



## wwPDB EM Validation Summary Report ⓘ

Apr 5, 2026 – 10:49 PM UTC

PDB ID : 9UAS / pdb\_00009uas  
EMDB ID : EMD-63994  
Title : PSI-LHCE-LHCII from Euglena gracilis  
Authors : Feng, Y.  
Deposited on : 2025-04-01  
Resolution : 2.35 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

---

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

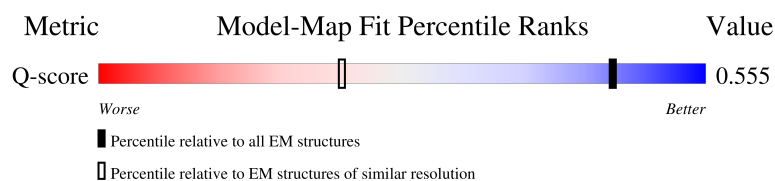
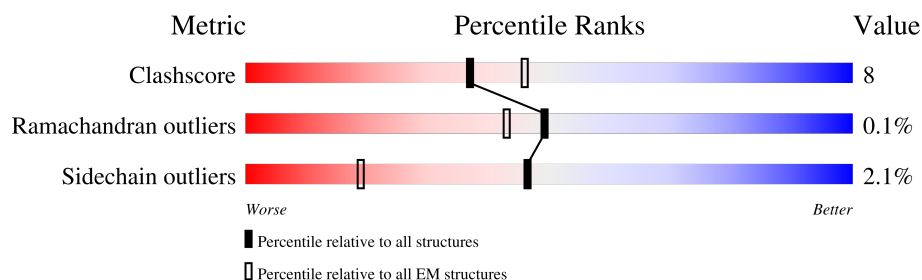
EMDB validation analysis : 0.0.1.dev132  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4-5-2 with Phenix2.0  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

# 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 2.35 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	4607 ( 1.85 - 2.85 )

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  $\geq 3$ , 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  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion  $< 40\%$ ). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	B	734	
2	C	81	
3	D	193	
4	E	158	

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Length	Quality of chain
5	F	325	
6	G	184	
6	P	184	
7	H	185	
8	I	184	
8	N	184	
9	J	39	
10	K	184	
10	Q	184	
11	L	187	
11	R	187	
12	M	31	
13	O	177	
14	S	180	
15	T	173	
16	U	209	
17	V	196	
18	W	228	
19	X	223	
20	A	756	

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
22	CLA	A	801	X	-	-	-
22	CLA	A	803	X	-	-	-
22	CLA	A	804	X	-	-	-

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	CLA	A	805	X	-	-	-
22	CLA	A	806	X	-	-	-
22	CLA	A	807	X	-	-	-
22	CLA	A	808	X	-	-	-
22	CLA	A	809	X	-	-	-
22	CLA	A	810	X	-	-	-
22	CLA	A	811	X	-	-	-
22	CLA	A	812	X	-	-	-
22	CLA	A	813	X	-	-	-
22	CLA	A	814	X	-	-	-
22	CLA	A	815	X	-	-	-
22	CLA	A	816	X	-	-	-
22	CLA	A	817	X	-	-	-
22	CLA	A	818	X	-	-	-
22	CLA	A	819	X	-	-	-
22	CLA	A	820	X	-	-	-
22	CLA	A	821	X	-	-	-
22	CLA	A	822	X	-	-	-
22	CLA	A	823	X	-	-	-
22	CLA	A	824	X	-	-	-
22	CLA	A	825	X	-	-	-
22	CLA	A	826	X	-	-	-
22	CLA	A	827	X	-	-	-
22	CLA	A	828	X	-	-	-
22	CLA	A	829	X	-	-	-
22	CLA	A	830	X	-	-	-
22	CLA	A	831	X	-	-	-
22	CLA	A	832	X	-	-	-
22	CLA	A	833	X	-	-	-
22	CLA	A	834	X	-	-	-
22	CLA	A	835	X	-	-	-
22	CLA	A	836	X	-	-	-
22	CLA	A	837	X	-	-	-
22	CLA	A	838	X	-	-	-
22	CLA	A	839	X	-	-	-
22	CLA	A	840	X	-	-	-
22	CLA	A	841	X	-	-	-
22	CLA	A	842	X	-	-	-
22	CLA	A	844	X	-	-	-
22	CLA	A	852	X	-	-	-
22	CLA	B	802	X	-	-	-
22	CLA	B	803	X	-	-	-

*Continued on next page...*



*Continued from previous page...*

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	CLA	B	804	X	-	-	-
22	CLA	B	805	X	-	-	-
22	CLA	B	806	X	-	-	-
22	CLA	B	807	X	-	-	-
22	CLA	B	808	X	-	-	-
22	CLA	B	809	X	-	-	-
22	CLA	B	810	X	-	-	-
22	CLA	B	811	X	-	-	-
22	CLA	B	812	X	-	-	-
22	CLA	B	813	X	-	-	-
22	CLA	B	814	X	-	-	-
22	CLA	B	815	X	-	-	-
22	CLA	B	816	X	-	-	-
22	CLA	B	817	X	-	-	-
22	CLA	B	818	X	-	-	-
22	CLA	B	819	X	-	-	-
22	CLA	B	820	X	-	-	-
22	CLA	B	821	X	-	-	-
22	CLA	B	822	X	-	-	-
22	CLA	B	823	X	-	-	-
22	CLA	B	824	X	-	-	-
22	CLA	B	825	X	-	-	-
22	CLA	B	826	X	-	-	-
22	CLA	B	827	X	-	-	-
22	CLA	B	828	X	-	-	-
22	CLA	B	829	X	-	-	-
22	CLA	B	830	X	-	-	-
22	CLA	B	831	X	-	-	-
22	CLA	B	832	X	-	-	-
22	CLA	B	833	X	-	-	-
22	CLA	B	834	X	-	-	-
22	CLA	B	835	X	-	-	-
22	CLA	B	836	X	-	-	-
22	CLA	B	837	X	-	-	-
22	CLA	B	838	X	-	-	-
22	CLA	B	839	X	-	-	-
22	CLA	B	859	X	-	-	-
22	CLA	F	403	X	-	-	-
22	CLA	F	404	X	-	-	-
22	CLA	F	405	X	-	-	-
22	CLA	G	601	X	-	-	-
22	CLA	G	602	X	-	-	-

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	CLA	G	603	X	-	-	-
22	CLA	G	604	X	-	-	-
22	CLA	G	605	X	-	-	-
22	CLA	G	606	X	-	-	-
22	CLA	G	607	X	-	-	-
22	CLA	G	608	X	-	-	-
22	CLA	G	609	X	-	-	-
22	CLA	G	610	X	-	-	-
22	CLA	G	611	X	-	-	-
22	CLA	H	302	X	-	-	-
22	CLA	H	303	X	-	-	-
22	CLA	H	304	X	-	-	-
22	CLA	H	305	X	-	-	-
22	CLA	H	306	X	-	-	-
22	CLA	H	307	X	-	-	-
22	CLA	H	308	X	-	-	-
22	CLA	H	309	X	-	-	-
22	CLA	H	310	X	-	-	-
22	CLA	H	311	X	-	-	-
22	CLA	H	312	X	-	-	-
22	CLA	H	313	X	-	-	-
22	CLA	H	318	X	-	-	-
22	CLA	I	601	X	-	-	-
22	CLA	I	602	X	-	-	-
22	CLA	I	603	X	-	-	-
22	CLA	I	604	X	-	-	-
22	CLA	I	605	X	-	-	-
22	CLA	I	606	X	-	-	-
22	CLA	I	607	X	-	-	-
22	CLA	I	608	X	-	-	-
22	CLA	I	609	X	-	-	-
22	CLA	I	610	X	-	-	-
22	CLA	I	611	X	-	-	-
22	CLA	J	102	X	-	-	-
22	CLA	K	602	X	-	-	-
22	CLA	K	603	X	-	-	-
22	CLA	K	604	X	-	-	-
22	CLA	K	605	X	-	-	-
22	CLA	K	606	X	-	-	-
22	CLA	K	607	X	-	-	-
22	CLA	K	608	X	-	-	-
22	CLA	K	609	X	-	-	-

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	CLA	K	610	X	-	-	-
22	CLA	K	611	X	-	-	-
22	CLA	K	612	X	-	-	-
22	CLA	K	613	X	-	-	-
22	CLA	K	617	X	-	-	-
22	CLA	L	402	X	-	-	-
22	CLA	L	403	X	-	-	-
22	CLA	L	404	X	-	-	-
22	CLA	L	405	X	-	-	-
22	CLA	L	406	X	-	-	-
22	CLA	L	407	X	-	-	-
22	CLA	L	408	X	-	-	-
22	CLA	L	409	X	-	-	-
22	CLA	L	410	X	-	-	-
22	CLA	L	411	X	-	-	-
22	CLA	L	412	X	-	-	-
22	CLA	L	417	X	-	-	-
22	CLA	N	601	X	-	-	-
22	CLA	N	602	X	-	-	-
22	CLA	N	603	X	-	-	-
22	CLA	N	604	X	-	-	-
22	CLA	N	605	X	-	-	-
22	CLA	N	606	X	-	-	-
22	CLA	N	607	X	-	-	-
22	CLA	N	608	X	-	-	-
22	CLA	N	609	X	-	-	-
22	CLA	N	610	X	-	-	-
22	CLA	N	611	X	-	-	-
22	CLA	O	305	X	-	-	-
22	CLA	O	306	X	-	-	-
22	CLA	O	307	X	-	-	-
22	CLA	O	308	X	-	-	-
22	CLA	O	309	X	-	-	-
22	CLA	O	310	X	-	-	-
22	CLA	O	311	X	-	-	-
22	CLA	O	312	X	-	-	-
22	CLA	O	313	X	-	-	-
22	CLA	O	314	X	-	-	-
22	CLA	O	315	X	-	-	-
22	CLA	O	319	X	-	-	-
22	CLA	P	602	X	-	-	-
22	CLA	P	604	X	-	-	-

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	CLA	P	605	X	-	-	-
22	CLA	P	606	X	-	-	-
22	CLA	P	607	X	-	-	-
22	CLA	P	608	X	-	-	-
22	CLA	P	609	X	-	-	-
22	CLA	P	610	X	-	-	-
22	CLA	P	611	X	-	-	-
22	CLA	Q	601	X	-	-	-
22	CLA	Q	603	X	-	-	-
22	CLA	Q	604	X	-	-	-
22	CLA	Q	605	X	-	-	-
22	CLA	Q	606	X	-	-	-
22	CLA	Q	607	X	-	-	-
22	CLA	Q	608	X	-	-	-
22	CLA	Q	609	X	-	-	-
22	CLA	Q	610	X	-	-	-
22	CLA	Q	611	X	-	-	-
22	CLA	Q	612	X	-	-	-
22	CLA	Q	613	X	-	-	-
22	CLA	Q	617	X	-	-	-
22	CLA	Q	618	X	-	-	-
22	CLA	R	601	X	-	-	-
22	CLA	R	602	X	-	-	-
22	CLA	R	603	X	-	-	-
22	CLA	R	604	X	-	-	-
22	CLA	R	605	X	-	-	-
22	CLA	R	606	X	-	-	-
22	CLA	R	607	X	-	-	-
22	CLA	R	608	X	-	-	-
22	CLA	R	609	X	-	-	-
22	CLA	R	610	X	-	-	-
22	CLA	R	611	X	-	-	-
22	CLA	R	615	X	-	-	-
22	CLA	S	601	X	-	-	-
22	CLA	S	602	X	-	-	-
22	CLA	S	603	X	-	-	-
22	CLA	S	604	X	-	-	-
22	CLA	S	605	X	-	-	-
22	CLA	S	606	X	-	-	-
22	CLA	S	607	X	-	-	-
22	CLA	S	608	X	-	-	-
22	CLA	S	610	X	-	-	-

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	CLA	S	614	X	-	-	-
22	CLA	S	615	X	-	-	-
22	CLA	T	601	X	-	-	-
22	CLA	T	602	X	-	-	-
22	CLA	T	603	X	-	-	-
22	CLA	T	604	X	-	-	-
22	CLA	T	605	X	-	-	-
22	CLA	T	606	X	-	-	-
22	CLA	T	607	X	-	-	-
22	CLA	T	608	X	-	-	-
22	CLA	T	609	X	-	-	-
22	CLA	T	610	X	-	-	-
22	CLA	T	611	X	-	-	-
22	CLA	U	401	X	-	-	-
22	CLA	U	403	X	-	-	-
22	CLA	U	404	X	-	-	-
22	CLA	U	405	X	-	-	-
22	CLA	U	406	X	-	-	-
22	CLA	U	409	X	-	-	-
22	CLA	U	410	X	-	-	-
22	CLA	U	411	X	-	-	-
22	CLA	U	412	X	-	-	-
22	CLA	U	413	X	-	-	-
22	CLA	U	414	X	-	-	-
22	CLA	U	415	X	-	-	-
22	CLA	U	420	X	-	-	-
22	CLA	V	601	X	-	-	-
22	CLA	V	602	X	-	-	-
22	CLA	V	603	X	-	-	-
22	CLA	V	604	X	-	-	-
22	CLA	V	607	X	-	-	-
22	CLA	V	608	X	-	-	-
22	CLA	V	609	X	-	-	-
22	CLA	V	610	X	-	-	-
22	CLA	V	611	X	-	-	-
22	CLA	V	612	X	-	-	-
22	CLA	V	613	X	-	-	-
22	CLA	V	617	X	-	-	-
22	CLA	W	402	X	-	-	-
22	CLA	W	403	X	-	-	-
22	CLA	W	404	X	-	-	-
22	CLA	W	405	X	-	-	-

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	CLA	W	406	X	-	-	-
22	CLA	W	409	X	-	-	-
22	CLA	W	410	X	-	-	-
22	CLA	W	411	X	-	-	-
22	CLA	W	412	X	-	-	-
22	CLA	W	413	X	-	-	-
22	CLA	W	414	X	-	-	-
22	CLA	W	415	X	-	-	-
22	CLA	W	419	X	-	-	-
22	CLA	X	402	X	-	-	-
22	CLA	X	403	X	-	-	-
22	CLA	X	404	X	-	-	-
22	CLA	X	405	X	-	-	-
22	CLA	X	407	X	-	-	-
22	CLA	X	408	X	-	-	-
22	CLA	X	409	X	-	-	-
22	CLA	X	410	X	-	-	-
22	CLA	X	411	X	-	-	-
22	CLA	X	412	X	-	-	-
22	CLA	X	413	X	-	-	-
22	CLA	X	417	X	-	-	-
22	CLA	X	419	X	-	-	-
31	CHL	U	407	X	-	-	-
31	CHL	U	408	X	-	-	-
31	CHL	V	605	X	-	-	-
31	CHL	V	606	X	-	-	-
31	CHL	W	407	X	-	-	-
31	CHL	W	408	X	-	-	-
31	CHL	W	422	X	-	-	-
31	CHL	X	406	X	-	-	-
33	CL0	A	802	X	-	-	-

## 2 Entry composition [i](#)

There are 33 unique types of molecules in this entry. The entry contains 60137 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 P700 chlorophyll a apoprotein A2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	B	732	Total	C	N	O	S	0	0
			5868	3859	985	1009	15		

- Molecule 2 is a protein called Photosystem I iron-sulfur center.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	80	Total	C	N	O	S	0	0
			596	363	104	118	11		

- Molecule 3 is a protein called PsaD.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	D	190	Total	C	N	O	S	0	0
			1489	948	254	285	2		

- Molecule 4 is a protein called PsaE.

Mol	Chain	Residues	Atoms				AltConf	Trace
4	E	63	Total	C	N	O	0	0
			509	324	86	99		

- Molecule 5 is a protein called PsaF.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	F	166	Total	C	N	O	S	0	0
			1262	811	210	239	2		

- Molecule 6 is a protein called Lhce5.7.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	G	175	Total	C	N	O	S	0	0
			1323	853	224	242	4		

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms					AltConf	Trace
6	P	164	Total	C	N	O	S	0	0
			1243	803	209	227	4		

- Molecule 7 is a protein called Lhce7.3.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	H	173	Total	C	N	O	S	0	0
			1342	862	233	242	5		

- Molecule 8 is a protein called Lhce5.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	I	165	Total	C	N	O	S	0	0
			1242	801	212	225	4		
8	N	170	Total	C	N	O	S	0	0
			1271	819	215	233	4		

- Molecule 9 is a protein called PsaJ.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	J	37	Total	C	N	O	S	0	0
			305	209	43	52	1		

- Molecule 10 is a protein called LhcE6.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	K	182	Total	C	N	O	S	0	0
			1444	939	246	253	6		
10	Q	182	Total	C	N	O	S	0	0
			1440	938	245	251	6		

- Molecule 11 is a protein called Lhce8.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	L	178	Total	C	N	O	S	0	0
			1364	876	237	247	4		
11	R	174	Total	C	N	O	S	0	0
			1331	852	232	243	4		

- Molecule 12 is a protein called PsaM.



Mol	Chain	Residues	Atoms					AltConf	Trace
12	M	31	Total	C	N	O	S	0	0
			242	162	37	42	1		

- Molecule 13 is a protein called LhcE7.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	O	175	Total	C	N	O	S	0	0
			1359	870	234	250	5		

- Molecule 14 is a protein called Lhce10.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	S	172	Total	C	N	O	S	0	0
			1327	858	219	246	4		

- Molecule 15 is a protein called Lhce11.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	T	167	Total	C	N	O	S	0	0
			1283	824	221	231	7		

- Molecule 16 is a protein called LhcbM4.6.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	U	199	Total	C	N	O	S	0	0
			1517	981	256	275	5		

- Molecule 17 is a protein called LhcbM4.10.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	V	196	Total	C	N	O	S	0	0
			1513	990	253	265	5		

- Molecule 18 is a protein called LhcbM2.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	W	220	Total	C	N	O	S	0	0
			1669	1088	275	302	4		

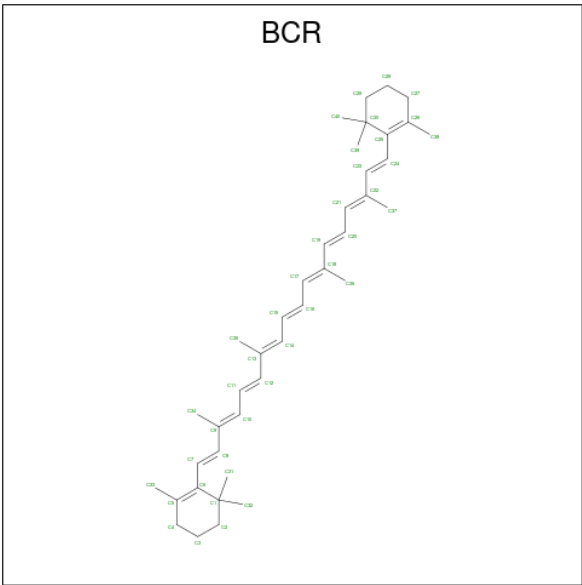
- Molecule 19 is a protein called LhcbM8.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	X	223	Total	C	N	O	S	0	0
			1688	1093	284	306	5		

- Molecule 20 is a protein called PsaA.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	A	740	Total	C	N	O	S	0	0
			5872	3855	992	1004	21		

- Molecule 21 is BETA-CAROTENE (CCD ID: BCR) (formula: C<sub>40</sub>H<sub>56</sub>) (labeled as "Ligand of Interest" by depositor).



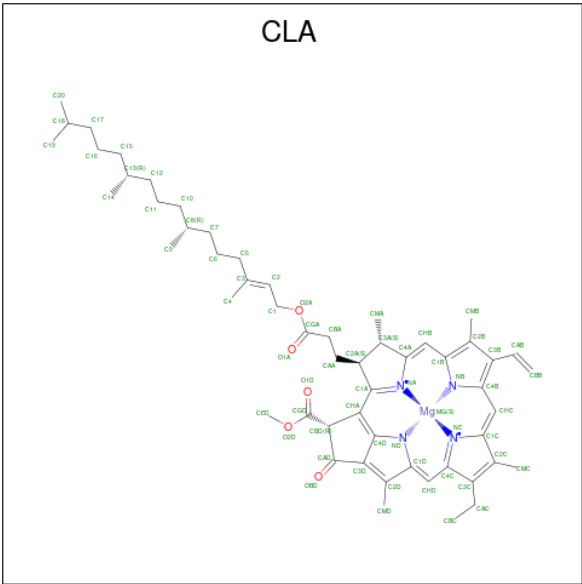
Mol	Chain	Residues	Atoms		AltConf
21	B	1	Total	C	0
			40	40	
21	B	1	Total	C	0
			40	40	
21	B	1	Total	C	0
			40	40	
21	B	1	Total	C	0
			40	40	
21	B	1	Total	C	0
			40	40	
21	B	1	Total	C	0
			40	40	
21	J	1	Total	C	0
			40	40	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		AltConf
21	M	1	Total	C	0
			40	40	
21	A	1	Total	C	0
			40	40	
21	A	1	Total	C	0
			40	40	
21	A	1	Total	C	0
			40	40	
21	A	1	Total	C	0
			40	40	

- Molecule 22 is CHLOROPHYLL A (CCD ID: CLA) (formula: C<sub>55</sub>H<sub>72</sub>MgN<sub>4</sub>O<sub>5</sub>) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
22	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	B	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
22	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	B	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
22	B	1	Total 55	C 45	Mg 1	N 4	O 5	0
22	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	B	1	Total 56	C 46	Mg 1	N 4	O 5	0
22	B	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	B	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	B	1	Total 52	C 42	Mg 1	N 4	O 5	0
22	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	B	1	Total 53	C 43	Mg 1	N 4	O 5	0
22	B	1	Total 53	C 43	Mg 1	N 4	O 5	0
22	B	1	Total 60	C 50	Mg 1	N 4	O 5	0
22	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	B	1	Total 58	C 48	Mg 1	N 4	O 5	0
22	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	B	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
22	B	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	B	1	Total 62	C 52	Mg 1	N 4	O 5	0
22	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	B	1	Total 51	C 41	Mg 1	N 4	O 5	0
22	B	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	B	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	F	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	F	1	Total 55	C 45	Mg 1	N 4	O 5	0
22	F	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	G	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	G	1	Total 60	C 50	Mg 1	N 4	O 5	0
22	G	1	Total 56	C 46	Mg 1	N 4	O 5	0
22	G	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	G	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	G	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
22	G	1	Total 60	C 50	Mg 1	N 4	O 5	0
22	G	1	Total 60	C 50	Mg 1	N 4	O 5	0
22	G	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	G	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	G	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	H	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	H	1	Total 60	C 50	Mg 1	N 4	O 5	0
22	H	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	H	1	Total 60	C 50	Mg 1	N 4	O 5	0
22	H	1	Total 55	C 45	Mg 1	N 4	O 5	0
22	H	1	Total 60	C 50	Mg 1	N 4	O 5	0
22	H	1	Total 60	C 50	Mg 1	N 4	O 5	0
22	H	1	Total 55	C 45	Mg 1	N 4	O 5	0
22	H	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	H	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	H	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	H	1	Total 58	C 48	Mg 1	N 4	O 5	0
22	H	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	I	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	I	1	Total 60	C 50	Mg 1	N 4	O 5	0
22	I	1	Total 56	C 46	Mg 1	N 4	O 5	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms					AltConf
22	I	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	I	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	I	1	Total 61	C 51	Mg 1	N 4	O 5	0
22	I	1	Total 55	C 45	Mg 1	N 4	O 5	0
22	I	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	I	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	I	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	I	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	J	1	Total 50	C 40	Mg 1	N 4	O 5	0
22	K	1	Total 60	C 50	Mg 1	N 4	O 5	0
22	K	1	Total 60	C 50	Mg 1	N 4	O 5	0
22	K	1	Total 64	C 55	Mg 1	N 4	O 4	0
22	K	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	K	1	Total 50	C 40	Mg 1	N 4	O 5	0
22	K	1	Total 57	C 47	Mg 1	N 4	O 5	0
22	K	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	K	1	Total 60	C 50	Mg 1	N 4	O 5	0
22	K	1	Total 56	C 46	Mg 1	N 4	O 5	0
22	K	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	K	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	K	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
22	K	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	L	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	L	1	Total 60	C 50	Mg 1	N 4	O 5	0
22	L	1	Total 56	C 46	Mg 1	N 4	O 5	0
22	L	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	L	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	L	1	Total 57	C 47	Mg 1	N 4	O 5	0
22	L	1	Total 60	C 50	Mg 1	N 4	O 5	0
22	L	1	Total 60	C 50	Mg 1	N 4	O 5	0
22	L	1	Total 60	C 50	Mg 1	N 4	O 5	0
22	L	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	L	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	L	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	N	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	N	1	Total 60	C 50	Mg 1	N 4	O 5	0
22	N	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	N	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	N	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	N	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	N	1	Total 60	C 50	Mg 1	N 4	O 5	0
22	N	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
22	N	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	N	1	Total 55	C 45	Mg 1	N 4	O 5	0
22	N	1	Total 40	C 32	Mg 1	N 4	O 3	0
22	O	1	Total 50	C 40	Mg 1	N 4	O 5	0
22	O	1	Total 60	C 50	Mg 1	N 4	O 5	0
22	O	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	O	1	Total 61	C 51	Mg 1	N 4	O 5	0
22	O	1	Total 50	C 40	Mg 1	N 4	O 5	0
22	O	1	Total 60	C 50	Mg 1	N 4	O 5	0
22	O	1	Total 60	C 50	Mg 1	N 4	O 5	0
22	O	1	Total 60	C 50	Mg 1	N 4	O 5	0
22	O	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	O	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	O	1	Total 50	C 40	Mg 1	N 4	O 5	0
22	O	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	P	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	P	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	P	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	P	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	P	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	P	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
22	P	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	P	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	P	1	Total 41	C 33	Mg 1	N 4	O 3	0
22	P	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	Q	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	Q	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	Q	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	Q	1	Total 56	C 46	Mg 1	N 4	O 5	0
22	Q	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	Q	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	Q	1	Total 50	C 40	Mg 1	N 4	O 5	0
22	Q	1	Total 60	C 50	Mg 1	N 4	O 5	0
22	Q	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	Q	1	Total 55	C 45	Mg 1	N 4	O 5	0
22	Q	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	Q	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	Q	1	Total 52	C 42	Mg 1	N 4	O 5	0
22	Q	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	R	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	R	1	Total 60	C 50	Mg 1	N 4	O 5	0
22	R	1	Total 56	C 46	Mg 1	N 4	O 5	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms					AltConf
22	R	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	R	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	R	1	Total 57	C 47	Mg 1	N 4	O 5	0
22	R	1	Total 60	C 50	Mg 1	N 4	O 5	0
22	R	1	Total 54	C 44	Mg 1	N 4	O 5	0
22	R	1	Total 41	C 33	Mg 1	N 4	O 3	0
22	R	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	R	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	R	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	S	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	S	1	Total 60	C 50	Mg 1	N 4	O 5	0
22	S	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	S	1	Total 60	C 50	Mg 1	N 4	O 5	0
22	S	1	Total 60	C 50	Mg 1	N 4	O 5	0
22	S	1	Total 50	C 40	Mg 1	N 4	O 5	0
22	S	1	Total 60	C 50	Mg 1	N 4	O 5	0
22	S	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	S	1	Total 55	C 45	Mg 1	N 4	O 5	0
22	S	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	S	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	S	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
22	T	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	T	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	T	1	Total 60	C 50	Mg 1	N 4	O 5	0
22	T	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	T	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	T	1	Total 50	C 40	Mg 1	N 4	O 5	0
22	T	1	Total 60	C 50	Mg 1	N 4	O 5	0
22	T	1	Total 60	C 50	Mg 1	N 4	O 5	0
22	T	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	T	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	T	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	U	1	Total 55	C 45	Mg 1	N 4	O 5	0
22	U	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	U	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	U	1	Total 57	C 47	Mg 1	N 4	O 5	0
22	U	1	Total 56	C 46	Mg 1	N 4	O 5	0
22	U	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	U	1	Total 55	C 45	Mg 1	N 4	O 5	0
22	U	1	Total 57	C 47	Mg 1	N 4	O 5	0
22	U	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	U	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
22	U	1	Total 61	C 51	Mg 1	N 4	O 5	0
22	U	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	U	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	V	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	V	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	V	1	Total 57	C 47	Mg 1	N 4	O 5	0
22	V	1	Total 56	C 46	Mg 1	N 4	O 5	0
22	V	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	V	1	Total 55	C 45	Mg 1	N 4	O 5	0
22	V	1	Total 57	C 47	Mg 1	N 4	O 5	0
22	V	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	V	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	V	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	V	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	V	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	W	1	Total 55	C 45	Mg 1	N 4	O 5	0
22	W	1	Total 52	C 42	Mg 1	N 4	O 5	0
22	W	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	W	1	Total 60	C 50	Mg 1	N 4	O 5	0
22	W	1	Total 56	C 46	Mg 1	N 4	O 5	0
22	W	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
22	W	1	Total 60	C 50	Mg 1	N 4	O 5	0
22	W	1	Total 60	C 50	Mg 1	N 4	O 5	0
22	W	1	Total 60	C 50	Mg 1	N 4	O 5	0
22	W	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	W	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	W	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	W	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	X	1	Total 55	C 45	Mg 1	N 4	O 5	0
22	X	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	X	1	Total 60	C 50	Mg 1	N 4	O 5	0
22	X	1	Total 56	C 46	Mg 1	N 4	O 5	0
22	X	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	X	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	X	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	X	1	Total 60	C 50	Mg 1	N 4	O 5	0
22	X	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	X	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	X	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	X	1	Total 50	C 40	Mg 1	N 4	O 5	0
22	X	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	A	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
22	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	A	1	Total 61	C 51	Mg 1	N 4	O 5	0
22	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	A	1	Total 53	C 43	Mg 1	N 4	O 5	0
22	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	A	1	Total 57	C 47	Mg 1	N 4	O 5	0
22	A	1	Total 57	C 47	Mg 1	N 4	O 5	0
22	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	A	1	Total 61	C 51	Mg 1	N 4	O 5	0
22	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	A	1	Total 53	C 43	Mg 1	N 4	O 5	0
22	A	1	Total 58	C 48	Mg 1	N 4	O 5	0
22	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	A	1	Total 45	C 35	Mg 1	N 4	O 5	0

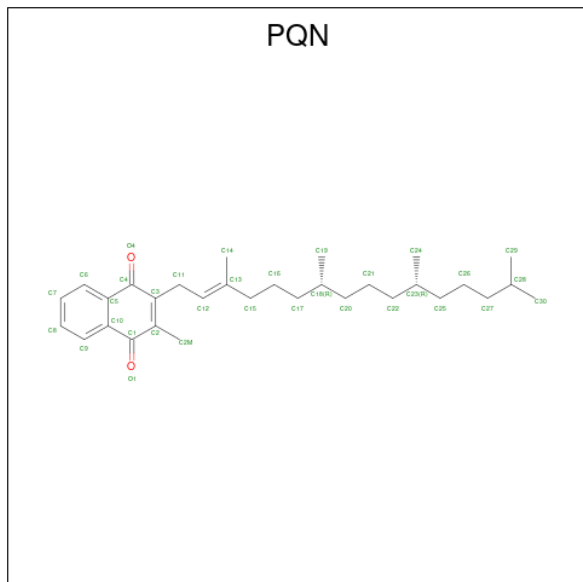
*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms					AltConf
22	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	A	1	Total 61	C 51	Mg 1	N 4	O 5	0
22	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	A	1	Total 62	C 52	Mg 1	N 4	O 5	0
22	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	A	1	Total 52	C 42	Mg 1	N 4	O 5	0
22	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	A	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	A	1	Total 61	C 51	Mg 1	N 4	O 5	0
22	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	A	1	Total 50	C 40	Mg 1	N 4	O 5	0
22	A	1	Total 52	C 42	Mg 1	N 4	O 5	0
22	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	A	1	Total 55	C 45	Mg 1	N 4	O 5	0
22	A	1	Total 65	C 55	Mg 1	N 4	O 5	0

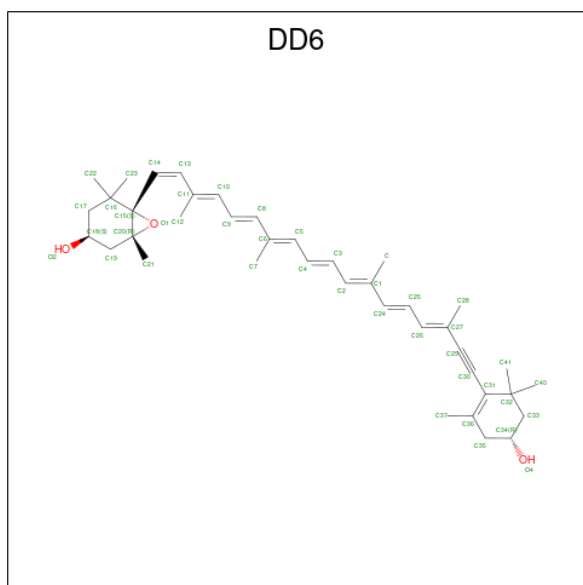


- Molecule 23 is PHYLLOQUINONE (CCD ID: PQN) (formula:  $C_{31}H_{46}O_2$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
23	B	1	Total	C	O	0
			33	31	2	
23	A	1	Total	C	O	0
			33	31	2	

- Molecule 24 is (3S,3'R,5R,6S,7cis)-7',8'-didehydro-5,6-dihydro-5,6-epoxy-beta,beta-carotene-3,3'-diol (CCD ID: DD6) (formula:  $C_{40}H_{54}O_3$ ) (labeled as "Ligand of Interest" by depositor).



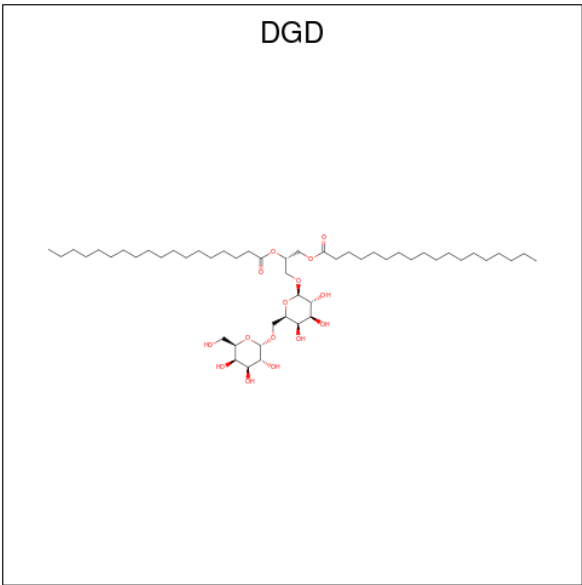
Mol	Chain	Residues	Atoms			AltConf
24	B	1	Total 43	C 40	O 3	0
24	F	1	Total 43	C 40	O 3	0
24	G	1	Total 43	C 40	O 3	0
24	G	1	Total 43	C 40	O 3	0
24	H	1	Total 43	C 40	O 3	0
24	H	1	Total 43	C 40	O 3	0
24	I	1	Total 43	C 40	O 3	0
24	I	1	Total 43	C 40	O 3	0
24	J	1	Total 43	C 40	O 3	0
24	K	1	Total 43	C 40	O 3	0
24	K	1	Total 43	C 40	O 3	0
24	L	1	Total 43	C 40	O 3	0
24	L	1	Total 43	C 40	O 3	0
24	L	1	Total 43	C 40	O 3	0
24	N	1	Total 43	C 40	O 3	0
24	N	1	Total 43	C 40	O 3	0
24	O	1	Total 43	C 40	O 3	0
24	O	1	Total 43	C 40	O 3	0
24	P	1	Total 43	C 40	O 3	0
24	P	1	Total 43	C 40	O 3	0
24	Q	1	Total 43	C 40	O 3	0
24	Q	1	Total 43	C 40	O 3	0

*Continued on next page...*

*Continued from previous page...*

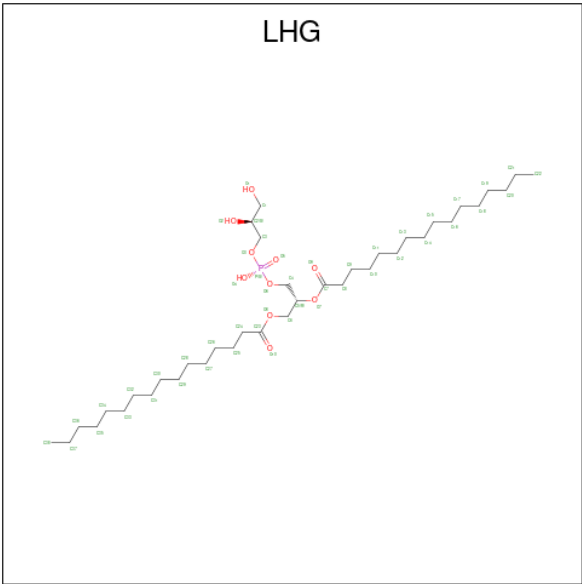
Mol	Chain	Residues	Atoms			AltConf
24	R	1	Total 43	C 40	O 3	0
24	R	1	Total 43	C 40	O 3	0
24	S	1	Total 43	C 40	O 3	0
24	S	1	Total 43	C 40	O 3	0
24	T	1	Total 43	C 40	O 3	0
24	T	1	Total 43	C 40	O 3	0
24	U	1	Total 43	C 40	O 3	0
24	U	1	Total 43	C 40	O 3	0
24	V	1	Total 43	C 40	O 3	0
24	V	1	Total 43	C 40	O 3	0
24	W	1	Total 43	C 40	O 3	0
24	W	1	Total 43	C 40	O 3	0
24	W	1	Total 43	C 40	O 3	0
24	X	1	Total 43	C 40	O 3	0
24	X	1	Total 43	C 40	O 3	0
24	X	1	Total 43	C 40	O 3	0
24	X	1	Total 43	C 40	O 3	0
24	A	1	Total 43	C 40	O 3	0
24	A	1	Total 43	C 40	O 3	0
24	A	1	Total 43	C 40	O 3	0

- Molecule 25 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula:  $C_{51}H_{96}O_{15}$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
25	B	1	Total	C	O	0
			66	51	15	
25	F	1	Total	C	O	0
			34	29	5	
25	O	1	Total	C	O	0
			60	45	15	

- Molecule 26 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: C<sub>38</sub>H<sub>75</sub>O<sub>10</sub>P) (labeled as "Ligand of Interest" by depositor).



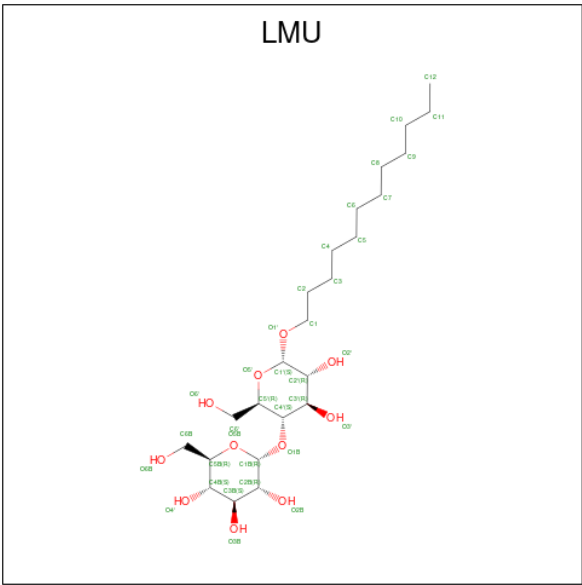
Mol	Chain	Residues	Atoms				AltConf
26	B	1	Total	C	O	P	0
			27	16	10	1	
26	B	1	Total	C	O	P	0
			42	31	10	1	
26	G	1	Total	C	O	P	0
			32	21	10	1	
26	H	1	Total	C	O	P	0
			27	16	10	1	
26	K	1	Total	C	O	P	0
			39	28	10	1	
26	K	1	Total	C	O	P	0
			33	22	10	1	
26	L	1	Total	C	O	P	0
			42	31	10	1	
26	N	1	Total	C	O	P	0
			28	17	10	1	
26	N	1	Total	C	O	P	0
			43	32	10	1	
26	O	1	Total	C	O	P	0
			34	23	10	1	
26	O	1	Total	C	O	P	0
			49	38	10	1	
26	O	1	Total	C	O	P	0
			43	32	10	1	
26	O	1	Total	C	O	P	0
			42	31	10	1	
26	P	1	Total	C	O	P	0
			40	29	10	1	
26	Q	1	Total	C	O	P	0
			44	33	10	1	
26	R	1	Total	C	O	P	0
			42	31	10	1	
26	S	1	Total	C	O	P	0
			32	21	10	1	
26	T	1	Total	C	O	P	0
			42	31	10	1	
26	U	1	Total	C	O	P	0
			25	16	8	1	
26	W	1	Total	C	O	P	0
			42	31	10	1	
26	X	1	Total	C	O	P	0
			42	31	10	1	
26	A	1	Total	C	O	P	0
			49	38	10	1	

*Continued on next page...*

Continued from previous page...

Mol	Chain	Residues	Atoms				AltConf
26	A	1	Total	C	O	P	0
			49	38	10	1	

- Molecule 27 is DODECYL-ALPHA-D-MALTOSIDE (CCD ID: LMU) (formula: C<sub>24</sub>H<sub>46</sub>O<sub>11</sub>) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
27	B	1	Total	C	O	0
			24	18	6	
27	B	1	Total	C	O	0
			24	18	6	
27	B	1	Total	C	O	0
			19	14	5	
27	B	1	Total	C	O	0
			24	18	6	
27	B	1	Total	C	O	0
			24	18	6	
27	B	1	Total	C	O	0
			35	24	11	
27	B	1	Total	C	O	0
			15	14	1	
27	F	1	Total	C	O	0
			21	15	6	
27	F	1	Total	C	O	0
			21	15	6	
27	G	1	Total	C	O	0
			21	15	6	

Continued on next page...

*Continued from previous page...*

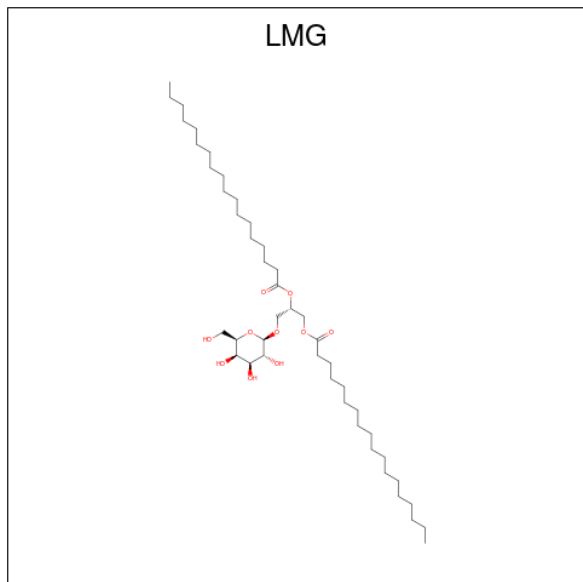
Mol	Chain	Residues	Atoms			AltConf
27	H	1	Total	C	O	0
			21	15	6	
27	H	1	Total	C	O	0
			24	18	6	
27	H	1	Total	C	O	0
			33	23	10	
27	J	1	Total	C	O	0
			34	24	10	
27	K	1	Total	C	O	0
			33	23	10	
27	L	1	Total	C	O	0
			24	18	6	
27	L	1	Total	C	O	0
			27	21	6	
27	L	1	Total	C	O	0
			34	24	10	
27	M	1	Total	C	O	0
			24	18	6	
27	O	1	Total	C	O	0
			24	18	6	
27	O	1	Total	C	O	0
			35	24	11	
27	O	1	Total	C	O	0
			26	22	4	
27	O	1	Total	C	O	0
			35	24	11	
27	T	1	Total	C	O	0
			21	15	6	
27	T	1	Total	C	O	0
			24	18	6	
27	T	1	Total	C	O	0
			24	18	6	
27	U	1	Total	C	O	0
			35	24	11	
27	U	1	Total	C	O	0
			35	24	11	
27	U	1	Total	C	O	0
			24	18	6	
27	W	1	Total	C	O	0
			24	18	6	
27	X	1	Total	C	O	0
			24	18	6	

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms			AltConf
27	X	1	Total	C	O	0
			35	24	11	
27	A	1	Total	C	O	0
			24	18	6	
27	A	1	Total	C	O	0
			35	24	11	
27	A	1	Total	C	O	0
			21	15	6	
27	A	1	Total	C	O	0
			24	18	6	

- Molecule 28 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula:  $C_{45}H_{86}O_{10}$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
28	B	1	Total	C	O	0
			43	33	10	
28	B	1	Total	C	O	0
			53	43	10	
28	F	1	Total	C	O	0
			42	32	10	
28	G	1	Total	C	O	0
			46	36	10	
28	H	1	Total	C	O	0
			43	33	10	
28	H	1	Total	C	O	0
			40	30	10	

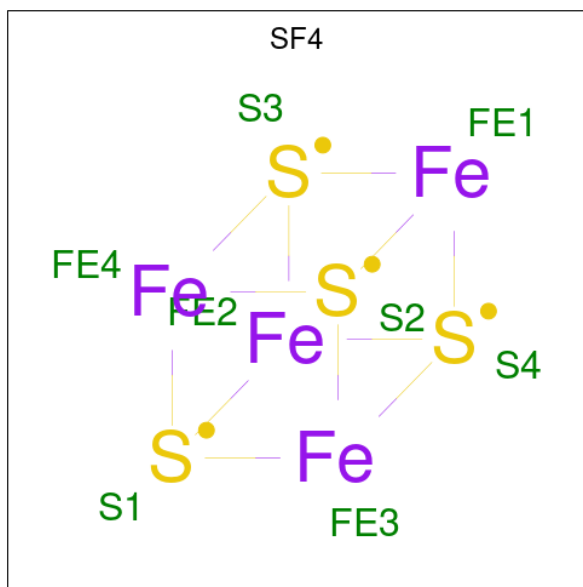
*Continued on next page...*



*Continued from previous page...*

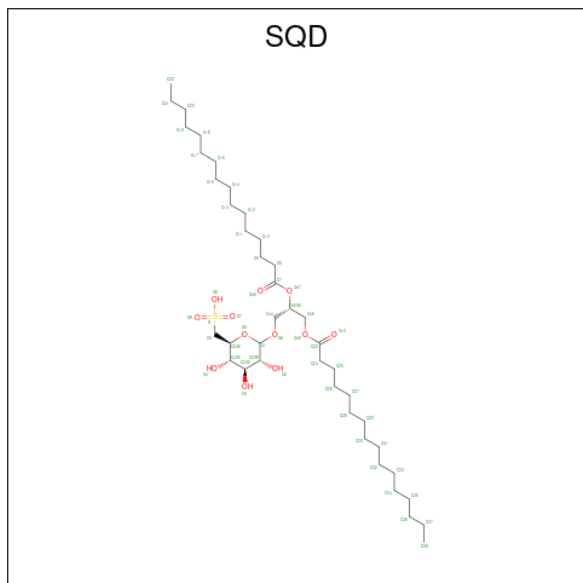
Mol	Chain	Residues	Atoms			AltConf
28	H	1	Total	C	O	0
			37	27	10	
28	I	1	Total	C	O	0
			37	27	10	
28	I	1	Total	C	O	0
			50	41	9	
28	J	1	Total	C	O	0
			55	45	10	
28	K	1	Total	C	O	0
			43	33	10	
28	K	1	Total	C	O	0
			49	39	10	
28	K	1	Total	C	O	0
			43	33	10	
28	L	1	Total	C	O	0
			51	41	10	
28	N	1	Total	C	O	0
			44	34	10	
28	Q	1	Total	C	O	0
			37	27	10	
28	T	1	Total	C	O	0
			41	31	10	
28	U	1	Total	C	O	0
			53	43	10	
28	U	1	Total	C	O	0
			49	39	10	
28	W	1	Total	C	O	0
			48	38	10	
28	A	1	Total	C	O	0
			41	31	10	

- Molecule 29 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula:  $\text{Fe}_4\text{S}_4$ ) (labeled as "Ligand of Interest" by depositor).



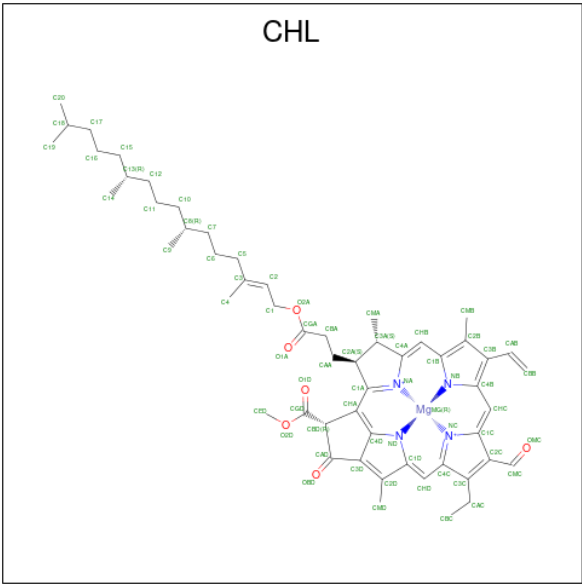
Mol	Chain	Residues	Atoms			AltConf
29	B	1	Total	Fe	S	0
			8	4	4	
29	C	1	Total	Fe	S	0
			8	4	4	
29	C	1	Total	Fe	S	0
			8	4	4	

- Molecule 30 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (CCD ID: SQD) (formula:  $C_{41}H_{78}O_{12}S$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
30	F	1	Total	C	O	S	0
			42	29	12	1	
30	K	1	Total	C	O	S	0
			43	30	12	1	
30	O	1	Total	C	O	S	0
			42	29	12	1	
30	V	1	Total	C	O	S	0
			27	16	10	1	

- Molecule 31 is CHLOROPHYLL B (CCD ID: CHL) (formula:  $C_{55}H_{70}MgN_4O_6$ ) (labeled as "Ligand of Interest" by depositor).



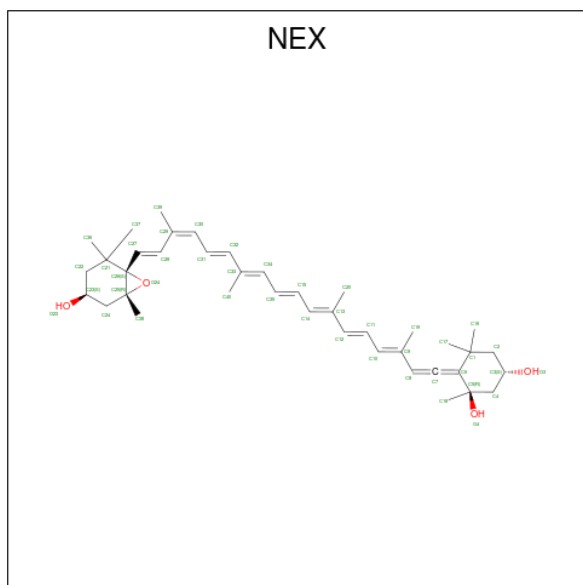
Mol	Chain	Residues	Atoms				AltConf
31	U	1	Total	C	Mg	N	O
			46	35	1	4	6
31	U	1	Total	C	Mg	N	O
			46	35	1	4	6
31	V	1	Total	C	Mg	N	O
			46	35	1	4	6
31	V	1	Total	C	Mg	N	O
			46	35	1	4	6
31	W	1	Total	C	Mg	N	O
			46	35	1	4	6
31	W	1	Total	C	Mg	N	O
			66	55	1	4	6
31	W	1	Total	C	Mg	N	O
			66	55	1	4	6

Continued on next page...

Continued from previous page...

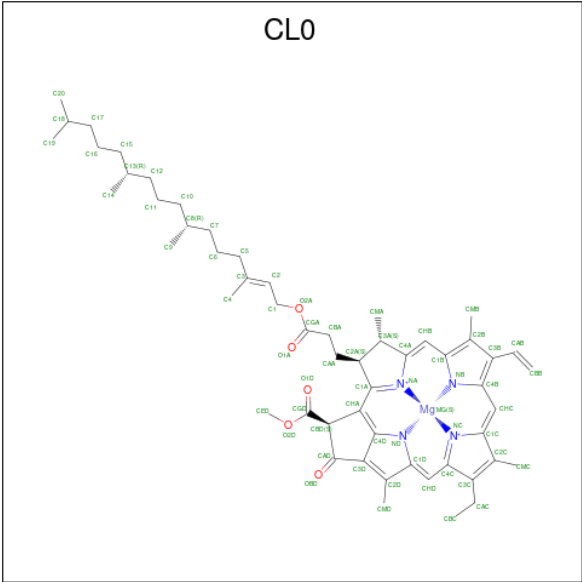
Mol	Chain	Residues	Atoms					AltConf
31	X	1	Total	C	Mg	N	O	0
			46	35	1	4	6	

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



Mol	Chain	Residues	Atoms			AltConf
32	U	1	Total	C	O	0
			44	40	4	
32	V	1	Total	C	O	0
			44	40	4	

- Molecule 33 is CHLOROPHYLL A ISOMER (CCD ID: CL0) (formula:  $C_{55}H_{72}MgN_4O_5$ ) (labeled as "Ligand of Interest" by depositor).

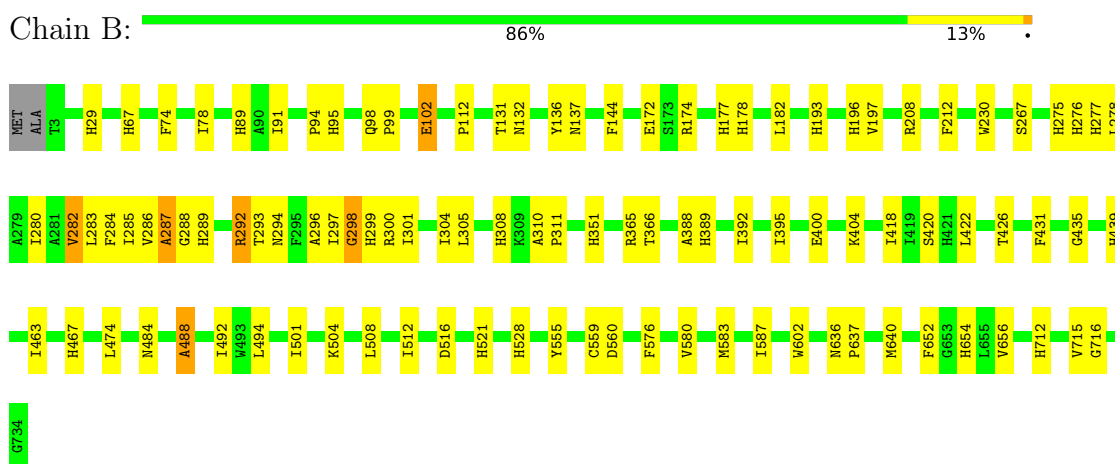


Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
33	A	1	65	55	1	4	5	0

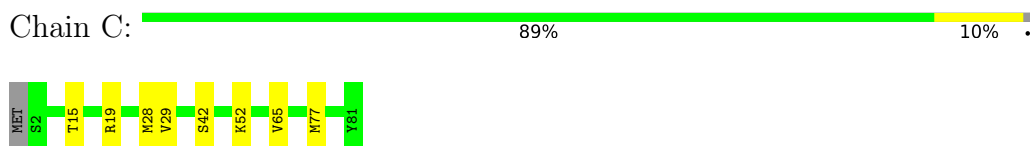
### 3 Residue-property plots

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 and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

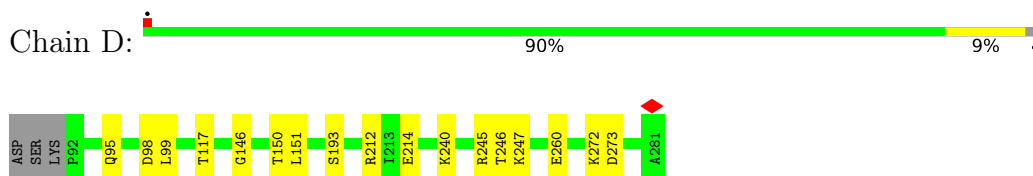
- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A2



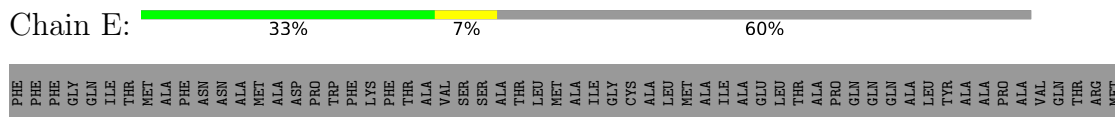
- Molecule 2: Photosystem I iron-sulfur center

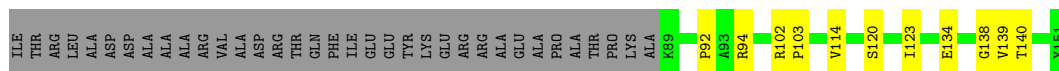


- Molecule 3: PsaD



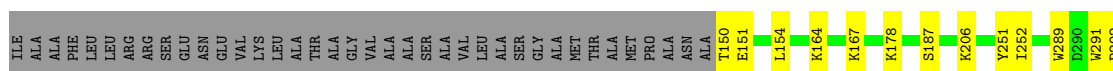
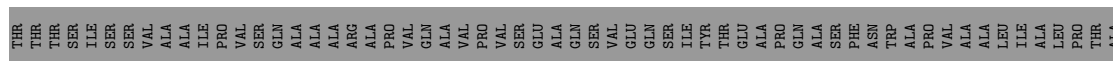
- Molecule 4: PsaE





- Molecule 5: PsaF

Chain F: 46% 5% 49%



- Molecule 6: Lhce5.7

Chain G: 83% 12% 5%



- Molecule 6: Lhce5.7

Chain P: 5% 60% 26% 11%



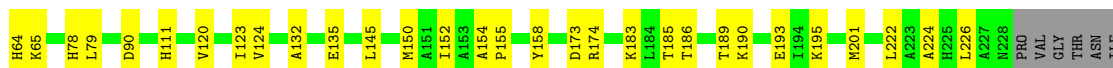
- Molecule 7: Lhce7.3

Chain H: 85% 8% 6%



- Molecule 8: Lhce5

Chain I: 73% 16% 10%



THR  
THR  
THR  
LEU  
ALA  
MET  
TVR  
SER  
THR  
SER  
GLY  
ASP  
LYS

• Molecule 8: Lhce5

Chain N: 75% 16% 8%

HIS  
LYS  
D66  
G67  
V68  
W69  
F70  
F71  
H78  
E108  
S115  
M116  
L117  
V120  
A132  
E135  
D141  
K144  
M150  
A151  
I152  
A153  
A154  
P155  
T156  
E157  
Y158  
W159  
R160  
G178  
F179  
D180  
L184  
T185  
T186  
D187  
Y188  
T189  
G197  
M201  
E216  
L222  
L226

T235  
THR  
THR  
LEU  
ALA  
MET  
TVR  
SER  
THR  
SER  
GLY  
ASP  
LYS

• Molecule 9: PsaJ

Chain J: 87% 8% 5%

LEU  
THR  
M7  
V20  
R37  
I42  
L43

• Molecule 10: LhcE6

Chain K: 88% 10% ..

E377  
P390  
L393  
V434  
E471  
R474  
W481  
K486  
Y487  
P492  
P496  
E508  
G521  
L522  
E523  
V524  
Q525  
V528  
H543  
P544  
L545  
A546  
A547  
N548  
T549  
P568  
PRO  
VAL

• Molecule 10: LhcE6

Chain Q: 83% 15% ..

GLU  
LYS  
Y379  
R380  
W383  
F384  
P385  
N386  
I387  
T388  
L408  
M418  
N425  
G426  
R458  
L461  
I462  
S463  
L464  
Q465  
V467  
T504  
I509  
R513  
M516  
V524  
L537  
I538  
E539  
H540  
L541  
R542  
L545  
A546  
A547  
N548  
I549  
G550  
V560

• Molecule 11: Lhce8

Chain L: 78% 16% 5%

VAL  
D194  
R195  
G201  
D226  
P227  
K228  
E231  
M245  
L257  
Y263  
V285  
V288  
L292  
N301  
F305  
T315  
E319  
G332  
L333  
E334  
V335  
Q336  
R337  
H338  
V339  
V342  
V346  
N347  
L348  
V349  
E350  
H351  
V352  
A361  
H366  
Q367  
V368  
F369  
V370  
A371  
MET

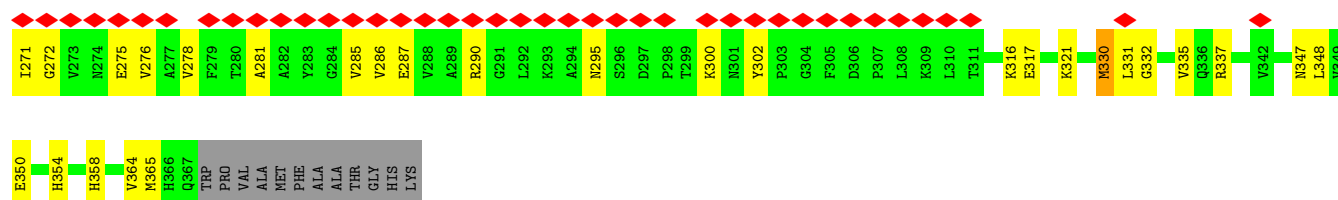
PHE  
ALA  
ALA  
THR  
GLY  
HIS  
LYS

• Molecule 11: Lhce8

Chain R: 38% 66% 25% 7%

VAL  
D194  
R195  
P196  
F199  
S206  
Y207  
L208  
T209  
G210  
Q211  
Y212  
F213  
F218  
A225  
D226  
P227  
K228  
V229  
R232  
M233  
R234  
V235  
S236  
E237  
V238  
Y239  
H240  
G241  
R242  
L243  
A244  
M245  
L246  
A247  
I248  
V253  
P254  
D255  
I256  
L257  
G258  
K259  
G260  
A261  
V262  
Y263  
E264  
A265  
A266  
Q267  
N268  
A269  
G270





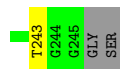
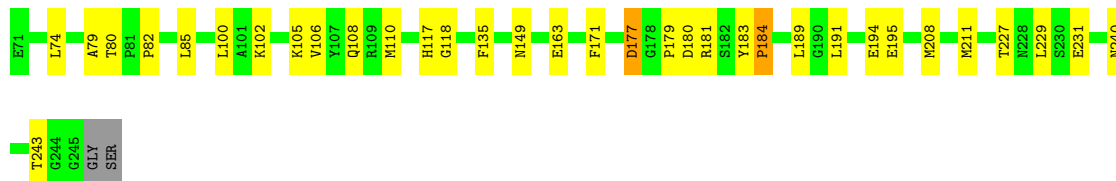
- Molecule 12: PsaM

Chain M: 84% 16%



- Molecule 13: LhcE7

Chain O: 80% 18% ..



- Molecule 14: Lhce10

Chain S: 81% 14% ..



- Molecule 15: Lhce11

Chain T: 92% 5% .



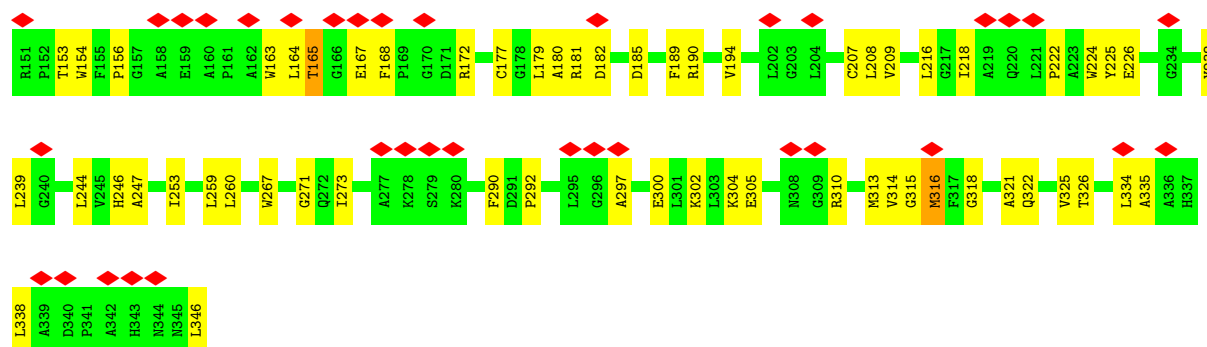
- Molecule 16: LhcbM4.6

Chain U: 88% 8% 5%



- Molecule 17: LhcbM4.10

Chain V: 18% 70% 29% .



• Molecule 18: LhcbM2

Chain W: 87% 9% .



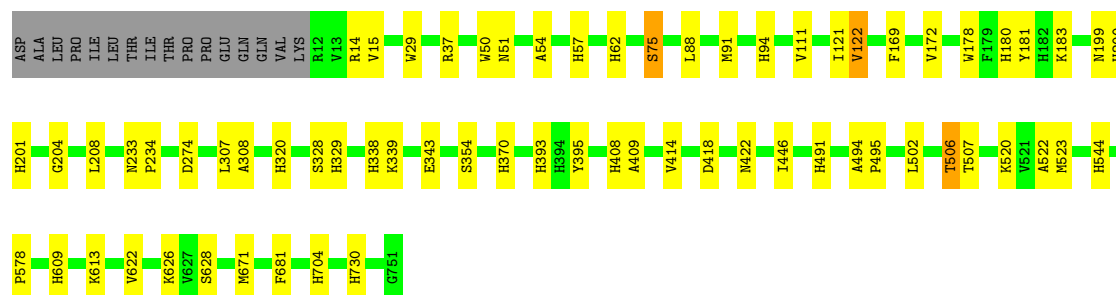
• Molecule 19: LhcbM8

Chain X: 93% 7% .



• Molecule 20: PsaA

Chain A: 89% 9% .



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	51871	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	50.0	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	0.393	Depositor
Minimum map value	-0.080	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.008	Depositor
Recommended contour level	0.04	Depositor
Map size ( $\text{\AA}$ )	496.64, 496.64, 496.64	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	0.97, 0.97, 0.97	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: PQN, BCR, DD6, SQD, LHG, NEX, CHL, DGD, CL0, CLA, LMU, SF4, LMG

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	B	0.35	1/6078 (0.0%)	0.49	4/8287 (0.0%)
2	C	0.33	0/606	0.53	0/819
3	D	0.14	0/1525	0.38	0/2065
4	E	0.13	0/521	0.31	0/707
5	F	0.17	0/1288	0.46	0/1747
6	G	0.17	0/1360	0.39	0/1855
6	P	0.41	0/1279	0.68	1/1744 (0.1%)
7	H	0.32	0/1381	0.52	3/1876 (0.2%)
8	I	0.31	0/1278	0.56	0/1741
8	N	0.24	0/1307	0.46	0/1784
9	J	0.14	0/314	0.32	0/429
10	K	0.21	0/1492	0.49	0/2035
10	Q	0.20	0/1489	0.48	0/2034
11	L	0.35	0/1401	0.58	2/1910 (0.1%)
11	R	0.16	0/1365	0.41	0/1858
12	M	0.13	0/246	0.32	0/332
13	O	0.20	0/1397	0.46	0/1898
14	S	0.26	0/1370	0.46	0/1865
15	T	0.16	0/1320	0.40	0/1784
16	U	0.15	0/1566	0.37	0/2141
17	V	0.14	0/1566	0.33	0/2141
18	W	0.16	0/1719	0.38	0/2343
19	X	0.17	0/1731	0.37	0/2351
20	A	0.35	0/6073	0.49	1/8279 (0.0%)
All	All	0.27	1/39672 (0.0%)	0.47	11/54025 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	287	ALA	CA-C	-6.82	1.46	1.53

The worst 5 of 11 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	P	395	GLY	N-CA-C	-9.42	102.67	114.92
1	B	298	GLY	N-CA-C	8.87	120.52	111.56
1	B	287	ALA	N-CA-C	-6.79	102.39	111.96
7	H	149	GLY	O-C-N	-6.78	115.67	122.18
7	H	152	VAL	CB-CA-C	-5.83	104.18	112.22

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	5868	0	5667	91	0
2	C	596	0	571	6	0
3	D	1489	0	1462	9	0
4	E	509	0	489	5	0
5	F	1262	0	1293	10	0
6	G	1323	0	1305	15	0
6	P	1243	0	1218	39	0
7	H	1342	0	1315	9	0
8	I	1242	0	1213	25	0
8	N	1271	0	1245	27	0
9	J	305	0	314	4	0
10	K	1444	0	1391	17	0
10	Q	1440	0	1388	26	0
11	L	1364	0	1346	27	0
11	R	1331	0	1315	45	0
12	M	242	0	258	8	0
13	O	1359	0	1328	29	0
14	S	1327	0	1271	18	0
15	T	1283	0	1238	6	0
16	U	1517	0	1466	14	0
17	V	1513	0	1467	56	0
18	W	1669	0	1647	15	0
19	X	1688	0	1693	10	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
20	A	5872	0	5735	55	0
21	A	160	0	224	8	0
21	B	240	0	336	21	0
21	J	40	0	56	1	0
21	M	40	0	56	3	0
22	A	2638	0	2742	77	0
22	B	2341	0	2395	78	0
22	F	165	0	154	6	0
22	G	571	0	498	10	0
22	H	698	0	626	10	0
22	I	567	0	490	17	0
22	J	50	0	39	1	0
22	K	765	0	758	33	0
22	L	703	0	694	30	0
22	N	570	0	504	19	0
22	O	651	0	585	20	0
22	P	446	0	326	10	0
22	Q	738	0	655	20	0
22	R	678	0	653	29	0
22	S	621	0	530	14	0
22	T	625	0	603	10	0
22	U	676	0	586	14	0
22	V	625	0	548	32	0
22	W	733	0	694	18	0
22	X	741	0	716	7	0
23	A	33	0	46	2	0
23	B	33	0	46	1	0
24	A	129	0	0	0	0
24	B	43	0	0	1	0
24	F	43	0	0	0	0
24	G	86	0	0	0	0
24	H	86	0	0	0	0
24	I	86	0	0	0	0
24	J	43	0	0	0	0
24	K	86	0	0	0	0
24	L	129	0	0	0	0
24	N	86	0	0	0	0
24	O	86	0	0	0	0
24	P	86	0	0	0	0
24	Q	86	0	0	1	0
24	R	86	0	0	0	0
24	S	86	0	0	1	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
24	T	86	0	0	0	0
24	U	86	0	0	0	0
24	V	86	0	0	0	0
24	W	129	0	0	0	0
24	X	172	0	0	0	0
25	B	66	0	96	6	0
25	F	34	0	50	2	0
25	O	60	0	81	3	0
26	A	98	0	148	3	0
26	B	69	0	81	8	0
26	G	32	0	34	0	0
26	H	27	0	24	0	0
26	K	72	0	84	3	0
26	L	42	0	57	3	0
26	N	71	0	82	2	0
26	O	168	0	228	4	0
26	P	40	0	53	1	0
26	Q	44	0	61	1	0
26	R	42	0	57	3	0
26	S	32	0	34	2	0
26	T	42	0	57	1	0
26	U	25	0	21	0	0
26	W	42	0	57	2	0
26	X	42	0	57	0	0
27	A	104	0	142	2	0
27	B	165	0	233	10	0
27	F	42	0	52	1	0
27	G	21	0	26	0	0
27	H	78	0	103	2	0
27	J	34	0	44	0	0
27	K	33	0	42	2	0
27	L	85	0	110	6	0
27	M	24	0	35	1	0
27	O	120	0	155	4	0
27	T	69	0	96	2	0
27	U	94	0	127	2	0
27	W	24	0	35	0	0
27	X	59	0	81	0	0
28	A	41	0	52	0	0
28	B	96	0	138	4	0
28	F	42	0	54	3	0
28	G	46	0	65	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
28	H	120	0	150	2	0
28	I	87	0	117	1	0
28	J	55	0	86	1	0
28	K	135	0	183	3	0
28	L	51	0	75	0	0
28	N	44	0	61	1	0
28	Q	37	0	44	2	0
28	T	41	0	52	2	0
28	U	102	0	150	4	0
28	W	48	0	69	3	0
29	B	8	0	0	0	0
29	C	16	0	0	0	0
30	F	42	0	48	2	0
30	K	43	0	50	1	0
30	O	42	0	48	8	0
30	V	27	0	25	1	0
31	U	92	0	62	7	0
31	V	92	0	62	14	0
31	W	178	0	171	10	0
31	X	46	0	31	0	0
32	U	44	0	56	4	0
32	V	44	0	56	9	0
33	A	65	0	72	6	0
All	All	60137	0	57815	901	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

The worst 5 of 901 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:B:840:PQN:H291	25:B:847:DGD:HBT1	1.23	1.10
31:V:605:CHL:HAB	31:V:606:CHL:OMC	1.50	1.08
8:N:184:LEU:HD12	22:N:607:CLA:H42	1.41	1.01
6:P:391:ALA:HB2	6:P:404:ASP:HB3	1.47	0.96
1:B:131:THR:HB	12:M:1:MET:HE1	1.46	0.94

There are no symmetry-related clashes.



## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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	B	730/734 (100%)	698 (96%)	29 (4%)	3 (0%)	30	34
2	C	78/81 (96%)	74 (95%)	4 (5%)	0	100	100
3	D	188/193 (97%)	182 (97%)	6 (3%)	0	100	100
4	E	61/158 (39%)	61 (100%)	0	0	100	100
5	F	164/325 (50%)	161 (98%)	3 (2%)	0	100	100
6	G	173/184 (94%)	169 (98%)	4 (2%)	0	100	100
6	P	162/184 (88%)	146 (90%)	16 (10%)	0	100	100
7	H	171/185 (92%)	165 (96%)	6 (4%)	0	100	100
8	I	163/184 (89%)	160 (98%)	3 (2%)	0	100	100
8	N	168/184 (91%)	155 (92%)	13 (8%)	0	100	100
9	J	35/39 (90%)	35 (100%)	0	0	100	100
10	K	180/184 (98%)	175 (97%)	5 (3%)	0	100	100
10	Q	180/184 (98%)	168 (93%)	12 (7%)	0	100	100
11	L	176/187 (94%)	167 (95%)	8 (4%)	1 (1%)	21	24
11	R	172/187 (92%)	163 (95%)	8 (5%)	1 (1%)	21	24
12	M	29/31 (94%)	29 (100%)	0	0	100	100
13	O	173/177 (98%)	160 (92%)	12 (7%)	1 (1%)	21	24
14	S	170/180 (94%)	166 (98%)	4 (2%)	0	100	100
15	T	165/173 (95%)	158 (96%)	7 (4%)	0	100	100
16	U	197/209 (94%)	186 (94%)	11 (6%)	0	100	100
17	V	194/196 (99%)	183 (94%)	11 (6%)	0	100	100
18	W	218/228 (96%)	209 (96%)	9 (4%)	0	100	100
19	X	221/223 (99%)	215 (97%)	6 (3%)	0	100	100
20	A	738/756 (98%)	715 (97%)	22 (3%)	1 (0%)	48	59
All	All	4906/5366 (91%)	4700 (96%)	199 (4%)	7 (0%)	49	59

5 of 7 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
11	R	196	PRO
1	B	288	GLY
1	B	284	PHE
11	L	367	GLN
1	B	488	ALA

### 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	B	608/609 (100%)	600 (99%)	8 (1%)	61	76
2	C	69/70 (99%)	67 (97%)	2 (3%)	37	49
3	D	157/160 (98%)	154 (98%)	3 (2%)	50	65
4	E	54/124 (44%)	52 (96%)	2 (4%)	30	40
5	F	132/251 (53%)	129 (98%)	3 (2%)	44	58
6	G	133/140 (95%)	132 (99%)	1 (1%)	73	84
6	P	124/140 (89%)	118 (95%)	6 (5%)	23	29
7	H	141/149 (95%)	139 (99%)	2 (1%)	59	73
8	I	120/136 (88%)	114 (95%)	6 (5%)	22	27
8	N	124/136 (91%)	120 (97%)	4 (3%)	34	46
9	J	34/36 (94%)	34 (100%)	0	100	100
10	K	144/146 (99%)	139 (96%)	5 (4%)	32	42
10	Q	144/146 (99%)	141 (98%)	3 (2%)	47	61
11	L	139/145 (96%)	134 (96%)	5 (4%)	31	41
11	R	136/145 (94%)	132 (97%)	4 (3%)	37	49
12	M	26/26 (100%)	26 (100%)	0	100	100
13	O	143/144 (99%)	138 (96%)	5 (4%)	32	42
14	S	133/137 (97%)	130 (98%)	3 (2%)	44	58
15	T	126/131 (96%)	125 (99%)	1 (1%)	73	84

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
16	U	152/158 (96%)	150 (99%)	2 (1%)	61	76
17	V	151/151 (100%)	148 (98%)	3 (2%)	48	63
18	W	167/172 (97%)	165 (99%)	2 (1%)	63	77
19	X	173/173 (100%)	171 (99%)	2 (1%)	63	77
20	A	621/636 (98%)	612 (99%)	9 (1%)	59	73
All	All	3951/4261 (93%)	3870 (98%)	81 (2%)	46	61

5 of 81 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
11	R	278	VAL
19	X	320	ASP
14	S	78	THR
17	V	165	THR
20	A	328	SER

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

Mol	Chain	Res	Type
17	V	322	GLN
19	X	123	HIS
20	A	34	HIS
11	L	336	GLN
11	L	211	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry

436 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
22	CLA	F	404	-	59,63,73	1.26	6 (10%)	70,101,113	1.35	6 (8%)
22	CLA	K	604	-	68,72,73	1.18	8 (11%)	80,111,113	1.26	6 (7%)
22	CLA	B	821	1	64,68,73	1.22	8 (12%)	76,107,113	1.29	5 (6%)
22	CLA	W	403	18	56,60,73	1.31	8 (14%)	65,97,113	1.38	6 (9%)
28	LMG	I	615	-	50,50,55	1.04	1 (2%)	56,57,63	1.41	6 (10%)
22	CLA	A	819	20	62,66,73	1.22	8 (12%)	73,104,113	1.44	7 (9%)
22	CLA	A	820	20	69,73,73	1.17	8 (11%)	82,113,113	1.25	7 (8%)
26	LHG	K	619	-	32,32,48	1.36	6 (18%)	35,38,54	1.12	2 (5%)
22	CLA	P	604	-	49,53,73	1.39	7 (14%)	58,89,113	1.42	4 (6%)
22	CLA	B	831	1	69,73,73	1.16	8 (11%)	82,113,113	1.24	8 (9%)
22	CLA	I	604	-	49,53,73	1.39	9 (18%)	58,89,113	1.42	4 (6%)
22	CLA	O	319	13	49,53,73	1.39	7 (14%)	58,89,113	1.42	4 (6%)
28	LMG	T	616	-	41,41,55	0.83	1 (2%)	49,49,63	1.24	3 (6%)
27	LMU	B	849	-	24,24,36	0.45	0	29,29,47	0.64	0
22	CLA	P	609	-	49,53,73	1.39	8 (16%)	58,89,113	1.39	3 (5%)
22	CLA	X	405	-	60,64,73	1.25	8 (13%)	71,102,113	1.32	5 (7%)
21	BCR	A	848	-	41,41,41	0.71	0	56,56,56	1.81	10 (17%)
22	CLA	S	610	14	49,53,73	1.40	7 (14%)	58,89,113	1.49	5 (8%)
22	CLA	W	412	26	64,68,73	1.23	8 (12%)	76,107,113	1.30	6 (7%)
22	CLA	A	818	20	57,61,73	1.28	8 (14%)	67,98,113	1.34	7 (10%)
22	CLA	I	607	8	59,63,73	1.26	8 (13%)	70,101,113	1.34	7 (10%)
24	DD6	S	611	-	40,45,45	1.54	2 (5%)	51,67,67	1.81	13 (25%)
22	CLA	A	844	26	59,63,73	1.27	9 (15%)	70,101,113	1.38	7 (10%)
28	LMG	H	322	-	37,37,55	0.84	1 (2%)	45,45,63	1.24	3 (6%)
28	LMG	I	614	-	37,37,55	0.85	1 (2%)	45,45,63	1.28	5 (11%)
22	CLA	Q	617	10	56,60,73	1.30	7 (12%)	65,97,113	1.38	6 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
22	CLA	B	807	1	69,73,73	1.16	8 (11%)	82,113,113	1.23	6 (7%)
31	CHL	U	408	-	40,54,74	2.38	10 (25%)	34,90,114	1.35	5 (14%)
22	CLA	K	606	-	54,58,73	1.32	8 (14%)	64,95,113	1.40	6 (9%)
24	DD6	U	416	-	40,45,45	1.57	2 (5%)	51,67,67	1.79	12 (23%)
22	CLA	W	410	18	64,68,73	1.21	8 (12%)	76,107,113	1.30	6 (7%)
22	CLA	U	420	16	49,53,73	1.39	8 (16%)	58,89,113	1.40	4 (6%)
26	LHG	K	616	22	38,38,48	1.27	6 (15%)	41,44,54	1.04	3 (7%)
22	CLA	B	824	-	69,73,73	1.17	8 (11%)	82,113,113	1.31	7 (8%)
22	CLA	R	604	-	49,53,73	1.40	7 (14%)	58,89,113	1.37	5 (8%)
22	CLA	W	411	18	64,68,73	1.21	9 (14%)	76,107,113	1.26	7 (9%)
27	LMU	H	321	-	34,34,36	0.48	0	42,44,47	0.77	2 (4%)
22	CLA	B	810	-	60,64,73	1.25	8 (13%)	71,102,113	1.30	5 (7%)
21	BCR	M	101	-	41,41,41	0.74	1 (2%)	56,56,56	2.02	15 (26%)
24	DD6	W	418	-	40,45,45	1.57	3 (7%)	51,67,67	1.88	15 (29%)
26	LHG	N	616	-	42,42,48	1.21	6 (14%)	45,48,54	0.99	2 (4%)
22	CLA	H	311	7	69,73,73	1.19	7 (10%)	82,113,113	1.27	6 (7%)
22	CLA	R	607	11	64,68,73	1.24	9 (14%)	76,107,113	1.30	6 (7%)
22	CLA	X	413	19	49,53,73	1.39	6 (12%)	58,89,113	1.40	4 (6%)
27	LMU	B	855	-	24,24,36	0.46	0	29,29,47	0.66	0
22	CLA	O	306	13	64,68,73	1.21	9 (14%)	76,107,113	1.27	6 (7%)
26	LHG	S	613	22	31,31,48	1.37	6 (19%)	34,37,54	1.14	3 (8%)
22	CLA	J	102	9	54,58,73	1.31	8 (14%)	64,95,113	1.38	5 (7%)
27	LMU	B	857	-	36,36,36	0.42	0	47,47,47	0.74	1 (2%)
24	DD6	V	614	-	40,45,45	1.53	2 (5%)	51,67,67	2.01	15 (29%)
22	CLA	X	412	19	69,73,73	1.18	7 (10%)	82,113,113	1.25	5 (6%)
22	CLA	B	817	1	69,73,73	1.17	8 (11%)	82,113,113	1.25	5 (6%)
22	CLA	T	606	15	54,58,73	1.31	7 (12%)	64,95,113	1.37	6 (9%)
22	CLA	S	602	14	64,68,73	1.22	7 (10%)	76,107,113	1.31	8 (10%)
22	CLA	V	609	17	61,65,73	1.25	8 (13%)	72,103,113	1.32	6 (8%)
27	LMU	T	615	-	21,21,36	0.47	0	26,26,47	0.58	0
27	LMU	H	301	-	21,21,36	0.50	0	26,26,47	0.71	0
22	CLA	X	411	-	49,53,73	1.39	7 (14%)	58,89,113	1.44	6 (10%)
22	CLA	N	606	8	69,73,73	1.19	7 (10%)	82,113,113	1.25	6 (7%)
27	LMU	B	854	-	24,24,36	0.46	0	29,29,47	0.80	1 (3%)
30	SQD	F	407	-	40,42,54	0.43	1 (2%)	50,53,65	0.47	1 (2%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
31	CHL	W	422	-	60,74,74	1.92	10 (16%)	58,114,114	1.12	5 (8%)
21	BCR	B	843	-	41,41,41	0.72	0	56,56,56	3.46	25 (44%)
31	CHL	X	406	-	40,54,74	2.36	10 (25%)	34,90,114	1.40	5 (14%)
22	CLA	B	829	-	49,53,73	1.34	9 (18%)	58,89,113	1.50	5 (8%)
27	LMU	A	854	-	36,36,36	0.42	0	47,47,47	0.70	1 (2%)
24	DD6	X	401	-	40,45,45	1.51	2 (5%)	51,67,67	1.81	11 (21%)
22	CLA	X	403	19	69,73,73	1.17	8 (11%)	82,113,113	1.25	5 (6%)
27	LMU	G	615	-	21,21,36	0.46	0	26,26,47	0.50	0
22	CLA	G	604	-	49,53,73	1.39	7 (14%)	58,89,113	1.44	6 (10%)
22	CLA	L	411	11	69,73,73	1.17	8 (11%)	82,113,113	1.25	6 (7%)
22	CLA	N	607	-	64,68,73	1.22	9 (14%)	76,107,113	1.26	6 (7%)
22	CLA	A	803	-	69,73,73	1.19	8 (11%)	82,113,113	1.25	7 (8%)
22	CLA	H	308	7	64,68,73	1.20	7 (10%)	76,107,113	1.28	7 (9%)
22	CLA	A	813	20	69,73,73	1.16	7 (10%)	82,113,113	1.18	6 (7%)
22	CLA	B	806	1	69,73,73	1.17	8 (11%)	82,113,113	1.26	6 (7%)
27	LMU	J	104	-	35,35,36	0.40	0	44,45,47	0.93	2 (4%)
28	LMG	A	855	-	41,41,55	0.84	0	49,49,63	1.26	6 (12%)
22	CLA	B	833	1	69,73,73	1.17	9 (13%)	82,113,113	1.25	5 (6%)
22	CLA	O	311	26	64,68,73	1.21	7 (10%)	76,107,113	1.27	6 (7%)
27	LMU	F	402	-	21,21,36	0.47	0	26,26,47	0.68	0
24	DD6	L	413	-	40,45,45	1.53	2 (5%)	51,67,67	1.76	13 (25%)
22	CLA	B	813	1	69,73,73	1.17	8 (11%)	82,113,113	1.20	5 (6%)
22	CLA	H	302	7	49,53,73	1.39	8 (16%)	58,89,113	1.39	4 (6%)
22	CLA	S	606	14	54,58,73	1.33	6 (11%)	64,95,113	1.36	6 (9%)
22	CLA	B	808	1	59,63,73	1.27	9 (15%)	70,101,113	1.32	6 (8%)
22	CLA	B	835	1	69,73,73	1.16	7 (10%)	82,113,113	1.29	6 (7%)
22	CLA	H	312	7	49,53,73	1.39	7 (14%)	58,89,113	1.37	4 (6%)
26	LHG	B	848	22	26,26,48	1.36	6 (23%)	29,32,54	1.17	2 (6%)
22	CLA	N	604	-	49,53,73	1.39	8 (16%)	58,89,113	1.41	4 (6%)
22	CLA	P	608	-	49,53,73	1.41	9 (18%)	58,89,113	1.42	5 (8%)
22	CLA	V	612	-	69,73,73	1.19	8 (11%)	82,113,113	1.24	4 (4%)
25	DGD	O	304	-	61,61,67	0.87	3 (4%)	75,75,81	1.13	6 (8%)
22	CLA	V	602	17	69,73,73	1.18	7 (10%)	82,113,113	1.26	5 (6%)
22	CLA	V	608	17	59,63,73	1.27	8 (13%)	70,101,113	1.30	5 (7%)
22	CLA	S	605	-	64,68,73	1.21	7 (10%)	76,107,113	1.42	5 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
27	LMU	T	618	-	24,24,36	0.45	0	29,29,47	0.65	0
22	CLA	H	313	7	62,66,73	1.24	7 (11%)	73,104,113	1.30	6 (8%)
24	DD6	H	315	-	40,45,45	1.53	2 (5%)	51,67,67	1.79	14 (27%)
22	CLA	K	613	-	57,61,73	1.29	9 (15%)	67,98,113	1.33	5 (7%)
22	CLA	G	601	6	49,53,73	1.38	8 (16%)	58,89,113	1.42	4 (6%)
26	LHG	T	614	22	41,41,48	1.24	6 (14%)	44,47,54	0.99	2 (4%)
27	LMU	O	322	-	36,36,36	0.49	0	47,47,47	1.10	5 (10%)
22	CLA	A	811	20	61,65,73	1.24	7 (11%)	72,103,113	1.39	9 (12%)
22	CLA	U	415	16	49,53,73	1.40	8 (16%)	58,89,113	1.38	4 (6%)
22	CLA	A	824	20	69,73,73	1.17	7 (10%)	82,113,113	1.26	7 (8%)
27	LMU	F	409	-	21,21,36	0.50	0	26,26,47	0.56	0
22	CLA	W	415	18	49,53,73	1.44	8 (16%)	58,89,113	1.42	5 (8%)
22	CLA	G	608	26	64,68,73	1.21	8 (12%)	76,107,113	1.33	5 (6%)
24	DD6	X	416	-	40,45,45	1.57	1 (2%)	51,67,67	2.21	14 (27%)
22	CLA	B	822	1	69,73,73	1.17	8 (11%)	82,113,113	1.27	5 (6%)
22	CLA	P	606	6	49,53,73	1.38	7 (14%)	58,89,113	1.42	5 (8%)
24	DD6	S	612	-	40,45,45	1.53	2 (5%)	51,67,67	1.81	13 (25%)
27	LMU	B	850	-	24,24,36	0.45	0	29,29,47	0.55	0
28	LMG	W	401	-	48,48,55	0.72	0	56,56,63	1.33	7 (12%)
22	CLA	V	607	-	49,53,73	1.39	6 (12%)	58,89,113	1.42	5 (8%)
24	DD6	W	417	-	40,45,45	1.52	2 (5%)	51,67,67	1.72	12 (23%)
22	CLA	G	605	-	49,53,73	1.38	8 (16%)	58,89,113	1.44	4 (6%)
22	CLA	L	402	11	69,73,73	1.16	8 (11%)	82,113,113	1.25	4 (4%)
22	CLA	R	610	11	69,73,73	1.19	7 (10%)	82,113,113	1.21	5 (6%)
22	CLA	W	402	18	59,63,73	1.26	8 (13%)	70,101,113	1.29	6 (8%)
22	CLA	Q	606	-	49,53,73	1.40	8 (16%)	58,89,113	1.42	4 (6%)
22	CLA	R	608	26	58,62,73	1.29	8 (13%)	68,99,113	1.30	5 (7%)
25	DGD	B	847	-	67,67,67	0.84	4 (5%)	81,81,81	1.01	5 (6%)
22	CLA	L	407	-	61,65,73	1.25	8 (13%)	72,103,113	1.31	5 (6%)
28	LMG	H	319	-	40,40,55	0.81	1 (2%)	48,48,63	1.21	3 (6%)
27	LMU	T	617	-	24,24,36	0.43	0	29,29,47	0.65	0
22	CLA	H	303	7	64,68,73	1.22	8 (12%)	76,107,113	1.28	5 (6%)
27	LMU	K	620	-	34,34,36	0.50	0	42,44,47	0.99	4 (9%)
26	LHG	A	845	-	48,48,48	1.15	6 (12%)	51,54,54	0.95	3 (5%)
22	CLA	A	852	-	69,73,73	1.16	8 (11%)	82,113,113	1.21	5 (6%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
22	CLA	U	405	16	61,65,73	1.26	8 (13%)	72,103,113	1.31	5 (6%)
22	CLA	A	806	20	69,73,73	1.17	8 (11%)	82,113,113	1.24	6 (7%)
22	CLA	U	401	-	59,63,73	1.27	9 (15%)	70,101,113	1.32	5 (7%)
24	DD6	P	613	-	40,45,45	1.55	2 (5%)	51,67,67	1.94	18 (35%)
24	DD6	A	858	-	40,45,45	1.53	2 (5%)	51,67,67	2.53	21 (41%)
22	CLA	N	608	26	49,53,73	1.39	7 (14%)	58,89,113	1.39	4 (6%)
22	CLA	Q	613	10	49,53,73	1.38	8 (16%)	58,89,113	1.43	5 (8%)
22	CLA	I	608	-	49,53,73	1.39	8 (16%)	58,89,113	1.41	4 (6%)
22	CLA	A	807	20	69,73,73	1.17	9 (13%)	82,113,113	1.30	5 (6%)
22	CLA	I	605	-	49,53,73	1.38	8 (16%)	58,89,113	1.44	5 (8%)
29	SF4	C	102	2	0,12,12	-	-	-	-	-
22	CLA	R	606	11	61,65,73	1.25	5 (8%)	72,103,113	1.27	5 (6%)
22	CLA	B	830	1	69,73,73	1.14	8 (11%)	82,113,113	1.31	8 (9%)
22	CLA	T	609	15	49,53,73	1.38	7 (14%)	58,89,113	1.42	6 (10%)
22	CLA	U	404	16	69,73,73	1.17	7 (10%)	82,113,113	1.25	6 (7%)
22	CLA	W	409	-	69,73,73	1.17	8 (11%)	82,113,113	1.26	7 (8%)
22	CLA	T	611	15	69,73,73	1.18	8 (11%)	82,113,113	1.26	6 (7%)
22	CLA	T	601	15	49,53,73	1.38	8 (16%)	58,89,113	1.43	4 (6%)
22	CLA	T	603	15	64,68,73	1.22	8 (12%)	76,107,113	1.28	7 (9%)
27	LMU	U	424	-	24,24,36	0.43	0	29,29,47	0.57	0
27	LMU	B	853	-	19,19,36	0.47	0	23,23,47	0.43	0
22	CLA	K	602	10	64,68,73	1.21	8 (12%)	76,107,113	1.28	7 (9%)
28	LMG	B	856	-	53,53,55	0.73	0	61,61,63	1.38	8 (13%)
26	LHG	O	323	-	42,42,48	1.23	6 (14%)	45,48,54	0.96	2 (4%)
26	LHG	O	318	22	33,33,48	1.34	6 (18%)	36,39,54	1.07	3 (8%)
27	LMU	X	418	-	24,24,36	0.44	0	29,29,47	0.54	0
22	CLA	H	309	26	59,63,73	1.28	8 (13%)	70,101,113	1.32	6 (8%)
22	CLA	T	608	26	64,68,73	1.22	8 (12%)	76,107,113	1.29	5 (6%)
28	LMG	F	408	-	42,42,55	0.85	2 (4%)	50,50,63	1.33	4 (8%)
22	CLA	F	405	5	49,53,73	1.40	8 (16%)	58,89,113	1.35	4 (6%)
22	CLA	G	603	6	60,64,73	1.26	8 (13%)	71,102,113	1.30	6 (8%)
22	CLA	B	819	1	57,61,73	1.33	6 (10%)	67,98,113	1.37	3 (4%)
22	CLA	A	841	20	69,73,73	1.17	8 (11%)	82,113,113	1.24	5 (6%)
22	CLA	A	808	20	69,73,73	1.17	8 (11%)	82,113,113	1.25	5 (6%)
22	CLA	Q	605	-	60,64,73	1.26	6 (10%)	71,102,113	1.32	7 (9%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
22	CLA	A	805	20	65,69,73	1.20	6 (9%)	77,108,113	1.28	7 (9%)
31	CHL	W	407	-	40,54,74	2.36	10 (25%)	34,90,114	1.42	5 (14%)
21	BCR	A	850	-	41,41,41	0.70	0	56,56,56	1.97	13 (23%)
22	CLA	O	308	-	65,69,73	1.21	7 (10%)	77,108,113	1.28	7 (9%)
22	CLA	V	610	-	49,53,73	1.40	6 (12%)	58,89,113	1.39	4 (6%)
24	DD6	A	859	-	40,45,45	1.58	2 (5%)	51,67,67	1.89	14 (27%)
22	CLA	W	404	18	69,73,73	1.16	7 (10%)	82,113,113	1.26	5 (6%)
26	LHG	L	416	22	41,41,48	1.22	6 (14%)	44,47,54	1.01	2 (4%)
22	CLA	V	611	-	49,53,73	1.41	7 (14%)	58,89,113	1.41	4 (6%)
22	CLA	N	601	8	49,53,73	1.38	8 (16%)	58,89,113	1.39	4 (6%)
22	CLA	H	304	7	49,53,73	1.38	7 (14%)	58,89,113	1.40	6 (10%)
26	LHG	O	324	-	41,41,48	1.23	5 (12%)	44,47,54	0.98	2 (4%)
22	CLA	B	823	-	69,73,73	1.16	8 (11%)	82,113,113	1.26	4 (4%)
22	CLA	B	826	1	62,66,73	1.24	7 (11%)	73,104,113	1.31	6 (8%)
26	LHG	H	316	22	26,26,48	1.45	6 (23%)	29,32,54	1.18	2 (6%)
28	LMG	Q	602	-	37,37,55	0.84	1 (2%)	45,45,63	1.29	6 (13%)
22	CLA	Q	604	10	69,73,73	1.16	8 (11%)	82,113,113	1.26	5 (6%)
30	SQD	K	621	-	41,43,54	0.43	1 (2%)	51,54,65	0.53	0
22	CLA	S	603	14	49,53,73	1.38	7 (14%)	58,89,113	1.40	6 (10%)
22	CLA	A	809	20	57,61,73	1.29	8 (14%)	67,98,113	1.34	5 (7%)
22	CLA	X	410	26	64,68,73	1.21	7 (10%)	76,107,113	1.29	5 (6%)
22	CLA	Q	618	-	49,53,73	1.40	8 (16%)	58,89,113	1.39	4 (6%)
21	BCR	B	846	-	41,41,41	0.68	0	56,56,56	1.84	17 (30%)
22	CLA	A	815	20	69,73,73	1.17	7 (10%)	82,113,113	1.27	7 (8%)
24	DD6	W	416	-	40,45,45	1.50	2 (5%)	51,67,67	1.77	11 (21%)
25	DGD	F	401	-	33,33,67	1.08	2 (6%)	35,35,81	1.33	5 (14%)
24	DD6	L	414	-	40,45,45	1.55	2 (5%)	51,67,67	1.80	15 (29%)
27	LMU	X	421	-	36,36,36	0.40	0	47,47,47	0.68	1 (2%)
22	CLA	A	827	-	66,70,73	1.18	7 (10%)	78,109,113	1.29	5 (6%)
24	DD6	N	613	-	40,45,45	1.54	2 (5%)	51,67,67	1.85	15 (29%)
22	CLA	I	610	8	49,53,73	1.39	8 (16%)	58,89,113	1.41	4 (6%)
22	CLA	F	403	-	69,73,73	1.17	9 (13%)	82,113,113	1.26	6 (7%)
31	CHL	V	606	-	40,54,74	2.39	10 (25%)	34,90,114	1.33	5 (14%)
24	DD6	O	316	-	40,45,45	1.53	2 (5%)	51,67,67	1.69	13 (25%)
27	LMU	O	320	-	27,27,36	0.54	0	30,31,47	0.80	1 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
22	CLA	B	832	1	66,70,73	1.19	8 (12%)	78,109,113	1.32	6 (7%)
22	CLA	A	817	20	69,73,73	1.17	8 (11%)	82,113,113	1.27	6 (7%)
22	CLA	A	804	-	69,73,73	1.17	7 (10%)	82,113,113	1.19	5 (6%)
22	CLA	A	816	20	65,69,73	1.20	9 (13%)	77,108,113	1.40	7 (9%)
22	CLA	W	419	18	49,53,73	1.39	7 (14%)	58,89,113	1.42	4 (6%)
22	CLA	R	603	-	60,64,73	1.26	7 (11%)	71,102,113	1.33	5 (7%)
24	DD6	A	847	-	40,45,45	1.53	2 (5%)	51,67,67	1.83	14 (27%)
22	CLA	T	602	15	69,73,73	1.17	8 (11%)	82,113,113	1.25	5 (6%)
22	CLA	T	604	15	69,73,73	1.16	8 (11%)	82,113,113	1.28	5 (6%)
21	BCR	A	851	-	41,41,41	0.70	0	56,56,56	2.11	16 (28%)
24	DD6	G	613	-	40,45,45	1.56	2 (5%)	51,67,67	1.90	16 (31%)
27	LMU	U	421	-	36,36,36	0.41	0	47,47,47	0.66	1 (2%)
22	CLA	A	842	20	69,73,73	1.17	7 (10%)	82,113,113	1.30	7 (8%)
22	CLA	S	604	-	64,68,73	1.22	8 (12%)	76,107,113	1.29	6 (7%)
22	CLA	H	310	7	49,53,73	1.38	7 (14%)	58,89,113	1.40	4 (6%)
22	CLA	A	826	-	69,73,73	1.16	8 (11%)	82,113,113	1.28	6 (7%)
26	LHG	R	614	22	41,41,48	1.22	6 (14%)	44,47,54	0.97	2 (4%)
21	BCR	A	849	-	41,41,41	0.72	0	56,56,56	1.89	13 (23%)
22	CLA	K	610	10	60,64,73	1.25	8 (13%)	71,102,113	1.30	6 (8%)
32	NEX	V	616	-	40,46,46	0.36	1 (2%)	50,70,70	0.66	1 (2%)
24	DD6	K	614	-	40,45,45	1.57	3 (7%)	51,67,67	1.83	14 (27%)
26	LHG	P	601	-	39,39,48	1.25	6 (15%)	42,45,54	1.00	2 (4%)
28	LMG	K	618	-	49,49,55	0.75	0	57,57,63	1.32	7 (12%)
22	CLA	O	315	13	54,58,73	1.34	8 (14%)	64,95,113	1.34	6 (9%)
22	CLA	P	607	6	49,53,73	1.39	8 (16%)	58,89,113	1.42	5 (8%)
21	BCR	B	844	-	41,41,41	0.69	0	56,56,56	1.81	12 (21%)
22	CLA	A	821	20	69,73,73	1.16	8 (11%)	82,113,113	1.30	6 (7%)
24	DD6	P	612	-	40,45,45	1.56	1 (2%)	51,67,67	2.93	17 (33%)
22	CLA	K	607	10	61,65,73	1.22	9 (14%)	72,103,113	1.44	6 (8%)
22	CLA	K	609	26	64,68,73	1.21	8 (12%)	76,107,113	1.28	4 (5%)
22	CLA	K	603	10	64,68,73	1.21	9 (14%)	76,107,113	1.28	5 (6%)
27	LMU	M	102	-	24,24,36	0.44	0	29,29,47	0.60	0
22	CLA	X	407	-	69,73,73	1.18	7 (10%)	82,113,113	1.26	5 (6%)
24	DD6	V	615	-	40,45,45	1.50	2 (5%)	51,67,67	1.85	14 (27%)
24	DD6	F	406	-	40,45,45	1.55	2 (5%)	51,67,67	1.88	16 (31%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
22	CLA	R	605	-	69,73,73	1.19	7 (10%)	82,113,113	1.26	5 (6%)
31	CHL	W	408	-	60,74,74	1.89	10 (16%)	58,114,114	1.16	6 (10%)
28	LMG	K	601	-	43,43,55	0.76	0	51,51,63	1.28	5 (9%)
22	CLA	G	610	6	49,53,73	1.38	8 (16%)	58,89,113	1.41	4 (6%)
22	CLA	X	404	19	64,68,73	1.23	7 (10%)	76,107,113	1.25	5 (6%)
22	CLA	N	602	8	64,68,73	1.21	9 (14%)	76,107,113	1.31	6 (7%)
31	CHL	V	605	-	40,54,74	2.36	10 (25%)	34,90,114	1.38	5 (14%)
22	CLA	G	606	6	69,73,73	1.17	7 (10%)	82,113,113	1.22	5 (6%)
21	BCR	B	801	-	41,41,41	0.69	0	56,56,56	1.97	17 (30%)
22	CLA	B	838	1	49,53,73	1.39	8 (16%)	58,89,113	1.39	4 (6%)
22	CLA	X	417	19	54,58,73	1.33	6 (11%)	64,95,113	1.38	7 (10%)
24	DD6	R	612	-	40,45,45	1.52	2 (5%)	51,67,67	1.84	11 (21%)
22	CLA	Q	611	10	59,63,73	1.27	7 (11%)	70,101,113	1.32	6 (8%)
22	CLA	L	410	11	64,68,73	1.21	7 (10%)	76,107,113	1.29	6 (7%)
22	CLA	A	837	20	54,58,73	1.32	8 (14%)	64,95,113	1.37	6 (9%)
22	CLA	B	814	1	49,53,73	1.37	7 (14%)	58,89,113	1.40	7 (12%)
22	CLA	Q	609	10	64,68,73	1.21	8 (12%)	76,107,113	1.26	6 (7%)
22	CLA	R	611	11	49,53,73	1.39	7 (14%)	58,89,113	1.38	4 (6%)
22	CLA	P	610	6	45,49,73	1.44	6 (13%)	54,84,113	1.51	6 (11%)
22	CLA	T	605	-	69,73,73	1.18	8 (11%)	82,113,113	1.24	5 (6%)
22	CLA	B	809	1	69,73,73	1.17	7 (10%)	82,113,113	1.28	6 (7%)
22	CLA	O	314	13	49,53,73	1.39	8 (16%)	58,89,113	1.38	4 (6%)
26	LHG	W	420	22	41,41,48	1.23	6 (14%)	44,47,54	0.91	2 (4%)
22	CLA	L	403	11	64,68,73	1.21	8 (12%)	76,107,113	1.30	8 (10%)
22	CLA	A	810	20	69,73,73	1.16	8 (11%)	82,113,113	1.26	7 (8%)
22	CLA	B	811	1	49,53,73	1.38	7 (14%)	58,89,113	1.45	6 (10%)
24	DD6	H	314	-	40,45,45	1.53	2 (5%)	51,67,67	1.87	15 (29%)
22	CLA	I	606	8	65,69,73	1.21	9 (13%)	77,108,113	1.27	5 (6%)
22	CLA	U	403	16	49,53,73	1.40	7 (14%)	58,89,113	1.46	5 (8%)
21	BCR	J	103	-	41,41,41	0.67	0	56,56,56	1.78	13 (23%)
22	CLA	B	859	-	69,73,73	1.18	8 (11%)	82,113,113	1.29	5 (6%)
22	CLA	K	608	10	69,73,73	1.14	8 (11%)	82,113,113	1.25	8 (9%)
22	CLA	Q	612	10	69,73,73	1.16	7 (10%)	82,113,113	1.26	4 (4%)
22	CLA	O	312	13	64,68,73	1.20	7 (10%)	76,107,113	1.31	8 (10%)
26	LHG	X	420	22	41,41,48	1.24	6 (14%)	44,47,54	1.00	2 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
28	LMG	J	101	-	55,55,55	0.70	1 (1%)	63,63,63	1.35	8 (12%)
31	CHL	U	407	-	40,54,74	2.36	10 (25%)	34,90,114	1.39	5 (14%)
22	CLA	B	836	1	55,59,73	1.30	8 (14%)	64,96,113	1.36	6 (9%)
22	CLA	Q	608	10	54,58,73	1.32	7 (12%)	64,95,113	1.36	6 (9%)
22	CLA	R	609	-	45,49,73	1.42	7 (15%)	54,84,113	1.48	7 (12%)
22	CLA	A	832	20	56,60,73	1.29	7 (12%)	65,97,113	1.35	6 (9%)
22	CLA	A	840	20	69,73,73	1.17	8 (11%)	82,113,113	1.26	6 (7%)
22	CLA	R	601	-	69,73,73	1.18	8 (11%)	82,113,113	1.25	7 (8%)
22	CLA	R	615	11	69,73,73	1.18	8 (11%)	82,113,113	1.26	6 (7%)
26	LHG	O	321	-	48,48,48	1.15	6 (12%)	51,54,54	0.93	2 (3%)
22	CLA	U	413	16	49,53,73	1.39	8 (16%)	58,89,113	1.45	5 (8%)
22	CLA	A	822	-	69,73,73	1.16	9 (13%)	82,113,113	1.24	5 (6%)
24	DD6	G	612	-	40,45,45	1.56	2 (5%)	51,67,67	1.75	12 (23%)
22	CLA	T	607	15	64,68,73	1.22	8 (12%)	76,107,113	1.28	8 (10%)
22	CLA	T	610	-	49,53,73	1.39	7 (14%)	58,89,113	1.39	4 (6%)
22	CLA	H	307	7	64,68,73	1.23	7 (10%)	76,107,113	1.28	6 (7%)
27	LMU	U	422	-	36,36,36	0.44	0	47,47,47	0.80	2 (4%)
26	LHG	A	846	22	48,48,48	1.15	6 (12%)	51,54,54	0.93	2 (3%)
24	DD6	K	615	-	40,45,45	1.58	3 (7%)	51,67,67	1.69	12 (23%)
22	CLA	K	617	10	69,73,73	1.17	8 (11%)	82,113,113	1.26	6 (7%)
22	CLA	I	602	8	64,68,73	1.22	8 (12%)	76,107,113	1.30	7 (9%)
22	CLA	U	410	16	59,63,73	1.27	8 (13%)	70,101,113	1.31	5 (7%)
22	CLA	V	617	-	49,53,73	1.40	7 (14%)	58,89,113	1.42	5 (8%)
22	CLA	B	805	1	69,73,73	1.16	8 (11%)	82,113,113	1.28	7 (8%)
22	CLA	A	814	20	69,73,73	1.16	6 (8%)	82,113,113	1.26	6 (7%)
26	LHG	Q	616	22	43,43,48	1.20	6 (13%)	46,49,54	0.95	2 (4%)
24	DD6	I	612	-	40,45,45	1.53	2 (5%)	51,67,67	1.69	10 (19%)
24	DD6	X	414	-	40,45,45	1.52	2 (5%)	51,67,67	1.79	13 (25%)
22	CLA	O	310	13	64,68,73	1.21	8 (12%)	76,107,113	1.33	6 (7%)
22	CLA	P	602	6	49,53,73	1.37	9 (18%)	58,89,113	1.45	4 (6%)
22	CLA	A	831	20	69,73,73	1.16	7 (10%)	82,113,113	1.28	7 (8%)
22	CLA	W	406	-	60,64,73	1.25	7 (11%)	71,102,113	1.30	4 (5%)
22	CLA	U	411	16	61,65,73	1.23	7 (11%)	72,103,113	1.30	7 (9%)
22	CLA	B	839	26	69,73,73	1.17	8 (11%)	82,113,113	1.27	7 (8%)
22	CLA	G	611	6	49,53,73	1.39	7 (14%)	58,89,113	1.41	4 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
28	LMG	L	401	-	51,51,55	0.71	1 (1%)	59,59,63	1.32	5 (8%)
24	DD6	X	415	-	40,45,45	1.50	2 (5%)	51,67,67	1.68	11 (21%)
28	LMG	H	317	-	43,43,55	0.79	1 (2%)	51,51,63	1.32	8 (15%)
22	CLA	G	607	-	64,68,73	1.21	8 (12%)	76,107,113	1.26	5 (6%)
22	CLA	S	608	26	49,53,73	1.41	8 (16%)	58,89,113	1.39	5 (8%)
22	CLA	H	306	-	59,63,73	1.27	8 (13%)	70,101,113	1.32	6 (8%)
22	CLA	W	413	-	49,53,73	1.38	8 (16%)	58,89,113	1.40	4 (6%)
22	CLA	A	833	20	69,73,73	1.17	8 (11%)	82,113,113	1.26	6 (7%)
22	CLA	N	610	8	59,63,73	1.27	7 (11%)	70,101,113	1.42	7 (10%)
22	CLA	S	609	14	59,63,73	1.27	7 (11%)	70,101,113	1.30	7 (10%)
22	CLA	H	318	7	49,53,73	1.39	8 (16%)	58,89,113	1.42	5 (8%)
24	DD6	Q	614	-	40,45,45	1.53	2 (5%)	51,67,67	1.76	11 (21%)
22	CLA	N	609	8	49,53,73	1.39	7 (14%)	58,89,113	1.38	4 (6%)
22	CLA	A	835	20	65,69,73	1.20	8 (12%)	77,108,113	1.28	6 (7%)
27	LMU	L	419	-	27,27,36	0.42	0	29,30,47	0.75	0
24	DD6	Q	615	-	40,45,45	1.55	2 (5%)	51,67,67	1.87	13 (25%)
22	CLA	S	601	14	49,53,73	1.39	6 (12%)	58,89,113	1.44	4 (6%)
22	CLA	Q	603	10	49,53,73	1.38	7 (14%)	58,89,113	1.45	6 (10%)
22	CLA	R	602	-	64,68,73	1.22	7 (10%)	76,107,113	1.26	5 (6%)
22	CLA	S	615	-	55,59,73	1.31	7 (12%)	64,96,113	1.38	6 (9%)
22	CLA	O	313	13	69,73,73	1.18	8 (11%)	82,113,113	1.23	5 (6%)
27	LMU	L	420	-	35,35,36	0.37	0	44,45,47	0.83	2 (4%)
22	CLA	I	601	8	69,73,73	1.18	8 (11%)	82,113,113	1.23	5 (6%)
22	CLA	W	405	18	64,68,73	1.22	9 (14%)	76,107,113	1.27	5 (6%)
22	CLA	B	812	1	69,73,73	1.17	8 (11%)	82,113,113	1.27	7 (8%)
22	CLA	I	603	8	60,64,73	1.27	8 (13%)	71,102,113	1.29	6 (8%)
22	CLA	V	603	17	61,65,73	1.25	7 (11%)	72,103,113	1.29	6 (8%)
24	DD6	L	415	-	40,45,45	1.54	2 (5%)	51,67,67	1.95	14 (27%)
22	CLA	G	609	-	49,53,73	1.39	7 (14%)	58,89,113	1.39	5 (8%)
22	CLA	B	828	1	69,73,73	1.17	8 (11%)	82,113,113	1.27	9 (10%)
27	LMU	O	303	-	36,36,36	0.42	0	47,47,47	0.72	1 (2%)
28	LMG	U	423	-	49,49,55	0.73	1 (2%)	57,57,63	1.31	3 (5%)
21	BCR	B	842	-	41,41,41	0.71	0	56,56,56	2.00	16 (28%)
22	CLA	K	605	-	69,73,73	1.17	8 (11%)	82,113,113	1.25	5 (6%)
30	SQD	V	618	-	25,27,54	0.54	1 (4%)	33,36,65	0.46	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
22	CLA	A	839	20	69,73,73	1.16	5 (7%)	82,113,113	1.38	8 (9%)
21	BCR	B	845	-	41,41,41	0.66	0	56,56,56	1.91	14 (25%)
22	CLA	O	305	13	54,58,73	1.31	8 (14%)	64,95,113	1.38	6 (9%)
22	CLA	I	609	8	49,53,73	1.39	7 (14%)	58,89,113	1.45	6 (10%)
22	CLA	S	614	-	49,53,73	1.38	7 (14%)	58,89,113	1.43	6 (10%)
22	CLA	L	406	-	69,73,73	1.18	8 (11%)	82,113,113	1.26	5 (6%)
22	CLA	A	828	20	69,73,73	1.17	9 (13%)	82,113,113	1.27	7 (8%)
23	PQN	B	840	-	34,34,34	1.64	2 (5%)	43,45,45	1.11	4 (9%)
22	CLA	V	613	-	49,53,73	1.41	7 (14%)	58,89,113	1.47	4 (6%)
22	CLA	U	414	16	65,69,73	1.22	8 (12%)	77,108,113	1.29	5 (6%)
22	CLA	V	601	17	49,53,73	1.41	6 (12%)	58,89,113	1.42	4 (6%)
27	LMU	A	856	-	21,21,36	0.47	0	26,26,47	0.49	0
32	NEX	U	418	-	40,46,46	0.35	1 (2%)	50,70,70	0.64	1 (2%)
22	CLA	A	838	20	56,60,73	1.30	8 (14%)	65,97,113	1.41	7 (10%)
22	CLA	A	801	-	69,73,73	1.13	8 (11%)	82,113,113	1.34	9 (10%)
22	CLA	B	804	1	69,73,73	1.16	8 (11%)	82,113,113	1.33	8 (9%)
28	LMG	B	852	-	43,43,55	0.84	0	51,51,63	1.27	4 (7%)
22	CLA	B	816	1	69,73,73	1.18	8 (11%)	82,113,113	1.26	5 (6%)
22	CLA	B	825	1	69,73,73	1.17	7 (10%)	82,113,113	1.29	7 (8%)
22	CLA	L	409	26	64,68,73	1.22	8 (12%)	76,107,113	1.29	5 (6%)
22	CLA	K	611	10	69,73,73	1.18	8 (11%)	82,113,113	1.28	6 (7%)
22	CLA	L	404	-	60,64,73	1.25	7 (11%)	71,102,113	1.34	5 (7%)
27	LMU	L	418	-	24,24,36	0.48	0	29,29,47	0.73	0
22	CLA	L	405	-	49,53,73	1.40	8 (16%)	58,89,113	1.44	4 (6%)
28	LMG	N	615	-	44,44,55	0.78	0	52,52,63	1.26	4 (7%)
22	CLA	P	605	-	49,53,73	1.38	7 (14%)	58,89,113	1.42	4 (6%)
22	CLA	G	602	6	64,68,73	1.21	8 (12%)	76,107,113	1.32	8 (10%)
22	CLA	X	402	19	59,63,73	1.26	8 (13%)	70,101,113	1.34	5 (7%)
24	DD6	T	612	-	40,45,45	1.55	2 (5%)	51,67,67	1.86	14 (27%)
22	CLA	B	837	-	49,53,73	1.39	8 (16%)	58,89,113	1.44	4 (6%)
22	CLA	I	611	8	49,53,73	1.43	8 (16%)	58,89,113	1.42	7 (12%)
24	DD6	B	841	-	40,45,45	1.53	2 (5%)	51,67,67	1.99	15 (29%)
22	CLA	B	820	1	57,61,73	1.31	6 (10%)	67,98,113	1.48	6 (8%)
22	CLA	O	309	13	54,58,73	1.31	8 (14%)	64,95,113	1.39	5 (7%)
24	DD6	N	612	-	40,45,45	1.57	3 (7%)	51,67,67	1.83	13 (25%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
27	LMU	O	301	-	24,24,36	0.44	0	29,29,47	0.56	0
22	CLA	L	412	11	49,53,73	1.39	8 (16%)	58,89,113	1.35	4 (6%)
22	CLA	H	305	7	64,68,73	1.22	7 (10%)	76,107,113	1.30	7 (9%)
26	LHG	U	419	22	24,24,48	1.49	6 (25%)	27,29,54	1.24	2 (7%)
22	CLA	N	611	-	44,48,73	1.45	6 (13%)	51,82,113	1.49	5 (9%)
22	CLA	B	827	1	69,73,73	1.16	8 (11%)	82,113,113	1.17	6 (7%)
22	CLA	P	611	6	49,53,73	1.40	6 (12%)	58,89,113	1.48	5 (8%)
22	CLA	A	823	20	49,53,73	1.39	7 (14%)	58,89,113	1.44	4 (6%)
22	CLA	N	603	8	69,73,73	1.18	7 (10%)	82,113,113	1.25	6 (7%)
22	CLA	L	408	11	64,68,73	1.20	9 (14%)	76,107,113	1.40	10 (13%)
22	CLA	P	603	6	49,53,73	1.40	6 (12%)	58,89,113	1.28	4 (6%)
22	CLA	V	604	-	60,64,73	1.26	8 (13%)	71,102,113	1.32	6 (8%)
22	CLA	B	818	-	69,73,73	1.18	8 (11%)	82,113,113	1.26	6 (7%)
27	LMU	B	858	-	14,14,36	0.30	0	13,13,47	0.58	0
27	LMU	W	421	-	24,24,36	0.44	0	29,29,47	0.56	0
22	CLA	X	409	19	69,73,73	1.17	7 (10%)	82,113,113	1.25	7 (8%)
24	DD6	T	613	-	40,45,45	1.52	2 (5%)	51,67,67	1.69	12 (23%)
22	CLA	A	812	20	61,65,73	1.23	8 (13%)	72,103,113	1.28	5 (6%)
23	PQN	A	843	-	34,34,34	1.62	2 (5%)	43,45,45	1.14	4 (9%)
22	CLA	Q	607	-	49,53,73	1.39	8 (16%)	58,89,113	1.40	4 (6%)
27	LMU	A	857	-	24,24,36	0.45	0	29,29,47	0.65	0
22	CLA	Q	610	26	69,73,73	1.18	8 (11%)	82,113,113	1.23	5 (6%)
29	SF4	B	860	1,20	0,12,12	-	-	-	-	-
22	CLA	B	834	1	69,73,73	1.17	8 (11%)	82,113,113	1.28	6 (7%)
22	CLA	B	815	1	56,60,73	1.30	8 (14%)	65,97,113	1.30	4 (6%)
24	DD6	O	317	-	40,45,45	1.55	2 (5%)	51,67,67	1.81	11 (21%)
29	SF4	C	101	2	0,12,12	-	-	-	-	-
28	LMG	K	622	-	43,43,55	0.80	1 (2%)	51,51,63	1.28	5 (9%)
22	CLA	X	408	19	69,73,73	1.17	8 (11%)	82,113,113	1.27	5 (6%)
22	CLA	A	829	20	69,73,73	1.17	8 (11%)	82,113,113	1.24	5 (6%)
26	LHG	N	614	22	27,27,48	1.43	6 (22%)	30,33,54	1.12	2 (6%)
22	CLA	K	612	10	49,53,73	1.39	7 (14%)	58,89,113	1.36	6 (10%)
28	LMG	G	616	-	46,46,55	0.81	1 (2%)	54,54,63	1.29	7 (12%)
22	CLA	W	414	18	69,73,73	1.18	7 (10%)	82,113,113	1.25	6 (7%)
24	DD6	J	105	-	40,45,45	1.52	2 (5%)	51,67,67	1.87	13 (25%)
22	CLA	U	406	-	60,64,73	1.26	8 (13%)	71,102,113	1.31	6 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
22	CLA	B	802	1	69,73,73	1.18	10 (14%)	82,113,113	1.30	6 (7%)
22	CLA	Q	601	-	49,53,73	1.41	9 (18%)	58,89,113	1.40	4 (6%)
26	LHG	G	614	22	31,31,48	1.37	6 (19%)	34,37,54	1.07	2 (5%)
24	DD6	I	613	-	40,45,45	1.58	2 (5%)	51,67,67	1.91	16 (31%)
33	CL0	A	802	20	58,73,73	2.85	19 (32%)	60,113,113	1.76	11 (18%)
22	CLA	A	836	20	69,73,73	1.16	7 (10%)	82,113,113	1.24	5 (6%)
22	CLA	B	803	1	60,64,73	1.25	7 (11%)	71,102,113	1.32	6 (8%)
22	CLA	X	419	19	49,53,73	1.40	8 (16%)	58,89,113	1.39	4 (6%)
22	CLA	A	830	20	69,73,73	1.16	8 (11%)	82,113,113	1.23	6 (7%)
28	LMG	U	402	-	53,53,55	0.72	0	61,61,63	1.31	4 (6%)
27	LMU	H	320	-	24,24,36	0.44	0	29,29,47	0.59	0
22	CLA	L	417	11	69,73,73	1.18	8 (11%)	82,113,113	1.28	6 (7%)
22	CLA	N	605	-	49,53,73	1.38	7 (14%)	58,89,113	1.45	6 (10%)
22	CLA	A	825	20	65,69,73	1.19	7 (10%)	77,108,113	1.27	5 (6%)
24	DD6	U	417	-	40,45,45	1.50	2 (5%)	51,67,67	1.79	16 (31%)
22	CLA	O	307	13	49,53,73	1.39	7 (14%)	58,89,113	1.39	5 (8%)
26	LHG	B	851	-	41,41,48	1.22	6 (14%)	44,47,54	1.00	3 (6%)
30	SQD	O	302	-	40,42,54	0.44	1 (2%)	50,53,65	0.51	1 (2%)
22	CLA	A	834	20	49,53,73	1.38	8 (16%)	58,89,113	1.38	4 (6%)
22	CLA	S	607	14	64,68,73	1.22	6 (9%)	76,107,113	1.28	5 (6%)
27	LMU	A	853	-	24,24,36	0.44	0	29,29,47	0.56	0
22	CLA	U	409	-	49,53,73	1.39	8 (16%)	58,89,113	1.43	5 (8%)
24	DD6	R	613	-	40,45,45	1.55	2 (5%)	51,67,67	2.03	17 (33%)
22	CLA	U	412	26	49,53,73	1.39	8 (16%)	58,89,113	1.42	4 (6%)

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
22	CLA	F	404	-	1/1/13/20	10/27/103/115	-
22	CLA	K	604	-	1/1/14/20	19/37/113/115	-
22	CLA	B	821	1	1/1/14/20	8/33/109/115	-
22	CLA	W	403	18	1/1/12/20	6/24/100/115	-
28	LMG	I	615	-	-	26/46/62/70	0/1/1/1

Continued on next page...



*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	A	819	20	1/1/13/20	11/31/107/115	-
22	CLA	A	820	20	1/1/15/20	10/39/115/115	-
26	LHG	K	619	-	-	18/37/37/53	-
22	CLA	P	604	-	1/1/11/20	5/15/91/115	-
22	CLA	B	831	1	1/1/15/20	6/39/115/115	-
22	CLA	I	604	-	1/1/11/20	1/15/91/115	-
22	CLA	O	319	13	1/1/11/20	0/15/91/115	-
28	LMG	T	616	-	-	16/36/56/70	0/1/1/1
27	LMU	B	849	-	-	1/15/35/61	0/1/1/2
22	CLA	P	609	-	1/1/11/20	9/15/91/115	-
22	CLA	X	405	-	1/1/13/20	8/29/105/115	-
21	BCR	A	848	-	-	0/29/63/63	0/2/2/2
22	CLA	S	610	14	1/1/11/20	3/15/91/115	-
22	CLA	W	412	26	1/1/14/20	5/33/109/115	-
22	CLA	A	818	20	1/1/12/20	3/25/101/115	-
22	CLA	I	607	8	1/1/13/20	3/27/103/115	-
24	DD6	S	611	-	-	1/26/80/80	0/3/3/3
22	CLA	A	844	26	1/1/13/20	11/27/103/115	-
28	LMG	H	322	-	-	15/32/52/70	0/1/1/1
28	LMG	I	614	-	-	12/32/52/70	0/1/1/1
22	CLA	Q	617	10	1/1/12/20	4/24/100/115	-
22	CLA	B	807	1	1/1/15/20	15/39/115/115	-
31	CHL	U	408	-	3/3/16/26	1/15/113/137	-
22	CLA	K	606	-	1/1/12/20	0/21/97/115	-
24	DD6	U	416	-	-	1/26/80/80	0/3/3/3
22	CLA	W	410	18	1/1/14/20	9/33/109/115	-
22	CLA	U	420	16	1/1/11/20	7/15/91/115	-
26	LHG	K	616	22	-	15/43/43/53	-
22	CLA	B	824	-	1/1/15/20	11/39/115/115	-
22	CLA	R	604	-	1/1/11/20	5/15/91/115	-
22	CLA	W	411	18	1/1/14/20	9/33/109/115	-
27	LMU	H	321	-	-	1/19/56/61	0/2/2/2
22	CLA	B	810	-	1/1/13/20	4/29/105/115	-
21	BCR	M	101	-	-	2/29/63/63	0/2/2/2
24	DD6	W	418	-	-	1/26/80/80	0/3/3/3
26	LHG	N	616	-	-	23/47/47/53	-

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	H	311	7	1/1/15/20	13/39/115/115	-
22	CLA	R	607	11	1/1/14/20	14/33/109/115	-
22	CLA	X	413	19	1/1/11/20	3/15/91/115	-
27	LMU	B	855	-	-	2/15/35/61	0/1/1/2
22	CLA	O	306	13	1/1/14/20	7/33/109/115	-
26	LHG	S	613	22	-	13/36/36/53	-
22	CLA	J	102	9	1/1/12/20	7/21/97/115	-
27	LMU	B	857	-	-	4/21/61/61	0/2/2/2
24	DD6	V	614	-	-	1/26/80/80	0/3/3/3
22	CLA	X	412	19	1/1/15/20	10/39/115/115	-
22	CLA	B	817	1	1/1/15/20	15/39/115/115	-
22	CLA	T	606	15	1/1/12/20	4/21/97/115	-
22	CLA	S	602	14	1/1/14/20	7/33/109/115	-
22	CLA	V	609	17	1/1/13/20	7/30/106/115	-
27	LMU	T	615	-	-	0/12/32/61	0/1/1/2
27	LMU	H	301	-	-	1/12/32/61	0/1/1/2
22	CLA	X	411	-	1/1/11/20	2/15/91/115	-
22	CLA	N	606	8	1/1/15/20	9/39/115/115	-
27	LMU	B	854	-	-	3/15/35/61	0/1/1/2
30	SQD	F	407	-	-	3/37/57/69	0/1/1/1
31	CHL	W	422	-	3/3/20/26	8/39/137/137	-
21	BCR	B	843	-	-	4/29/63/63	0/2/2/2
31	CHL	X	406	-	3/3/16/26	0/15/113/137	-
22	CLA	B	829	-	1/1/11/20	6/15/91/115	-
27	LMU	A	854	-	-	2/21/61/61	0/2/2/2
24	DD6	X	401	-	-	0/26/80/80	0/3/3/3
22	CLA	X	403	19	1/1/15/20	8/39/115/115	-
27	LMU	G	615	-	-	0/12/32/61	0/1/1/2
22	CLA	G	604	-	1/1/11/20	0/15/91/115	-
22	CLA	L	411	11	1/1/15/20	11/39/115/115	-
22	CLA	N	607	-	1/1/14/20	13/33/109/115	-
22	CLA	A	803	-	1/1/15/20	12/39/115/115	-
22	CLA	H	308	7	1/1/14/20	5/33/109/115	-
22	CLA	A	813	20	1/1/15/20	10/39/115/115	-
22	CLA	B	806	1	1/1/15/20	11/39/115/115	-

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	LMU	J	104	-	-	9/21/57/61	0/2/2/2
28	LMG	A	855	-	-	12/36/56/70	0/1/1/1
22	CLA	B	833	1	1/1/15/20	9/39/115/115	-
22	CLA	O	311	26	1/1/14/20	9/33/109/115	-
27	LMU	F	402	-	-	1/12/32/61	0/1/1/2
24	DD6	L	413	-	-	1/26/80/80	0/3/3/3
22	CLA	B	813	1	1/1/15/20	9/39/115/115	-
22	CLA	H	302	7	1/1/11/20	2/15/91/115	-
22	CLA	S	606	14	1/1/12/20	4/21/97/115	-
22	CLA	B	808	1	1/1/13/20	6/27/103/115	-
22	CLA	B	835	1	1/1/15/20	11/39/115/115	-
22	CLA	H	312	7	1/1/11/20	3/15/91/115	-
26	LHG	B	848	22	-	10/31/31/53	-
22	CLA	N	604	-	1/1/11/20	4/15/91/115	-
22	CLA	P	608	-	1/1/11/20	9/15/91/115	-
22	CLA	V	612	-	1/1/15/20	13/39/115/115	-
25	DGD	O	304	-	-	31/49/89/95	0/2/2/2
22	CLA	V	602	17	1/1/15/20	7/39/115/115	-
22	CLA	V	608	17	1/1/13/20	9/27/103/115	-
22	CLA	S	605	-	1/1/14/20	13/33/109/115	-
27	LMU	T	618	-	-	1/15/35/61	0/1/1/2
22	CLA	H	313	7	1/1/13/20	10/31/107/115	-
24	DD6	H	315	-	-	1/26/80/80	0/3/3/3
22	CLA	K	613	-	1/1/12/20	4/25/101/115	-
22	CLA	G	601	6	1/1/11/20	4/15/91/115	-
26	LHG	T	614	22	-	27/46/46/53	-
27	LMU	O	322	-	-	4/21/61/61	0/2/2/2
22	CLA	A	811	20	1/1/13/20	10/30/106/115	-
22	CLA	U	415	16	1/1/11/20	7/15/91/115	-
22	CLA	A	824	20	1/1/15/20	21/39/115/115	-
27	LMU	F	409	-	-	4/12/32/61	0/1/1/2
22	CLA	W	415	18	1/1/11/20	6/15/91/115	-
22	CLA	G	608	26	1/1/14/20	16/33/109/115	-
24	DD6	X	416	-	-	5/26/80/80	0/3/3/3
22	CLA	B	822	1	1/1/15/20	10/39/115/115	-

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	P	606	6	1/1/11/20	6/15/91/115	-
24	DD6	S	612	-	-	1/26/80/80	0/3/3/3
27	LMU	B	850	-	-	3/15/35/61	0/1/1/2
28	LMG	W	401	-	-	18/43/63/70	0/1/1/1
22	CLA	V	607	-	1/1/11/20	3/15/91/115	-
24	DD6	W	417	-	-	1/26/80/80	0/3/3/3
22	CLA	G	605	-	1/1/11/20	2/15/91/115	-
22	CLA	L	402	11	1/1/15/20	14/39/115/115	-
22	CLA	R	610	11	1/1/15/20	14/39/115/115	-
22	CLA	W	402	18	1/1/13/20	2/27/103/115	-
22	CLA	Q	606	-	1/1/11/20	6/15/91/115	-
22	CLA	R	608	26	1/1/12/20	10/26/102/115	-
25	DGD	B	847	-	-	33/55/95/95	0/2/2/2
22	CLA	L	407	-	1/1/13/20	5/30/106/115	-
28	LMG	H	319	-	-	19/35/55/70	0/1/1/1
27	LMU	T	617	-	-	3/15/35/61	0/1/1/2
22	CLA	H	303	7	1/1/14/20	9/33/109/115	-
27	LMU	K	620	-	-	6/19/56/61	0/2/2/2
26	LHG	A	845	-	-	25/53/53/53	-
22	CLA	A	852	-	1/1/15/20	14/39/115/115	-
22	CLA	U	405	16	1/1/13/20	2/30/106/115	-
22	CLA	A	806	20	1/1/15/20	12/39/115/115	-
22	CLA	U	401	-	1/1/13/20	9/27/103/115	-
24	DD6	P	613	-	-	4/26/80/80	0/3/3/3
24	DD6	A	858	-	-	5/26/80/80	0/3/3/3
22	CLA	N	608	26	1/1/11/20	7/15/91/115	-
22	CLA	Q	613	10	1/1/11/20	6/15/91/115	-
22	CLA	I	608	-	1/1/11/20	4/15/91/115	-
22	CLA	A	807	20	1/1/15/20	8/39/115/115	-
22	CLA	I	605	-	1/1/11/20	2/15/91/115	-
29	SF4	C	102	2	-	-	0/6/5/5
22	CLA	R	606	11	1/1/13/20	9/30/106/115	-
22	CLA	B	830	1	1/1/15/20	8/39/115/115	-
22	CLA	T	609	15	1/1/11/20	4/15/91/115	-
22	CLA	U	404	16	1/1/15/20	12/39/115/115	-

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	W	409	-	1/1/15/20	9/39/115/115	-
22	CLA	T	611	15	1/1/15/20	13/39/115/115	-
22	CLA	T	601	15	1/1/11/20	3/15/91/115	-
22	CLA	T	603	15	1/1/14/20	8/33/109/115	-
27	LMU	U	424	-	-	2/15/35/61	0/1/1/2
27	LMU	B	853	-	-	0/10/27/61	0/1/1/2
22	CLA	K	602	10	1/1/14/20	9/33/109/115	-
28	LMG	B	856	-	-	27/48/68/70	0/1/1/1
26	LHG	O	323	-	-	18/47/47/53	-
26	LHG	O	318	22	-	16/38/38/53	-
27	LMU	X	418	-	-	1/15/35/61	0/1/1/2
22	CLA	H	309	26	1/1/13/20	9/27/103/115	-
22	CLA	T	608	26	1/1/14/20	2/33/109/115	-
28	LMG	F	408	-	-	18/37/57/70	0/1/1/1
22	CLA	F	405	5	1/1/11/20	6/15/91/115	-
22	CLA	G	603	6	1/1/13/20	6/29/105/115	-
22	CLA	B	819	1	1/1/12/20	10/25/101/115	-
22	CLA	A	841	20	1/1/15/20	10/39/115/115	-
22	CLA	A	808	20	1/1/15/20	10/39/115/115	-
22	CLA	Q	605	-	1/1/13/20	3/29/105/115	-
22	CLA	A	805	20	1/1/14/20	11/35/111/115	-
31	CHL	W	407	-	3/3/16/26	2/15/113/137	-
22	CLA	O	308	-	1/1/14/20	14/35/111/115	-
21	BCR	A	850	-	-	4/29/63/63	0/2/2/2
22	CLA	V	610	-	1/1/11/20	4/15/91/115	-
24	DD6	A	859	-	-	1/26/80/80	0/3/3/3
22	CLA	W	404	18	1/1/15/20	7/39/115/115	-
26	LHG	L	416	22	-	20/46/46/53	-
22	CLA	V	611	-	1/1/11/20	6/15/91/115	-
22	CLA	N	601	8	1/1/11/20	6/15/91/115	-
22	CLA	H	304	7	1/1/11/20	7/15/91/115	-
26	LHG	O	324	-	-	25/46/46/53	-
22	CLA	B	823	-	1/1/15/20	11/39/115/115	-
22	CLA	B	826	1	1/1/13/20	10/31/107/115	-
26	LHG	H	316	22	-	5/31/31/53	-

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	LMG	Q	602	-	-	11/32/52/70	0/1/1/1
22	CLA	Q	604	10	1/1/15/20	15/39/115/115	-
30	SQD	K	621	-	-	3/38/58/69	0/1/1/1
22	CLA	S	603	14	1/1/11/20	2/15/91/115	-
22	CLA	A	809	20	1/1/12/20	0/25/101/115	-
22	CLA	X	410	26	1/1/14/20	10/33/109/115	-
22	CLA	Q	618	-	1/1/11/20	9/15/91/115	-
21	BCR	B	846	-	-	6/29/63/63	0/2/2/2
22	CLA	A	815	20	1/1/15/20	5/39/115/115	-
24	DD6	W	416	-	-	1/26/80/80	0/3/3/3
25	DGD	F	401	-	-	19/35/35/95	-
24	DD6	L	414	-	-	2/26/80/80	0/3/3/3
27	LMU	X	421	-	-	2/21/61/61	0/2/2/2
22	CLA	A	827	-	1/1/14/20	4/36/112/115	-
24	DD6	N	613	-	-	4/26/80/80	0/3/3/3
22	CLA	I	610	8	1/1/11/20	5/15/91/115	-
22	CLA	F	403	-	1/1/15/20	9/39/115/115	-
31	CHL	V	606	-	3/3/16/26	1/15/113/137	-
24	DD6	O	316	-	-	1/26/80/80	0/3/3/3
27	LMU	O	320	-	-	0/17/35/61	1/2/2/2
22	CLA	B	832	1	1/1/14/20	13/36/112/115	-
22	CLA	A	817	20	1/1/15/20	13/39/115/115	-
22	CLA	A	804	-	1/1/15/20	6/39/115/115	-
22	CLA	A	816	20	1/1/14/20	14/35/111/115	-
22	CLA	W	419	18	1/1/11/20	5/15/91/115	-
22	CLA	R	603	-	1/1/13/20	9/29/105/115	-
24	DD6	A	847	-	-	1/26/80/80	0/3/3/3
22	CLA	T	602	15	1/1/15/20	7/39/115/115	-
22	CLA	T	604	15	1/1/15/20	17/39/115/115	-
21	BCR	A	851	-	-	4/29/63/63	0/2/2/2
24	DD6	G	613	-	-	0/26/80/80	0/3/3/3
27	LMU	U	421	-	-	7/21/61/61	0/2/2/2
22	CLA	A	842	20	1/1/15/20	12/39/115/115	-
22	CLA	S	604	-	1/1/14/20	9/33/109/115	-
22	CLA	H	310	7	1/1/11/20	4/15/91/115	-

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	A	826	-	1/1/15/20	9/39/115/115	-
26	LHG	R	614	22	-	19/46/46/53	-
21	BCR	A	849	-	-	0/29/63/63	0/2/2/2
22	CLA	K	610	10	1/1/13/20	8/29/105/115	-
32	NEX	V	616	-	-	4/27/83/83	0/3/3/3
24	DD6	K	614	-	-	0/26/80/80	0/3/3/3
26	LHG	P	601	-	-	22/44/44/53	-
28	LMG	K	618	-	-	24/44/64/70	0/1/1/1
22	CLA	O	315	13	1/1/12/20	4/21/97/115	-
22	CLA	P	607	6	1/1/11/20	4/15/91/115	-
21	BCR	B	844	-	-	0/29/63/63	0/2/2/2
22	CLA	A	821	20	1/1/15/20	12/39/115/115	-
24	DD6	P	612	-	-	6/26/80/80	0/3/3/3
22	CLA	K	607	10	1/1/13/20	8/30/106/115	-
22	CLA	K	609	26	1/1/14/20	11/33/109/115	-
22	CLA	K	603	10	1/1/14/20	6/33/109/115	-
27	LMU	M	102	-	-	4/15/35/61	0/1/1/2
22	CLA	X	407	-	1/1/15/20	4/39/115/115	-
24	DD6	V	615	-	-	3/26/80/80	0/3/3/3
24	DD6	F	406	-	-	8/26/80/80	0/3/3/3
22	CLA	R	605	-	1/1/15/20	15/39/115/115	-
31	CHL	W	408	-	3/3/20/26	4/39/137/137	-
28	LMG	K	601	-	-	24/38/58/70	0/1/1/1
22	CLA	G	610	6	1/1/11/20	5/15/91/115	-
22	CLA	X	404	19	1/1/14/20	9/33/109/115	-
22	CLA	N	602	8	1/1/14/20	3/33/109/115	-
31	CHL	V	605	-	3/3/16/26	0/15/113/137	-
22	CLA	G	606	6	1/1/15/20	12/39/115/115	-
21	BCR	B	801	-	-	4/29/63/63	0/2/2/2
22	CLA	B	838	1	1/1/11/20	6/15/91/115	-
22	CLA	X	417	19	1/1/12/20	3/21/97/115	-
24	DD6	R	612	-	-	1/26/80/80	0/3/3/3
22	CLA	Q	611	10	1/1/13/20	8/27/103/115	-
22	CLA	L	410	11	1/1/14/20	9/33/109/115	-
22	CLA	A	837	20	1/1/12/20	4/21/97/115	-

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	B	814	1	1/1/11/20	7/15/91/115	-
22	CLA	Q	609	10	1/1/14/20	8/33/109/115	-
22	CLA	R	611	11	1/1/11/20	4/15/91/115	-
22	CLA	P	610	6	1/1/10/20	4/10/86/115	-
22	CLA	T	605	-	1/1/15/20	15/39/115/115	-
22	CLA	B	809	1	1/1/15/20	3/39/115/115	-
22	CLA	O	314	13	1/1/11/20	0/15/91/115	-
26	LHG	W	420	22	-	21/46/46/53	-
22	CLA	L	403	11	1/1/14/20	6/33/109/115	-
22	CLA	A	810	20	1/1/15/20	10/39/115/115	-
22	CLA	B	811	1	1/1/11/20	1/15/91/115	-
24	DD6	H	314	-	-	1/26/80/80	0/3/3/3
22	CLA	I	606	8	1/1/14/20	11/35/111/115	-
22	CLA	U	403	16	1/1/11/20	6/15/91/115	-
21	BCR	J	103	-	-	2/29/63/63	0/2/2/2
22	CLA	B	859	-	1/1/15/20	11/39/115/115	-
22	CLA	K	608	10	1/1/15/20	9/39/115/115	-
22	CLA	Q	612	10	1/1/15/20	14/39/115/115	-
22	CLA	O	312	13	1/1/14/20	6/33/109/115	-
26	LHG	X	420	22	-	27/46/46/53	-
28	LMG	J	101	-	-	24/50/70/70	0/1/1/1
31	CHL	U	407	-	3/3/16/26	0/15/113/137	-
22	CLA	B	836	1	1/1/12/20	1/23/99/115	-
22	CLA	Q	608	10	1/1/12/20	2/21/97/115	-
22	CLA	R	609	-	1/1/10/20	4/10/86/115	-
22	CLA	A	832	20	1/1/12/20	4/24/100/115	-
22	CLA	A	840	20	1/1/15/20	14/39/115/115	-
22	CLA	R	601	-	1/1/15/20	15/39/115/115	-
22	CLA	R	615	11	1/1/15/20	11/39/115/115	-
26	LHG	O	321	-	-	29/53/53/53	-
22	CLA	U	413	16	1/1/11/20	4/15/91/115	-
22	CLA	A	822	-	1/1/15/20	8/39/115/115	-
24	DD6	G	612	-	-	0/26/80/80	0/3/3/3
22	CLA	T	607	15	1/1/14/20	9/33/109/115	-
22	CLA	T	610	-	1/1/11/20	6/15/91/115	-

*Continued on next page...*



*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	H	307	7	1/1/14/20	8/33/109/115	-
27	LMU	U	422	-	-	5/21/61/61	0/2/2/2
26	LHG	A	846	22	-	26/53/53/53	-
24	DD6	K	615	-	-	0/26/80/80	0/3/3/3
22	CLA	K	617	10	1/1/15/20	8/39/115/115	-
22	CLA	I	602	8	1/1/14/20	1/33/109/115	-
22	CLA	U	410	16	1/1/13/20	6/27/103/115	-
22	CLA	V	617	-	1/1/11/20	8/15/91/115	-
22	CLA	B	805	1	1/1/15/20	7/39/115/115	-
22	CLA	A	814	20	1/1/15/20	7/39/115/115	-
26	LHG	Q	616	22	-	15/48/48/53	-
24	DD6	I	612	-	-	0/26/80/80	0/3/3/3
24	DD6	X	414	-	-	1/26/80/80	0/3/3/3
22	CLA	O	310	13	1/1/14/20	8/33/109/115	-
22	CLA	P	602	6	1/1/11/20	9/15/91/115	-
22	CLA	A	831	20	1/1/15/20	6/39/115/115	-
22	CLA	W	406	-	1/1/13/20	2/29/105/115	-
22	CLA	U	411	16	1/1/13/20	7/30/106/115	-
22	CLA	B	839	26	1/1/15/20	2/39/115/115	-
22	CLA	G	611	6	1/1/11/20	5/15/91/115	-
28	LMG	L	401	-	-	19/46/66/70	0/1/1/1
24	DD6	X	415	-	-	1/26/80/80	0/3/3/3
28	LMG	H	317	-	-	13/38/58/70	0/1/1/1
22	CLA	G	607	-	1/1/14/20	2/33/109/115	-
22	CLA	S	608	26	1/1/11/20	8/15/91/115	-
22	CLA	H	306	-	1/1/13/20	9/27/103/115	-
22	CLA	W	413	-	1/1/11/20	4/15/91/115	-
22	CLA	A	833	20	1/1/15/20	6/39/115/115	-
22	CLA	N	610	8	1/1/13/20	16/27/103/115	-
22	CLA	S	609	14	-	9/27/103/115	-
22	CLA	H	318	7	1/1/11/20	6/15/91/115	-
24	DD6	Q	614	-	-	0/26/80/80	0/3/3/3
22	CLA	N	609	8	1/1/11/20	4/15/91/115	-
22	CLA	A	835	20	1/1/14/20	9/35/111/115	-
27	LMU	L	419	-	-	6/21/34/61	1/1/1/2

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	DD6	Q	615	-	-	0/26/80/80	0/3/3/3
22	CLA	S	601	14	1/1/11/20	6/15/91/115	-
22	CLA	Q	603	10	1/1/11/20	4/15/91/115	-
22	CLA	R	602	-	1/1/14/20	11/33/109/115	-
22	CLA	S	615	-	1/1/12/20	4/23/99/115	-
22	CLA	O	313	13	1/1/15/20	14/39/115/115	-
27	LMU	L	420	-	-	4/21/57/61	0/2/2/2
22	CLA	I	601	8	1/1/15/20	14/39/115/115	-
22	CLA	W	405	18	1/1/14/20	1/33/109/115	-
22	CLA	B	812	1	1/1/15/20	17/39/115/115	-
22	CLA	I	603	8	1/1/13/20	7/29/105/115	-
22	CLA	V	603	17	1/1/13/20	10/30/106/115	-
22	CLA	G	609	-	1/1/11/20	4/15/91/115	-
24	DD6	L	415	-	-	3/26/80/80	0/3/3/3
22	CLA	B	828	1	1/1/15/20	12/39/115/115	-
27	LMU	O	303	-	-	2/21/61/61	0/2/2/2
28	LMG	U	423	-	-	20/44/64/70	0/1/1/1
21	BCR	B	842	-	-	2/29/63/63	0/2/2/2
22	CLA	K	605	-	1/1/15/20	18/39/115/115	-
30	SQD	V	618	-	-	4/19/39/69	0/1/1/1
22	CLA	A	839	20	1/1/15/20	5/39/115/115	-
21	BCR	B	845	-	-	2/29/63/63	0/2/2/2
22	CLA	O	305	13	1/1/12/20	2/21/97/115	-
22	CLA	I	609	8	1/1/11/20	4/15/91/115	-
22	CLA	S	614	-	1/1/11/20	0/15/91/115	-
22	CLA	L	406	-	1/1/15/20	8/39/115/115	-
22	CLA	A	828	20	1/1/15/20	7/39/115/115	-
23	PQN	B	840	-	-	0/23/43/43	0/2/2/2
22	CLA	V	613	-	1/1/11/20	9/15/91/115	-
22	CLA	U	414	16	1/1/14/20	14/35/111/115	-
22	CLA	V	601	17	1/1/11/20	6/15/91/115	-
27	LMU	A	856	-	-	0/12/32/61	0/1/1/2
32	NEX	U	418	-	-	4/27/83/83	0/3/3/3
22	CLA	A	838	20	1/1/12/20	5/24/100/115	-
22	CLA	A	801	-	1/1/15/20	15/39/115/115	-

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	B	804	1	1/1/15/20	13/39/115/115	-
28	LMG	B	852	-	-	15/38/58/70	0/1/1/1
22	CLA	B	816	1	1/1/15/20	10/39/115/115	-
22	CLA	B	825	1	1/1/15/20	6/39/115/115	-
22	CLA	L	409	26	1/1/14/20	5/33/109/115	-
22	CLA	K	611	10	1/1/15/20	10/39/115/115	-
22	CLA	L	404	-	1/1/13/20	11/29/105/115	-
27	LMU	L	418	-	-	0/15/35/61	0/1/1/2
22	CLA	L	405	-	1/1/11/20	2/15/91/115	-
28	LMG	N	615	-	-	24/39/59/70	0/1/1/1
22	CLA	P	605	-	1/1/11/20	5/15/91/115	-
22	CLA	G	602	6	1/1/14/20	4/33/109/115	-
22	CLA	X	402	19	1/1/13/20	9/27/103/115	-
24	DD6	T	612	-	-	1/26/80/80	0/3/3/3
22	CLA	B	837	-	1/1/11/20	2/15/91/115	-
22	CLA	I	611	8	1/1/11/20	4/15/91/115	-
24	DD6	B	841	-	-	1/26/80/80	0/3/3/3
22	CLA	B	820	1	1/1/12/20	9/25/101/115	-
22	CLA	O	309	13	1/1/12/20	4/21/97/115	-
24	DD6	N	612	-	-	0/26/80/80	0/3/3/3
27	LMU	O	301	-	-	1/15/35/61	0/1/1/2
22	CLA	L	412	11	1/1/11/20	5/15/91/115	-
22	CLA	H	305	7	1/1/14/20	10/33/109/115	-
26	LHG	U	419	22	-	15/28/28/53	-
22	CLA	N	611	-	1/1/9/20	4/10/82/115	-
22	CLA	B	827	1	1/1/15/20	6/39/115/115	-
22	CLA	P	611	6	1/1/11/20	7/15/91/115	-
22	CLA	A	823	20	1/1/11/20	5/15/91/115	-
22	CLA	N	603	8	1/1/15/20	8/39/115/115	-
22	CLA	L	408	11	1/1/14/20	5/33/109/115	-
22	CLA	P	603	6	-	6/15/91/115	-
22	CLA	V	604	-	1/1/13/20	7/29/105/115	-
22	CLA	B	818	-	1/1/15/20	11/39/115/115	-
27	LMU	B	858	-	-	2/12/12/61	-
27	LMU	W	421	-	-	4/15/35/61	0/1/1/2

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	X	409	19	1/1/15/20	9/39/115/115	-
24	DD6	T	613	-	-	1/26/80/80	0/3/3/3
22	CLA	A	812	20	1/1/13/20	7/30/106/115	-
23	PQN	A	843	-	-	4/23/43/43	0/2/2/2
22	CLA	Q	607	-	1/1/11/20	4/15/91/115	-
27	LMU	A	857	-	-	3/15/35/61	0/1/1/2
22	CLA	Q	610	26	1/1/15/20	12/39/115/115	-
29	SF4	B	860	1,20	-	-	0/6/5/5
22	CLA	B	834	1	1/1/15/20	6/39/115/115	-
22	CLA	B	815	1	1/1/12/20	3/24/100/115	-
24	DD6	O	317	-	-	0/26/80/80	0/3/3/3
29	SF4	C	101	2	-	-	0/6/5/5
28	LMG	K	622	-	-	15/38/58/70	0/1/1/1
22	CLA	X	408	19	1/1/15/20	12/39/115/115	-
22	CLA	A	829	20	1/1/15/20	14/39/115/115	-
26	LHG	N	614	22	-	9/32/32/53	-
22	CLA	K	612	10	1/1/11/20	2/15/91/115	-
28	LMG	G	616	-	-	21/41/61/70	0/1/1/1
22	CLA	W	414	18	1/1/15/20	9/39/115/115	-
24	DD6	J	105	-	-	3/26/80/80	0/3/3/3
22	CLA	U	406	-	1/1/13/20	7/29/105/115	-
22	CLA	B	802	1	1/1/15/20	5/39/115/115	-
22	CLA	Q	601	-	1/1/11/20	5/15/91/115	-
26	LHG	G	614	22	-	13/36/36/53	-
24	DD6	I	613	-	-	0/26/80/80	0/3/3/3
33	CL0	A	802	20	3/3/20/25	8/37/135/135	-
22	CLA	A	836	20	1/1/15/20	10/39/115/115	-
22	CLA	B	803	1	1/1/13/20	7/29/105/115	-
22	CLA	X	419	19	1/1/11/20	8/15/91/115	-
22	CLA	A	830	20	1/1/15/20	13/39/115/115	-
28	LMG	U	402	-	-	26/48/68/70	0/1/1/1
27	LMU	H	320	-	-	2/15/35/61	0/1/1/2
22	CLA	L	417	11	1/1/15/20	8/39/115/115	-
22	CLA	N	605	-	1/1/11/20	2/15/91/115	-
22	CLA	A	825	20	1/1/14/20	14/35/111/115	-

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	DD6	U	417	-	-	1/26/80/80	0/3/3/3
22	CLA	O	307	13	1/1/11/20	5/15/91/115	-
26	LHG	B	851	-	-	22/46/46/53	-
30	SQD	O	302	-	-	5/37/57/69	0/1/1/1
22	CLA	A	834	20	1/1/11/20	4/15/91/115	-
22	CLA	S	607	14	1/1/14/20	10/33/109/115	-
27	LMU	A	853	-	-	0/15/35/61	0/1/1/2
22	CLA	U	409	-	1/1/11/20	5/15/91/115	-
24	DD6	R	613	-	-	1/26/80/80	0/3/3/3
22	CLA	U	412	26	1/1/11/20	3/15/91/115	-

The worst 5 of 2484 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	A	859	DD6	C30-C31	-8.58	1.25	1.42
24	P	612	DD6	C30-C31	-8.58	1.25	1.42
24	P	613	DD6	C30-C31	-8.56	1.25	1.42
24	N	612	DD6	C30-C31	-8.54	1.25	1.42
24	G	613	DD6	C30-C31	-8.51	1.26	1.42

The worst 5 of 2573 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	B	843	BCR	C40-C30-C25	-13.78	88.64	110.24
24	P	612	DD6	C9-C10-C11	-10.08	113.14	127.28
24	P	612	DD6	C4-C5-C6	-9.22	114.35	127.28
21	B	843	BCR	C40-C30-C39	-9.02	82.82	108.63
24	X	416	DD6	C4-C5-C6	-8.51	115.34	127.28

5 of 304 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
22	B	802	CLA	ND
22	B	803	CLA	ND
22	B	804	CLA	ND
22	B	805	CLA	ND
22	B	806	CLA	ND

5 of 3251 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
21	B	801	BCR	C7-C8-C9-C10
21	B	801	BCR	C7-C8-C9-C34
21	B	842	BCR	C21-C22-C23-C24
21	B	842	BCR	C37-C22-C23-C24
21	B	845	BCR	C21-C22-C23-C24

All (2) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
27	O	320	LMU	C1'-C2'-C3'-C4'-C5'-O5'
27	L	419	LMU	C1'-C2'-C3'-C4'-C5'-O5'

291 monomers are involved in 581 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	F	404	CLA	4	0
22	K	604	CLA	6	0
22	B	821	CLA	2	0
28	I	615	LMG	1	0
22	A	819	CLA	1	0
22	A	820	CLA	1	0
22	B	831	CLA	2	0
28	T	616	LMG	2	0
22	P	609	CLA	1	0
21	A	848	BCR	2	0
22	S	610	CLA	2	0
22	W	412	CLA	2	0
22	I	607	CLA	3	0
24	S	611	DD6	1	0
22	A	844	CLA	4	0
28	H	322	LMG	1	0
22	B	807	CLA	2	0
31	U	408	CHL	4	0
22	K	606	CLA	2	0
22	W	410	CLA	3	0
22	U	420	CLA	1	0
26	K	616	LHG	3	0
22	B	824	CLA	3	0
22	R	604	CLA	5	0
22	W	411	CLA	2	0
27	H	321	LMU	1	0
22	B	810	CLA	1	0
21	M	101	BCR	3	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Clashes	Symm-Clashes
26	N	616	LHG	1	0
22	H	311	CLA	2	0
22	R	607	CLA	3	0
22	X	413	CLA	1	0
27	B	855	LMU	1	0
26	S	613	LHG	2	0
22	J	102	CLA	1	0
22	B	817	CLA	1	0
22	T	606	CLA	1	0
22	S	602	CLA	1	0
22	V	609	CLA	2	0
27	H	301	LMU	1	0
22	X	411	CLA	1	0
22	N	606	CLA	4	0
27	B	854	LMU	8	0
30	F	407	SQD	2	0
31	W	422	CHL	2	0
21	B	843	BCR	3	0
22	B	829	CLA	3	0
27	A	854	LMU	1	0
22	X	403	CLA	1	0
22	L	411	CLA	1	0
22	N	607	CLA	7	0
22	A	803	CLA	1	0
22	H	308	CLA	2	0
22	A	813	CLA	2	0
22	B	806	CLA	4	0
22	B	833	CLA	4	0
22	O	311	CLA	3	0
22	B	813	CLA	3	0
22	S	606	CLA	1	0
22	B	835	CLA	2	0
22	H	312	CLA	3	0
26	B	848	LHG	1	0
22	N	604	CLA	1	0
22	P	608	CLA	2	0
22	V	612	CLA	7	0
25	O	304	DGD	3	0
22	V	602	CLA	5	0
22	V	608	CLA	1	0
22	S	605	CLA	4	0
27	T	618	LMU	2	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	H	313	CLA	1	0
22	K	613	CLA	4	0
22	G	601	CLA	1	0
26	T	614	LHG	1	0
22	A	811	CLA	1	0
22	U	415	CLA	2	0
22	A	824	CLA	4	0
27	F	409	LMU	1	0
22	W	415	CLA	1	0
22	G	608	CLA	4	0
22	B	822	CLA	3	0
22	P	606	CLA	3	0
28	W	401	LMG	3	0
22	V	607	CLA	2	0
22	L	402	CLA	2	0
22	R	610	CLA	3	0
22	W	402	CLA	2	0
25	B	847	DGD	6	0
28	H	319	LMG	1	0
27	K	620	LMU	2	0
26	A	845	LHG	1	0
22	A	852	CLA	4	0
22	U	405	CLA	3	0
22	A	806	CLA	4	0
22	U	401	CLA	2	0
22	Q	613	CLA	2	0
22	I	608	CLA	2	0
22	A	807	CLA	1	0
22	R	606	CLA	3	0
22	B	830	CLA	4	0
22	U	404	CLA	2	0
22	W	409	CLA	4	0
22	T	611	CLA	1	0
27	U	424	LMU	1	0
28	B	856	LMG	4	0
26	O	318	LHG	1	0
22	T	608	CLA	2	0
28	F	408	LMG	3	0
22	G	603	CLA	2	0
22	B	819	CLA	1	0
22	A	841	CLA	3	0
22	A	808	CLA	1	0

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	Q	605	CLA	1	0
22	A	805	CLA	2	0
31	W	407	CHL	6	0
22	O	308	CLA	4	0
22	W	404	CLA	2	0
26	L	416	LHG	3	0
22	N	601	CLA	1	0
22	B	823	CLA	3	0
28	Q	602	LMG	2	0
22	Q	604	CLA	5	0
30	K	621	SQD	1	0
22	A	809	CLA	1	0
21	B	846	BCR	1	0
22	A	815	CLA	2	0
25	F	401	DGD	2	0
22	A	827	CLA	2	0
22	F	403	CLA	2	0
31	V	606	CHL	14	0
22	B	832	CLA	3	0
22	A	817	CLA	2	0
22	A	804	CLA	3	0
22	A	816	CLA	2	0
22	T	604	CLA	1	0
21	A	851	BCR	3	0
27	U	421	LMU	1	0
22	A	842	CLA	4	0
22	S	604	CLA	1	0
22	H	310	CLA	1	0
26	R	614	LHG	3	0
21	A	849	BCR	3	0
32	V	616	NEX	9	0
26	P	601	LHG	1	0
22	O	315	CLA	2	0
22	P	607	CLA	1	0
21	B	844	BCR	5	0
22	A	821	CLA	1	0
22	K	607	CLA	9	0
22	K	609	CLA	2	0
22	K	603	CLA	2	0
27	M	102	LMU	1	0
22	R	605	CLA	5	0
31	W	408	CHL	8	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Clashes	Symm-Clashes
28	K	601	LMG	3	0
22	G	610	CLA	1	0
22	X	404	CLA	1	0
22	N	602	CLA	1	0
31	V	605	CHL	12	0
21	B	801	BCR	8	0
22	B	838	CLA	3	0
22	Q	611	CLA	1	0
22	L	410	CLA	3	0
22	B	814	CLA	1	0
22	Q	609	CLA	1	0
22	R	611	CLA	2	0
22	P	610	CLA	1	0
22	T	605	CLA	4	0
22	B	809	CLA	4	0
22	O	314	CLA	1	0
26	W	420	LHG	2	0
22	B	811	CLA	1	0
22	I	606	CLA	2	0
21	J	103	BCR	1	0
22	B	859	CLA	2	0
22	K	608	CLA	4	0
22	Q	612	CLA	1	0
22	O	312	CLA	1	0
28	J	101	LMG	1	0
31	U	407	CHL	3	0
22	B	836	CLA	2	0
22	Q	608	CLA	3	0
22	A	832	CLA	3	0
22	A	840	CLA	3	0
22	R	601	CLA	6	0
22	R	615	CLA	2	0
26	O	321	LHG	3	0
22	A	822	CLA	3	0
22	T	607	CLA	1	0
22	H	307	CLA	1	0
26	A	846	LHG	2	0
22	K	617	CLA	2	0
22	I	602	CLA	1	0
22	V	617	CLA	1	0
22	B	805	CLA	1	0
22	A	814	CLA	4	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Clashes	Symm-Clashes
26	Q	616	LHG	1	0
22	O	310	CLA	1	0
22	P	602	CLA	2	0
22	A	831	CLA	2	0
22	W	406	CLA	3	0
22	U	411	CLA	1	0
22	B	839	CLA	2	0
22	G	611	CLA	1	0
22	S	608	CLA	2	0
22	W	413	CLA	2	0
22	A	833	CLA	1	0
22	N	610	CLA	3	0
22	S	609	CLA	1	0
24	Q	614	DD6	1	0
27	L	419	LMU	4	0
22	S	601	CLA	1	0
22	Q	603	CLA	1	0
22	R	602	CLA	4	0
22	O	313	CLA	3	0
27	L	420	LMU	2	0
22	I	601	CLA	2	0
22	B	812	CLA	1	0
22	I	603	CLA	3	0
22	V	603	CLA	2	0
22	G	609	CLA	3	0
22	B	828	CLA	2	0
28	U	423	LMG	2	0
21	B	842	BCR	2	0
22	K	605	CLA	3	0
30	V	618	SQD	1	0
22	A	839	CLA	1	0
21	B	845	BCR	2	0
22	O	305	CLA	1	0
22	L	406	CLA	1	0
22	A	828	CLA	4	0
23	B	840	PQN	1	0
22	V	613	CLA	1	0
22	V	601	CLA	4	0
32	U	418	NEX	4	0
22	A	838	CLA	3	0
22	A	801	CLA	1	0
22	B	804	CLA	2	0

*Continued on next page...*

*Continued from previous page...*

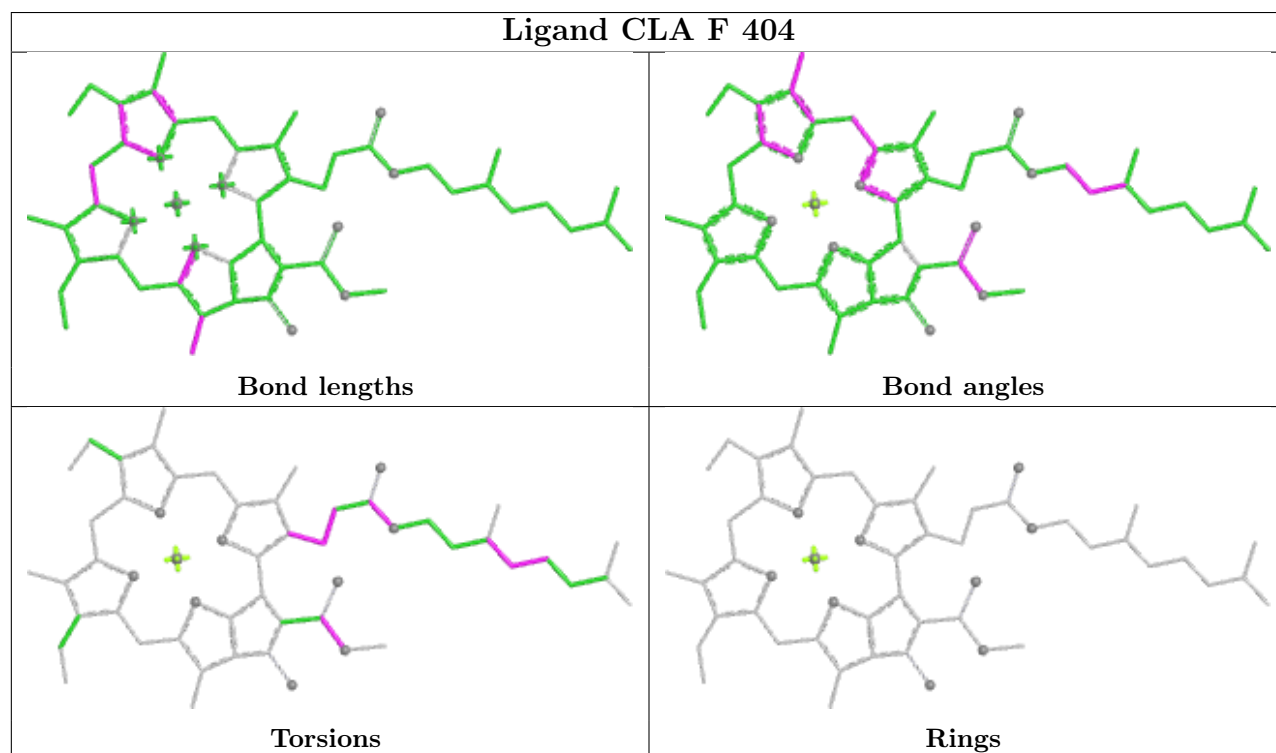
Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	B	816	CLA	2	0
22	B	825	CLA	3	0
22	L	409	CLA	2	0
22	K	611	CLA	3	0
22	L	404	CLA	6	0
28	N	615	LMG	1	0
22	P	605	CLA	1	0
22	G	602	CLA	1	0
22	I	611	CLA	4	0
24	B	841	DD6	1	0
22	B	820	CLA	1	0
22	O	309	CLA	3	0
27	O	301	LMU	4	0
22	L	412	CLA	3	0
22	H	305	CLA	1	0
22	B	827	CLA	1	0
22	A	823	CLA	1	0
22	N	603	CLA	2	0
22	L	408	CLA	12	0
22	P	603	CLA	1	0
22	V	604	CLA	7	0
22	B	818	CLA	1	0
27	B	858	LMU	1	0
22	X	409	CLA	1	0
22	A	812	CLA	3	0
23	A	843	PQN	2	0
22	Q	607	CLA	2	0
27	A	857	LMU	1	0
22	Q	610	CLA	2	0
22	B	834	CLA	5	0
22	B	815	CLA	3	0
22	X	408	CLA	1	0
22	A	829	CLA	1	0
26	N	614	LHG	1	0
22	W	414	CLA	1	0
22	U	406	CLA	1	0
22	B	802	CLA	2	0
22	Q	601	CLA	1	0
33	A	802	CL0	6	0
22	A	836	CLA	2	0
22	B	803	CLA	2	0
22	X	419	CLA	2	0

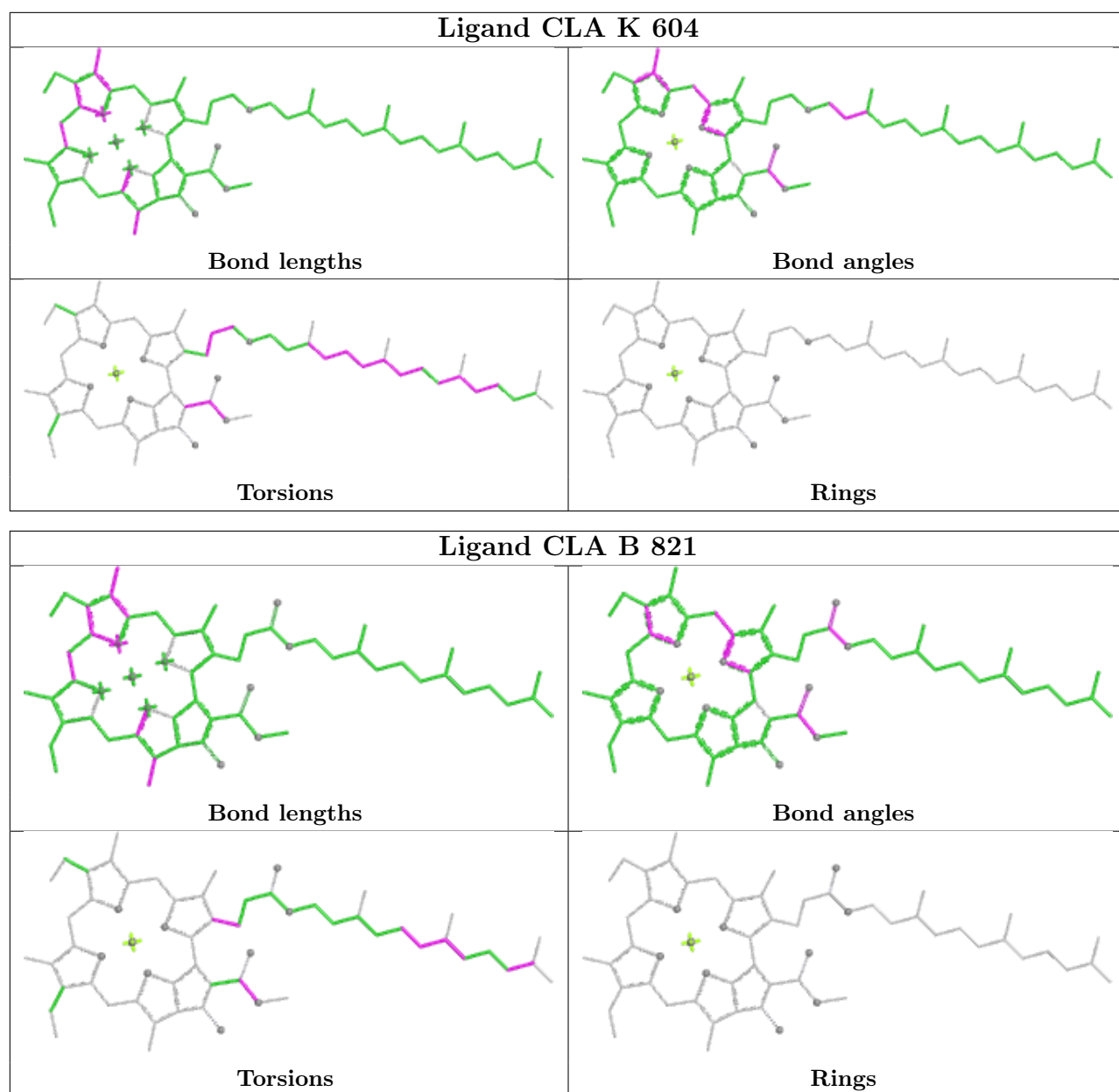
*Continued on next page...*

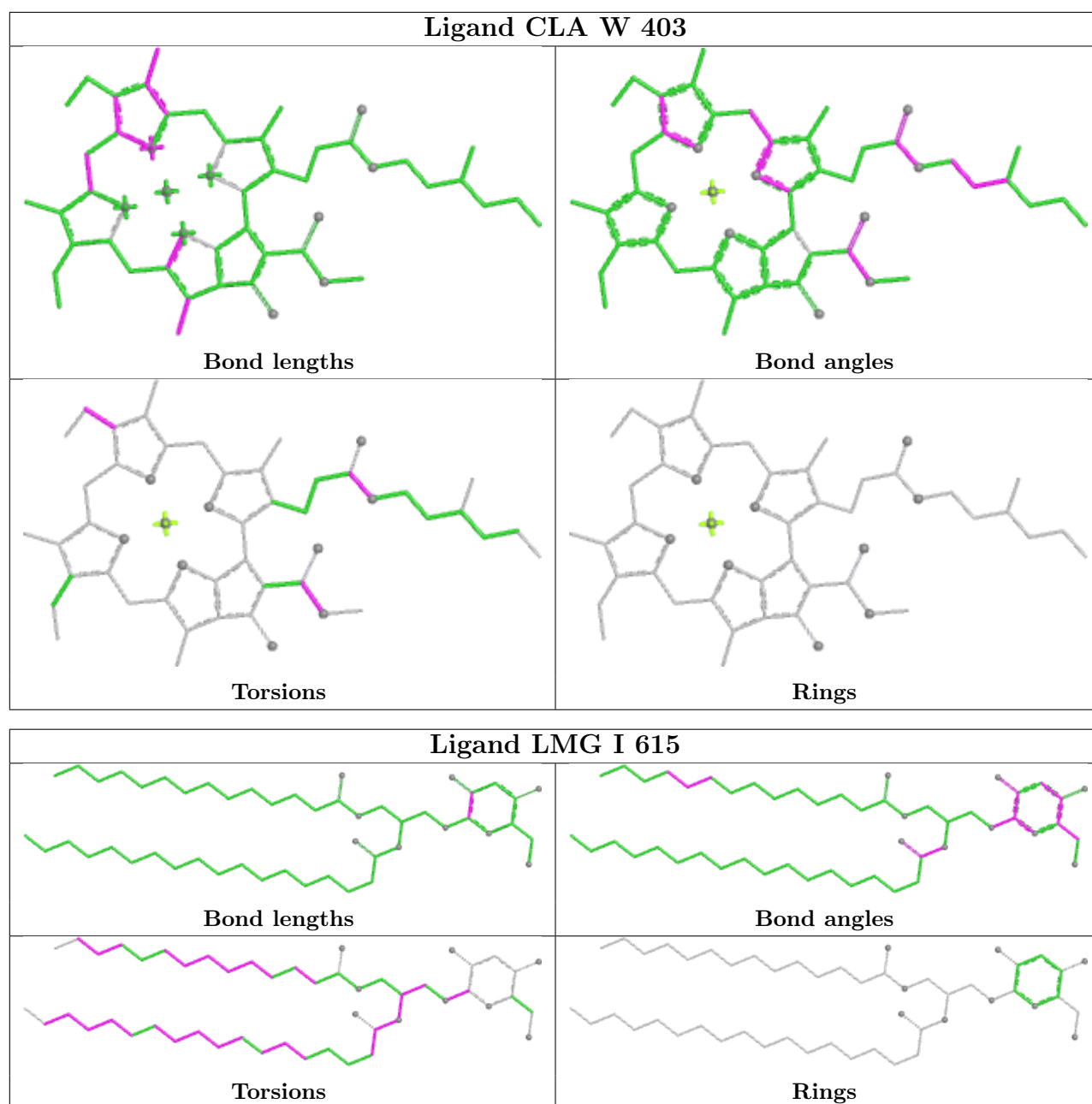
*Continued from previous page...*

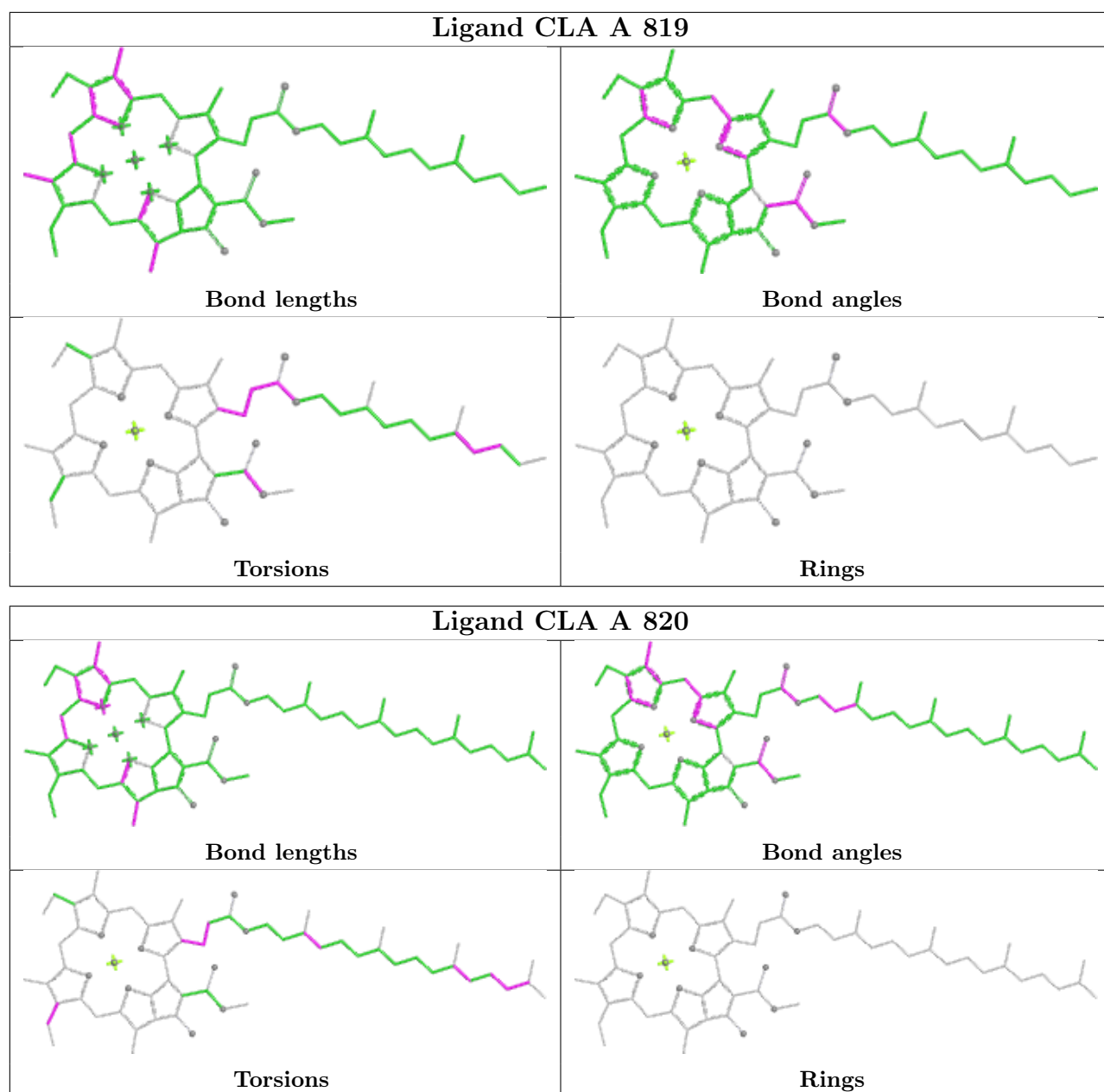
Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	A	830	CLA	1	0
28	U	402	LMG	2	0
22	L	417	CLA	7	0
22	A	825	CLA	2	0
22	O	307	CLA	1	0
26	B	851	LHG	7	0
30	O	302	SQD	8	0
22	A	834	CLA	1	0
22	S	607	CLA	1	0
22	U	409	CLA	1	0
22	U	412	CLA	1	0

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

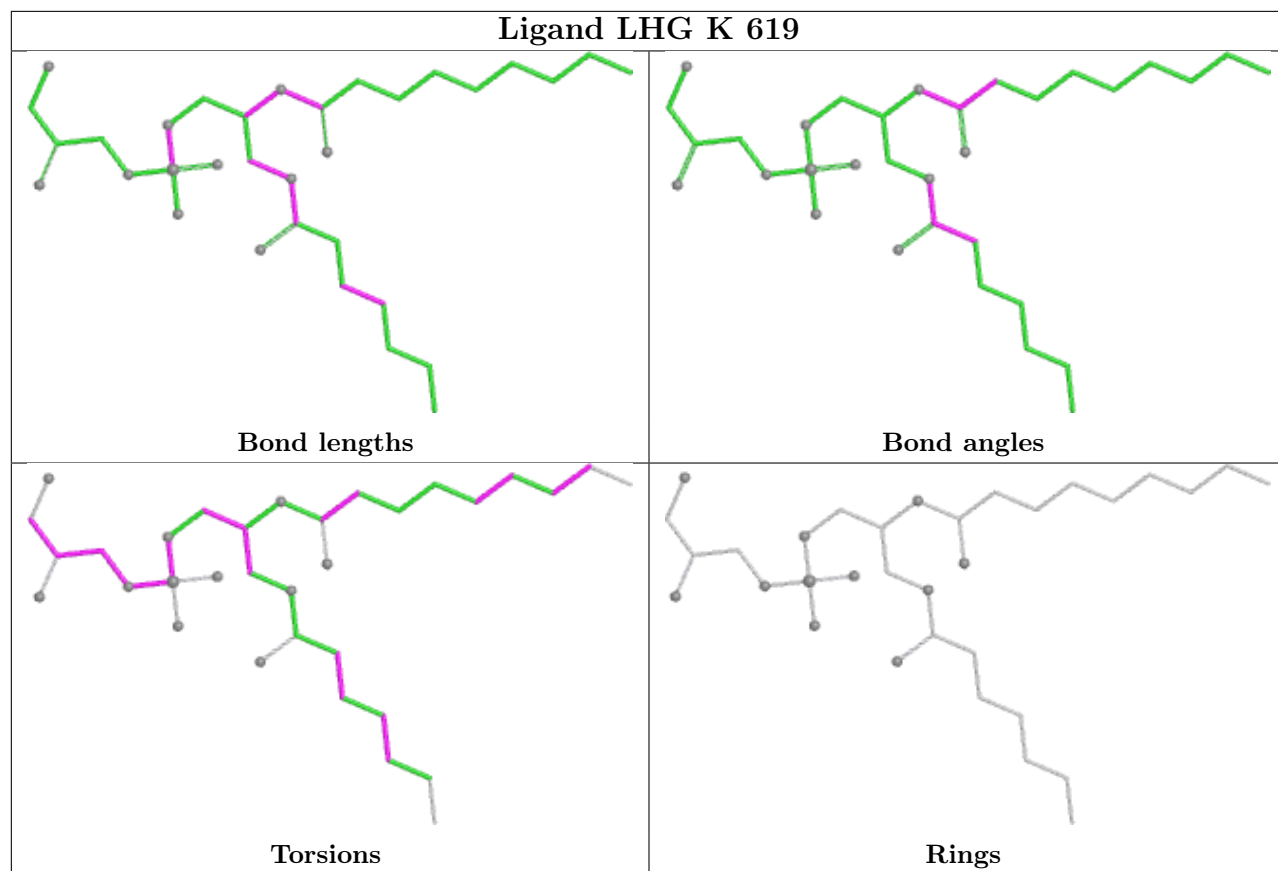




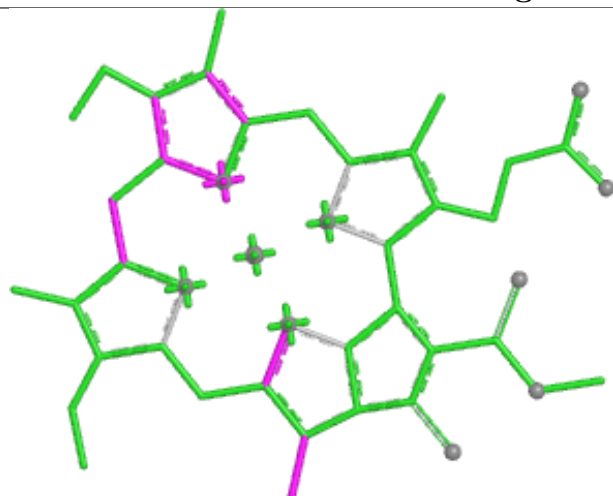








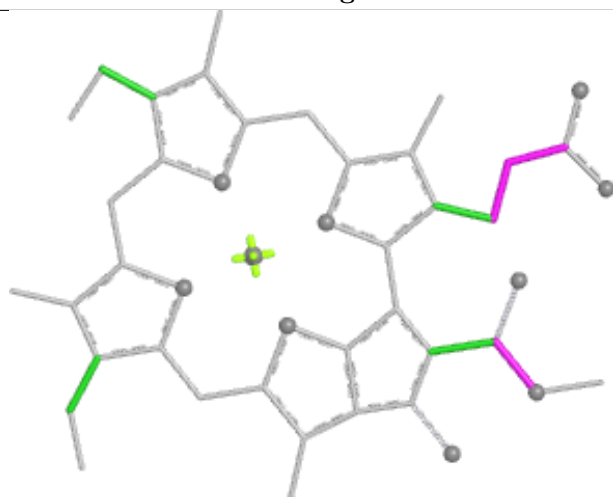
## Ligand CLA P 604



Bond lengths



Bond angles

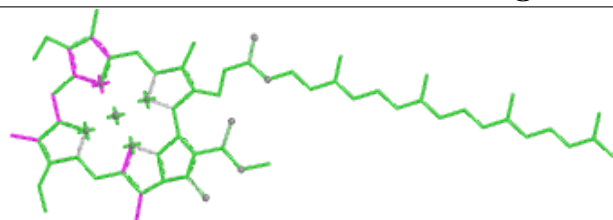


Torsions

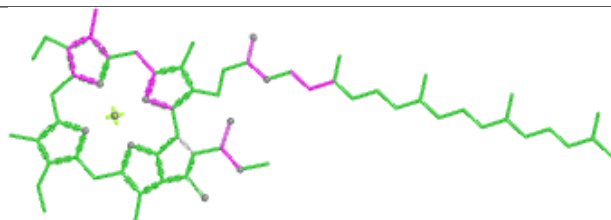


Rings

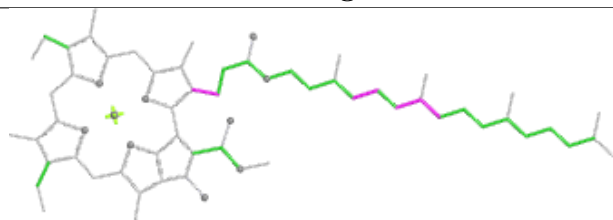
## Ligand CLA B 831



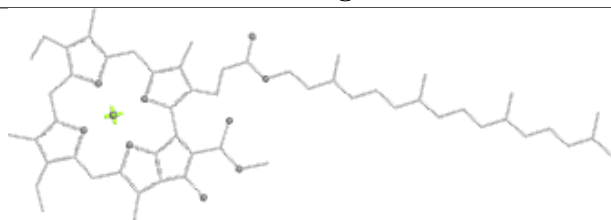
Bond lengths



Bond angles

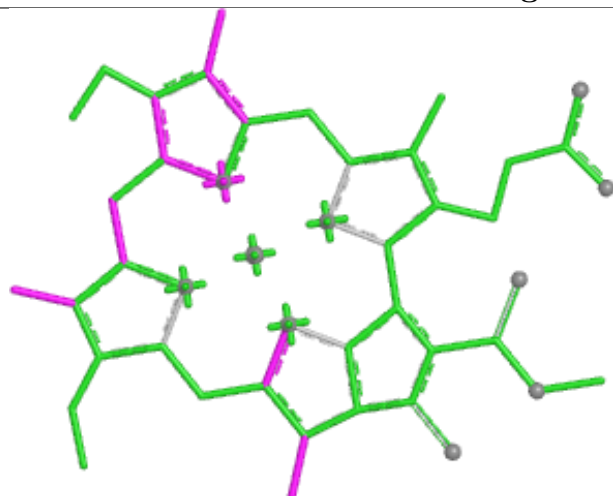


Torsions



Rings

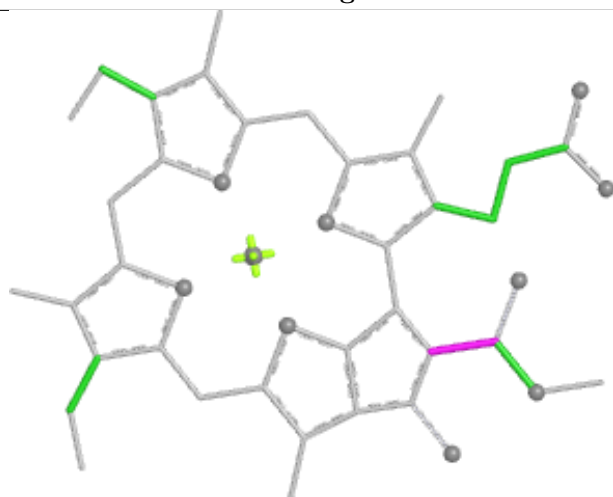
## Ligand CLA I 604



Bond lengths



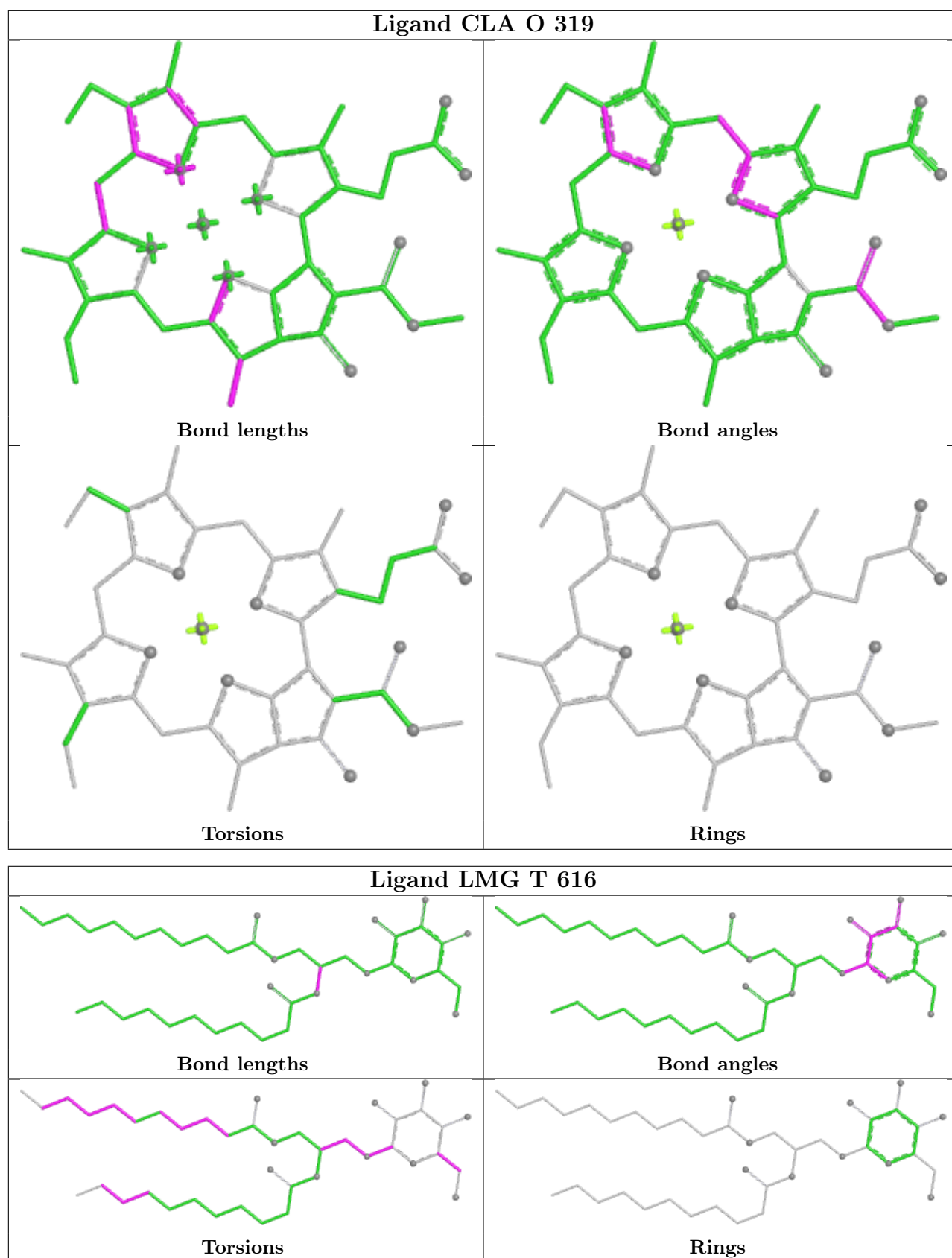
Bond angles

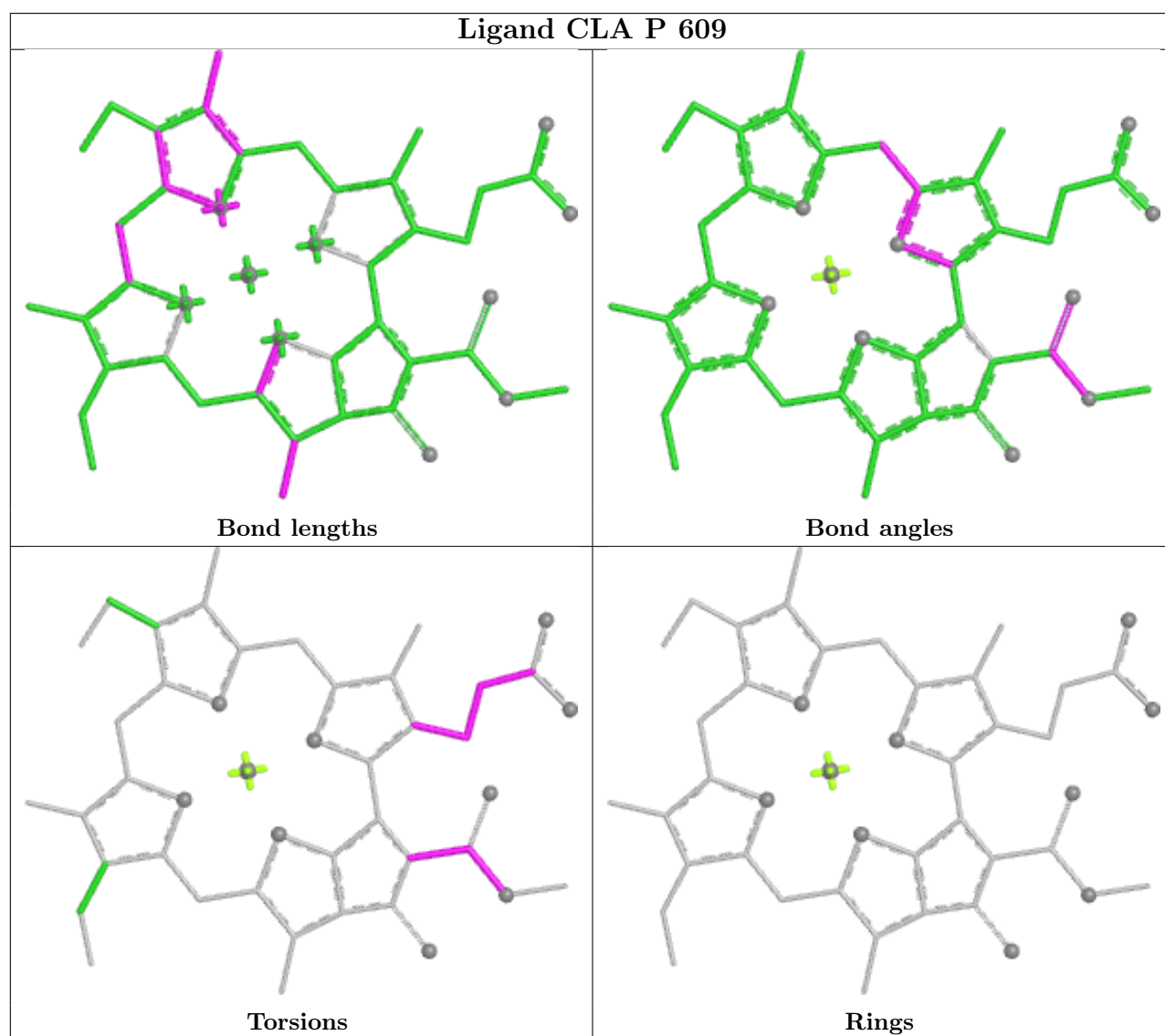
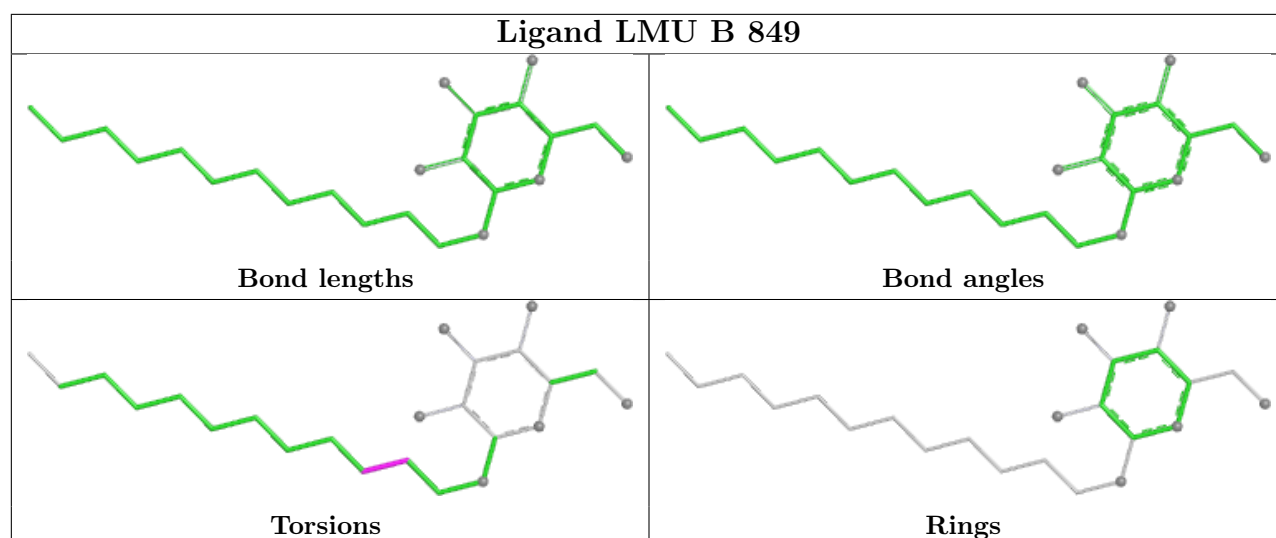


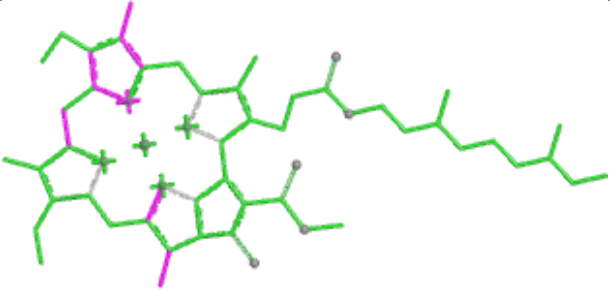
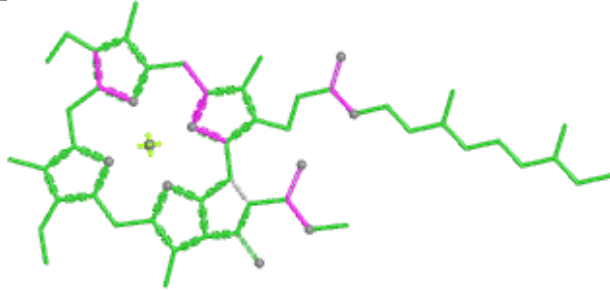
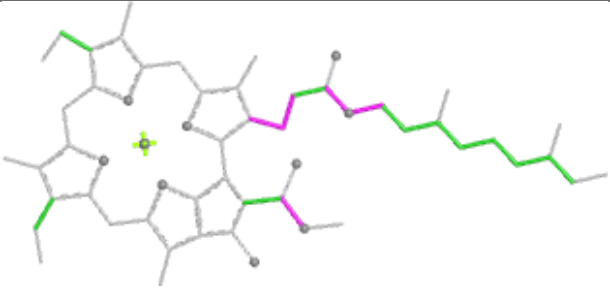
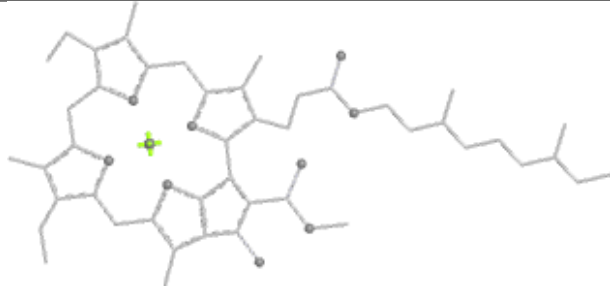
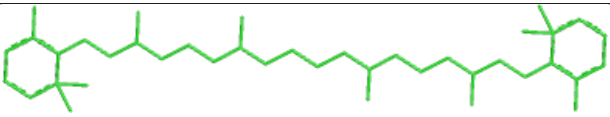
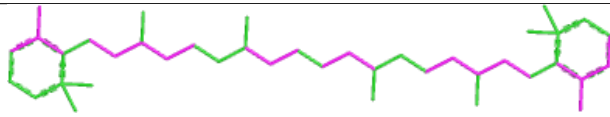
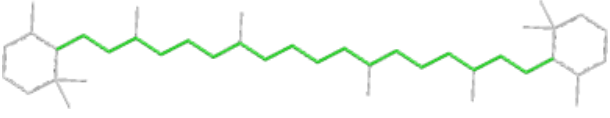
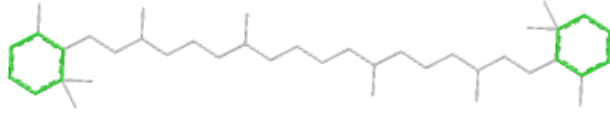
Torsions



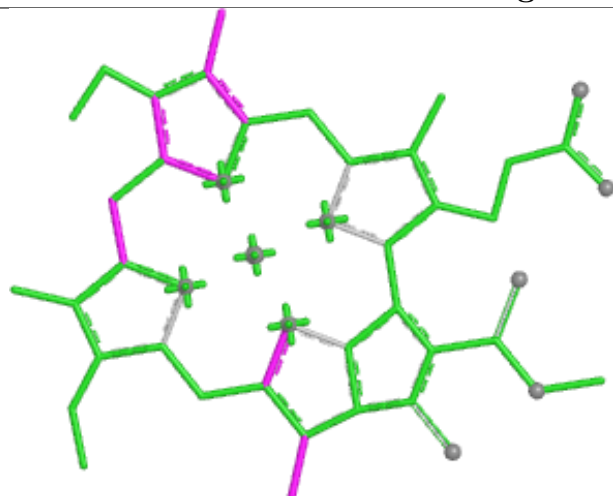
Rings



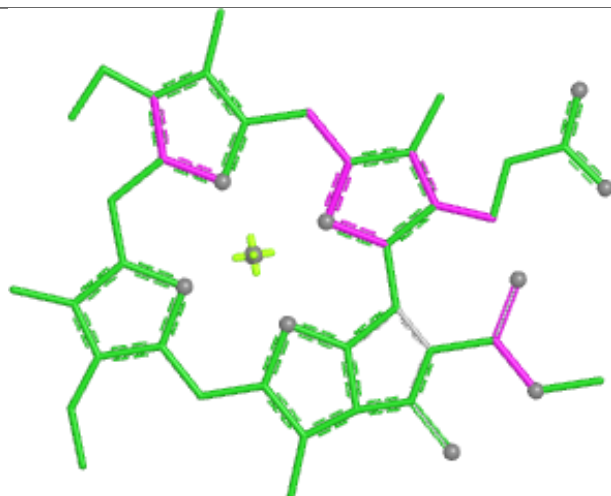


Ligand CLA X 405	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>
Ligand BCR A 848	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>

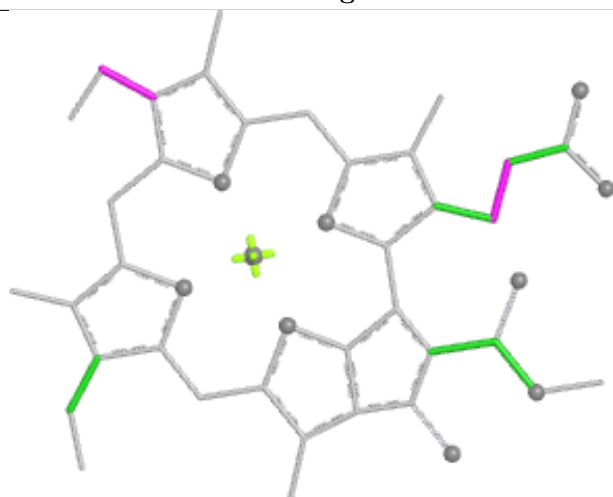
## Ligand CLA S 610



Bond lengths



Bond angles

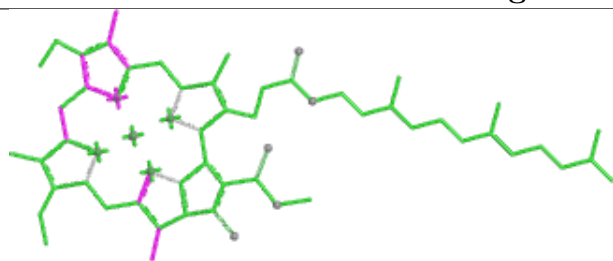


Torsions

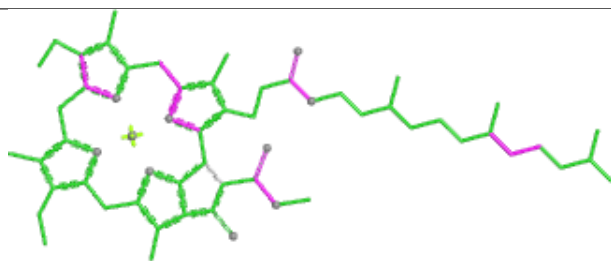


Rings

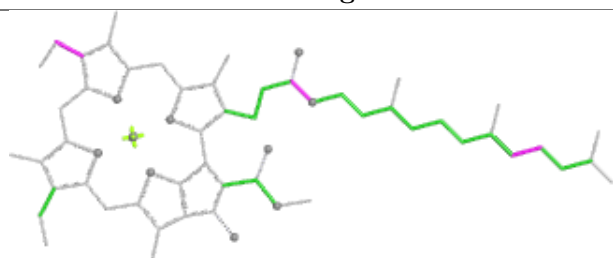
## Ligand CLA W 412



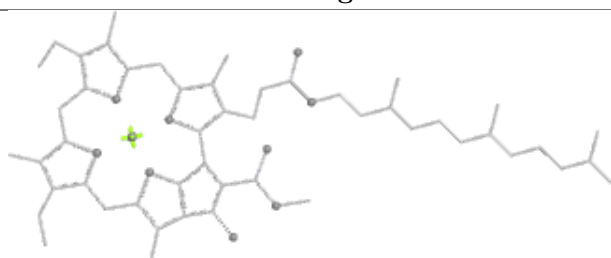
Bond lengths



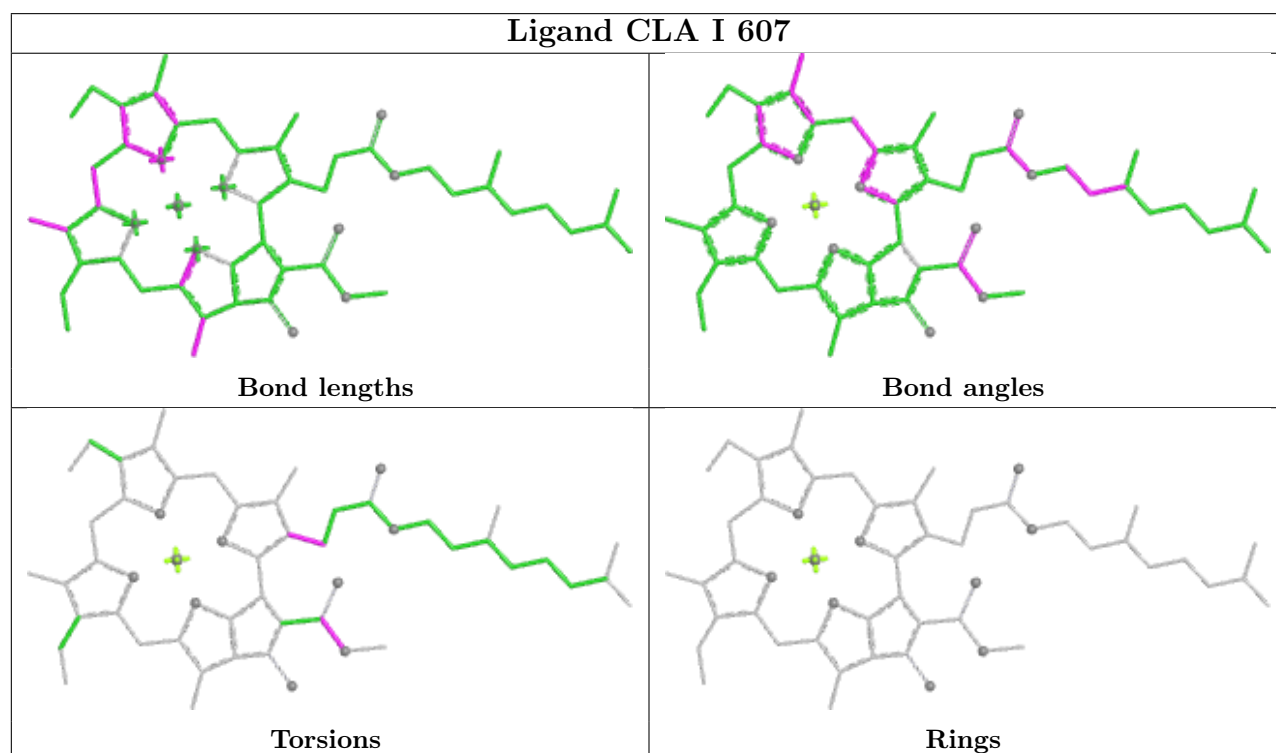
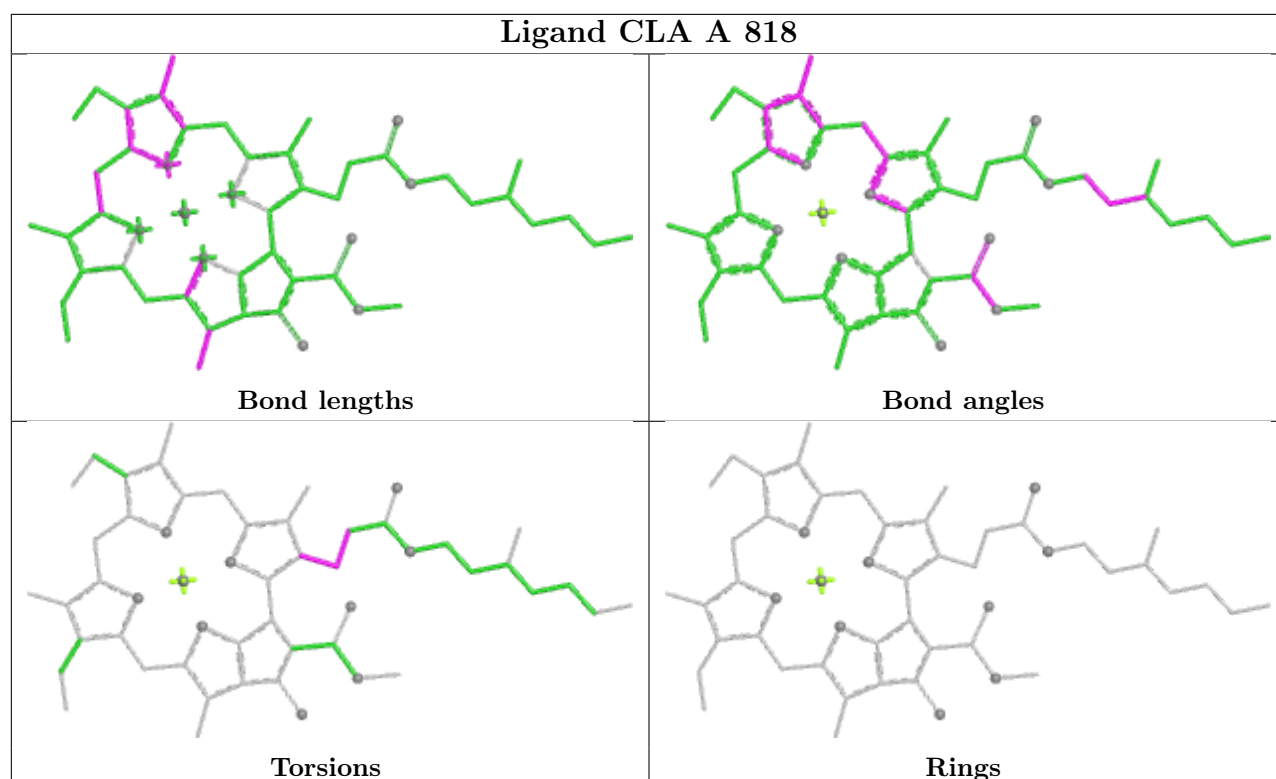
Bond angles



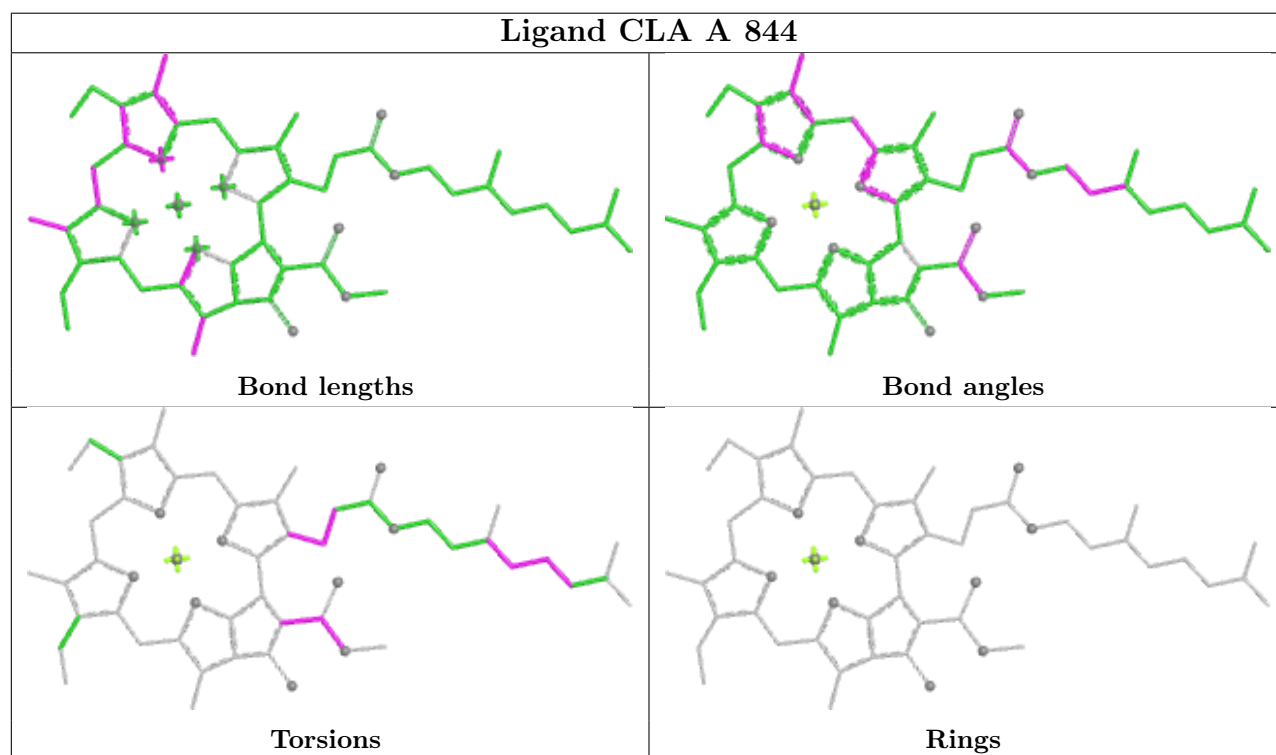
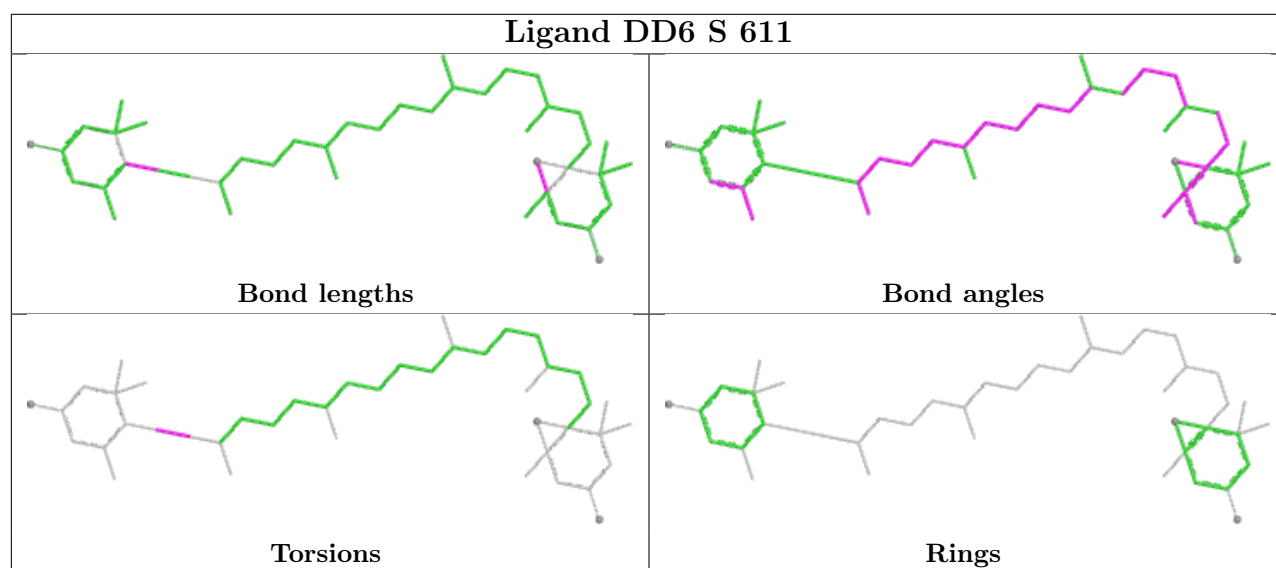
Torsions

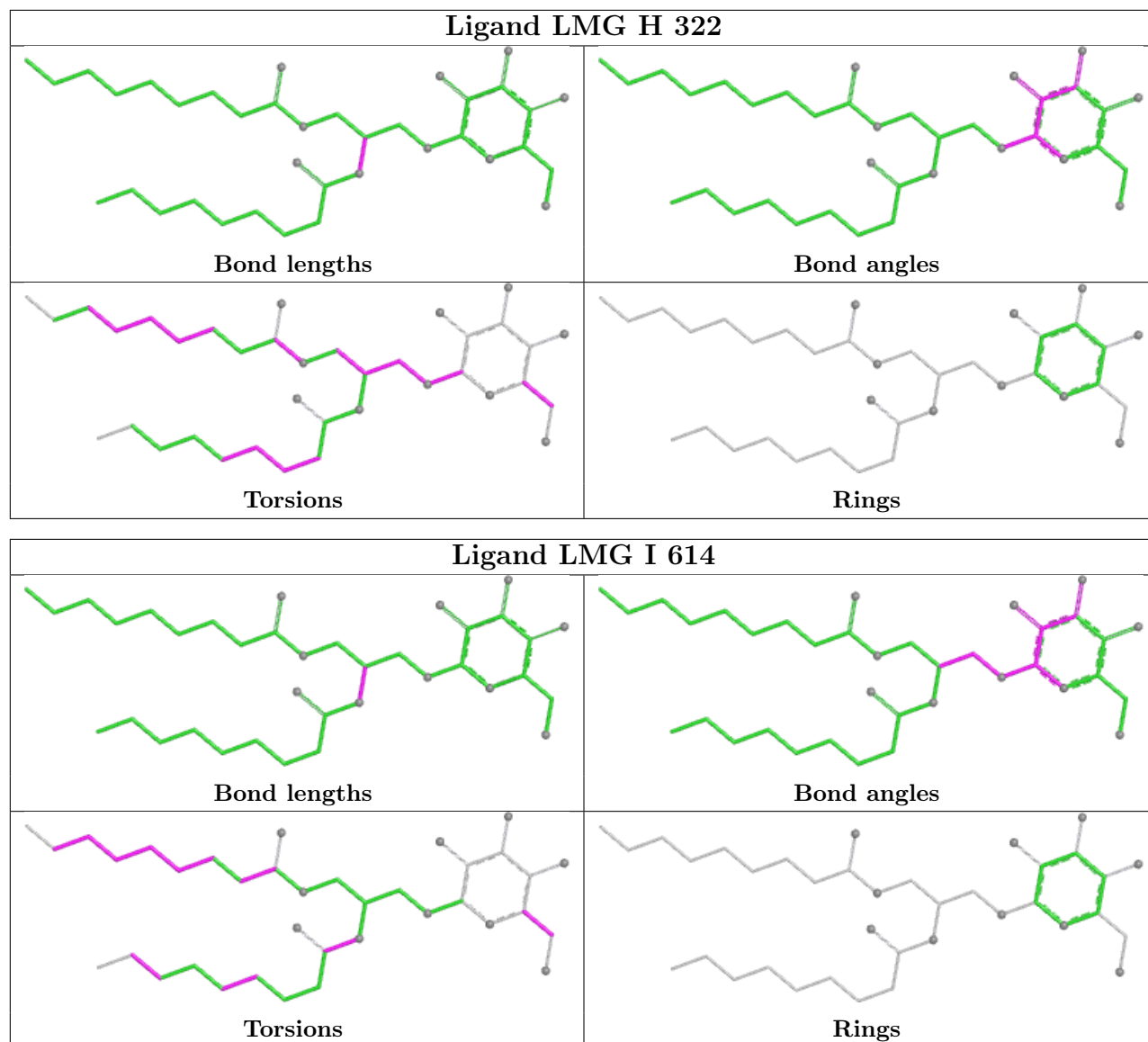


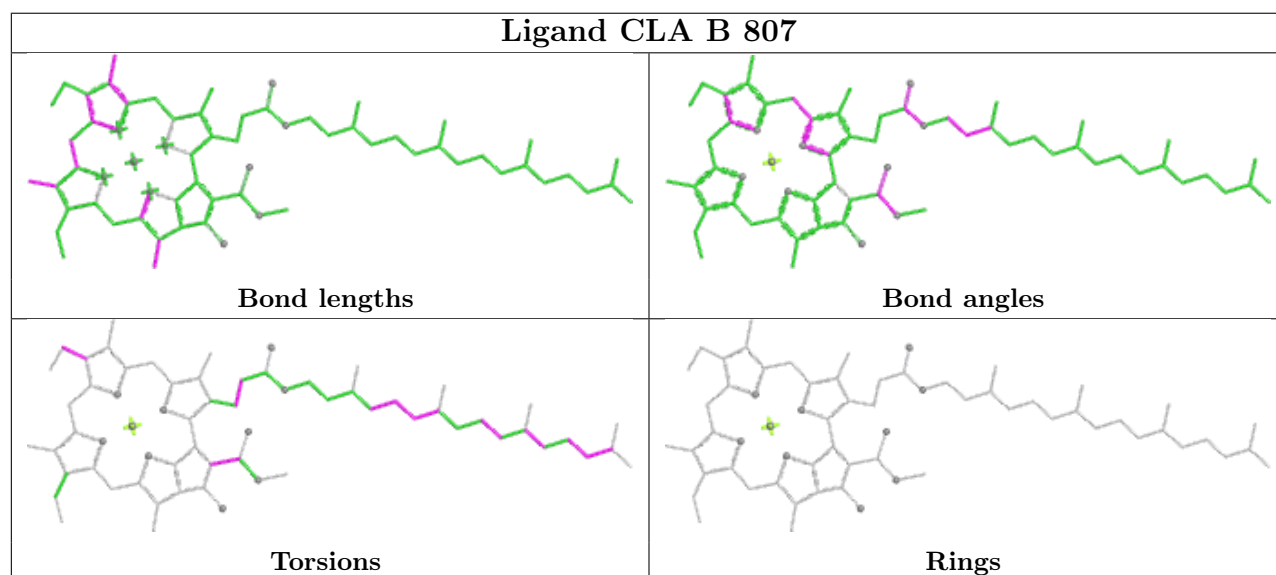
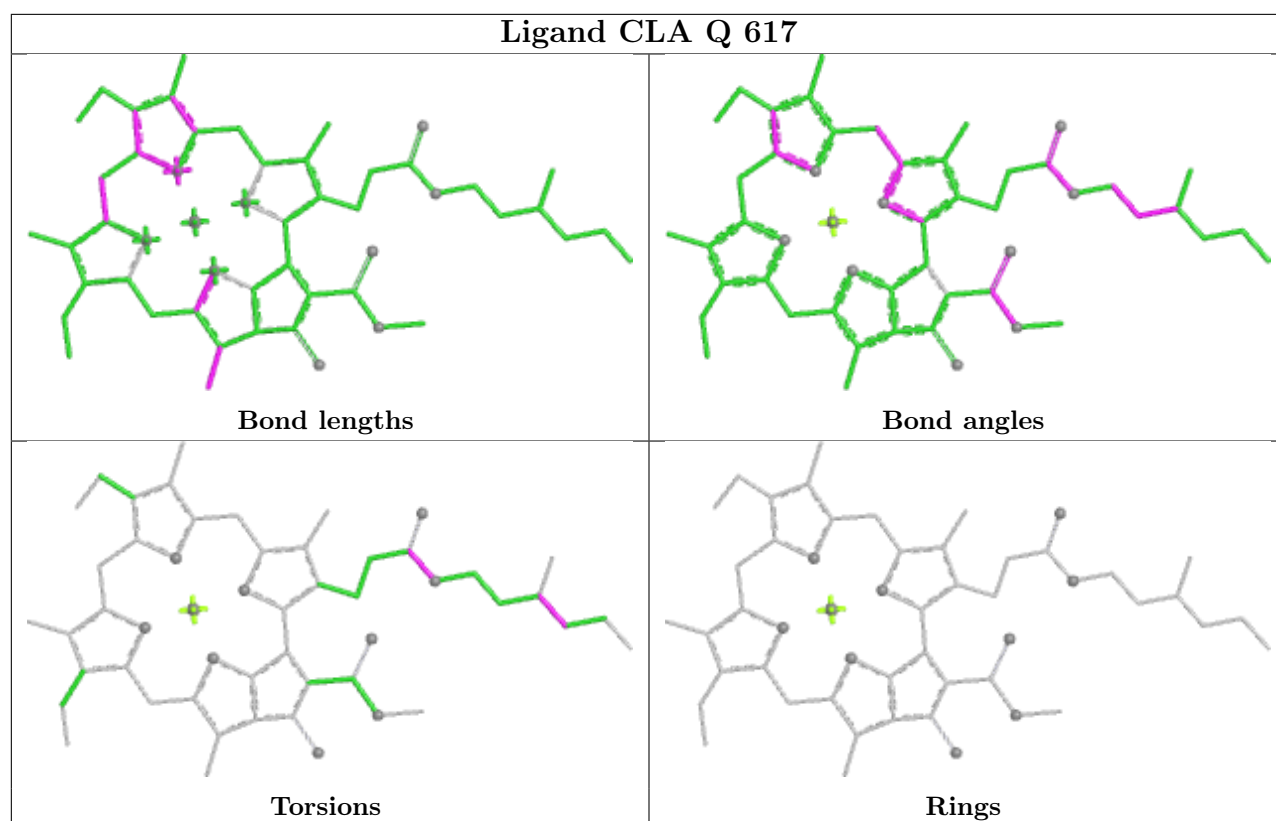
Rings

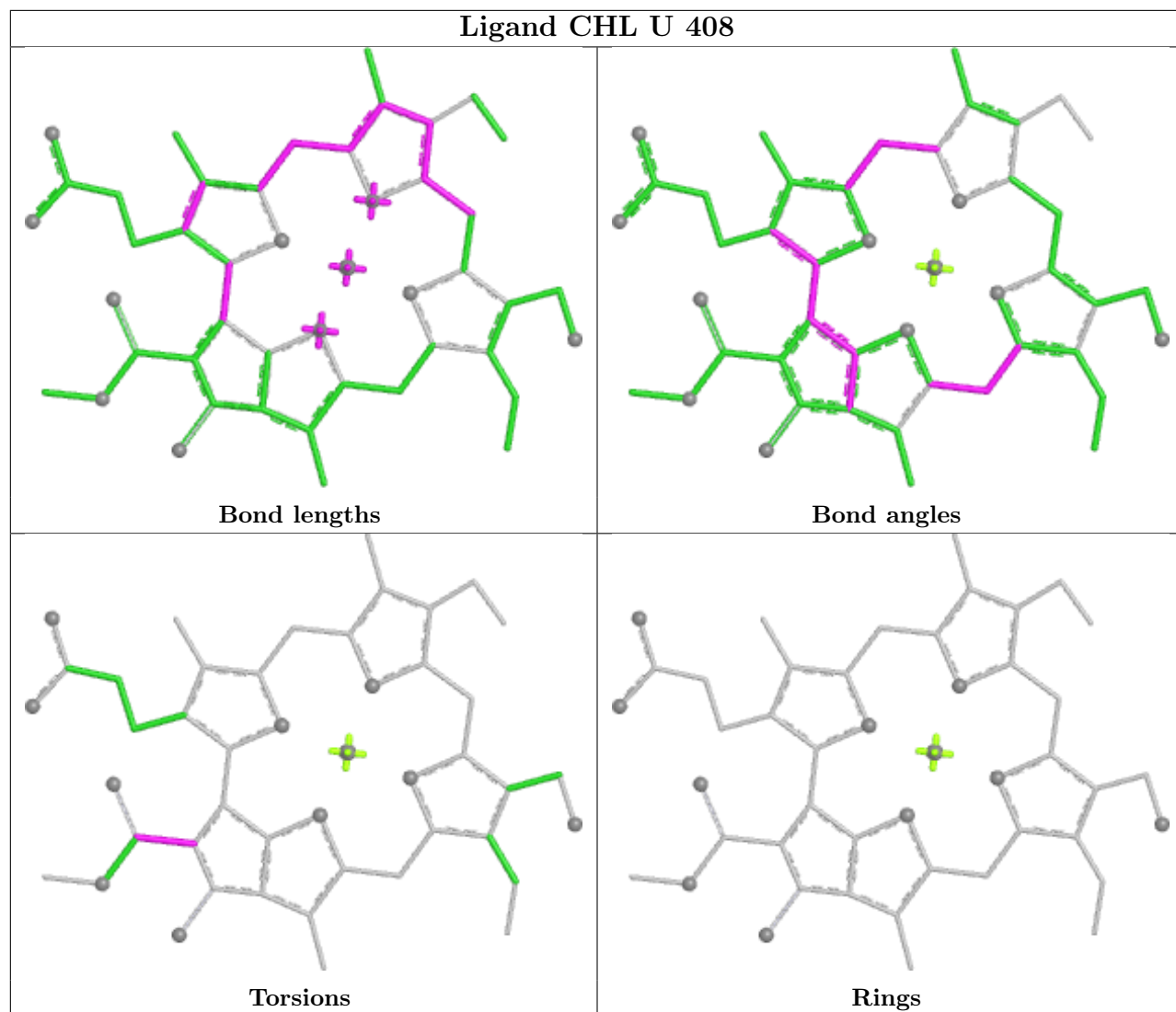




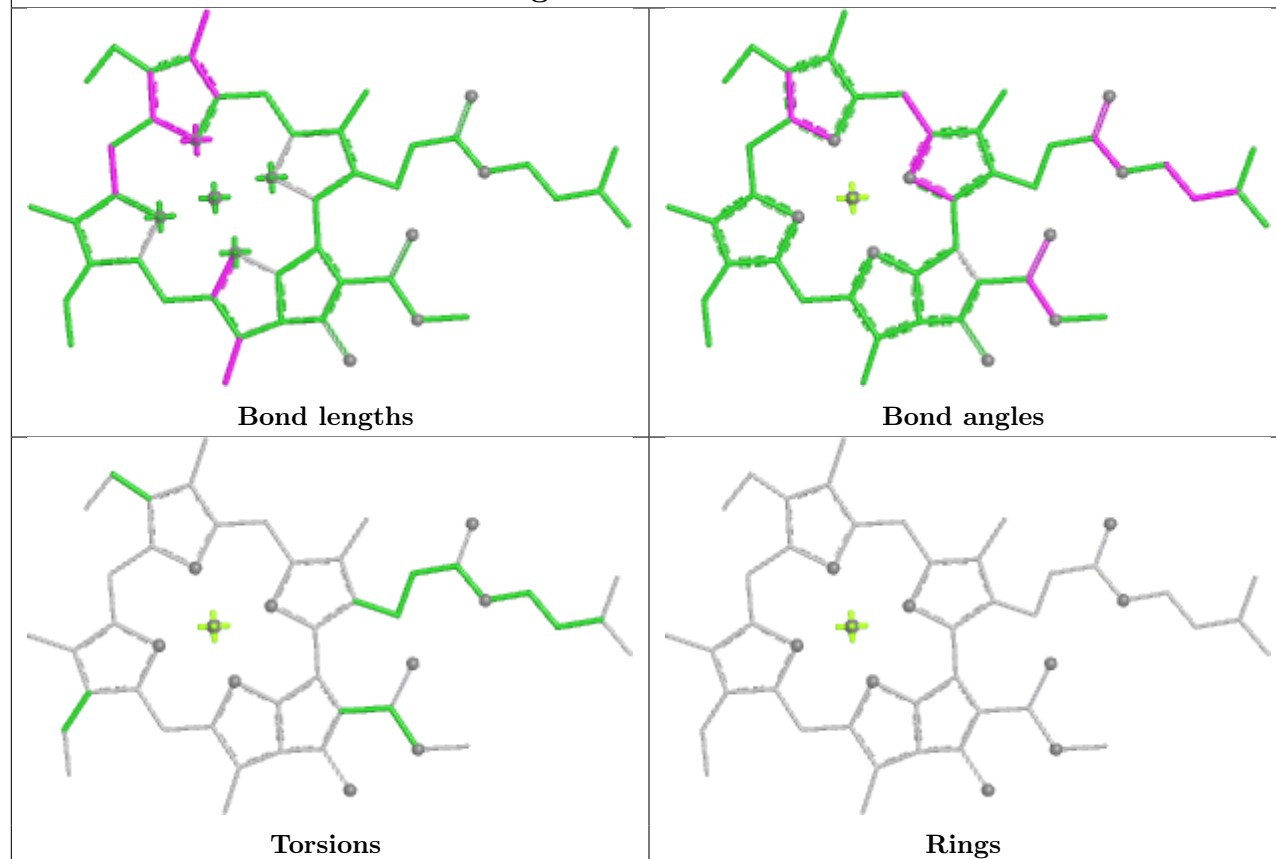




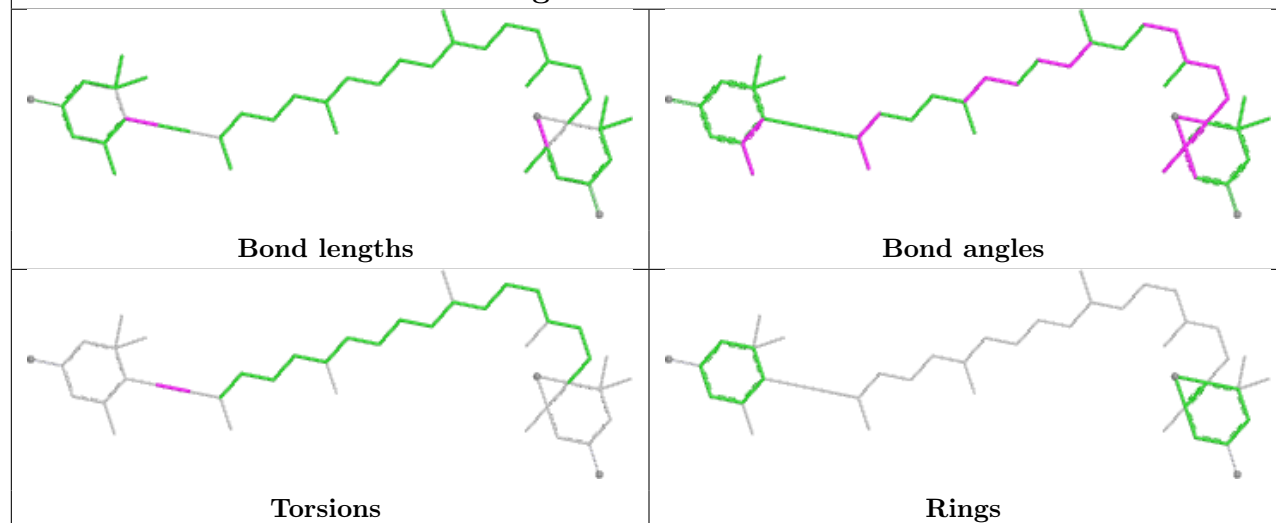


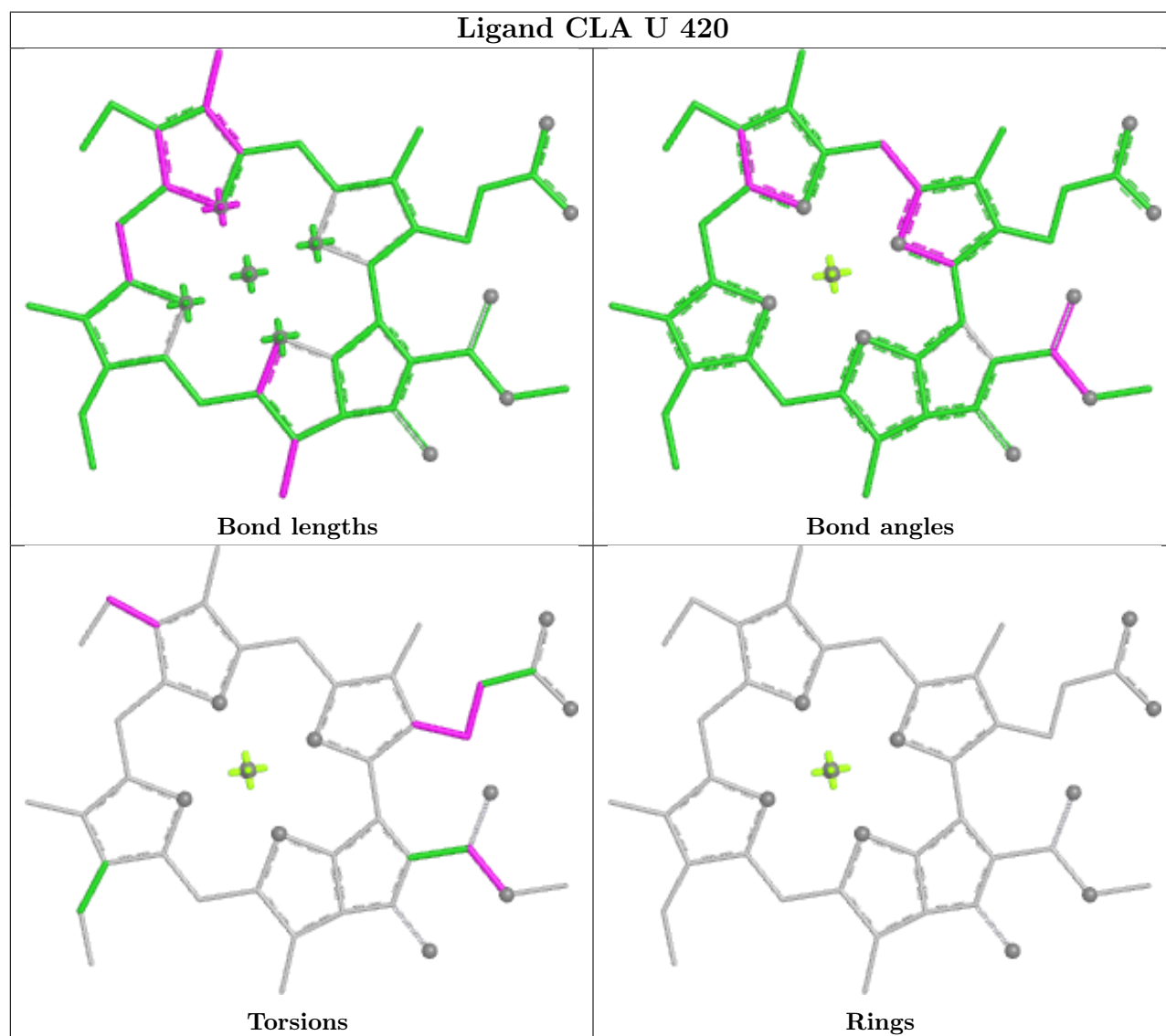
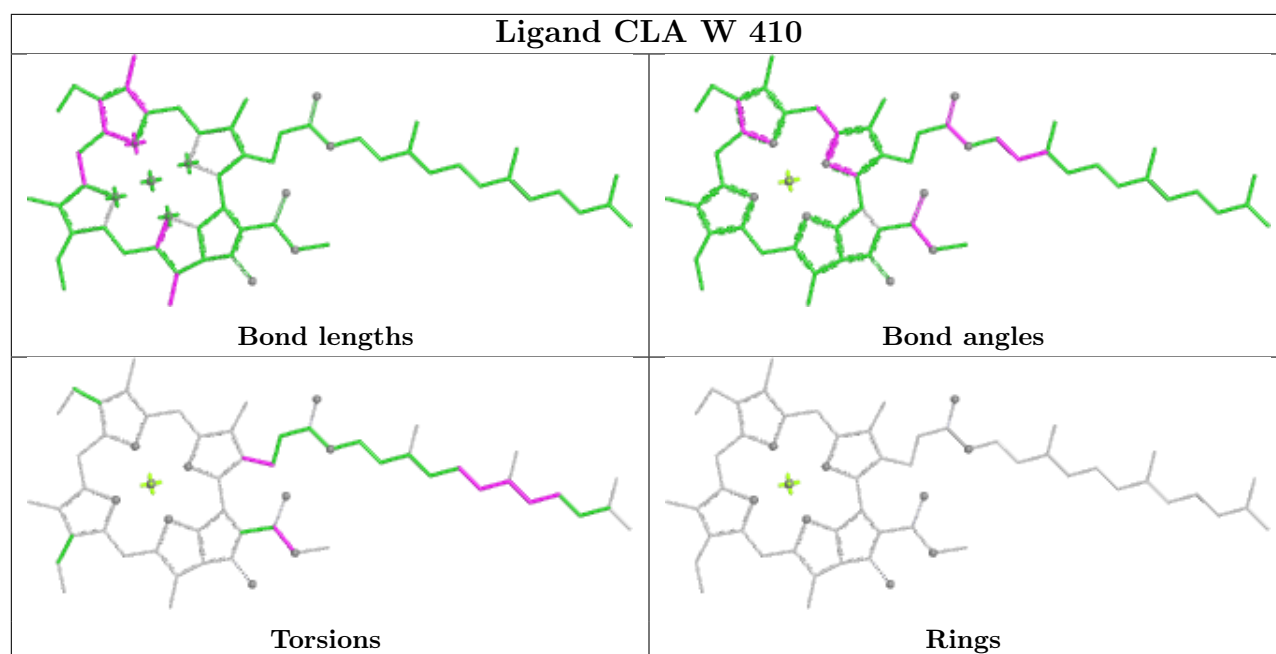


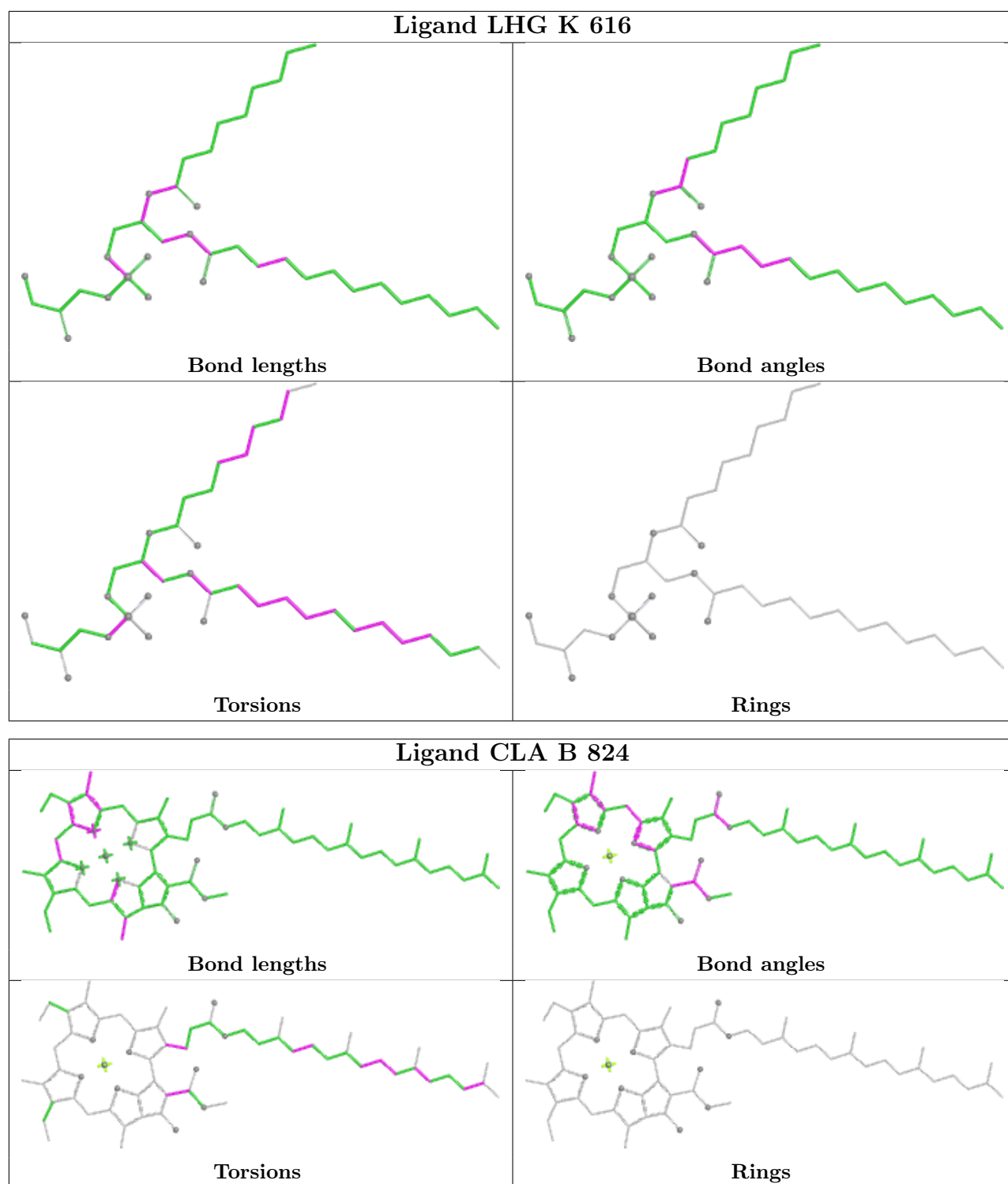
## Ligand CLA K 606



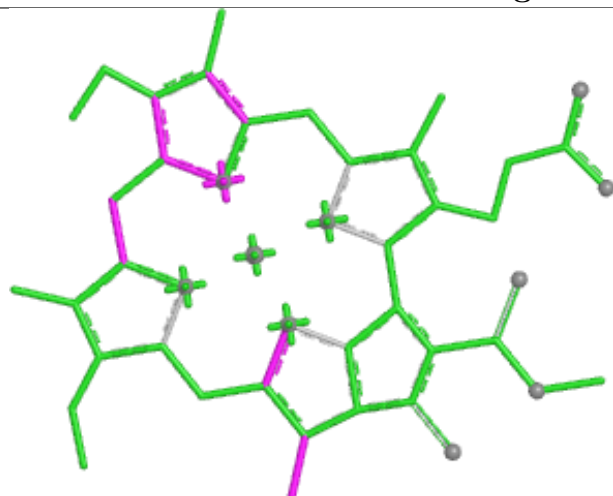
## Ligand DD6 U 416



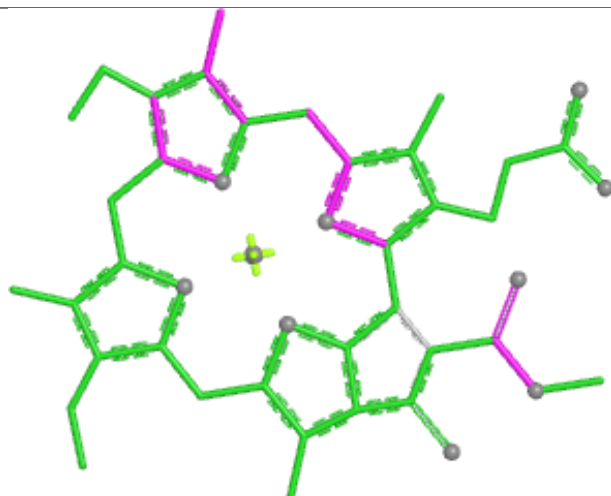




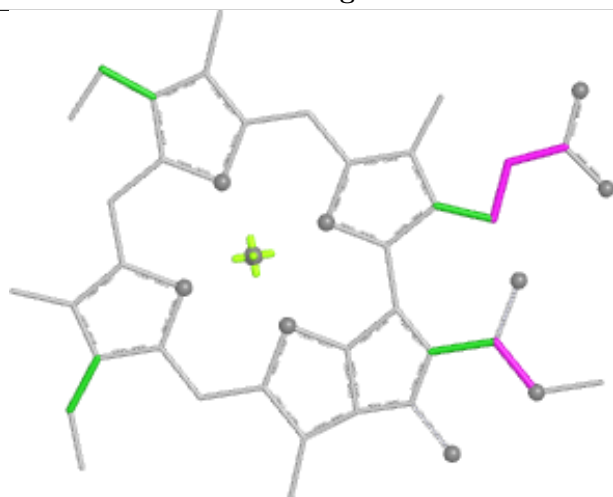
## Ligand CLA R 604



Bond lengths



Bond angles

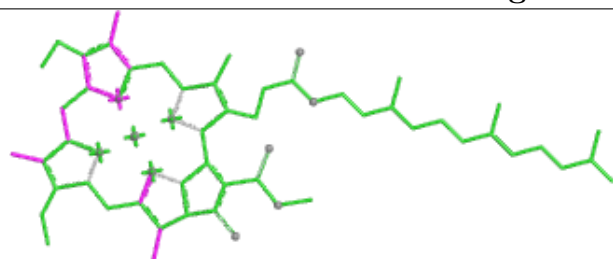


Torsions

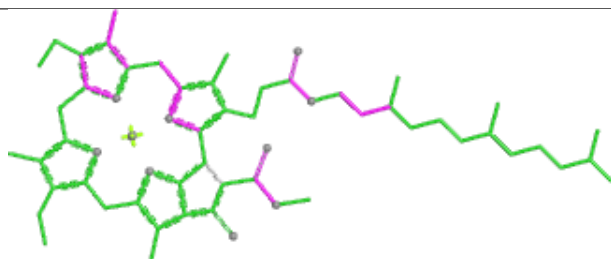


Rings

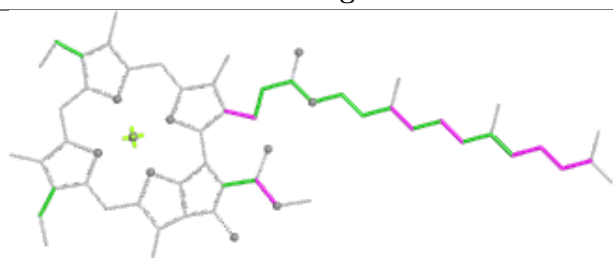
## Ligand CLA W 411



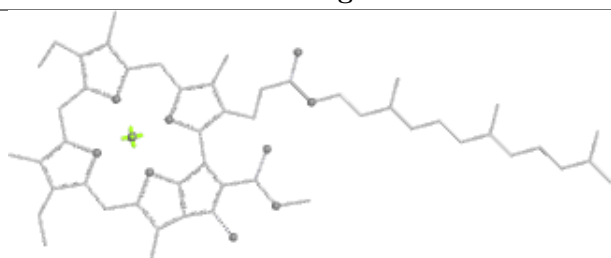
Bond lengths



Bond angles

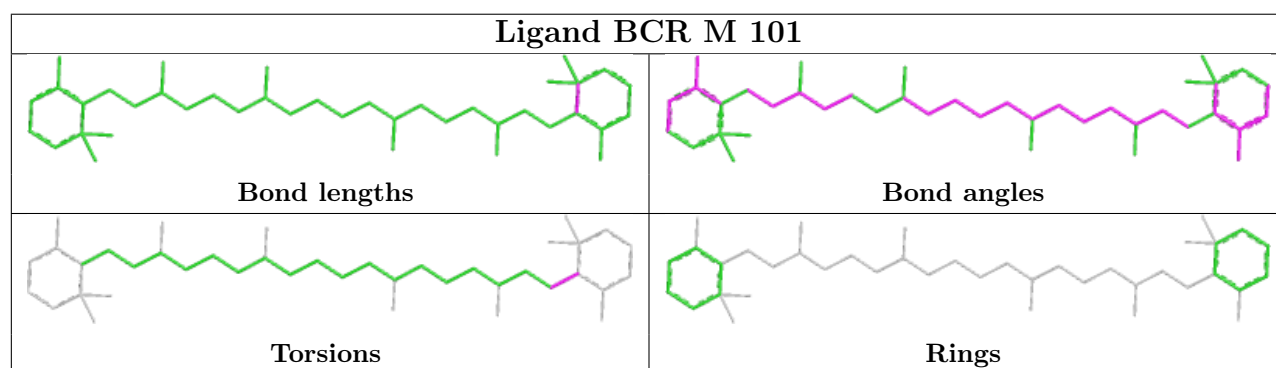
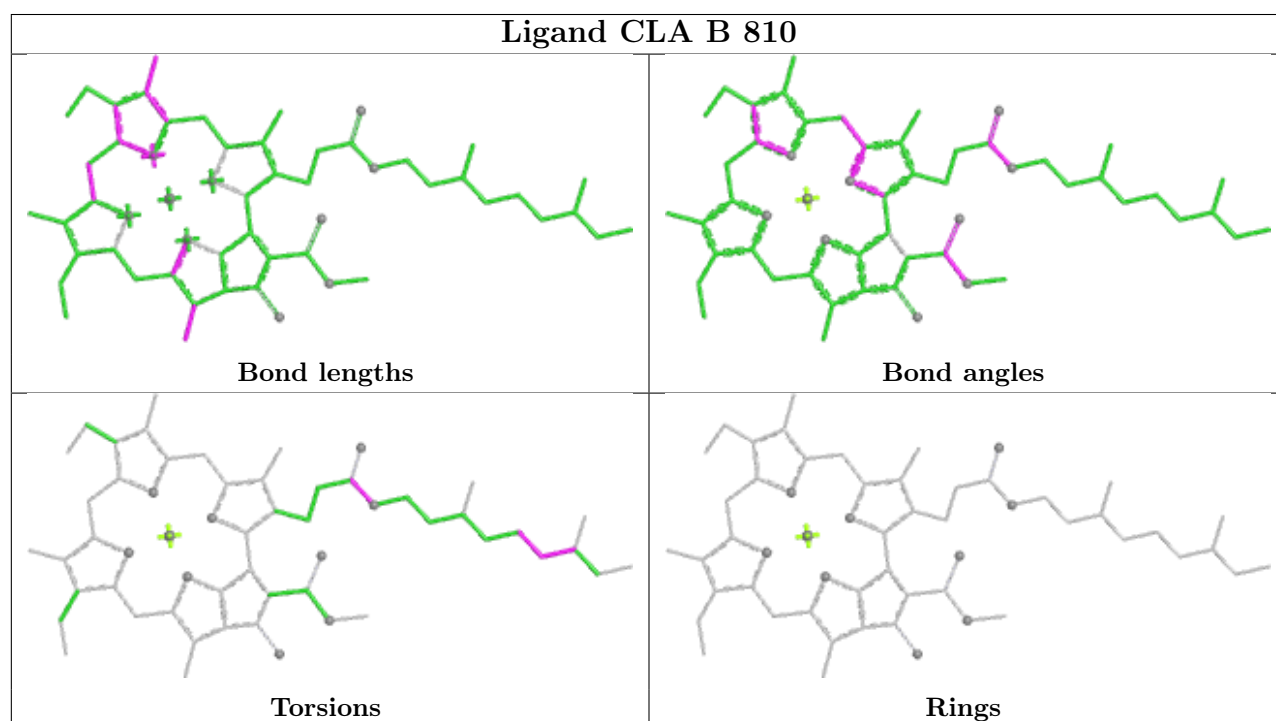
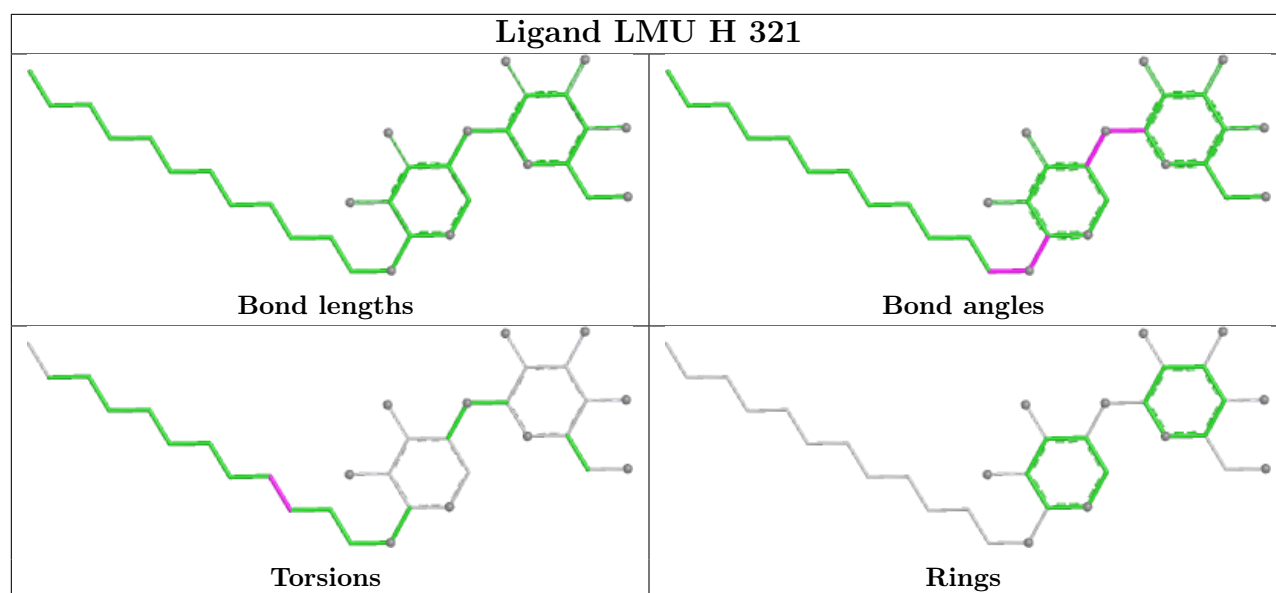


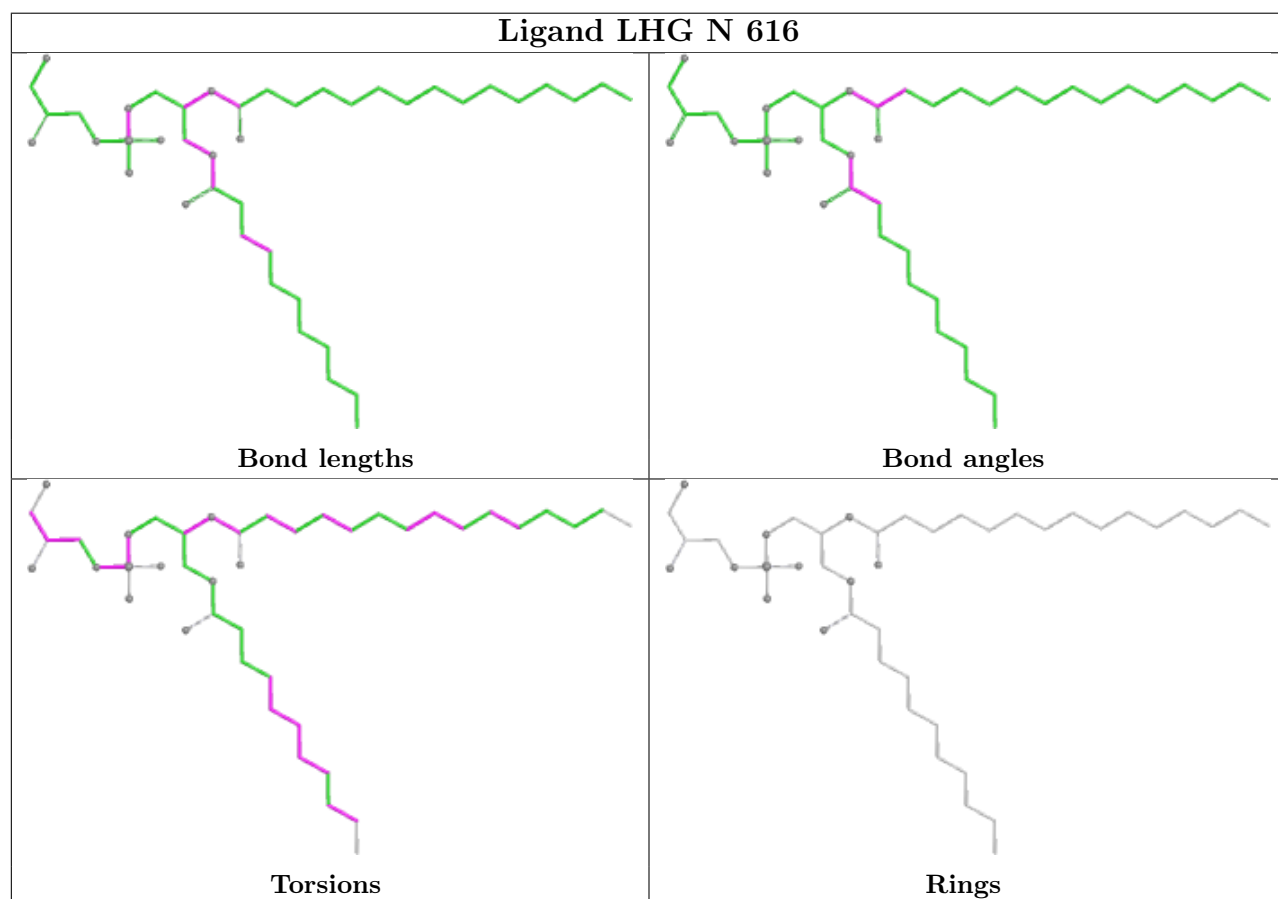
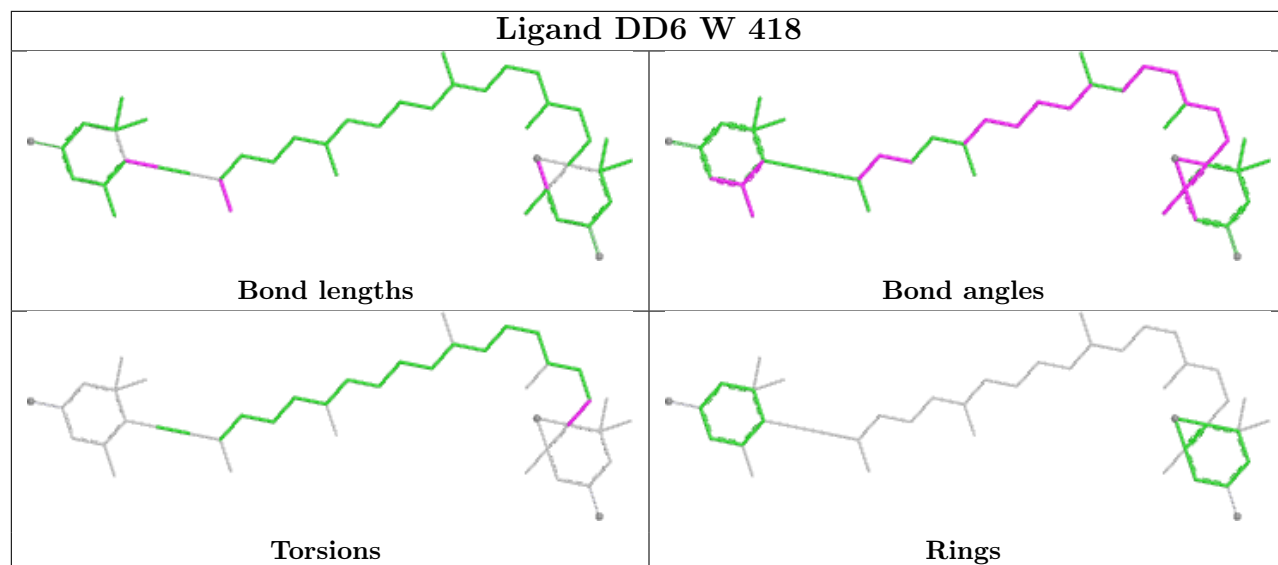
Torsions

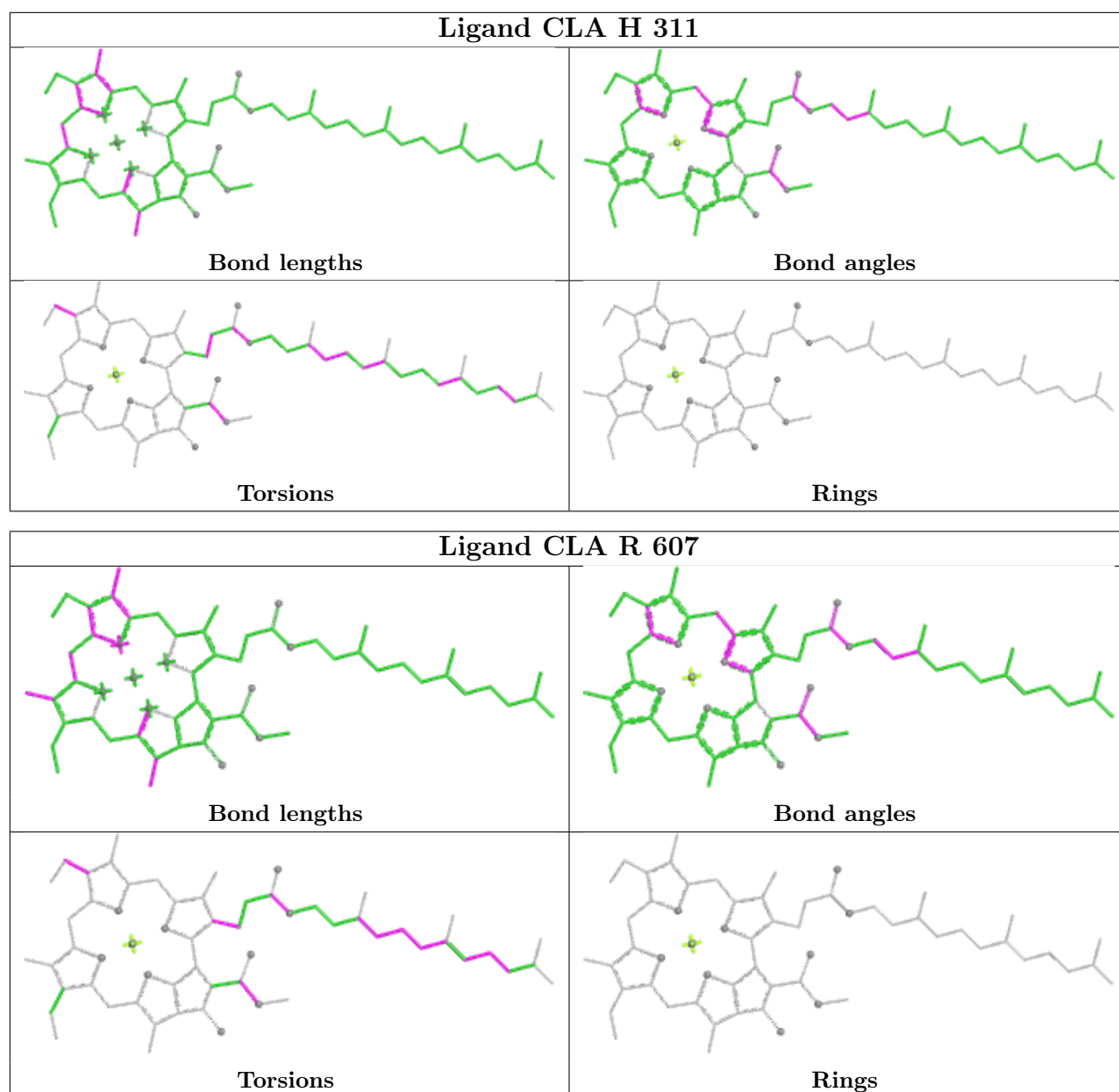


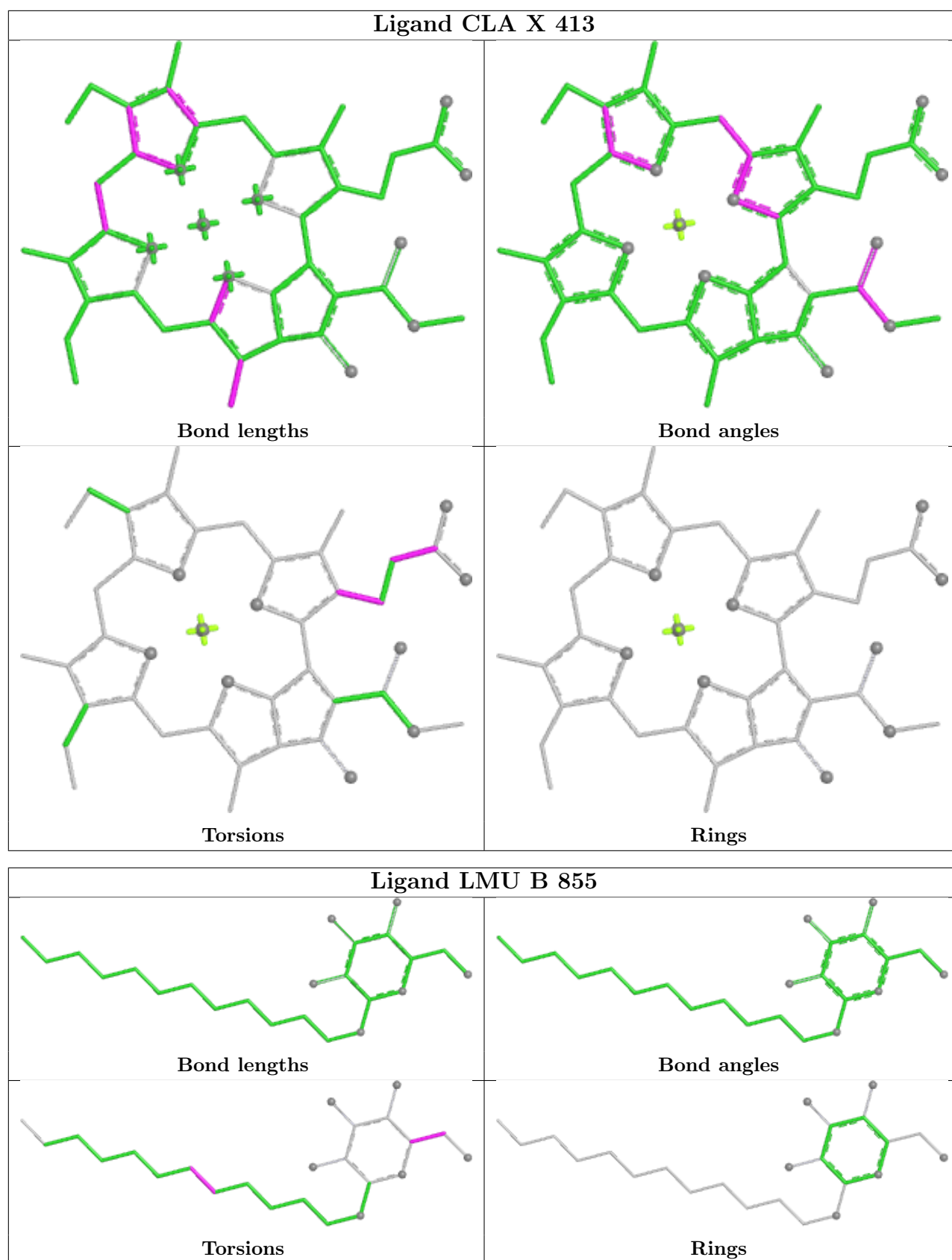
Rings

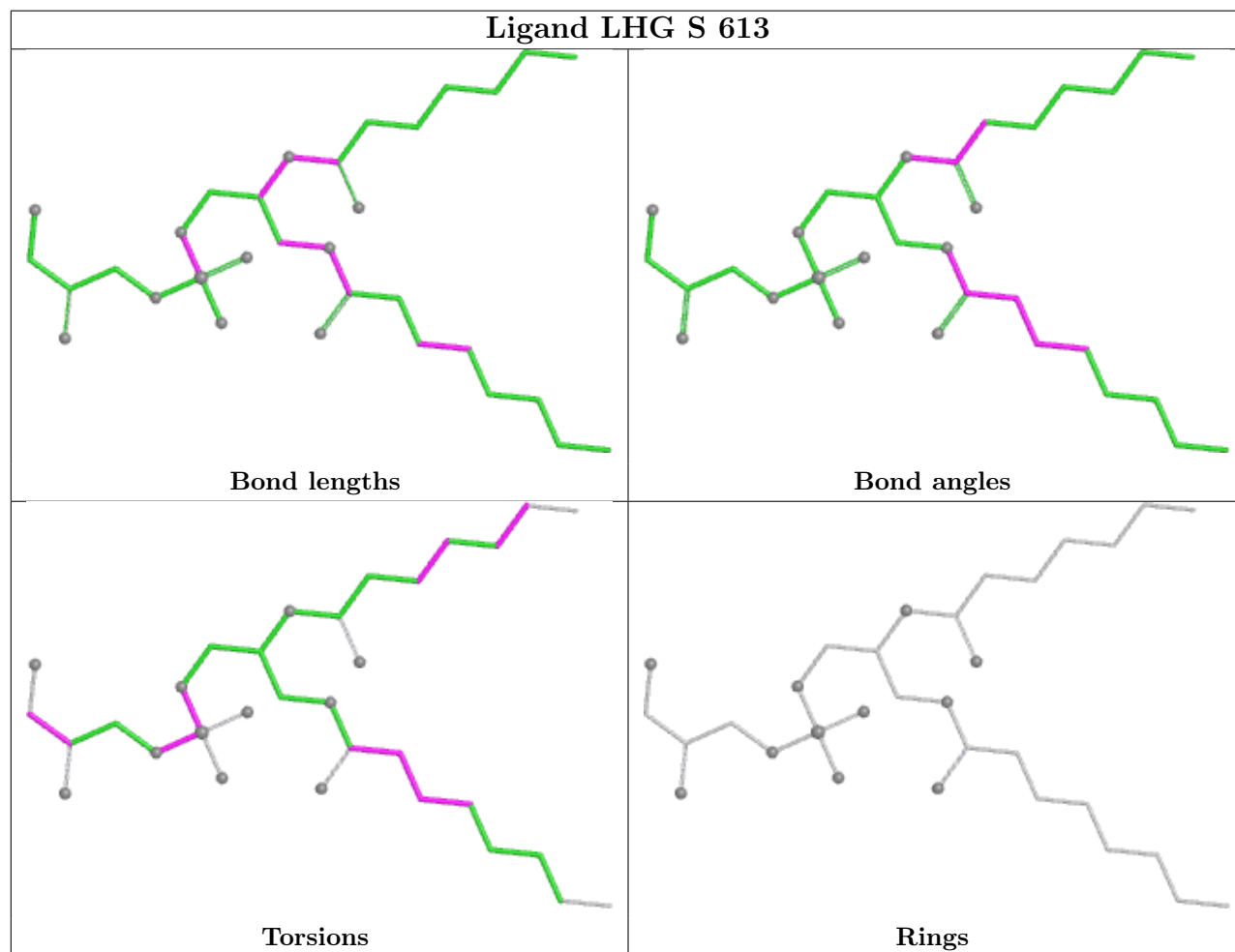
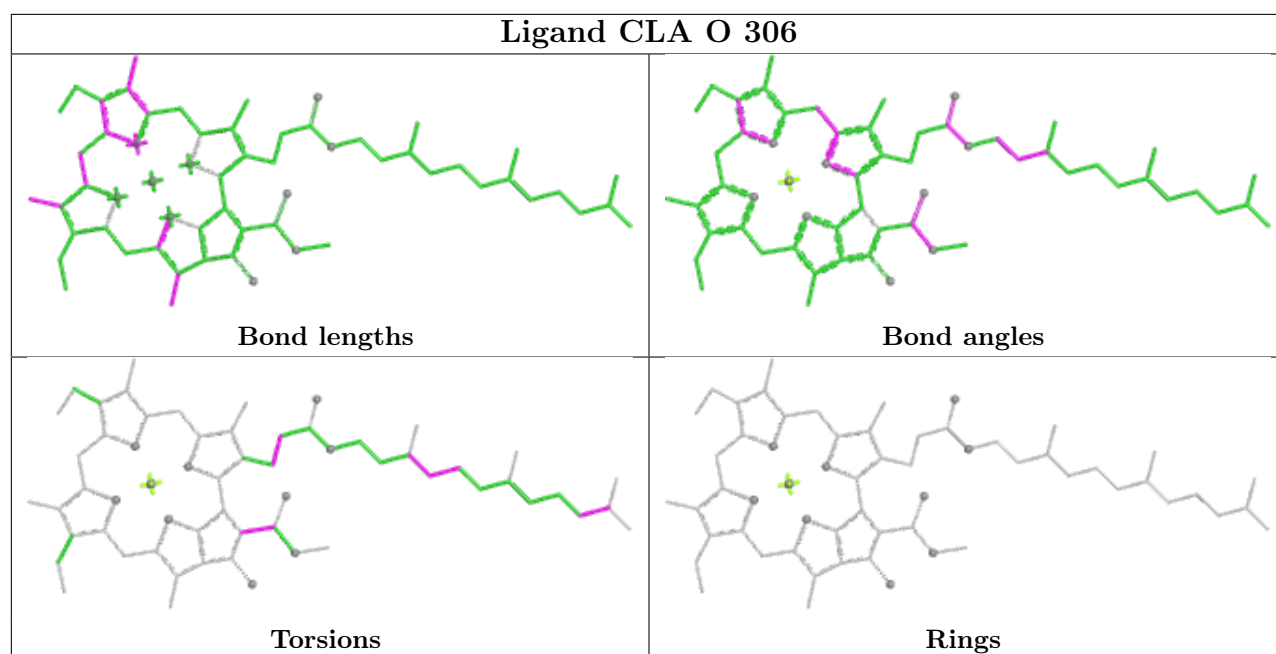




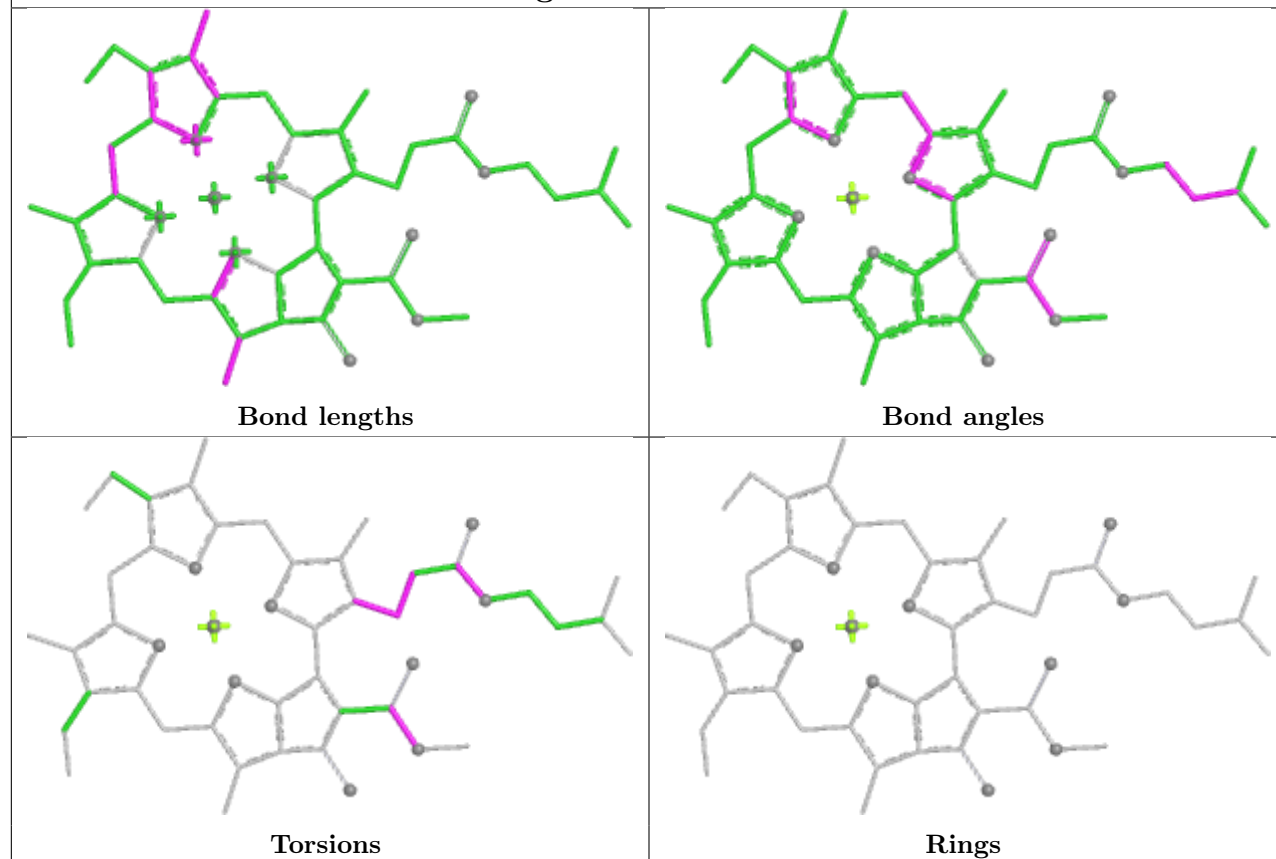




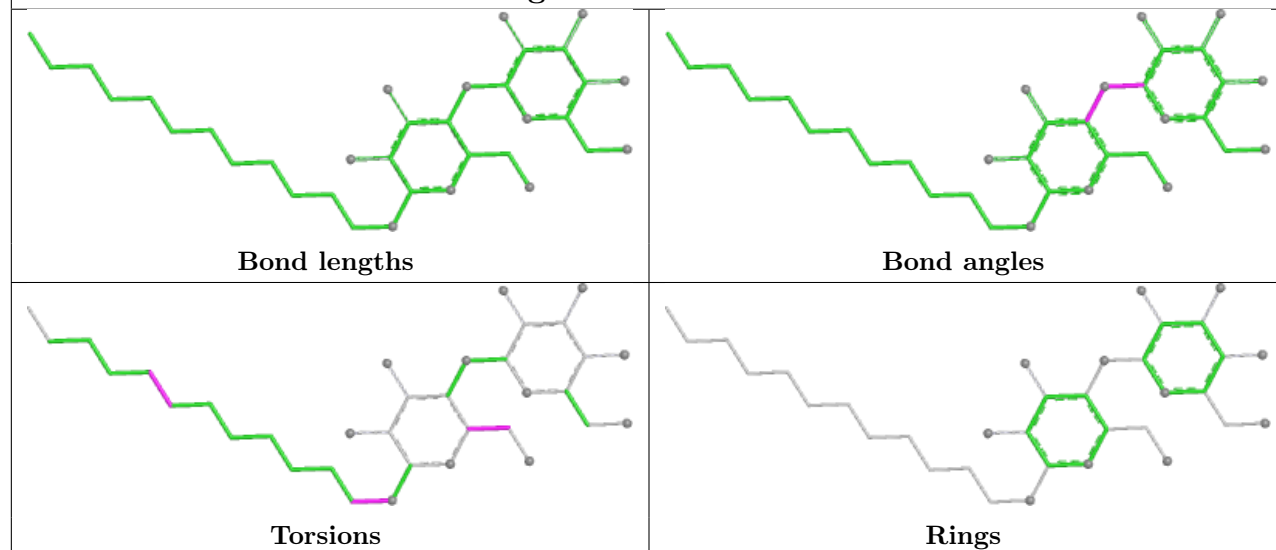


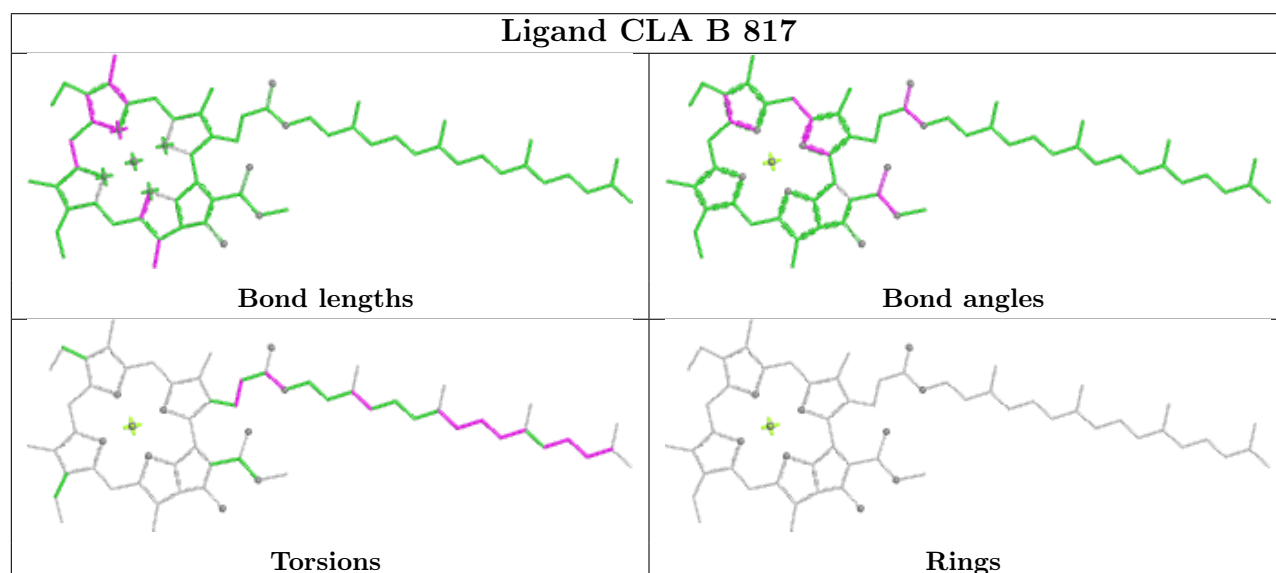
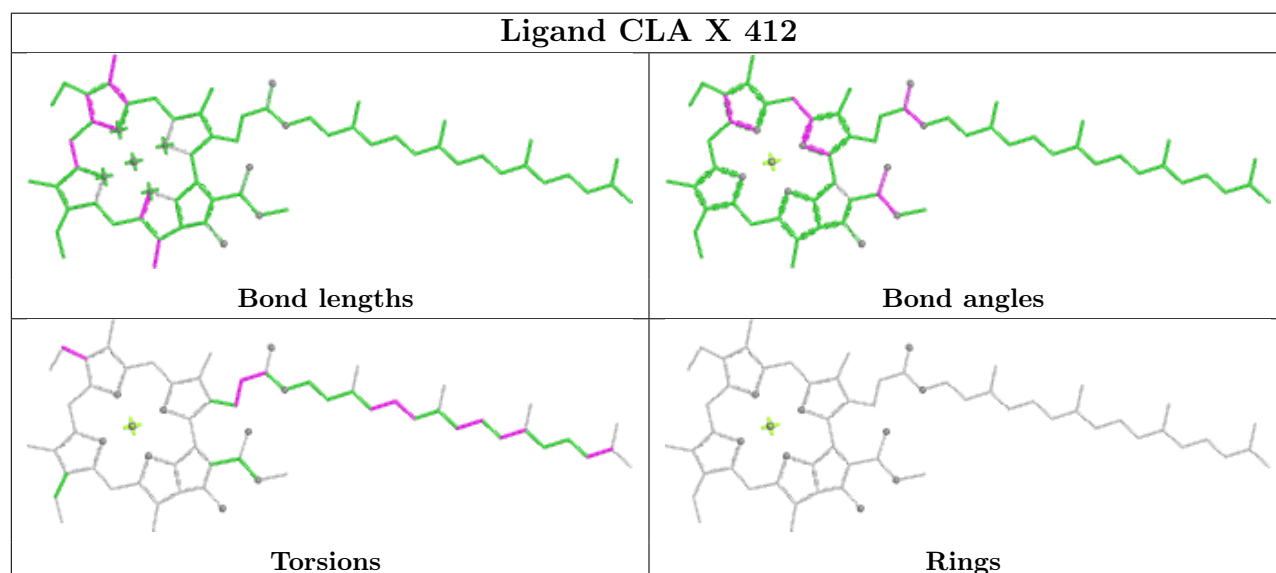
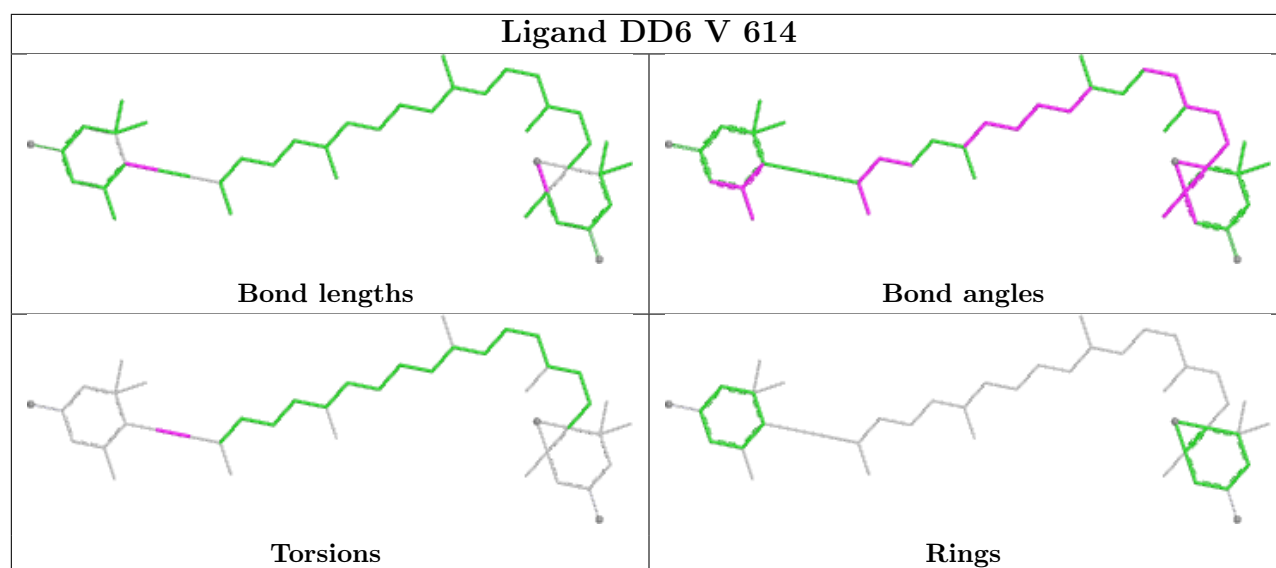


## Ligand CLA J 102

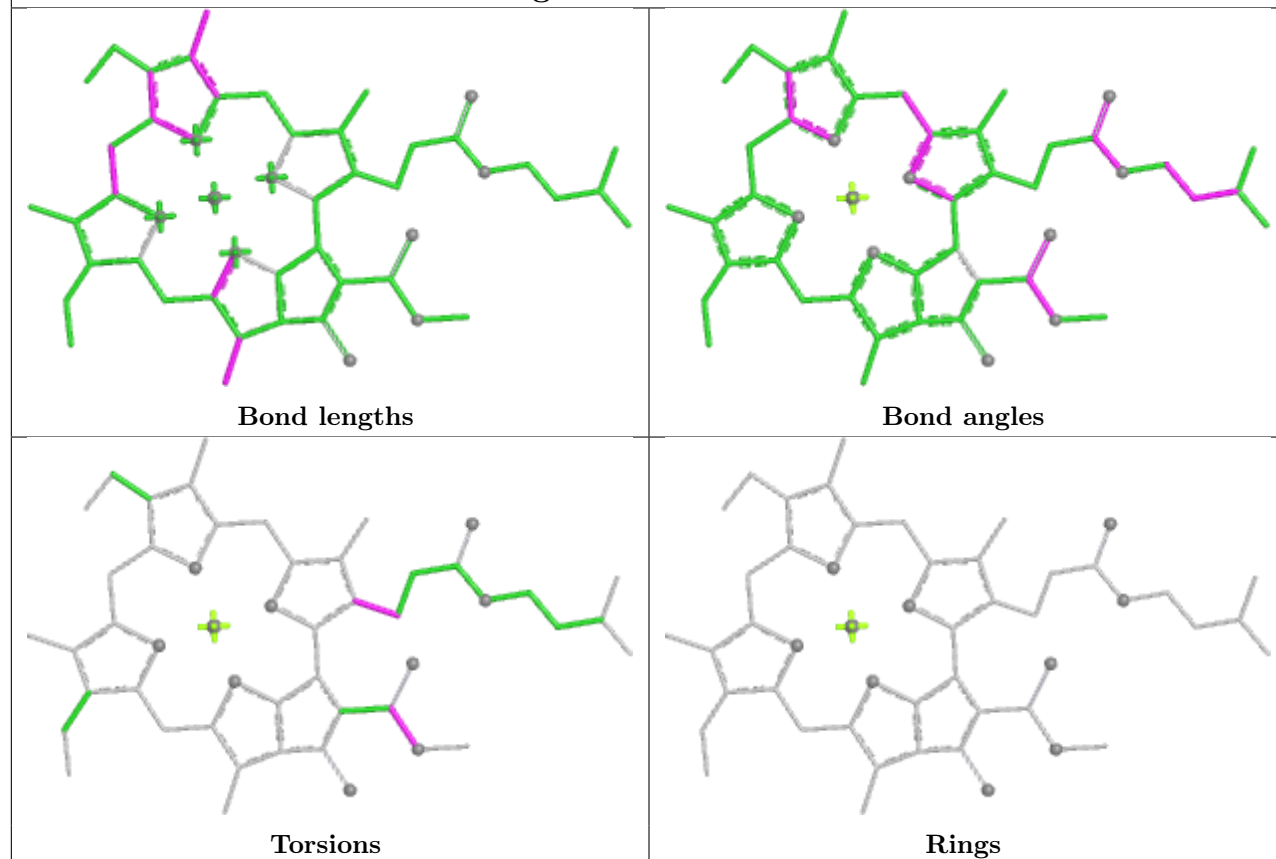


## Ligand LMU B 857

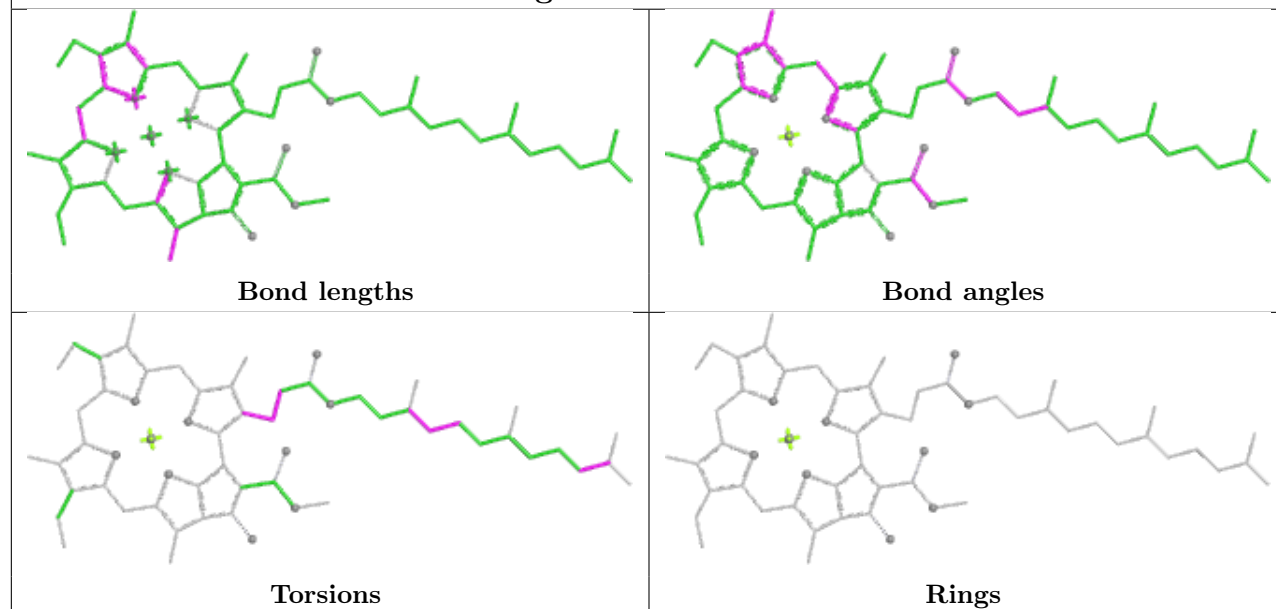




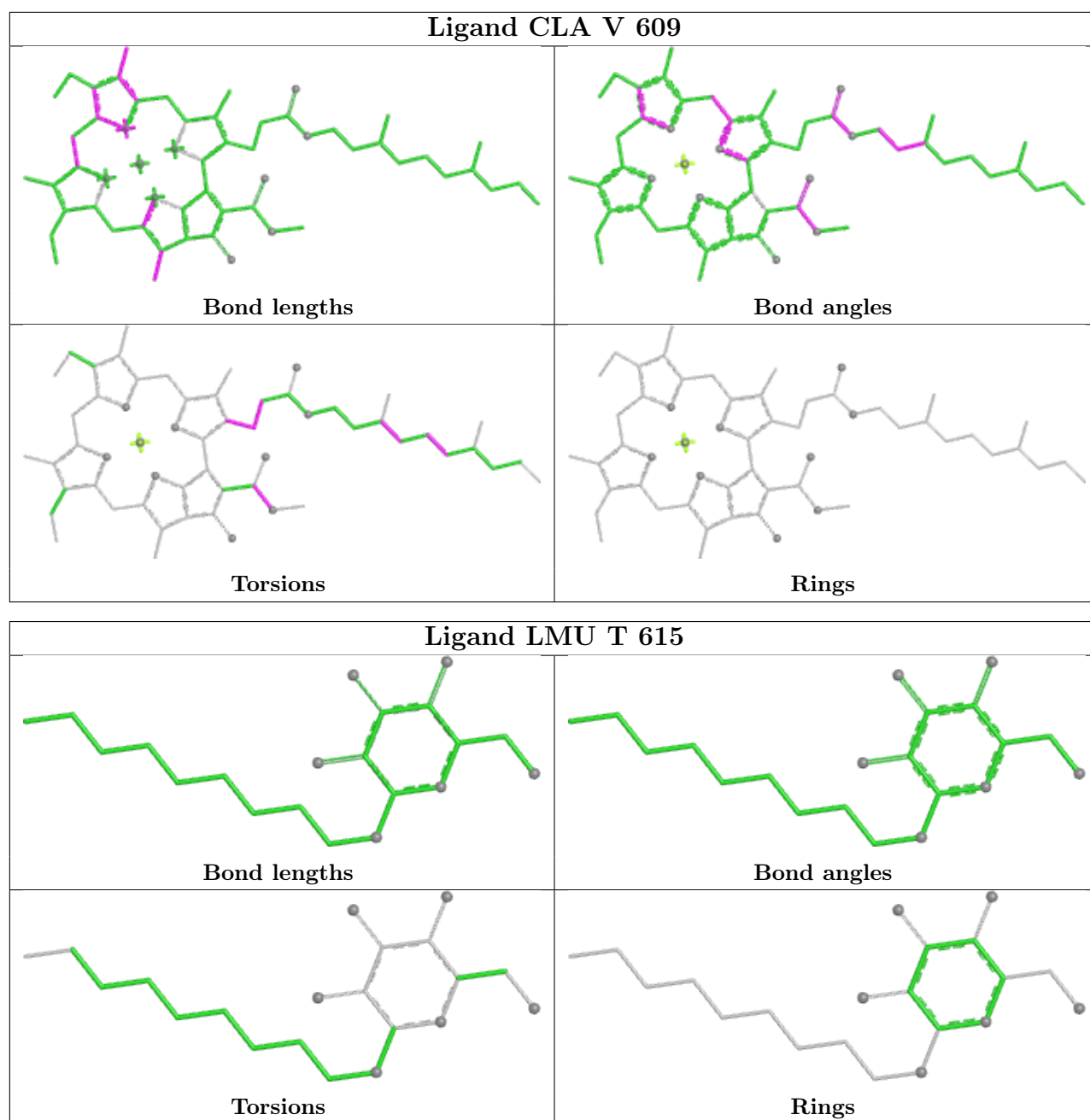
## Ligand CLA T 606

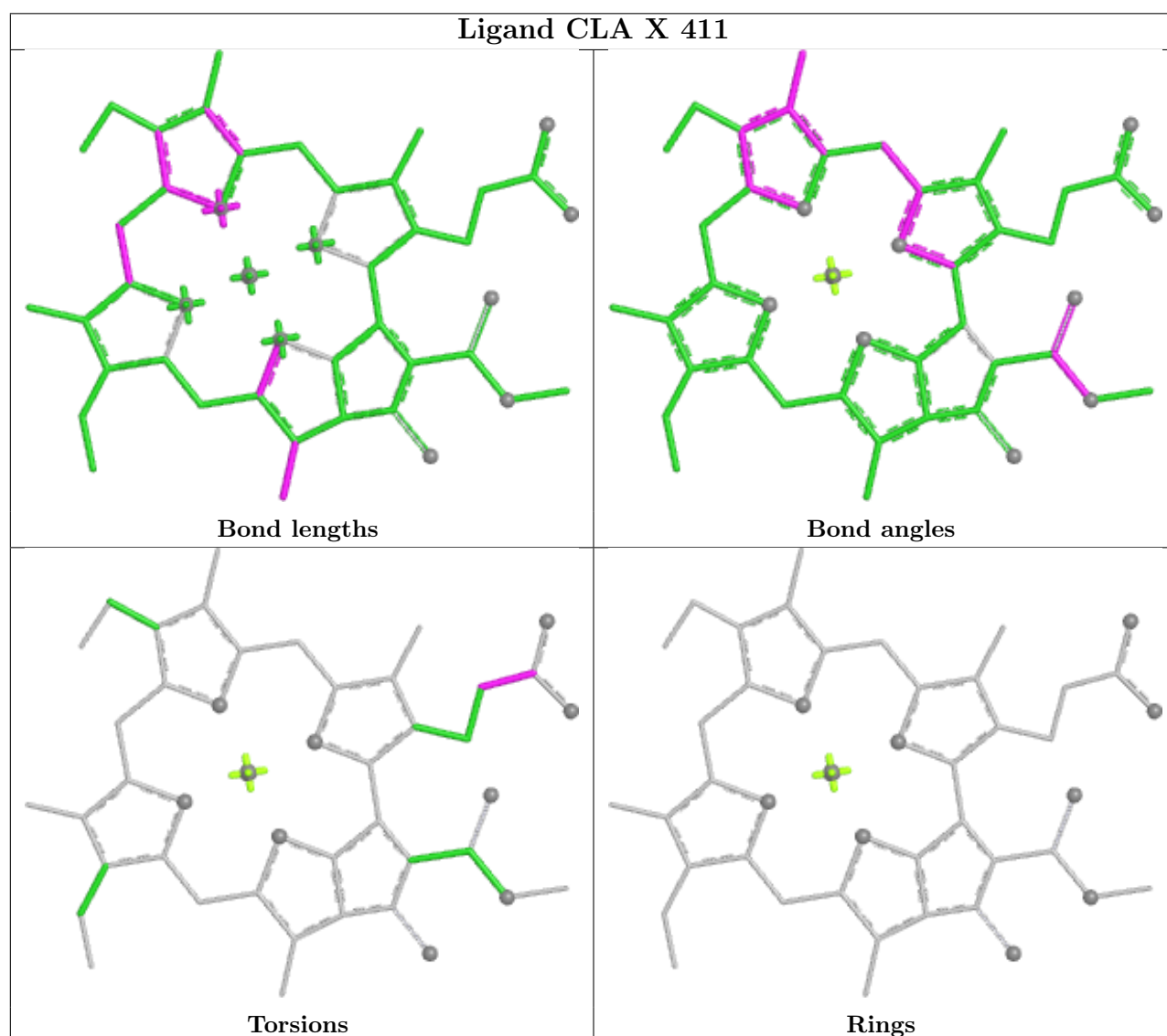
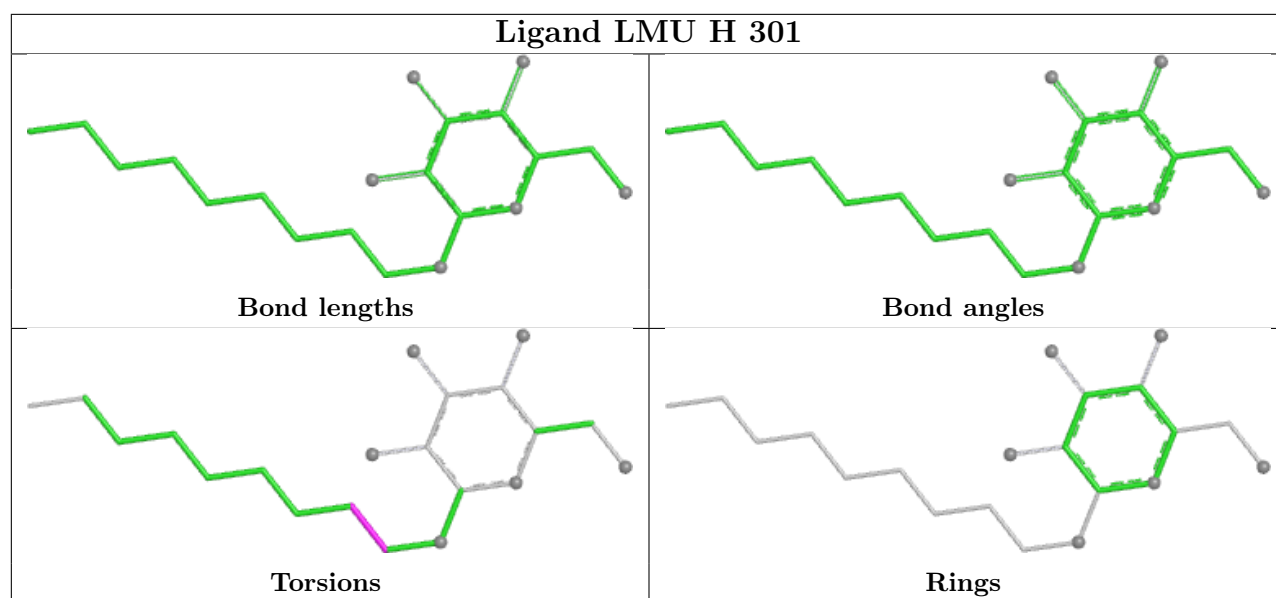


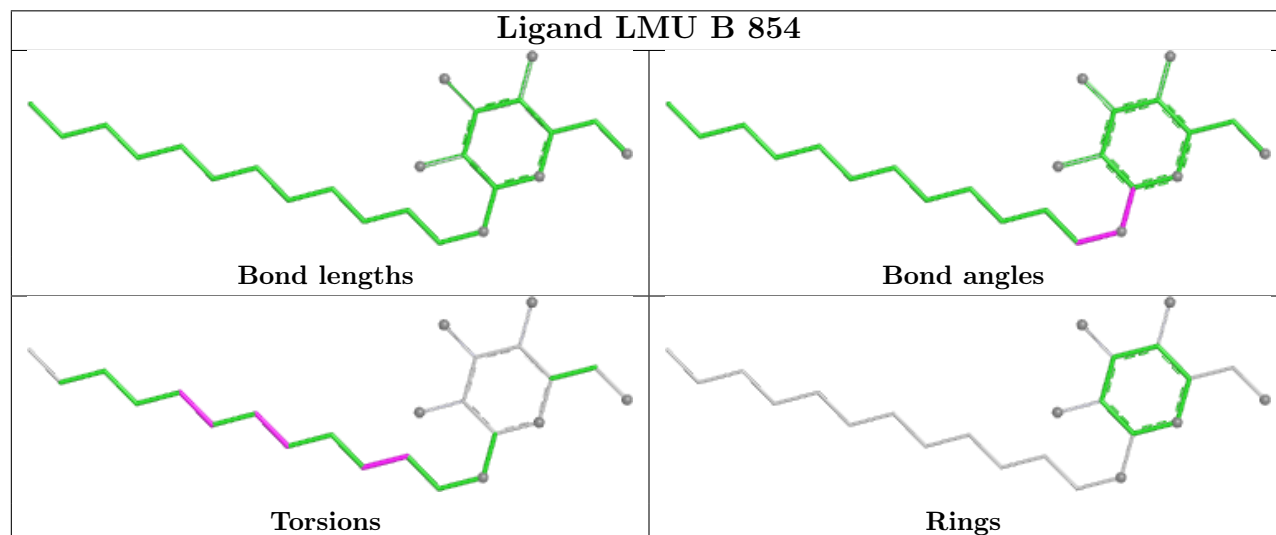
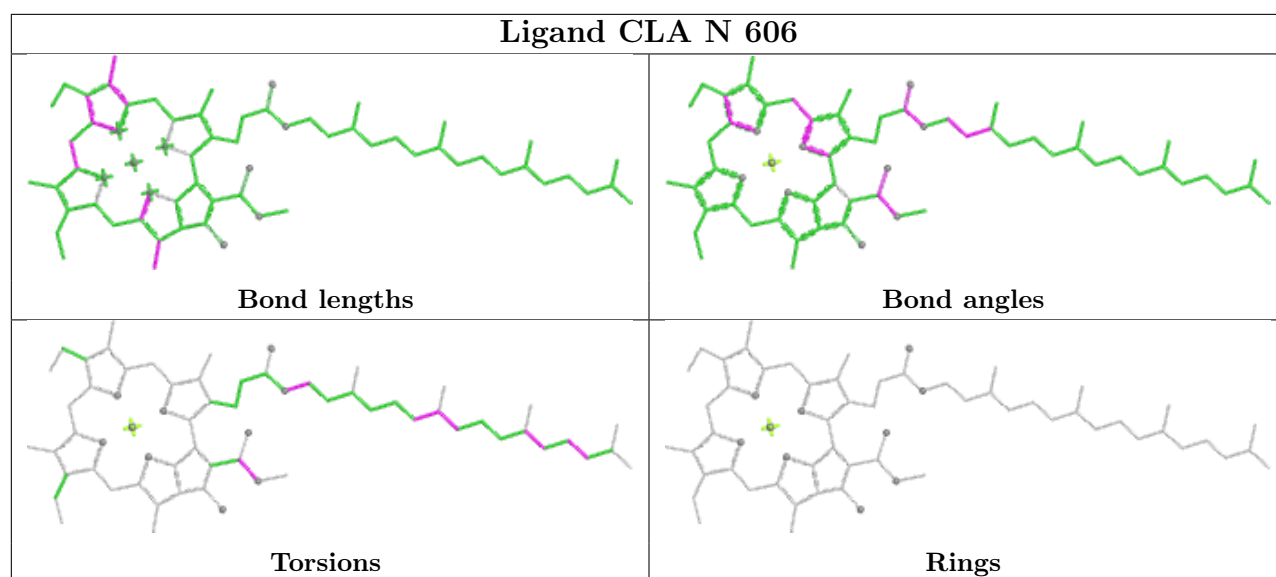
## Ligand CLA S 602

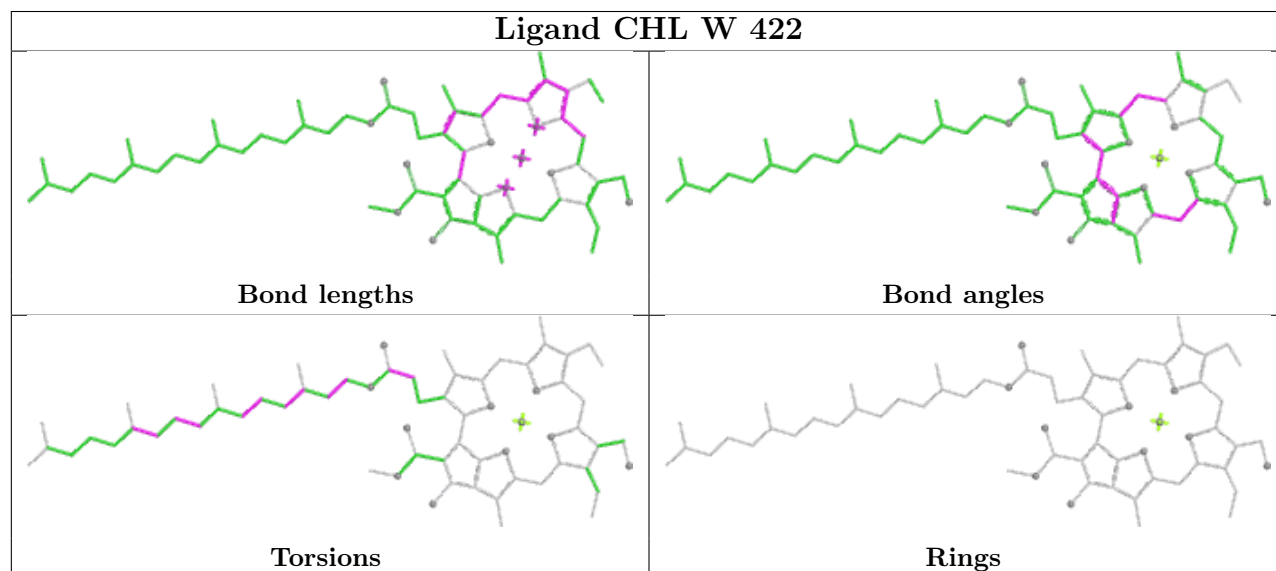
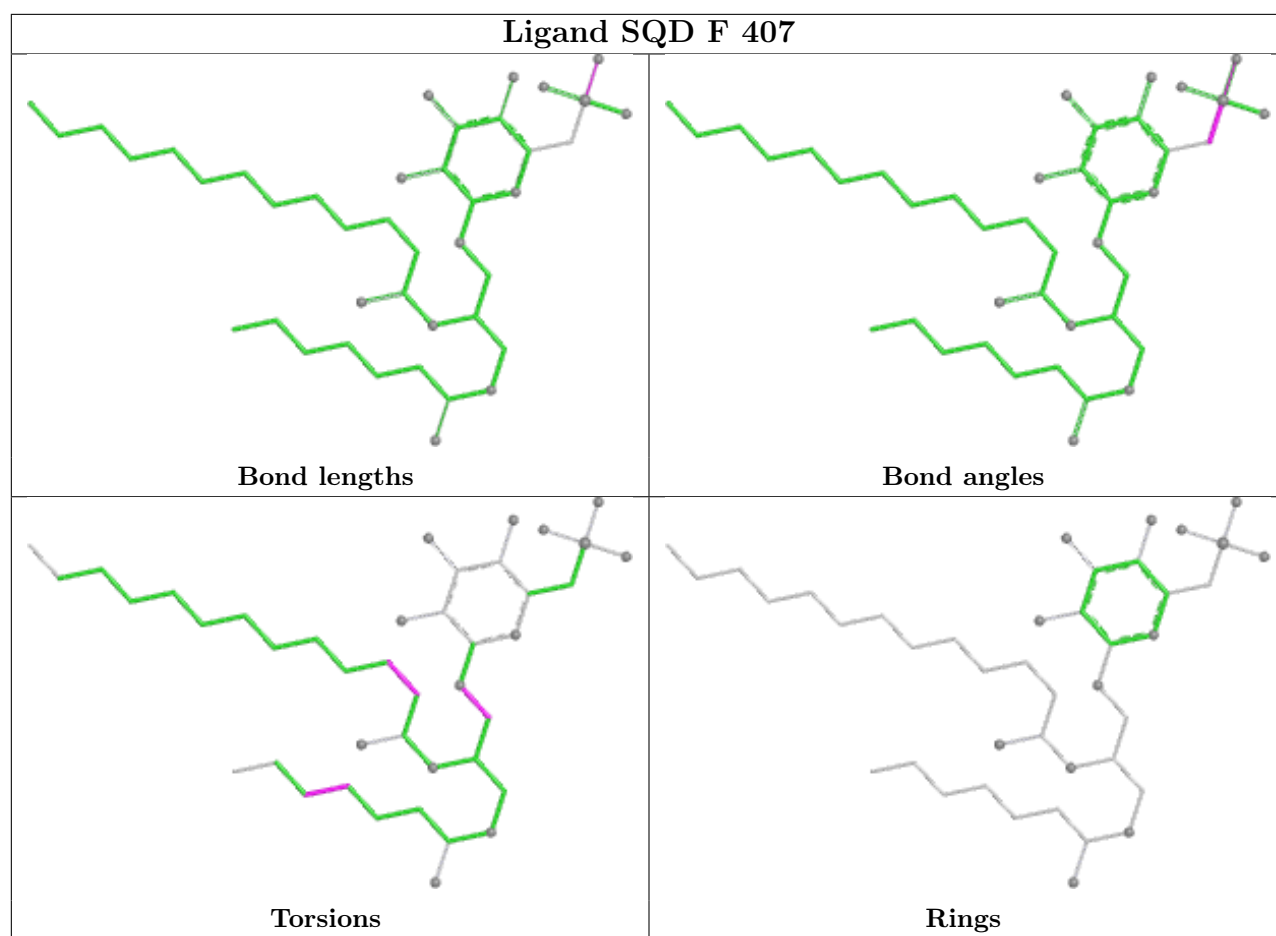


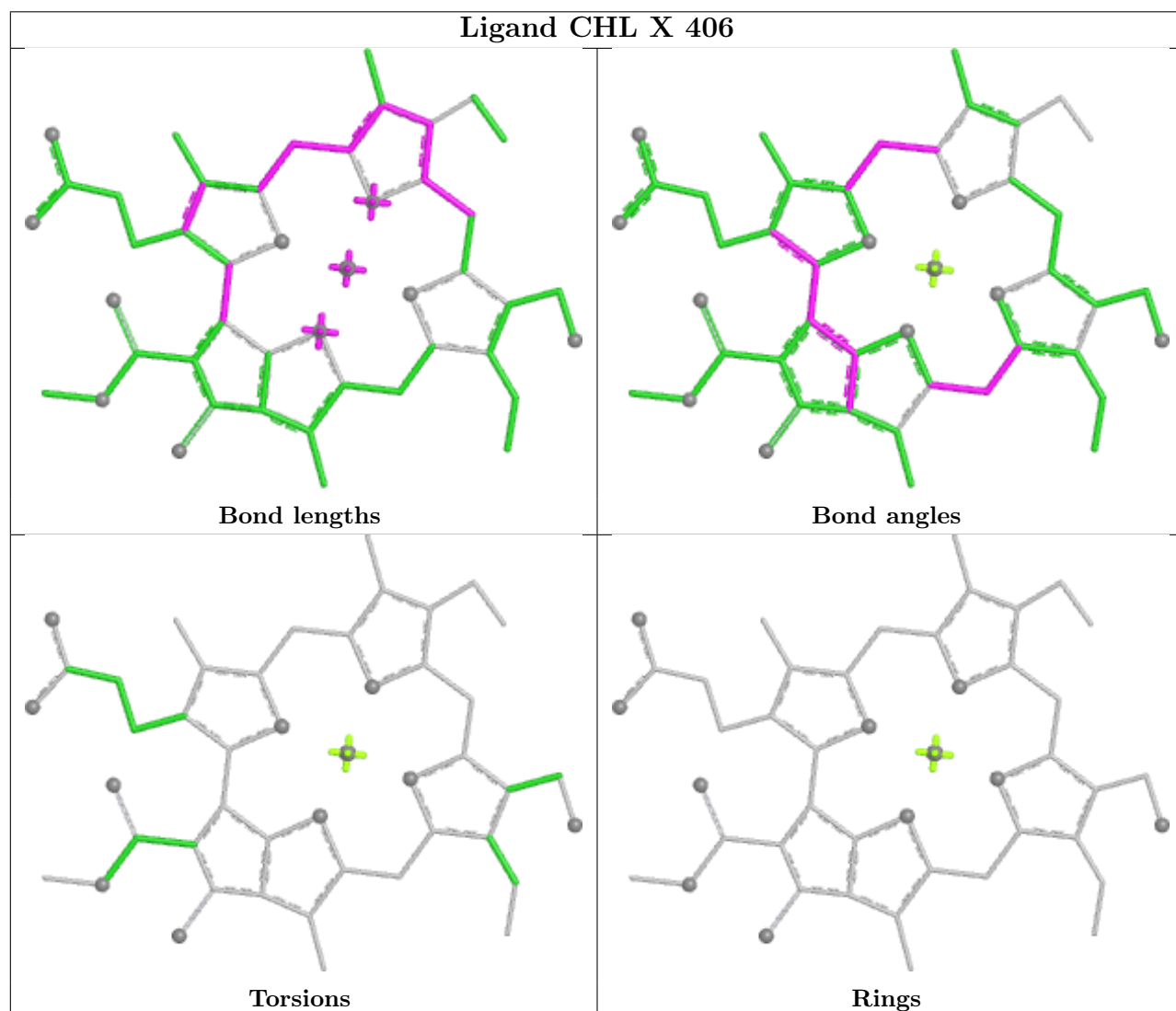
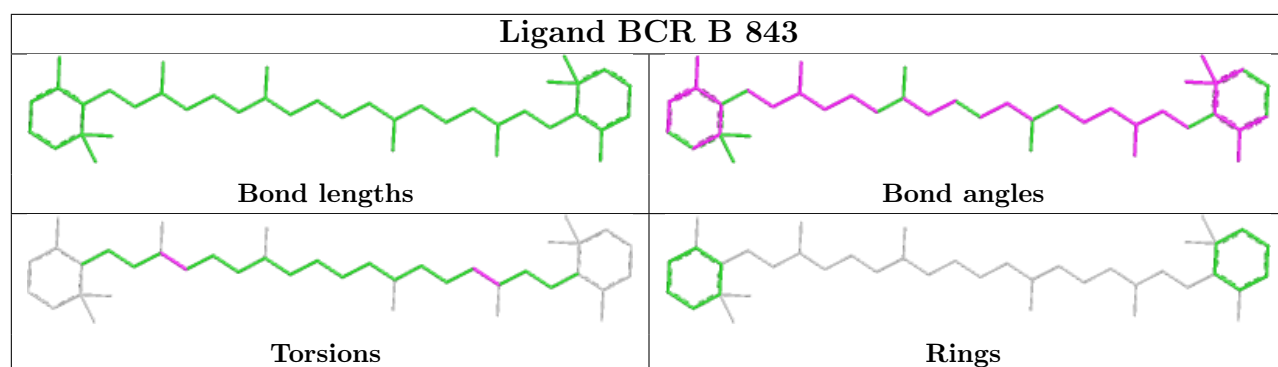




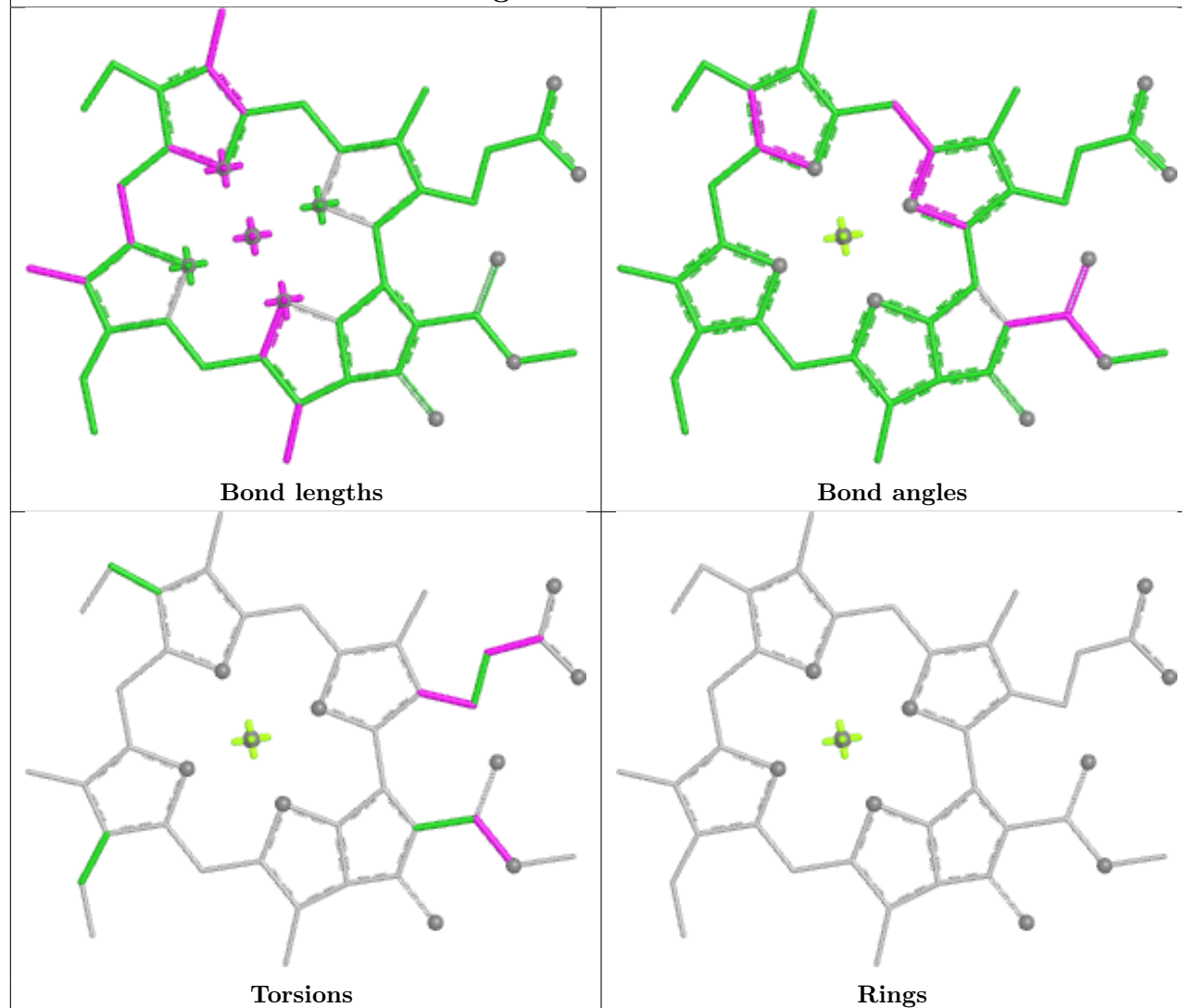




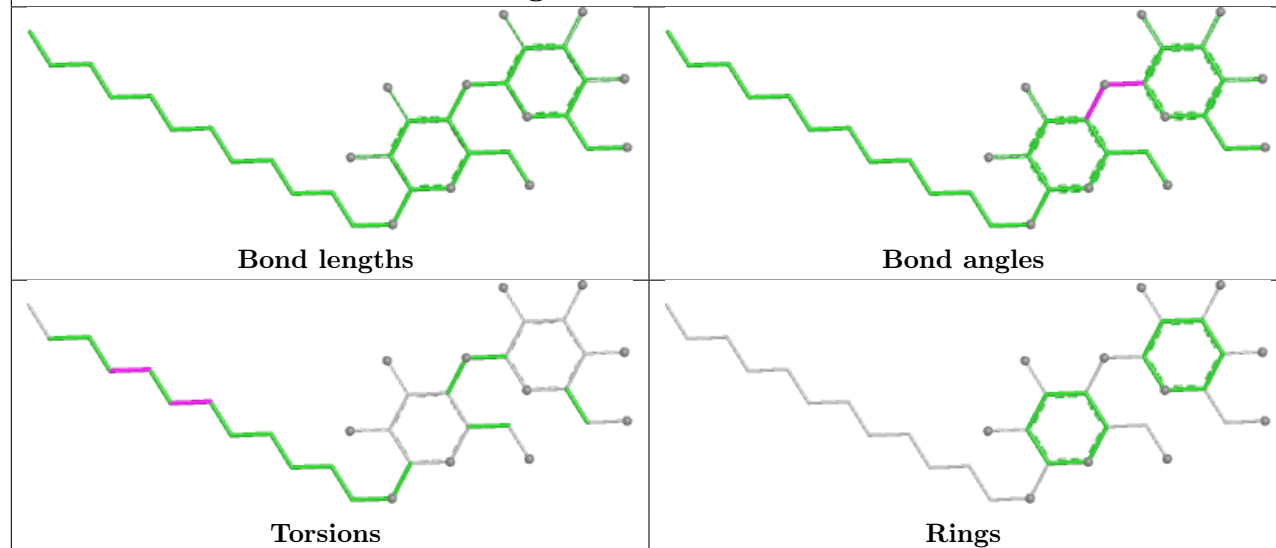


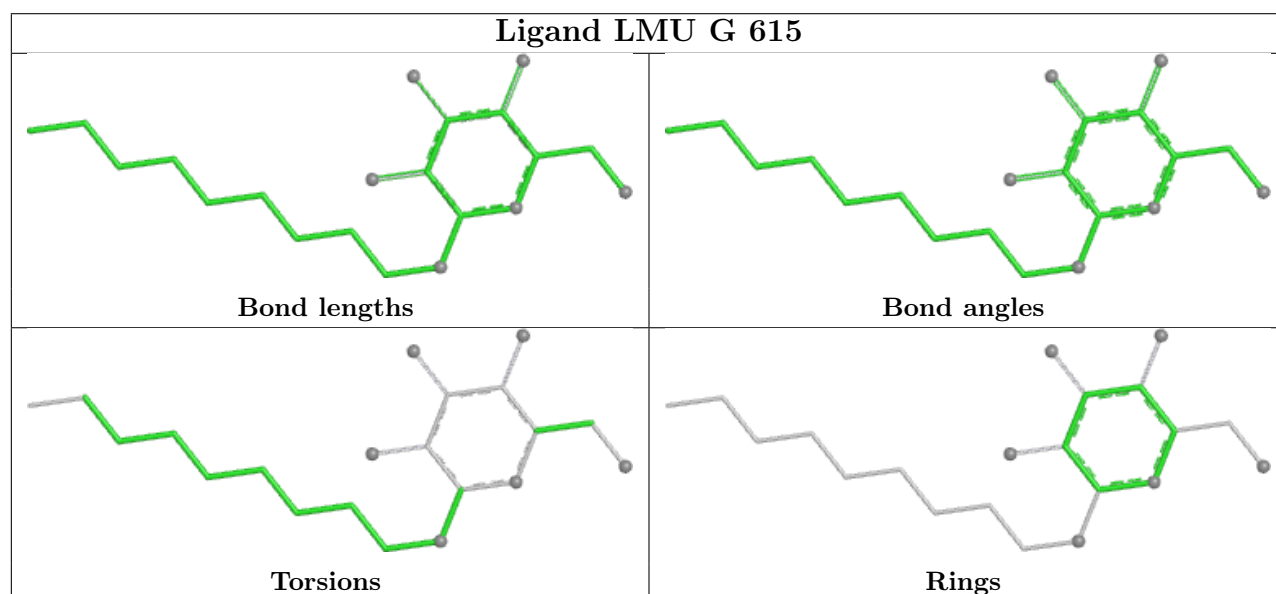
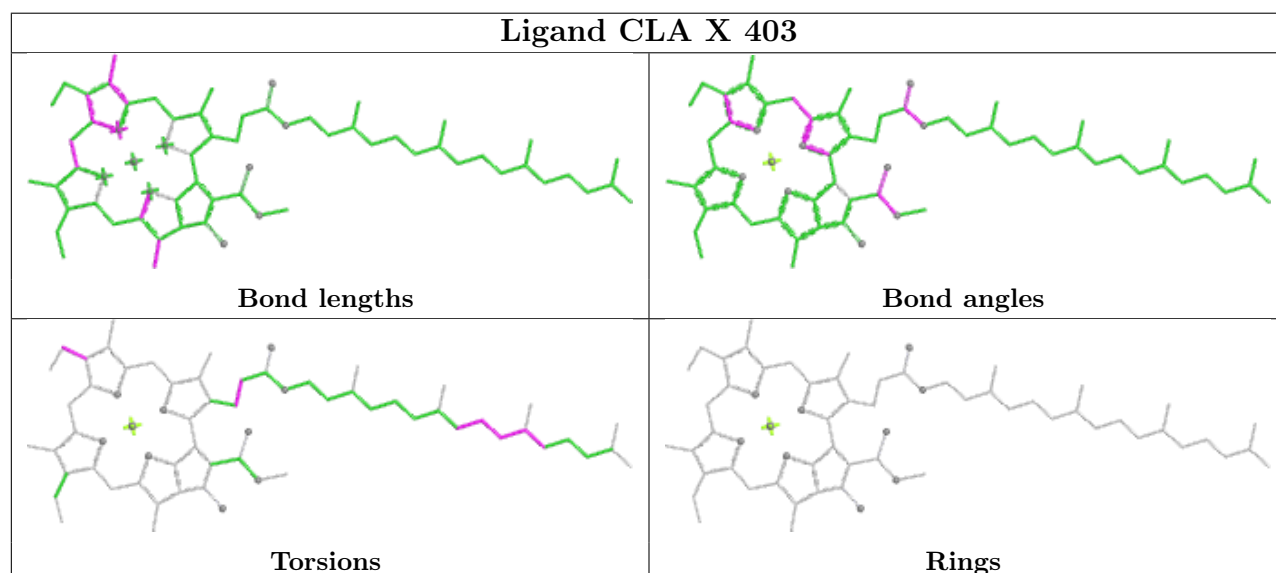
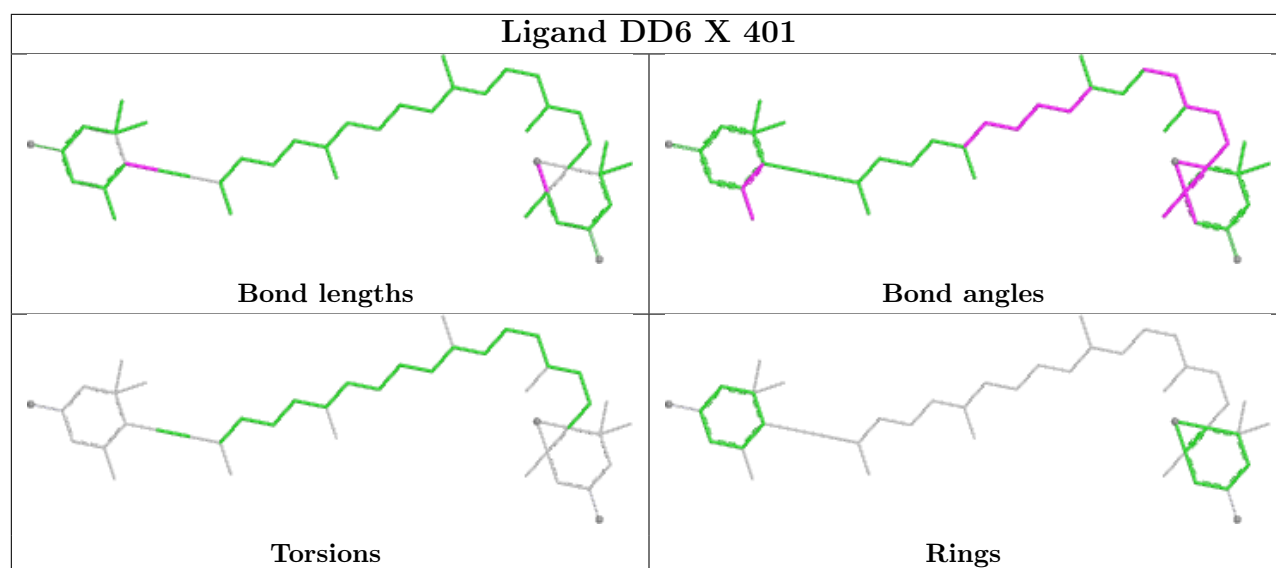


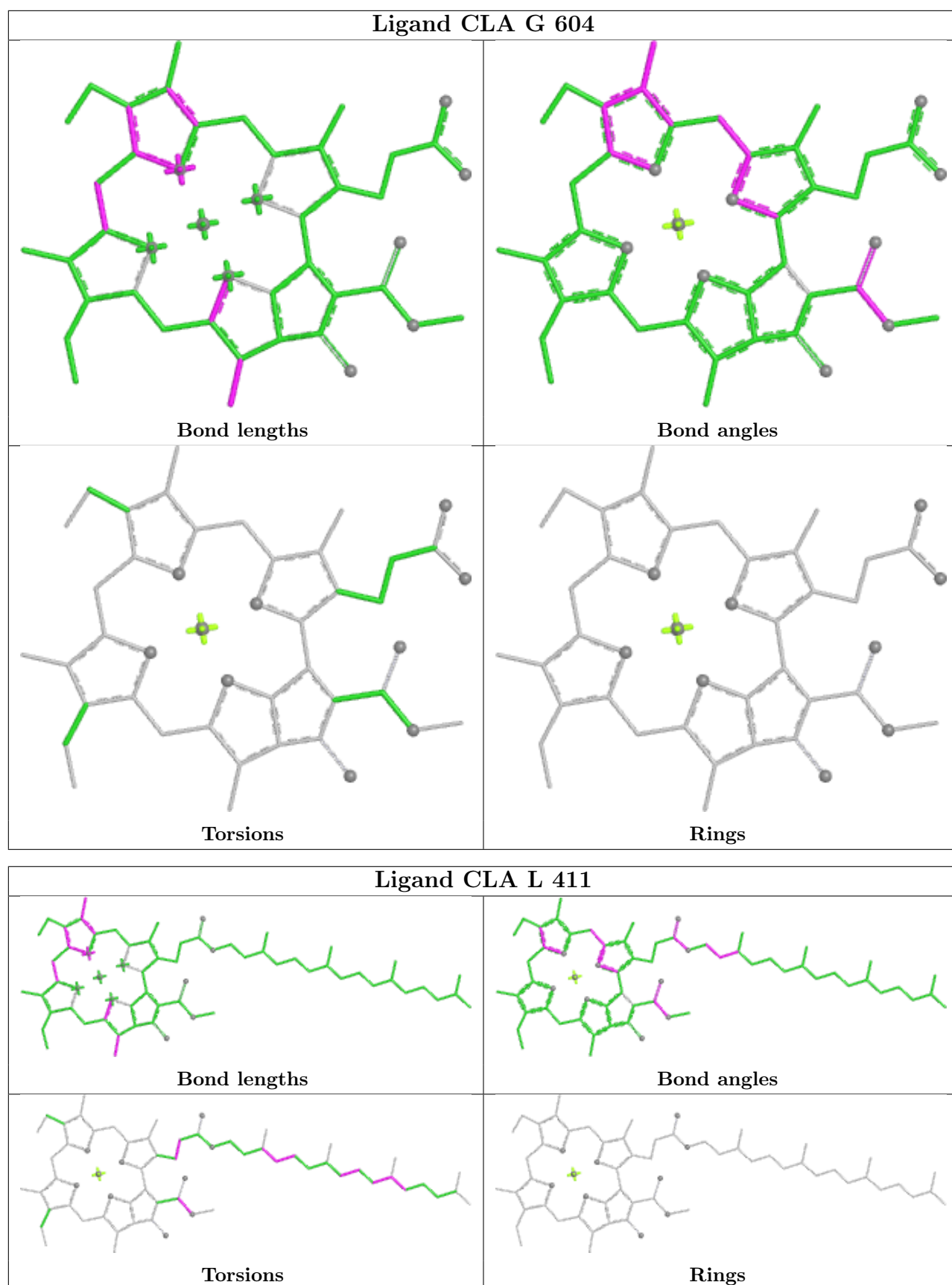
## Ligand CLA B 829



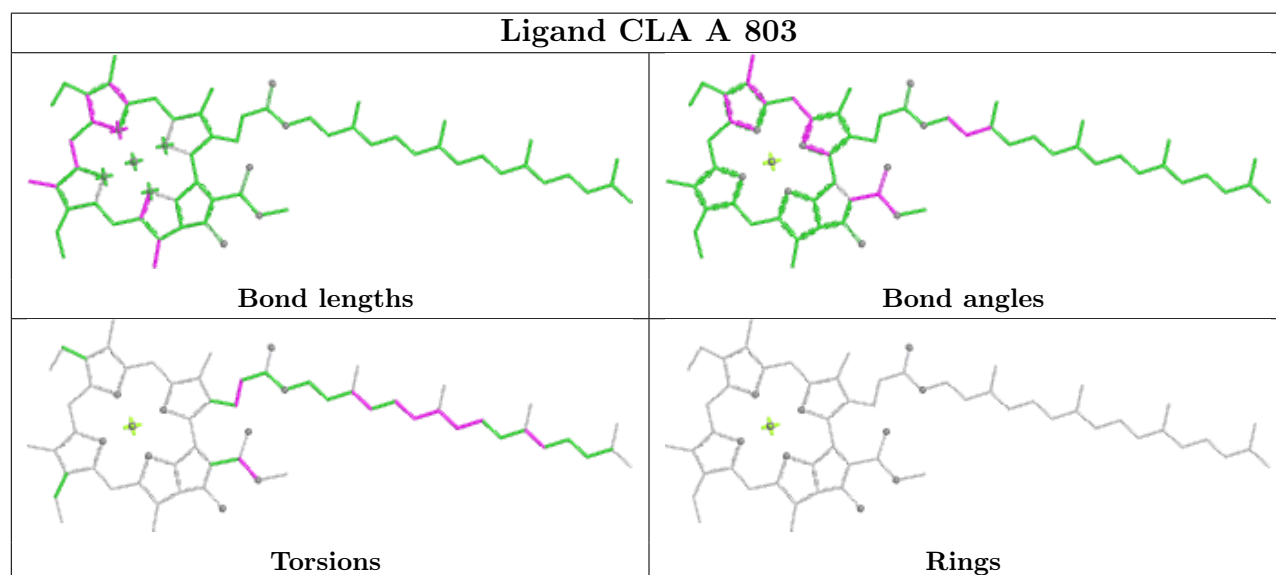
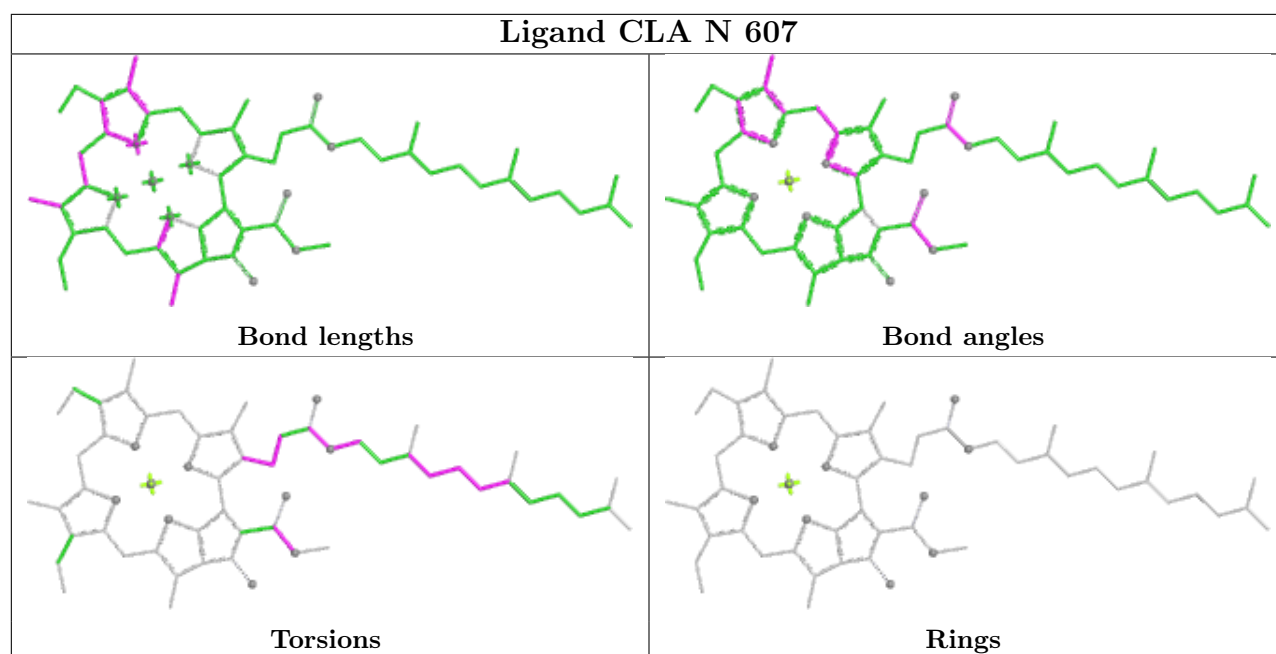
## Ligand LMU A 854

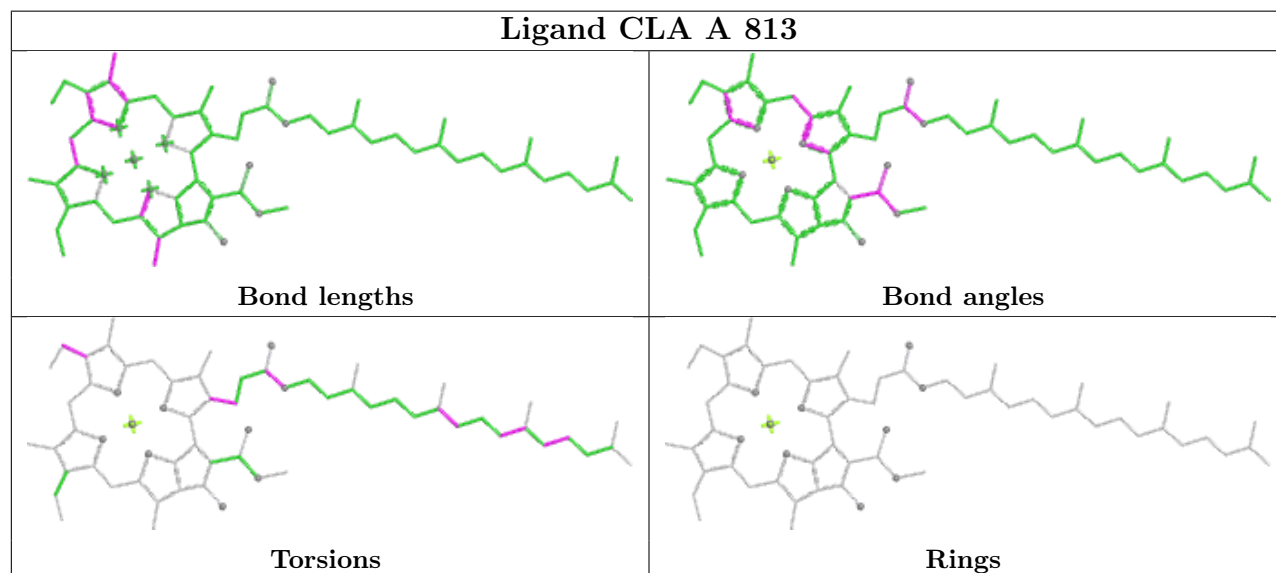
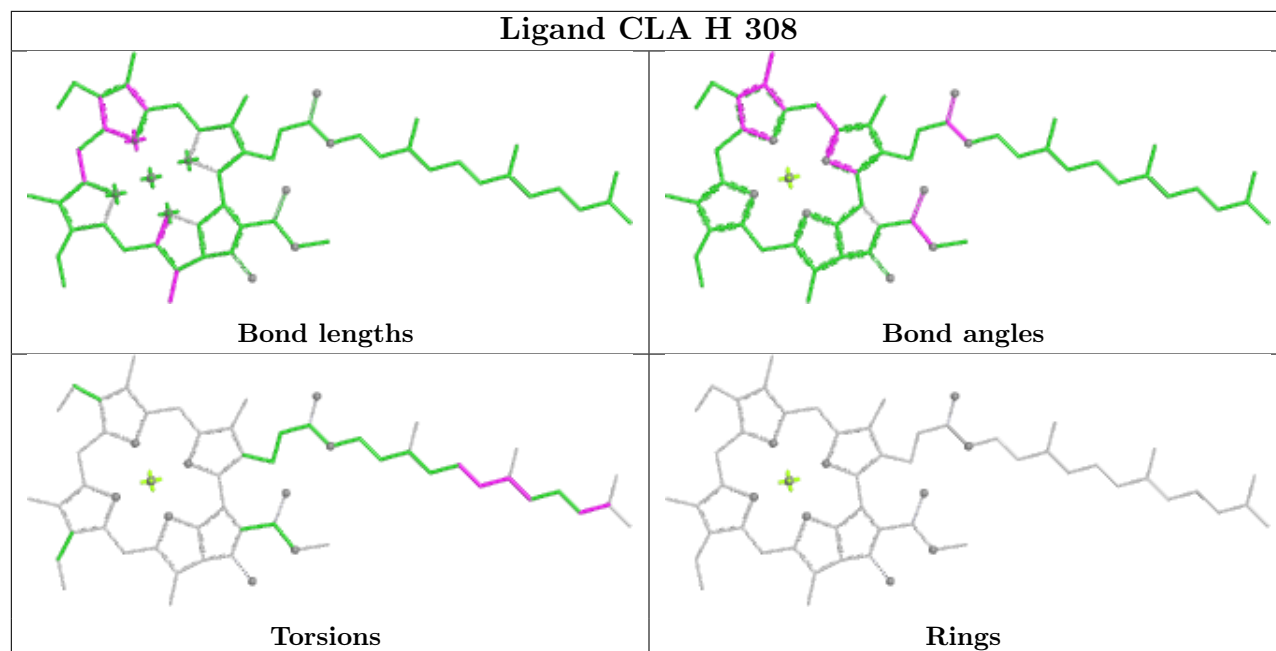


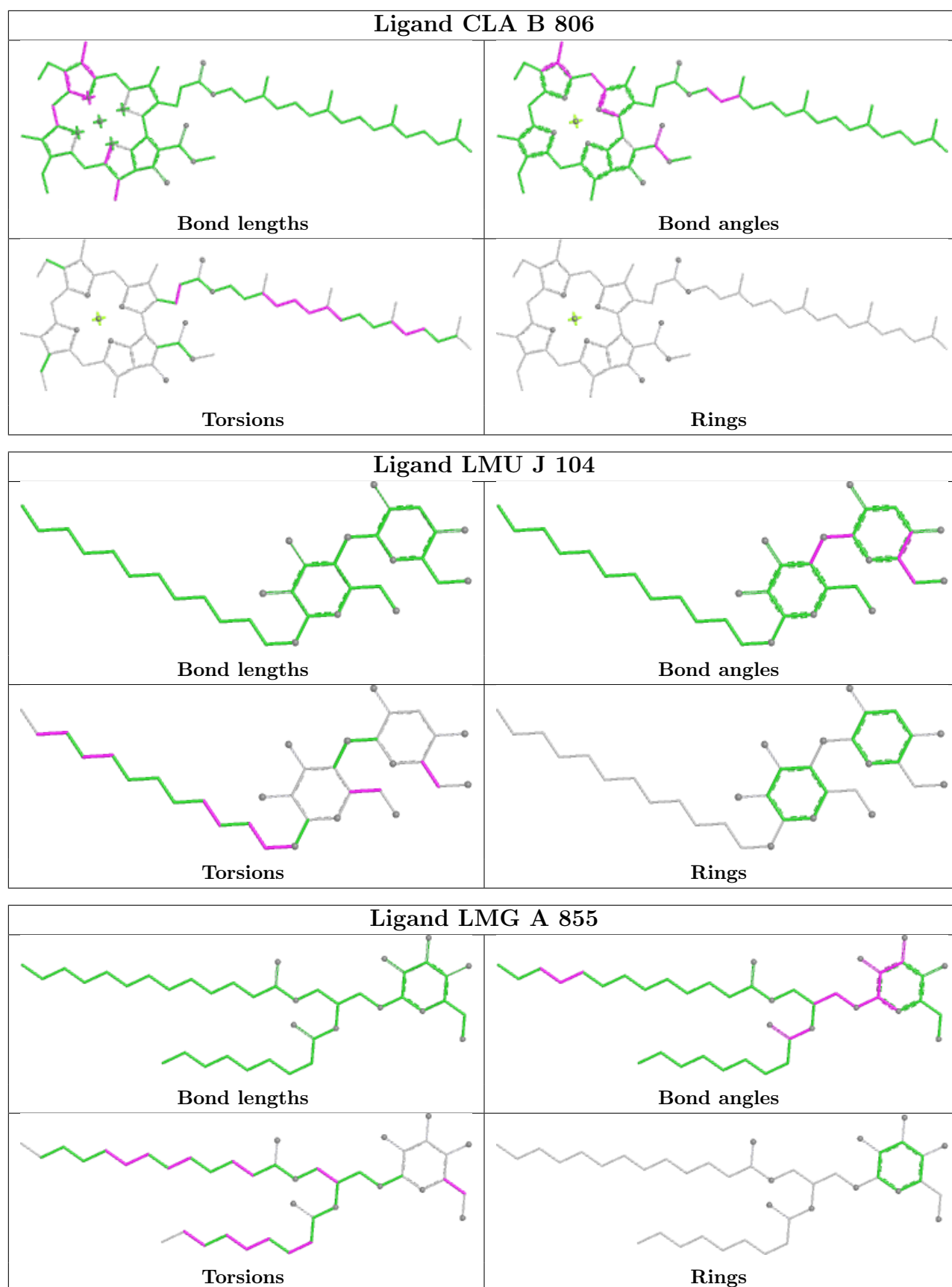


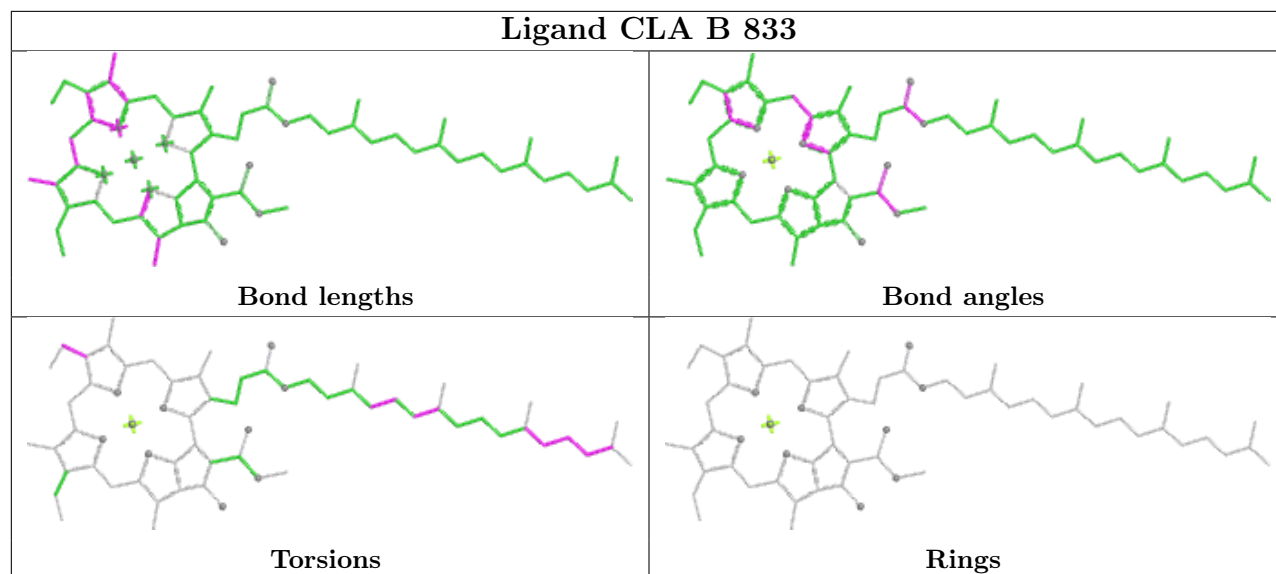
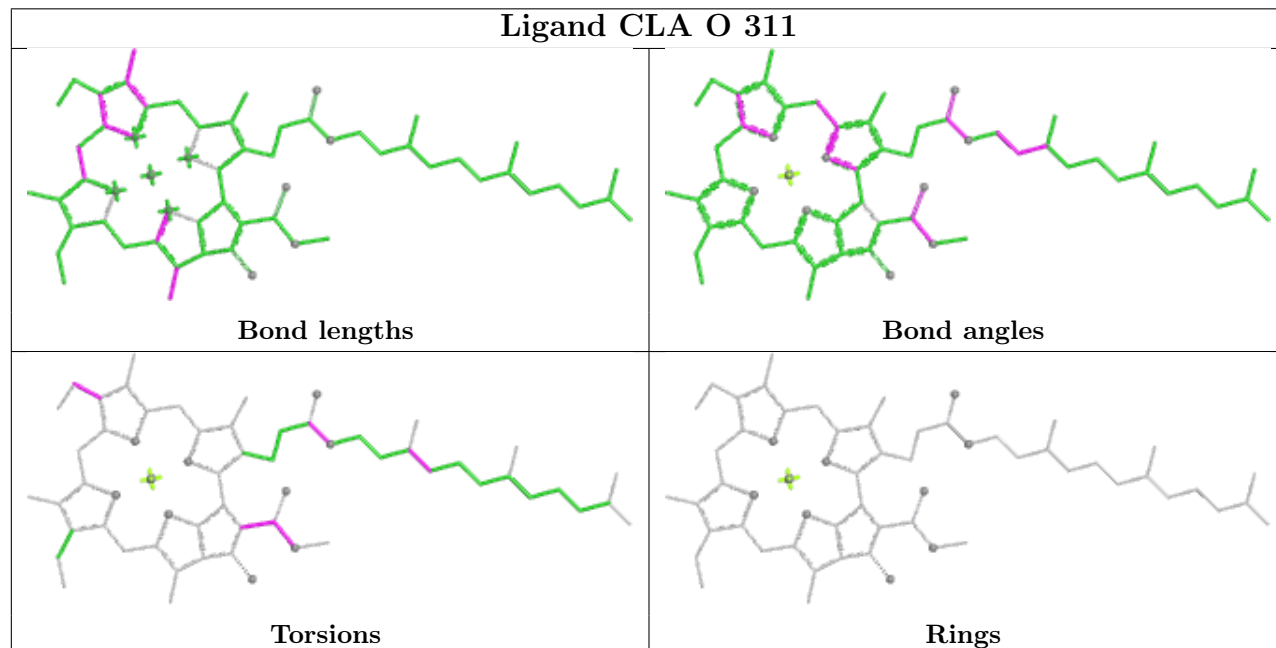


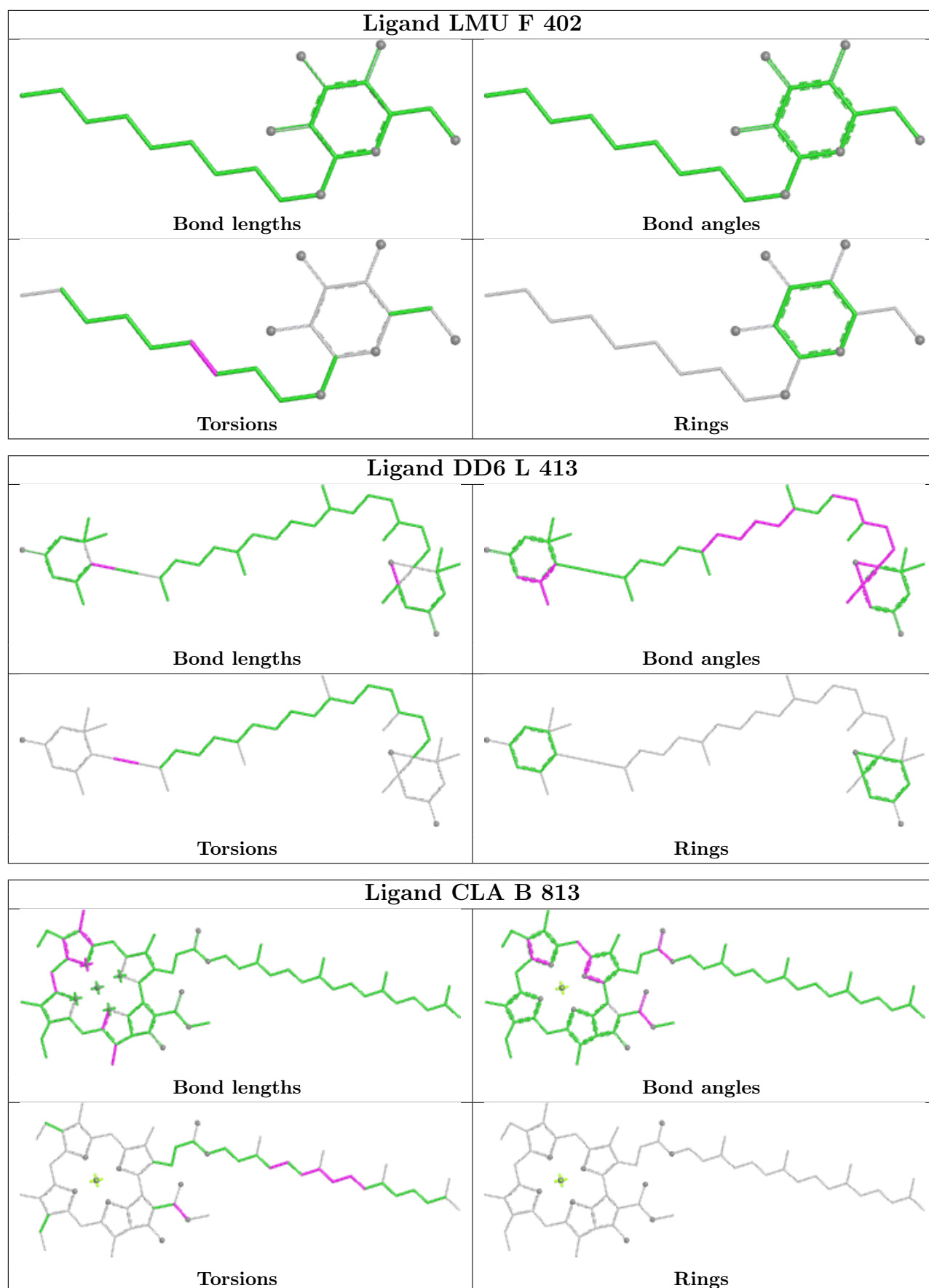




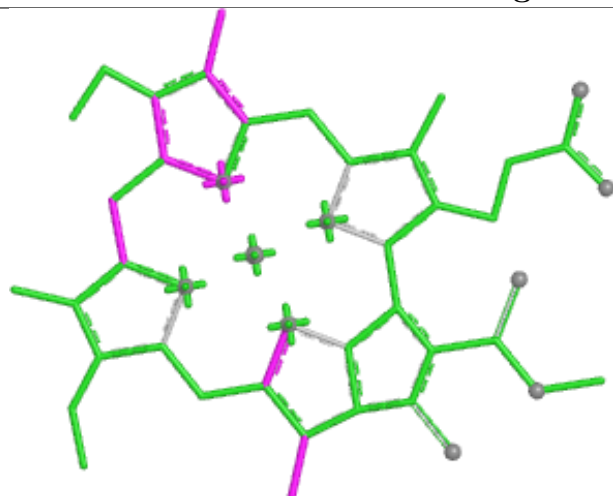




**Ligand CLA B 833****Ligand CLA O 311**



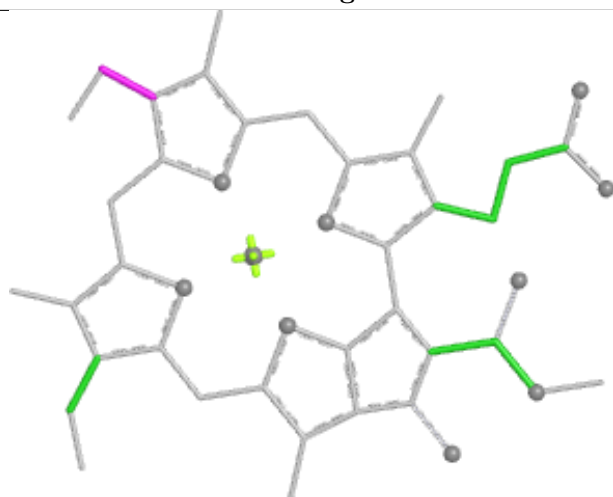
## Ligand CLA H 302



Bond lengths



Bond angles

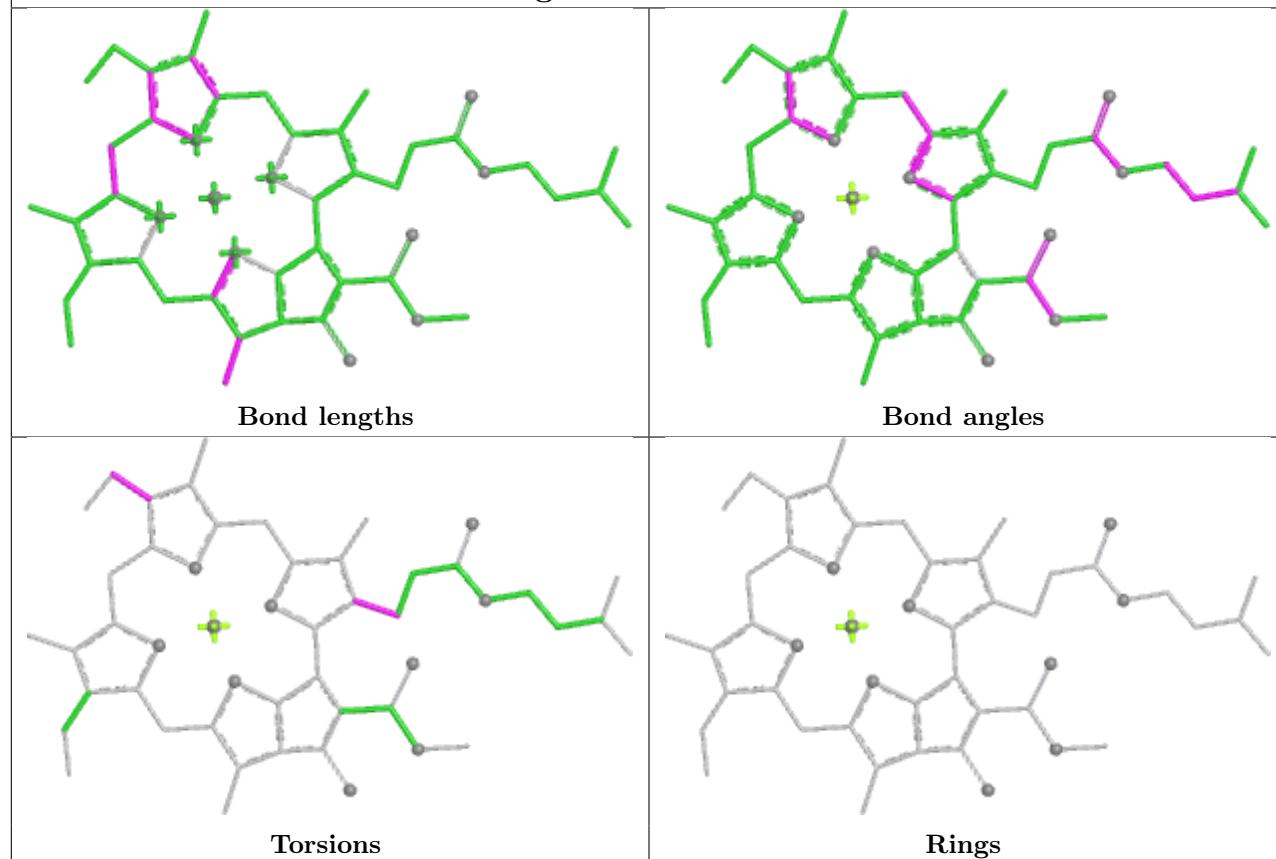


Torsions

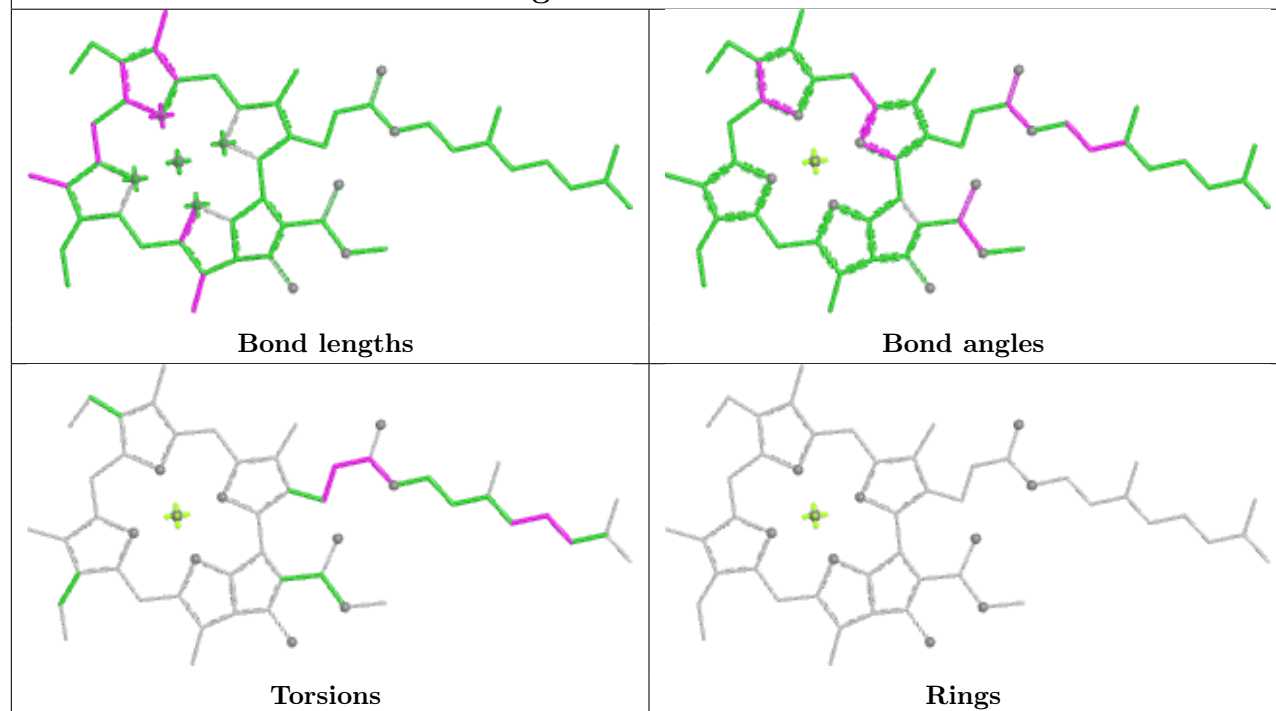


Rings

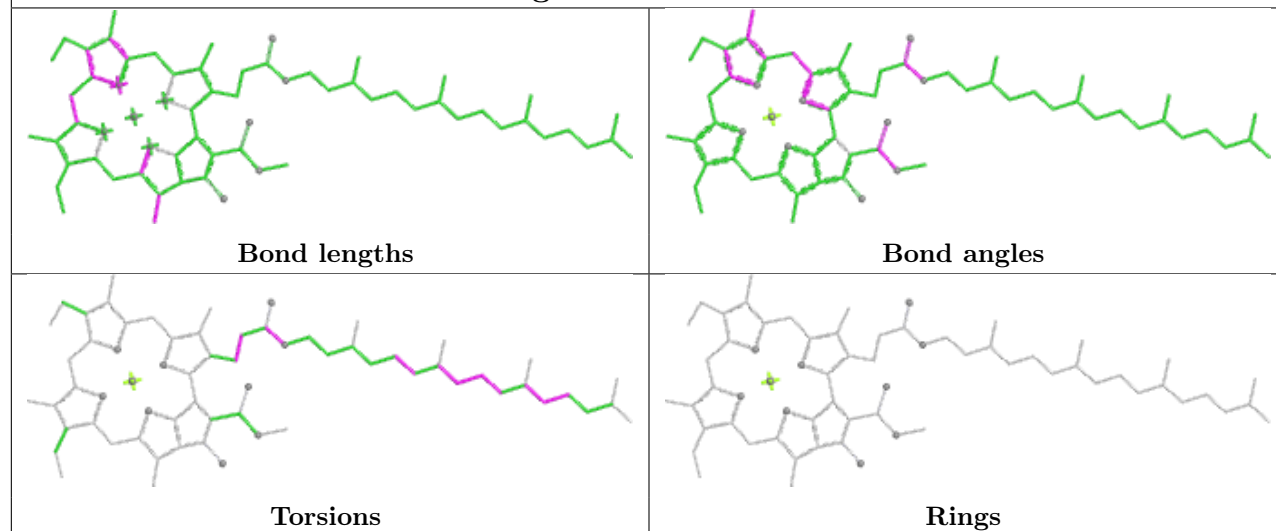
## Ligand CLA S 606



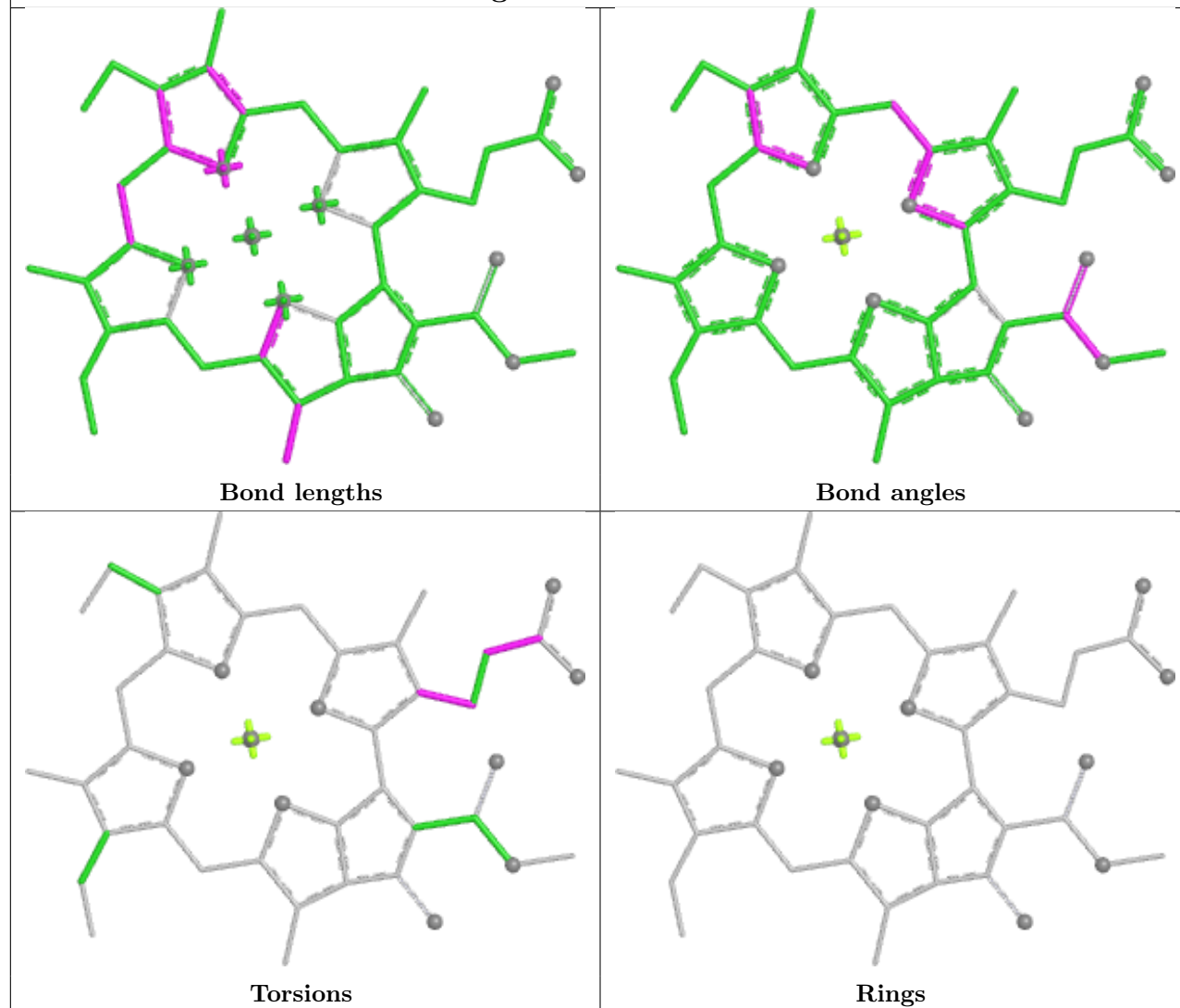
## Ligand CLA B 808



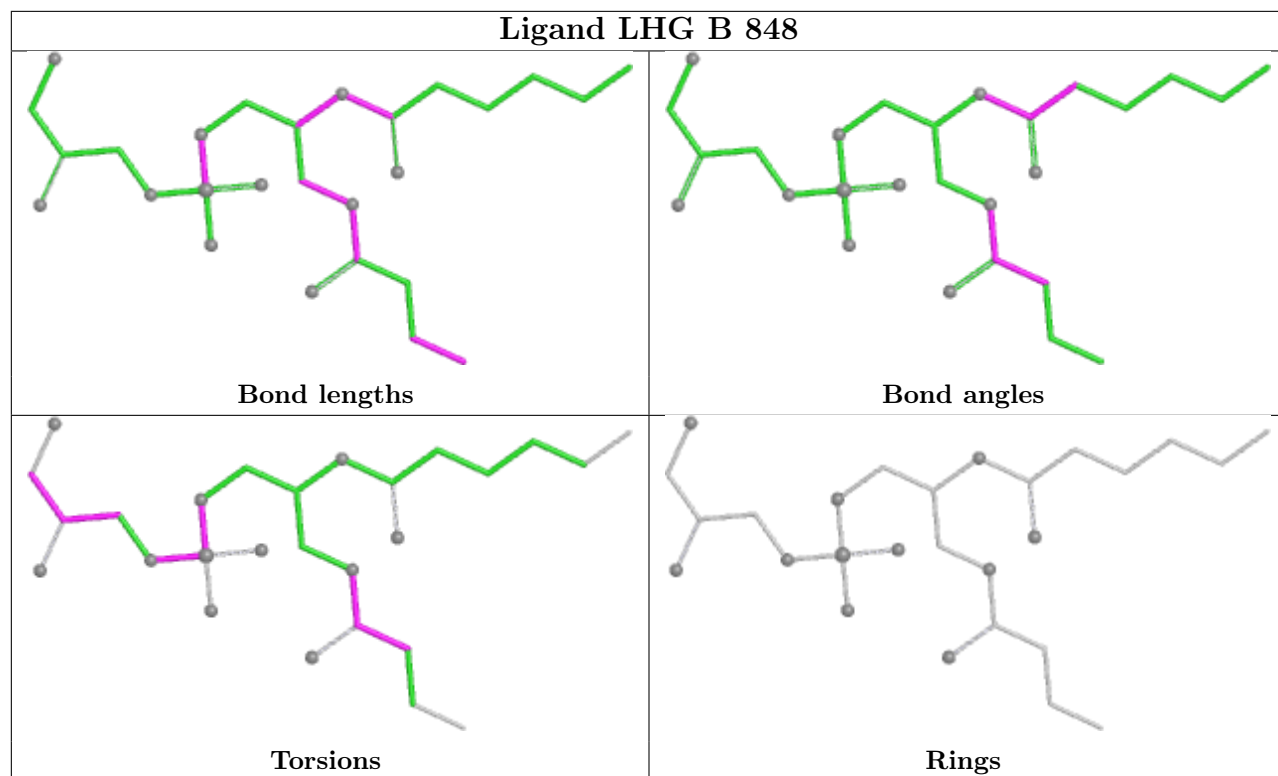
## Ligand CLA B 835

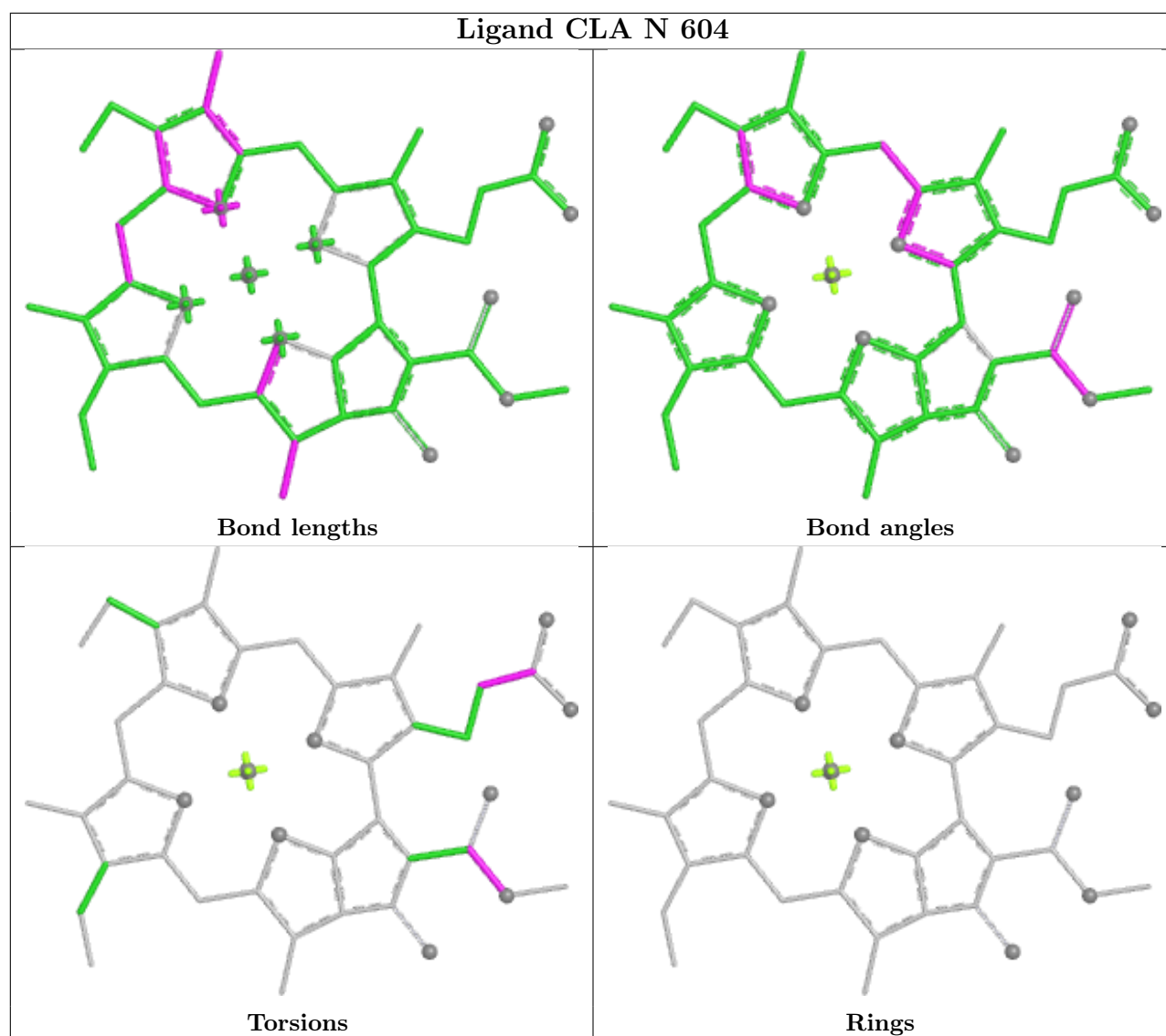


## Ligand CLA H 312

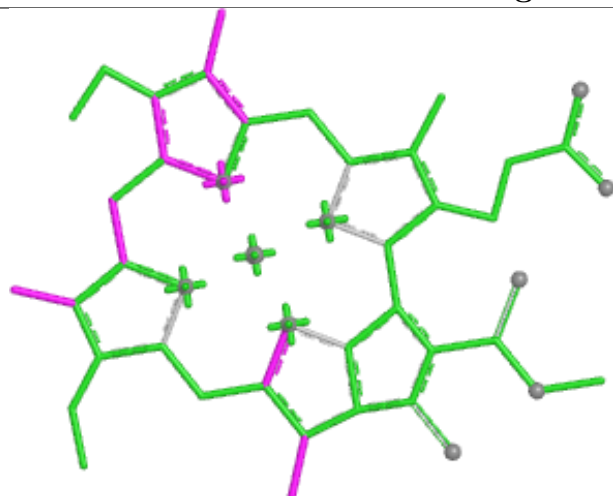




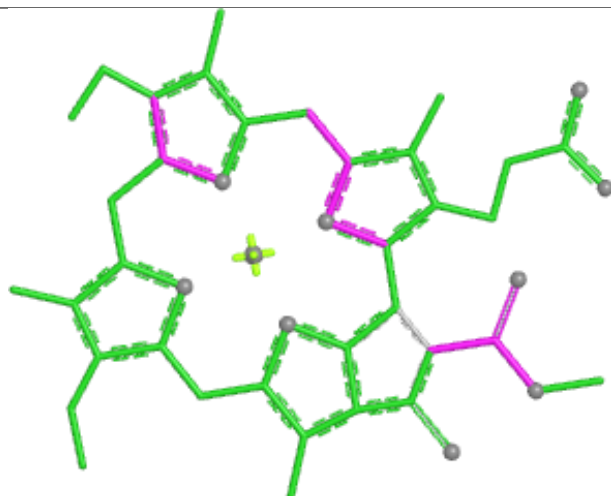




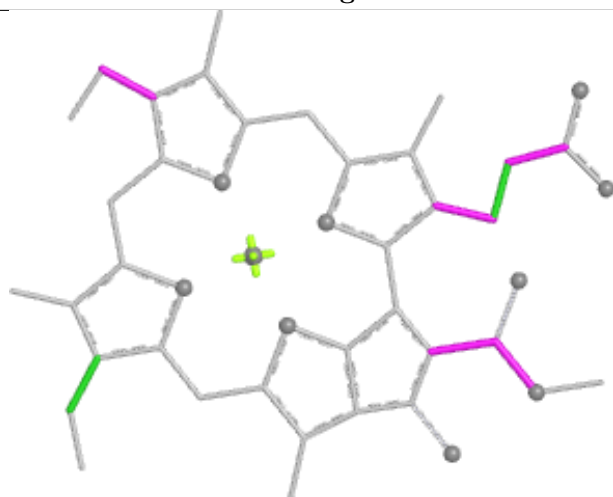
## Ligand CLA P 608



Bond lengths



Bond angles

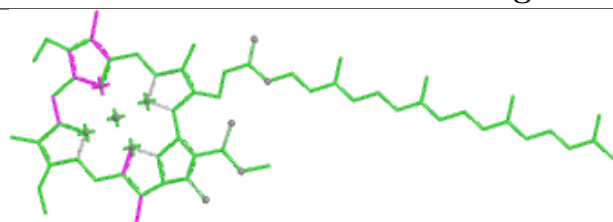


Torsions

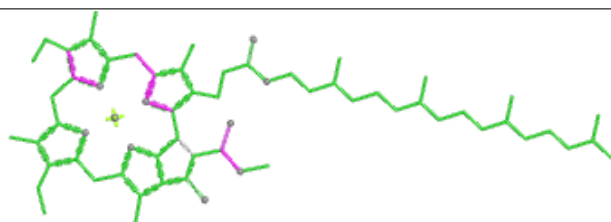


Rings

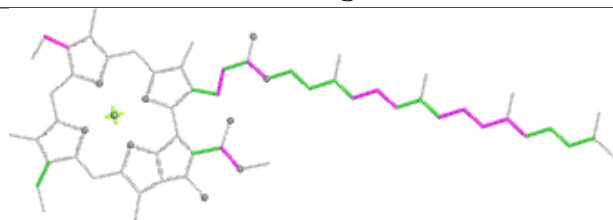
## Ligand CLA V 612



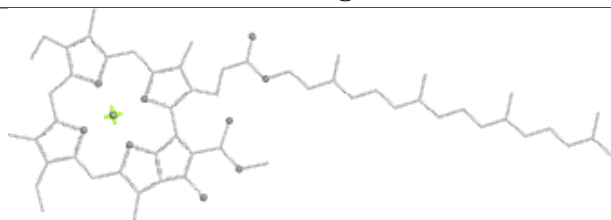
Bond lengths



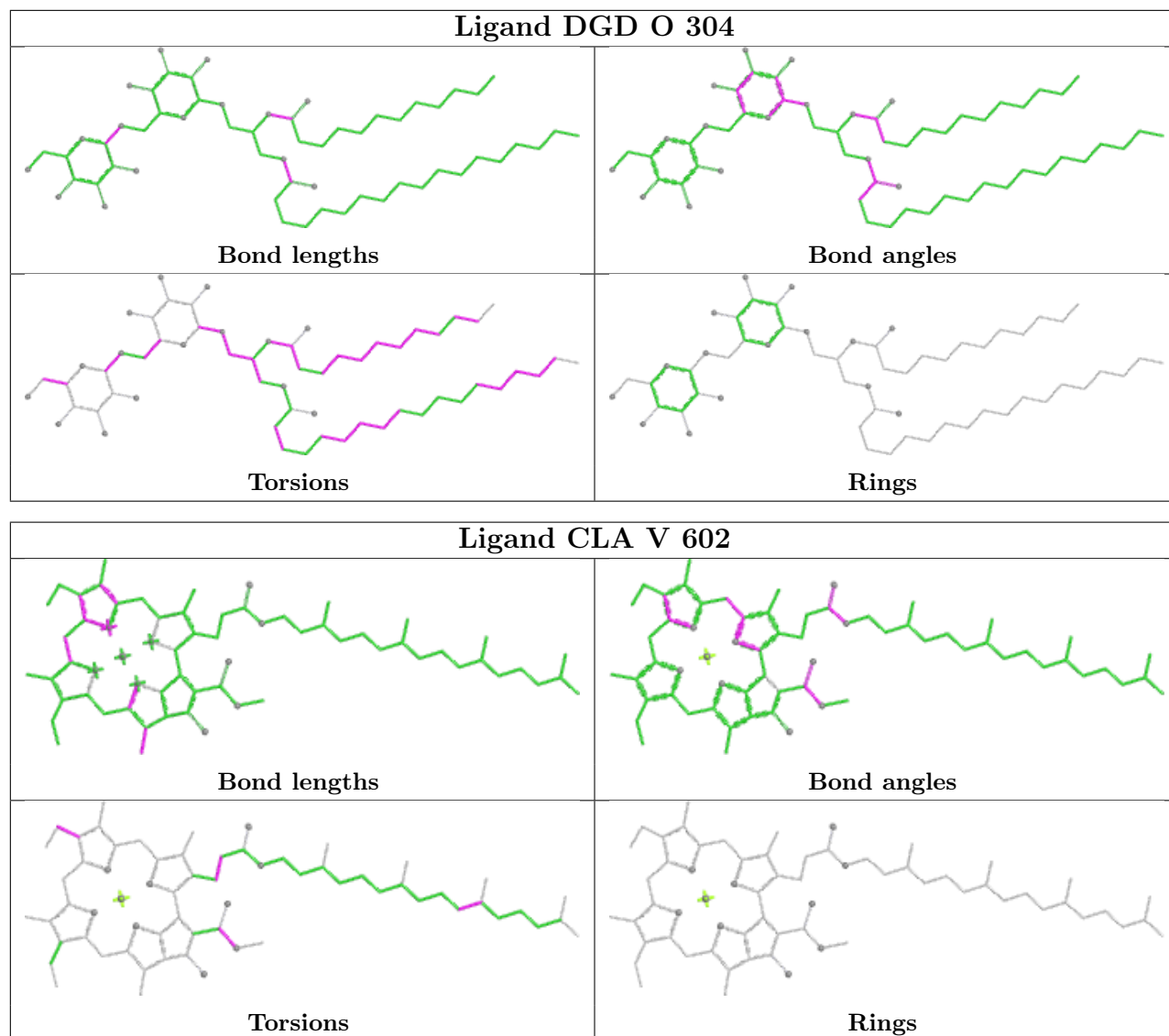
Bond angles



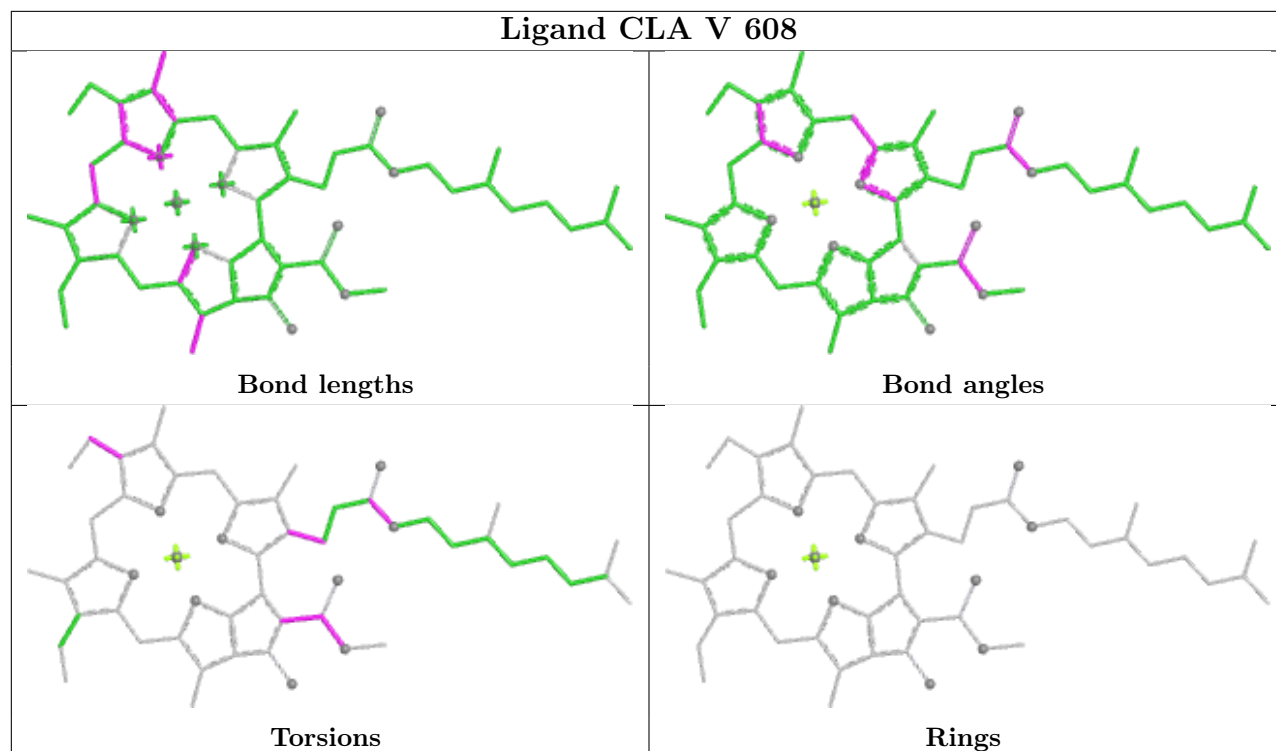
Torsions



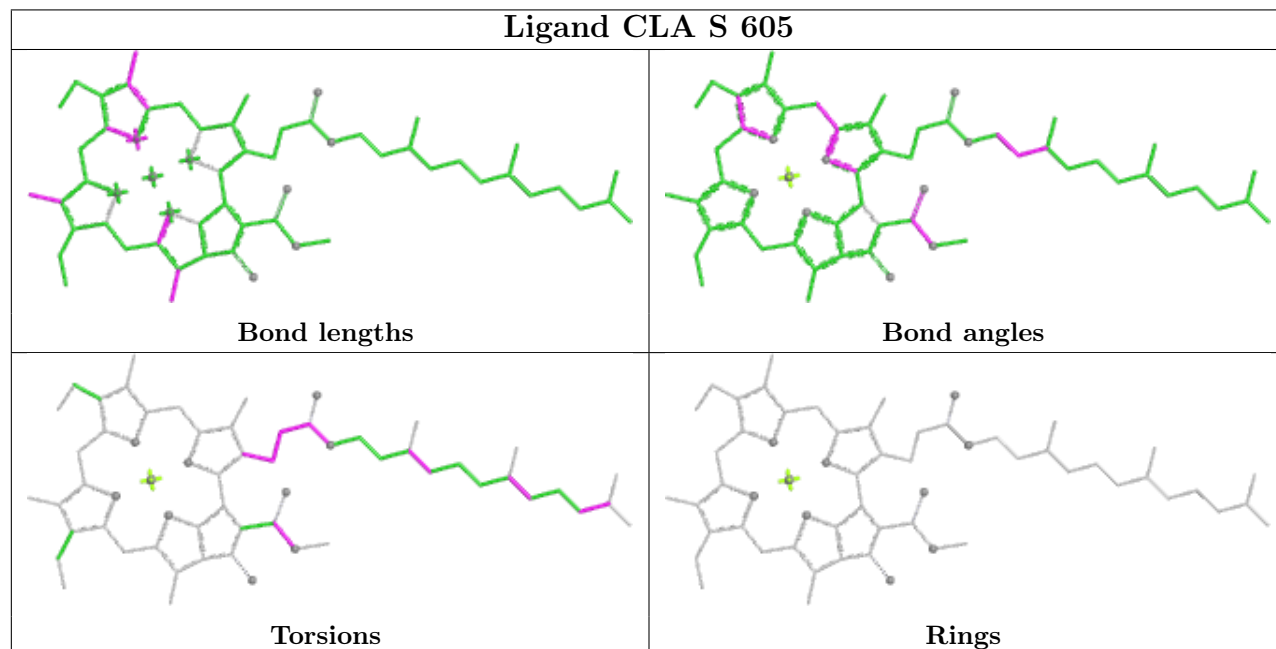
Rings

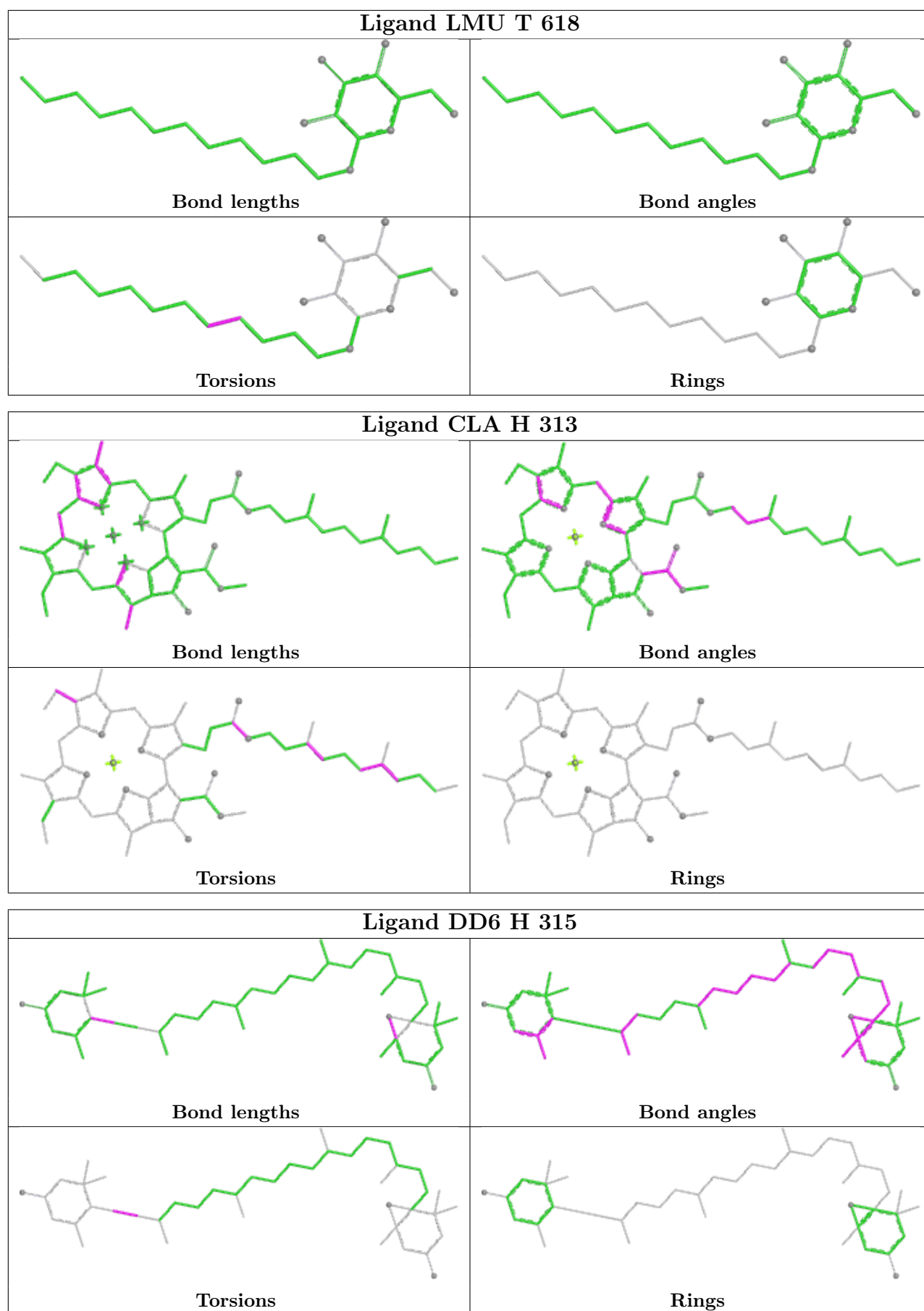


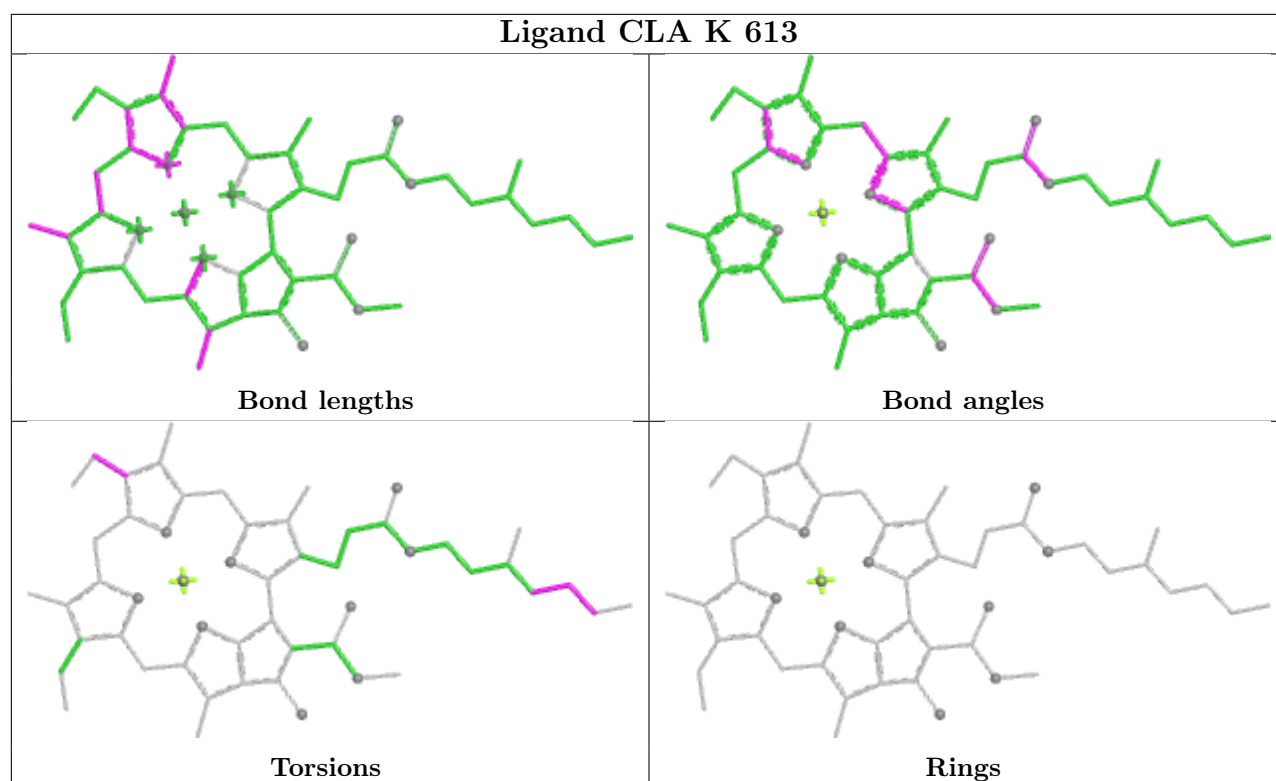
## Ligand CLA V 608

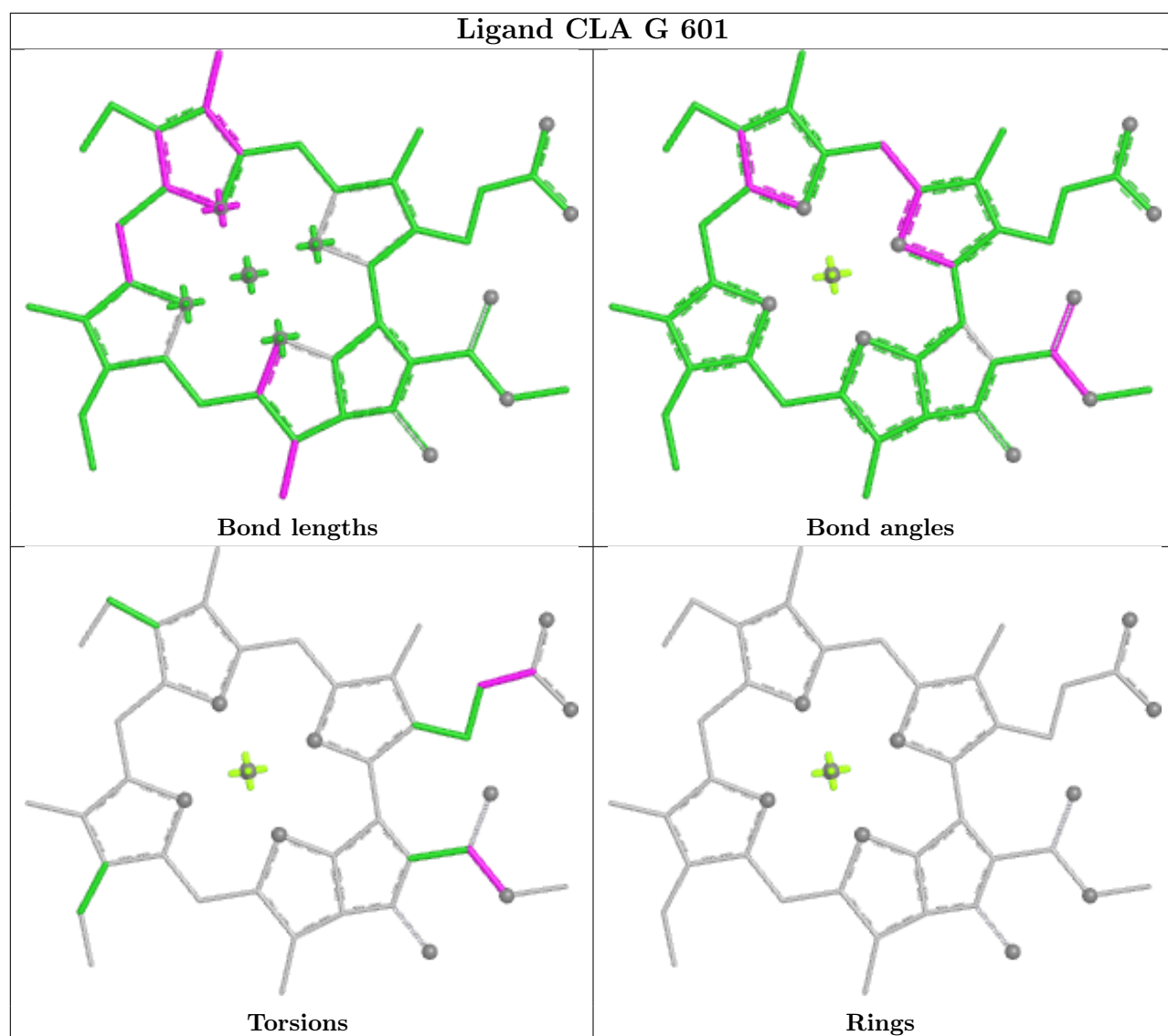


## Ligand CLA S 605

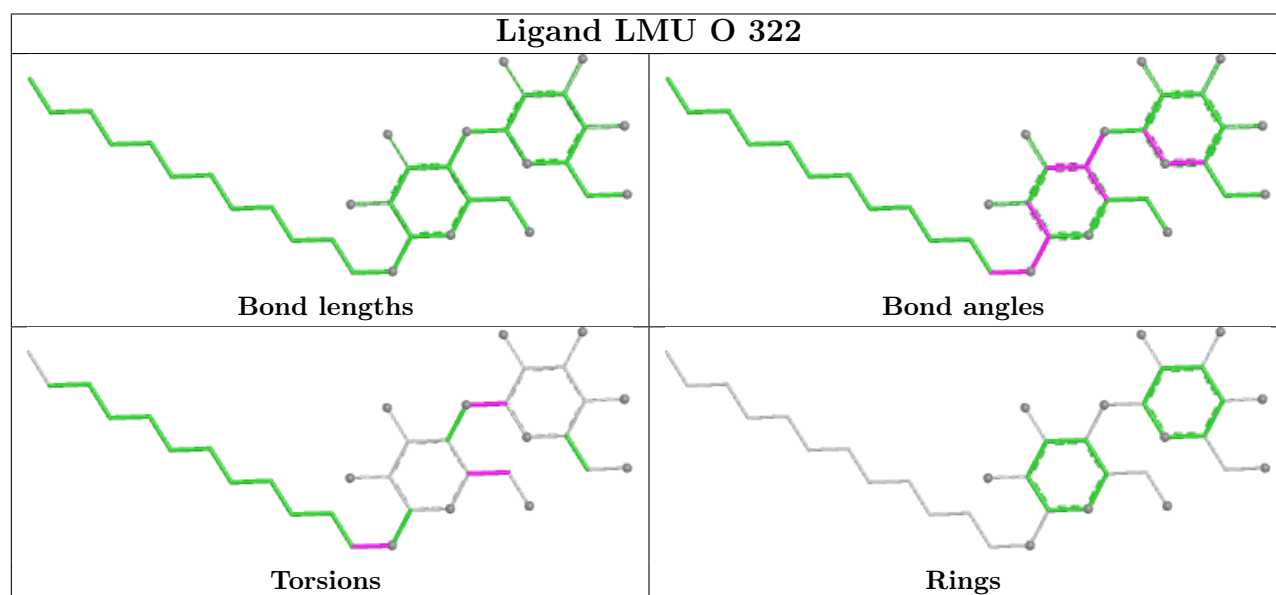
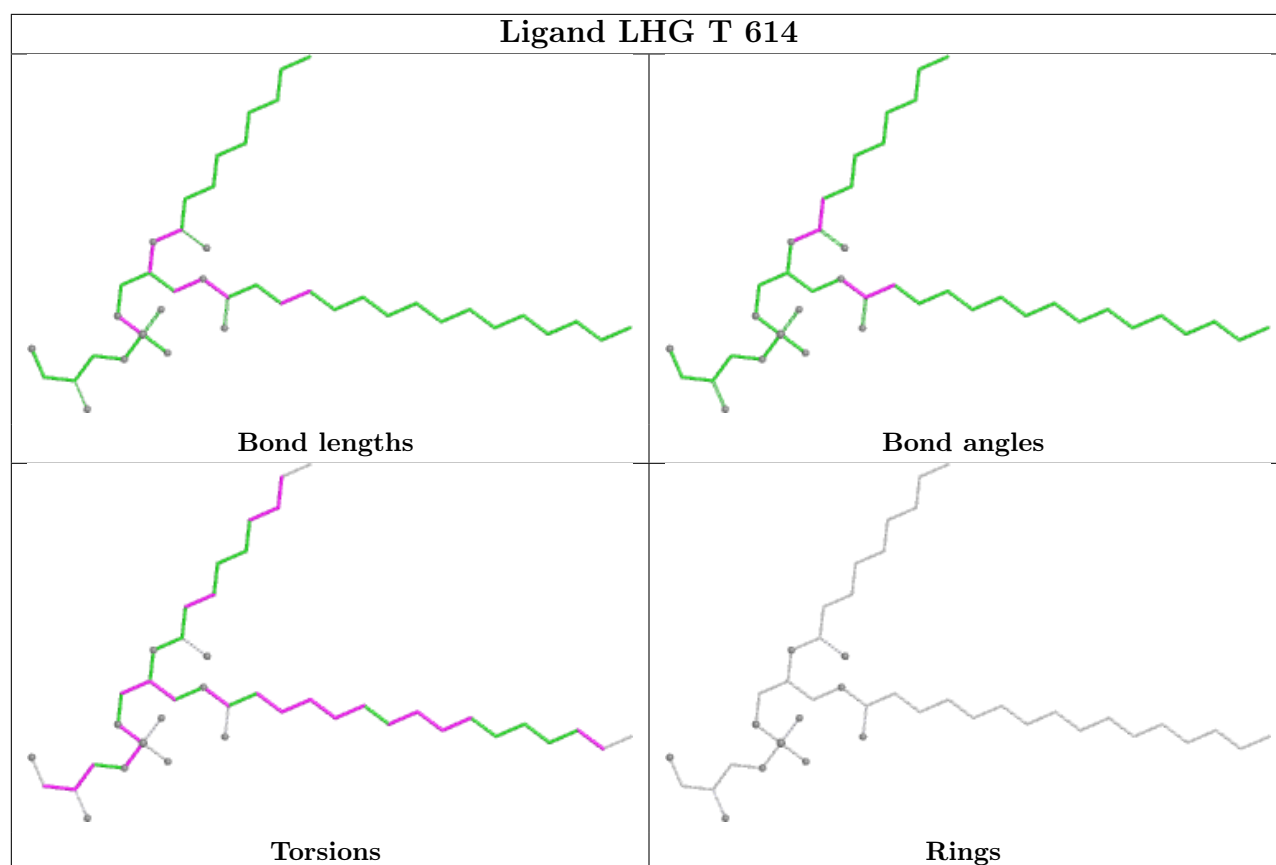


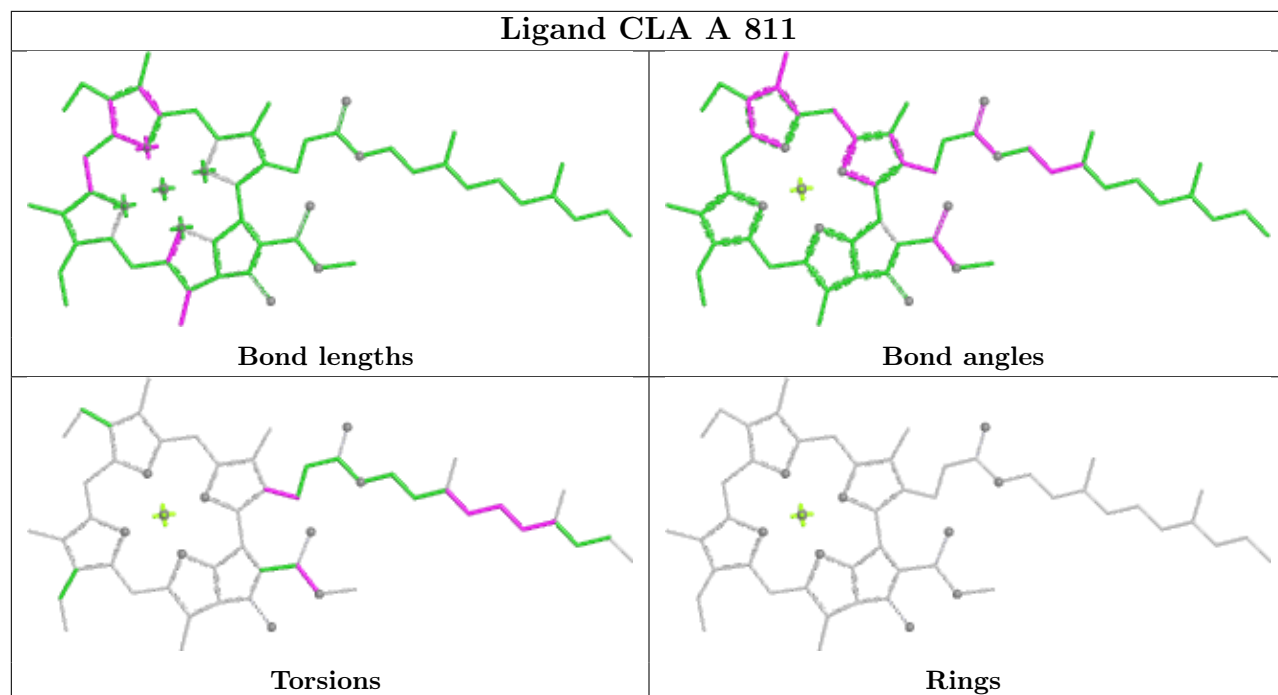




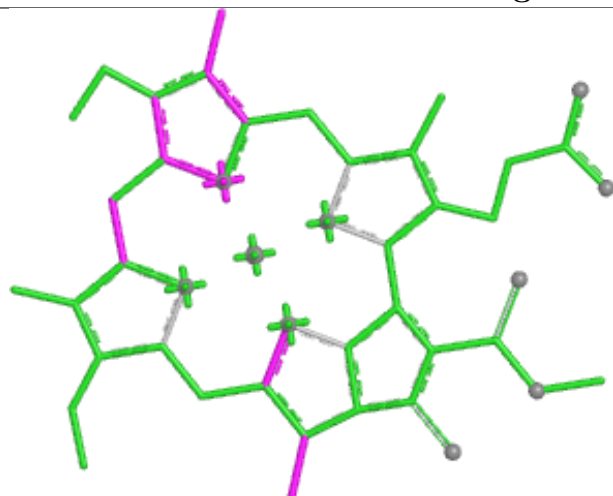




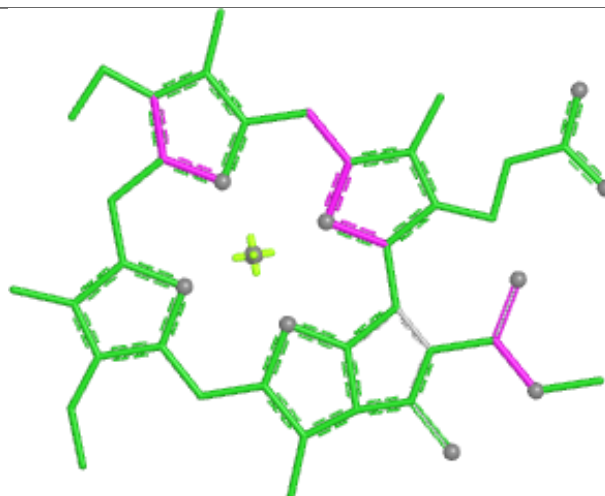




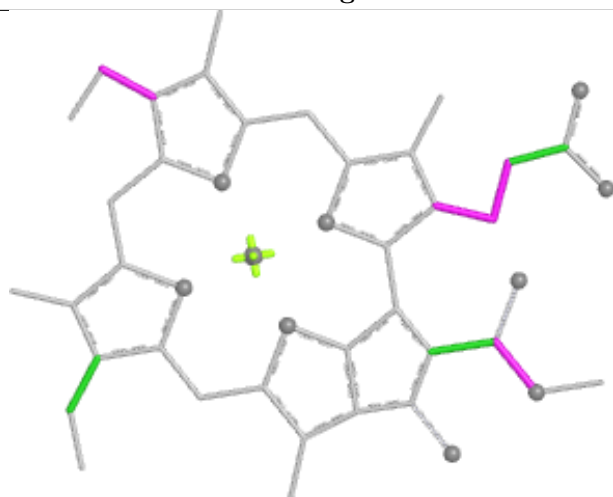
## Ligand CLA U 415



Bond lengths



Bond angles

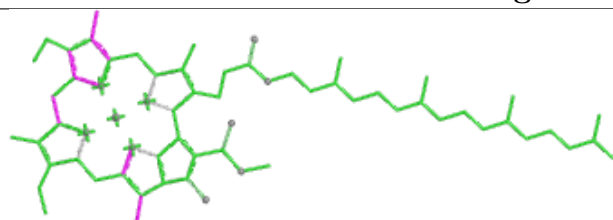


Torsions

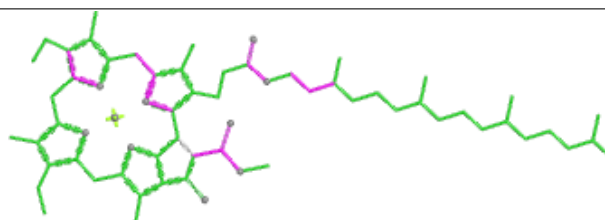


Rings

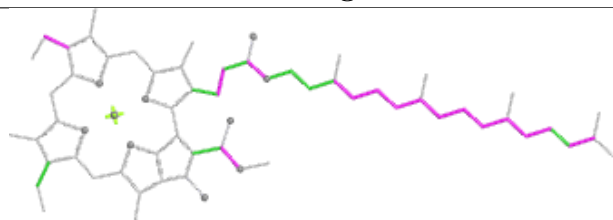
## Ligand CLA A 824



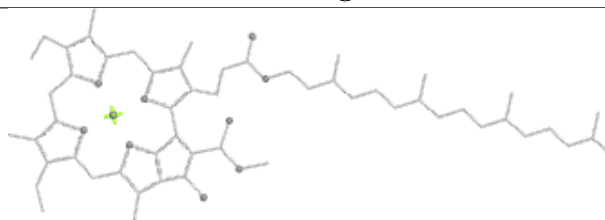
Bond lengths



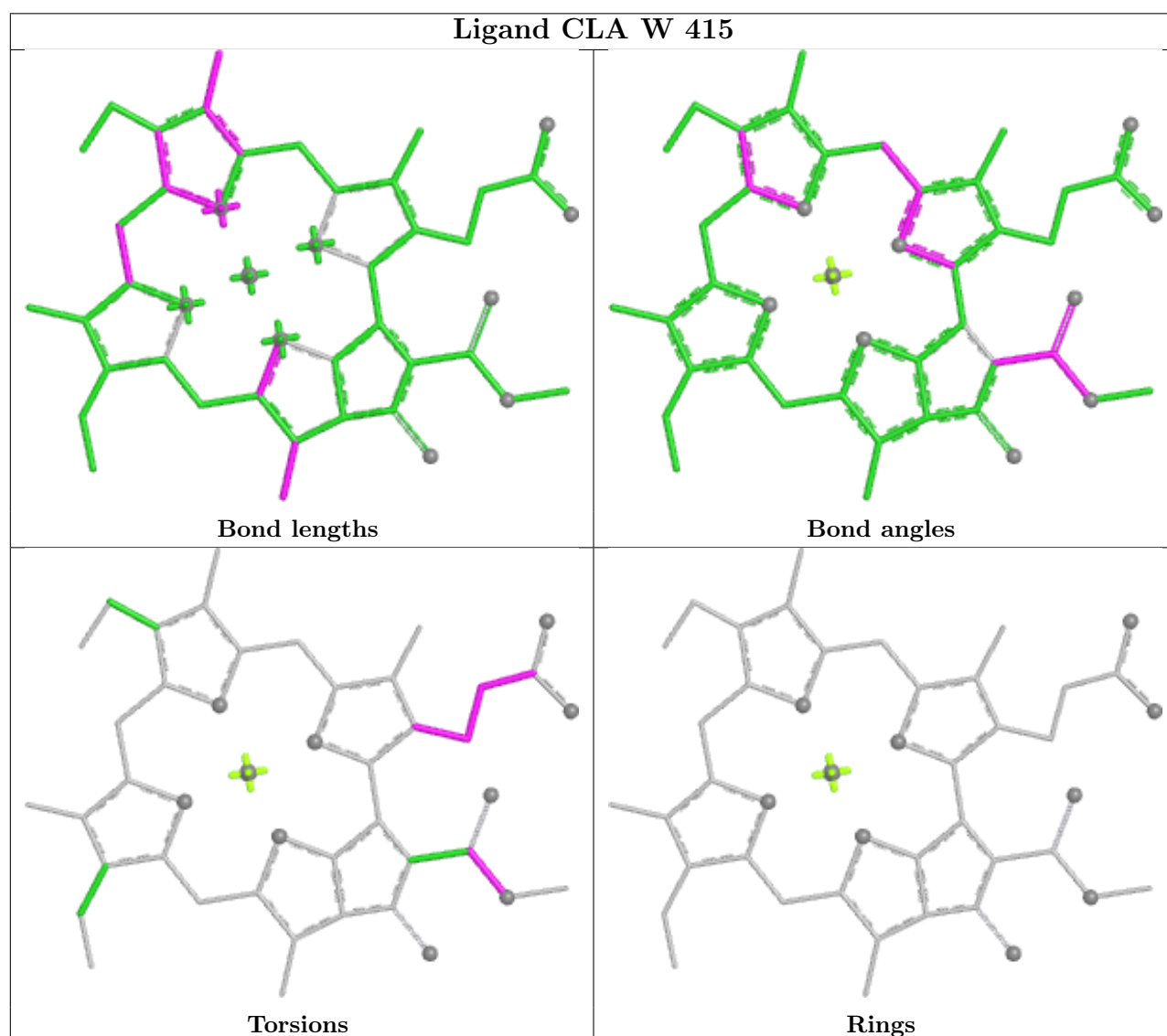
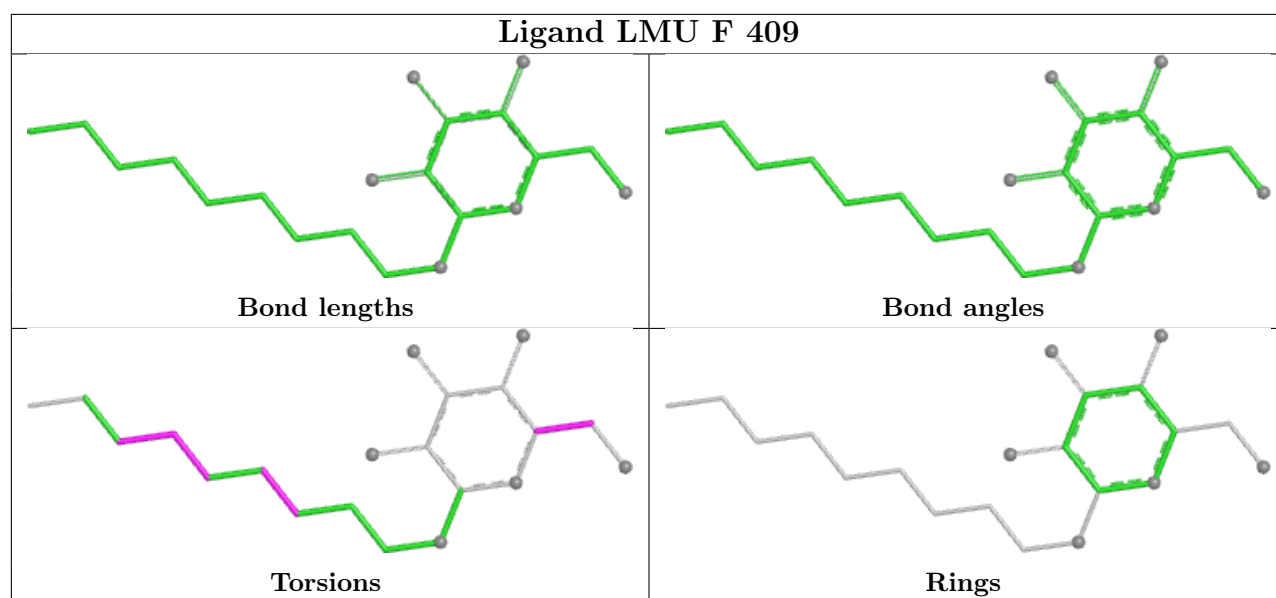
Bond angles

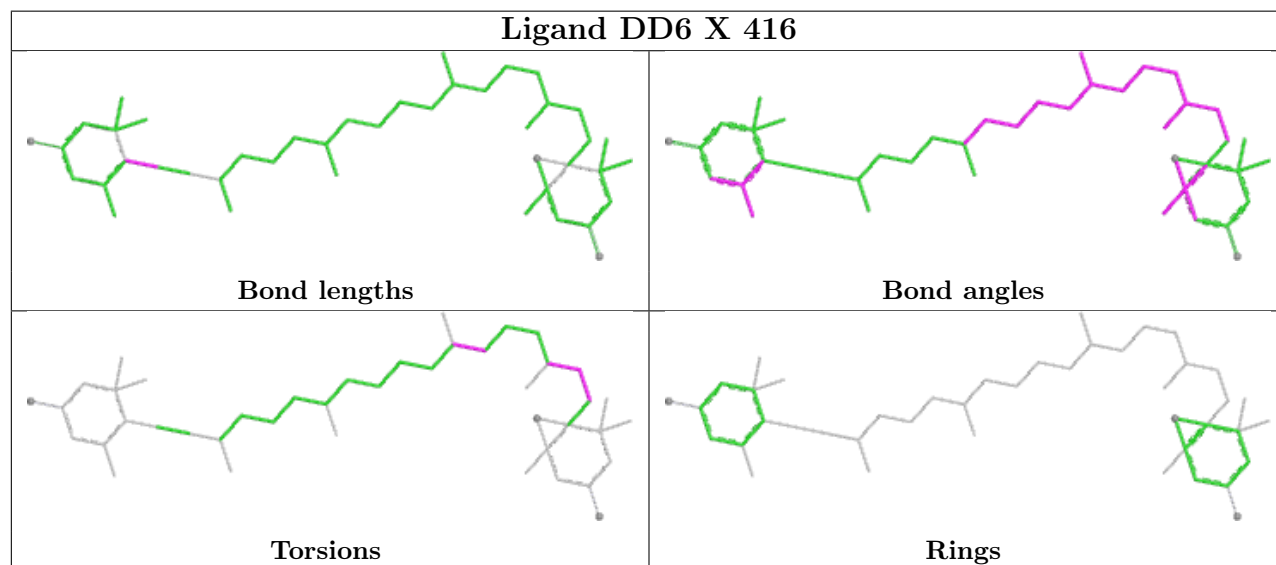
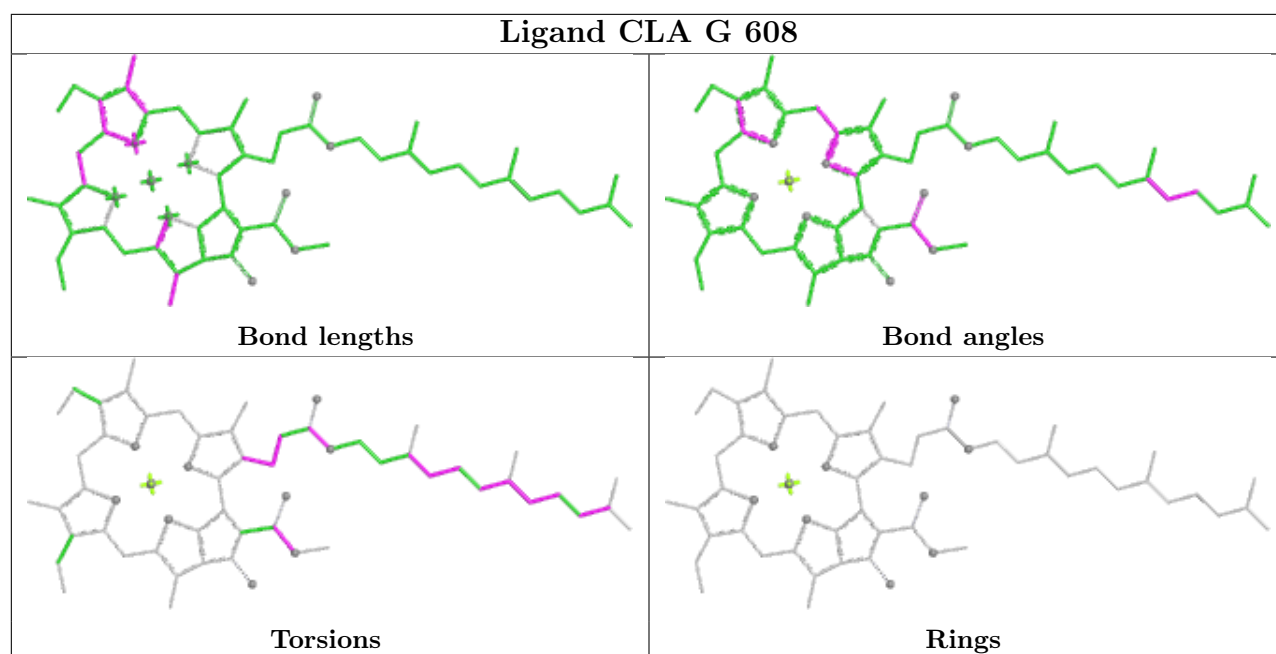


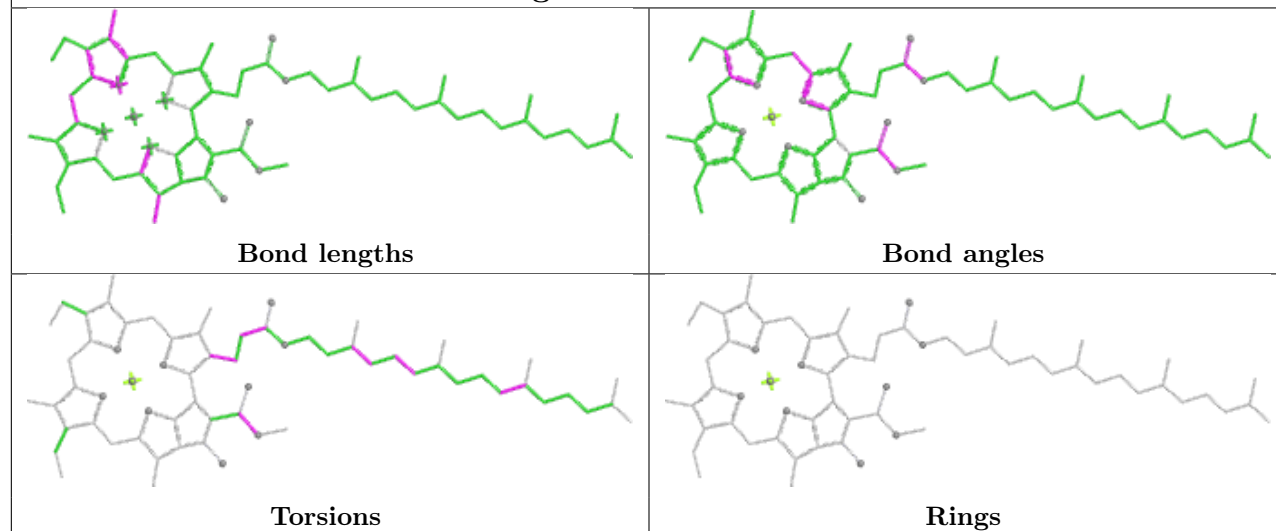
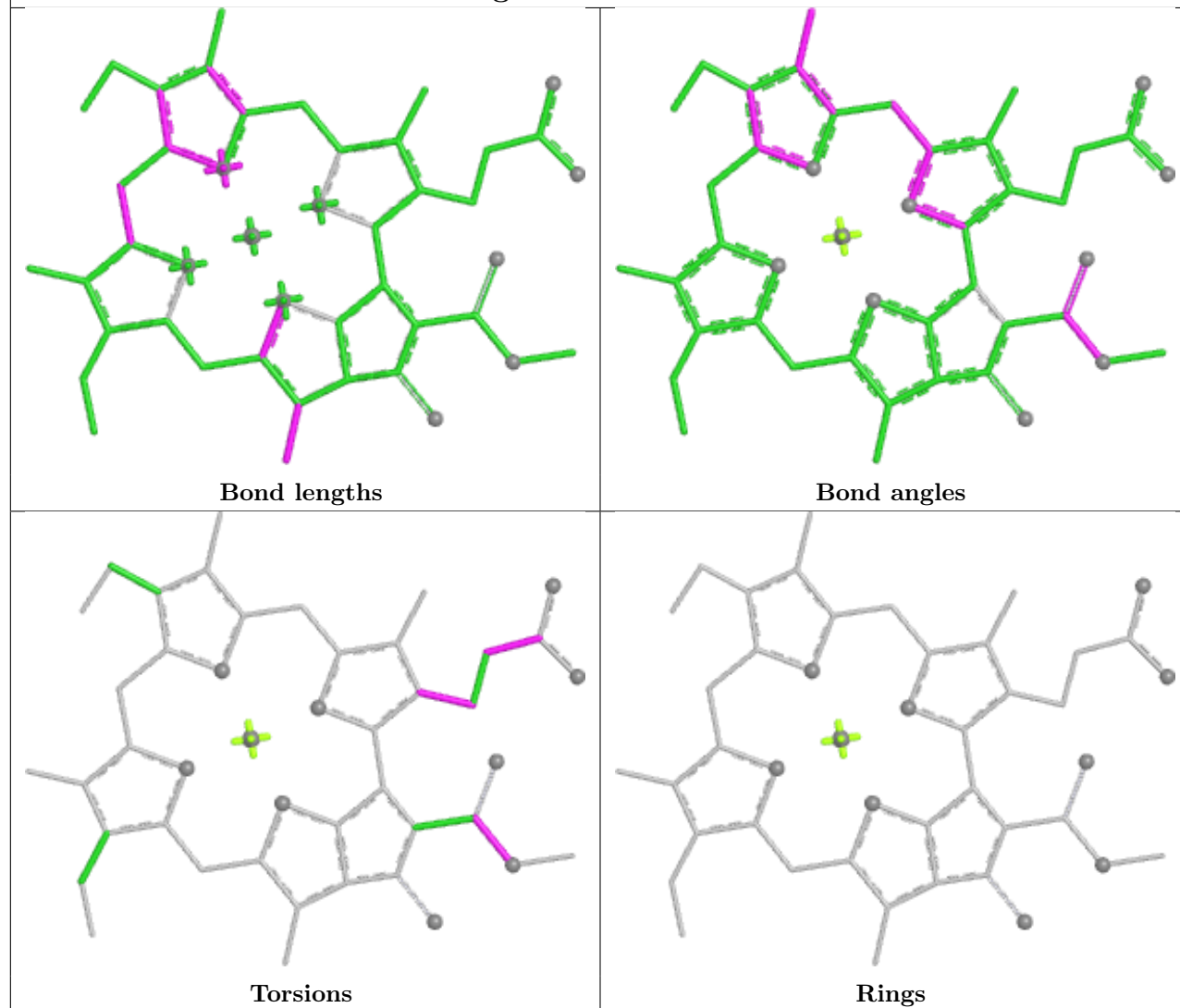
Torsions

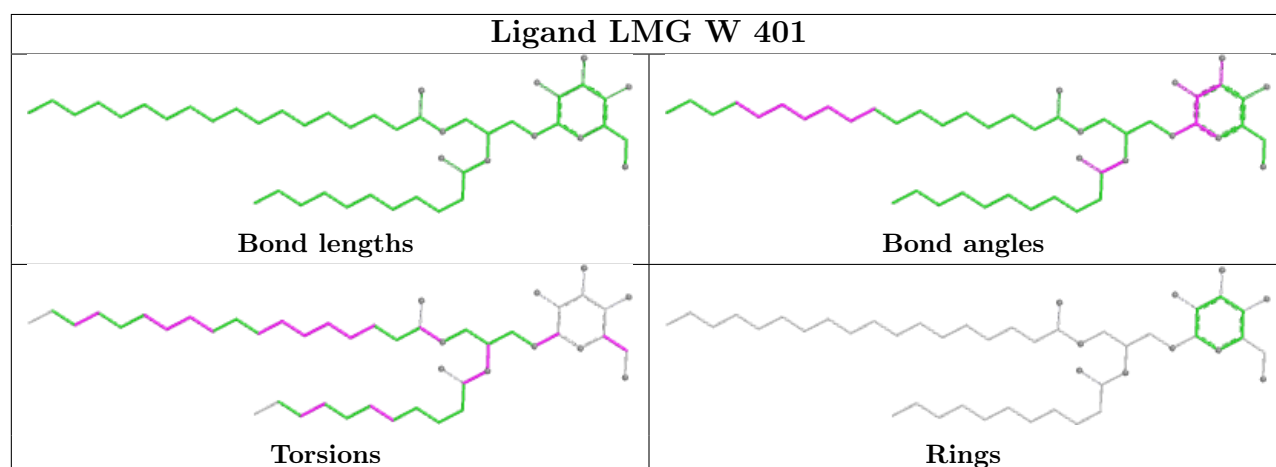
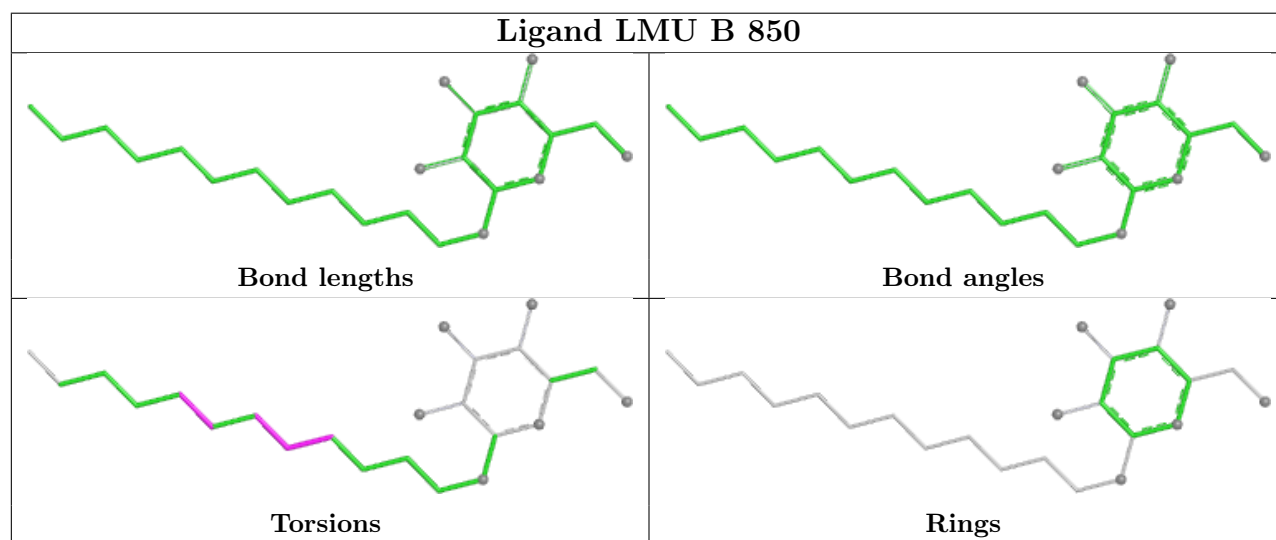
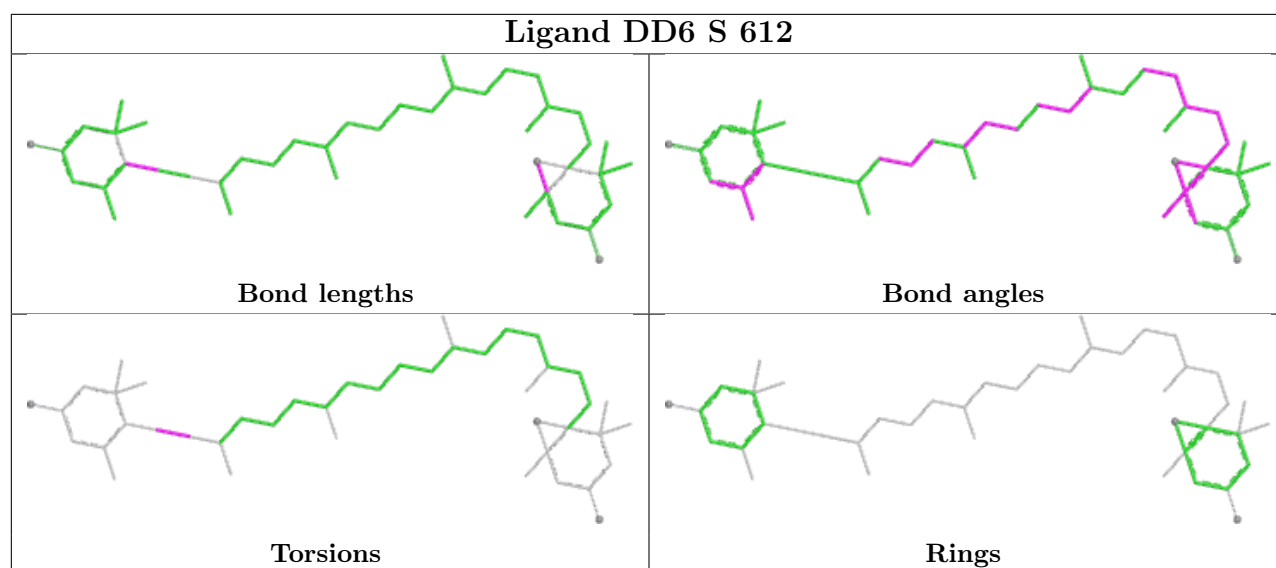


Rings

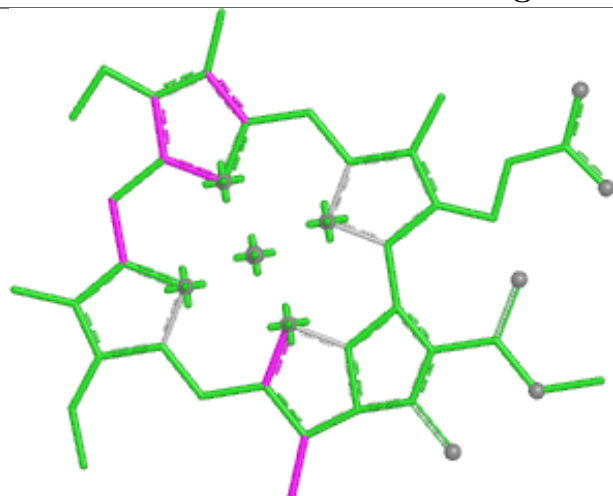




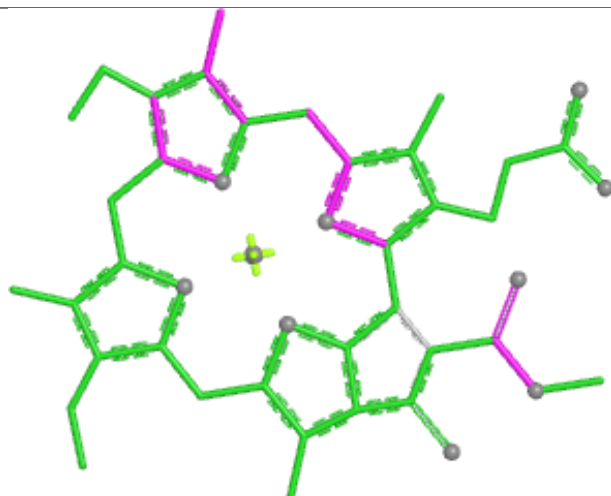
**Ligand CLA B 822****Ligand CLA P 606**



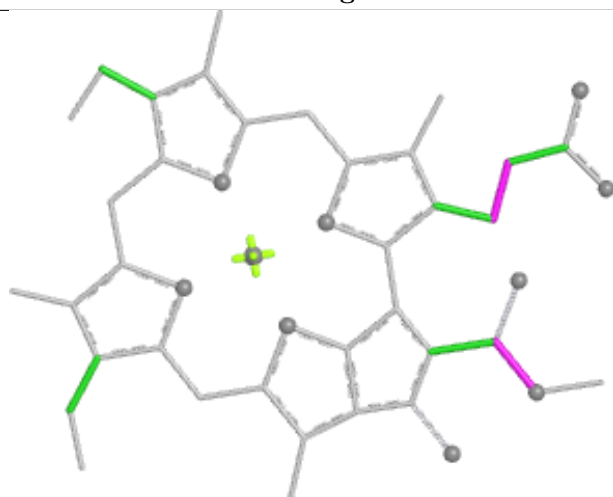
## Ligand CLA V 607



Bond lengths



Bond angles

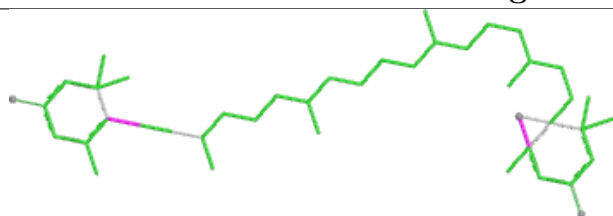


Torsions

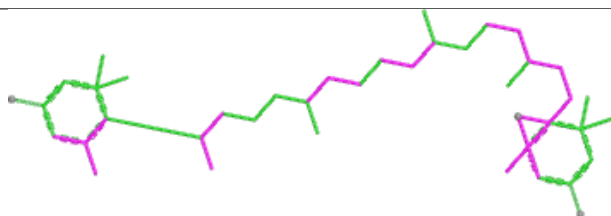


Rings

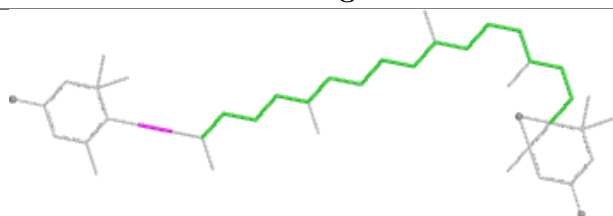
## Ligand DD6 W 417



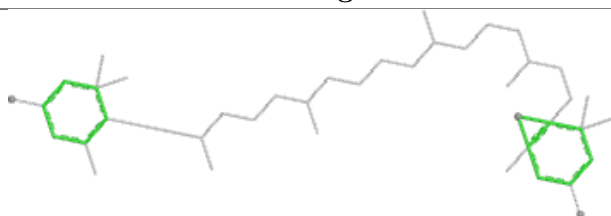
Bond lengths



Bond angles

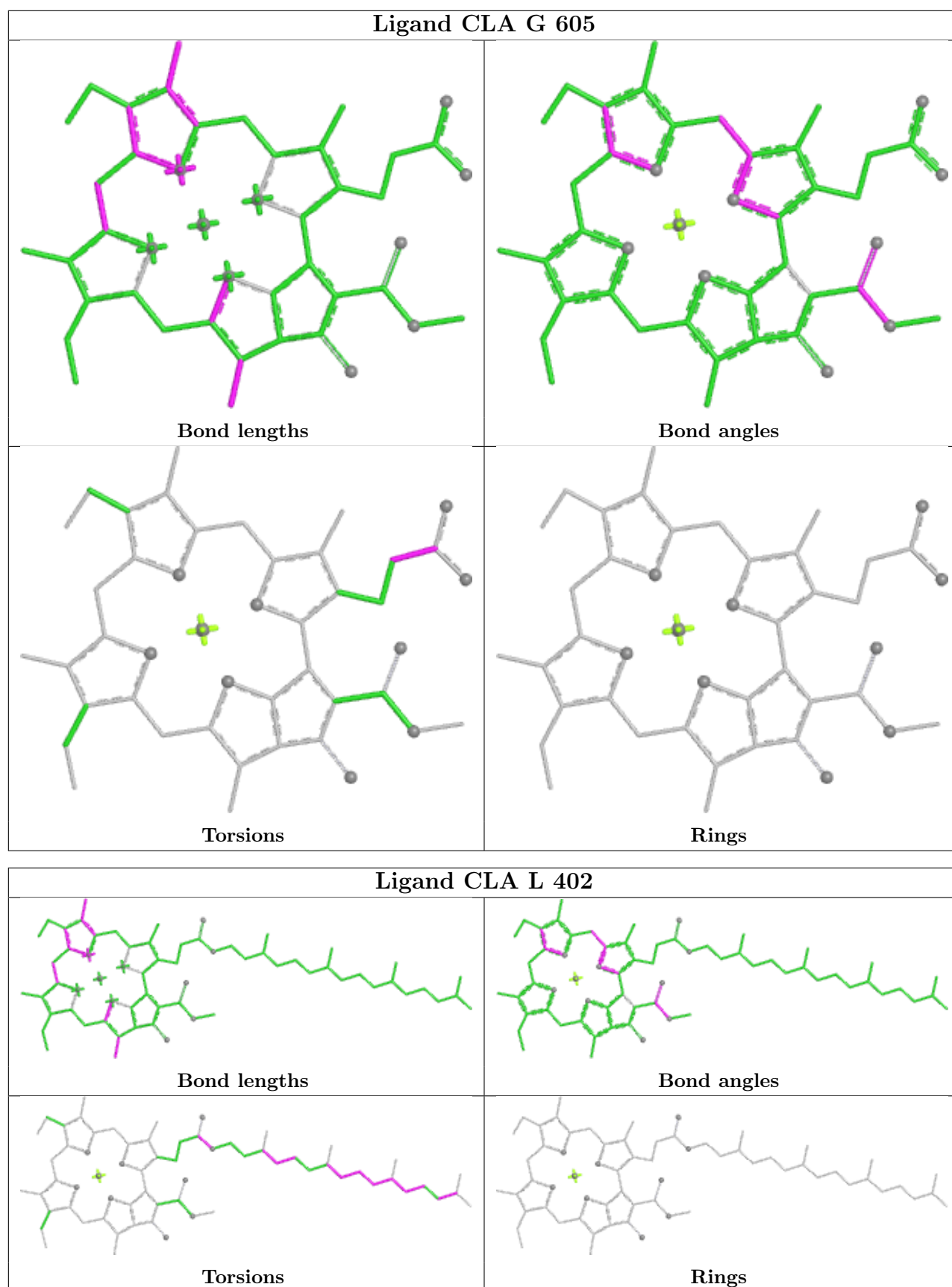


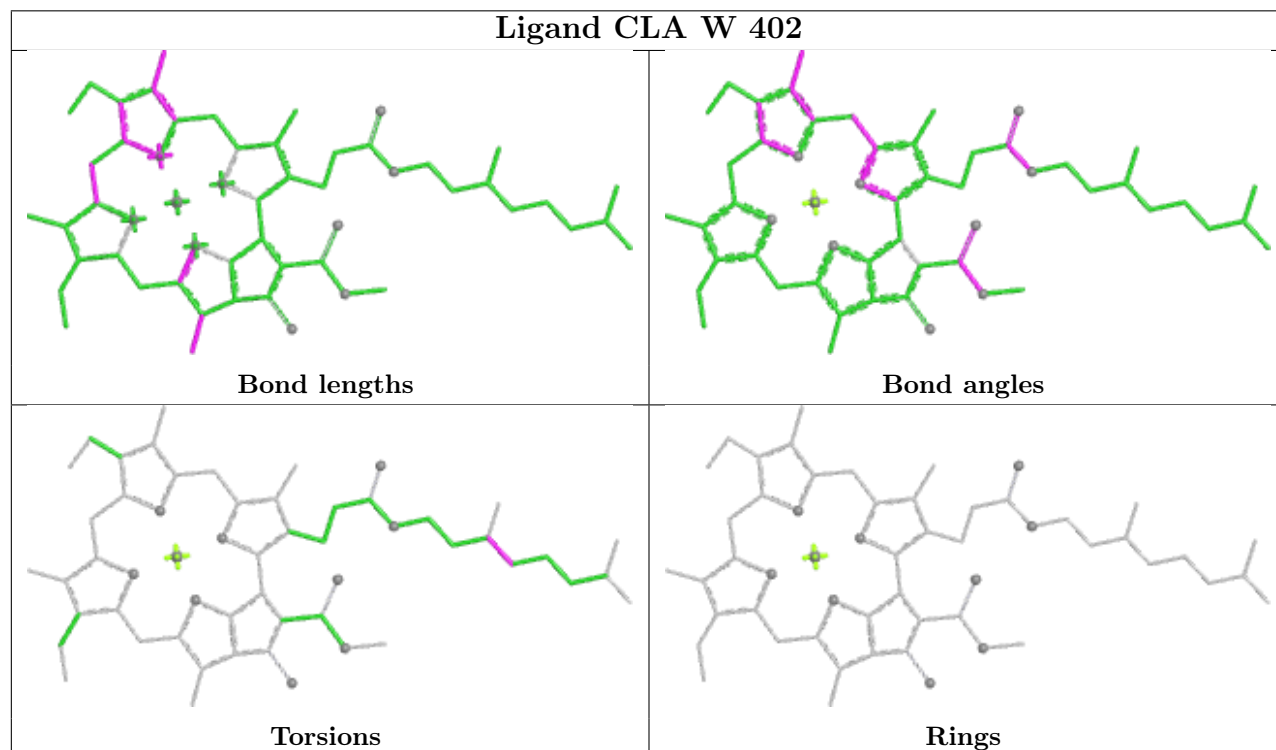
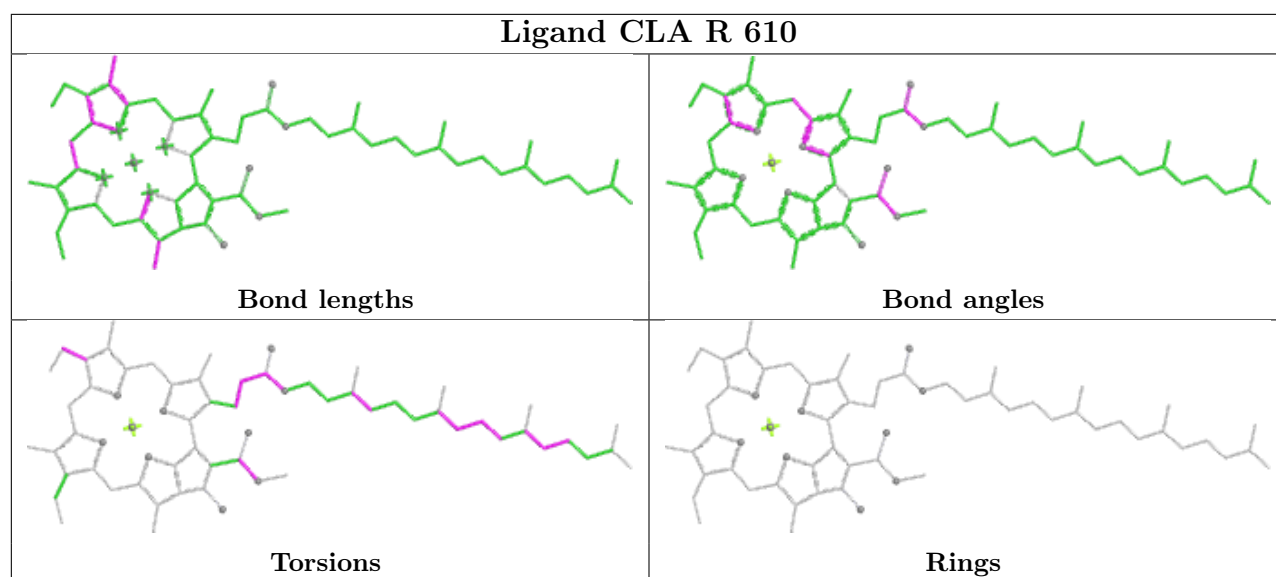
Torsions

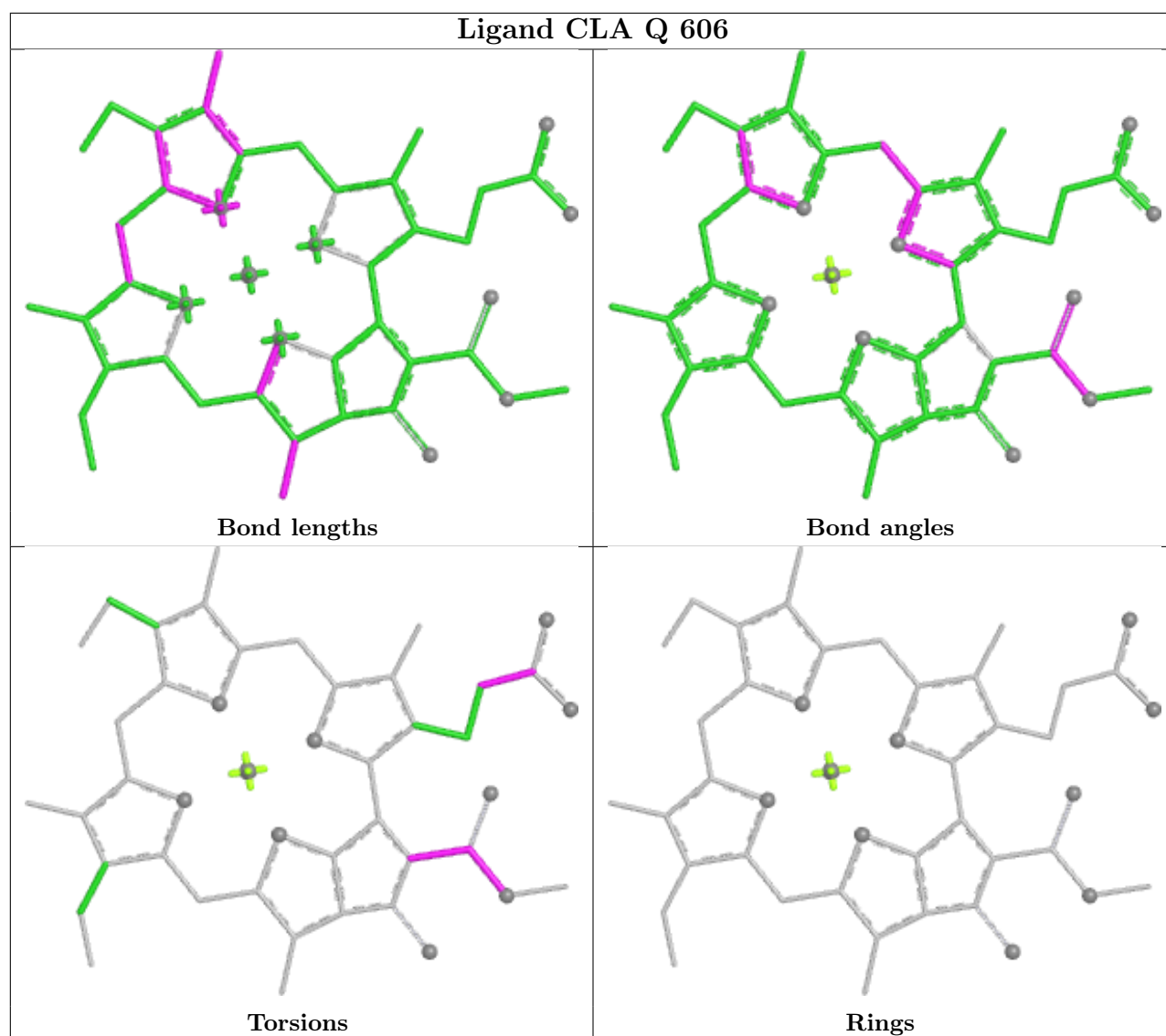


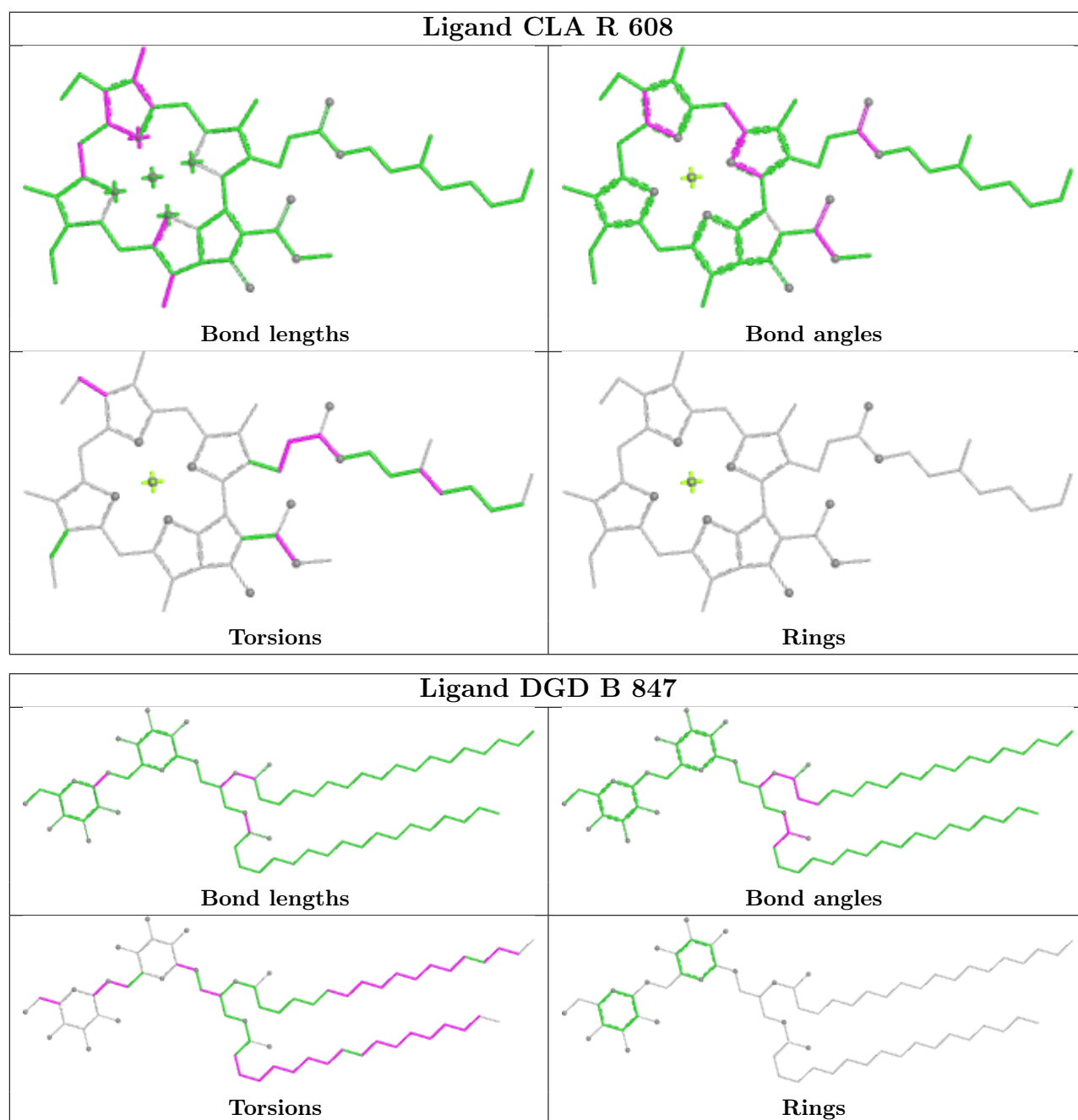
Rings

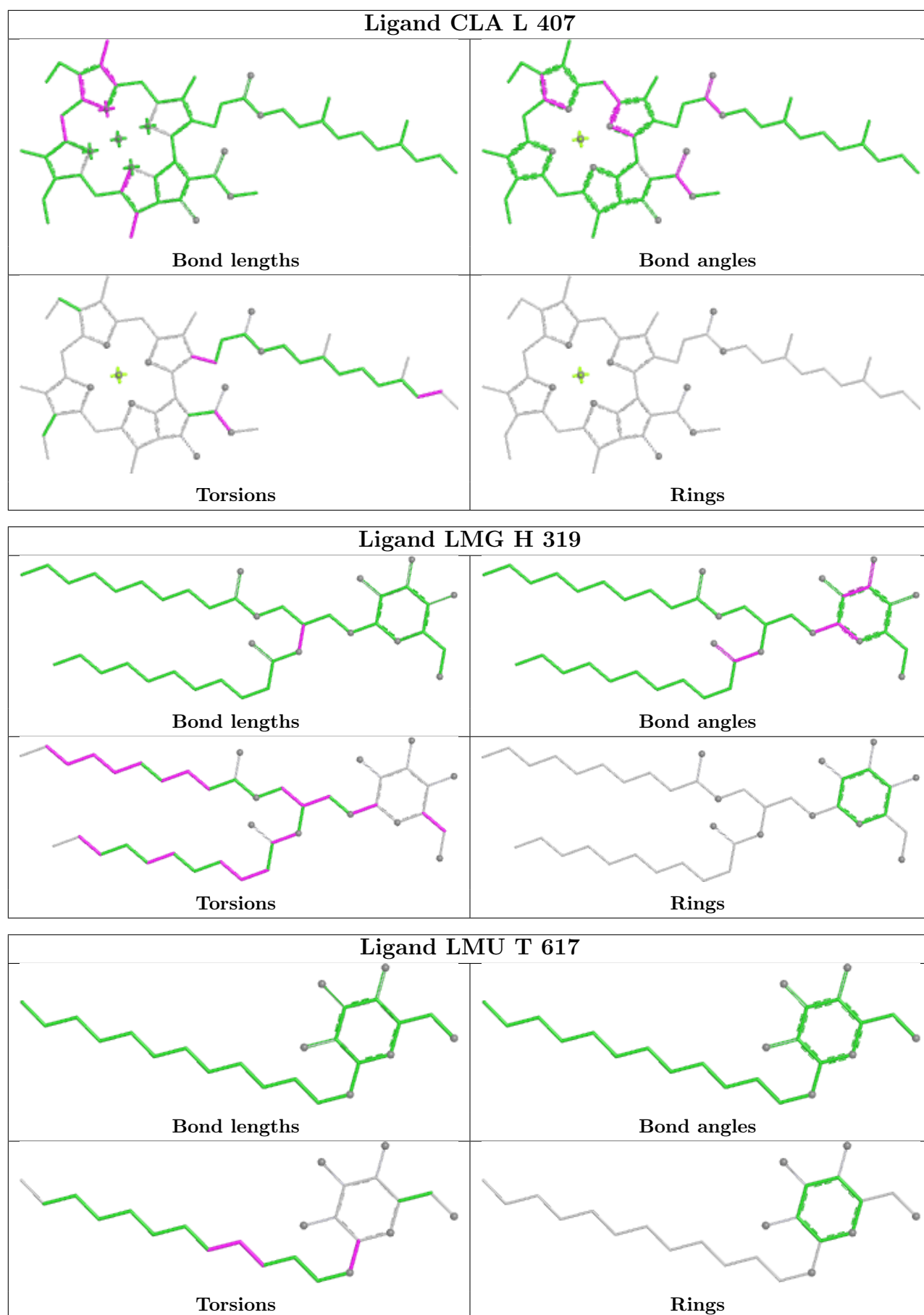


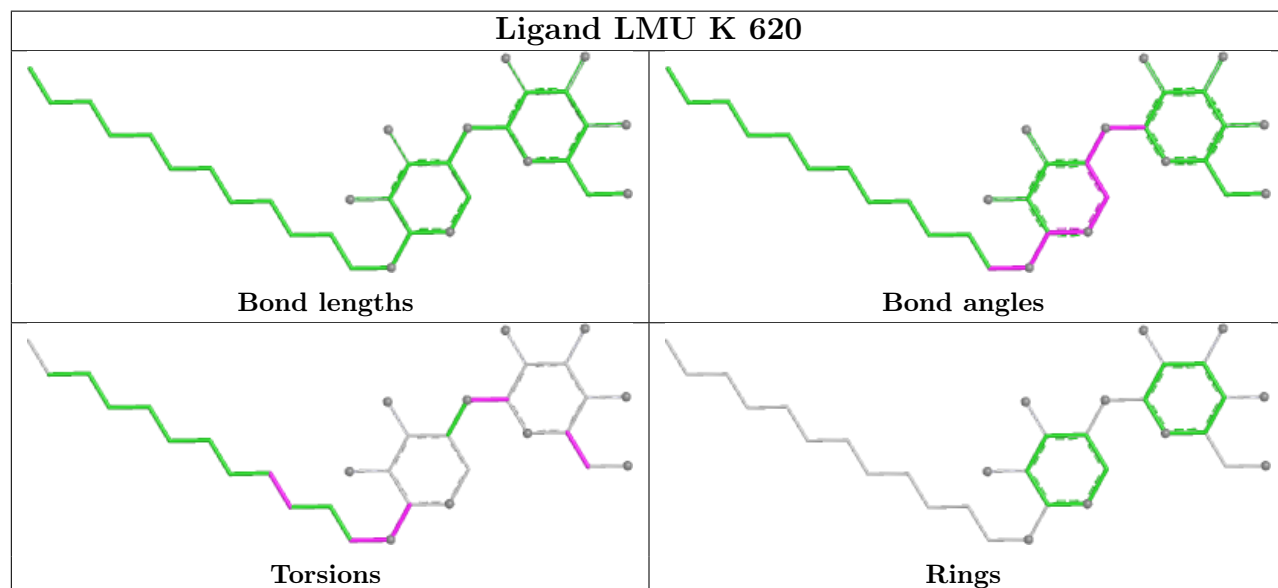
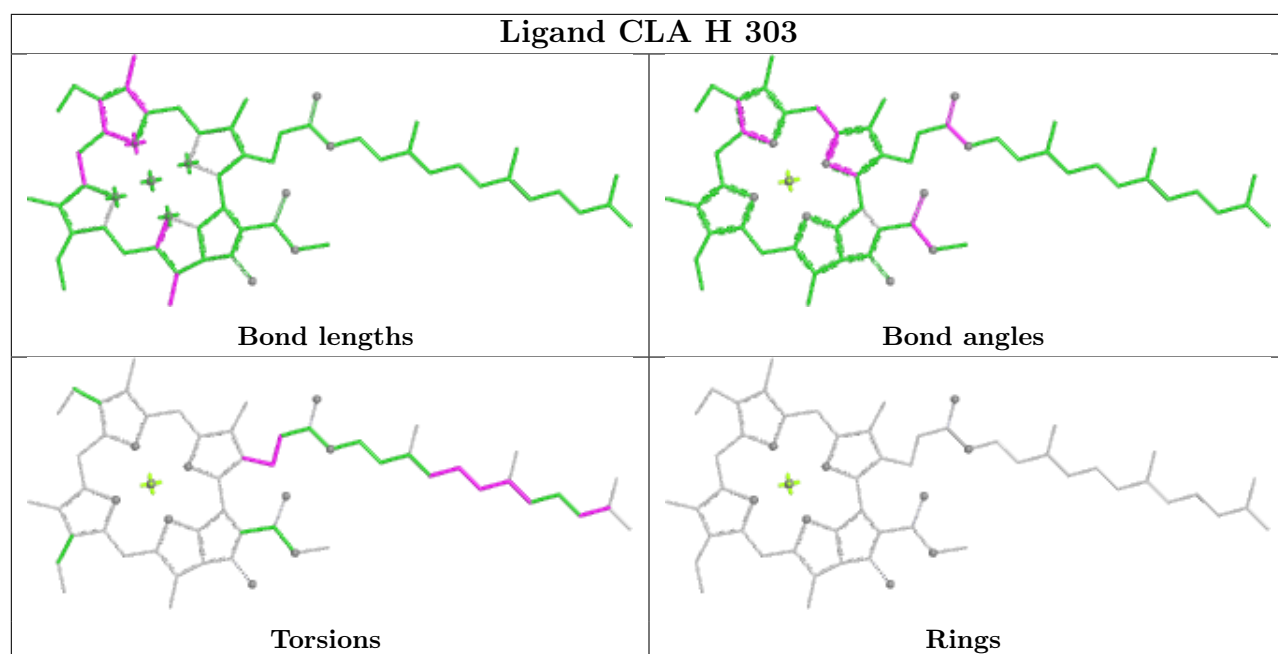


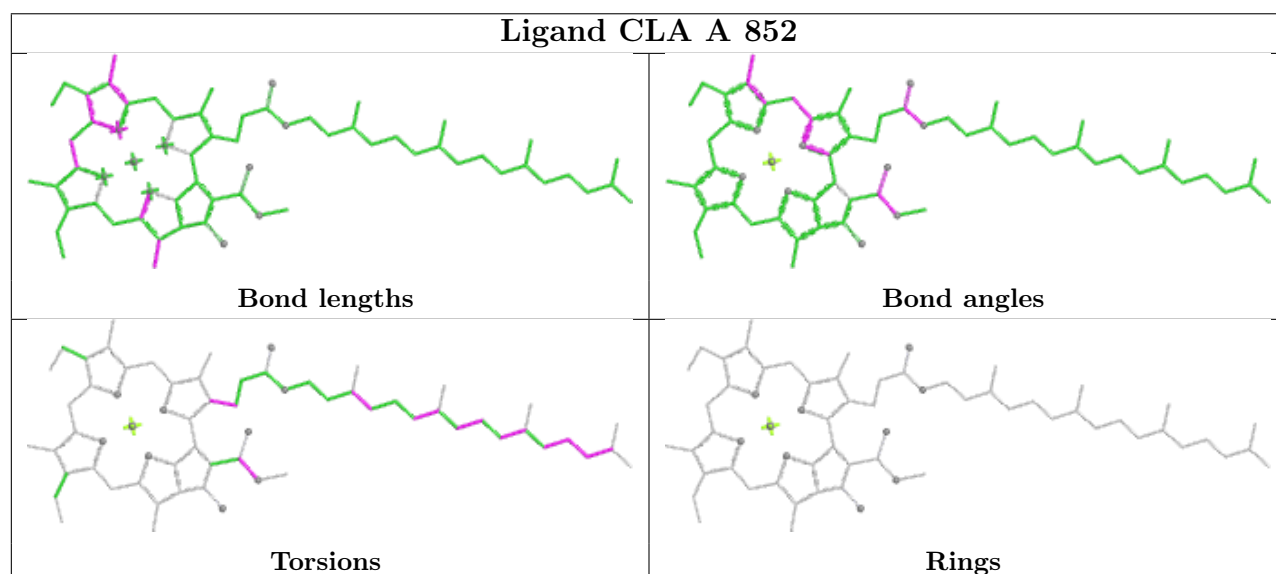
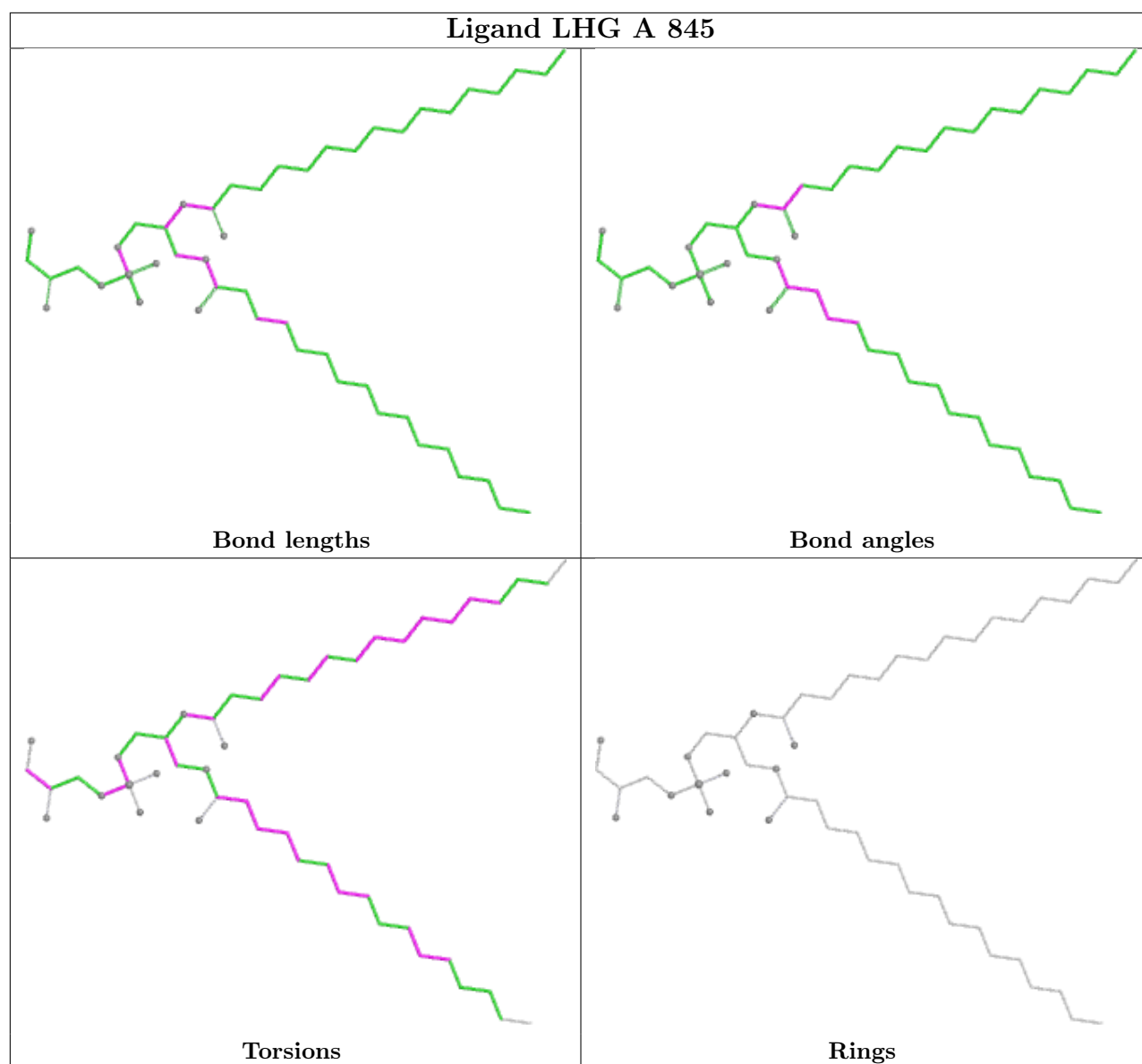


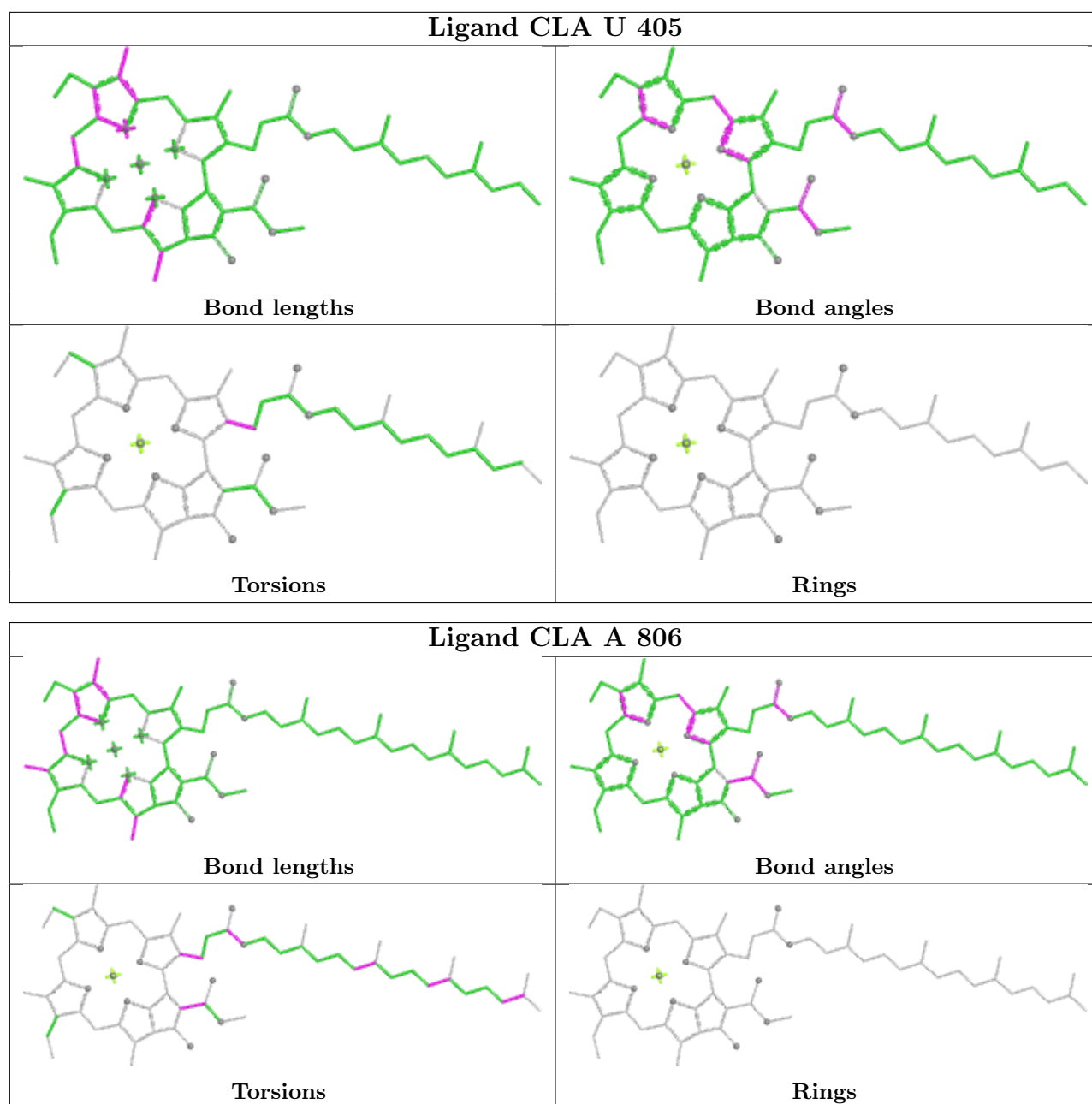




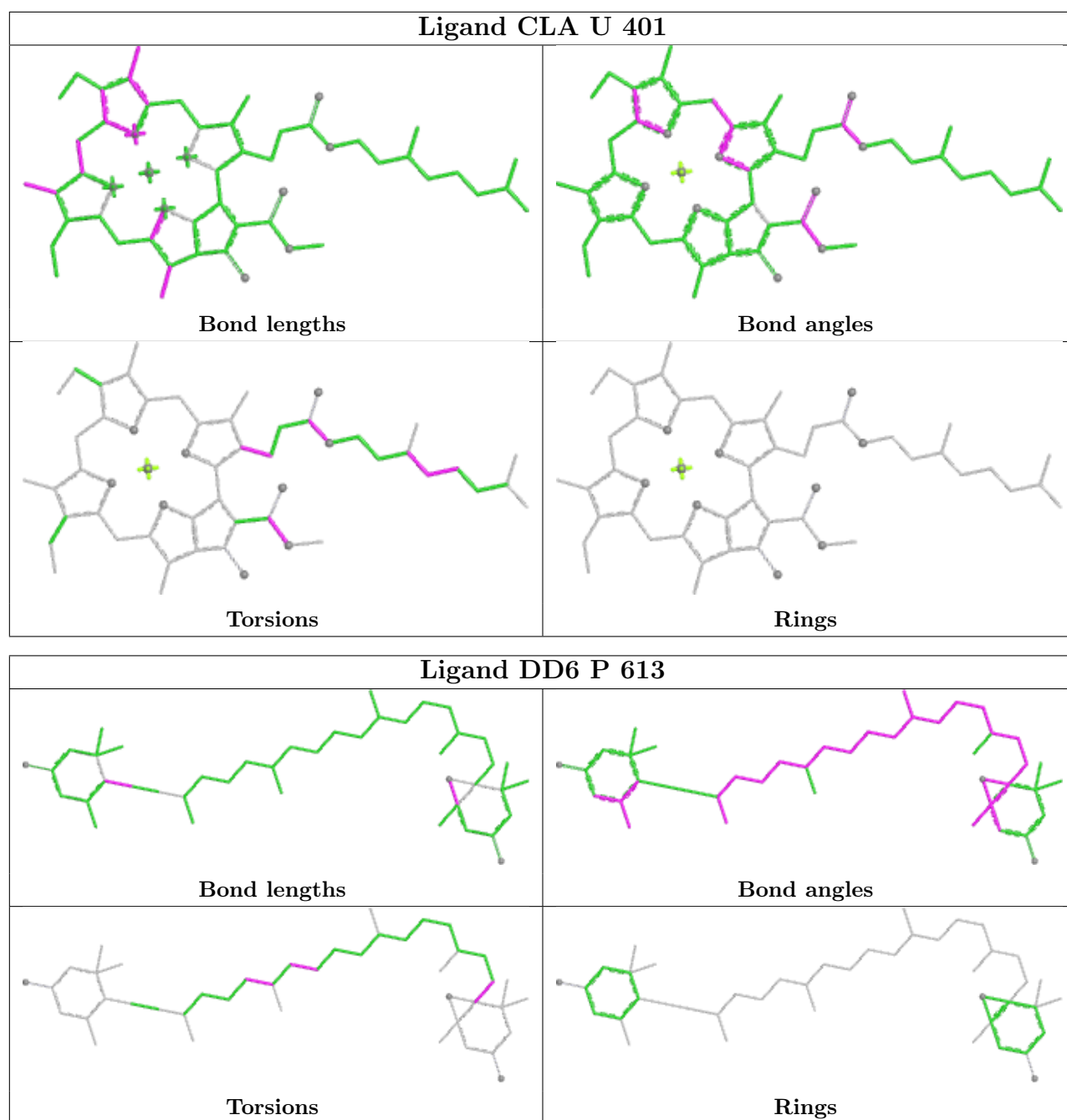


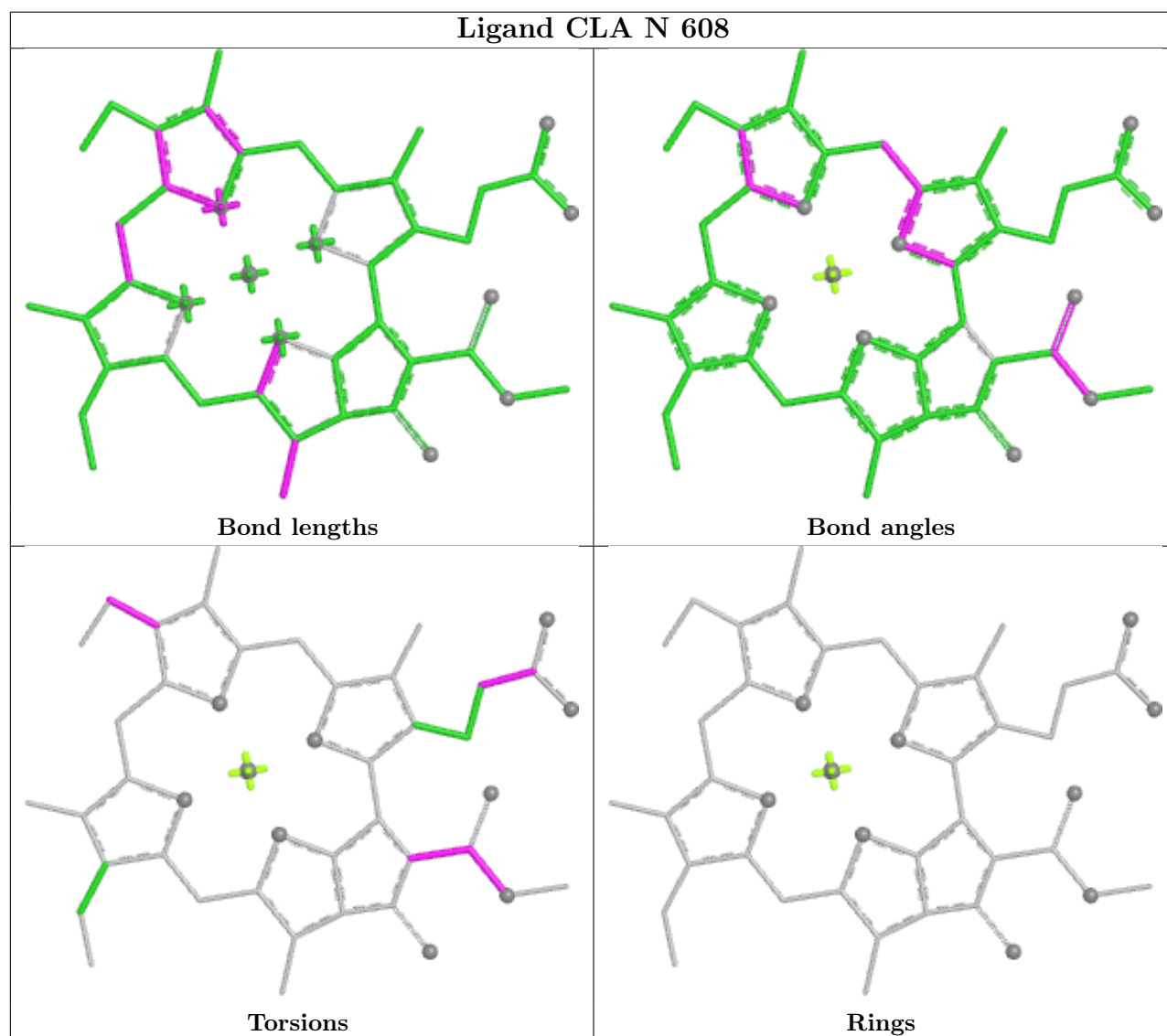
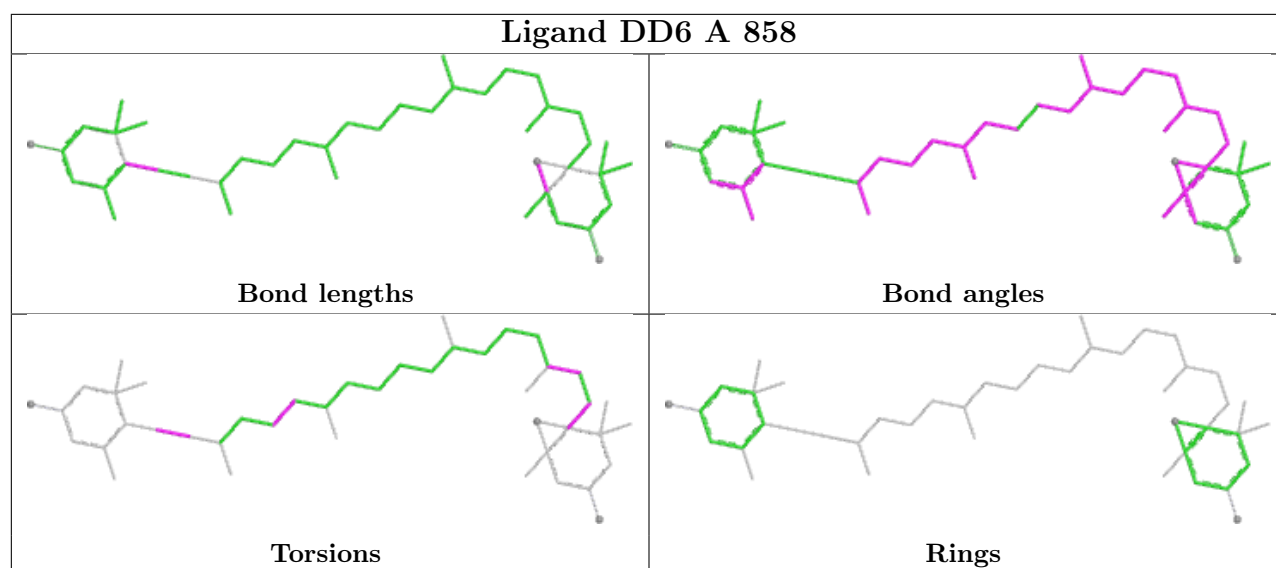




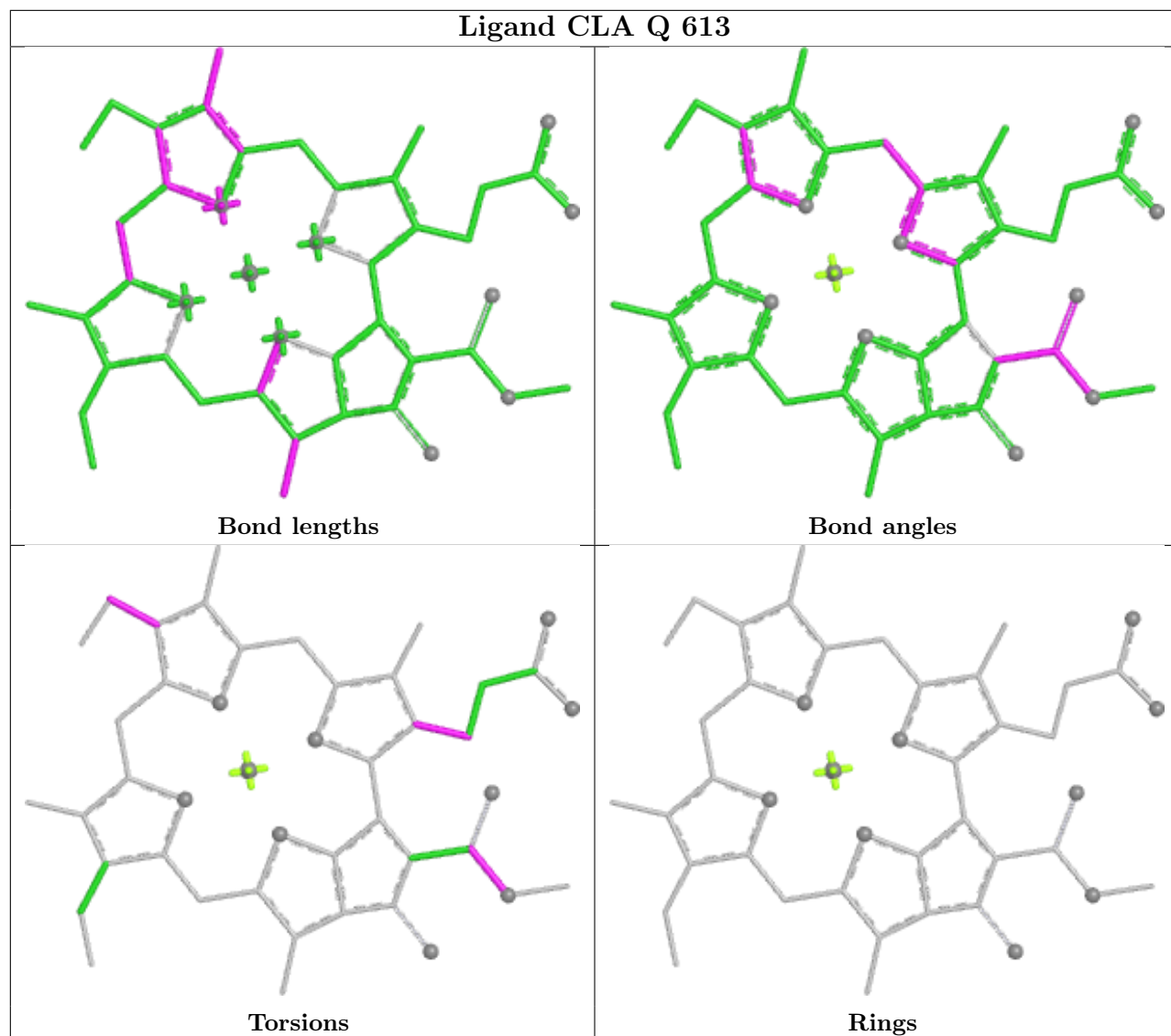




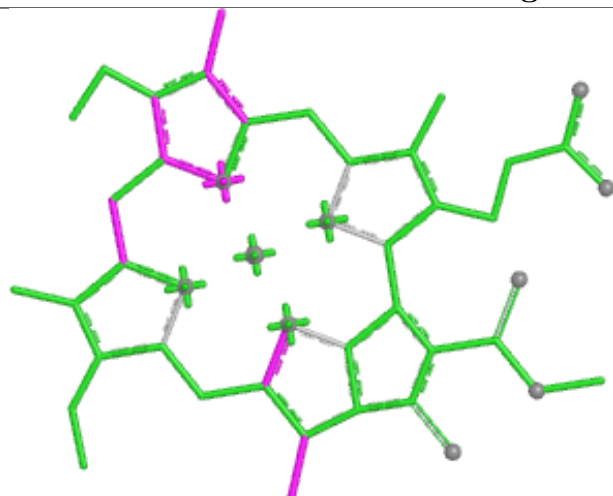




## Ligand CLA Q 613



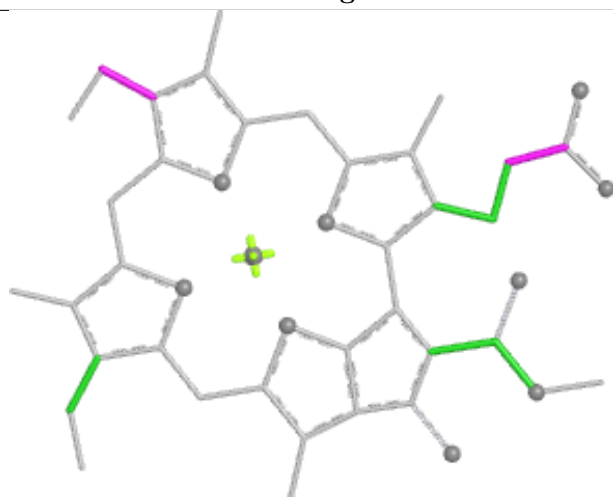
## Ligand CLA I 608



Bond lengths



Bond angles

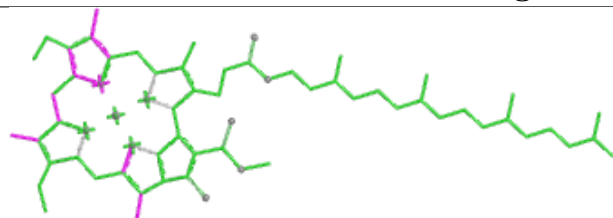


Torsions

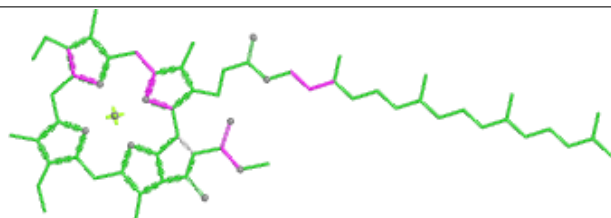


Rings

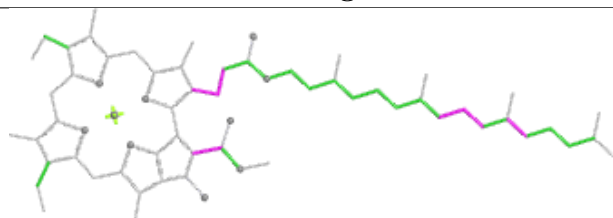
## Ligand CLA A 807



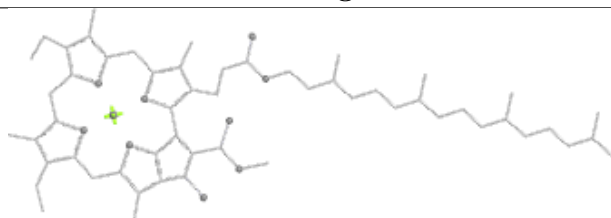
Bond lengths



Bond angles

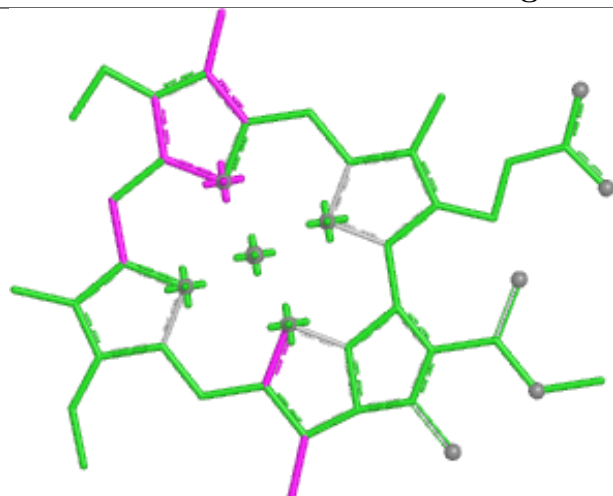


Torsions

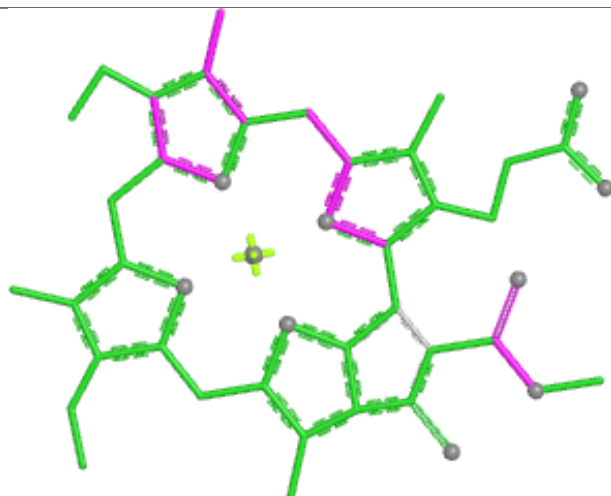


Rings

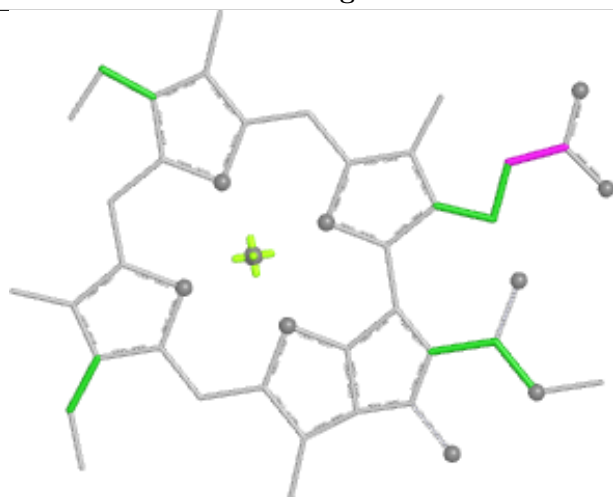
## Ligand CLA I 605



Bond lengths



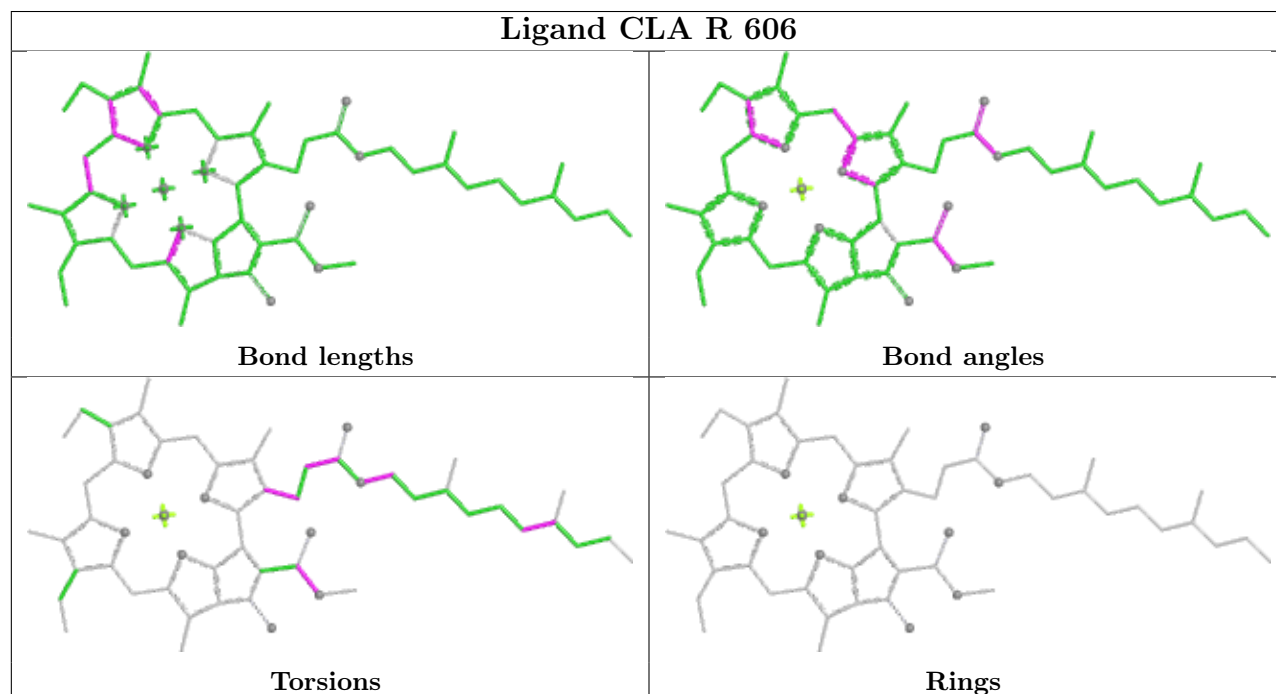
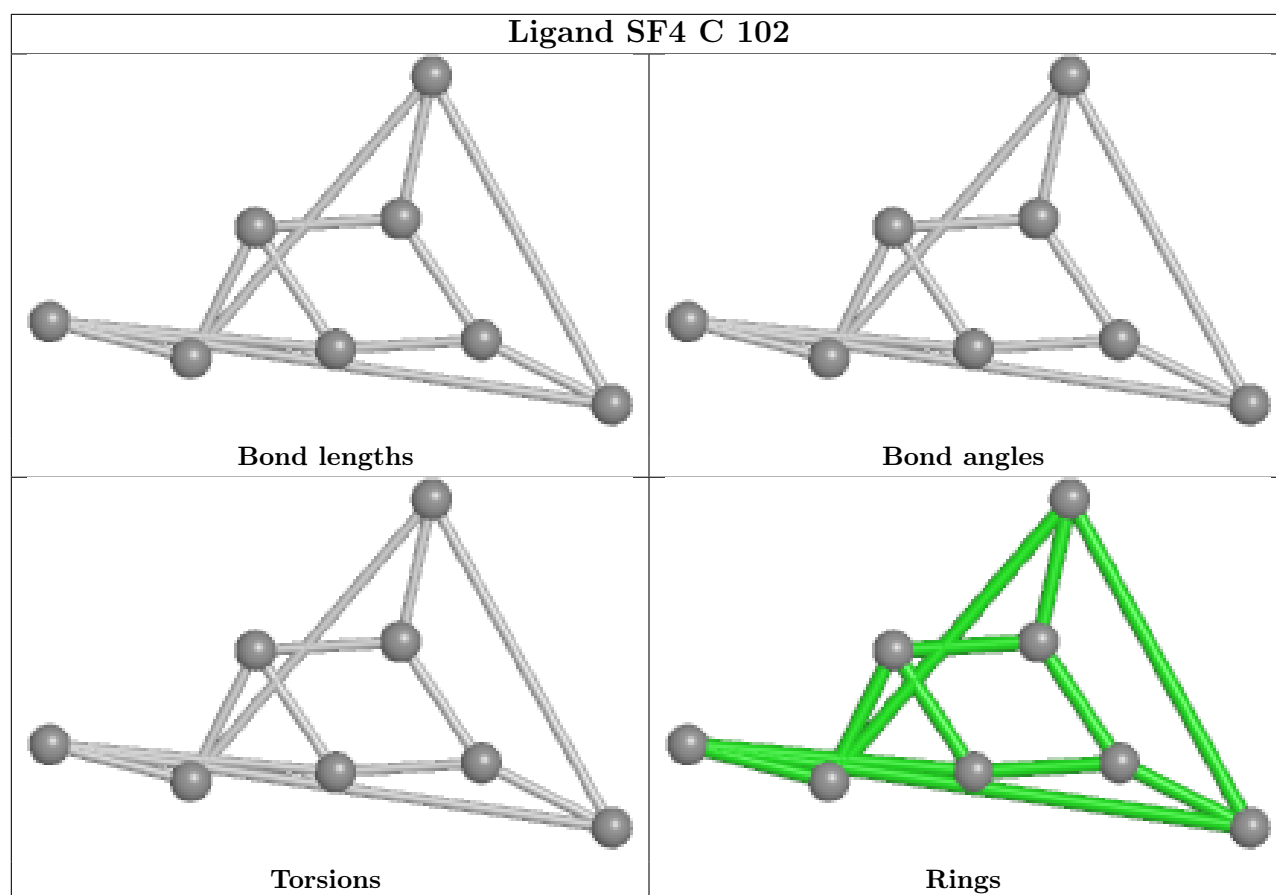
Bond angles



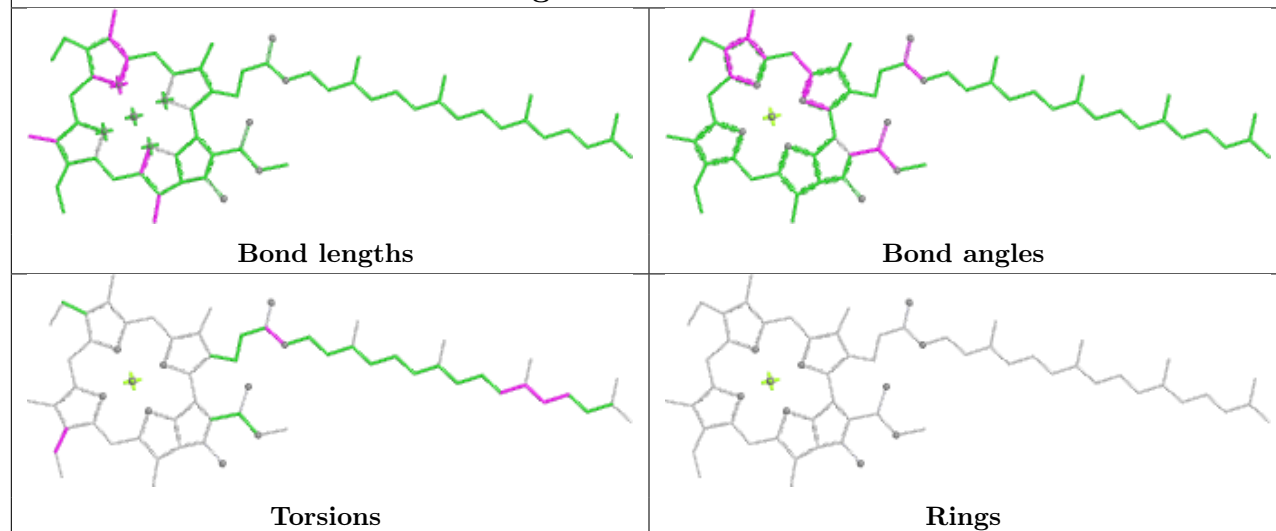
Torsions



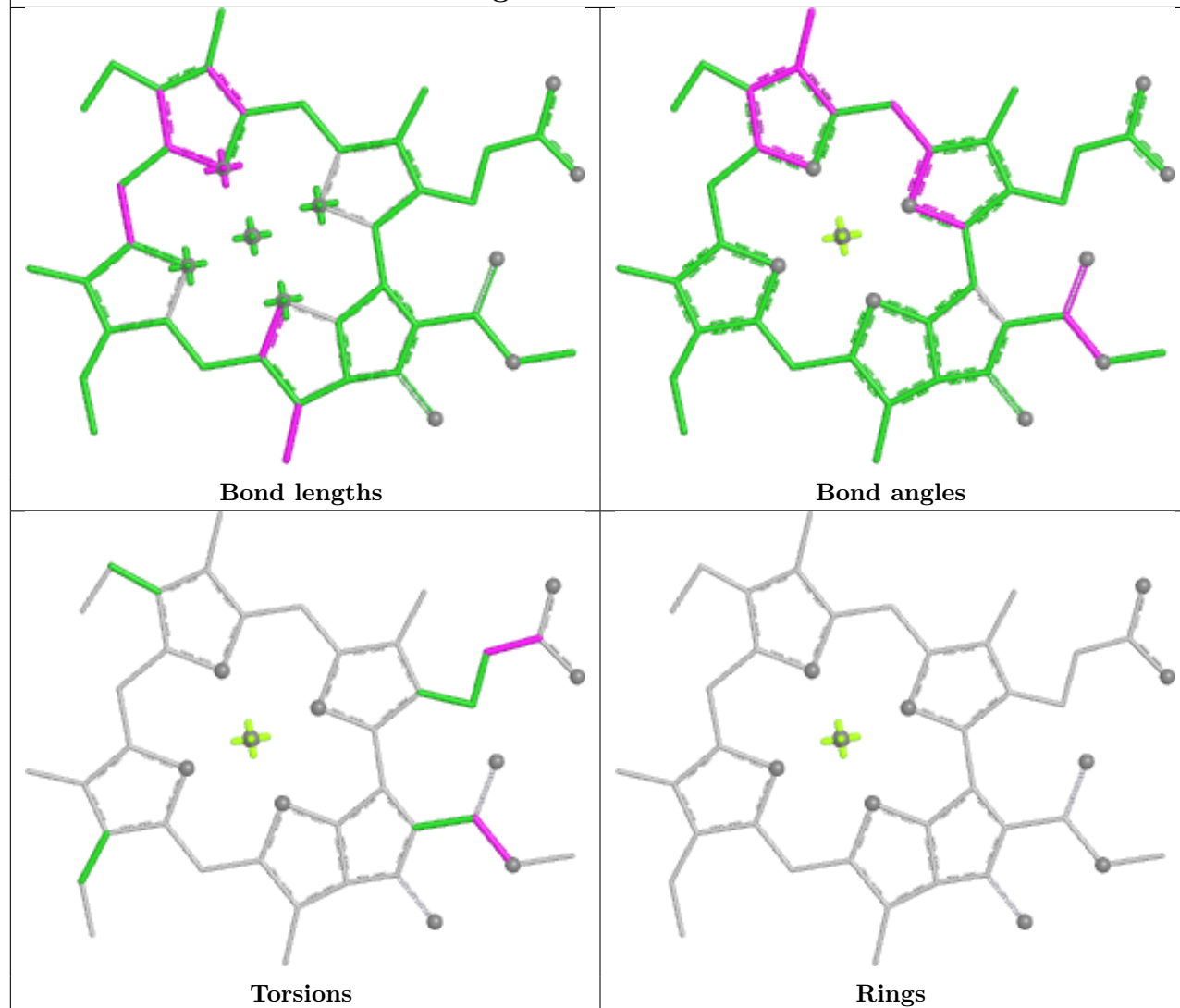
Rings

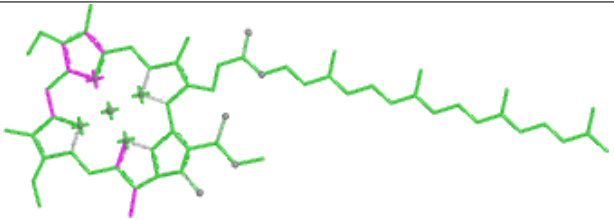
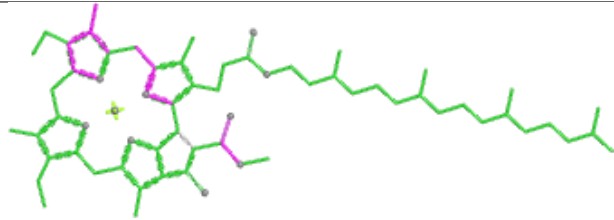
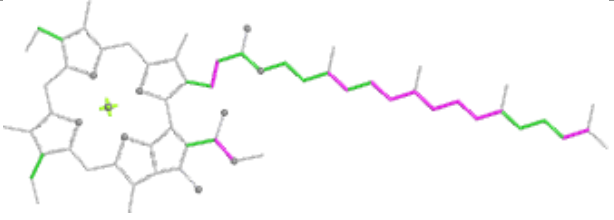
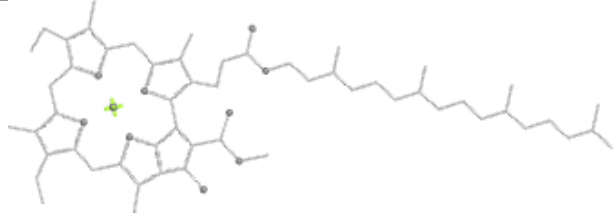


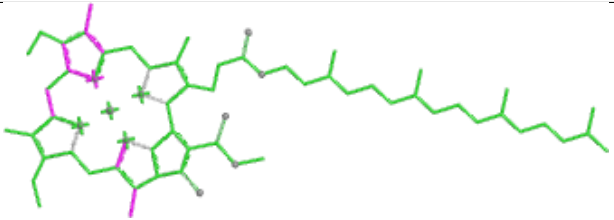
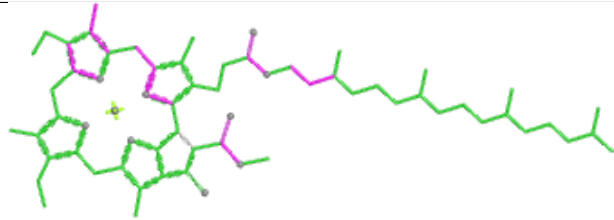
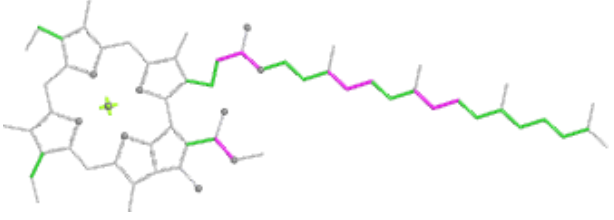
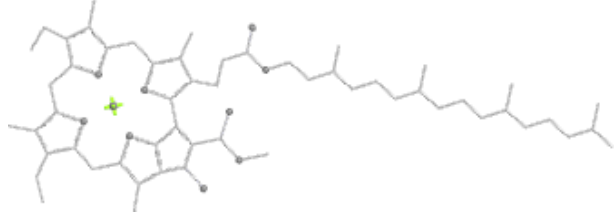
## Ligand CLA B 830

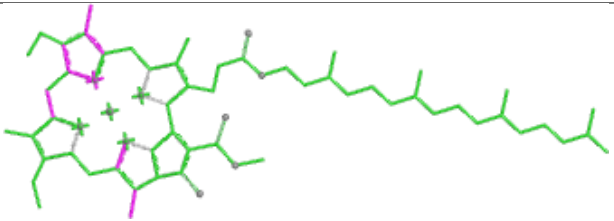
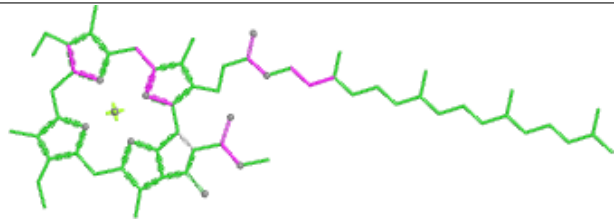
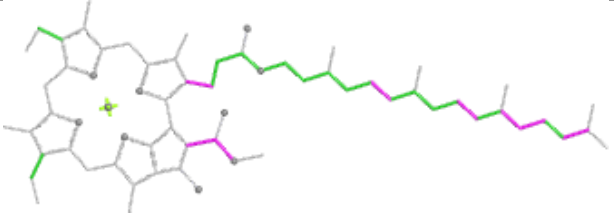
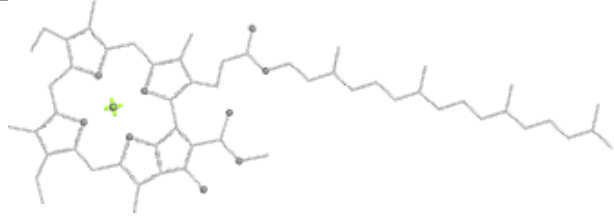


## Ligand CLA T 609



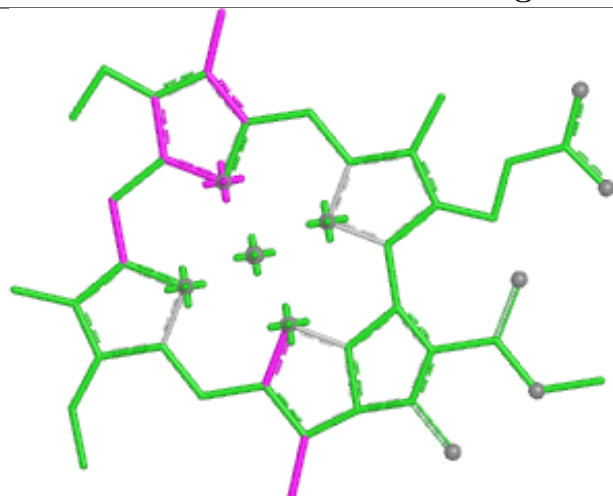
Ligand CLA U 404	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA W 409	
	
Bond lengths	Bond angles
	
Torsions	Rings

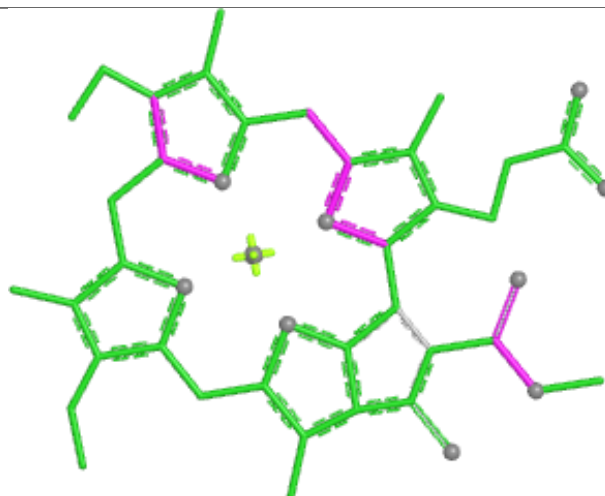
Ligand CLA T 611	
	
Bond lengths	Bond angles
	
Torsions	Rings



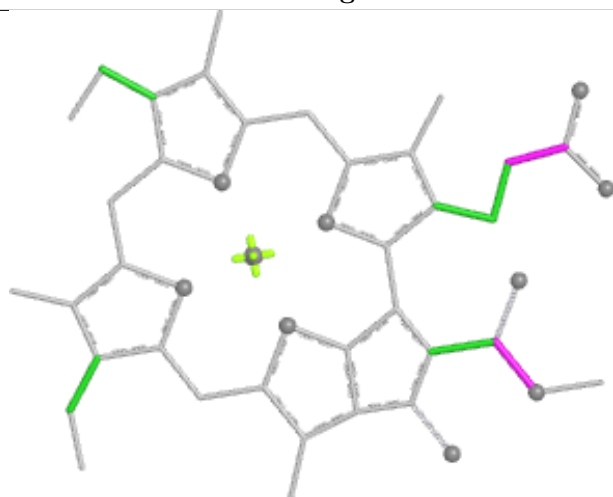
## Ligand CLA T 601



Bond lengths



Bond angles

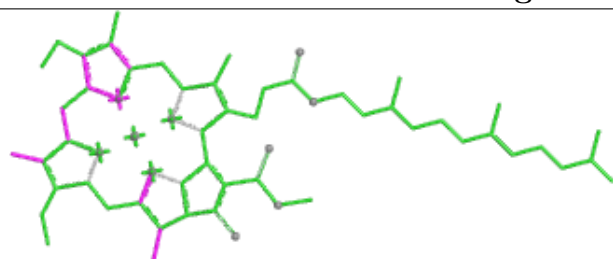


Torsions

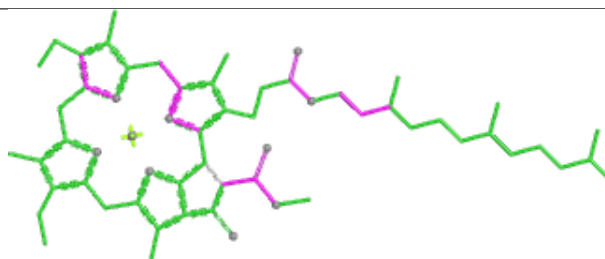


Rings

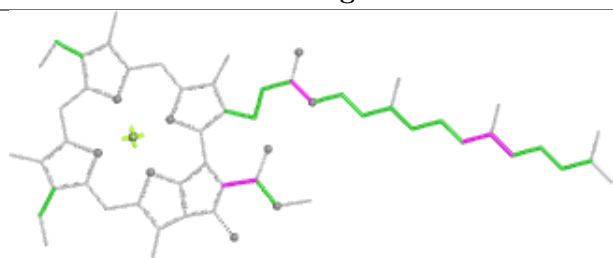
## Ligand CLA T 603



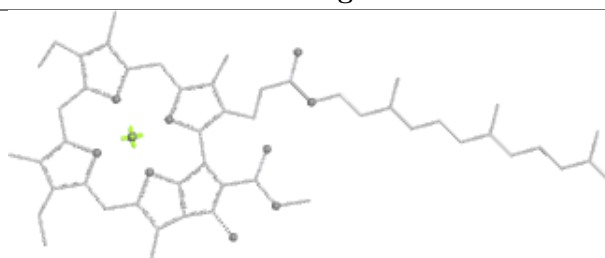
Bond lengths



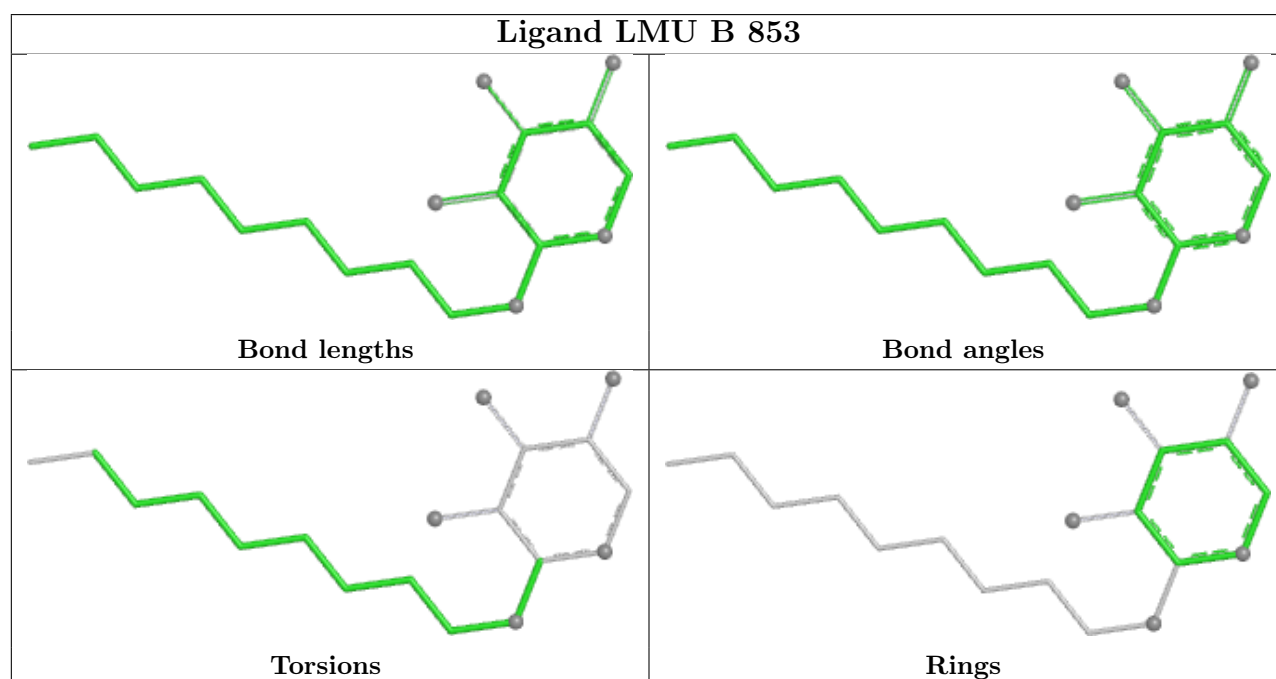
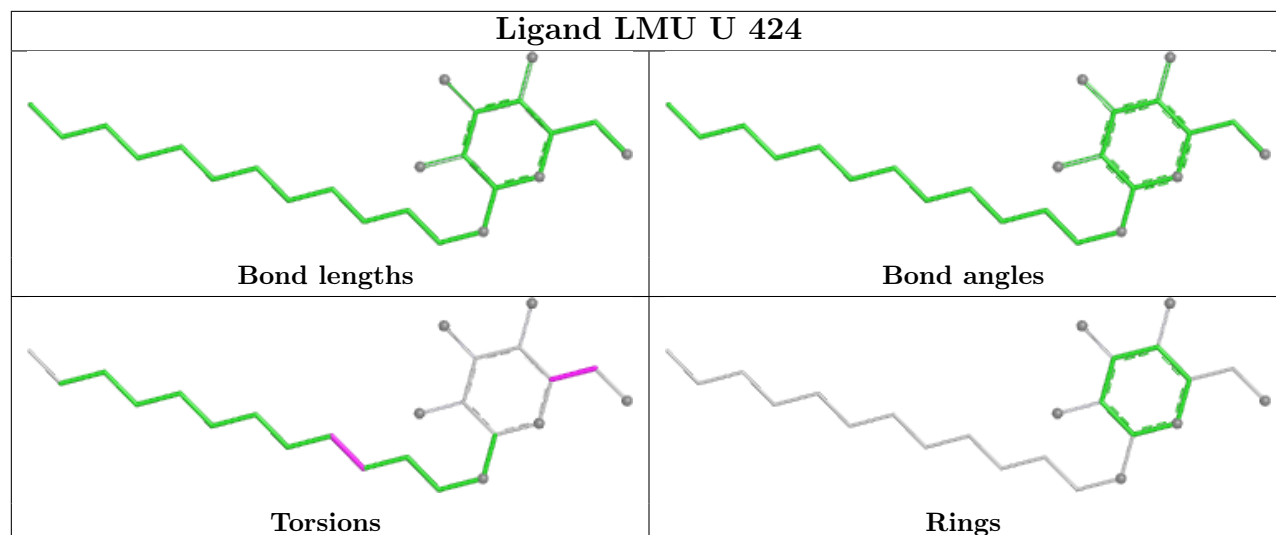
Bond angles

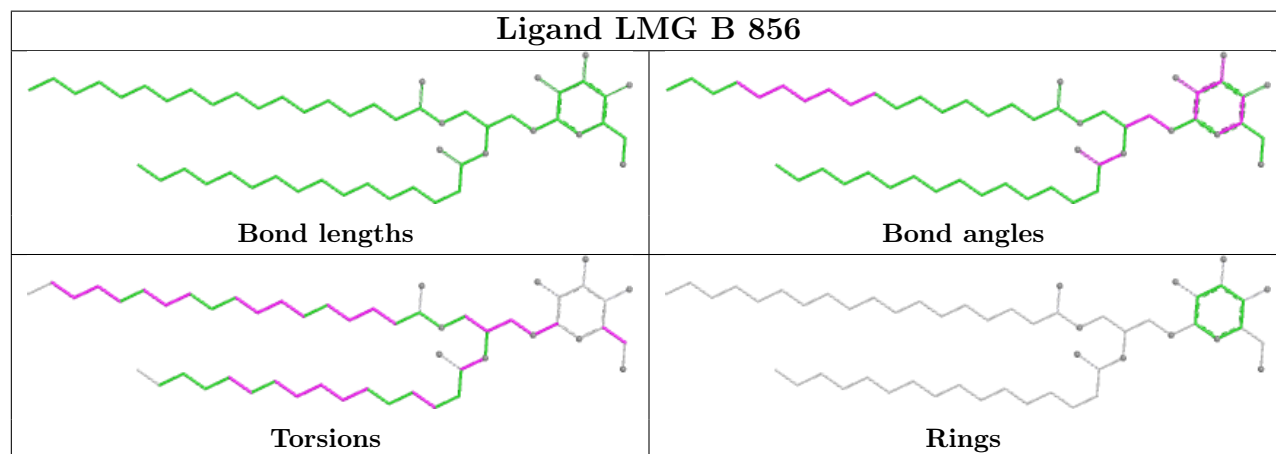
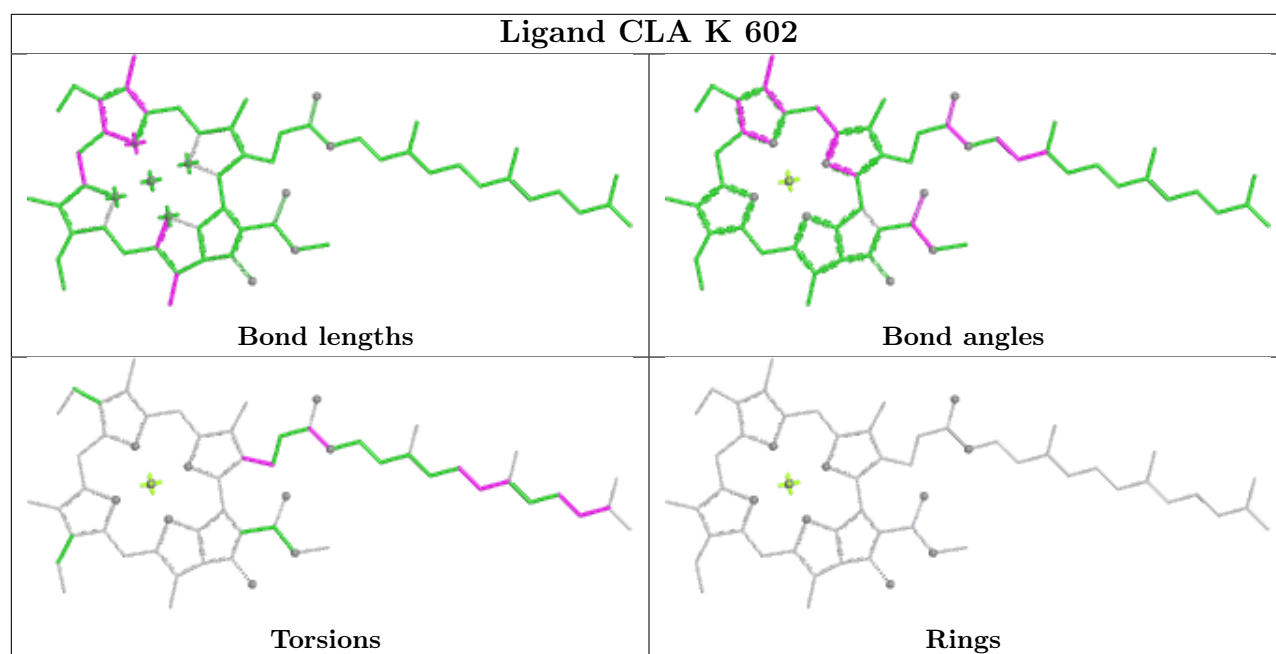


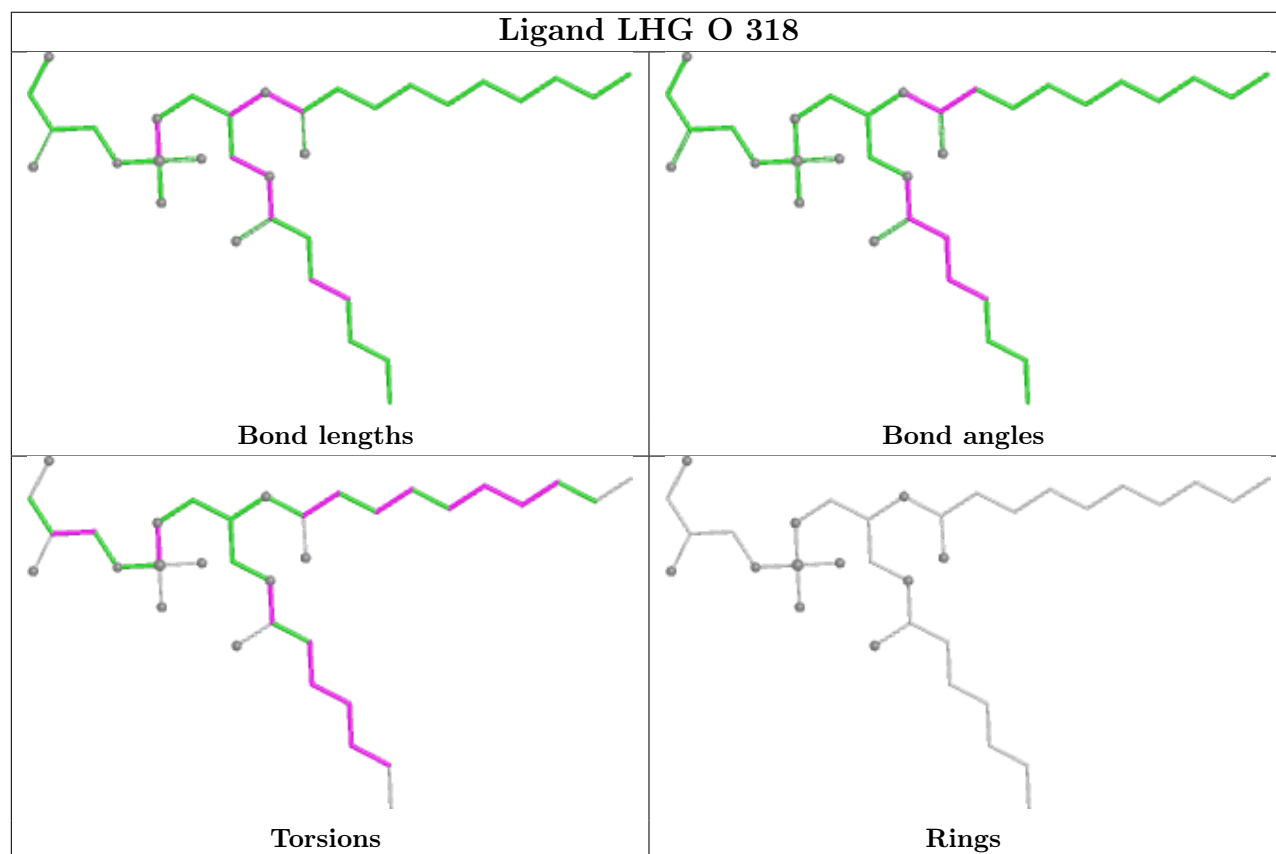
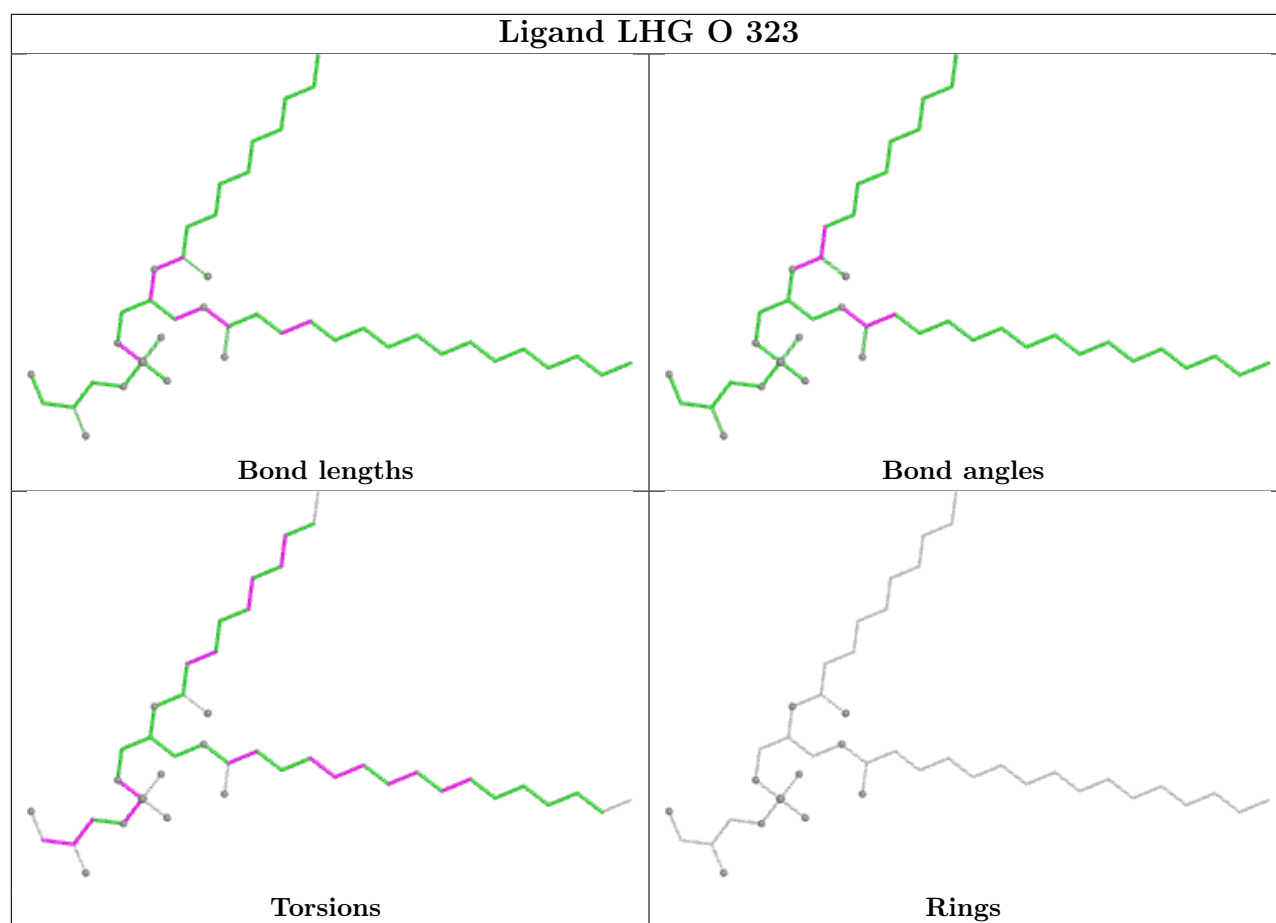
Torsions

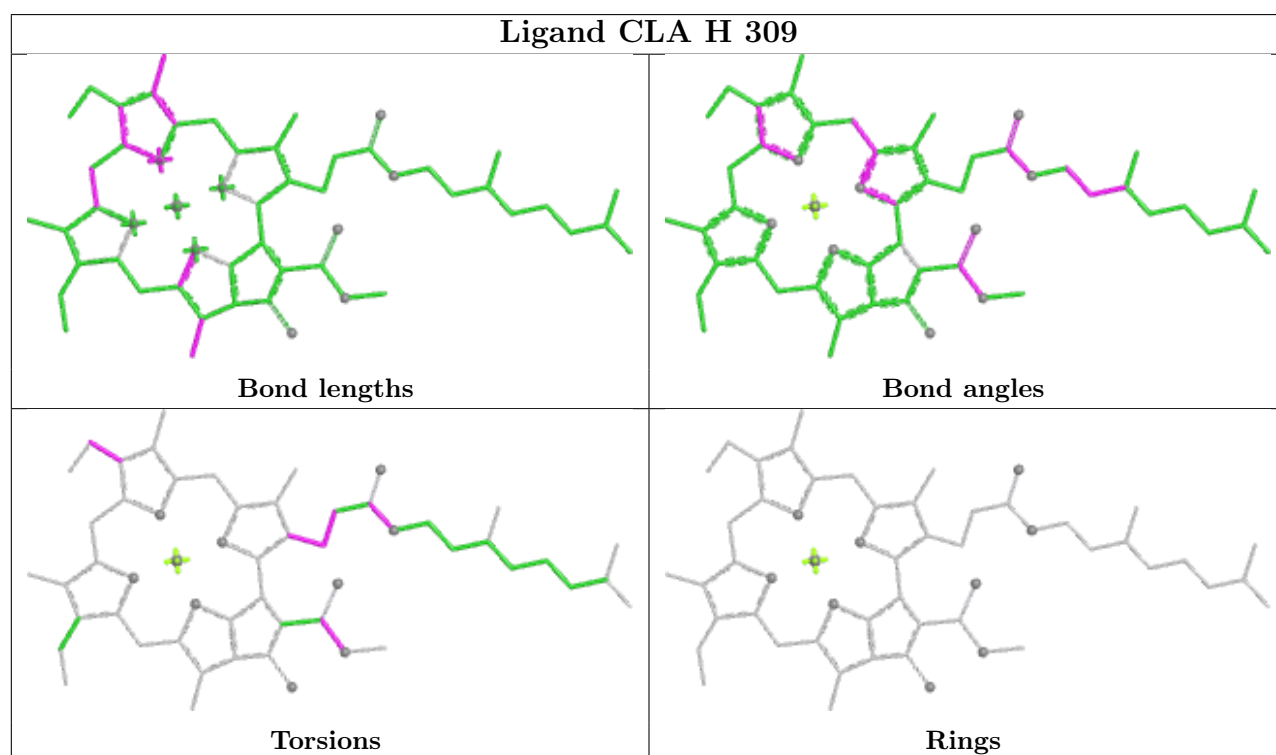
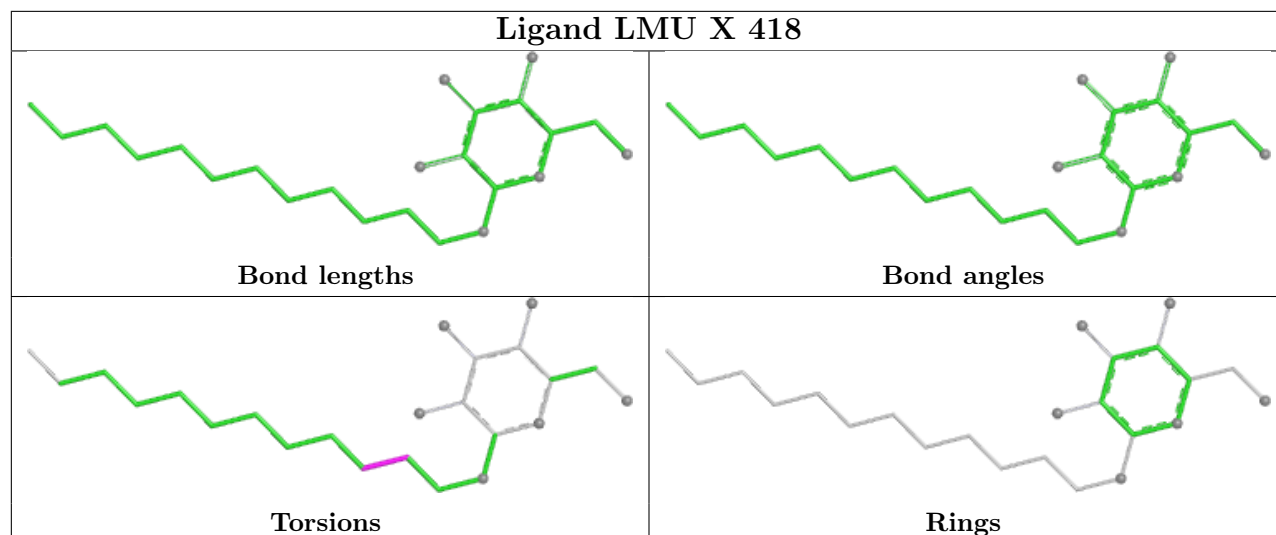


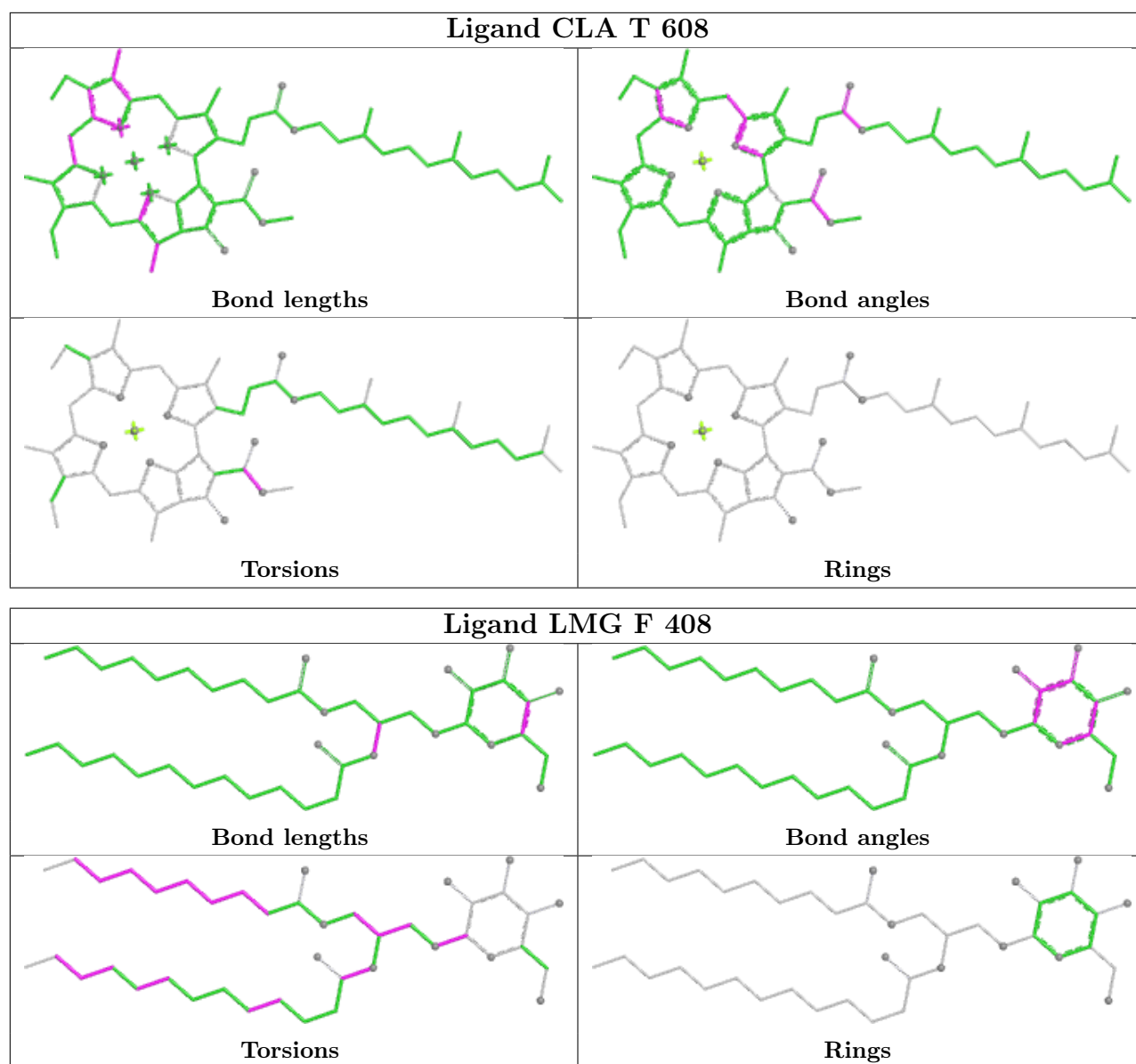
Rings



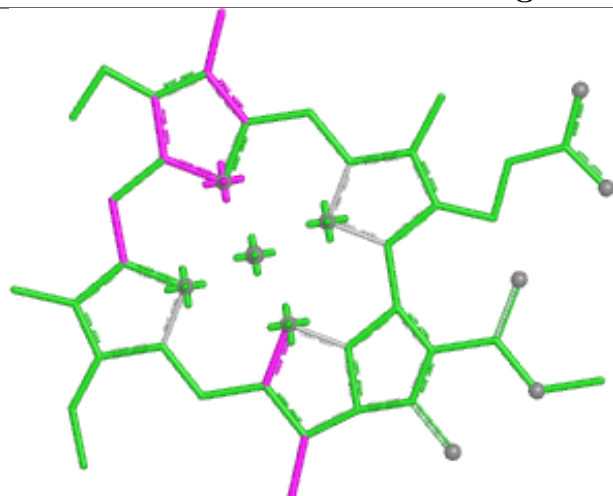




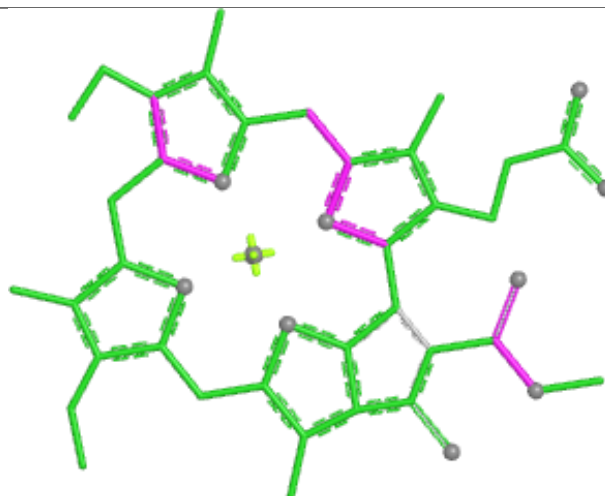




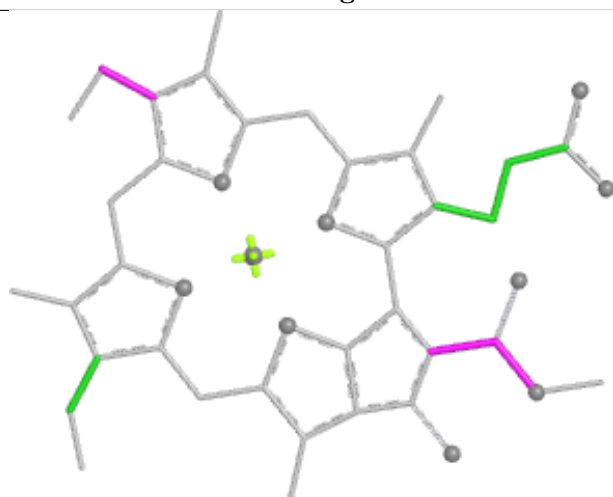
## Ligand CLA F 405



Bond lengths



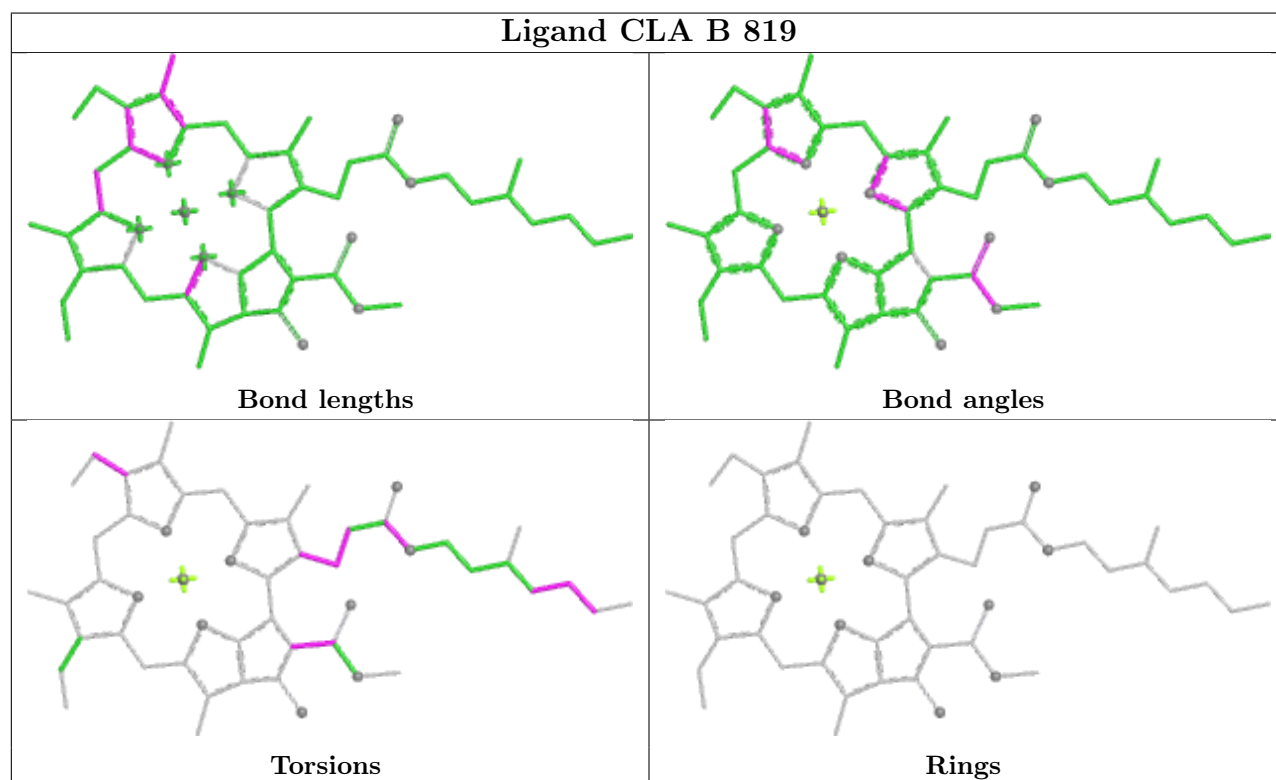
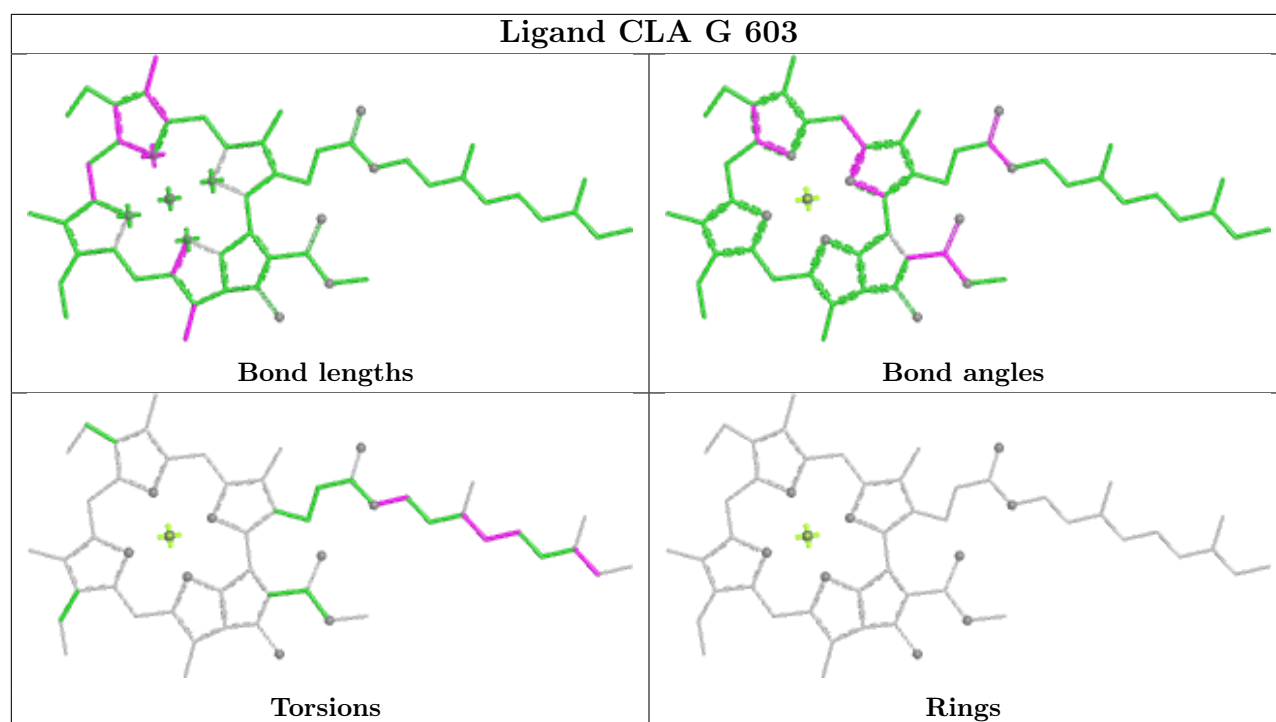
Bond angles



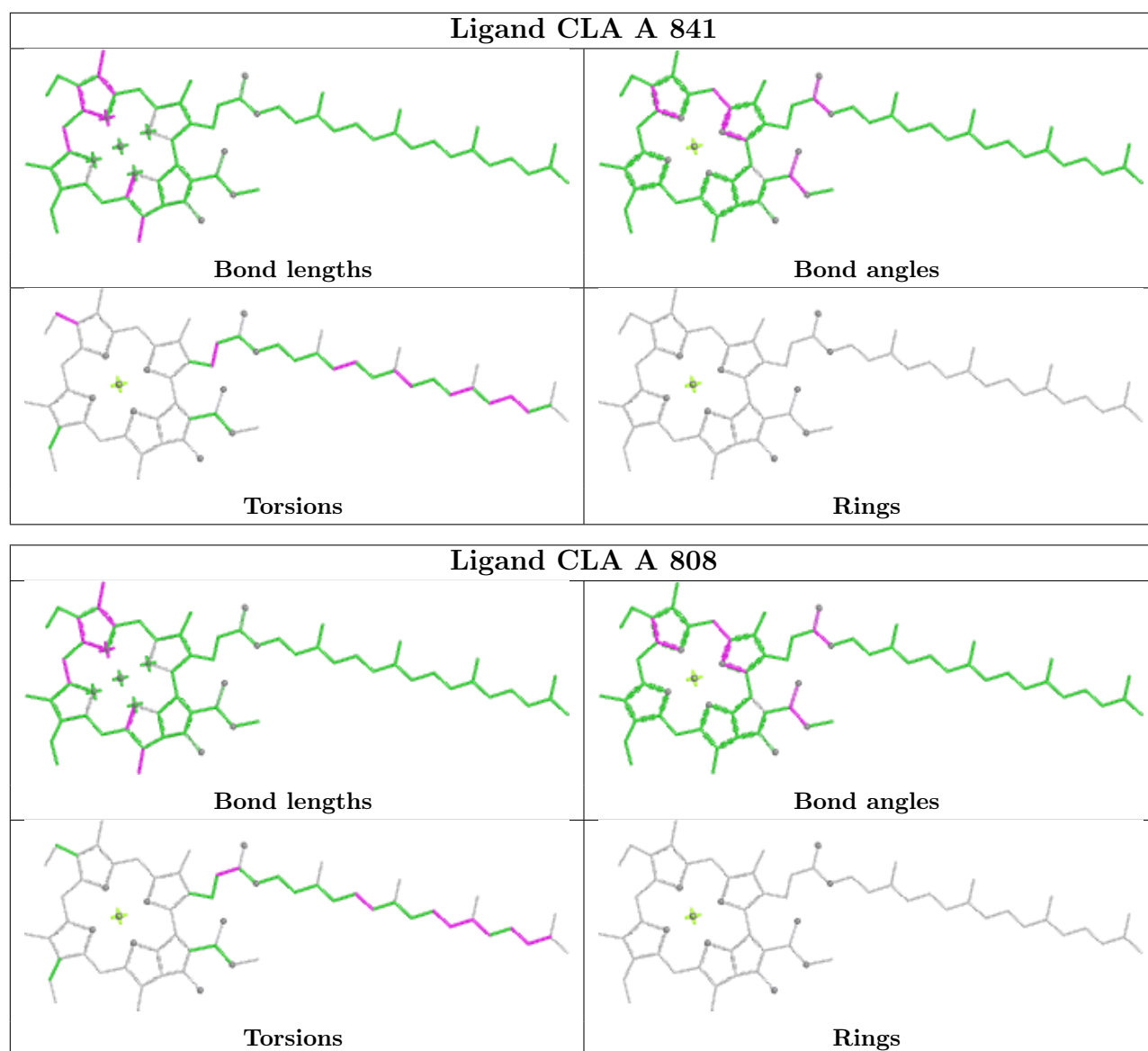
Torsions

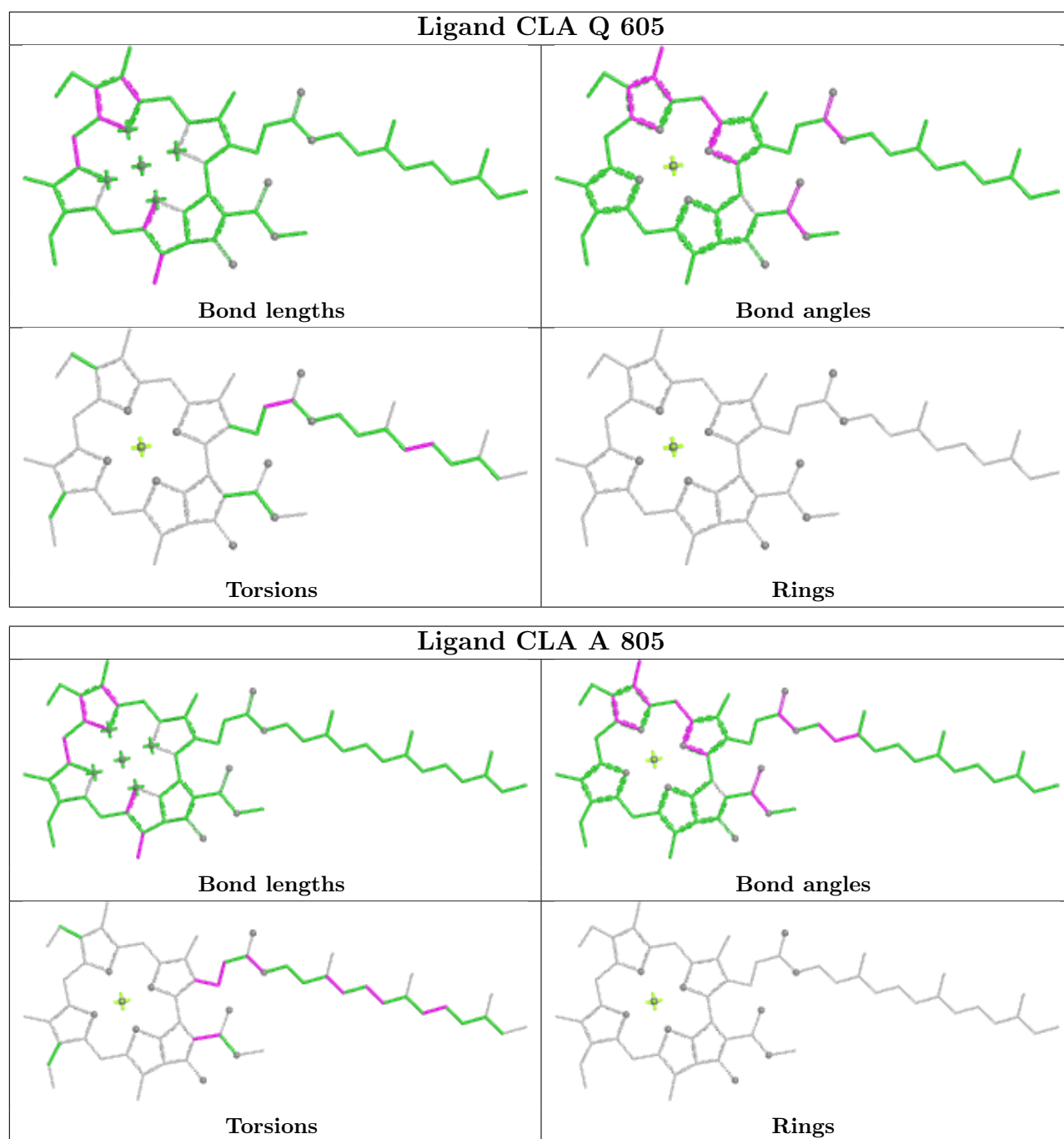


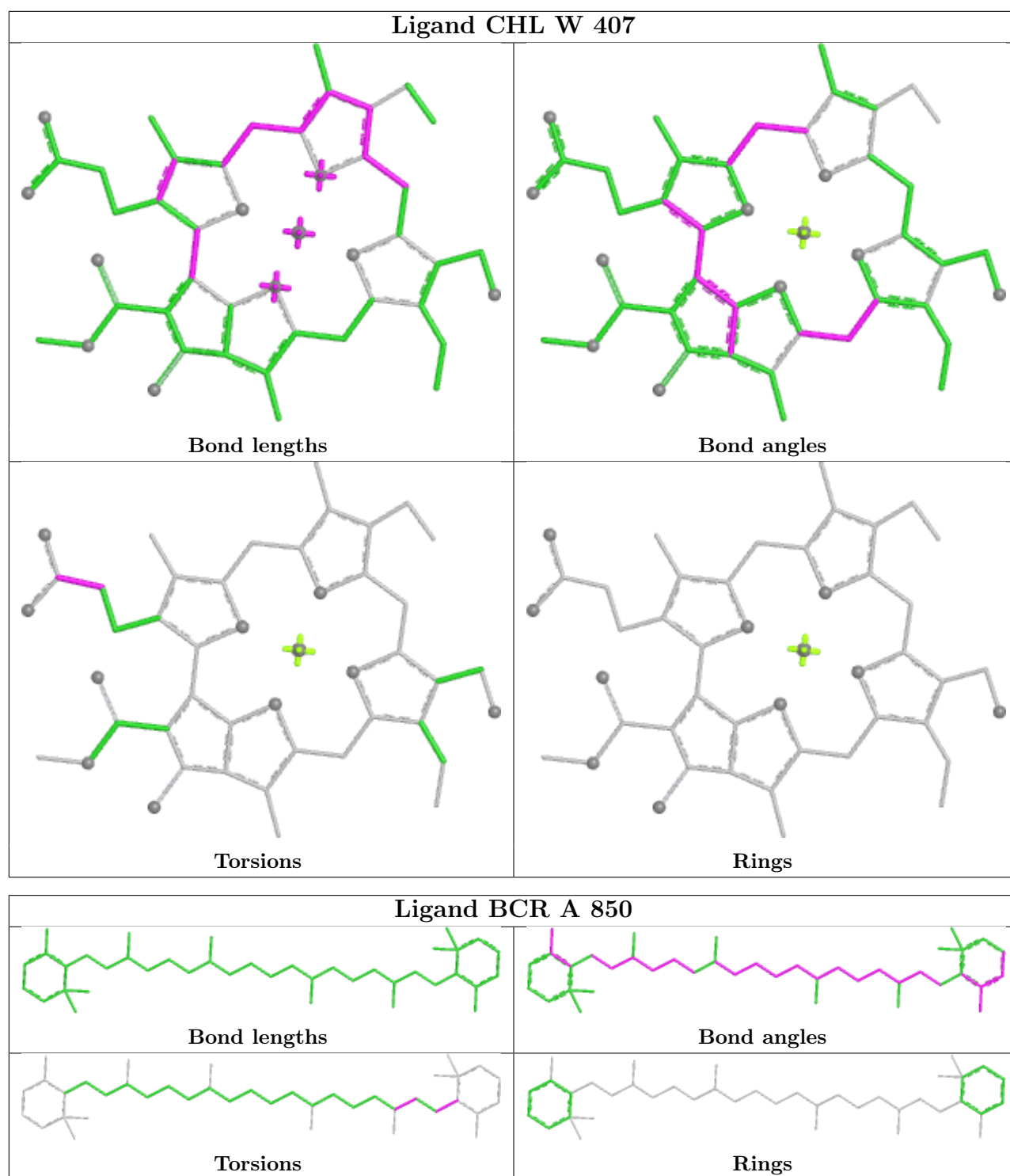
Rings



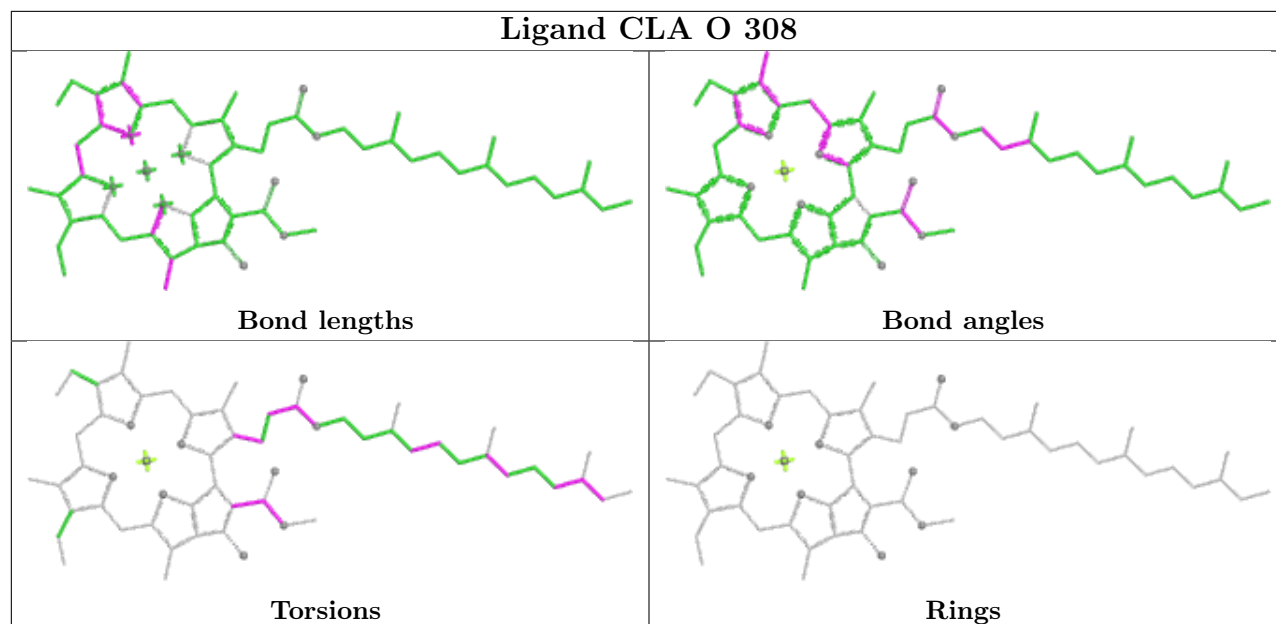




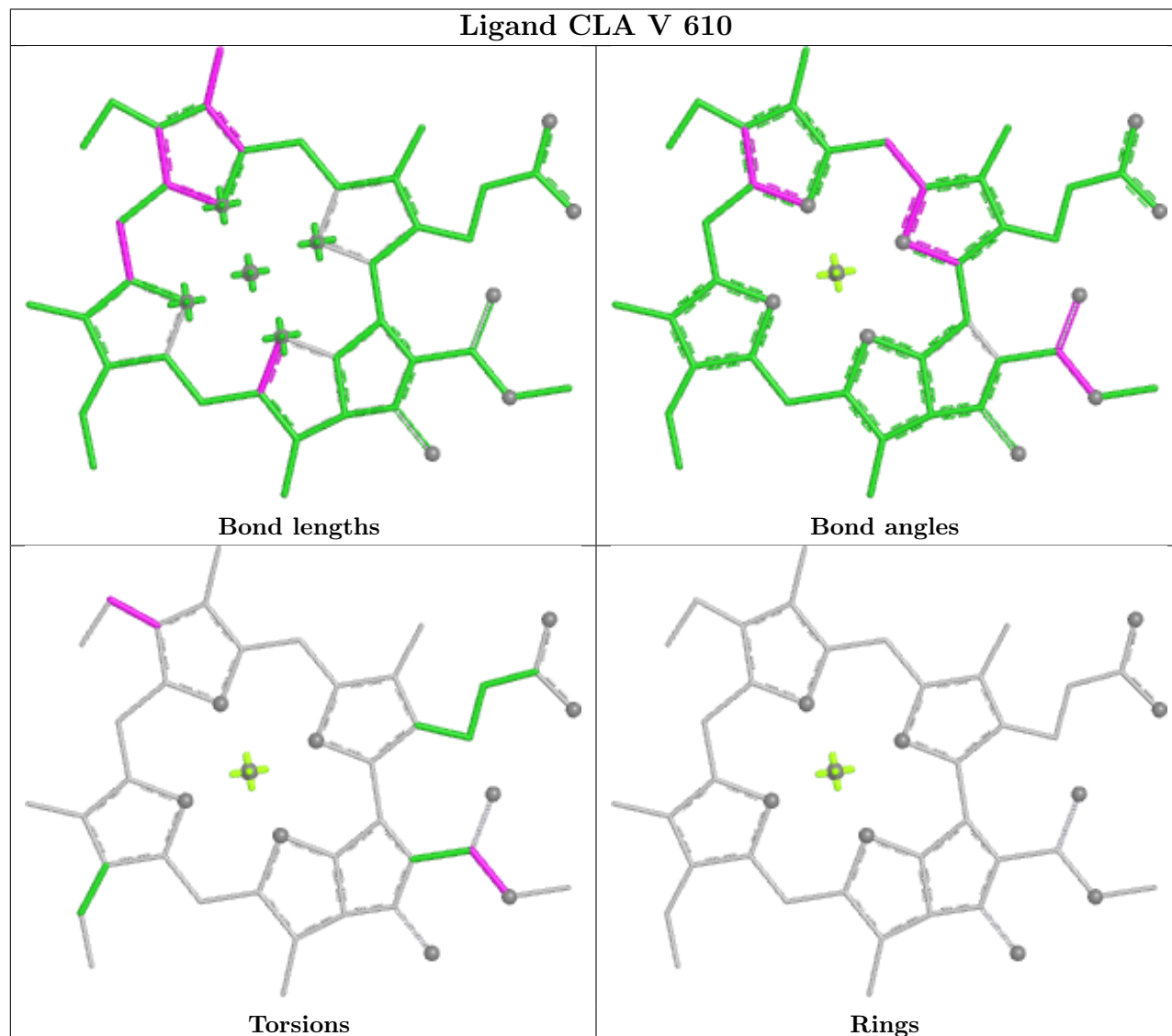


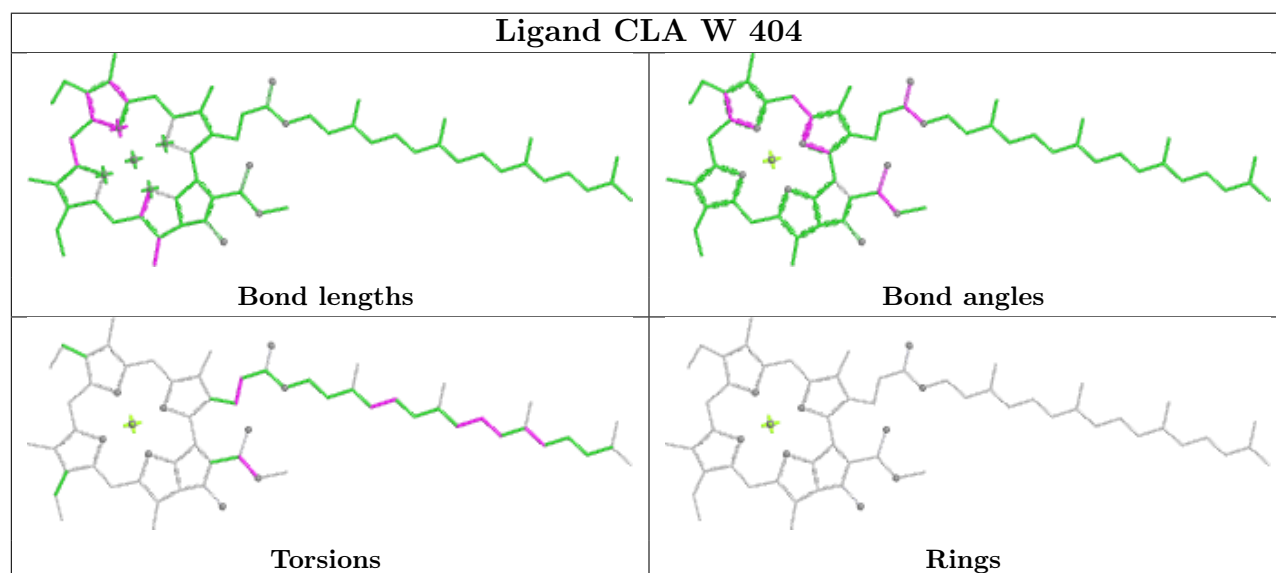
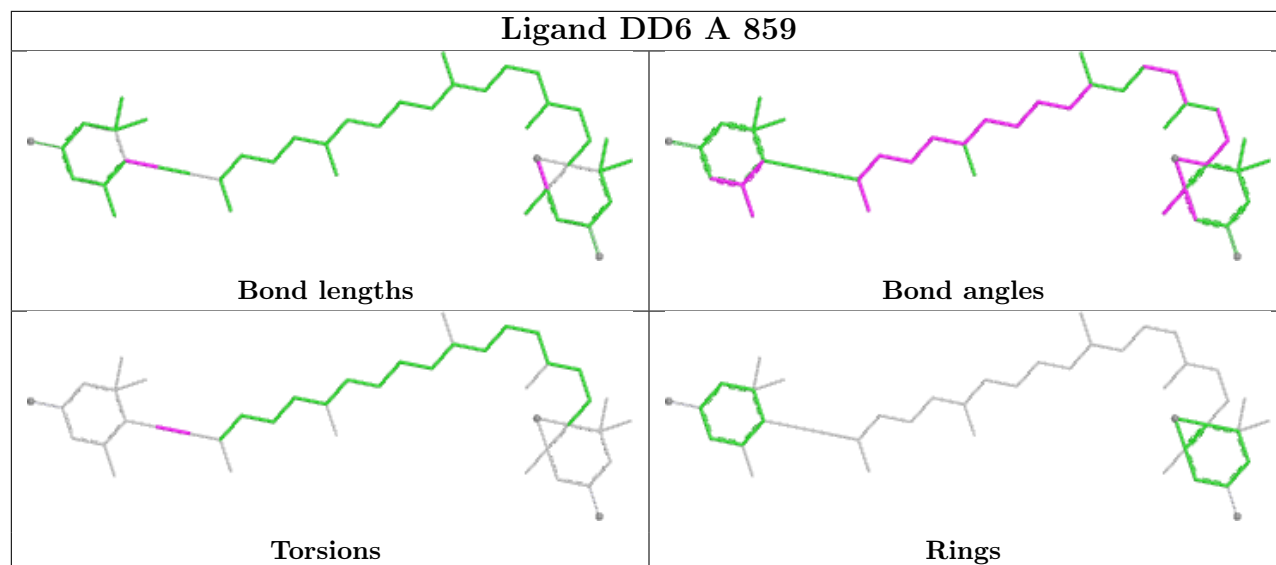


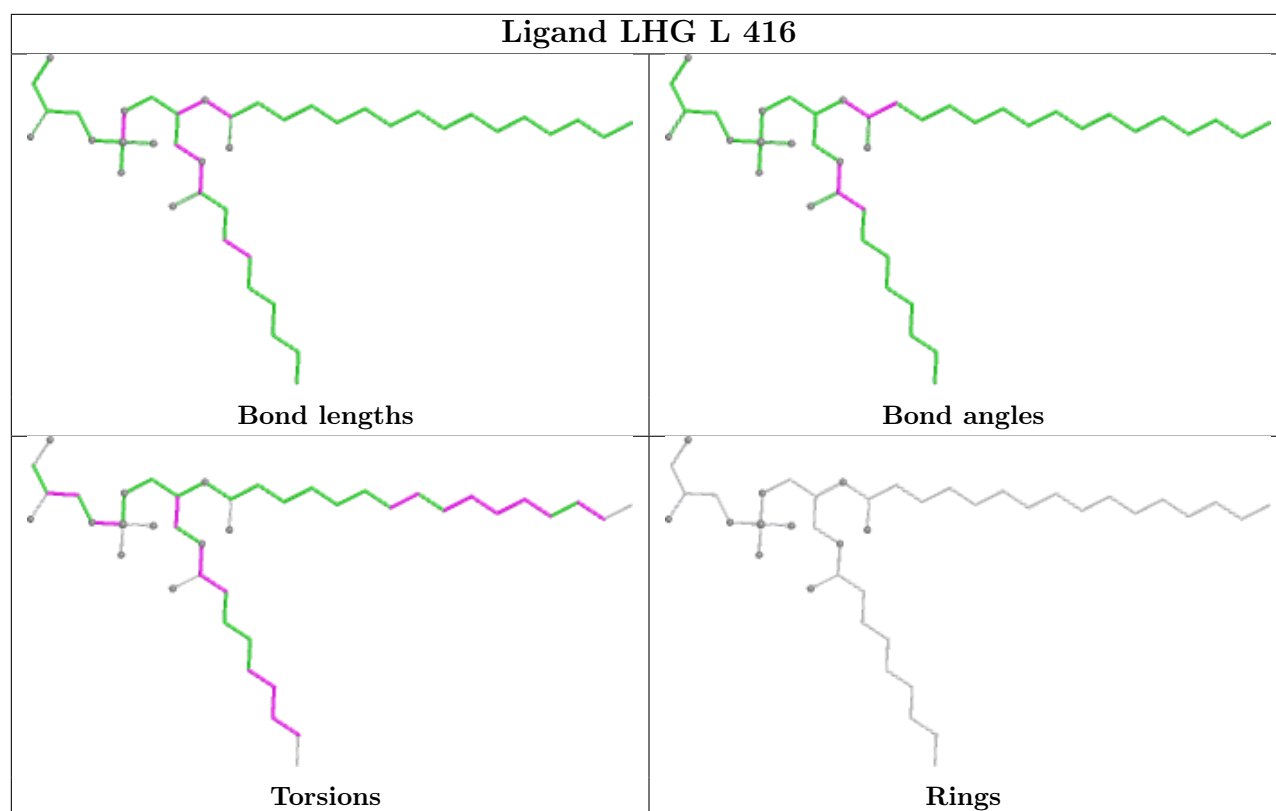
## Ligand CLA O 308



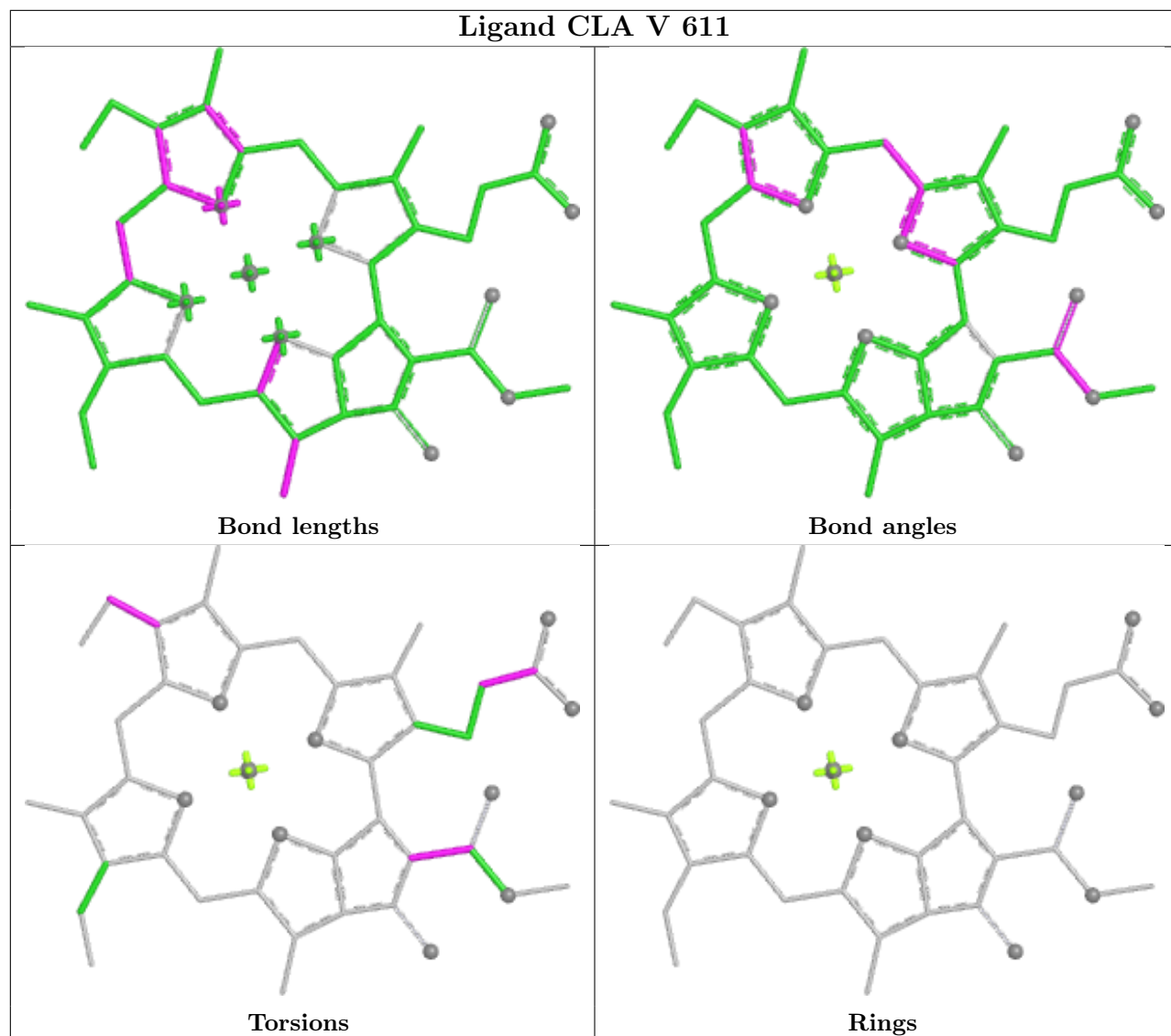
## Ligand CLA V 610



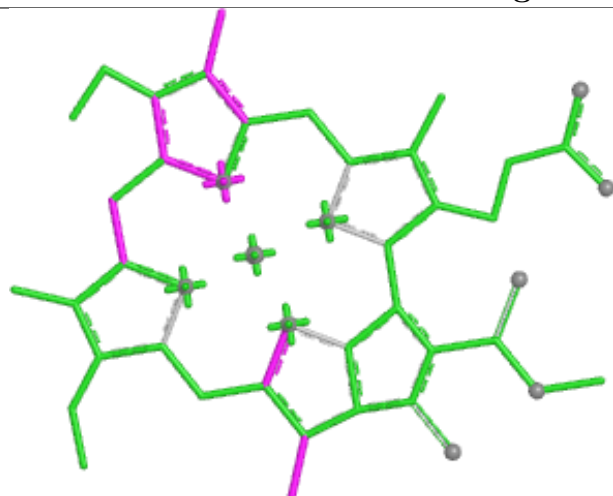




## Ligand CLA V 611



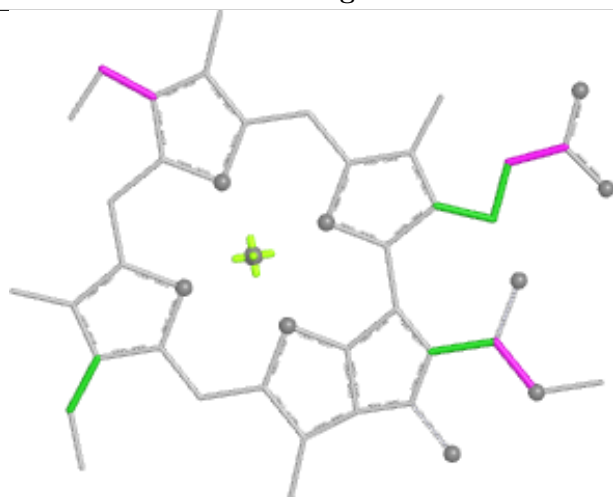
## Ligand CLA N 601



Bond lengths



Bond angles



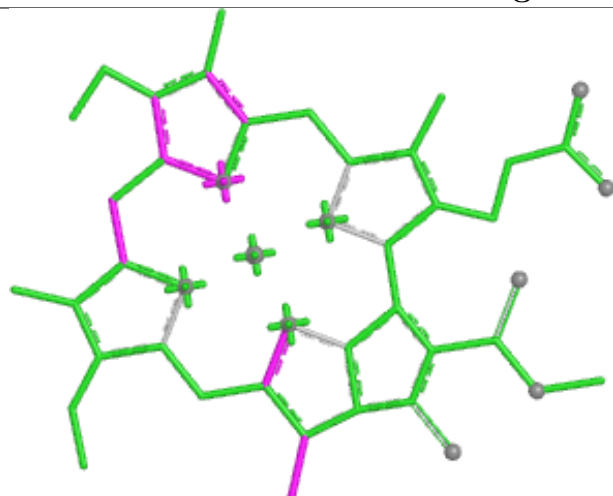
Torsions



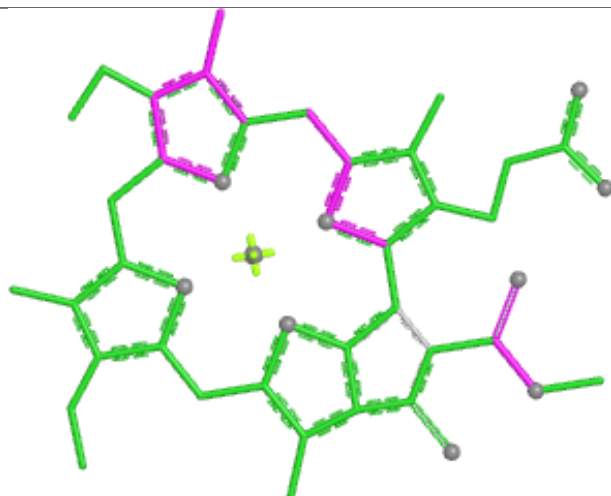
Rings



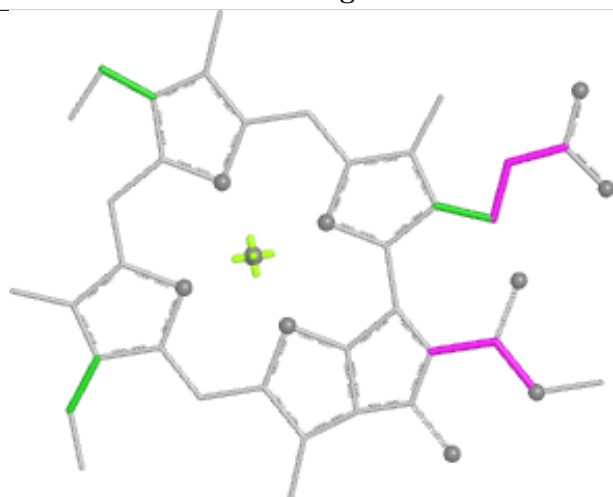
## Ligand CLA H 304



Bond lengths



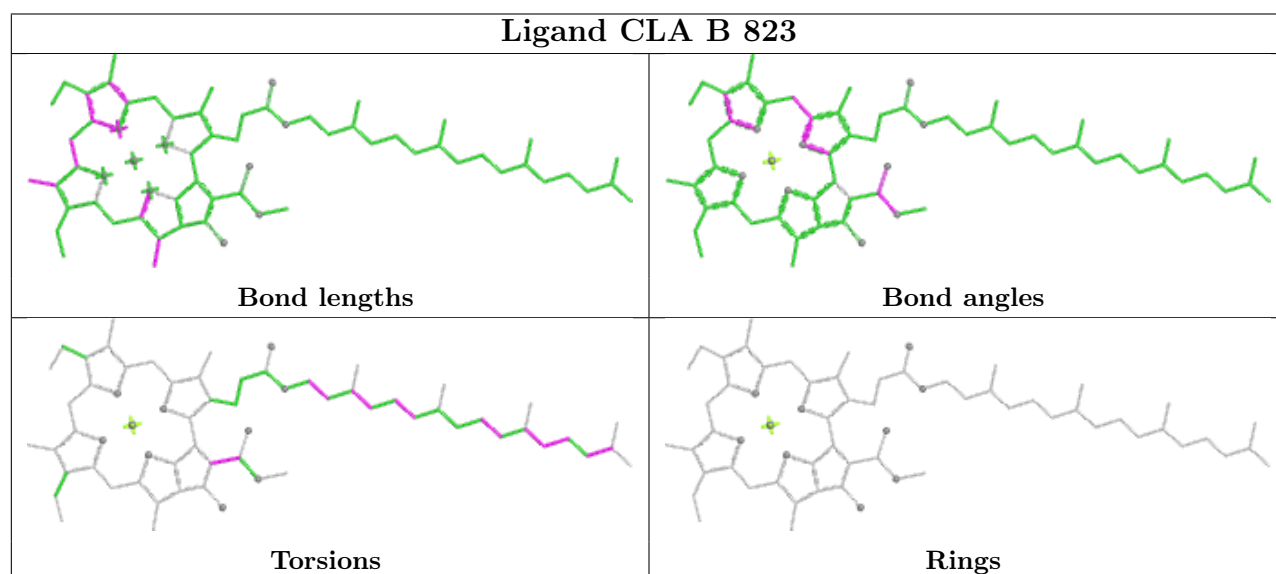
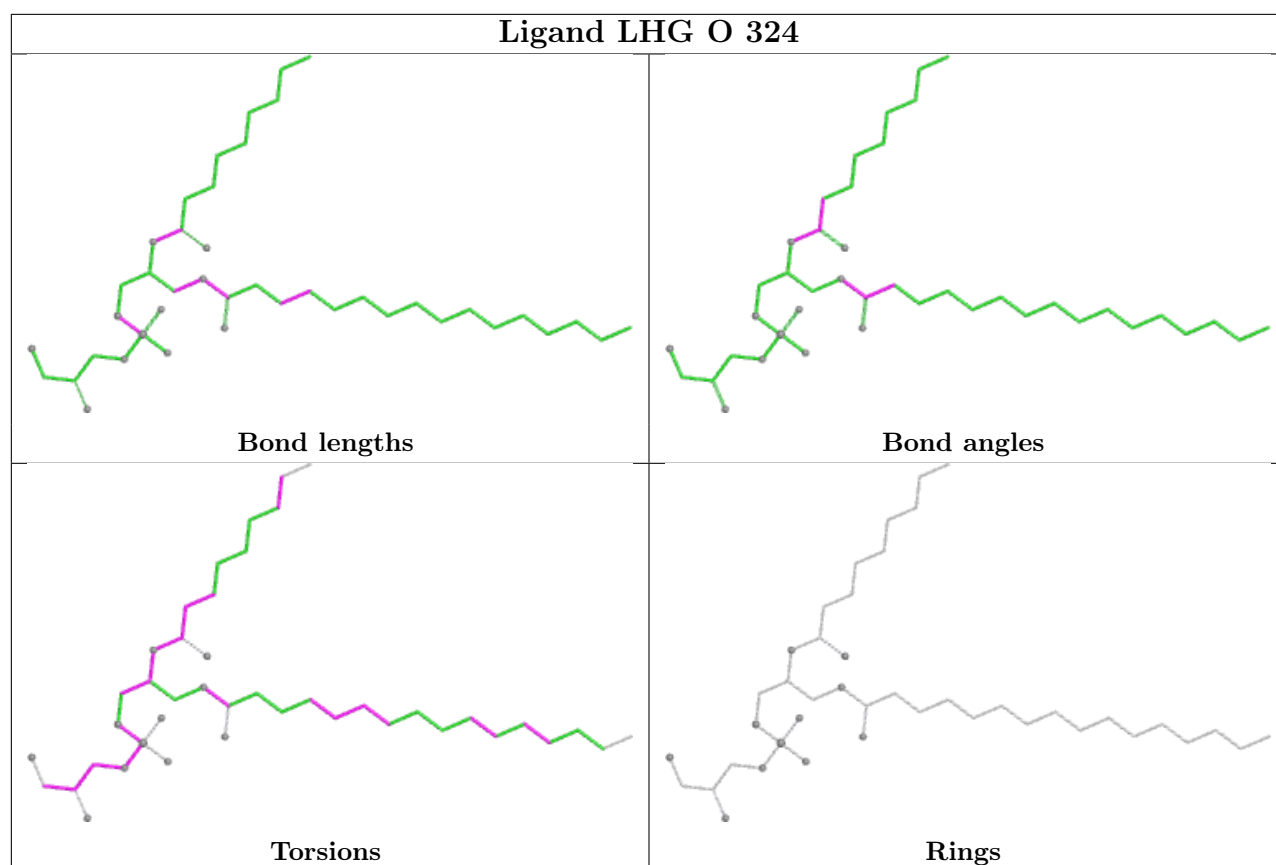
Bond angles



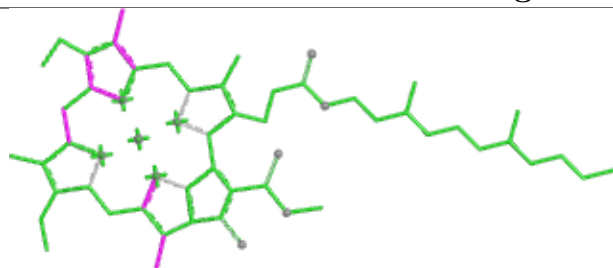
Torsions



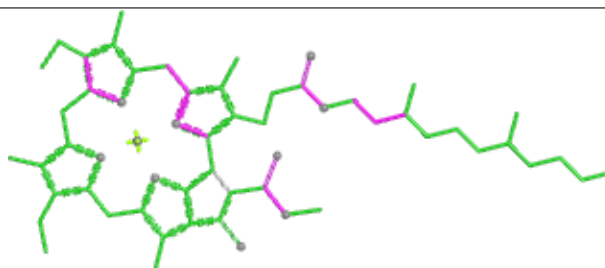
Rings



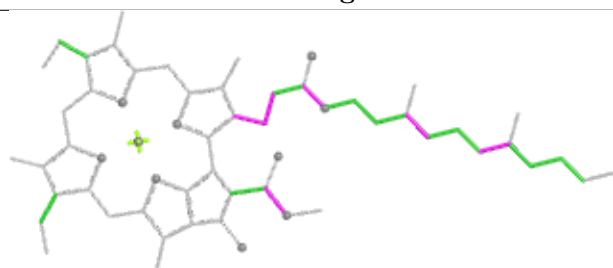
## Ligand CLA B 826



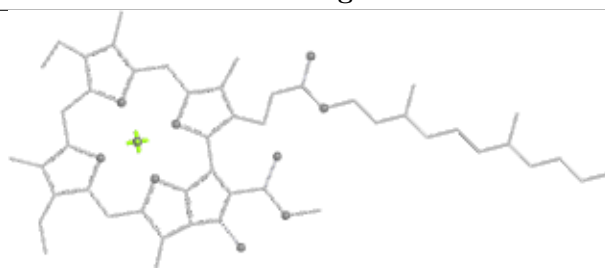
Bond lengths



Bond angles

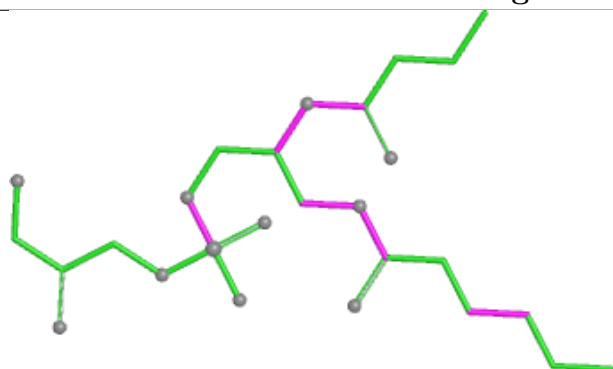


Torsions

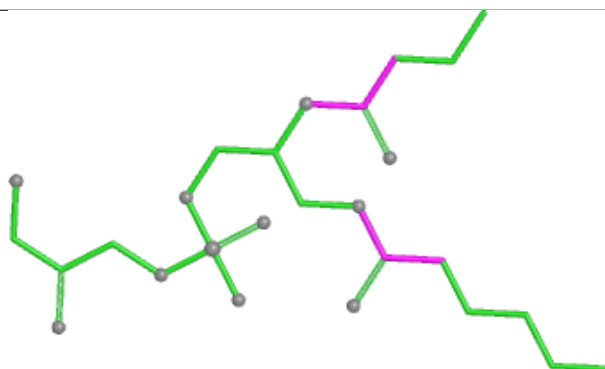


Rings

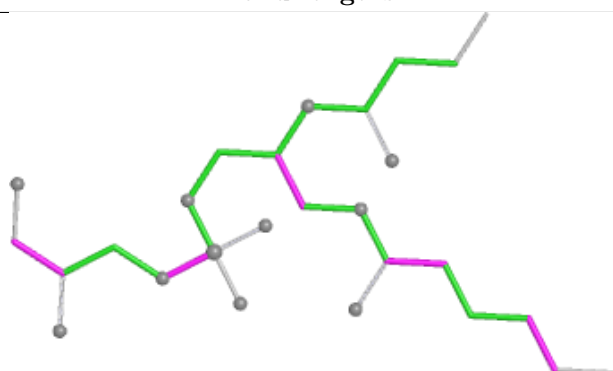
## Ligand LHG H 316



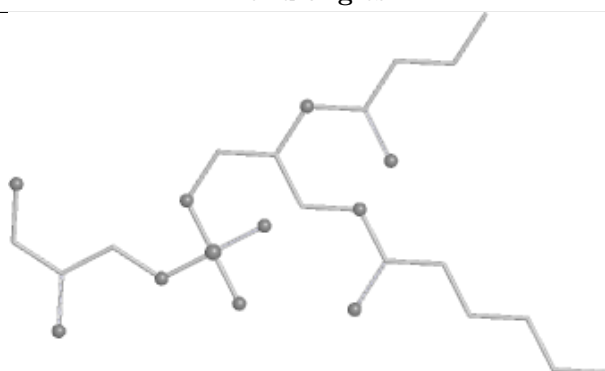
Bond lengths



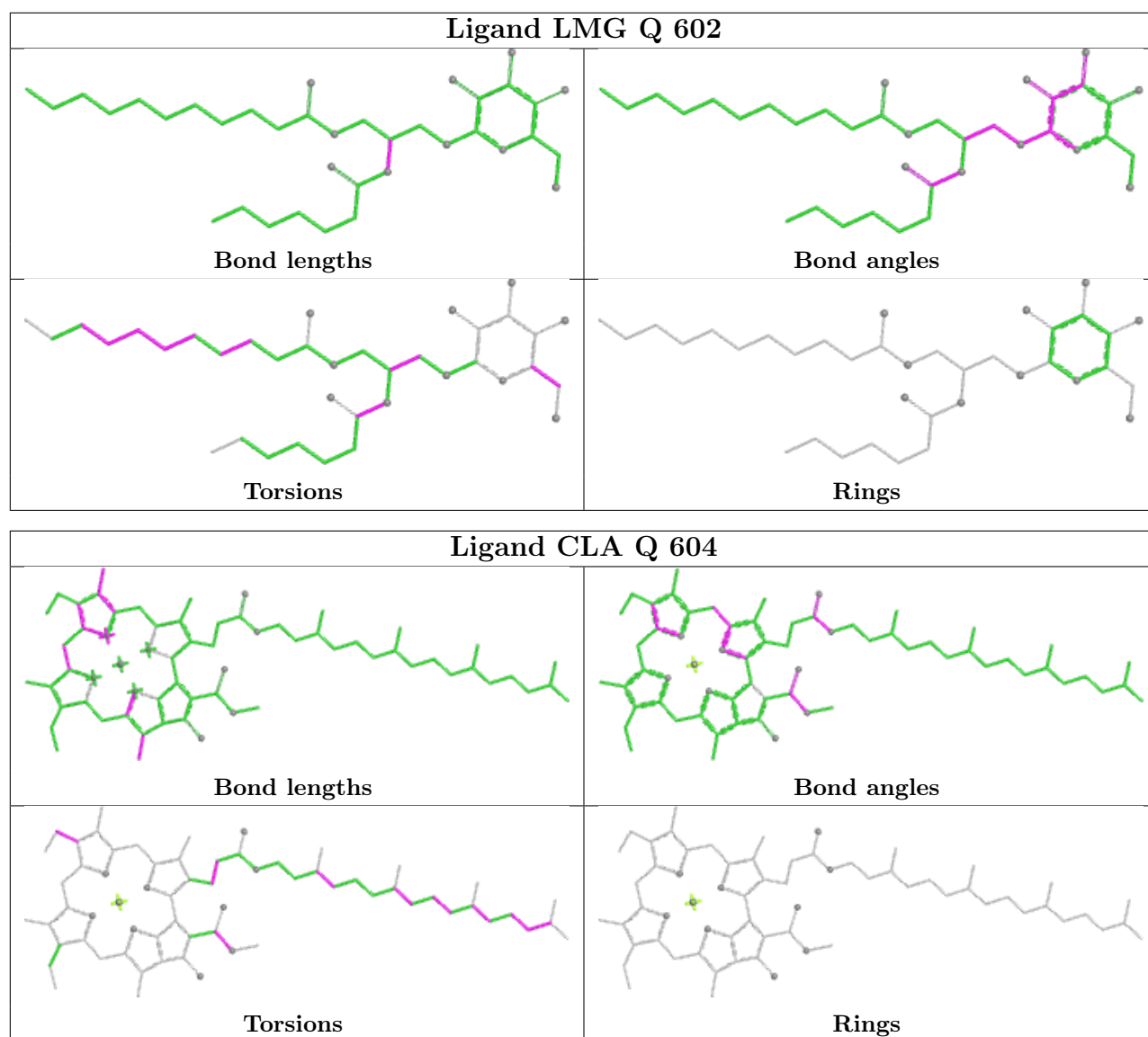
Bond angles

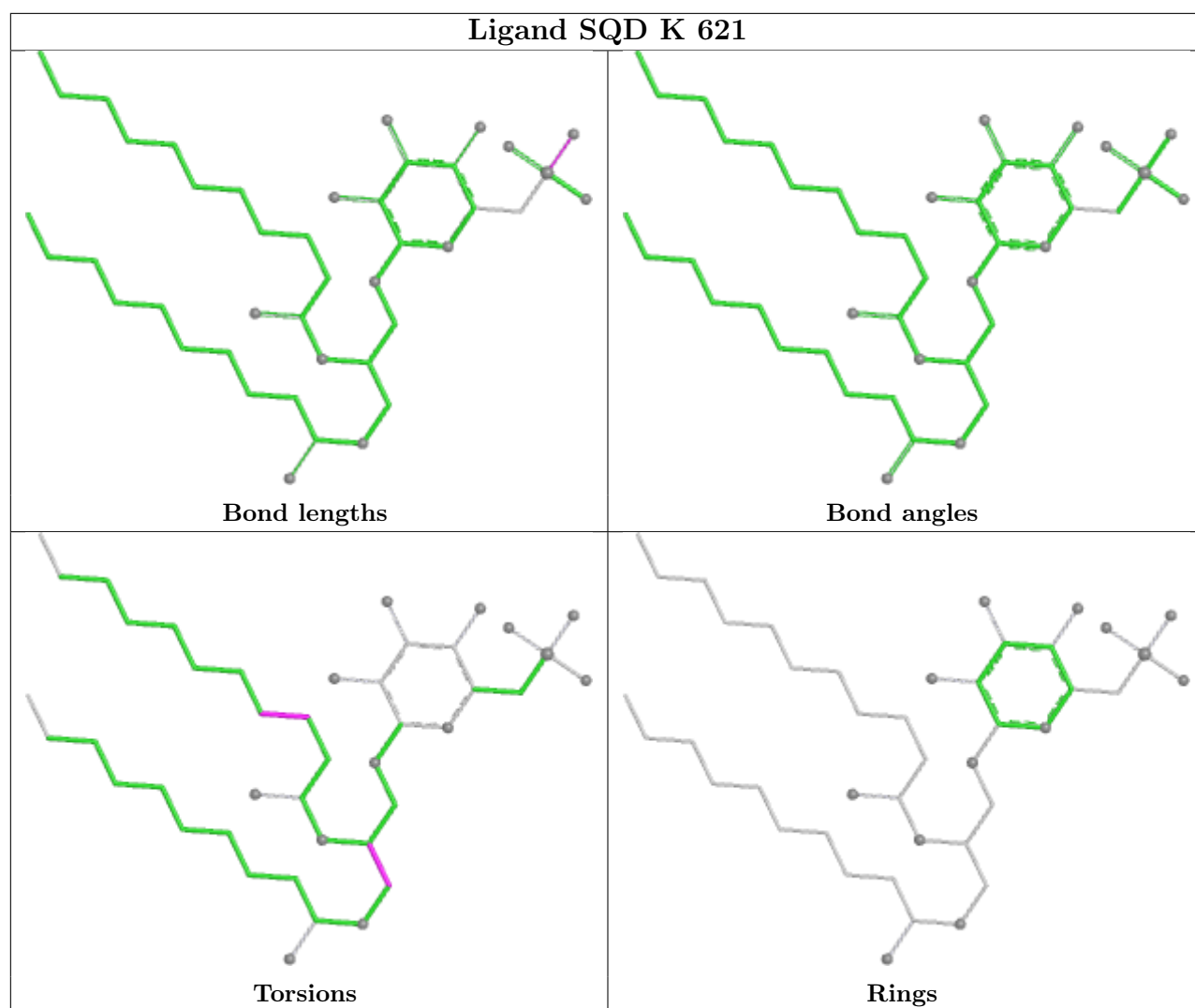


Torsions

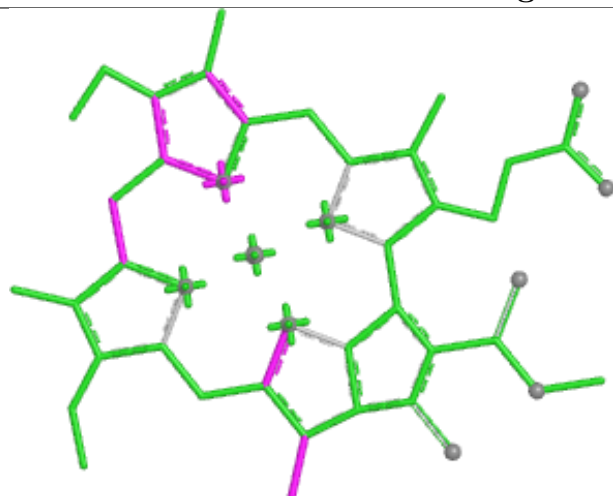


Rings

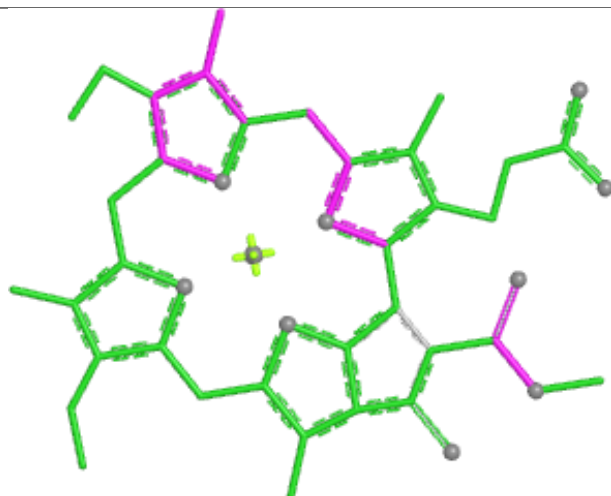




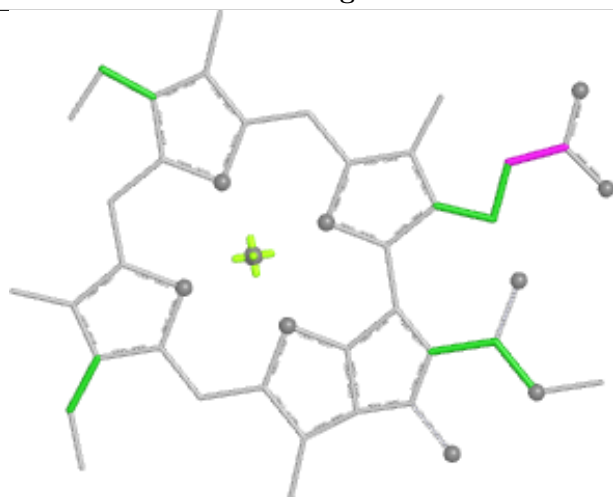
## Ligand CLA S 603



Bond lengths



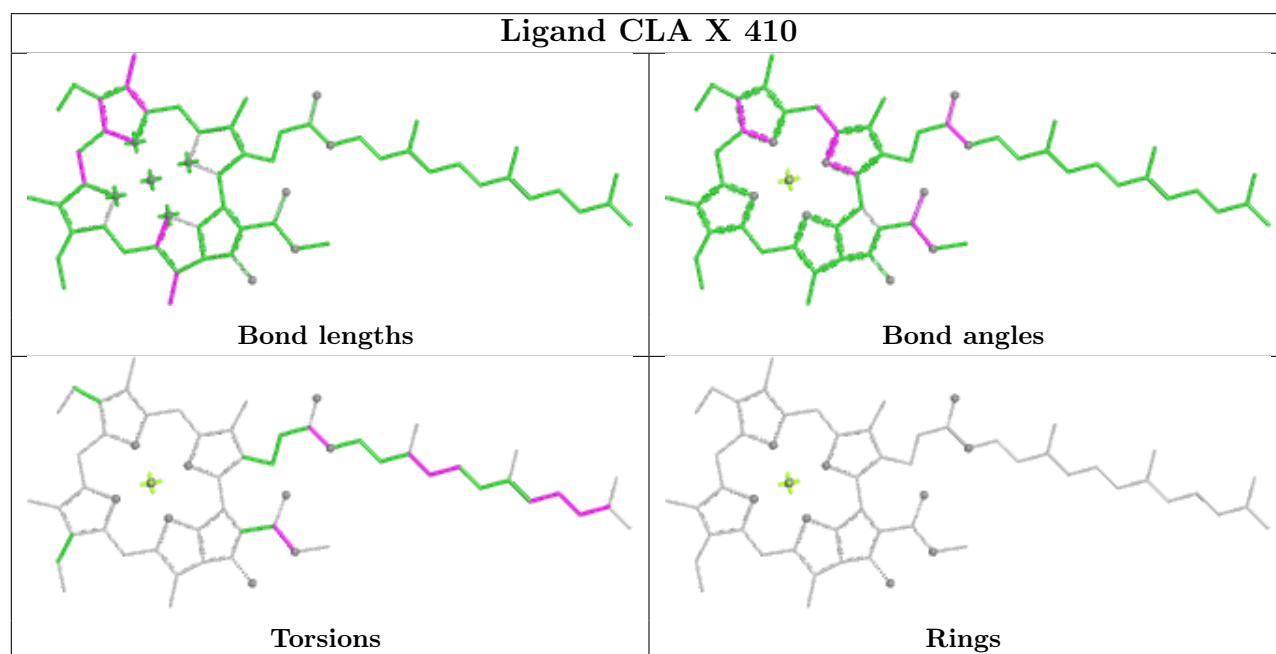
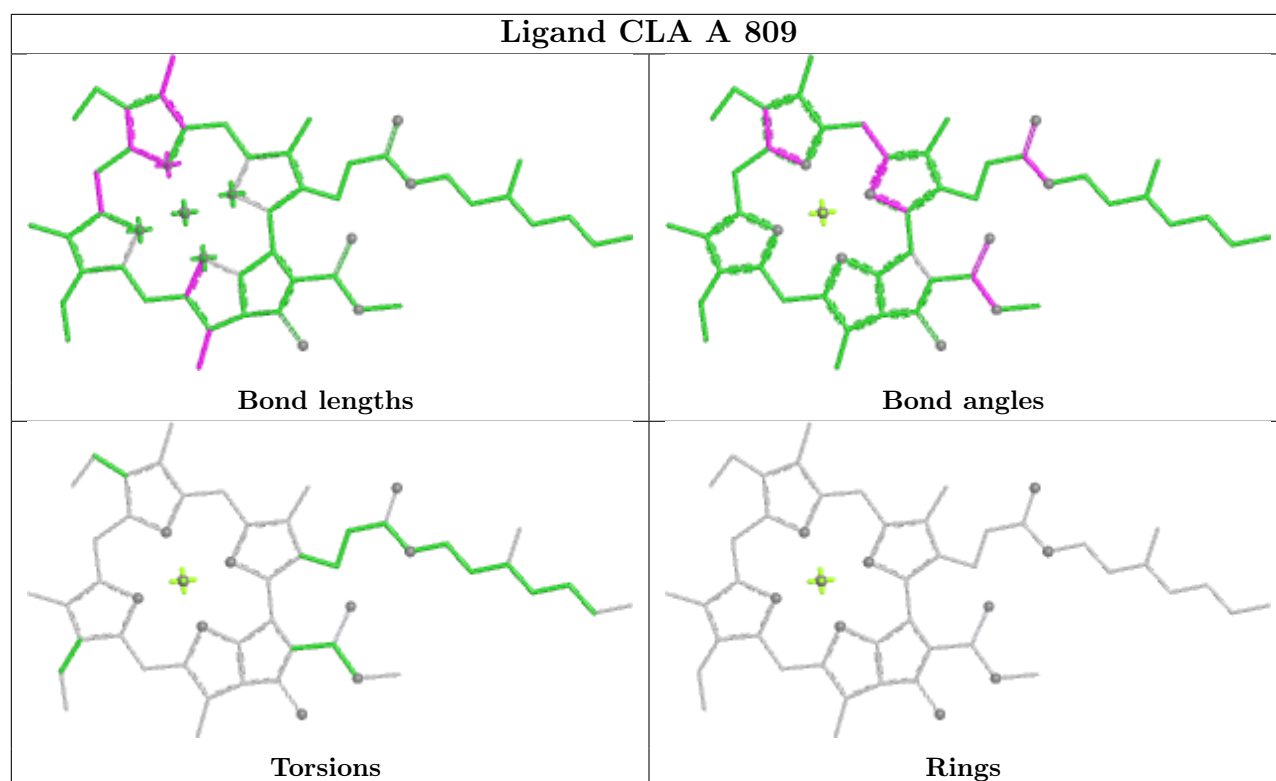
Bond angles

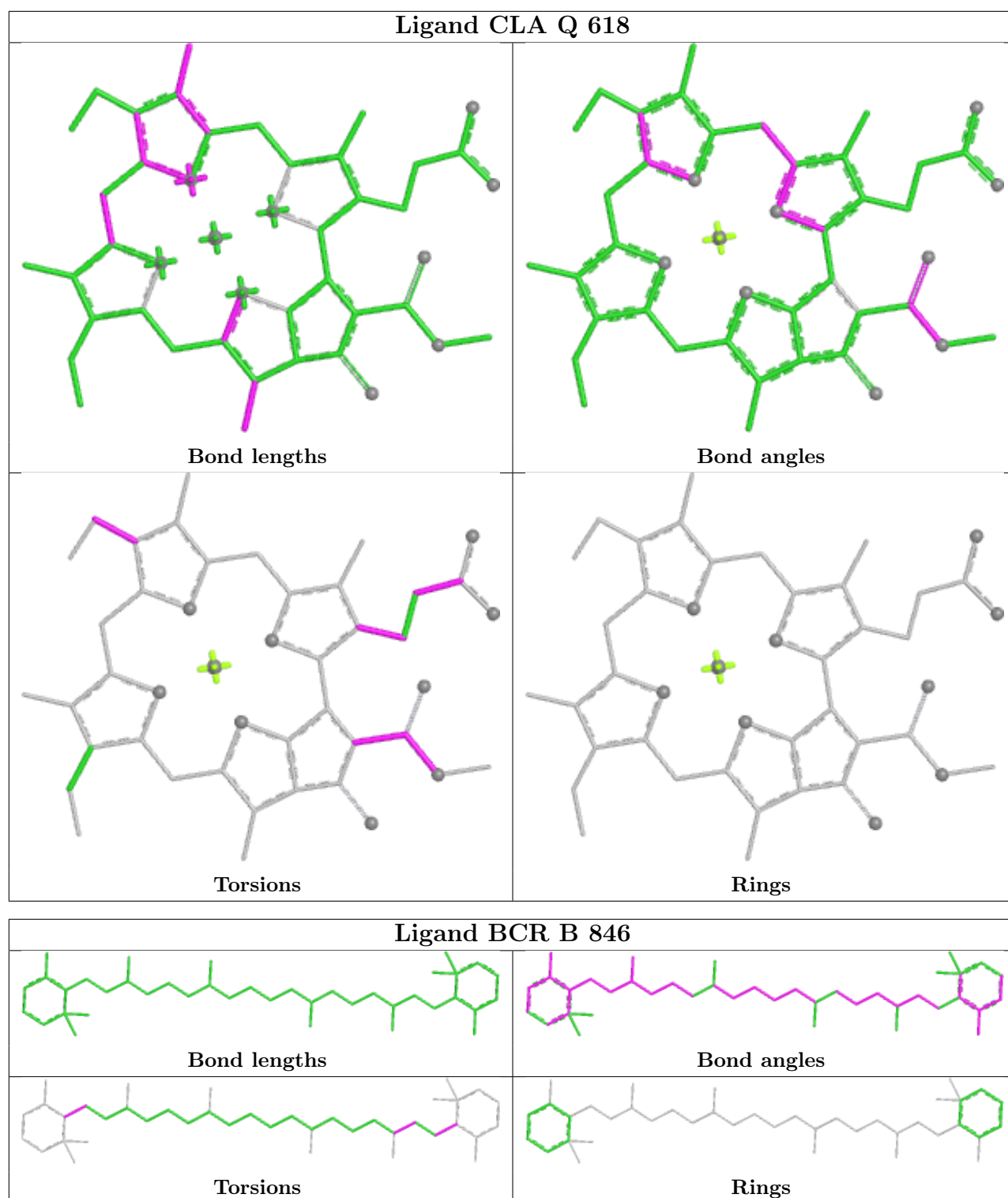


Torsions

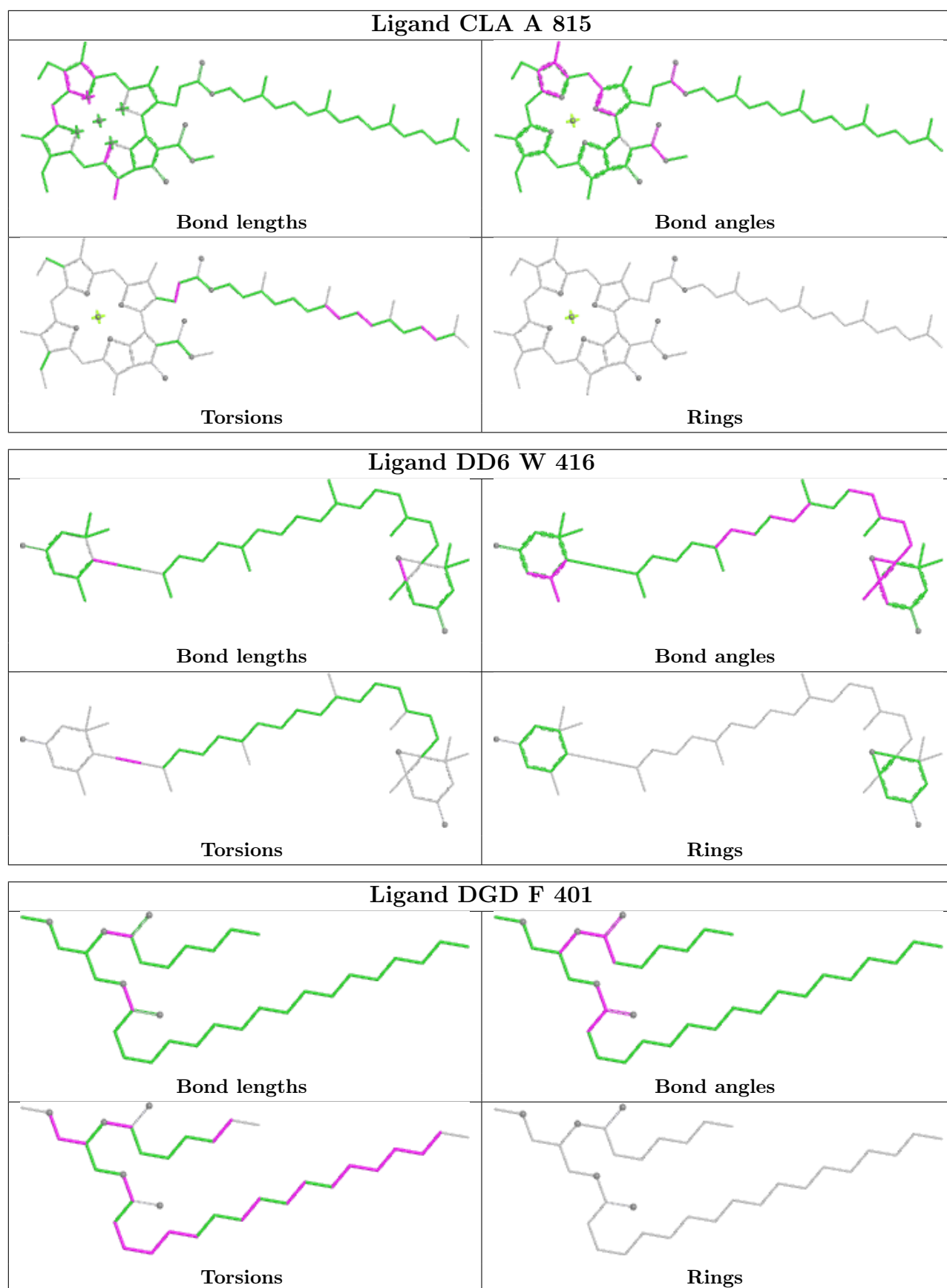


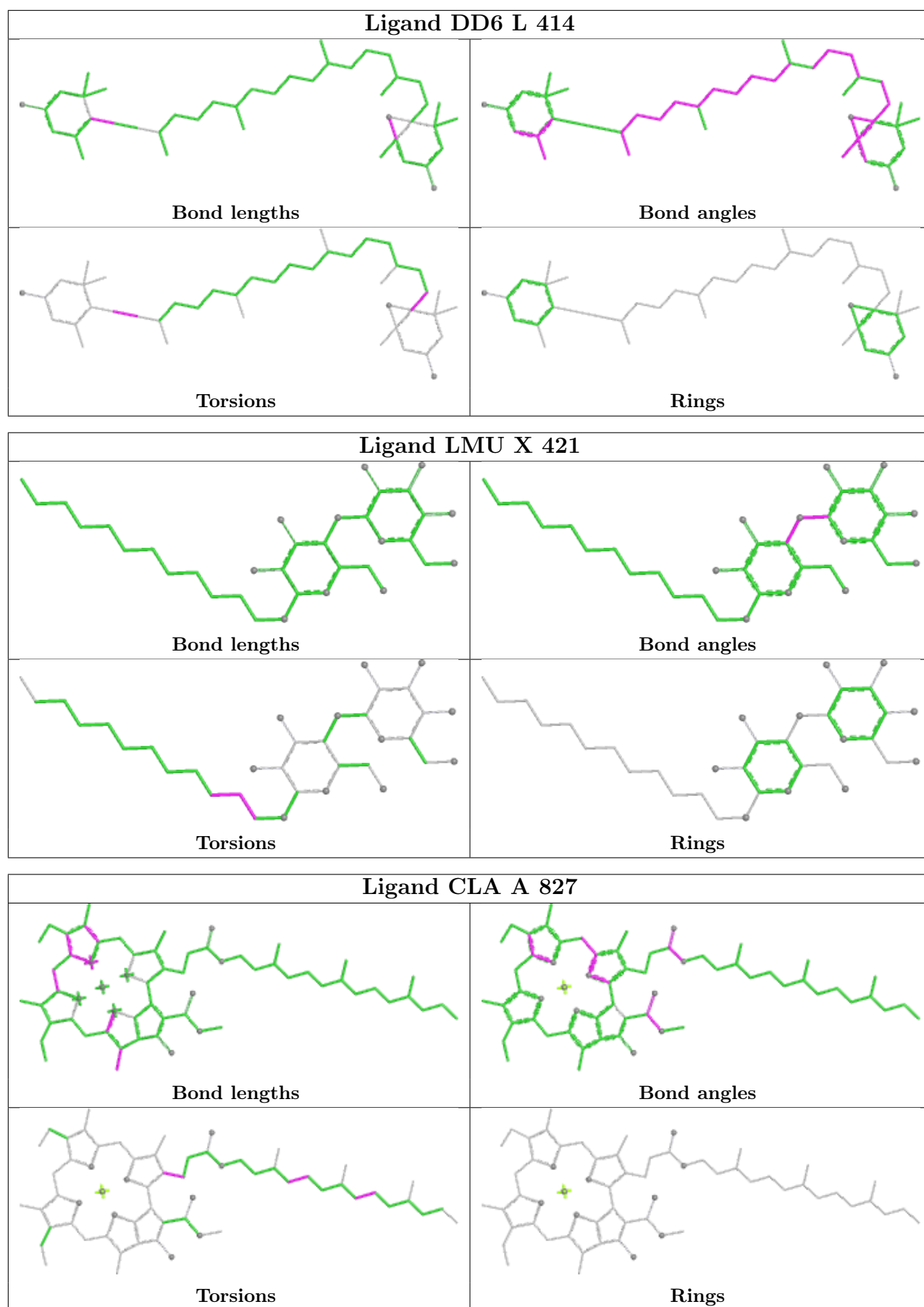
Rings

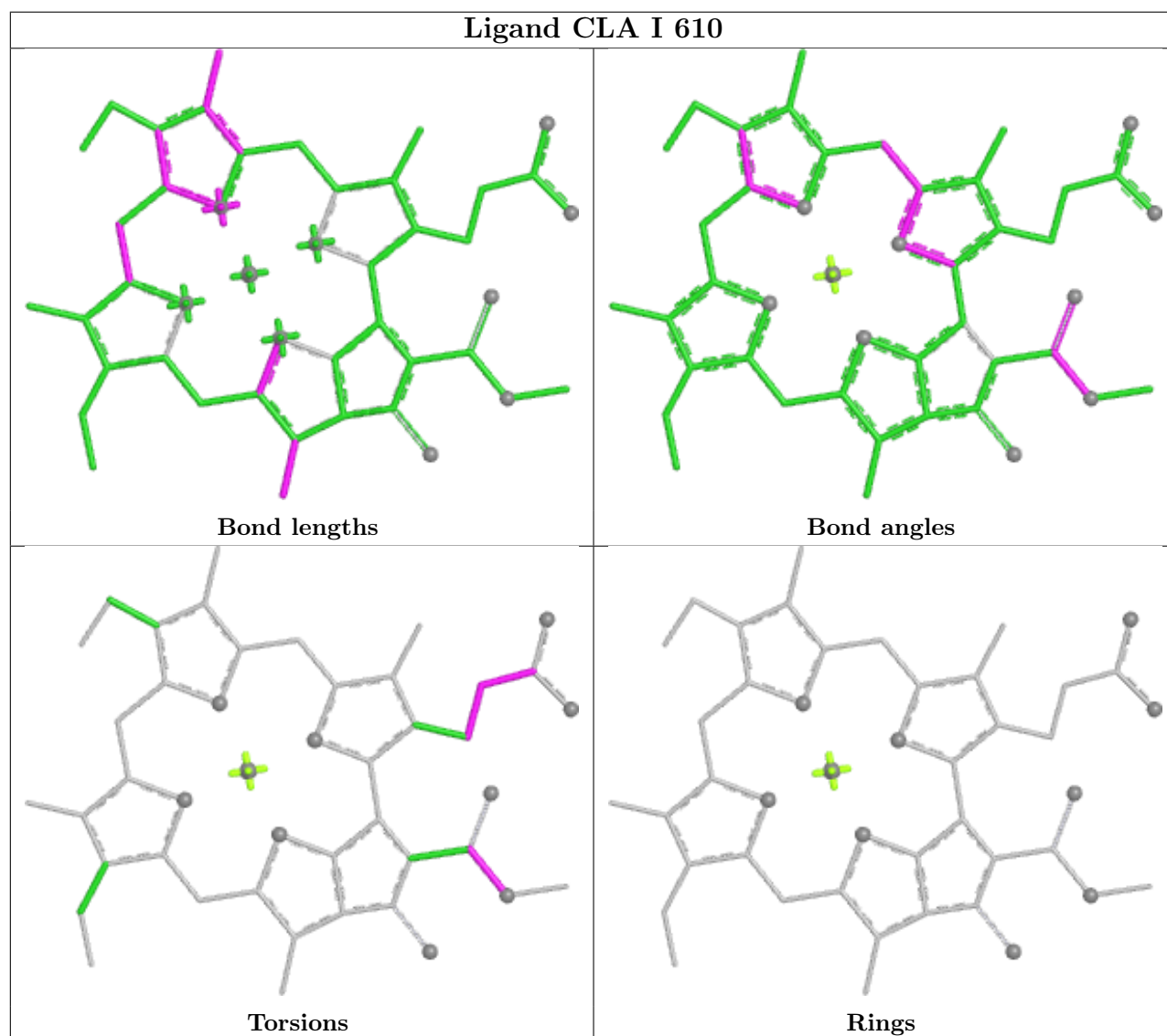
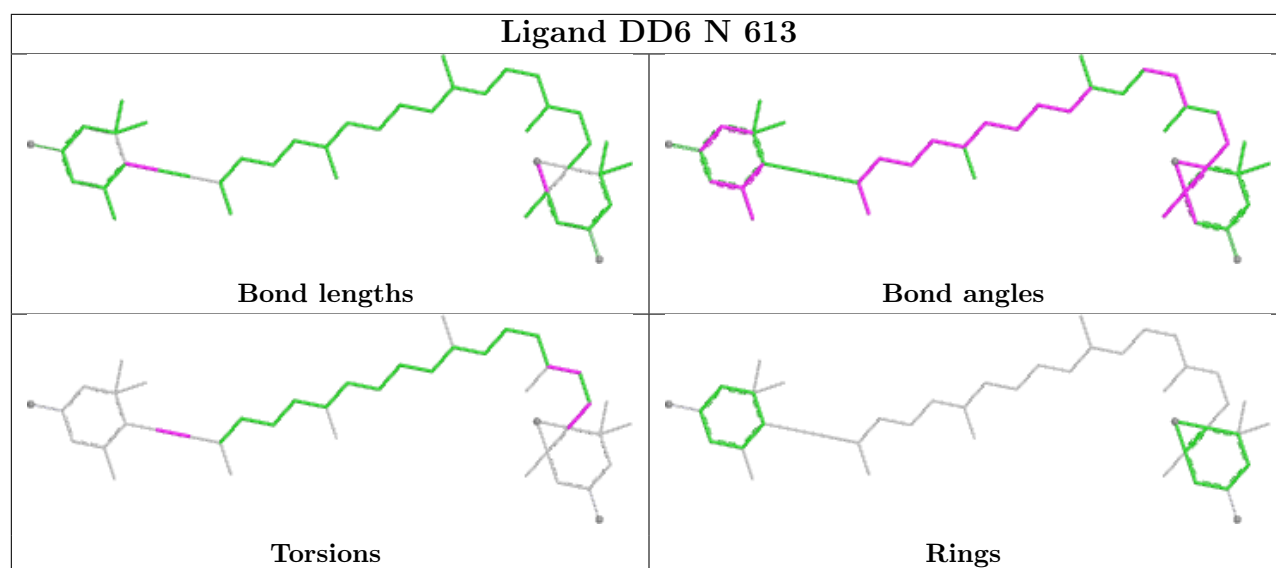




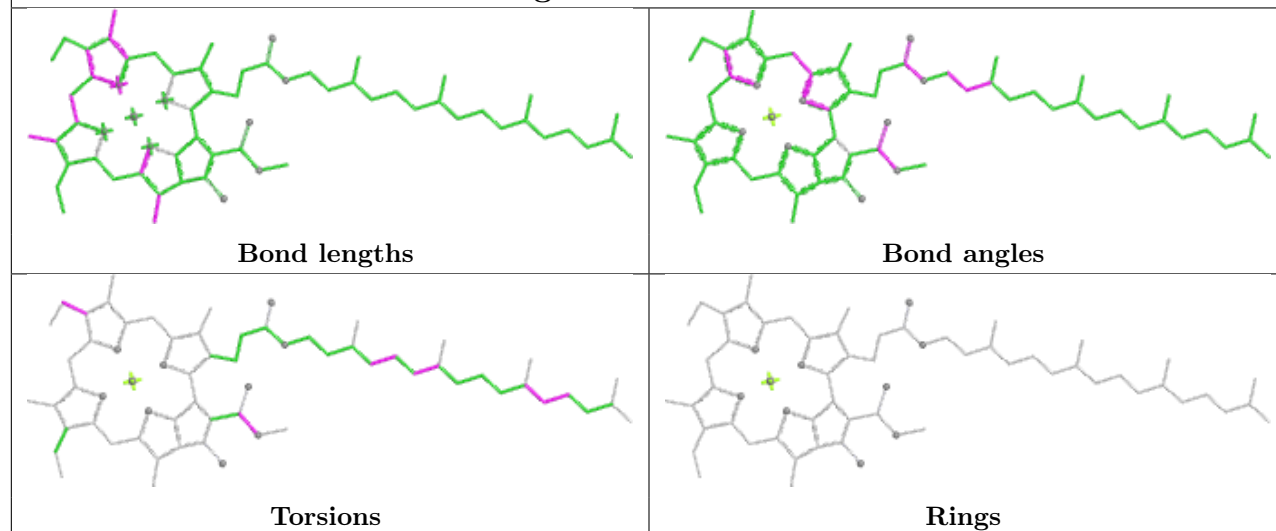




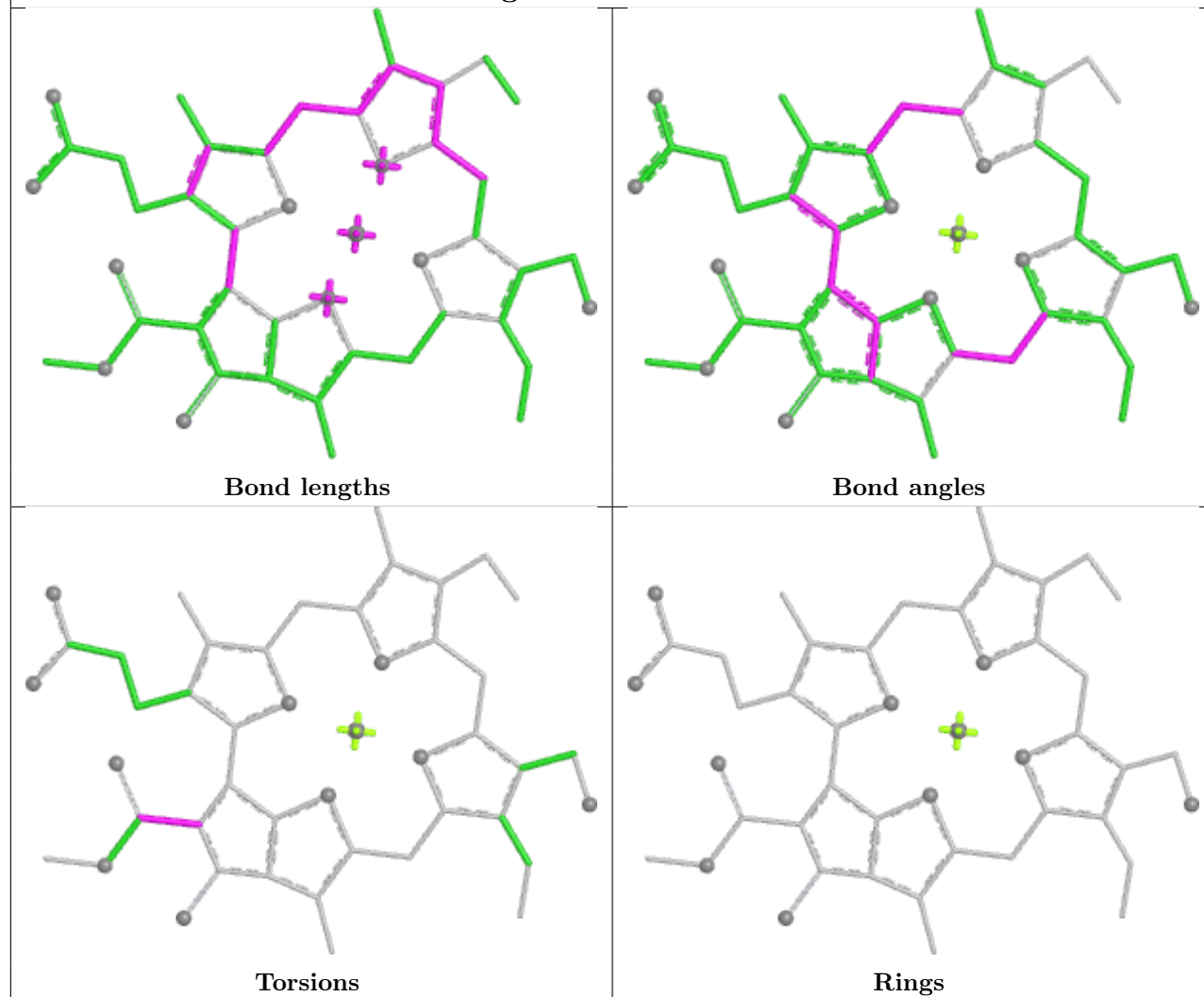


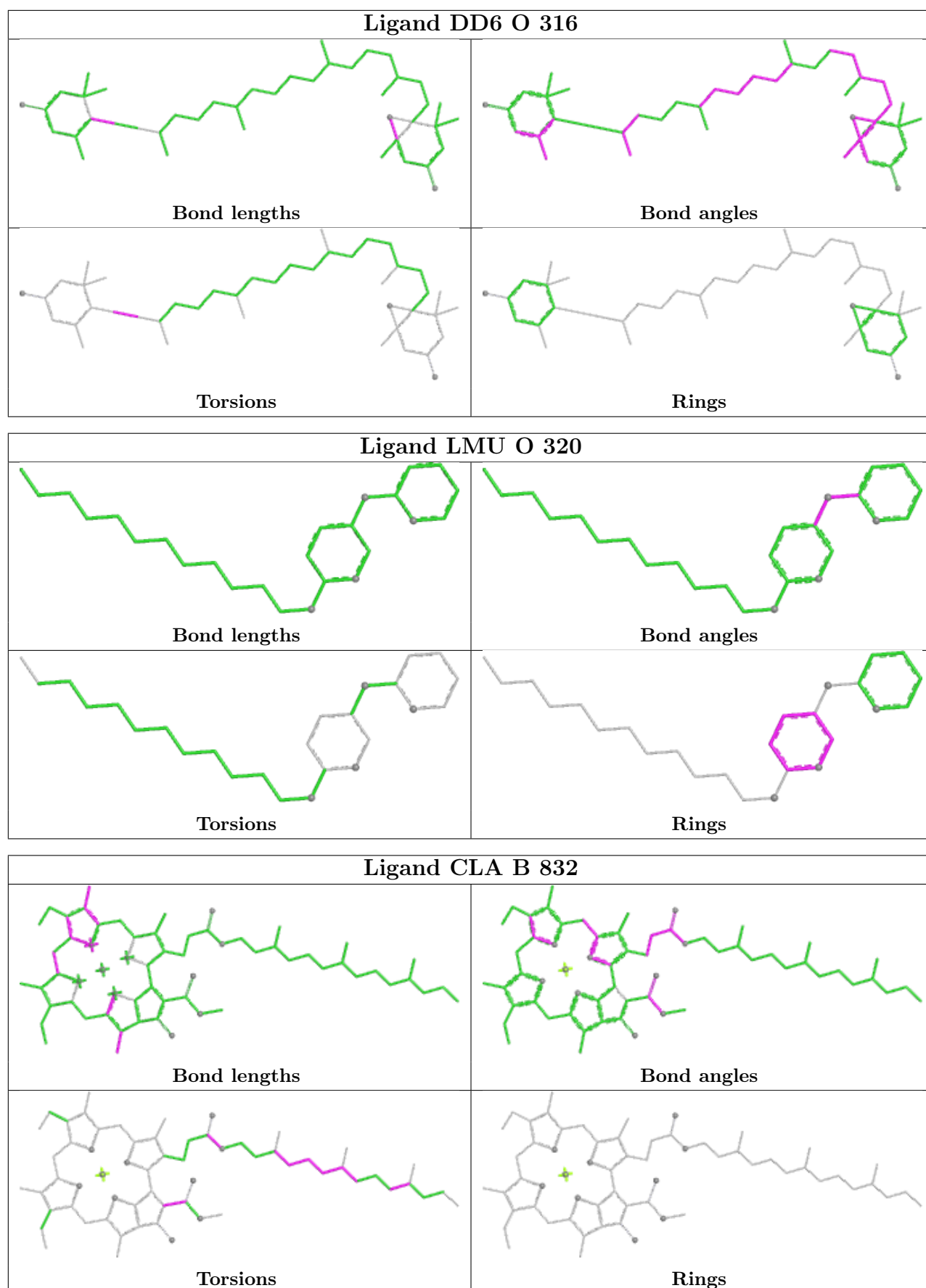


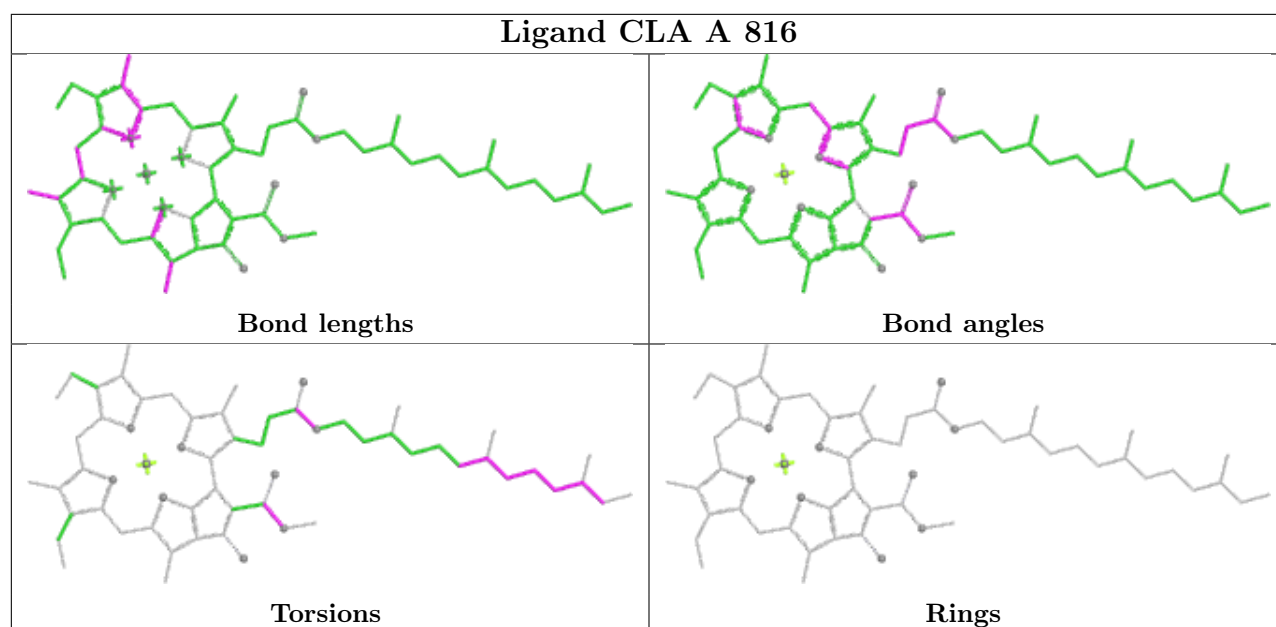
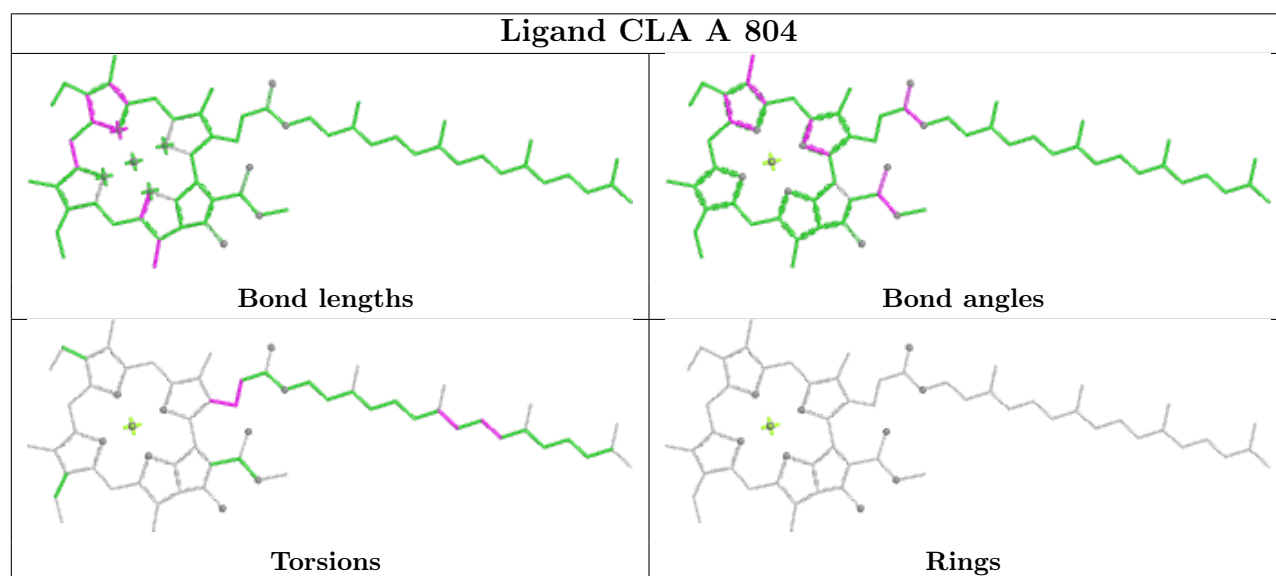
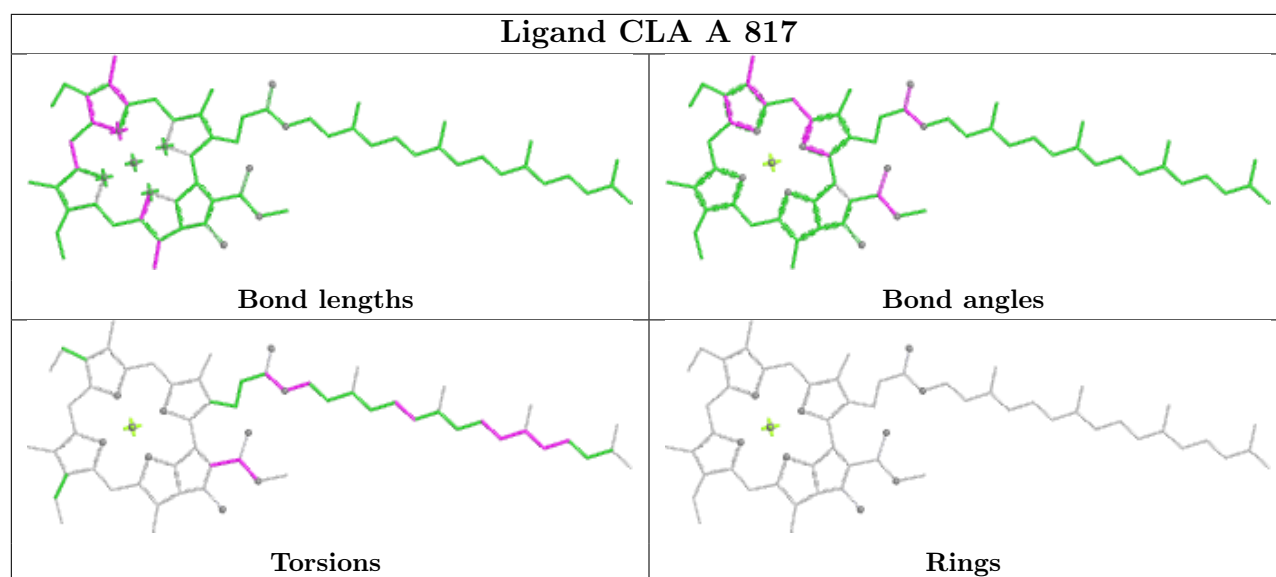
## Ligand CLA F 403

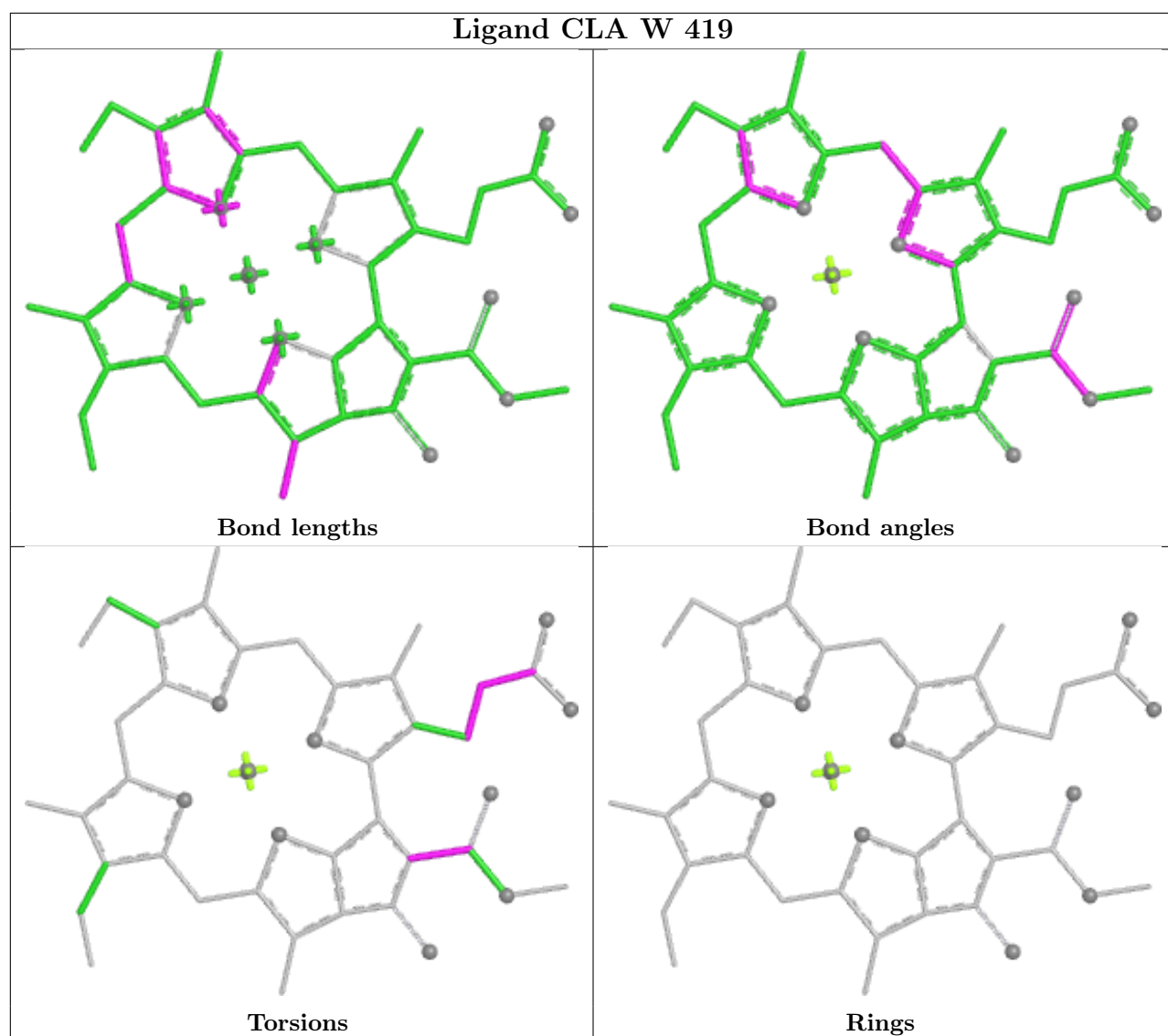


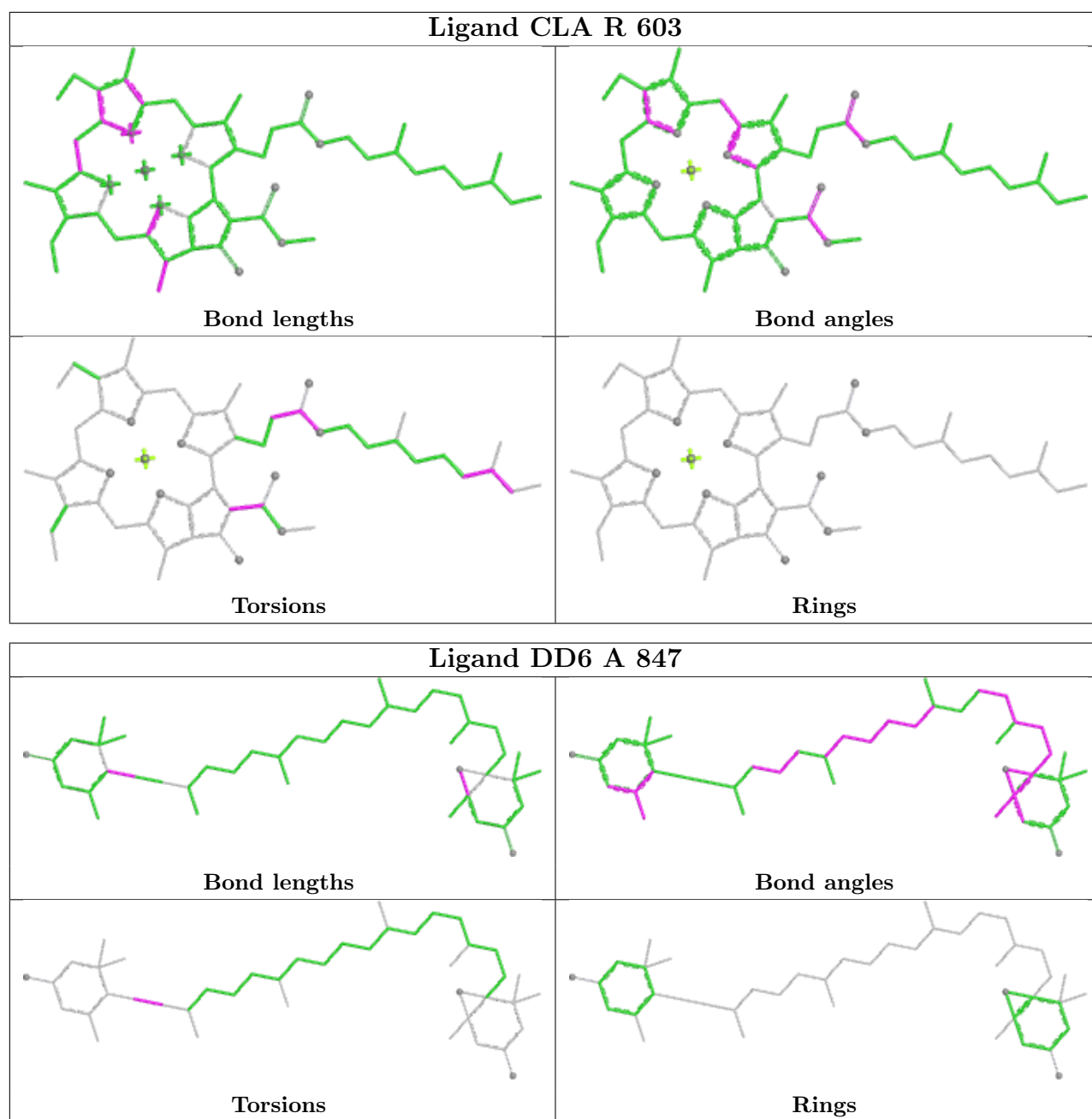
## Ligand CHL V 606



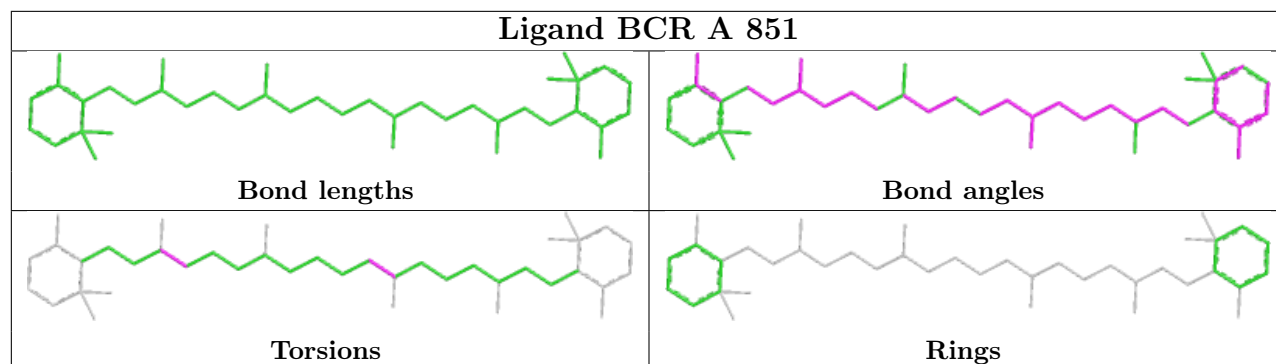
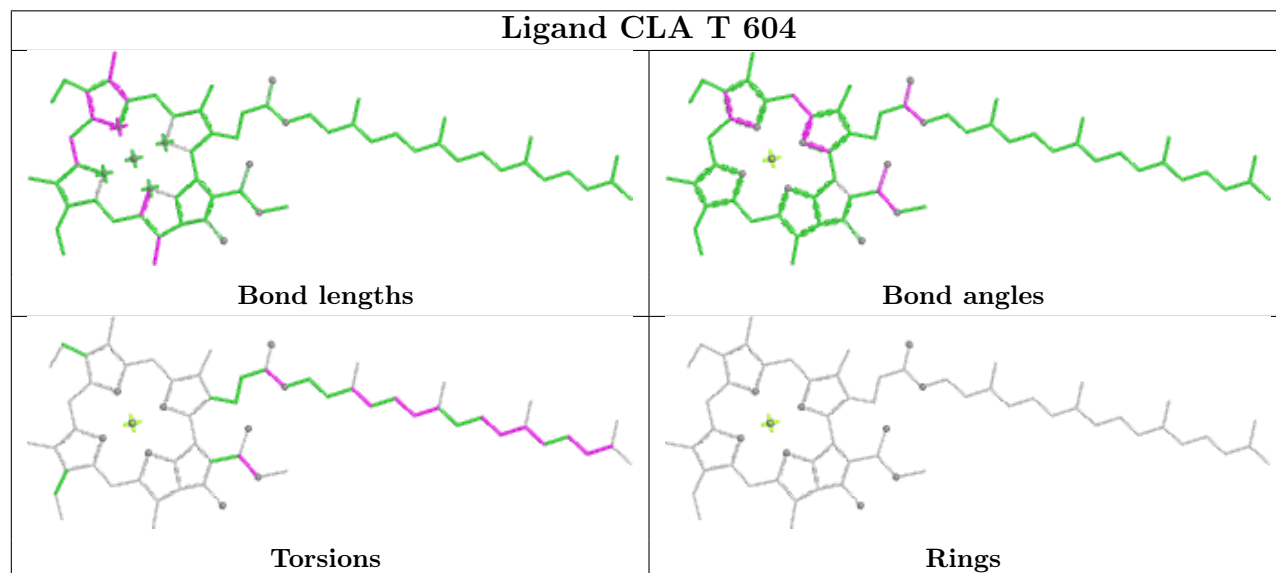
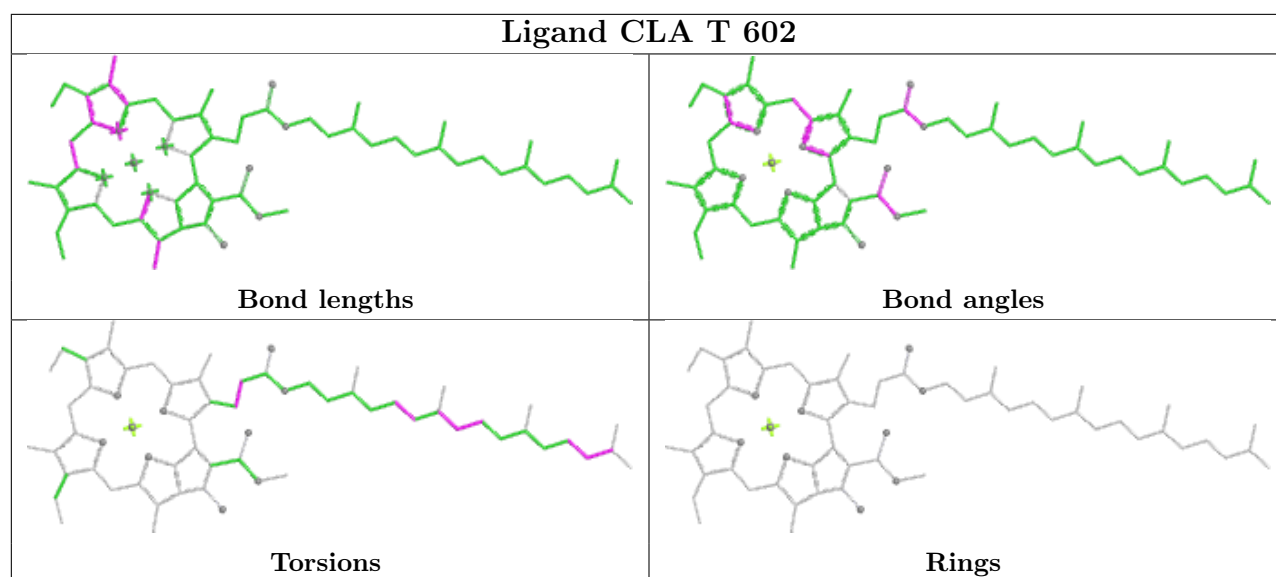


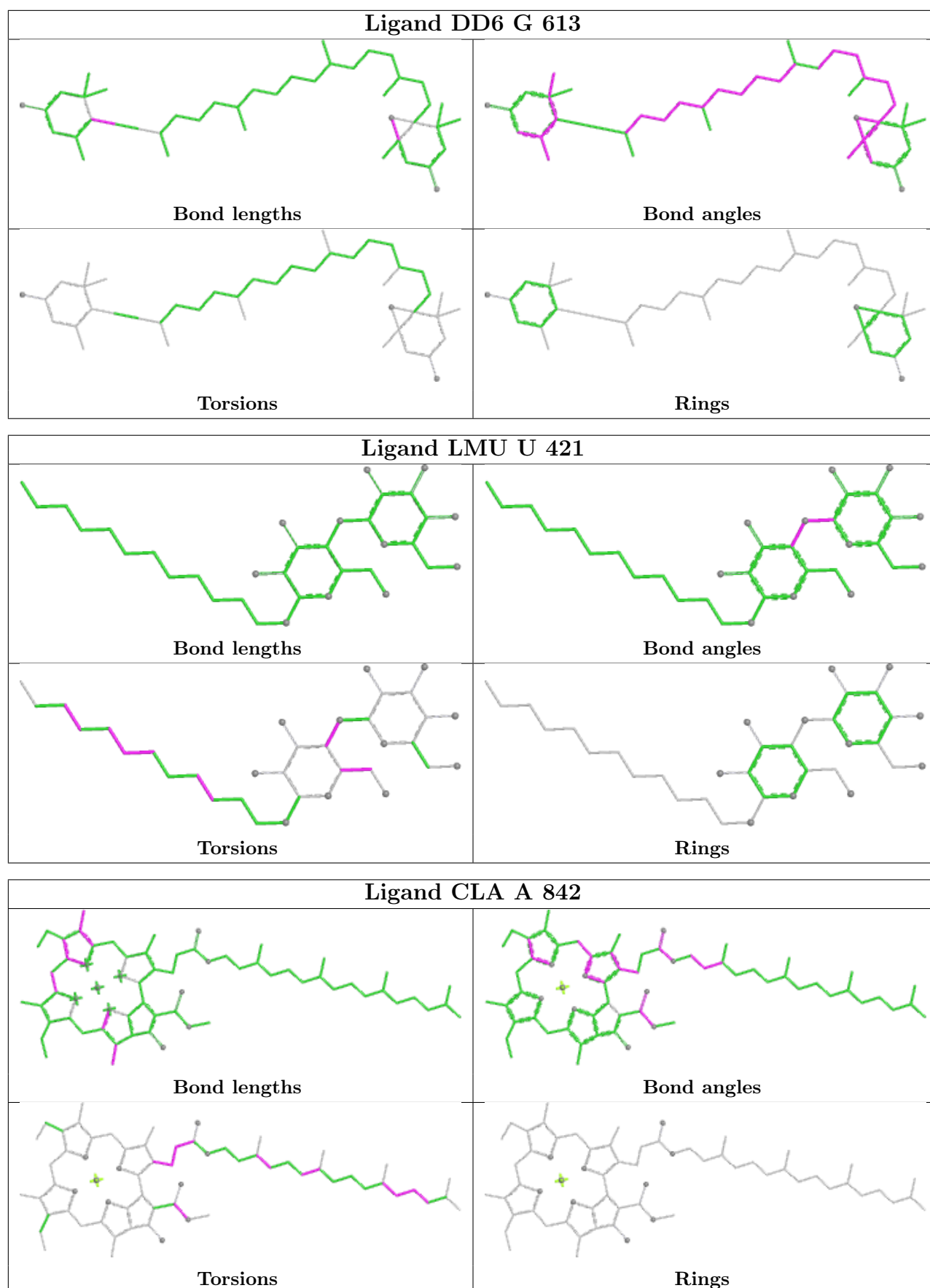




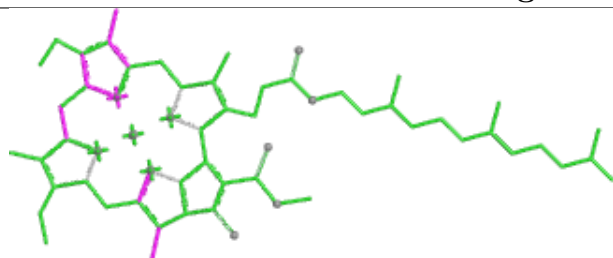




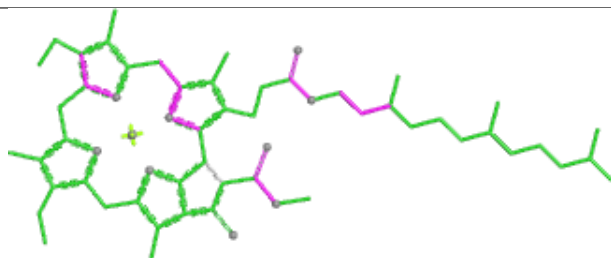




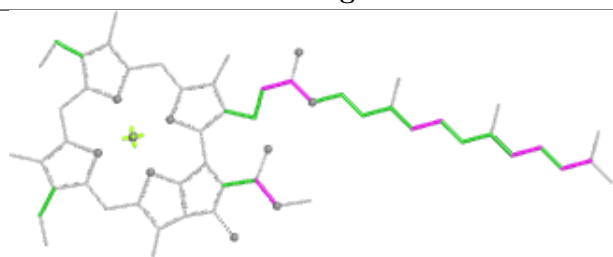
## Ligand CLA S 604



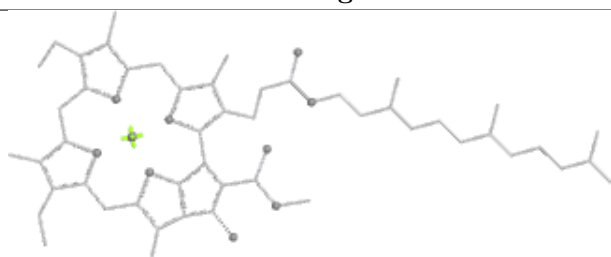
Bond lengths



Bond angles

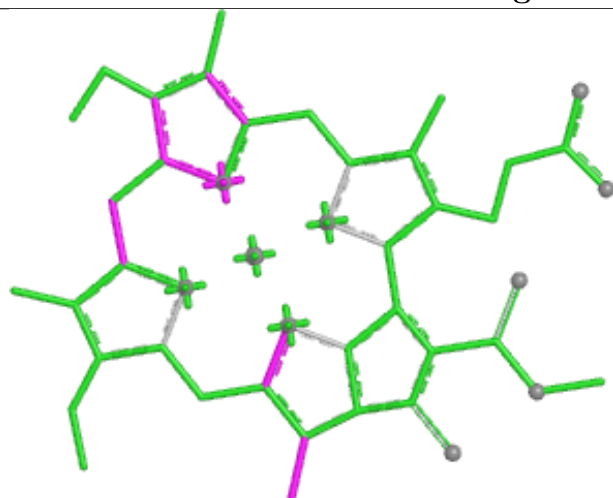


Torsions

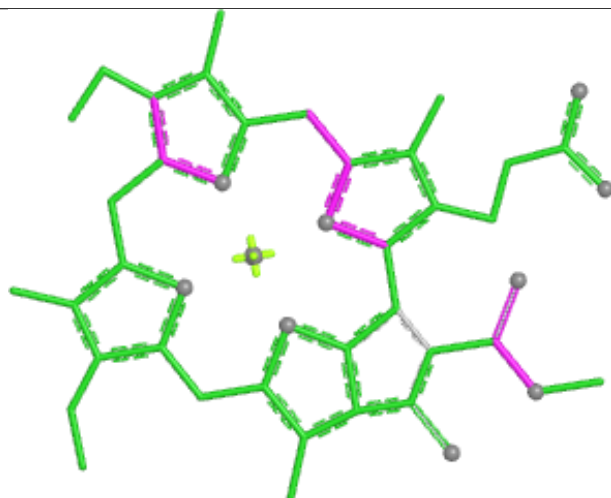


Rings

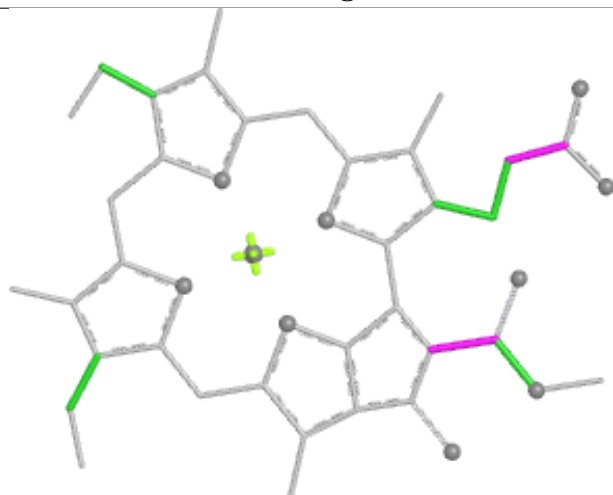
## Ligand CLA H 310



Bond lengths



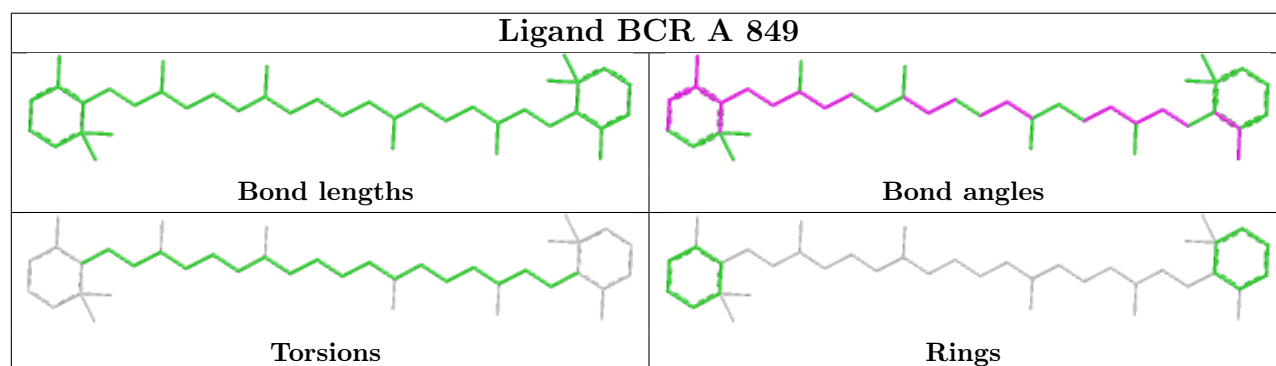
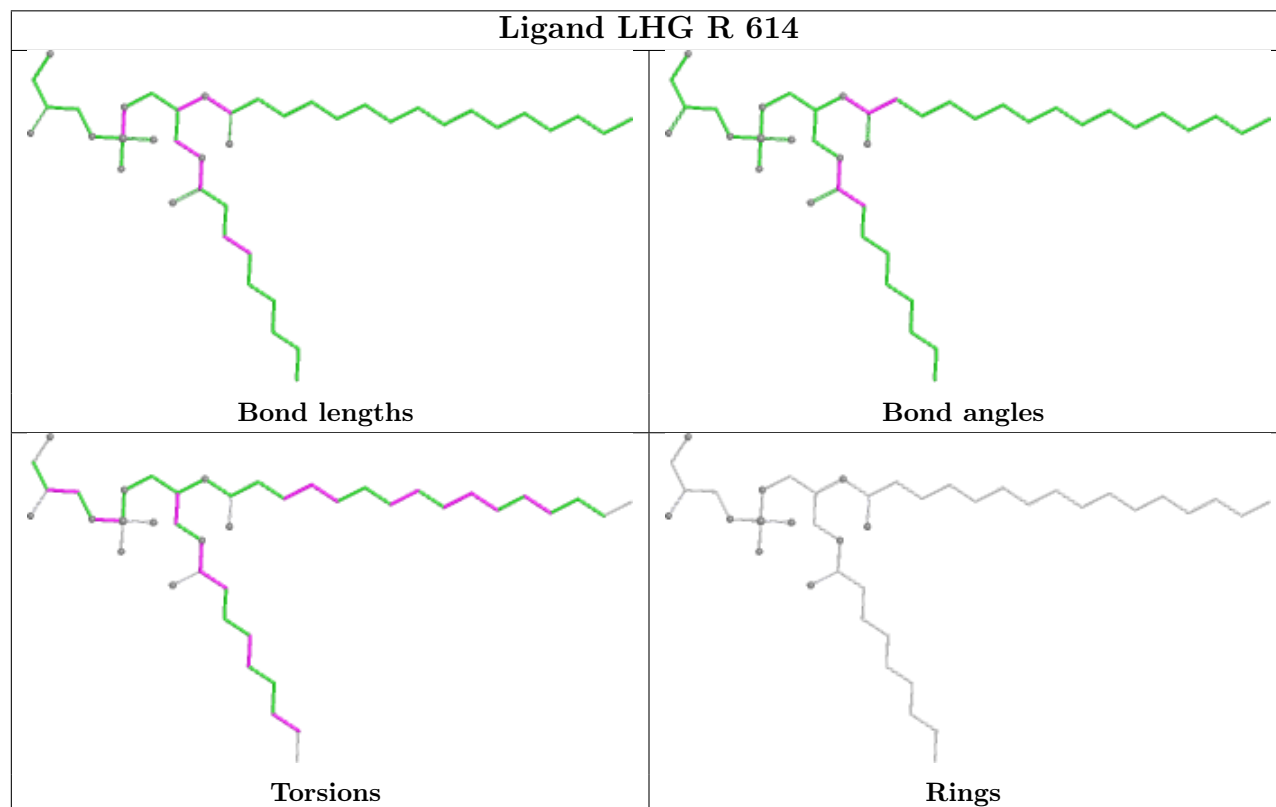
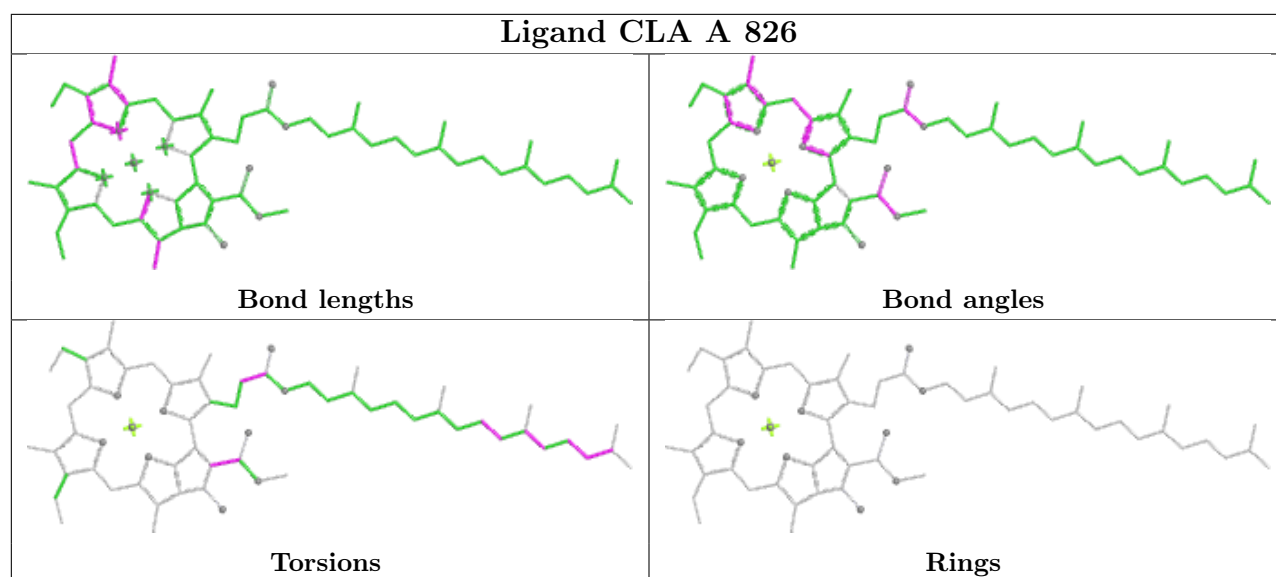
Bond angles

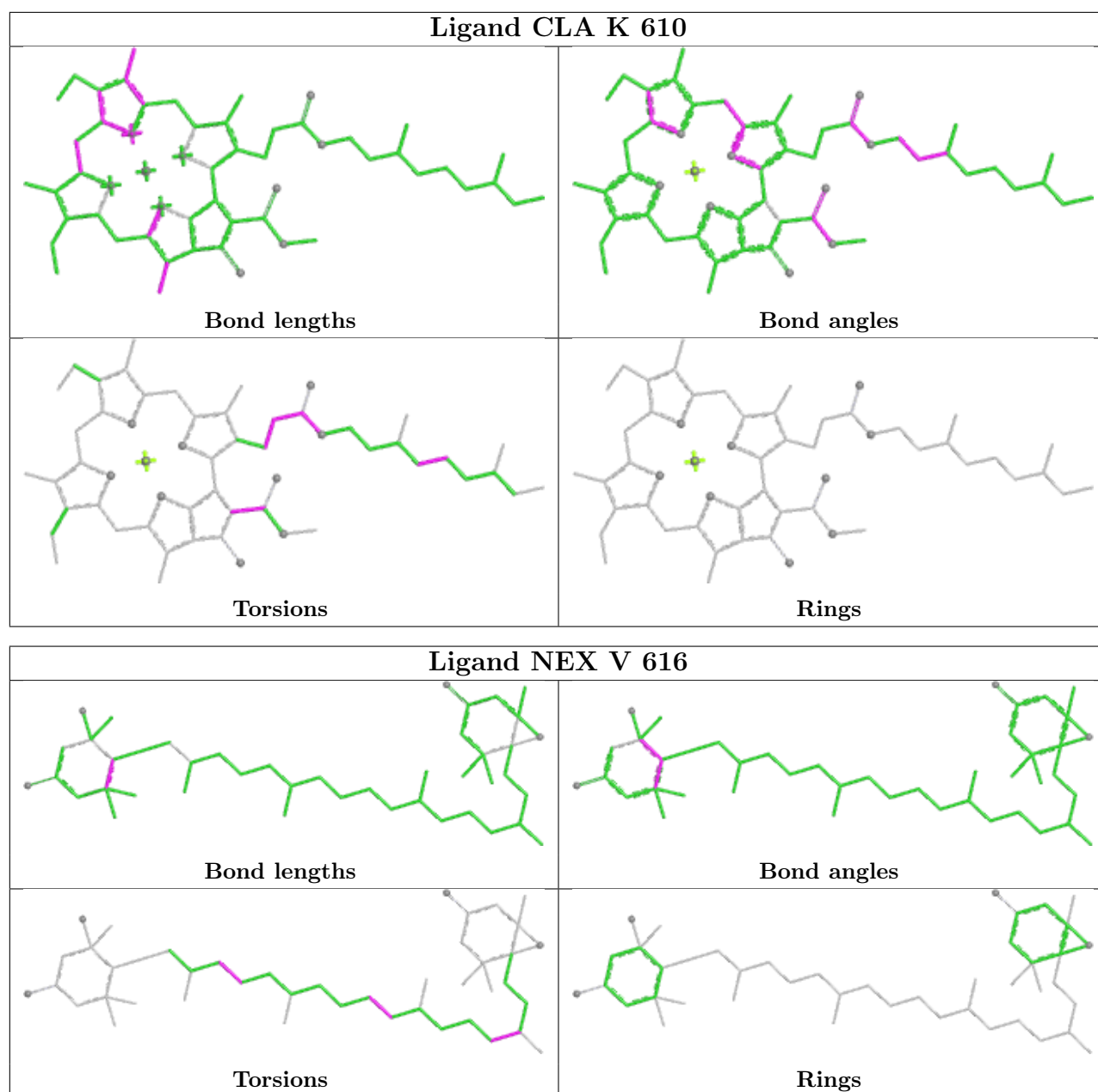


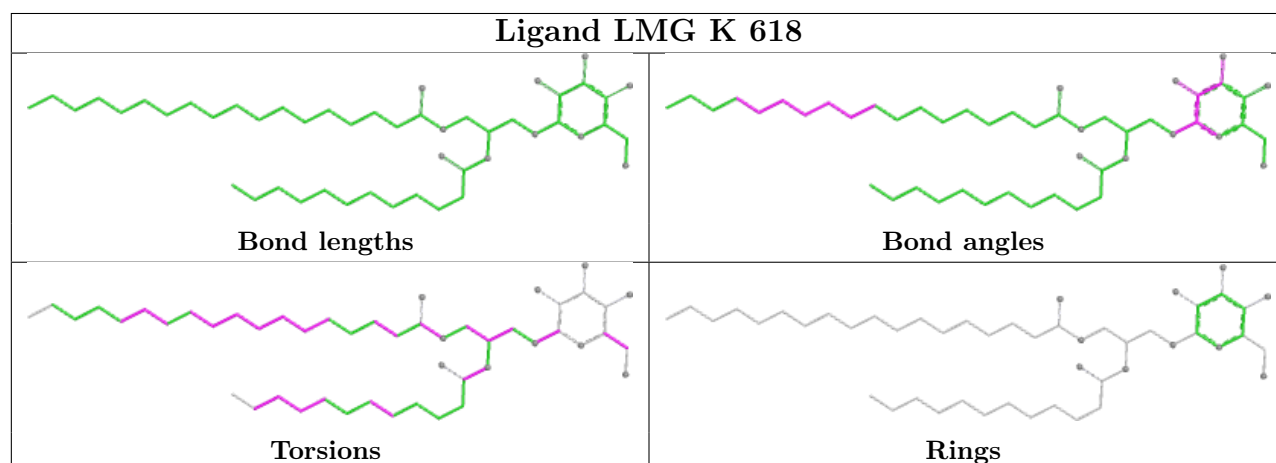
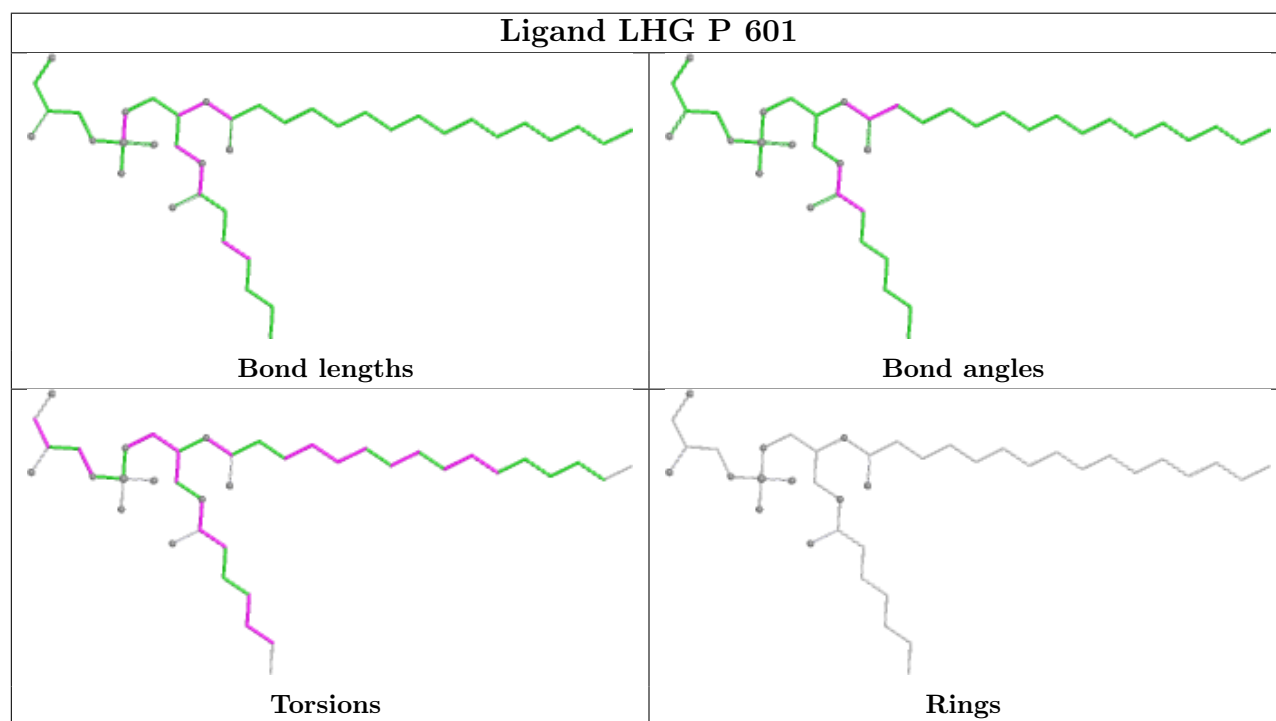
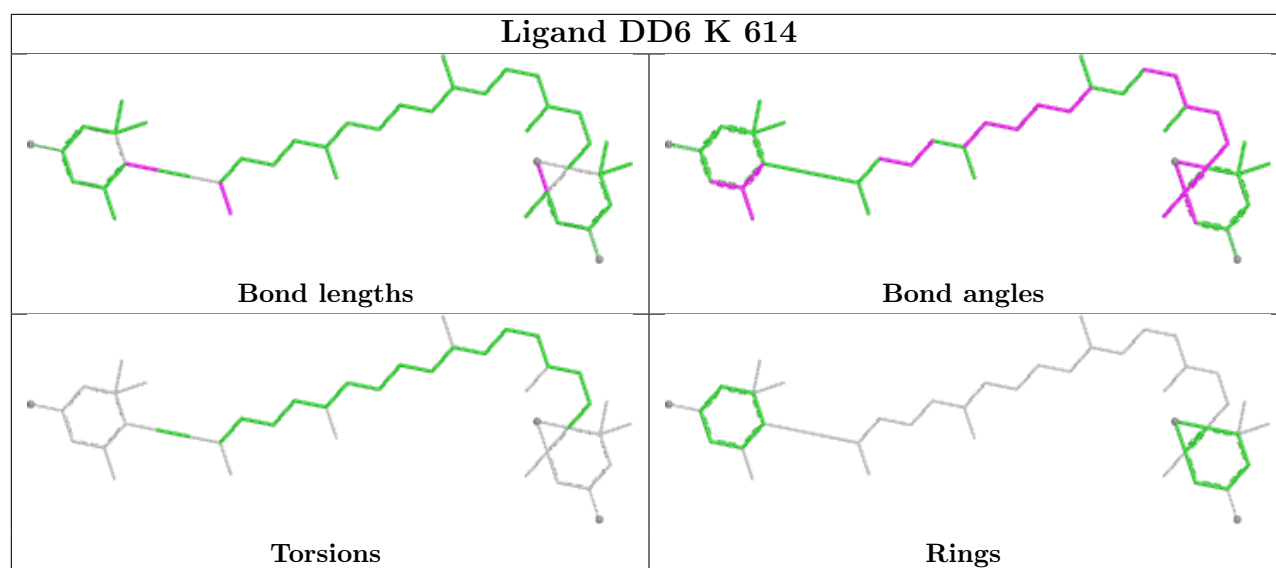
Torsions

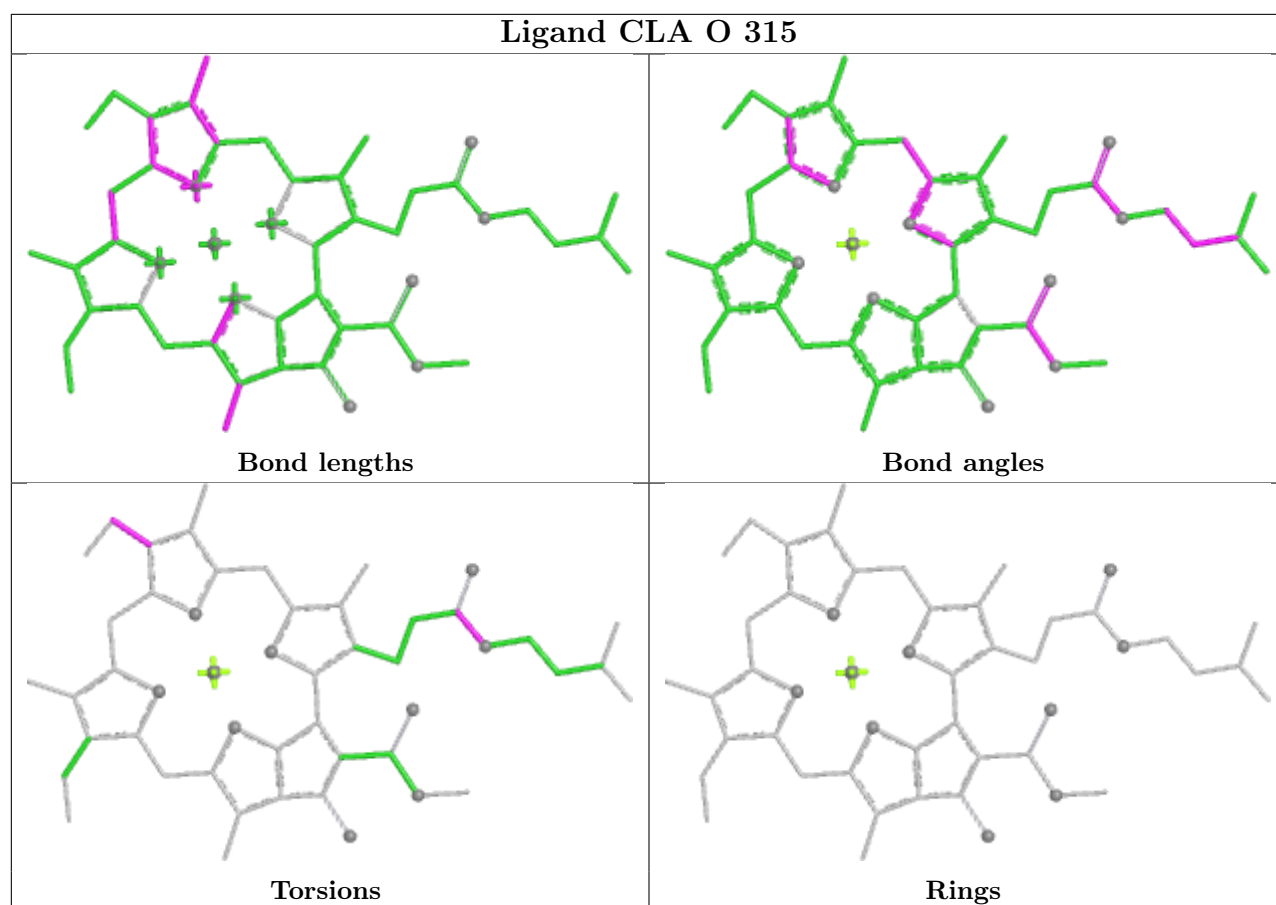


Rings

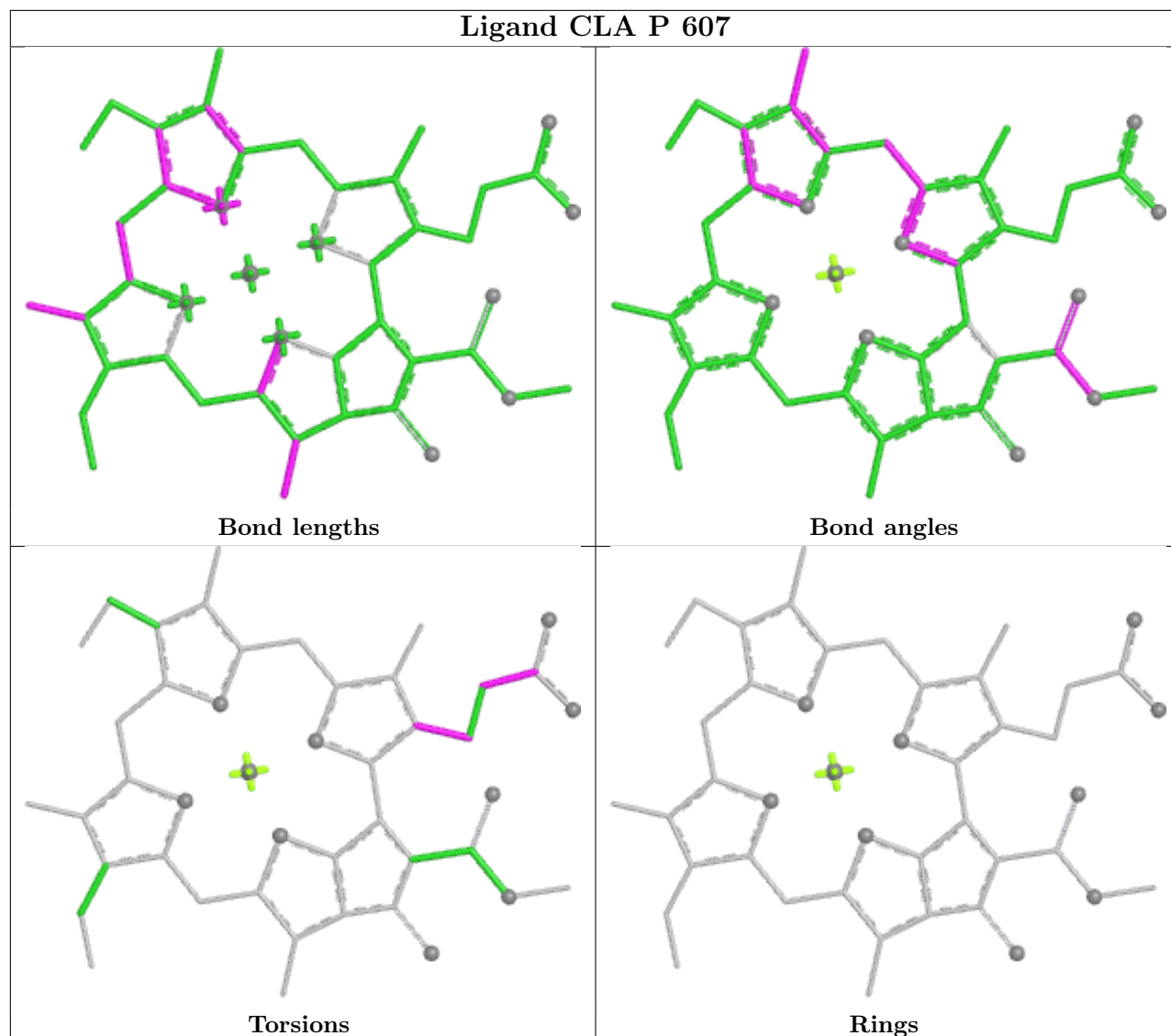




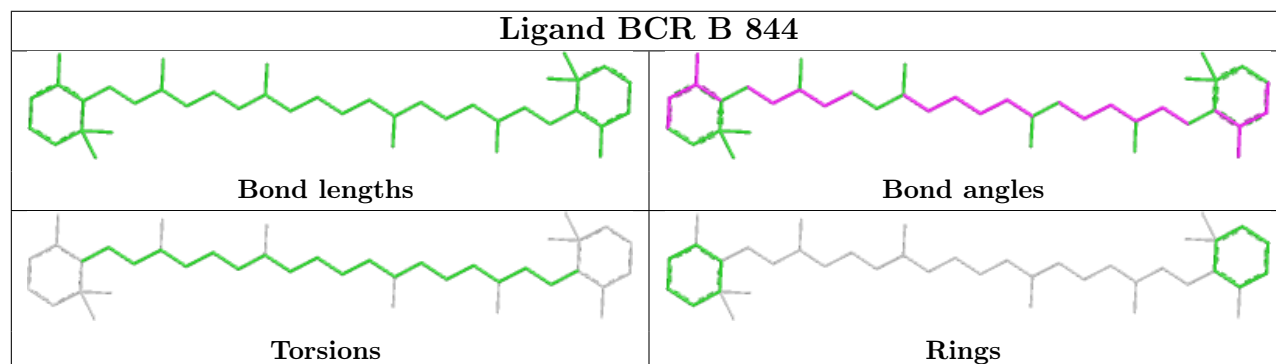




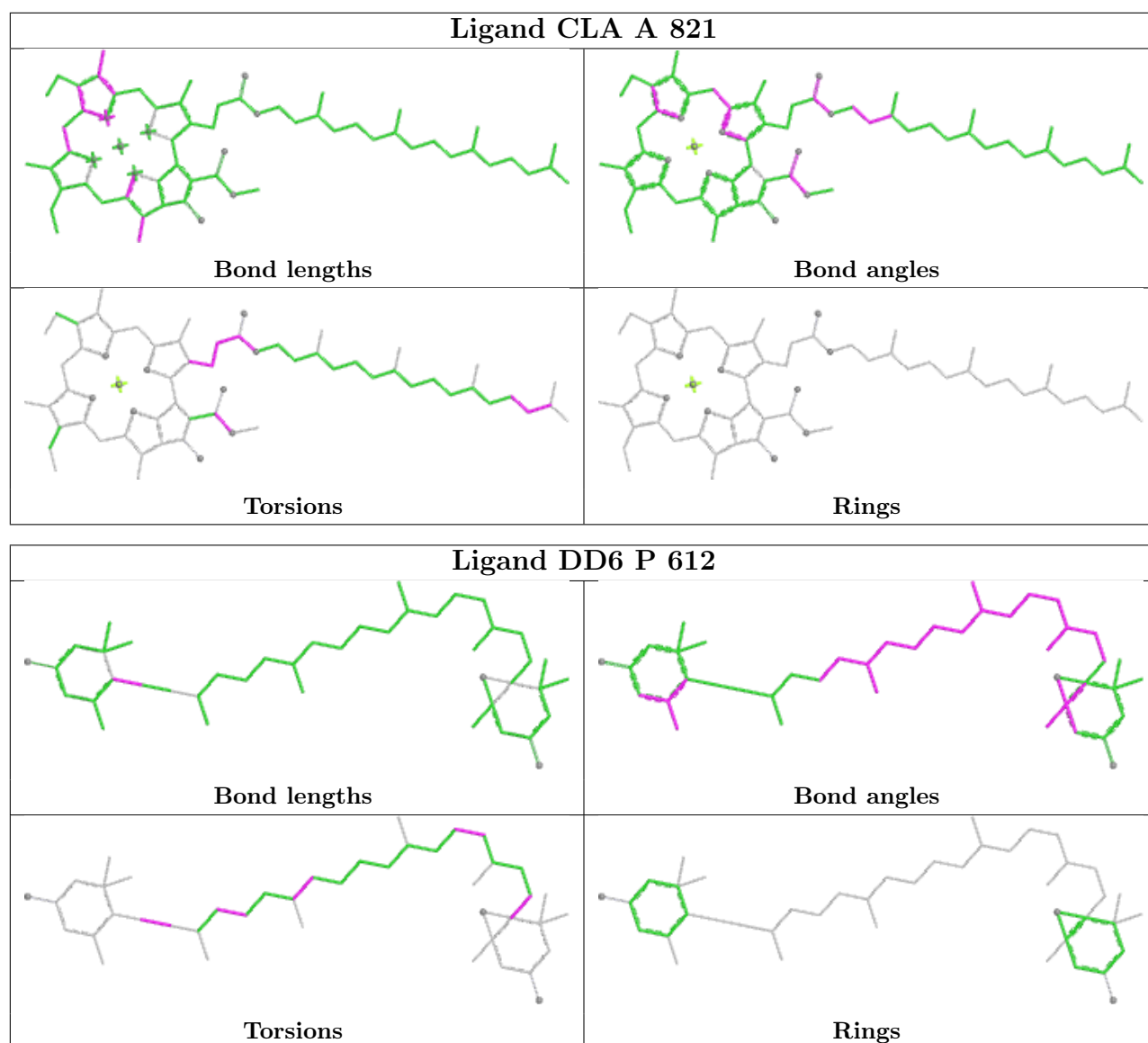
## Ligand CLA P 607

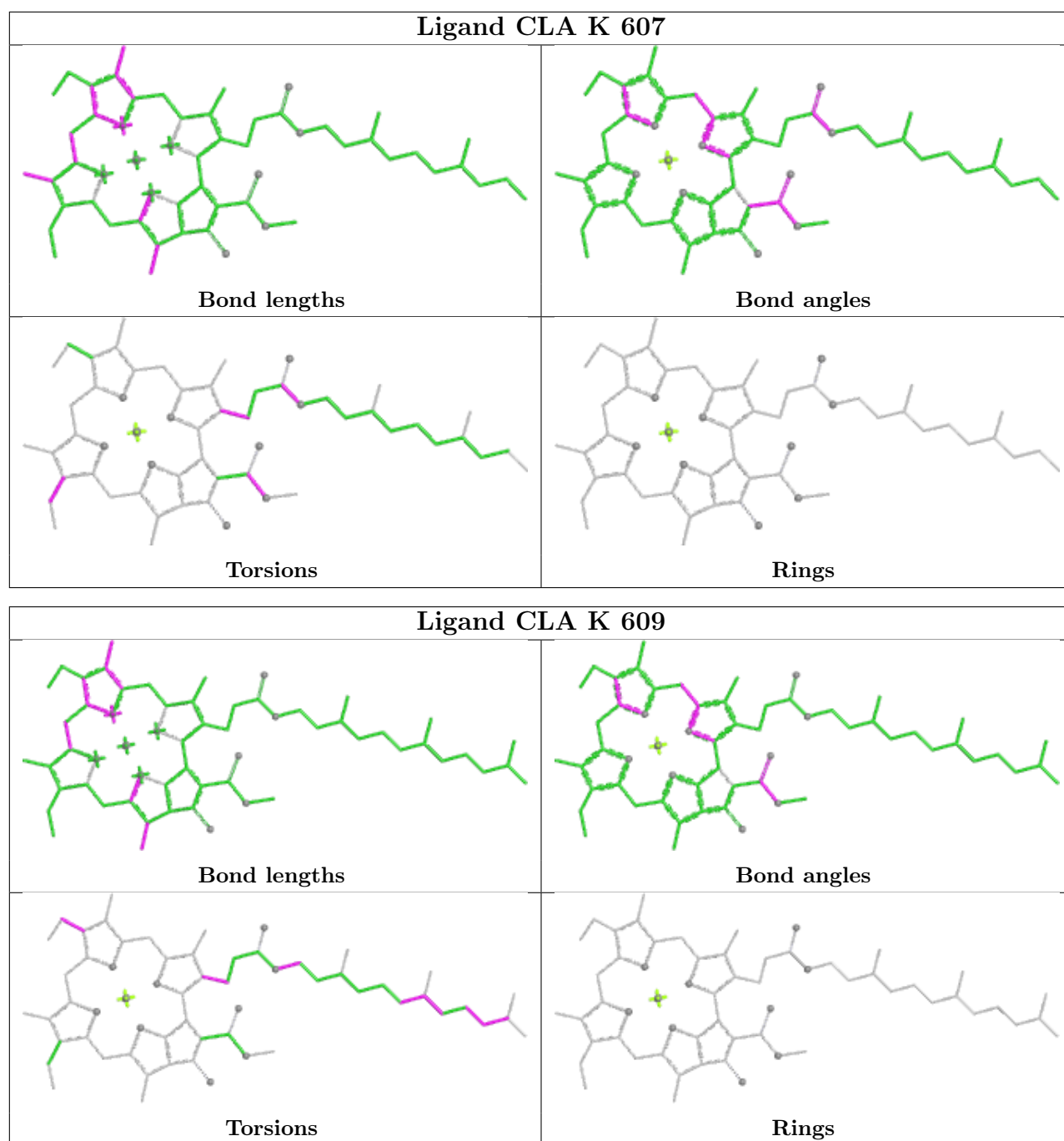


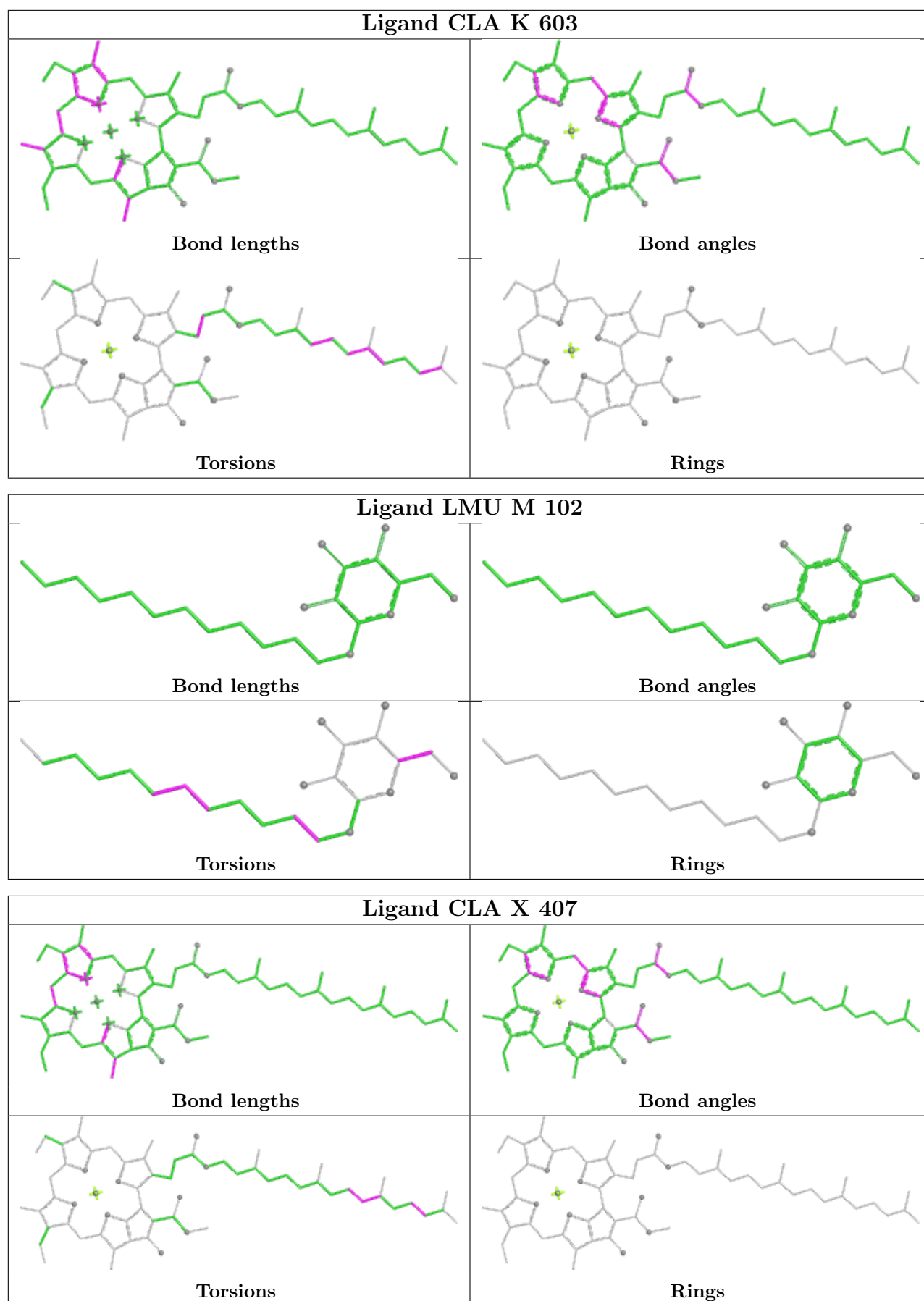
## Ligand BCR B 844

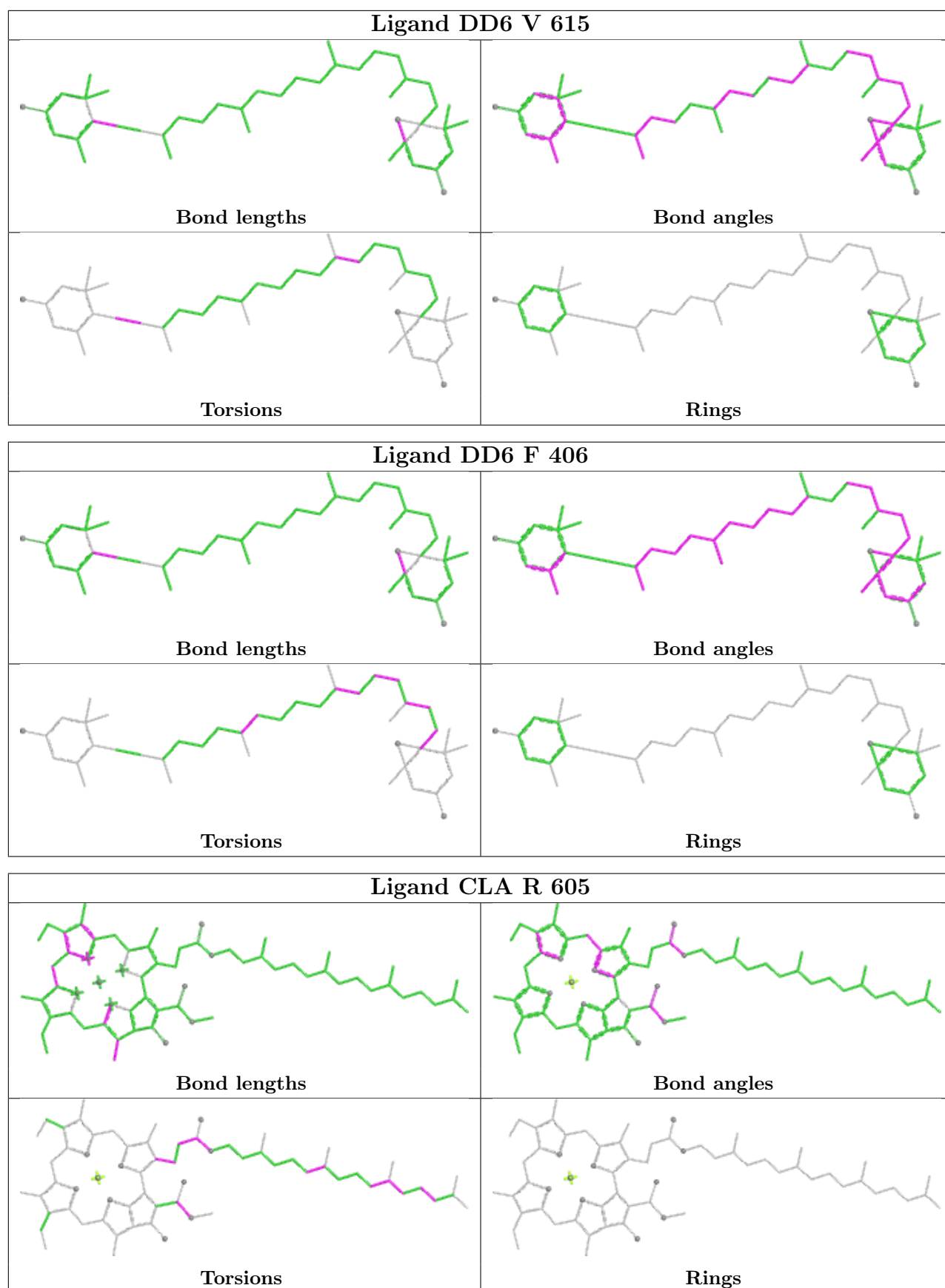


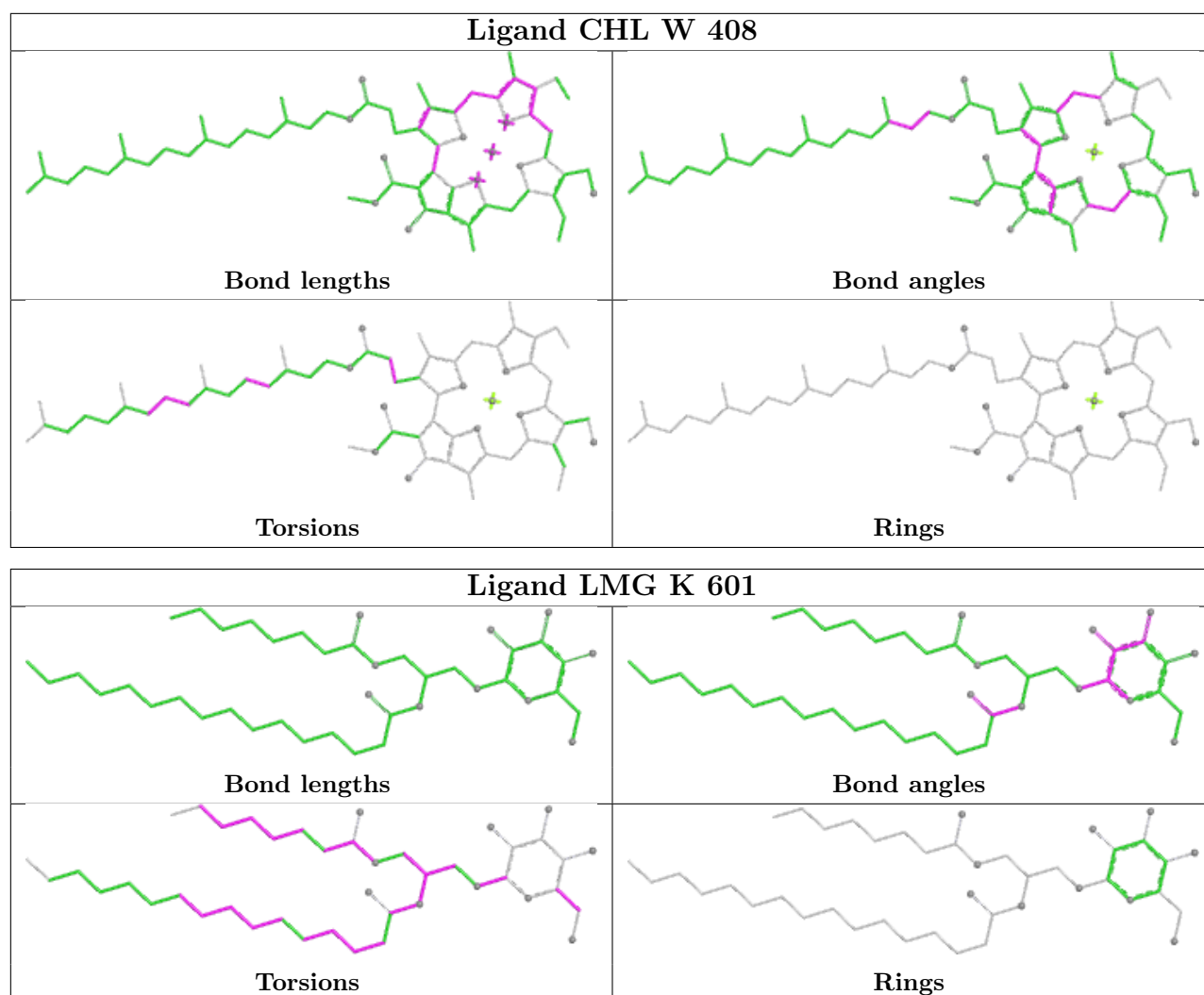




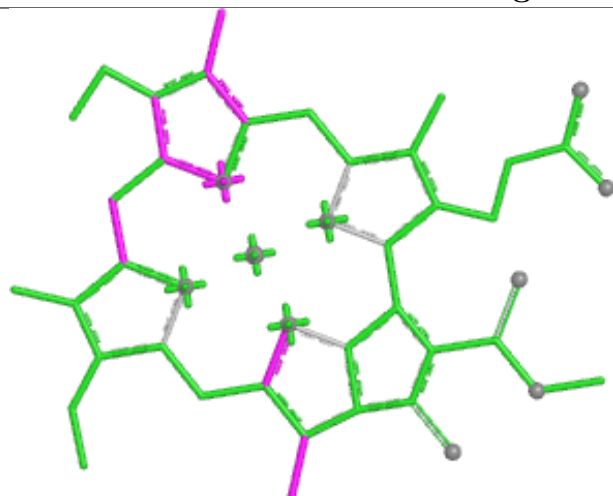




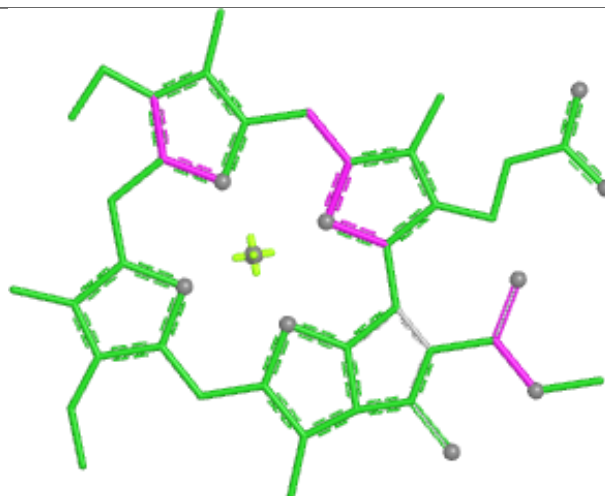




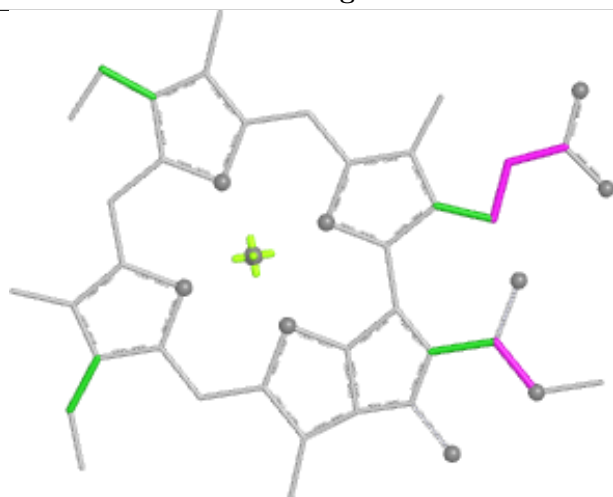
## Ligand CLA G 610



Bond lengths



Bond angles

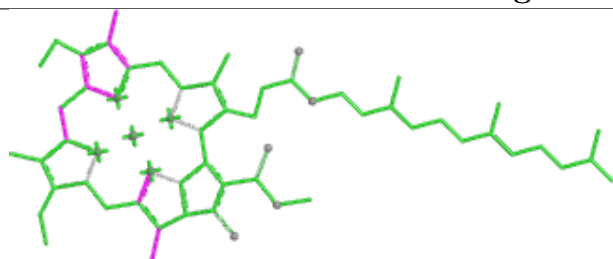


Torsions

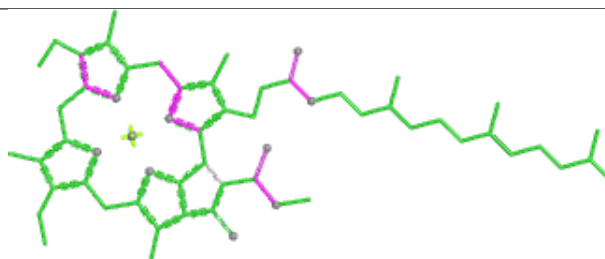


Rings

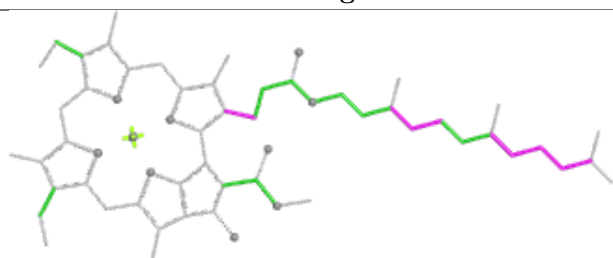
## Ligand CLA X 404



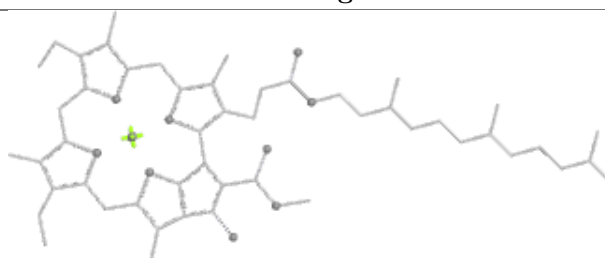
Bond lengths



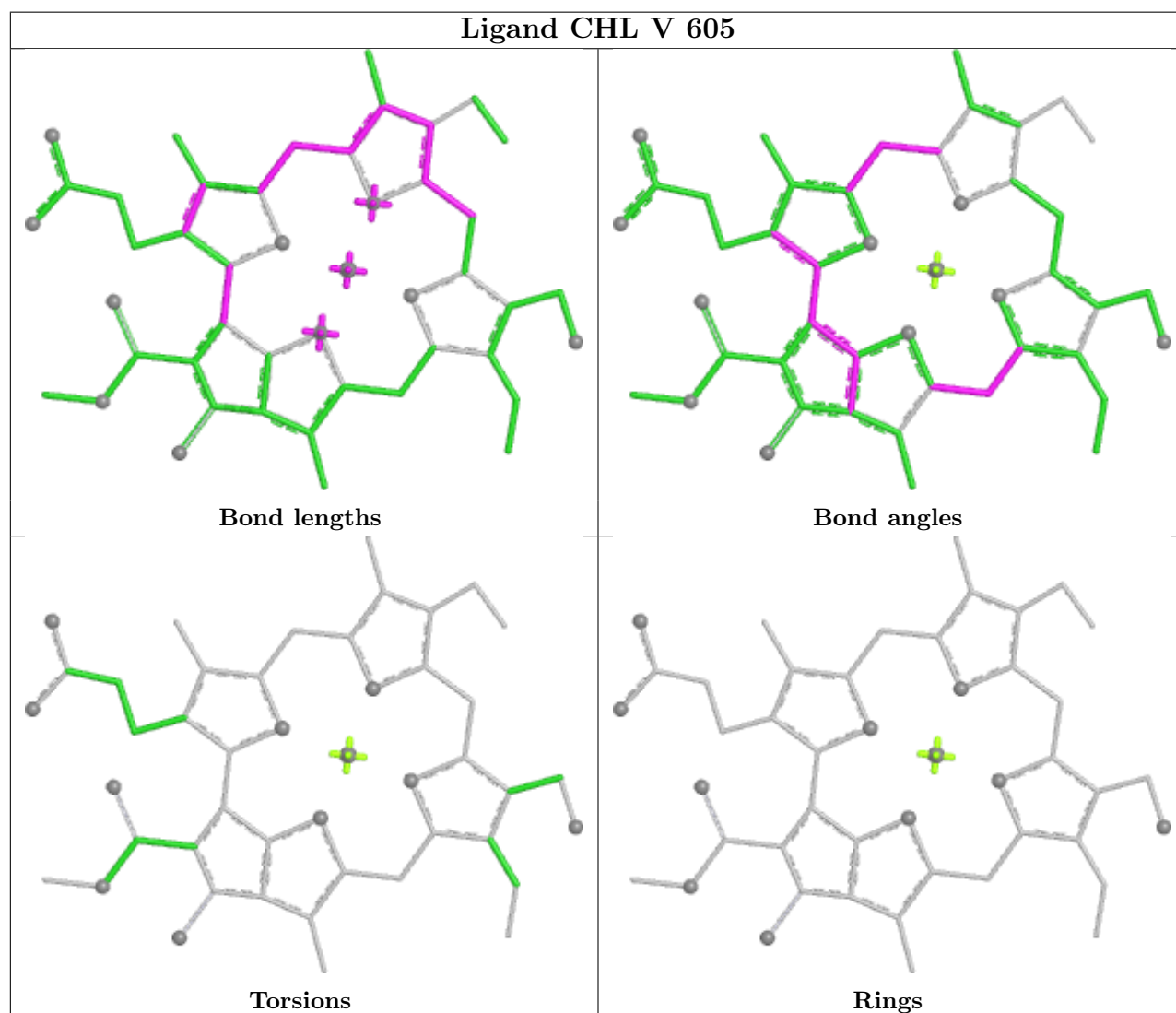
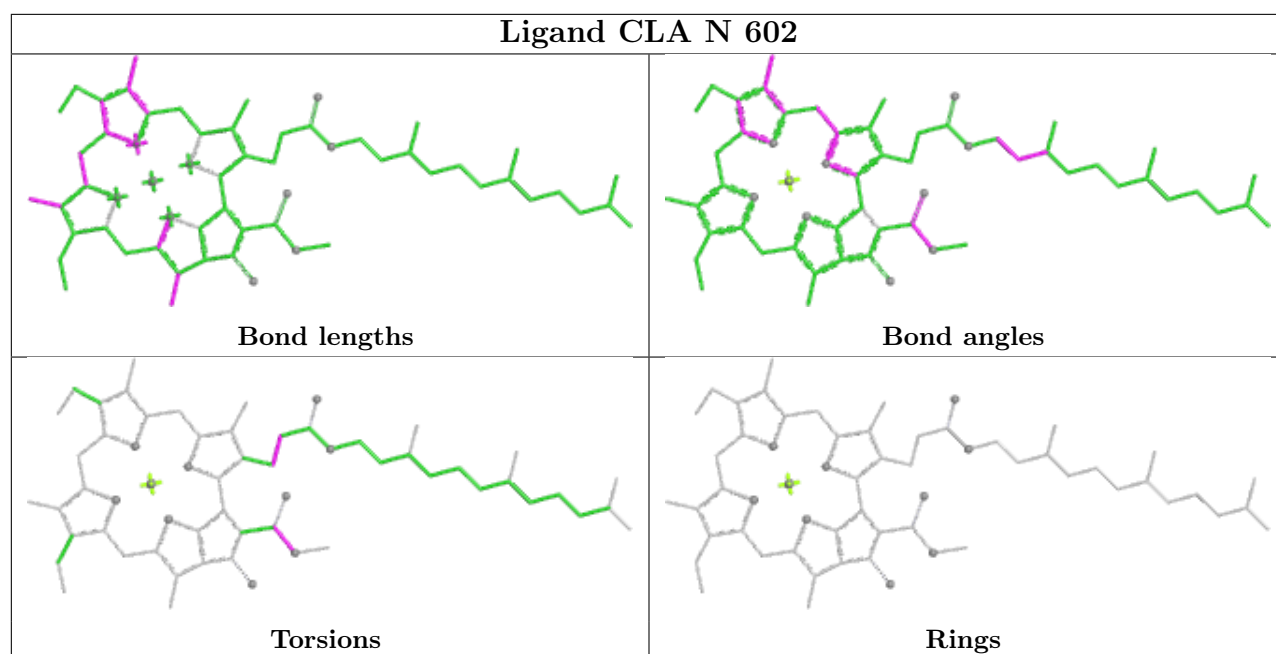
Bond angles

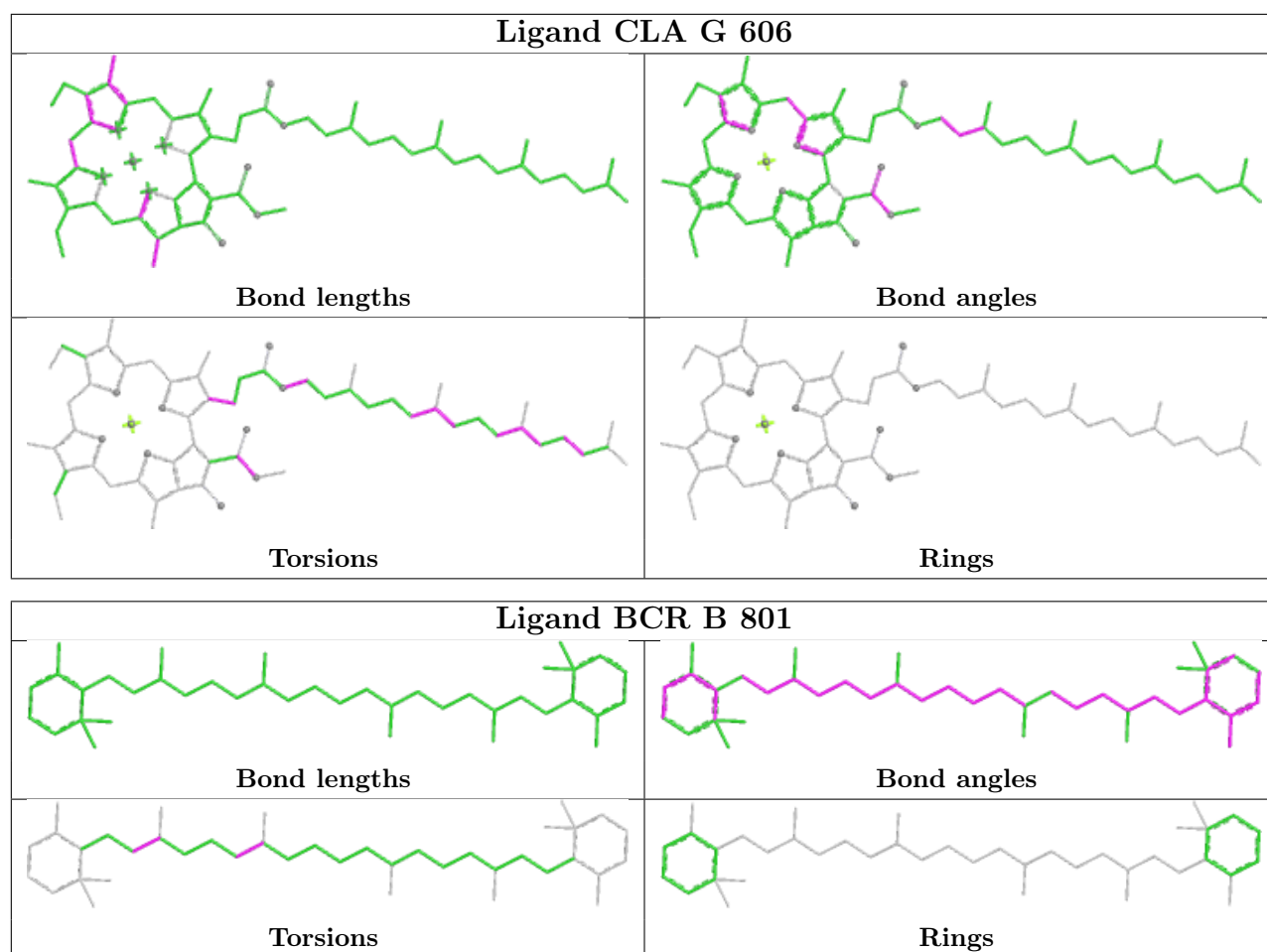


Torsions



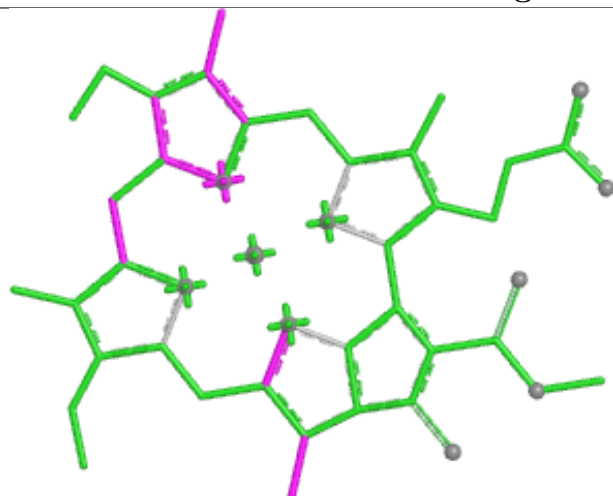
Rings



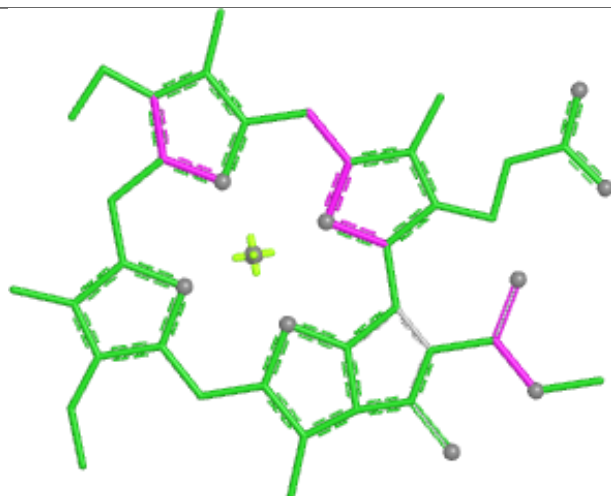




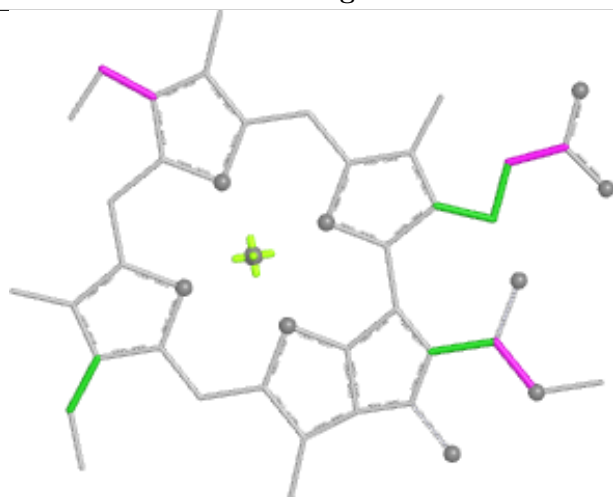
## Ligand CLA B 838



Bond lengths



Bond angles

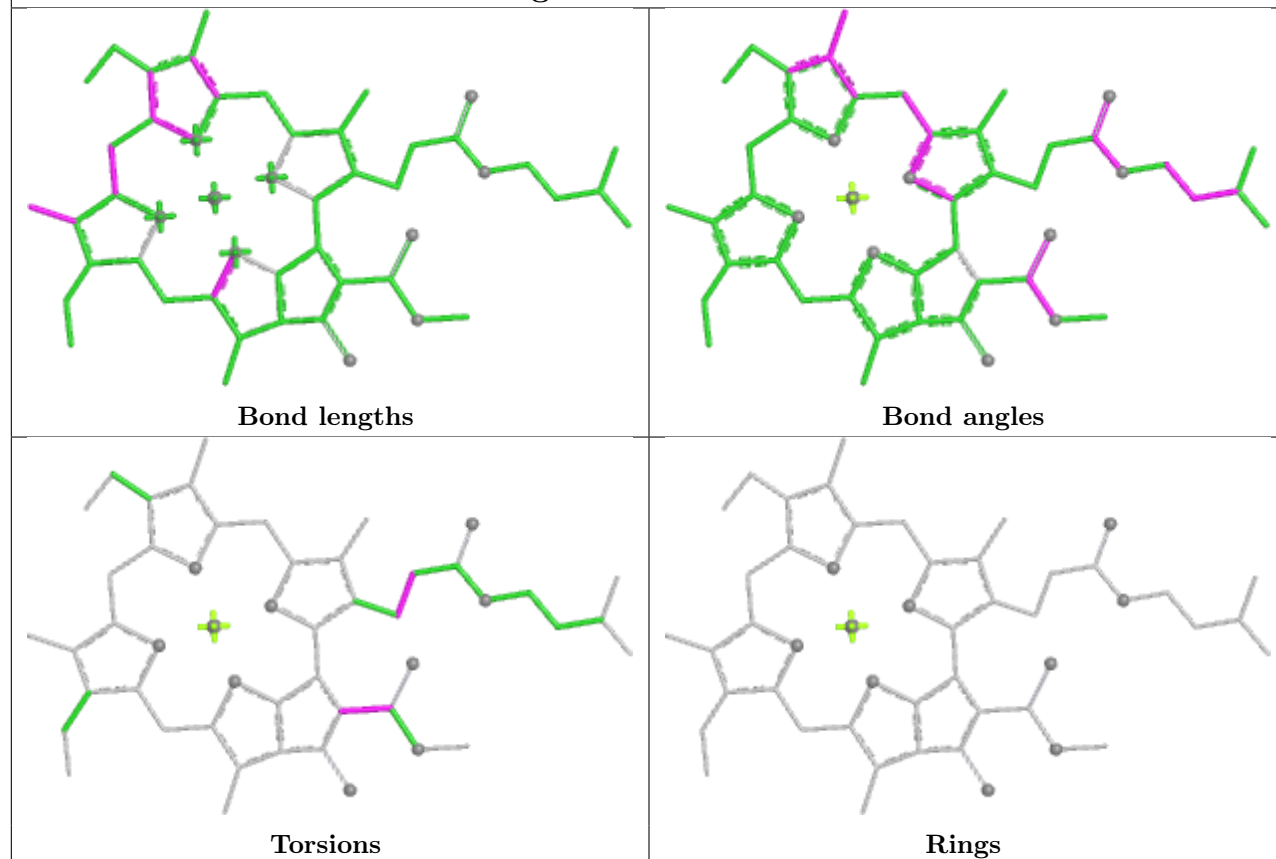


Torsions

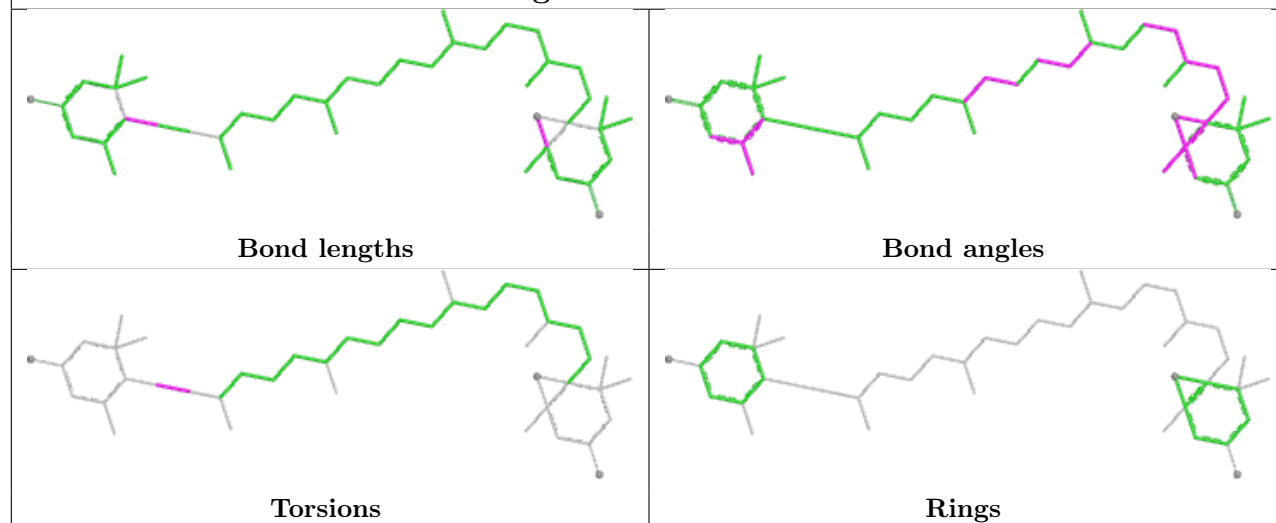


Rings

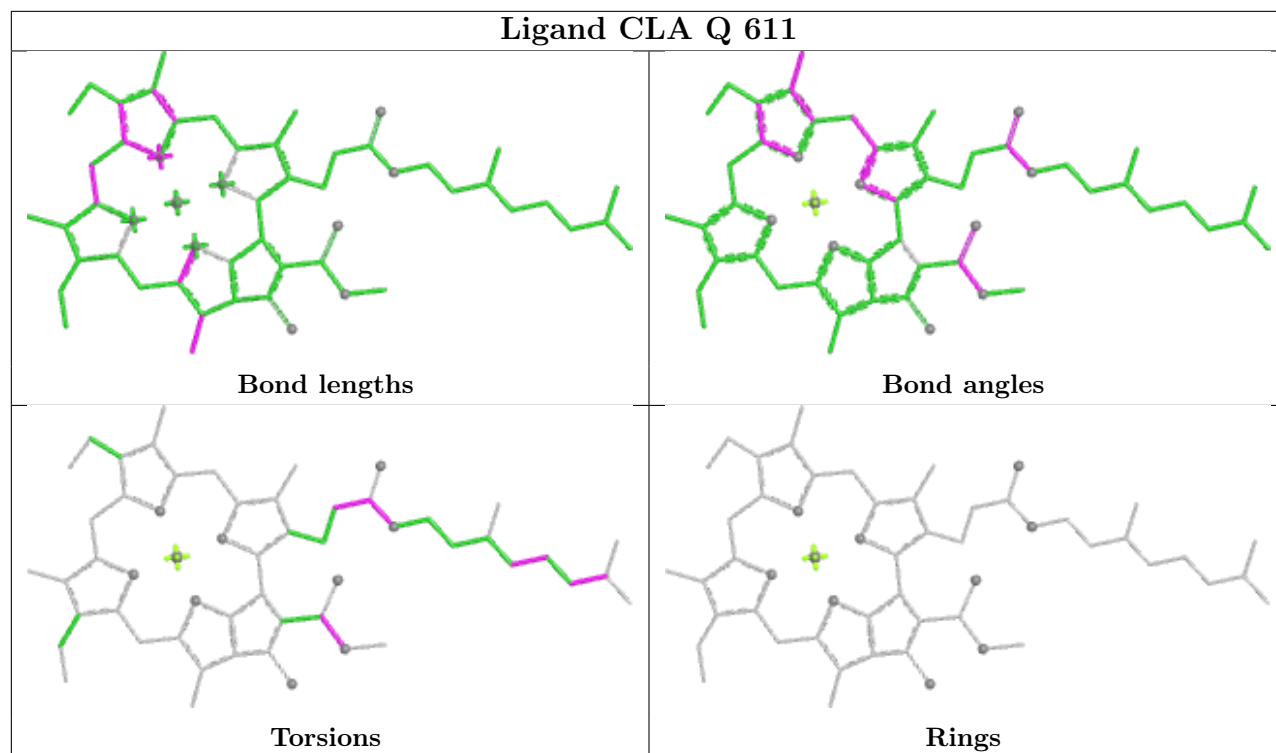
## Ligand CLA X 417



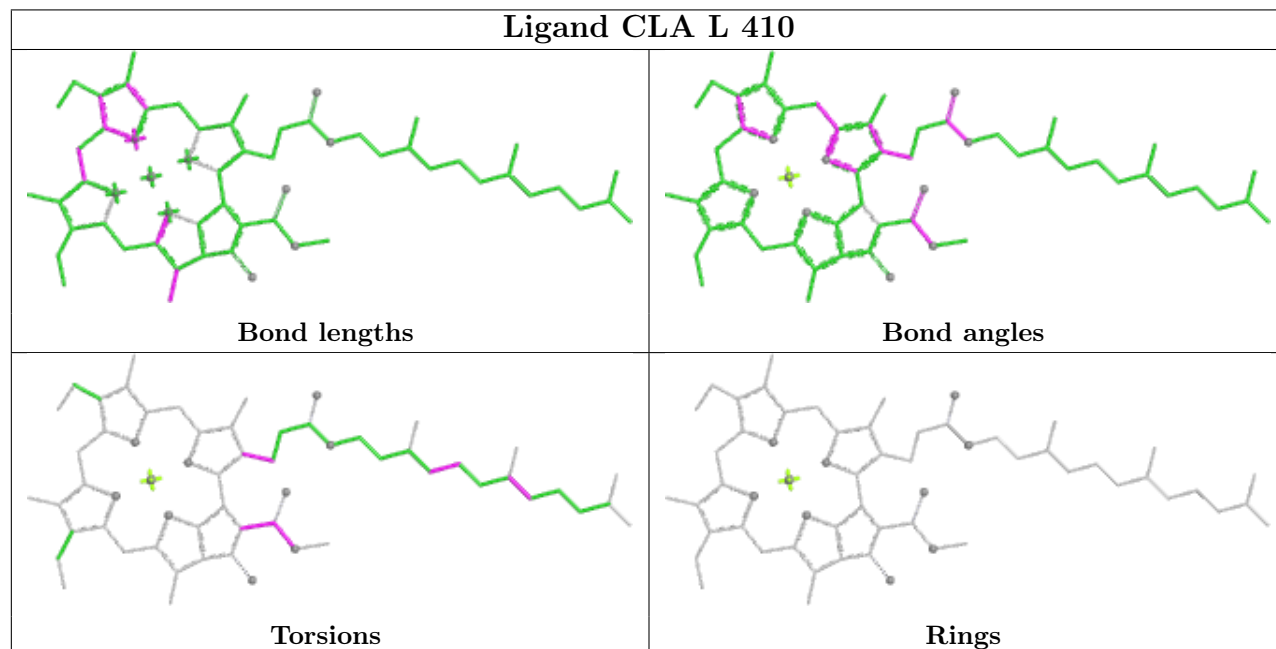
## Ligand DD6 R 612

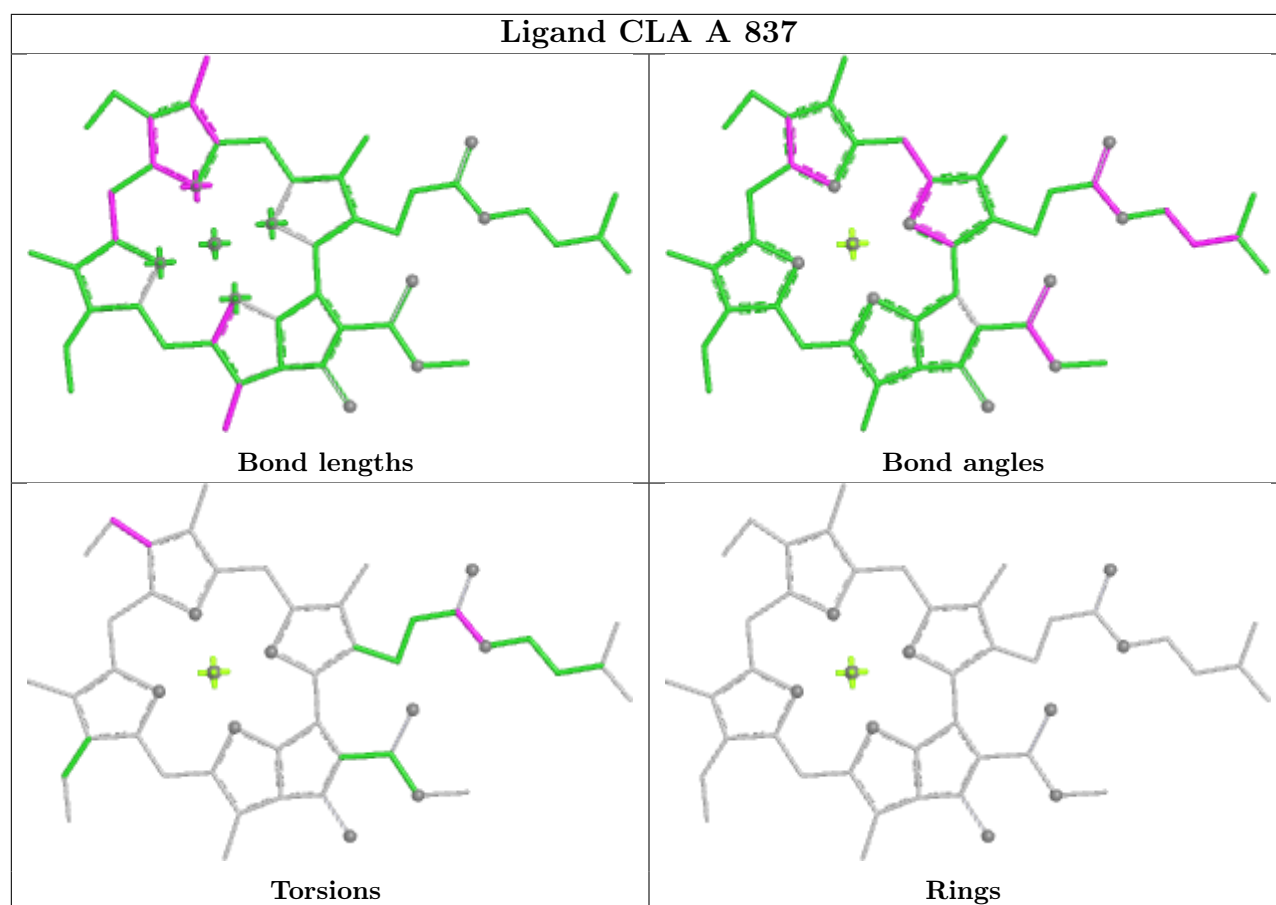


## Ligand CLA Q 611

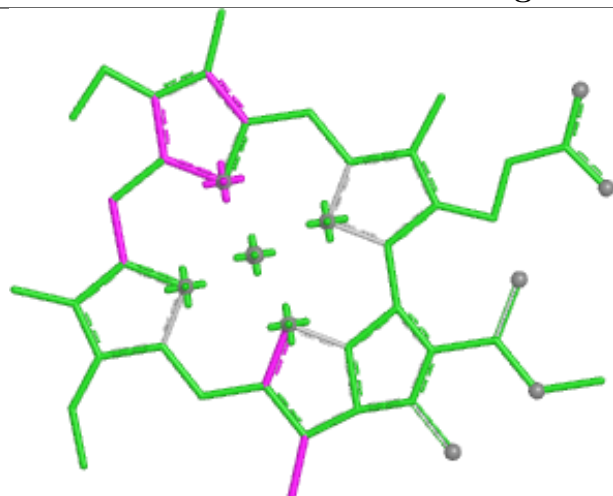


## Ligand CLA L 410

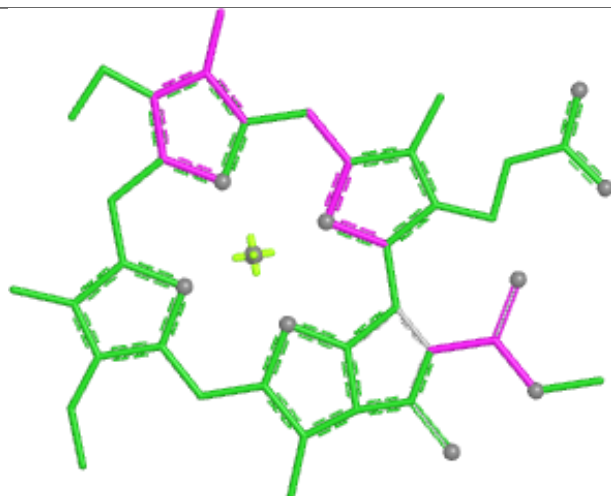




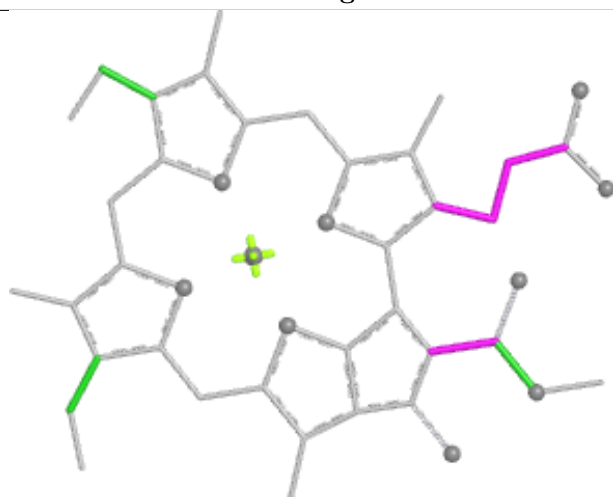
## Ligand CLA B 814



Bond lengths



Bond angles

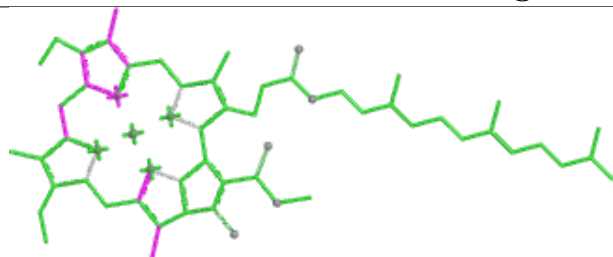


Torsions

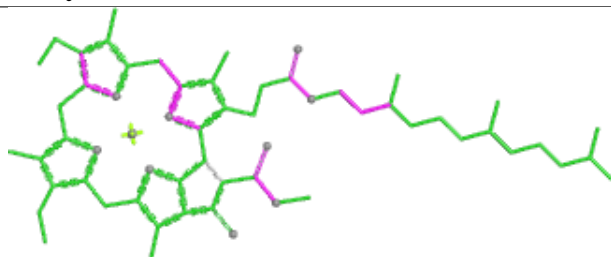


Rings

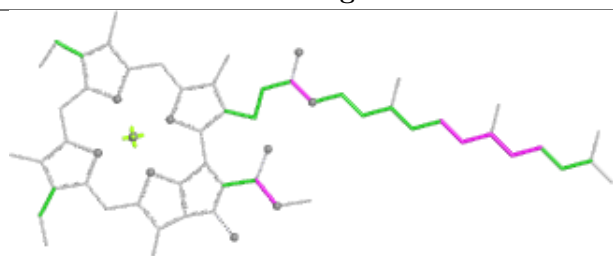
## Ligand CLA Q 609



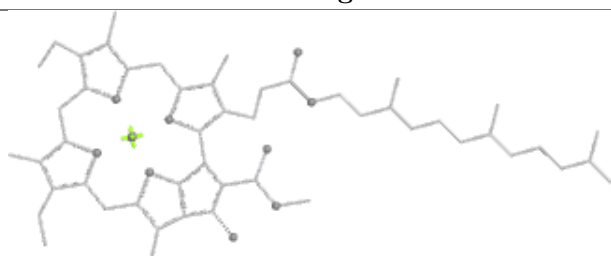
Bond lengths



Bond angles

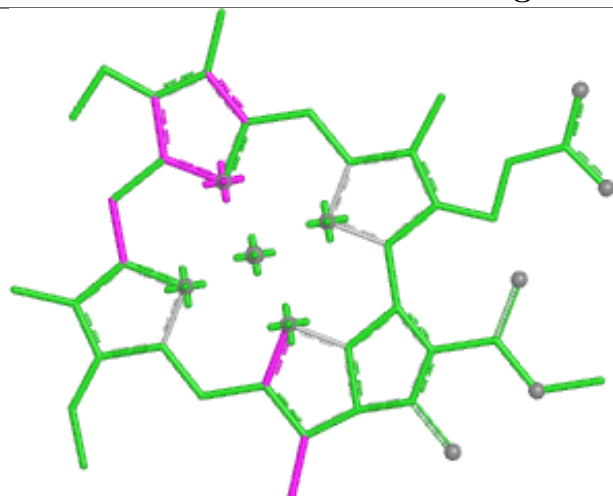


Torsions



Rings

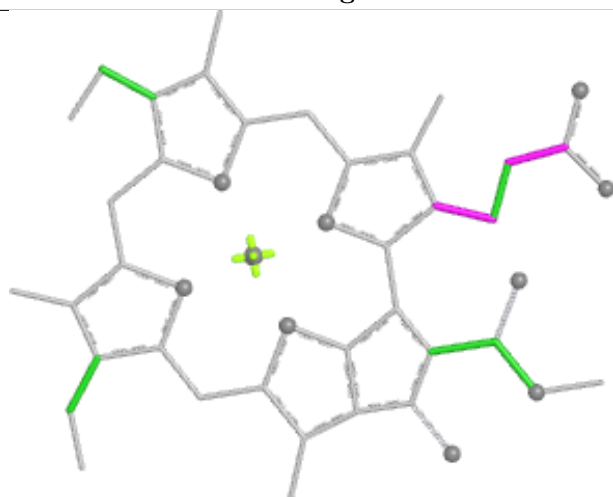
## Ligand CLA R 611



Bond lengths



Bond angles

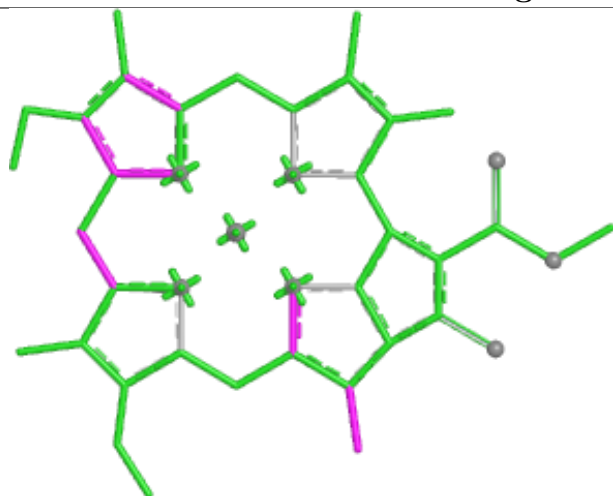


Torsions

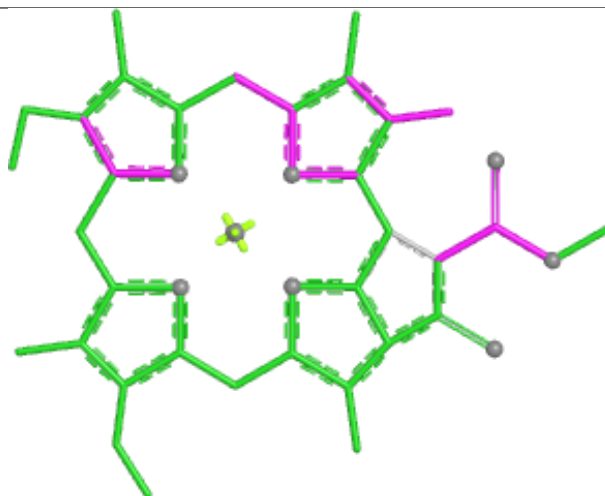


Rings

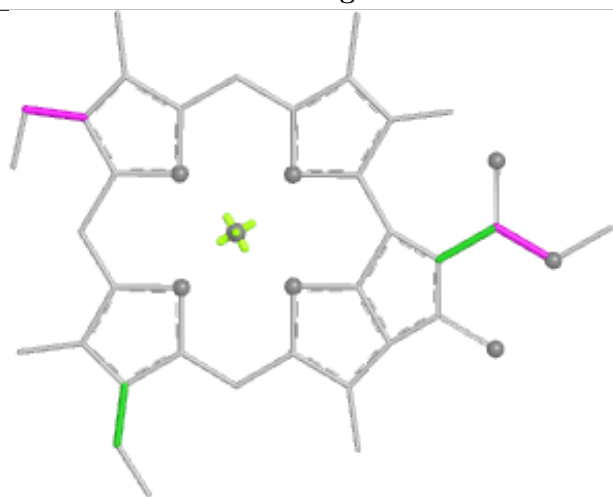
## Ligand CLA P 610



Bond lengths



Bond angles

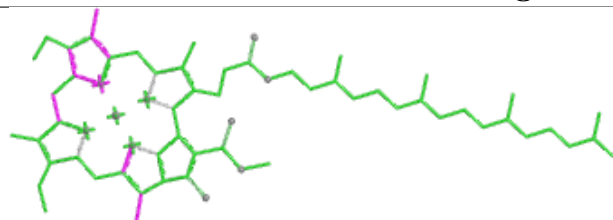


Torsions

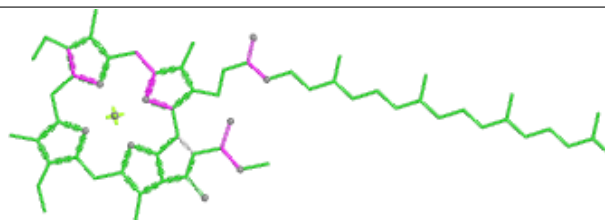


Rings

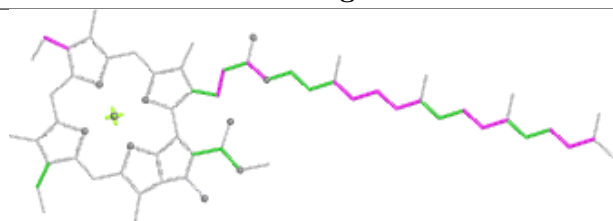
## Ligand CLA T 605



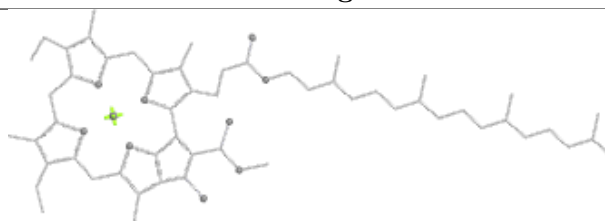
Bond lengths



Bond angles

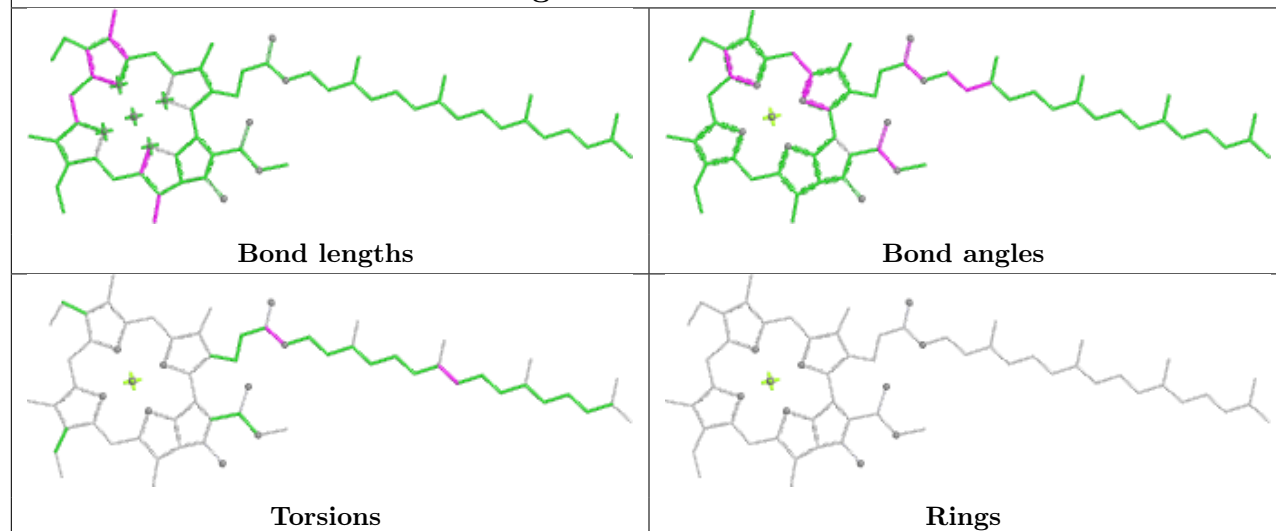


Torsions

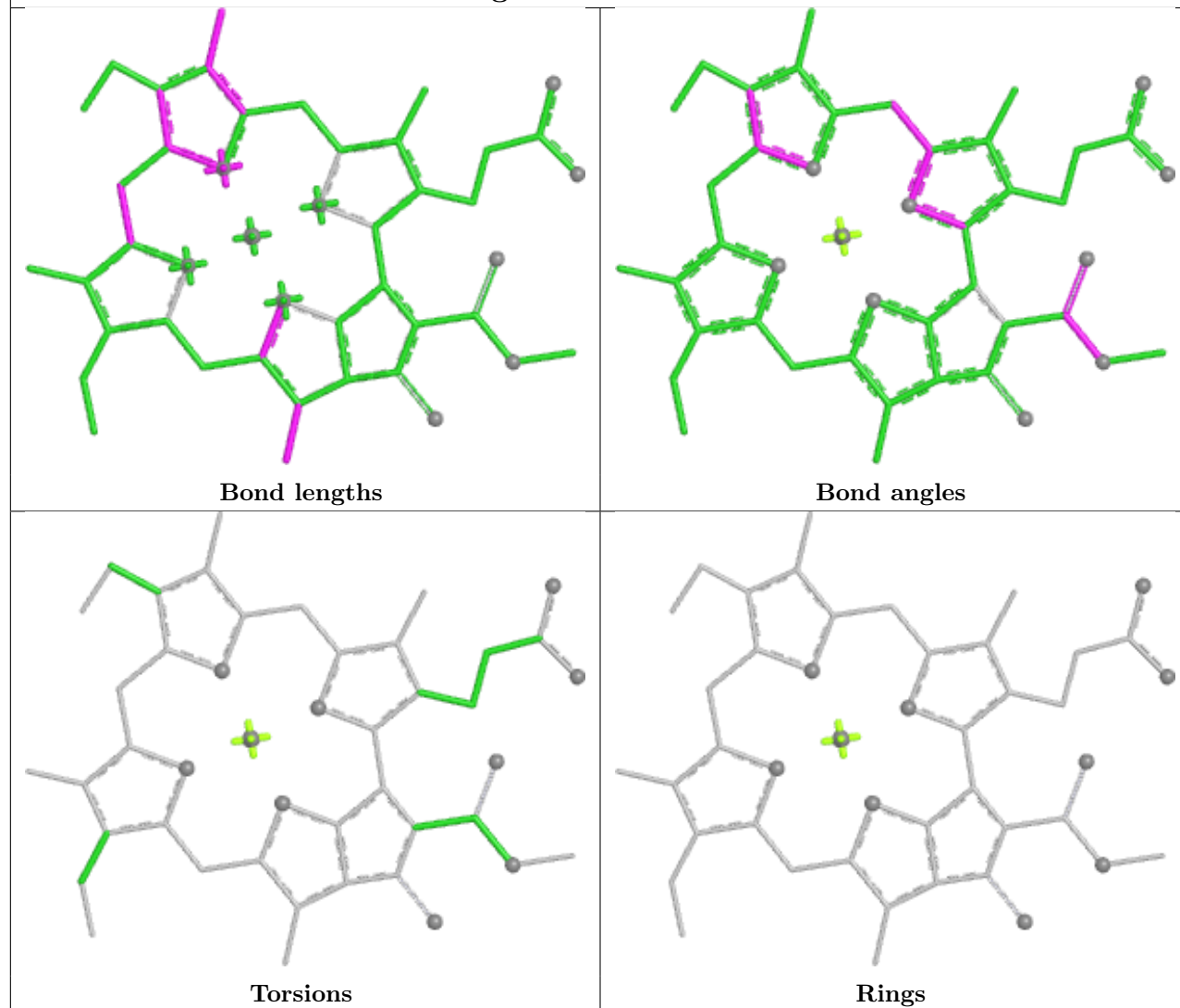


Rings

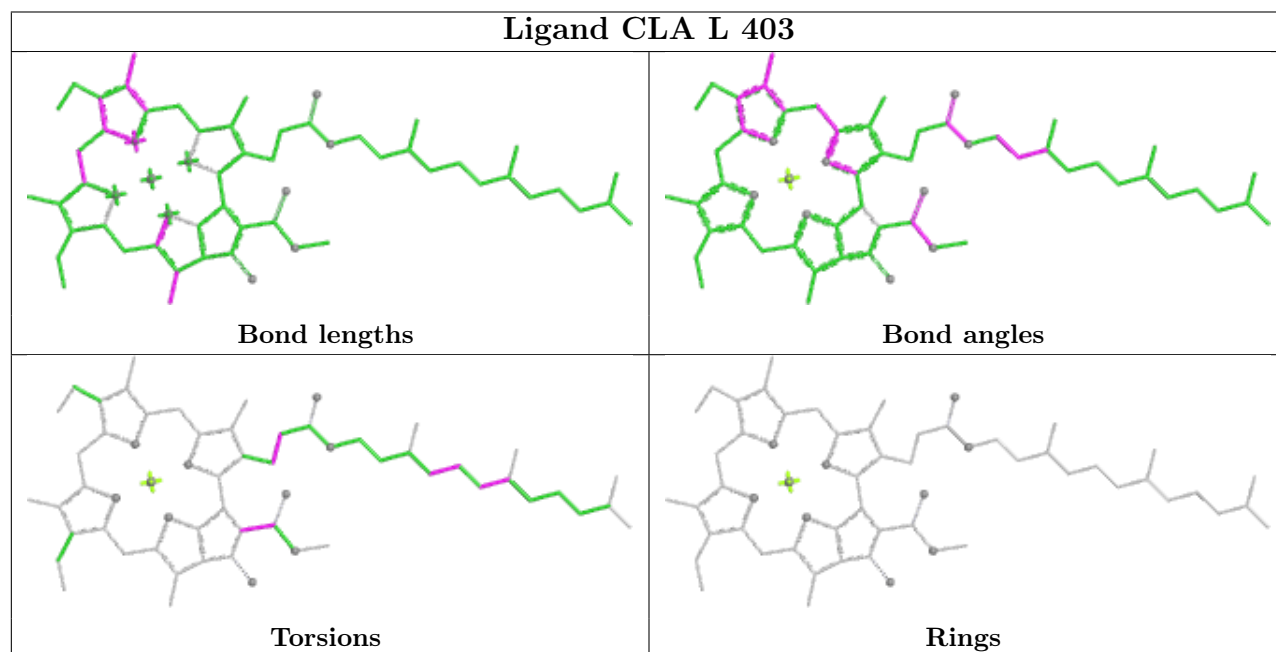
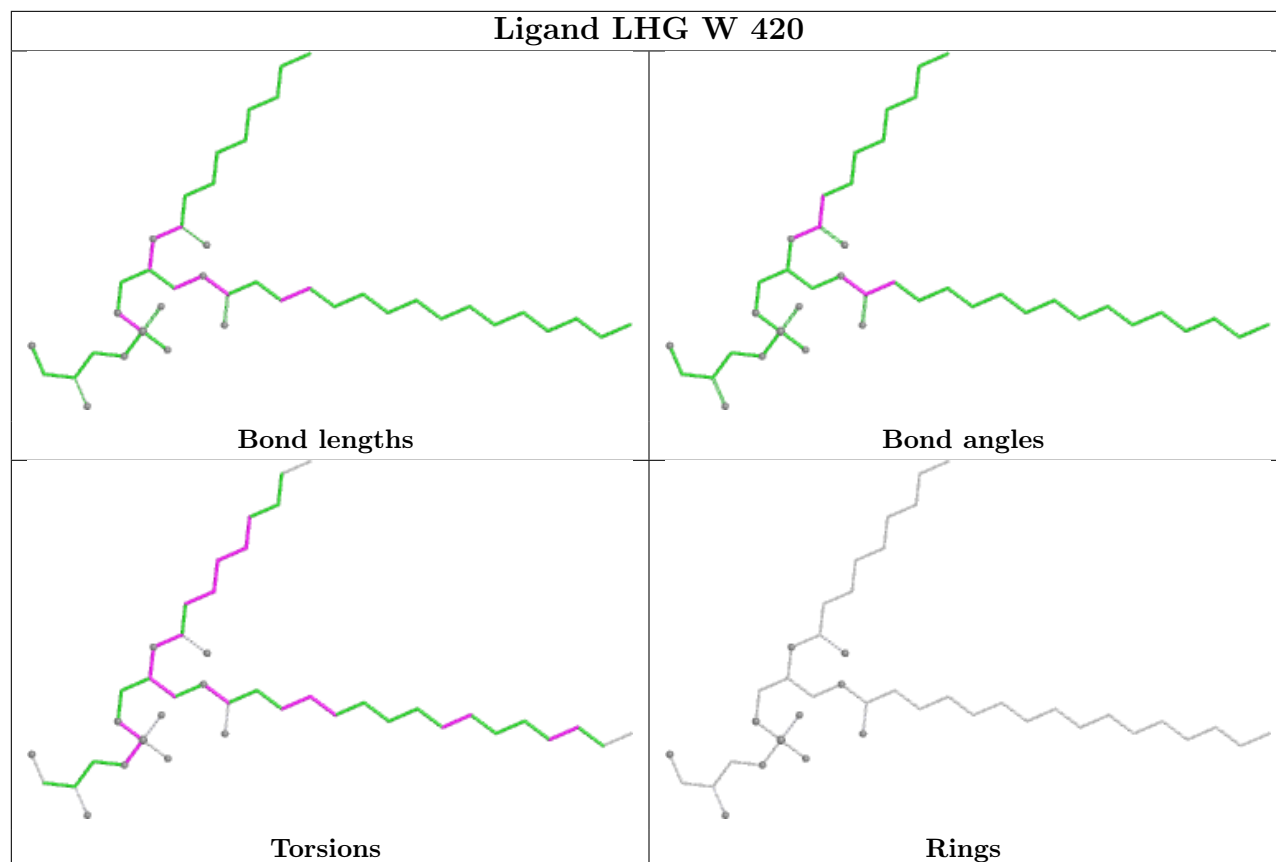
## Ligand CLA B 809

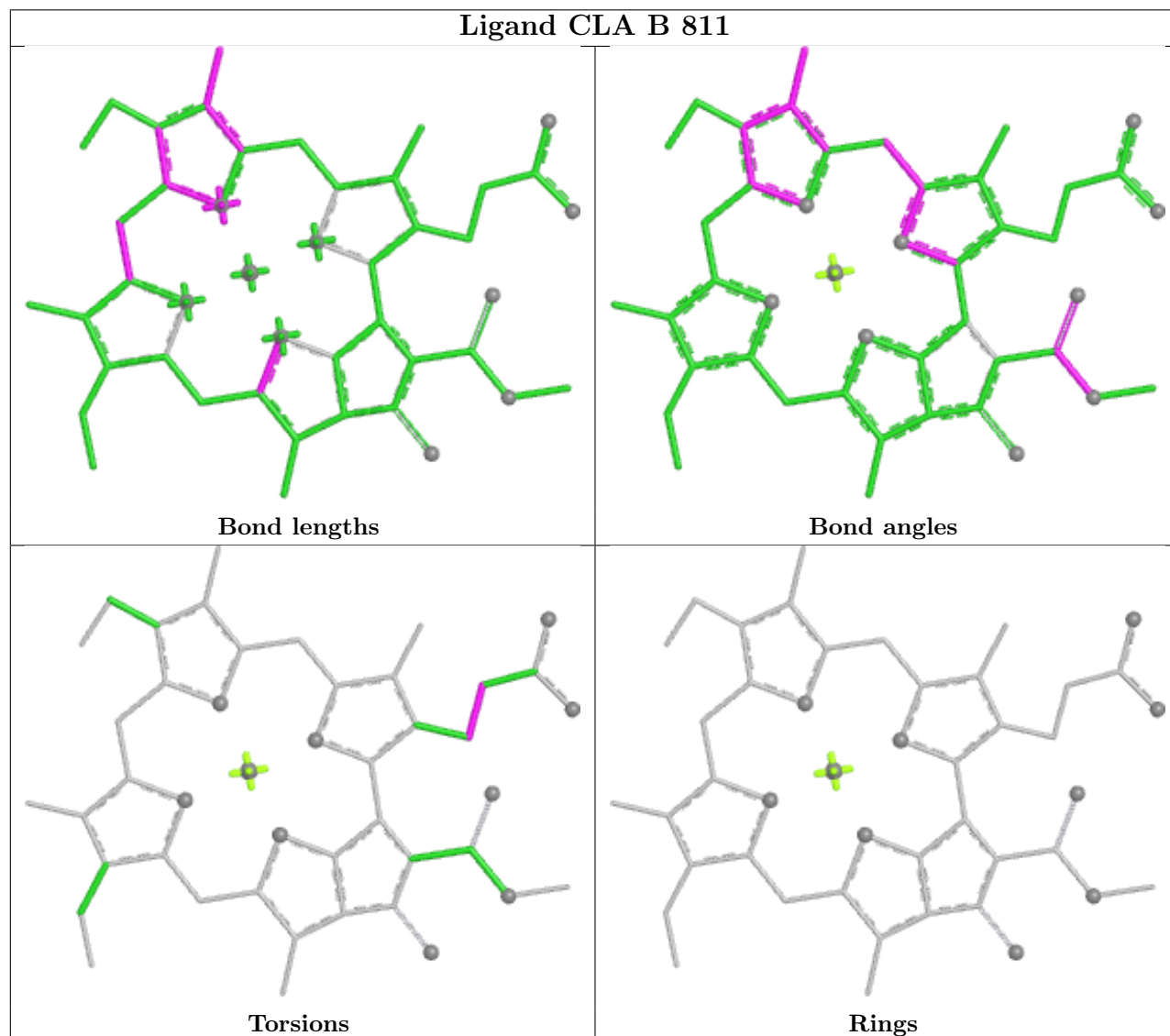
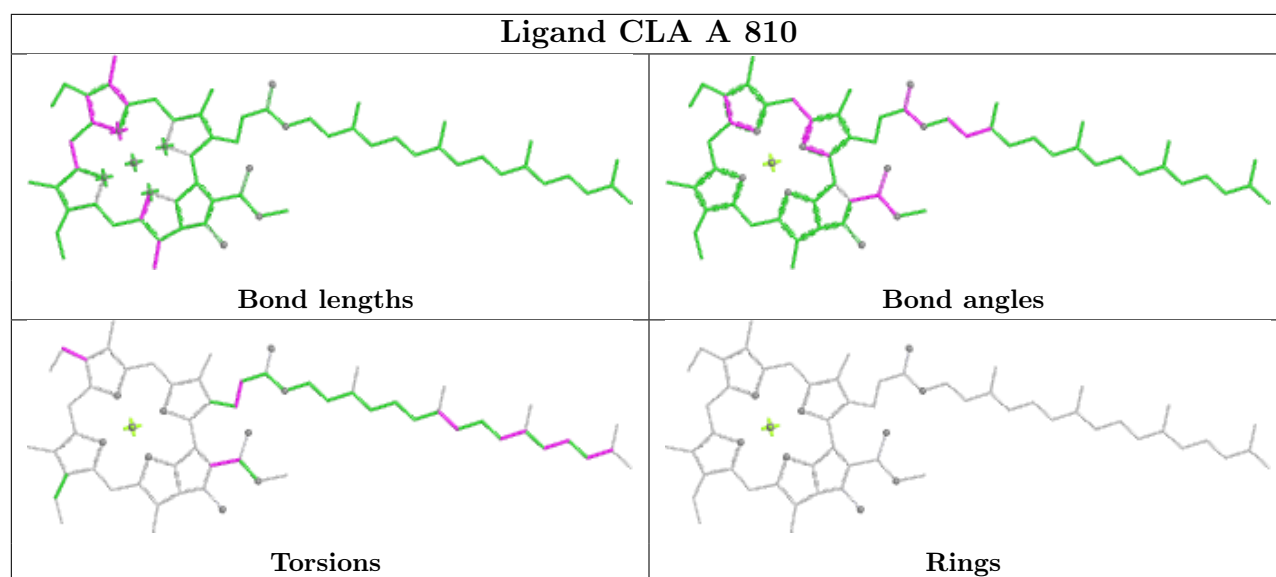


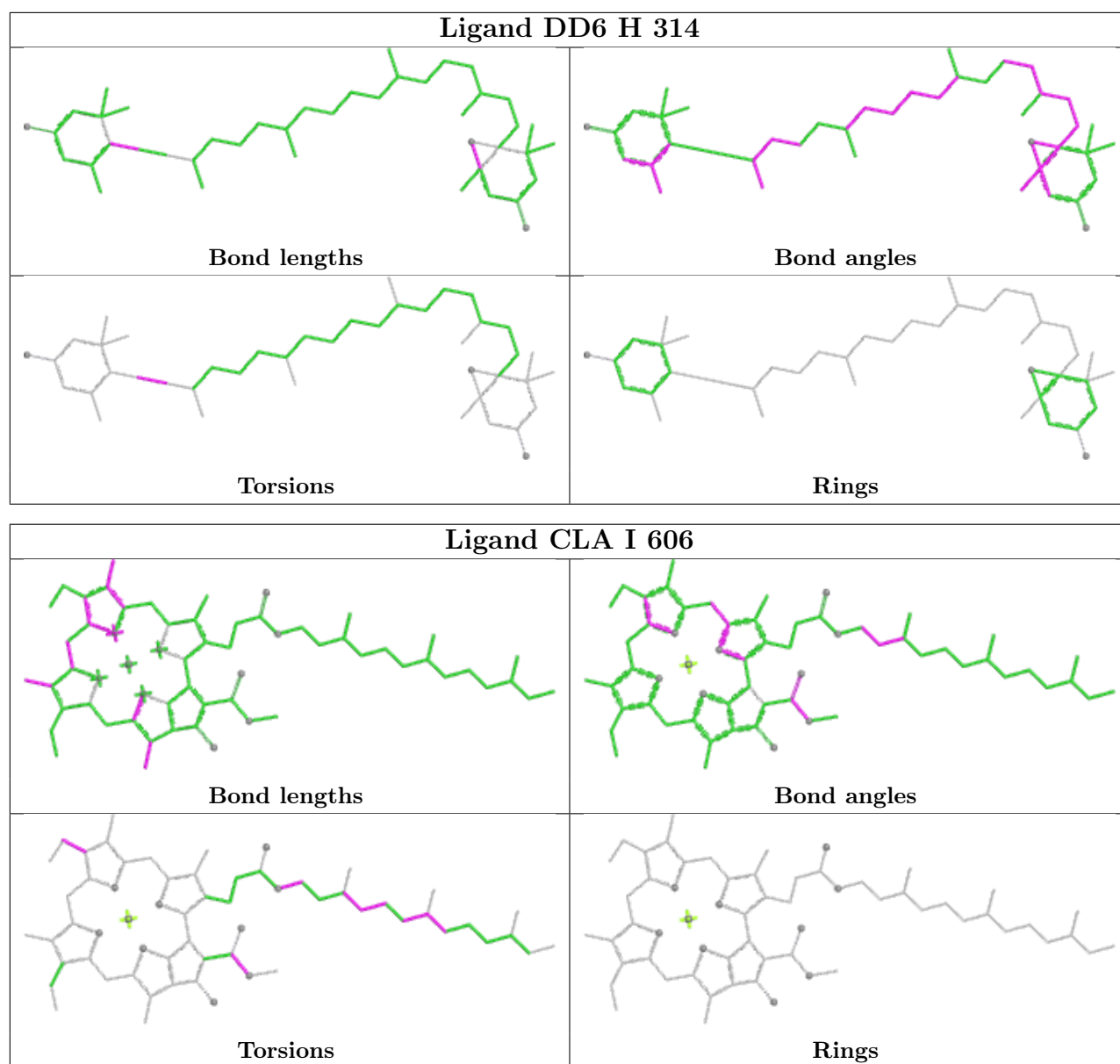
## Ligand CLA O 314

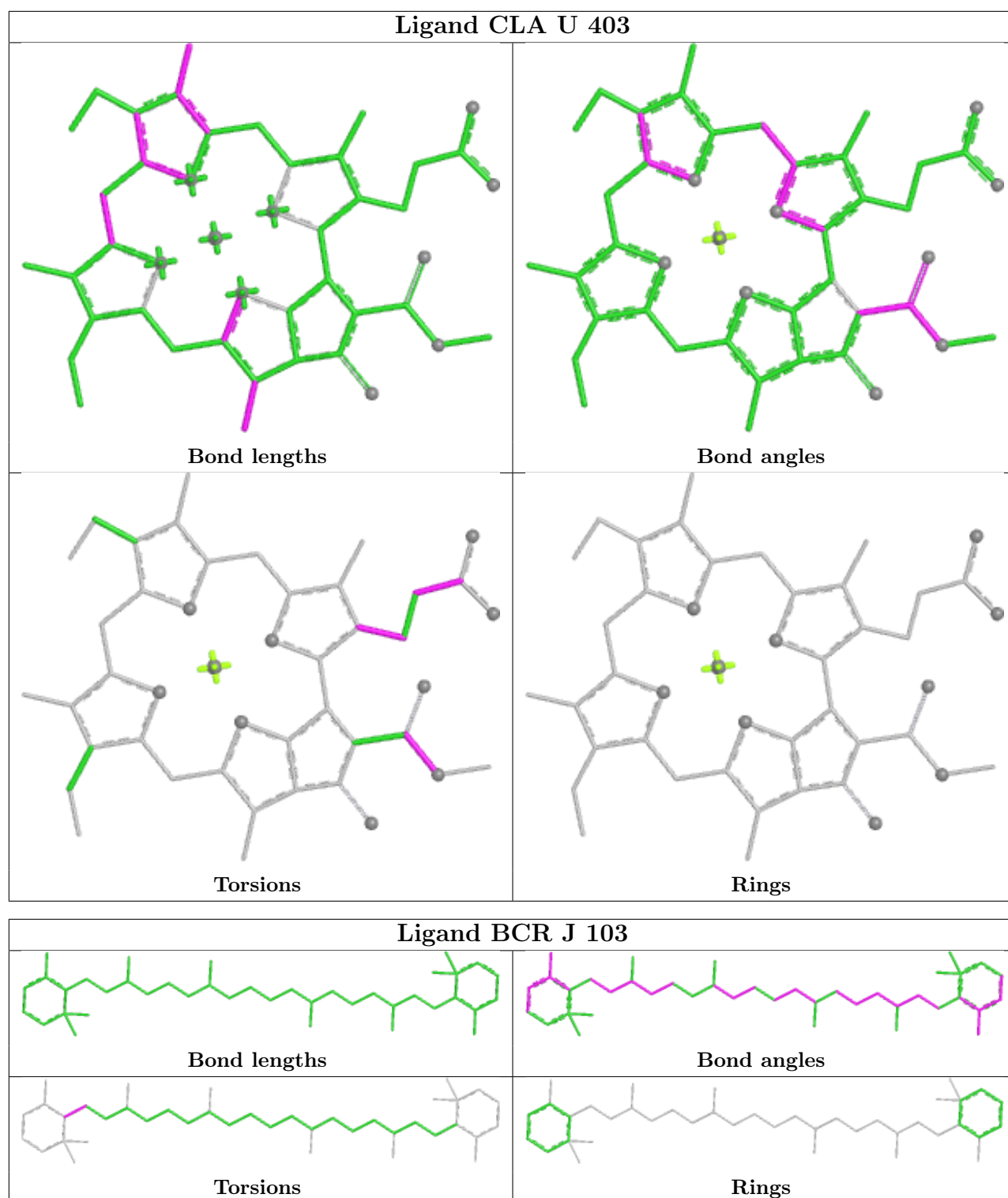


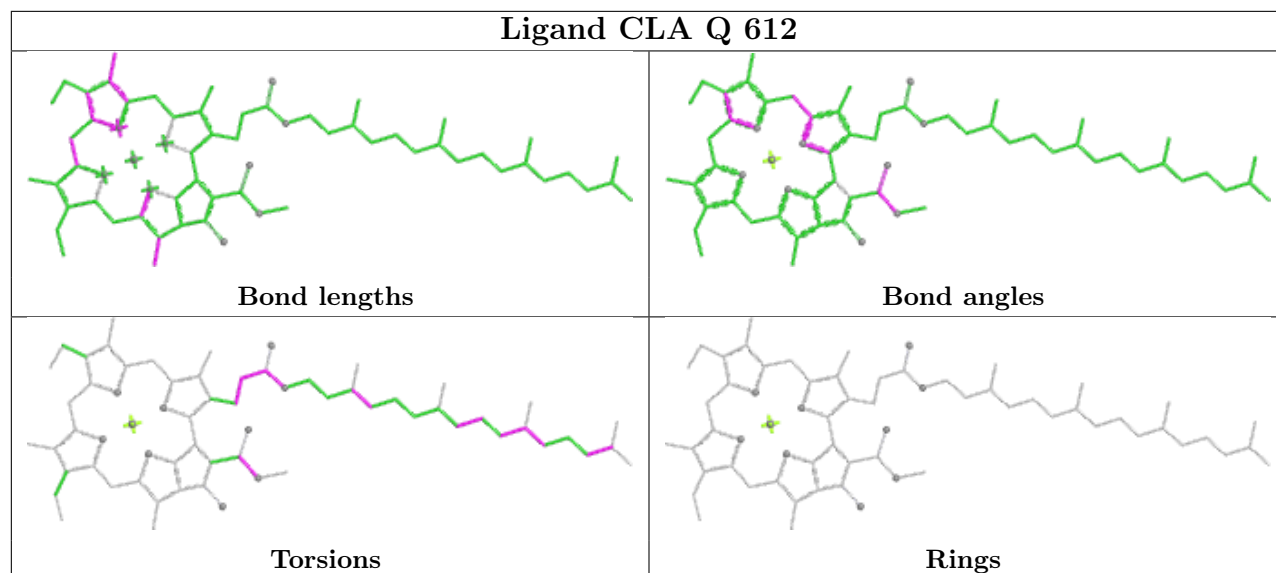
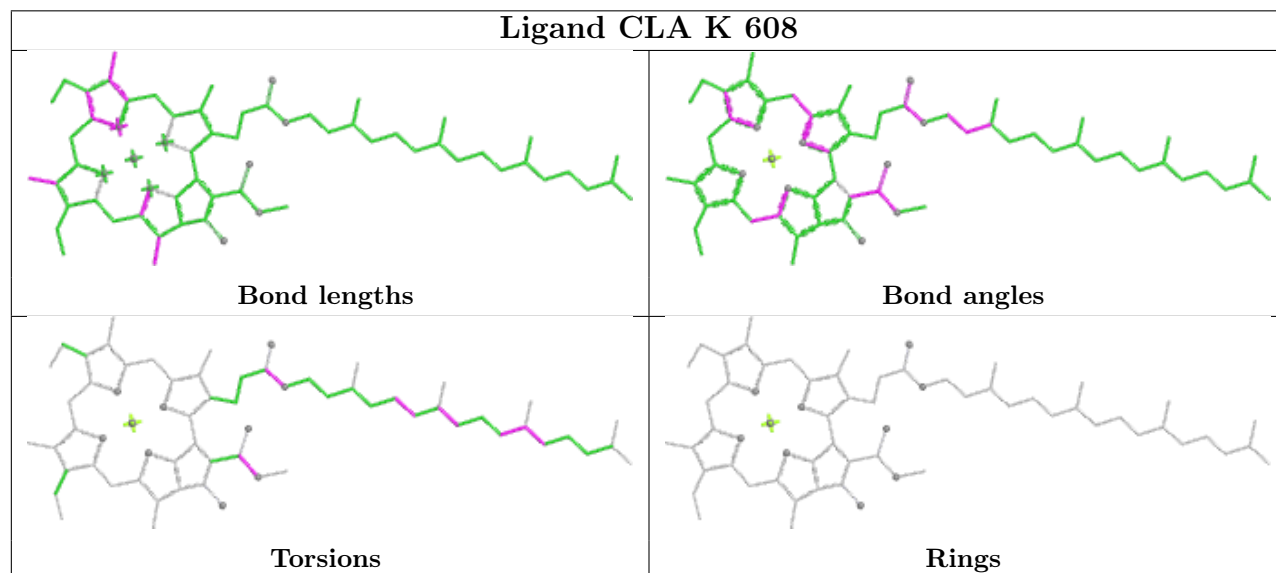
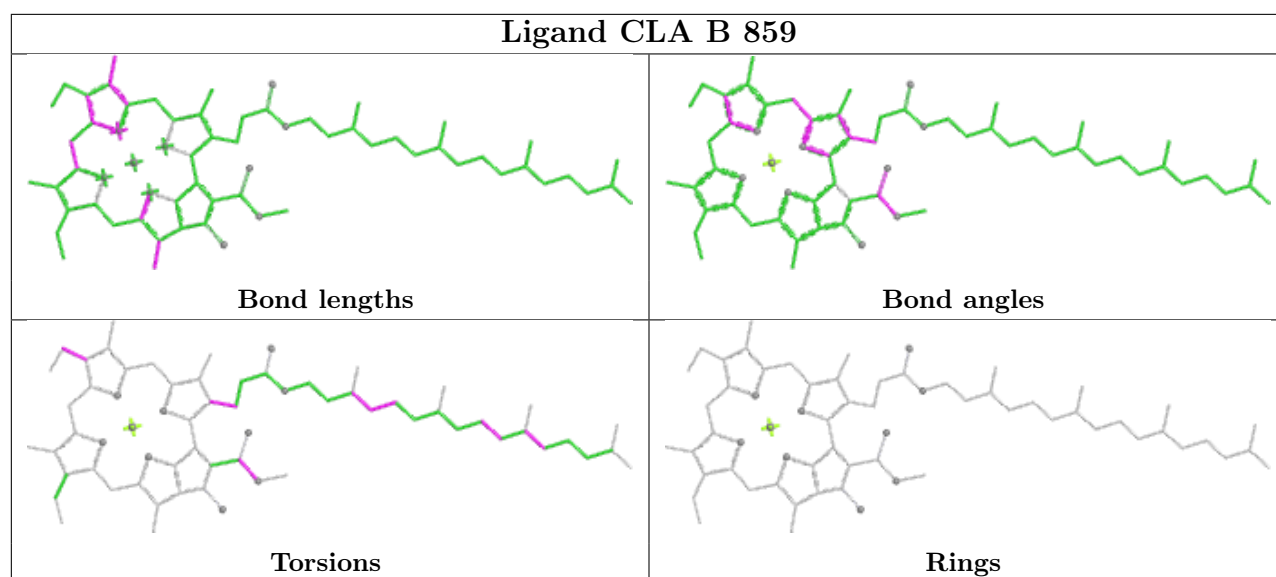


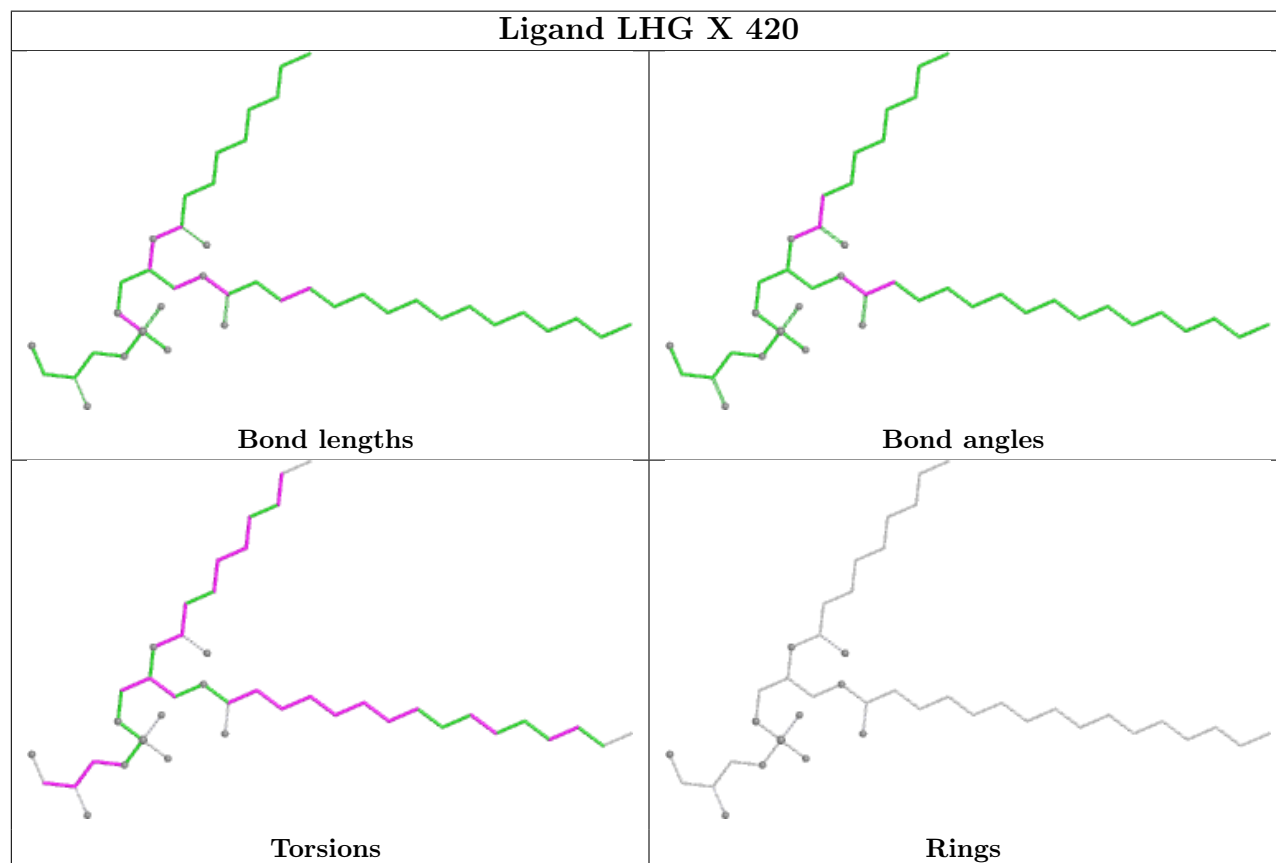
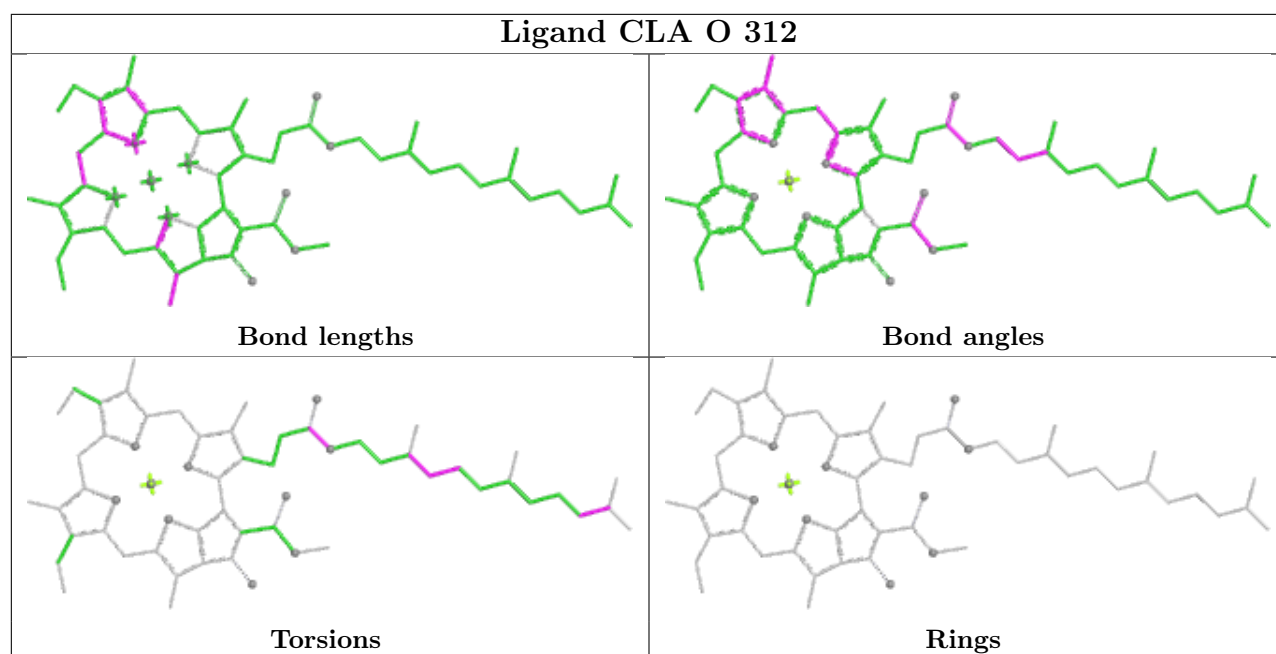


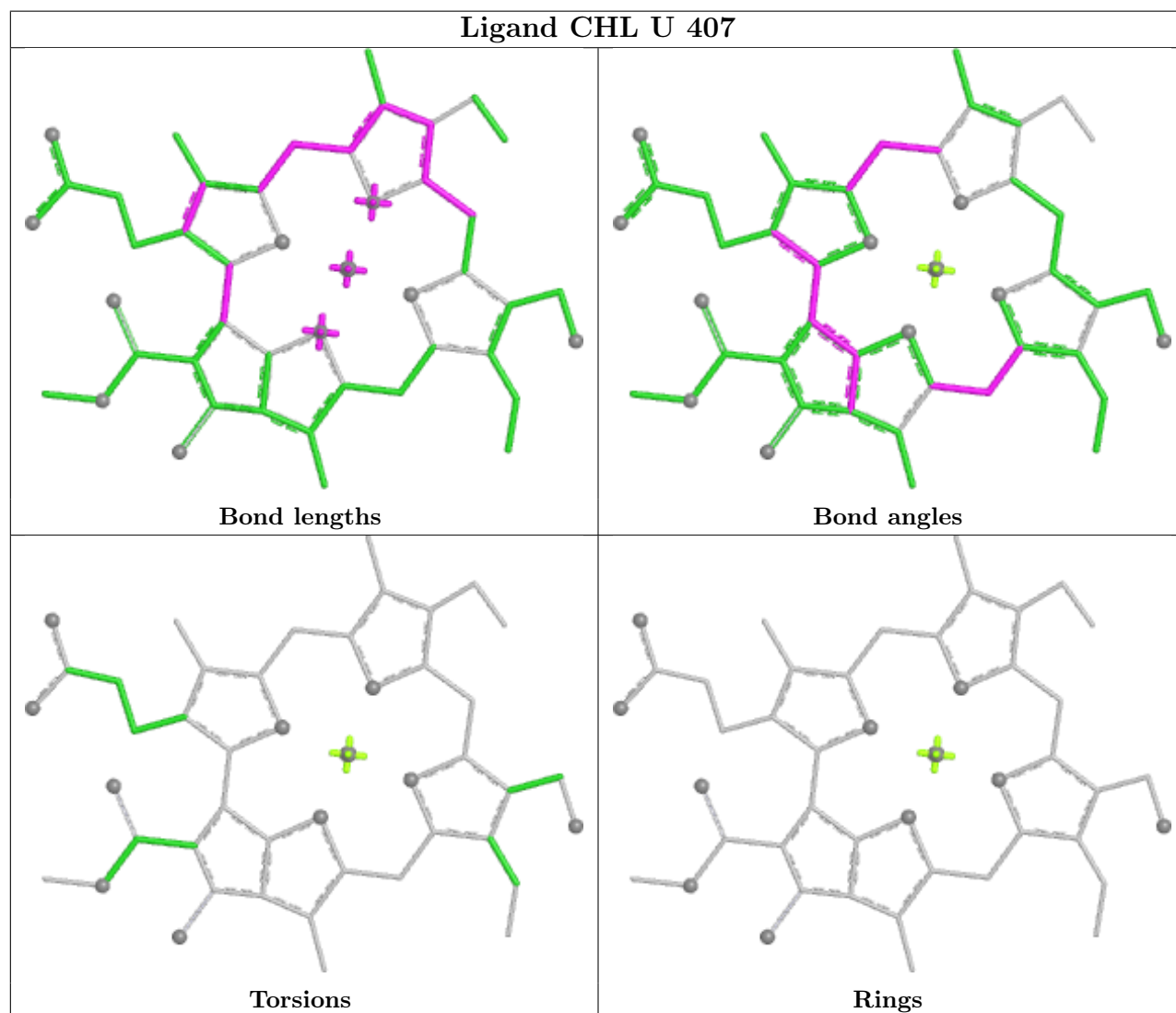
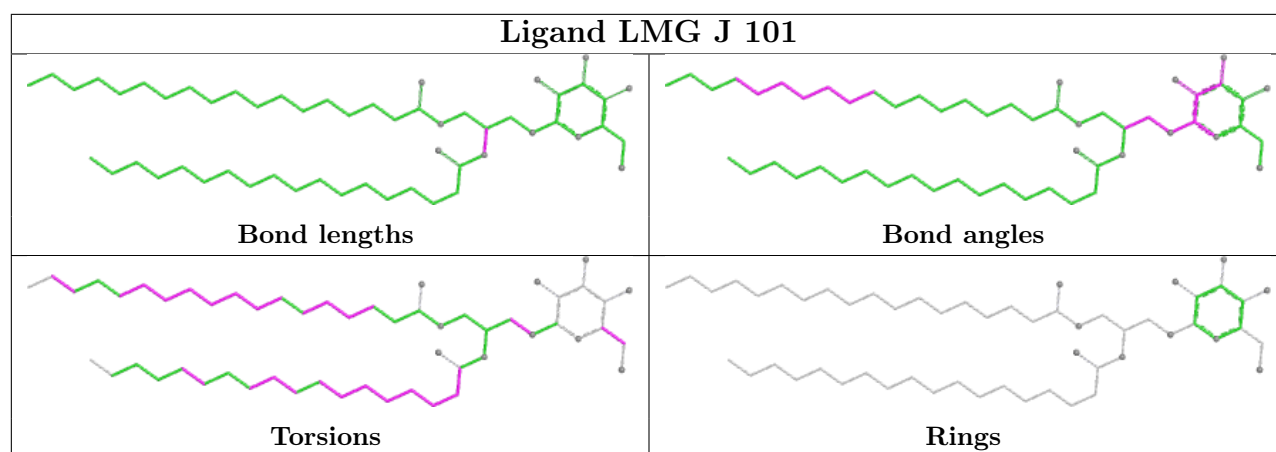




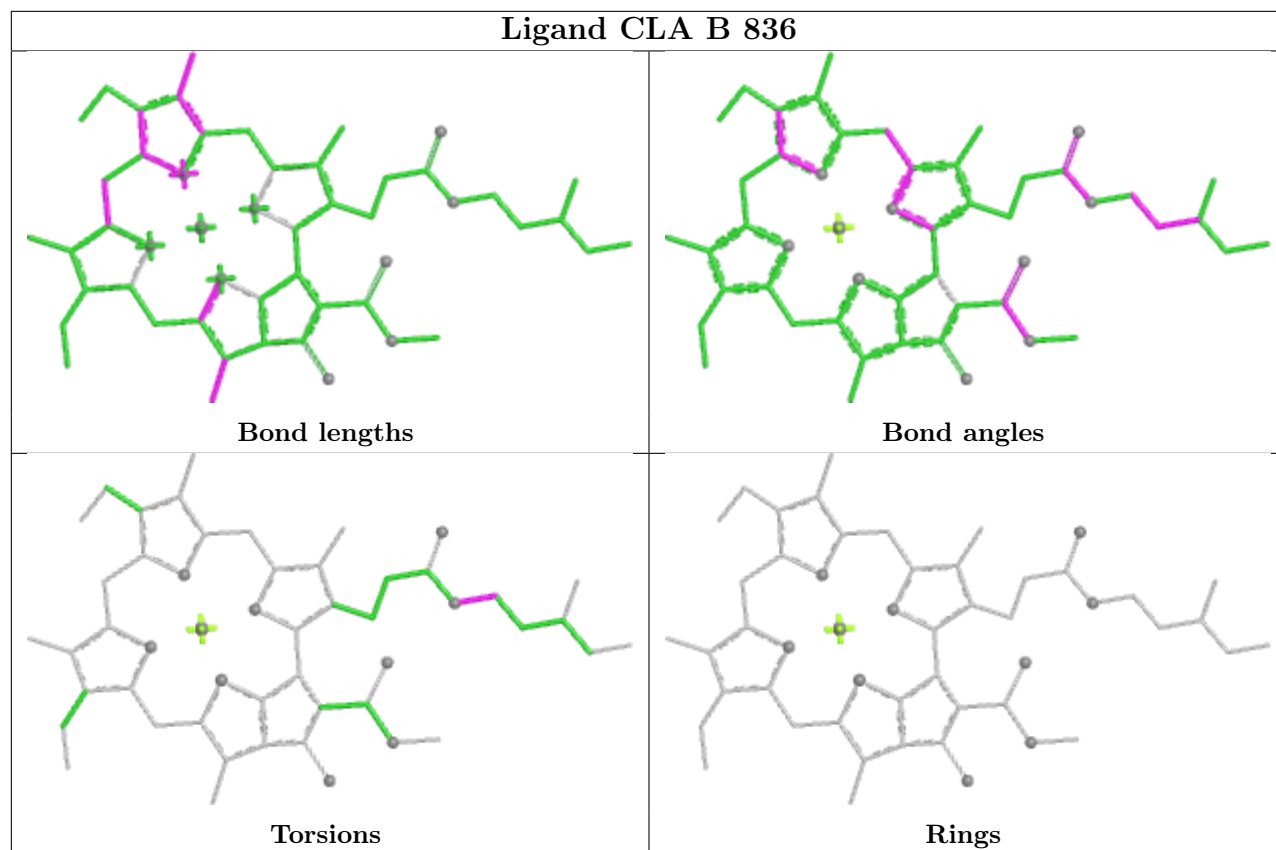




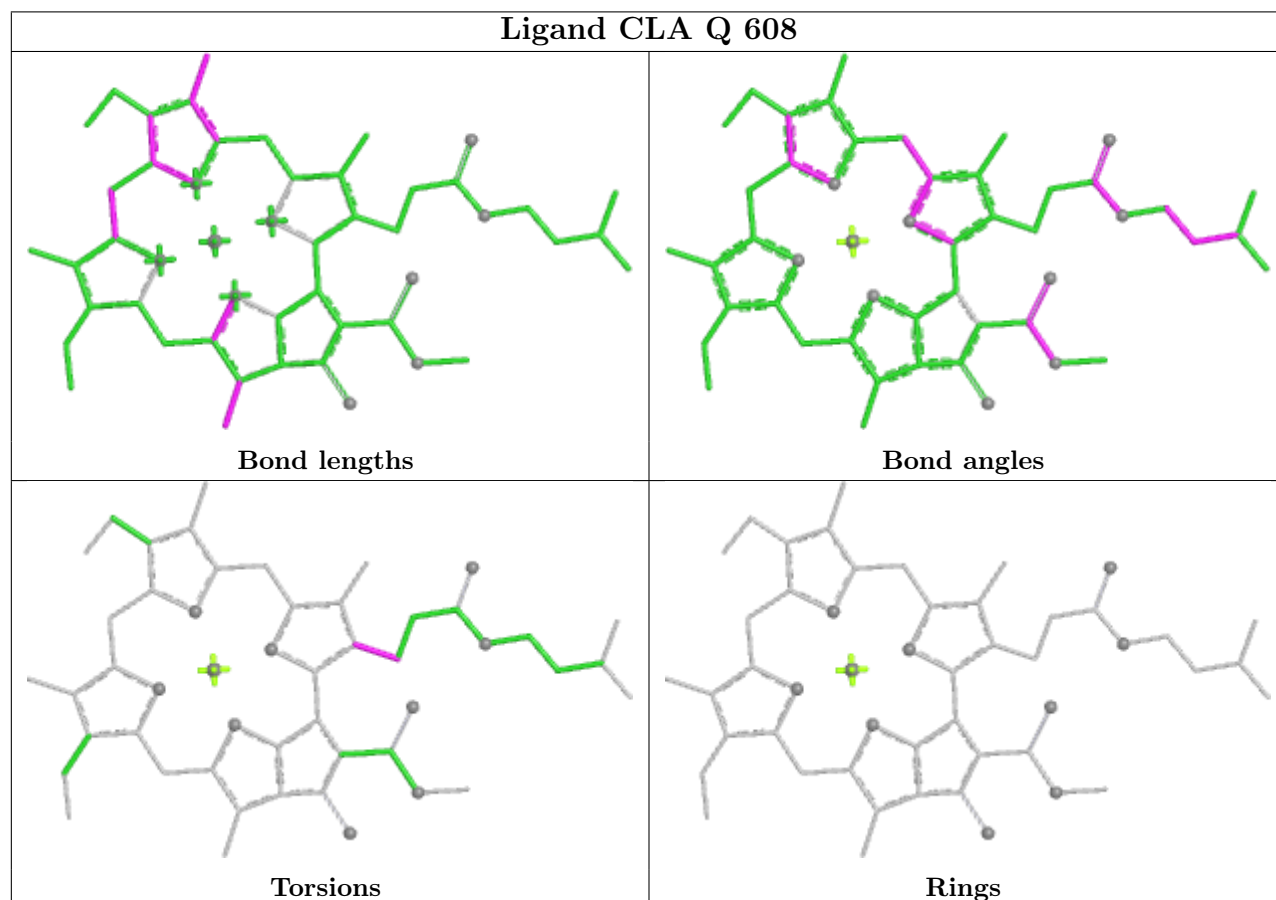




## Ligand CLA B 836

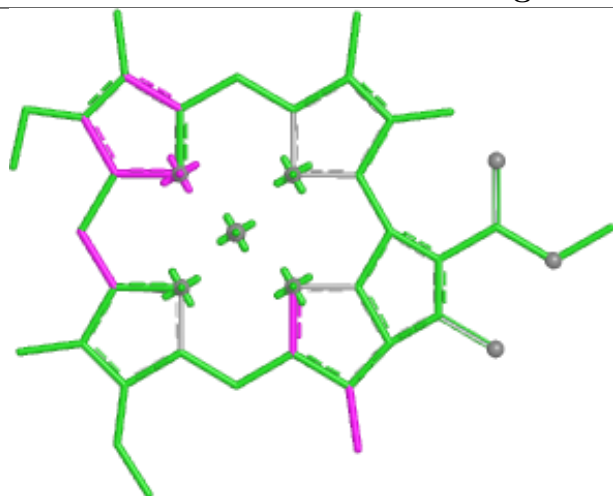


## Ligand CLA Q 608

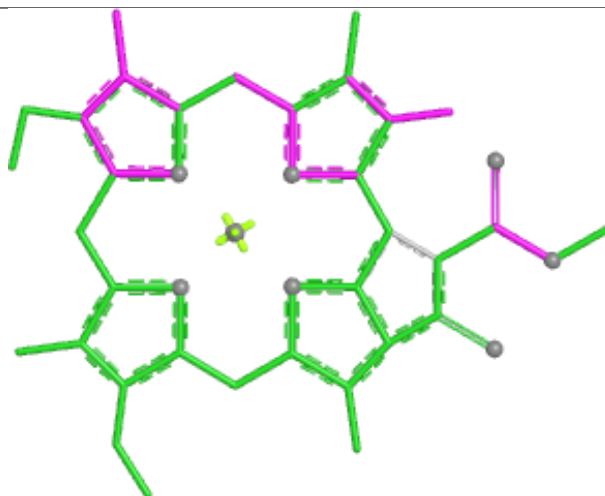




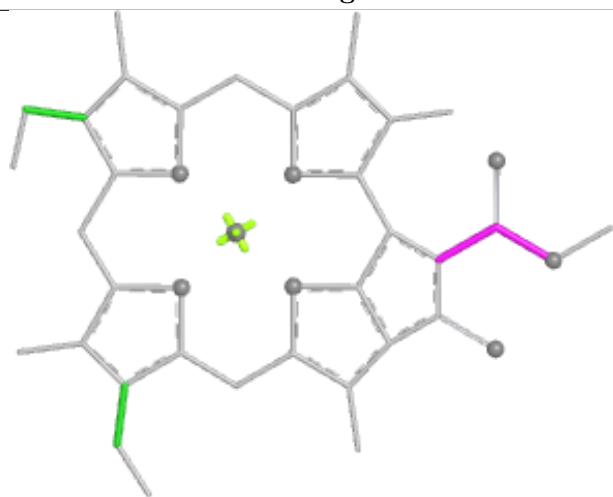
## Ligand CLA R 609



Bond lengths



Bond angles

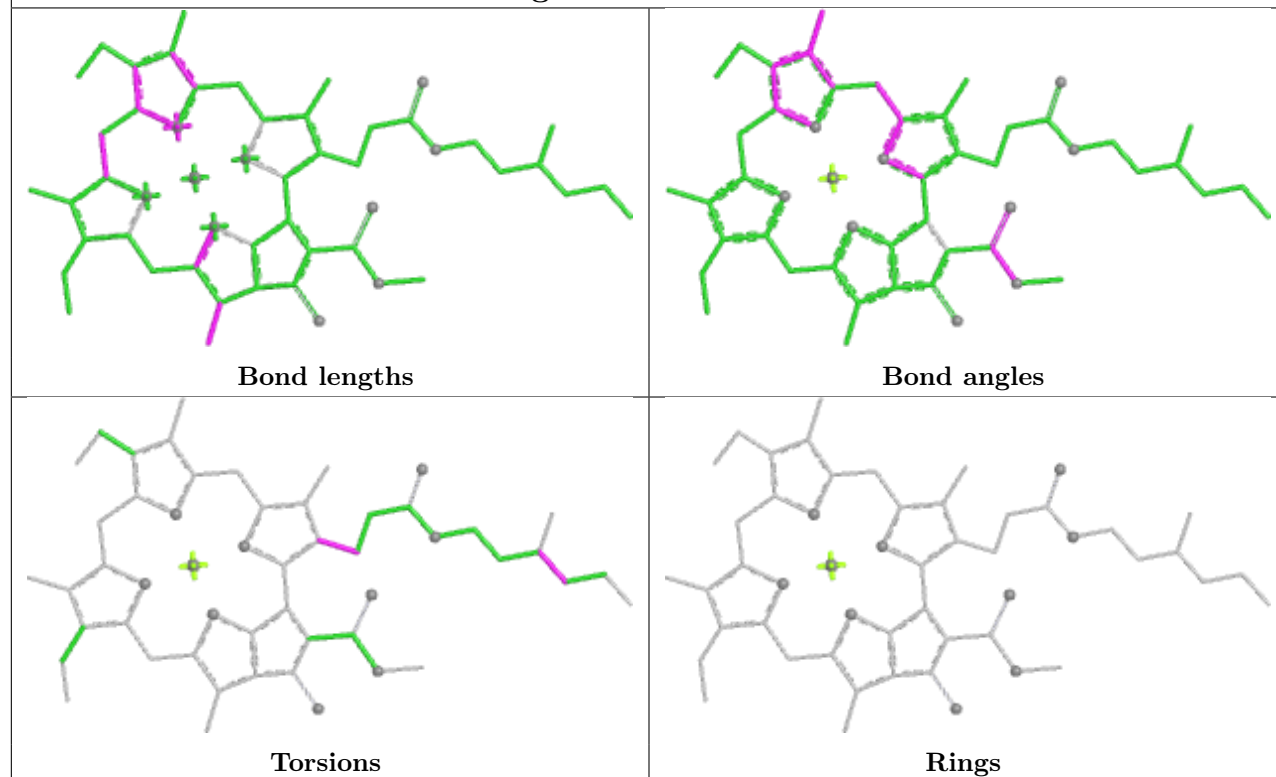


Torsions

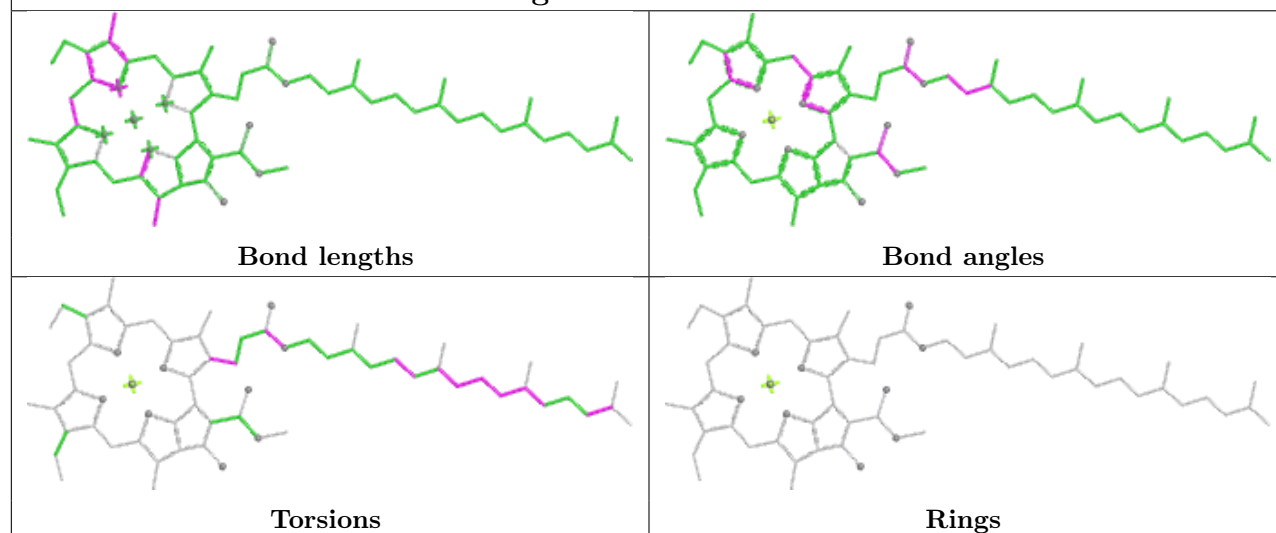


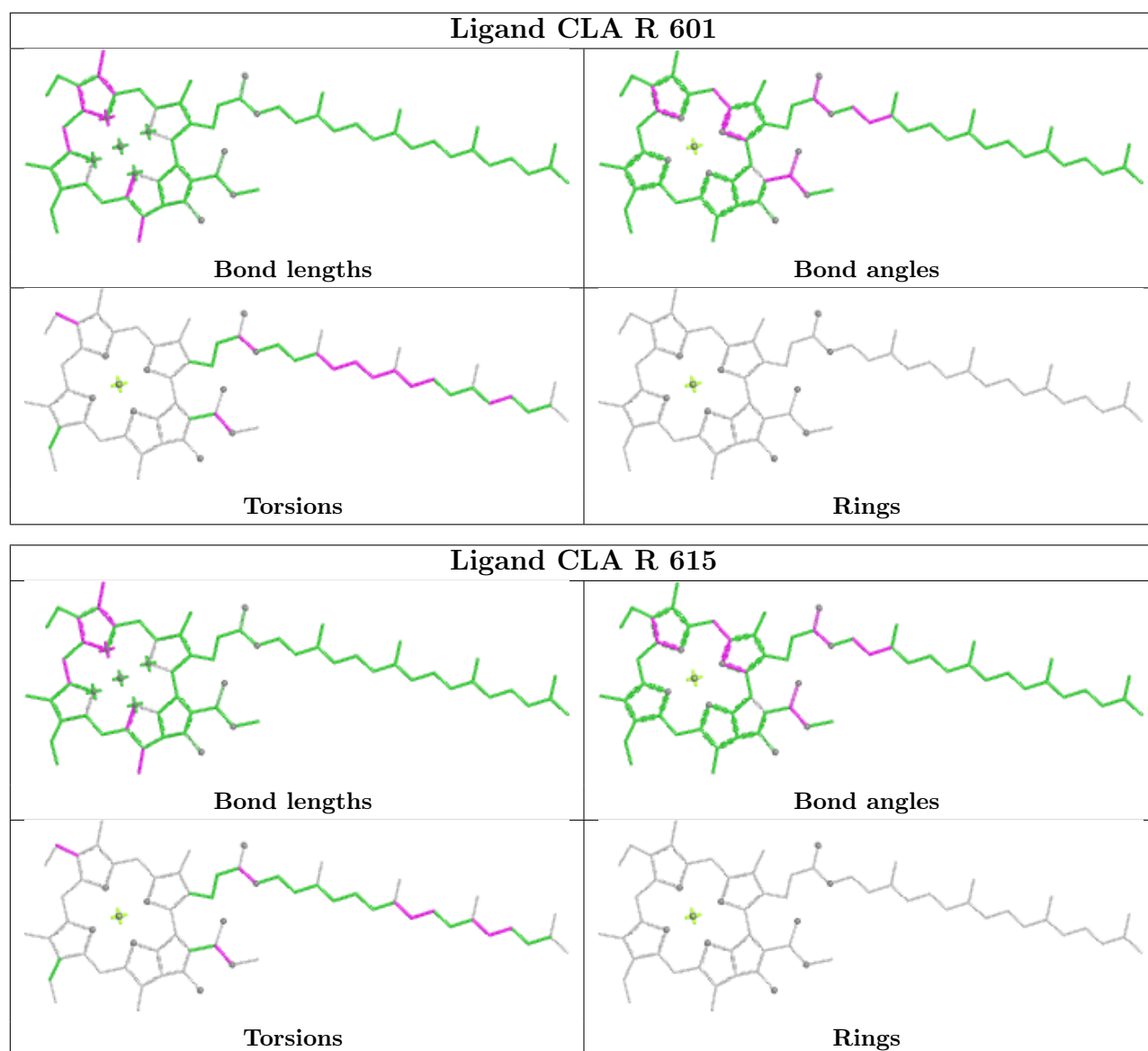
Rings

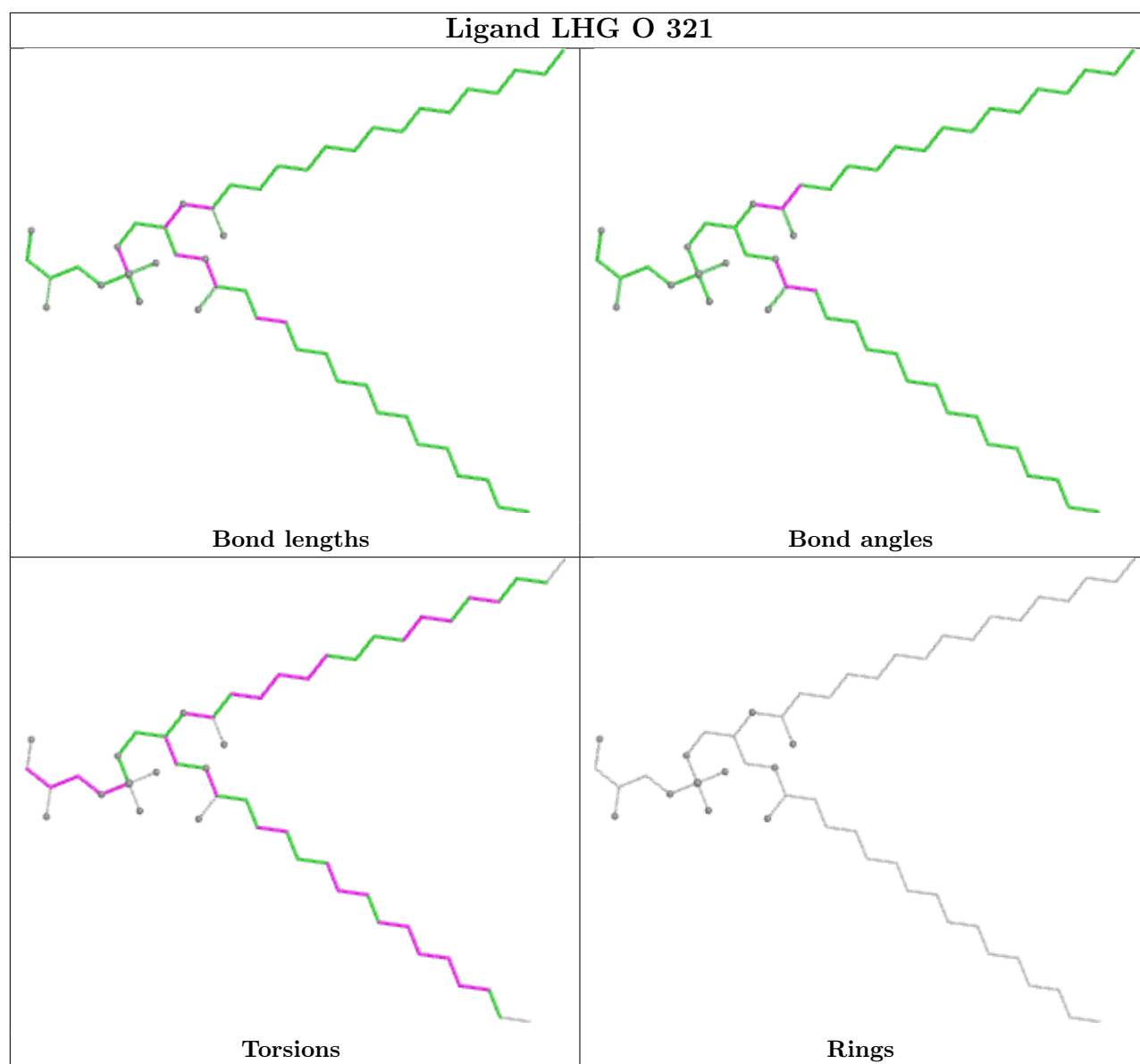
## Ligand CLA A 832



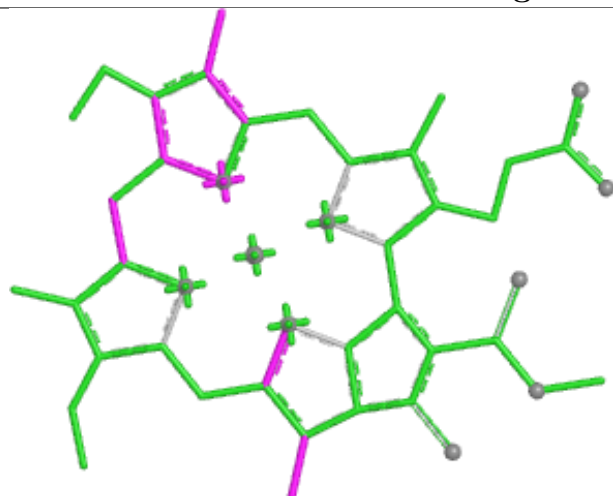
## Ligand CLA A 840



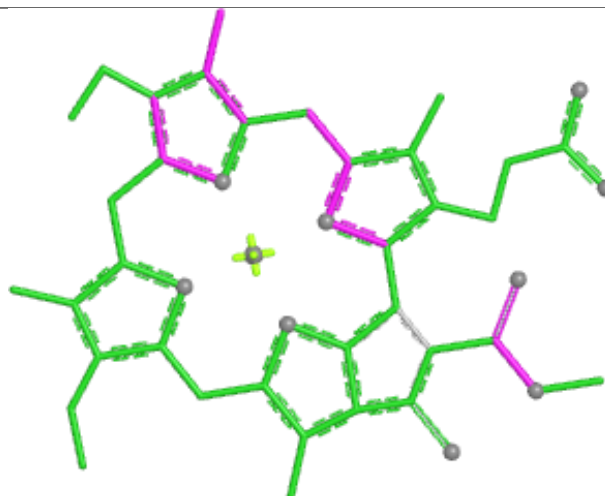




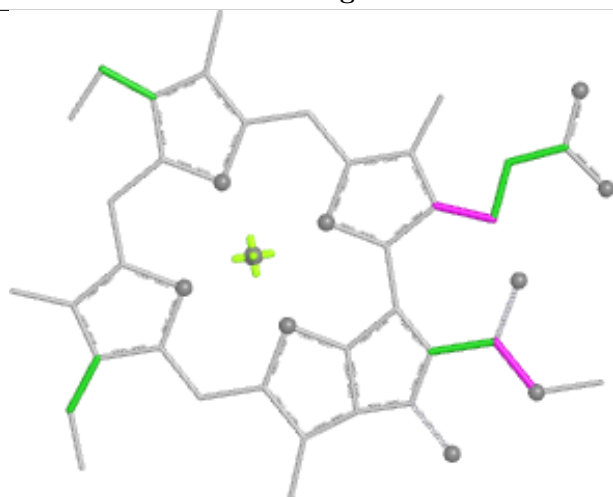
## Ligand CLA U 413



Bond lengths



Bond angles

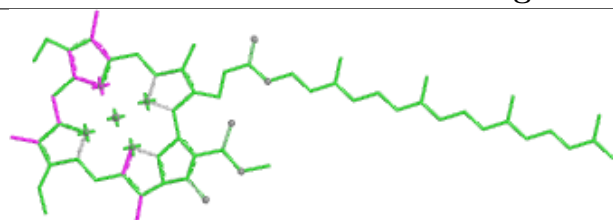


Torsions

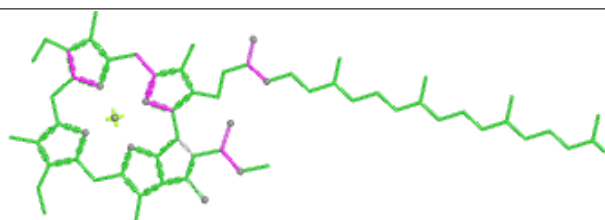


Rings

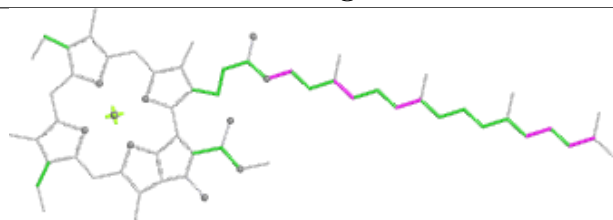
## Ligand CLA A 822



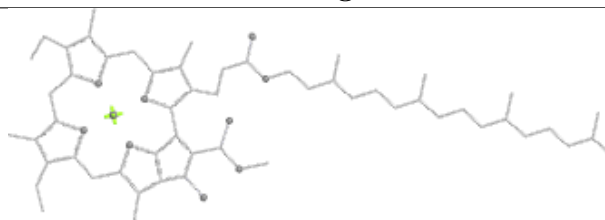
Bond lengths



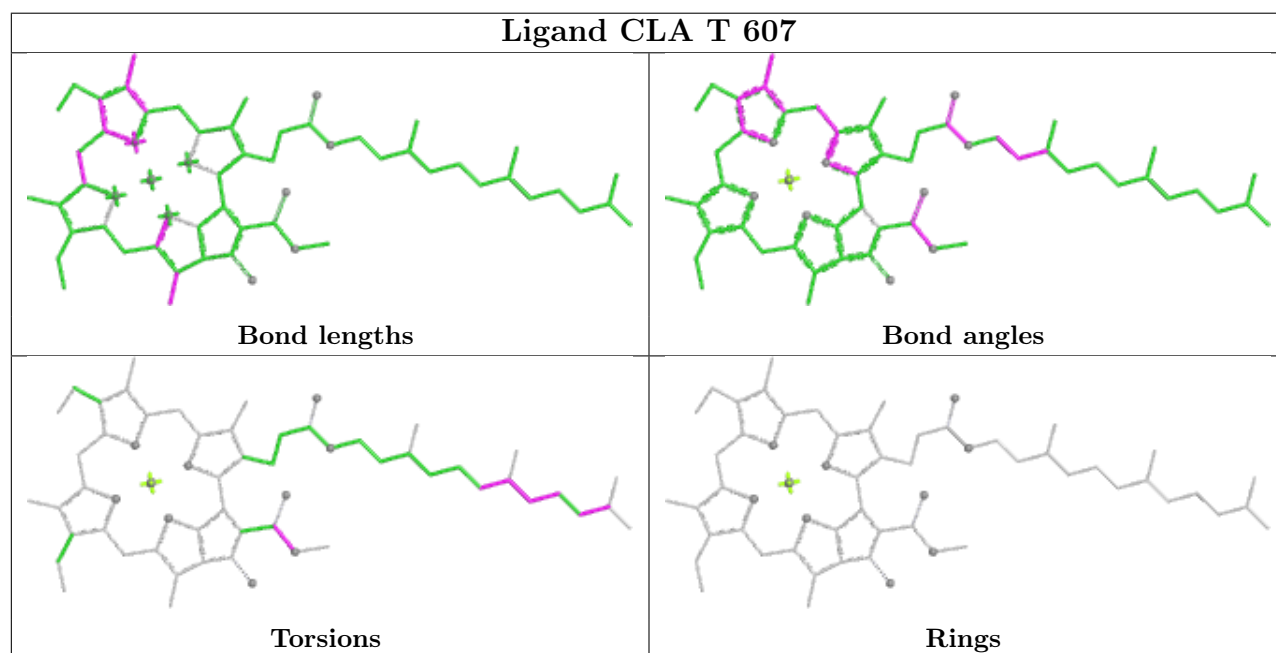
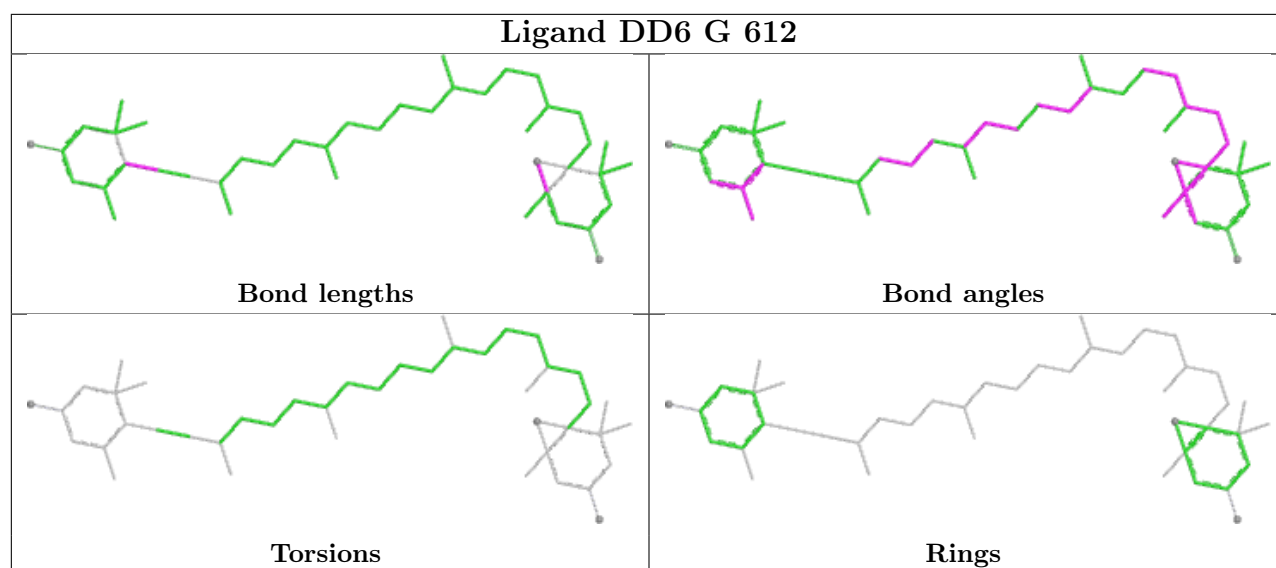
Bond angles



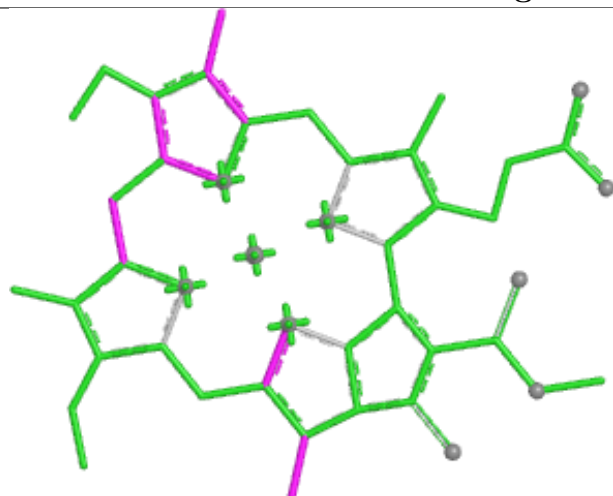
Torsions



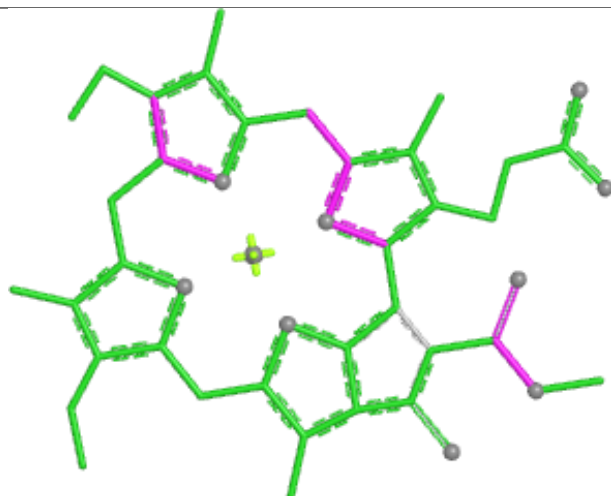
Rings



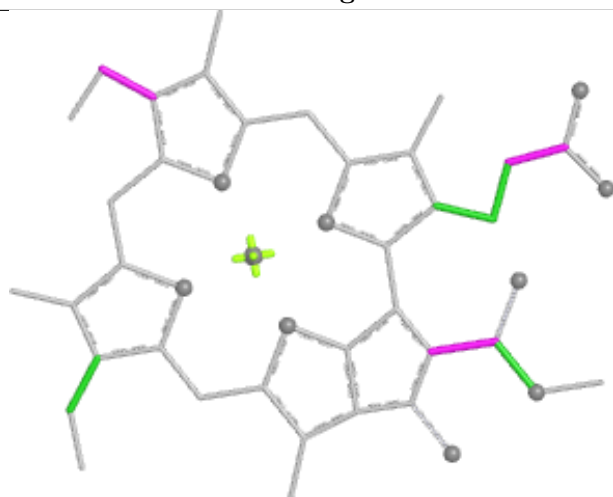
## Ligand CLA T 610



Bond lengths



Bond angles

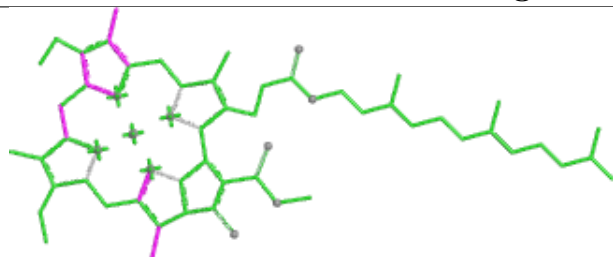


Torsions

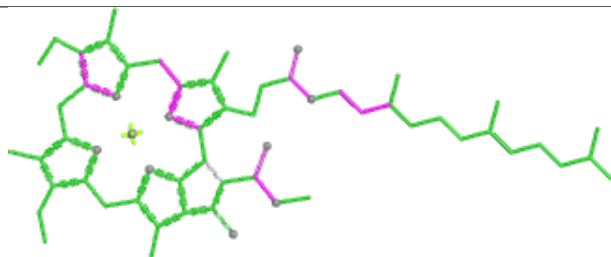


Rings

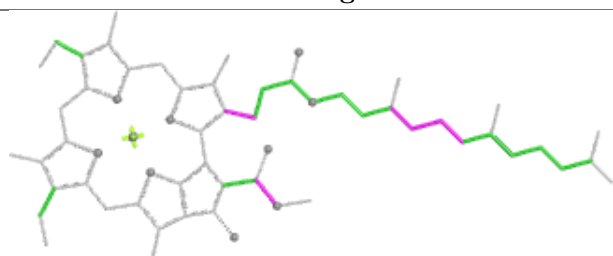
## Ligand CLA H 307



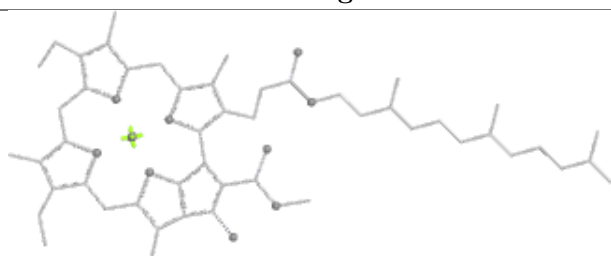
Bond lengths



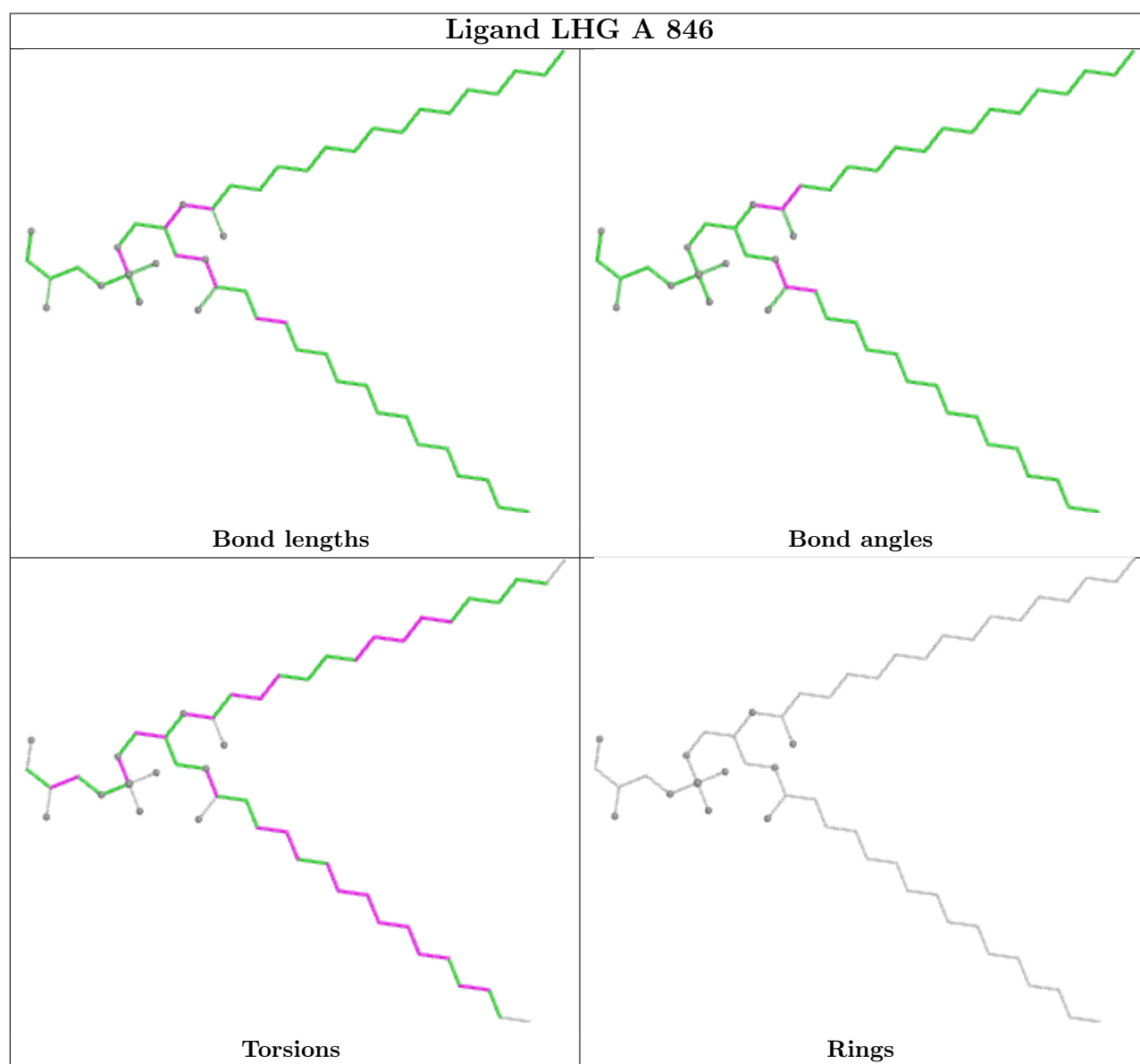
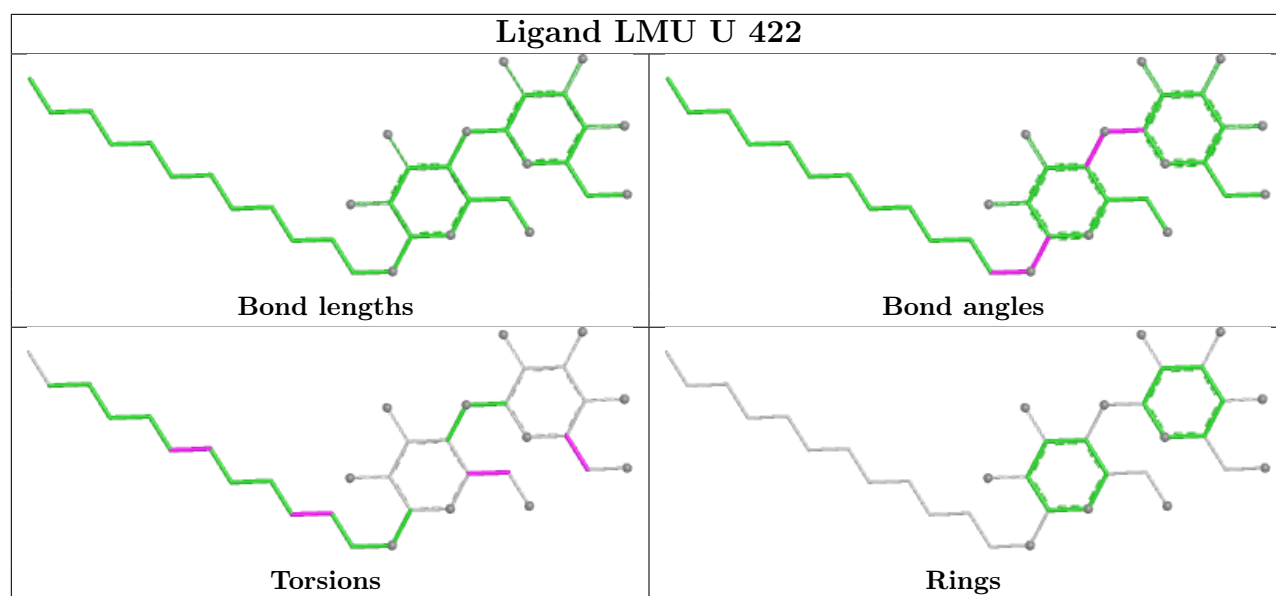
Bond angles



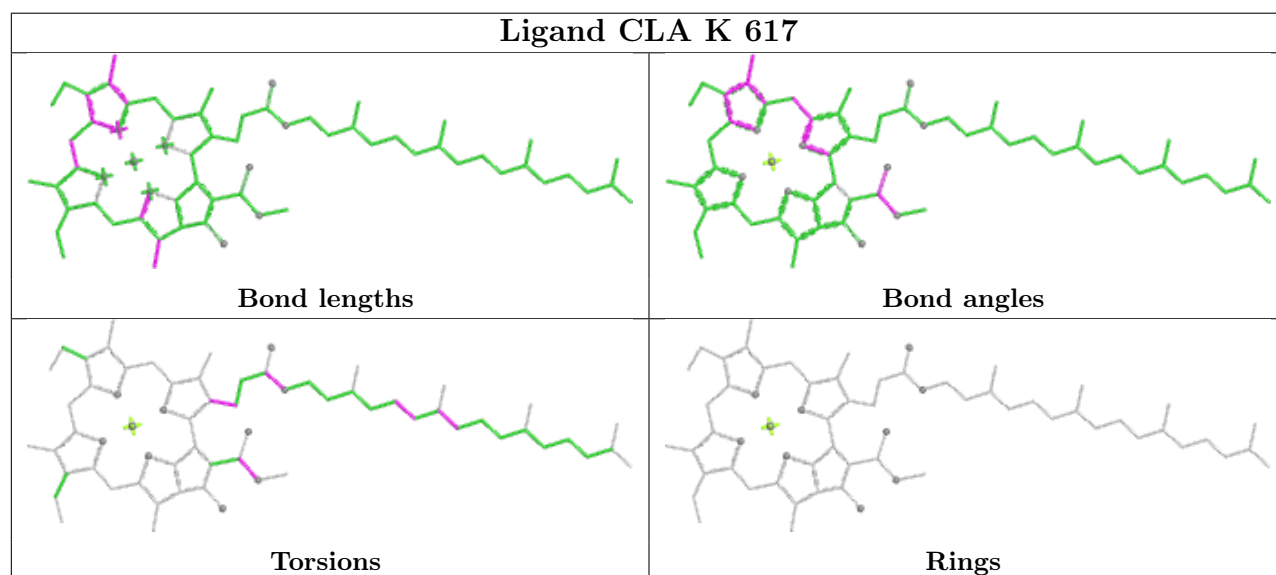
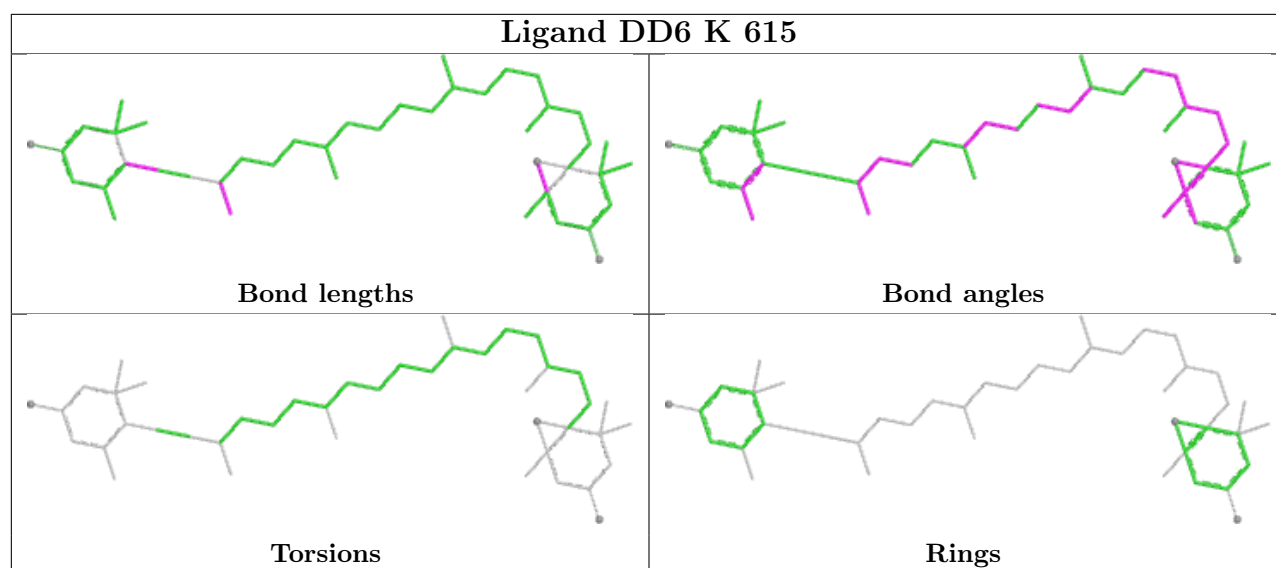
Torsions

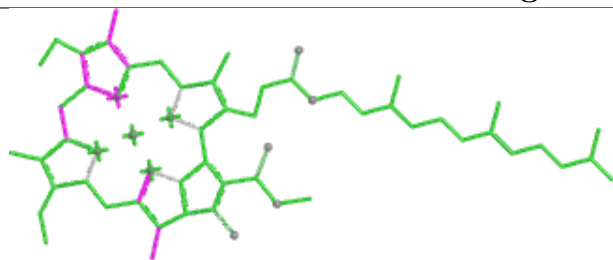
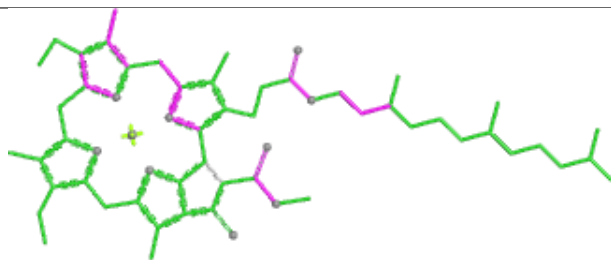
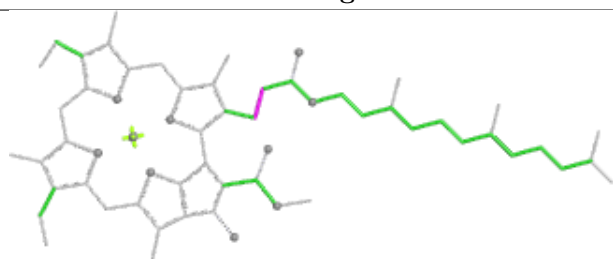
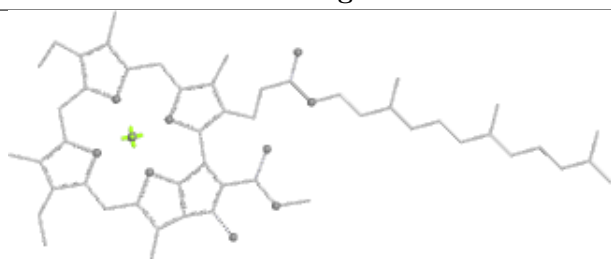
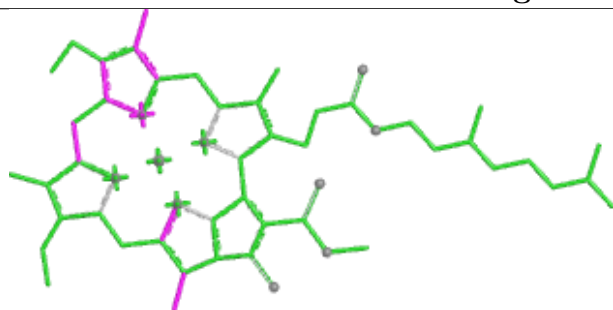
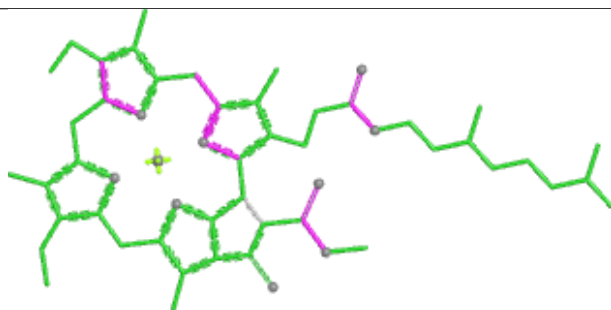
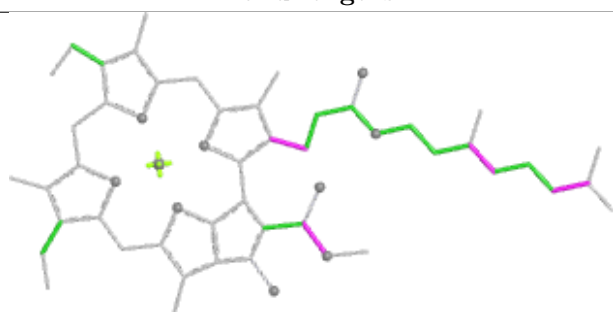
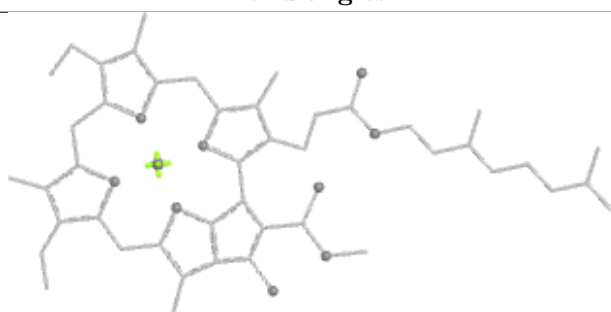


Rings

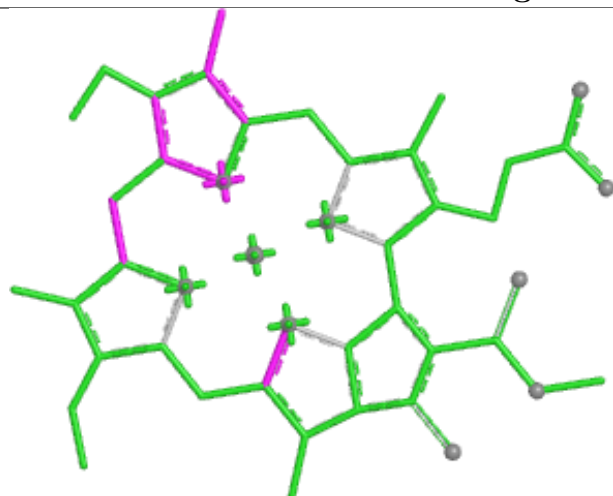




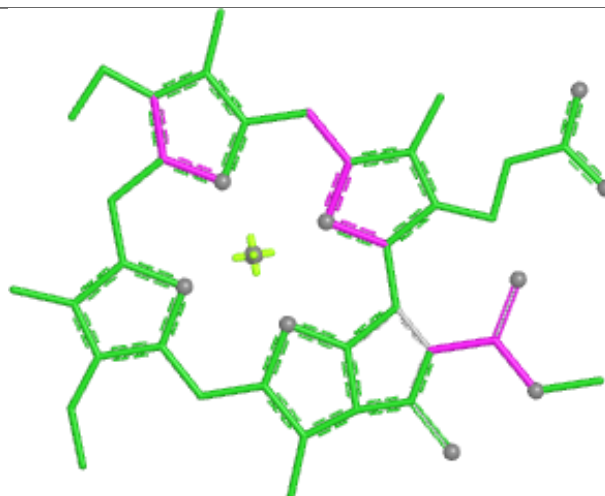


**Ligand CLA I 602****Bond lengths****Bond angles****Torsions****Rings****Ligand CLA U 410****Bond lengths****Bond angles****Torsions****Rings**

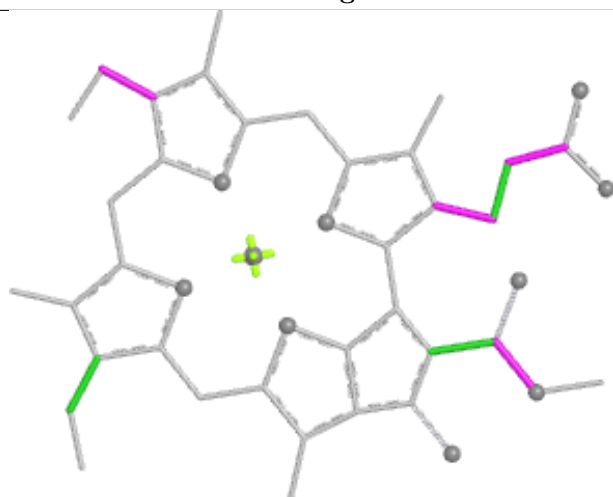
## Ligand CLA V 617



Bond lengths



Bond angles

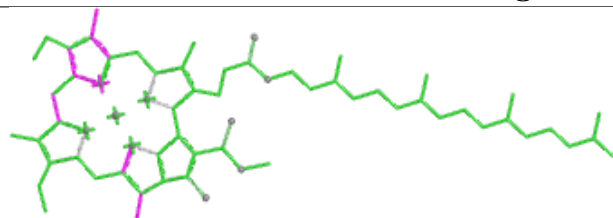


Torsions

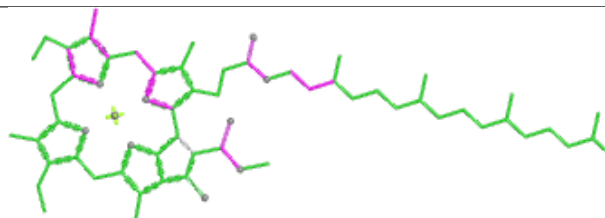


Rings

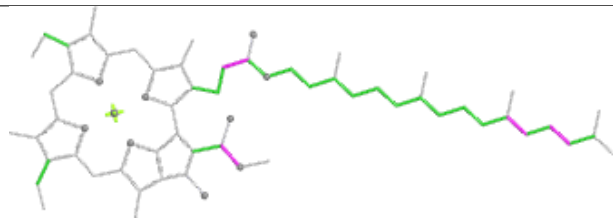
## Ligand CLA B 805



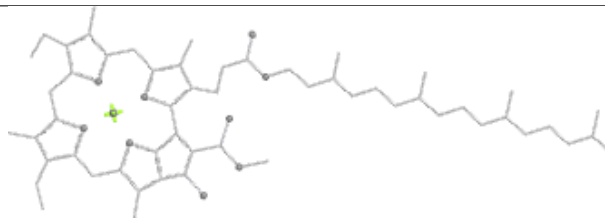
Bond lengths



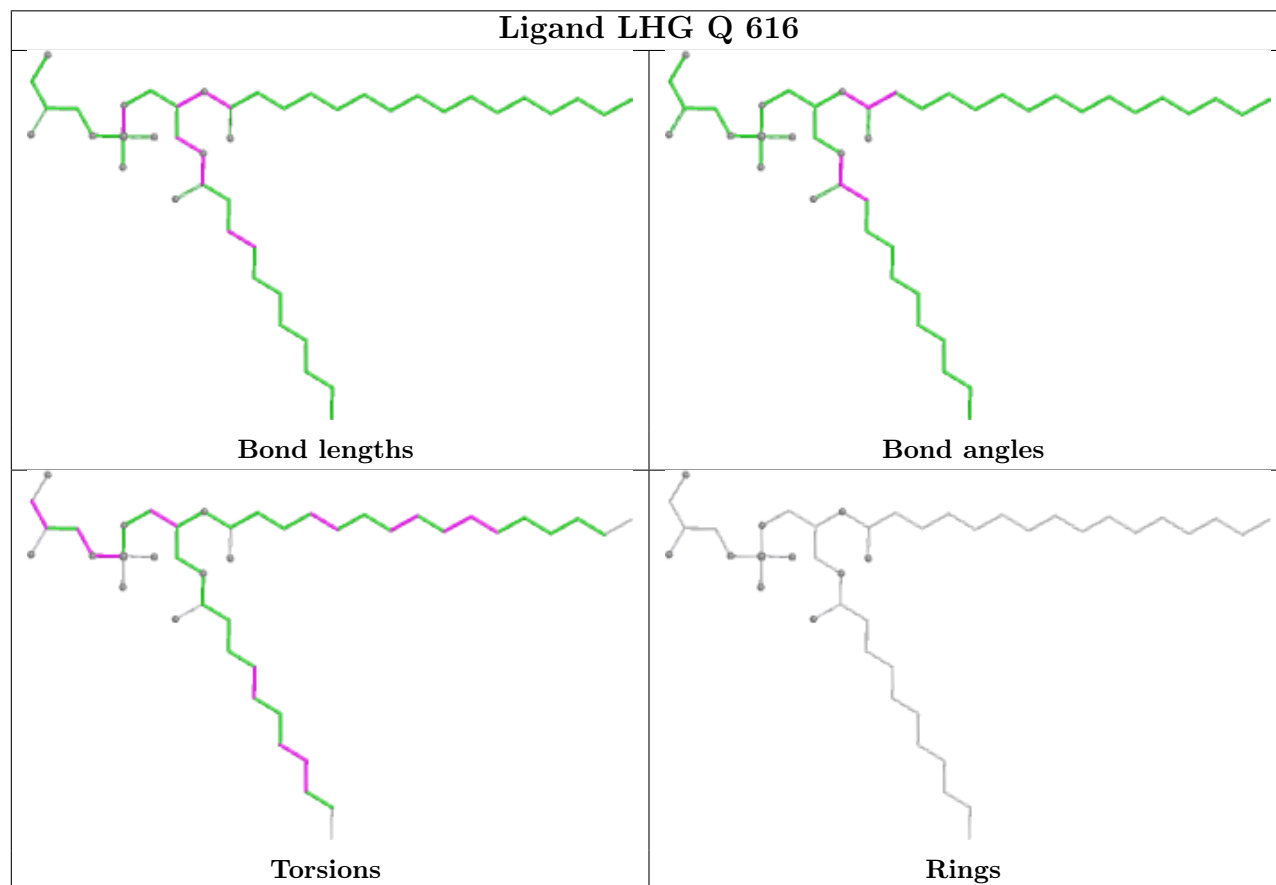
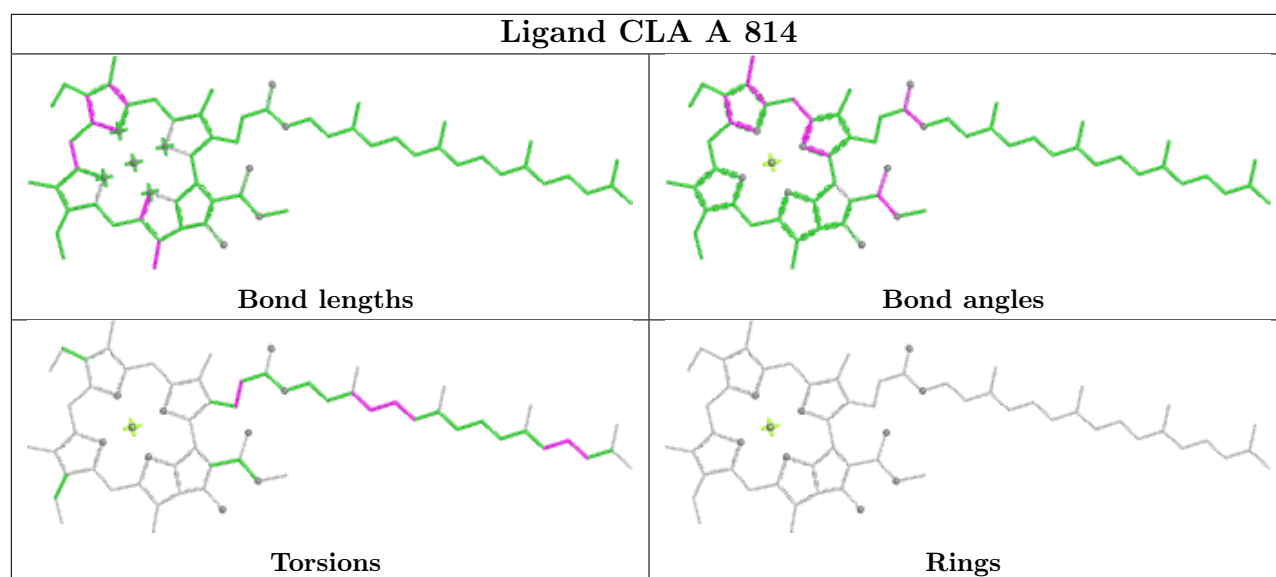
Bond angles

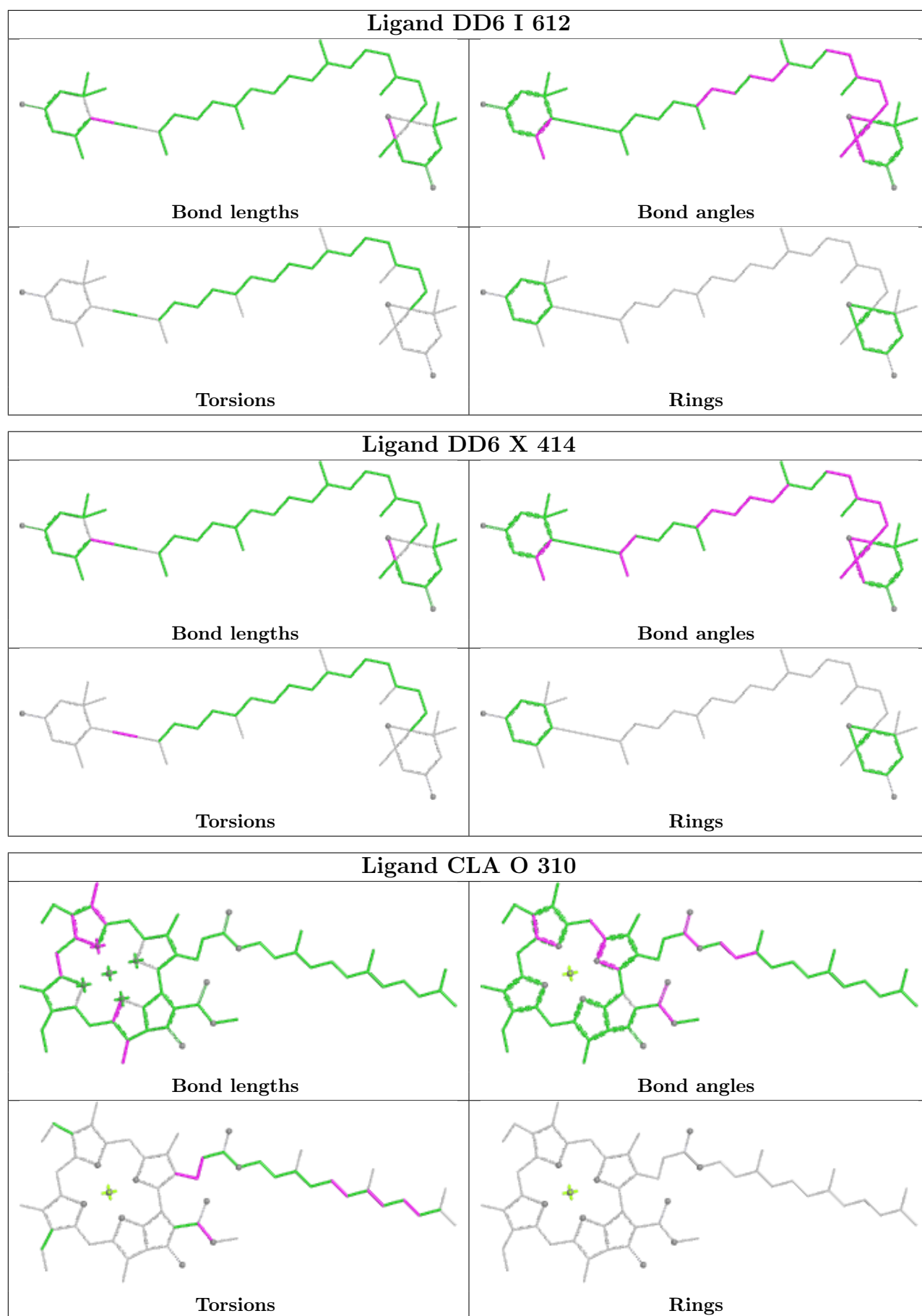


Torsions

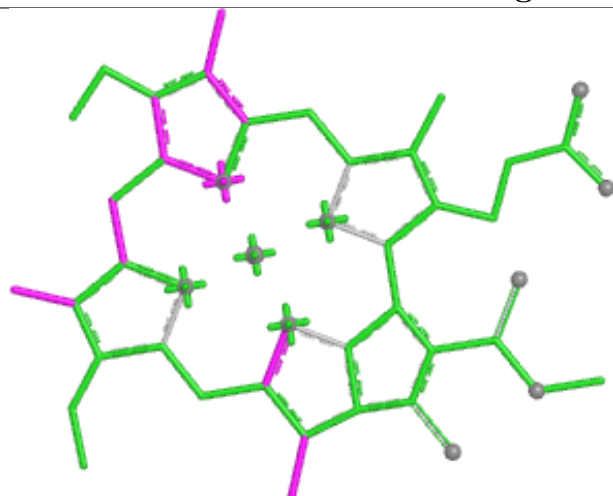


Rings





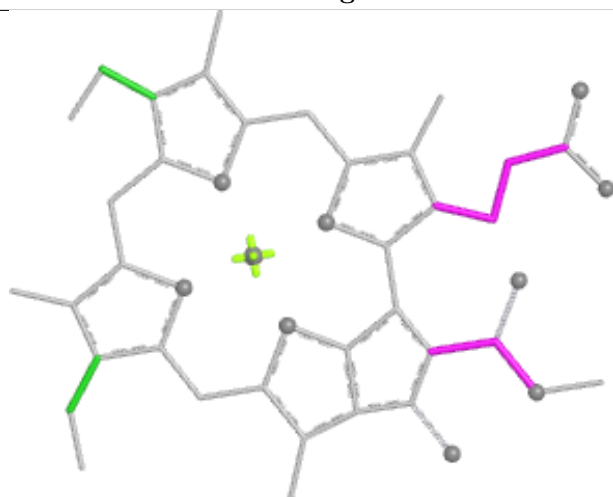
## Ligand CLA P 602



Bond lengths



Bond angles

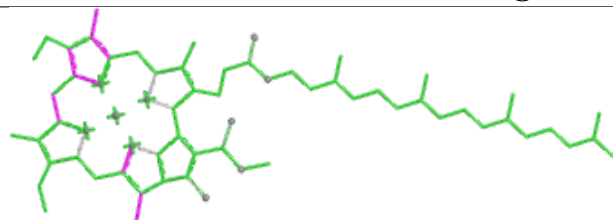


Torsions

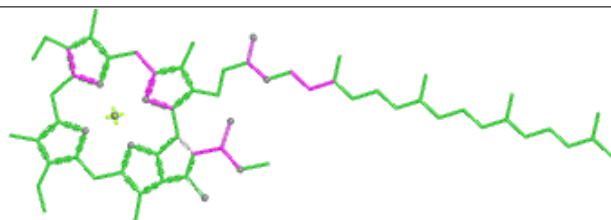


Rings

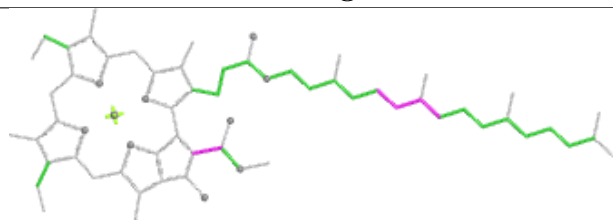
## Ligand CLA A 831



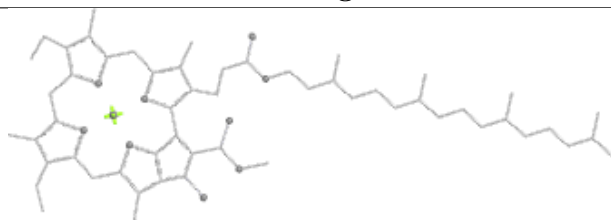
Bond lengths



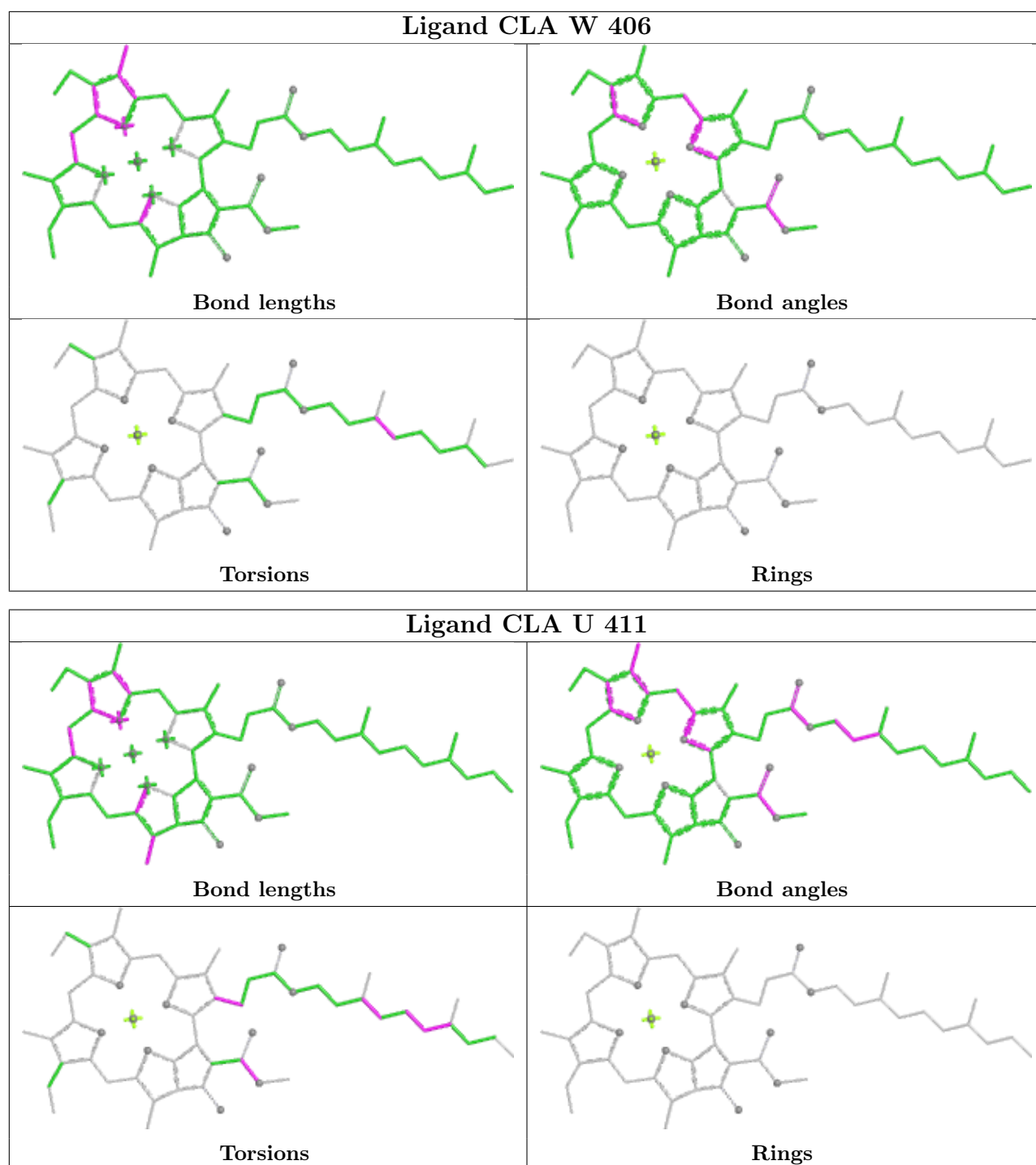
Bond angles



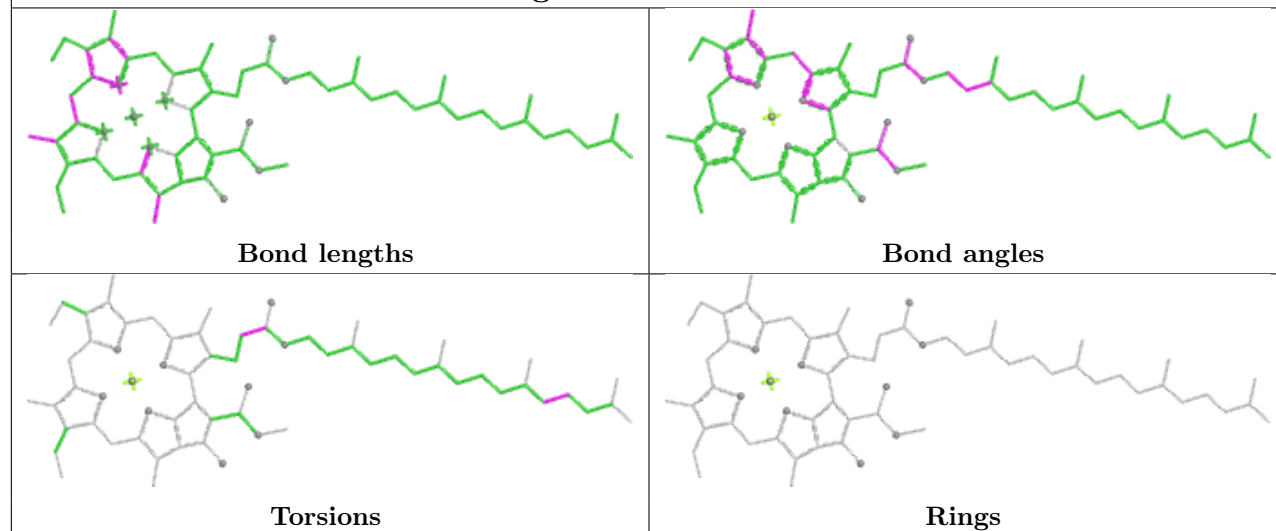
Torsions



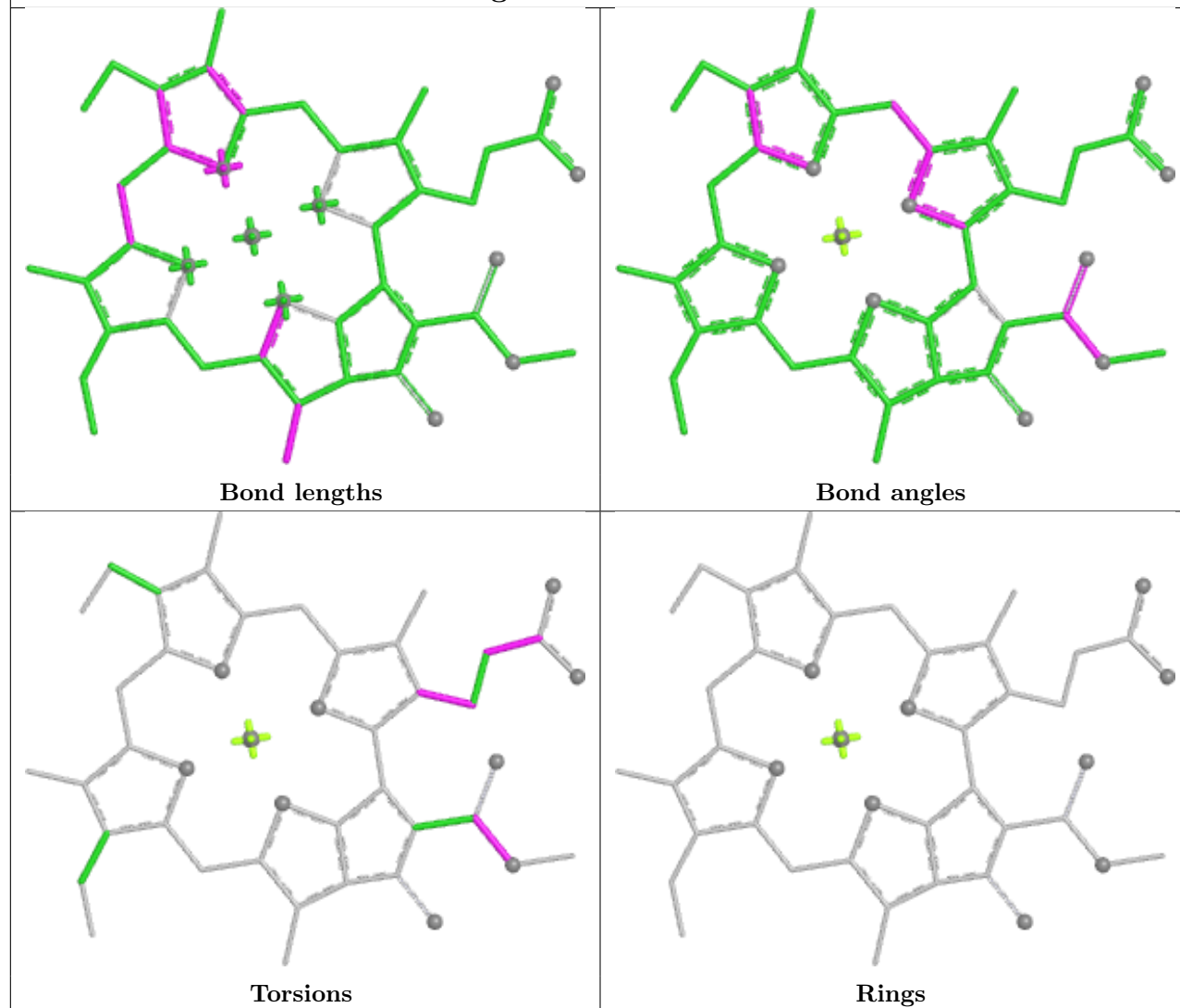
Rings



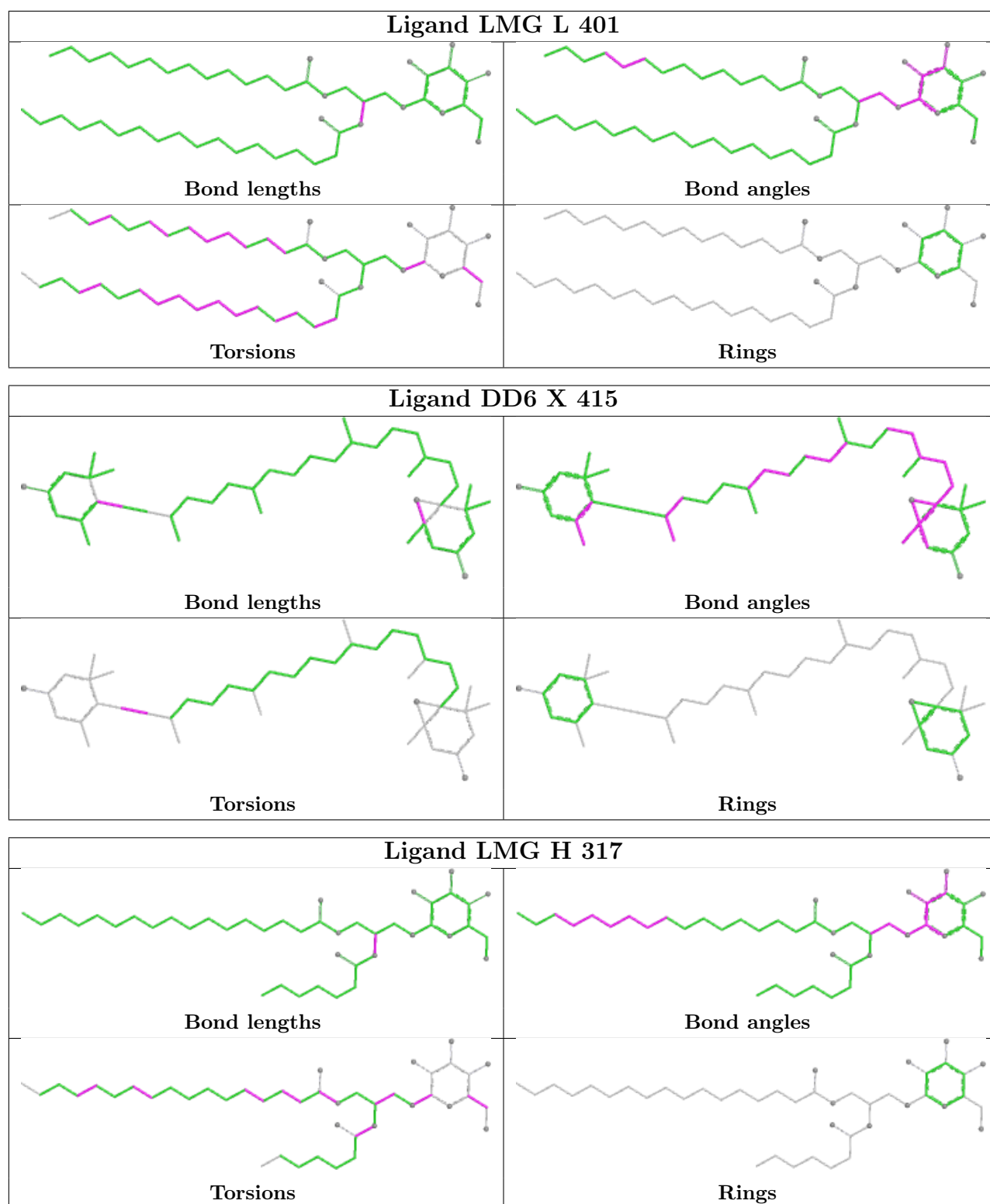
## Ligand CLA B 839



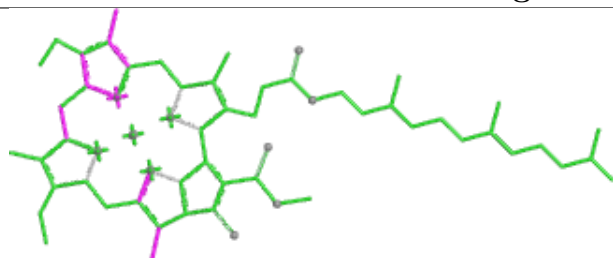
## Ligand CLA G 611



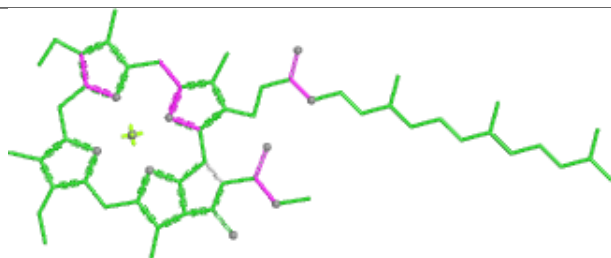




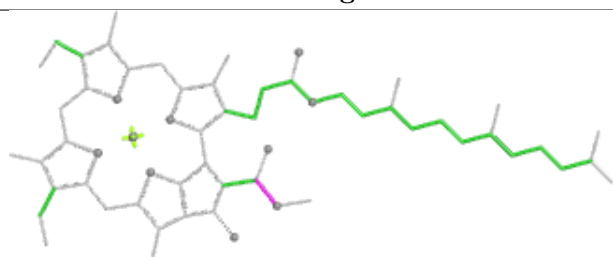
## Ligand CLA G 607



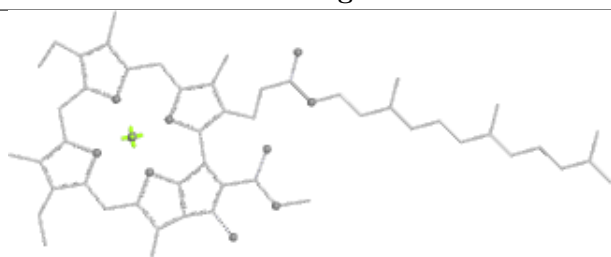
Bond lengths



Bond angles

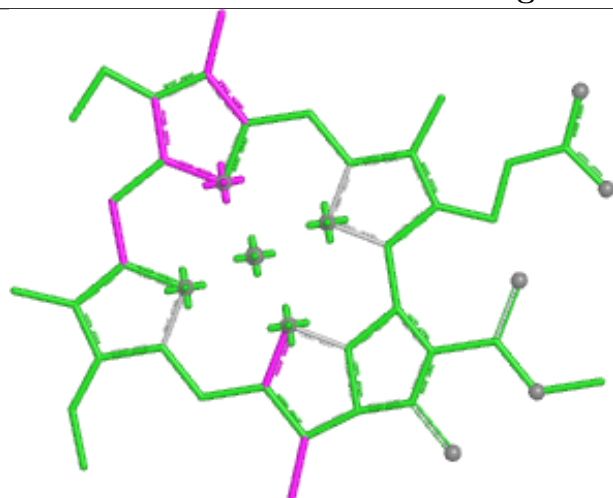


Torsions

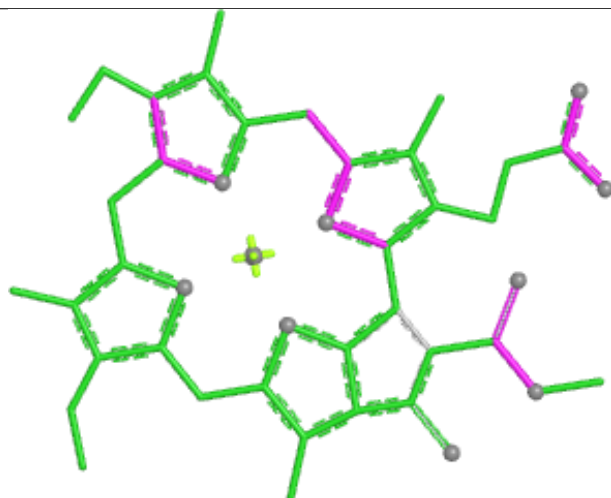


Rings

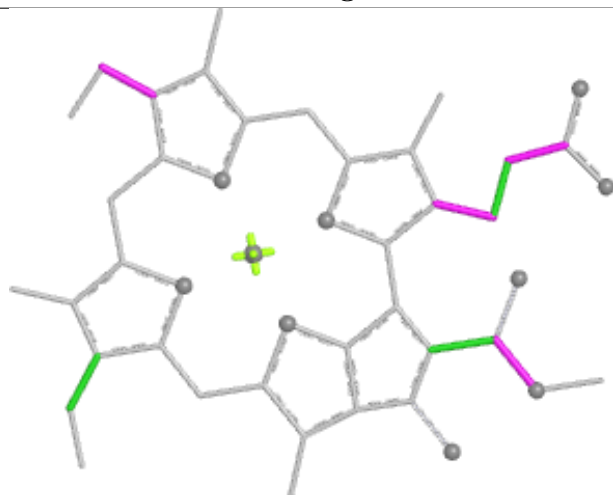
## Ligand CLA S 608



Bond lengths



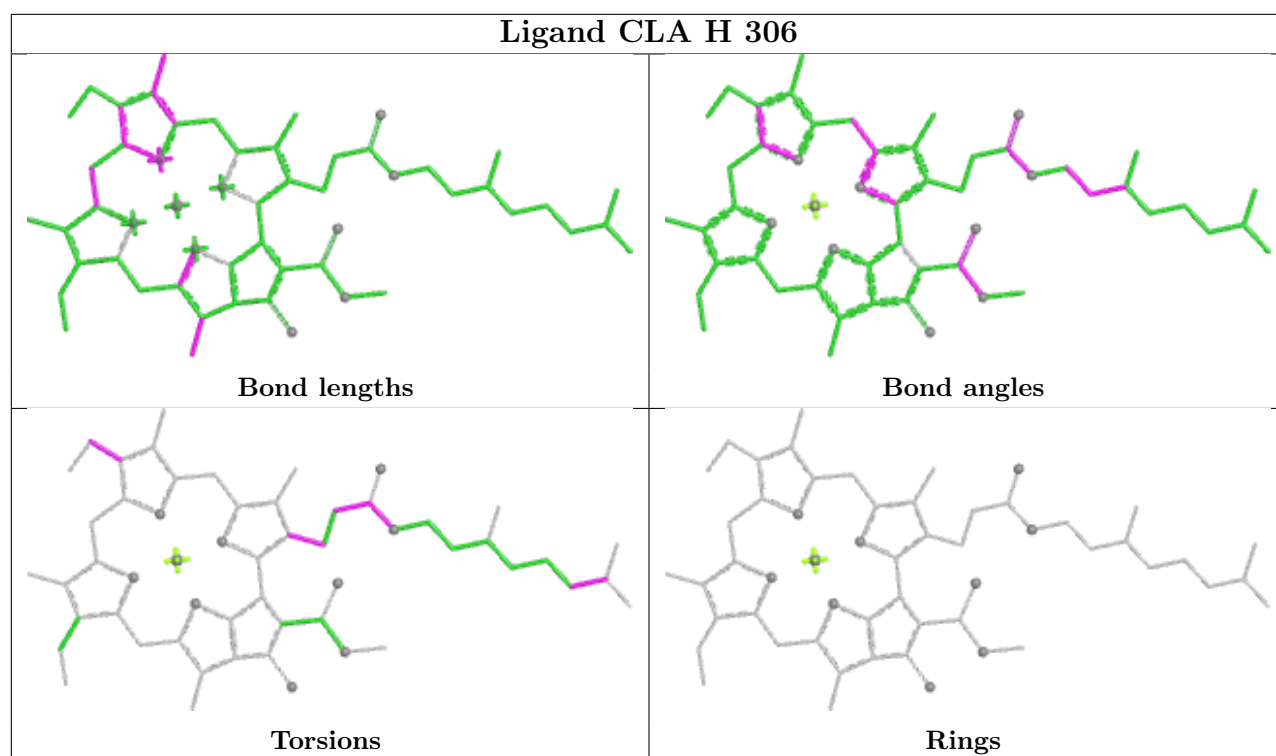
Bond angles

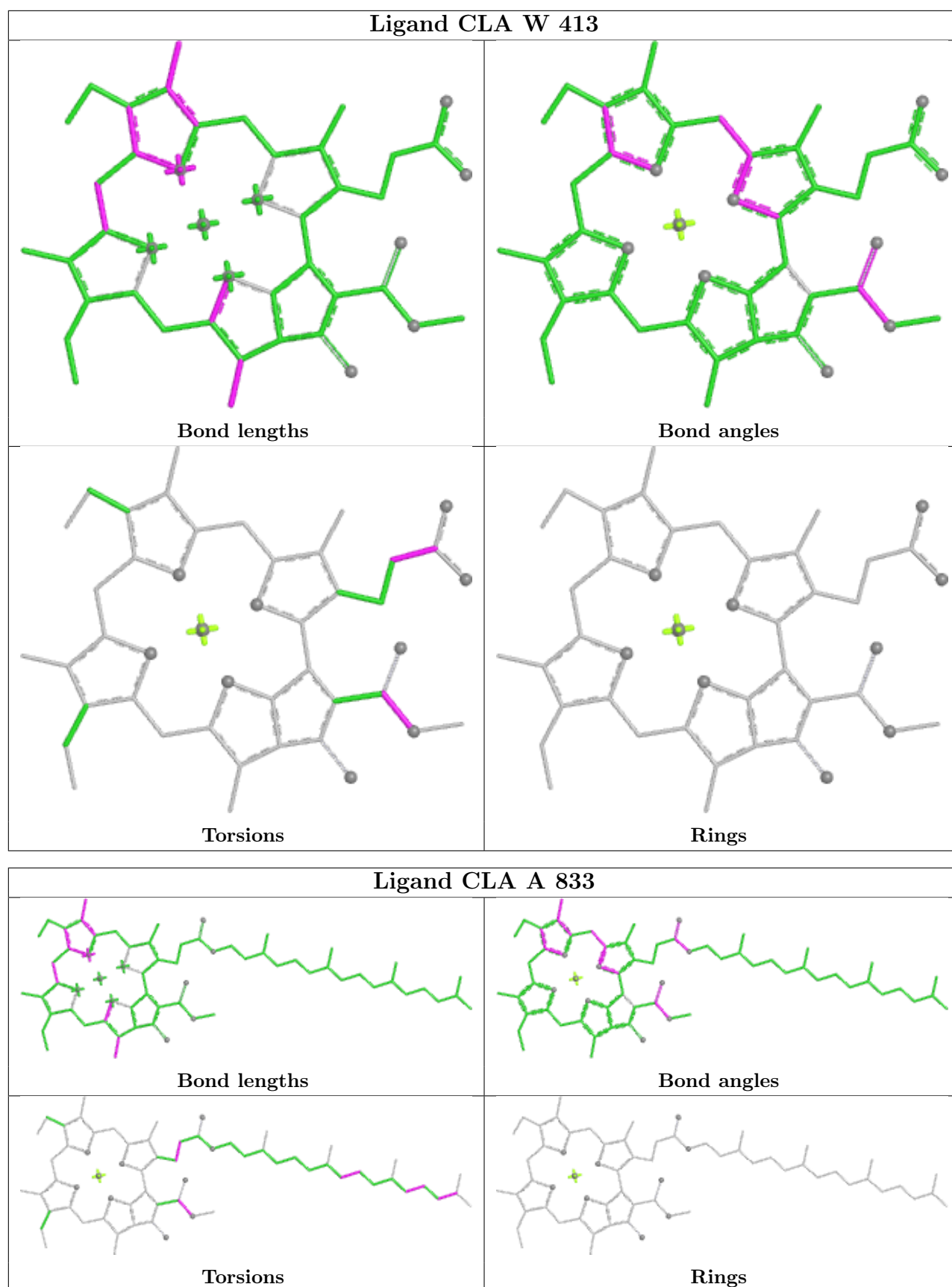


Torsions

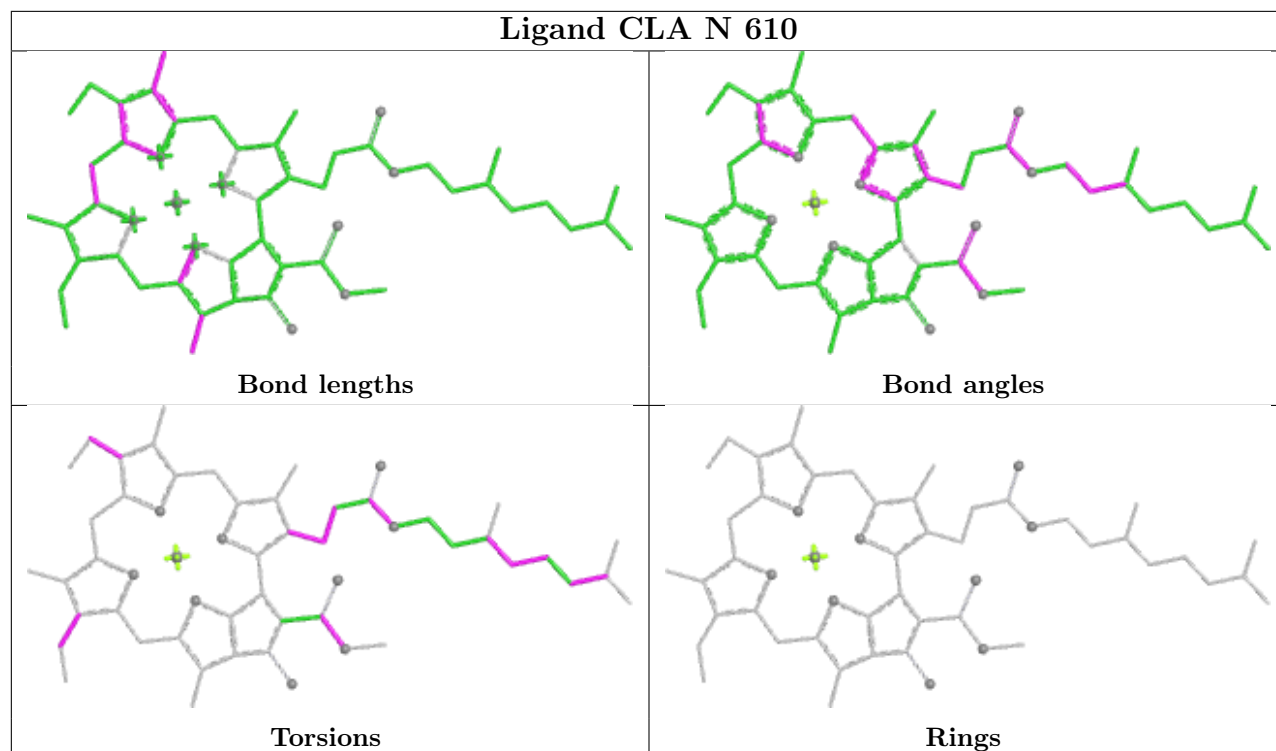


Rings

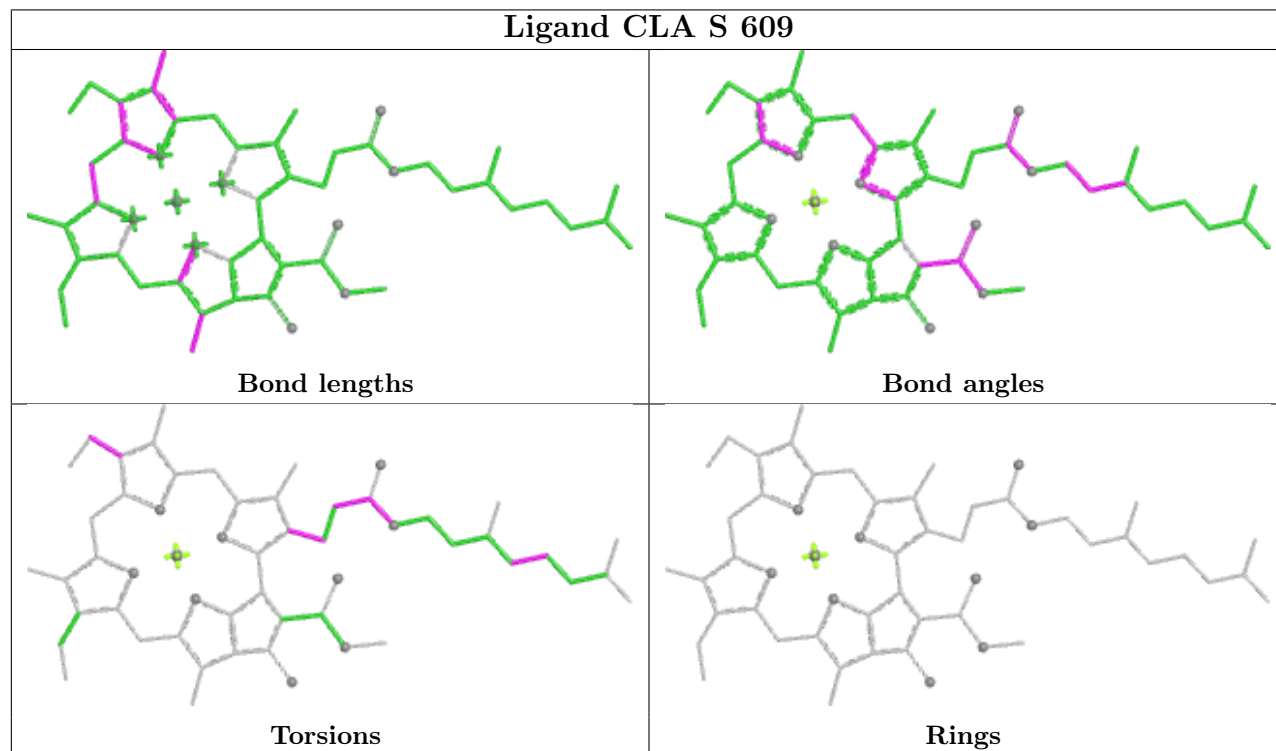


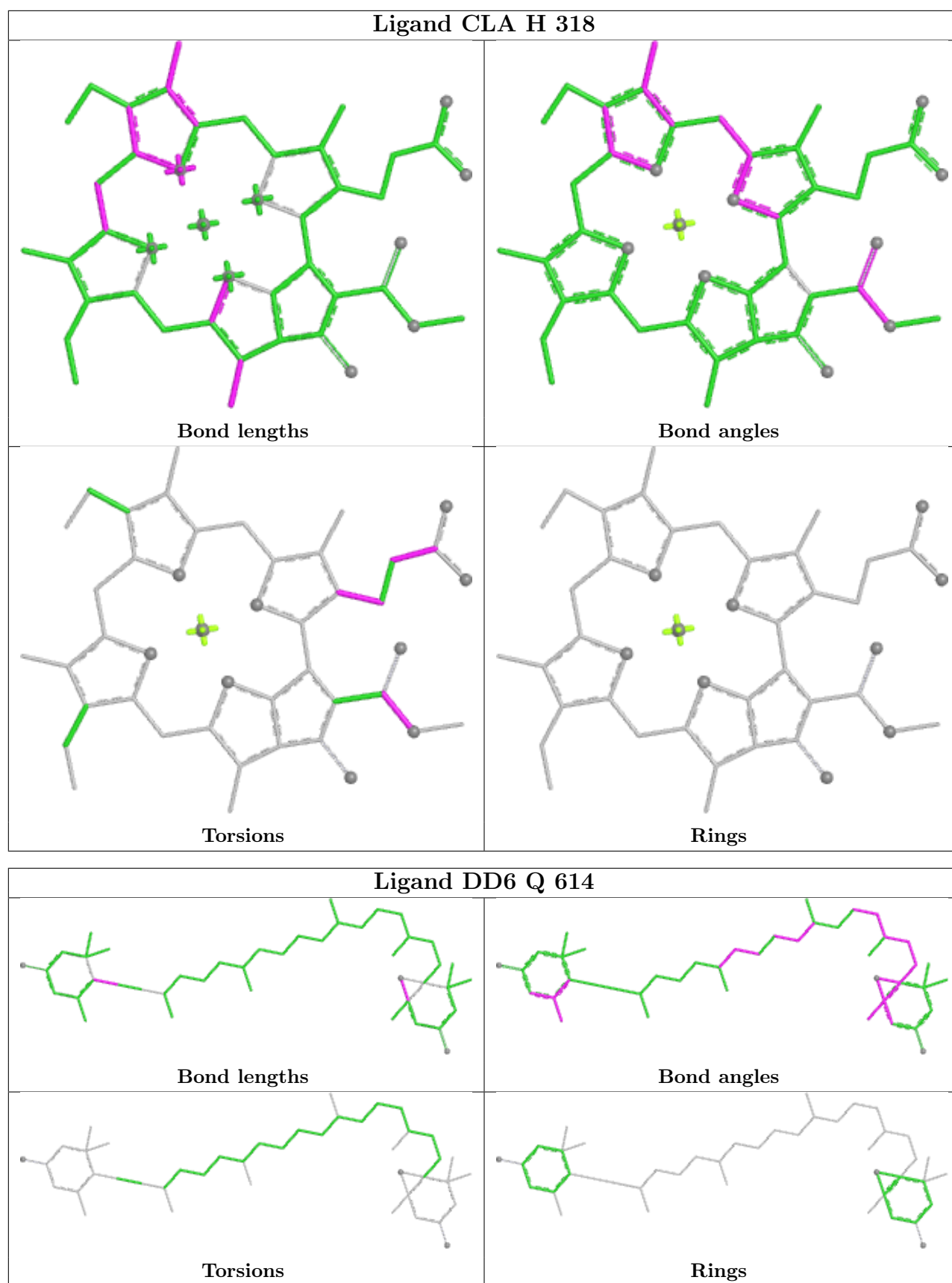


## Ligand CLA N 610

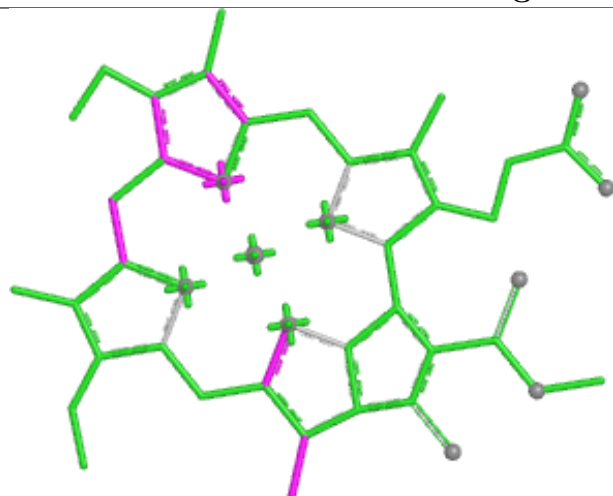


## Ligand CLA S 609

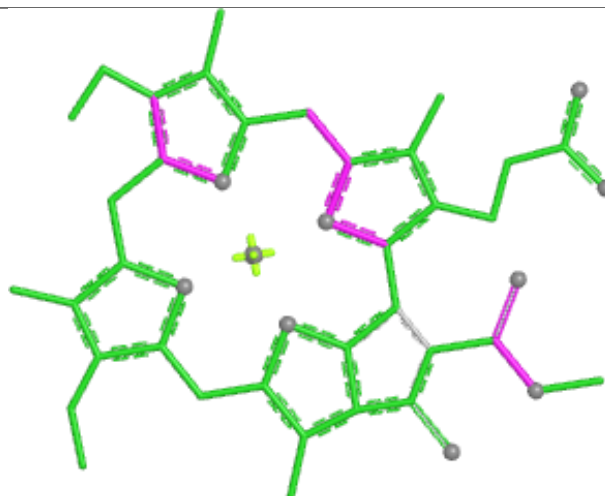




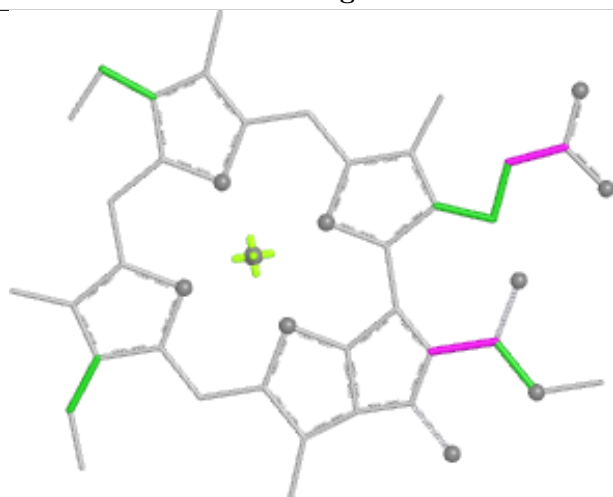
## Ligand CLA N 609



Bond lengths



Bond angles

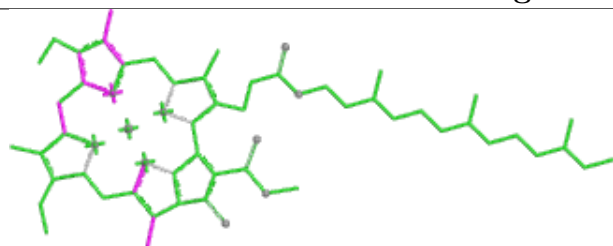


Torsions

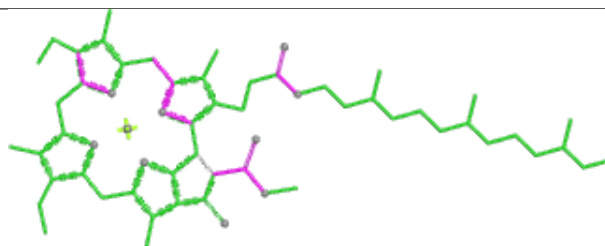


Rings

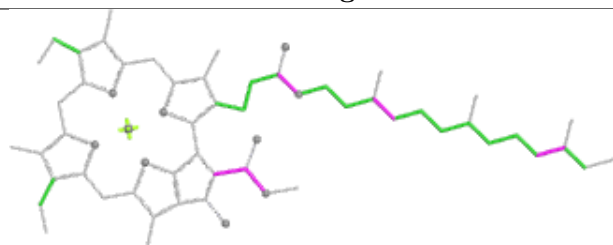
## Ligand CLA A 835



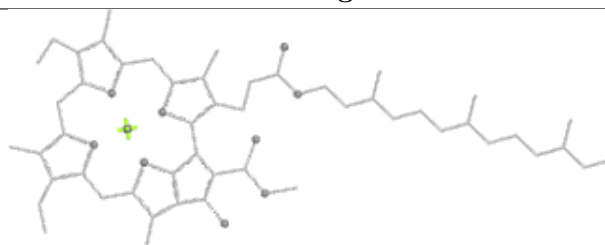
Bond lengths



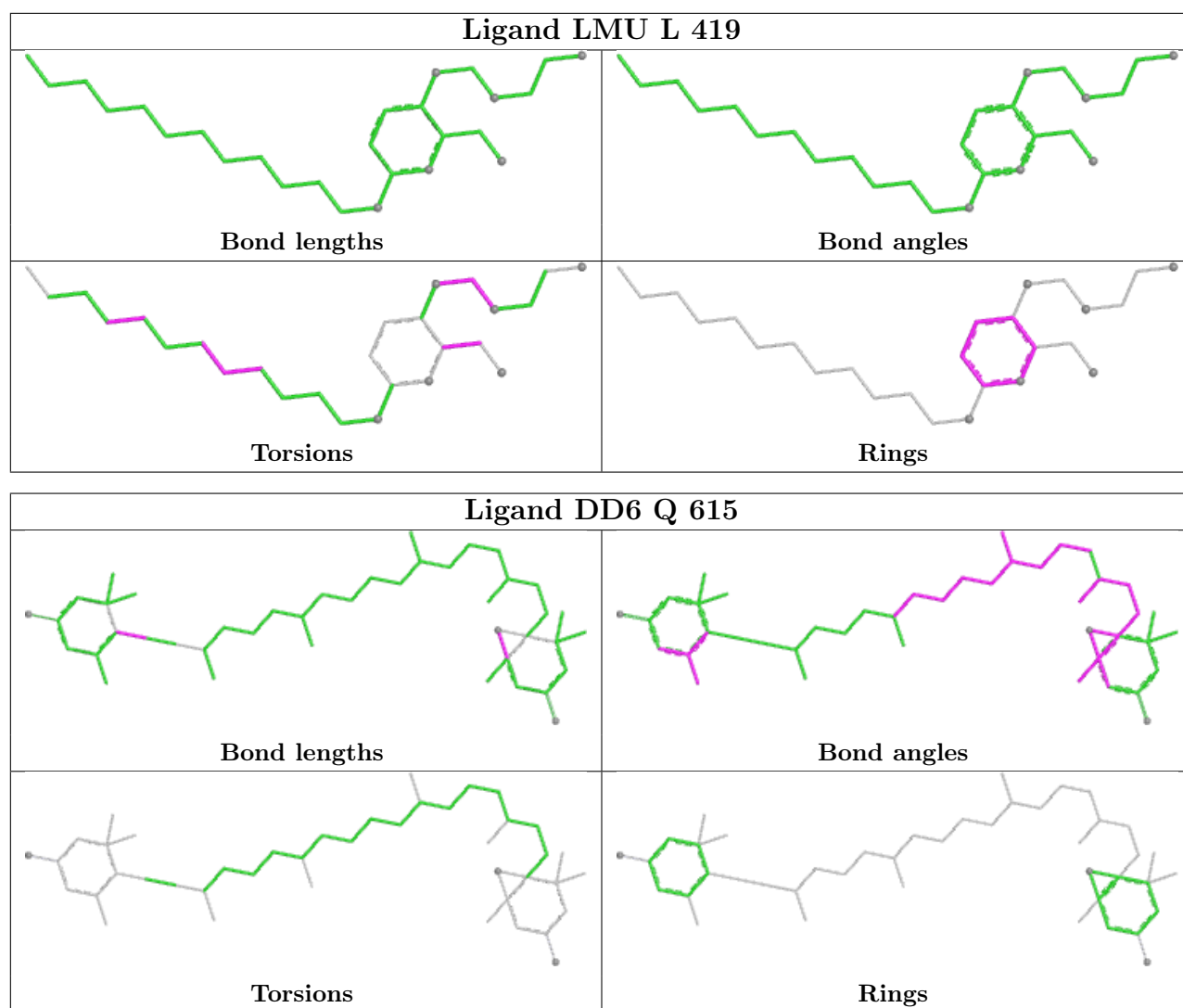
Bond angles



Torsions

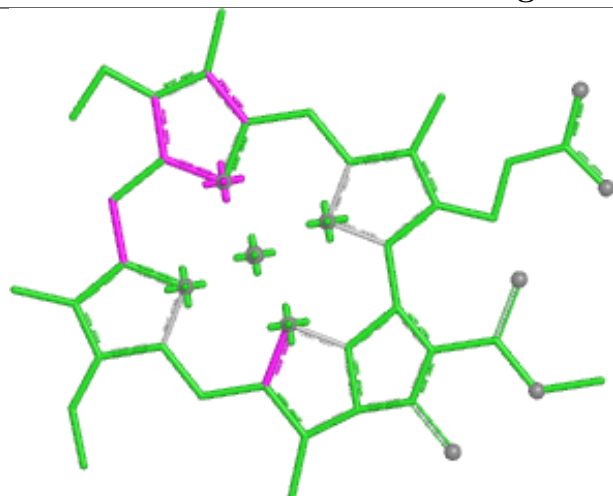


Rings

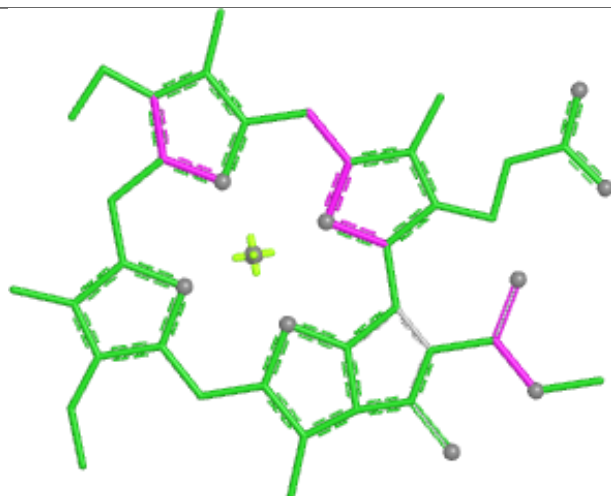




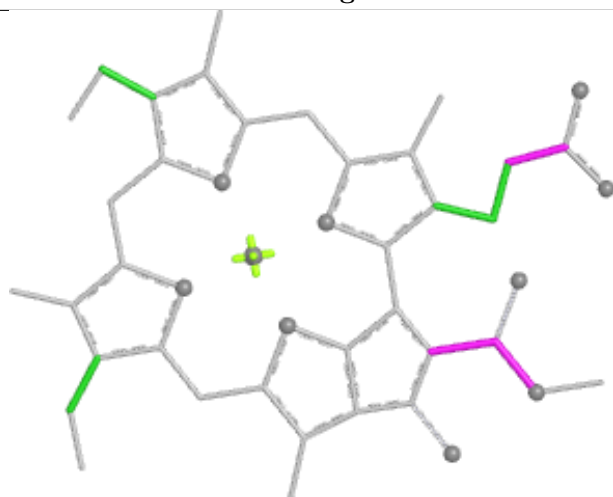
## Ligand CLA S 601



Bond lengths



Bond angles

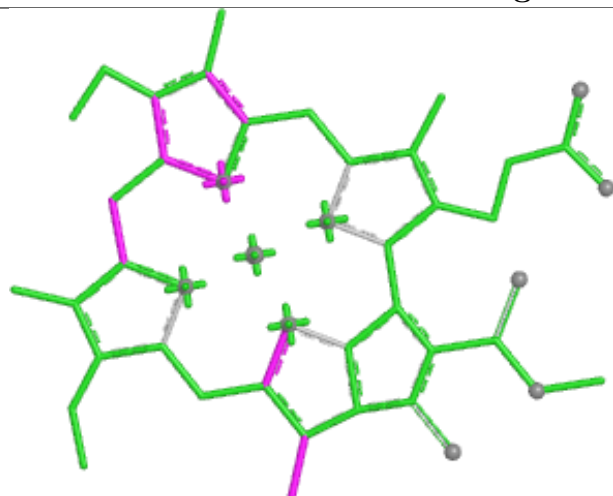


Torsions

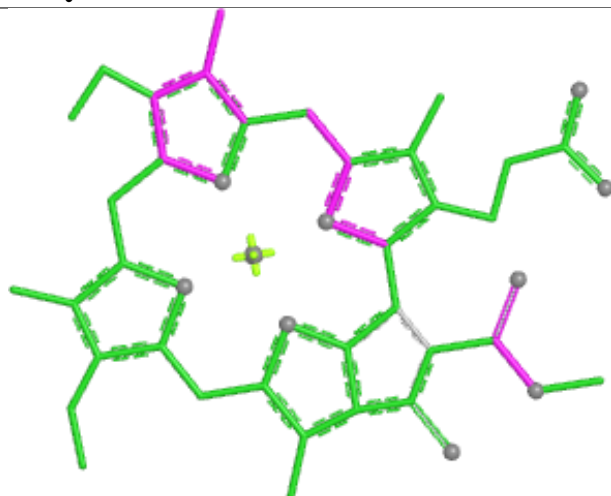


Rings

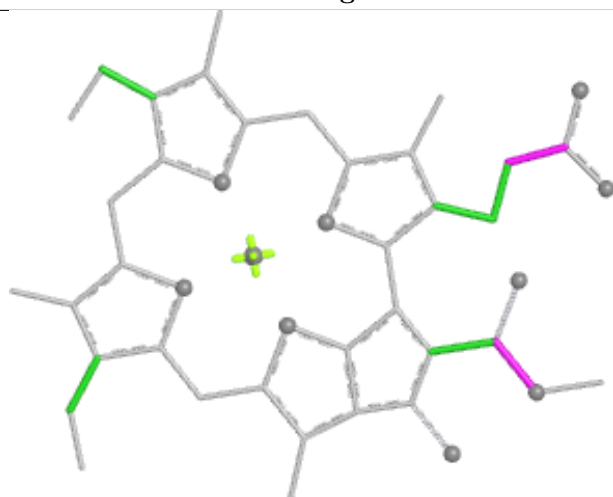
## Ligand CLA Q 603



Bond lengths



Bond angles

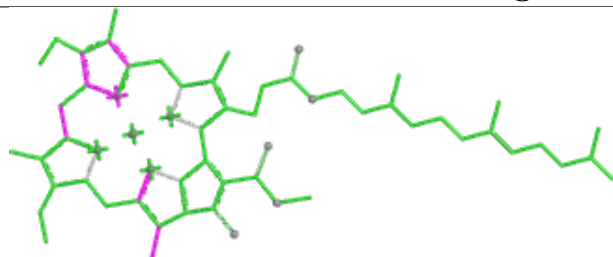


Torsions

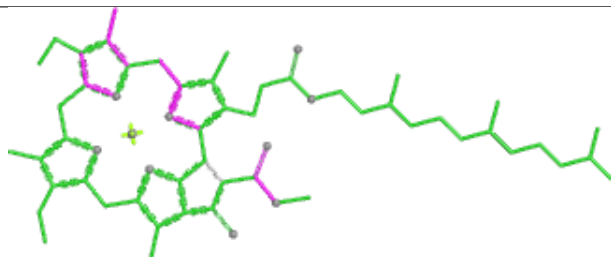


Rings

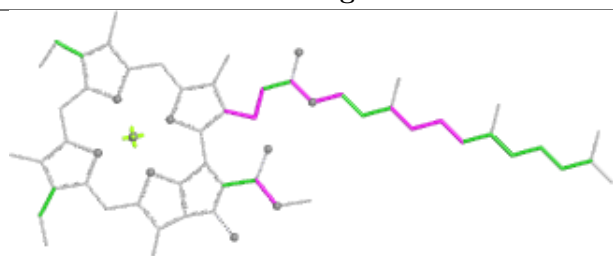
## Ligand CLA R 602



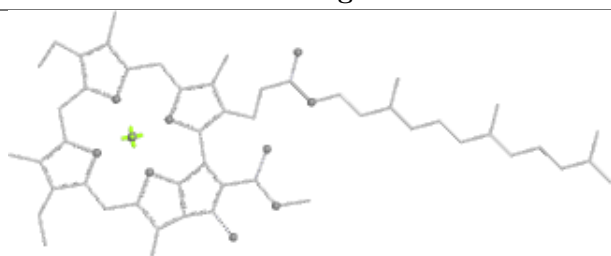
Bond lengths



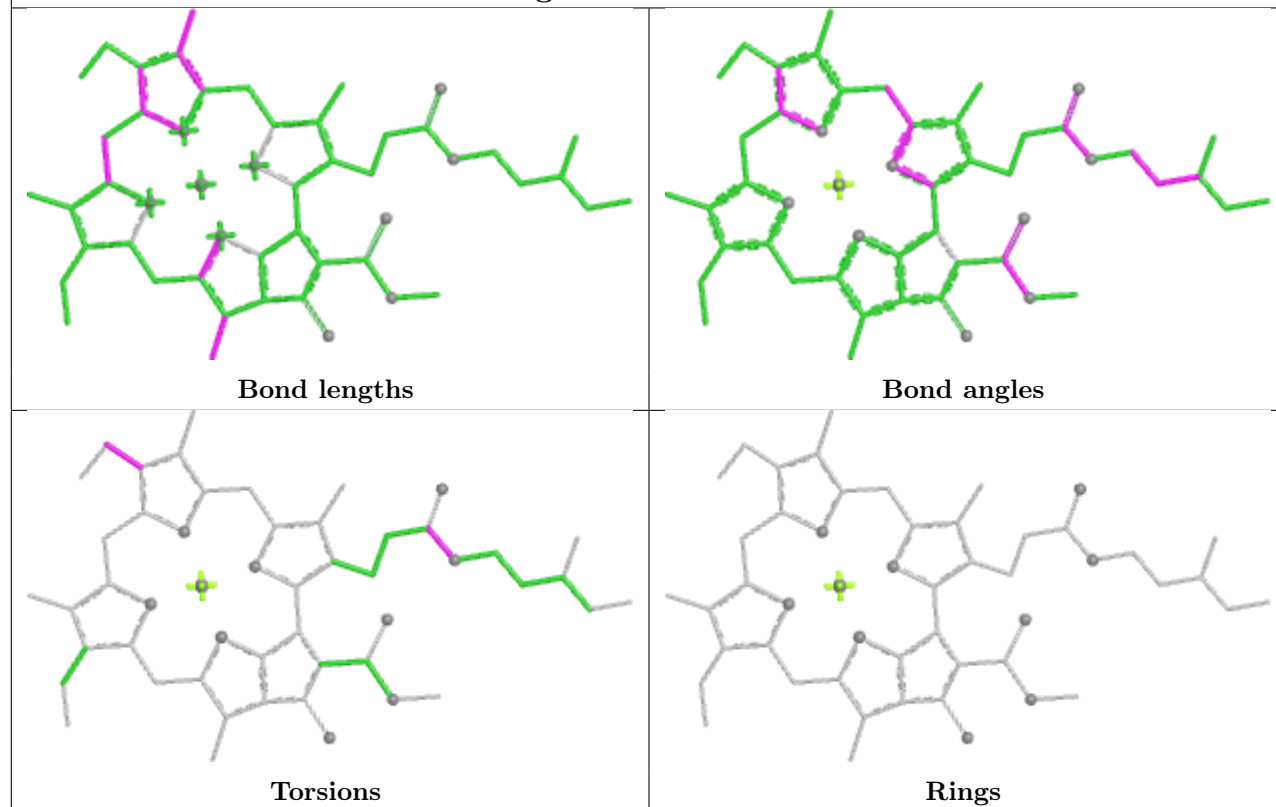
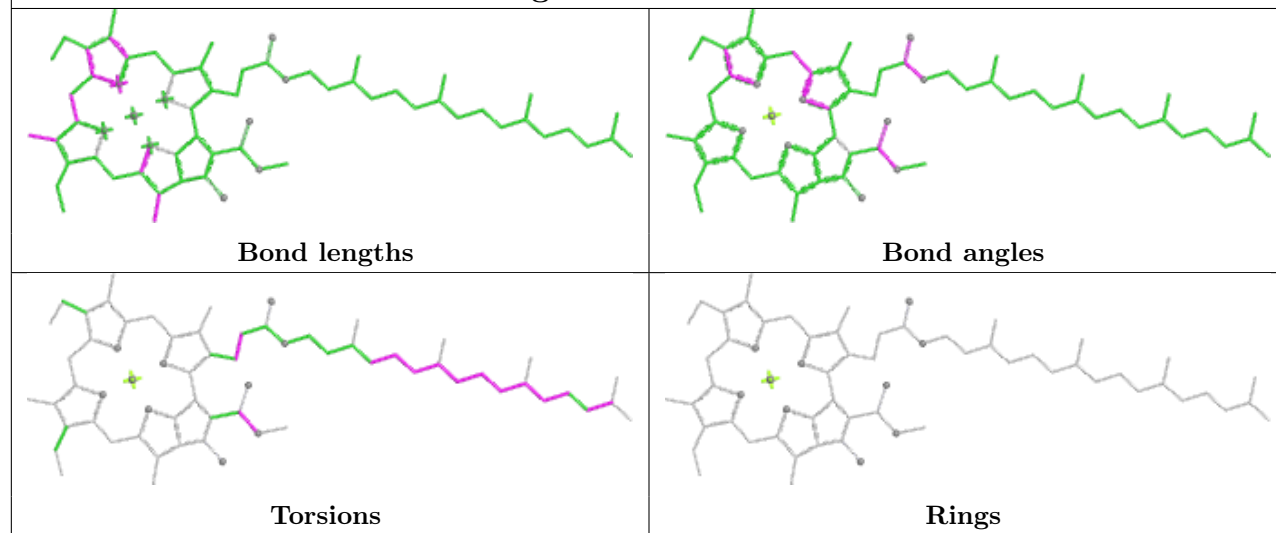
Bond angles

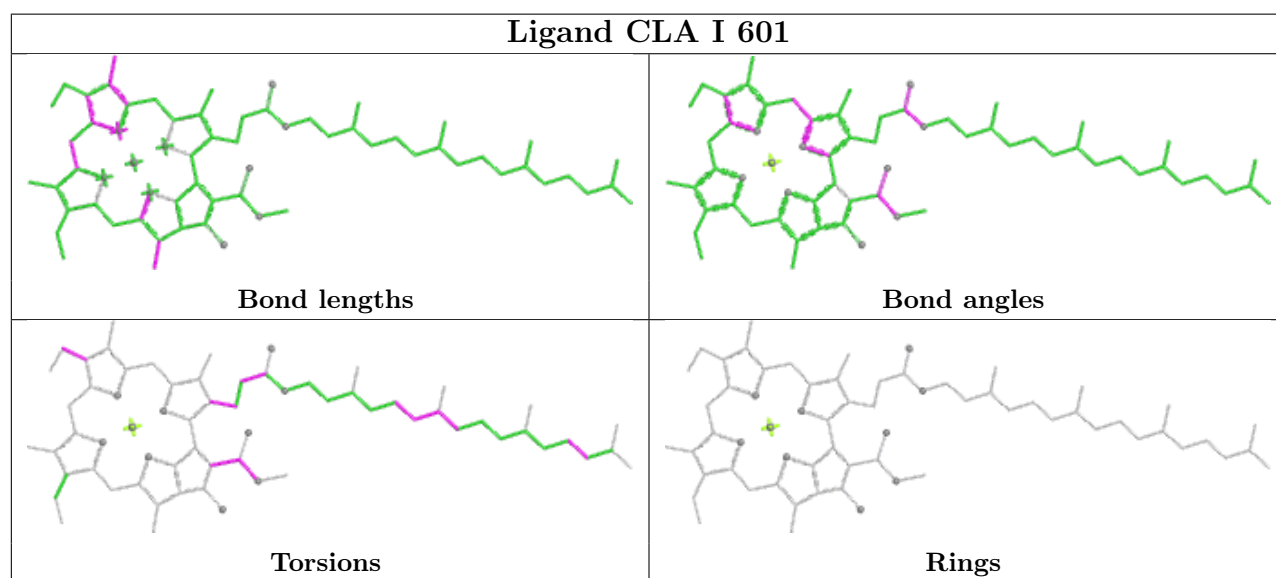
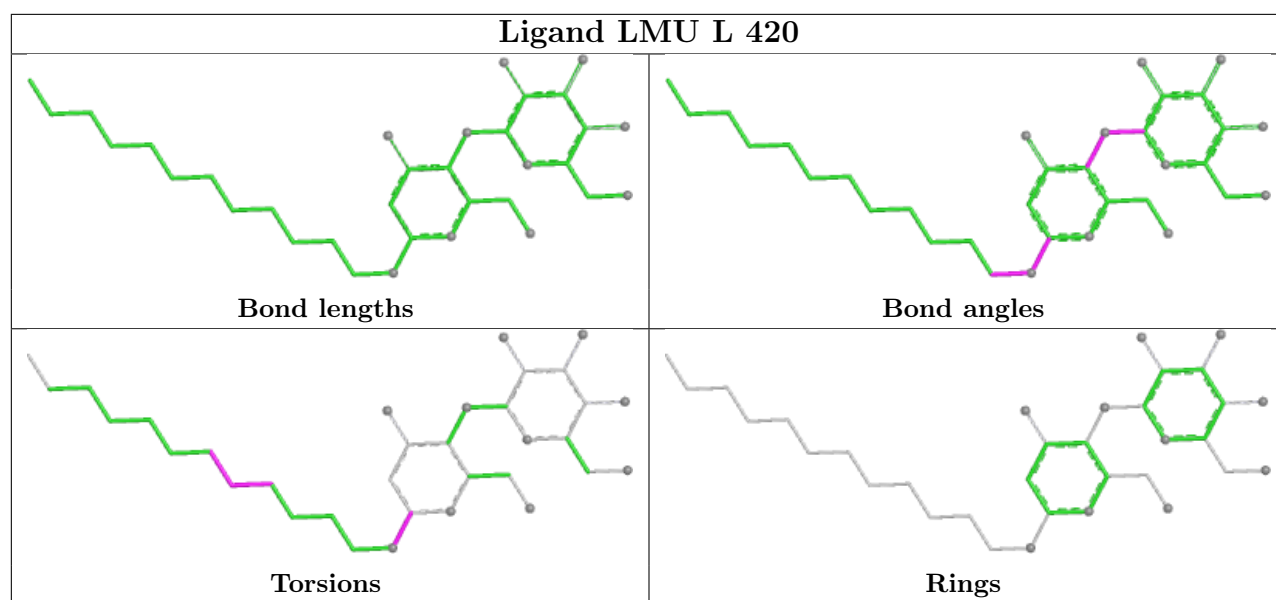


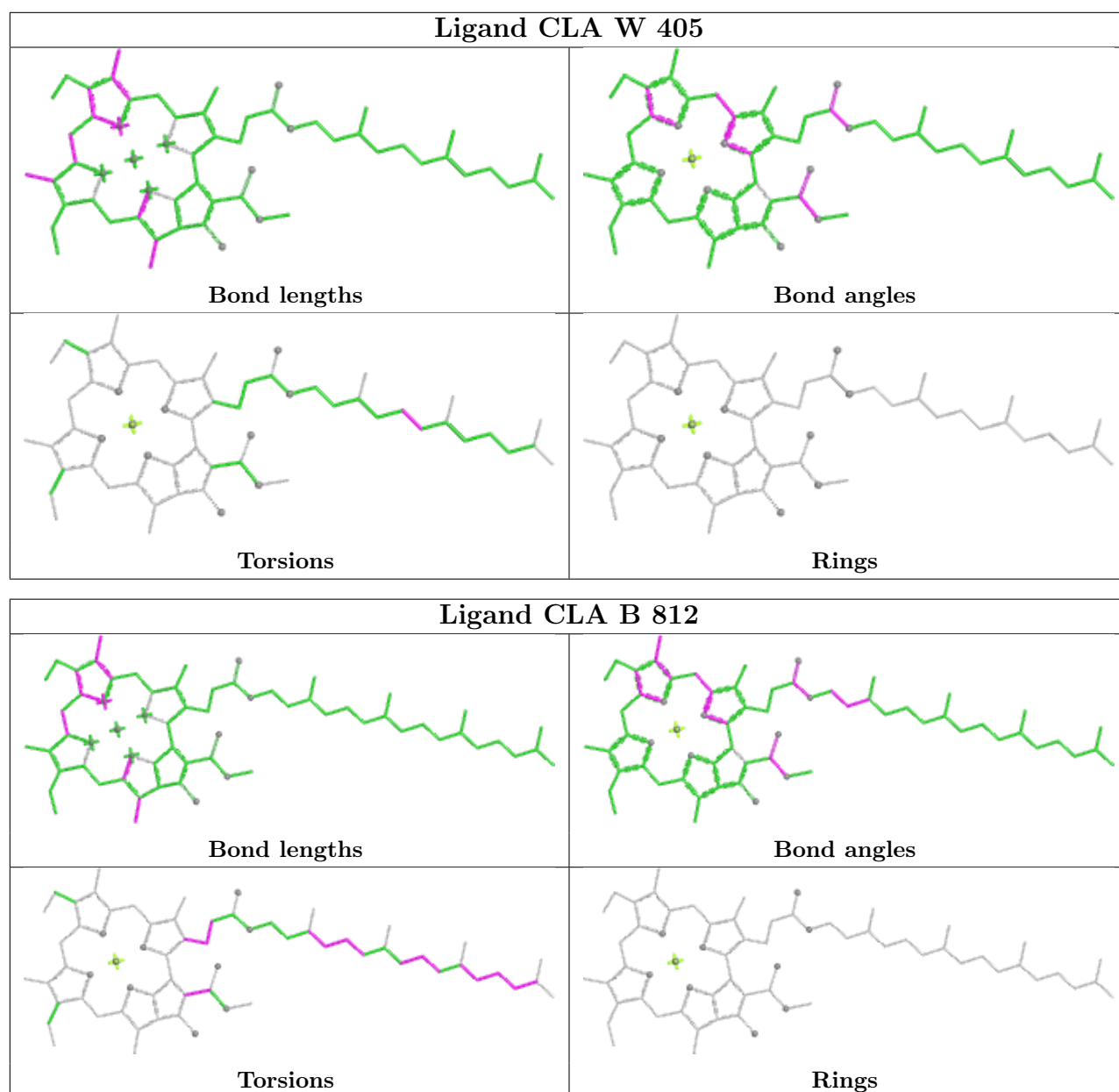
Torsions

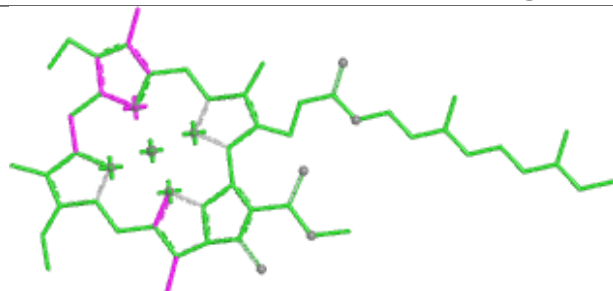


Rings

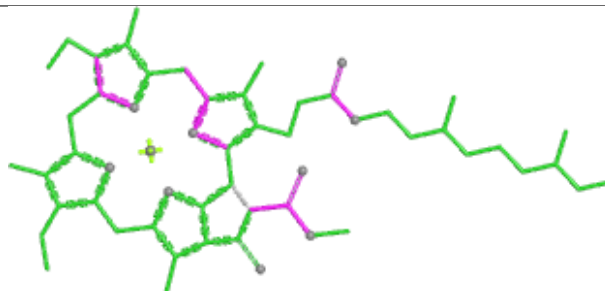
**Ligand CLA S 615****Ligand CLA O 313**



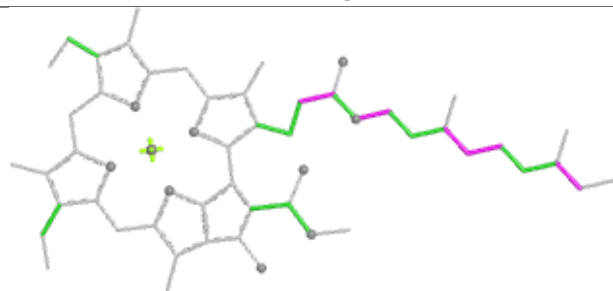


**Ligand CLA I 603**

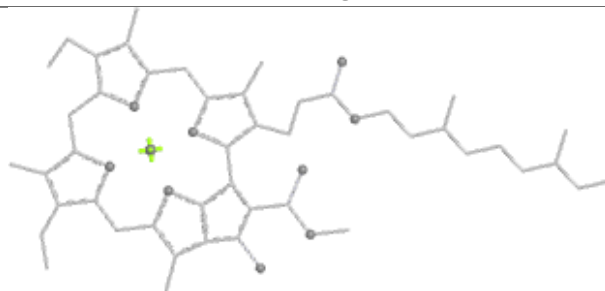
Bond lengths



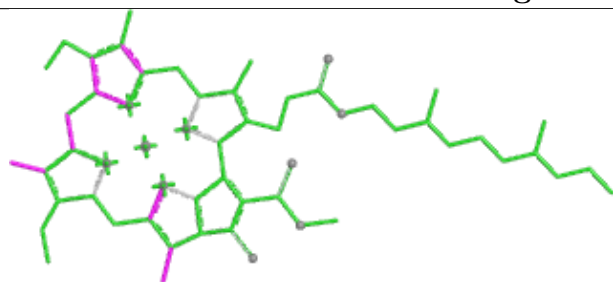
Bond angles



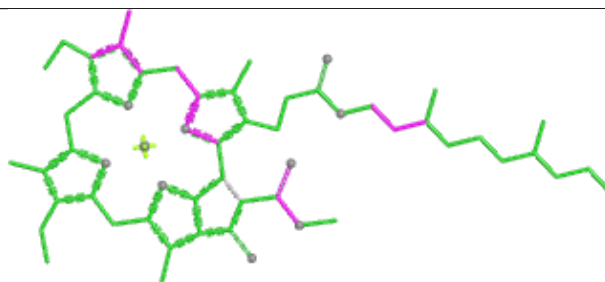
Torsions



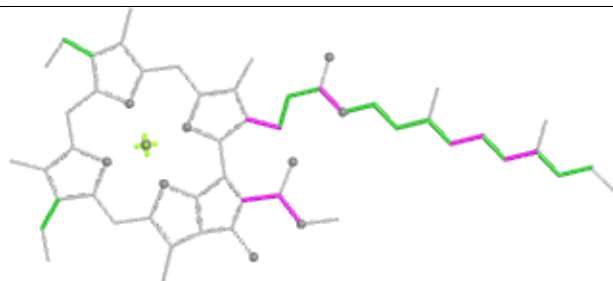
Rings

**Ligand CLA V 603**

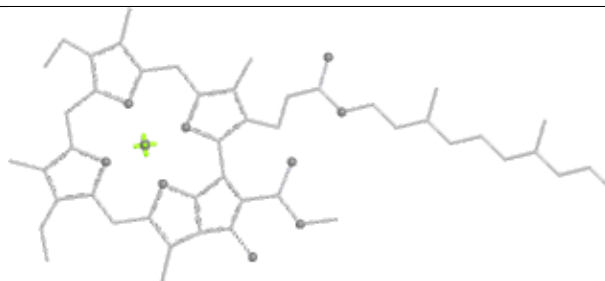
Bond lengths



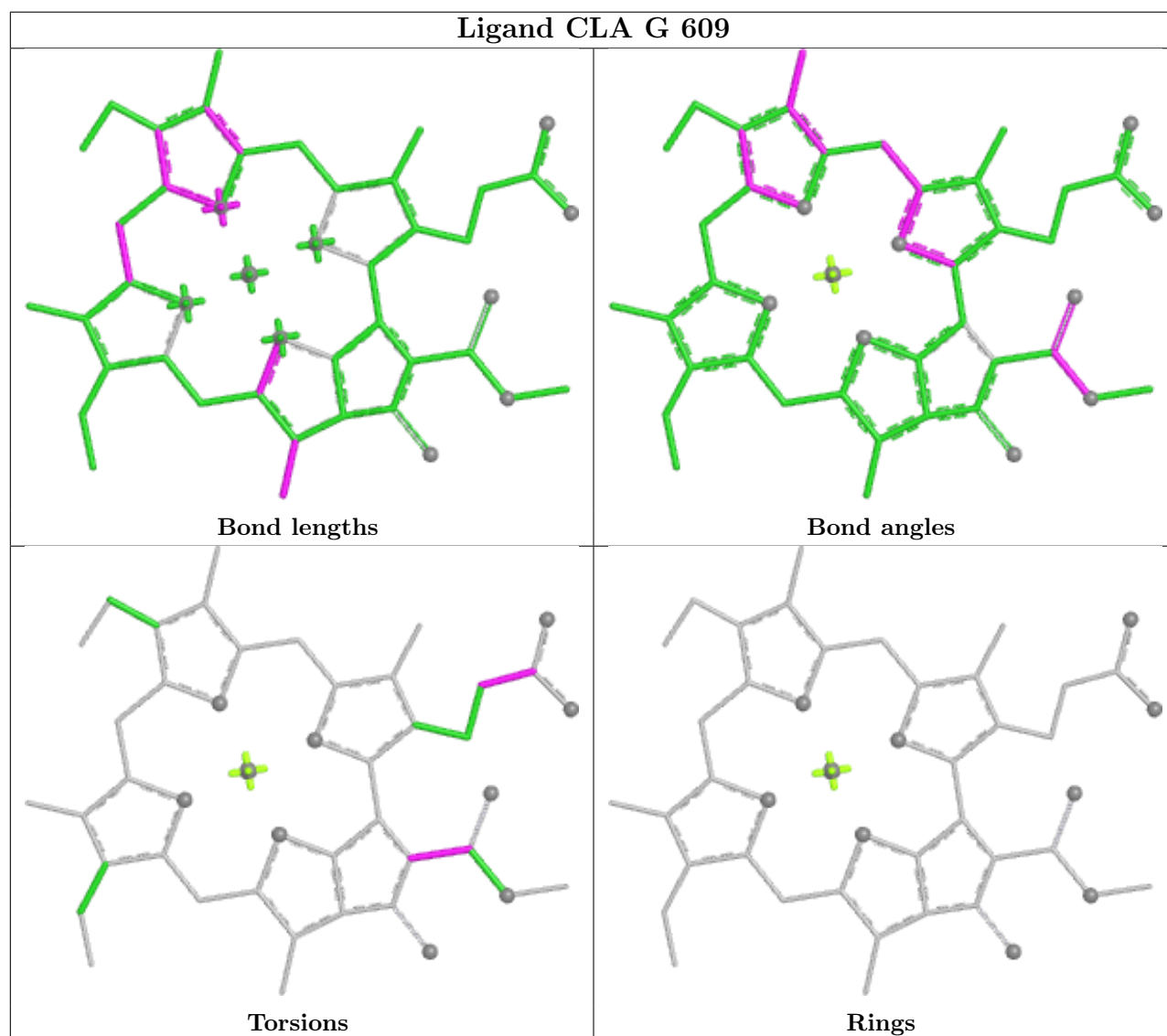
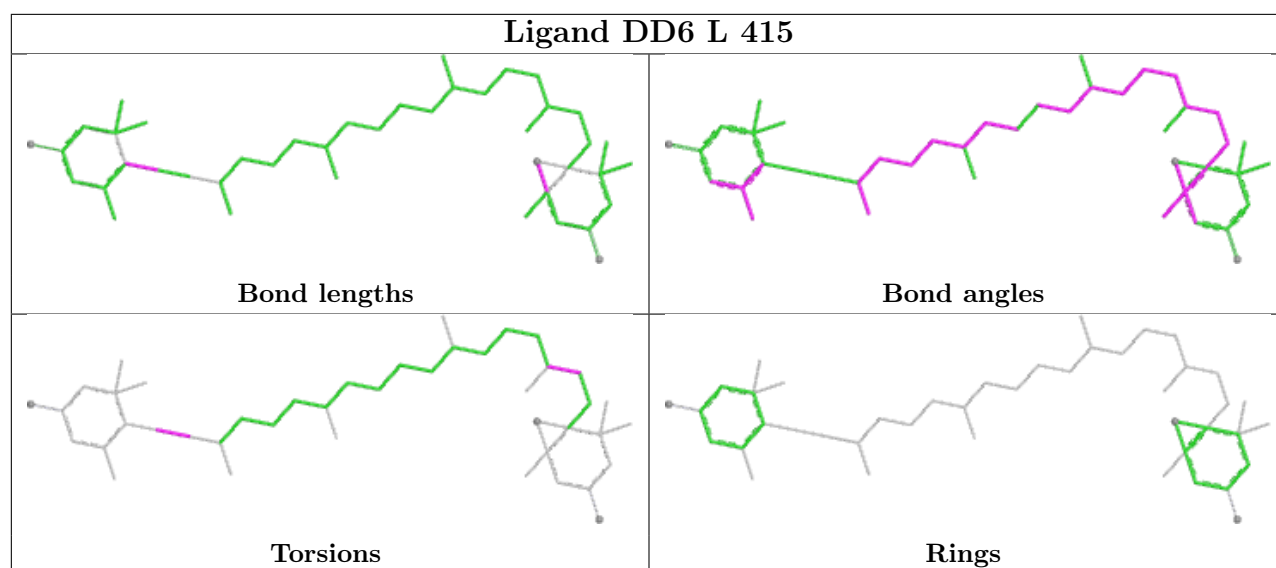
Bond angles

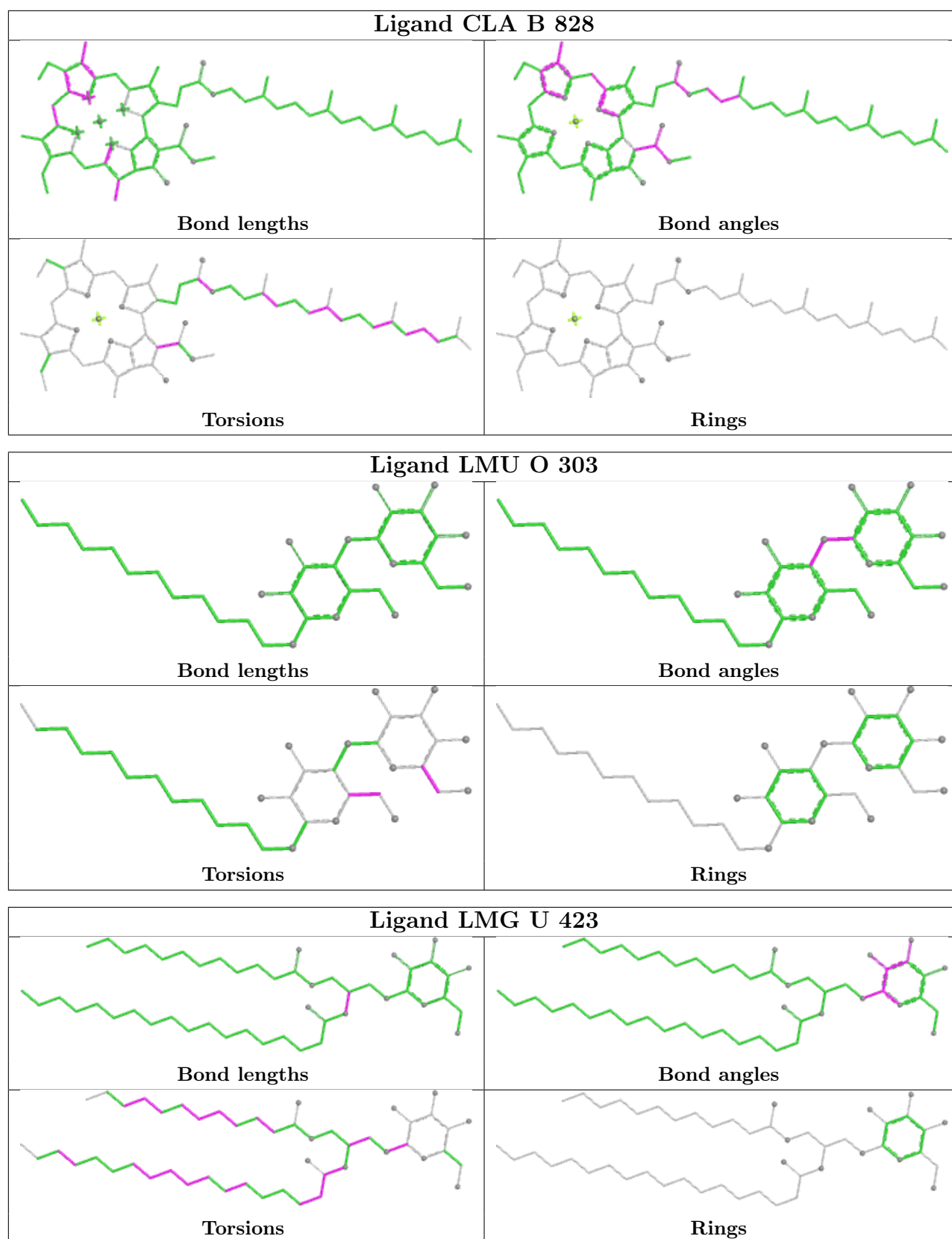


Torsions

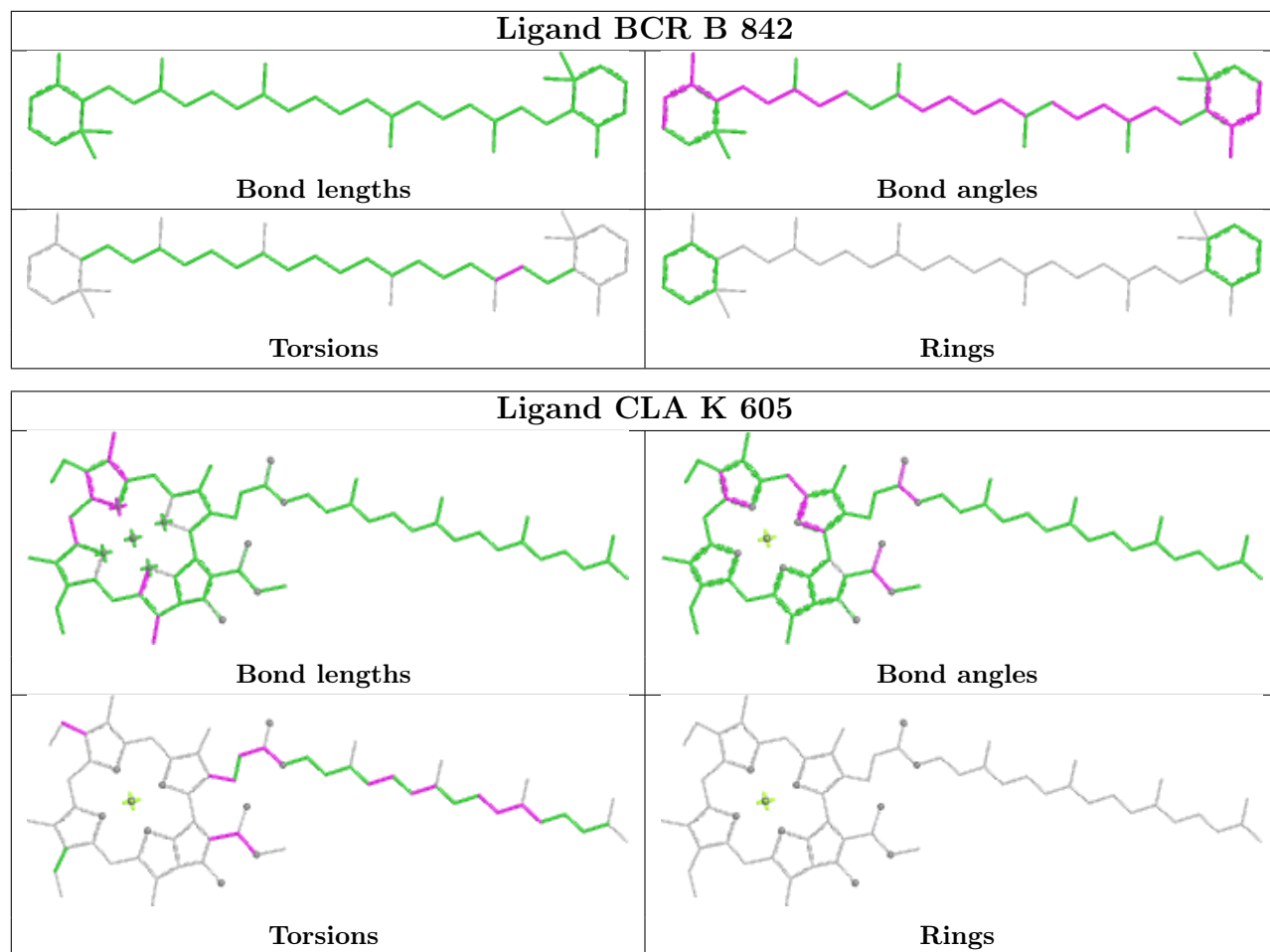


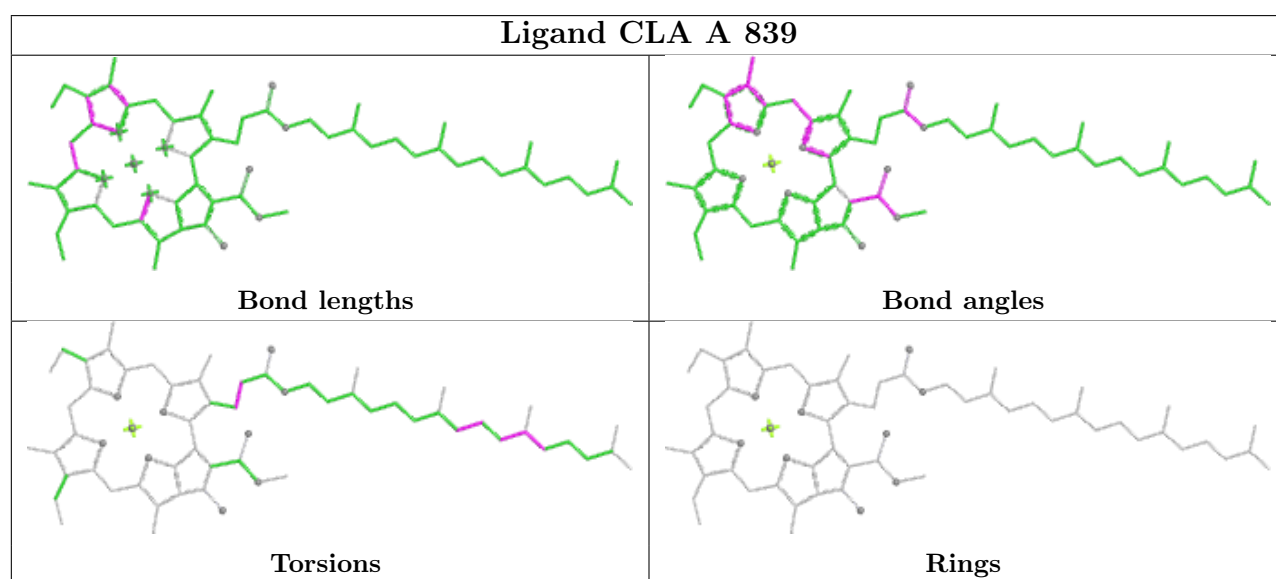
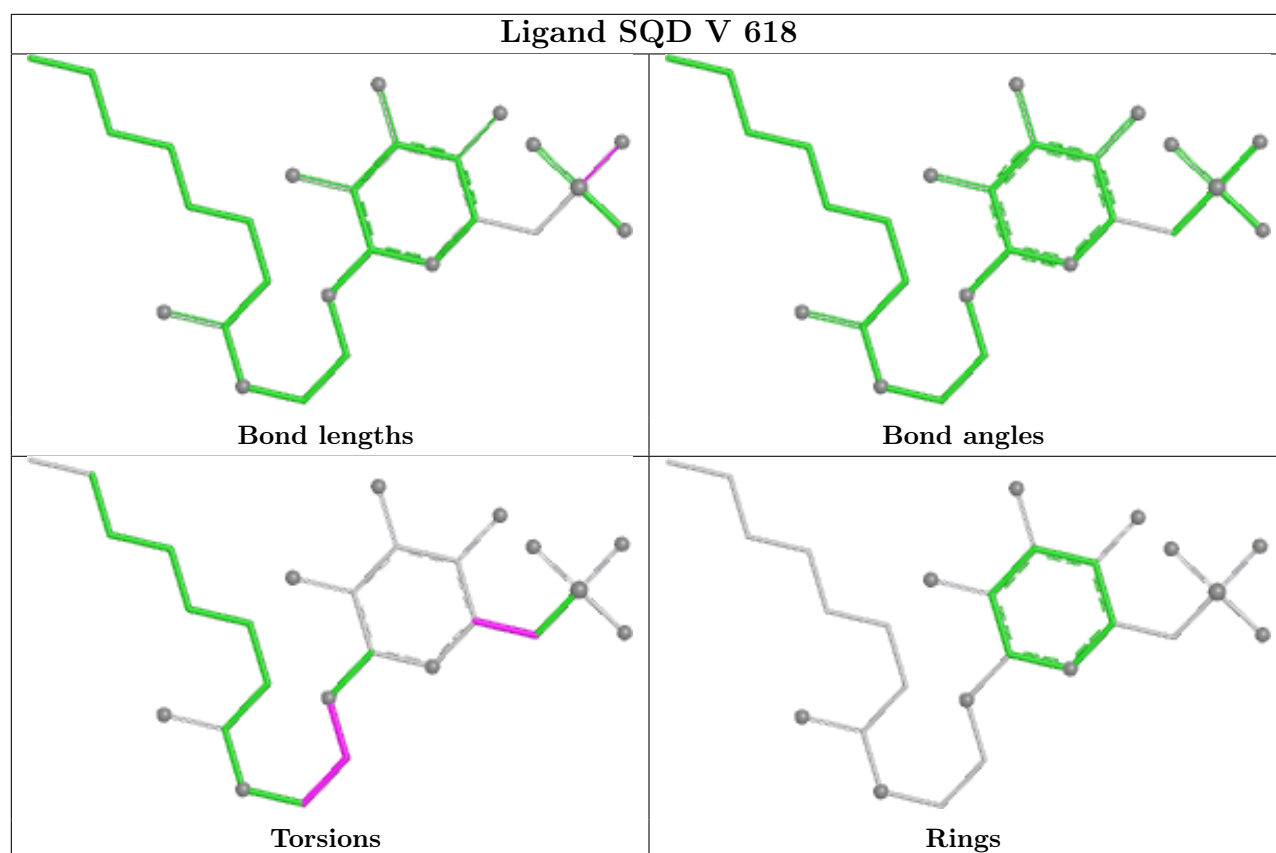
Rings

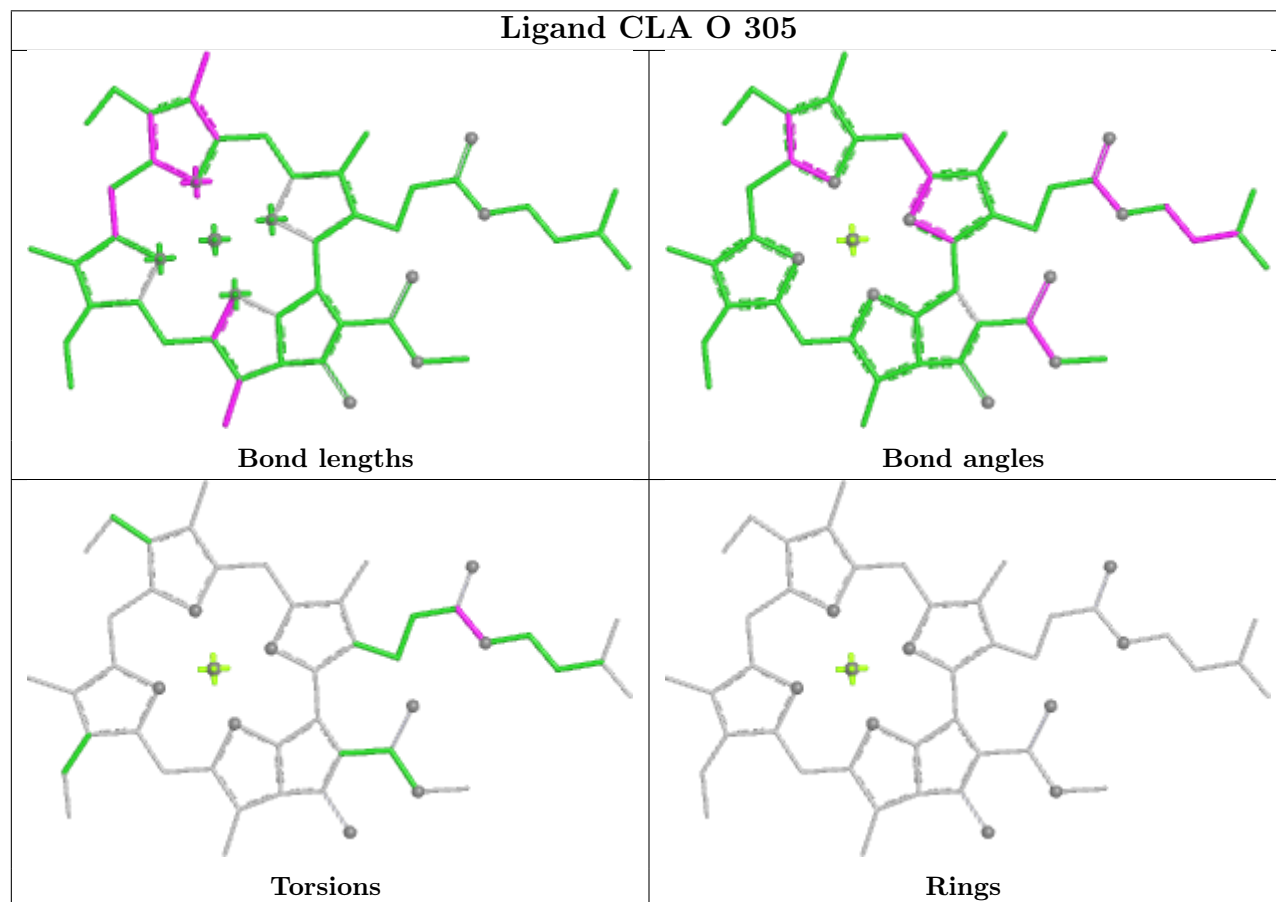
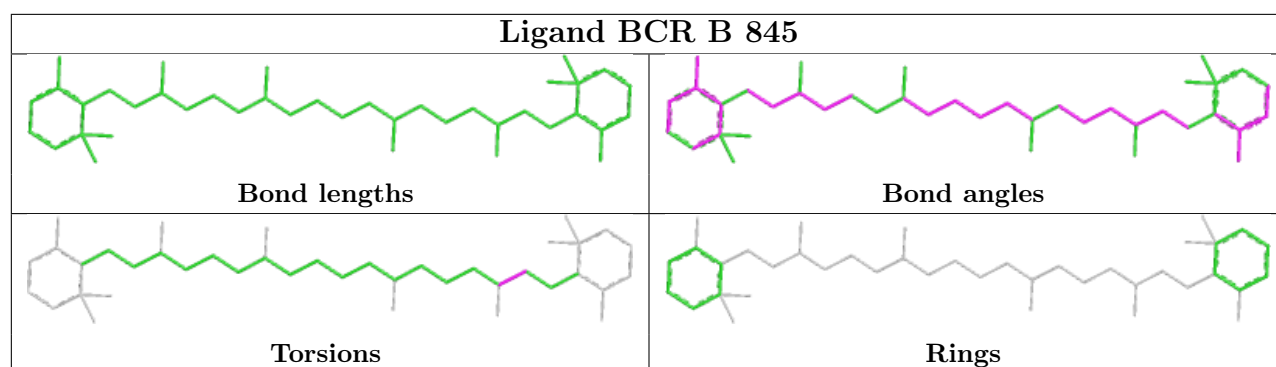




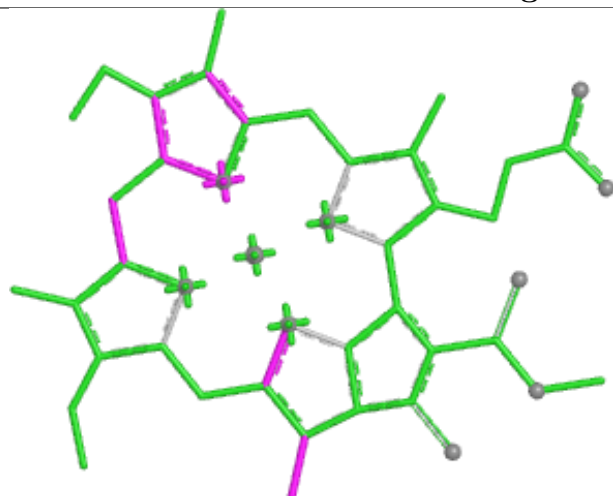




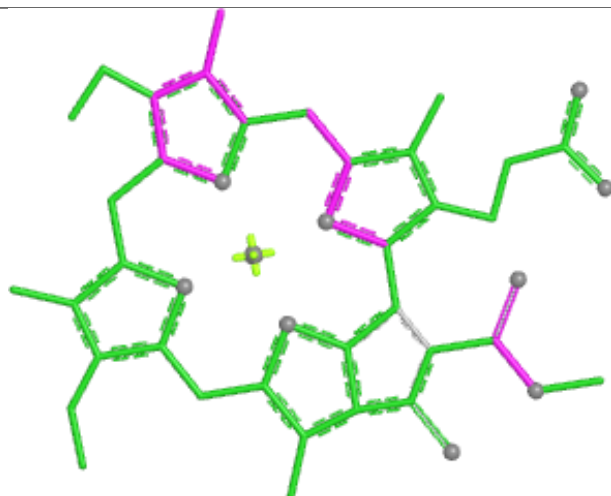




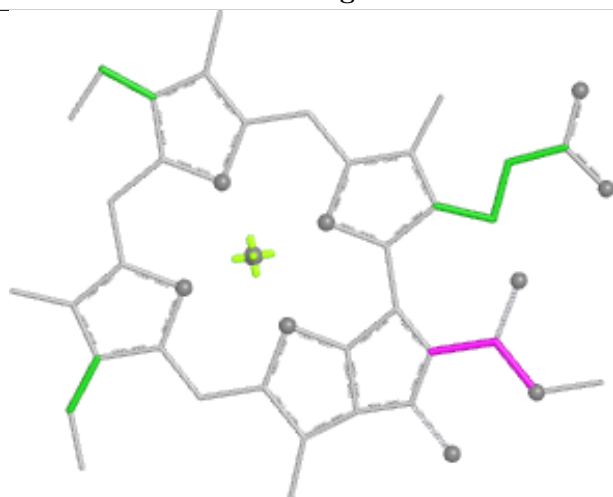
## Ligand CLA I 609



Bond lengths



Bond angles

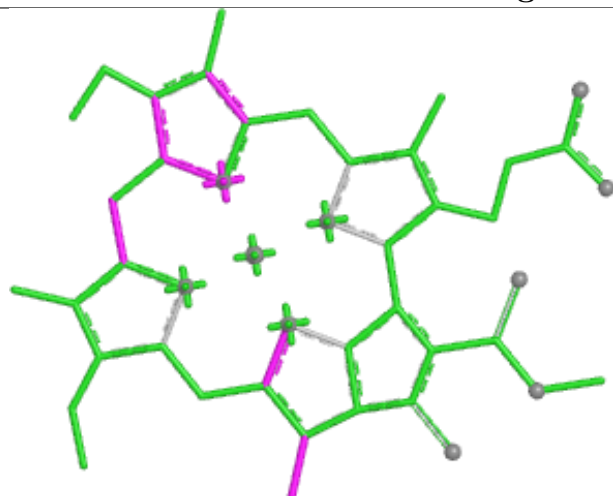


Torsions

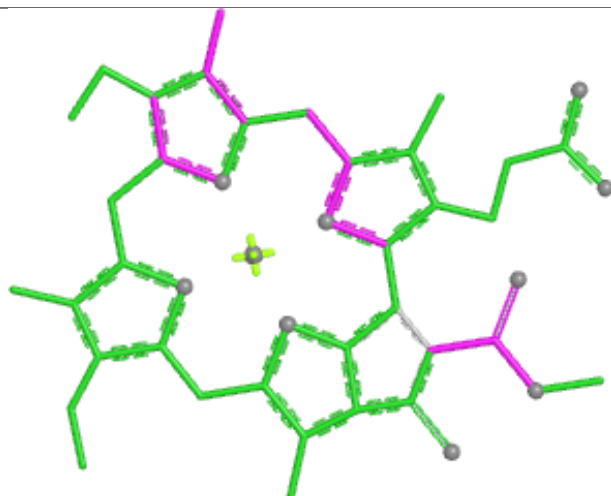


Rings

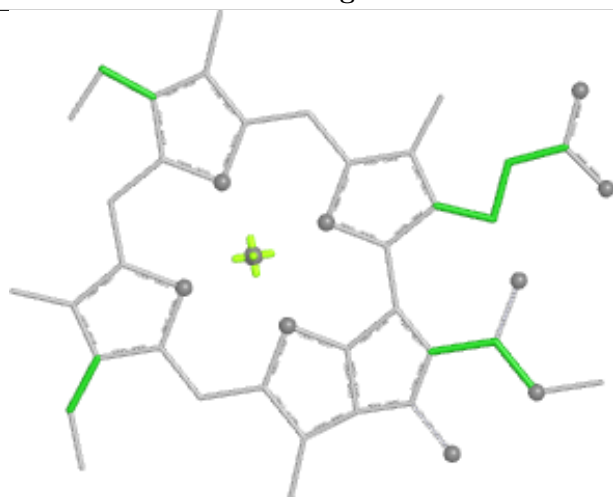
## Ligand CLA S 614



Bond lengths



Bond angles

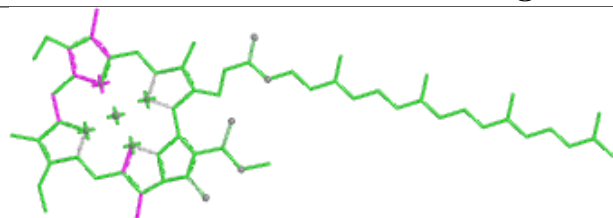


Torsions

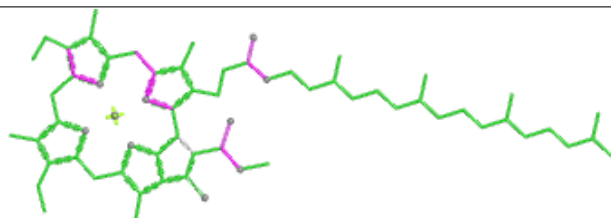


Rings

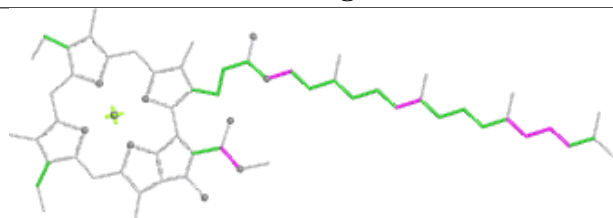
## Ligand CLA L 406



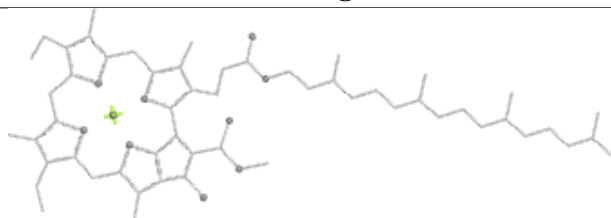
Bond lengths



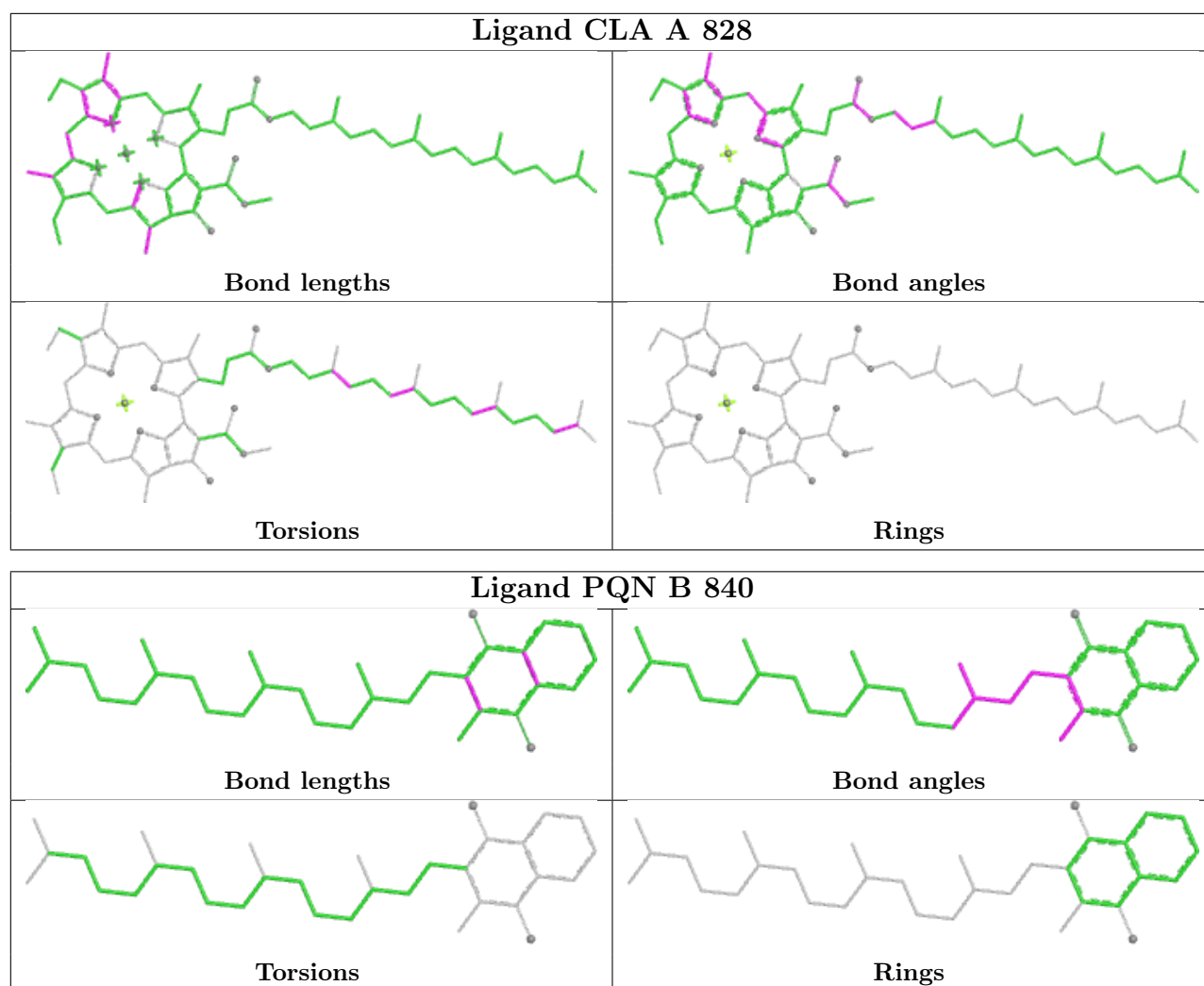
Bond angles



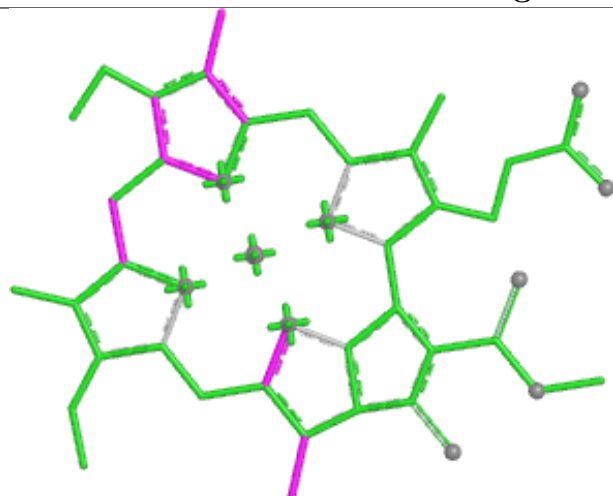
Torsions



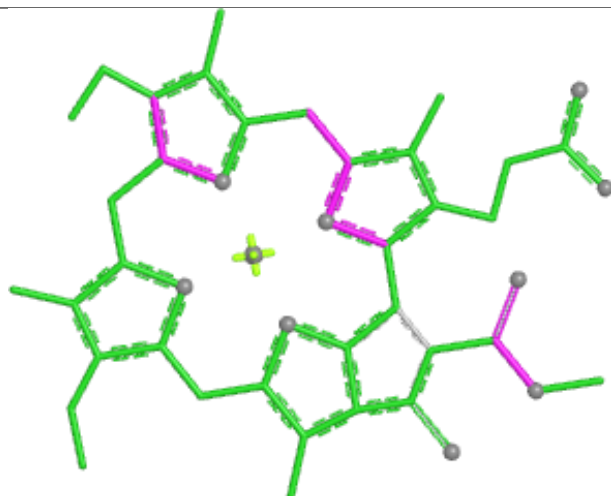
Rings



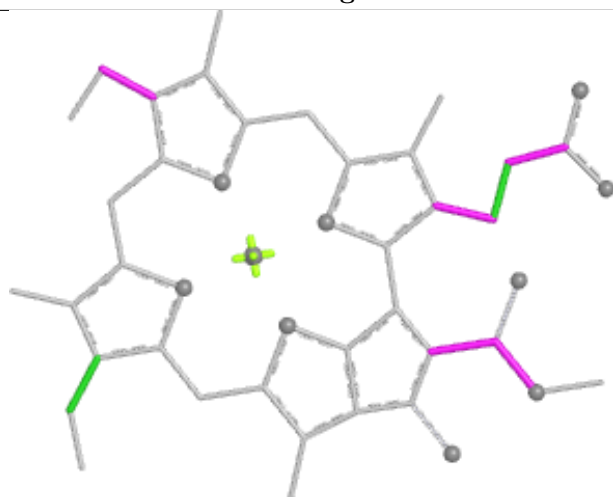
## Ligand CLA V 613



Bond lengths



Bond angles

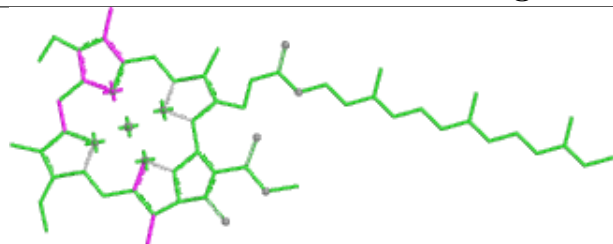


Torsions

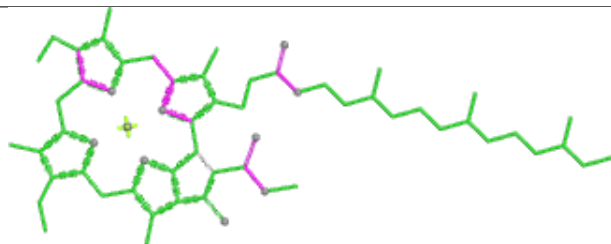


Rings

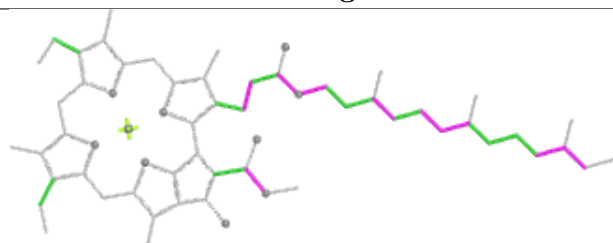
## Ligand CLA U 414



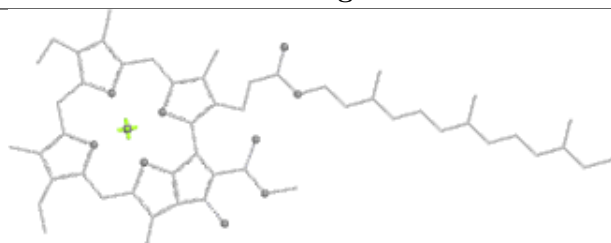
Bond lengths



Bond angles

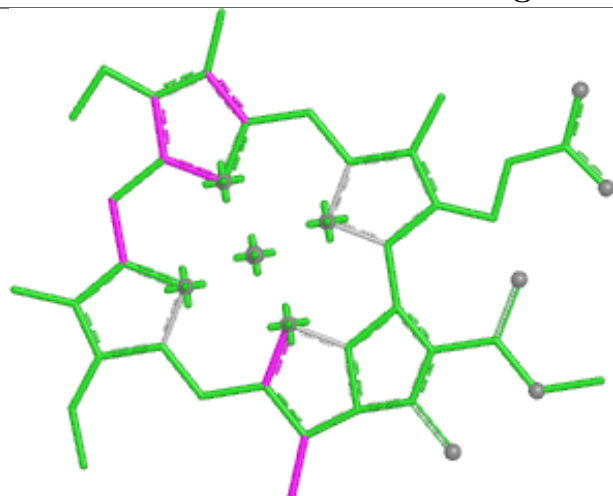


Torsions

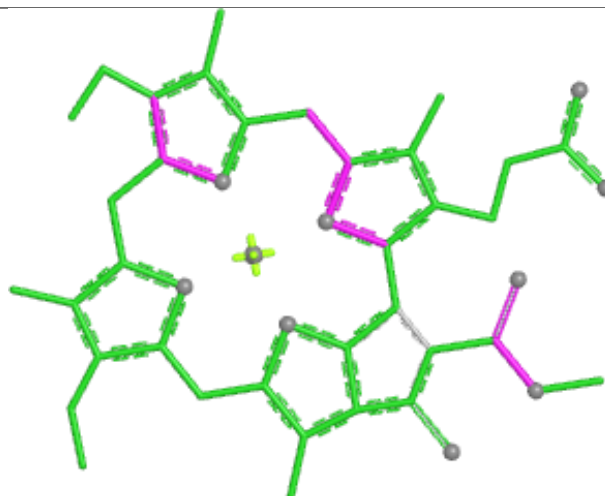


Rings

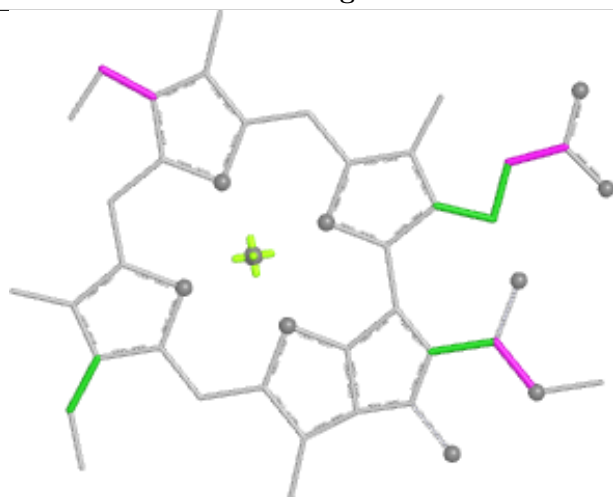
## Ligand CLA V 601



Bond lengths



Bond angles

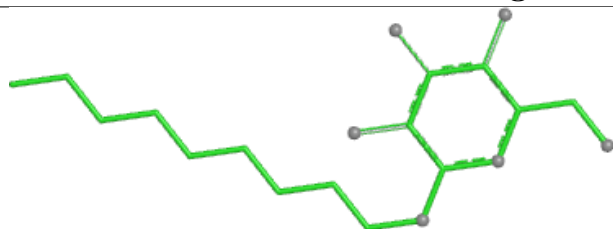


Torsions

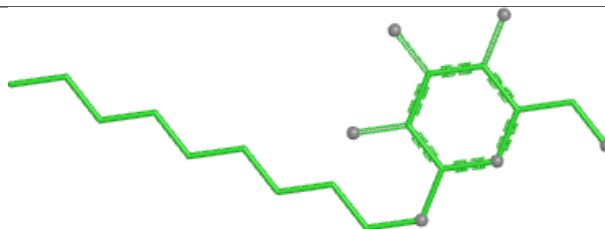


Rings

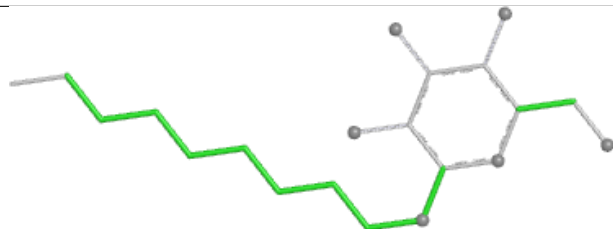
## Ligand LMU A 856



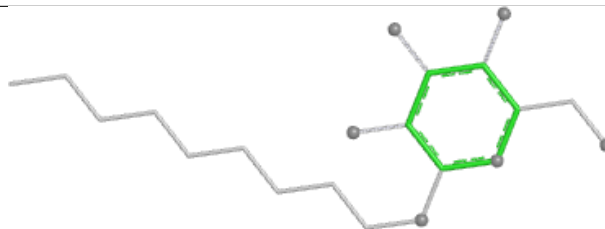
Bond lengths



Bond angles

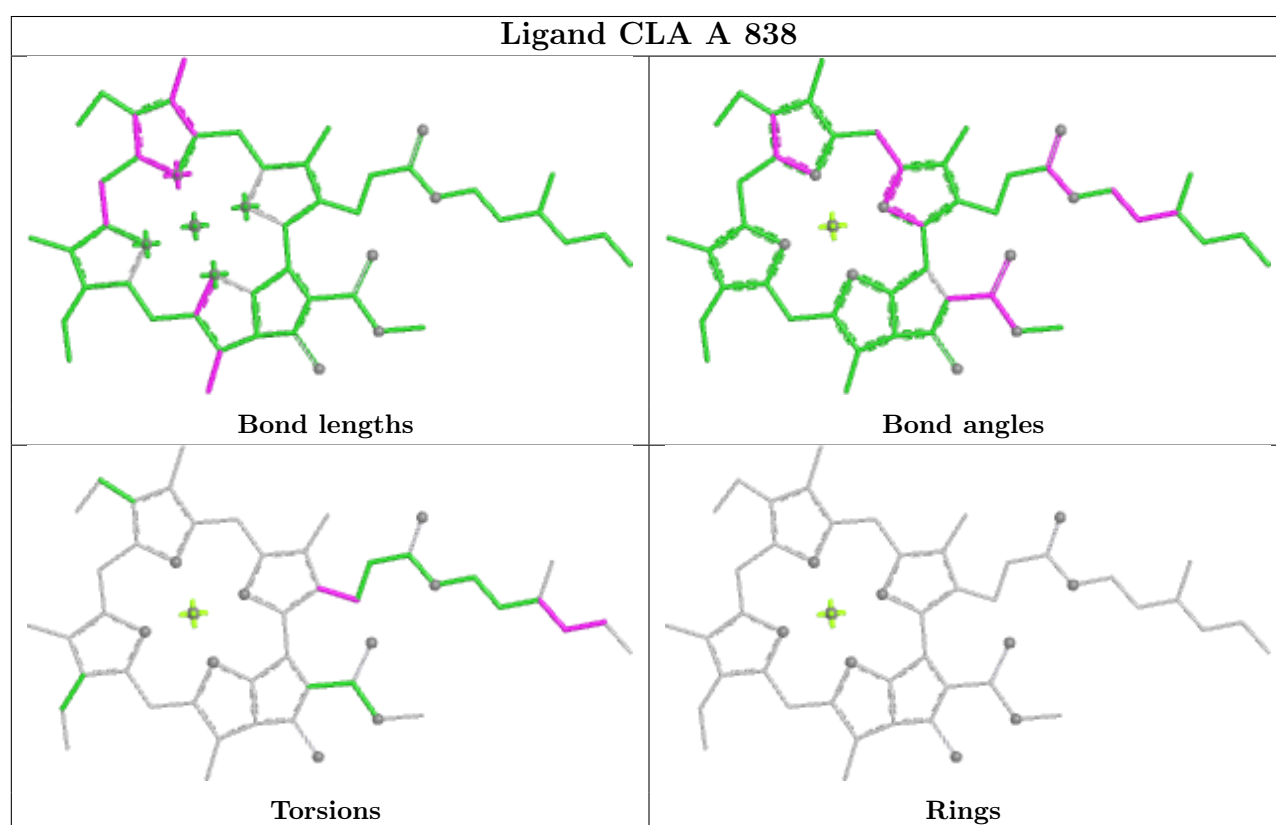
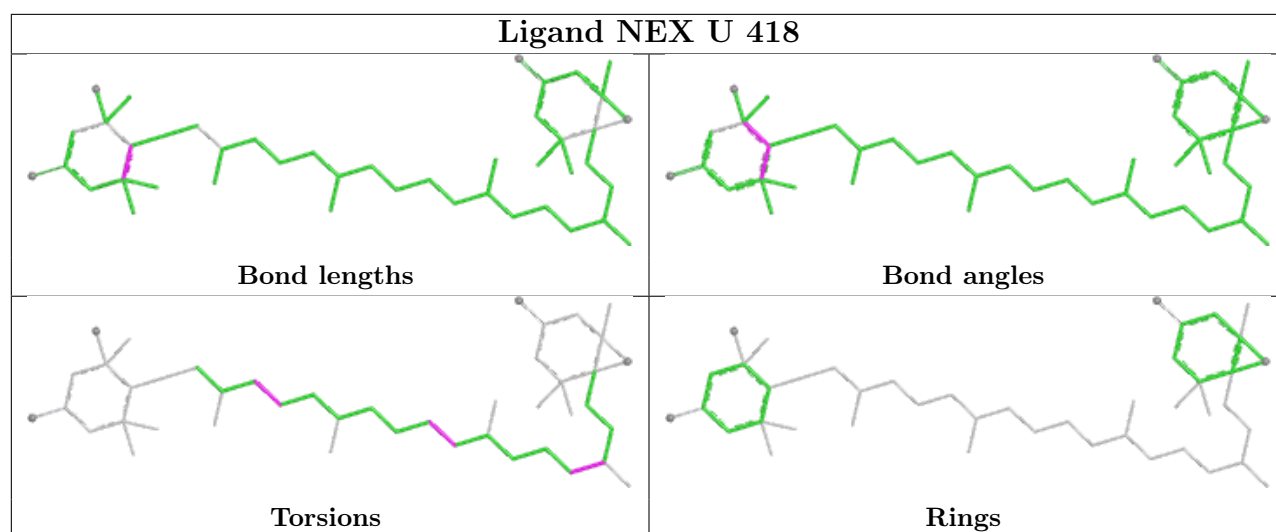


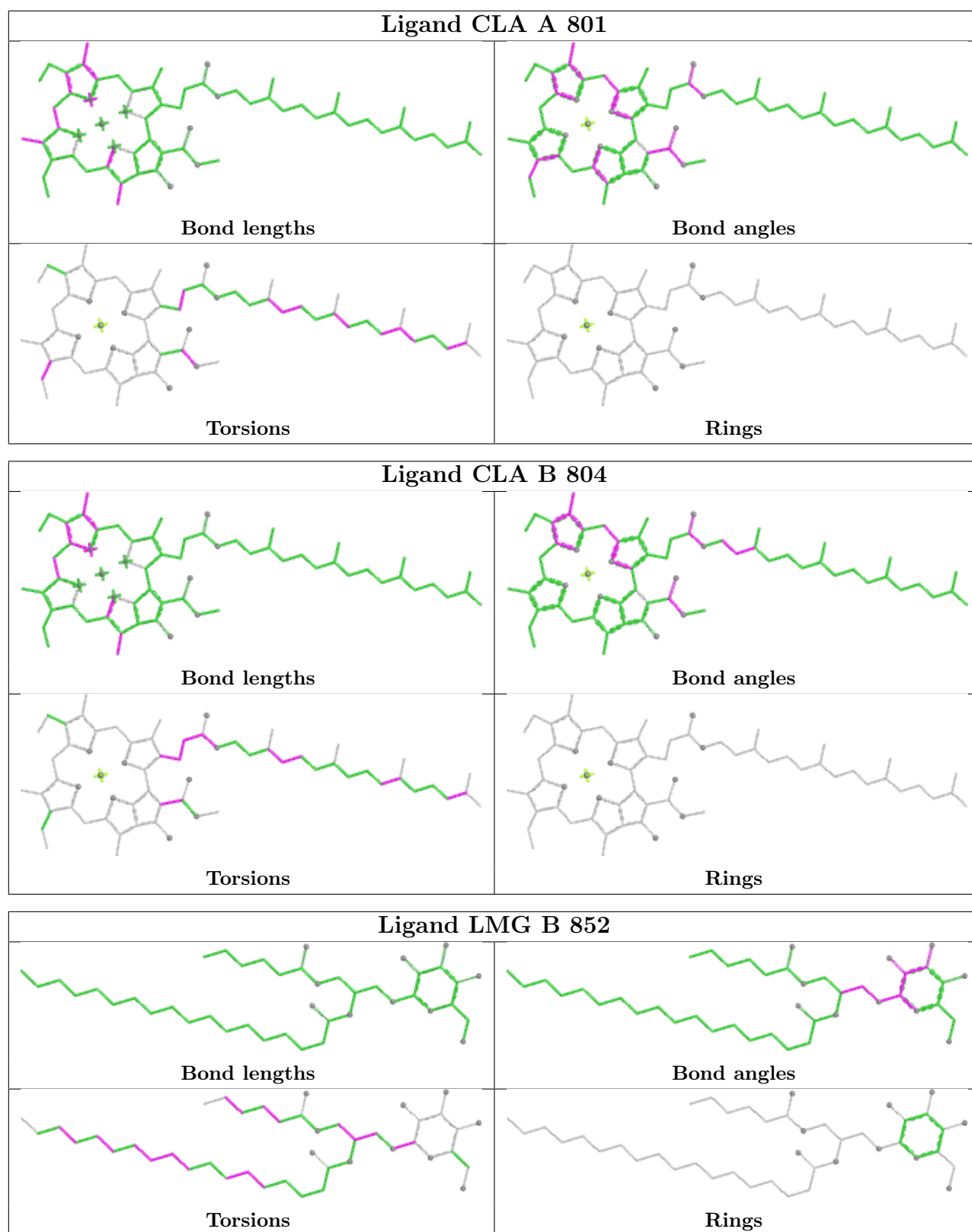
Torsions

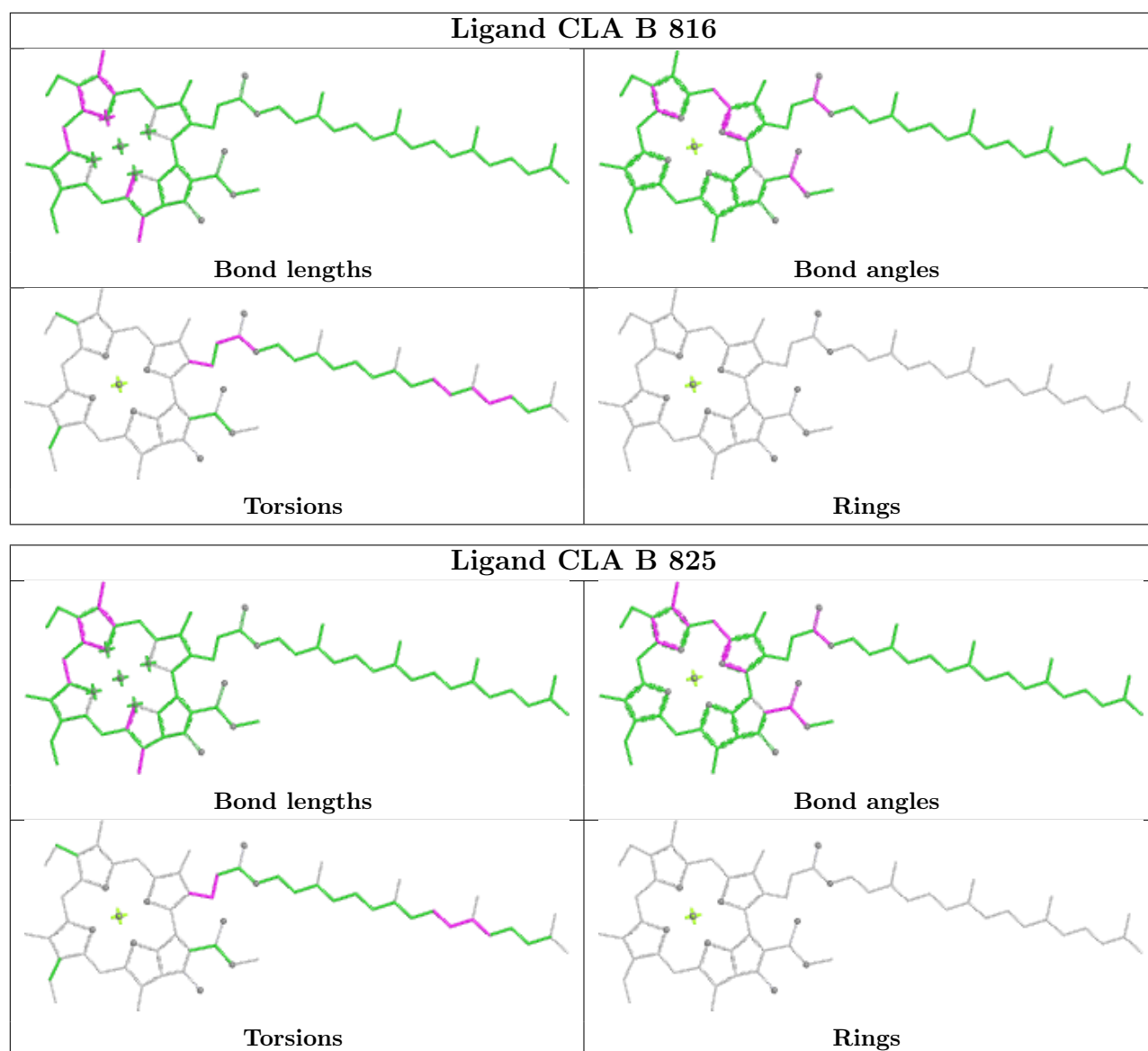


Rings

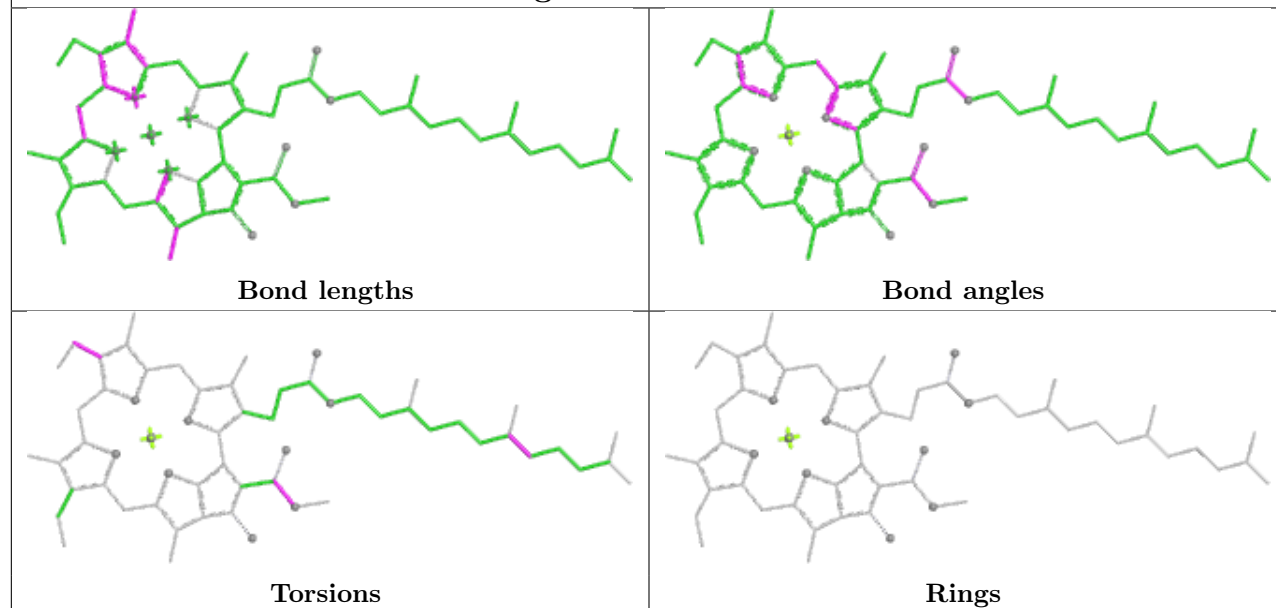




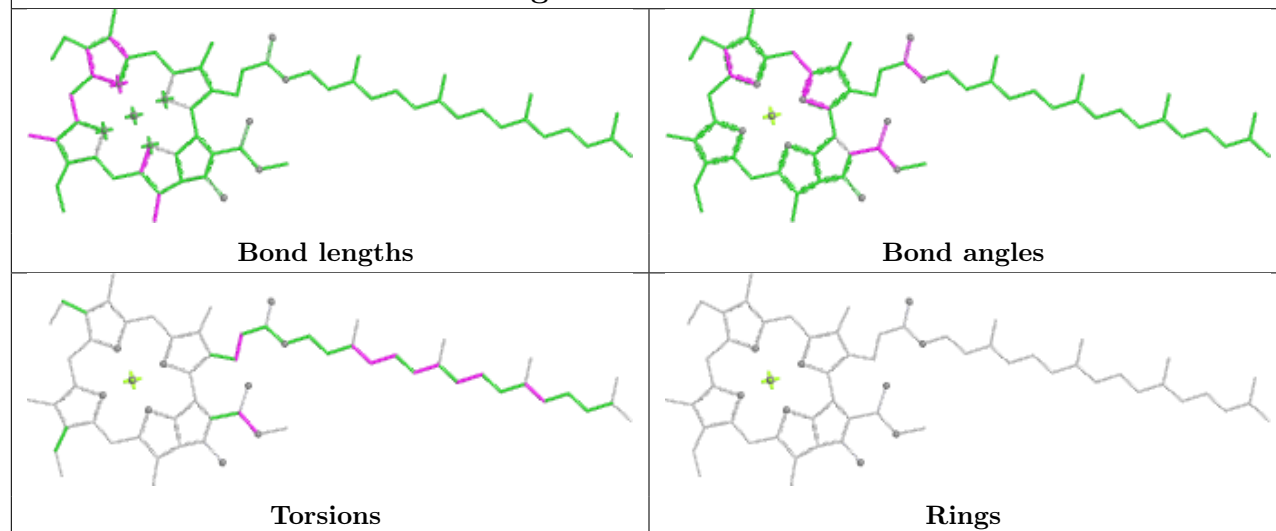


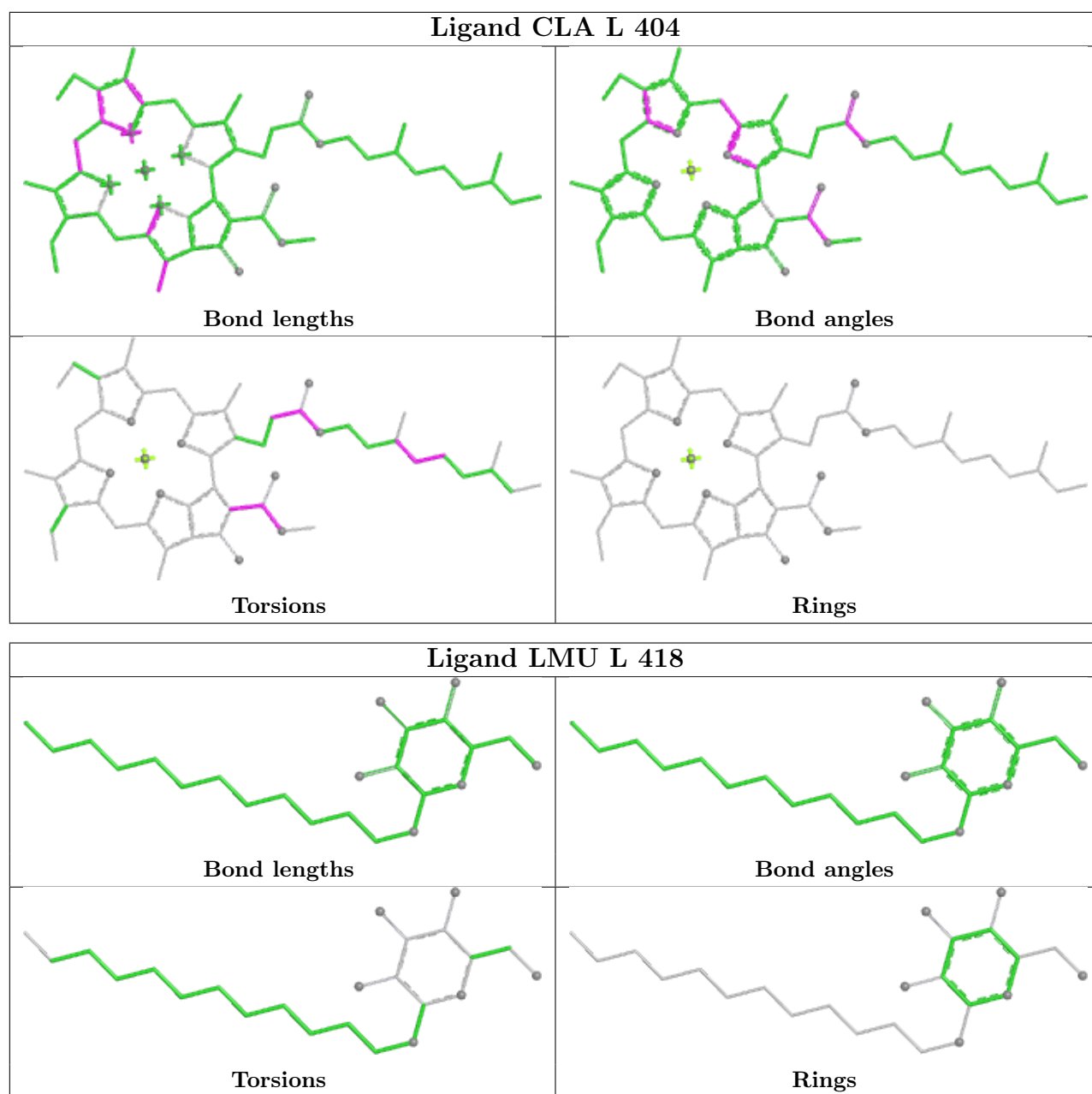


## Ligand CLA L 409

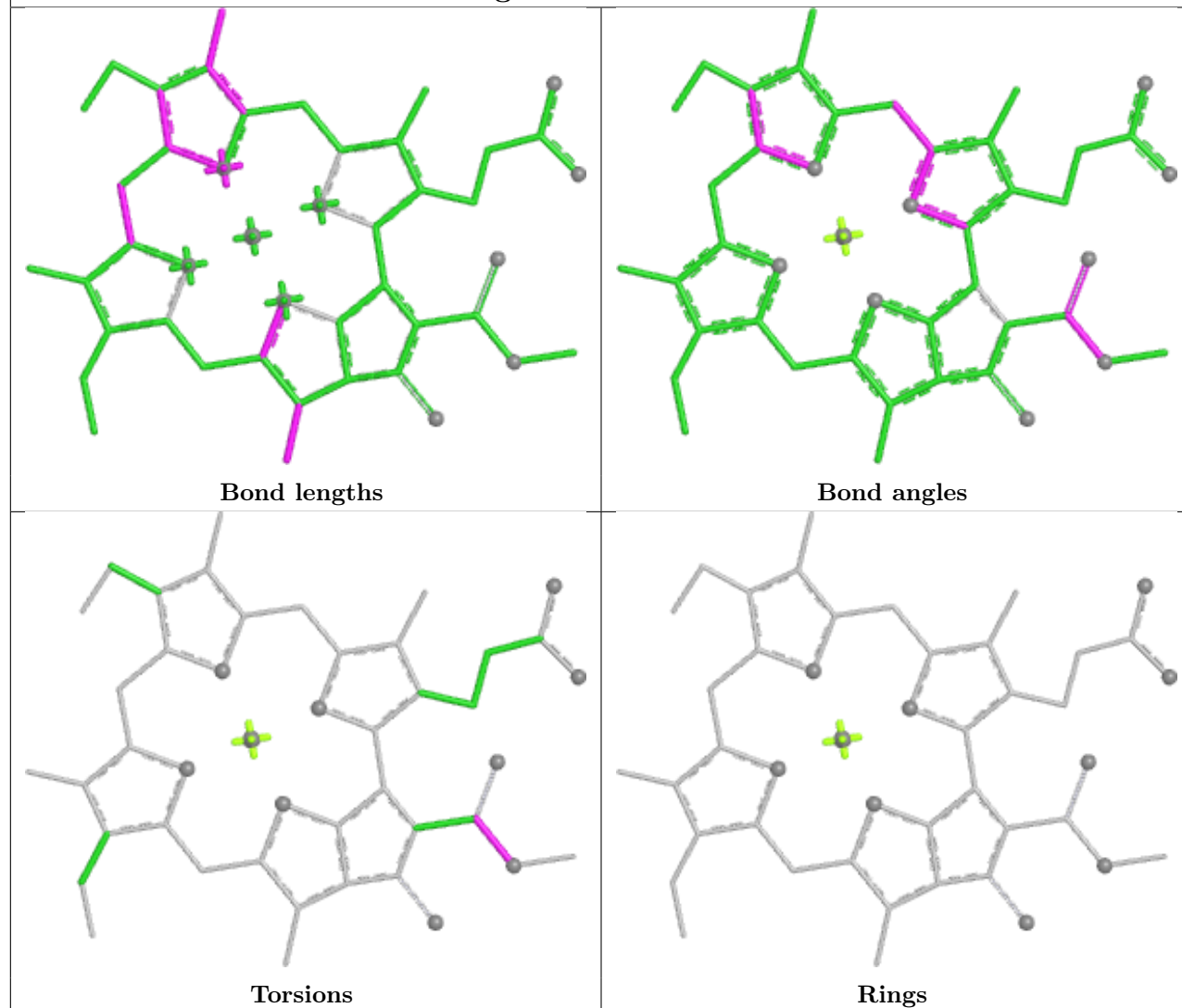


## Ligand CLA K 611

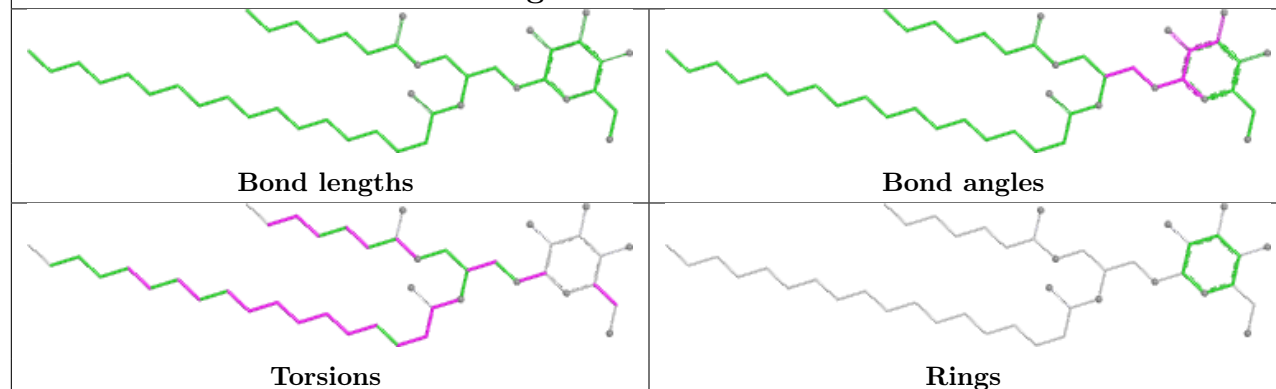




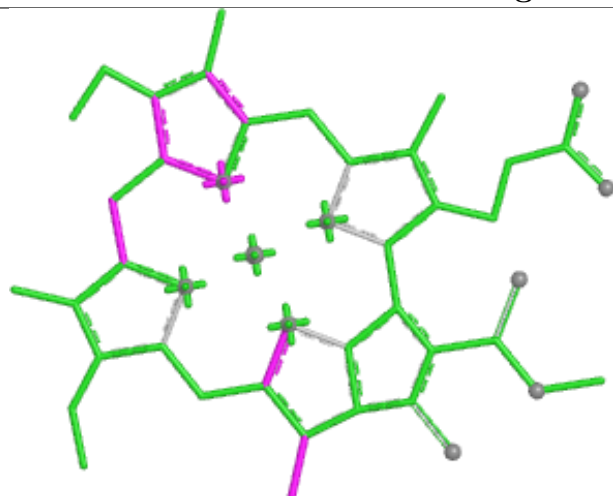
## Ligand CLA L 405



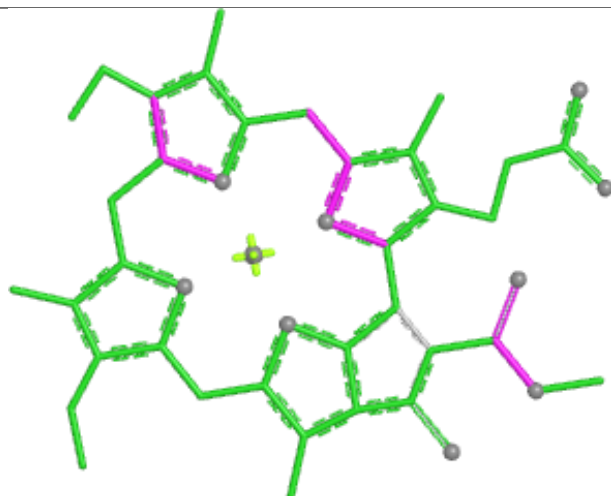
## Ligand LMG N 615



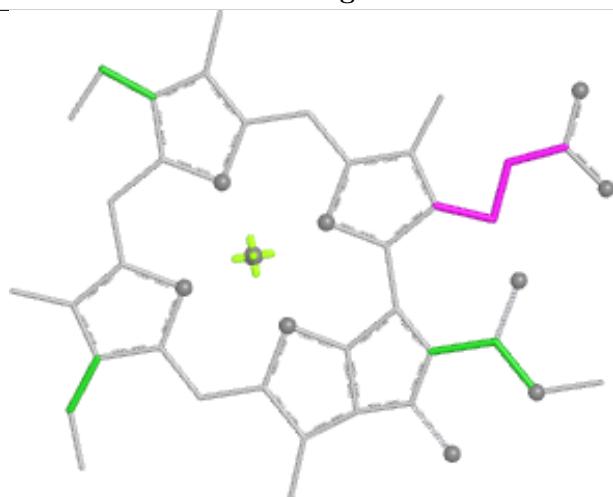
## Ligand CLA P 605



Bond lengths



Bond angles

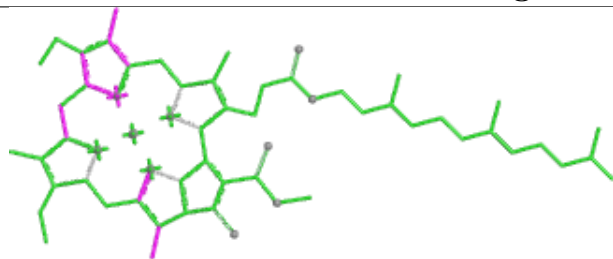


Torsions

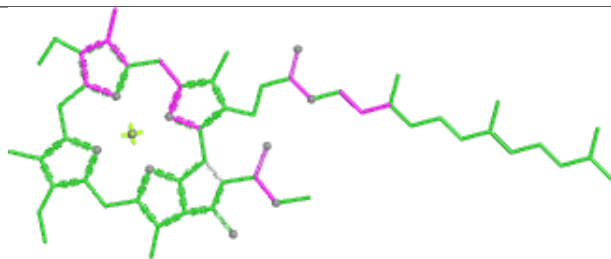


Rings

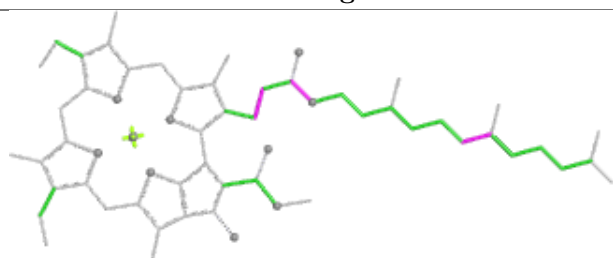
## Ligand CLA G 602



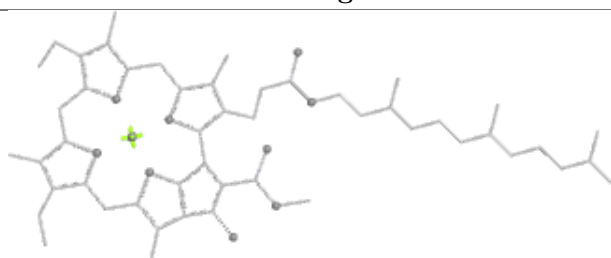
Bond lengths



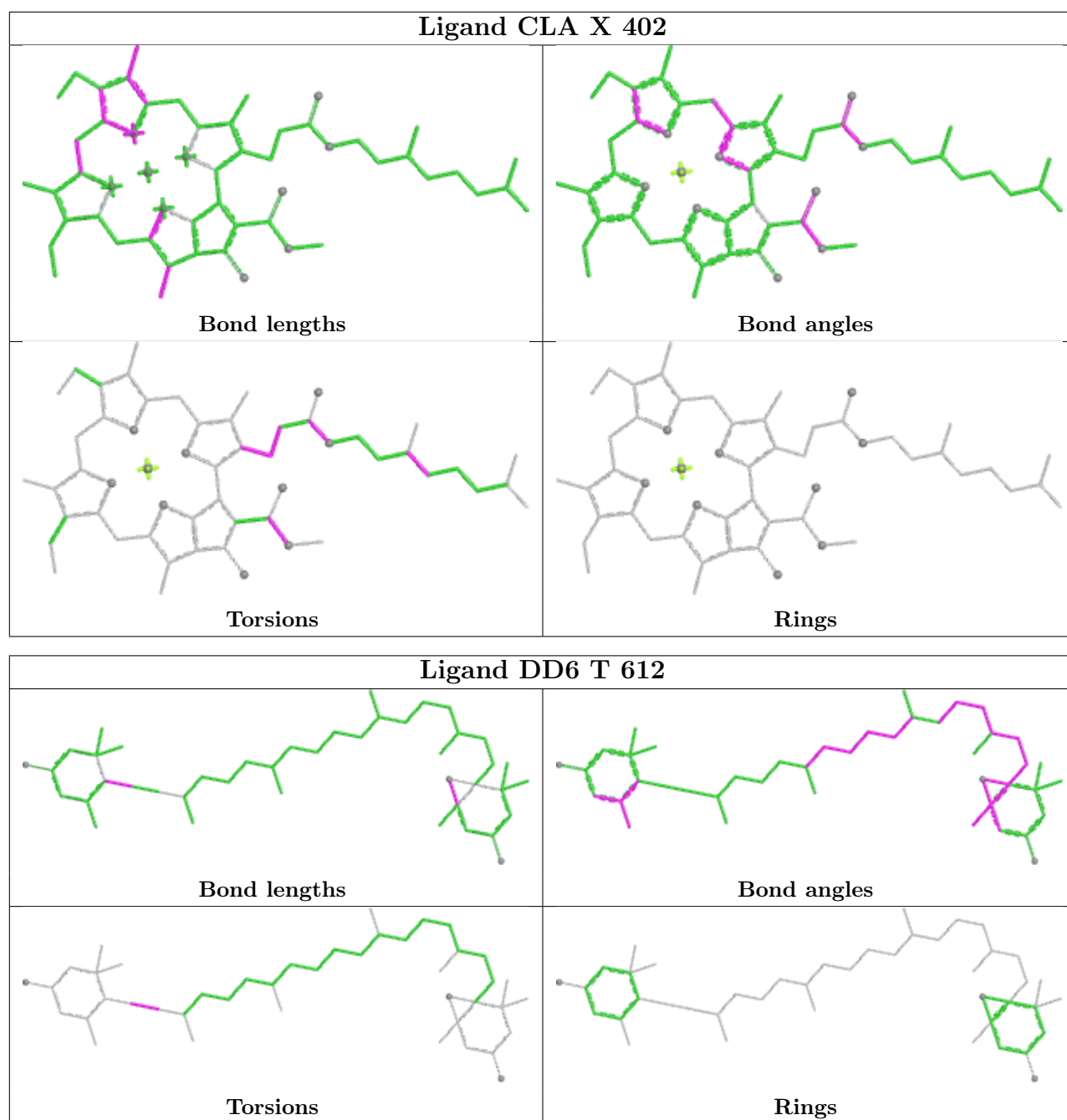
Bond angles



Torsions

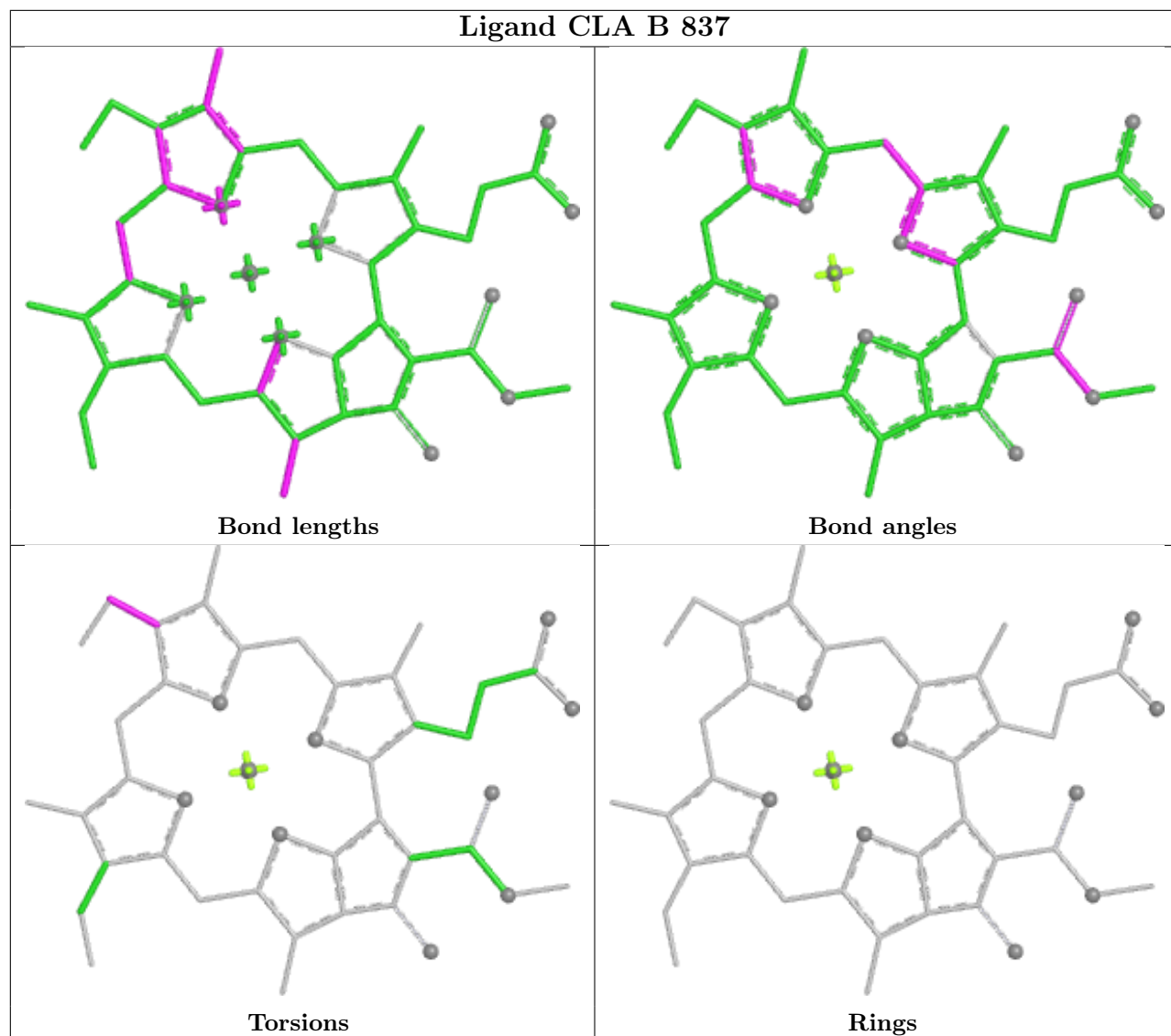


Rings

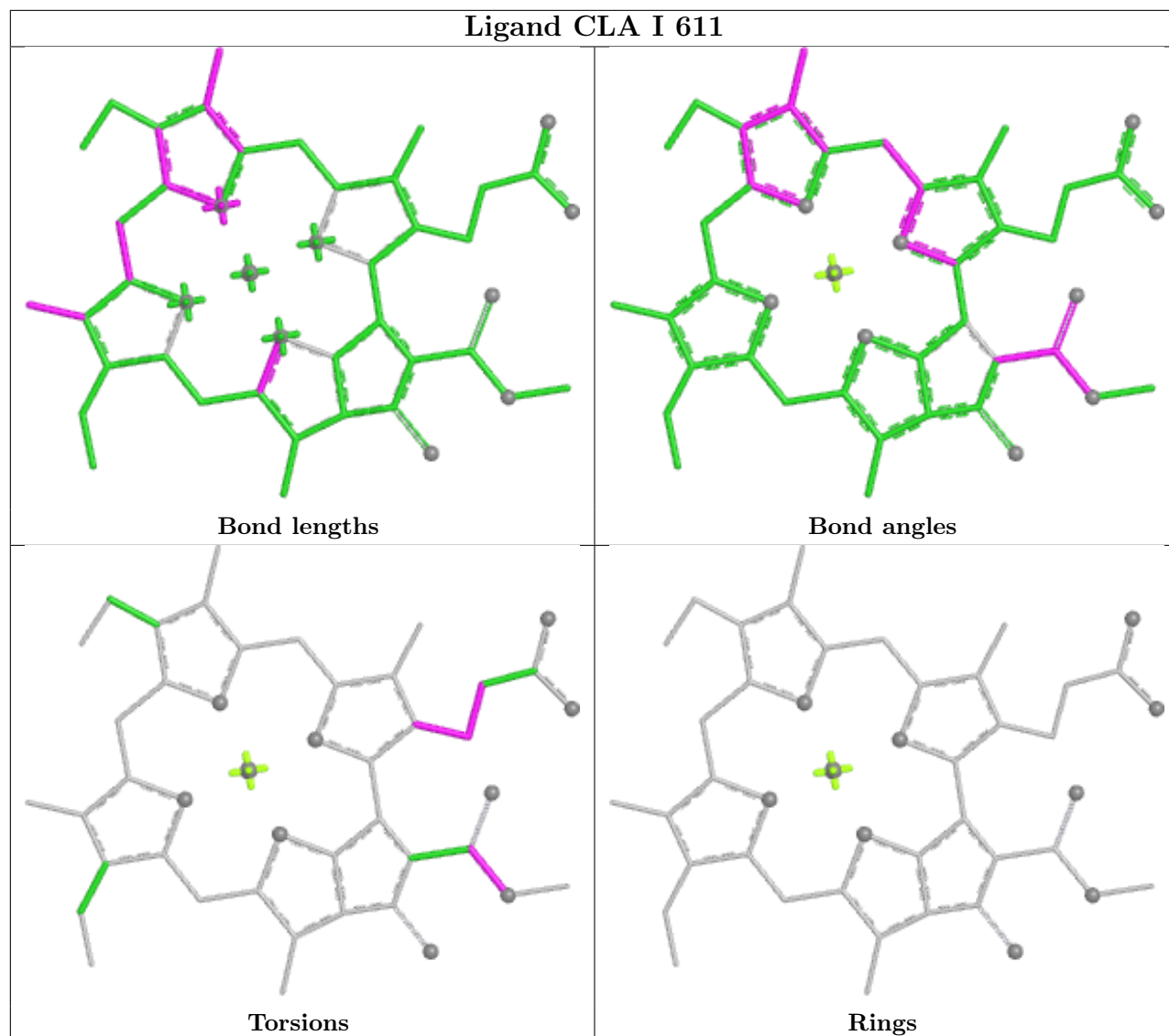




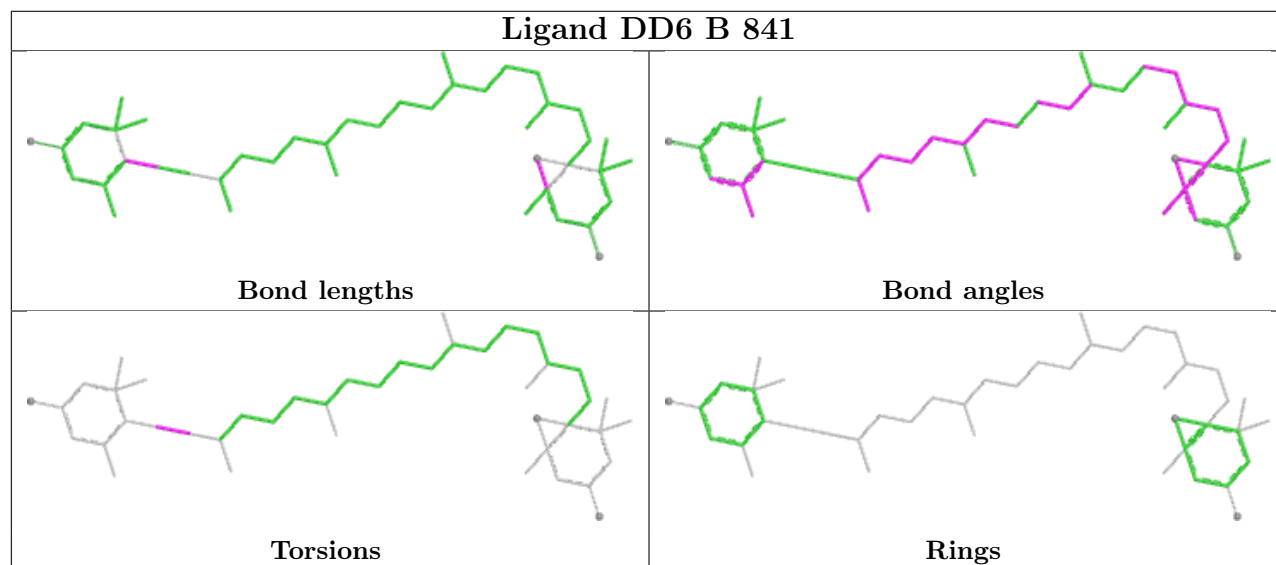
## Ligand CLA B 837



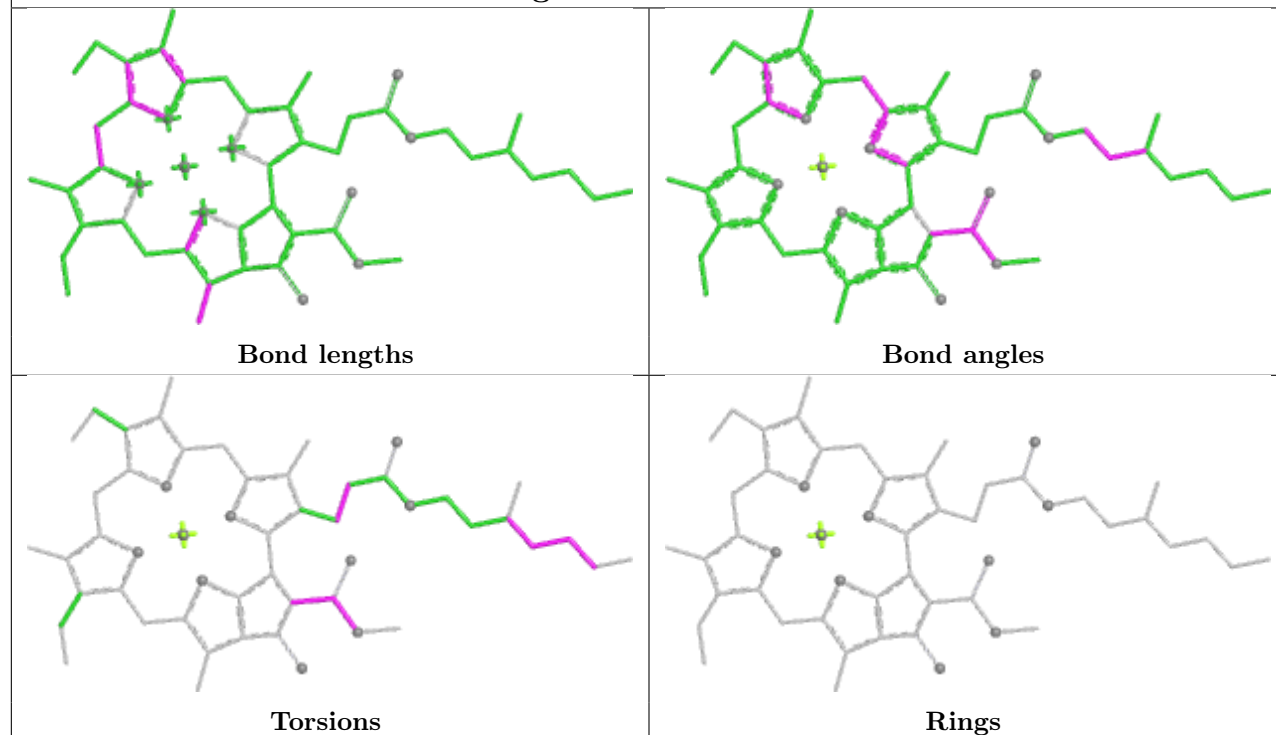
## Ligand CLA I 611



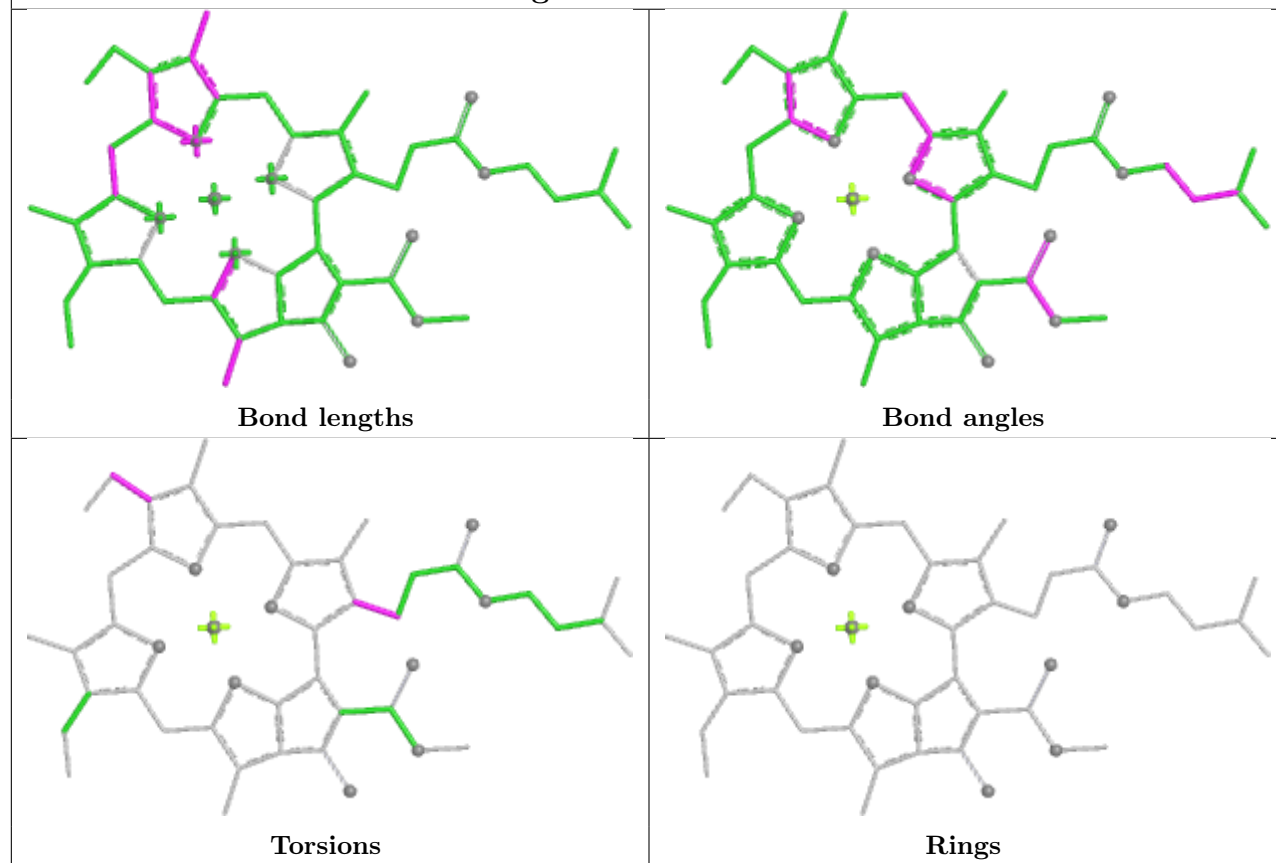
## Ligand DD6 B 841

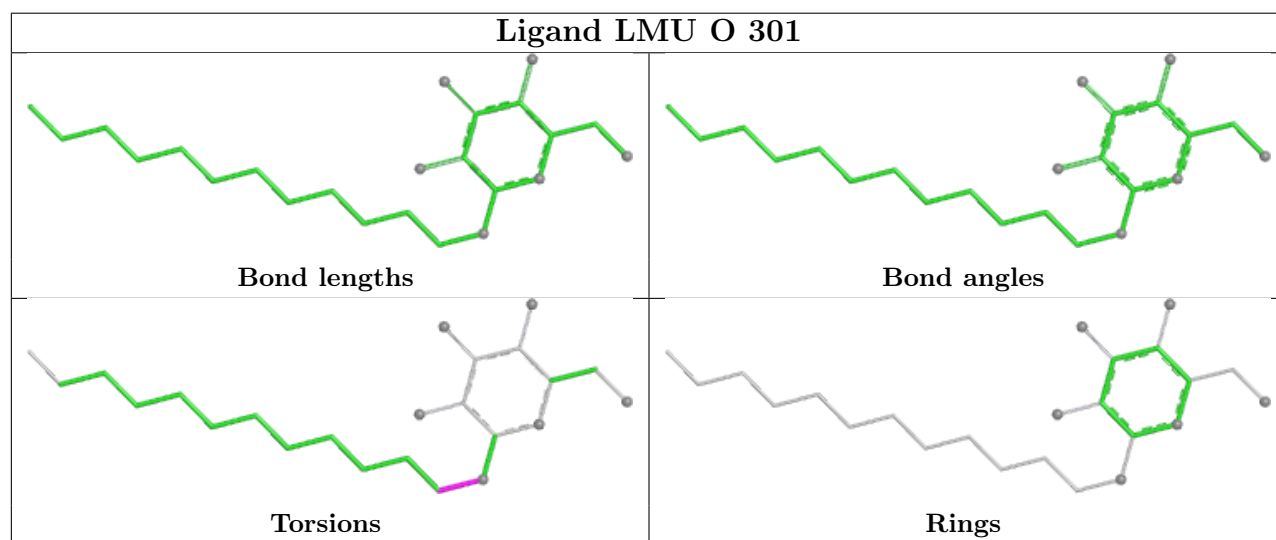
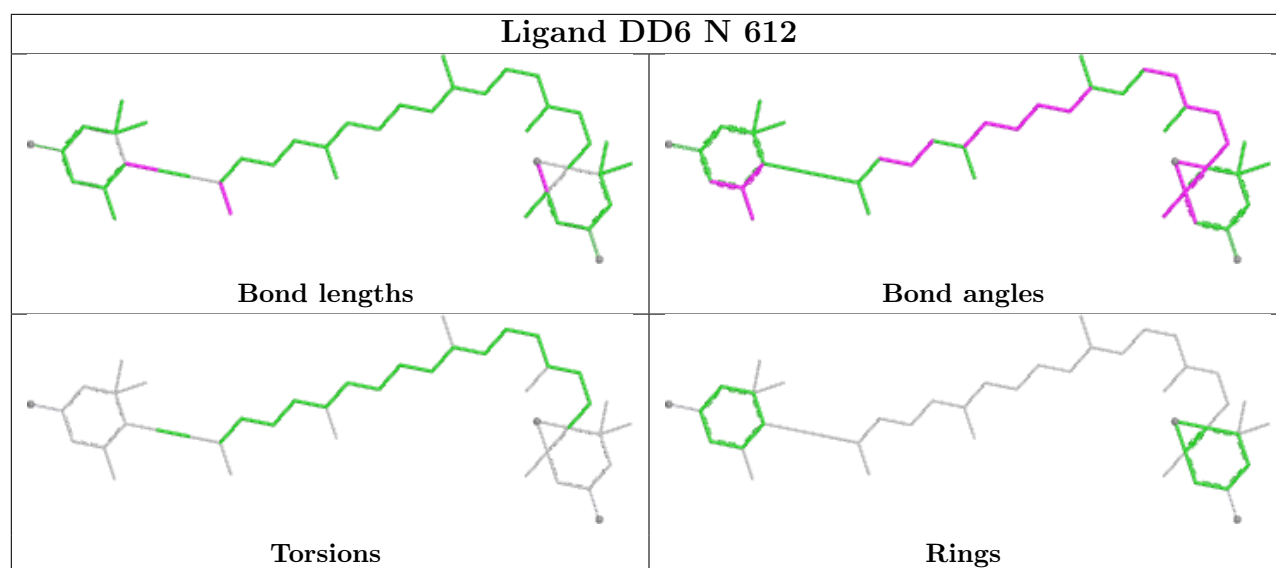


## Ligand CLA B 820

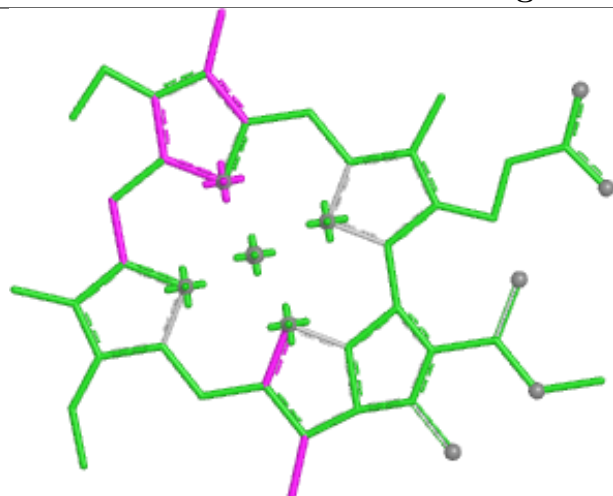


## Ligand CLA O 309

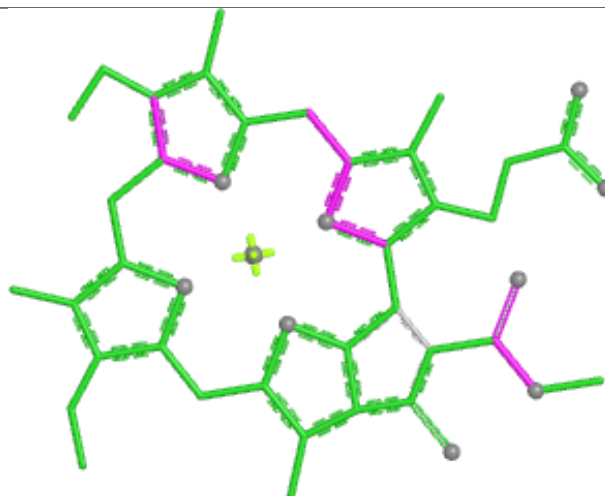




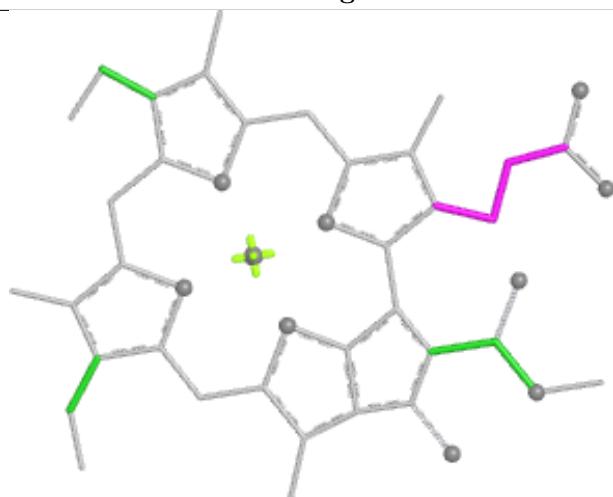
## Ligand CLA L 412



Bond lengths



Bond angles

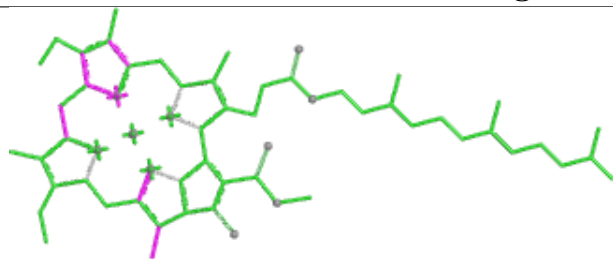


Torsions

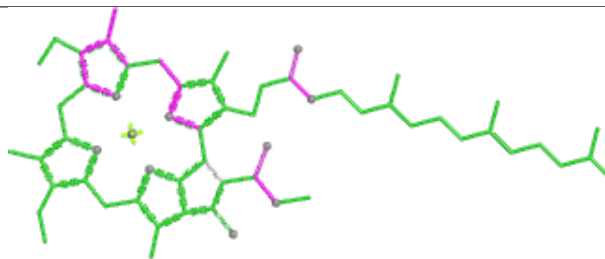


Rings

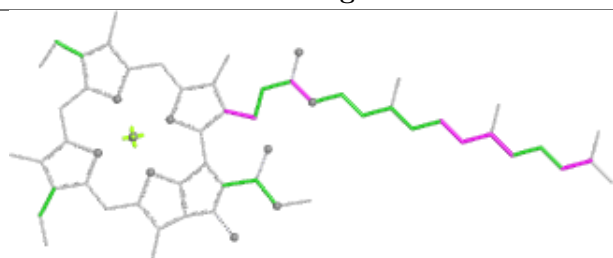
## Ligand CLA H 305



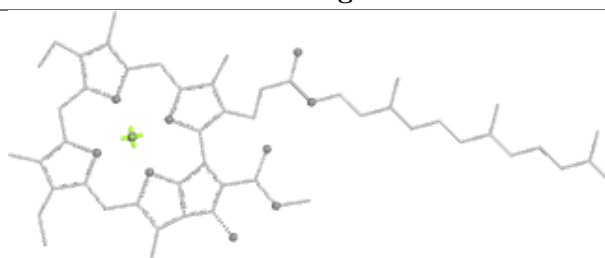
Bond lengths



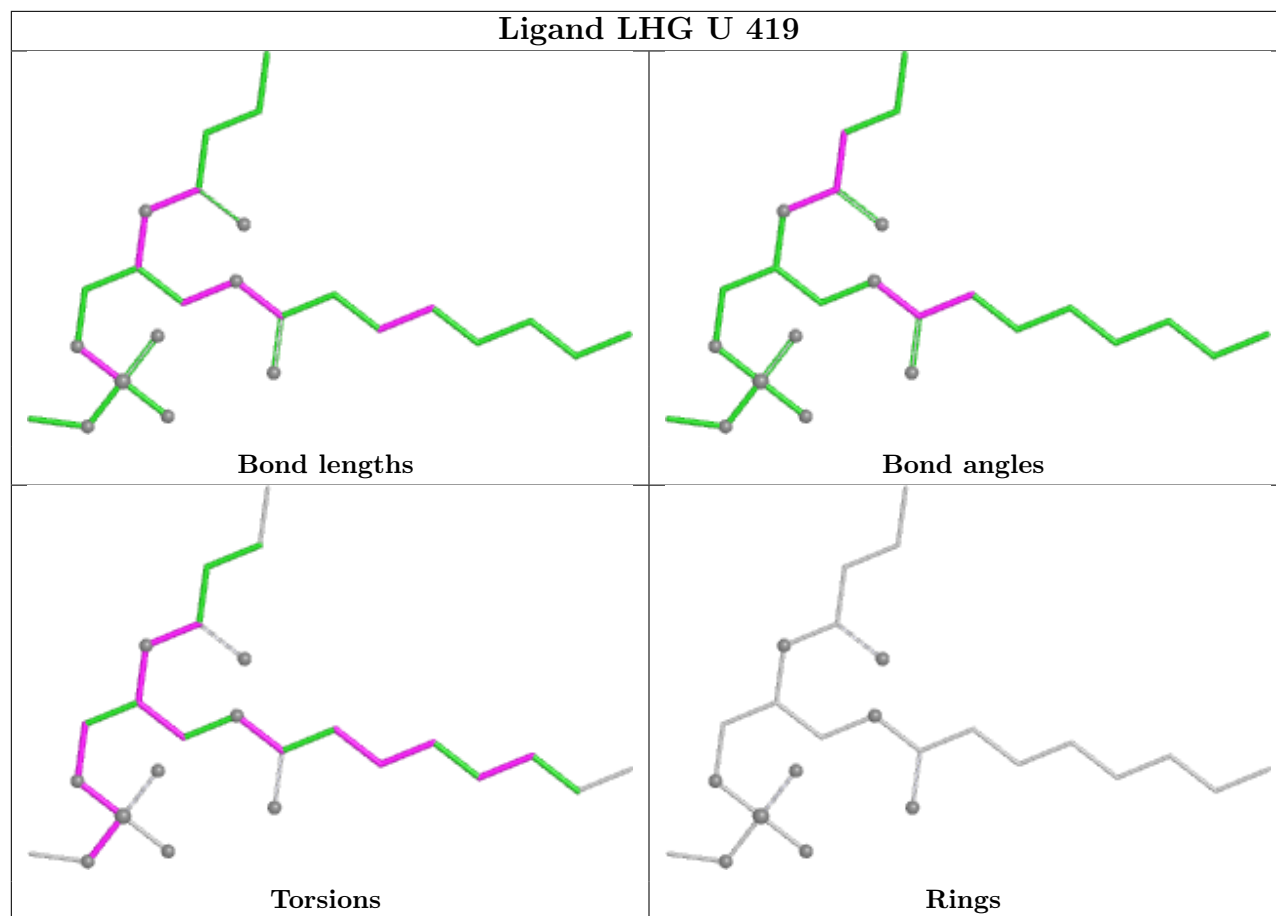
Bond angles



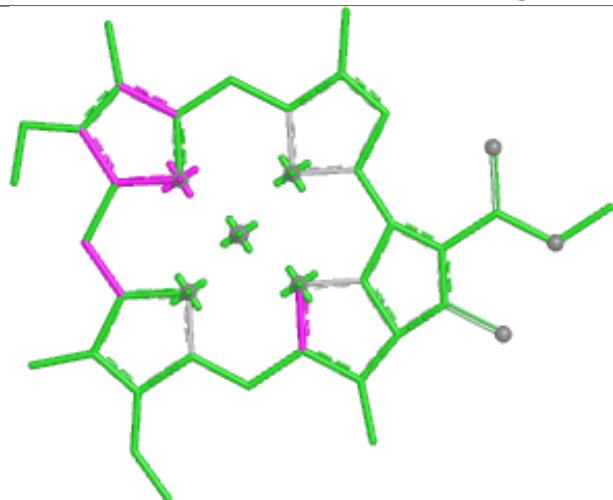
Torsions



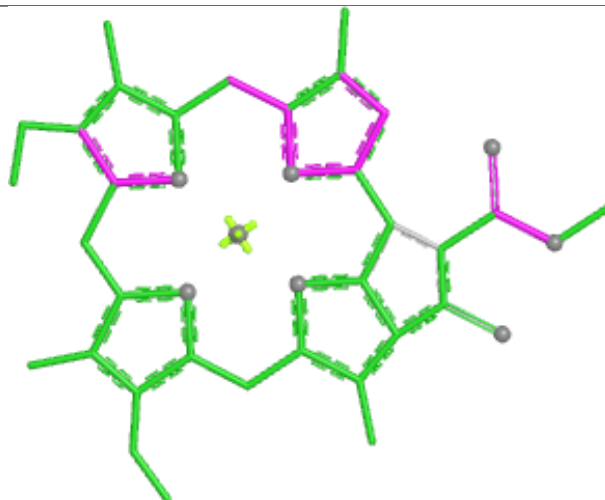
Rings



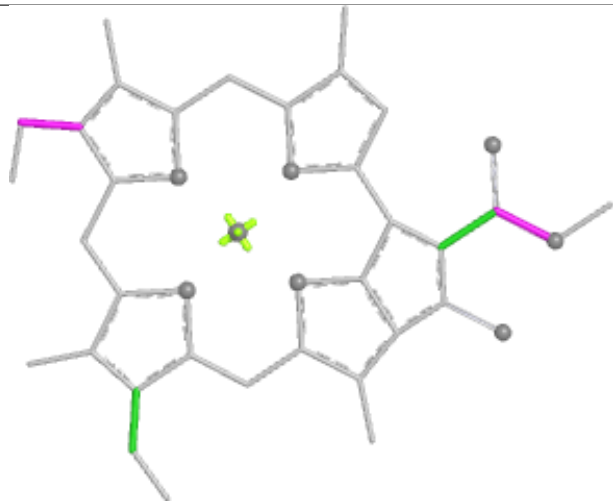
## Ligand CLA N 611



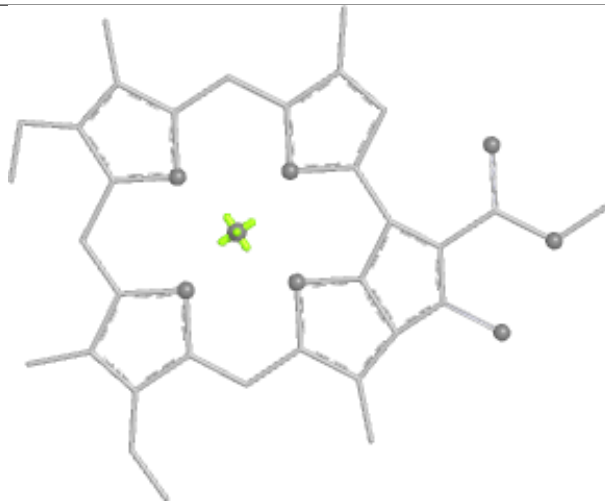
Bond lengths



Bond angles

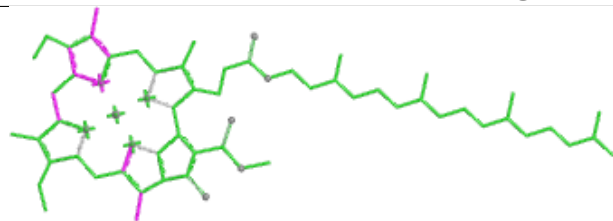


Torsions

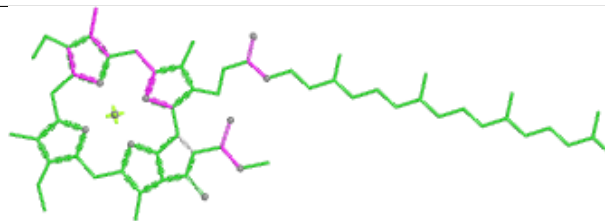


Rings

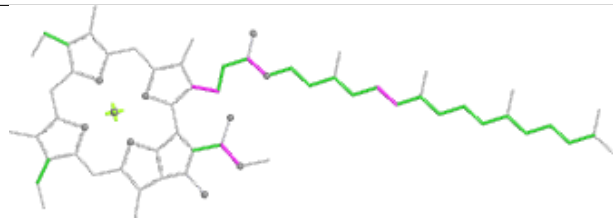
## Ligand CLA B 827



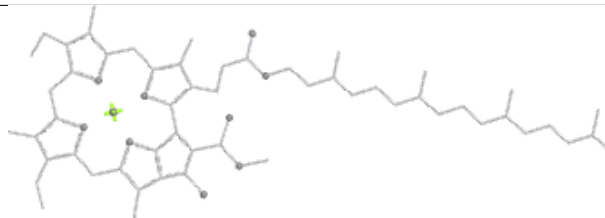
Bond lengths



Bond angles

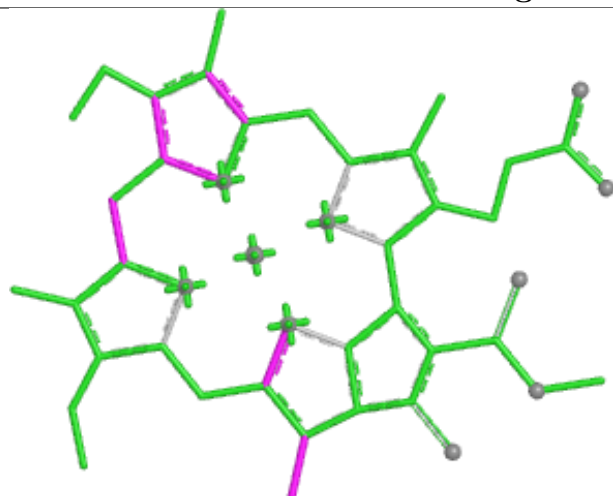


Torsions

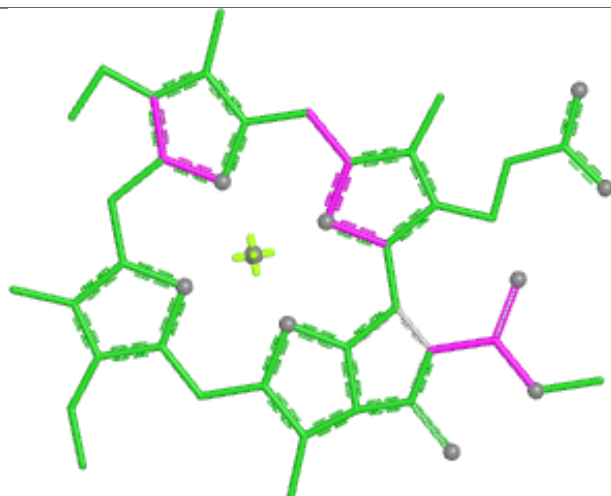


Rings

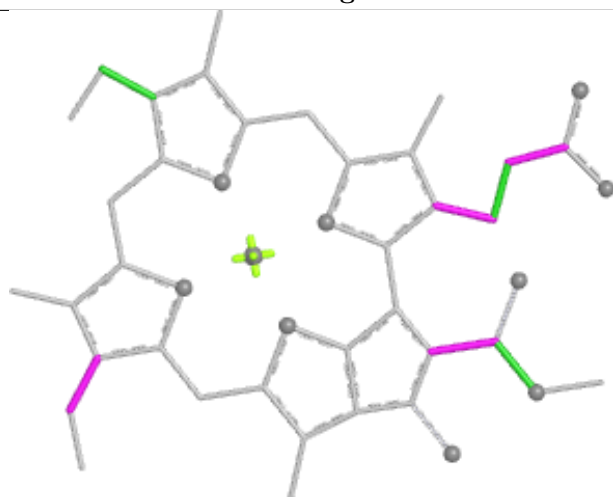
## Ligand CLA P 611



Bond lengths



Bond angles



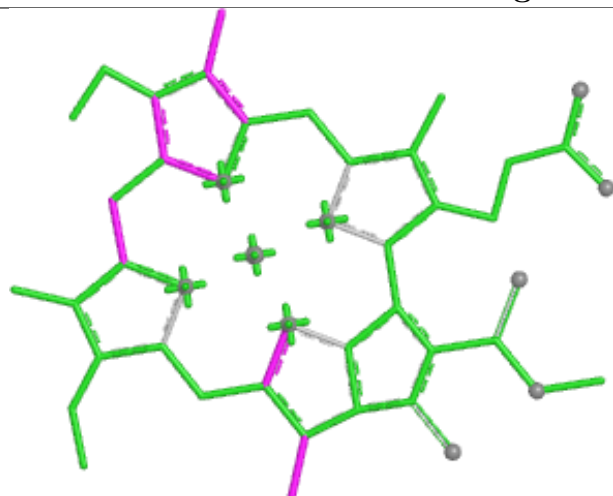
Torsions



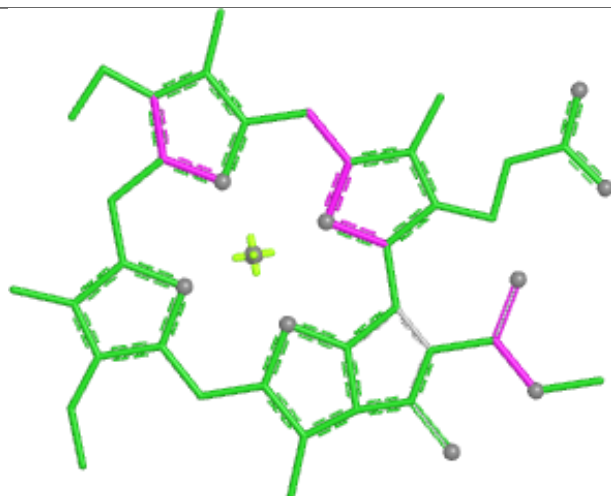
Rings



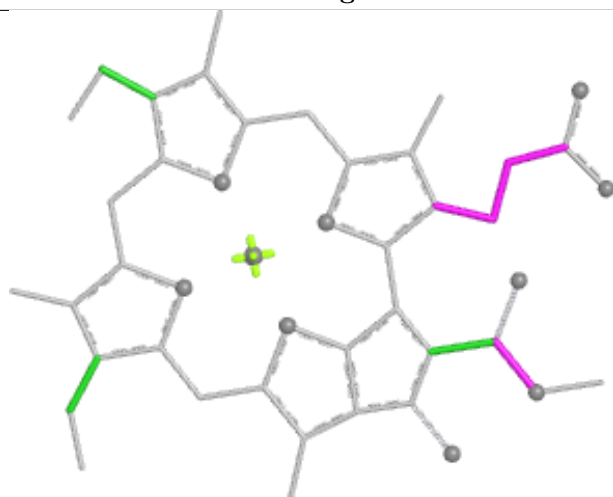
## Ligand CLA A 823



Bond lengths



Bond angles

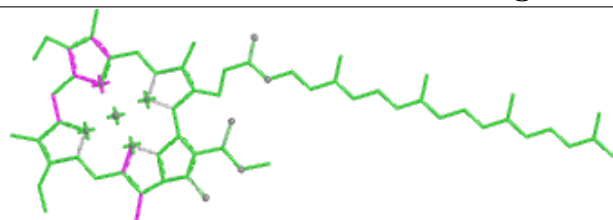


Torsions

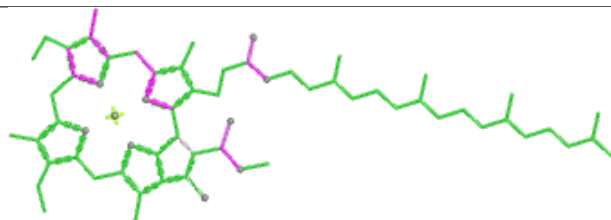


Rings

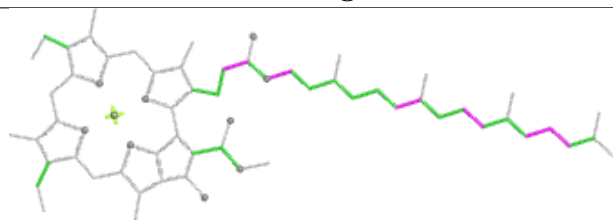
## Ligand CLA N 603



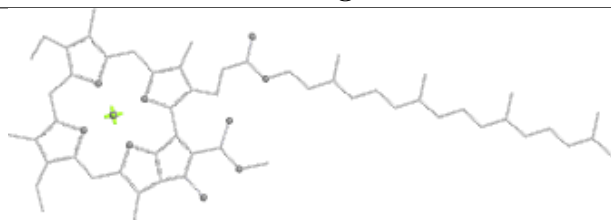
Bond lengths



Bond angles

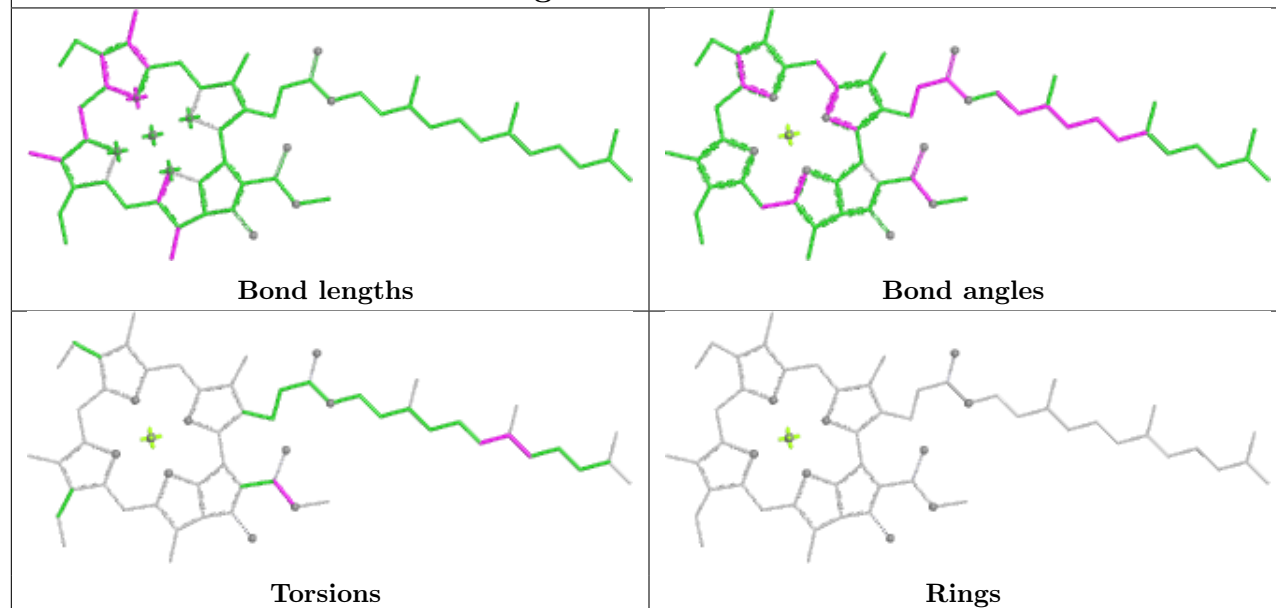


Torsions

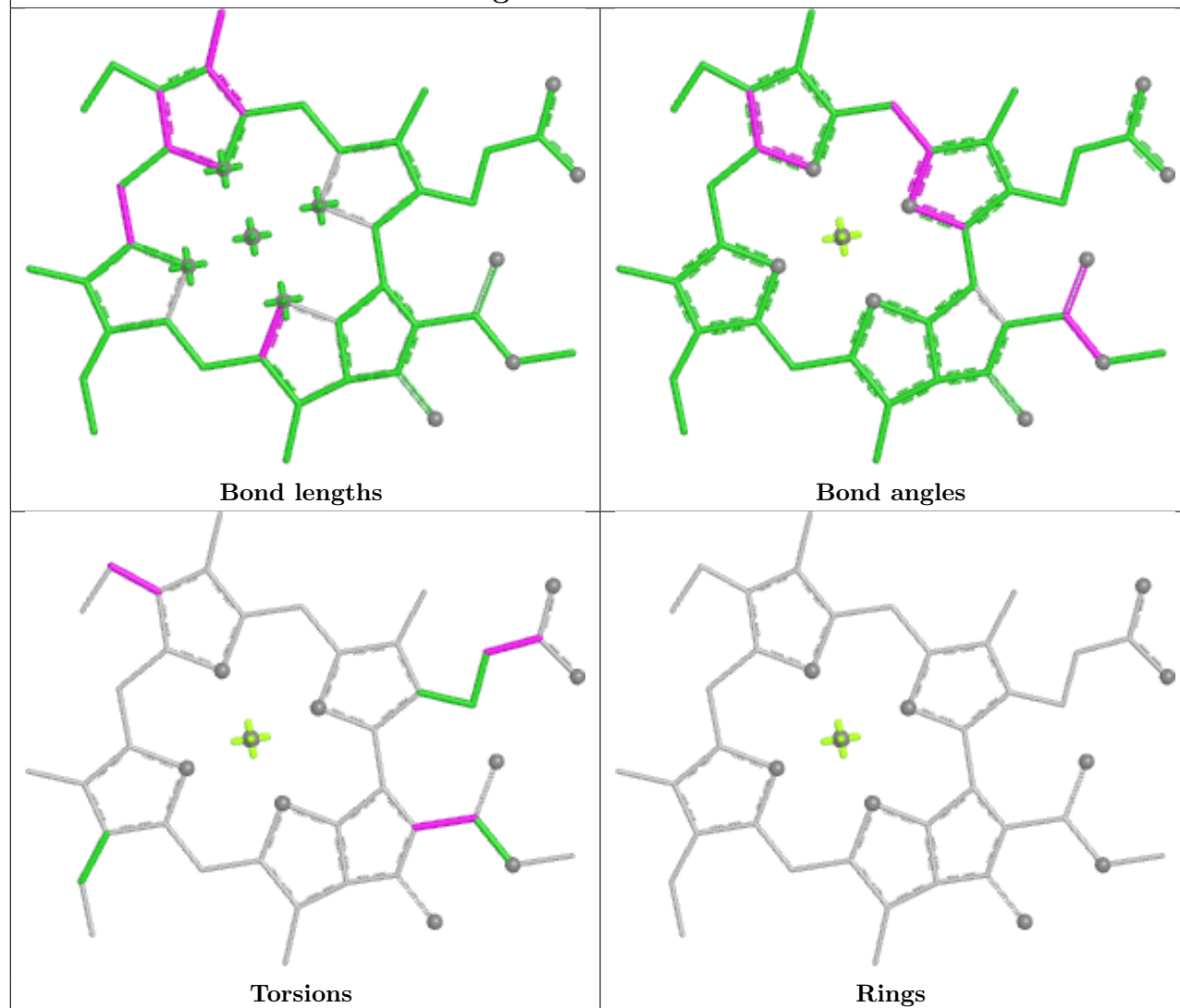


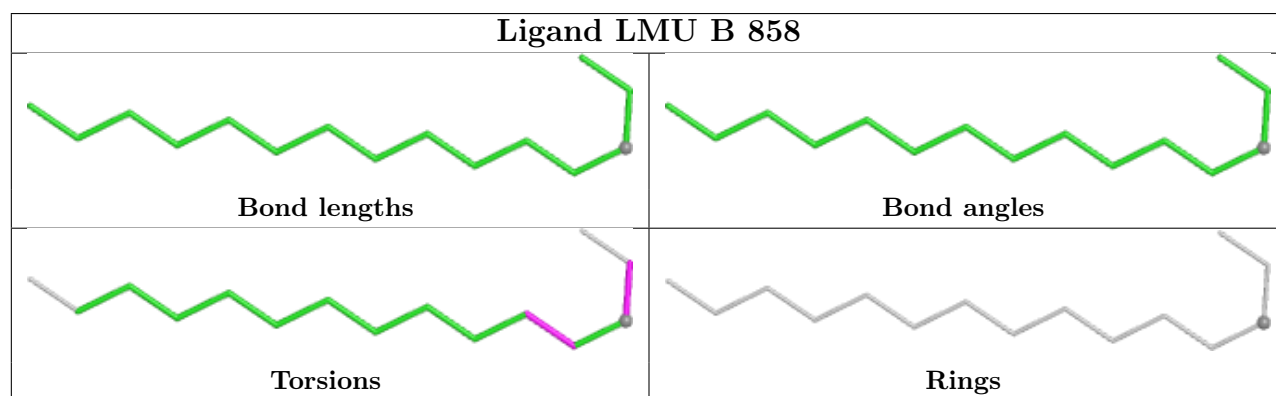
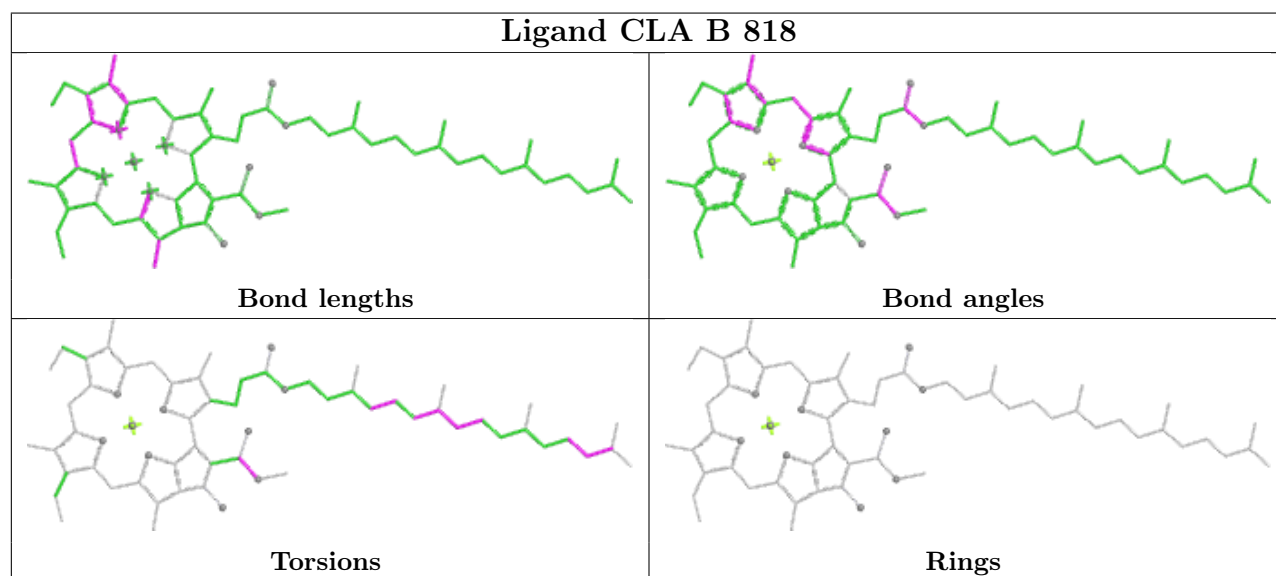
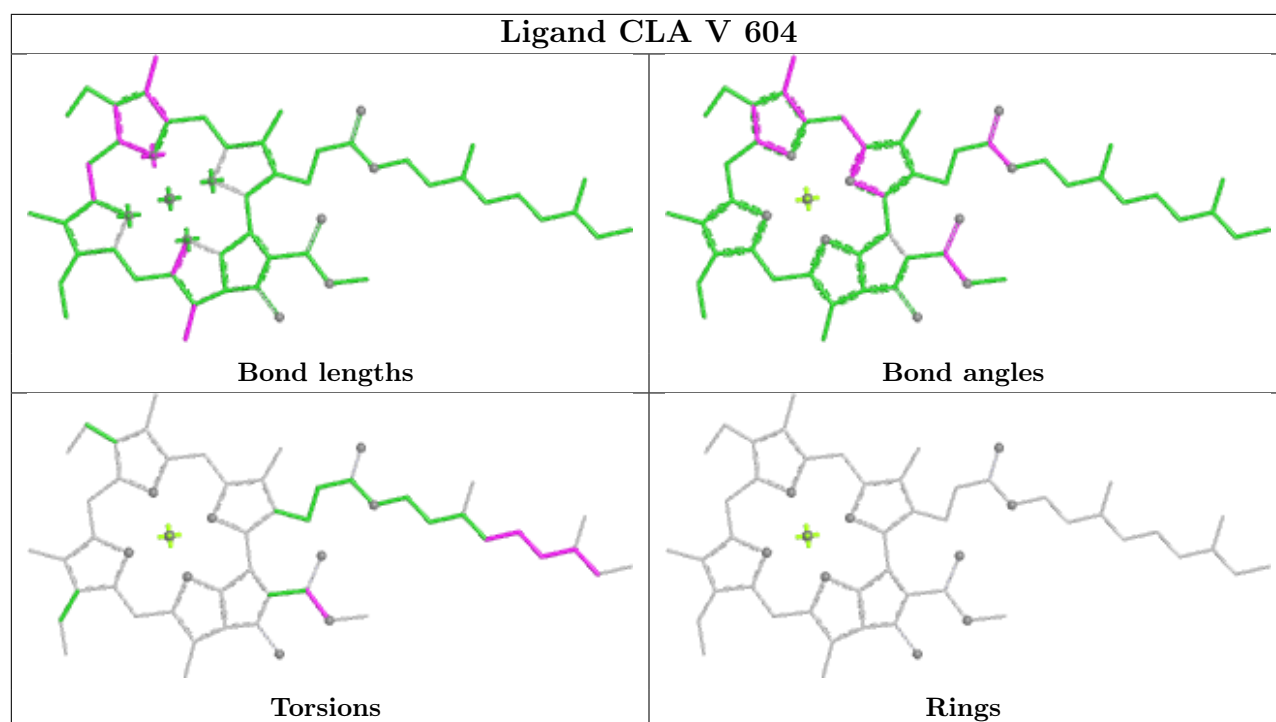
Rings

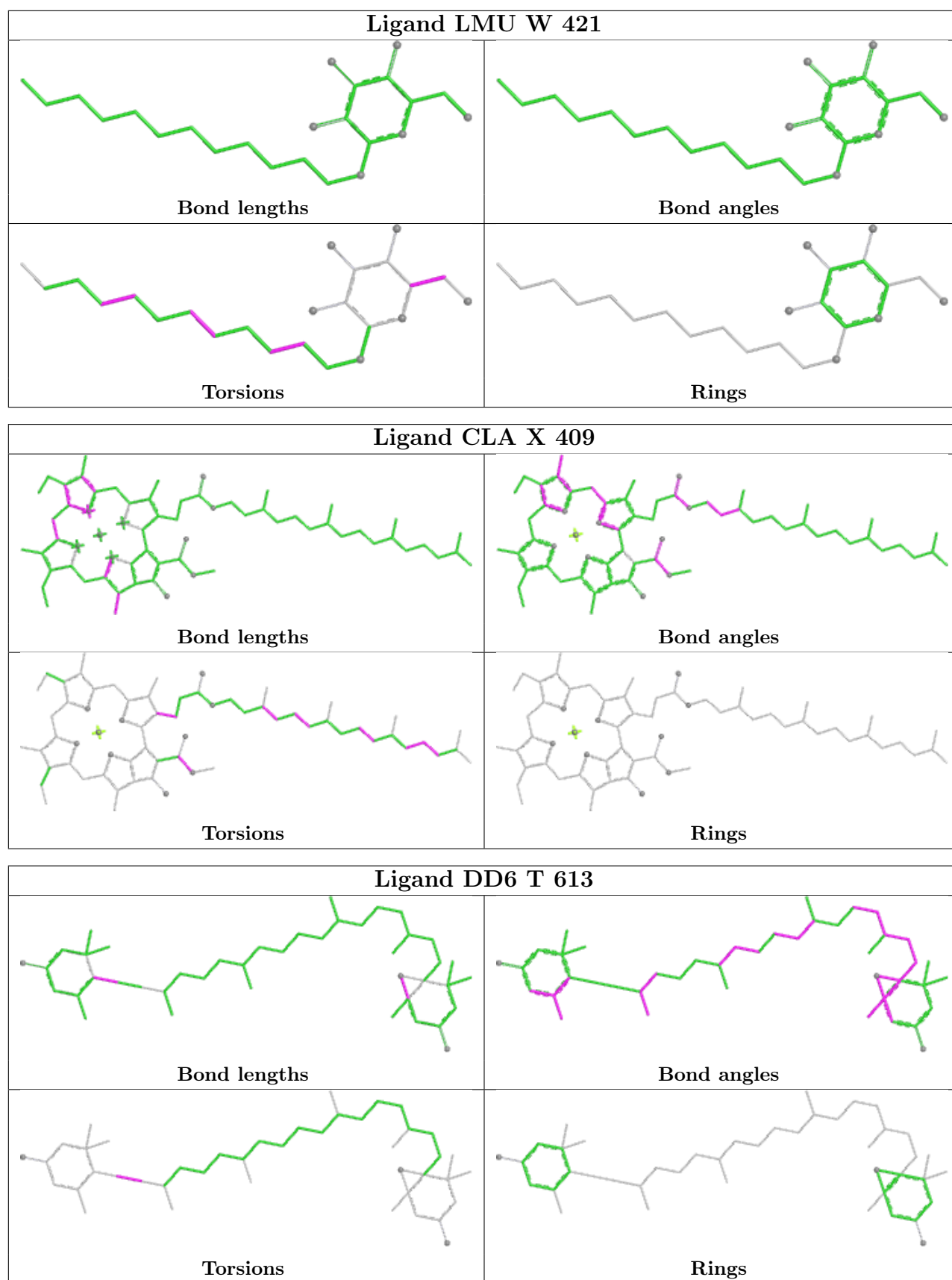
## Ligand CLA L 408

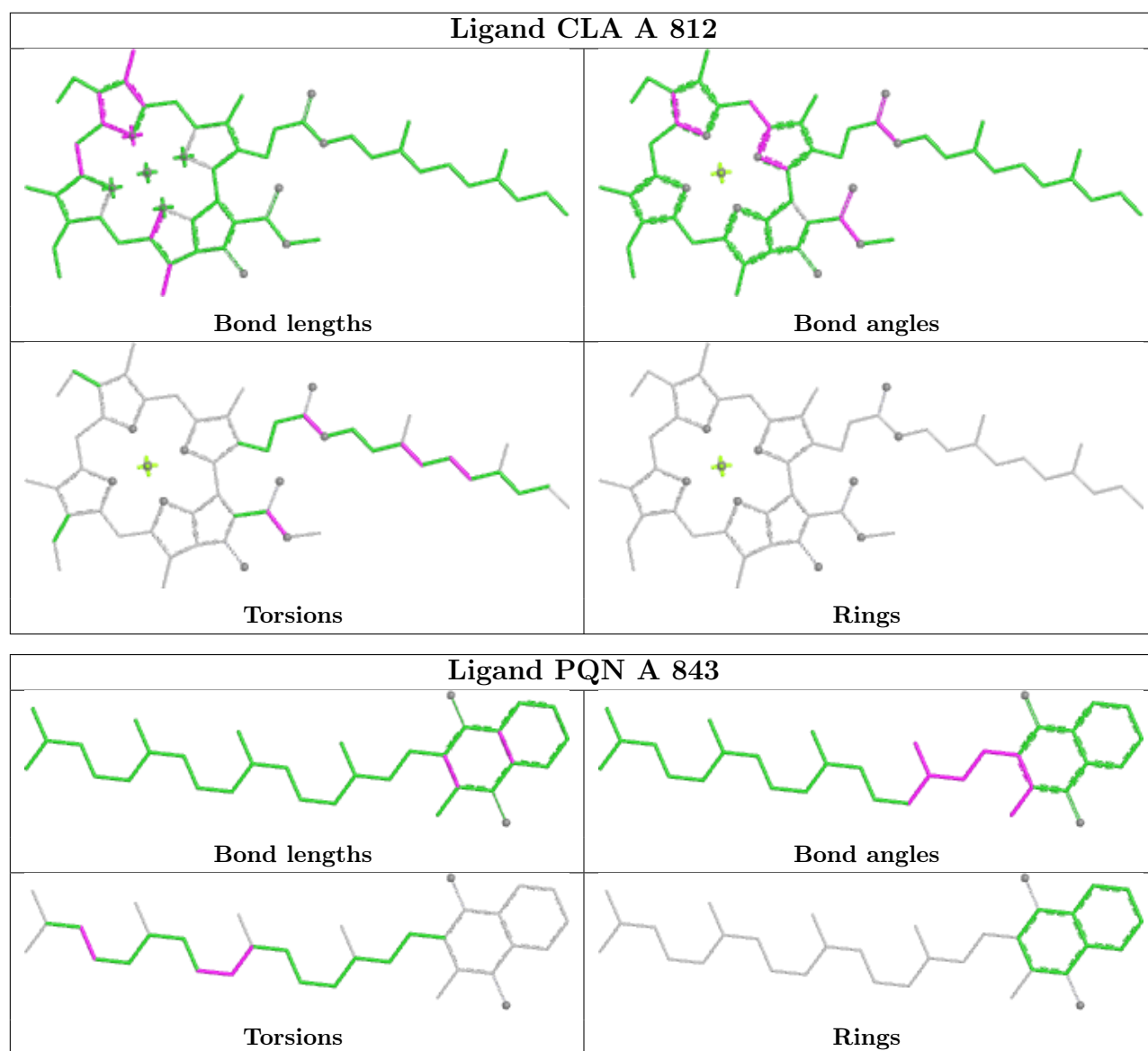


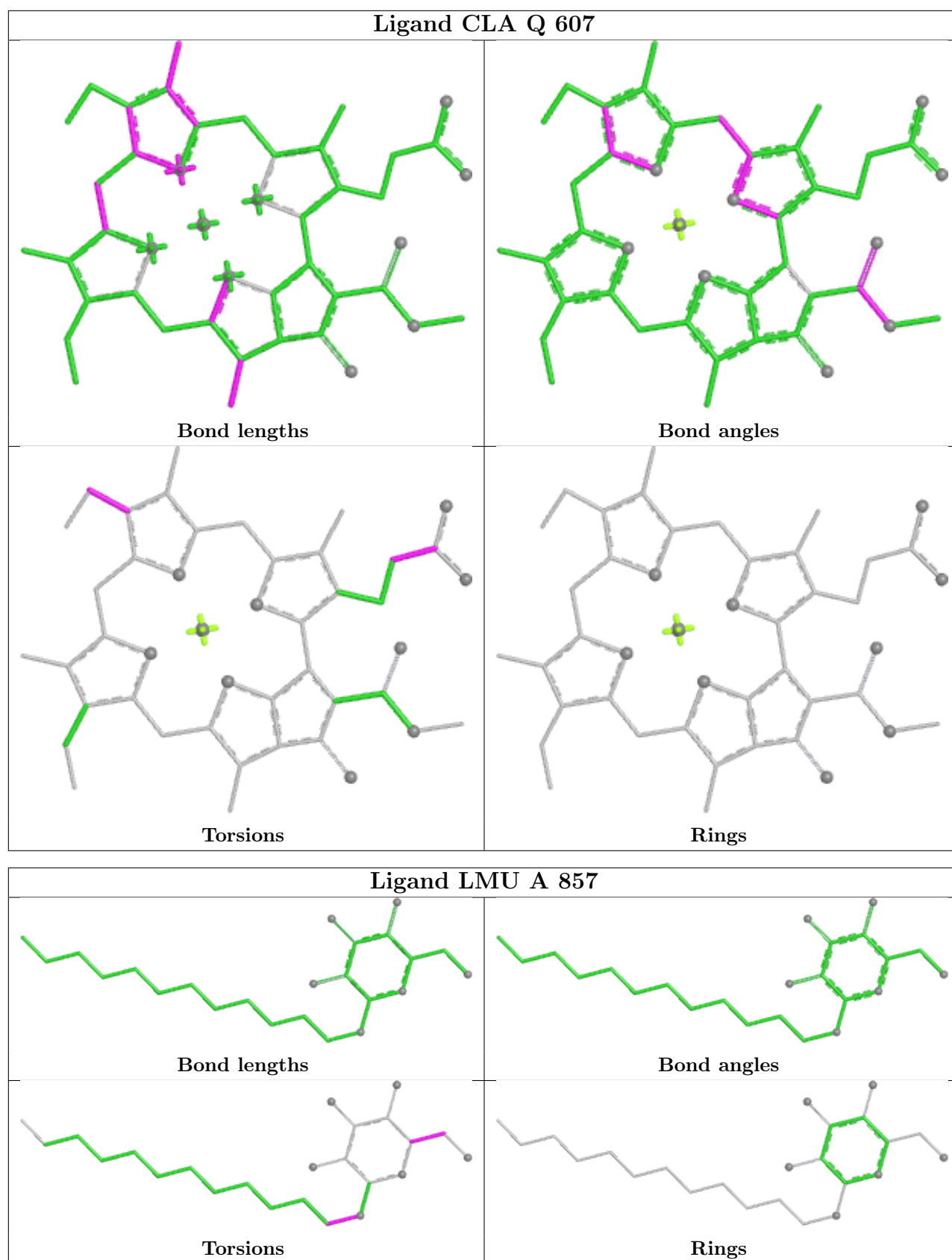
## Ligand CLA P 603



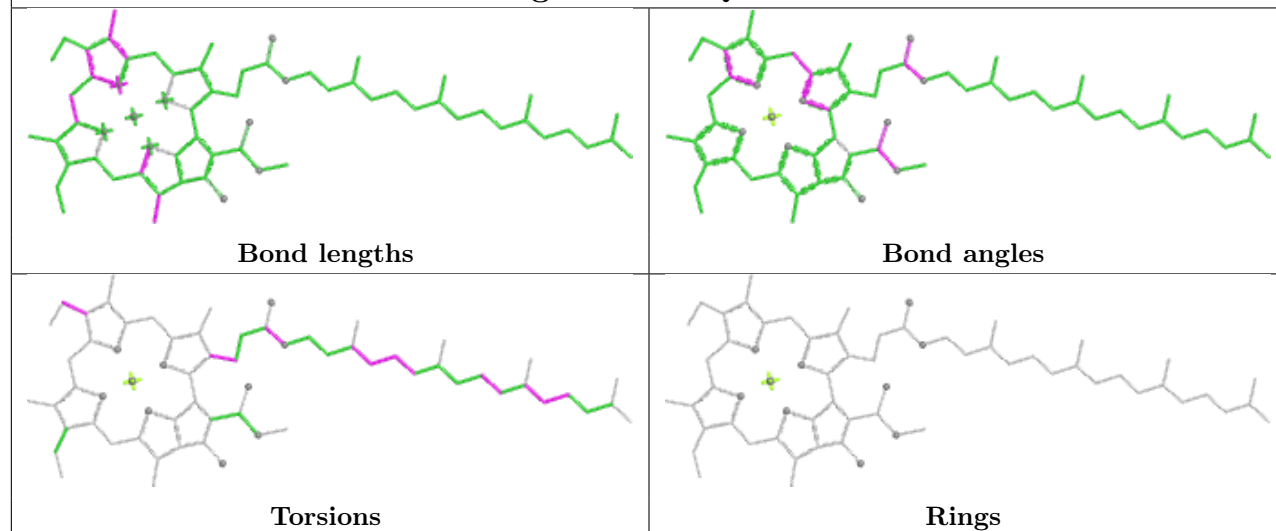




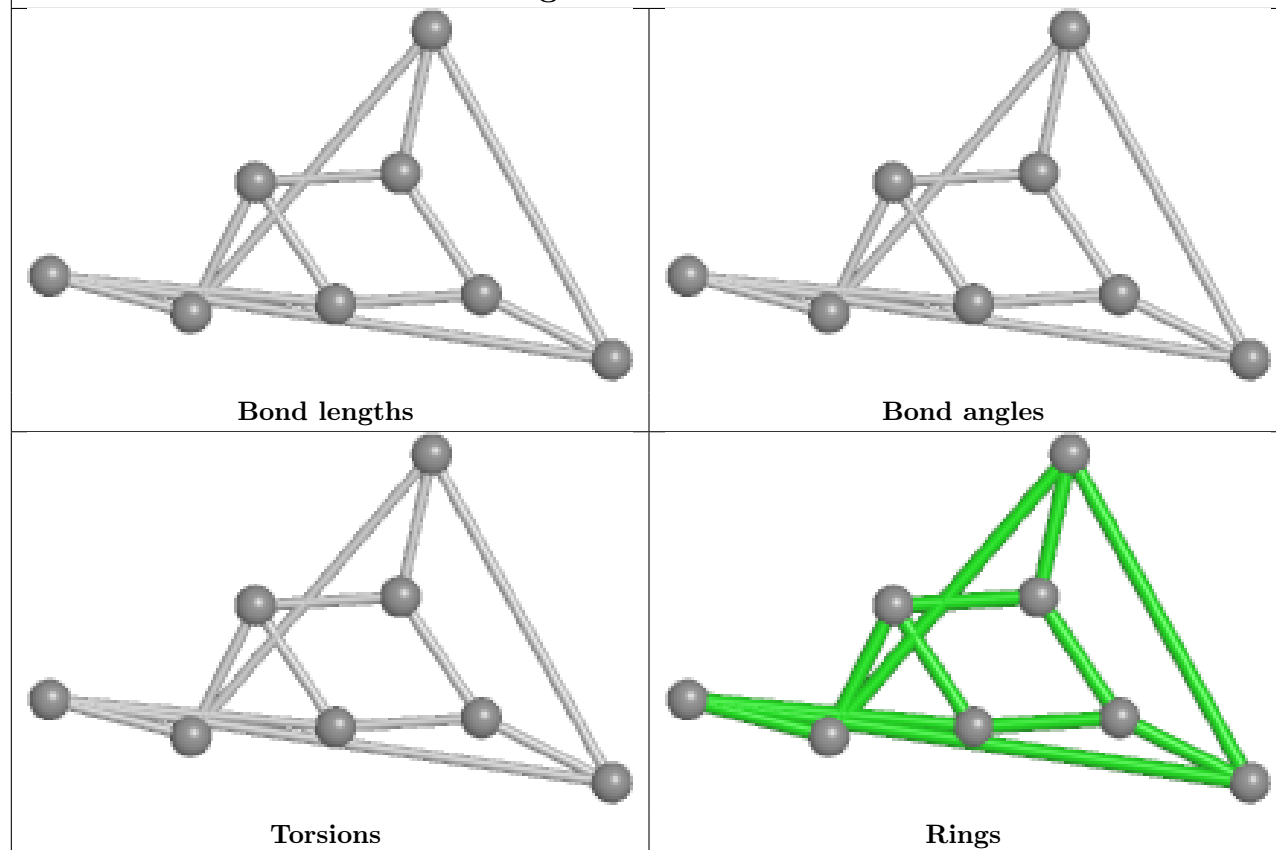


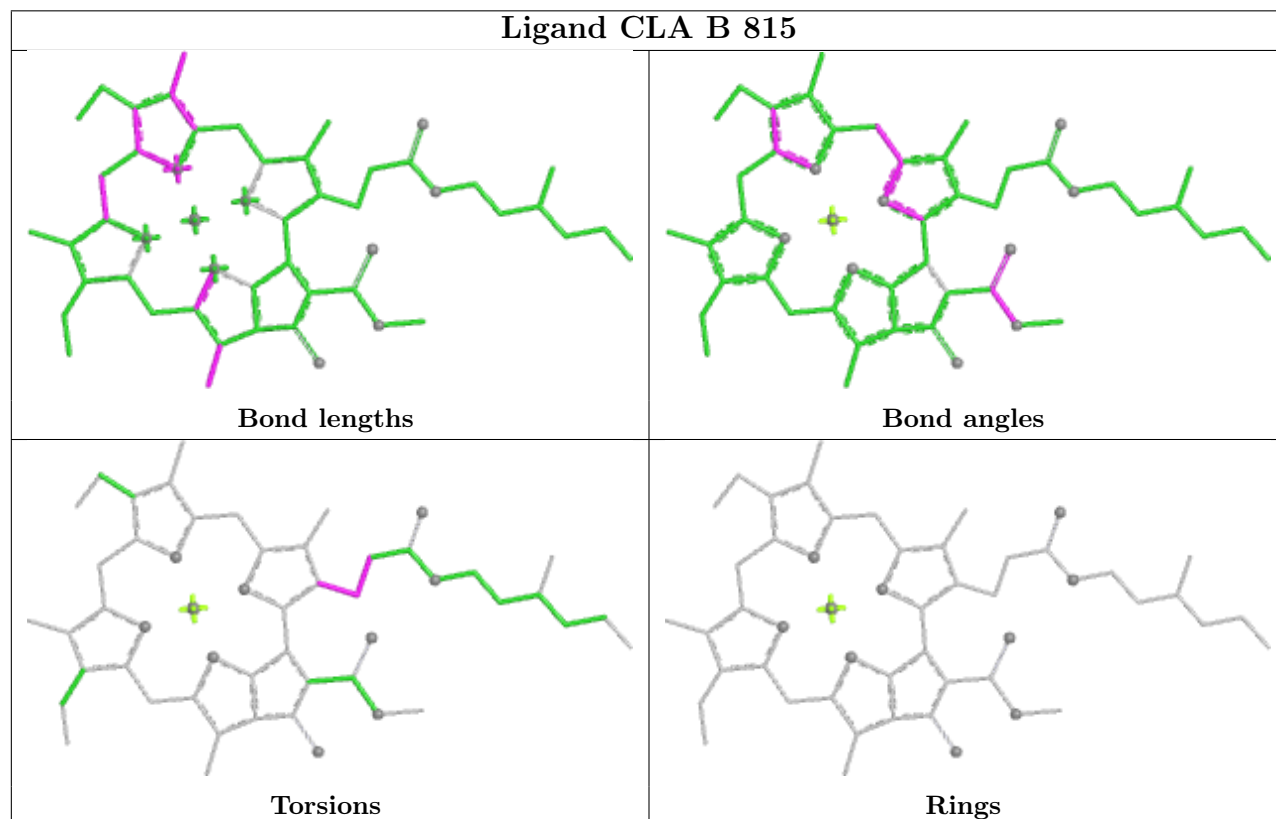
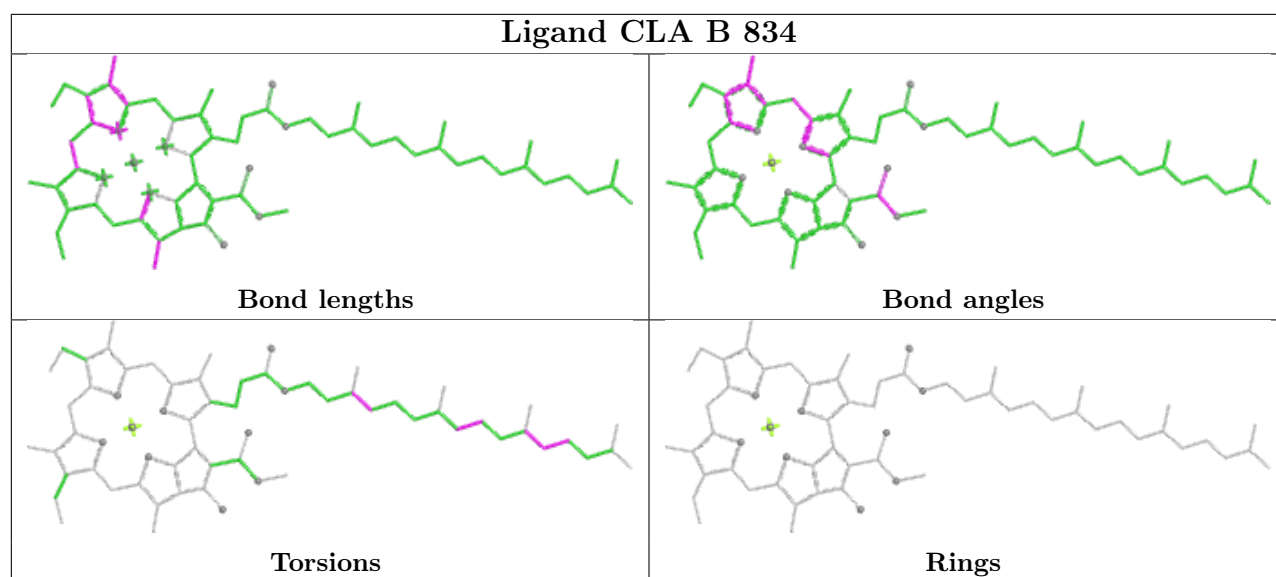


## Ligand CLA Q 610

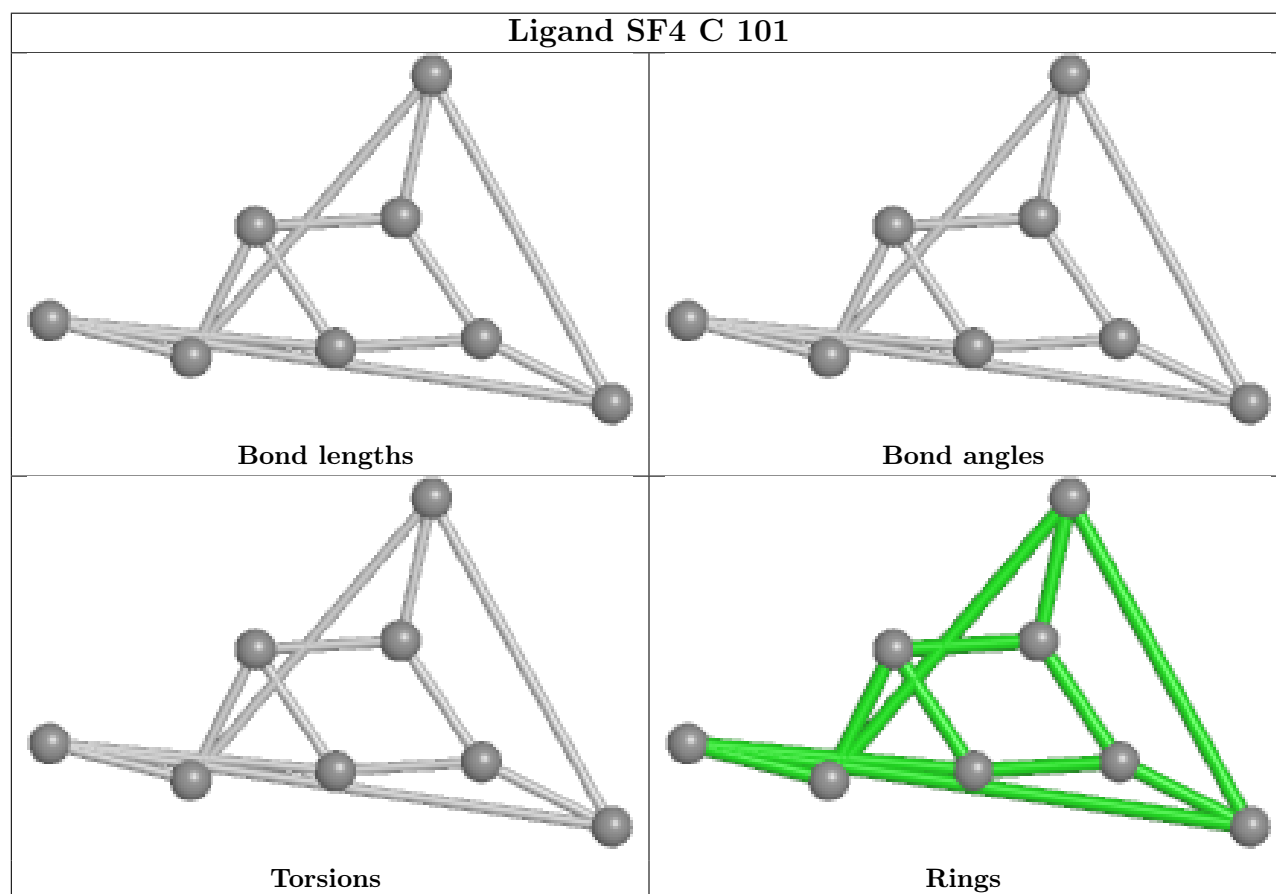
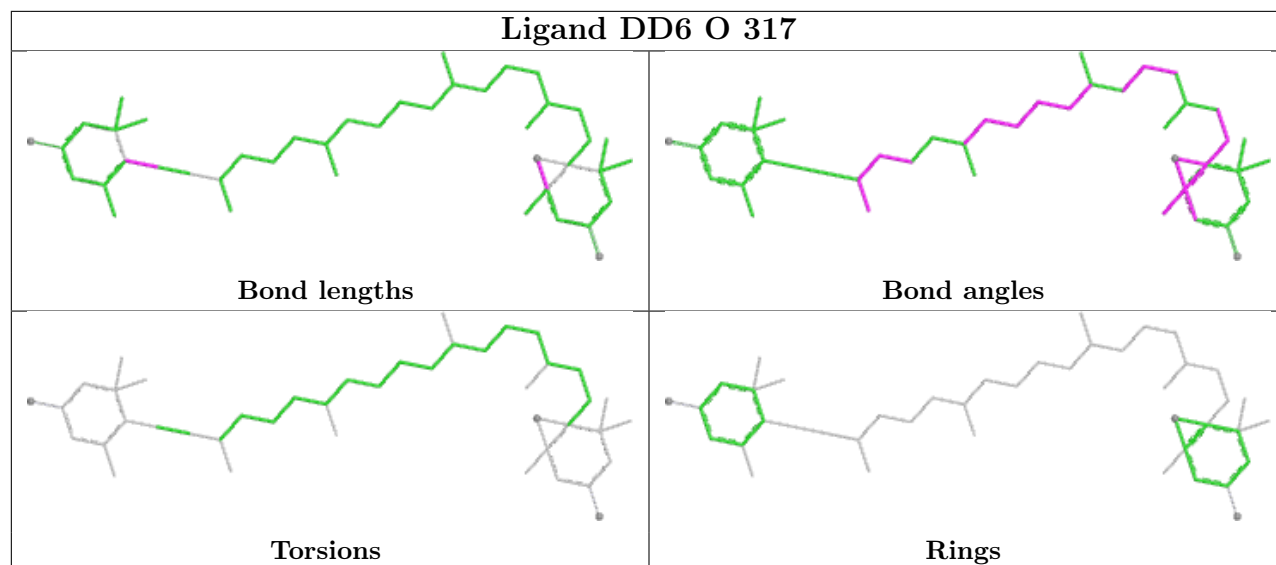


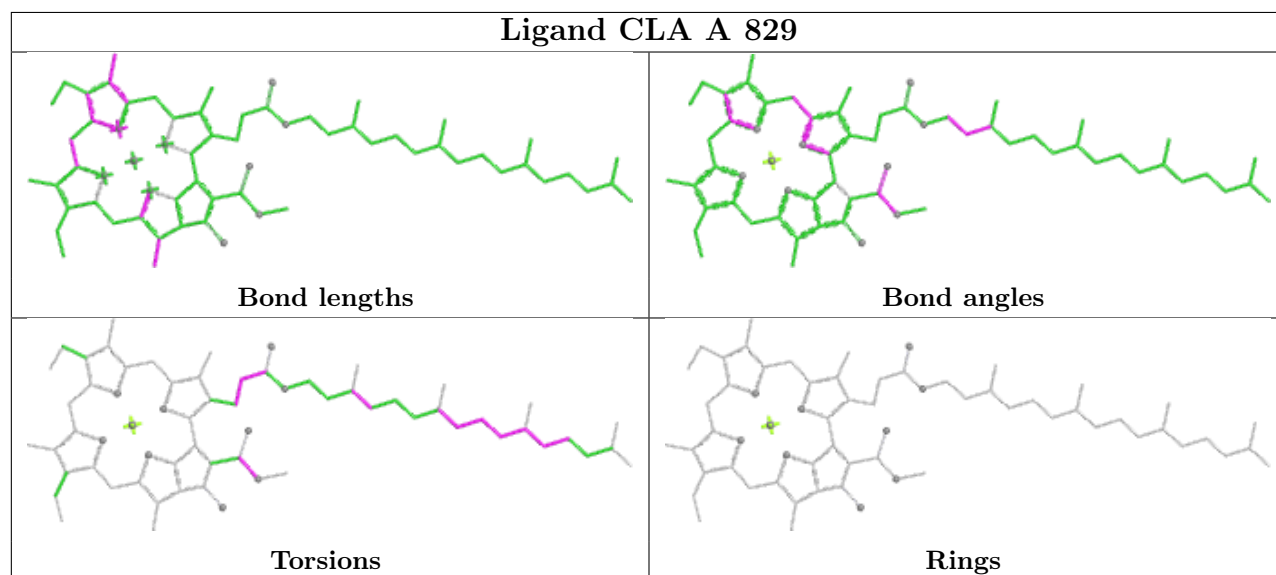
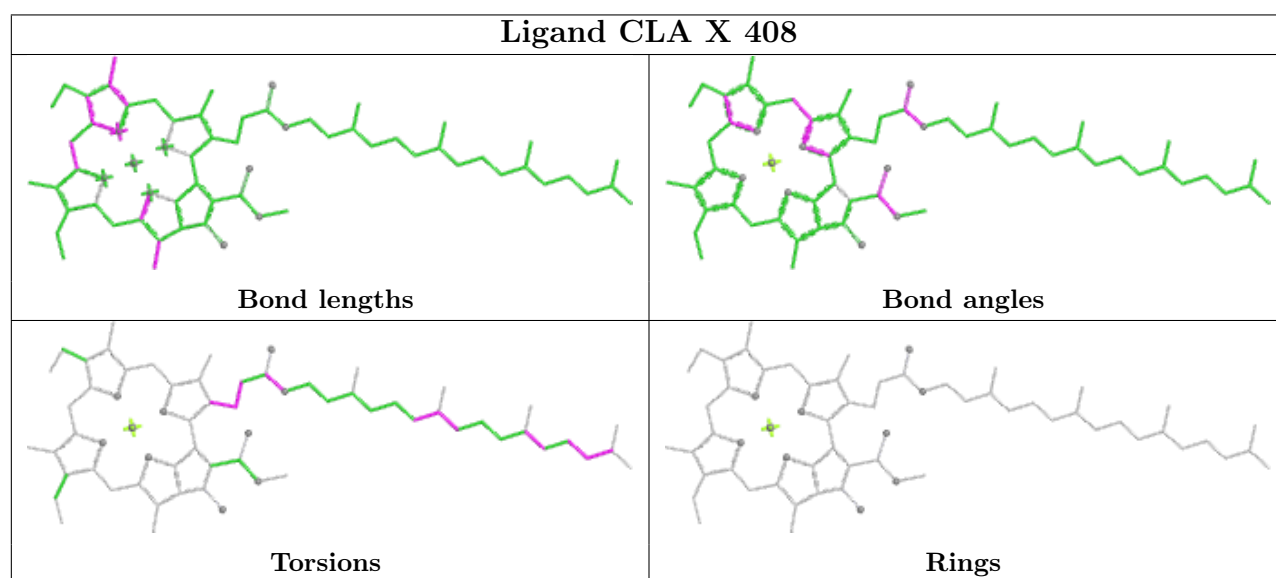
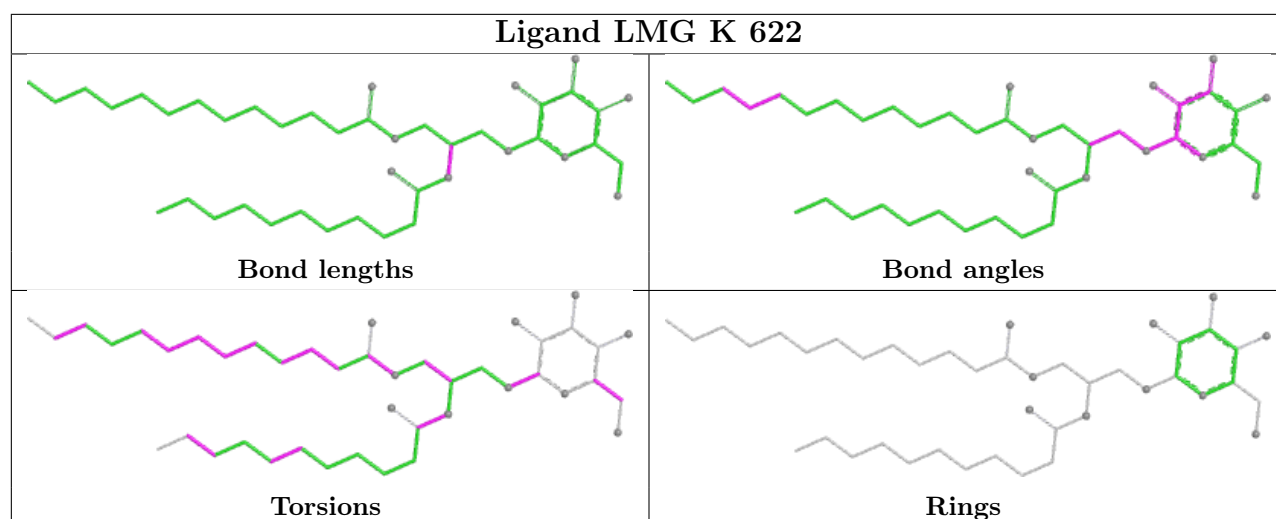
## Ligand SF4 B 860

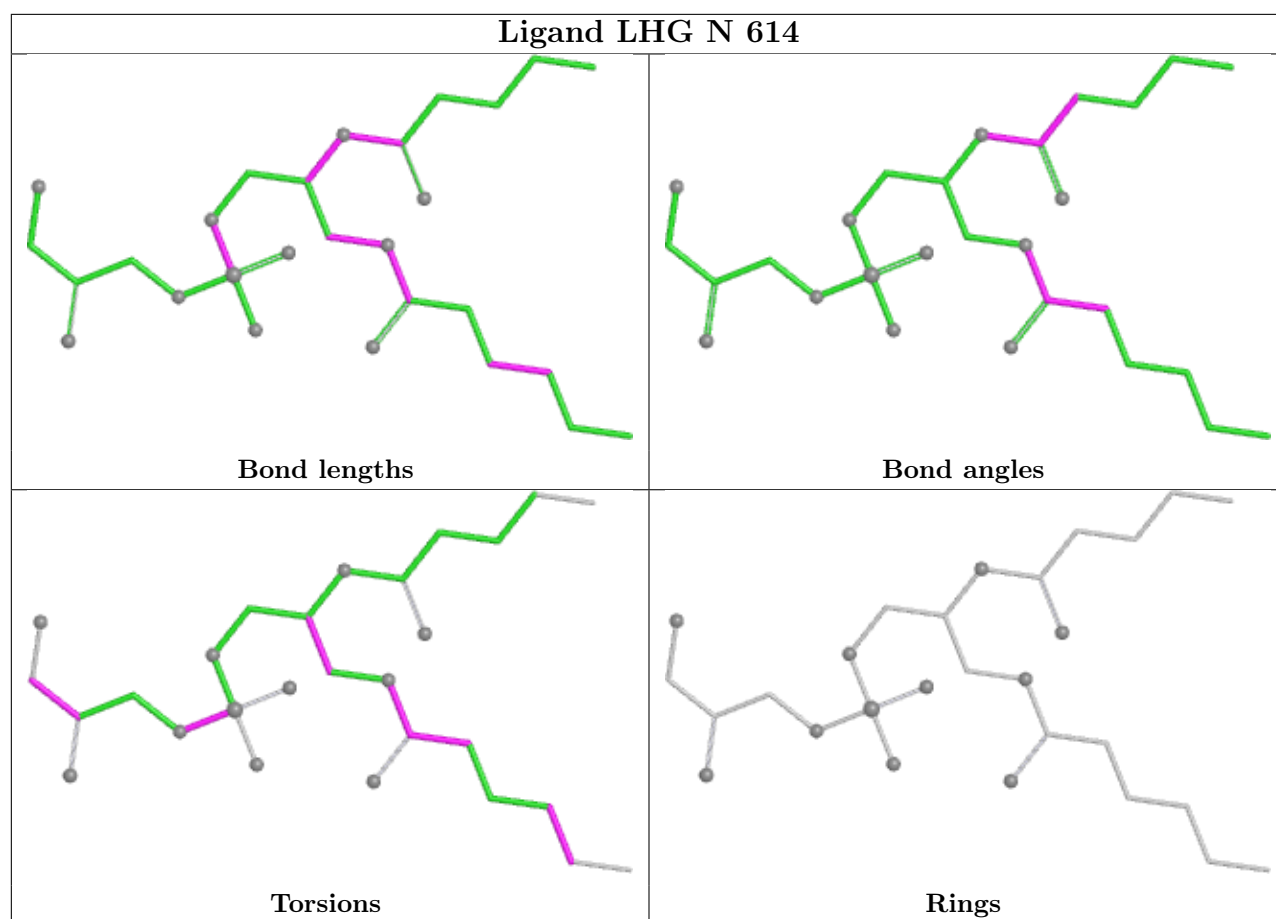


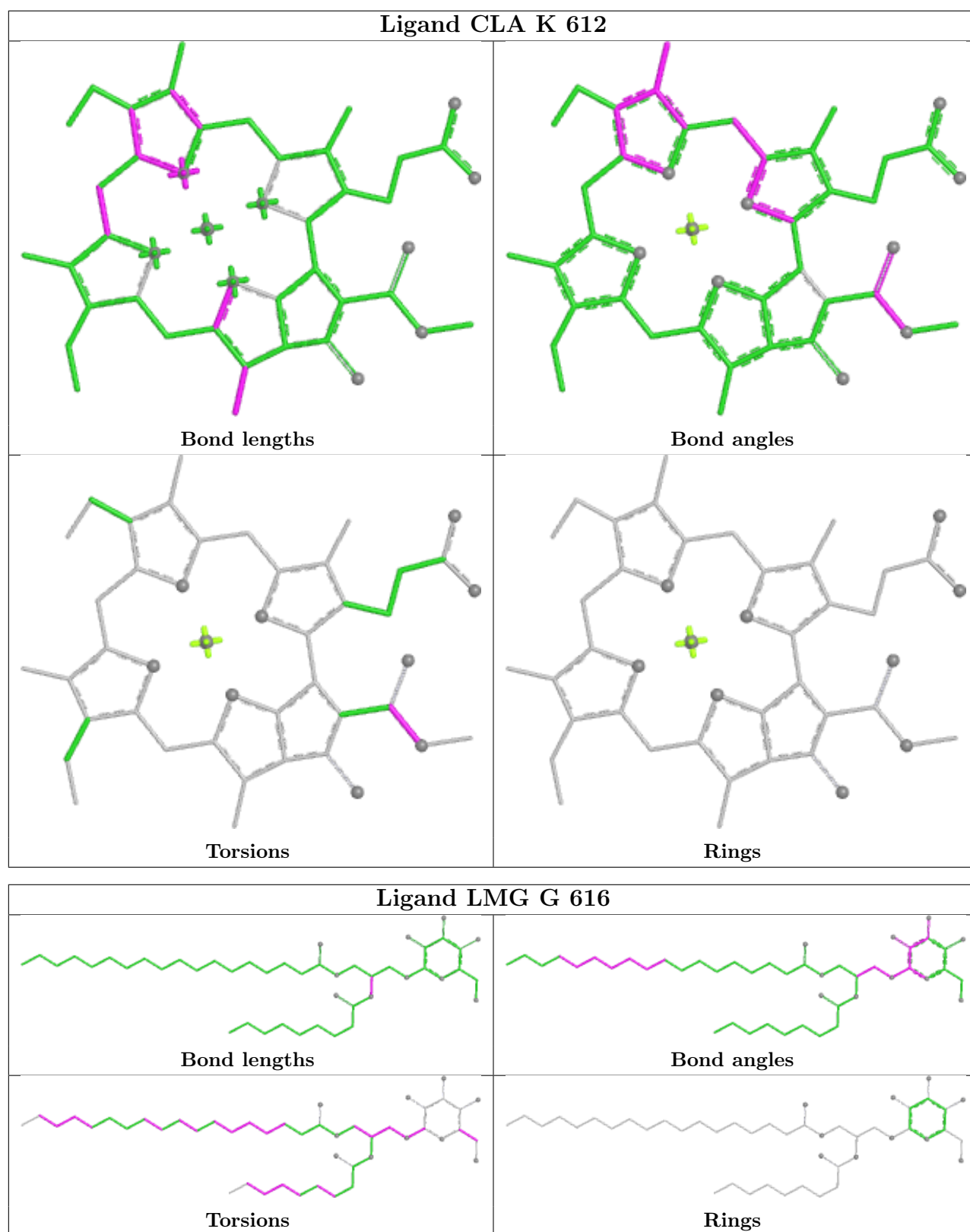


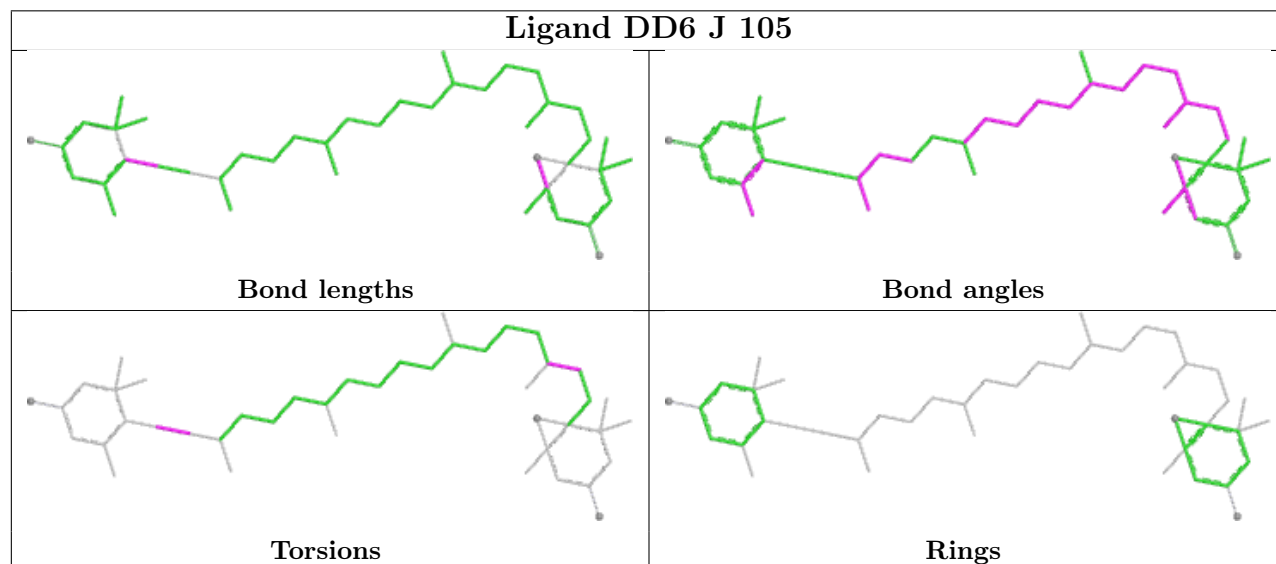
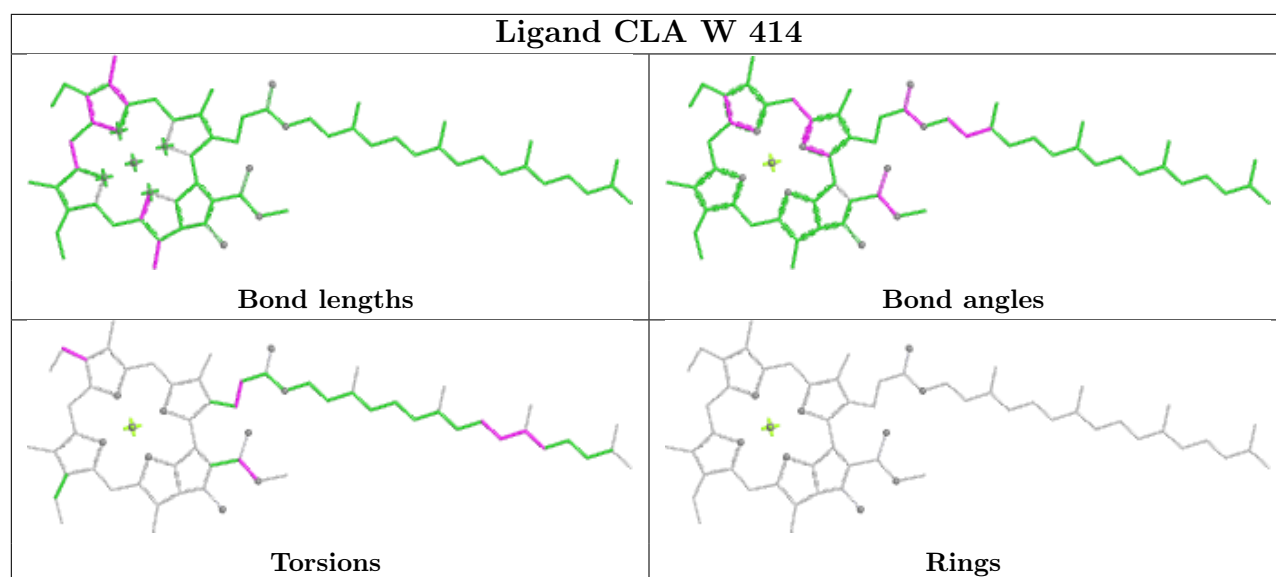


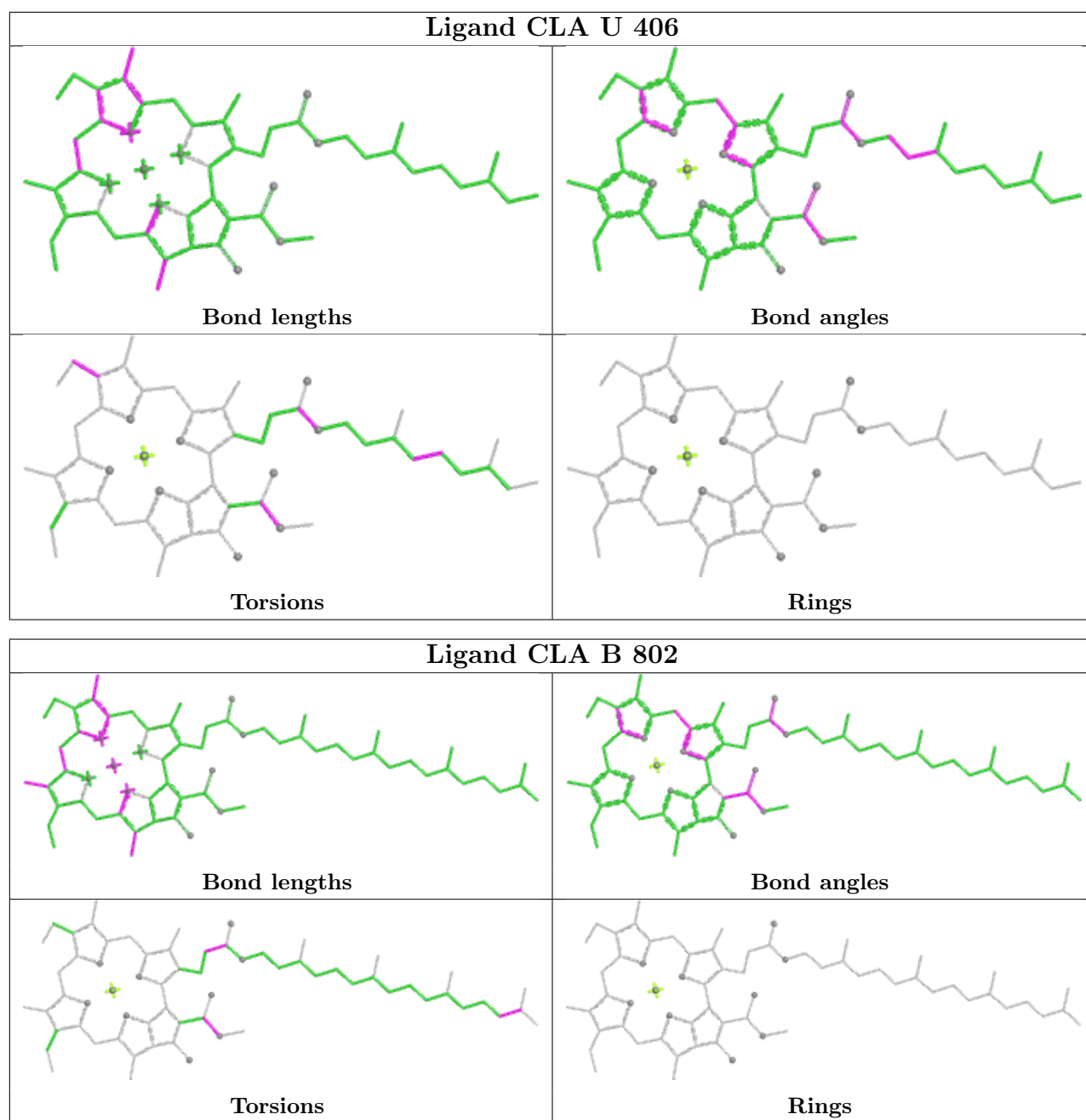




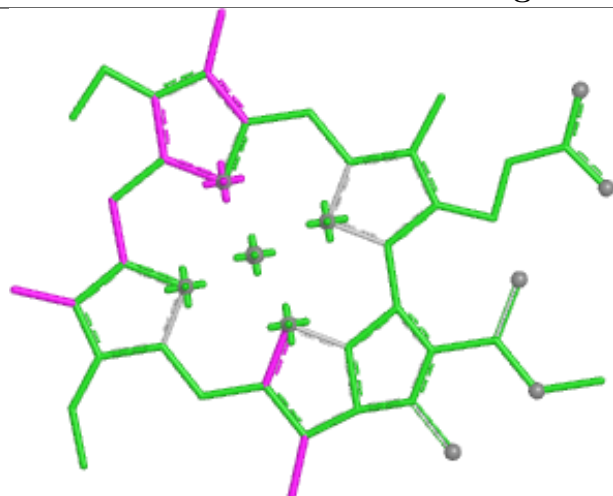




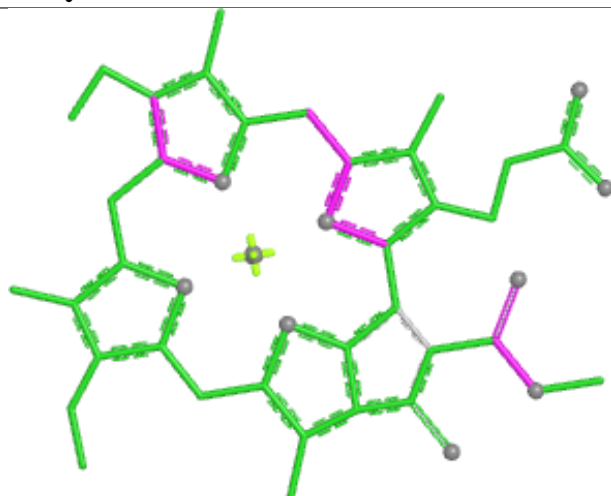




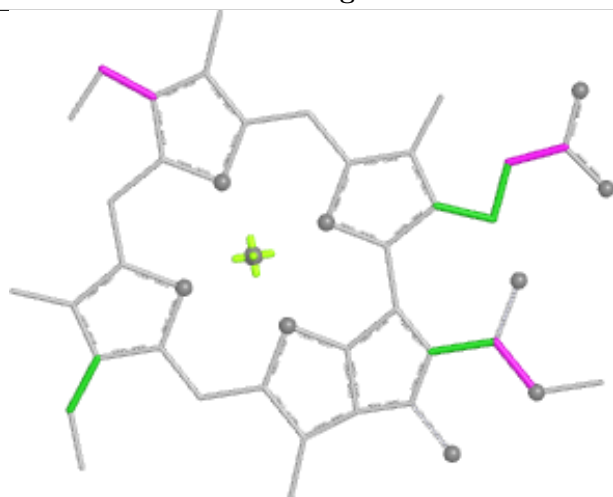
## Ligand CLA Q 601



Bond lengths



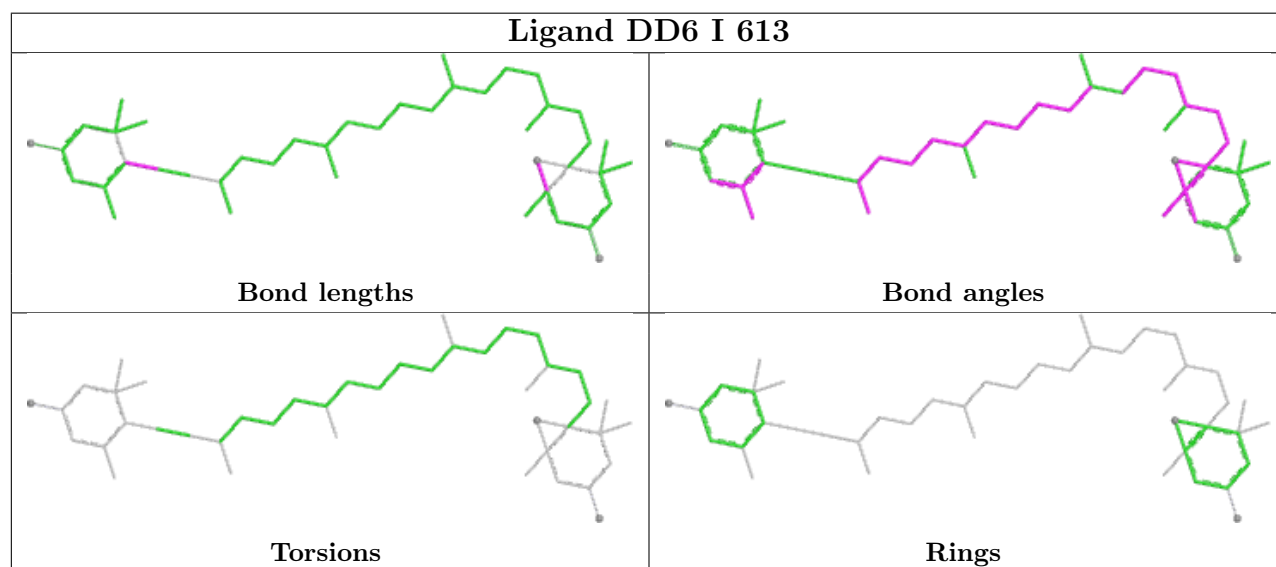
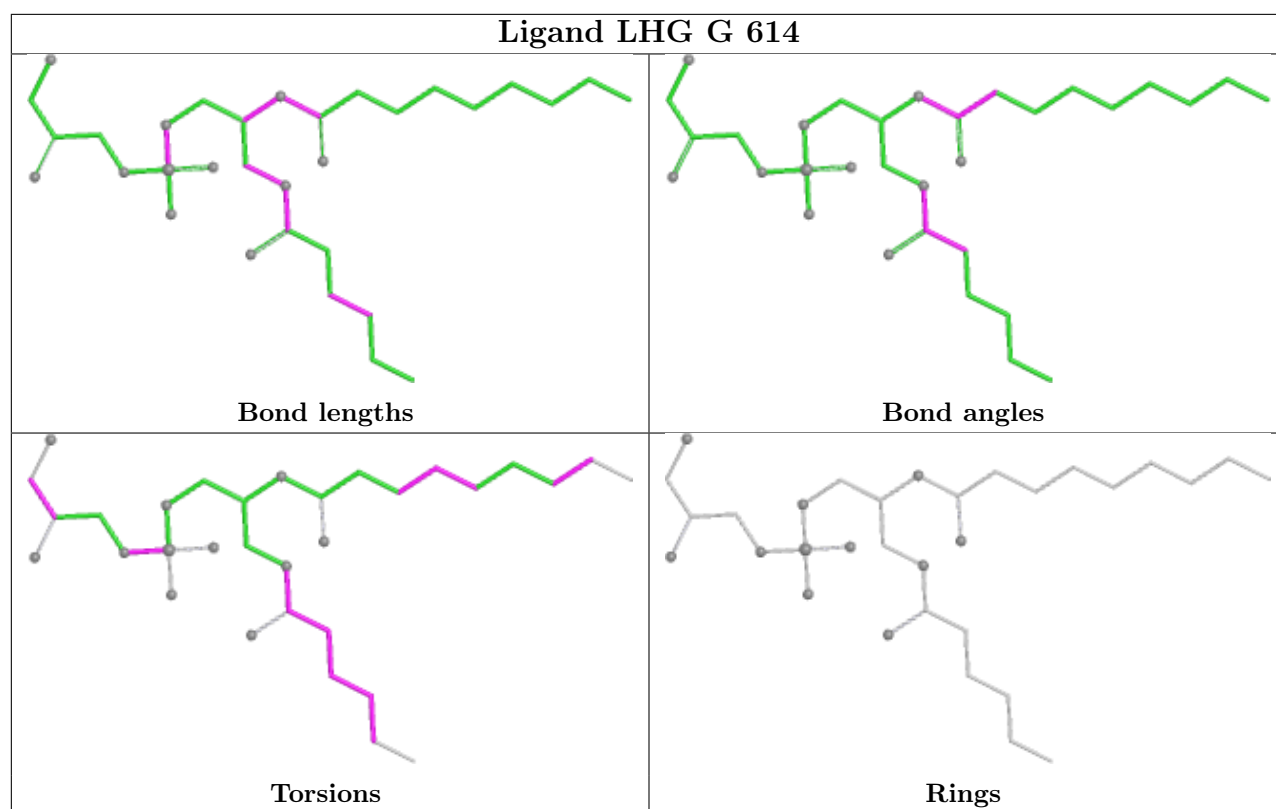
Bond angles



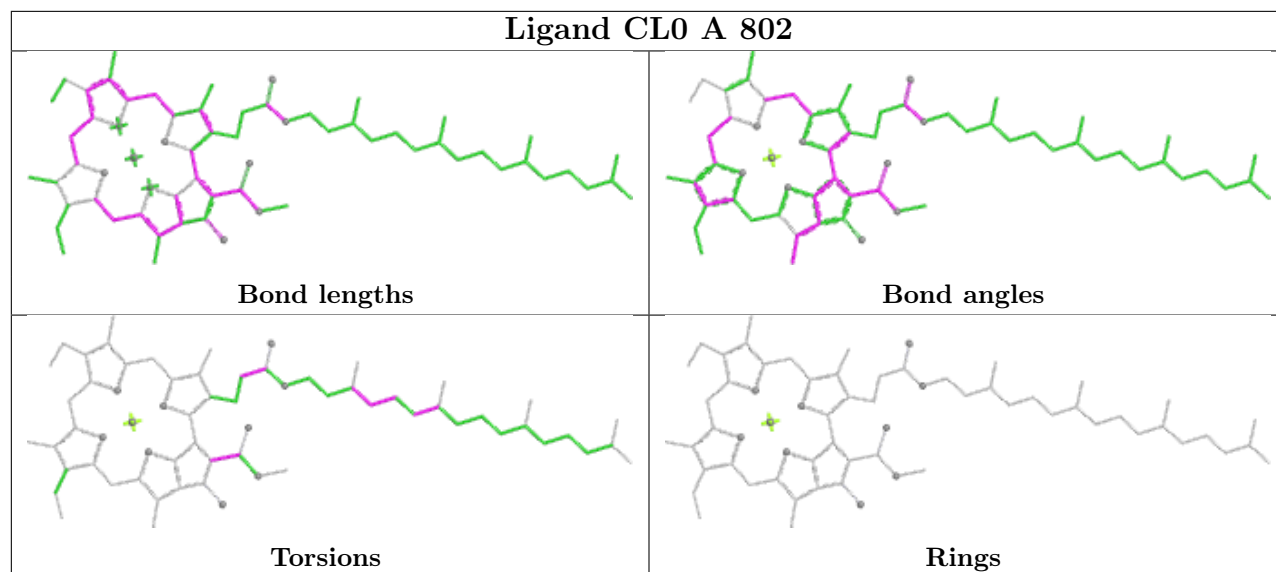
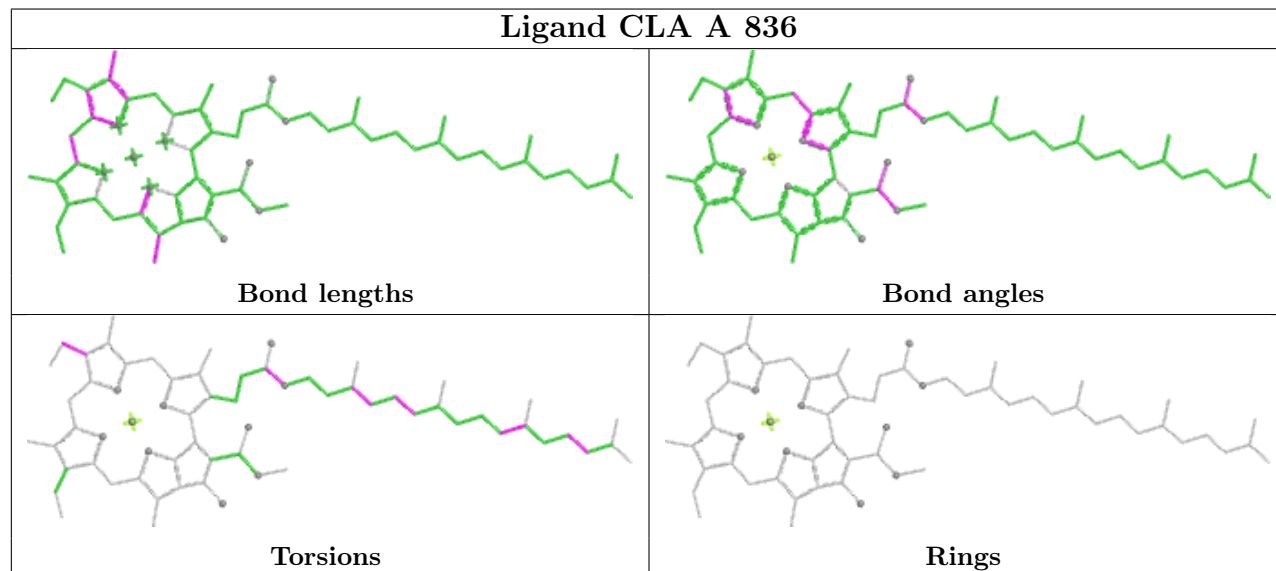
Torsions

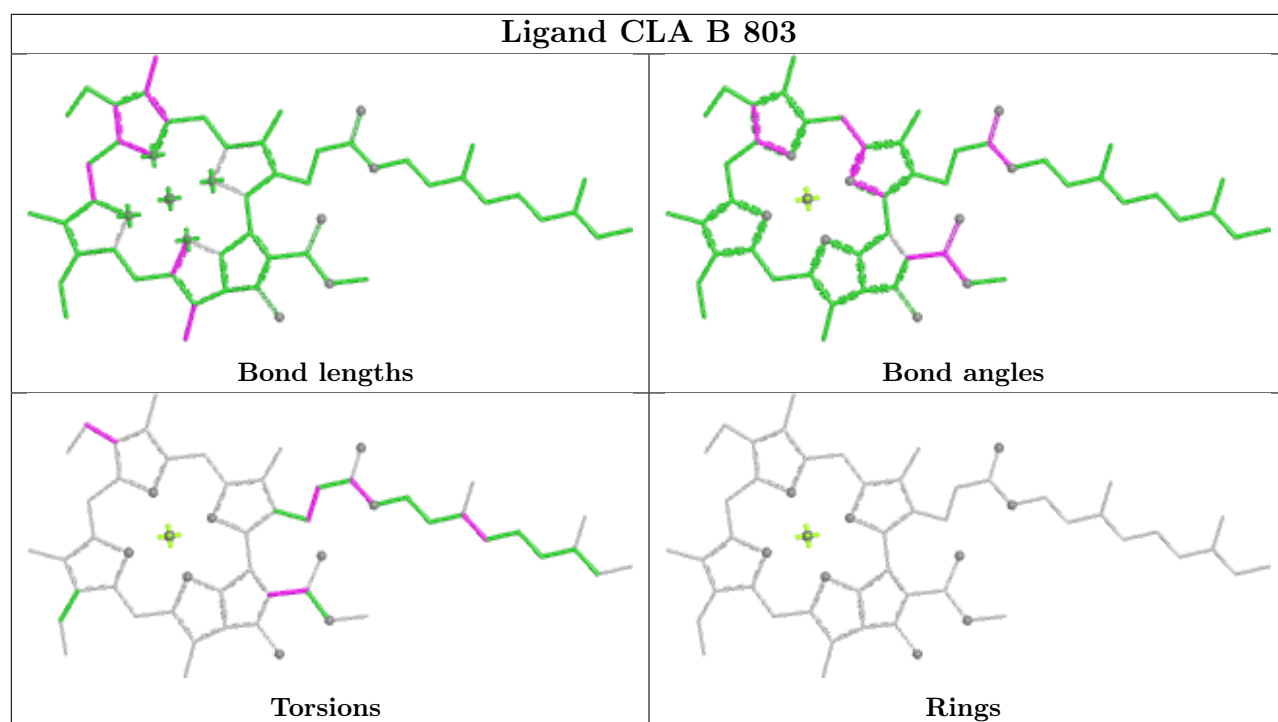


Rings

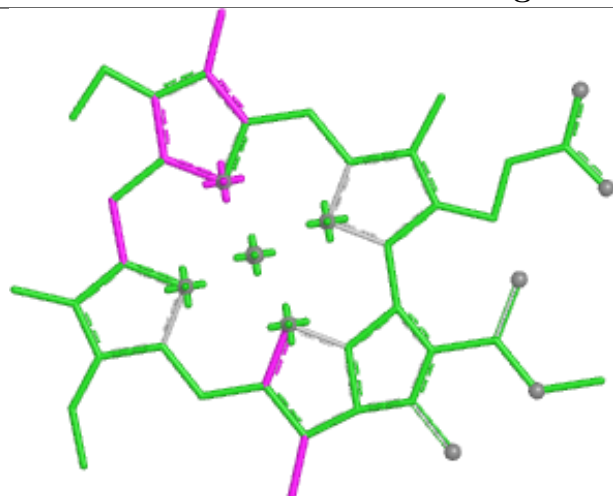




**Ligand CL0 A 802****Ligand CLA A 836**



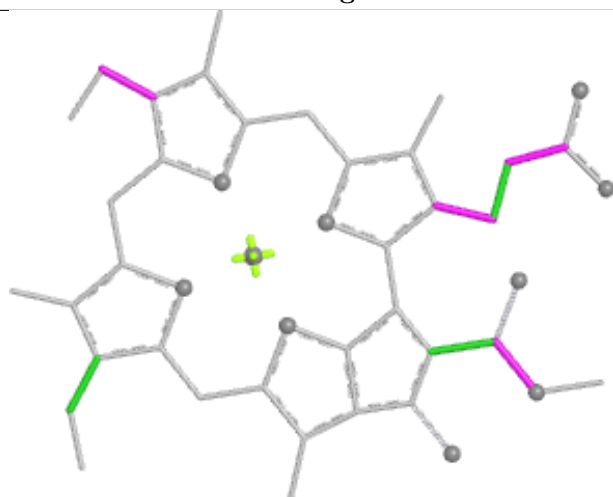
## Ligand CLA X 419



Bond lengths



Bond angles

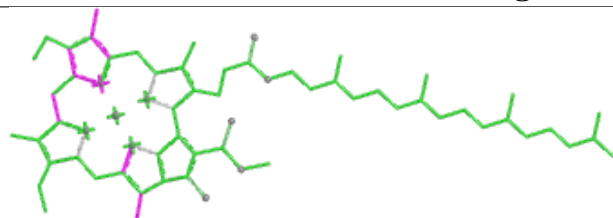


Torsions

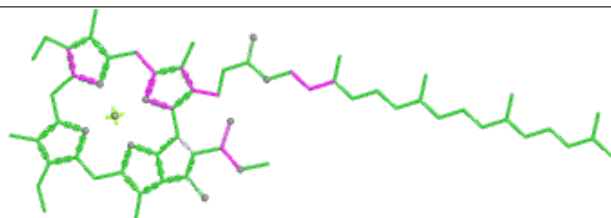


Rings

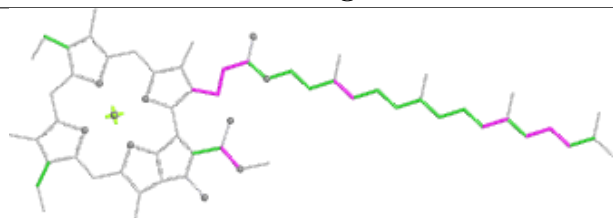
## Ligand CLA A 830



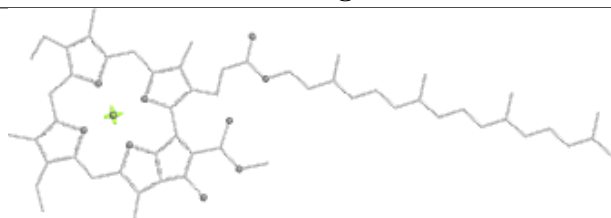
Bond lengths



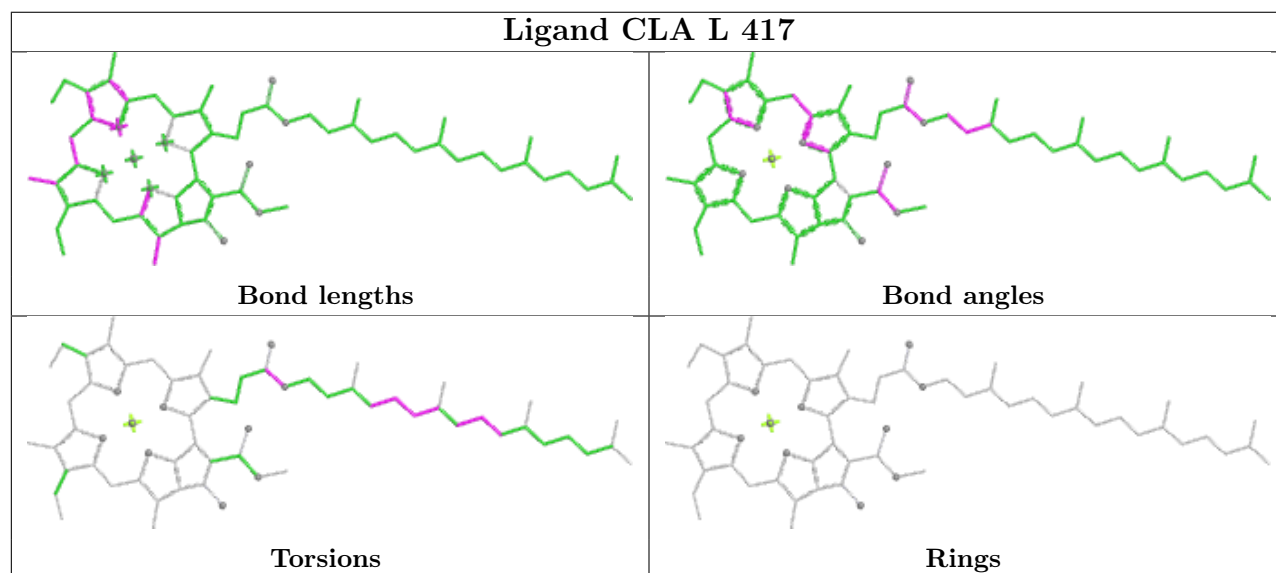
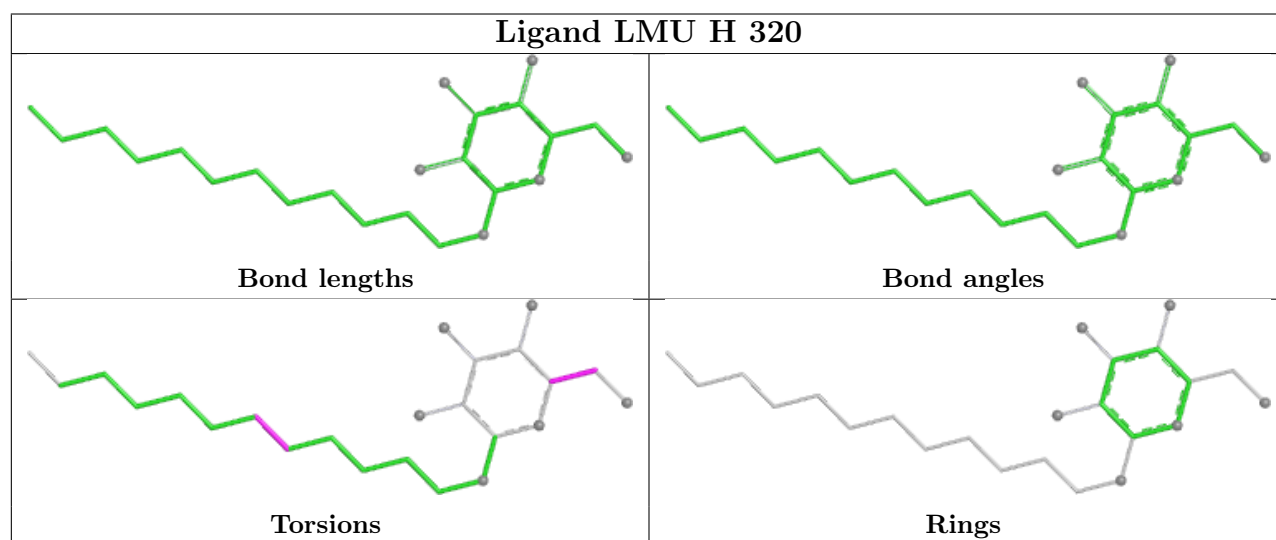
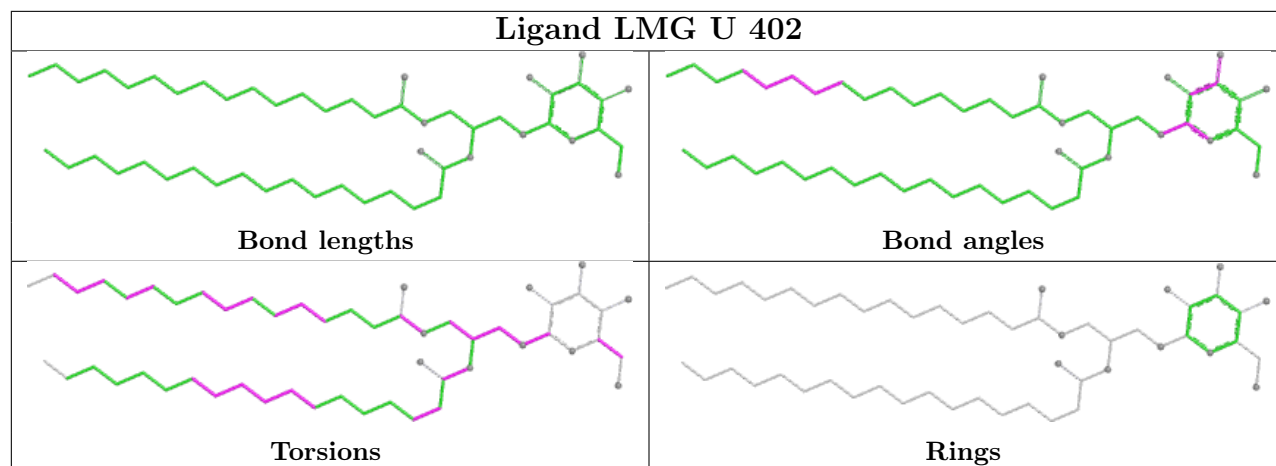
Bond angles



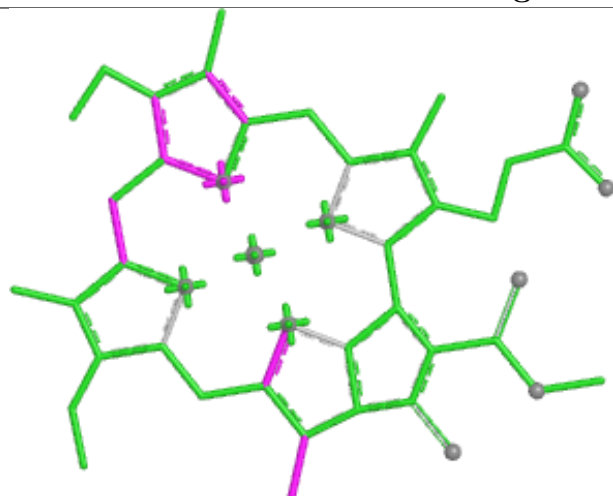
Torsions



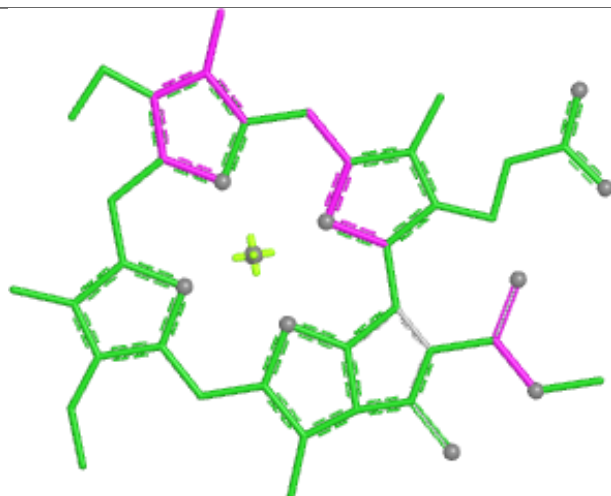
Rings



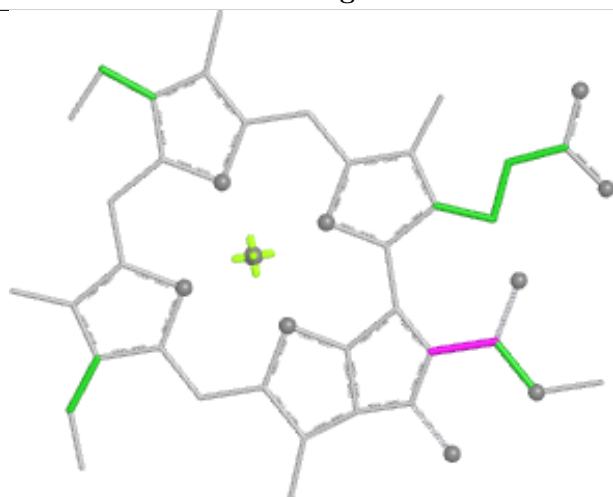
## Ligand CLA N 605



Bond lengths



Bond angles

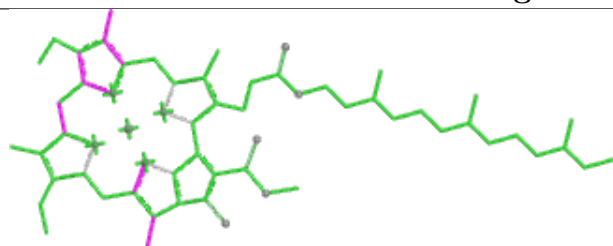


Torsions

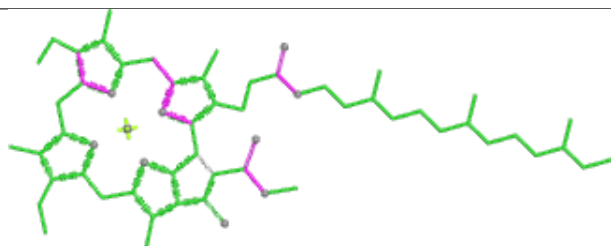


Rings

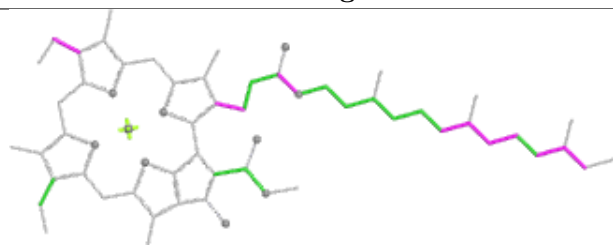
## Ligand CLA A 825



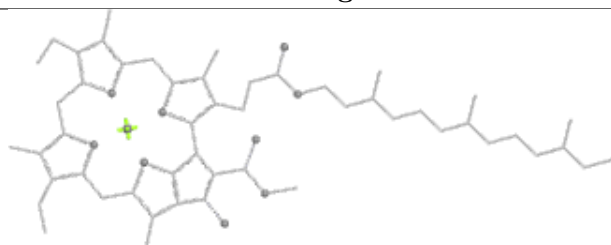
Bond lengths



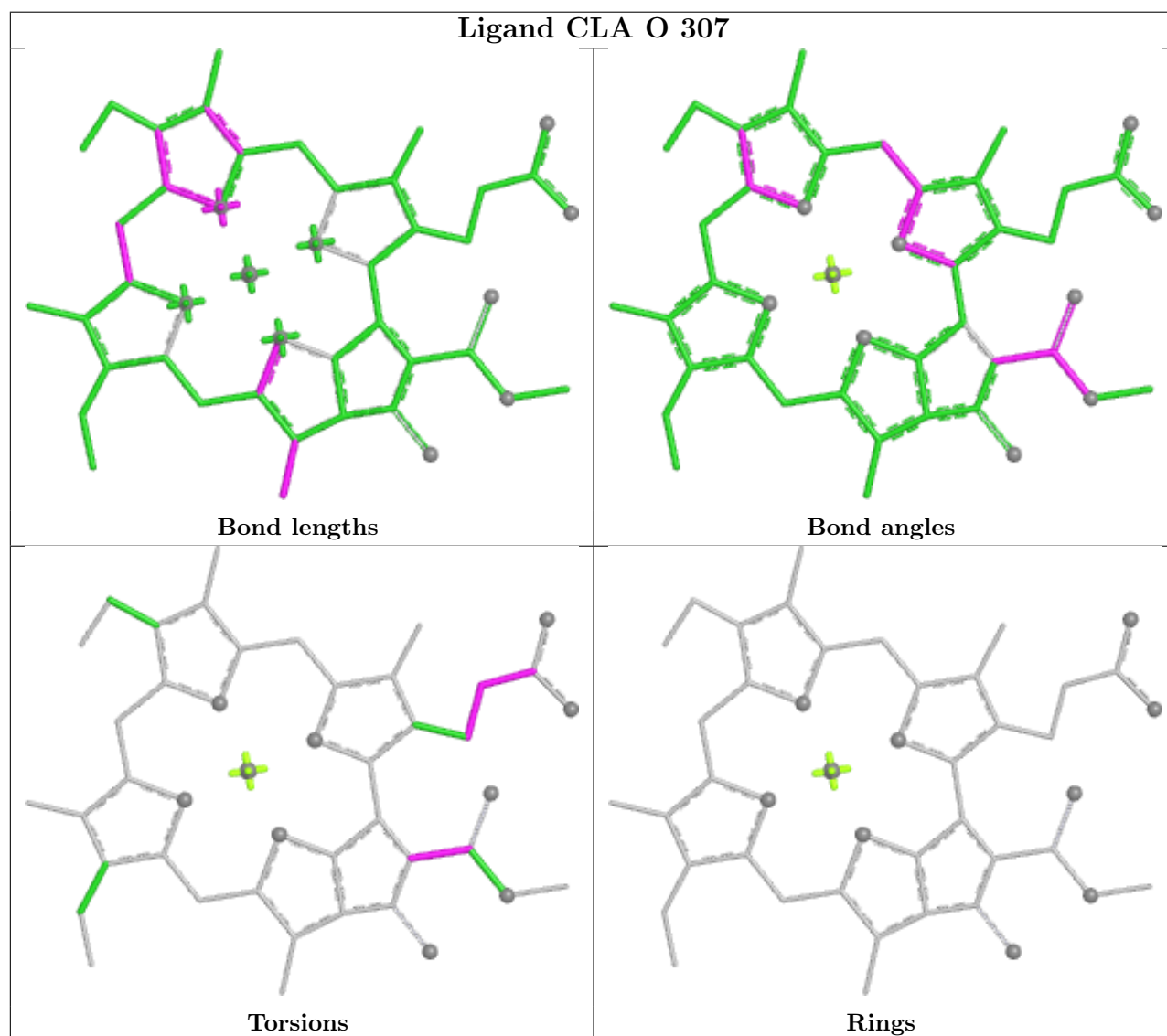
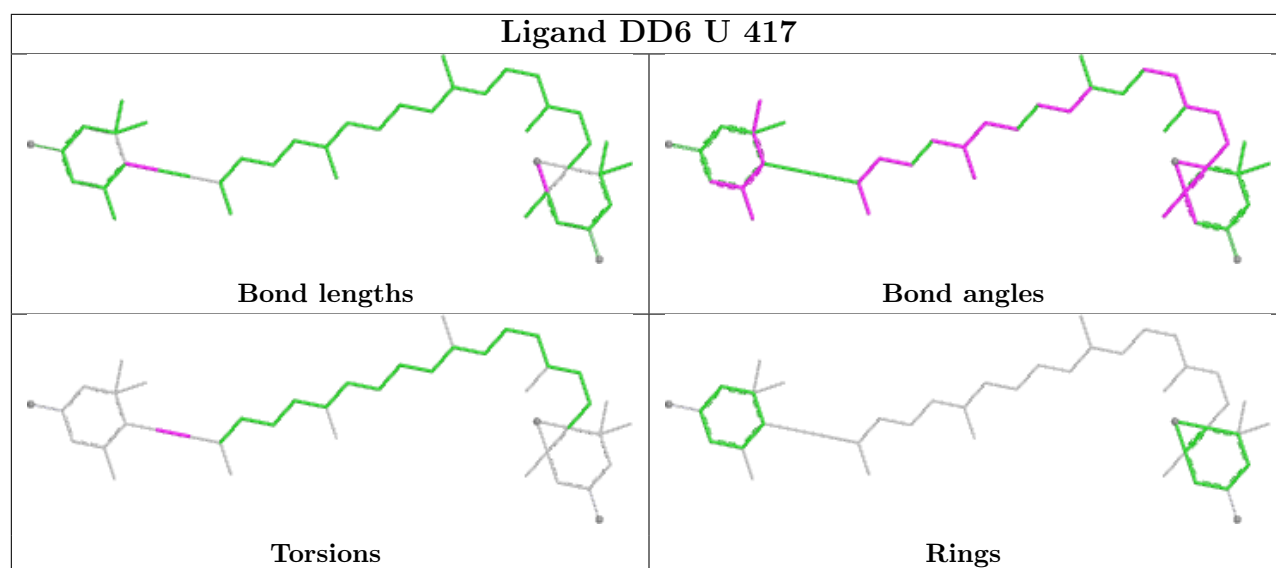
Bond angles

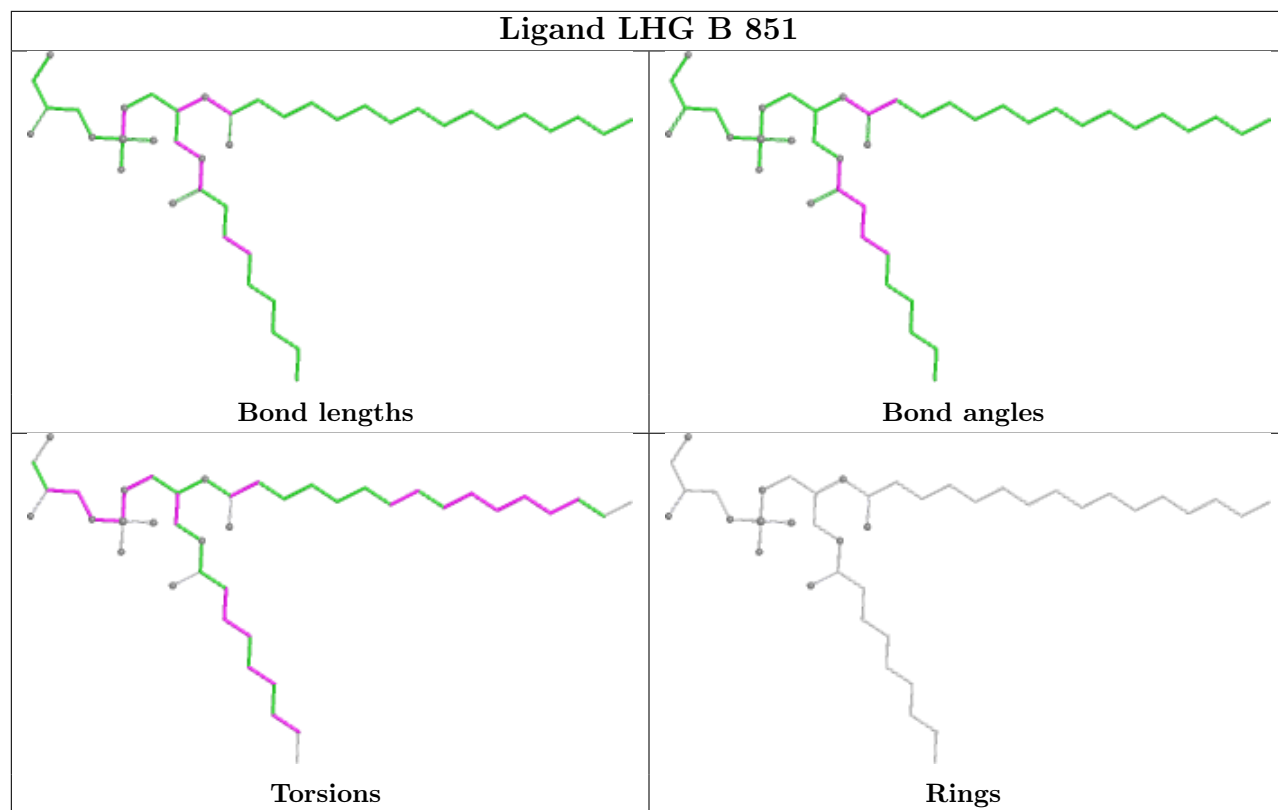


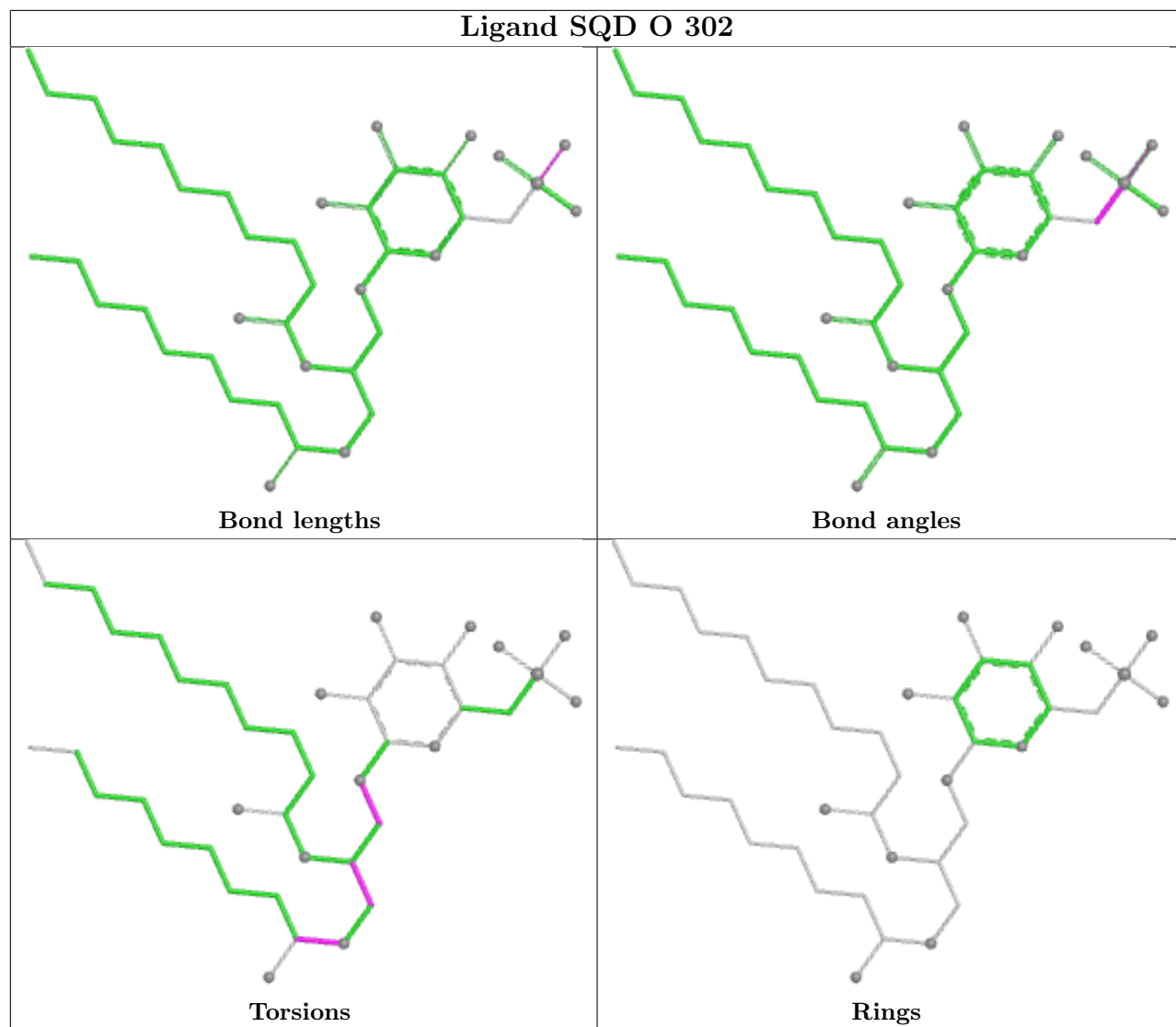
Torsions



Rings

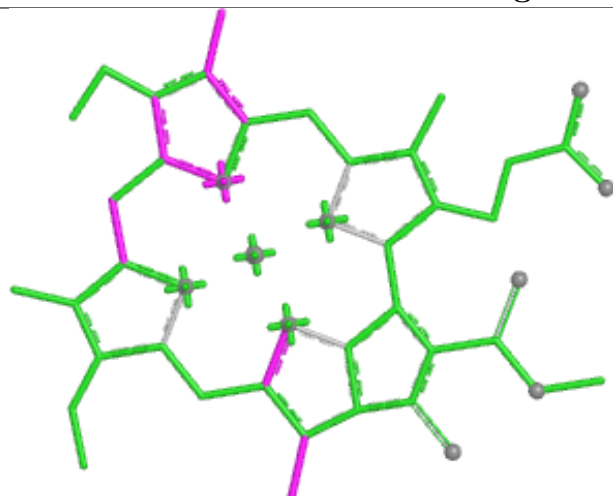




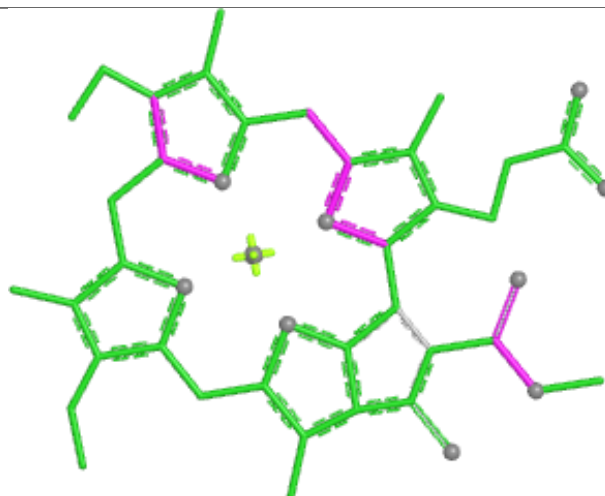




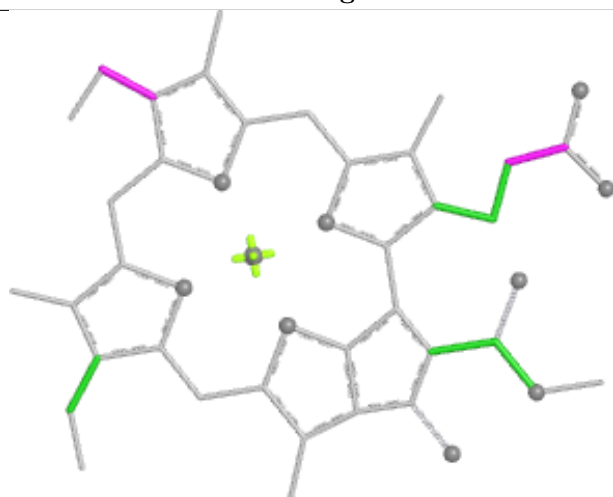
## Ligand CLA A 834



Bond lengths



Bond angles

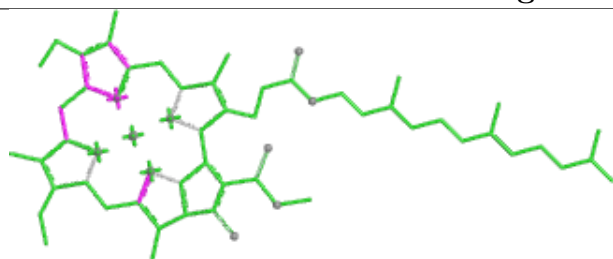


Torsions

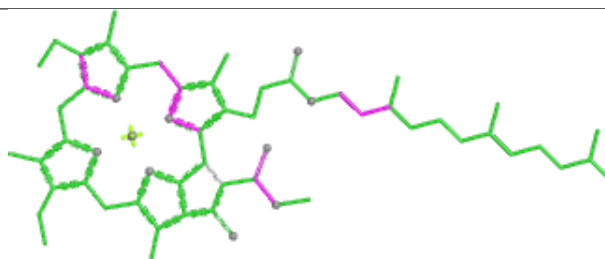


Rings

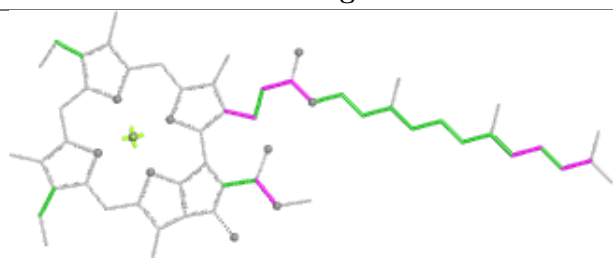
## Ligand CLA S 607



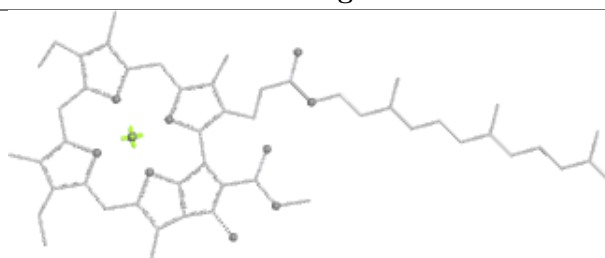
Bond lengths



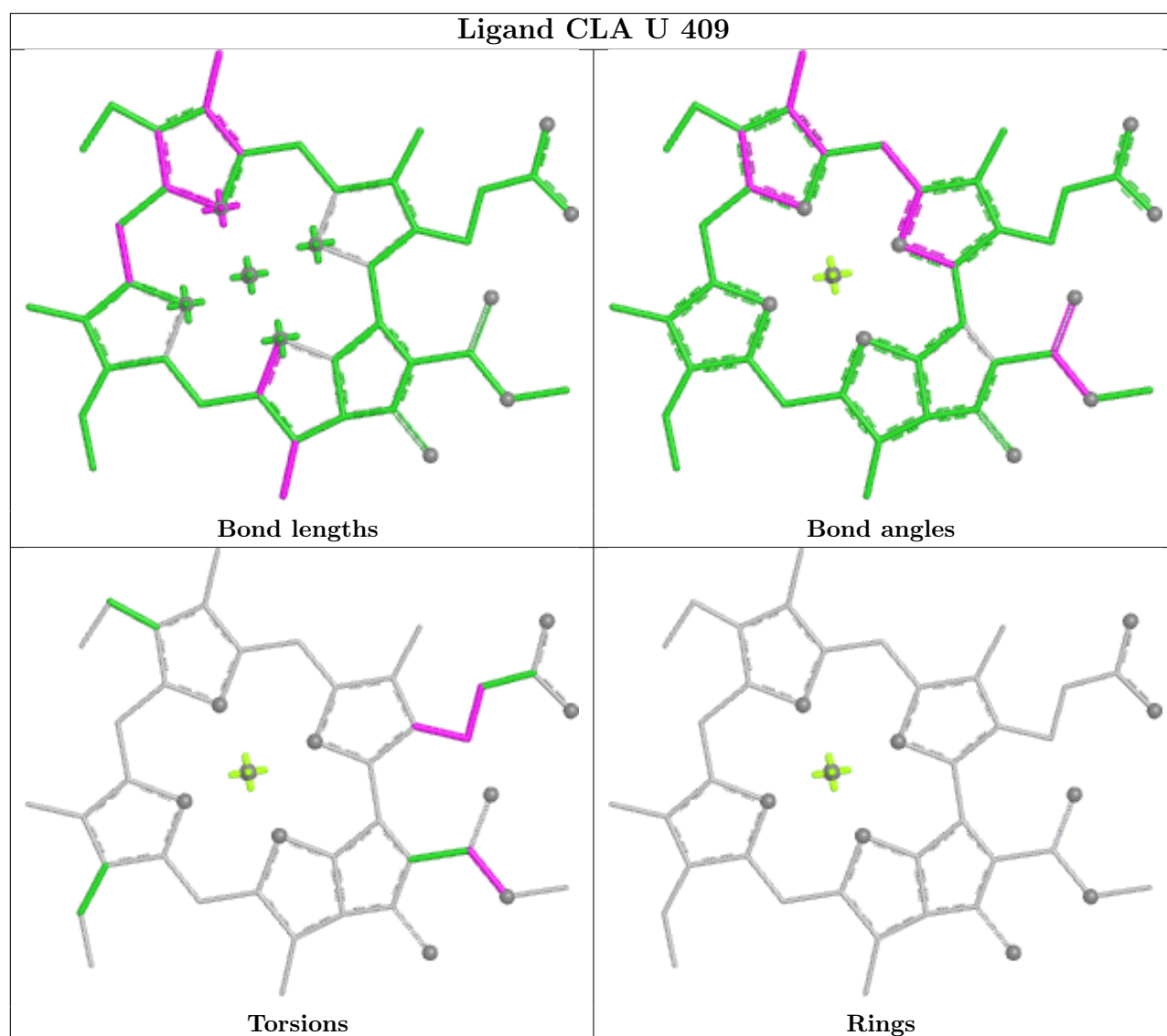
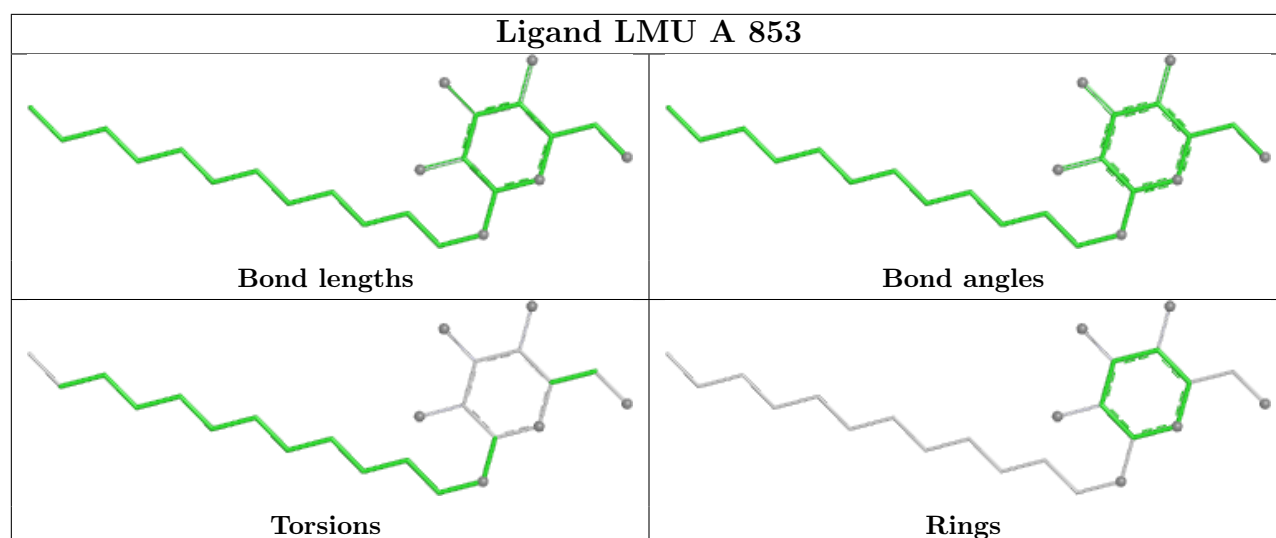
Bond angles

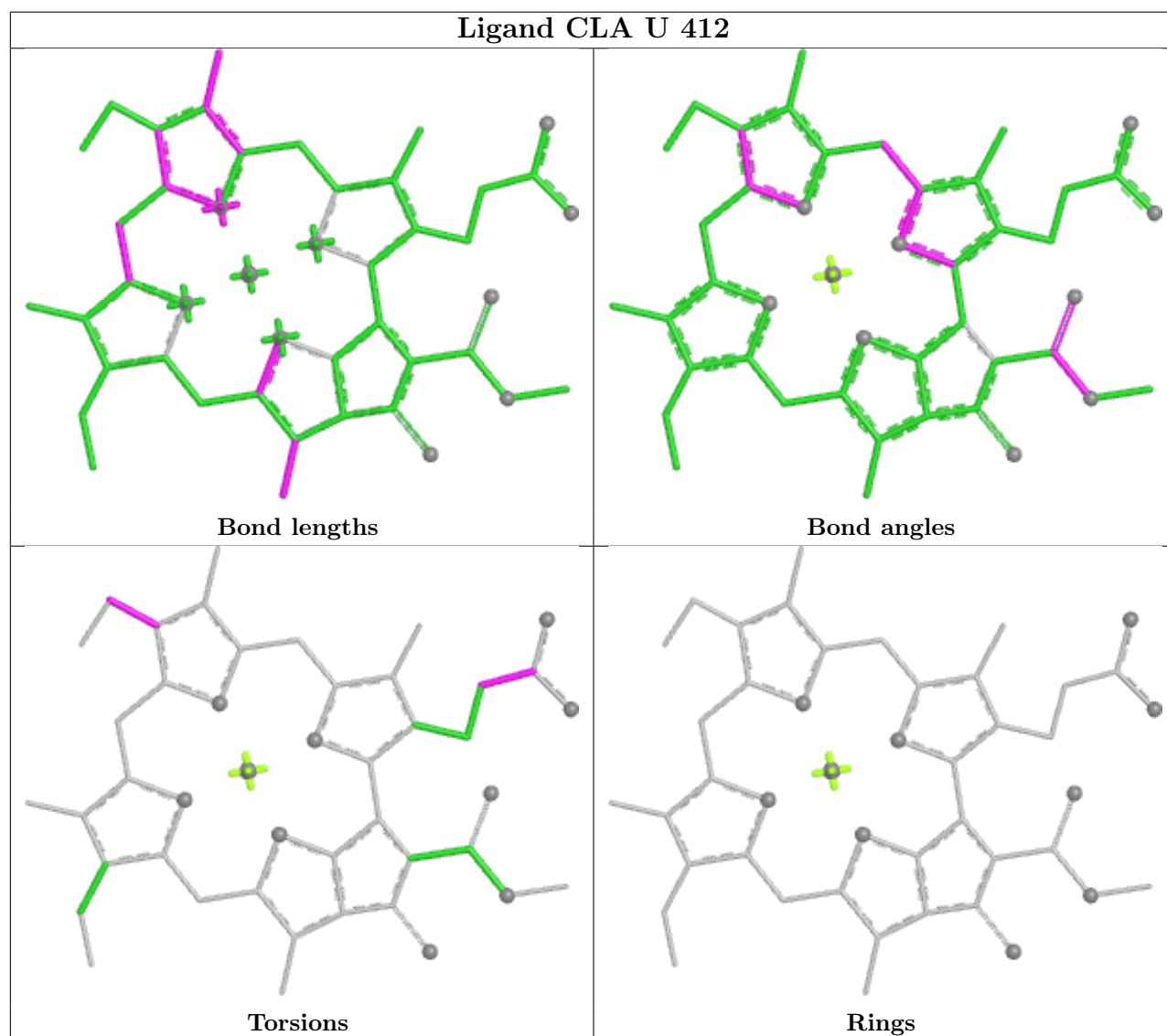
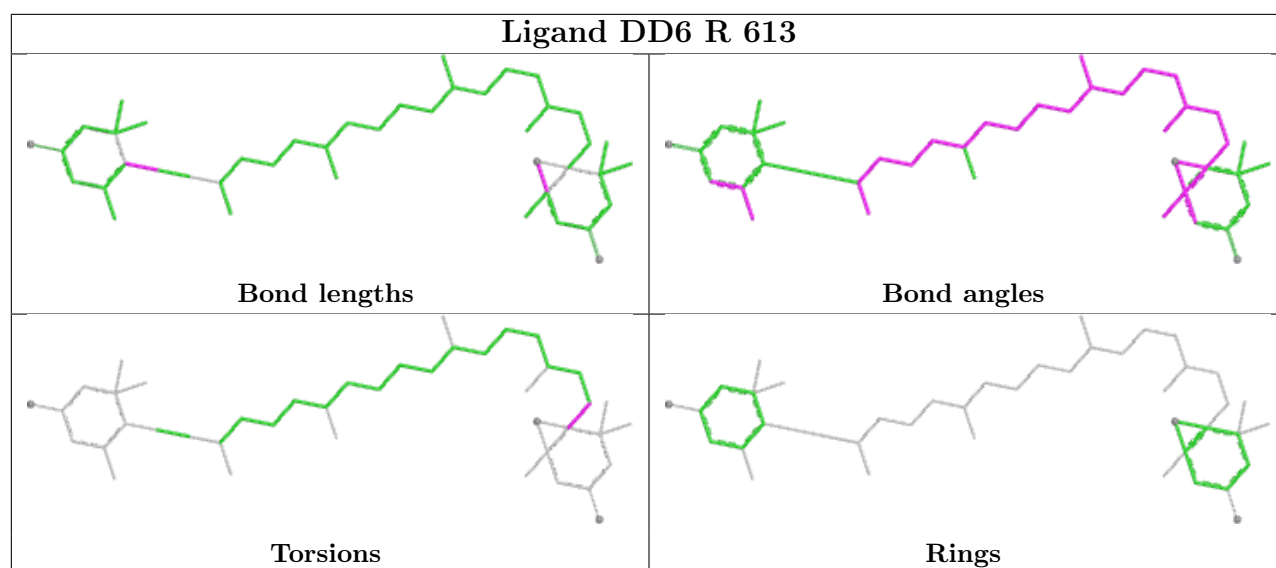


Torsions



Rings





## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

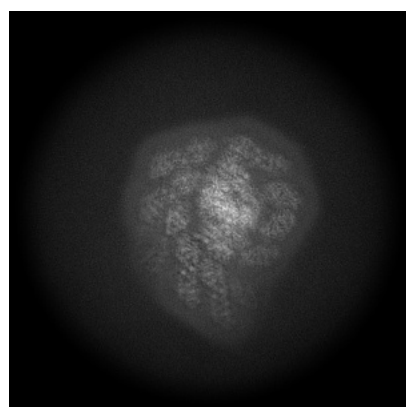
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-63994. These allow visual inspection of the internal detail of the map and identification of artifacts.

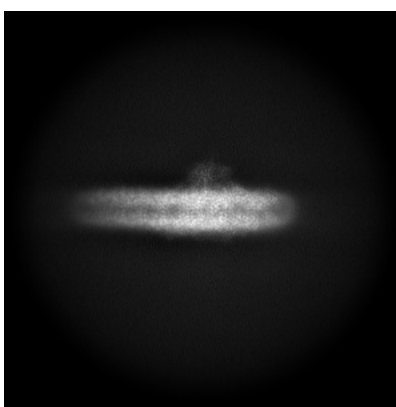
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

### 6.1 Orthogonal projections [i](#)

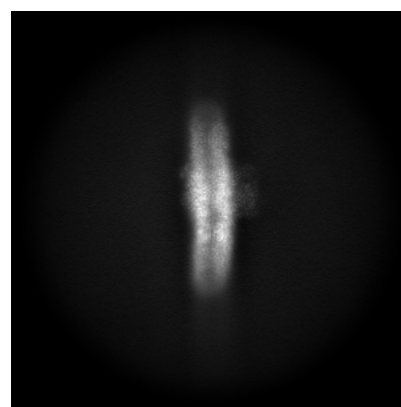
#### 6.1.1 Primary map



X



Y

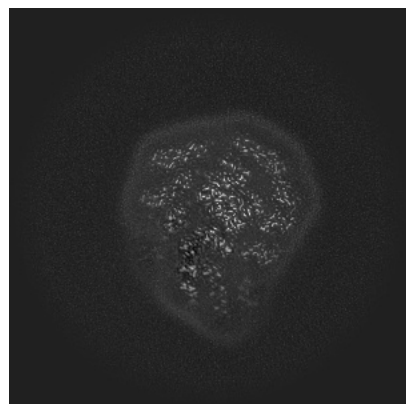


Z

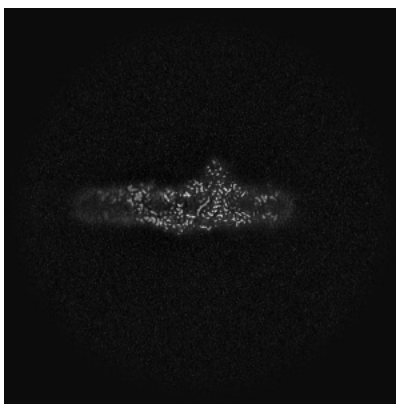
The images above show the map projected in three orthogonal directions.

### 6.2 Central slices [i](#)

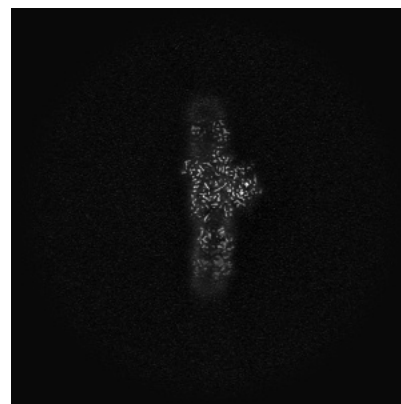
#### 6.2.1 Primary map



X Index: 256



Y Index: 256

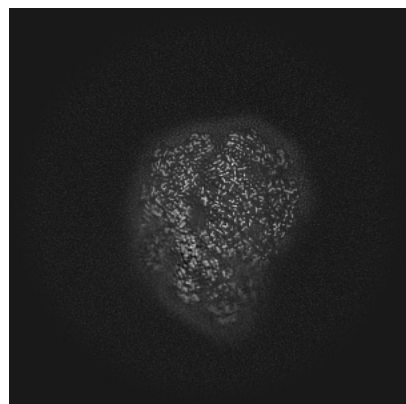


Z Index: 256

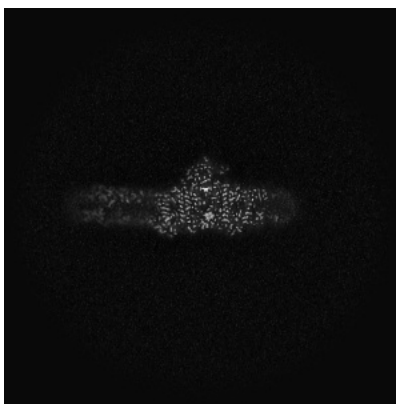
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

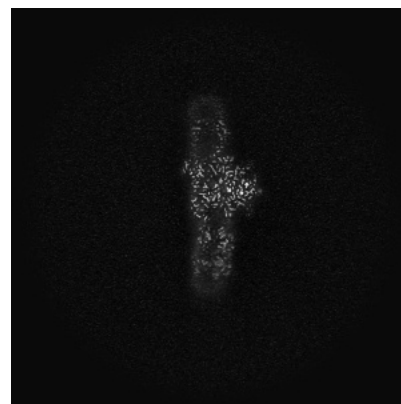
### 6.3.1 Primary map



X Index: 270



Y Index: 278

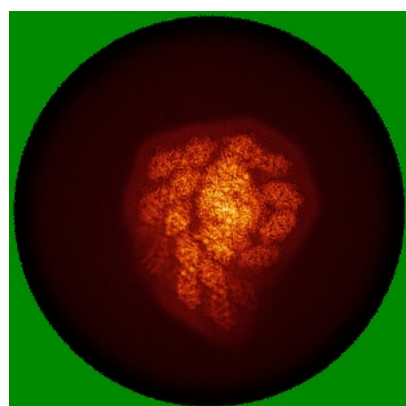


Z Index: 257

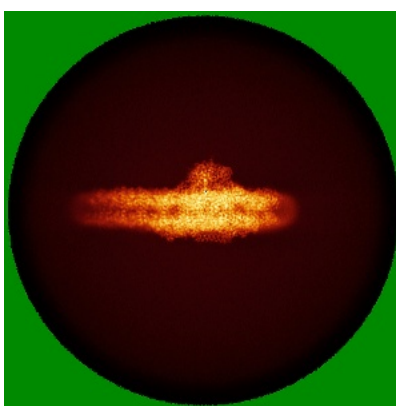
The images above show the largest variance slices of the map in three orthogonal directions.

## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

### 6.4.1 Primary map



X



Y



Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.04. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

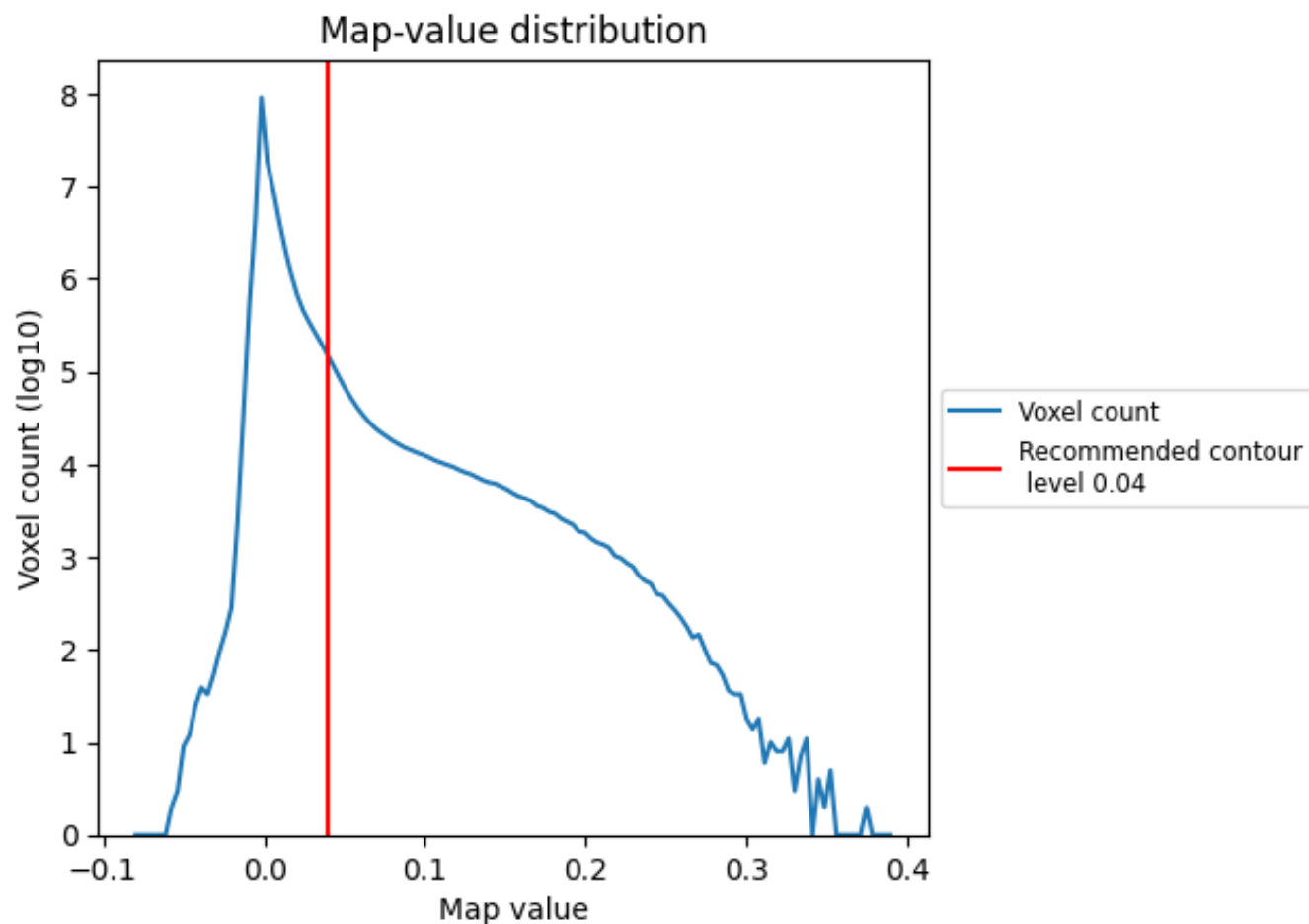
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

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

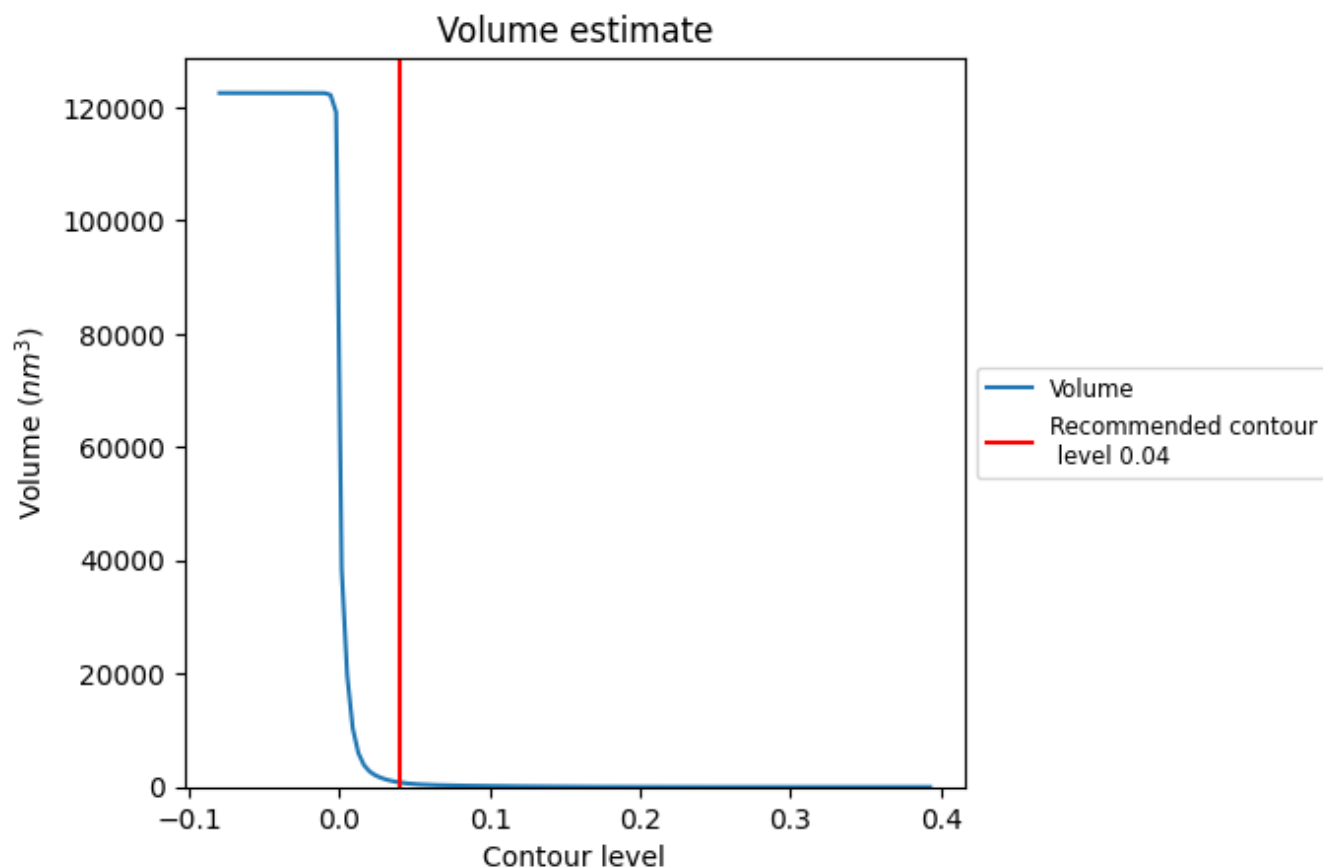
### 7.1 Map-value distribution [i](#)



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



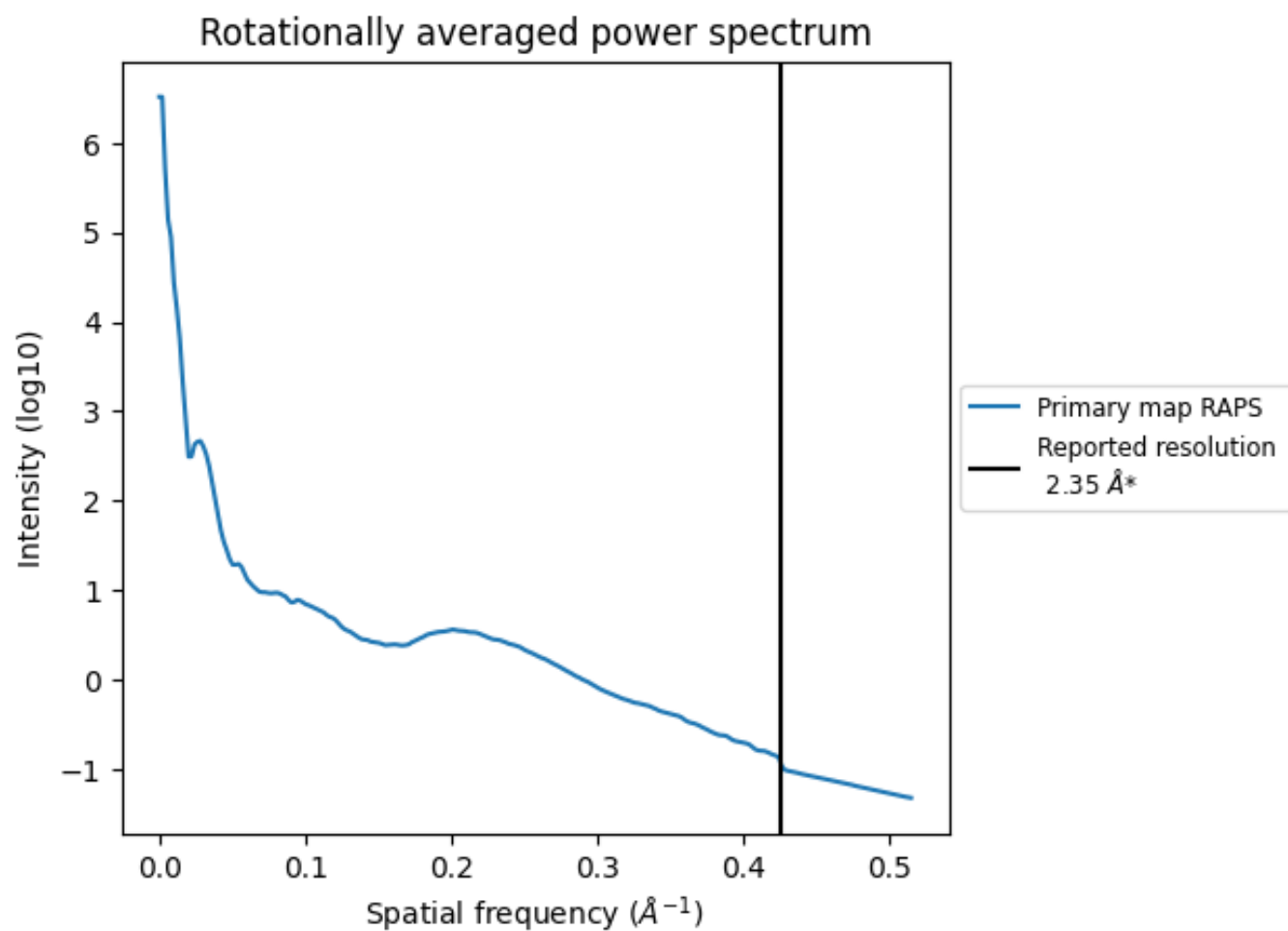
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 801  $\text{nm}^3$ ; this corresponds to an approximate mass of 724 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

### 7.3 Rotationally averaged power spectrum ⓘ

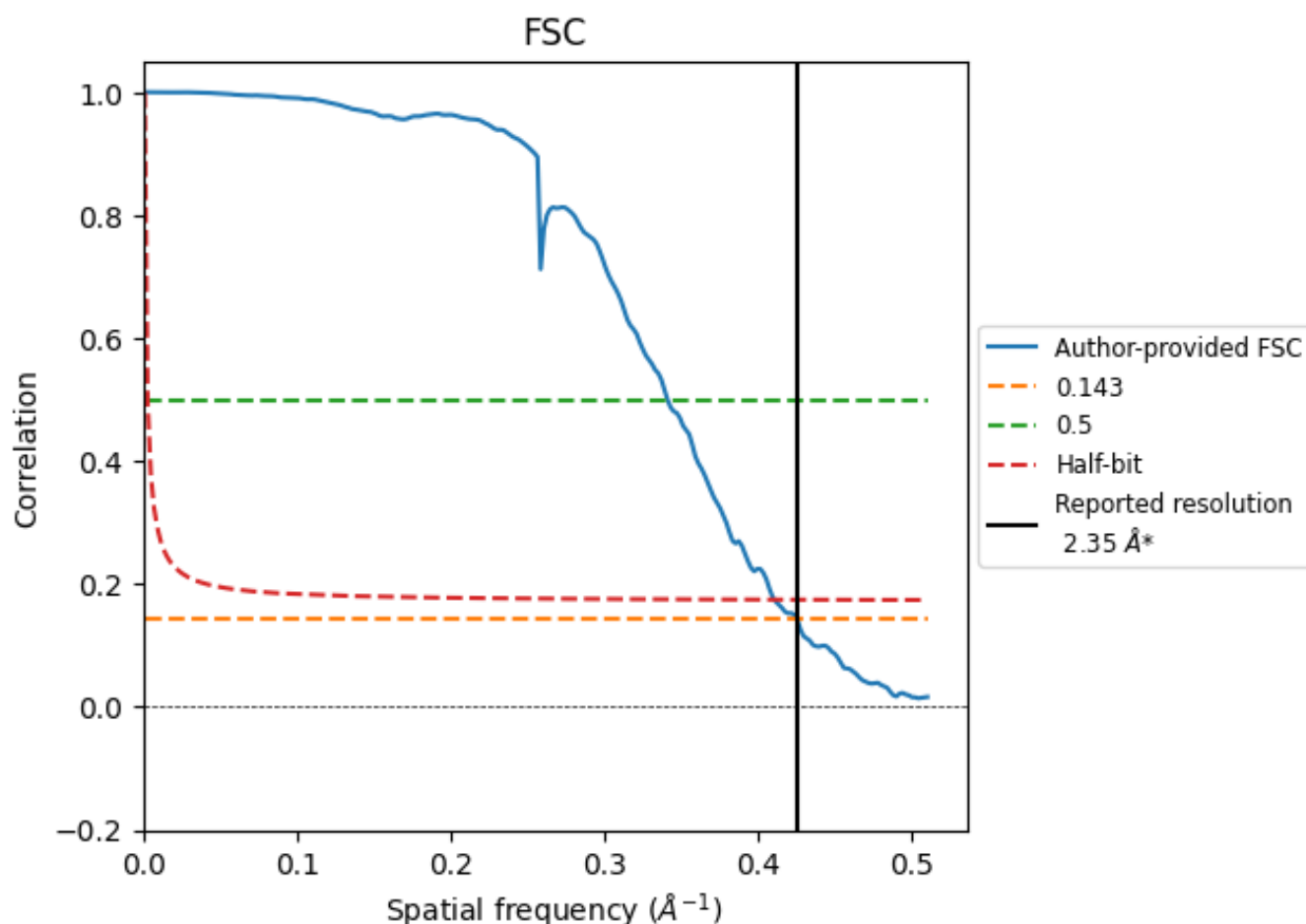


\*Reported resolution corresponds to spatial frequency of 0.426 Å<sup>-1</sup>

## 8 Fourier-Shell correlation [i](#)

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

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of 0.426 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

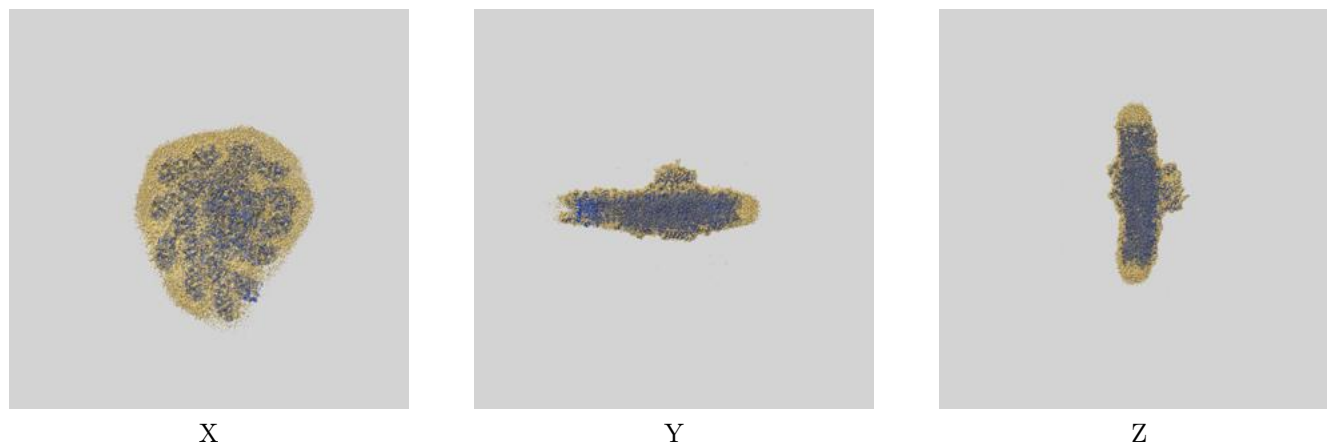
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.35	-	-
Author-provided FSC curve	2.35	2.93	2.43
Unmasked-calculated*	-	-	-

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

## 9 Map-model fit [i](#)

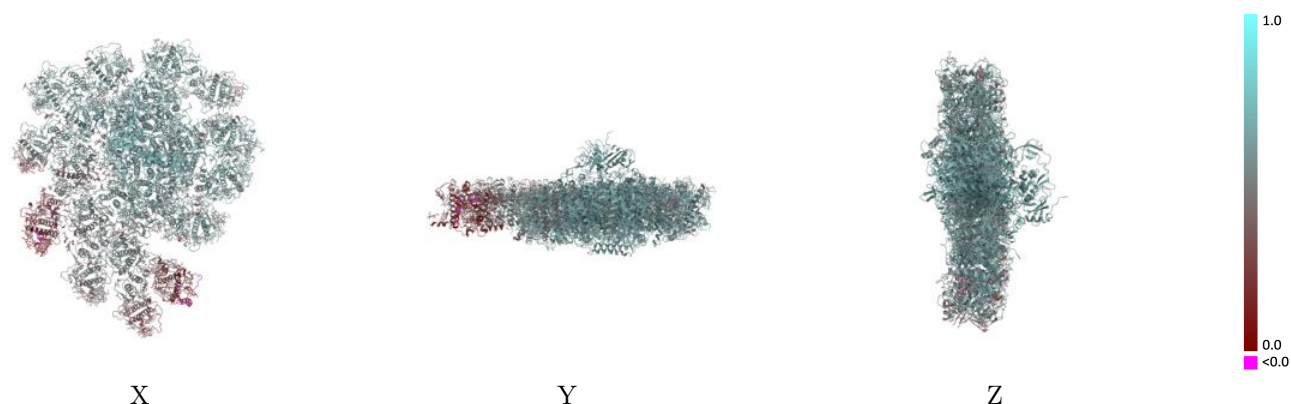
This section contains information regarding the fit between EMDB map EMD-63994 and PDB model 9UAS. Per-residue inclusion information can be found in section [3](#) on page [42](#).

### 9.1 Map-model overlay [i](#)



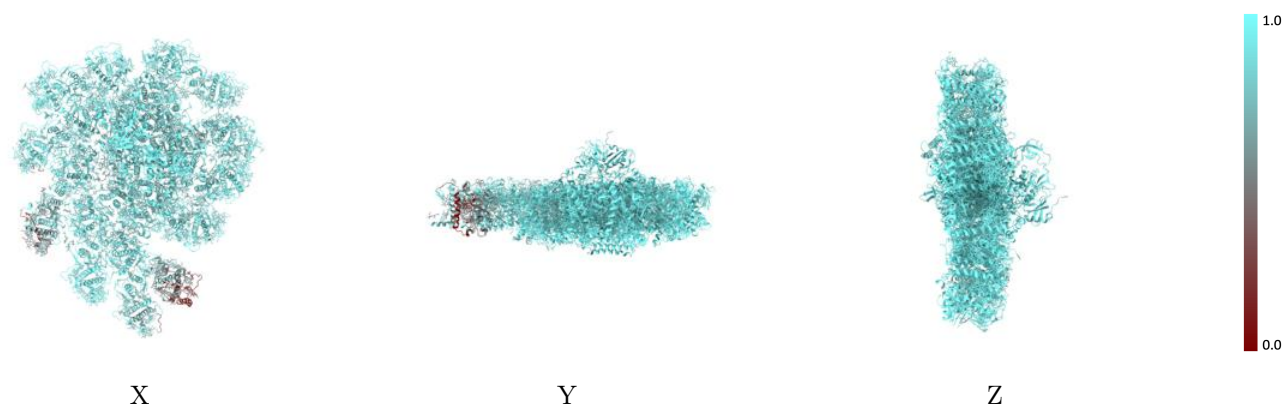
The images above show the 3D surface view of the map at the recommended contour level 0.04 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

## 9.2 Q-score mapped to coordinate model [i](#)



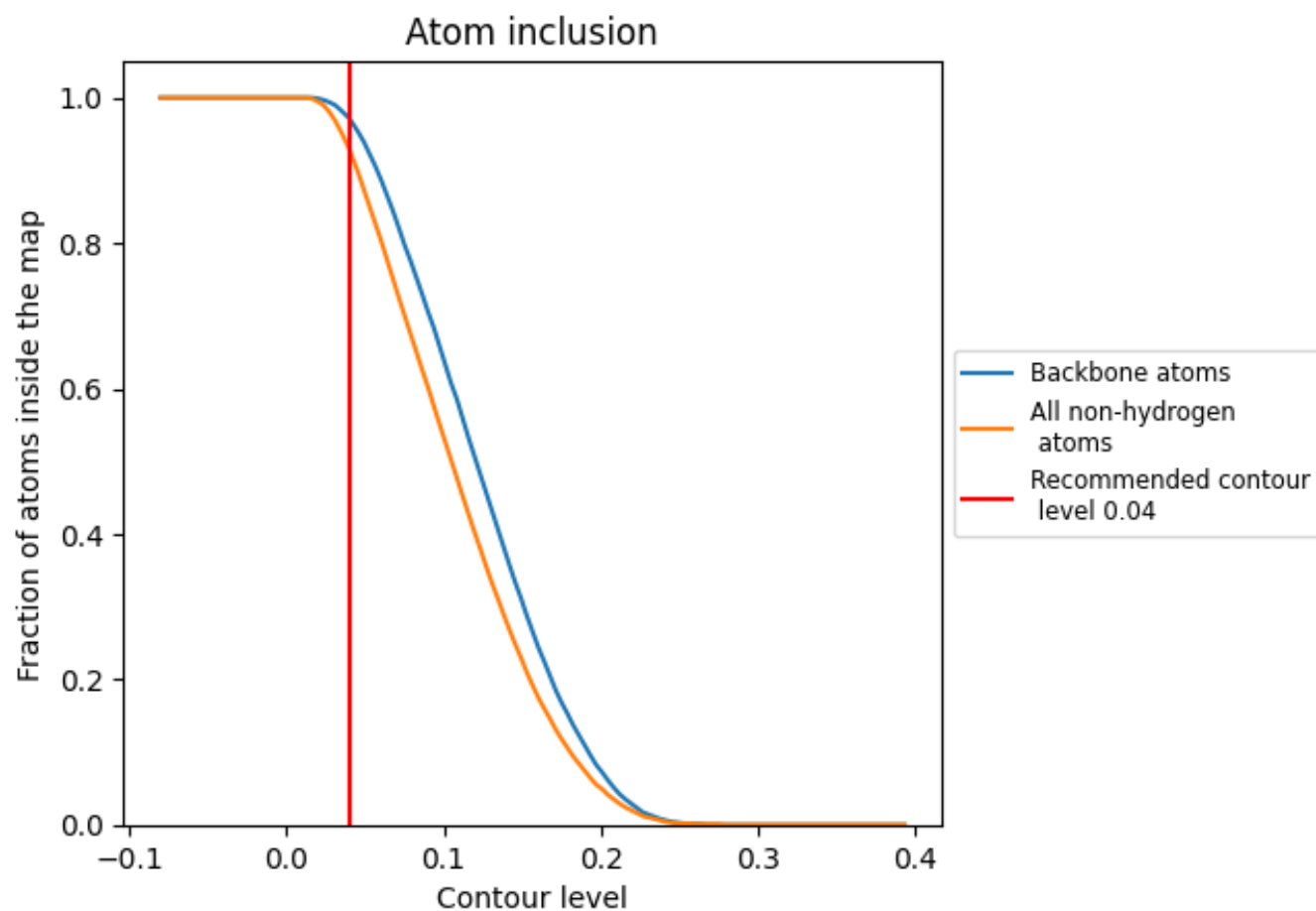
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

## 9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.04).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 97% of all backbone atoms, 93% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.04) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.9300	<div></div> 0.5550
A	<div></div> 0.9840	<div></div> 0.6580
B	<div></div> 0.9780	<div></div> 0.6190
C	<div></div> 0.9970	<div></div> 0.6770
D	<div></div> 0.9510	<div></div> 0.6400
E	<div></div> 0.9560	<div></div> 0.6350
F	<div></div> 0.9620	<div></div> 0.6150
G	<div></div> 0.9560	<div></div> 0.5620
H	<div></div> 0.9670	<div></div> 0.5870
I	<div></div> 0.9400	<div></div> 0.4830
J	<div></div> 0.9420	<div></div> 0.6280
K	<div></div> 0.9690	<div></div> 0.6110
L	<div></div> 0.9710	<div></div> 0.5060
M	<div></div> 0.9840	<div></div> 0.5760
N	<div></div> 0.9490	<div></div> 0.4660
O	<div></div> 0.9660	<div></div> 0.4920
P	<div></div> 0.7790	<div></div> 0.3540
Q	<div></div> 0.9570	<div></div> 0.5030
R	<div></div> 0.4970	<div></div> 0.2490
S	<div></div> 0.9380	<div></div> 0.5600
T	<div></div> 0.9500	<div></div> 0.6030
U	<div></div> 0.9200	<div></div> 0.5570
V	<div></div> 0.6770	<div></div> 0.2230
W	<div></div> 0.9550	<div></div> 0.6060
X	<div></div> 0.9420	<div></div> 0.6030

