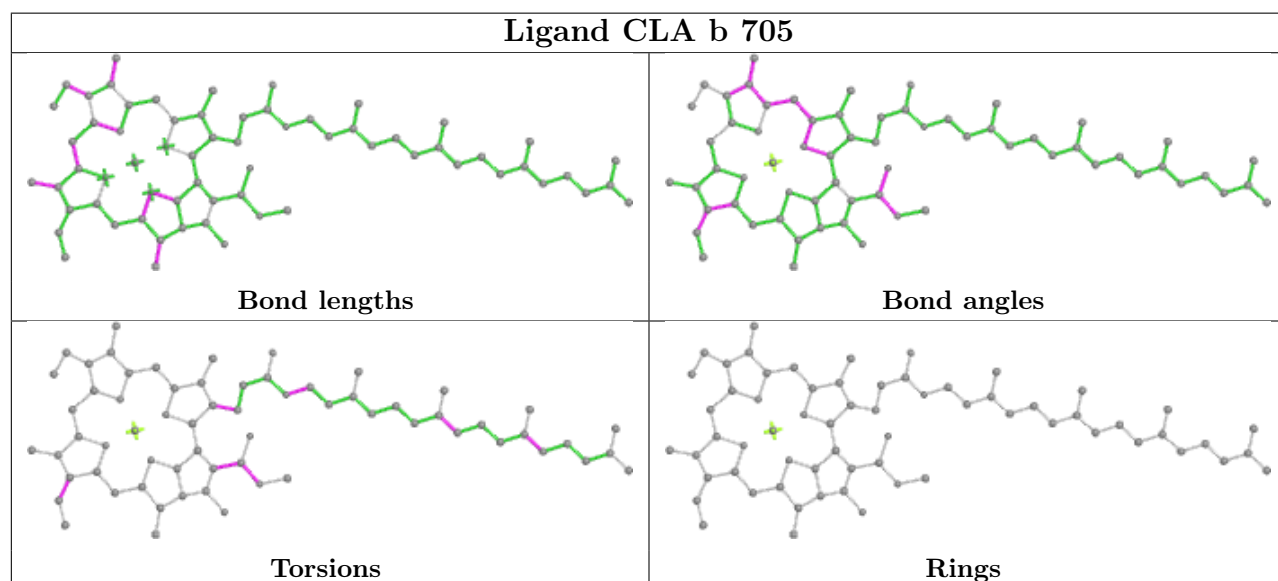
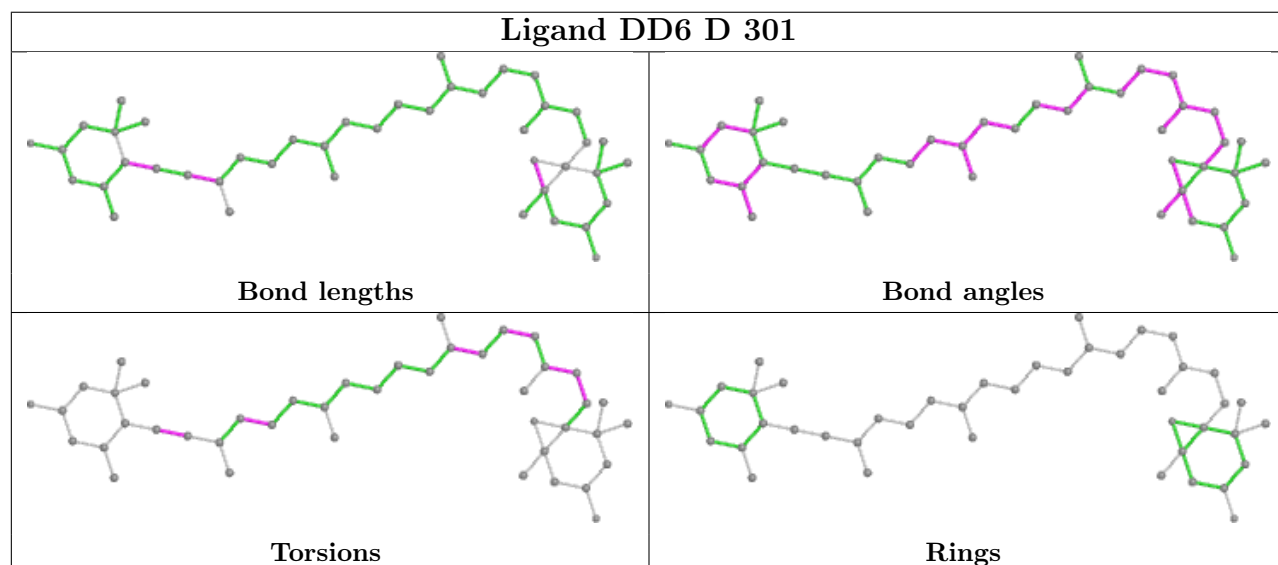
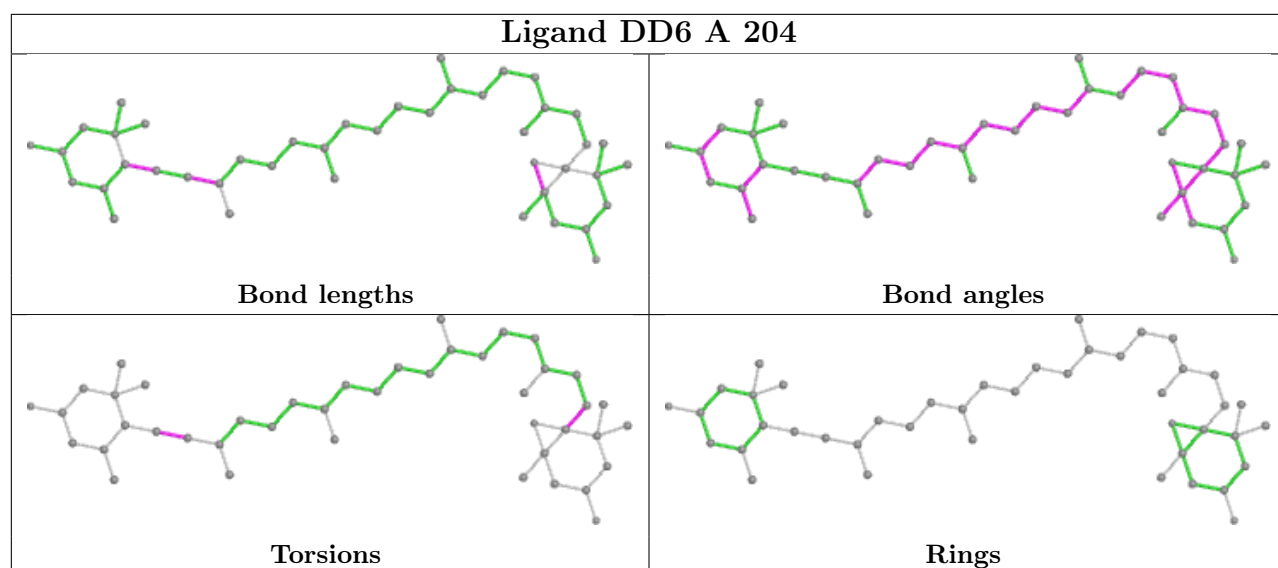
Bond angles

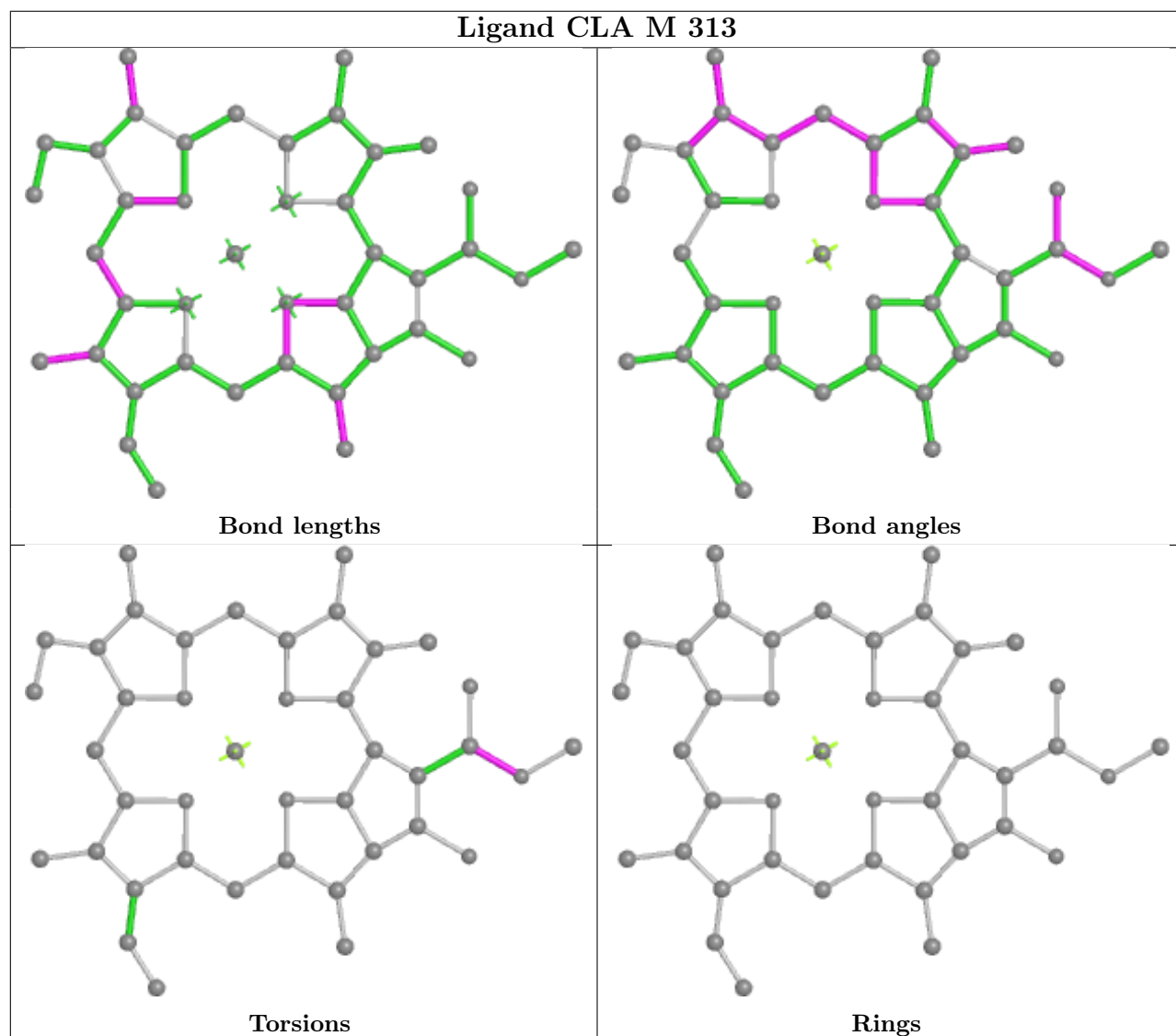
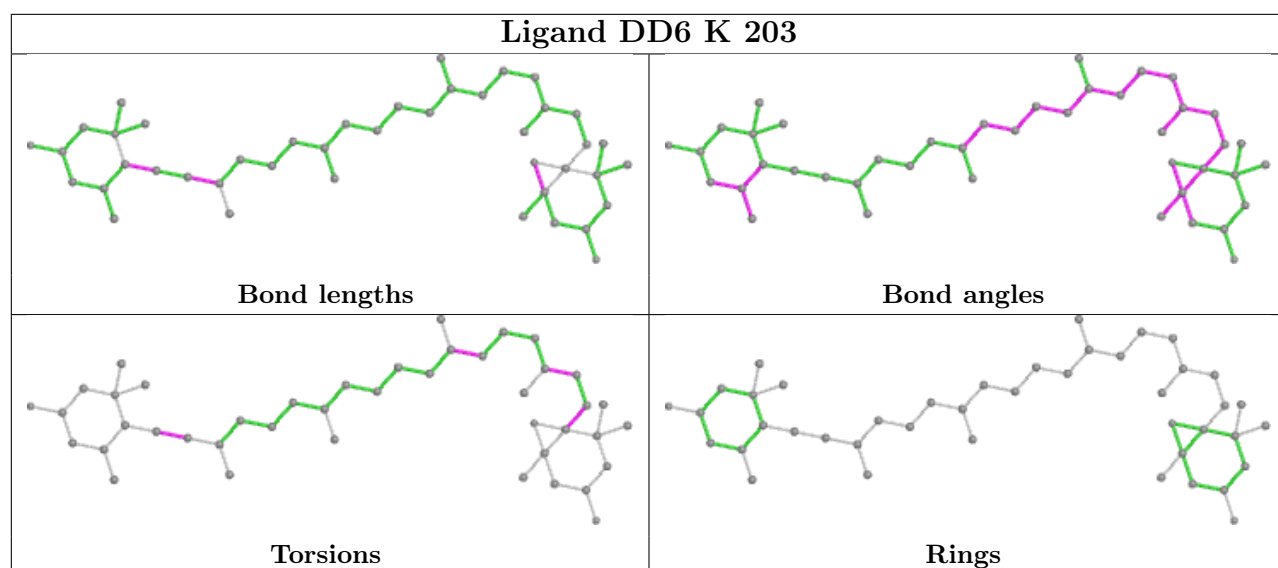


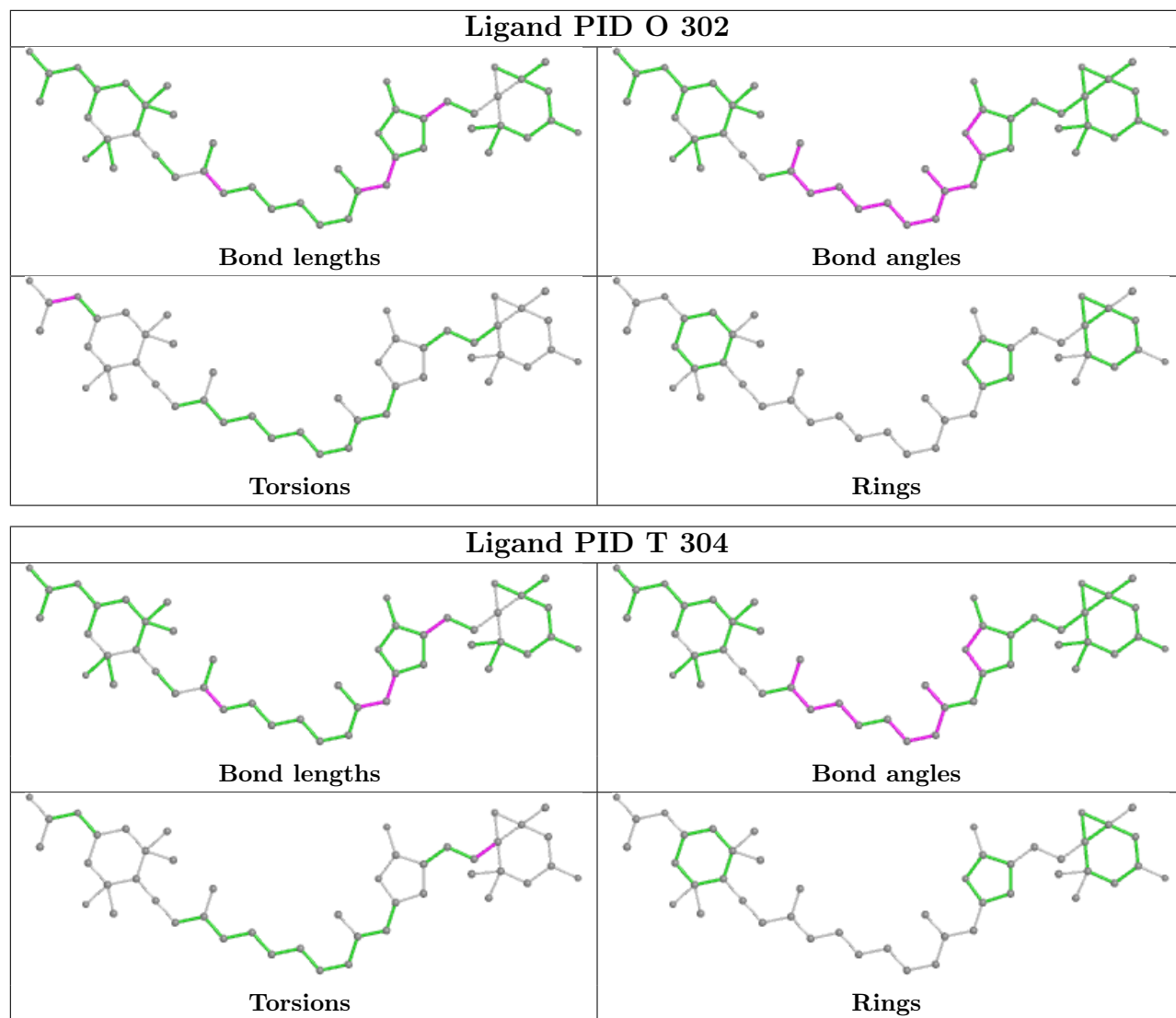
Torsions

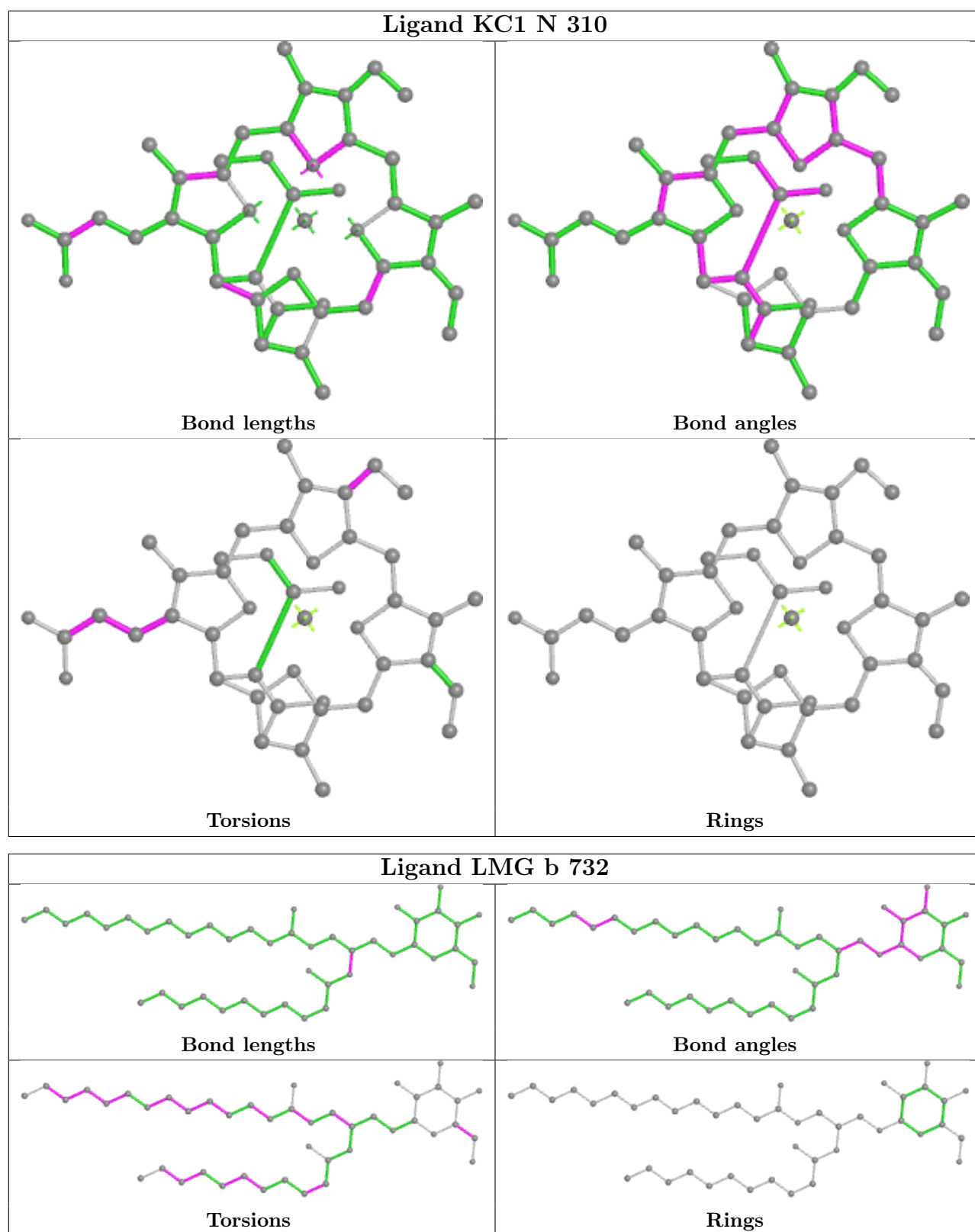


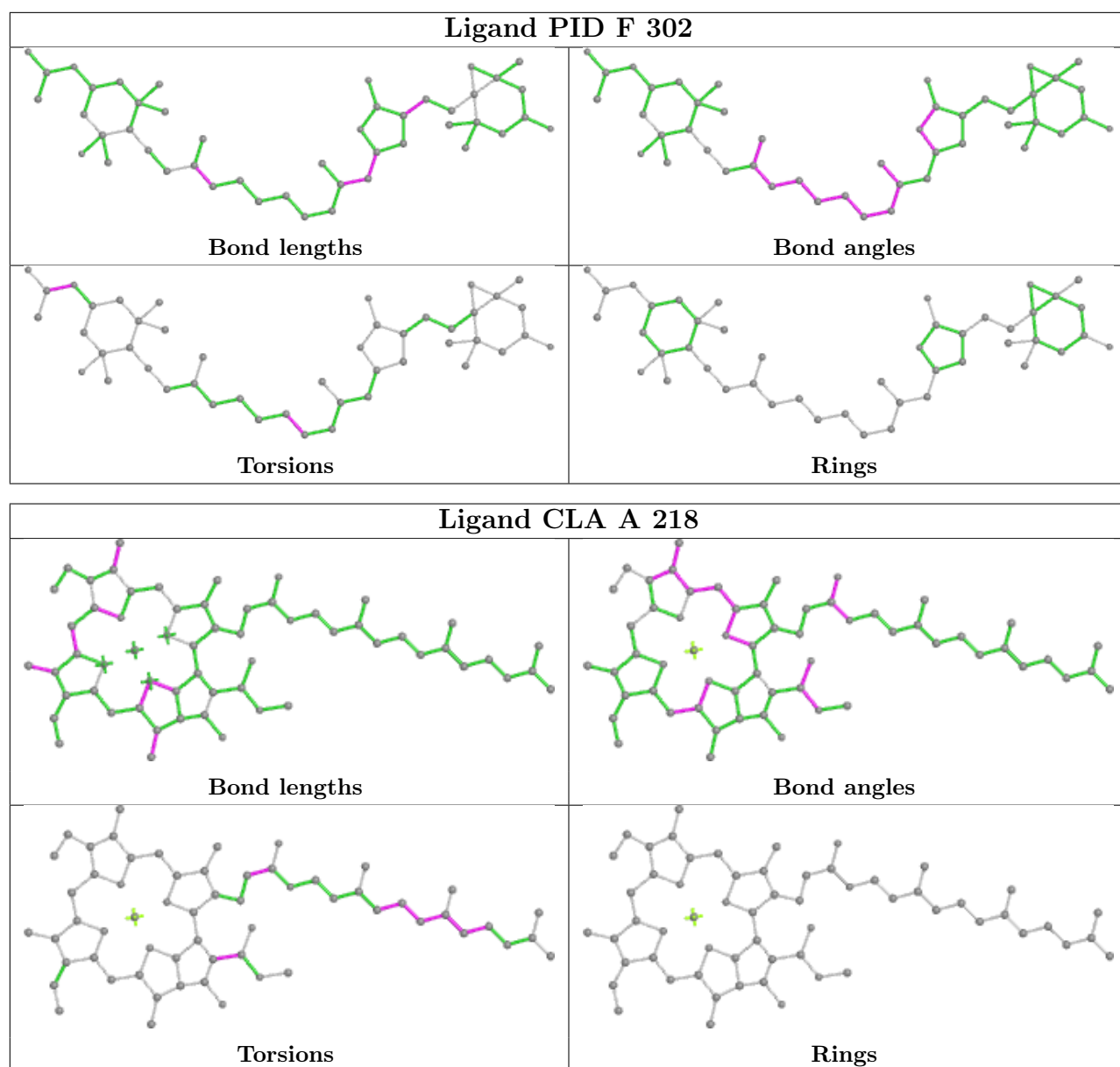
Rings



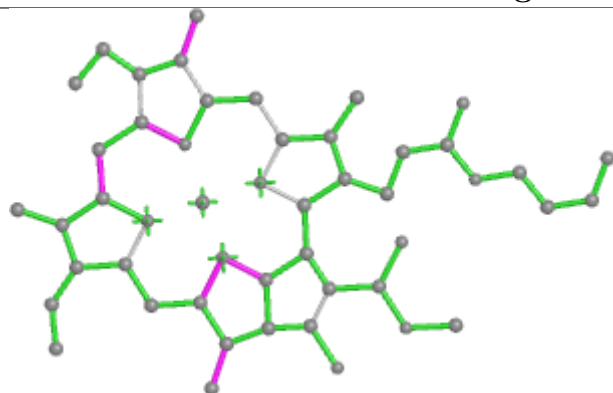




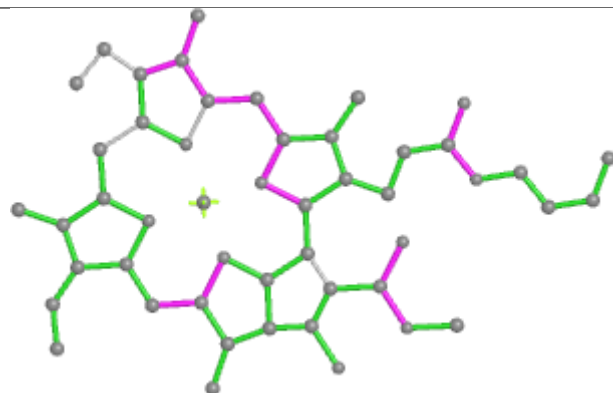




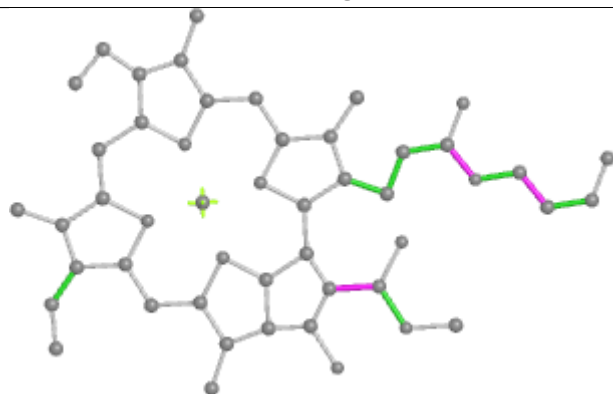
Ligand CLA B 306



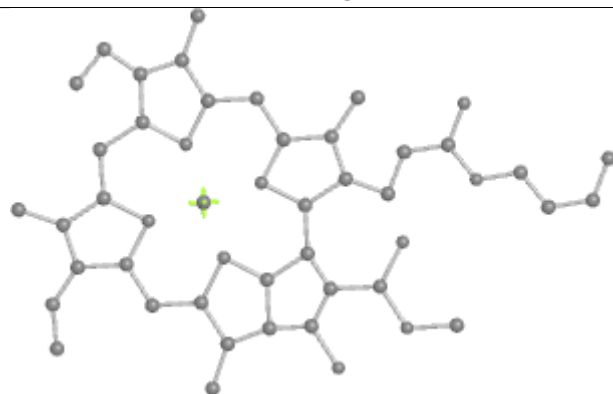
Bond lengths



Bond angles

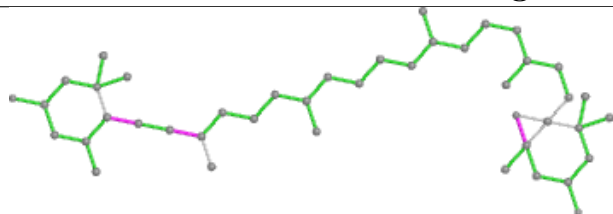


Torsions

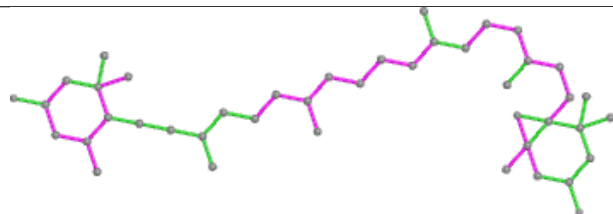


Rings

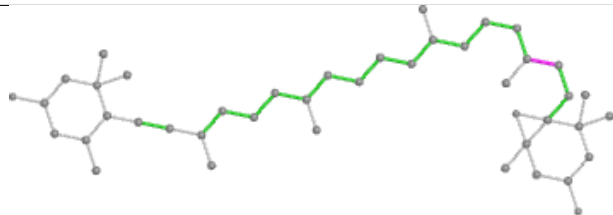
Ligand DD6 M 301



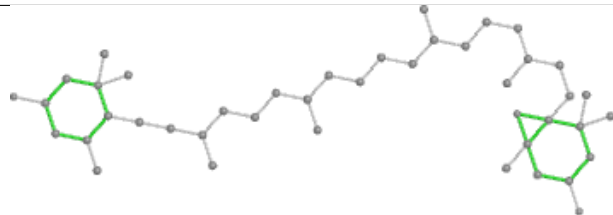
Bond lengths



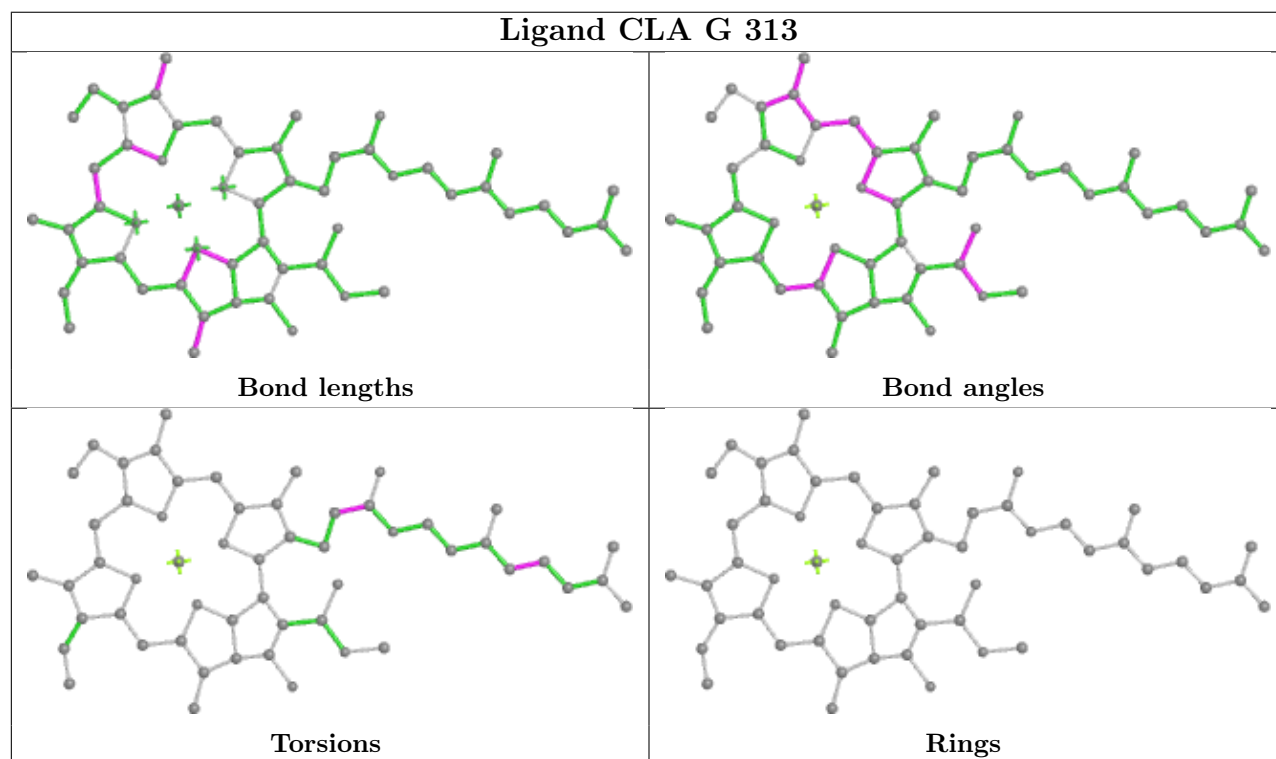
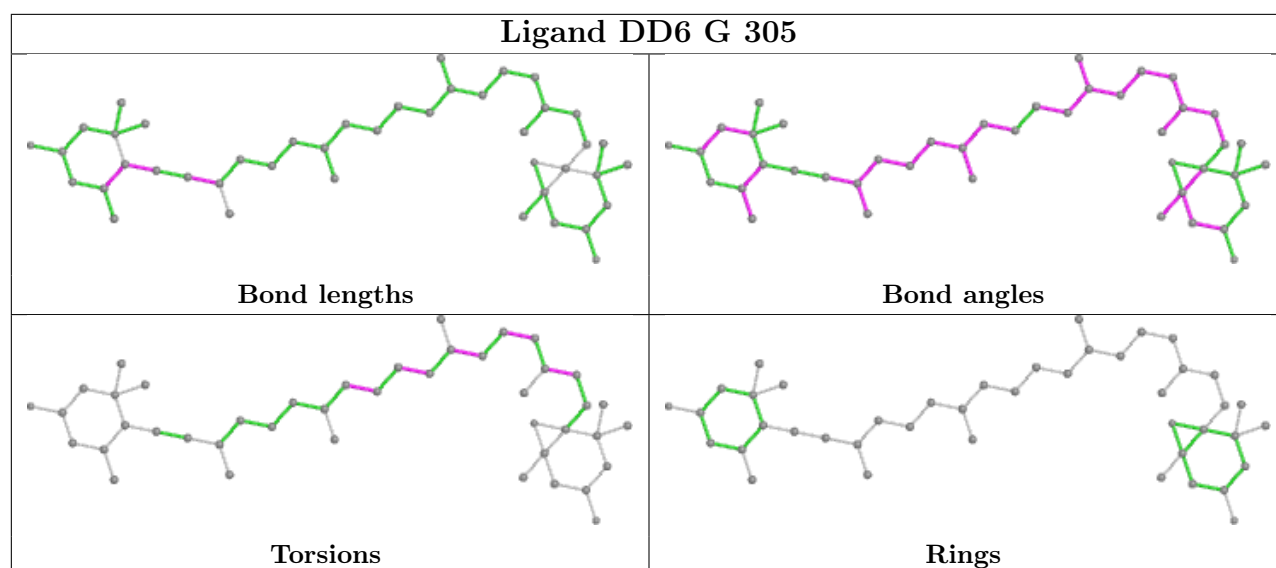
Bond angles

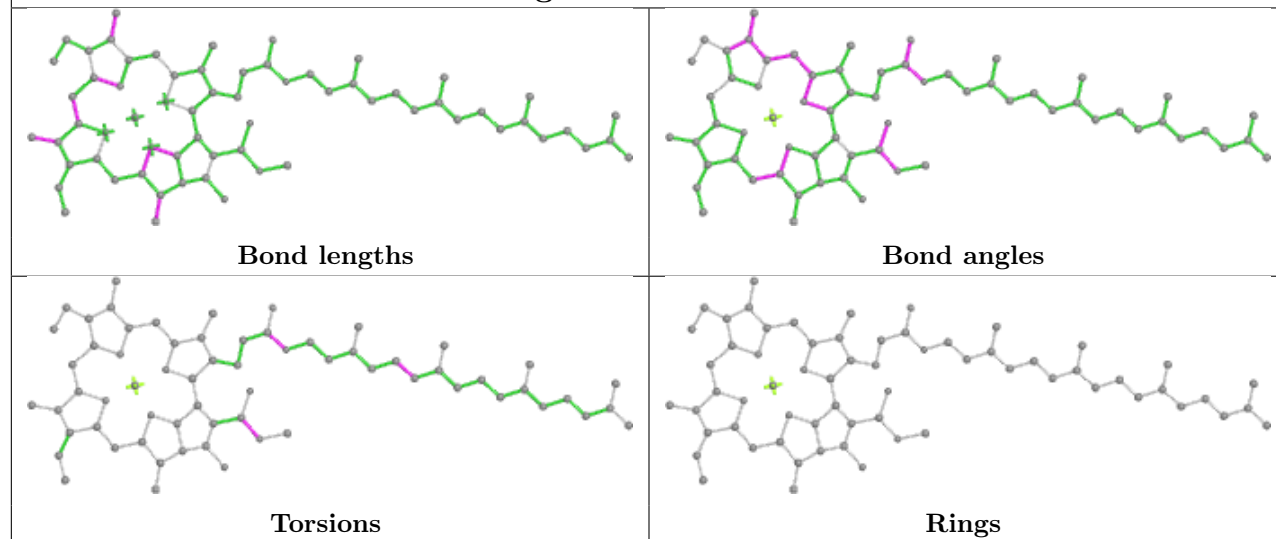
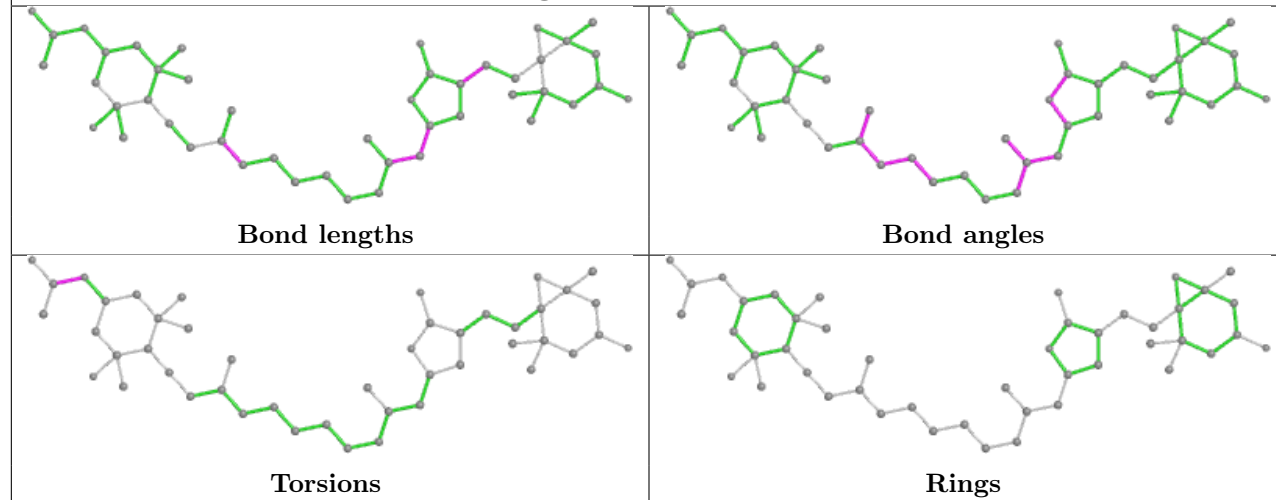


Torsions

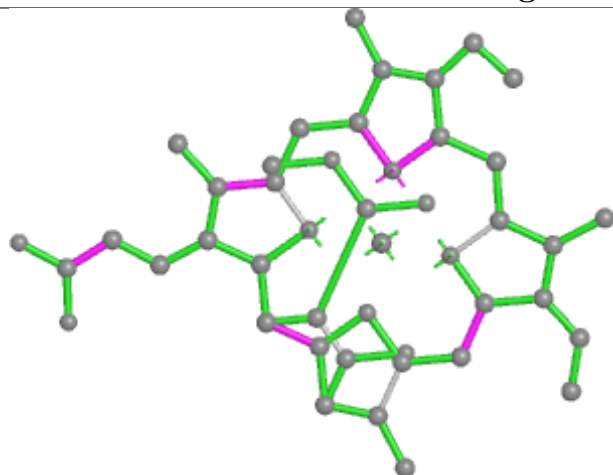


Rings

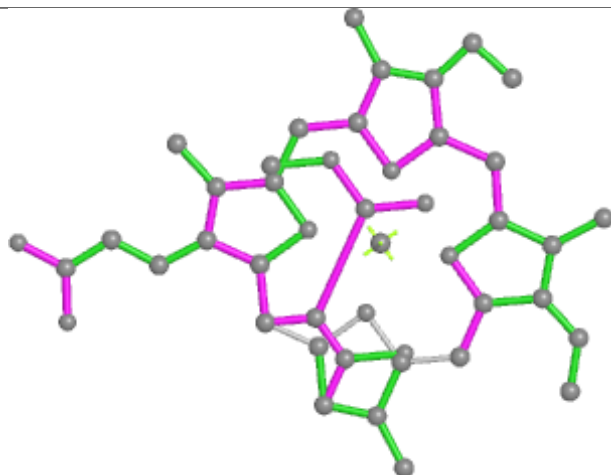


Ligand CLA b 723**Ligand PID N 302**

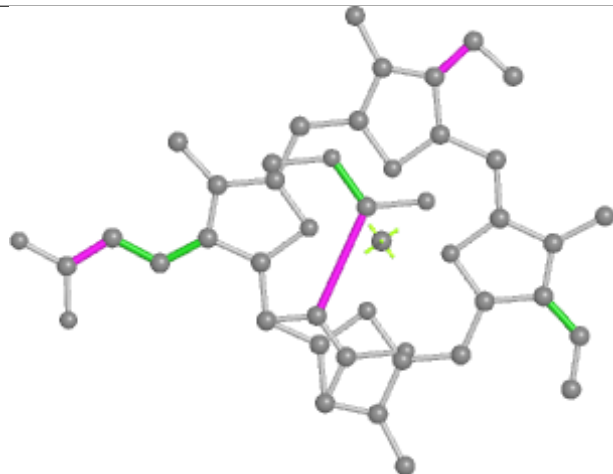
Ligand KC1 L 306



Bond lengths



Bond angles

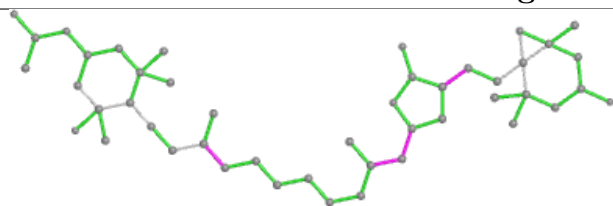


Torsions

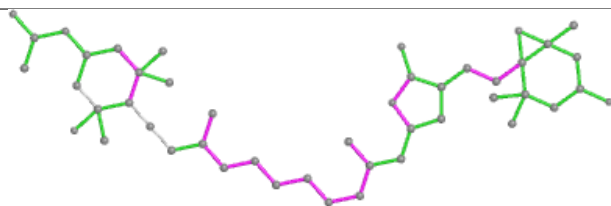


Rings

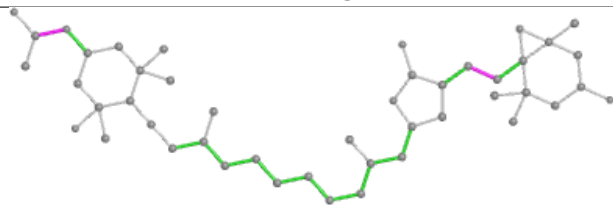
Ligand PID H 305



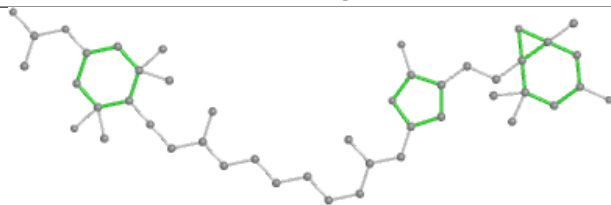
Bond lengths



Bond angles

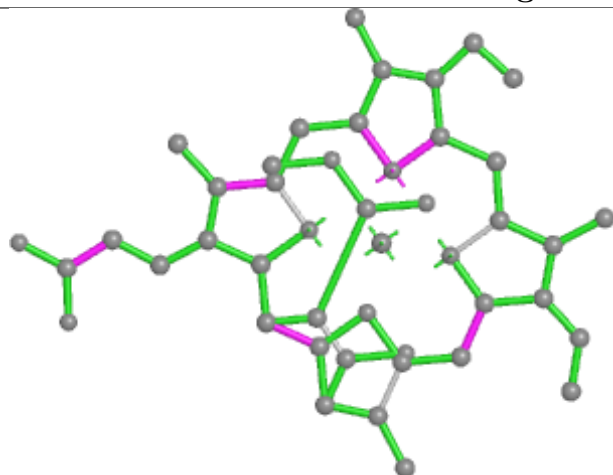


Torsions

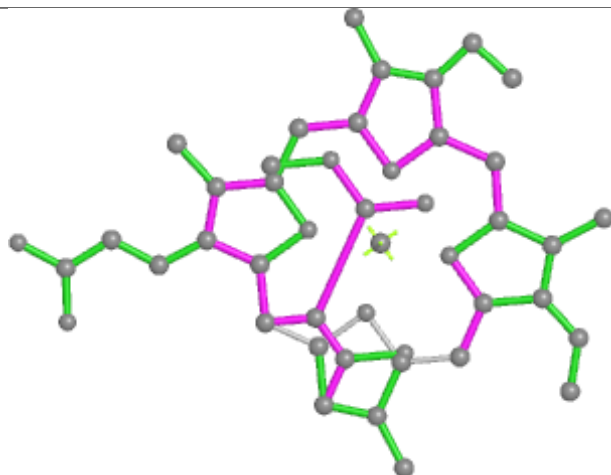


Rings

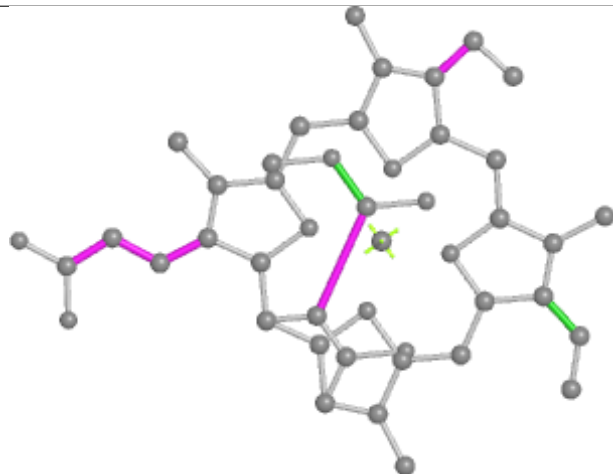
Ligand KC1 P 211



Bond lengths



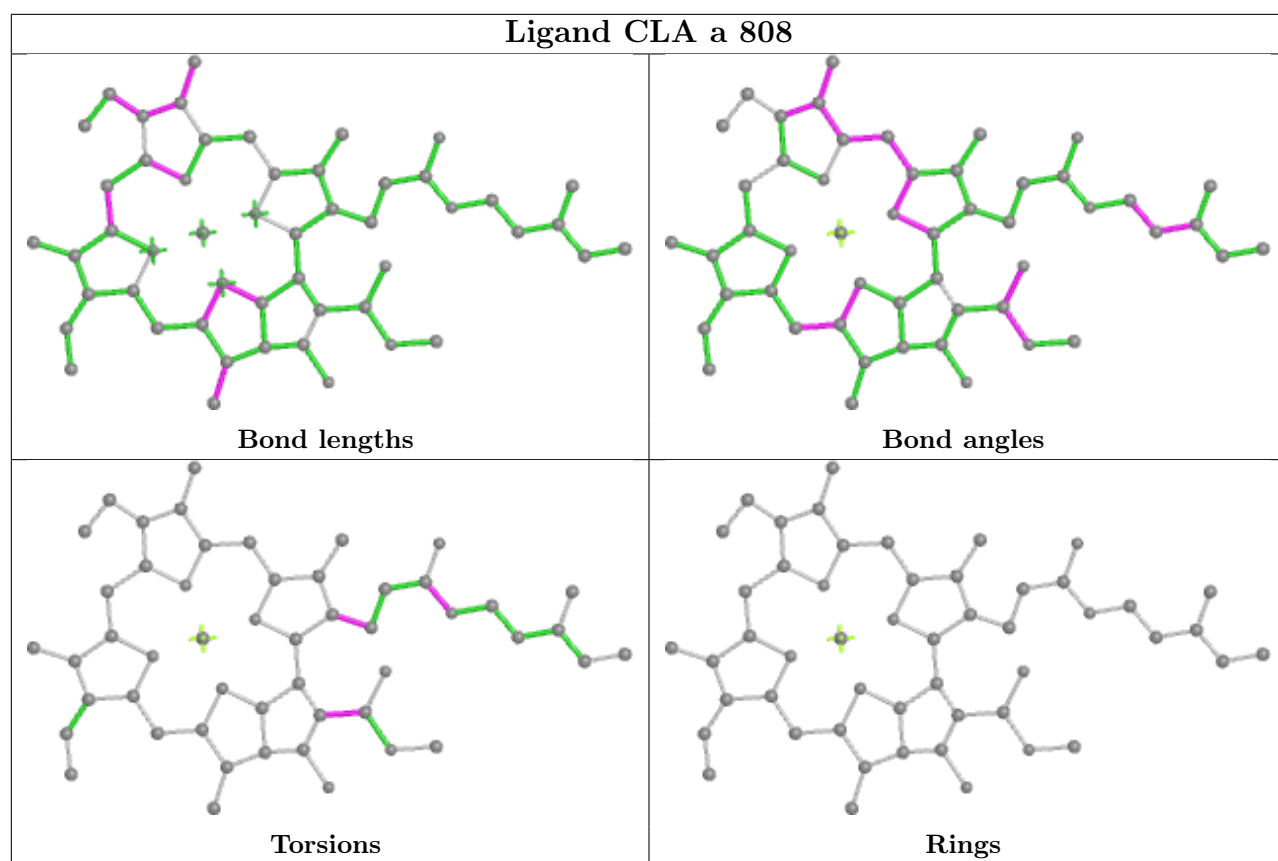
Bond angles



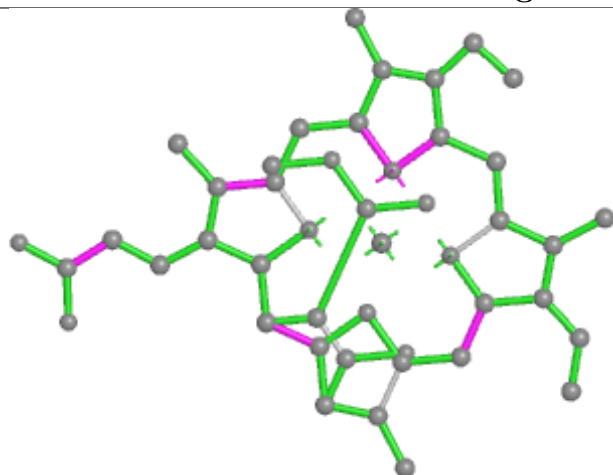
Torsions



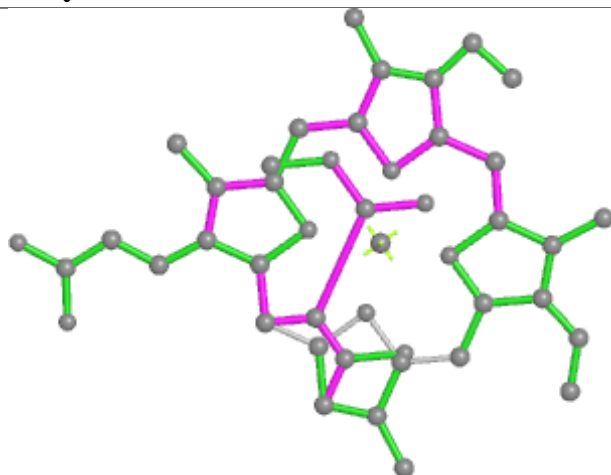
Rings



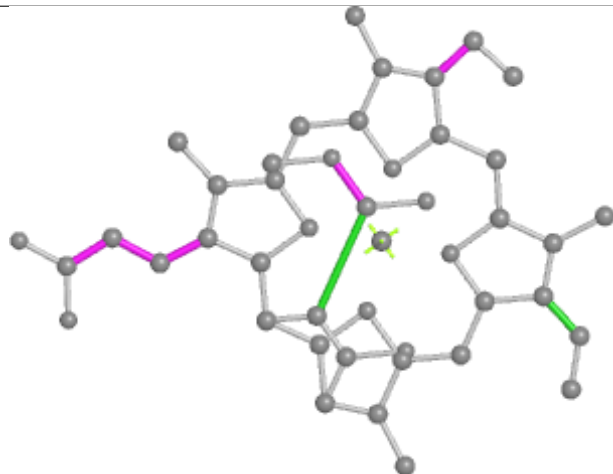
Ligand KC1 Q 314



Bond lengths



Bond angles

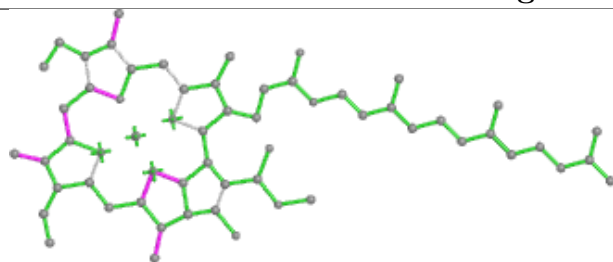


Torsions

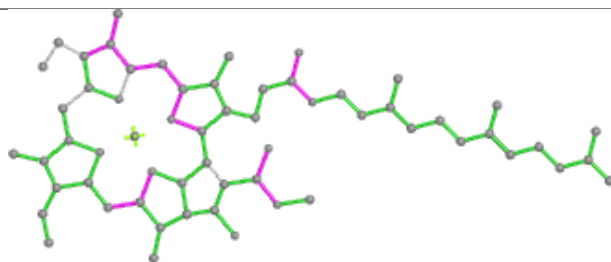


Rings

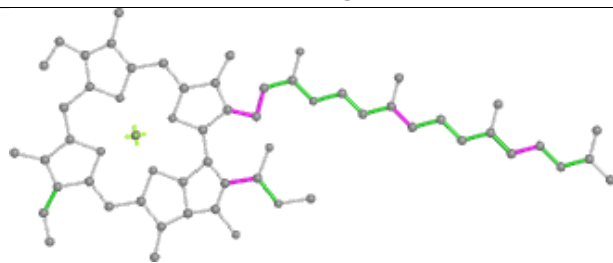
Ligand CLA h 201



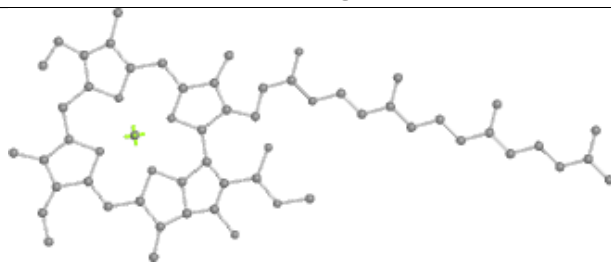
Bond lengths



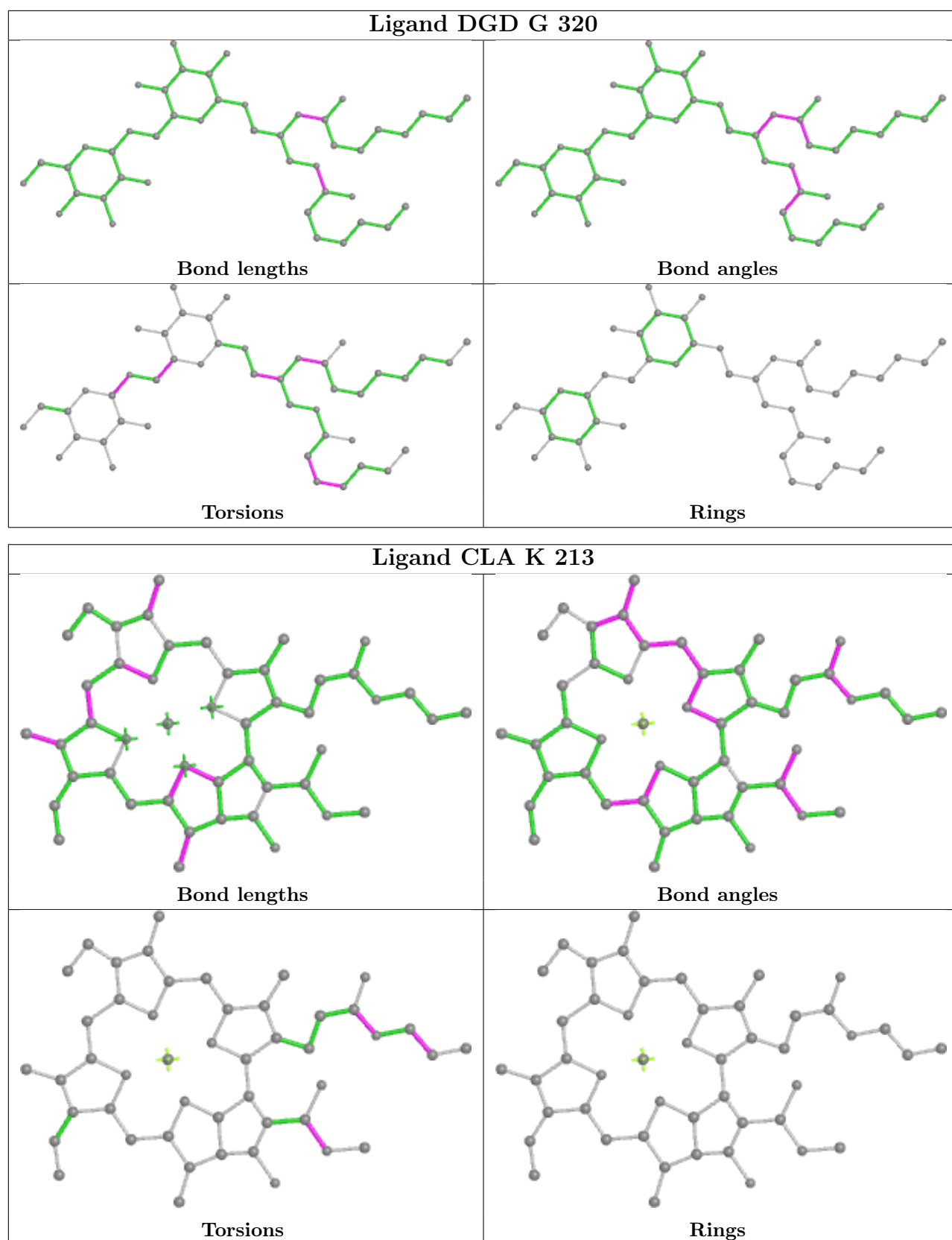
Bond angles



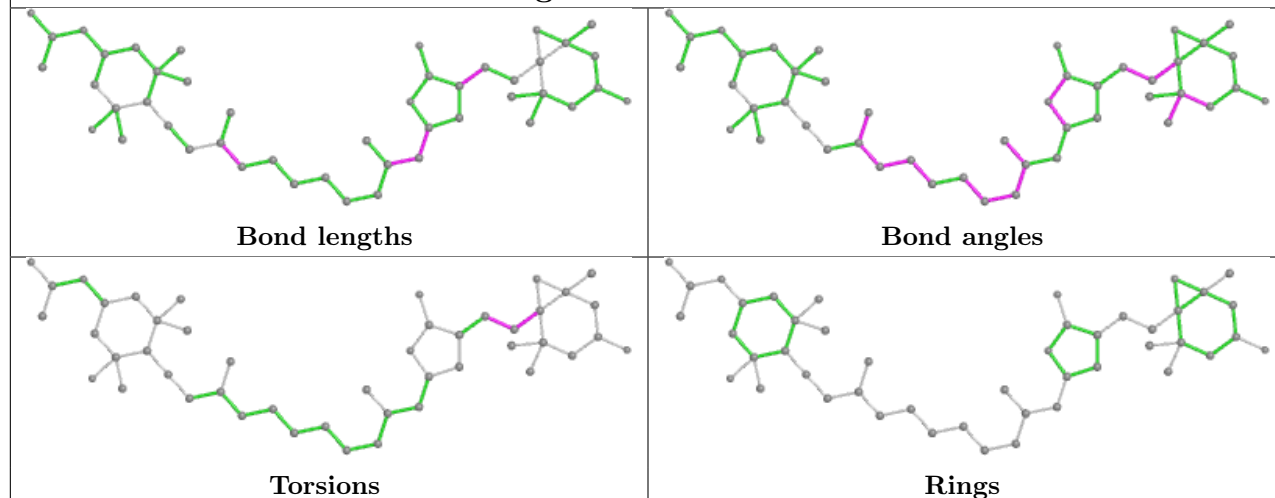
Torsions



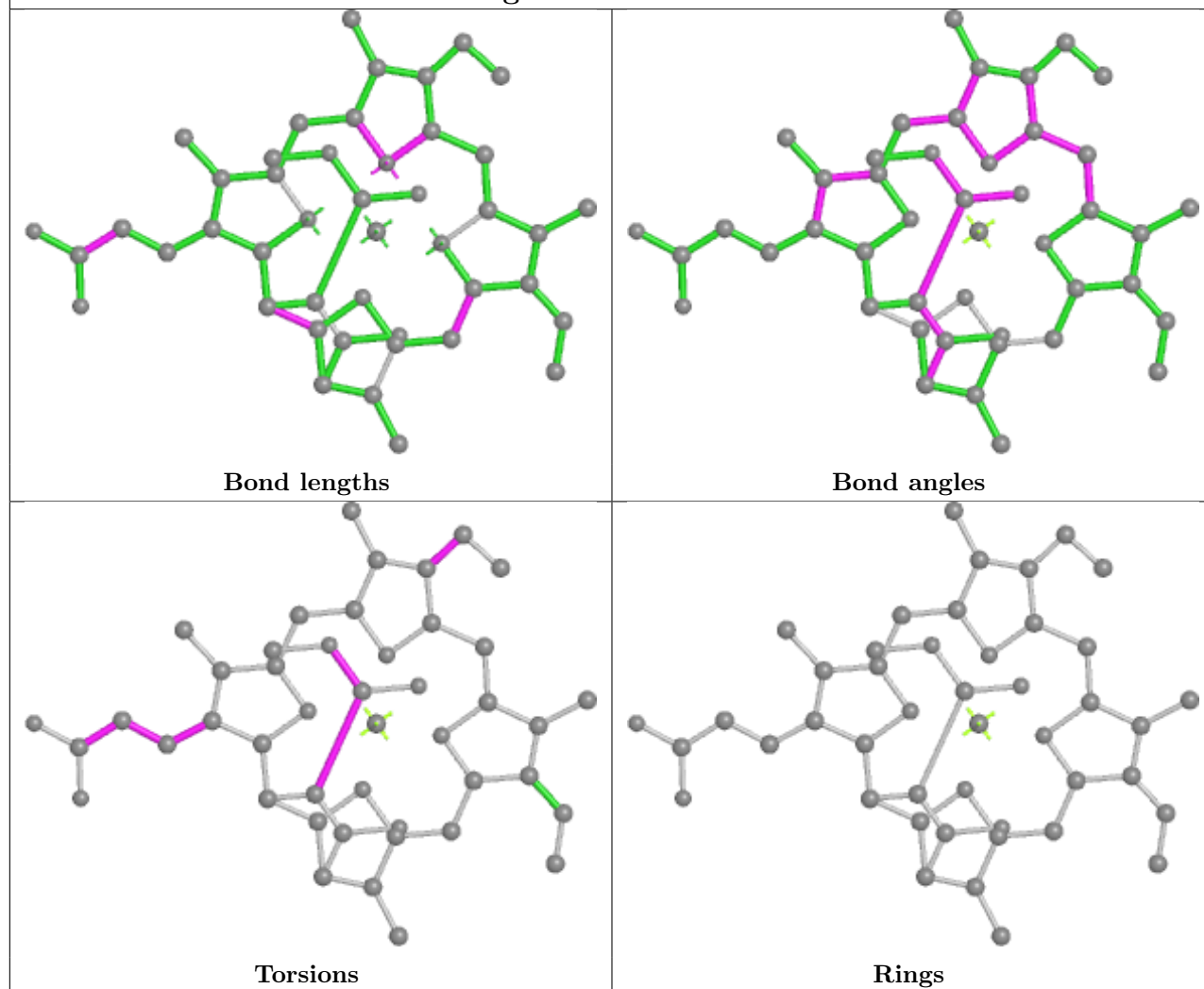
Rings



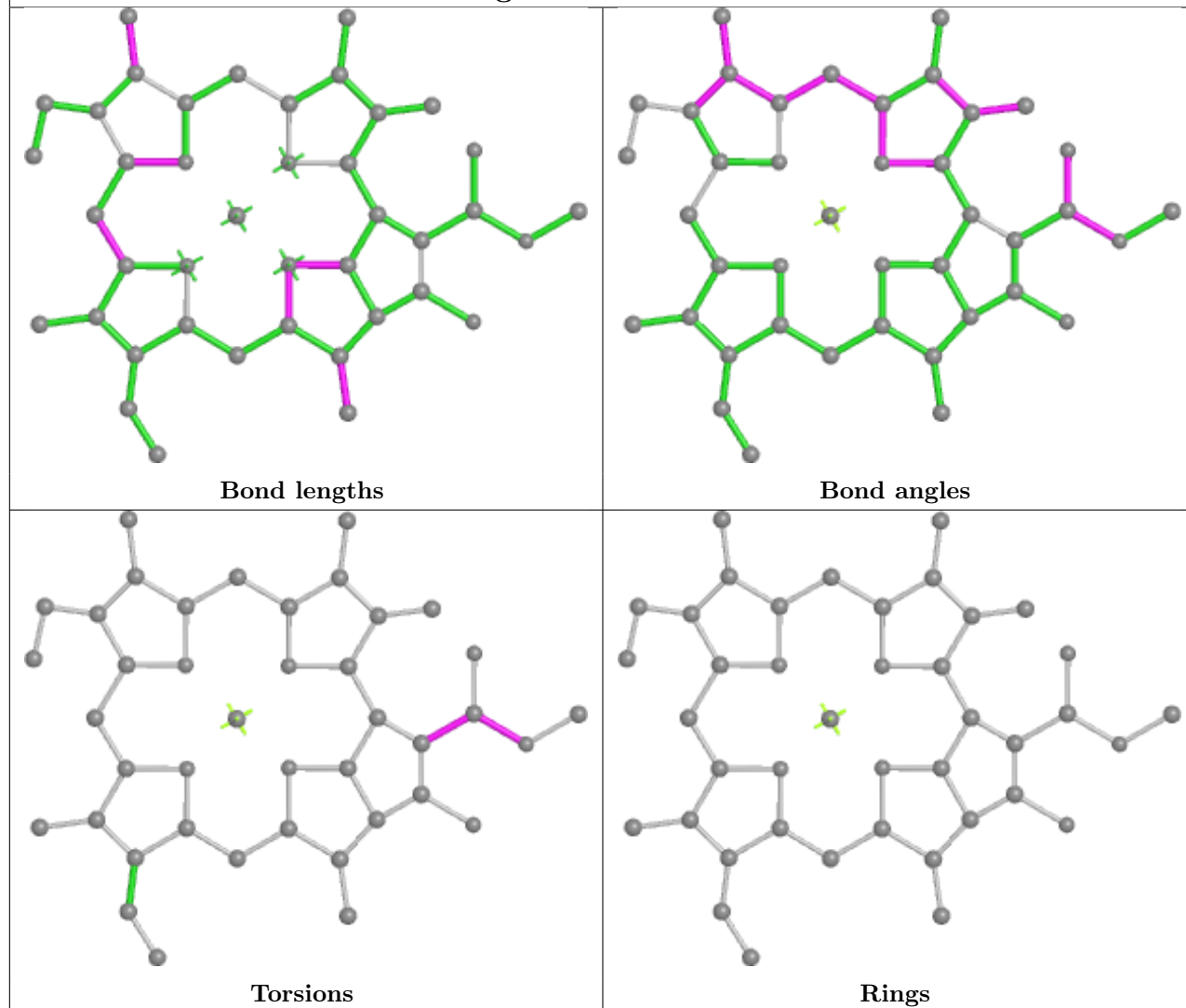
Ligand PID O 307



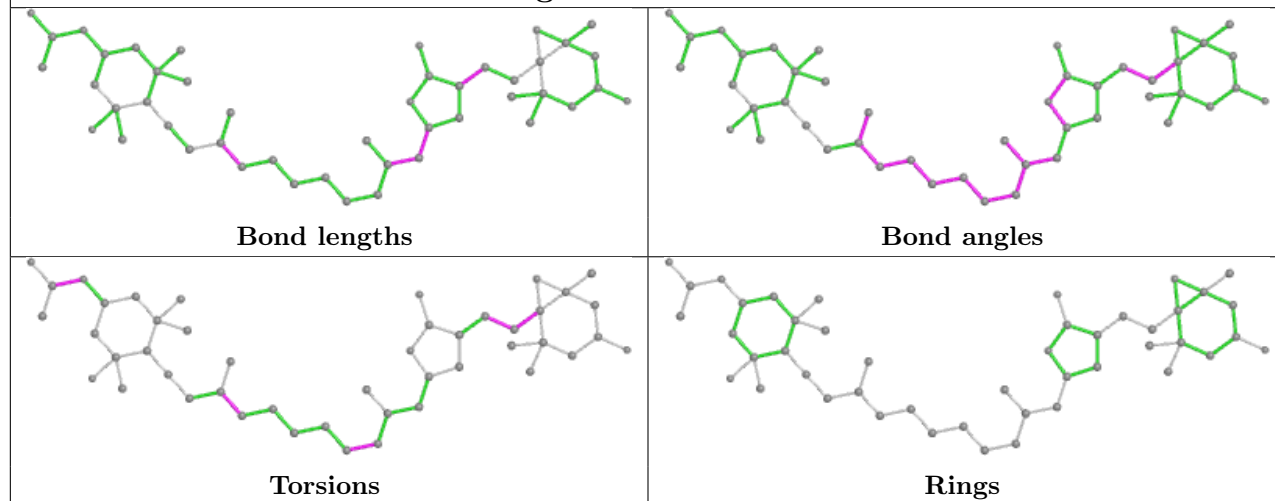
Ligand KC1 O 315

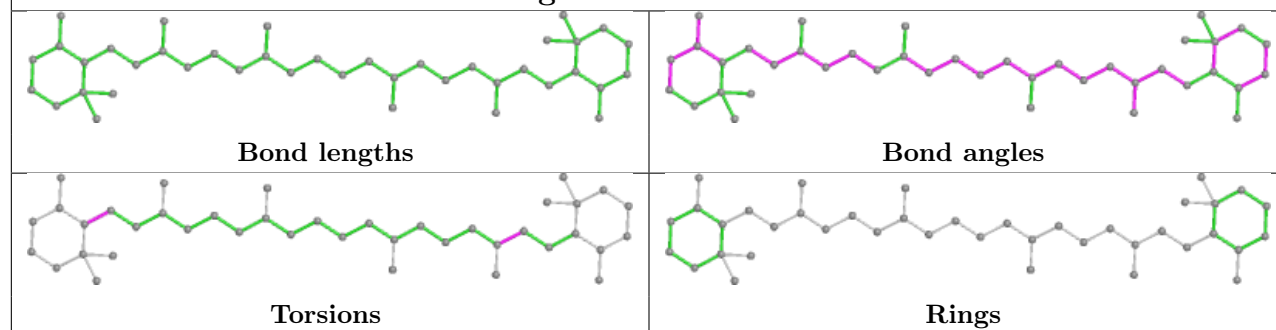
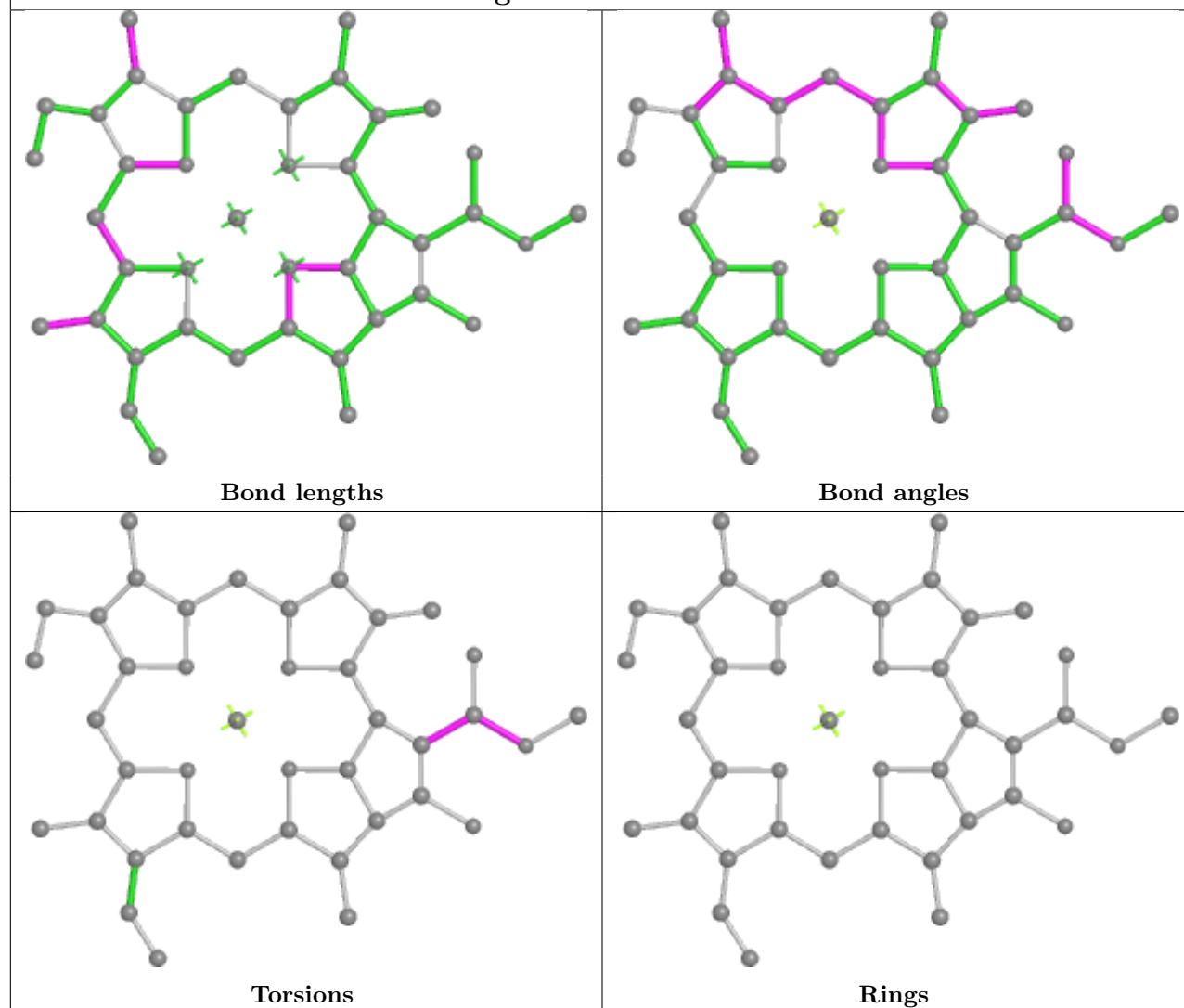


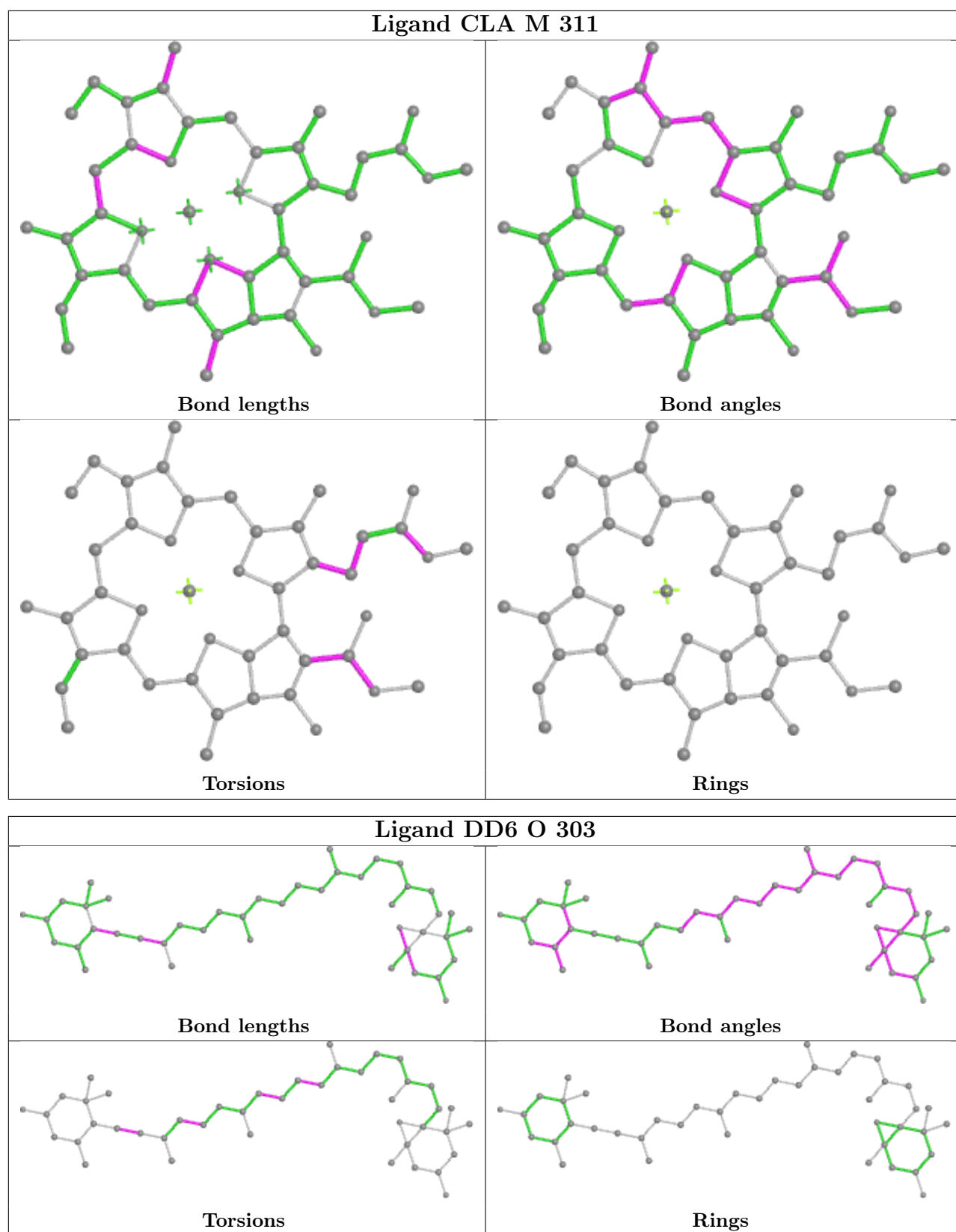
Ligand CLA F 316



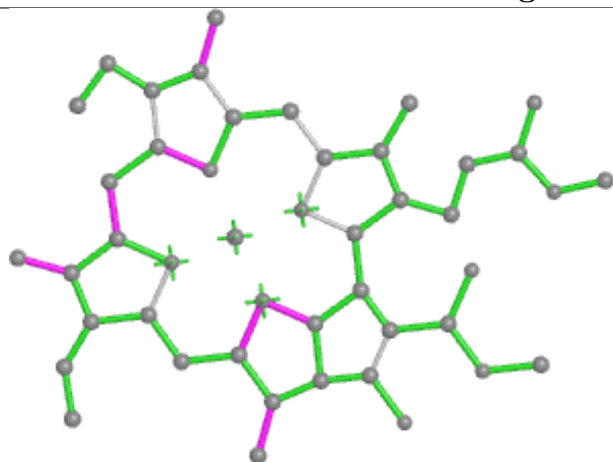
Ligand PID C 305



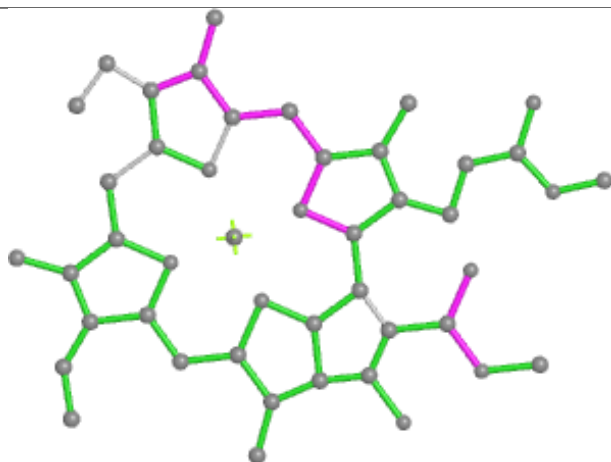
Ligand BCR i 204**Ligand CLA P 217**



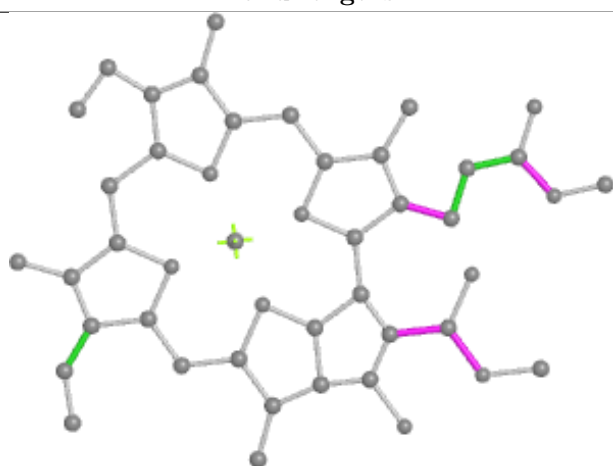
Ligand CLA a 828



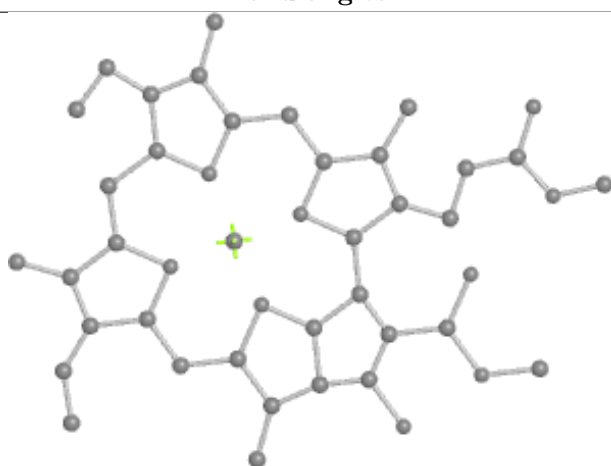
Bond lengths



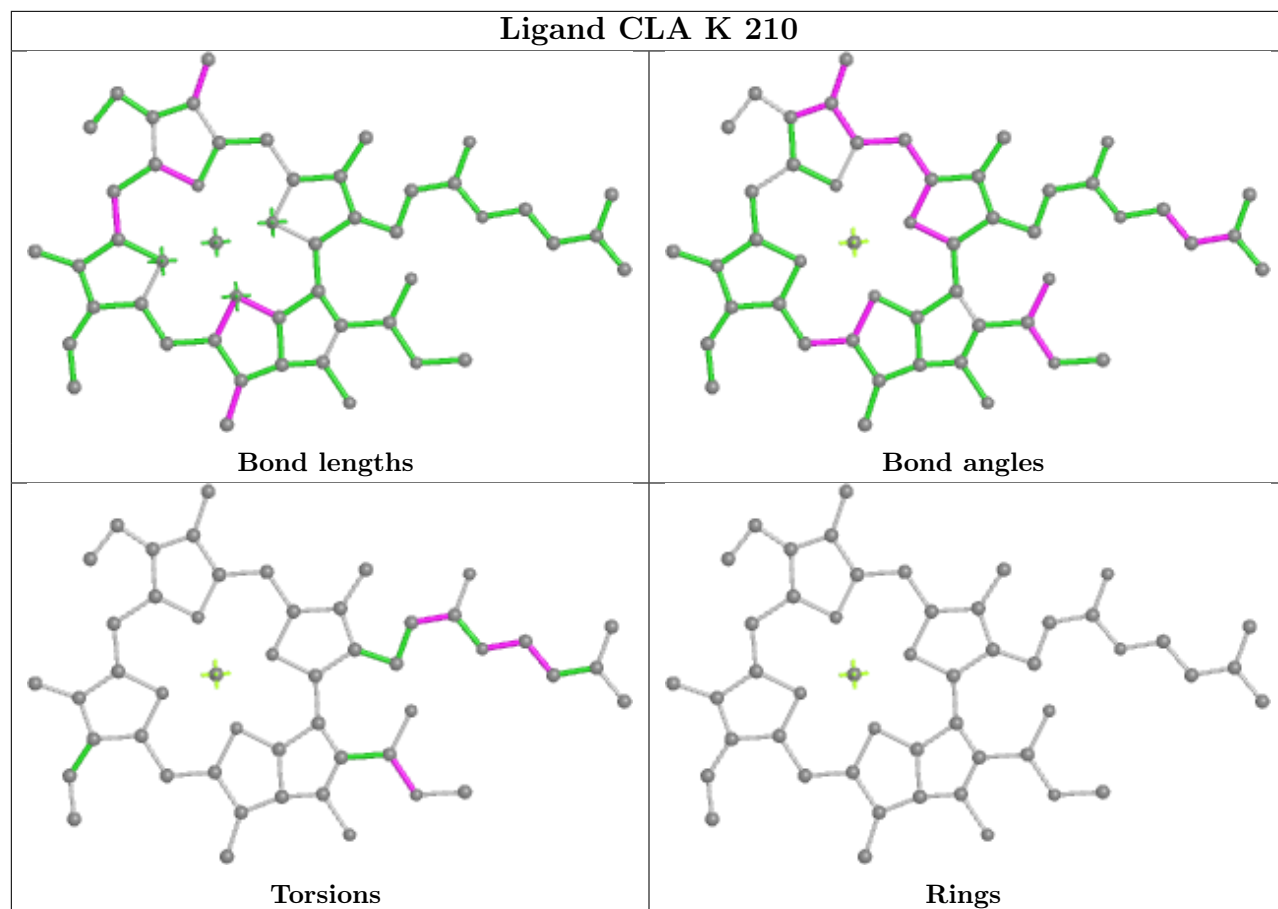
Bond angles



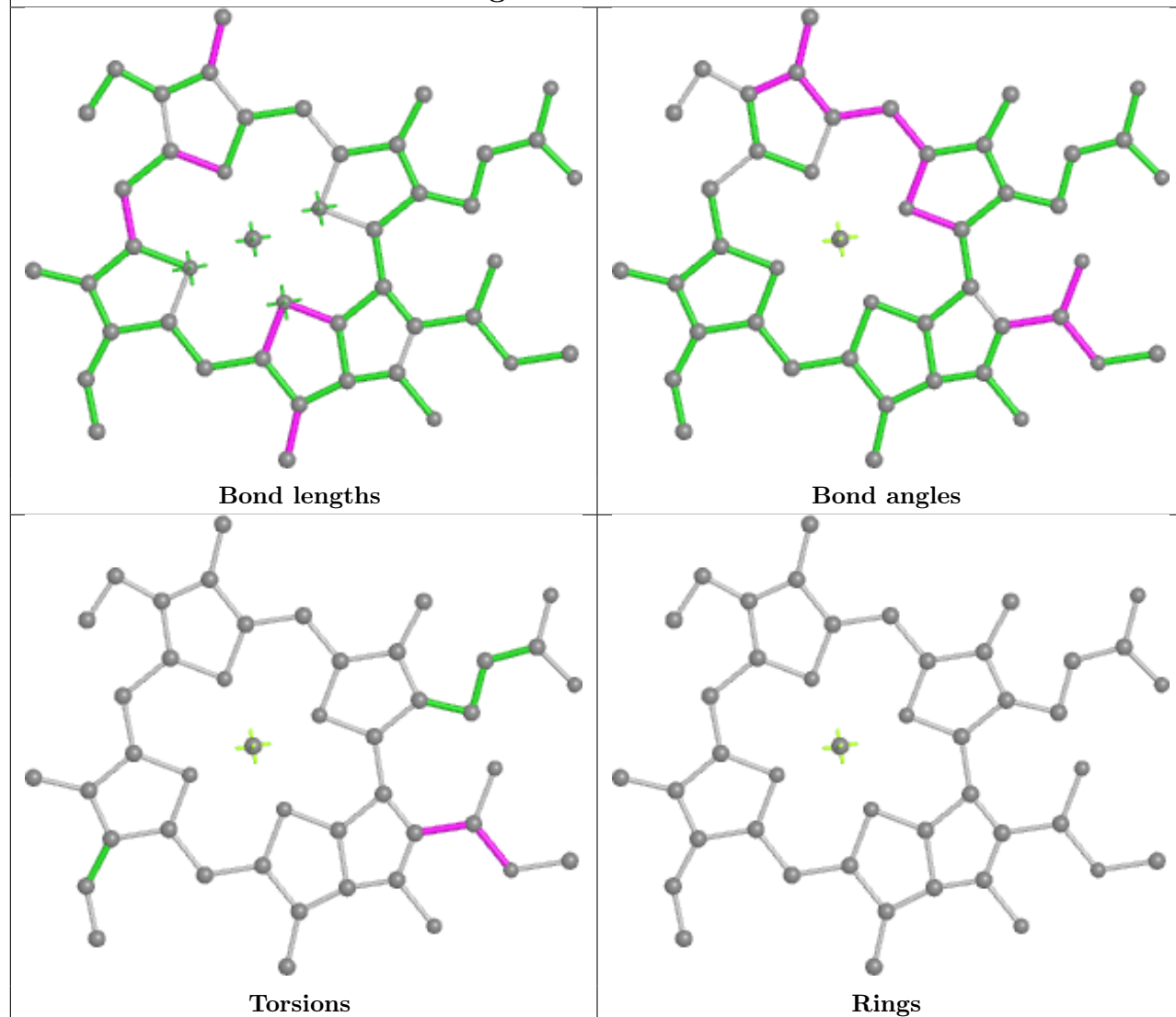
Torsions



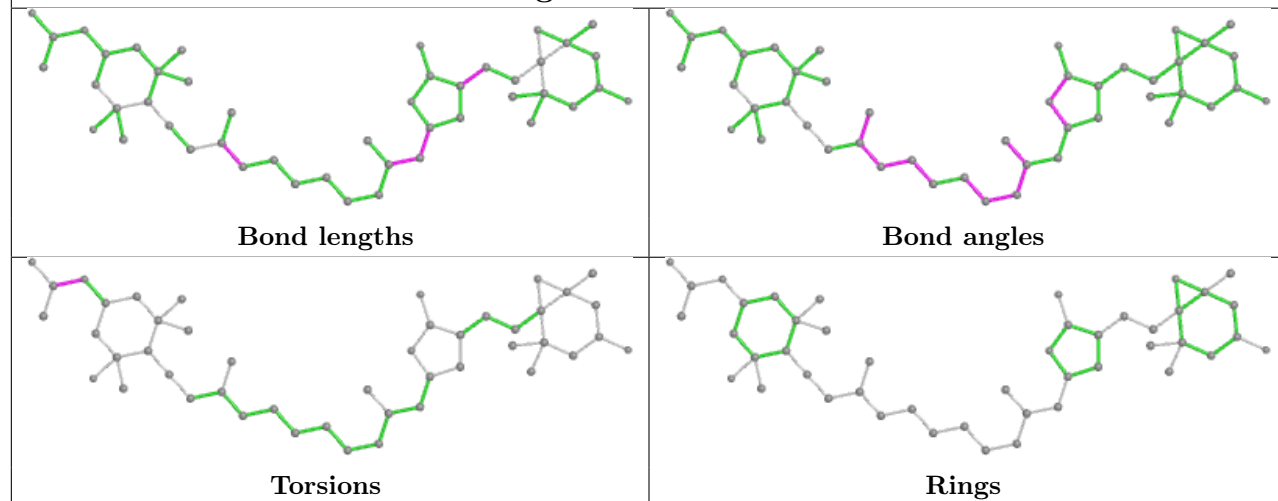
Rings

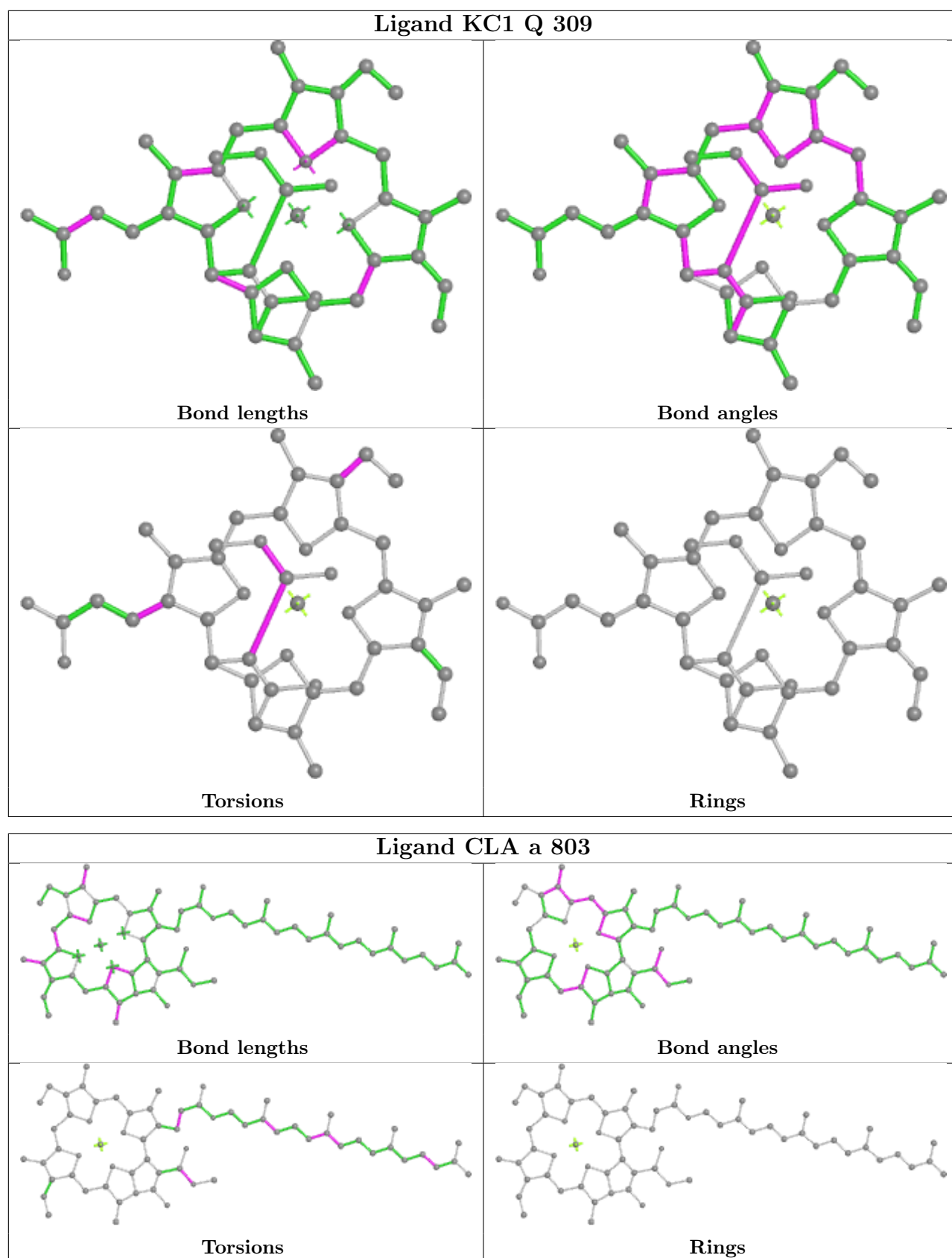


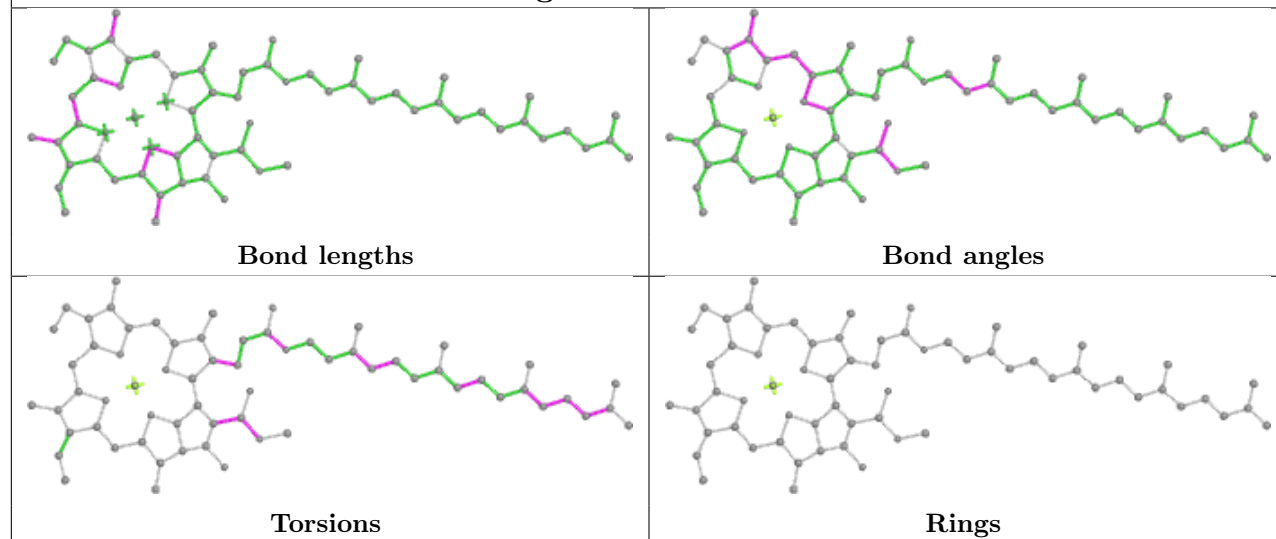
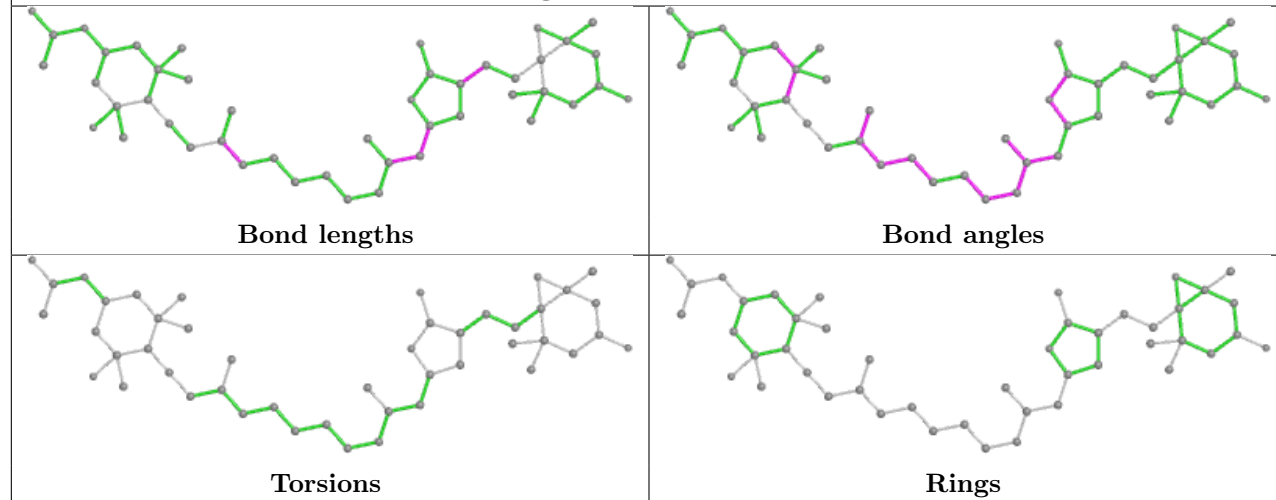
Ligand CLA A 206



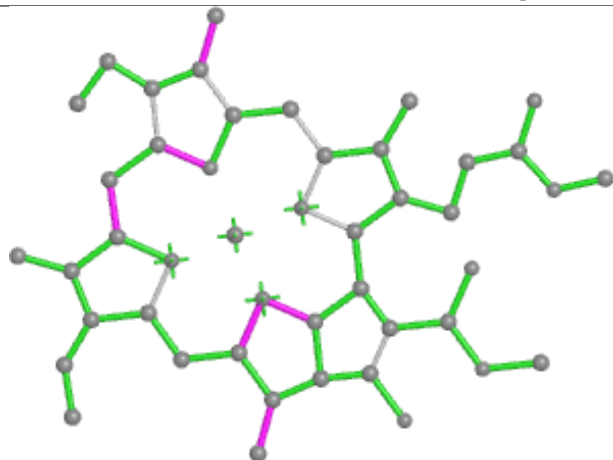
Ligand PID H 301



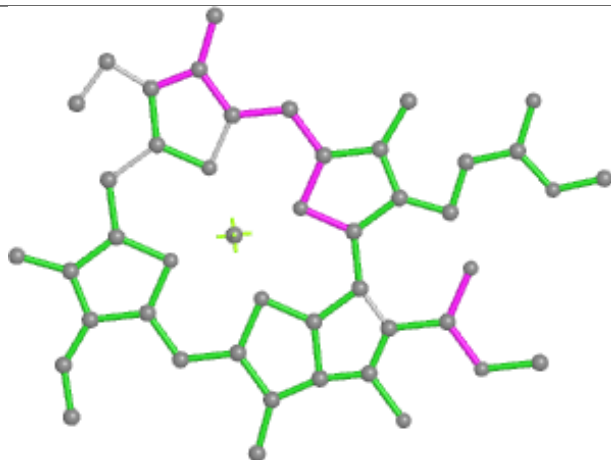


Ligand CLA J 306**Ligand PID T 305**

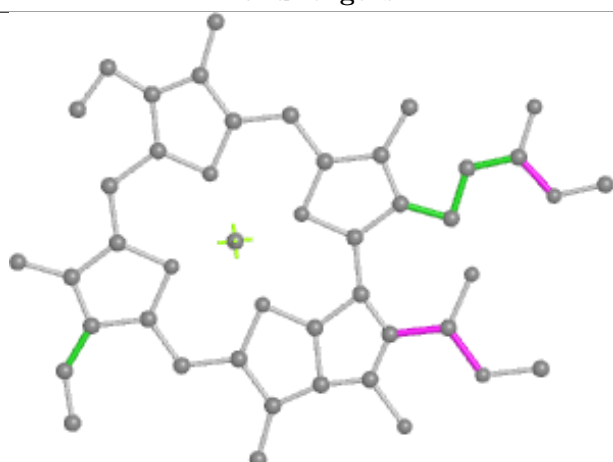
Ligand CLA C 313



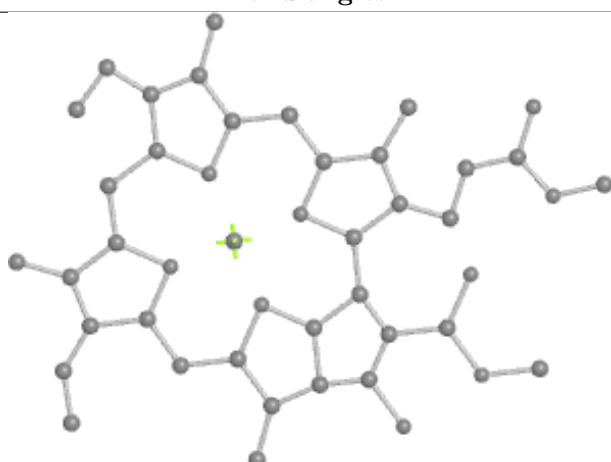
Bond lengths



Bond angles

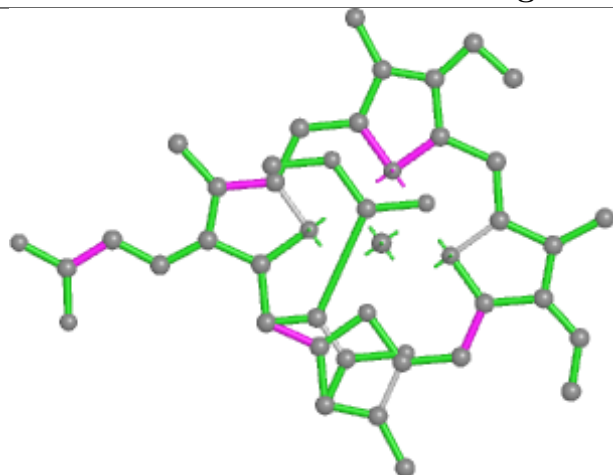


Torsions

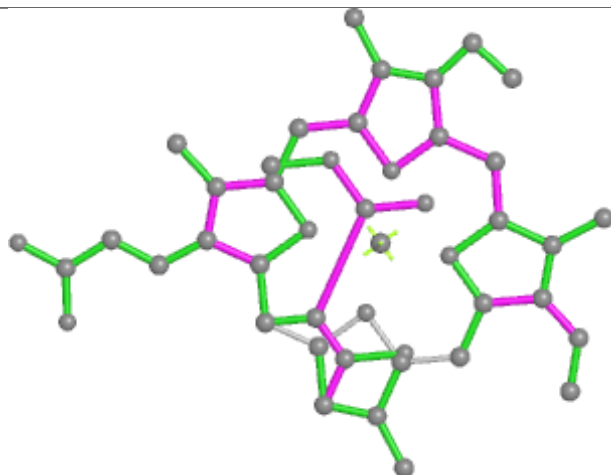


Rings

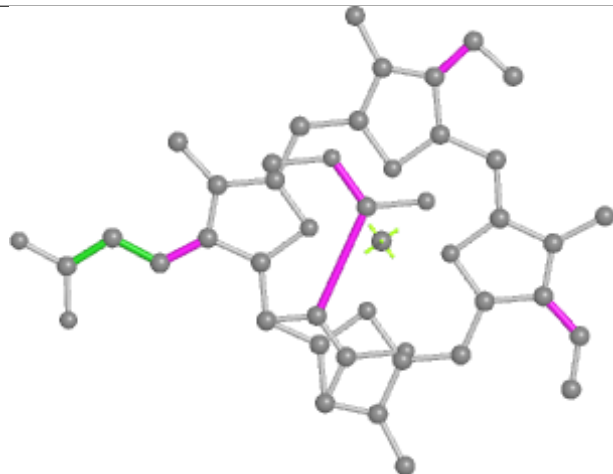
Ligand KC1 E 312



Bond lengths



Bond angles

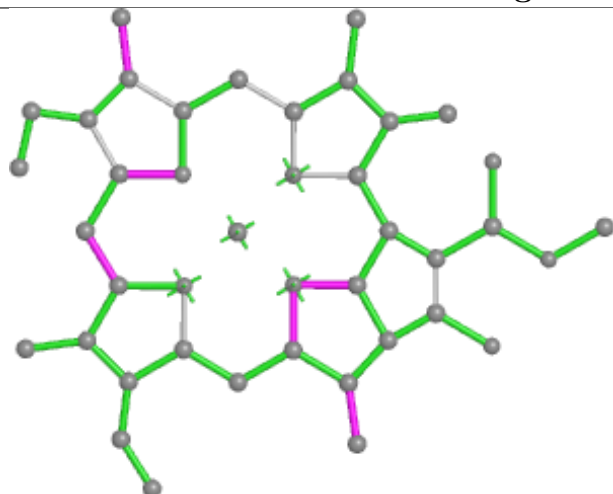


Torsions

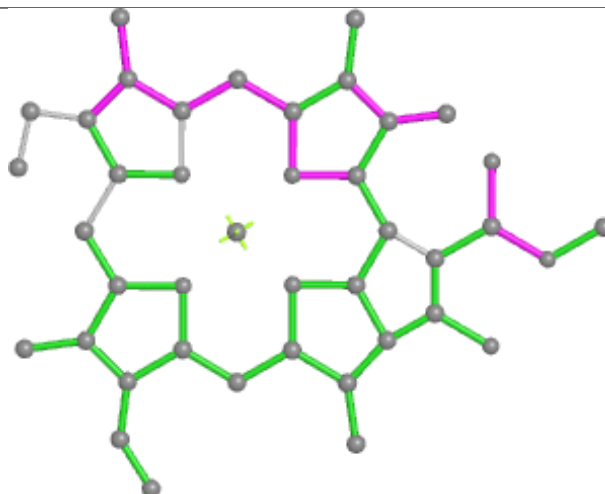


Rings

Ligand CLA C 316



Bond lengths



Bond angles

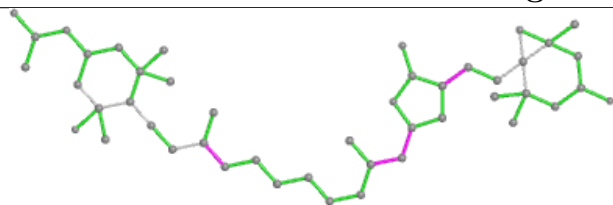


Torsions

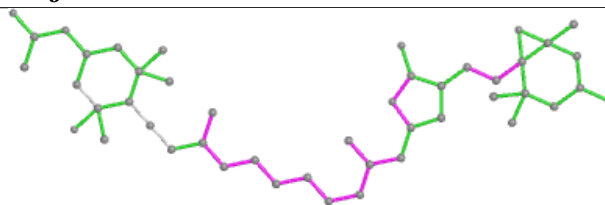


Rings

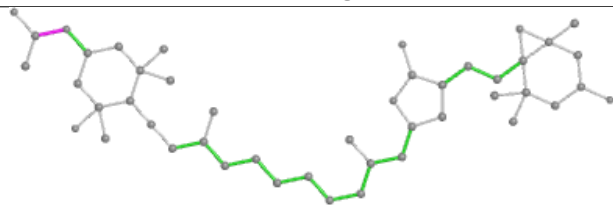
Ligand PID j 101



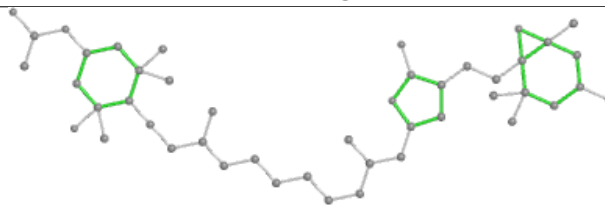
Bond lengths



Bond angles

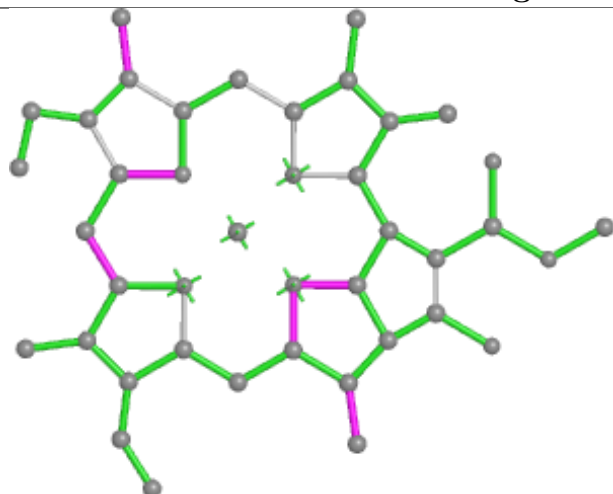


Torsions

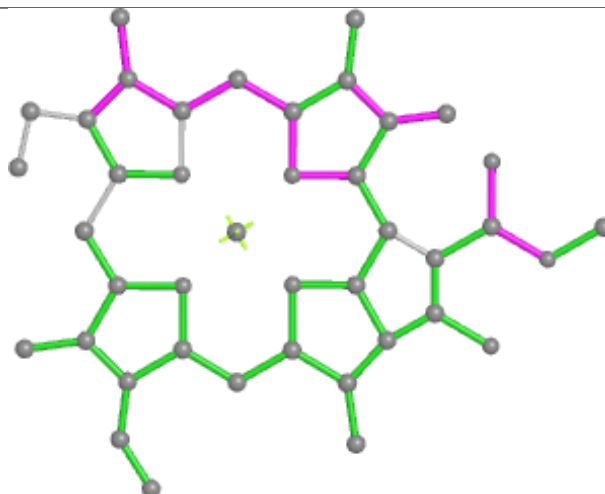


Rings

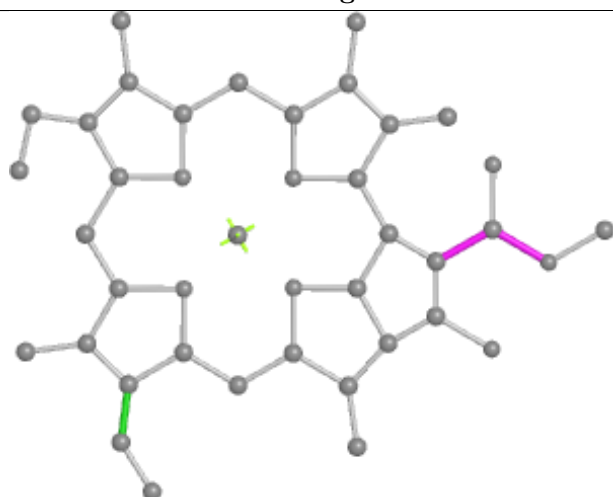
Ligand CLA G 319



Bond lengths



Bond angles

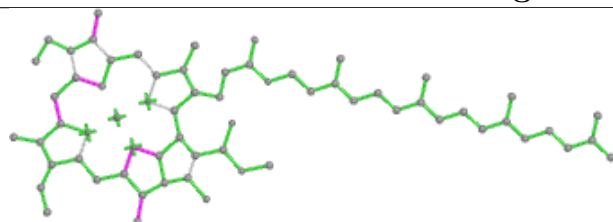


Torsions

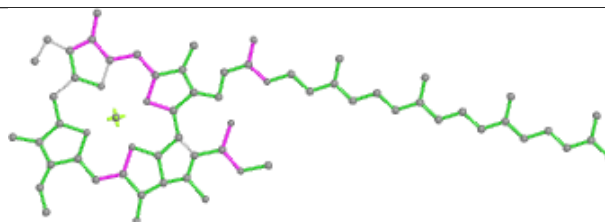


Rings

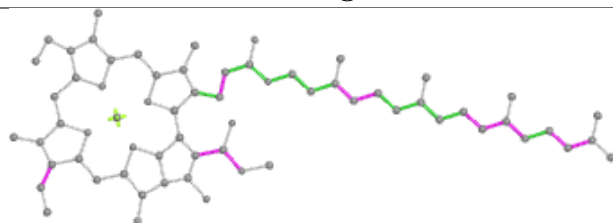
Ligand CLA N 309



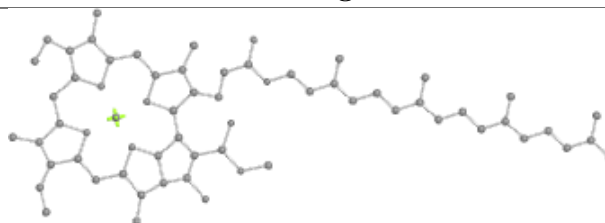
Bond lengths



Bond angles

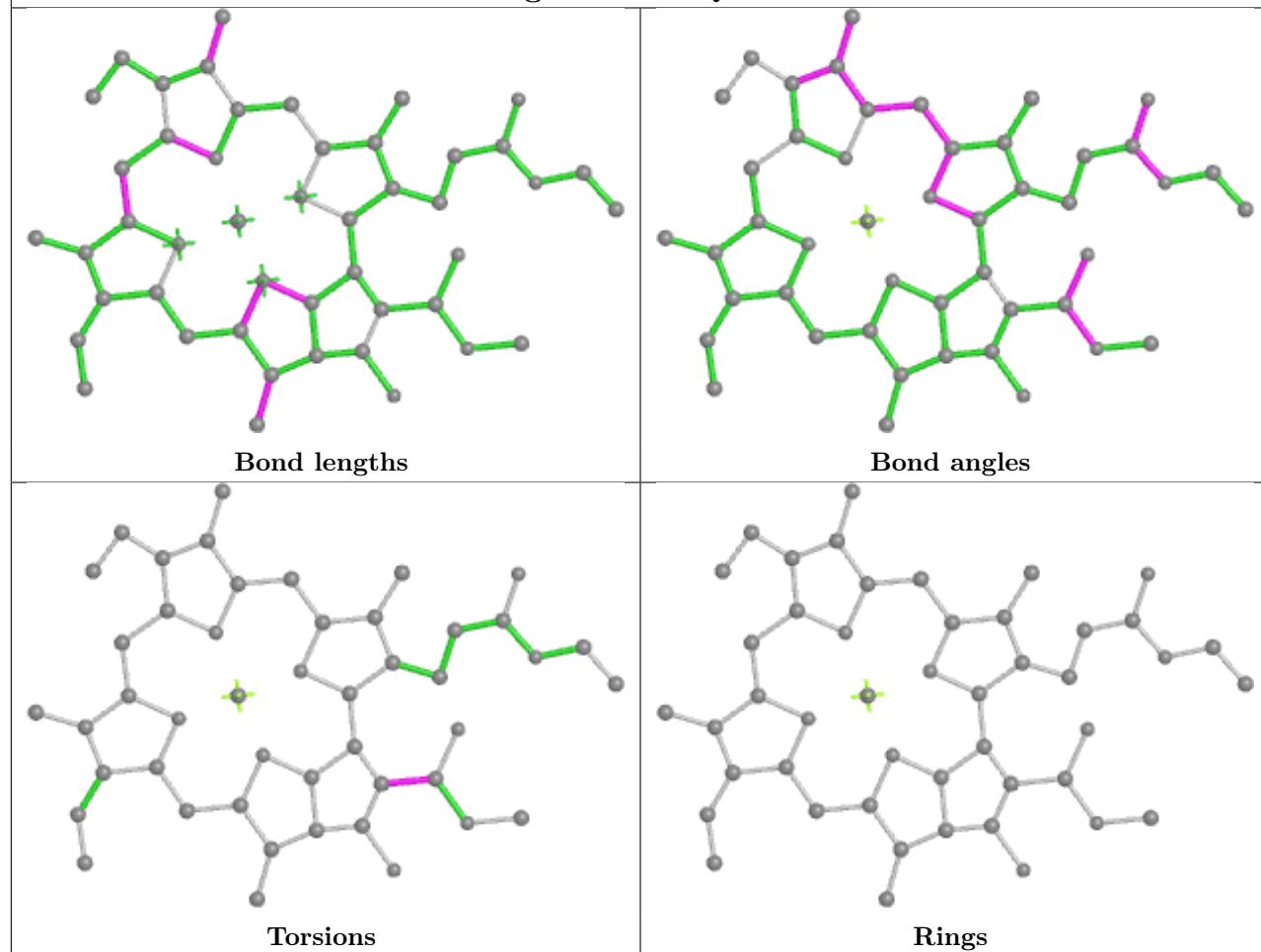


Torsions

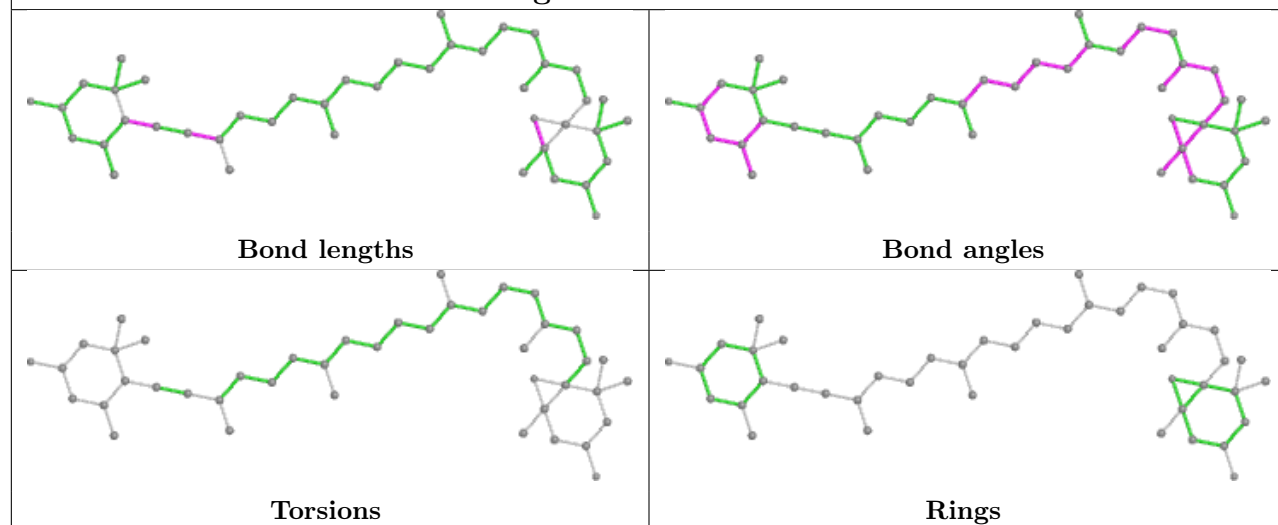


Rings

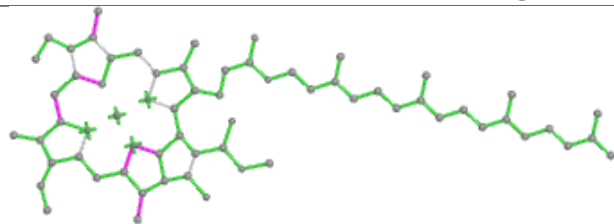
Ligand CLA Q 307



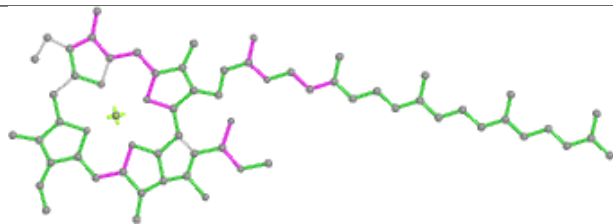
Ligand DD6 B 303



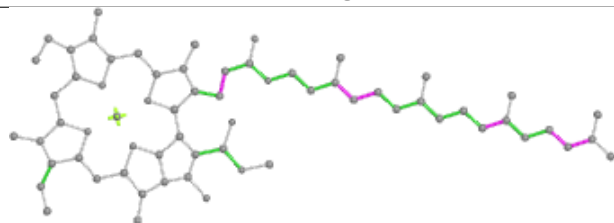
Ligand CLA H 308



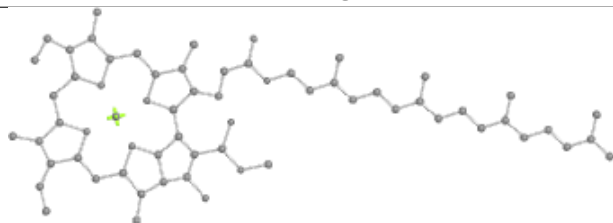
Bond lengths



Bond angles

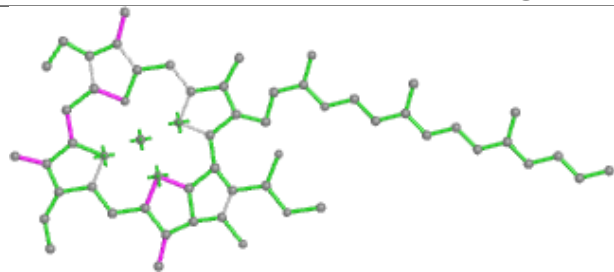


Torsions

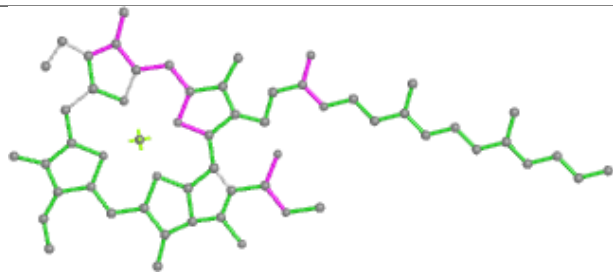


Rings

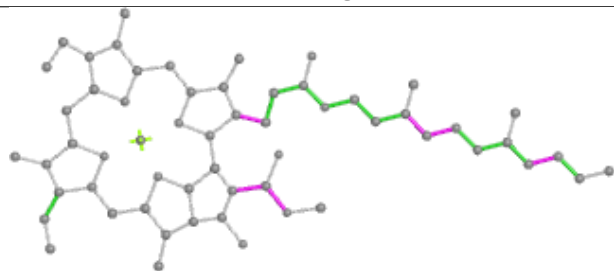
Ligand CLA b 722



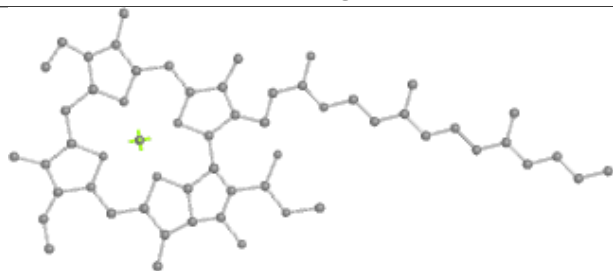
Bond lengths



Bond angles

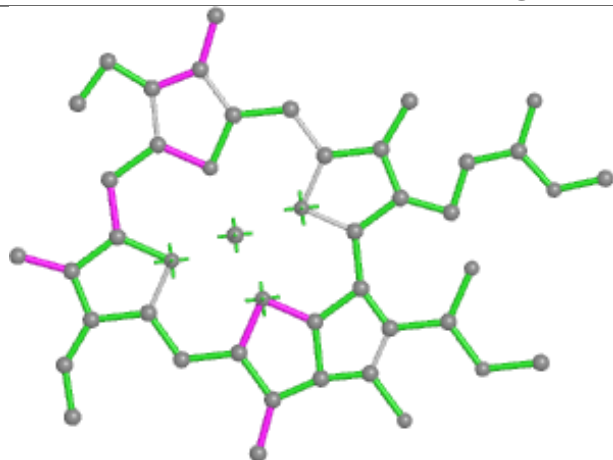


Torsions

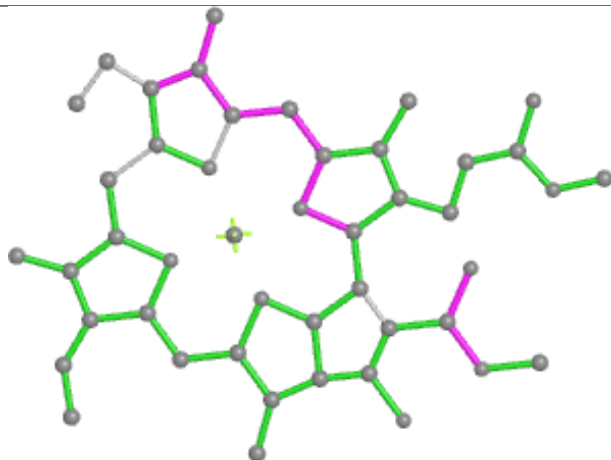


Rings

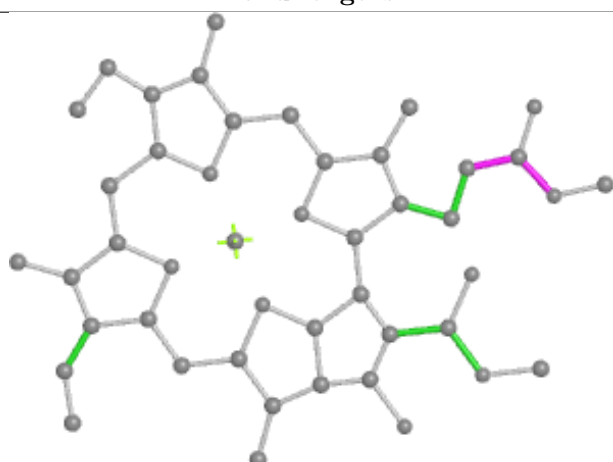
Ligand CLA K 217



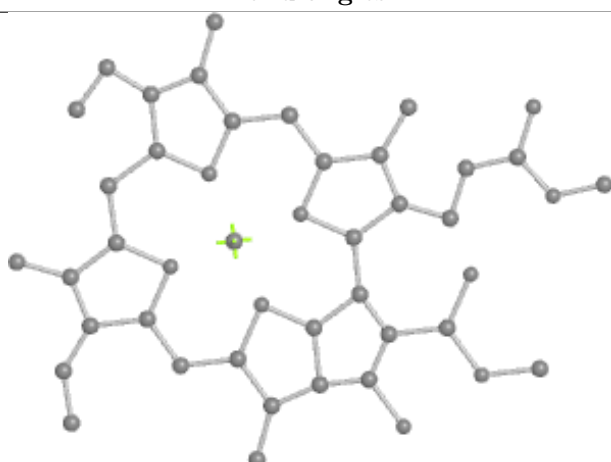
Bond lengths



Bond angles

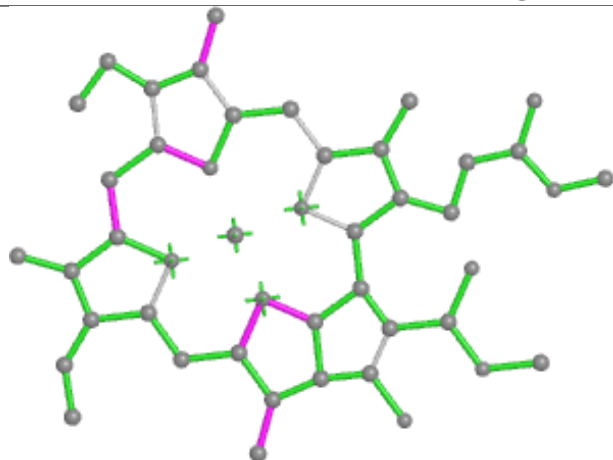


Torsions

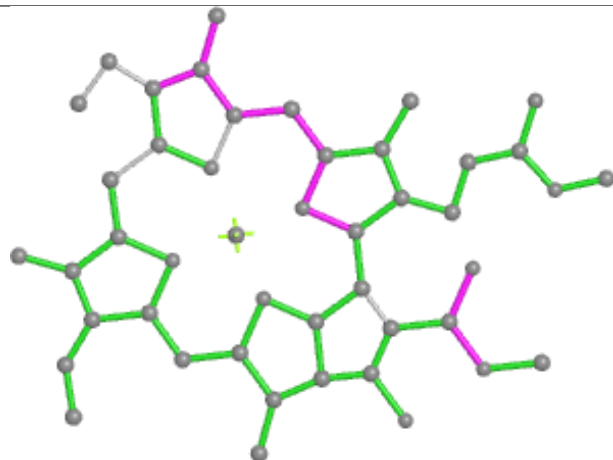


Rings

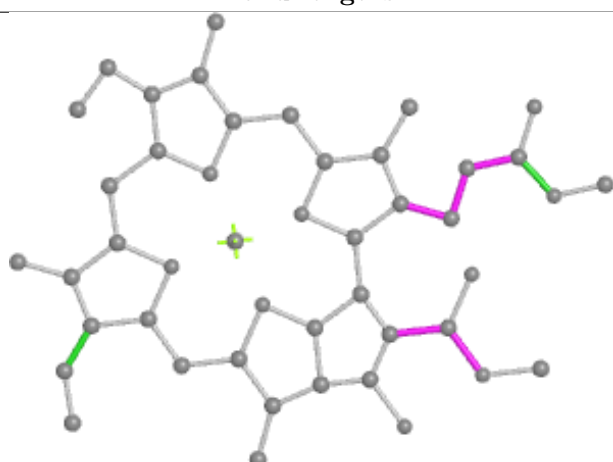
Ligand CLA H 312



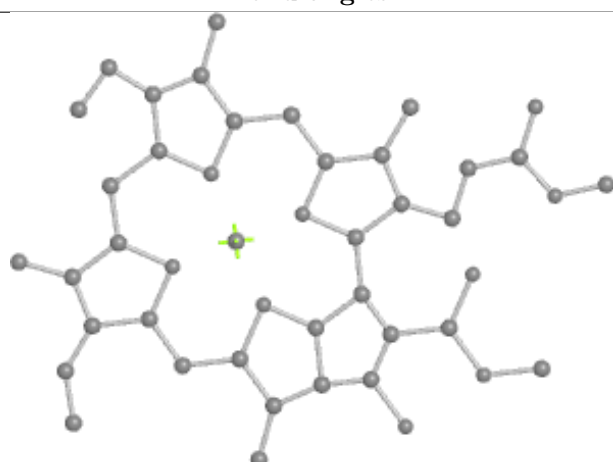
Bond lengths



Bond angles

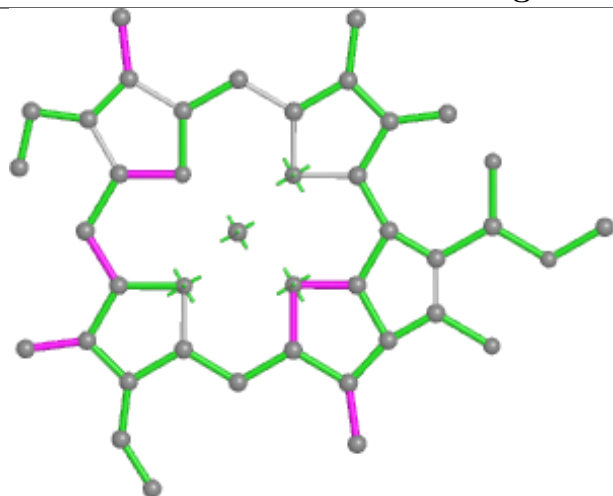


Torsions

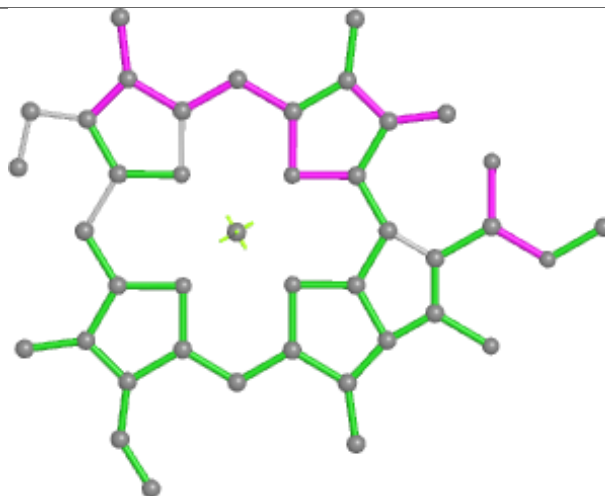


Rings

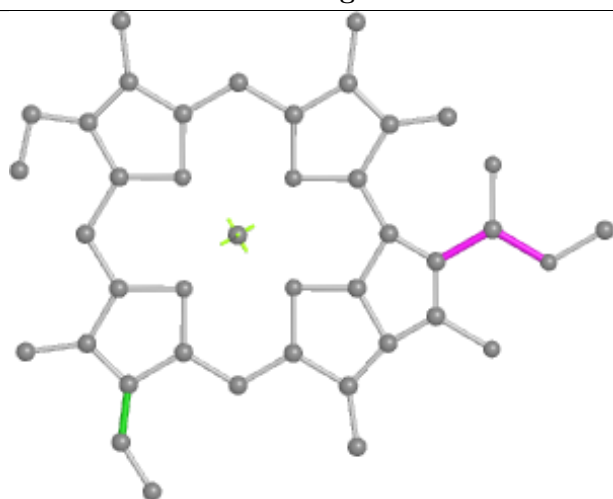
Ligand CLA K 216



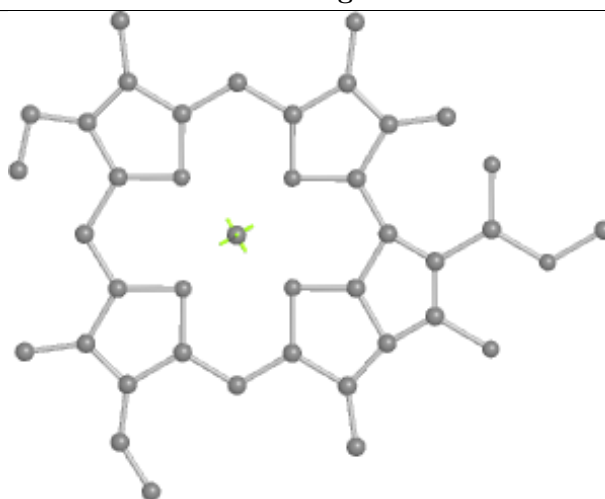
Bond lengths



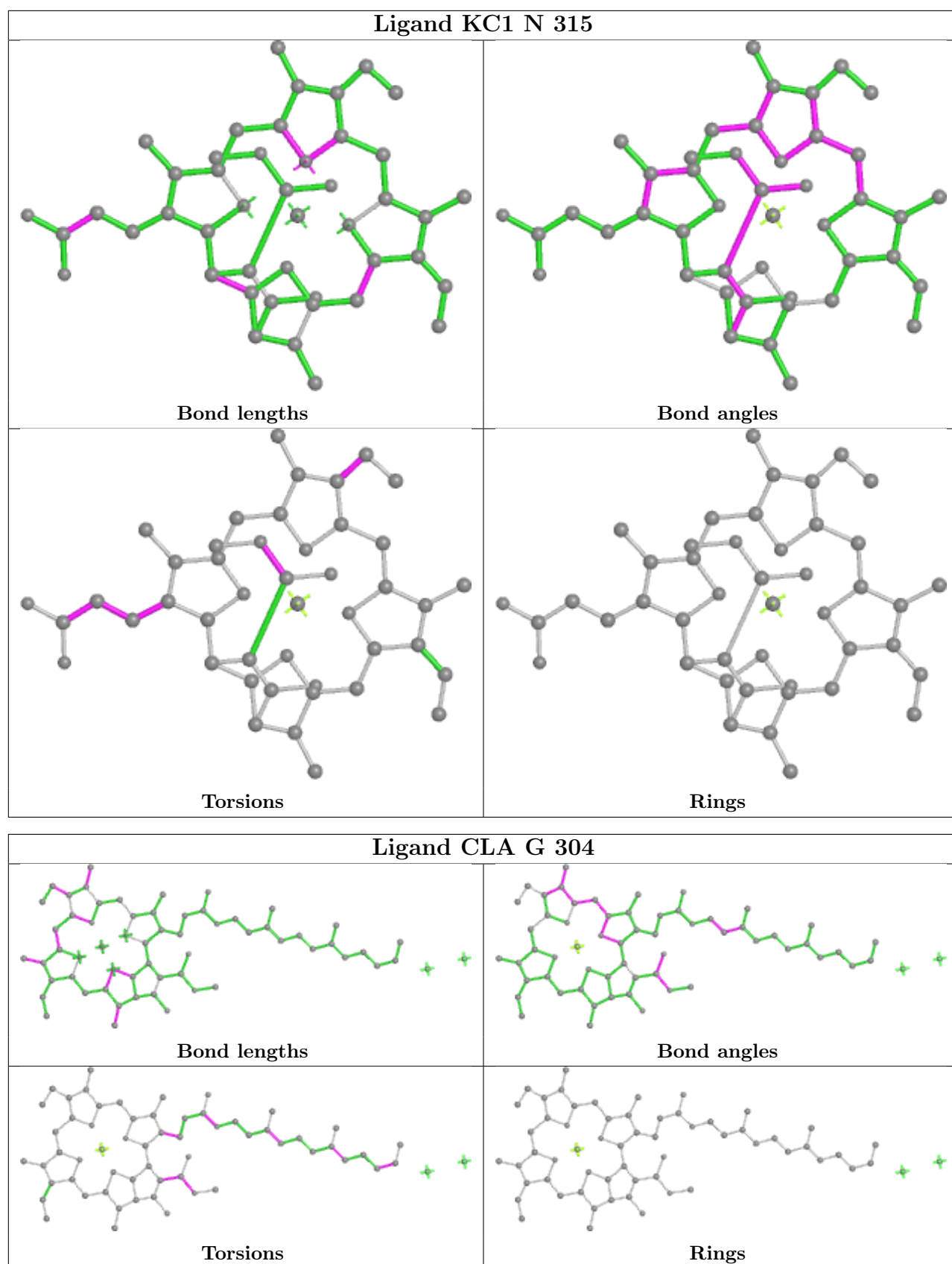
Bond angles

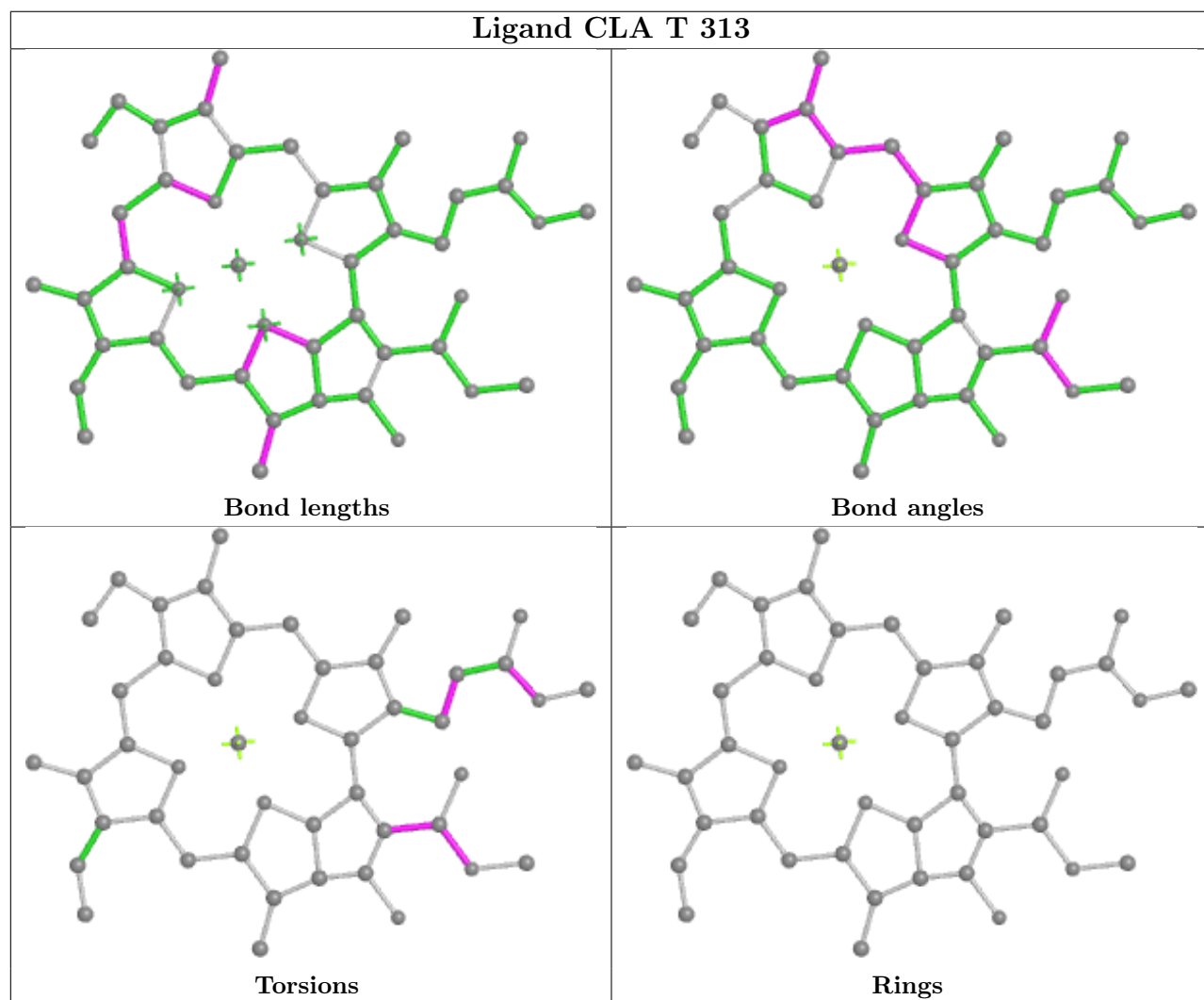
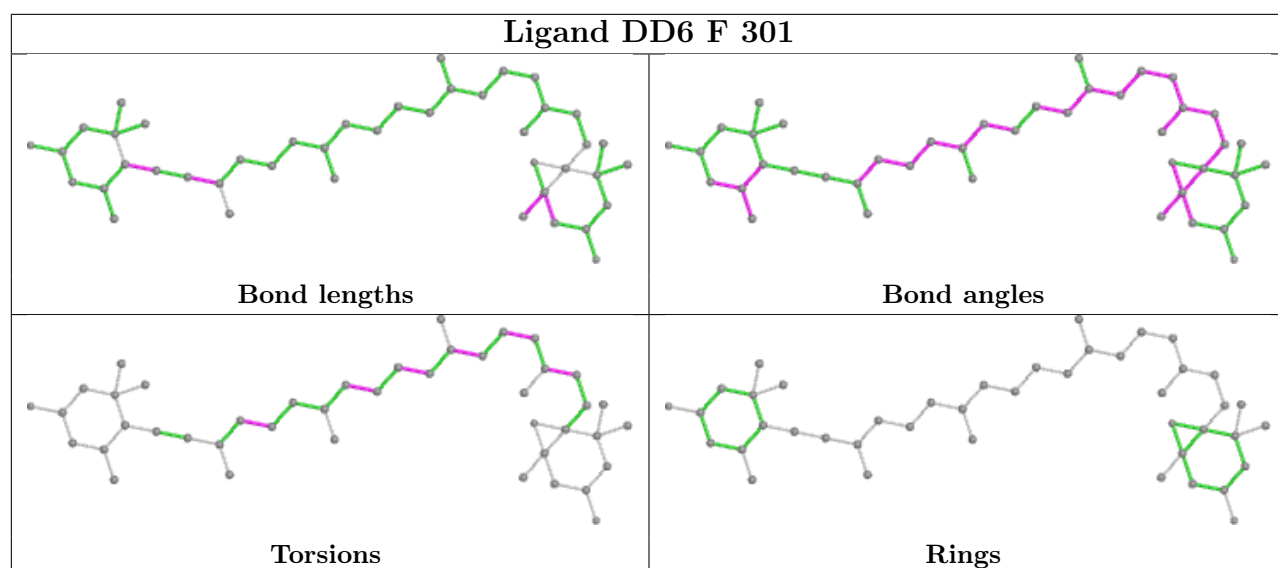


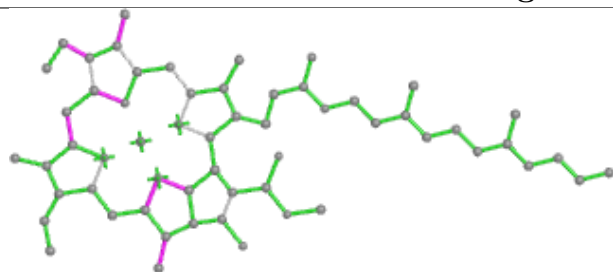
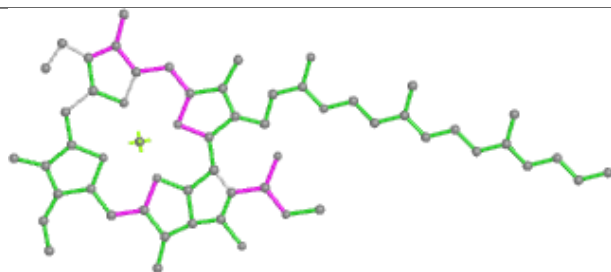
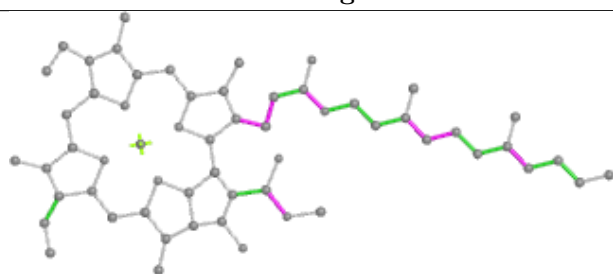
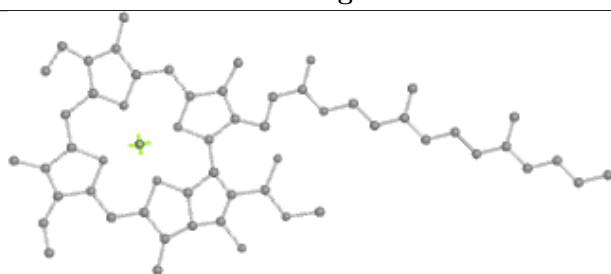
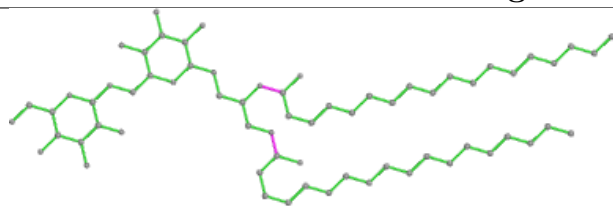
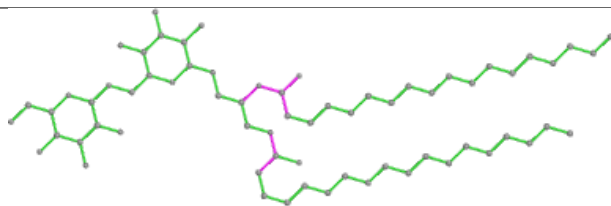
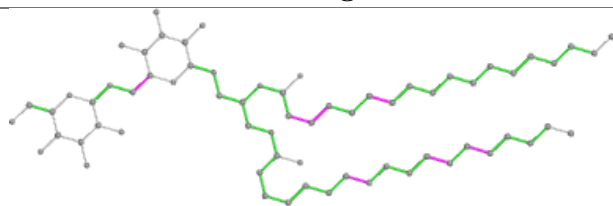
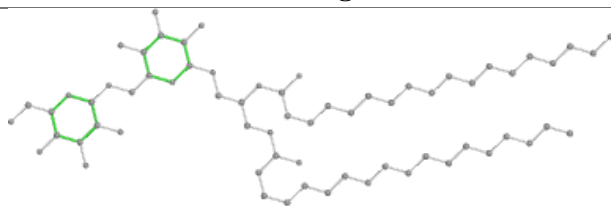
Torsions



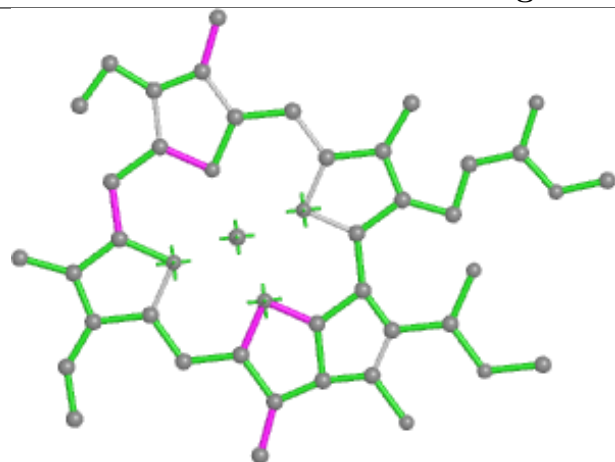
Rings



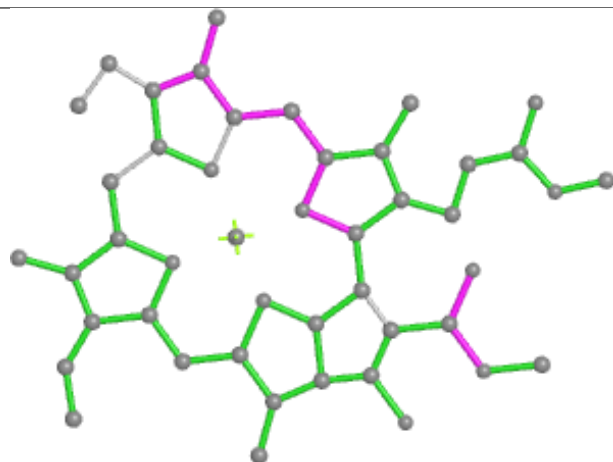


Ligand CLA b 711**Bond lengths****Bond angles****Torsions****Rings****Ligand DGD m 102****Bond lengths****Bond angles****Torsions****Rings**

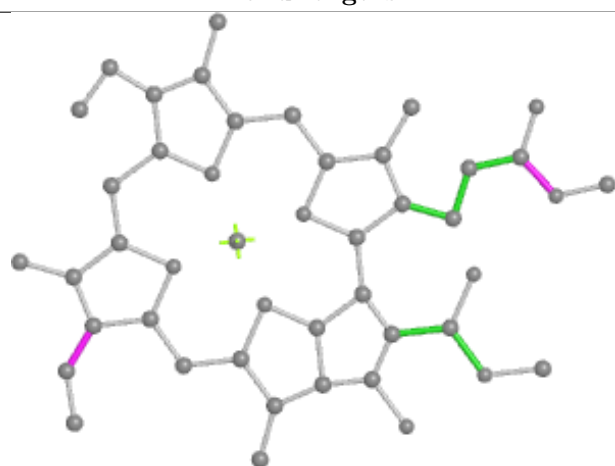
Ligand CLA B 315



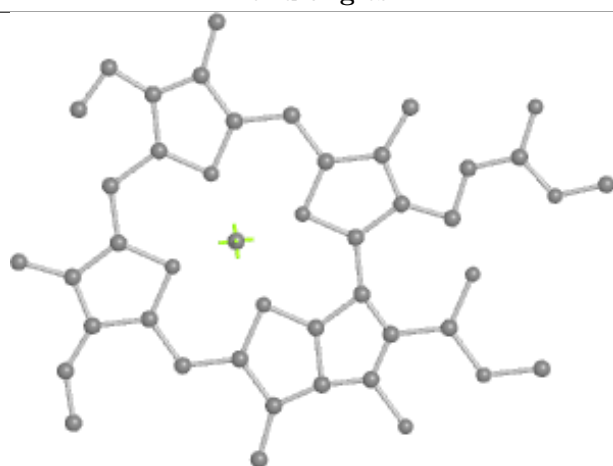
Bond lengths



Bond angles

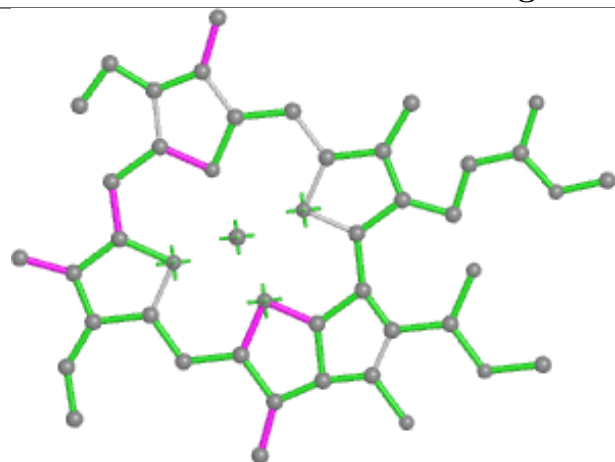


Torsions

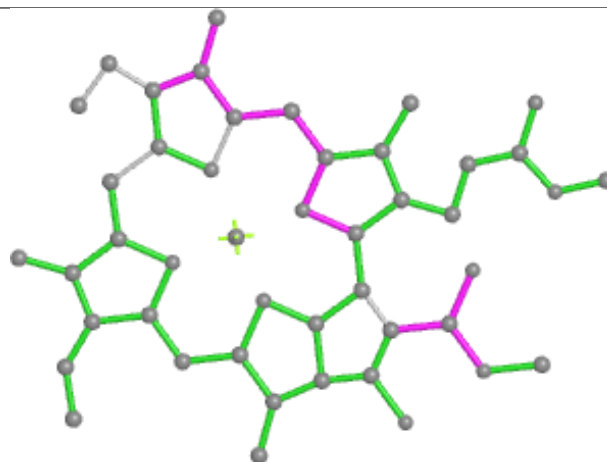


Rings

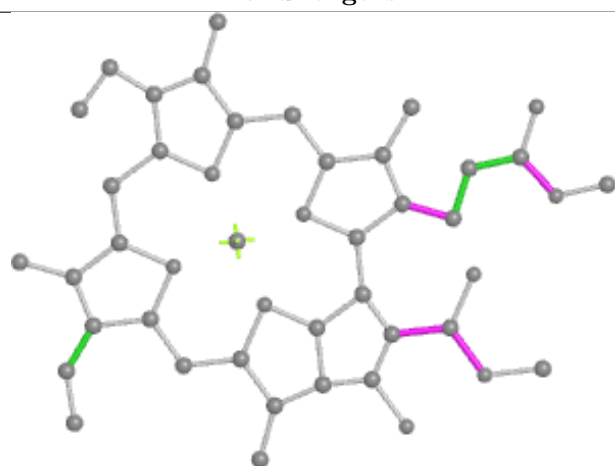
Ligand CLA F 310



Bond lengths



Bond angles

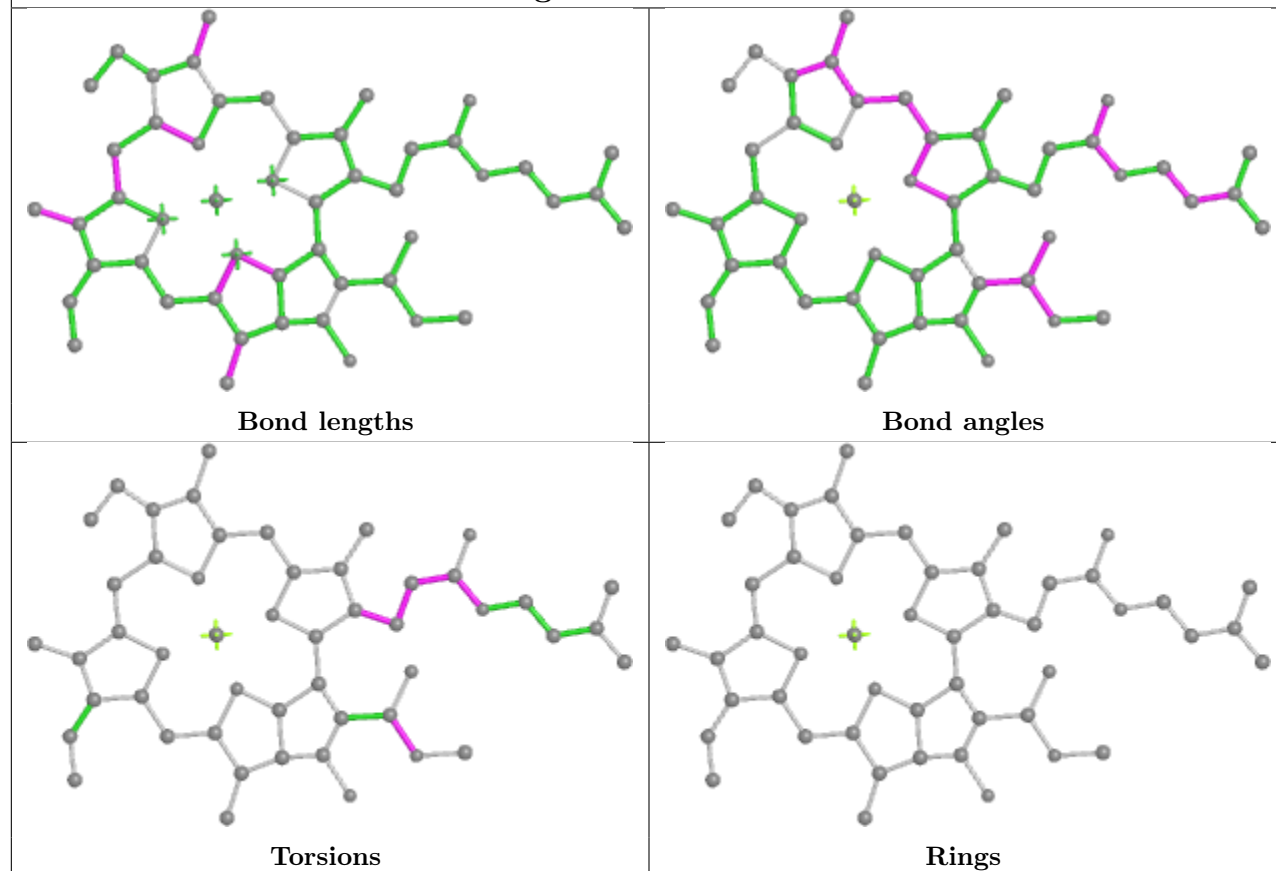


Torsions

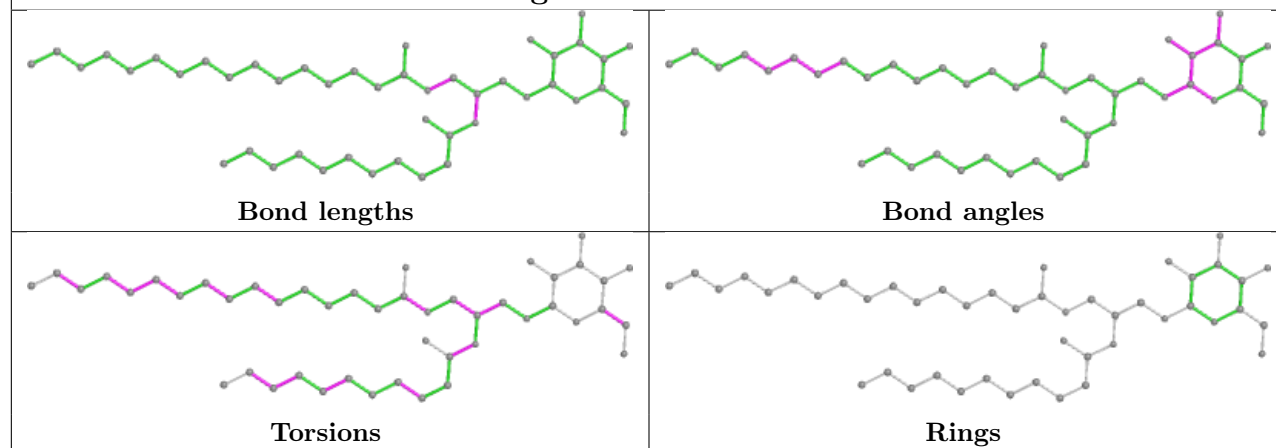


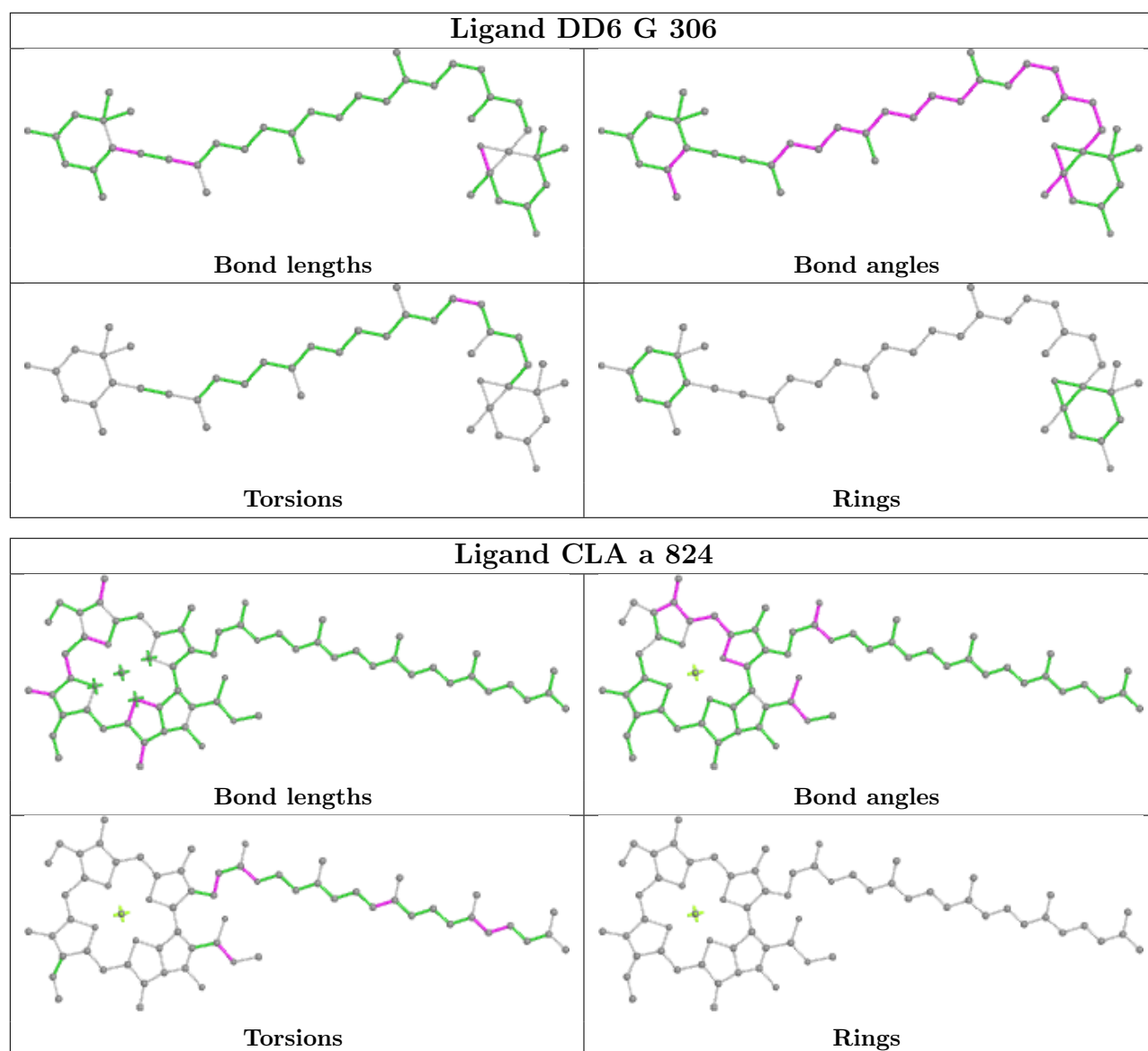
Rings

Ligand CLA L 307

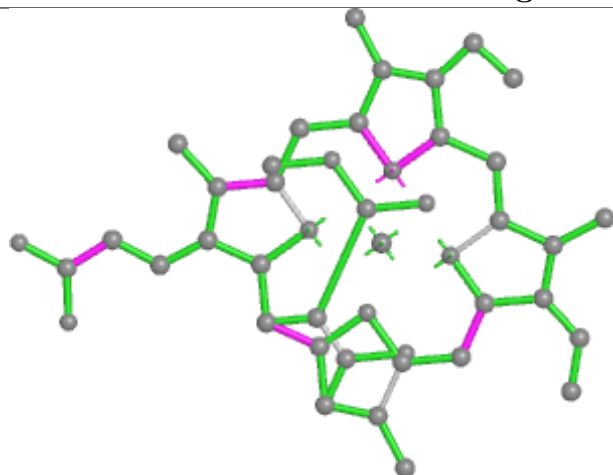


Ligand LMG b 730

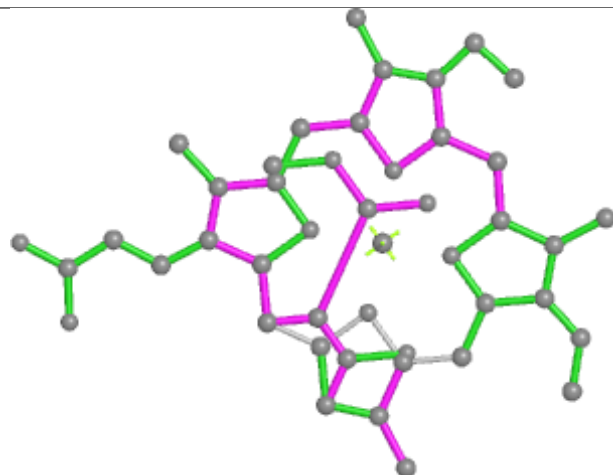




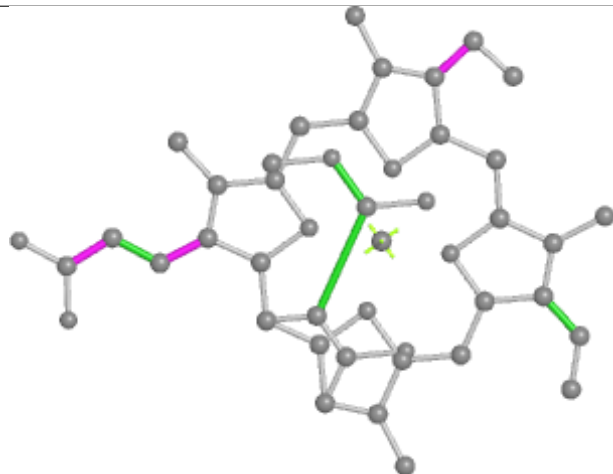
Ligand KC1 O 310



Bond lengths



Bond angles

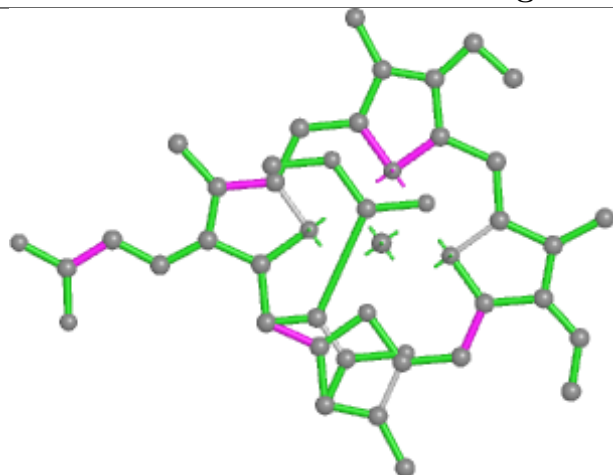


Torsions

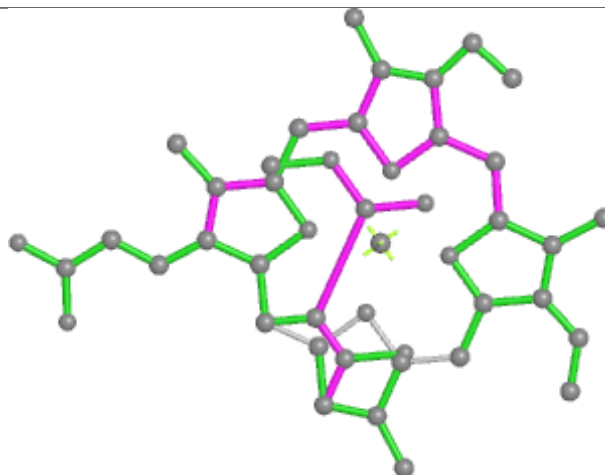


Rings

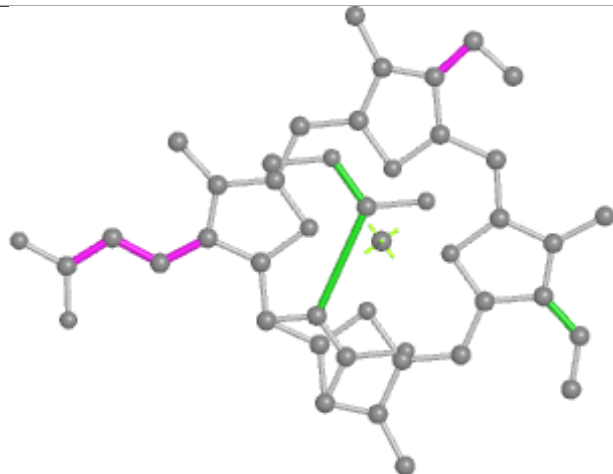
Ligand KC1 P 216



Bond lengths



Bond angles

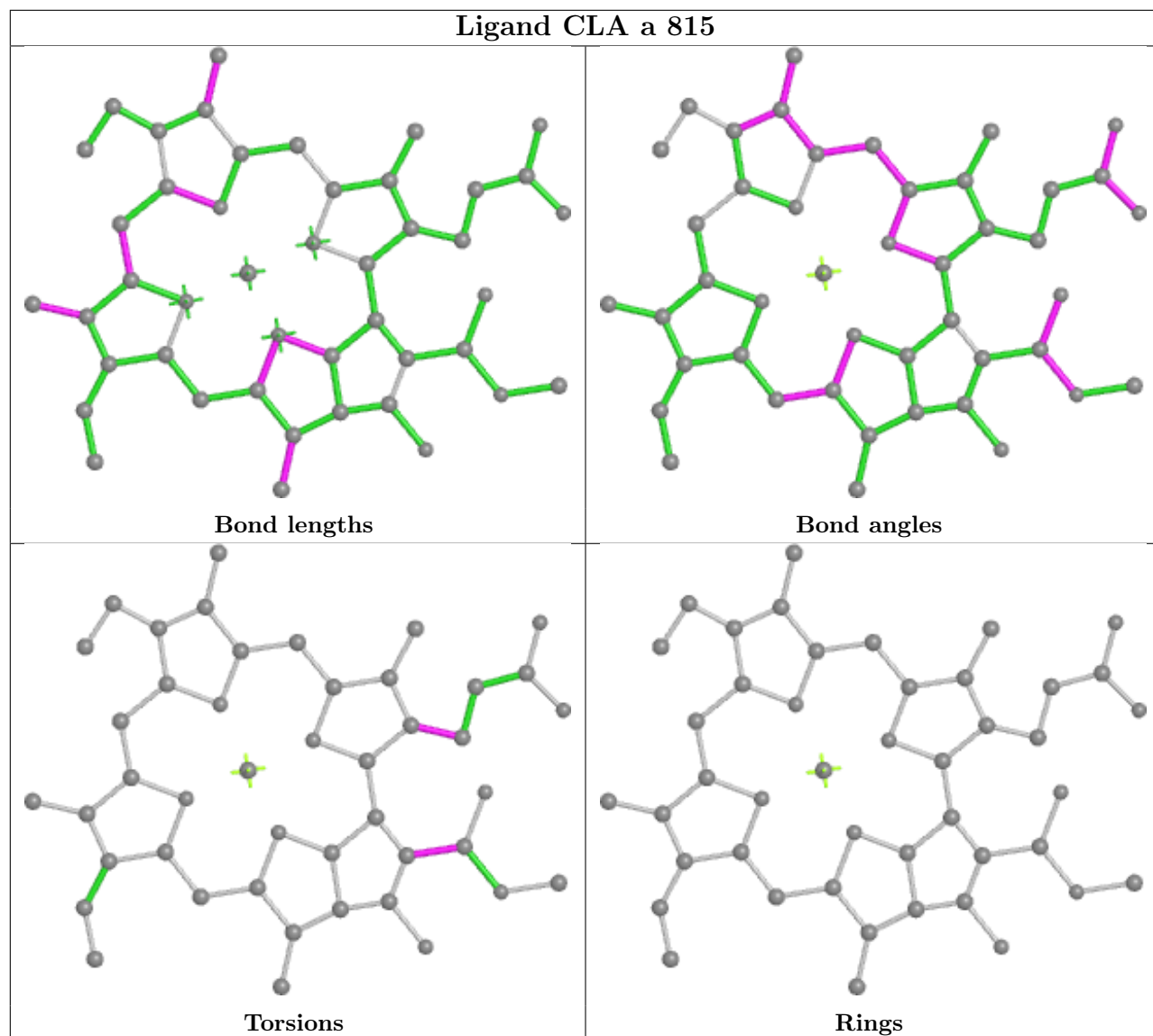


Torsions

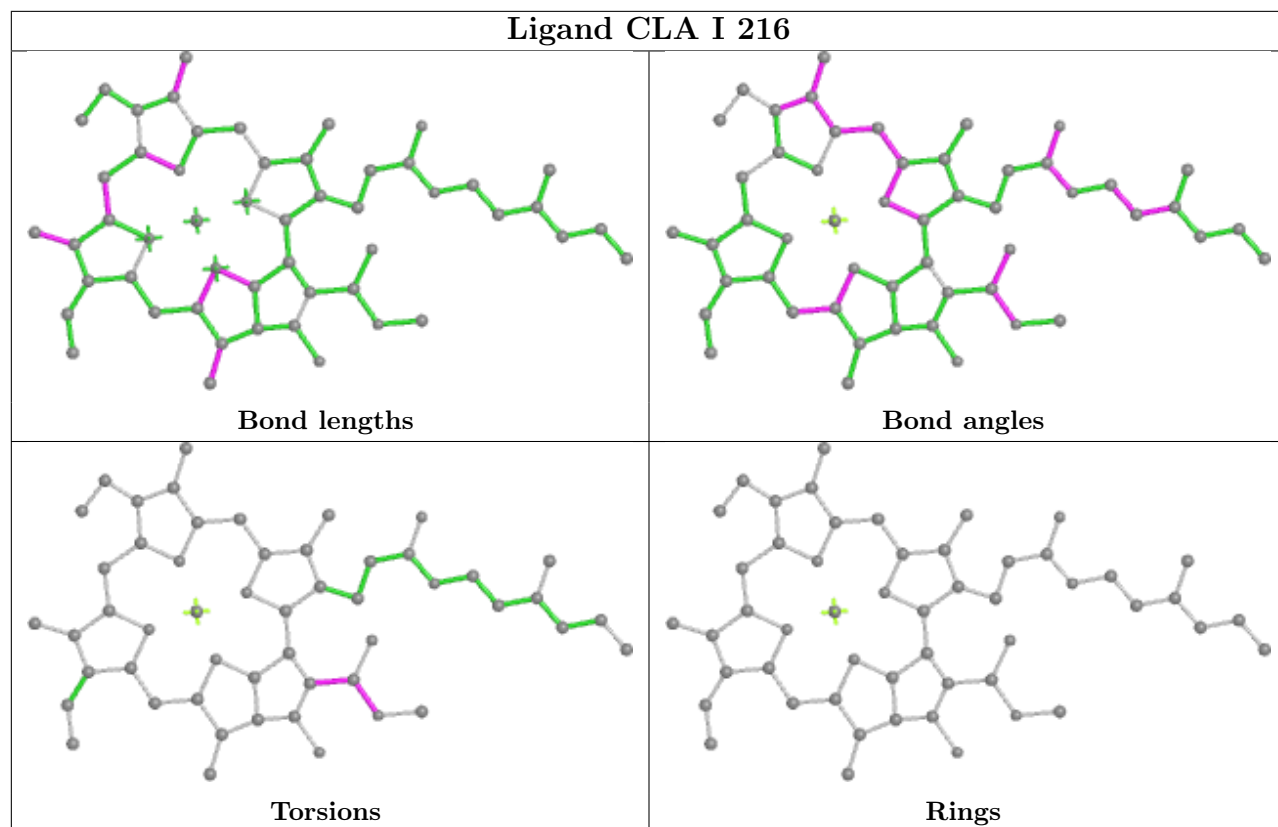


Rings

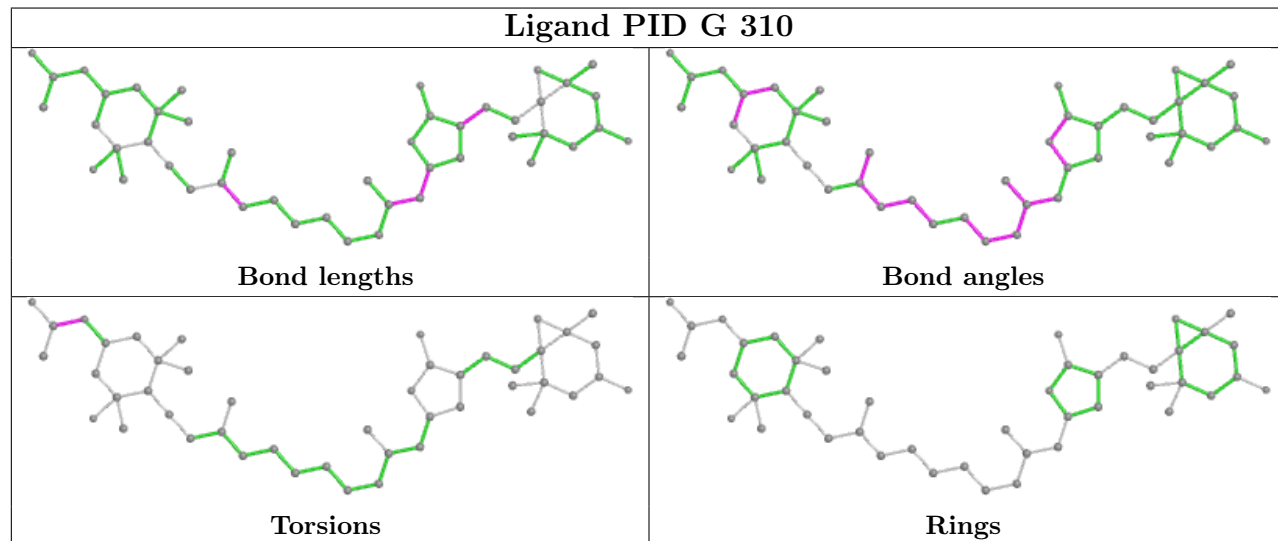
Ligand CLA a 815



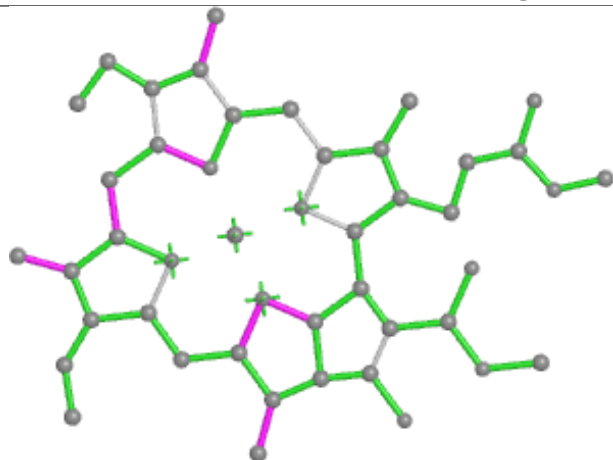
Ligand CLA I 216



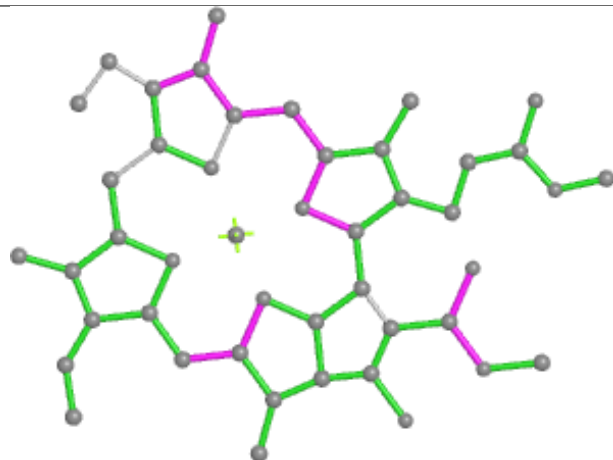
Ligand PID G 310



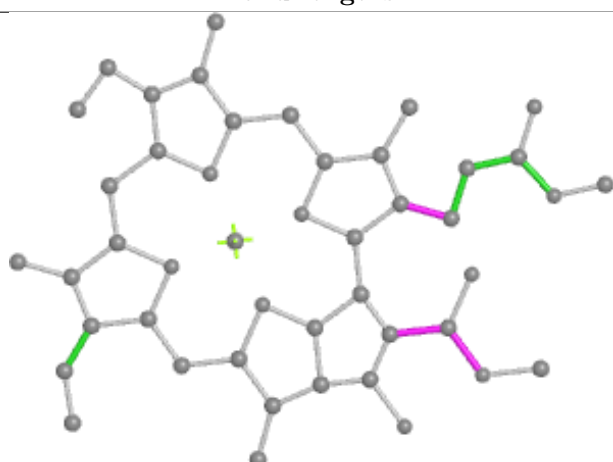
Ligand CLA T 309



Bond lengths



Bond angles

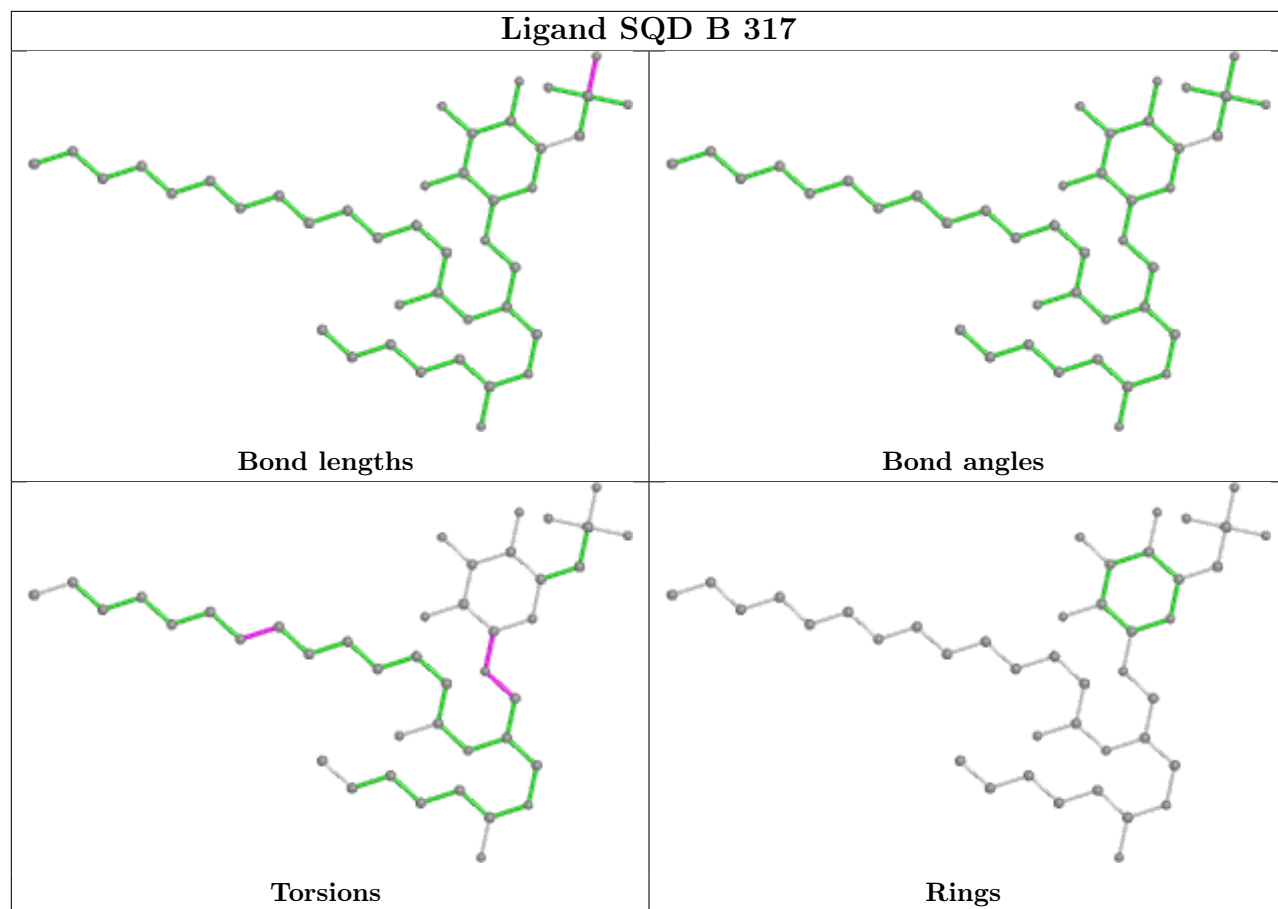


Torsions

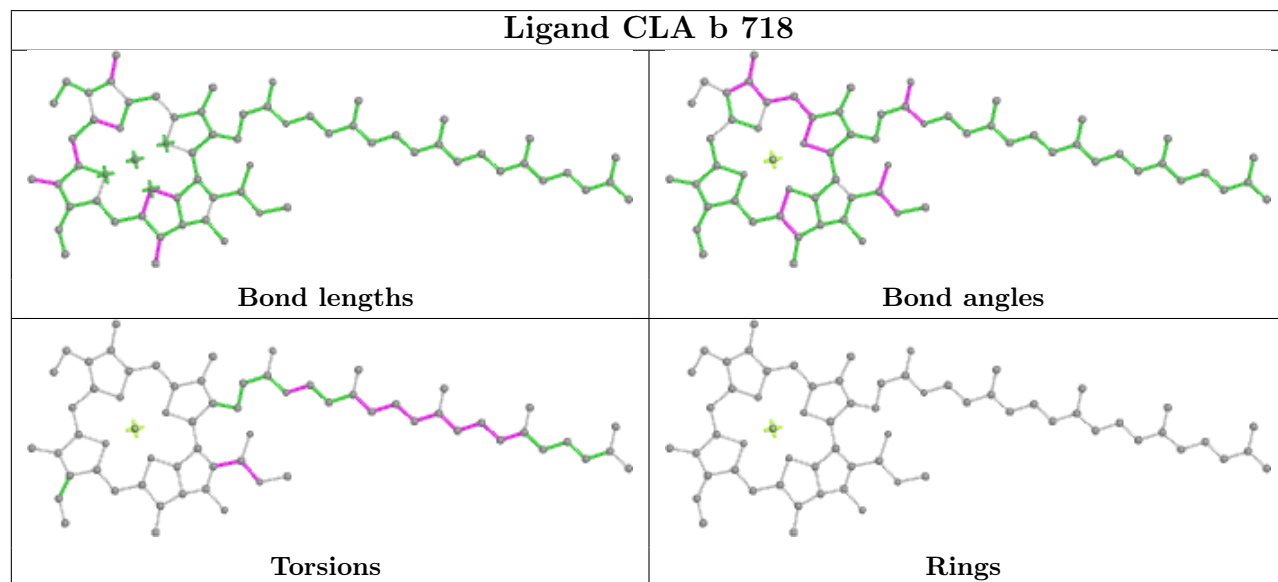


Rings

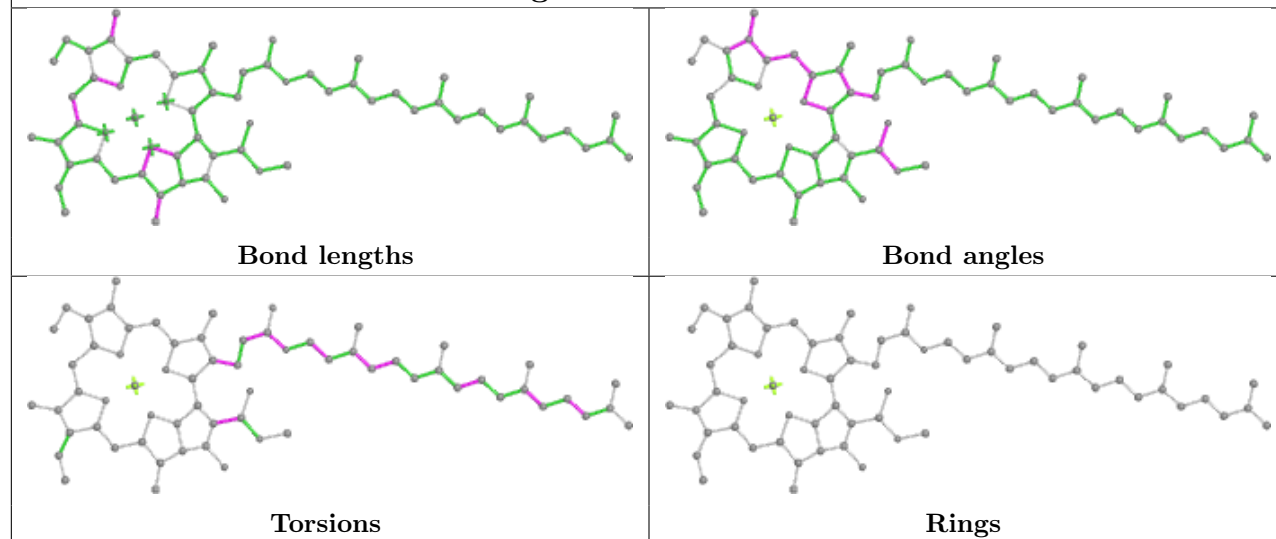
Ligand SQD B 317



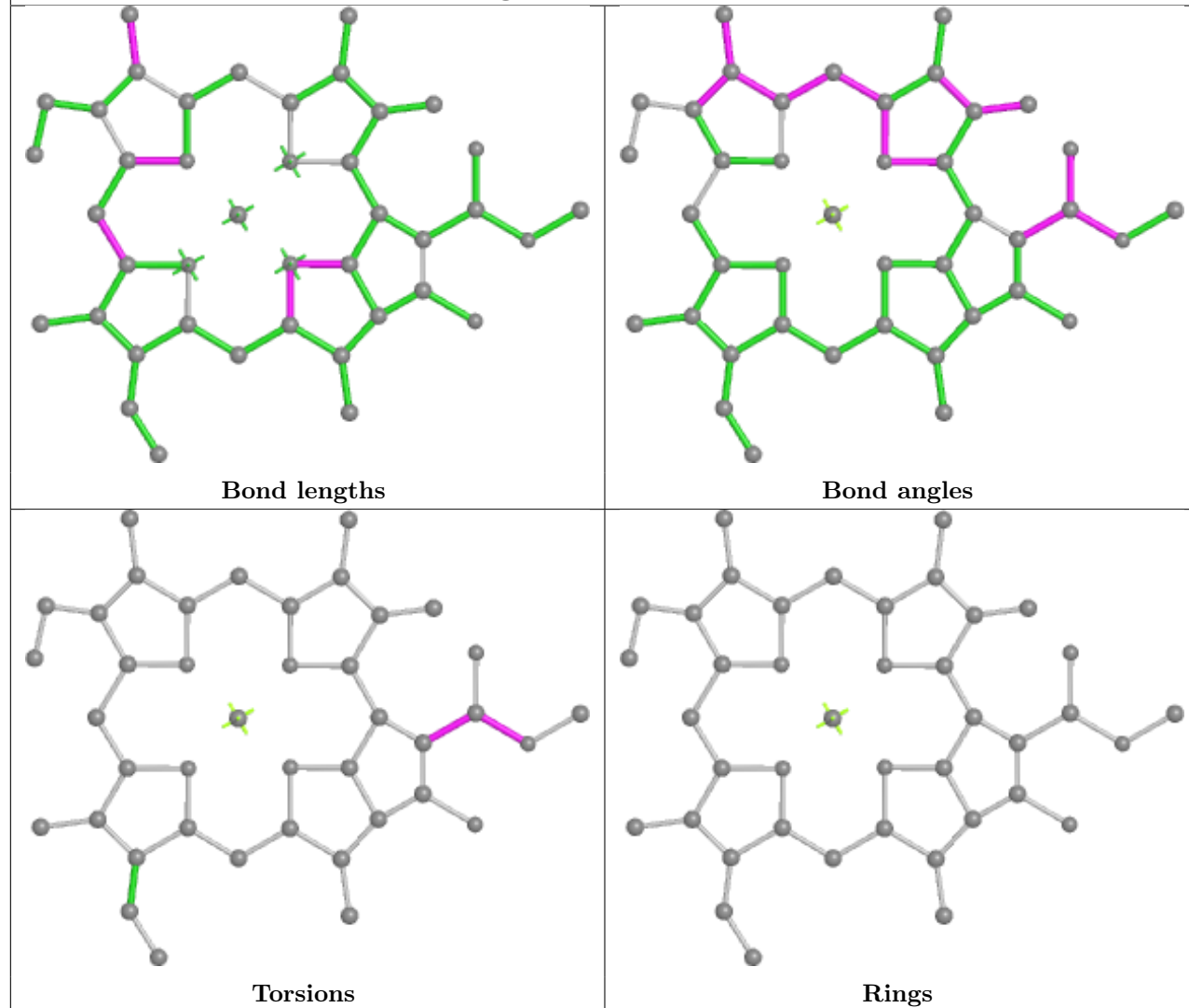
Ligand CLA b 718



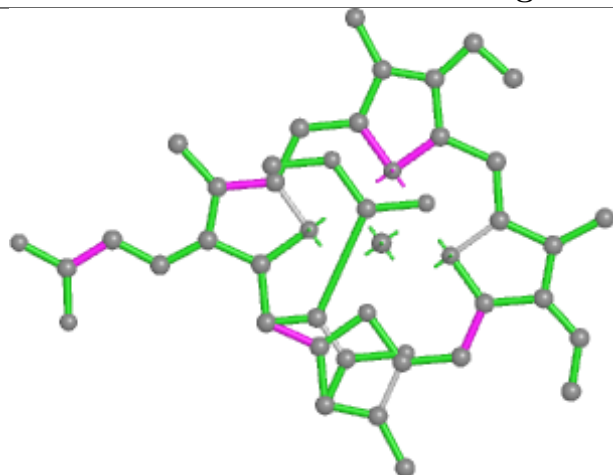
Ligand CLA G 302



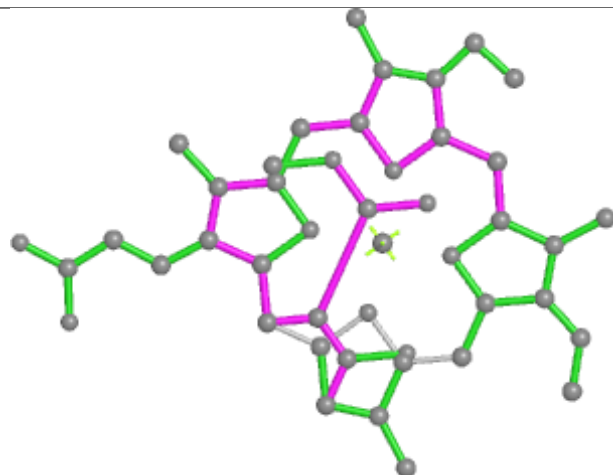
Ligand CLA F 315



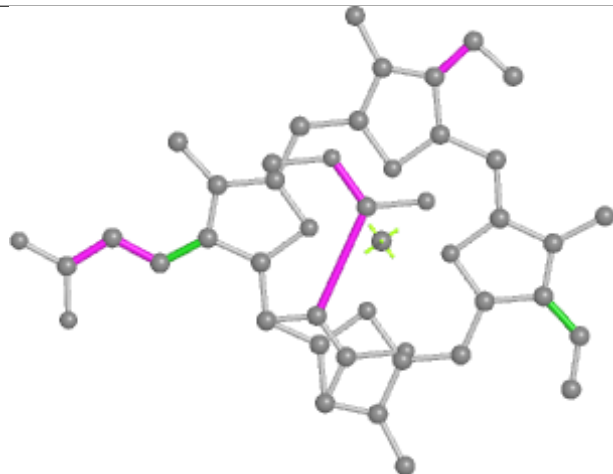
Ligand KC1 C 312



Bond lengths



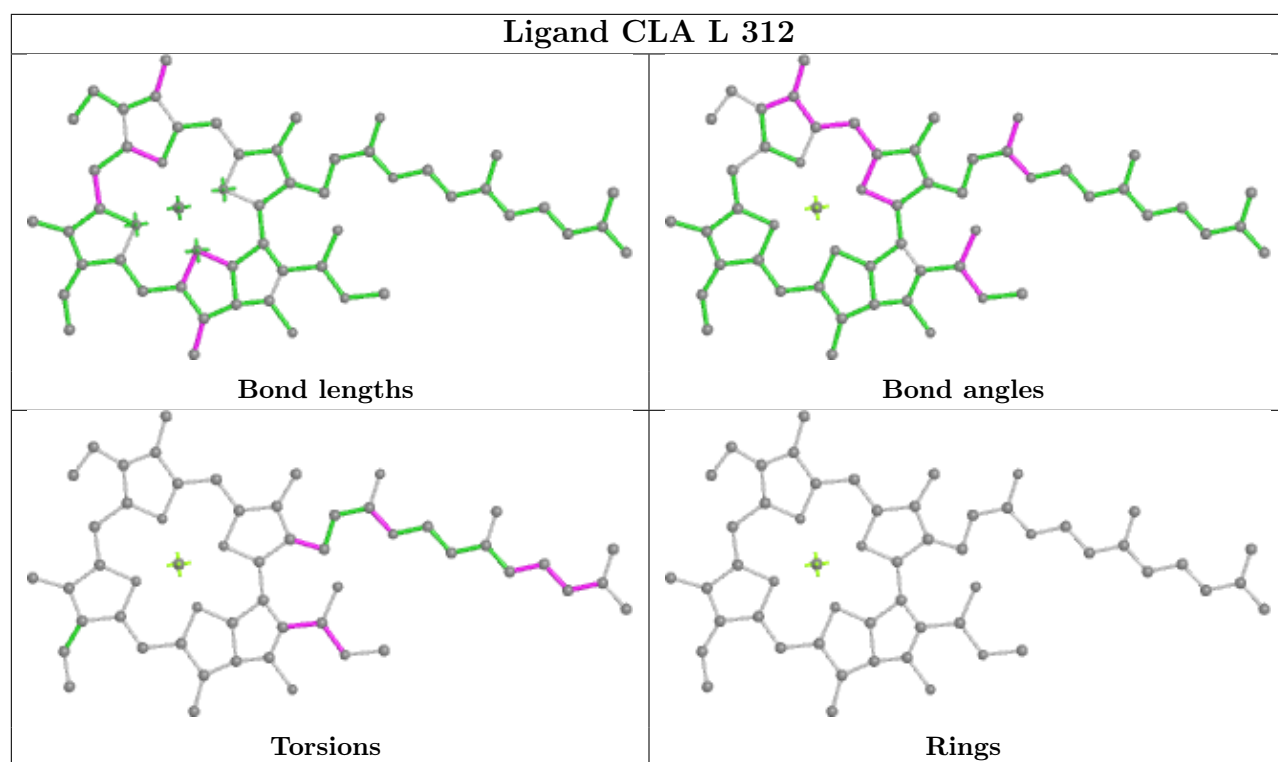
Bond angles



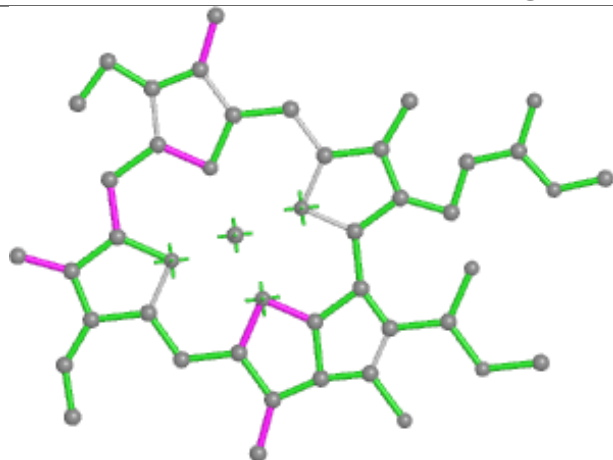
Torsions



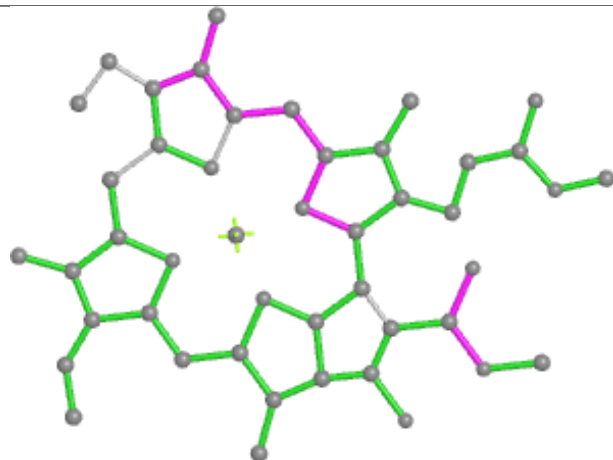
Rings



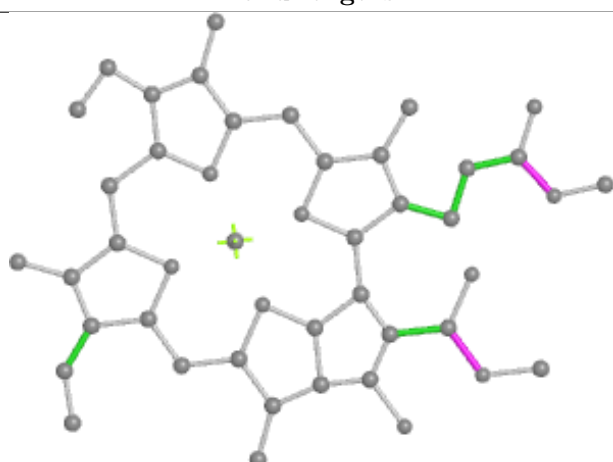
Ligand CLA f 802



Bond lengths



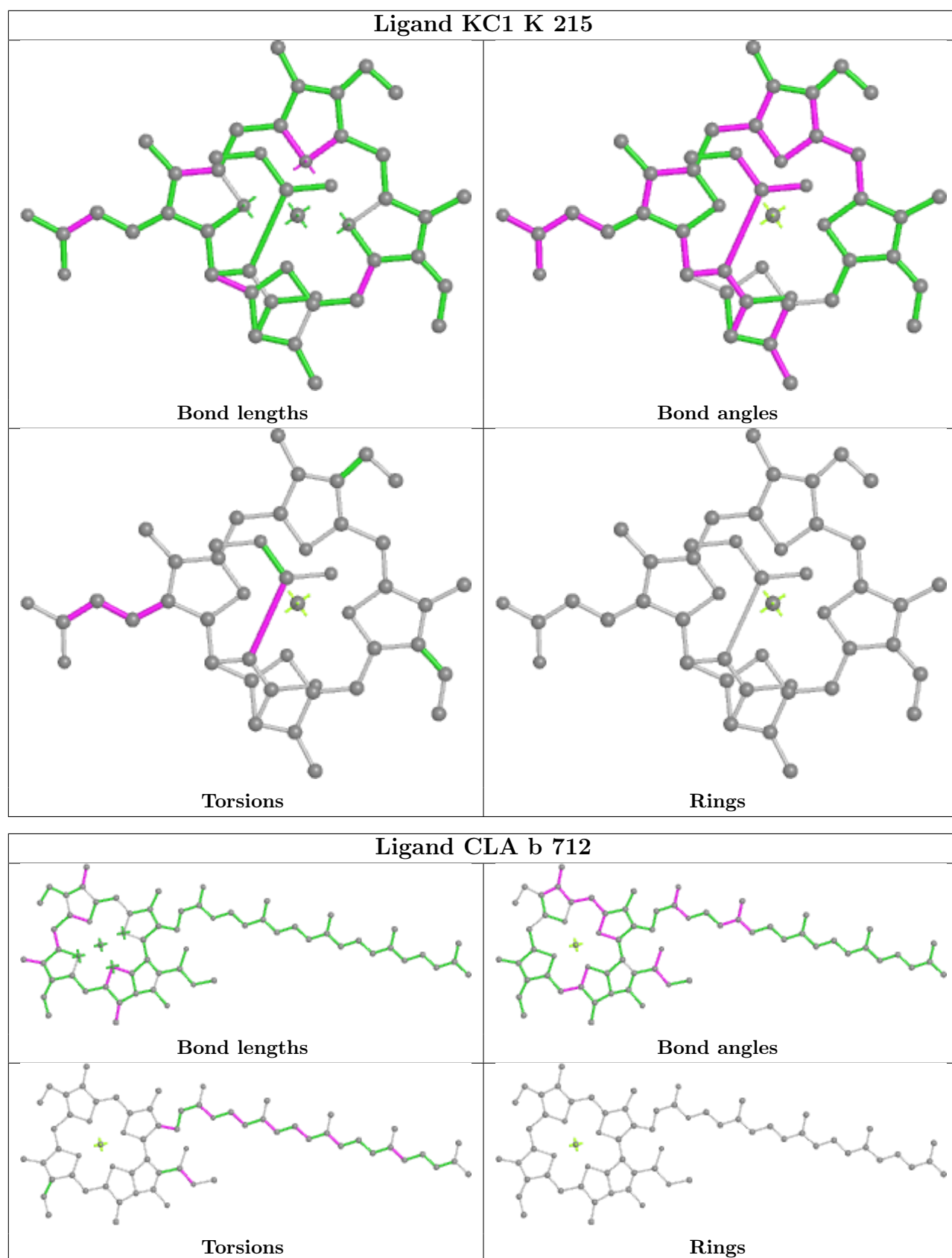
Bond angles



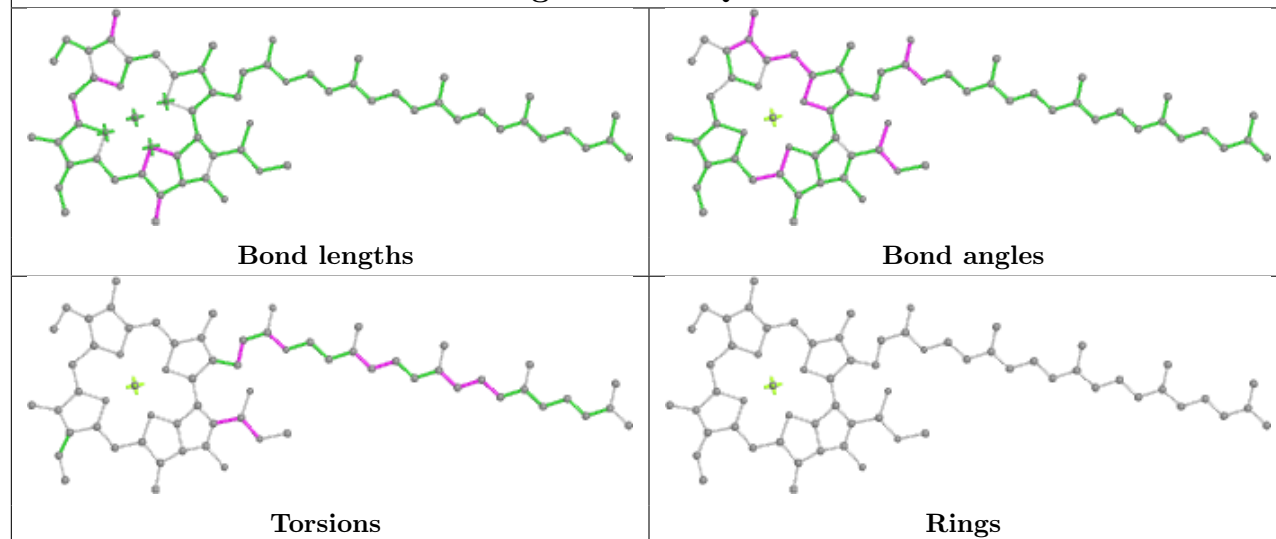
Torsions



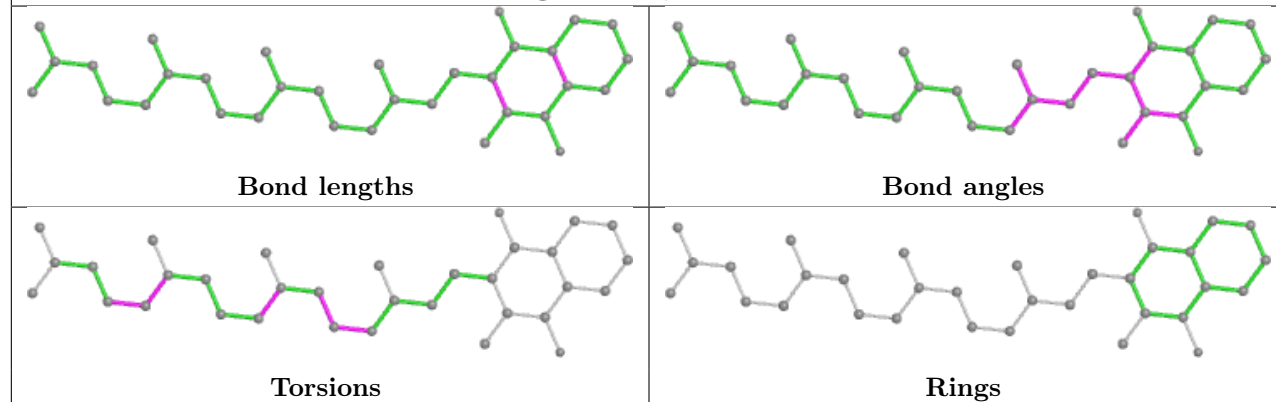
Rings



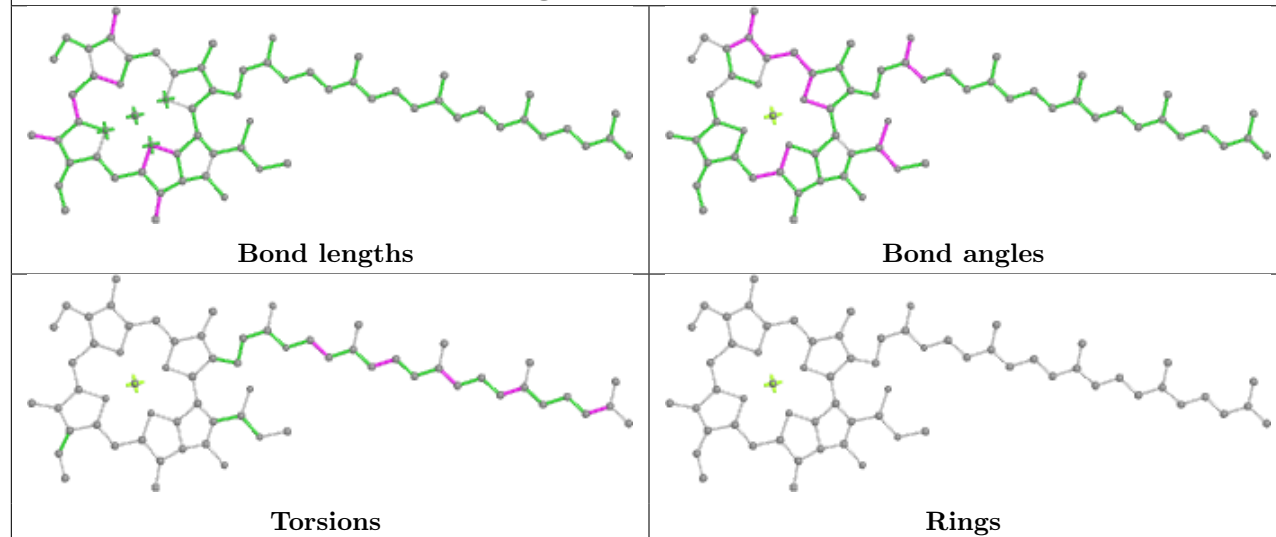
Ligand CLA Q 310



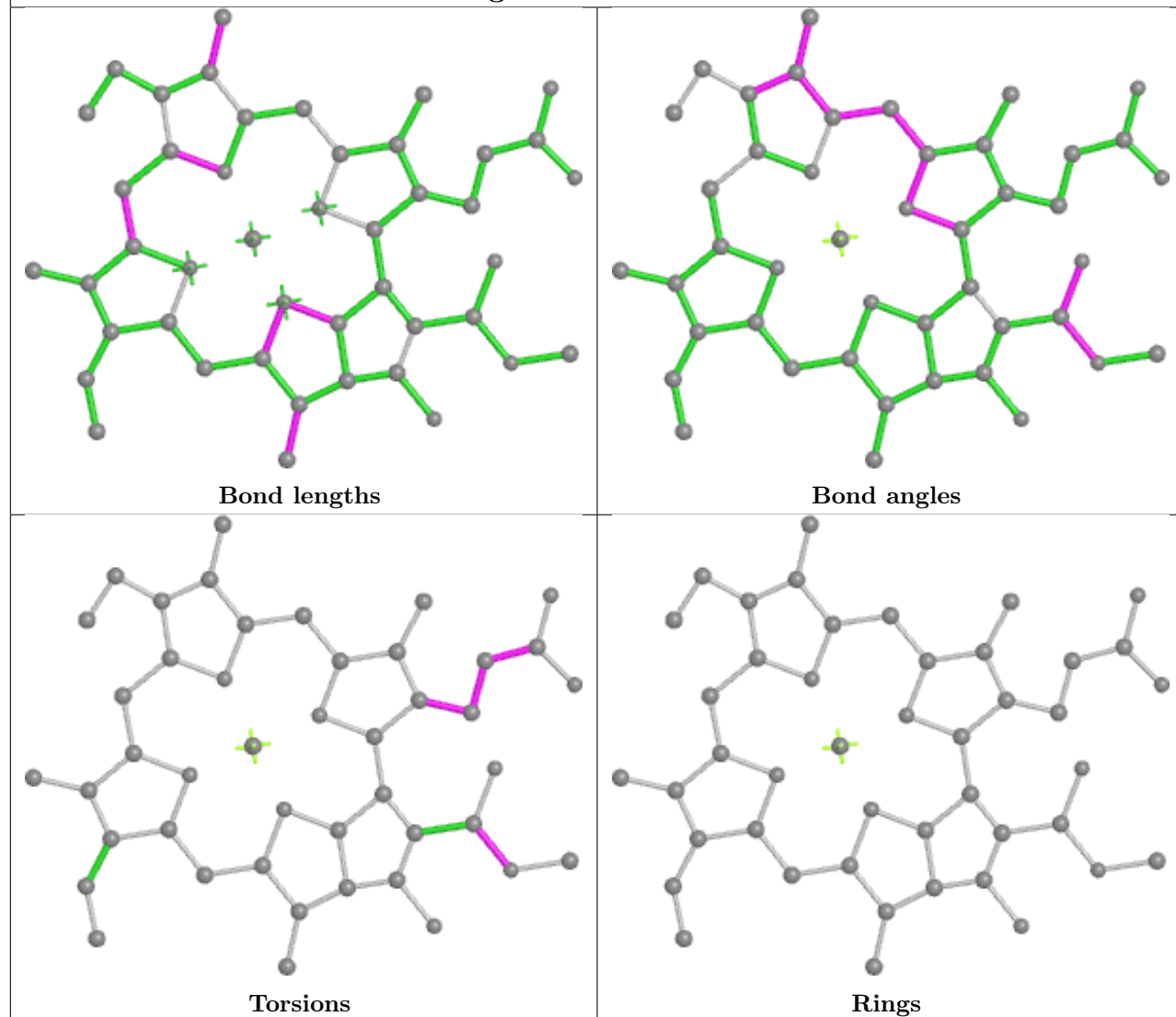
Ligand PQN a 832



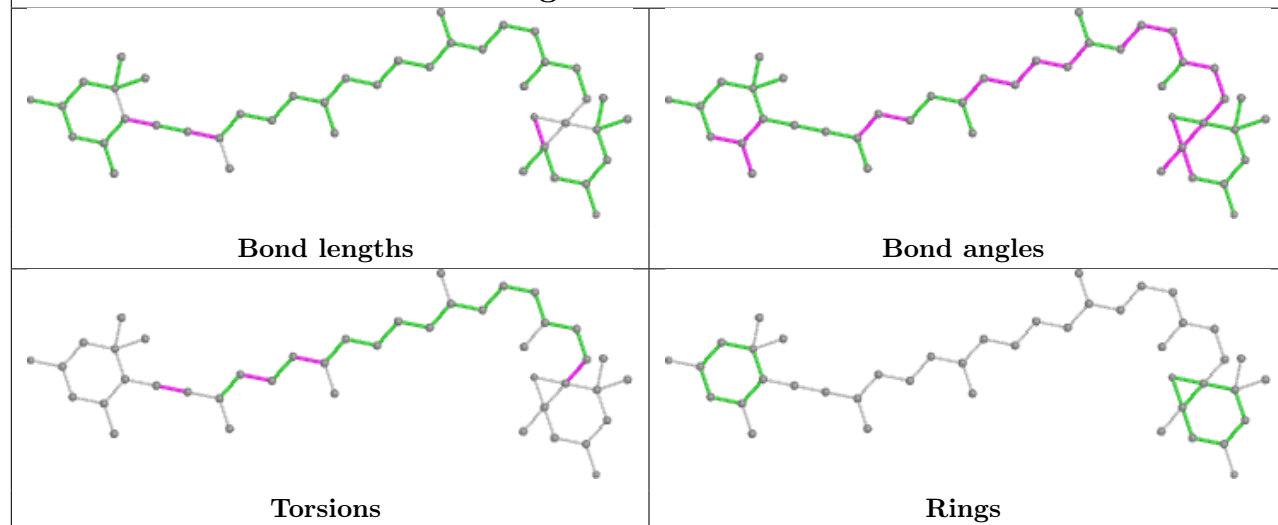
Ligand CLA b 726

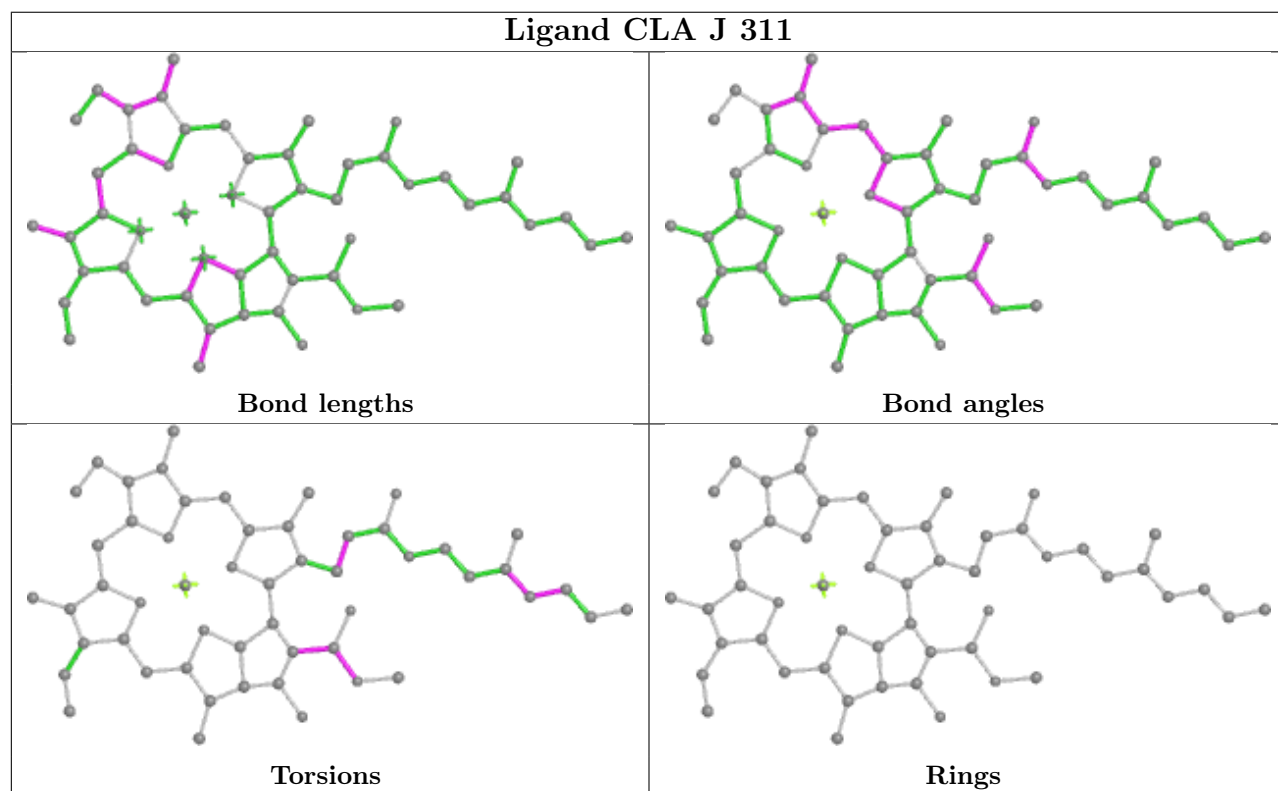
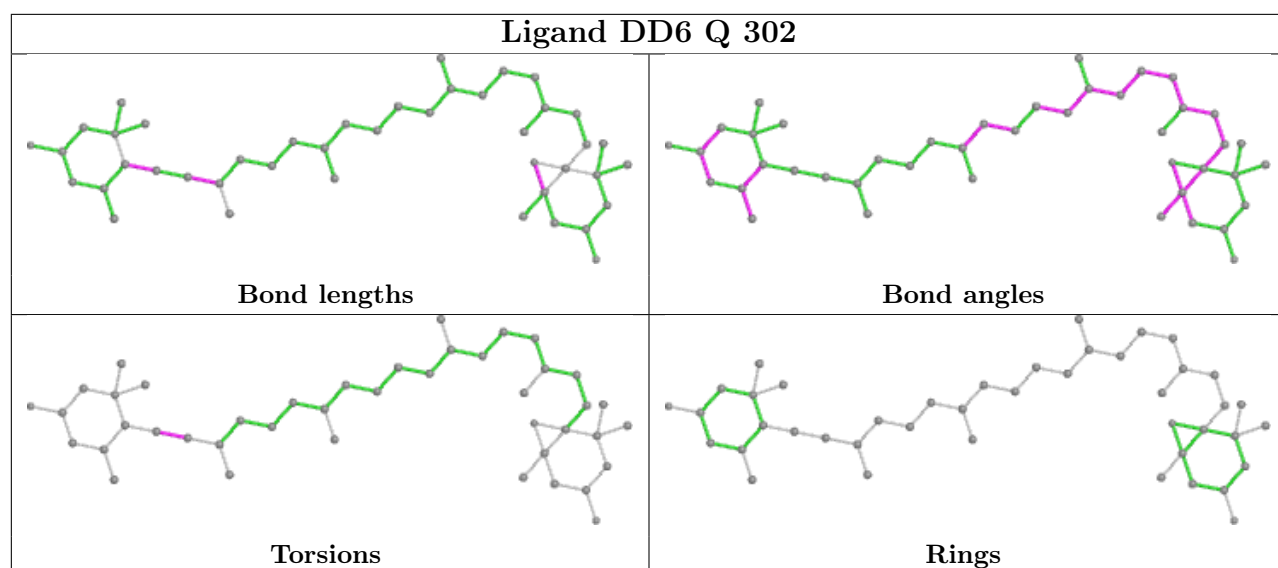


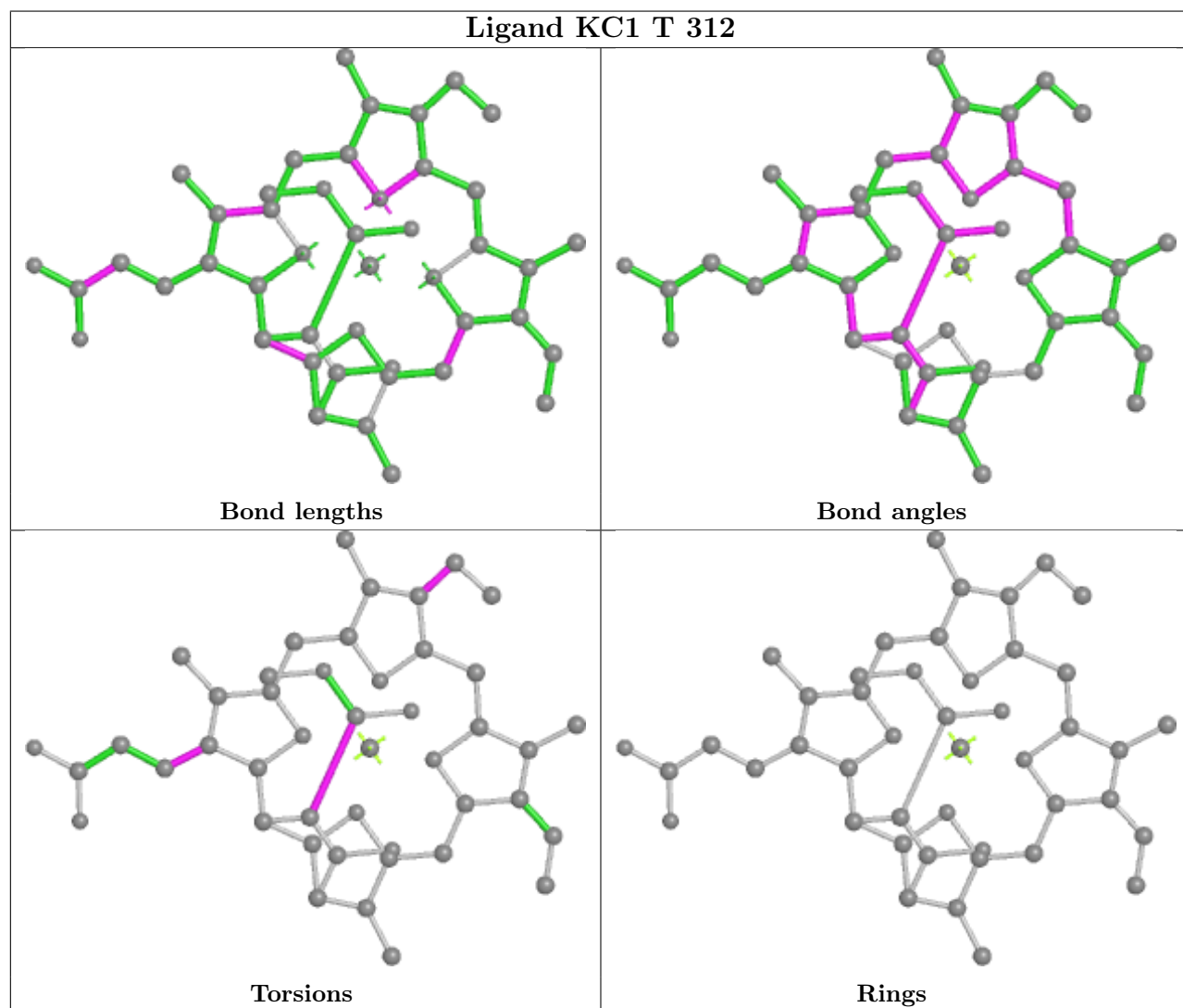
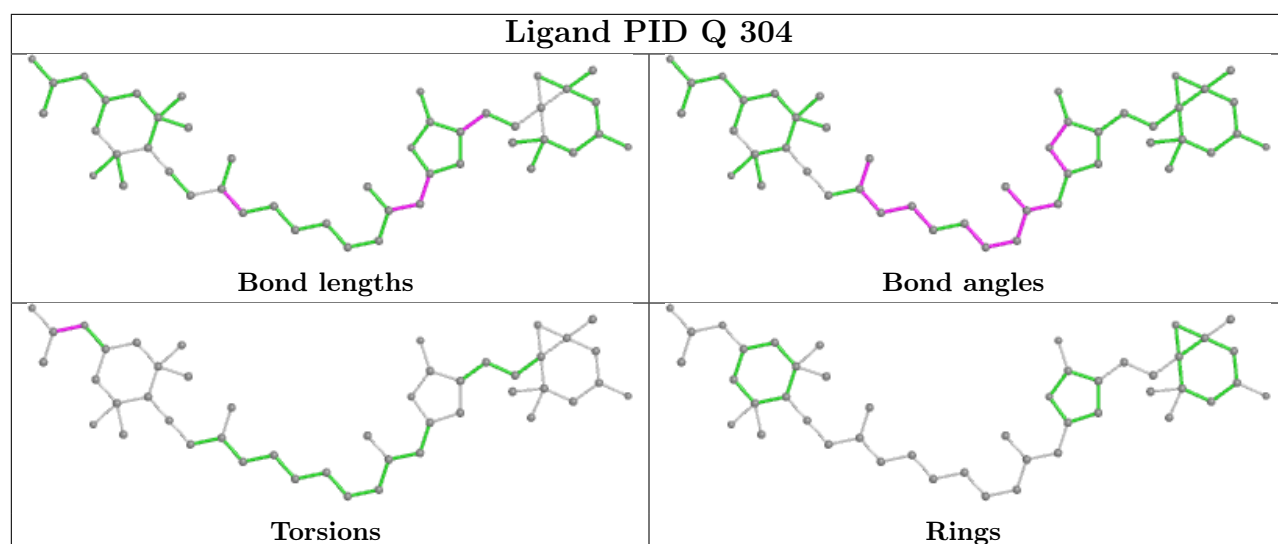
Ligand CLA K 218

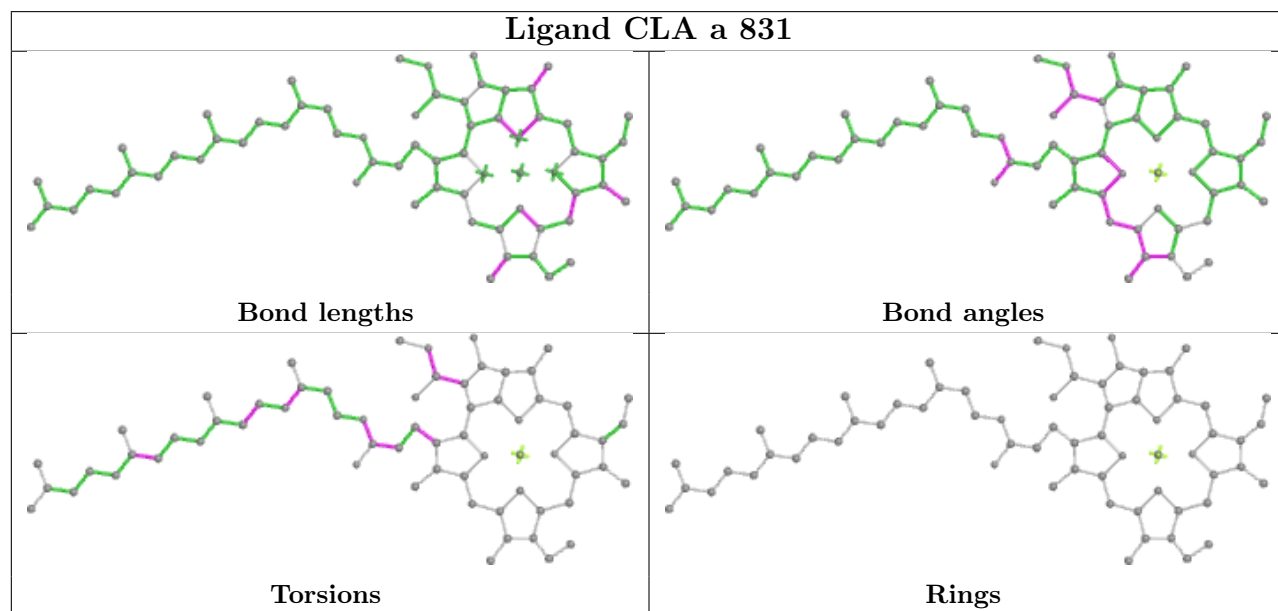
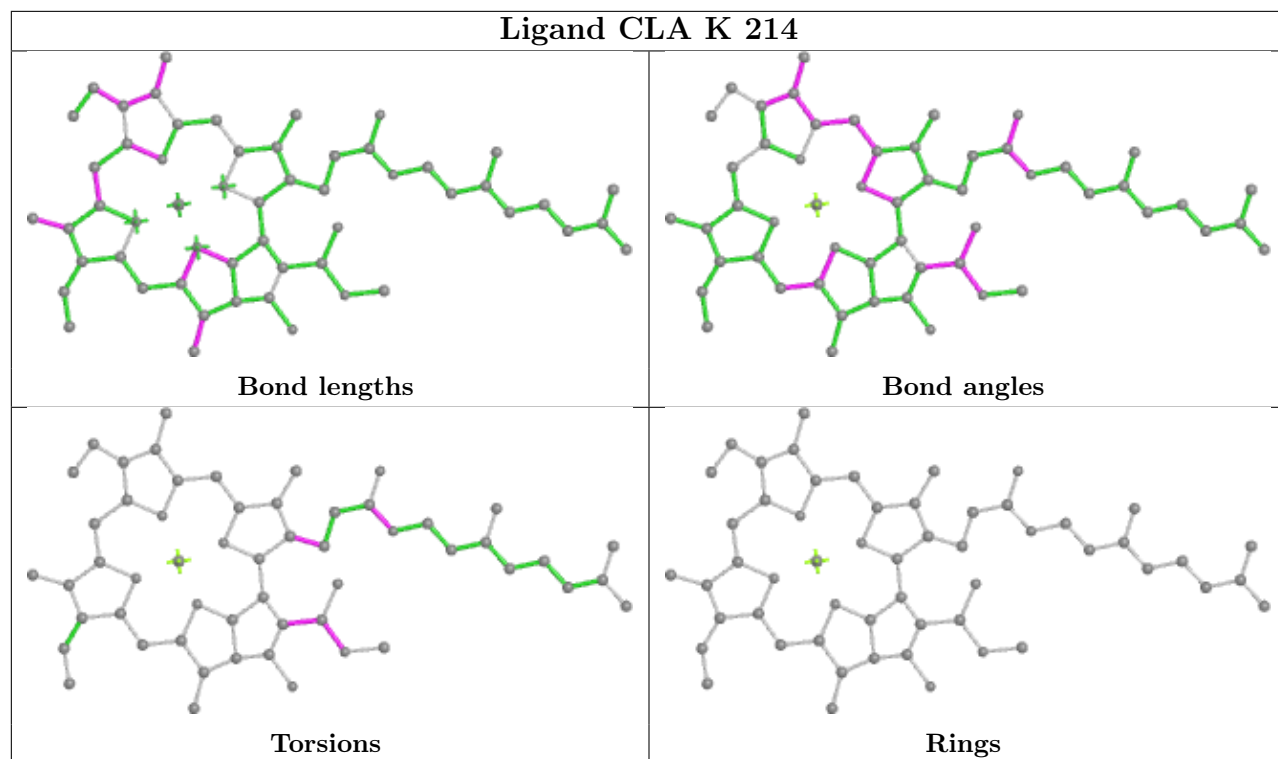


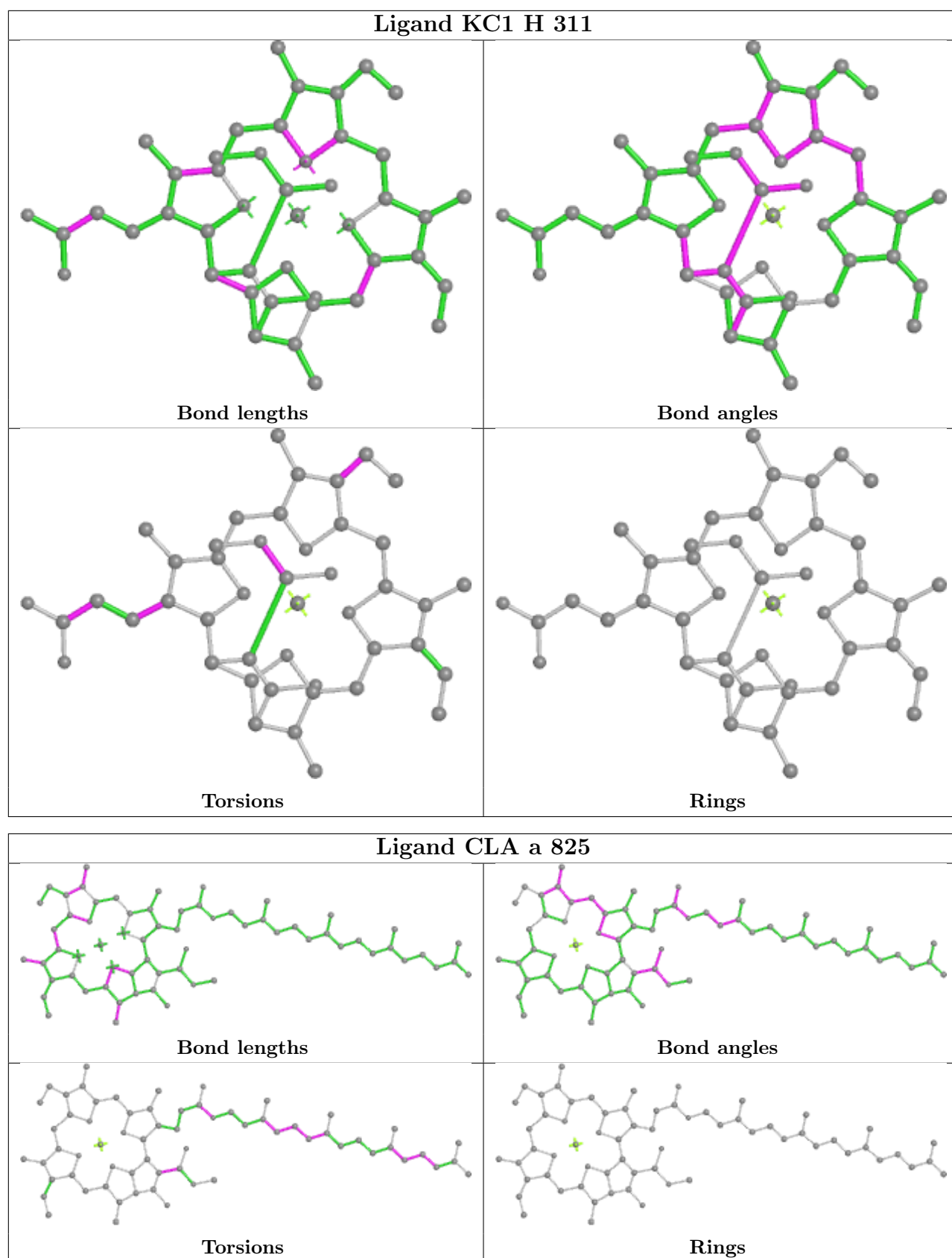
Ligand DD6 I 202



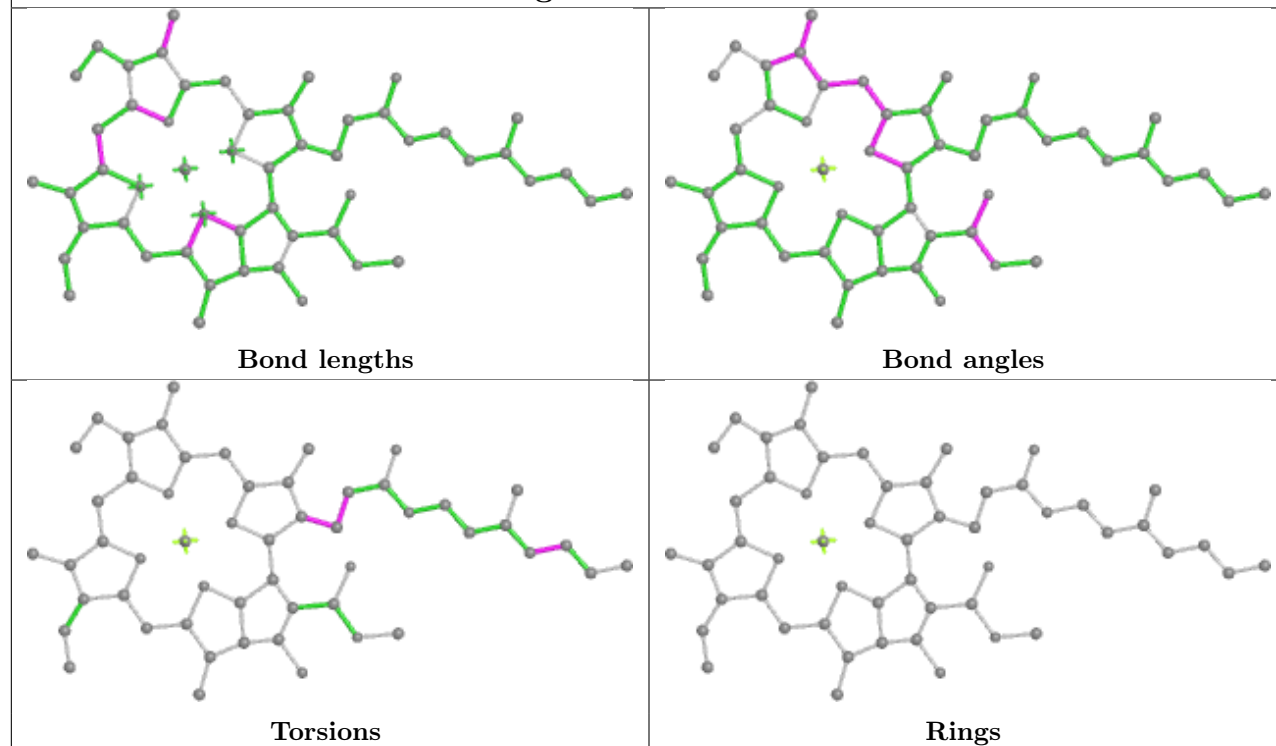




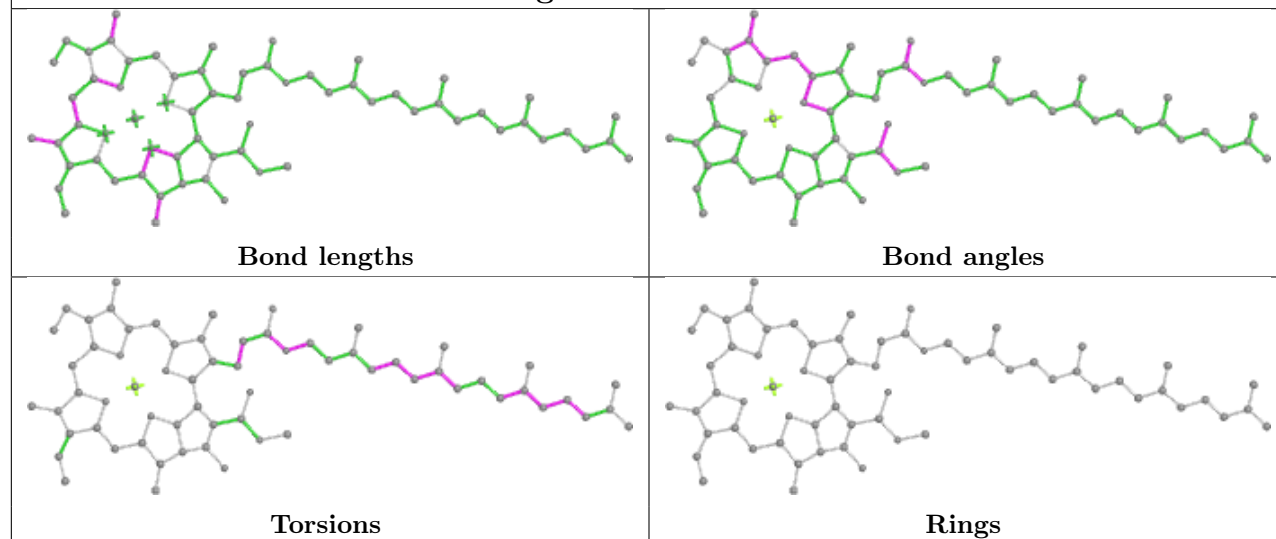




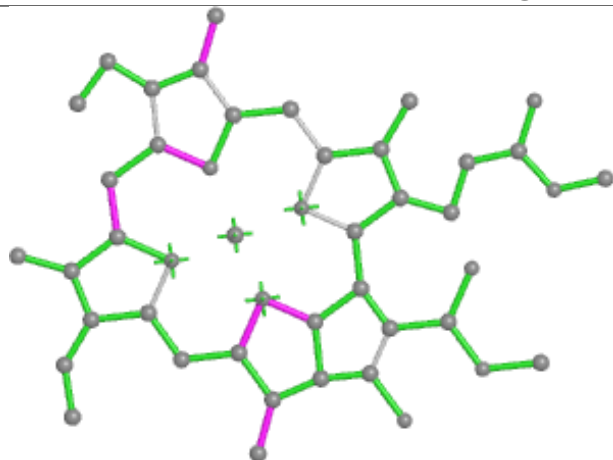
Ligand CLA b 713



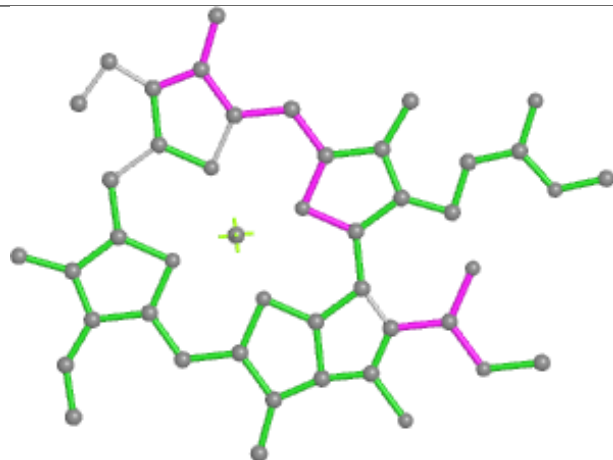
Ligand CLA a 829



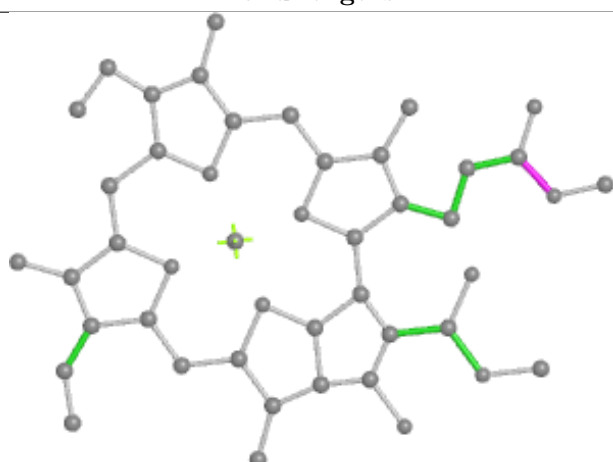
Ligand CLA F 307



Bond lengths



Bond angles

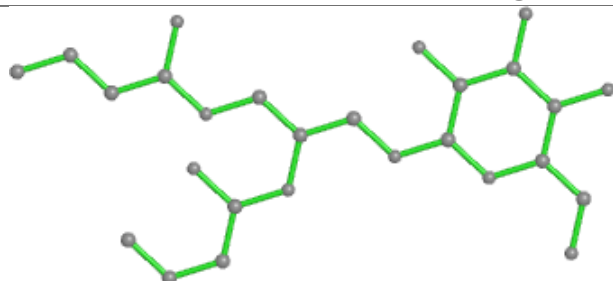


Torsions

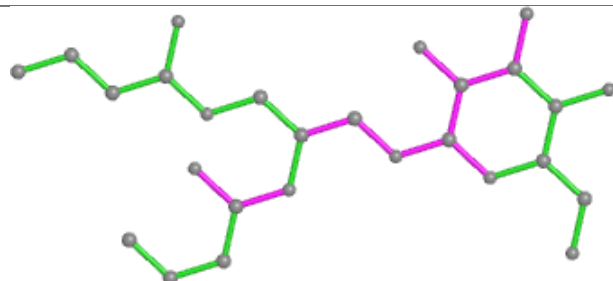


Rings

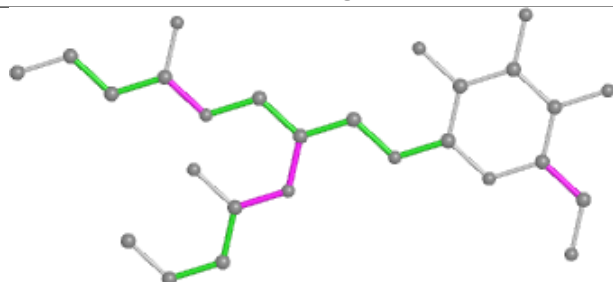
Ligand LMG P 201



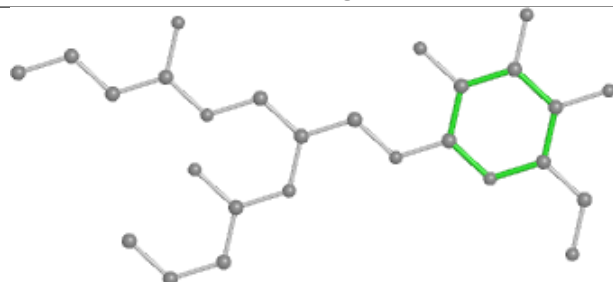
Bond lengths



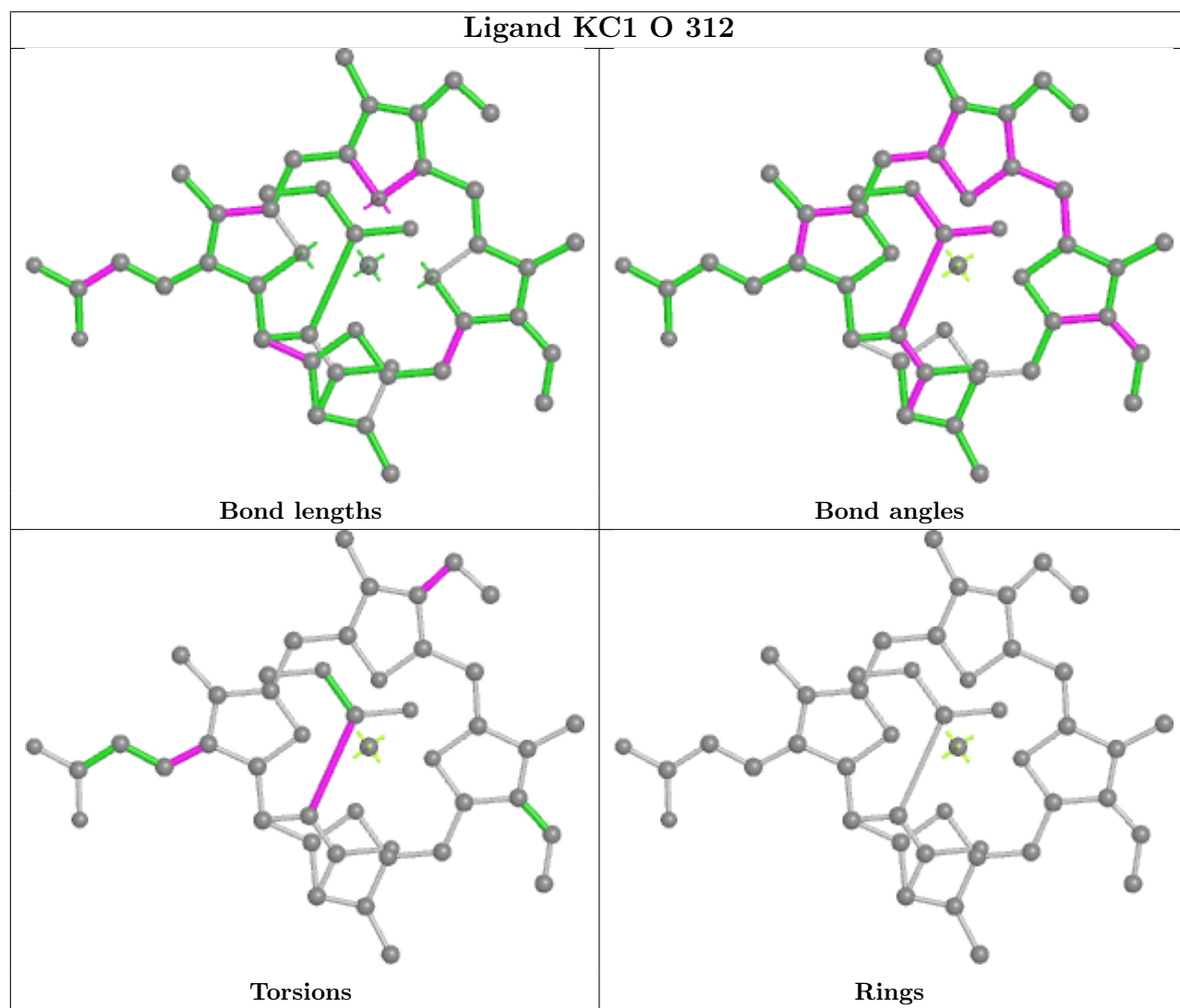
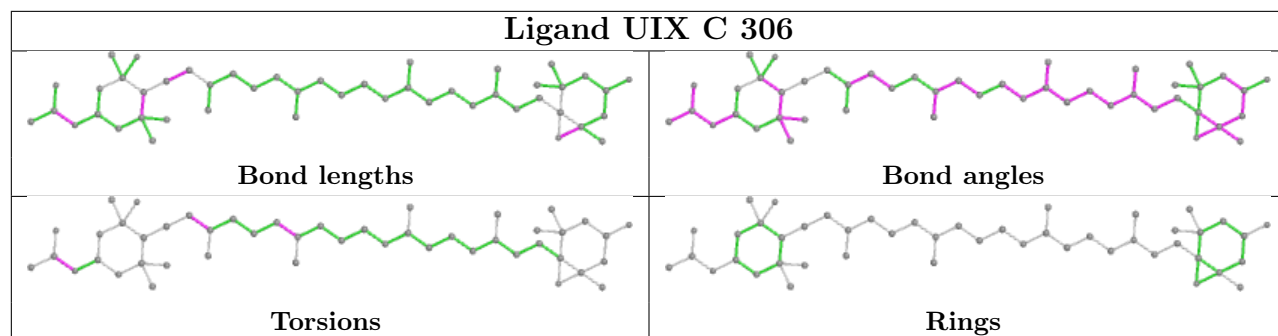
Bond angles



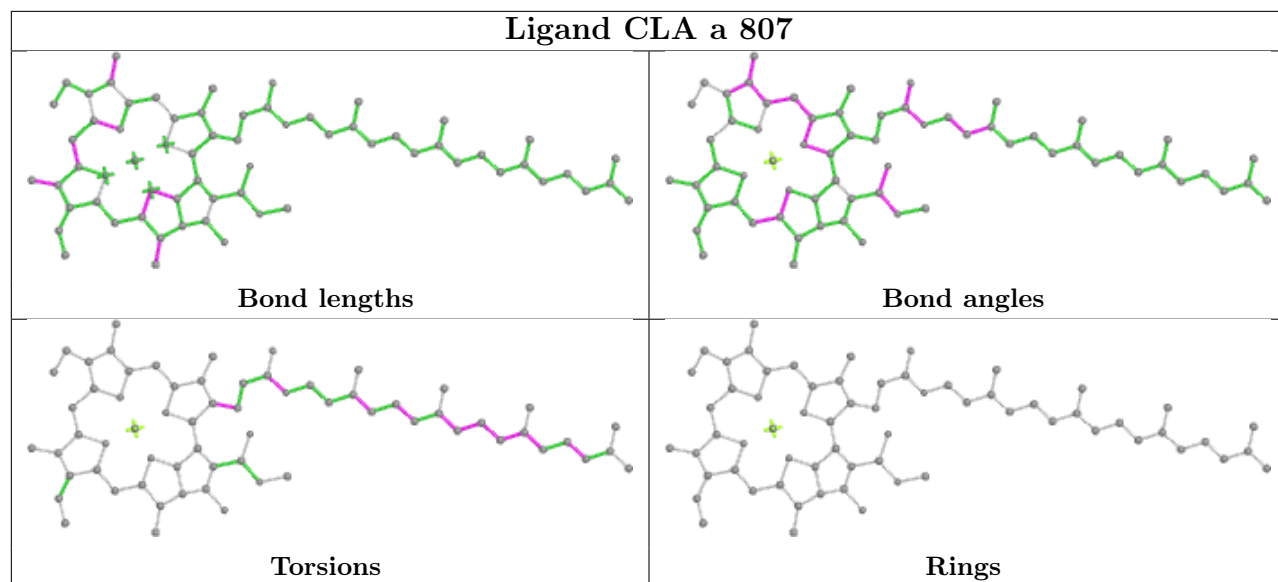
Torsions



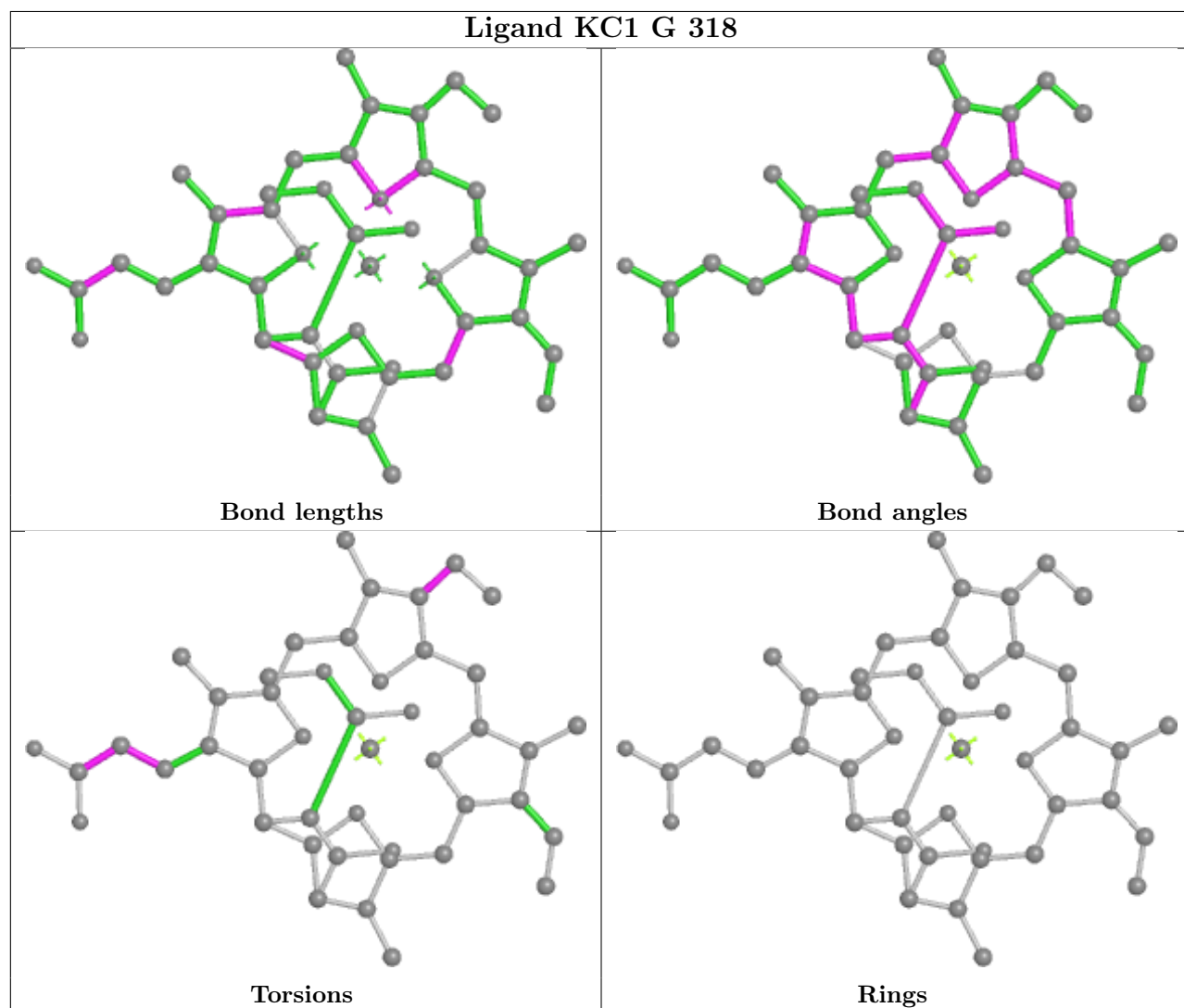
Rings

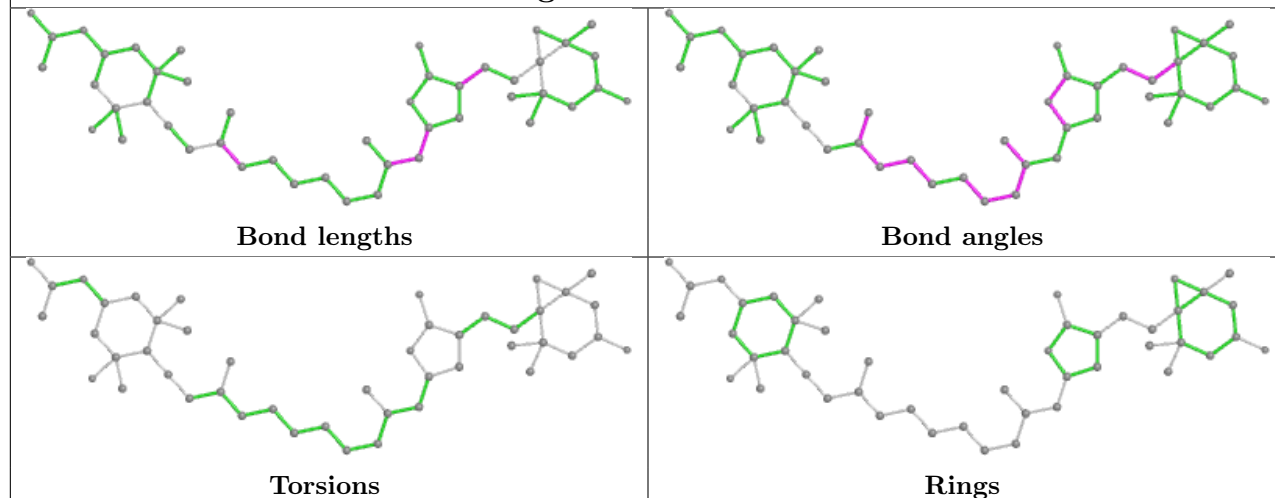
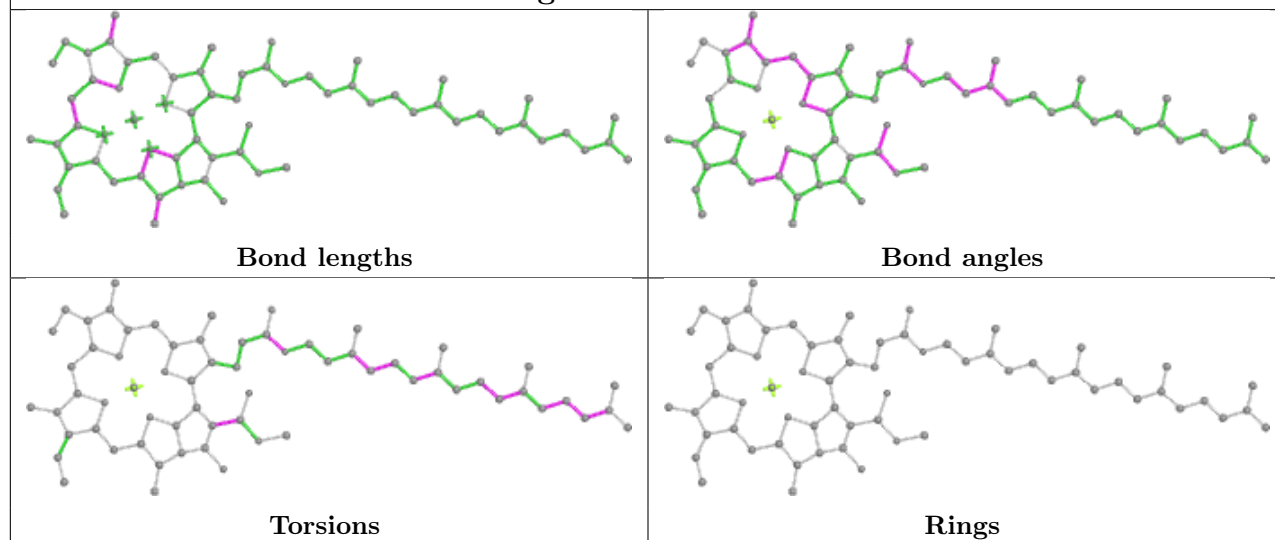
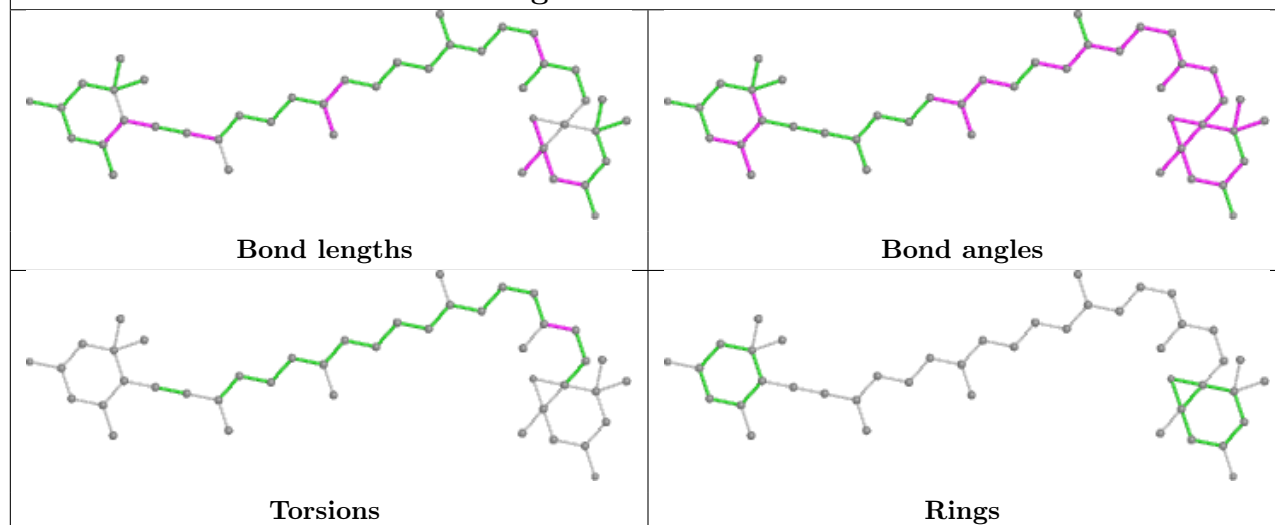


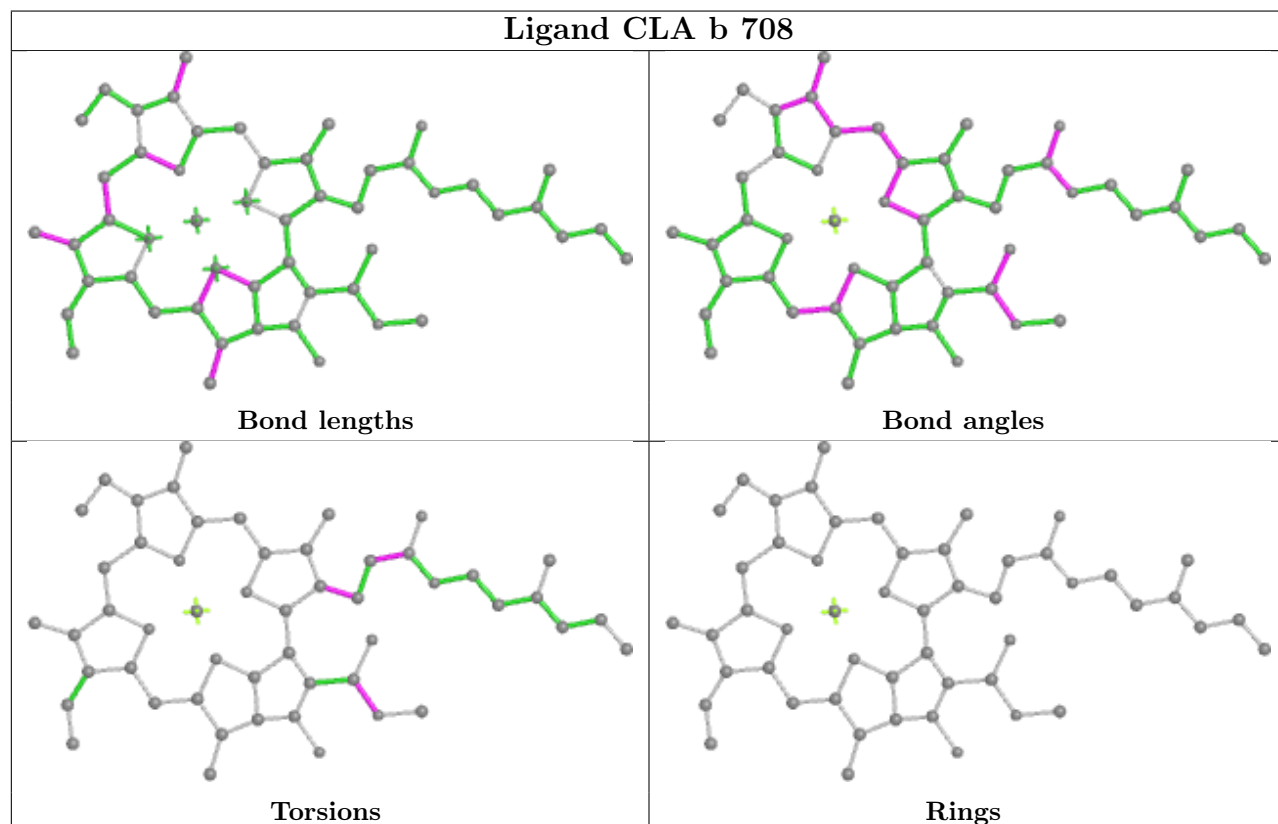
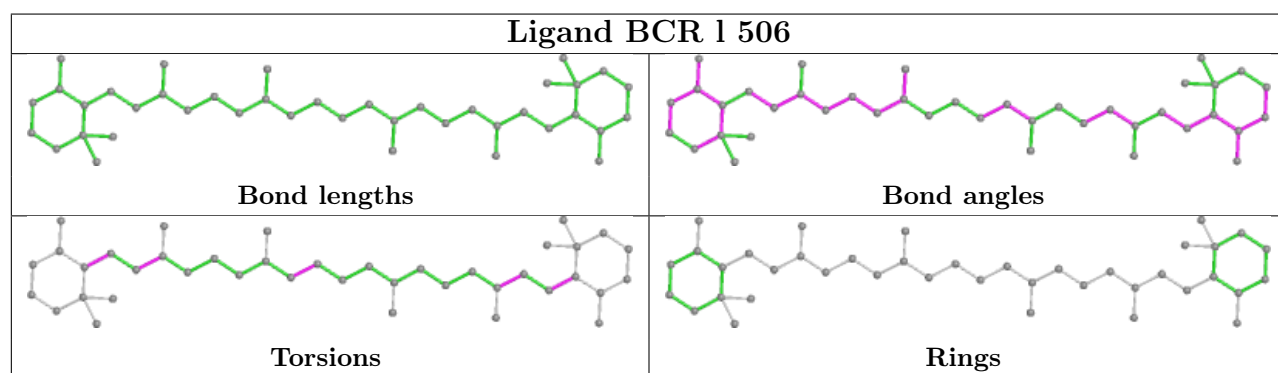
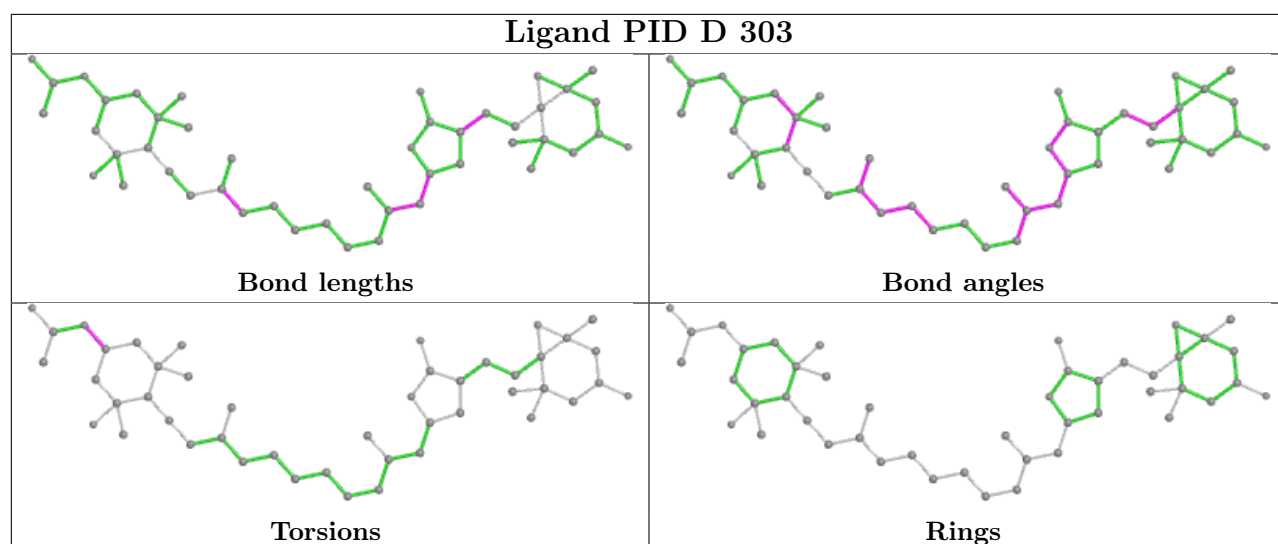
Ligand CLA a 807



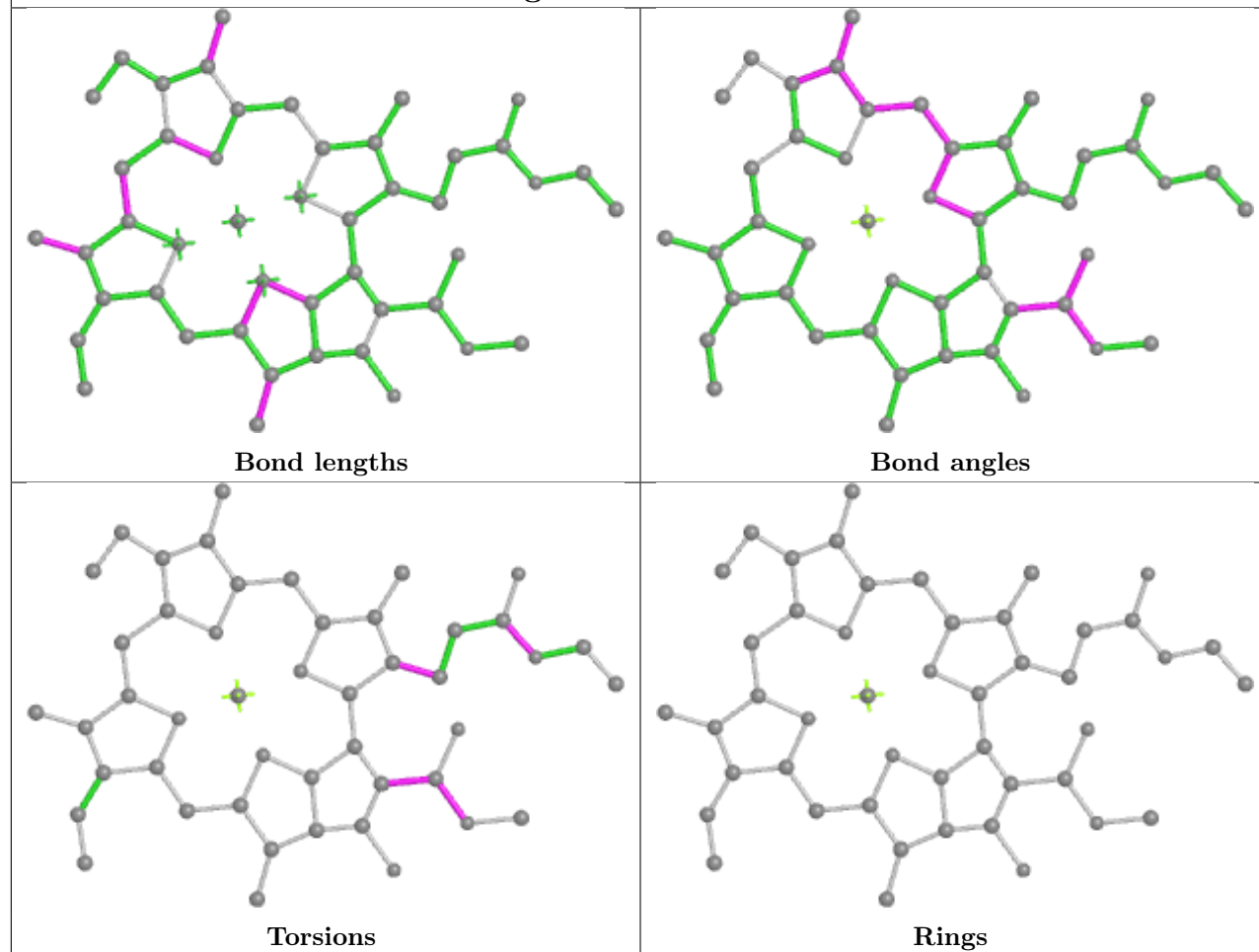
Ligand KC1 G 318



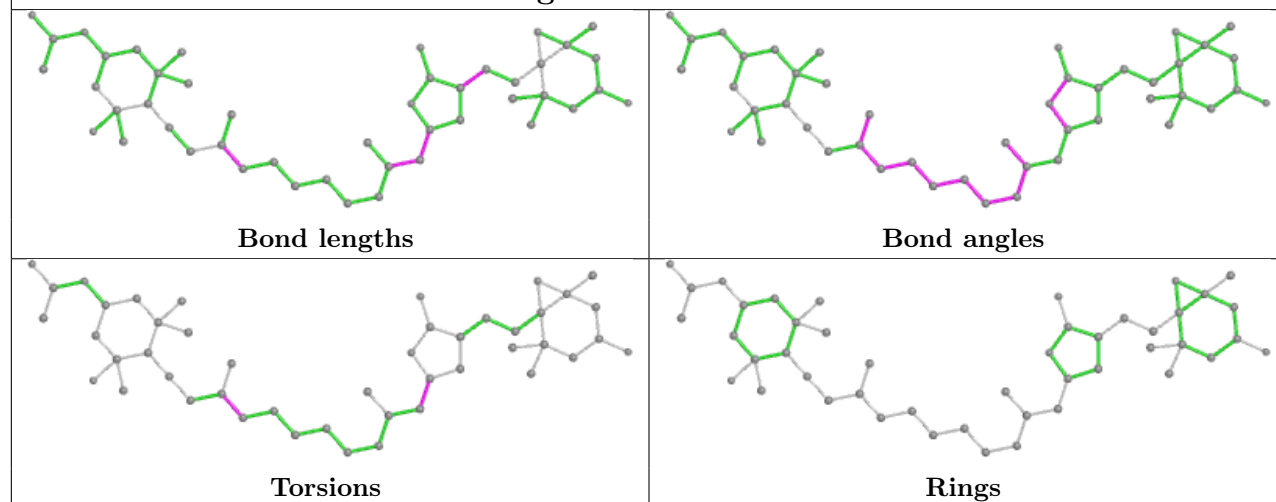
Ligand PID F 306**Ligand CLA I 213****Ligand DD6 G 307**

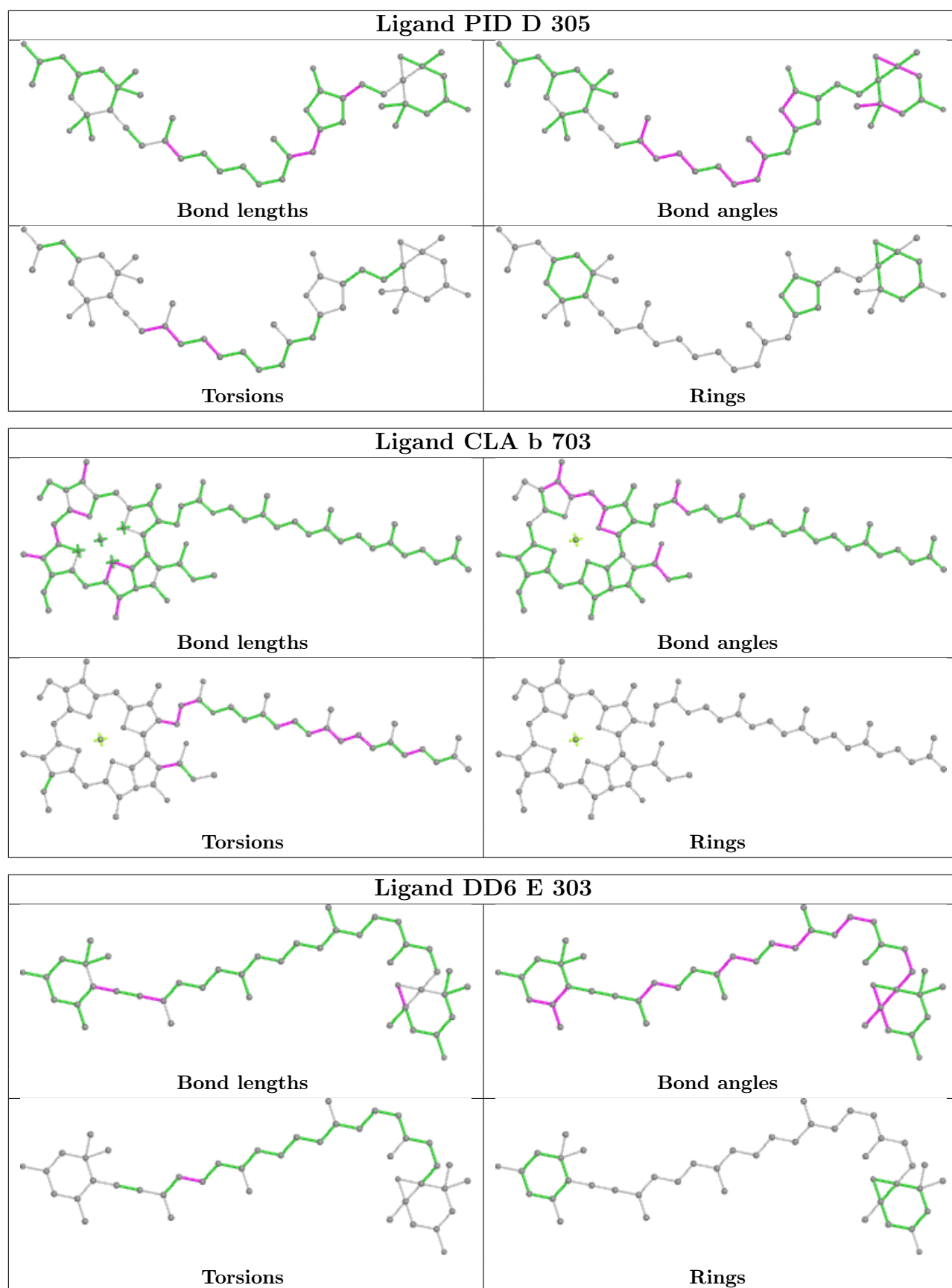


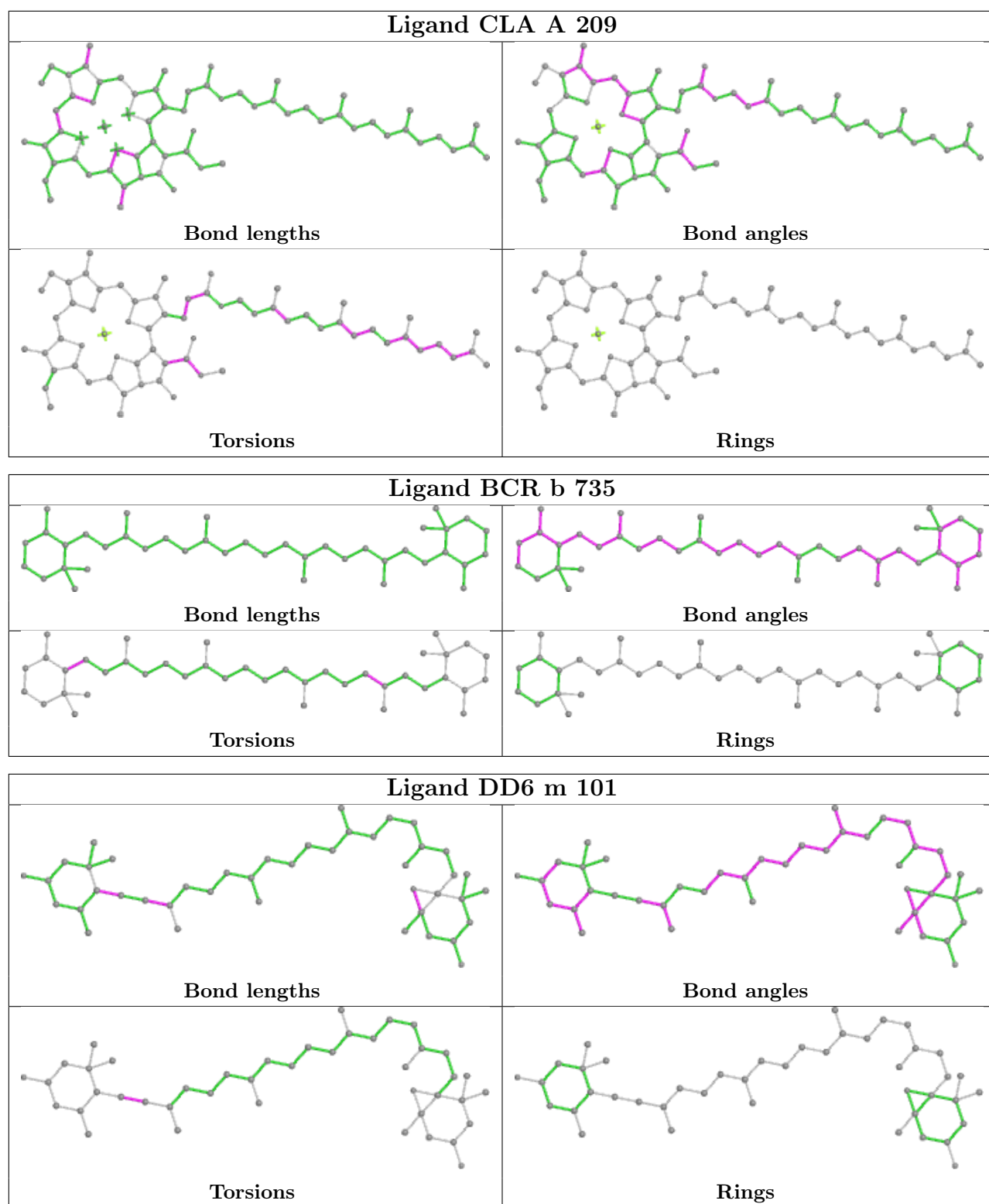
Ligand CLA D 314

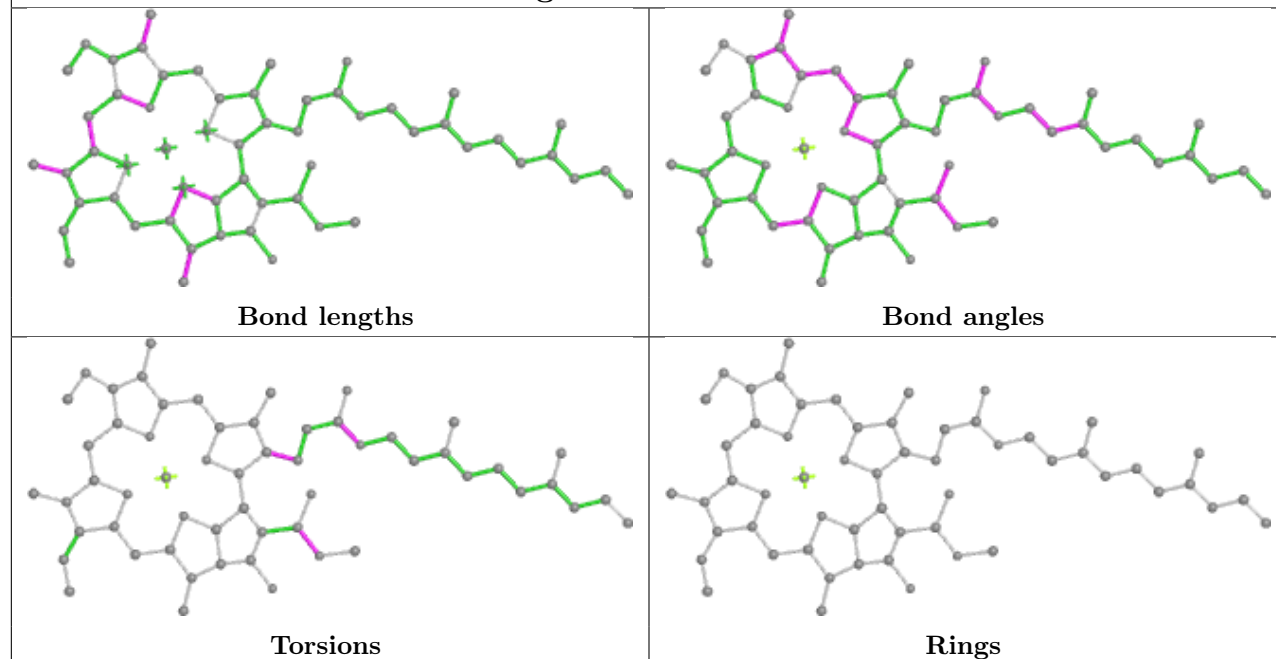
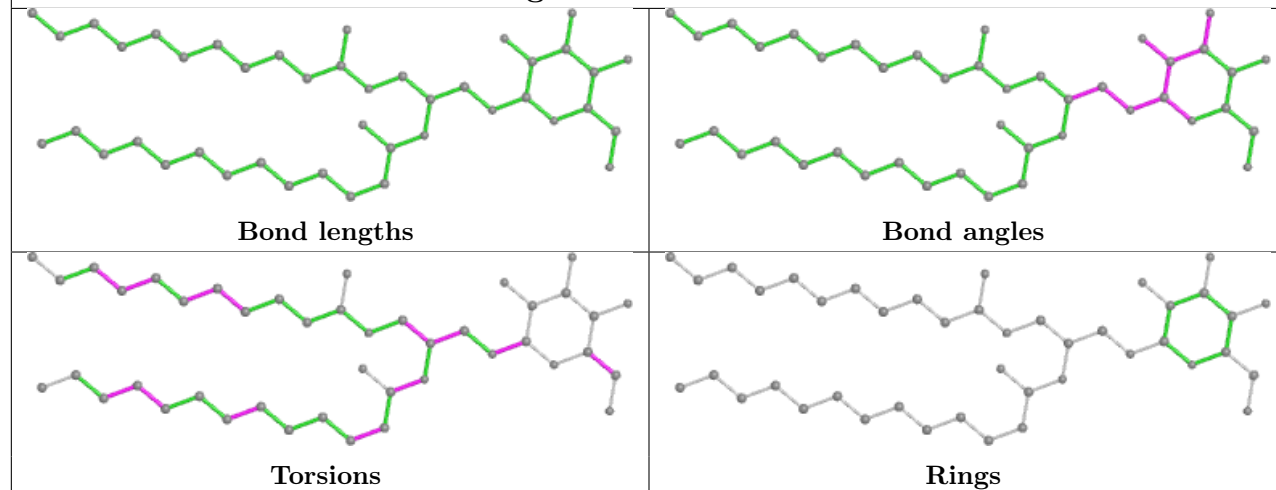


Ligand PID C 304

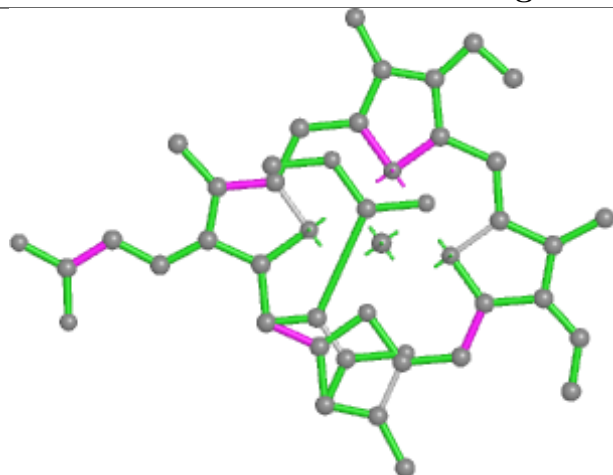




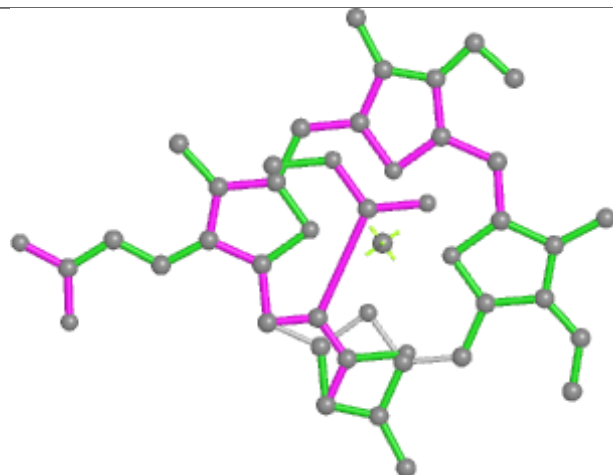


Ligand CLA a 819**Ligand LMG K 201**

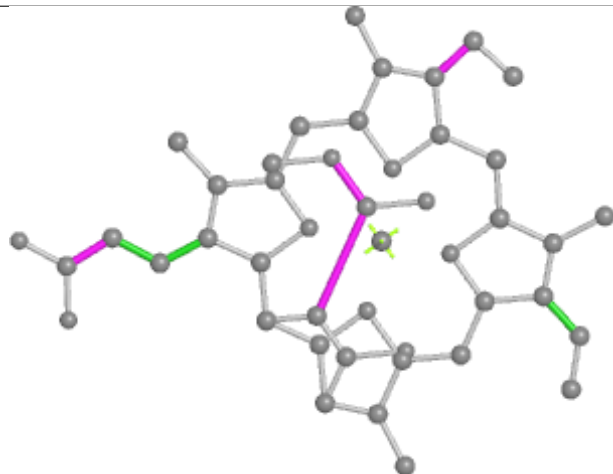
Ligand KC1 A 205



Bond lengths



Bond angles

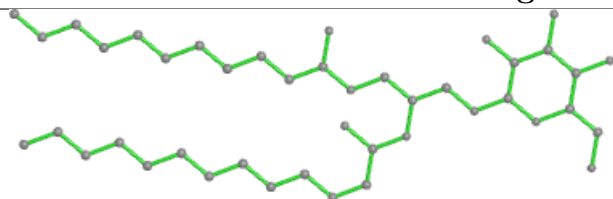


Torsions

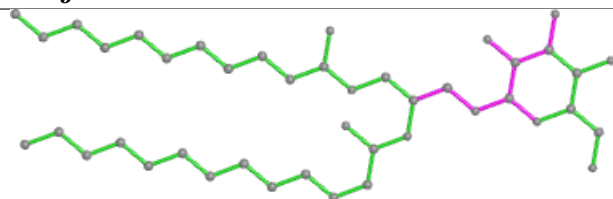


Rings

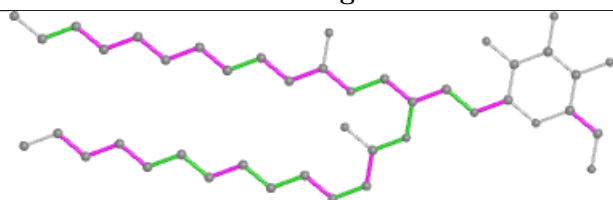
Ligand LMG j 102



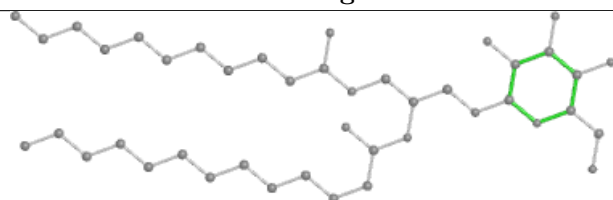
Bond lengths



Bond angles

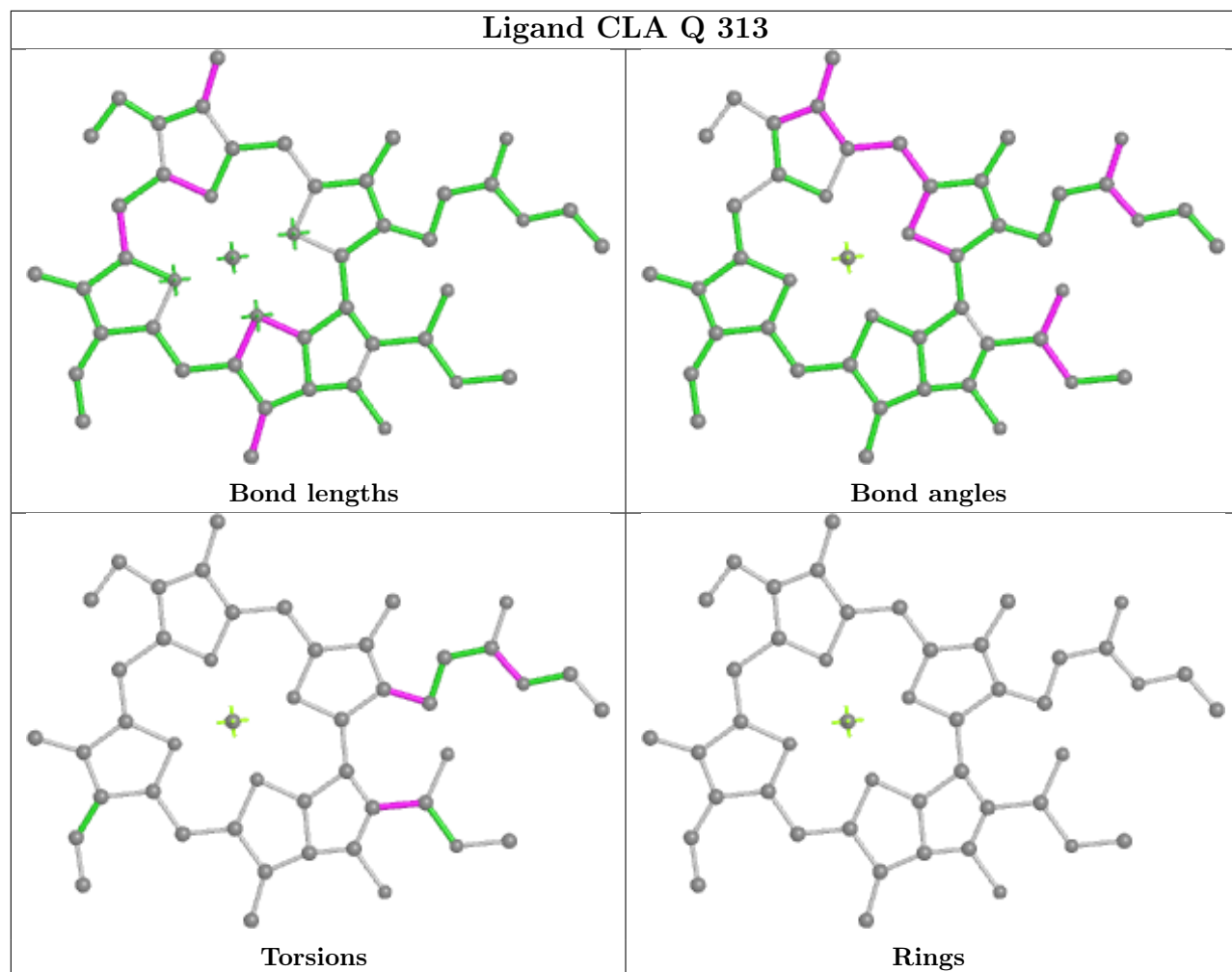


Torsions

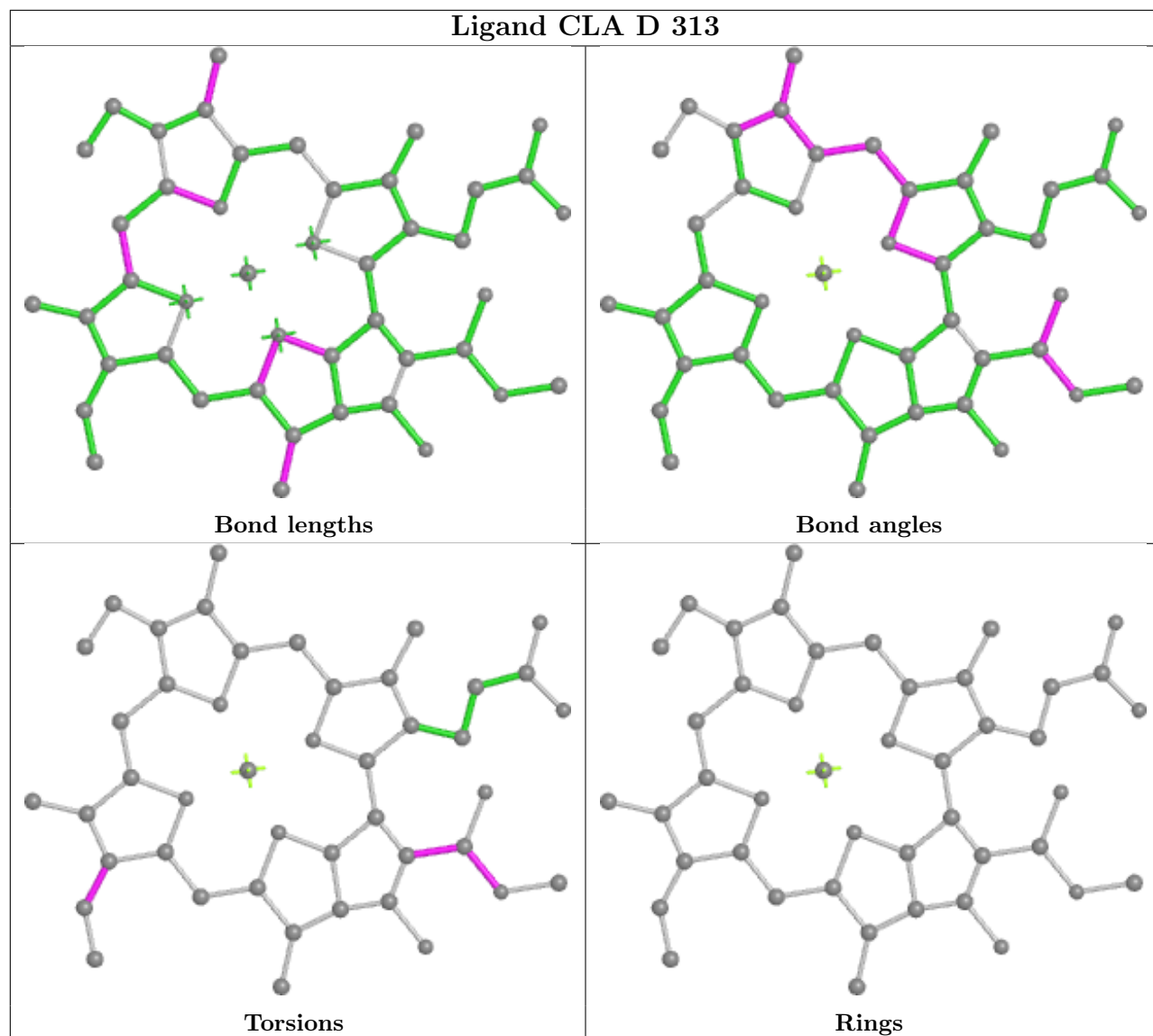


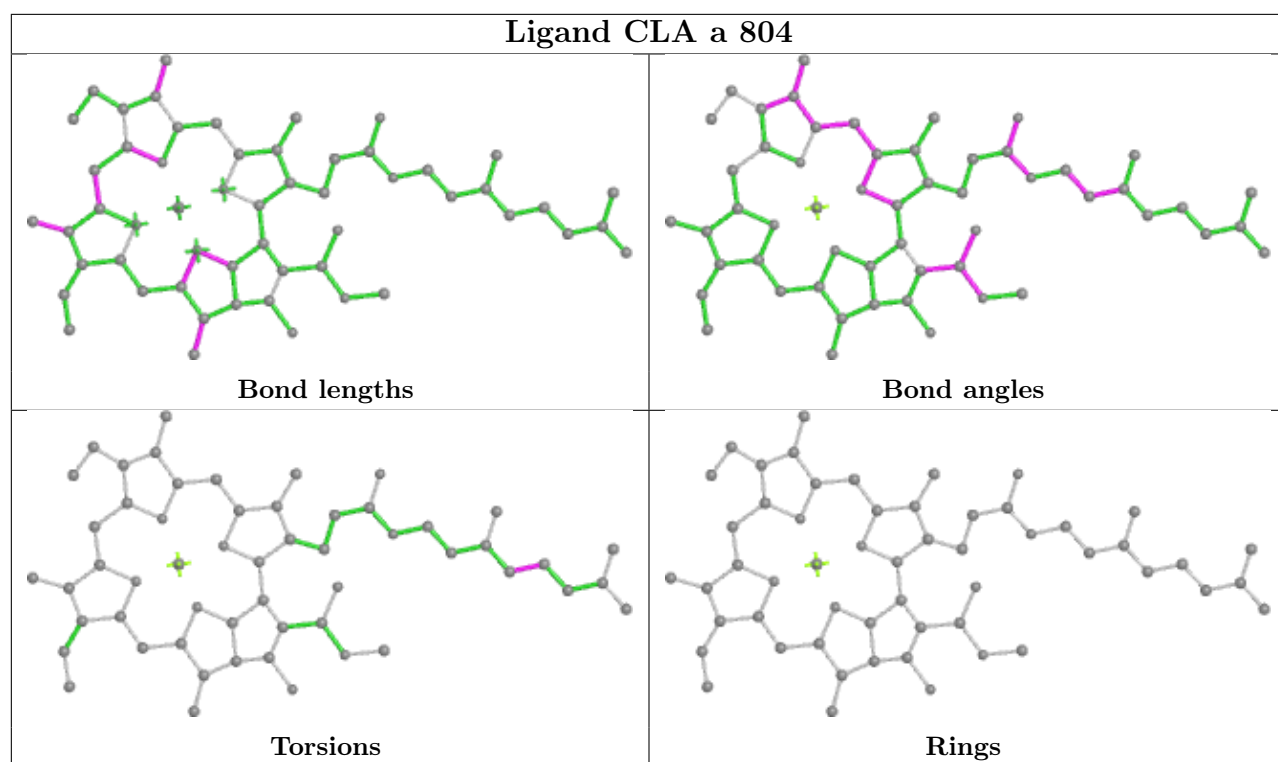
Rings

Ligand CLA Q 313

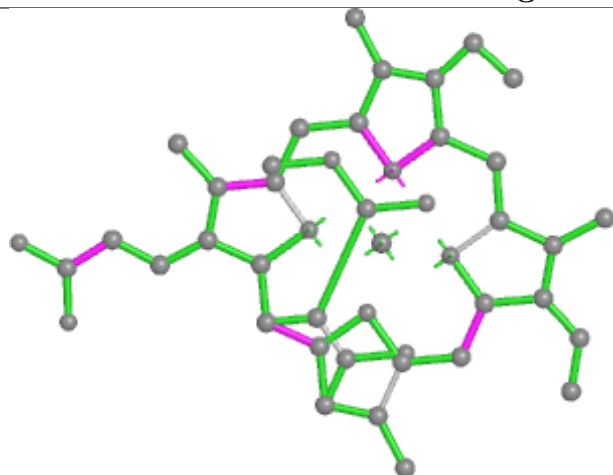


Ligand CLA D 313

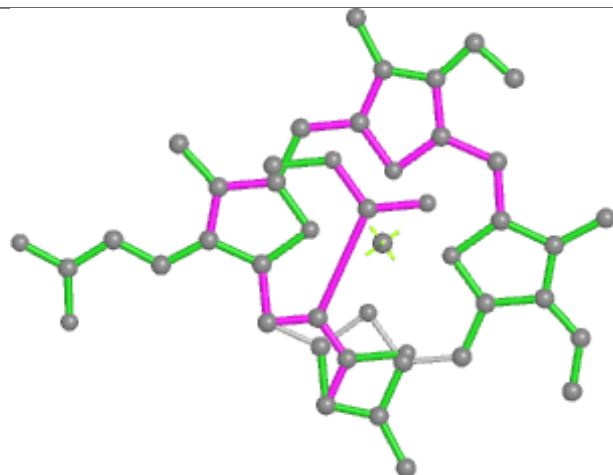




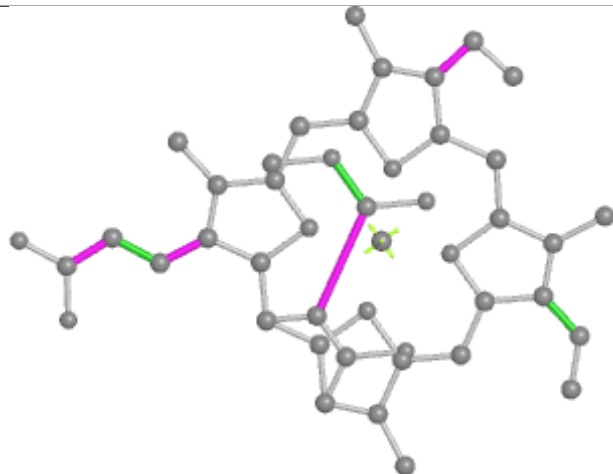
Ligand KC1 F 309



Bond lengths



Bond angles

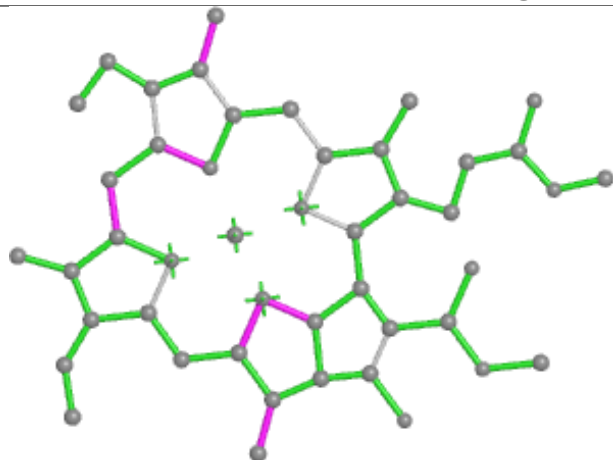


Torsions

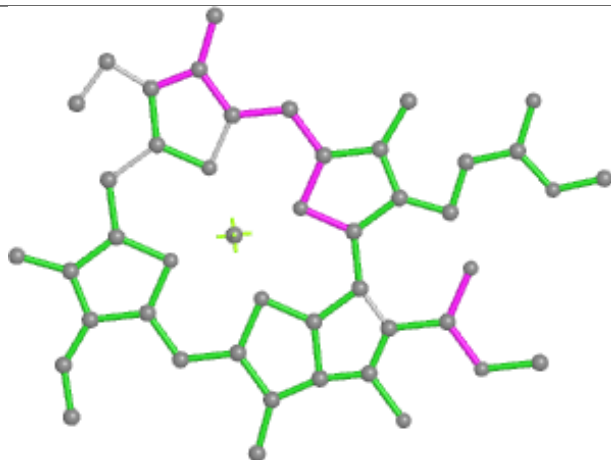


Rings

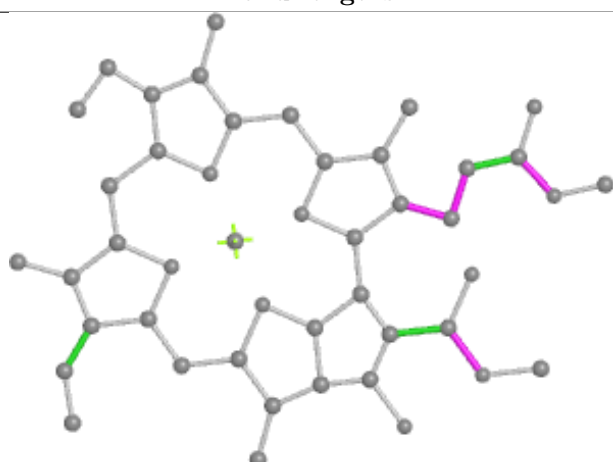
Ligand CLA P 214



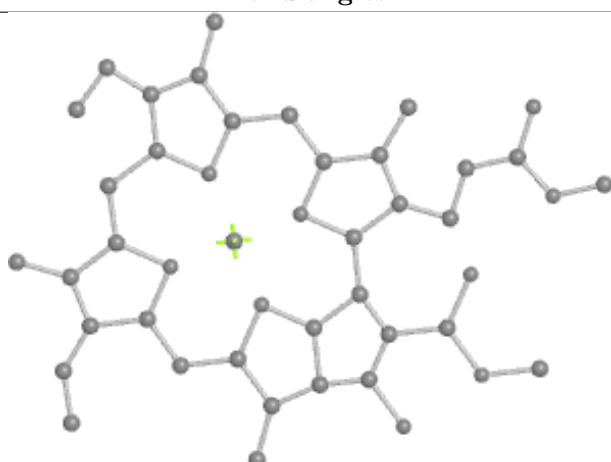
Bond lengths



Bond angles

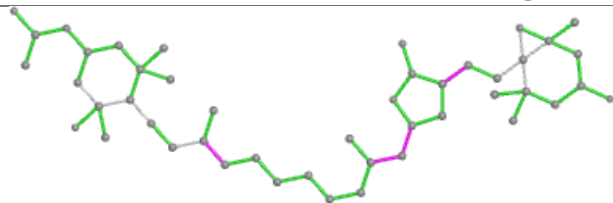


Torsions

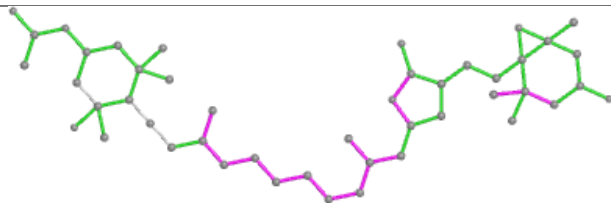


Rings

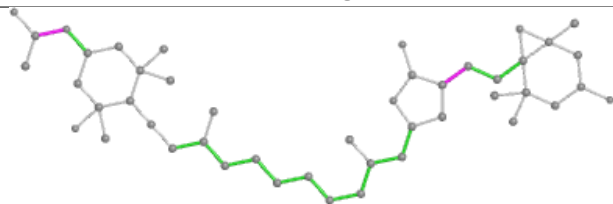
Ligand PID T 307



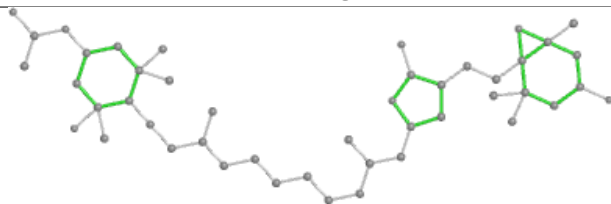
Bond lengths



Bond angles

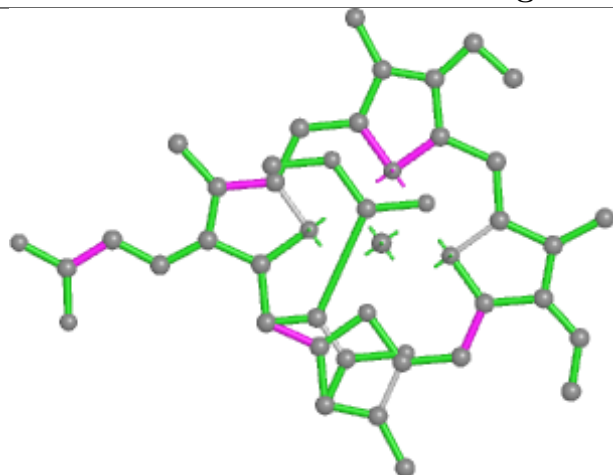


Torsions

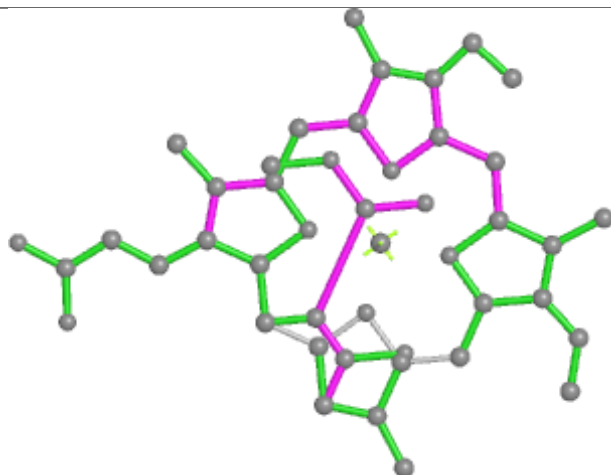


Rings

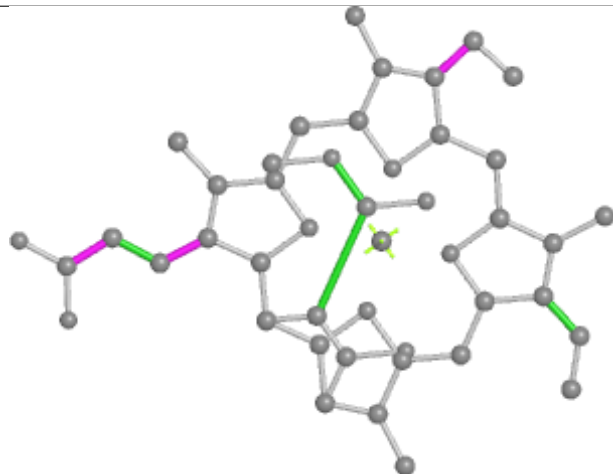
Ligand KC1 T 315



Bond lengths



Bond angles

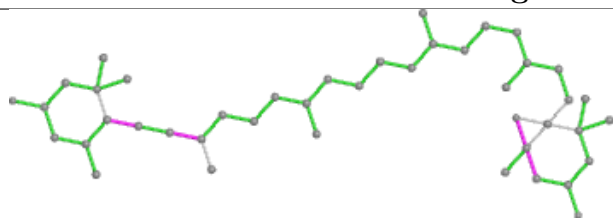


Torsions

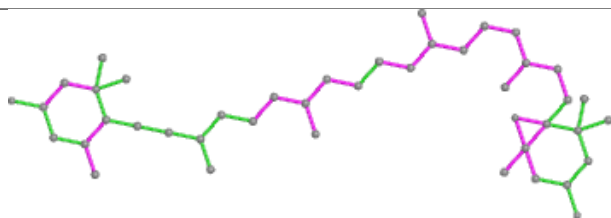


Rings

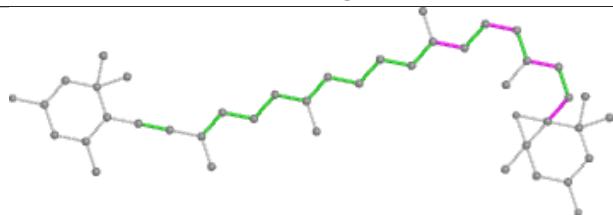
Ligand DD6 M 303



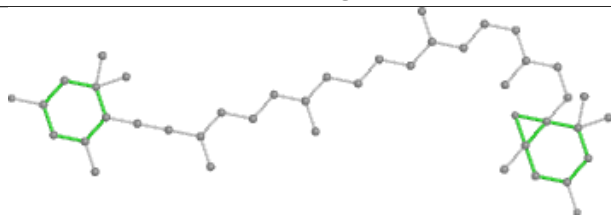
Bond lengths



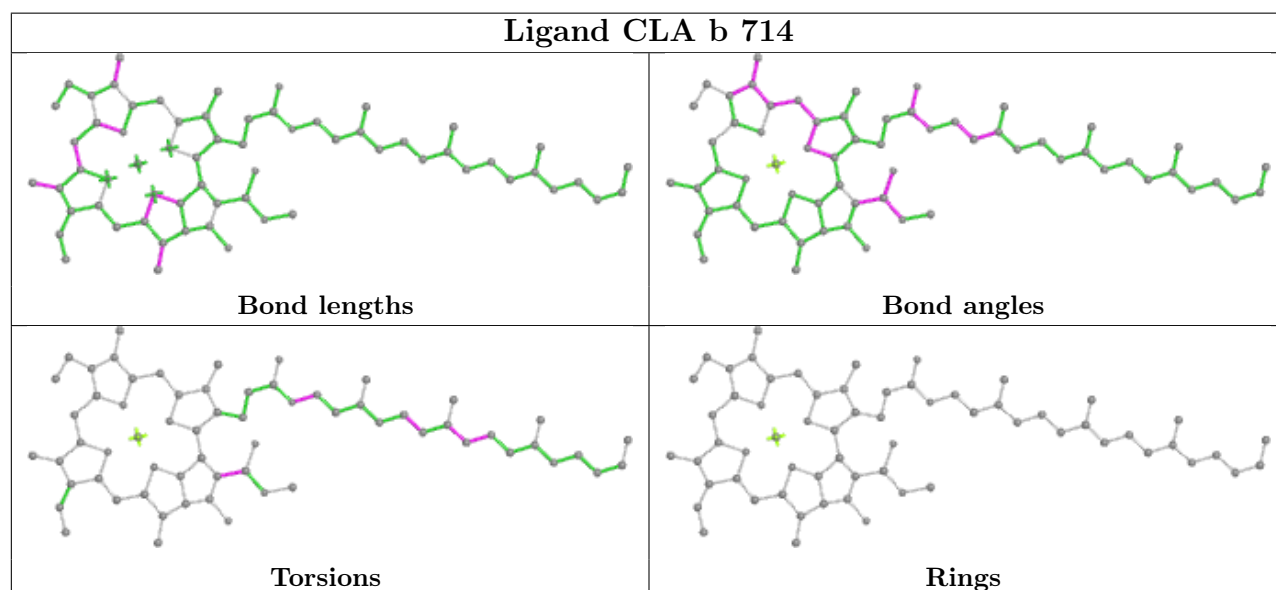
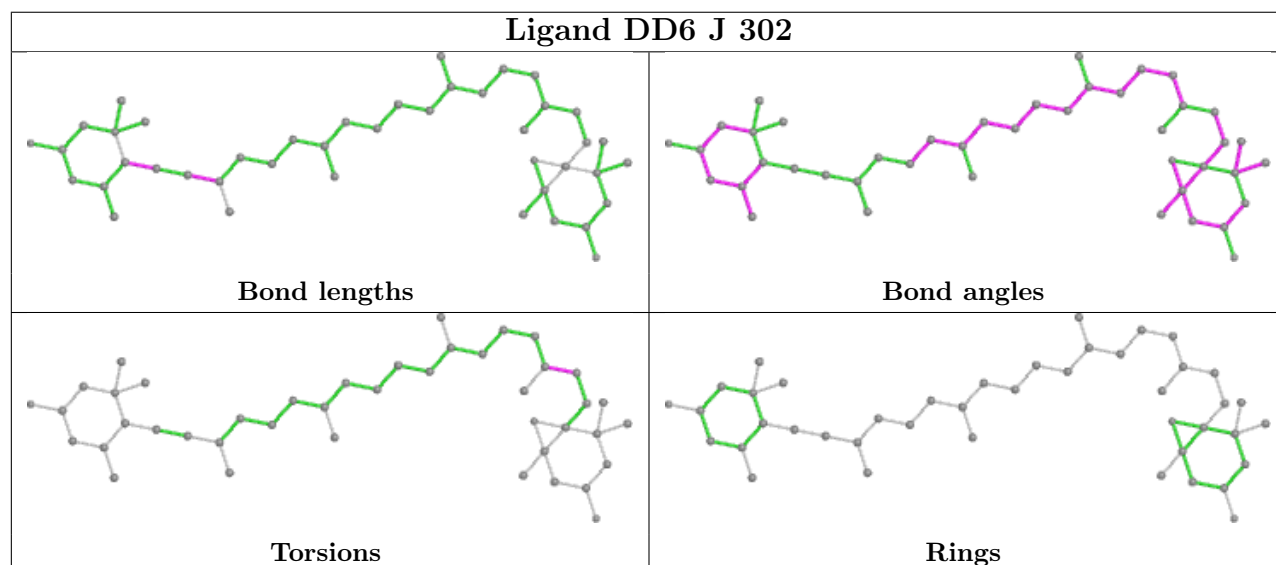
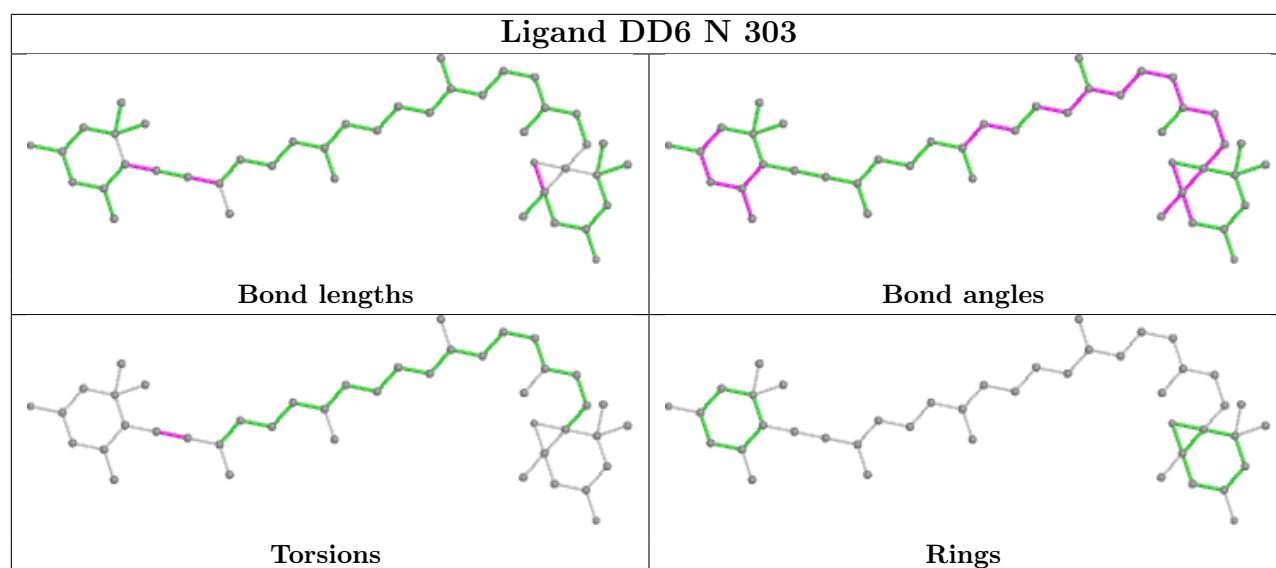
Bond angles



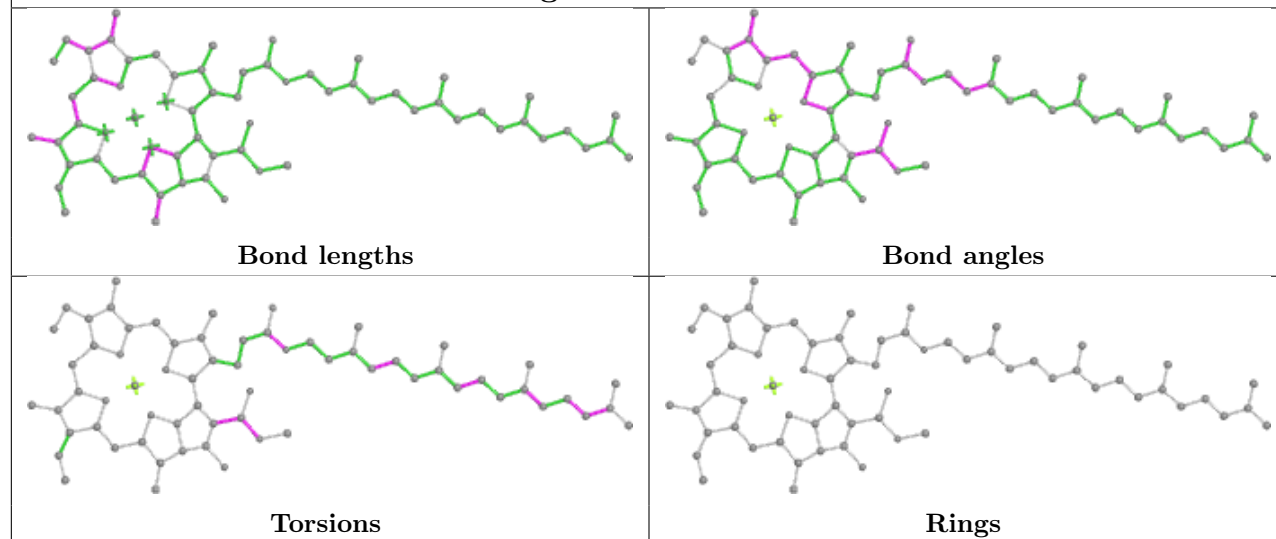
Torsions



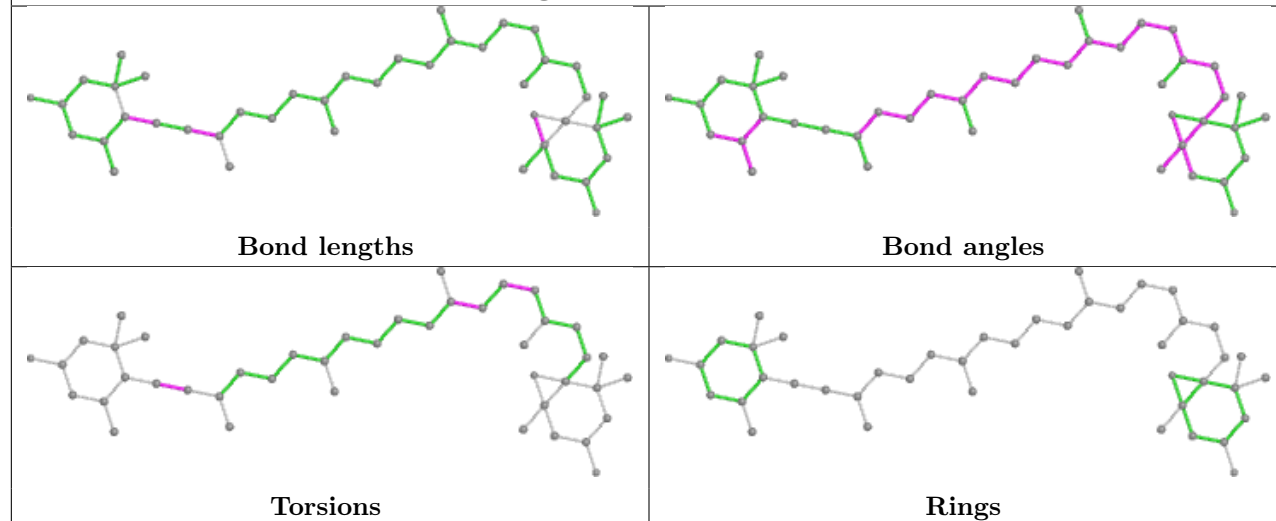
Rings



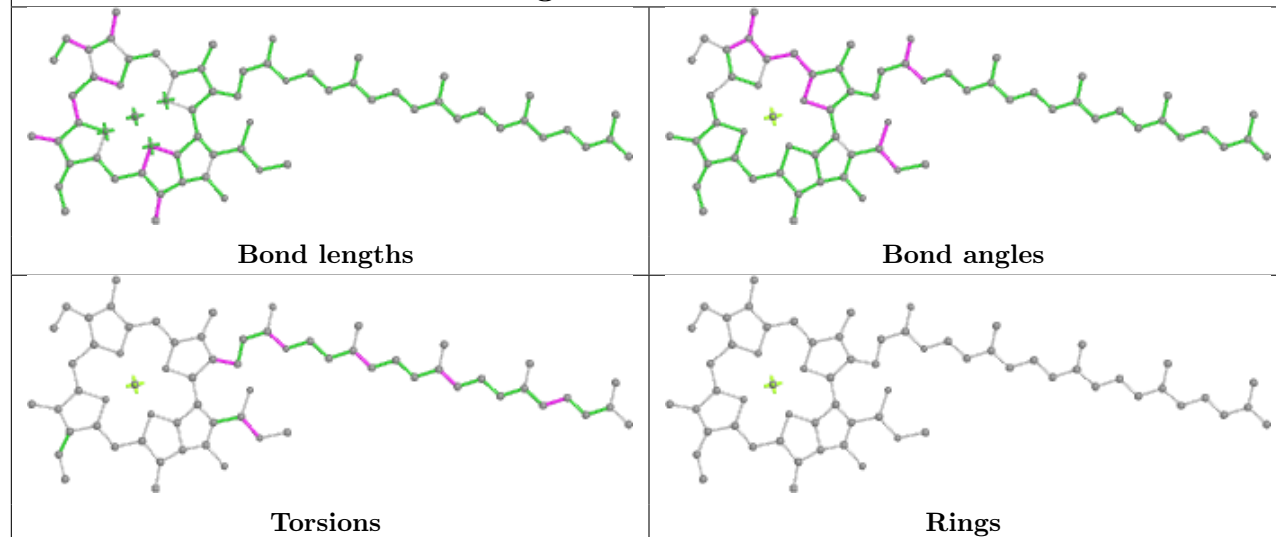
Ligand CLA l 502

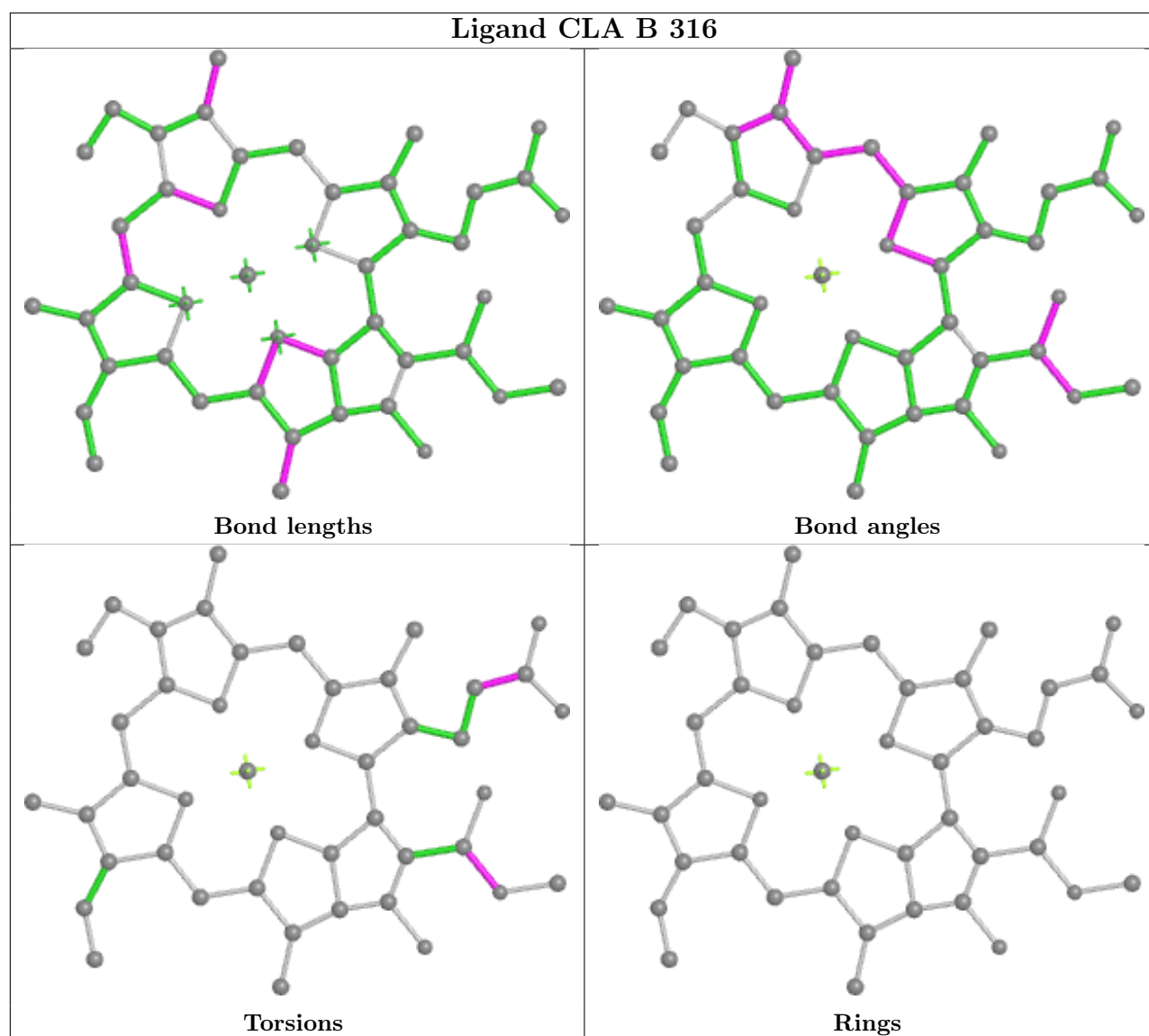


Ligand DD6 L 305



Ligand CLA a 820





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.