



wwPDB EM Validation Summary Report ⓘ

Jun 3, 2026 – 04:33 PM JST

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

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:

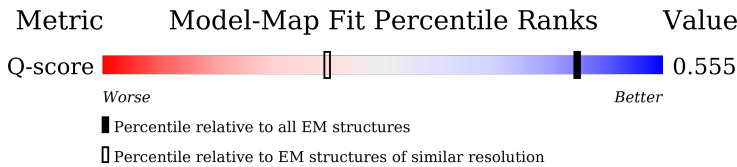
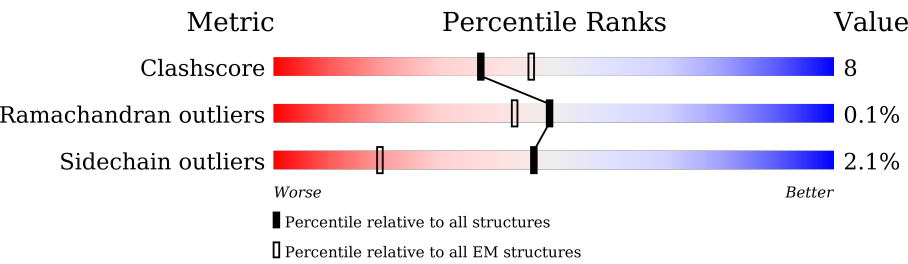
EMDB validation analysis : 0.0.1.dev132
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using 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 i

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 ≥ 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	86%13%
2	C	81	89%10%
3	D	193	90%9%
4	E	158	33%7% 60%

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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	

2 Entry composition

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		

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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		

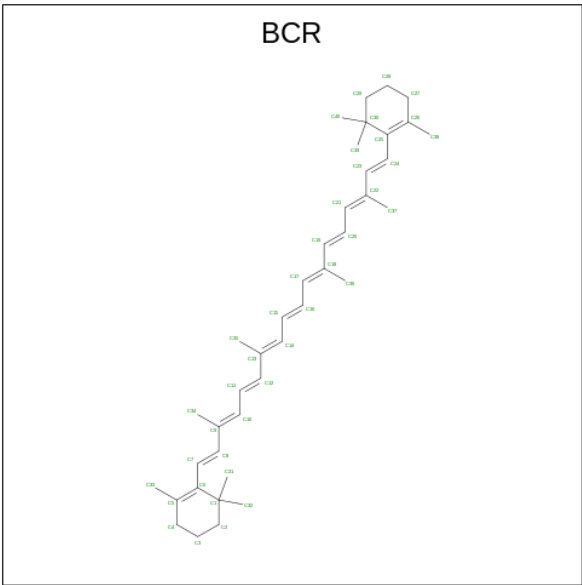
- Molecule 19 is a protein called LhcbM8.

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: C₄₀H₅₆) (labeled as "Ligand of Interest" by depositor).



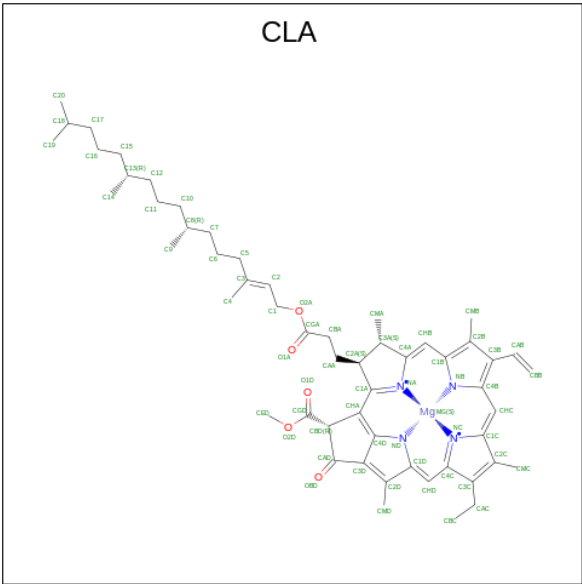
Mol	Chain	Residues	Atoms		AltConf
21	B	1	Total	C	0
			40	40	
21	B	1	Total	C	0
			40	40	
21	B	1	Total	C	0
			40	40	
21	B	1	Total	C	0
			40	40	
21	B	1	Total	C	0
			40	40	
21	B	1	Total	C	0
			40	40	
21	J	1	Total	C	0
			40	40	

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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: C₅₅H₇₂MgN₄O₅) (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	

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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

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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

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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

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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

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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

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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

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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

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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

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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

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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

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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

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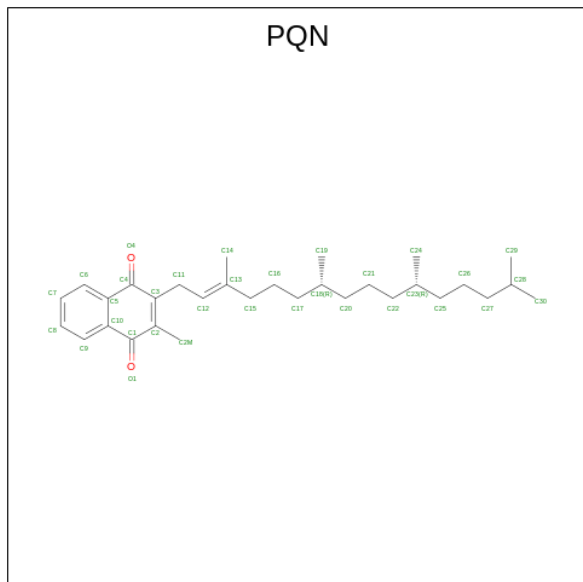
Mol	Chain	Residues	Atoms					AltConf
22	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	A	1	Total 61	C 51	Mg 1	N 4	O 5	0
22	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	A	1	Total 53	C 43	Mg 1	N 4	O 5	0
22	A	1	Total 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

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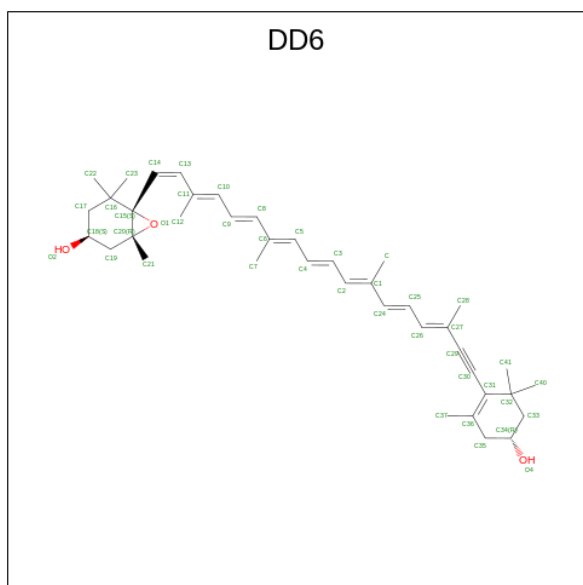
Mol	Chain	Residues	Atoms					AltConf
22	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	A	1	Total 61	C 51	Mg 1	N 4	O 5	0
22	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	A	1	Total 62	C 52	Mg 1	N 4	O 5	0
22	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	A	1	Total 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).



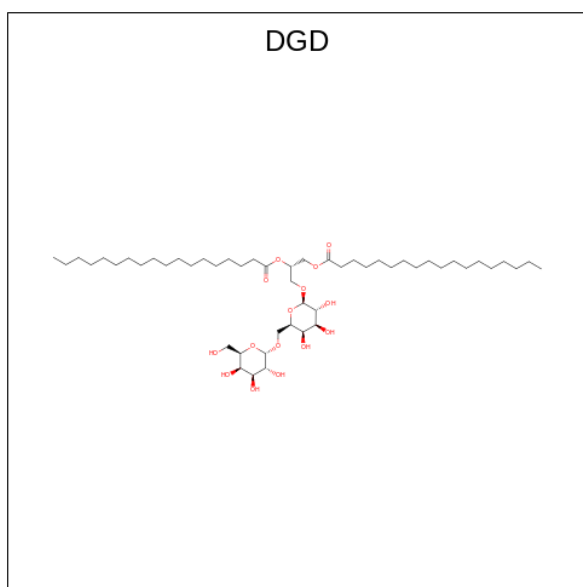
Mol	Chain	Residues	Atoms			AltConf
24	B	1	Total 43	C 40	O 3	0
24	F	1	Total 43	C 40	O 3	0
24	G	1	Total 43	C 40	O 3	0
24	G	1	Total 43	C 40	O 3	0
24	H	1	Total 43	C 40	O 3	0
24	H	1	Total 43	C 40	O 3	0
24	I	1	Total 43	C 40	O 3	0
24	I	1	Total 43	C 40	O 3	0
24	J	1	Total 43	C 40	O 3	0
24	K	1	Total 43	C 40	O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

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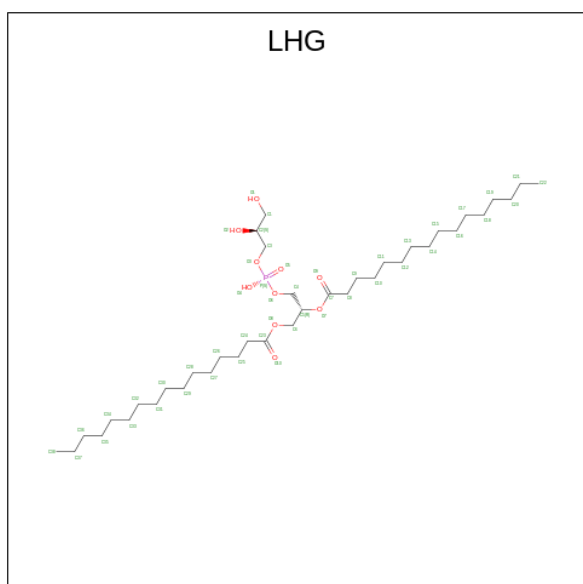
Mol	Chain	Residues	Atoms			AltConf
24	R	1	Total 43	C 40	O 3	0
24	R	1	Total 43	C 40	O 3	0
24	S	1	Total 43	C 40	O 3	0
24	S	1	Total 43	C 40	O 3	0
24	T	1	Total 43	C 40	O 3	0
24	T	1	Total 43	C 40	O 3	0
24	U	1	Total 43	C 40	O 3	0
24	U	1	Total 43	C 40	O 3	0
24	V	1	Total 43	C 40	O 3	0
24	V	1	Total 43	C 40	O 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: $C_{38}H_{75}O_{10}P$) (labeled as "Ligand of Interest" by depositor).



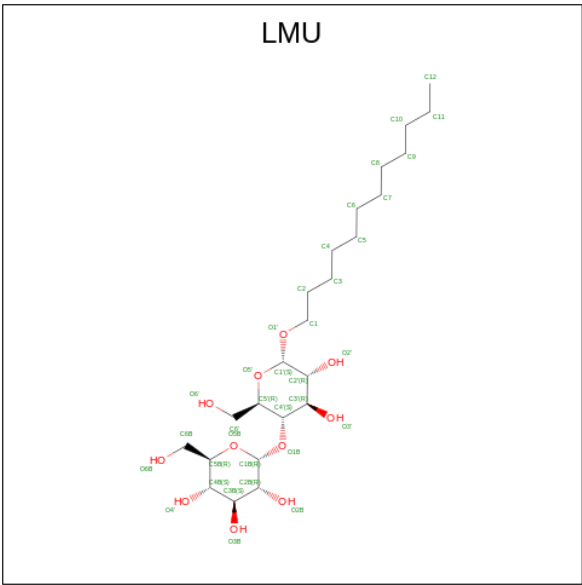
Mol	Chain	Residues	Atoms				AltConf
26	B	1	Total	C	O	P	0
			27	16	10	1	
26	B	1	Total	C	O	P	0
			42	31	10	1	
26	G	1	Total	C	O	P	0
			32	21	10	1	
26	H	1	Total	C	O	P	0
			27	16	10	1	
26	K	1	Total	C	O	P	0
			39	28	10	1	
26	K	1	Total	C	O	P	0
			33	22	10	1	
26	L	1	Total	C	O	P	0
			42	31	10	1	
26	N	1	Total	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	

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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: C₂₄H₄₆O₁₁) (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	

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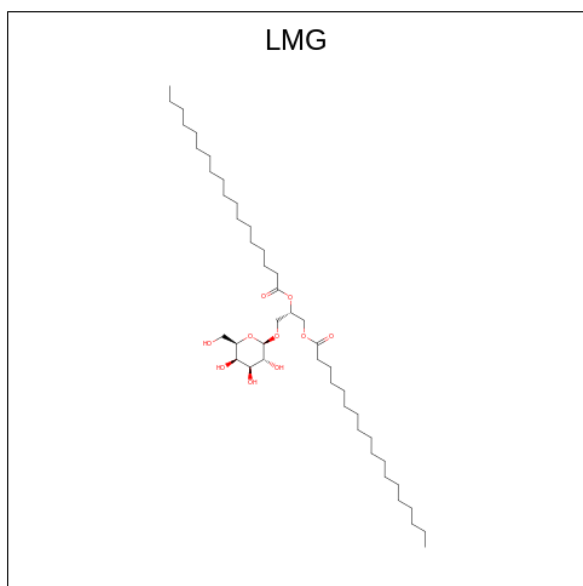
Mol	Chain	Residues	Atoms			AltConf
27	H	1	Total	C	O	0
			21	15	6	
27	H	1	Total	C	O	0
			24	18	6	
27	H	1	Total	C	O	0
			33	23	10	
27	J	1	Total	C	O	0
			34	24	10	
27	K	1	Total	C	O	0
			33	23	10	
27	L	1	Total	C	O	0
			24	18	6	
27	L	1	Total	C	O	0
			27	21	6	
27	L	1	Total	C	O	0
			34	24	10	
27	M	1	Total	C	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	

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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).



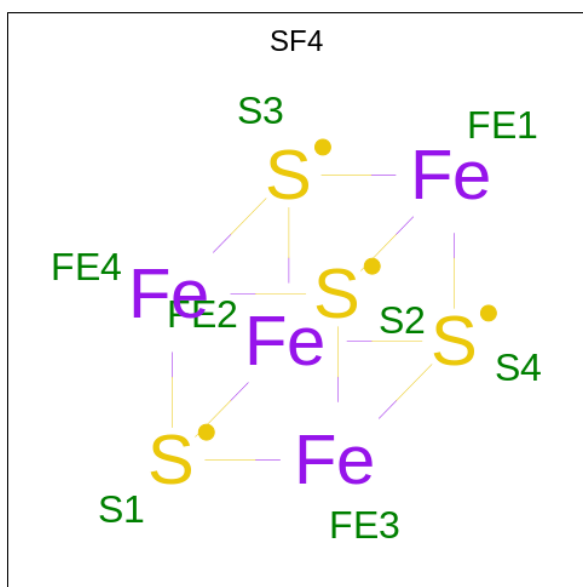
Mol	Chain	Residues	Atoms			AltConf
28	B	1	Total	C	O	0
			43	33	10	
28	B	1	Total	C	O	0
			53	43	10	
28	F	1	Total	C	O	0
			42	32	10	
28	G	1	Total	C	O	0
			46	36	10	
28	H	1	Total	C	O	0
			43	33	10	
28	H	1	Total	C	O	0
			40	30	10	

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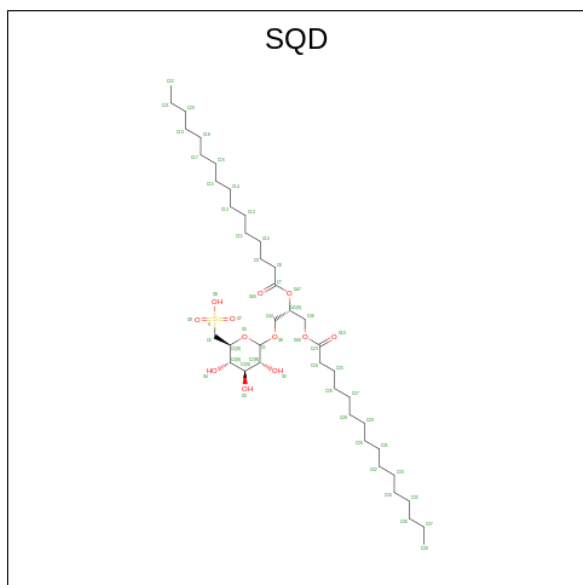
Mol	Chain	Residues	Atoms			AltConf
28	H	1	Total	C	O	0
			37	27	10	
28	I	1	Total	C	O	0
			37	27	10	
28	I	1	Total	C	O	0
			50	41	9	
28	J	1	Total	C	O	0
			55	45	10	
28	K	1	Total	C	O	0
			43	33	10	
28	K	1	Total	C	O	0
			49	39	10	
28	K	1	Total	C	O	0
			43	33	10	
28	L	1	Total	C	O	0
			51	41	10	
28	N	1	Total	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: Fe_4S_4) (labeled as "Ligand of Interest" by depositor).



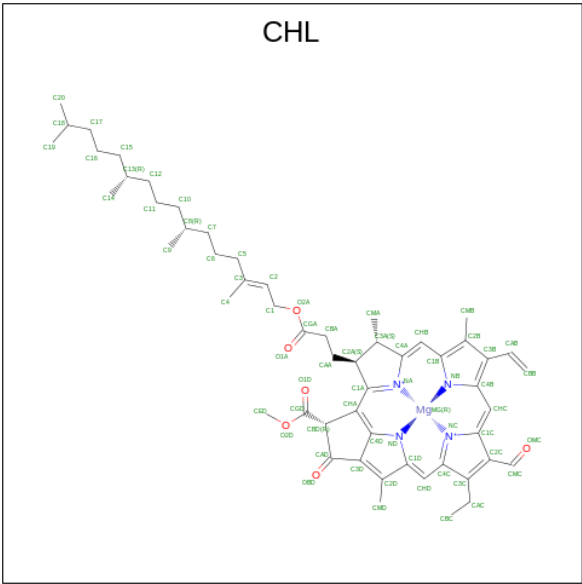
Mol	Chain	Residues	Atoms			AltConf
29	B	1	Total	Fe	S	0
			8	4	4	
29	C	1	Total	Fe	S	0
			8	4	4	
29	C	1	Total	Fe	S	0
			8	4	4	

- 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: C₅₅H₇₀MgN₄O₆) (labeled as "Ligand of Interest" by depositor).



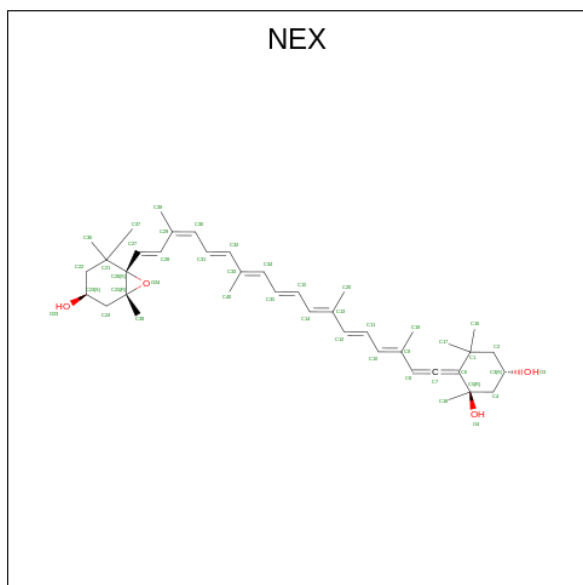
Mol	Chain	Residues	Atoms					AltConf
31	U	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
31	U	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
31	V	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
31	V	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
31	W	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
31	W	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
31	W	1	Total	C	Mg	N	O	0
			66	55	1	4	6	

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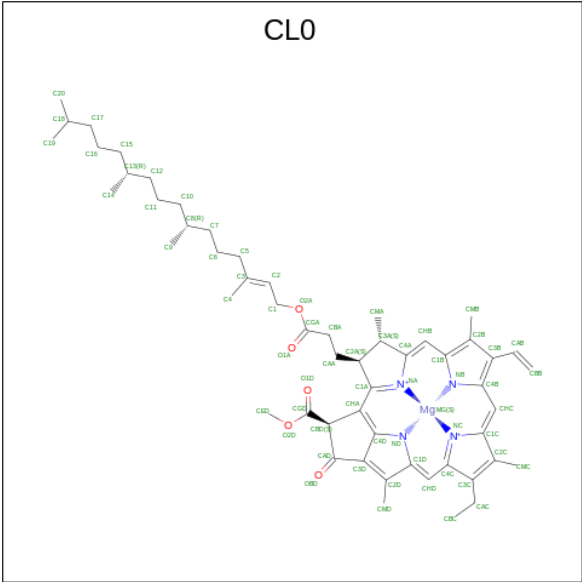
Mol	Chain	Residues	Atoms					AltConf
31	X	1	Total	C	Mg	N	O	0
			46	35	1	4	6	

- 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: C₄₀H₅₆O₄) (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: C₅₅H₇₂MgN₄O₅) (labeled as "Ligand of Interest" by depositor).

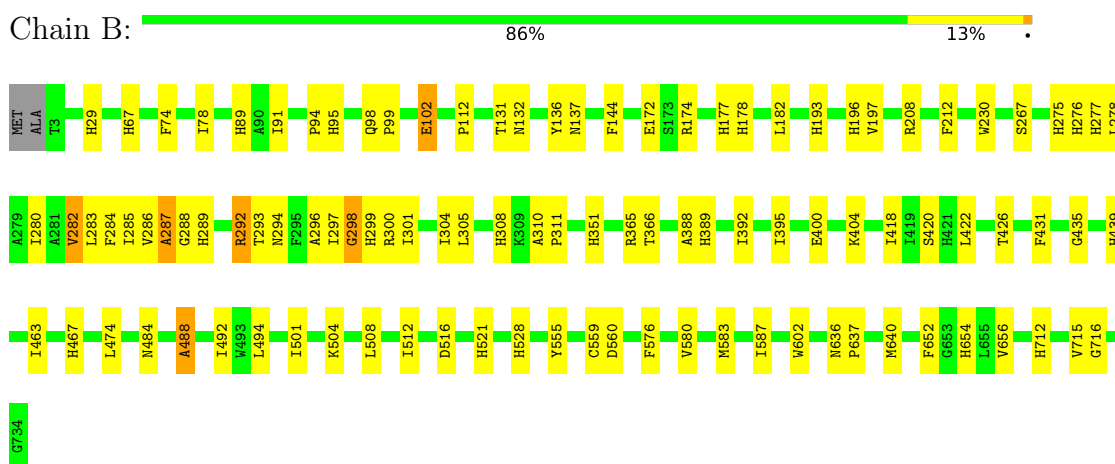


Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
33	A	1	65	55	1	4	5	0

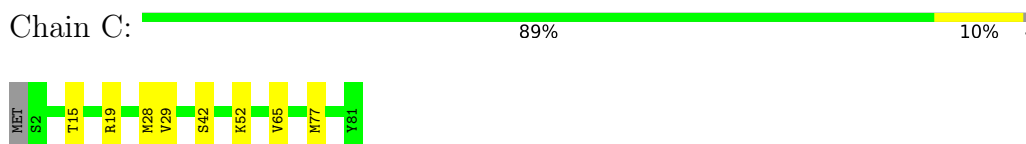
3 Residue-property plots

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.

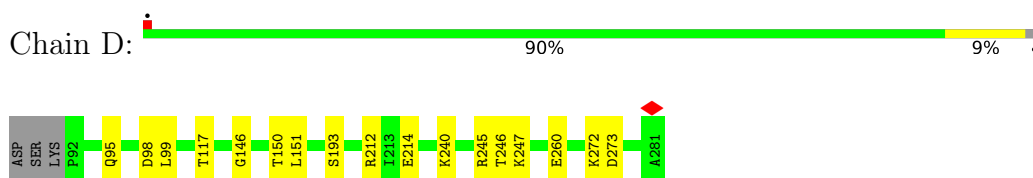
- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A2



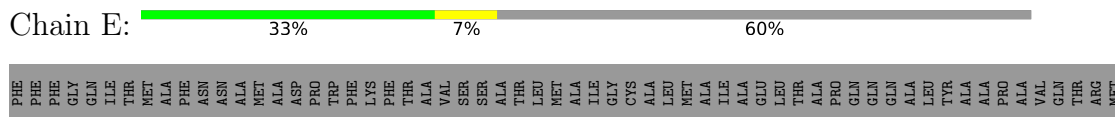
- Molecule 2: Photosystem I iron-sulfur center



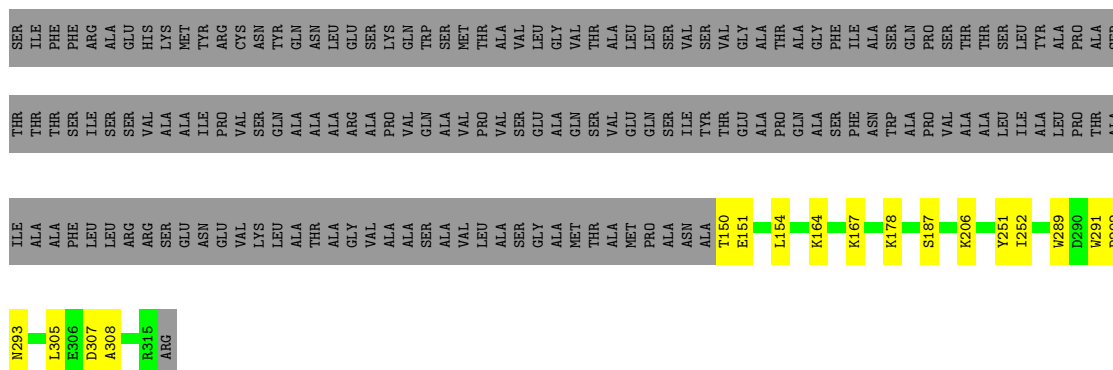
- Molecule 3: PsaD



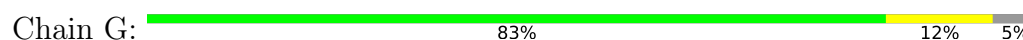
- Molecule 4: PsaE



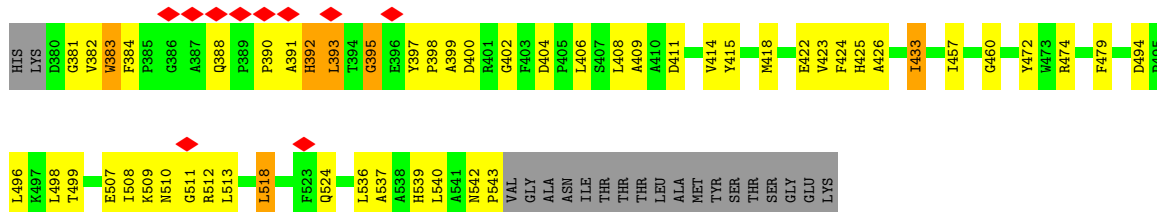
- Molecule 5: PsaF



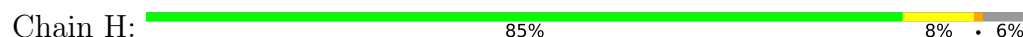
- Molecule 6: Lhce5.7



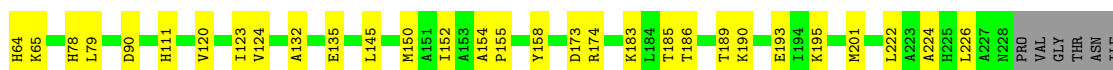
- Molecule 6: Lhce5.7



- Molecule 7: Lhce7.3



- Molecule 8: Lhce5



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
V466
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%

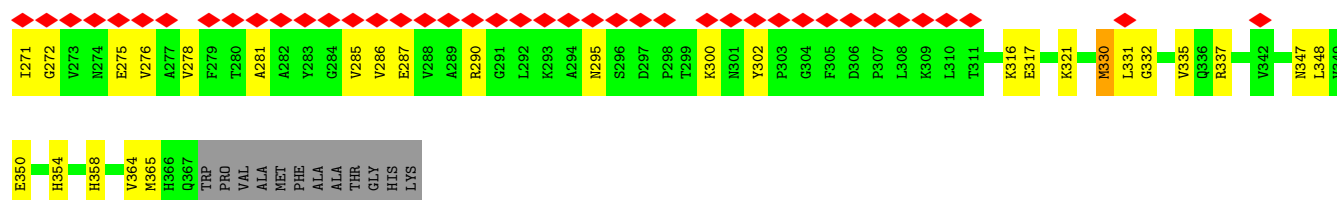
VAL
D194
R195
G201
D226
P227
K228
E231
M245
L257
Y263
V285
V288
L292
N301
F305
T315
E319
G332
L333
E334
V335
Q336
R337
H338
V339
V342
V346
N347
L348
V349
E350
H351
V352
A361
H366
Q367
V368
F369
V370
A371
MET

PHE
ALA
ALA
THR
GLY
HIS
LYS

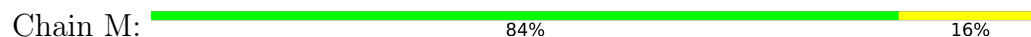
• Molecule 11: Lhce8

Chain R: 38% 66% 25% 7%

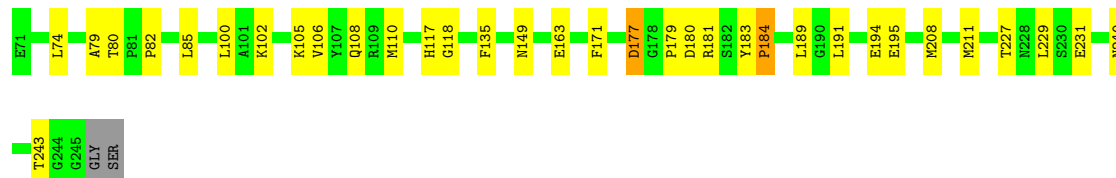
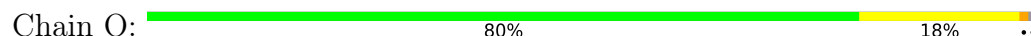
VAL
D194
R195
P196
F199
S206
Y207
L208
T209
G210
Q211
Y212
F213
F218
A225
D226
P227
K228
V229
R232
M233
R234
V235
S236
E237
V238
Y239
H240
G241
R242
L243
A244
M245
L246
A247
I248
V253
P254
D255
I256
L257
G258
K259
G260
A261
V262
Y263
E264
A265
A266
Q267
N268
A269
G270



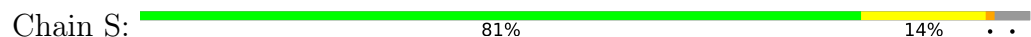
- Molecule 12: PsaM



- Molecule 13: LhcE7



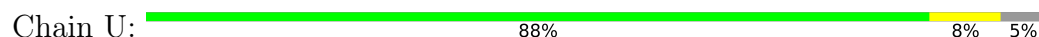
- Molecule 14: Lhce10



- Molecule 15: Lhce11

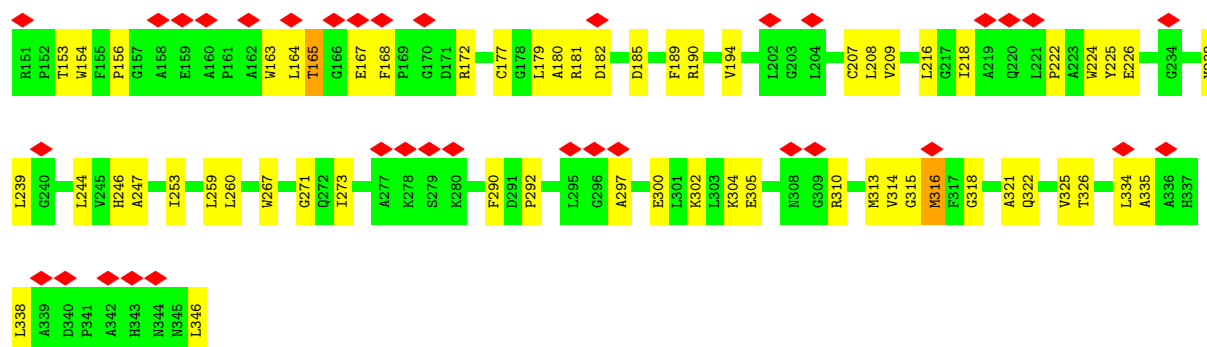


- Molecule 16: LhcbM4.6



- Molecule 17: LhcbM4.10





• Molecule 18: LhcbM2

Chain W: 87% 9% .



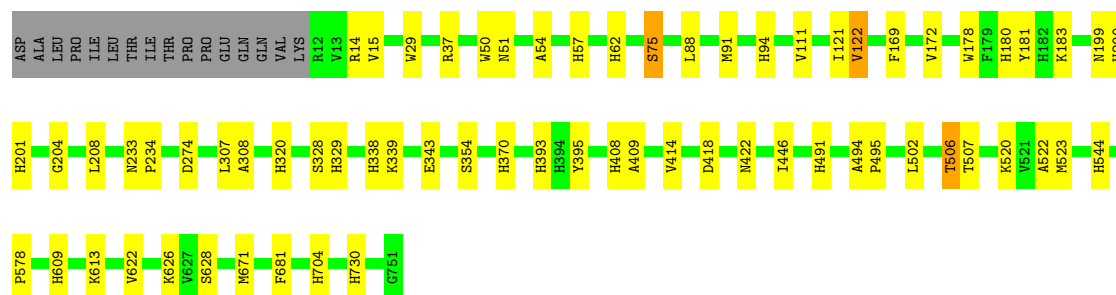
• Molecule 19: LhcbM8

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: DGD, LMU, CLA, LHG, CL0, CHL, LMG, BCR, NEX, PQN, DD6, SF4, SQD

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

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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

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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

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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

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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
24	DD6	H	314	-	39,45,45	1.99	3 (7%)	52,67,67	1.88	12 (23%)
22	CLA	O	315	13	54,58,73	1.43	9 (16%)	65,95,113	1.36	8 (12%)
22	CLA	B	838	1	49,53,73	1.49	9 (18%)	59,89,113	1.41	6 (10%)
29	SF4	C	101	2	0,12,12	-	-	-	-	-
24	DD6	P	612	-	39,45,45	2.04	2 (5%)	52,67,67	2.96	18 (34%)
22	CLA	O	314	13	49,53,73	1.48	8 (16%)	59,89,113	1.40	5 (8%)
22	CLA	L	407	-	61,65,73	1.33	8 (13%)	73,103,113	1.33	5 (6%)
27	LMU	T	618	-	24,24,36	0.44	0	29,29,47	0.66	0
22	CLA	A	828	20	69,73,73	1.25	7 (10%)	83,113,113	1.29	7 (8%)
22	CLA	L	411	11	69,73,73	1.25	8 (11%)	83,113,113	1.27	7 (8%)
22	CLA	G	602	6	64,68,73	1.30	8 (12%)	77,107,113	1.33	8 (10%)
27	LMU	X	418	-	24,24,36	0.43	0	29,29,47	0.55	0
26	LHG	L	416	22	41,41,48	1.17	6 (14%)	44,47,54	0.99	2 (4%)
22	CLA	W	402	18	59,63,73	1.35	8 (13%)	71,101,113	1.31	7 (9%)
24	DD6	V	614	-	39,45,45	2.00	3 (7%)	52,67,67	2.03	13 (25%)
28	LMG	U	423	-	49,49,55	0.73	0	57,57,63	1.31	3 (5%)
22	CLA	S	602	14	64,68,73	1.30	7 (10%)	77,107,113	1.33	8 (10%)
28	LMG	H	319	-	40,40,55	0.81	0	48,48,63	1.21	3 (6%)
22	CLA	B	830	1	69,73,73	1.24	10 (14%)	83,113,113	1.34	9 (10%)
22	CLA	X	410	26	64,68,73	1.31	7 (10%)	77,107,113	1.30	6 (7%)
22	CLA	B	812	1	69,73,73	1.26	7 (10%)	83,113,113	1.29	8 (9%)
30	SQD	K	621	-	42,43,54	0.42	1 (2%)	51,54,65	0.53	0
24	DD6	J	105	-	39,45,45	1.96	2 (5%)	52,67,67	1.88	13 (25%)
22	CLA	B	835	1	69,73,73	1.25	8 (11%)	83,113,113	1.31	7 (8%)
24	DD6	B	841	-	39,45,45	1.99	3 (7%)	52,67,67	1.99	13 (25%)
22	CLA	L	404	-	60,64,73	1.35	8 (13%)	72,102,113	1.36	6 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	CLA	S	606	14	54,58,73	1.42	7 (12%)	65,95,113	1.38	6 (9%)
32	NEX	V	616	-	38,46,46	0.37	1 (2%)	50,70,70	0.70	2 (4%)
22	CLA	A	841	20	69,73,73	1.24	9 (13%)	83,113,113	1.27	5 (6%)
21	BCR	A	849	-	41,41,41	0.73	0	56,56,56	1.89	13 (23%)
27	LMU	B	853	-	19,19,36	0.46	0	23,23,47	0.44	0
22	CLA	V	602	17	69,73,73	1.26	7 (10%)	83,113,113	1.28	7 (8%)
22	CLA	B	810	-	60,64,73	1.34	8 (13%)	72,102,113	1.33	5 (6%)
22	CLA	B	808	1	59,63,73	1.36	8 (13%)	71,101,113	1.34	4 (5%)
27	LMU	M	102	-	24,24,36	0.44	0	29,29,47	0.61	0
27	LMU	X	421	-	36,36,36	0.40	0	47,47,47	0.67	1 (2%)
22	CLA	B	809	1	69,73,73	1.25	8 (11%)	83,113,113	1.29	5 (6%)
22	CLA	B	821	1	64,68,73	1.31	8 (12%)	77,107,113	1.31	5 (6%)
24	DD6	G	612	-	39,45,45	2.00	3 (7%)	52,67,67	1.81	11 (21%)
22	CLA	B	831	1	69,73,73	1.24	7 (10%)	83,113,113	1.26	8 (9%)
22	CLA	U	412	26	49,53,73	1.49	8 (16%)	59,89,113	1.45	4 (6%)
27	LMU	O	322	-	36,36,36	0.49	0	47,47,47	1.09	5 (10%)
22	CLA	Q	617	10	56,60,73	1.39	8 (14%)	67,97,113	1.40	6 (8%)
22	CLA	B	823	-	69,73,73	1.25	7 (10%)	83,113,113	1.28	4 (4%)
22	CLA	P	610	6	45,49,73	1.54	7 (15%)	54,84,113	1.54	7 (12%)
22	CLA	W	414	18	69,73,73	1.27	8 (11%)	83,113,113	1.27	8 (9%)
21	BCR	B	844	-	41,41,41	0.71	0	56,56,56	1.80	13 (23%)
22	CLA	O	308	-	65,69,73	1.29	8 (12%)	78,108,113	1.30	7 (8%)
22	CLA	H	302	7	49,53,73	1.49	8 (16%)	59,89,113	1.42	5 (8%)
28	LMG	J	101	-	55,55,55	0.70	0	63,63,63	1.35	7 (11%)
22	CLA	V	612	-	69,73,73	1.27	8 (11%)	83,113,113	1.26	6 (7%)
22	CLA	I	607	8	59,63,73	1.35	8 (13%)	71,101,113	1.35	7 (9%)
24	DD6	U	416	-	39,45,45	2.01	3 (7%)	52,67,67	1.80	11 (21%)
22	CLA	A	807	20	69,73,73	1.25	8 (11%)	83,113,113	1.32	6 (7%)
22	CLA	H	310	7	49,53,73	1.48	8 (16%)	59,89,113	1.42	6 (10%)
22	CLA	S	601	14	49,53,73	1.49	7 (14%)	59,89,113	1.46	4 (6%)
27	LMU	A	857	-	24,24,36	0.45	0	29,29,47	0.66	0
22	CLA	K	608	10	69,73,73	1.24	9 (13%)	83,113,113	1.29	8 (9%)
21	BCR	B	843	-	41,41,41	0.71	0	56,56,56	3.38	24 (42%)
22	CLA	F	403	-	69,73,73	1.26	8 (11%)	83,113,113	1.28	7 (8%)
26	LHG	O	323	-	42,42,48	1.18	6 (14%)	45,48,54	0.95	2 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	CLA	N	602	8	64,68,73	1.30	8 (12%)	77,107,113	1.33	7 (9%)
22	CLA	K	613	-	57,61,73	1.38	8 (14%)	68,98,113	1.35	6 (8%)
22	CLA	N	601	8	49,53,73	1.48	8 (16%)	59,89,113	1.41	4 (6%)
24	DD6	W	417	-	39,45,45	1.96	3 (7%)	52,67,67	1.76	11 (21%)
28	LMG	F	408	-	42,42,55	0.85	1 (2%)	50,50,63	1.32	4 (8%)
27	LMU	H	320	-	24,24,36	0.44	0	29,29,47	0.59	0
22	CLA	B	826	1	62,66,73	1.32	7 (11%)	74,104,113	1.33	5 (6%)
28	LMG	K	601	-	43,43,55	0.77	0	51,51,63	1.27	4 (7%)
22	CLA	V	611	-	49,53,73	1.50	8 (16%)	59,89,113	1.43	4 (6%)
24	DD6	S	612	-	39,45,45	1.99	3 (7%)	52,67,67	1.83	12 (23%)
22	CLA	T	608	26	64,68,73	1.30	7 (10%)	77,107,113	1.31	5 (6%)
26	LHG	H	316	22	26,26,48	1.40	6 (23%)	29,32,54	1.16	2 (6%)
22	CLA	A	822	-	69,73,73	1.24	7 (10%)	83,113,113	1.26	6 (7%)
24	DD6	Q	614	-	39,45,45	1.97	3 (7%)	52,67,67	1.79	11 (21%)
24	DD6	I	613	-	39,45,45	2.05	3 (7%)	52,67,67	1.90	16 (30%)
22	CLA	R	603	-	60,64,73	1.35	8 (13%)	72,102,113	1.35	6 (8%)
26	LHG	S	613	22	31,31,48	1.32	6 (19%)	34,37,54	1.12	3 (8%)
22	CLA	I	601	8	69,73,73	1.27	9 (13%)	83,113,113	1.25	6 (7%)
24	DD6	N	612	-	39,45,45	1.99	3 (7%)	52,67,67	1.87	13 (25%)
22	CLA	P	603	6	49,53,73	1.49	6 (12%)	59,89,113	1.30	4 (6%)
22	CLA	R	601	-	69,73,73	1.26	8 (11%)	83,113,113	1.27	7 (8%)
22	CLA	A	818	20	57,61,73	1.37	8 (14%)	68,98,113	1.37	8 (11%)
22	CLA	U	405	16	61,65,73	1.34	8 (13%)	73,103,113	1.33	4 (5%)
22	CLA	G	608	26	64,68,73	1.30	7 (10%)	77,107,113	1.35	6 (7%)
22	CLA	A	830	20	69,73,73	1.24	8 (11%)	83,113,113	1.25	6 (7%)
27	LMU	T	617	-	24,24,36	0.42	0	29,29,47	0.66	0
22	CLA	L	408	11	64,68,73	1.30	10 (15%)	77,107,113	1.43	11 (14%)
22	CLA	A	811	20	61,65,73	1.33	8 (13%)	73,103,113	1.40	10 (13%)
31	CHL	U	408	-	45,54,74	3.24	13 (28%)	35,90,114	1.52	6 (17%)
22	CLA	Q	603	10	49,53,73	1.48	8 (16%)	59,89,113	1.47	6 (10%)
22	CLA	A	815	20	69,73,73	1.25	7 (10%)	83,113,113	1.29	8 (9%)
28	LMG	G	616	-	46,46,55	0.81	0	54,54,63	1.29	7 (12%)
24	DD6	P	613	-	39,45,45	2.03	3 (7%)	52,67,67	1.94	18 (34%)
22	CLA	W	411	18	64,68,73	1.29	8 (12%)	77,107,113	1.28	7 (9%)
27	LMU	J	104	-	34,35,36	0.36	0	42,45,47	0.89	2 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	CLA	G	610	6	49,53,73	1.48	7 (14%)	59,89,113	1.43	5 (8%)
24	DD6	G	613	-	39,45,45	2.03	3 (7%)	52,67,67	1.90	16 (30%)
24	DD6	I	612	-	39,45,45	1.99	3 (7%)	52,67,67	1.72	10 (19%)
28	LMG	N	615	-	44,44,55	0.78	0	52,52,63	1.26	4 (7%)
26	LHG	K	619	-	32,32,48	1.31	6 (18%)	35,38,54	1.10	2 (5%)
27	LMU	L	420	-	35,35,36	0.37	0	43,45,47	0.81	2 (4%)
24	DD6	R	612	-	39,45,45	1.99	3 (7%)	52,67,67	1.85	12 (23%)
28	LMG	B	856	-	53,53,55	0.72	0	61,61,63	1.37	7 (11%)
22	CLA	A	808	20	69,73,73	1.25	9 (13%)	83,113,113	1.27	6 (7%)
22	CLA	W	413	-	49,53,73	1.48	8 (16%)	59,89,113	1.43	5 (8%)
22	CLA	X	413	19	49,53,73	1.49	6 (12%)	59,89,113	1.42	4 (6%)
22	CLA	A	803	-	69,73,73	1.24	8 (11%)	83,113,113	1.29	10 (12%)
28	LMG	W	401	-	48,48,55	0.73	0	56,56,63	1.33	8 (14%)
22	CLA	N	608	26	49,53,73	1.49	8 (16%)	59,89,113	1.41	4 (6%)
22	CLA	B	811	1	49,53,73	1.48	7 (14%)	59,89,113	1.47	6 (10%)
22	CLA	T	605	-	69,73,73	1.26	9 (13%)	83,113,113	1.25	6 (7%)
22	CLA	B	828	1	69,73,73	1.25	9 (13%)	83,113,113	1.28	9 (10%)
22	CLA	G	609	-	49,53,73	1.48	8 (16%)	59,89,113	1.42	6 (10%)
22	CLA	Q	609	10	64,68,73	1.29	9 (14%)	77,107,113	1.27	5 (6%)
22	CLA	P	605	-	49,53,73	1.48	8 (16%)	59,89,113	1.44	6 (10%)
22	CLA	H	303	7	64,68,73	1.31	9 (14%)	77,107,113	1.30	6 (7%)
22	CLA	V	609	17	61,65,73	1.34	8 (13%)	73,103,113	1.34	6 (8%)
22	CLA	J	102	9	54,58,73	1.41	8 (14%)	65,95,113	1.40	5 (7%)
24	DD6	N	613	-	39,45,45	2.00	3 (7%)	52,67,67	1.86	15 (28%)
26	LHG	O	318	22	33,33,48	1.29	6 (18%)	36,39,54	1.06	3 (8%)
21	BCR	B	845	-	41,41,41	0.68	0	56,56,56	1.90	15 (26%)
22	CLA	K	602	10	64,68,73	1.30	9 (14%)	77,107,113	1.30	7 (9%)
22	CLA	O	307	13	49,53,73	1.48	8 (16%)	59,89,113	1.42	5 (8%)
27	LMU	W	421	-	24,24,36	0.44	0	29,29,47	0.56	0
22	CLA	R	615	11	69,73,73	1.27	7 (10%)	83,113,113	1.28	6 (7%)
32	NEX	U	418	-	38,46,46	0.35	1 (2%)	50,70,70	0.67	2 (4%)
22	CLA	B	827	1	69,73,73	1.24	8 (11%)	83,113,113	1.20	7 (8%)
22	CLA	A	814	20	69,73,73	1.24	7 (10%)	83,113,113	1.27	5 (6%)
22	CLA	X	403	19	69,73,73	1.25	8 (11%)	83,113,113	1.27	6 (7%)
22	CLA	I	608	-	49,53,73	1.48	9 (18%)	59,89,113	1.43	6 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	CLA	V	617	-	49,53,73	1.50	7 (14%)	59,89,113	1.44	4 (6%)
27	LMU	O	320	-	27,27,36	0.53	0	28,31,47	0.82	2 (7%)
22	CLA	B	802	1	69,73,73	1.26	12 (17%)	83,113,113	1.31	7 (8%)
22	CLA	A	819	20	62,66,73	1.32	9 (14%)	74,104,113	1.46	8 (10%)
22	CLA	A	827	-	66,70,73	1.27	7 (10%)	79,109,113	1.30	7 (8%)
22	CLA	A	813	20	69,73,73	1.25	7 (10%)	83,113,113	1.20	6 (7%)
27	LMU	L	418	-	24,24,36	0.48	0	29,29,47	0.74	0
22	CLA	K	617	10	69,73,73	1.25	9 (13%)	83,113,113	1.27	7 (8%)
22	CLA	O	313	13	69,73,73	1.26	8 (11%)	83,113,113	1.26	4 (4%)
22	CLA	R	607	11	64,68,73	1.32	9 (14%)	77,107,113	1.32	7 (9%)
22	CLA	F	404	-	59,63,73	1.35	7 (11%)	71,101,113	1.37	7 (9%)
22	CLA	O	319	13	49,53,73	1.48	7 (14%)	59,89,113	1.45	6 (10%)
22	CLA	B	819	1	57,61,73	1.42	7 (12%)	68,98,113	1.38	4 (5%)
27	LMU	B	857	-	36,36,36	0.41	0	47,47,47	0.73	1 (2%)
22	CLA	A	826	-	69,73,73	1.24	8 (11%)	83,113,113	1.29	5 (6%)
26	LHG	O	321	-	48,48,48	1.11	6 (12%)	51,54,54	0.92	2 (3%)
22	CLA	K	610	10	60,64,73	1.34	8 (13%)	72,102,113	1.32	5 (6%)
22	CLA	H	311	7	69,73,73	1.27	7 (10%)	83,113,113	1.29	8 (9%)
22	CLA	U	420	16	49,53,73	1.49	8 (16%)	59,89,113	1.43	5 (8%)
22	CLA	P	604	-	49,53,73	1.49	7 (14%)	59,89,113	1.44	6 (10%)
22	CLA	X	419	19	49,53,73	1.50	8 (16%)	59,89,113	1.41	5 (8%)
22	CLA	G	603	6	60,64,73	1.34	9 (15%)	72,102,113	1.33	8 (11%)
22	CLA	H	312	7	49,53,73	1.49	7 (14%)	59,89,113	1.40	5 (8%)
31	CHL	V	606	-	45,54,74	3.26	13 (28%)	35,90,114	1.50	6 (17%)
22	CLA	L	405	-	49,53,73	1.50	9 (18%)	59,89,113	1.46	4 (6%)
22	CLA	V	610	-	49,53,73	1.50	6 (12%)	59,89,113	1.42	7 (11%)
31	CHL	W	407	-	45,54,74	3.25	12 (26%)	35,90,114	1.61	6 (17%)
24	DD6	X	415	-	39,45,45	1.94	2 (5%)	52,67,67	1.71	10 (19%)
28	LMG	U	402	-	53,53,55	0.72	0	61,61,63	1.31	4 (6%)
31	CHL	U	407	-	45,54,74	3.24	14 (31%)	35,90,114	1.57	6 (17%)
27	LMU	F	409	-	21,21,36	0.49	0	26,26,47	0.57	0
24	DD6	L	415	-	39,45,45	2.01	2 (5%)	52,67,67	1.96	17 (32%)
22	CLA	I	611	8	49,53,73	1.53	8 (16%)	59,89,113	1.45	9 (15%)
22	CLA	V	604	-	60,64,73	1.35	8 (13%)	72,102,113	1.33	6 (8%)
22	CLA	A	829	20	69,73,73	1.25	8 (11%)	83,113,113	1.26	6 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	CLA	W	410	18	64,68,73	1.29	8 (12%)	77,107,113	1.32	6 (7%)
21	BCR	A	850	-	41,41,41	0.71	0	56,56,56	1.97	12 (21%)
24	DD6	K	615	-	39,45,45	1.95	2 (5%)	52,67,67	1.69	11 (21%)
24	DD6	X	414	-	39,45,45	1.97	3 (7%)	52,67,67	1.81	12 (23%)
22	CLA	A	821	20	69,73,73	1.24	9 (13%)	83,113,113	1.32	6 (7%)
22	CLA	V	603	17	61,65,73	1.34	7 (11%)	73,103,113	1.31	4 (5%)
27	LMU	T	615	-	21,21,36	0.47	0	26,26,47	0.59	0
22	CLA	T	606	15	54,58,73	1.41	6 (11%)	65,95,113	1.38	6 (9%)
22	CLA	K	604	-	68,72,73	1.26	8 (11%)	81,111,113	1.28	5 (6%)
22	CLA	V	601	17	49,53,73	1.51	6 (12%)	59,89,113	1.44	5 (8%)
22	CLA	G	611	6	49,53,73	1.49	7 (14%)	59,89,113	1.44	6 (10%)
22	CLA	U	409	-	49,53,73	1.48	8 (16%)	59,89,113	1.45	6 (10%)
22	CLA	B	820	1	57,61,73	1.39	7 (12%)	68,98,113	1.50	5 (7%)
22	CLA	B	818	-	69,73,73	1.26	9 (13%)	83,113,113	1.28	6 (7%)
22	CLA	W	404	18	69,73,73	1.25	7 (10%)	83,113,113	1.28	5 (6%)
24	DD6	T	612	-	39,45,45	2.03	3 (7%)	52,67,67	1.84	13 (25%)
22	CLA	N	606	8	69,73,73	1.28	7 (10%)	83,113,113	1.26	7 (8%)
22	CLA	L	406	-	69,73,73	1.26	8 (11%)	83,113,113	1.28	6 (7%)
22	CLA	K	607	10	61,65,73	1.31	9 (14%)	73,103,113	1.48	9 (12%)
22	CLA	Q	612	10	69,73,73	1.24	7 (10%)	83,113,113	1.28	4 (4%)
22	CLA	S	605	-	64,68,73	1.30	9 (14%)	77,107,113	1.43	7 (9%)
22	CLA	B	837	-	49,53,73	1.48	9 (18%)	59,89,113	1.46	5 (8%)
22	CLA	A	816	20	65,69,73	1.29	11 (16%)	78,108,113	1.42	10 (12%)
27	LMU	F	402	-	21,21,36	0.46	0	26,26,47	0.69	0
22	CLA	F	405	5	49,53,73	1.49	8 (16%)	59,89,113	1.38	4 (6%)
22	CLA	B	824	-	69,73,73	1.25	8 (11%)	83,113,113	1.32	7 (8%)
22	CLA	T	604	15	69,73,73	1.24	7 (10%)	83,113,113	1.29	6 (7%)
22	CLA	A	812	20	61,65,73	1.32	8 (13%)	73,103,113	1.30	6 (8%)
22	CLA	X	405	-	60,64,73	1.34	8 (13%)	72,102,113	1.34	6 (8%)
26	LHG	W	420	22	41,41,48	1.19	6 (14%)	44,47,54	0.89	2 (4%)
22	CLA	I	606	8	65,69,73	1.30	9 (13%)	78,108,113	1.29	5 (6%)
22	CLA	U	410	16	59,63,73	1.35	8 (13%)	71,101,113	1.33	5 (7%)
26	LHG	P	601	-	39,39,48	1.20	6 (15%)	42,45,54	0.98	2 (4%)
22	CLA	Q	610	26	69,73,73	1.26	9 (13%)	83,113,113	1.25	5 (6%)
22	CLA	G	605	-	49,53,73	1.48	8 (16%)	59,89,113	1.46	4 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	CLA	G	604	-	49,53,73	1.49	8 (16%)	59,89,113	1.46	6 (10%)
26	LHG	G	614	22	31,31,48	1.32	6 (19%)	34,37,54	1.06	2 (5%)
22	CLA	L	417	11	69,73,73	1.27	7 (10%)	83,113,113	1.30	5 (6%)
22	CLA	W	415	18	49,53,73	1.53	9 (18%)	59,89,113	1.45	8 (13%)
22	CLA	K	612	10	49,53,73	1.48	8 (16%)	59,89,113	1.39	7 (11%)
22	CLA	B	836	1	55,59,73	1.40	8 (14%)	66,96,113	1.37	5 (7%)
22	CLA	W	405	18	64,68,73	1.31	7 (10%)	77,107,113	1.29	6 (7%)
22	CLA	U	406	-	60,64,73	1.35	7 (11%)	72,102,113	1.33	6 (8%)
22	CLA	Q	606	-	49,53,73	1.49	8 (16%)	59,89,113	1.45	5 (8%)
22	CLA	I	604	-	49,53,73	1.49	8 (16%)	59,89,113	1.44	5 (8%)
22	CLA	A	809	20	57,61,73	1.38	8 (14%)	68,98,113	1.36	7 (10%)
22	CLA	B	859	-	69,73,73	1.26	9 (13%)	83,113,113	1.31	6 (7%)
22	CLA	Q	601	-	49,53,73	1.51	9 (18%)	59,89,113	1.43	5 (8%)
22	CLA	R	605	-	69,73,73	1.27	8 (11%)	83,113,113	1.29	6 (7%)
22	CLA	R	609	-	45,49,73	1.52	7 (15%)	54,84,113	1.50	7 (12%)
22	CLA	K	609	26	64,68,73	1.29	8 (12%)	77,107,113	1.30	4 (5%)
25	DGD	F	401	-	33,33,67	1.08	2 (6%)	35,35,81	1.31	4 (11%)
22	CLA	B	814	1	49,53,73	1.47	8 (16%)	59,89,113	1.42	7 (11%)
26	LHG	X	420	22	41,41,48	1.19	6 (14%)	44,47,54	0.99	2 (4%)
22	CLA	B	834	1	69,73,73	1.25	8 (11%)	83,113,113	1.30	7 (8%)
26	LHG	N	614	22	27,27,48	1.38	6 (22%)	30,33,54	1.10	2 (6%)
22	CLA	T	602	15	69,73,73	1.26	8 (11%)	83,113,113	1.27	7 (8%)
22	CLA	W	409	-	69,73,73	1.25	9 (13%)	83,113,113	1.28	7 (8%)
22	CLA	A	838	20	56,60,73	1.39	9 (16%)	67,97,113	1.43	9 (13%)
22	CLA	X	404	19	64,68,73	1.31	7 (10%)	77,107,113	1.27	6 (7%)
22	CLA	W	406	-	60,64,73	1.34	8 (13%)	72,102,113	1.32	5 (6%)
22	CLA	A	842	20	69,73,73	1.26	7 (10%)	83,113,113	1.30	6 (7%)
22	CLA	B	804	1	69,73,73	1.25	9 (13%)	83,113,113	1.34	7 (8%)
27	LMU	B	849	-	24,24,36	0.45	0	29,29,47	0.65	0
31	CHL	W	408	-	65,74,74	2.71	13 (20%)	59,114,114	1.30	7 (11%)
22	CLA	S	603	14	49,53,73	1.48	8 (16%)	59,89,113	1.43	5 (8%)
22	CLA	H	309	26	59,63,73	1.37	8 (13%)	71,101,113	1.34	6 (8%)
27	LMU	H	301	-	21,21,36	0.49	0	26,26,47	0.72	0
22	CLA	G	607	-	64,68,73	1.29	8 (12%)	77,107,113	1.27	5 (6%)
31	CHL	V	605	-	45,54,74	3.25	14 (31%)	35,90,114	1.56	6 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	CLA	X	411	-	49,53,73	1.49	8 (16%)	59,89,113	1.46	7 (11%)
26	LHG	O	324	-	41,41,48	1.18	5 (12%)	44,47,54	0.97	2 (4%)
22	CLA	Q	611	10	59,63,73	1.36	8 (13%)	71,101,113	1.33	7 (9%)
22	CLA	B	817	1	69,73,73	1.25	8 (11%)	83,113,113	1.27	5 (6%)
22	CLA	A	834	20	49,53,73	1.49	9 (18%)	59,89,113	1.41	6 (10%)
21	BCR	M	101	-	41,41,41	0.75	0	56,56,56	2.02	16 (28%)
24	DD6	S	611	-	39,45,45	1.99	3 (7%)	52,67,67	1.78	13 (25%)
22	CLA	A	836	20	69,73,73	1.25	7 (10%)	83,113,113	1.26	6 (7%)
22	CLA	A	805	20	65,69,73	1.29	7 (10%)	78,108,113	1.30	7 (8%)
22	CLA	A	801	-	69,73,73	1.23	11 (15%)	83,113,113	1.36	10 (12%)
22	CLA	O	311	26	64,68,73	1.29	7 (10%)	77,107,113	1.29	6 (7%)
21	BCR	B	842	-	41,41,41	0.72	0	56,56,56	1.99	15 (26%)
22	CLA	V	607	-	49,53,73	1.49	7 (14%)	59,89,113	1.44	6 (10%)
22	CLA	R	604	-	49,53,73	1.49	7 (14%)	59,89,113	1.40	7 (11%)
22	CLA	A	837	20	54,58,73	1.42	9 (16%)	65,95,113	1.39	8 (12%)
28	LMG	L	401	-	51,51,55	0.71	0	59,59,63	1.32	5 (8%)
22	CLA	H	305	7	64,68,73	1.30	8 (12%)	77,107,113	1.31	7 (9%)
22	CLA	X	407	-	69,73,73	1.26	8 (11%)	83,113,113	1.28	7 (8%)
28	LMG	H	317	-	43,43,55	0.79	1 (2%)	51,51,63	1.31	7 (13%)
22	CLA	N	609	8	49,53,73	1.49	8 (16%)	59,89,113	1.40	5 (8%)
26	LHG	B	851	-	41,41,48	1.17	6 (14%)	44,47,54	0.99	3 (6%)
22	CLA	R	608	26	58,62,73	1.38	8 (13%)	69,99,113	1.32	5 (7%)
22	CLA	A	824	20	69,73,73	1.25	8 (11%)	83,113,113	1.28	7 (8%)
22	CLA	S	604	-	64,68,73	1.31	8 (12%)	77,107,113	1.30	6 (7%)
22	CLA	P	608	-	49,53,73	1.51	8 (16%)	59,89,113	1.44	6 (10%)
22	CLA	A	852	-	69,73,73	1.25	7 (10%)	83,113,113	1.23	6 (7%)
22	CLA	B	829	-	49,53,73	1.44	11 (22%)	59,89,113	1.53	5 (8%)
22	CLA	G	601	6	49,53,73	1.48	7 (14%)	59,89,113	1.45	5 (8%)
22	CLA	L	409	26	64,68,73	1.30	9 (14%)	77,107,113	1.30	5 (6%)
22	CLA	Q	608	10	54,58,73	1.42	7 (12%)	65,95,113	1.38	7 (10%)
22	CLA	A	831	20	69,73,73	1.24	8 (11%)	83,113,113	1.29	6 (7%)
22	CLA	I	602	8	64,68,73	1.31	8 (12%)	77,107,113	1.32	8 (10%)
22	CLA	N	604	-	49,53,73	1.49	8 (16%)	59,89,113	1.43	4 (6%)
22	CLA	B	816	1	69,73,73	1.26	9 (13%)	83,113,113	1.29	6 (7%)
24	DD6	X	416	-	39,45,45	2.01	2 (5%)	52,67,67	2.23	15 (28%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	CLA	B	825	1	69,73,73	1.25	6 (8%)	83,113,113	1.30	7 (8%)
28	LMG	I	614	-	37,37,55	0.85	0	45,45,63	1.27	5 (11%)
22	CLA	B	839	26	69,73,73	1.25	8 (11%)	83,113,113	1.29	7 (8%)
22	CLA	H	306	-	59,63,73	1.36	9 (15%)	71,101,113	1.34	5 (7%)
24	DD6	X	401	-	39,45,45	1.98	3 (7%)	52,67,67	1.83	11 (21%)
28	LMG	I	615	-	49,50,55	0.75	0	54,57,63	1.38	4 (7%)
22	CLA	S	607	14	64,68,73	1.31	7 (10%)	77,107,113	1.29	5 (6%)
22	CLA	T	607	15	64,68,73	1.31	8 (12%)	77,107,113	1.30	8 (10%)
24	DD6	A	858	-	39,45,45	1.97	2 (5%)	52,67,67	2.54	18 (34%)
27	LMU	U	424	-	24,24,36	0.42	0	29,29,47	0.58	0
22	CLA	N	611	-	43,48,73	1.56	7 (16%)	52,82,113	1.52	7 (13%)
24	DD6	L	413	-	39,45,45	2.00	3 (7%)	52,67,67	1.78	12 (23%)
26	LHG	N	616	-	42,42,48	1.17	6 (14%)	45,48,54	0.98	2 (4%)
22	CLA	X	409	19	69,73,73	1.25	8 (11%)	83,113,113	1.26	7 (8%)
28	LMG	Q	602	-	37,37,55	0.84	1 (2%)	45,45,63	1.28	5 (11%)
24	DD6	H	315	-	39,45,45	1.99	3 (7%)	52,67,67	1.78	13 (25%)
22	CLA	A	817	20	69,73,73	1.25	8 (11%)	83,113,113	1.29	7 (8%)
28	LMG	K	622	-	43,43,55	0.80	0	51,51,63	1.27	5 (9%)
27	LMU	A	854	-	36,36,36	0.42	0	47,47,47	0.69	1 (2%)
22	CLA	K	611	10	69,73,73	1.26	7 (10%)	83,113,113	1.30	5 (6%)
27	LMU	L	419	-	27,27,36	0.41	0	30,30,47	0.75	0
24	DD6	Q	615	-	39,45,45	2.03	3 (7%)	52,67,67	1.90	14 (26%)
26	LHG	U	419	22	24,24,48	1.42	5 (20%)	27,29,54	1.22	2 (7%)
31	CHL	X	406	-	45,54,74	3.28	13 (28%)	35,90,114	1.58	6 (17%)
24	DD6	A	859	-	39,45,45	2.07	3 (7%)	52,67,67	1.88	13 (25%)
28	LMG	K	618	-	49,49,55	0.76	0	57,57,63	1.31	7 (12%)
22	CLA	L	410	11	64,68,73	1.30	7 (10%)	77,107,113	1.31	6 (7%)
26	LHG	B	848	22	26,26,48	1.33	5 (19%)	29,32,54	1.15	2 (6%)
22	CLA	T	609	15	49,53,73	1.48	8 (16%)	59,89,113	1.44	7 (11%)
28	LMG	H	322	-	37,37,55	0.85	0	45,45,63	1.23	4 (8%)
23	PQN	B	840	-	34,34,34	1.61	2 (5%)	42,45,45	1.07	3 (7%)
22	CLA	U	403	16	49,53,73	1.50	7 (14%)	59,89,113	1.47	6 (10%)
28	LMG	B	852	-	43,43,55	0.84	0	51,51,63	1.27	4 (7%)
27	LMU	O	303	-	36,36,36	0.42	0	47,47,47	0.71	1 (2%)
26	LHG	A	845	-	48,48,48	1.10	6 (12%)	51,54,54	0.94	3 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	CLA	L	402	11	69,73,73	1.24	9 (13%)	83,113,113	1.27	5 (6%)
22	CLA	R	602	-	64,68,73	1.31	8 (12%)	77,107,113	1.28	5 (6%)
22	CLA	Q	613	10	49,53,73	1.48	8 (16%)	59,89,113	1.46	7 (11%)
22	CLA	B	805	1	69,73,73	1.25	8 (11%)	83,113,113	1.30	6 (7%)
22	CLA	X	412	19	69,73,73	1.27	8 (11%)	83,113,113	1.27	6 (7%)
22	CLA	O	306	13	64,68,73	1.30	8 (12%)	77,107,113	1.29	7 (9%)
22	CLA	T	610	-	49,53,73	1.49	6 (12%)	59,89,113	1.41	4 (6%)
22	CLA	H	313	7	62,66,73	1.33	7 (11%)	74,104,113	1.32	6 (8%)
22	CLA	S	609	14	59,63,73	1.36	6 (10%)	71,101,113	1.31	6 (8%)
24	DD6	T	613	-	39,45,45	1.98	3 (7%)	52,67,67	1.73	11 (21%)
22	CLA	R	606	11	61,65,73	1.34	6 (9%)	73,103,113	1.29	6 (8%)
22	CLA	T	601	15	49,53,73	1.48	8 (16%)	59,89,113	1.45	4 (6%)
22	CLA	I	609	8	49,53,73	1.49	8 (16%)	59,89,113	1.47	5 (8%)
22	CLA	P	606	6	49,53,73	1.47	8 (16%)	59,89,113	1.43	5 (8%)
22	CLA	A	820	20	69,73,73	1.25	8 (11%)	83,113,113	1.27	9 (10%)
22	CLA	A	825	20	65,69,73	1.27	6 (9%)	78,108,113	1.29	6 (7%)
22	CLA	O	312	13	64,68,73	1.29	8 (12%)	77,107,113	1.32	9 (11%)
21	BCR	A	851	-	41,41,41	0.70	0	56,56,56	2.11	16 (28%)
22	CLA	A	839	20	69,73,73	1.24	6 (8%)	83,113,113	1.38	8 (9%)
22	CLA	P	607	6	49,53,73	1.49	9 (18%)	59,89,113	1.43	5 (8%)
22	CLA	V	608	17	59,63,73	1.35	7 (11%)	71,101,113	1.31	6 (8%)
22	CLA	A	844	26	59,63,73	1.36	9 (15%)	71,101,113	1.39	7 (9%)
22	CLA	W	403	18	56,60,73	1.41	9 (16%)	67,97,113	1.39	7 (10%)
25	DGD	O	304	-	61,61,67	0.87	3 (4%)	75,75,81	1.14	8 (10%)
22	CLA	B	806	1	69,73,73	1.26	8 (11%)	83,113,113	1.28	6 (7%)
22	CLA	S	614	-	49,53,73	1.48	8 (16%)	59,89,113	1.45	5 (8%)
24	DD6	W	416	-	39,45,45	1.97	3 (7%)	52,67,67	1.80	11 (21%)
22	CLA	T	603	15	64,68,73	1.31	8 (12%)	77,107,113	1.30	6 (7%)
22	CLA	Q	605	-	60,64,73	1.34	7 (11%)	72,102,113	1.34	8 (11%)
22	CLA	A	840	20	69,73,73	1.25	8 (11%)	83,113,113	1.28	7 (8%)
22	CLA	A	833	20	69,73,73	1.25	8 (11%)	83,113,113	1.28	8 (9%)
22	CLA	K	606	-	54,58,73	1.42	8 (14%)	65,95,113	1.42	6 (9%)
22	CLA	N	610	8	59,63,73	1.36	7 (11%)	71,101,113	1.43	8 (11%)
27	LMU	B	858	-	14,14,36	0.31	0	13,13,47	0.58	0
25	DGD	B	847	-	67,67,67	0.83	2 (2%)	81,81,81	1.01	5 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	CLA	X	408	19	69,73,73	1.25	8 (11%)	83,113,113	1.29	5 (6%)
28	LMG	A	855	-	41,41,55	0.84	0	49,49,63	1.26	5 (10%)
22	CLA	U	413	16	49,53,73	1.49	7 (14%)	59,89,113	1.47	6 (10%)
22	CLA	R	610	11	69,73,73	1.27	7 (10%)	83,113,113	1.24	7 (8%)
22	CLA	N	607	-	64,68,73	1.31	7 (10%)	77,107,113	1.28	6 (7%)
22	CLA	R	611	11	49,53,73	1.50	7 (14%)	59,89,113	1.41	5 (8%)
24	DD6	R	613	-	39,45,45	2.01	3 (7%)	52,67,67	2.01	18 (34%)
22	CLA	B	803	1	60,64,73	1.34	6 (10%)	72,102,113	1.34	7 (9%)
22	CLA	W	419	18	49,53,73	1.49	7 (14%)	59,89,113	1.44	4 (6%)
24	DD6	L	414	-	39,45,45	2.01	3 (7%)	52,67,67	1.80	15 (28%)
22	CLA	S	610	14	49,53,73	1.50	7 (14%)	59,89,113	1.51	5 (8%)
22	CLA	A	832	20	56,60,73	1.39	8 (14%)	67,97,113	1.36	6 (8%)
28	LMG	T	616	-	41,41,55	0.84	0	49,49,63	1.24	3 (6%)
27	LMU	B	855	-	24,24,36	0.45	0	29,29,47	0.67	0
22	CLA	I	610	8	49,53,73	1.49	9 (18%)	59,89,113	1.44	5 (8%)
22	CLA	T	611	15	69,73,73	1.26	7 (10%)	83,113,113	1.28	5 (6%)
22	CLA	H	307	7	64,68,73	1.31	7 (10%)	77,107,113	1.29	4 (5%)
22	CLA	P	602	6	49,53,73	1.47	10 (20%)	59,89,113	1.48	6 (10%)
22	CLA	N	603	8	69,73,73	1.26	8 (11%)	83,113,113	1.26	7 (8%)
22	CLA	U	415	16	49,53,73	1.49	8 (16%)	59,89,113	1.40	5 (8%)
24	DD6	O	316	-	39,45,45	1.96	3 (7%)	52,67,67	1.72	12 (23%)
27	LMU	G	615	-	21,21,36	0.46	0	26,26,47	0.51	0
22	CLA	B	822	1	69,73,73	1.26	8 (11%)	83,113,113	1.28	6 (7%)
22	CLA	Q	618	-	49,53,73	1.50	7 (14%)	59,89,113	1.41	4 (6%)
22	CLA	V	613	-	49,53,73	1.51	6 (12%)	59,89,113	1.48	4 (6%)
24	DD6	V	615	-	39,45,45	1.94	3 (7%)	52,67,67	1.87	13 (25%)
21	BCR	J	103	-	41,41,41	0.68	0	56,56,56	1.78	12 (21%)
22	CLA	L	403	11	64,68,73	1.30	8 (12%)	77,107,113	1.31	7 (9%)
22	CLA	A	835	20	65,69,73	1.29	8 (12%)	78,108,113	1.29	6 (7%)
22	CLA	U	414	16	65,69,73	1.30	8 (12%)	78,108,113	1.31	5 (6%)
27	LMU	B	850	-	24,24,36	0.44	0	29,29,47	0.55	0
26	LHG	Q	616	22	43,43,48	1.16	6 (13%)	46,49,54	0.94	2 (4%)
22	CLA	I	603	8	60,64,73	1.36	8 (13%)	72,102,113	1.31	7 (9%)
27	LMU	H	321	-	34,34,36	0.48	0	44,44,47	0.79	2 (4%)
22	CLA	K	603	10	64,68,73	1.30	8 (12%)	77,107,113	1.30	6 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
30	SQD	O	302	-	41,42,54	0.43	1 (2%)	50,53,65	0.52	1 (2%)
24	DD6	U	417	-	39,45,45	1.93	3 (7%)	52,67,67	1.87	15 (28%)
22	CLA	B	813	1	69,73,73	1.25	8 (11%)	83,113,113	1.22	6 (7%)
22	CLA	U	411	16	61,65,73	1.32	7 (11%)	73,103,113	1.31	6 (8%)
22	CLA	L	412	11	49,53,73	1.49	8 (16%)	59,89,113	1.38	5 (8%)
22	CLA	H	308	7	64,68,73	1.29	7 (10%)	77,107,113	1.29	6 (7%)
24	DD6	W	418	-	39,45,45	2.02	3 (7%)	52,67,67	1.89	14 (26%)
26	LHG	K	616	22	38,38,48	1.22	5 (13%)	41,44,54	1.03	3 (7%)
22	CLA	N	605	-	49,53,73	1.48	8 (16%)	59,89,113	1.47	6 (10%)
27	LMU	A	853	-	24,24,36	0.43	0	29,29,47	0.57	0
22	CLA	S	608	26	49,53,73	1.50	7 (14%)	59,89,113	1.42	6 (10%)
30	SQD	V	618	-	26,27,54	0.52	1 (3%)	33,36,65	0.45	0
21	BCR	B	846	-	41,41,41	0.71	0	56,56,56	1.82	17 (30%)
22	CLA	A	810	20	69,73,73	1.24	7 (10%)	83,113,113	1.27	6 (7%)
22	CLA	U	401	-	59,63,73	1.36	8 (13%)	71,101,113	1.34	7 (9%)
24	DD6	F	406	-	39,45,45	2.01	3 (7%)	52,67,67	1.89	16 (30%)
22	CLA	A	806	20	69,73,73	1.25	7 (10%)	83,113,113	1.26	6 (7%)
22	CLA	A	804	-	69,73,73	1.25	7 (10%)	83,113,113	1.21	5 (6%)
22	CLA	X	417	19	54,58,73	1.42	6 (11%)	65,95,113	1.41	8 (12%)
22	CLA	P	609	-	49,53,73	1.49	9 (18%)	59,89,113	1.41	4 (6%)
22	CLA	G	606	6	69,73,73	1.26	8 (11%)	83,113,113	1.23	5 (6%)
22	CLA	I	605	-	49,53,73	1.48	8 (16%)	59,89,113	1.46	7 (11%)
29	SF4	B	860	20,1	0,12,12	-	-	-	-	-
22	CLA	A	823	20	49,53,73	1.48	8 (16%)	59,89,113	1.47	6 (10%)
27	LMU	K	620	-	34,34,36	0.50	0	44,44,47	1.04	5 (11%)
21	BCR	A	848	-	41,41,41	0.71	0	56,56,56	1.81	10 (17%)
22	CLA	K	605	-	69,73,73	1.25	7 (10%)	83,113,113	1.27	4 (4%)
22	CLA	P	611	6	49,53,73	1.50	6 (12%)	59,89,113	1.48	5 (8%)
22	CLA	O	309	13	54,58,73	1.40	9 (16%)	65,95,113	1.41	5 (7%)
24	DD6	O	317	-	39,45,45	2.01	3 (7%)	52,67,67	1.79	14 (26%)
22	CLA	S	615	-	55,59,73	1.40	8 (14%)	66,96,113	1.39	6 (9%)
26	LHG	A	846	22	48,48,48	1.11	6 (12%)	51,54,54	0.92	2 (3%)
22	CLA	U	404	16	69,73,73	1.25	8 (11%)	83,113,113	1.27	7 (8%)
22	CLA	X	402	19	59,63,73	1.35	7 (11%)	71,101,113	1.36	7 (9%)
27	LMU	O	301	-	24,24,36	0.44	0	29,29,47	0.57	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
27	LMU	U	422	-	36,36,36	0.44	0	47,47,47	0.79	2 (4%)
21	BCR	B	801	-	41,41,41	0.69	0	56,56,56	1.96	16 (28%)
27	LMU	U	421	-	36,36,36	0.41	0	47,47,47	0.65	1 (2%)
33	CL0	A	802	20	63,73,73	2.83	21 (33%)	61,113,113	1.91	12 (19%)
27	LMU	A	856	-	21,21,36	0.46	0	26,26,47	0.50	0
26	LHG	T	614	22	41,41,48	1.19	6 (14%)	44,47,54	0.98	2 (4%)
22	CLA	Q	604	10	69,73,73	1.25	7 (10%)	83,113,113	1.28	7 (8%)
22	CLA	Q	607	-	49,53,73	1.49	7 (14%)	59,89,113	1.42	5 (8%)
31	CHL	W	422	-	65,74,74	2.67	13 (20%)	59,114,114	1.27	6 (10%)
22	CLA	B	815	1	56,60,73	1.39	9 (16%)	67,97,113	1.32	6 (8%)
24	DD6	K	614	-	39,45,45	1.98	3 (7%)	52,67,67	1.86	15 (28%)
29	SF4	C	102	2	0,12,12	-	-	-	-	-
22	CLA	H	304	7	49,53,73	1.48	8 (16%)	59,89,113	1.43	7 (11%)
22	CLA	O	310	13	64,68,73	1.29	9 (14%)	77,107,113	1.34	6 (7%)
30	SQD	F	407	-	41,42,54	0.42	1 (2%)	50,53,65	0.49	1 (2%)
23	PQN	A	843	-	34,34,34	1.59	2 (5%)	42,45,45	1.08	3 (7%)
26	LHG	R	614	22	41,41,48	1.18	6 (14%)	44,47,54	0.96	2 (4%)
24	DD6	A	847	-	39,45,45	1.98	3 (7%)	52,67,67	1.85	15 (28%)
22	CLA	B	807	1	69,73,73	1.24	9 (13%)	83,113,113	1.24	5 (6%)
22	CLA	H	318	7	49,53,73	1.49	7 (14%)	59,89,113	1.44	5 (8%)
27	LMU	B	854	-	24,24,36	0.46	0	29,29,47	0.81	1 (3%)
22	CLA	O	305	13	54,58,73	1.40	8 (14%)	65,95,113	1.41	8 (12%)
22	CLA	B	832	1	66,70,73	1.27	8 (12%)	79,109,113	1.34	7 (8%)
22	CLA	B	833	1	69,73,73	1.25	8 (11%)	83,113,113	1.26	5 (6%)
22	CLA	W	412	26	64,68,73	1.31	9 (14%)	77,107,113	1.32	6 (7%)

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
24	DD6	H	314	-	-	1/26/80/80	0/3/3/3
22	CLA	O	315	13	-	4/21/97/115	-
22	CLA	B	838	1	-	7/15/91/115	-
29	SF4	C	101	2	-	-	0/6/5/5
24	DD6	P	612	-	-	6/26/80/80	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	O	314	13	-	1/15/91/115	-
22	CLA	L	407	-	-	11/30/106/115	-
27	LMU	T	618	-	-	1/15/35/61	0/1/1/2
22	CLA	A	828	20	-	8/39/115/115	-
22	CLA	L	411	11	-	14/39/115/115	-
22	CLA	G	602	6	-	4/33/109/115	-
27	LMU	X	418	-	-	1/15/35/61	0/1/1/2
26	LHG	L	416	22	-	20/46/46/53	-
22	CLA	W	402	18	-	2/27/103/115	-
24	DD6	V	614	-	-	1/26/80/80	0/3/3/3
28	LMG	U	423	-	-	20/44/64/70	0/1/1/1
22	CLA	S	602	14	-	9/33/109/115	-
28	LMG	H	319	-	-	19/35/55/70	0/1/1/1
22	CLA	B	830	1	-	9/39/115/115	-
22	CLA	X	410	26	-	12/33/109/115	-
22	CLA	B	812	1	-	18/39/115/115	-
30	SQD	K	621	-	-	5/38/58/69	0/1/1/1
24	DD6	J	105	-	-	3/26/80/80	0/3/3/3
22	CLA	B	835	1	-	11/39/115/115	-
24	DD6	B	841	-	-	1/26/80/80	0/3/3/3
22	CLA	L	404	-	-	12/29/105/115	-
22	CLA	S	606	14	-	4/21/97/115	-
32	NEX	V	616	-	-	4/27/83/83	0/3/3/3
22	CLA	A	841	20	-	12/39/115/115	-
21	BCR	A	849	-	-	0/29/63/63	0/2/2/2
27	LMU	B	853	-	-	0/10/27/61	0/1/1/2
22	CLA	V	602	17	-	8/39/115/115	-
22	CLA	B	810	-	-	4/29/105/115	-
22	CLA	B	808	1	-	7/27/103/115	-
27	LMU	M	102	-	-	4/15/35/61	0/1/1/2
27	LMU	X	421	-	-	3/21/61/61	0/2/2/2
22	CLA	B	809	1	-	3/39/115/115	-
22	CLA	B	821	1	-	11/33/109/115	-
24	DD6	G	612	-	-	0/26/80/80	0/3/3/3
22	CLA	B	831	1	-	7/39/115/115	-
22	CLA	U	412	26	-	3/15/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	LMU	O	322	-	-	5/21/61/61	0/2/2/2
22	CLA	Q	617	10	-	5/24/100/115	-
22	CLA	B	823	-	-	10/39/115/115	-
22	CLA	P	610	6	-	5/10/86/115	-
22	CLA	W	414	18	-	10/39/115/115	-
21	BCR	B	844	-	-	1/29/63/63	0/2/2/2
22	CLA	O	308	-	-	14/35/111/115	-
22	CLA	H	302	7	-	4/15/91/115	-
28	LMG	J	101	-	-	23/50/70/70	0/1/1/1
22	CLA	V	612	-	-	15/39/115/115	-
22	CLA	I	607	8	-	4/27/103/115	-
24	DD6	U	416	-	-	1/26/80/80	0/3/3/3
22	CLA	A	807	20	-	13/39/115/115	-
22	CLA	H	310	7	-	3/15/91/115	-
22	CLA	S	601	14	-	6/15/91/115	-
27	LMU	A	857	-	-	3/15/35/61	0/1/1/2
22	CLA	K	608	10	-	11/39/115/115	-
21	BCR	B	843	-	-	4/29/63/63	0/2/2/2
22	CLA	F	403	-	-	11/39/115/115	-
26	LHG	O	323	-	-	19/47/47/53	-
22	CLA	N	602	8	-	5/33/109/115	-
22	CLA	K	613	-	-	5/25/101/115	-
22	CLA	N	601	8	-	6/15/91/115	-
24	DD6	W	417	-	-	1/26/80/80	0/3/3/3
28	LMG	F	408	-	-	18/37/57/70	0/1/1/1
27	LMU	H	320	-	-	2/15/35/61	0/1/1/2
22	CLA	B	826	1	-	10/31/107/115	-
28	LMG	K	601	-	-	24/38/58/70	0/1/1/1
22	CLA	V	611	-	-	5/15/91/115	-
24	DD6	S	612	-	-	1/26/80/80	0/3/3/3
22	CLA	T	608	26	-	4/33/109/115	-
26	LHG	H	316	22	-	5/31/31/53	-
22	CLA	A	822	-	-	8/39/115/115	-
24	DD6	Q	614	-	-	1/26/80/80	0/3/3/3
24	DD6	I	613	-	-	0/26/80/80	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	R	603	-	-	10/29/105/115	-
26	LHG	S	613	22	-	13/36/36/53	-
22	CLA	I	601	8	-	15/39/115/115	-
24	DD6	N	612	-	-	0/26/80/80	0/3/3/3
22	CLA	P	603	6	-	5/15/91/115	-
22	CLA	R	601	-	-	19/39/115/115	-
22	CLA	A	818	20	-	4/25/101/115	-
22	CLA	U	405	16	-	5/30/106/115	-
22	CLA	G	608	26	-	16/33/109/115	-
22	CLA	A	830	20	-	13/39/115/115	-
27	LMU	T	617	-	-	3/15/35/61	0/1/1/2
22	CLA	L	408	11	-	6/33/109/115	-
22	CLA	A	811	20	-	10/30/106/115	-
31	CHL	U	408	-	-	1/15/113/137	-
22	CLA	Q	603	10	-	4/15/91/115	-
22	CLA	A	815	20	-	6/39/115/115	-
28	LMG	G	616	-	-	21/41/61/70	0/1/1/1
24	DD6	P	613	-	-	4/26/80/80	0/3/3/3
22	CLA	W	411	18	-	10/33/109/115	-
27	LMU	J	104	-	-	9/21/57/61	0/2/2/2
22	CLA	G	610	6	-	5/15/91/115	-
24	DD6	G	613	-	-	1/26/80/80	0/3/3/3
24	DD6	I	612	-	-	0/26/80/80	0/3/3/3
28	LMG	N	615	-	-	24/39/59/70	0/1/1/1
26	LHG	K	619	-	-	19/37/37/53	-
27	LMU	L	420	-	-	4/21/57/61	1/2/2/2
24	DD6	R	612	-	-	1/26/80/80	0/3/3/3
28	LMG	B	856	-	-	26/48/68/70	0/1/1/1
22	CLA	A	808	20	-	12/39/115/115	-
22	CLA	W	413	-	-	6/15/91/115	-
22	CLA	X	413	19	-	3/15/91/115	-
22	CLA	A	803	-	-	12/39/115/115	-
28	LMG	W	401	-	-	19/43/63/70	0/1/1/1
22	CLA	N	608	26	-	7/15/91/115	-
22	CLA	B	811	1	-	2/15/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	T	605	-	-	15/39/115/115	-
22	CLA	B	828	1	-	15/39/115/115	-
22	CLA	G	609	-	-	4/15/91/115	-
22	CLA	Q	609	10	-	9/33/109/115	-
22	CLA	P	605	-	-	8/15/91/115	-
22	CLA	H	303	7	-	11/33/109/115	-
22	CLA	V	609	17	-	8/30/106/115	-
22	CLA	J	102	9	-	7/21/97/115	-
24	DD6	N	613	-	-	4/26/80/80	0/3/3/3
26	LHG	O	318	22	-	16/38/38/53	-
21	BCR	B	845	-	-	2/29/63/63	0/2/2/2
22	CLA	K	602	10	-	11/33/109/115	-
22	CLA	O	307	13	-	3/15/91/115	-
27	LMU	W	421	-	-	4/15/35/61	0/1/1/2
22	CLA	R	615	11	-	13/39/115/115	-
32	NEX	U	418	-	-	4/27/83/83	0/3/3/3
22	CLA	B	827	1	-	9/39/115/115	-
22	CLA	A	814	20	-	9/39/115/115	-
22	CLA	X	403	19	-	9/39/115/115	-
22	CLA	I	608	-	-	5/15/91/115	-
22	CLA	V	617	-	-	10/15/91/115	-
27	LMU	O	320	-	-	1/17/35/61	0/2/2/2
22	CLA	B	802	1	-	6/39/115/115	-
22	CLA	A	819	20	-	11/31/107/115	-
22	CLA	A	827	-	-	5/36/112/115	-
22	CLA	A	813	20	-	10/39/115/115	-
27	LMU	L	418	-	-	0/15/35/61	0/1/1/2
22	CLA	K	617	10	-	12/39/115/115	-
22	CLA	O	313	13	-	14/39/115/115	-
22	CLA	R	607	11	-	17/33/109/115	-
22	CLA	F	404	-	-	10/27/103/115	-
22	CLA	O	319	13	-	1/15/91/115	-
22	CLA	B	819	1	-	9/25/101/115	-
27	LMU	B	857	-	-	4/21/61/61	0/2/2/2
22	CLA	A	826	-	-	8/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	LHG	O	321	-	-	30/53/53/53	-
22	CLA	K	610	10	-	8/29/105/115	-
22	CLA	H	311	7	-	16/39/115/115	-
22	CLA	U	420	16	-	9/15/91/115	-
22	CLA	P	604	-	-	6/15/91/115	-
22	CLA	X	419	19	-	9/15/91/115	-
22	CLA	G	603	6	-	10/29/105/115	-
22	CLA	H	312	7	-	3/15/91/115	-
31	CHL	V	606	-	-	1/15/113/137	-
22	CLA	L	405	-	-	3/15/91/115	-
22	CLA	V	610	-	-	4/15/91/115	-
31	CHL	W	407	-	-	2/15/113/137	-
24	DD6	X	415	-	-	1/26/80/80	0/3/3/3
28	LMG	U	402	-	-	25/48/68/70	0/1/1/1
31	CHL	U	407	-	-	0/15/113/137	-
27	LMU	F	409	-	-	4/12/32/61	0/1/1/2
24	DD6	L	415	-	-	3/26/80/80	0/3/3/3
22	CLA	I	611	8	-	6/15/91/115	-
22	CLA	V	604	-	-	9/29/105/115	-
22	CLA	A	829	20	-	15/39/115/115	-
22	CLA	W	410	18	-	10/33/109/115	-
21	BCR	A	850	-	-	4/29/63/63	0/2/2/2
24	DD6	K	615	-	-	0/26/80/80	0/3/3/3
24	DD6	X	414	-	-	1/26/80/80	0/3/3/3
22	CLA	A	821	20	-	15/39/115/115	-
22	CLA	V	603	17	-	11/30/106/115	-
27	LMU	T	615	-	-	0/12/32/61	0/1/1/2
22	CLA	T	606	15	-	5/21/97/115	-
22	CLA	K	604	-	-	19/37/113/115	-
22	CLA	V	601	17	-	6/15/91/115	-
22	CLA	G	611	6	-	5/15/91/115	-
22	CLA	U	409	-	-	6/15/91/115	-
22	CLA	B	820	1	-	8/25/101/115	-
22	CLA	B	818	-	-	12/39/115/115	-
22	CLA	W	404	18	-	10/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	DD6	T	612	-	-	1/26/80/80	0/3/3/3
22	CLA	N	606	8	-	13/39/115/115	-
22	CLA	L	406	-	-	10/39/115/115	-
22	CLA	K	607	10	-	9/30/106/115	-
22	CLA	Q	612	10	-	15/39/115/115	-
22	CLA	S	605	-	-	14/33/109/115	-
22	CLA	B	837	-	-	3/15/91/115	-
22	CLA	A	816	20	-	14/35/111/115	-
27	LMU	F	402	-	-	1/12/32/61	0/1/1/2
22	CLA	F	405	5	-	7/15/91/115	-
22	CLA	B	824	-	-	11/39/115/115	-
22	CLA	T	604	15	-	18/39/115/115	-
22	CLA	A	812	20	-	10/30/106/115	-
22	CLA	X	405	-	-	8/29/105/115	-
26	LHG	W	420	22	-	22/46/46/53	-
22	CLA	I	606	8	-	12/35/111/115	-
22	CLA	U	410	16	-	7/27/103/115	-
26	LHG	P	601	-	-	23/44/44/53	-
22	CLA	Q	610	26	-	16/39/115/115	-
22	CLA	G	605	-	-	3/15/91/115	-
22	CLA	G	604	-	-	0/15/91/115	-
26	LHG	G	614	22	-	13/36/36/53	-
22	CLA	L	417	11	-	8/39/115/115	-
22	CLA	W	415	18	-	6/15/91/115	-
22	CLA	K	612	10	-	2/15/91/115	-
22	CLA	B	836	1	-	2/23/99/115	-
22	CLA	W	405	18	-	3/33/109/115	-
22	CLA	U	406	-	-	7/29/105/115	-
22	CLA	Q	606	-	-	7/15/91/115	-
22	CLA	I	604	-	-	1/15/91/115	-
22	CLA	A	809	20	-	1/25/101/115	-
22	CLA	B	859	-	-	12/39/115/115	-
22	CLA	Q	601	-	-	6/15/91/115	-
22	CLA	R	605	-	-	15/39/115/115	-
22	CLA	R	609	-	-	3/10/86/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	K	609	26	-	13/33/109/115	-
25	DGD	F	401	-	-	19/35/35/95	-
22	CLA	B	814	1	-	6/15/91/115	-
26	LHG	X	420	22	-	28/46/46/53	-
22	CLA	B	834	1	-	7/39/115/115	-
26	LHG	N	614	22	-	9/32/32/53	-
22	CLA	T	602	15	-	9/39/115/115	-
22	CLA	W	409	-	-	10/39/115/115	-
22	CLA	A	838	20	-	7/24/100/115	-
22	CLA	X	404	19	-	8/33/109/115	-
22	CLA	W	406	-	-	2/29/105/115	-
22	CLA	A	842	20	-	12/39/115/115	-
22	CLA	B	804	1	-	15/39/115/115	-
27	LMU	B	849	-	-	2/15/35/61	0/1/1/2
31	CHL	W	408	-	-	4/39/137/137	-
22	CLA	S	603	14	-	3/15/91/115	-
22	CLA	H	309	26	-	10/27/103/115	-
27	LMU	H	301	-	-	2/12/32/61	0/1/1/2
22	CLA	G	607	-	-	3/33/109/115	-
31	CHL	V	605	-	-	0/15/113/137	-
22	CLA	X	411	-	-	3/15/91/115	-
26	LHG	O	324	-	-	25/46/46/53	-
22	CLA	Q	611	10	-	9/27/103/115	-
22	CLA	B	817	1	-	15/39/115/115	-
22	CLA	A	834	20	-	5/15/91/115	-
21	BCR	M	101	-	-	2/29/63/63	0/2/2/2
24	DD6	S	611	-	-	1/26/80/80	0/3/3/3
22	CLA	A	836	20	-	12/39/115/115	-
22	CLA	A	805	20	-	9/35/111/115	-
22	CLA	A	801	-	-	15/39/115/115	-
22	CLA	O	311	26	-	9/33/109/115	-
21	BCR	B	842	-	-	2/29/63/63	0/2/2/2
22	CLA	V	607	-	-	3/15/91/115	-
22	CLA	R	604	-	-	5/15/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	A	837	20	-	6/21/97/115	-
28	LMG	L	401	-	-	20/46/66/70	0/1/1/1
22	CLA	H	305	7	-	11/33/109/115	-
22	CLA	X	407	-	-	4/39/115/115	-
28	LMG	H	317	-	-	13/38/58/70	0/1/1/1
22	CLA	N	609	8	-	4/15/91/115	-
26	LHG	B	851	-	-	22/46/46/53	-
22	CLA	R	608	26	-	10/26/102/115	-
22	CLA	A	824	20	-	25/39/115/115	-
22	CLA	S	604	-	-	9/33/109/115	-
22	CLA	P	608	-	-	9/15/91/115	-
22	CLA	A	852	-	-	14/39/115/115	-
22	CLA	B	829	-	-	7/15/91/115	-
22	CLA	G	601	6	-	6/15/91/115	-
22	CLA	L	409	26	-	6/33/109/115	-
22	CLA	Q	608	10	-	3/21/97/115	-
22	CLA	A	831	20	-	6/39/115/115	-
22	CLA	I	602	8	-	3/33/109/115	-
22	CLA	N	604	-	-	6/15/91/115	-
22	CLA	B	816	1	-	13/39/115/115	-
24	DD6	X	416	-	-	5/26/80/80	0/3/3/3
22	CLA	B	825	1	-	10/39/115/115	-
28	LMG	I	614	-	-	10/32/52/70	0/1/1/1
22	CLA	B	839	26	-	3/39/115/115	-
22	CLA	H	306	-	-	10/27/103/115	-
24	DD6	X	401	-	-	0/26/80/80	0/3/3/3
28	LMG	I	615	-	-	26/46/62/70	0/1/1/1
22	CLA	S	607	14	-	9/33/109/115	-
22	CLA	T	607	15	-	9/33/109/115	-
24	DD6	A	858	-	-	5/26/80/80	0/3/3/3
27	LMU	U	424	-	-	2/15/35/61	0/1/1/2
22	CLA	N	611	-	-	4/10/82/115	-
24	DD6	L	413	-	-	1/26/80/80	0/3/3/3
26	LHG	N	616	-	-	23/47/47/53	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	X	409	19	-	10/39/115/115	-
28	LMG	Q	602	-	-	11/32/52/70	0/1/1/1
24	DD6	H	315	-	-	1/26/80/80	0/3/3/3
22	CLA	A	817	20	-	16/39/115/115	-
28	LMG	K	622	-	-	15/38/58/70	0/1/1/1
27	LMU	A	854	-	-	3/21/61/61	0/2/2/2
22	CLA	K	611	10	-	11/39/115/115	-
27	LMU	L	419	-	-	6/21/34/61	1/1/1/2
24	DD6	Q	615	-	-	0/26/80/80	0/3/3/3
26	LHG	U	419	22	-	15/28/28/53	-
31	CHL	X	406	-	-	0/15/113/137	-
24	DD6	A	859	-	-	1/26/80/80	0/3/3/3
28	LMG	K	618	-	-	24/44/64/70	0/1/1/1
22	CLA	L	410	11	-	8/33/109/115	-
26	LHG	B	848	22	-	10/31/31/53	-
22	CLA	T	609	15	-	5/15/91/115	-
28	LMG	H	322	-	-	15/32/52/70	0/1/1/1
23	PQN	B	840	-	-	0/23/43/43	0/2/2/2
22	CLA	U	403	16	-	8/15/91/115	-
28	LMG	B	852	-	-	15/38/58/70	0/1/1/1
27	LMU	O	303	-	-	2/21/61/61	0/2/2/2
26	LHG	A	845	-	-	25/53/53/53	-
22	CLA	L	402	11	-	17/39/115/115	-
22	CLA	R	602	-	-	12/33/109/115	-
22	CLA	Q	613	10	-	6/15/91/115	-
22	CLA	B	805	1	-	7/39/115/115	-
22	CLA	X	412	19	-	12/39/115/115	-
22	CLA	O	306	13	-	7/33/109/115	-
22	CLA	T	610	-	-	7/15/91/115	-
22	CLA	H	313	7	-	10/31/107/115	-
22	CLA	S	609	14	-	9/27/103/115	-
24	DD6	T	613	-	-	1/26/80/80	0/3/3/3
22	CLA	R	606	11	-	12/30/106/115	-
22	CLA	T	601	15	-	5/15/91/115	-
22	CLA	I	609	8	-	4/15/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	P	606	6	-	6/15/91/115	-
22	CLA	A	820	20	-	12/39/115/115	-
22	CLA	A	825	20	-	17/35/111/115	-
22	CLA	O	312	13	-	8/33/109/115	-
21	BCR	A	851	-	-	4/29/63/63	0/2/2/2
22	CLA	A	839	20	-	6/39/115/115	-
22	CLA	P	607	6	-	4/15/91/115	-
22	CLA	V	608	17	-	8/27/103/115	-
22	CLA	A	844	26	-	12/27/103/115	-
22	CLA	W	403	18	-	7/24/100/115	-
25	DGD	O	304	-	-	31/49/89/95	0/2/2/2
22	CLA	B	806	1	-	13/39/115/115	-
22	CLA	S	614	-	-	0/15/91/115	-
24	DD6	W	416	-	-	1/26/80/80	0/3/3/3
22	CLA	T	603	15	-	8/33/109/115	-
22	CLA	Q	605	-	-	3/29/105/115	-
22	CLA	A	840	20	-	16/39/115/115	-
22	CLA	A	833	20	-	6/39/115/115	-
22	CLA	K	606	-	-	1/21/97/115	-
22	CLA	N	610	8	-	18/27/103/115	-
27	LMU	B	858	-	-	2/12/12/61	-
25	DGD	B	847	-	-	33/55/95/95	0/2/2/2
22	CLA	X	408	19	-	12/39/115/115	-
28	LMG	A	855	-	-	12/36/56/70	0/1/1/1
22	CLA	U	413	16	-	5/15/91/115	-
22	CLA	R	610	11	-	12/39/115/115	-
22	CLA	N	607	-	-	14/33/109/115	-
22	CLA	R	611	11	-	6/15/91/115	-
24	DD6	R	613	-	-	1/26/80/80	0/3/3/3
22	CLA	B	803	1	-	7/29/105/115	-
22	CLA	W	419	18	-	6/15/91/115	-
24	DD6	L	414	-	-	2/26/80/80	0/3/3/3
22	CLA	S	610	14	-	4/15/91/115	-
22	CLA	A	832	20	-	5/24/100/115	-
28	LMG	T	616	-	-	16/36/56/70	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	LMU	B	855	-	-	2/15/35/61	0/1/1/2
22	CLA	I	610	8	-	8/15/91/115	-
22	CLA	T	611	15	-	15/39/115/115	-
22	CLA	H	307	7	-	11/33/109/115	-
22	CLA	P	602	6	-	10/15/91/115	-
22	CLA	N	603	8	-	10/39/115/115	-
22	CLA	U	415	16	-	7/15/91/115	-
24	DD6	O	316	-	-	1/26/80/80	0/3/3/3
27	LMU	G	615	-	-	0/12/32/61	0/1/1/2
22	CLA	B	822	1	-	10/39/115/115	-
22	CLA	Q	618	-	-	9/15/91/115	-
22	CLA	V	613	-	-	11/15/91/115	-
24	DD6	V	615	-	-	3/26/80/80	0/3/3/3
21	BCR	J	103	-	-	2/29/63/63	0/2/2/2
22	CLA	L	403	11	-	5/33/109/115	-
22	CLA	A	835	20	-	9/35/111/115	-
22	CLA	U	414	16	-	14/35/111/115	-
27	LMU	B	850	-	-	3/15/35/61	0/1/1/2
26	LHG	Q	616	22	-	15/48/48/53	-
22	CLA	I	603	8	-	9/29/105/115	-
27	LMU	H	321	-	-	1/19/56/61	0/2/2/2
22	CLA	K	603	10	-	7/33/109/115	-
30	SQD	O	302	-	-	5/37/57/69	0/1/1/1
24	DD6	U	417	-	-	1/26/80/80	0/3/3/3
22	CLA	B	813	1	-	10/39/115/115	-
22	CLA	U	411	16	-	7/30/106/115	-
22	CLA	L	412	11	-	5/15/91/115	-
22	CLA	H	308	7	-	6/33/109/115	-
24	DD6	W	418	-	-	1/26/80/80	0/3/3/3
26	LHG	K	616	22	-	18/43/43/53	-
22	CLA	N	605	-	-	1/15/91/115	-
27	LMU	A	853	-	-	0/15/35/61	0/1/1/2
22	CLA	S	608	26	-	9/15/91/115	-
30	SQD	V	618	-	-	4/19/39/69	0/1/1/1
21	BCR	B	846	-	-	6/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	A	810	20	-	10/39/115/115	-
22	CLA	U	401	-	-	9/27/103/115	-
24	DD6	F	406	-	-	7/26/80/80	0/3/3/3
22	CLA	A	806	20	-	10/39/115/115	-
22	CLA	A	804	-	-	6/39/115/115	-
22	CLA	X	417	19	-	5/21/97/115	-
22	CLA	P	609	-	-	8/15/91/115	-
22	CLA	G	606	6	-	12/39/115/115	-
22	CLA	I	605	-	-	2/15/91/115	-
29	SF4	B	860	20,1	-	-	0/6/5/5
22	CLA	A	823	20	-	5/15/91/115	-
27	LMU	K	620	-	-	6/19/56/61	0/2/2/2
21	BCR	A	848	-	-	0/29/63/63	0/2/2/2
22	CLA	K	605	-	-	19/39/115/115	-
22	CLA	P	611	6	-	6/15/91/115	-
22	CLA	O	309	13	-	4/21/97/115	-
24	DD6	O	317	-	-	0/26/80/80	0/3/3/3
22	CLA	S	615	-	-	4/23/99/115	-
26	LHG	A	846	22	-	27/53/53/53	-
22	CLA	U	404	16	-	14/39/115/115	-
22	CLA	X	402	19	-	11/27/103/115	-
27	LMU	O	301	-	-	1/15/35/61	0/1/1/2
27	LMU	U	422	-	-	5/21/61/61	0/2/2/2
21	BCR	B	801	-	-	4/29/63/63	0/2/2/2
27	LMU	U	421	-	-	7/21/61/61	0/2/2/2
33	CL0	A	802	20	-	8/37/135/135	-
27	LMU	A	856	-	-	0/12/32/61	0/1/1/2
26	LHG	T	614	22	-	27/46/46/53	-
22	CLA	Q	604	10	-	16/39/115/115	-
22	CLA	Q	607	-	-	5/15/91/115	-
31	CHL	W	422	-	-	9/39/137/137	-
22	CLA	B	815	1	-	3/24/100/115	-
24	DD6	K	614	-	-	0/26/80/80	0/3/3/3
29	SF4	C	102	2	-	-	0/6/5/5
22	CLA	H	304	7	-	6/15/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	O	310	13	-	9/33/109/115	-
30	SQD	F	407	-	-	2/37/57/69	0/1/1/1
23	PQN	A	843	-	-	4/23/43/43	0/2/2/2
26	LHG	R	614	22	-	20/46/46/53	-
24	DD6	A	847	-	-	1/26/80/80	0/3/3/3
22	CLA	B	807	1	-	15/39/115/115	-
22	CLA	H	318	7	-	6/15/91/115	-
27	LMU	B	854	-	-	3/15/35/61	0/1/1/2
22	CLA	O	305	13	-	4/21/97/115	-
22	CLA	B	832	1	-	12/36/112/115	-
22	CLA	B	833	1	-	9/39/115/115	-
22	CLA	W	412	26	-	5/33/109/115	-

The worst 5 of 2588 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	W	408	CHL	C4C-NC	15.74	1.49	1.35
31	X	406	CHL	C4C-NC	15.66	1.49	1.35
31	W	407	CHL	C4C-NC	15.51	1.49	1.35
31	V	605	CHL	C4C-NC	15.34	1.48	1.35
31	U	407	CHL	C4C-NC	15.32	1.48	1.35

The worst 5 of 2716 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	B	843	BCR	C40-C30-C25	-13.35	88.64	110.30
24	P	612	DD6	C9-C10-C11	-9.93	113.14	127.31
24	P	612	DD6	C4-C5-C6	-9.08	114.35	127.31
24	X	416	DD6	C4-C5-C6	-8.39	115.34	127.31
21	B	843	BCR	C40-C30-C39	-8.38	82.82	108.53

There are no chirality outliers.

5 of 3517 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

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Mol	Chain	Res	Type	Atoms
21	B	845	BCR	C21-C22-C23-C24

All (2) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
27	L	420	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	O	315	CLA	2	0
22	B	838	CLA	3	0
22	O	314	CLA	1	0
27	T	618	LMU	2	0
22	A	828	CLA	4	0
22	L	411	CLA	1	0
22	G	602	CLA	1	0
26	L	416	LHG	3	0
22	W	402	CLA	2	0
28	U	423	LMG	2	0
22	S	602	CLA	1	0
28	H	319	LMG	1	0
22	B	830	CLA	4	0
22	B	812	CLA	1	0
30	K	621	SQD	1	0
22	B	835	CLA	2	0
24	B	841	DD6	1	0
22	L	404	CLA	6	0
22	S	606	CLA	1	0
32	V	616	NEX	9	0
22	A	841	CLA	3	0
21	A	849	BCR	3	0
22	V	602	CLA	5	0
22	B	810	CLA	1	0
27	M	102	LMU	1	0
22	B	809	CLA	4	0
22	B	821	CLA	2	0
22	B	831	CLA	2	0
22	U	412	CLA	1	0
22	B	823	CLA	3	0
22	P	610	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	W	414	CLA	1	0
21	B	844	BCR	5	0
22	O	308	CLA	4	0
28	J	101	LMG	1	0
22	V	612	CLA	7	0
22	I	607	CLA	3	0
22	A	807	CLA	1	0
22	H	310	CLA	1	0
22	S	601	CLA	1	0
27	A	857	LMU	1	0
22	K	608	CLA	4	0
21	B	843	BCR	3	0
22	F	403	CLA	2	0
22	N	602	CLA	1	0
22	K	613	CLA	4	0
22	N	601	CLA	1	0
28	F	408	LMG	3	0
28	K	601	LMG	3	0
22	T	608	CLA	2	0
22	A	822	CLA	3	0
24	Q	614	DD6	1	0
26	S	613	LHG	2	0
22	I	601	CLA	2	0
22	P	603	CLA	1	0
22	R	601	CLA	6	0
22	U	405	CLA	3	0
22	G	608	CLA	4	0
22	A	830	CLA	1	0
22	L	408	CLA	12	0
22	A	811	CLA	1	0
31	U	408	CHL	4	0
22	Q	603	CLA	1	0
22	A	815	CLA	2	0
22	W	411	CLA	2	0
22	G	610	CLA	1	0
28	N	615	LMG	1	0
27	L	420	LMU	2	0
28	B	856	LMG	4	0
22	A	808	CLA	1	0
22	W	413	CLA	2	0
22	X	413	CLA	1	0
22	A	803	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
28	W	401	LMG	3	0
22	B	811	CLA	1	0
22	T	605	CLA	4	0
22	B	828	CLA	2	0
22	G	609	CLA	3	0
22	Q	609	CLA	1	0
22	P	605	CLA	1	0
22	V	609	CLA	2	0
22	J	102	CLA	1	0
26	O	318	LHG	1	0
21	B	845	BCR	2	0
22	O	307	CLA	1	0
22	R	615	CLA	2	0
32	U	418	NEX	4	0
22	B	827	CLA	1	0
22	A	814	CLA	4	0
22	X	403	CLA	1	0
22	I	608	CLA	2	0
22	V	617	CLA	1	0
22	B	802	CLA	2	0
22	A	819	CLA	1	0
22	A	827	CLA	2	0
22	A	813	CLA	2	0
22	K	617	CLA	2	0
22	O	313	CLA	3	0
22	R	607	CLA	3	0
22	F	404	CLA	4	0
22	B	819	CLA	1	0
26	O	321	LHG	3	0
22	H	311	CLA	2	0
22	U	420	CLA	1	0
22	X	419	CLA	2	0
22	G	603	CLA	2	0
22	H	312	CLA	3	0
31	V	606	CHL	14	0
31	W	407	CHL	6	0
28	U	402	LMG	2	0
31	U	407	CHL	3	0
27	F	409	LMU	1	0
22	I	611	CLA	4	0
22	V	604	CLA	7	0
22	A	829	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	W	410	CLA	3	0
22	A	821	CLA	1	0
22	V	603	CLA	2	0
22	T	606	CLA	1	0
22	K	604	CLA	6	0
22	V	601	CLA	4	0
22	G	611	CLA	1	0
22	U	409	CLA	1	0
22	B	820	CLA	1	0
22	B	818	CLA	1	0
22	W	404	CLA	2	0
22	N	606	CLA	4	0
22	L	406	CLA	1	0
22	K	607	CLA	9	0
22	Q	612	CLA	1	0
22	S	605	CLA	4	0
22	A	816	CLA	2	0
22	B	824	CLA	3	0
22	T	604	CLA	1	0
22	A	812	CLA	3	0
26	W	420	LHG	2	0
22	I	606	CLA	2	0
26	P	601	LHG	1	0
22	Q	610	CLA	2	0
22	L	417	CLA	7	0
22	W	415	CLA	1	0
22	B	836	CLA	2	0
22	U	406	CLA	1	0
22	A	809	CLA	1	0
22	B	859	CLA	2	0
22	Q	601	CLA	1	0
22	R	605	CLA	5	0
22	K	609	CLA	2	0
25	F	401	DGD	2	0
22	B	814	CLA	1	0
22	B	834	CLA	5	0
26	N	614	LHG	1	0
22	W	409	CLA	4	0
22	A	838	CLA	3	0
22	X	404	CLA	1	0
22	W	406	CLA	3	0
22	A	842	CLA	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	B	804	CLA	2	0
31	W	408	CHL	8	0
27	H	301	LMU	1	0
31	V	605	CHL	12	0
22	X	411	CLA	1	0
22	Q	611	CLA	1	0
22	B	817	CLA	1	0
22	A	834	CLA	1	0
21	M	101	BCR	3	0
24	S	611	DD6	1	0
22	A	836	CLA	2	0
22	A	805	CLA	2	0
22	A	801	CLA	1	0
22	O	311	CLA	3	0
21	B	842	BCR	2	0
22	V	607	CLA	2	0
22	R	604	CLA	5	0
22	H	305	CLA	1	0
26	B	851	LHG	7	0
22	A	824	CLA	4	0
22	S	604	CLA	1	0
22	P	608	CLA	2	0
22	A	852	CLA	4	0
22	B	829	CLA	3	0
22	G	601	CLA	1	0
22	L	409	CLA	2	0
22	Q	608	CLA	3	0
22	A	831	CLA	2	0
22	I	602	CLA	1	0
22	N	604	CLA	1	0
22	B	816	CLA	2	0
22	B	825	CLA	3	0
22	B	839	CLA	2	0
28	I	615	LMG	1	0
22	S	607	CLA	1	0
22	T	607	CLA	1	0
27	U	424	LMU	1	0
26	N	616	LHG	1	0
22	X	409	CLA	1	0
28	Q	602	LMG	2	0
22	A	817	CLA	2	0
27	A	854	LMU	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	K	611	CLA	3	0
27	L	419	LMU	4	0
22	L	410	CLA	3	0
26	B	848	LHG	1	0
28	H	322	LMG	1	0
23	B	840	PQN	1	0
26	A	845	LHG	1	0
22	L	402	CLA	2	0
22	R	602	CLA	4	0
22	Q	613	CLA	2	0
22	B	805	CLA	1	0
22	H	313	CLA	1	0
22	S	609	CLA	1	0
22	R	606	CLA	3	0
22	P	606	CLA	3	0
22	A	820	CLA	1	0
22	A	825	CLA	2	0
22	O	312	CLA	1	0
21	A	851	BCR	3	0
22	A	839	CLA	1	0
22	P	607	CLA	1	0
22	V	608	CLA	1	0
22	A	844	CLA	4	0
25	O	304	DGD	3	0
22	B	806	CLA	4	0
22	Q	605	CLA	1	0
22	A	840	CLA	3	0
22	A	833	CLA	1	0
22	K	606	CLA	2	0
22	N	610	CLA	3	0
27	B	858	LMU	1	0
25	B	847	DGD	6	0
22	X	408	CLA	1	0
22	R	610	CLA	3	0
22	N	607	CLA	7	0
22	R	611	CLA	2	0
22	B	803	CLA	2	0
22	S	610	CLA	2	0
22	A	832	CLA	3	0
28	T	616	LMG	2	0
27	B	855	LMU	1	0
22	T	611	CLA	1	0

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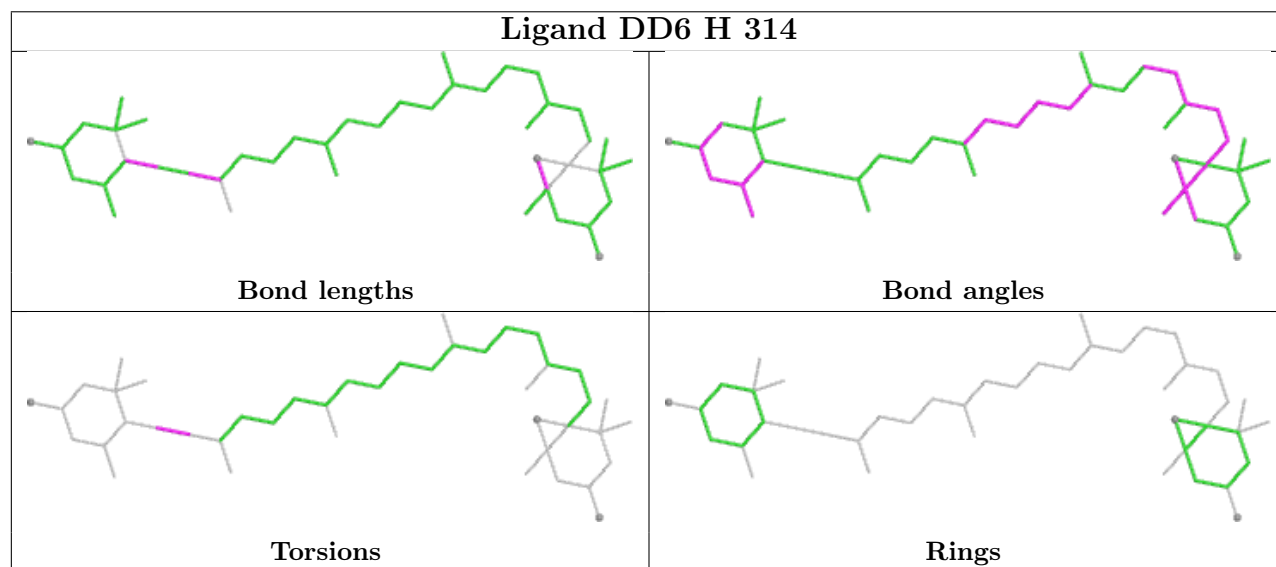
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22	P	602	CLA	2	0
22	N	603	CLA	2	0
22	U	415	CLA	2	0
22	B	822	CLA	3	0
22	V	613	CLA	1	0
21	J	103	BCR	1	0
26	Q	616	LHG	1	0
22	I	603	CLA	3	0
27	H	321	LMU	1	0
22	K	603	CLA	2	0
30	O	302	SQD	8	0
22	B	813	CLA	3	0
22	U	411	CLA	1	0
22	L	412	CLA	3	0
22	H	308	CLA	2	0
26	K	616	LHG	3	0
22	S	608	CLA	2	0
30	V	618	SQD	1	0
21	B	846	BCR	1	0
22	U	401	CLA	2	0
22	A	806	CLA	4	0
22	A	804	CLA	3	0
22	P	609	CLA	1	0
22	A	823	CLA	1	0
27	K	620	LMU	2	0
21	A	848	BCR	2	0
22	K	605	CLA	3	0
22	O	309	CLA	3	0
26	A	846	LHG	2	0
22	U	404	CLA	2	0
27	O	301	LMU	4	0
21	B	801	BCR	8	0
27	U	421	LMU	1	0
33	A	802	CL0	6	0
26	T	614	LHG	1	0
22	Q	604	CLA	5	0
22	Q	607	CLA	2	0
31	W	422	CHL	2	0
22	B	815	CLA	3	0
22	O	310	CLA	1	0
30	F	407	SQD	2	0

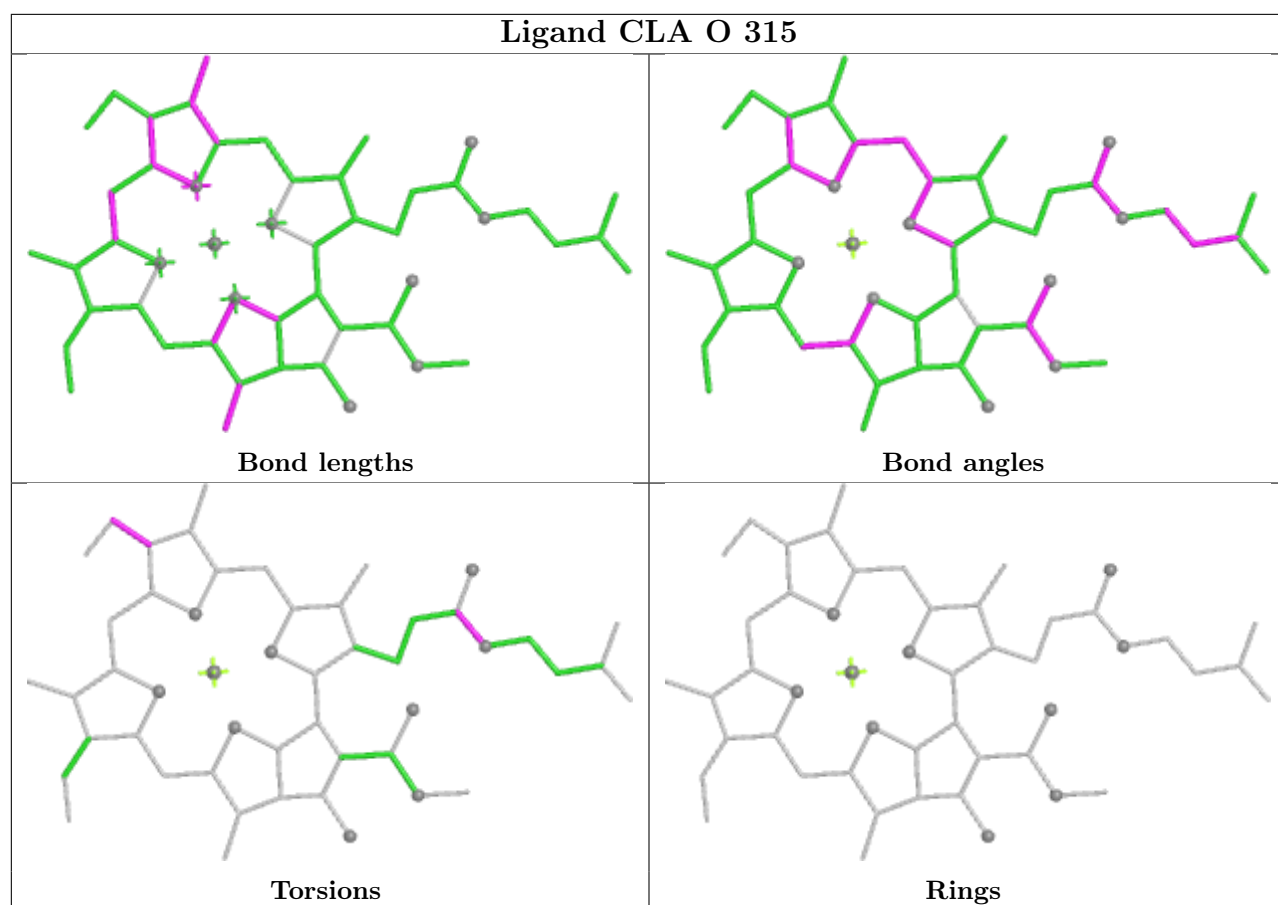
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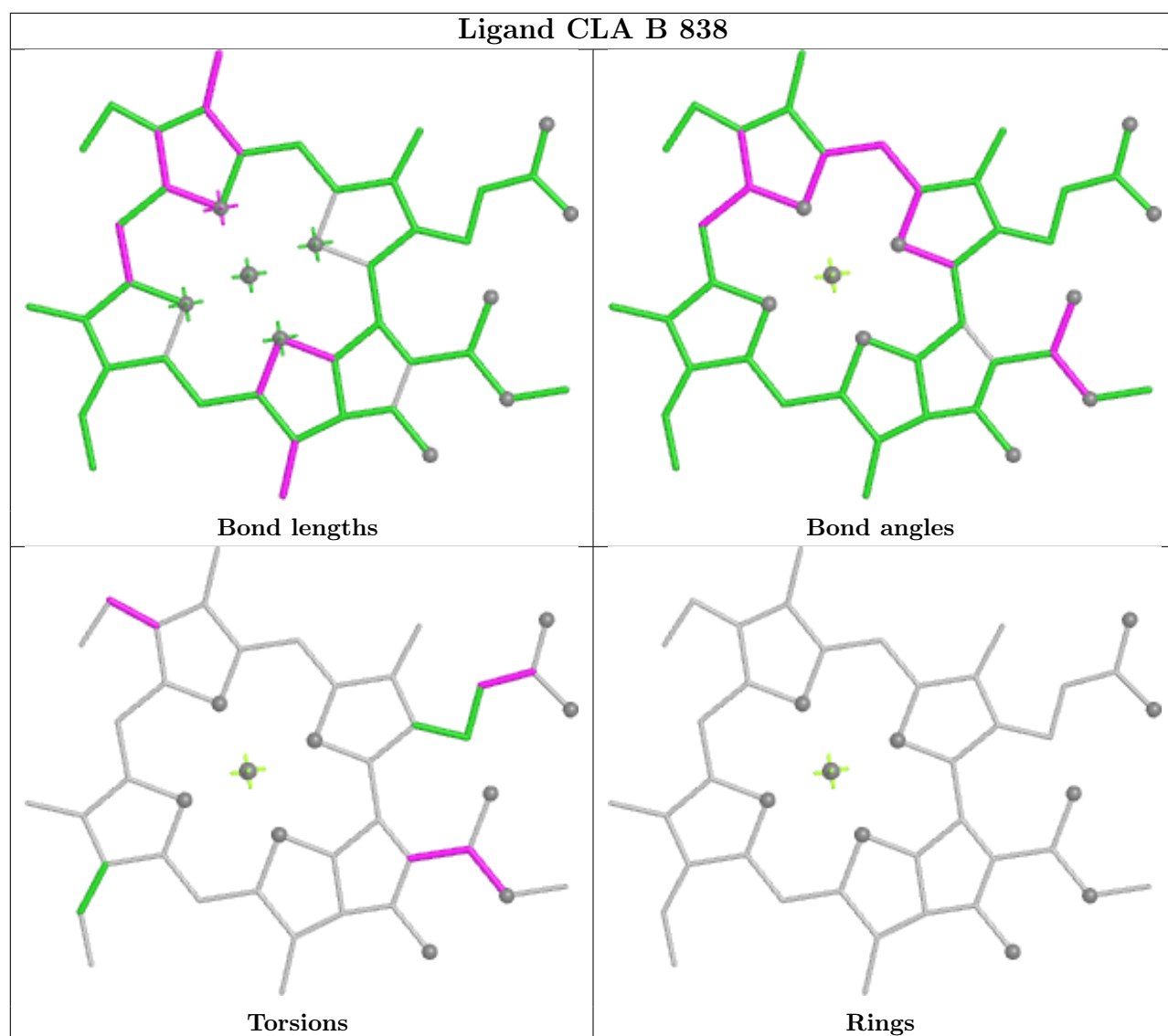
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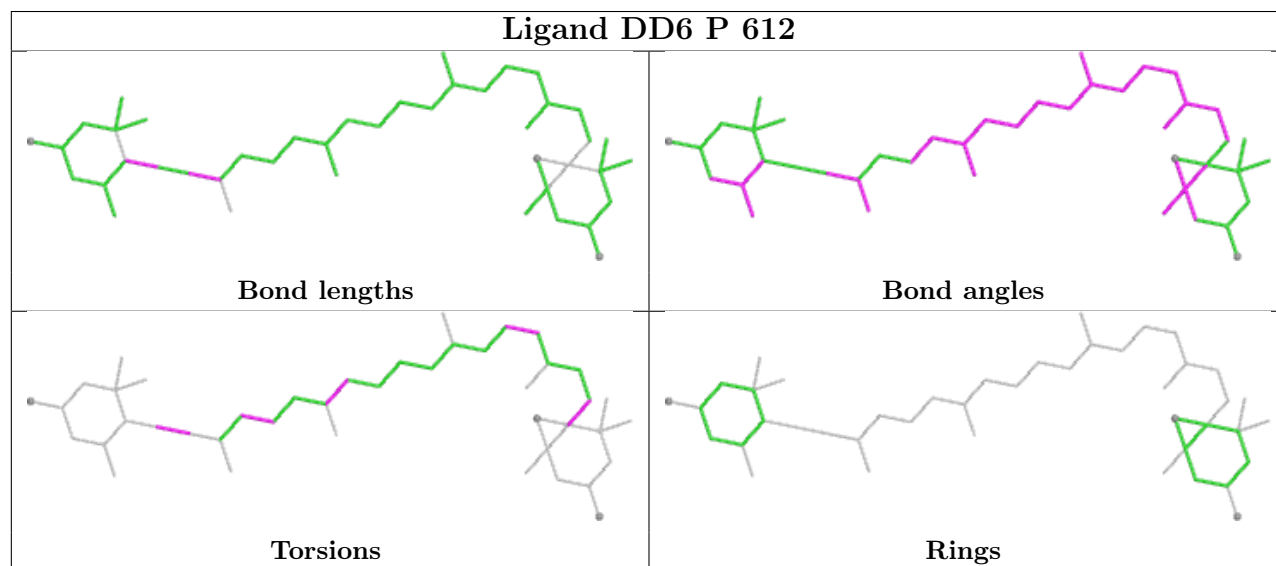
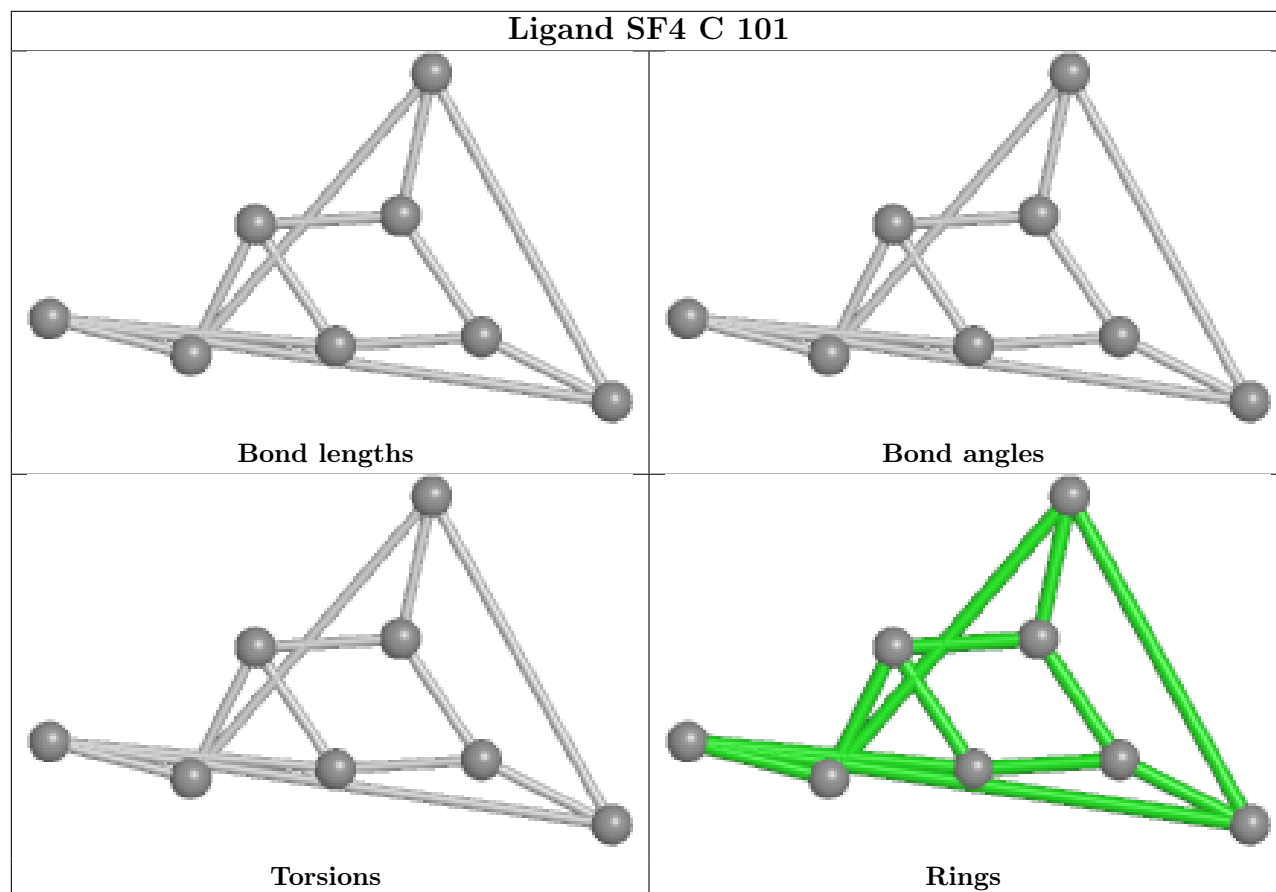
Mol	Chain	Res	Type	Clashes	Symm-Clashes
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26	R	614	LHG	3	0
22	B	807	CLA	2	0
27	B	854	LMU	8	0
22	O	305	CLA	1	0
22	B	832	CLA	3	0
22	B	833	CLA	4	0
22	W	412	CLA	2	0

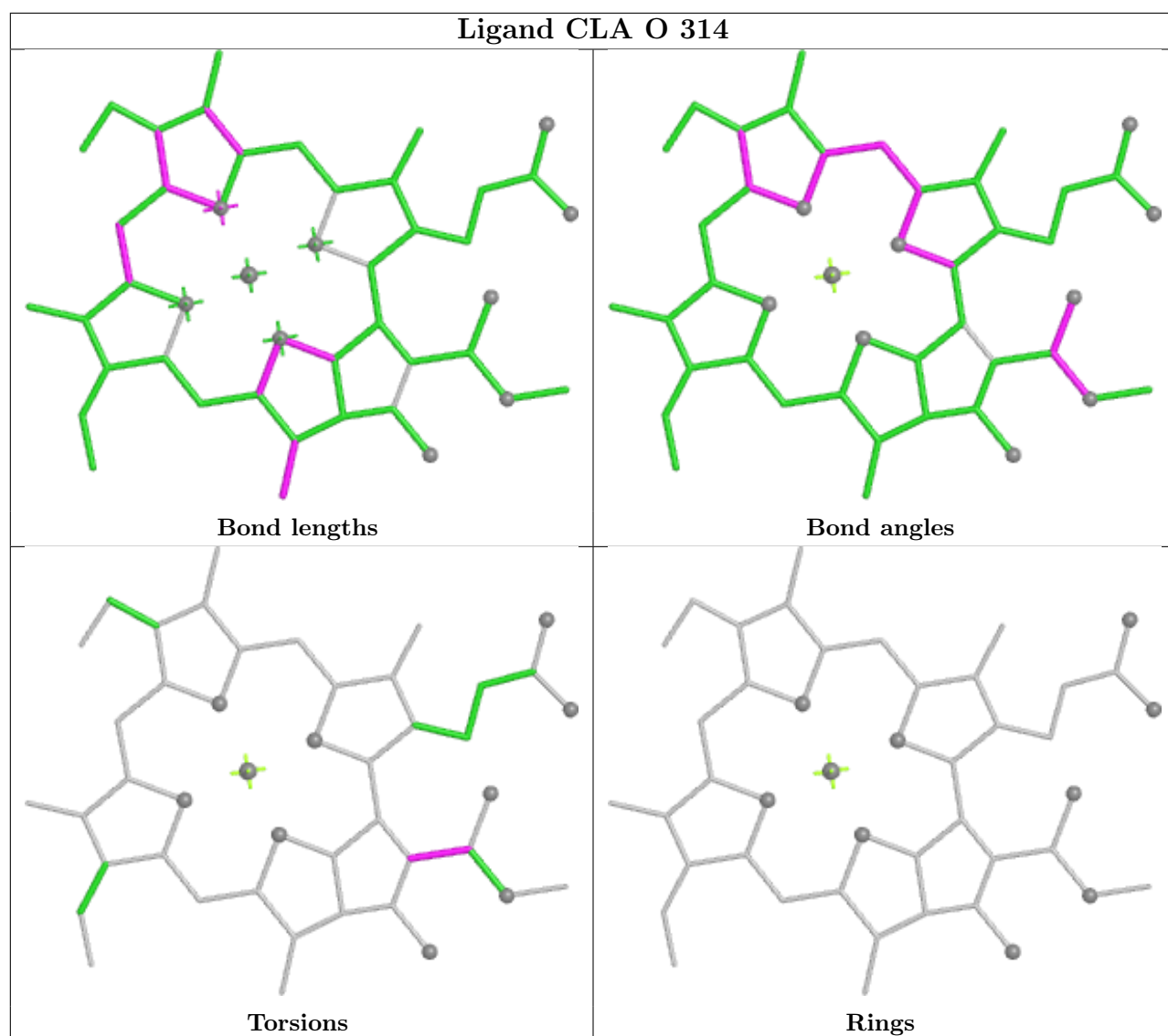
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

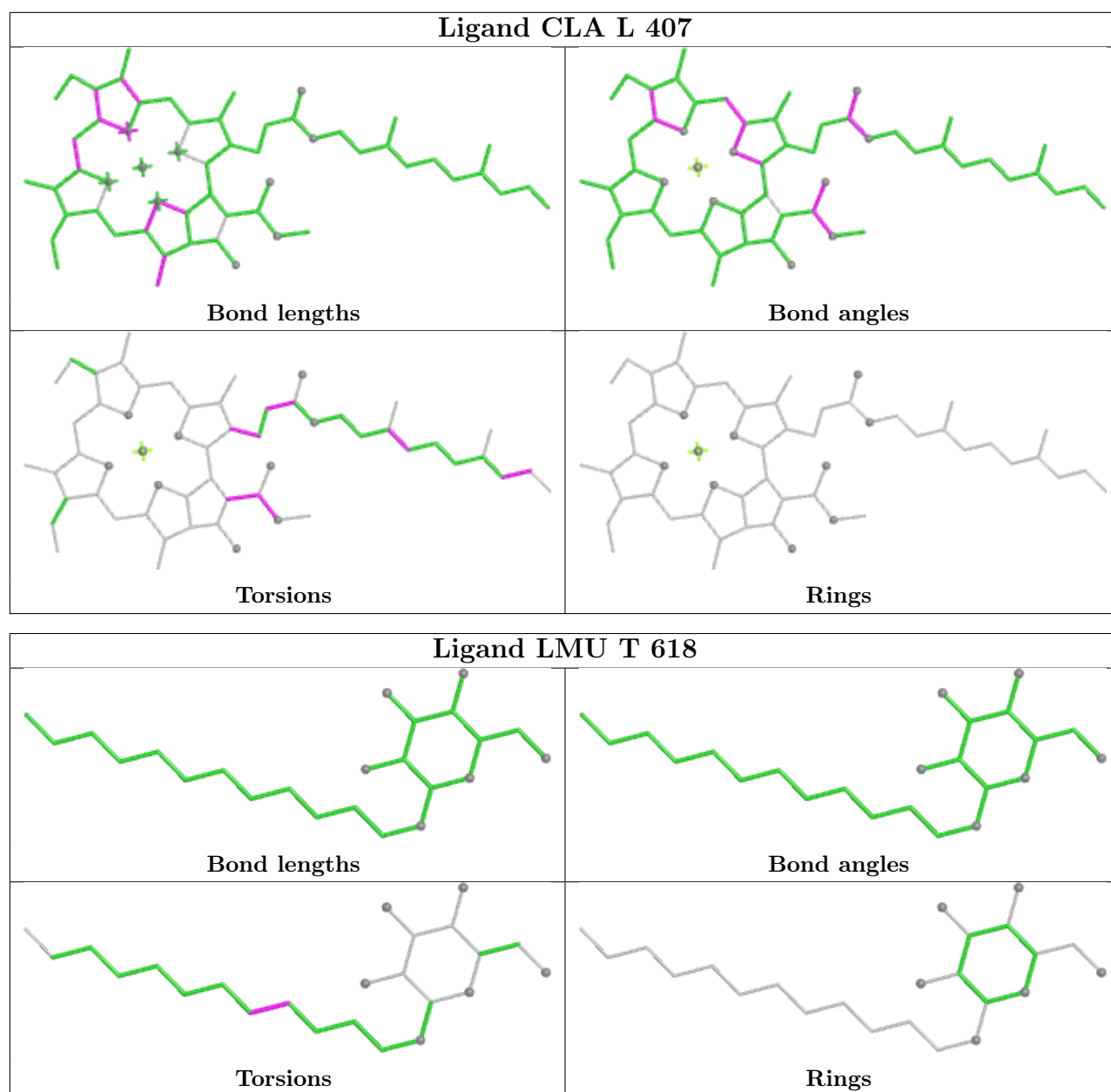


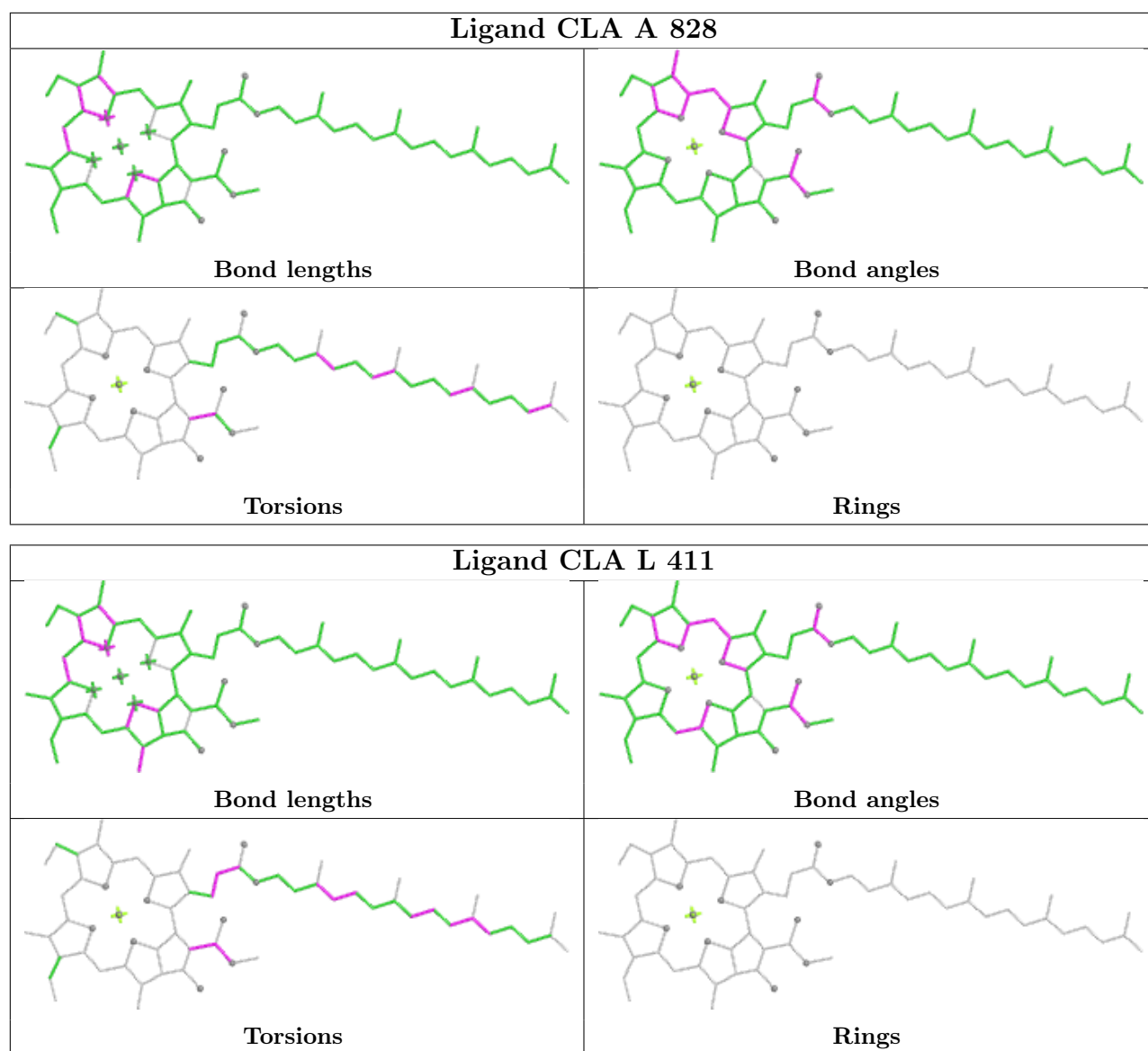


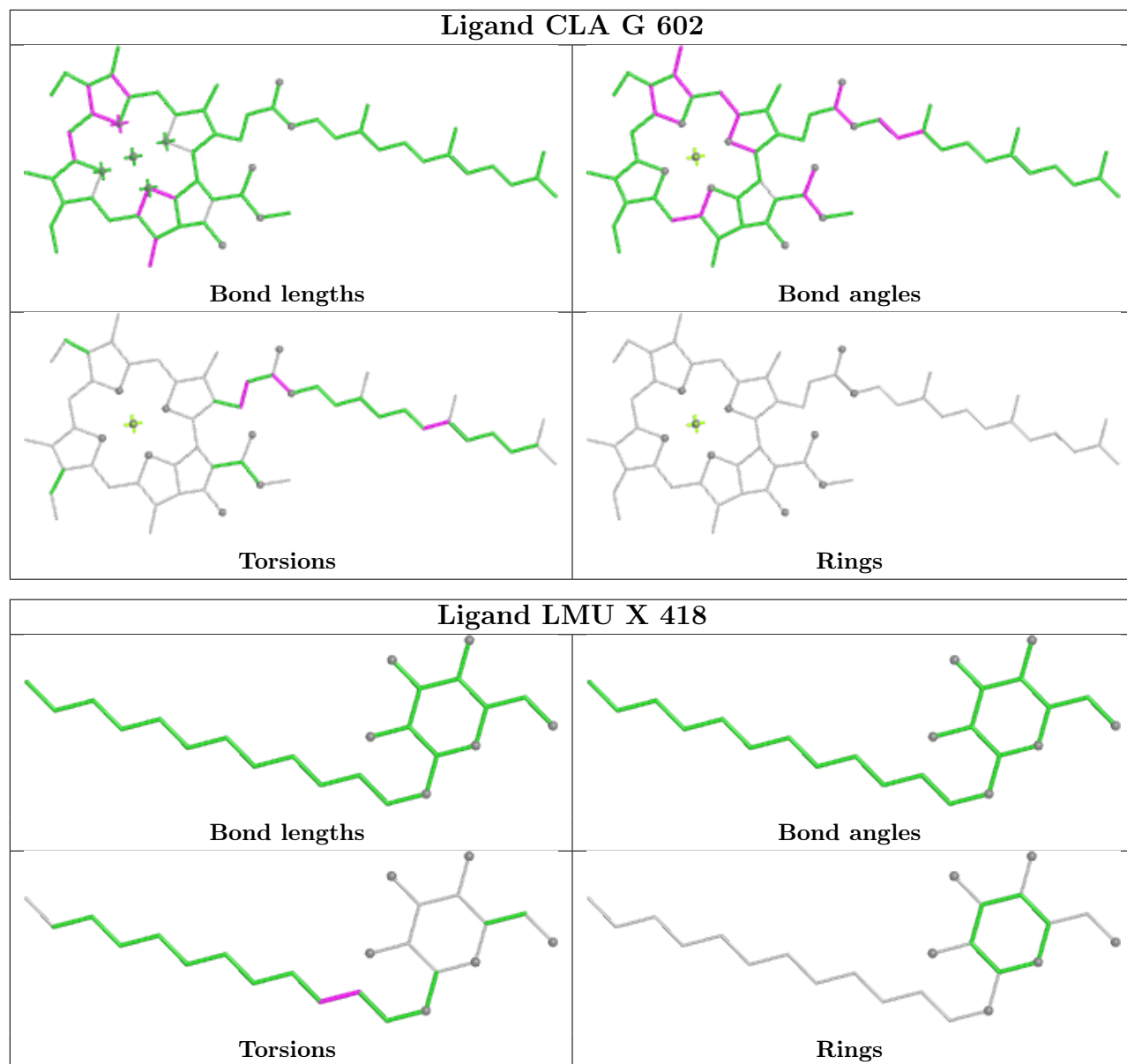


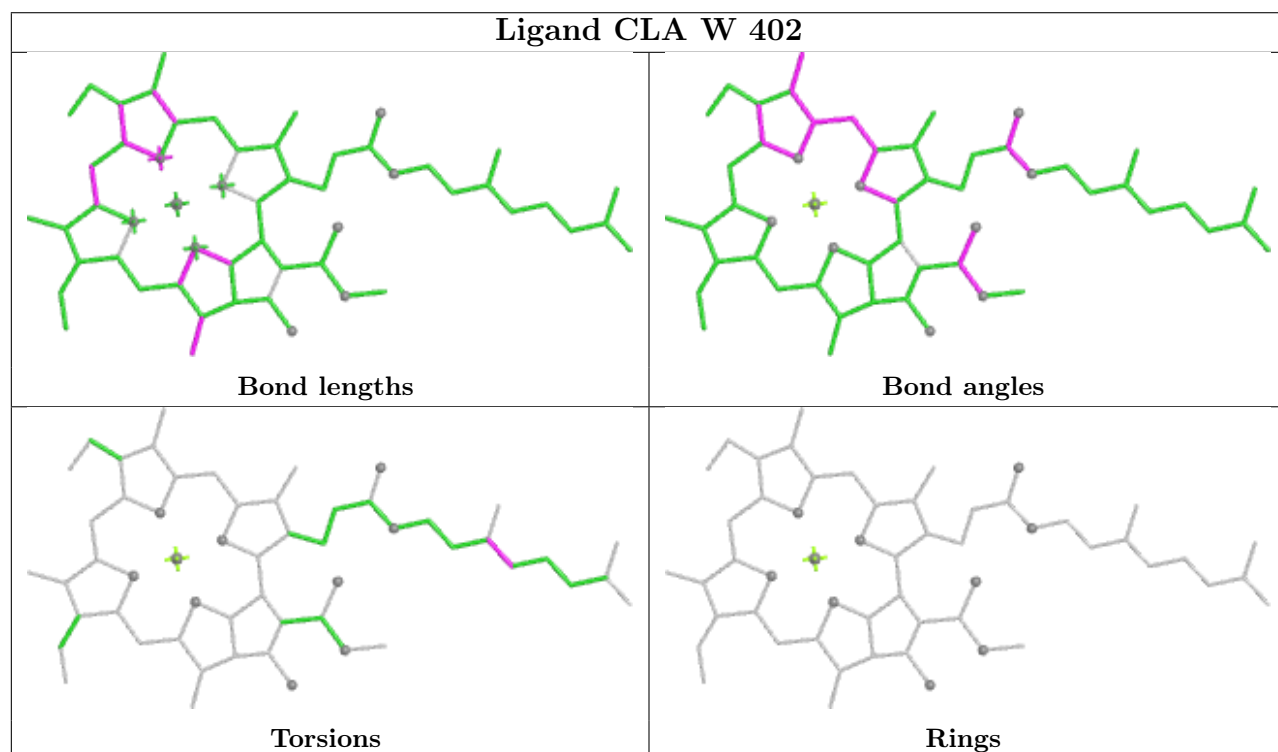
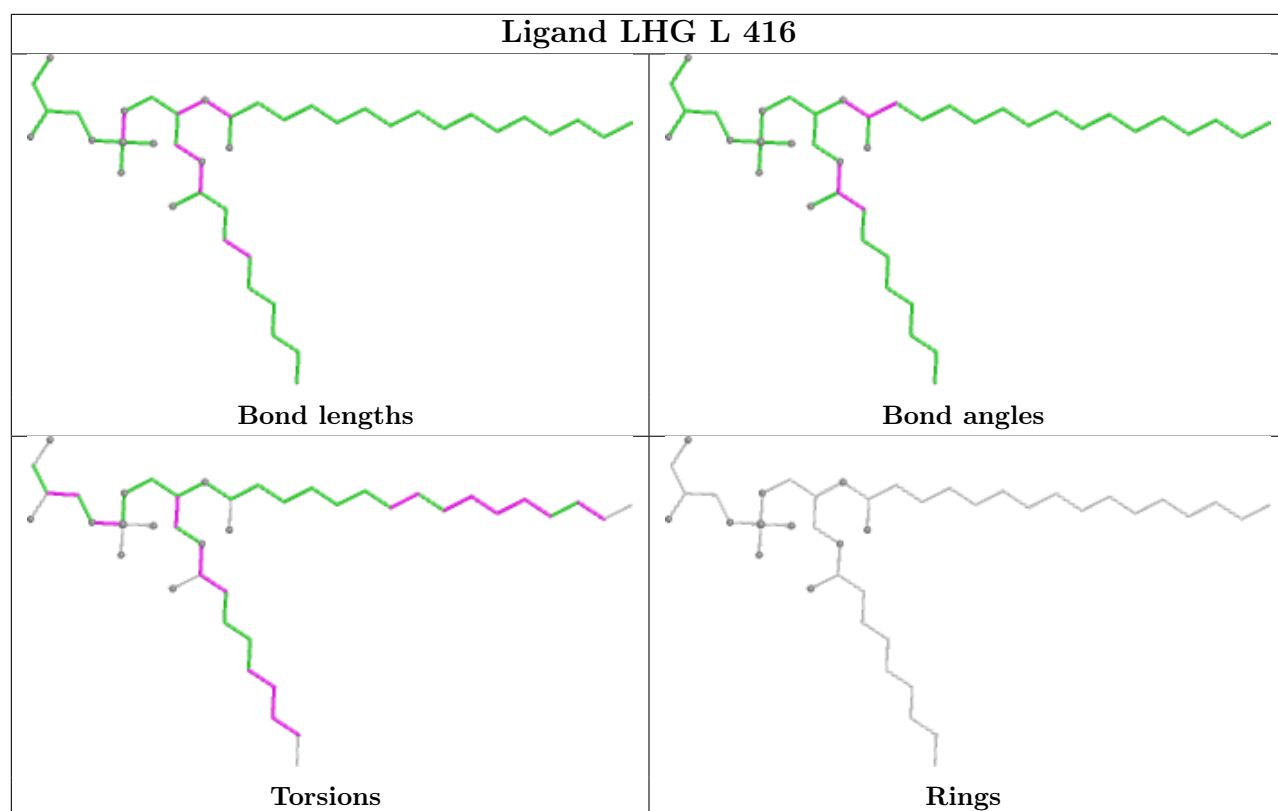


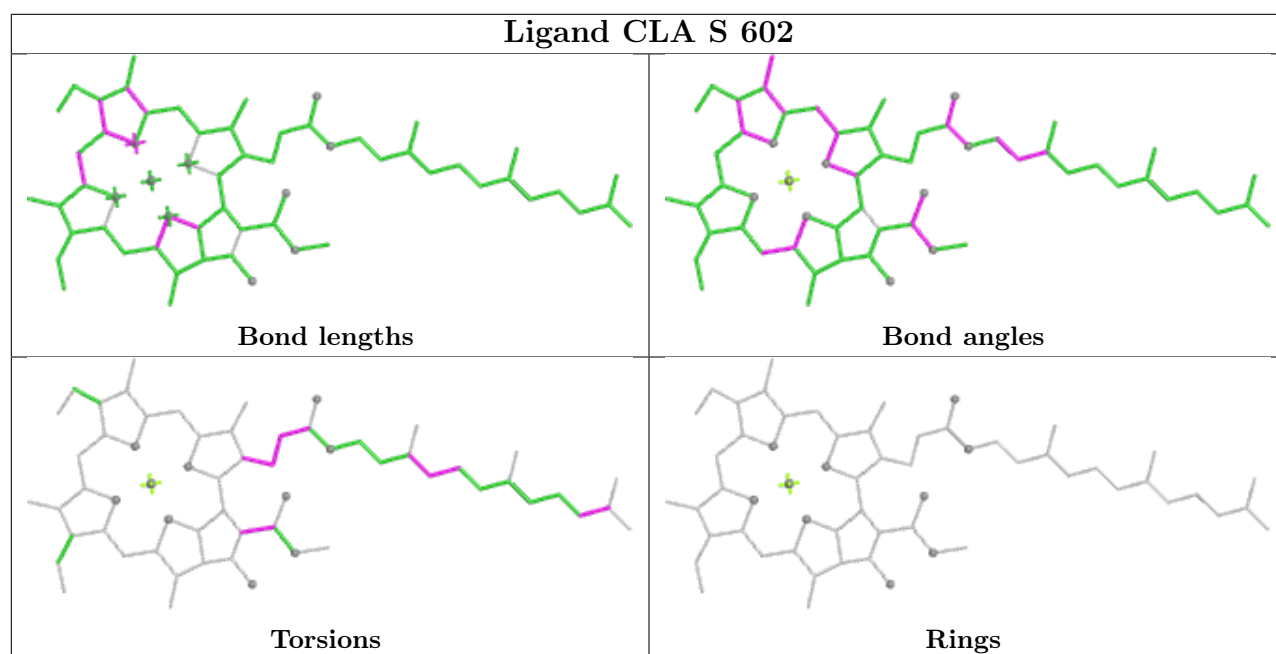
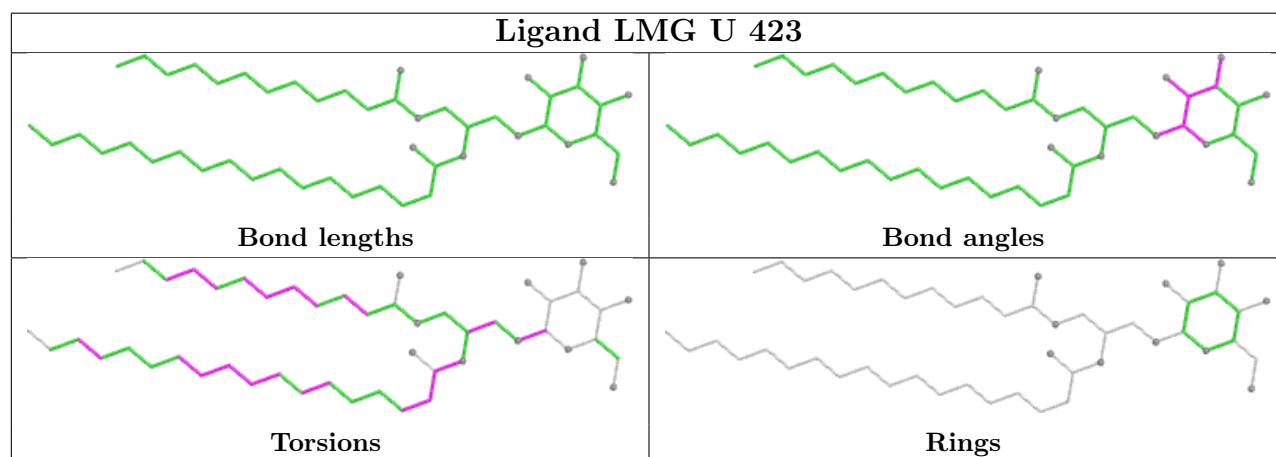
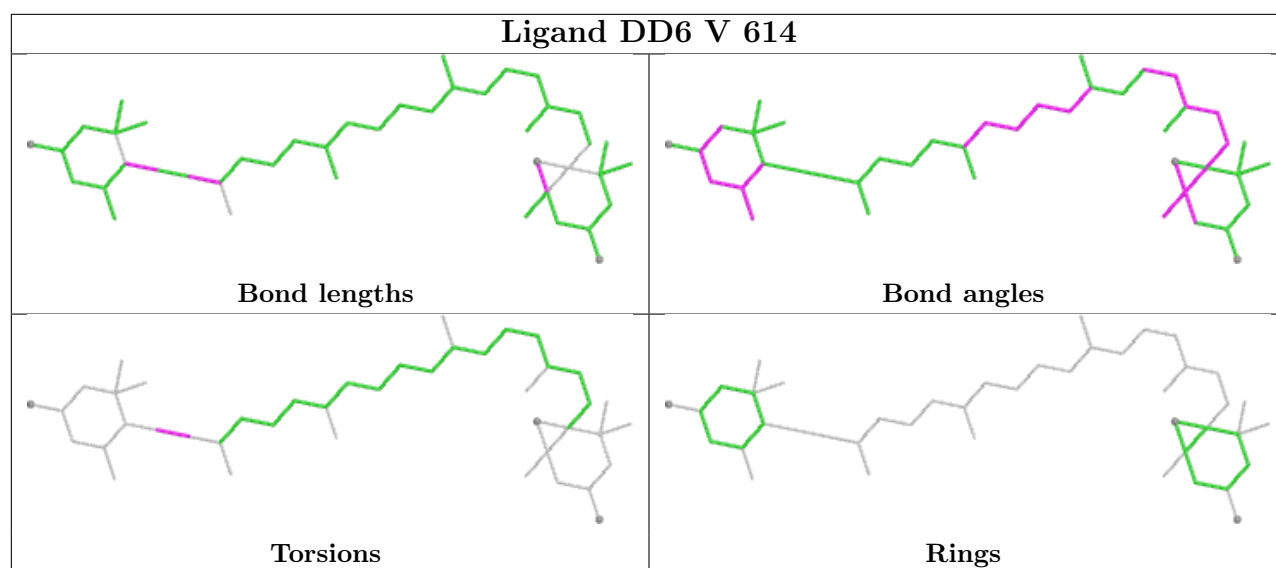


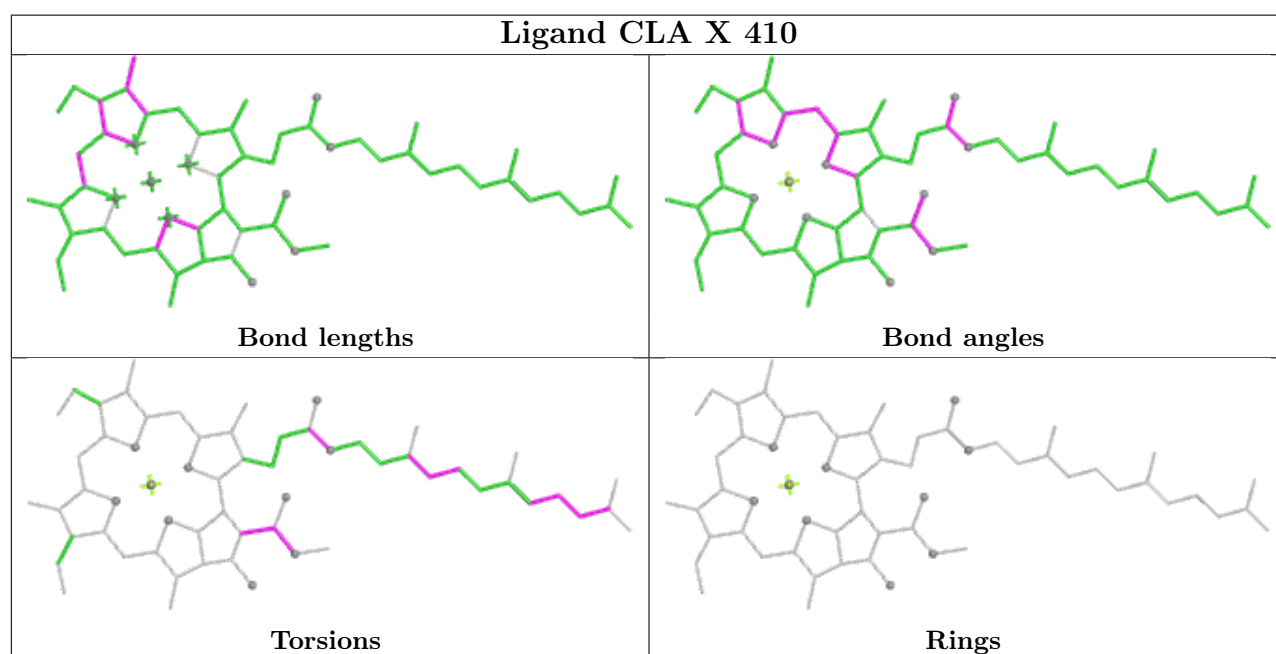
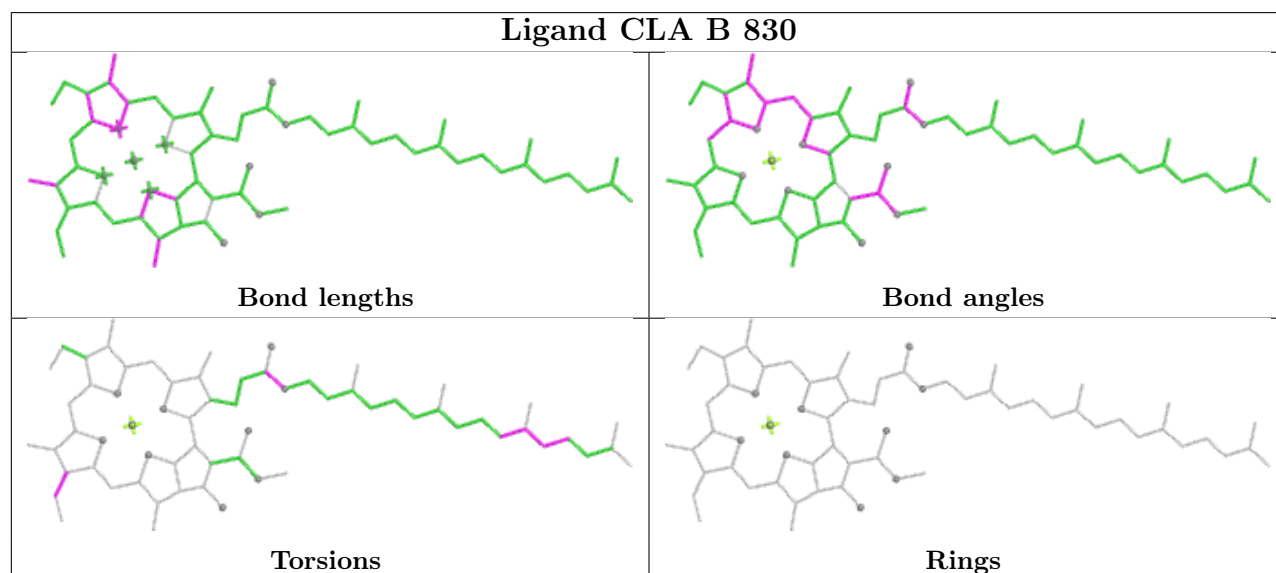
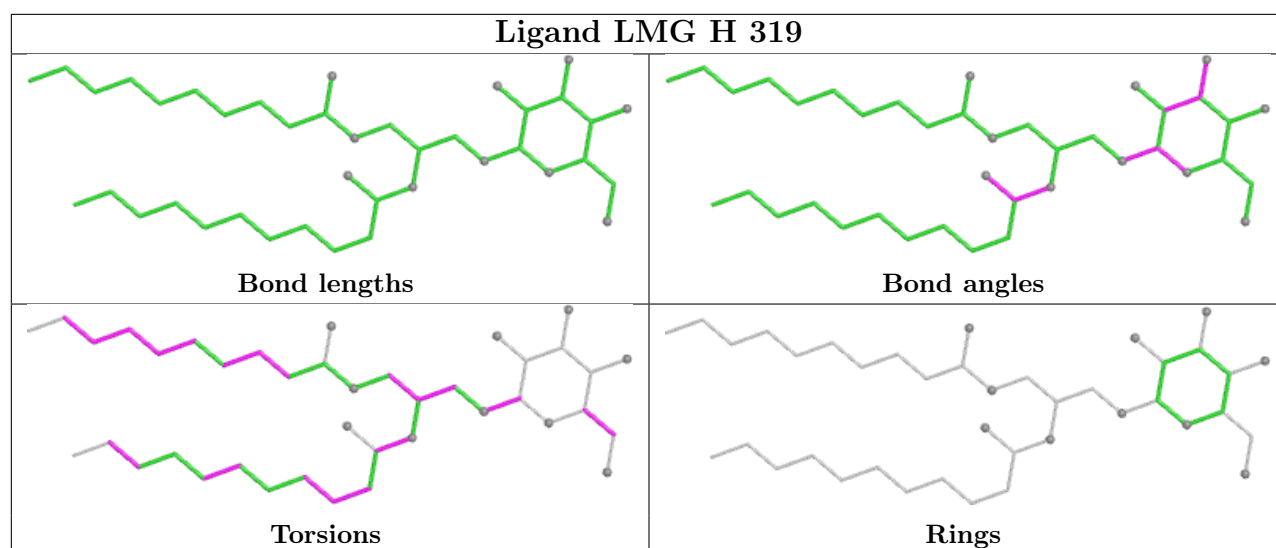


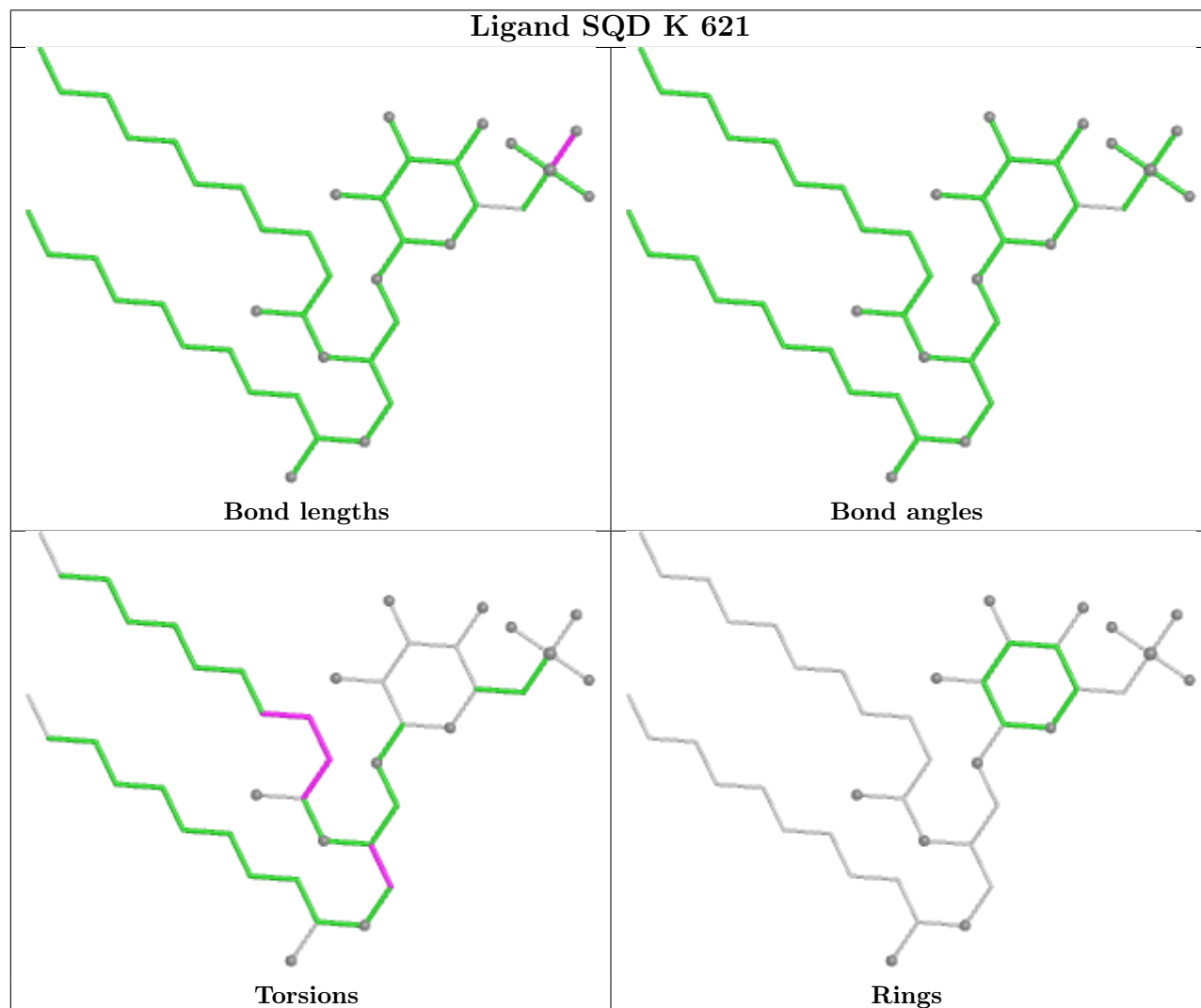
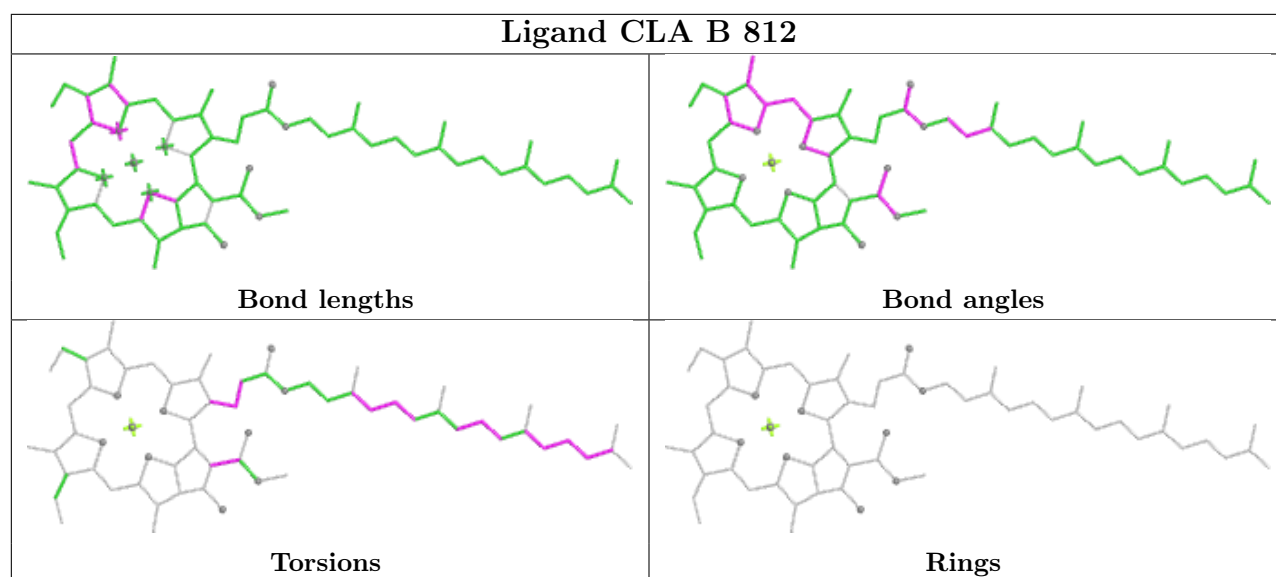


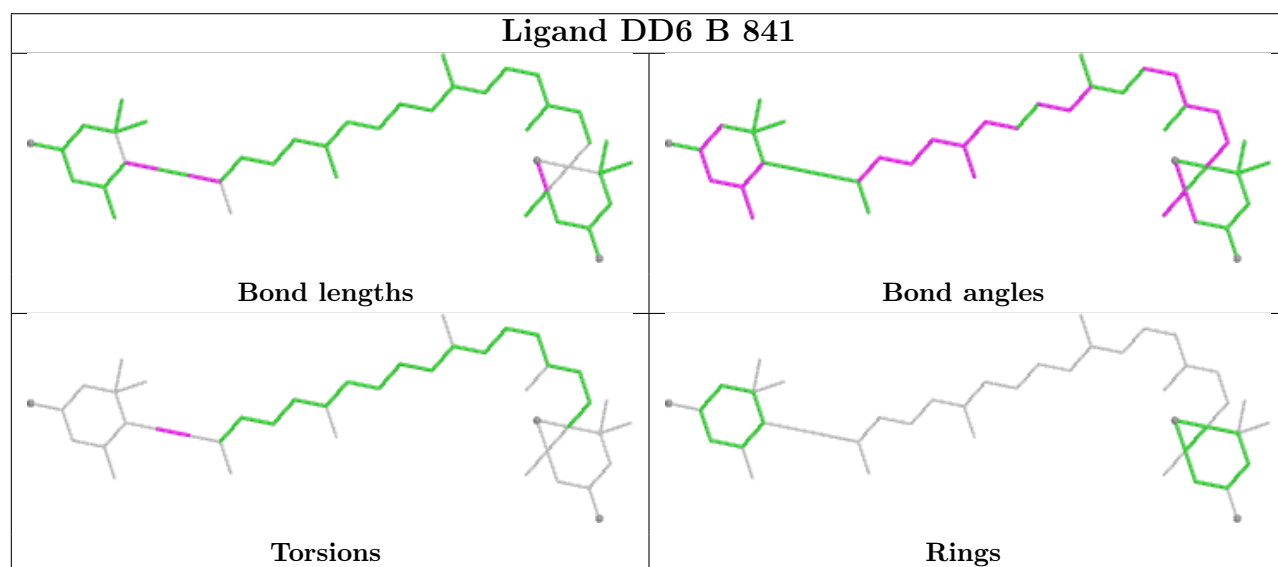
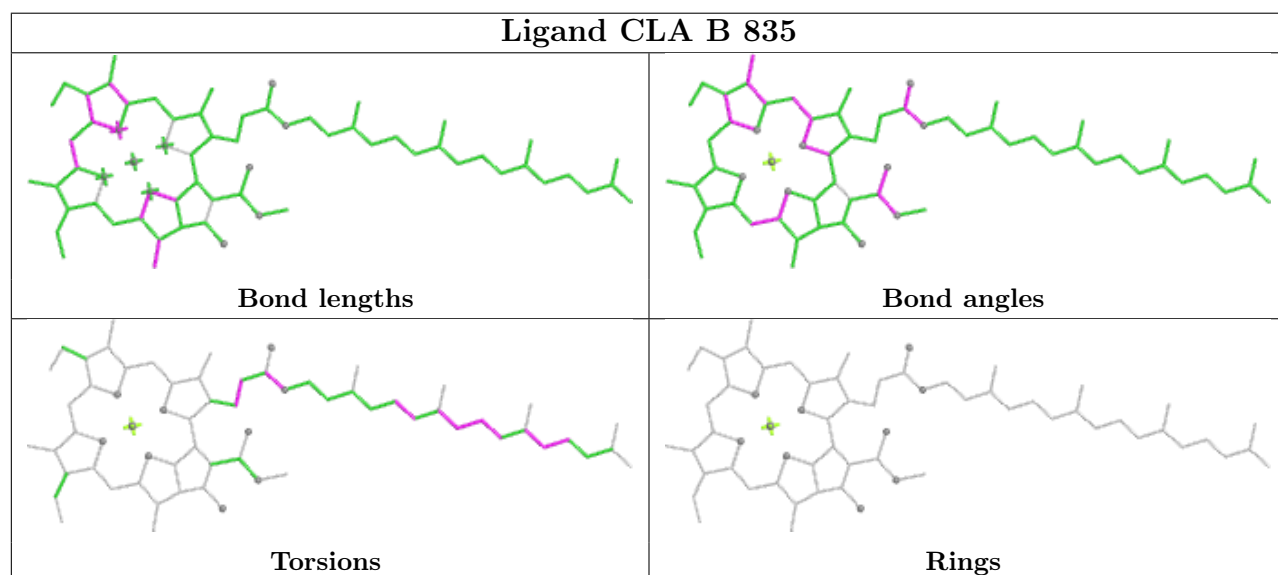
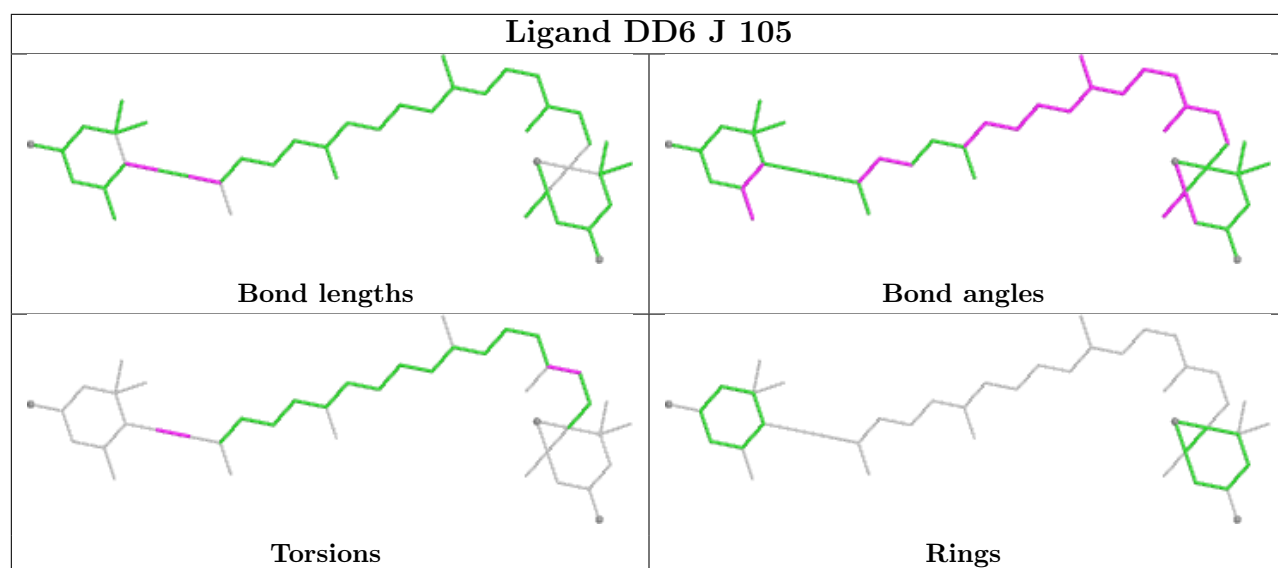




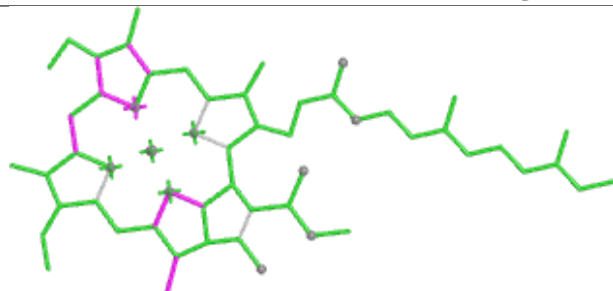




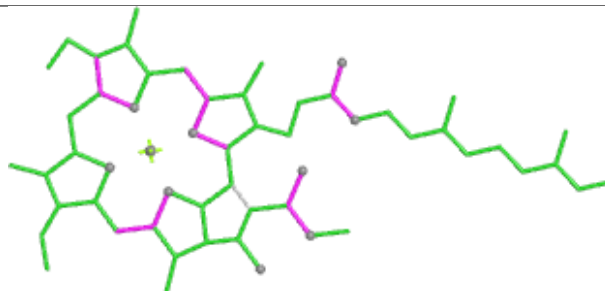




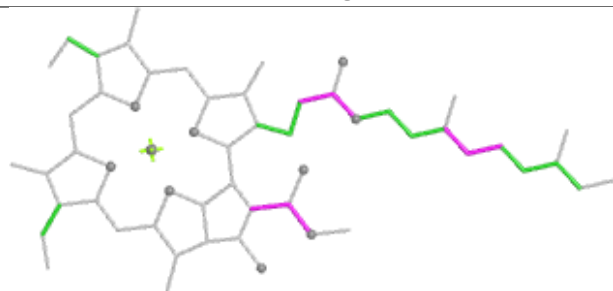
Ligand CLA L 404



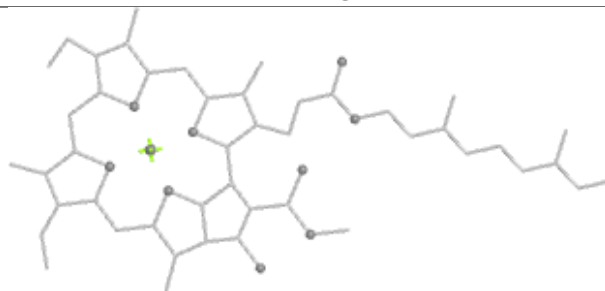
Bond lengths



Bond angles

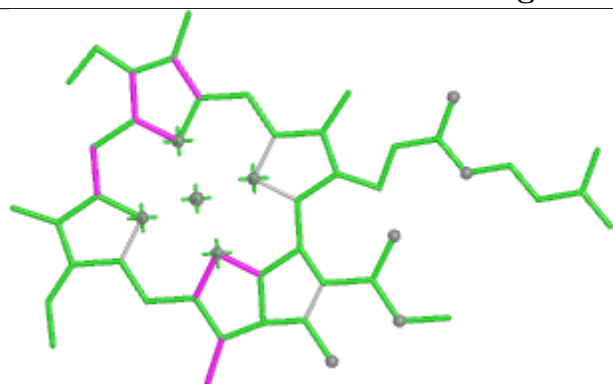


Torsions

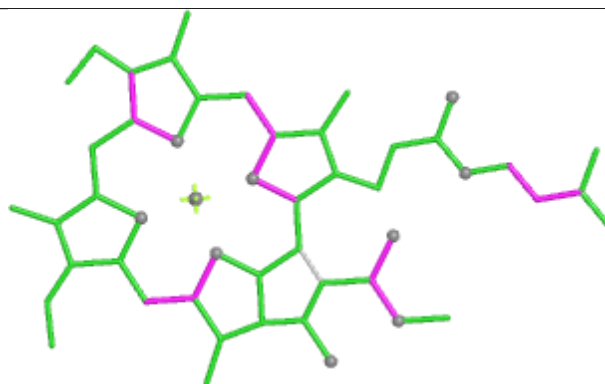


Rings

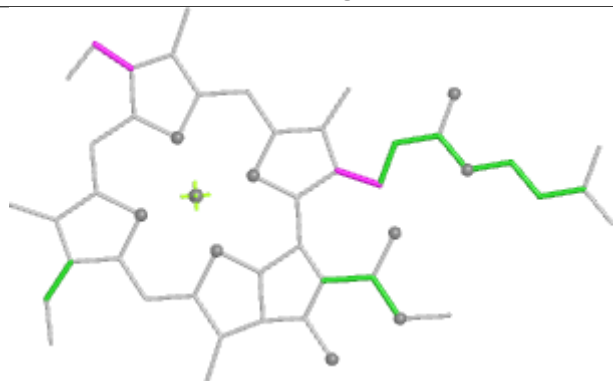
Ligand CLA S 606



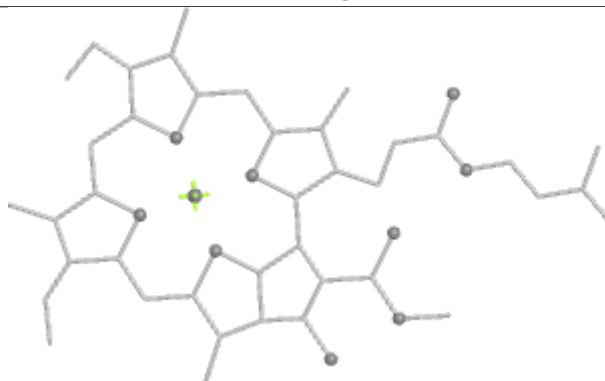
Bond lengths



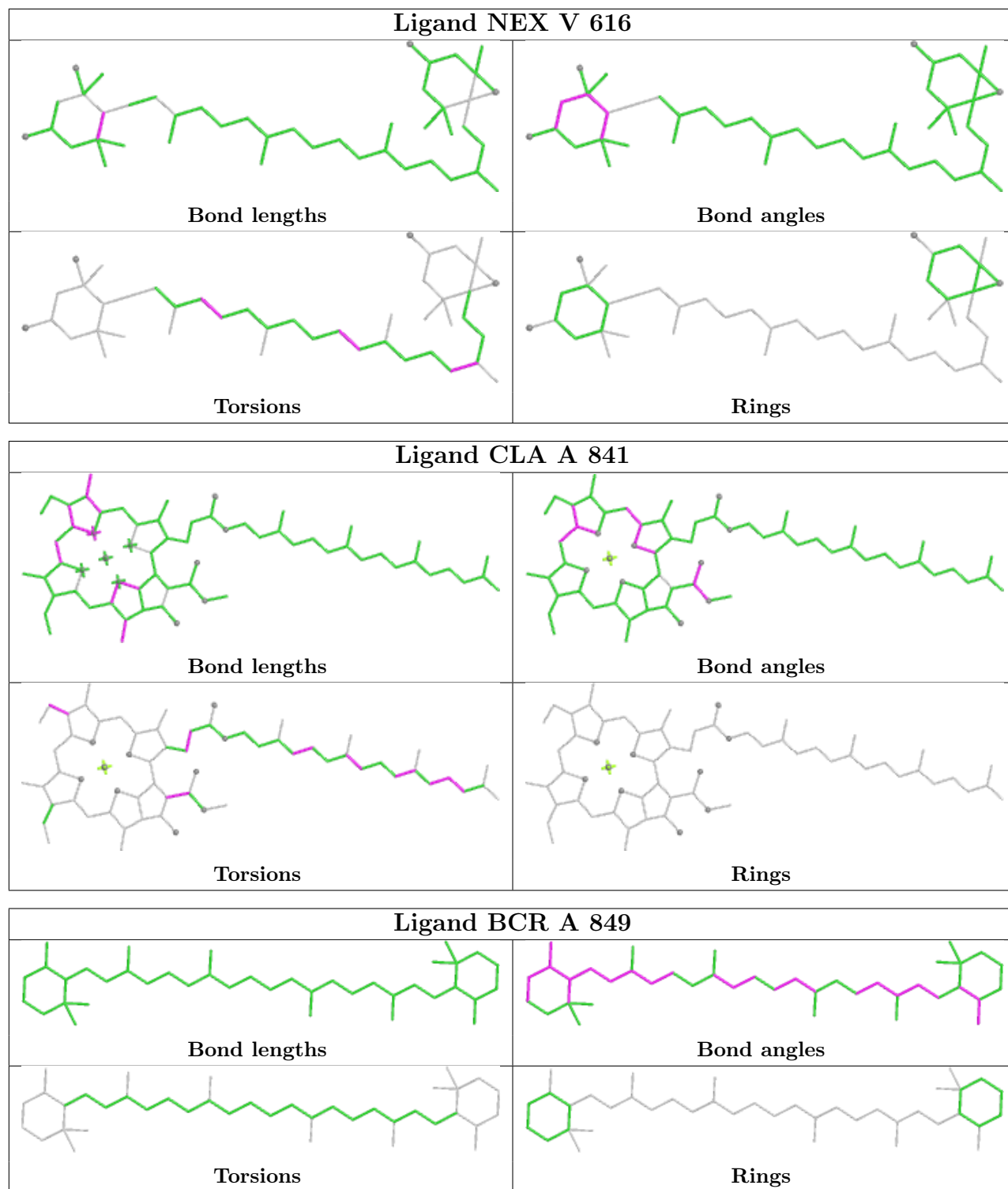
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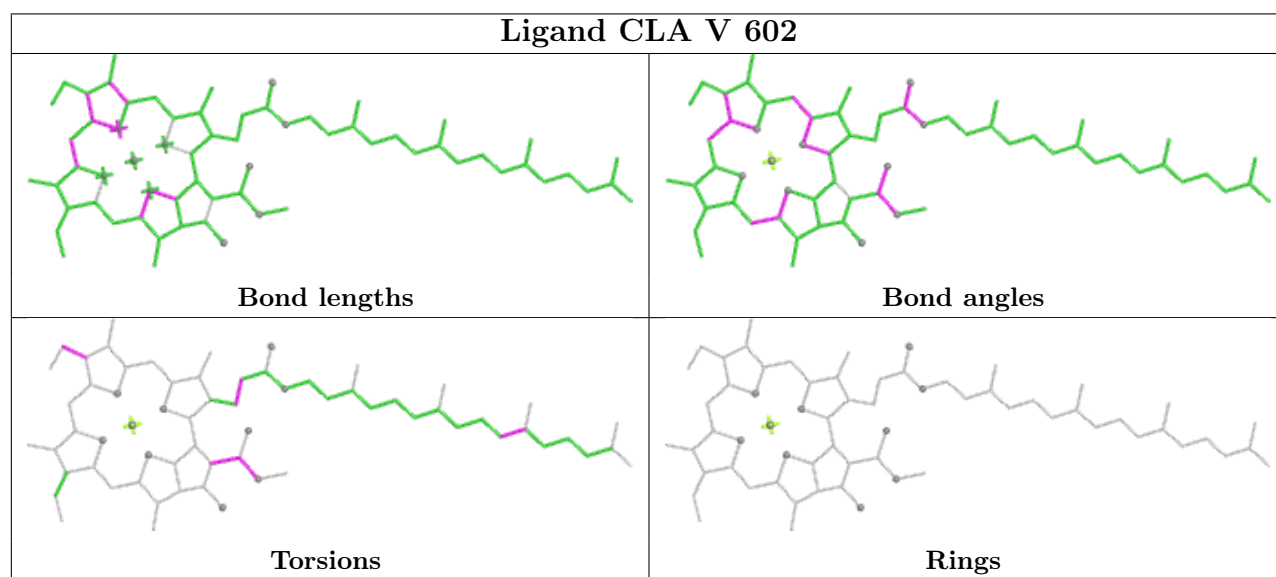
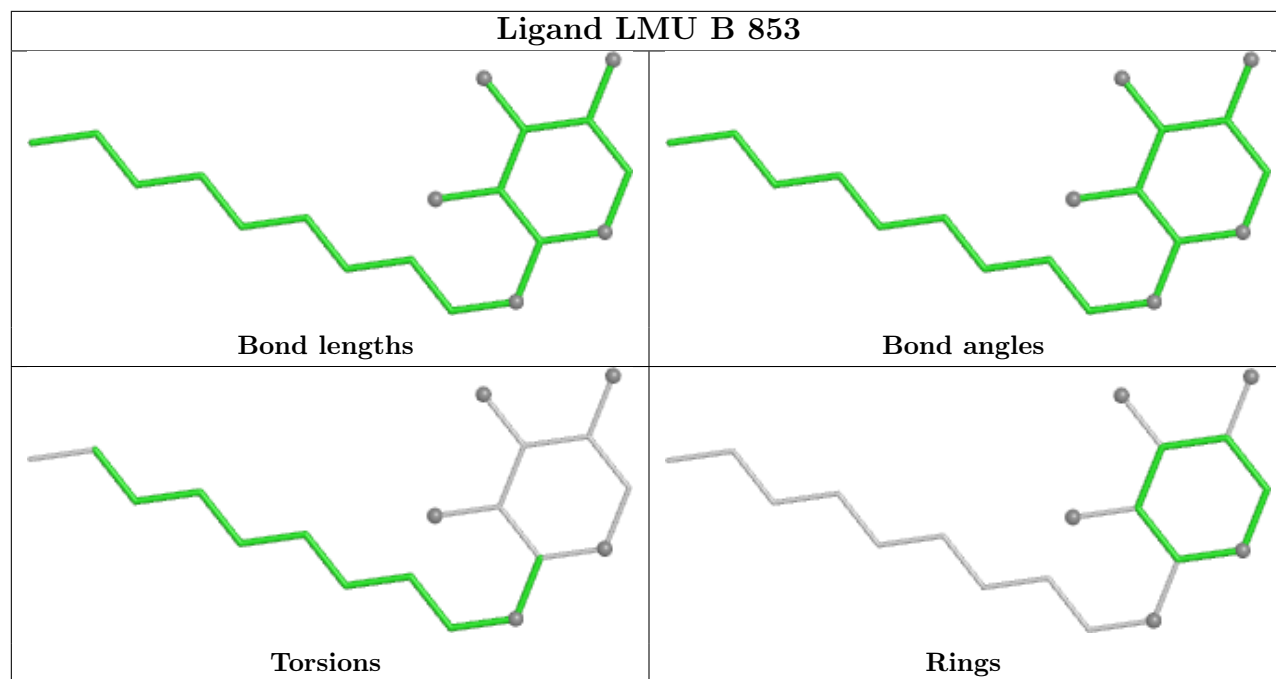


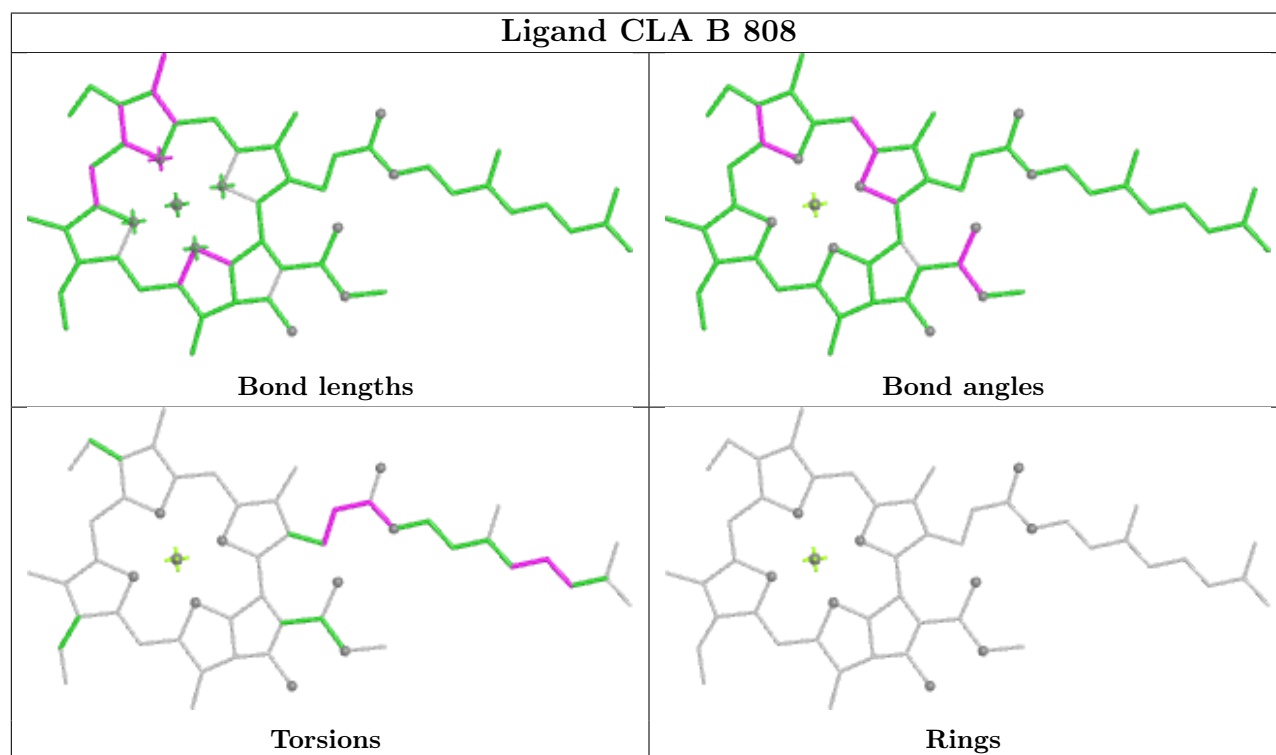
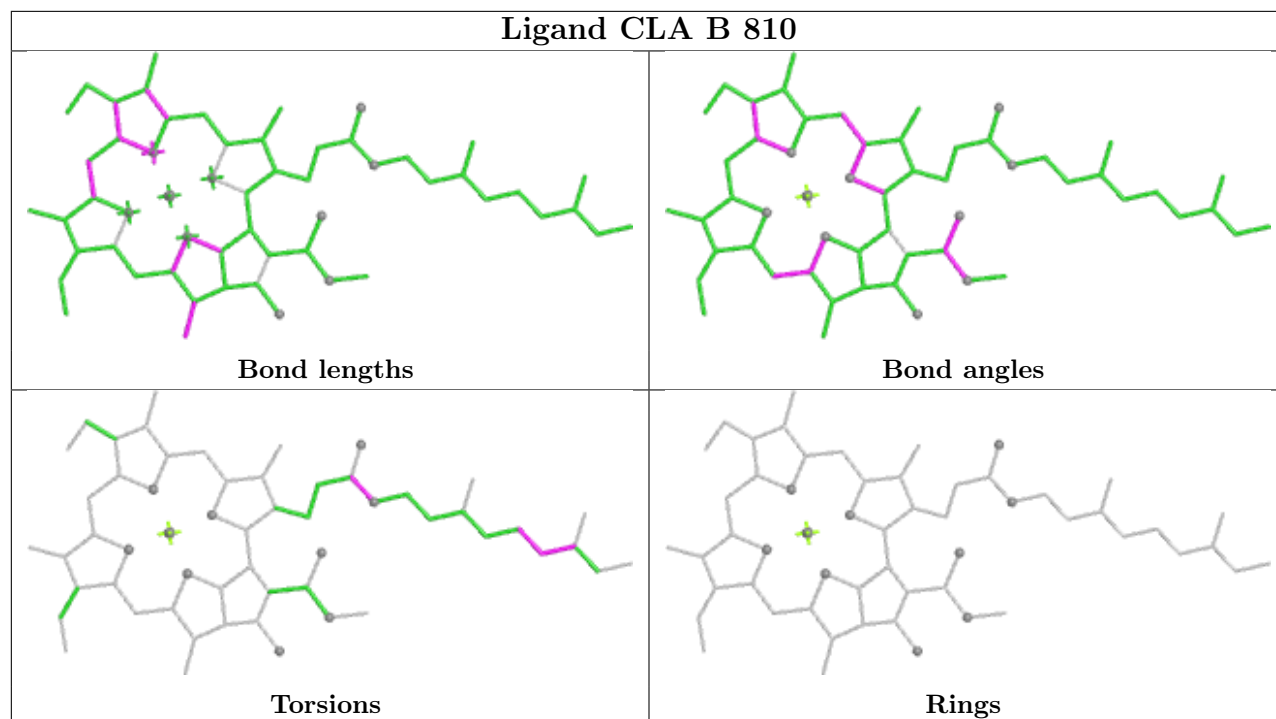
Torsions

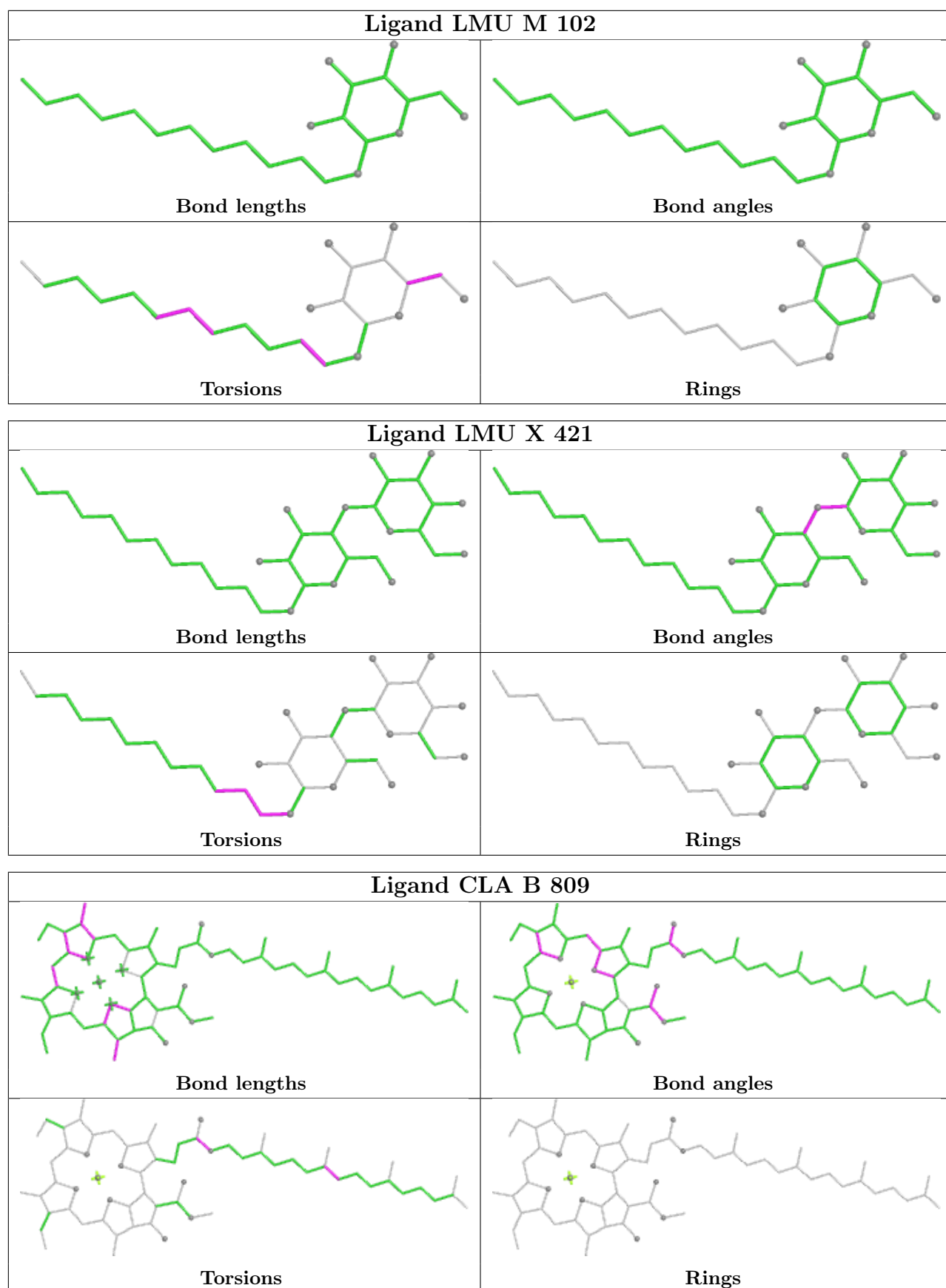


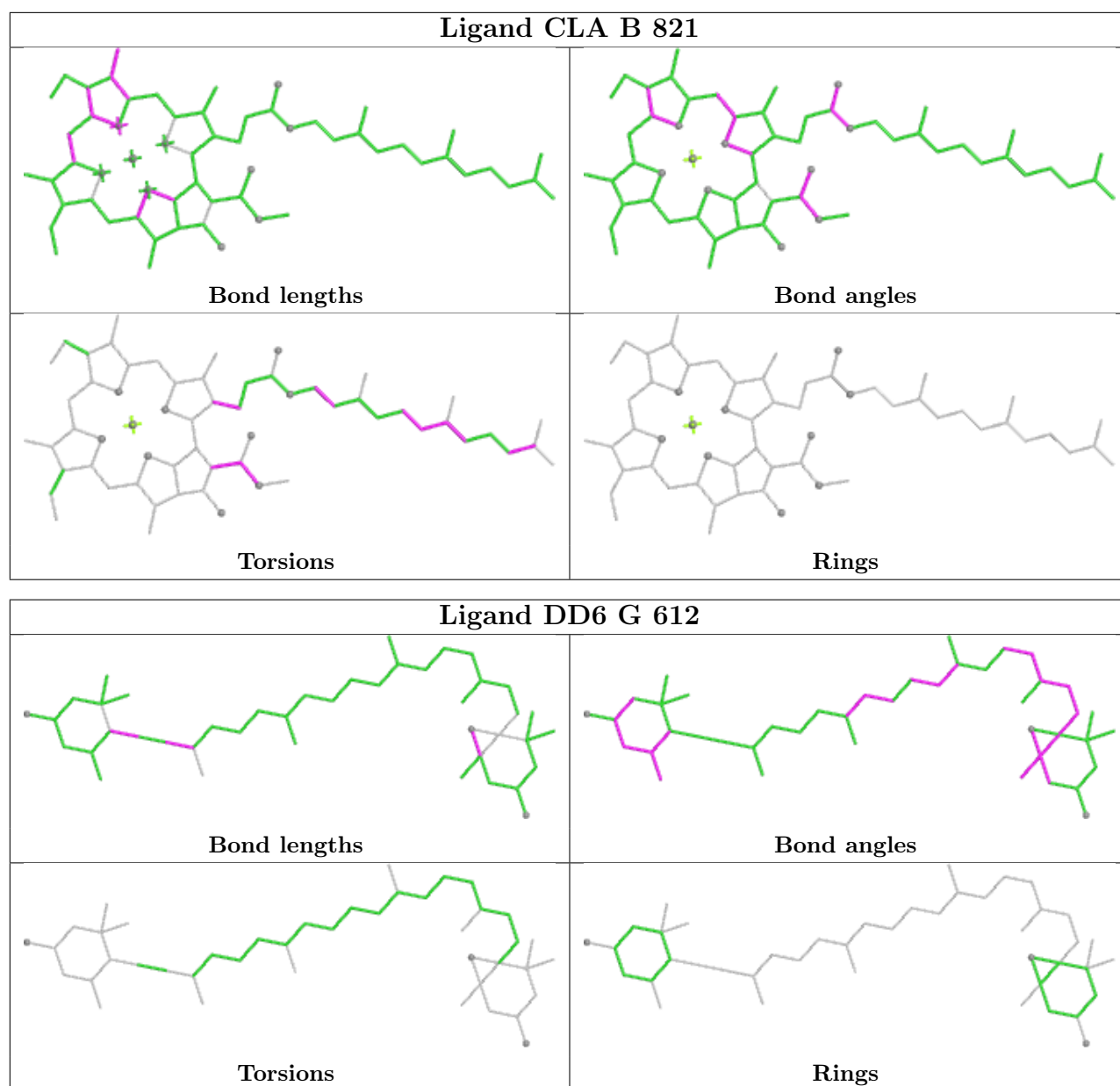
Rings



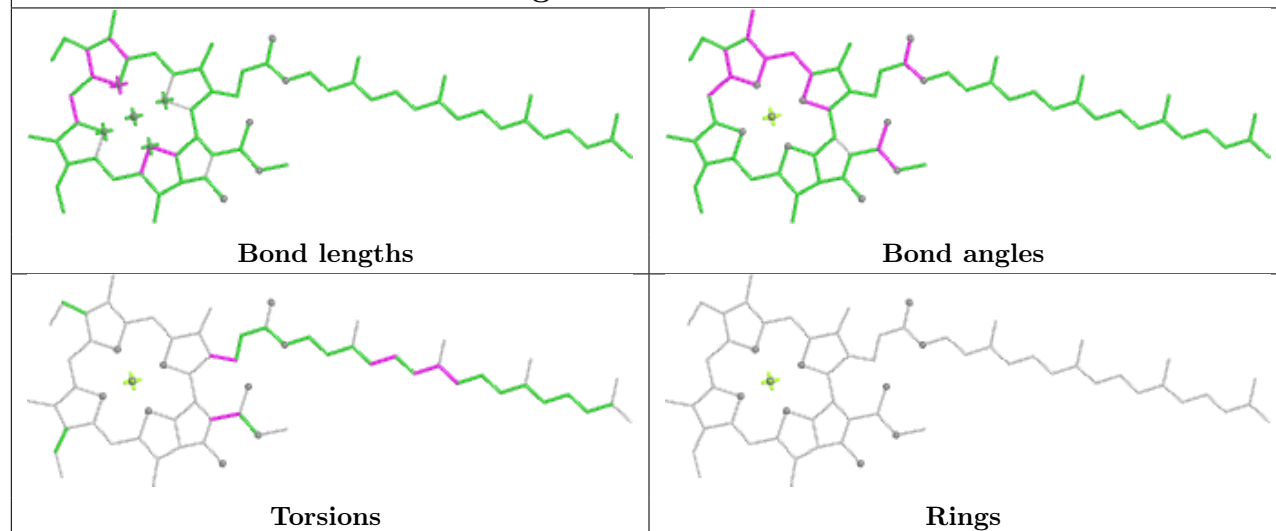




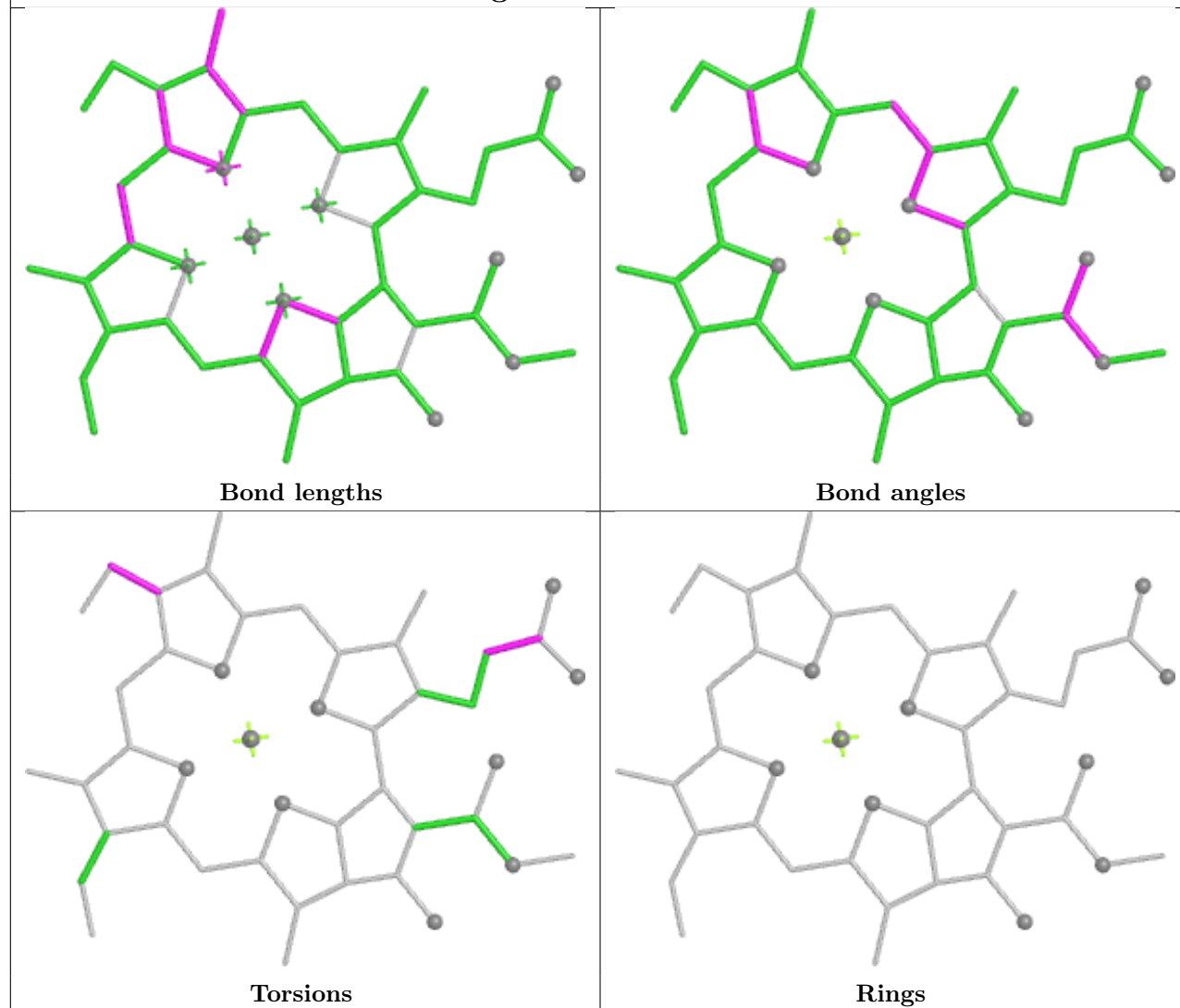


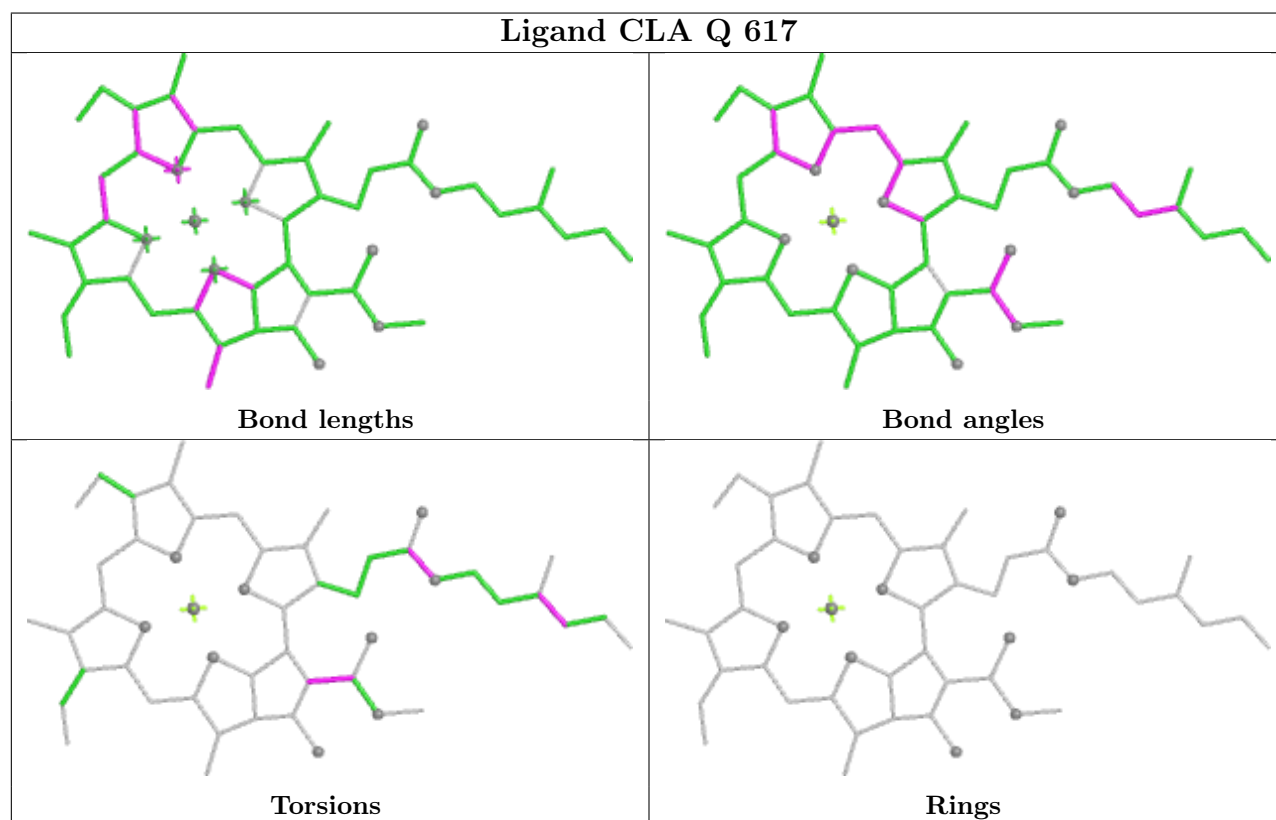
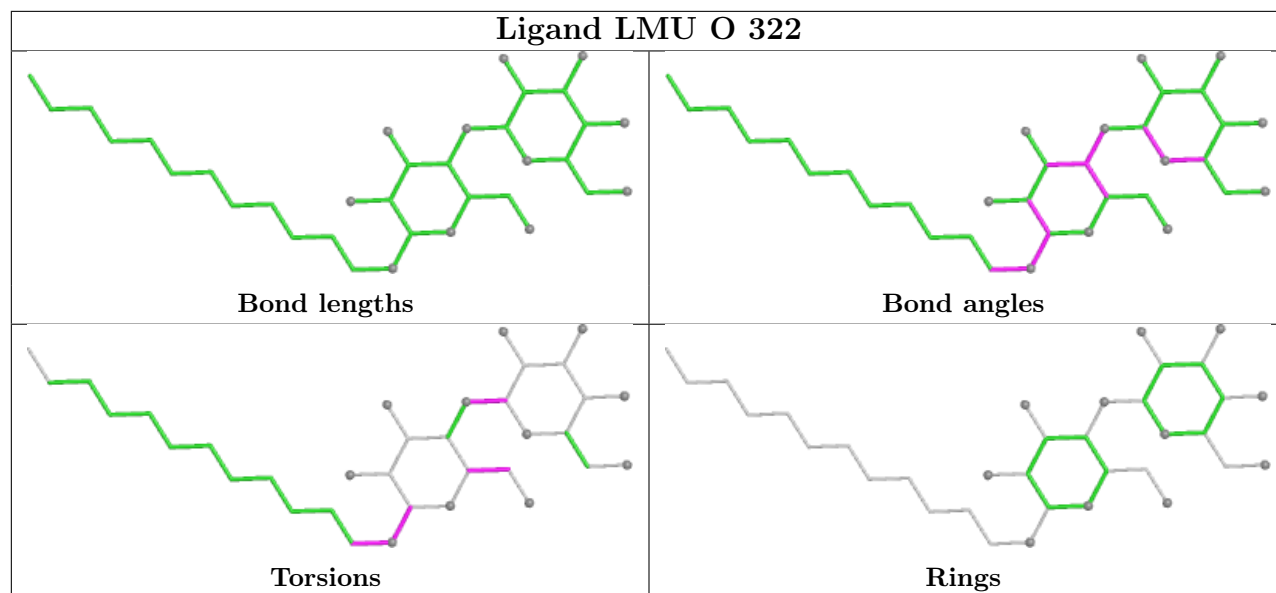


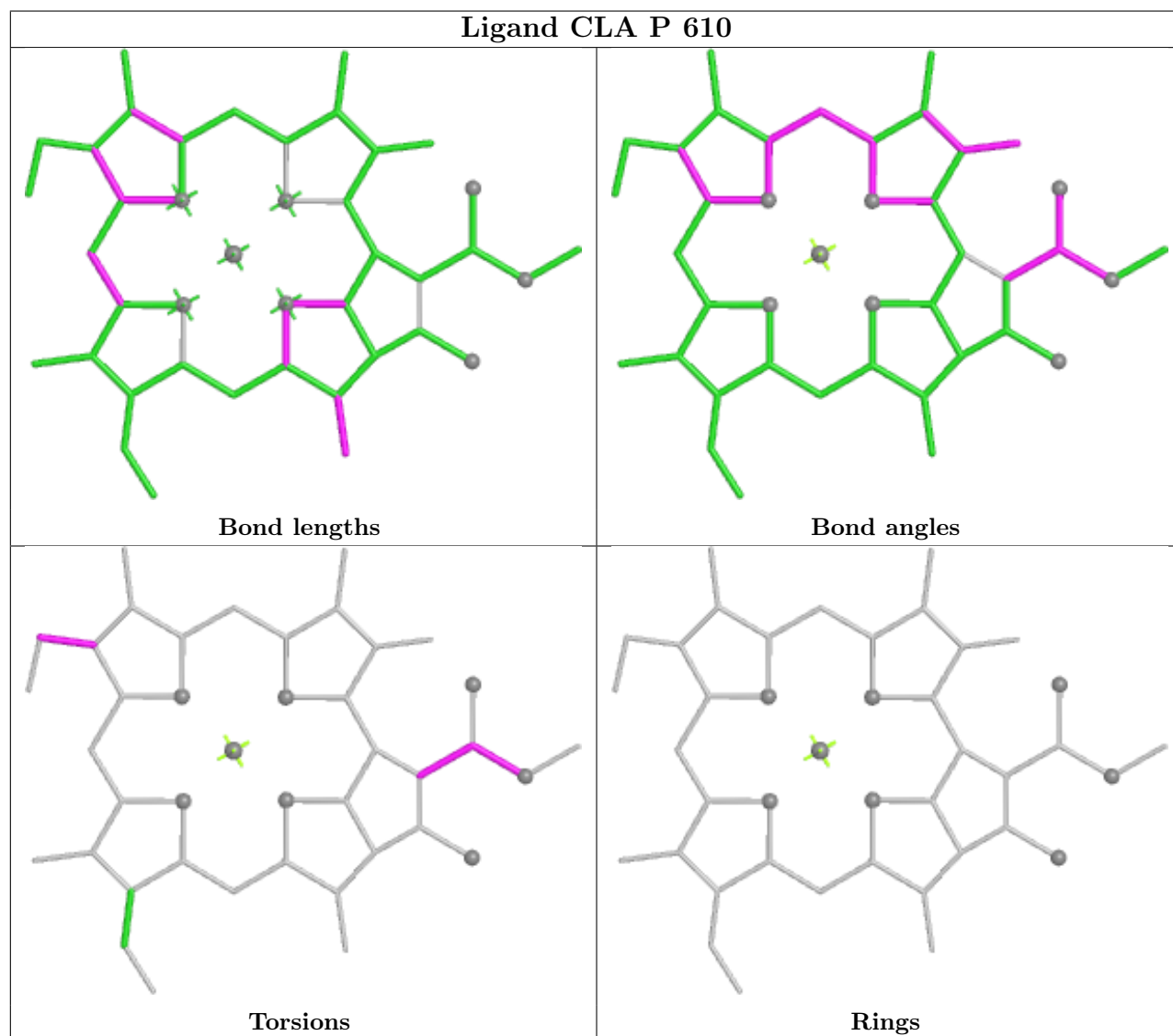
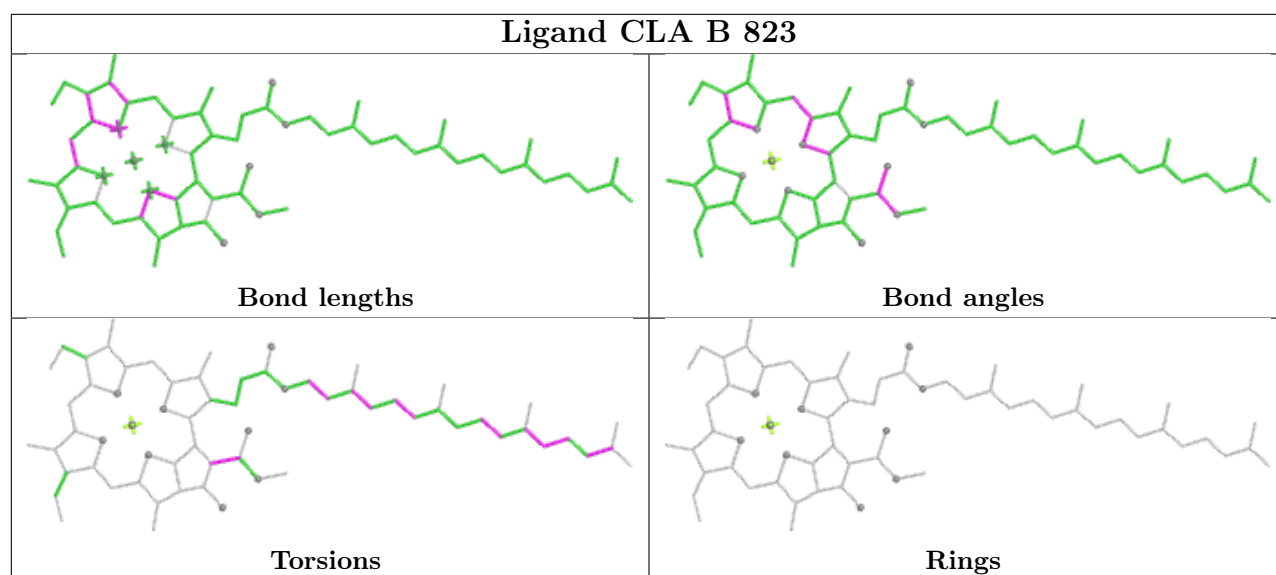
Ligand CLA B 831

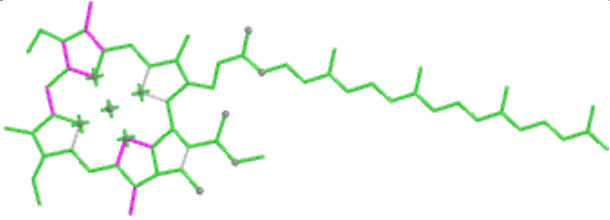
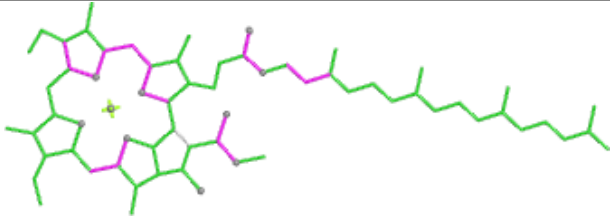
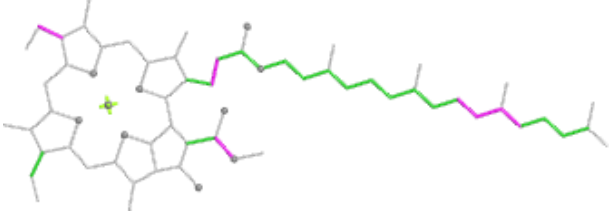
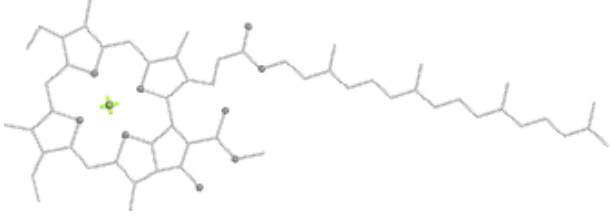
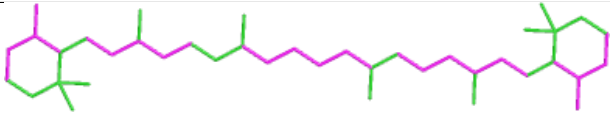
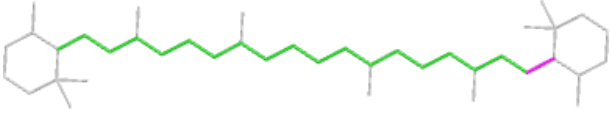
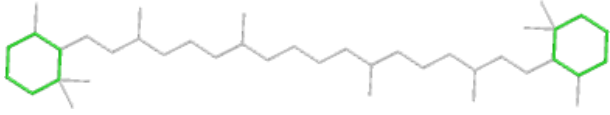
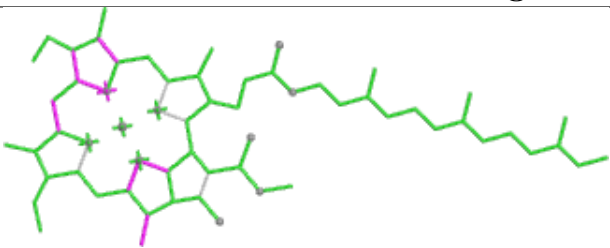
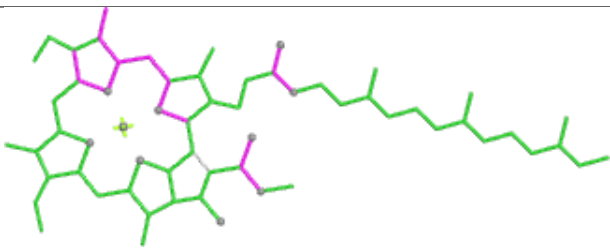
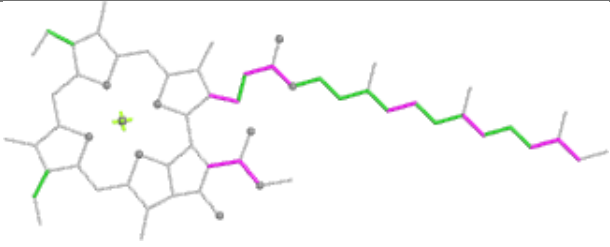
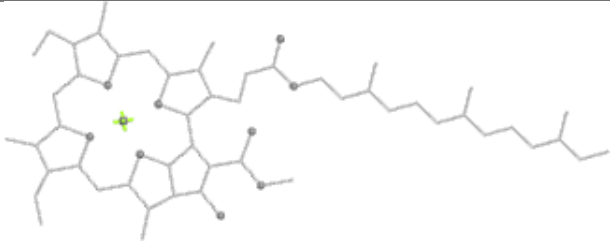


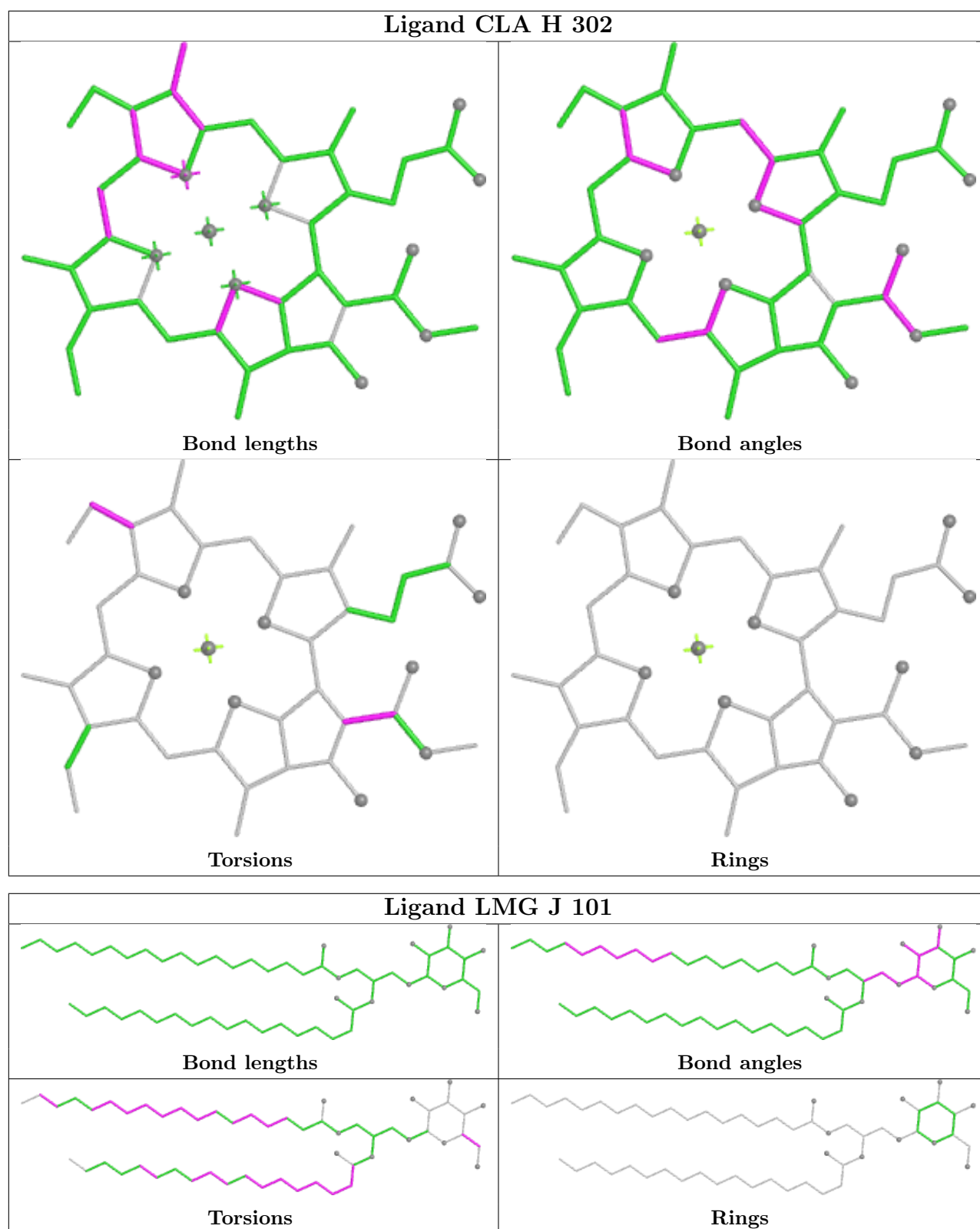
Ligand CLA U 412

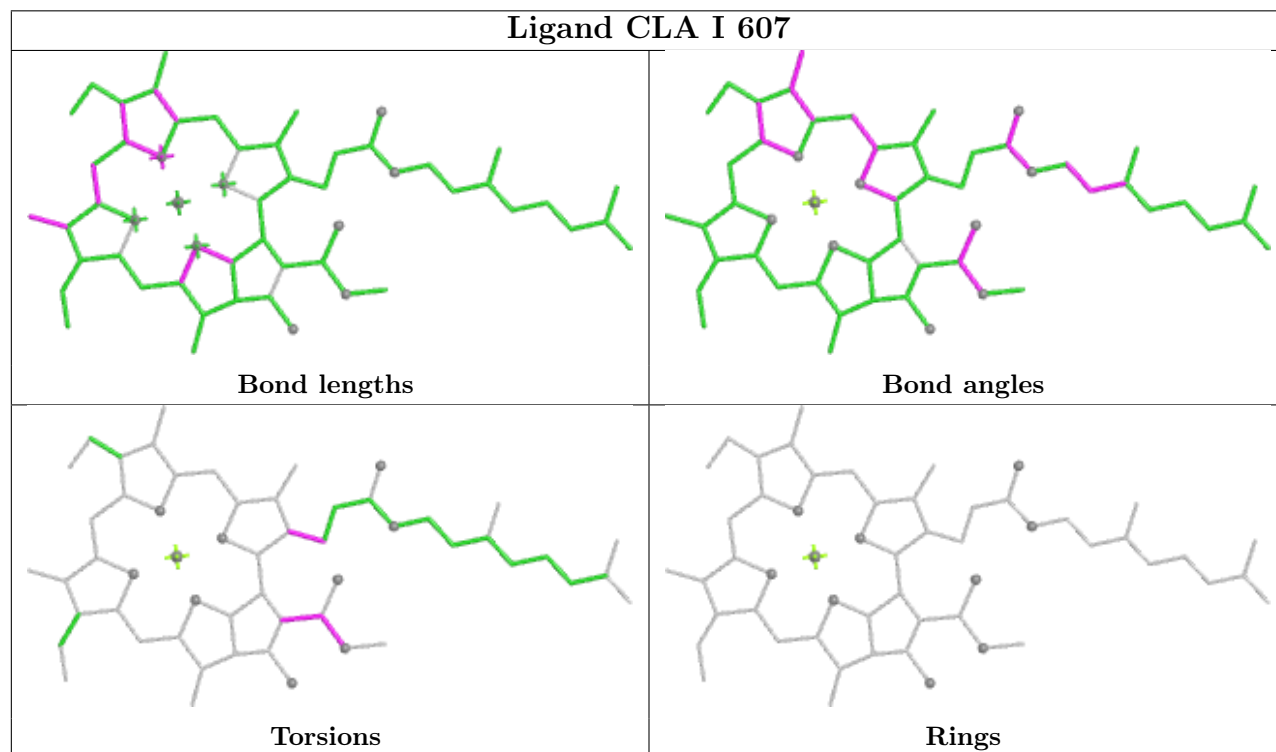
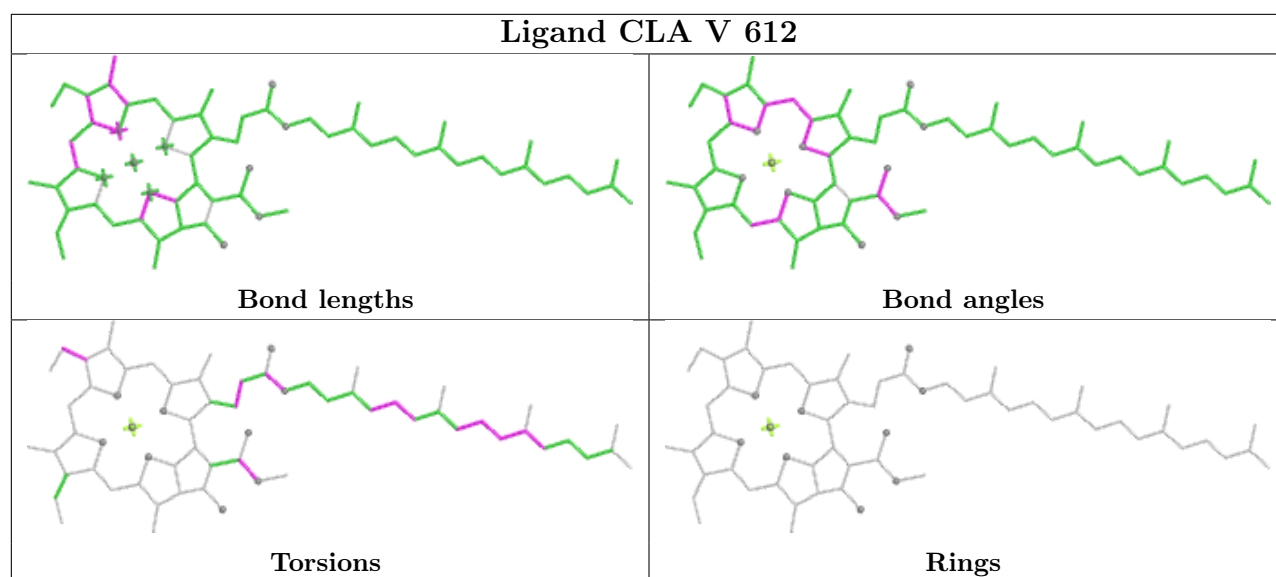


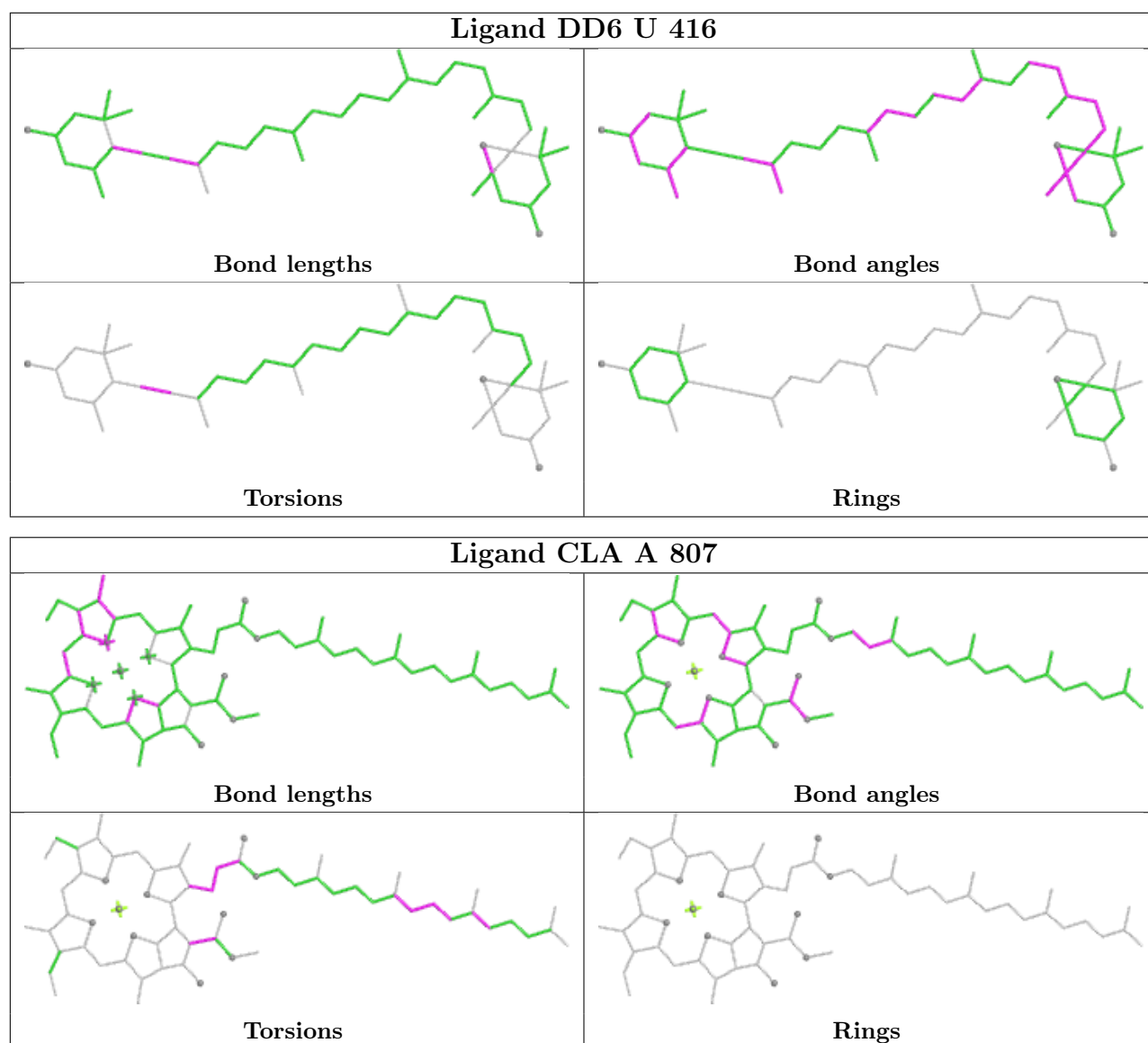


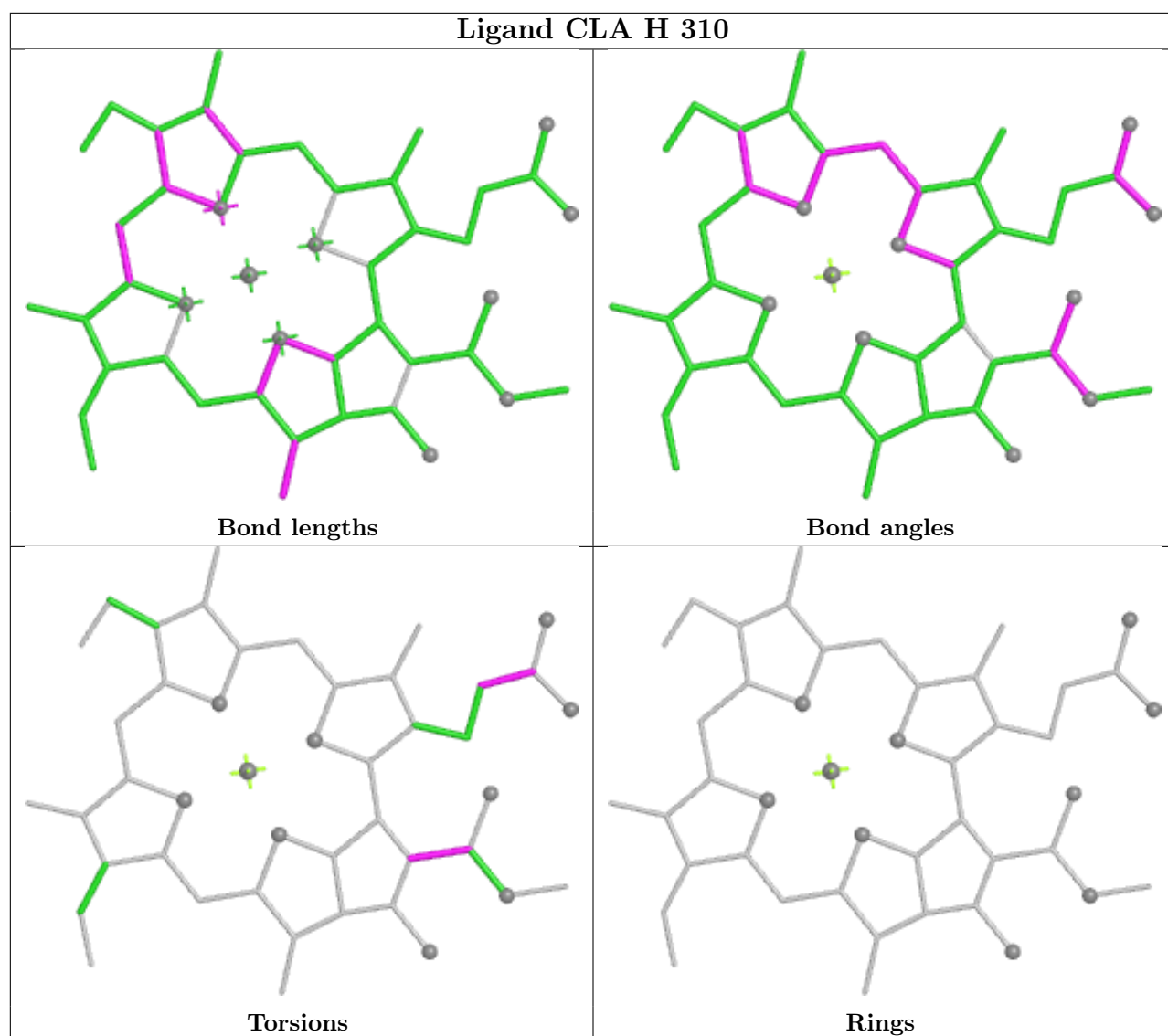


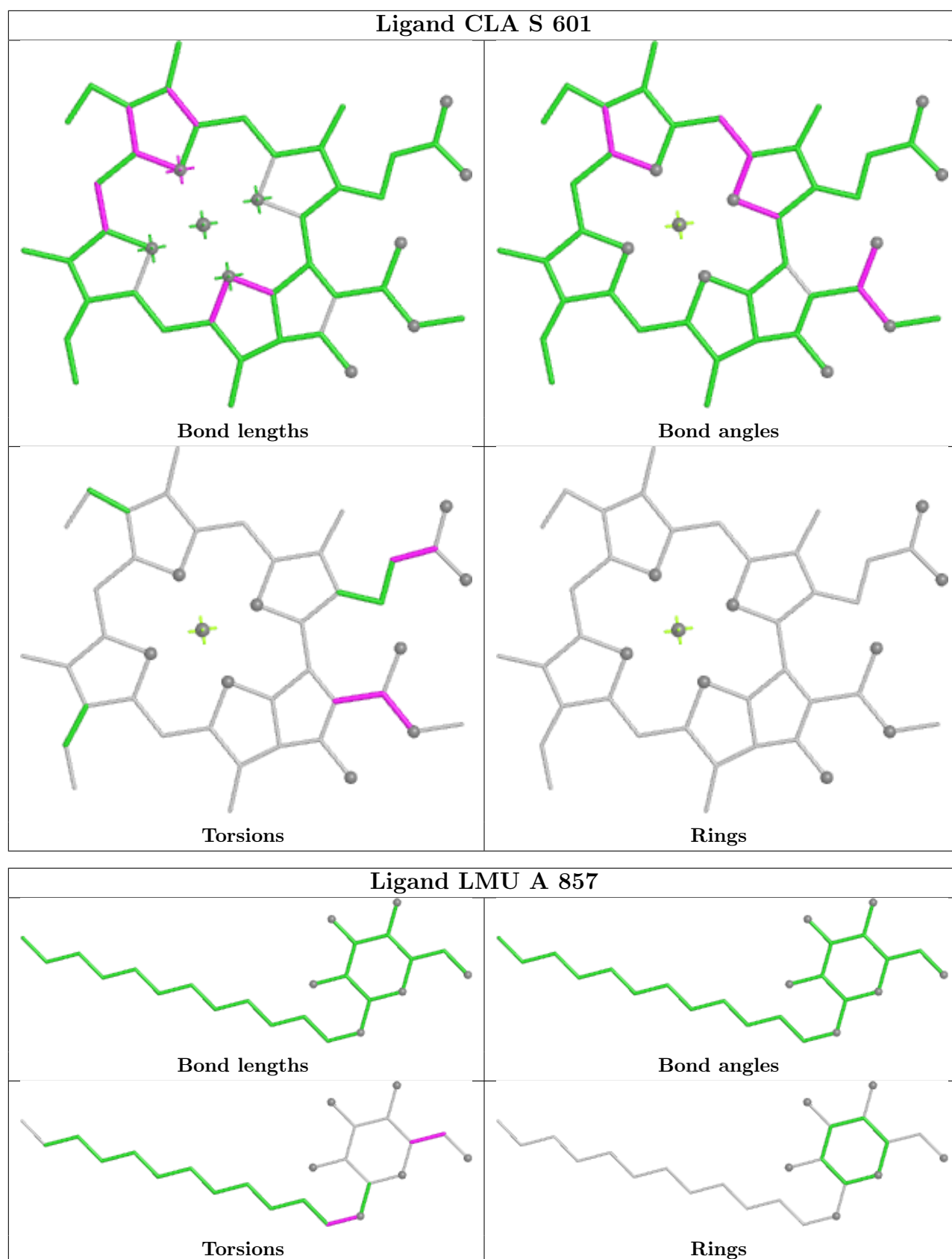
Ligand CLA W 414	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCR B 844	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand CLA O 308	
 Bond lengths	 Bond angles
 Torsions	 Rings

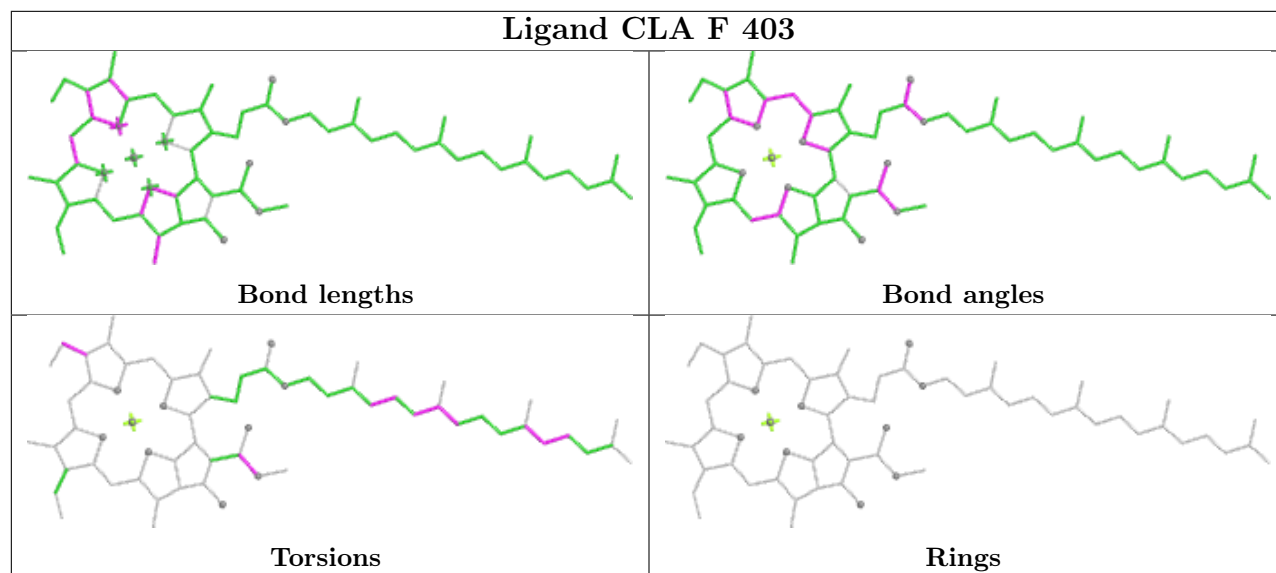
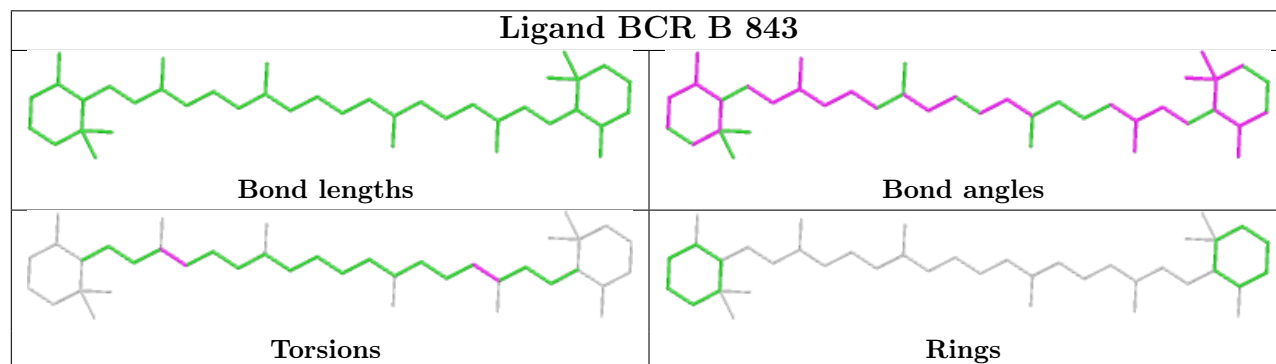
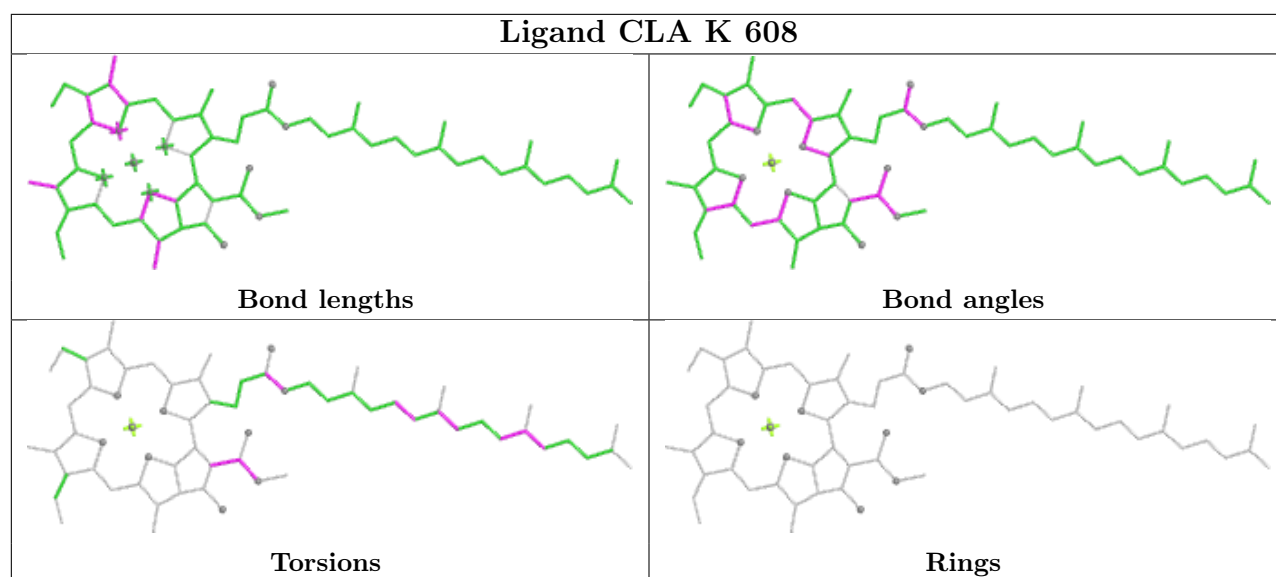


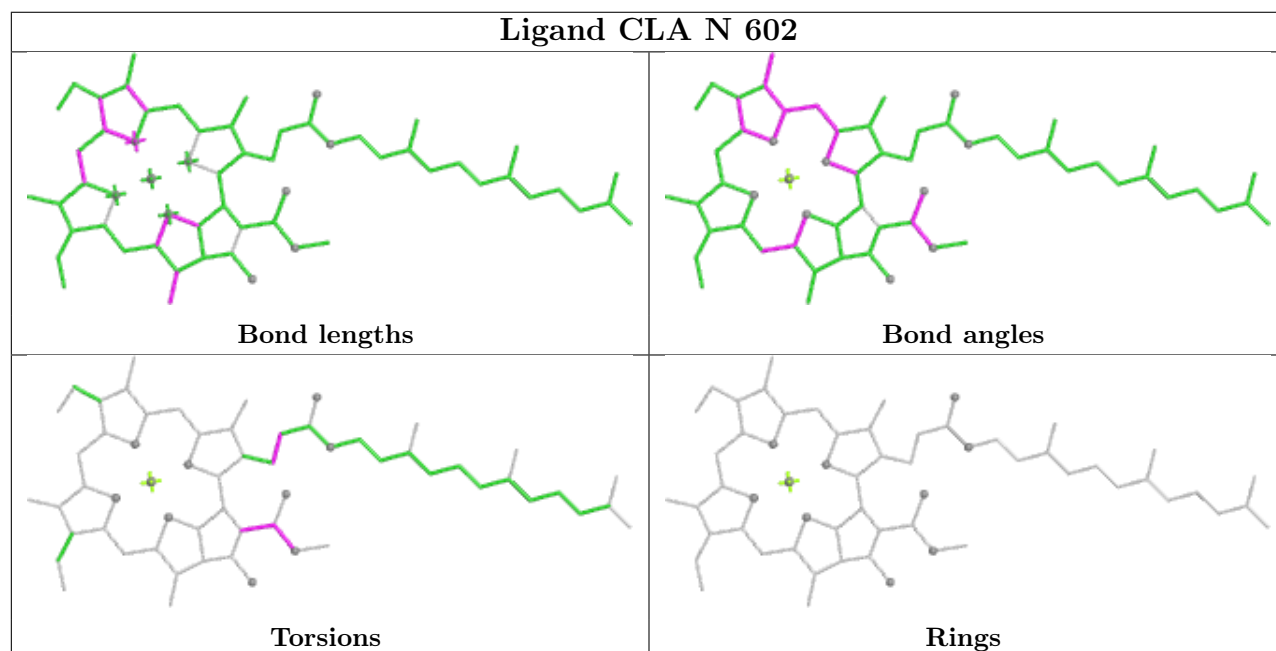
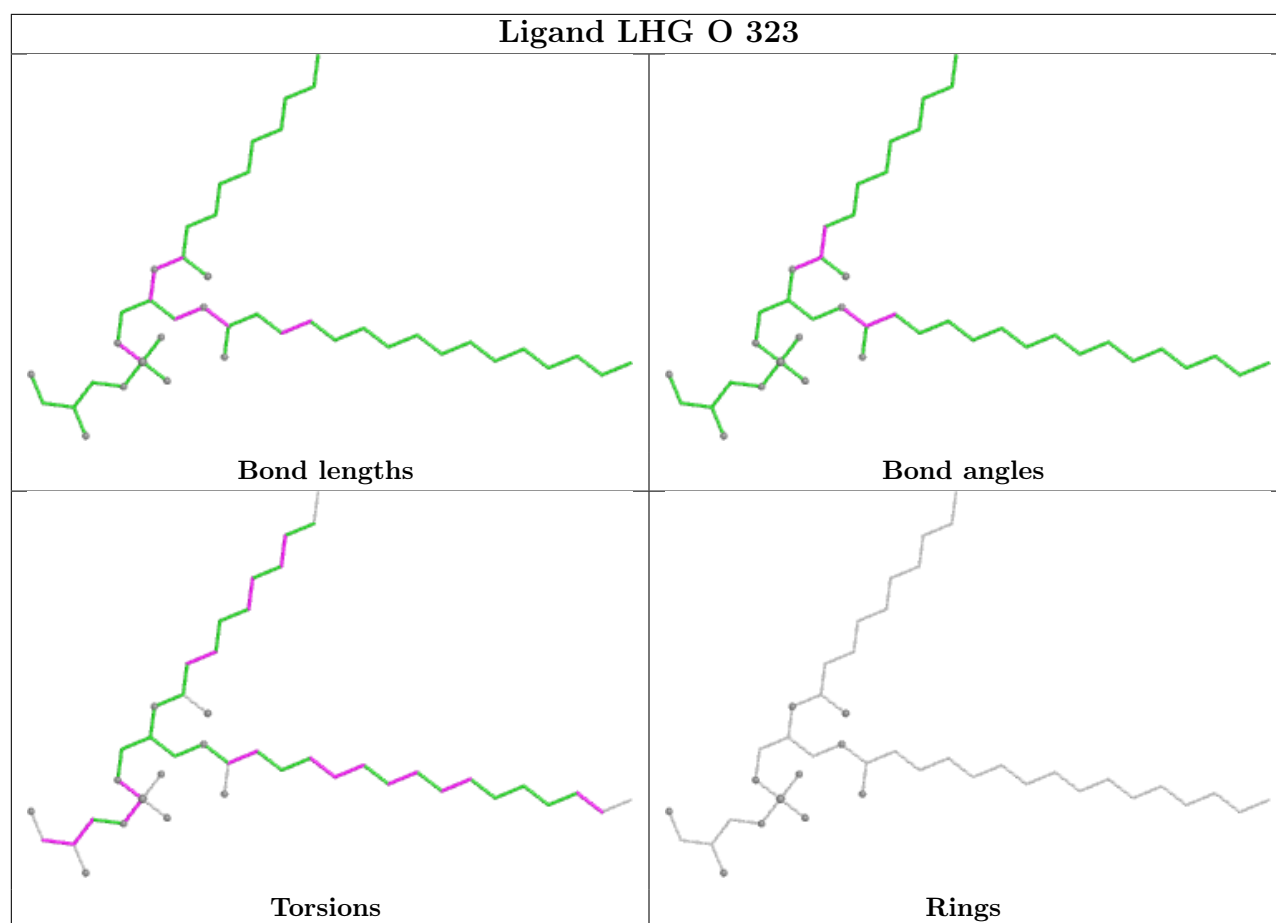


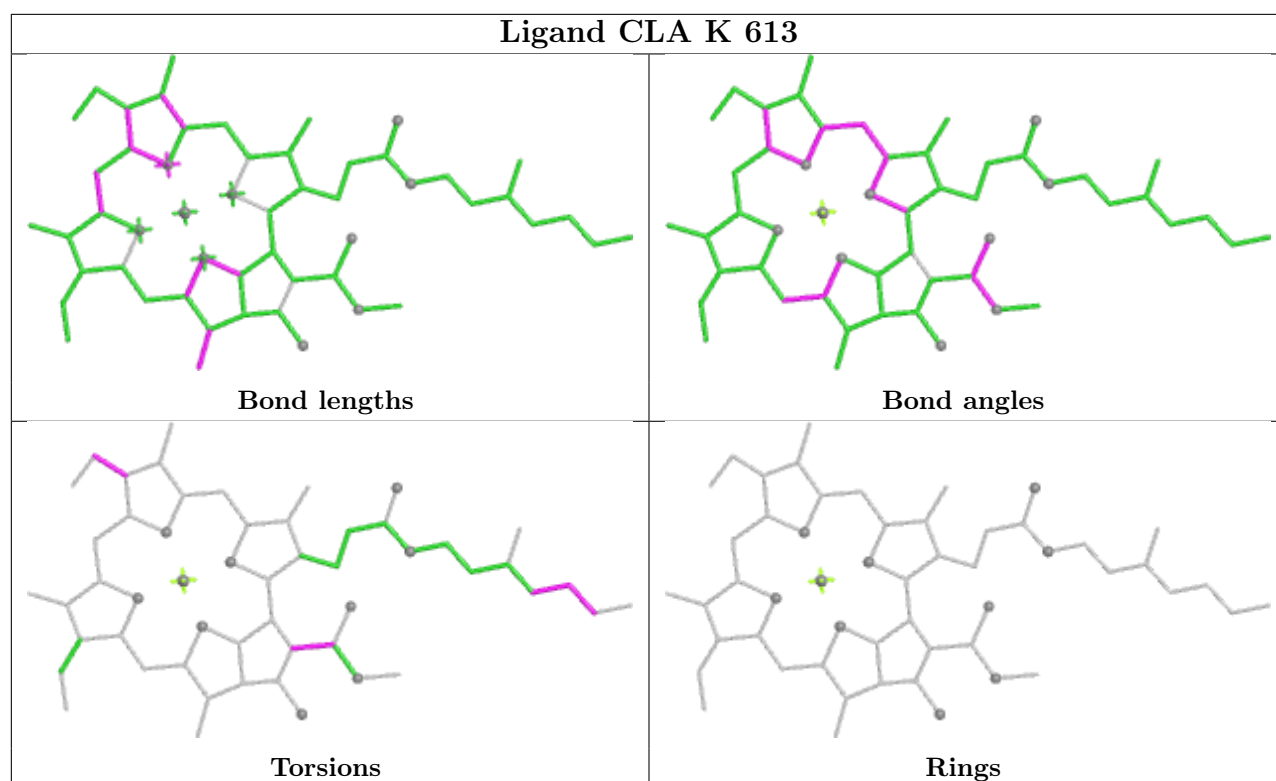


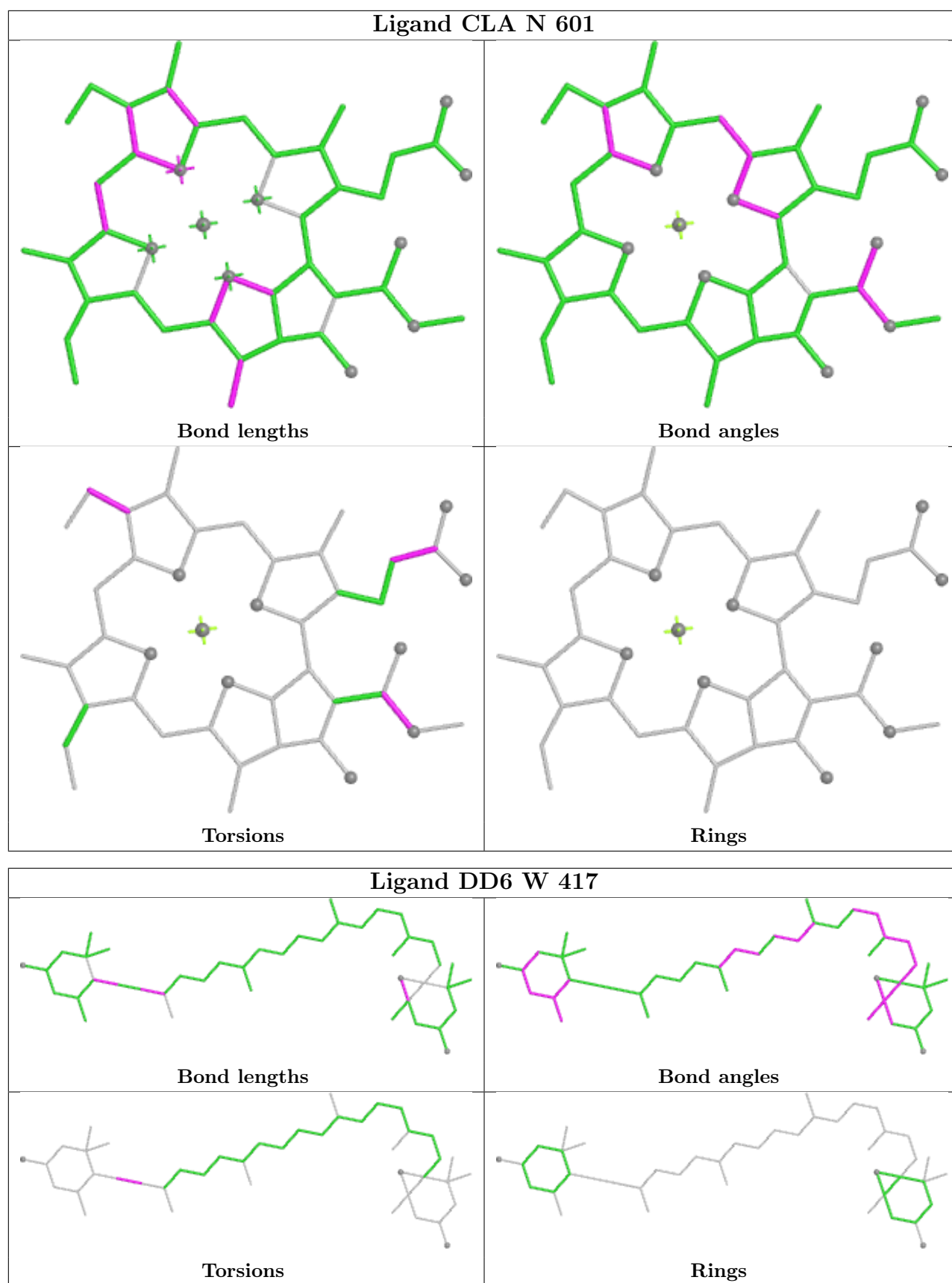


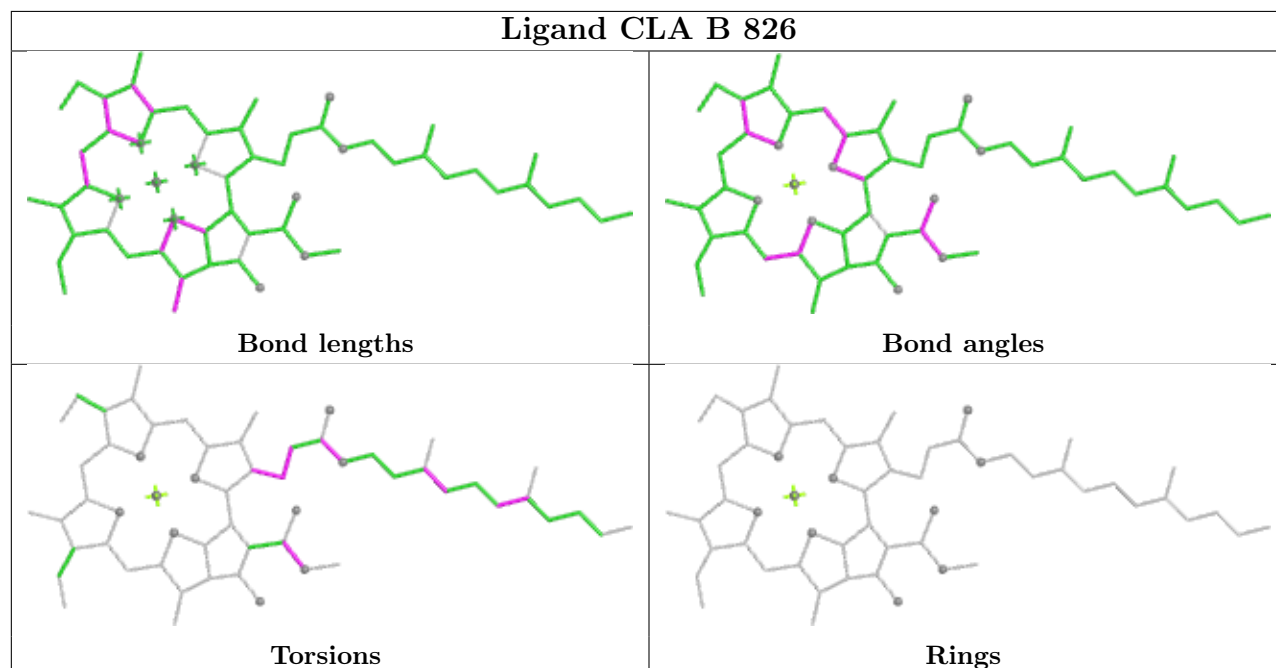
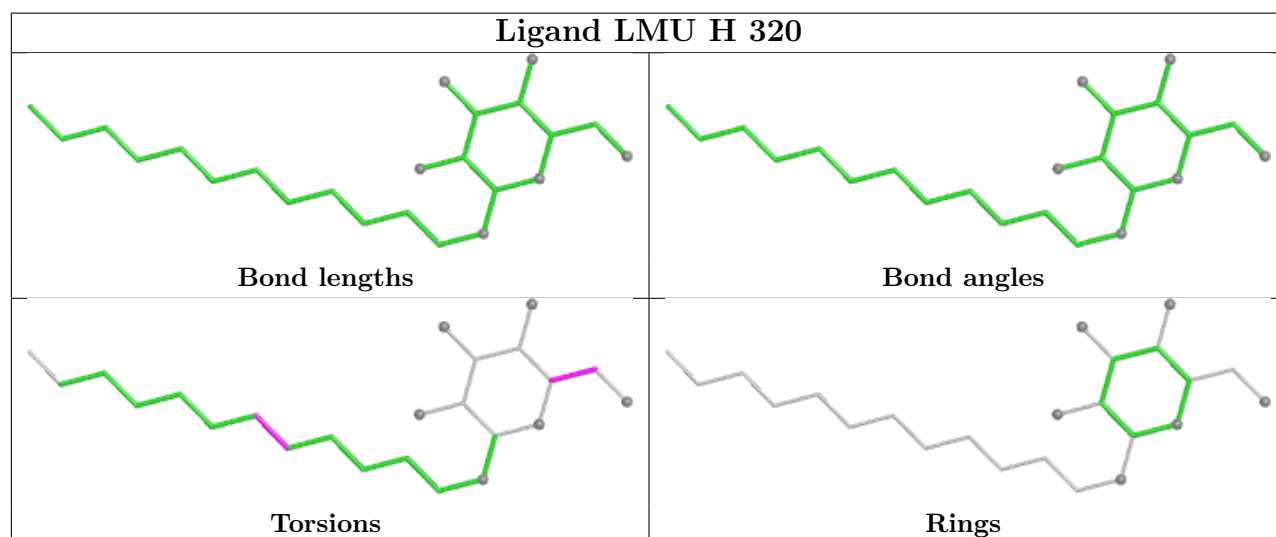
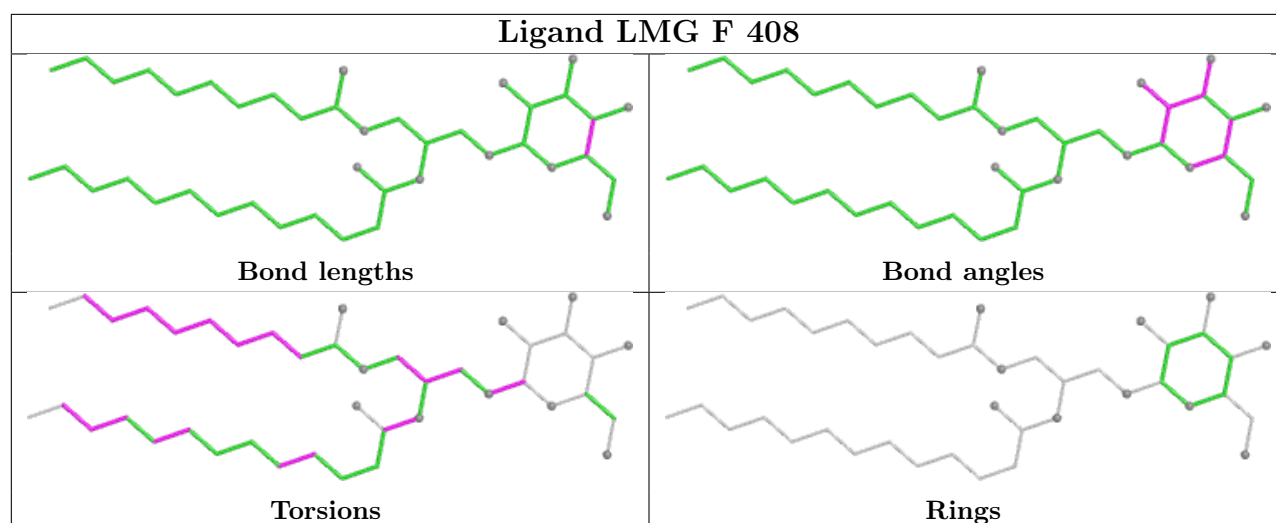


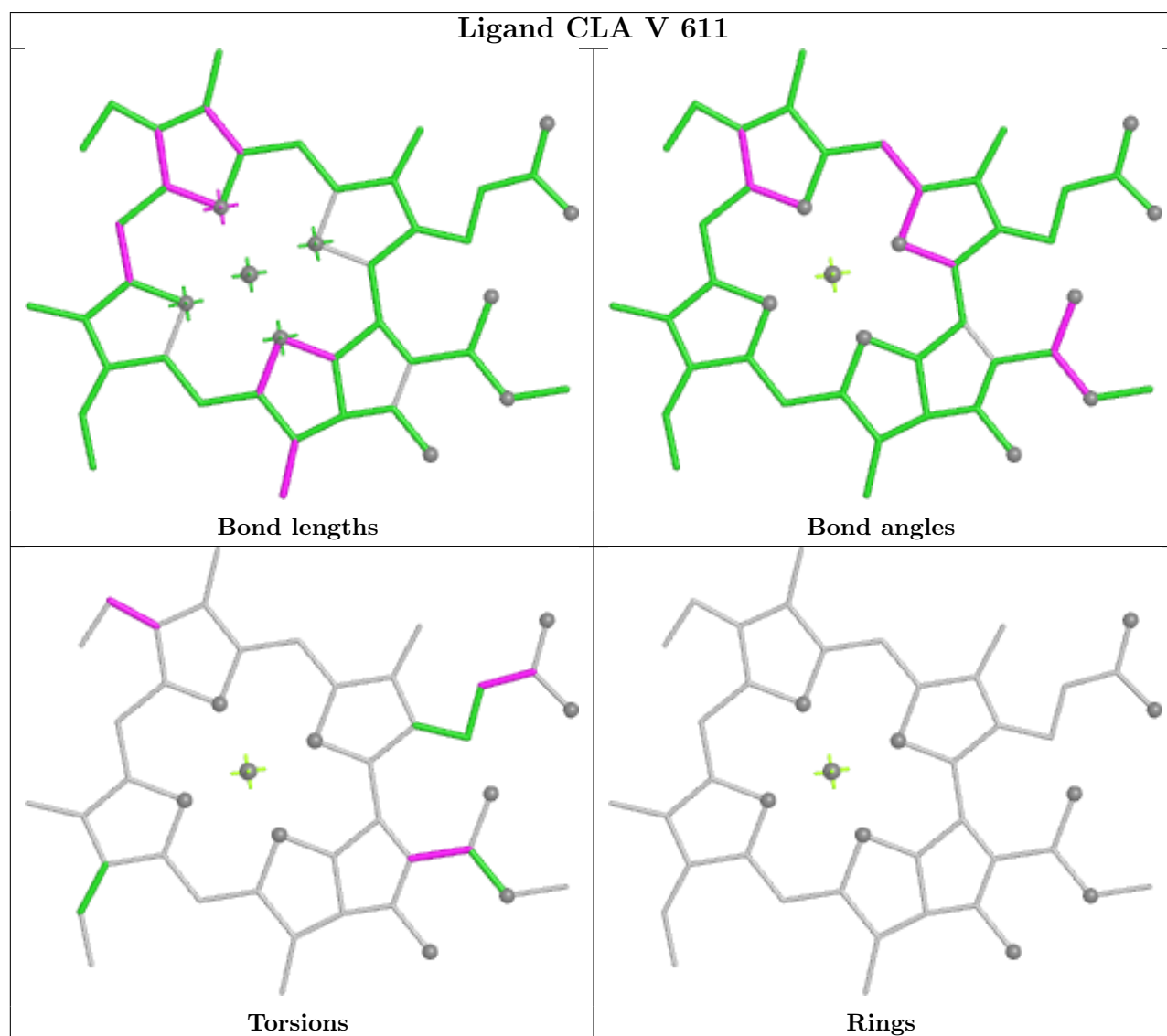
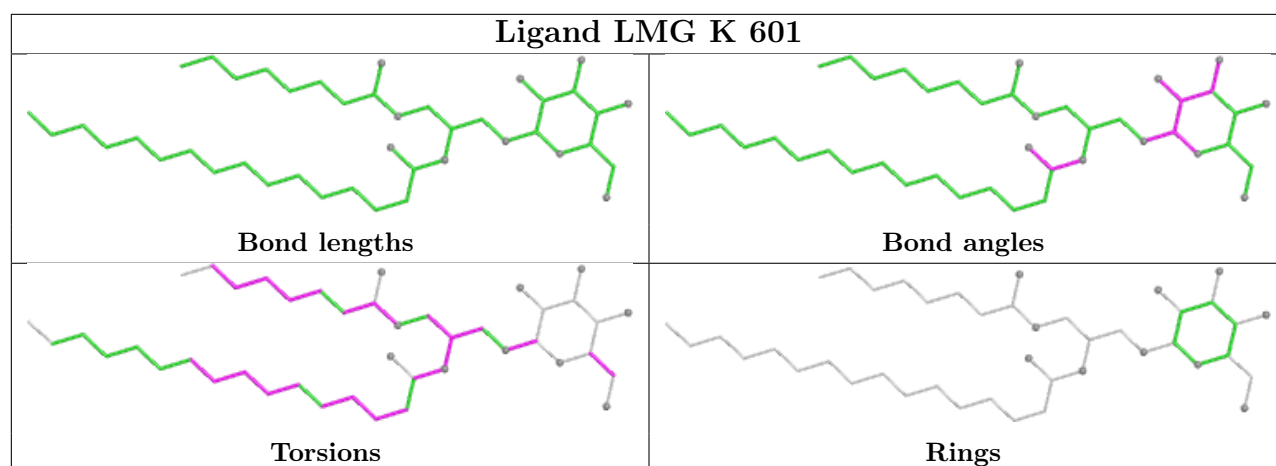


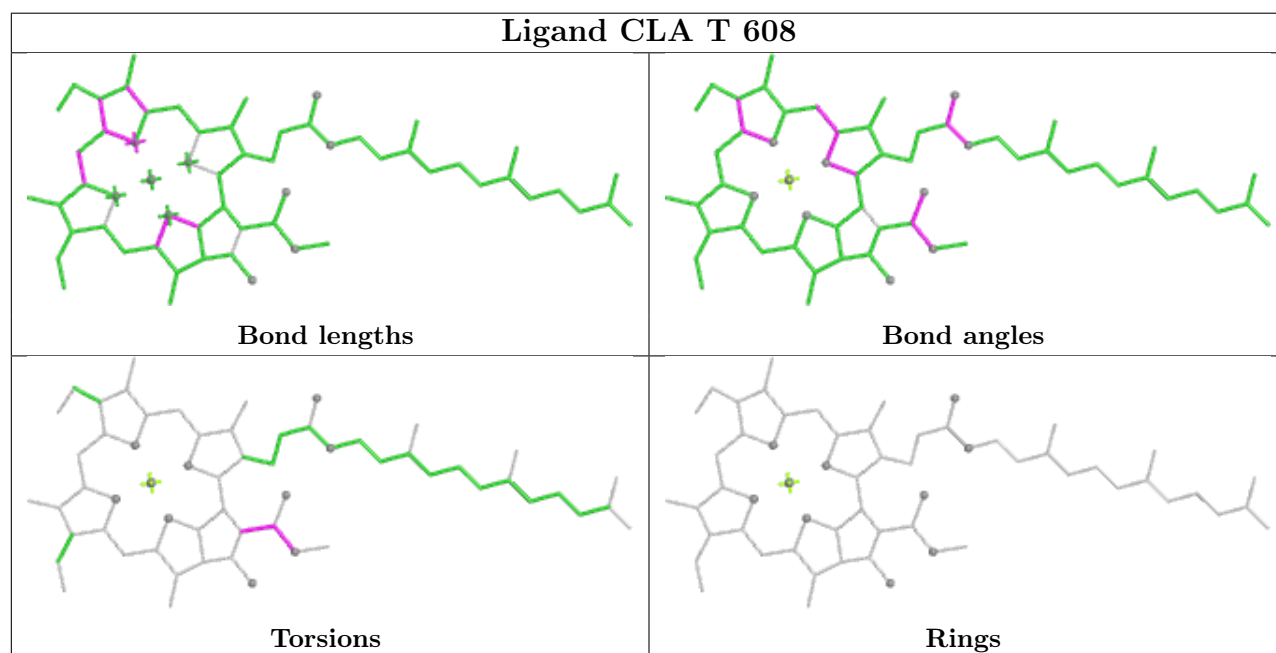
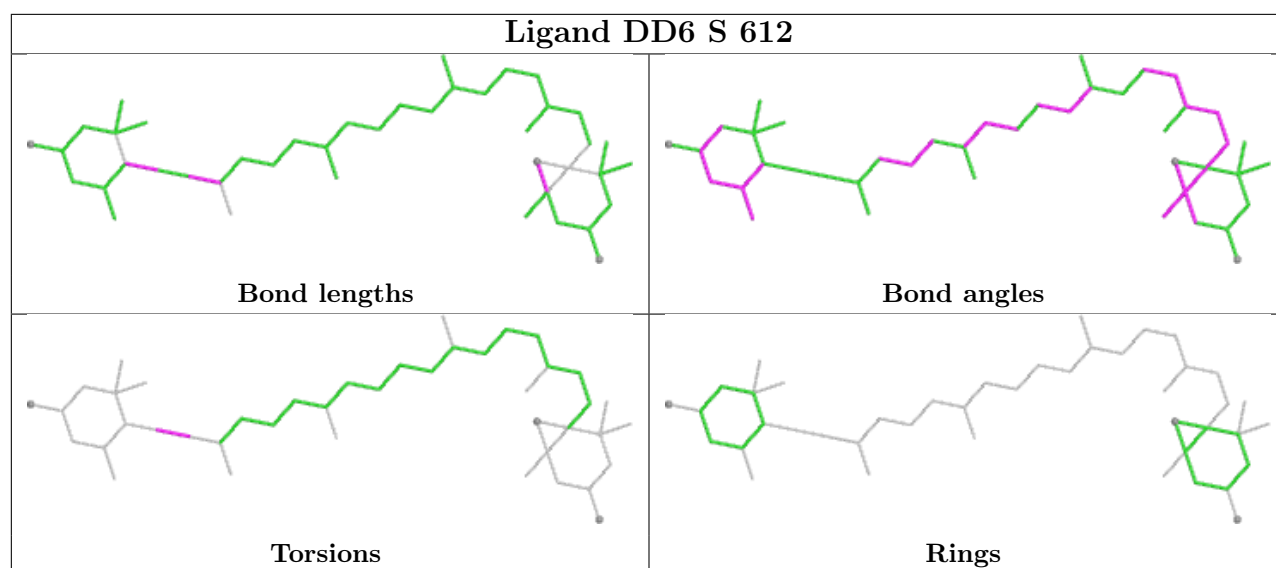


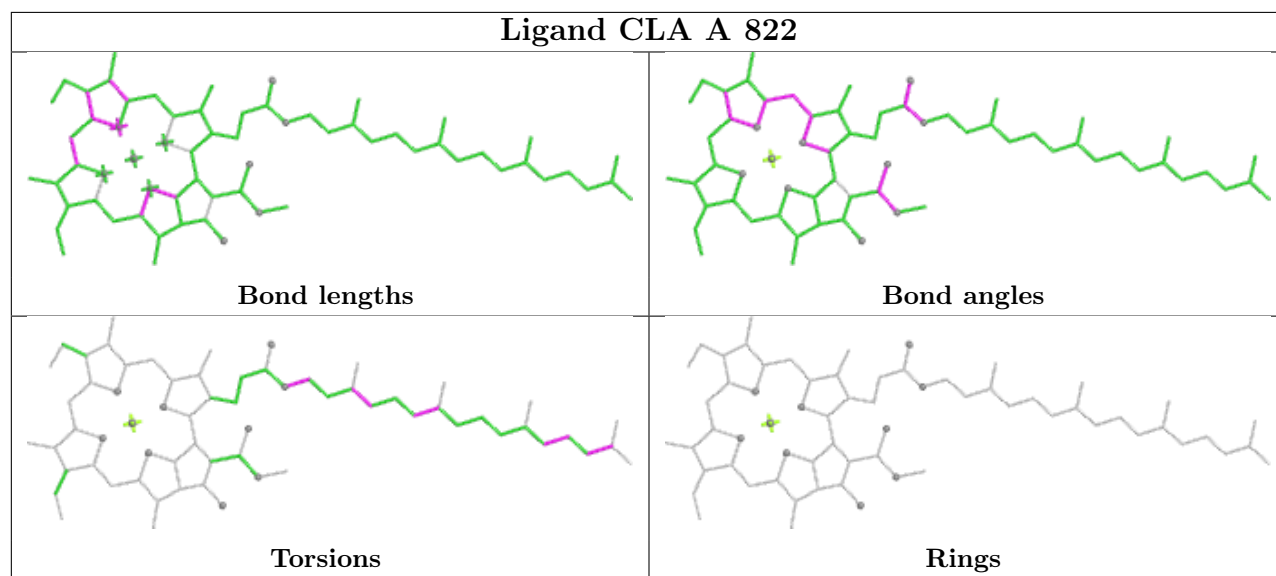
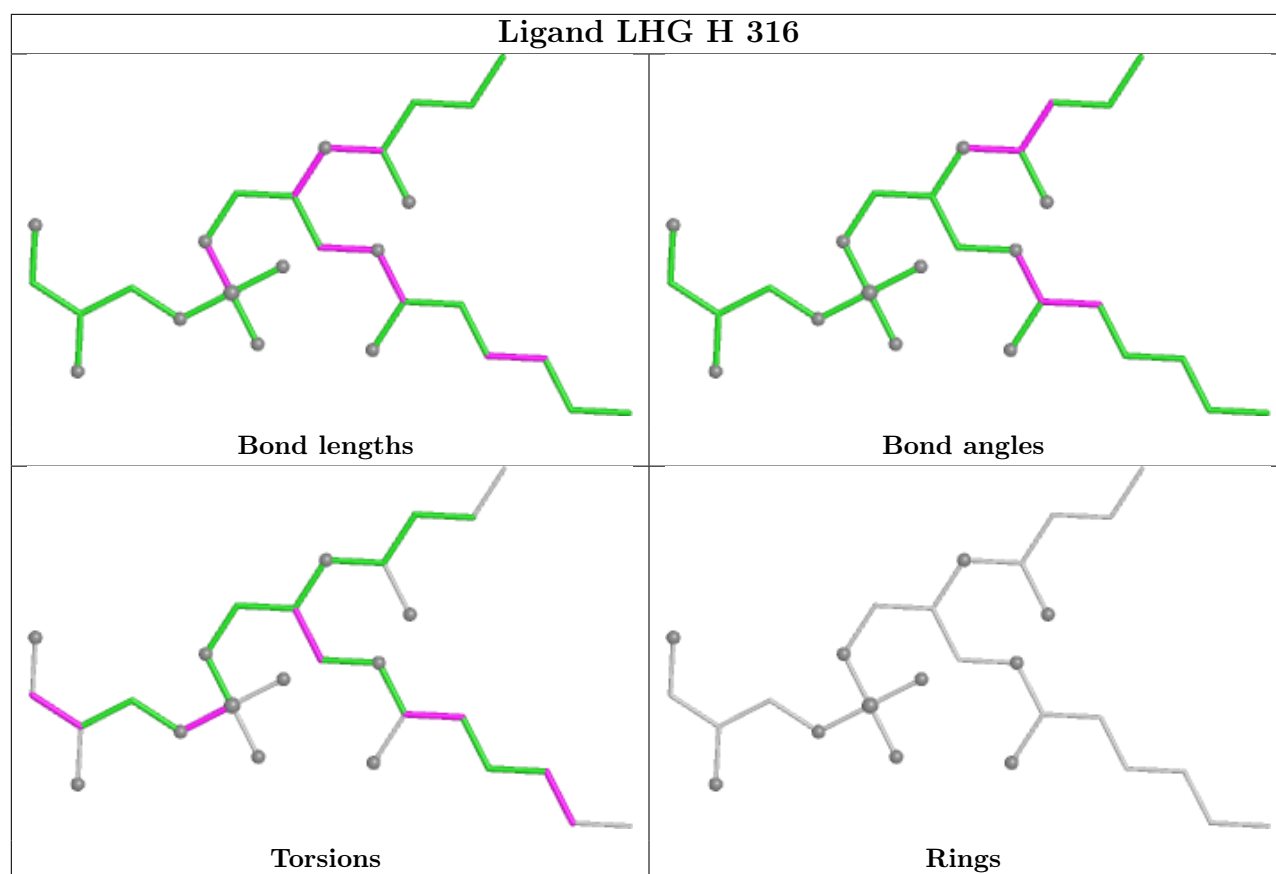


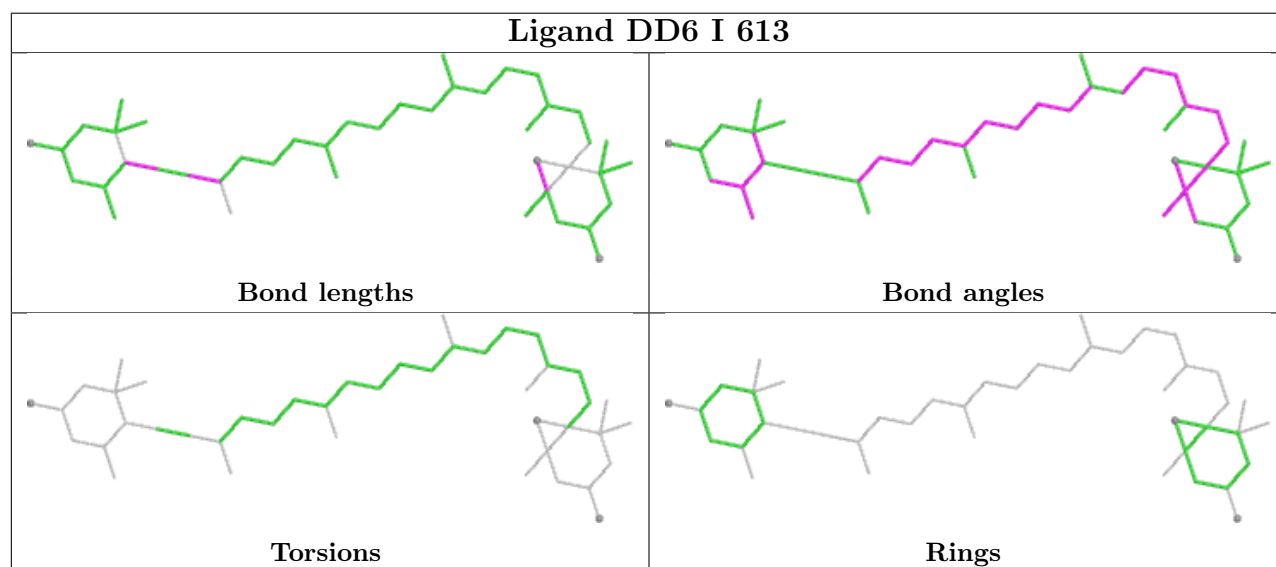
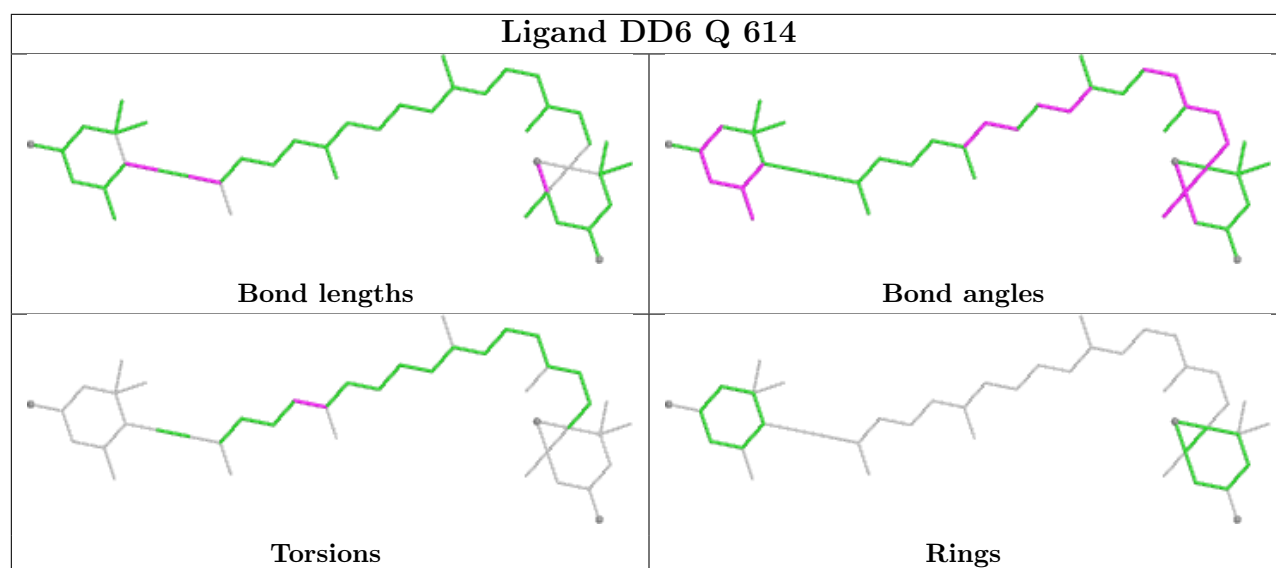


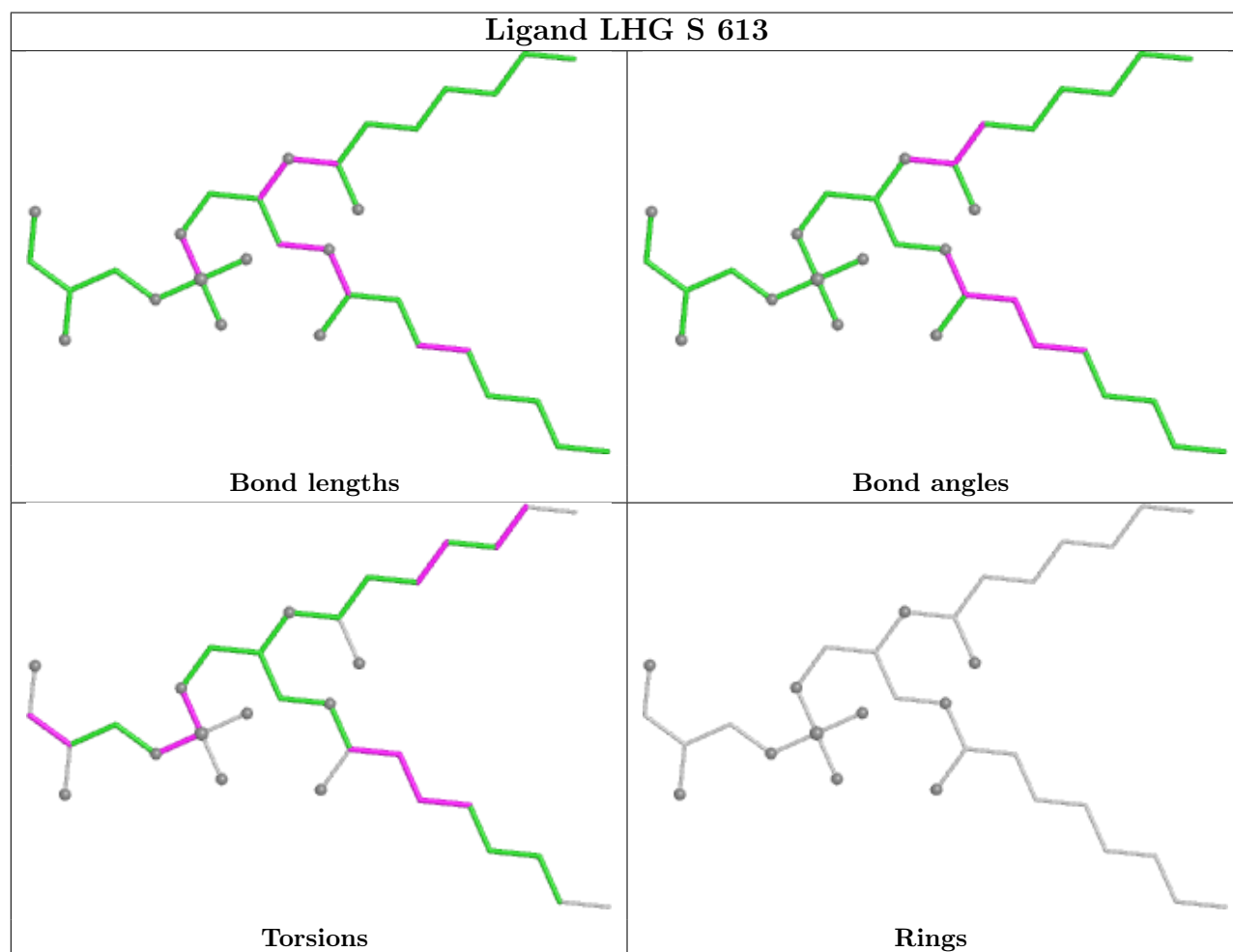
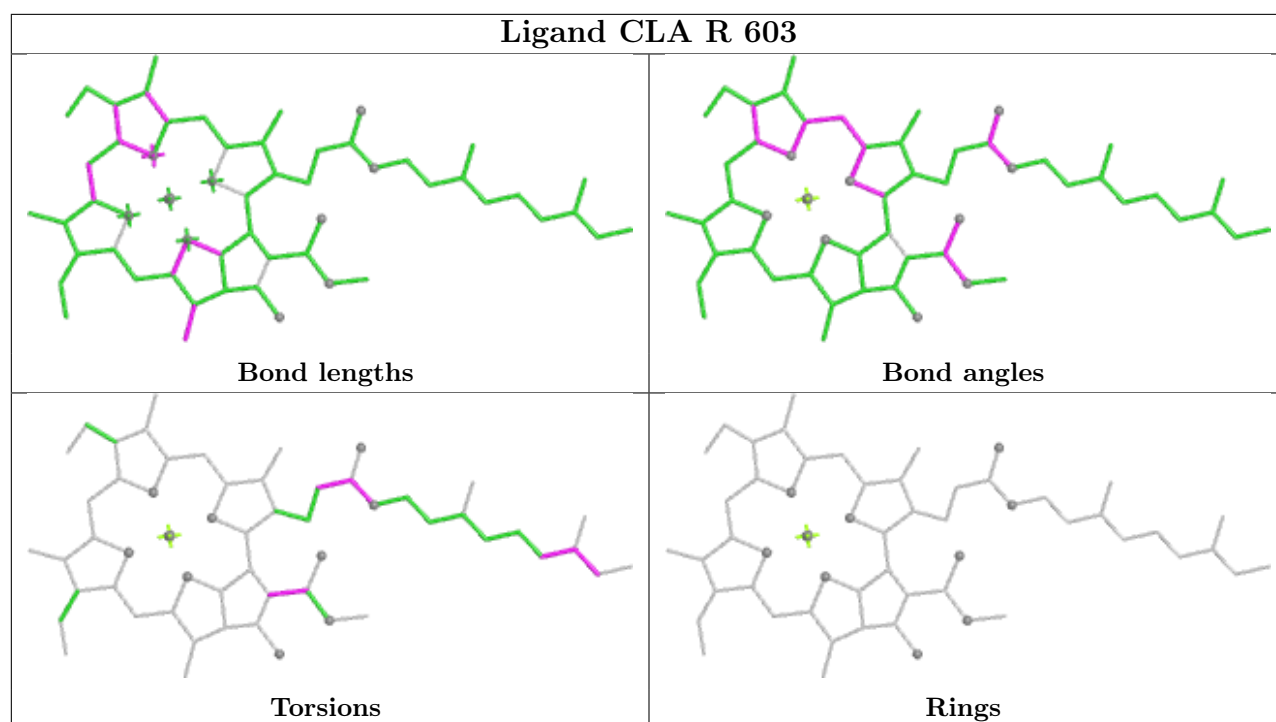


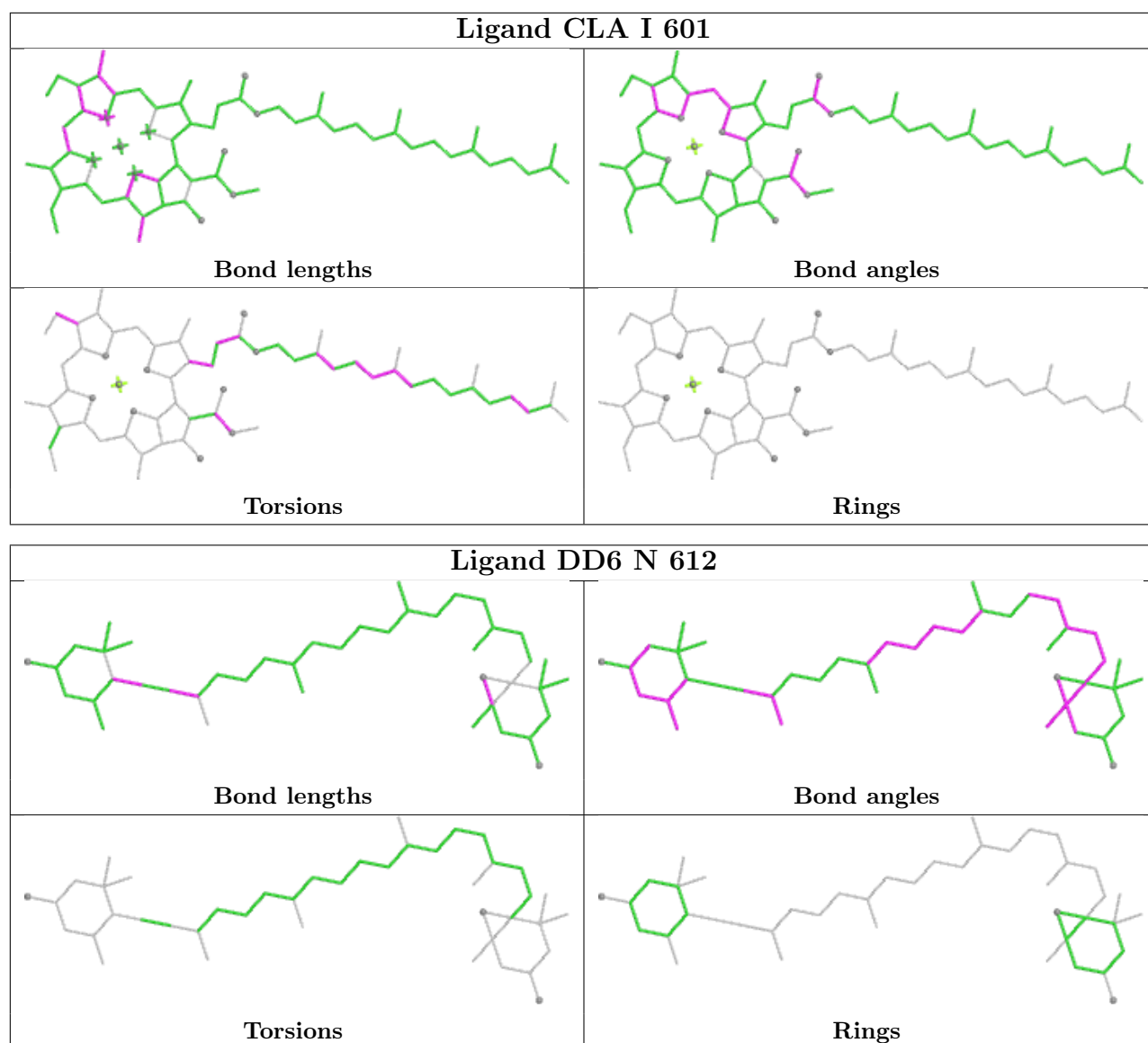


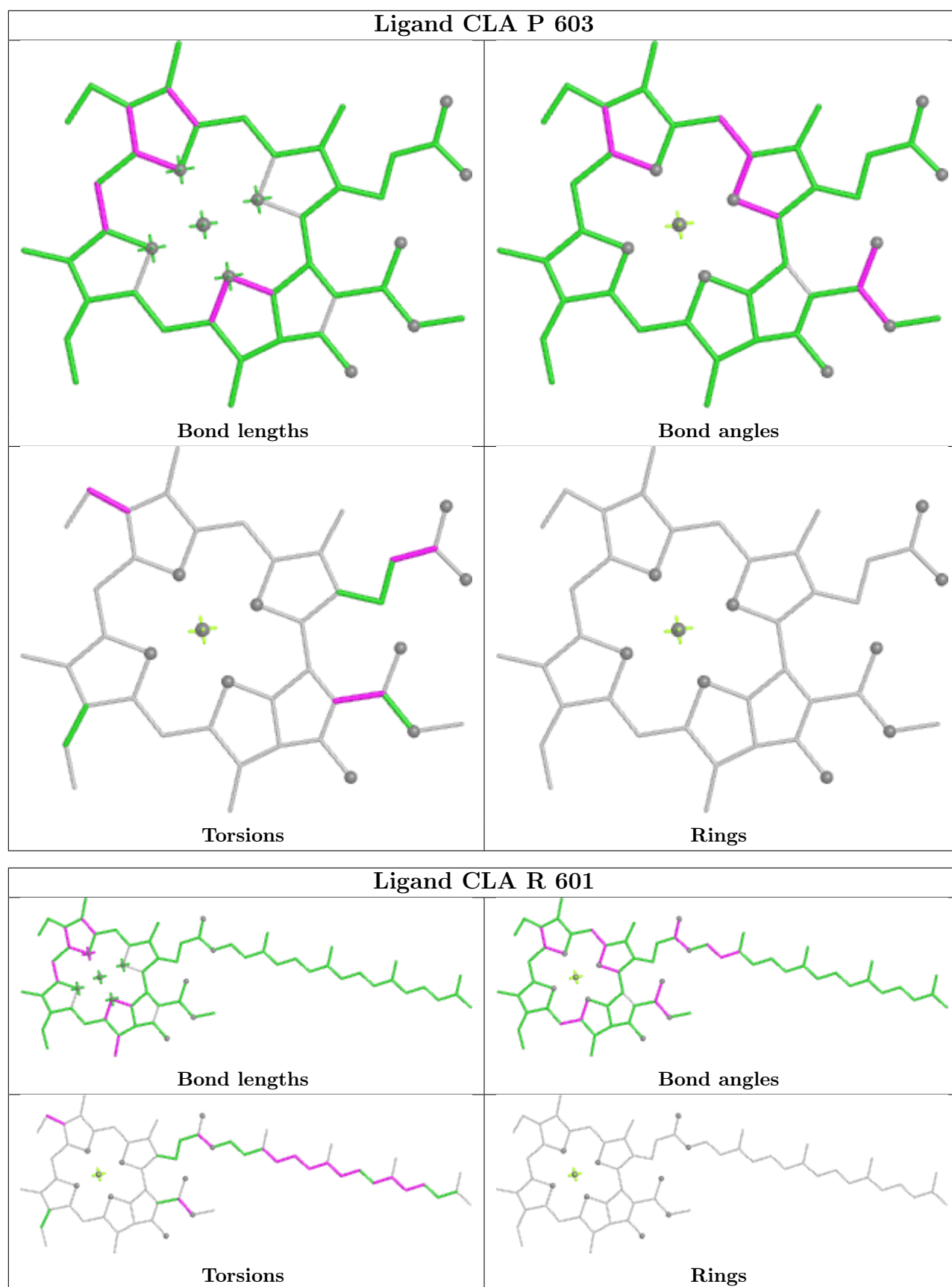




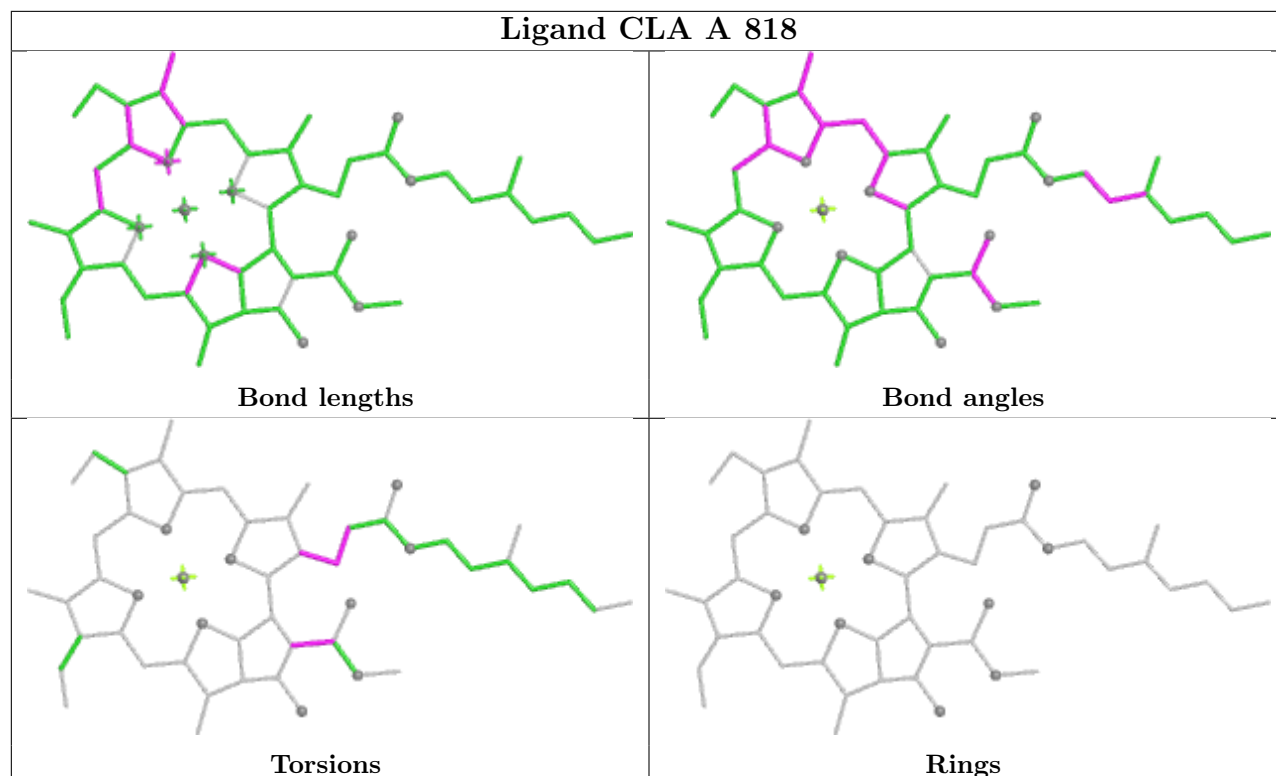




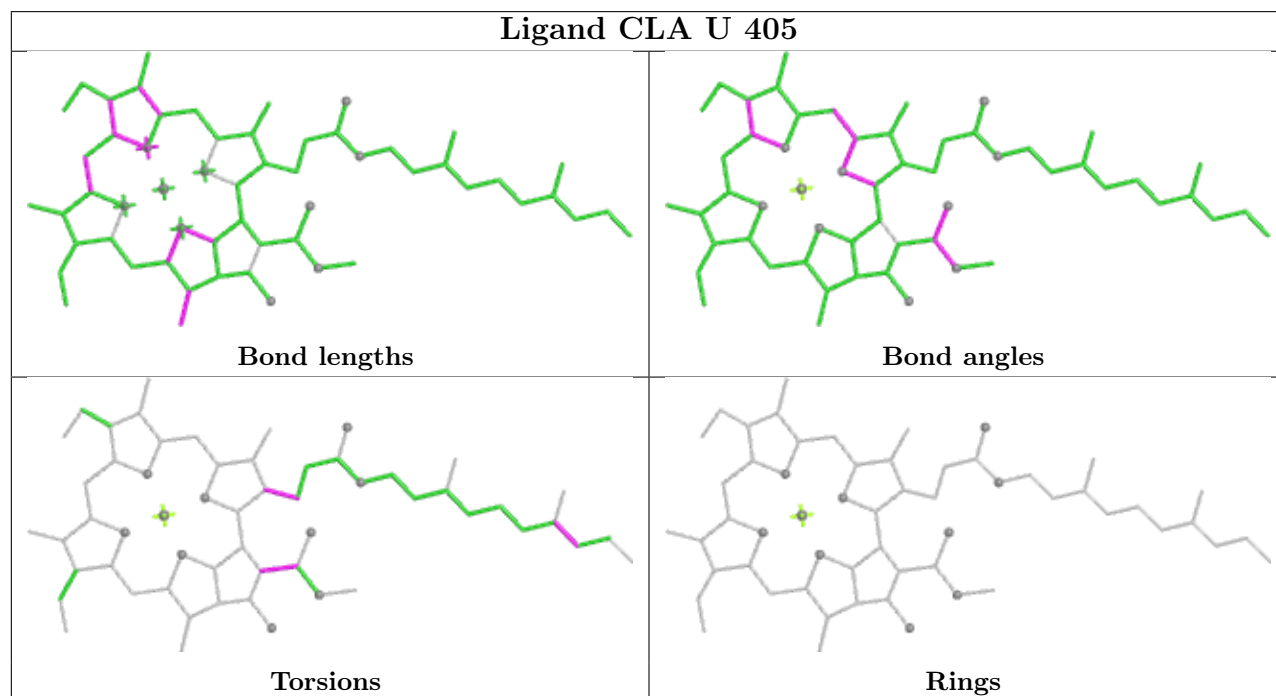


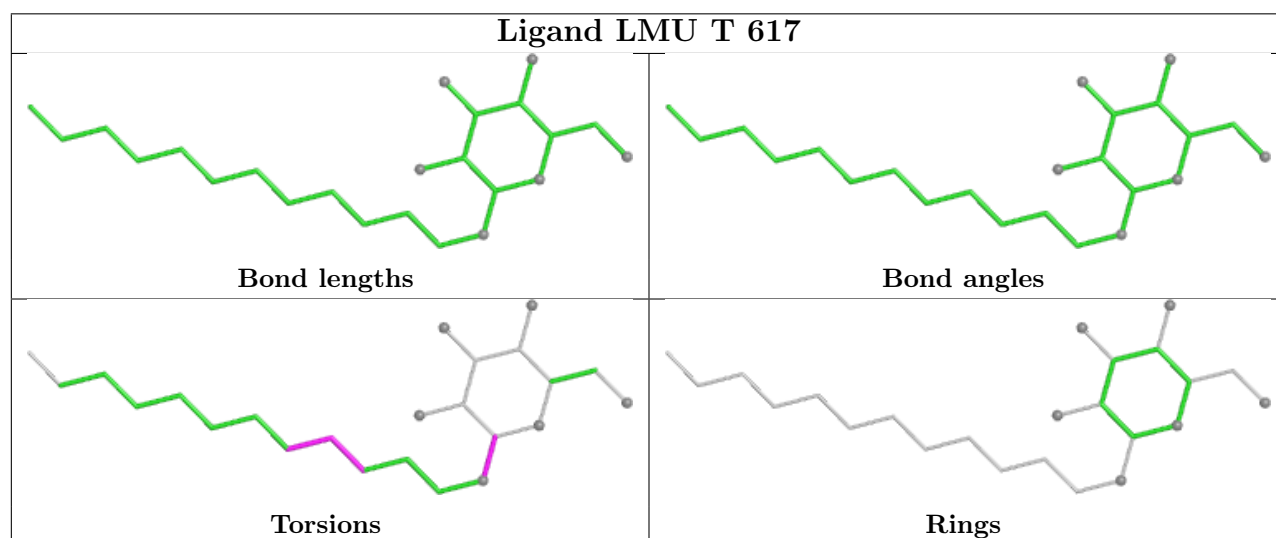
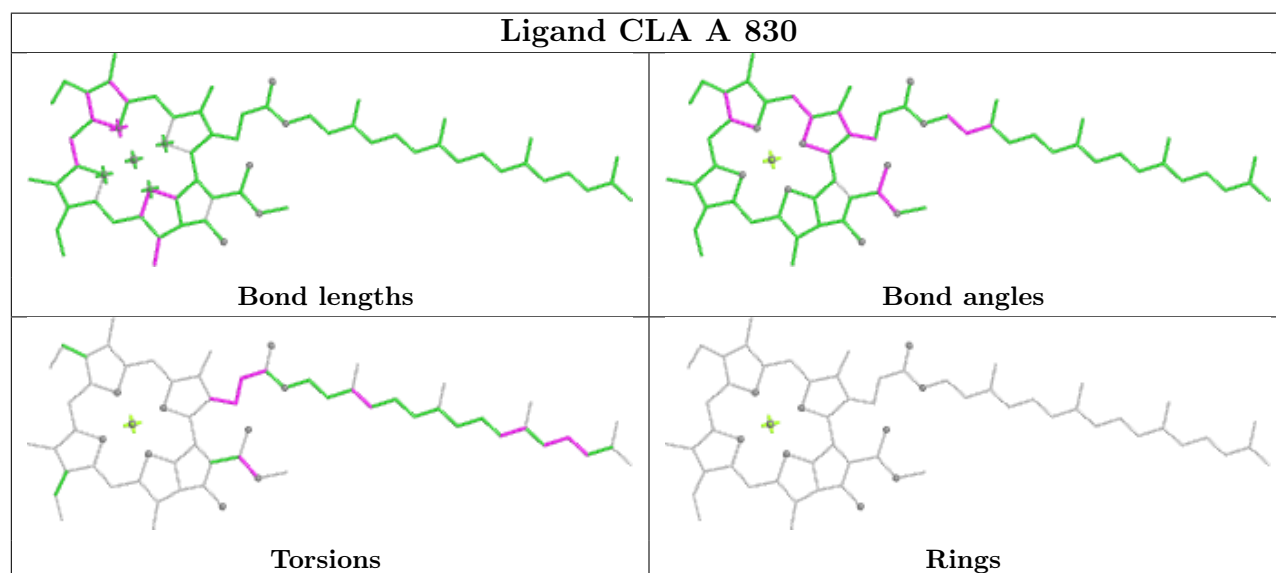
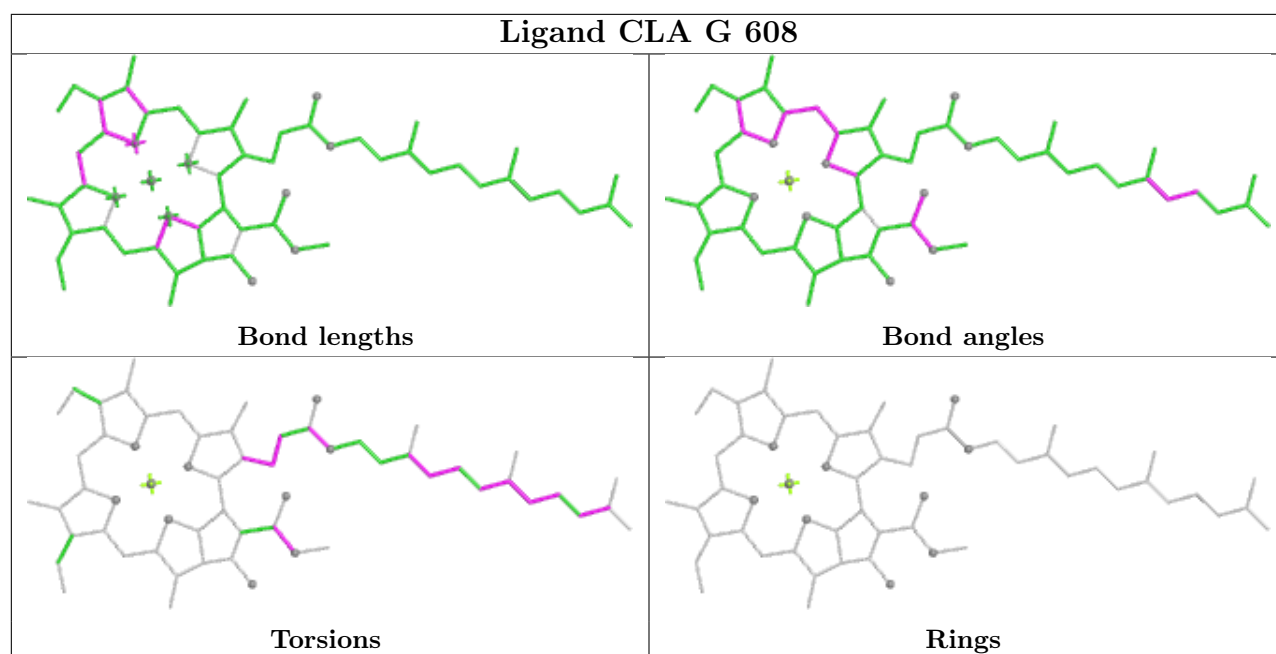


Ligand CLA A 818

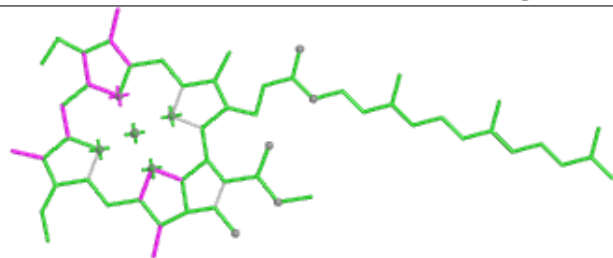


Ligand CLA U 405

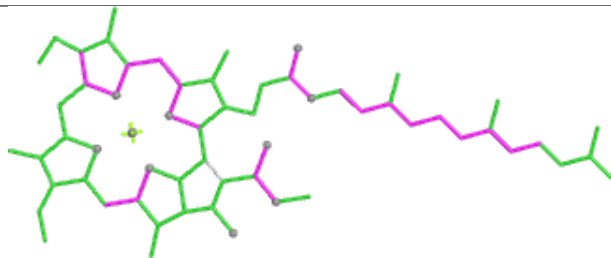




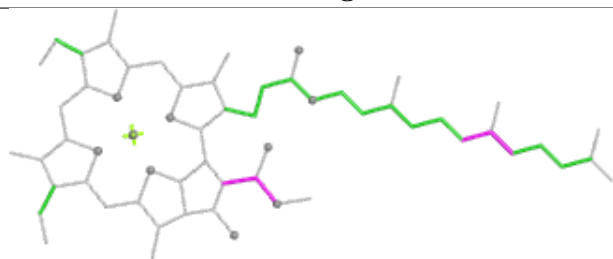
Ligand CLA L 408



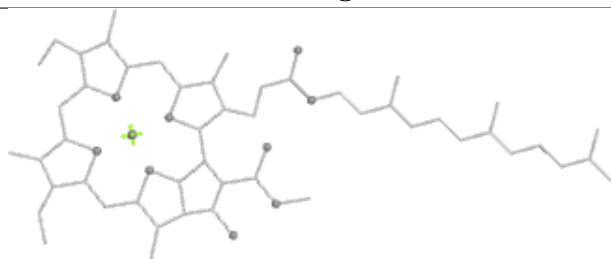
Bond lengths



Bond angles

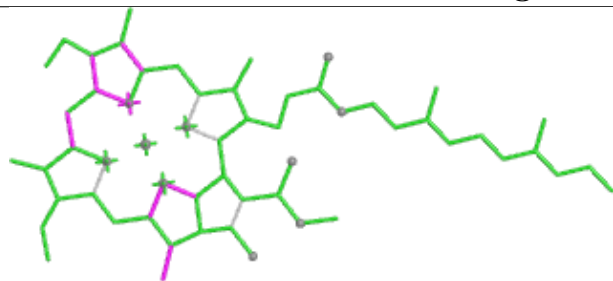


Torsions

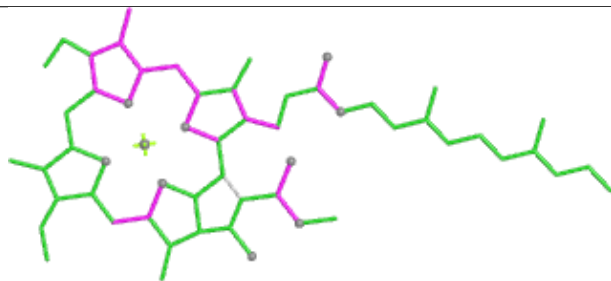


Rings

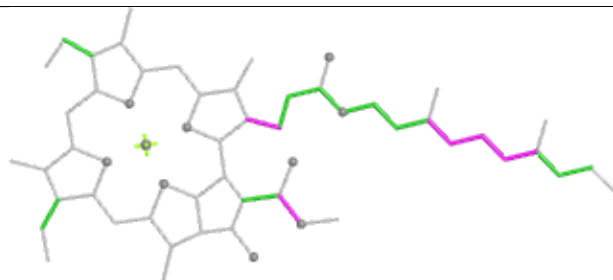
Ligand CLA A 811



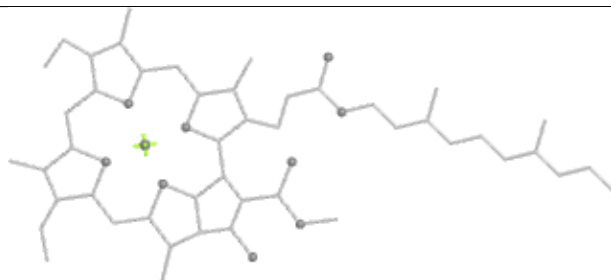
Bond lengths



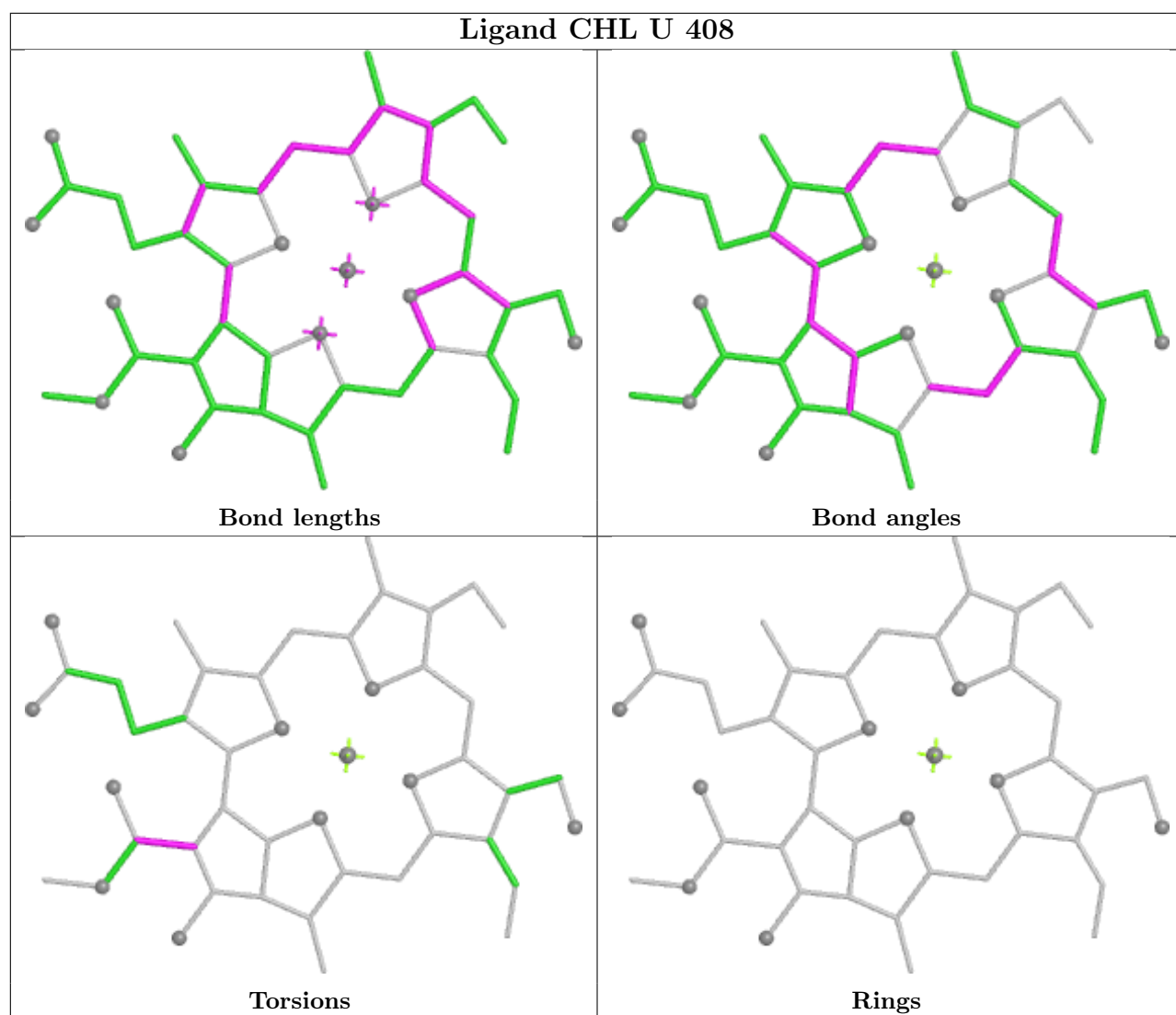
Bond angles

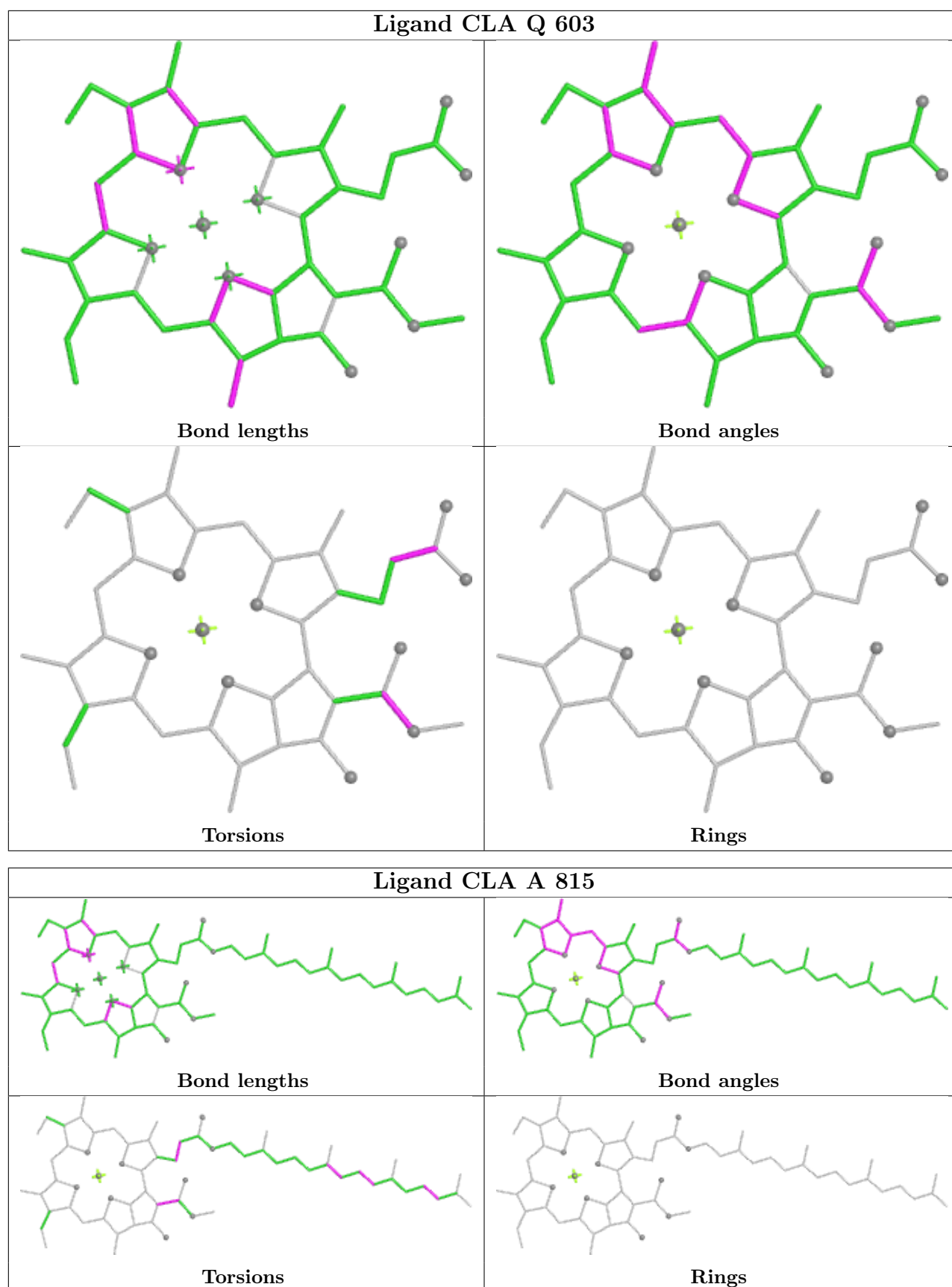


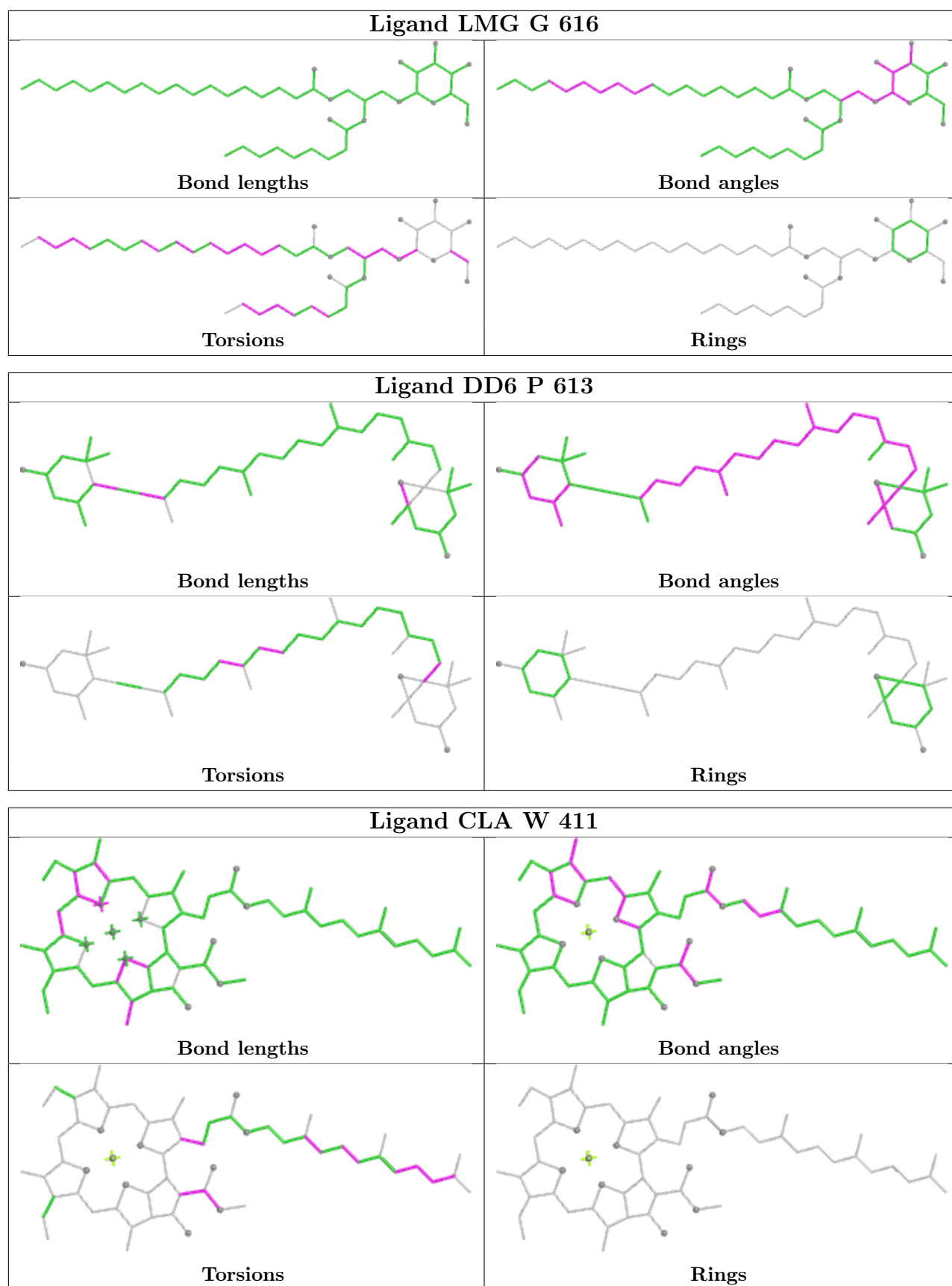
Torsions

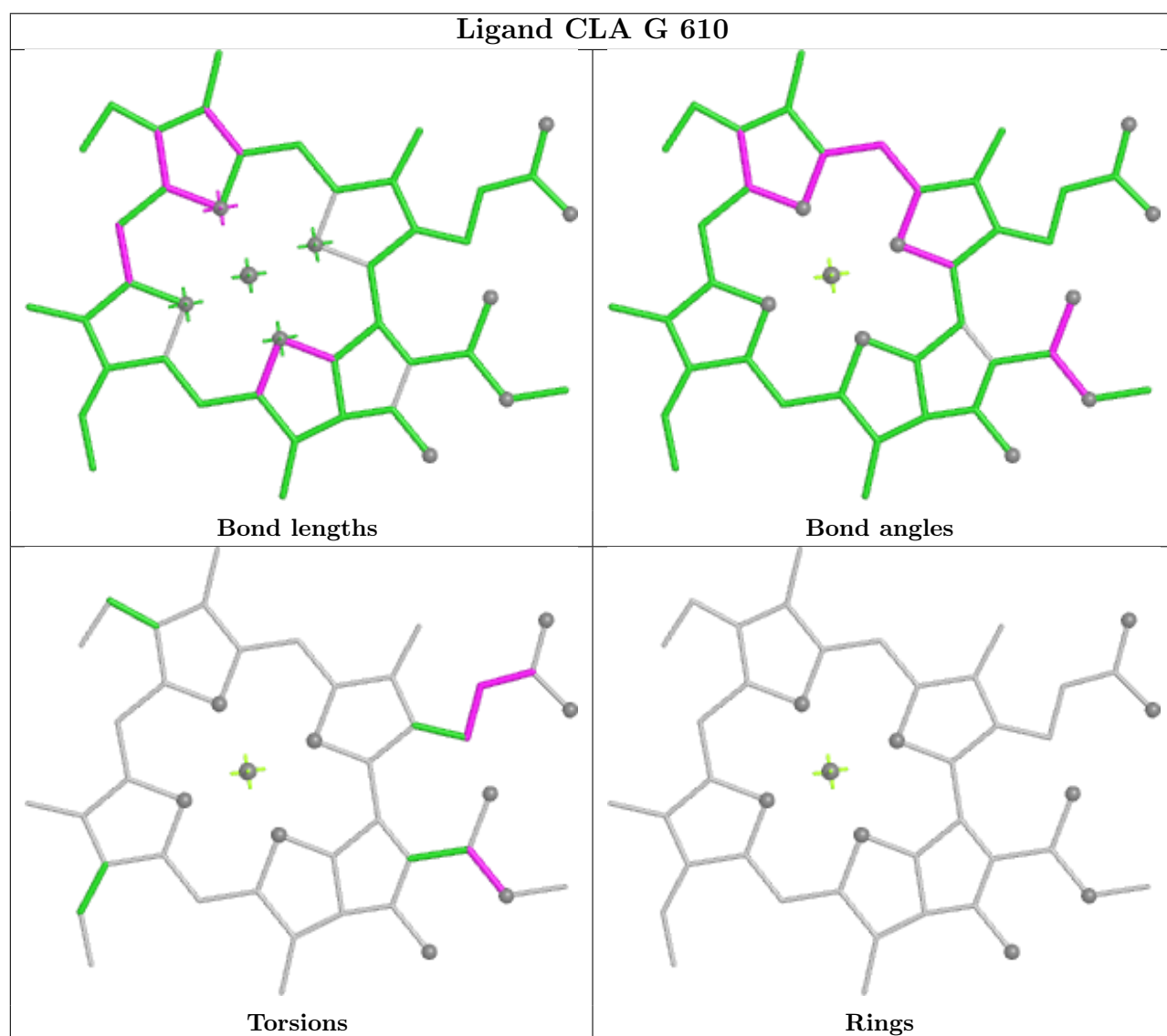
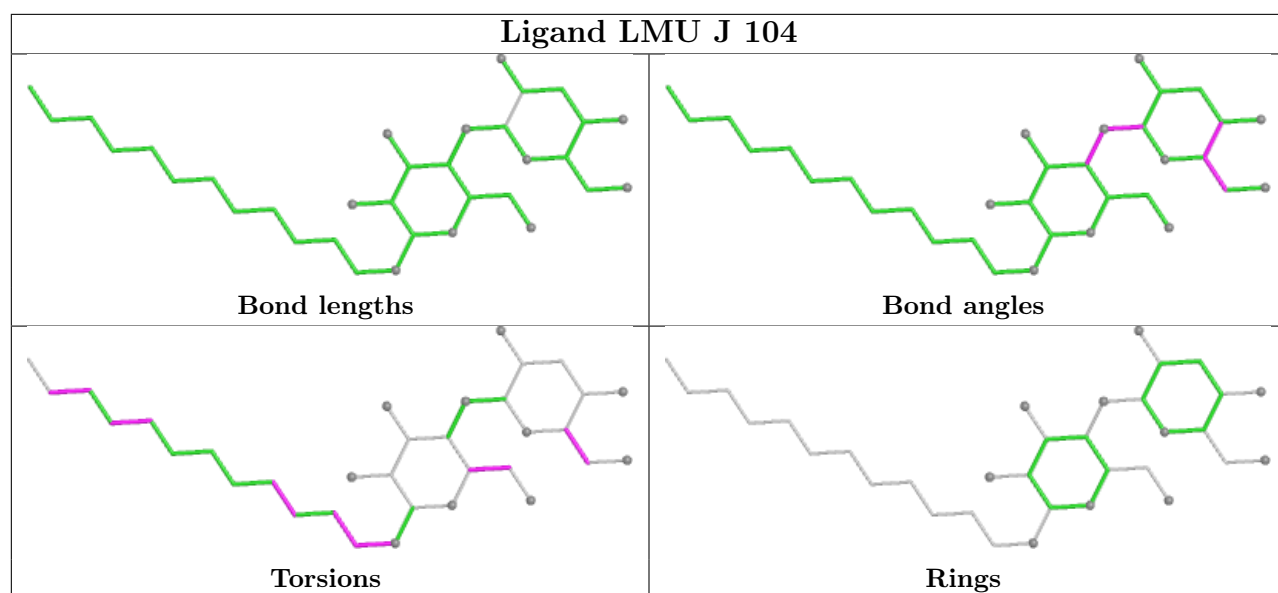


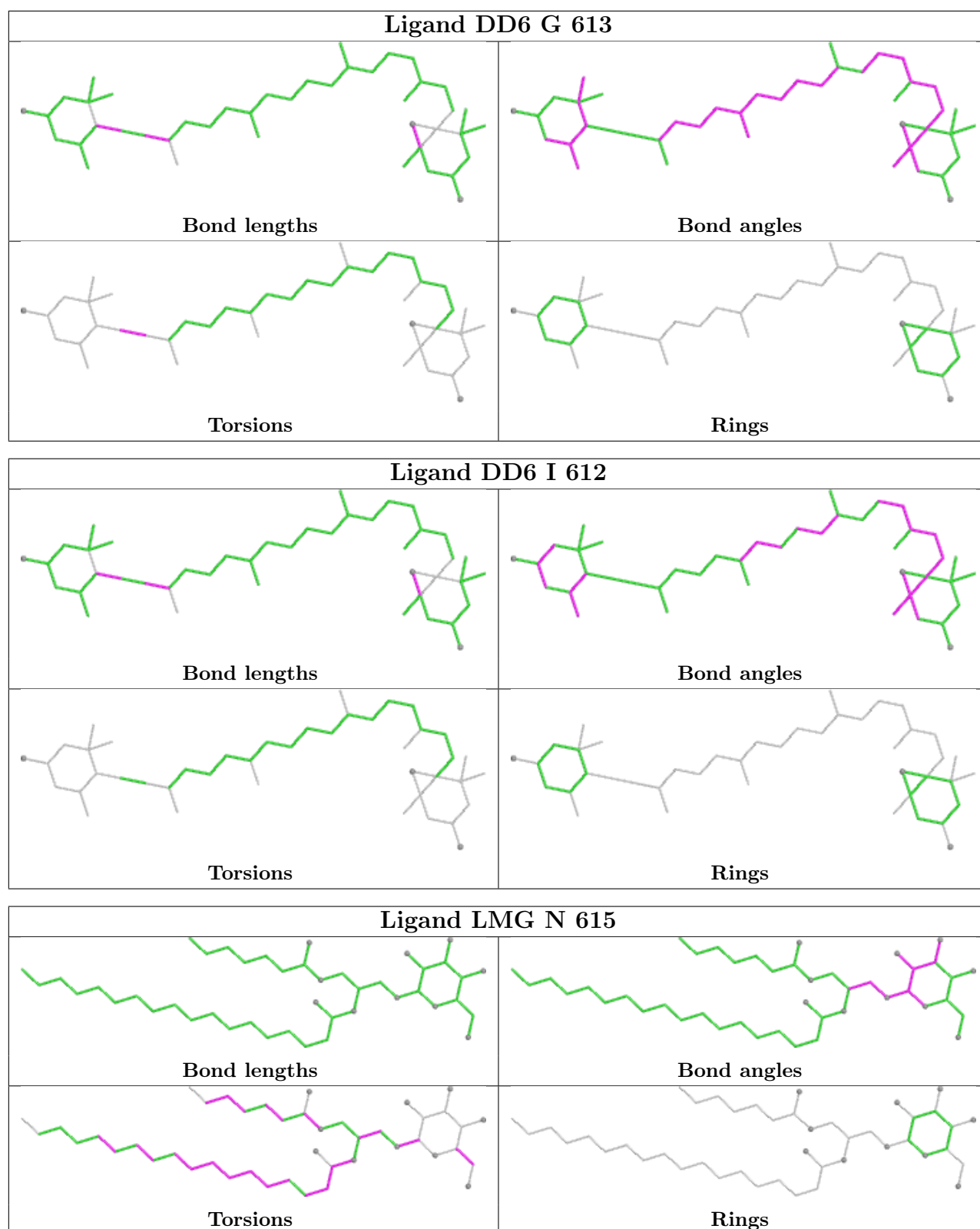
Rings

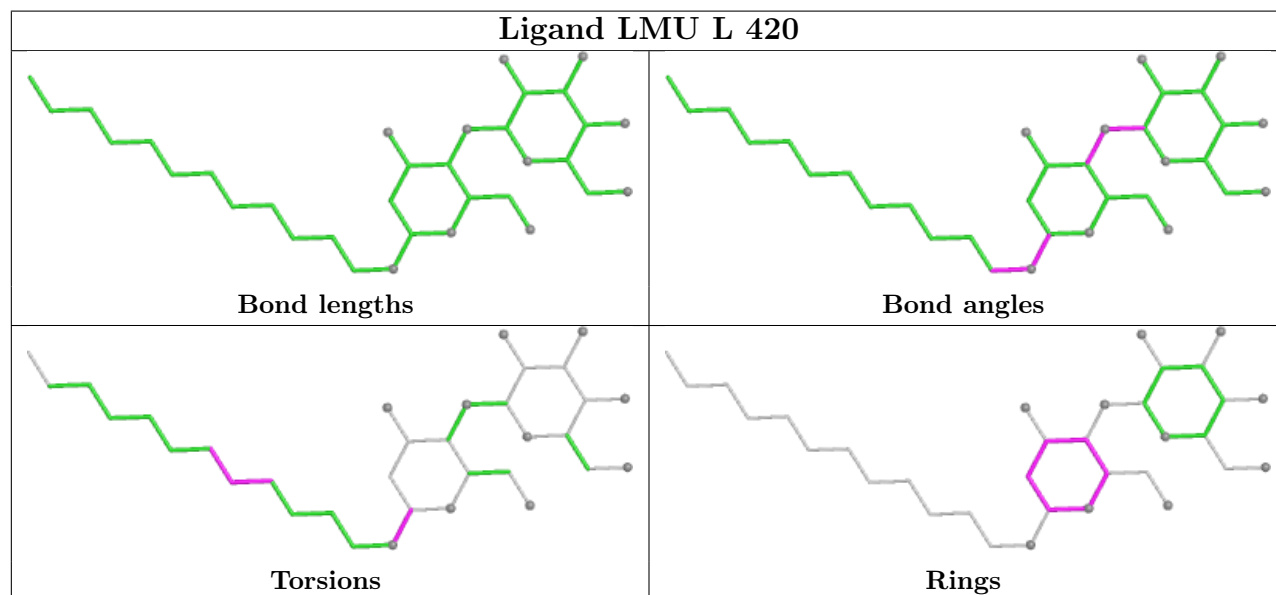
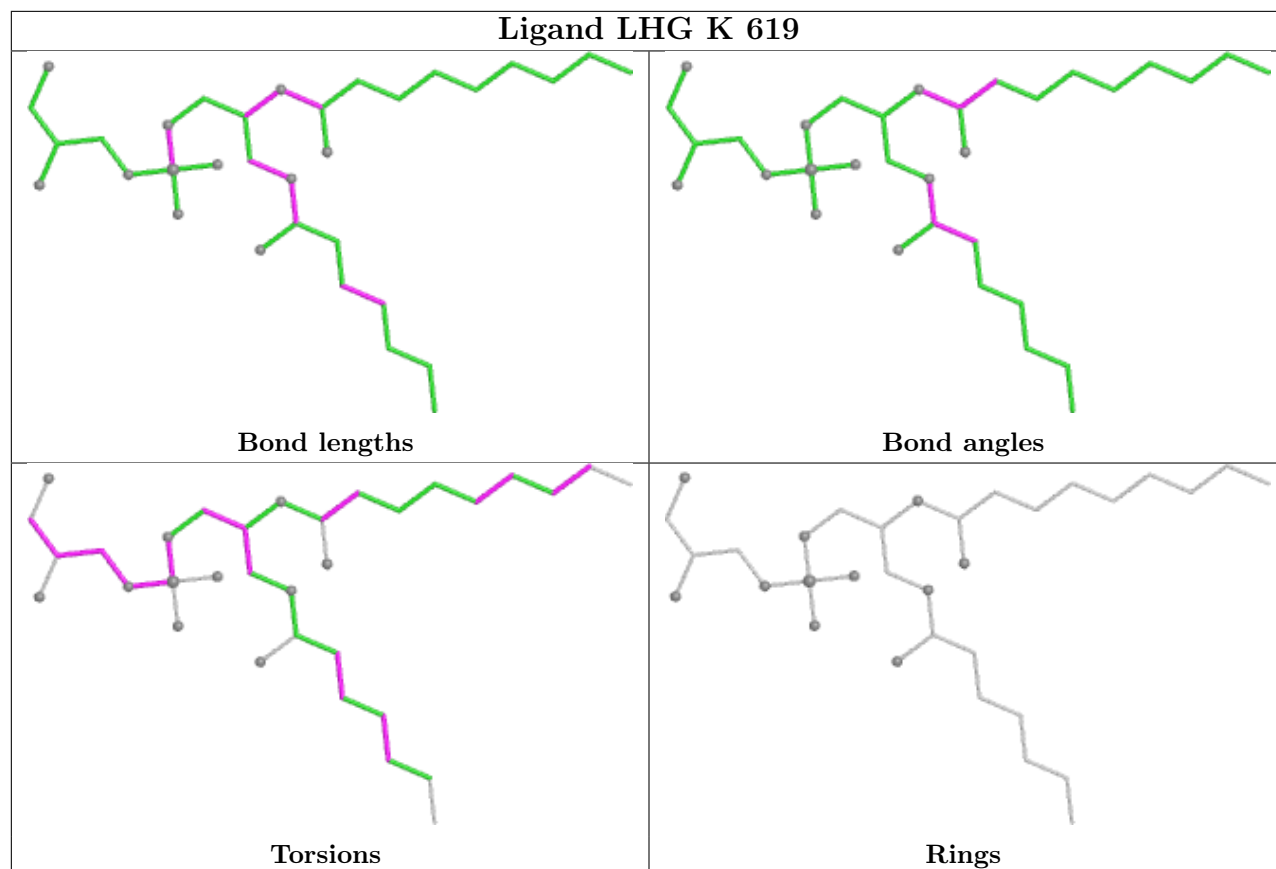


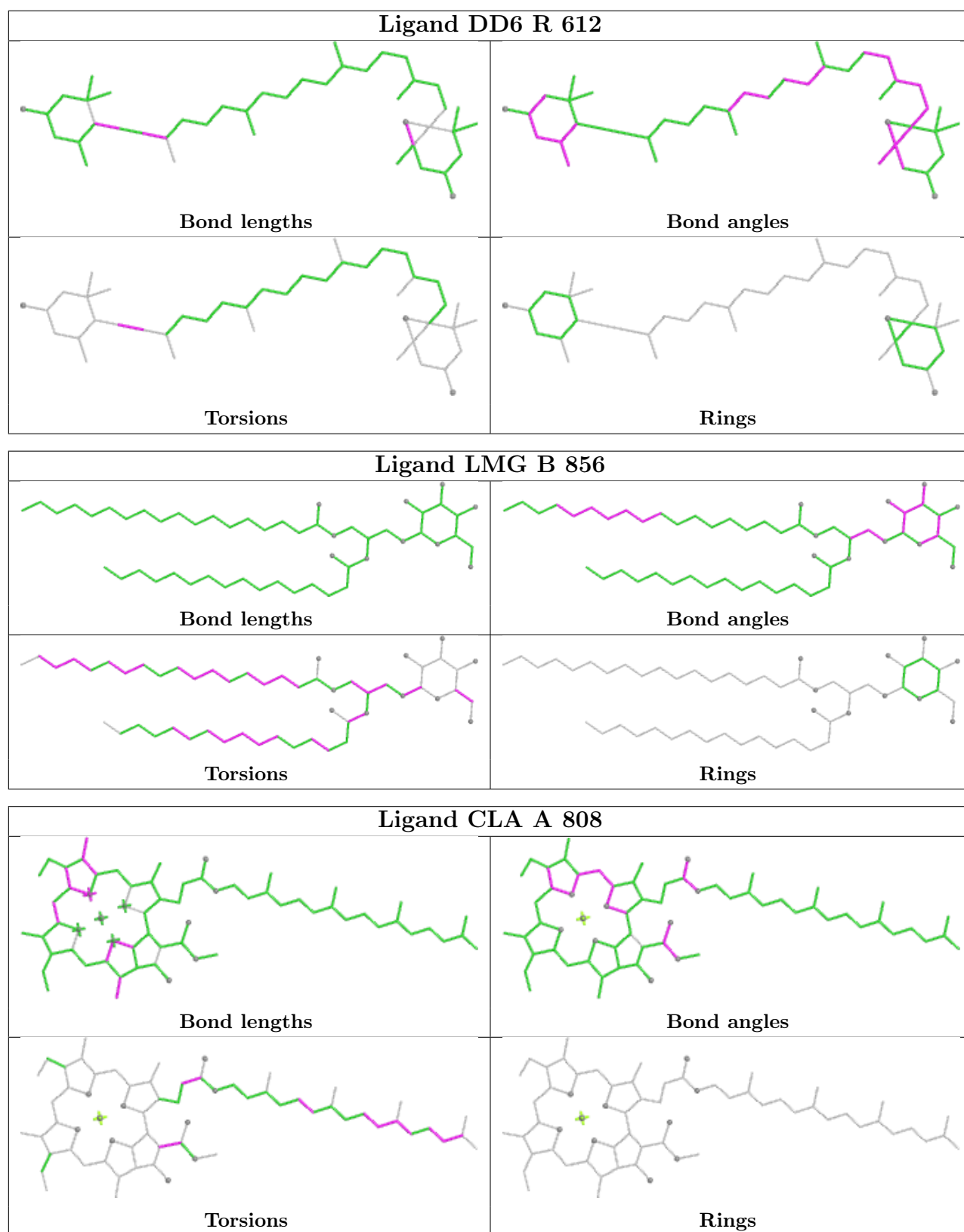


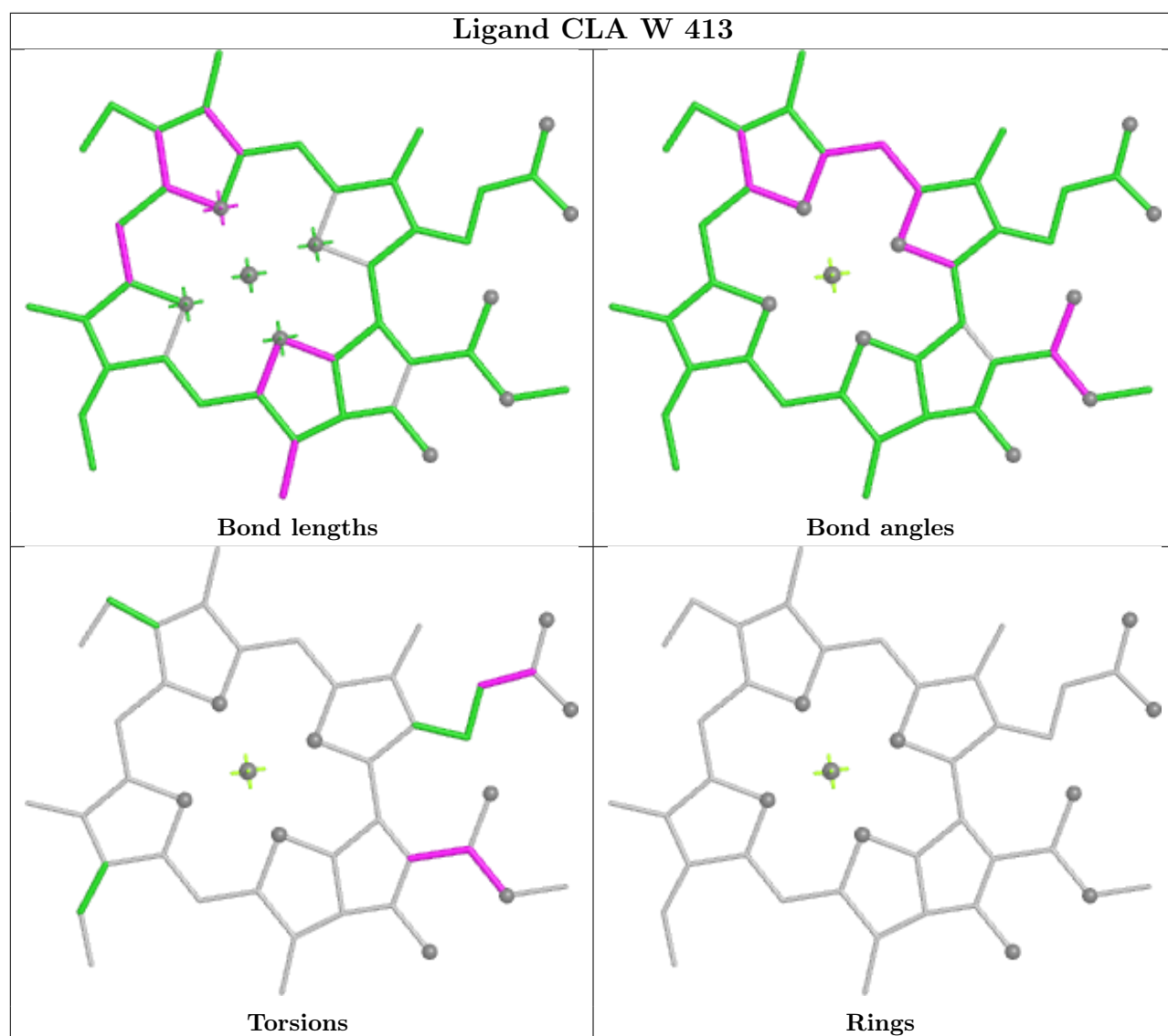


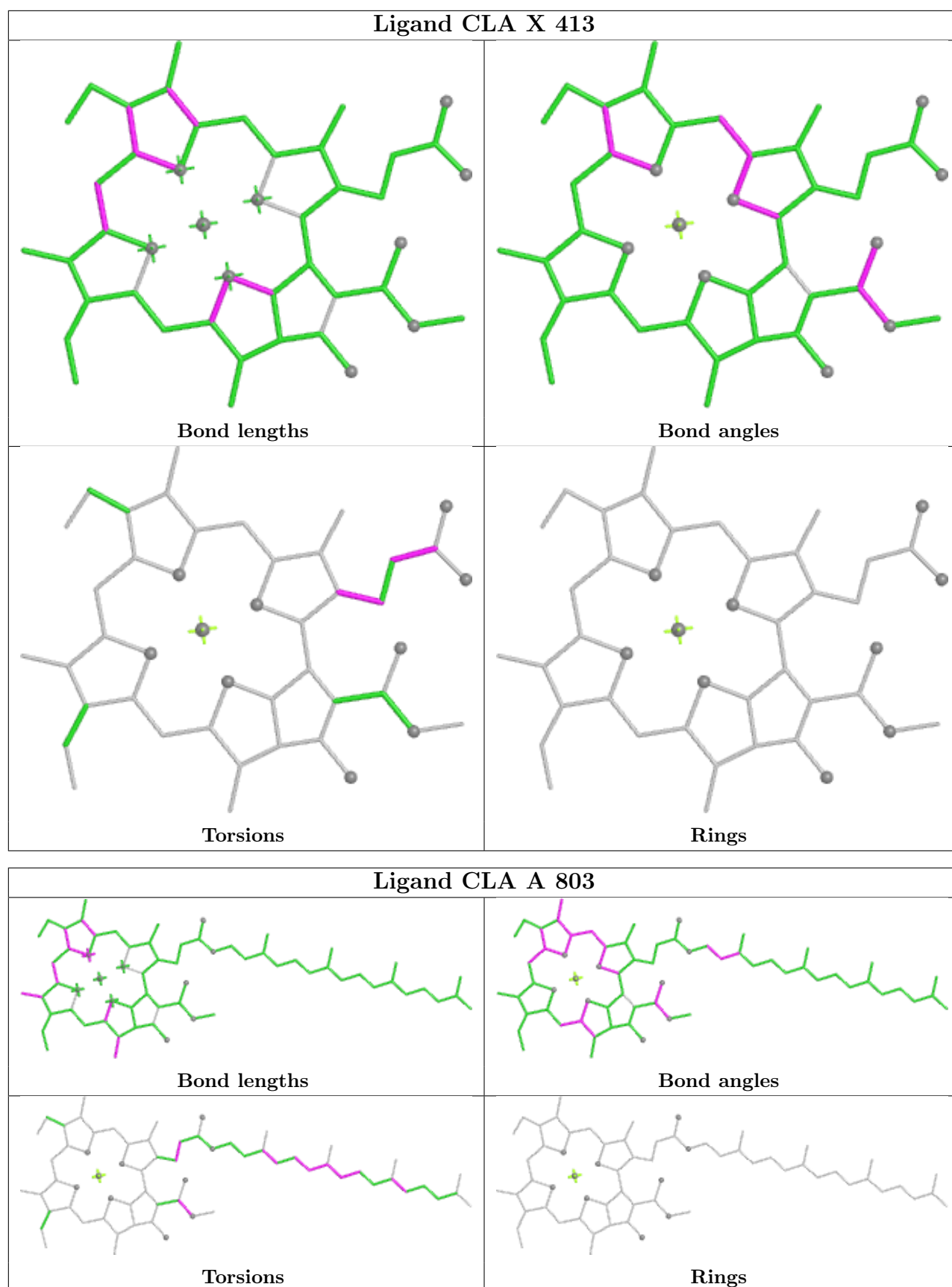


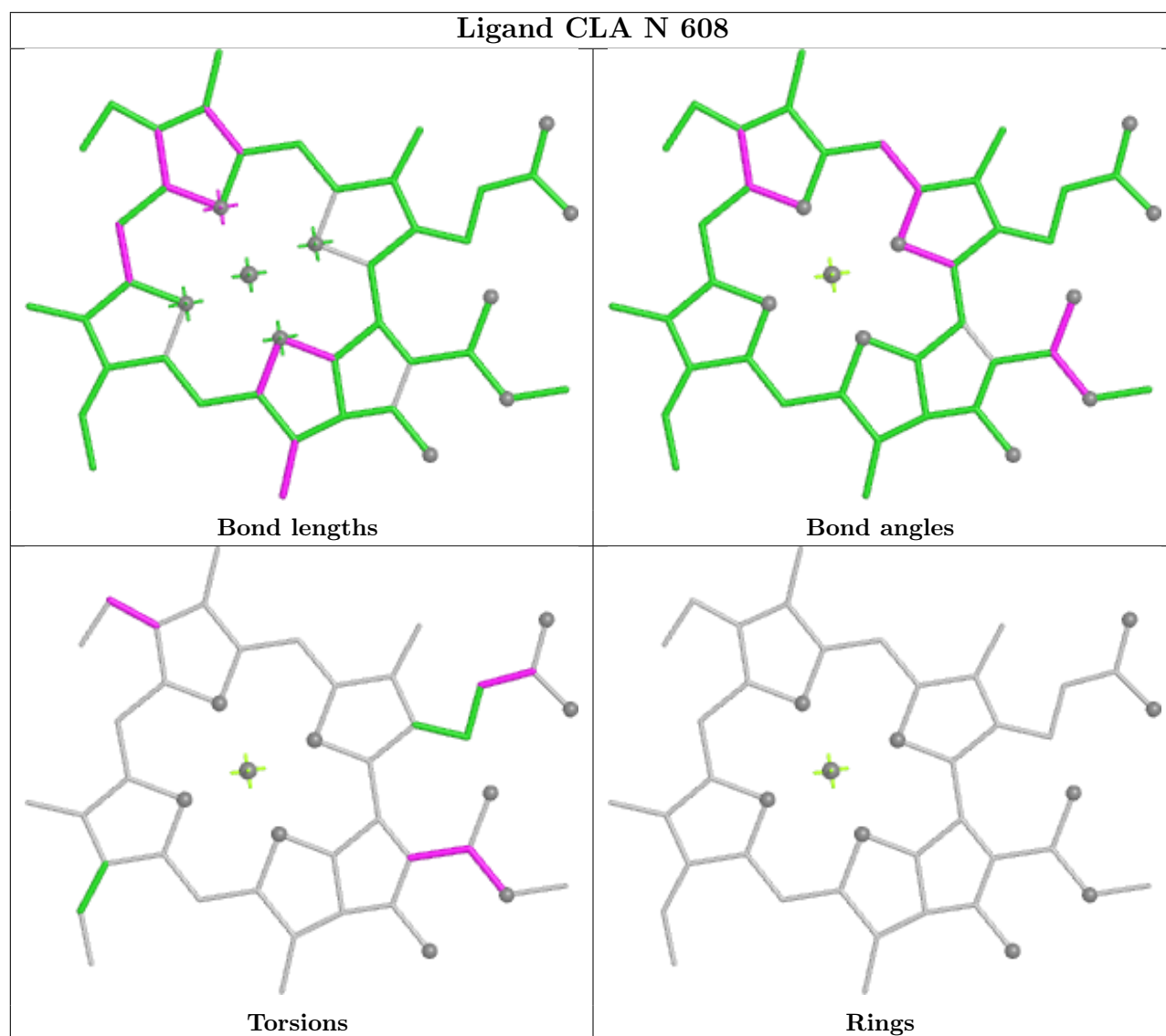
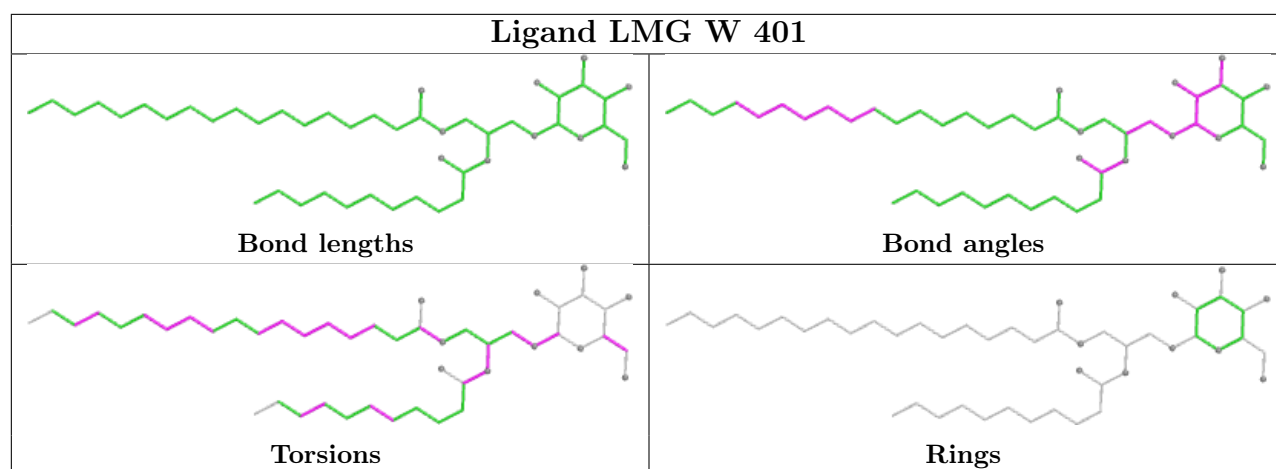




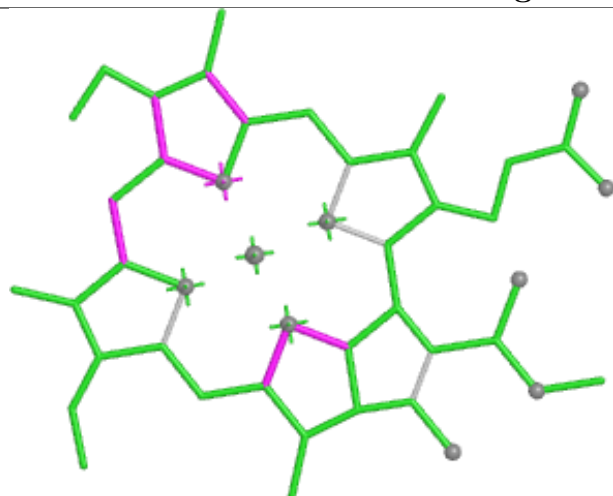




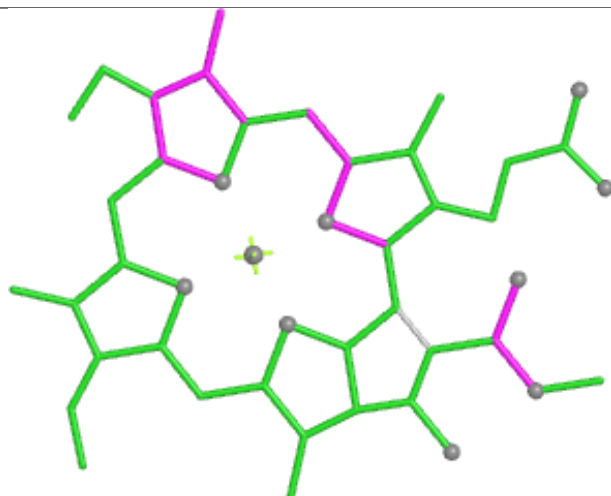




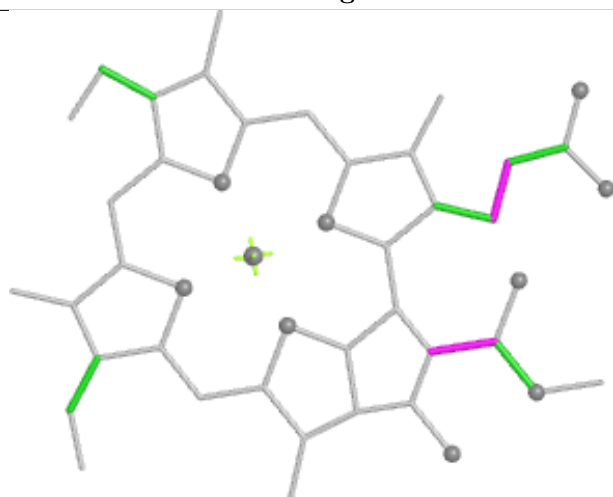
Ligand CLA B 811



Bond lengths



Bond angles

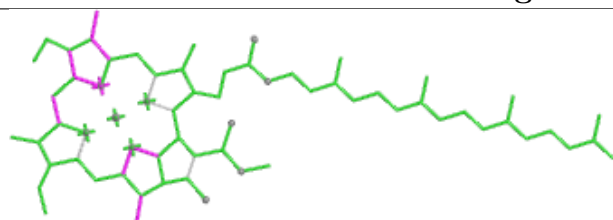


Torsions

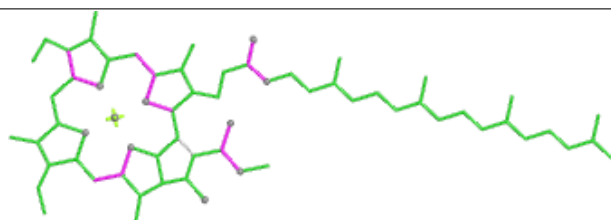


Rings

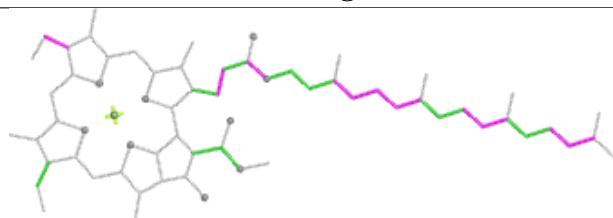
Ligand CLA T 605



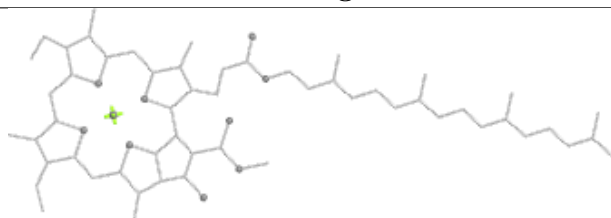
Bond lengths



Bond angles

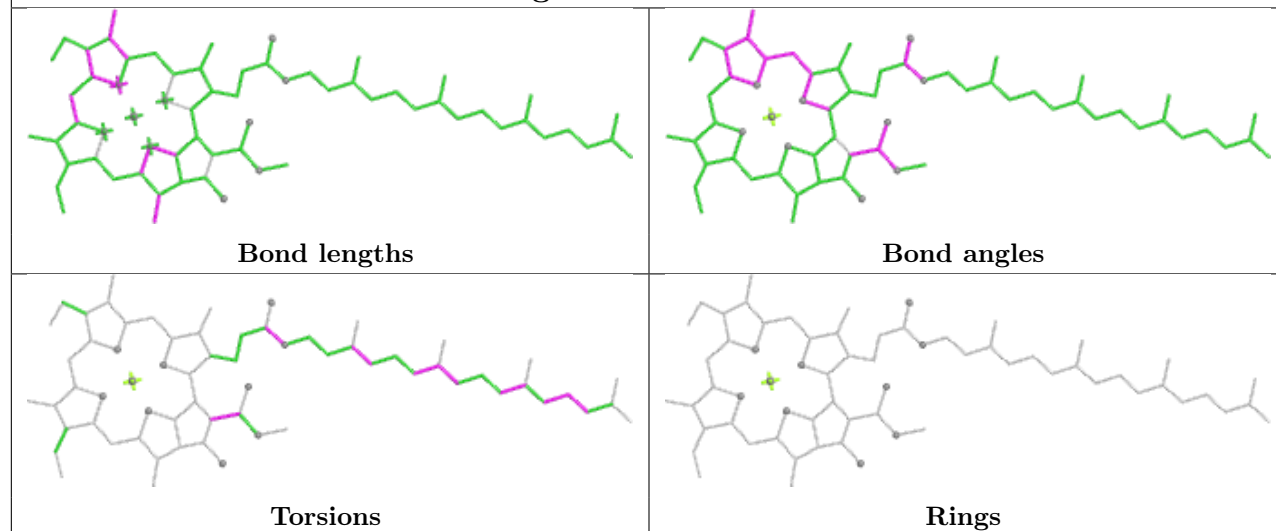


Torsions

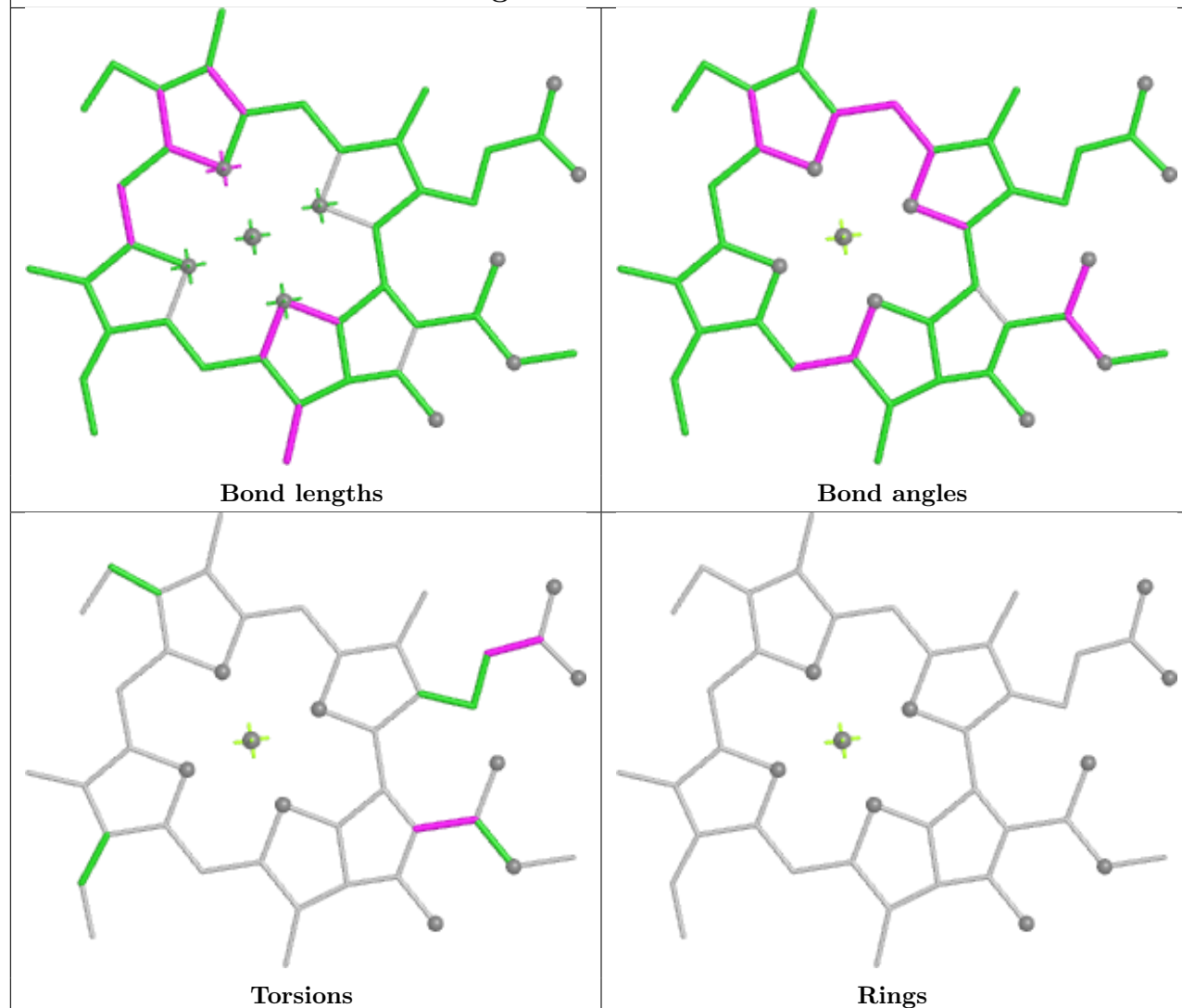


Rings

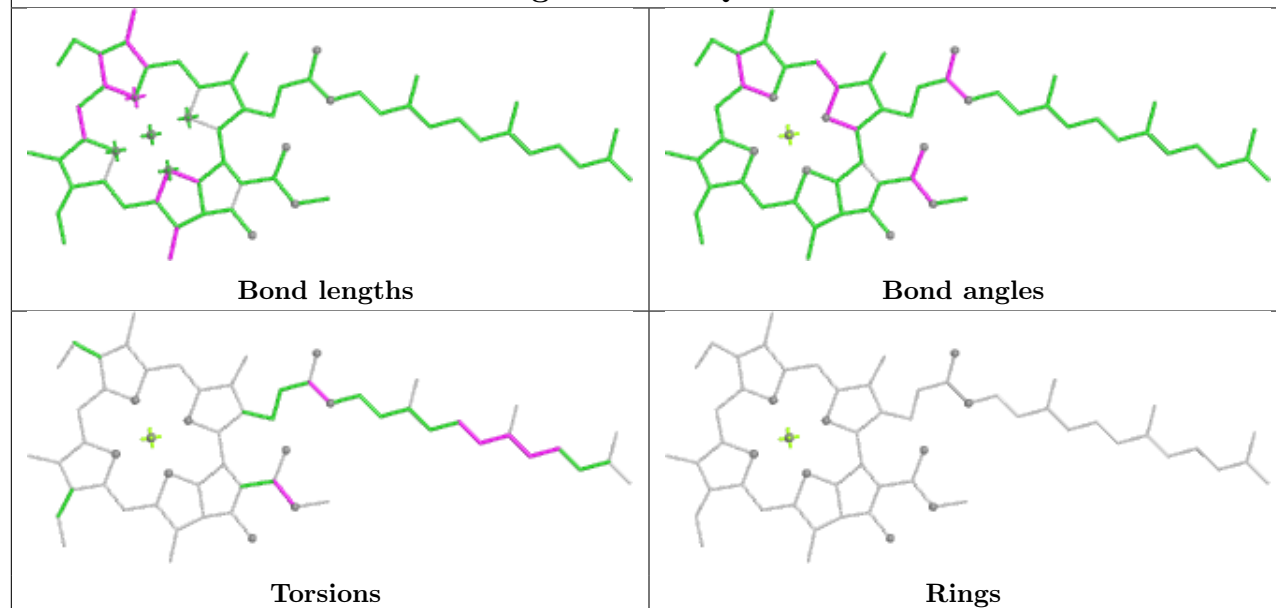
Ligand CLA B 828



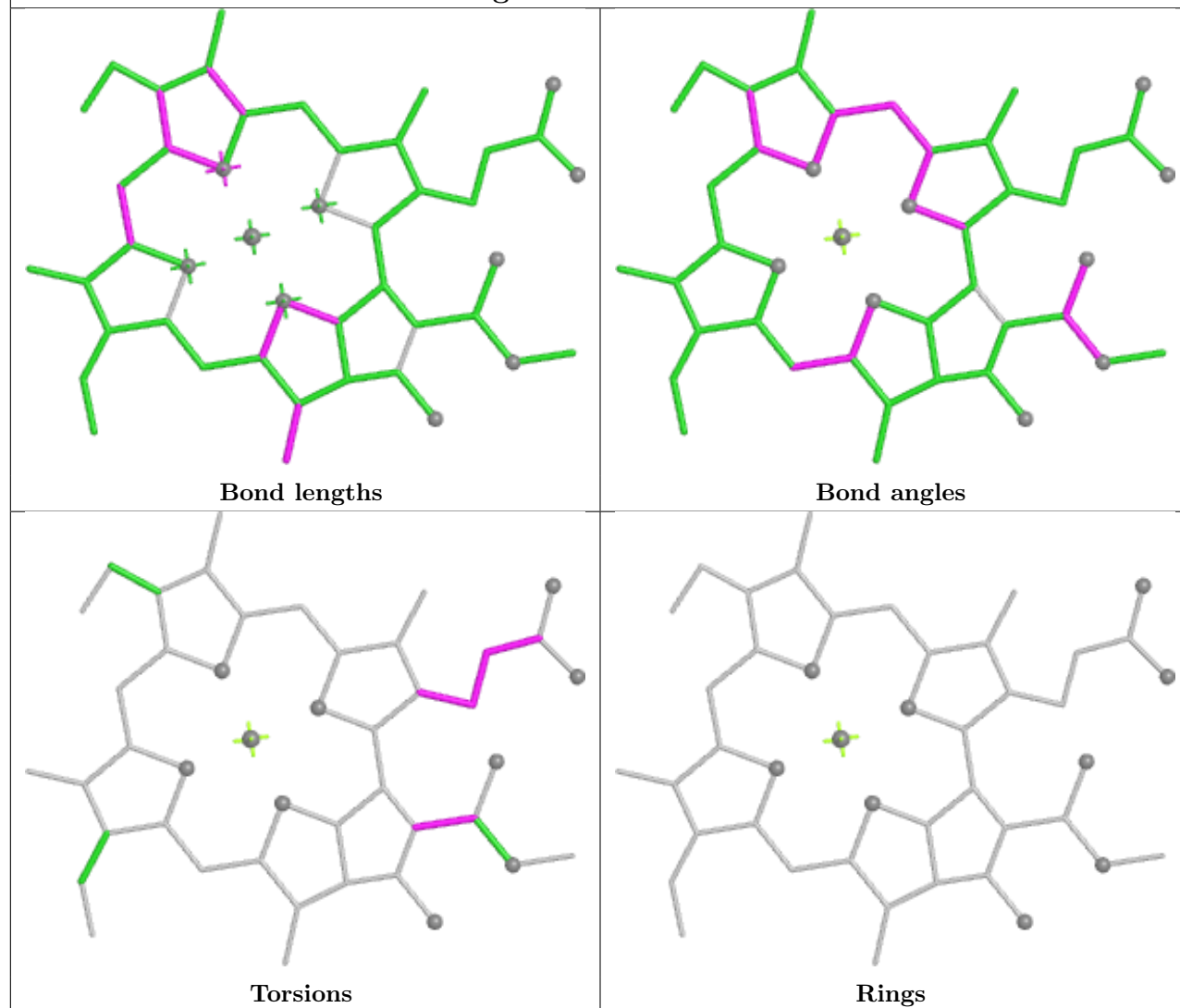
Ligand CLA G 609

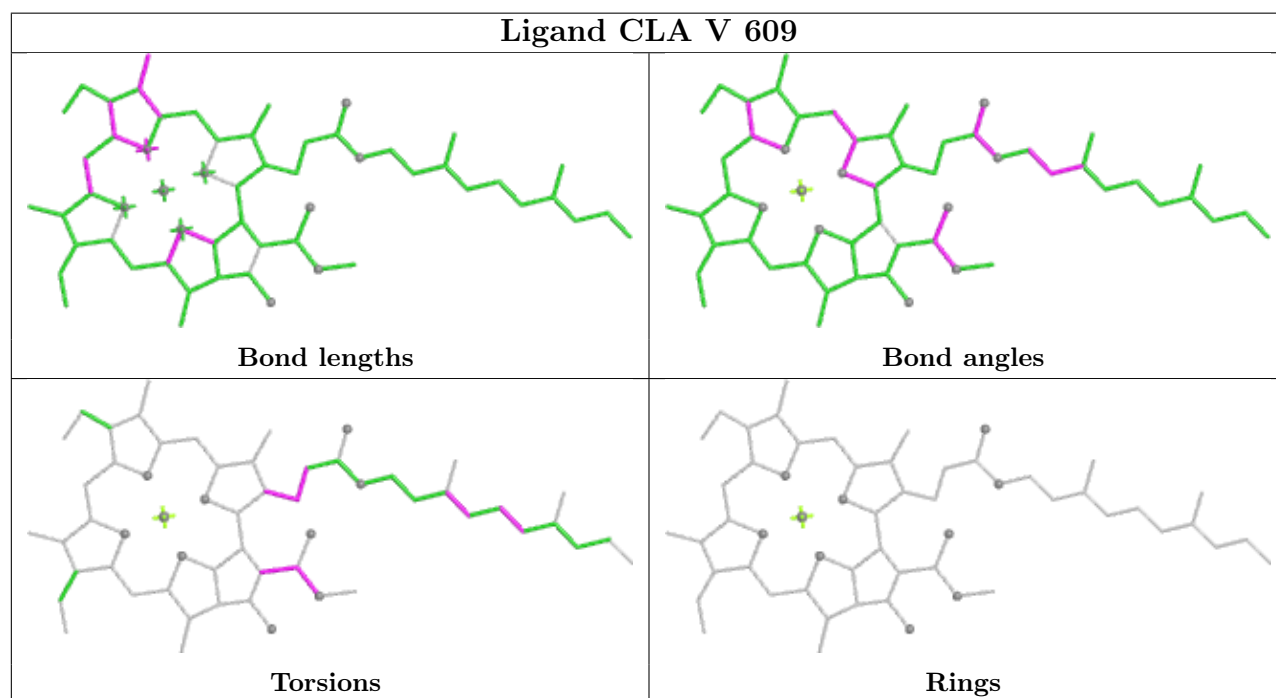
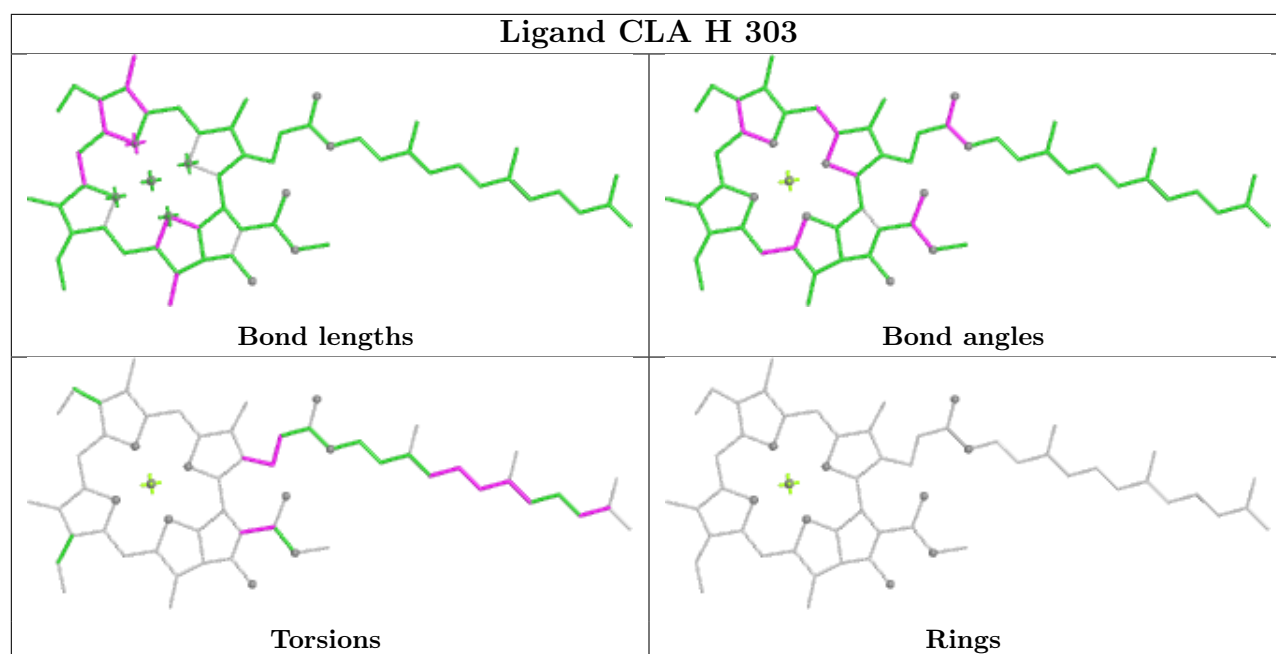


Ligand CLA Q 609

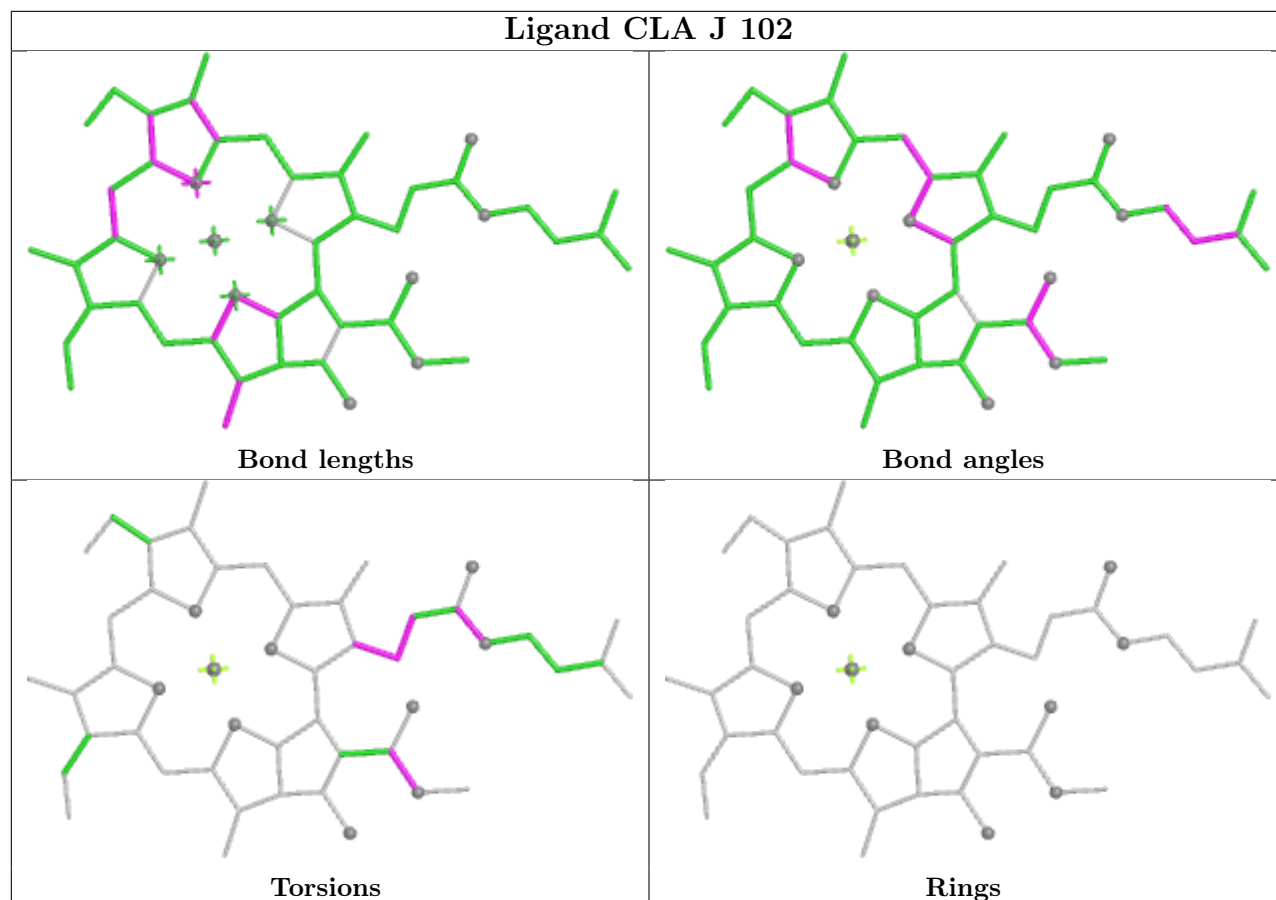


Ligand CLA P 605

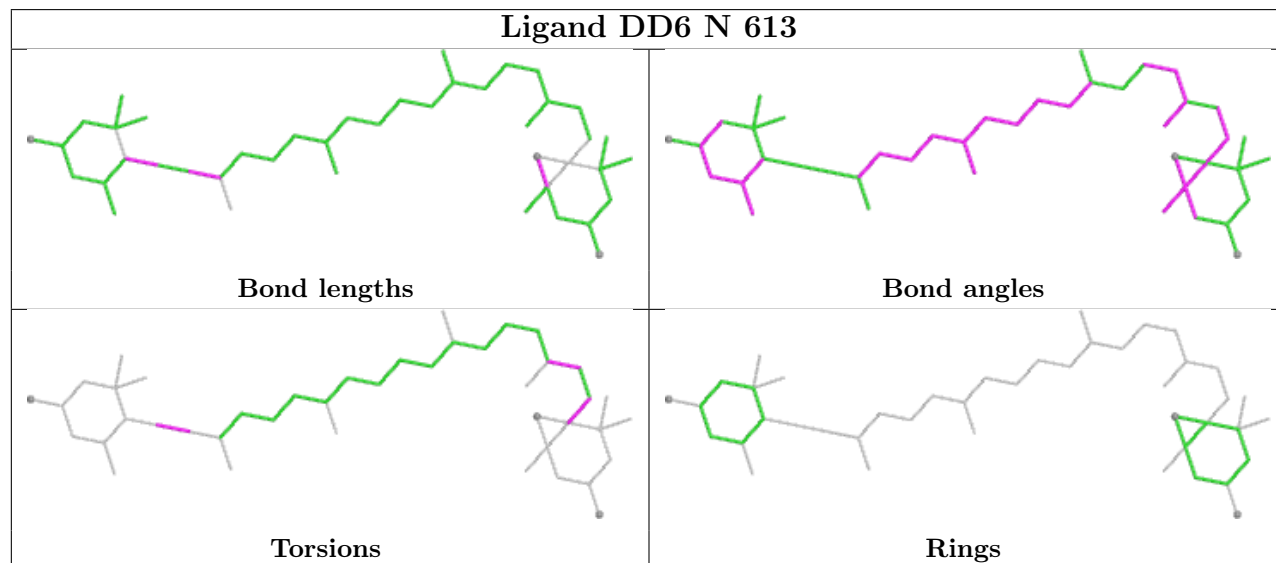


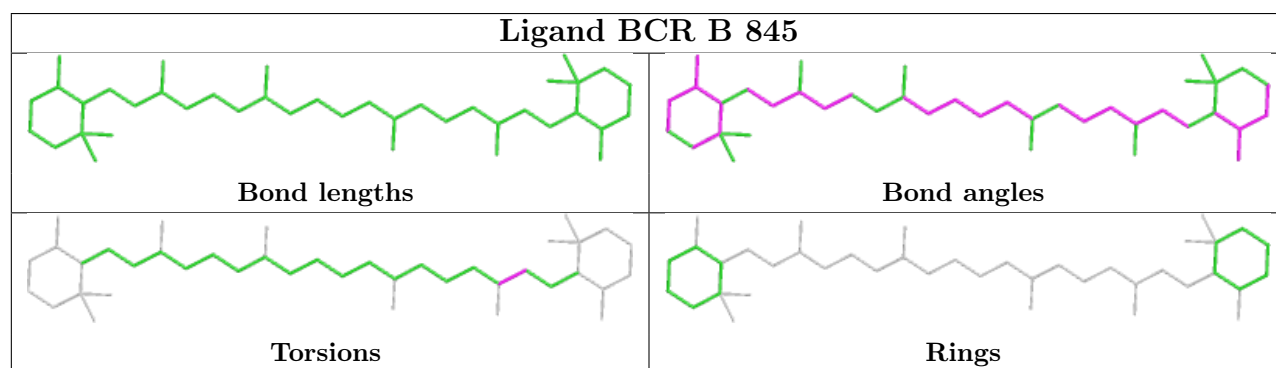
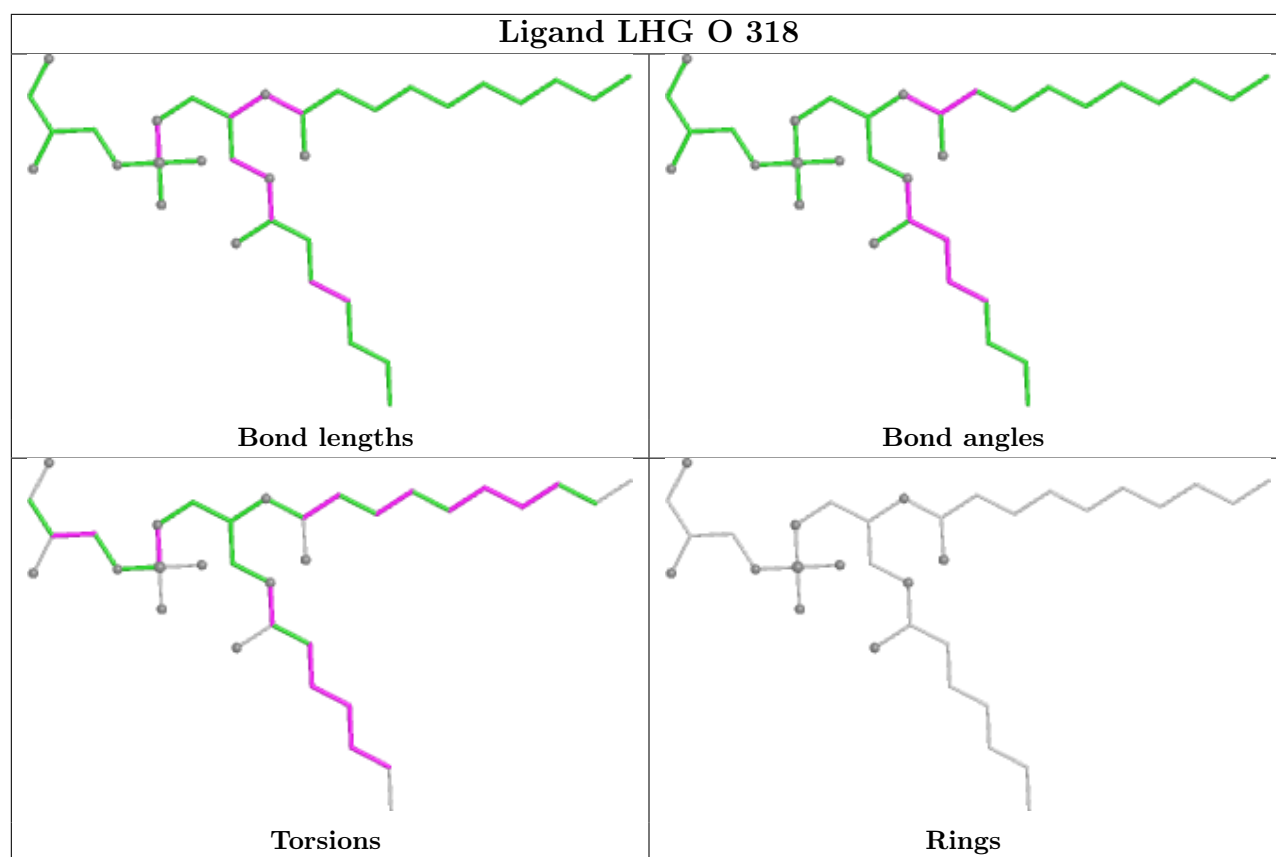


Ligand CLA J 102

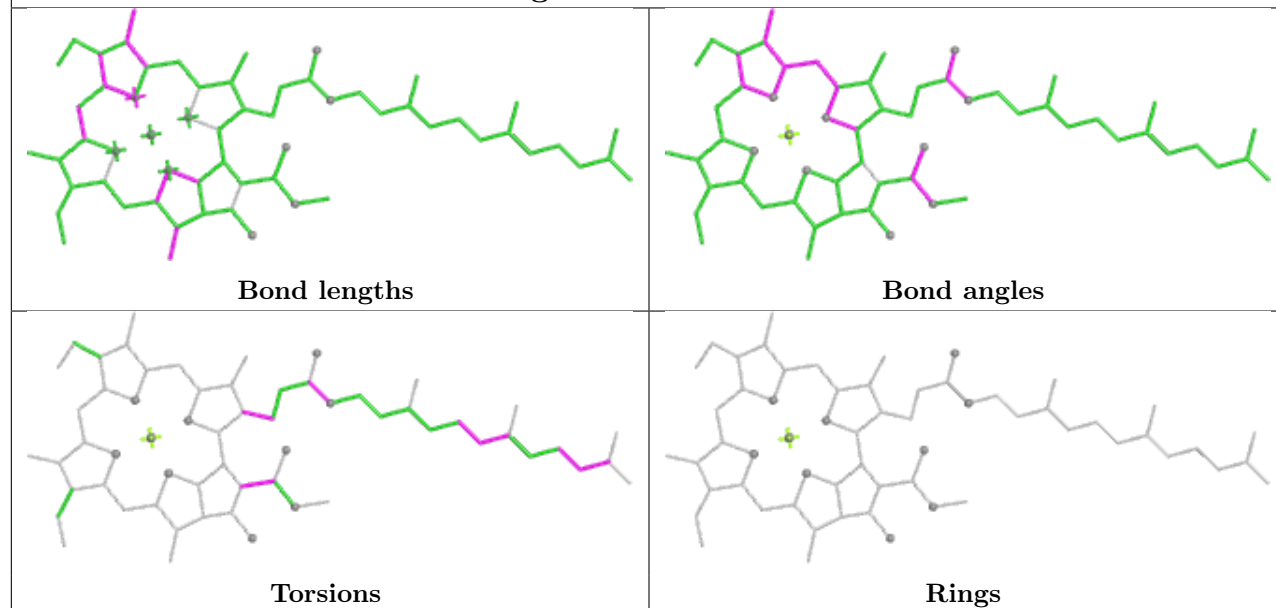


Ligand DD6 N 613

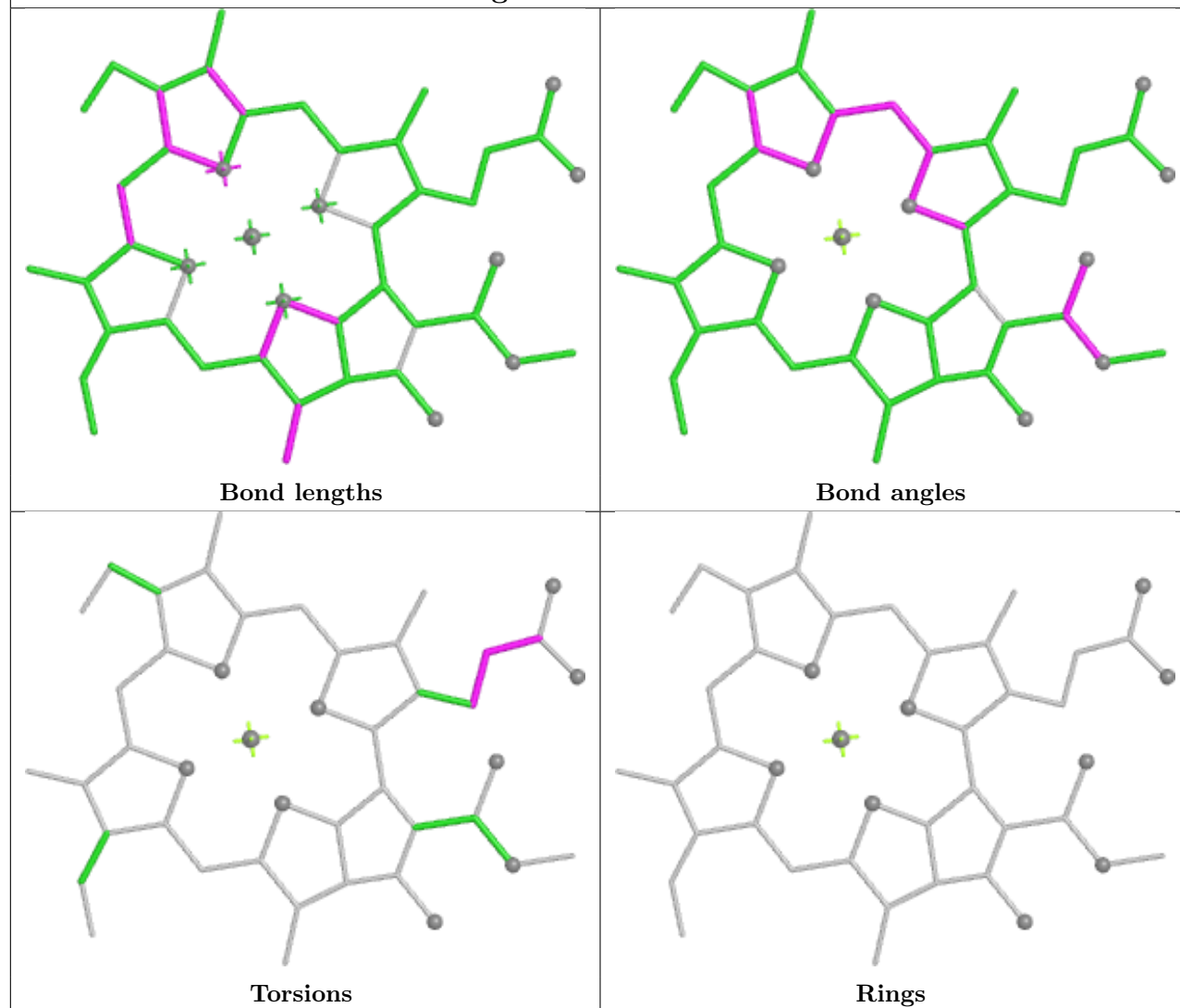


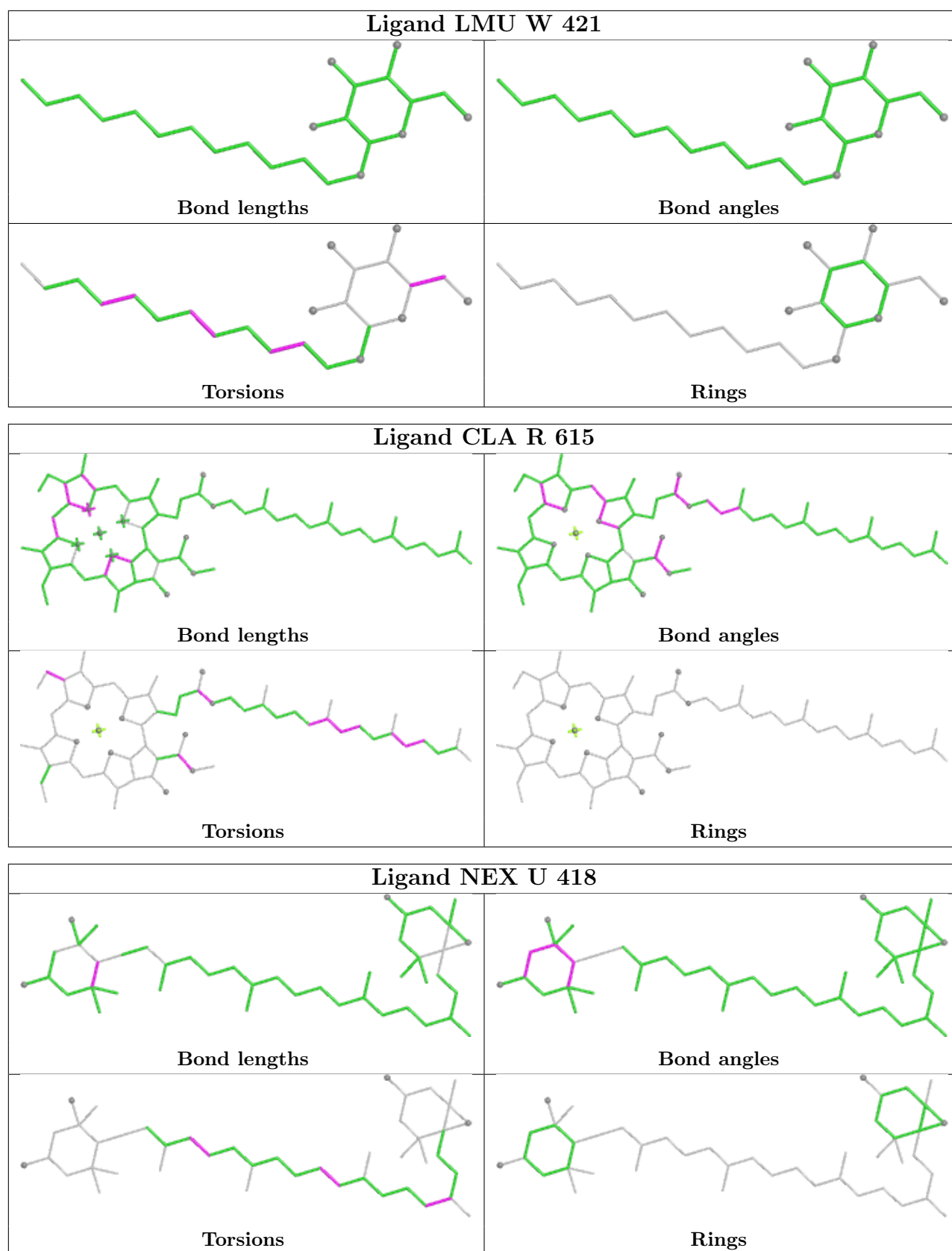


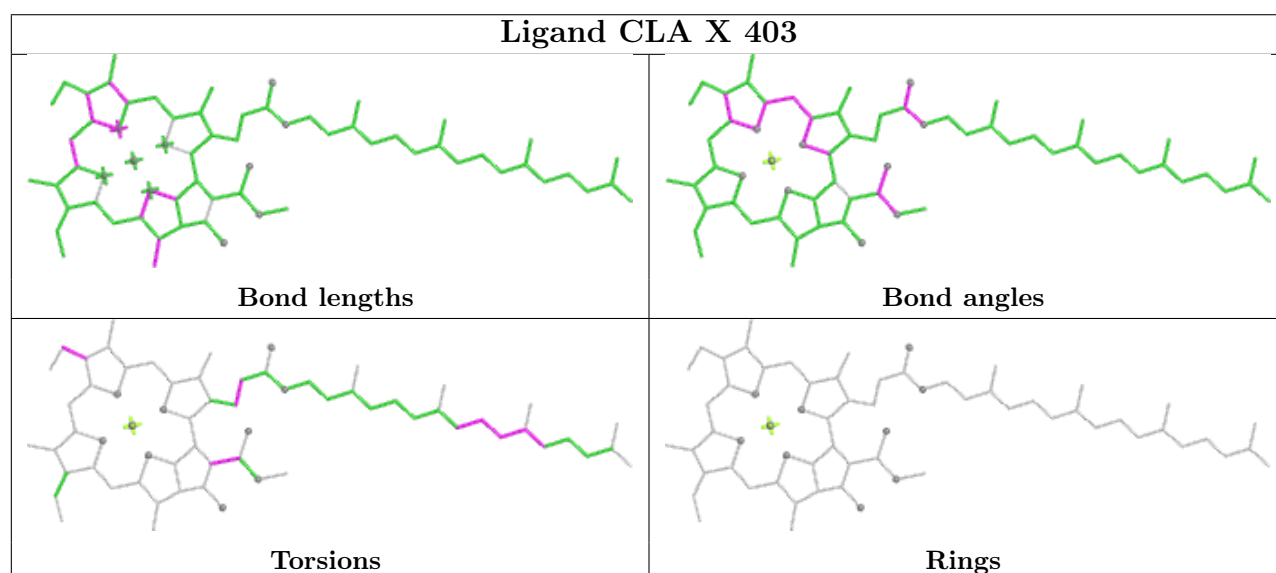
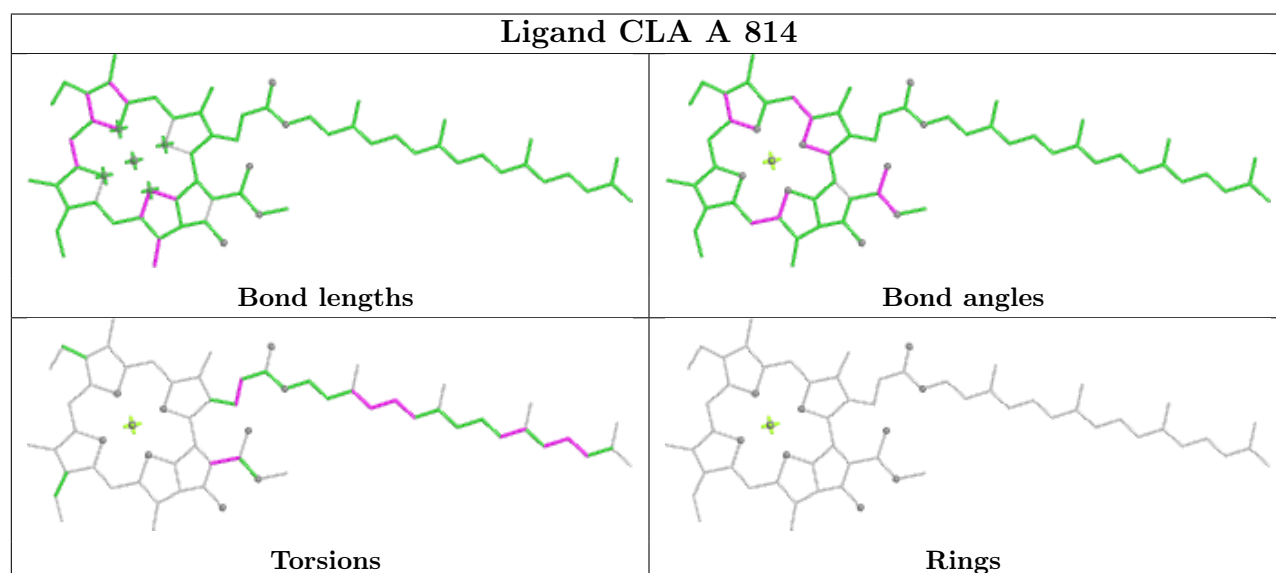
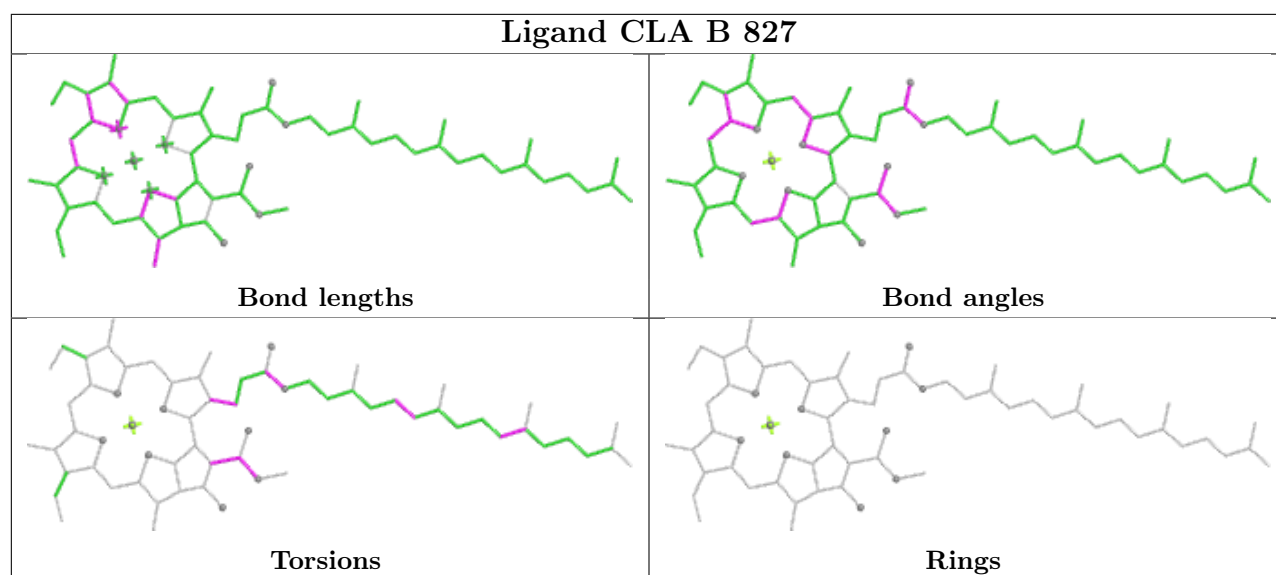
Ligand CLA K 602



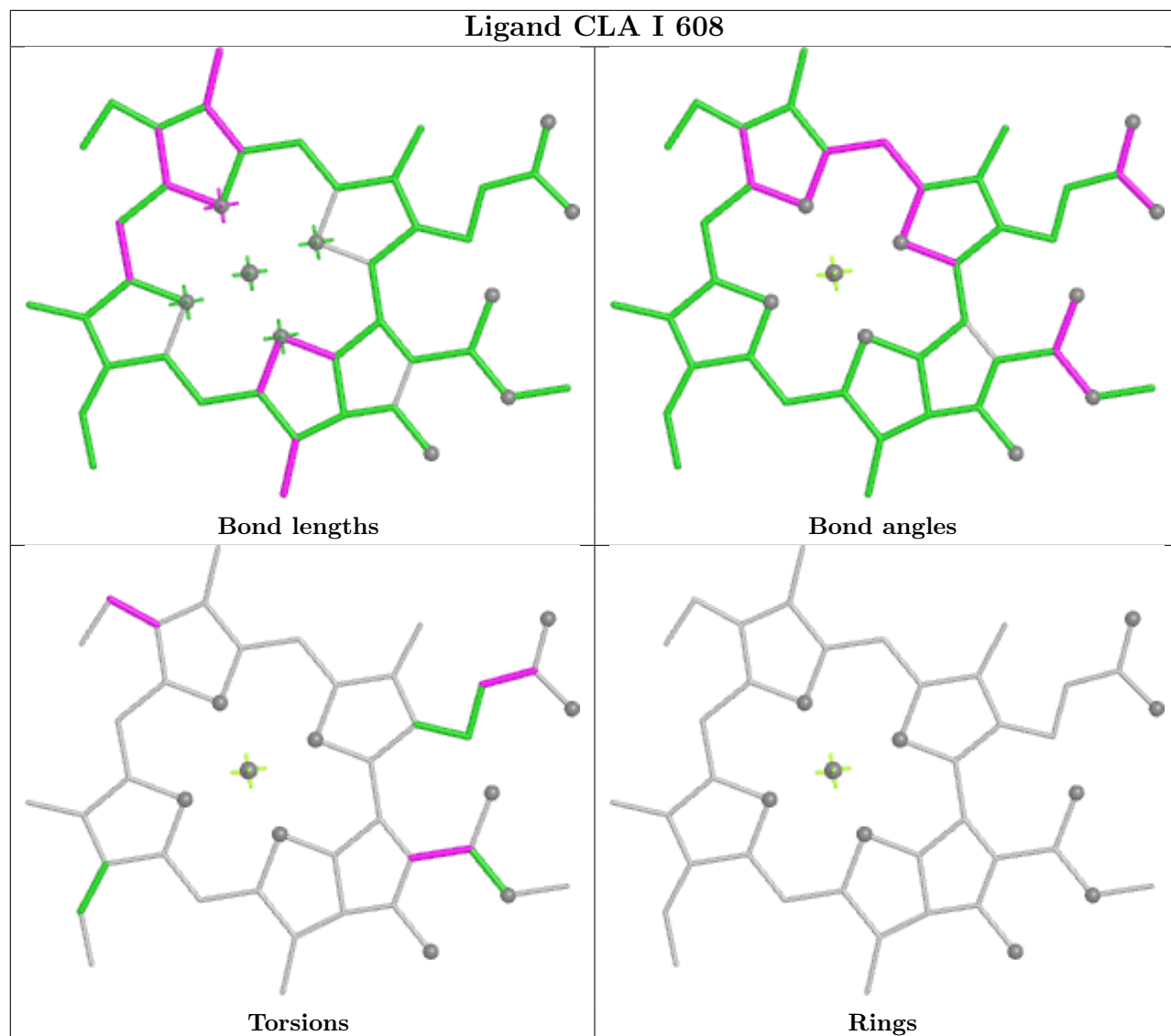
Ligand CLA O 307

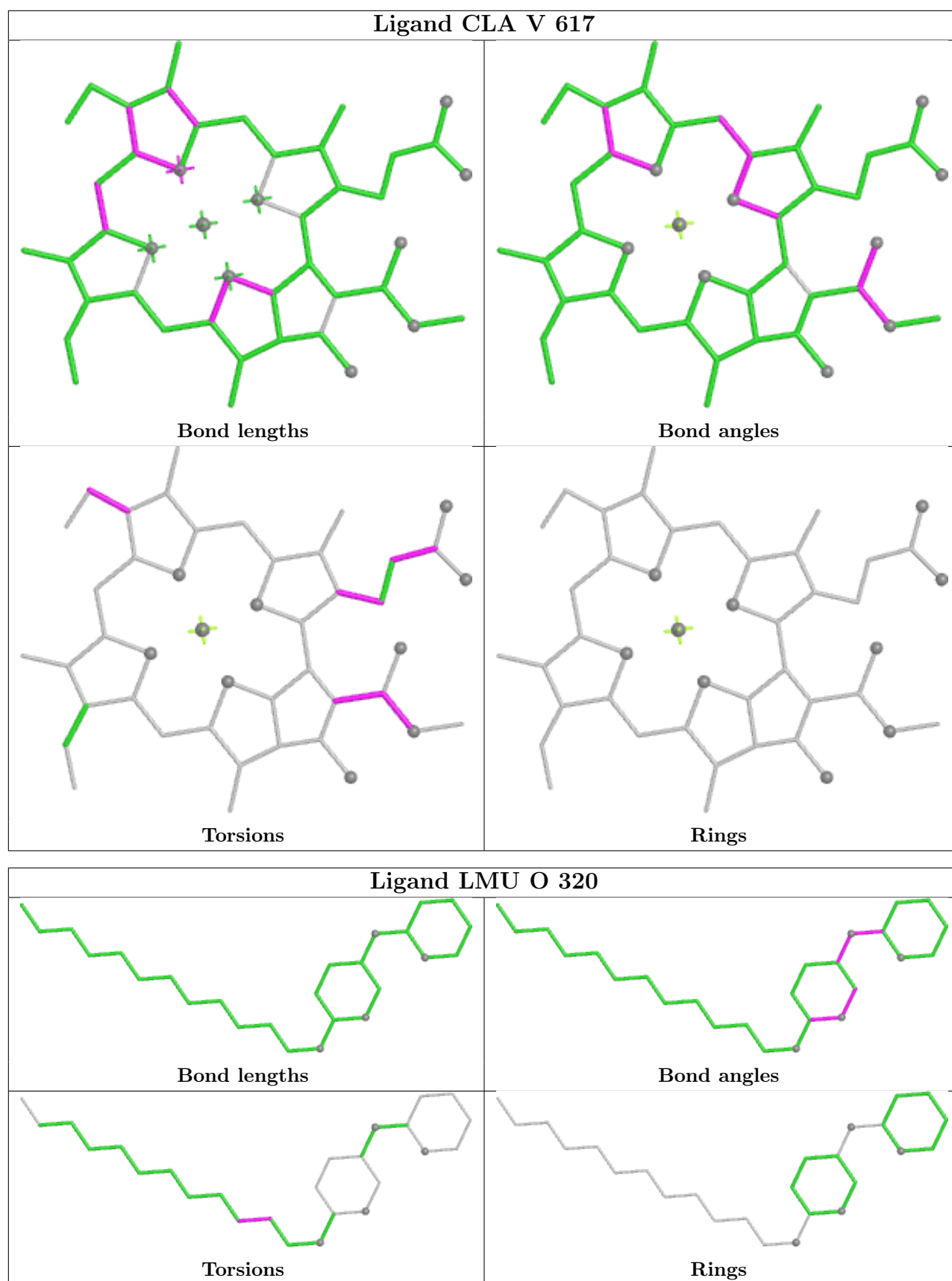


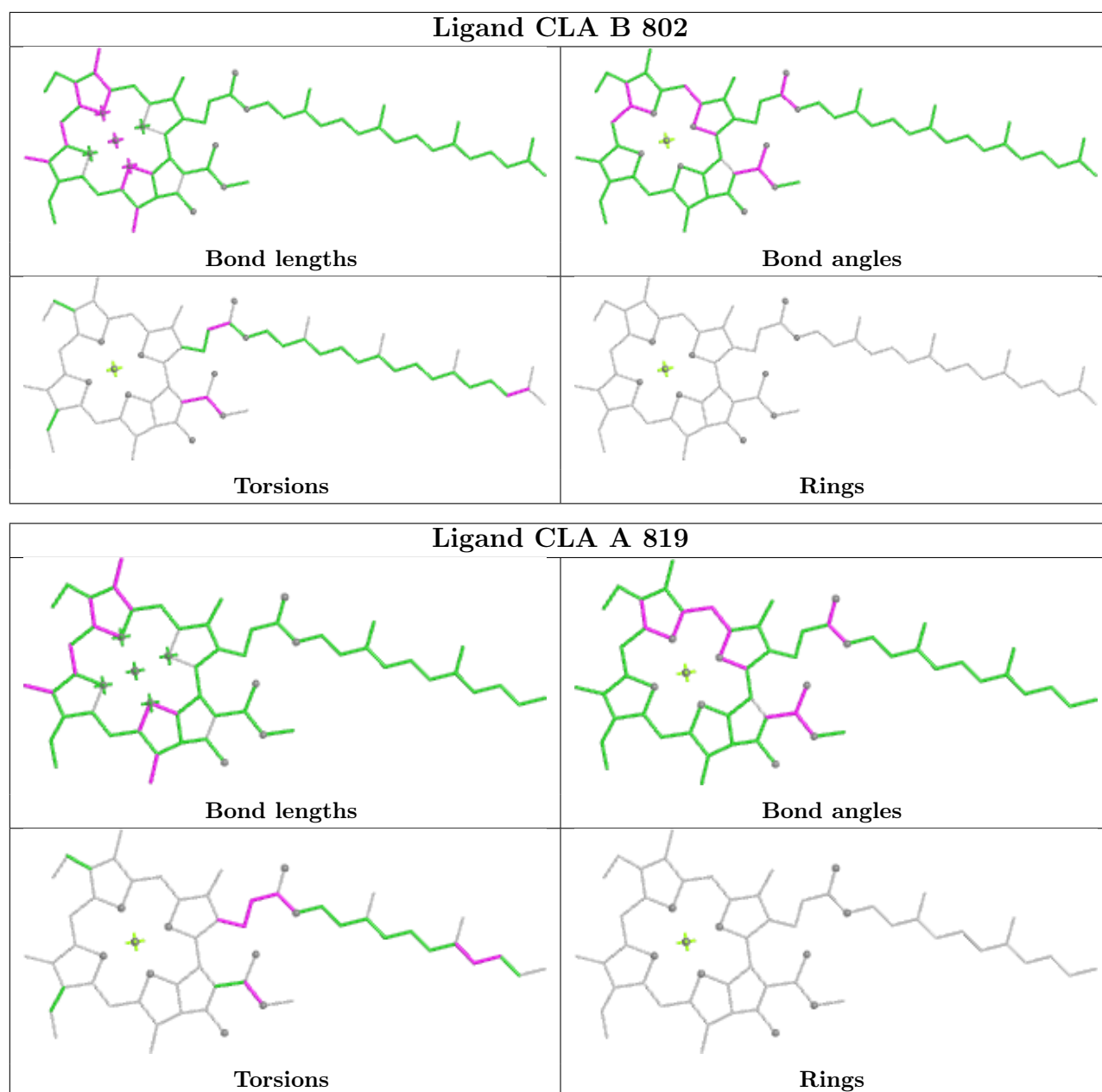


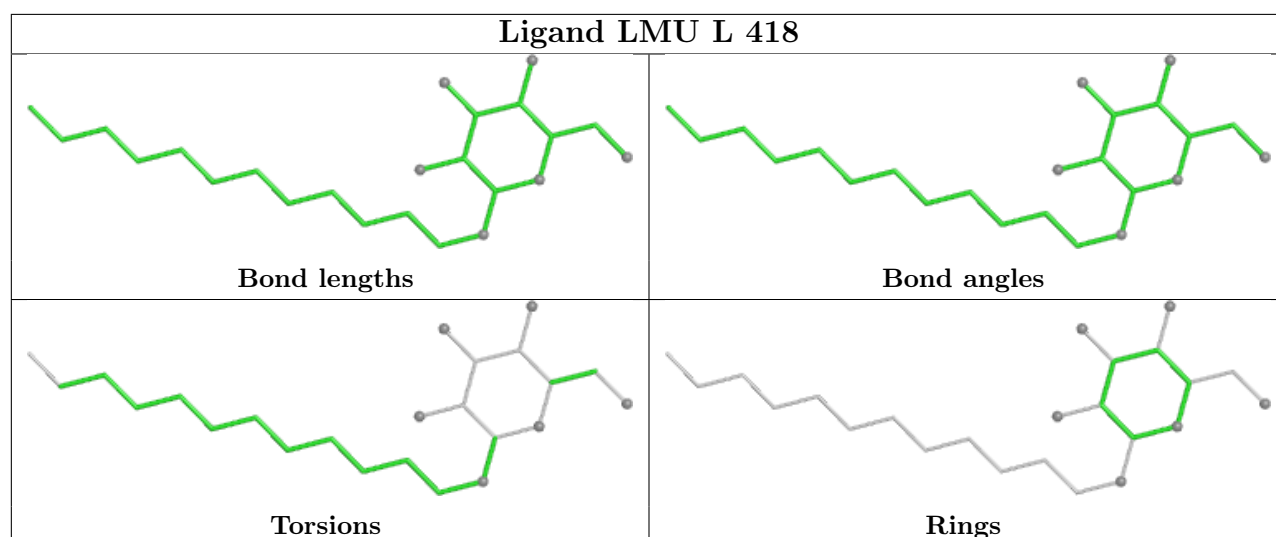
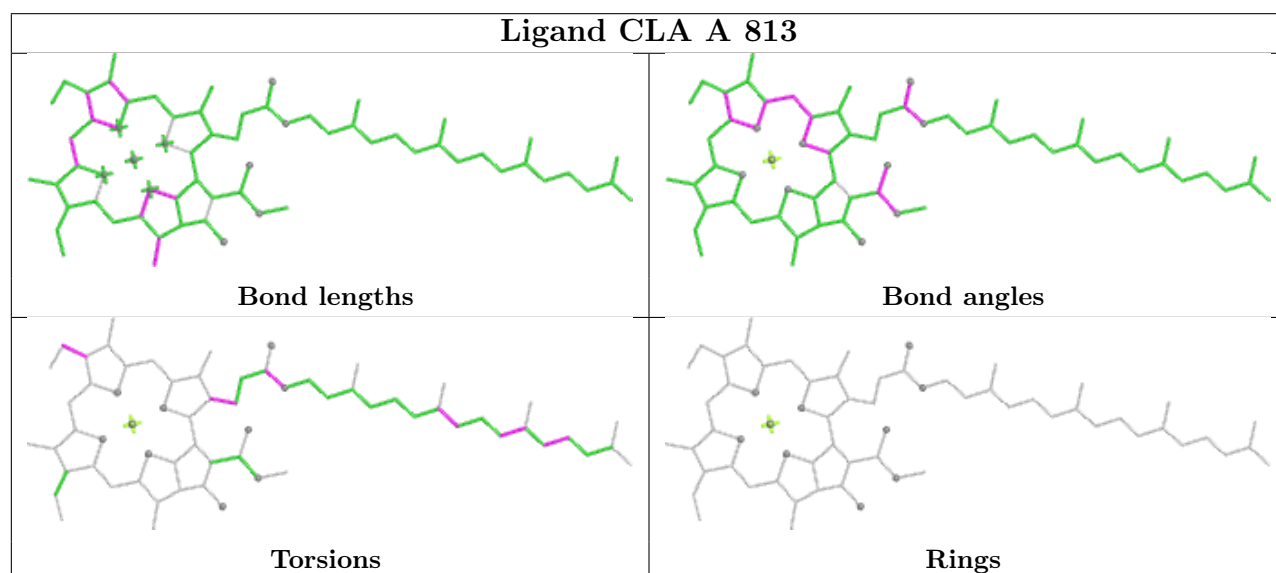
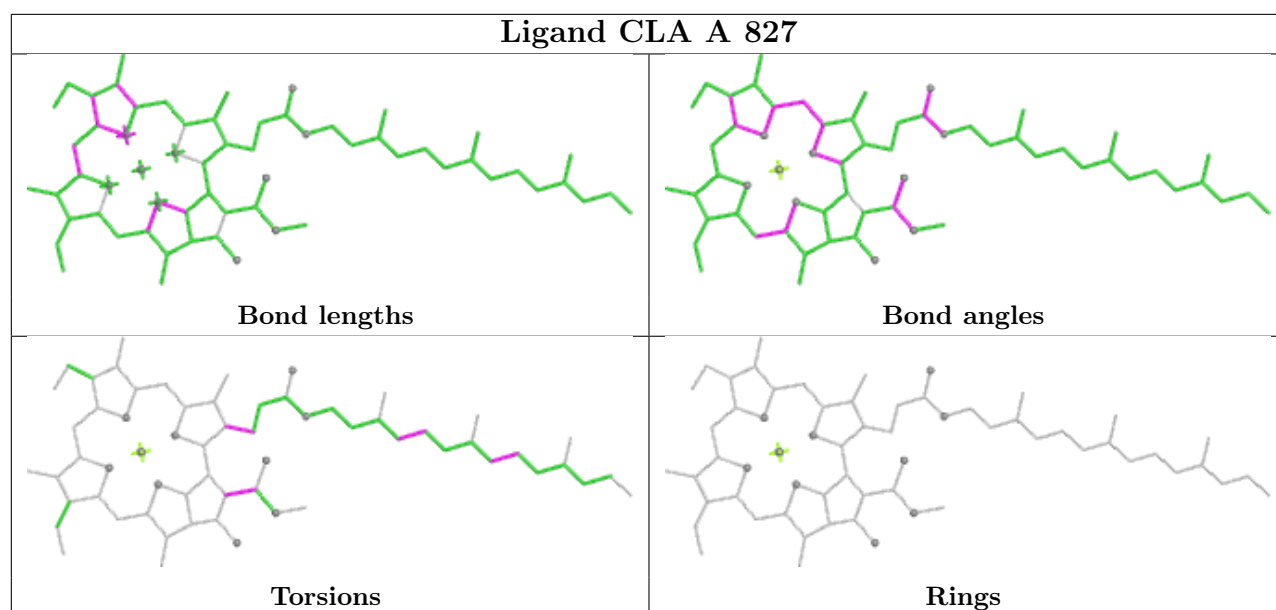


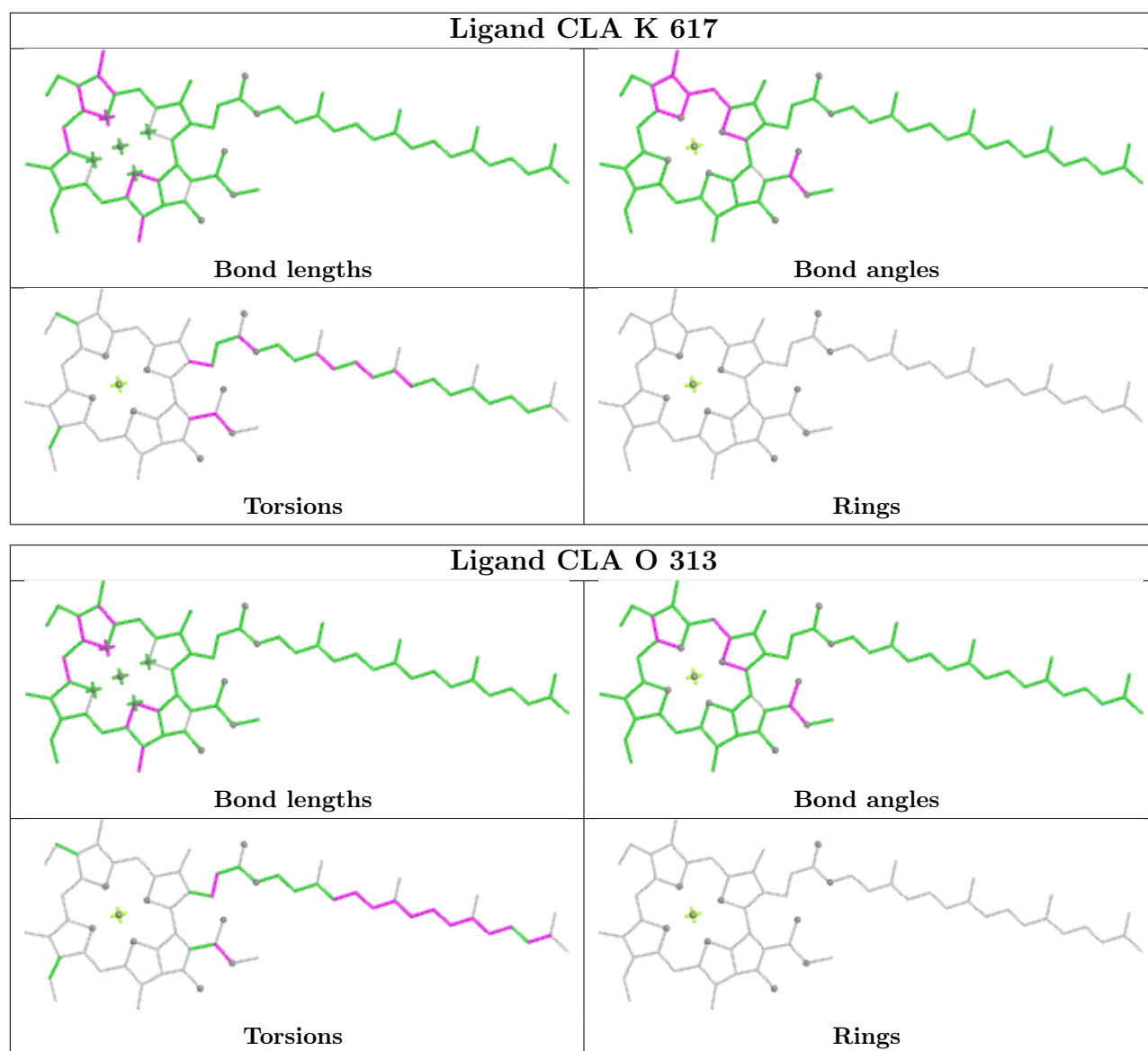
Ligand CLA I 608

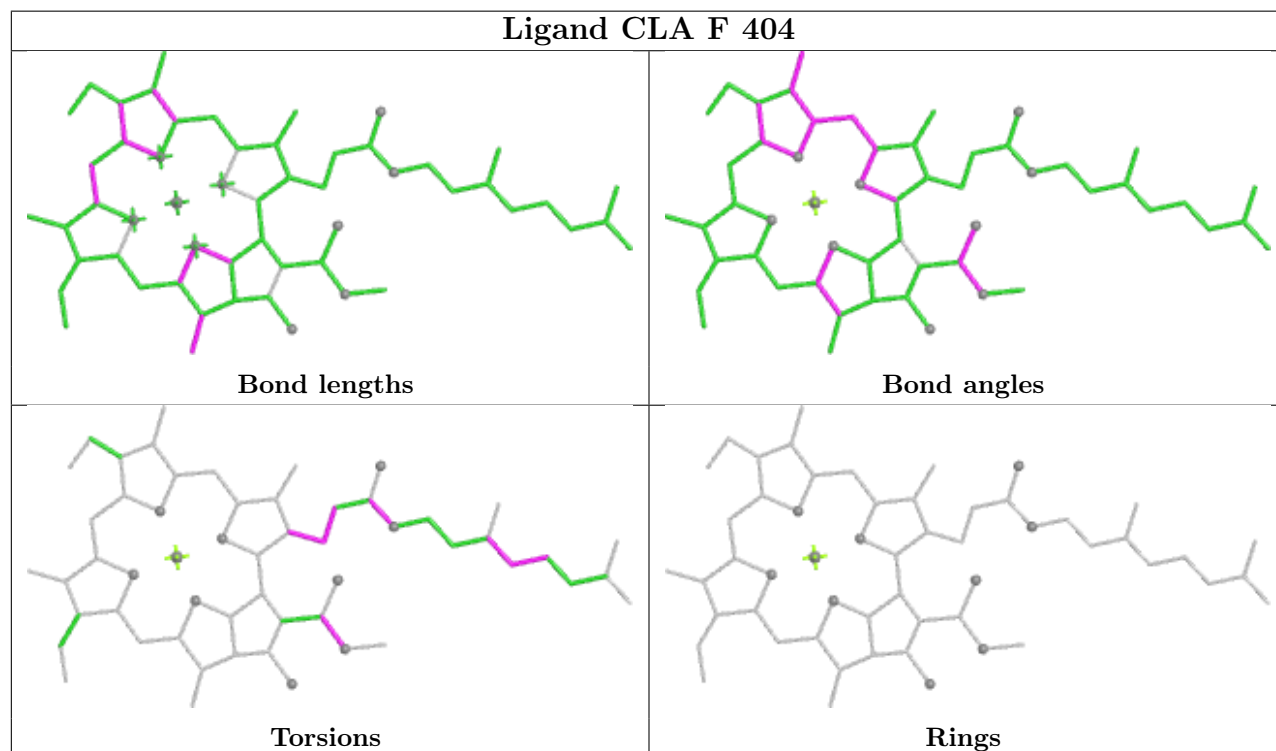
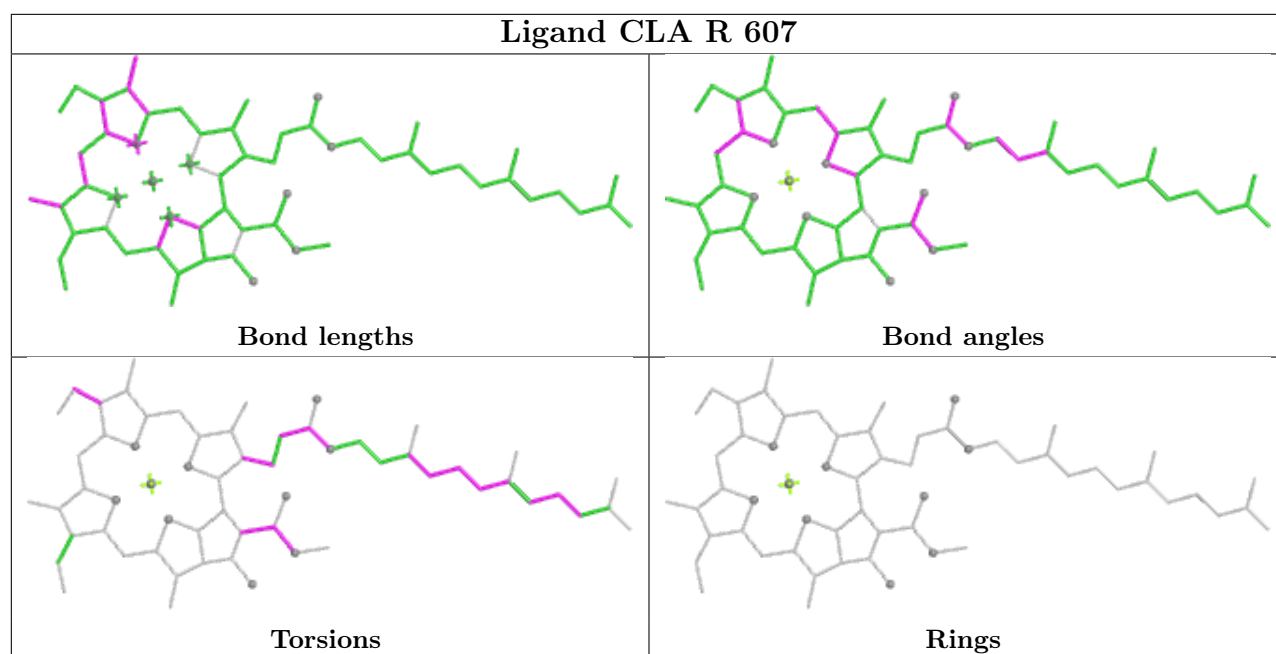




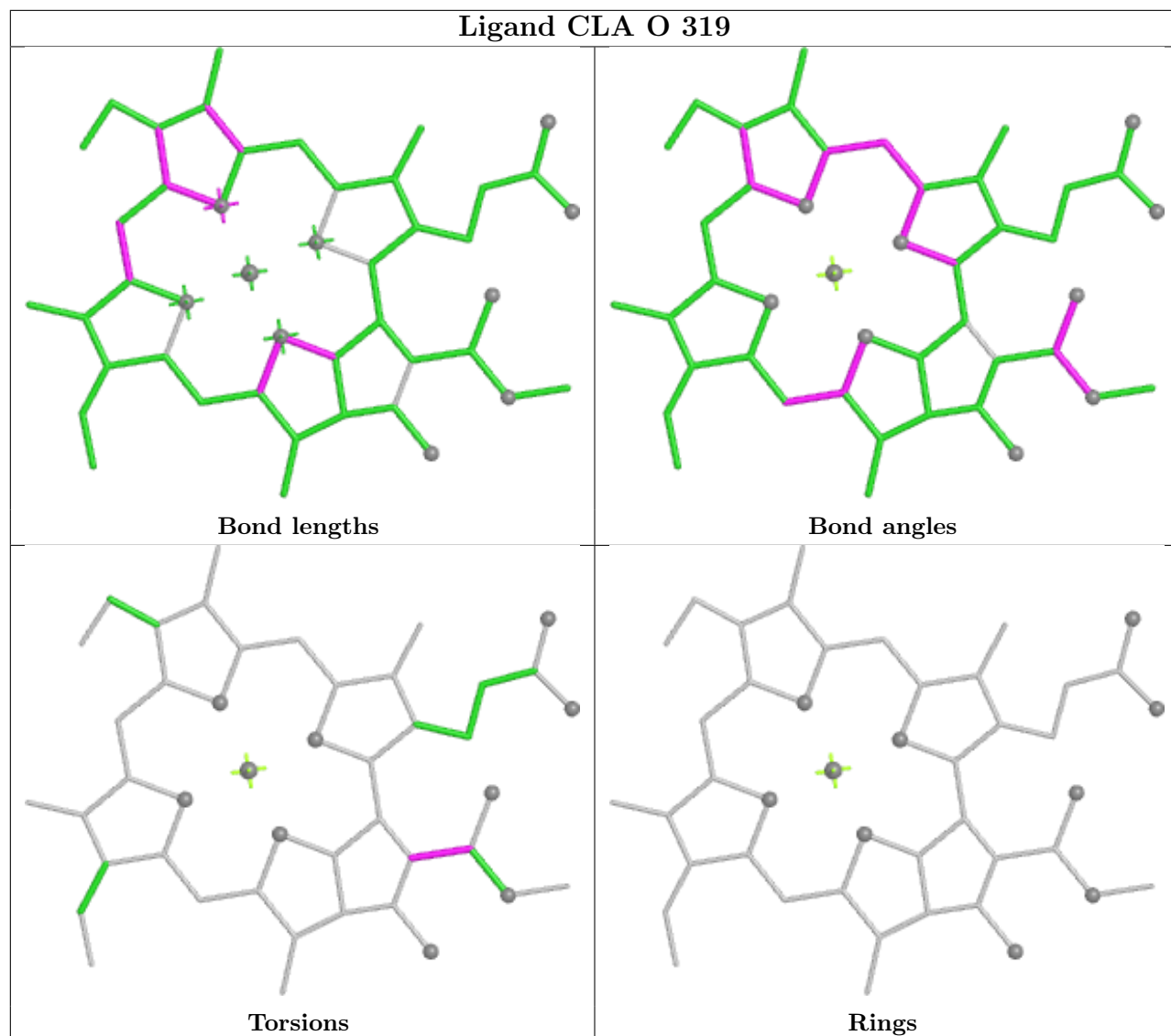


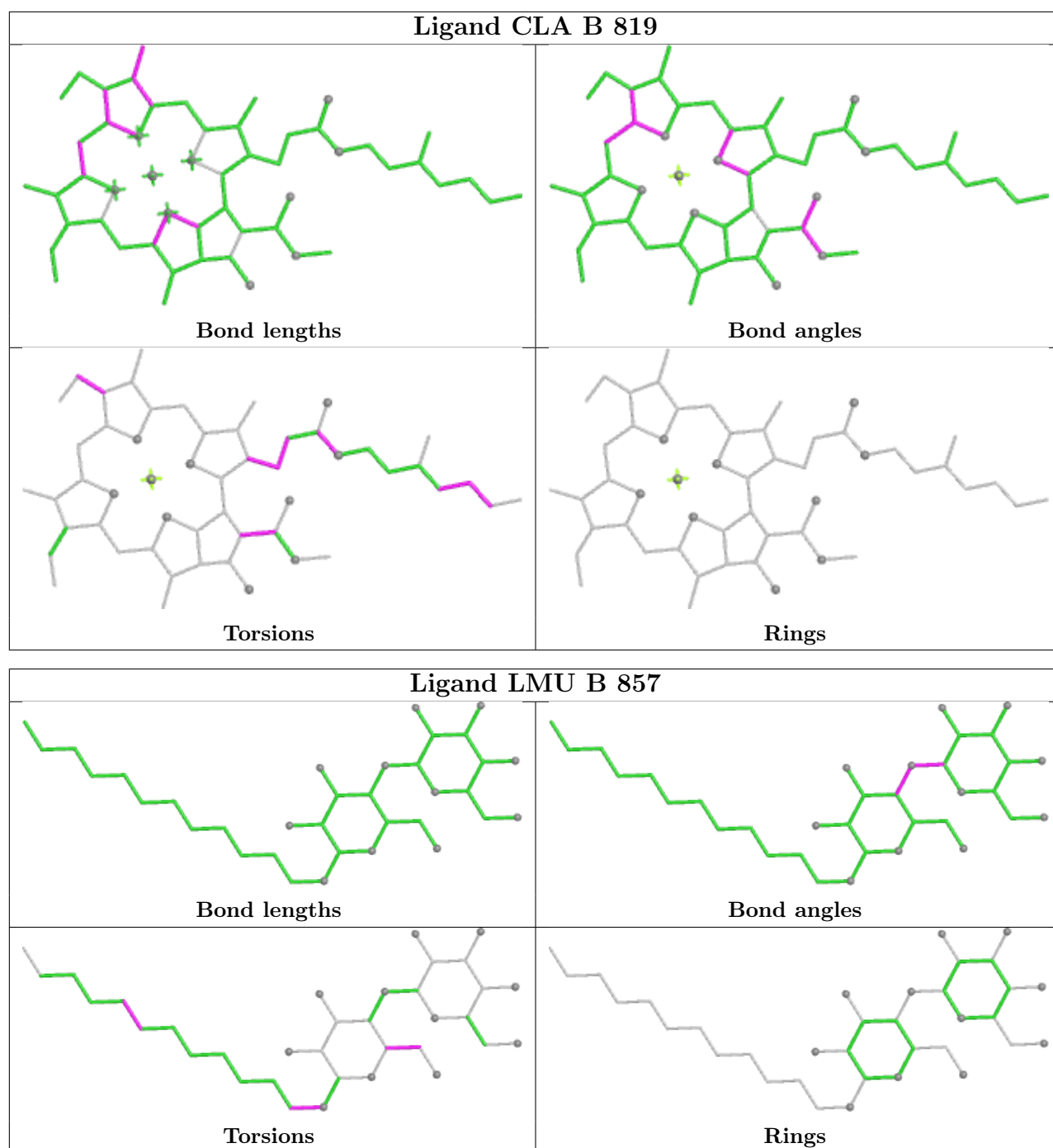


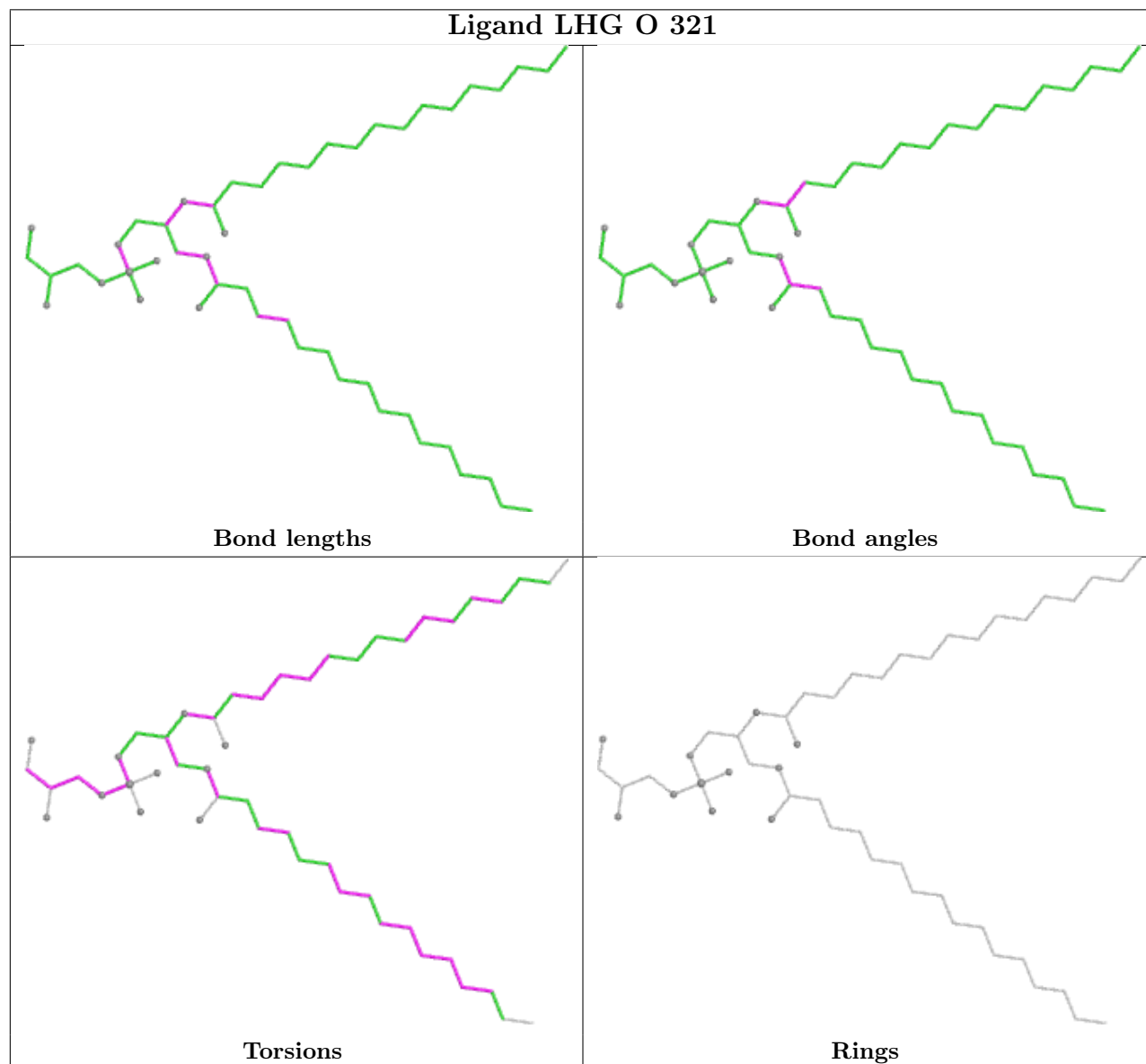
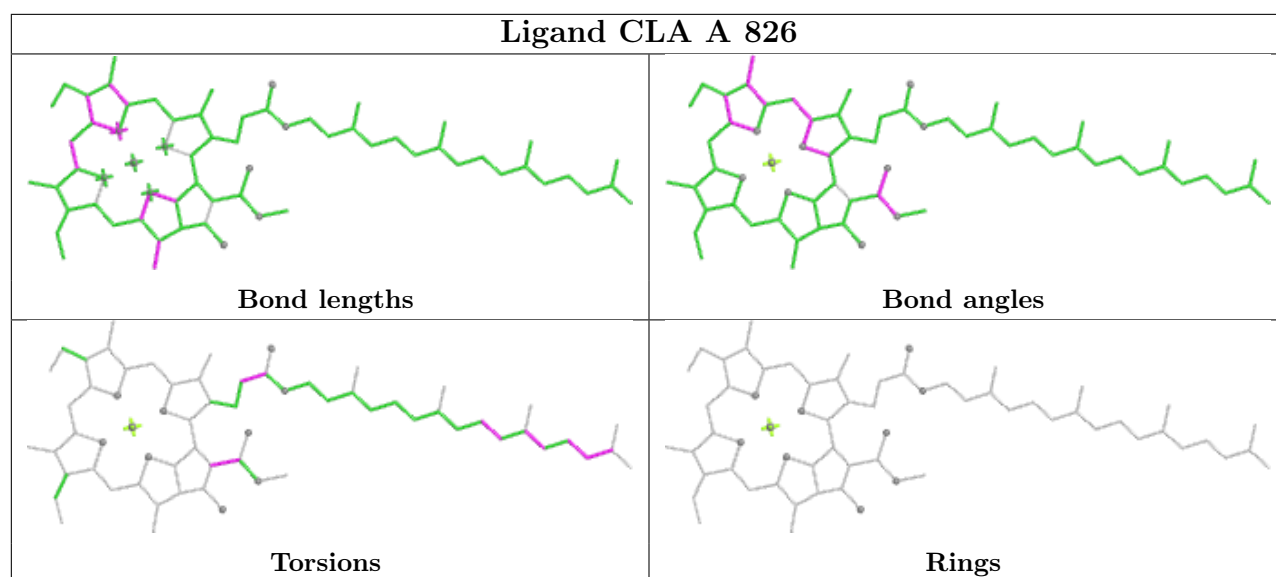


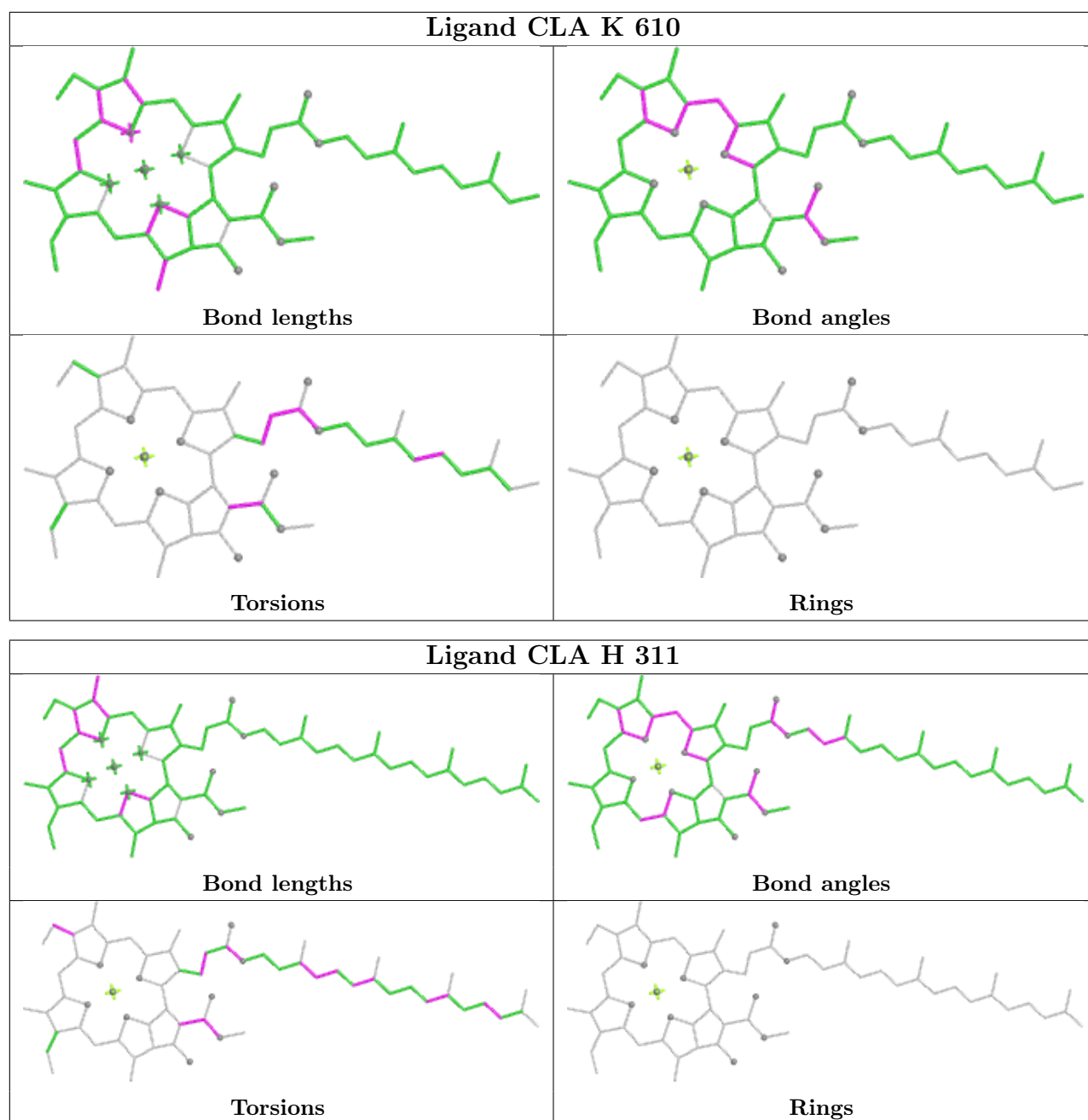


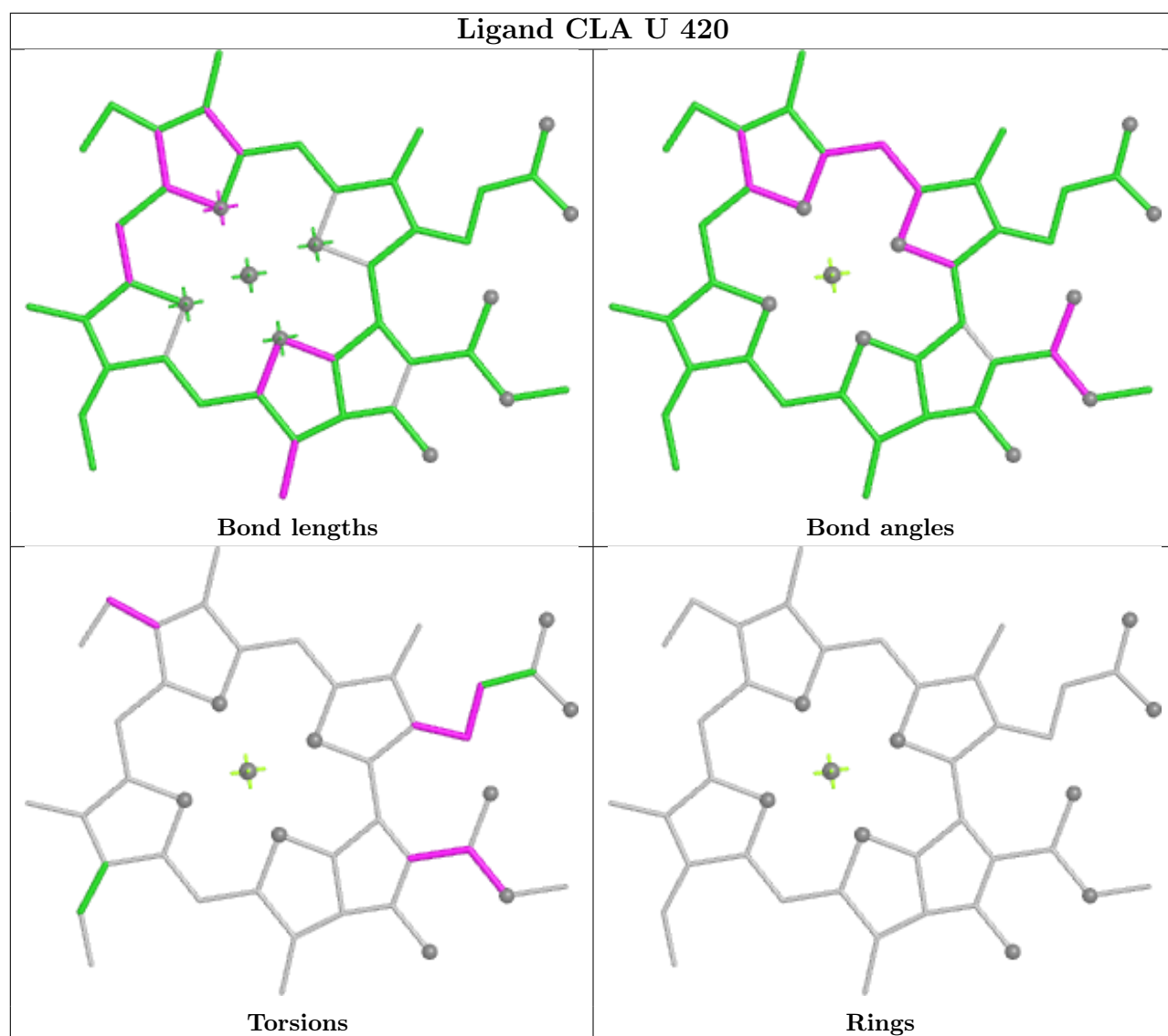
Ligand CLA O 319



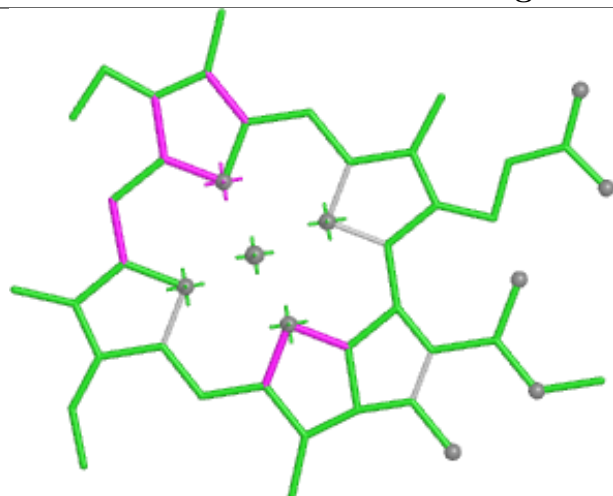




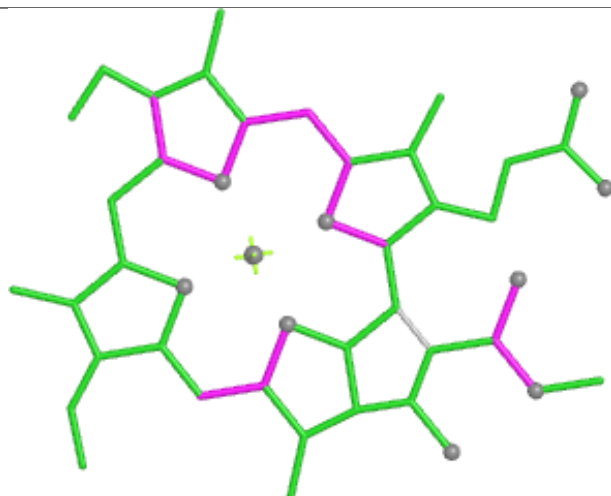




Ligand CLA P 604



Bond lengths



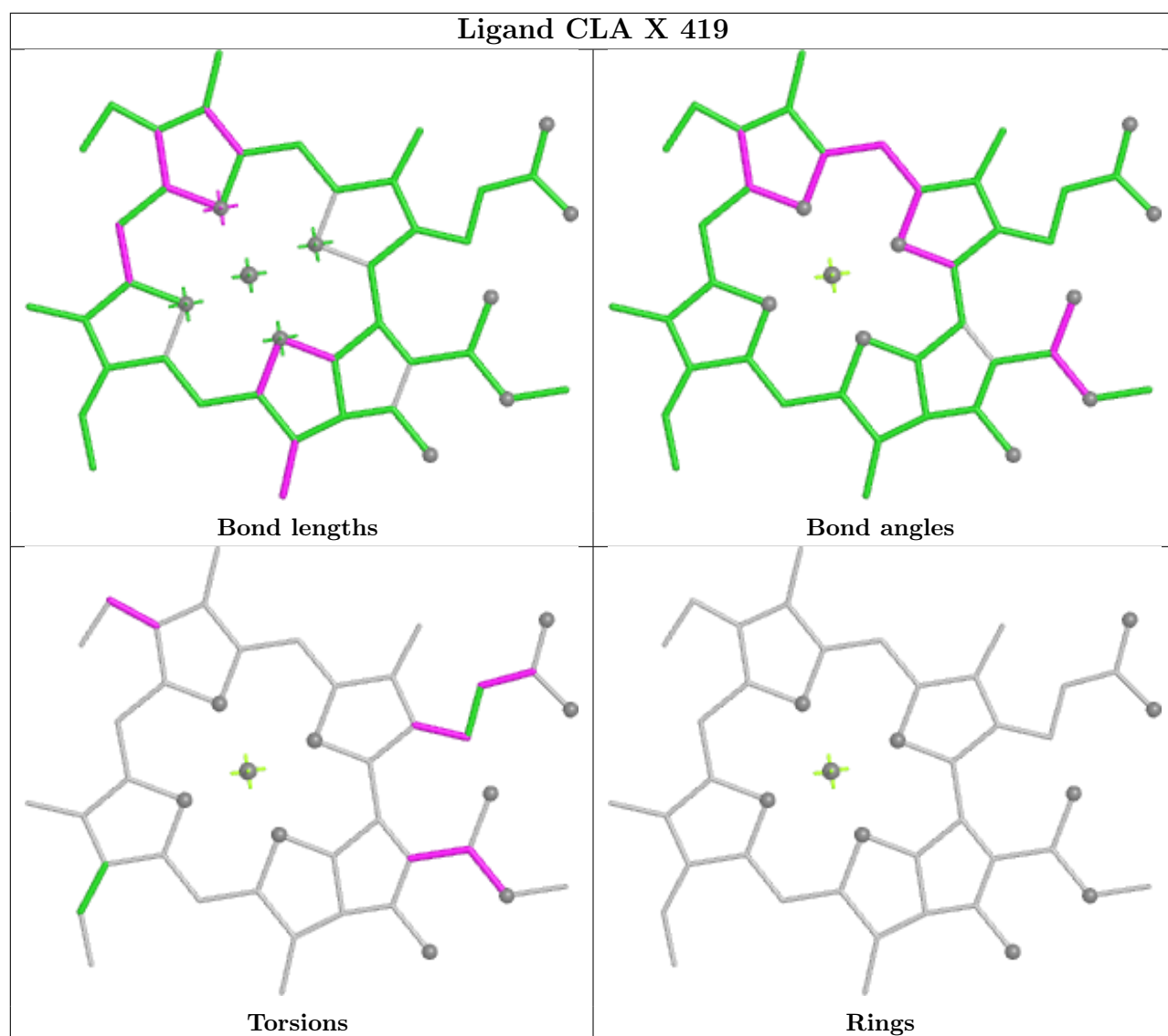
Bond angles

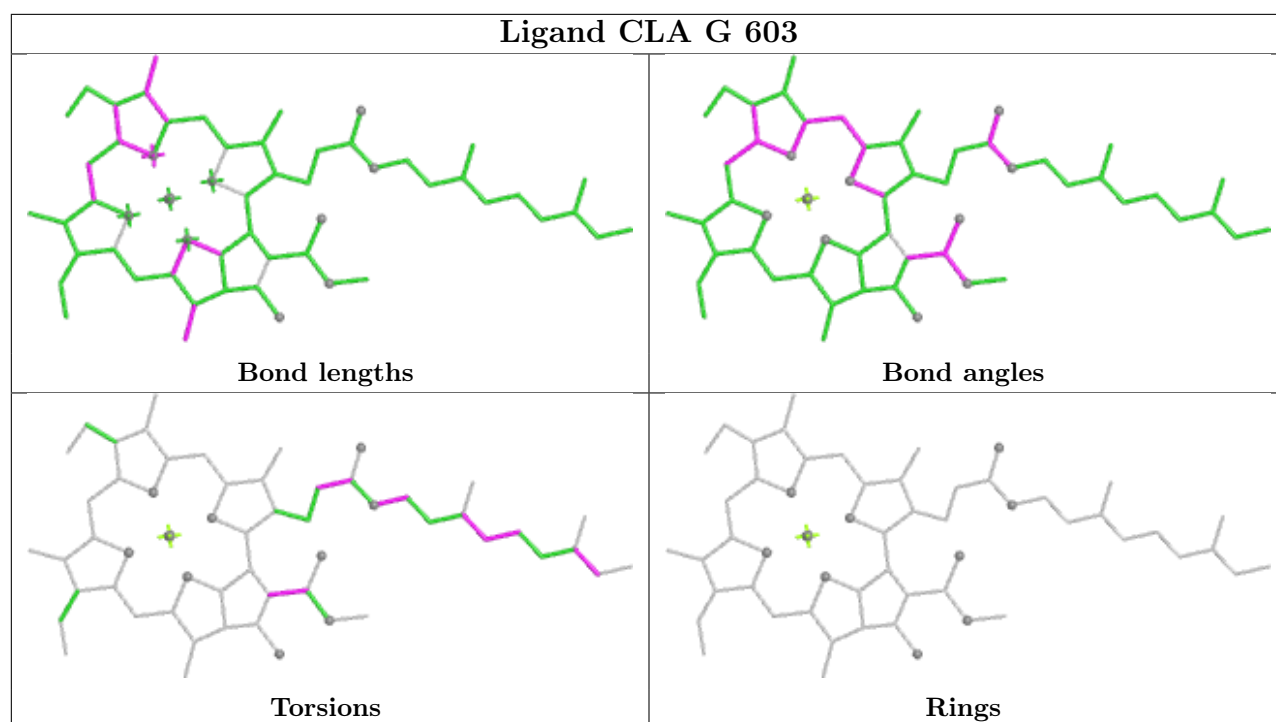


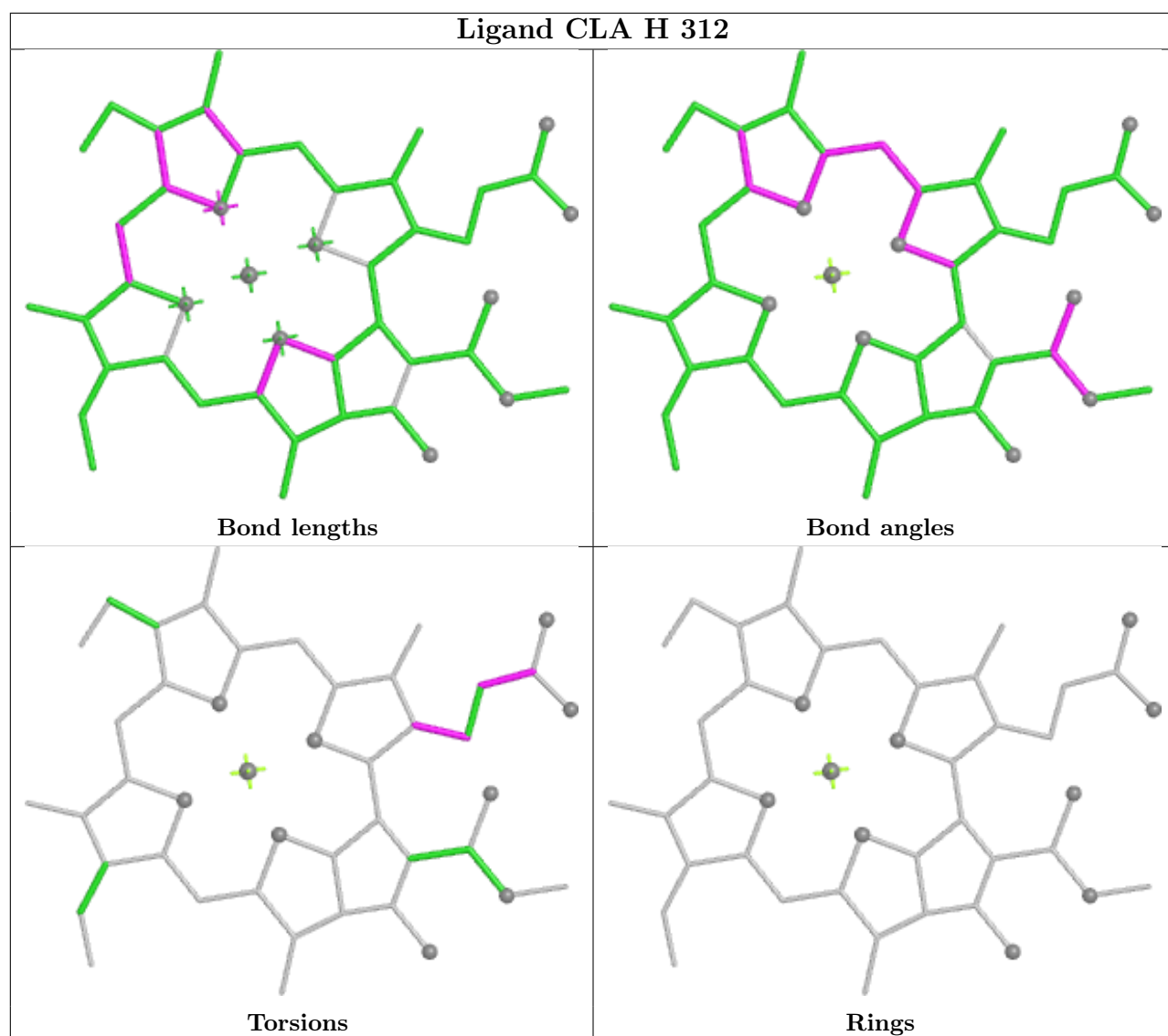
Torsions

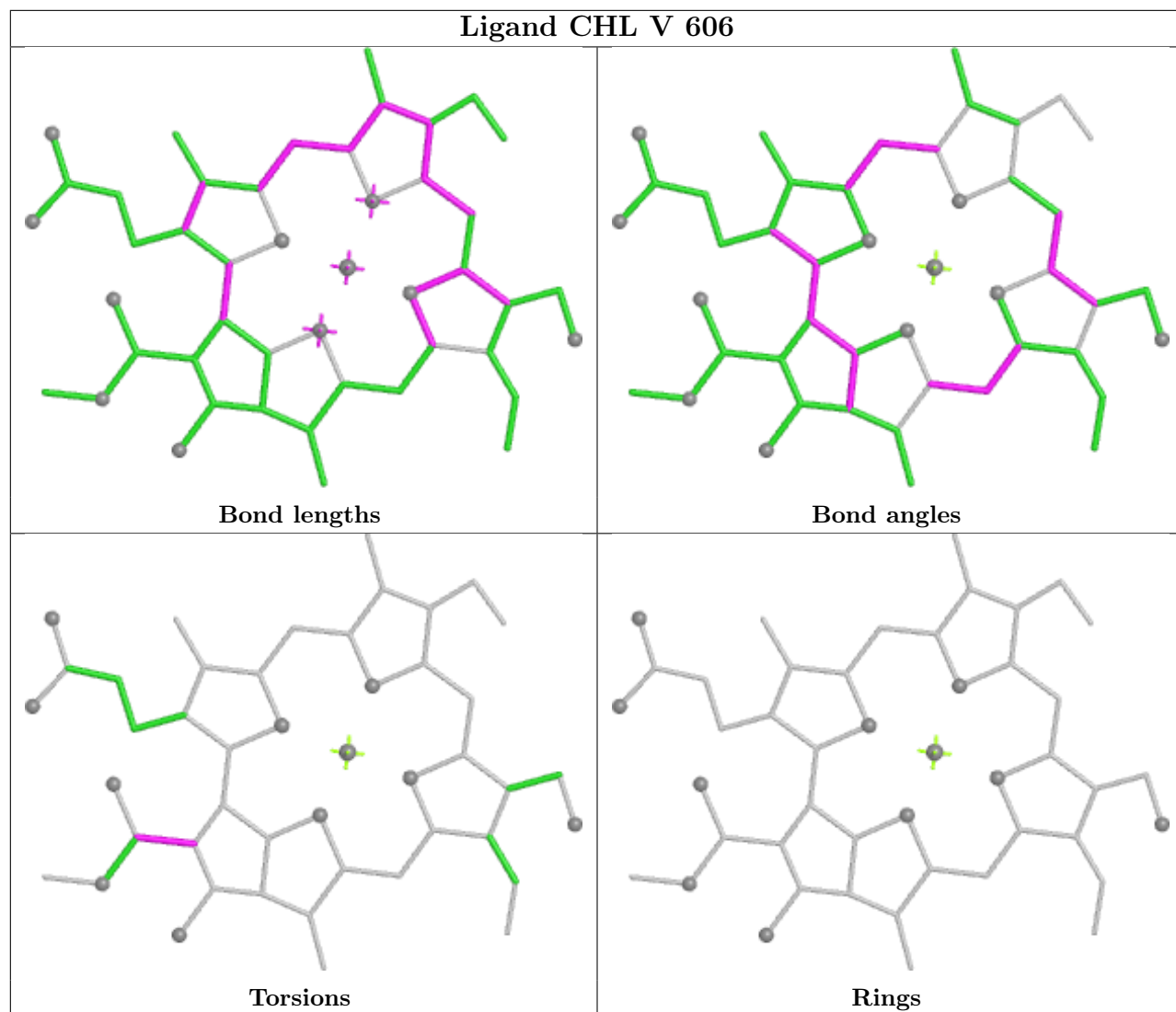


Rings

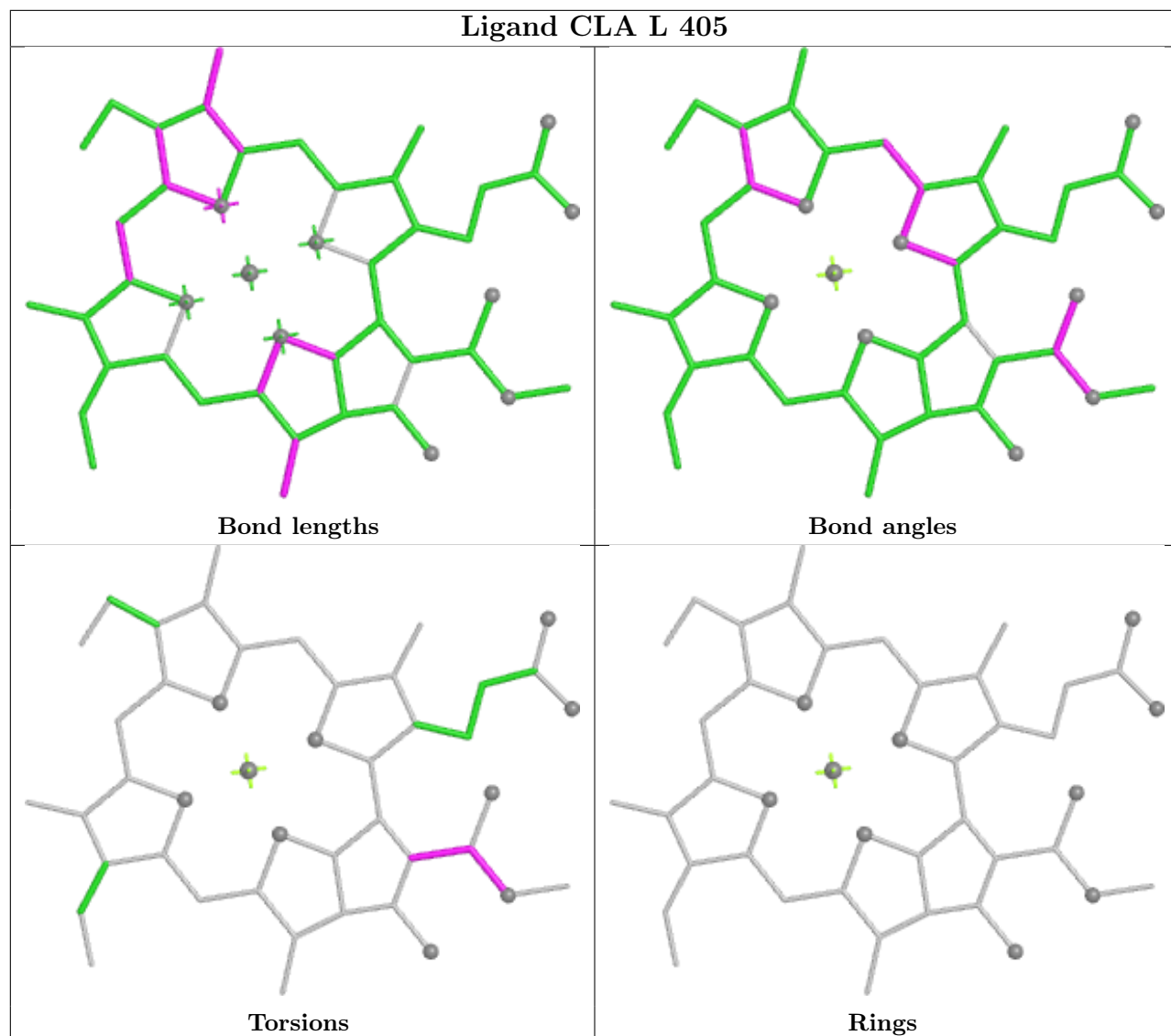




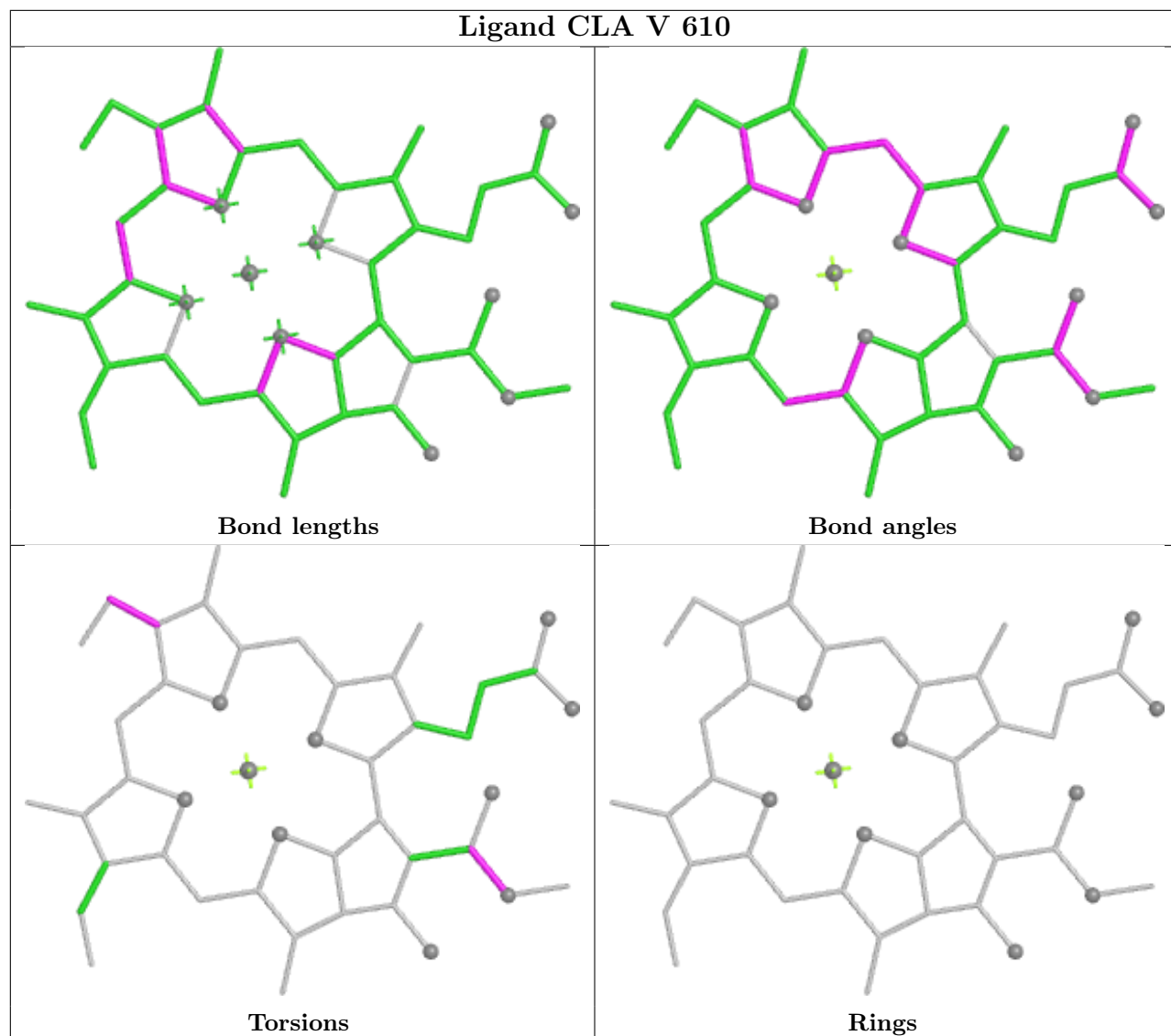


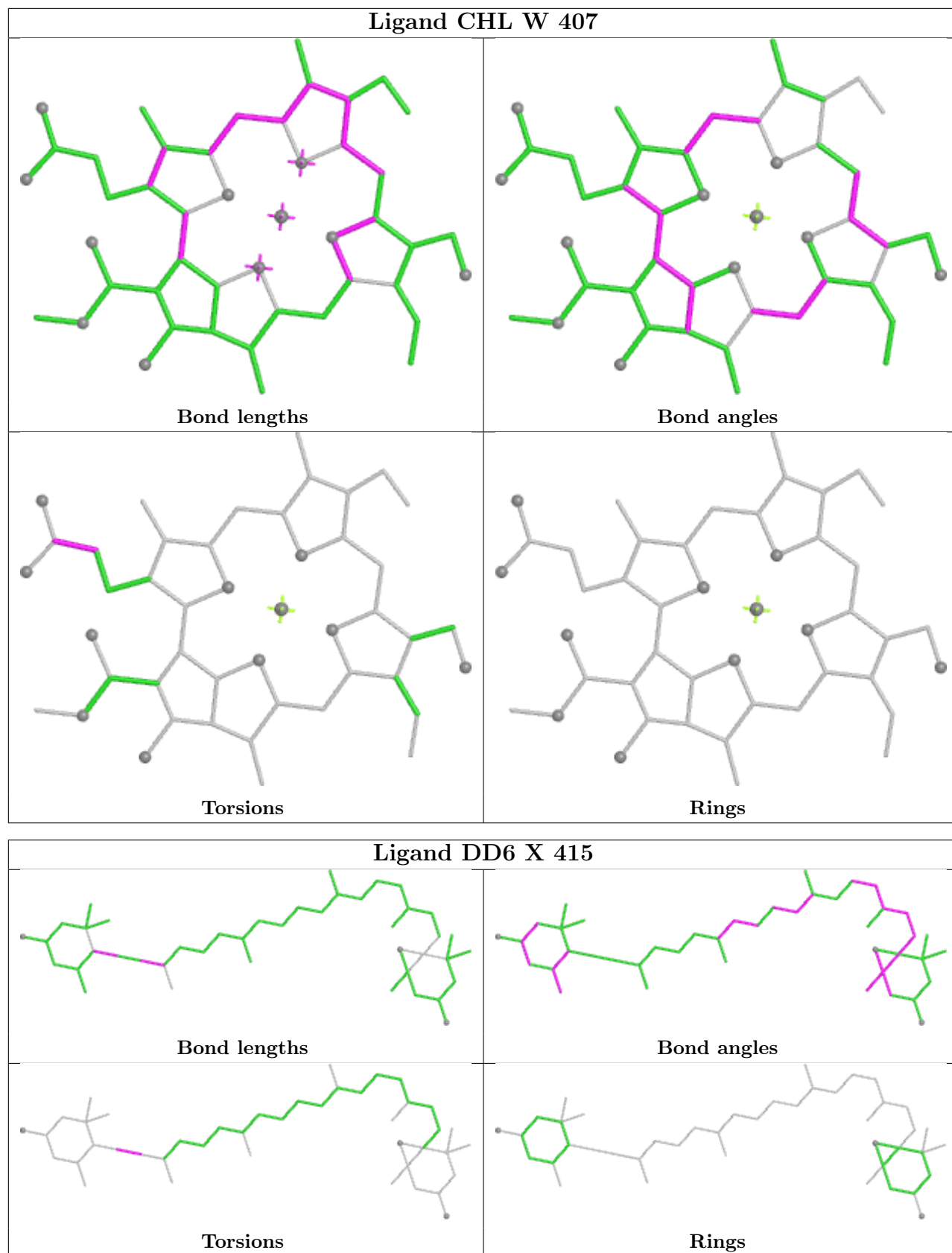


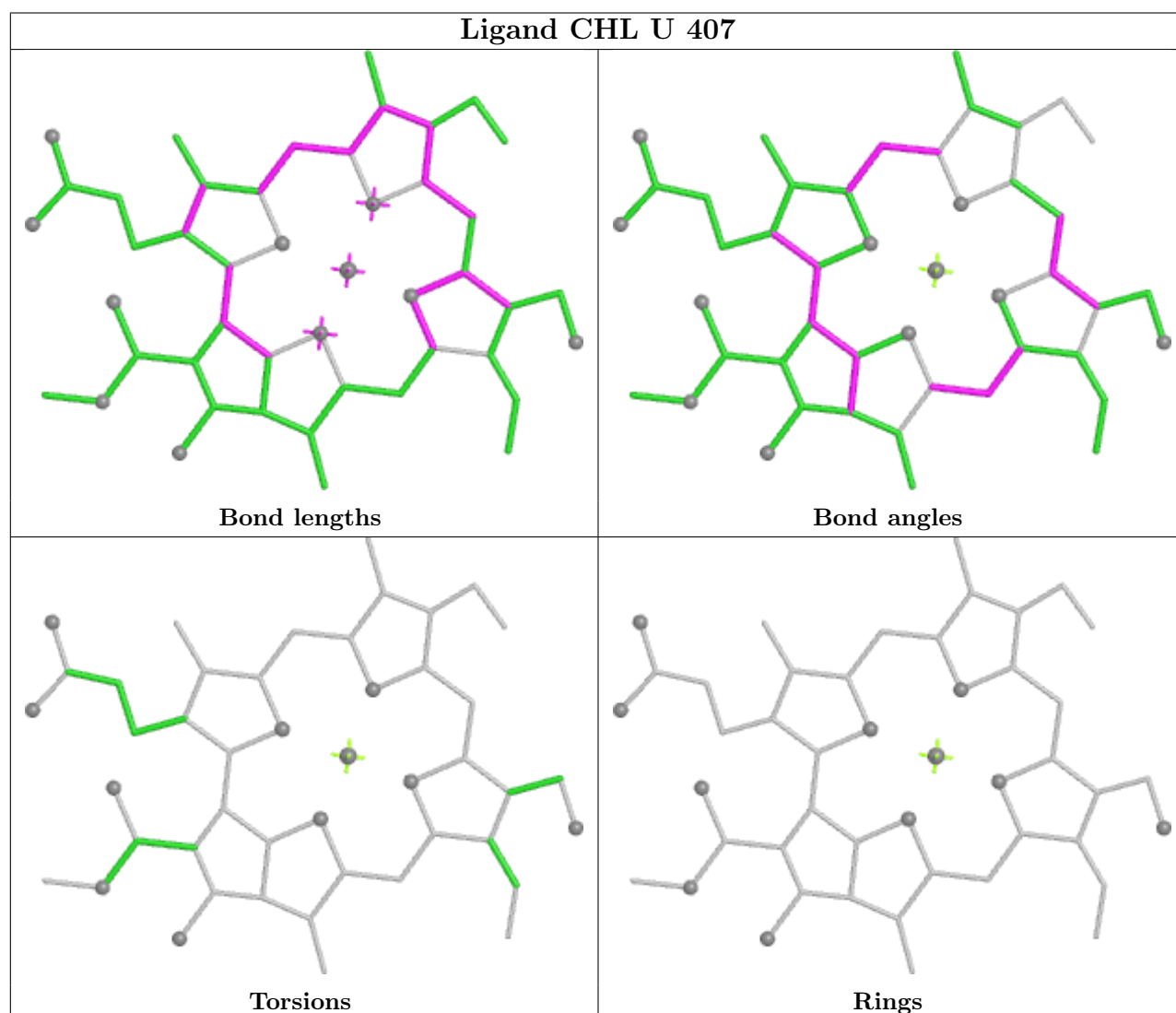
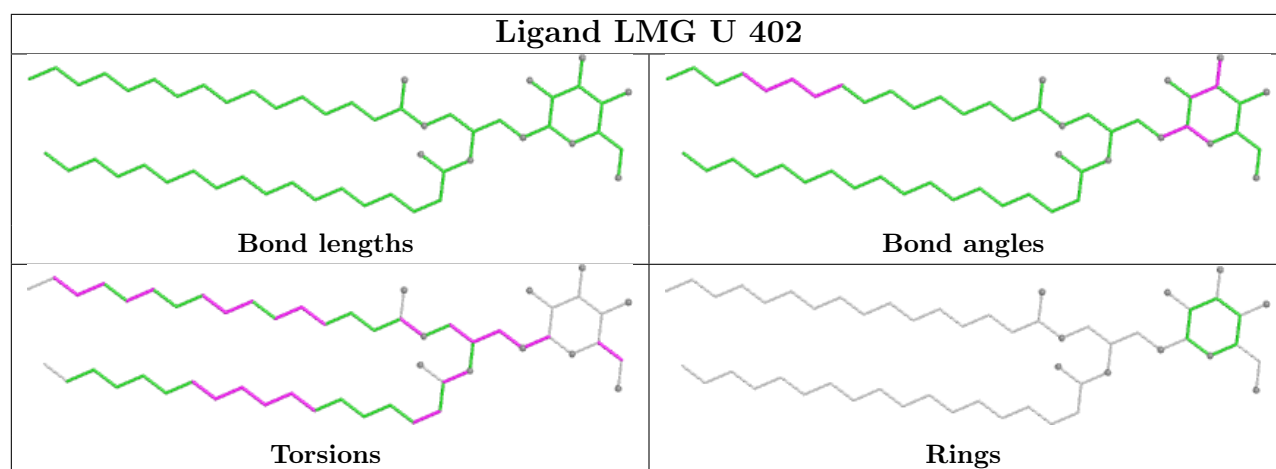
Ligand CLA L 405

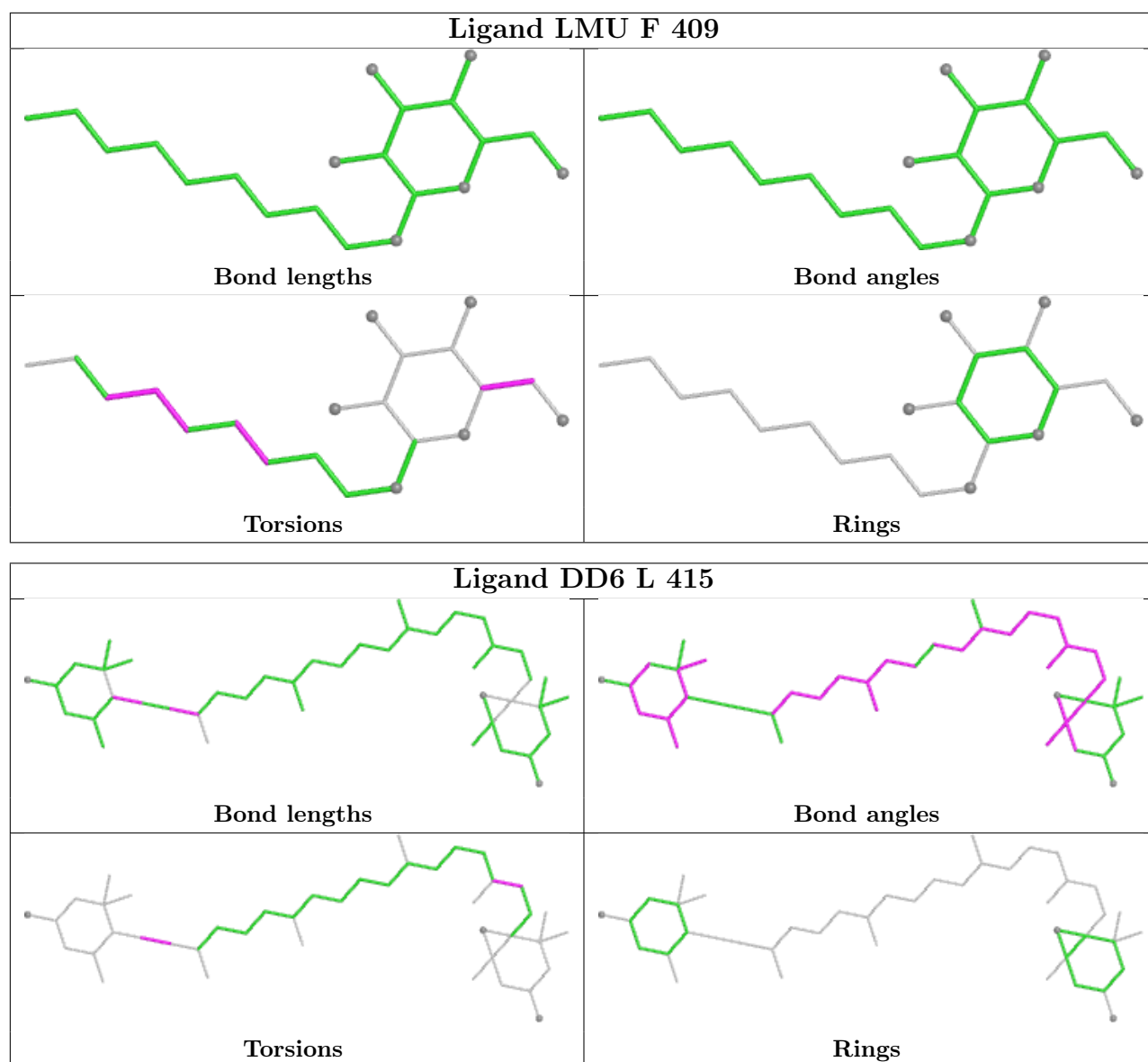


Ligand CLA V 610

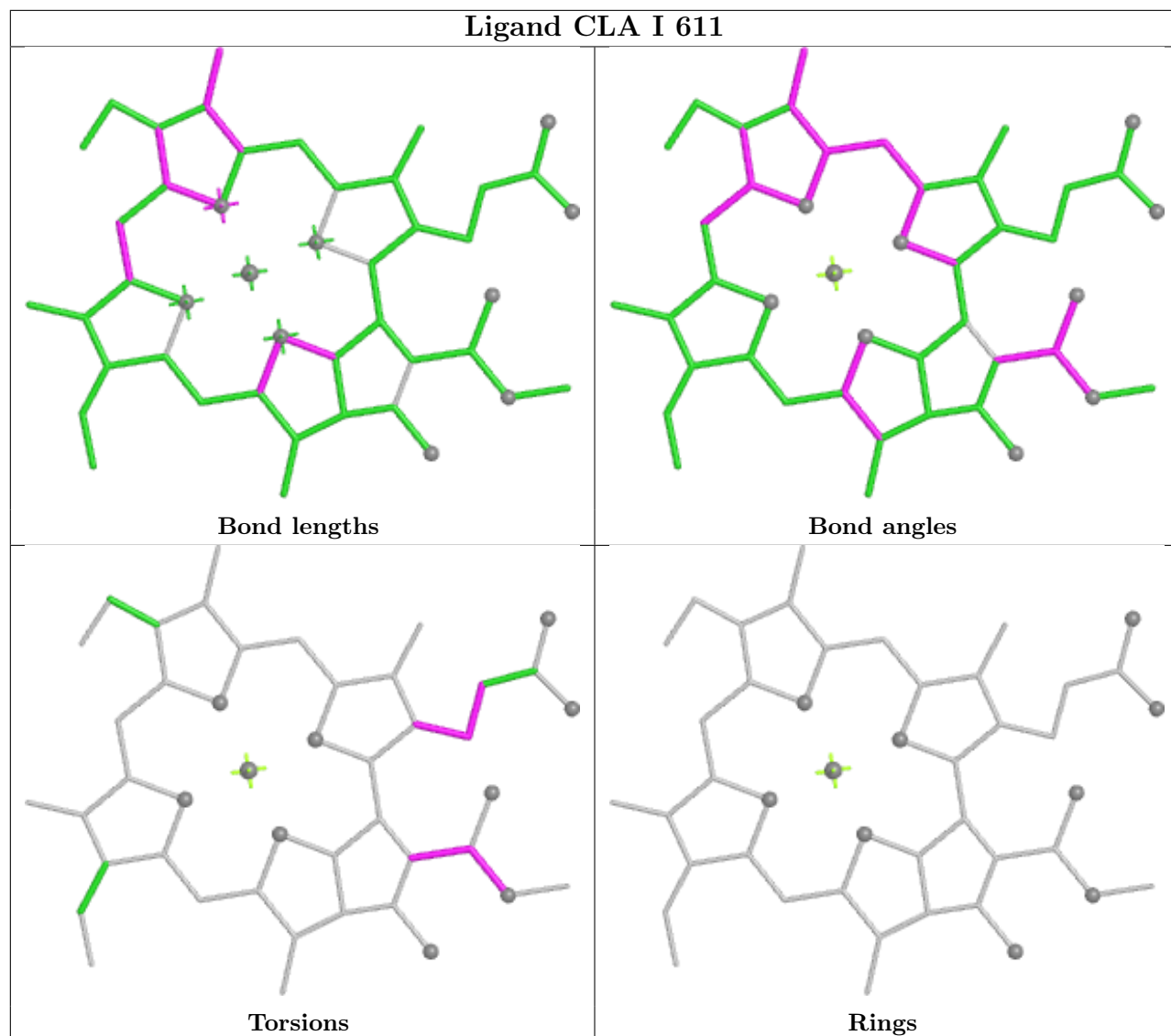


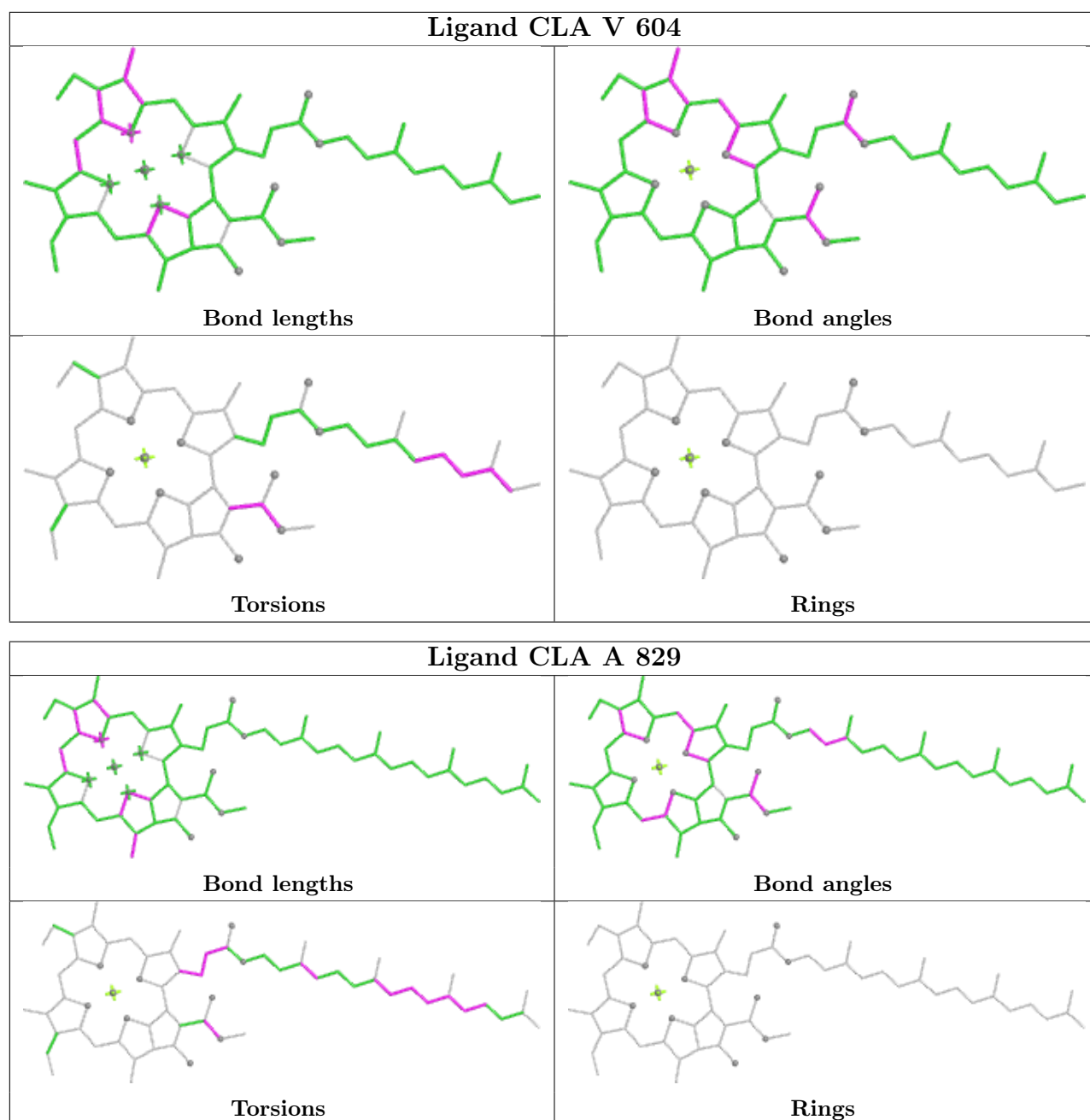


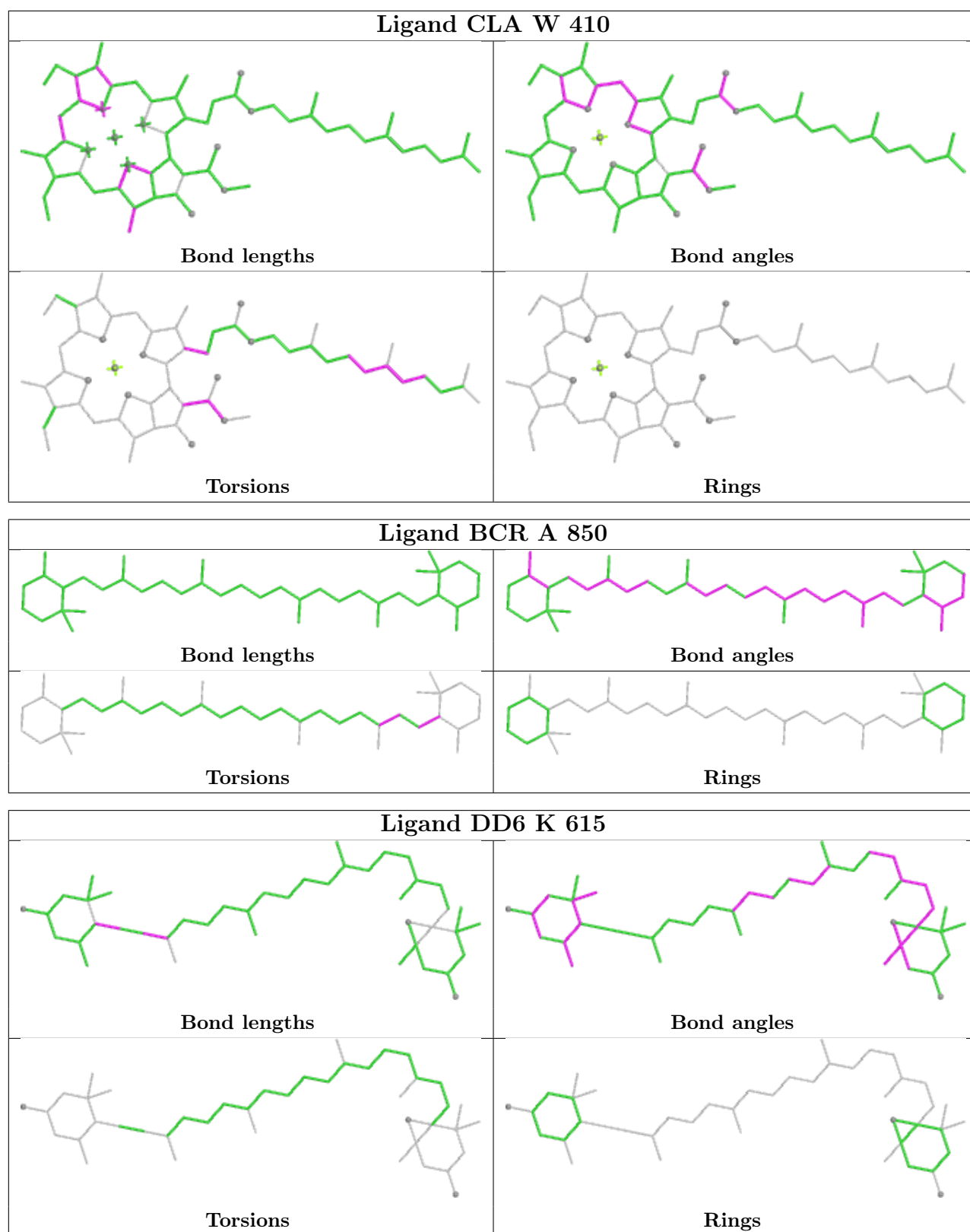


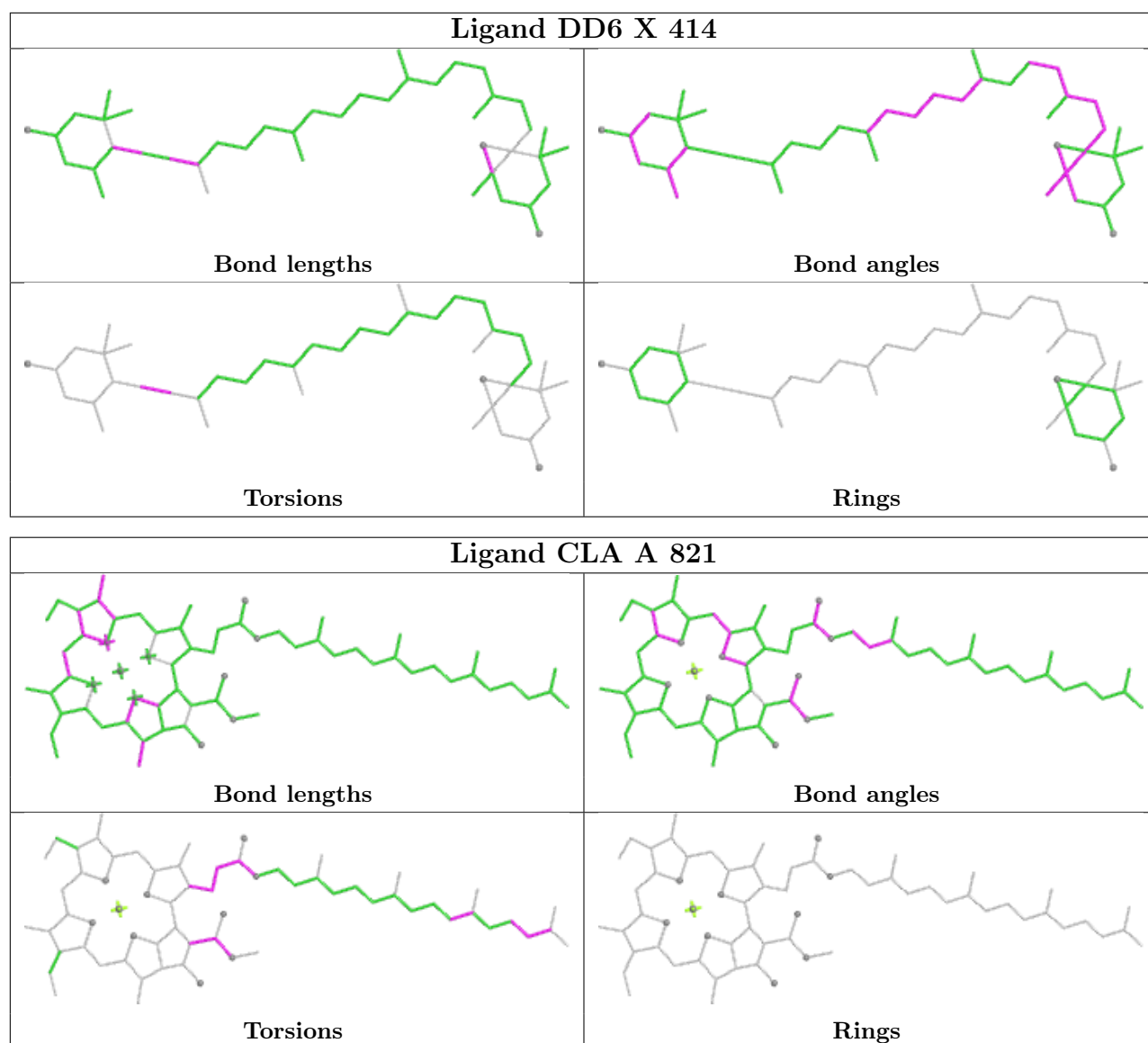


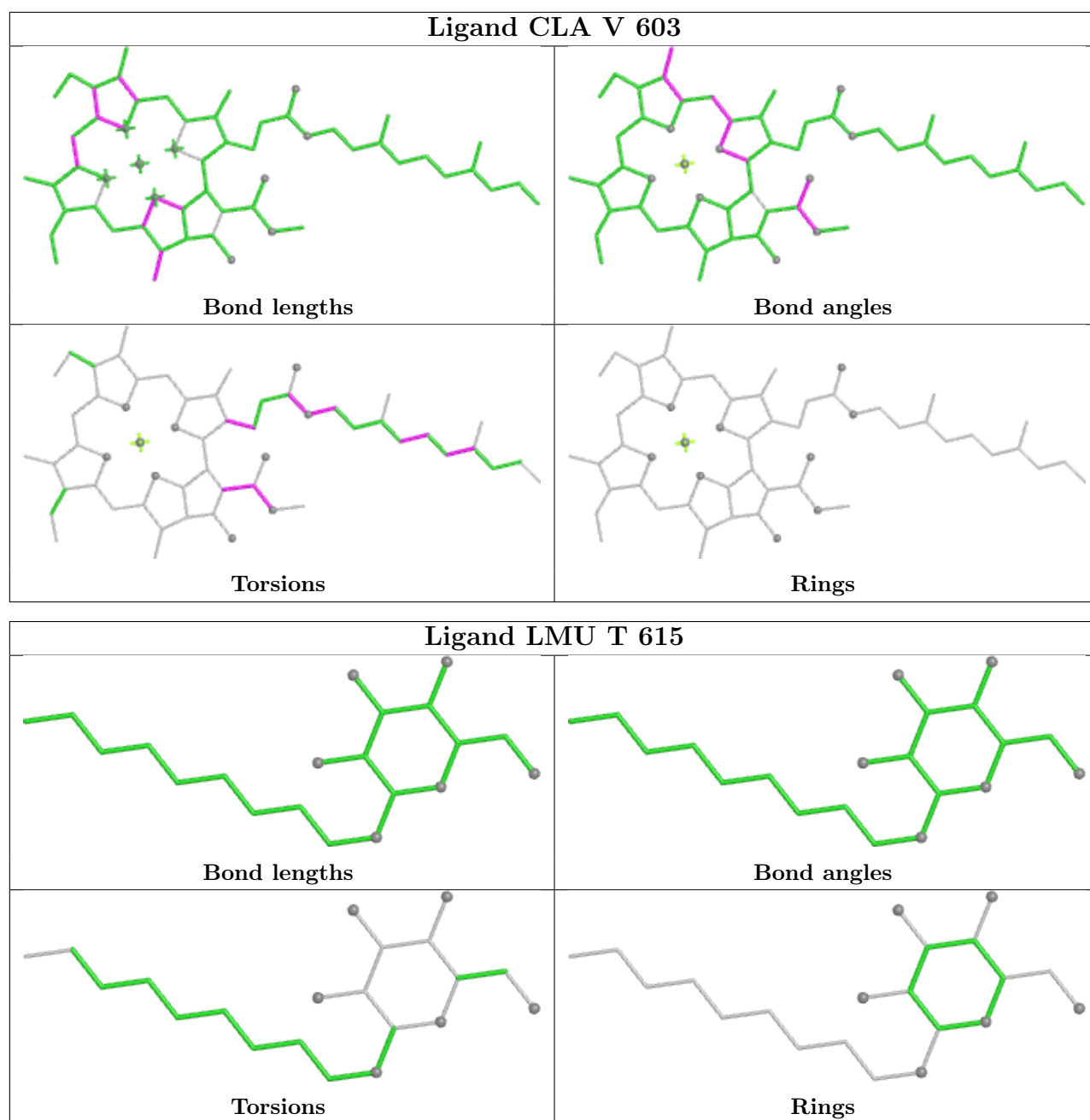
Ligand CLA I 611



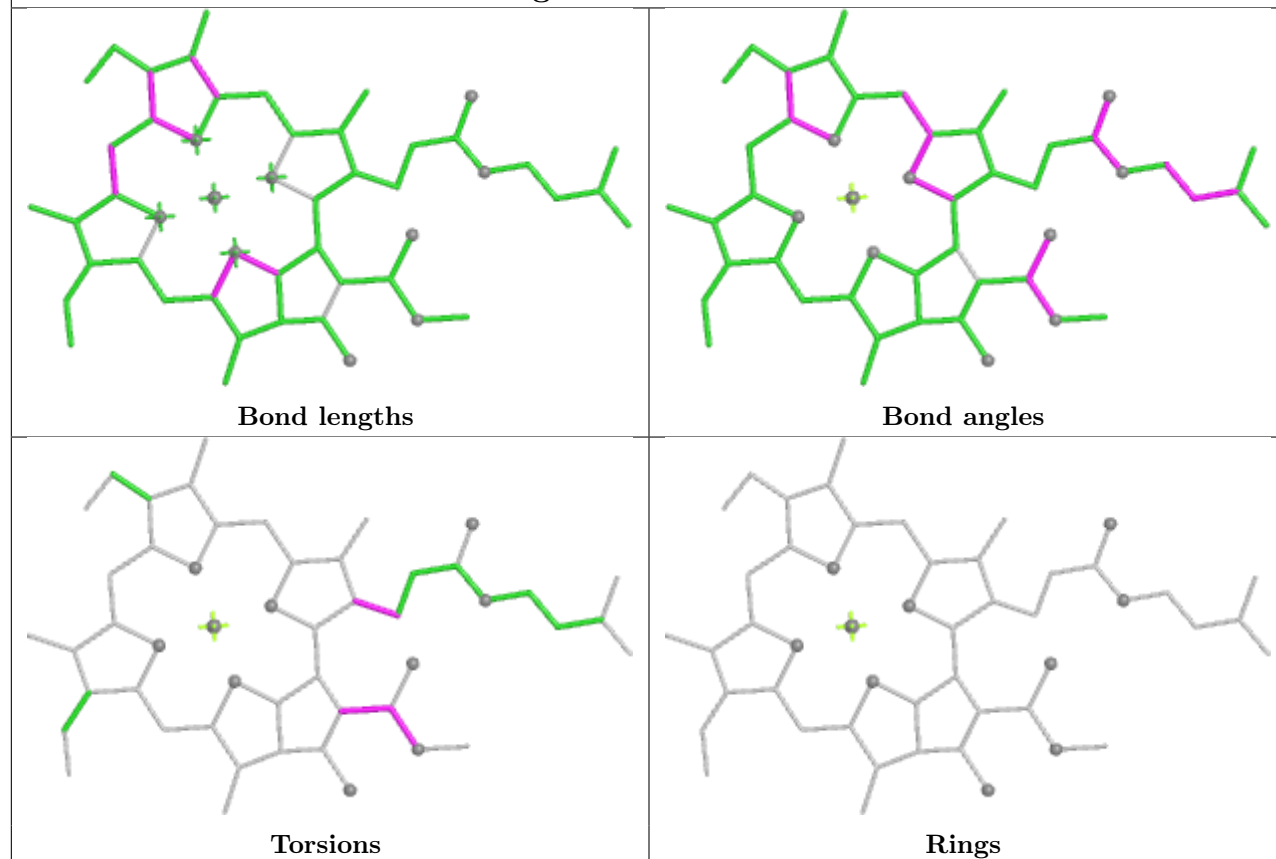




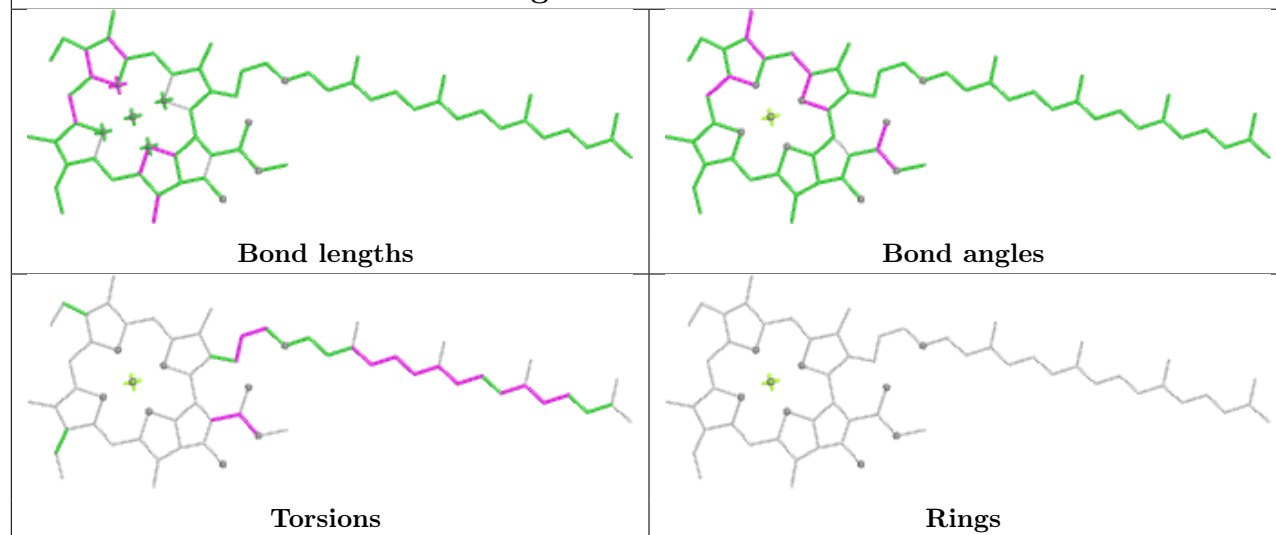


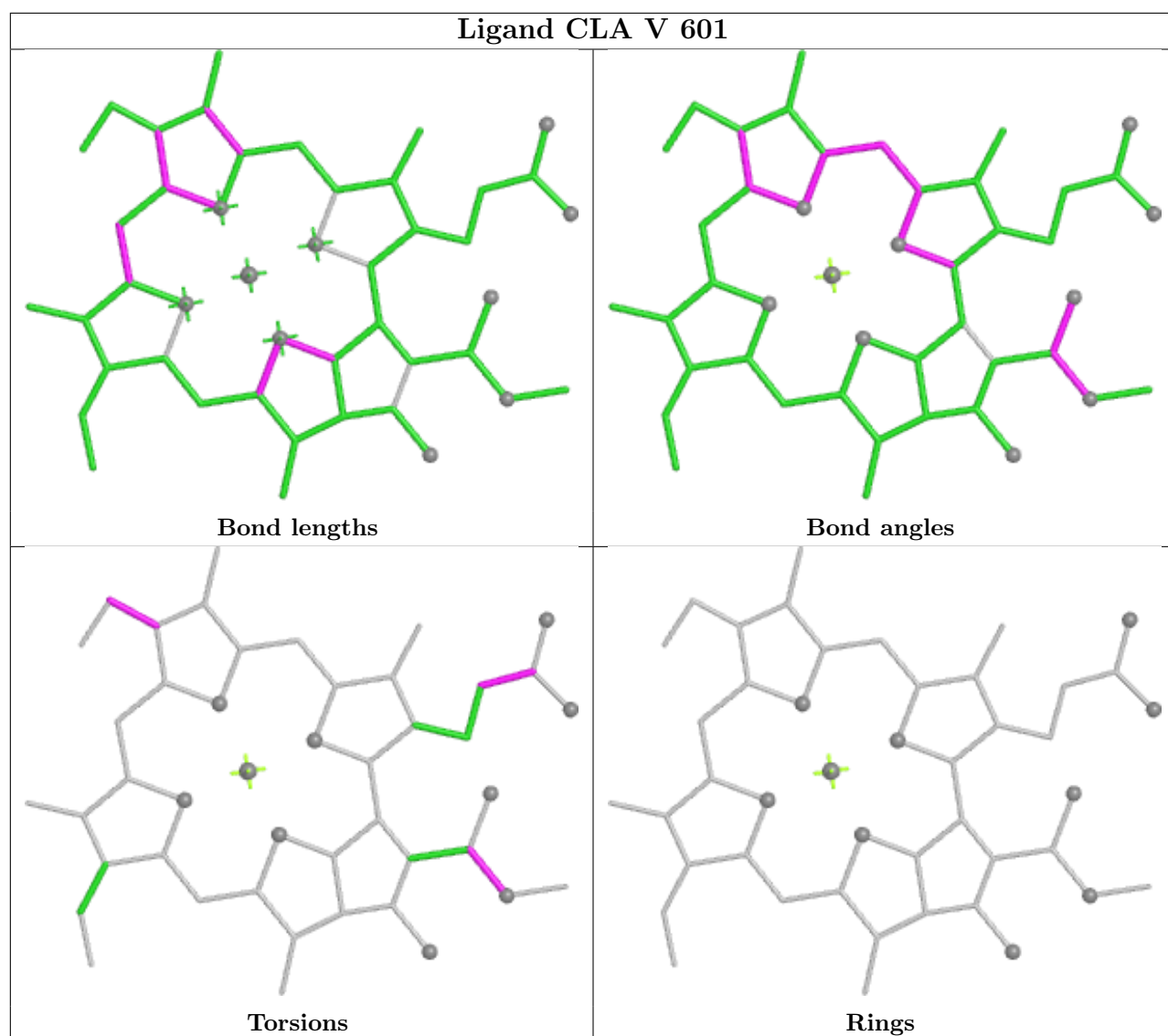


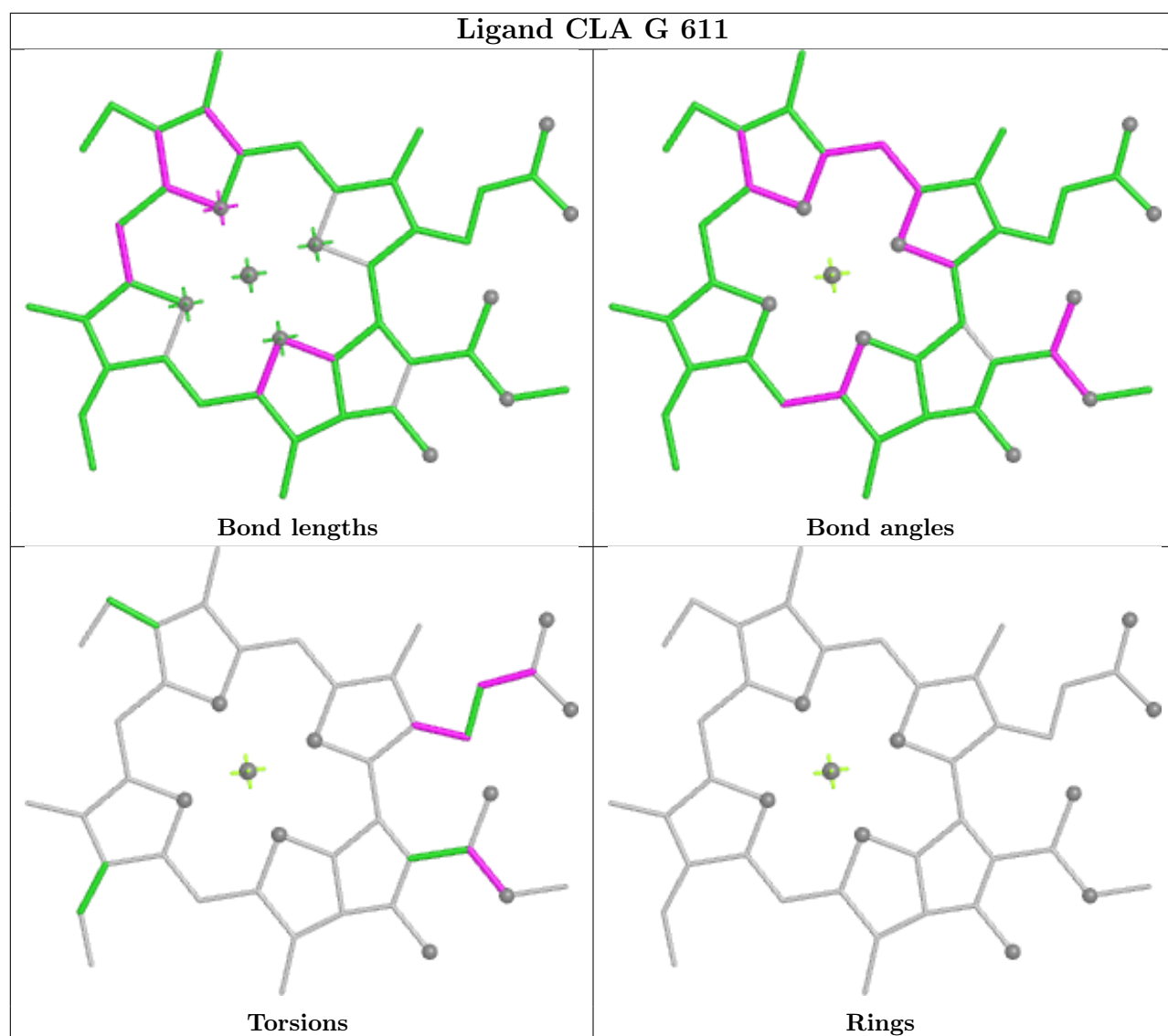
Ligand CLA T 606



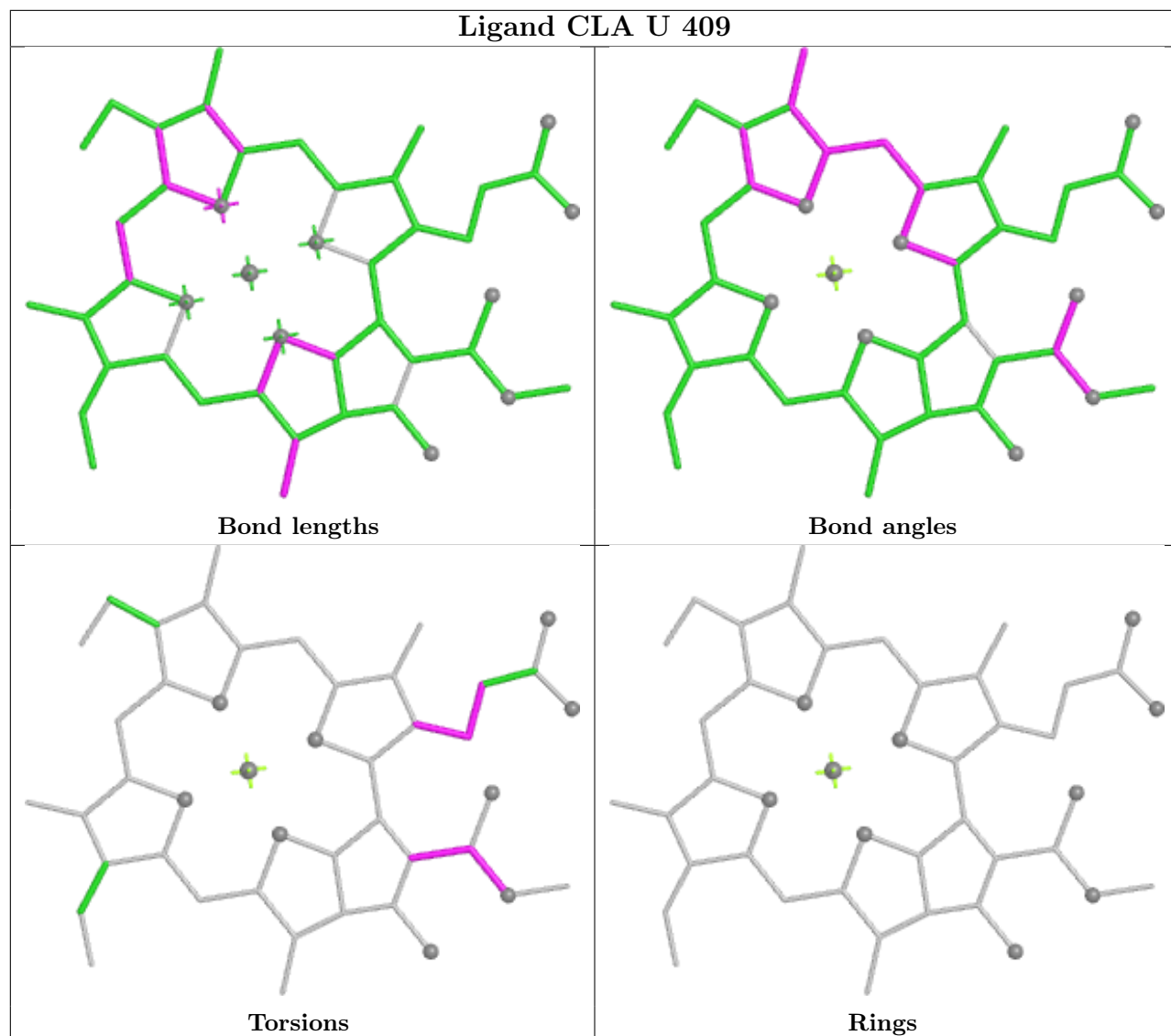
Ligand CLA K 604

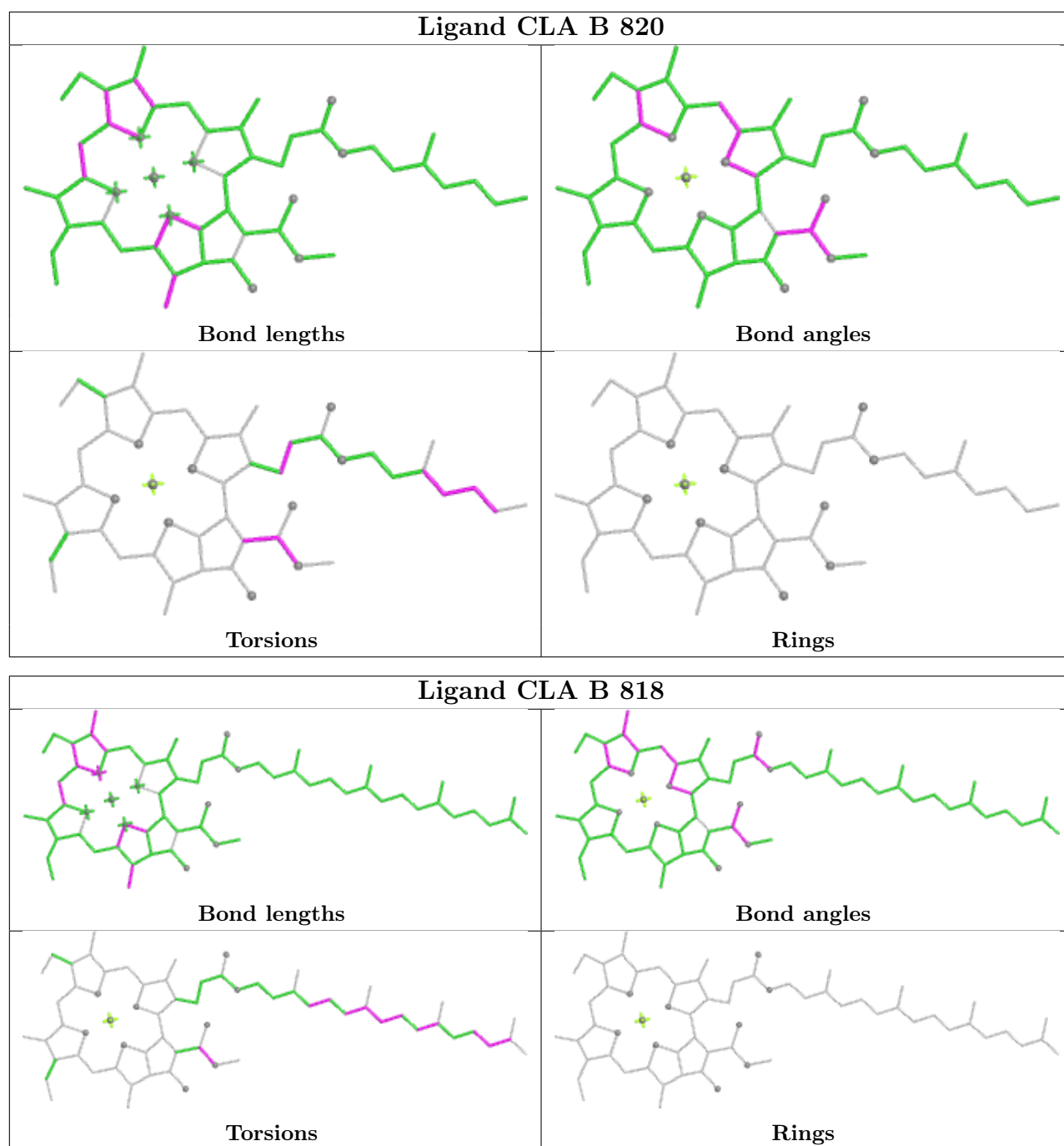


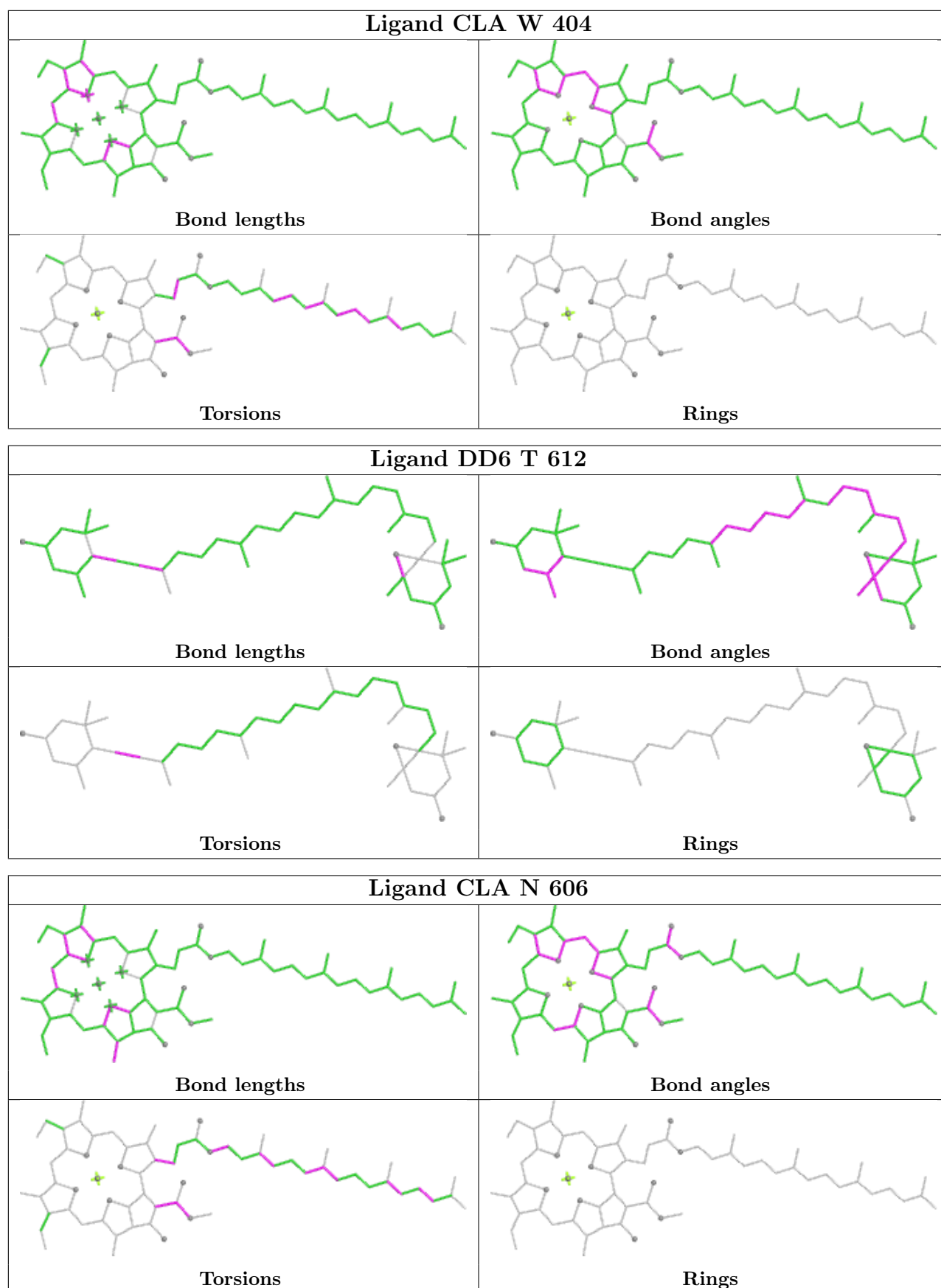


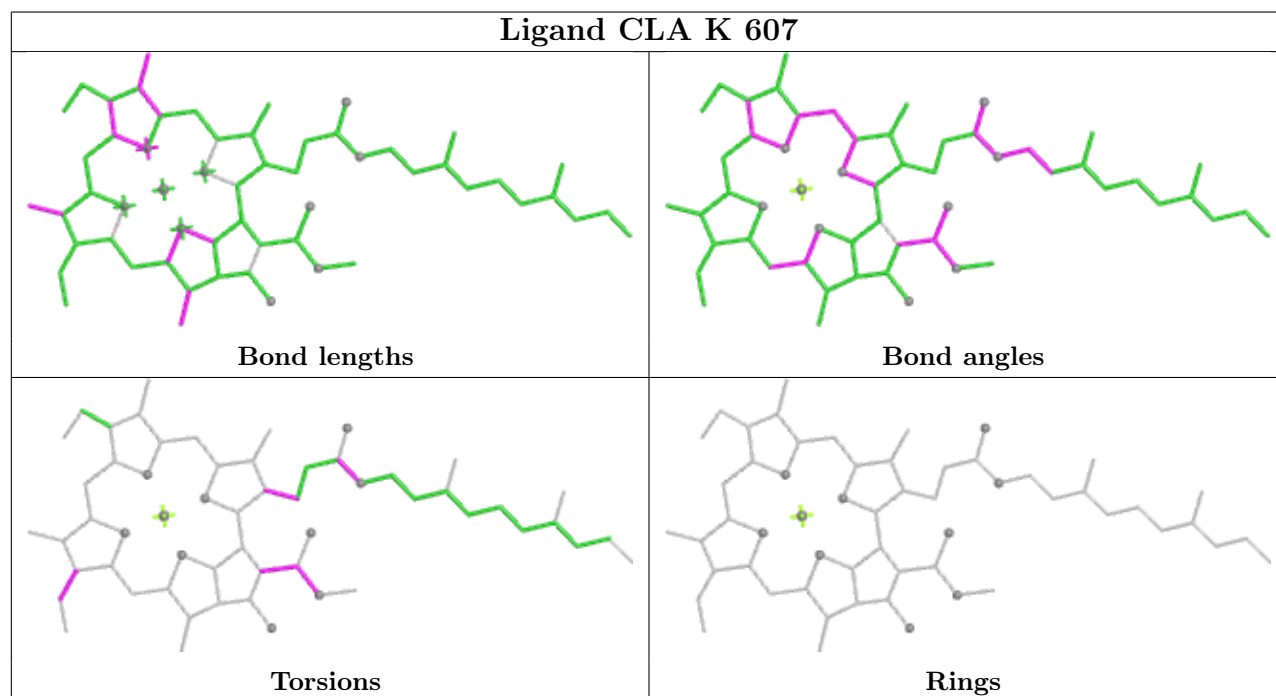
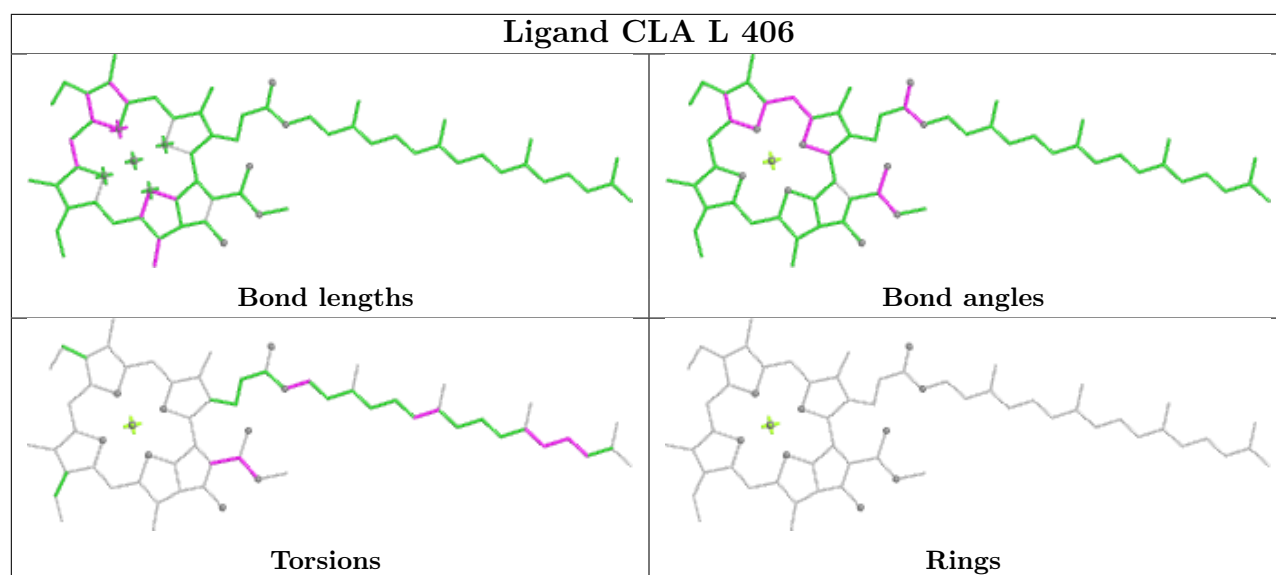


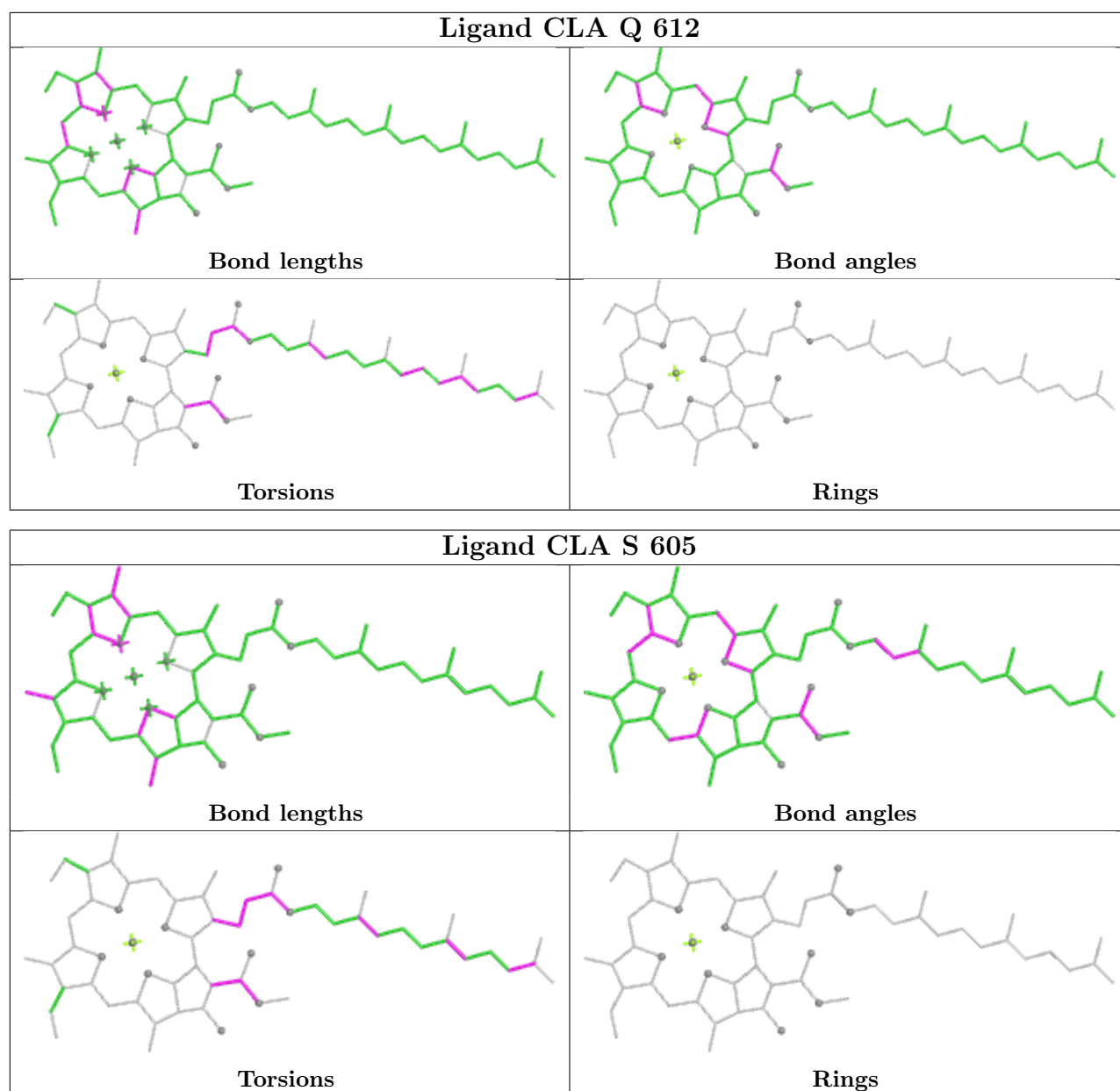
Ligand CLA U 409



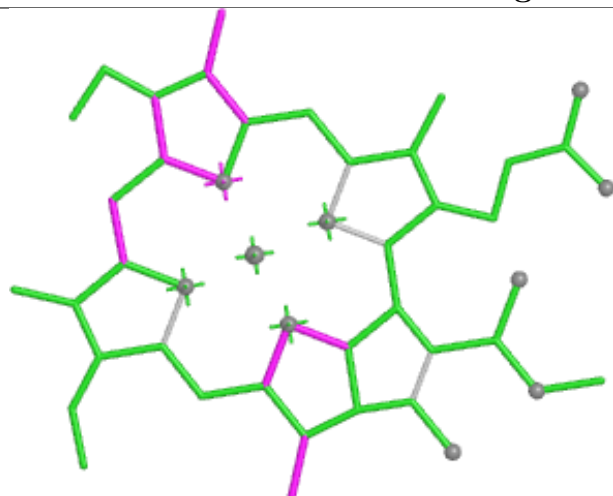




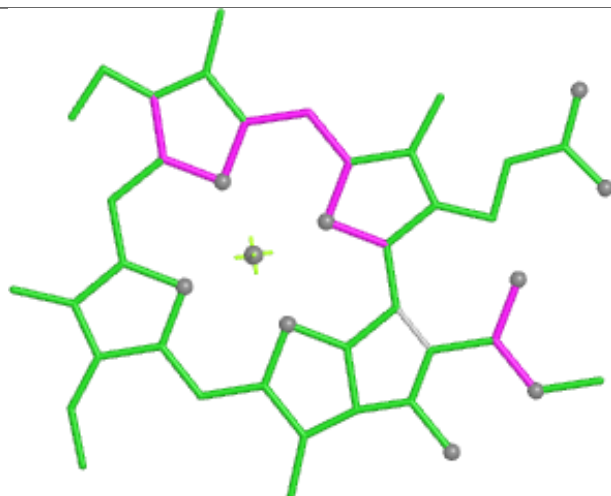




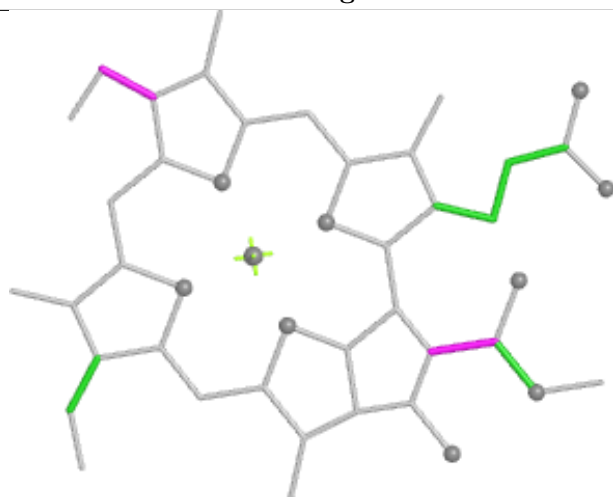
Ligand CLA B 837



Bond lengths



Bond angles

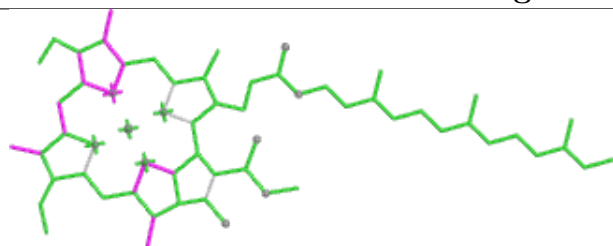


Torsions

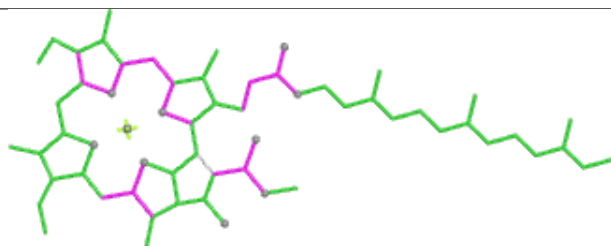


Rings

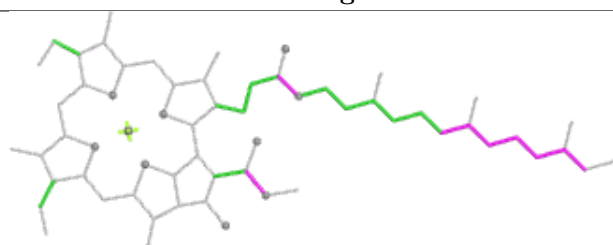
Ligand CLA A 816



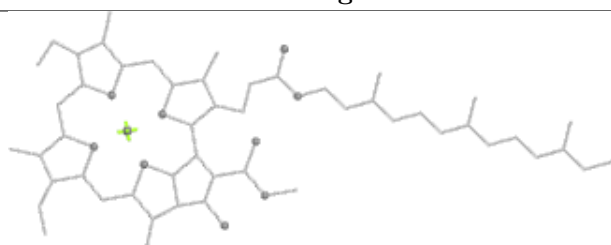
Bond lengths



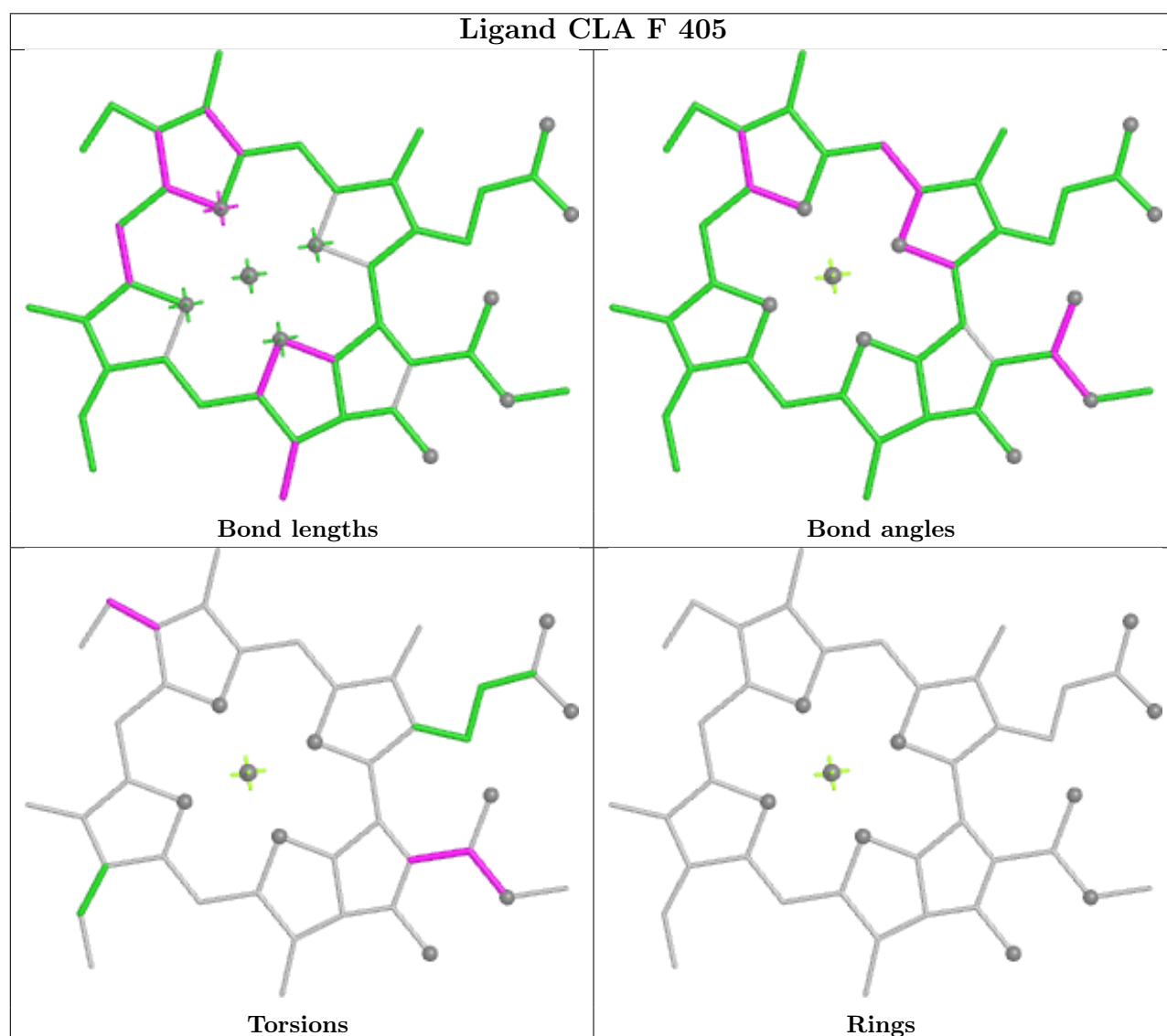
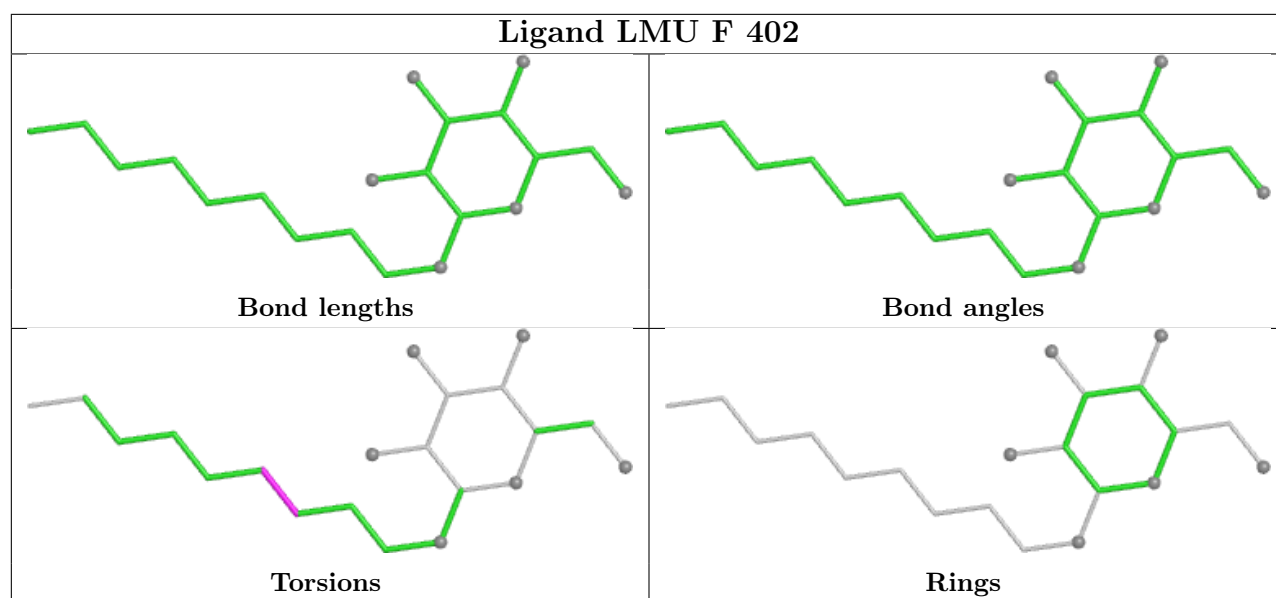
Bond angles

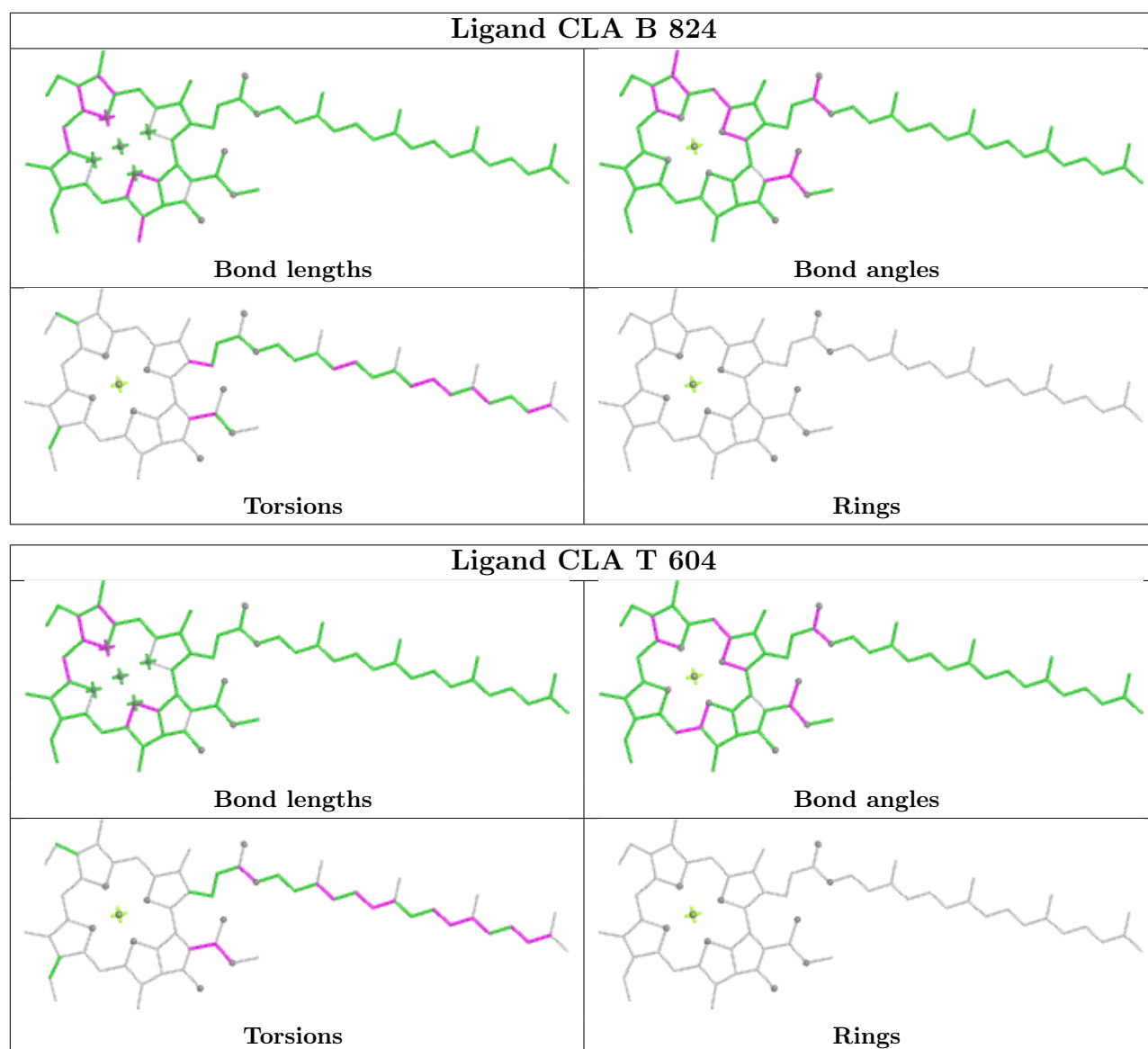


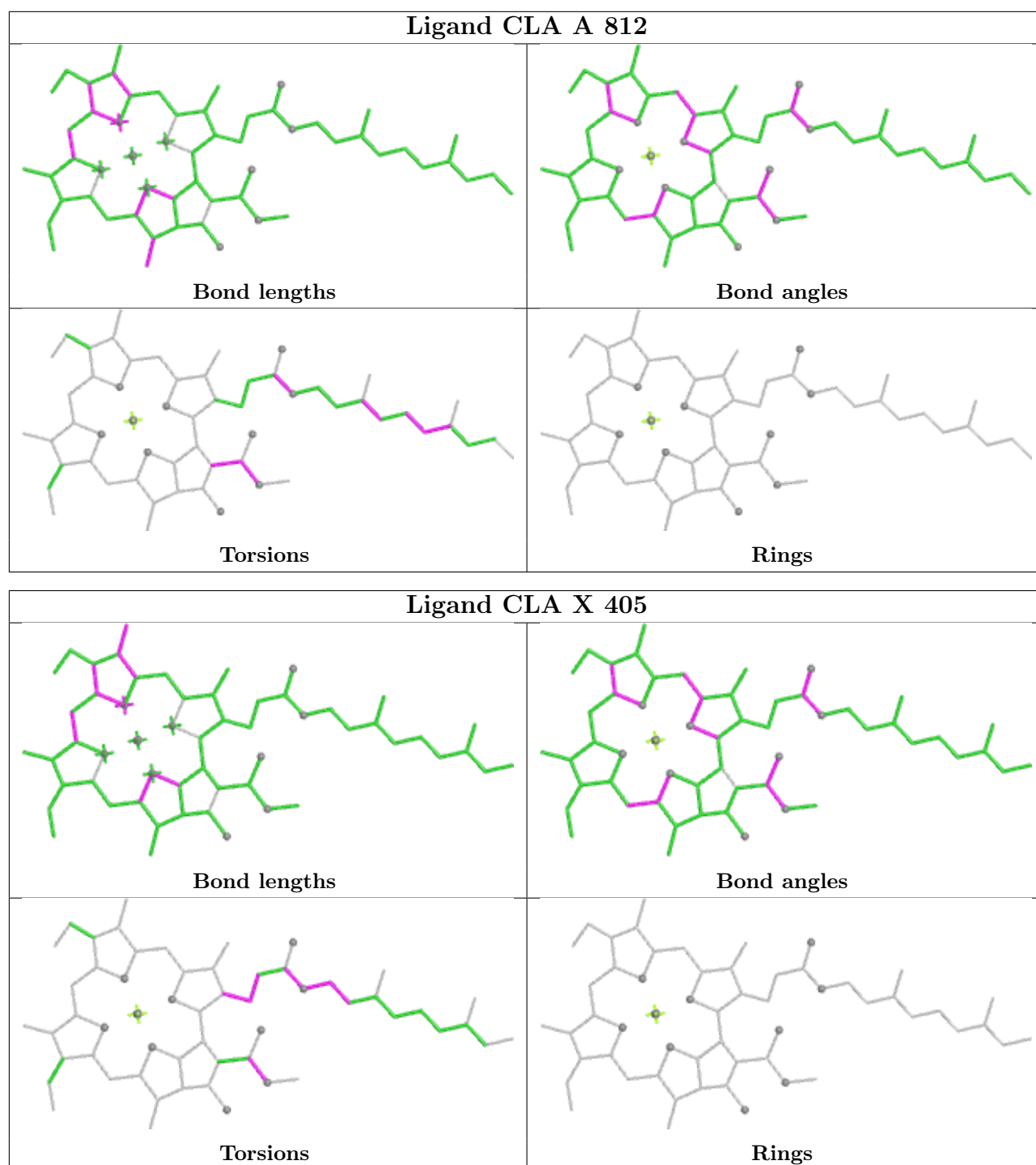
Torsions

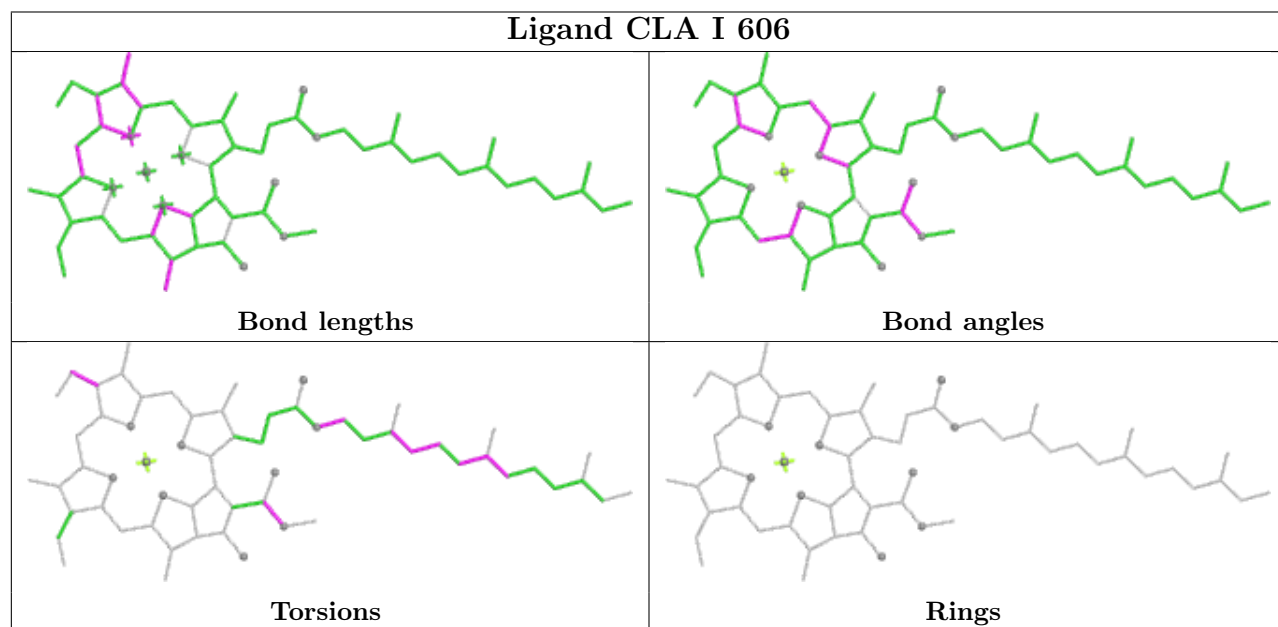
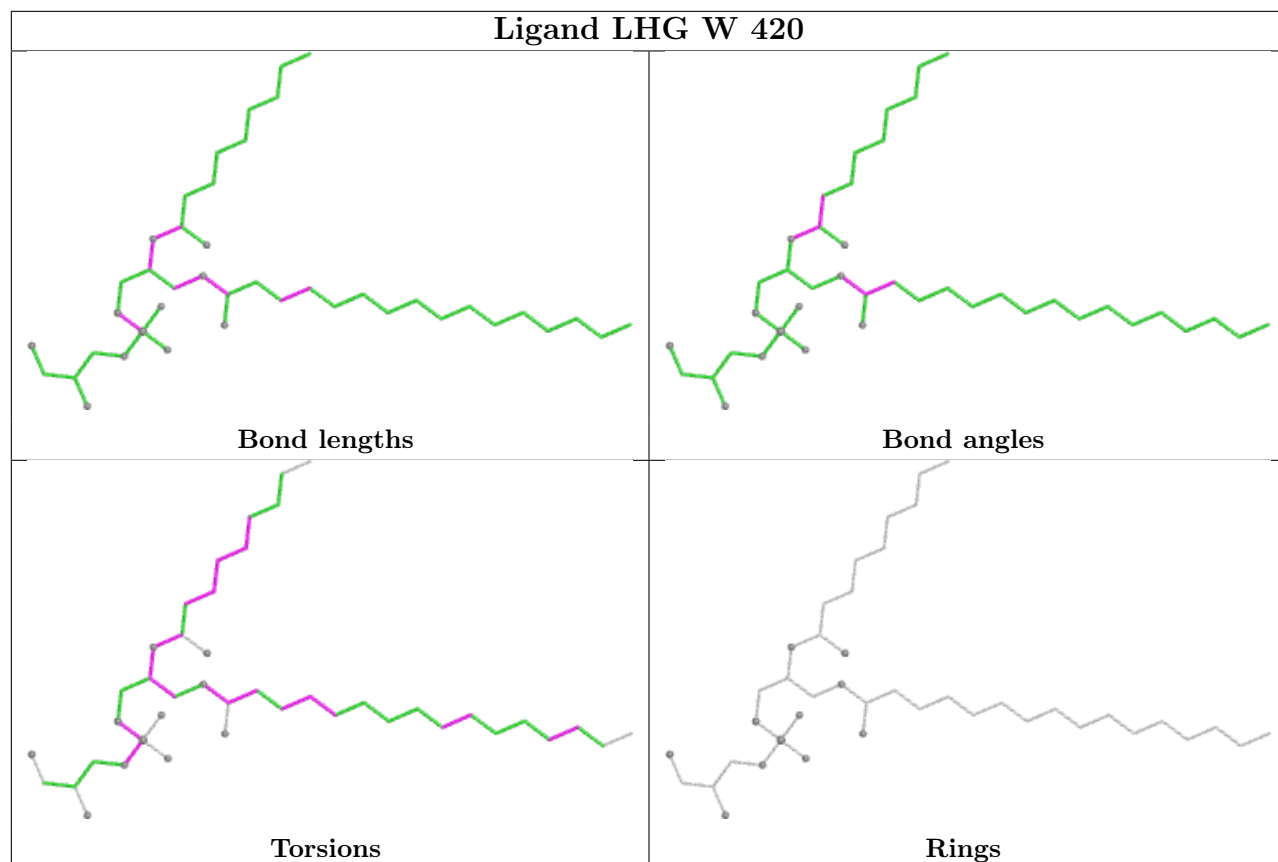


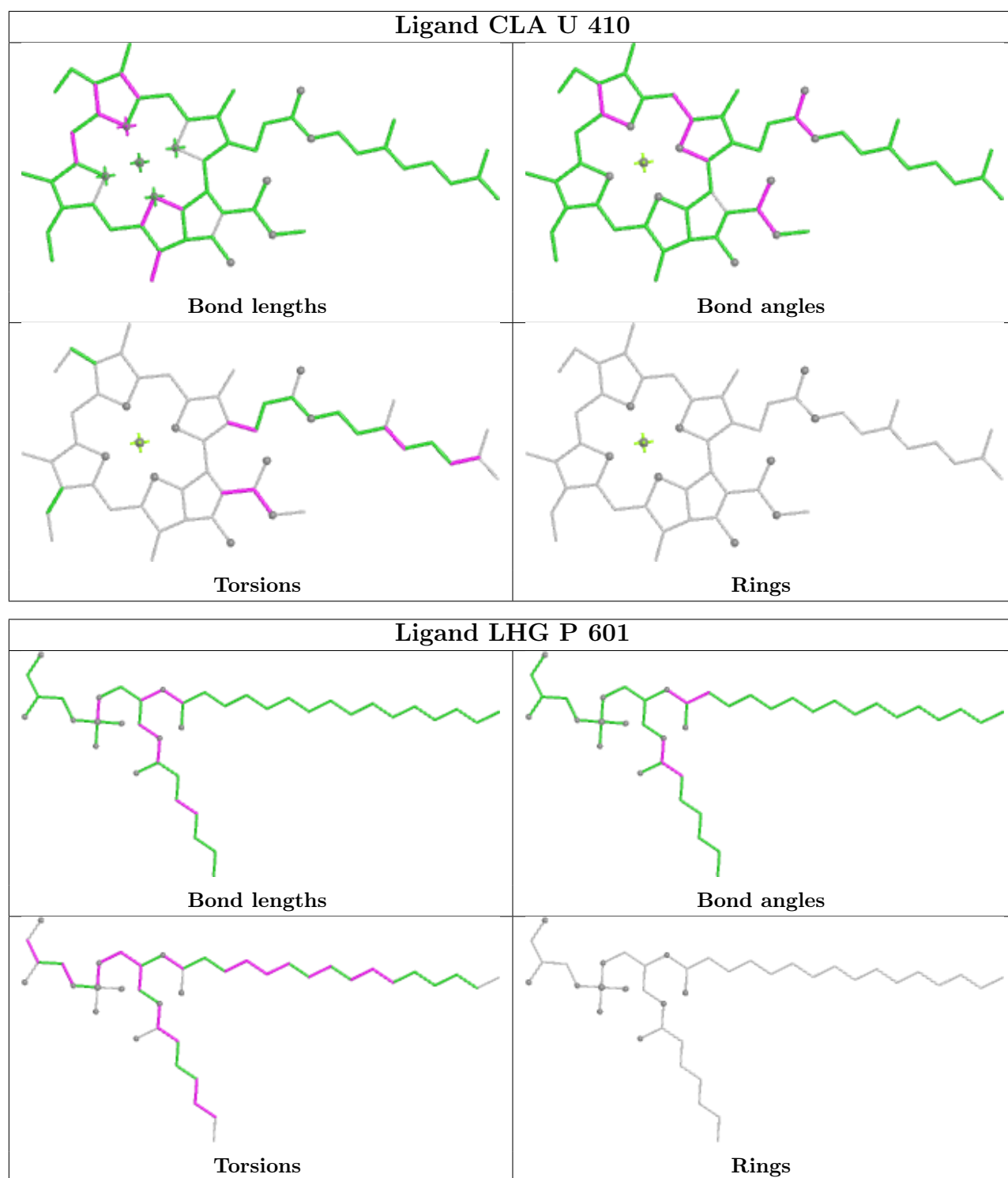
Rings

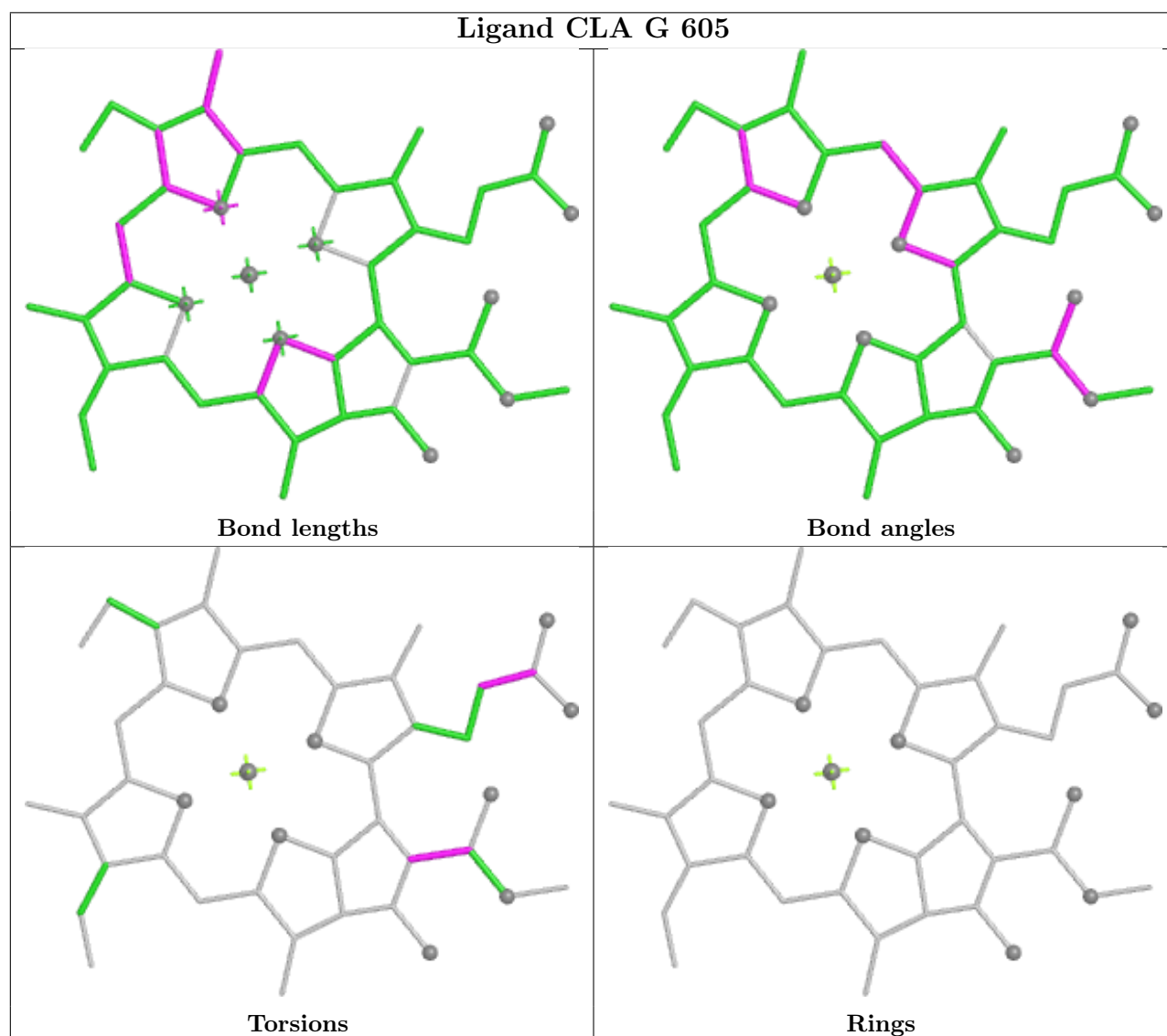
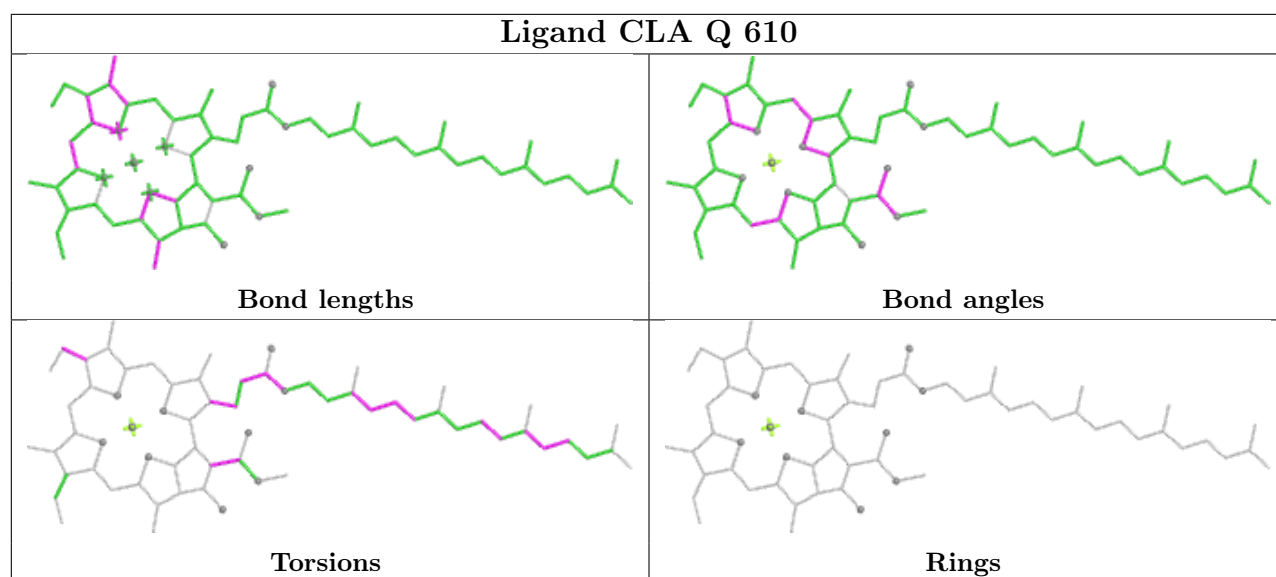


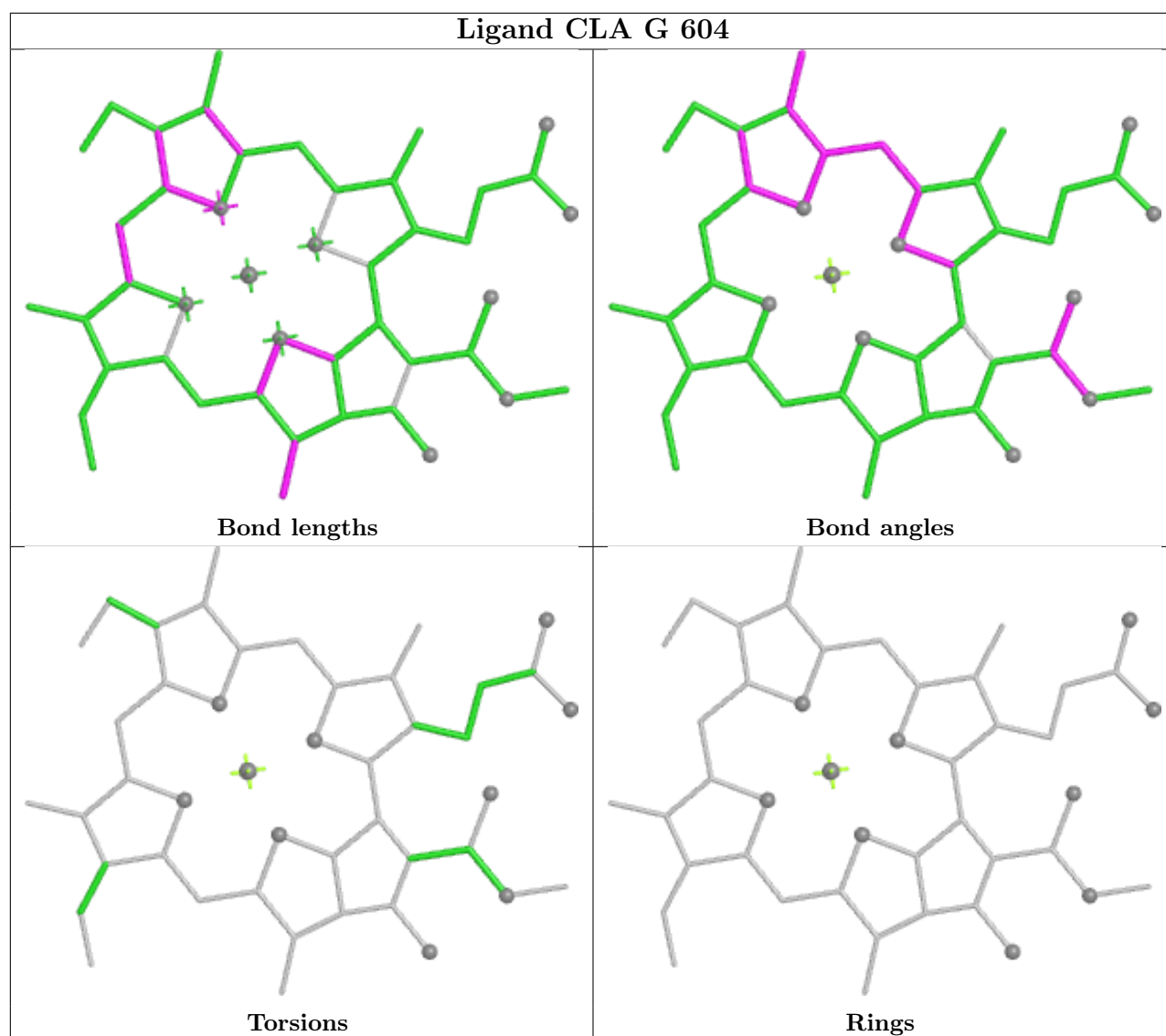


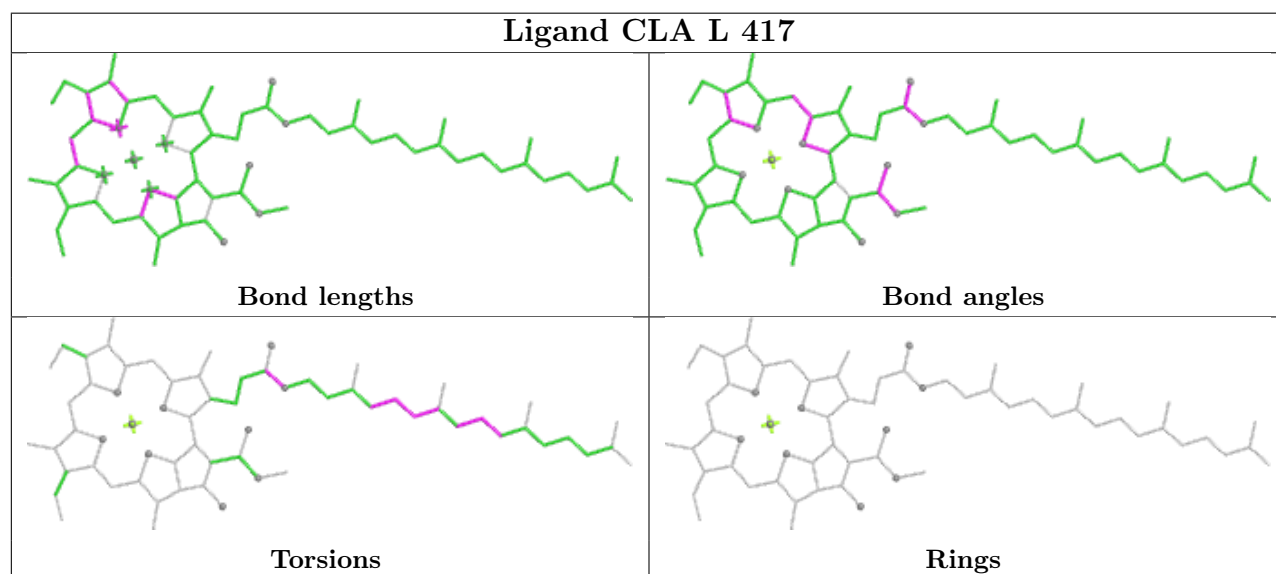
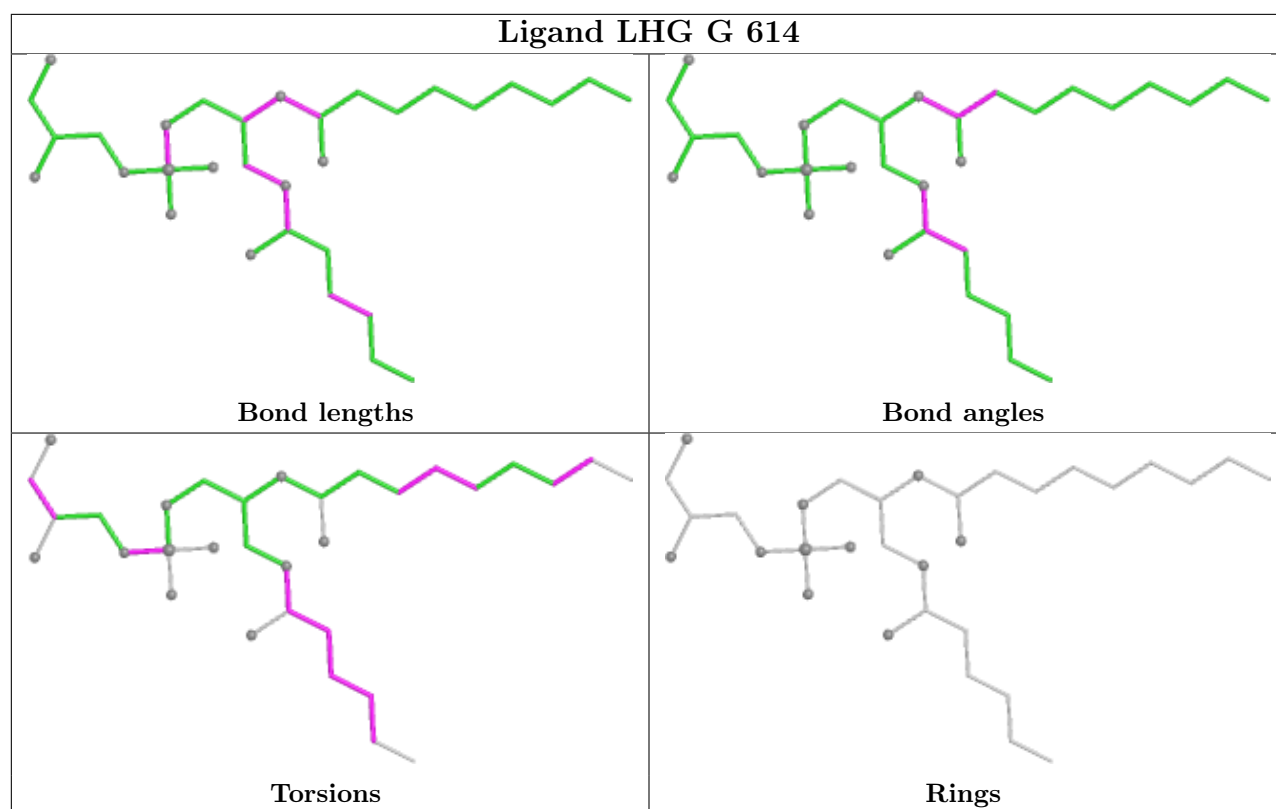


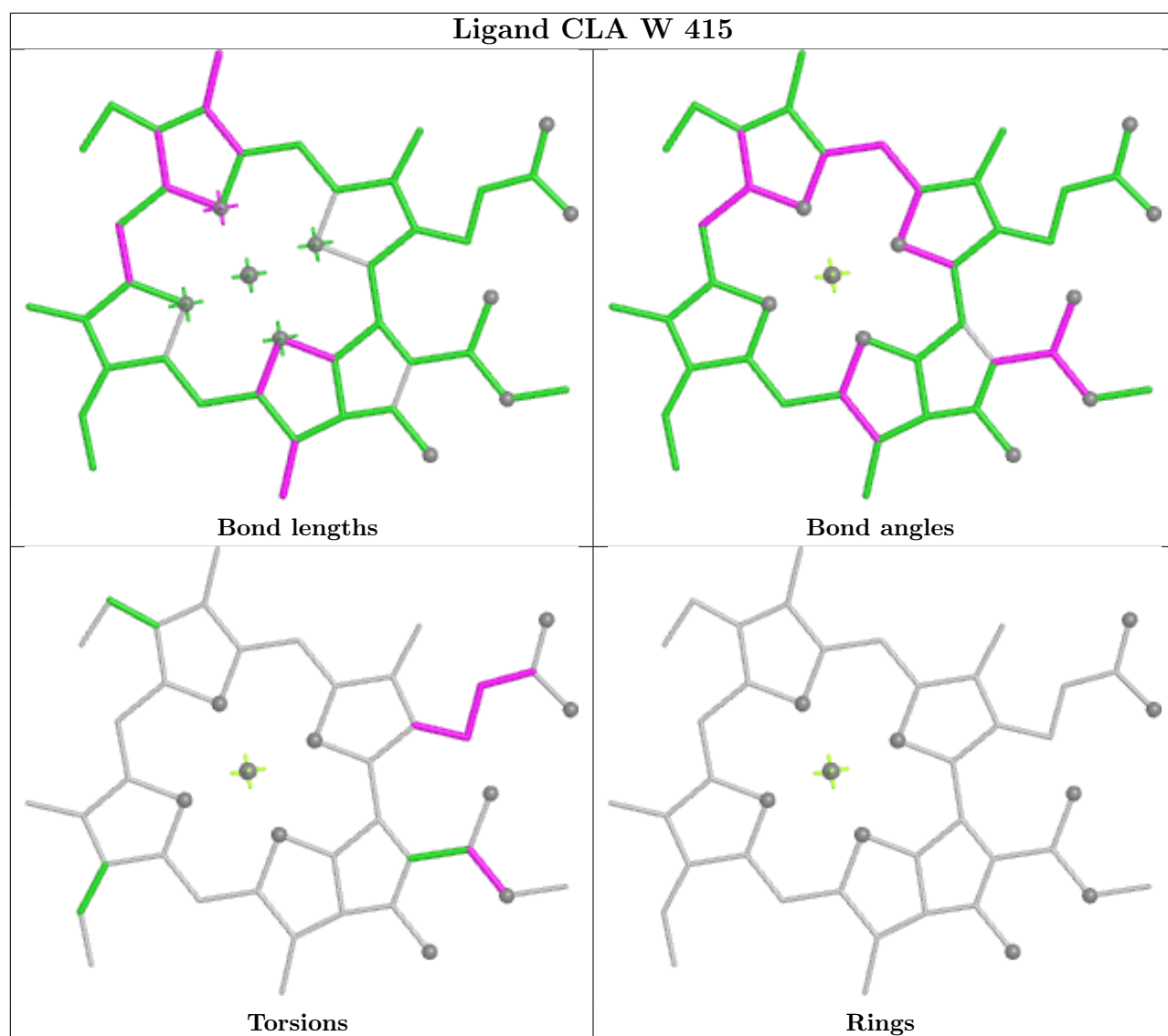




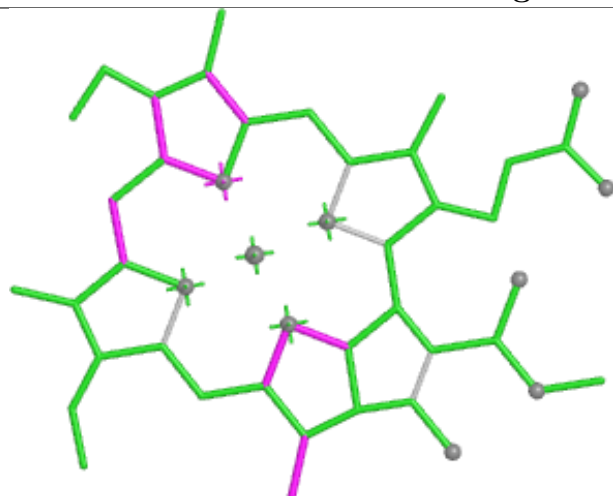




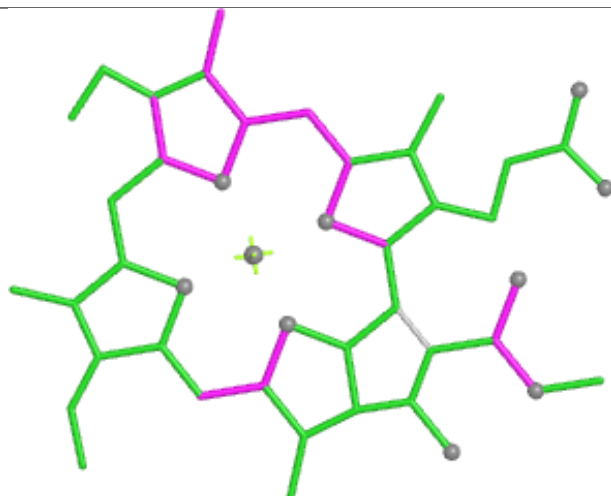




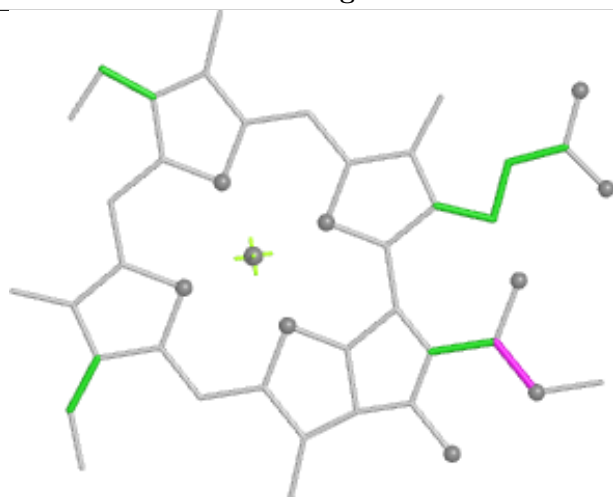
Ligand CLA K 612



Bond lengths



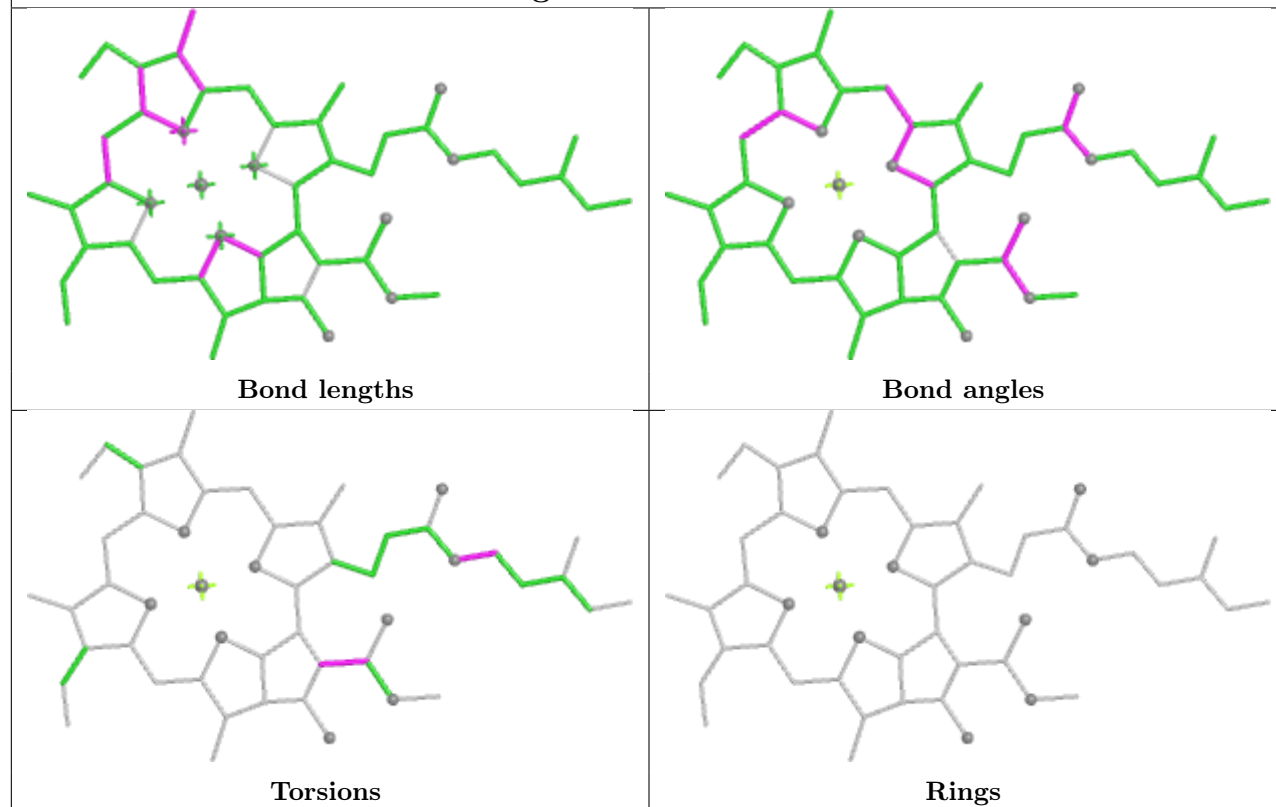
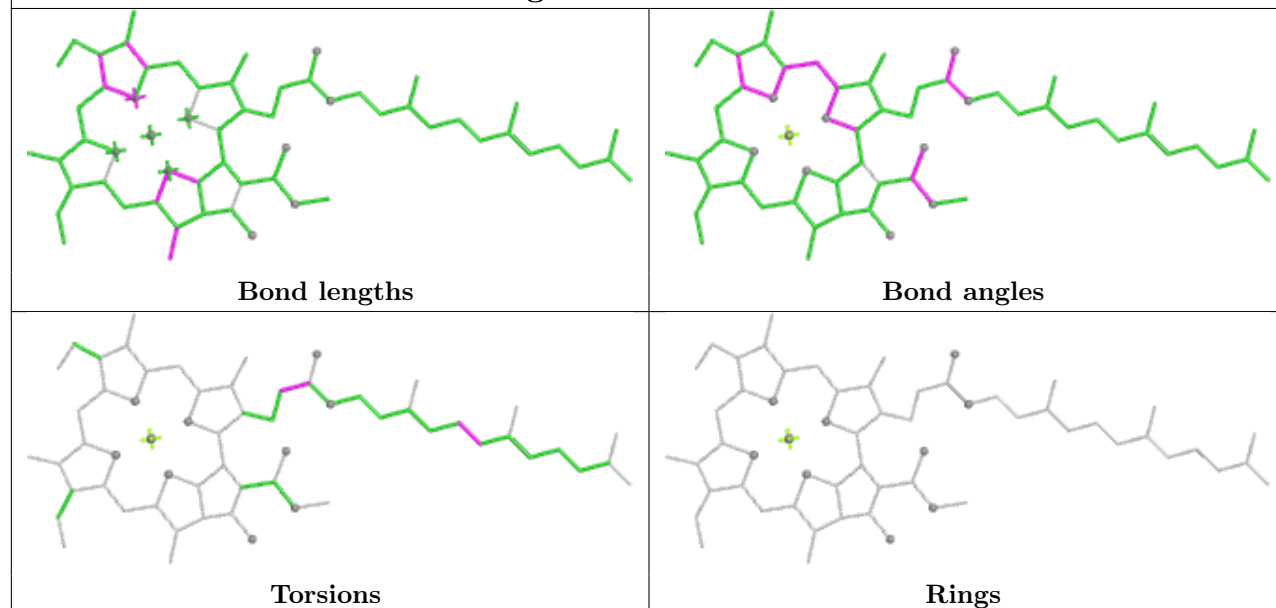
Bond angles

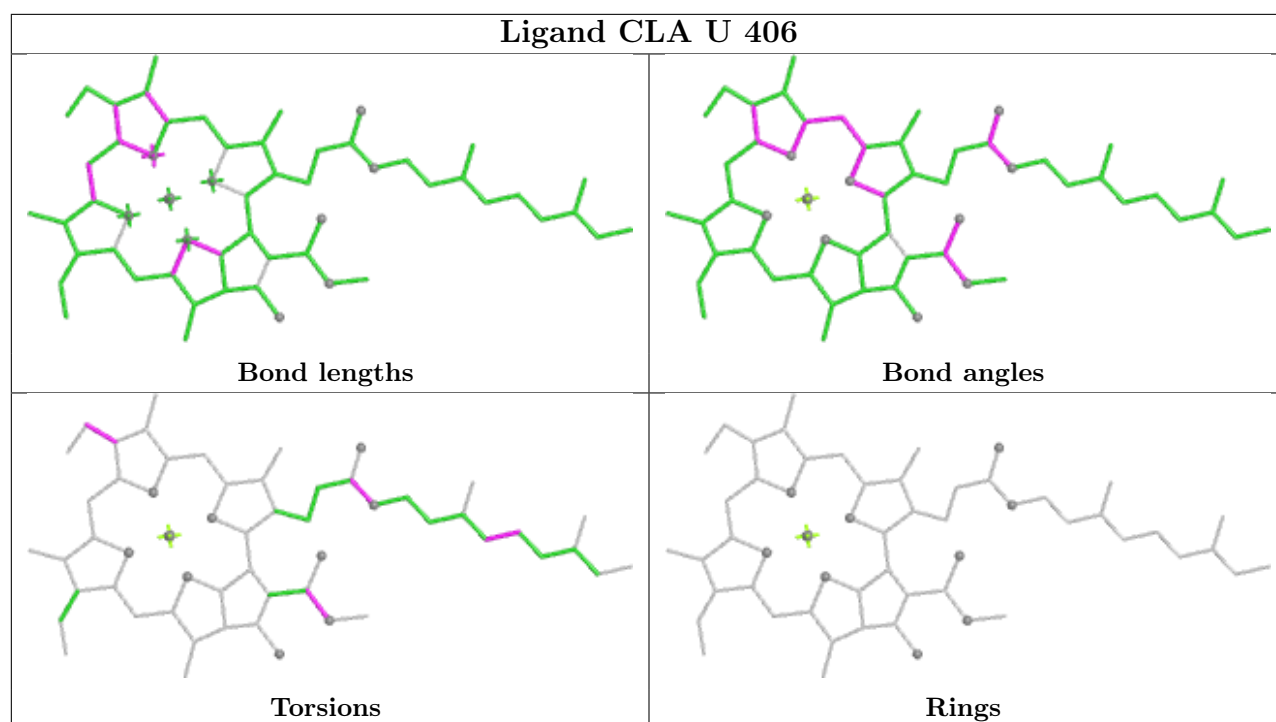


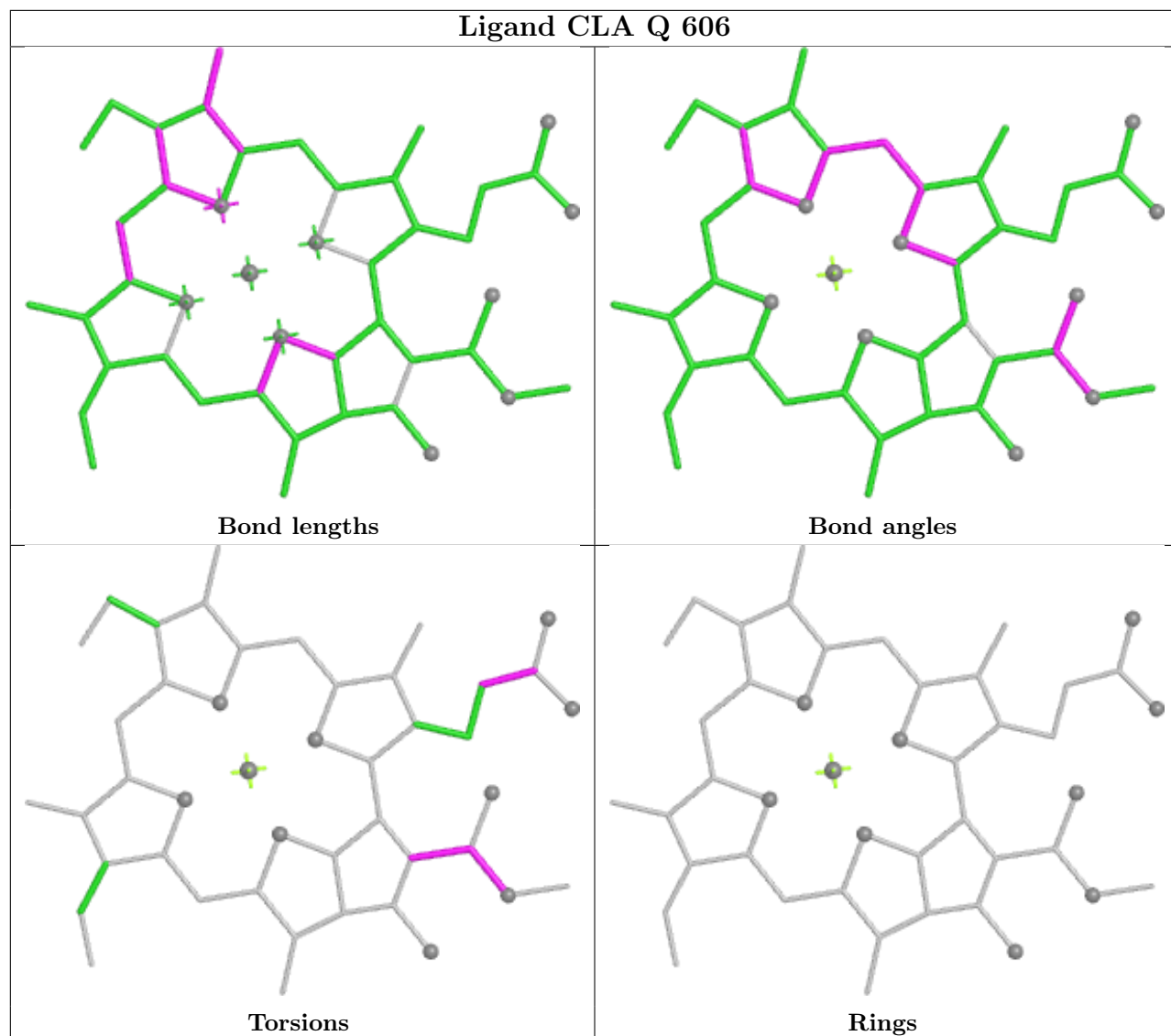
Torsions



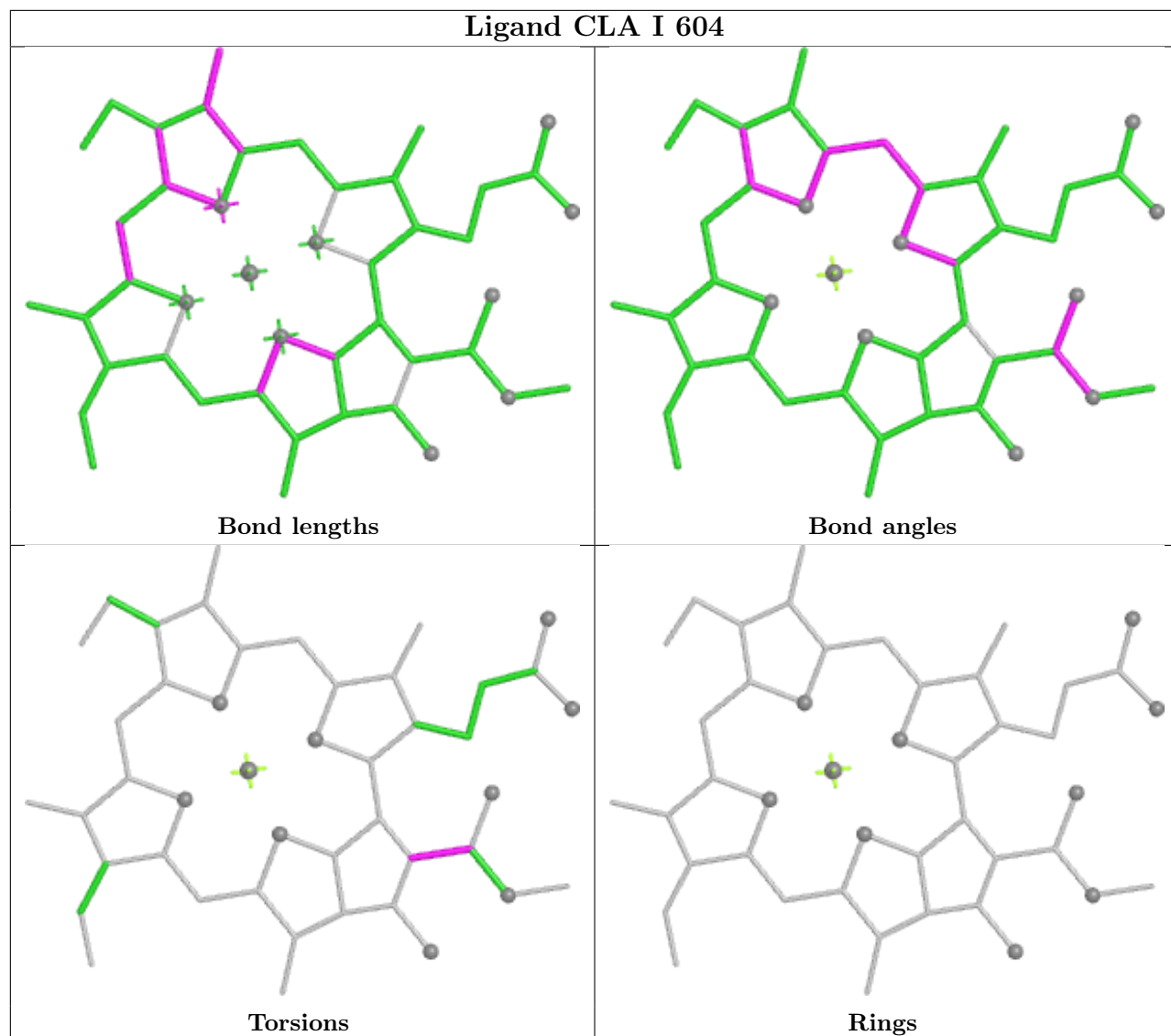
Rings

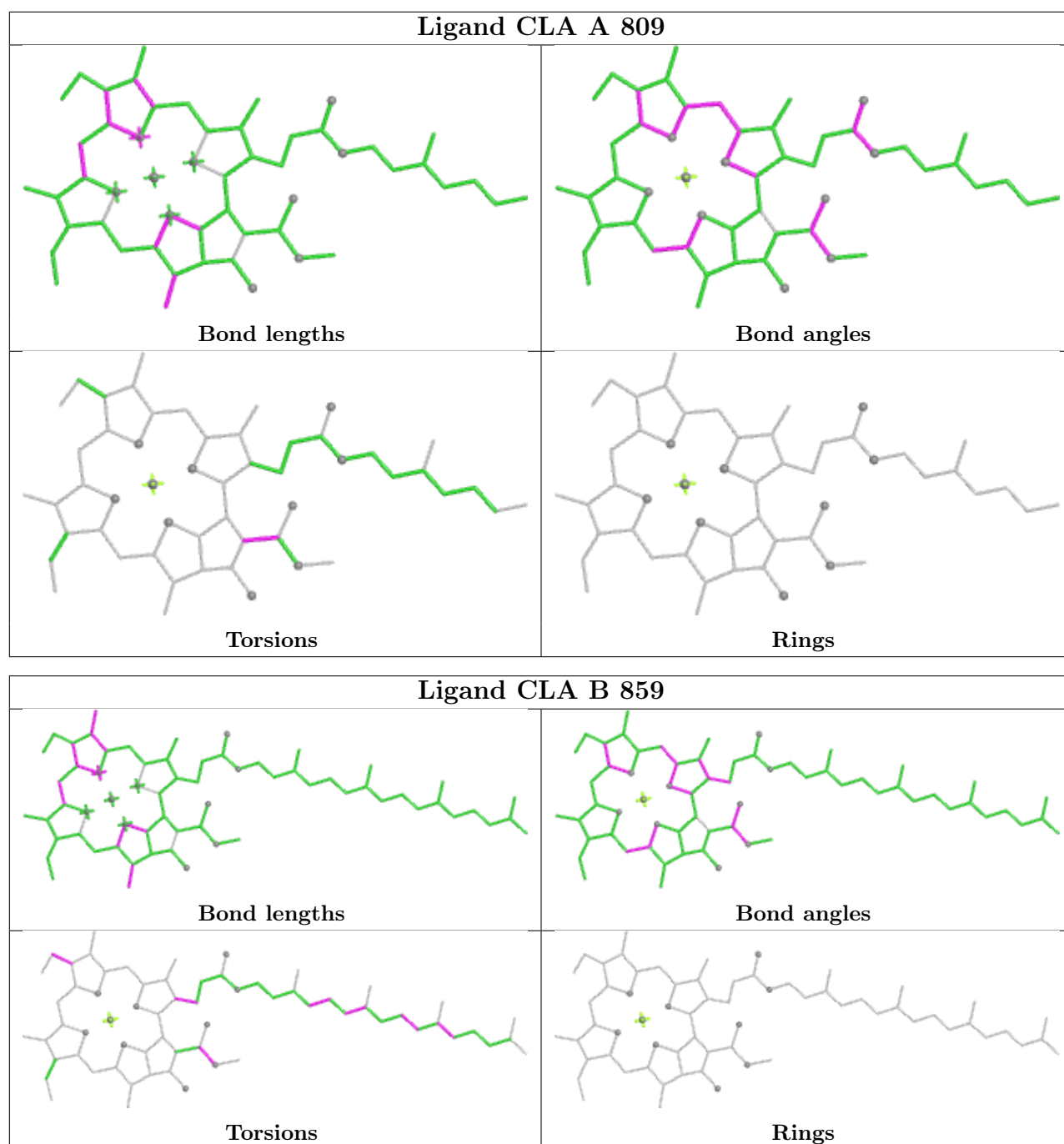
Ligand CLA B 836**Ligand CLA W 405**

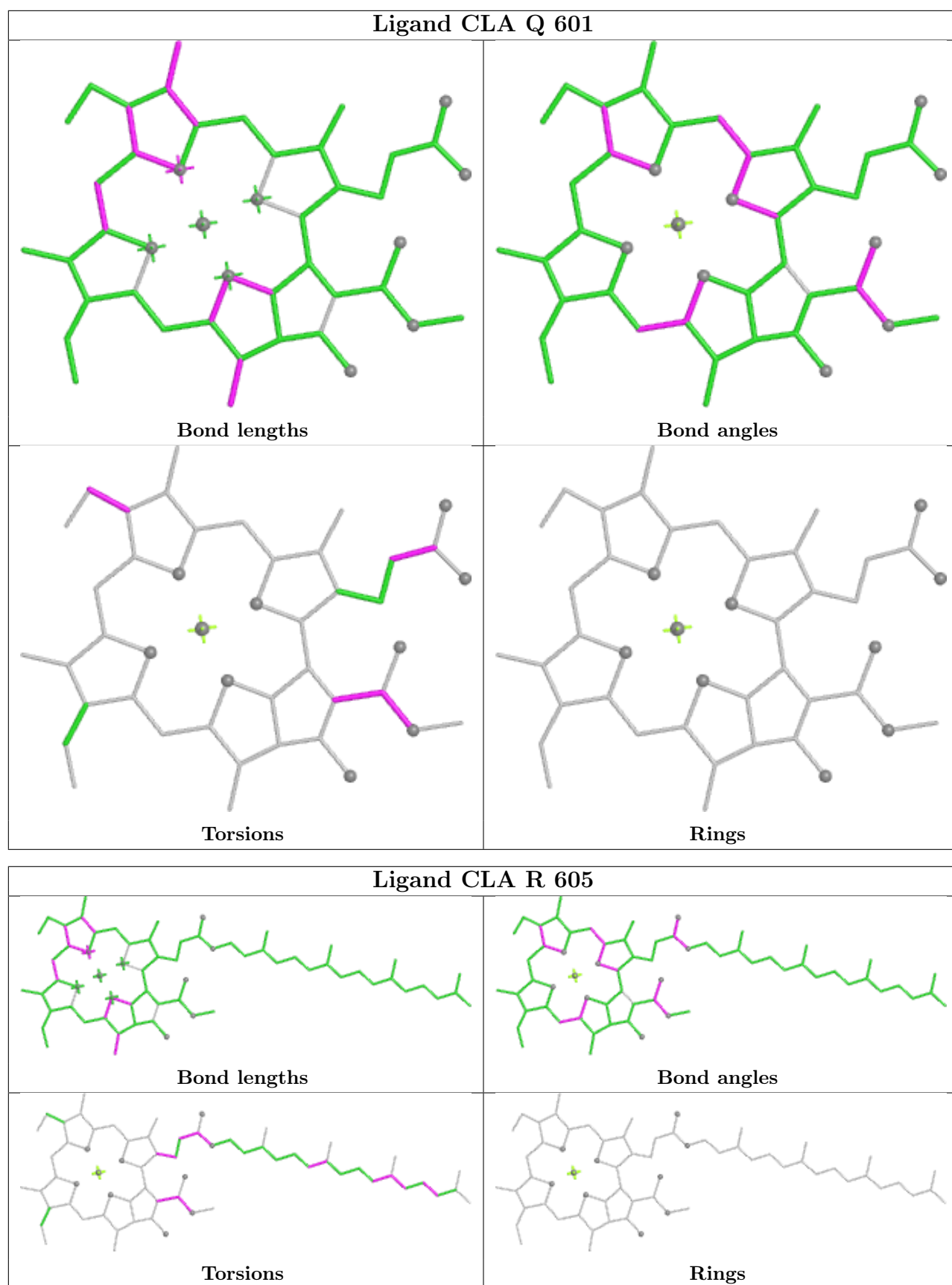




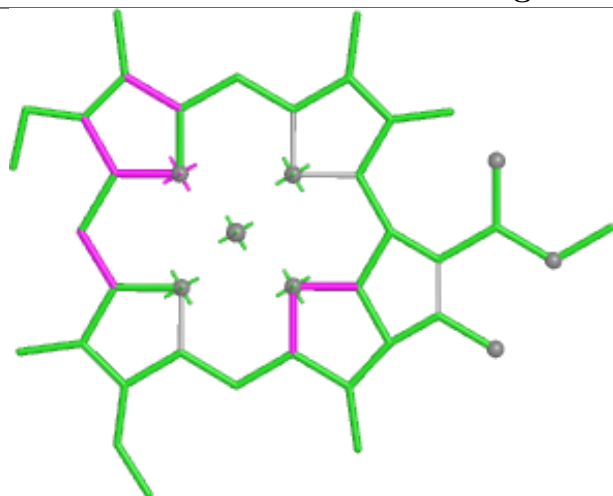
Ligand CLA I 604



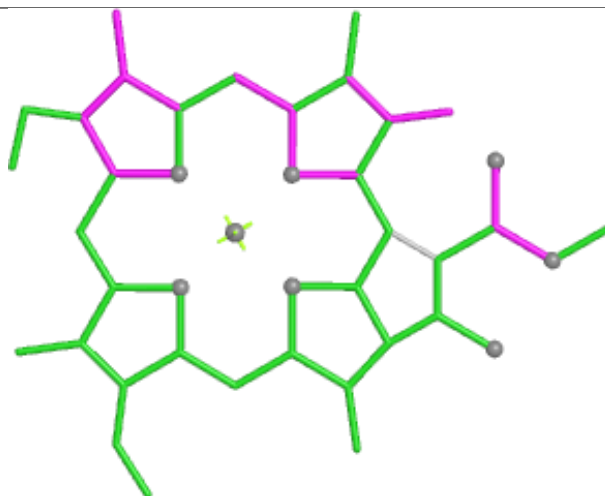




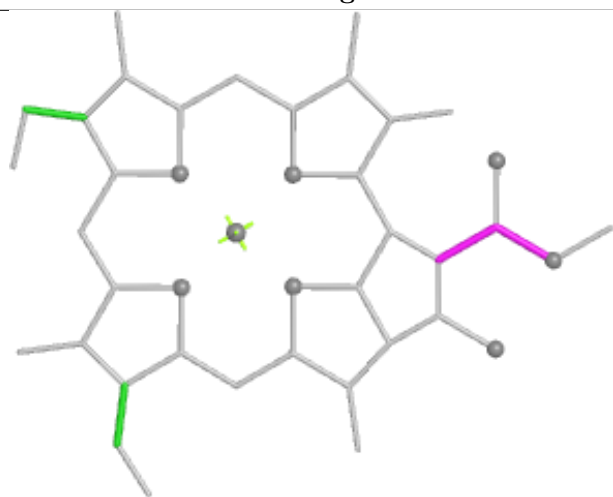
Ligand CLA R 609



Bond lengths



Bond angles

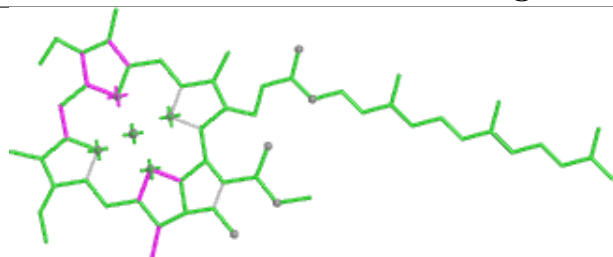


Torsions

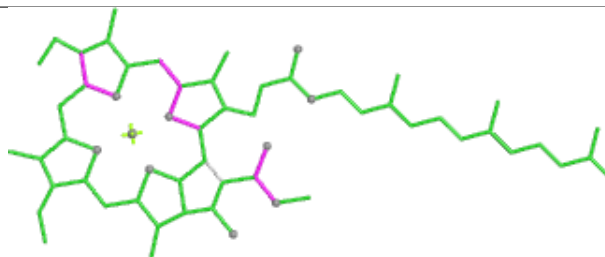


Rings

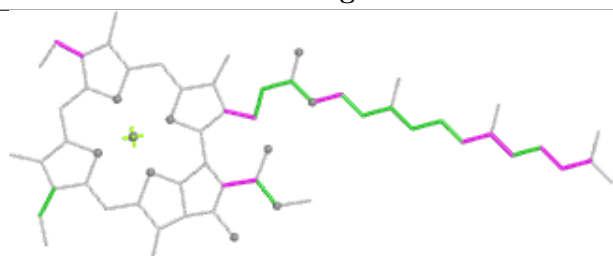
Ligand CLA K 609



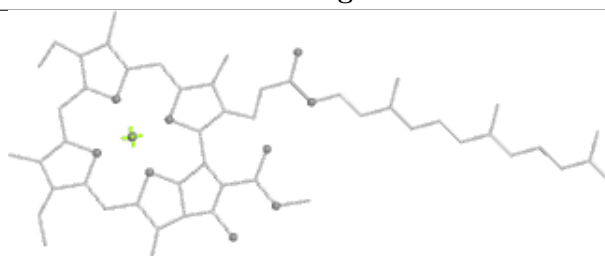
Bond lengths



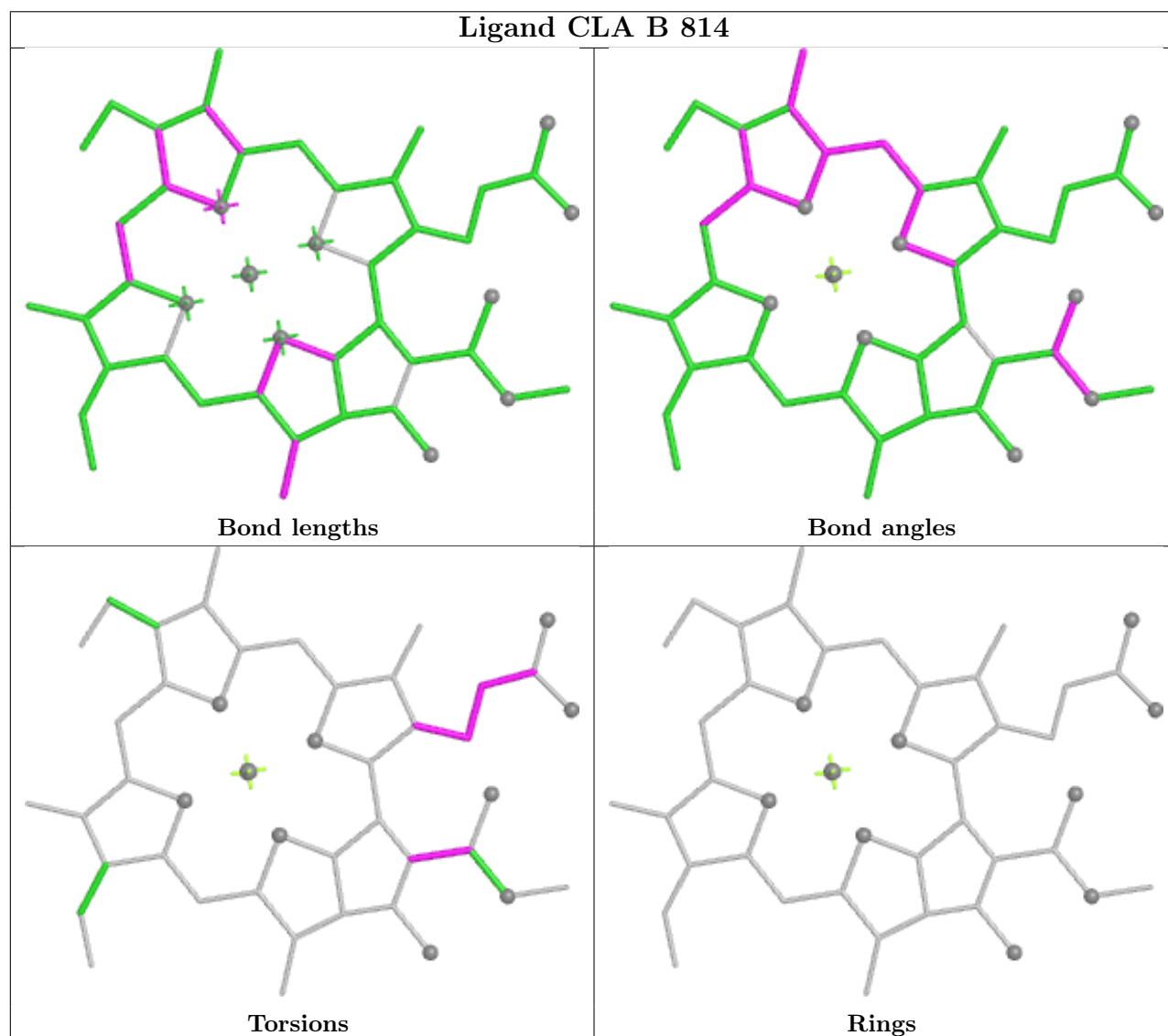
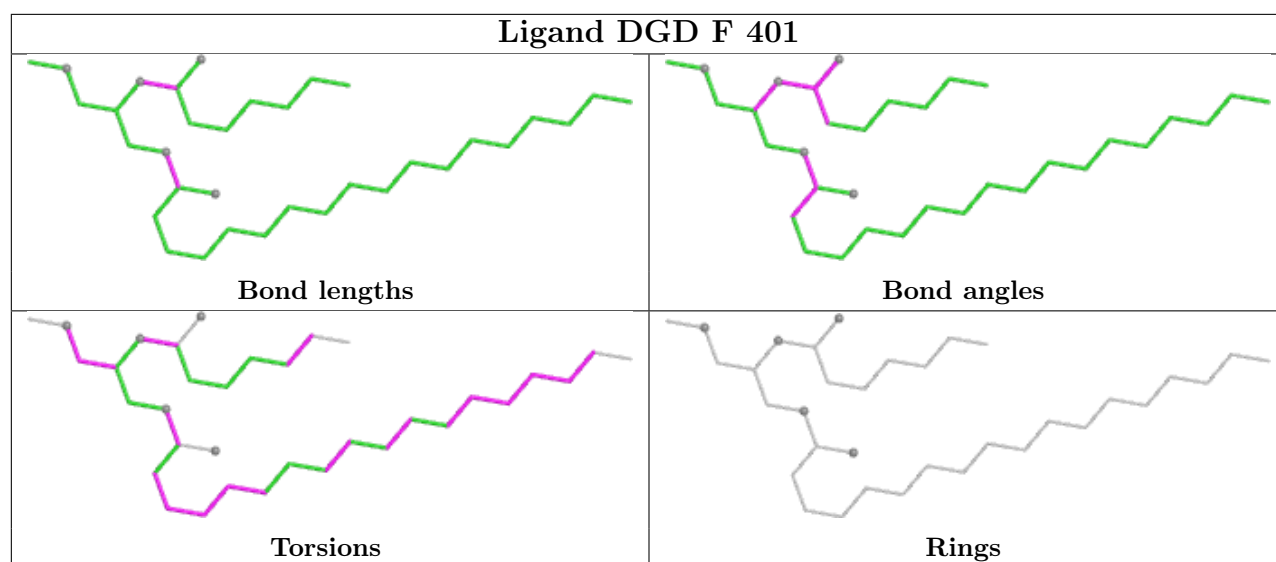
Bond angles

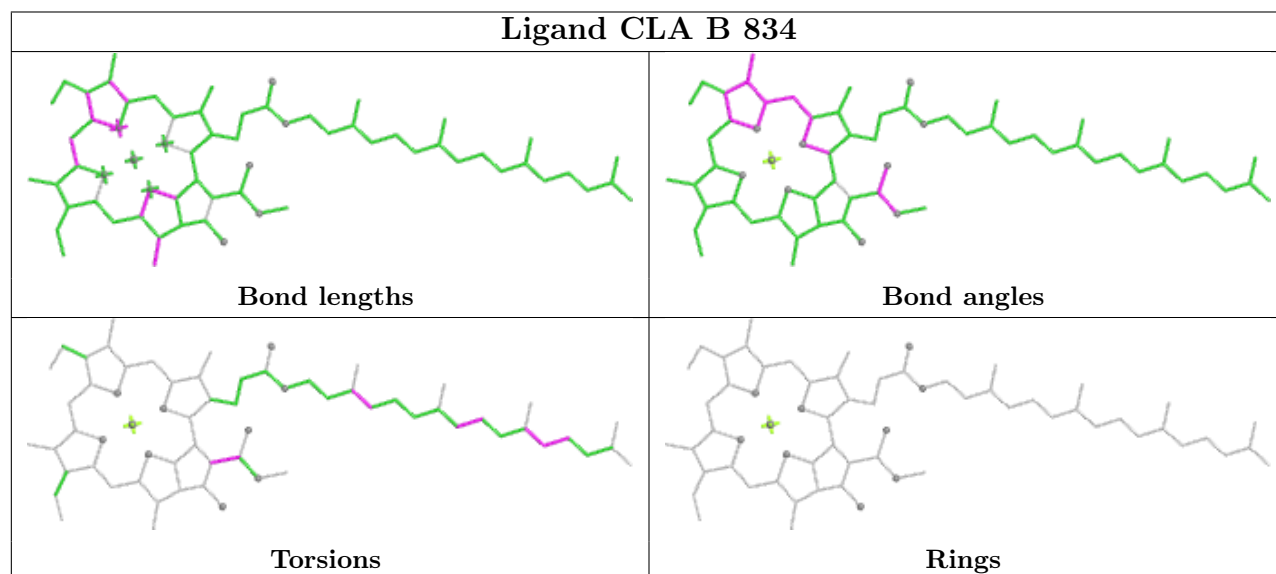
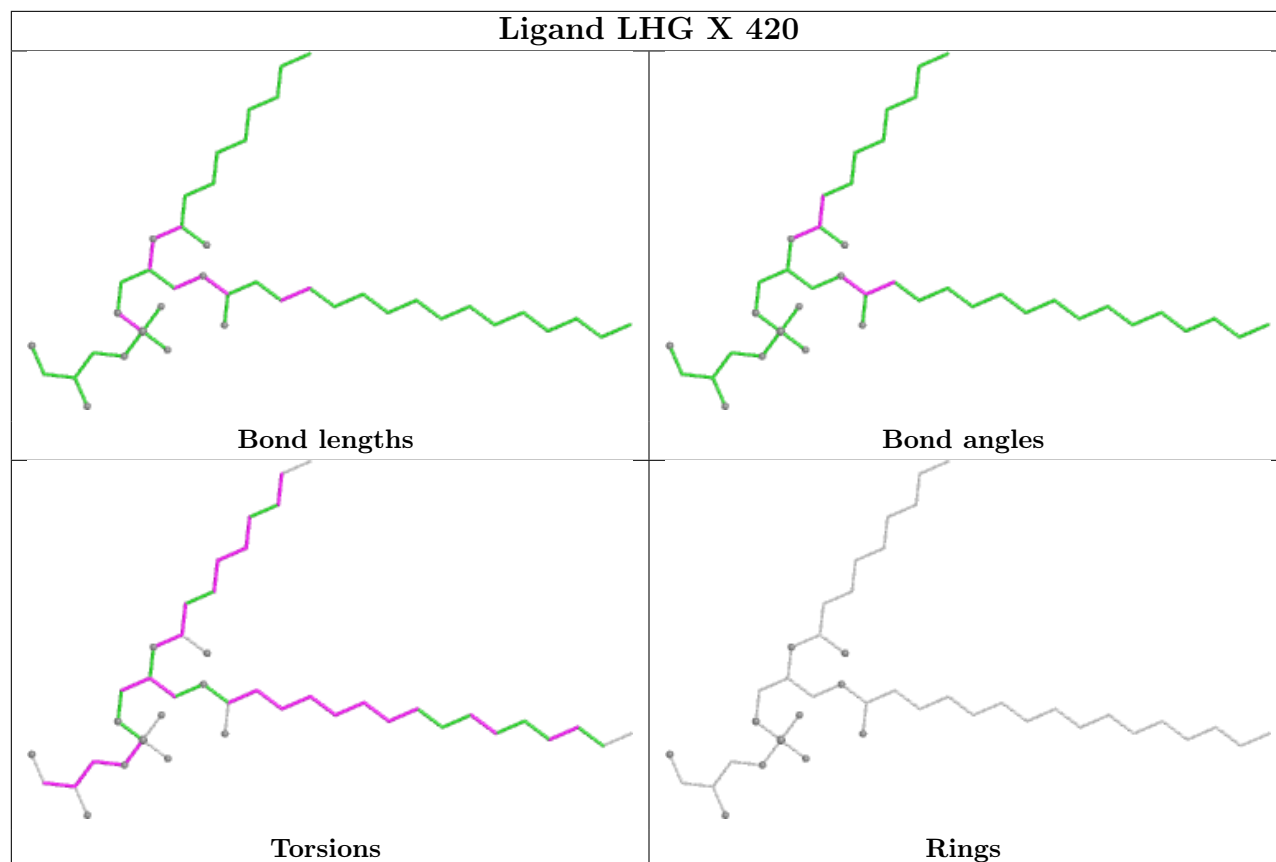


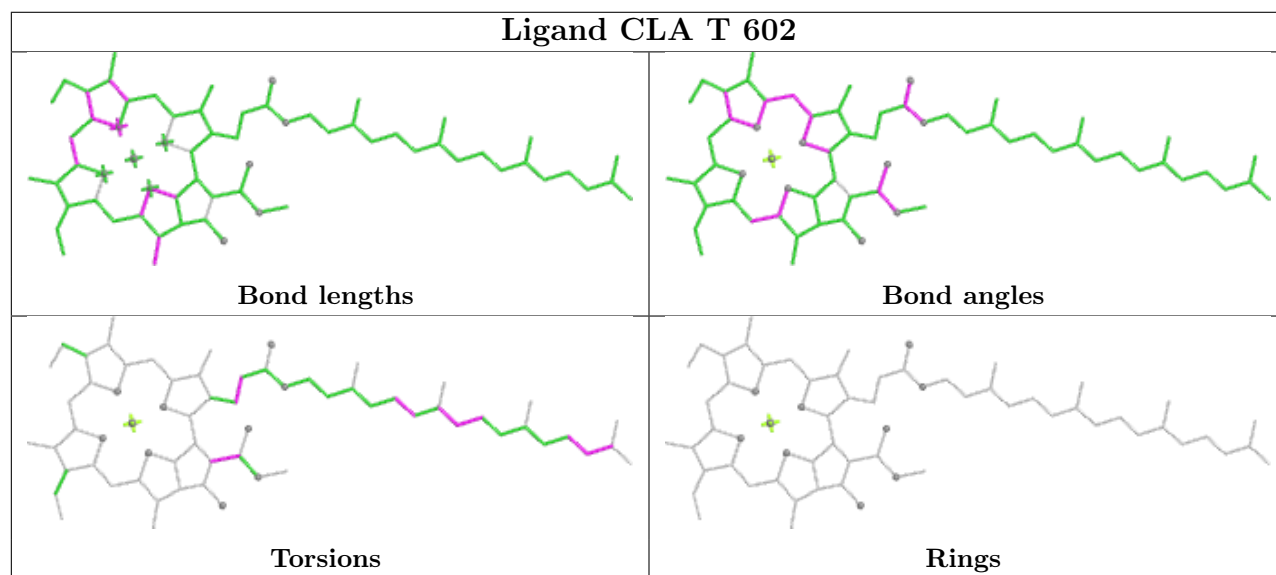
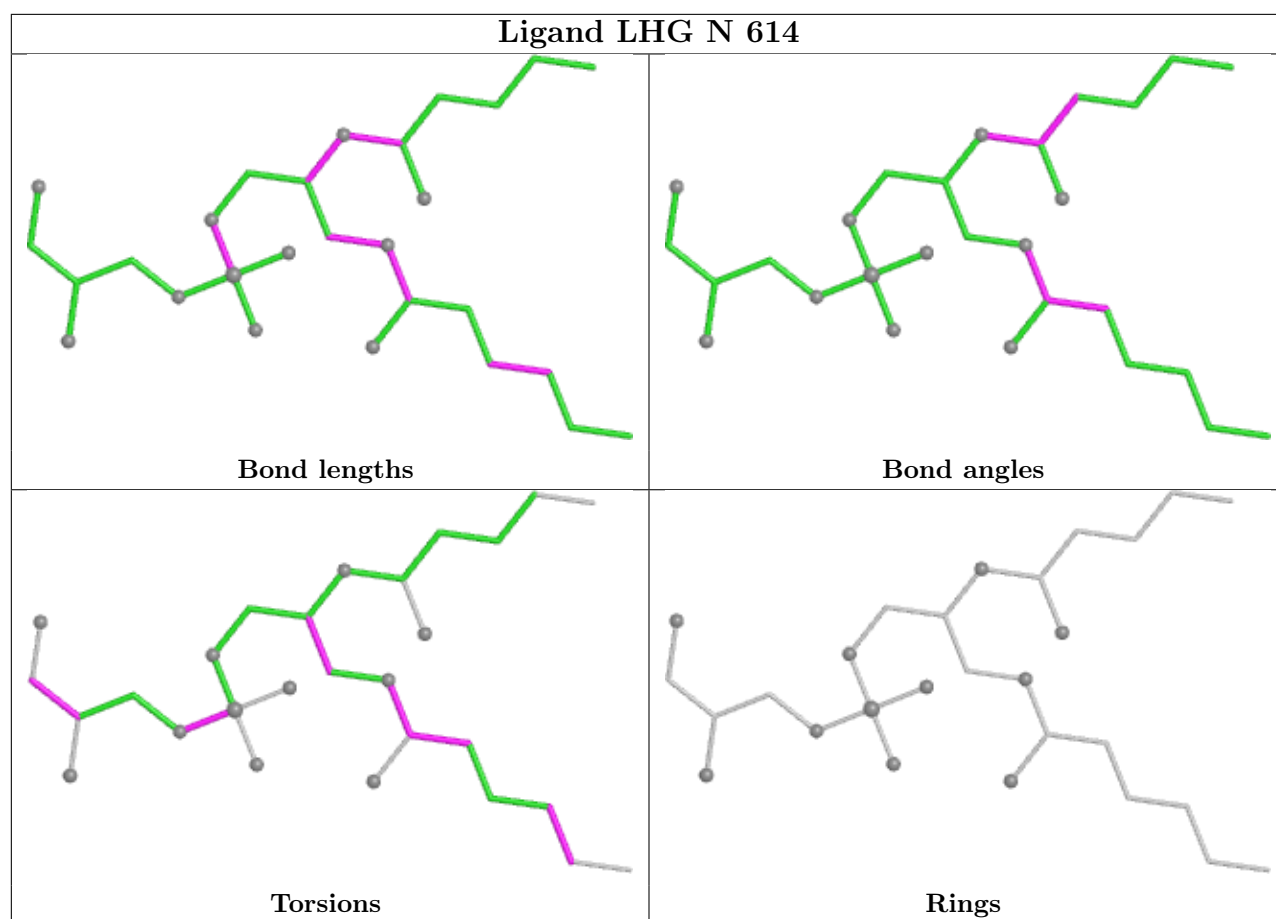
Torsions

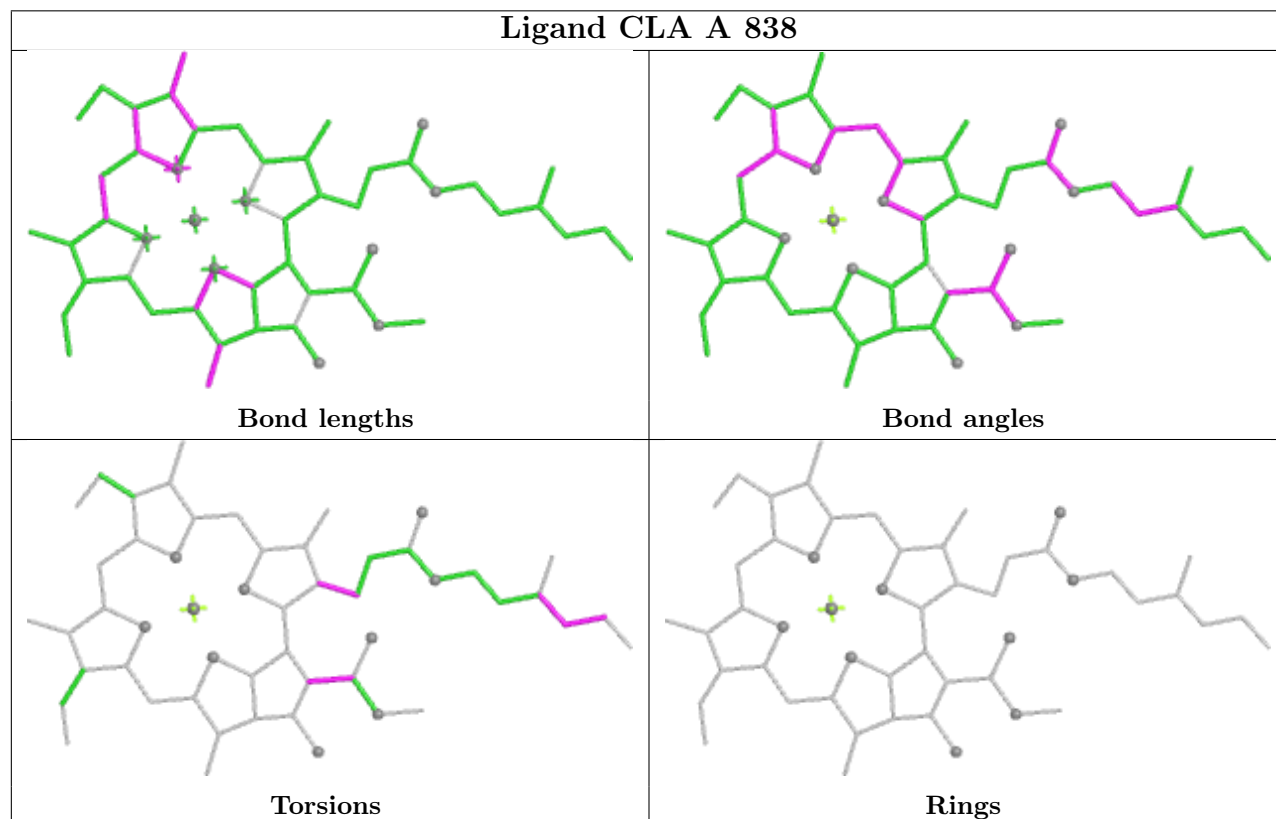
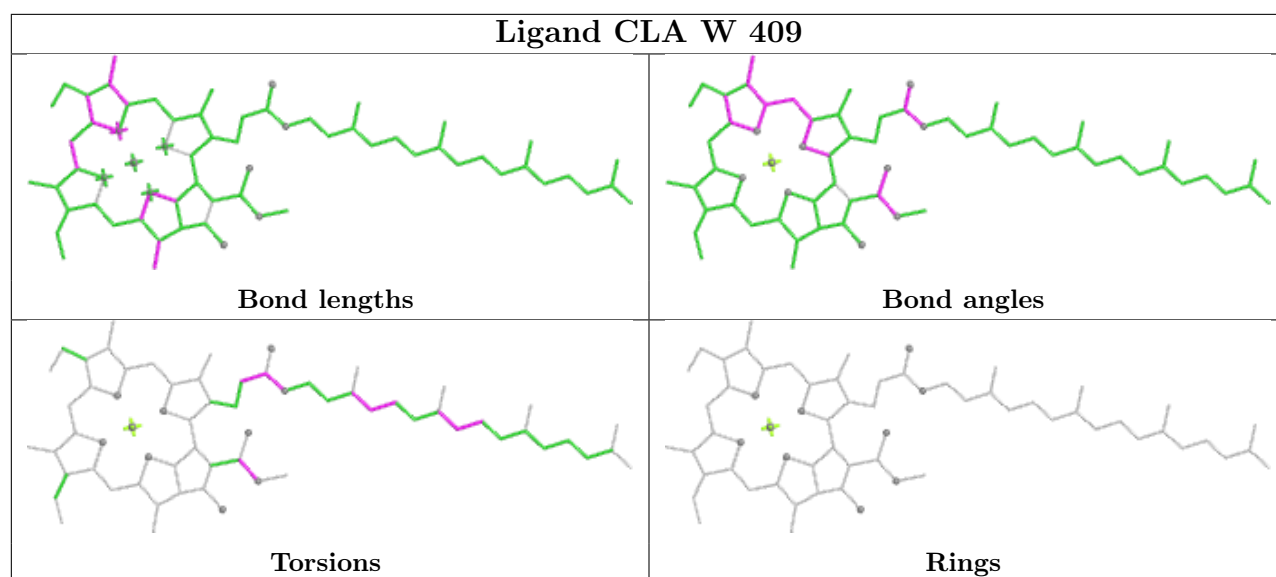


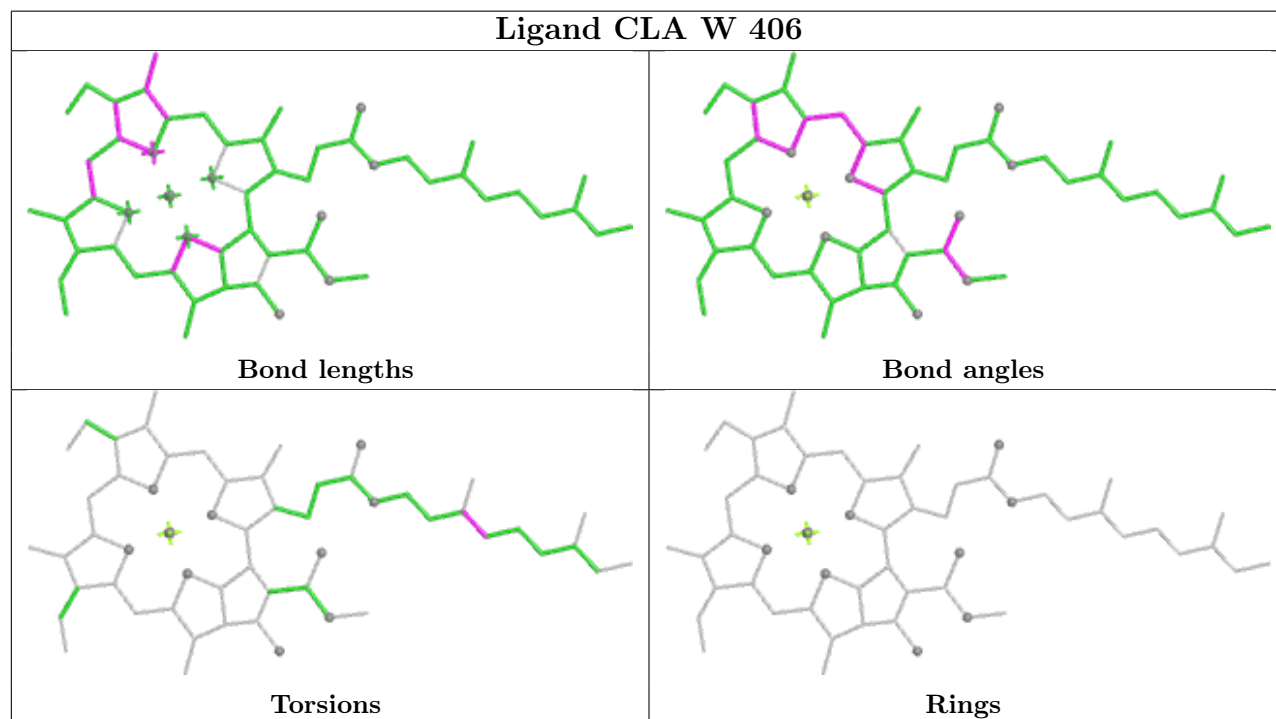
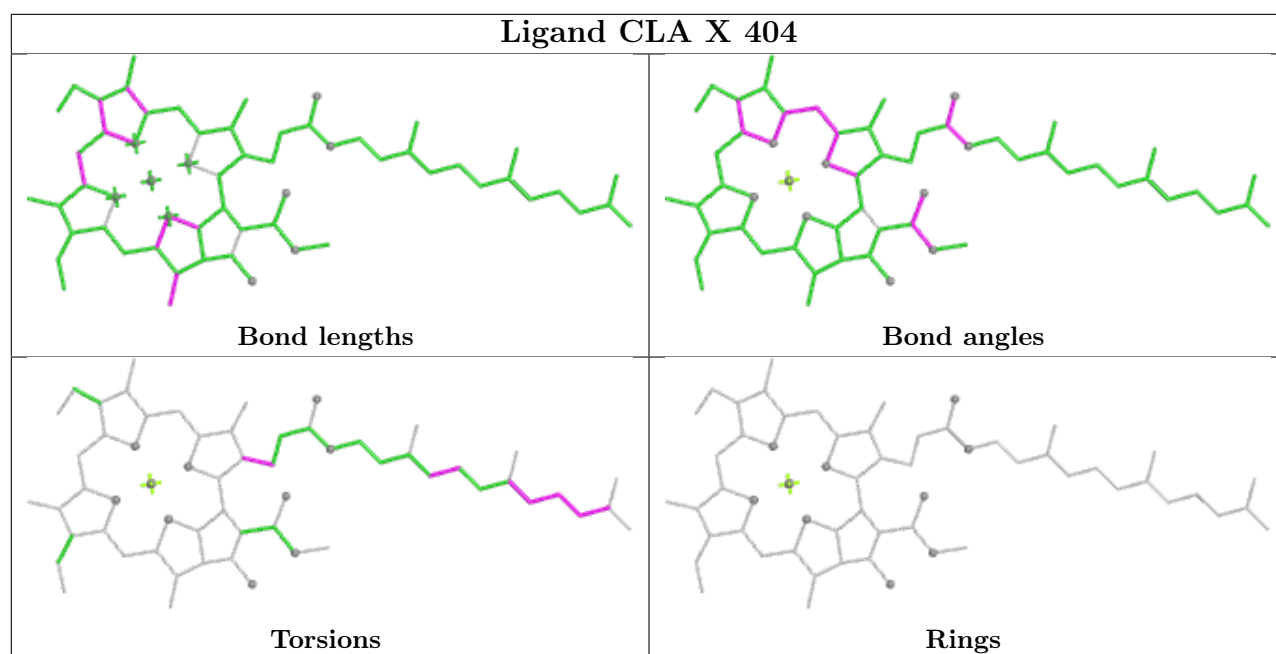
Rings

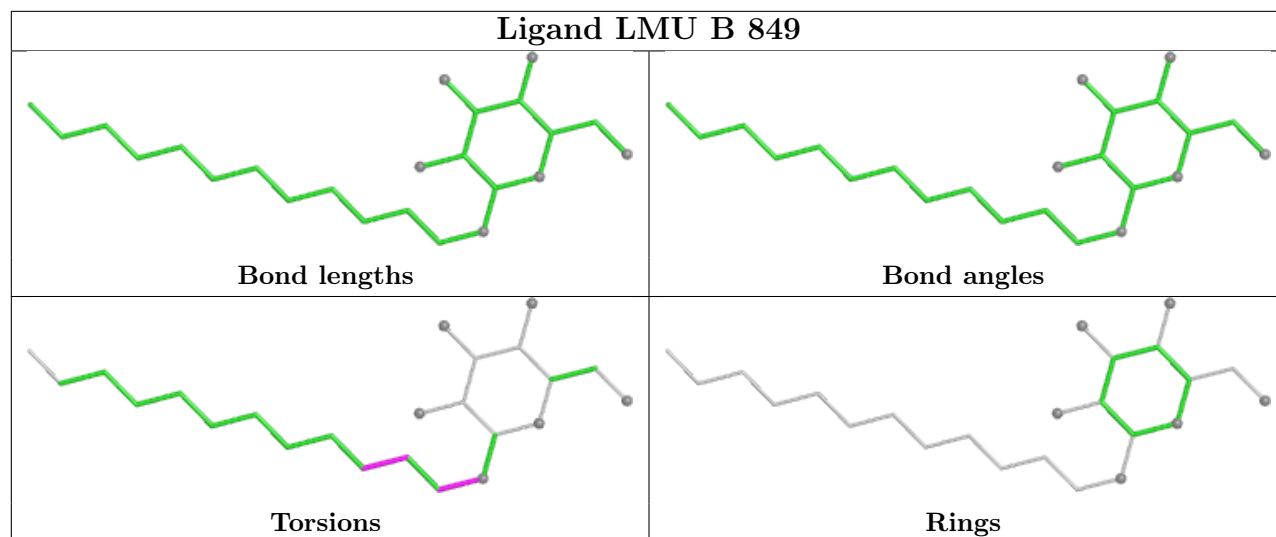
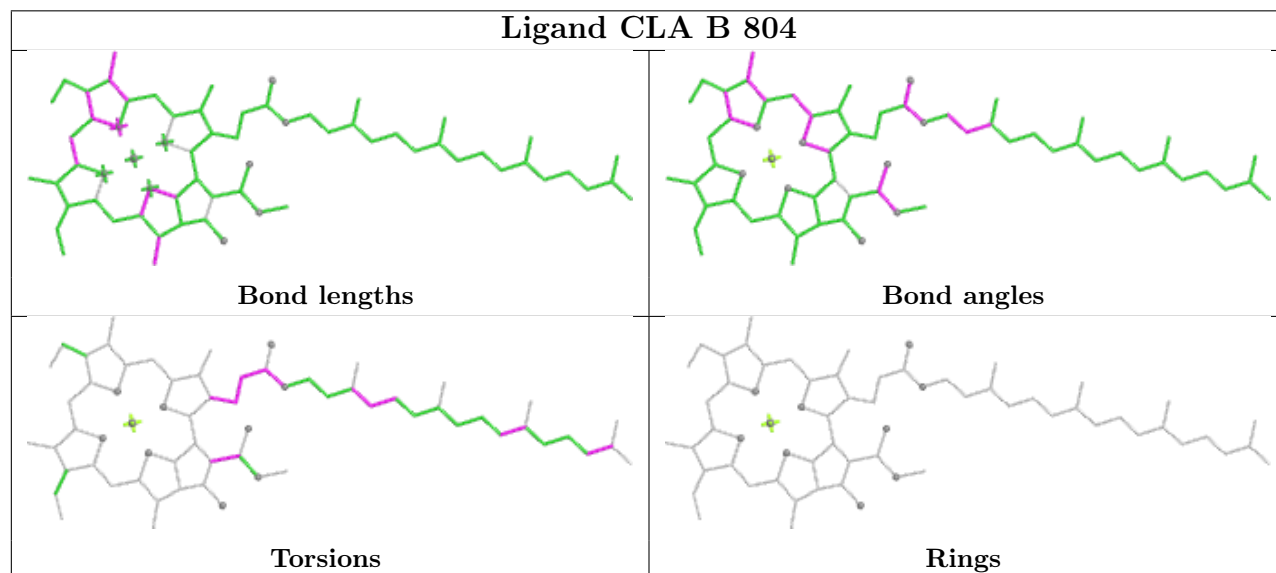
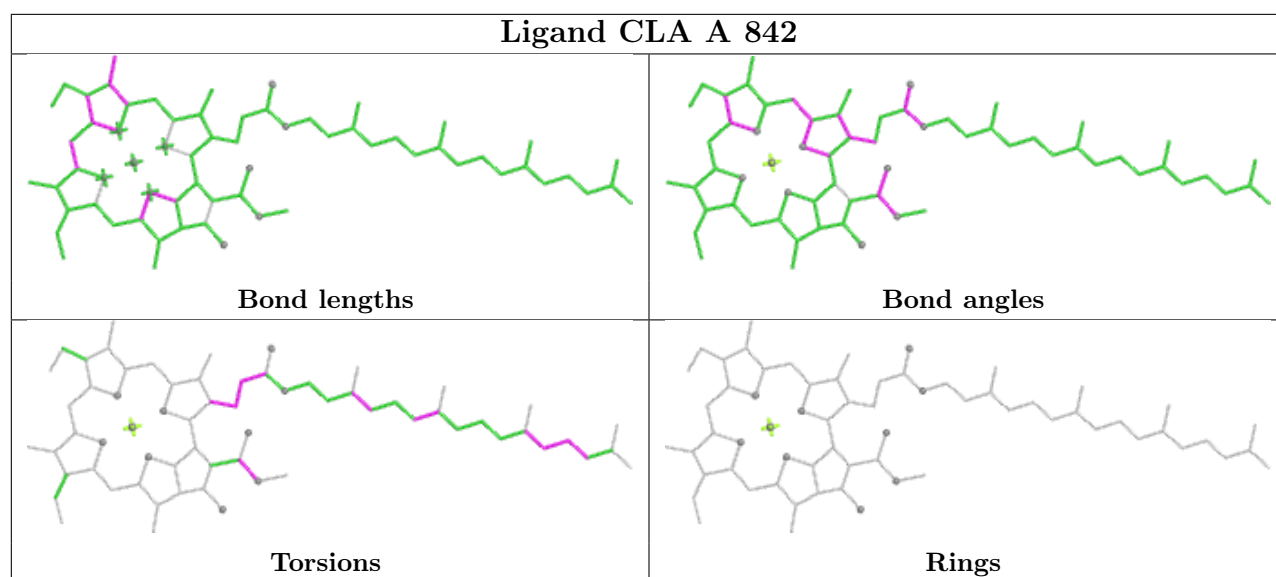


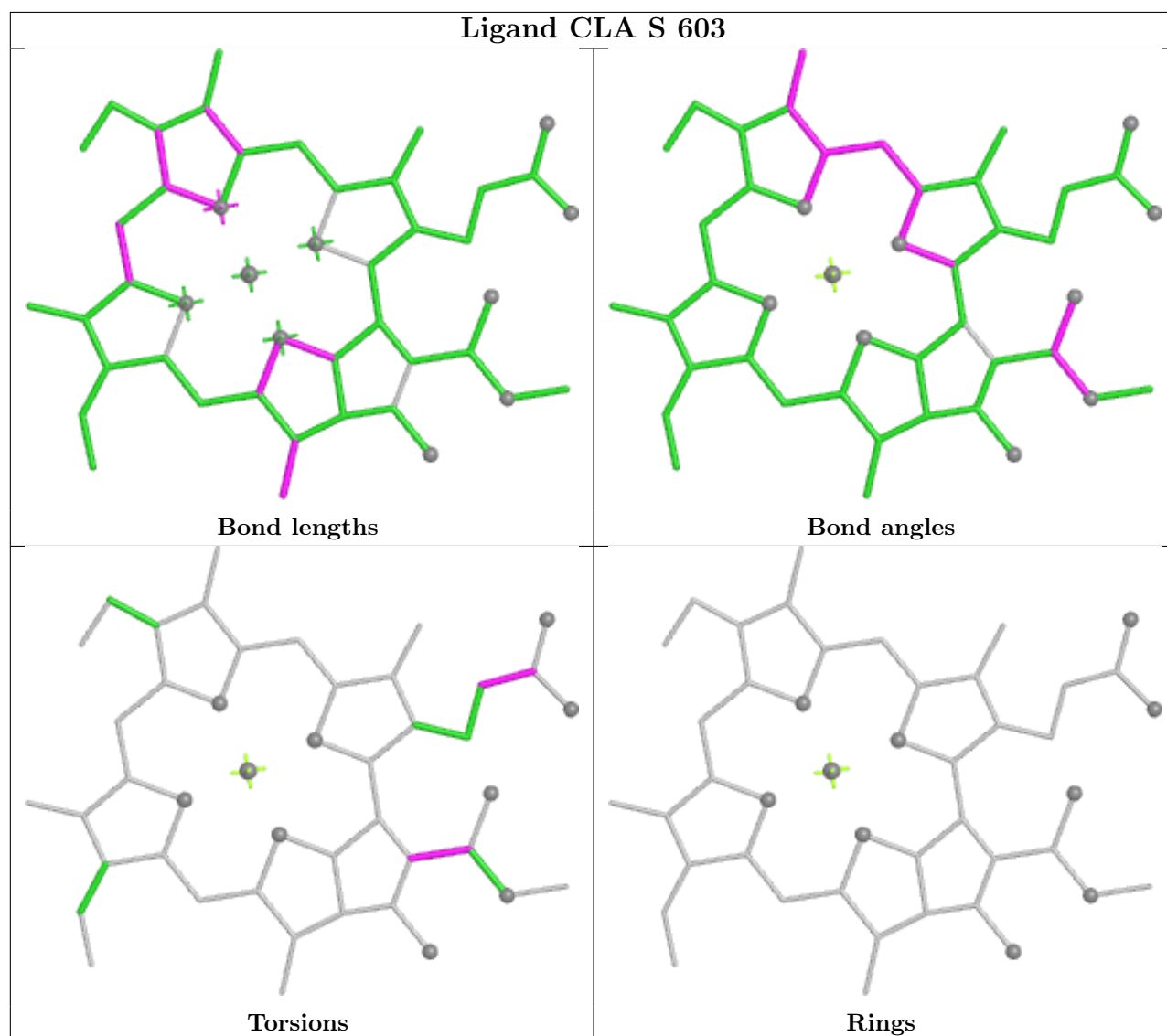
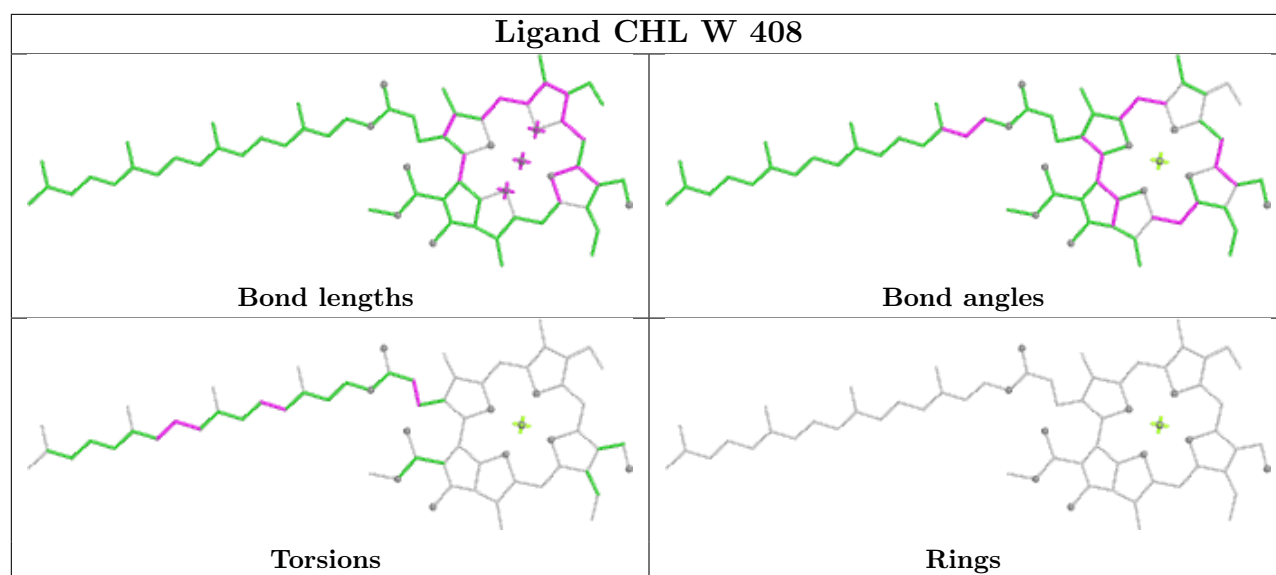


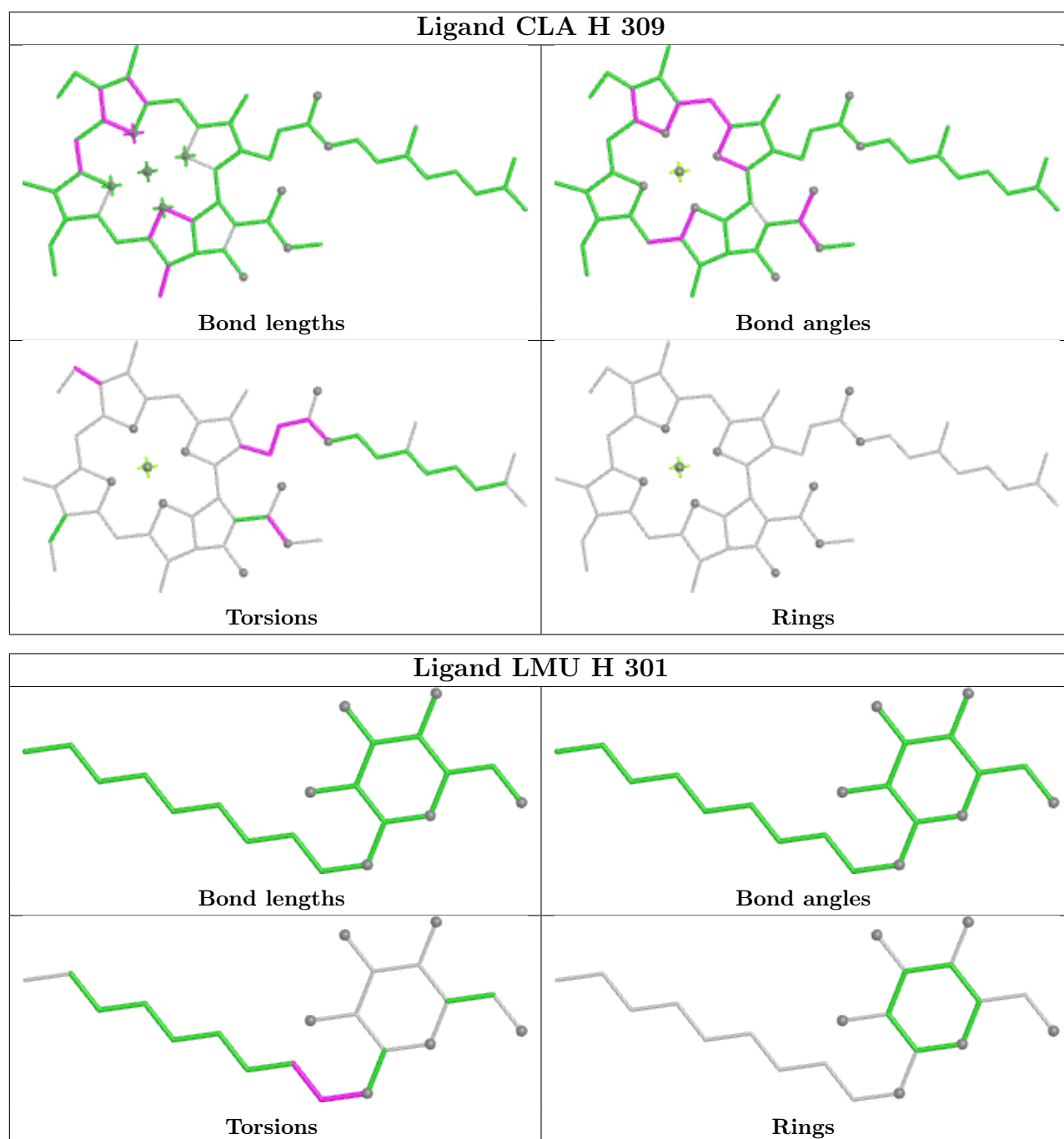


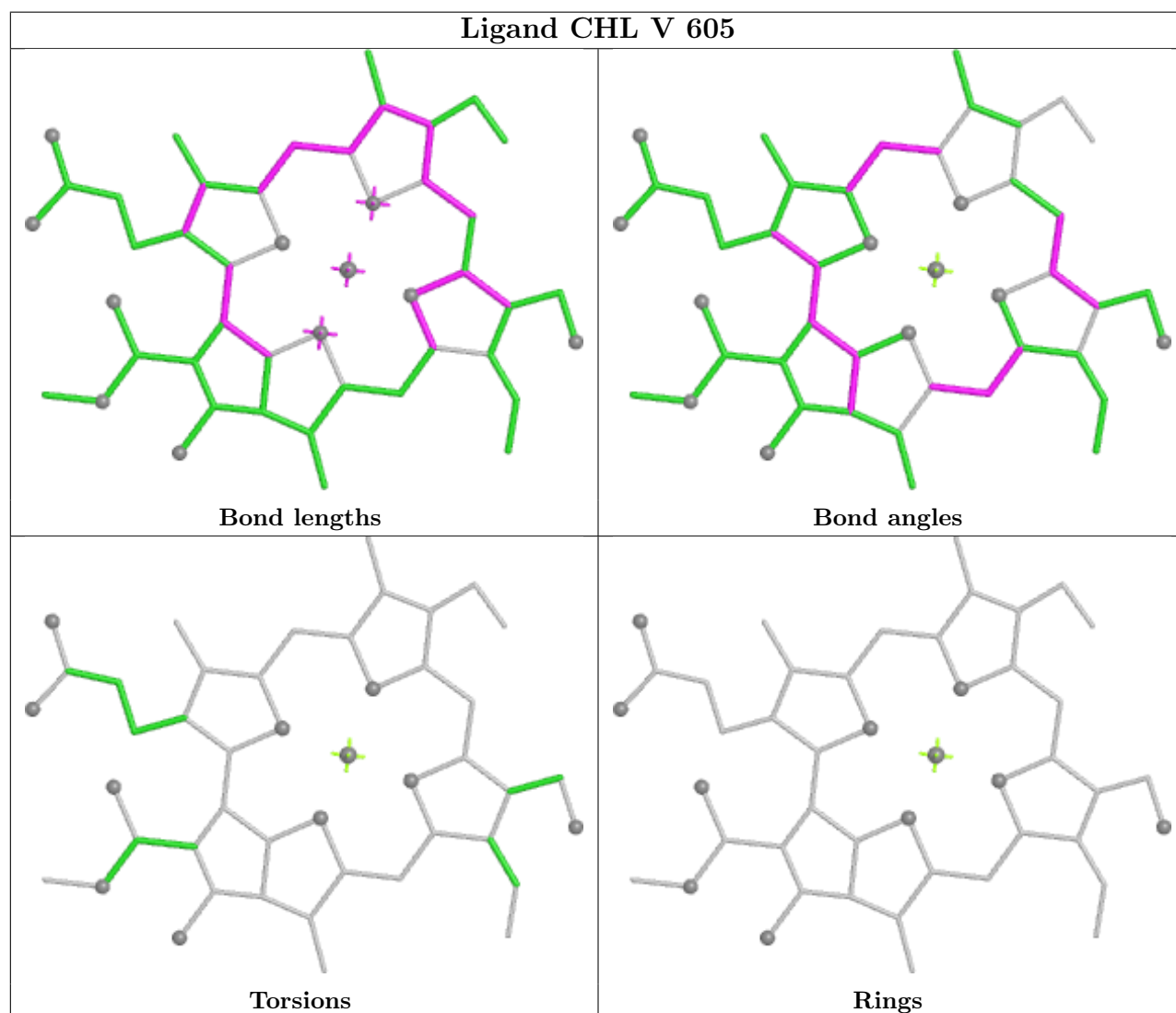
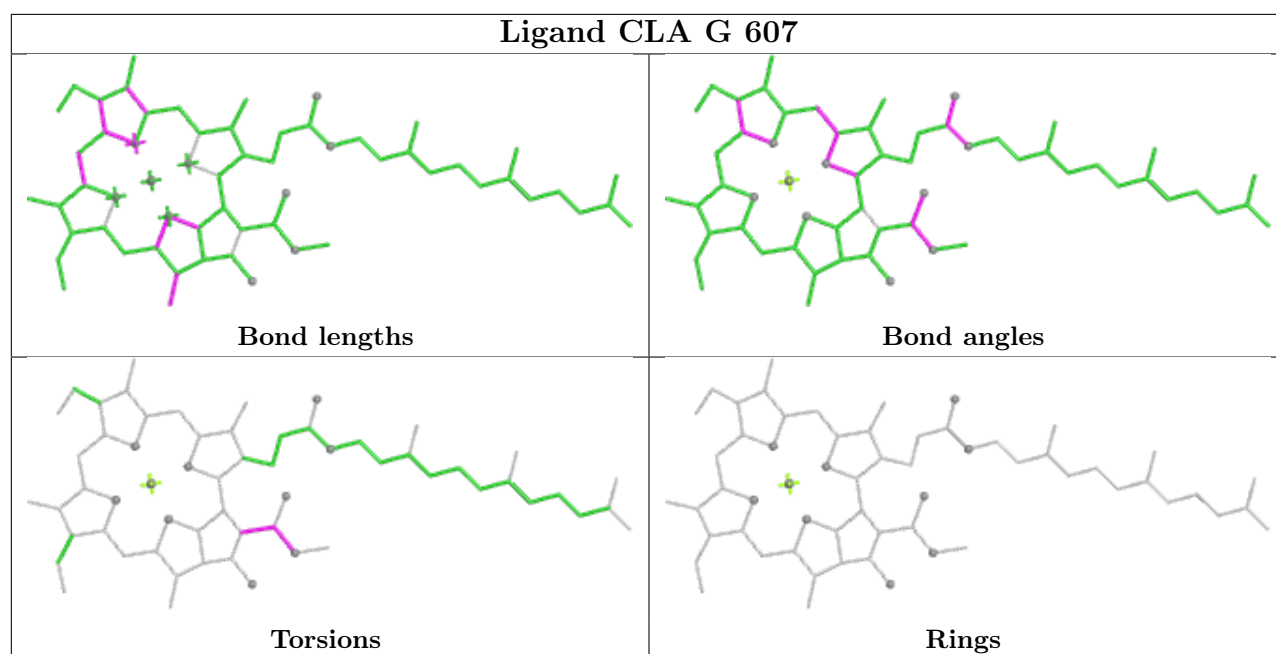


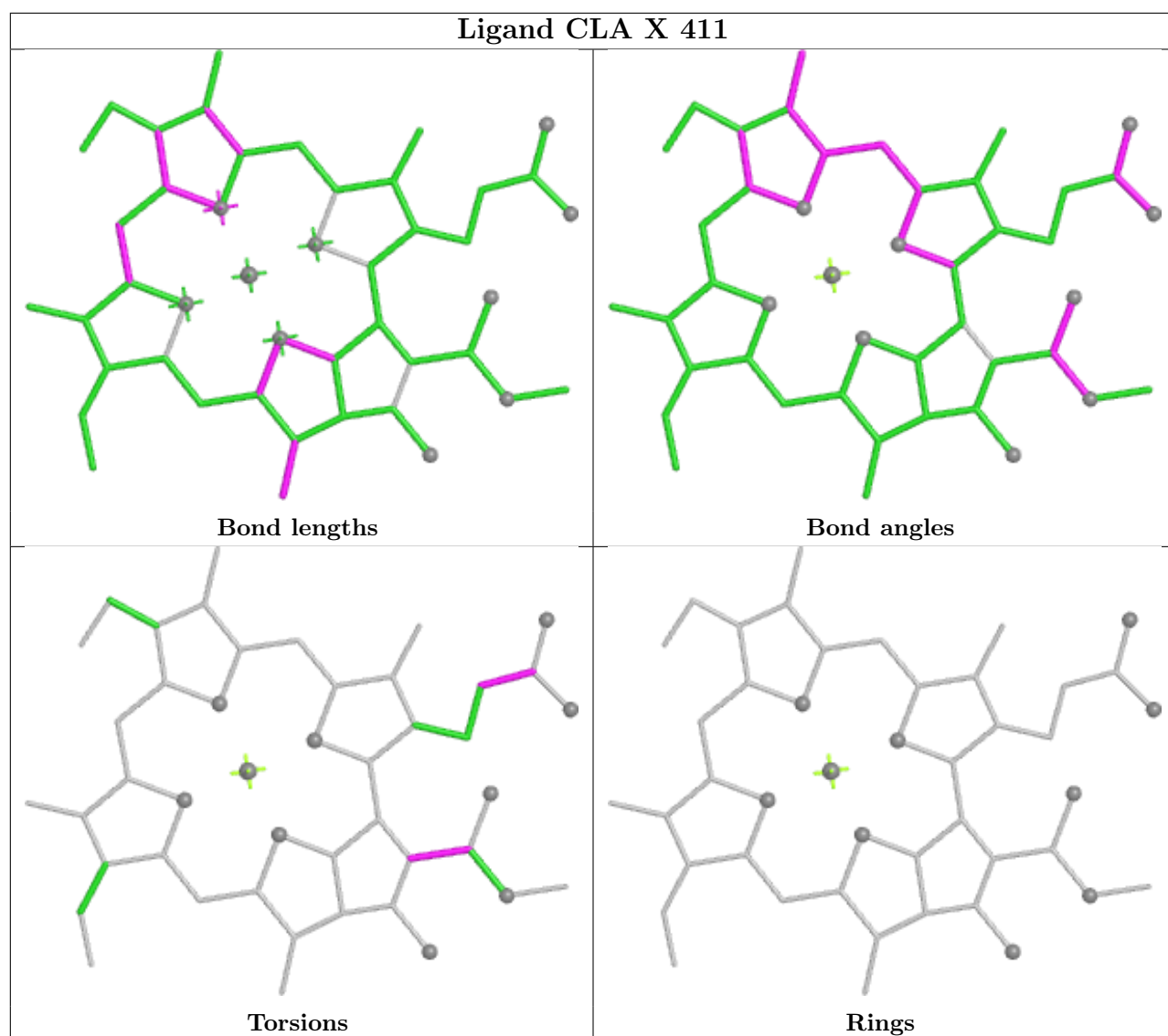


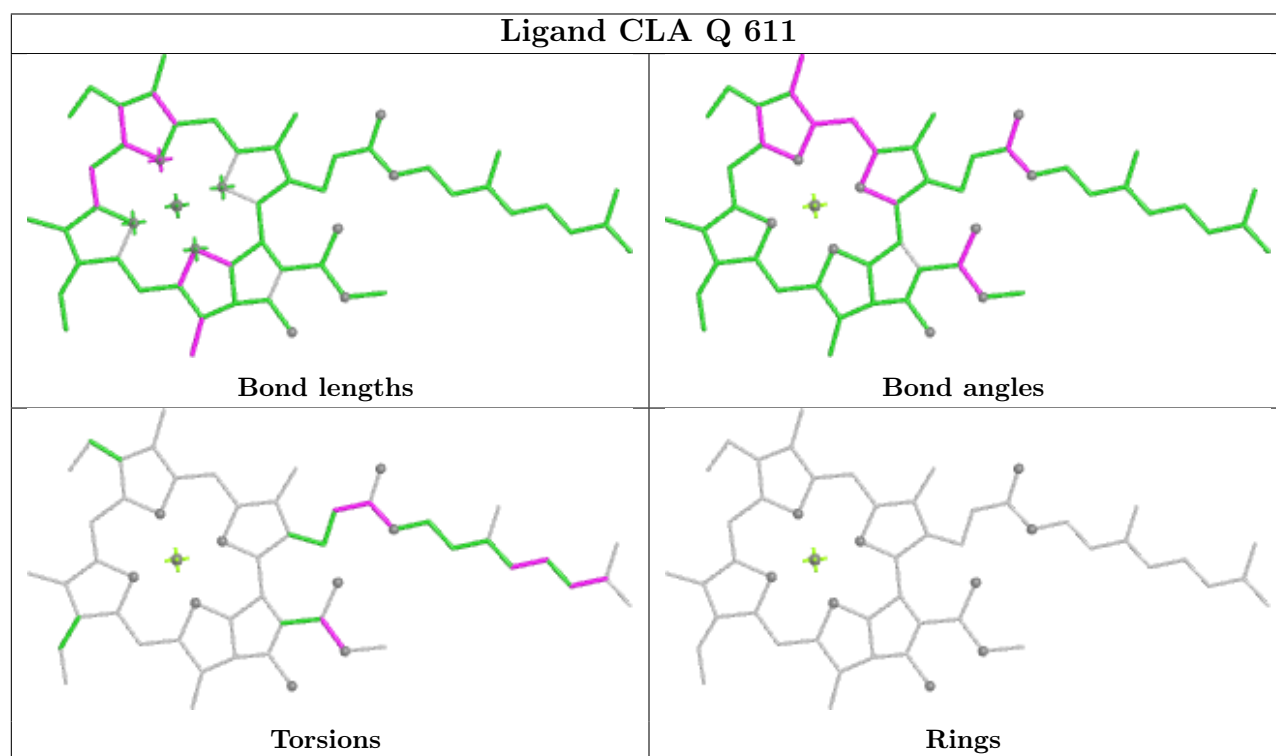
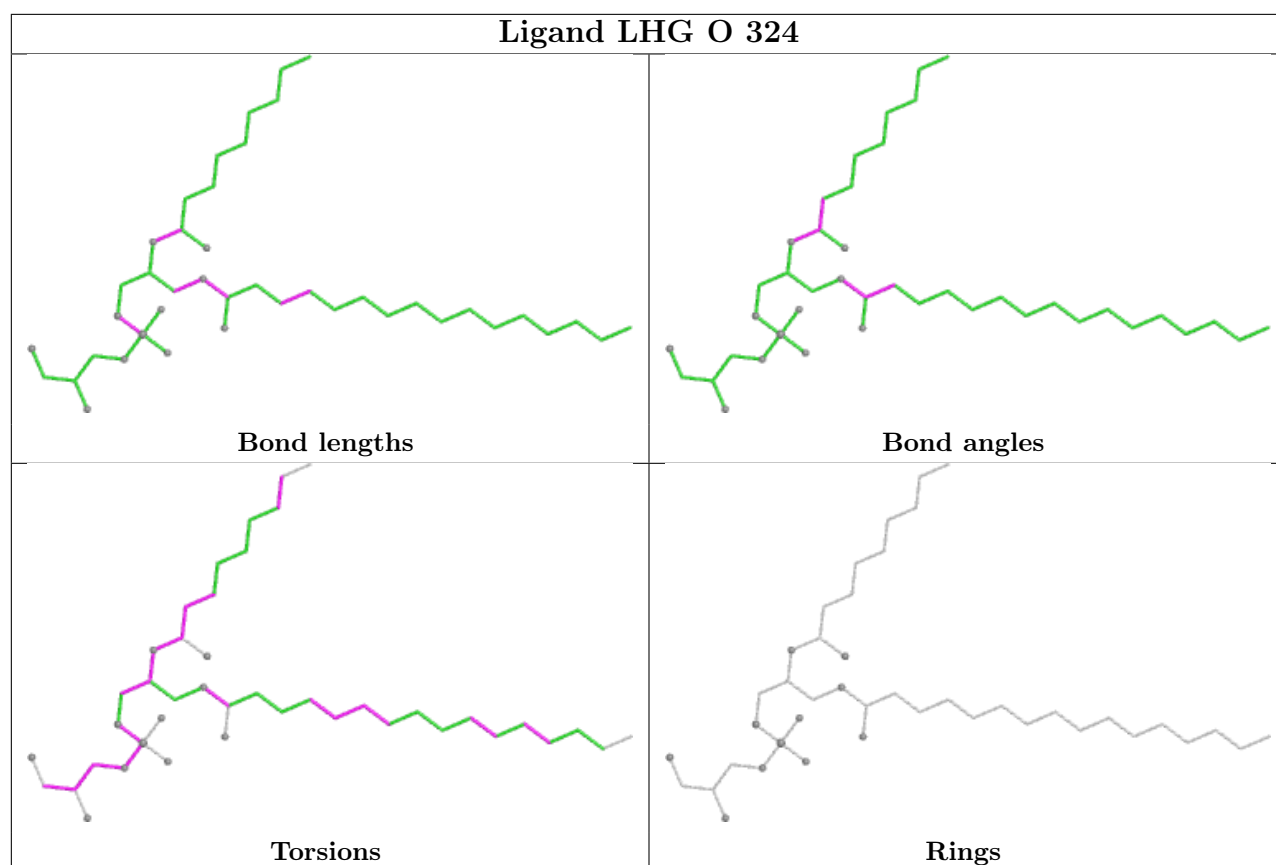


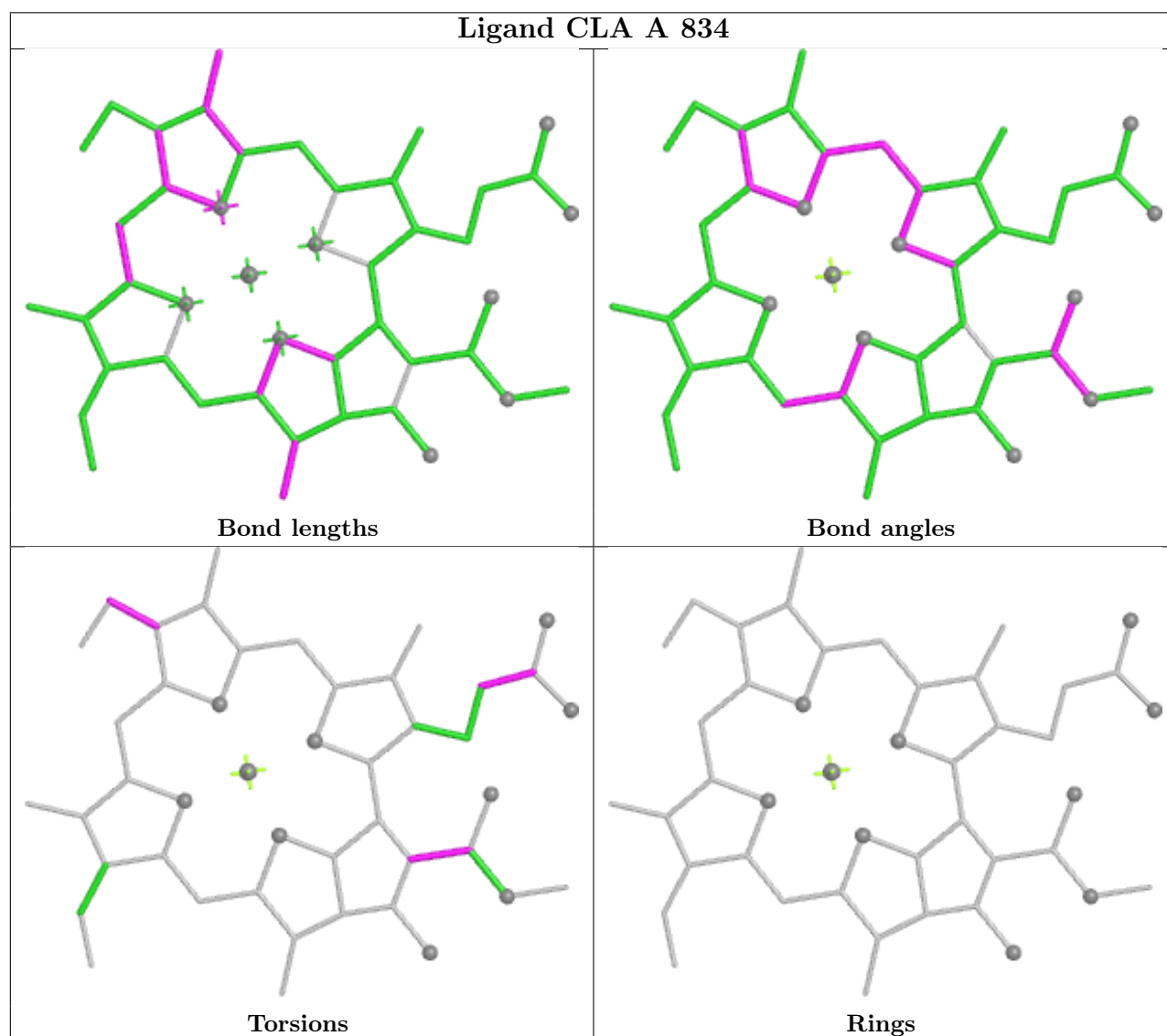
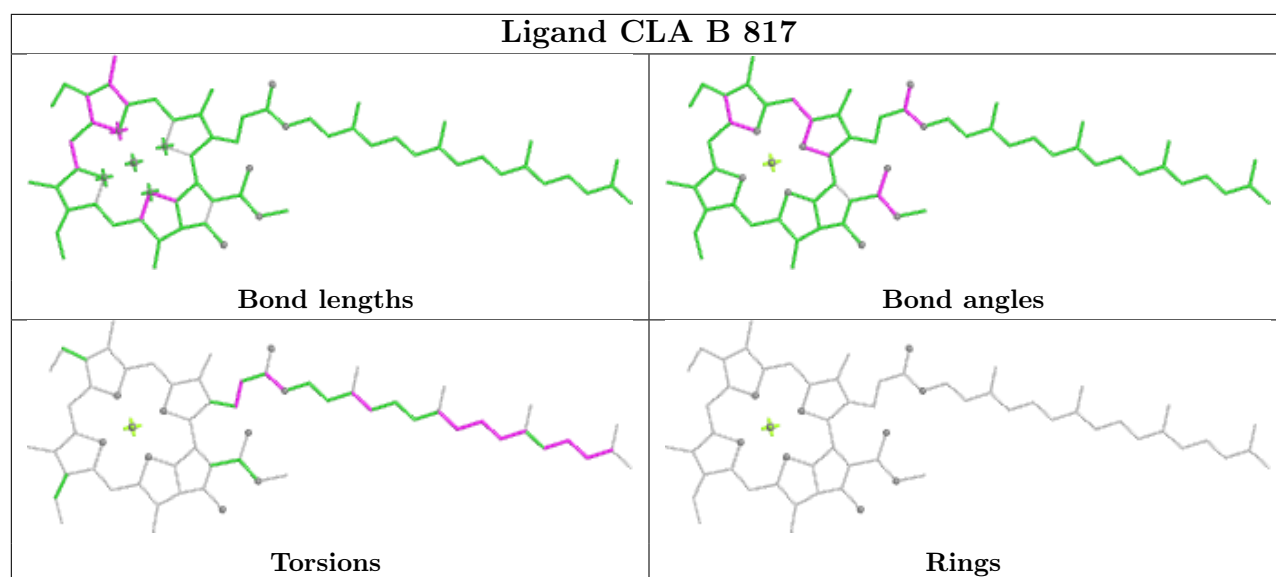


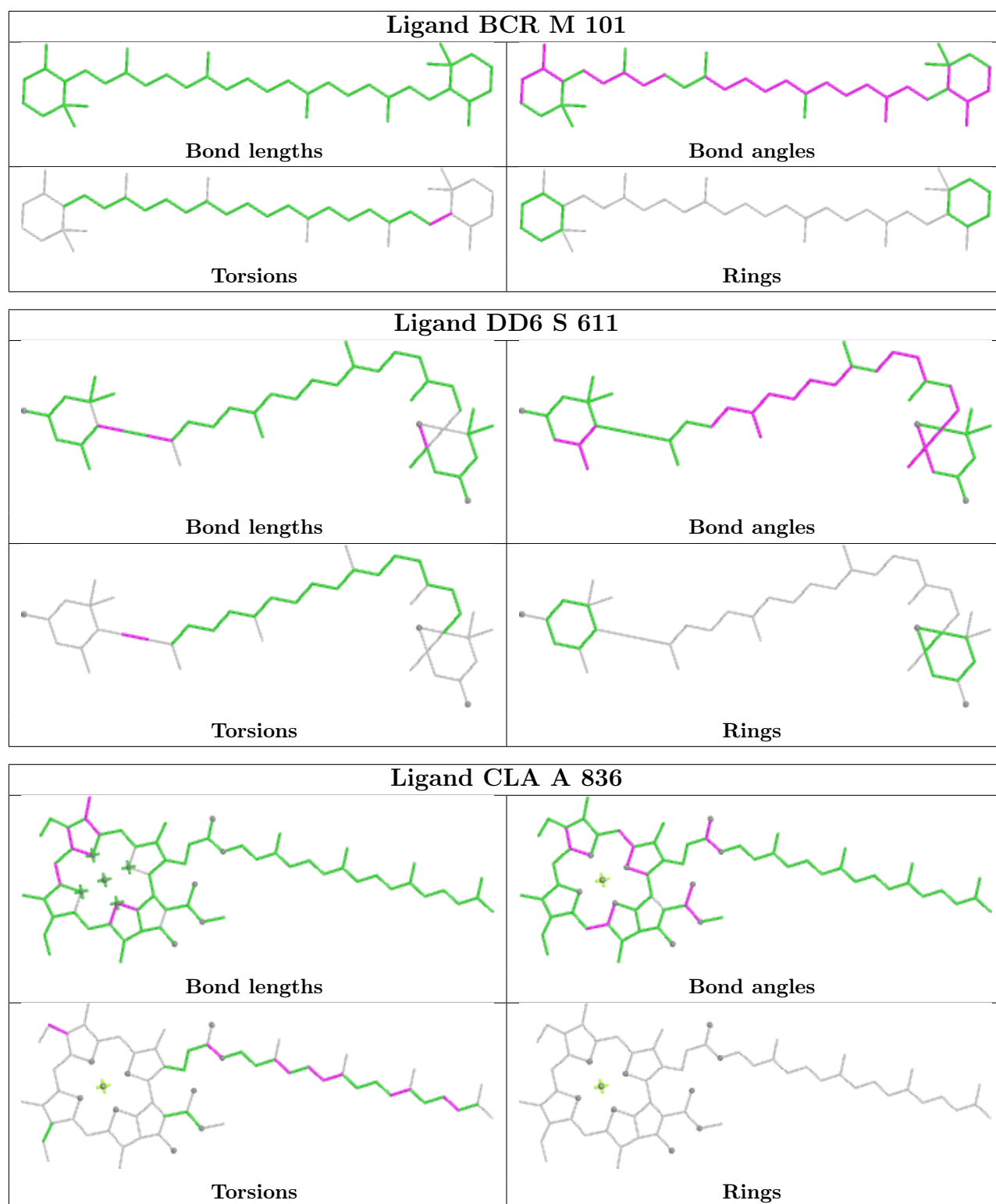


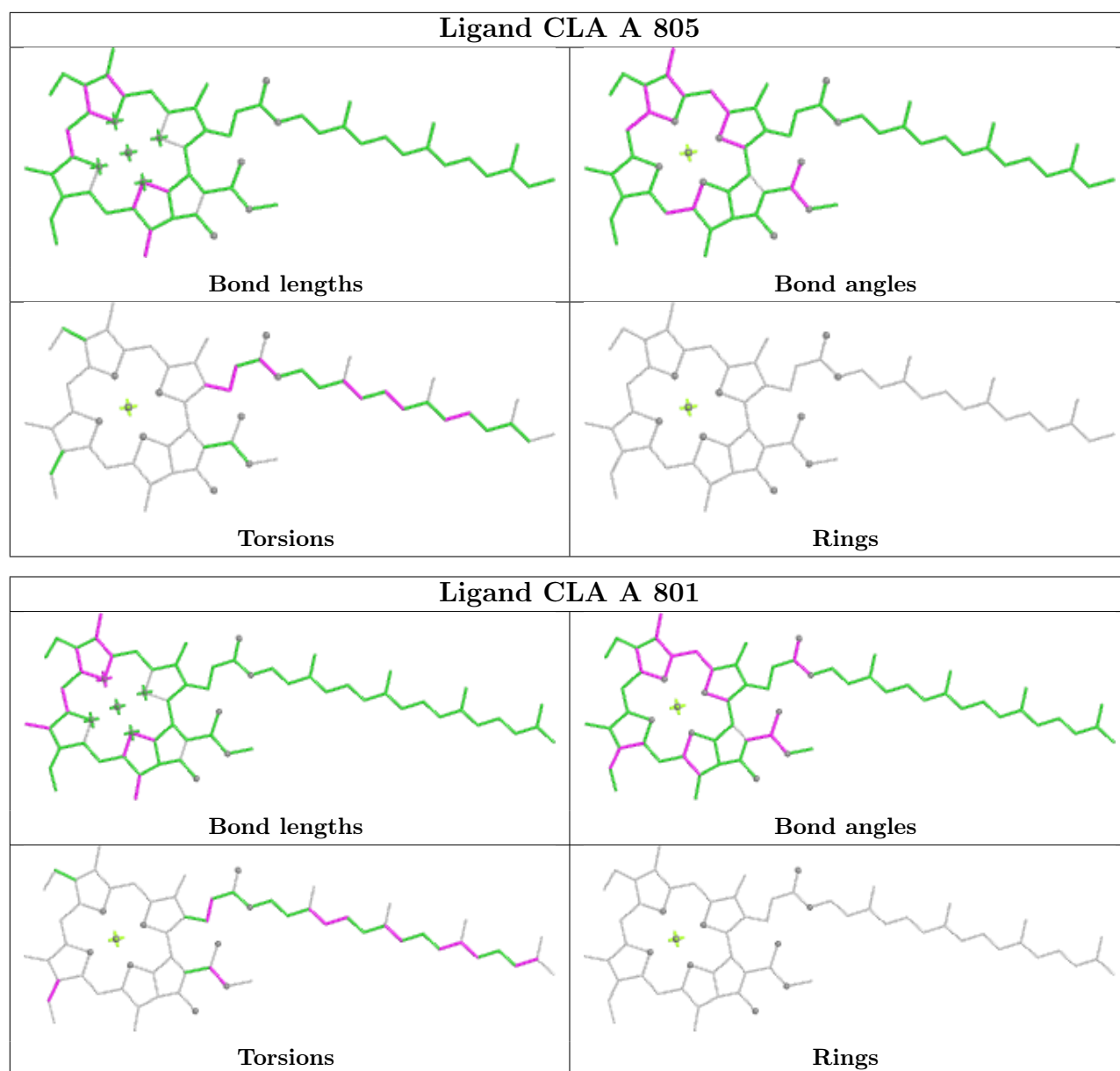


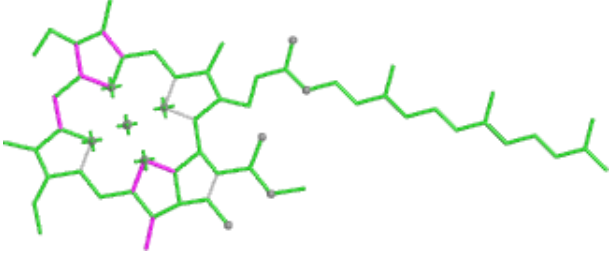
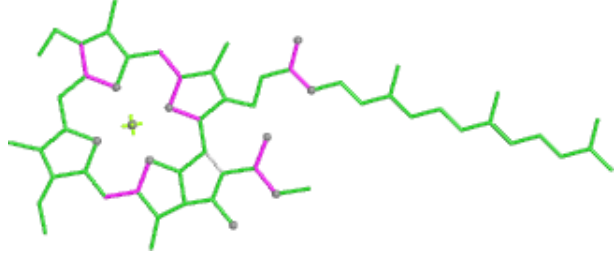
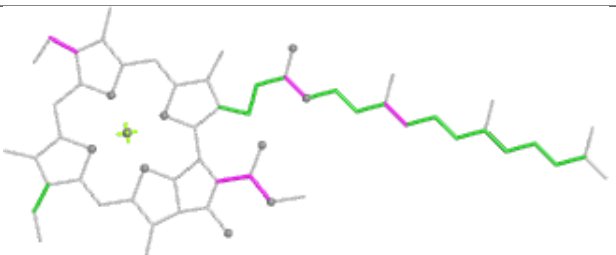
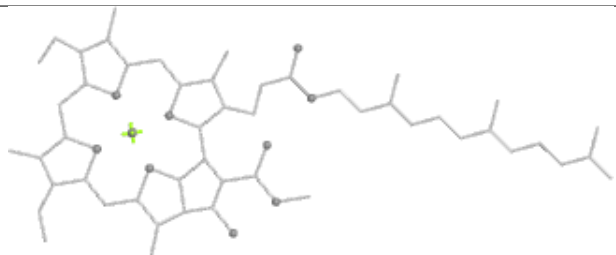
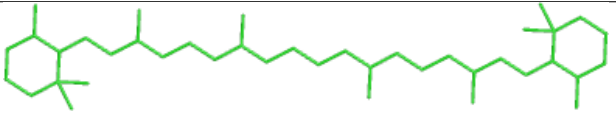
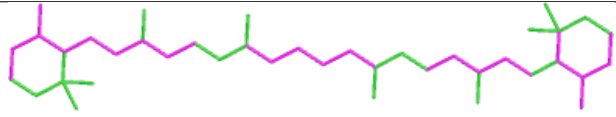
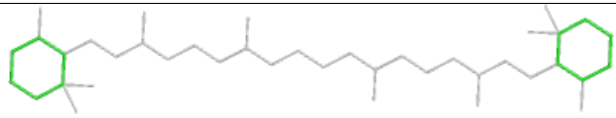


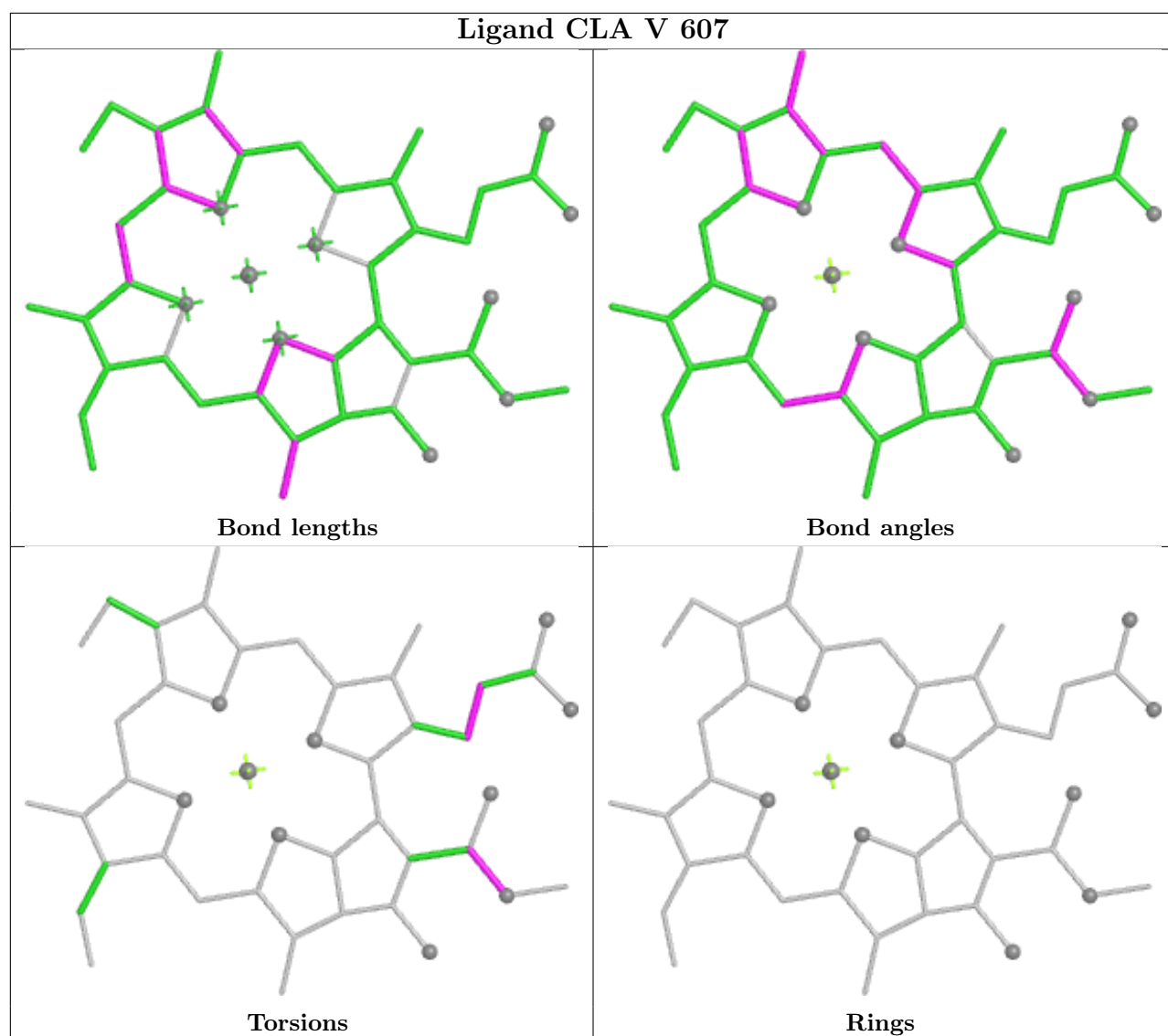


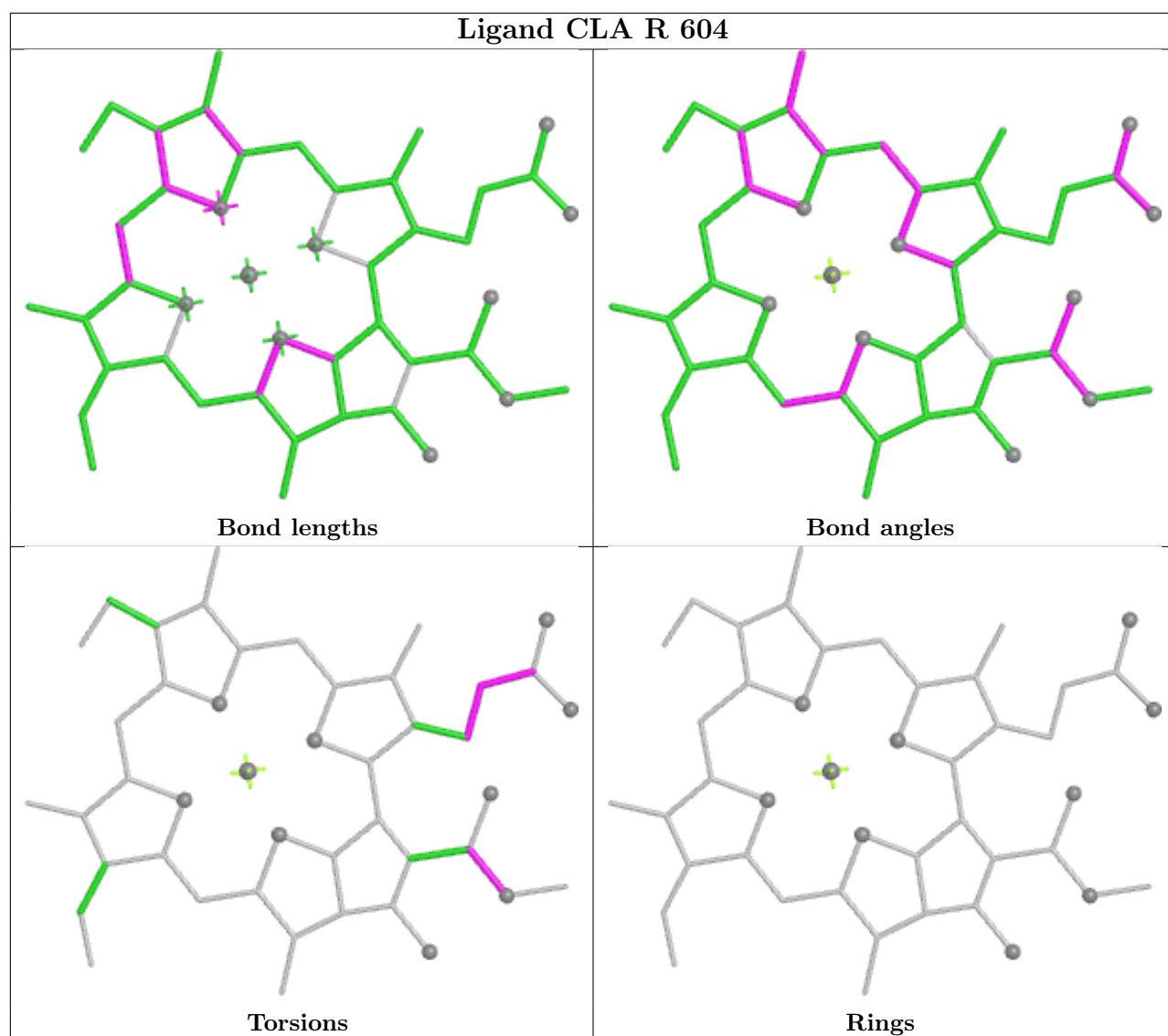




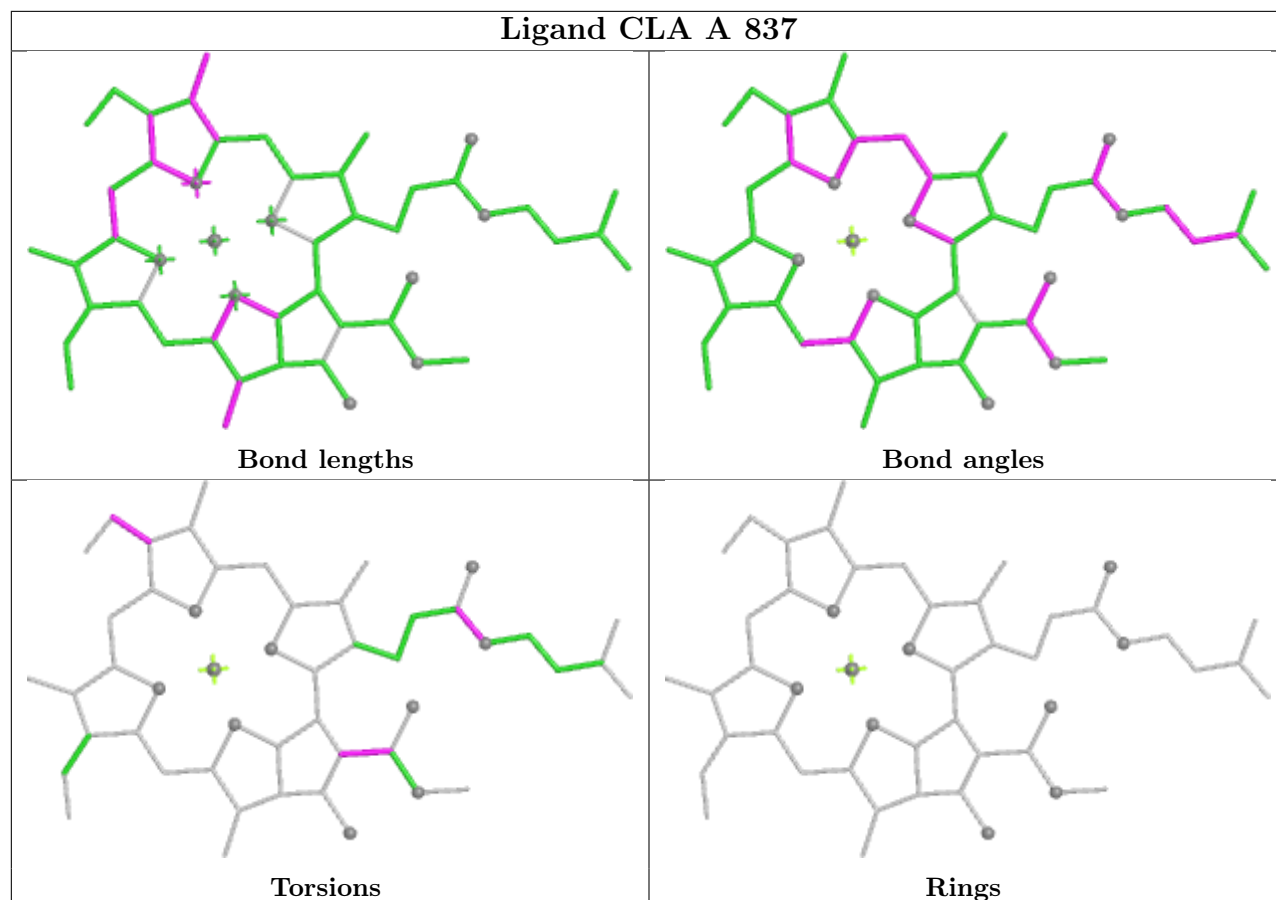


Ligand CLA O 311	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCR B 842	
 Bond lengths	 Bond angles
 Torsions	 Rings

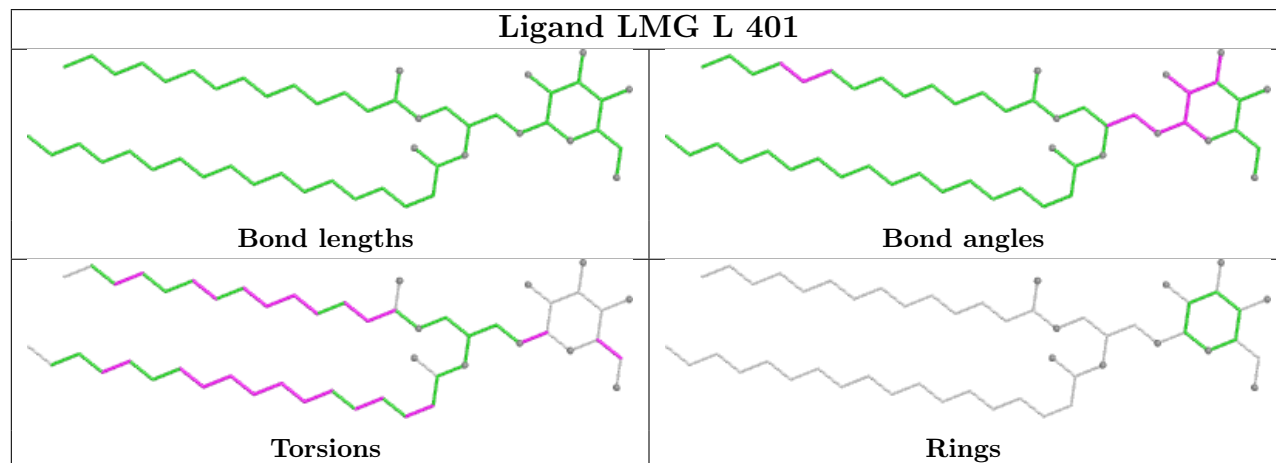


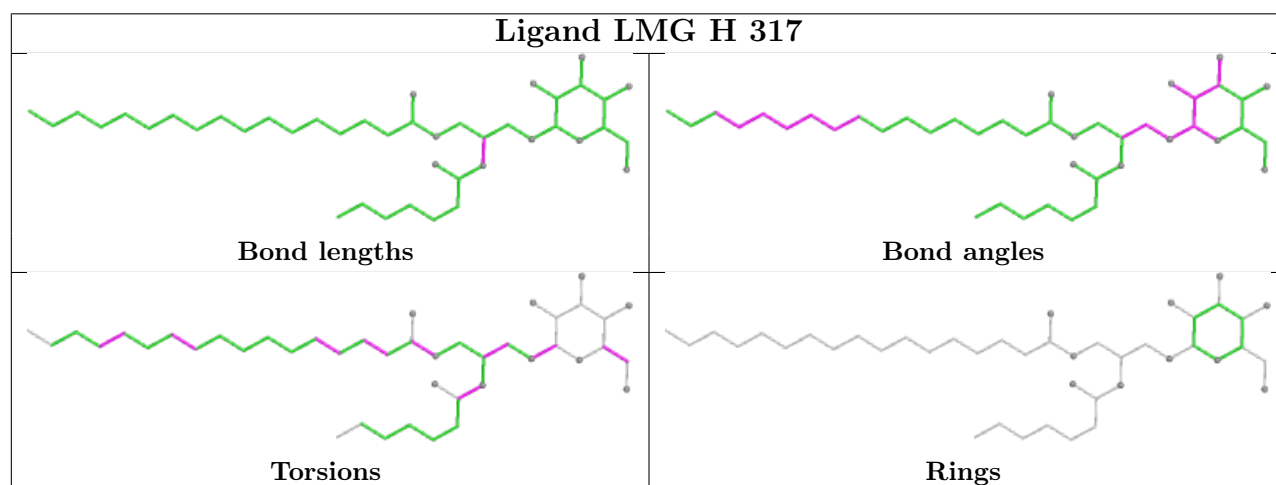
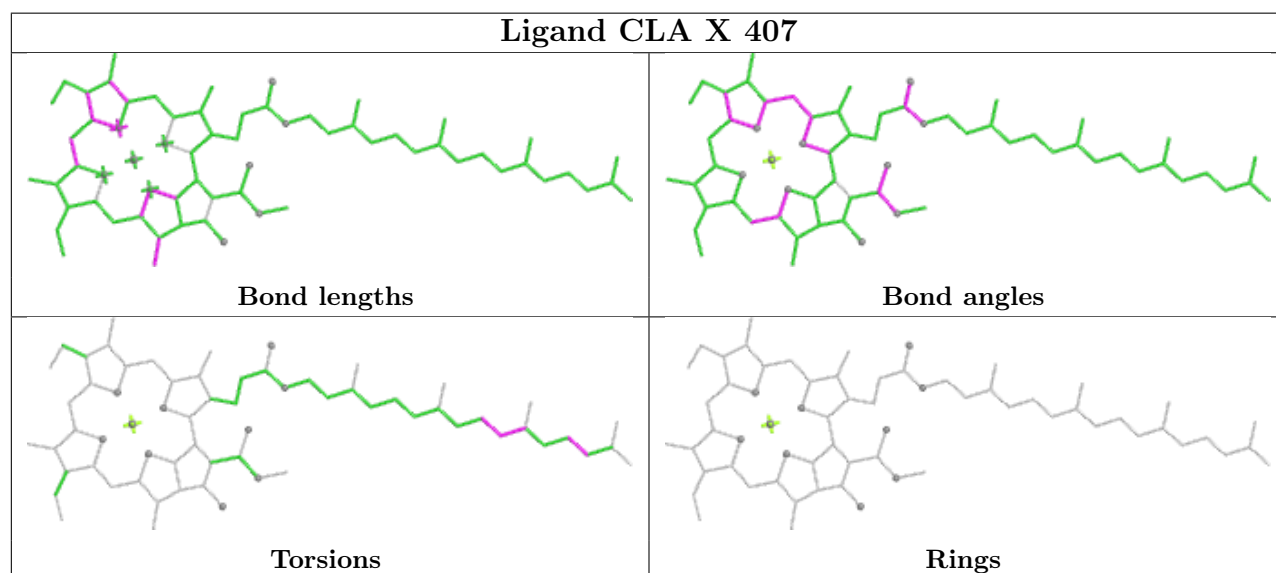
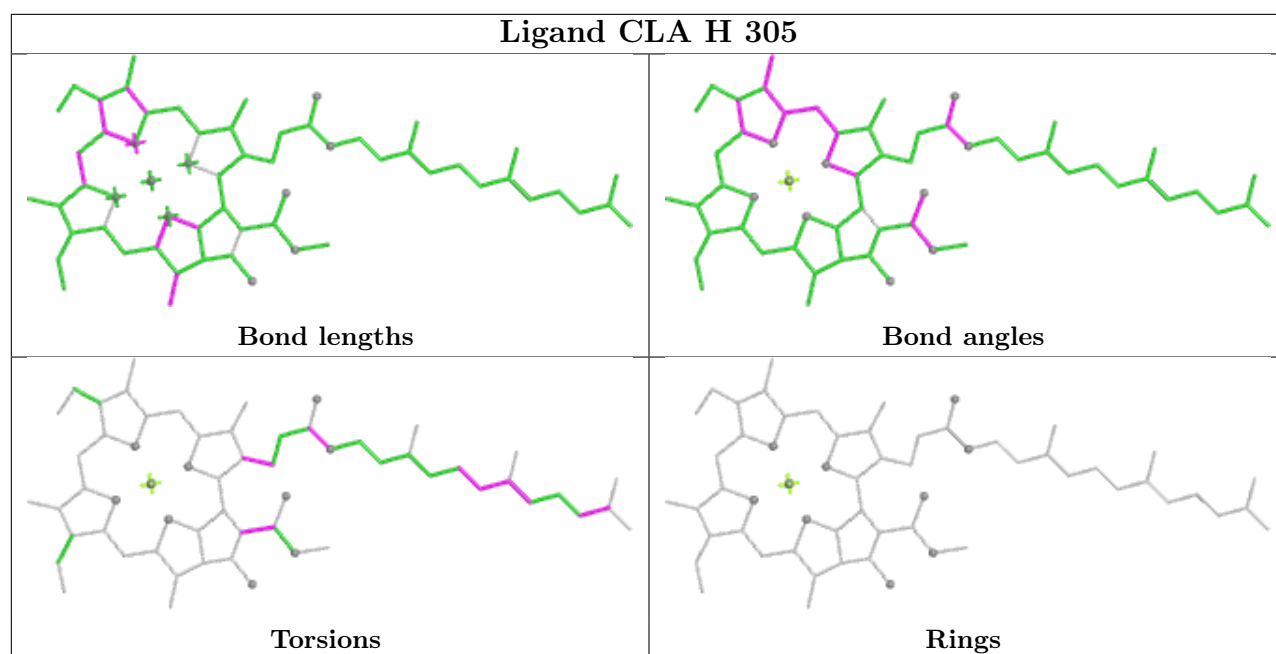


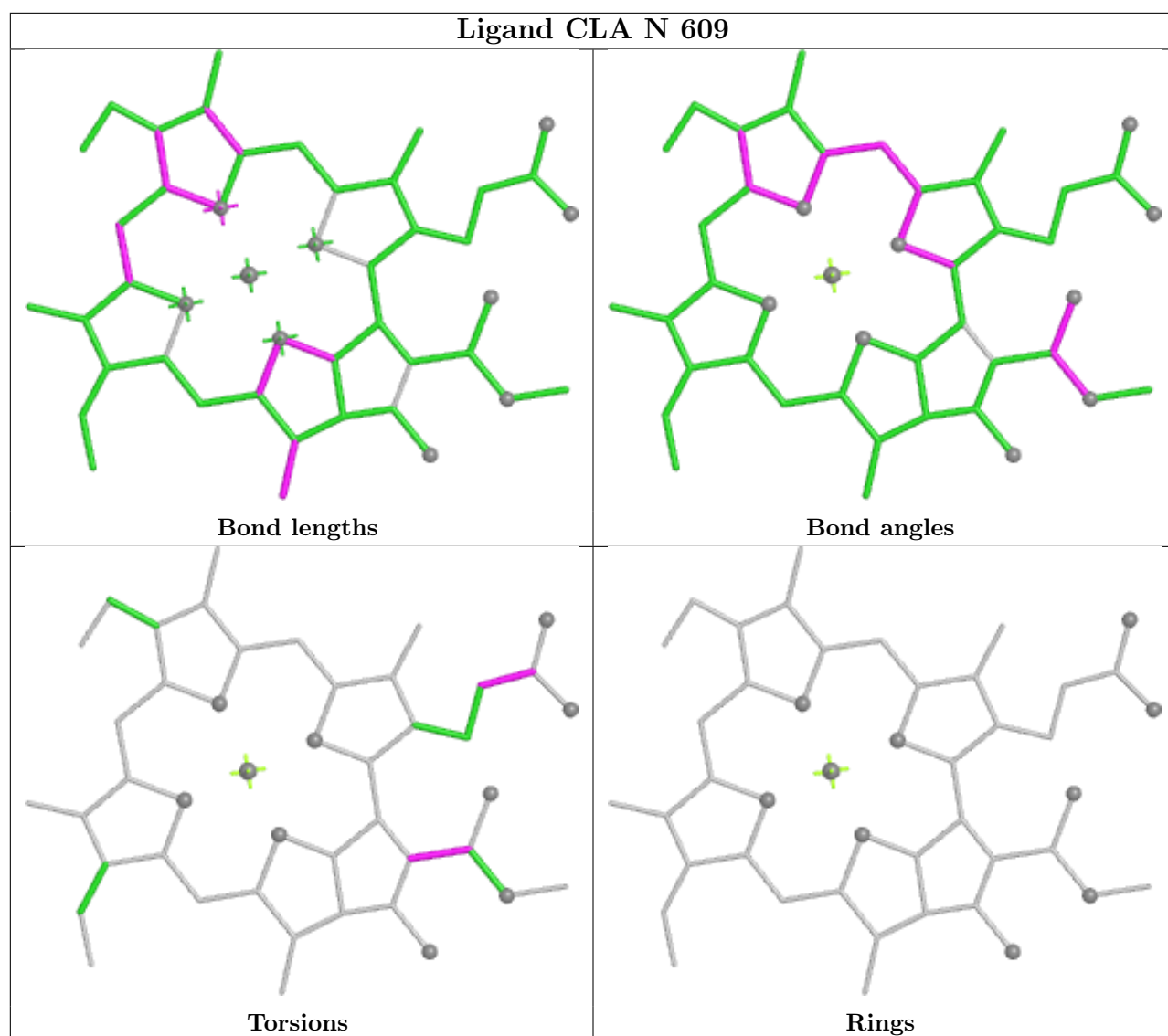
Ligand CLA A 837

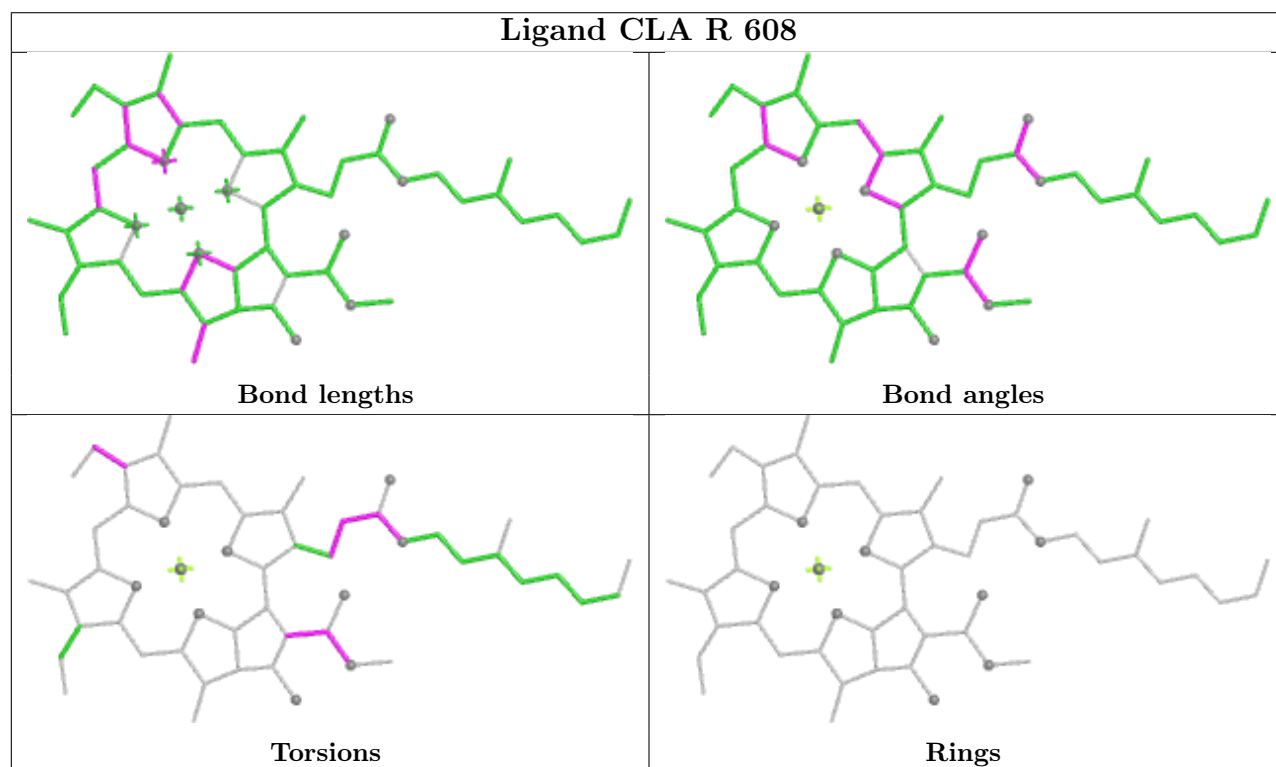
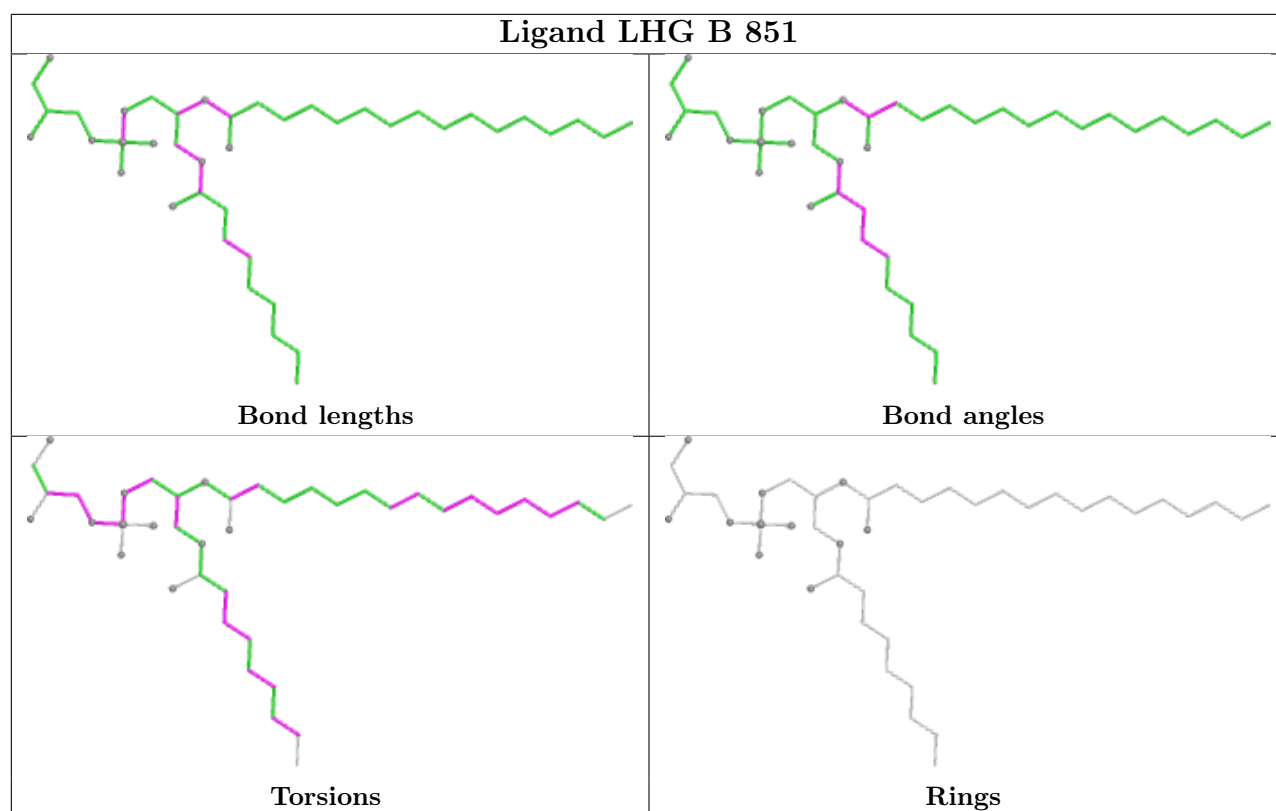


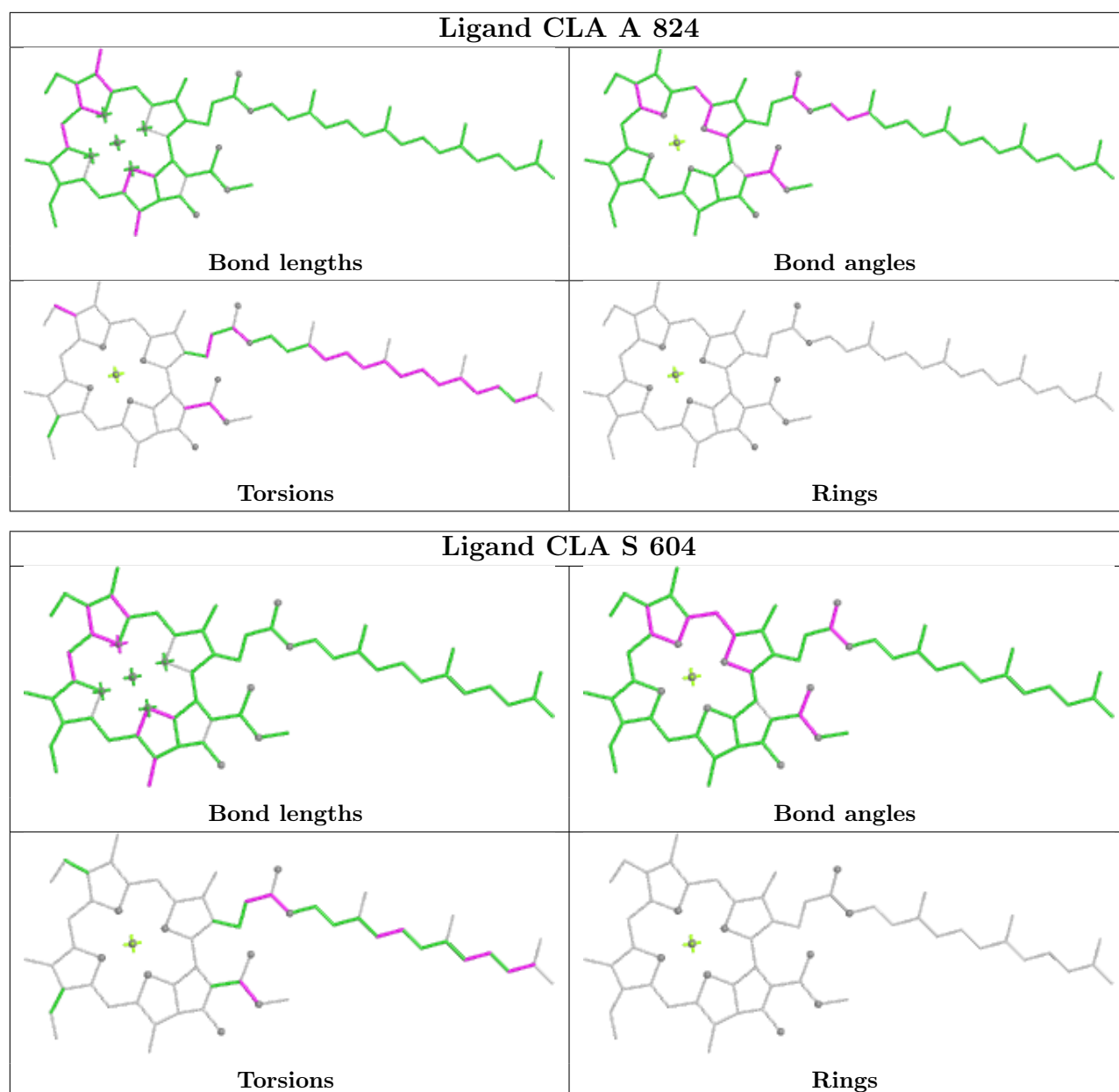
Ligand LMG L 401



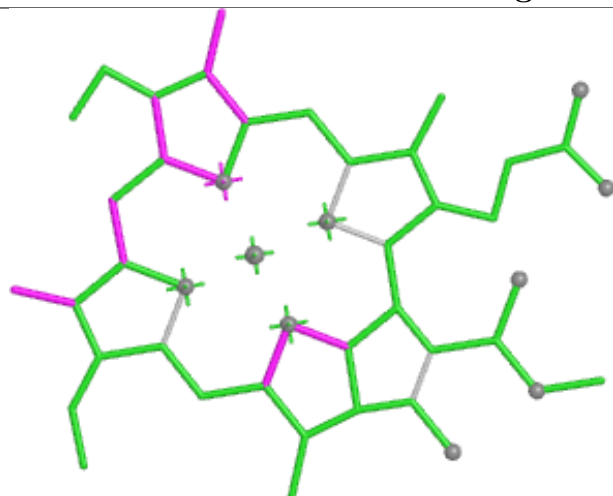




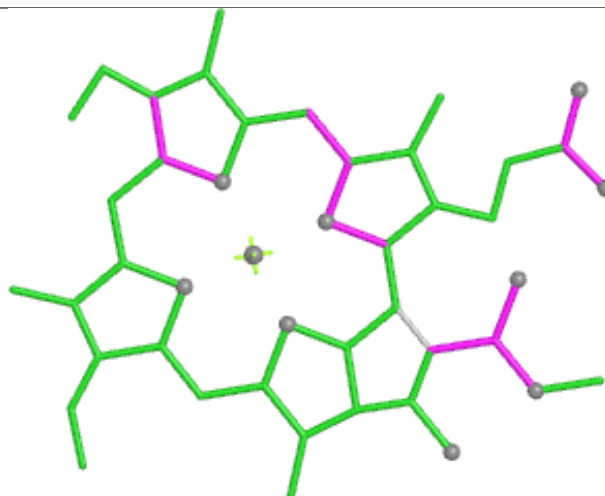




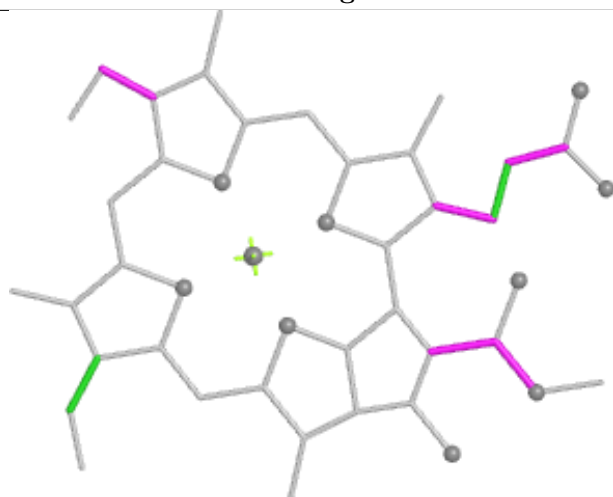
Ligand CLA P 608



Bond lengths



Bond angles

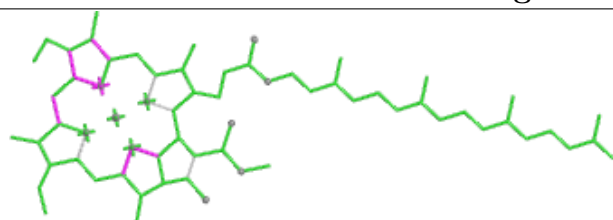


Torsions

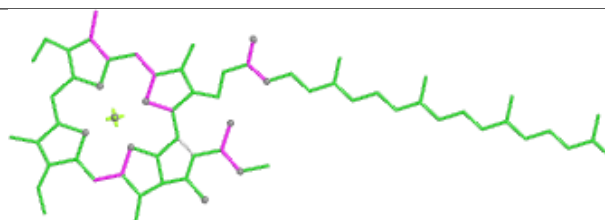


Rings

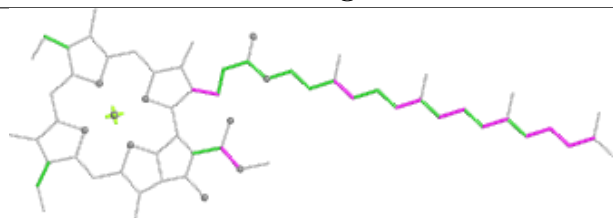
Ligand CLA A 852



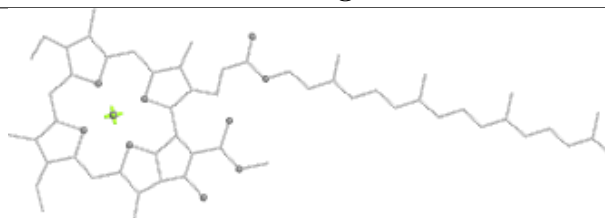
Bond lengths



Bond angles

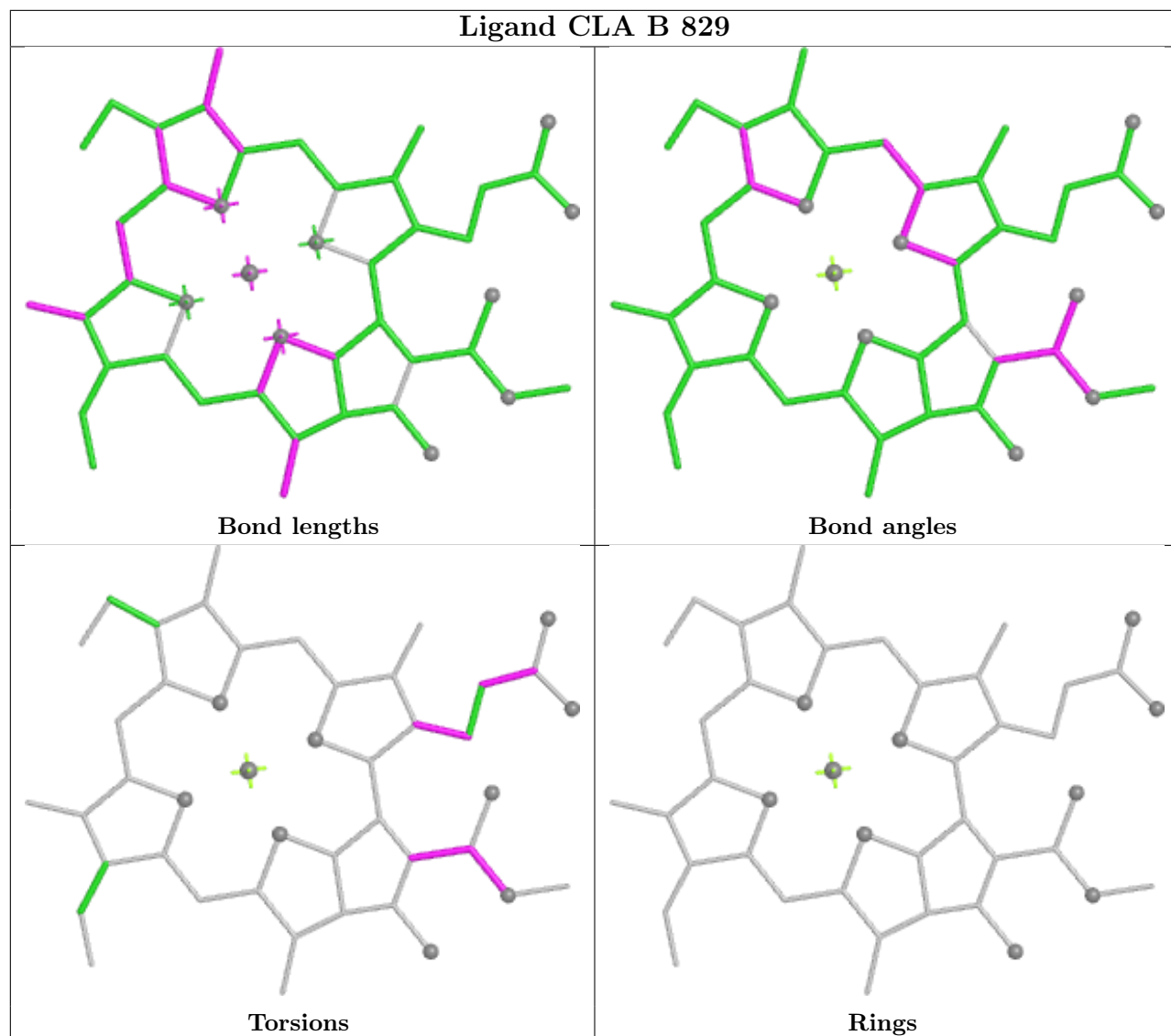


Torsions

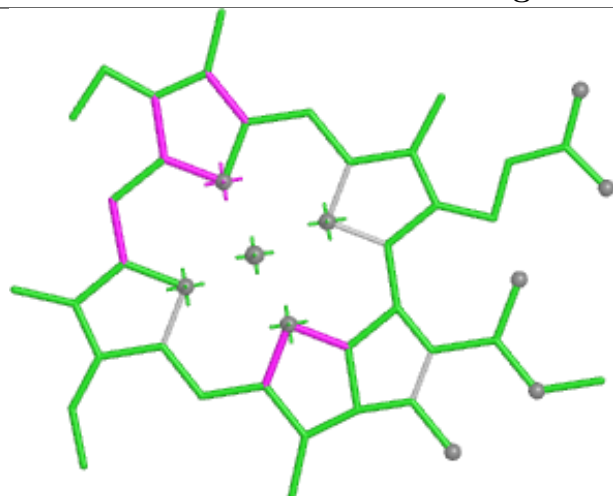


Rings

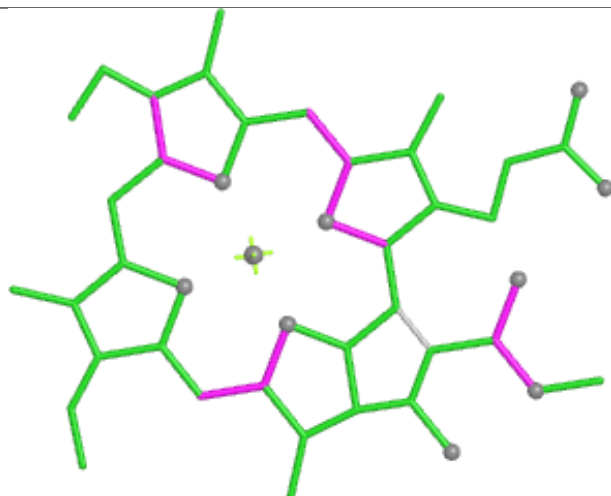
Ligand CLA B 829



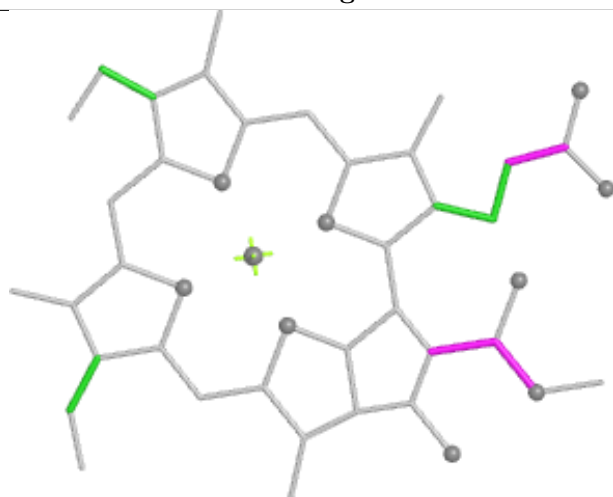
Ligand CLA G 601



Bond lengths



Bond angles

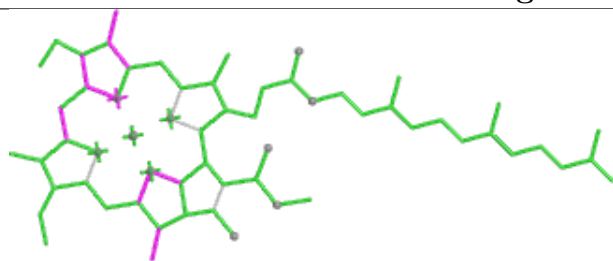


Torsions

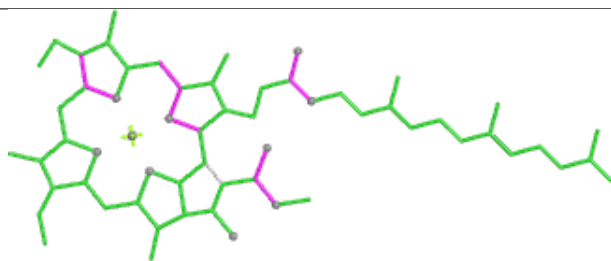


Rings

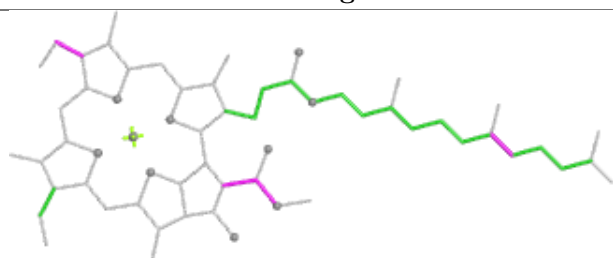
Ligand CLA L 409



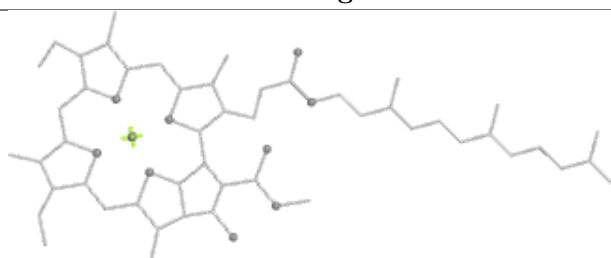
Bond lengths



Bond angles

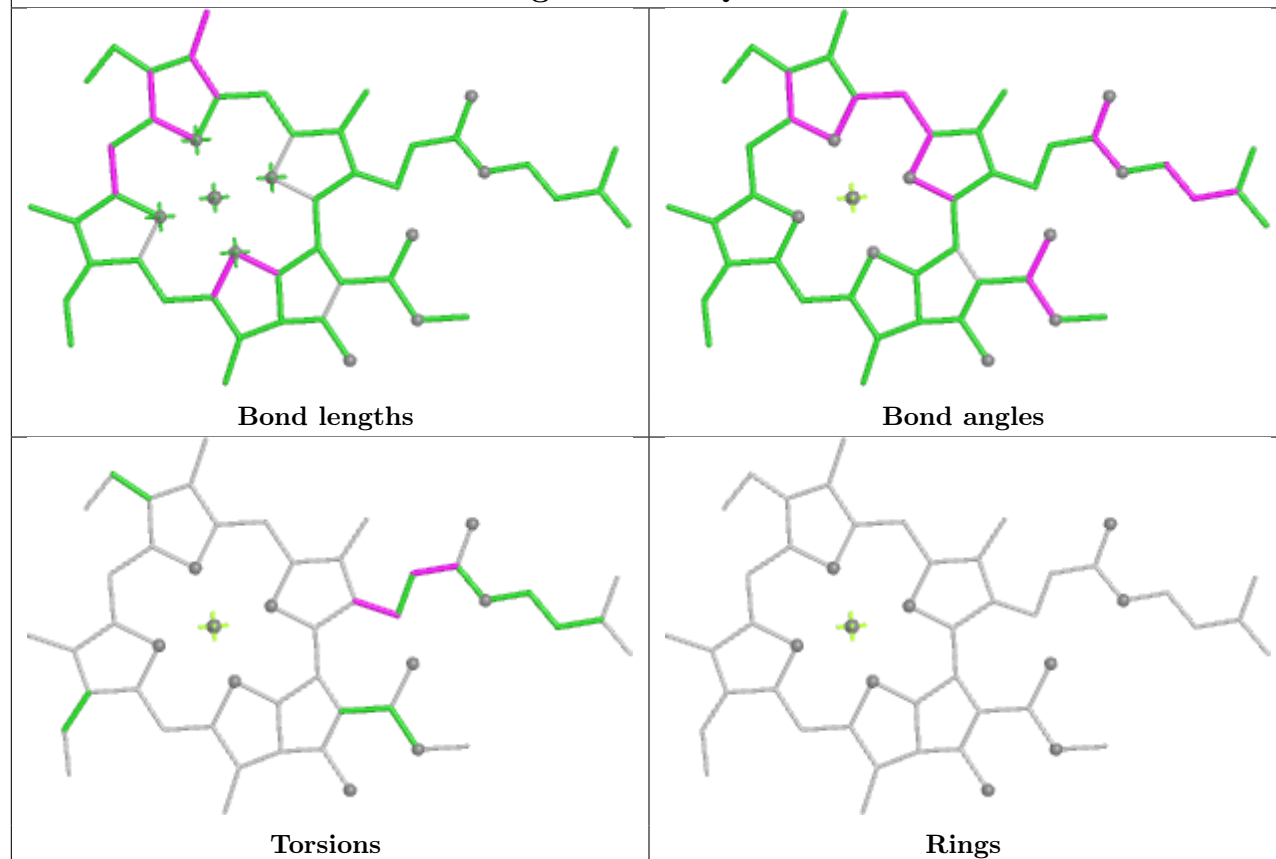


Torsions

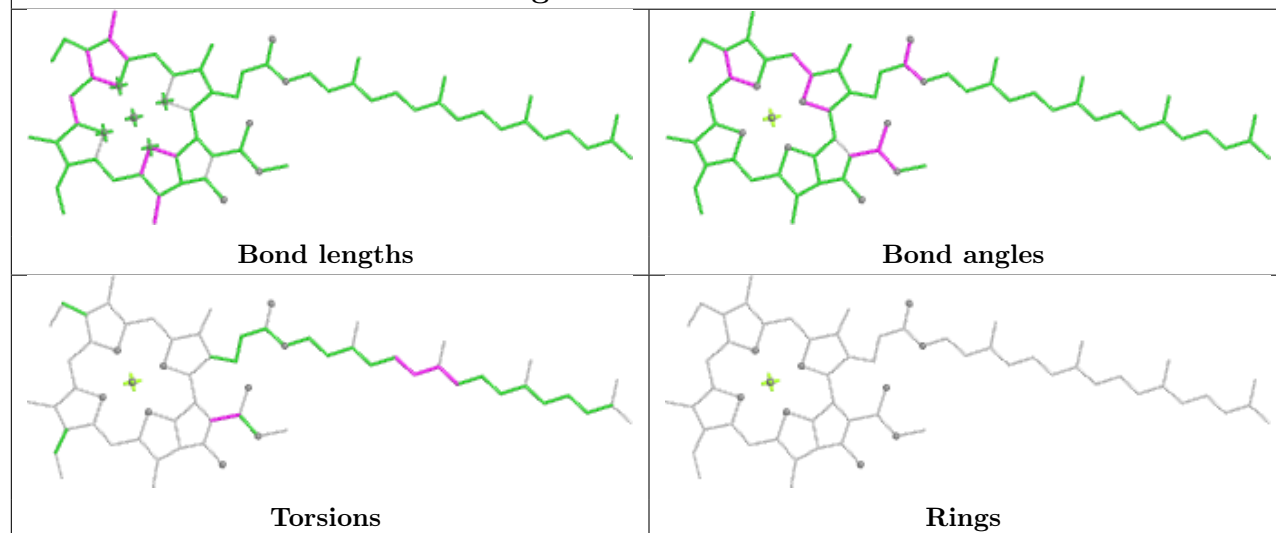


Rings

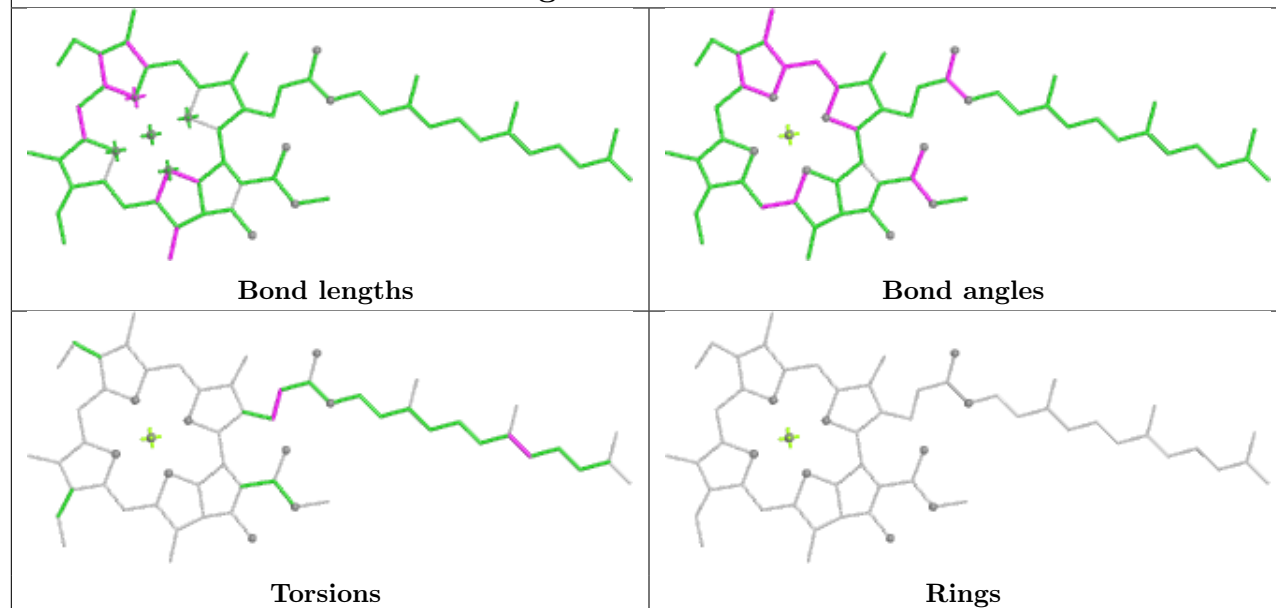
Ligand CLA Q 608



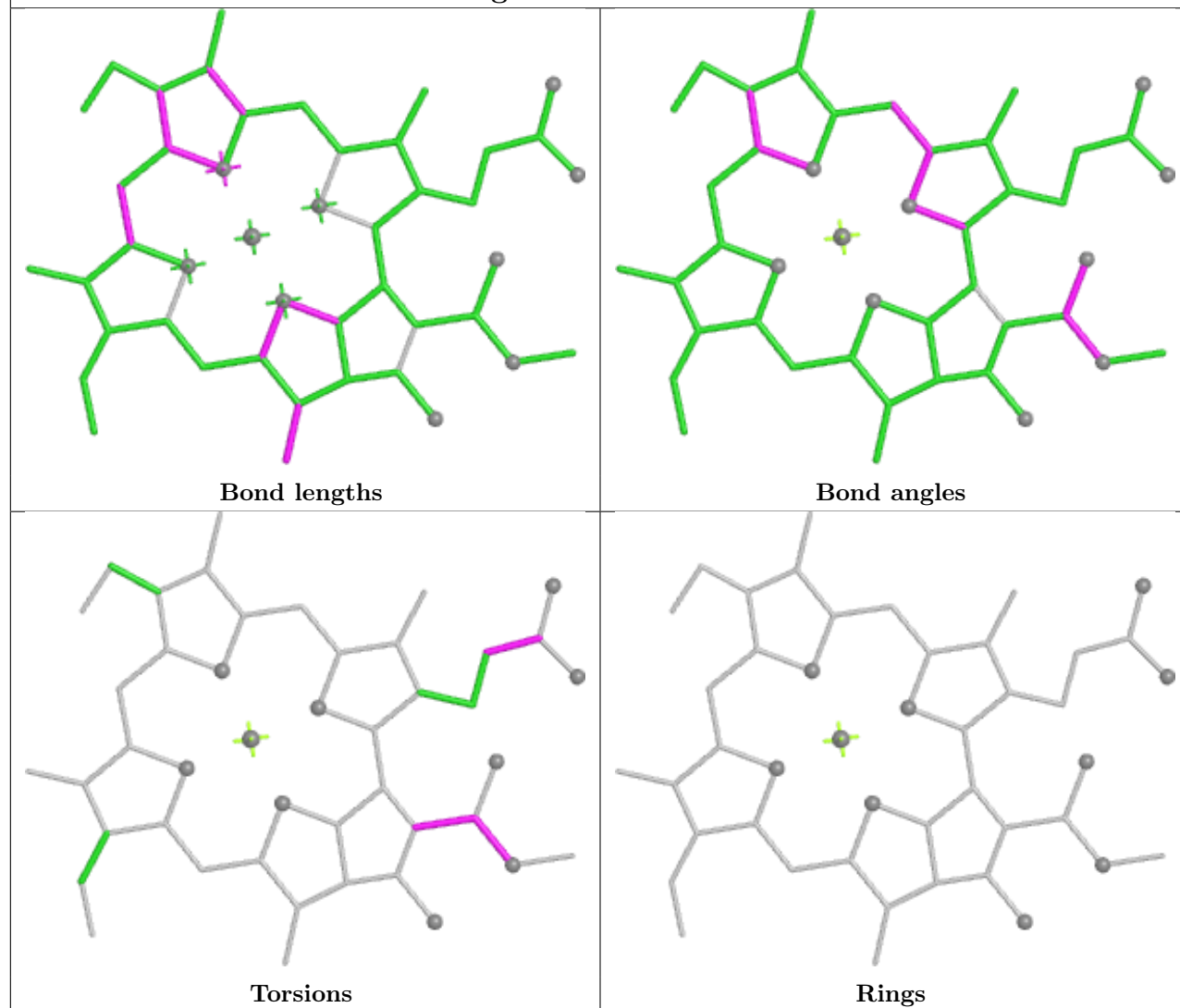
Ligand CLA A 831

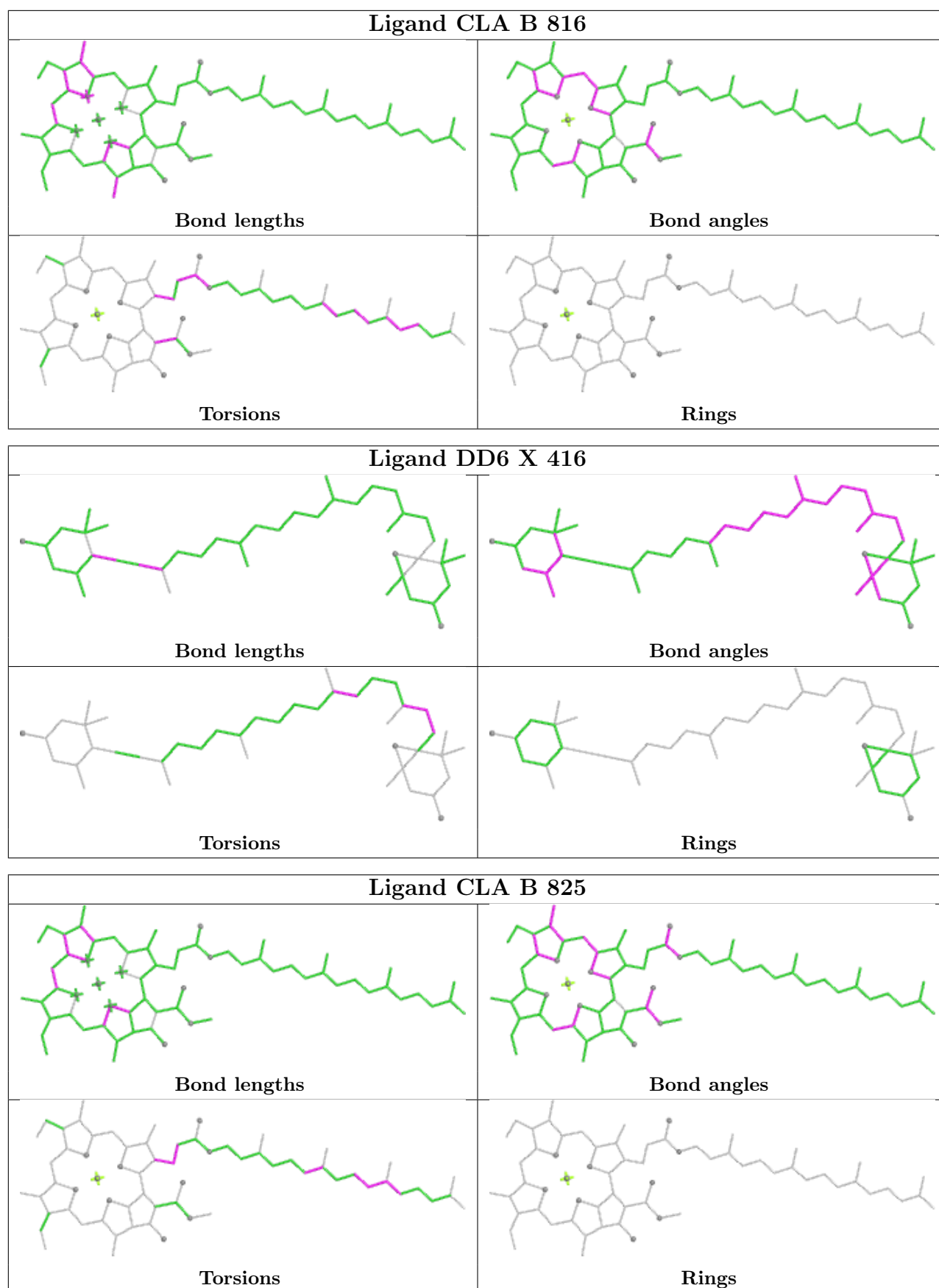


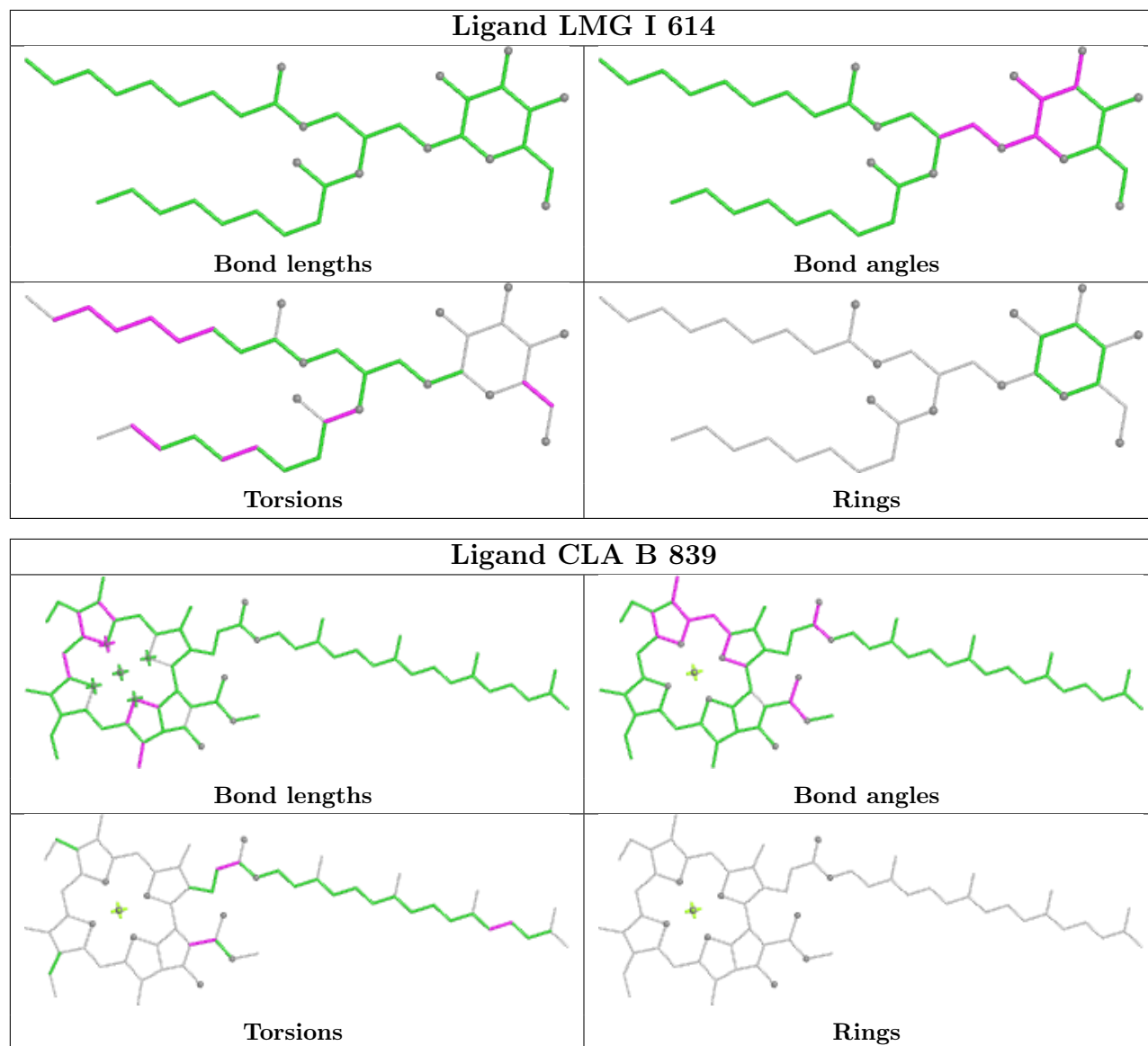
Ligand CLA I 602

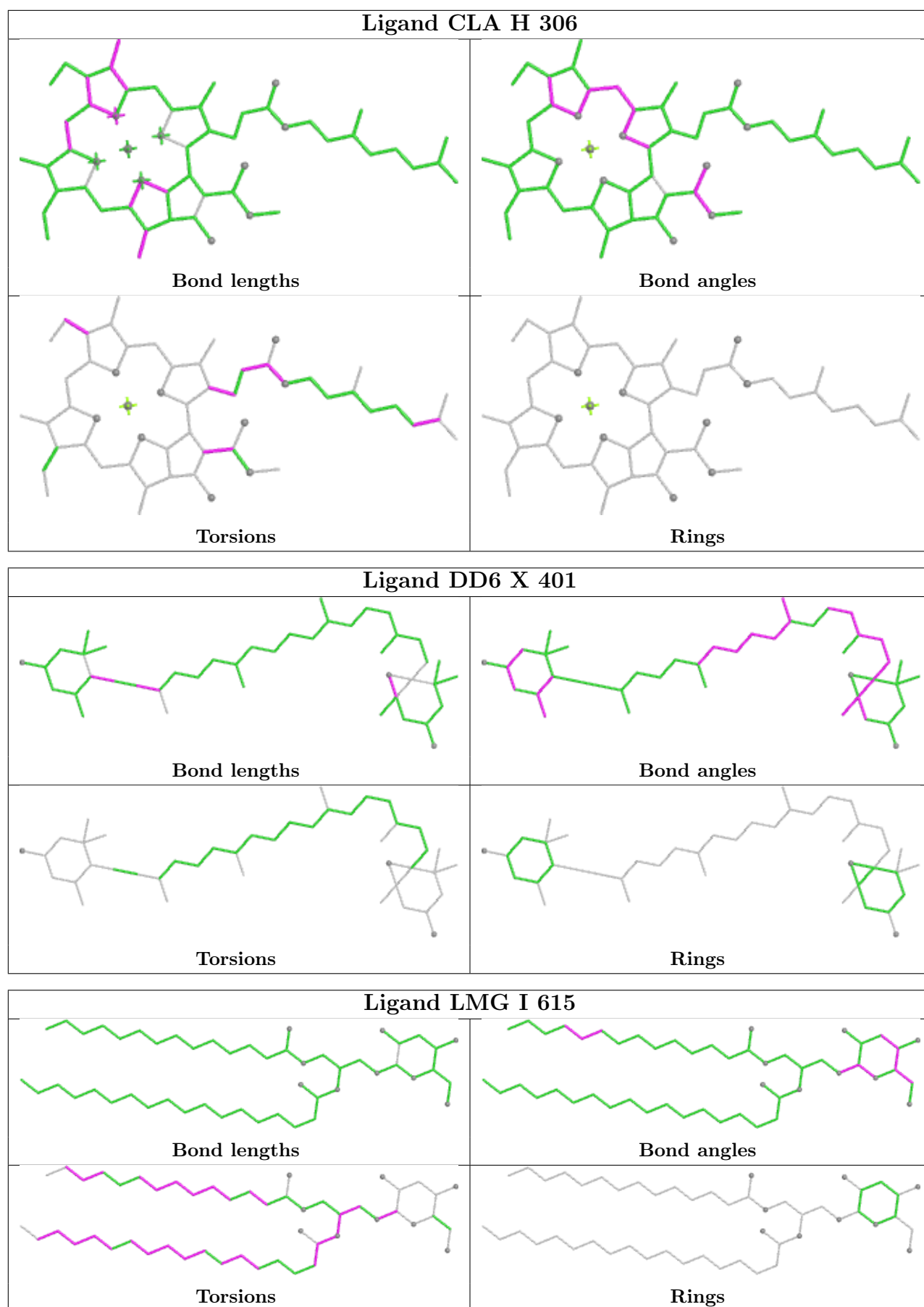


Ligand CLA N 604

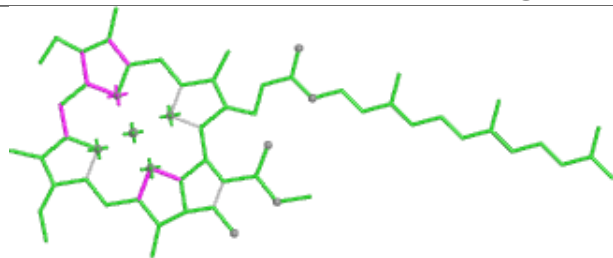




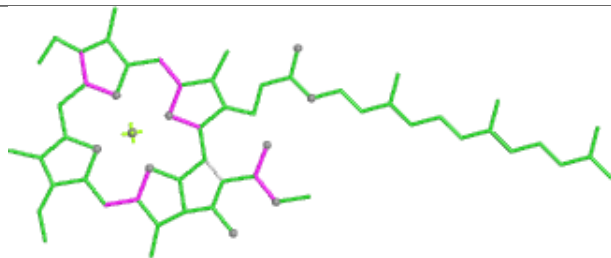




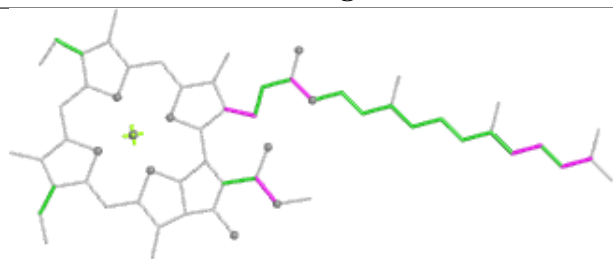
Ligand CLA S 607



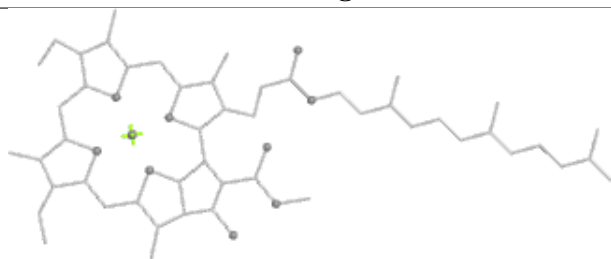
Bond lengths



Bond angles

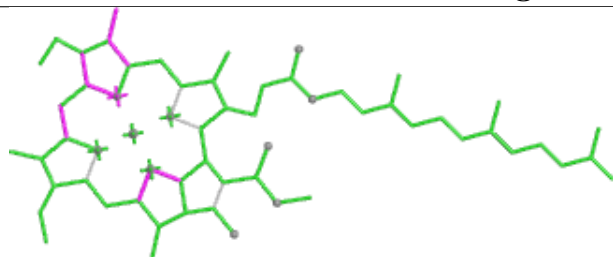


Torsions

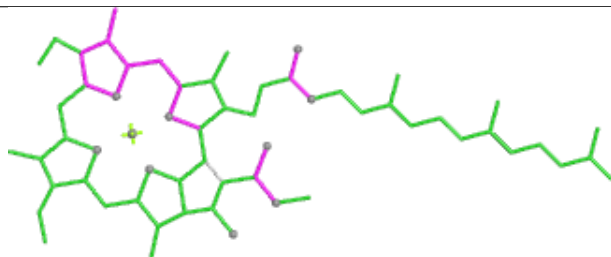


Rings

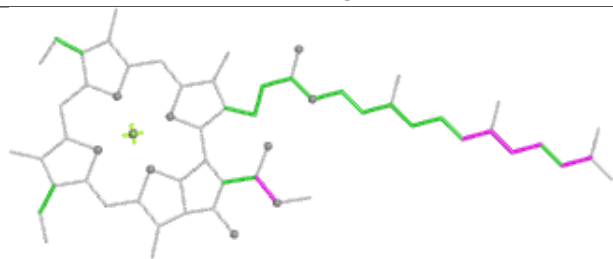
Ligand CLA T 607



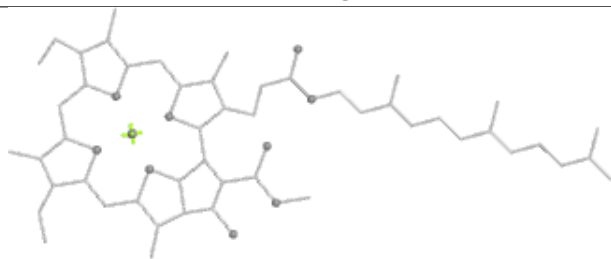
Bond lengths



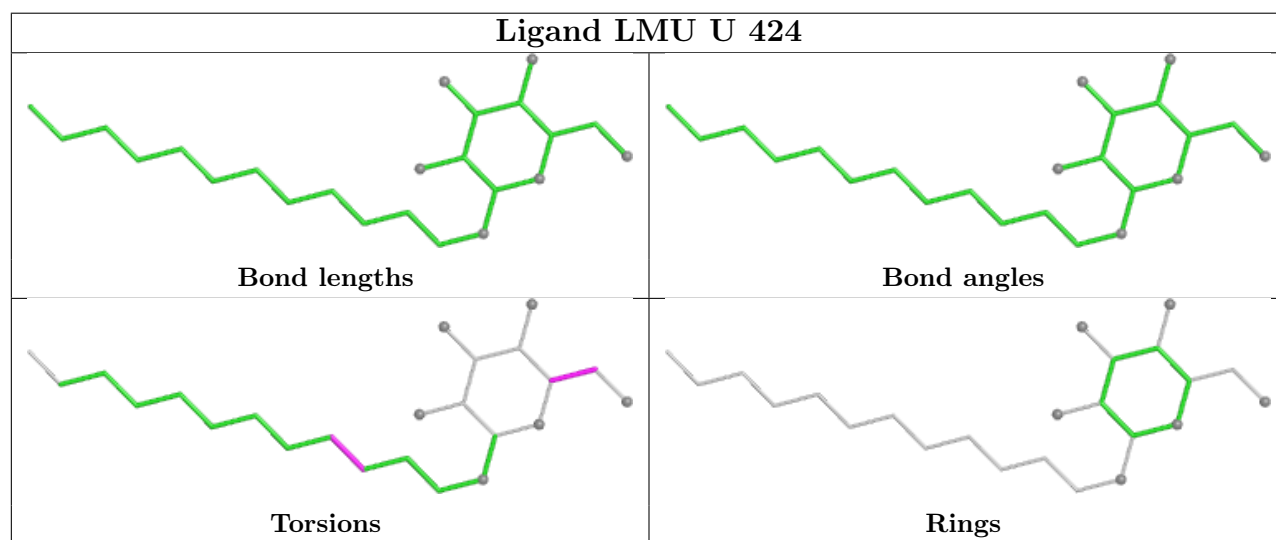
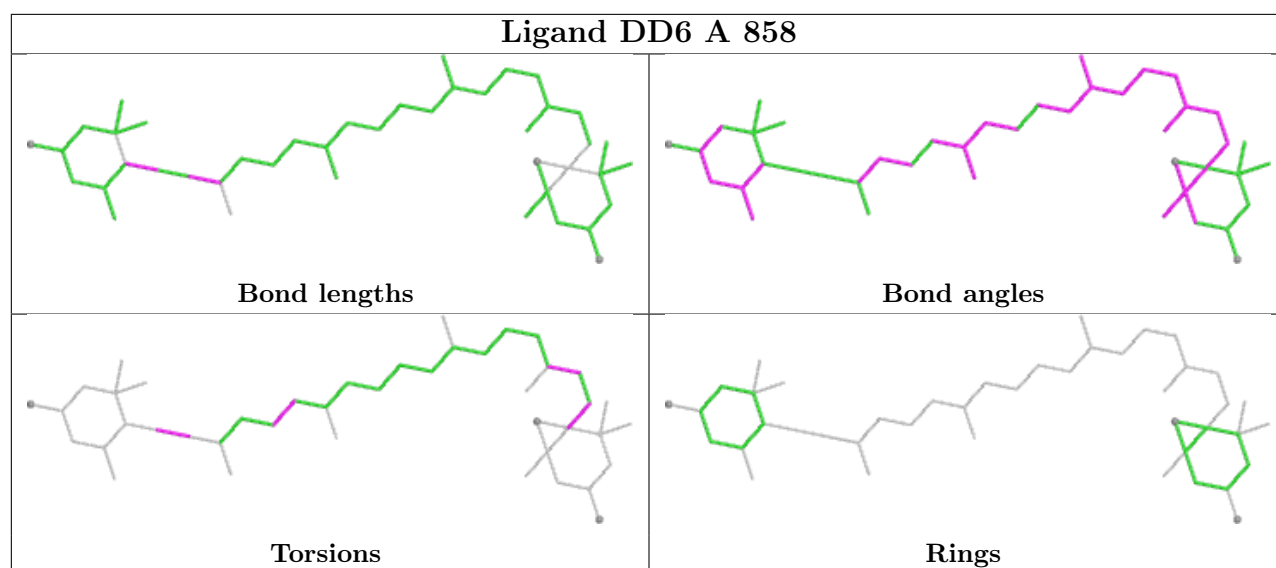
Bond angles

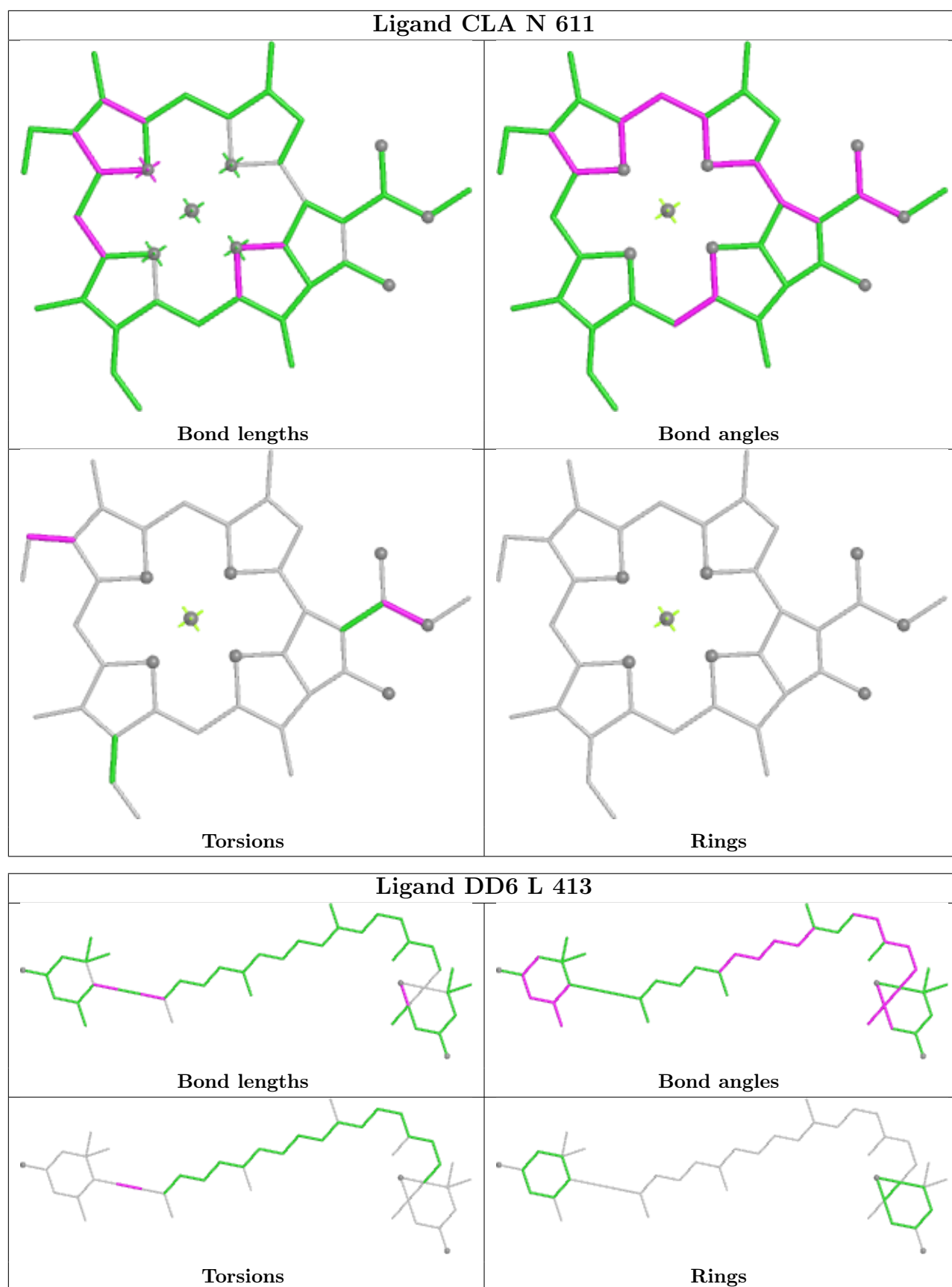


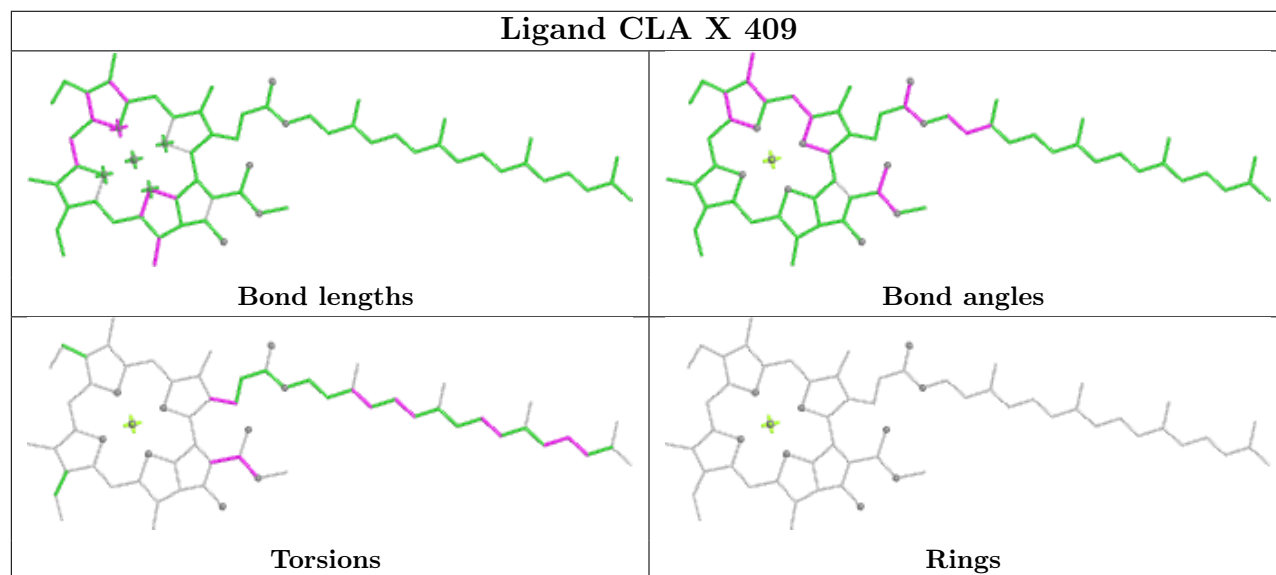
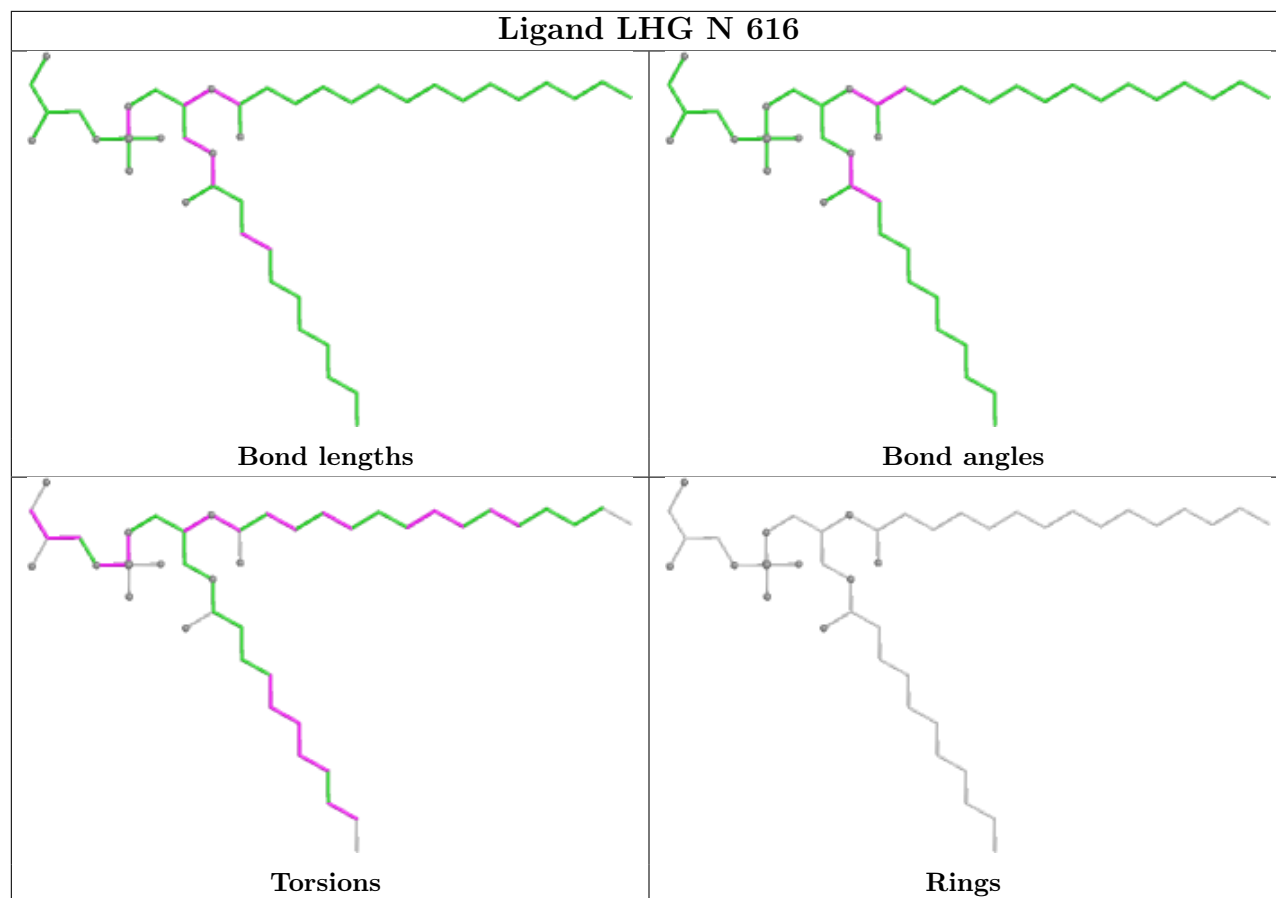
Torsions

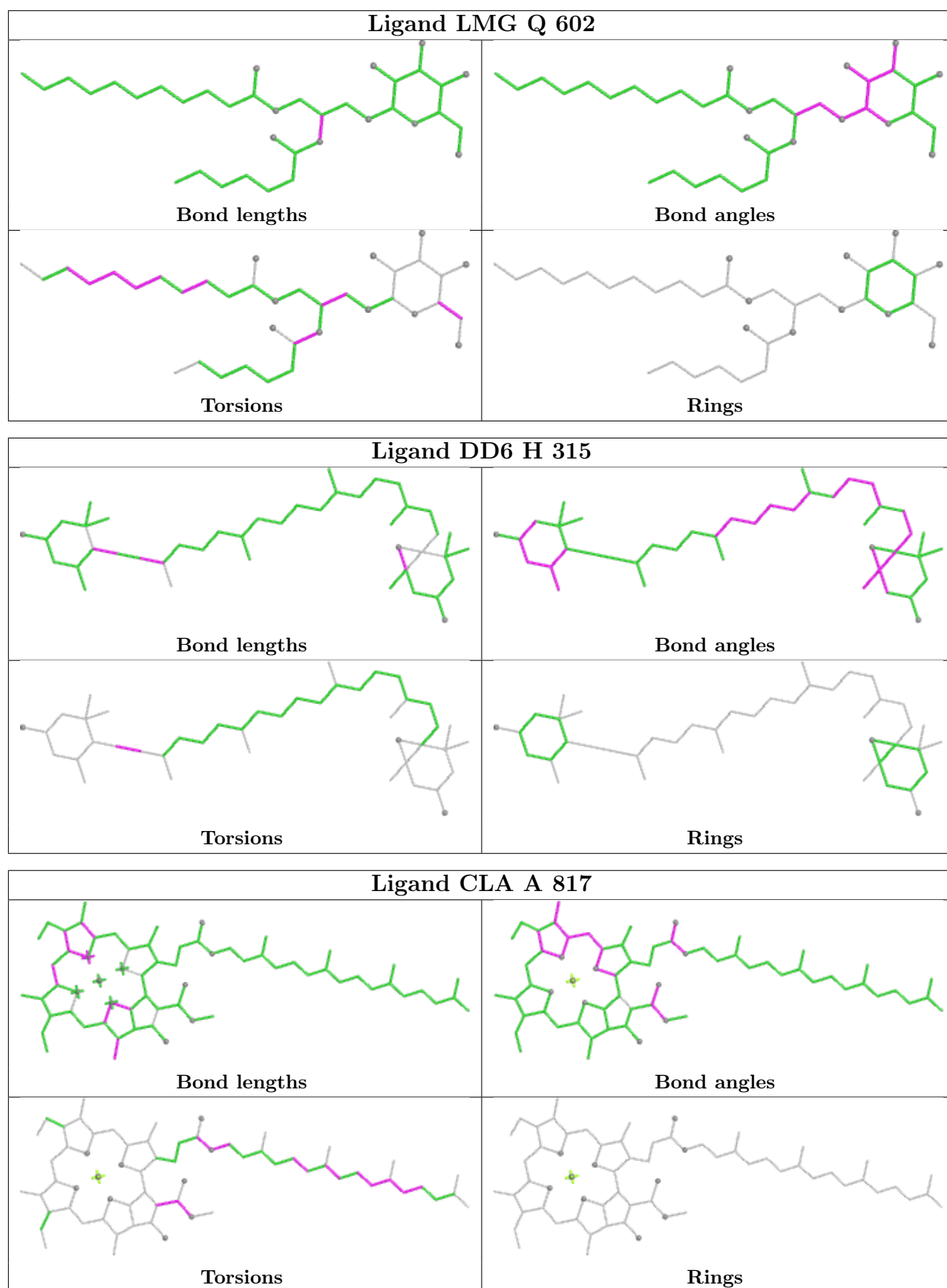


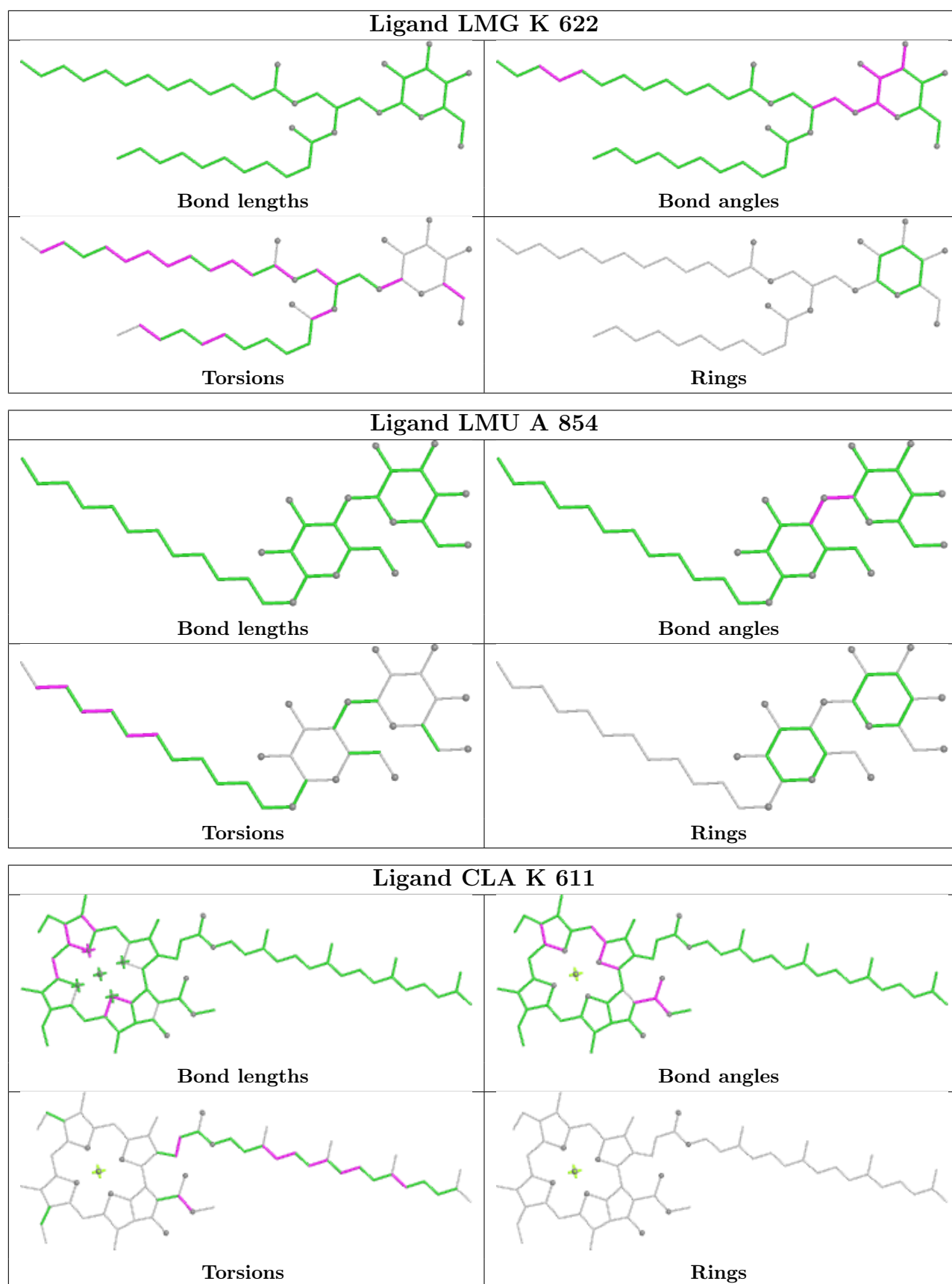
Rings

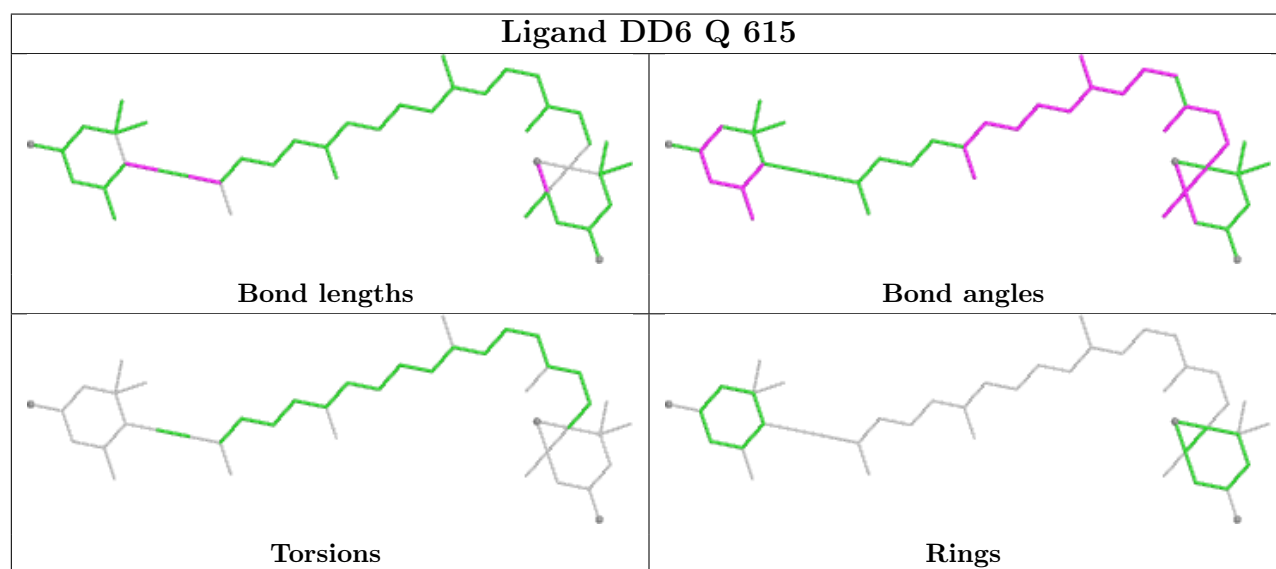
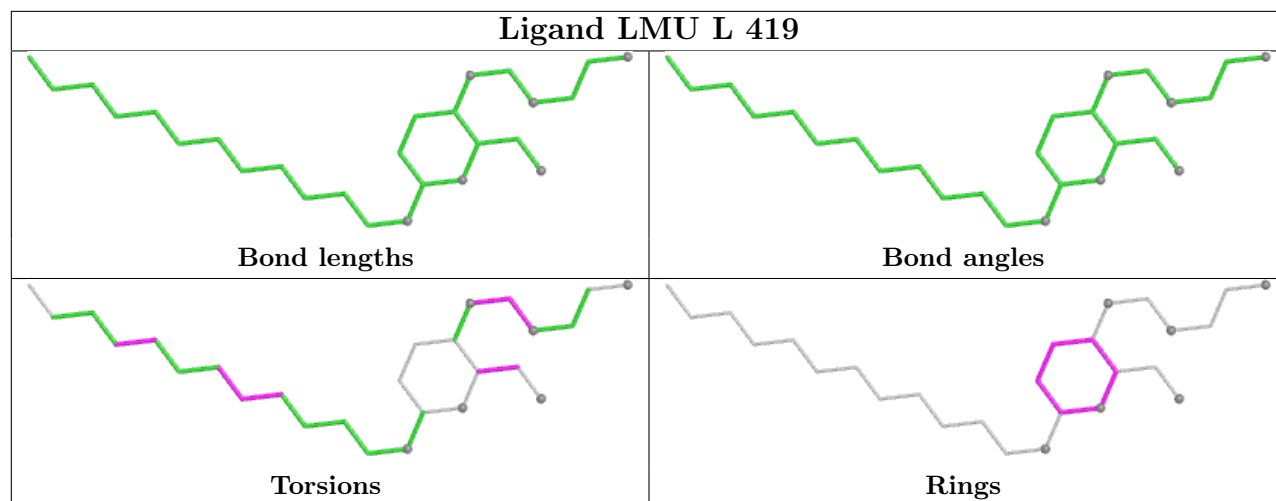


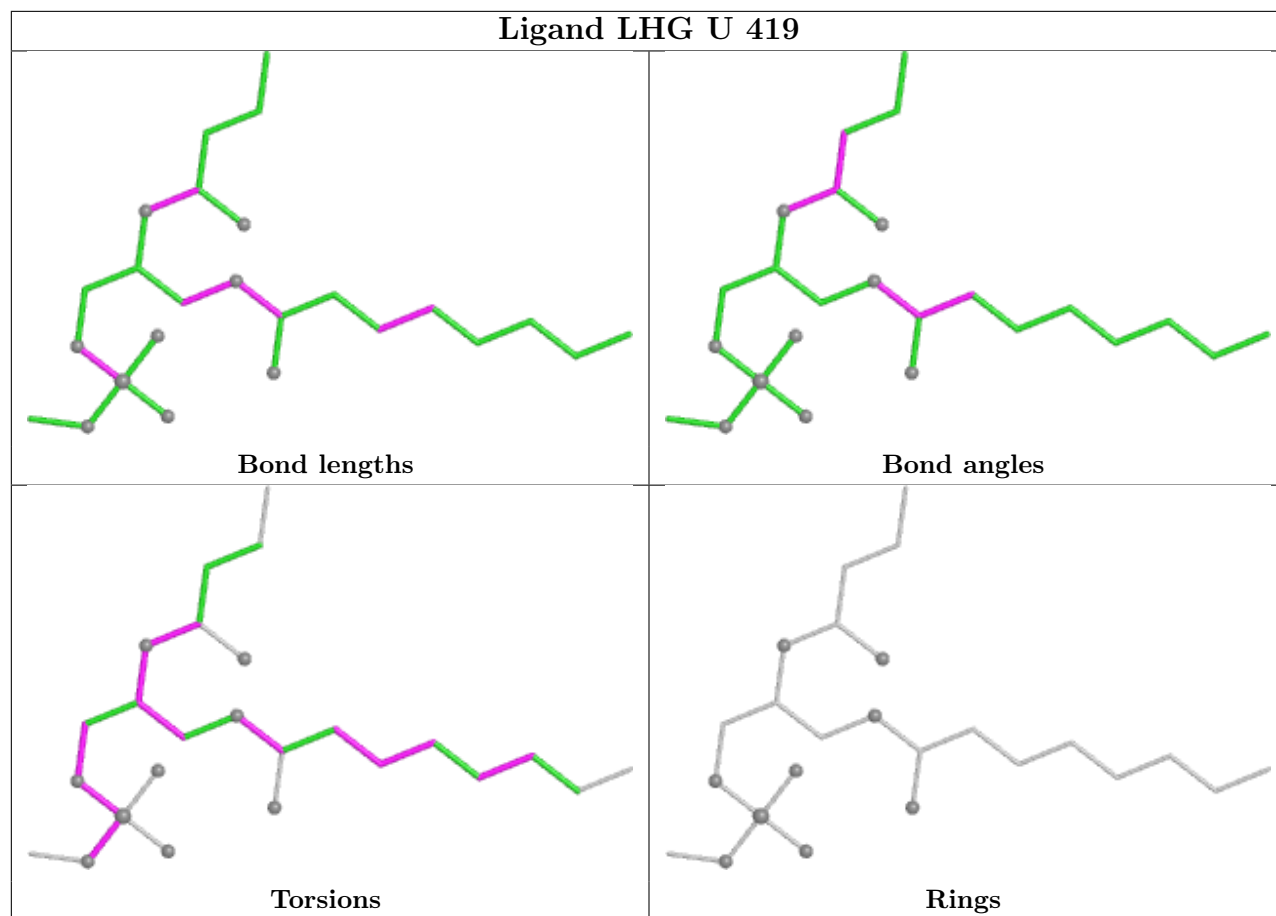


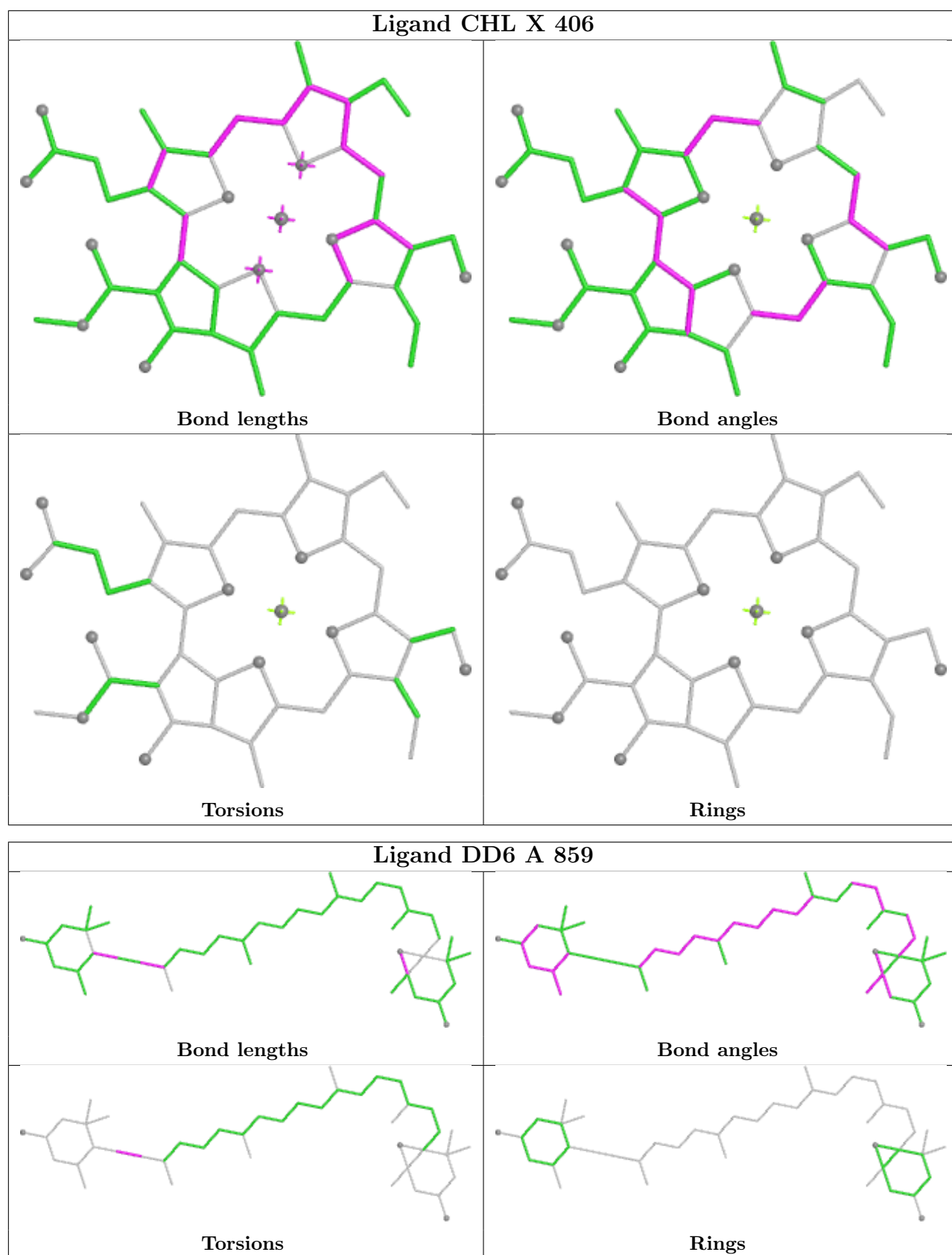


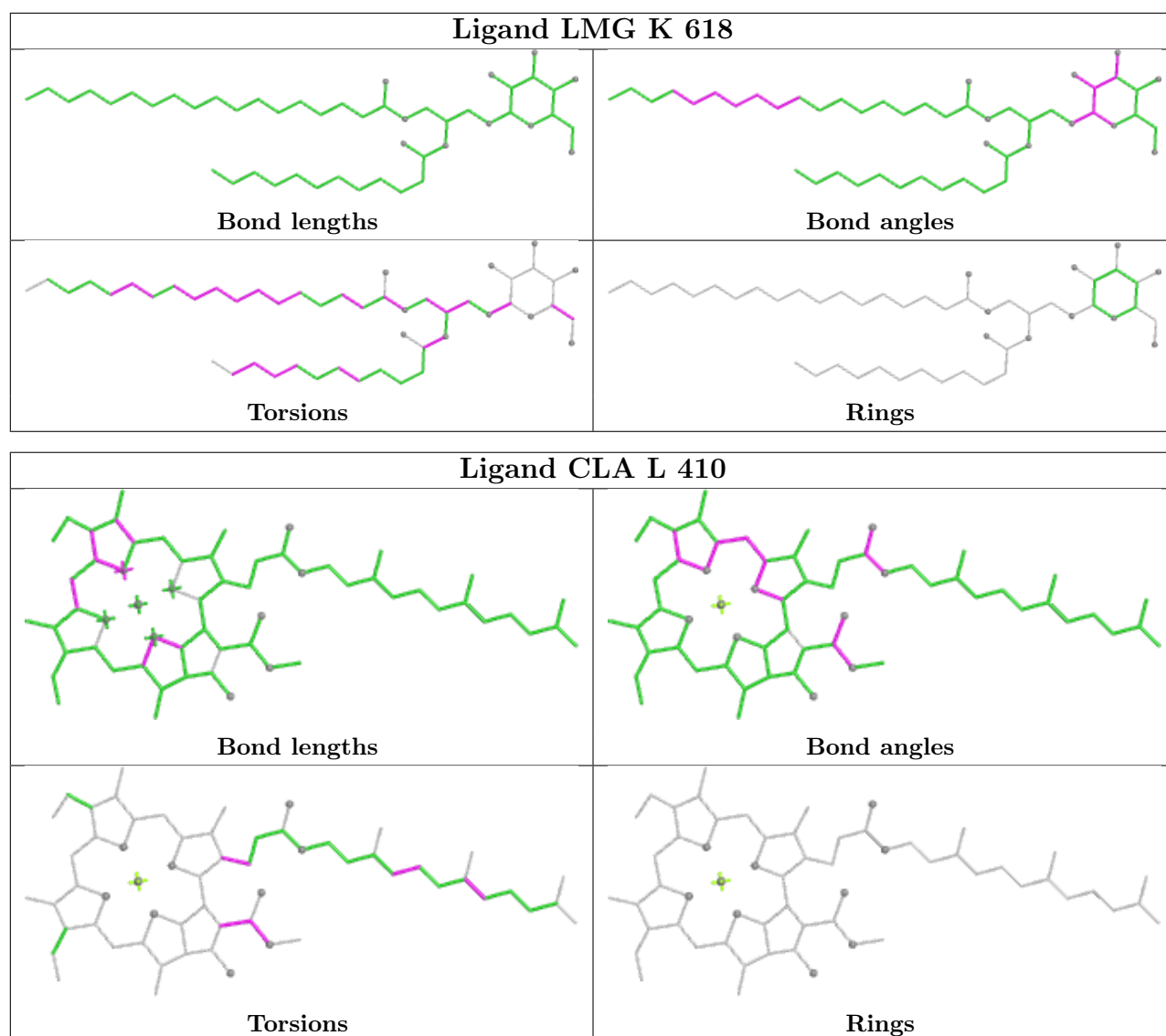


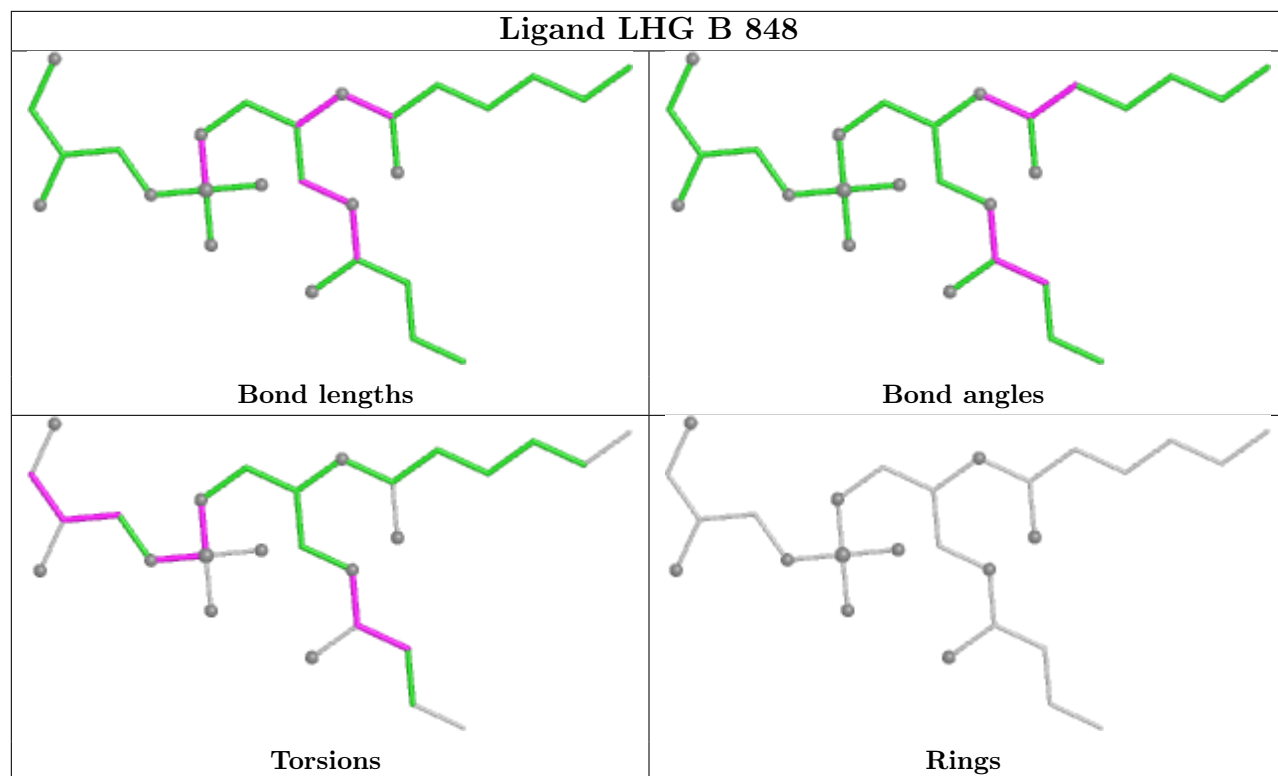


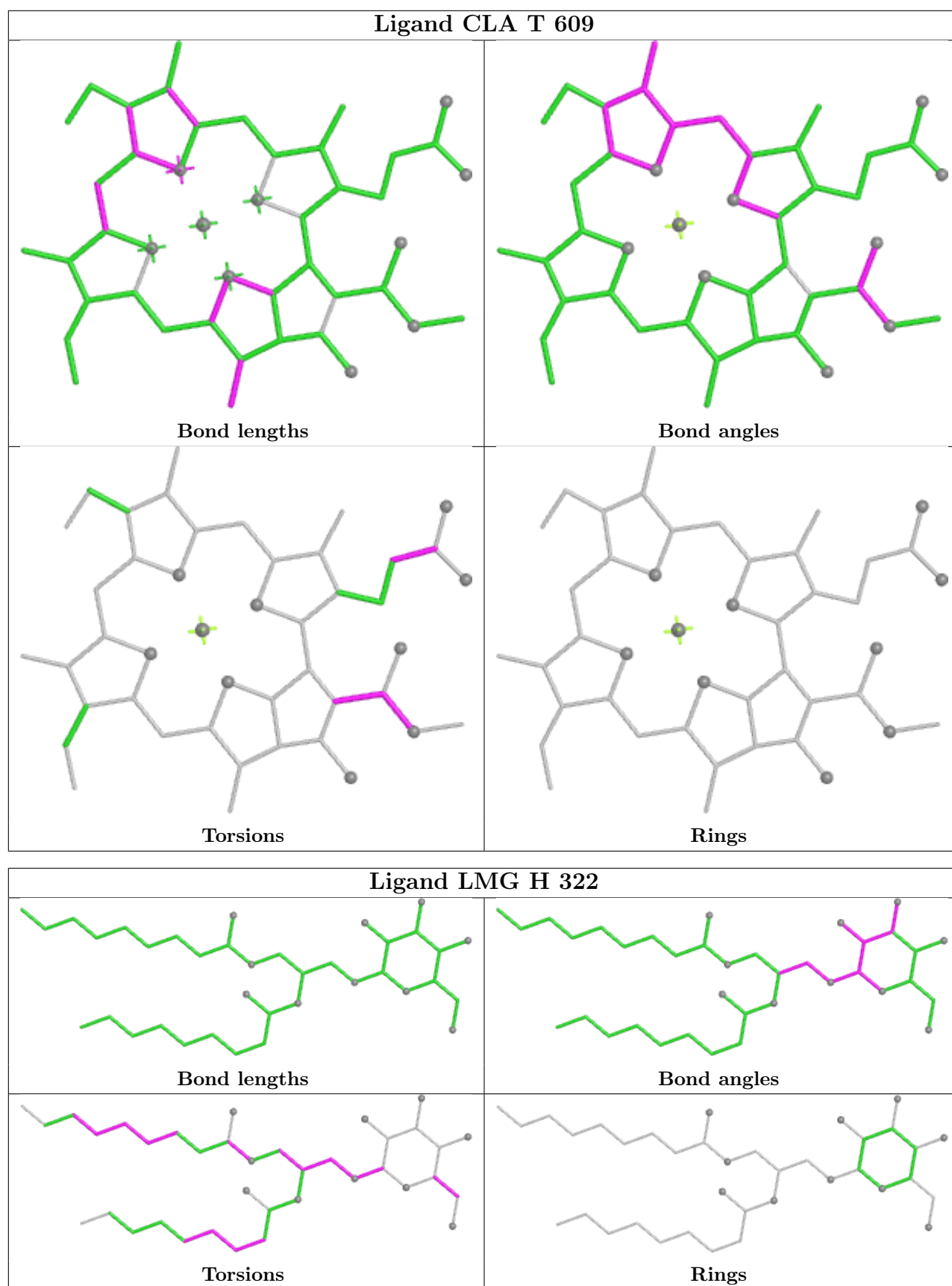


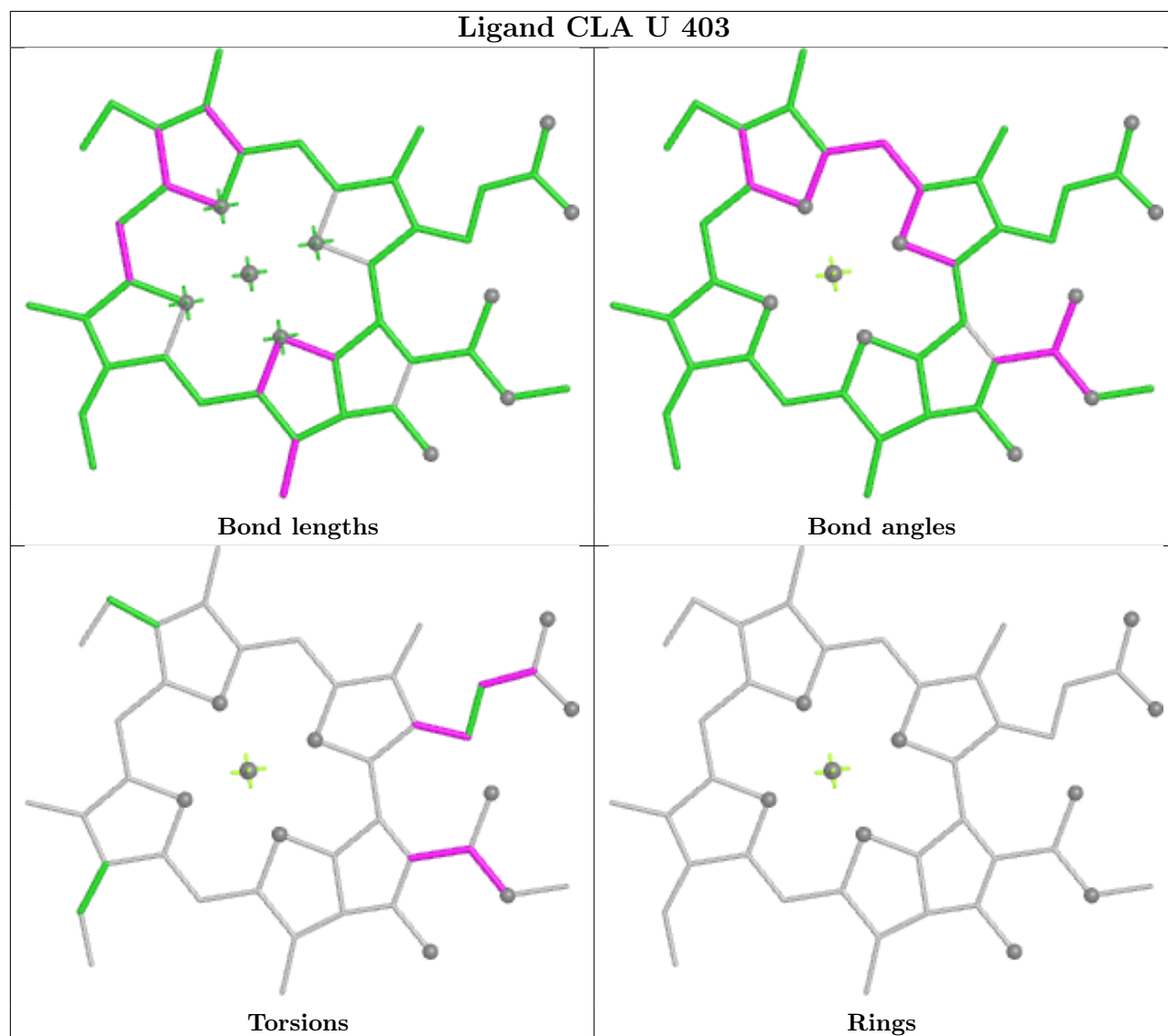
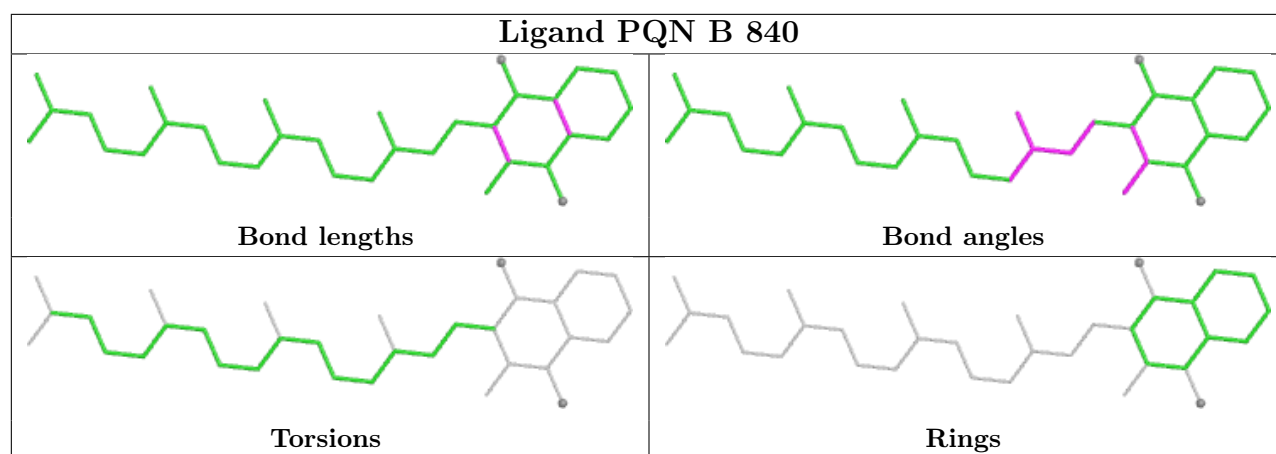


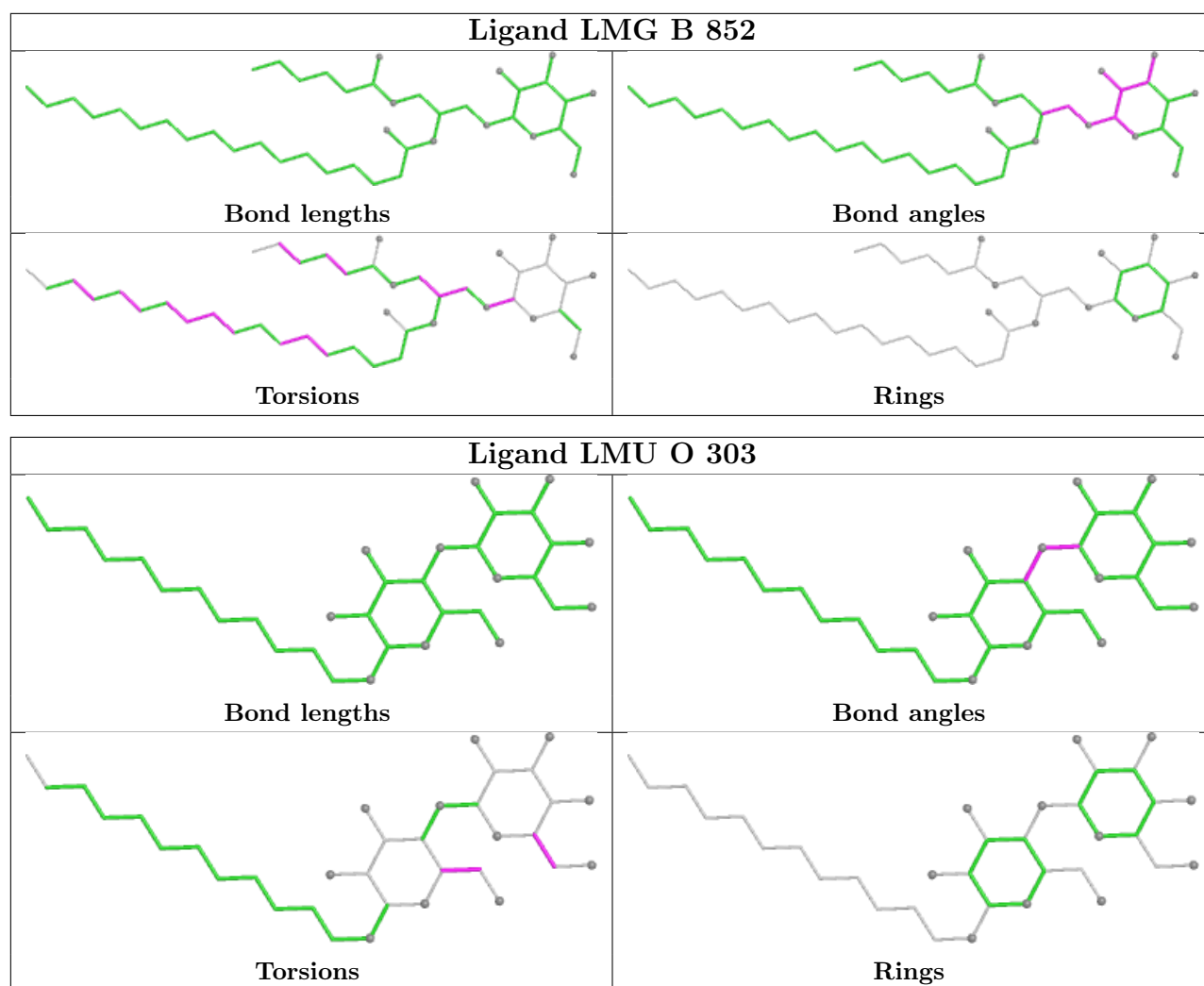


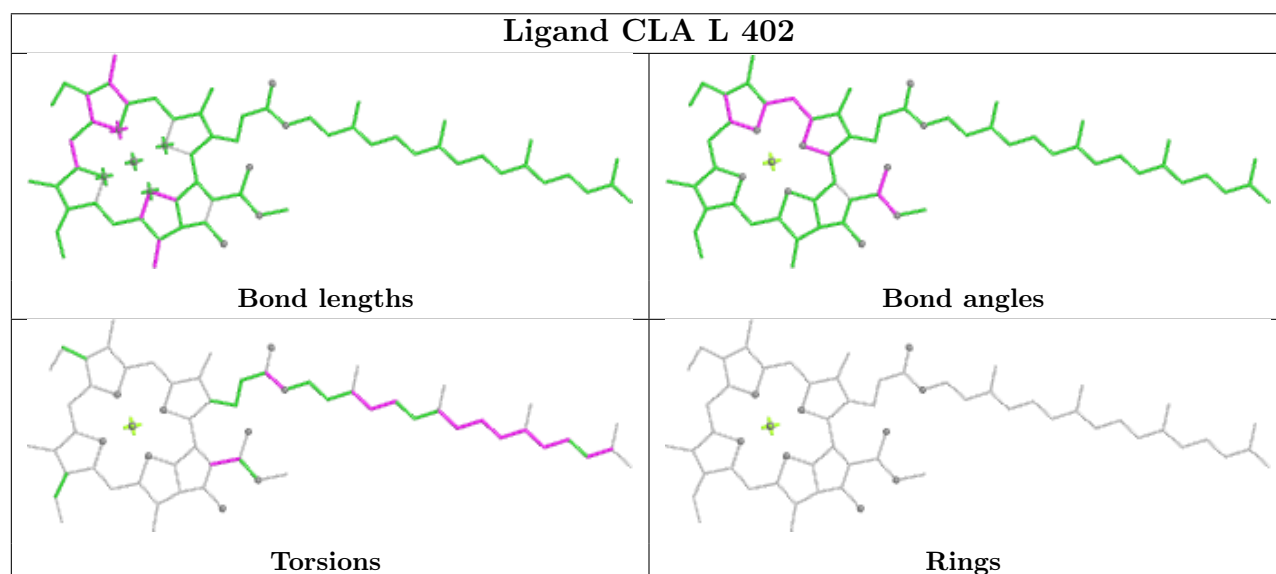
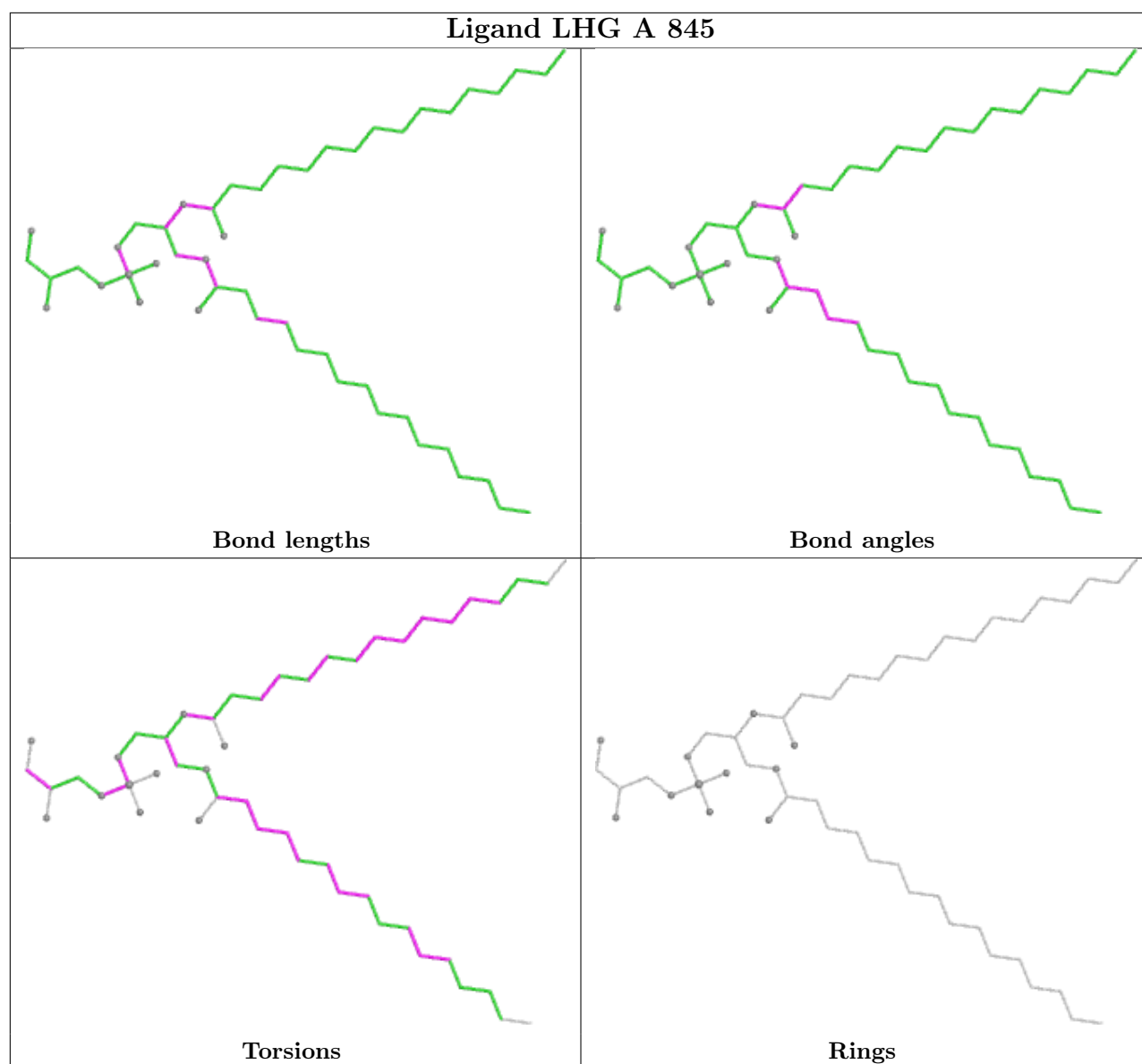




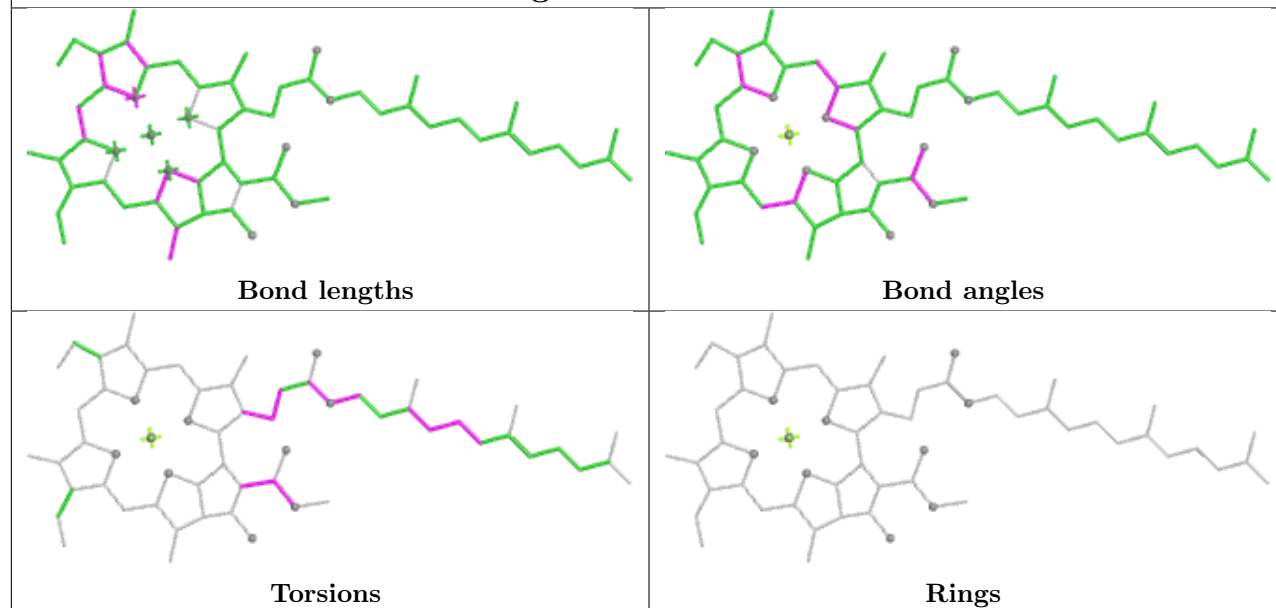




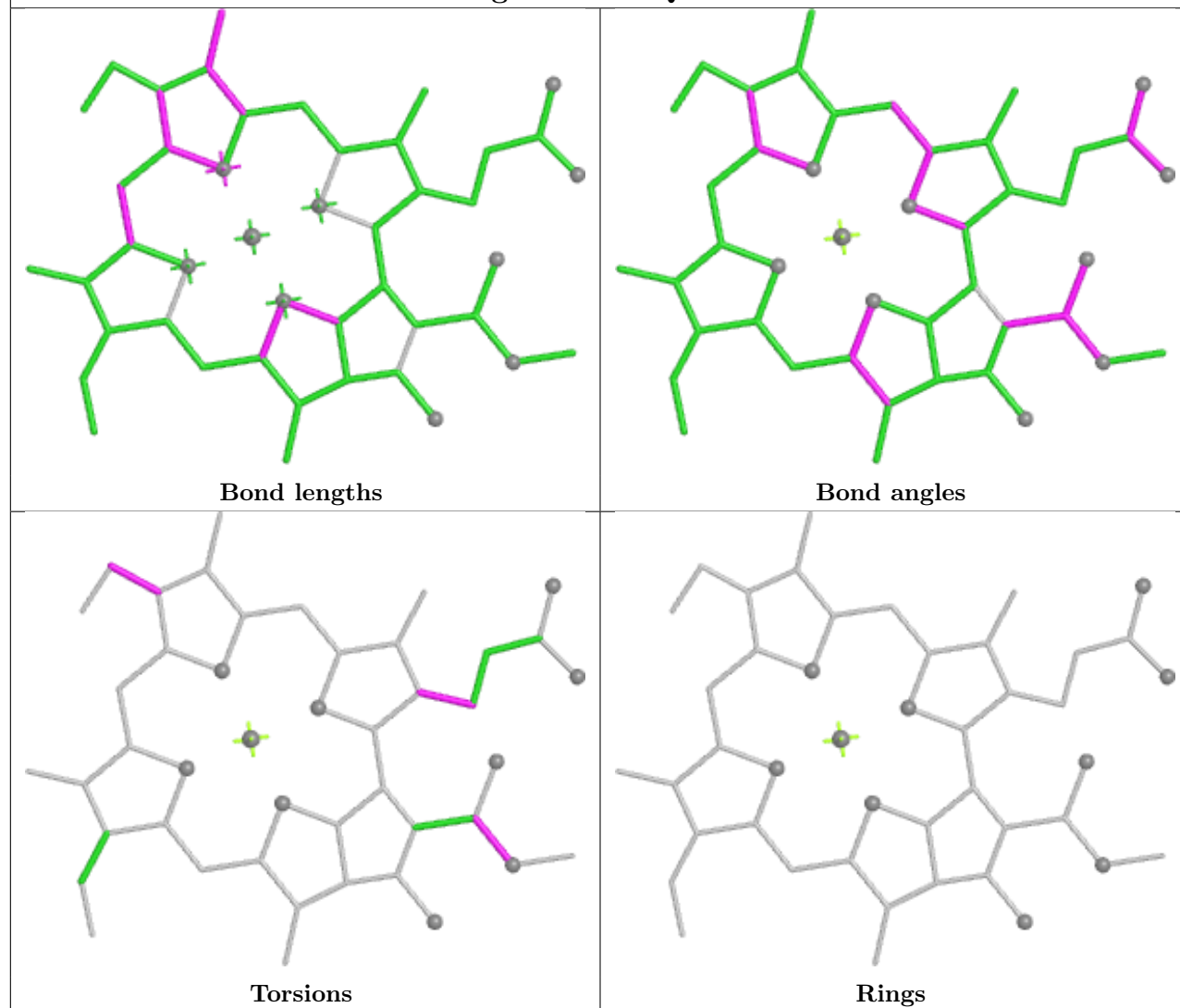


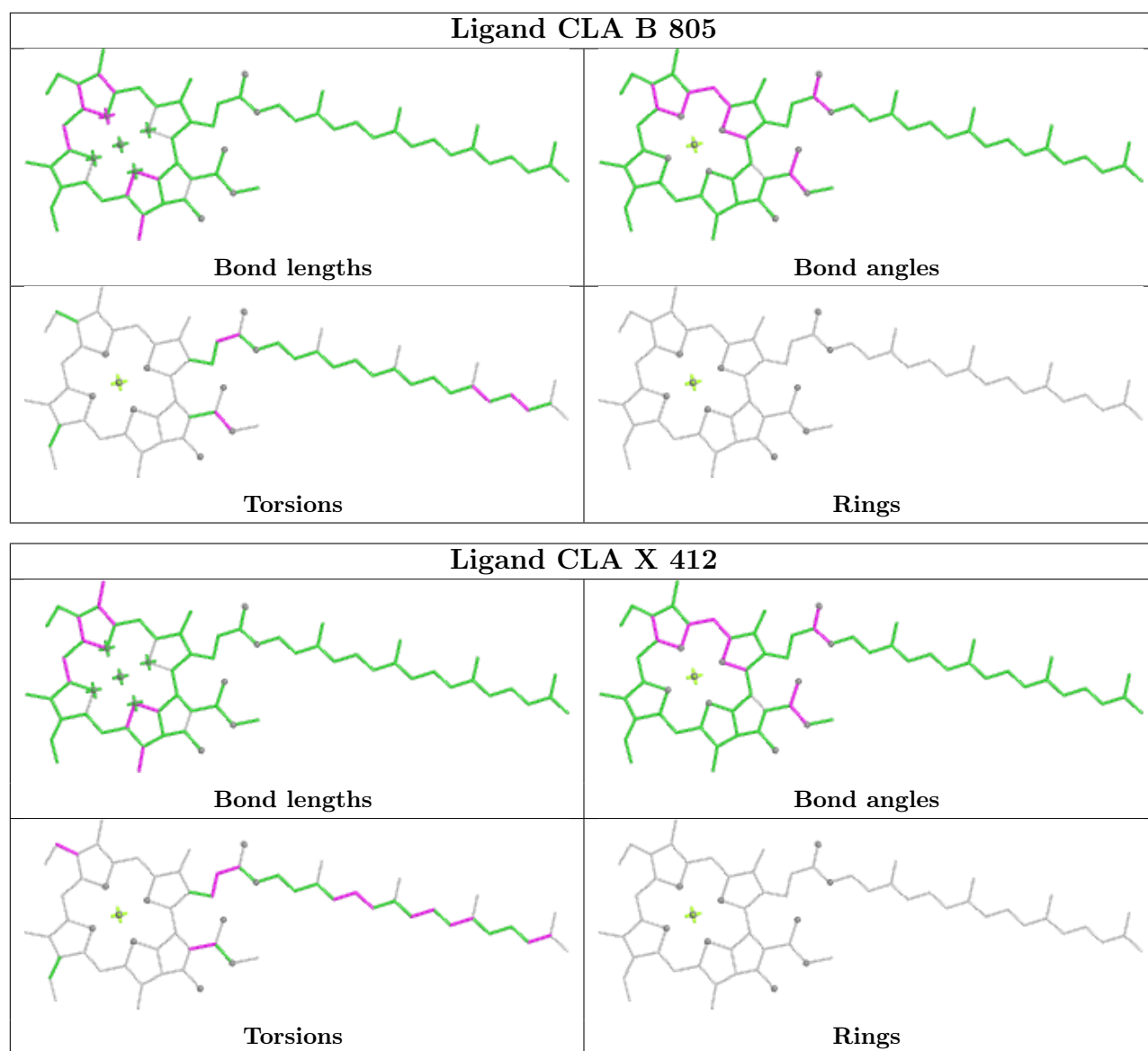


Ligand CLA R 602

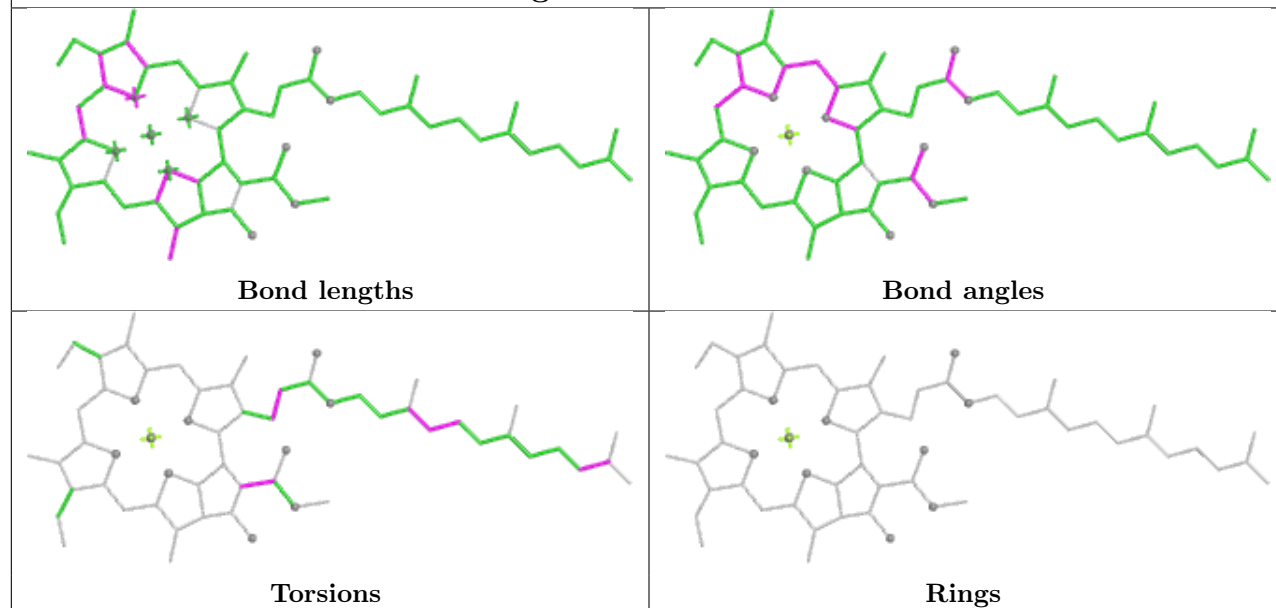


Ligand CLA Q 613

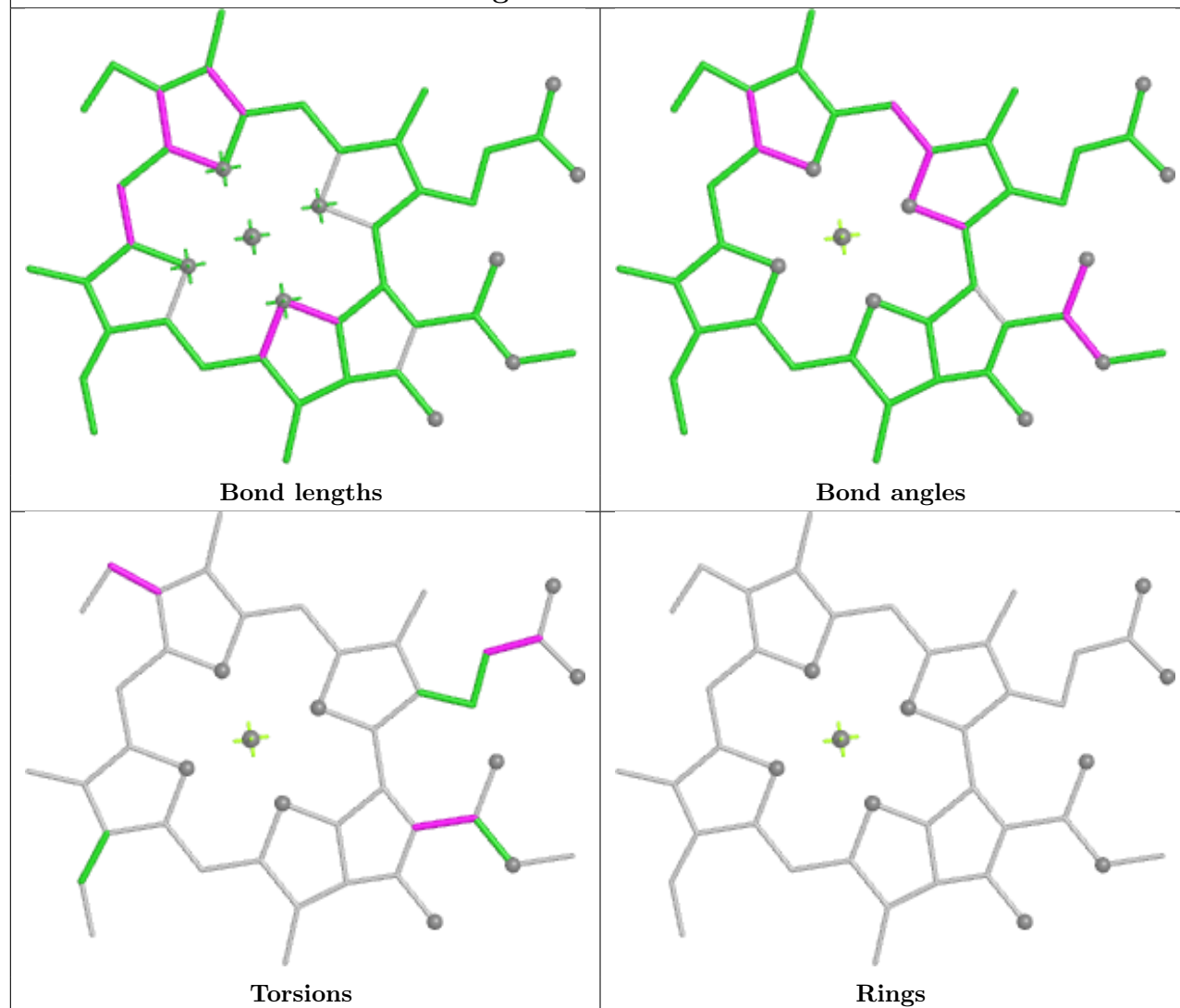




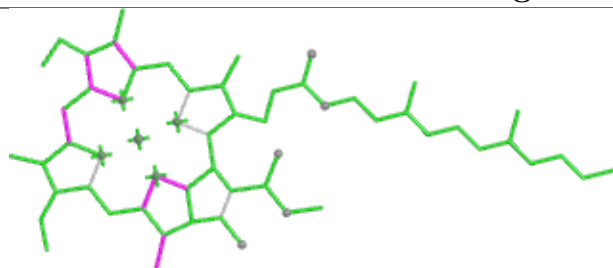
Ligand CLA O 306



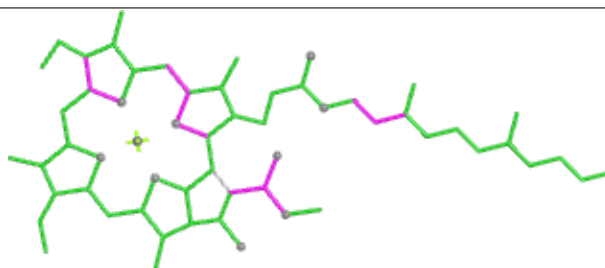
Ligand CLA T 610



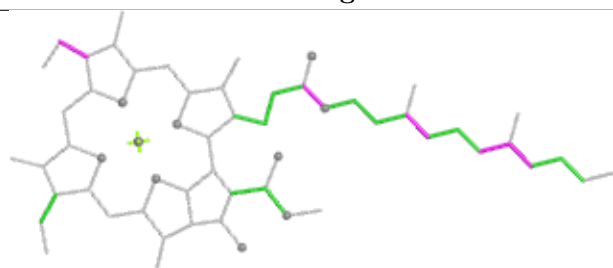
Ligand CLA H 313



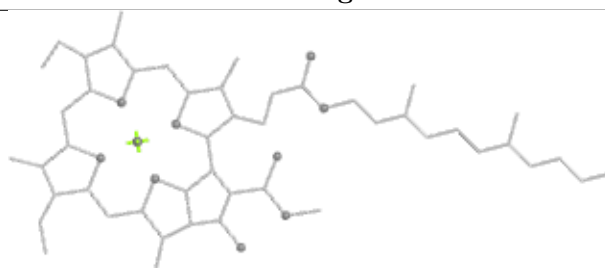
Bond lengths



Bond angles

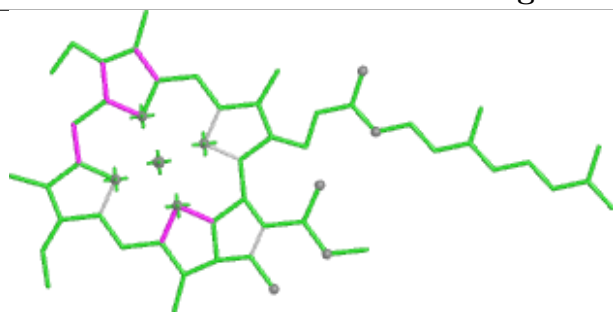


Torsions

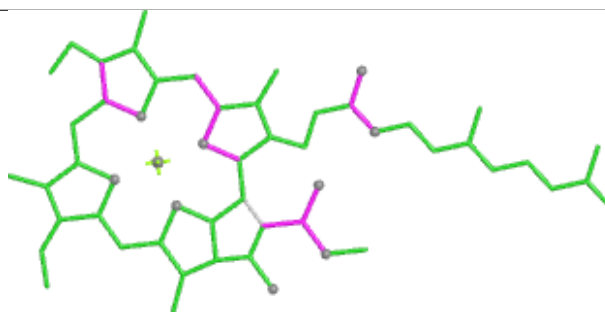


Rings

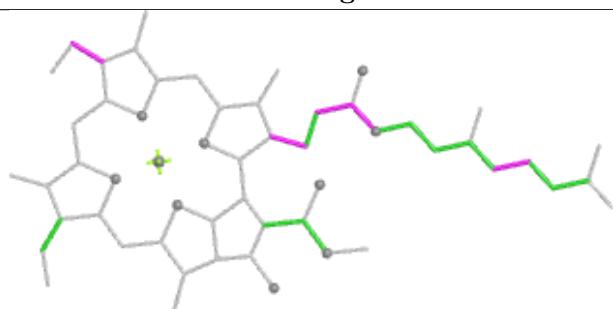
Ligand CLA S 609



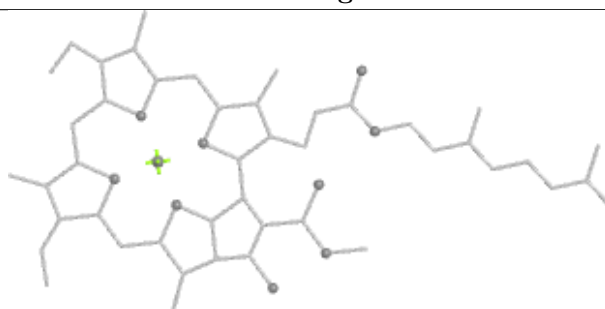
Bond lengths



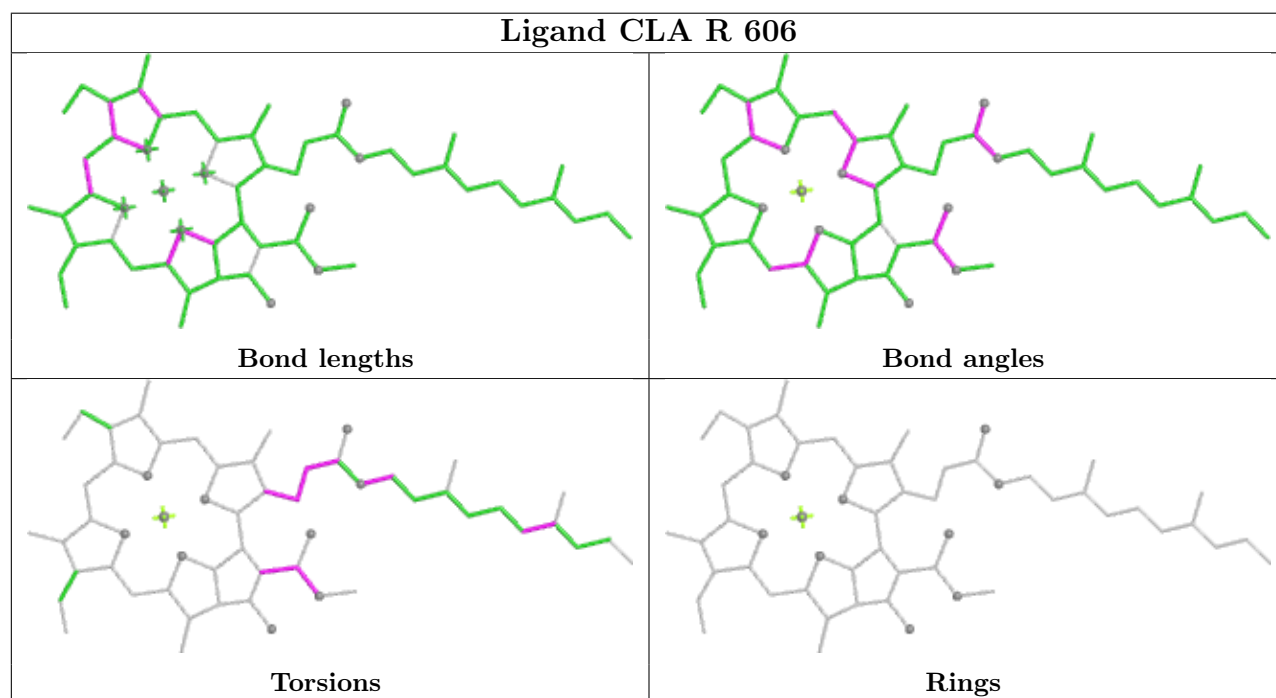
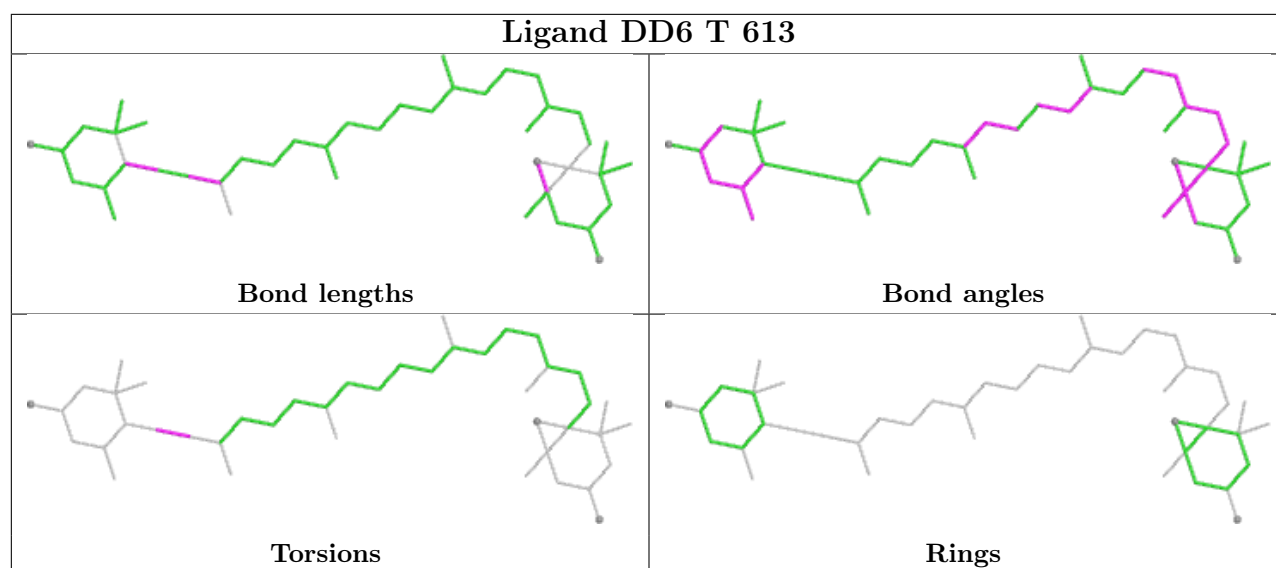
Bond angles



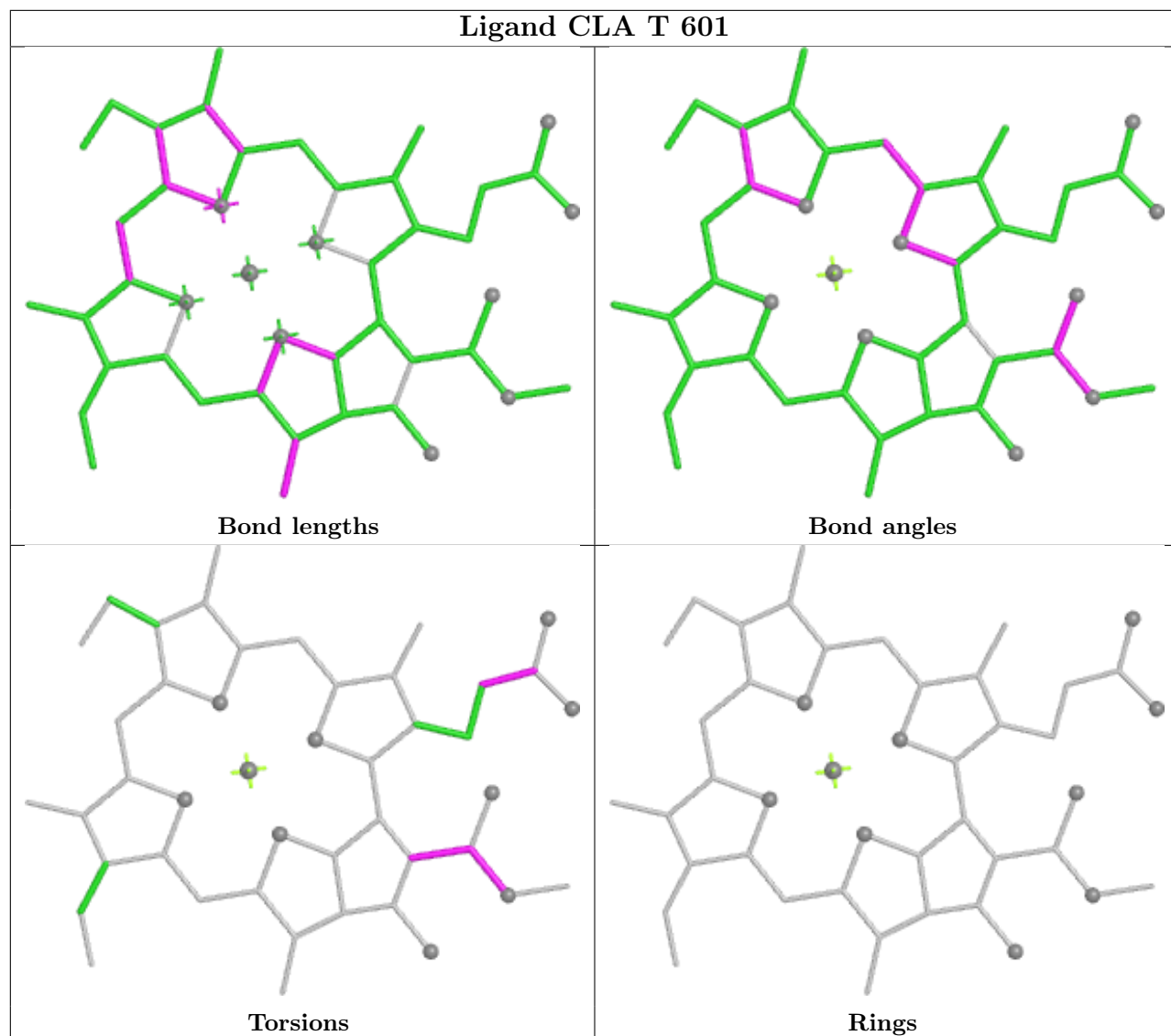
Torsions



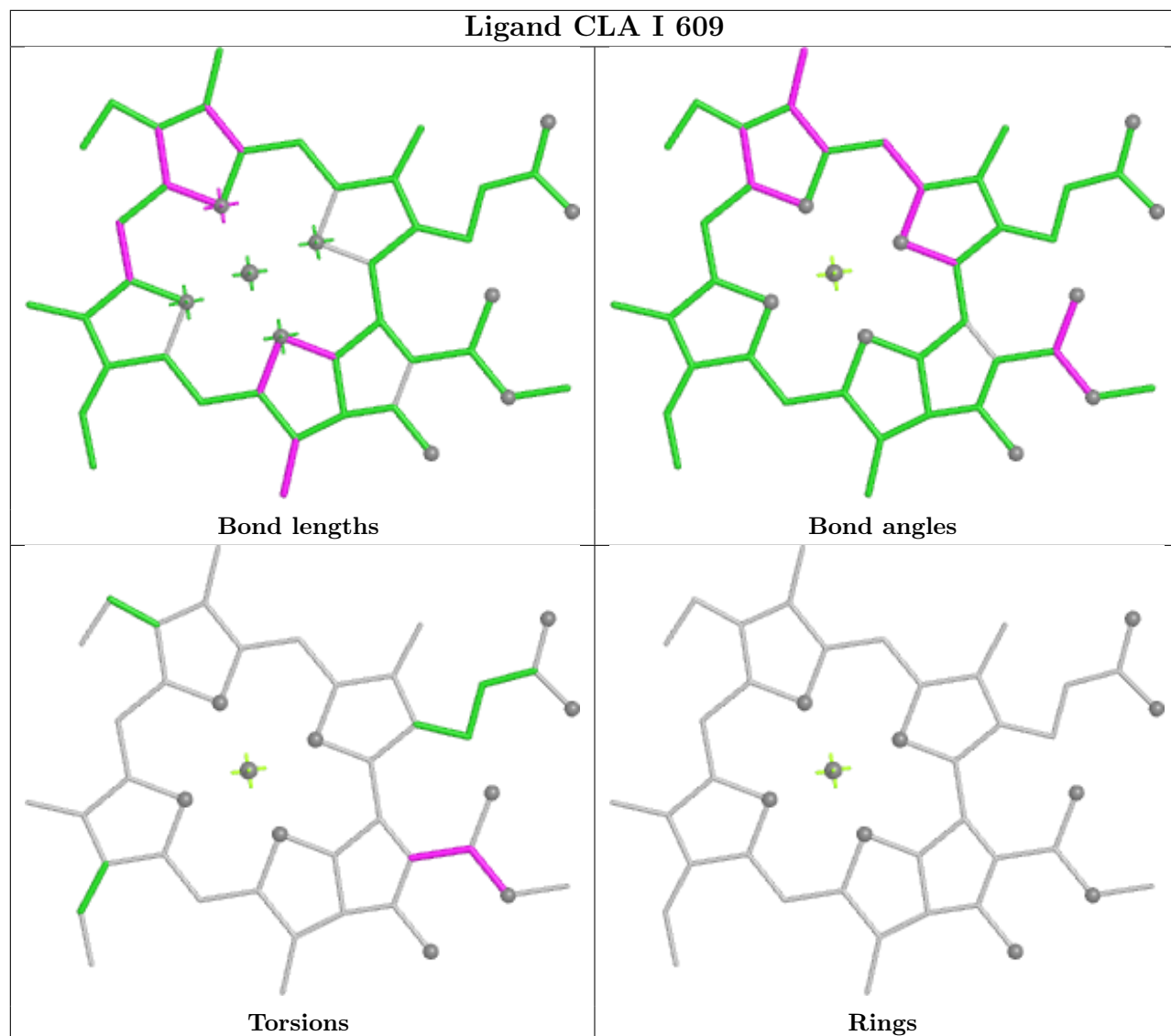
Rings

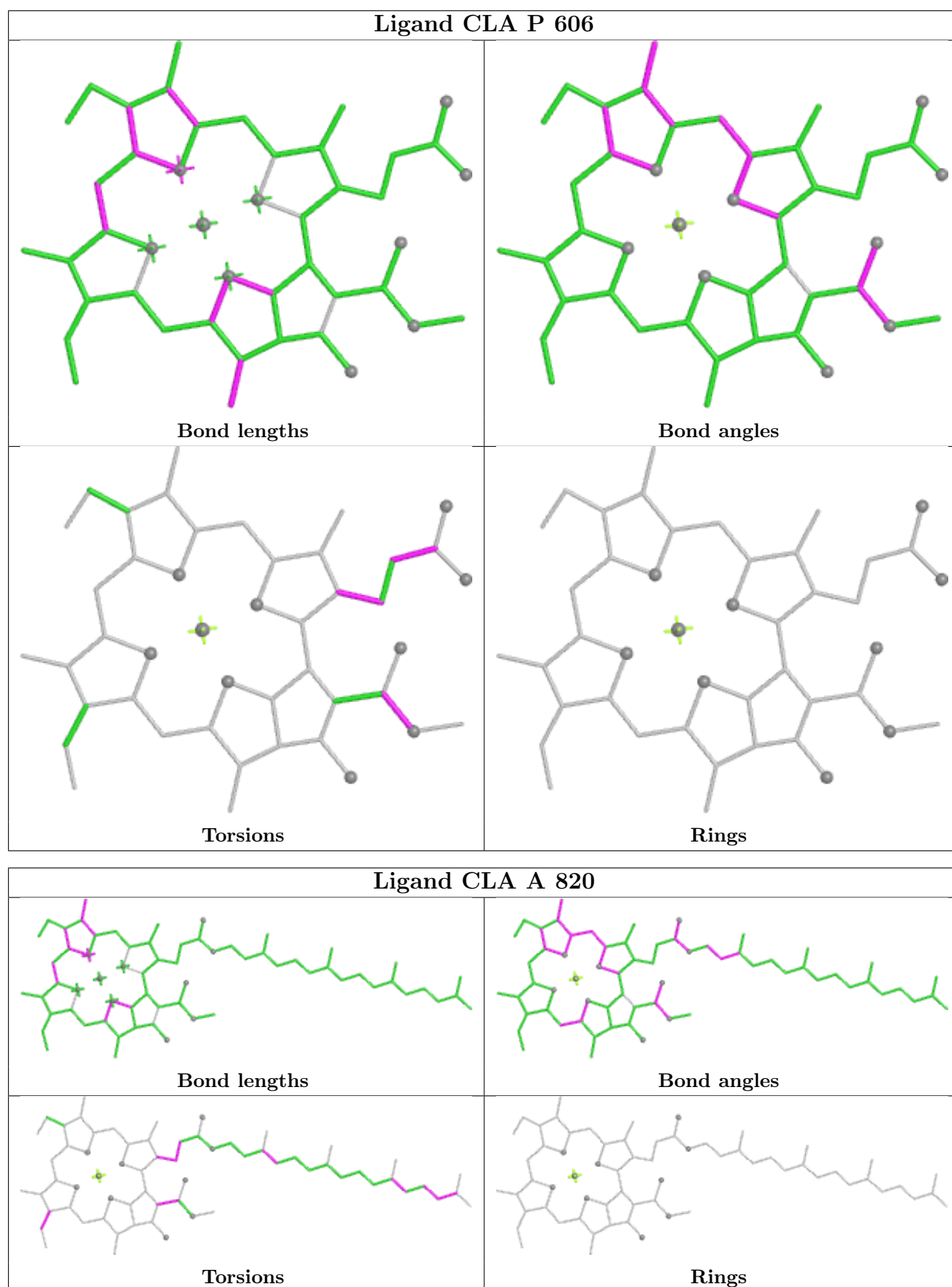


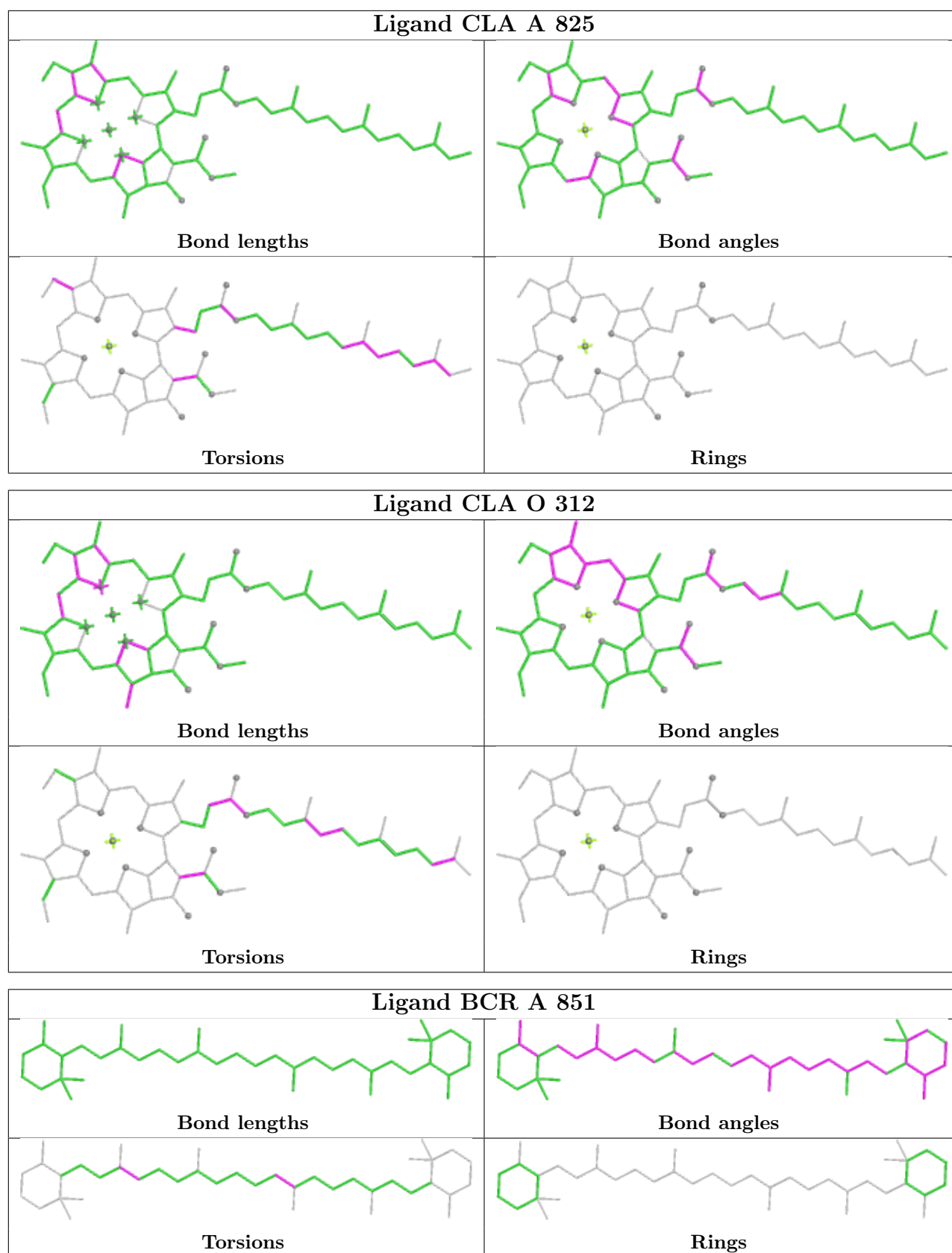
Ligand CLA T 601



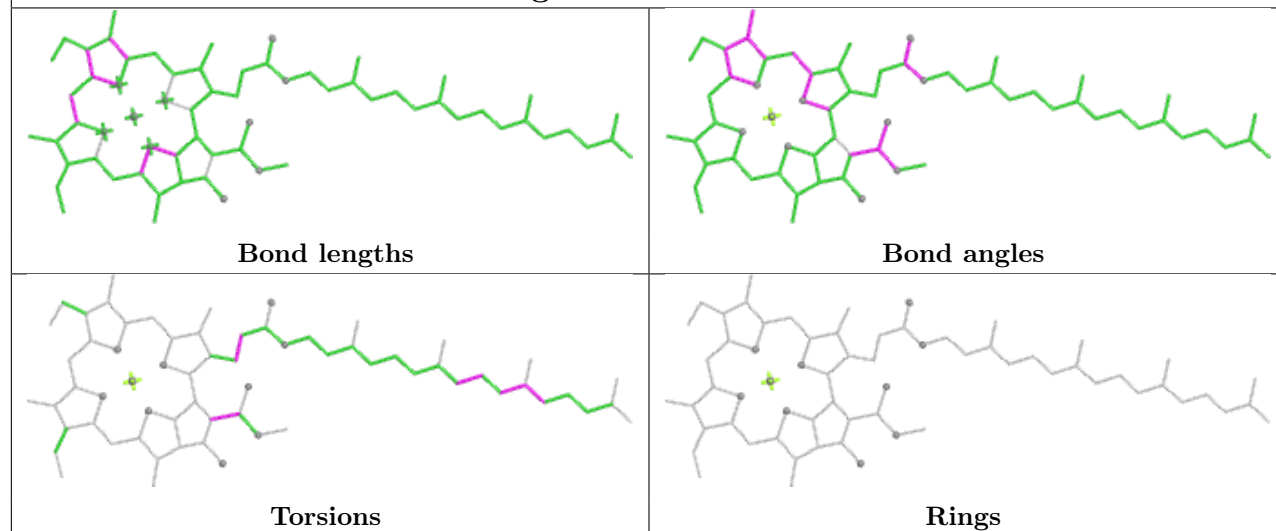
Ligand CLA I 609



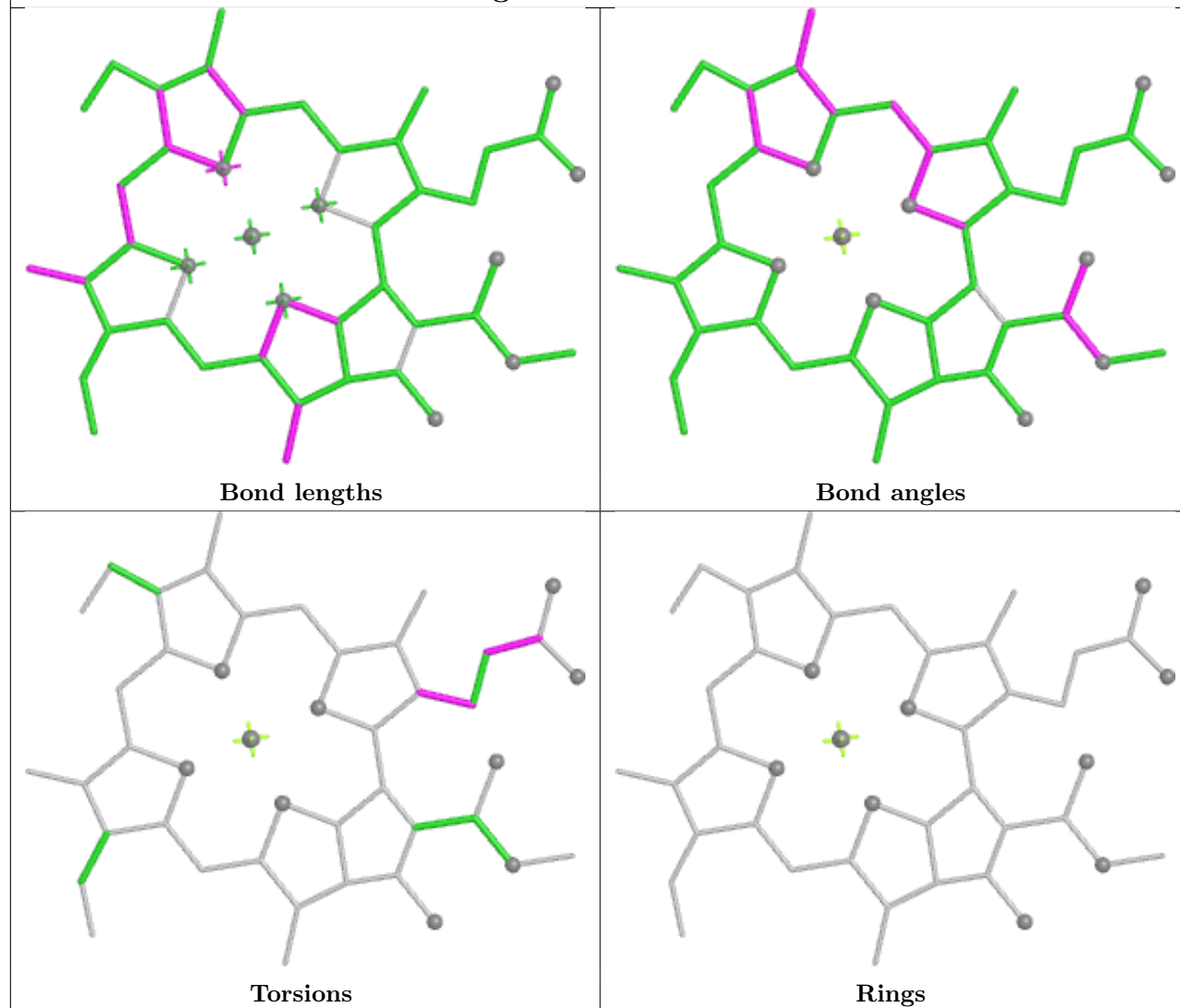




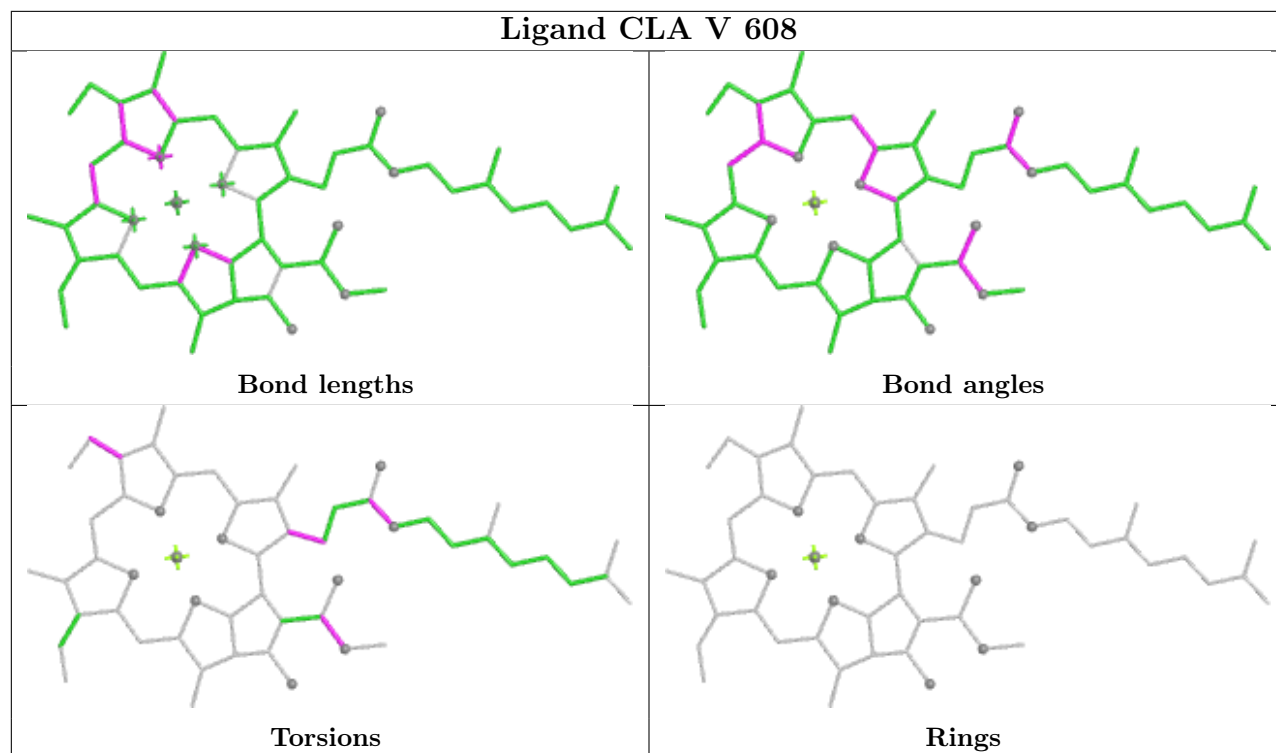
Ligand CLA A 839



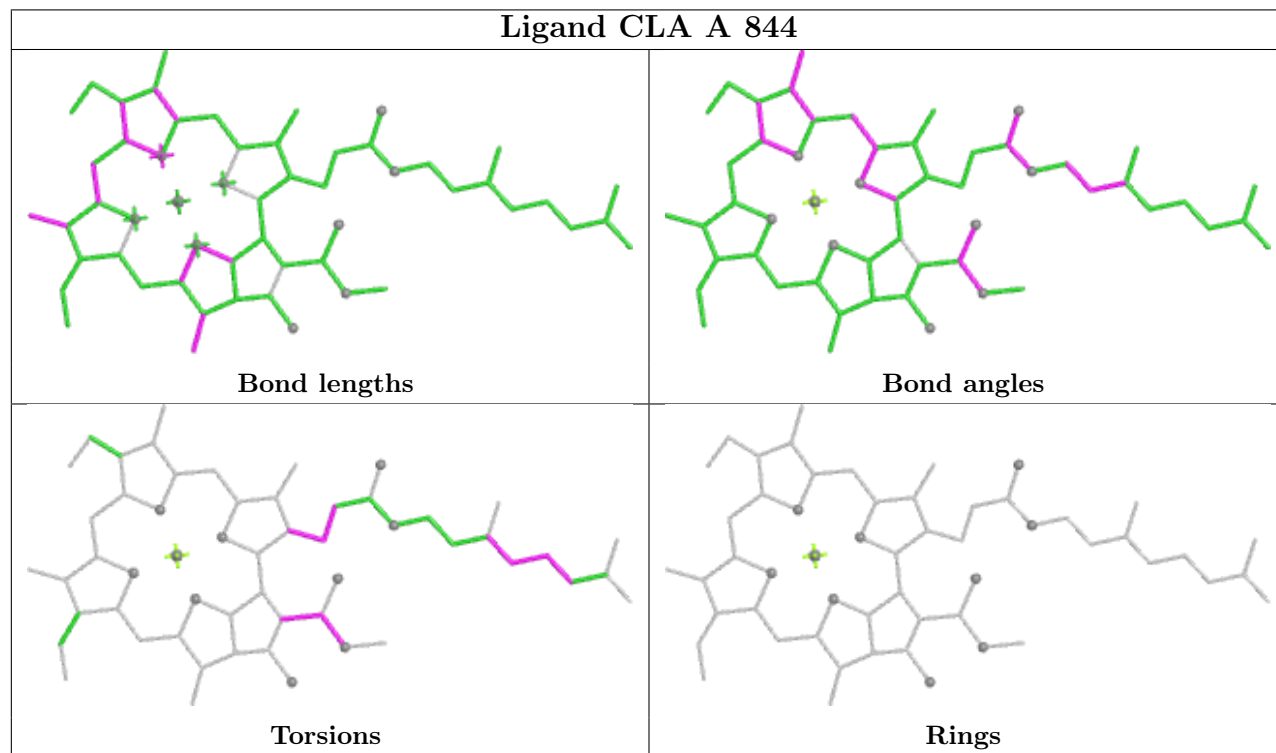
Ligand CLA P 607

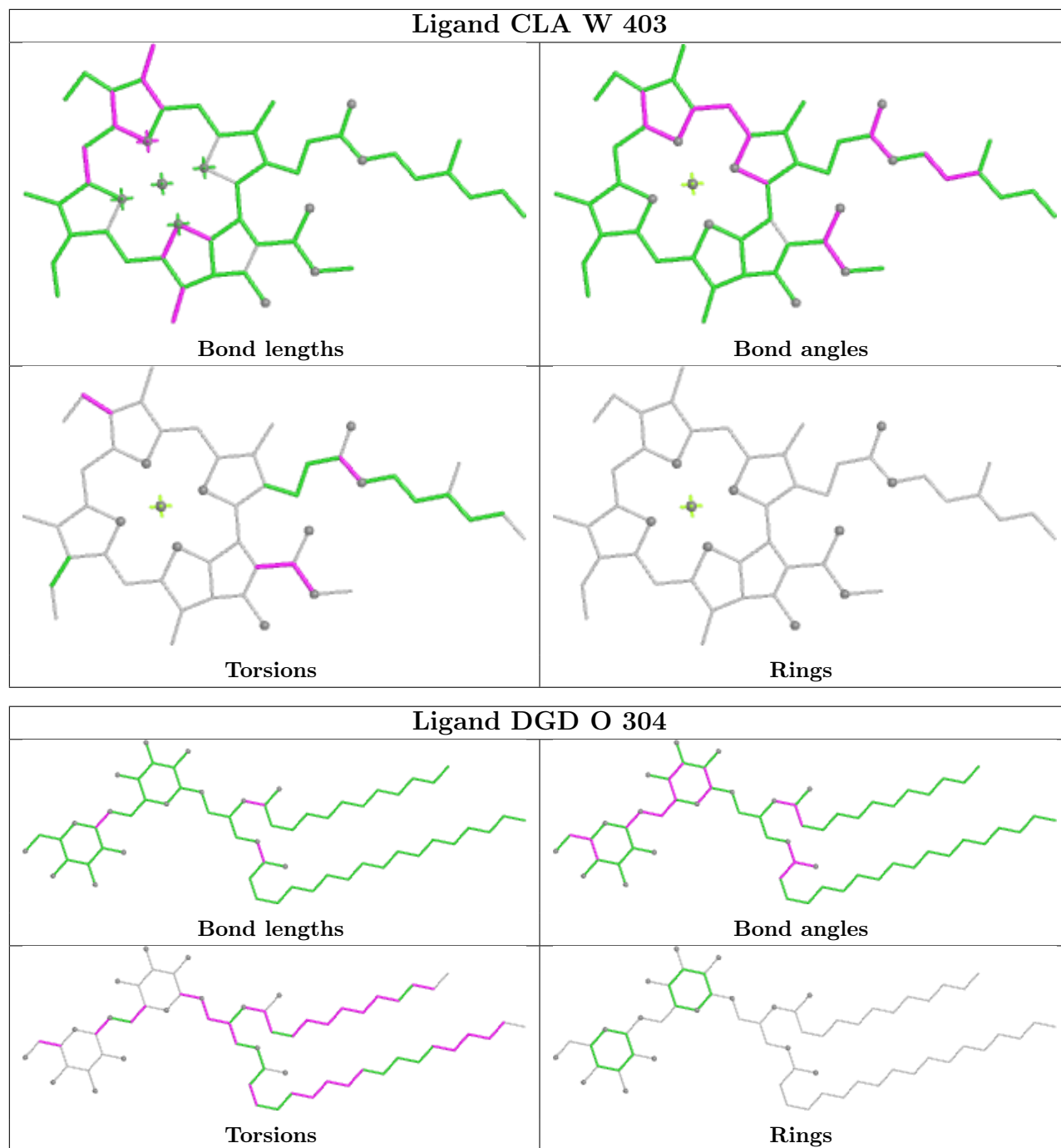


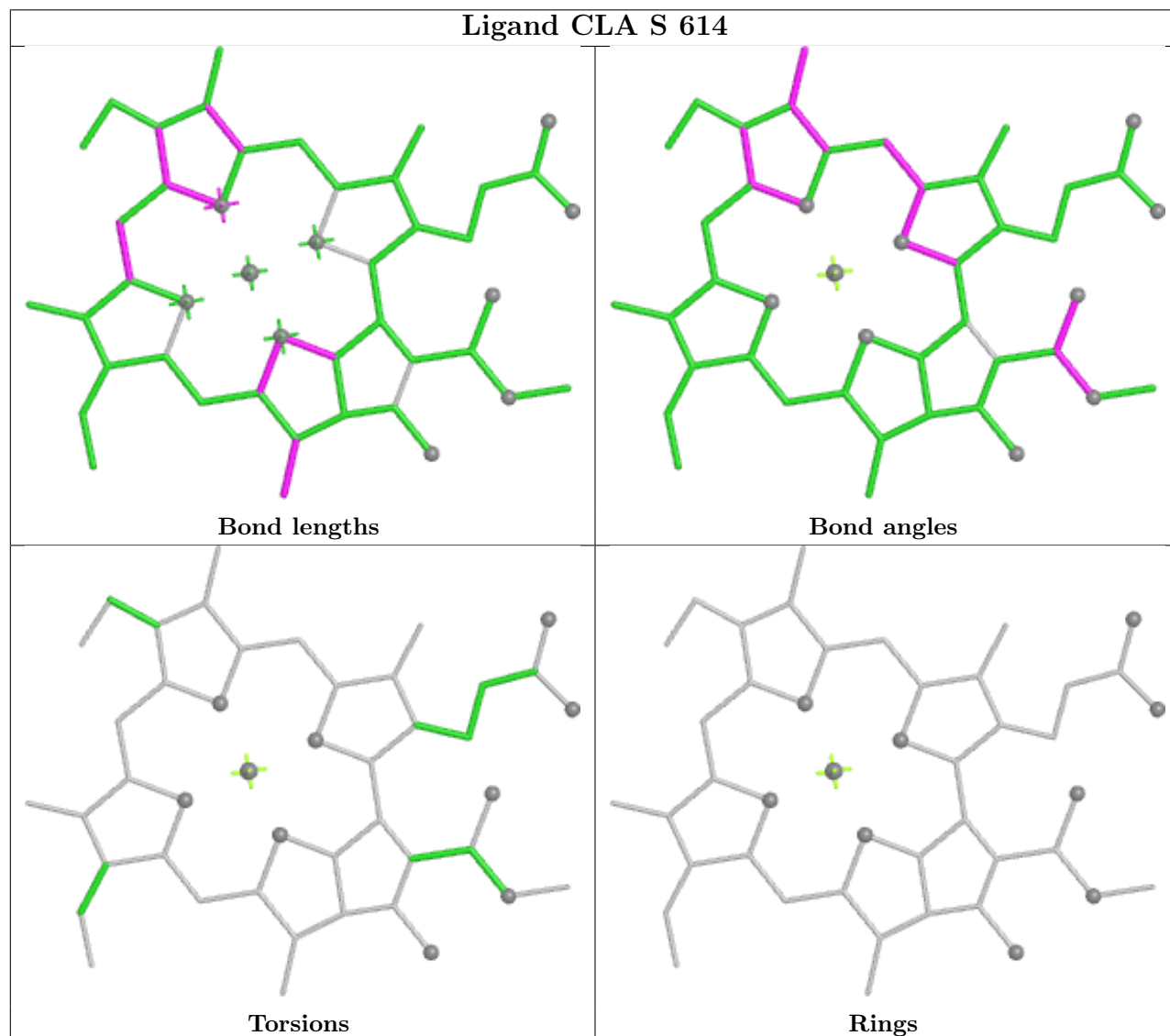
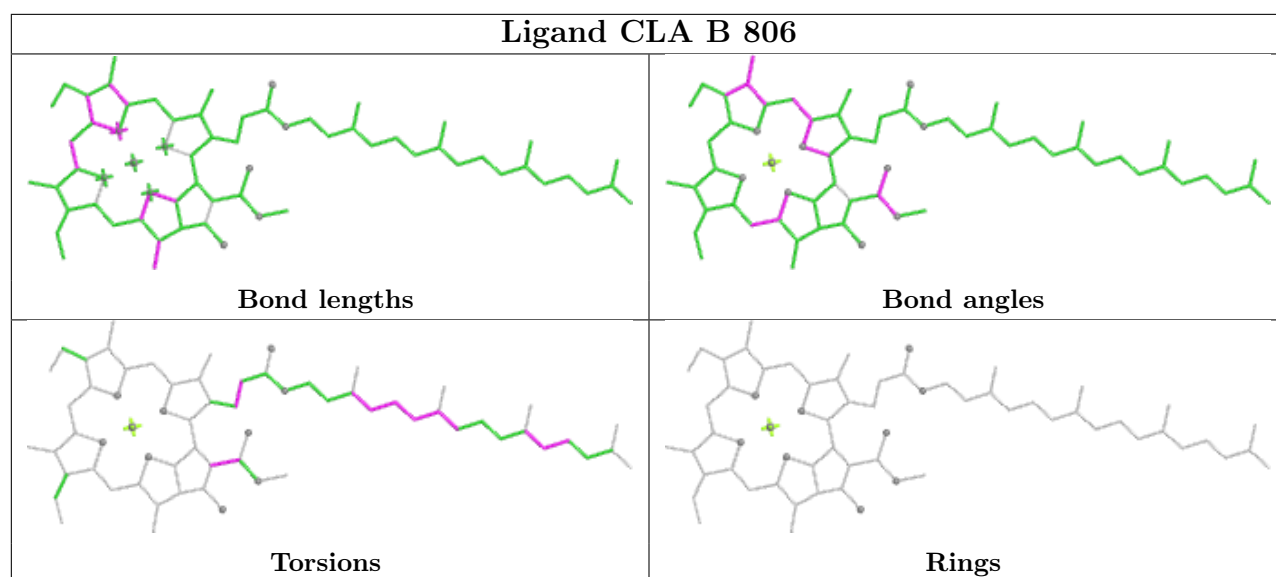
Ligand CLA V 608

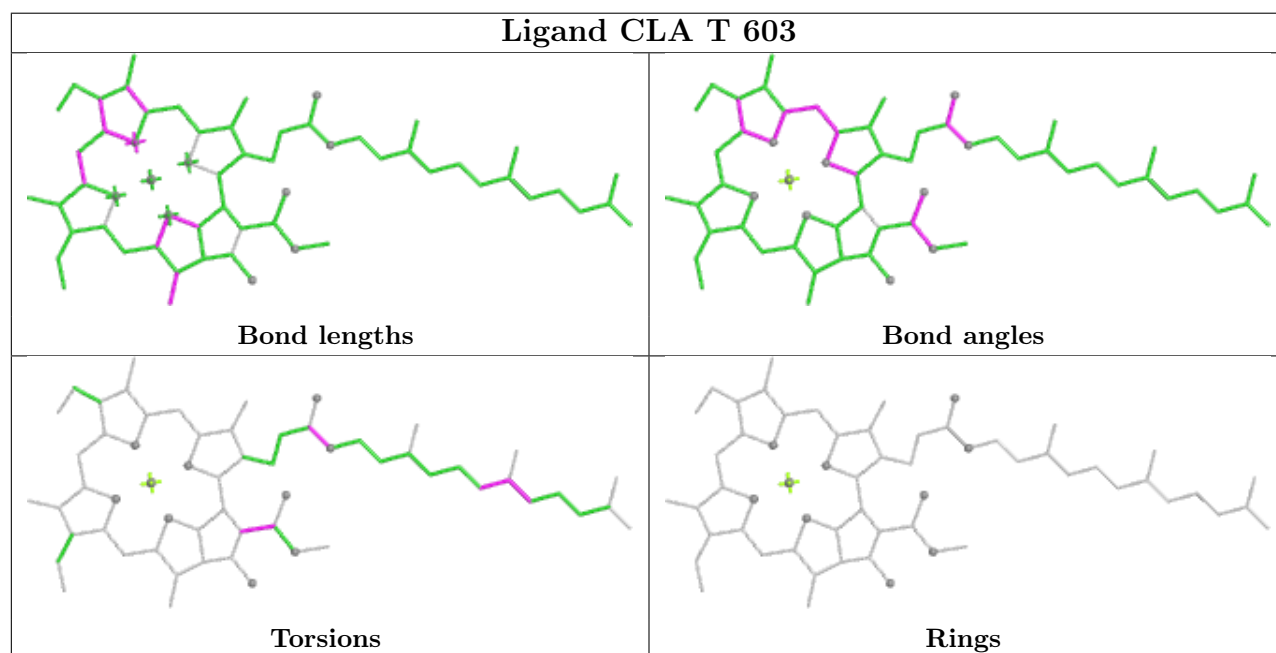
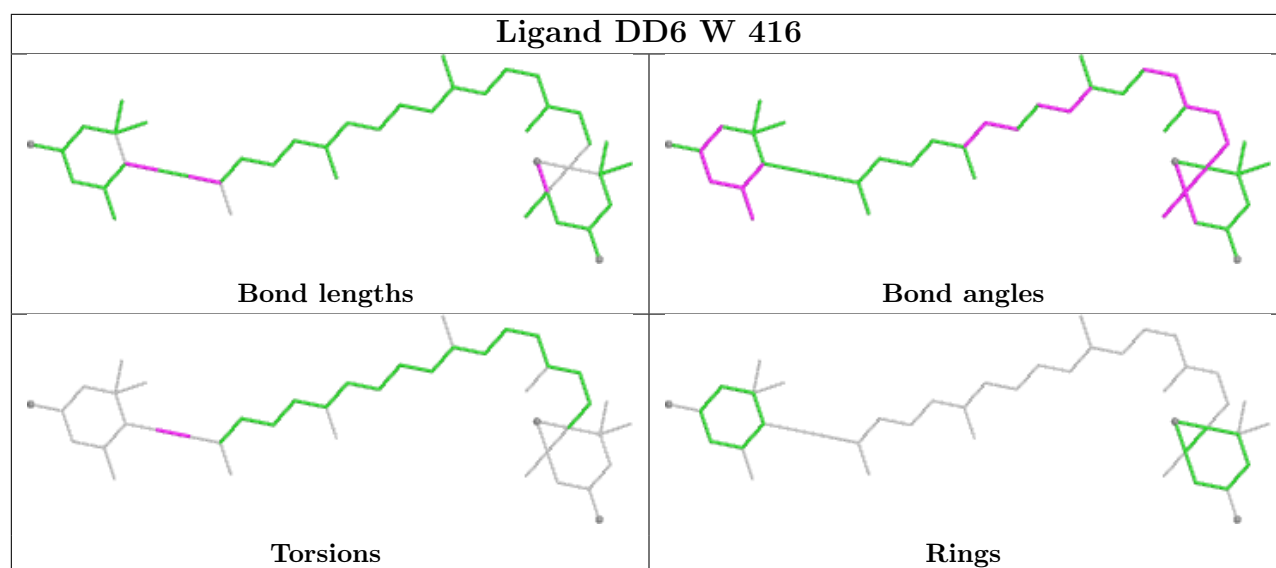


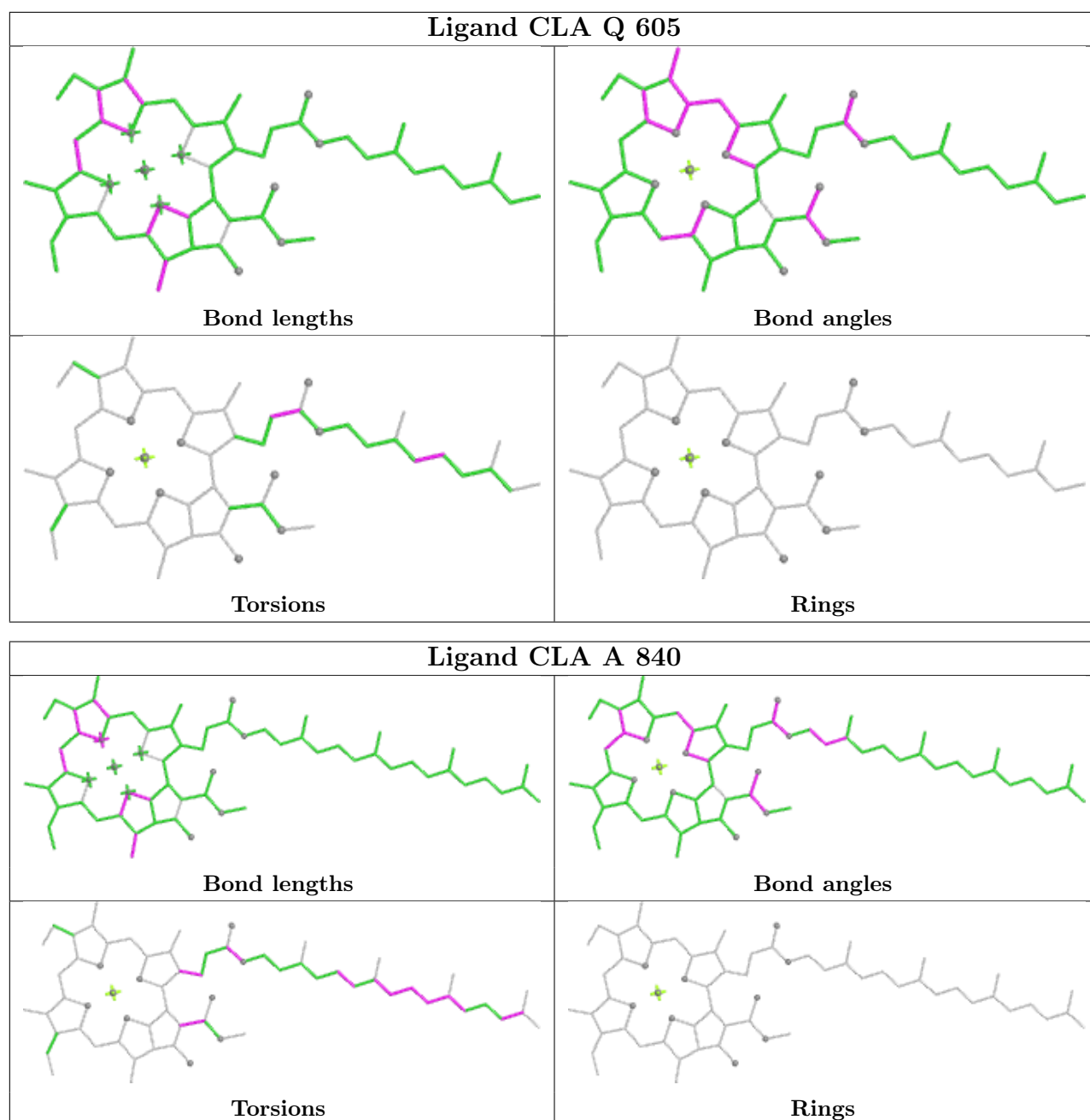
Ligand CLA A 844

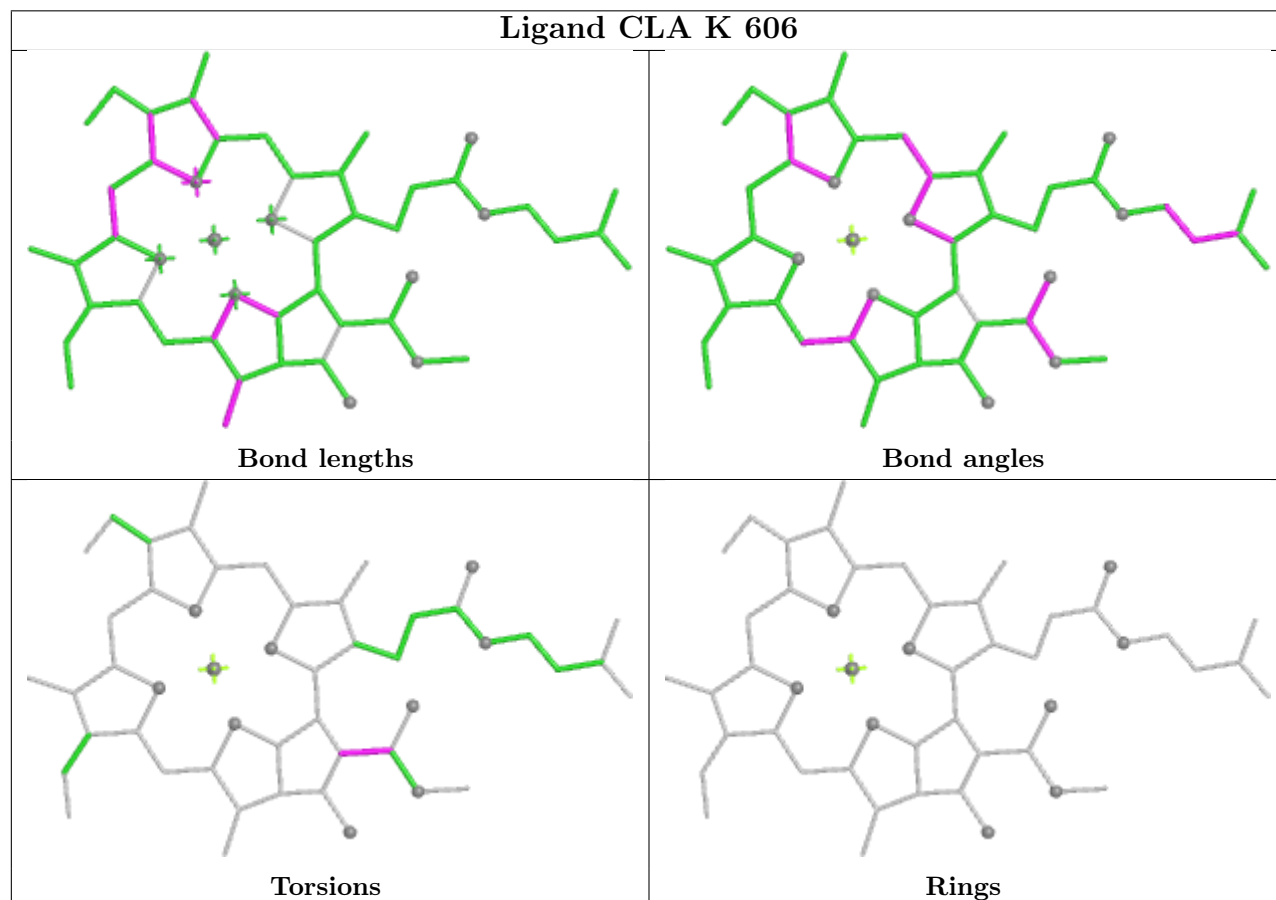
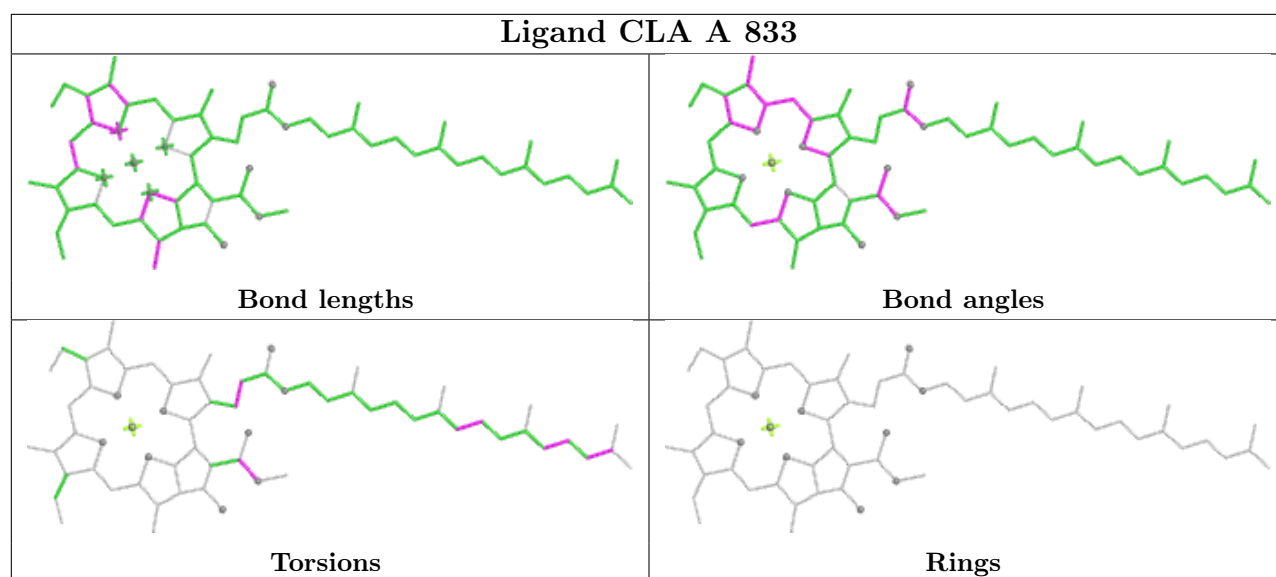


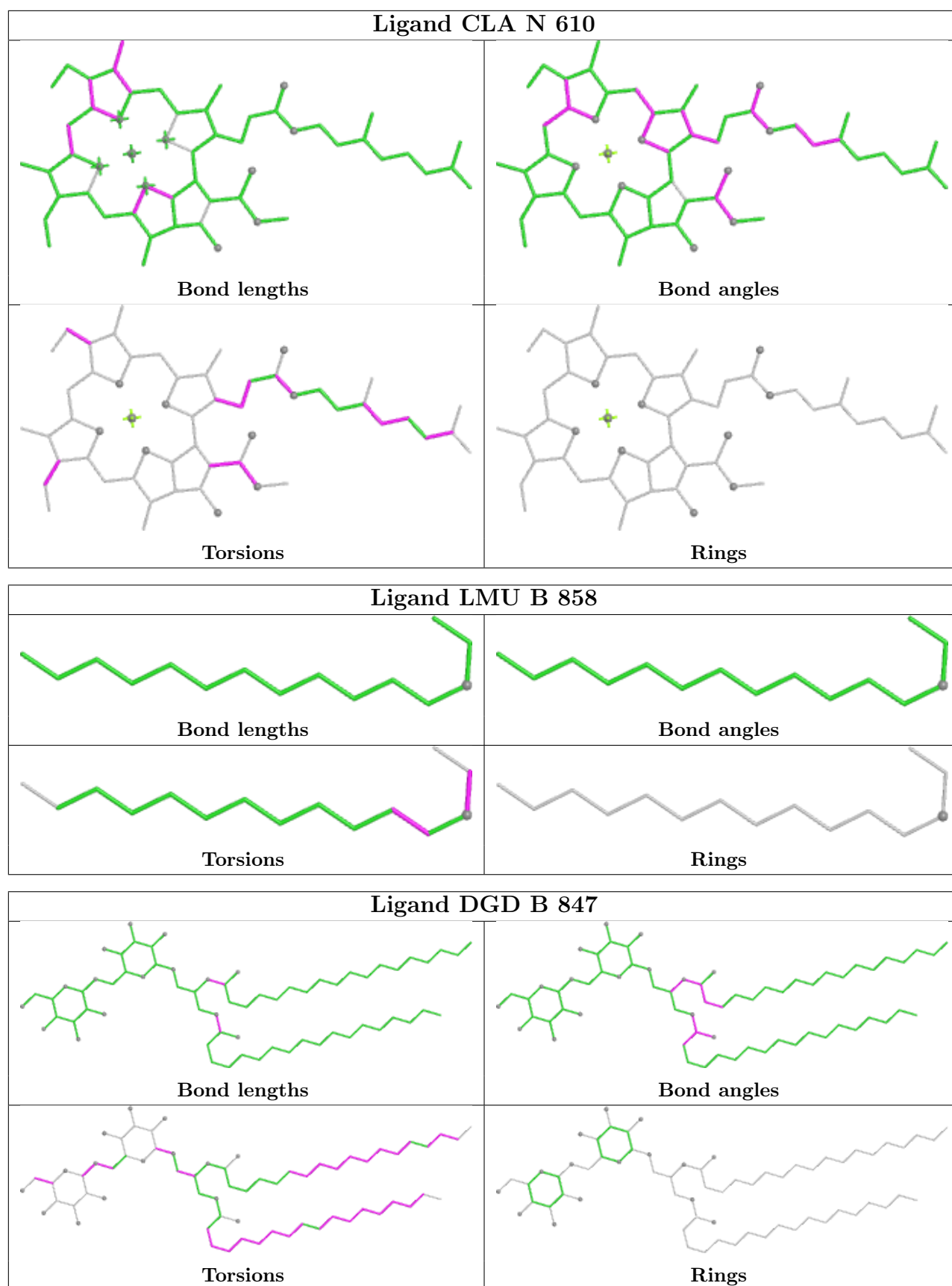


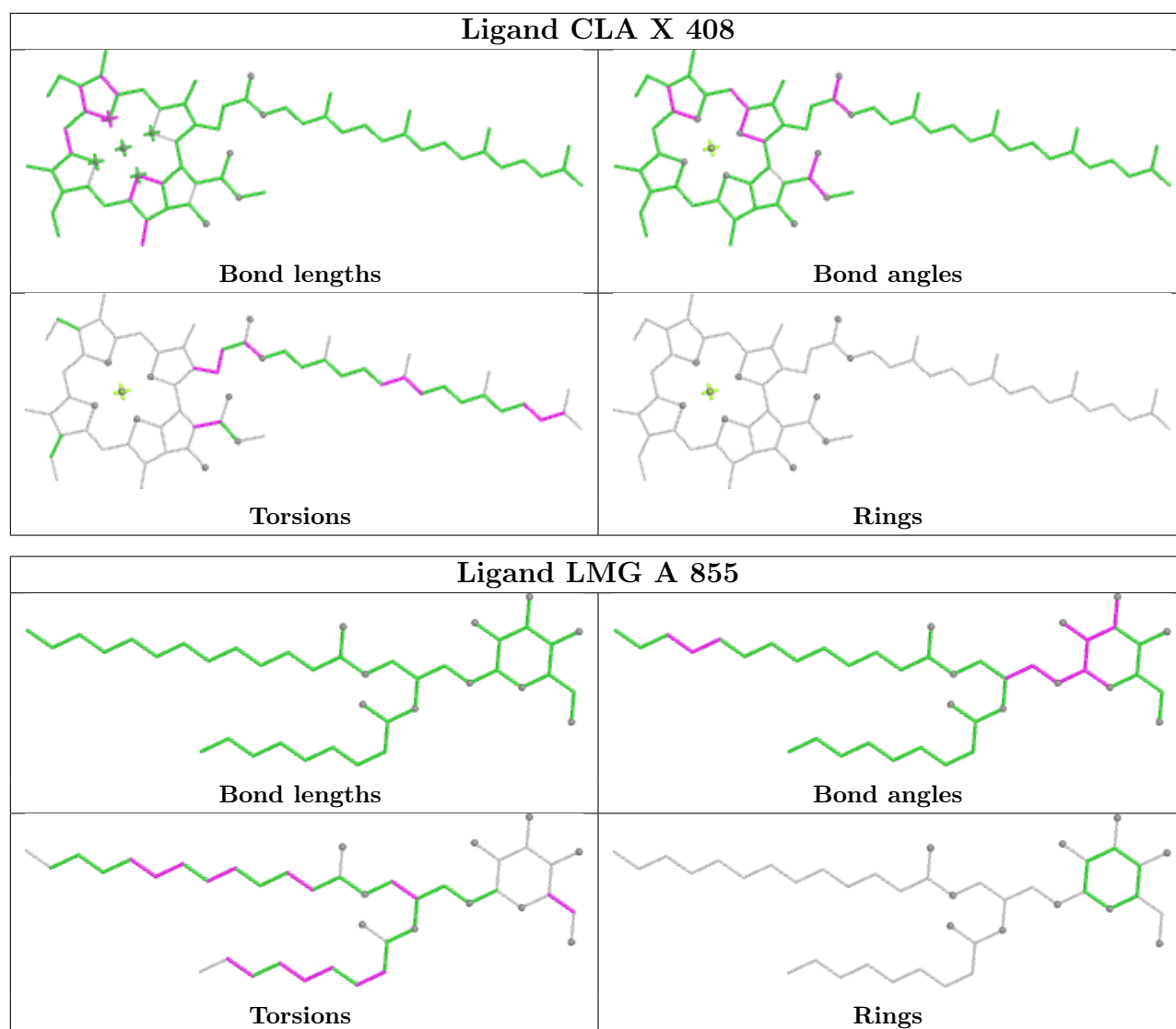


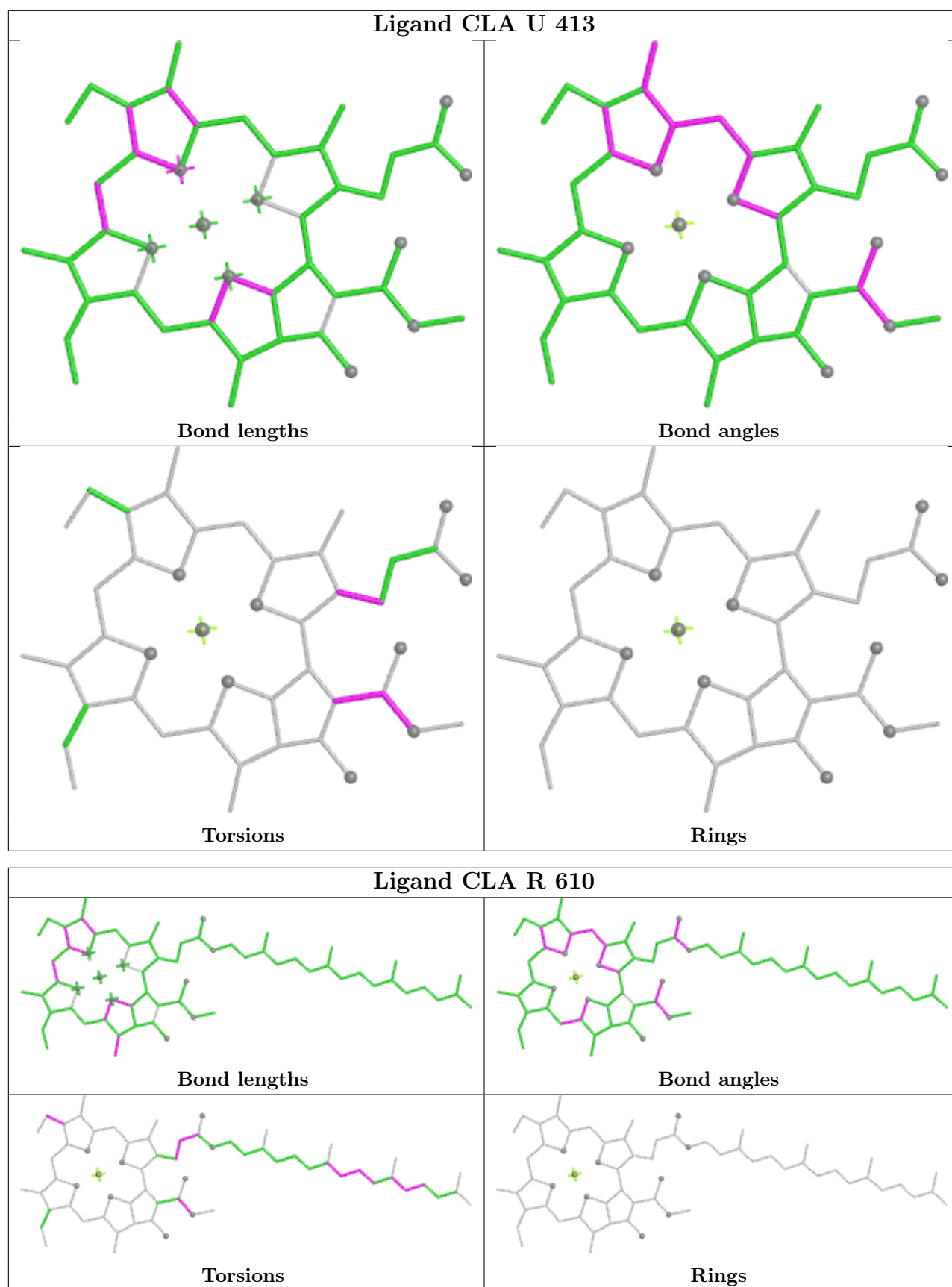




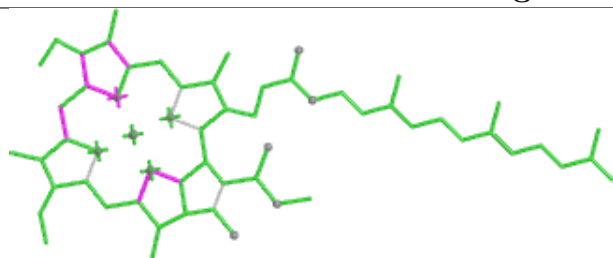




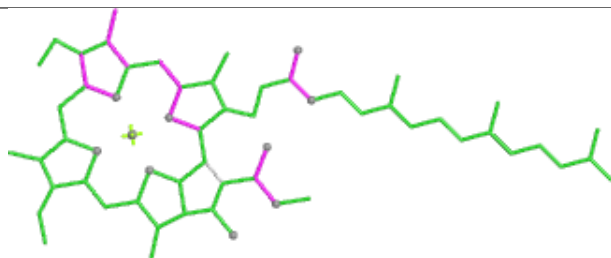




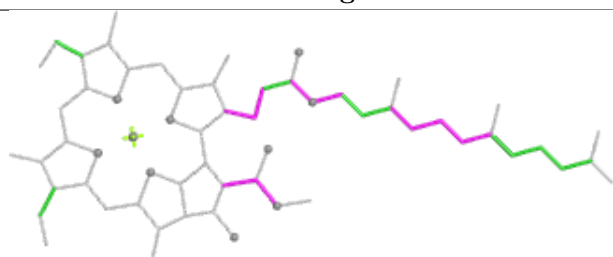
Ligand CLA N 607



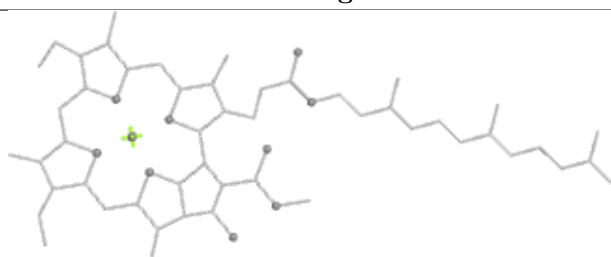
Bond lengths



Bond angles

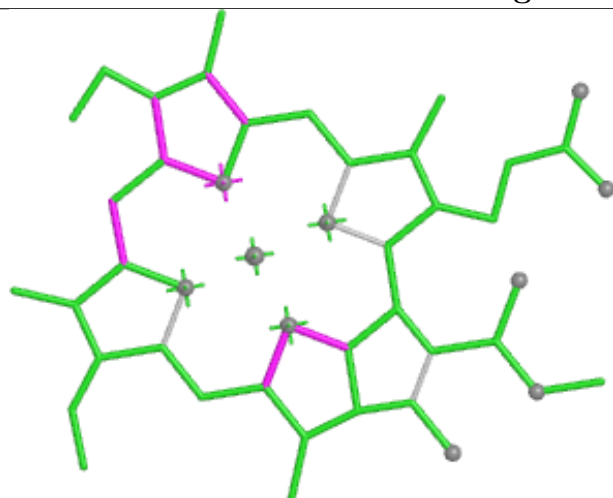


Torsions

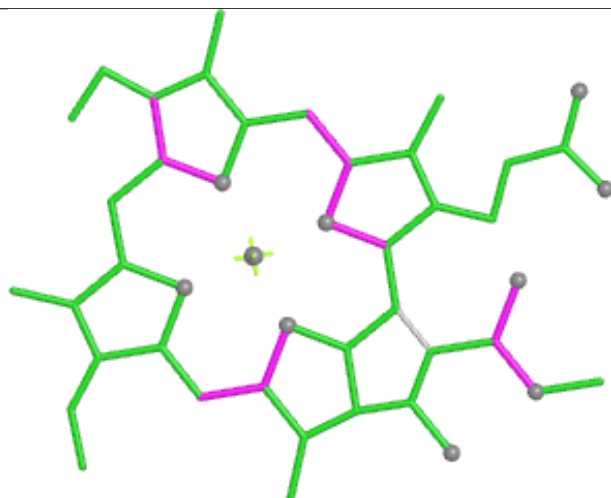


Rings

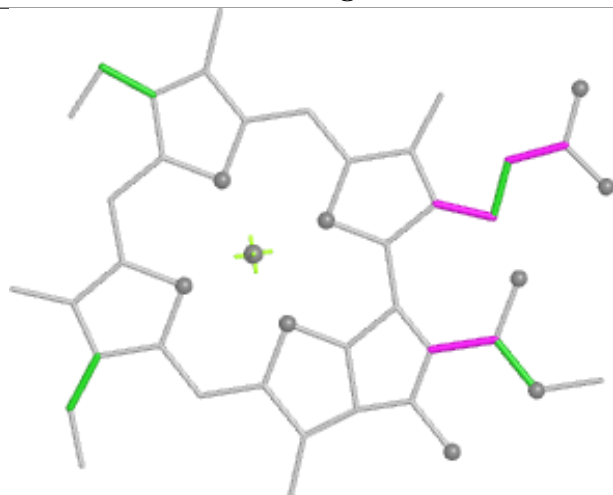
Ligand CLA R 611



Bond lengths



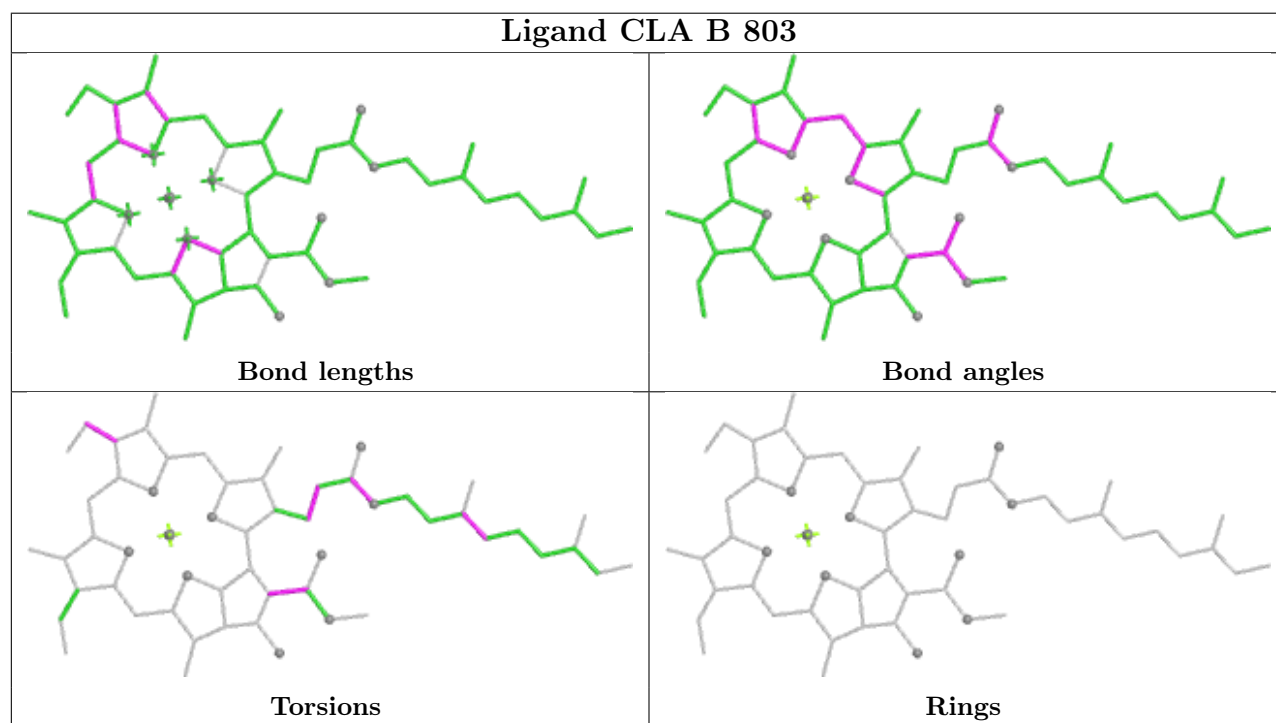
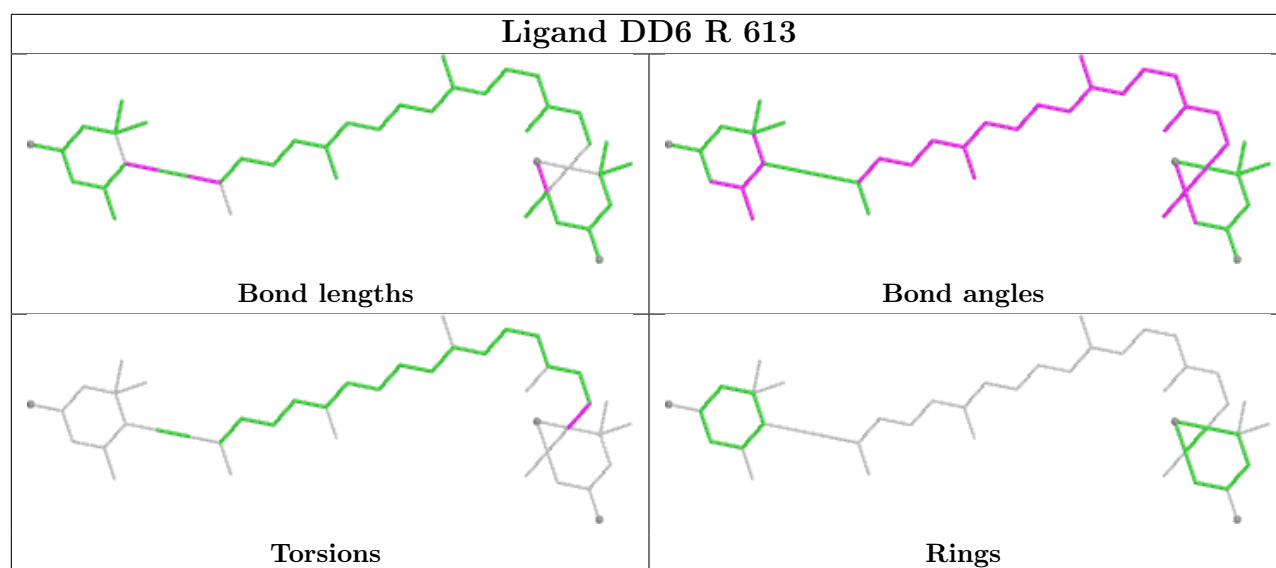
Bond angles

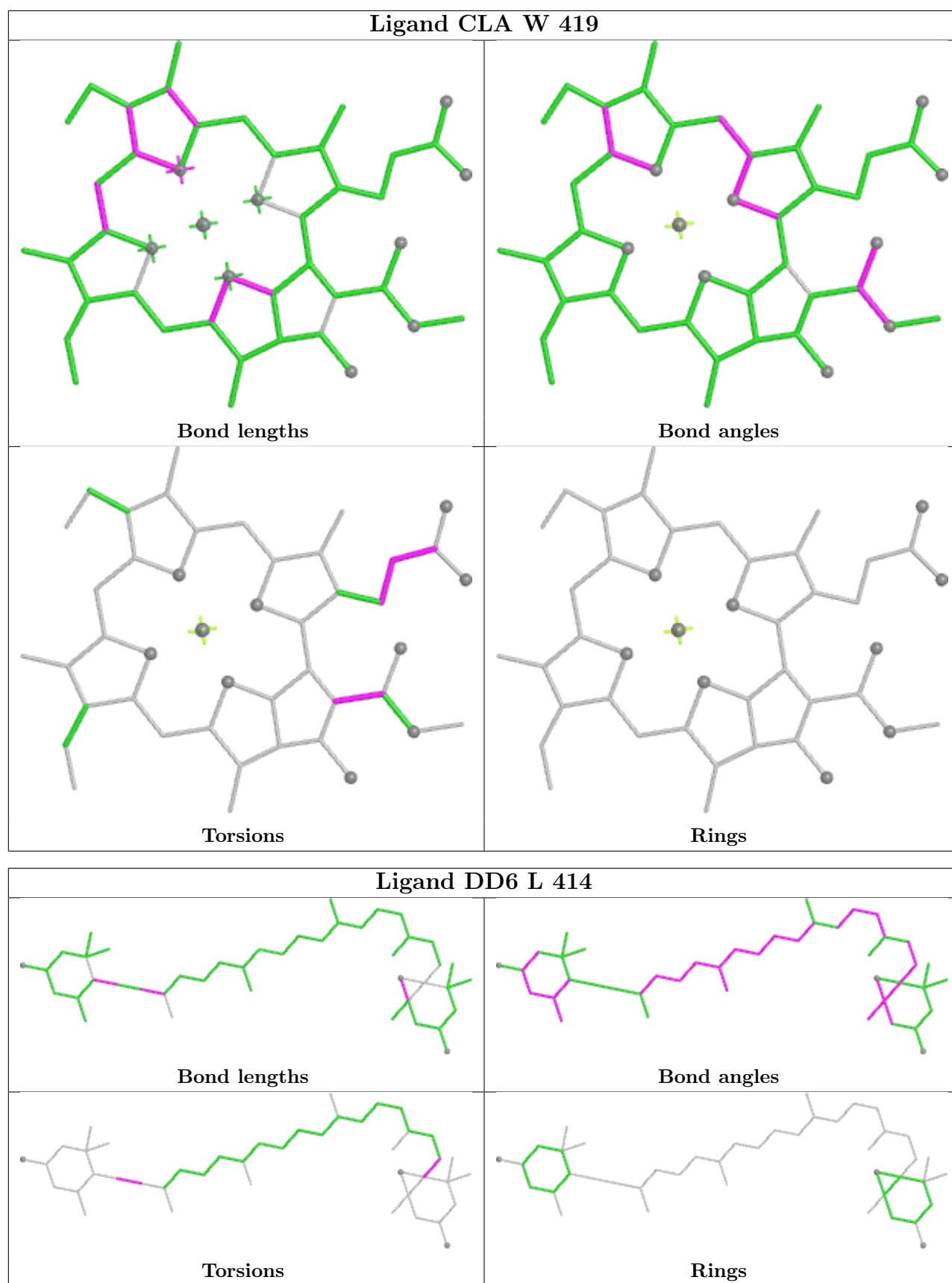


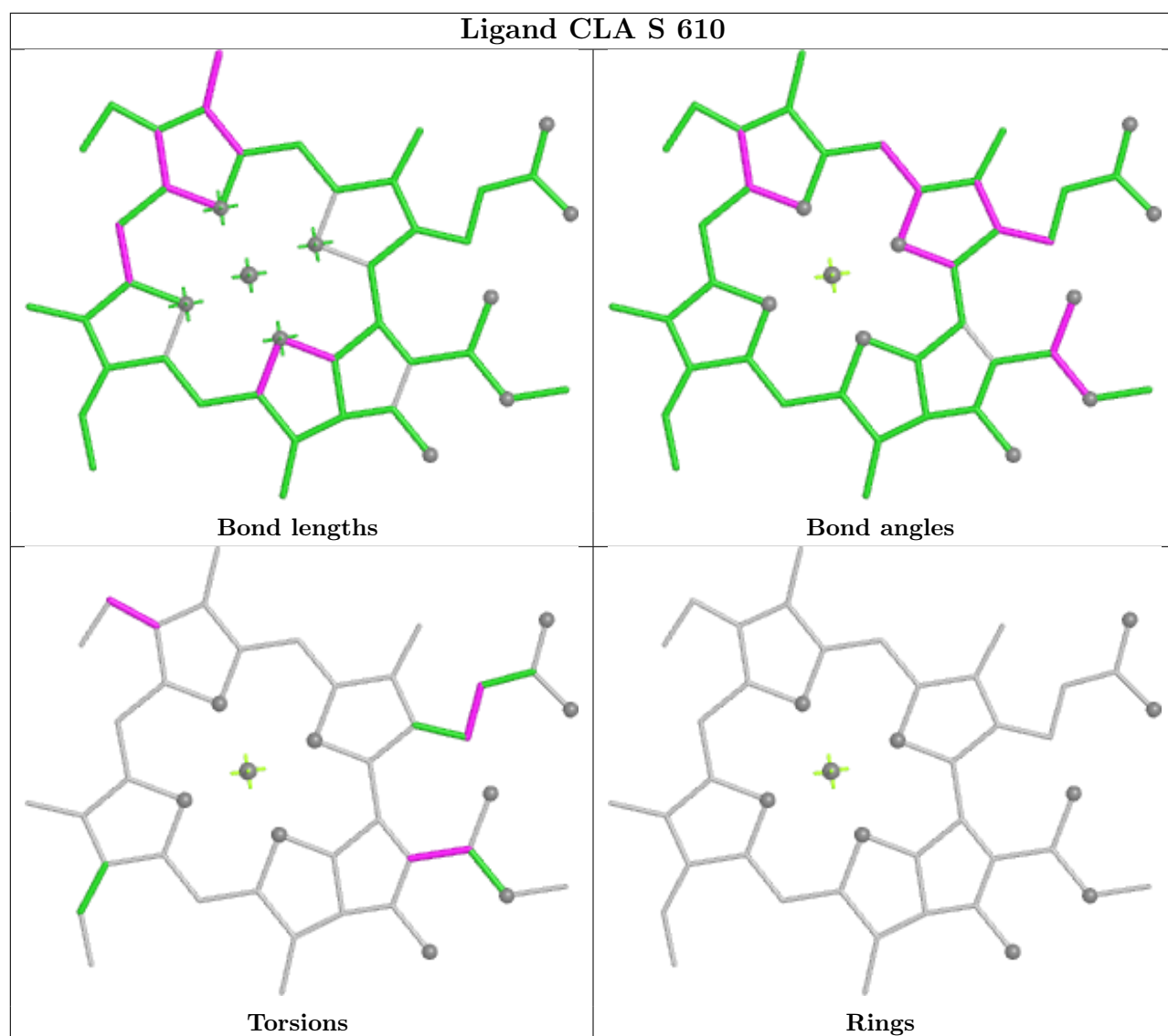
Torsions

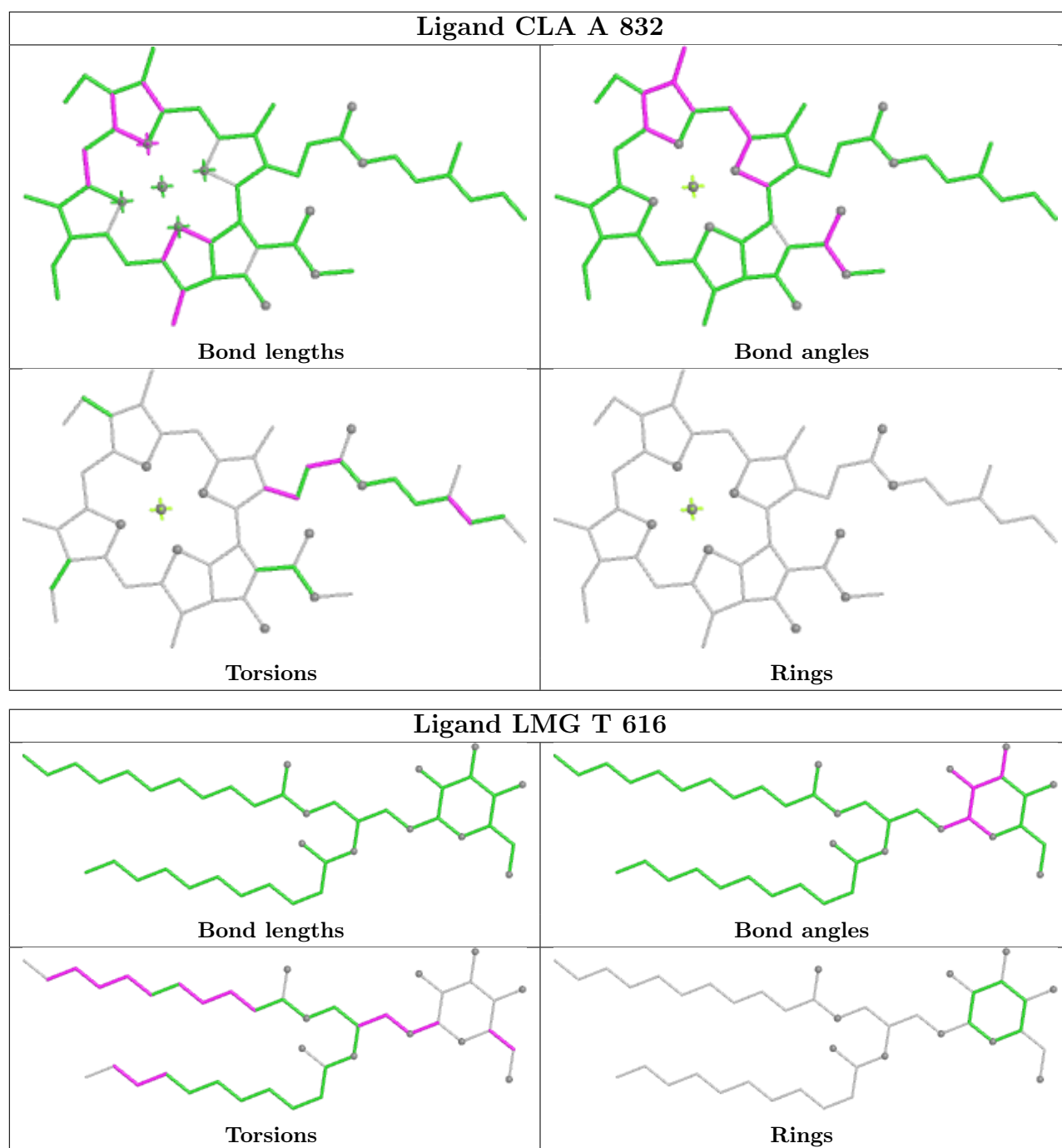


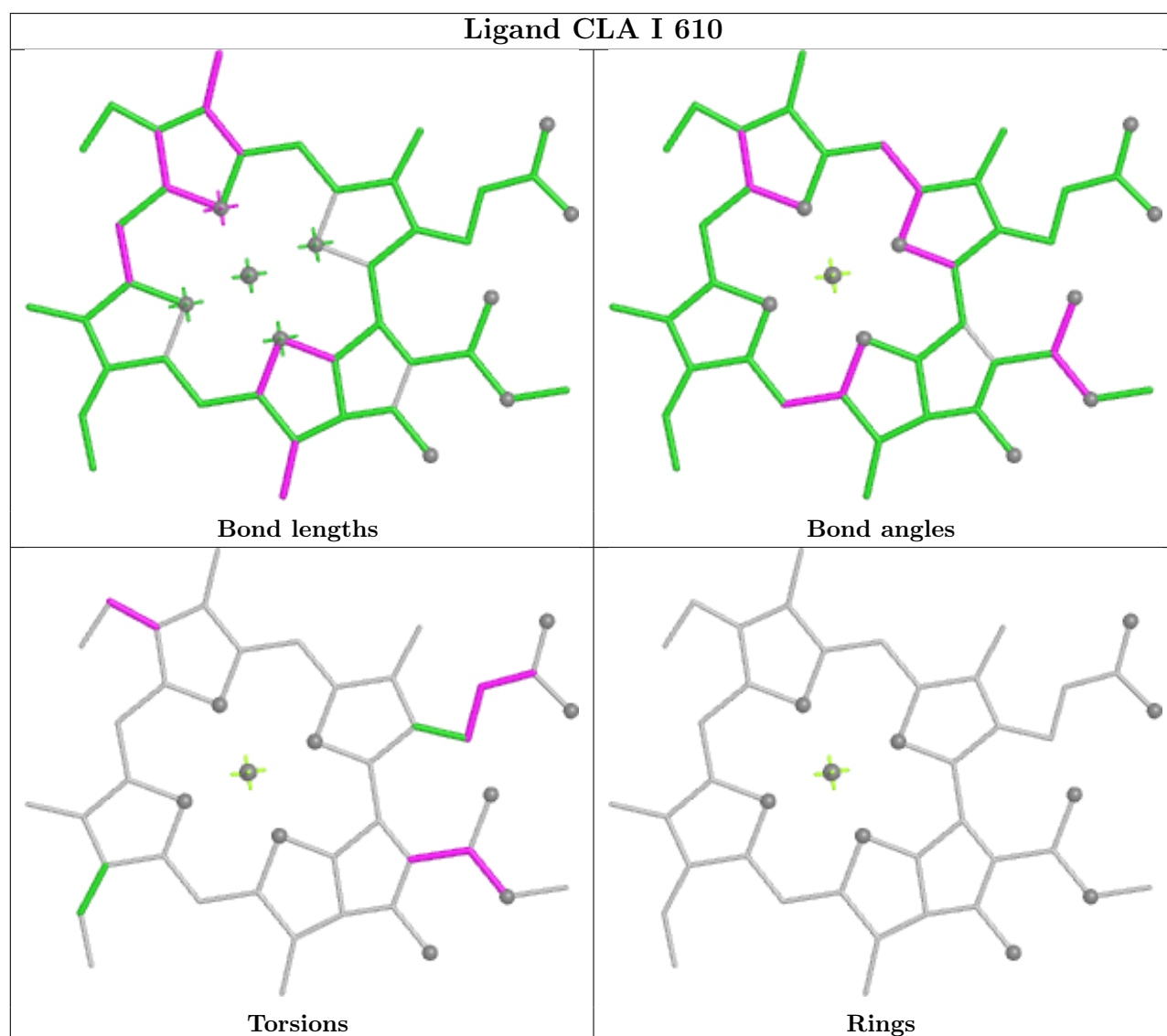
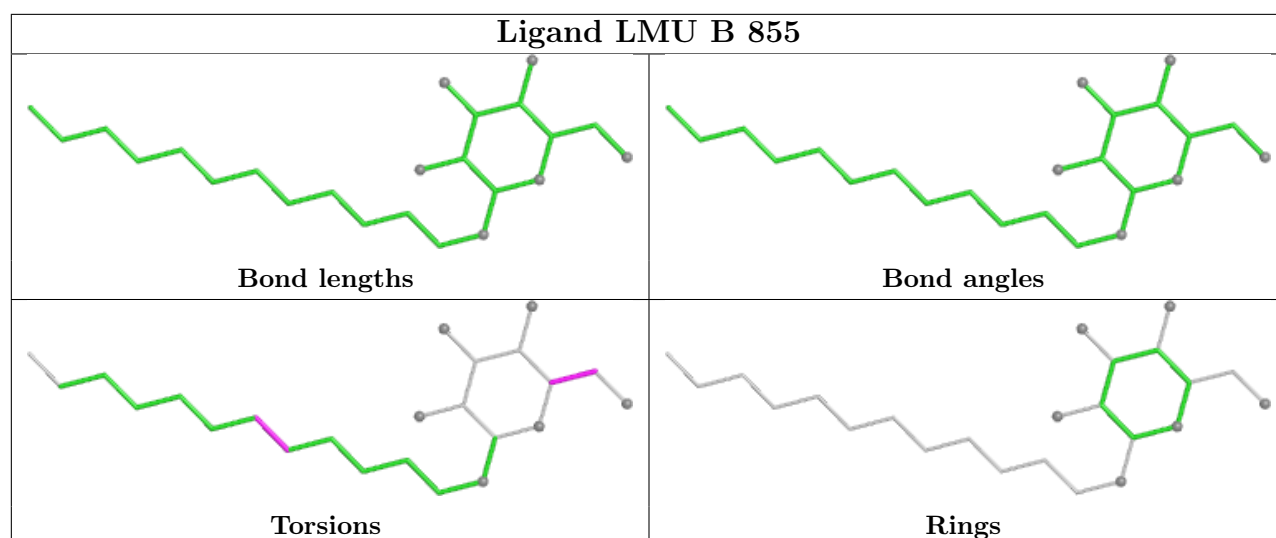
Rings

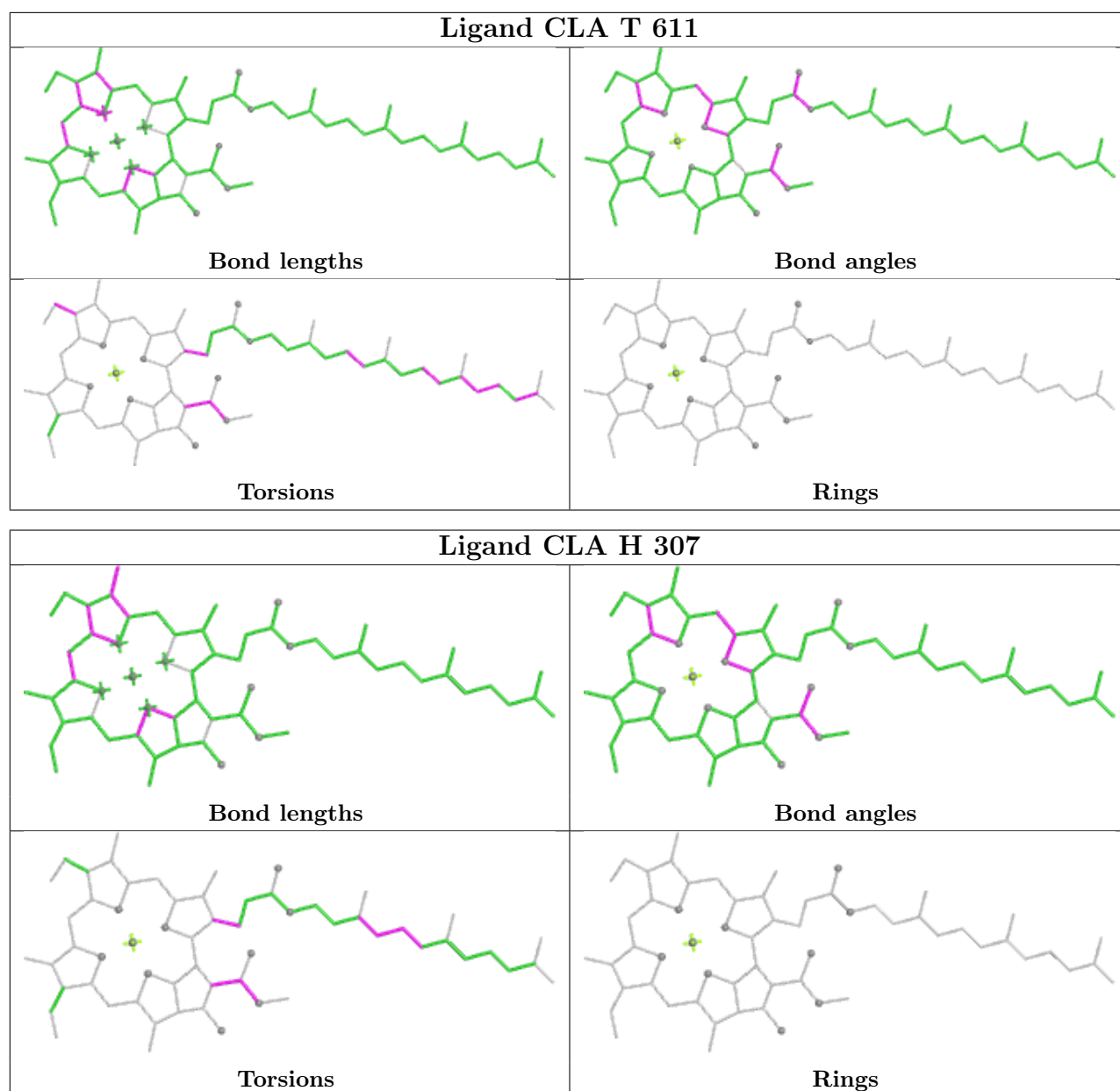




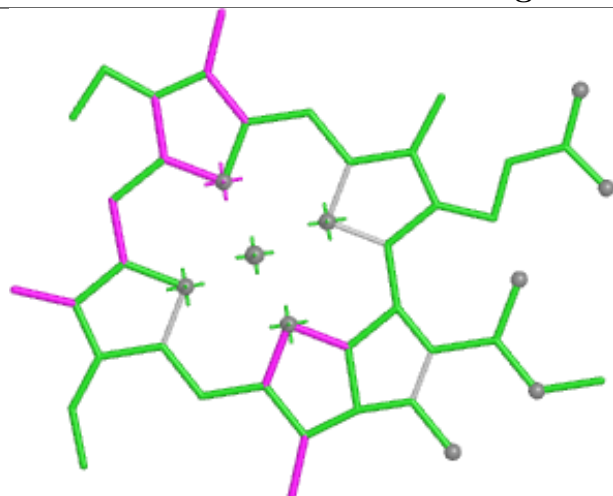




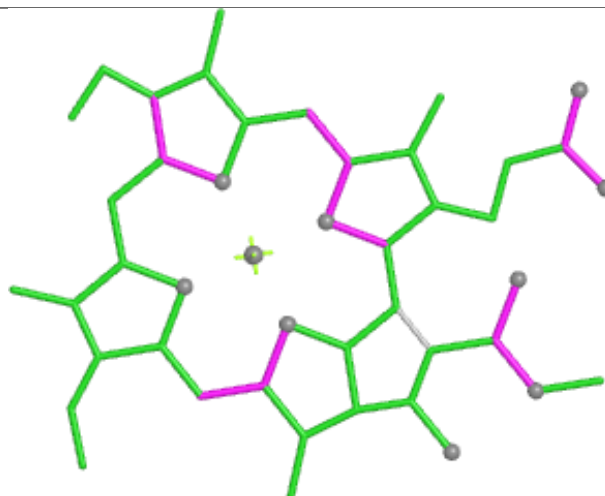




Ligand CLA P 602



Bond lengths



Bond angles

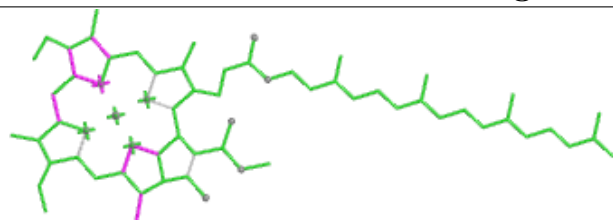


Torsions

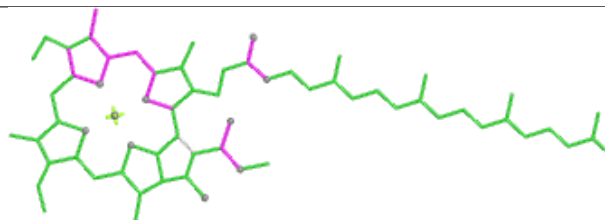


Rings

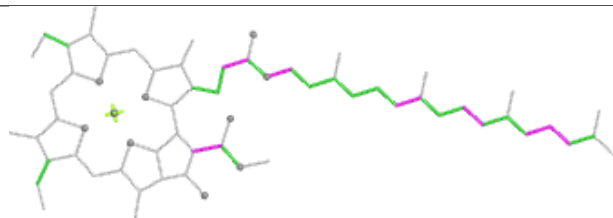
Ligand CLA N 603



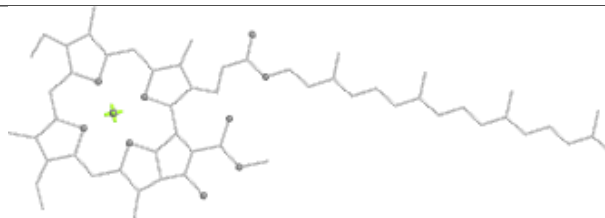
Bond lengths



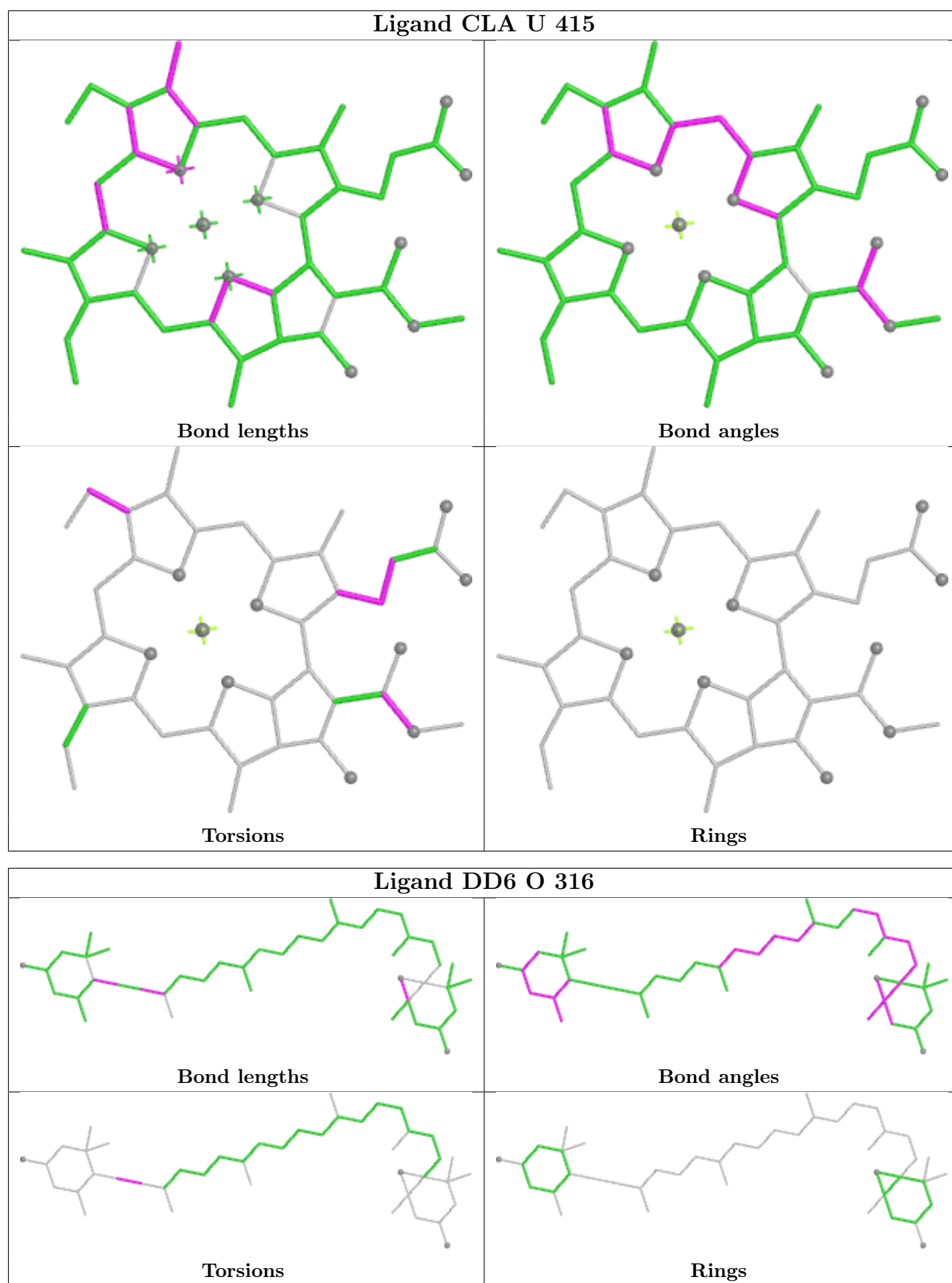
Bond angles

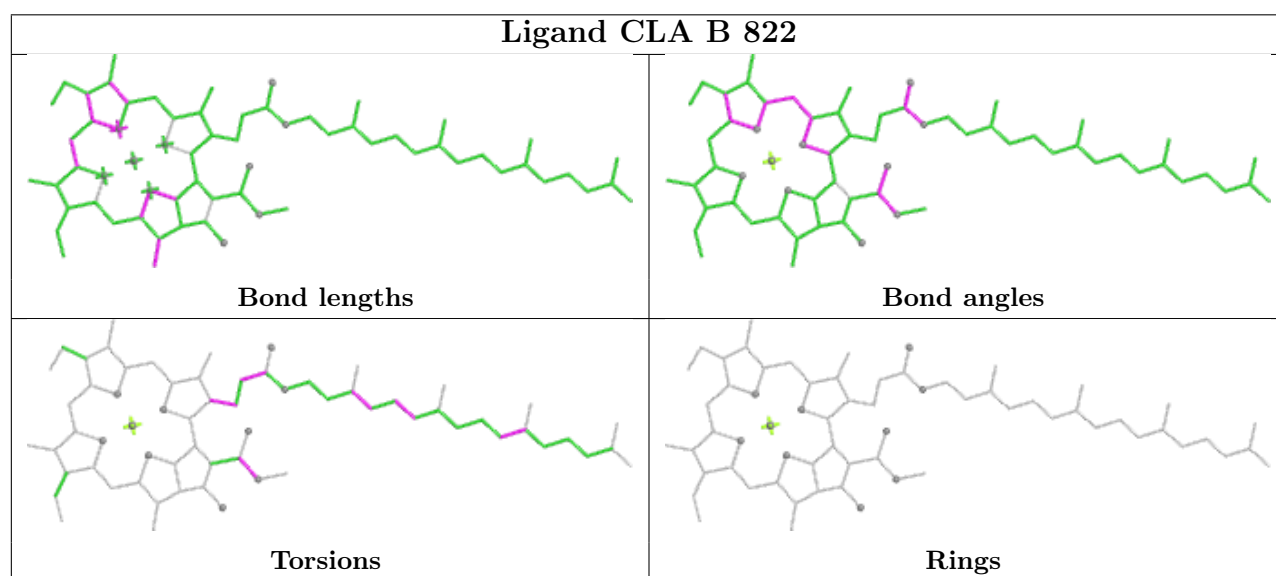
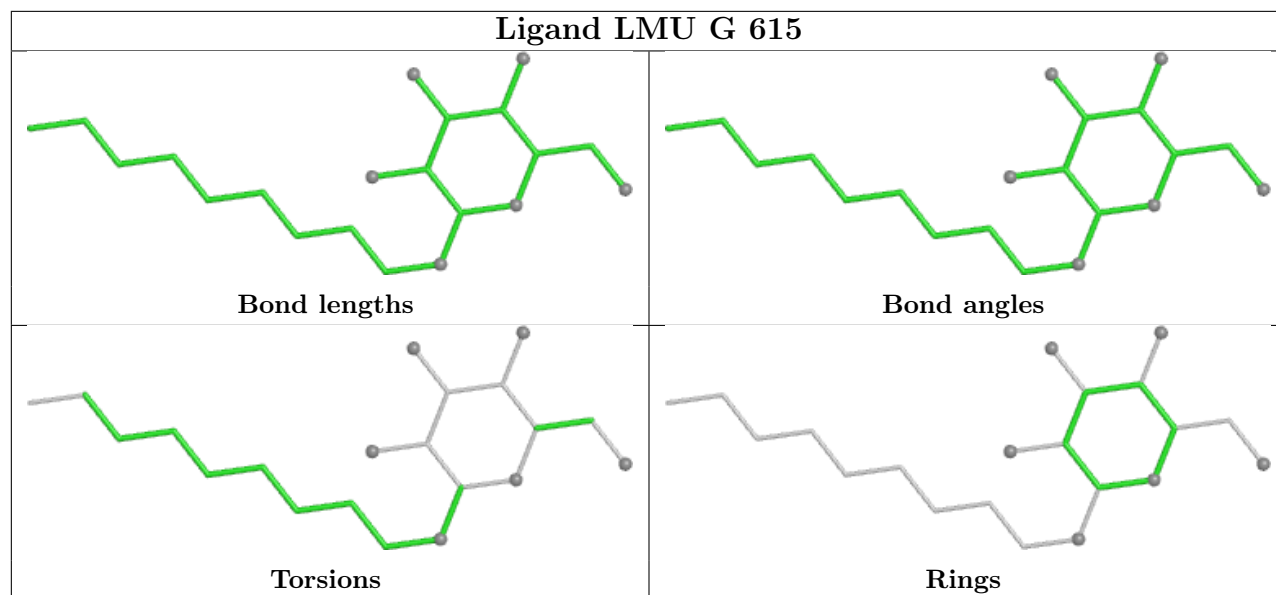


Torsions

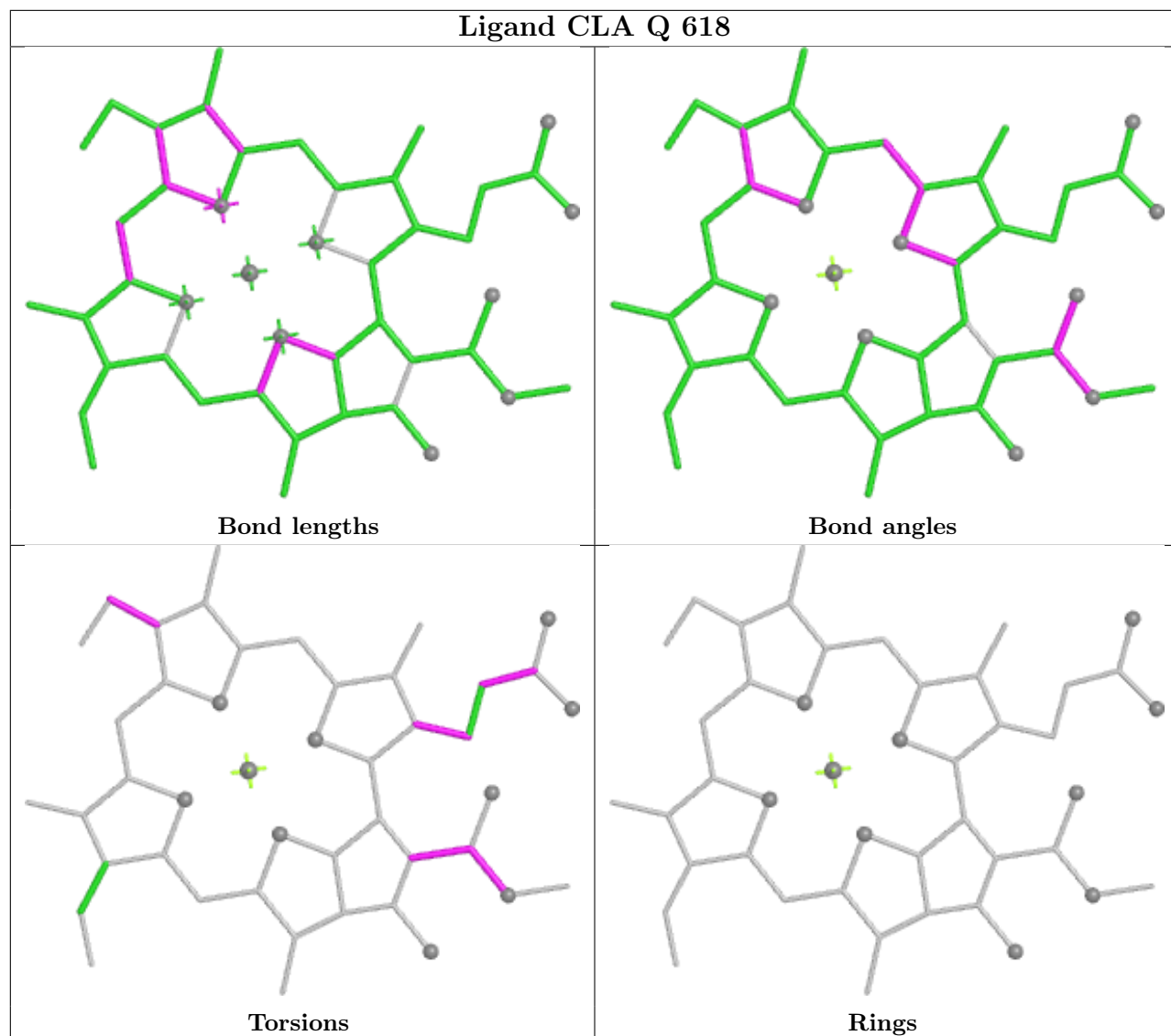


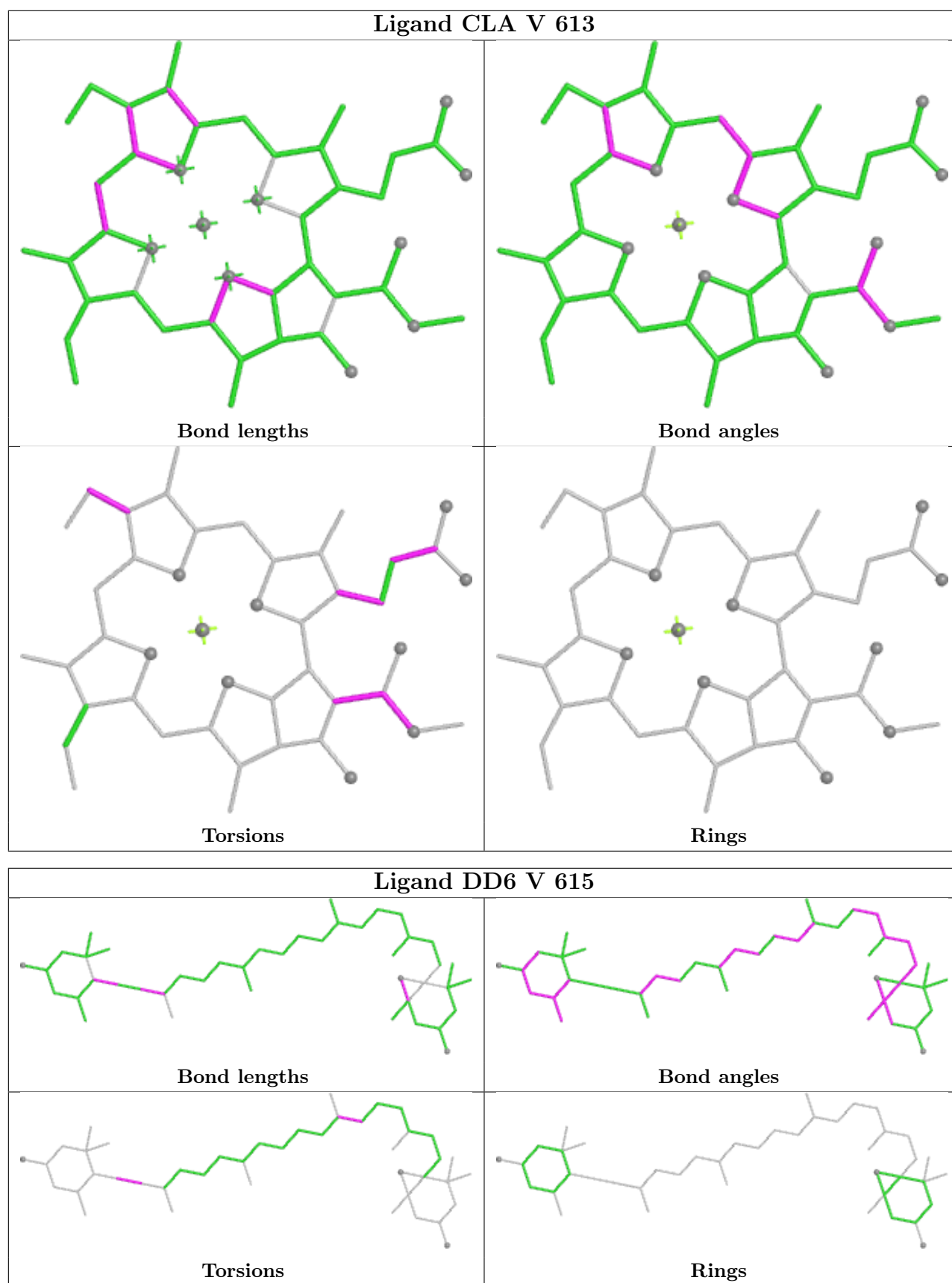
Rings

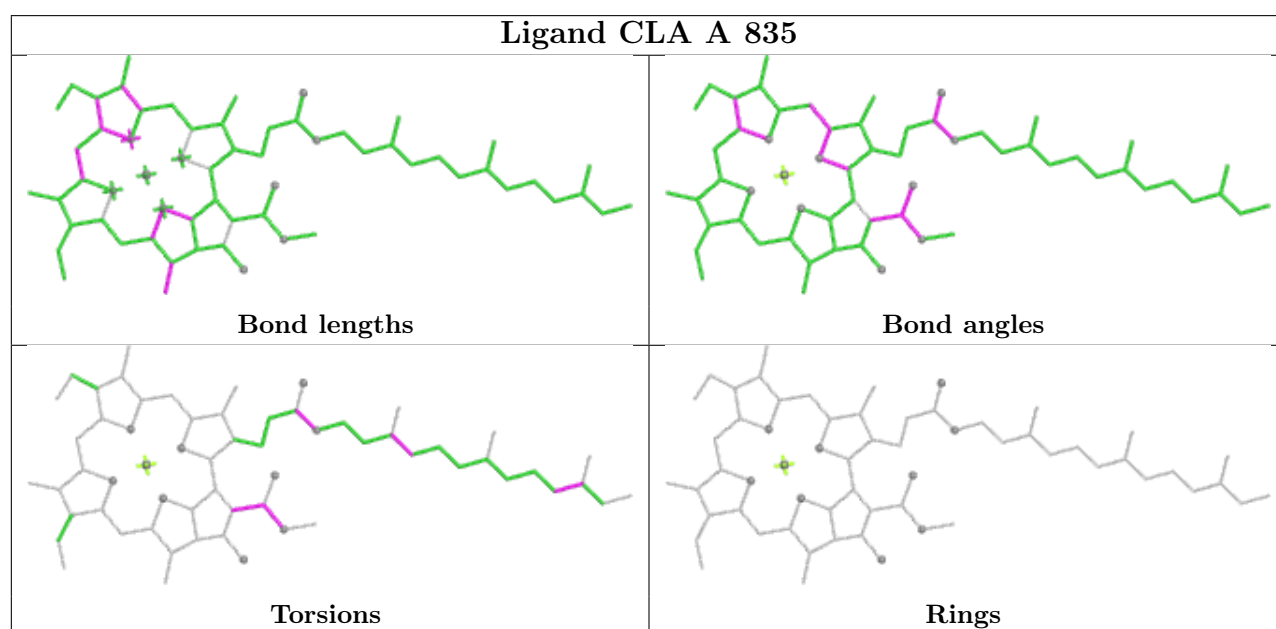
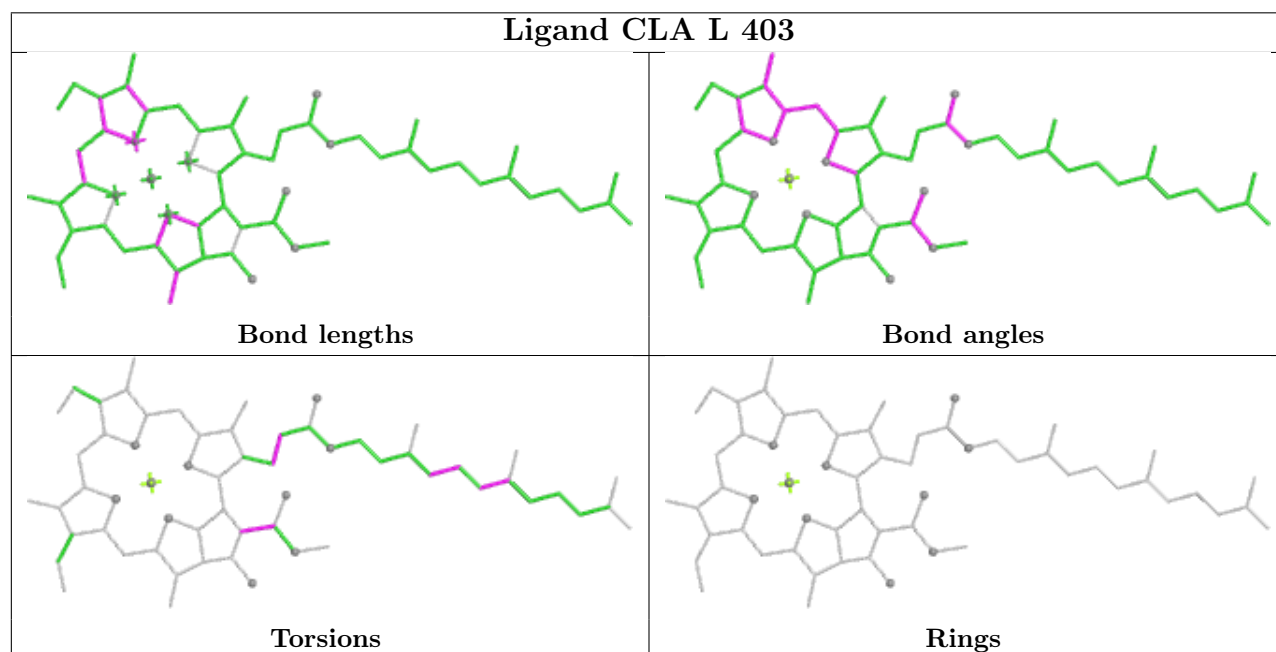
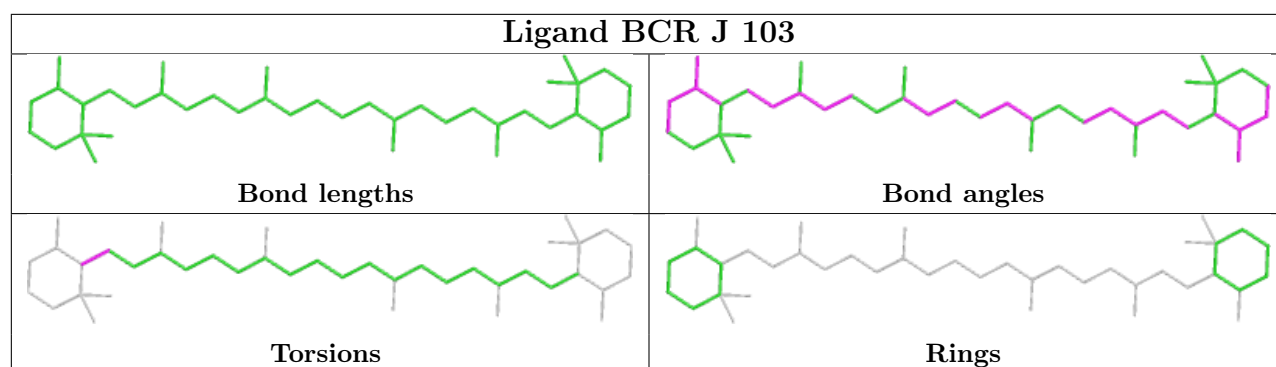


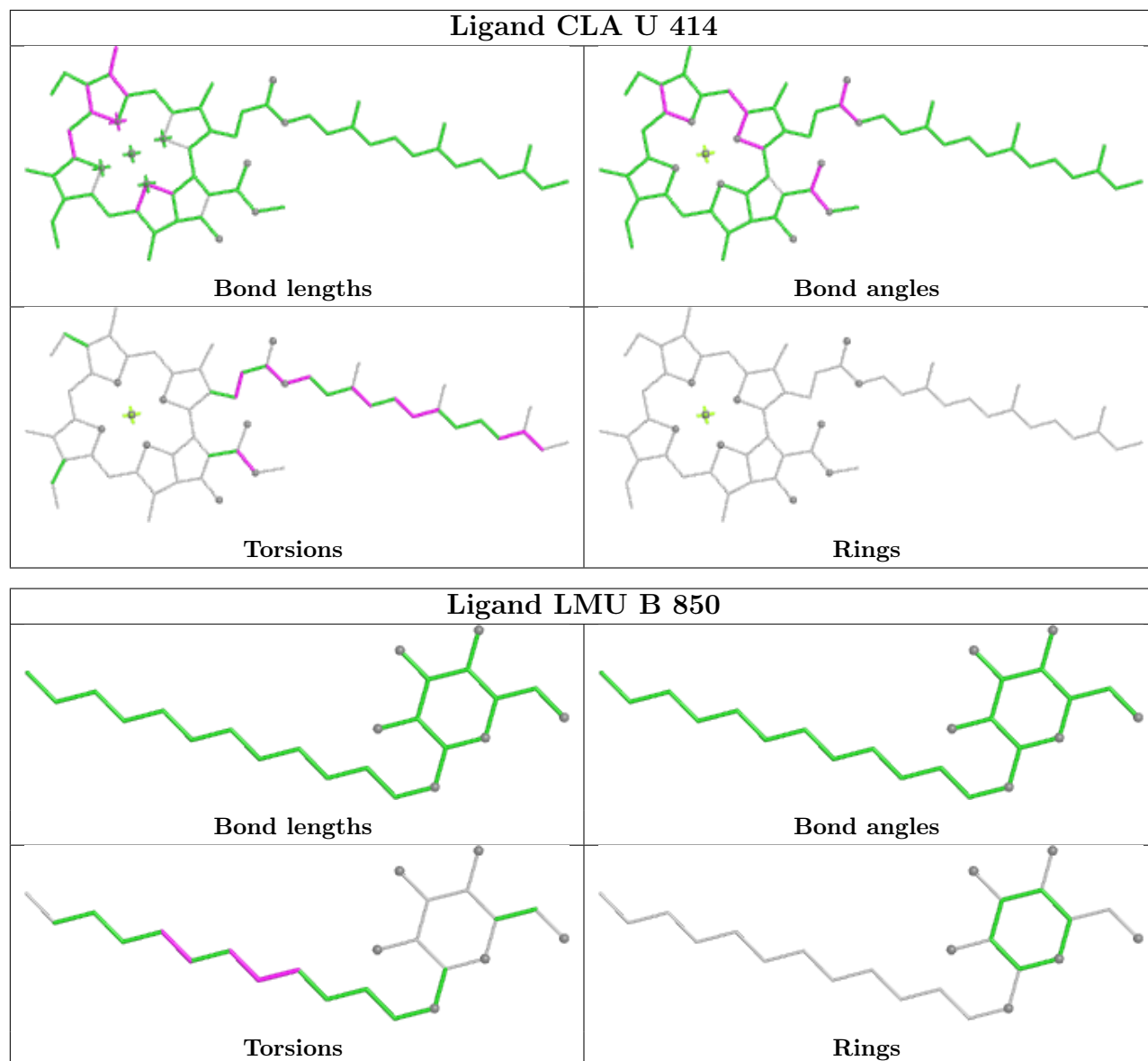


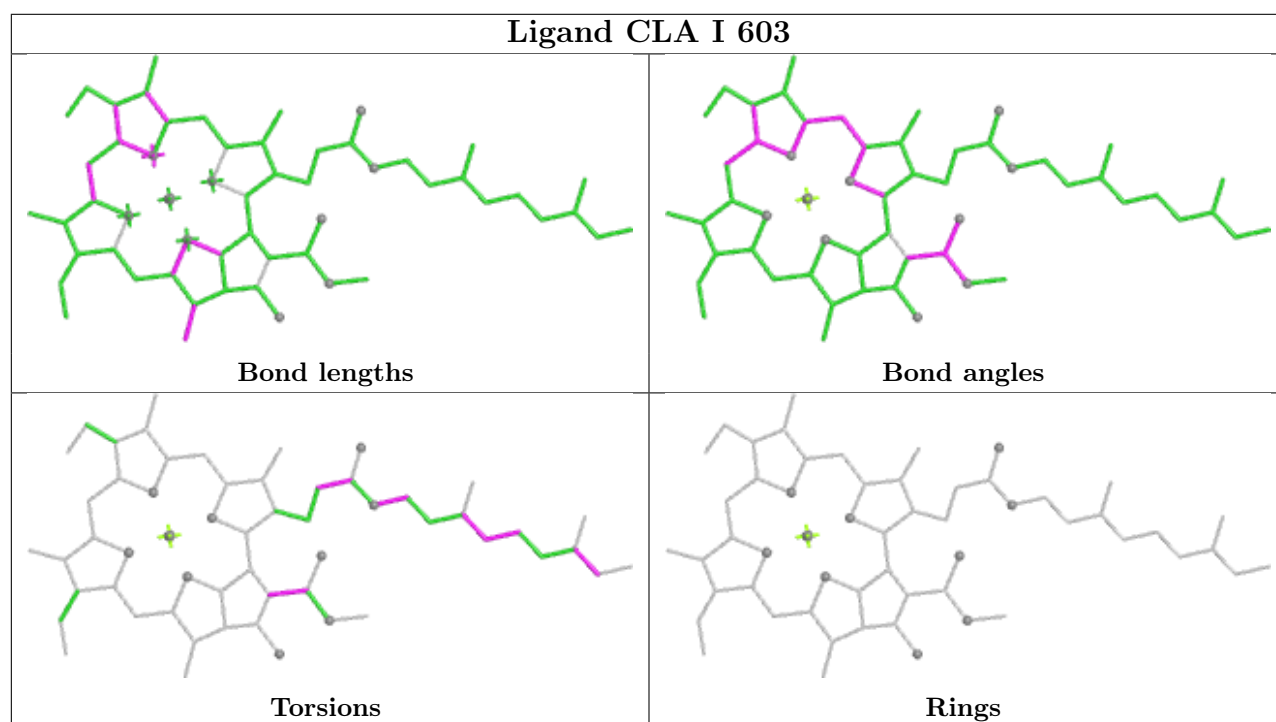
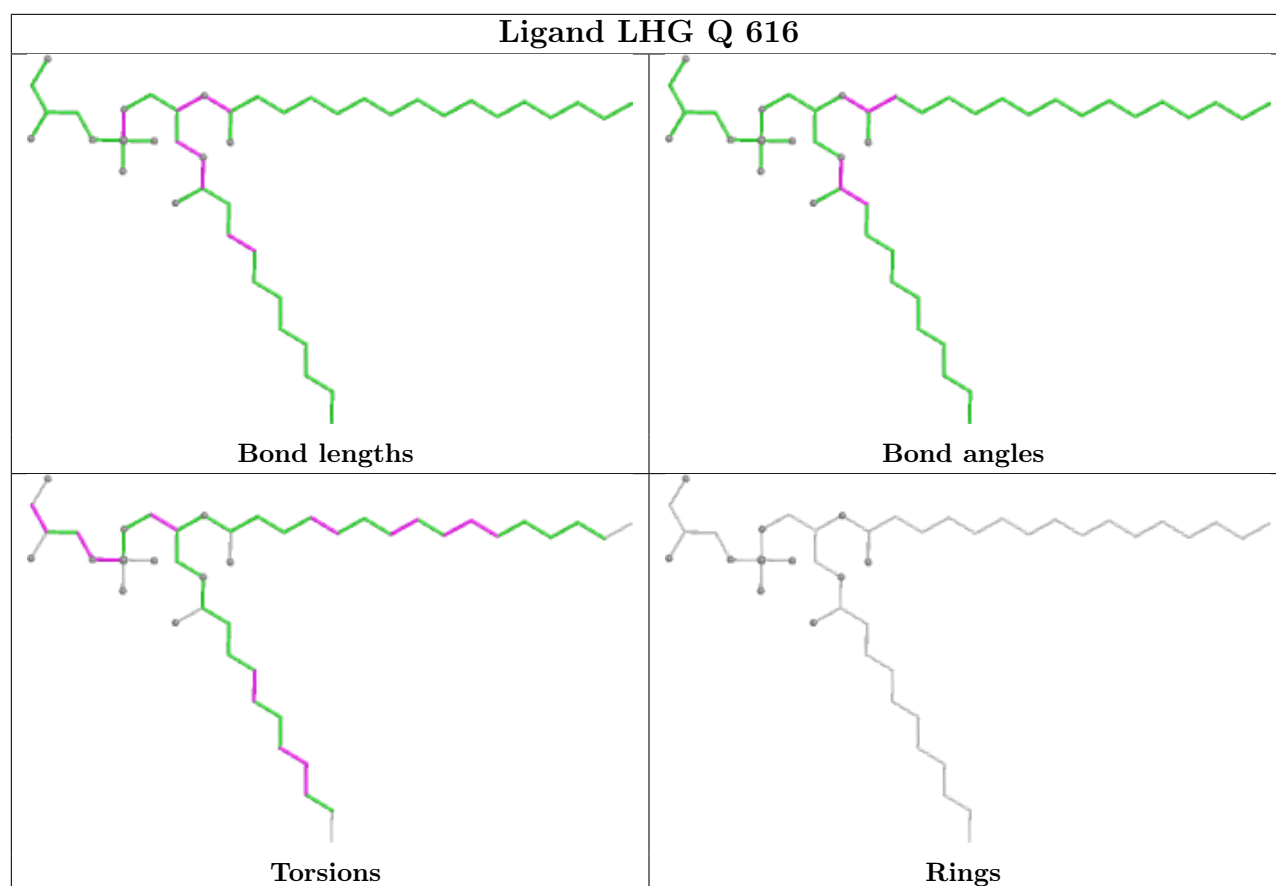
Ligand CLA Q 618

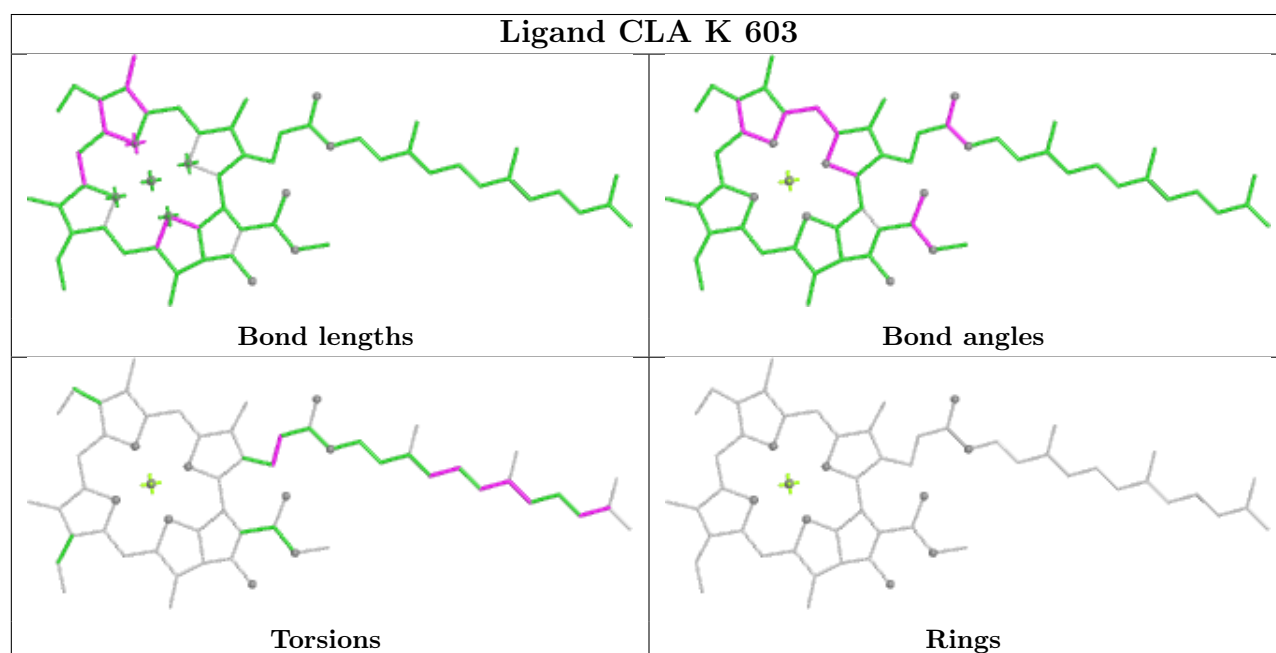
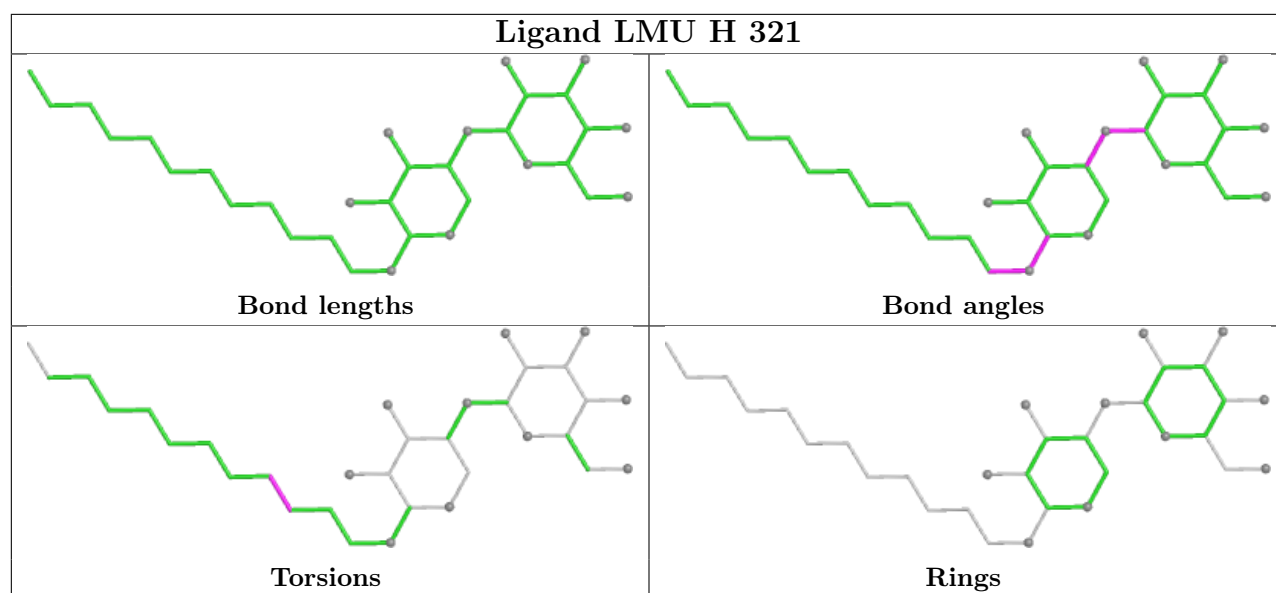


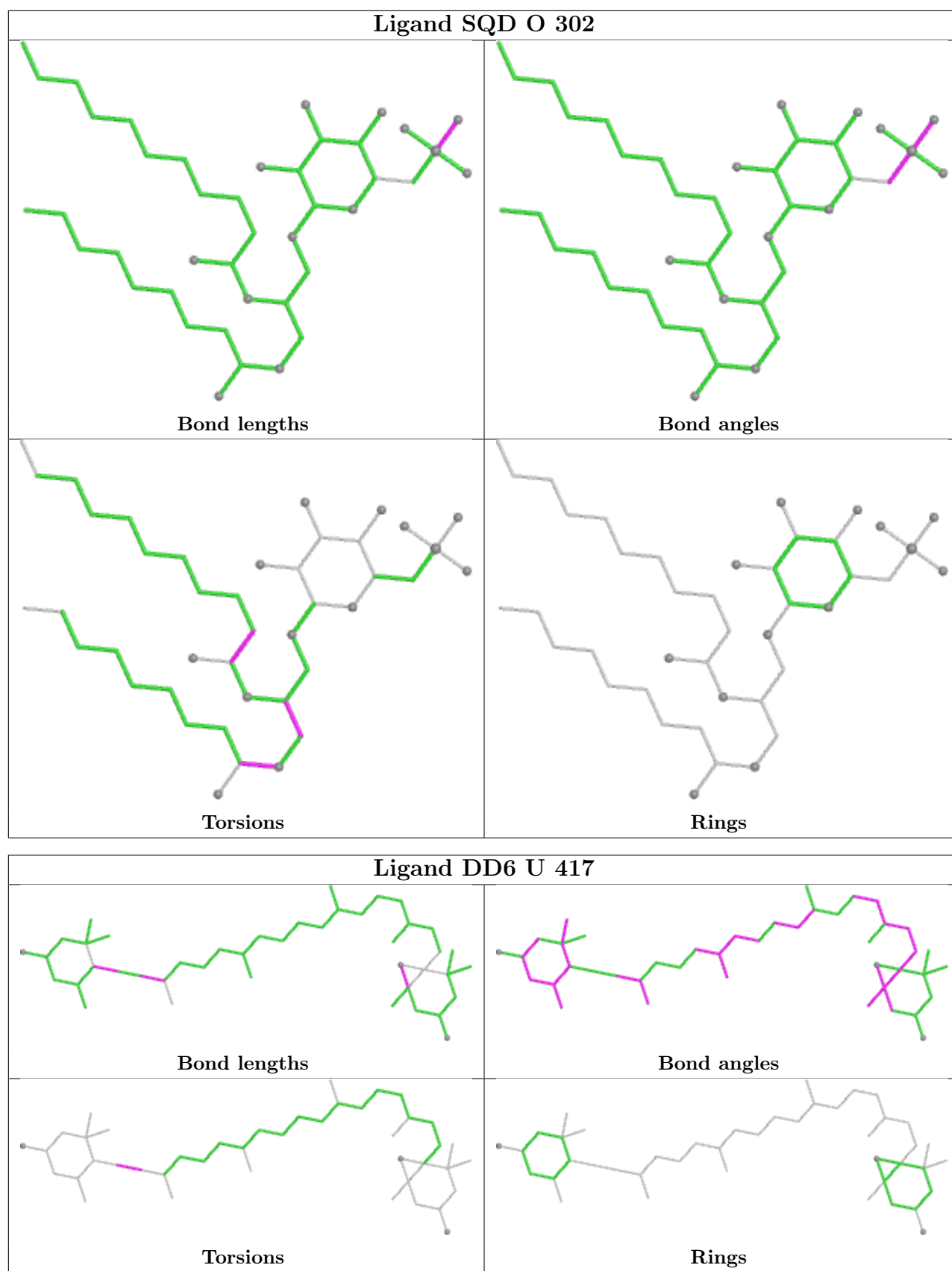




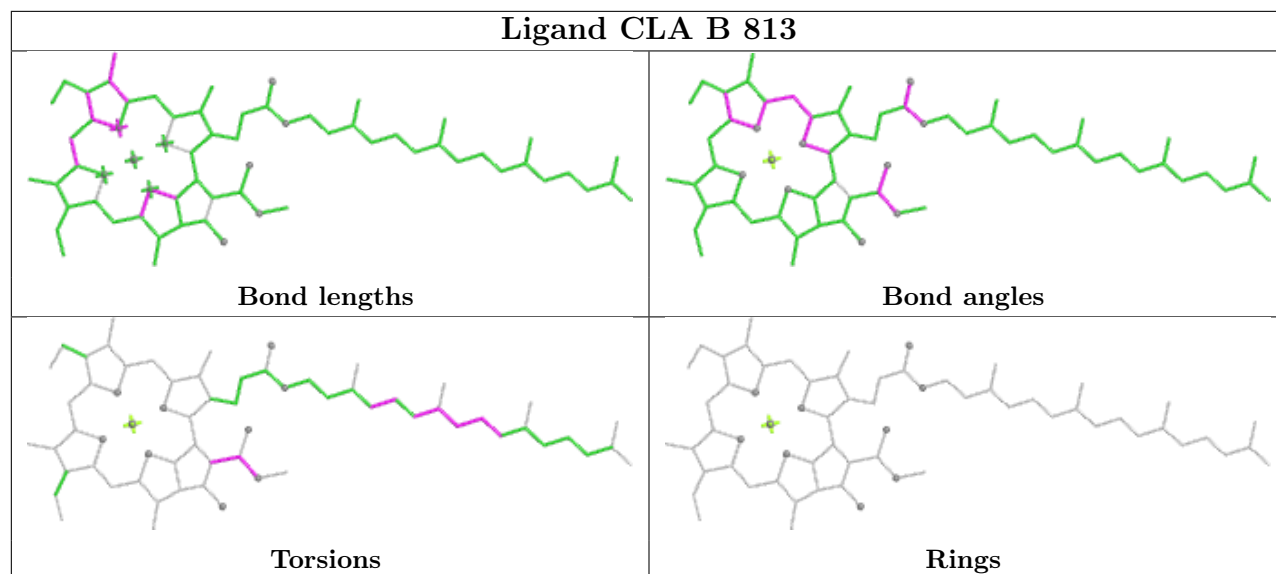




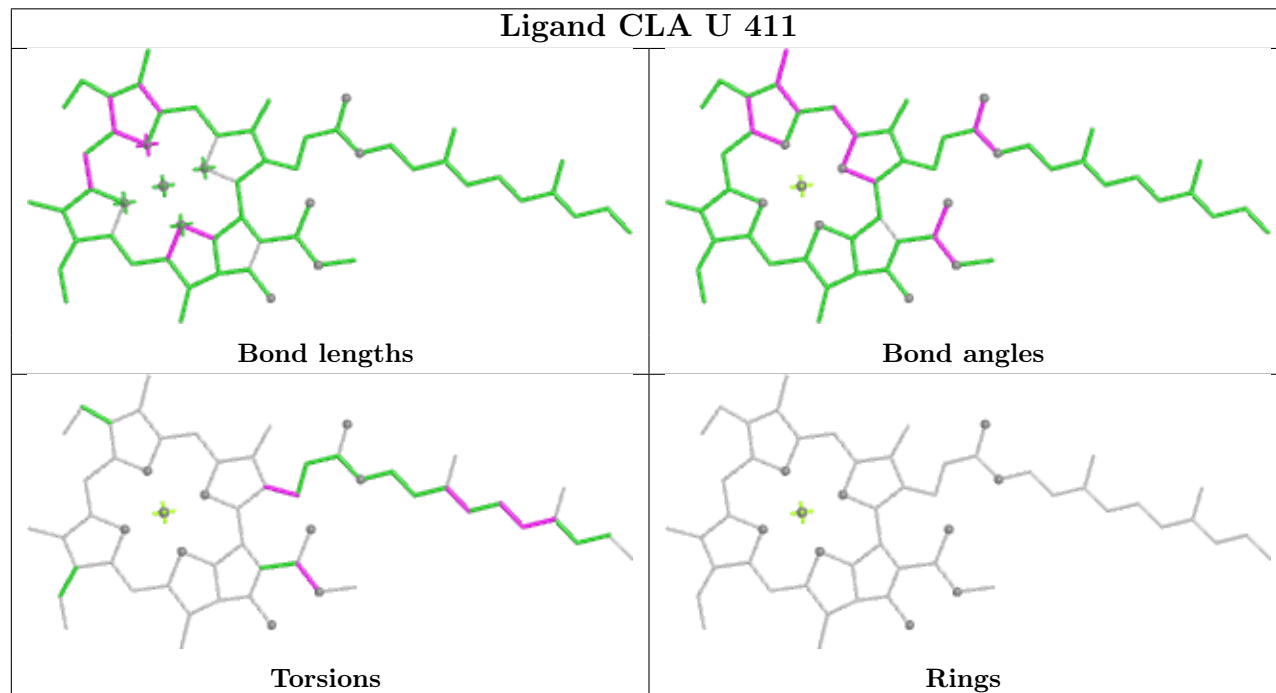




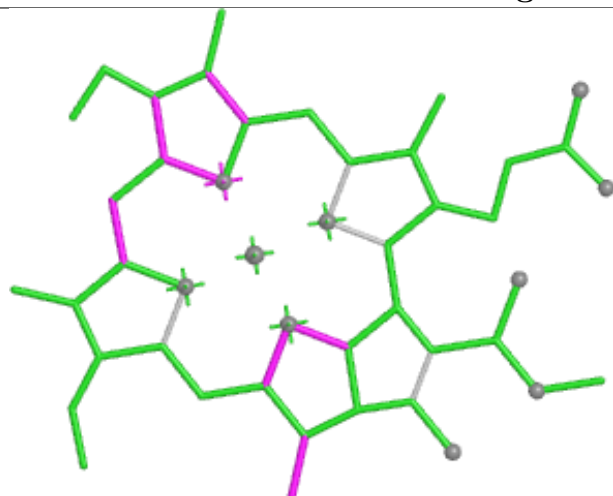
Ligand CLA B 813



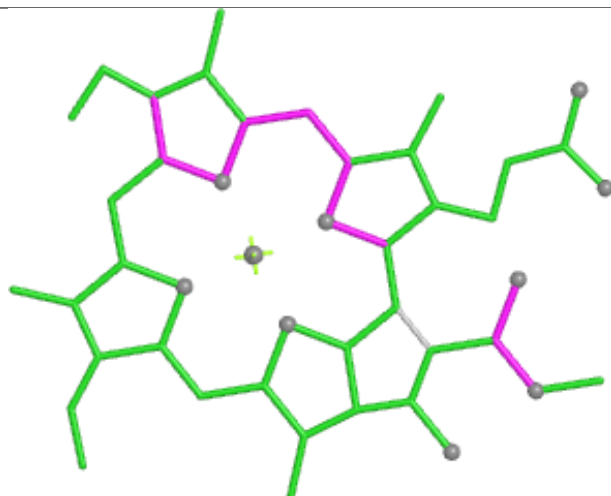
Ligand CLA U 411



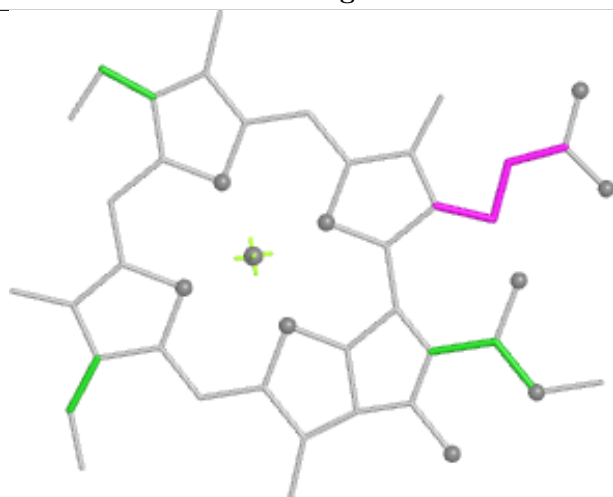
Ligand CLA L 412



Bond lengths



Bond angles

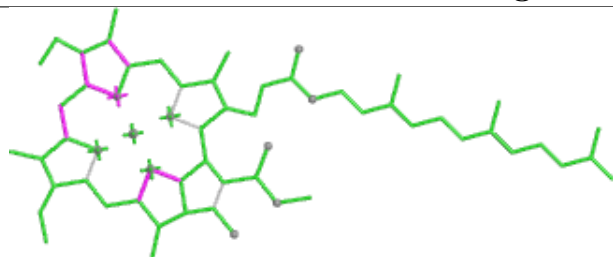


Torsions

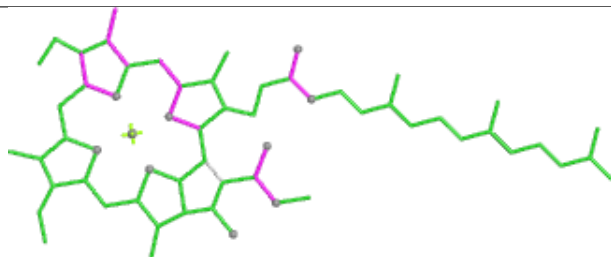


Rings

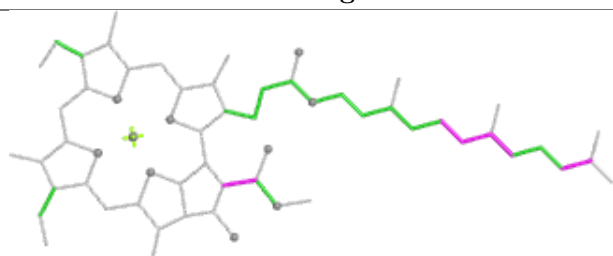
Ligand CLA H 308



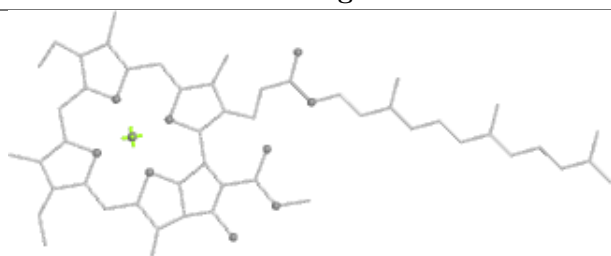
Bond lengths



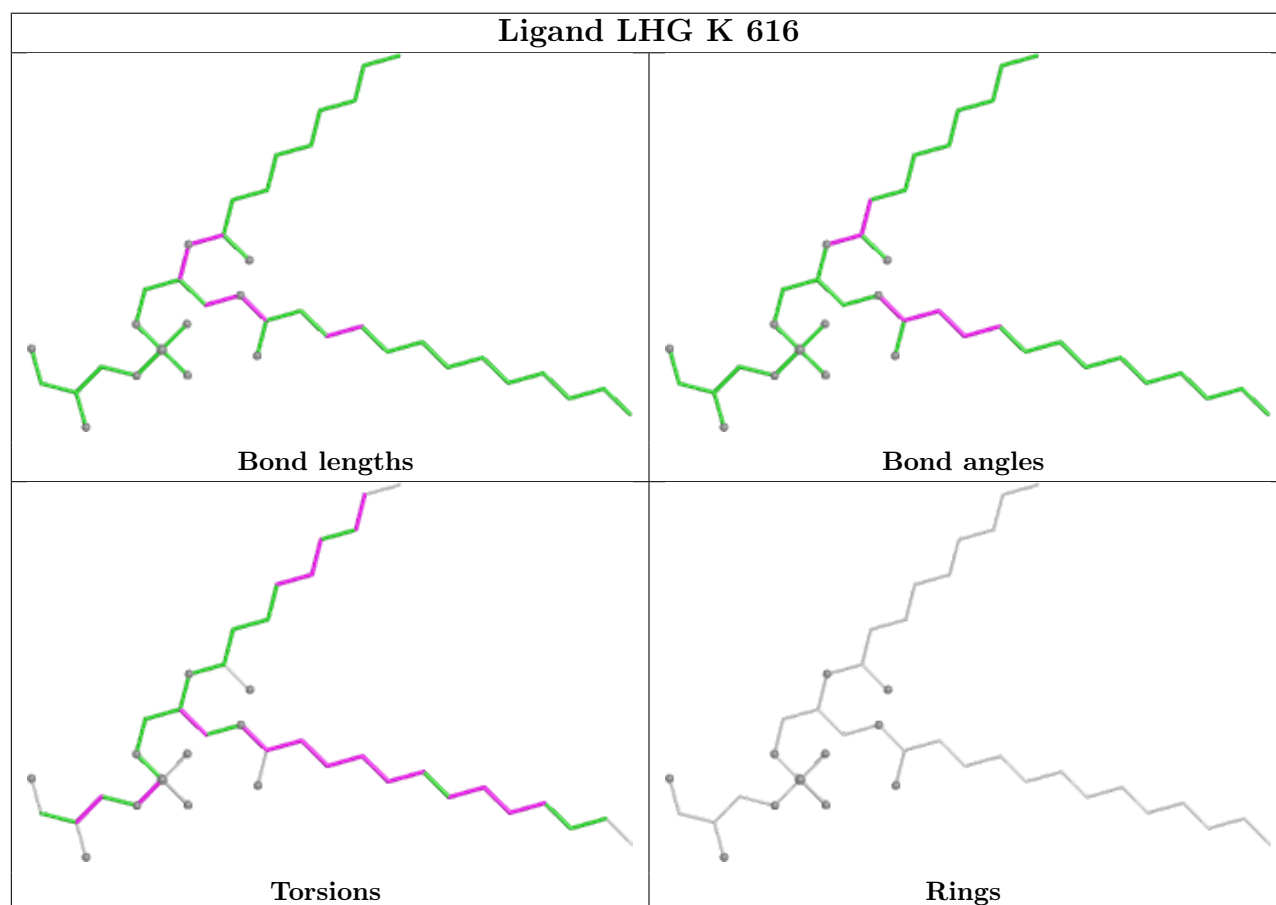
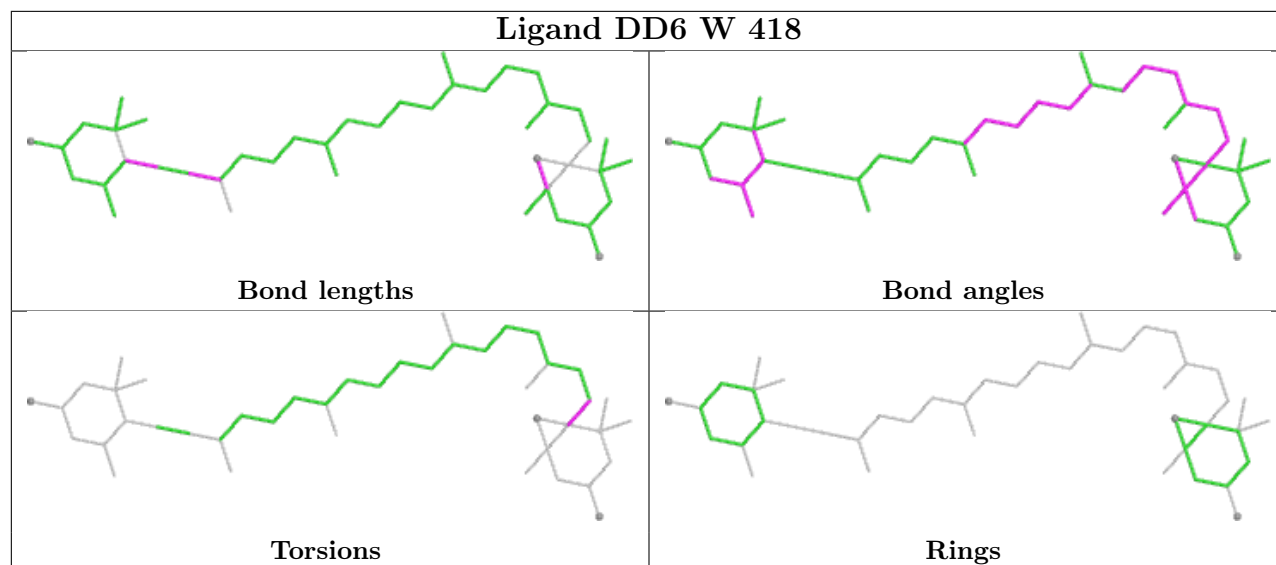
Bond angles

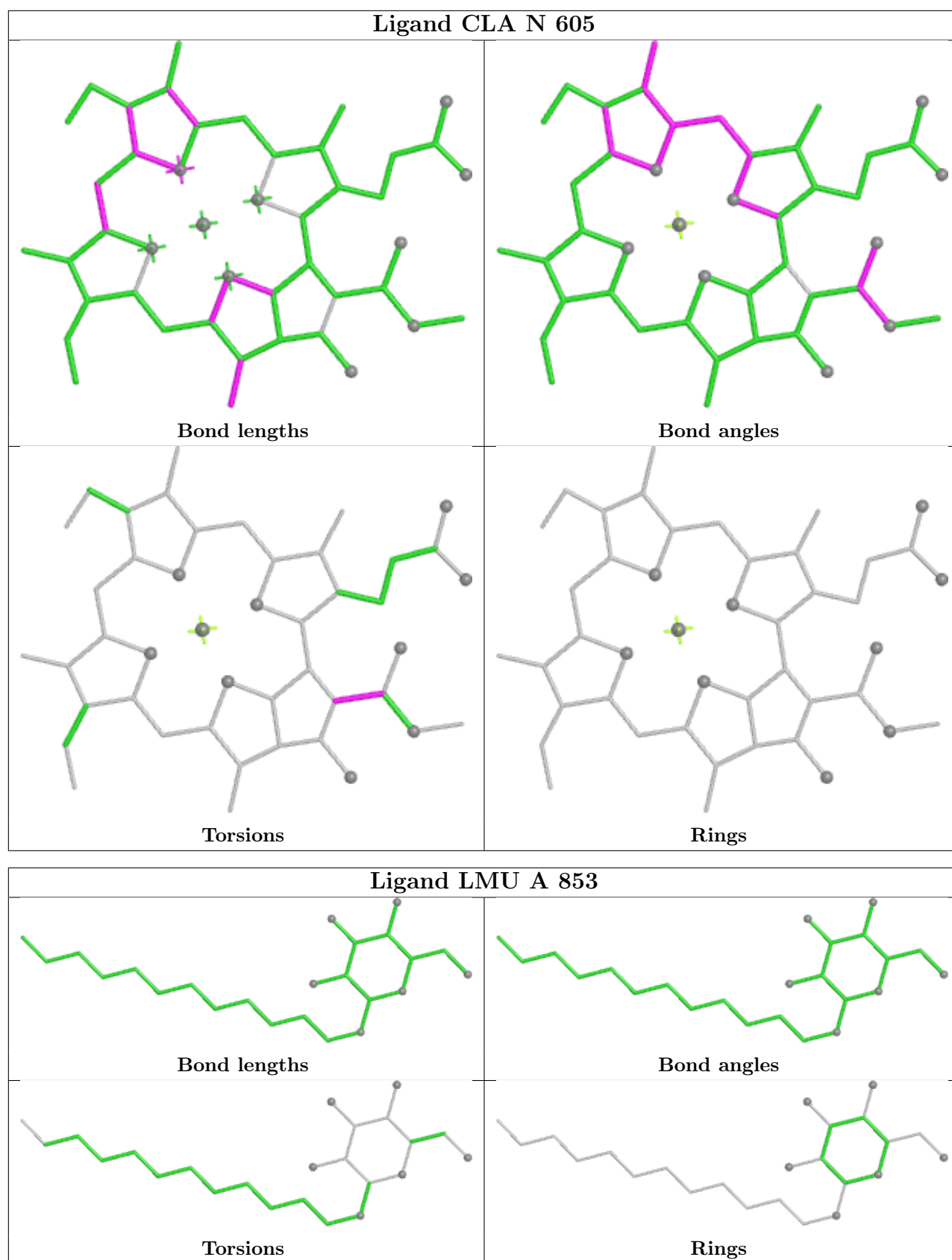


Torsions

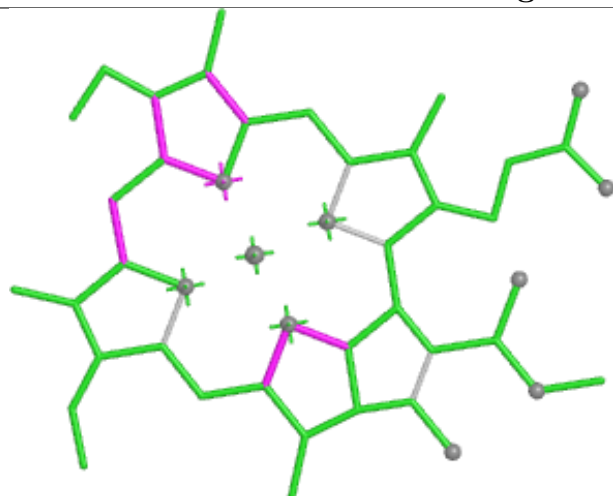


Rings

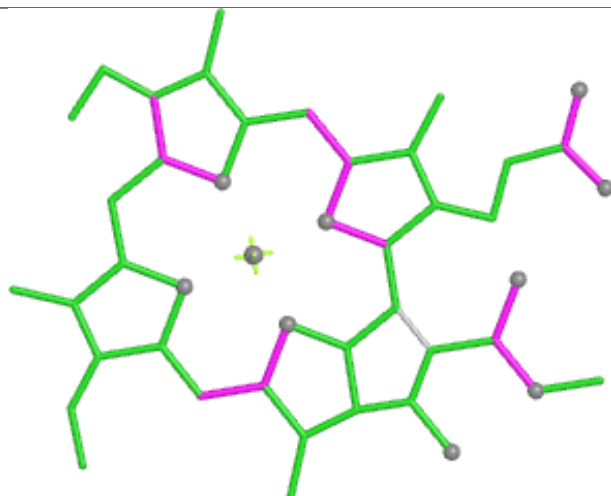




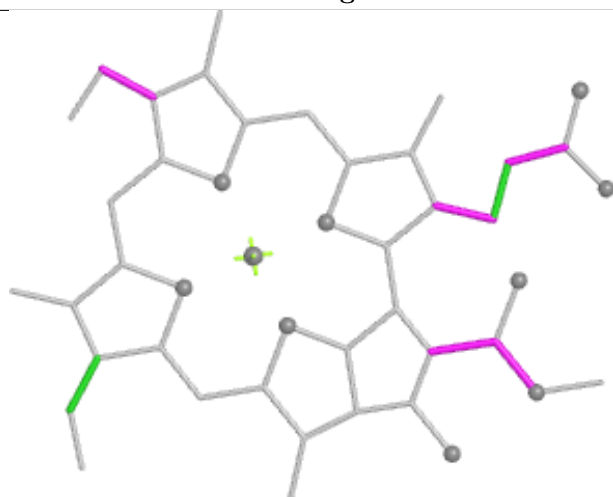
Ligand CLA S 608



Bond lengths



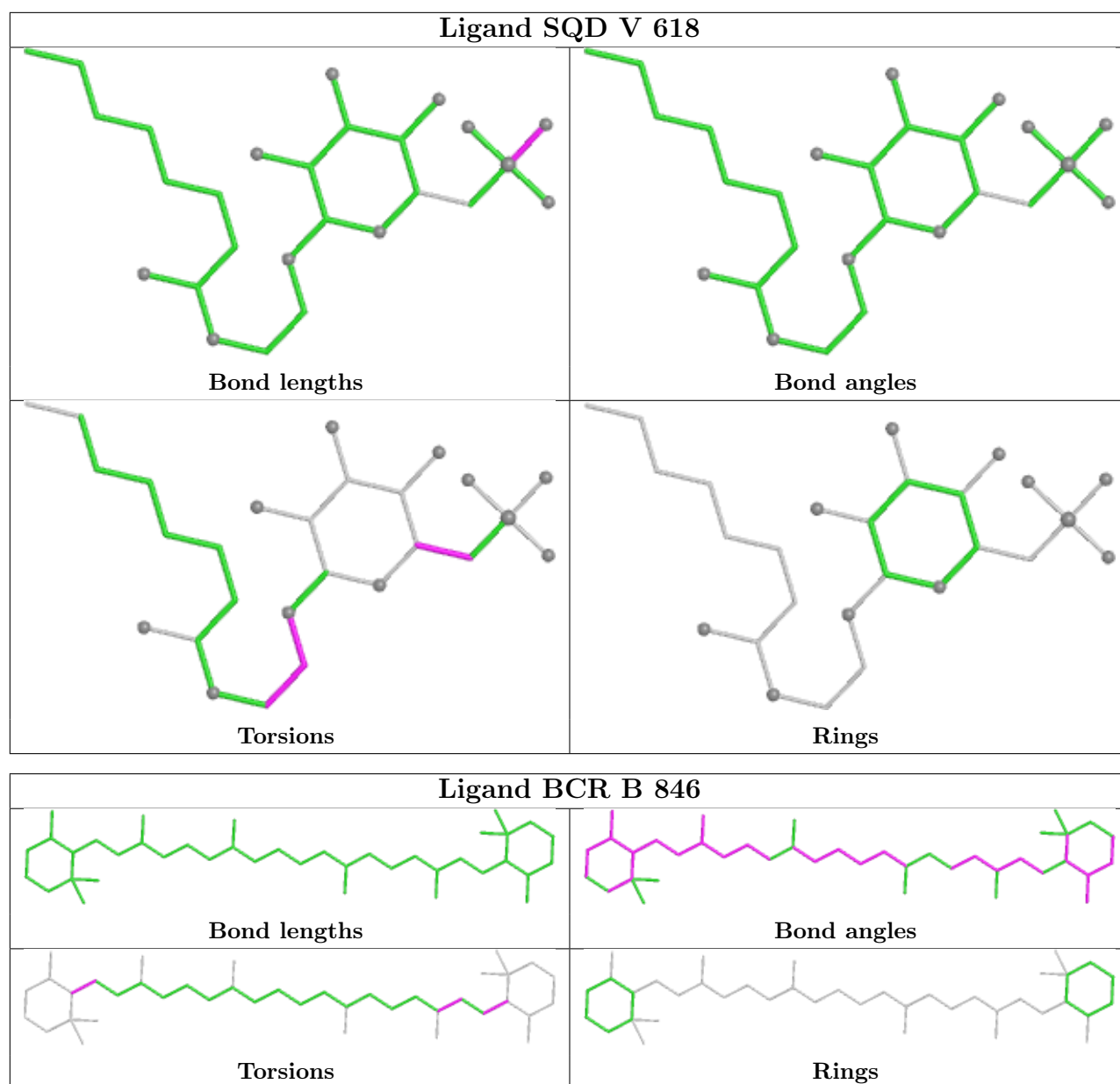
Bond angles

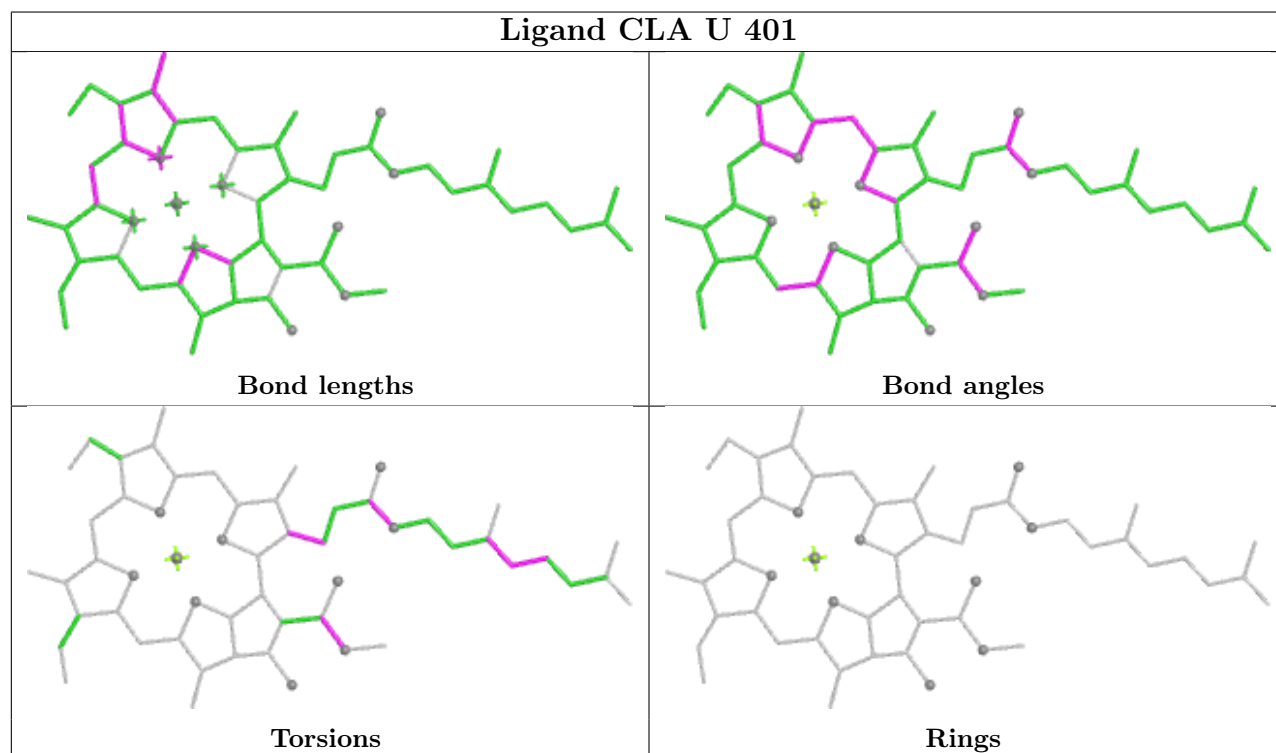
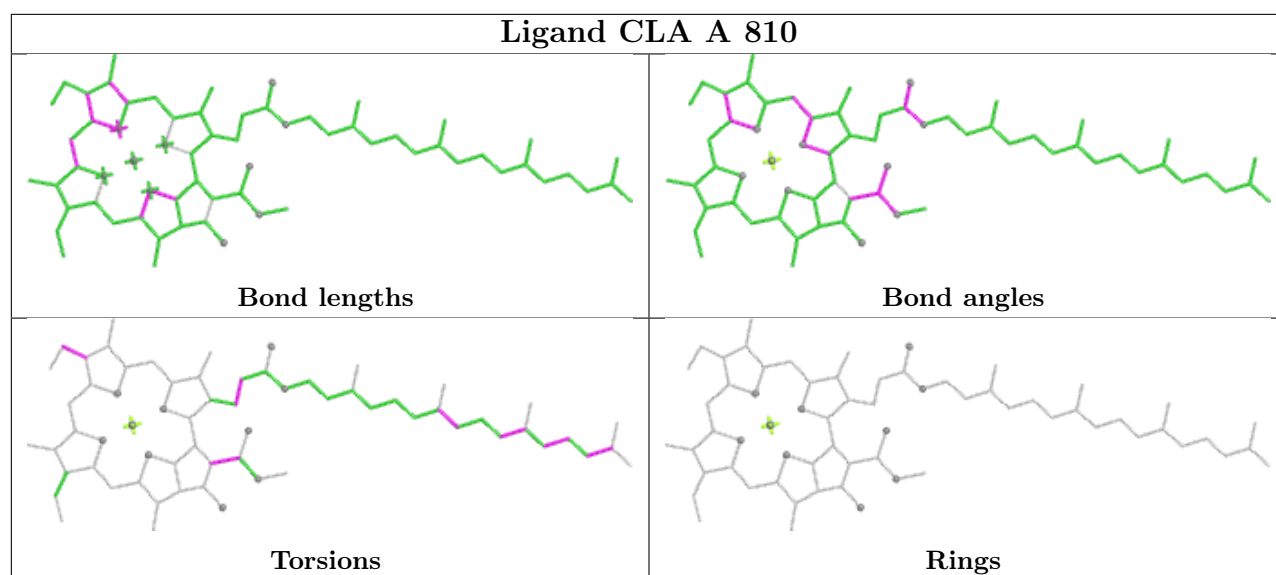


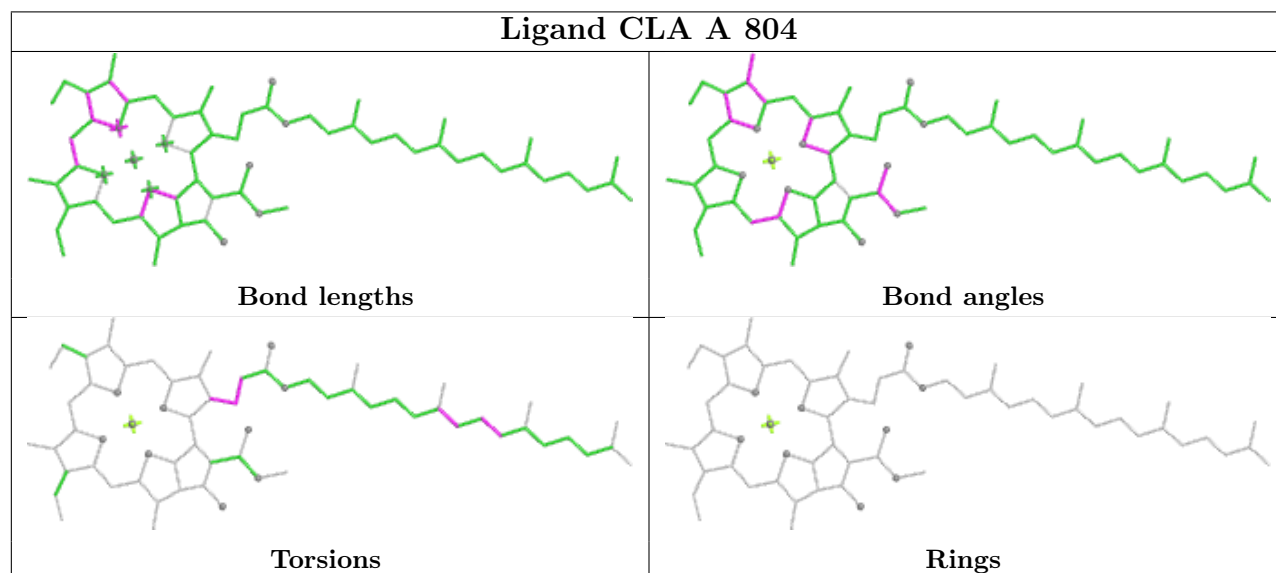
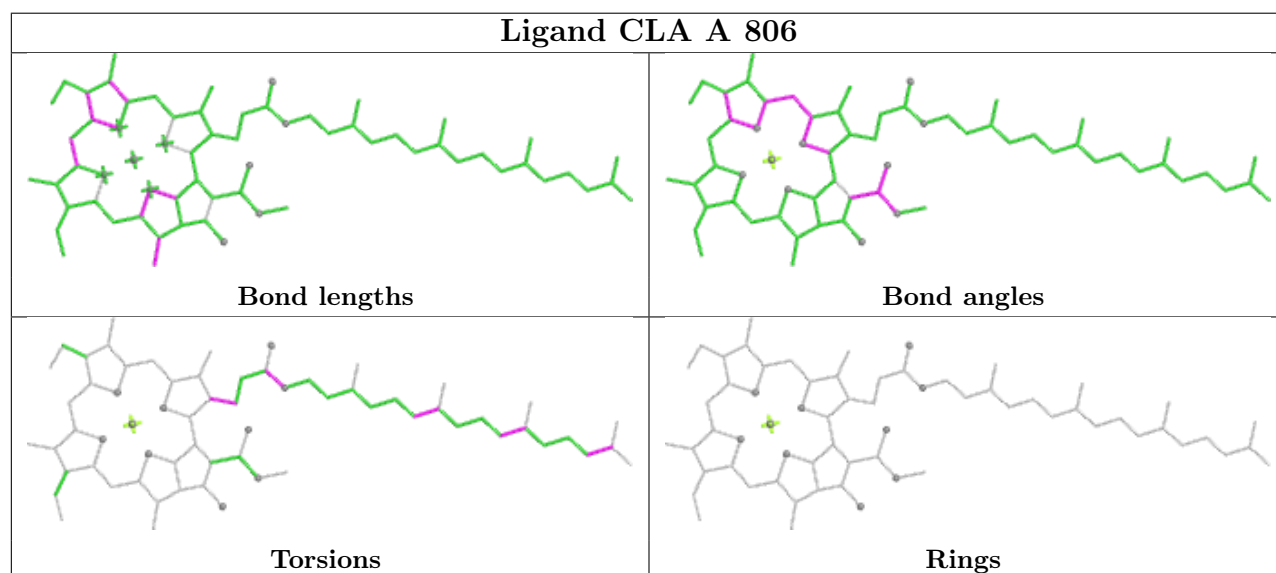
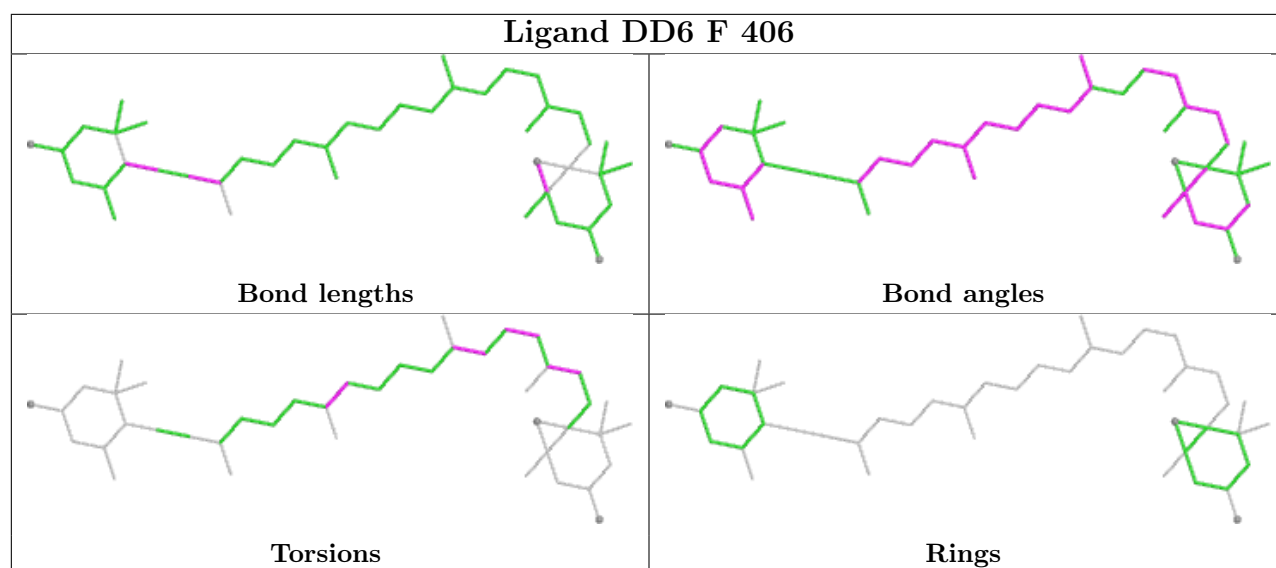
Torsions

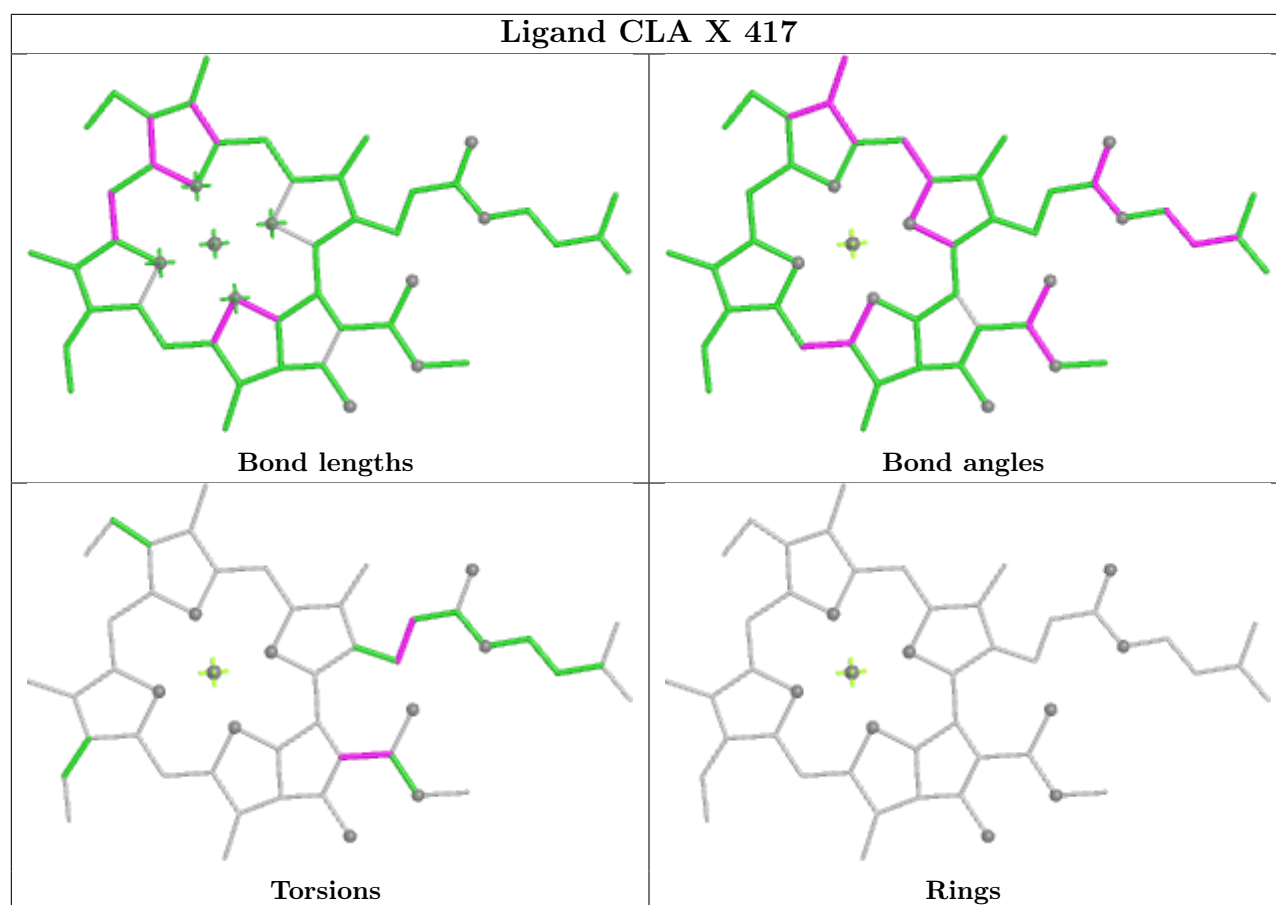


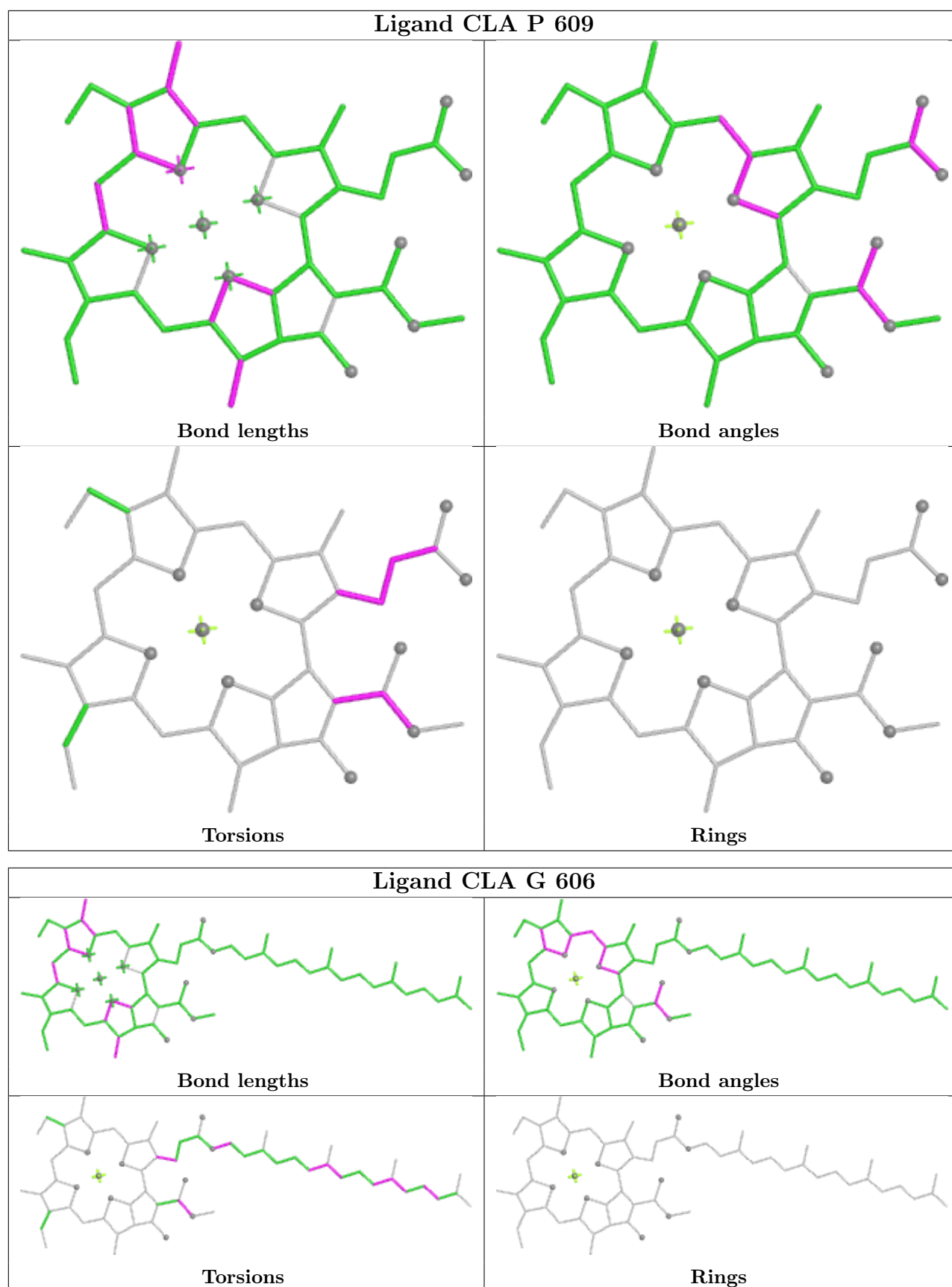
Rings



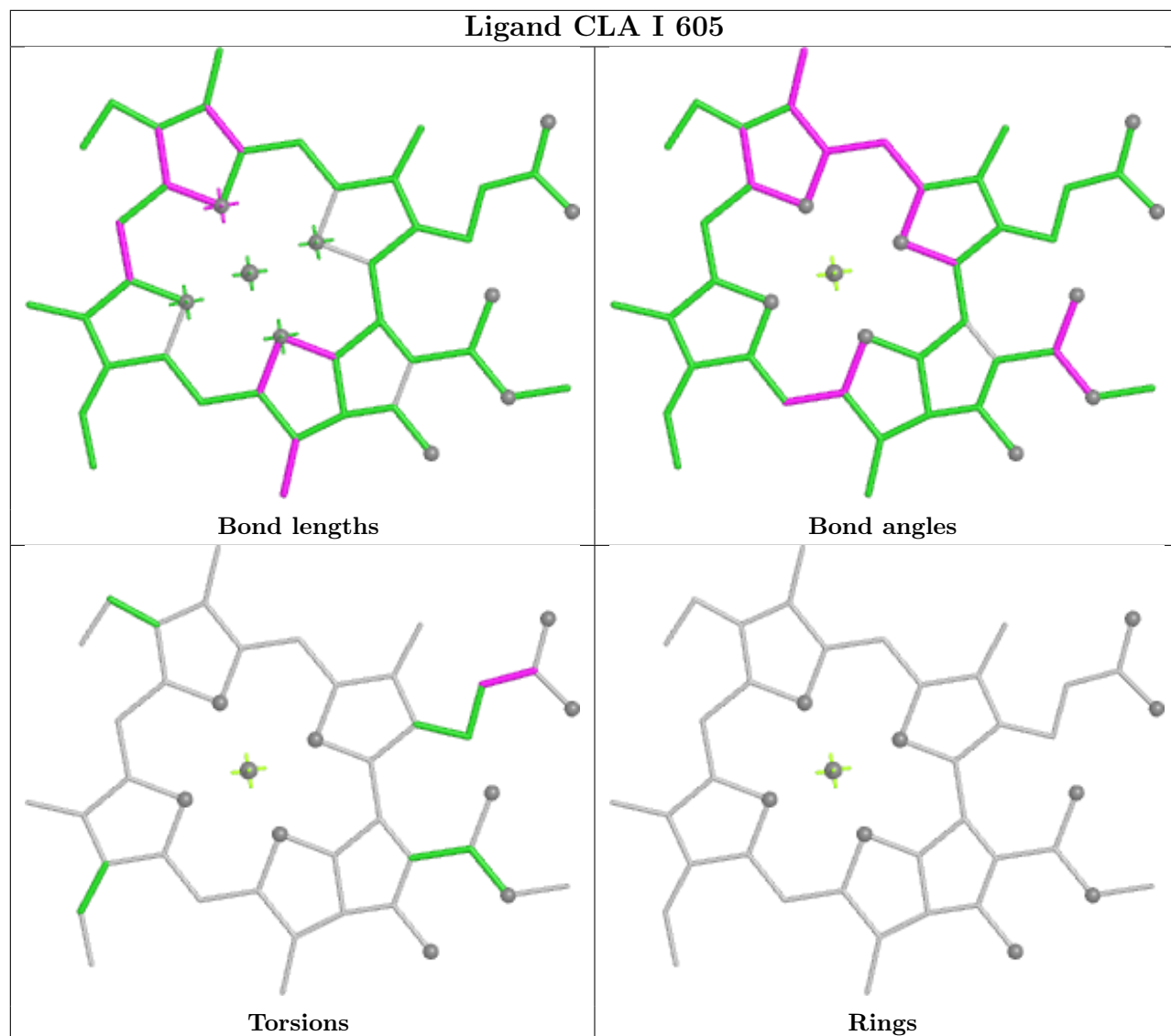


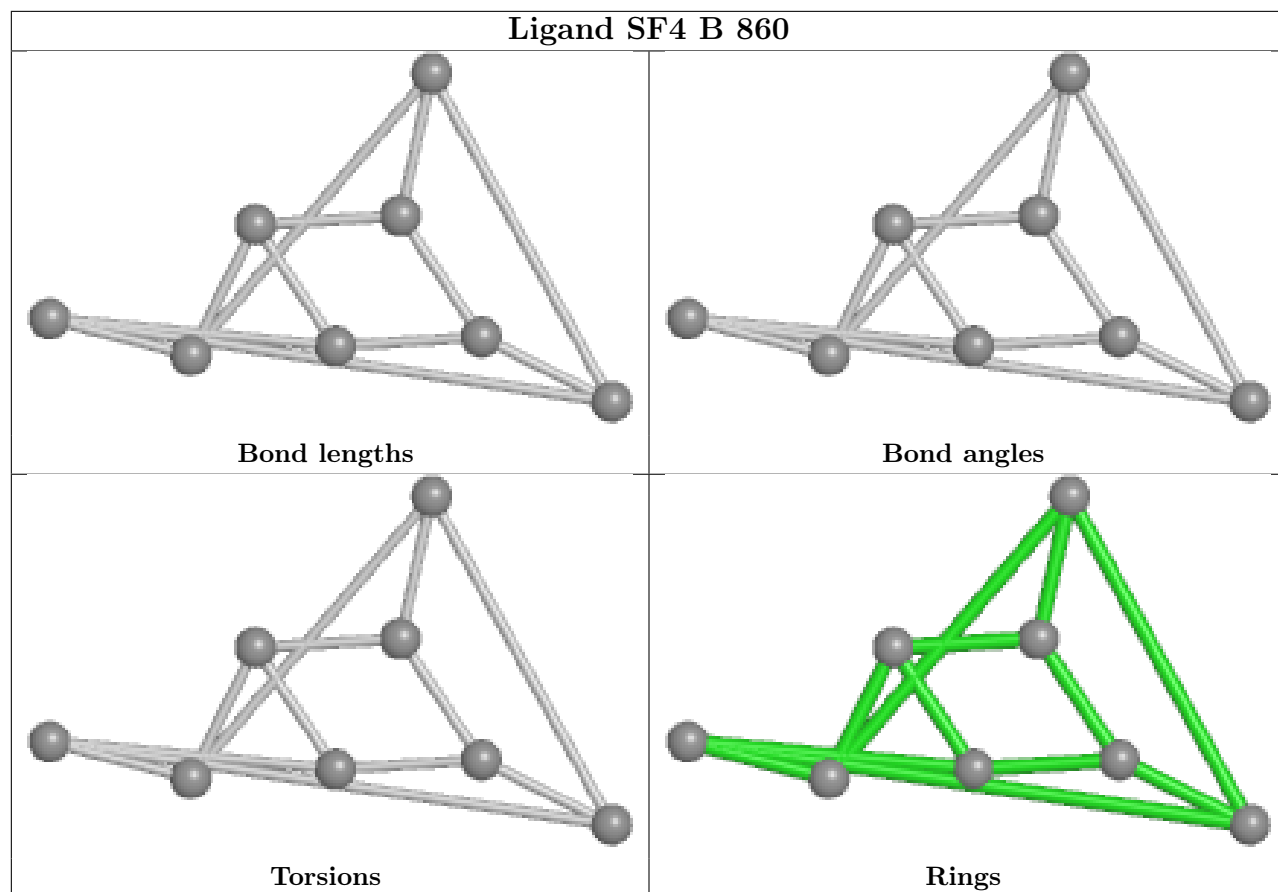


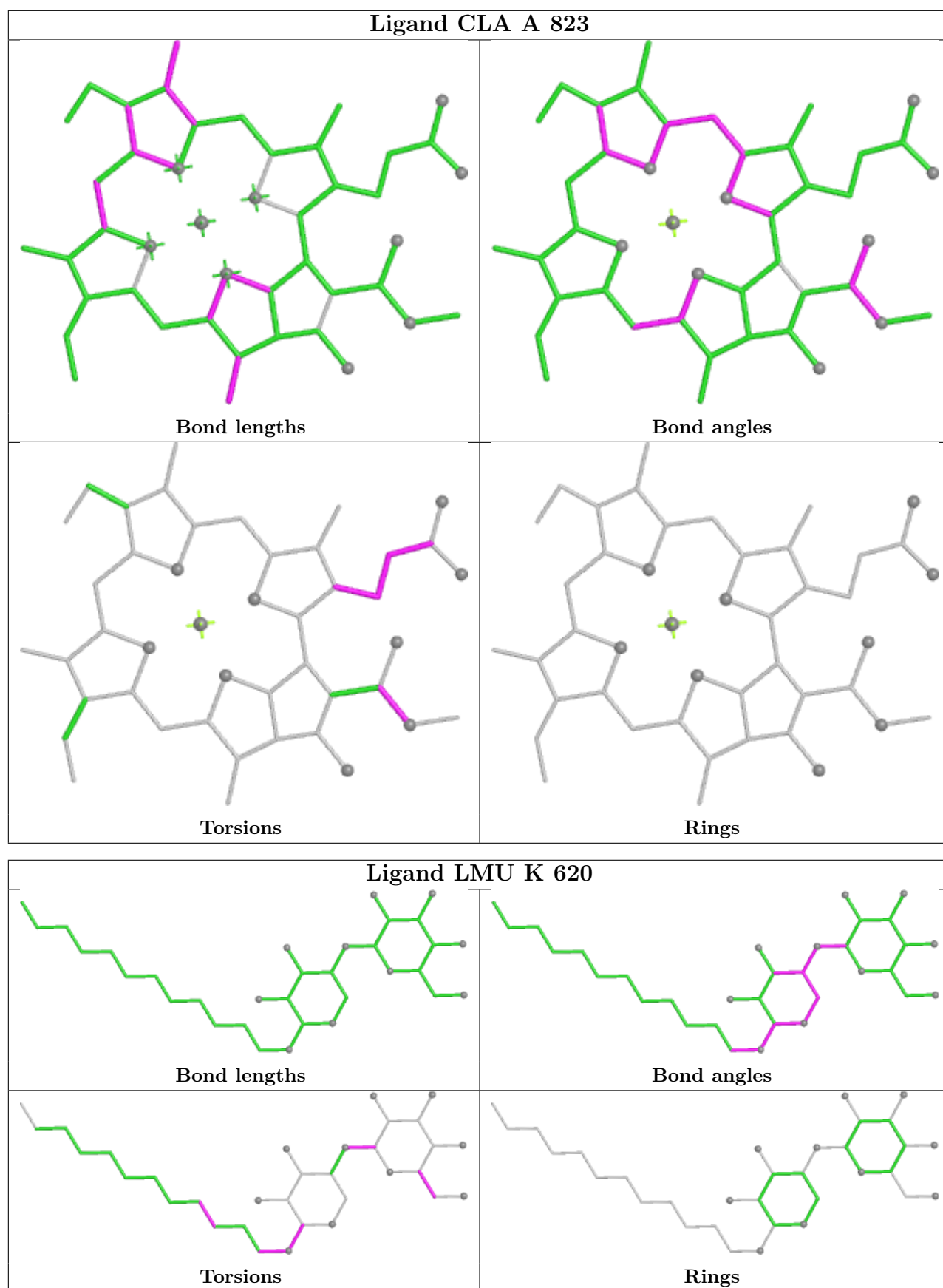


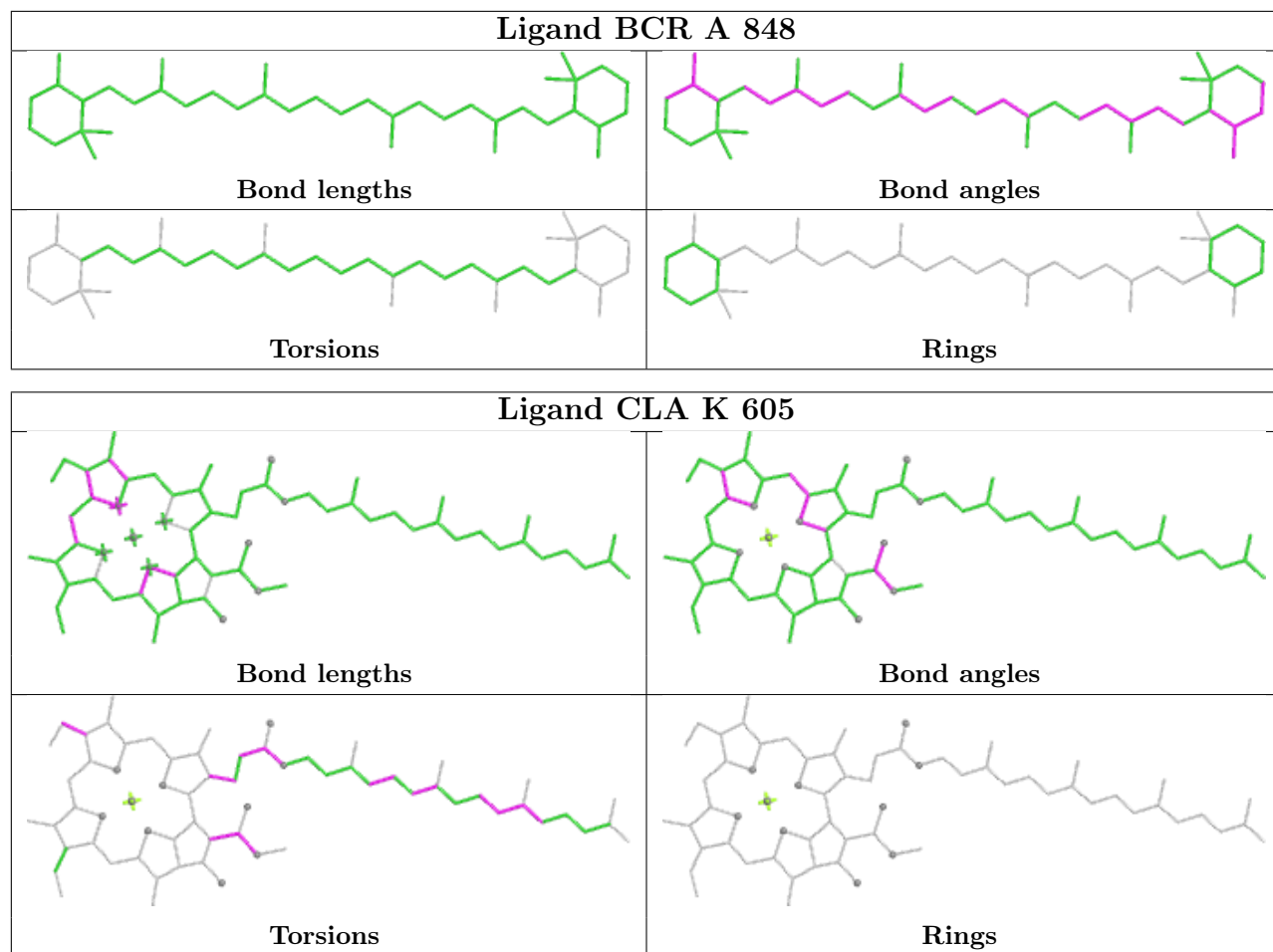


Ligand CLA I 605

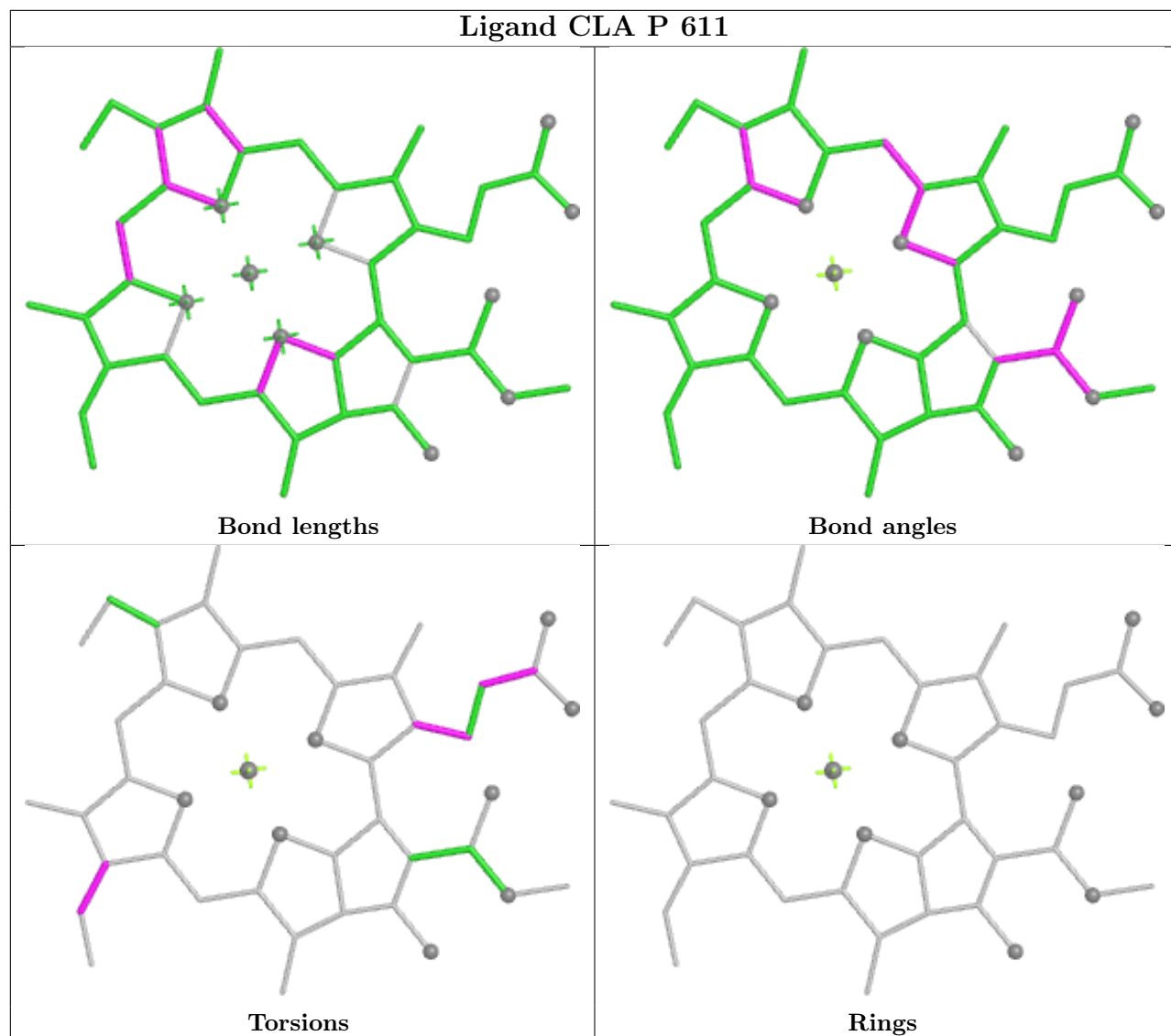




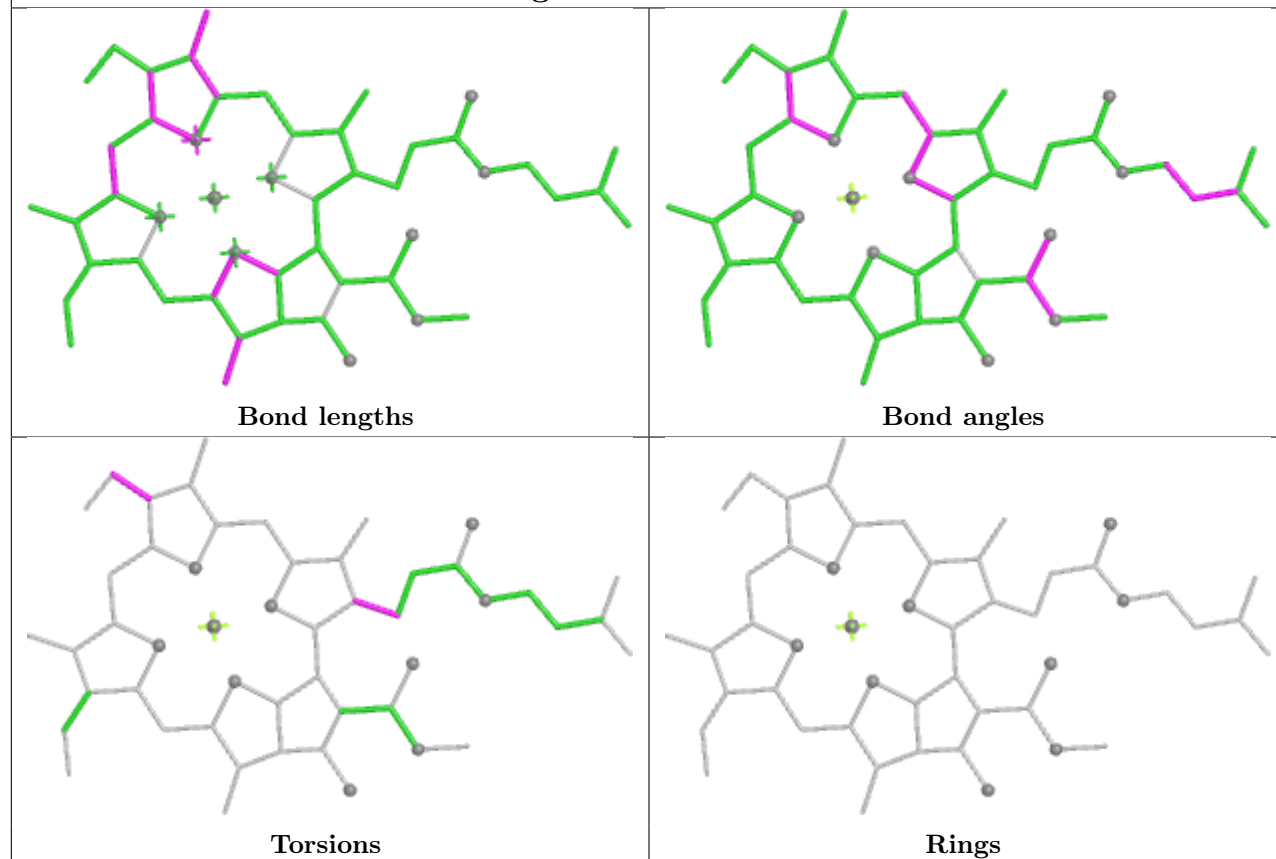




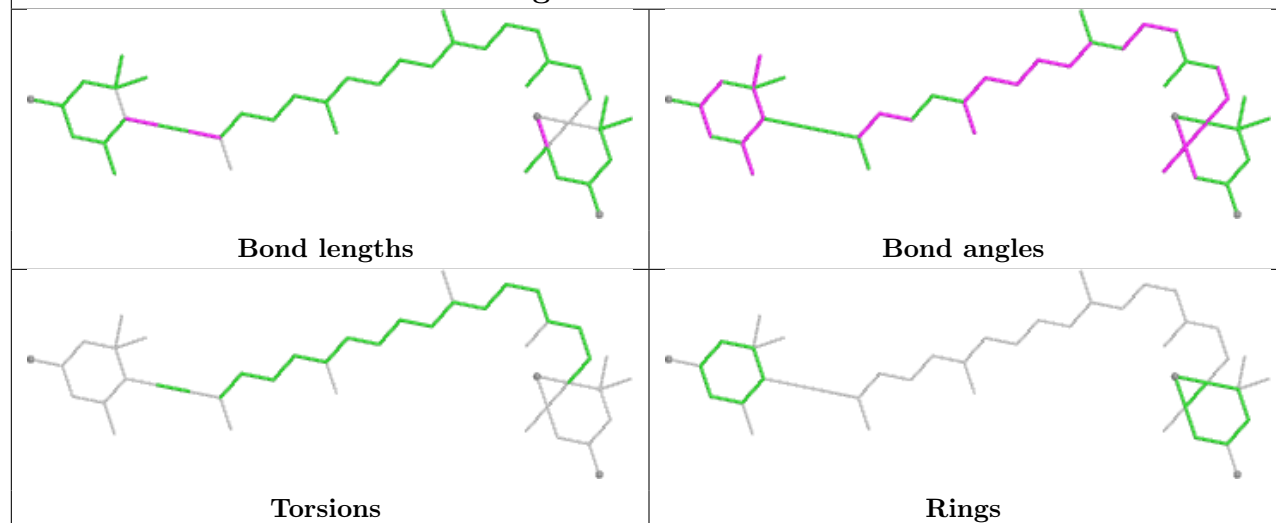
Ligand CLA P 611

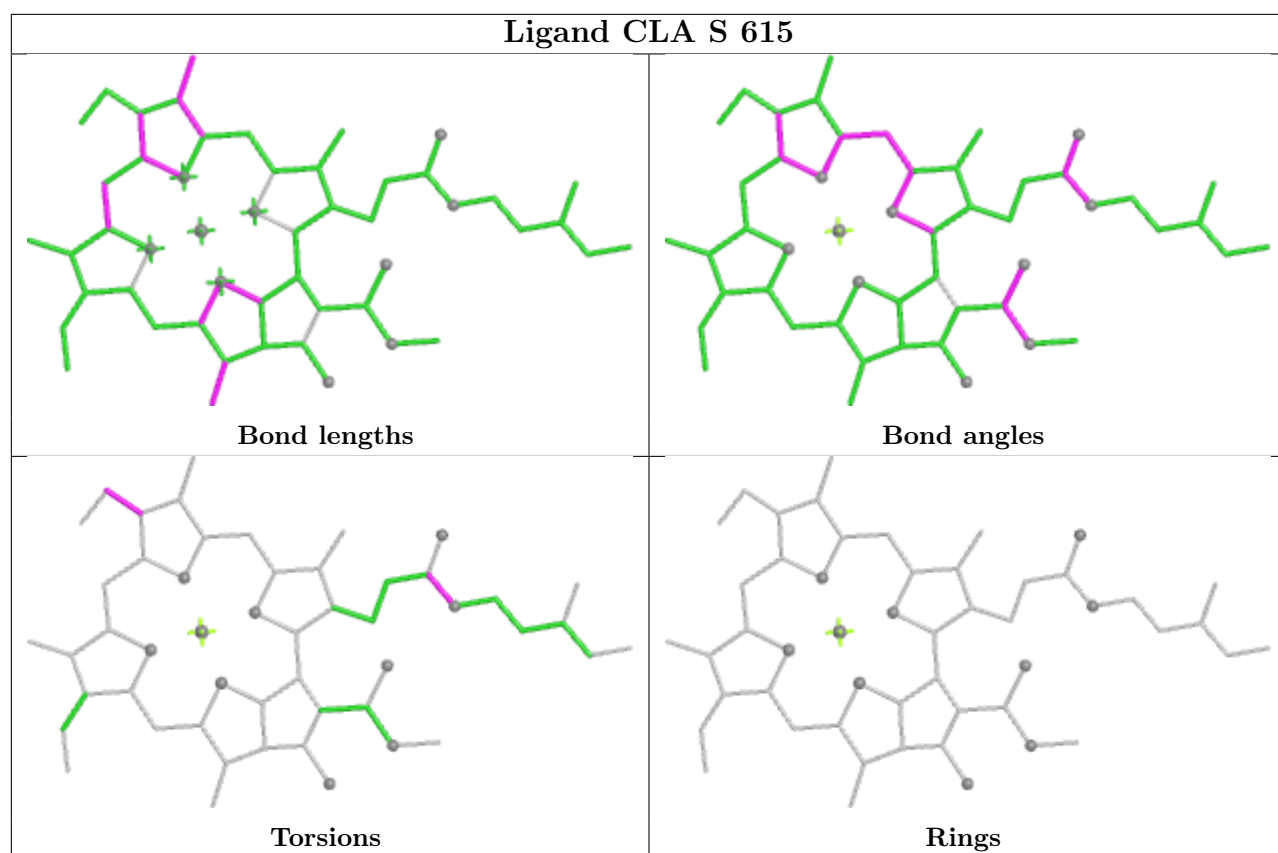


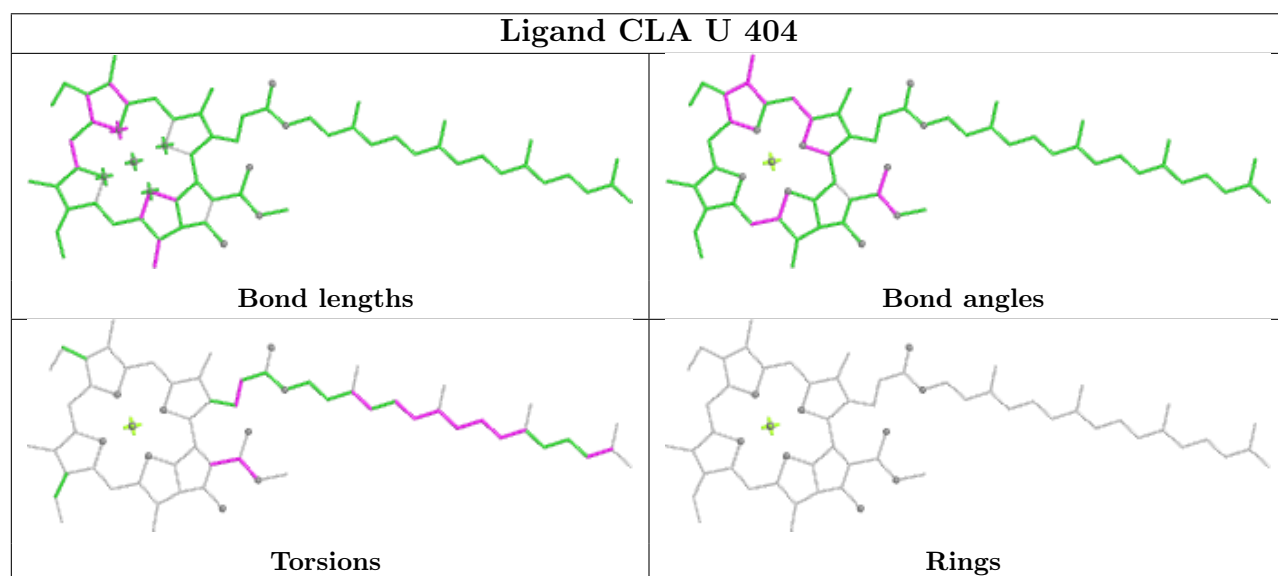
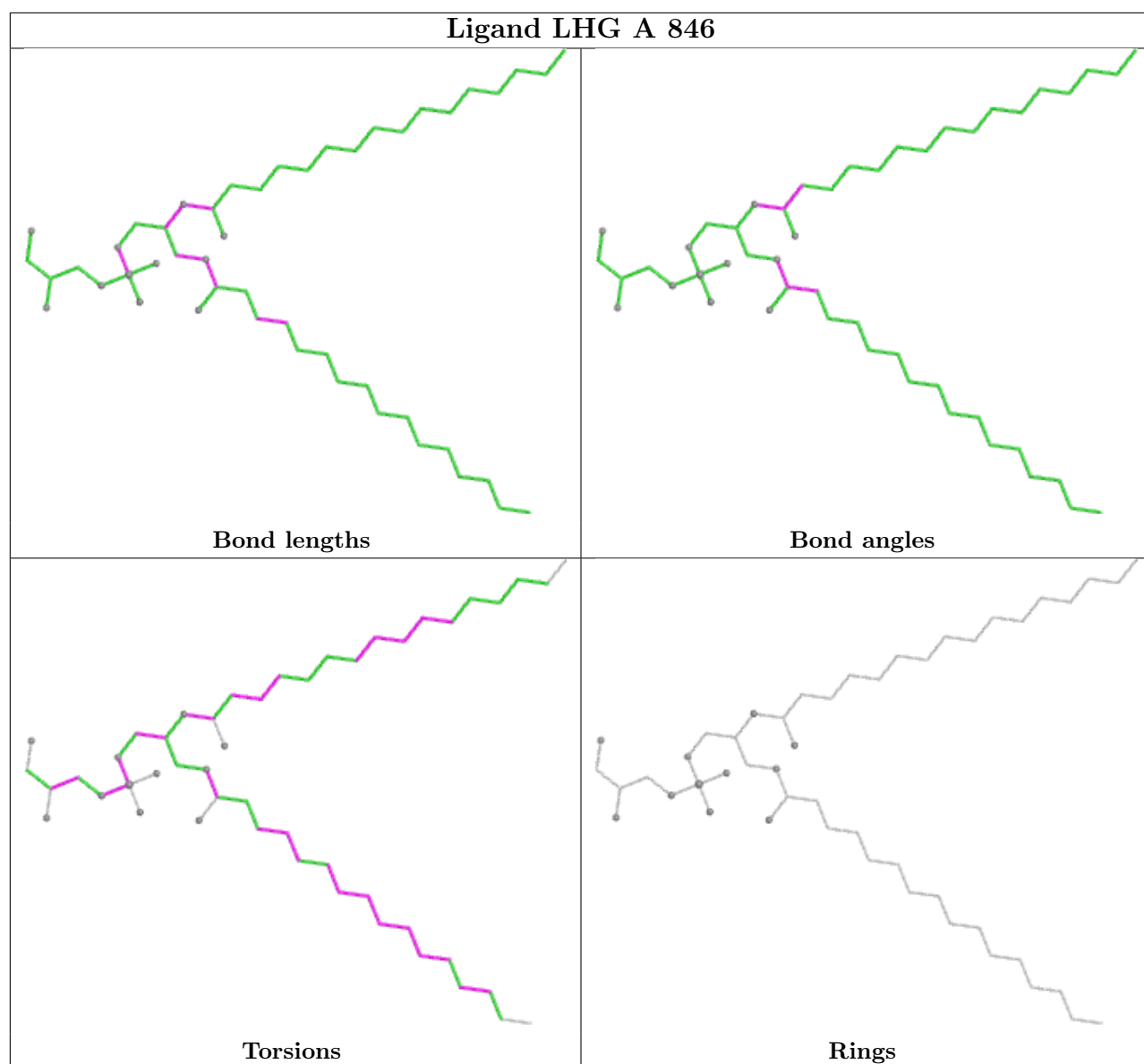
Ligand CLA O 309

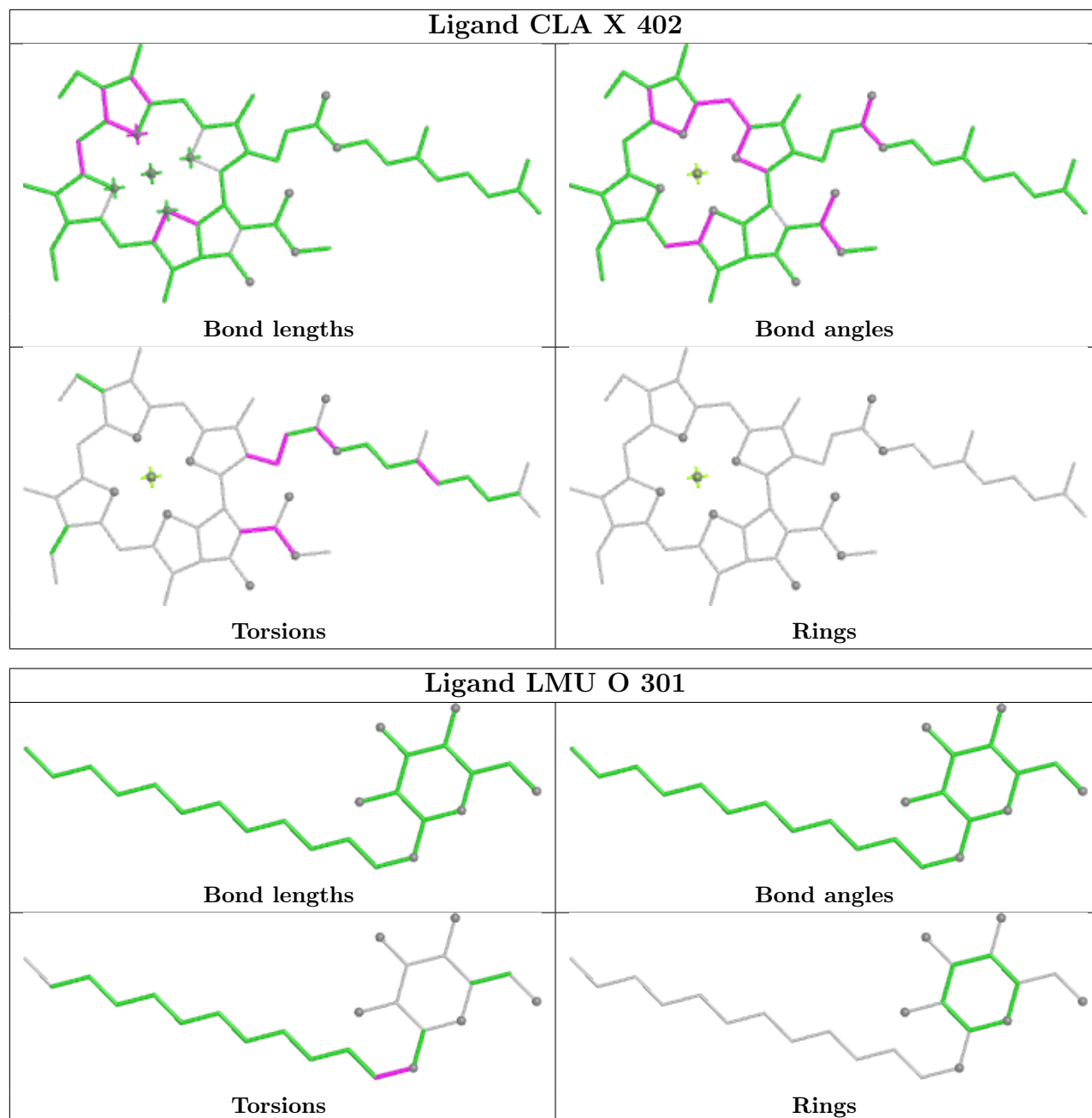


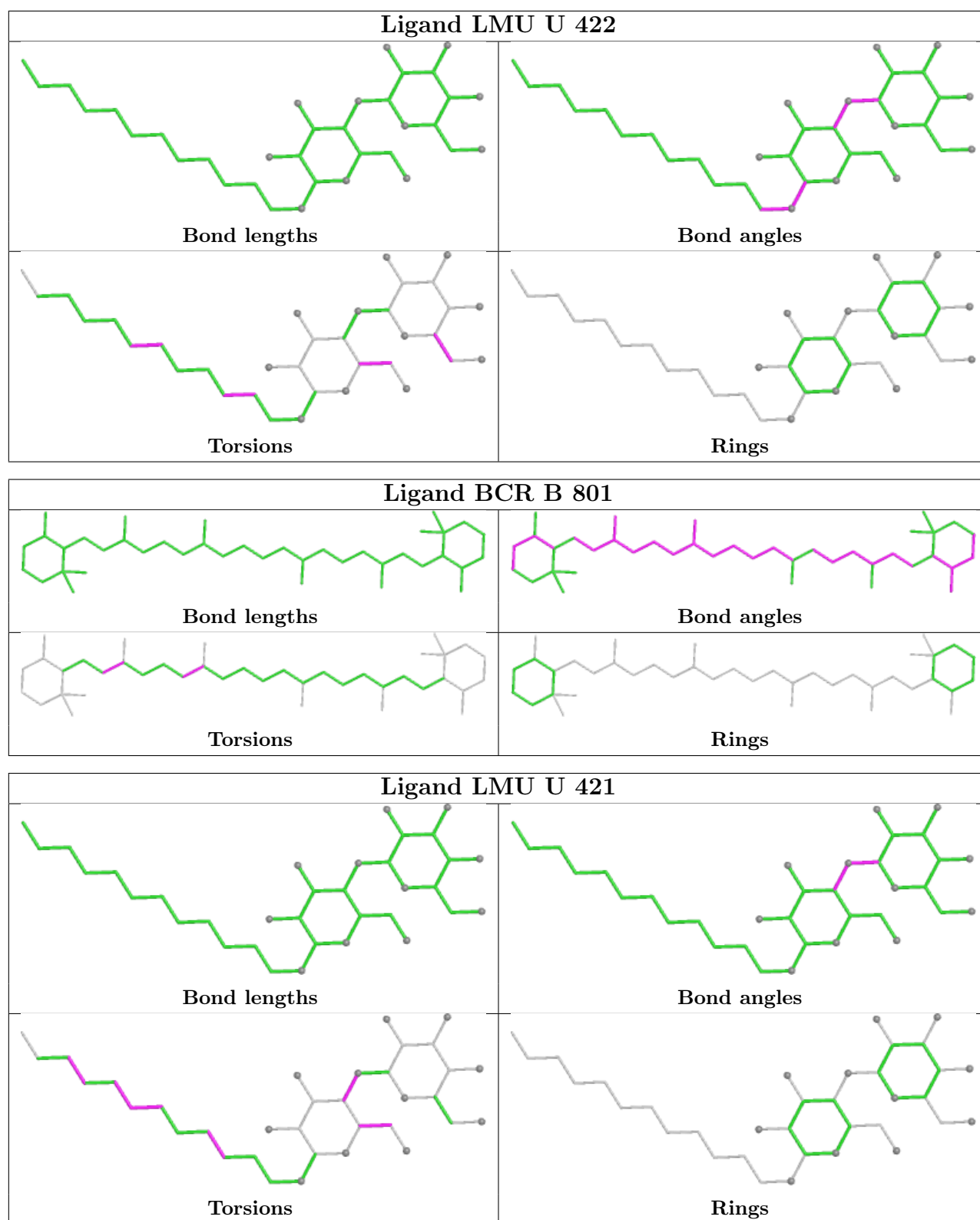
Ligand DD6 O 317

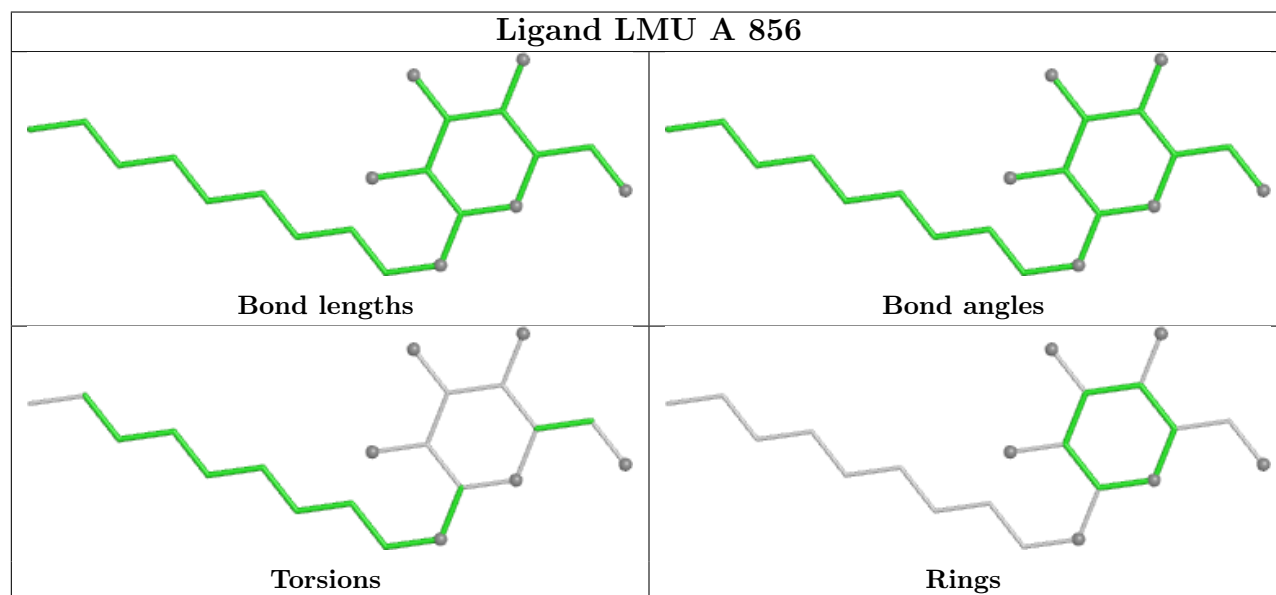
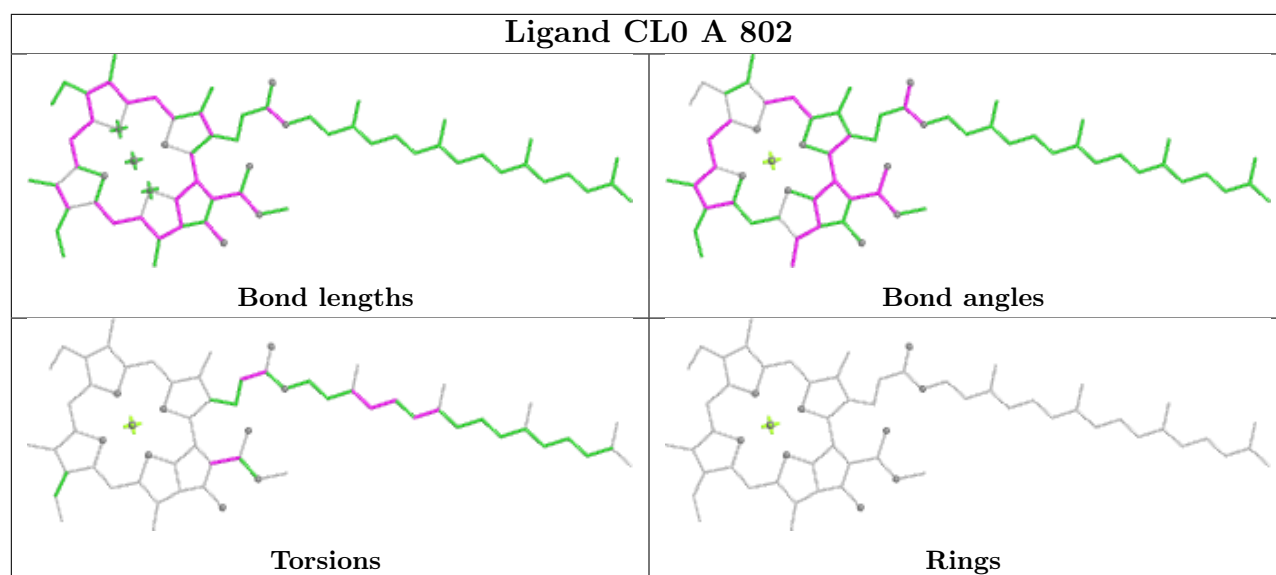


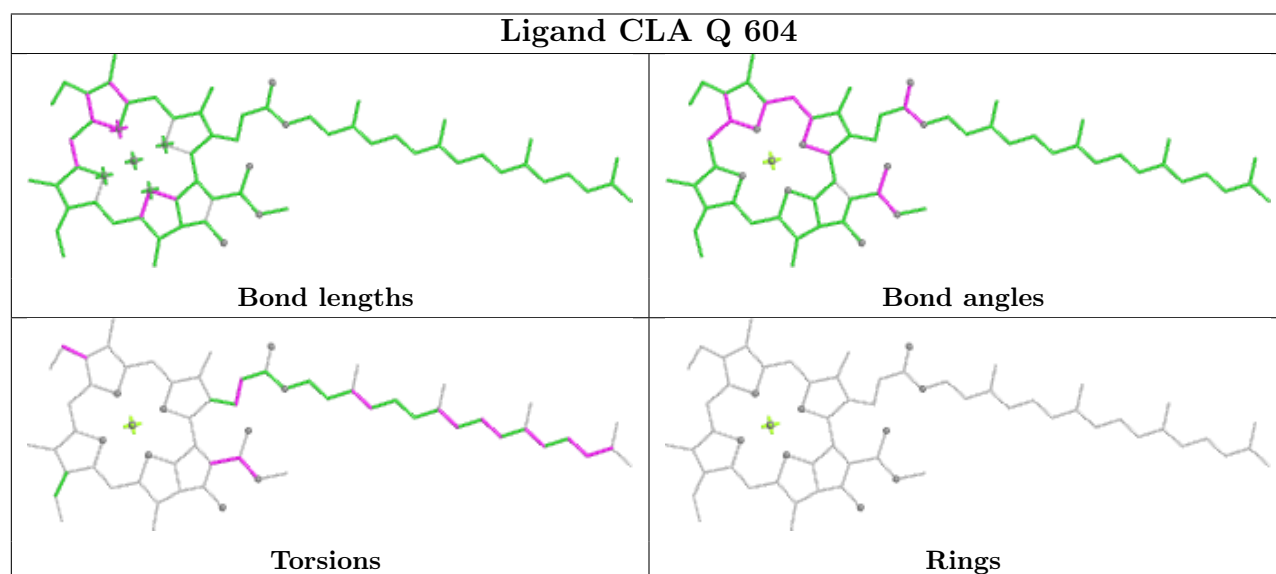
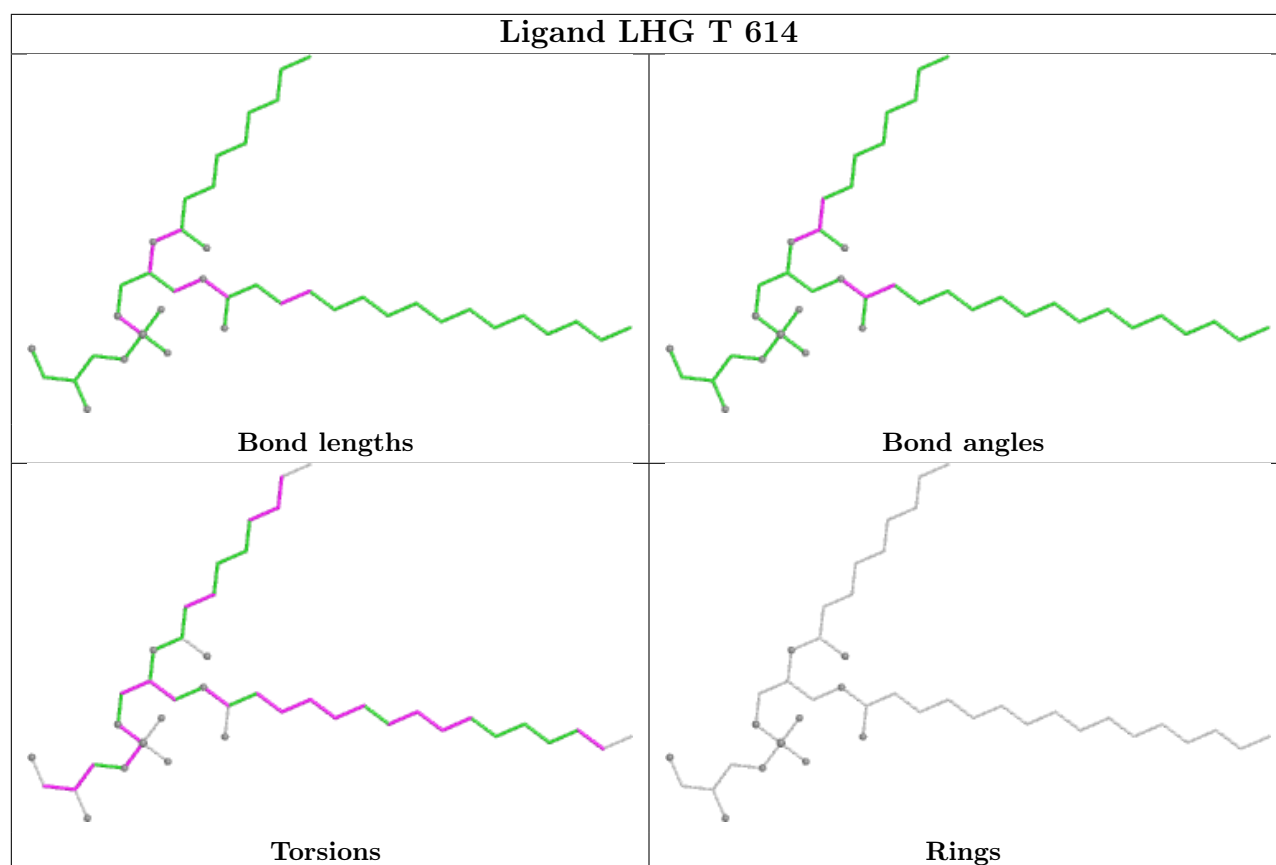


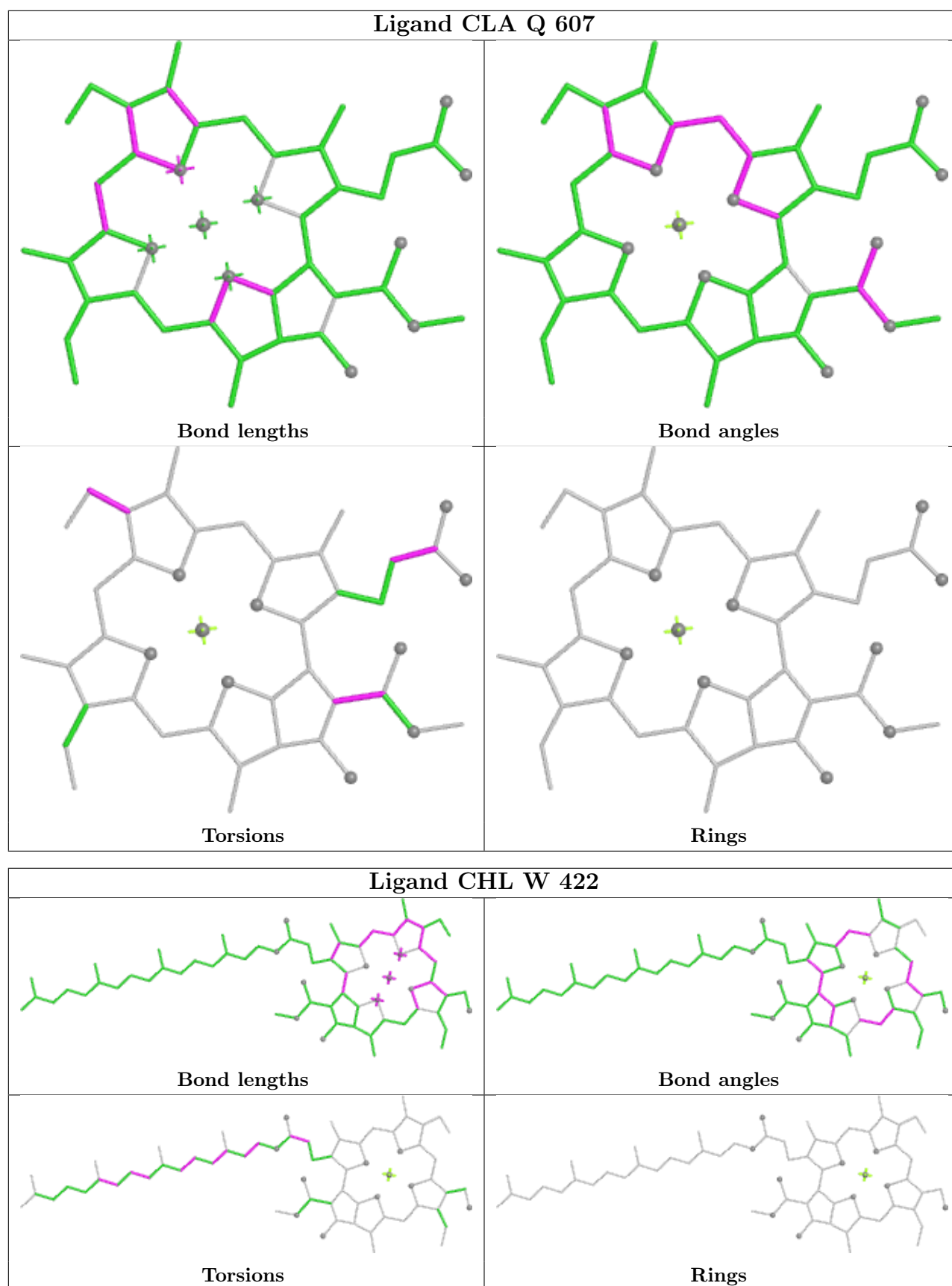


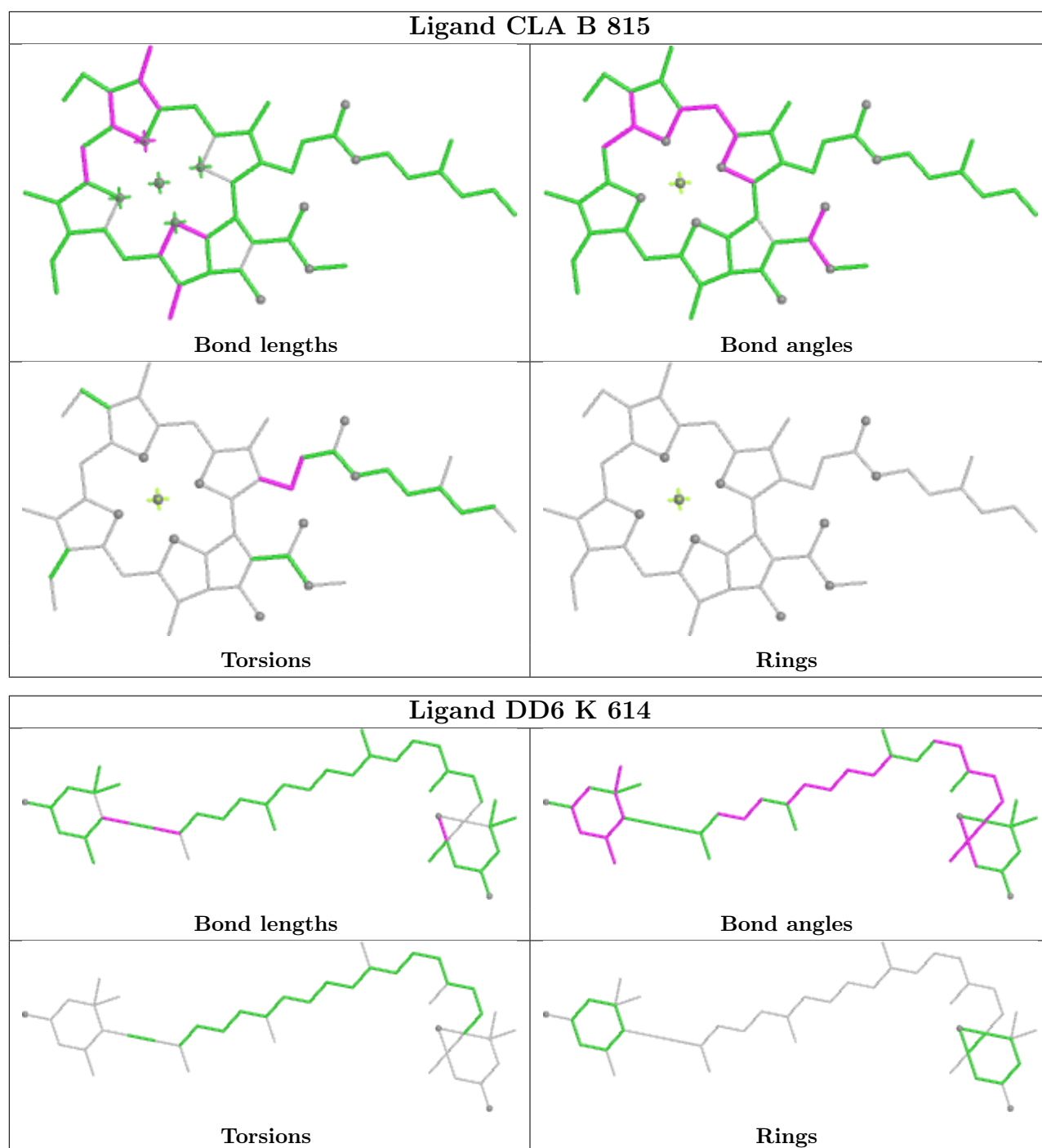


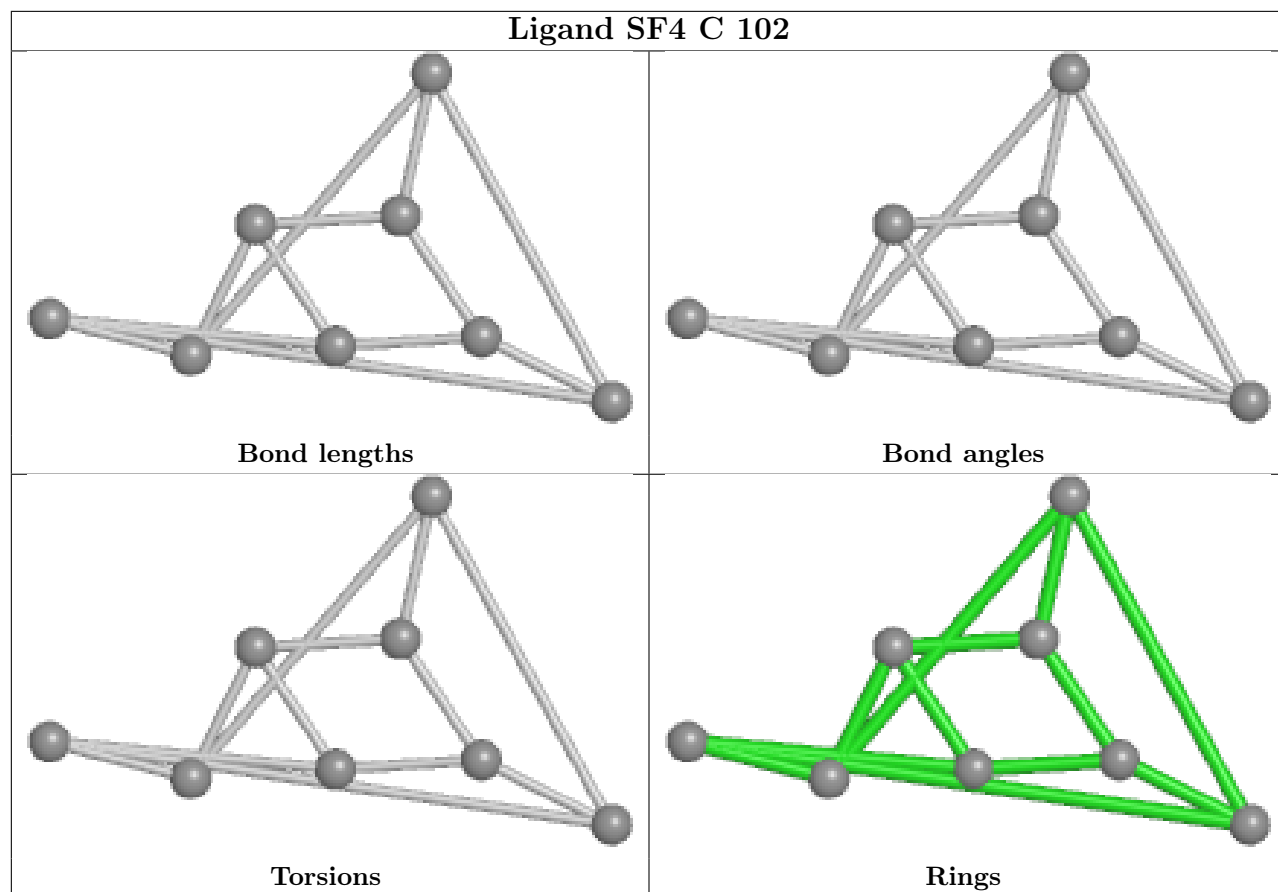




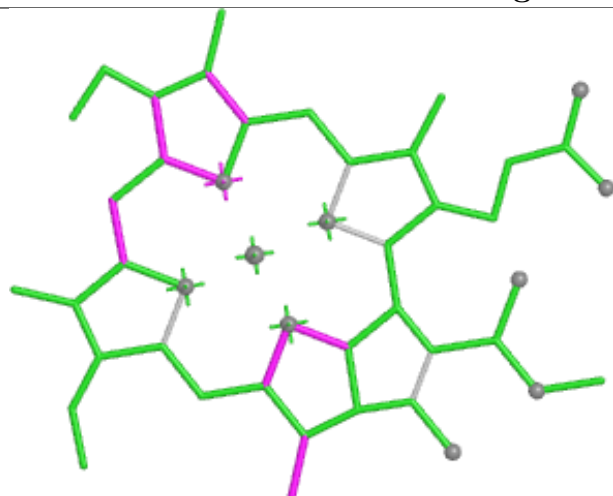




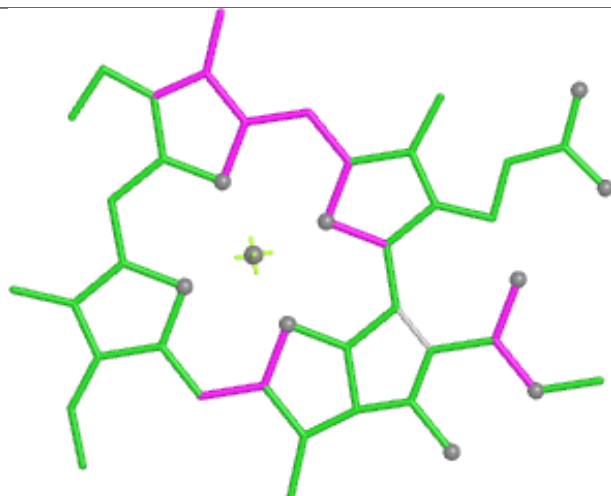




Ligand CLA H 304



Bond lengths



Bond angles

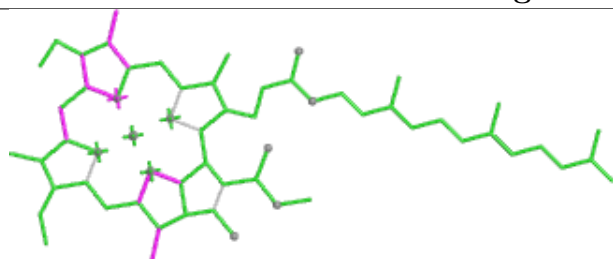


Torsions

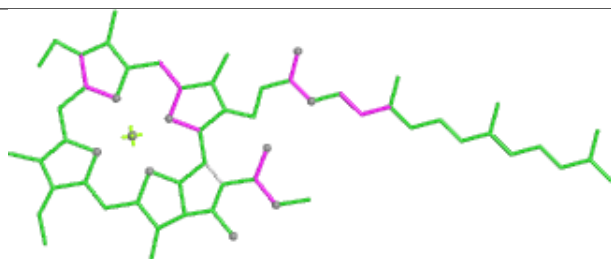


Rings

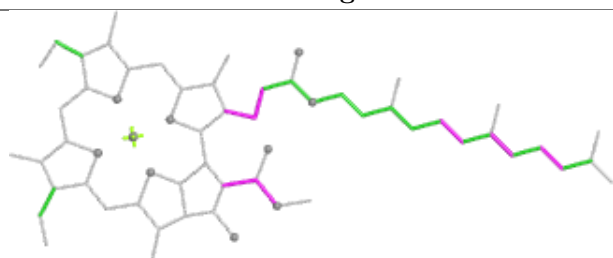
Ligand CLA O 310



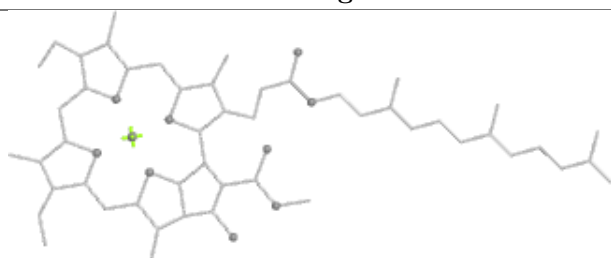
Bond lengths



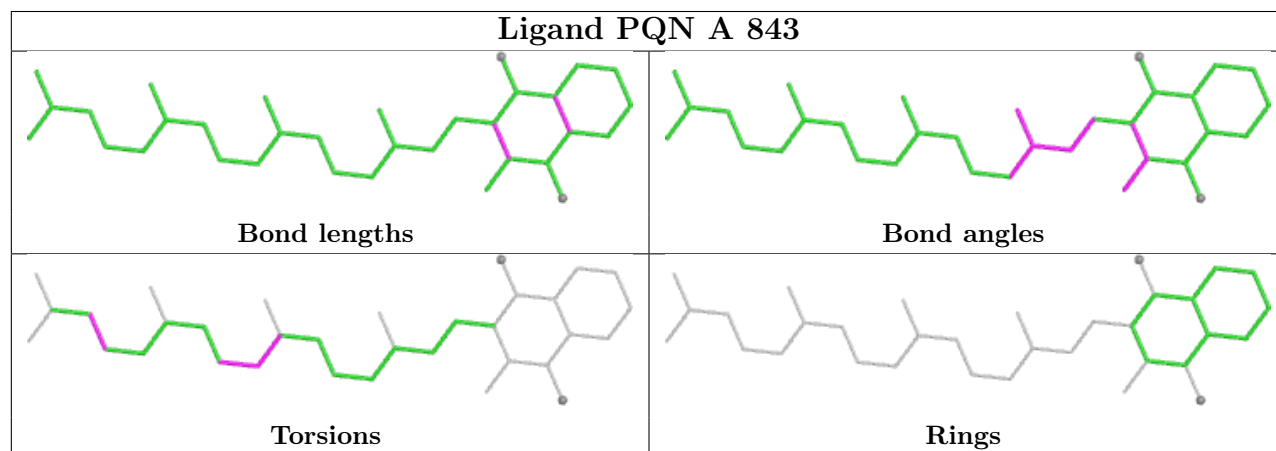
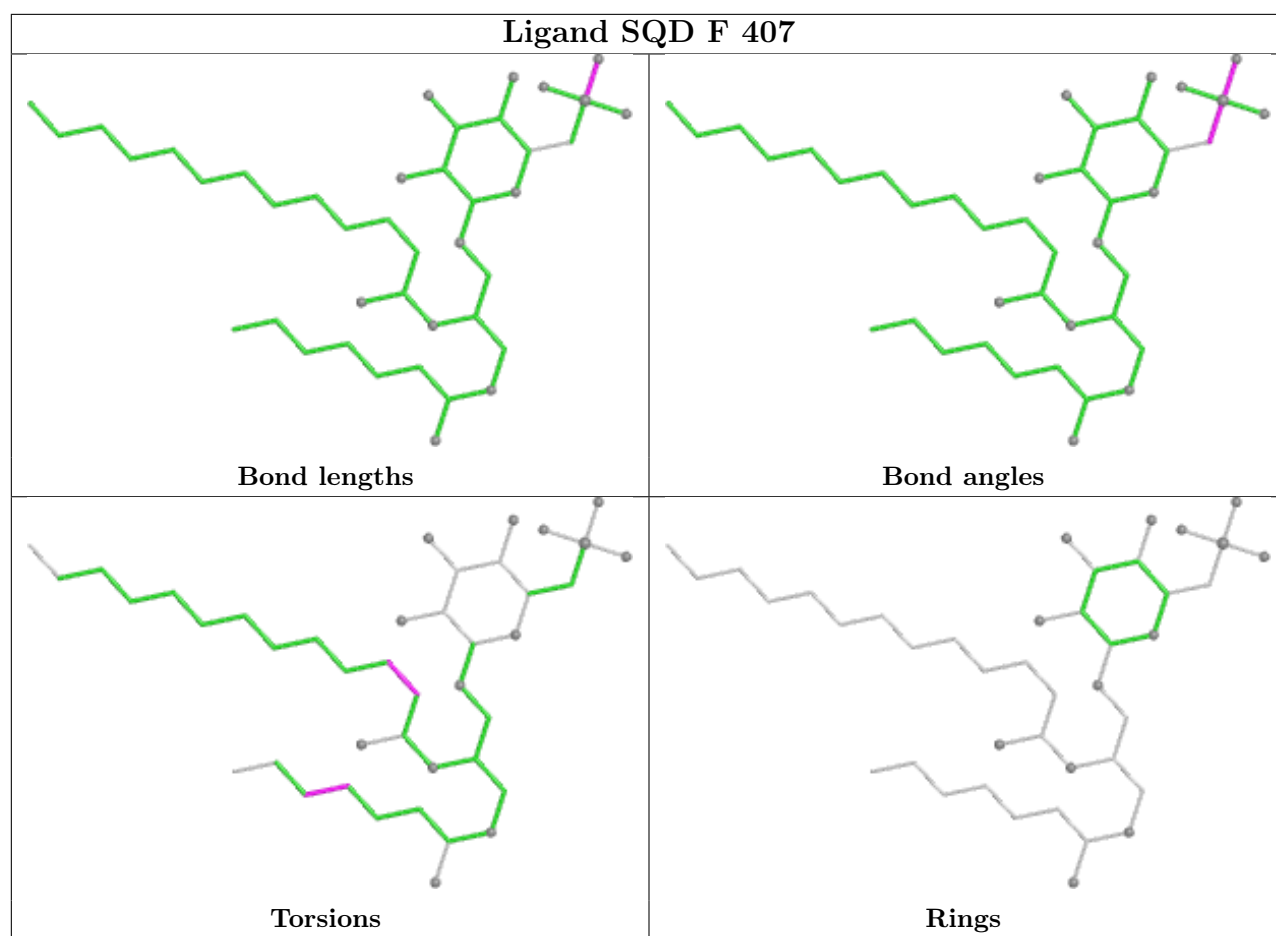
Bond angles

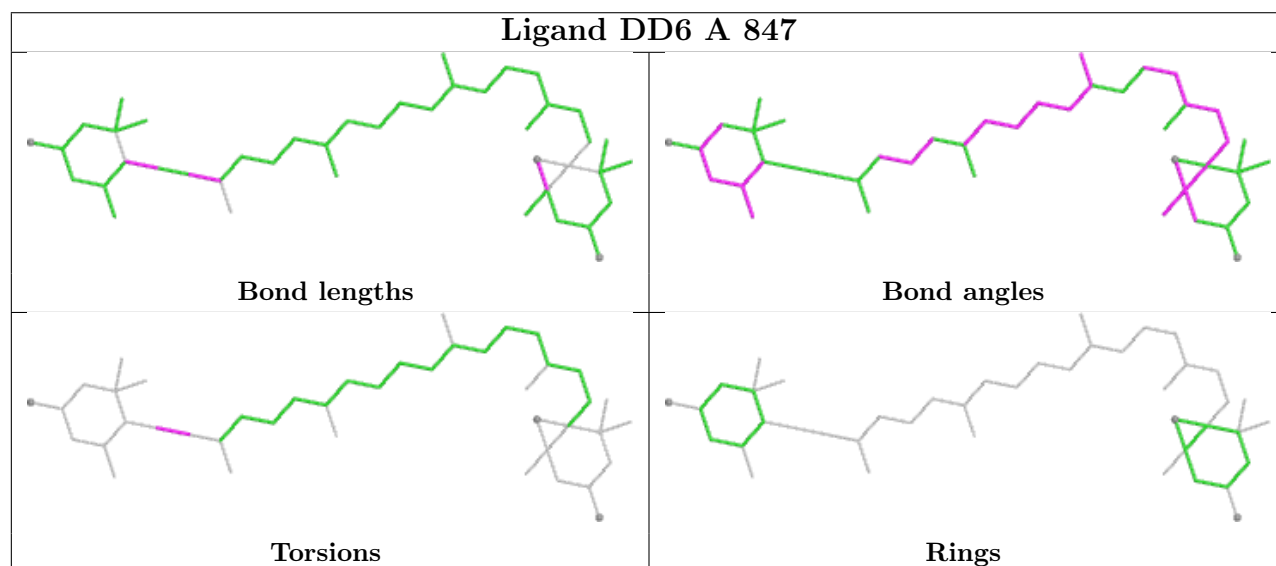
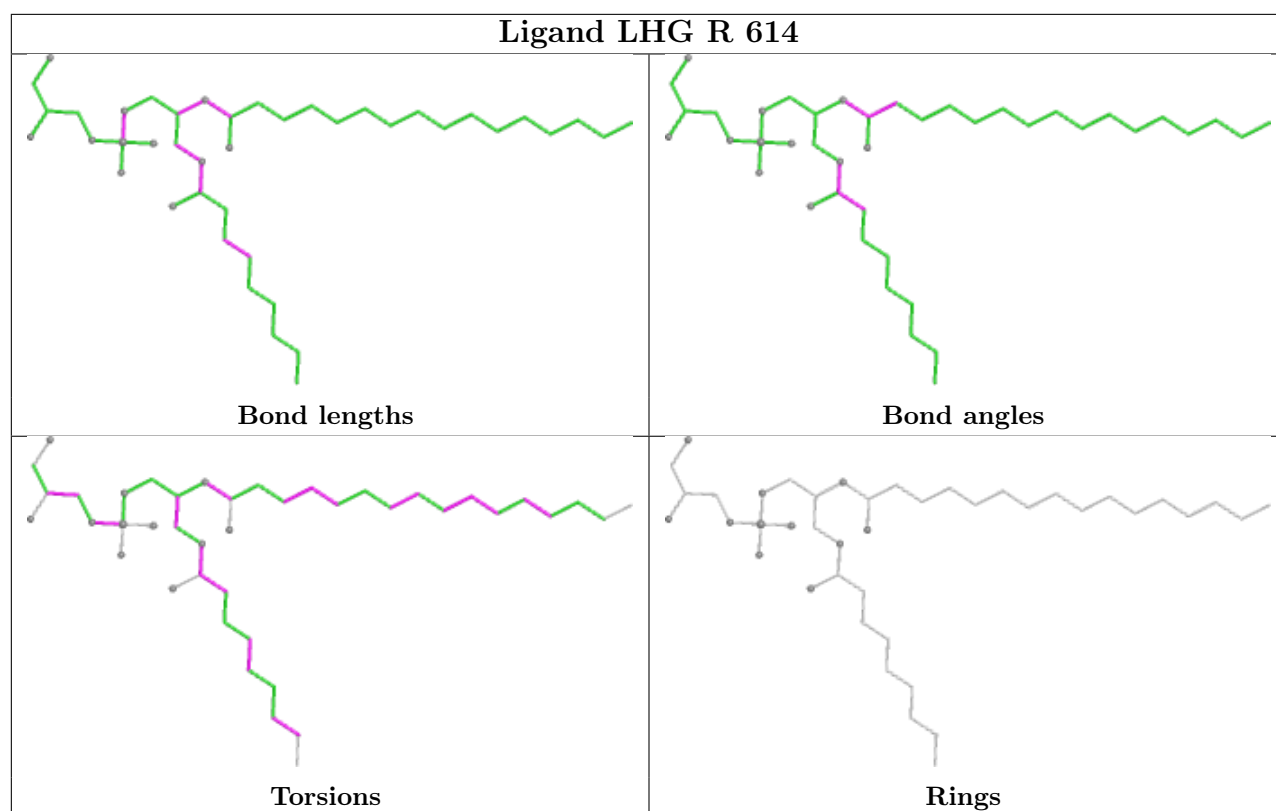


Torsions

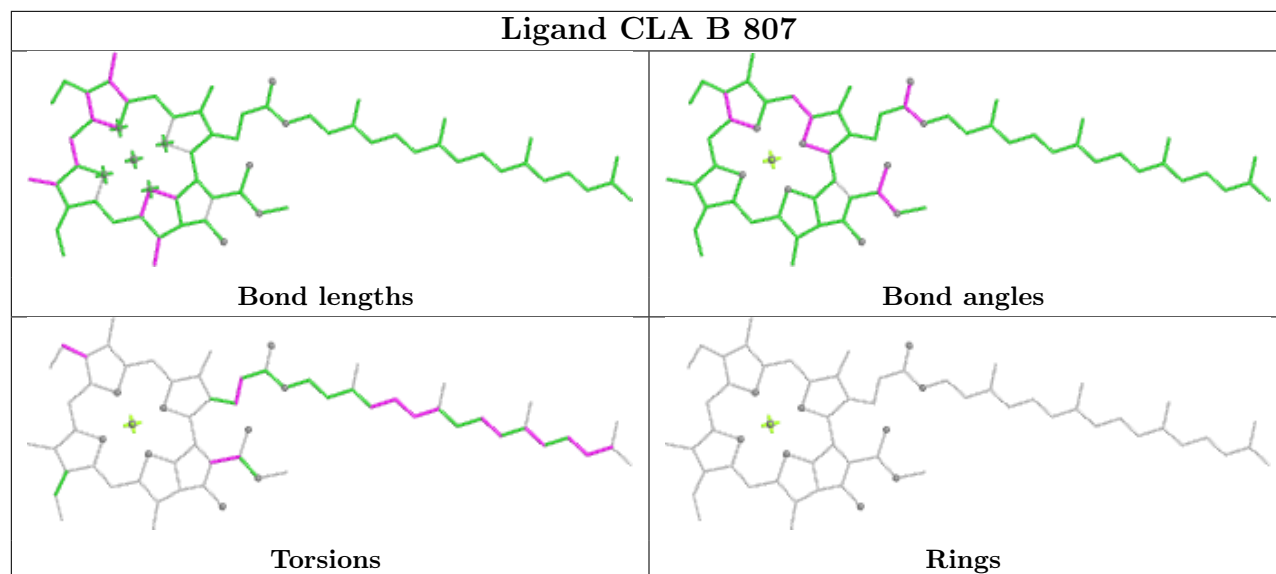


Rings

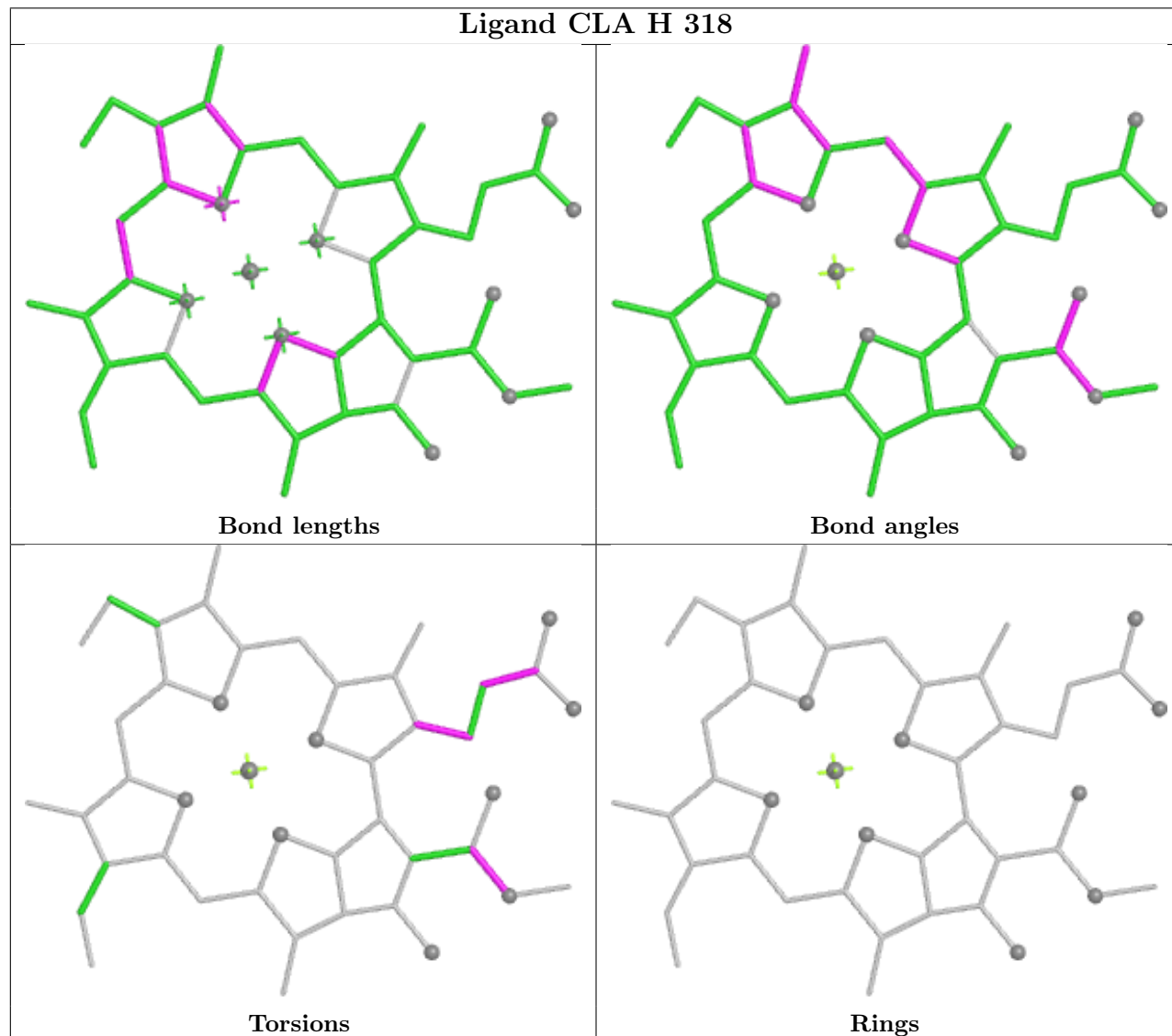


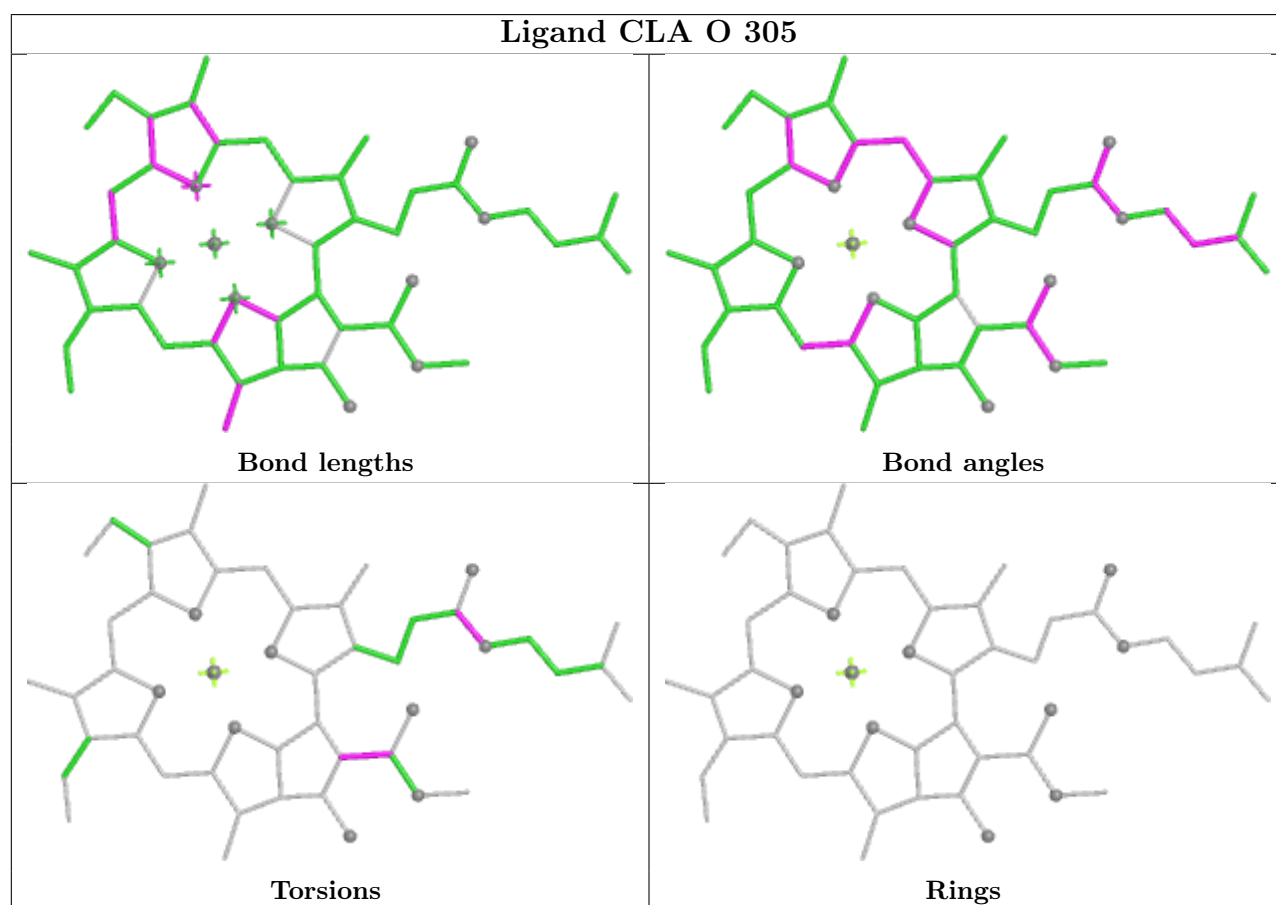
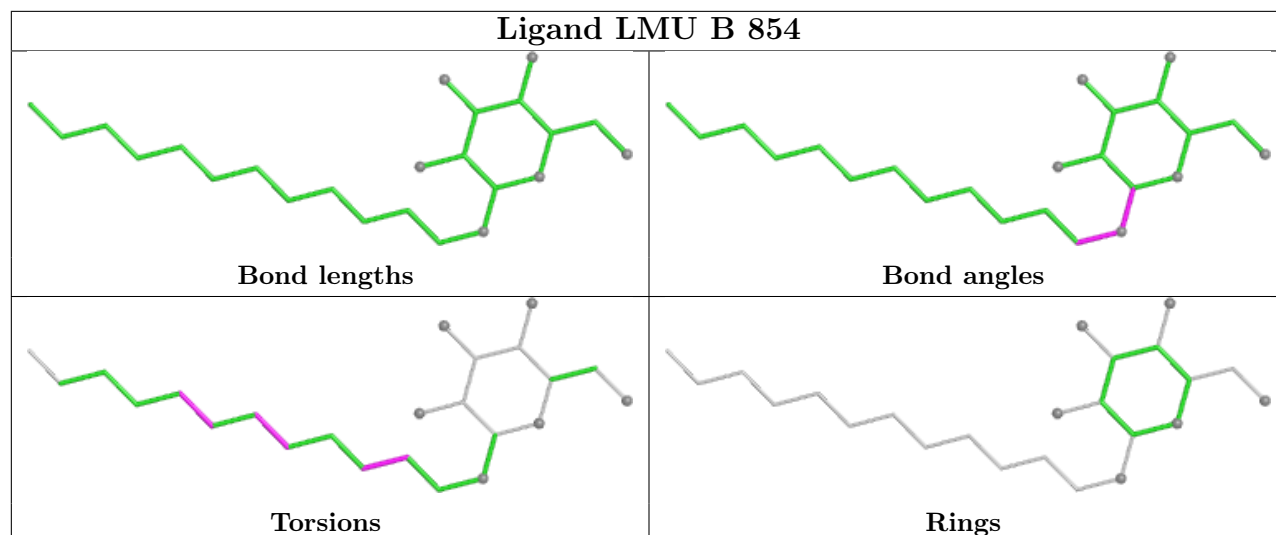


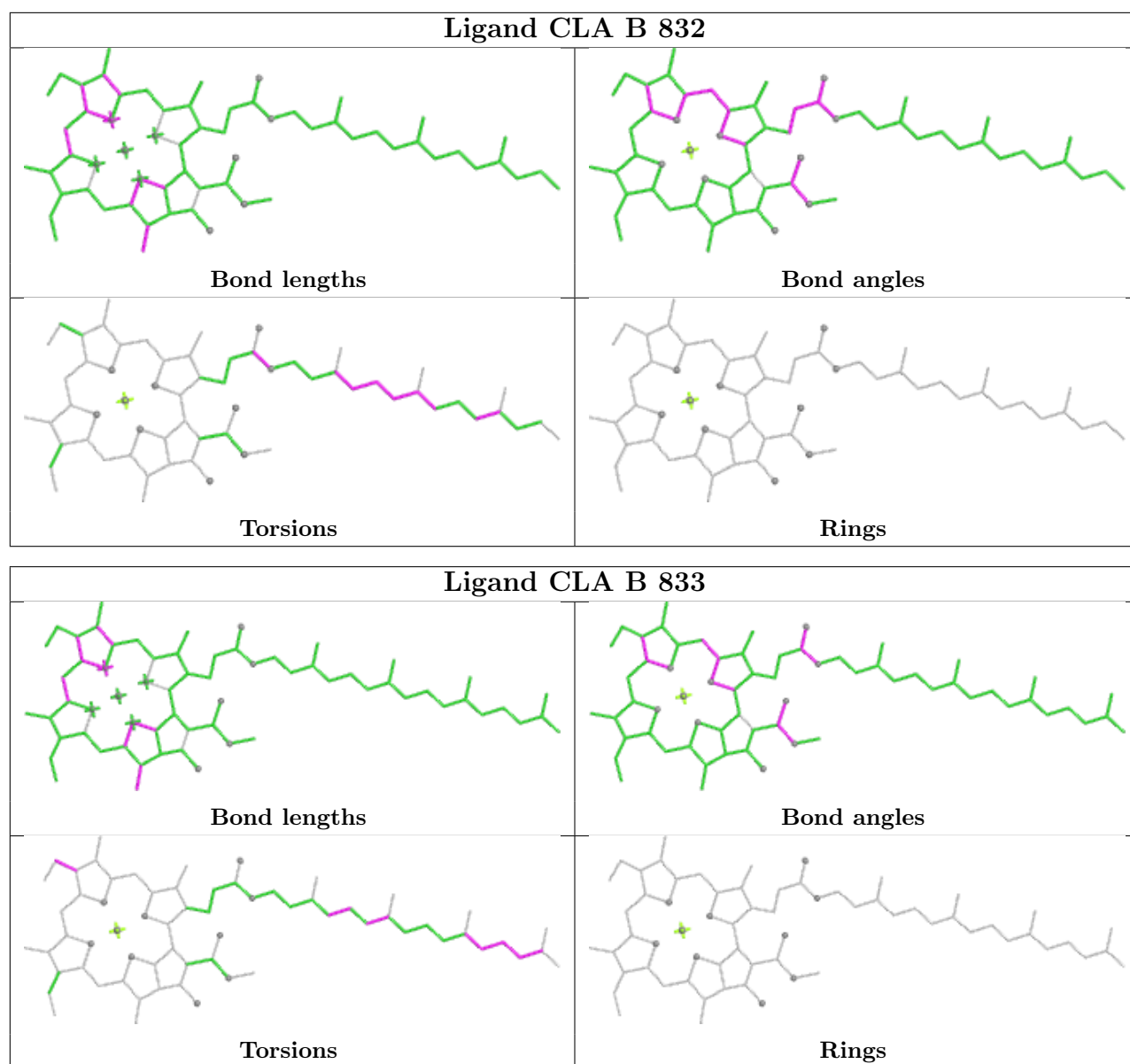
Ligand CLA B 807

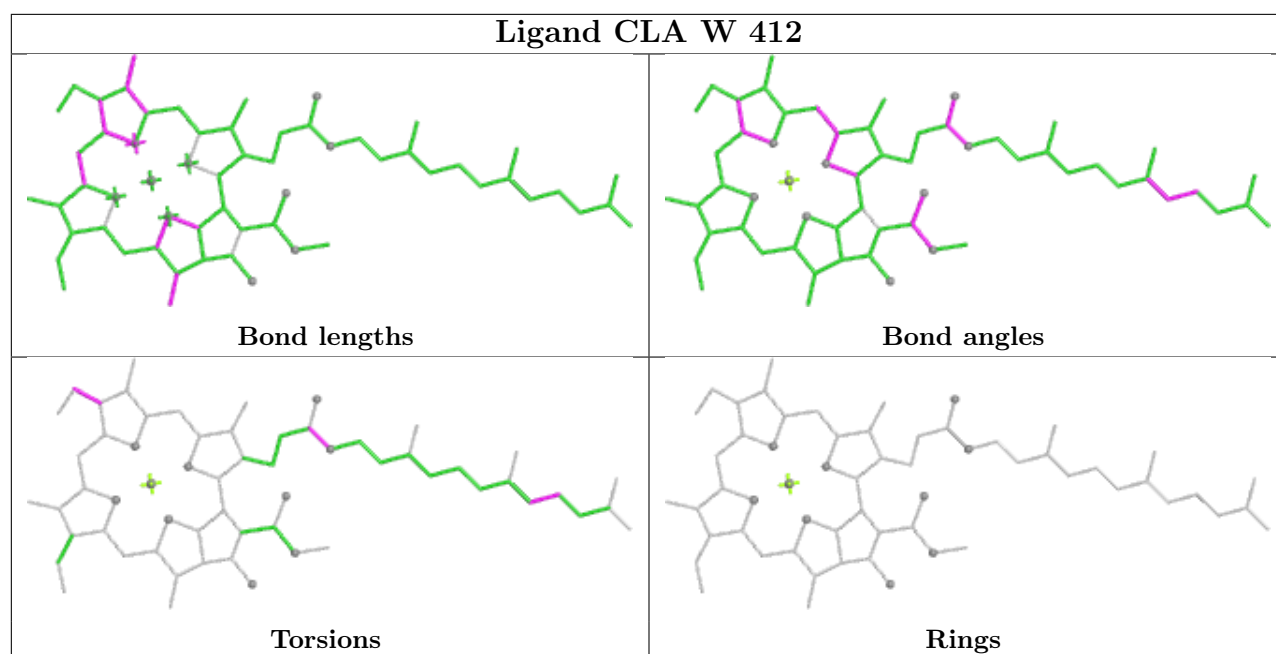


Ligand CLA H 318









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.

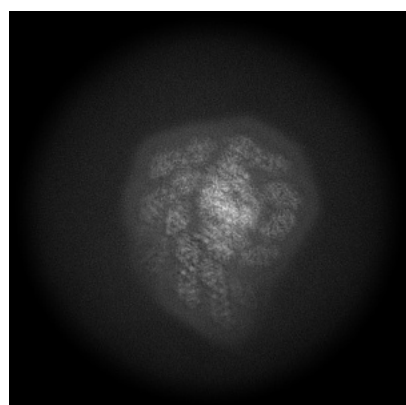
6 Map visualisation [i](#)

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.

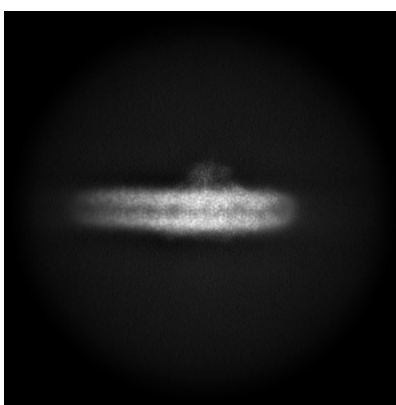
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

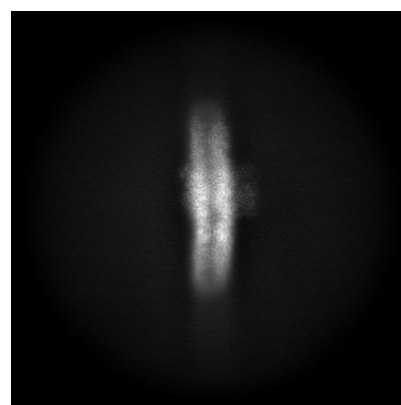
6.1.1 Primary map



X



Y

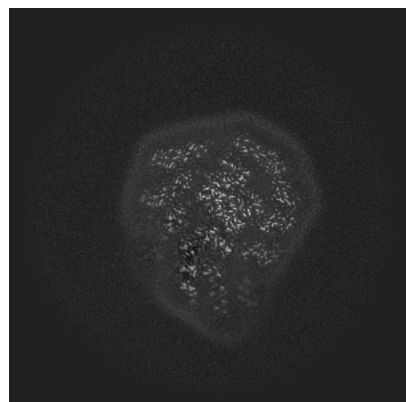


Z

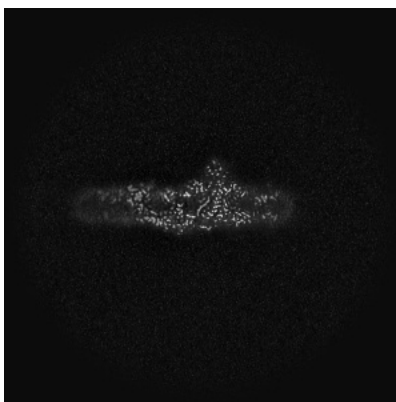
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

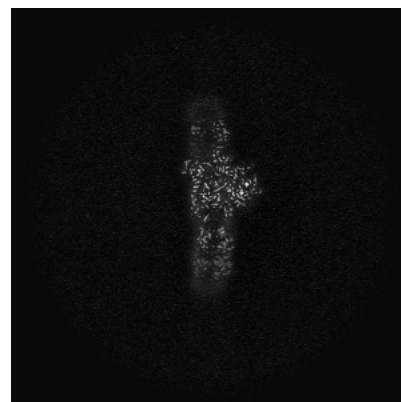
6.2.1 Primary map



X Index: 256



Y Index: 256

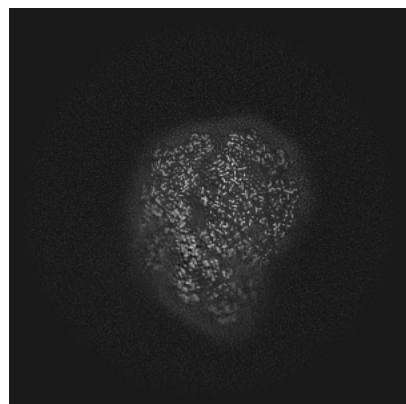


Z Index: 256

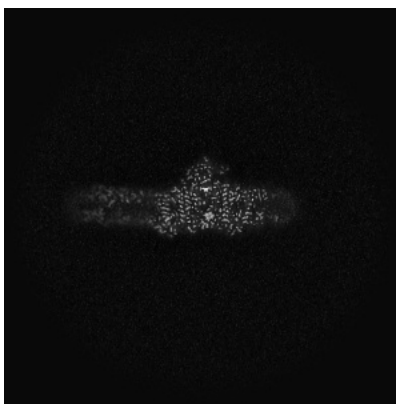
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

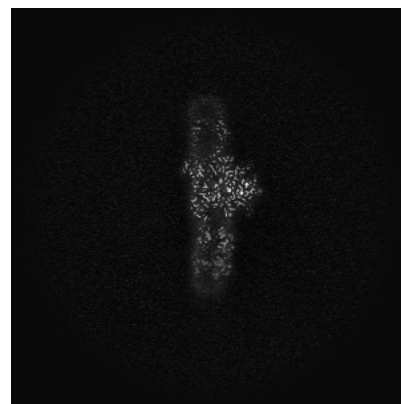
6.3.1 Primary map



X Index: 270



Y Index: 278

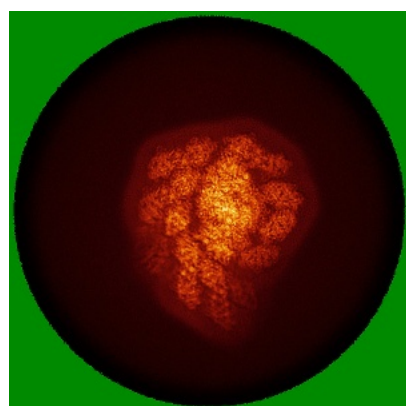


Z Index: 257

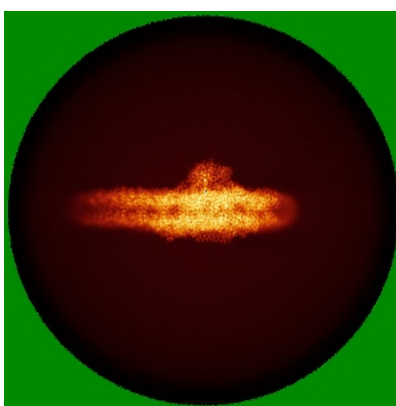
The images above show the largest variance slices of the map in three orthogonal directions.

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.

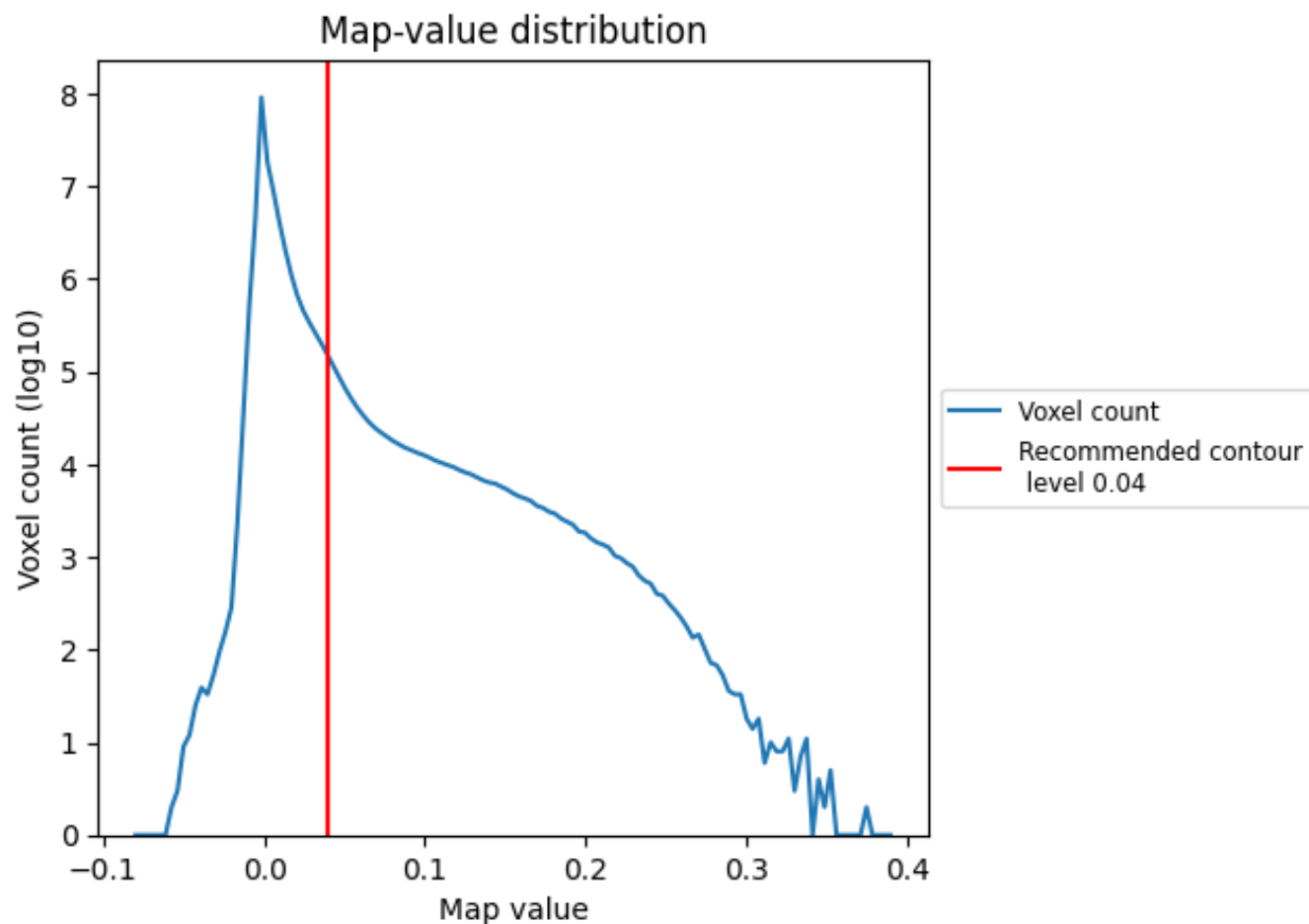
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

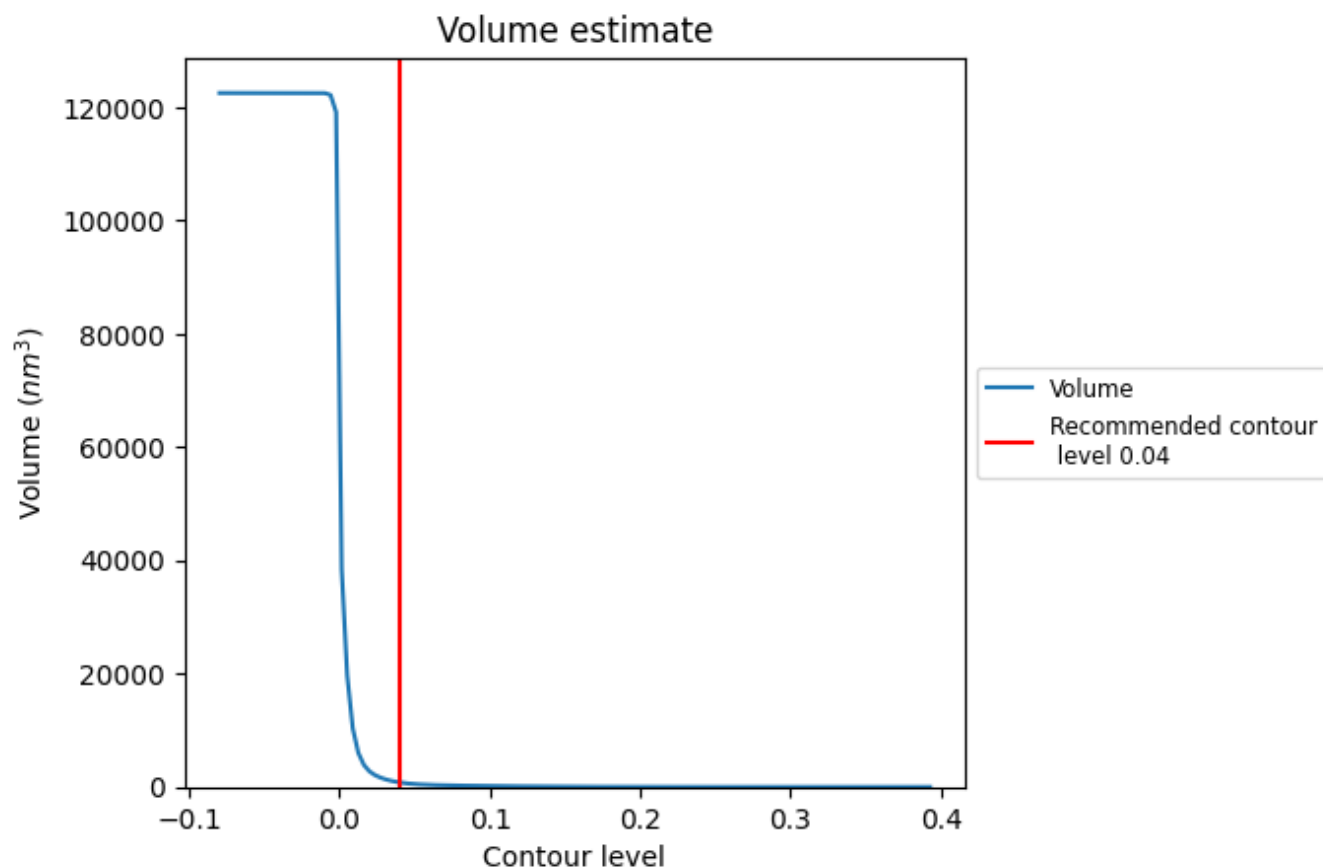
This section contains the results of statistical analysis of the map.

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.

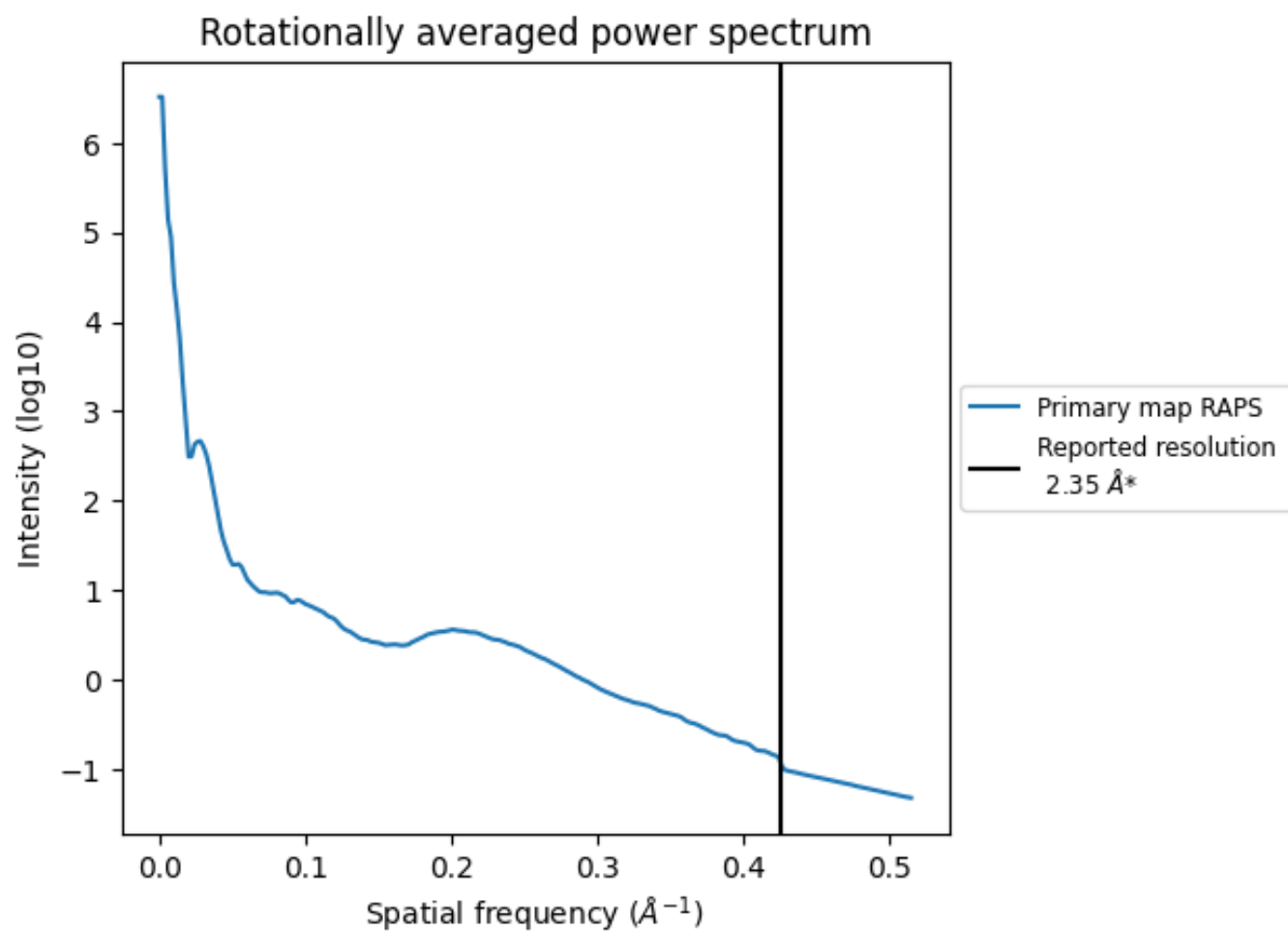
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 801 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 ⓘ

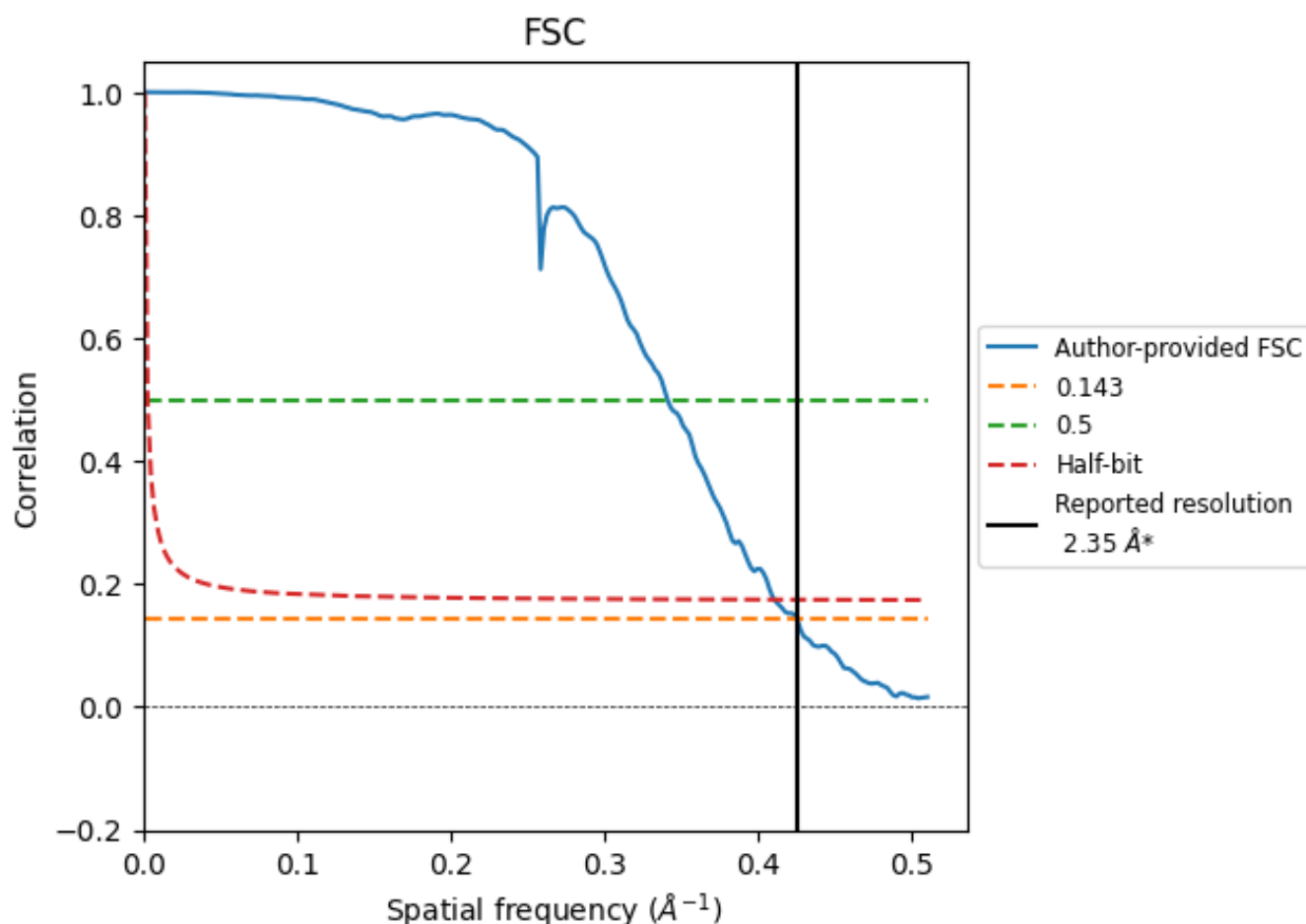


*Reported resolution corresponds to spatial frequency of 0.426 Å⁻¹

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⁻¹

8.2 Resolution estimates [i](#)

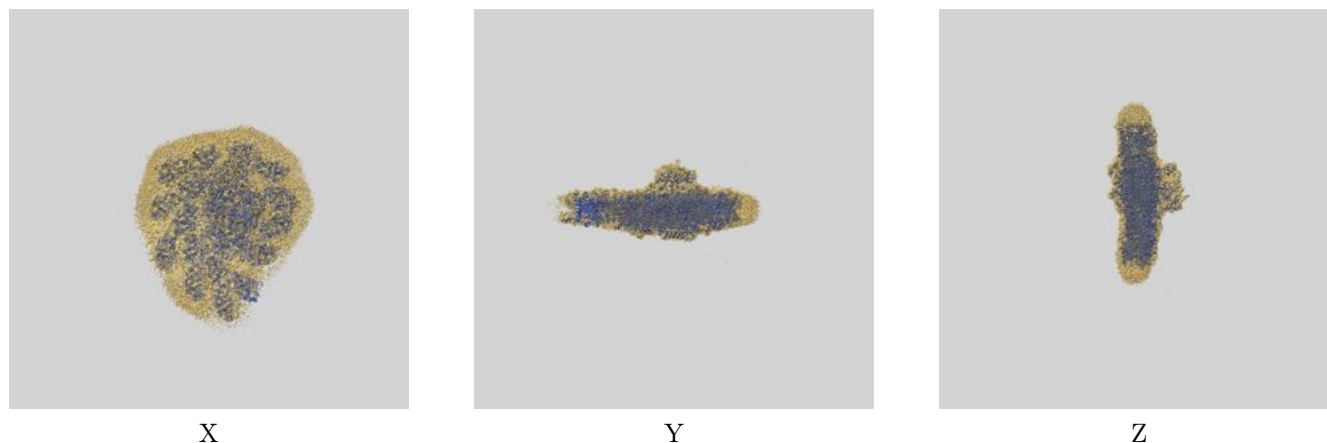
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.35	-	-
Author-provided FSC curve	2.35	2.93	2.43
Unmasked-calculated*	-	-	-

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

9 Map-model fit [i](#)

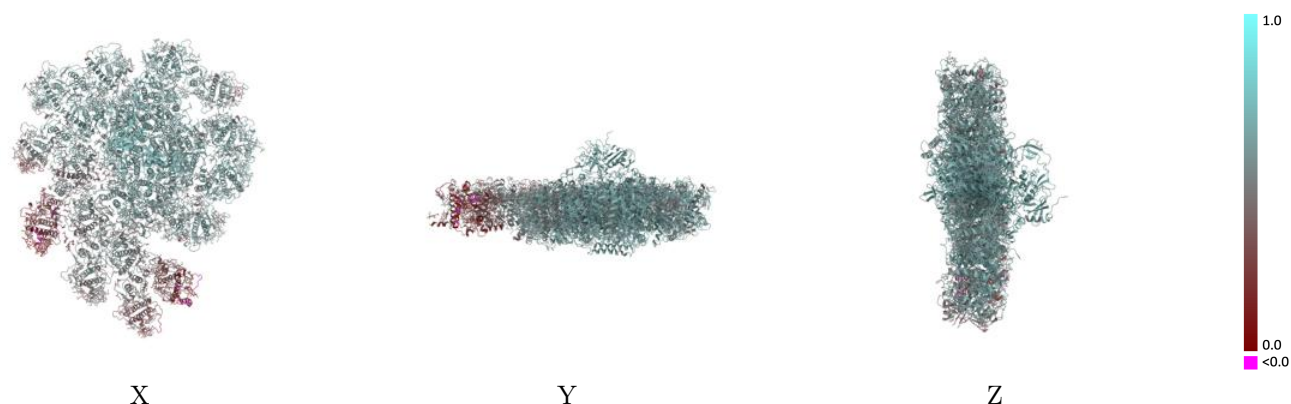
This section contains information regarding the fit between EMDB map EMD-63994 and PDB model 9UAS. Per-residue inclusion information can be found in section [3](#) on page [35](#).

9.1 Map-model overlay [i](#)



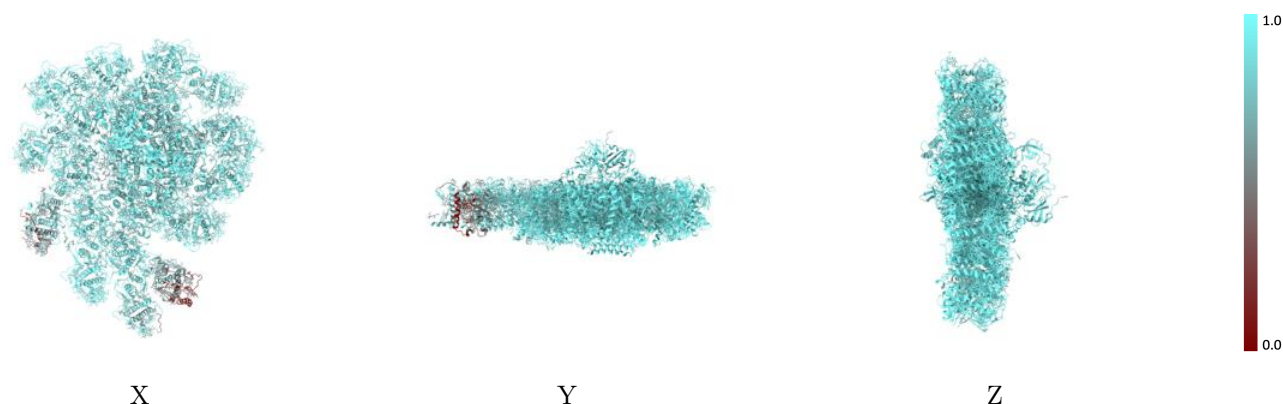
The images above show the 3D surface view of the map at the recommended contour level 0.04 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



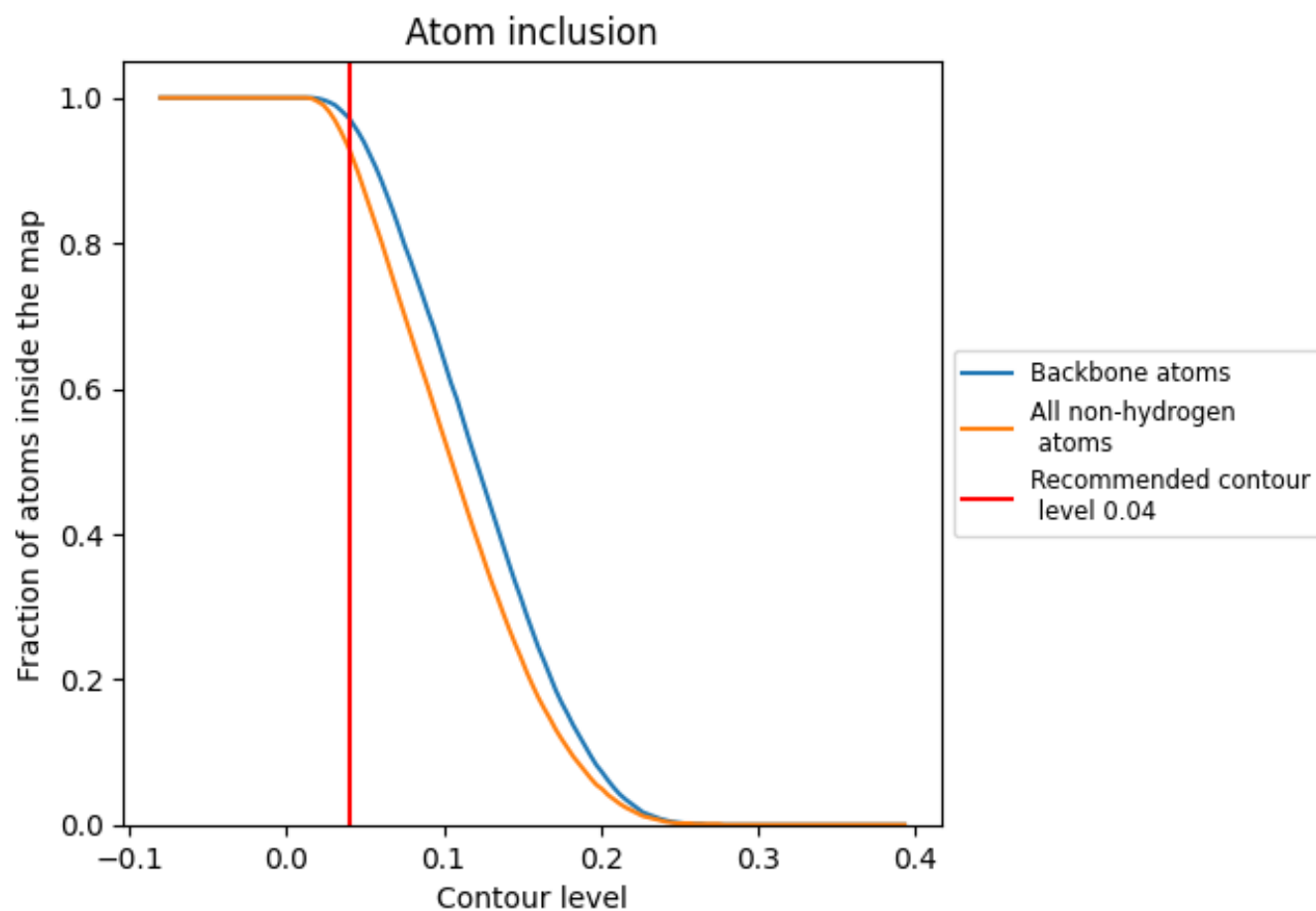
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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	 0.9300	 0.5550
A	 0.9840	 0.6580
B	 0.9780	 0.6190
C	 0.9970	 0.6770
D	 0.9510	 0.6400
E	 0.9560	 0.6350
F	 0.9620	 0.6150
G	 0.9560	 0.5620
H	 0.9670	 0.5870
I	 0.9400	 0.4830
J	 0.9420	 0.6280
K	 0.9690	 0.6110
L	 0.9710	 0.5060
M	 0.9840	 0.5760
N	 0.9490	 0.4660
O	 0.9660	 0.4920
P	 0.7790	 0.3540
Q	 0.9570	 0.5030
R	 0.4970	 0.2490
S	 0.9380	 0.5600
T	 0.9500	 0.6030
U	 0.9200	 0.5570
V	 0.6770	 0.2230
W	 0.9550	 0.6060
X	 0.9420	 0.6030

