



wwPDB EM Validation Summary Report ⓘ

Oct 1, 2024 – 12:08 PM JST

PDB ID : 7DZ8
EMDB ID : EMD-30926
Title : State transition supercomplex PSI-LHCI-LHCII from the LhcbM1 lacking mutant of *Chlamydomonas reinhardtii*
Authors : Pan, X.W.; Li, A.J.; Liu, Z.F.; Li, M.
Deposited on : 2021-01-23
Resolution : 3.16 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.dev113
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

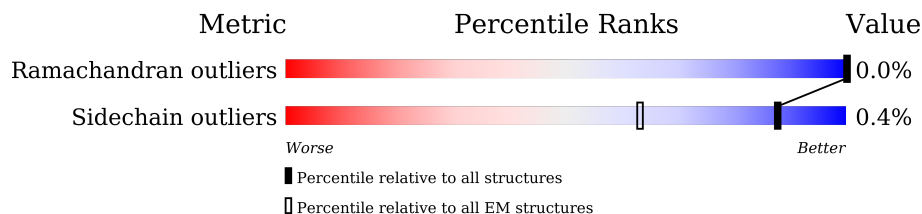
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.16 Å.

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














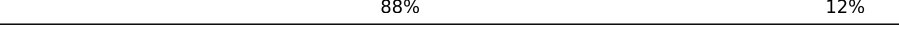

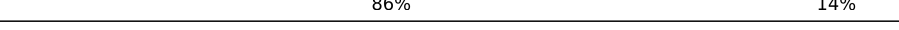






Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	751	
2	B	735	
3	C	81	
4	D	196	
5	E	97	
6	F	227	
7	G	126	
8	H	130	
9	I	106	

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Mol	Chain	Length	Quality of chain
10	J	41	 100%
11	K	113	 76% 24%
12	L	196	 81% 19%
13	O	126	 77% 23%
14	1	228	 83% 15%
14	a	228	 83% 15%
15	2	246	 87% 12%
16	3	298	 74% 26%
17	4	264	 80% 20%
18	5	257	 88% 12%
19	6	257	 89% 11%
20	7	241	 88% 12%
21	8	243	 89% 11%
22	9	213	 86% 14%
23	W	249	 88% 12%
23	X	249	 88% 11%
24	U	257	 85% 15%
24	Y	257	 85% 15%
24	Z	257	 86% 14%
25	V	268	 88% 11%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
26	CLA	1	602	X	-	-	-
26	CLA	1	603	X	-	-	-
26	CLA	1	604	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
26	CLA	1	606	X	-	-	-
26	CLA	1	607	X	-	-	-
26	CLA	1	608	X	-	-	-
26	CLA	1	609	X	-	-	-
26	CLA	1	610	X	-	-	-
26	CLA	1	611	X	-	-	-
26	CLA	1	612	X	-	-	-
26	CLA	1	613	X	-	-	-
26	CLA	1	614	X	-	-	-
26	CLA	1	616	X	-	-	-
26	CLA	2	601	X	-	-	-
26	CLA	2	602	X	-	-	-
26	CLA	2	603	X	-	-	-
26	CLA	2	604	X	-	-	-
26	CLA	2	606	X	-	-	-
26	CLA	2	607	X	-	-	-
26	CLA	2	609	X	-	-	-
26	CLA	2	610	X	-	-	-
26	CLA	2	611	X	-	-	-
26	CLA	2	612	X	-	-	-
26	CLA	2	613	X	-	-	-
26	CLA	2	614	X	-	-	-
26	CLA	2	616	X	-	-	-
26	CLA	3	602	X	-	-	-
26	CLA	3	603	X	-	-	-
26	CLA	3	604	X	-	-	-
26	CLA	3	606	X	-	-	-
26	CLA	3	607	X	-	-	-
26	CLA	3	608	X	-	-	-
26	CLA	3	609	X	-	-	-
26	CLA	3	610	X	-	-	-
26	CLA	3	611	X	-	-	-
26	CLA	3	612	X	-	-	-
26	CLA	3	613	X	-	-	-
26	CLA	3	614	X	-	-	-
26	CLA	3	615	X	-	-	-
26	CLA	3	617	X	-	-	-
26	CLA	4	601	X	-	-	-
26	CLA	4	602	X	-	-	-
26	CLA	4	603	X	-	-	-
26	CLA	4	604	X	-	-	-
26	CLA	4	606	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
26	CLA	4	607	X	-	-	-
26	CLA	4	608	X	-	-	-
26	CLA	4	609	X	-	-	-
26	CLA	4	610	X	-	-	-
26	CLA	4	611	X	-	-	-
26	CLA	4	612	X	-	-	-
26	CLA	4	613	X	-	-	-
26	CLA	4	616	X	-	-	-
26	CLA	4	618	X	-	-	-
26	CLA	5	601	X	-	-	-
26	CLA	5	602	X	-	-	-
26	CLA	5	603	X	-	-	-
26	CLA	5	604	X	-	-	-
26	CLA	5	607	X	-	-	-
26	CLA	5	608	X	-	-	-
26	CLA	5	609	X	-	-	-
26	CLA	5	610	X	-	-	-
26	CLA	5	611	X	-	-	-
26	CLA	5	612	X	-	-	-
26	CLA	5	613	X	-	-	-
26	CLA	5	614	X	-	-	-
26	CLA	5	616	X	-	-	-
26	CLA	5	617	X	-	-	-
26	CLA	5	618	X	-	-	-
26	CLA	5	619	X	-	-	-
26	CLA	6	601	X	-	-	-
26	CLA	6	603	X	-	-	-
26	CLA	6	604	X	-	-	-
26	CLA	6	606	X	-	-	-
26	CLA	6	607	X	-	-	-
26	CLA	6	609	X	-	-	-
26	CLA	6	610	X	-	-	-
26	CLA	6	611	X	-	-	-
26	CLA	6	612	X	-	-	-
26	CLA	6	614	X	-	-	-
26	CLA	6	616	X	-	-	-
26	CLA	6	617	X	-	-	-
26	CLA	6	618	X	-	-	-
26	CLA	6	620	X	-	-	-
26	CLA	7	601	X	-	-	-
26	CLA	7	602	X	-	-	-
26	CLA	7	603	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
26	CLA	7	604	X	-	-	-
26	CLA	7	606	X	-	-	-
26	CLA	7	607	X	-	-	-
26	CLA	7	609	X	-	-	-
26	CLA	7	610	X	-	-	-
26	CLA	7	611	X	-	-	-
26	CLA	7	612	X	-	-	-
26	CLA	7	613	X	-	-	-
26	CLA	7	614	X	-	-	-
26	CLA	7	615	X	-	-	-
26	CLA	7	616	X	-	-	-
26	CLA	8	601	X	-	-	-
26	CLA	8	603	X	-	-	-
26	CLA	8	604	X	-	-	-
26	CLA	8	606	X	-	-	-
26	CLA	8	607	X	-	-	-
26	CLA	8	609	X	-	-	-
26	CLA	8	610	X	-	-	-
26	CLA	8	611	X	-	-	-
26	CLA	8	612	X	-	-	-
26	CLA	8	613	X	-	-	-
26	CLA	8	614	X	-	-	-
26	CLA	8	616	X	-	-	-
26	CLA	9	601	X	-	-	-
26	CLA	9	602	X	-	-	-
26	CLA	9	603	X	-	-	-
26	CLA	9	604	X	-	-	-
26	CLA	9	606	X	-	-	-
26	CLA	9	609	X	-	-	-
26	CLA	9	610	X	-	-	-
26	CLA	9	611	X	-	-	-
26	CLA	9	612	X	-	-	-
26	CLA	9	613	X	-	-	-
26	CLA	9	614	X	-	-	-
26	CLA	A	801	X	-	-	-
26	CLA	A	802	X	-	-	-
26	CLA	A	803	X	-	-	-
26	CLA	A	804	X	-	-	-
26	CLA	A	806	X	-	-	-
26	CLA	A	807	X	-	-	-
26	CLA	A	808	X	-	-	-
26	CLA	A	809	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
26	CLA	A	811	X	-	-	-
26	CLA	A	812	X	-	-	-
26	CLA	A	813	X	-	-	-
26	CLA	A	814	X	-	-	-
26	CLA	A	815	X	-	-	-
26	CLA	A	816	X	-	-	-
26	CLA	A	819	X	-	-	-
26	CLA	A	820	X	-	-	-
26	CLA	A	822	X	-	-	-
26	CLA	A	823	X	-	-	-
26	CLA	A	824	X	-	-	-
26	CLA	A	825	X	-	-	-
26	CLA	A	826	X	-	-	-
26	CLA	A	827	X	-	-	-
26	CLA	A	828	X	-	-	-
26	CLA	A	829	X	-	-	-
26	CLA	A	830	X	-	-	-
26	CLA	A	831	X	-	-	-
26	CLA	A	832	X	-	-	-
26	CLA	A	833	X	-	-	-
26	CLA	A	834	X	-	-	-
26	CLA	A	836	X	-	-	-
26	CLA	A	837	X	-	-	-
26	CLA	A	838	X	-	-	-
26	CLA	A	839	X	-	-	-
26	CLA	A	841	X	-	-	-
26	CLA	A	842	X	-	-	-
26	CLA	A	843	X	-	-	-
26	CLA	A	845	X	-	-	-
26	CLA	A	854	X	-	-	-
26	CLA	B	802	X	-	-	-
26	CLA	B	803	X	-	-	-
26	CLA	B	804	X	-	-	-
26	CLA	B	805	X	-	-	-
26	CLA	B	806	X	-	-	-
26	CLA	B	808	X	-	-	-
26	CLA	B	809	X	-	-	-
26	CLA	B	810	X	-	-	-
26	CLA	B	811	X	-	-	-
26	CLA	B	812	X	-	-	-
26	CLA	B	813	X	-	-	-
26	CLA	B	814	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
26	CLA	B	815	X	-	-	-
26	CLA	B	816	X	-	-	-
26	CLA	B	817	X	-	-	-
26	CLA	B	819	X	-	-	-
26	CLA	B	820	X	-	-	-
26	CLA	B	821	X	-	-	-
26	CLA	B	823	X	-	-	-
26	CLA	B	824	X	-	-	-
26	CLA	B	826	X	-	-	-
26	CLA	B	827	X	-	-	-
26	CLA	B	828	X	-	-	-
26	CLA	B	829	X	-	-	-
26	CLA	B	830	X	-	-	-
26	CLA	B	831	X	-	-	-
26	CLA	B	832	X	-	-	-
26	CLA	B	833	X	-	-	-
26	CLA	B	834	X	-	-	-
26	CLA	B	835	X	-	-	-
26	CLA	B	836	X	-	-	-
26	CLA	B	838	X	-	-	-
26	CLA	B	839	X	-	-	-
26	CLA	B	840	X	-	-	-
26	CLA	B	841	X	-	-	-
26	CLA	F	301	X	-	-	-
26	CLA	G	203	X	-	-	-
26	CLA	G	204	X	-	-	-
26	CLA	H	202	X	-	-	-
26	CLA	H	203	X	-	-	-
26	CLA	J	101	X	-	-	-
26	CLA	K	201	X	-	-	-
26	CLA	K	204	X	-	-	-
26	CLA	K	206	X	-	-	-
26	CLA	L	302	X	-	-	-
26	CLA	L	304	X	-	-	-
26	CLA	L	306	X	-	-	-
26	CLA	L	307	X	-	-	-
26	CLA	O	2001	X	-	-	-
26	CLA	O	2002	X	-	-	-
26	CLA	O	2003	X	-	-	-
26	CLA	U	602	X	-	-	-
26	CLA	U	603	X	-	-	-
26	CLA	U	604	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
26	CLA	U	610	X	-	-	-
26	CLA	U	611	X	-	-	-
26	CLA	U	612	X	-	-	-
26	CLA	U	613	X	-	-	-
26	CLA	U	614	X	-	-	-
26	CLA	V	602	X	-	-	-
26	CLA	V	603	X	-	-	-
26	CLA	V	604	X	-	-	-
26	CLA	V	610	X	-	-	-
26	CLA	V	611	X	-	-	-
26	CLA	V	612	X	-	-	-
26	CLA	V	613	X	-	-	-
26	CLA	V	614	X	-	-	-
26	CLA	W	602	X	-	-	-
26	CLA	W	603	X	-	-	-
26	CLA	W	604	X	-	-	-
26	CLA	W	610	X	-	-	-
26	CLA	W	611	X	-	-	-
26	CLA	W	612	X	-	-	-
26	CLA	W	613	X	-	-	-
26	CLA	W	614	X	-	-	-
26	CLA	X	602	X	-	-	-
26	CLA	X	603	X	-	-	-
26	CLA	X	604	X	-	-	-
26	CLA	X	610	X	-	-	-
26	CLA	X	611	X	-	-	-
26	CLA	X	612	X	-	-	-
26	CLA	X	613	X	-	-	-
26	CLA	X	614	X	-	-	-
26	CLA	Y	602	X	-	-	-
26	CLA	Y	603	X	-	-	-
26	CLA	Y	604	X	-	-	-
26	CLA	Y	610	X	-	-	-
26	CLA	Y	611	X	-	-	-
26	CLA	Y	612	X	-	-	-
26	CLA	Y	614	X	-	-	-
26	CLA	Z	602	X	-	-	-
26	CLA	Z	603	X	-	-	-
26	CLA	Z	604	X	-	-	-
26	CLA	Z	610	X	-	-	-
26	CLA	Z	611	X	-	-	-
26	CLA	Z	612	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
26	CLA	Z	613	X	-	-	-
26	CLA	Z	614	X	-	-	-
26	CLA	a	602	X	-	-	-
26	CLA	a	603	X	-	-	-
26	CLA	a	604	X	-	-	-
26	CLA	a	606	X	-	-	-
26	CLA	a	607	X	-	-	-
26	CLA	a	608	X	-	-	-
26	CLA	a	609	X	-	-	-
26	CLA	a	610	X	-	-	-
26	CLA	a	611	X	-	-	-
26	CLA	a	612	X	-	-	-
26	CLA	a	613	X	-	-	-
26	CLA	a	614	X	-	-	-
26	CLA	a	616	X	-	-	-
37	CHL	U	601	X	-	-	-
37	CHL	U	605	X	-	-	-
37	CHL	U	606	X	-	-	-
37	CHL	U	607	X	-	-	-
37	CHL	U	608	X	-	-	-
37	CHL	U	609	X	-	-	-
37	CHL	V	601	X	-	-	-
37	CHL	V	605	X	-	-	-
37	CHL	V	606	X	-	-	-
37	CHL	V	607	X	-	-	-
37	CHL	V	608	X	-	-	-
37	CHL	V	609	X	-	-	-
37	CHL	W	601	X	-	-	-
37	CHL	W	605	X	-	-	-
37	CHL	W	606	X	-	-	-
37	CHL	W	607	X	-	-	-
37	CHL	W	608	X	-	-	-
37	CHL	W	609	X	-	-	-
37	CHL	X	601	X	-	-	-
37	CHL	X	605	X	-	-	-
37	CHL	X	606	X	-	-	-
37	CHL	X	607	X	-	-	-
37	CHL	X	608	X	-	-	-
37	CHL	X	609	X	-	-	-
37	CHL	Y	601	X	-	-	-
37	CHL	Y	605	X	-	-	-
37	CHL	Y	606	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
37	CHL	Y	607	X	-	-	-
37	CHL	Y	608	X	-	-	-
37	CHL	Y	609	X	-	-	-
37	CHL	Z	601	X	-	-	-
37	CHL	Z	605	X	-	-	-
37	CHL	Z	606	X	-	-	-
37	CHL	Z	607	X	-	-	-
37	CHL	Z	608	X	-	-	-
37	CHL	Z	609	X	-	-	-

2 Entry composition [i](#)

There are 37 unique types of molecules in this entry. The entry contains 69460 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 A1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	741	5819	3805	993	999	22	0	0

- Molecule 2 is a protein called Photosystem I P700 chlorophyll a apoprotein A2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	733	5824	3825	977	1004	18	0	0

- Molecule 3 is a protein called Photosystem I iron-sulfur center.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	80	600	369	103	116	12	0	0

- Molecule 4 is a protein called Photosystem I reaction center subunit II, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	D	143	1124	719	199	199	7	0	0

- Molecule 5 is a protein called Photosystem I reaction center subunit IV, chloroplastic.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
5	E	63	496	316	87	93	0	0

- Molecule 6 is a protein called Photosystem I reaction center subunit III, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	F	165	1265	817	213	232	3	0	0

- Molecule 7 is a protein called Photosystem I reaction center subunit V, chloroplastic.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
7	G	94	699	449	118	132	0	0

- Molecule 8 is a protein called Photosystem I reaction center subunit VI, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	H	100	776	482	138	154	2	0	0

- Molecule 9 is a protein called Photosystem I reaction center subunit VIII.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	I	42	316	217	45	53	1	0	0

- Molecule 10 is a protein called Photosystem I reaction center subunit IX.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	J	41	337	231	47	58	1	0	0

- Molecule 11 is a protein called Photosystem I reaction center subunit psaK, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	K	86	582	370	100	110	2	0	0

- Molecule 12 is a protein called PSI subunit V.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	L	159	1161	757	189	212	3	0	0

- Molecule 13 is a protein called Photosystem I subunit O.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
13	O	97	758	503	123	132	0	0

- Molecule 14 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	1	194	Total	C	N	O	S	0	0
			1444	941	240	260	3		
14	a	194	Total	C	N	O	S	0	0
			1444	941	240	260	3		

- Molecule 15 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	2	217	Total	C	N	O	S	0	0
			1682	1094	274	304	10		

- Molecule 16 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	3	220	Total	C	N	O	S	0	0
			1678	1097	270	303	8		

- Molecule 17 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	4	210	Total	C	N	O	S	0	0
			1631	1071	263	292	5		

- Molecule 18 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	5	227	Total	C	N	O	S	0	0
			1774	1154	297	315	8		

- Molecule 19 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	6	230	Total	C	N	O	S	0	0
			1771	1167	293	305	6		

- Molecule 20 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	7	213	Total	C	N	O	S	0	0
			1649	1072	274	297	6		

- Molecule 21 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	8	216	Total	C	N	O	S	0	0
			1641	1067	279	291	4		

- Molecule 22 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	9	183	Total	C	N	O	S	0	0
			1403	909	235	252	7		

- Molecule 23 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	X	221	Total	C	N	O	S	0	0
			1680	1091	274	310	5		
23	W	220	Total	C	N	O	S	0	0
			1671	1085	273	308	5		

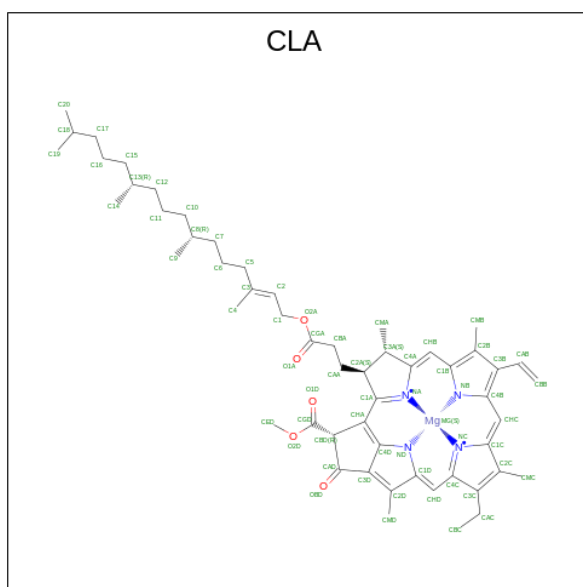
- Molecule 24 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	Y	219	Total	C	N	O	S	0	0
			1675	1084	272	314	5		
24	Z	221	Total	C	N	O	S	0	0
			1684	1089	274	316	5		
24	U	219	Total	C	N	O	S	0	0
			1669	1080	272	312	5		

- Molecule 25 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace	
25	V	238	Total	C	N	O	P	S	0	0
			1815	1176	300	333	1	5		

- Molecule 26 is CHLOROPHYLL A (three-letter code: CLA) (formula: $C_{55}H_{72}MgN_4O_5$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf	
26	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	A	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
26	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	A	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
26	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	A	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
26	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	A	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
26	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
26	A	1	50	40	1	4	5	0
26	A	1	65	55	1	4	5	0
26	A	1	45	35	1	4	5	0
26	A	1	60	50	1	4	5	0
26	A	1	59	49	1	4	5	0
26	A	1	65	55	1	4	5	0
26	A	1	53	43	1	4	5	0
26	A	1	65	55	1	4	5	0
26	A	1	42	34	1	4	3	0
26	A	1	65	55	1	4	5	0
26	A	1	65	55	1	4	5	0
26	A	1	64	55	1	4	4	0
26	A	1	58	48	1	4	5	0
26	A	1	65	55	1	4	5	0
26	A	1	65	55	1	4	5	0
26	A	1	65	55	1	4	5	0
26	A	1	50	40	1	4	5	0
26	A	1	45	35	1	4	5	0
26	A	1	65	55	1	4	5	0
26	A	1	61	51	1	4	5	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
26	A	1	65	55	1	4	5	0
26	A	1	45	35	1	4	5	0
26	A	1	50	40	1	4	5	0
26	A	1	55	45	1	4	5	0
26	A	1	52	42	1	4	5	0
26	A	1	65	55	1	4	5	0
26	A	1	65	55	1	4	5	0
26	A	1	64	54	1	4	5	0
26	A	1	50	40	1	4	5	0
26	A	1	65	55	1	4	5	0
26	B	1	65	55	1	4	5	0
26	B	1	65	55	1	4	5	0
26	B	1	41	33	1	4	3	0
26	B	1	65	55	1	4	5	0
26	B	1	65	55	1	4	5	0
26	B	1	52	42	1	4	5	0
26	B	1	65	55	1	4	5	0
26	B	1	65	55	1	4	5	0
26	B	1	64	55	1	4	4	0
26	B	1	52	43	1	4	4	0
26	B	1	43	35	1	4	3	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
26	B	1	65	55	1	4	5	0
26	B	1	64	54	1	4	5	0
26	B	1	43	35	1	4	3	0
26	B	1	54	45	1	4	4	0
26	B	1	59	49	1	4	5	0
26	B	1	60	50	1	4	5	0
26	B	1	55	45	1	4	5	0
26	B	1	50	40	1	4	5	0
26	B	1	43	33	1	4	5	0
26	B	1	42	34	1	4	3	0
26	B	1	45	35	1	4	5	0
26	B	1	65	55	1	4	5	0
26	B	1	49	39	1	4	5	0
26	B	1	62	52	1	4	5	0
26	B	1	62	52	1	4	5	0
26	B	1	65	55	1	4	5	0
26	B	1	65	55	1	4	5	0
26	B	1	43	35	1	4	3	0
26	B	1	65	55	1	4	5	0
26	B	1	60	50	1	4	5	0
26	B	1	65	55	1	4	5	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
26	B	1	60	50	1	4	5	0
26	B	1	45	35	1	4	5	0
26	B	1	50	40	1	4	5	0
26	B	1	65	55	1	4	5	0
26	B	1	46	36	1	4	5	0
26	B	1	65	55	1	4	5	0
26	B	1	65	55	1	4	5	0
26	B	1	65	55	1	4	5	0
26	F	1	57	47	1	4	5	0
26	F	1	42	34	1	4	3	0
26	F	1	41	33	1	4	3	0
26	G	1	42	34	1	4	3	0
26	G	1	45	35	1	4	5	0
26	H	1	39	31	1	4	3	0
26	H	1	65	55	1	4	5	0
26	J	1	42	34	1	4	3	0
26	K	1	45	35	1	4	5	0
26	K	1	56	46	1	4	5	0
26	K	1	45	35	1	4	5	0
26	K	1	45	35	1	4	5	0
26	L	1	45	35	1	4	5	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
26	L	1	65	55	1	4	5	0
26	L	1	45	35	1	4	5	0
26	L	1	40	32	1	4	3	0
26	L	1	40	32	1	4	3	0
26	O	1	38	30	1	4	3	0
26	O	1	38	30	1	4	3	0
26	O	1	40	32	1	4	3	0
26	1	1	54	44	1	4	5	0
26	1	1	61	51	1	4	5	0
26	1	1	53	44	1	4	4	0
26	1	1	49	39	1	4	5	0
26	1	1	39	32	1	4	2	0
26	1	1	40	32	1	4	3	0
26	1	1	44	34	1	4	5	0
26	1	1	40	32	1	4	3	0
26	1	1	39	31	1	4	3	0
26	1	1	57	47	1	4	5	0
26	1	1	45	35	1	4	5	0
26	1	1	65	55	1	4	5	0
26	1	1	37	29	1	4	3	0
26	1	1	43	33	1	4	5	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
26	a	1	54	44	1	4	5	0
26	a	1	61	51	1	4	5	0
26	a	1	54	45	1	4	4	0
26	a	1	49	39	1	4	5	0
26	a	1	44	35	1	4	4	0
26	a	1	45	35	1	4	5	0
26	a	1	44	34	1	4	5	0
26	a	1	64	54	1	4	5	0
26	a	1	59	49	1	4	5	0
26	a	1	38	30	1	4	3	0
26	a	1	45	35	1	4	5	0
26	a	1	54	44	1	4	5	0
26	a	1	54	44	1	4	5	0
26	a	1	45	35	1	4	5	0
26	2	1	65	55	1	4	5	0
26	2	1	63	54	1	3	5	0
26	2	1	44	34	1	4	5	0
26	2	1	42	34	1	4	3	0
26	2	1	43	35	1	4	3	0
26	2	1	44	34	1	4	5	0
26	2	1	45	35	1	4	5	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
26	2	1	Total 55	C 45	Mg 1	N 4	O 5	0
26	2	1	Total 42	C 34	Mg 1	N 4	O 3	0
26	2	1	Total 44	C 34	Mg 1	N 4	O 5	0
26	2	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	2	1	Total 42	C 34	Mg 1	N 4	O 3	0
26	2	1	Total 43	C 33	Mg 1	N 4	O 5	0
26	3	1	Total 60	C 50	Mg 1	N 4	O 5	0
26	3	1	Total 55	C 45	Mg 1	N 4	O 5	0
26	3	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	3	1	Total 54	C 44	Mg 1	N 4	O 5	0
26	3	1	Total 56	C 46	Mg 1	N 4	O 5	0
26	3	1	Total 55	C 45	Mg 1	N 4	O 5	0
26	3	1	Total 60	C 50	Mg 1	N 4	O 5	0
26	3	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	3	1	Total 38	C 30	Mg 1	N 4	O 3	0
26	3	1	Total 43	C 35	Mg 1	N 4	O 3	0
26	3	1	Total 53	C 44	Mg 1	N 4	O 4	0
26	3	1	Total 40	C 32	Mg 1	N 4	O 3	0
26	3	1	Total 40	C 32	Mg 1	N 4	O 3	0
26	3	1	Total 40	C 32	Mg 1	N 4	O 3	0
26	4	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
26	4	1	60	50	1	4	5	0
26	4	1	44	34	1	4	5	0
26	4	1	54	44	1	4	5	0
26	4	1	40	32	1	4	3	0
26	4	1	45	35	1	4	5	0
26	4	1	65	55	1	4	5	0
26	4	1	57	47	1	4	5	0
26	4	1	61	51	1	4	5	0
26	4	1	42	34	1	4	3	0
26	4	1	41	33	1	4	3	0
26	4	1	65	55	1	4	5	0
26	4	1	56	46	1	4	5	0
26	4	1	43	33	1	4	5	0
26	4	1	40	32	1	4	3	0
26	5	1	56	46	1	4	5	0
26	5	1	65	55	1	4	5	0
26	5	1	54	44	1	4	5	0
26	5	1	63	53	1	4	5	0
26	5	1	40	32	1	4	3	0
26	5	1	65	55	1	4	5	0
26	5	1	50	40	1	4	5	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
26	5	1	65	55	1	4	5	0
26	5	1	54	44	1	4	5	0
26	5	1	42	34	1	4	3	0
26	5	1	41	33	1	4	3	0
26	5	1	64	55	1	4	4	0
26	5	1	44	34	1	4	5	0
26	5	1	42	33	1	4	4	0
26	5	1	50	40	1	4	5	0
26	5	1	40	32	1	4	3	0
26	5	1	43	33	1	4	5	0
26	6	1	65	55	1	4	5	0
26	6	1	65	55	1	4	5	0
26	6	1	51	41	1	4	5	0
26	6	1	65	55	1	4	5	0
26	6	1	40	32	1	4	3	0
26	6	1	41	33	1	4	3	0
26	6	1	45	35	1	4	5	0
26	6	1	45	35	1	4	5	0
26	6	1	65	55	1	4	5	0
26	6	1	42	34	1	4	3	0
26	6	1	41	33	1	4	3	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
26	6	1	64	54	1	4	5	0
26	6	1	60	50	1	4	5	0
26	6	1	65	55	1	4	5	0
26	6	1	45	35	1	4	5	0
26	6	1	40	32	1	4	3	0
26	6	1	64	54	1	4	5	0
26	7	1	60	50	1	4	5	0
26	7	1	65	55	1	4	5	0
26	7	1	44	34	1	4	5	0
26	7	1	50	40	1	4	5	0
26	7	1	41	33	1	4	3	0
26	7	1	42	34	1	4	3	0
26	7	1	50	40	1	4	5	0
26	7	1	44	35	1	4	4	0
26	7	1	65	55	1	4	5	0
26	7	1	59	49	1	4	5	0
26	7	1	44	34	1	4	5	0
26	7	1	65	55	1	4	5	0
26	7	1	42	34	1	4	3	0
26	7	1	42	33	1	4	4	0
26	7	1	43	33	1	4	5	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
26	8	1	65	55	1	4	5	0
26	8	1	60	50	1	4	5	0
26	8	1	44	34	1	4	5	0
26	8	1	50	40	1	4	5	0
26	8	1	64	54	1	4	5	0
26	8	1	41	33	1	4	3	0
26	8	1	51	41	1	4	5	0
26	8	1	45	35	1	4	5	0
26	8	1	60	50	1	4	5	0
26	8	1	42	34	1	4	3	0
26	8	1	41	33	1	4	3	0
26	8	1	65	55	1	4	5	0
26	8	1	53	43	1	4	5	0
26	8	1	43	33	1	4	5	0
26	9	1	45	35	1	4	5	0
26	9	1	60	50	1	4	5	0
26	9	1	44	34	1	4	5	0
26	9	1	50	40	1	4	5	0
26	9	1	40	32	1	4	3	0
26	9	1	45	35	1	4	5	0
26	9	1	61	51	1	4	5	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
26	9	1	57	47	1	4	5	0
26	9	1	42	34	1	4	3	0
26	9	1	41	33	1	4	3	0
26	9	1	65	55	1	4	5	0
26	9	1	45	35	1	4	5	0
26	X	1	65	55	1	4	5	0
26	X	1	62	52	1	4	5	0
26	X	1	49	39	1	4	5	0
26	X	1	65	55	1	4	5	0
26	X	1	45	35	1	4	5	0
26	X	1	43	35	1	4	3	0
26	X	1	65	55	1	4	5	0
26	X	1	42	34	1	4	3	0
26	Y	1	58	48	1	4	5	0
26	Y	1	55	45	1	4	5	0
26	Y	1	50	40	1	4	5	0
26	Y	1	65	55	1	4	5	0
26	Y	1	43	35	1	4	3	0
26	Y	1	45	35	1	4	5	0
26	Y	1	65	55	1	4	5	0
26	Y	1	48	38	1	4	5	0

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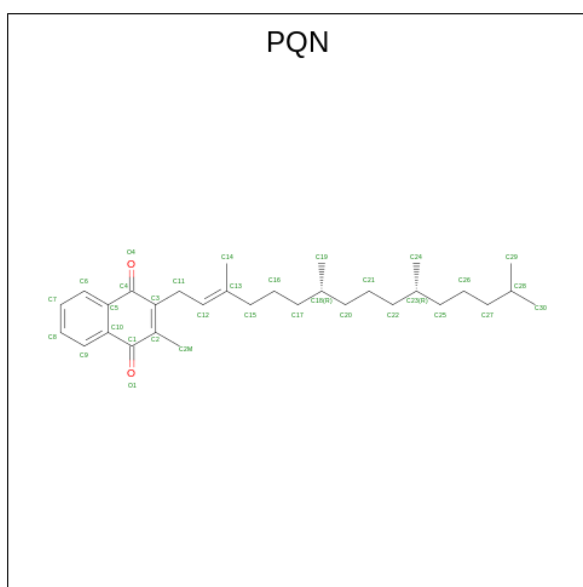
Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
26	Z	1	58	48	1	4	5	0
26	Z	1	55	45	1	4	5	0
26	Z	1	49	40	1	4	4	0
26	Z	1	65	55	1	4	5	0
26	Z	1	42	34	1	4	3	0
26	Z	1	45	35	1	4	5	0
26	Z	1	65	55	1	4	5	0
26	Z	1	48	38	1	4	5	0
26	U	1	59	49	1	4	5	0
26	U	1	52	42	1	4	5	0
26	U	1	48	39	1	4	4	0
26	U	1	56	46	1	4	5	0
26	U	1	42	34	1	4	3	0
26	U	1	42	34	1	4	3	0
26	U	1	59	49	1	4	5	0
26	U	1	42	34	1	4	3	0
26	V	1	60	50	1	4	5	0
26	V	1	45	35	1	4	5	0
26	V	1	50	40	1	4	5	0
26	V	1	62	52	1	4	5	0
26	V	1	43	35	1	4	3	0

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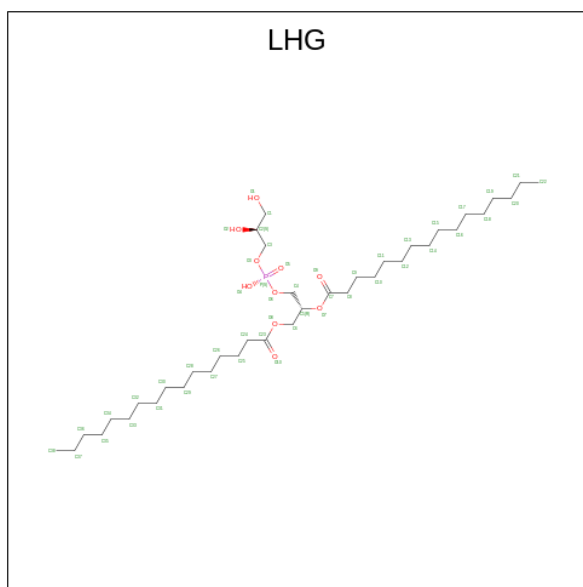
Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
26	V	1	Total 45	C 35	Mg 1	N 4	O 5	0
26	V	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	V	1	Total 45	C 35	Mg 1	N 4	O 5	0
26	W	1	Total 60	C 50	Mg 1	N 4	O 5	0
26	W	1	Total 52	C 42	Mg 1	N 4	O 5	0
26	W	1	Total 47	C 37	Mg 1	N 4	O 5	0
26	W	1	Total 55	C 45	Mg 1	N 4	O 5	0
26	W	1	Total 57	C 47	Mg 1	N 4	O 5	0
26	W	1	Total 45	C 35	Mg 1	N 4	O 5	0
26	W	1	Total 65	C 55	Mg 1	N 4	O 5	0
26	W	1	Total 45	C 35	Mg 1	N 4	O 5	0

- Molecule 27 is PHYLLOQUINONE (three-letter code: PQN) (formula: C₃₁H₄₆O₂).



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

- Molecule 28 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula: $C_{38}H_{75}O_{10}P$).



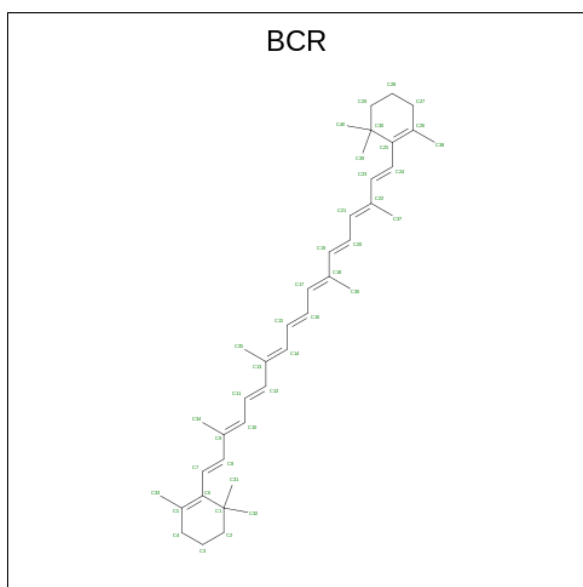
Mol	Chain	Residues	Atoms				AltConf
28	A	1	Total	C	O	P	0
			49	38	10	1	
28	A	1	Total	C	O	P	0
			30	19	10	1	
28	A	1	Total	C	O	P	0
			49	38	10	1	
28	B	1	Total	C	O	P	0
			38	27	10	1	
28	H	1	Total	C	O	P	0
			49	38	10	1	
28	O	1	Total	C	O	P	0
			36	25	10	1	
28	1	1	Total	C	O	P	0
			49	38	10	1	
28	a	1	Total	C	O	P	0
			43	32	10	1	
28	2	1	Total	C	O	P	0
			36	25	10	1	

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
28	3	1	45	34	10	1	0
28	3	1	49	38	10	1	0
28	4	1	49	38	10	1	0
28	5	1	49	38	10	1	0
28	5	1	49	38	10	1	0
28	6	1	48	37	10	1	0
28	7	1	37	26	10	1	0
28	8	1	49	38	10	1	0
28	8	1	40	29	10	1	0
28	9	1	30	19	10	1	0
28	9	1	49	38	10	1	0
28	9	1	49	38	10	1	0
28	X	1	49	38	10	1	0
28	Y	1	49	38	10	1	0
28	Z	1	49	38	10	1	0
28	U	1	49	38	10	1	0
28	V	1	36	25	10	1	0
28	W	1	34	23	10	1	0

- Molecule 29 is BETA-CAROTENE (three-letter code: BCR) (formula: C₄₀H₅₆).



Mol	Chain	Residues	Atoms	AltConf
29	A	1	Total C 40 40	0
29	A	1	Total C 40 40	0
29	A	1	Total C 40 40	0
29	A	1	Total C 40 40	0
29	A	1	Total C 40 40	0
29	A	1	Total C 40 40	0
29	B	1	Total C 40 40	0
29	B	1	Total C 40 40	0
29	B	1	Total C 40 40	0
29	B	1	Total C 40 40	0
29	B	1	Total C 40 40	0
29	B	1	Total C 40 40	0
29	B	1	Total C 40 40	0
29	B	1	Total C 40 40	0

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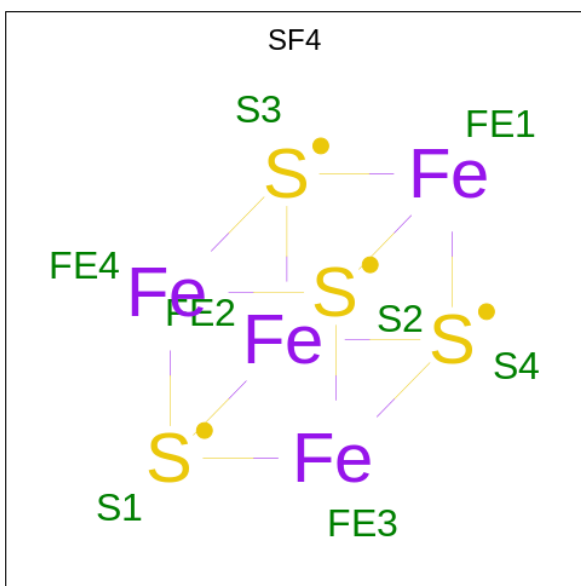
Mol	Chain	Residues	Atoms	AltConf
29	B	1	Total C 40 40	0
29	B	1	Total C 40 40	0
29	F	1	Total C 40 40	0
29	G	1	Total C 40 40	0
29	J	1	Total C 40 40	0
29	K	1	Total C 40 40	0
29	K	1	Total C 40 40	0
29	L	1	Total C 40 40	0
29	L	1	Total C 40 40	0
29	L	1	Total C 40 40	0
29	L	1	Total C 40 40	0
29	O	1	Total C 40 40	0
29	O	1	Total C 40 40	0
29	1	1	Total C 40 40	0
29	a	1	Total C 40 40	0
29	2	1	Total C 40 40	0
29	3	1	Total C 40 40	0
29	3	1	Total C 40 40	0
29	3	1	Total C 40 40	0
29	4	1	Total C 40 40	0
29	5	1	Total C 40 40	0

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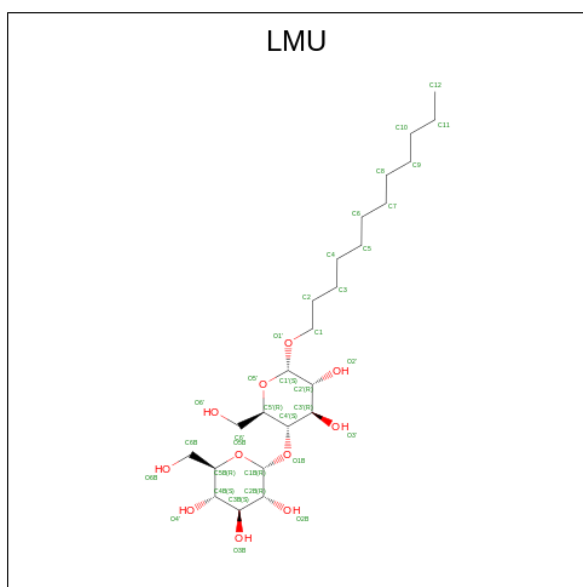
Mol	Chain	Residues	Atoms	AltConf
29	6	1	Total C 40 40	0
29	7	1	Total C 40 40	0
29	7	1	Total C 40 40	0
29	8	1	Total C 40 40	0
29	9	1	Total C 40 40	0

- Molecule 30 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe₄S₄).



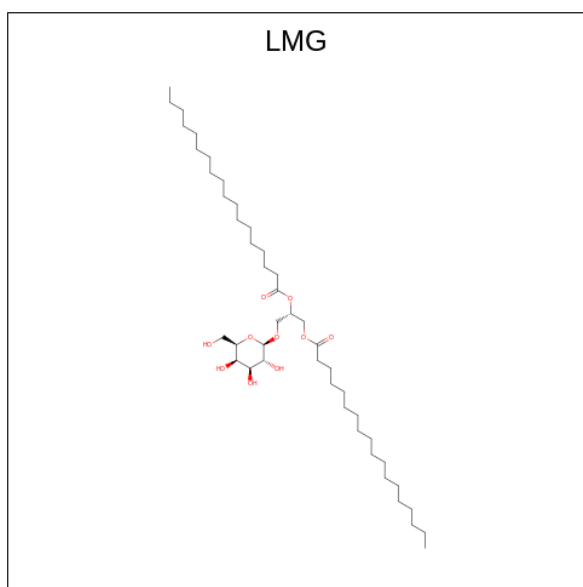
Mol	Chain	Residues	Atoms	AltConf
30	A	1	Total Fe S 8 4 4	0
30	C	1	Total Fe S 8 4 4	0
30	C	1	Total Fe S 8 4 4	0

- Molecule 31 is DODECYL-ALPHA-D-MALTOSIDE (three-letter code: LMU) (formula: C₂₄H₄₆O₁₁).



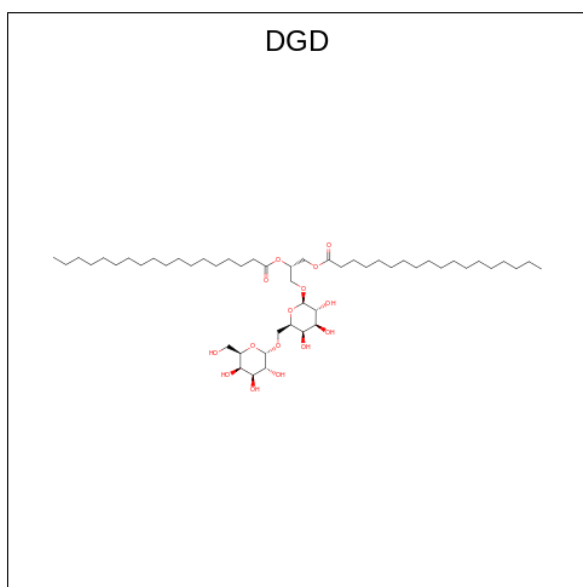
Mol	Chain	Residues	Atoms			AltConf
31	A	1	Total	C	O	0
			35	24	11	
31	A	1	Total	C	O	0
			34	24	10	
31	K	1	Total	C	O	0
			35	24	11	
31	1	1	Total	C	O	0
			35	24	11	
31	5	1	Total	C	O	0
			33	22	11	
31	5	1	Total	C	O	0
			32	21	11	
31	8	1	Total	C	O	0
			35	24	11	

- Molecule 32 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: LMG) (formula: C₄₅H₈₆O₁₀).



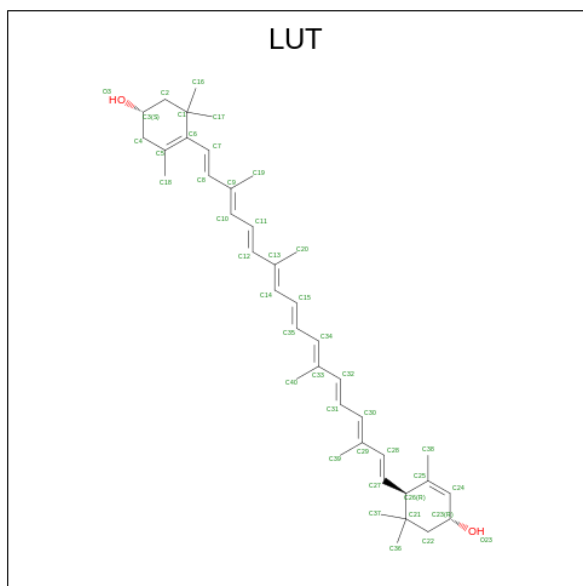
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
32	A	1	40	30	10	0
32	H	1	55	45	10	0
32	J	1	42	32	10	0
32	J	1	40	30	10	0
32	L	1	37	27	10	0
32	4	1	40	30	10	0
32	4	1	40	30	10	0
32	5	1	40	30	10	0
32	8	1	46	36	10	0
32	9	1	55	45	10	0
32	V	1	55	45	10	0

- Molecule 33 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (three-letter code: DGD) (formula: $C_{51}H_{96}O_{15}$).



Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
33	B	1	62	47	15	0

- Molecule 34 is (3R,3'R,6S)-4,5-DIDEHYDRO-5,6-DIHYDRO-BETA,BETA-CAROTENE-3,3'-DIOL (three-letter code: LUT) (formula: $C_{40}H_{56}O_2$).



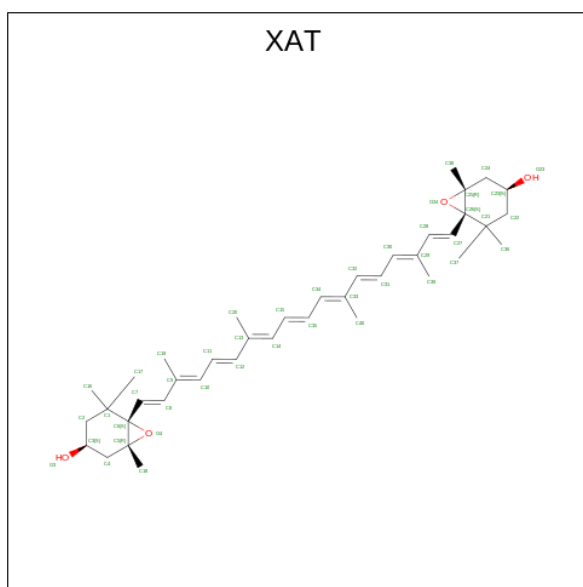
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
34	1	1	42	40	2	0
34	a	1	42	40	2	0

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Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
34	2	1	42	40	2	0
34	3	1	42	40	2	0
34	4	1	42	40	2	0
34	5	1	42	40	2	0
34	6	1	42	40	2	0
34	7	1	42	40	2	0
34	8	1	42	40	2	0
34	9	1	42	40	2	0
34	X	1	42	40	2	0
34	X	1	42	40	2	0
34	Y	1	42	40	2	0
34	Y	1	42	40	2	0
34	Z	1	42	40	2	0
34	Z	1	42	40	2	0
34	U	1	42	40	2	0
34	U	1	42	40	2	0
34	V	1	42	40	2	0
34	V	1	42	40	2	0
34	W	1	42	40	2	0
34	W	1	42	40	2	0

- Molecule 35 is (3S,5R,6S,3'S,5'R,6'S)-5,6,5',6'-DIEPOXY-5,6,5',6'- TETRAHYDRO-BETA ,BETA-CAROTENE-3,3'-DIOL (three-letter code: XAT) (formula: C₄₀H₅₆O₄).



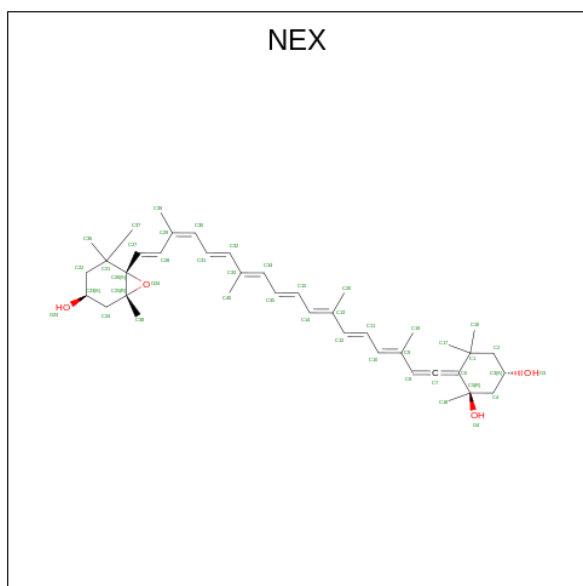
Mol	Chain	Residues	Atoms			AltConf
35	1	1	Total	C	O	0
			44	40	4	
35	a	1	Total	C	O	0
			44	40	4	
35	2	1	Total	C	O	0
			44	40	4	
35	3	1	Total	C	O	0
			44	40	4	
35	4	1	Total	C	O	0
			44	40	4	
35	5	1	Total	C	O	0
			44	40	4	
35	6	1	Total	C	O	0
			44	40	4	
35	7	1	Total	C	O	0
			44	40	4	
35	8	1	Total	C	O	0
			44	40	4	
35	9	1	Total	C	O	0
			44	40	4	
35	X	1	Total	C	O	0
			44	40	4	
35	Y	1	Total	C	O	0
			44	40	4	
35	Z	1	Total	C	O	0
			44	40	4	
35	U	1	Total	C	O	0
			44	40	4	

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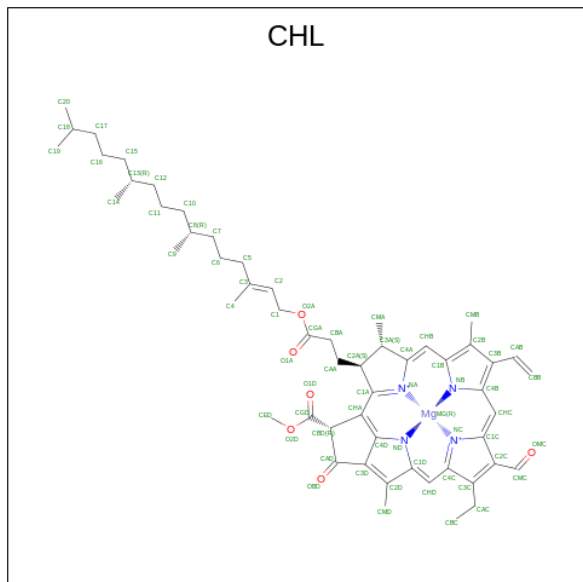
Mol	Chain	Residues	Atoms			AltConf
35	V	1	Total	C	O	0
			44	40	4	
35	W	1	Total	C	O	0
			44	40	4	

- Molecule 36 is (1R,3R)-6-[(3E,5E,7E,9E,11E,13E,15E,17E)-18-[(1S,4R,6R)-4-HYDROXY-2,6-TRIMETHYL-7-OXABICYCLO[4.1.0]HEPT-1-YL]-3,7,12,16-TETRAMETHYLOCTADEC-1,3,5,7,9,11,13,15,17-NONAENYLIDENE]-1,5,5-TRIMETHYLCYCLOHEXANE-1,3-DIOL (three-letter code: NEX) (formula: C₄₀H₅₆O₄).



Mol	Chain	Residues	Atoms			AltConf
36	5	1	Total	C	O	0
			44	40	4	
36	6	1	Total	C	O	0
			44	40	4	
36	X	1	Total	C	O	0
			44	40	4	
36	Y	1	Total	C	O	0
			44	40	4	
36	Z	1	Total	C	O	0
			44	40	4	
36	U	1	Total	C	O	0
			44	40	4	
36	V	1	Total	C	O	0
			44	40	4	
36	W	1	Total	C	O	0
			44	40	4	

- Molecule 37 is CHLOROPHYLL B (three-letter code: CHL) (formula: $C_{55}H_{70}MgN_4O_6$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf		
			Total	C	Mg	N		O	
37	X	1	Total	66	55	1	4	6	0
37	X	1	Total	46	35	1	4	6	0
37	X	1	Total	44	35	1	4	4	0
37	X	1	Total	66	55	1	4	6	0
37	X	1	Total	65	55	1	4	5	0
37	X	1	Total	66	55	1	4	6	0
37	Y	1	Total	66	55	1	4	6	0
37	Y	1	Total	42	33	1	4	4	0
37	Y	1	Total	46	35	1	4	6	0
37	Y	1	Total	66	55	1	4	6	0
37	Y	1	Total	49	38	1	4	6	0
37	Y	1	Total	66	55	1	4	6	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
37	Z	1	66	55	1	4	6	0
37	Z	1	42	33	1	4	4	0
37	Z	1	46	35	1	4	6	0
37	Z	1	66	55	1	4	6	0
37	Z	1	49	38	1	4	6	0
37	Z	1	66	55	1	4	6	0
37	U	1	66	55	1	4	6	0
37	U	1	43	34	1	4	4	0
37	U	1	44	35	1	4	4	0
37	U	1	46	35	1	4	6	0
37	U	1	44	35	1	4	4	0
37	U	1	60	49	1	4	6	0
37	V	1	66	55	1	4	6	0
37	V	1	44	35	1	4	4	0
37	V	1	44	35	1	4	4	0
37	V	1	46	35	1	4	6	0
37	V	1	48	37	1	4	6	0
37	V	1	61	50	1	4	6	0
37	W	1	66	55	1	4	6	0
37	W	1	46	35	1	4	6	0
37	W	1	46	35	1	4	6	0

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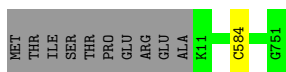
Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
37	W	1	Total 65	54	1	4	6	0
37	W	1	Total 47	36	1	4	6	0
37	W	1	Total 66	55	1	4	6	0

3 Residue-property plots [i](#)

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

- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1

Chain A:  99%



- Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

Chain B:  99%



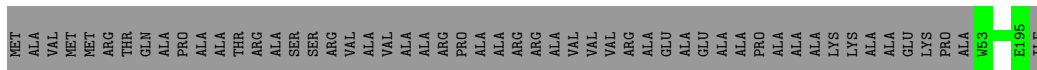
- Molecule 3: Photosystem I iron-sulfur center

Chain C:  96%



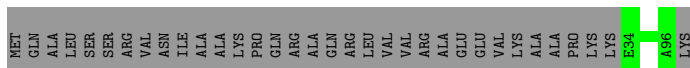
- Molecule 4: Photosystem I reaction center subunit II, chloroplastic

Chain D:  73%  27%



- Molecule 5: Photosystem I reaction center subunit IV, chloroplastic

Chain E:  65%  35%




- Molecule 6: Photosystem I reaction center subunit III, chloroplastic

Chain F:  73% 27%

MET ALA LEU THR MET ARG ASN PRO ALA VAL LYS SER SER ARG VAL ALA PRO SER SER ARG ARG ALA LEU ARG VAL ALA CYS GLN ALA GLN LYS ASN GLU THR ALA SER LYS VAL GLY THR ALA LEU ALA ALA SER ALA LEU ALA VAL SER LEU SER PRO SER ALA


MET ALA D63 R227

- Molecule 7: Photosystem I reaction center subunit V, chloroplastic

Chain G:  75% 25%

MET GLN THR LEU ALA SER ARG PRO SER LEU ARG ALA SER ALA VAL SER VAL PRO ARG ARG ALA PRO ARG ARG VAL THR LYS ALA ALA L82 S65 T66 T72 L125 SER

- Molecule 8: Photosystem I reaction center subunit VI, chloroplastic

Chain H:  77% 23%

MET ALA LEU VAL ALA ARG PRO VAL LEU SER ALA ALA ARG VAL ALA SER VAL ARG PRO ARG VAL ALA ALA K31 L130

- Molecule 9: Photosystem I reaction center subunit VIII

Chain I:  40% 60%

MET ALA LEU ARG ALA VAL SER ALA LYS SER ALA VAL ARG PRO THR VAL ALA ARG ALA SER VAL VAL LYS LEU LEU LYS PRO ALA GLN LYS MET ALA LEU ALA GLY ALA ALA VAL VAL LEU LEU ALA ALA SER SER SER SER ALA ALA GLU ALA SER GLN VAL ILE ALA THR VAL


ALA SER A63 F104 SER SER

- Molecule 10: Photosystem I reaction center subunit IX

Chain J:  100%


There are no outlier residues recorded for this chain.

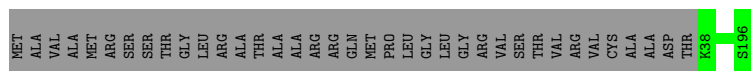
- Molecule 11: Photosystem I reaction center subunit psaK, chloroplastic

Chain K:  76% 24%

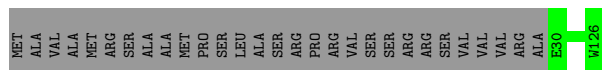
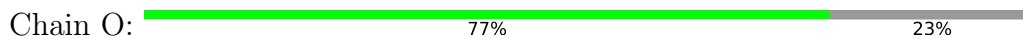
MET GLN ALA LEU THR ARG PRO ALA ILE ARG PRO THR LYS ALA ARG ARG SER SER VAL VAL VAL ARG ALA ASP G28 L113

- Molecule 12: PSI subunit V

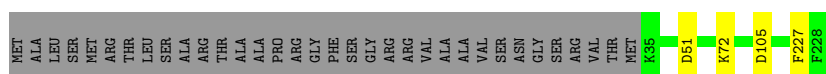
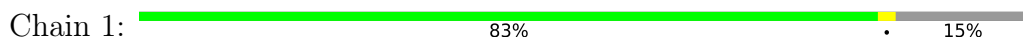
Chain L:  81% 19%



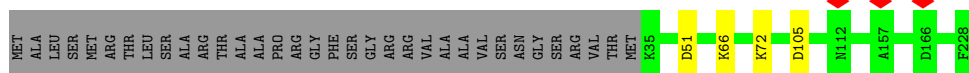
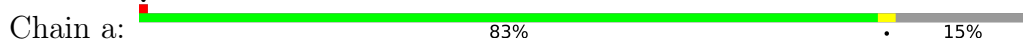
• Molecule 13: Photosystem I subunit O



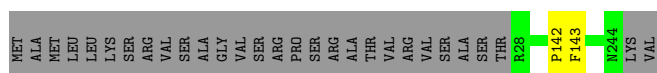
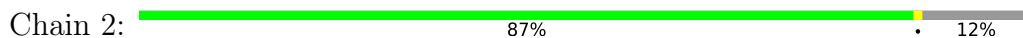
• Molecule 14: Chlorophyll a-b binding protein, chloroplastic



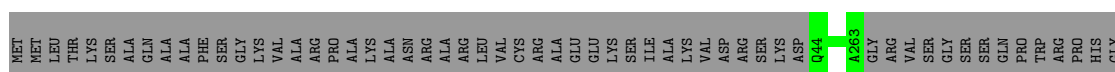
• Molecule 14: Chlorophyll a-b binding protein, chloroplastic



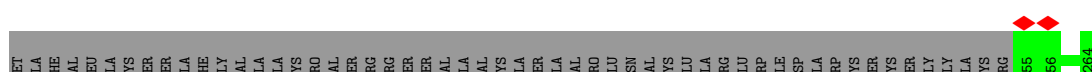
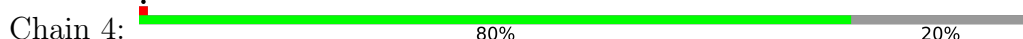
• Molecule 15: Chlorophyll a-b binding protein, chloroplastic




• Molecule 16: Chlorophyll a-b binding protein, chloroplastic



• Molecule 17: Chlorophyll a-b binding protein, chloroplastic




• Molecule 18: Chlorophyll a-b binding protein, chloroplastic

Chain Y:  85% 15%


MET ALA PHE LEU SER PHE SER ARG LYS LEU ALA GLN VAL SER LYS ALA ALA THR GLY LYS LYS GLY THR GLY LYS THR ALA ALA LYS LYS GLN ALA PRO ALA ALA SER SER SER GLY I39 H145 S256 ALA

- Molecule 24: Chlorophyll a-b binding protein, chloroplastic

Chain Z:  86% 14%


MET ALA PHE ALA LEU SER PHE SER ARG LYS ALA LEU GLN VAL SER LYS ALA ALA THR GLY LYS LYS GLY THR GLY LYS THR ALA ALA LYS LYS GLN ALA PRO ALA ALA SER SER SER G37 A257

- Molecule 24: Chlorophyll a-b binding protein, chloroplastic

Chain U:  85% 15%

MET ALA PHE ALA LEU SER PHE SER ARG LYS ALA LEU GLN VAL SER LYS ALA ALA THR GLY LYS LYS GLY THR GLY LYS THR ALA ALA LYS LYS GLN ALA PRO ALA ALA SER SER SER G39 A257 ILE

- Molecule 25: Chlorophyll a-b binding protein, chloroplastic

Chain V:  88% 11%

MET MET LEU SER THR VAL VAL ASN VAL GLN LYS LEU THR LYS LYS GLY ALA PRO ALA ALA SER SER ALA GLN K31 K32 T33 Q268

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	123997	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	1.5625	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.116	Depositor
Minimum map value	-0.049	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.005	Depositor
Map size (\AA)	360.0, 360.0, 360.0	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.0, 1.0, 1.0	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NEX, BCR, LUT, CLA, LHG, SF4, DGD, TPO, XAT, CHL, LMU, PQN, LMG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.58	0/6015	0.48	0/8201
2	B	0.58	0/6036	0.49	0/8242
3	C	0.56	0/610	0.58	0/826
4	D	0.52	0/1152	0.52	0/1556
5	E	0.55	0/506	0.46	0/689
6	F	0.46	0/1291	0.47	0/1747
7	G	0.35	0/714	0.45	0/972
8	H	0.44	0/788	0.48	0/1059
9	I	0.58	0/329	0.45	0/456
10	J	0.52	0/349	0.43	0/478
11	K	0.39	0/587	0.48	0/795
12	L	0.54	0/1190	0.48	0/1628
13	O	0.46	0/784	0.49	0/1069
14	1	0.42	0/1490	0.47	0/2028
14	a	0.41	0/1490	0.47	0/2028
15	2	0.42	0/1730	0.47	0/2353
16	3	0.49	0/1726	0.45	0/2342
17	4	0.36	0/1686	0.42	0/2300
18	5	0.43	0/1829	0.46	0/2492
19	6	0.42	0/1833	0.45	0/2505
20	7	0.50	0/1701	0.43	0/2310
21	8	0.45	0/1692	0.45	0/2304
22	9	0.41	0/1444	0.47	0/1964
23	W	0.29	0/1721	0.52	0/2341
23	X	0.32	0/1730	0.55	0/2355
24	U	0.31	0/1717	0.54	0/2336
24	Y	0.32	0/1723	0.53	0/2345
24	Z	0.32	0/1732	0.52	0/2357
25	V	0.31	0/1856	0.47	0/2518
All	All	0.46	0/47451	0.48	0/64596

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	739/751 (98%)	713 (96%)	26 (4%)	0	100	100
2	B	731/735 (100%)	701 (96%)	30 (4%)	0	100	100
3	C	78/81 (96%)	67 (86%)	11 (14%)	0	100	100
4	D	141/196 (72%)	135 (96%)	6 (4%)	0	100	100
5	E	61/97 (63%)	57 (93%)	4 (7%)	0	100	100
6	F	163/227 (72%)	156 (96%)	7 (4%)	0	100	100
7	G	92/126 (73%)	86 (94%)	6 (6%)	0	100	100
8	H	98/130 (75%)	94 (96%)	4 (4%)	0	100	100
9	I	40/106 (38%)	35 (88%)	5 (12%)	0	100	100
10	J	39/41 (95%)	38 (97%)	1 (3%)	0	100	100
11	K	84/113 (74%)	78 (93%)	6 (7%)	0	100	100
12	L	157/196 (80%)	146 (93%)	11 (7%)	0	100	100
13	O	95/126 (75%)	87 (92%)	8 (8%)	0	100	100
14	1	192/228 (84%)	186 (97%)	6 (3%)	0	100	100
14	a	192/228 (84%)	186 (97%)	6 (3%)	0	100	100
15	2	215/246 (87%)	203 (94%)	10 (5%)	2 (1%)	14	45

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
16	3	218/298 (73%)	211 (97%)	7 (3%)	0	100	100
17	4	208/264 (79%)	202 (97%)	6 (3%)	0	100	100
18	5	225/257 (88%)	211 (94%)	14 (6%)	0	100	100
19	6	228/257 (89%)	210 (92%)	18 (8%)	0	100	100
20	7	211/241 (88%)	197 (93%)	14 (7%)	0	100	100
21	8	214/243 (88%)	210 (98%)	4 (2%)	0	100	100
22	9	181/213 (85%)	165 (91%)	16 (9%)	0	100	100
23	W	218/249 (88%)	202 (93%)	16 (7%)	0	100	100
23	X	219/249 (88%)	194 (89%)	25 (11%)	0	100	100
24	U	217/257 (84%)	196 (90%)	21 (10%)	0	100	100
24	Y	217/257 (84%)	198 (91%)	19 (9%)	0	100	100
24	Z	219/257 (85%)	204 (93%)	15 (7%)	0	100	100
25	V	235/268 (88%)	222 (94%)	13 (6%)	0	100	100
All	All	5927/6937 (85%)	5590 (94%)	335 (6%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
15	2	142	PRO
15	2	143	PHE

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	601/610 (98%)	600 (100%)	1 (0%)	92	96
2	B	596/597 (100%)	594 (100%)	2 (0%)	91	95
3	C	69/70 (99%)	67 (97%)	2 (3%)	37	63
4	D	120/152 (79%)	120 (100%)	0	100	100
5	E	54/81 (67%)	54 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	F	127/169 (75%)	127 (100%)	0	100	100
7	G	70/94 (74%)	70 (100%)	0	100	100
8	H	81/102 (79%)	81 (100%)	0	100	100
9	I	33/76 (43%)	33 (100%)	0	100	100
10	J	37/37 (100%)	37 (100%)	0	100	100
11	K	59/80 (74%)	59 (100%)	0	100	100
12	L	121/148 (82%)	121 (100%)	0	100	100
13	O	78/101 (77%)	78 (100%)	0	100	100
14	1	137/162 (85%)	133 (97%)	4 (3%)	37	63
14	a	137/162 (85%)	133 (97%)	4 (3%)	37	63
15	2	173/198 (87%)	173 (100%)	0	100	100
16	3	167/230 (73%)	167 (100%)	0	100	100
17	4	165/205 (80%)	165 (100%)	0	100	100
18	5	184/206 (89%)	184 (100%)	0	100	100
19	6	184/203 (91%)	184 (100%)	0	100	100
20	7	164/181 (91%)	164 (100%)	0	100	100
21	8	162/183 (88%)	162 (100%)	0	100	100
22	9	140/159 (88%)	140 (100%)	0	100	100
23	W	164/187 (88%)	163 (99%)	1 (1%)	84	91
23	X	165/187 (88%)	162 (98%)	3 (2%)	54	74
24	U	168/194 (87%)	168 (100%)	0	100	100
24	Y	170/194 (88%)	169 (99%)	1 (1%)	84	91
24	Z	170/194 (88%)	170 (100%)	0	100	100
25	V	178/201 (89%)	178 (100%)	0	100	100
All	All	4674/5363 (87%)	4656 (100%)	18 (0%)	88	94

5 of 18 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
23	X	156	GLU
23	W	237	ASN
24	Y	145	HIS
14	1	227	PHE
23	X	104	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 13 such sidechains are listed below:

Mol	Chain	Res	Type
16	3	245	ASN
18	5	76	GLN
22	9	161	ASN
19	6	41	HIS
20	7	234	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is 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
25	TPO	V	33	25	8,10,11	1.56	1 (12%)	10,14,16	1.95	2 (20%)

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
25	TPO	V	33	25	-	3/9/11/13	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	V	33	TPO	P-O1P	3.28	1.61	1.50

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	V	33	TPO	P-OG1-CB	-5.21	107.48	123.21
25	V	33	TPO	CG2-CB-CA	-2.55	108.14	113.16

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
25	V	33	TPO	N-CA-CB-CG2
25	V	33	TPO	N-CA-CB-OG1
25	V	33	TPO	C-CA-CB-CG2

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

471 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$
26	CLA	A	805	-	52,60,73	1.67	12 (23%)	60,97,113	1.66	9 (15%)
26	CLA	4	611	28	42,50,73	1.78	8 (19%)	48,85,113	1.54	7 (14%)
29	BCR	A	852	-	41,41,41	0.97	1 (2%)	56,56,56	2.56	26 (46%)
37	CHL	X	607	-	66,74,74	1.85	14 (21%)	73,114,114	2.75	20 (27%)
28	LHG	9	622	26	29,29,48	1.18	2 (6%)	32,35,54	1.02	1 (3%)
26	CLA	Z	614	-	48,56,73	1.76	7 (14%)	55,92,113	1.42	7 (12%)
26	CLA	V	603	-	45,53,73	1.79	6 (13%)	52,89,113	1.63	7 (13%)
29	BCR	8	621	-	41,41,41	0.75	0	56,56,56	2.77	21 (37%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
26	CLA	V	611	28	43,51,73	1.86	7 (16%)	49,86,113	1.43	6 (12%)
26	CLA	6	610	19	65,73,73	1.55	9 (13%)	76,113,113	1.24	8 (10%)
35	XAT	3	619	-	39,47,47	0.98	2 (5%)	54,74,74	2.60	19 (35%)
26	CLA	8	609	21	45,53,73	1.78	8 (17%)	52,89,113	1.53	7 (13%)
26	CLA	8	602	21	60,68,73	1.57	7 (11%)	70,107,113	1.50	9 (12%)
26	CLA	1	606	-	37,47,73	1.96	9 (24%)	41,80,113	1.54	7 (17%)
26	CLA	3	609	16	60,68,73	1.59	10 (16%)	70,107,113	1.38	8 (11%)
29	BCR	K	207	-	41,41,41	0.85	1 (2%)	56,56,56	2.72	21 (37%)
26	CLA	a	610	14	59,67,73	1.55	7 (11%)	69,106,113	1.31	7 (10%)
26	CLA	1	604	-	49,57,73	1.74	9 (18%)	55,93,113	1.47	8 (14%)
26	CLA	A	845	28	50,58,73	1.68	7 (14%)	58,95,113	1.62	7 (12%)
26	CLA	Z	603	-	55,63,73	1.62	7 (12%)	64,101,113	1.51	10 (15%)
29	BCR	6	622	-	41,41,41	0.75	0	56,56,56	2.46	25 (44%)
26	CLA	V	614	-	45,53,73	1.81	7 (15%)	52,89,113	1.49	7 (13%)
34	LUT	8	619	-	42,43,43	0.86	1 (2%)	51,60,60	1.87	11 (21%)
26	CLA	B	812	-	43,51,73	1.80	8 (18%)	49,86,113	1.40	6 (12%)
28	LHG	A	847	26	29,29,48	1.16	2 (6%)	32,35,54	1.04	3 (9%)
26	CLA	4	608	-	65,73,73	1.50	9 (13%)	76,113,113	1.27	9 (11%)
26	CLA	2	604	-	42,50,73	1.82	7 (16%)	48,85,113	1.58	7 (14%)
26	CLA	K	201	11	45,53,73	1.76	8 (17%)	52,89,113	1.37	7 (13%)
26	CLA	6	601	19	65,73,73	1.48	10 (15%)	76,113,113	1.24	8 (10%)
26	CLA	a	613	-	54,62,73	1.62	9 (16%)	62,99,113	1.43	6 (9%)
26	CLA	8	608	-	51,59,73	1.68	11 (21%)	59,96,113	1.53	8 (13%)
26	CLA	W	602	23	60,68,73	1.58	7 (11%)	70,107,113	1.33	9 (12%)
26	CLA	Y	602	24	58,66,73	1.58	7 (12%)	67,104,113	1.40	9 (13%)
36	NEX	Z	1623	-	38,46,46	1.02	1 (2%)	50,70,70	2.64	19 (38%)
26	CLA	7	607	-	42,50,73	1.82	10 (23%)	48,85,113	1.39	7 (14%)
34	LUT	Z	1621	-	42,43,43	0.79	0	51,60,60	1.41	8 (15%)
26	CLA	Y	611	28	43,51,73	1.85	7 (16%)	49,86,113	1.44	6 (12%)
26	CLA	5	618	18	39,48,73	1.94	8 (20%)	48,83,113	1.57	9 (18%)
26	CLA	8	613	21	65,73,73	1.53	9 (13%)	76,113,113	1.25	7 (9%)
26	CLA	9	612	22	40,49,73	1.90	6 (15%)	45,84,113	1.41	6 (13%)
26	CLA	7	614	-	42,50,73	1.80	9 (21%)	48,85,113	1.45	6 (12%)
26	CLA	A	802	-	65,73,73	1.48	10 (15%)	76,113,113	1.55	10 (13%)
26	CLA	L	303	-	65,73,73	1.49	10 (15%)	76,113,113	1.37	10 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
26	CLA	7	616	20	43,51,73	1.87	8 (18%)	54,87,113	1.53	8 (14%)
26	CLA	K	203	-	56,64,73	1.60	10 (17%)	65,102,113	1.48	10 (15%)
26	CLA	W	604	-	47,55,73	1.80	6 (12%)	54,91,113	1.48	7 (12%)
26	CLA	3	602	16	60,68,73	1.55	9 (15%)	70,107,113	1.33	10 (14%)
26	CLA	1	603	-	52,61,73	1.64	8 (15%)	59,98,113	1.49	7 (11%)
28	LHG	5	623	26	48,48,48	0.93	2 (4%)	51,54,54	0.87	2 (3%)
26	CLA	B	823	-	45,53,73	1.79	10 (22%)	52,89,113	1.46	8 (15%)
26	CLA	2	611	28	42,50,73	1.81	7 (16%)	48,85,113	1.50	7 (14%)
26	CLA	9	602	22	60,68,73	1.55	7 (11%)	70,107,113	1.44	8 (11%)
26	CLA	B	838	-	46,54,73	1.74	7 (15%)	53,90,113	1.58	7 (13%)
26	CLA	5	616	18	41,50,73	1.90	10 (24%)	50,85,113	1.47	8 (16%)
28	LHG	U	2630	26	48,48,48	0.94	2 (4%)	51,54,54	1.08	4 (7%)
26	CLA	A	830	-	65,73,73	1.49	10 (15%)	76,113,113	1.29	8 (10%)
26	CLA	7	603	-	43,52,73	1.82	11 (25%)	49,88,113	1.63	8 (16%)
26	CLA	U	603	-	52,60,73	1.67	7 (13%)	60,97,113	1.48	9 (15%)
34	LUT	X	1621	-	42,43,43	0.81	0	51,60,60	1.74	15 (29%)
28	LHG	Z	2630	26	48,48,48	0.92	2 (4%)	51,54,54	0.97	2 (3%)
37	CHL	Y	605	24	42,50,74	2.50	17 (40%)	44,85,114	3.27	20 (45%)
26	CLA	A	821	-	53,61,73	1.64	9 (16%)	61,98,113	1.43	9 (14%)
26	CLA	U	610	24	56,64,73	1.57	7 (12%)	65,102,113	1.44	8 (12%)
26	CLA	A	817	-	45,53,73	1.81	10 (22%)	52,89,113	1.54	9 (17%)
26	CLA	Z	610	24	65,73,73	1.53	9 (13%)	76,113,113	1.28	8 (10%)
26	CLA	6	602	19	65,73,73	1.53	9 (13%)	76,113,113	1.24	9 (11%)
32	LMG	8	626	-	46,46,55	0.97	2 (4%)	54,54,63	1.10	4 (7%)
37	CHL	U	601	24	66,74,74	1.96	17 (25%)	73,114,114	2.52	20 (27%)
34	LUT	9	619	-	42,43,43	0.87	1 (2%)	51,60,60	1.90	14 (27%)
29	BCR	A	850	-	41,41,41	0.93	1 (2%)	56,56,56	2.02	14 (25%)
26	CLA	a	602	14	61,69,73	1.54	8 (13%)	71,108,113	1.43	8 (11%)
28	LHG	2	622	26	35,35,48	1.05	2 (5%)	38,41,54	1.16	3 (7%)
34	LUT	W	1621	-	42,43,43	0.69	0	51,60,60	1.78	13 (25%)
26	CLA	A	834	-	65,73,73	1.50	10 (15%)	76,113,113	1.47	8 (10%)
34	LUT	W	1620	-	42,43,43	0.72	0	51,60,60	1.59	11 (21%)
37	CHL	Y	606	-	46,54,74	2.24	15 (32%)	49,90,114	3.12	18 (36%)
37	CHL	U	607	-	46,54,74	2.28	14 (30%)	49,90,114	3.11	18 (36%)
26	CLA	A	819	-	59,67,73	1.53	11 (18%)	68,105,113	1.50	6 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
37	CHL	X	606	-	44,52,74	2.29	14 (31%)	46,87,114	3.19	18 (39%)
37	CHL	X	609	23	66,74,74	1.95	16 (24%)	73,114,114	2.72	23 (31%)
26	CLA	A	835	-	61,69,73	1.55	11 (18%)	71,108,113	1.35	9 (12%)
26	CLA	a	612	14	45,53,73	1.80	8 (17%)	52,89,113	1.51	6 (11%)
37	CHL	Z	601	24	66,74,74	1.89	16 (24%)	73,114,114	2.67	19 (26%)
26	CLA	6	606	-	39,48,73	1.90	8 (20%)	44,83,113	1.35	5 (11%)
26	CLA	W	613	23	65,73,73	1.53	8 (12%)	76,113,113	1.27	6 (7%)
26	CLA	6	609	19	45,53,73	1.83	10 (22%)	52,89,113	1.45	7 (13%)
26	CLA	B	819	-	55,63,73	1.65	9 (16%)	64,101,113	1.36	8 (12%)
26	CLA	A	814	-	65,73,73	1.47	11 (16%)	76,113,113	1.54	10 (13%)
27	PQN	B	842	-	34,34,34	3.33	8 (23%)	42,45,45	2.02	7 (16%)
26	CLA	2	612	15	44,52,73	1.80	8 (18%)	51,88,113	1.42	6 (11%)
26	CLA	1	610	14	38,47,73	1.89	7 (18%)	44,81,113	1.62	8 (18%)
34	LUT	3	618	-	42,43,43	0.83	1 (2%)	51,60,60	2.01	12 (23%)
26	CLA	A	836	-	65,73,73	1.47	11 (16%)	76,113,113	1.38	9 (11%)
26	CLA	U	602	24	59,67,73	1.57	7 (11%)	68,105,113	1.36	8 (11%)
37	CHL	U	609	24	60,68,74	2.01	14 (23%)	65,106,114	2.79	22 (33%)
29	BCR	3	620	-	41,41,41	0.80	0	56,56,56	2.38	23 (41%)
26	CLA	8	601	21	65,73,73	1.57	9 (13%)	76,113,113	1.26	7 (9%)
26	CLA	G	204	7	45,53,73	1.82	8 (17%)	52,89,113	1.45	7 (13%)
26	CLA	W	610	23	55,63,73	1.62	5 (9%)	64,101,113	1.43	10 (15%)
26	CLA	3	612	16	43,51,73	1.86	7 (16%)	49,86,113	1.41	6 (12%)
26	CLA	5	619	-	43,51,73	1.91	9 (20%)	54,87,113	1.60	10 (18%)
31	LMU	5	629	-	33,33,36	1.21	2 (6%)	44,44,47	1.27	6 (13%)
26	CLA	V	602	25	60,68,73	1.53	7 (11%)	70,107,113	1.42	8 (11%)
26	CLA	A	838	-	50,58,73	1.65	11 (22%)	58,95,113	1.54	9 (15%)
26	CLA	Z	612	24	45,53,73	1.82	7 (15%)	52,89,113	1.45	7 (13%)
26	CLA	1	614	-	37,45,73	2.10	8 (21%)	44,79,113	1.72	9 (20%)
26	CLA	A	824	-	65,73,73	1.47	10 (15%)	76,113,113	1.41	8 (10%)
26	CLA	8	610	21	60,68,73	1.52	7 (11%)	70,107,113	1.51	9 (12%)
28	LHG	O	2631	-	35,35,48	1.07	2 (5%)	38,41,54	1.12	3 (7%)
26	CLA	4	604	-	54,62,73	1.67	8 (14%)	67,100,113	1.46	10 (14%)
35	XAT	Y	1622	-	39,47,47	0.92	0	54,74,74	2.75	22 (40%)
34	LUT	a	617	-	42,43,43	0.80	1 (2%)	51,60,60	1.90	16 (31%)
28	LHG	4	622	26	48,48,48	0.91	2 (4%)	51,54,54	0.82	2 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
36	NEX	Y	1623	-	38,46,46	0.98	1 (2%)	50,70,70	2.52	16 (32%)
26	CLA	9	607	-	45,53,73	1.78	9 (20%)	52,89,113	1.38	7 (13%)
29	BCR	B	848	-	41,41,41	0.84	1 (2%)	56,56,56	2.53	14 (25%)
37	CHL	Z	606	-	46,54,74	2.29	16 (34%)	49,90,114	3.16	21 (42%)
26	CLA	Z	602	24	58,66,73	1.58	7 (12%)	67,104,113	1.37	6 (8%)
26	CLA	1	607	-	39,48,73	1.99	9 (23%)	44,83,113	1.40	7 (15%)
26	CLA	O	2003	-	39,48,73	1.87	9 (23%)	44,83,113	1.46	6 (13%)
26	CLA	a	601	14	53,62,73	1.65	9 (16%)	61,100,113	1.31	8 (13%)
26	CLA	9	604	-	50,58,73	1.76	8 (16%)	62,95,113	1.45	9 (14%)
26	CLA	A	816	-	65,73,73	1.48	10 (15%)	76,113,113	1.40	9 (11%)
26	CLA	3	604	-	65,73,73	1.50	10 (15%)	76,113,113	1.32	9 (11%)
35	XAT	1	618	-	39,47,47	0.91	0	54,74,74	2.46	21 (38%)
26	CLA	A	820	-	65,73,73	1.48	11 (16%)	76,113,113	1.42	9 (11%)
37	CHL	Z	609	24	66,74,74	1.94	14 (21%)	73,114,114	2.64	22 (30%)
29	BCR	A	851	-	41,41,41	0.91	1 (2%)	56,56,56	2.29	24 (42%)
26	CLA	A	826	-	64,72,73	1.47	8 (12%)	74,111,113	1.45	7 (9%)
26	CLA	4	614	-	56,64,73	1.61	7 (12%)	65,102,113	1.37	8 (12%)
26	CLA	H	203	-	65,73,73	1.48	9 (13%)	76,113,113	1.37	8 (10%)
26	CLA	7	609	20	43,52,73	1.84	10 (23%)	48,87,113	1.41	6 (12%)
26	CLA	X	602	23	65,73,73	1.50	7 (10%)	76,113,113	1.36	6 (7%)
26	CLA	A	810	1	50,58,73	1.73	9 (18%)	58,95,113	1.52	10 (17%)
26	CLA	8	611	28	42,50,73	1.83	10 (23%)	48,85,113	1.44	7 (14%)
26	CLA	1	609	14	40,48,73	1.88	8 (20%)	50,83,113	1.69	10 (20%)
26	CLA	W	614	-	45,53,73	1.80	6 (13%)	52,89,113	1.56	6 (11%)
26	CLA	B	831	-	65,73,73	1.49	9 (13%)	76,113,113	1.30	8 (10%)
26	CLA	6	612	19	40,49,73	1.85	8 (20%)	45,84,113	1.44	7 (15%)
37	CHL	W	608	-	47,55,74	2.26	15 (31%)	50,91,114	3.07	17 (34%)
26	CLA	B	832	-	60,68,73	1.58	9 (15%)	70,107,113	1.44	10 (14%)
26	CLA	9	611	28	42,50,73	1.88	7 (16%)	48,85,113	1.43	5 (10%)
33	DGD	B	850	-	63,63,67	0.83	2 (3%)	77,77,81	1.24	7 (9%)
26	CLA	1	602	14	61,69,73	1.54	7 (11%)	71,108,113	1.44	8 (11%)
26	CLA	Y	604	-	50,58,73	1.77	8 (16%)	58,95,113	1.41	6 (10%)
26	CLA	B	802	-	65,73,73	1.47	11 (16%)	76,113,113	1.33	8 (10%)
37	CHL	Z	608	-	49,57,74	2.23	16 (32%)	52,93,114	3.07	19 (36%)
28	LHG	H	204	-	48,48,48	0.92	2 (4%)	51,54,54	0.94	2 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
26	CLA	A	827	-	58,66,73	1.58	10 (17%)	67,104,113	1.32	7 (10%)
26	CLA	A	828	-	65,73,73	1.46	10 (15%)	76,113,113	1.42	8 (10%)
26	CLA	7	613	20	65,73,73	1.49	10 (15%)	76,113,113	1.35	8 (10%)
26	CLA	7	602	20	65,73,73	1.57	10 (15%)	76,113,113	1.26	8 (10%)
37	CHL	U	606	-	44,52,74	2.18	15 (34%)	46,87,114	3.21	18 (39%)
26	CLA	A	801	-	65,73,73	1.48	11 (16%)	76,113,113	1.36	9 (11%)
26	CLA	6	611	28	42,50,73	1.82	7 (16%)	48,85,113	1.44	6 (12%)
28	LHG	Y	2630	26	48,48,48	0.92	2 (4%)	51,54,54	1.01	2 (3%)
26	CLA	K	206	11	45,53,73	1.84	8 (17%)	52,89,113	1.39	6 (11%)
26	CLA	B	829	-	65,73,73	1.55	10 (15%)	76,113,113	1.50	10 (13%)
26	CLA	5	606	-	39,48,73	1.95	9 (23%)	44,83,113	1.38	5 (11%)
35	XAT	Z	1622	-	39,47,47	0.93	0	54,74,74	2.87	21 (38%)
26	CLA	X	603	-	62,70,73	1.56	6 (9%)	72,109,113	1.40	8 (11%)
29	BCR	7	623	-	41,41,41	0.87	0	56,56,56	2.01	17 (30%)
26	CLA	X	611	28	45,53,73	1.81	6 (13%)	52,89,113	1.43	6 (11%)
26	CLA	4	618	17	39,48,73	1.95	7 (17%)	48,83,113	1.54	8 (16%)
29	BCR	a	619	-	41,41,41	0.84	0	56,56,56	2.38	22 (39%)
26	CLA	B	815	-	43,51,73	1.80	10 (23%)	49,86,113	1.42	6 (12%)
26	CLA	3	617	16	39,48,73	1.86	9 (23%)	44,83,113	1.58	7 (15%)
29	BCR	A	856	-	41,41,41	0.91	2 (4%)	56,56,56	1.97	17 (30%)
26	CLA	B	836	-	50,58,73	1.63	9 (18%)	58,95,113	1.72	8 (13%)
26	CLA	1	601	14	53,62,73	1.64	9 (16%)	61,100,113	1.30	8 (13%)
37	CHL	X	601	23	66,74,74	1.89	16 (24%)	73,114,114	2.64	25 (34%)
34	LUT	V	1621	-	42,43,43	0.79	0	51,60,60	1.99	16 (31%)
26	CLA	B	820	-	50,58,73	1.69	9 (18%)	58,95,113	1.51	7 (12%)
34	LUT	Y	1620	-	42,43,43	0.80	0	51,60,60	3.18	18 (35%)
26	CLA	L	304	-	45,53,73	1.76	9 (20%)	52,89,113	1.45	8 (15%)
30	SF4	A	853	1,2	0,12,12	-	-	-	-	-
31	LMU	1	621	-	36,36,36	1.15	2 (5%)	47,47,47	1.00	1 (2%)
26	CLA	5	609	18	65,73,73	1.55	10 (15%)	76,113,113	1.32	8 (10%)
26	CLA	6	604	-	65,73,73	1.48	10 (15%)	76,113,113	1.21	8 (10%)
26	CLA	7	601	20	60,68,73	1.54	10 (16%)	70,107,113	1.48	8 (11%)
34	LUT	X	1620	-	42,43,43	0.73	0	51,60,60	1.54	9 (17%)
35	XAT	7	620	-	39,47,47	0.99	2 (5%)	54,74,74	2.50	18 (33%)
29	BCR	2	623	-	41,41,41	0.86	1 (2%)	56,56,56	2.36	20 (35%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
37	CHL	Y	607	-	66,74,74	1.86	14 (21%)	73,114,114	2.67	19 (26%)
26	CLA	F	301	-	57,65,73	1.62	9 (15%)	66,103,113	1.30	7 (10%)
26	CLA	W	603	-	52,60,73	1.64	6 (11%)	60,97,113	1.57	8 (13%)
26	CLA	W	611	28	57,65,73	1.62	5 (8%)	66,103,113	1.27	7 (10%)
26	CLA	A	803	-	65,73,73	1.53	12 (18%)	76,113,113	1.41	5 (6%)
26	CLA	A	831	-	65,73,73	1.52	10 (15%)	76,113,113	1.37	9 (11%)
26	CLA	A	833	-	45,53,73	1.77	9 (20%)	52,89,113	1.72	11 (21%)
26	CLA	B	830	-	43,51,73	1.87	9 (20%)	49,86,113	1.54	11 (22%)
29	BCR	B	853	-	41,41,41	0.87	3 (7%)	56,56,56	1.81	14 (25%)
26	CLA	B	806	2	65,73,73	1.48	12 (18%)	76,113,113	1.50	11 (14%)
34	LUT	U	1621	-	42,43,43	0.75	0	51,60,60	1.55	9 (17%)
26	CLA	6	618	19	39,48,73	1.92	9 (23%)	48,83,113	1.60	8 (16%)
29	BCR	L	308	-	41,41,41	0.81	0	56,56,56	2.33	23 (41%)
30	SF4	C	101	3	0,12,12	-	-	-	-	-
37	CHL	V	601	25	66,74,74	1.94	16 (24%)	73,114,114	2.60	20 (27%)
29	BCR	B	801	-	41,41,41	0.94	1 (2%)	56,56,56	2.10	18 (32%)
32	LMG	J	104	-	40,40,55	1.02	2 (5%)	48,48,63	1.30	6 (12%)
26	CLA	A	842	-	65,73,73	1.54	11 (16%)	76,113,113	1.48	10 (13%)
26	CLA	A	832	-	50,58,73	1.75	11 (22%)	58,95,113	1.59	10 (17%)
26	CLA	A	812	-	65,73,73	1.51	10 (15%)	76,113,113	1.30	8 (10%)
26	CLA	3	615	-	39,48,73	1.87	9 (23%)	44,83,113	1.47	6 (13%)
26	CLA	Y	612	24	45,53,73	1.85	7 (15%)	52,89,113	1.48	7 (13%)
26	CLA	A	811	-	65,73,73	1.52	10 (15%)	76,113,113	1.36	8 (10%)
26	CLA	5	601	18	56,64,73	1.59	8 (14%)	65,102,113	1.44	8 (12%)
26	CLA	Z	604	-	50,57,73	1.80	8 (16%)	53,93,113	1.57	8 (15%)
26	CLA	2	616	-	43,51,73	1.88	8 (18%)	54,87,113	1.52	8 (14%)
26	CLA	X	612	23	43,51,73	1.83	7 (16%)	49,86,113	1.50	8 (16%)
29	BCR	A	848	-	41,41,41	1.01	3 (7%)	56,56,56	2.24	14 (25%)
37	CHL	V	605	25	44,52,74	2.32	15 (34%)	46,87,114	3.17	17 (36%)
26	CLA	B	814	-	64,72,73	1.48	10 (15%)	74,111,113	1.43	9 (12%)
26	CLA	B	837	-	65,73,73	1.54	10 (15%)	76,113,113	1.39	10 (13%)
35	XAT	W	1622	-	39,47,47	0.92	1 (2%)	54,74,74	4.26	25 (46%)
26	CLA	B	821	-	43,51,73	1.93	9 (20%)	48,86,113	1.54	9 (18%)
36	NEX	W	1623	-	38,46,46	0.90	2 (5%)	50,70,70	2.54	12 (24%)
26	CLA	3	608	-	55,63,73	1.67	11 (20%)	64,101,113	1.27	6 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
26	CLA	1	612	14	45,53,73	1.79	8 (17%)	52,89,113	1.51	6 (11%)
34	LUT	Z	1620	-	42,43,43	0.78	0	51,60,60	1.80	12 (23%)
26	CLA	U	604	-	49,56,73	1.82	7 (14%)	50,91,113	1.58	7 (14%)
31	LMU	A	858	-	34,35,36	1.26	4 (11%)	42,45,47	0.99	2 (4%)
28	LHG	9	623	-	48,48,48	0.91	2 (4%)	51,54,54	0.96	2 (3%)
26	CLA	W	612	23	45,53,73	1.80	9 (20%)	52,89,113	1.55	8 (15%)
26	CLA	A	815	-	50,58,73	1.70	9 (18%)	58,95,113	1.49	7 (12%)
37	CHL	Z	605	24	42,50,74	2.37	15 (35%)	44,85,114	3.42	20 (45%)
28	LHG	V	2630	26	35,35,48	1.07	2 (5%)	38,41,54	1.08	2 (5%)
37	CHL	X	608	-	66,73,74	1.98	14 (21%)	68,112,114	2.63	18 (26%)
28	LHG	3	623	-	44,44,48	0.93	2 (4%)	47,50,54	1.00	3 (6%)
37	CHL	Y	609	24	66,74,74	1.92	14 (21%)	73,114,114	2.67	22 (30%)
26	CLA	Z	611	28	42,50,73	1.87	8 (19%)	52,85,113	1.59	9 (17%)
34	LUT	4	619	-	42,43,43	0.80	1 (2%)	51,60,60	2.02	18 (35%)
26	CLA	6	608	-	45,53,73	1.83	9 (20%)	52,89,113	1.46	8 (15%)
32	LMG	4	624	-	40,40,55	1.03	2 (5%)	48,48,63	1.15	5 (10%)
26	CLA	F	303	-	42,50,73	1.86	10 (23%)	48,85,113	1.55	7 (14%)
34	LUT	5	620	-	42,43,43	0.84	1 (2%)	51,60,60	1.91	15 (29%)
26	CLA	A	829	-	65,73,73	1.48	8 (12%)	76,113,113	1.55	8 (10%)
29	BCR	7	621	-	41,41,41	0.80	1 (2%)	56,56,56	2.28	22 (39%)
26	CLA	7	610	20	65,73,73	1.56	9 (13%)	76,113,113	1.19	7 (9%)
26	CLA	A	843	-	64,72,73	1.53	10 (15%)	74,111,113	1.35	9 (12%)
29	BCR	L	301	-	41,41,41	0.80	0	56,56,56	2.26	24 (42%)
26	CLA	4	602	17	60,68,73	1.63	8 (13%)	70,107,113	1.32	8 (11%)
32	LMG	H	205	-	55,55,55	0.86	2 (3%)	63,63,63	1.11	6 (9%)
32	LMG	V	2631	-	55,55,55	0.87	2 (3%)	63,63,63	1.11	5 (7%)
26	CLA	A	809	1	65,73,73	1.48	11 (16%)	76,113,113	1.43	8 (10%)
26	CLA	4	603	17	44,52,73	1.84	9 (20%)	55,88,113	1.54	10 (18%)
29	BCR	O	2005	-	41,41,41	0.88	1 (2%)	56,56,56	3.05	23 (41%)
28	LHG	a	620	26	42,42,48	0.98	2 (4%)	45,48,54	0.82	2 (4%)
28	LHG	6	623	26	47,47,48	0.91	2 (4%)	50,53,54	0.96	3 (6%)
34	LUT	1	617	-	42,43,43	0.80	1 (2%)	51,60,60	1.89	16 (31%)
37	CHL	X	605	-	46,54,74	2.45	16 (34%)	49,90,114	2.96	18 (36%)
26	CLA	5	607	-	65,73,73	1.50	10 (15%)	76,113,113	1.28	8 (10%)
26	CLA	7	615	-	41,50,73	1.91	8 (19%)	50,85,113	1.60	7 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
26	CLA	3	614	-	39,48,73	1.93	9 (23%)	44,83,113	1.52	6 (13%)
26	CLA	A	854	-	65,73,73	1.52	10 (15%)	76,113,113	1.52	8 (10%)
26	CLA	5	614	-	45,52,73	1.90	10 (22%)	48,87,113	1.47	6 (12%)
26	CLA	a	608	-	43,52,73	1.83	8 (18%)	49,88,113	1.46	8 (16%)
37	CHL	V	607	-	46,54,74	2.29	16 (34%)	49,90,114	3.02	20 (40%)
28	LHG	A	846	-	48,48,48	0.91	2 (4%)	51,54,54	0.87	2 (3%)
26	CLA	B	817	-	59,67,73	1.59	11 (18%)	68,105,113	1.41	7 (10%)
37	CHL	V	606	-	44,52,74	2.17	14 (31%)	46,87,114	3.18	21 (45%)
26	CLA	U	614	-	42,50,73	1.83	6 (14%)	48,85,113	1.55	7 (14%)
26	CLA	2	613	15	65,73,73	1.47	8 (12%)	76,113,113	1.25	7 (9%)
34	LUT	7	619	-	42,43,43	0.91	2 (4%)	51,60,60	1.99	14 (27%)
28	LHG	B	851	26	37,37,48	1.04	2 (5%)	40,43,54	1.14	4 (10%)
28	LHG	A	861	-	48,48,48	0.94	2 (4%)	51,54,54	1.00	2 (3%)
26	CLA	B	825	-	49,57,73	1.69	9 (18%)	55,93,113	1.56	9 (16%)
26	CLA	X	614	-	42,50,73	1.87	7 (16%)	48,85,113	1.46	7 (14%)
29	BCR	1	619	-	41,41,41	0.83	0	56,56,56	2.38	22 (39%)
26	CLA	3	611	28	37,46,73	1.98	7 (18%)	46,81,113	1.54	7 (15%)
26	CLA	4	612	17	40,49,73	1.88	8 (20%)	45,84,113	1.45	6 (13%)
26	CLA	5	603	-	54,62,73	1.69	10 (18%)	67,100,113	1.48	9 (13%)
26	CLA	B	826	-	62,70,73	1.52	9 (14%)	72,109,113	1.56	8 (11%)
26	CLA	6	614	-	60,68,73	1.56	8 (13%)	70,107,113	1.32	9 (12%)
29	BCR	B	843	-	41,41,41	1.04	4 (9%)	56,56,56	1.94	18 (32%)
32	LMG	9	625	-	55,55,55	0.88	2 (3%)	63,63,63	1.03	6 (9%)
26	CLA	F	304	6	41,49,73	1.91	10 (24%)	47,84,113	1.52	8 (17%)
26	CLA	3	610	16	65,73,73	1.55	9 (13%)	76,113,113	1.22	7 (9%)
26	CLA	8	616	21	43,51,73	1.88	6 (13%)	54,87,113	1.53	11 (20%)
26	CLA	B	839	-	65,73,73	1.48	11 (16%)	76,113,113	1.32	8 (10%)
31	LMU	5	628	-	34,34,36	1.19	2 (5%)	45,45,47	1.14	5 (11%)
37	CHL	V	609	25	61,69,74	2.00	15 (24%)	67,108,114	2.83	21 (31%)
32	LMG	5	627	-	40,40,55	1.03	2 (5%)	48,48,63	1.02	3 (6%)
26	CLA	a	616	14	45,53,73	1.78	6 (13%)	52,89,113	1.59	7 (13%)
26	CLA	9	601	22	45,53,73	1.81	8 (17%)	52,89,113	1.46	8 (15%)
28	LHG	W	2630	26	33,33,48	1.13	2 (6%)	36,39,54	1.17	3 (8%)
26	CLA	Y	610	24	65,73,73	1.55	8 (12%)	76,113,113	1.24	8 (10%)
29	BCR	5	622	-	41,41,41	0.87	2 (4%)	56,56,56	2.31	19 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
26	CLA	U	611	28	42,50,73	1.86	5 (11%)	48,85,113	1.51	7 (14%)
26	CLA	6	603	-	51,59,73	1.71	8 (15%)	63,96,113	1.53	9 (14%)
26	CLA	5	612	18	40,49,73	1.85	7 (17%)	45,84,113	1.49	6 (13%)
29	BCR	B	845	-	41,41,41	0.93	1 (2%)	56,56,56	2.50	23 (41%)
26	CLA	B	807	-	52,60,73	1.71	11 (21%)	60,97,113	1.48	9 (15%)
26	CLA	5	610	18	54,62,73	1.69	9 (16%)	62,99,113	1.30	7 (11%)
32	LMG	A	860	-	40,40,55	1.00	2 (5%)	48,48,63	1.09	4 (8%)
32	LMG	L	2631	-	37,37,55	1.08	2 (5%)	45,45,63	1.18	4 (8%)
26	CLA	7	608	-	50,58,73	1.71	11 (22%)	58,95,113	1.45	9 (15%)
26	CLA	K	204	-	45,53,73	1.75	10 (22%)	52,89,113	1.61	7 (13%)
26	CLA	B	811	-	53,60,73	1.74	10 (18%)	62,97,113	1.48	11 (17%)
34	LUT	2	619	-	42,43,43	0.91	2 (4%)	51,60,60	1.95	14 (27%)
36	NEX	5	624	-	38,46,46	1.08	1 (2%)	50,70,70	2.27	18 (36%)
26	CLA	A	825	-	65,73,73	1.49	10 (15%)	76,113,113	1.31	8 (10%)
26	CLA	B	804	-	41,49,73	1.80	9 (21%)	47,84,113	1.56	6 (12%)
26	CLA	7	612	20	44,52,73	1.78	7 (15%)	51,88,113	1.46	6 (11%)
26	CLA	U	612	24	42,50,73	1.84	5 (11%)	48,85,113	1.60	7 (14%)
26	CLA	A	823	-	42,50,73	1.79	8 (19%)	48,85,113	1.56	7 (14%)
26	CLA	4	610	17	61,69,73	1.53	7 (11%)	71,108,113	1.39	8 (11%)
29	BCR	B	852	-	41,41,41	0.82	0	56,56,56	4.21	30 (53%)
28	LHG	7	622	26	36,36,48	1.05	2 (5%)	39,42,54	1.02	3 (7%)
26	CLA	B	834	-	60,68,73	1.52	11 (18%)	70,107,113	1.39	9 (12%)
26	CLA	Y	614	-	48,56,73	1.75	6 (12%)	55,92,113	1.42	8 (14%)
29	BCR	G	205	-	41,41,41	0.80	1 (2%)	56,56,56	1.97	15 (26%)
35	XAT	V	1622	-	39,47,47	0.87	0	54,74,74	2.68	20 (37%)
36	NEX	V	1623	-	38,46,46	0.94	2 (5%)	50,70,70	2.30	18 (36%)
37	CHL	Y	608	-	49,57,74	2.19	15 (30%)	52,93,114	3.13	20 (38%)
26	CLA	4	616	17	43,51,73	1.90	8 (18%)	54,87,113	1.48	7 (12%)
26	CLA	1	611	28	57,65,73	1.60	7 (12%)	66,103,113	1.31	9 (13%)
26	CLA	A	804	-	65,73,73	1.45	11 (16%)	76,113,113	1.38	9 (11%)
26	CLA	B	808	-	65,73,73	1.54	10 (15%)	76,113,113	1.32	11 (14%)
26	CLA	X	604	-	49,57,73	1.78	5 (10%)	55,93,113	1.43	7 (12%)
37	CHL	U	605	24	43,51,74	2.41	15 (34%)	45,86,114	3.09	18 (40%)
37	CHL	W	607	-	65,73,74	2.00	16 (24%)	73,113,114	2.54	21 (28%)
29	BCR	3	622	-	41,41,41	0.89	1 (2%)	56,56,56	2.23	18 (32%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
26	CLA	A	806	-	65,73,73	1.50	12 (18%)	76,113,113	1.54	11 (14%)
26	CLA	B	840	-	65,73,73	1.58	11 (16%)	76,113,113	1.39	8 (10%)
26	CLA	5	602	18	65,73,73	1.52	9 (13%)	76,113,113	1.26	8 (10%)
29	BCR	B	847	-	41,41,41	0.92	2 (4%)	56,56,56	2.20	16 (28%)
26	CLA	9	606	-	39,48,73	1.90	9 (23%)	44,83,113	1.50	6 (13%)
28	LHG	8	622	26	48,48,48	0.91	2 (4%)	51,54,54	0.86	2 (3%)
26	CLA	A	818	-	60,68,73	1.52	9 (15%)	70,107,113	1.44	8 (11%)
29	BCR	3	621	-	41,41,41	0.83	1 (2%)	56,56,56	1.84	15 (26%)
26	CLA	3	606	-	53,62,73	1.61	10 (18%)	61,100,113	1.46	9 (14%)
35	XAT	4	620	-	39,47,47	0.94	2 (5%)	54,74,74	2.49	24 (44%)
29	BCR	K	202	-	41,41,41	0.94	2 (4%)	56,56,56	2.28	21 (37%)
29	BCR	L	309	-	41,41,41	0.78	0	56,56,56	2.40	25 (44%)
26	CLA	4	607	-	45,53,73	1.84	9 (20%)	52,89,113	1.43	7 (13%)
29	BCR	9	621	-	41,41,41	0.76	1 (2%)	56,56,56	2.90	18 (32%)
35	XAT	U	1622	-	39,47,47	0.92	1 (2%)	54,74,74	4.40	22 (40%)
26	CLA	a	611	28	37,46,73	1.99	8 (21%)	46,81,113	1.58	11 (23%)
37	CHL	W	609	23	66,74,74	1.98	15 (22%)	73,114,114	2.64	20 (27%)
26	CLA	B	818	-	60,68,73	1.57	11 (18%)	70,107,113	1.47	9 (12%)
26	CLA	A	822	-	65,73,73	1.51	10 (15%)	76,113,113	1.45	10 (13%)
26	CLA	9	609	22	61,69,73	1.54	10 (16%)	71,108,113	1.35	7 (9%)
26	CLA	7	604	-	50,58,73	1.69	9 (18%)	58,95,113	1.37	7 (12%)
26	CLA	8	606	-	64,72,73	1.53	9 (14%)	75,112,113	1.18	8 (10%)
35	XAT	X	1622	-	39,47,47	0.87	0	54,74,74	2.63	20 (37%)
35	XAT	5	621	-	39,47,47	0.95	2 (5%)	54,74,74	2.52	18 (33%)
26	CLA	V	612	25	45,53,73	1.81	8 (17%)	52,89,113	1.50	8 (15%)
29	BCR	B	844	-	41,41,41	1.08	4 (9%)	56,56,56	2.60	26 (46%)
26	CLA	6	616	19	65,73,73	1.49	10 (15%)	76,113,113	1.38	10 (13%)
26	CLA	Y	613	24	65,73,73	1.51	7 (10%)	76,113,113	1.30	7 (9%)
26	CLA	V	604	-	50,58,73	1.70	7 (14%)	58,95,113	1.52	7 (12%)
26	CLA	5	617	-	50,58,73	1.69	11 (22%)	58,95,113	1.38	8 (13%)
26	CLA	J	101	10	42,50,73	1.86	9 (21%)	48,85,113	1.41	7 (14%)
26	CLA	A	840	-	52,60,73	1.64	11 (21%)	60,97,113	1.56	8 (13%)
34	LUT	6	619	-	42,43,43	0.77	1 (2%)	51,60,60	2.07	18 (35%)
26	CLA	B	835	-	45,53,73	1.77	10 (22%)	52,89,113	1.50	7 (13%)
26	CLA	2	610	15	55,63,73	1.66	9 (16%)	64,101,113	1.30	8 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
26	CLA	a	604	-	49,57,73	1.73	9 (18%)	55,93,113	1.46	7 (12%)
26	CLA	2	601	15	65,73,73	1.43	9 (13%)	76,113,113	1.48	7 (9%)
26	CLA	H	202	-	38,47,73	1.96	8 (21%)	43,82,113	1.42	6 (13%)
28	LHG	5	625	-	48,48,48	0.91	2 (4%)	51,54,54	1.02	3 (5%)
37	CHL	W	601	23	66,74,74	1.97	16 (24%)	73,114,114	2.57	21 (28%)
26	CLA	3	613	16	52,61,73	1.70	9 (17%)	59,98,113	1.30	6 (10%)
26	CLA	L	306	-	39,48,73	1.88	9 (23%)	44,83,113	1.53	6 (13%)
26	CLA	9	613	22	65,73,73	1.51	9 (13%)	76,113,113	1.35	8 (10%)
26	CLA	6	607	-	41,49,73	1.91	8 (19%)	51,84,113	1.52	8 (15%)
26	CLA	2	603	15	43,52,73	1.88	10 (23%)	49,88,113	1.39	7 (14%)
26	CLA	B	809	2	65,73,73	1.53	11 (16%)	76,113,113	1.37	8 (10%)
26	CLA	V	610	25	62,70,73	1.52	8 (12%)	72,109,113	1.33	9 (12%)
26	CLA	A	807	1	65,73,73	1.52	11 (16%)	76,113,113	1.36	7 (9%)
26	CLA	2	607	-	43,52,73	1.81	9 (20%)	49,88,113	1.48	8 (16%)
27	PQN	A	844	-	34,34,34	3.31	9 (26%)	42,45,45	2.07	4 (9%)
34	LUT	V	1620	-	42,43,43	0.75	0	51,60,60	1.65	10 (19%)
26	CLA	5	604	-	63,71,73	1.59	8 (12%)	78,111,113	1.33	10 (12%)
26	CLA	B	824	-	65,73,73	1.49	10 (15%)	76,113,113	1.29	7 (9%)
26	CLA	5	613	18	64,72,73	1.48	9 (14%)	74,111,113	1.37	9 (12%)
37	CHL	W	605	23	46,54,74	2.31	17 (36%)	49,90,114	3.20	19 (38%)
26	CLA	6	620	-	64,72,73	1.51	10 (15%)	74,111,113	1.28	8 (10%)
26	CLA	O	2002	-	37,46,73	1.99	8 (21%)	46,81,113	1.62	9 (19%)
29	BCR	A	849	-	41,41,41	0.85	0	56,56,56	2.22	21 (37%)
29	BCR	B	846	-	41,41,41	0.81	1 (2%)	56,56,56	2.34	21 (37%)
26	CLA	4	613	17	65,73,73	1.56	9 (13%)	76,113,113	1.34	10 (13%)
29	BCR	4	621	-	41,41,41	0.83	1 (2%)	56,56,56	2.03	18 (32%)
26	CLA	a	609	14	63,72,73	1.51	9 (14%)	73,112,113	1.29	8 (10%)
26	CLA	2	614	-	41,50,73	1.86	8 (19%)	46,85,113	1.54	7 (15%)
26	CLA	A	841	-	65,73,73	1.48	10 (15%)	76,113,113	1.28	7 (9%)
26	CLA	a	603	-	54,62,73	1.61	8 (14%)	62,99,113	1.48	7 (11%)
26	CLA	X	613	23	65,73,73	1.51	7 (10%)	76,113,113	1.25	8 (10%)
26	CLA	2	609	15	45,53,73	1.86	9 (20%)	52,89,113	1.39	8 (15%)
28	LHG	8	623	-	39,39,48	1.03	2 (5%)	42,45,54	1.07	2 (4%)
29	BCR	B	849	-	41,41,41	0.93	2 (4%)	56,56,56	2.53	19 (33%)
37	CHL	U	608	-	44,52,74	2.22	13 (29%)	46,87,114	3.32	19 (41%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
26	CLA	6	617	-	45,53,73	1.76	9 (20%)	52,89,113	1.48	8 (15%)
37	CHL	W	606	-	46,54,74	2.21	15 (32%)	49,90,114	3.12	20 (40%)
26	CLA	B	841	28	65,73,73	1.49	9 (13%)	76,113,113	1.32	8 (10%)
26	CLA	B	803	-	65,73,73	1.45	11 (16%)	76,113,113	1.41	6 (7%)
34	LUT	U	1620	-	42,43,43	0.74	0	51,60,60	1.60	10 (19%)
37	CHL	Z	607	-	66,74,74	1.90	15 (22%)	73,114,114	2.67	18 (24%)
26	CLA	L	307	8	39,48,73	1.81	8 (20%)	44,83,113	1.66	6 (13%)
26	CLA	B	833	-	65,73,73	1.49	10 (15%)	76,113,113	1.28	8 (10%)
26	CLA	B	816	-	54,62,73	1.62	9 (16%)	62,99,113	1.42	8 (12%)
26	CLA	A	839	-	55,63,73	1.66	11 (20%)	64,101,113	1.41	9 (14%)
28	LHG	1	620	26	48,48,48	0.92	2 (4%)	51,54,54	0.79	2 (3%)
31	LMU	K	208	-	36,36,36	1.14	2 (5%)	47,47,47	1.00	3 (6%)
26	CLA	B	822	-	42,50,73	1.81	10 (23%)	48,85,113	1.44	7 (14%)
26	CLA	4	609	17	57,65,73	1.61	9 (15%)	66,103,113	1.24	6 (9%)
26	CLA	2	602	15	58,69,73	1.14	6 (10%)	69,102,113	1.04	4 (5%)
26	CLA	a	606	-	43,52,73	1.86	8 (18%)	48,87,113	1.39	5 (10%)
26	CLA	7	611	28	59,67,73	1.55	10 (16%)	68,105,113	1.32	8 (11%)
26	CLA	1	608	-	43,52,73	1.83	8 (18%)	49,88,113	1.45	8 (16%)
26	CLA	8	614	-	53,61,73	1.64	9 (16%)	61,98,113	1.43	8 (13%)
26	CLA	B	805	-	65,73,73	1.47	11 (16%)	76,113,113	1.40	9 (11%)
26	CLA	8	612	21	40,49,73	1.85	9 (22%)	45,84,113	1.51	6 (13%)
26	CLA	6	613	-	63,72,73	1.59	10 (15%)	73,112,113	1.31	9 (12%)
26	CLA	9	614	-	45,53,73	1.84	8 (17%)	52,89,113	1.35	7 (13%)
32	LMG	4	623	-	40,40,55	1.07	2 (5%)	48,48,63	1.15	5 (10%)
26	CLA	B	828	-	65,73,73	1.51	10 (15%)	76,113,113	1.29	7 (9%)
26	CLA	A	837	1	45,53,73	1.81	10 (22%)	52,89,113	1.62	8 (15%)
26	CLA	V	613	25	65,73,73	1.49	7 (10%)	76,113,113	1.28	6 (7%)
26	CLA	8	603	-	44,52,73	1.86	8 (18%)	55,88,113	1.65	8 (14%)
26	CLA	3	603	-	55,63,73	1.60	11 (20%)	64,101,113	1.52	8 (12%)
26	CLA	4	606	-	39,48,73	1.90	9 (23%)	44,83,113	1.39	6 (13%)
26	CLA	B	827	-	62,70,73	1.51	10 (16%)	72,109,113	1.49	9 (12%)
26	CLA	9	603	22	44,52,73	1.88	9 (20%)	55,88,113	1.52	7 (12%)
30	SF4	C	102	3	0,12,12	-	-	-	-	-
26	CLA	B	810	-	64,72,73	1.48	10 (15%)	74,111,113	1.52	11 (14%)
26	CLA	1	616	14	43,51,73	1.86	7 (16%)	54,87,113	1.63	9 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
26	CLA	L	302	12	45,53,73	1.86	10 (22%)	52,89,113	1.53	7 (13%)
26	CLA	Z	613	24	65,73,73	1.51	7 (10%)	76,113,113	1.28	6 (7%)
31	LMU	A	857	-	36,36,36	1.09	2 (5%)	47,47,47	1.37	8 (17%)
32	LMG	J	103	-	42,42,55	0.98	2 (4%)	50,50,63	1.22	6 (12%)
26	CLA	O	2001	-	36,46,73	1.99	9 (25%)	41,80,113	1.49	6 (14%)
29	BCR	O	2004	-	41,41,41	0.82	0	56,56,56	1.96	14 (25%)
36	NEX	X	1623	-	38,46,46	0.90	1 (2%)	50,70,70	4.33	20 (40%)
26	CLA	5	608	-	50,58,73	1.71	10 (20%)	58,95,113	1.32	7 (12%)
31	LMU	8	625	-	36,36,36	1.10	2 (5%)	47,47,47	1.24	3 (6%)
29	BCR	L	305	-	41,41,41	0.89	0	56,56,56	2.52	25 (44%)
26	CLA	4	601	17	65,73,73	1.49	10 (15%)	76,113,113	1.36	8 (10%)
26	CLA	A	813	-	54,62,73	1.66	10 (18%)	62,99,113	1.42	8 (12%)
29	BCR	F	305	-	41,41,41	0.89	1 (2%)	56,56,56	2.34	20 (35%)
26	CLA	8	604	-	50,58,73	1.68	7 (14%)	58,95,113	1.59	9 (15%)
26	CLA	Y	603	-	55,63,73	1.64	8 (14%)	64,101,113	1.51	9 (14%)
26	CLA	a	614	-	55,62,73	1.72	8 (14%)	60,99,113	1.46	7 (11%)
26	CLA	2	606	-	43,51,73	1.81	10 (23%)	49,86,113	1.49	8 (16%)
26	CLA	9	610	22	57,65,73	1.67	8 (14%)	66,103,113	1.35	9 (13%)
26	CLA	B	813	-	65,73,73	1.52	10 (15%)	76,113,113	1.31	8 (10%)
26	CLA	7	606	-	41,49,73	1.84	9 (21%)	47,84,113	1.44	6 (12%)
29	BCR	J	102	-	41,41,41	0.93	2 (4%)	56,56,56	2.40	22 (39%)
26	CLA	A	808	-	50,58,73	1.67	10 (20%)	58,95,113	1.53	8 (13%)
26	CLA	G	203	-	42,50,73	1.82	9 (21%)	48,85,113	1.53	8 (16%)
35	XAT	8	620	-	39,47,47	1.02	2 (5%)	54,74,74	2.45	24 (44%)
28	LHG	3	624	26	48,48,48	0.91	2 (4%)	51,54,54	0.97	3 (5%)
26	CLA	a	607	-	45,53,73	1.87	9 (20%)	52,89,113	1.35	7 (13%)
28	LHG	9	624	-	48,48,48	0.93	2 (4%)	51,54,54	0.87	2 (3%)
28	LHG	X	2630	26	48,48,48	0.92	2 (4%)	51,54,54	1.02	3 (5%)
35	XAT	6	621	-	39,47,47	0.98	3 (7%)	54,74,74	2.42	23 (42%)
26	CLA	1	613	-	65,73,73	1.48	9 (13%)	76,113,113	1.31	6 (7%)
37	CHL	Y	601	24	66,74,74	1.94	16 (24%)	73,114,114	2.63	21 (28%)
36	NEX	6	624	-	38,46,46	1.13	3 (7%)	50,70,70	2.40	18 (36%)
34	LUT	Y	1621	-	42,43,43	0.87	1 (2%)	51,60,60	1.87	14 (27%)
35	XAT	9	620	-	39,47,47	0.99	2 (5%)	54,74,74	2.51	19 (35%)
26	CLA	X	610	23	65,73,73	1.55	7 (10%)	76,113,113	1.26	7 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
37	CHL	V	608	-	48,56,74	2.18	14 (29%)	51,92,114	3.21	20 (39%)
26	CLA	8	607	-	41,49,73	1.91	8 (19%)	51,84,113	1.53	8 (15%)
35	XAT	a	618	-	39,47,47	0.90	0	54,74,74	2.47	21 (38%)
26	CLA	U	613	24	59,67,73	1.61	7 (11%)	68,105,113	1.33	9 (13%)
35	XAT	2	620	-	39,47,47	1.05	2 (5%)	54,74,74	2.48	26 (48%)
26	CLA	3	607	16	56,64,73	1.64	8 (14%)	69,102,113	1.39	10 (14%)
36	NEX	U	1623	-	38,46,46	0.93	1 (2%)	50,70,70	2.60	20 (40%)
26	CLA	5	611	28	42,50,73	1.81	6 (14%)	48,85,113	1.44	7 (14%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	CLA	A	805	-	-	7/22/100/115	-
26	CLA	4	611	28	1/1/10/20	7/10/88/115	-
29	BCR	A	852	-	-	8/29/63/63	0/2/2/2
37	CHL	X	607	-	3/3/20/26	25/39/137/137	-
28	LHG	9	622	26	-	10/34/34/53	-
26	CLA	Z	614	-	1/1/11/20	7/17/95/115	-
26	CLA	V	603	-	1/1/11/20	4/13/91/115	-
29	BCR	8	621	-	-	2/29/63/63	0/2/2/2
26	CLA	V	611	28	1/1/10/20	5/11/89/115	-
26	CLA	6	610	19	1/1/15/20	10/37/115/115	-
35	XAT	3	619	-	-	0/31/93/93	0/4/4/4
26	CLA	8	609	21	1/1/11/20	2/13/91/115	-
26	CLA	8	602	21	-	14/31/109/115	-
26	CLA	1	606	-	1/1/8/20	2/5/79/115	-
26	CLA	3	609	16	1/1/14/20	12/31/109/115	-
29	BCR	K	207	-	-	2/29/63/63	0/2/2/2
26	CLA	a	610	14	1/1/14/20	7/29/107/115	-
26	CLA	1	604	-	1/1/11/20	7/18/96/115	-
26	CLA	A	845	28	1/1/12/20	7/19/97/115	-
26	CLA	Z	603	-	1/1/13/20	9/25/103/115	-
29	BCR	6	622	-	-	2/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	CLA	V	614	-	1/1/11/20	4/13/91/115	-
34	LUT	8	619	-	-	4/29/67/67	0/2/2/2
26	CLA	B	812	-	1/1/10/20	3/11/89/115	-
28	LHG	A	847	26	-	6/34/34/53	-
26	CLA	4	608	-	1/1/15/20	9/37/115/115	-
26	CLA	2	604	-	1/1/10/20	3/9/87/115	-
26	CLA	K	201	11	1/1/11/20	5/13/91/115	-
26	CLA	6	601	19	1/1/15/20	17/37/115/115	-
26	CLA	a	613	-	1/1/12/20	9/24/102/115	-
26	CLA	8	608	-	-	5/21/99/115	-
26	CLA	W	602	23	1/1/14/20	10/31/109/115	-
26	CLA	Y	602	24	1/1/13/20	12/29/107/115	-
36	NEX	Z	1623	-	-	6/27/83/83	0/3/3/3
26	CLA	7	607	-	1/1/10/20	1/10/88/115	-
34	LUT	Z	1621	-	-	3/29/67/67	0/2/2/2
26	CLA	Y	611	28	1/1/10/20	7/11/89/115	-
26	CLA	5	618	18	1/1/10/20	3/8/84/115	-
26	CLA	8	613	21	1/1/15/20	16/37/115/115	-
26	CLA	9	612	22	1/1/10/20	2/8/86/115	-
26	CLA	7	614	-	1/1/10/20	1/10/88/115	-
26	CLA	A	802	-	1/1/15/20	12/37/115/115	-
26	CLA	L	303	-	-	12/37/115/115	-
26	CLA	7	616	20	1/1/11/20	8/11/87/115	-
26	CLA	K	203	-	-	10/27/105/115	-
26	CLA	W	604	-	1/1/11/20	6/16/94/115	-
26	CLA	3	602	16	1/1/14/20	3/31/109/115	-
26	CLA	1	603	-	1/1/12/20	5/21/99/115	-
28	LHG	5	623	26	-	15/53/53/53	-
26	CLA	B	823	-	1/1/11/20	6/13/91/115	-
26	CLA	2	611	28	1/1/10/20	2/10/88/115	-
26	CLA	9	602	22	1/1/14/20	7/31/109/115	-
26	CLA	B	838	-	1/1/11/20	3/15/93/115	-
26	CLA	5	616	18	1/1/10/20	4/8/84/115	-
28	LHG	U	2630	26	-	21/53/53/53	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	CLA	A	830	-	1/1/15/20	13/37/115/115	-
26	CLA	7	603	-	1/1/11/20	5/11/89/115	-
26	CLA	U	603	-	1/1/12/20	8/22/100/115	-
34	LUT	X	1621	-	-	3/29/67/67	0/2/2/2
28	LHG	Z	2630	26	-	19/53/53/53	-
37	CHL	Y	605	24	3/3/15/26	4/10/108/137	-
26	CLA	A	821	-	-	12/23/101/115	-
26	CLA	U	610	24	1/1/13/20	4/27/105/115	-
26	CLA	A	817	-	-	0/13/91/115	-
26	CLA	Z	610	24	1/1/15/20	7/37/115/115	-
26	CLA	6	602	19	-	8/37/115/115	-
37	CHL	U	601	24	3/3/20/26	19/39/137/137	-
32	LMG	8	626	-	-	16/41/61/70	0/1/1/1
34	LUT	9	619	-	-	4/29/67/67	0/2/2/2
29	BCR	A	850	-	-	2/29/63/63	0/2/2/2
26	CLA	a	602	14	1/1/14/20	5/33/111/115	-
28	LHG	2	622	26	-	9/40/40/53	-
34	LUT	W	1621	-	-	5/29/67/67	0/2/2/2
26	CLA	A	834	-	1/1/15/20	10/37/115/115	-
34	LUT	W	1620	-	-	6/29/67/67	0/2/2/2
37	CHL	Y	606	-	3/3/16/26	8/15/113/137	-
37	CHL	U	607	-	3/3/16/26	9/15/113/137	-
26	CLA	A	819	-	1/1/13/20	5/30/108/115	-
37	CHL	X	606	-	3/3/15/26	6/13/111/137	-
37	CHL	X	609	23	3/3/20/26	24/39/137/137	-
26	CLA	A	835	-	-	12/33/111/115	-
26	CLA	a	612	14	1/1/11/20	6/13/91/115	-
37	CHL	Z	601	24	3/3/20/26	16/39/137/137	-
26	CLA	6	606	-	1/1/10/20	0/6/84/115	-
26	CLA	W	613	23	1/1/15/20	20/37/115/115	-
26	CLA	6	609	19	1/1/11/20	5/13/91/115	-
26	CLA	B	819	-	1/1/13/20	6/25/103/115	-
26	CLA	A	814	-	1/1/15/20	18/37/115/115	-
27	PQN	B	842	-	-	7/23/43/43	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	CLA	2	612	15	1/1/11/20	5/11/89/115	-
26	CLA	1	610	14	1/1/9/20	2/6/80/115	-
34	LUT	3	618	-	-	4/29/67/67	0/2/2/2
26	CLA	A	836	-	1/1/15/20	9/37/115/115	-
26	CLA	U	602	24	1/1/13/20	16/30/108/115	-
37	CHL	U	609	24	3/3/18/26	12/32/130/137	-
29	BCR	3	620	-	-	4/29/63/63	0/2/2/2
26	CLA	8	601	21	1/1/15/20	14/37/115/115	-
26	CLA	G	204	7	1/1/11/20	5/13/91/115	-
26	CLA	W	610	23	1/1/13/20	5/25/103/115	-
26	CLA	3	612	16	1/1/10/20	5/11/89/115	-
26	CLA	5	619	-	1/1/11/20	10/11/87/115	-
31	LMU	5	629	-	-	11/18/58/61	0/2/2/2
26	CLA	V	602	25	1/1/14/20	8/31/109/115	-
26	CLA	A	838	-	1/1/12/20	8/19/97/115	-
26	CLA	Z	612	24	1/1/11/20	6/13/91/115	-
26	CLA	1	614	-	1/1/9/20	0/4/76/115	-
26	CLA	A	824	-	1/1/15/20	9/37/115/115	-
26	CLA	8	610	21	1/1/14/20	9/31/109/115	-
28	LHG	O	2631	-	-	13/40/40/53	-
26	CLA	4	604	-	1/1/13/20	9/25/101/115	-
35	XAT	Y	1622	-	-	3/31/93/93	0/4/4/4
34	LUT	a	617	-	-	4/29/67/67	0/2/2/2
28	LHG	4	622	26	-	8/53/53/53	-
36	NEX	Y	1623	-	-	6/27/83/83	0/3/3/3
26	CLA	9	607	-	-	9/13/91/115	-
29	BCR	B	848	-	-	4/29/63/63	0/2/2/2
37	CHL	Z	606	-	3/3/16/26	8/15/113/137	-
26	CLA	Z	602	24	1/1/13/20	5/29/107/115	-
26	CLA	1	607	-	1/1/10/20	0/6/84/115	-
26	CLA	O	2003	-	1/1/10/20	4/6/84/115	-
26	CLA	a	601	14	-	2/23/101/115	-
26	CLA	9	604	-	1/1/12/20	8/20/96/115	-
26	CLA	A	816	-	1/1/15/20	15/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	CLA	3	604	-	1/1/15/20	7/37/115/115	-
35	XAT	1	618	-	-	0/31/93/93	0/4/4/4
26	CLA	A	820	-	1/1/15/20	8/37/115/115	-
37	CHL	Z	609	24	3/3/20/26	16/39/137/137	-
29	BCR	A	851	-	-	2/29/63/63	0/2/2/2
26	CLA	A	826	-	1/1/14/20	8/35/113/115	-
26	CLA	4	614	-	-	7/27/105/115	-
26	CLA	H	203	-	1/1/15/20	15/37/115/115	-
26	CLA	7	609	20	1/1/10/20	6/10/88/115	-
26	CLA	X	602	23	1/1/15/20	13/37/115/115	-
26	CLA	A	810	1	-	5/19/97/115	-
26	CLA	8	611	28	1/1/10/20	4/10/88/115	-
26	CLA	1	609	14	1/1/10/20	3/8/84/115	-
26	CLA	W	614	-	1/1/11/20	6/13/91/115	-
26	CLA	B	831	-	1/1/15/20	12/37/115/115	-
26	CLA	6	612	19	1/1/10/20	3/8/86/115	-
37	CHL	W	608	-	3/3/16/26	9/17/115/137	-
26	CLA	B	832	-	1/1/14/20	12/31/109/115	-
26	CLA	9	611	28	1/1/10/20	3/10/88/115	-
33	DGD	B	850	-	-	15/51/91/95	0/2/2/2
26	CLA	1	602	14	1/1/14/20	5/33/111/115	-
26	CLA	Y	604	-	1/1/12/20	6/19/97/115	-
26	CLA	B	802	-	1/1/15/20	16/37/115/115	-
37	CHL	Z	608	-	3/3/16/26	6/19/117/137	-
28	LHG	H	204	-	-	15/53/53/53	-
26	CLA	A	827	-	1/1/13/20	5/29/107/115	-
26	CLA	A	828	-	1/1/15/20	16/37/115/115	-
26	CLA	7	613	20	1/1/15/20	16/37/115/115	-
26	CLA	7	602	20	1/1/15/20	10/37/115/115	-
37	CHL	U	606	-	3/3/15/26	6/13/111/137	-
26	CLA	A	801	-	1/1/15/20	10/37/115/115	-
26	CLA	6	611	28	1/1/10/20	3/10/88/115	-
28	LHG	Y	2630	26	-	13/53/53/53	-
26	CLA	K	206	11	1/1/11/20	4/13/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	CLA	B	829	-	1/1/15/20	8/37/115/115	-
26	CLA	5	606	-	-	1/6/84/115	-
35	XAT	Z	1622	-	-	4/31/93/93	0/4/4/4
26	CLA	X	603	-	1/1/14/20	13/34/112/115	-
29	BCR	7	623	-	-	3/29/63/63	0/2/2/2
26	CLA	X	611	28	1/1/11/20	4/13/91/115	-
26	CLA	4	618	17	1/1/10/20	2/8/84/115	-
29	BCR	a	619	-	-	3/29/63/63	0/2/2/2
26	CLA	B	815	-	1/1/10/20	2/11/89/115	-
26	CLA	3	617	16	1/1/10/20	0/6/84/115	-
29	BCR	A	856	-	-	2/29/63/63	0/2/2/2
26	CLA	B	836	-	1/1/12/20	4/19/97/115	-
37	CHL	X	601	23	3/3/20/26	19/39/137/137	-
26	CLA	1	601	14	-	2/23/101/115	-
34	LUT	V	1621	-	-	3/29/67/67	0/2/2/2
26	CLA	B	820	-	1/1/12/20	1/19/97/115	-
34	LUT	Y	1620	-	-	5/29/67/67	0/2/2/2
26	CLA	L	304	-	1/1/11/20	3/13/91/115	-
30	SF4	A	853	1,2	-	-	0/6/5/5
31	LMU	1	621	-	-	7/21/61/61	0/2/2/2
26	CLA	5	609	18	1/1/15/20	11/37/115/115	-
26	CLA	6	604	-	1/1/15/20	16/37/115/115	-
26	CLA	7	601	20	1/1/14/20	8/31/109/115	-
34	LUT	X	1620	-	-	4/29/67/67	0/2/2/2
35	XAT	7	620	-	-	0/31/93/93	0/4/4/4
37	CHL	Y	607	-	3/3/20/26	19/39/137/137	-
29	BCR	2	623	-	-	4/29/63/63	0/2/2/2
26	CLA	F	301	-	1/1/13/20	12/28/106/115	-
26	CLA	W	603	-	1/1/12/20	9/22/100/115	-
26	CLA	W	611	28	1/1/13/20	7/28/106/115	-
26	CLA	A	803	-	1/1/15/20	9/37/115/115	-
26	CLA	A	831	-	1/1/15/20	16/37/115/115	-
26	CLA	A	833	-	1/1/11/20	5/13/91/115	-
26	CLA	B	830	-	1/1/10/20	2/11/89/115	-
29	BCR	B	853	-	-	4/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	CLA	B	806	2	1/1/15/20	19/37/115/115	-
34	LUT	U	1621	-	-	5/29/67/67	0/2/2/2
26	CLA	6	618	19	1/1/10/20	1/8/84/115	-
29	BCR	L	308	-	-	6/29/63/63	0/2/2/2
37	CHL	V	601	25	3/3/20/26	13/39/137/137	-
30	SF4	C	101	3	-	-	0/6/5/5
29	BCR	B	801	-	-	4/29/63/63	0/2/2/2
32	LMG	J	104	-	-	12/35/55/70	0/1/1/1
26	CLA	A	842	-	1/1/15/20	16/37/115/115	-
26	CLA	A	832	-	1/1/12/20	9/19/97/115	-
26	CLA	A	812	-	1/1/15/20	7/37/115/115	-
26	CLA	3	615	-	1/1/10/20	3/6/84/115	-
26	CLA	Y	612	24	1/1/11/20	5/13/91/115	-
26	CLA	A	811	-	1/1/15/20	15/37/115/115	-
26	CLA	5	601	18	1/1/13/20	1/27/105/115	-
26	CLA	Z	604	-	1/1/11/20	5/19/93/115	-
26	CLA	2	616	-	1/1/11/20	3/11/87/115	-
26	CLA	X	612	23	1/1/10/20	6/11/89/115	-
37	CHL	V	605	25	3/3/15/26	5/13/111/137	-
29	BCR	A	848	-	-	3/29/63/63	0/2/2/2
26	CLA	B	814	-	1/1/14/20	15/36/114/115	-
26	CLA	B	837	-	-	8/37/115/115	-
35	XAT	W	1622	-	-	2/31/93/93	0/4/4/4
26	CLA	B	821	-	1/1/11/20	3/11/89/115	-
36	NEX	W	1623	-	-	6/27/83/83	0/3/3/3
26	CLA	3	608	-	1/1/13/20	8/25/103/115	-
26	CLA	1	612	14	1/1/11/20	6/13/91/115	-
34	LUT	Z	1620	-	-	5/29/67/67	0/2/2/2
26	CLA	U	604	-	1/1/10/20	7/18/92/115	-
31	LMU	A	858	-	-	10/21/57/61	0/2/2/2
28	LHG	9	623	-	-	20/53/53/53	-
26	CLA	W	612	23	1/1/11/20	5/13/91/115	-
26	CLA	A	815	-	1/1/12/20	10/19/97/115	-
37	CHL	Z	605	24	3/3/15/26	4/10/108/137	-
28	LHG	V	2630	26	-	6/40/40/53	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
37	CHL	X	608	-	3/3/19/26	21/39/133/137	-
37	CHL	Y	609	24	3/3/20/26	15/39/137/137	-
28	LHG	3	623	-	-	15/49/49/53	-
26	CLA	Z	611	28	1/1/10/20	5/11/87/115	-
34	LUT	4	619	-	-	4/29/67/67	0/2/2/2
26	CLA	6	608	-	-	6/13/91/115	-
32	LMG	4	624	-	-	5/35/55/70	0/1/1/1
26	CLA	F	303	-	-	5/10/88/115	-
34	LUT	5	620	-	-	0/29/67/67	0/2/2/2
26	CLA	A	829	-	1/1/15/20	10/37/115/115	-
29	BCR	7	621	-	-	2/29/63/63	0/2/2/2
26	CLA	7	610	20	1/1/15/20	5/37/115/115	-
26	CLA	A	843	-	1/1/14/20	14/35/113/115	-
29	BCR	L	301	-	-	4/29/63/63	0/2/2/2
26	CLA	4	602	17	1/1/14/20	6/31/109/115	-
32	LMG	H	205	-	-	14/50/70/70	0/1/1/1
32	LMG	V	2631	-	-	12/50/70/70	0/1/1/1
26	CLA	A	809	1	1/1/15/20	9/37/115/115	-
26	CLA	4	603	17	1/1/11/20	5/13/89/115	-
29	BCR	O	2005	-	-	2/29/63/63	0/2/2/2
28	LHG	a	620	26	-	7/47/47/53	-
28	LHG	6	623	26	-	19/52/52/53	-
34	LUT	1	617	-	-	4/29/67/67	0/2/2/2
37	CHL	X	605	-	3/3/16/26	7/15/113/137	-
26	CLA	5	607	-	1/1/15/20	13/37/115/115	-
26	CLA	7	615	-	1/1/10/20	6/8/84/115	-
26	CLA	3	614	-	1/1/10/20	0/6/84/115	-
26	CLA	A	854	-	1/1/15/20	9/37/115/115	-
26	CLA	5	614	-	1/1/10/20	7/13/87/115	-
26	CLA	a	608	-	1/1/11/20	2/11/89/115	-
37	CHL	V	607	-	3/3/16/26	10/15/113/137	-
28	LHG	A	846	-	-	15/53/53/53	-
26	CLA	B	817	-	1/1/13/20	8/30/108/115	-
37	CHL	V	606	-	3/3/15/26	4/13/111/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	CLA	U	614	-	1/1/10/20	3/10/88/115	-
26	CLA	2	613	15	1/1/15/20	8/37/115/115	-
34	LUT	7	619	-	-	2/29/67/67	0/2/2/2
28	LHG	B	851	26	-	14/42/42/53	-
28	LHG	A	861	-	-	18/53/53/53	-
26	CLA	B	825	-	-	4/18/96/115	-
26	CLA	X	614	-	1/1/10/20	1/10/88/115	-
29	BCR	1	619	-	-	3/29/63/63	0/2/2/2
26	CLA	3	611	28	1/1/10/20	3/4/80/115	-
26	CLA	4	612	17	1/1/10/20	4/8/86/115	-
26	CLA	5	603	-	1/1/13/20	5/25/101/115	-
26	CLA	B	826	-	1/1/14/20	14/34/112/115	-
26	CLA	6	614	-	1/1/14/20	7/31/109/115	-
29	BCR	B	843	-	-	4/29/63/63	0/2/2/2
32	LMG	9	625	-	-	11/50/70/70	0/1/1/1
26	CLA	3	610	16	1/1/15/20	12/37/115/115	-
26	CLA	8	616	21	1/1/11/20	5/11/87/115	-
26	CLA	F	304	6	-	3/8/86/115	-
26	CLA	B	839	-	1/1/15/20	14/37/115/115	-
31	LMU	5	628	-	-	10/19/59/61	0/2/2/2
37	CHL	V	609	25	3/3/19/26	11/33/131/137	-
32	LMG	5	627	-	-	7/35/55/70	0/1/1/1
26	CLA	a	616	14	1/1/11/20	7/13/91/115	-
26	CLA	9	601	22	1/1/11/20	6/13/91/115	-
28	LHG	W	2630	26	-	13/38/38/53	-
26	CLA	Y	610	24	1/1/15/20	8/37/115/115	-
29	BCR	5	622	-	-	1/29/63/63	0/2/2/2
26	CLA	U	611	28	1/1/10/20	2/10/88/115	-
26	CLA	6	603	-	1/1/12/20	5/22/98/115	-
26	CLA	5	612	18	1/1/10/20	2/8/86/115	-
29	BCR	B	845	-	-	9/29/63/63	0/2/2/2
26	CLA	B	807	-	-	2/22/100/115	-
26	CLA	5	610	18	1/1/12/20	4/24/102/115	-
32	LMG	A	860	-	-	9/35/55/70	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	LMG	L	2631	-	-	4/32/52/70	0/1/1/1
26	CLA	7	608	-	-	2/19/97/115	-
26	CLA	K	204	-	1/1/11/20	3/13/91/115	-
26	CLA	B	811	-	1/1/12/20	11/23/95/115	-
34	LUT	2	619	-	-	2/29/67/67	0/2/2/2
36	NEX	5	624	-	-	2/27/83/83	0/3/3/3
26	CLA	A	825	-	1/1/15/20	15/37/115/115	-
26	CLA	B	804	-	1/1/10/20	3/8/86/115	-
26	CLA	7	612	20	1/1/11/20	4/11/89/115	-
26	CLA	U	612	24	1/1/10/20	3/10/88/115	-
26	CLA	A	823	-	1/1/10/20	1/10/88/115	-
26	CLA	4	610	17	1/1/14/20	8/33/111/115	-
29	BCR	B	852	-	-	6/29/63/63	0/2/2/2
28	LHG	7	622	26	-	19/41/41/53	-
26	CLA	B	834	-	1/1/14/20	5/31/109/115	-
26	CLA	Y	614	-	1/1/11/20	8/17/95/115	-
29	BCR	G	205	-	-	2/29/63/63	0/2/2/2
35	XAT	V	1622	-	-	2/31/93/93	0/4/4/4
36	NEX	V	1623	-	-	7/27/83/83	0/3/3/3
37	CHL	Y	608	-	3/3/16/26	6/19/117/137	-
26	CLA	4	616	17	1/1/11/20	7/11/87/115	-
26	CLA	1	611	28	1/1/13/20	5/28/106/115	-
26	CLA	A	804	-	1/1/15/20	16/37/115/115	-
26	CLA	B	808	-	1/1/15/20	13/37/115/115	-
26	CLA	X	604	-	1/1/11/20	9/18/96/115	-
37	CHL	U	605	24	3/3/15/26	4/12/110/137	-
37	CHL	W	607	-	3/3/20/26	21/37/135/137	-
29	BCR	3	622	-	-	3/29/63/63	0/2/2/2
26	CLA	A	806	-	1/1/15/20	13/37/115/115	-
26	CLA	B	840	-	1/1/15/20	7/37/115/115	-
26	CLA	5	602	18	1/1/15/20	10/37/115/115	-
29	BCR	B	847	-	-	2/29/63/63	0/2/2/2
26	CLA	9	606	-	1/1/10/20	2/6/84/115	-
28	LHG	8	622	26	-	13/53/53/53	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	CLA	A	818	-	-	15/31/109/115	-
29	BCR	3	621	-	-	0/29/63/63	0/2/2/2
26	CLA	3	606	-	1/1/13/20	2/23/101/115	-
35	XAT	4	620	-	-	2/31/93/93	0/4/4/4
29	BCR	K	202	-	-	4/29/63/63	0/2/2/2
29	BCR	L	309	-	-	3/29/63/63	0/2/2/2
26	CLA	4	607	-	1/1/11/20	5/13/91/115	-
29	BCR	9	621	-	-	4/29/63/63	0/2/2/2
35	XAT	U	1622	-	-	4/31/93/93	0/4/4/4
26	CLA	a	611	28	1/1/10/20	0/4/80/115	-
37	CHL	W	609	23	3/3/20/26	11/39/137/137	-
26	CLA	B	818	-	-	11/31/109/115	-
26	CLA	A	822	-	1/1/15/20	6/37/115/115	-
26	CLA	9	609	22	1/1/14/20	4/33/111/115	-
26	CLA	7	604	-	1/1/12/20	7/19/97/115	-
26	CLA	8	606	-	1/1/15/20	7/35/113/115	-
35	XAT	X	1622	-	-	3/31/93/93	0/4/4/4
35	XAT	5	621	-	-	0/31/93/93	0/4/4/4
26	CLA	V	612	25	1/1/11/20	5/13/91/115	-
29	BCR	B	844	-	-	2/29/63/63	0/2/2/2
26	CLA	6	616	19	1/1/15/20	18/37/115/115	-
26	CLA	V	604	-	1/1/12/20	8/19/97/115	-
26	CLA	Y	613	24	-	14/37/115/115	-
26	CLA	5	617	-	1/1/12/20	10/19/97/115	-
26	CLA	J	101	10	1/1/10/20	5/10/88/115	-
26	CLA	A	840	-	-	5/22/100/115	-
34	LUT	6	619	-	-	4/29/67/67	0/2/2/2
26	CLA	B	835	-	1/1/11/20	2/13/91/115	-
26	CLA	2	610	15	1/1/13/20	3/25/103/115	-
26	CLA	a	604	-	1/1/11/20	7/18/96/115	-
26	CLA	2	601	15	1/1/15/20	8/37/115/115	-
26	CLA	H	202	-	1/1/10/20	2/4/82/115	-
28	LHG	5	625	-	-	14/53/53/53	-
37	CHL	W	601	23	3/3/20/26	19/39/137/137	-
26	CLA	3	613	16	1/1/12/20	5/21/99/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	CLA	L	306	-	1/1/10/20	1/6/84/115	-
26	CLA	9	613	22	1/1/15/20	12/37/115/115	-
26	CLA	6	607	-	1/1/10/20	2/10/86/115	-
26	CLA	2	603	15	1/1/11/20	5/11/89/115	-
26	CLA	B	809	2	1/1/15/20	11/37/115/115	-
26	CLA	V	610	25	1/1/14/20	7/34/112/115	-
26	CLA	A	807	1	1/1/15/20	20/37/115/115	-
26	CLA	2	607	-	1/1/11/20	0/11/89/115	-
27	PQN	A	844	-	-	6/23/43/43	0/2/2/2
34	LUT	V	1620	-	-	4/29/67/67	0/2/2/2
26	CLA	5	604	-	1/1/15/20	12/35/111/115	-
26	CLA	B	824	-	1/1/15/20	10/37/115/115	-
26	CLA	5	613	18	1/1/14/20	14/35/113/115	-
37	CHL	W	605	23	3/3/16/26	10/15/113/137	-
26	CLA	6	620	-	1/1/14/20	10/35/113/115	-
26	CLA	O	2002	-	1/1/10/20	0/4/80/115	-
29	BCR	A	849	-	-	5/29/63/63	0/2/2/2
29	BCR	B	846	-	-	0/29/63/63	0/2/2/2
26	CLA	4	613	17	1/1/15/20	11/37/115/115	-
29	BCR	4	621	-	-	2/29/63/63	0/2/2/2
26	CLA	a	609	14	1/1/15/20	13/35/113/115	-
26	CLA	2	614	-	1/1/10/20	0/9/87/115	-
26	CLA	A	841	-	1/1/15/20	16/37/115/115	-
26	CLA	a	603	-	1/1/12/20	8/23/101/115	-
26	CLA	X	613	23	1/1/15/20	12/37/115/115	-
26	CLA	2	609	15	1/1/11/20	3/13/91/115	-
28	LHG	8	623	-	-	12/44/44/53	-
29	BCR	B	849	-	-	5/29/63/63	0/2/2/2
37	CHL	U	608	-	3/3/15/26	5/13/111/137	-
26	CLA	6	617	-	1/1/11/20	7/13/91/115	-
37	CHL	W	606	-	3/3/16/26	2/15/113/137	-
26	CLA	B	841	28	1/1/15/20	15/37/115/115	-
26	CLA	B	803	-	1/1/15/20	12/37/115/115	-
34	LUT	U	1620	-	-	7/29/67/67	0/2/2/2
37	CHL	Z	607	-	3/3/20/26	21/39/137/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	CLA	L	307	8	1/1/10/20	2/6/84/115	-
26	CLA	B	833	-	1/1/15/20	11/37/115/115	-
26	CLA	B	816	-	1/1/12/20	10/23/101/115	-
26	CLA	A	839	-	1/1/13/20	8/25/103/115	-
28	LHG	1	620	26	-	9/53/53/53	-
31	LMU	K	208	-	-	10/21/61/61	0/2/2/2
26	CLA	B	822	-	-	7/10/88/115	-
26	CLA	4	609	17	1/1/13/20	3/28/106/115	-
26	CLA	2	602	15	1/1/15/20	14/39/99/115	-
26	CLA	a	606	-	1/1/10/20	7/10/88/115	-
26	CLA	7	611	28	1/1/13/20	6/29/107/115	-
26	CLA	1	608	-	1/1/11/20	2/11/89/115	-
26	CLA	8	614	-	1/1/12/20	8/23/101/115	-
26	CLA	B	805	-	1/1/15/20	11/37/115/115	-
26	CLA	8	612	21	1/1/10/20	2/8/86/115	-
26	CLA	6	613	-	-	13/35/113/115	-
26	CLA	9	614	-	1/1/11/20	3/13/91/115	-
32	LMG	4	623	-	-	6/35/55/70	0/1/1/1
26	CLA	B	828	-	1/1/15/20	17/37/115/115	-
26	CLA	A	837	1	1/1/11/20	7/13/91/115	-
26	CLA	V	613	25	1/1/15/20	18/37/115/115	-
26	CLA	8	603	-	1/1/11/20	4/13/89/115	-
26	CLA	3	603	-	1/1/13/20	10/25/103/115	-
26	CLA	4	606	-	1/1/10/20	2/6/84/115	-
26	CLA	B	827	-	1/1/14/20	12/34/112/115	-
26	CLA	9	603	22	1/1/11/20	5/13/89/115	-
30	SF4	C	102	3	-	-	0/6/5/5
26	CLA	B	810	-	1/1/14/20	20/35/113/115	-
26	CLA	1	616	14	1/1/11/20	7/11/87/115	-
26	CLA	L	302	12	1/1/11/20	8/13/91/115	-
26	CLA	Z	613	24	1/1/15/20	6/37/115/115	-
31	LMU	A	857	-	-	9/21/61/61	0/2/2/2
32	LMG	J	103	-	-	10/37/57/70	0/1/1/1
26	CLA	O	2001	-	1/1/9/20	2/4/78/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	BCR	O	2004	-	-	2/29/63/63	0/2/2/2
36	NEX	X	1623	-	-	5/27/83/83	0/3/3/3
26	CLA	5	608	-	1/1/12/20	4/19/97/115	-
31	LMU	8	625	-	-	12/21/61/61	0/2/2/2
29	BCR	L	305	-	-	2/29/63/63	0/2/2/2
26	CLA	4	601	17	1/1/15/20	14/37/115/115	-
26	CLA	A	813	-	1/1/12/20	5/24/102/115	-
29	BCR	F	305	-	-	6/29/63/63	0/2/2/2
26	CLA	8	604	-	1/1/12/20	6/19/97/115	-
26	CLA	Y	603	-	1/1/13/20	10/25/103/115	-
26	CLA	a	614	-	1/1/12/20	7/25/99/115	-
26	CLA	2	606	-	1/1/10/20	3/11/89/115	-
26	CLA	9	610	22	1/1/13/20	3/28/106/115	-
26	CLA	B	813	-	1/1/15/20	20/37/115/115	-
26	CLA	7	606	-	1/1/10/20	2/8/86/115	-
29	BCR	J	102	-	-	2/29/63/63	0/2/2/2
26	CLA	A	808	-	1/1/12/20	3/19/97/115	-
26	CLA	G	203	-	1/1/10/20	3/10/88/115	-
35	XAT	8	620	-	-	0/31/93/93	0/4/4/4
28	LHG	3	624	26	-	14/53/53/53	-
26	CLA	a	607	-	1/1/11/20	4/13/91/115	-
28	LHG	9	624	-	-	17/53/53/53	-
28	LHG	X	2630	26	-	13/53/53/53	-
35	XAT	6	621	-	-	0/31/93/93	0/4/4/4
26	CLA	1	613	-	1/1/15/20	17/37/115/115	-
37	CHL	Y	601	24	3/3/20/26	19/39/137/137	-
36	NEX	6	624	-	-	3/27/83/83	0/3/3/3
34	LUT	Y	1621	-	-	3/29/67/67	0/2/2/2
35	XAT	9	620	-	-	0/31/93/93	0/4/4/4
26	CLA	X	610	23	1/1/15/20	11/37/115/115	-
37	CHL	V	608	-	3/3/16/26	5/18/116/137	-
26	CLA	8	607	-	1/1/10/20	2/10/86/115	-
35	XAT	a	618	-	-	0/31/93/93	0/4/4/4
26	CLA	U	613	24	1/1/13/20	11/30/108/115	-
35	XAT	2	620	-	-	0/31/93/93	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	CLA	3	607	16	1/1/13/20	6/28/104/115	-
36	NEX	U	1623	-	-	6/27/83/83	0/3/3/3
26	CLA	5	611	28	1/1/10/20	0/10/88/115	-

The worst 5 of 3353 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	B	842	PQN	C12-C13	9.58	1.56	1.33
27	A	844	PQN	C12-C13	9.30	1.55	1.33
26	X	604	CLA	C4B-NB	8.04	1.42	1.35
26	3	612	CLA	C4B-NB	8.03	1.42	1.35
26	Y	604	CLA	C4B-NB	8.01	1.42	1.35

The worst 5 of 4786 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	X	1623	NEX	C17-C1-C6	-20.23	92.37	110.47
35	U	1622	XAT	C37-C21-C36	-17.41	81.69	107.37
35	W	1622	XAT	C37-C21-C36	-17.39	81.72	107.37
29	B	852	BCR	C32-C1-C6	-16.31	83.85	110.30
35	U	1622	XAT	C37-C21-C22	-15.46	82.13	108.98

5 of 378 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
26	A	801	CLA	ND
26	A	802	CLA	ND
26	A	803	CLA	ND
26	A	804	CLA	ND
26	A	806	CLA	ND

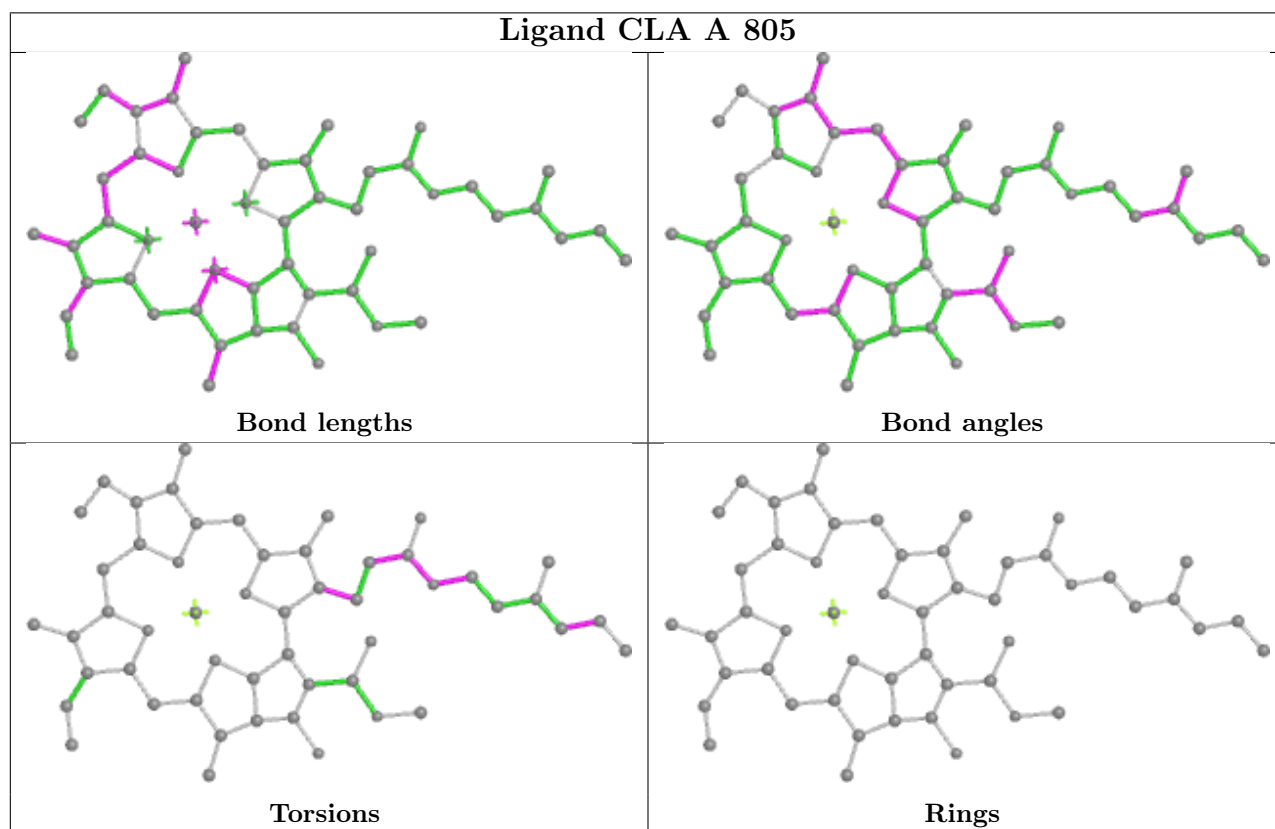
5 of 3427 torsion outliers are listed below:

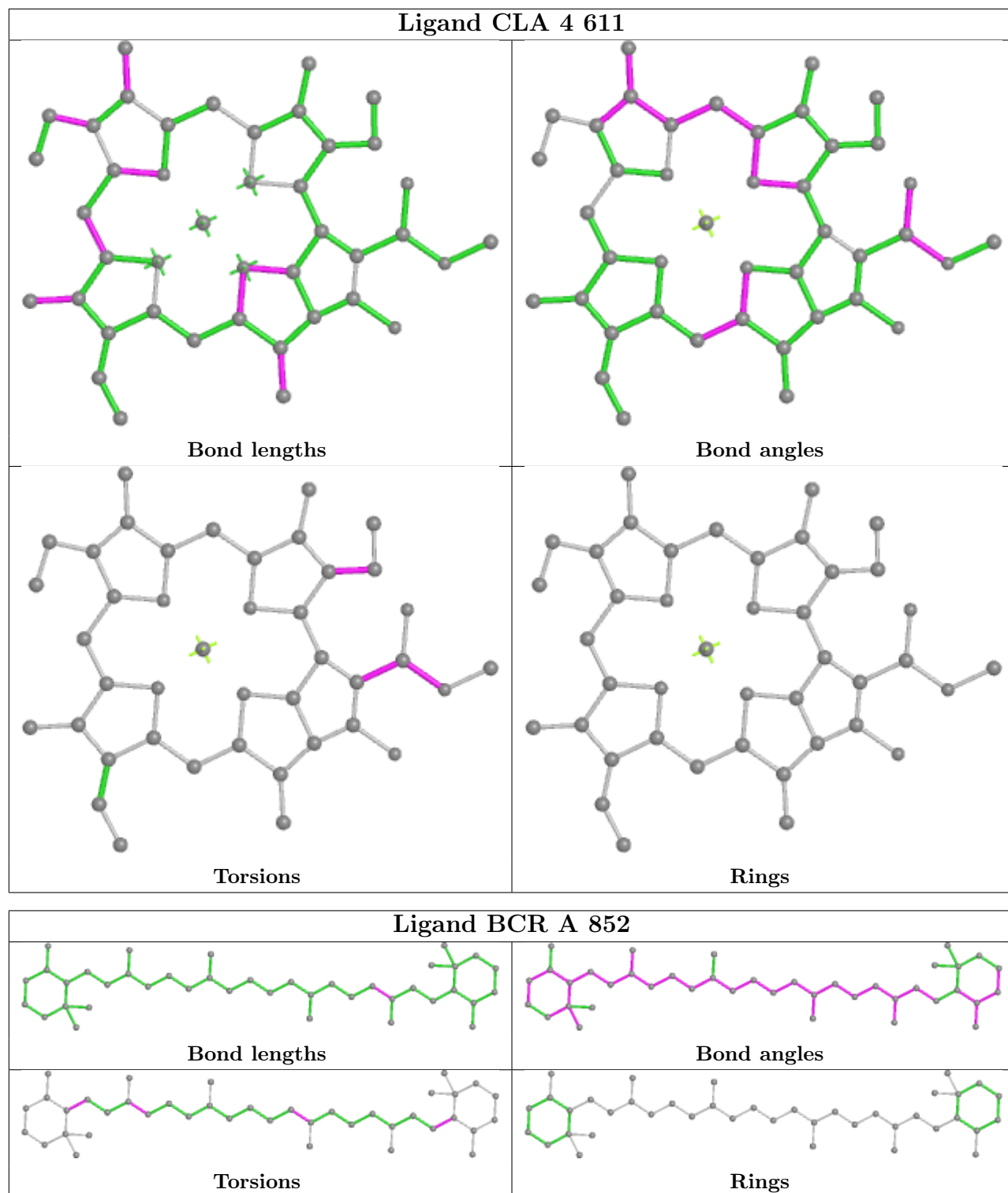
Mol	Chain	Res	Type	Atoms
26	A	801	CLA	CBD-CGD-O2D-CED
26	A	801	CLA	O1D-CGD-O2D-CED
26	A	804	CLA	C1A-C2A-CAA-CBA
26	A	804	CLA	C3A-C2A-CAA-CBA
26	A	804	CLA	CHA-CBD-CGD-O1D

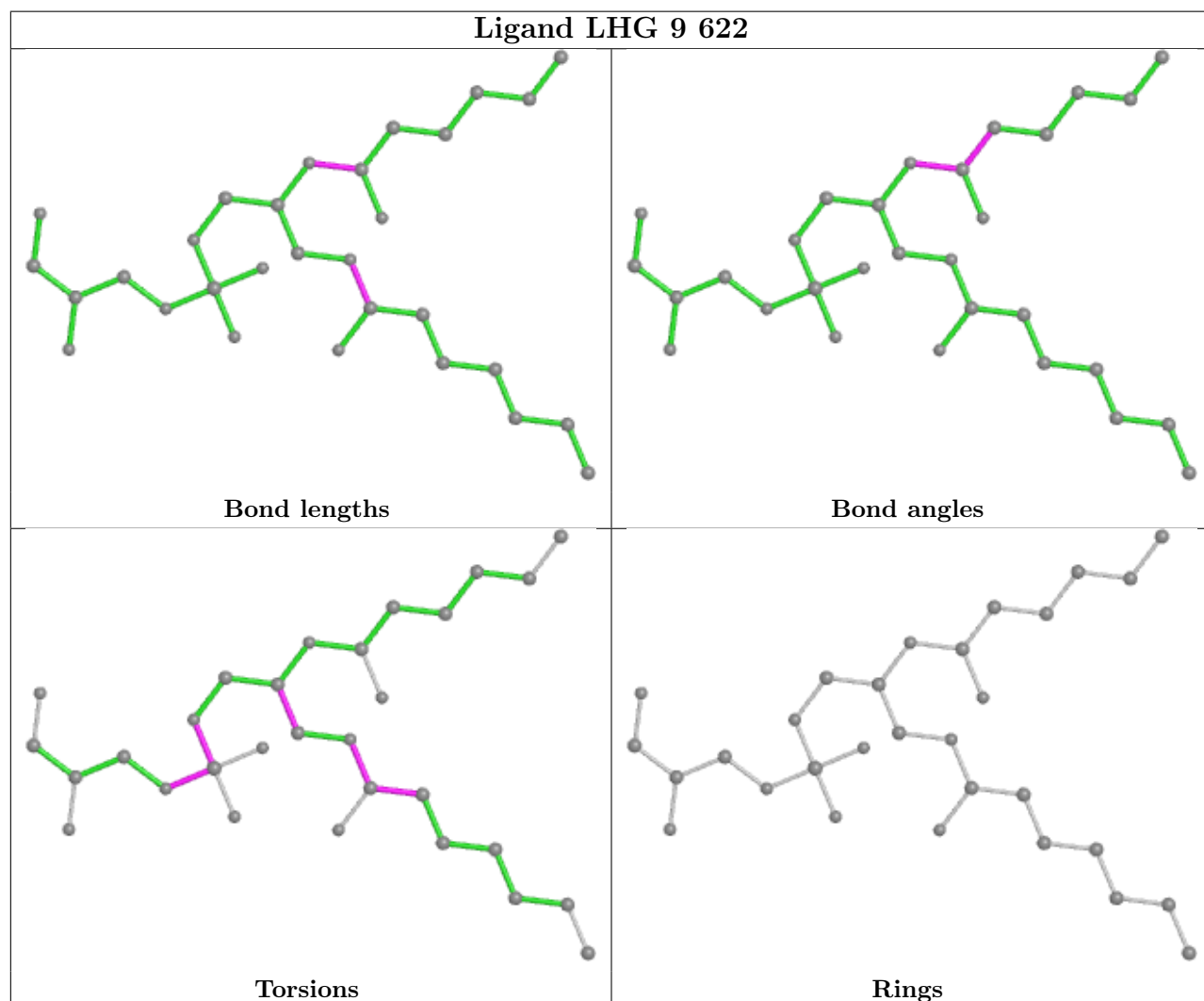
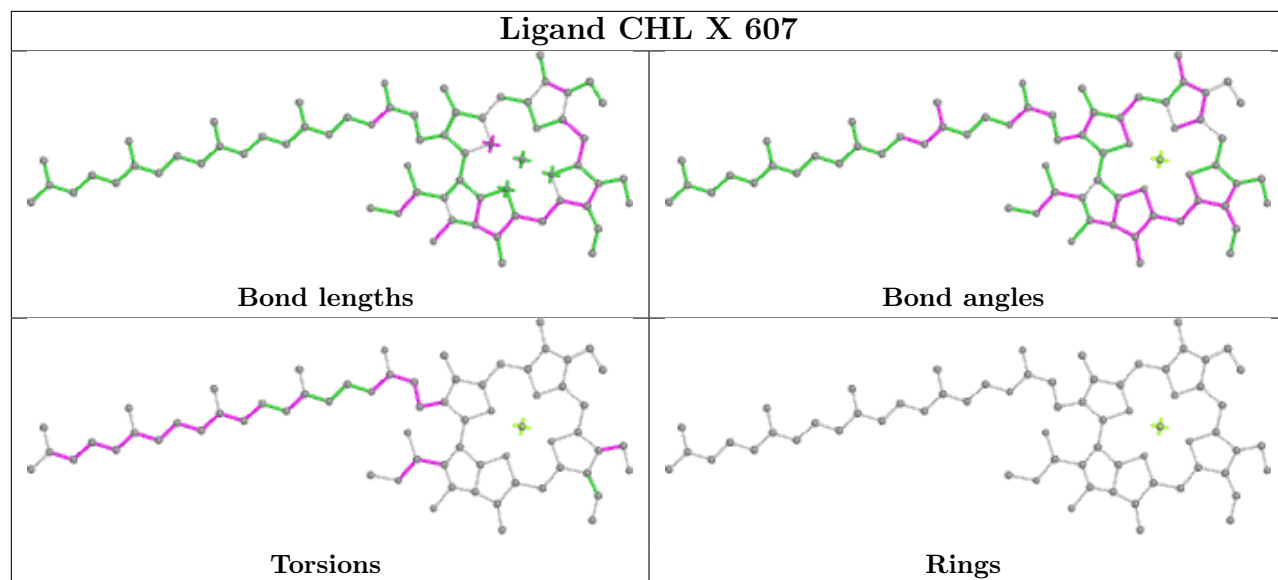
There are no ring outliers.

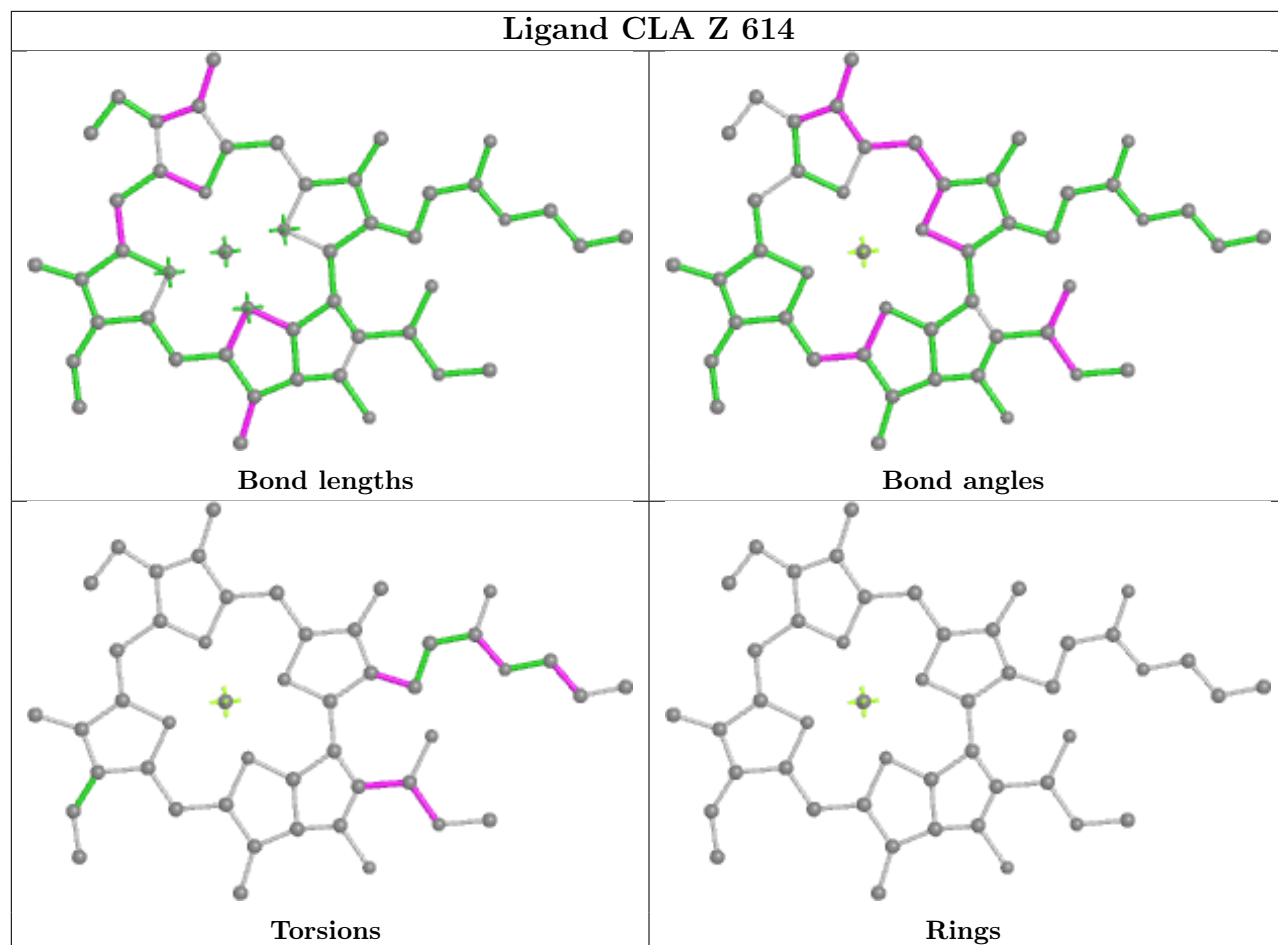
No monomer is involved in short contacts.

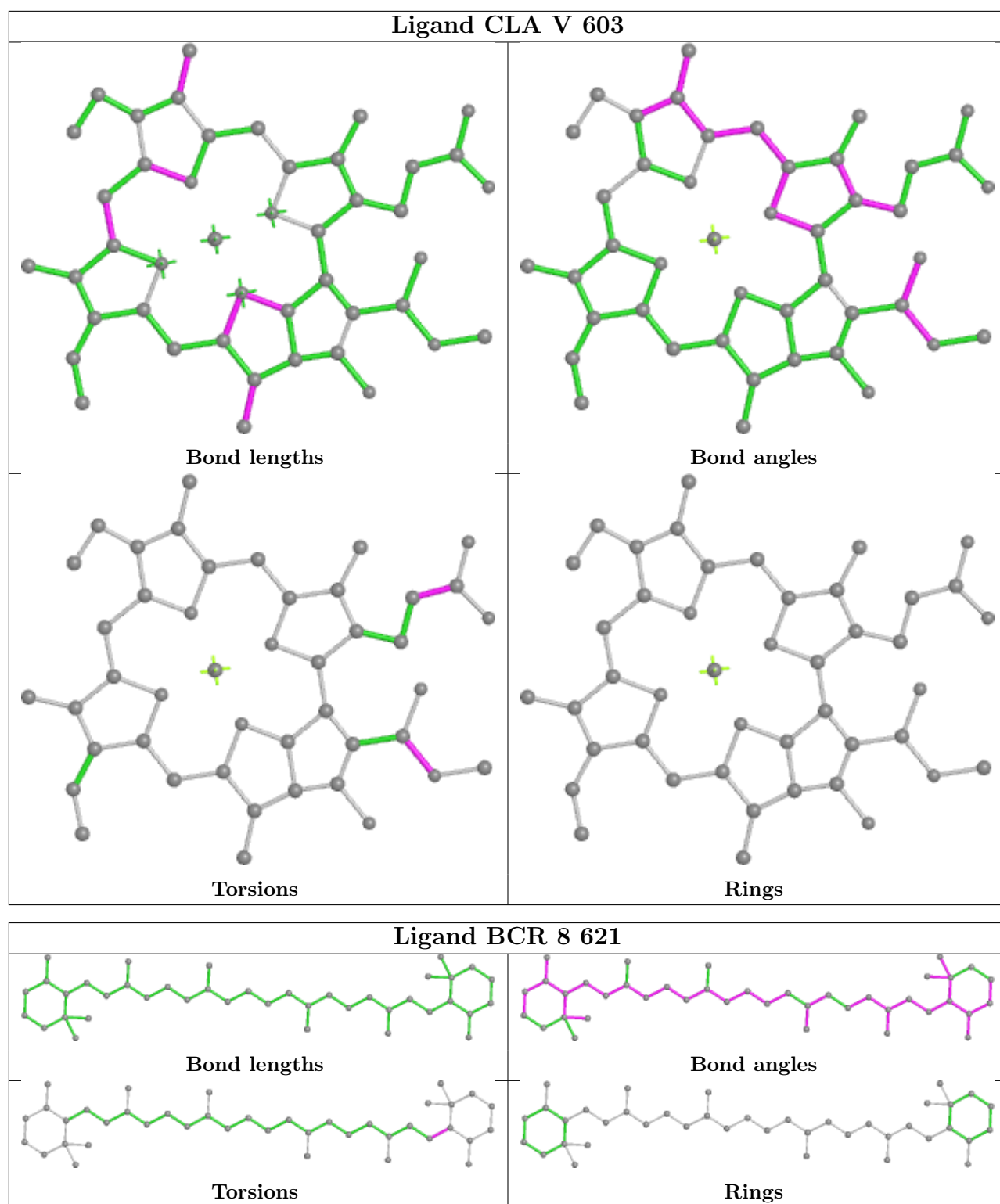
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

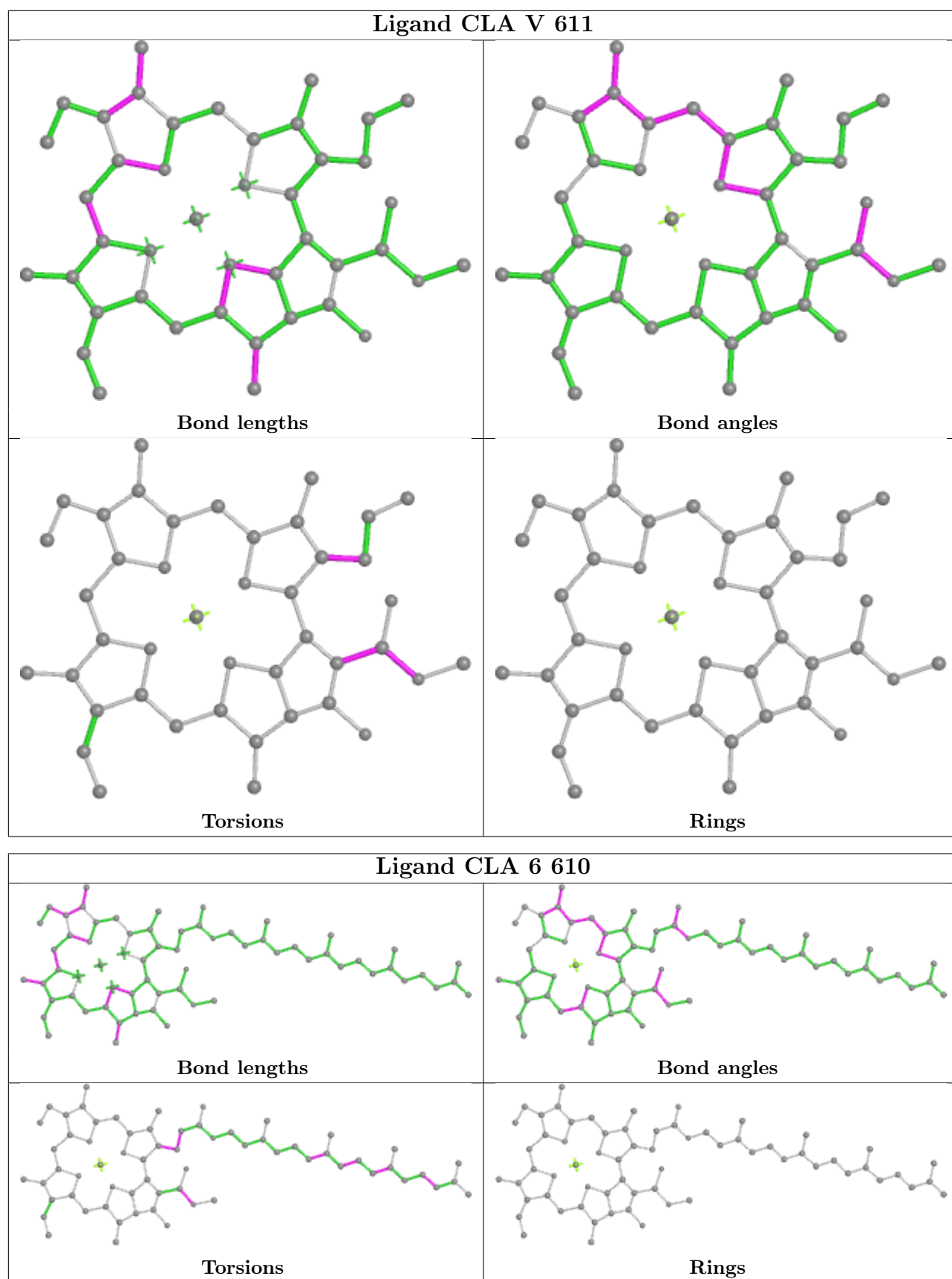


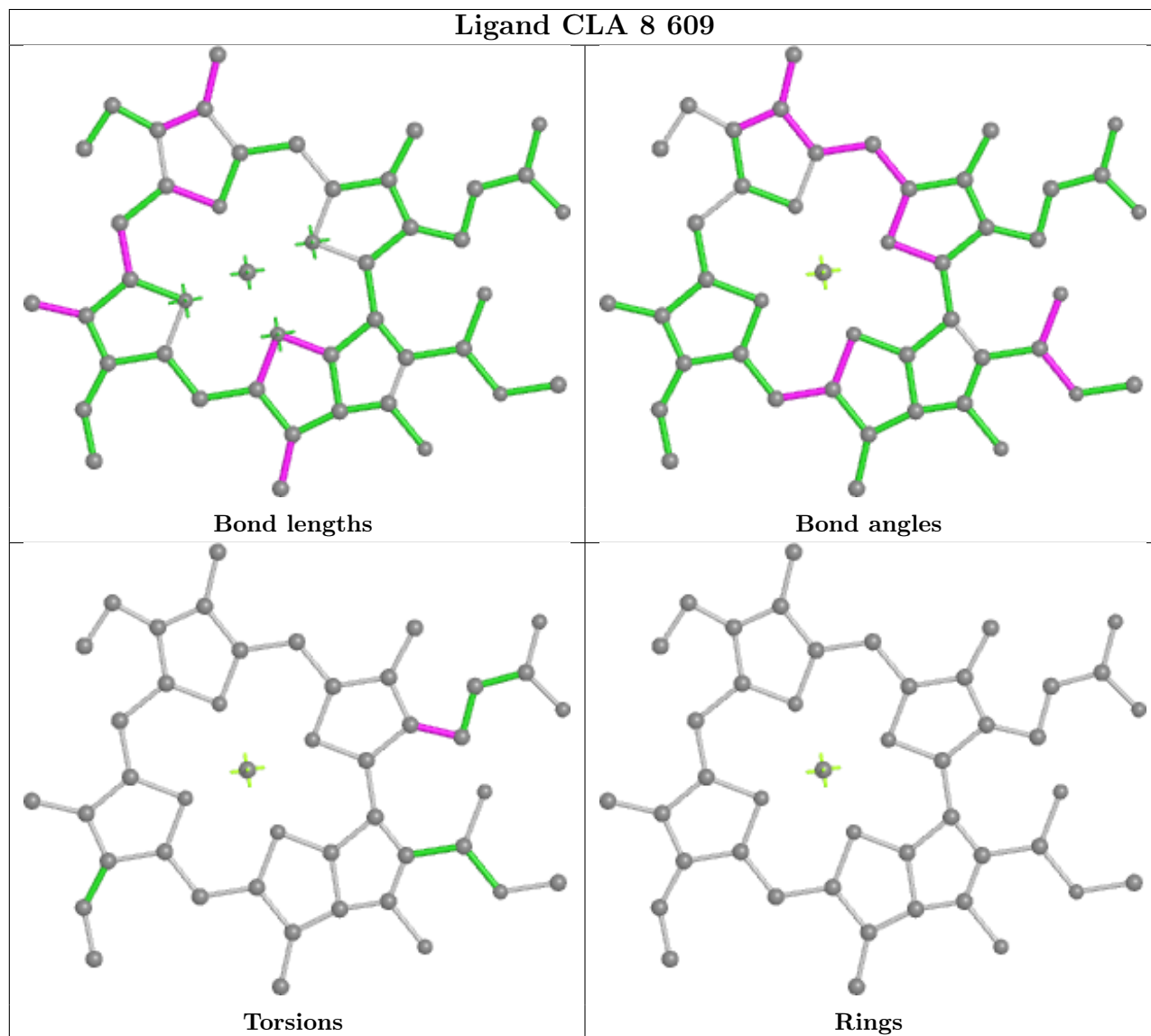
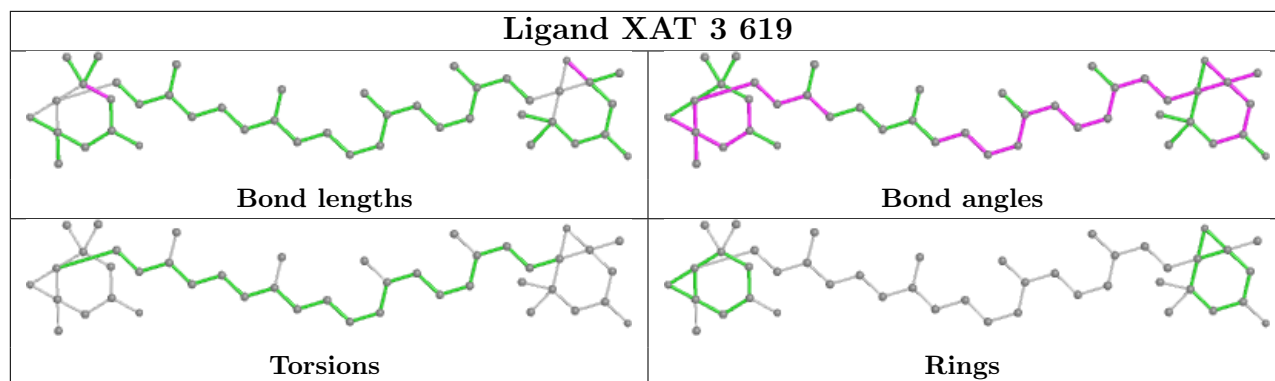


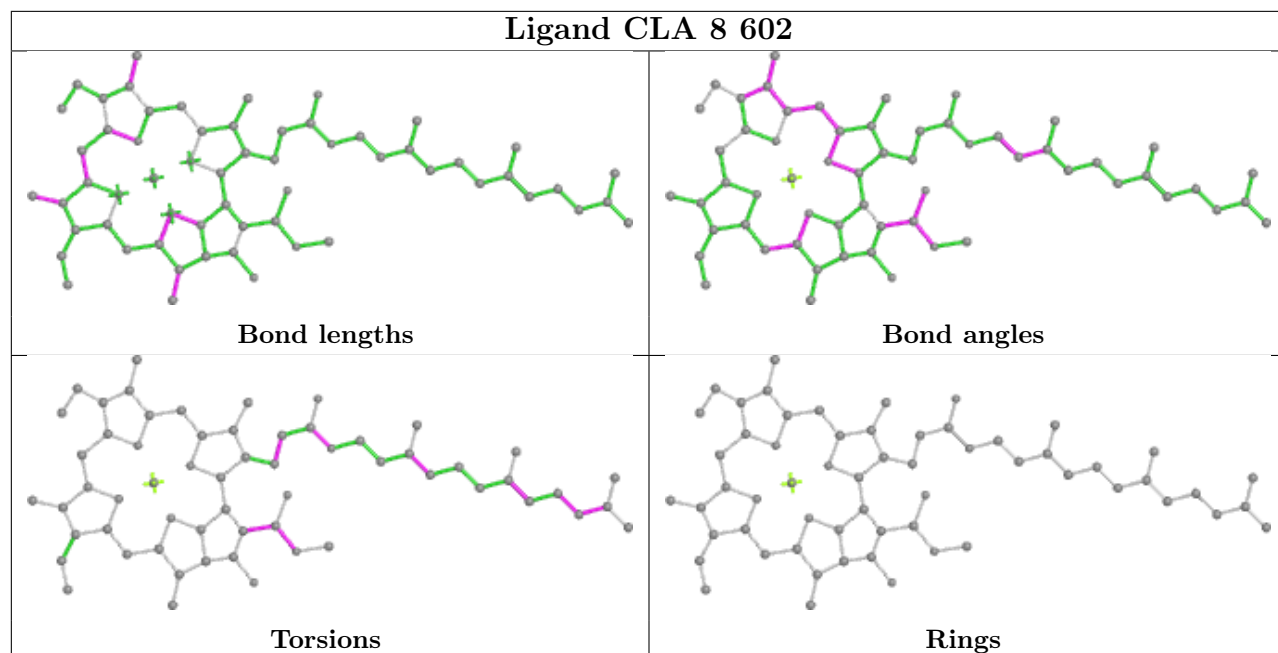


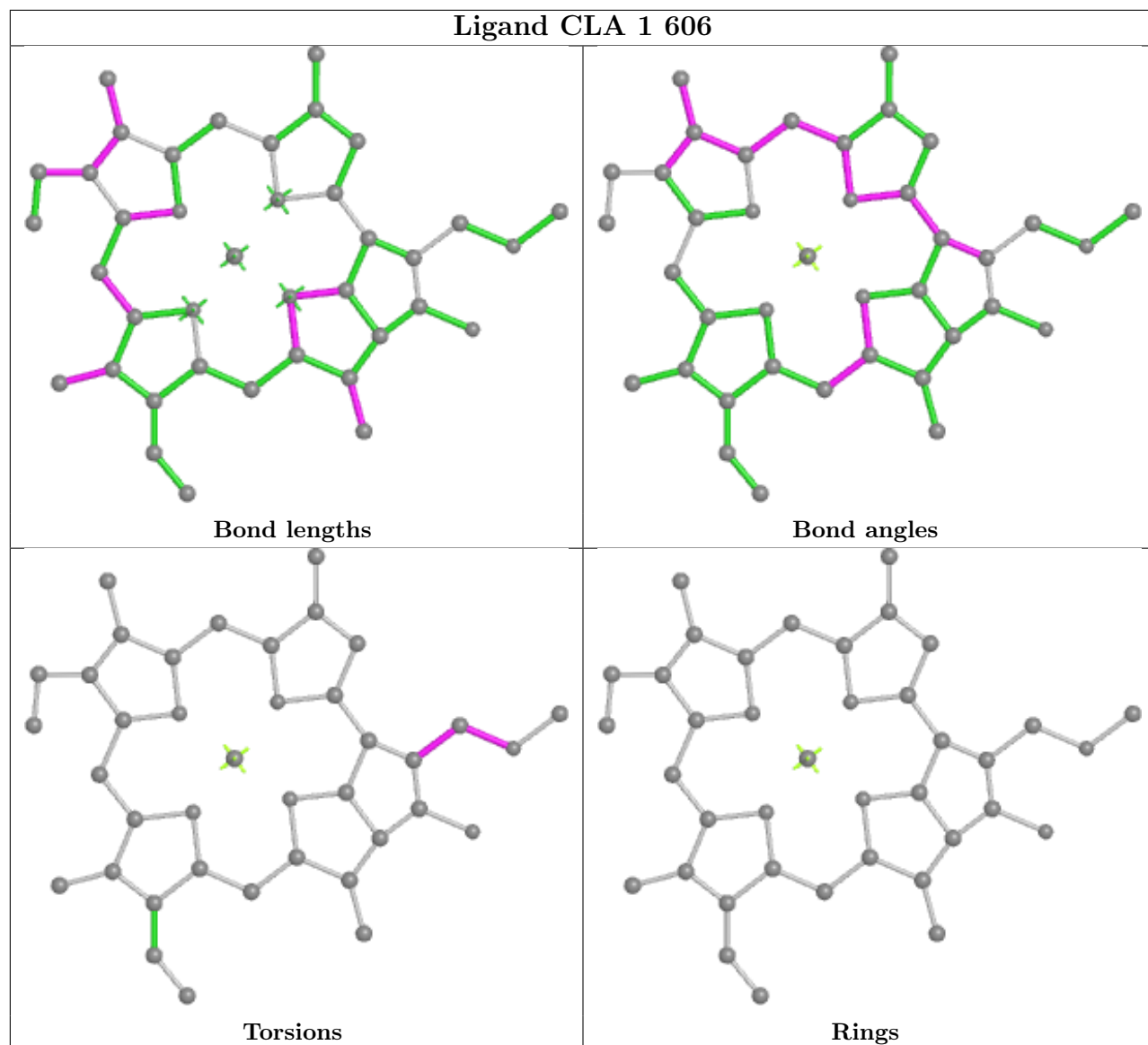


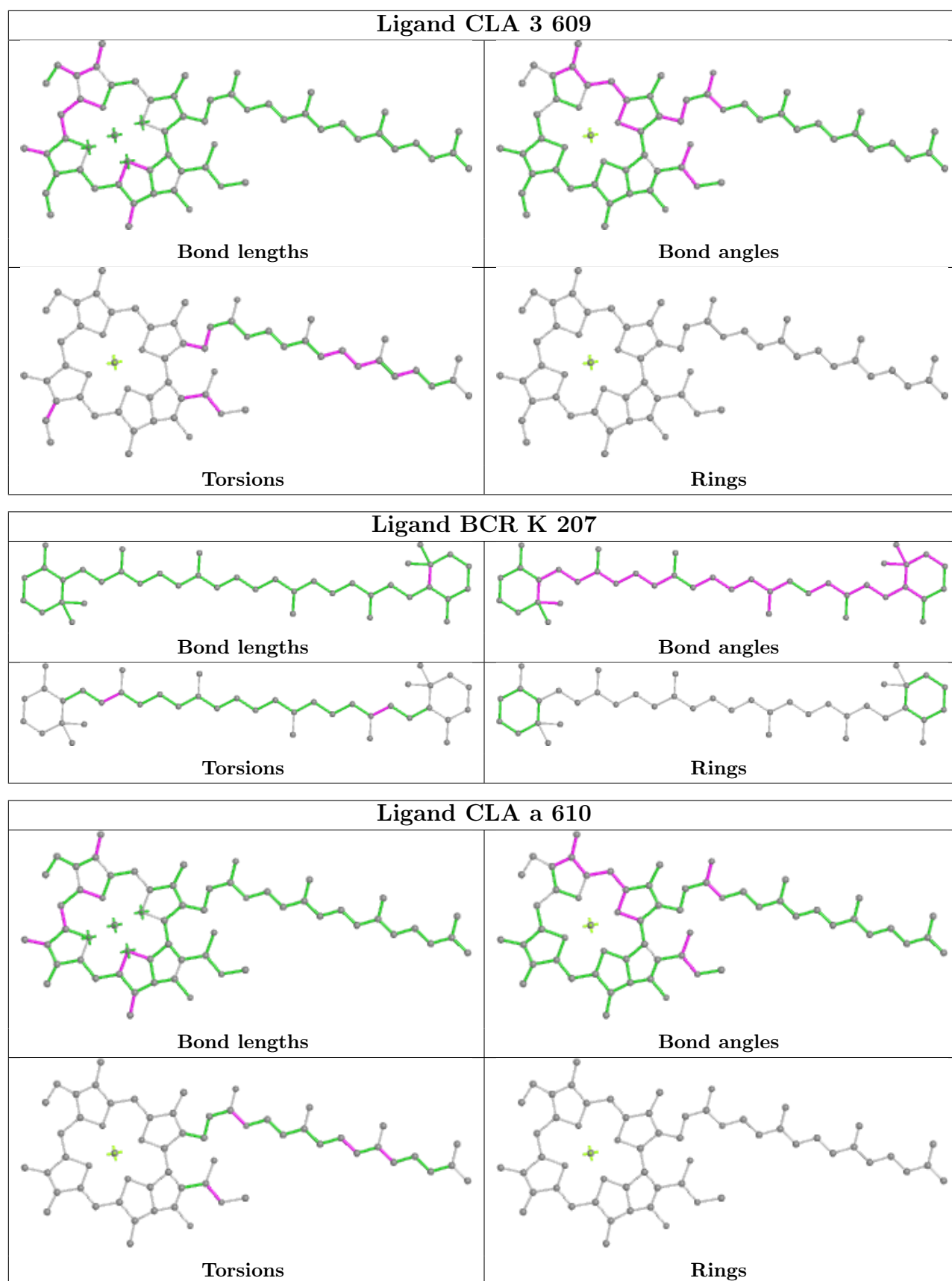


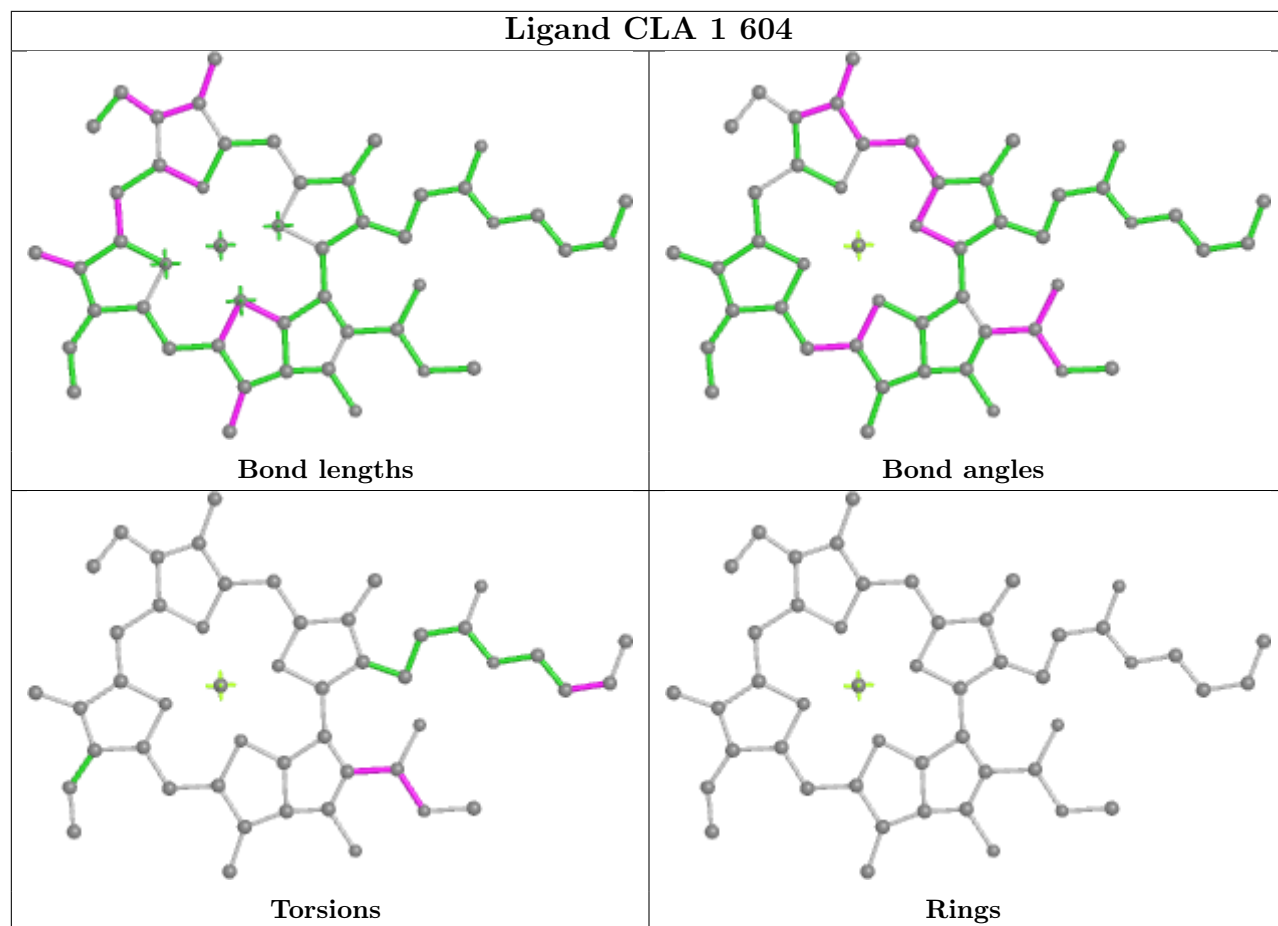


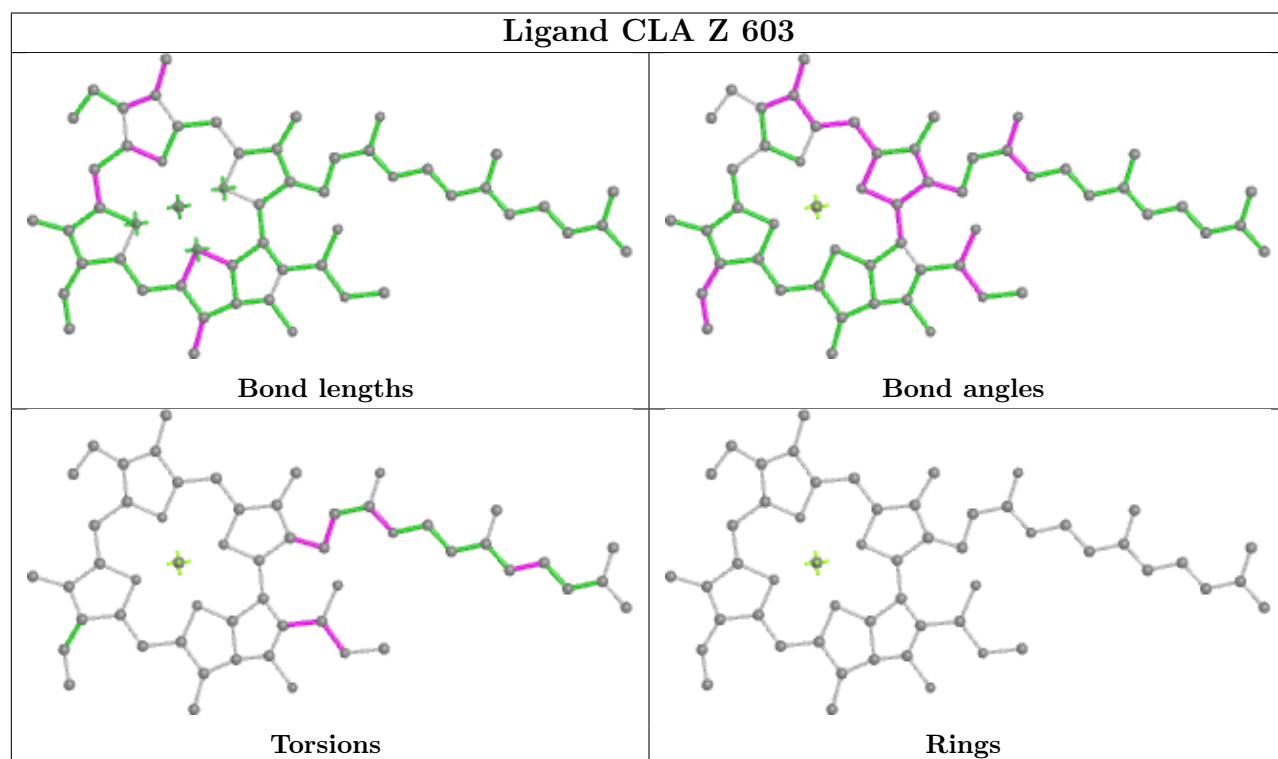
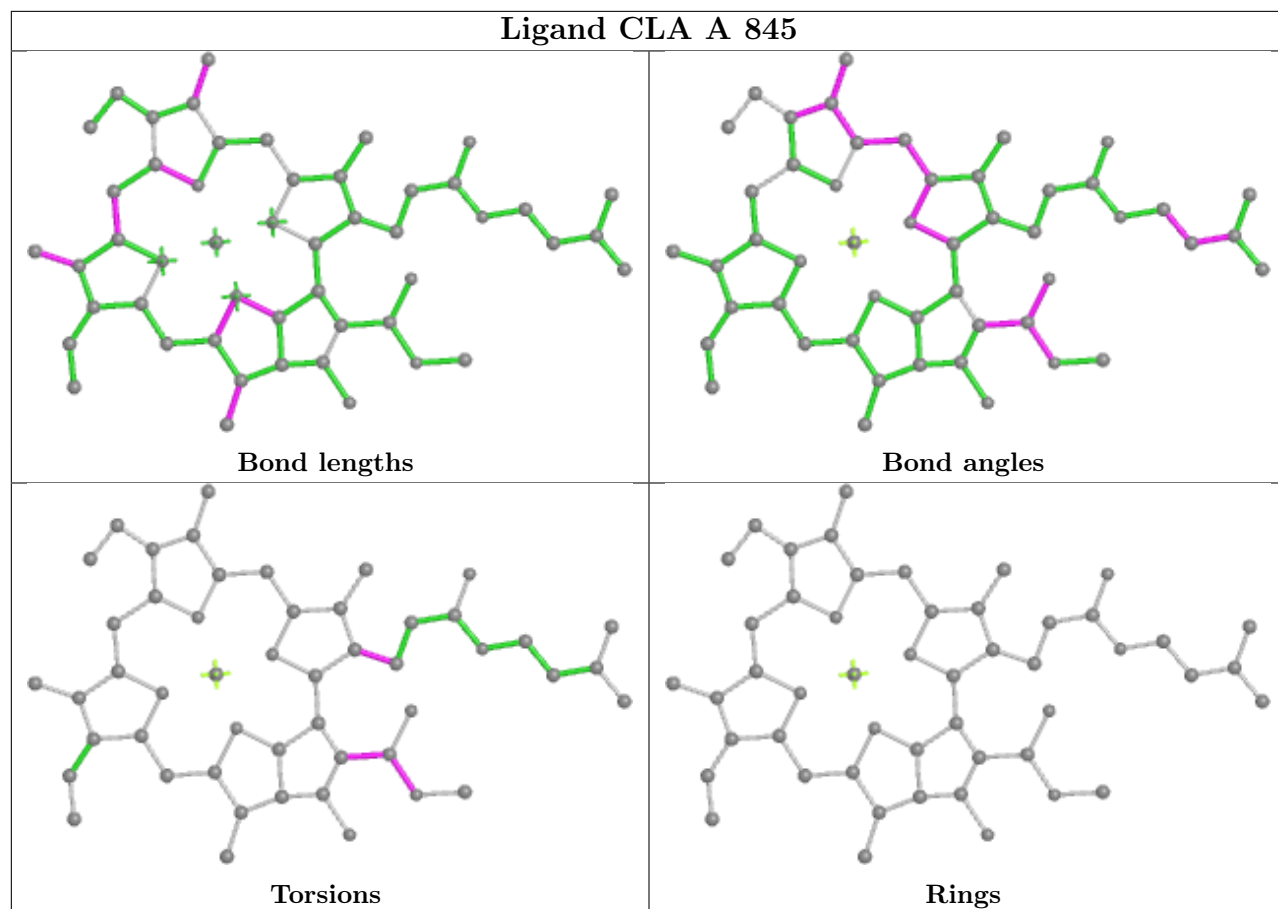


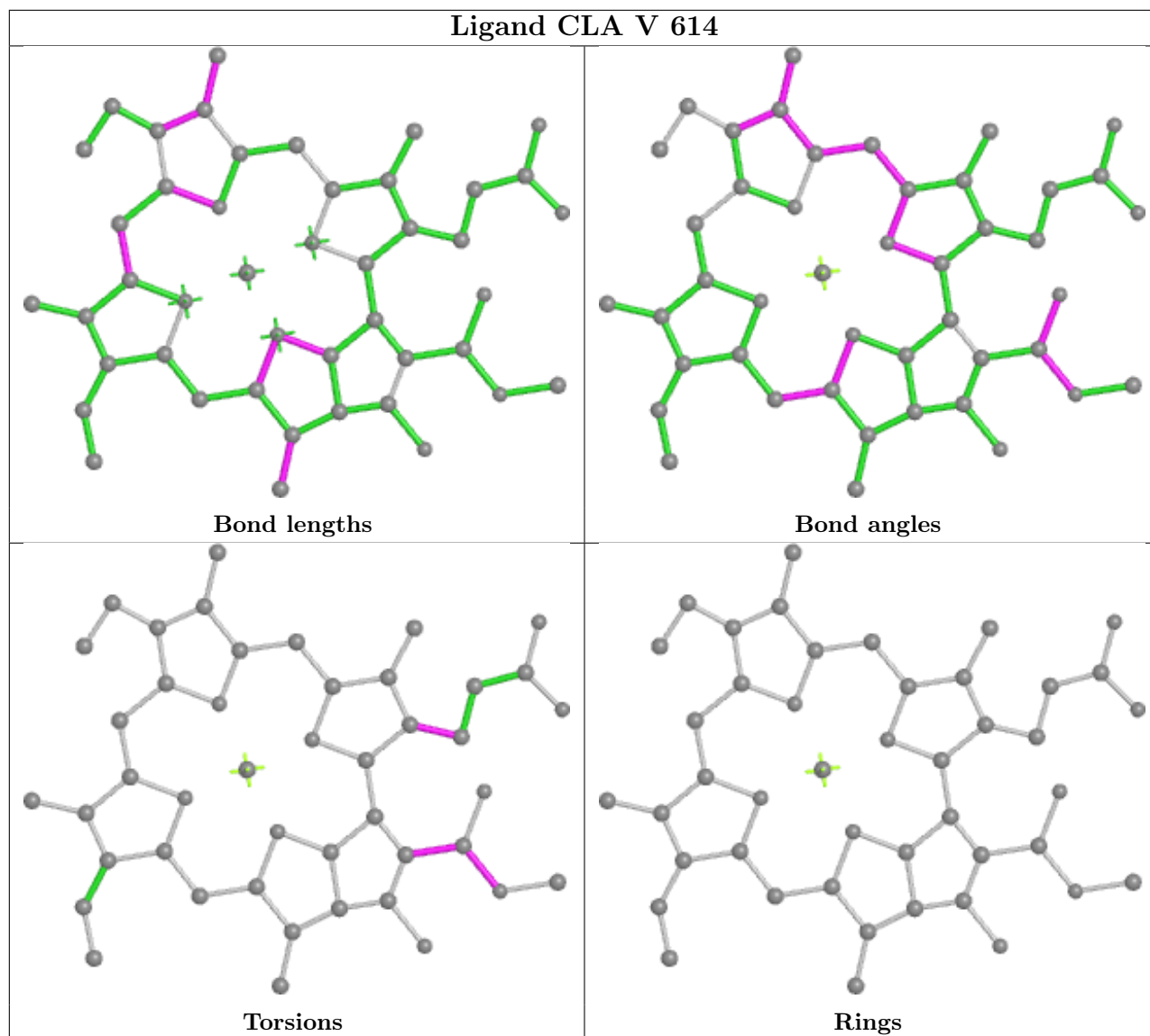
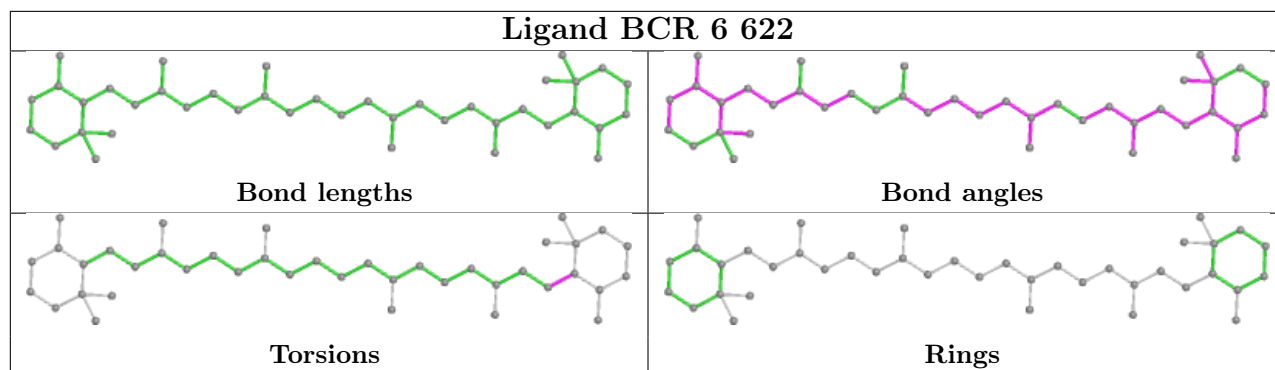


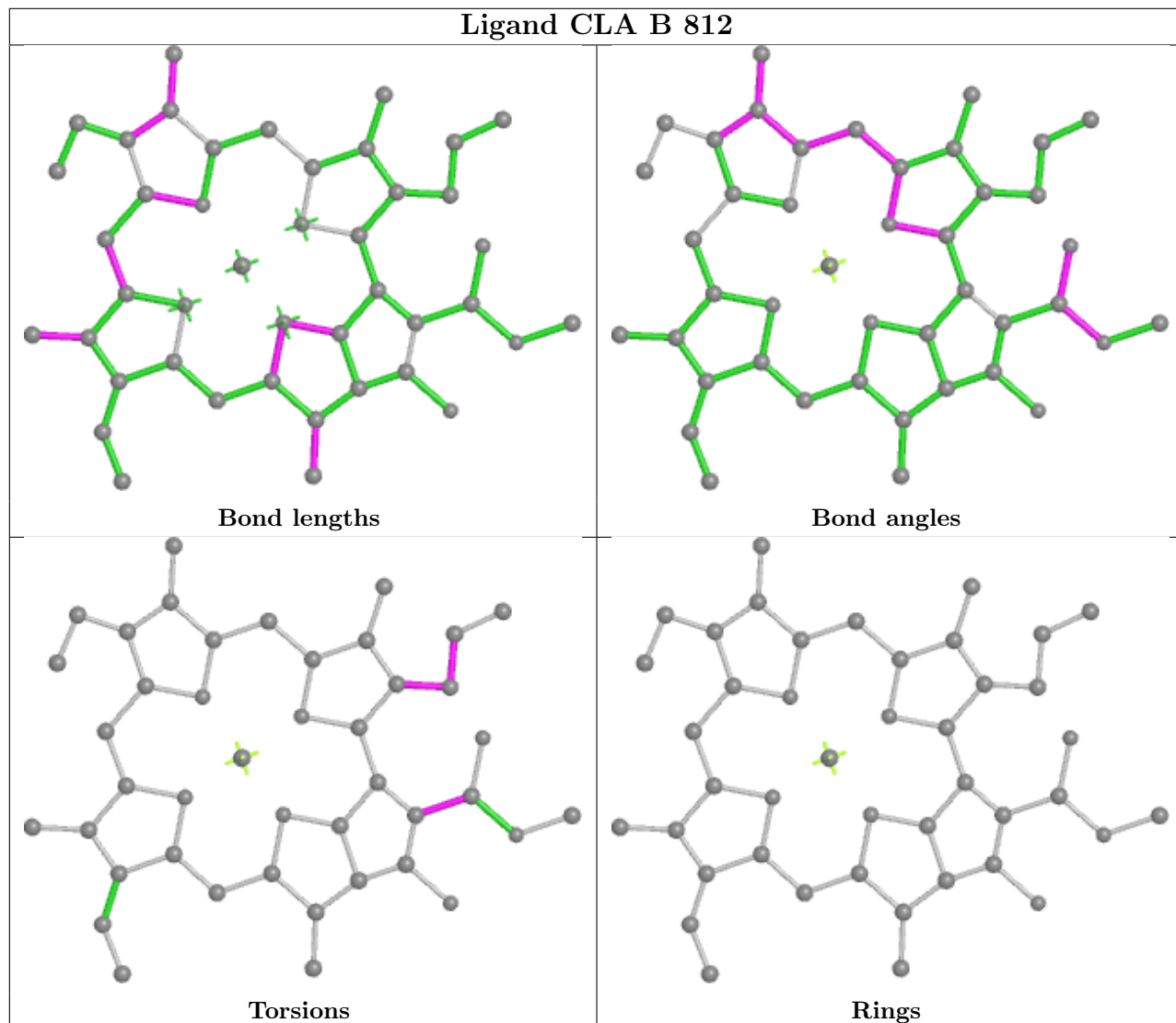
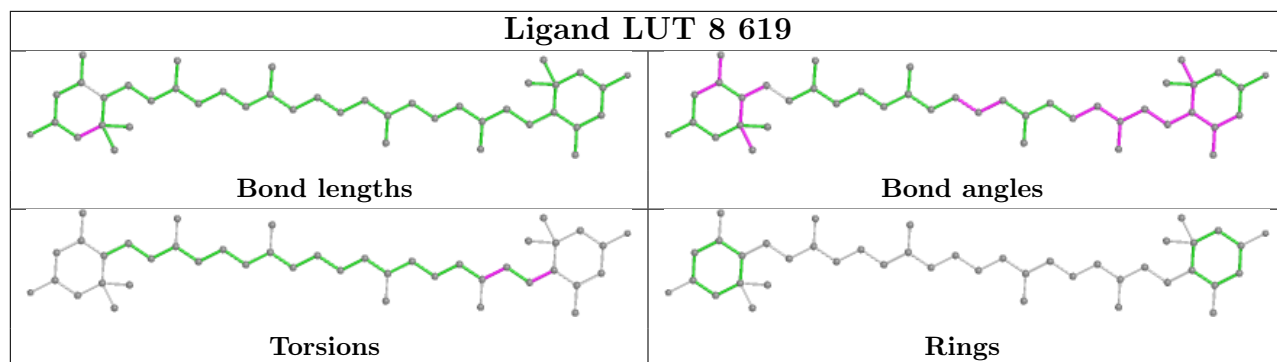


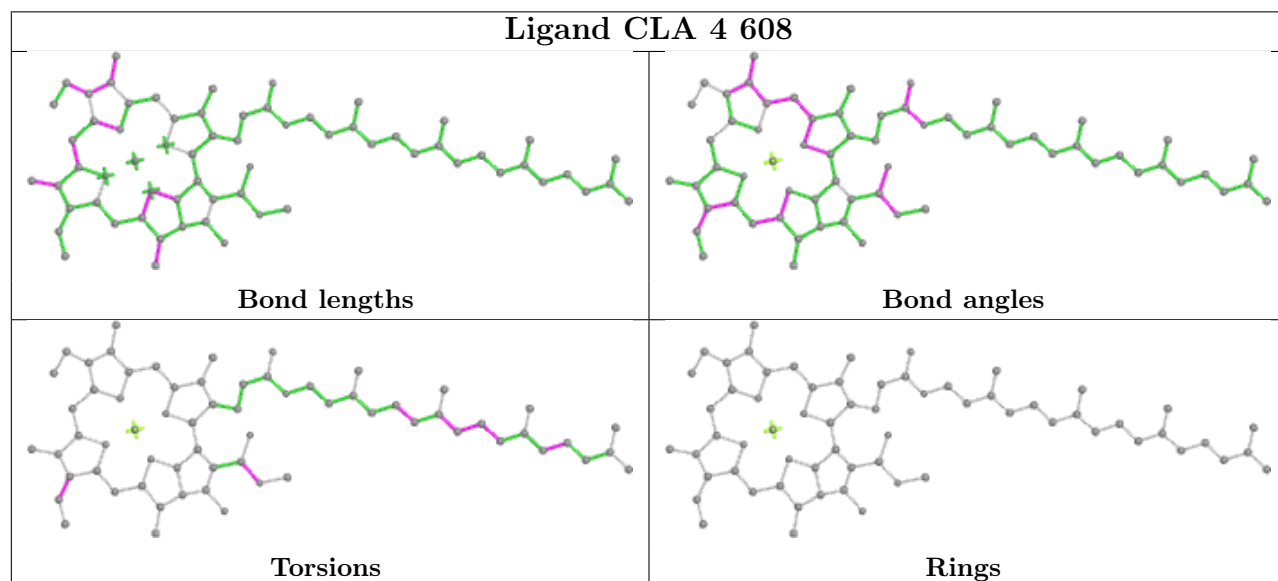
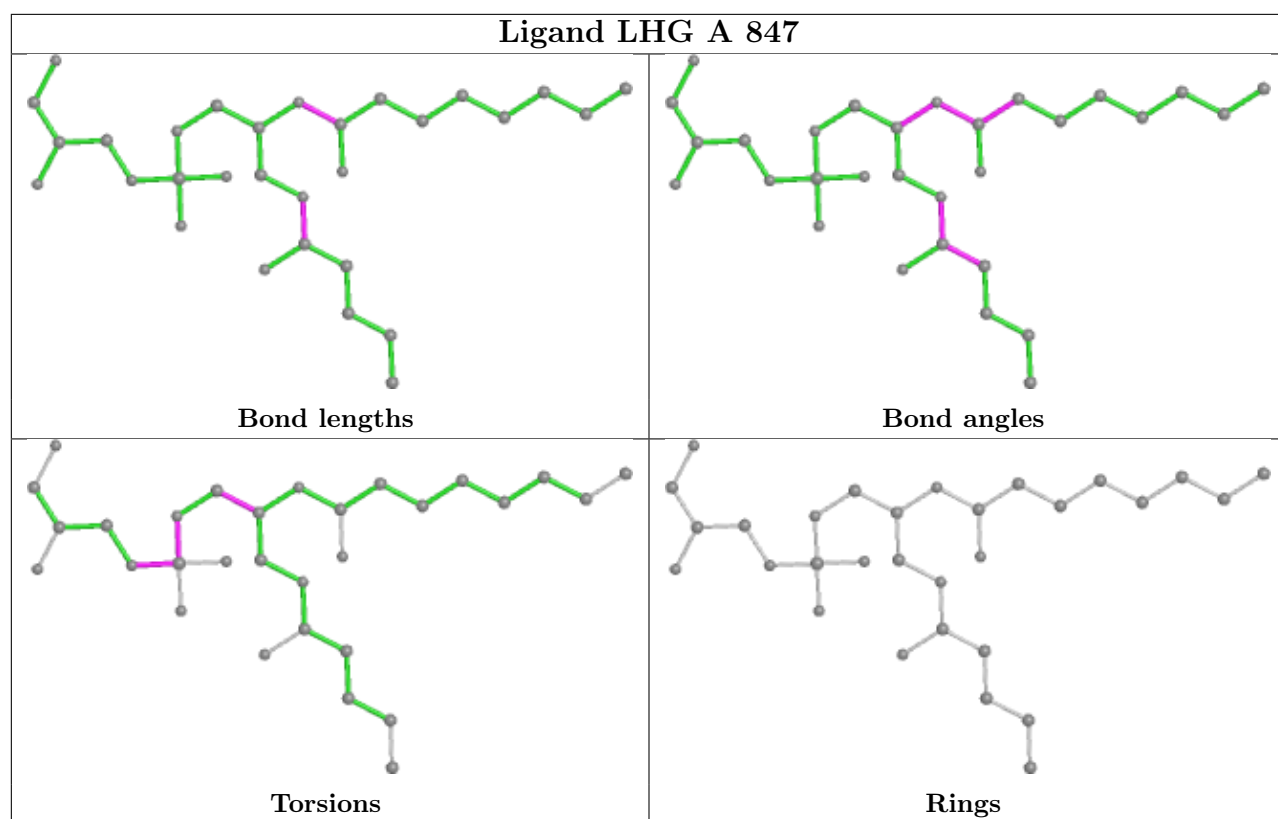


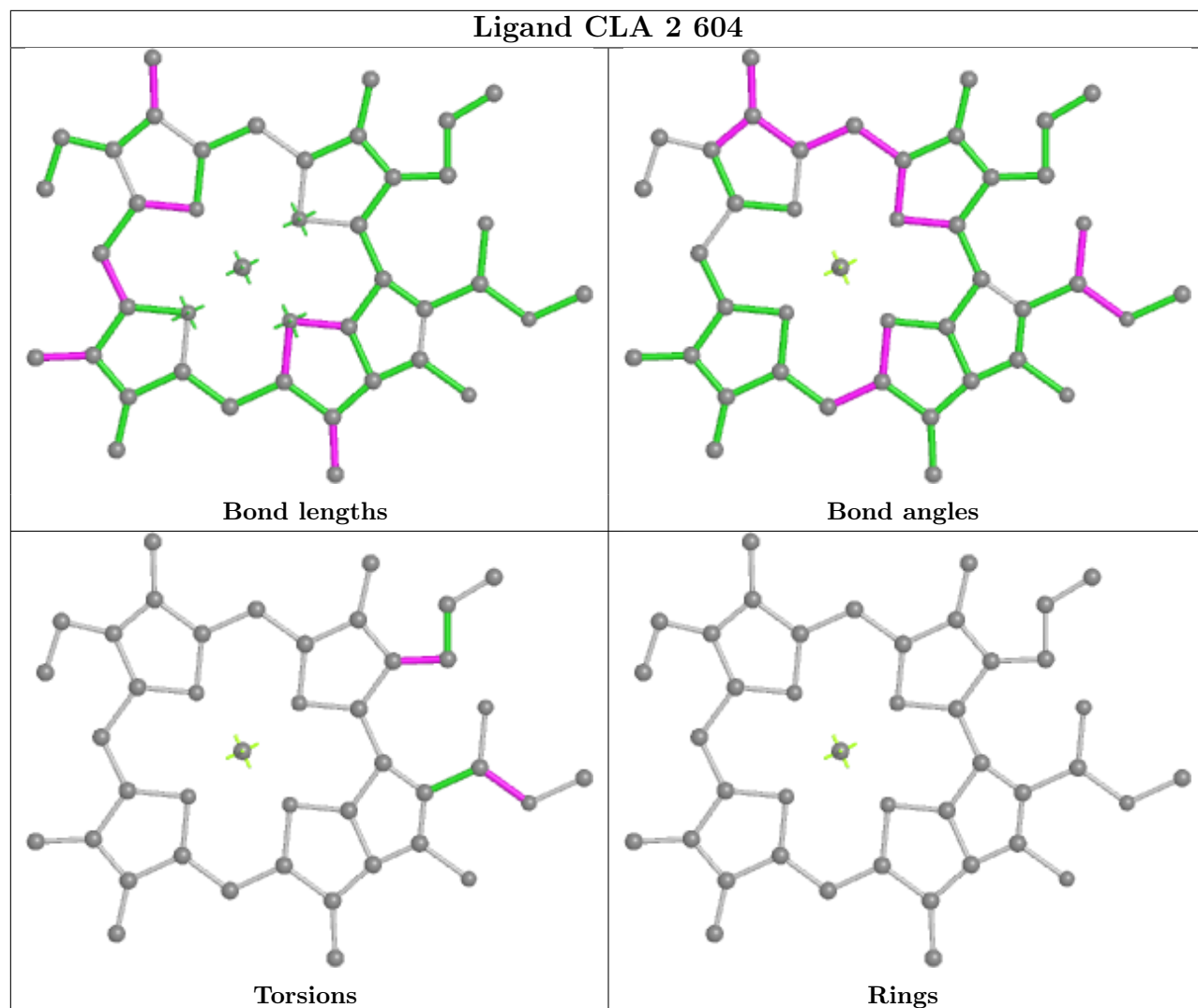


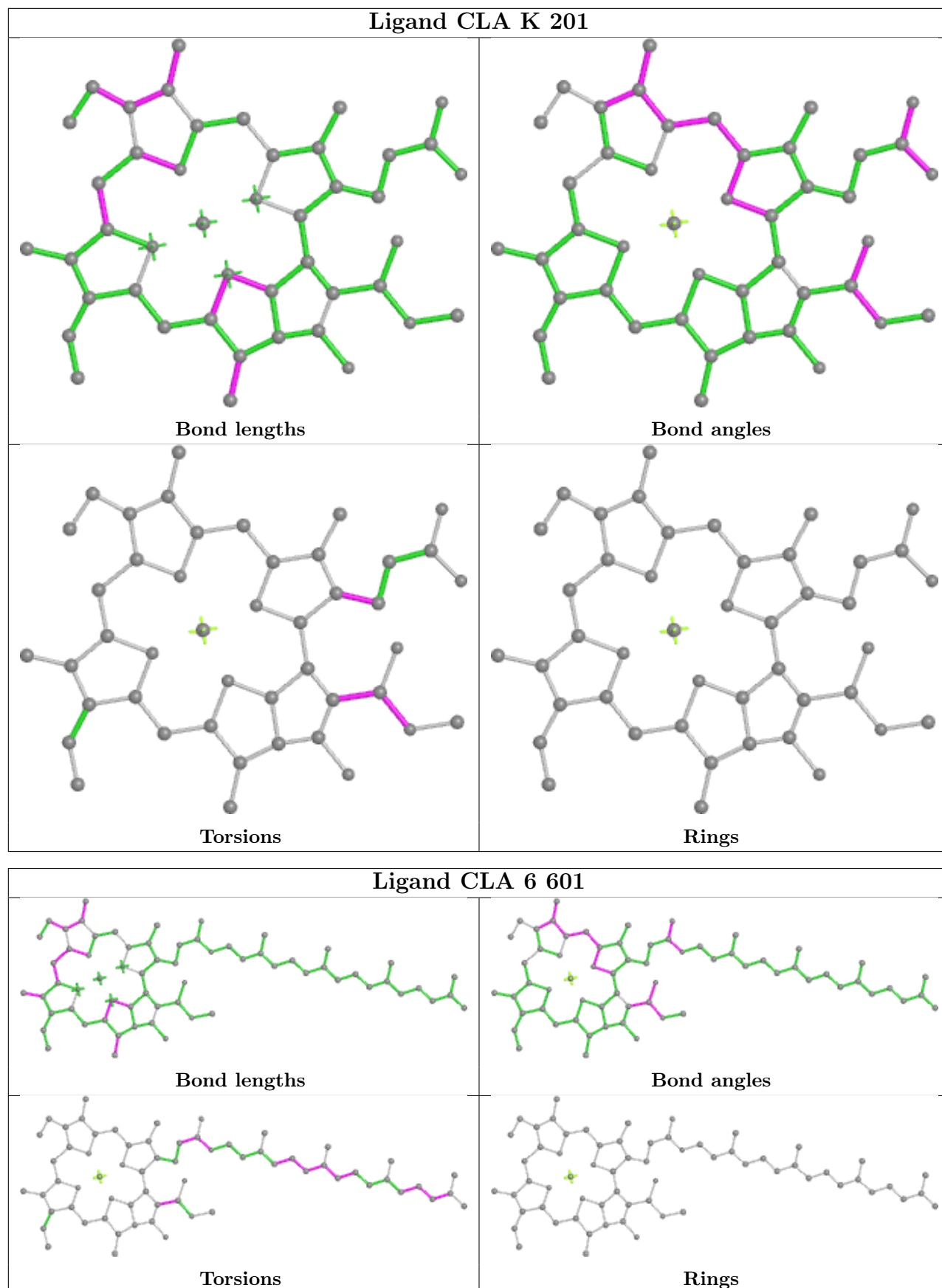


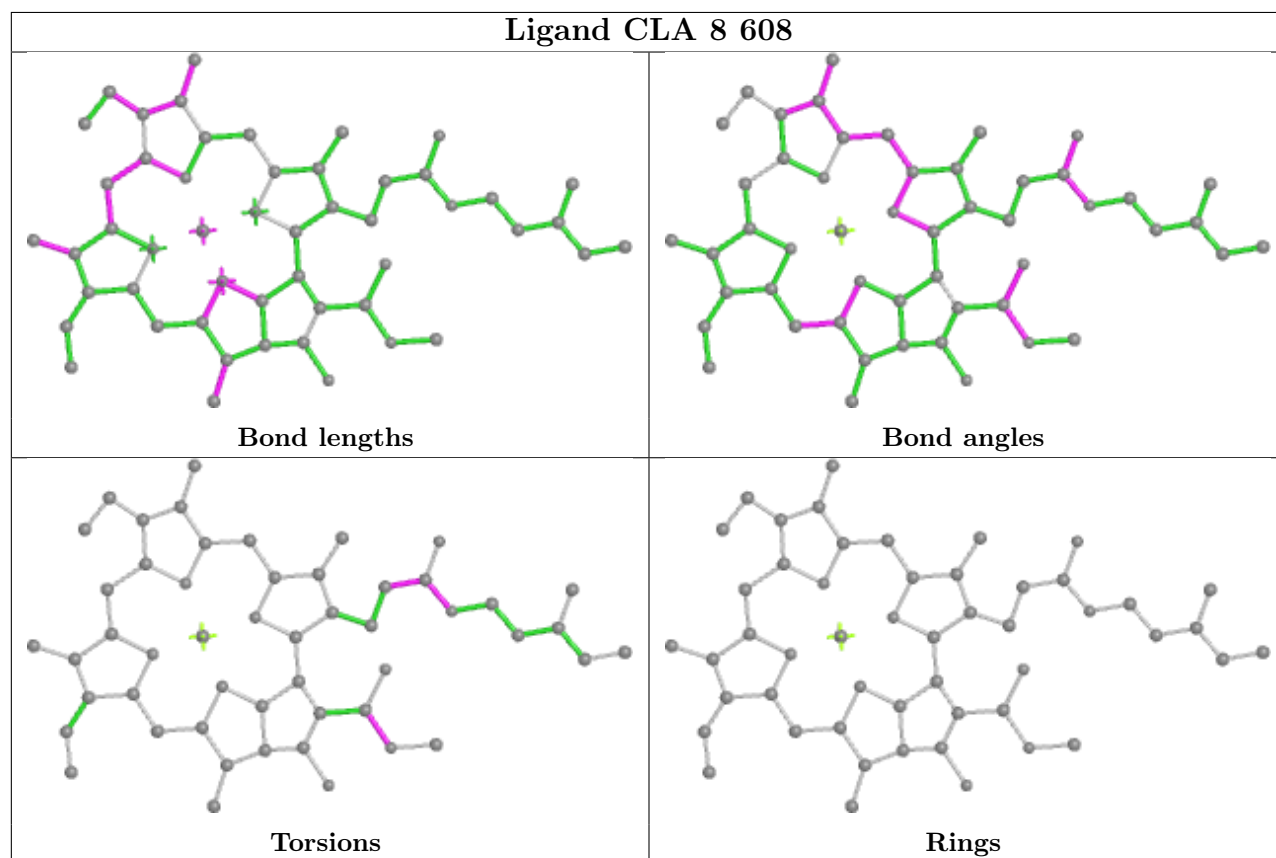
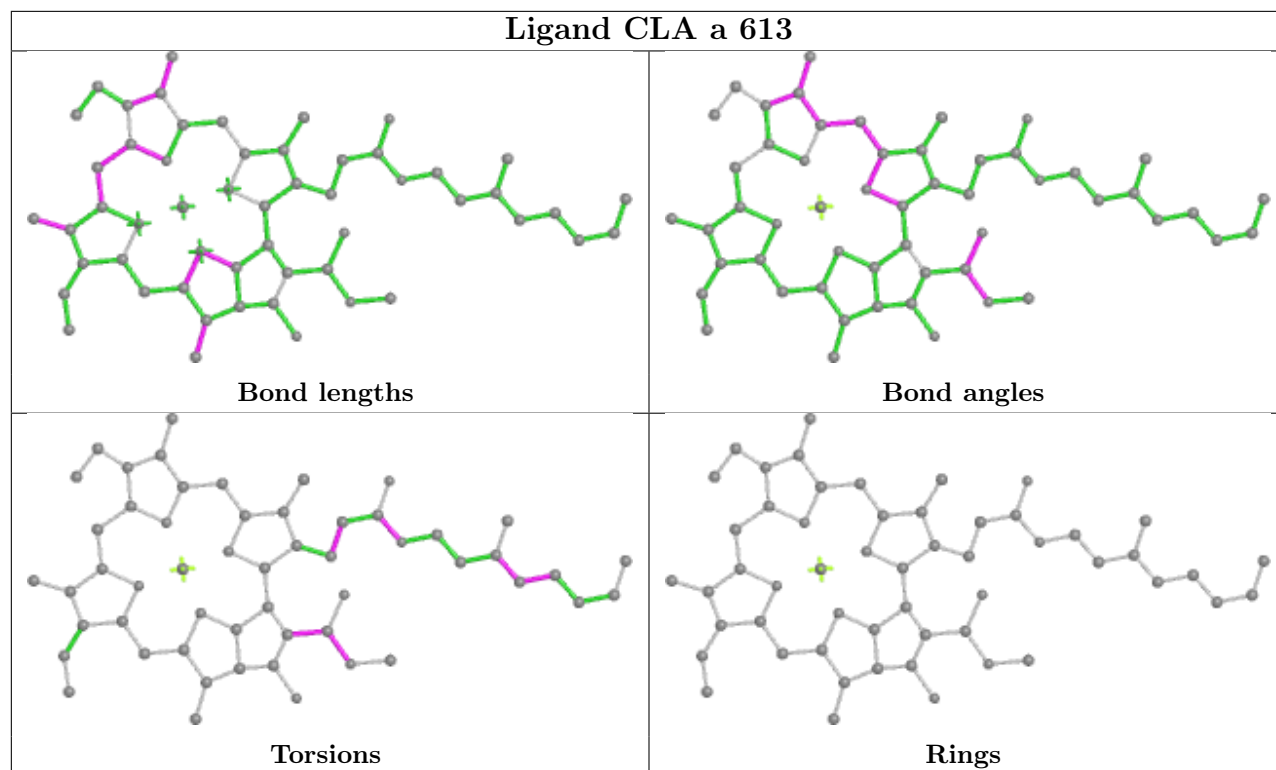


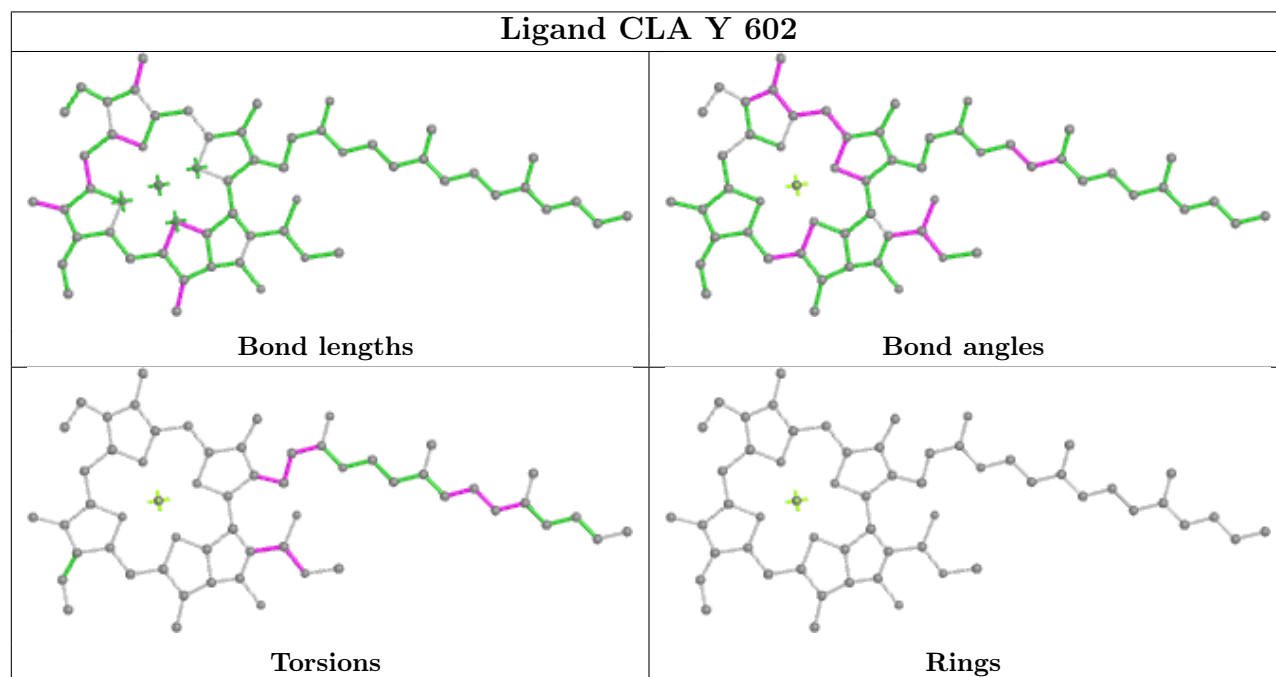
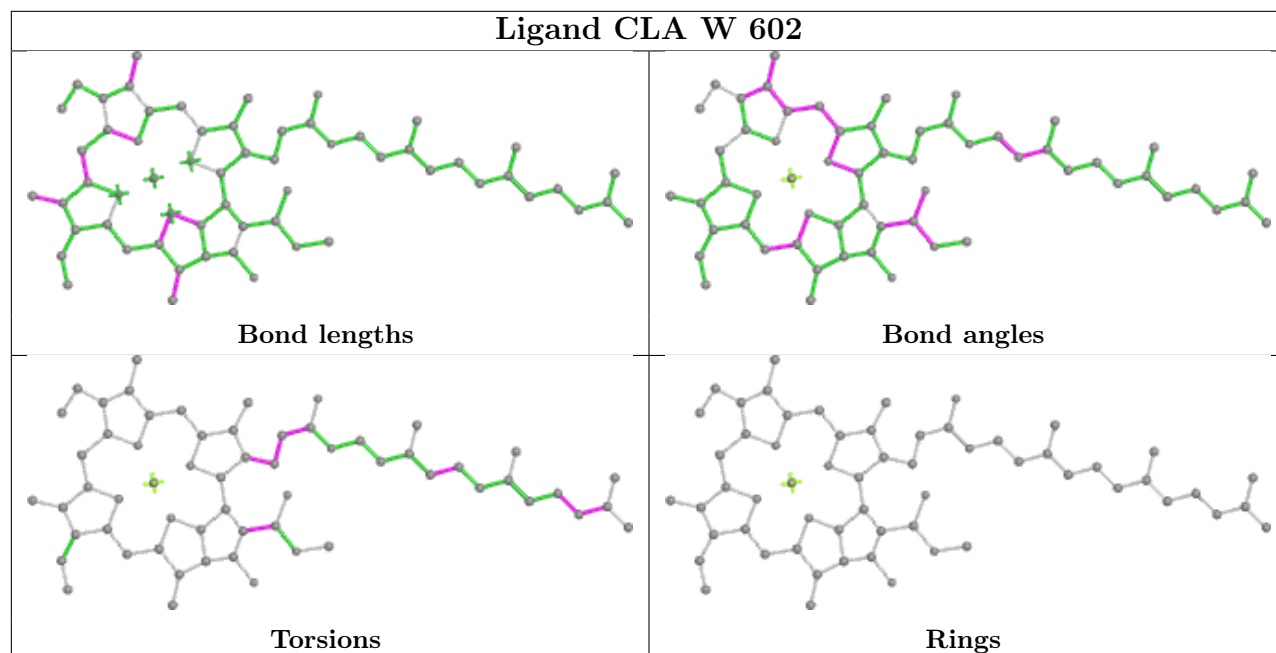


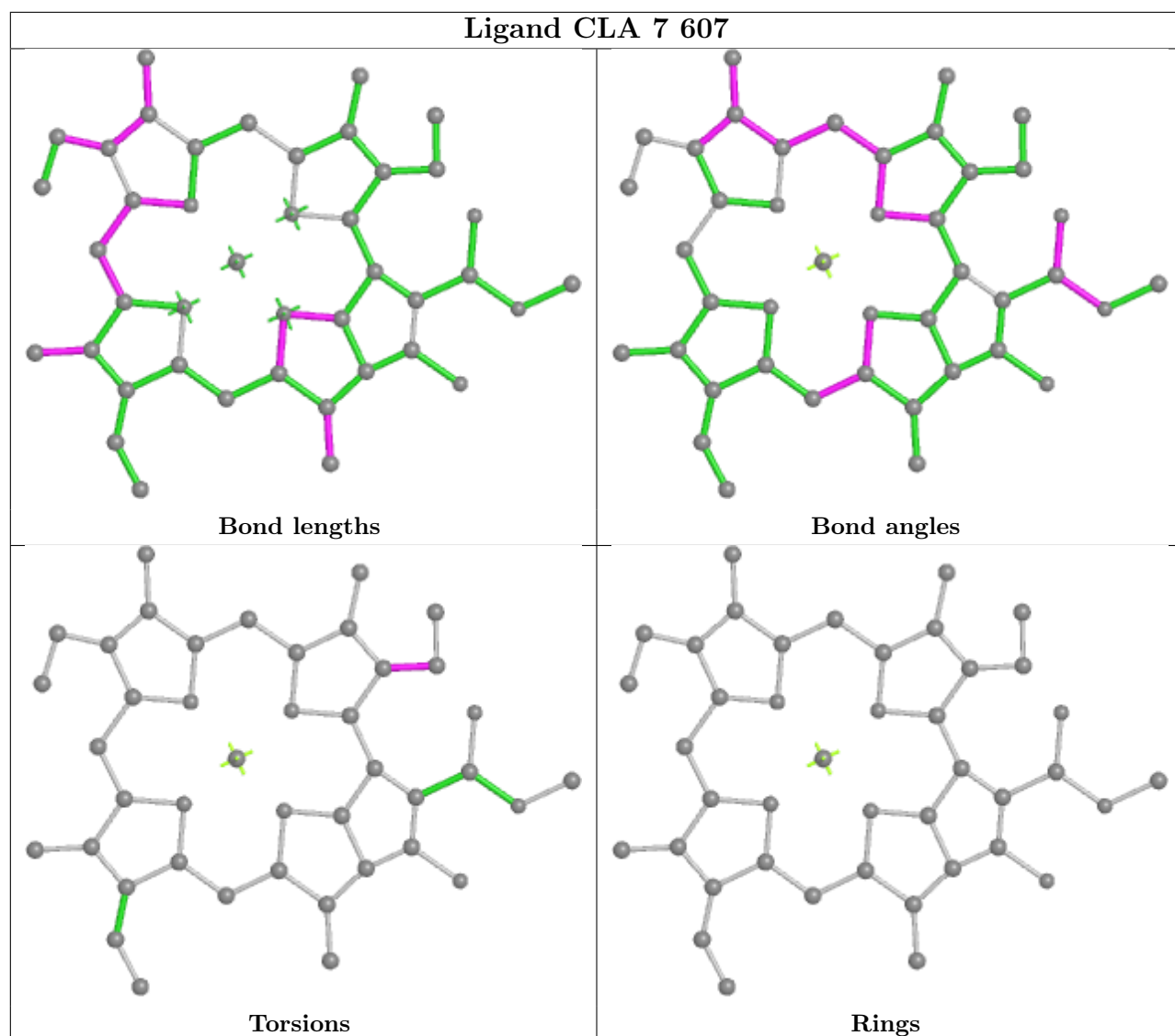
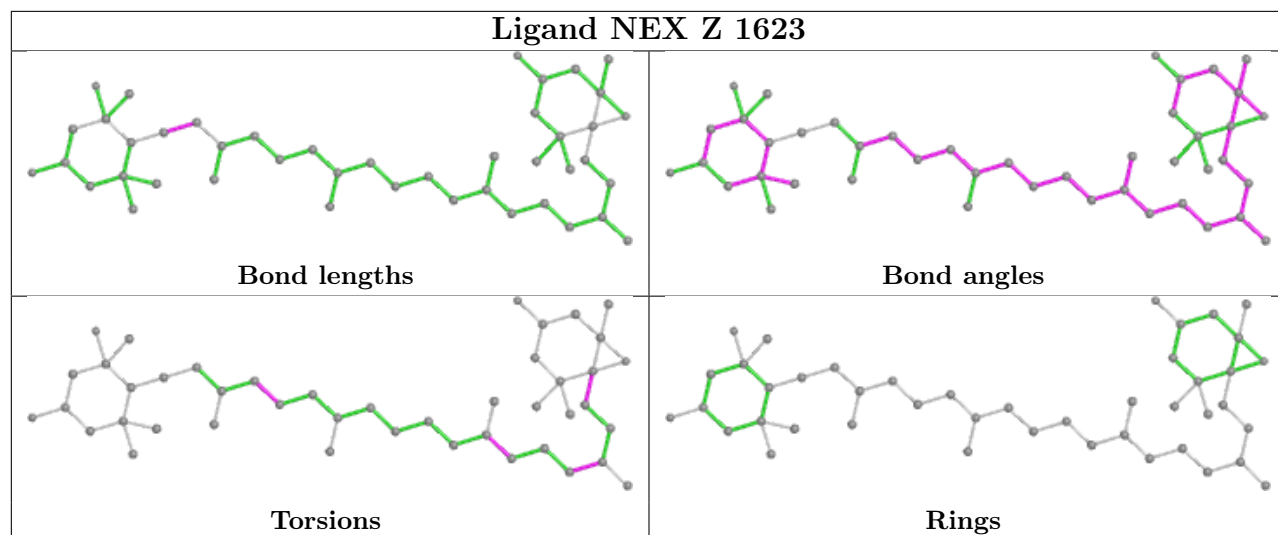


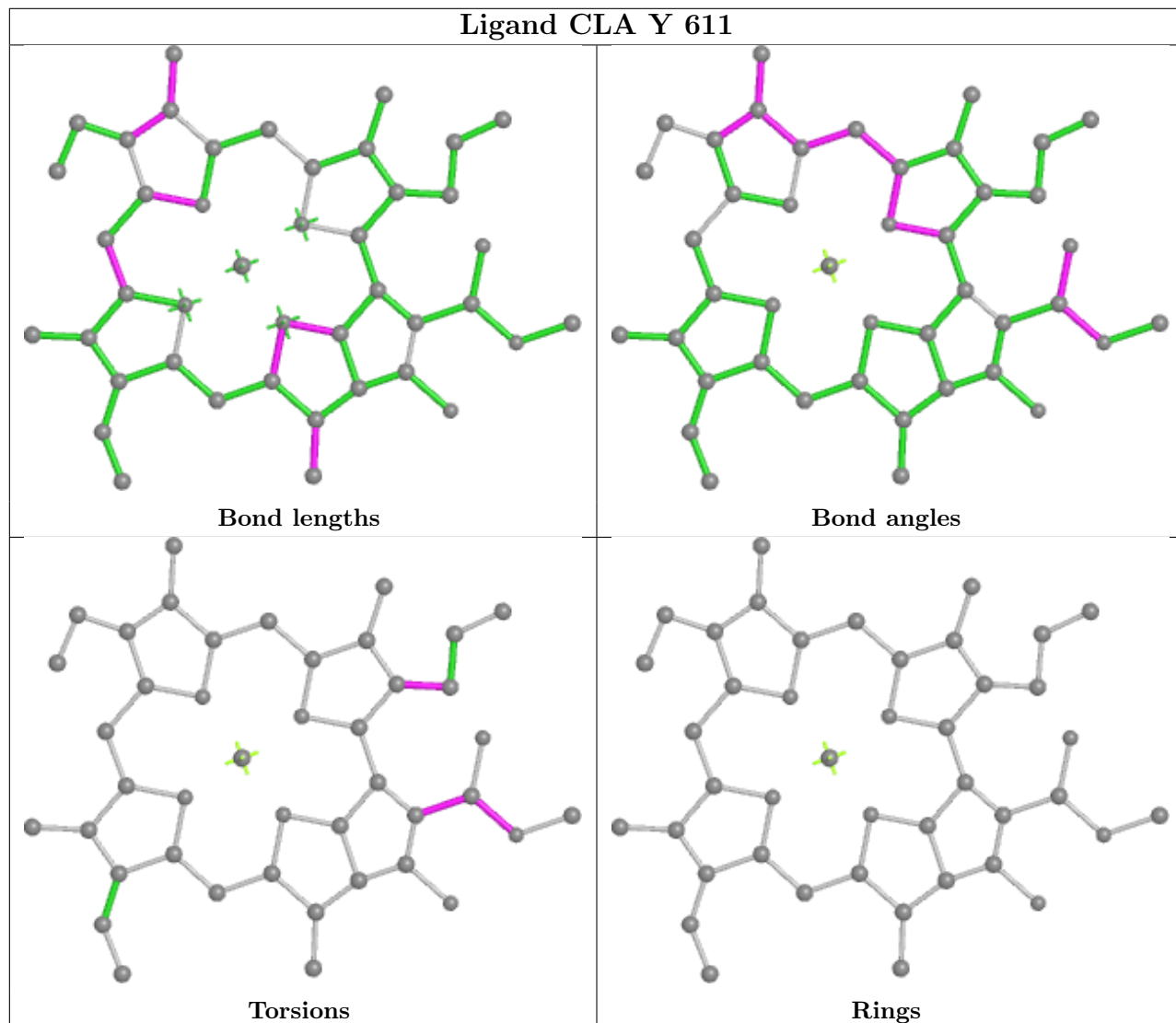
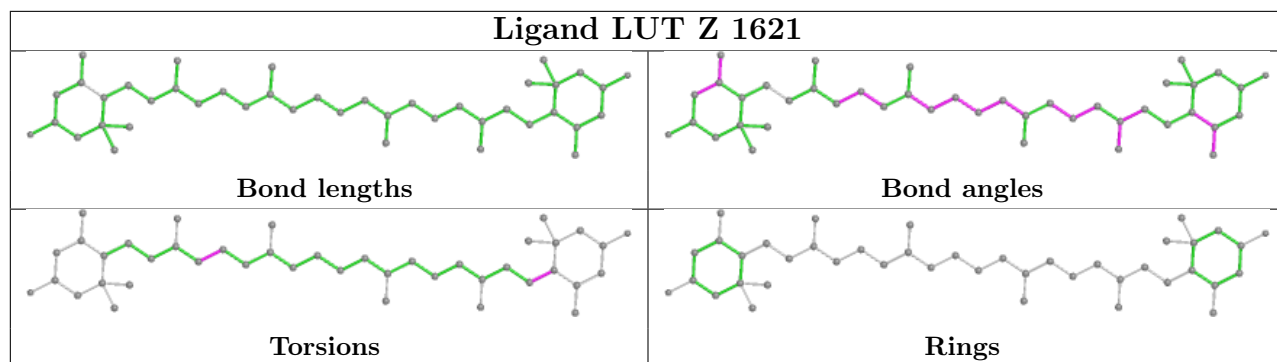


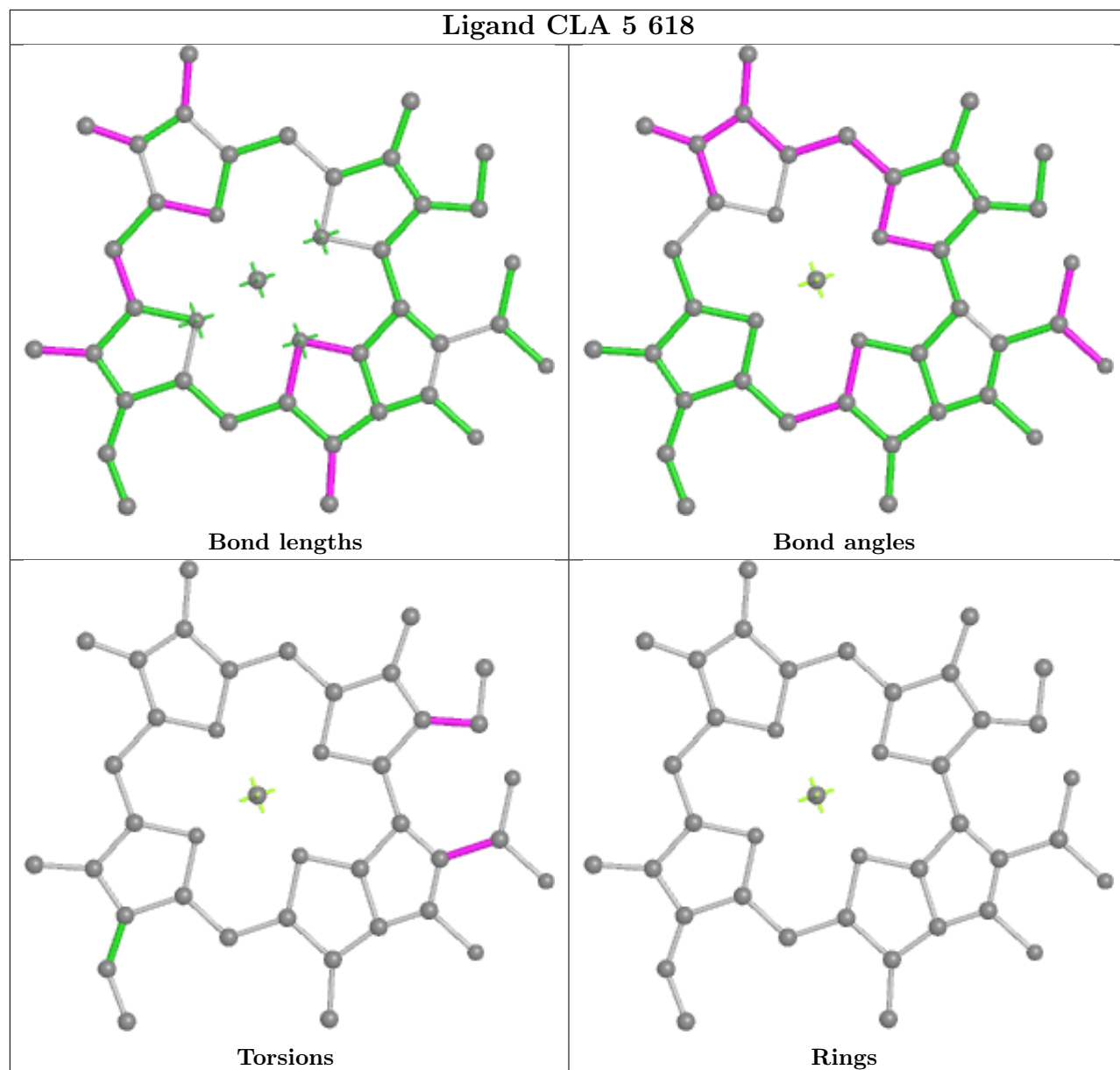


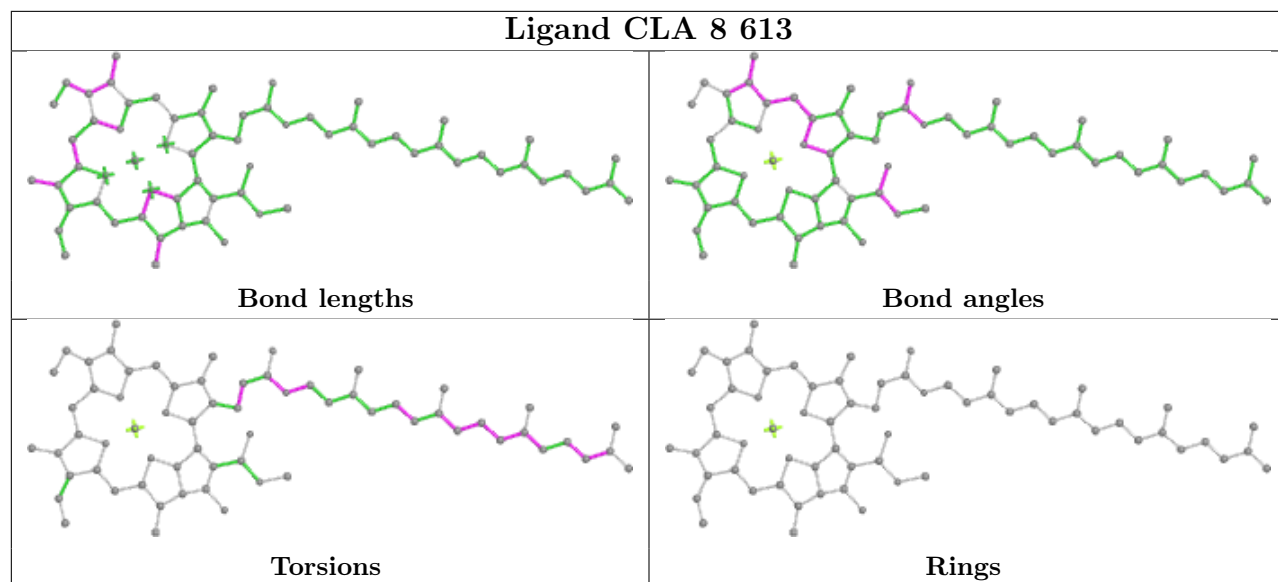


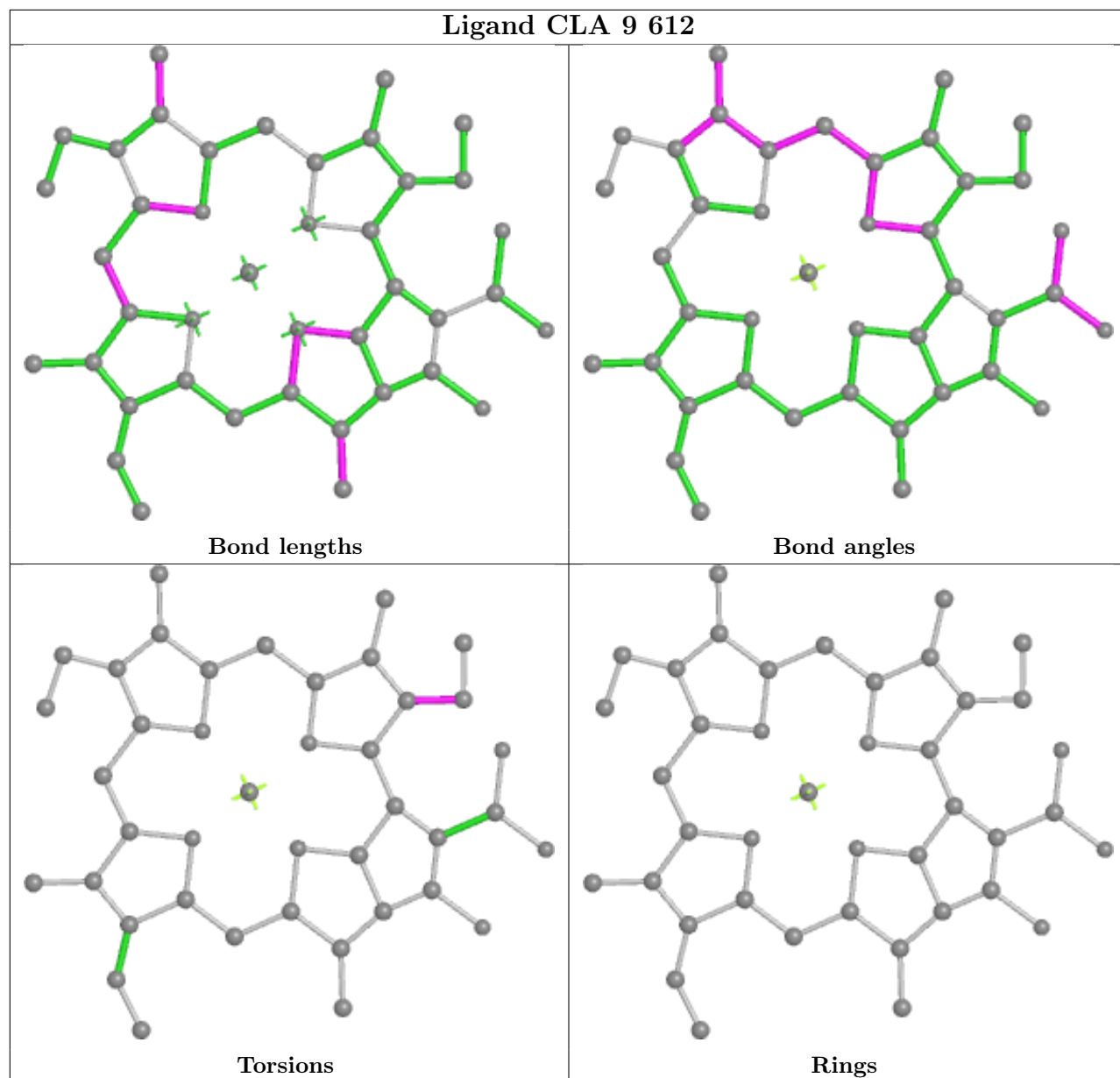




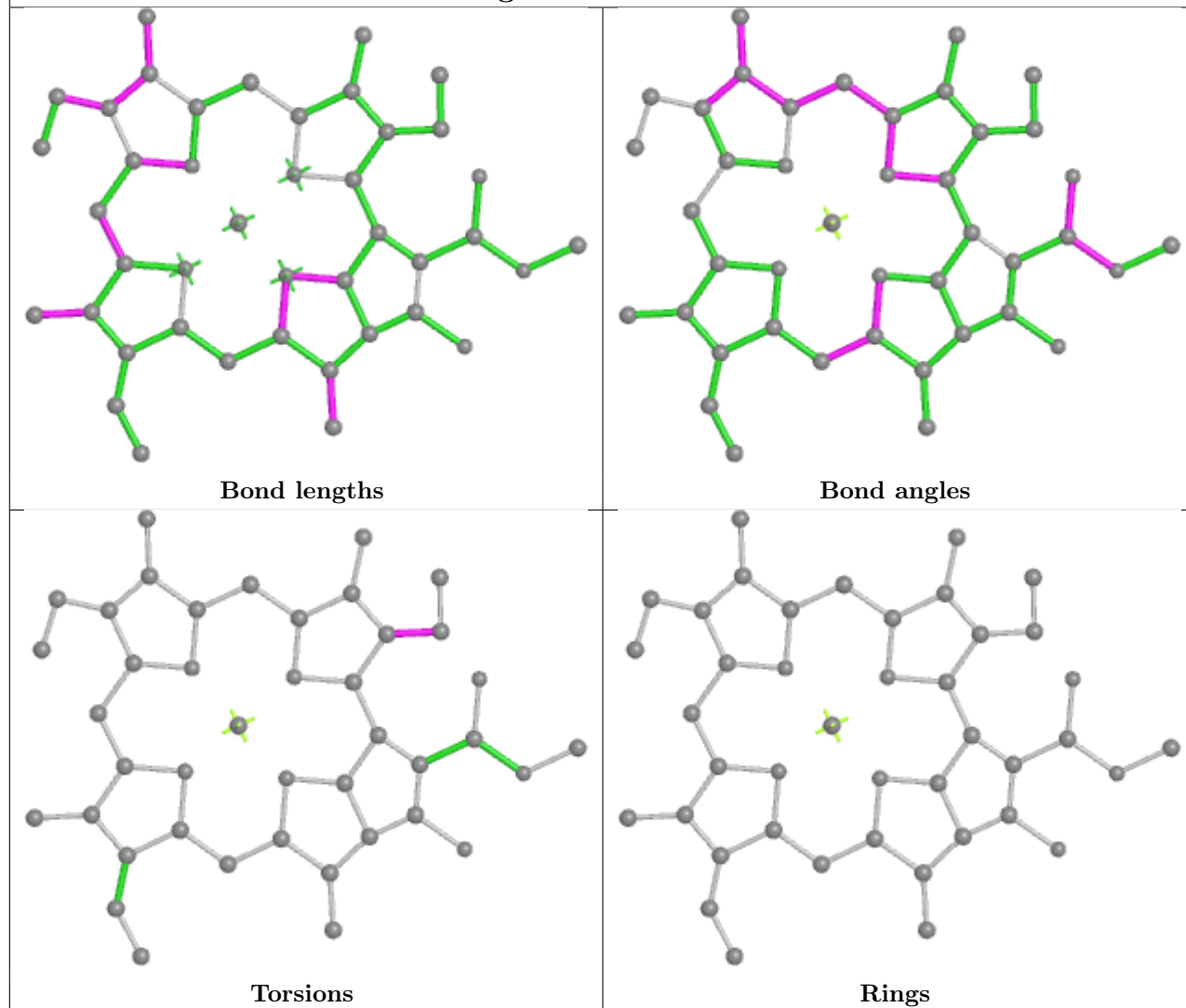




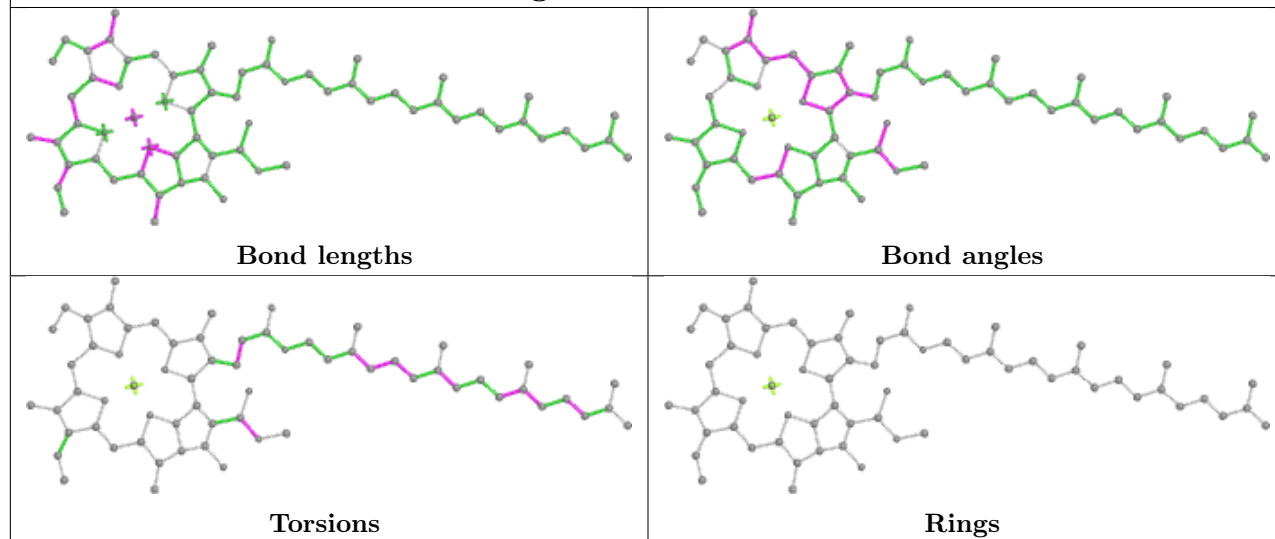


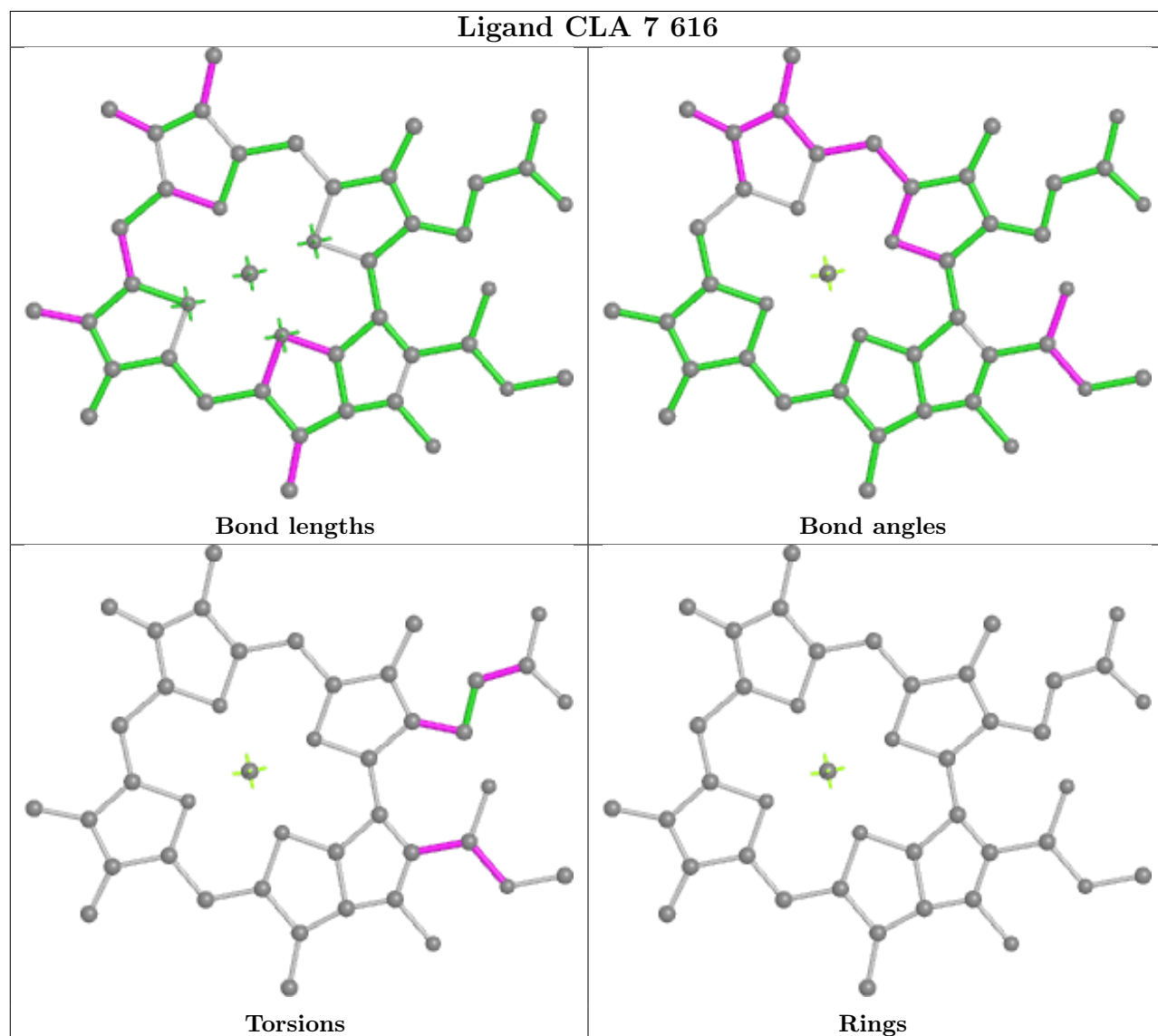
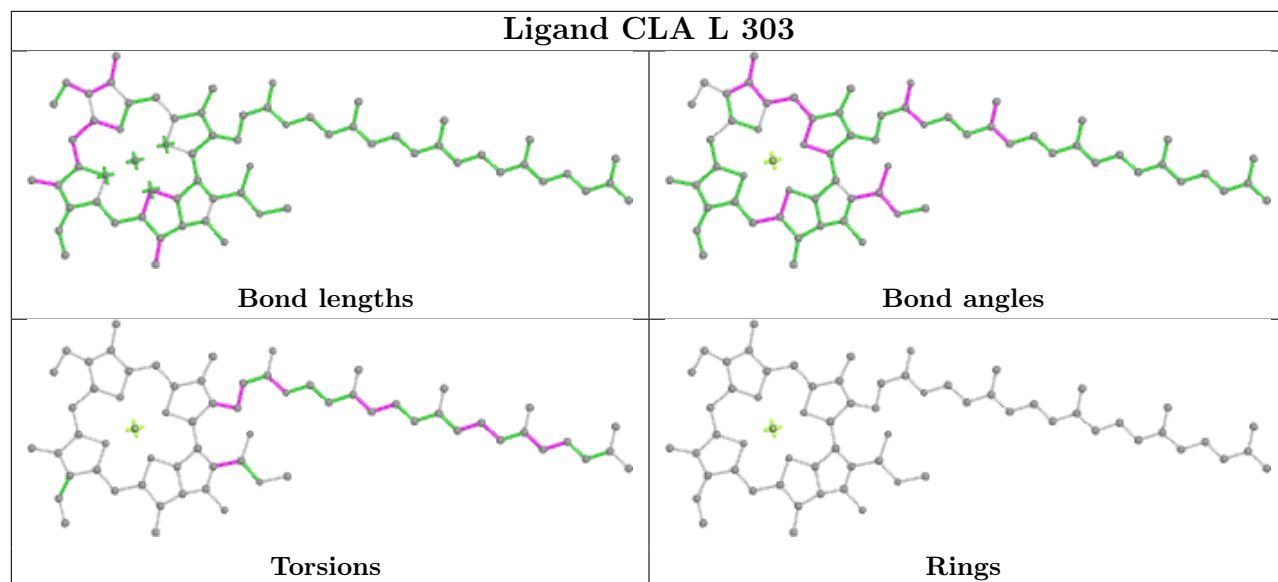


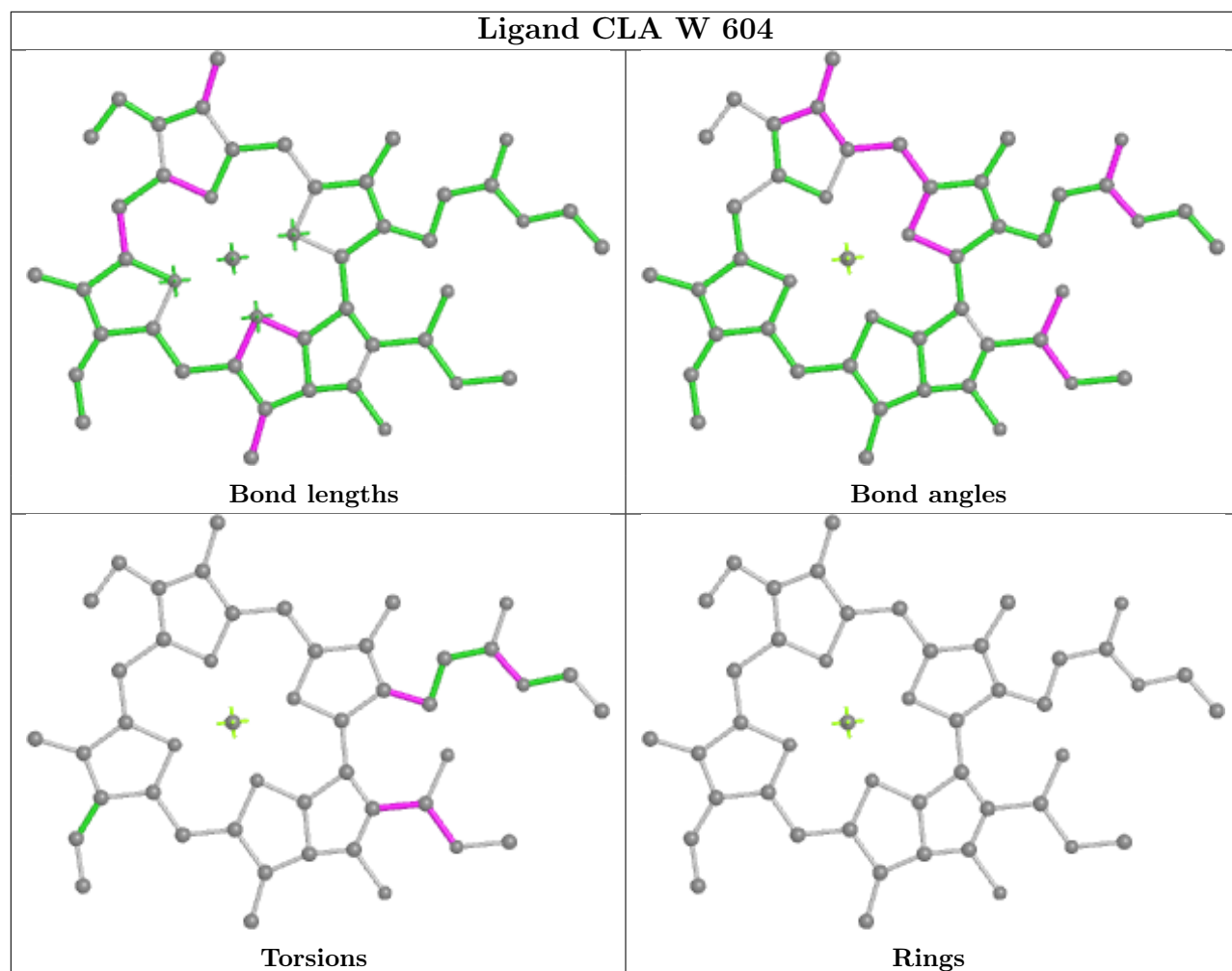
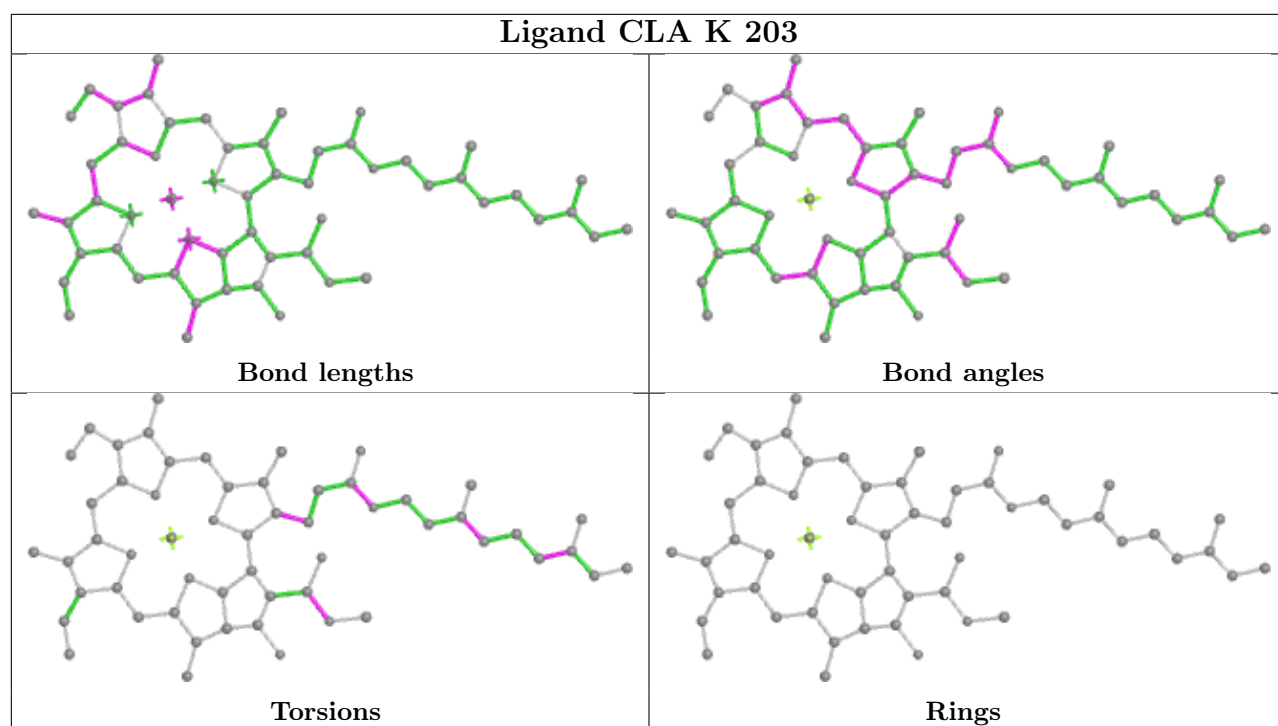
Ligand CLA 7 614

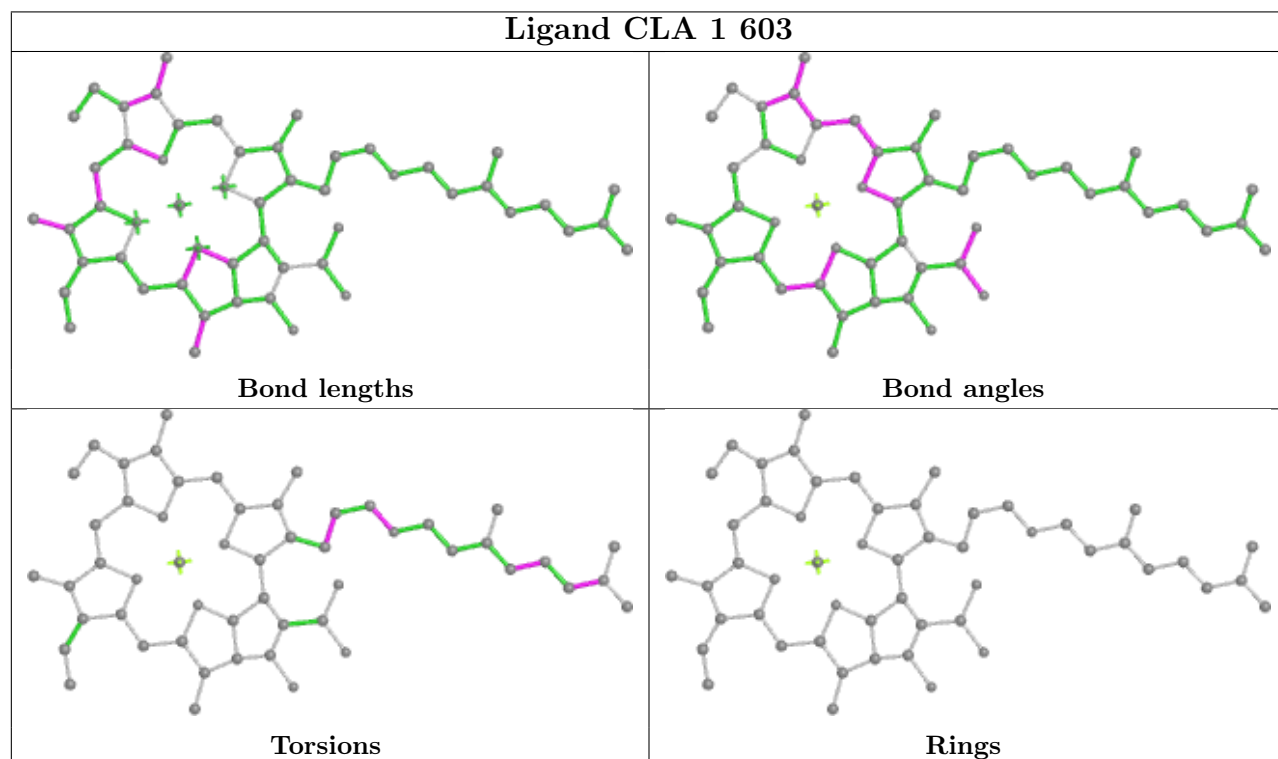
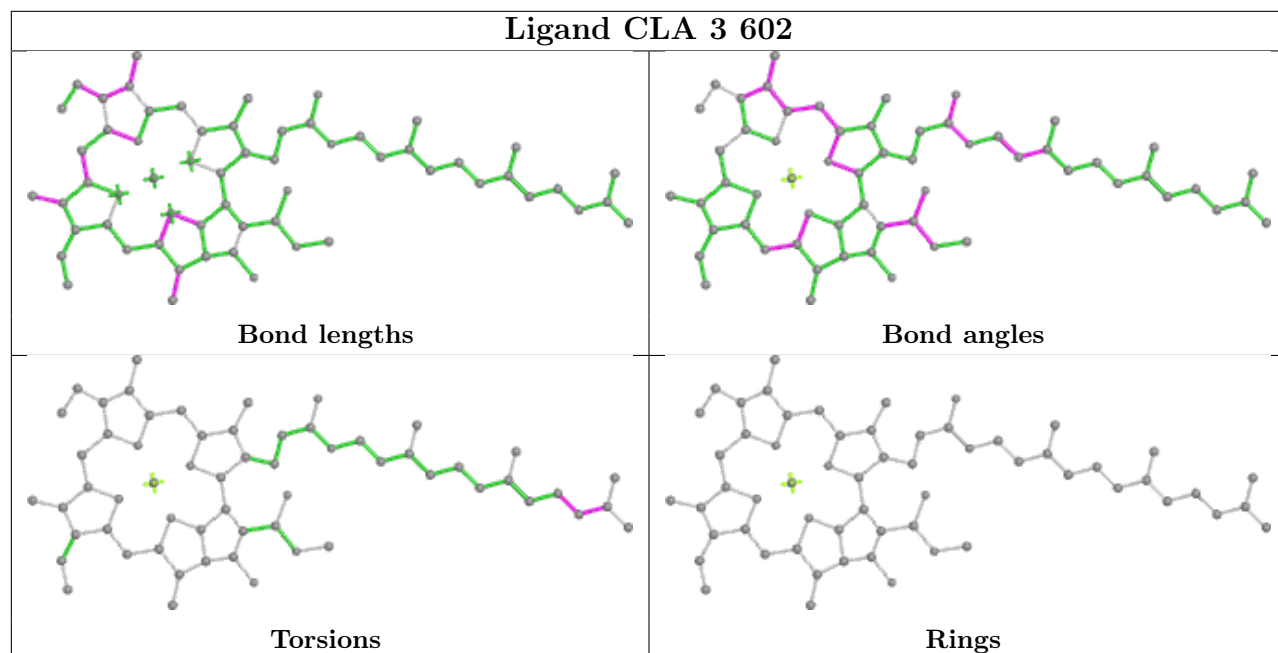


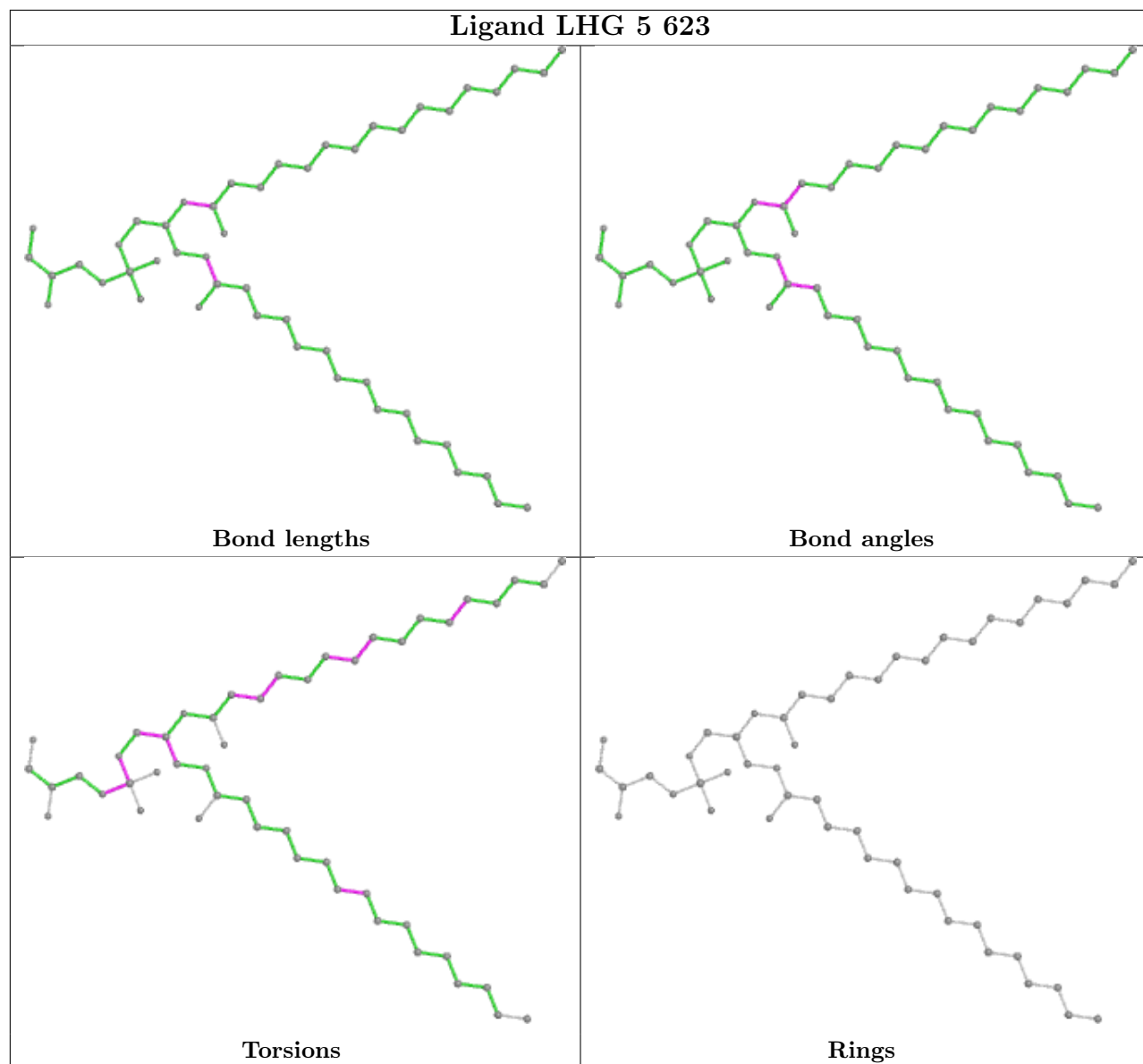
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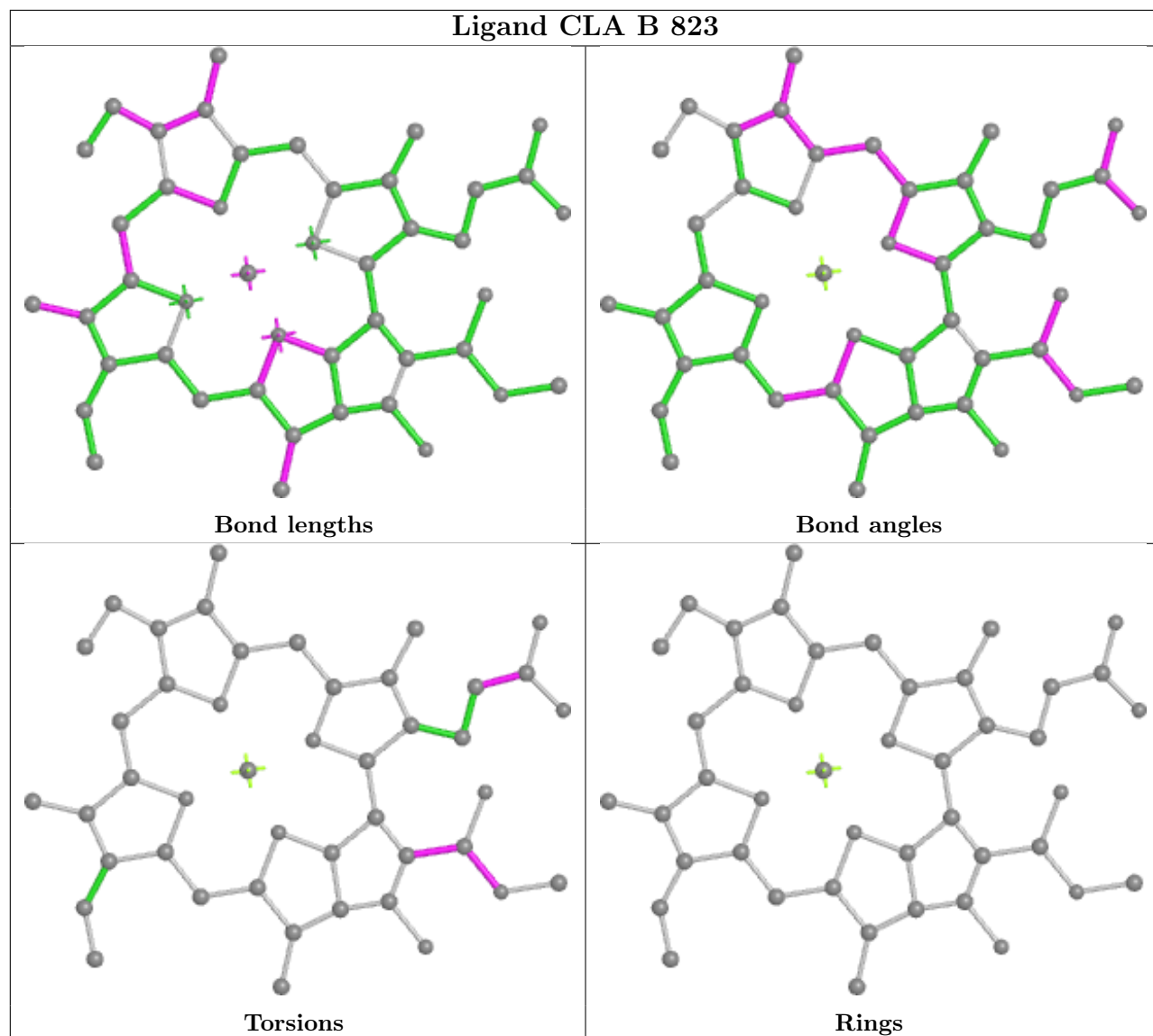


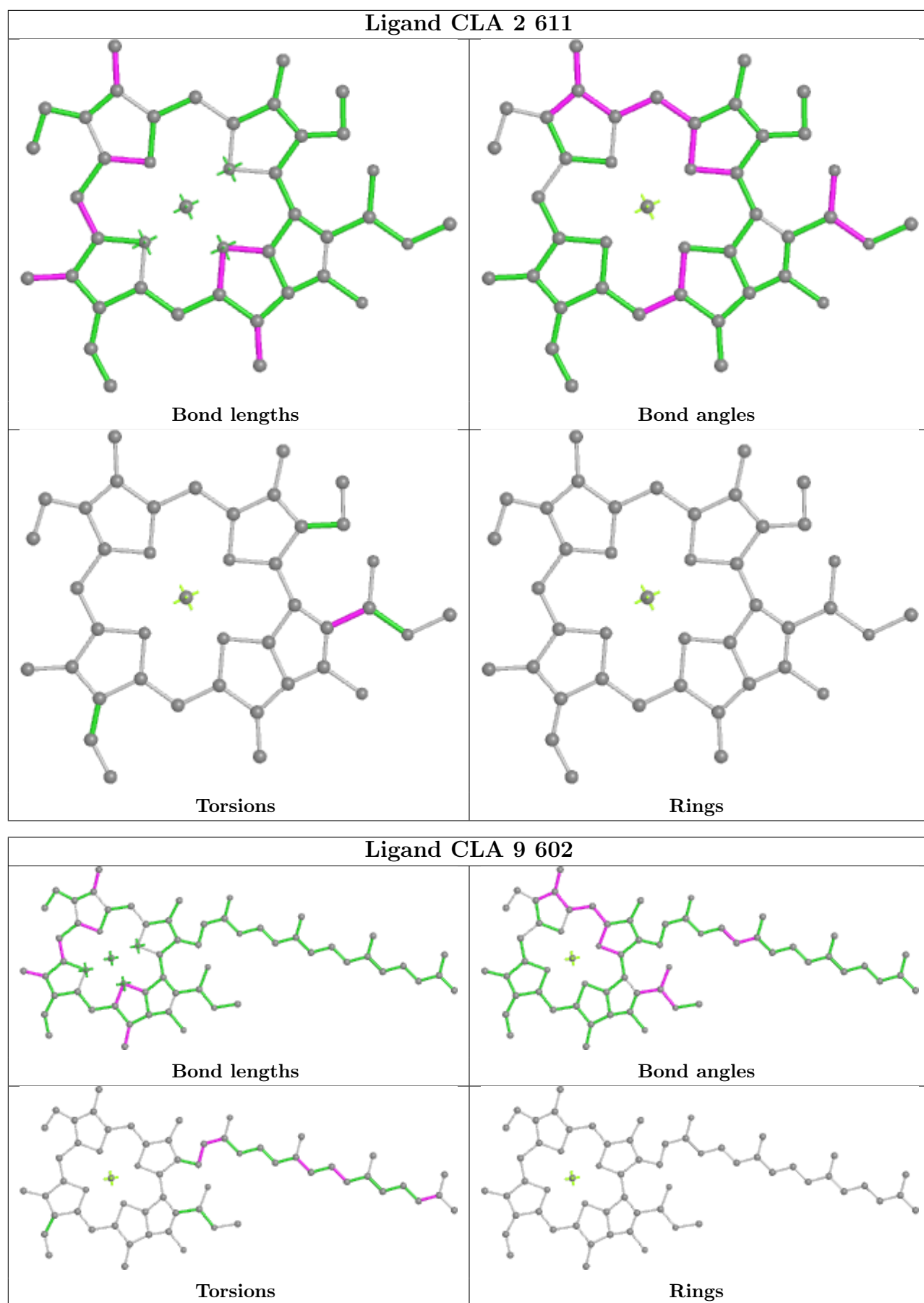


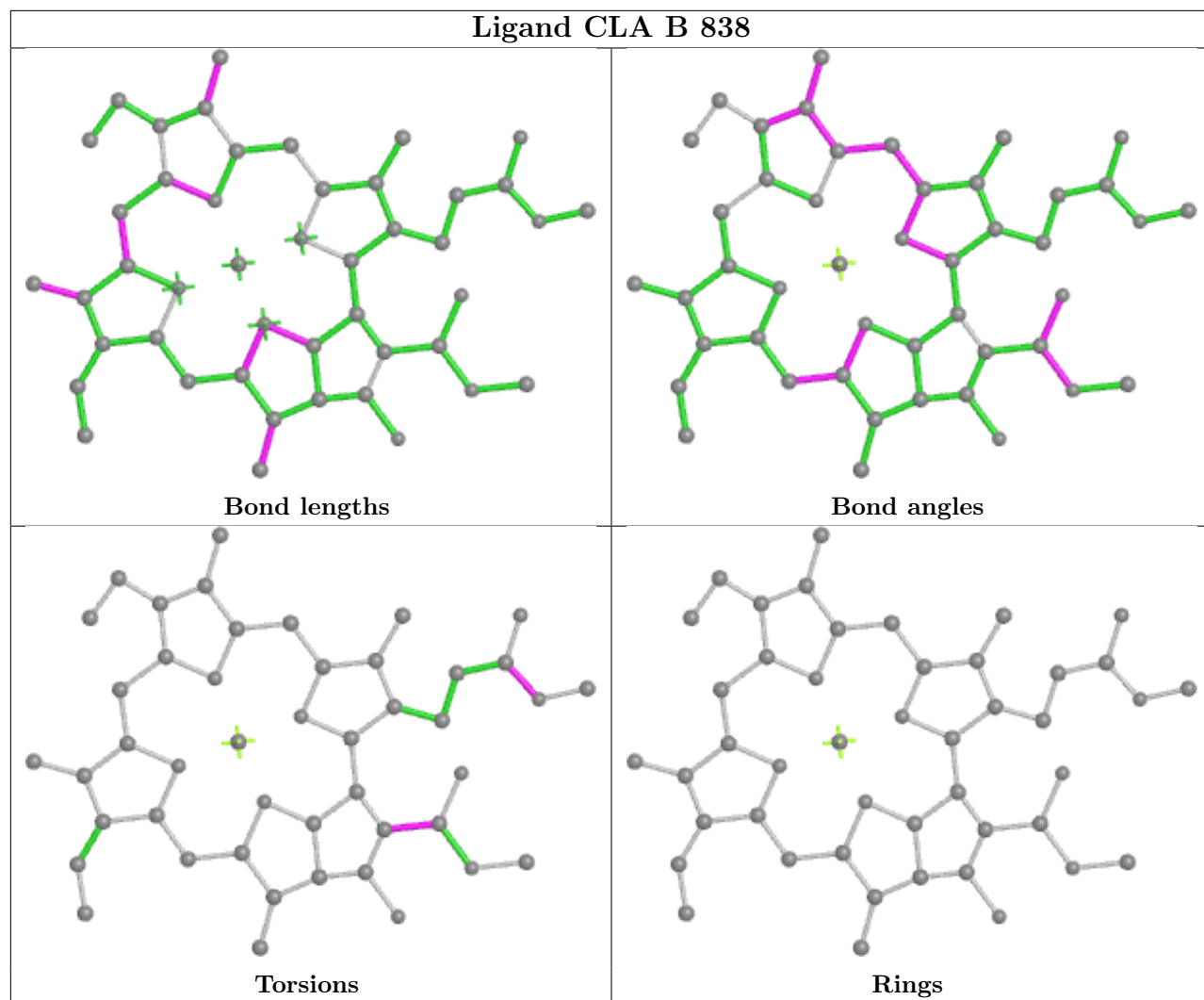


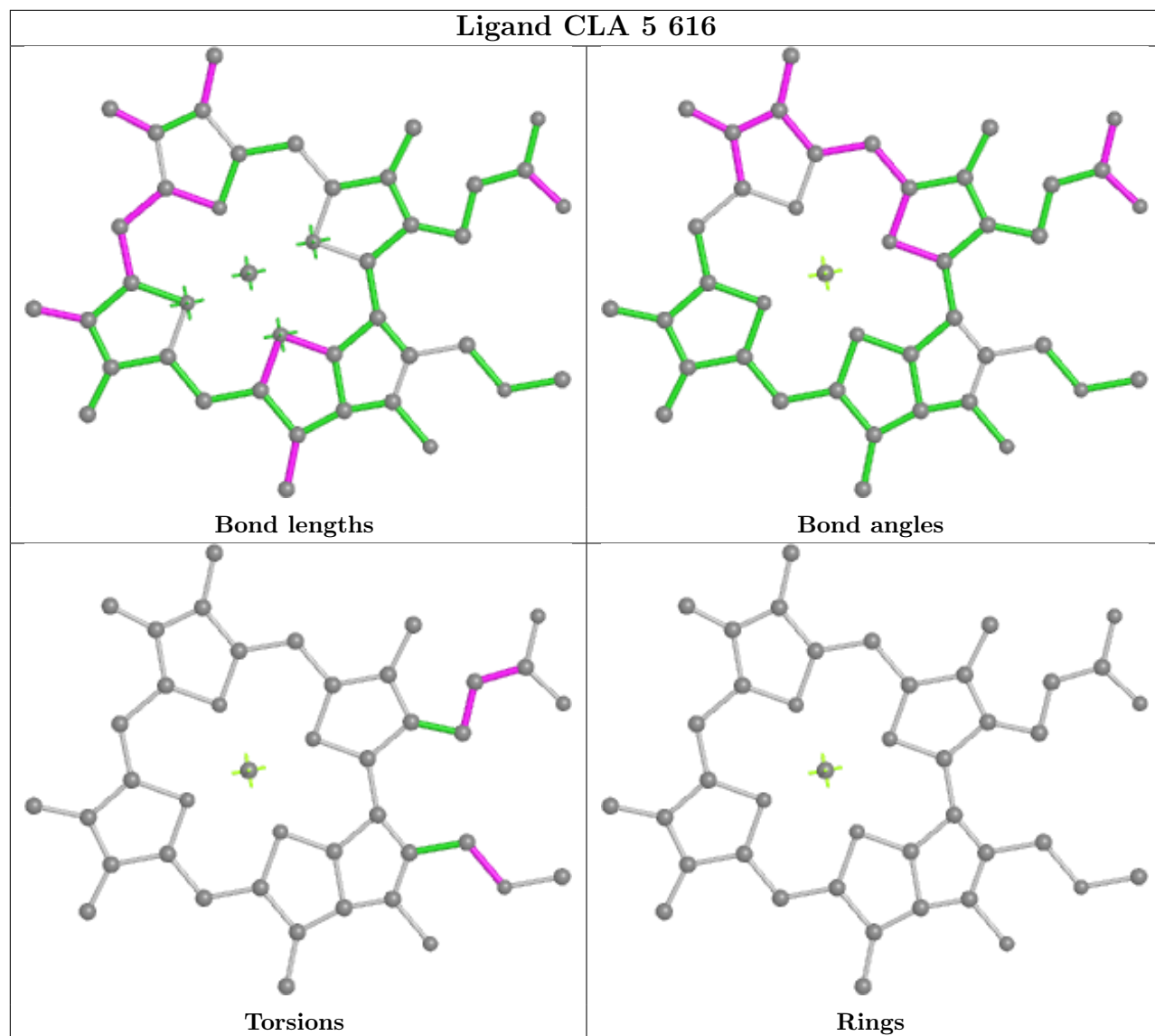


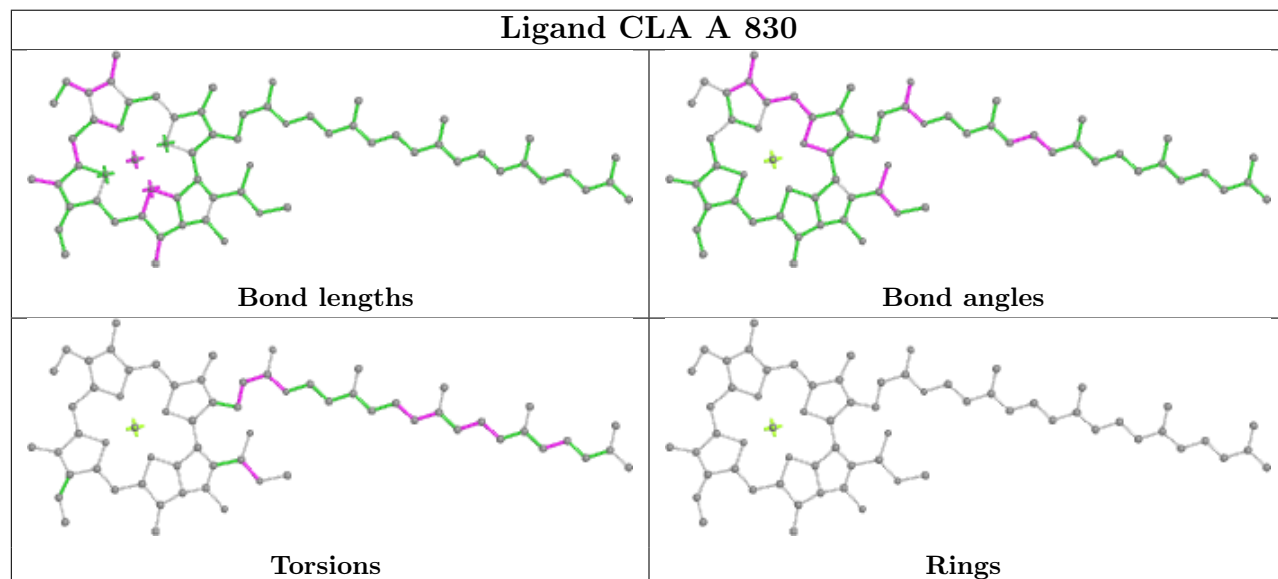
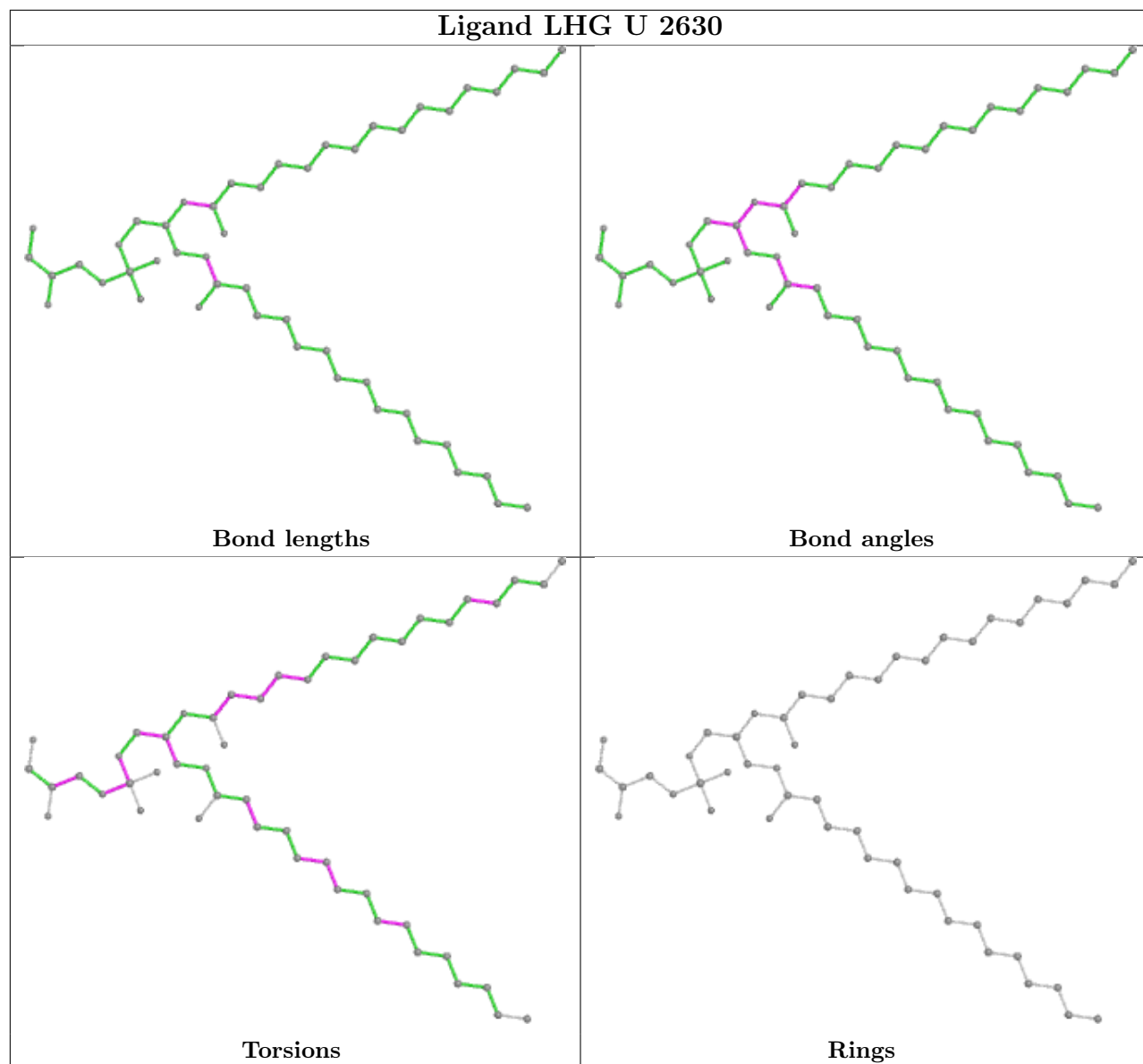


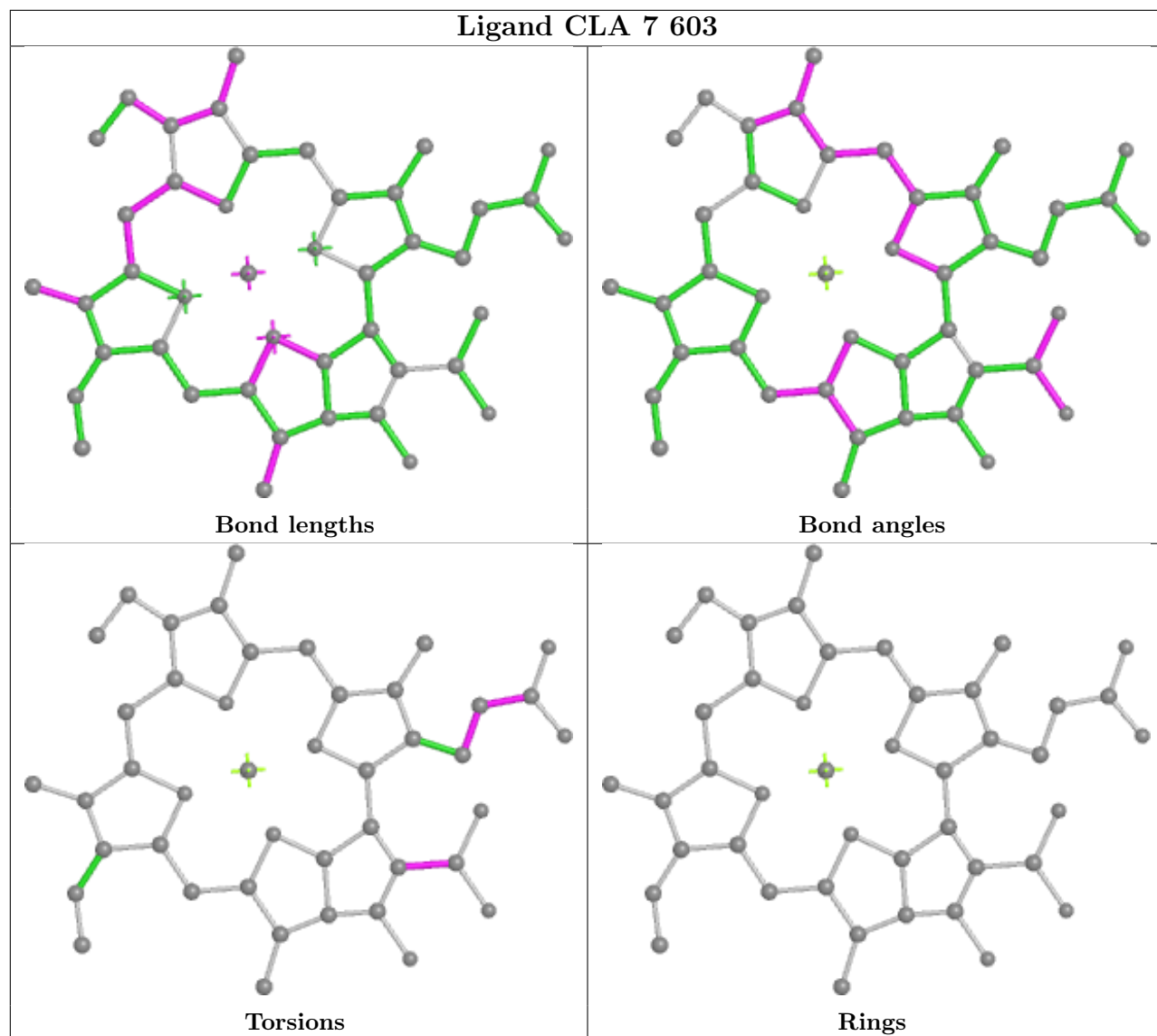


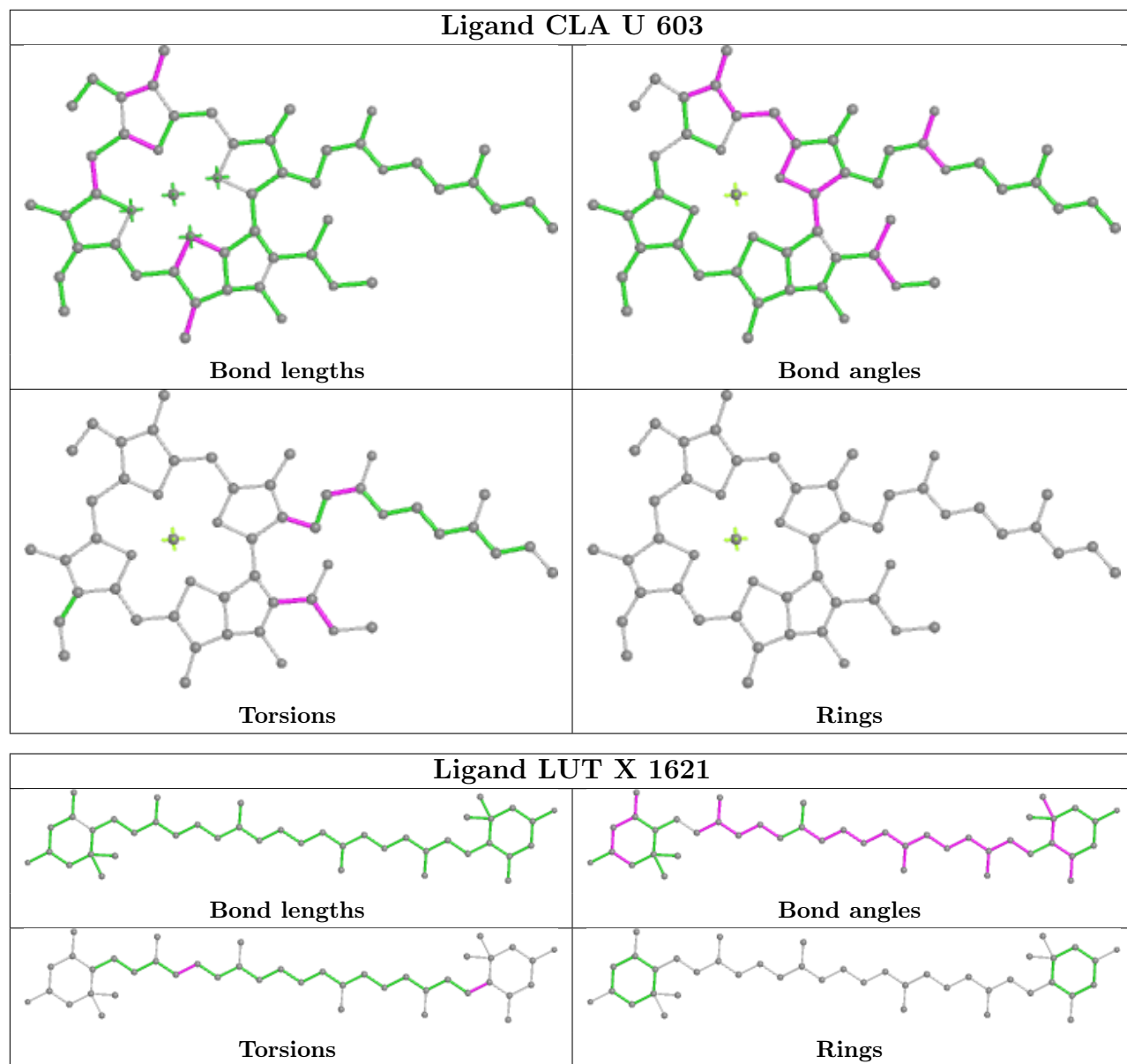


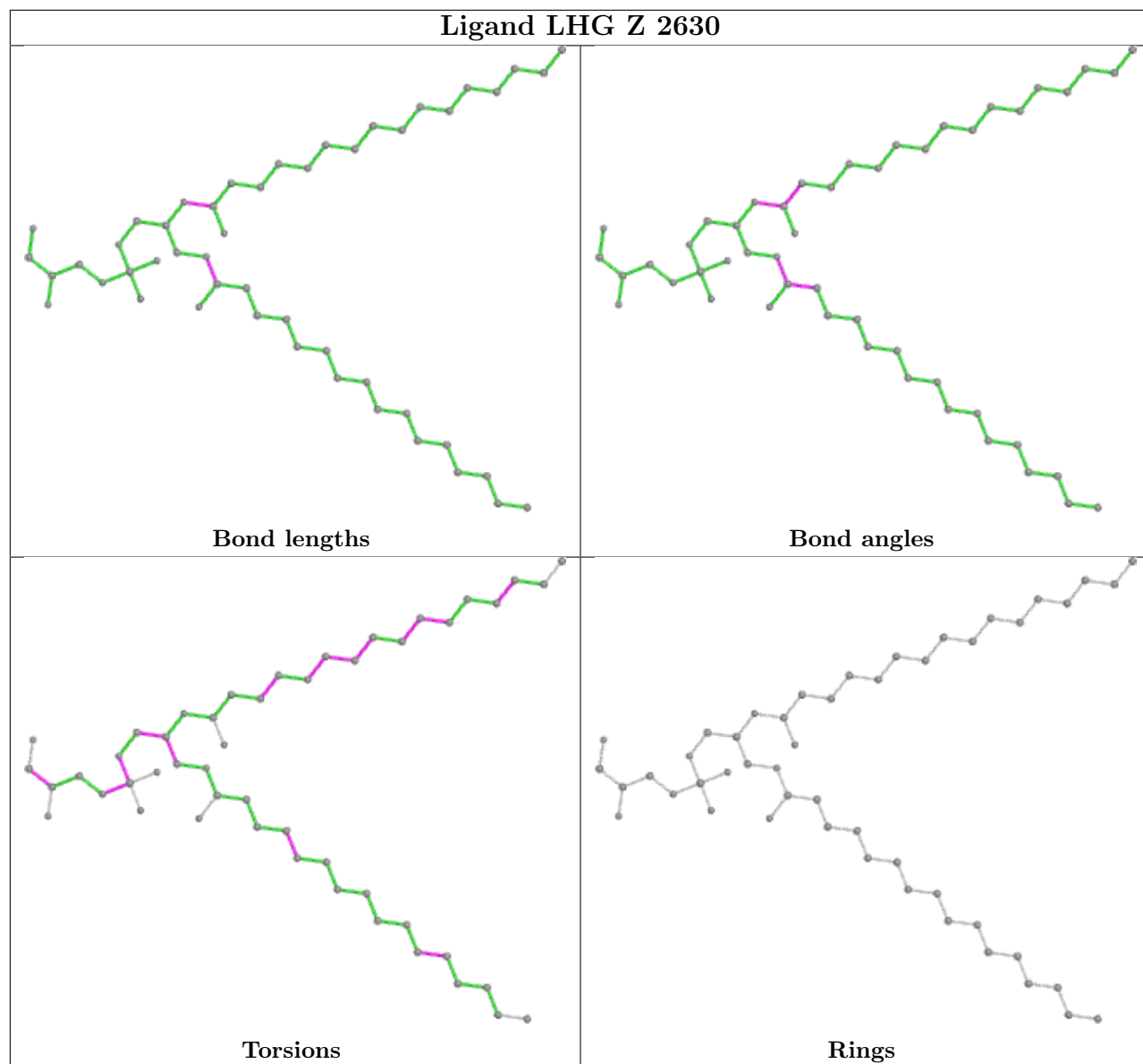


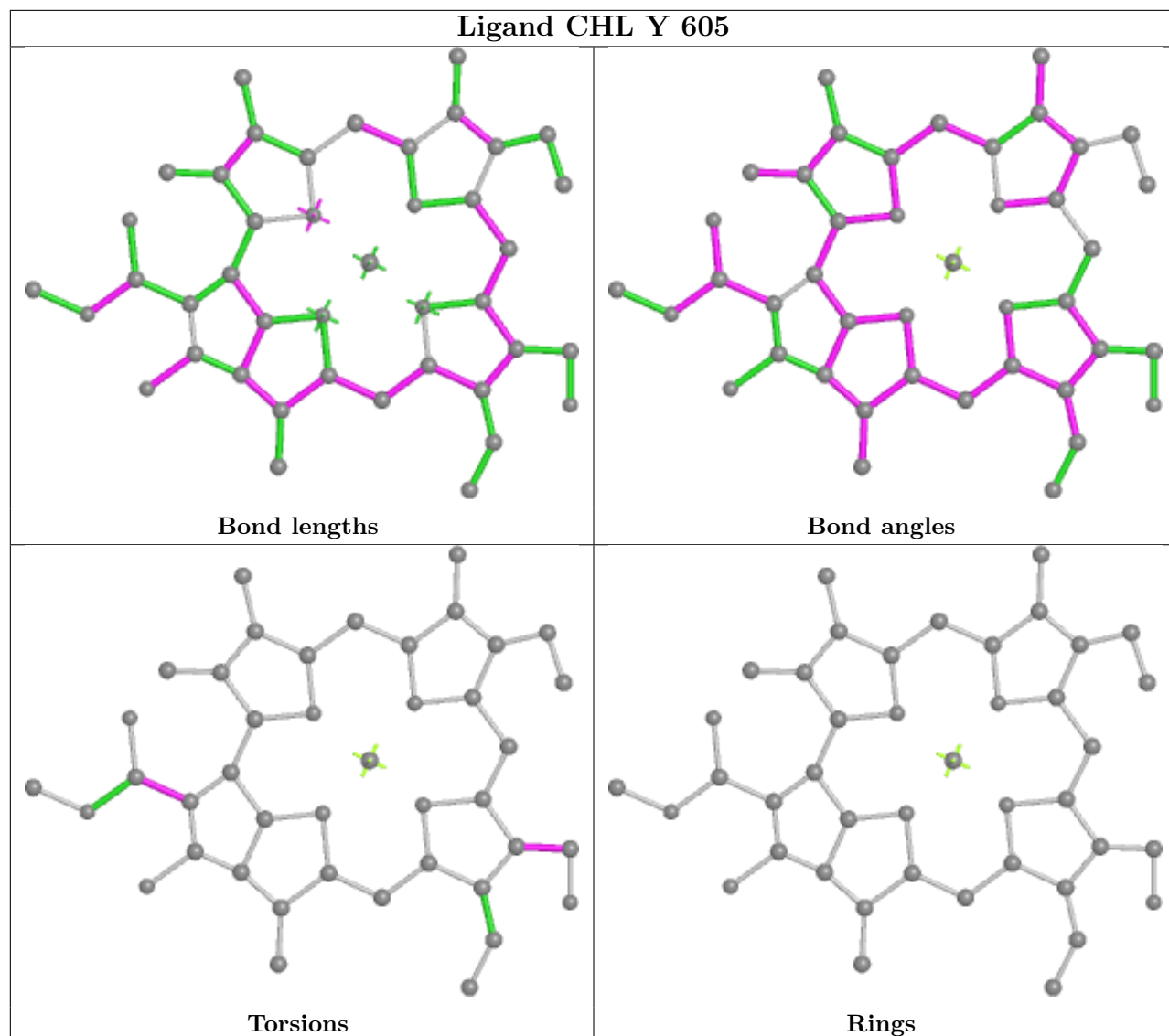


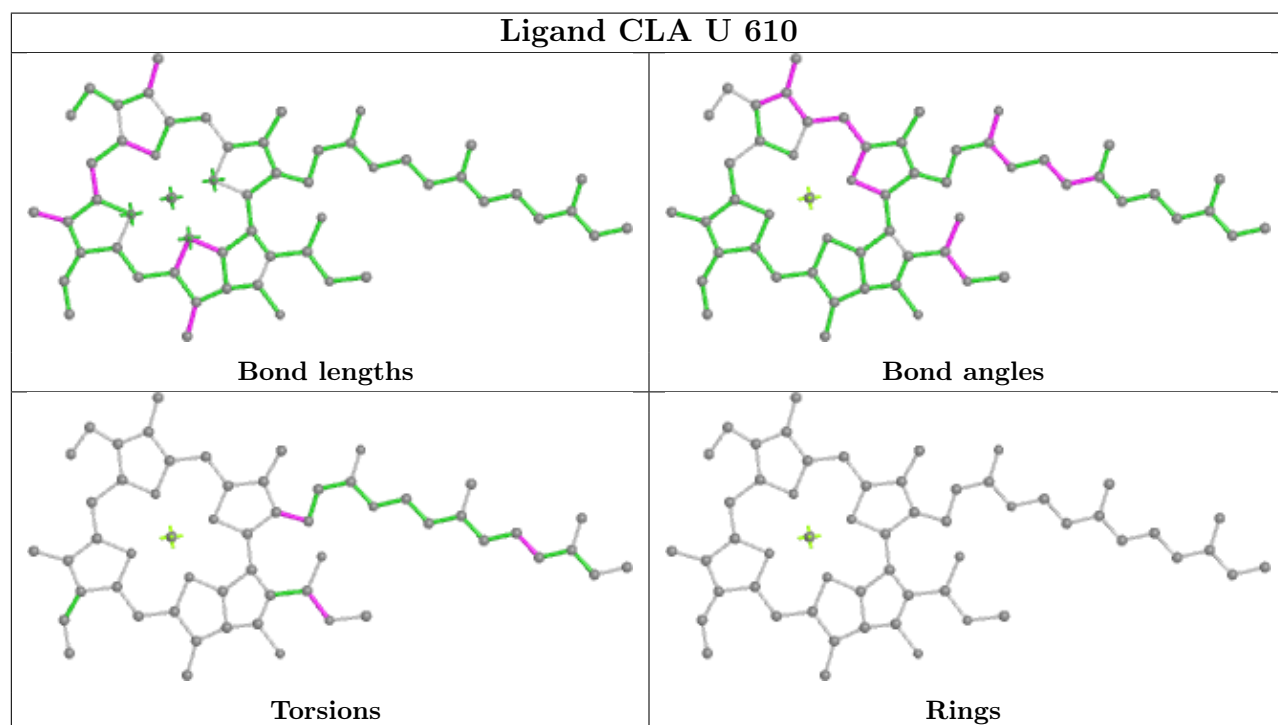
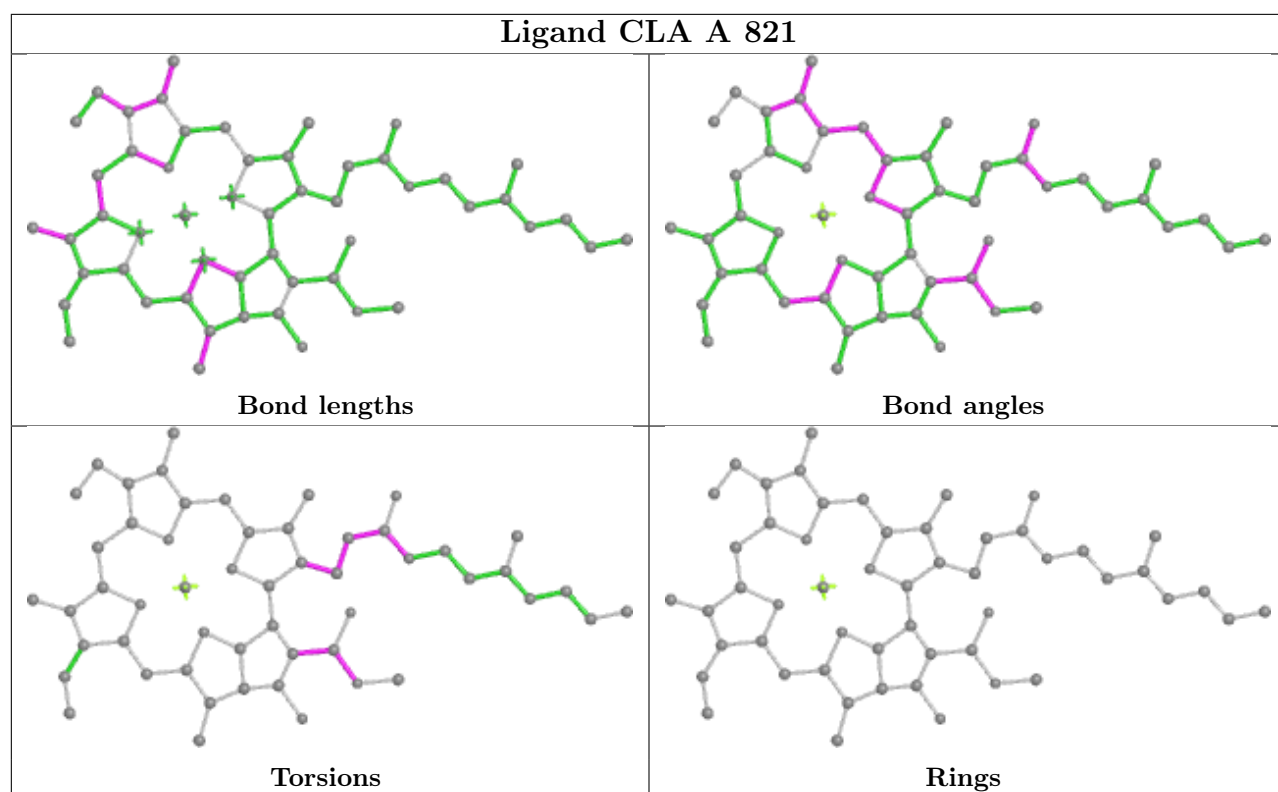


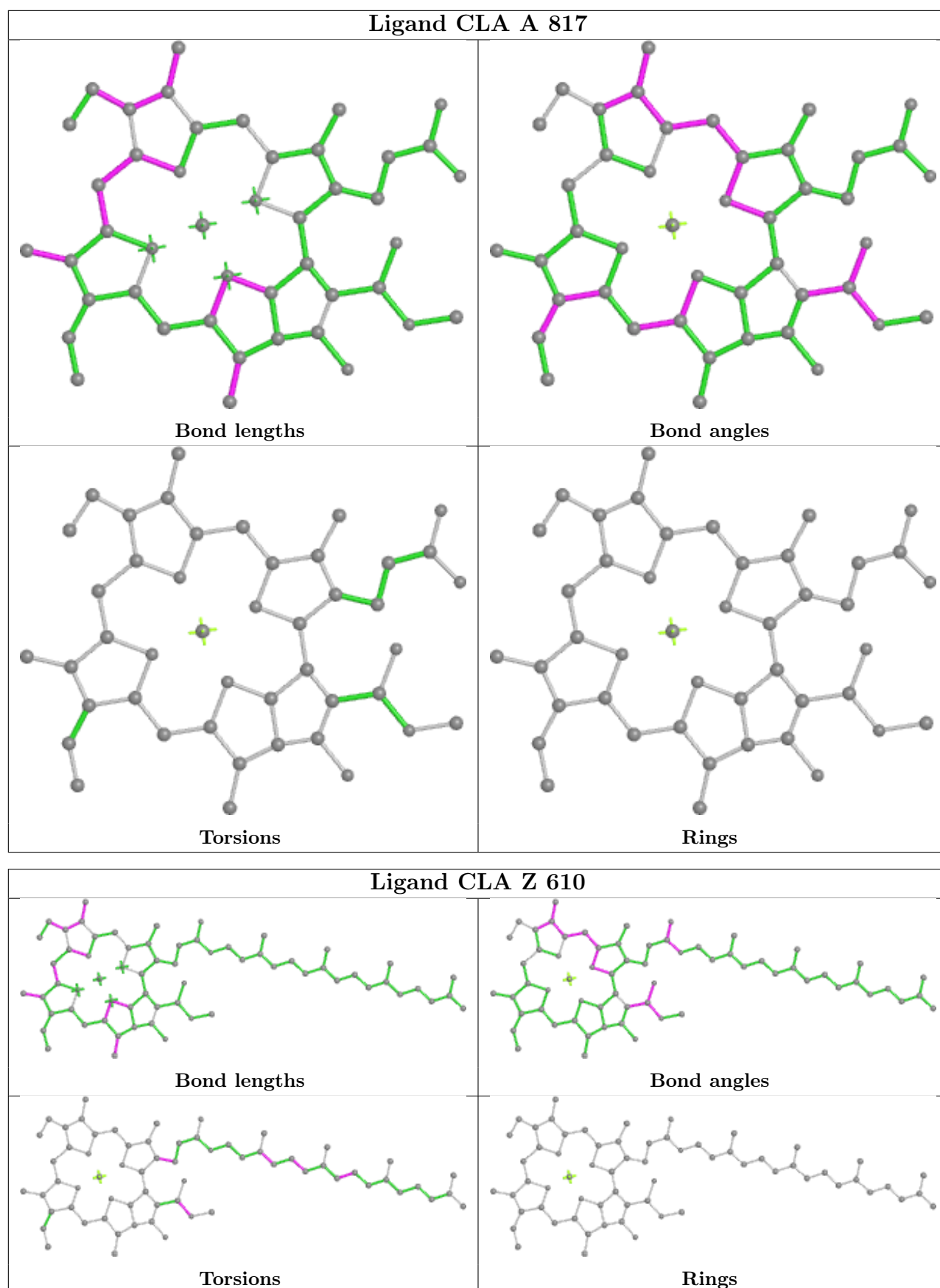


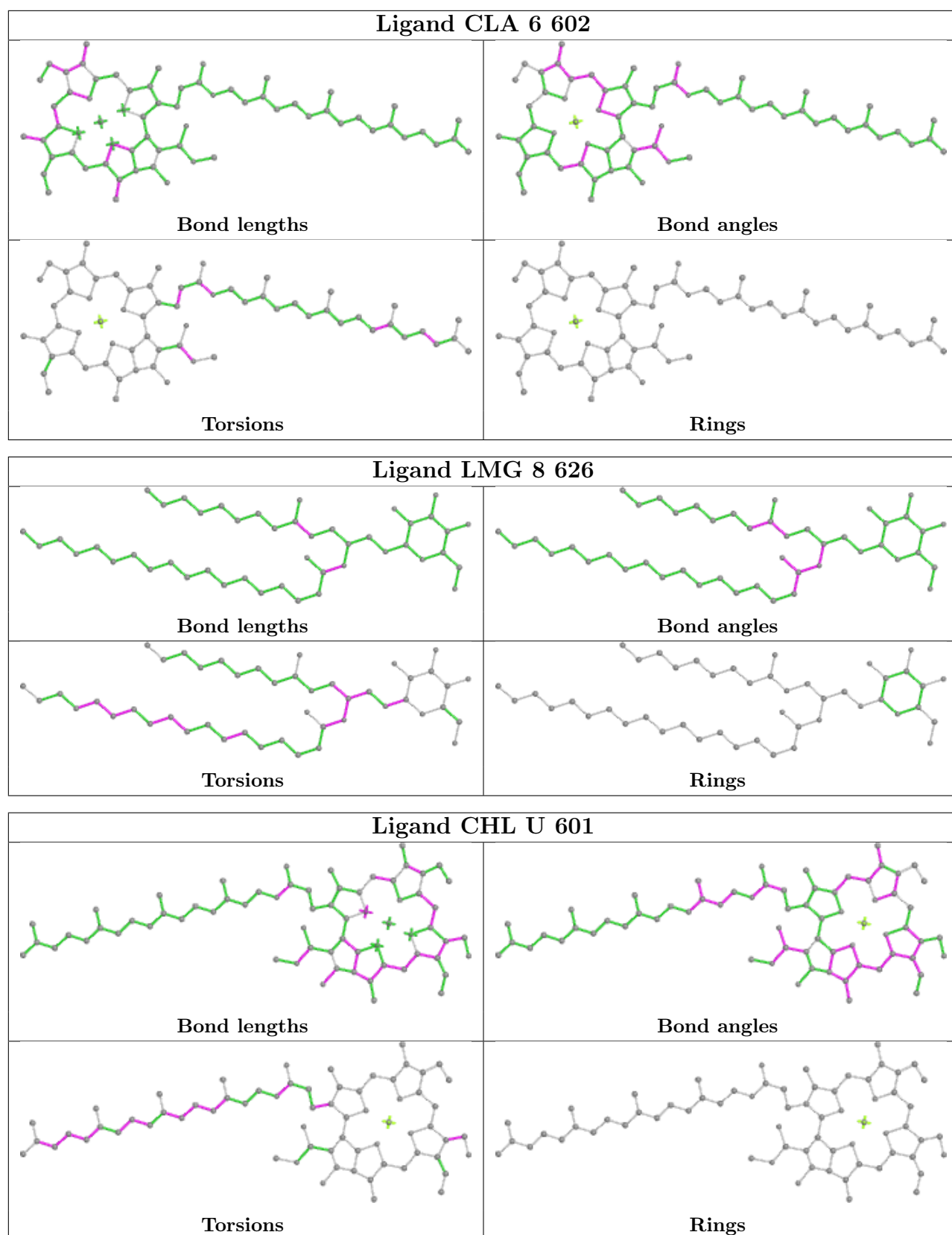


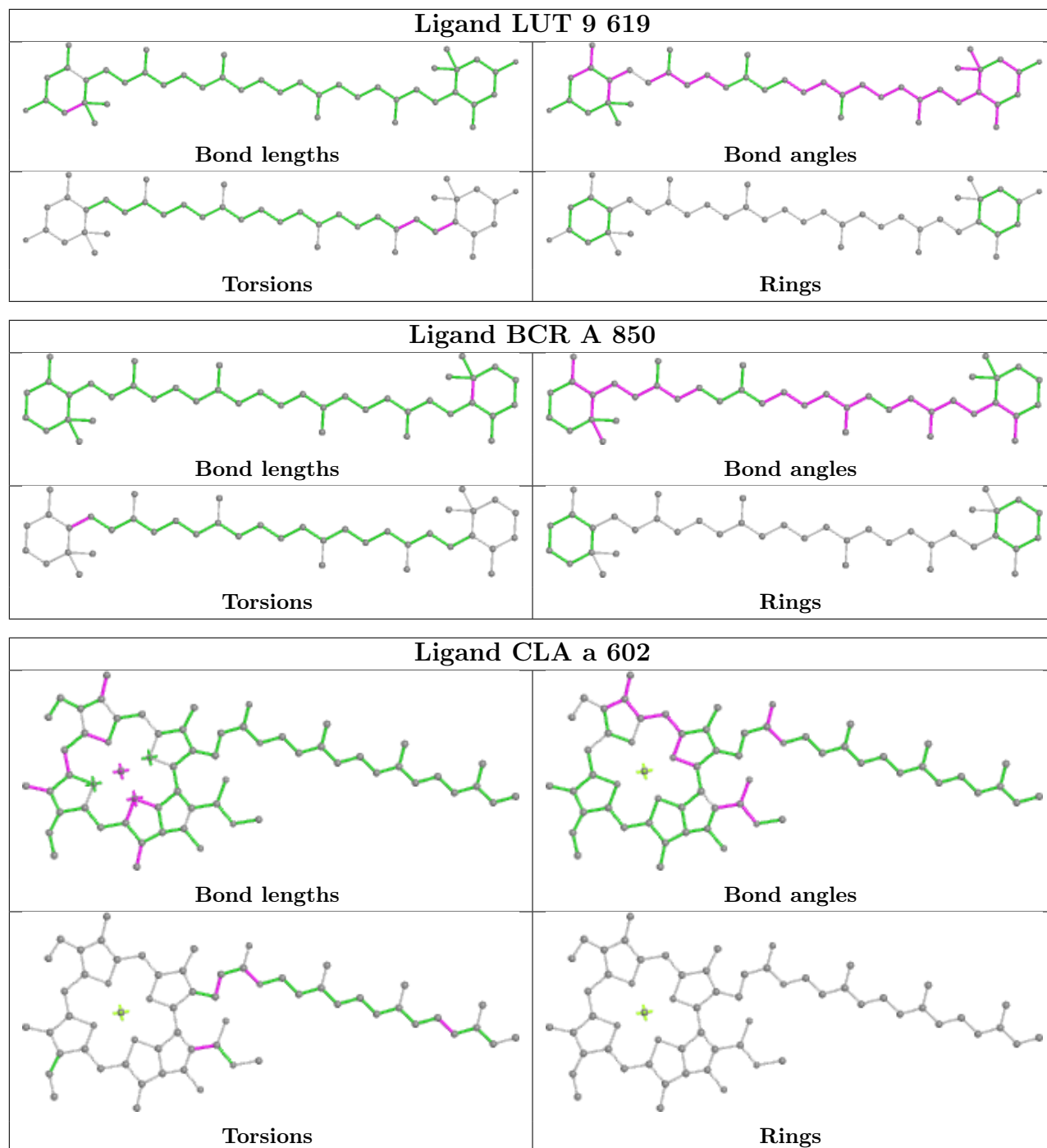


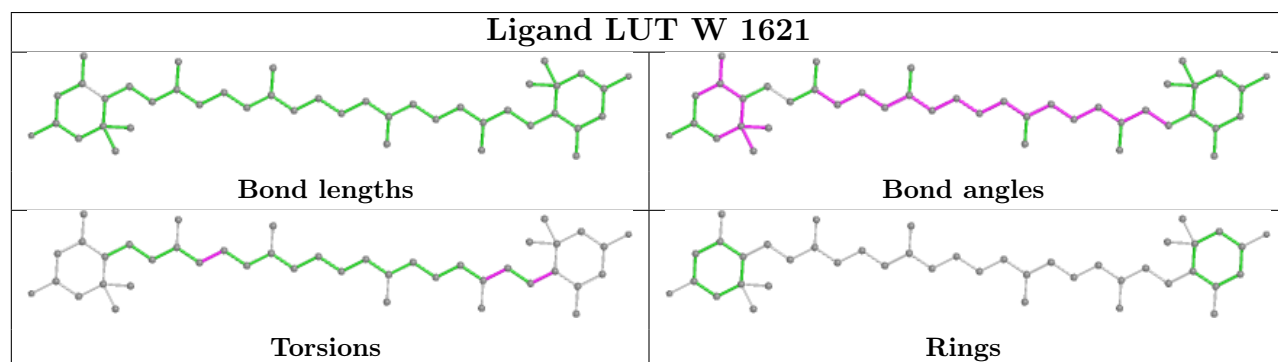
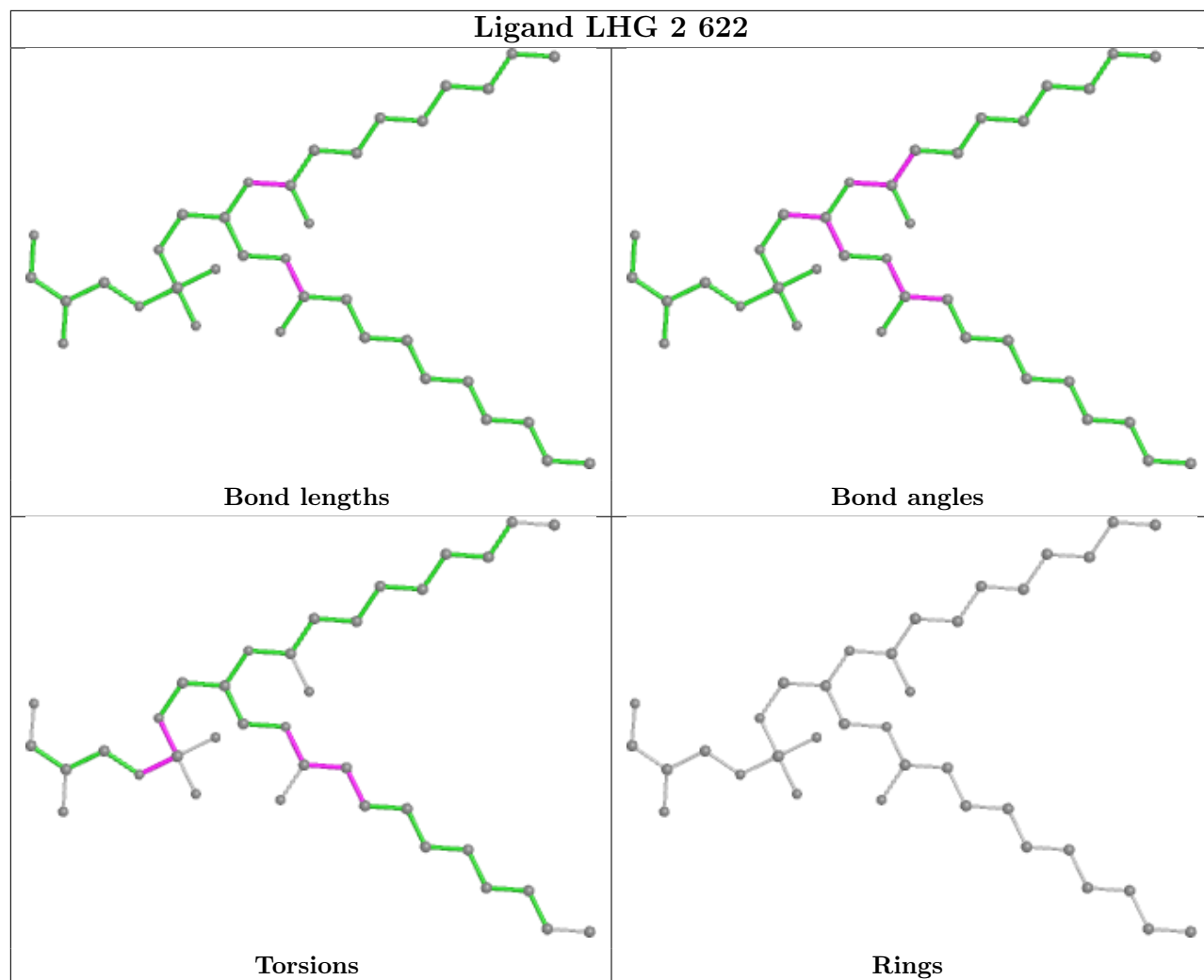


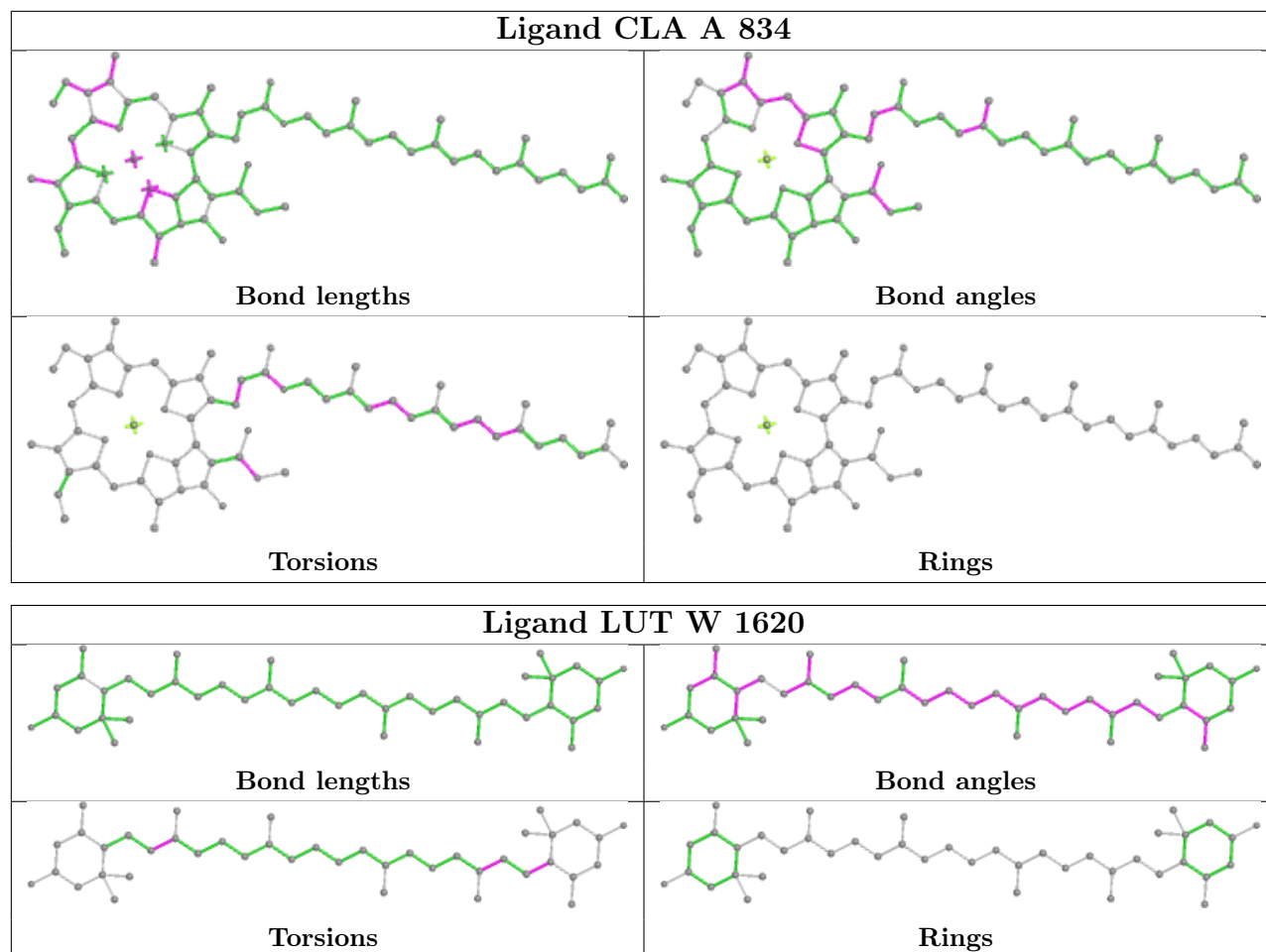


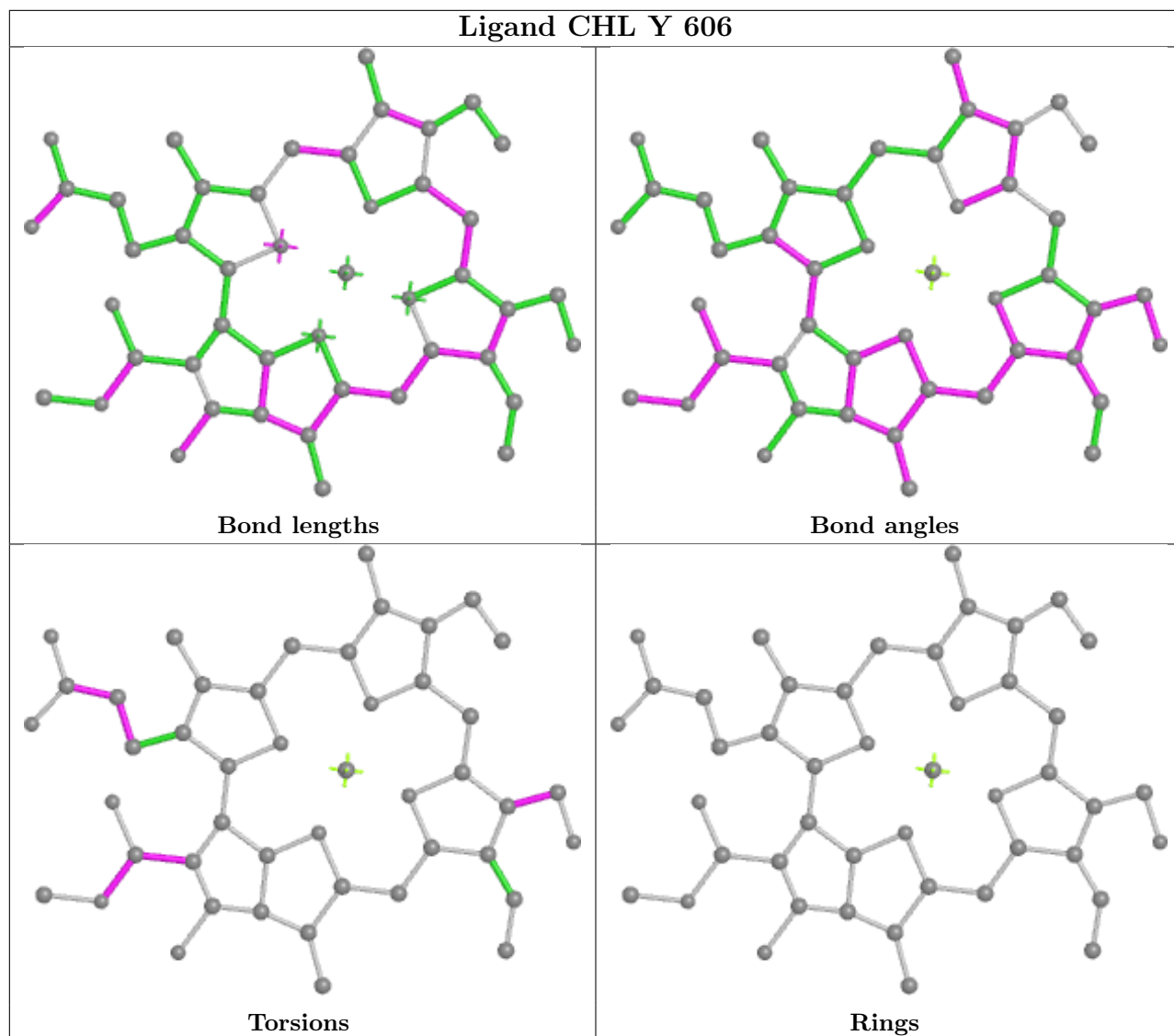


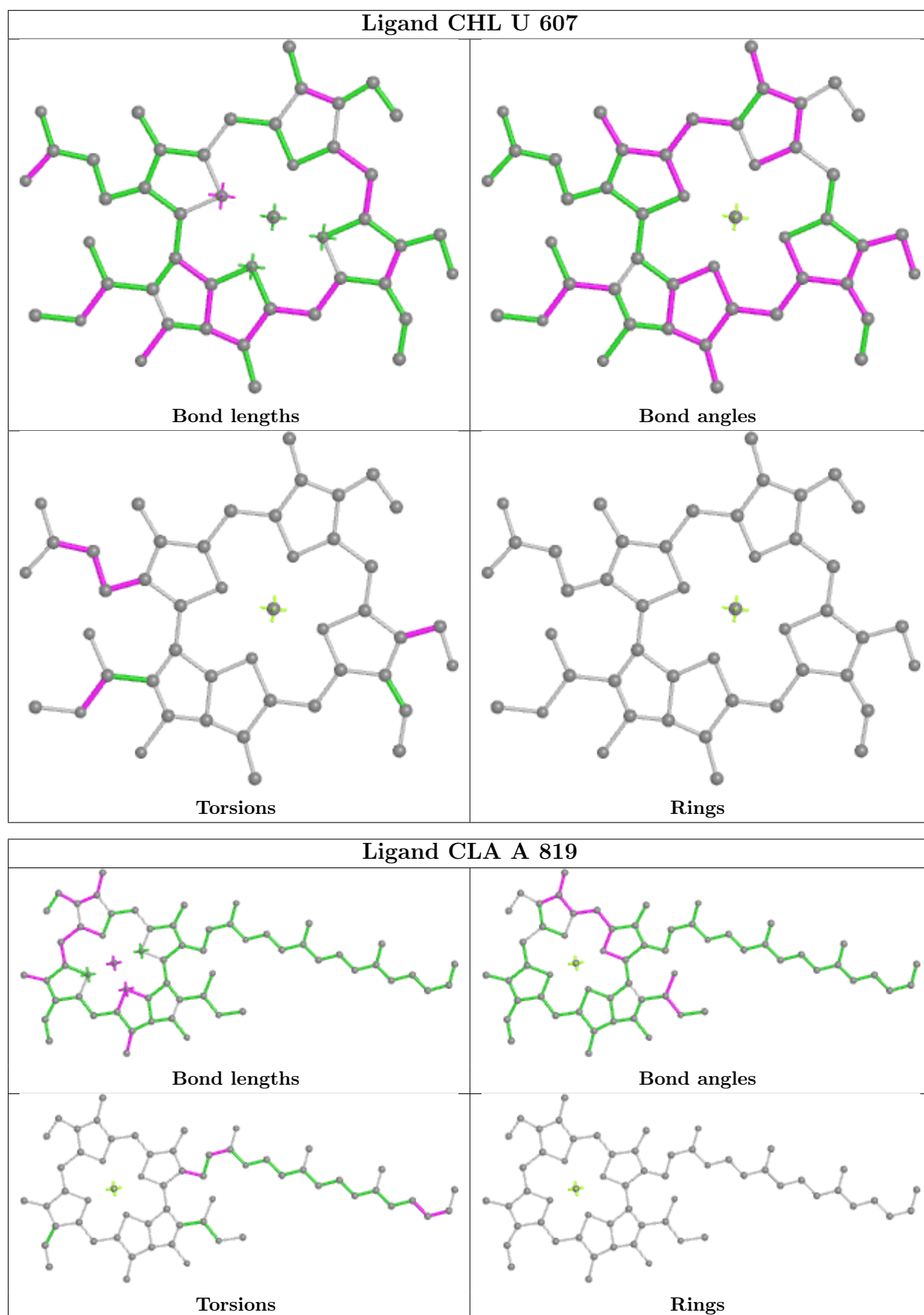


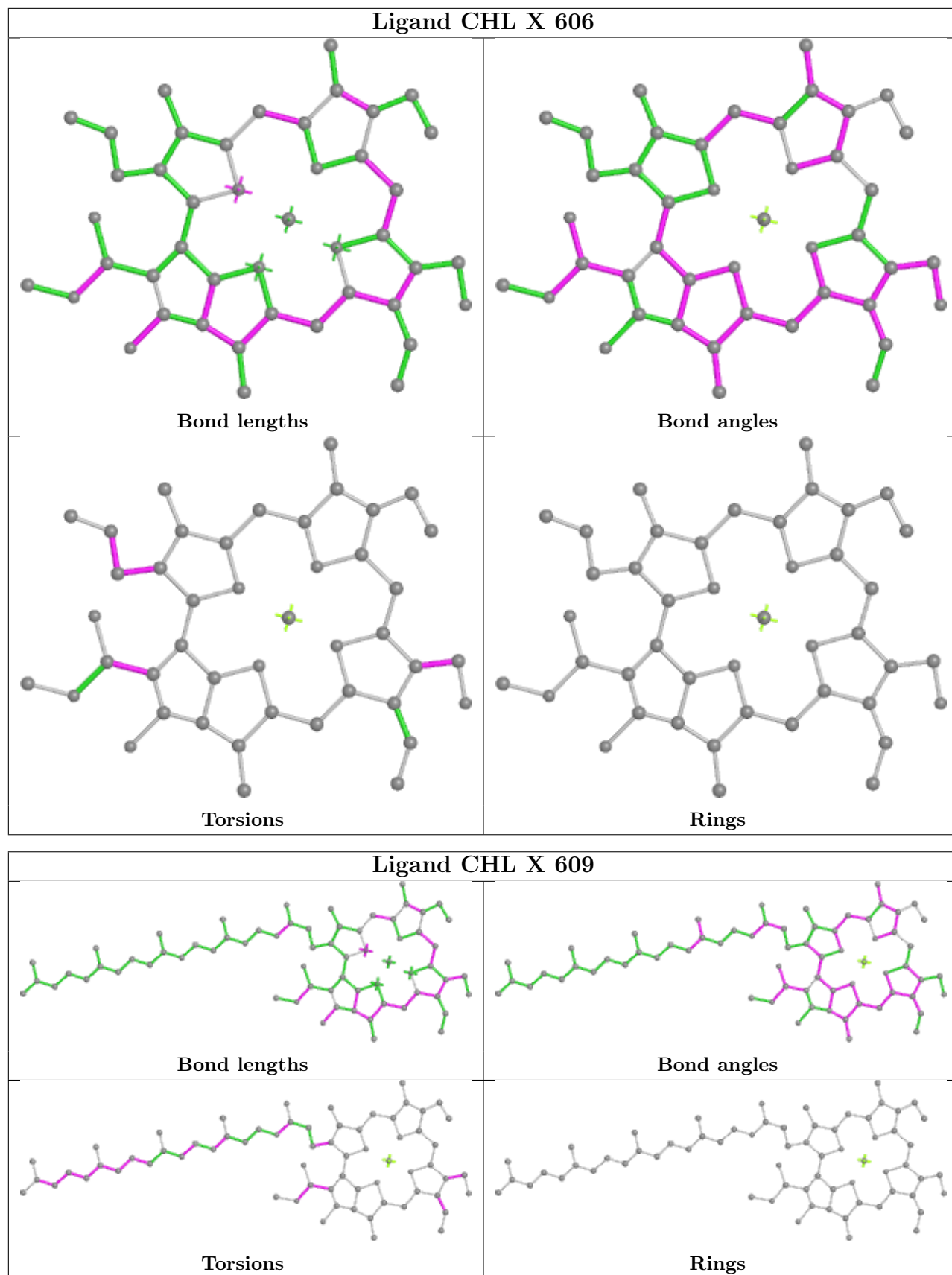


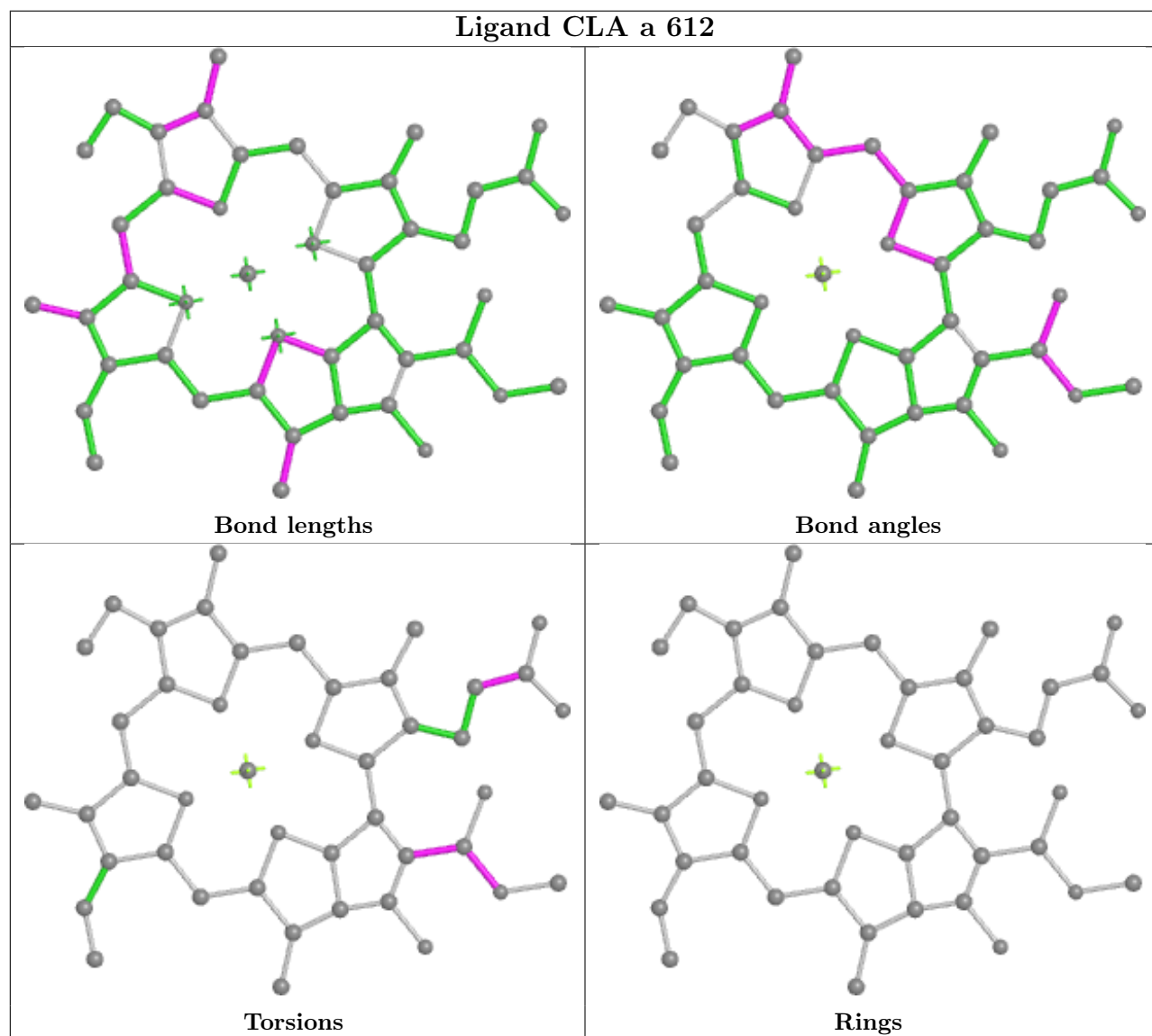
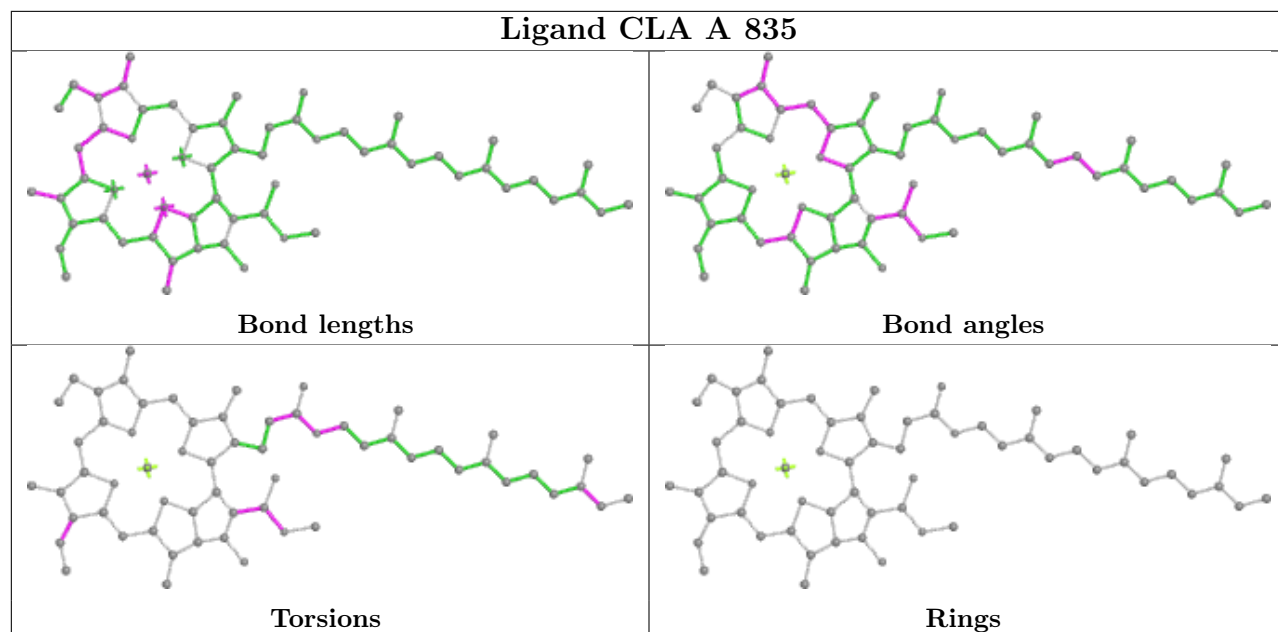


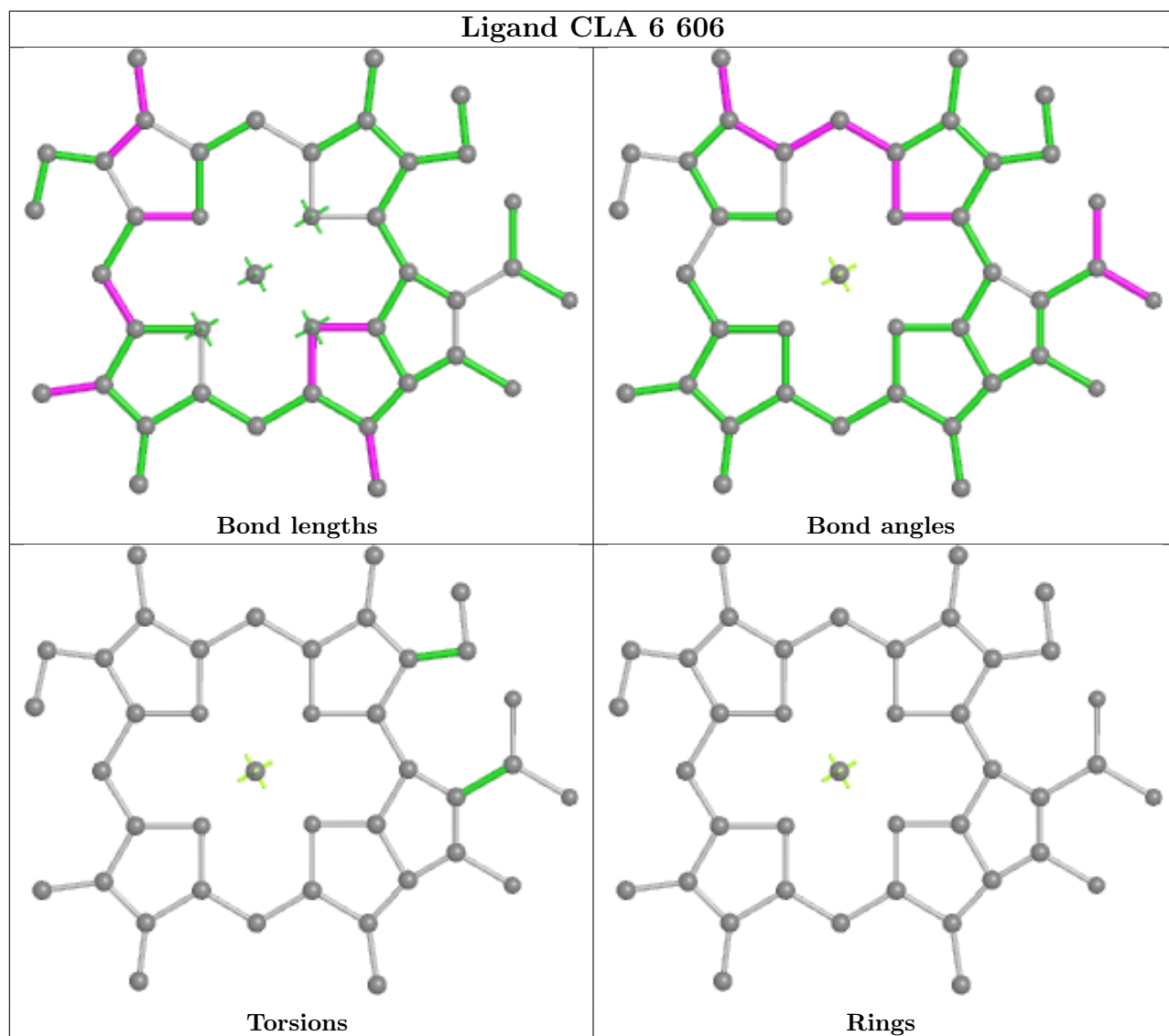
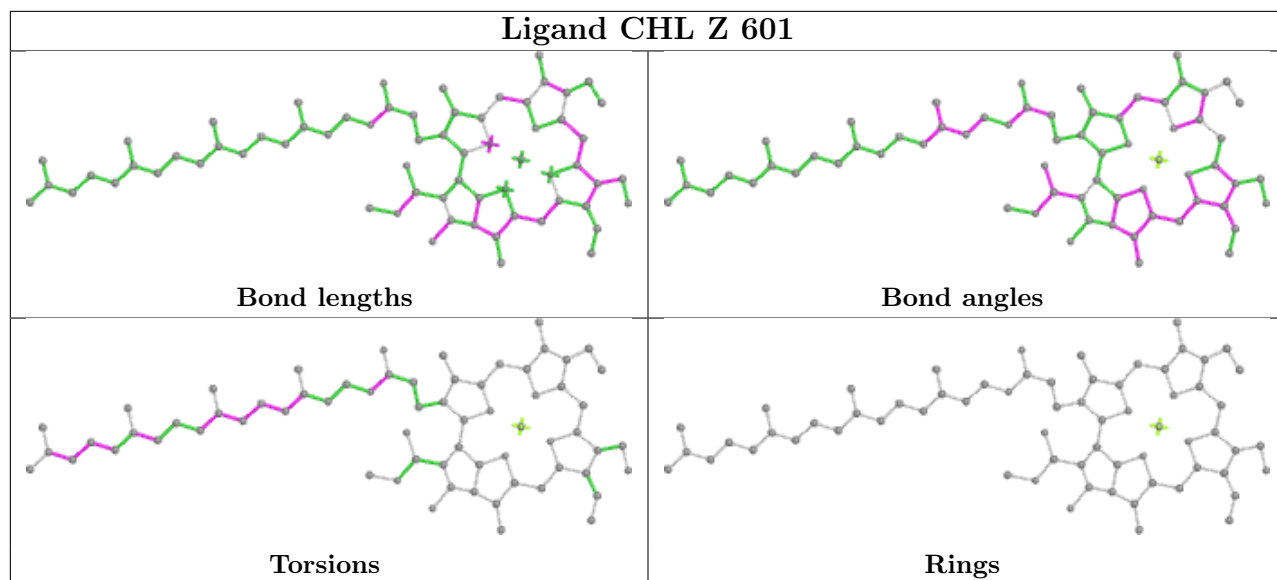


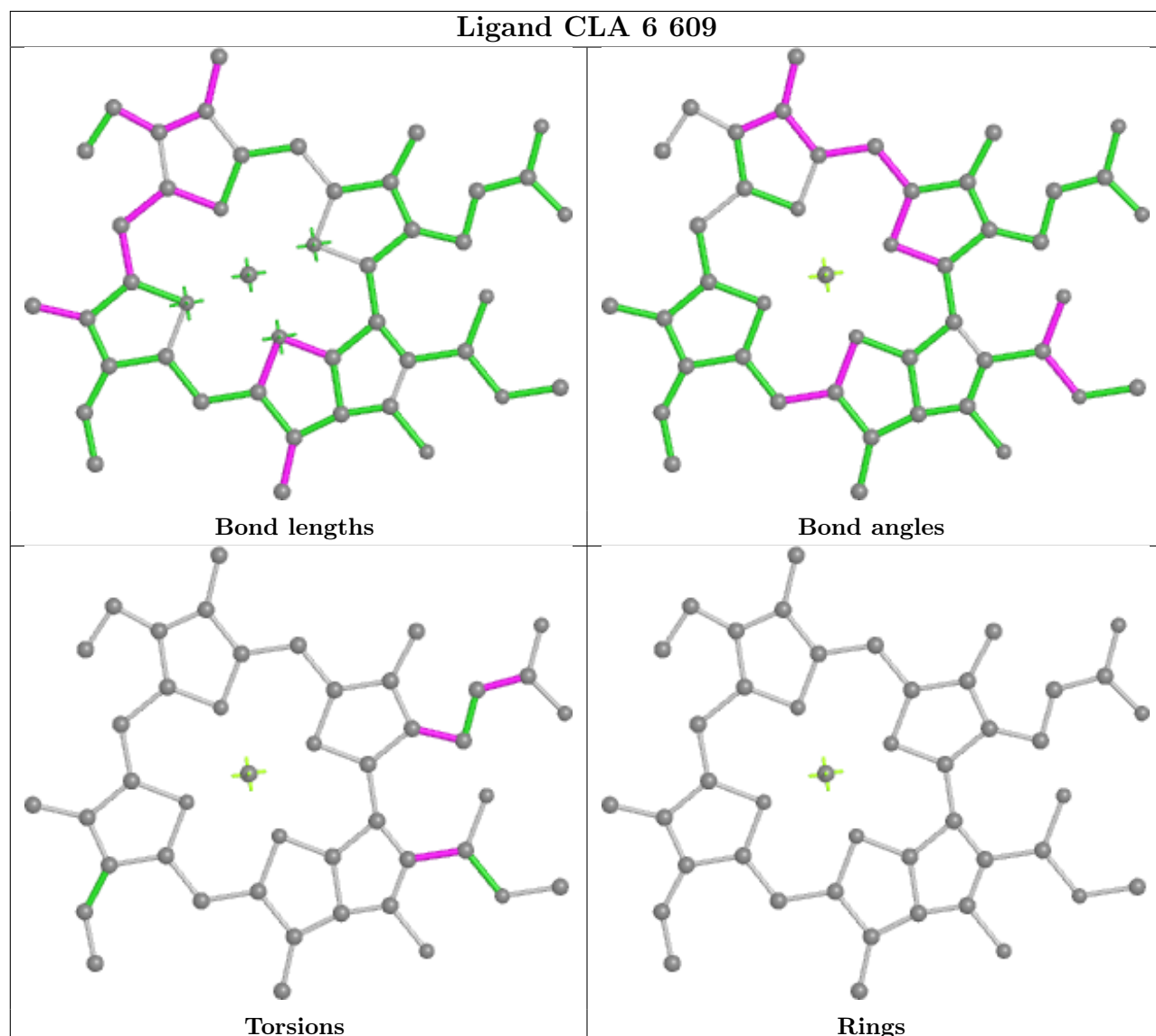
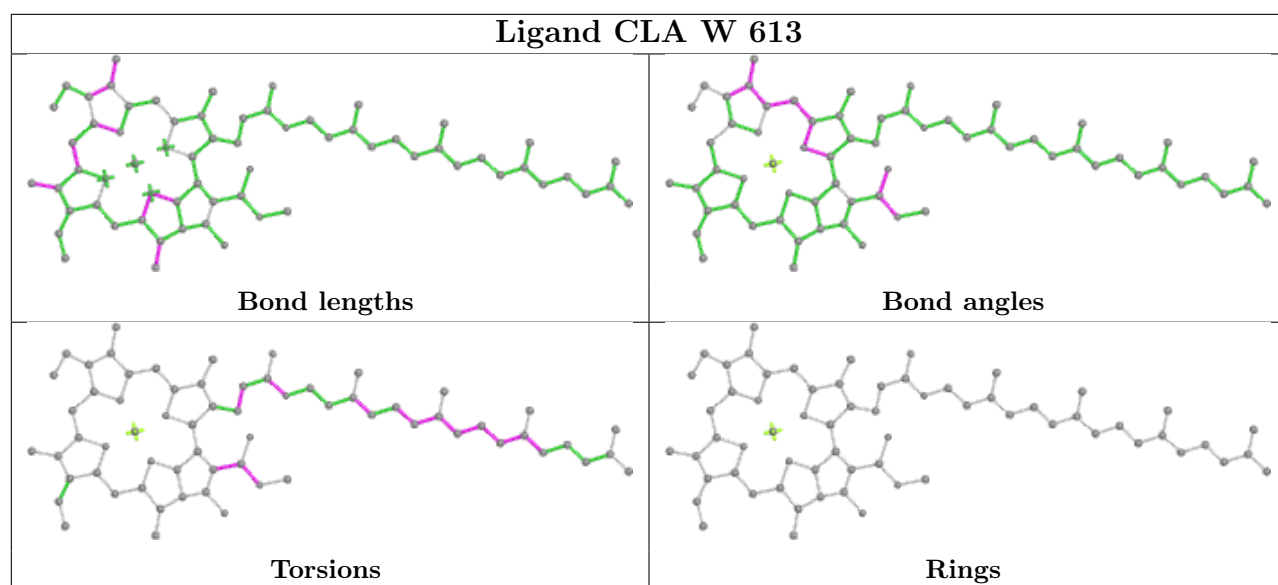


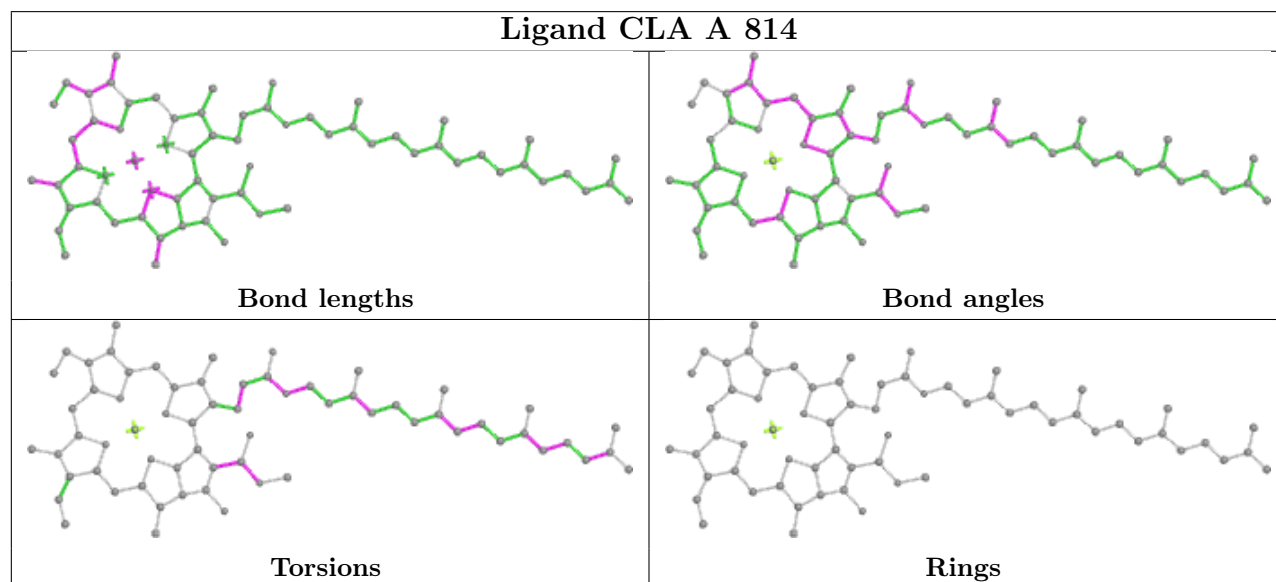
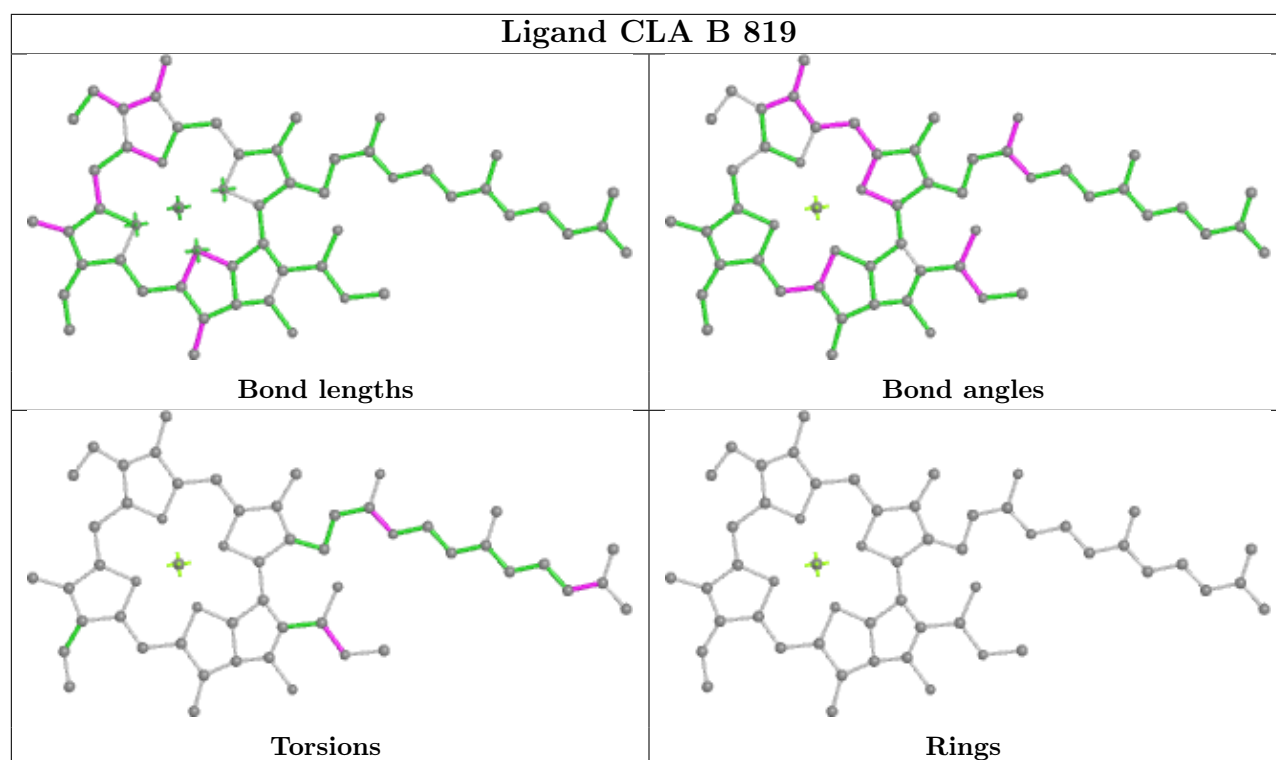


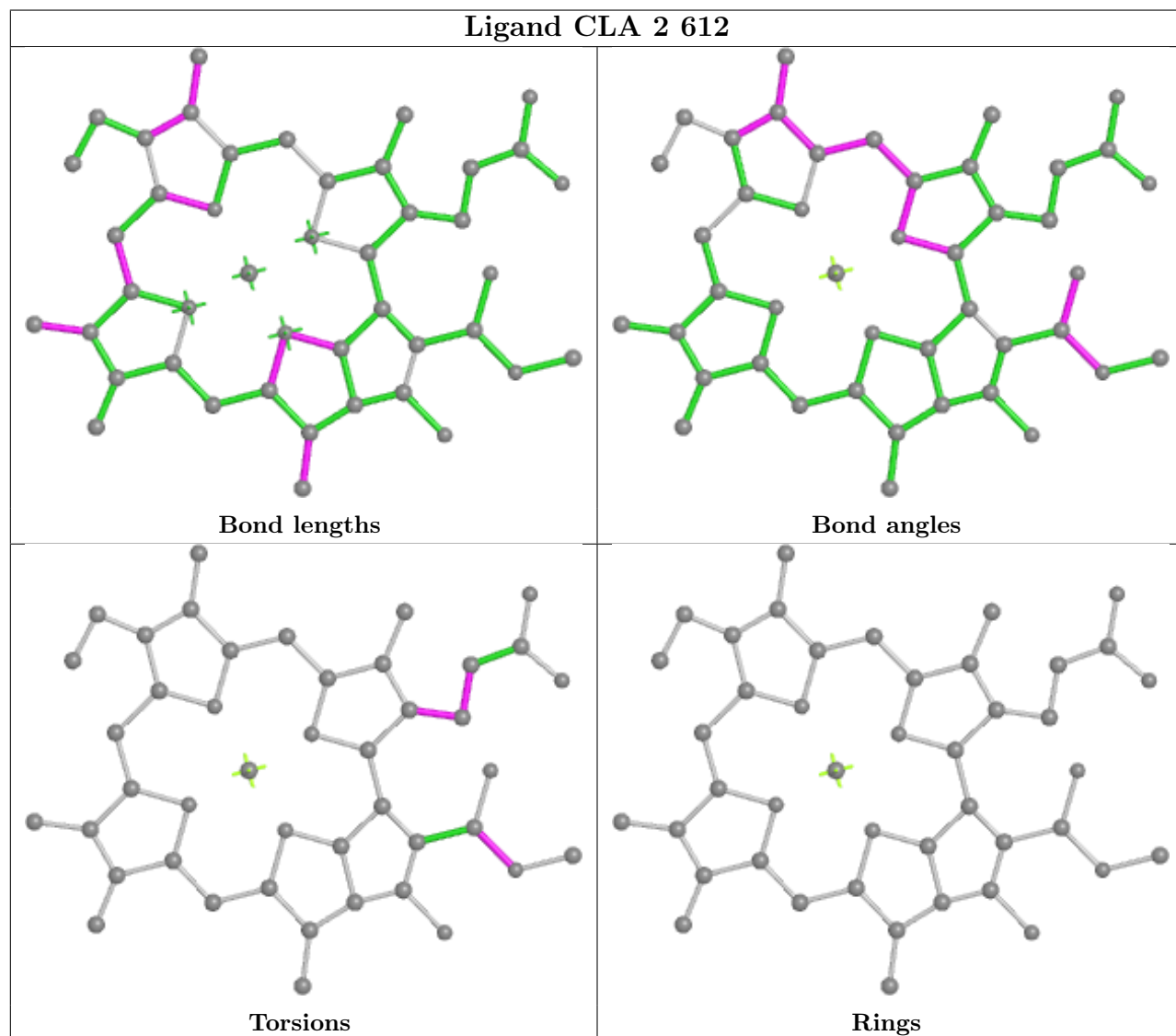
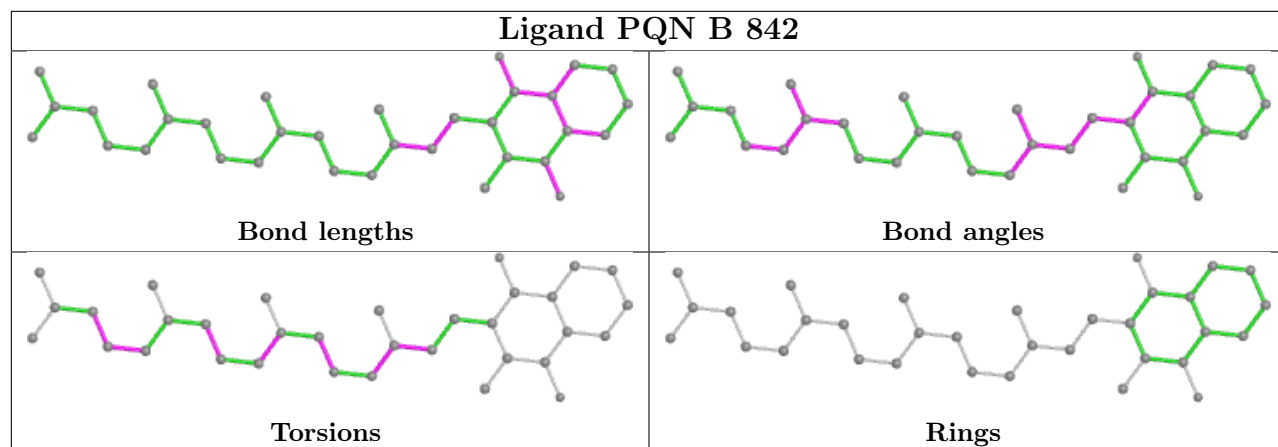


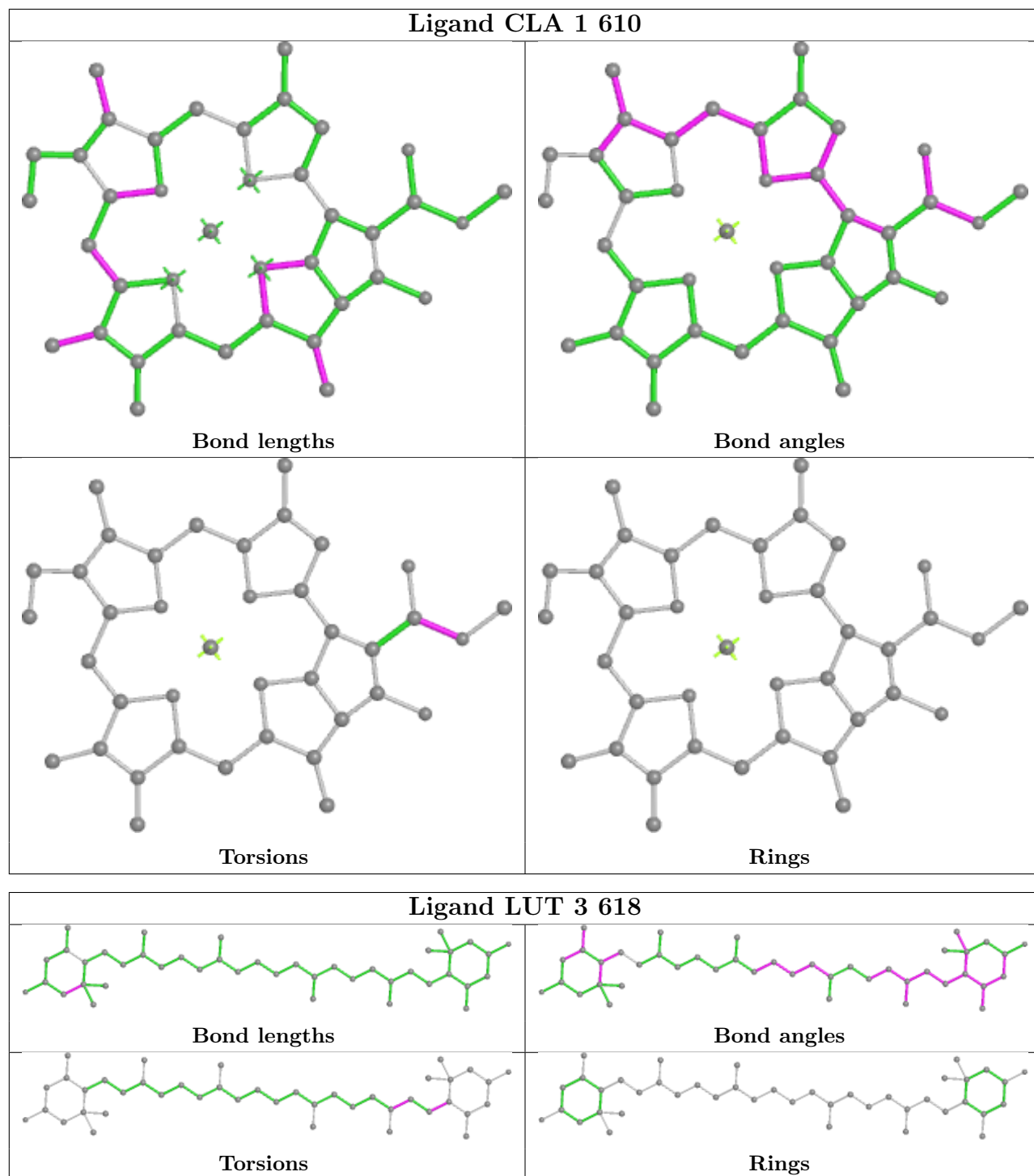


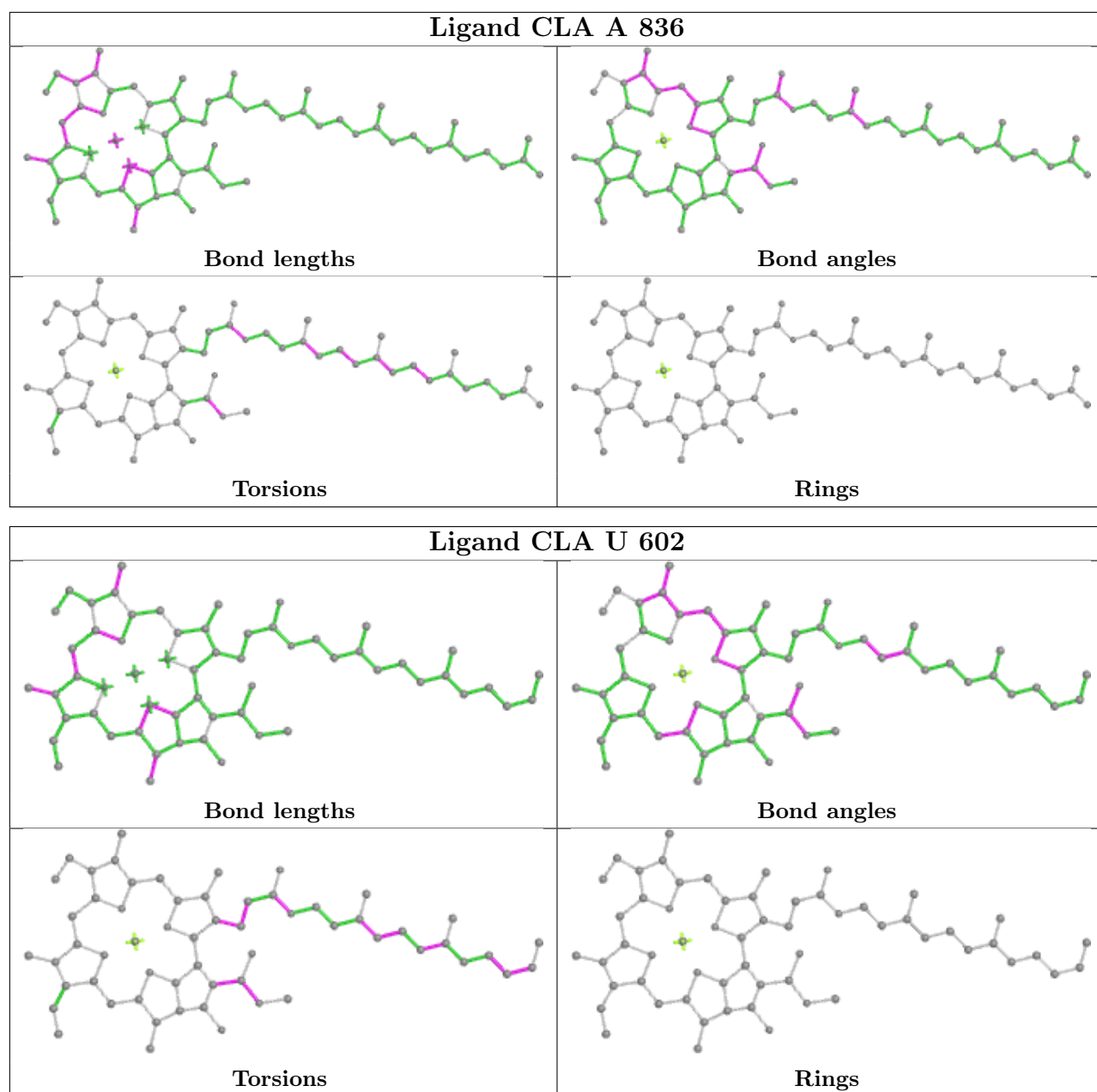


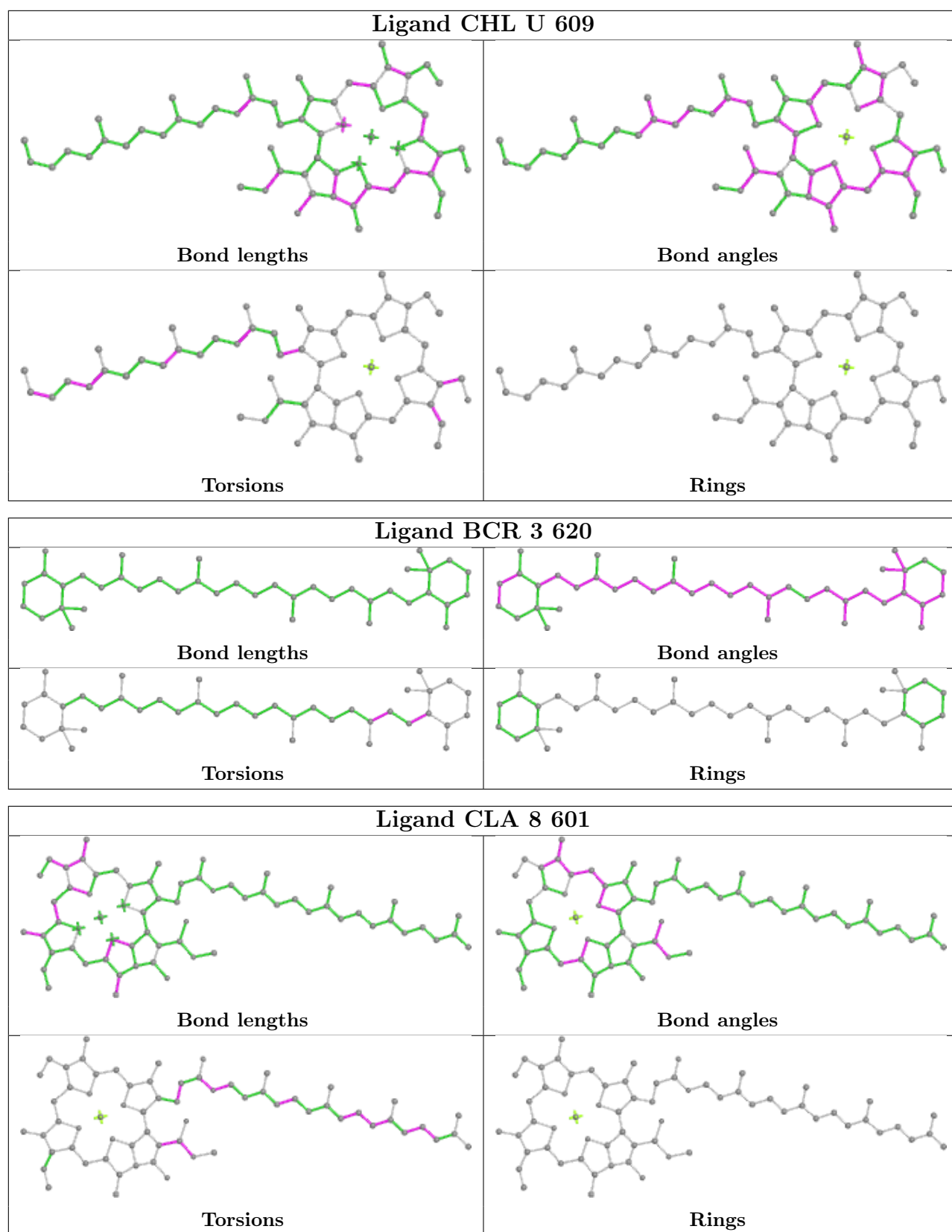


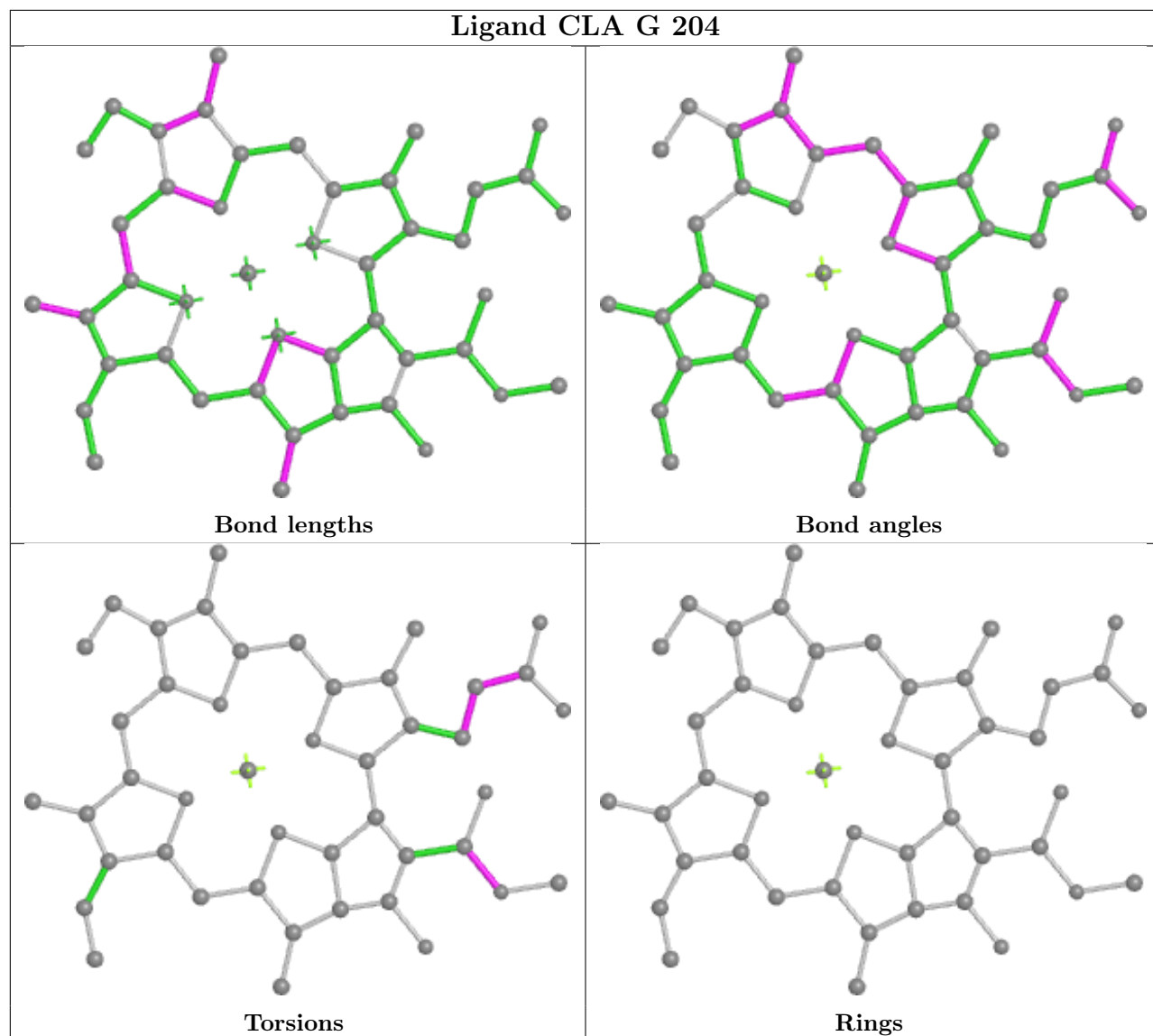


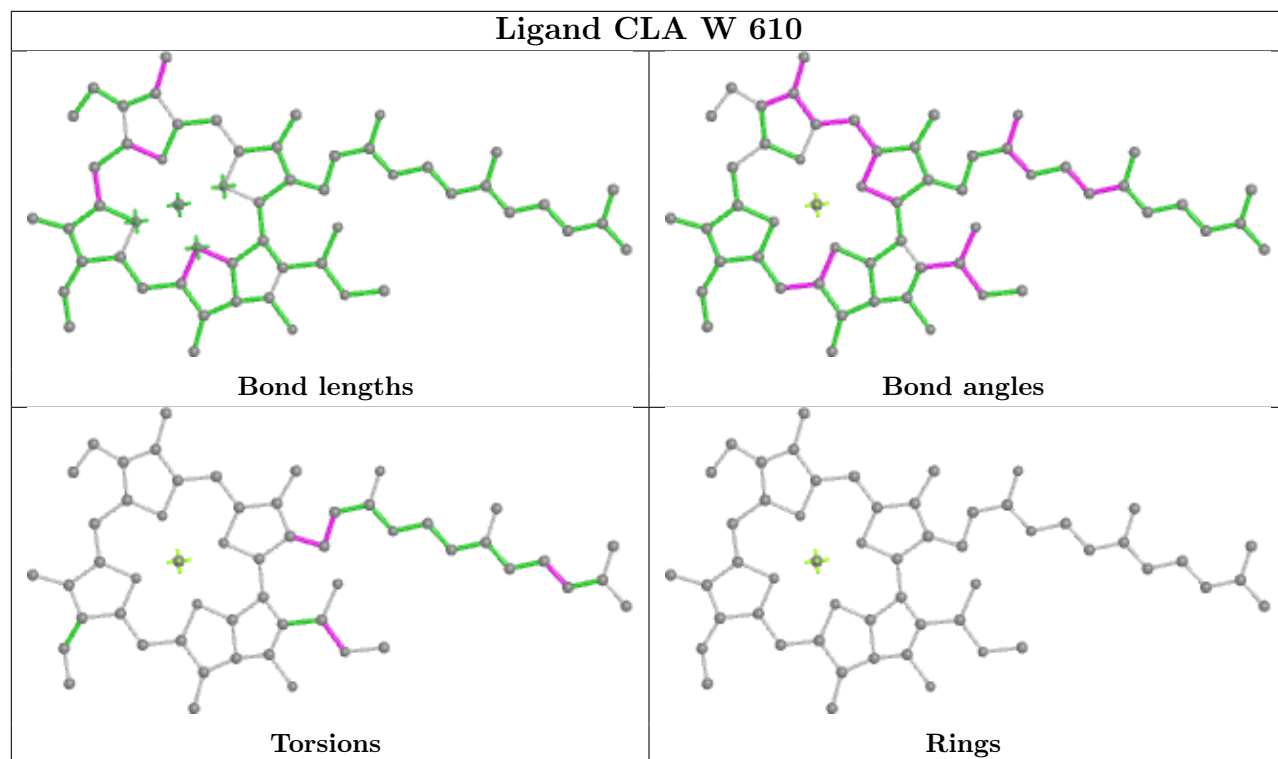


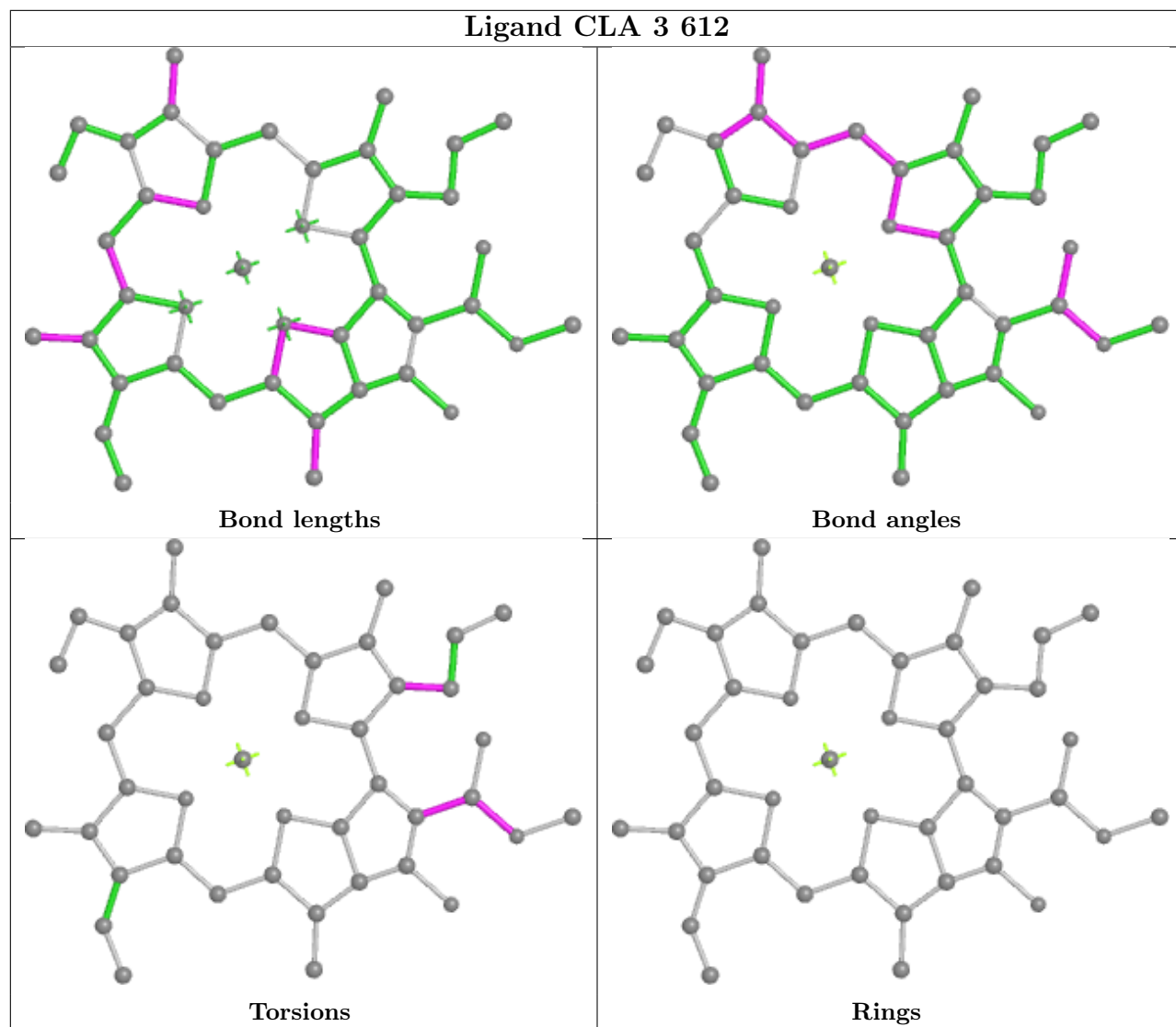




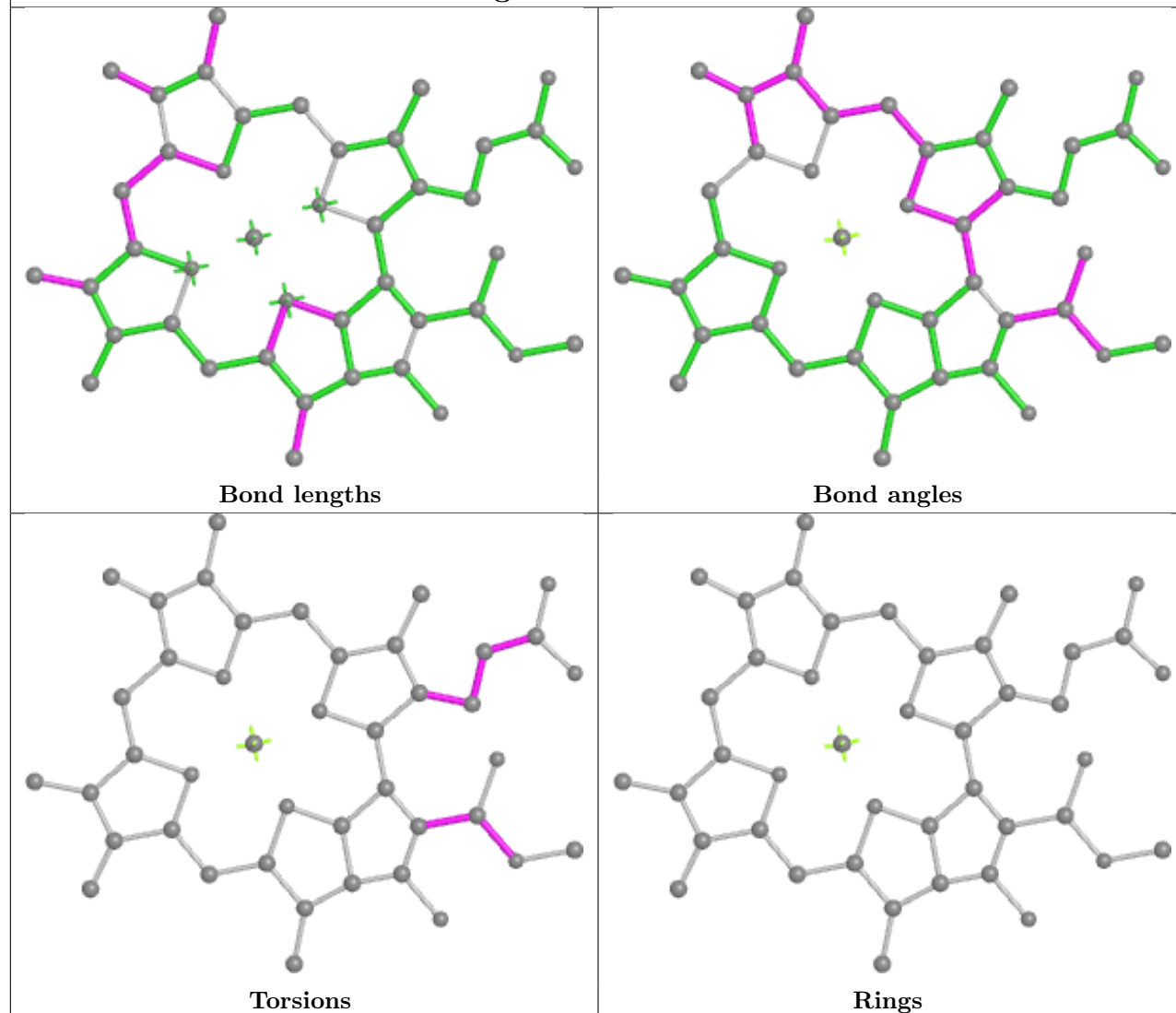




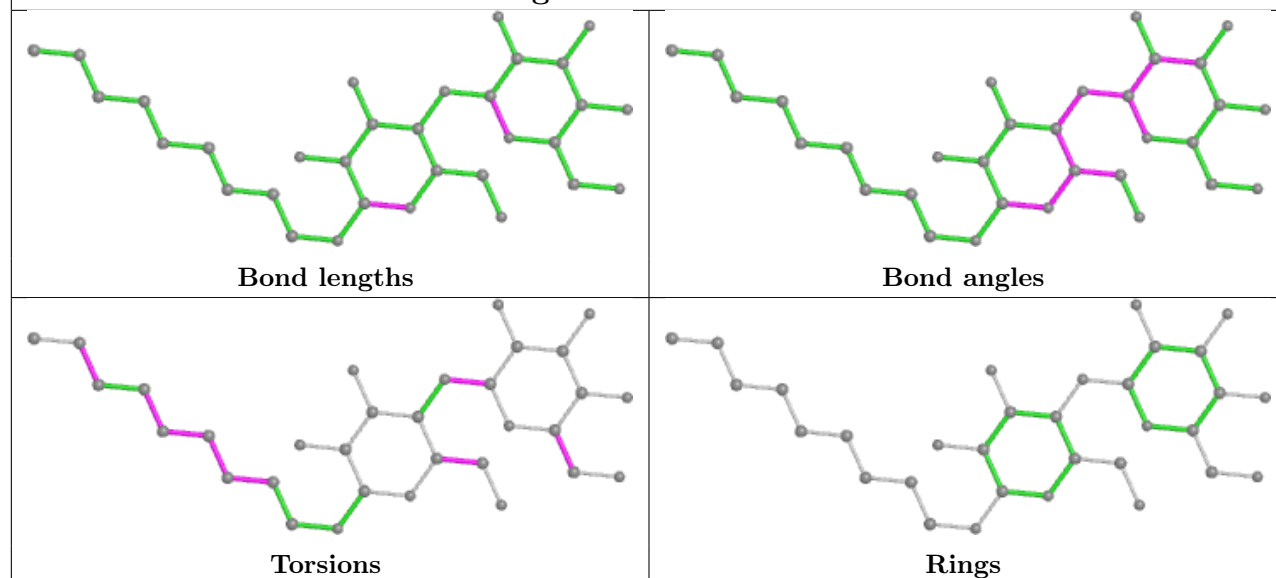


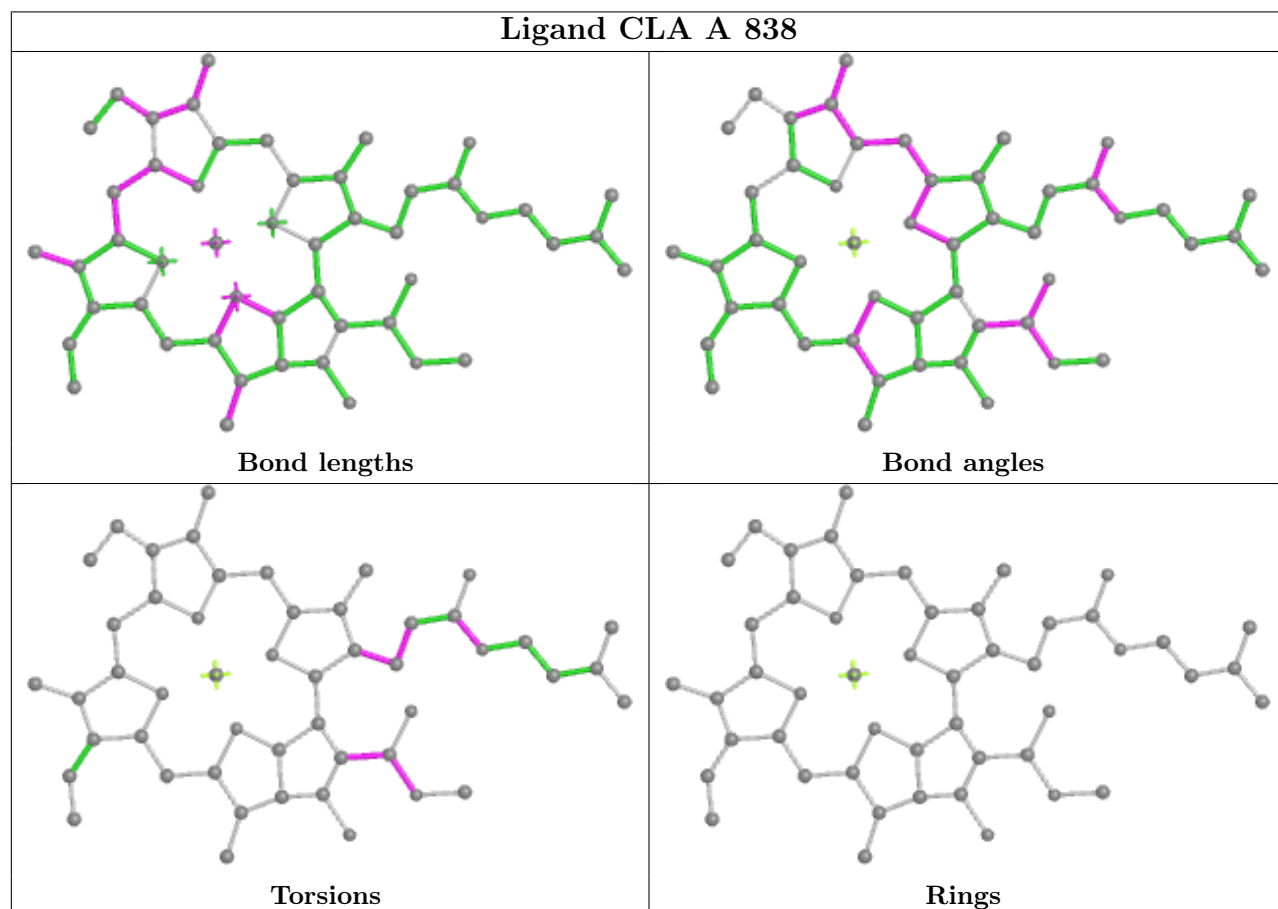
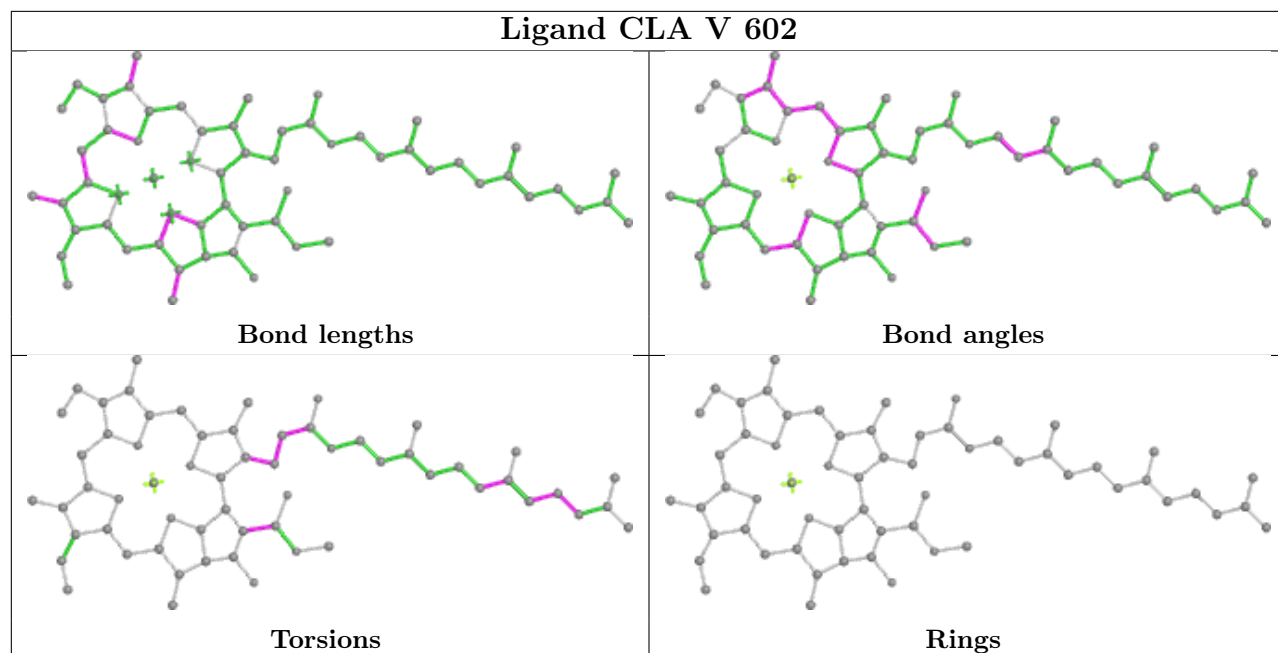


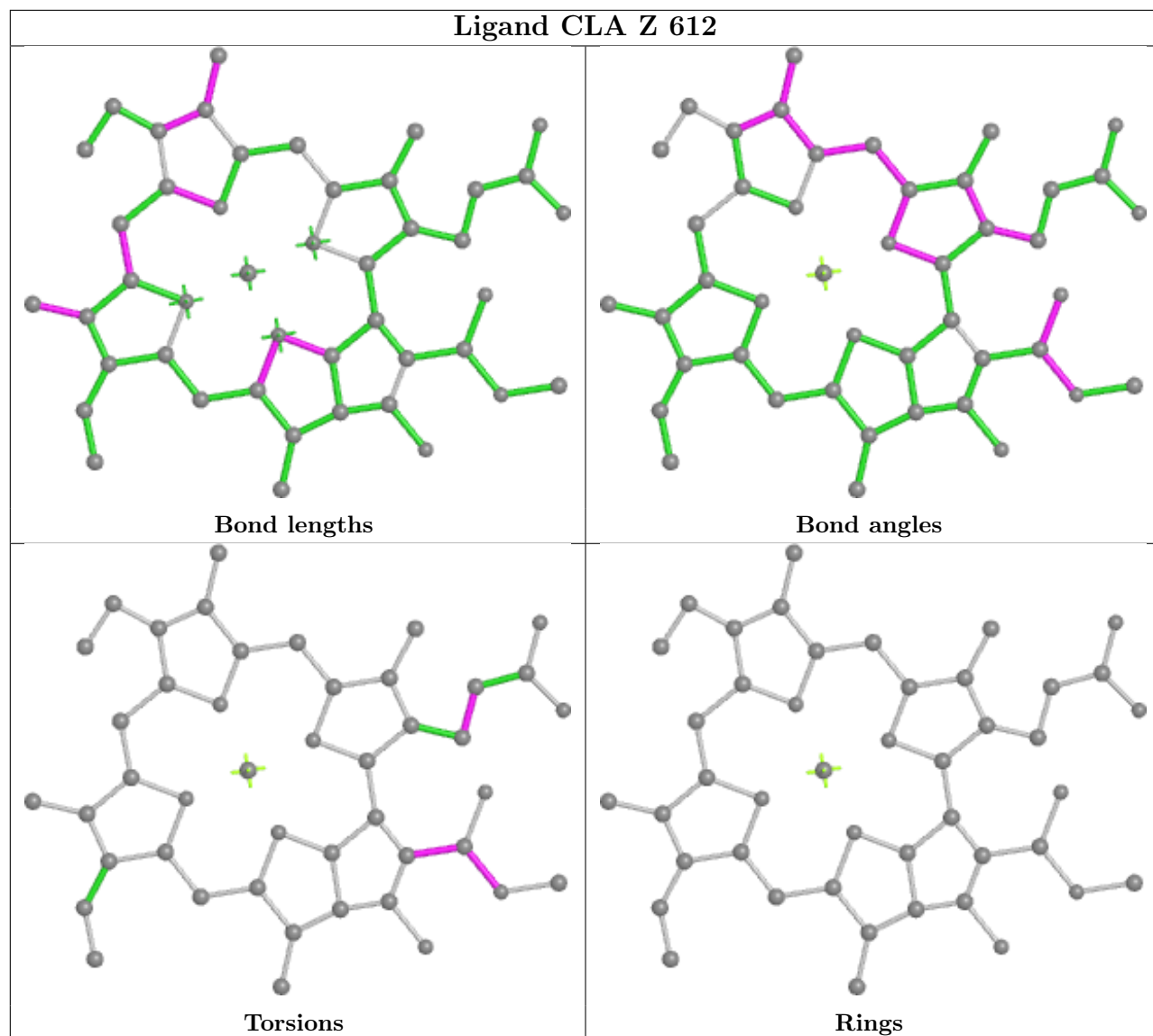
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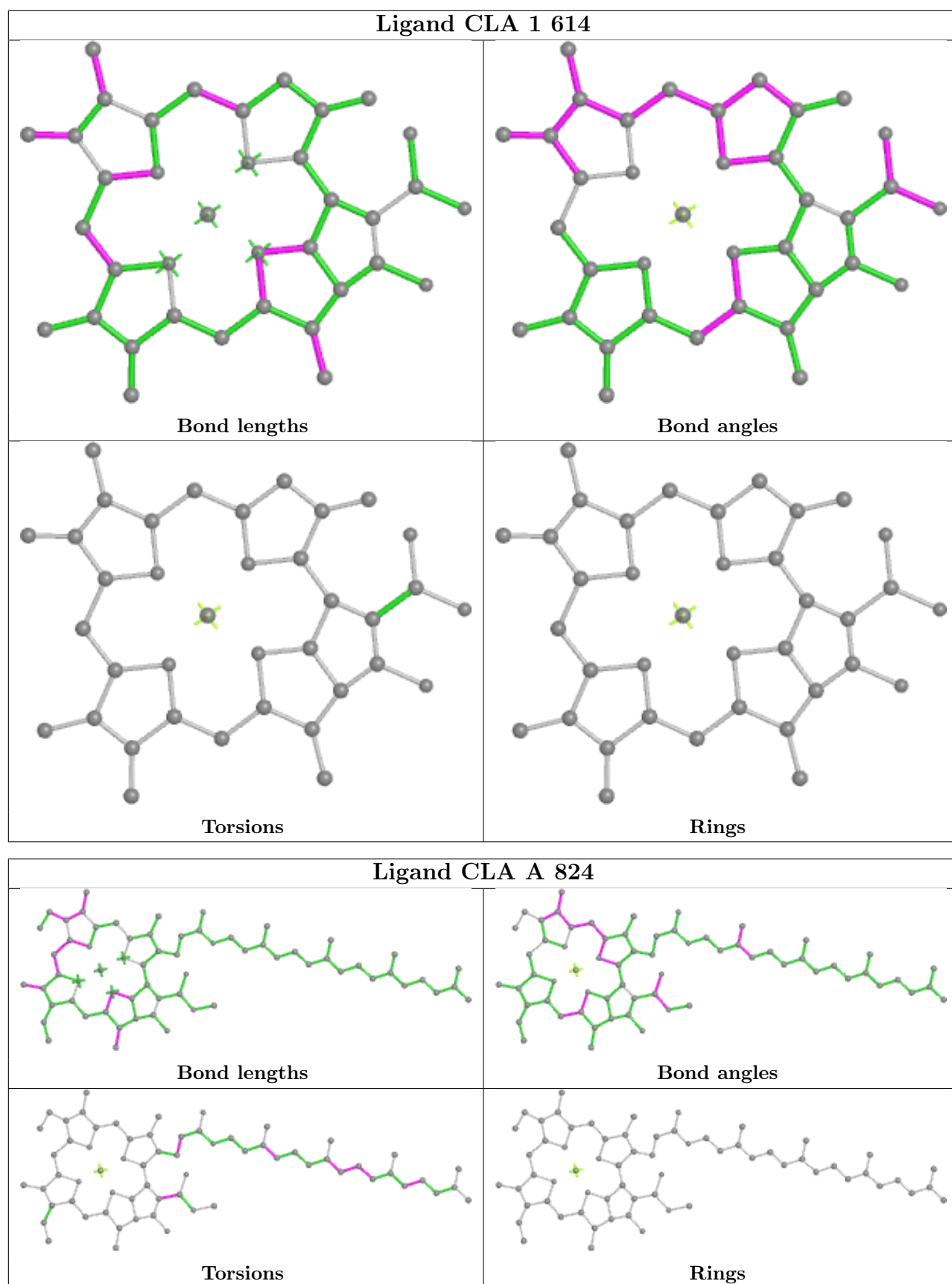


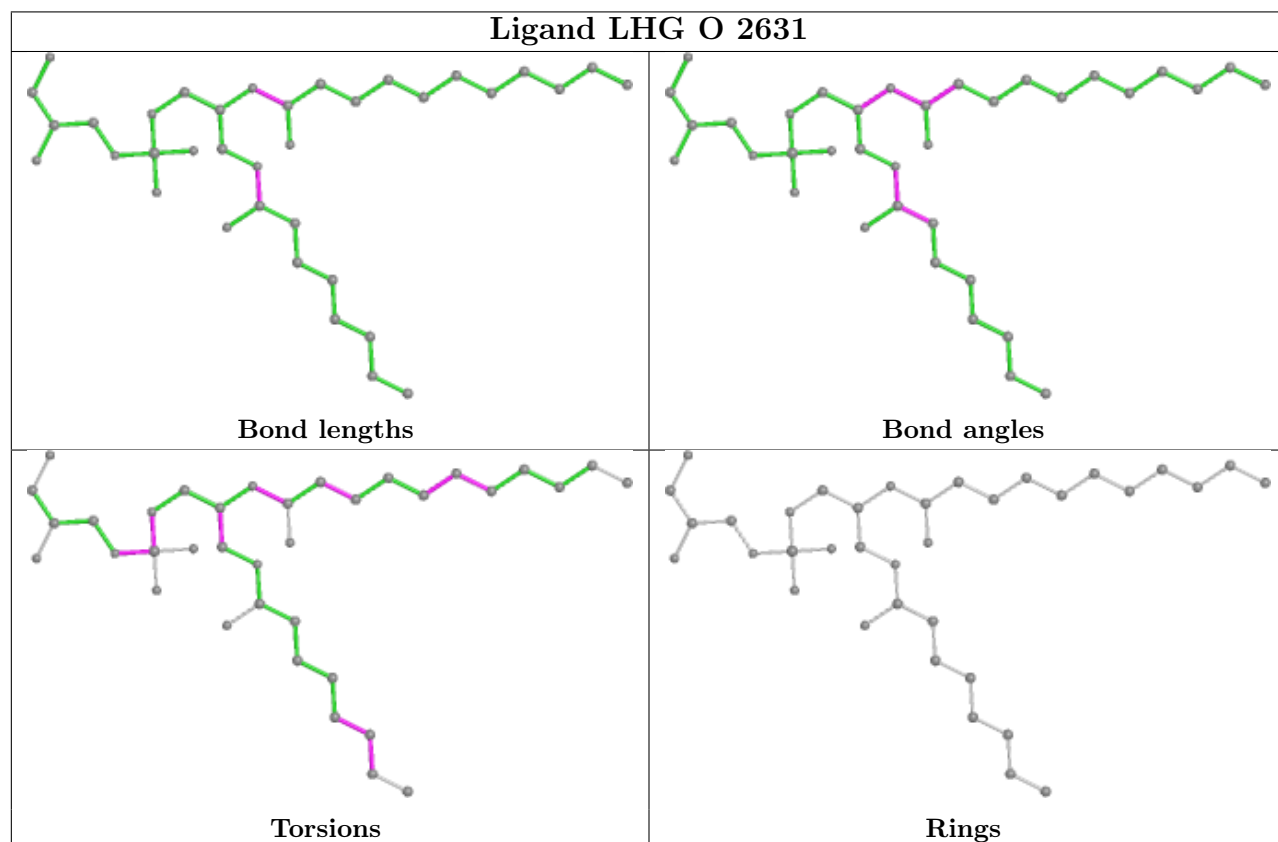
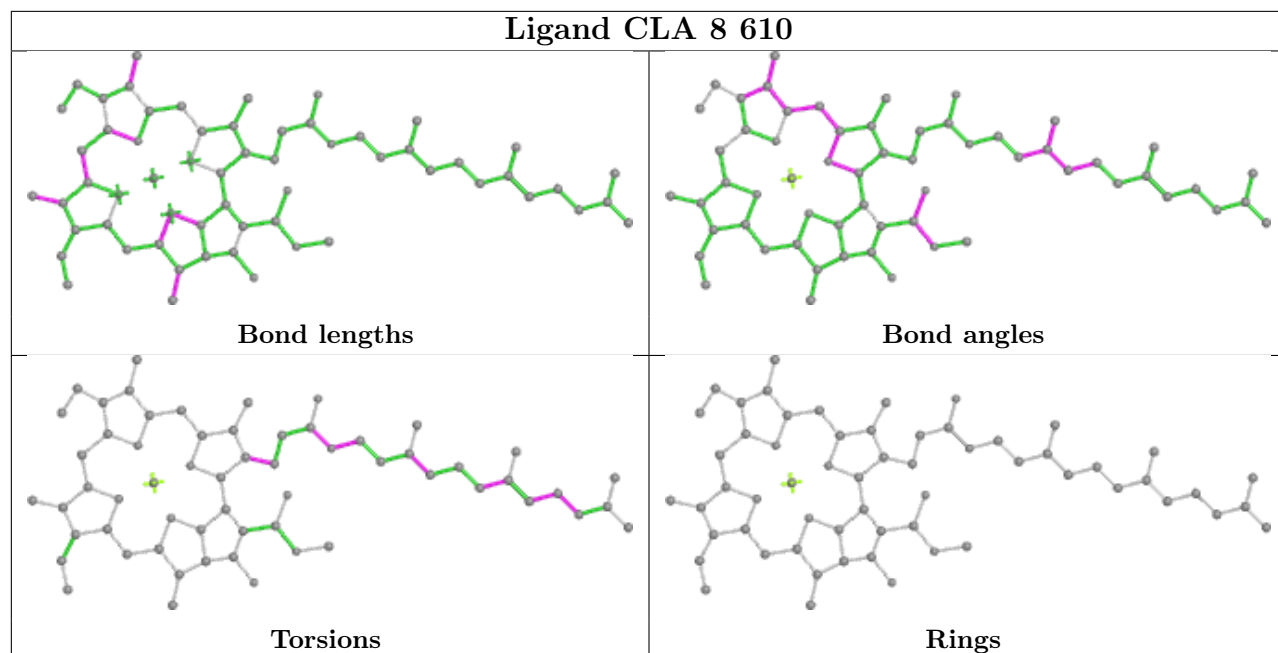
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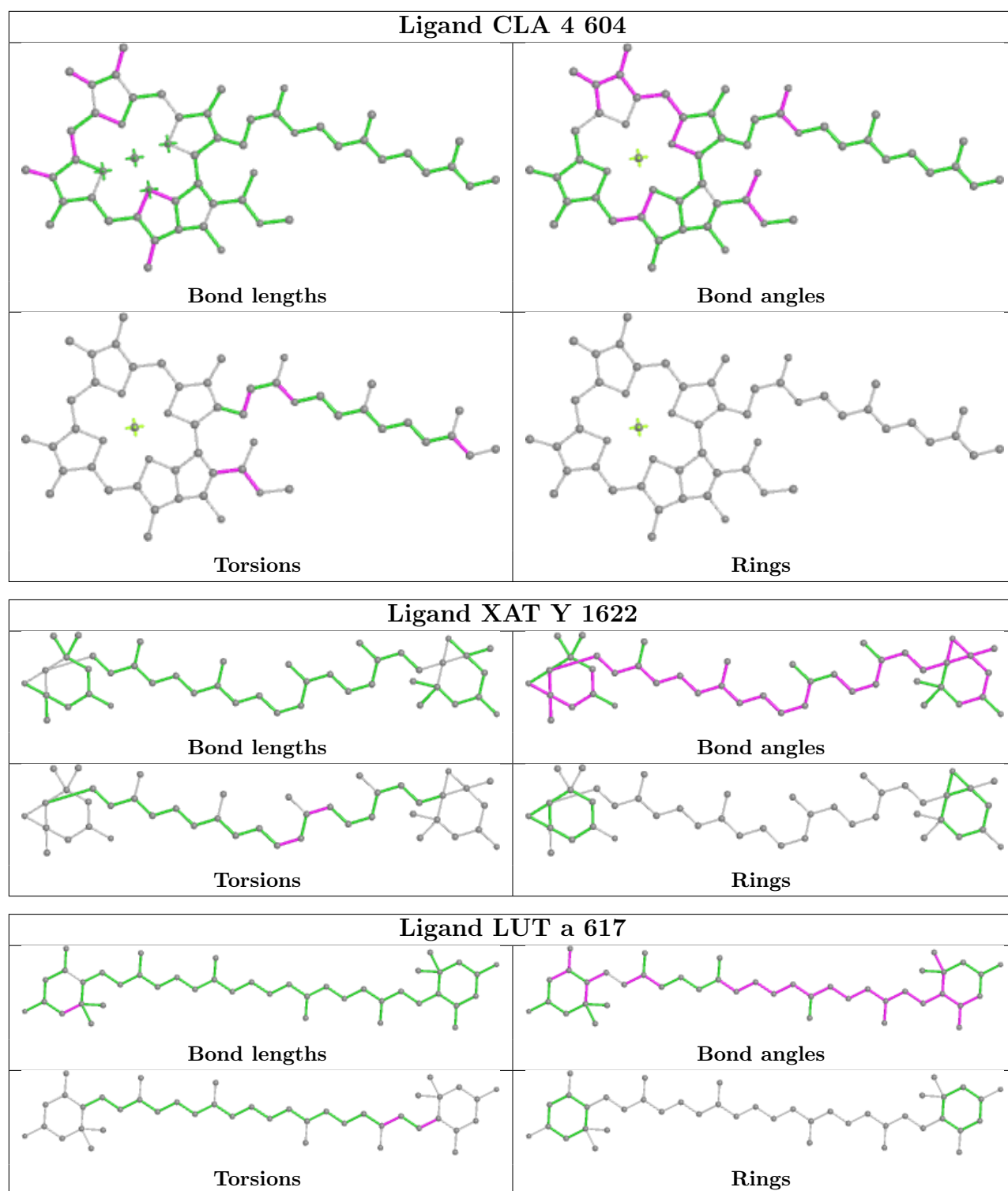


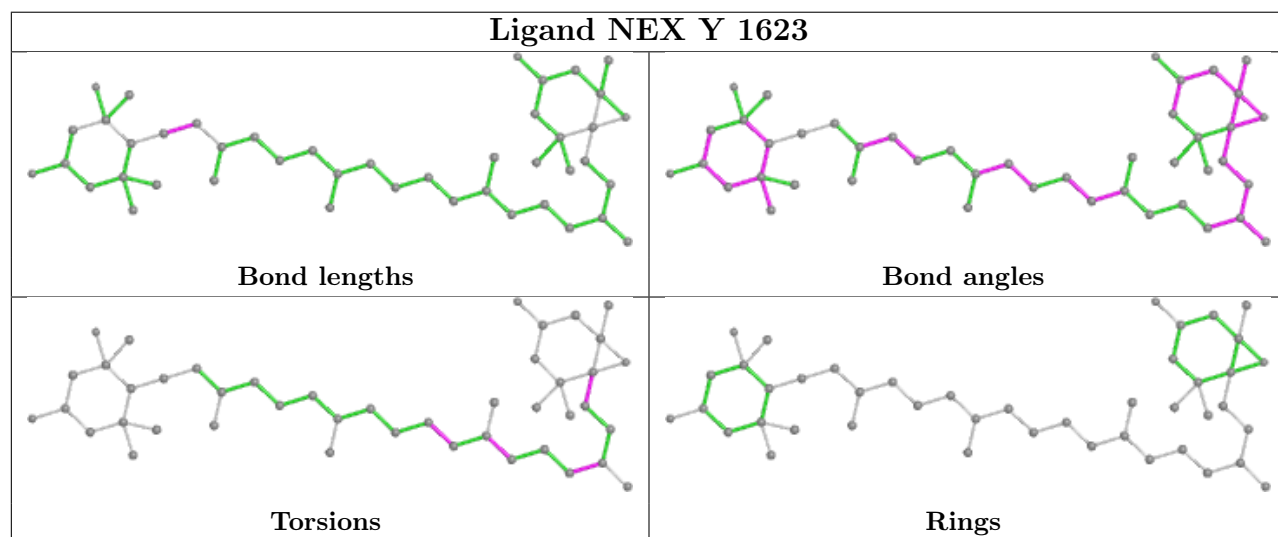
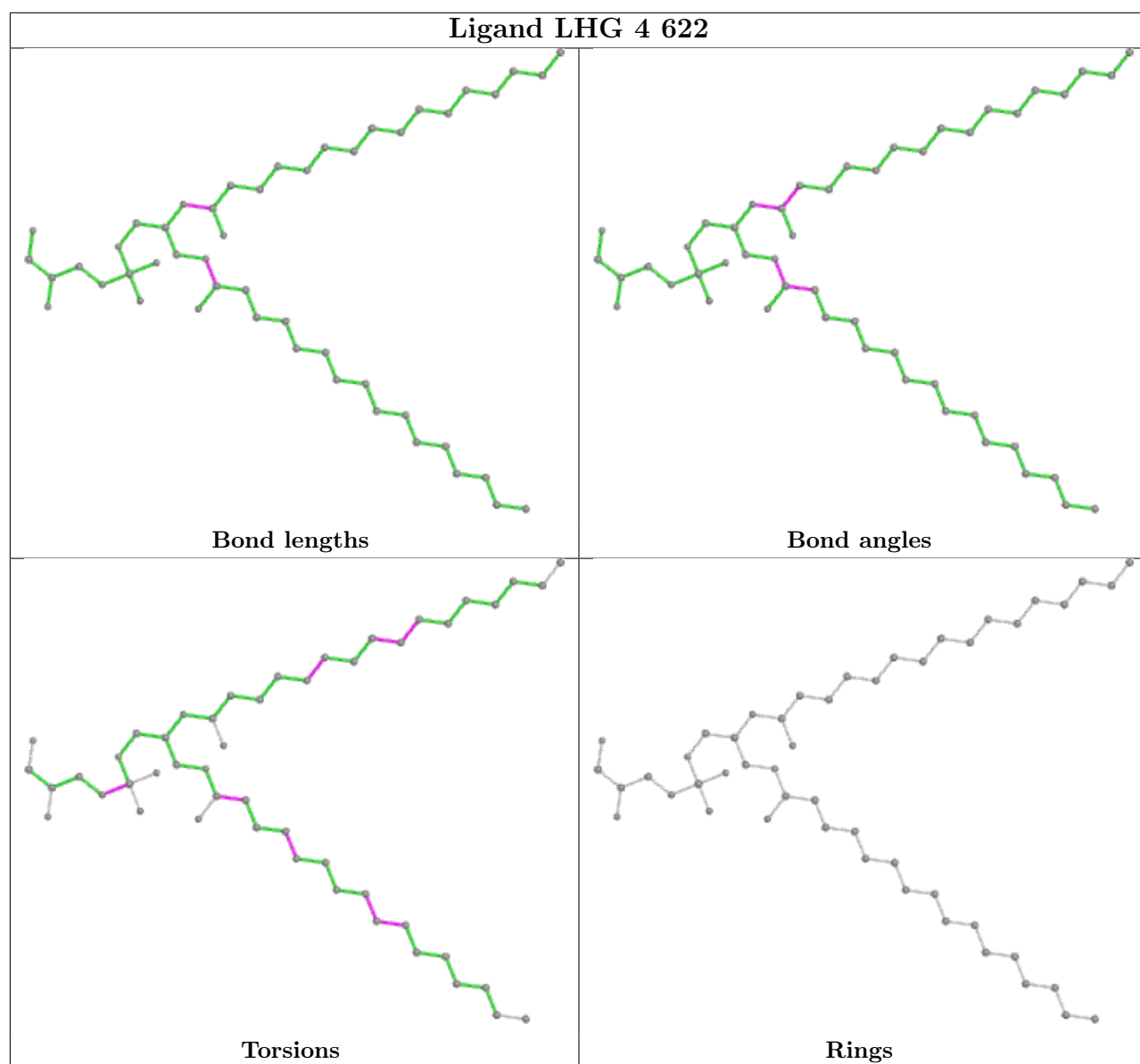


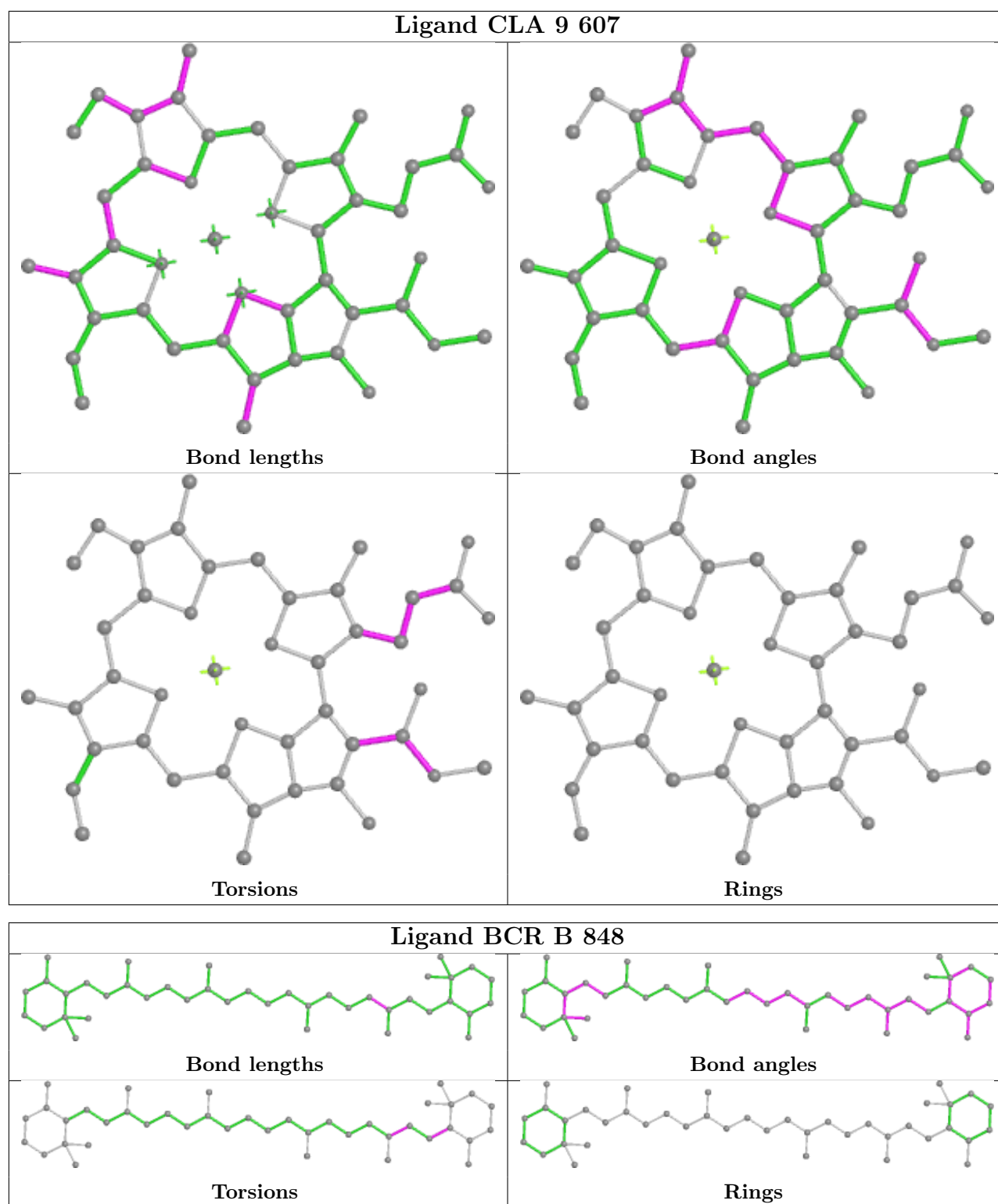


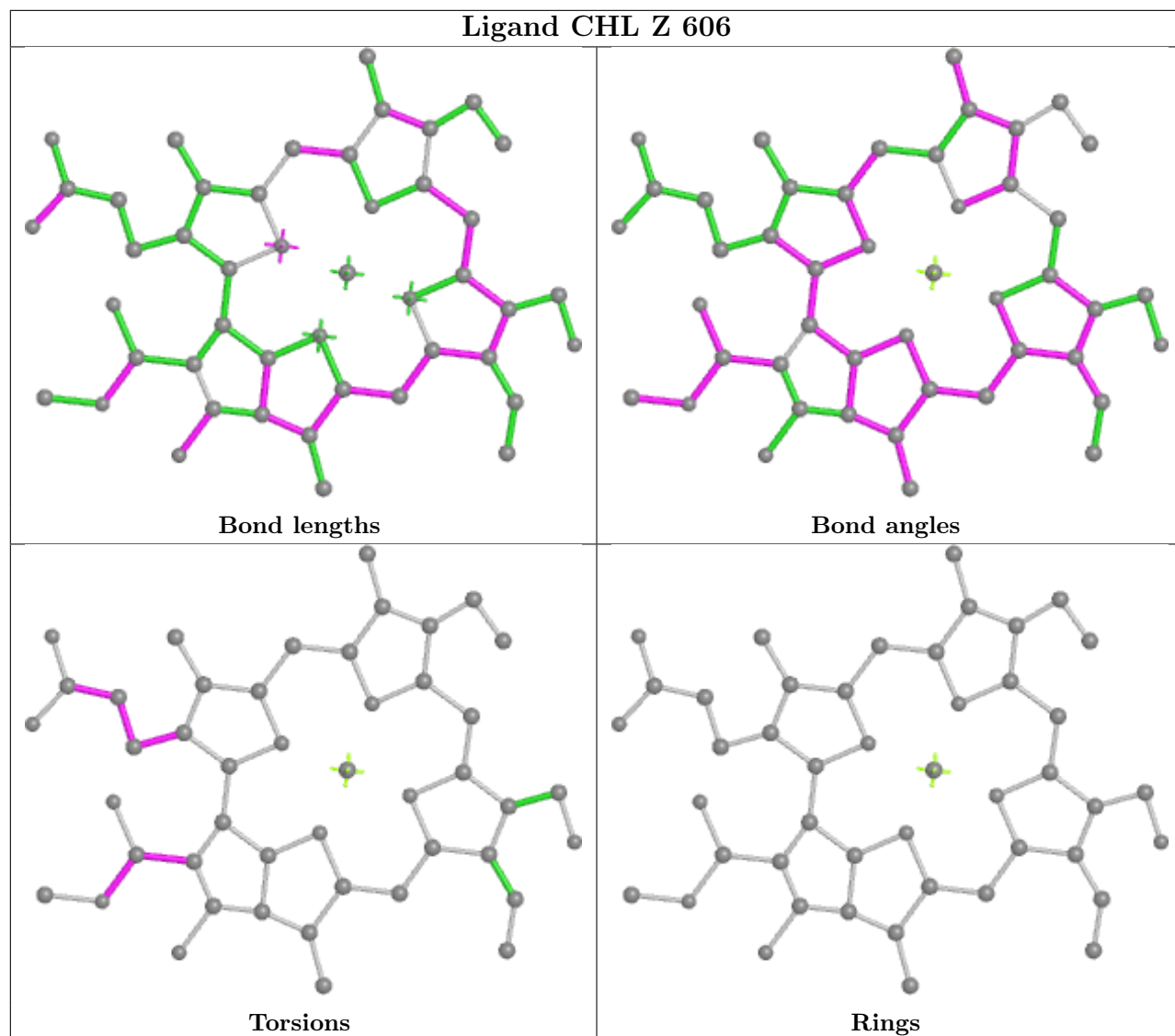


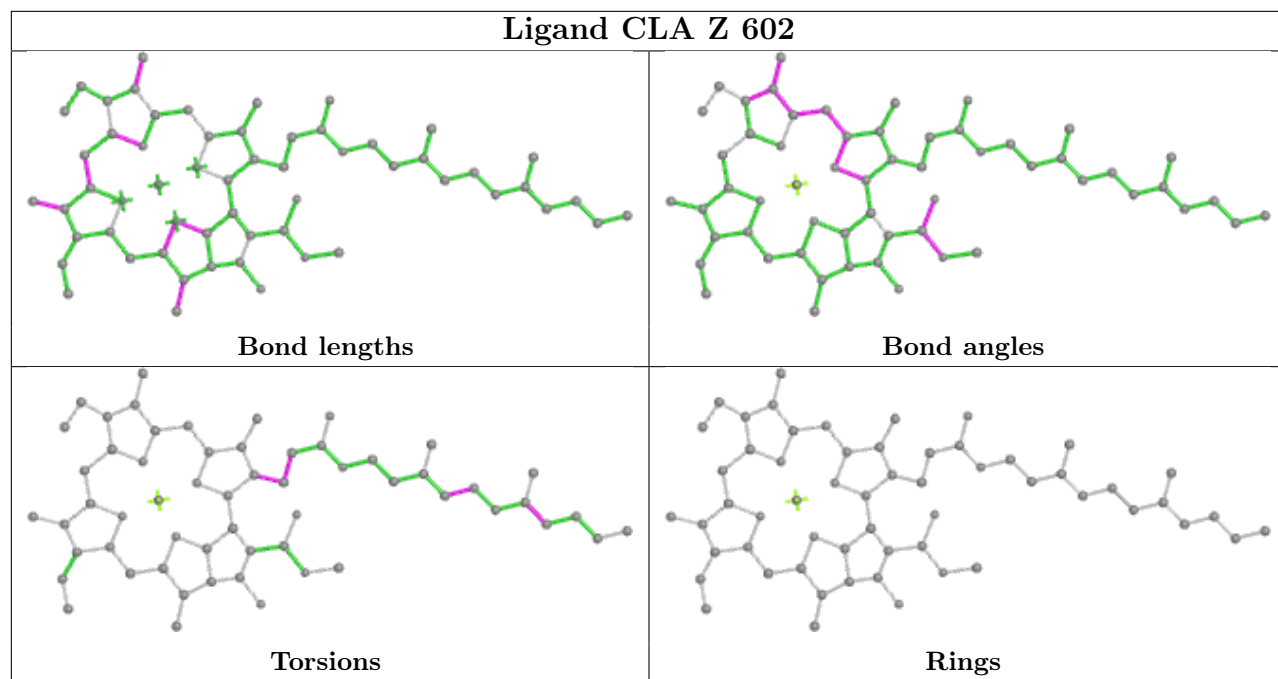


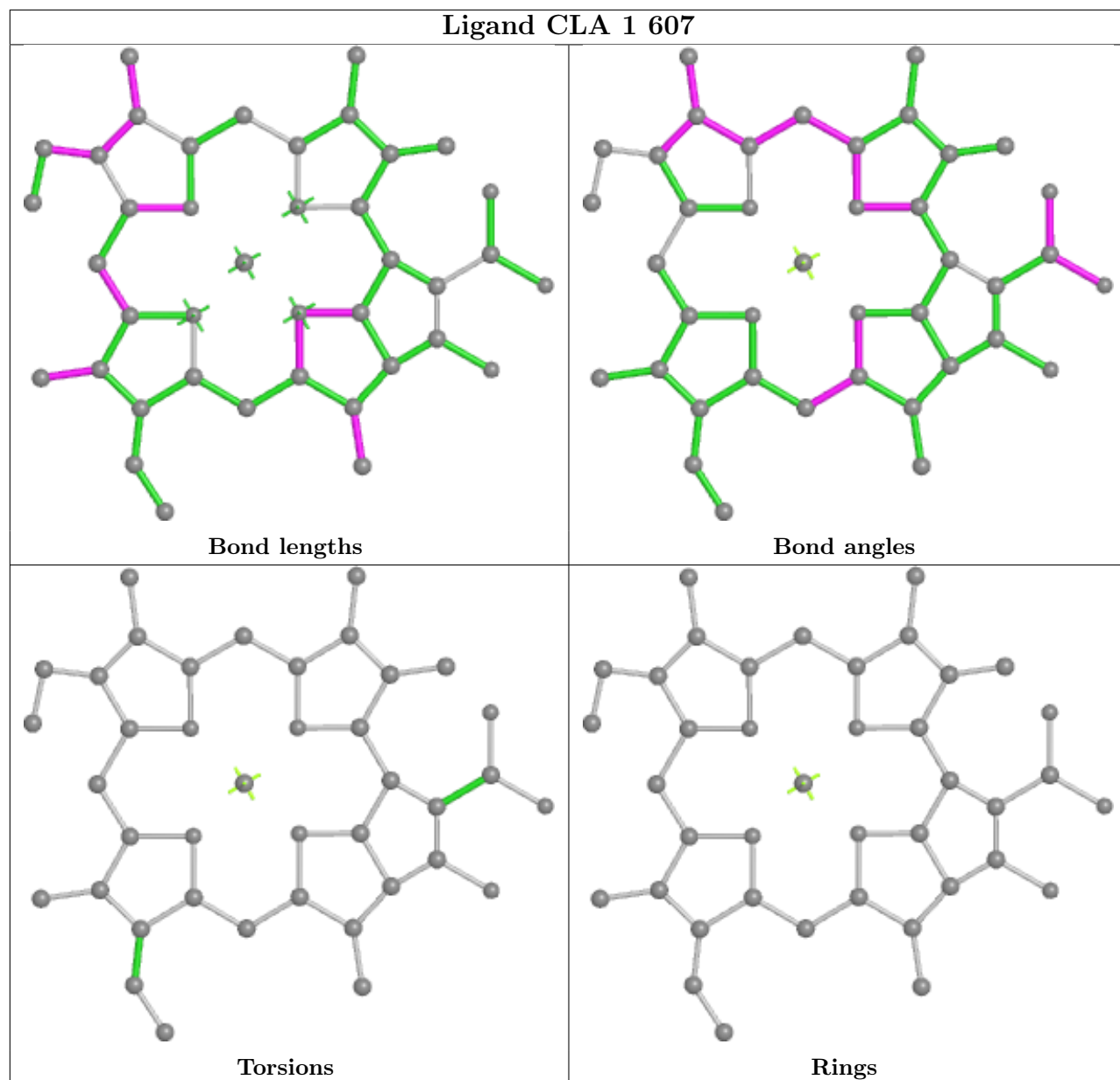


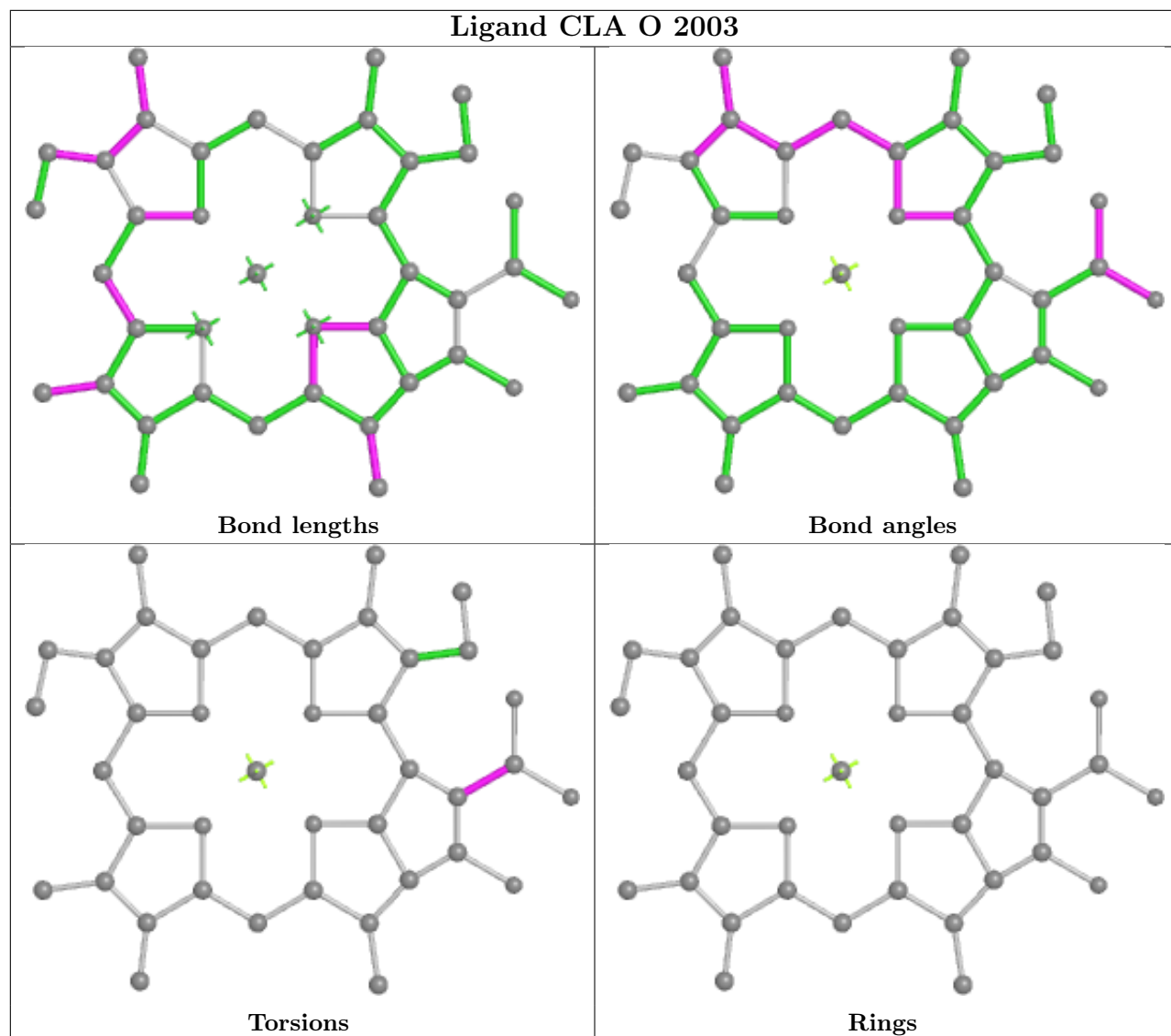


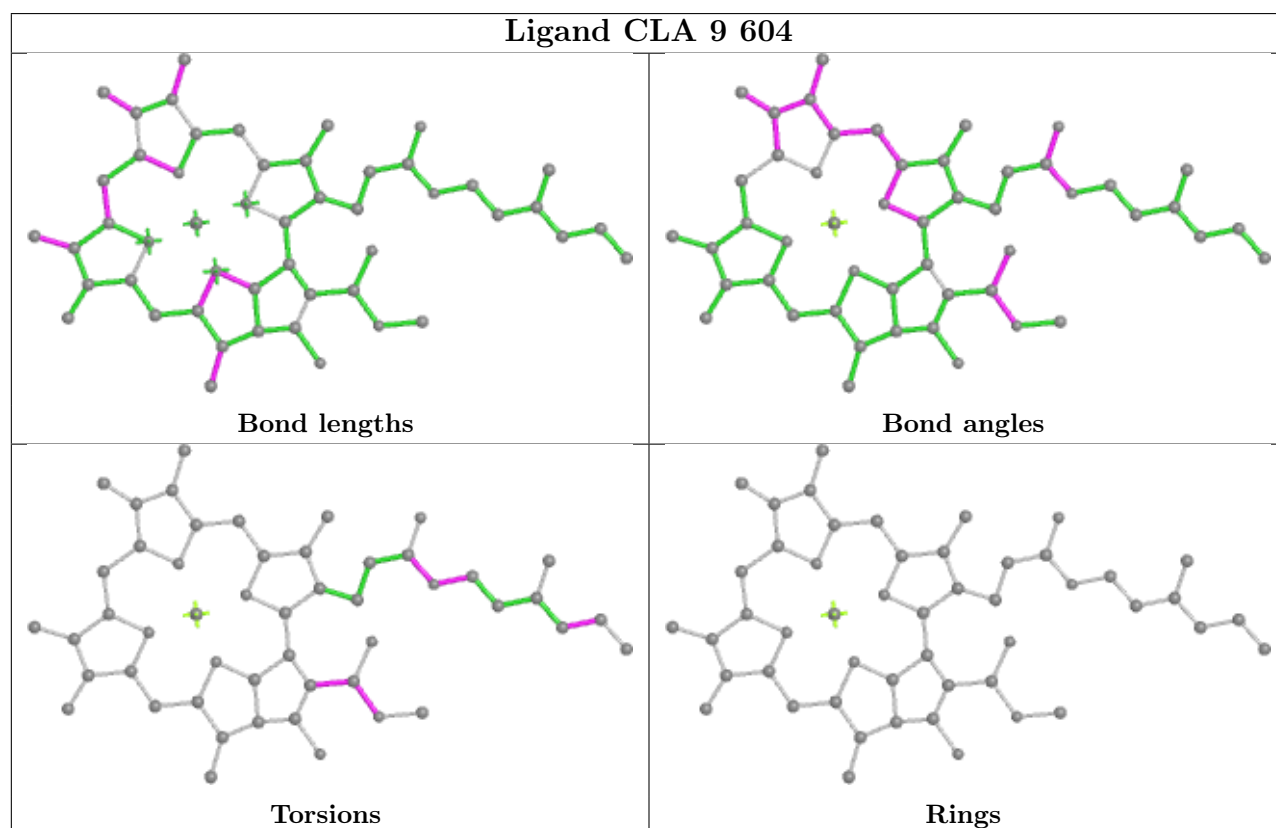
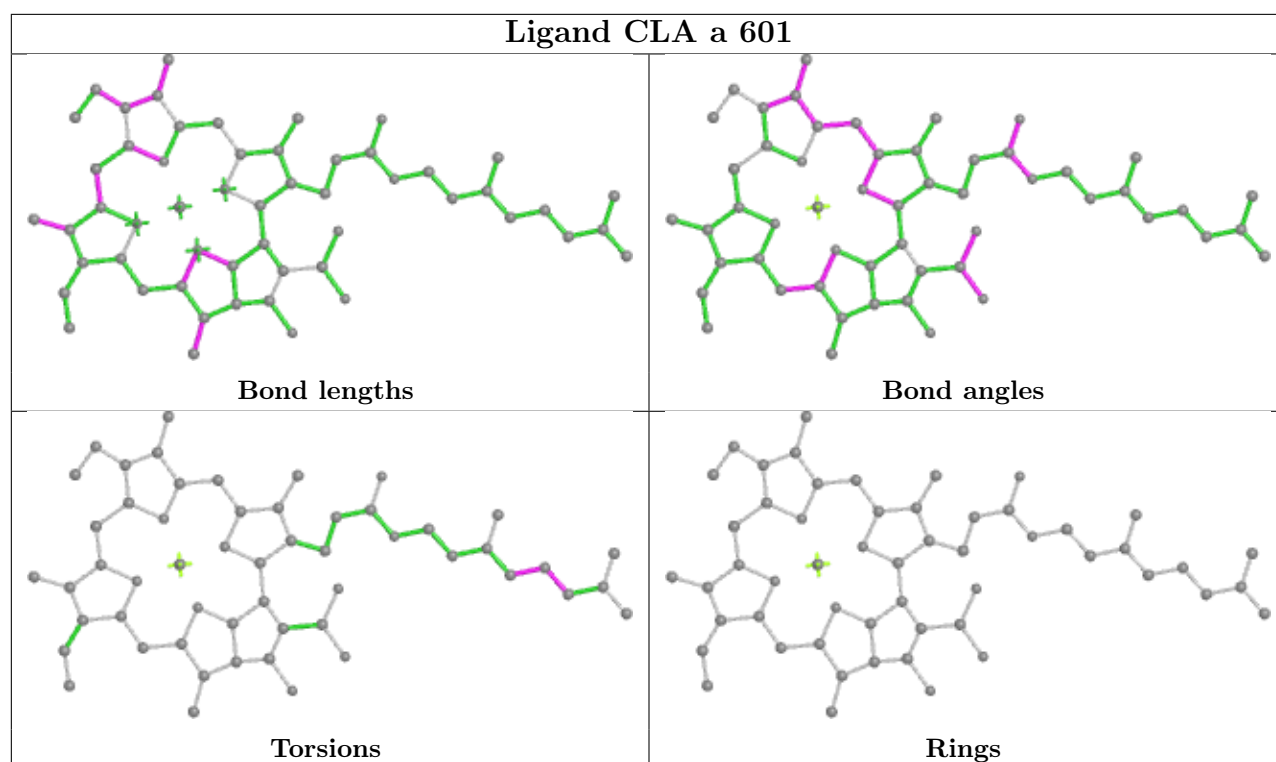


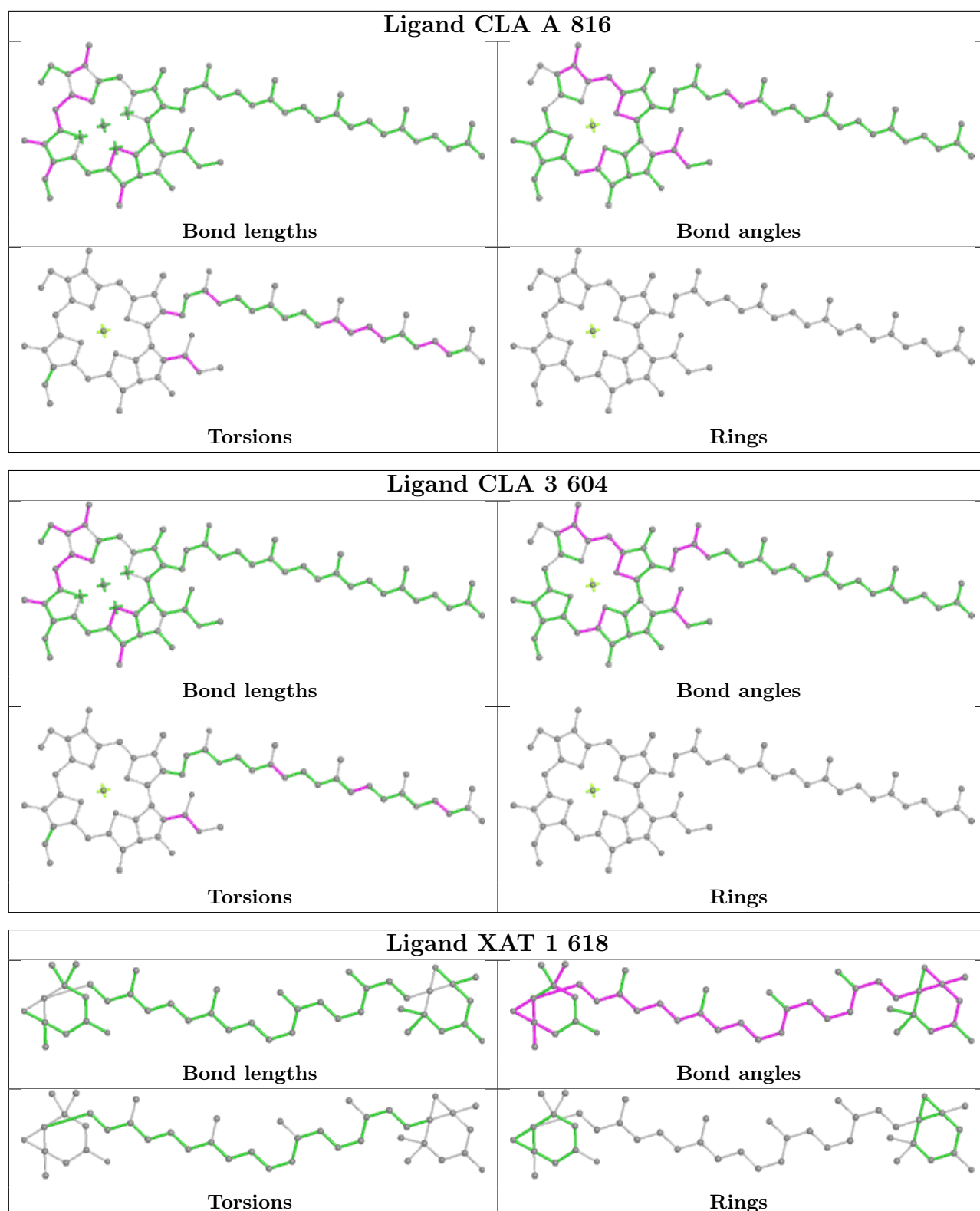


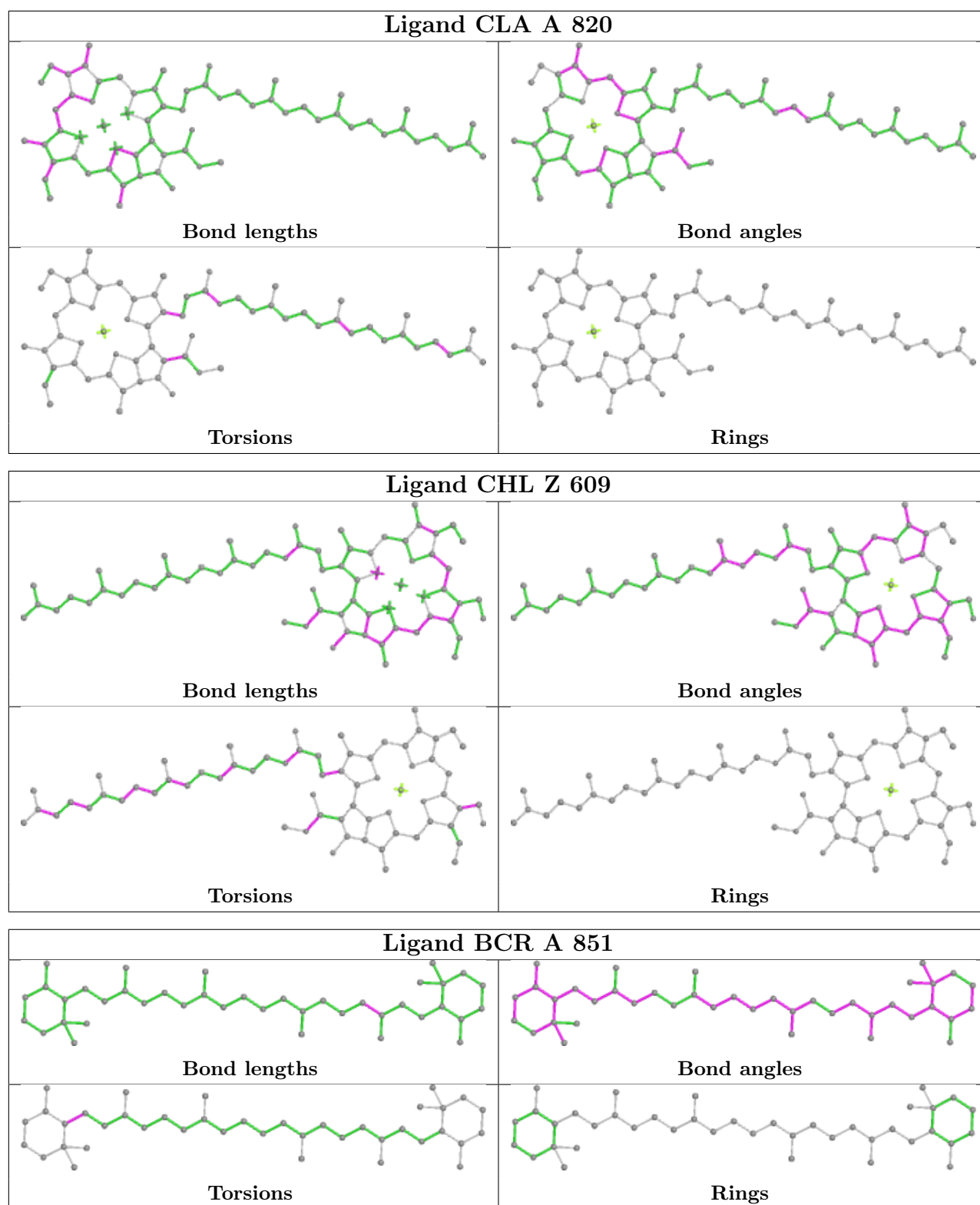


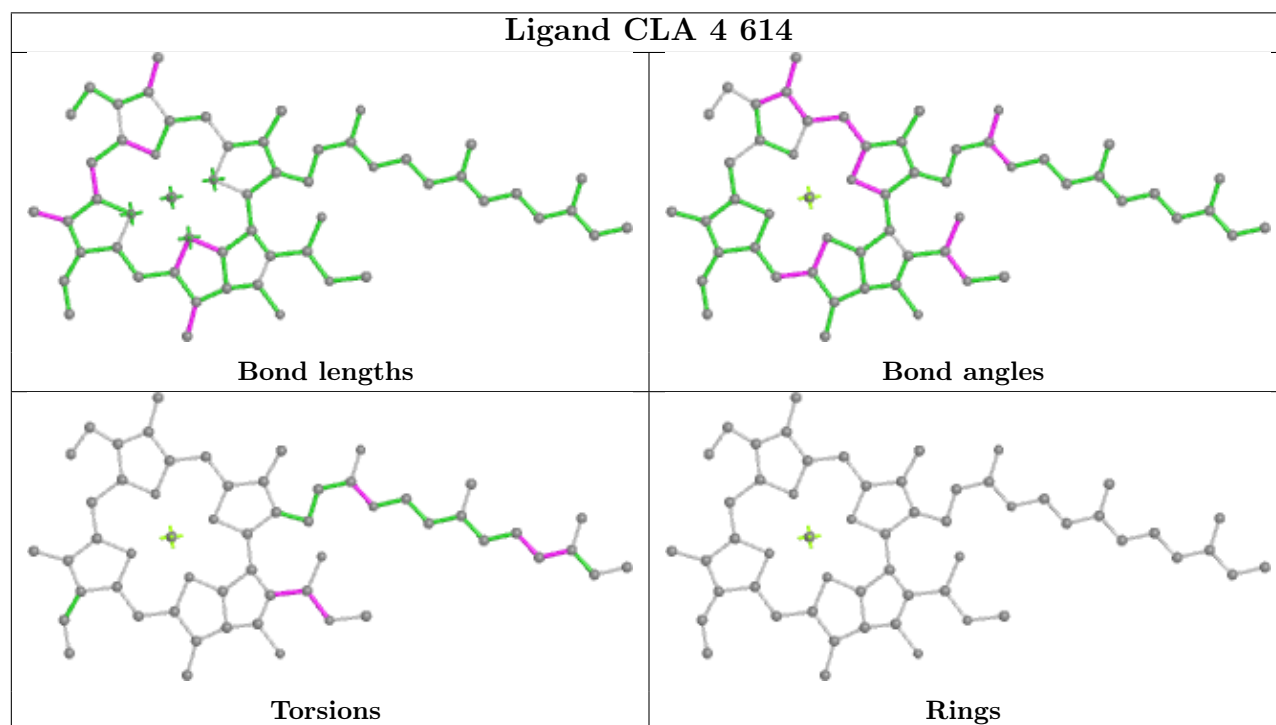
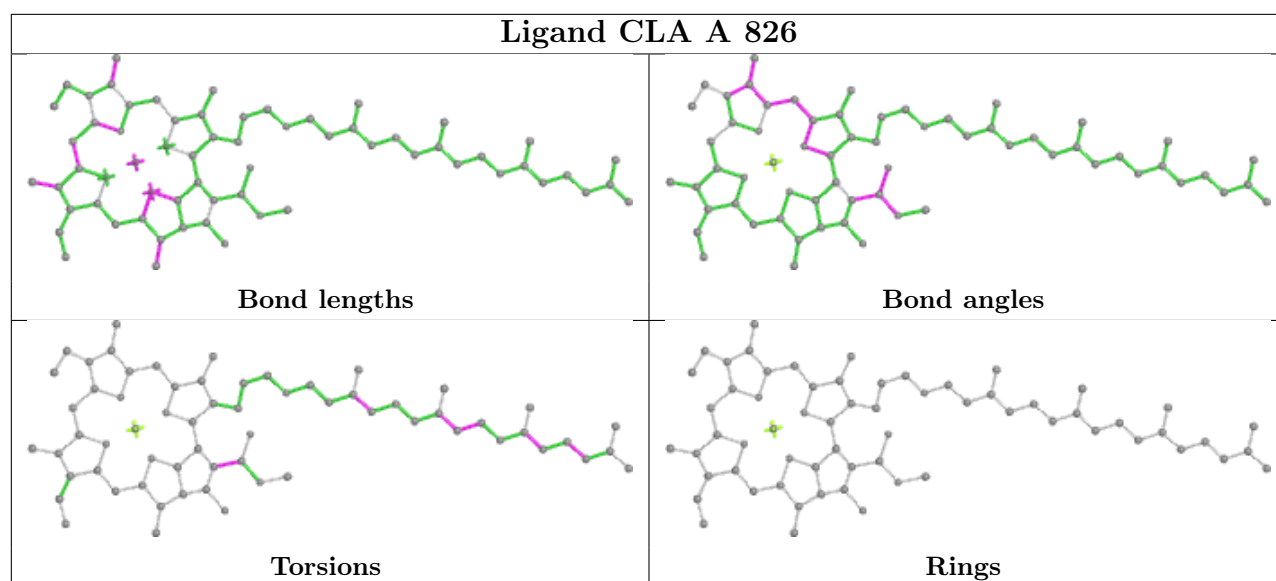


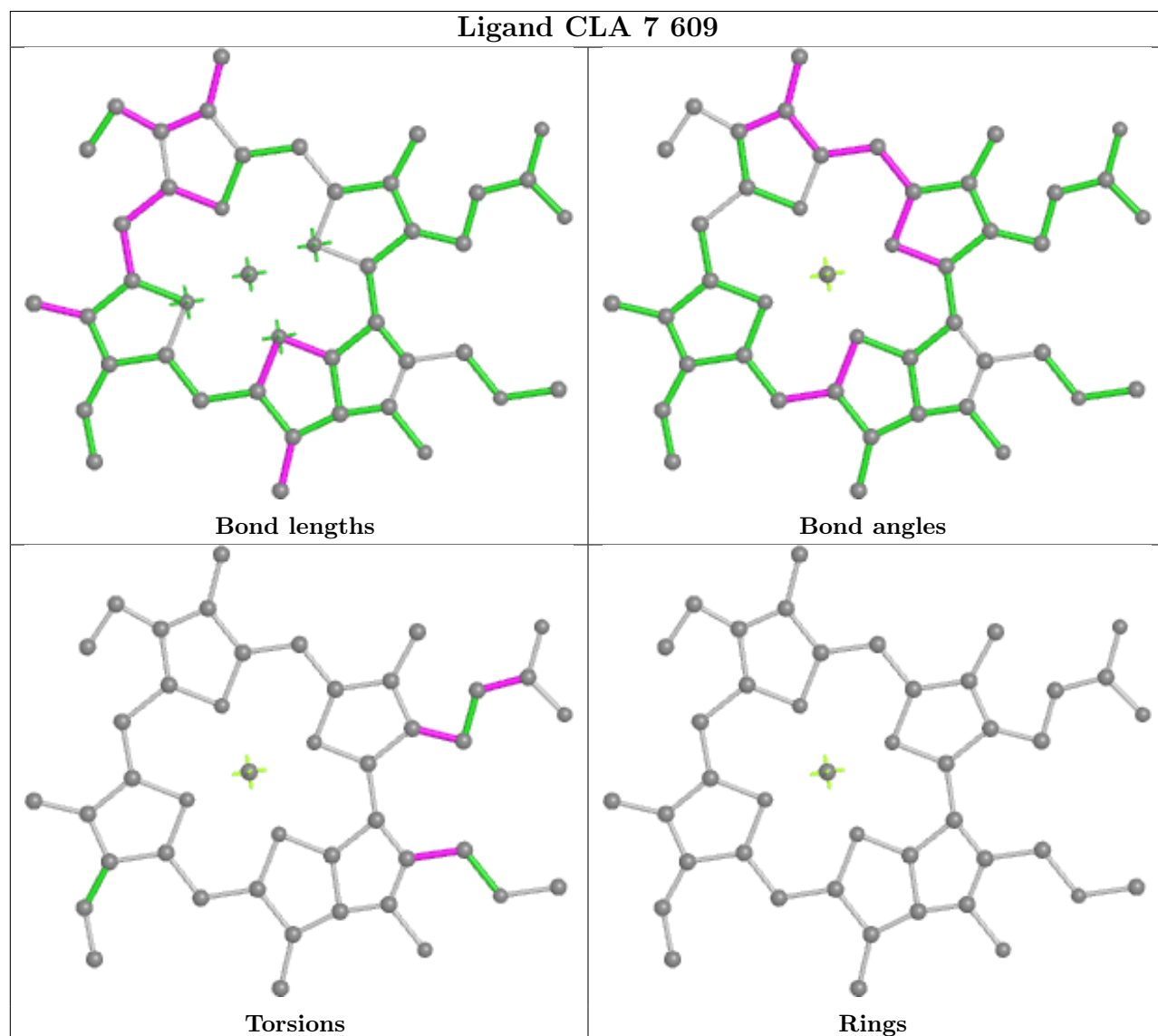
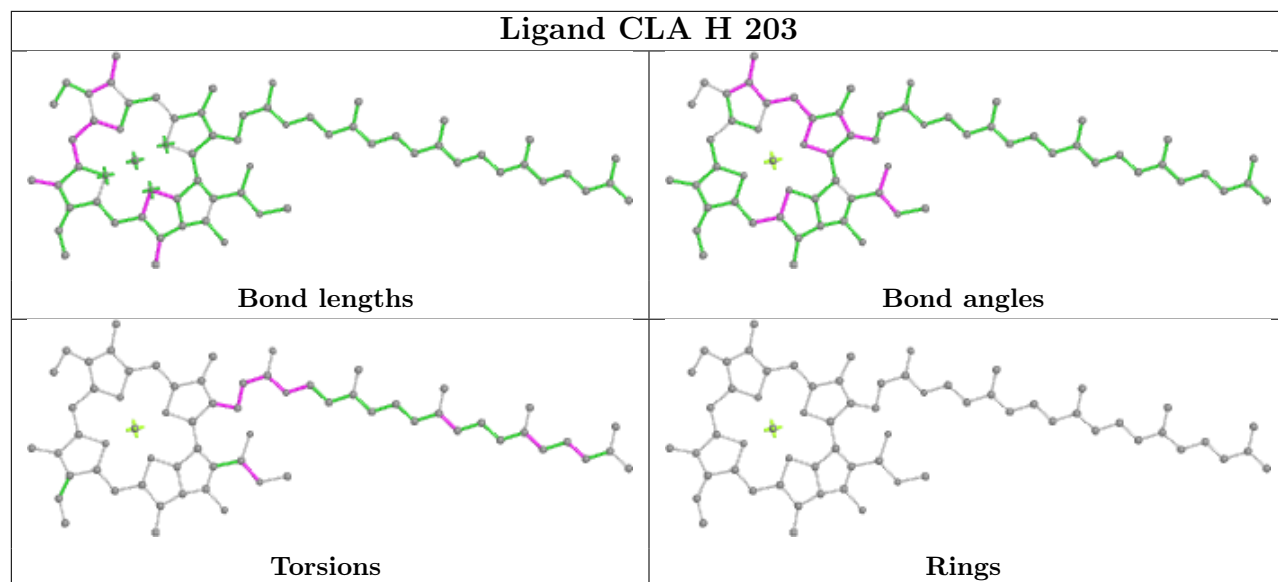


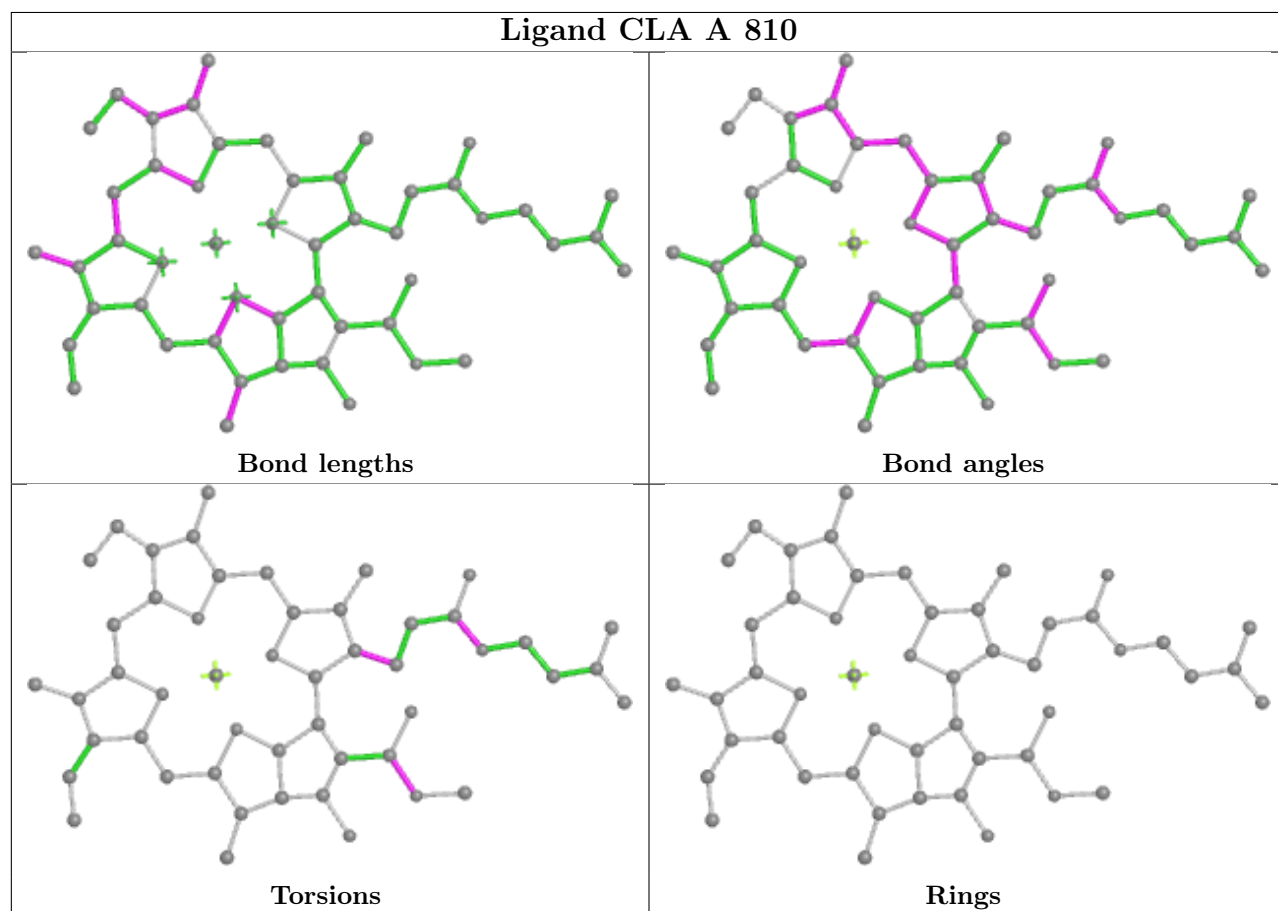
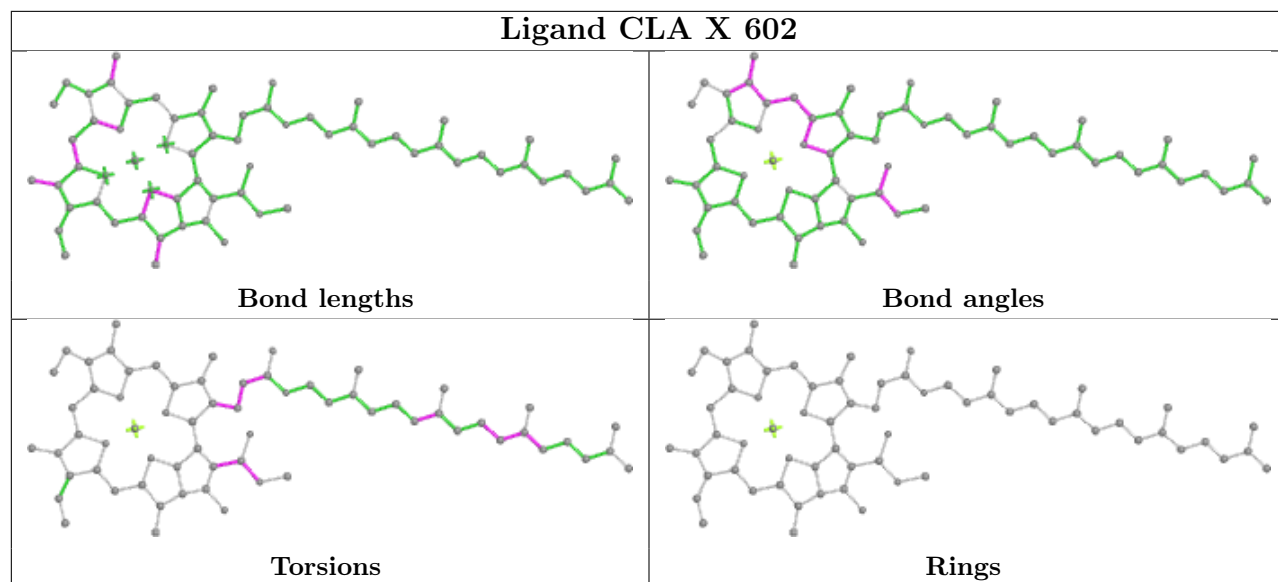




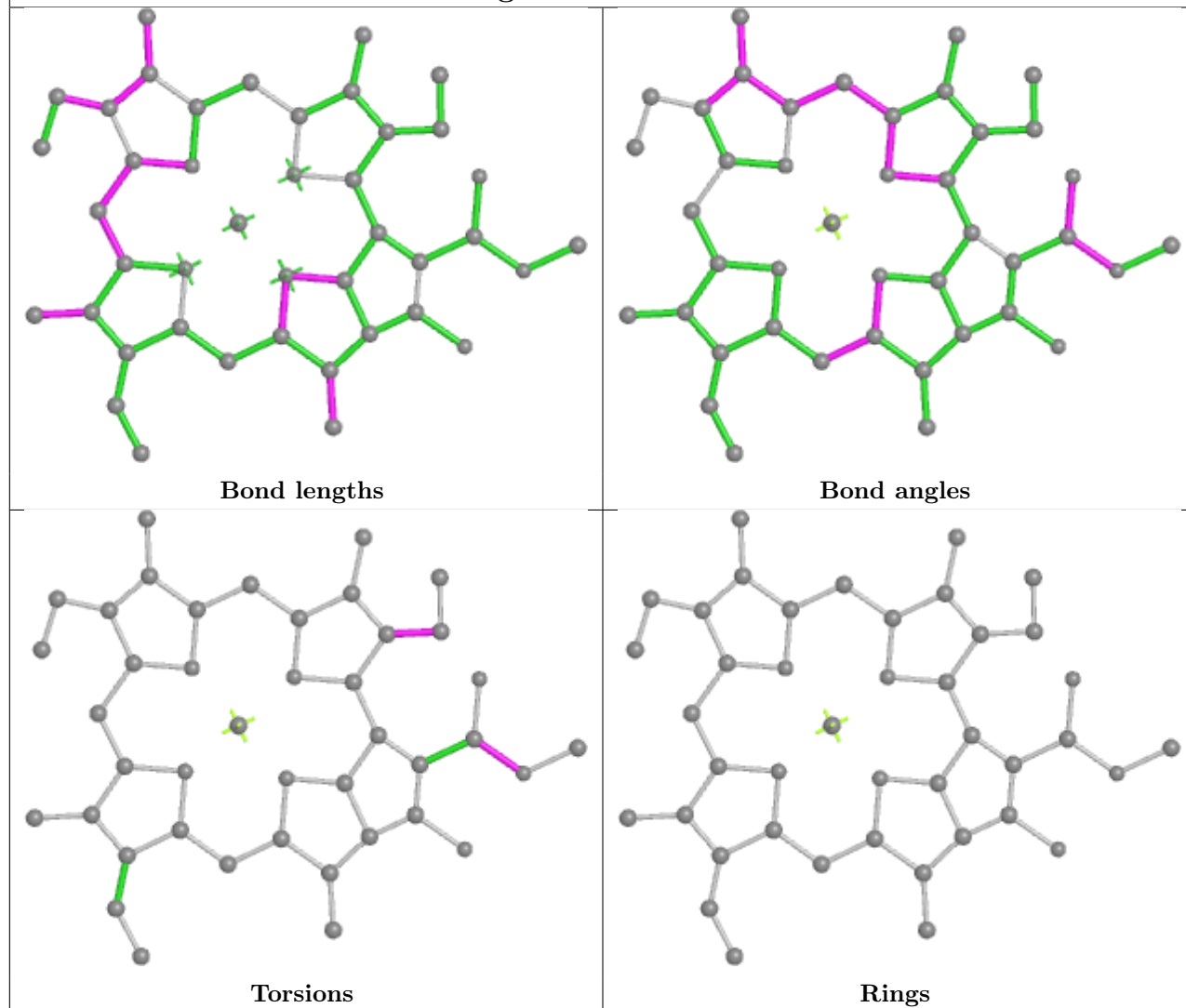


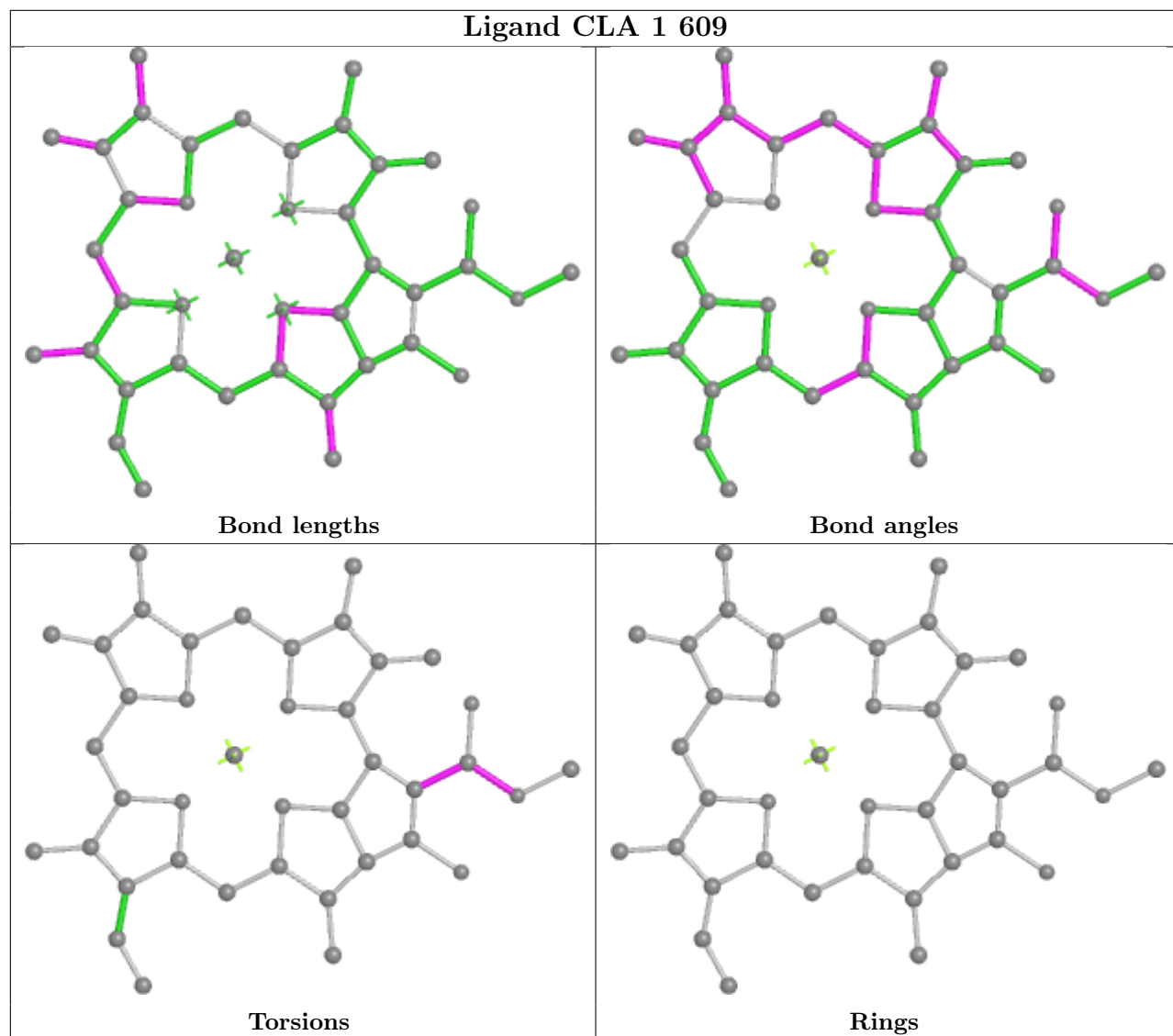


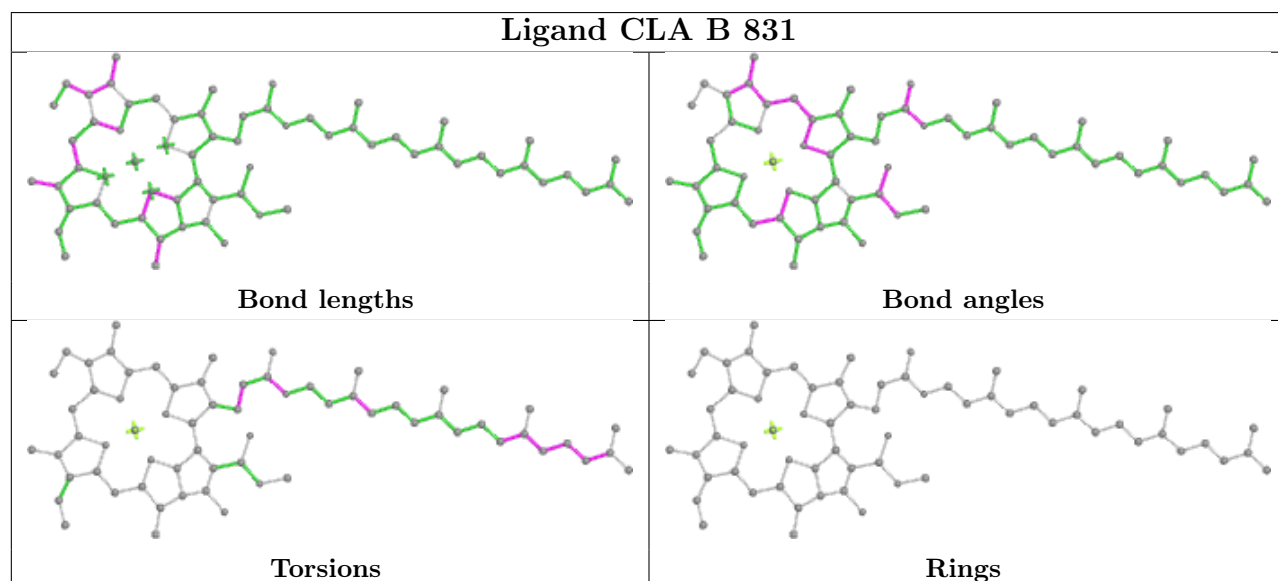
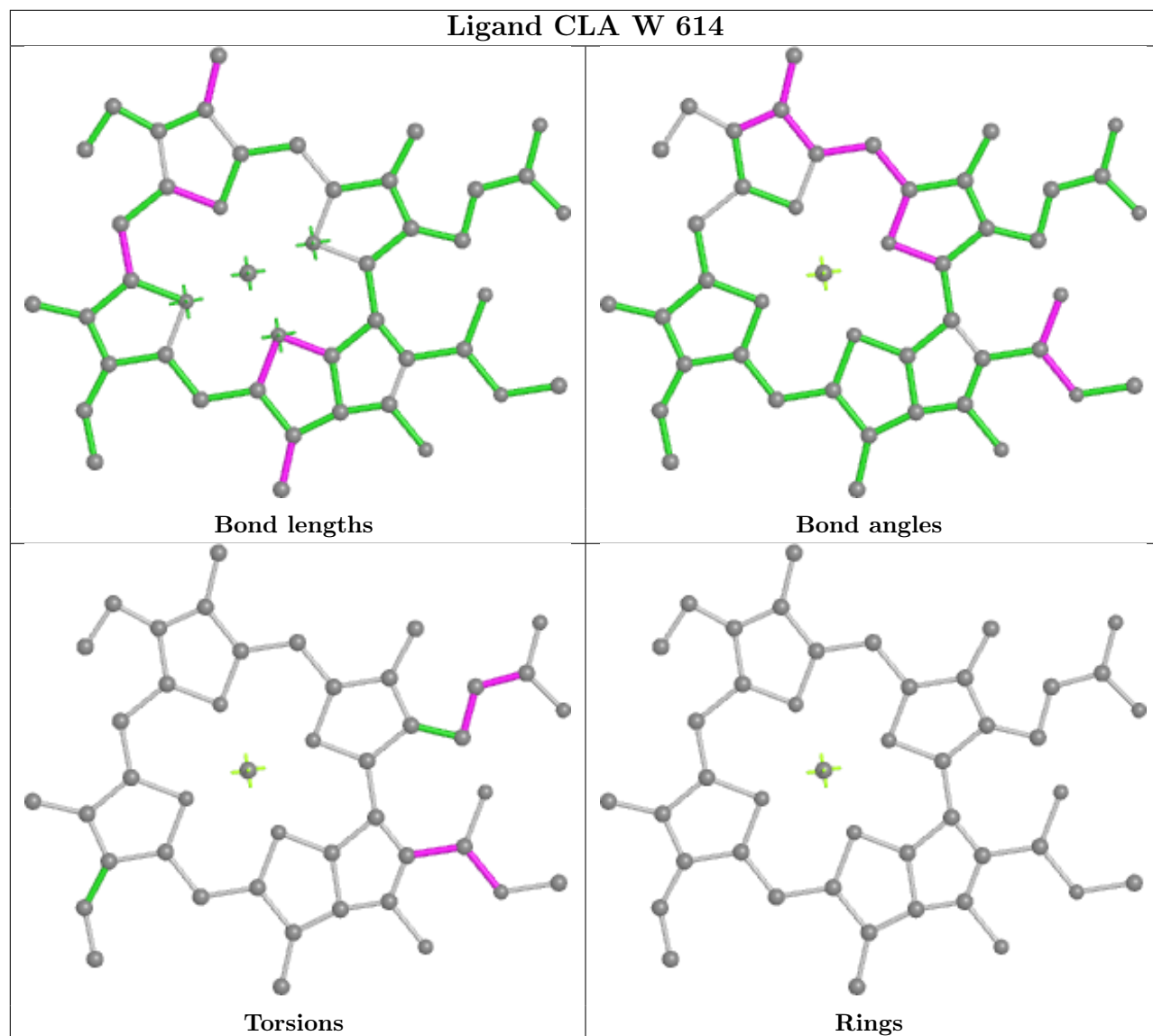


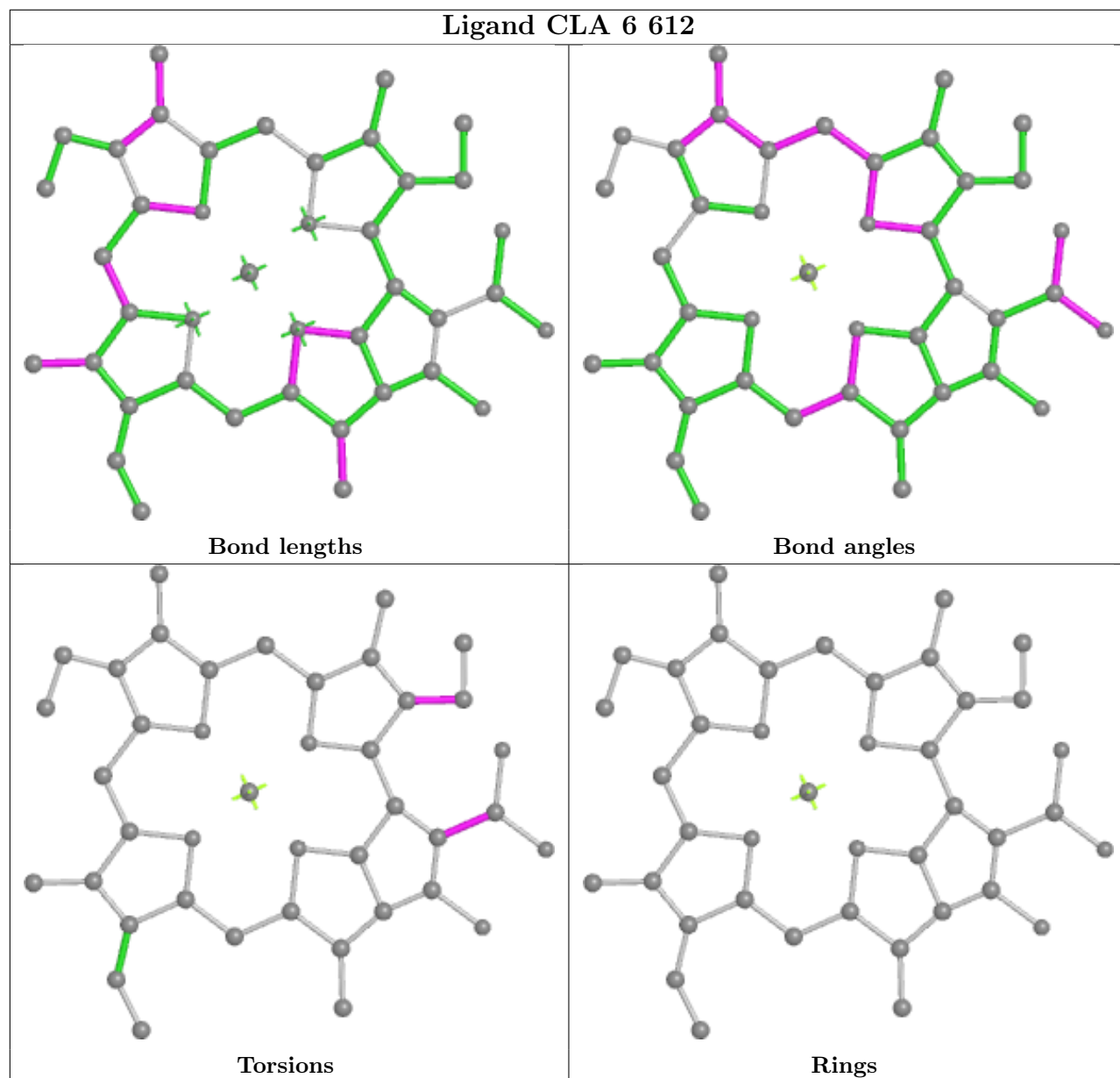


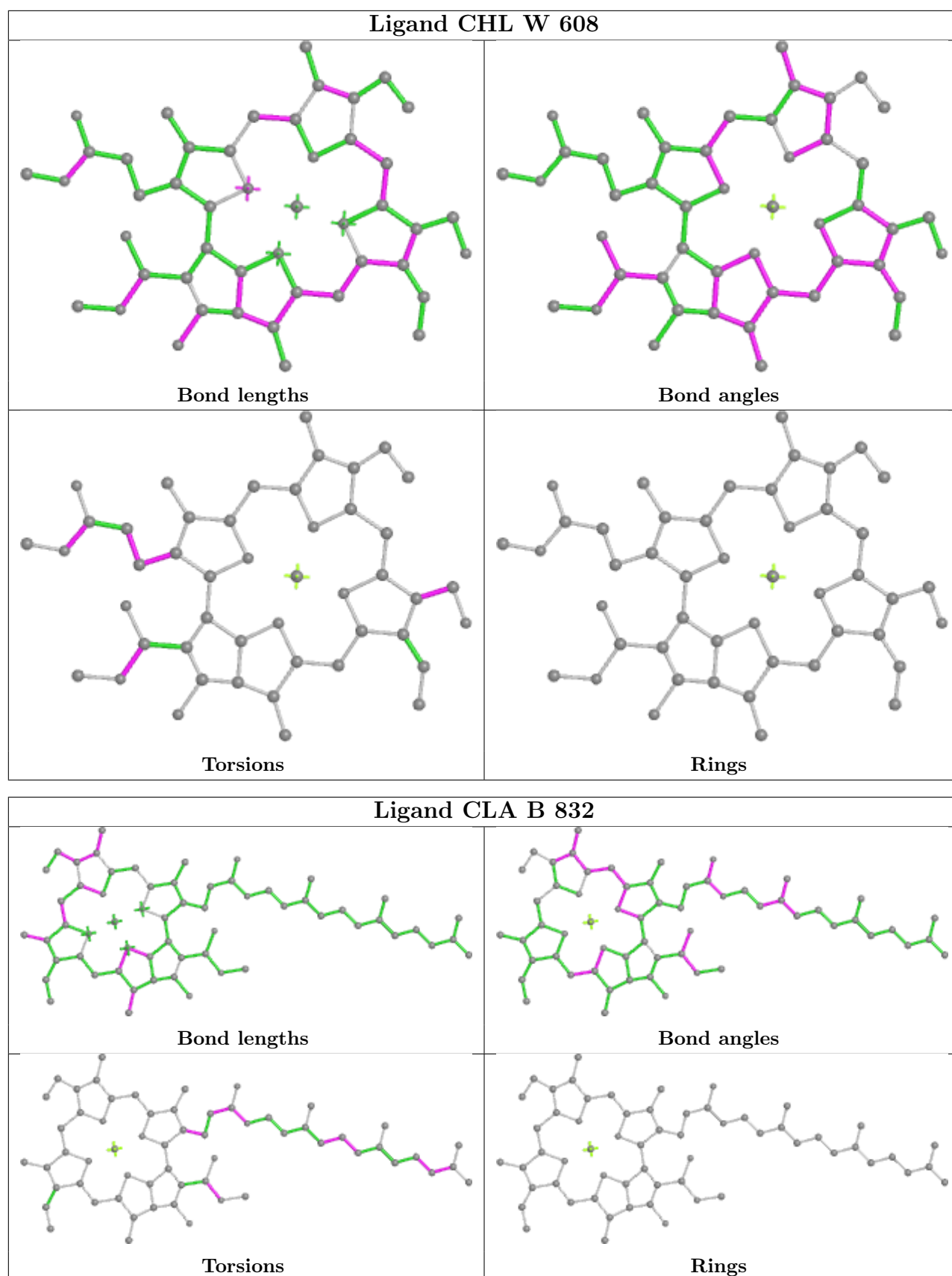
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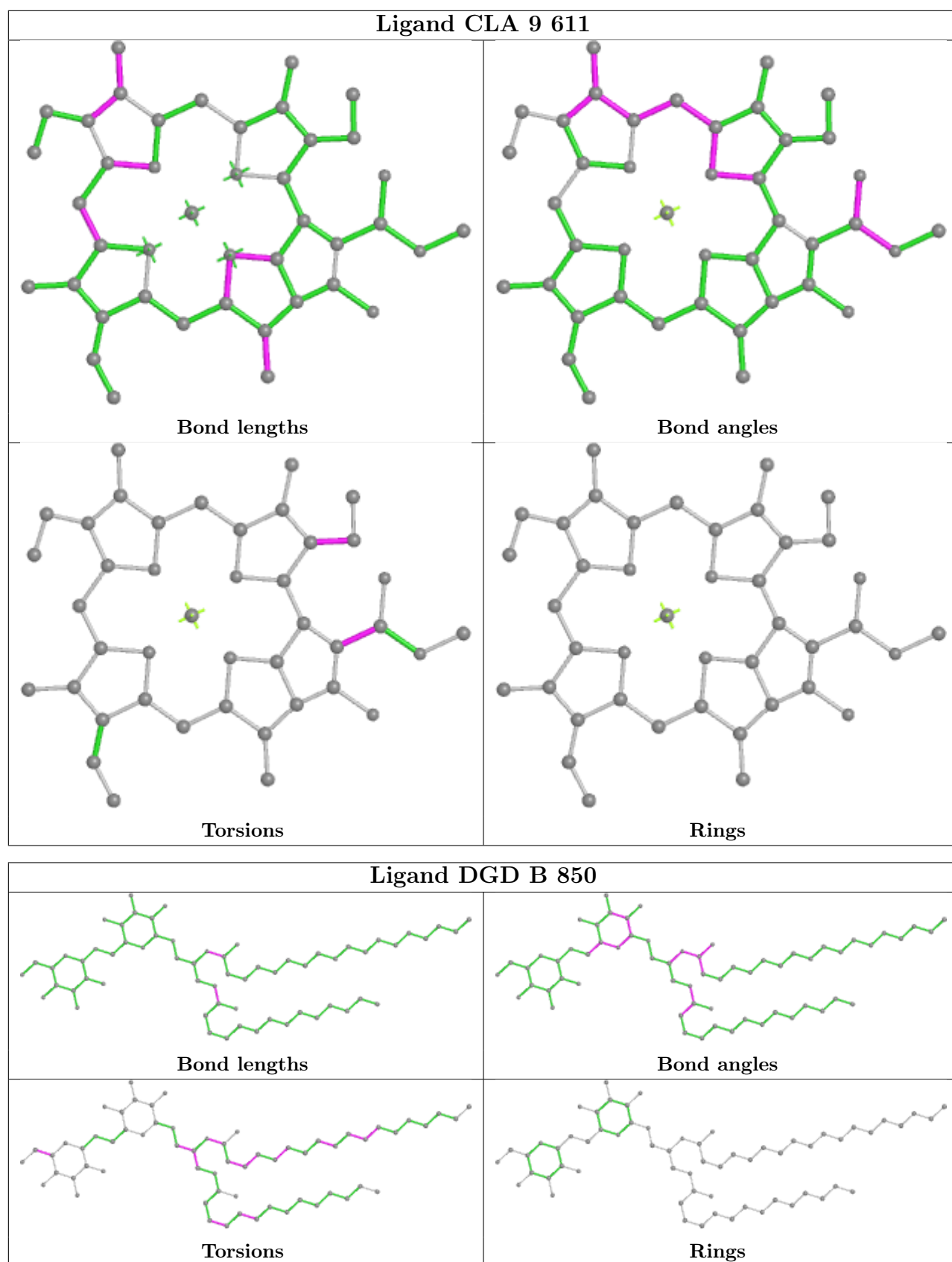


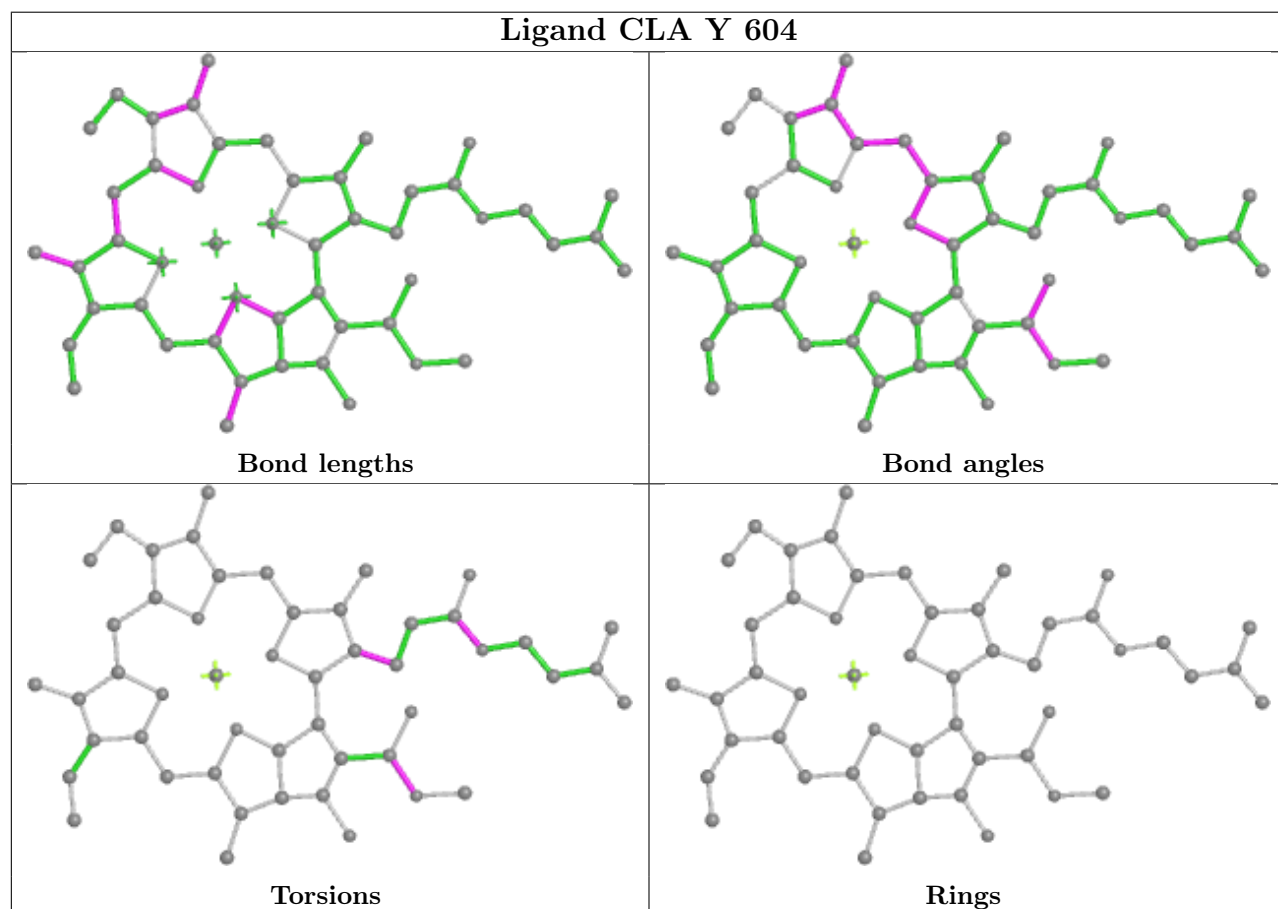
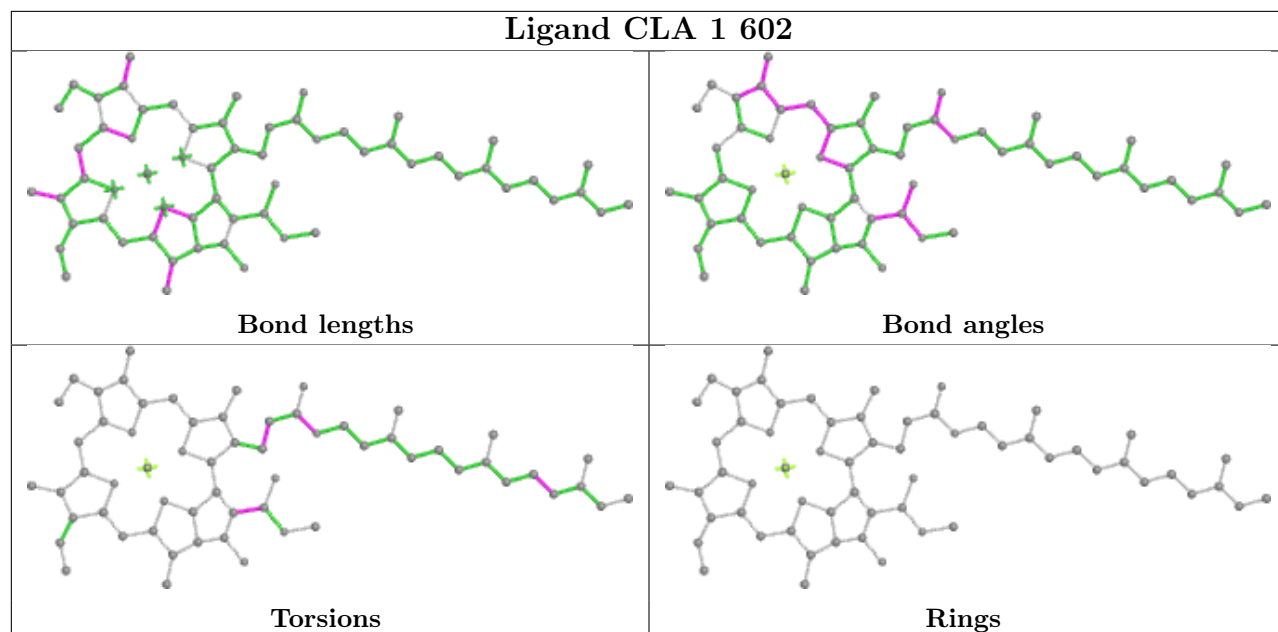


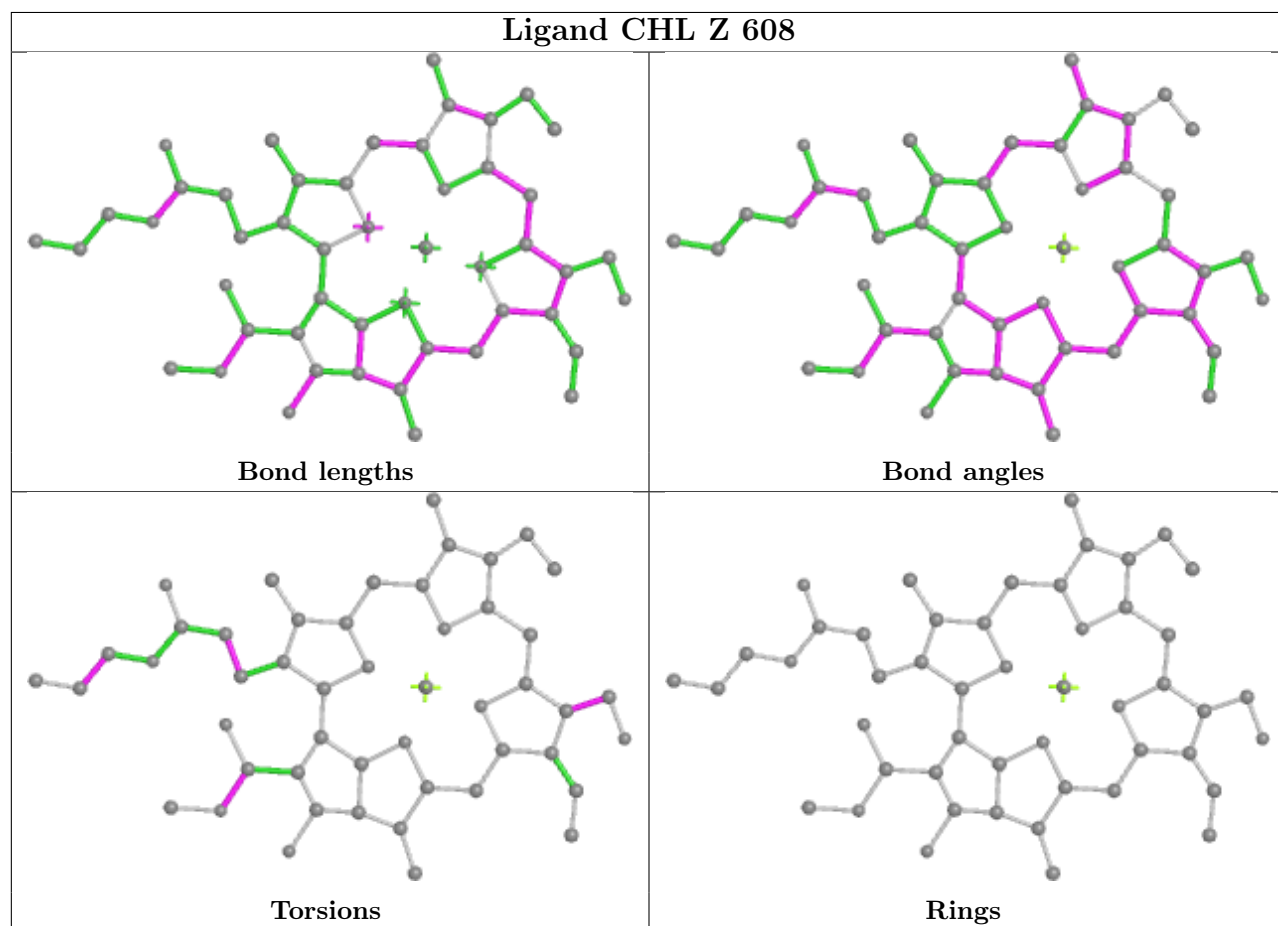
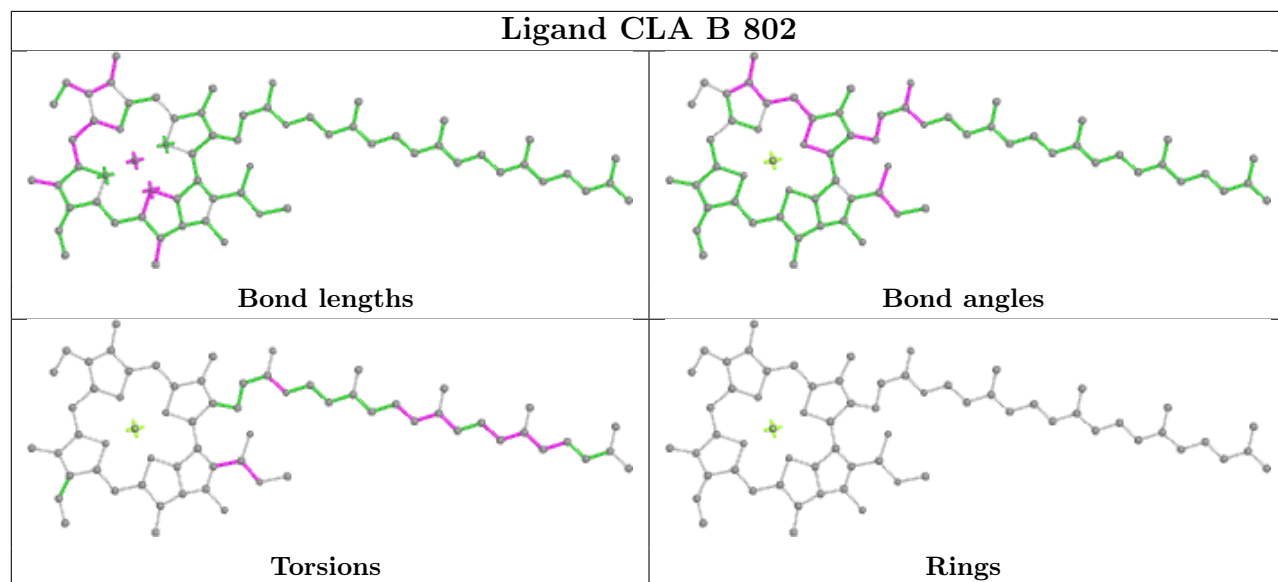


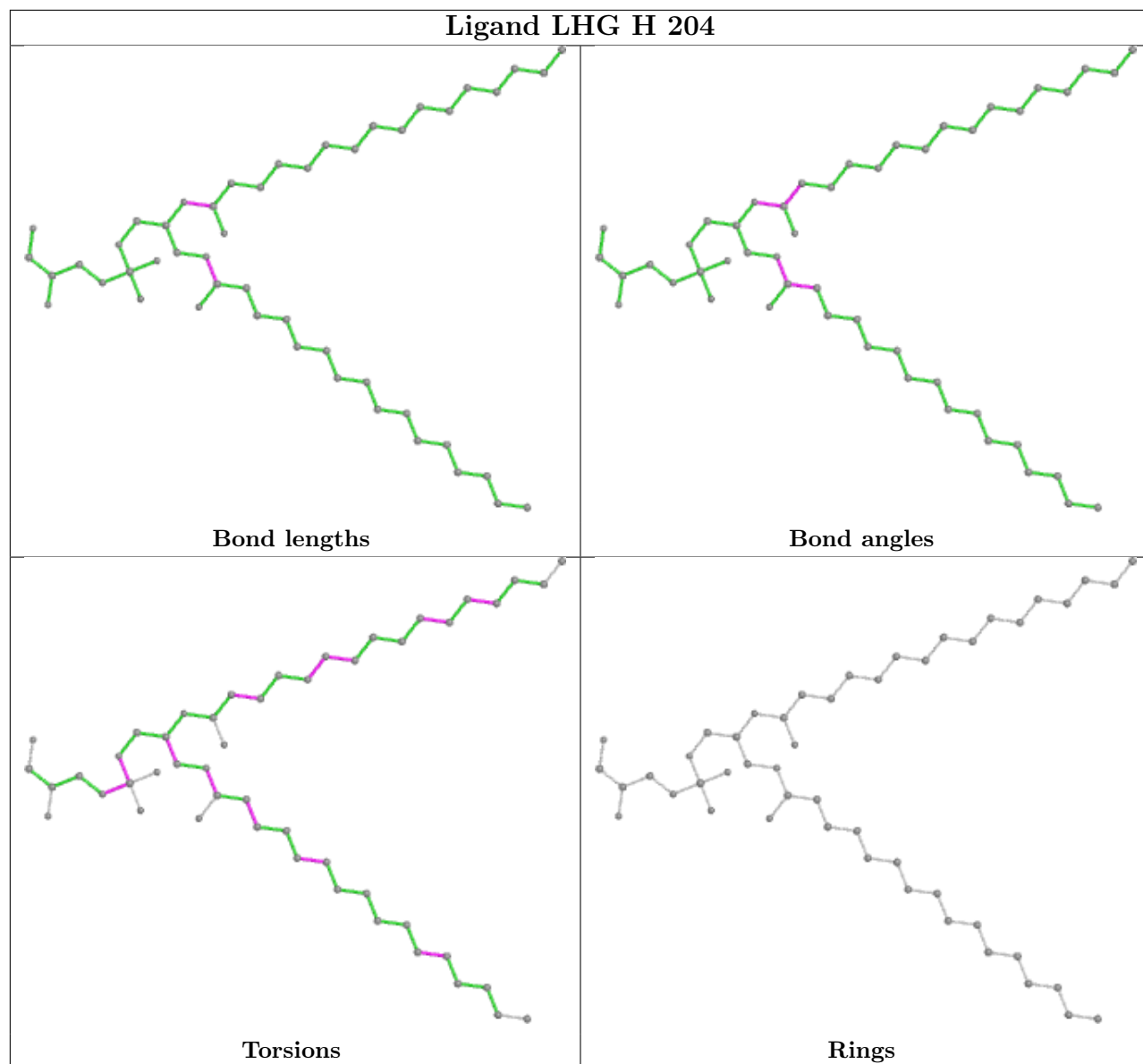


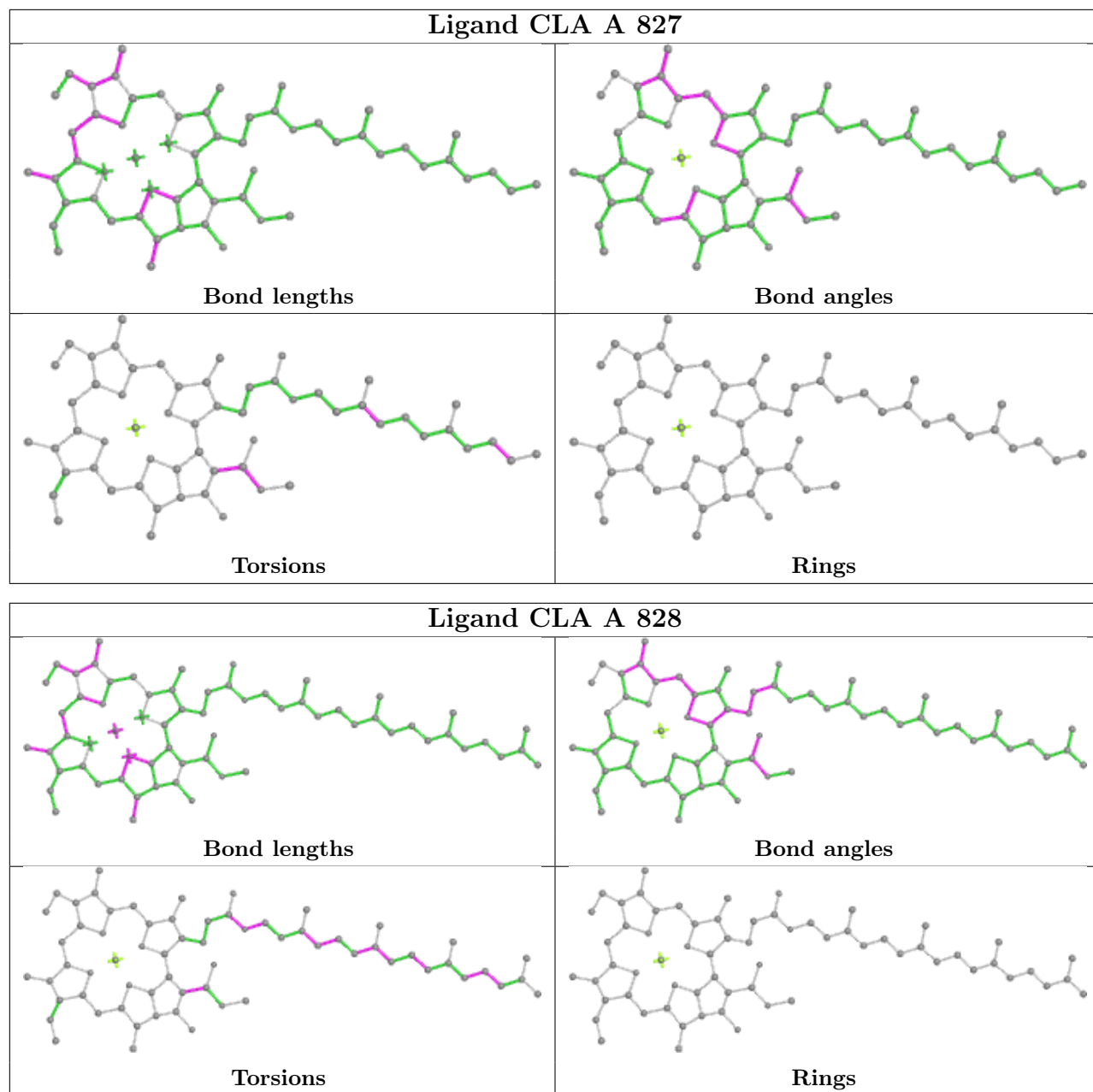


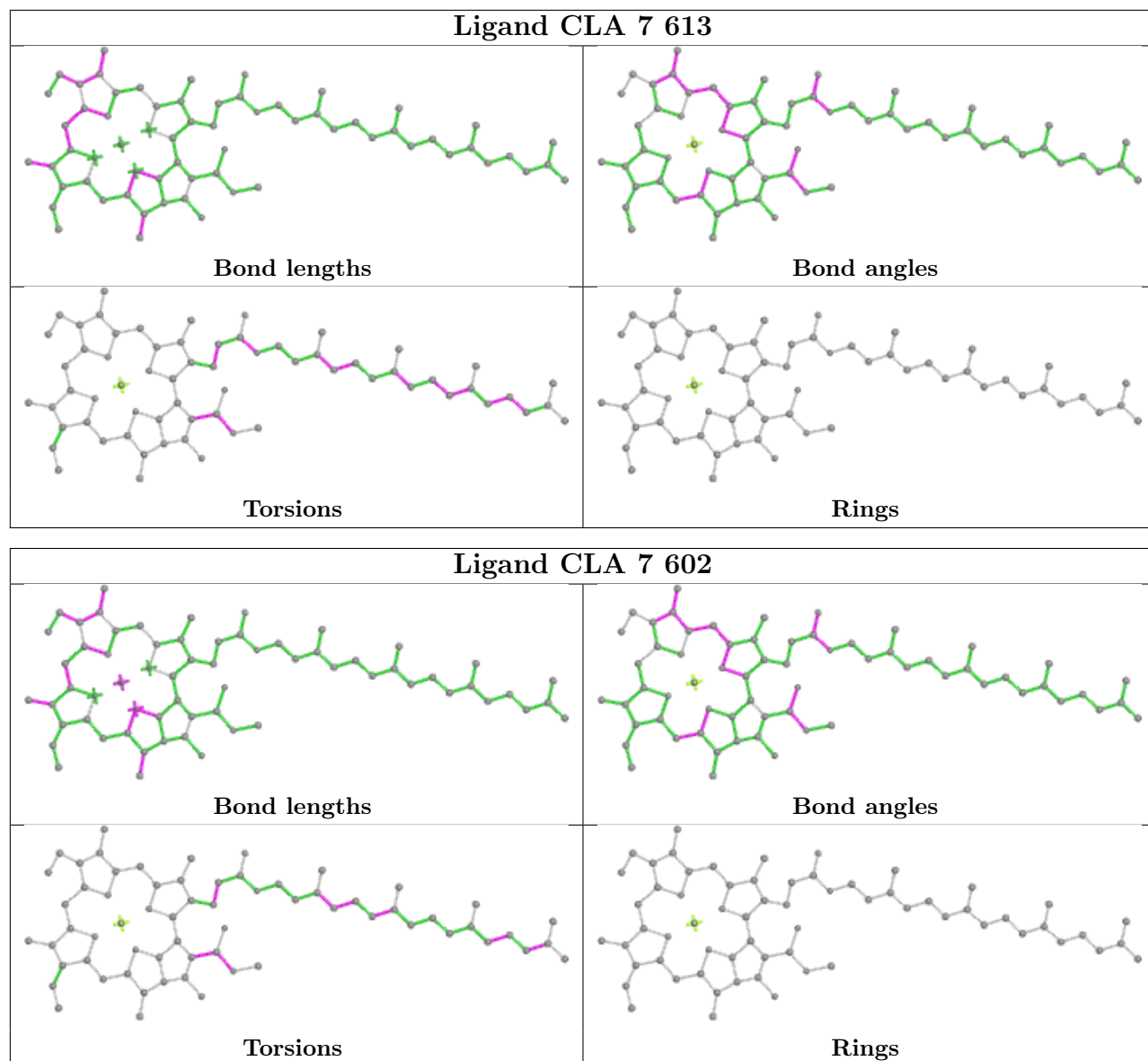


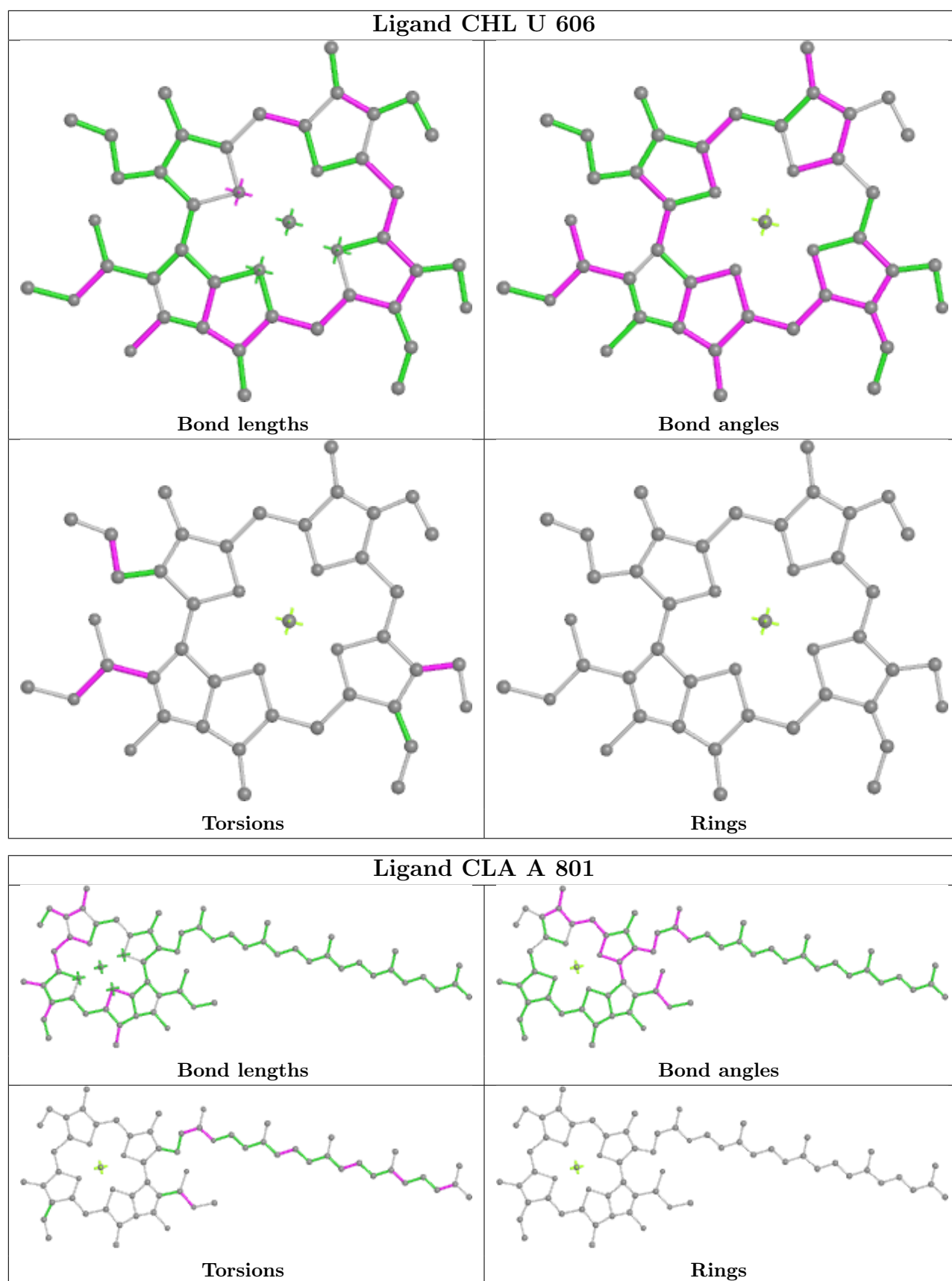




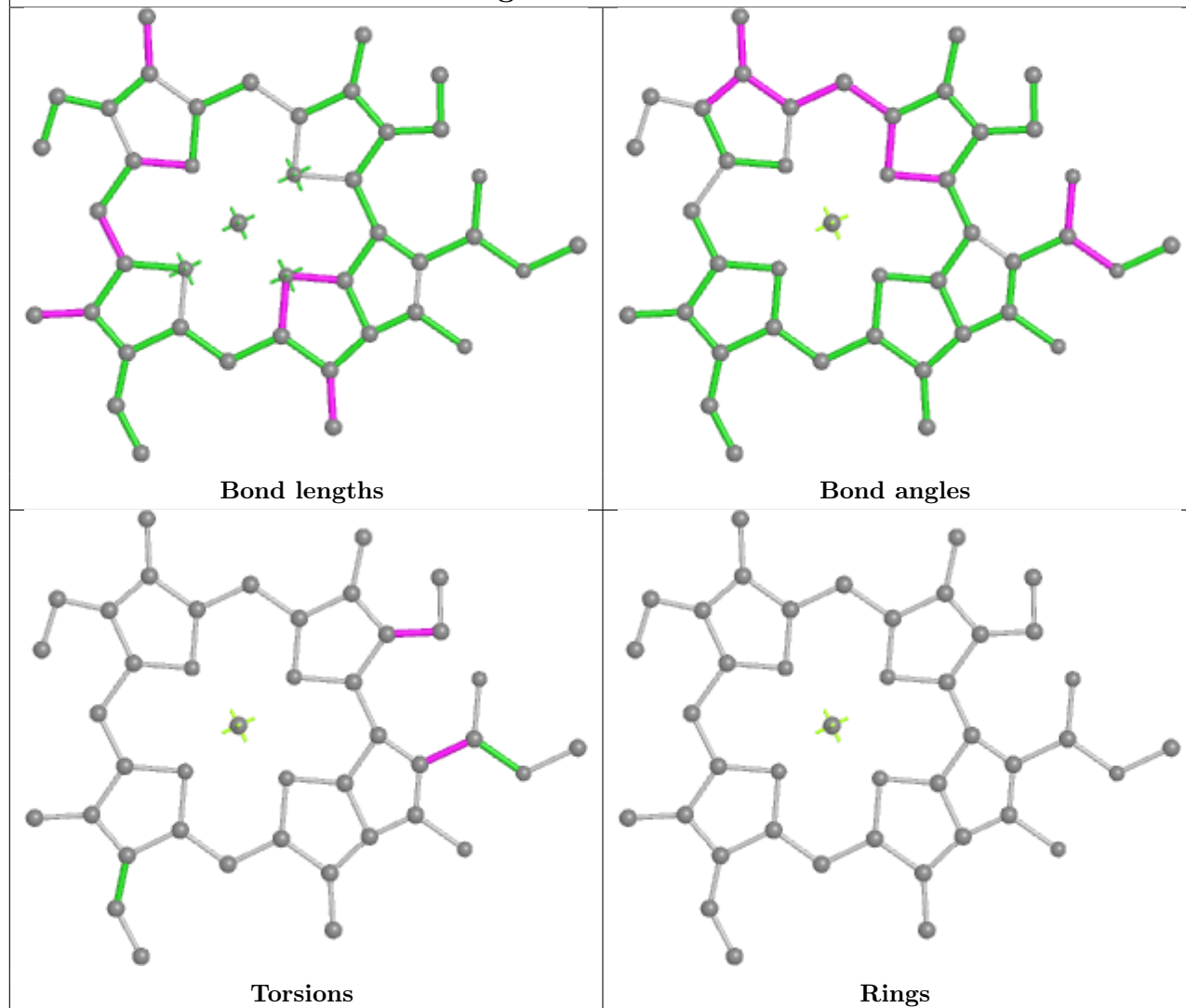


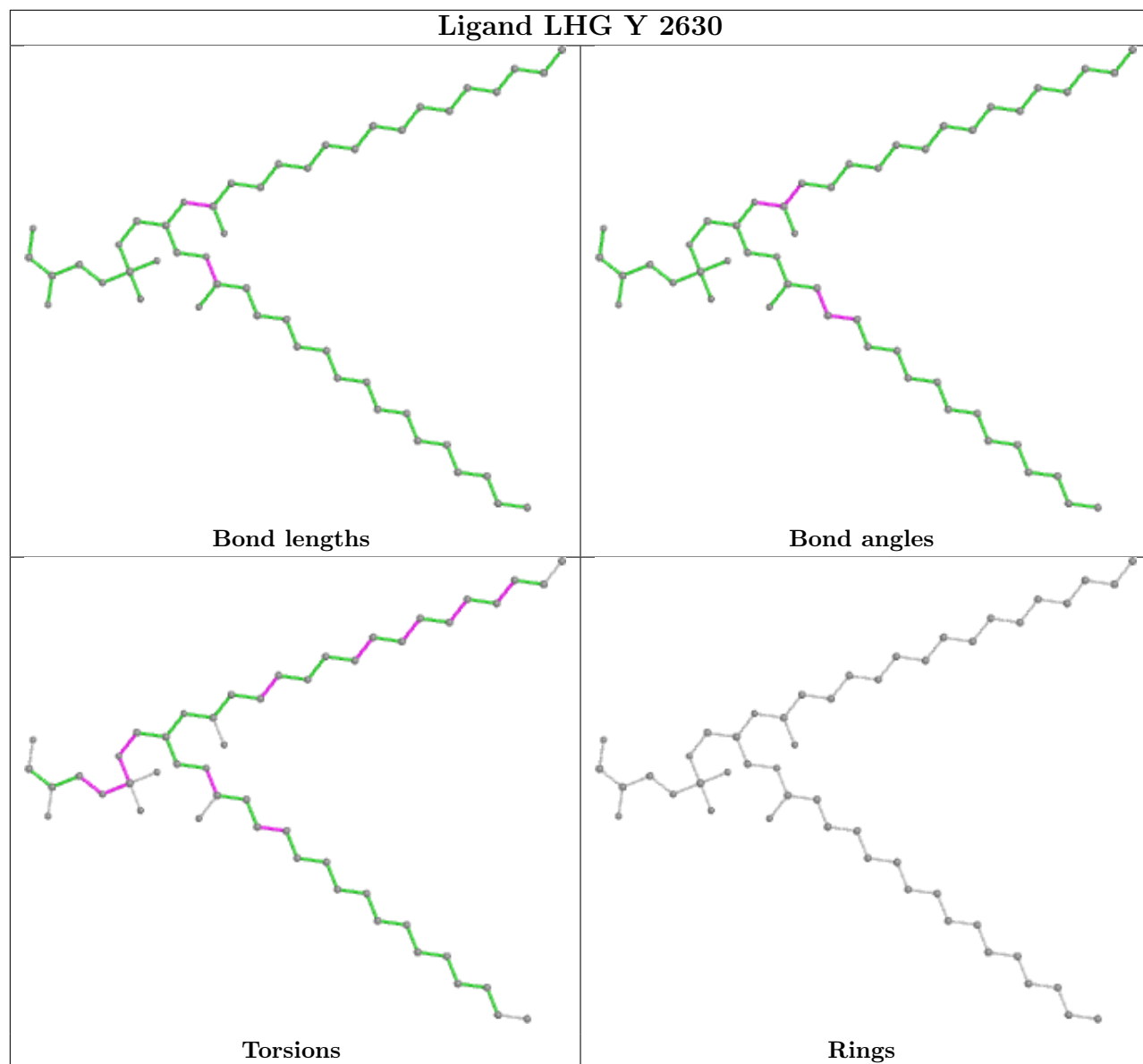


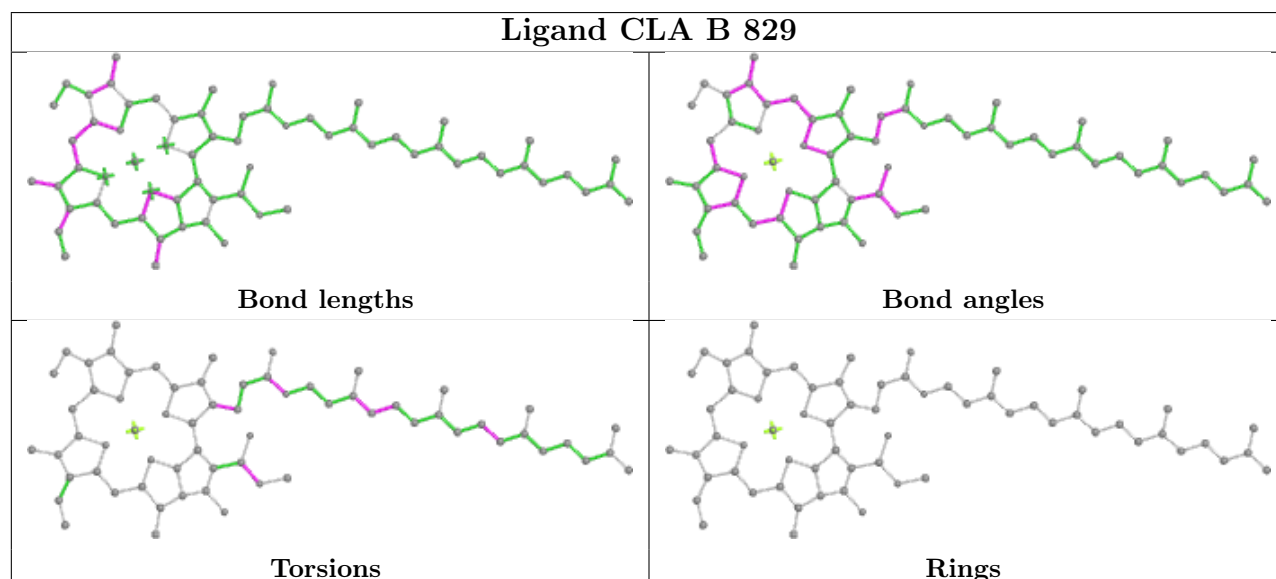
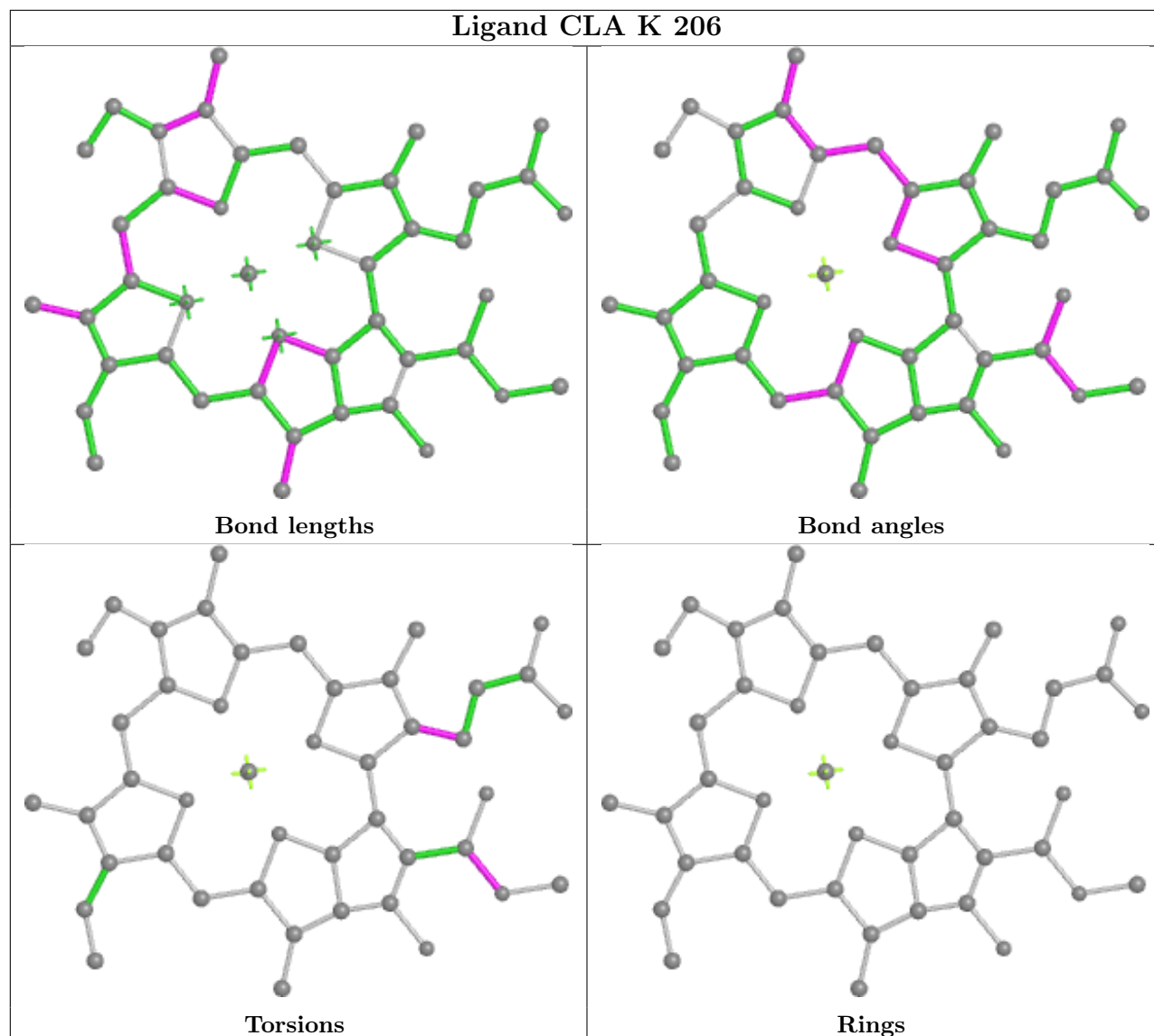


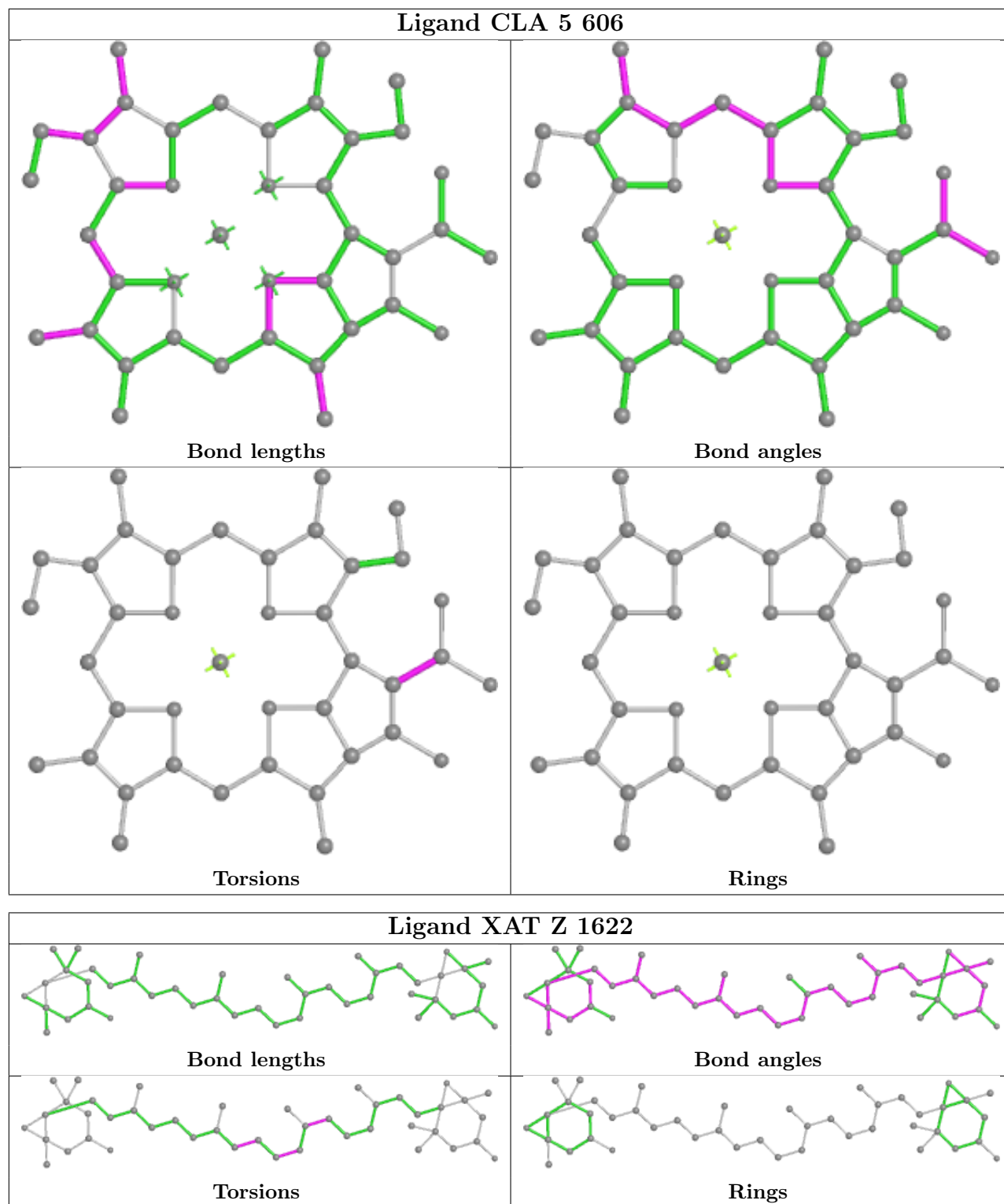


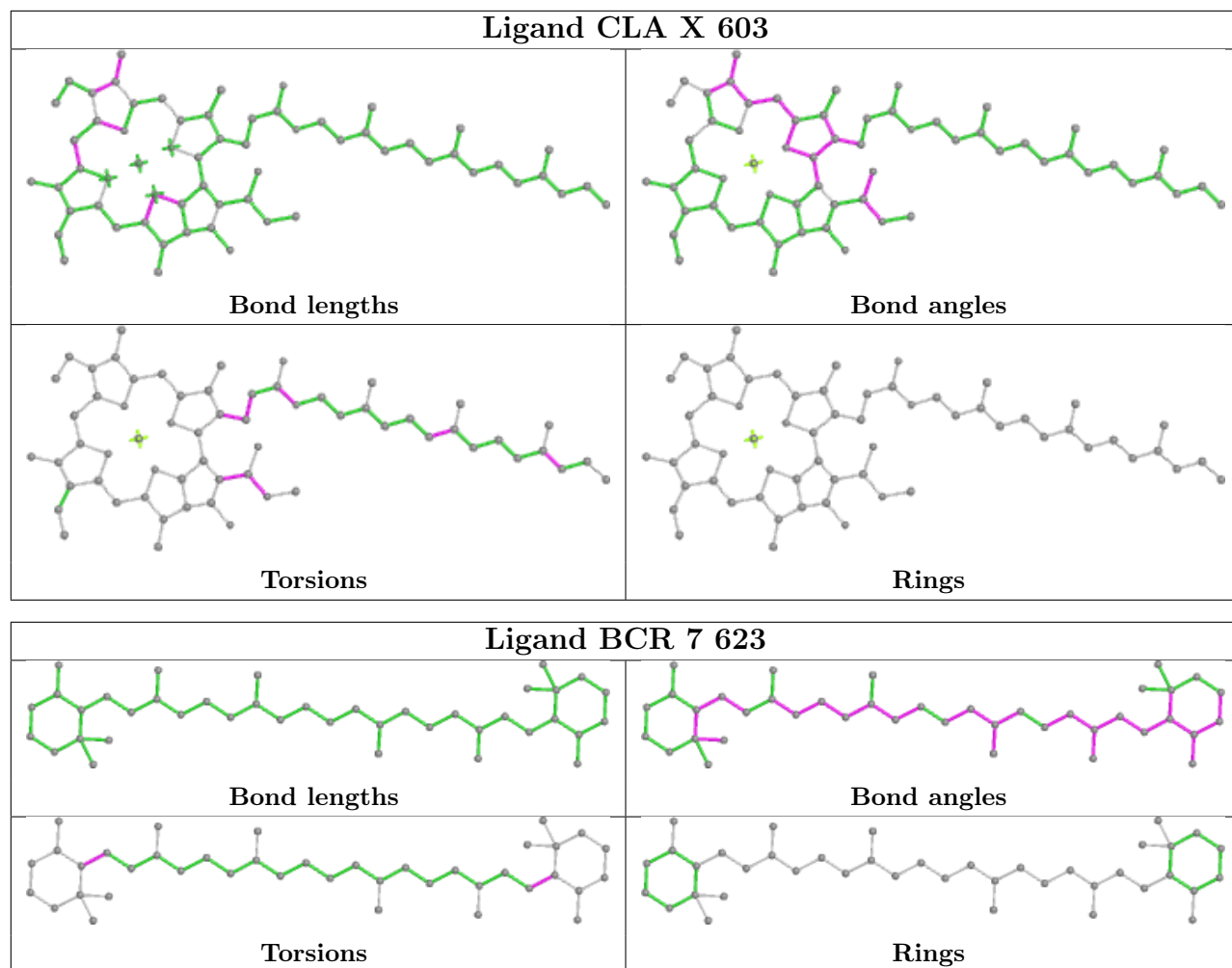
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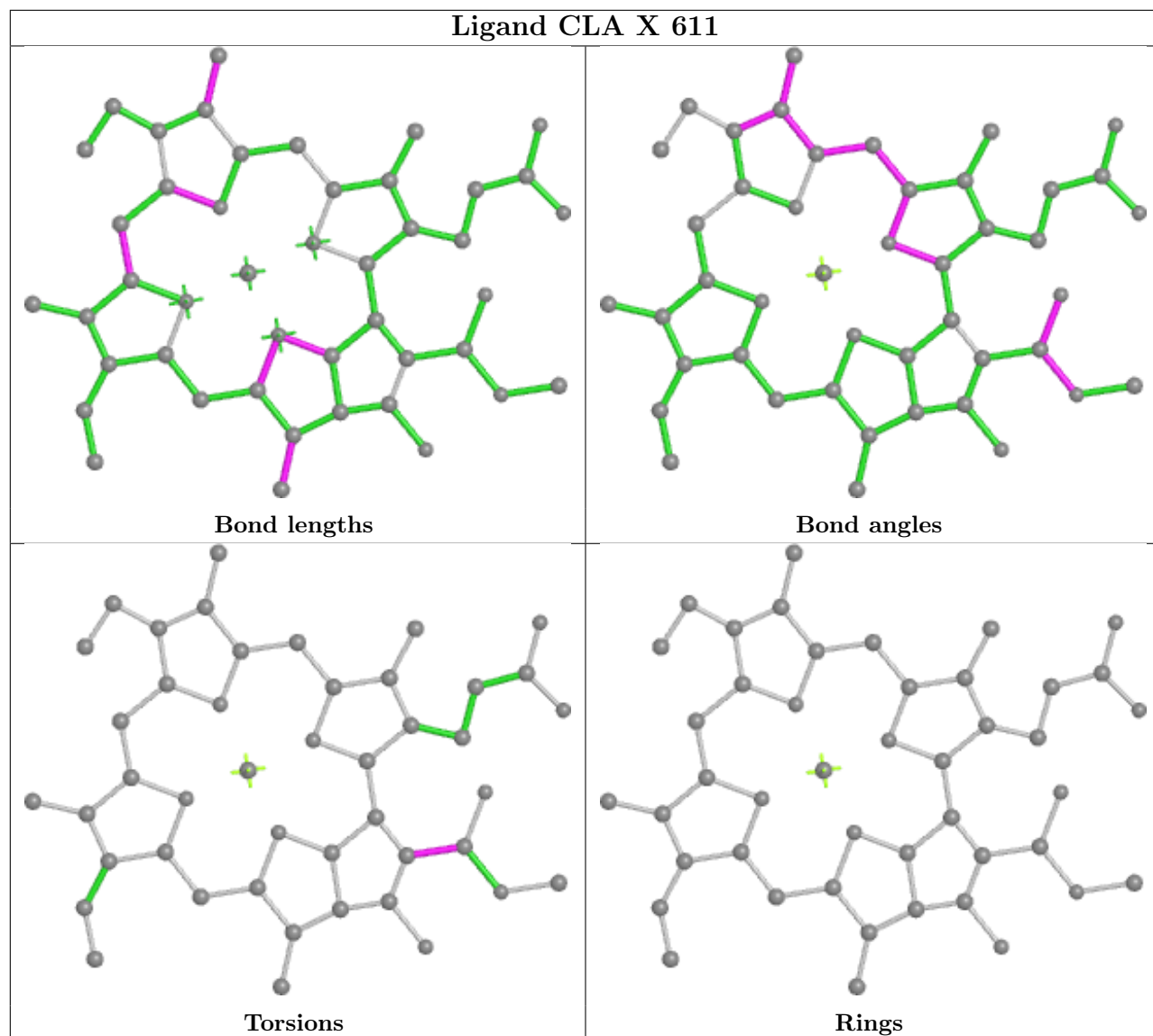


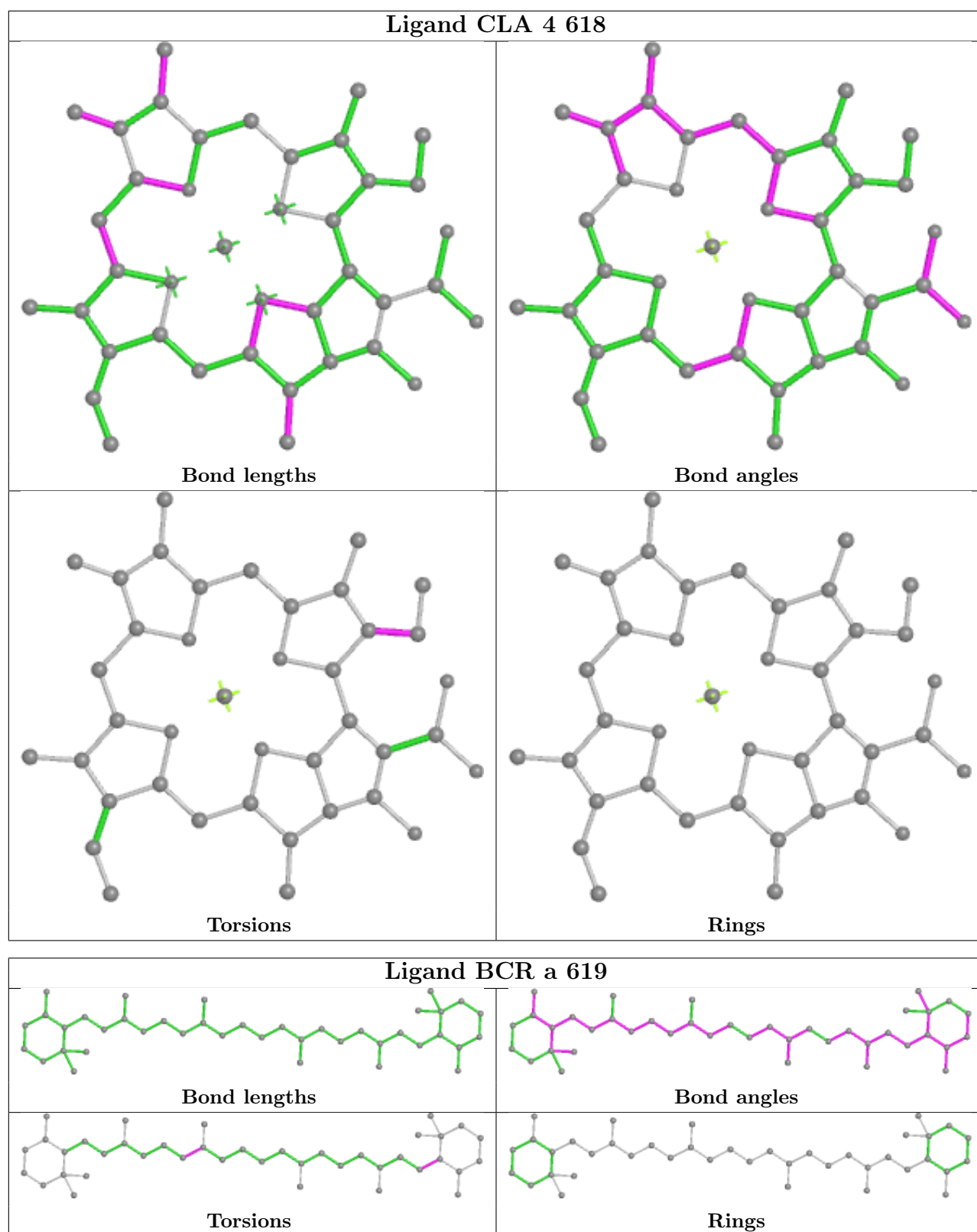


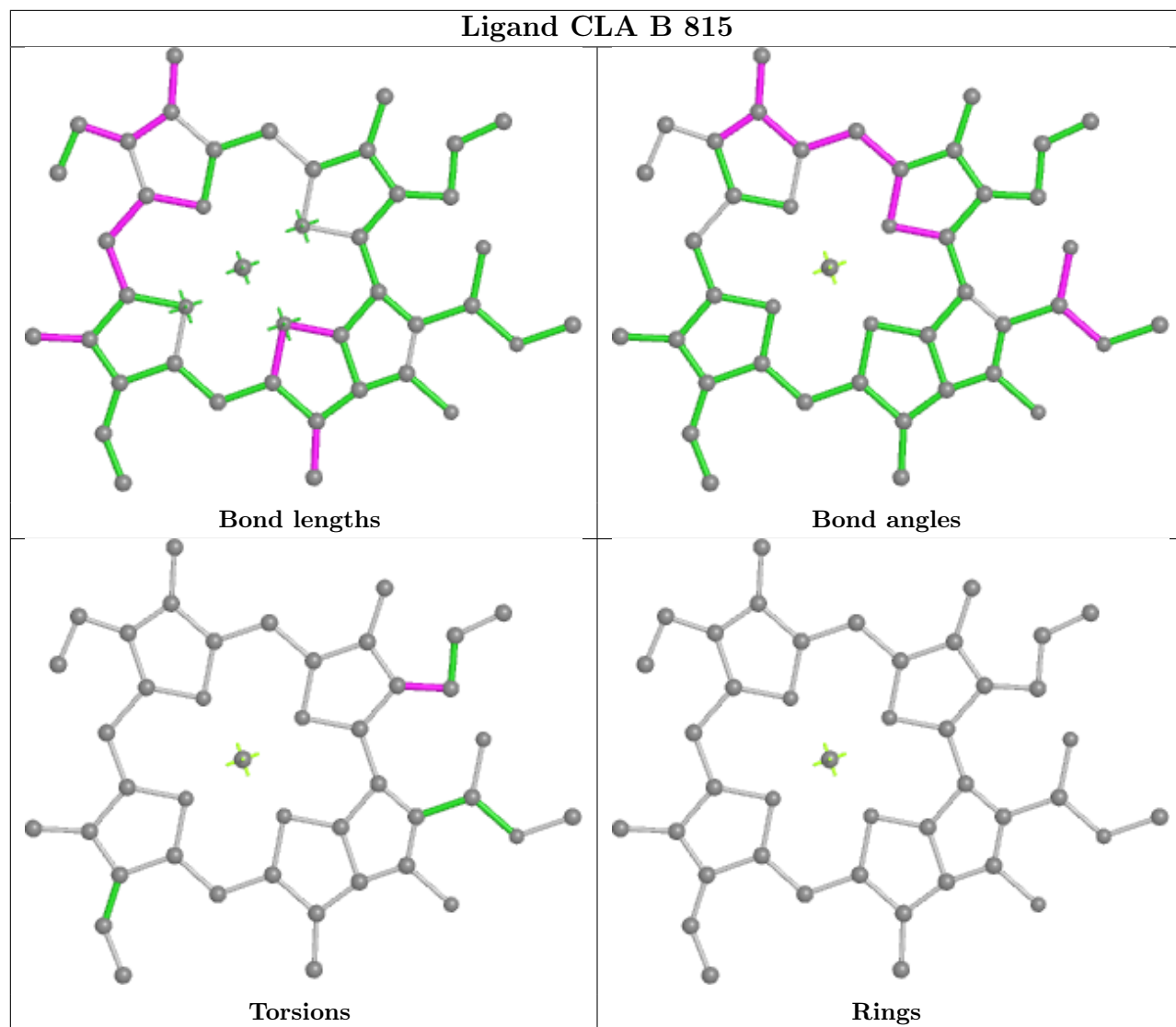


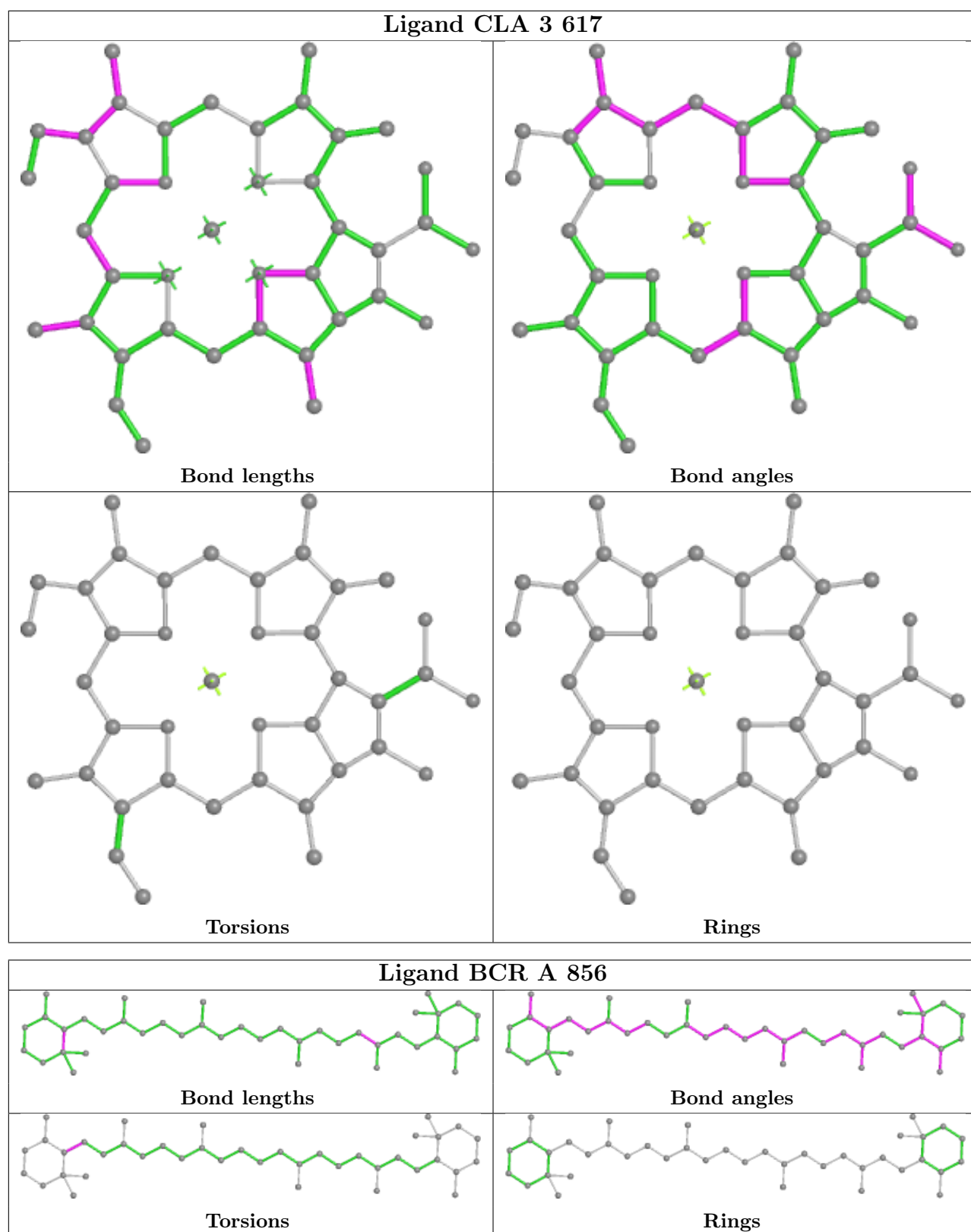


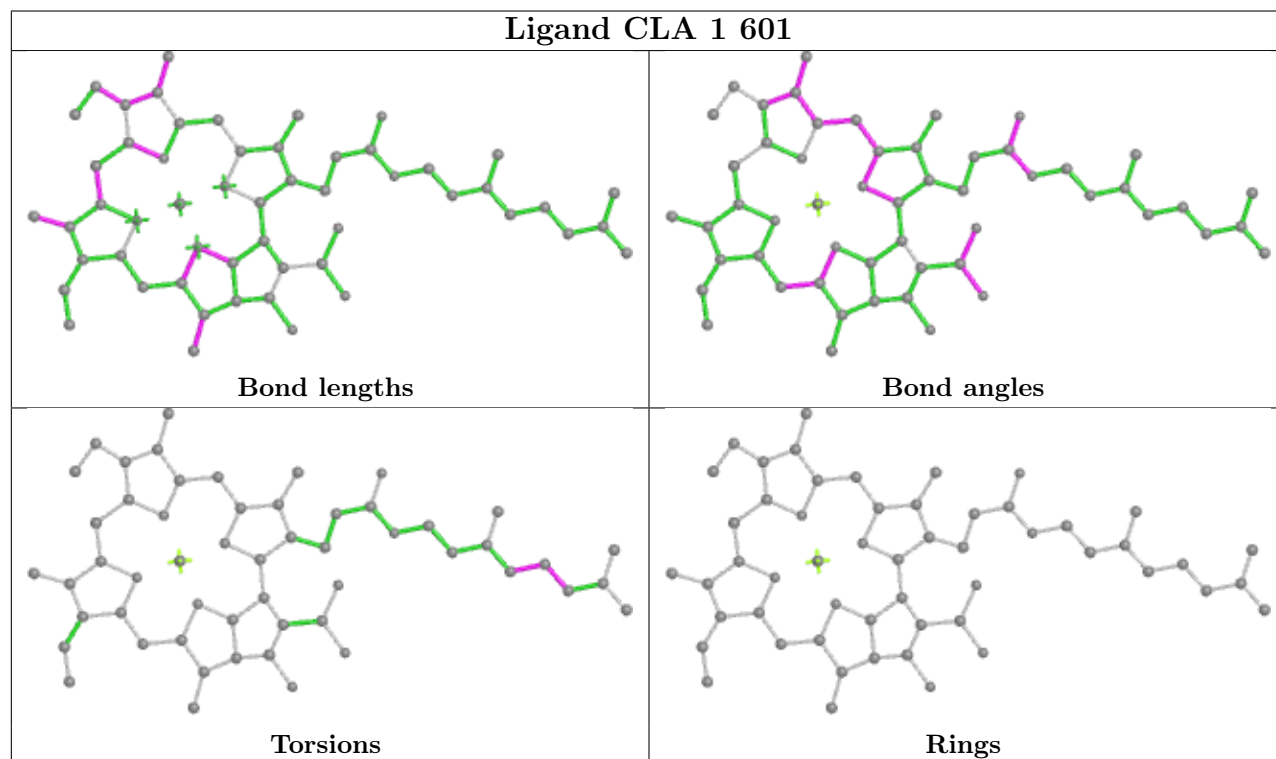
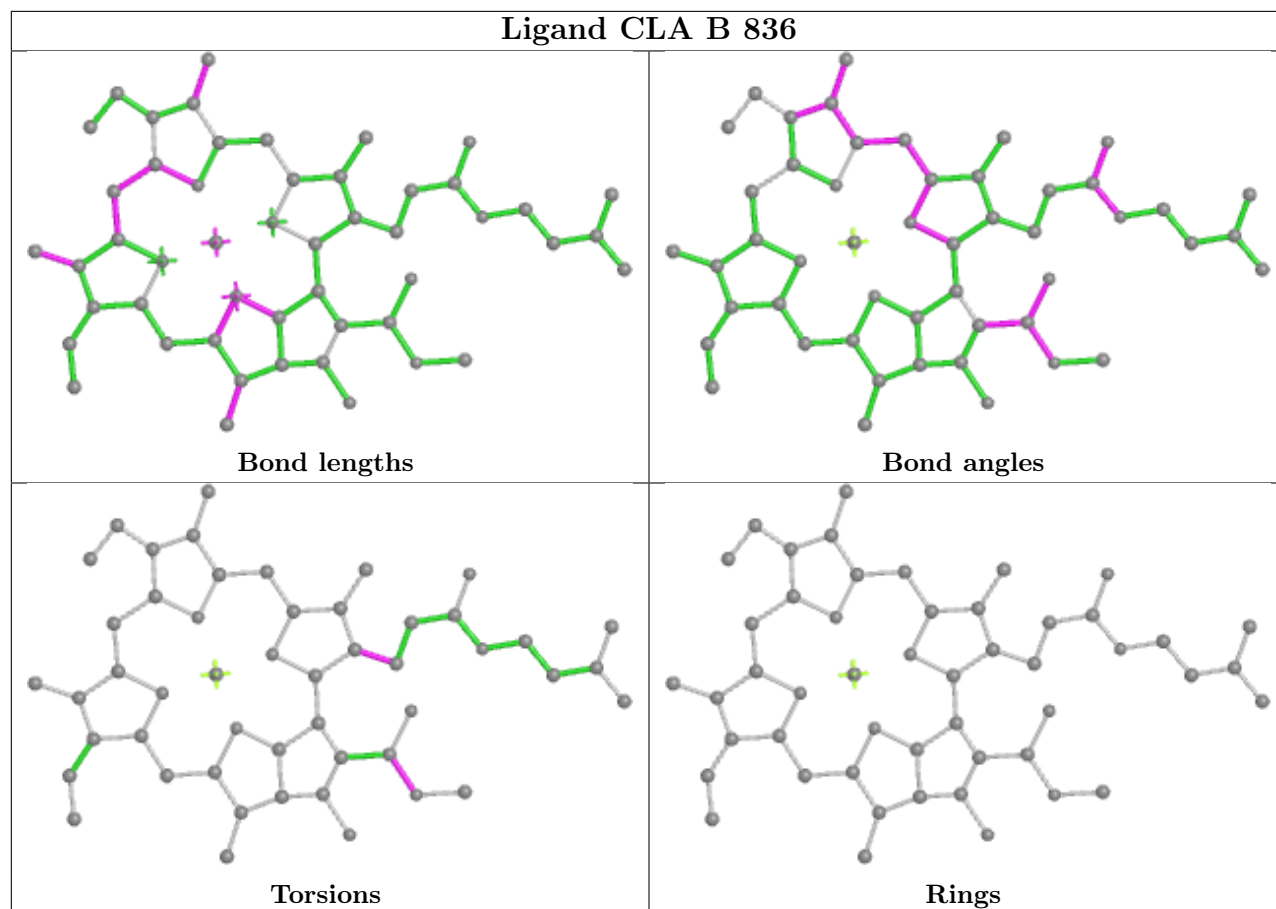


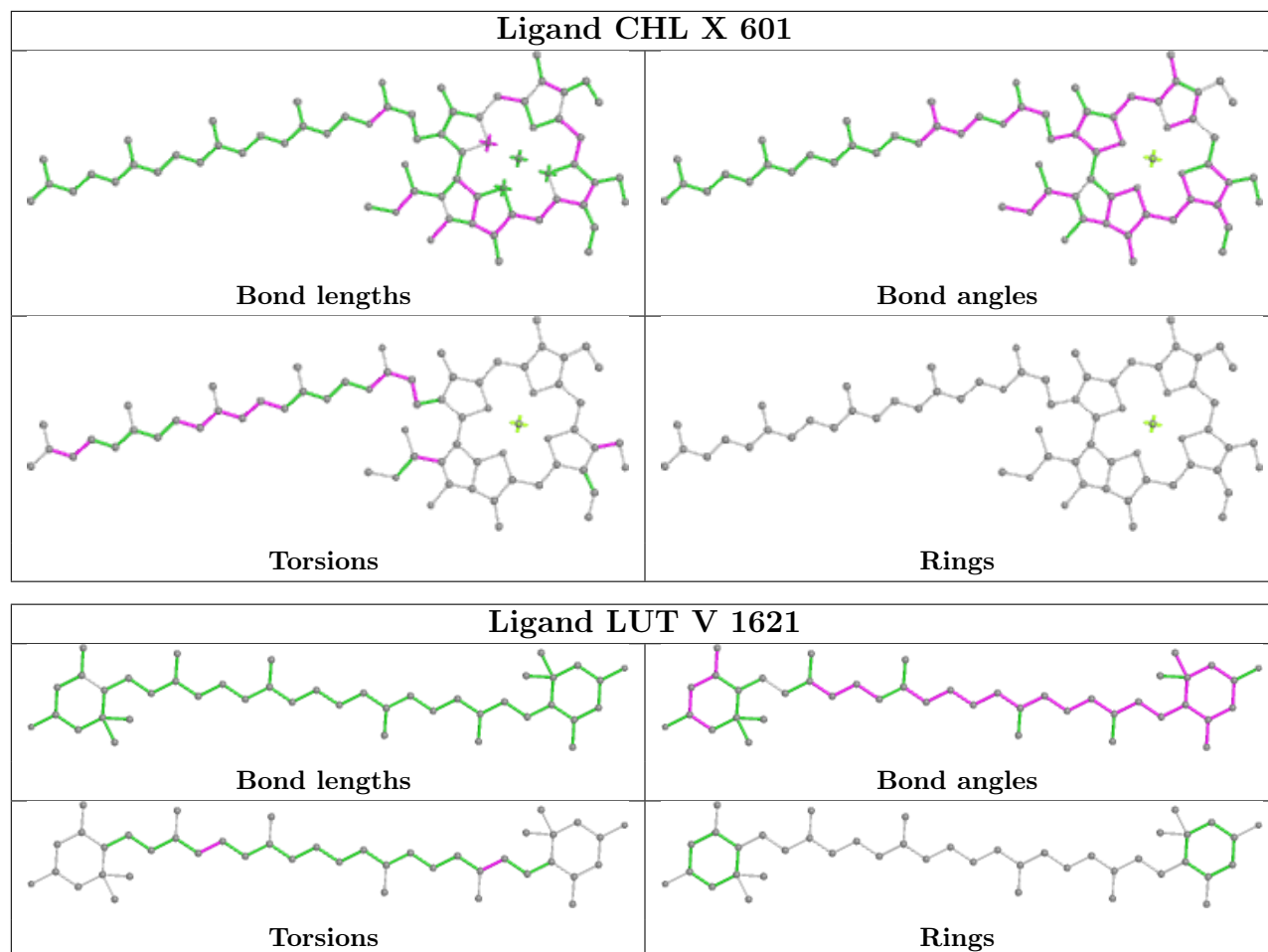


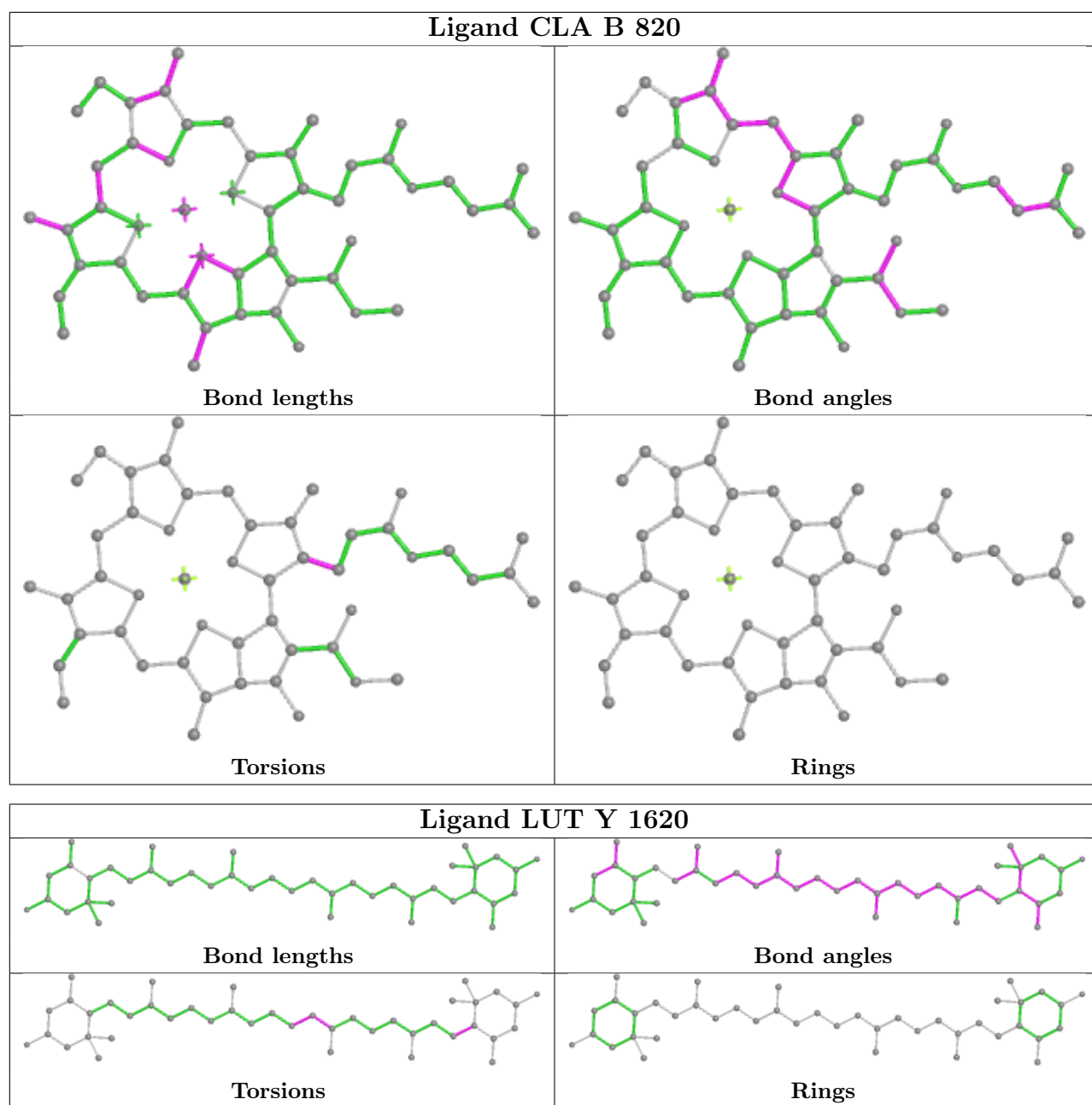


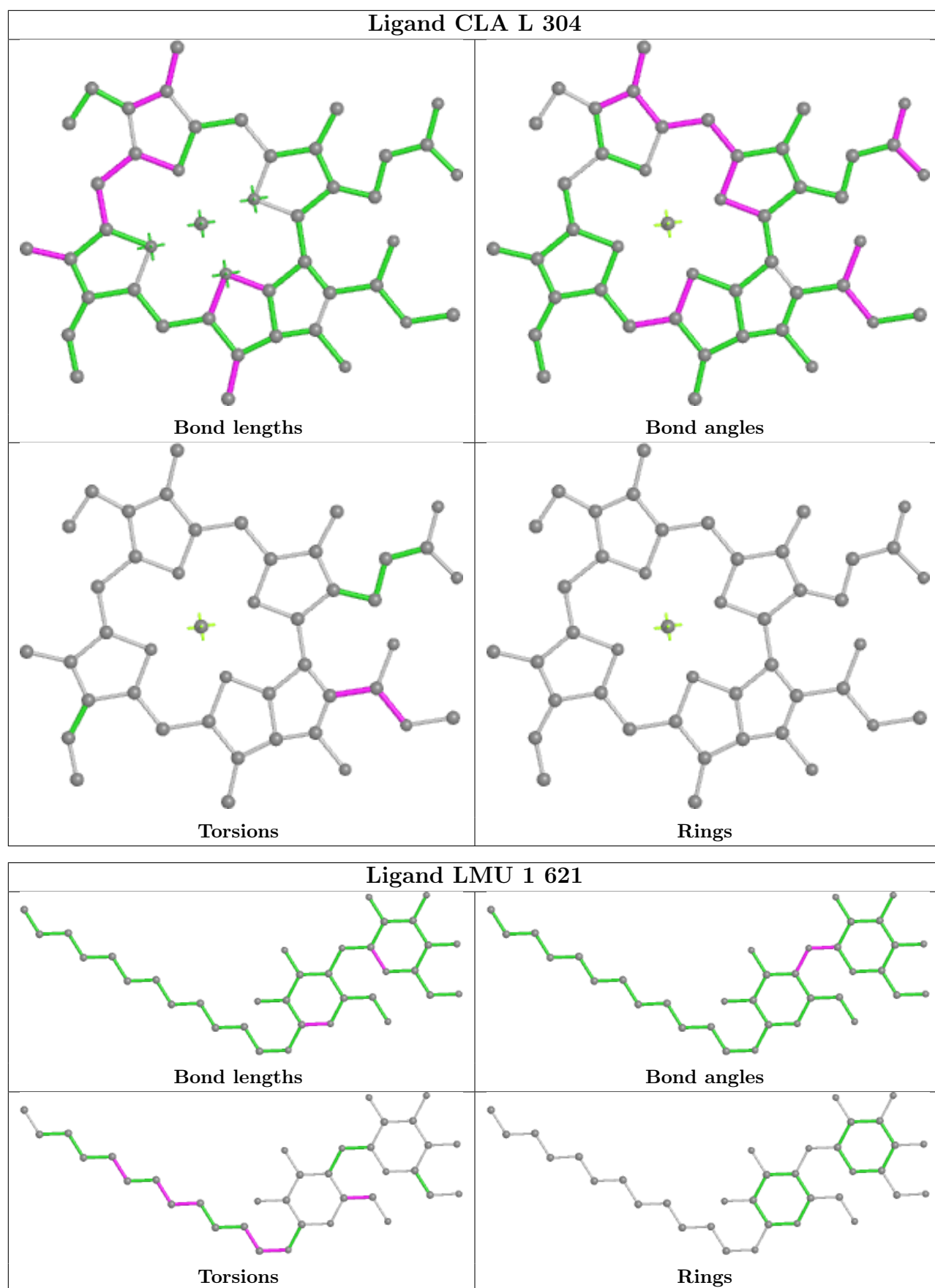


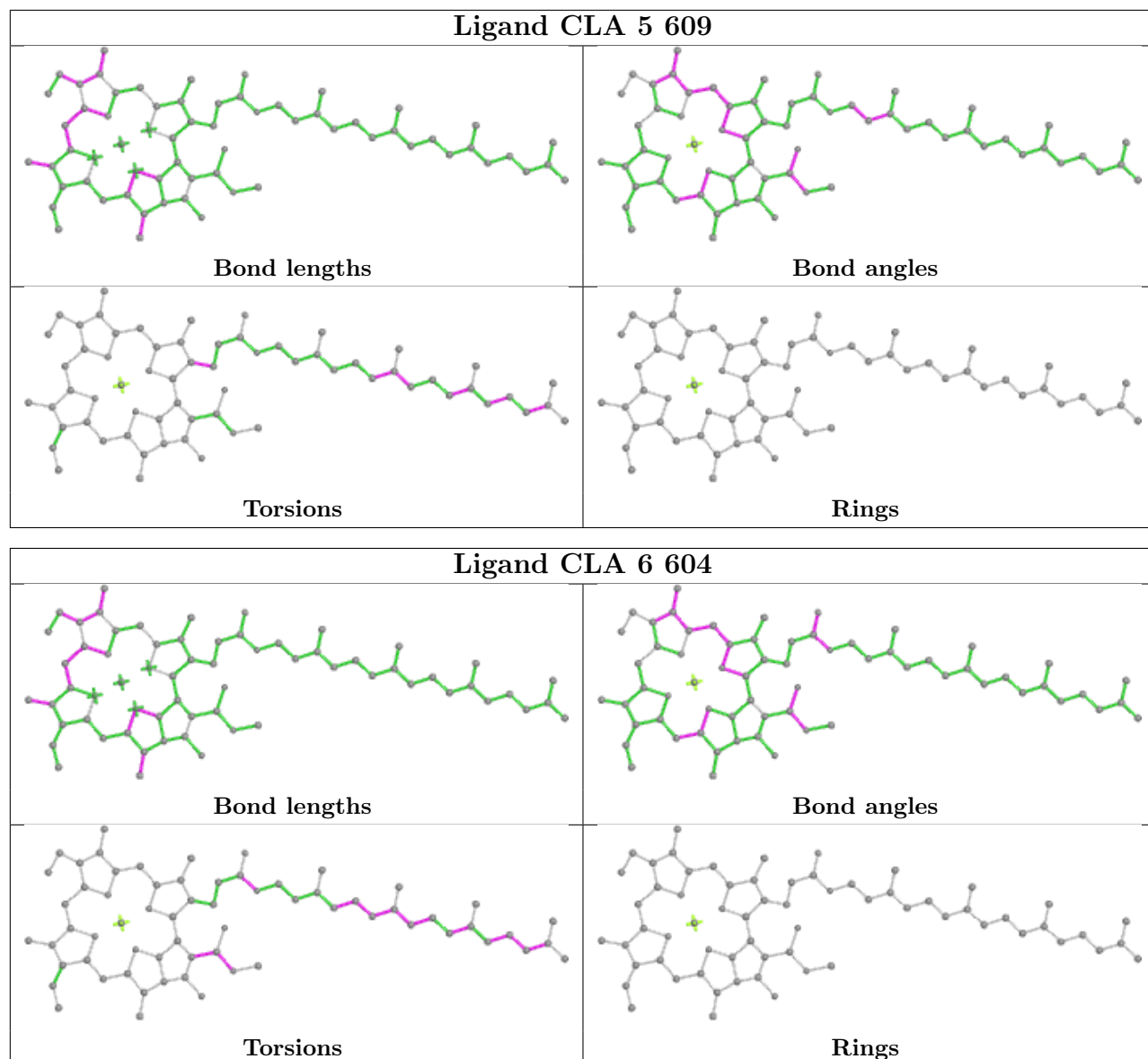


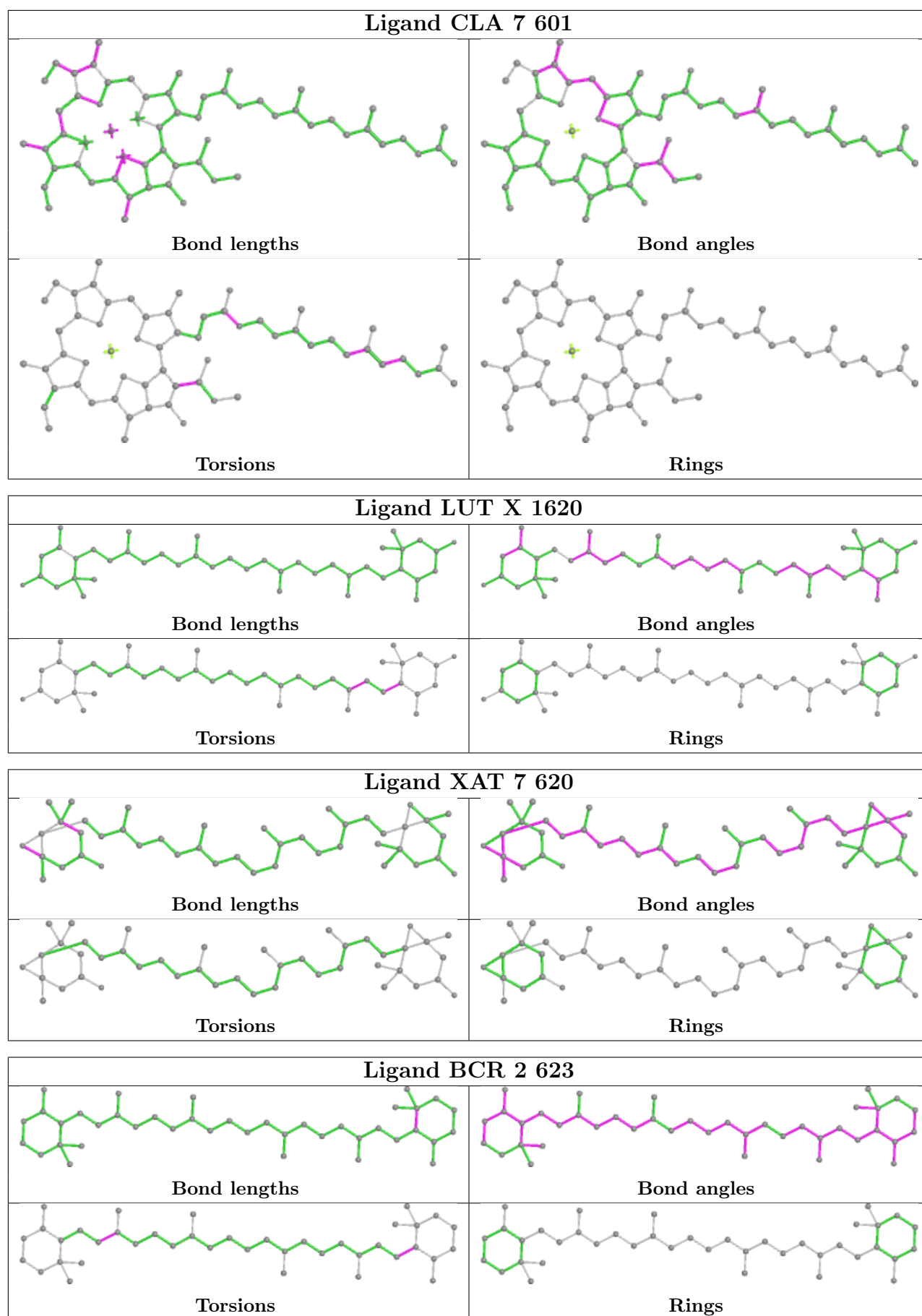


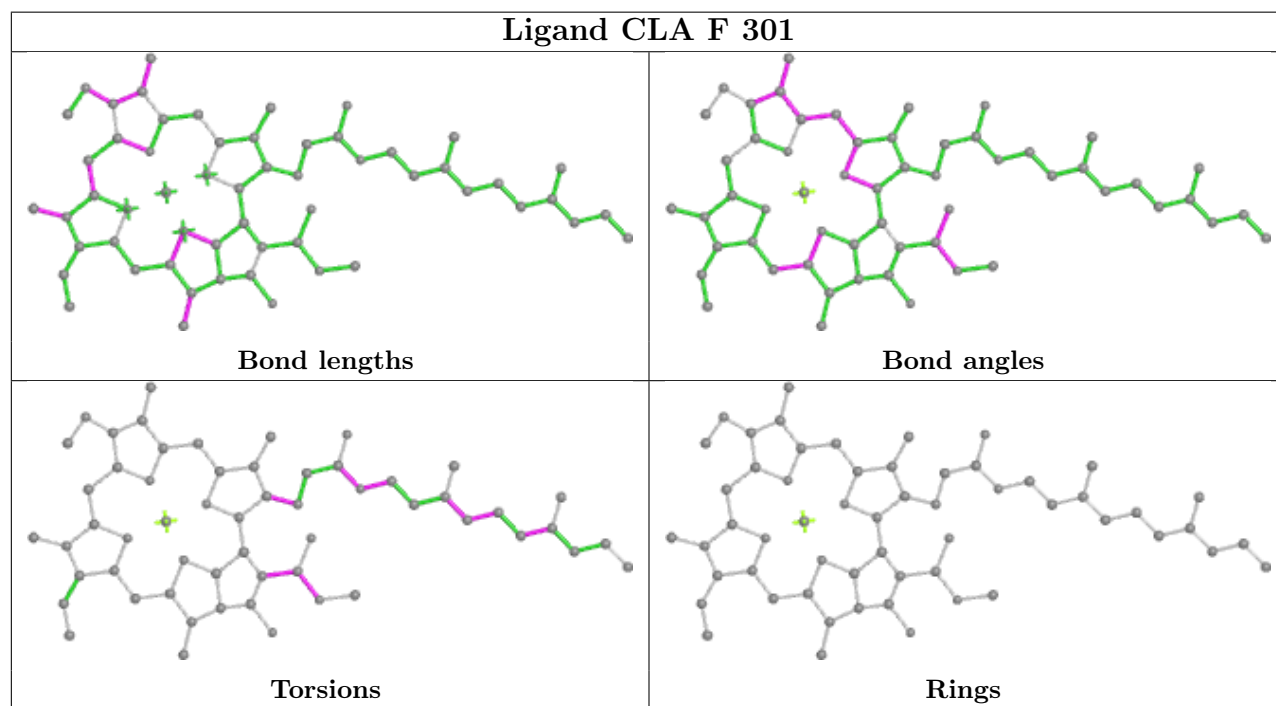
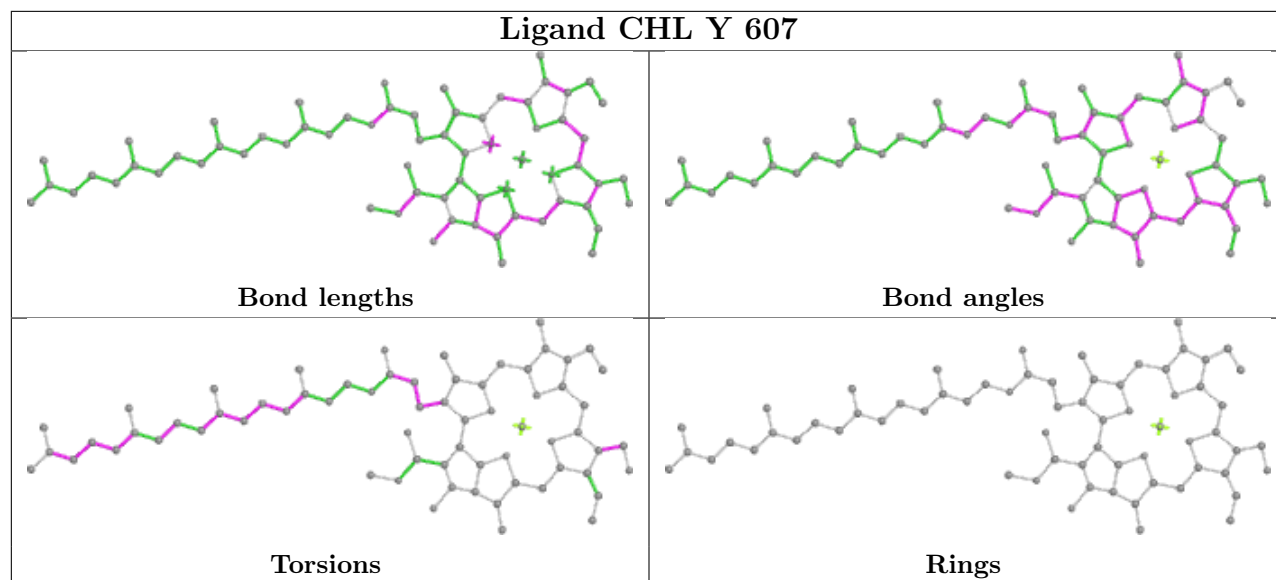


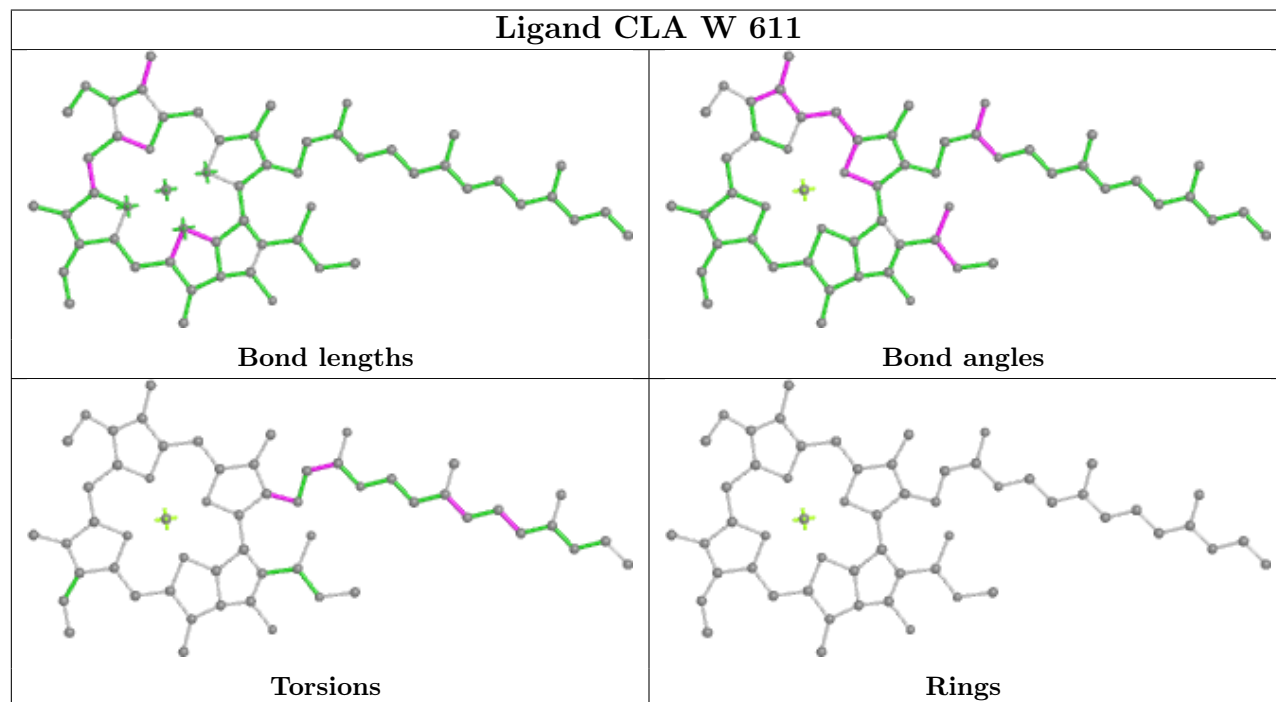
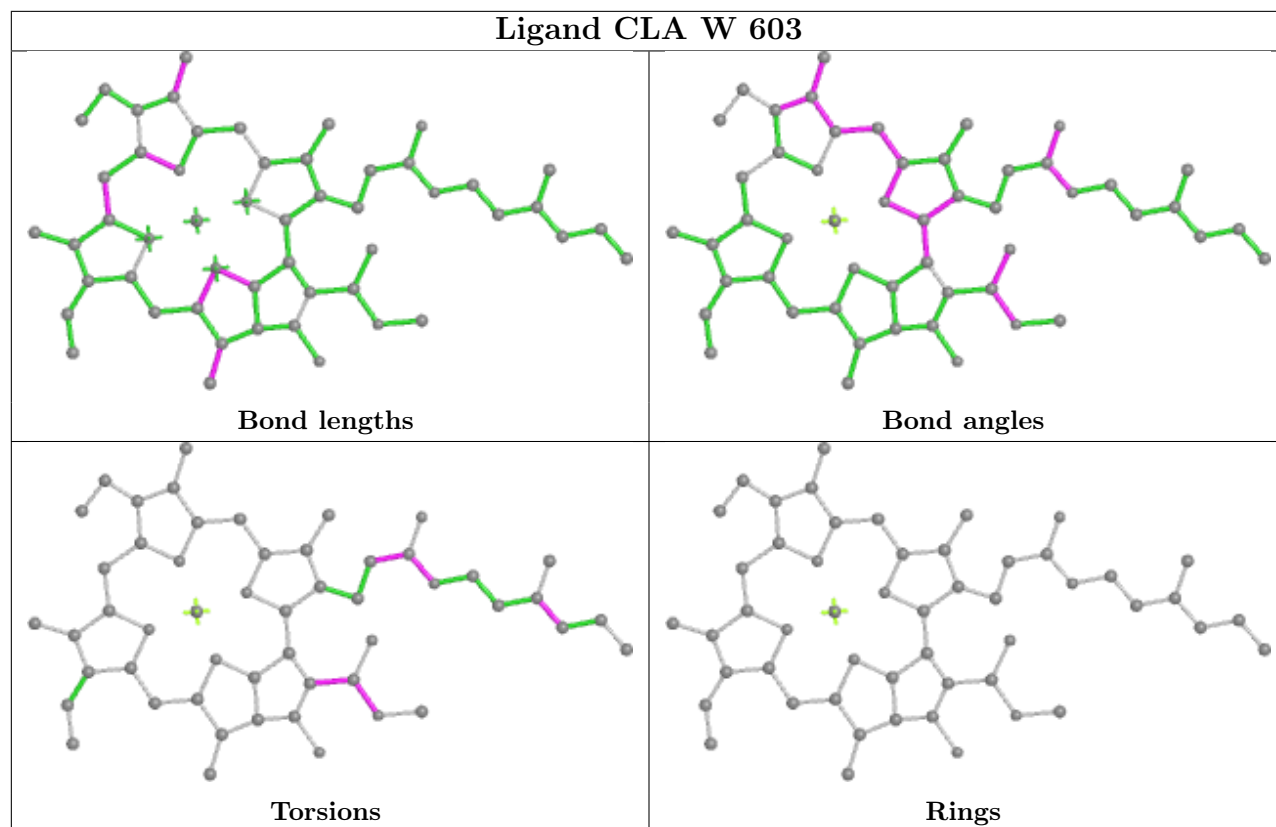


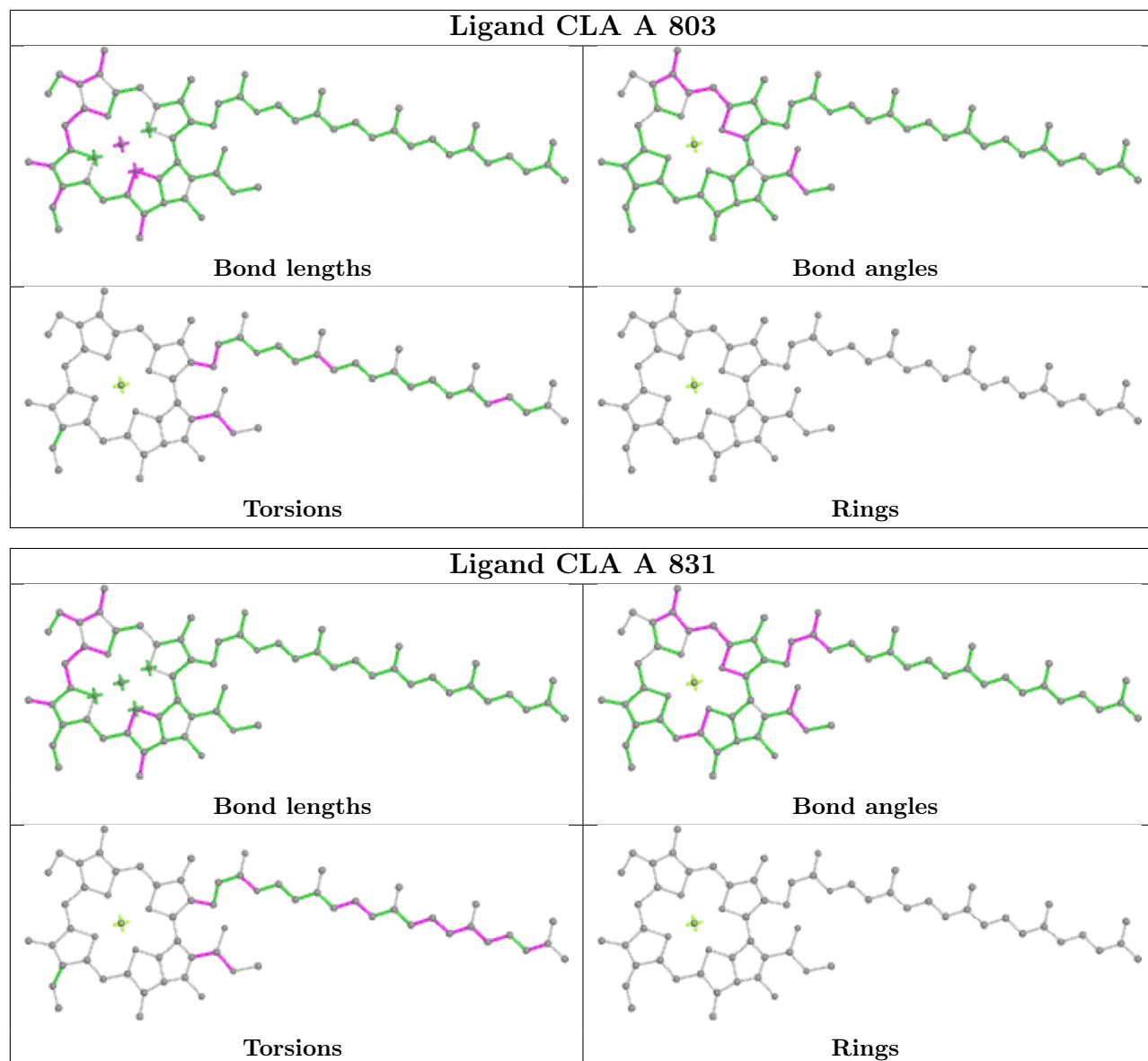


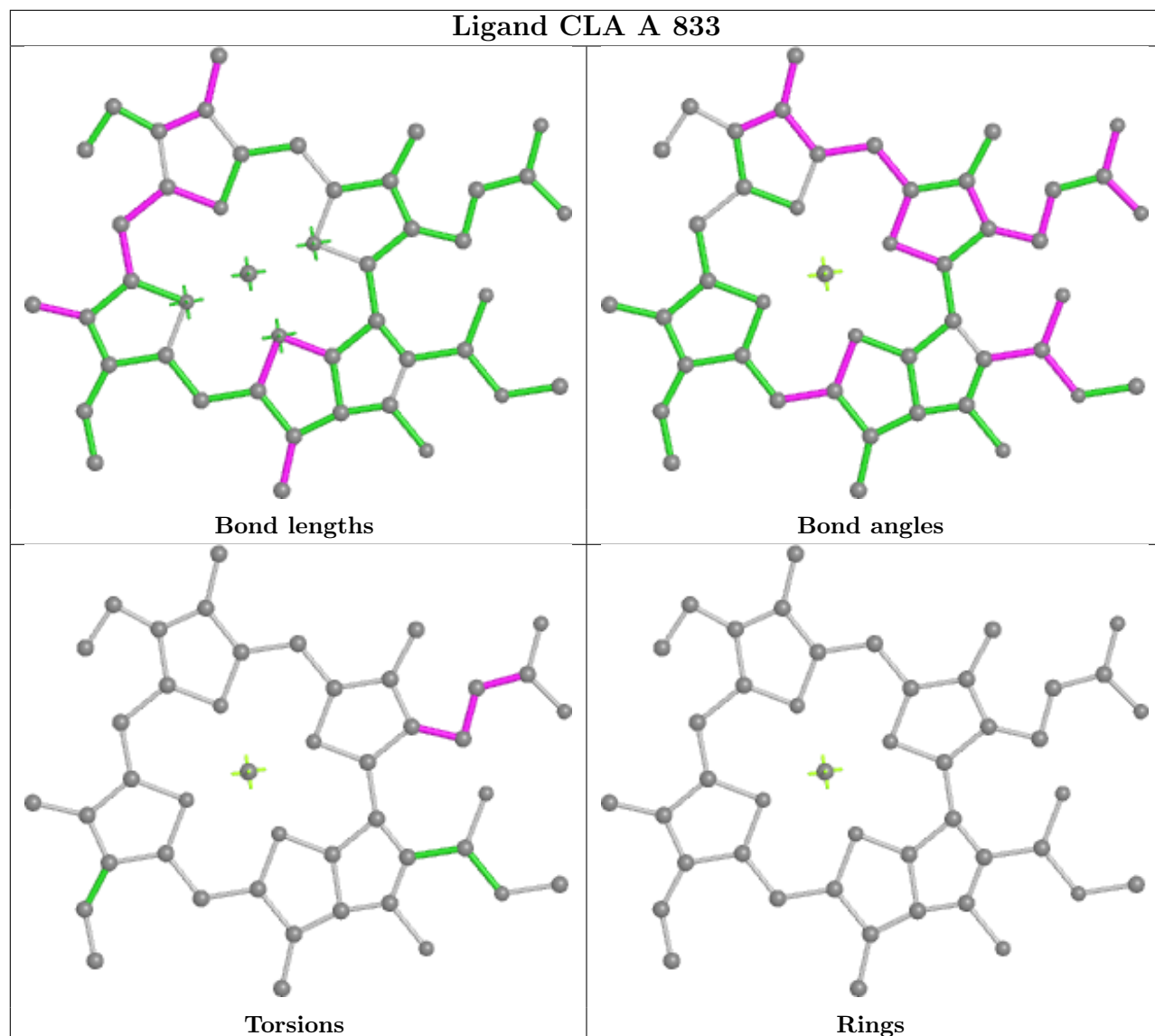


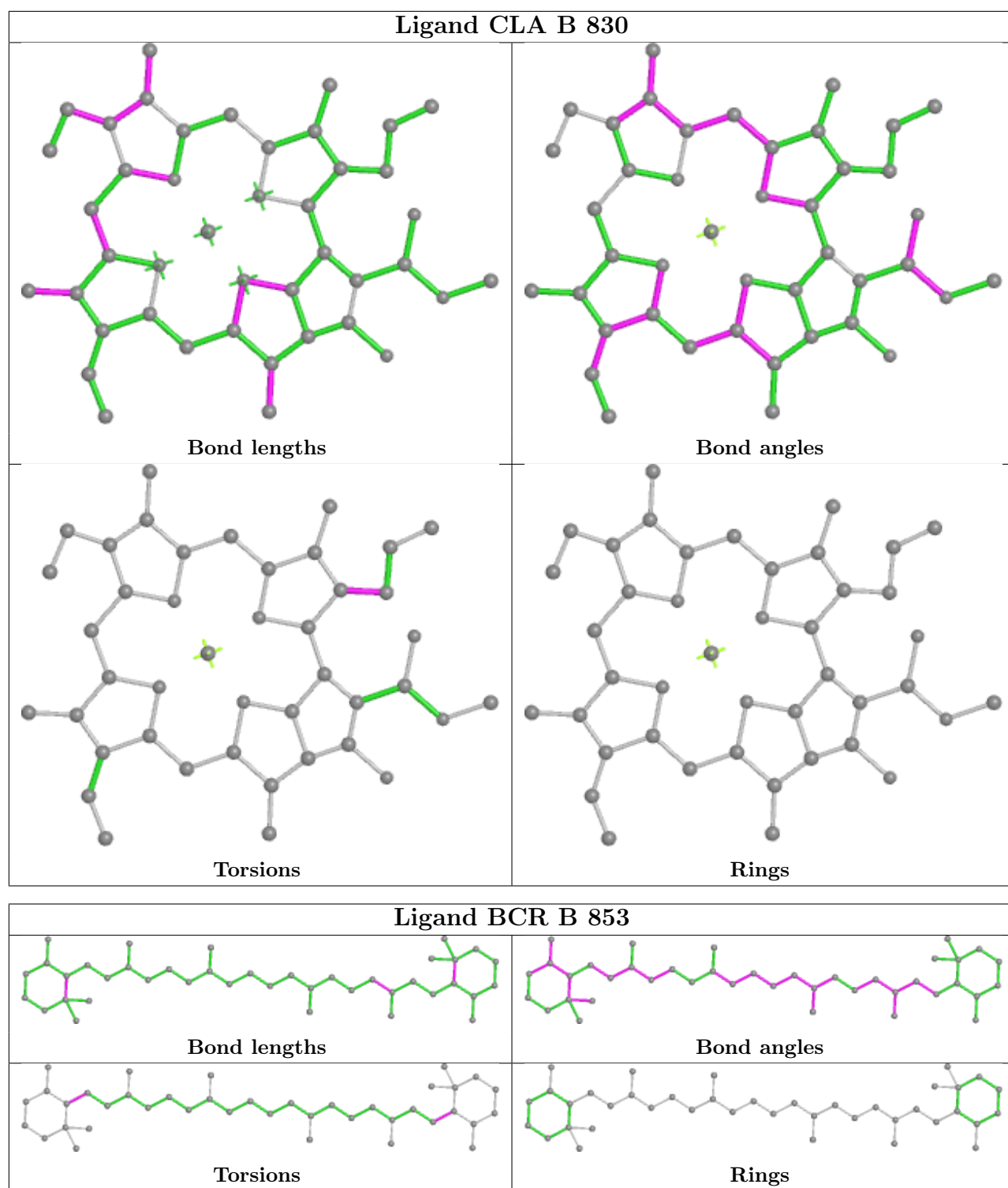


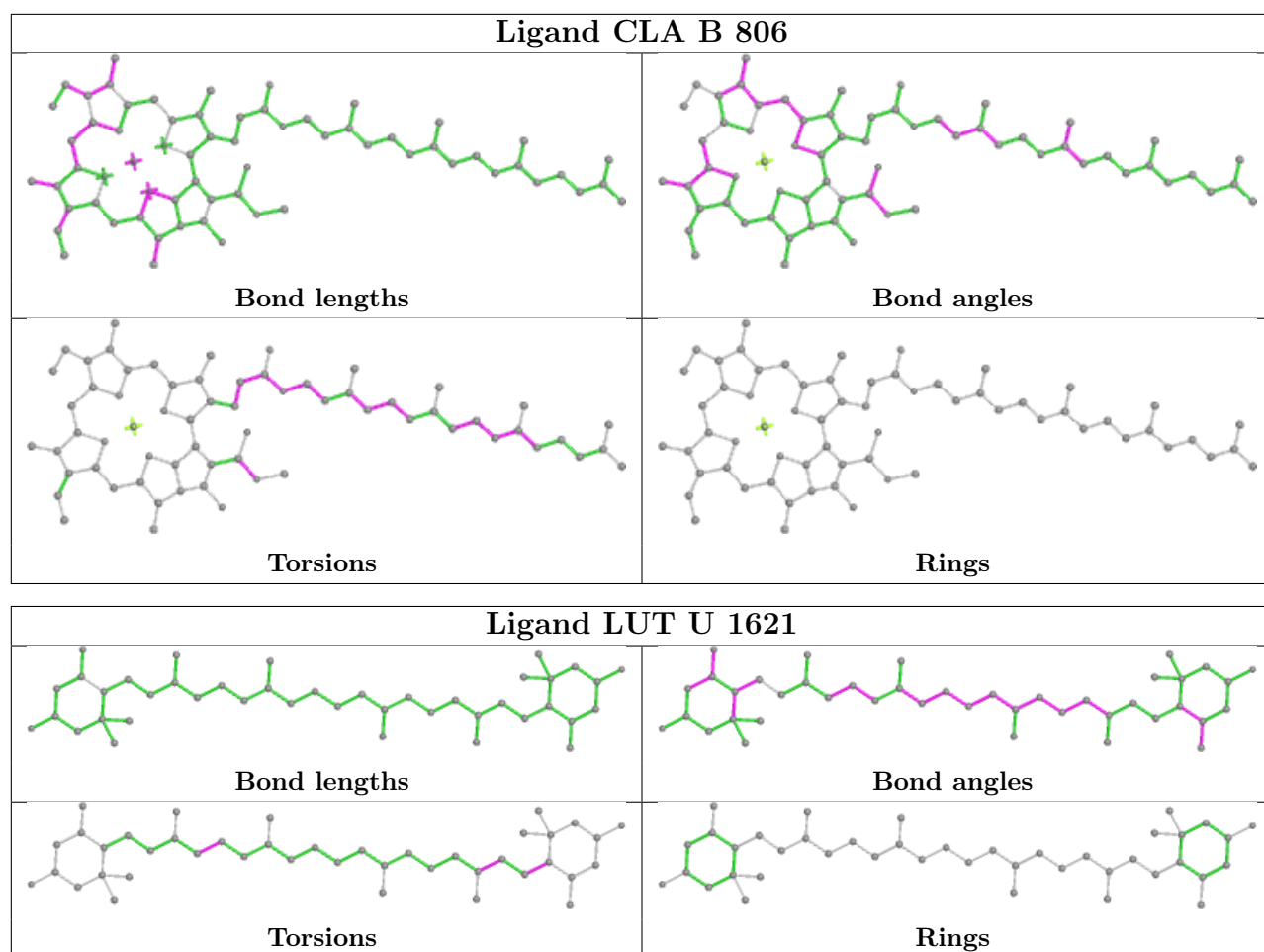


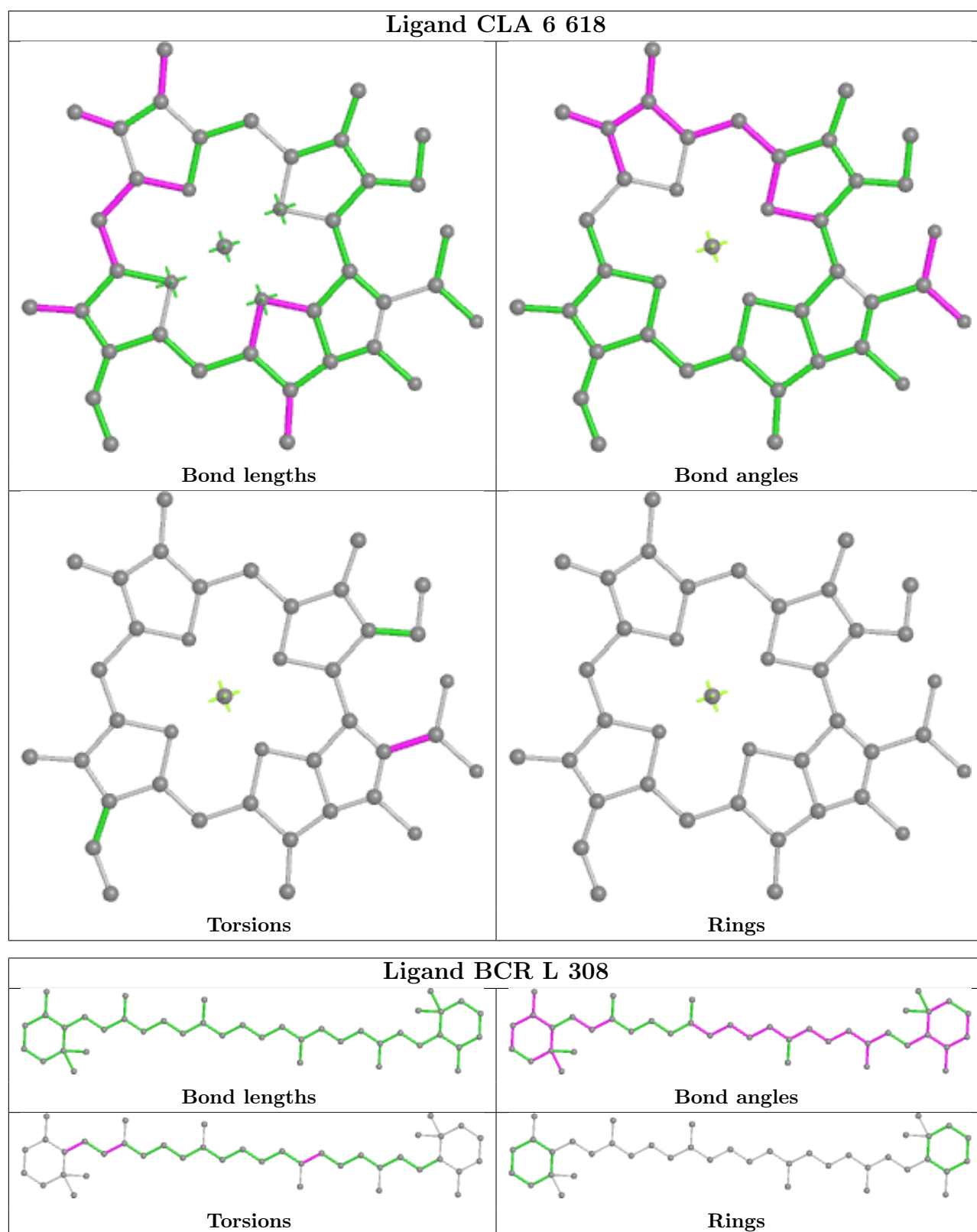


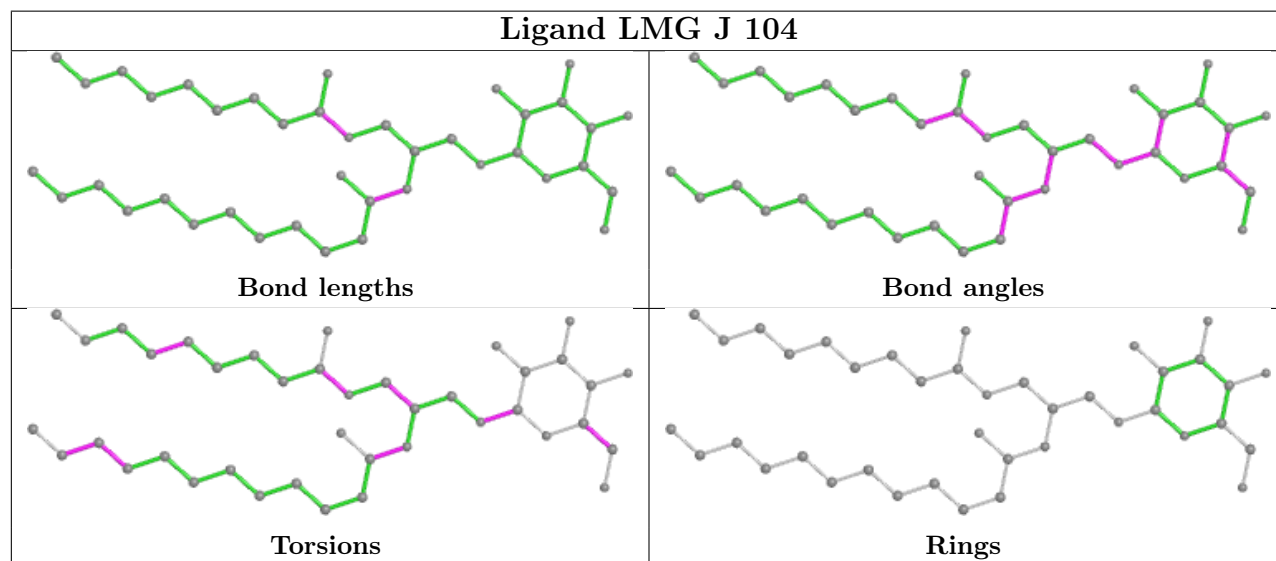
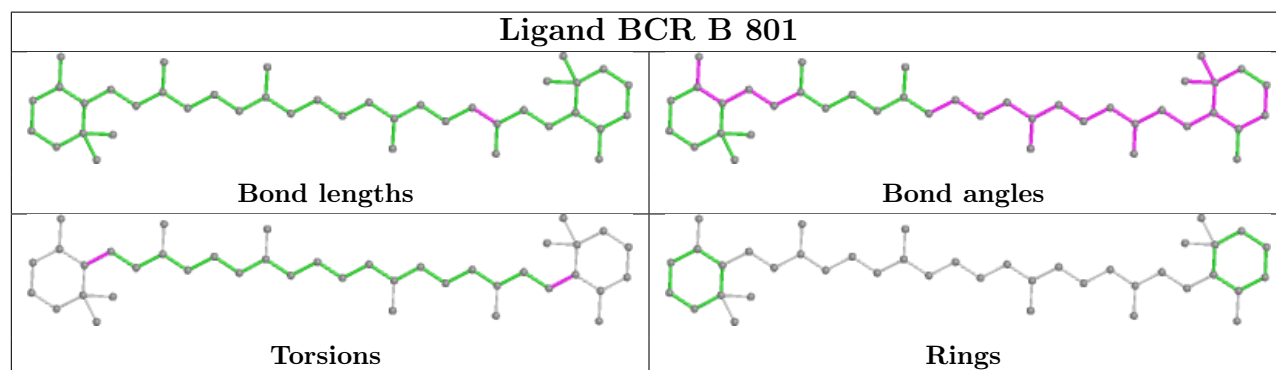
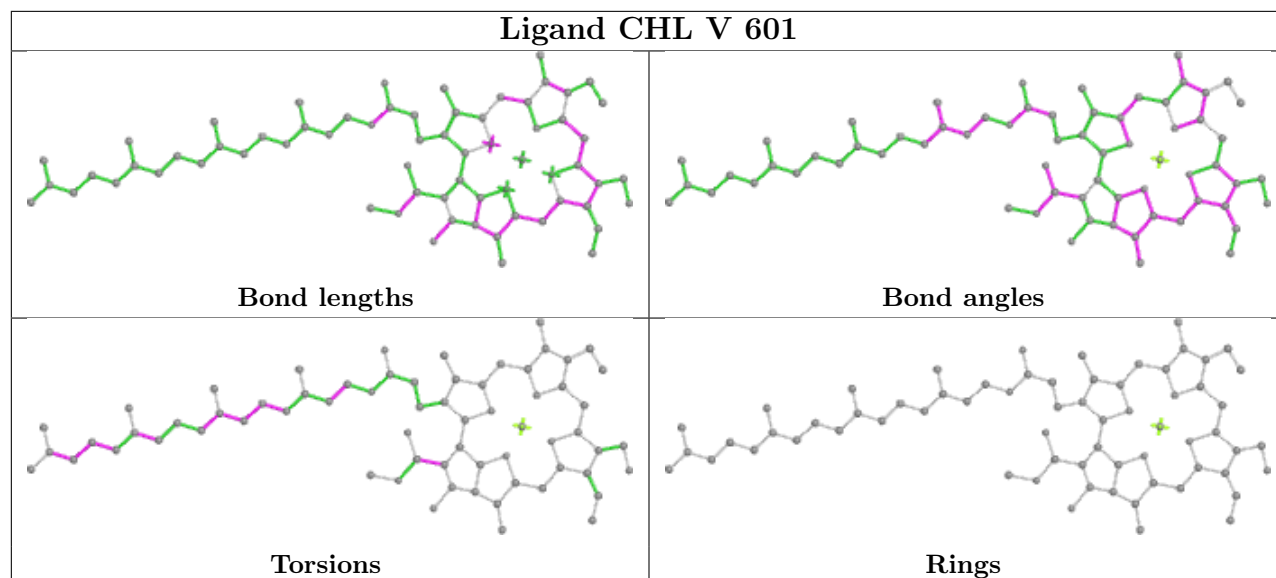


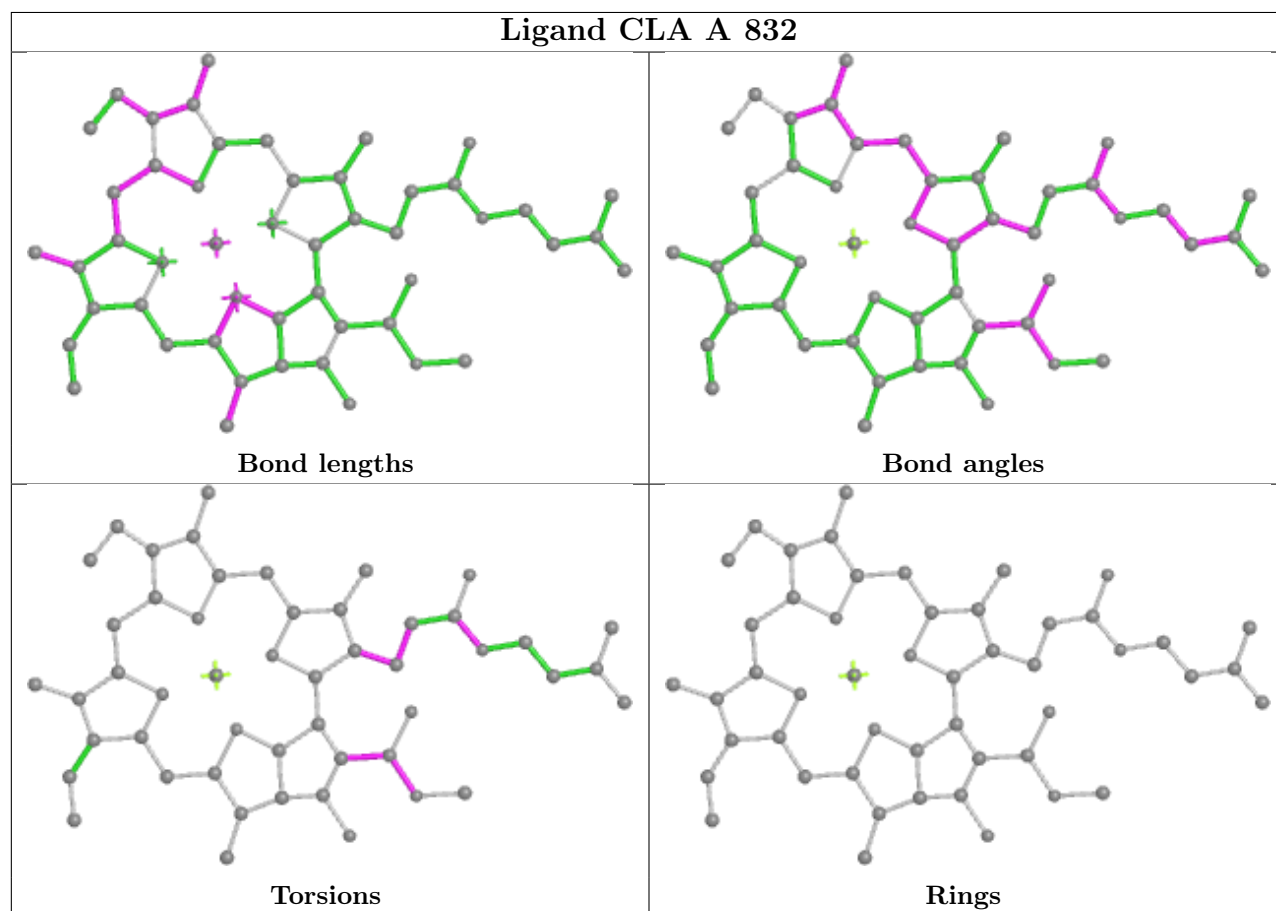
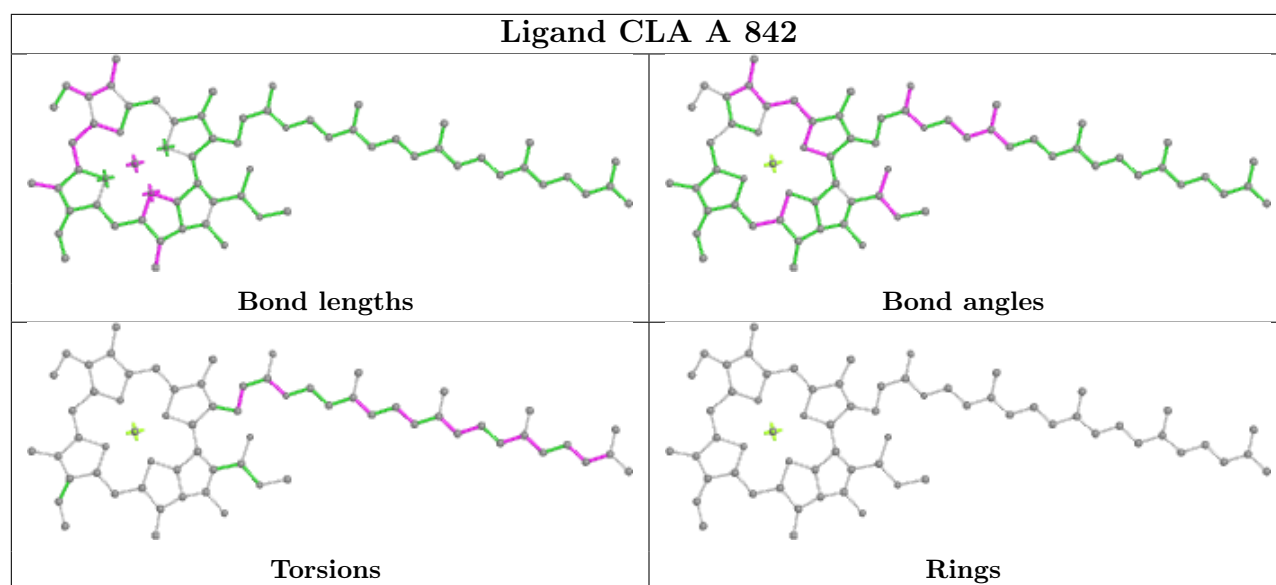


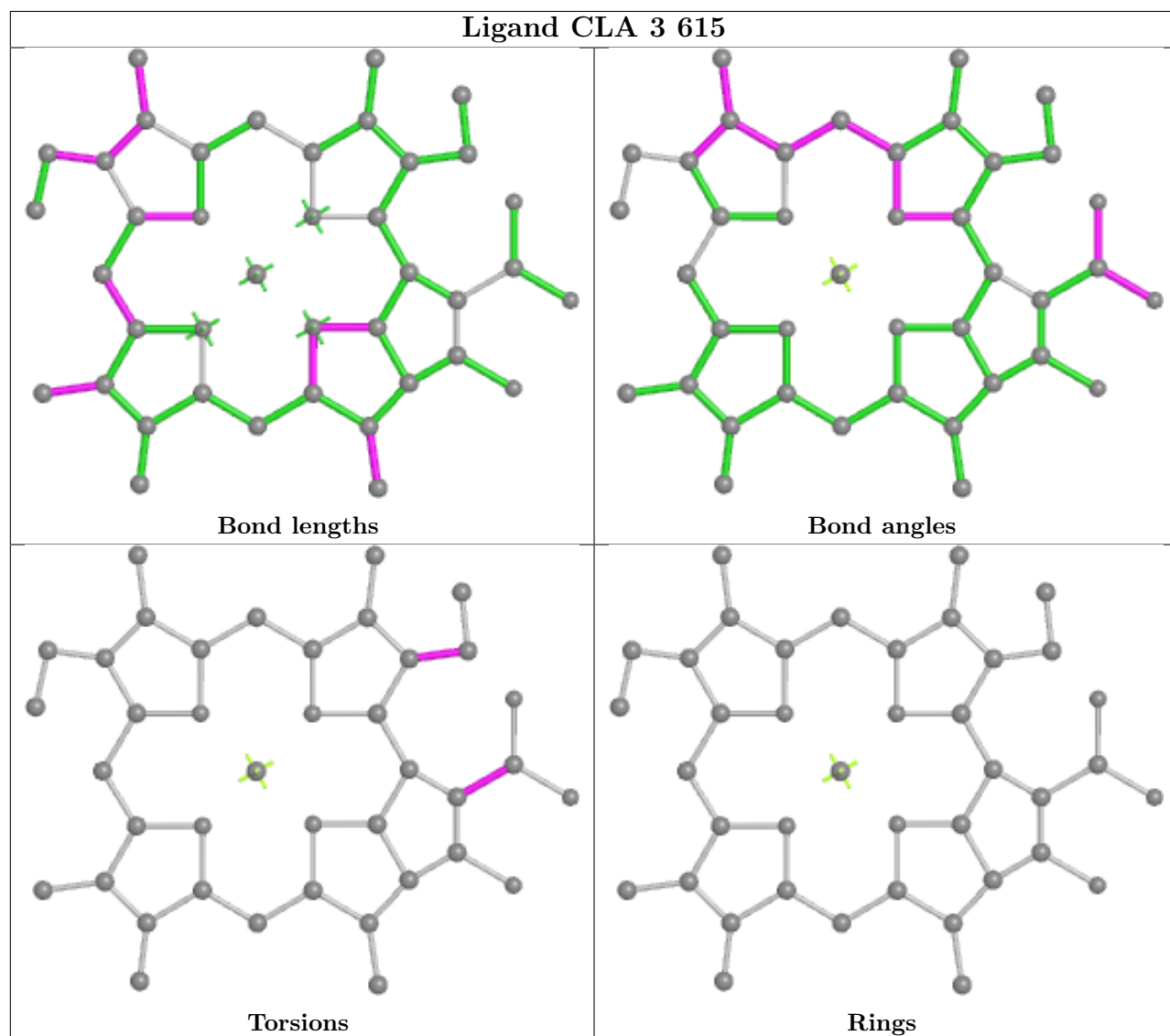
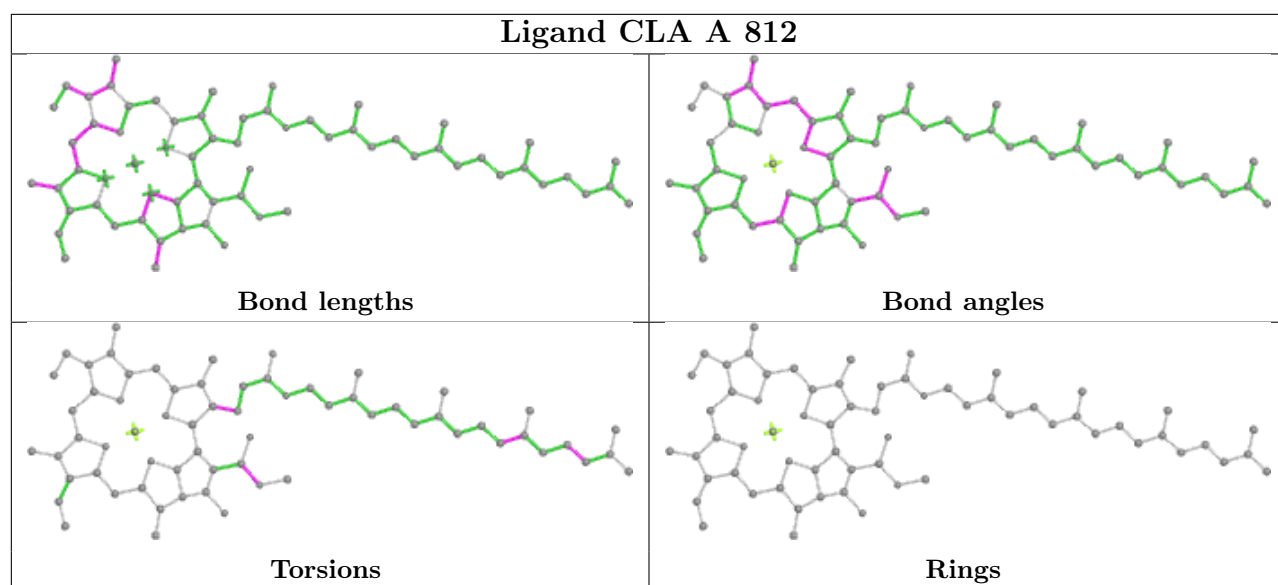


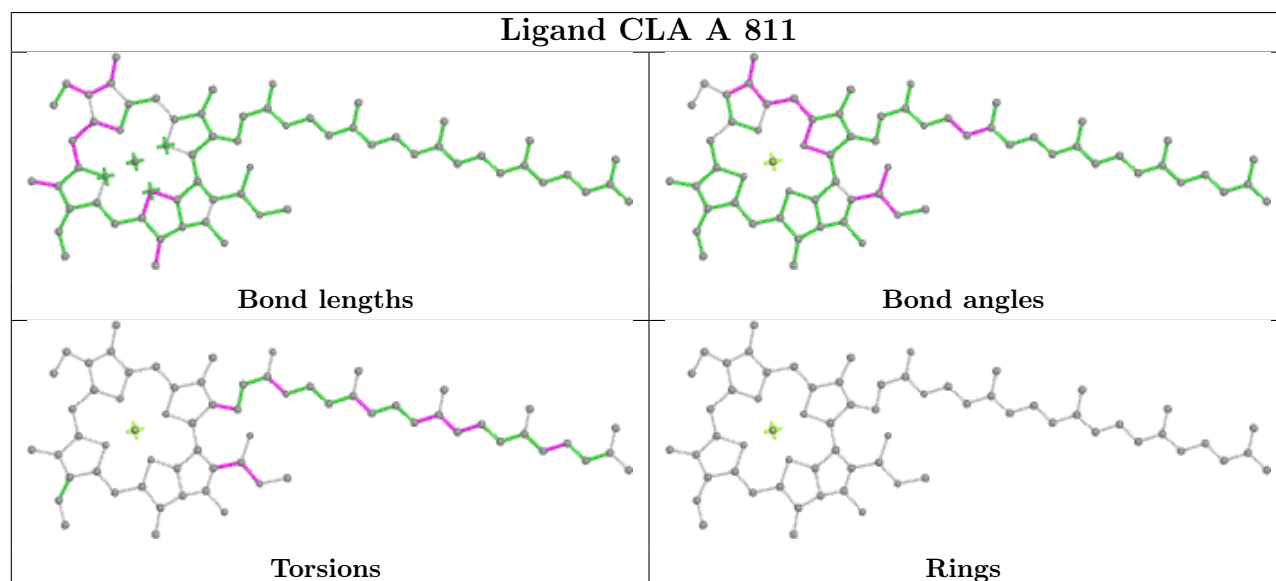
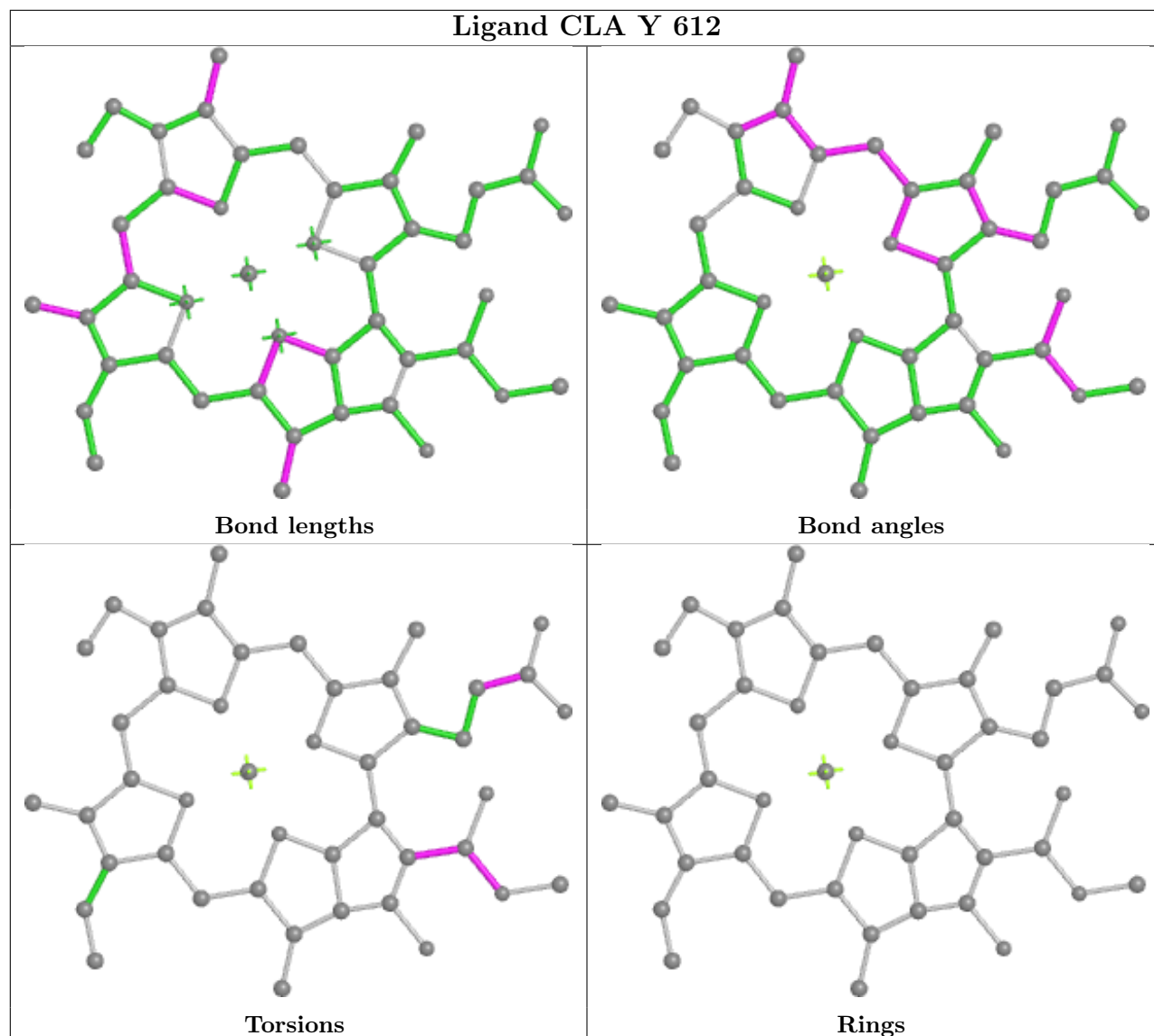


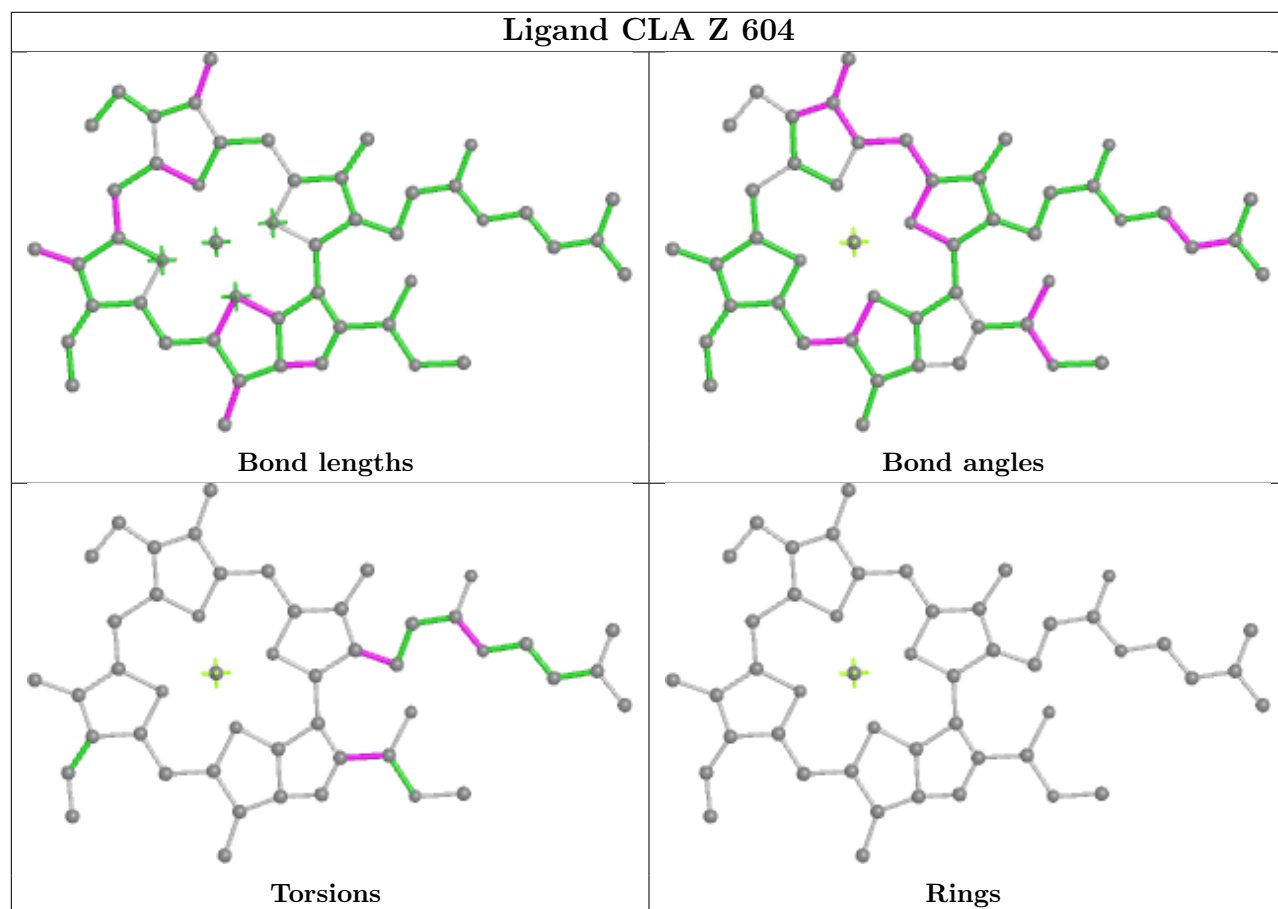
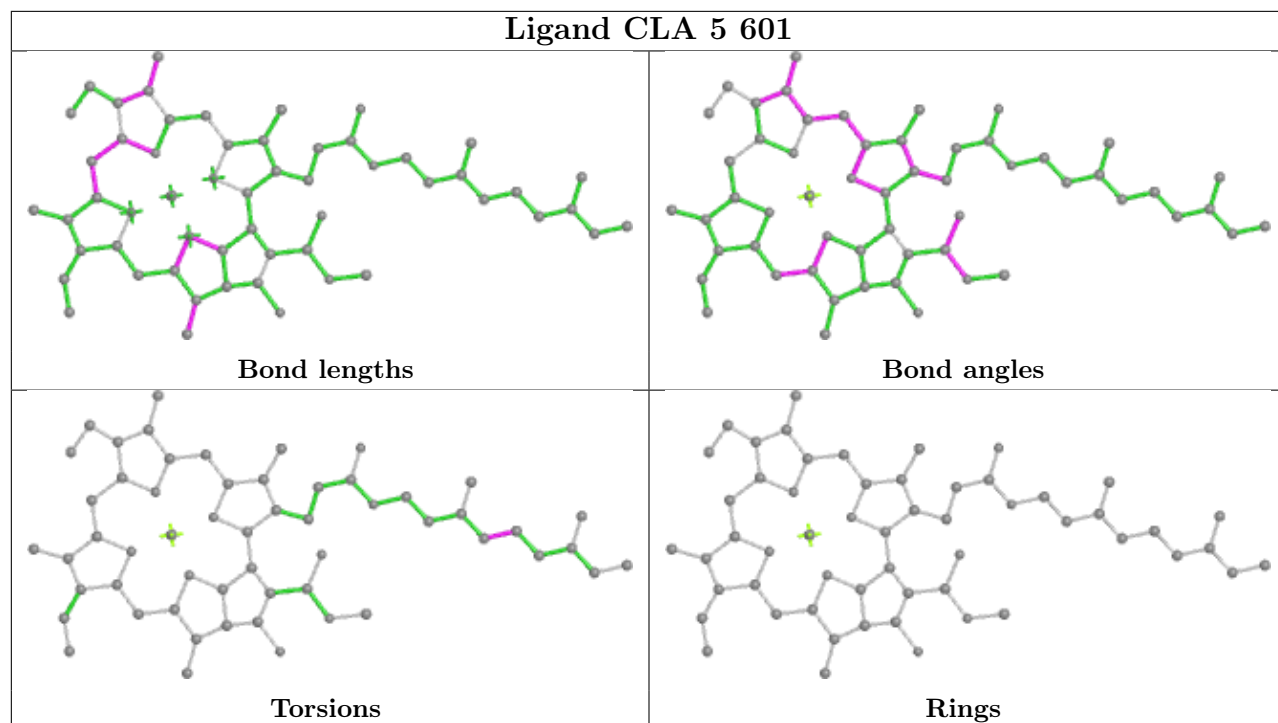


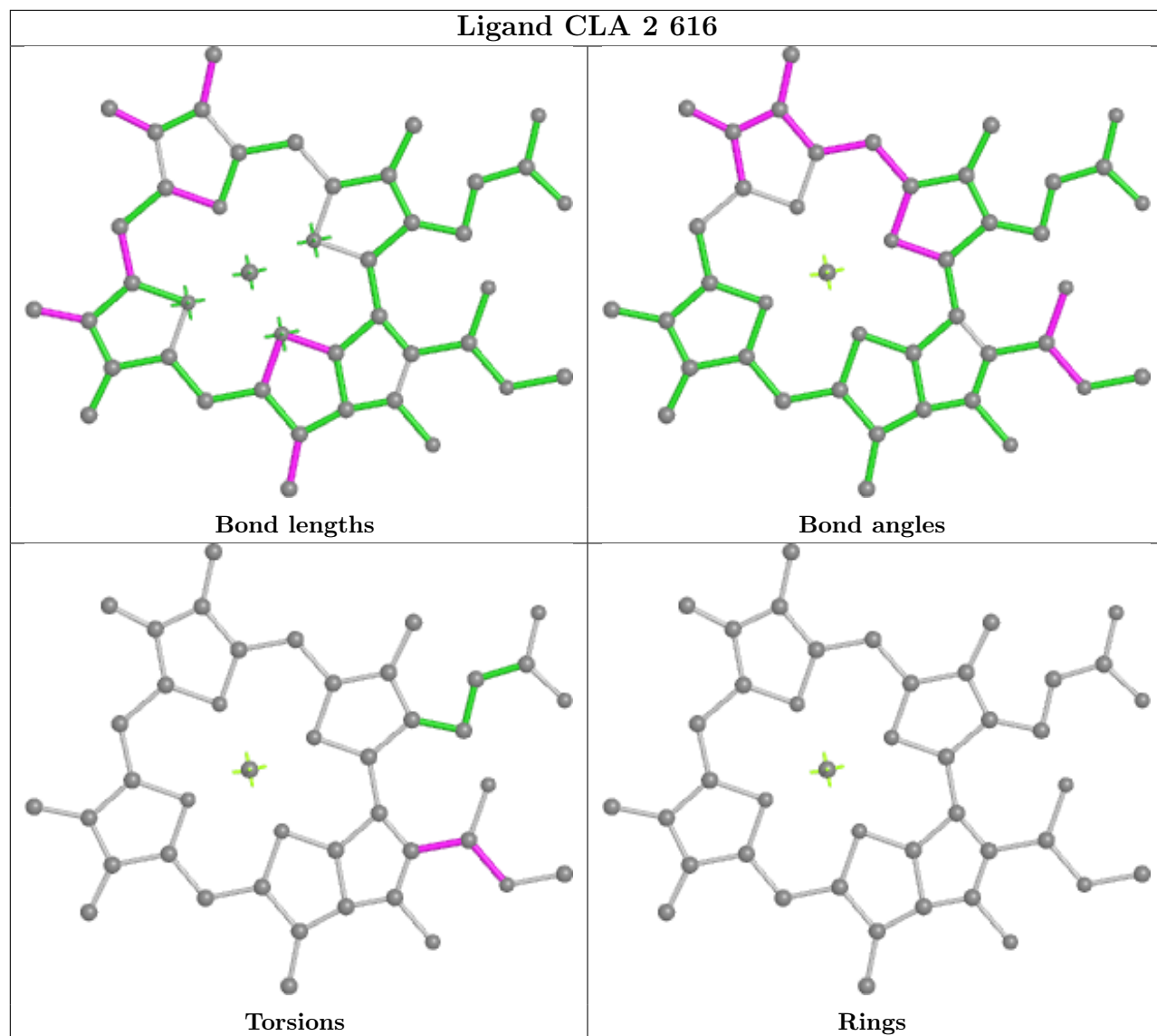


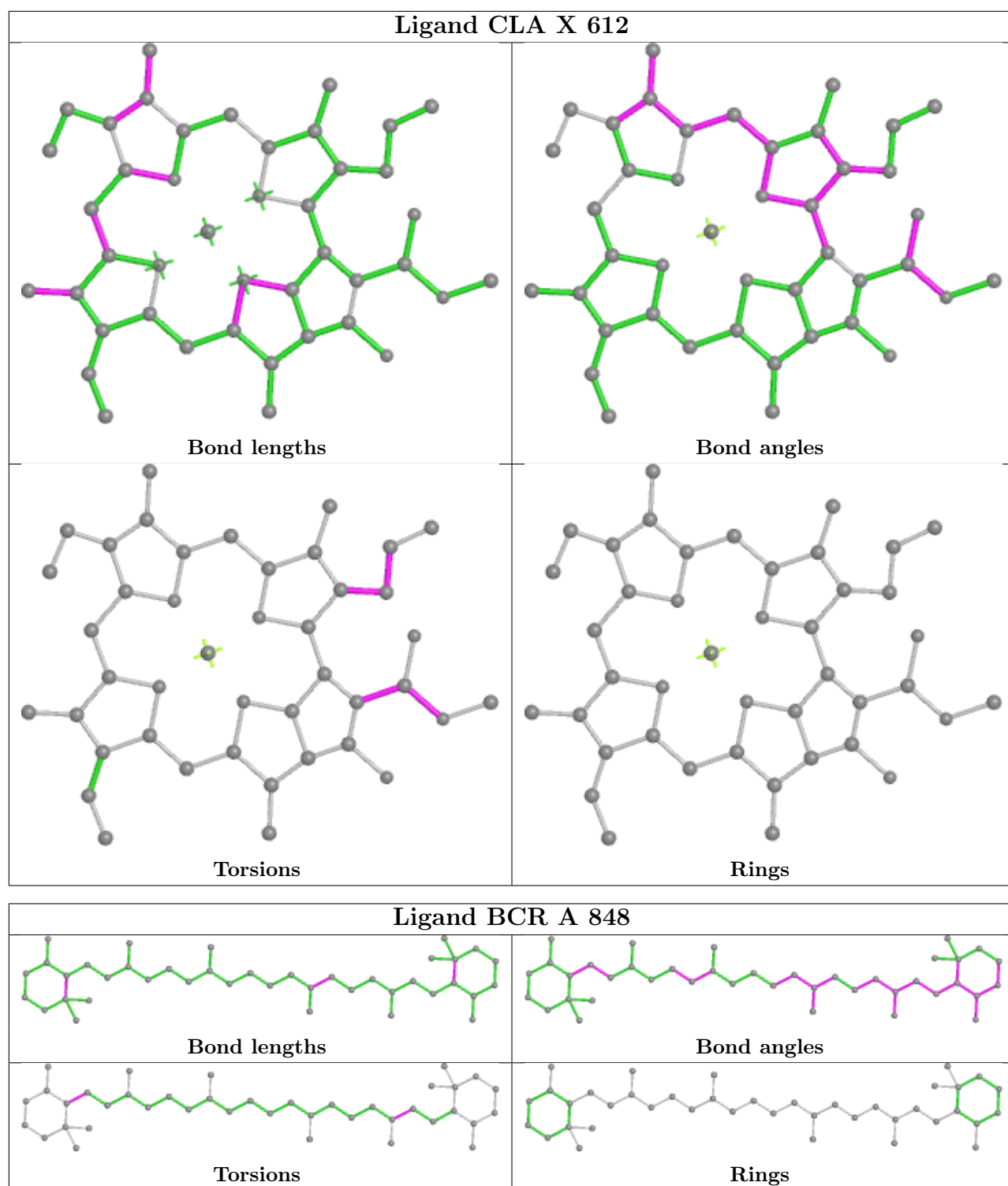


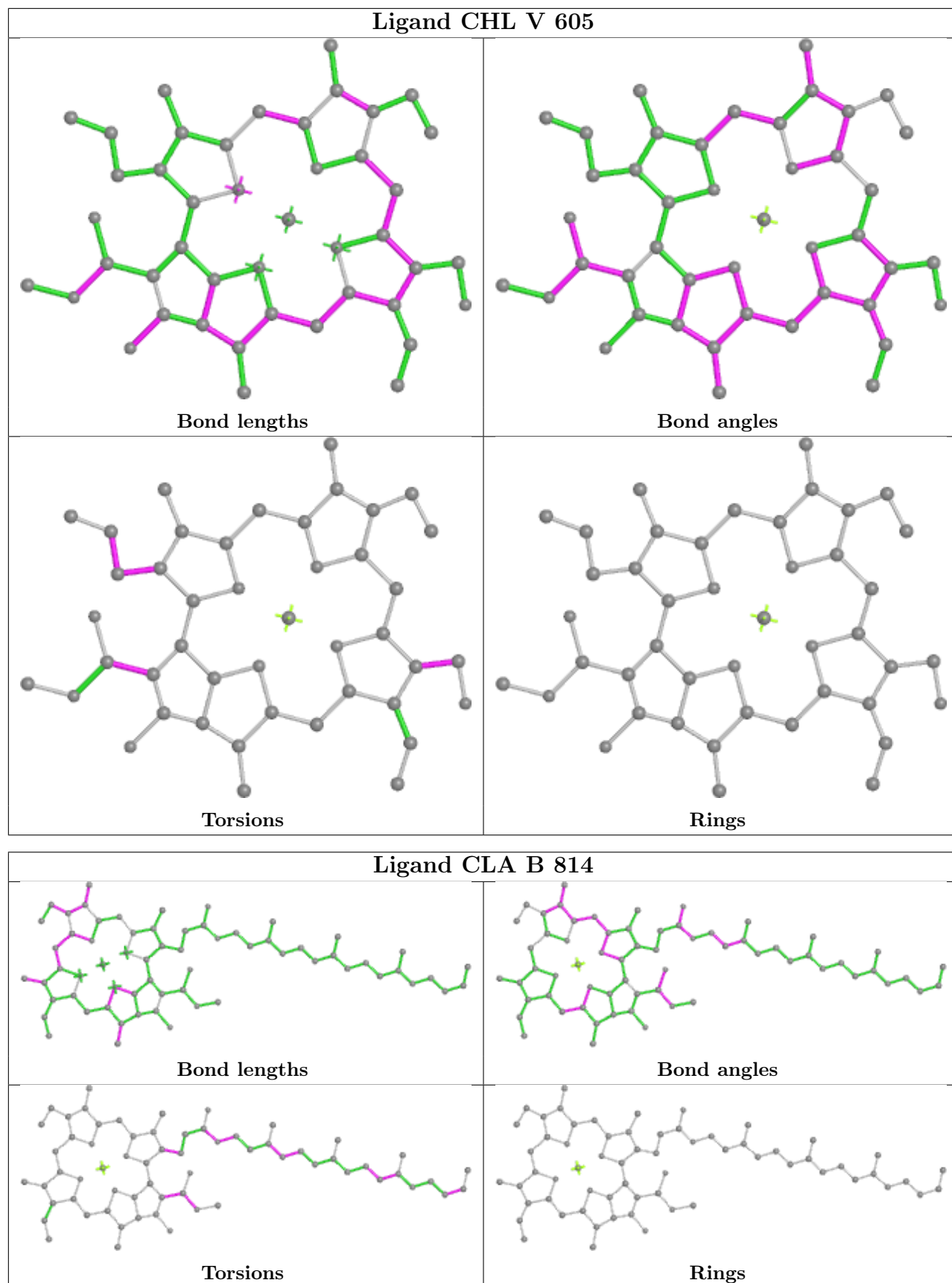


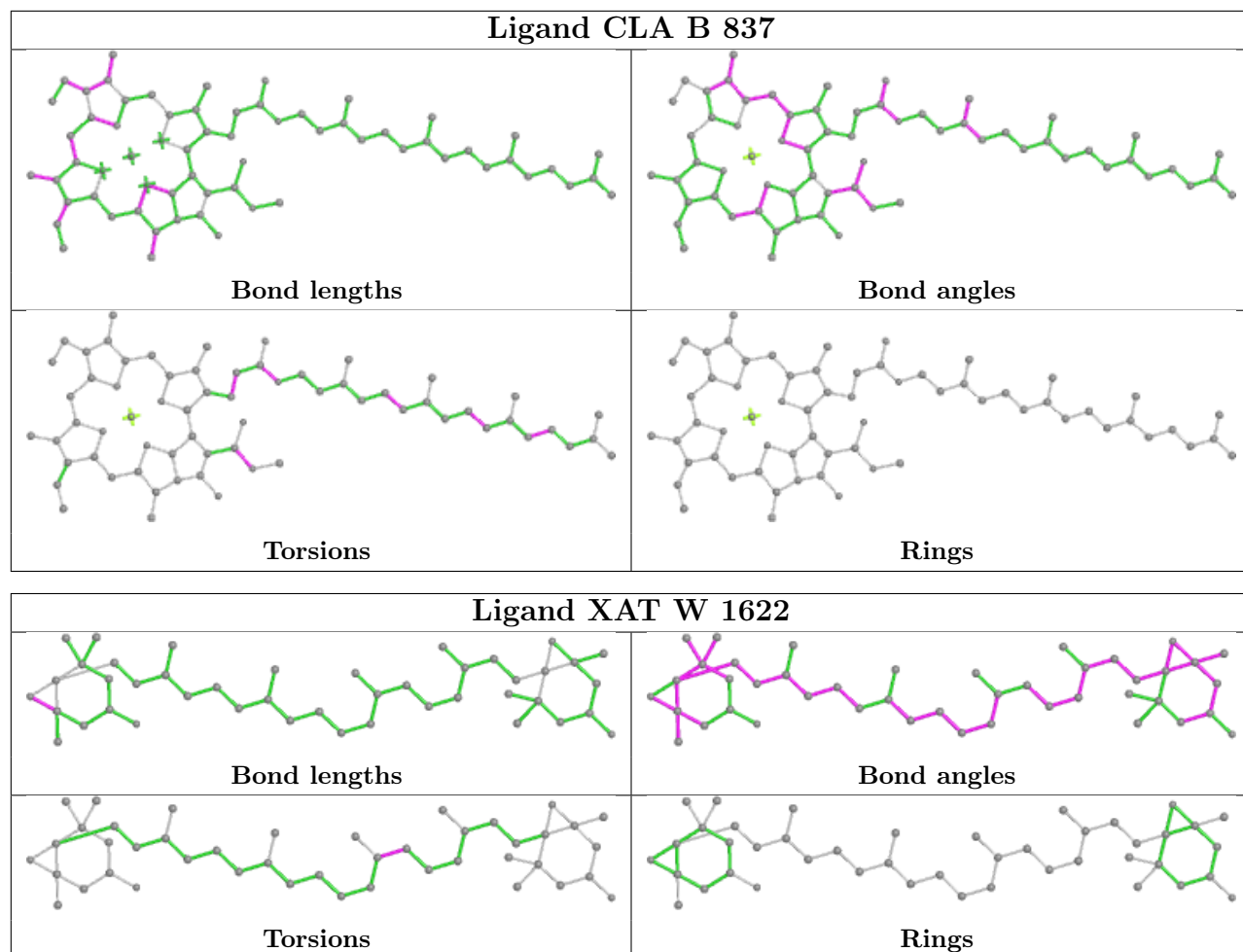


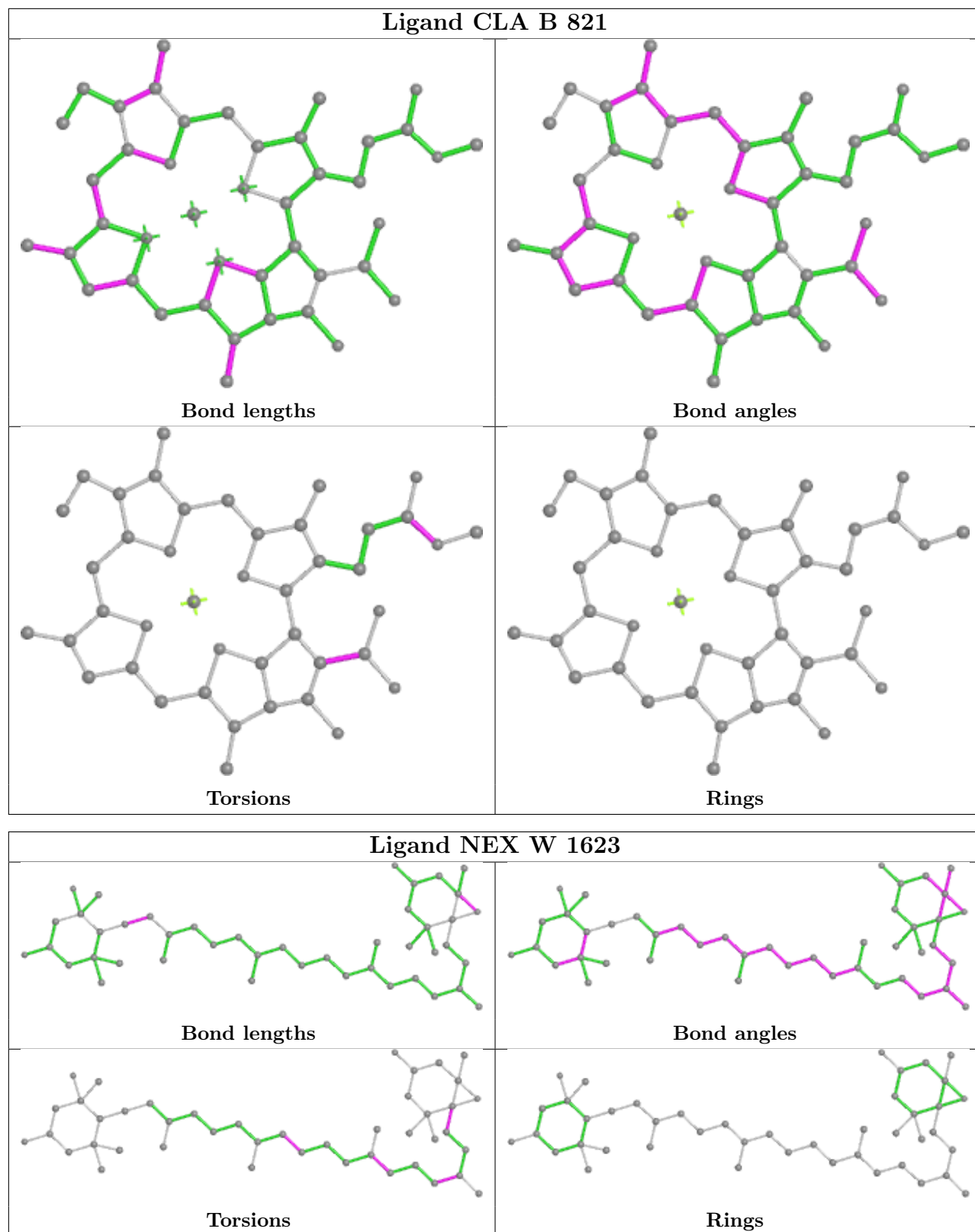


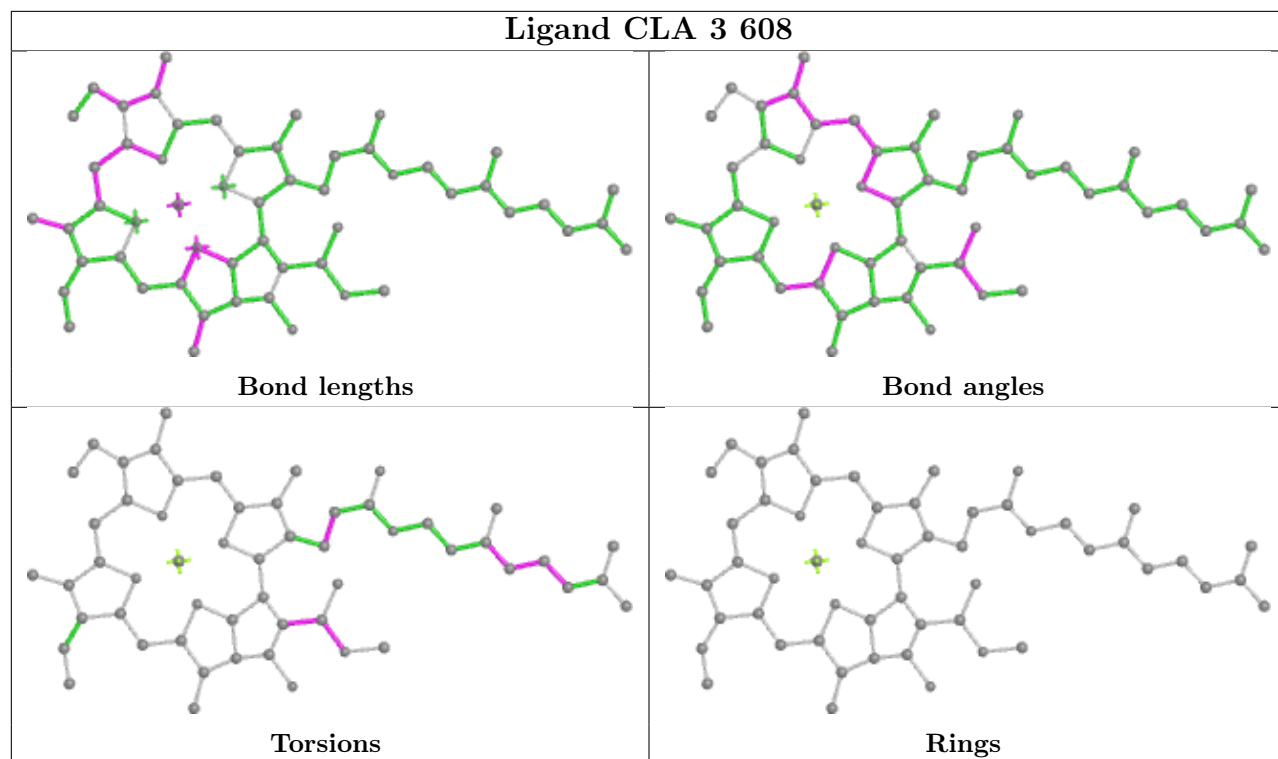


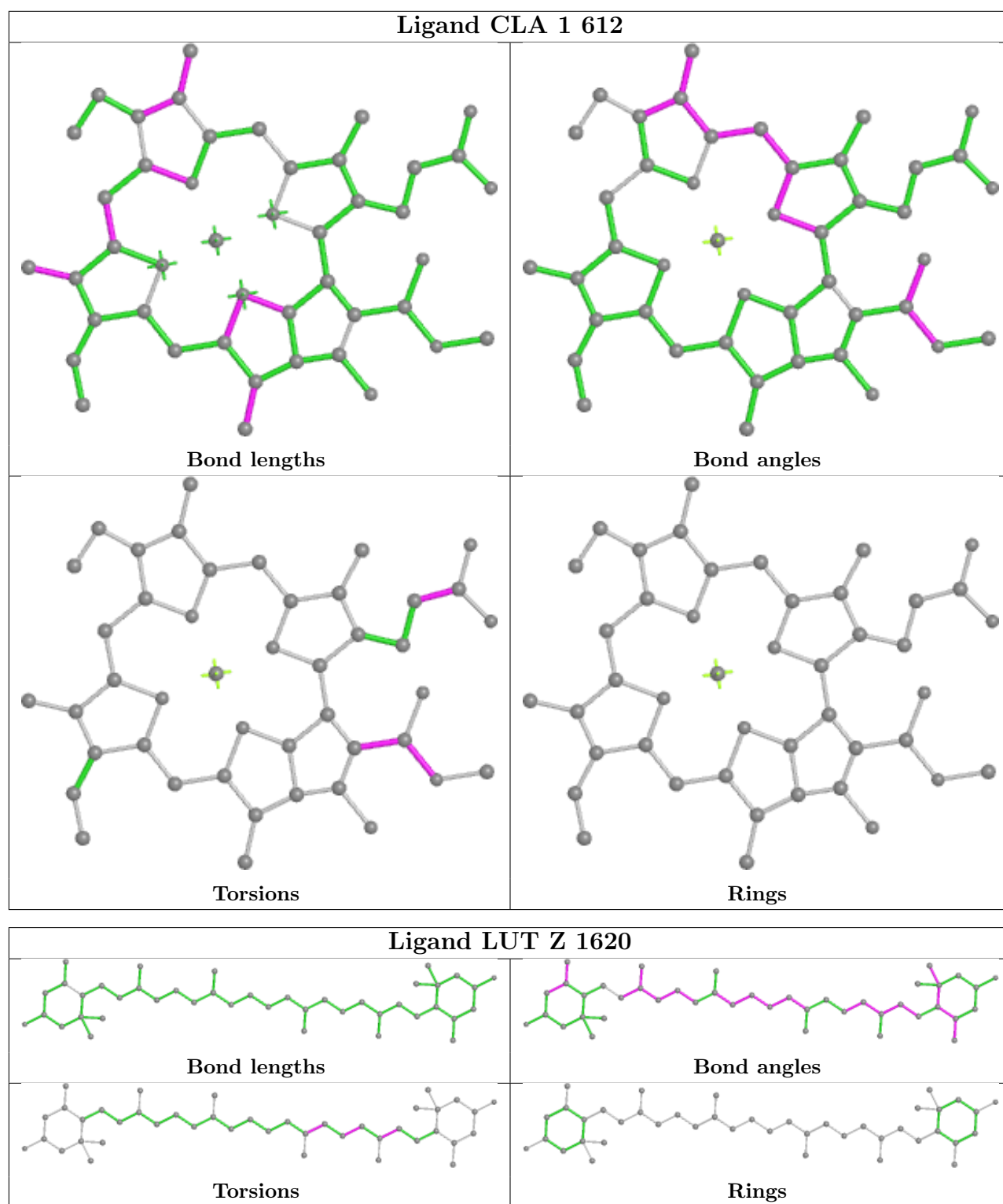


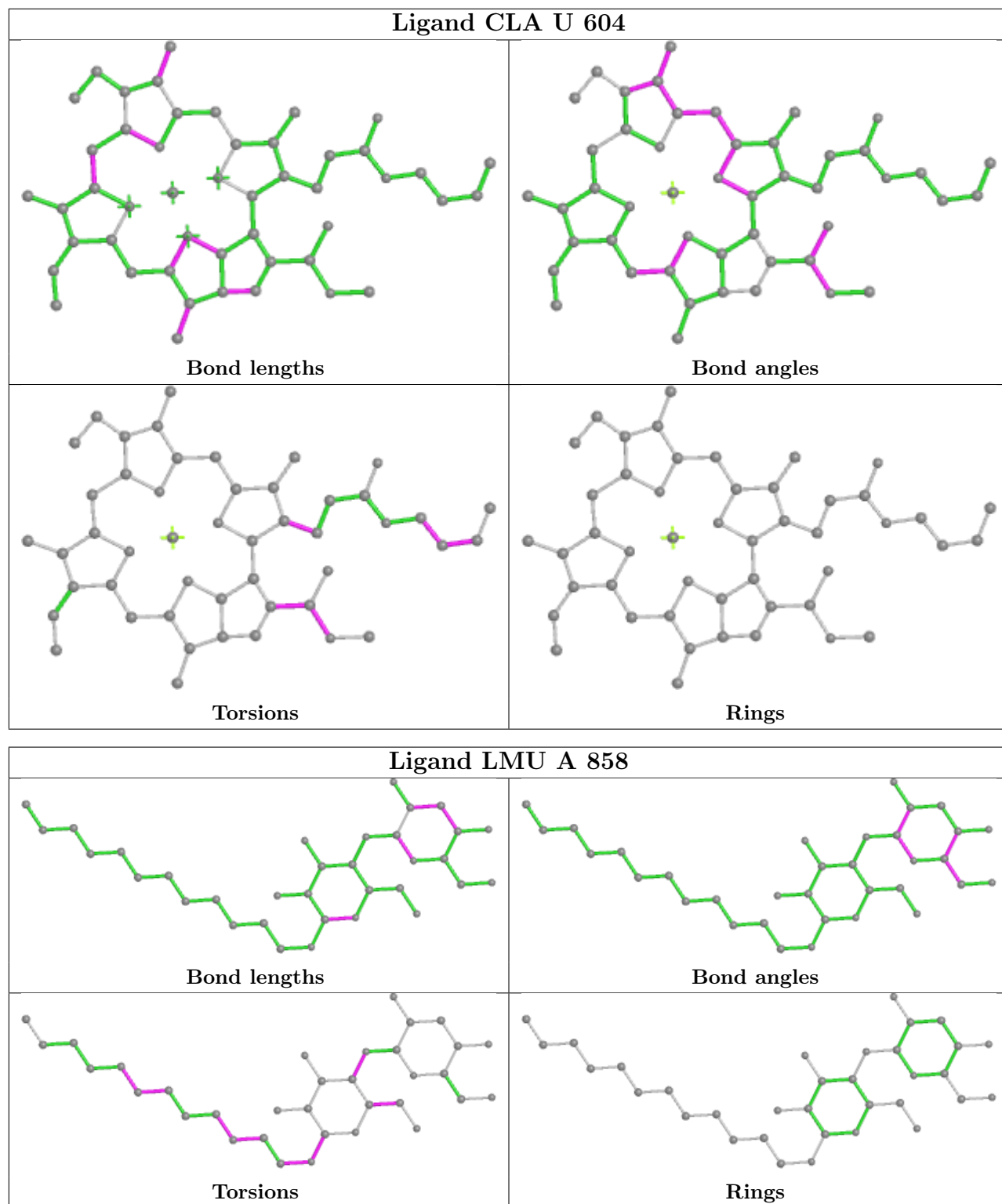


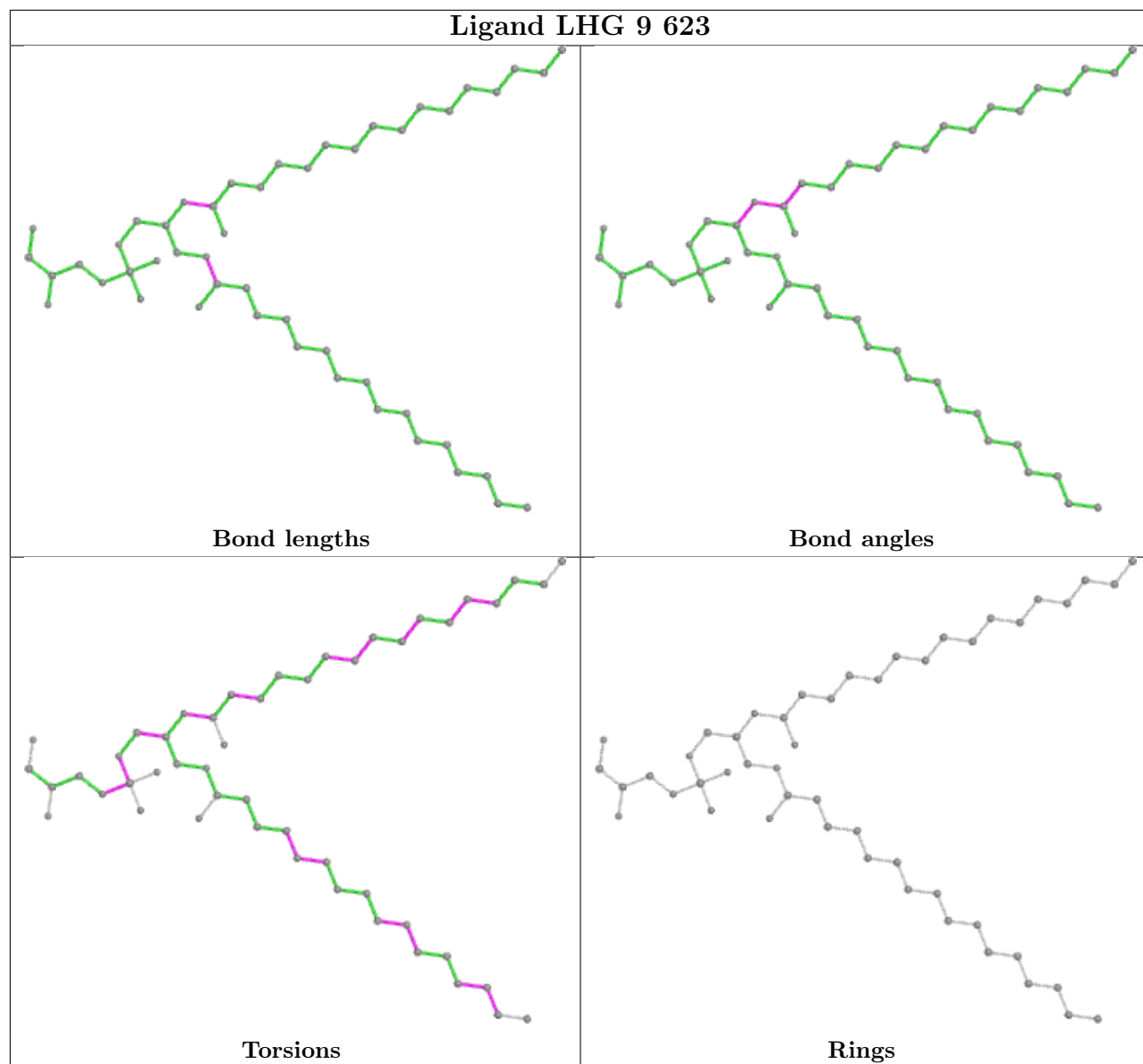


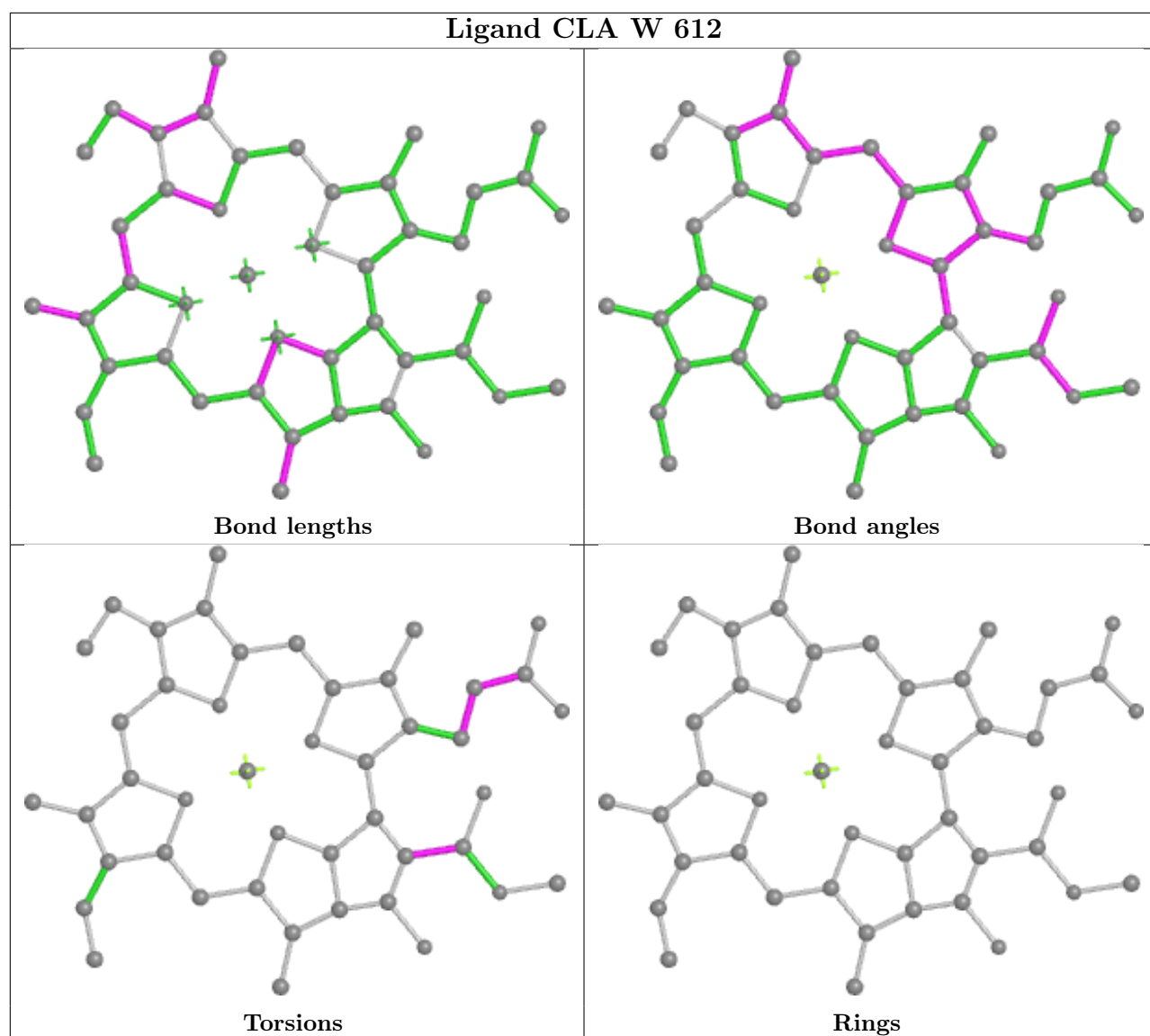


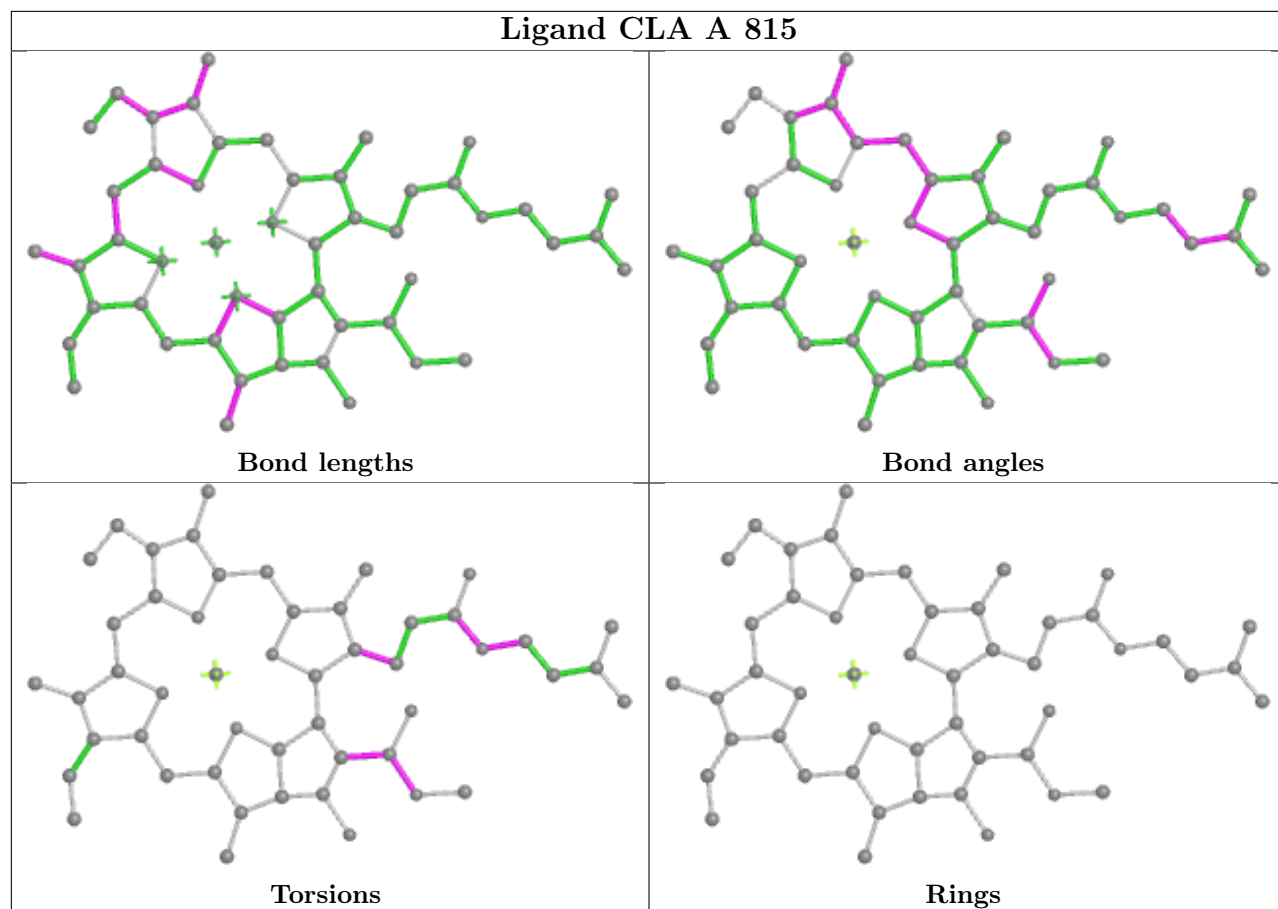


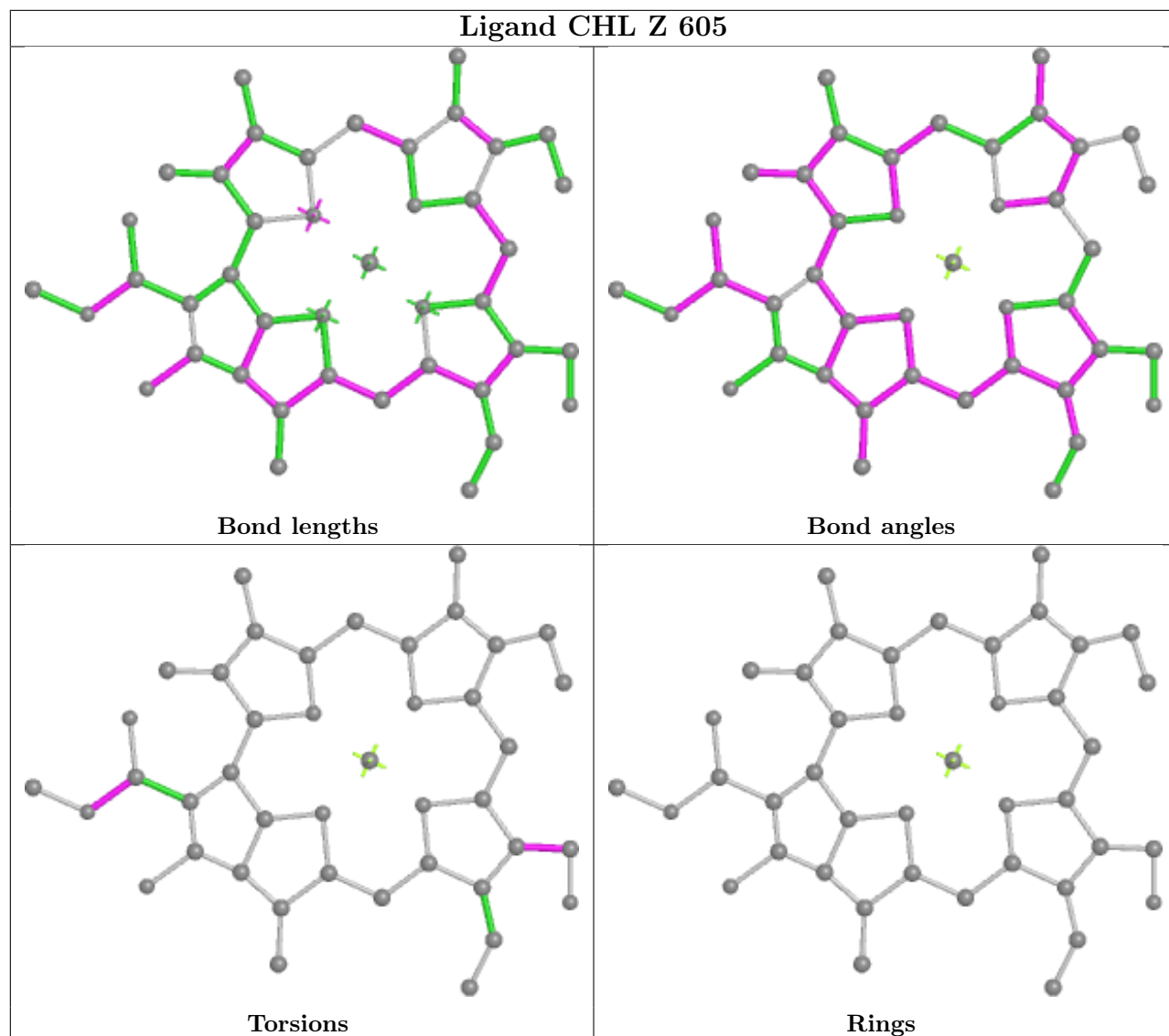


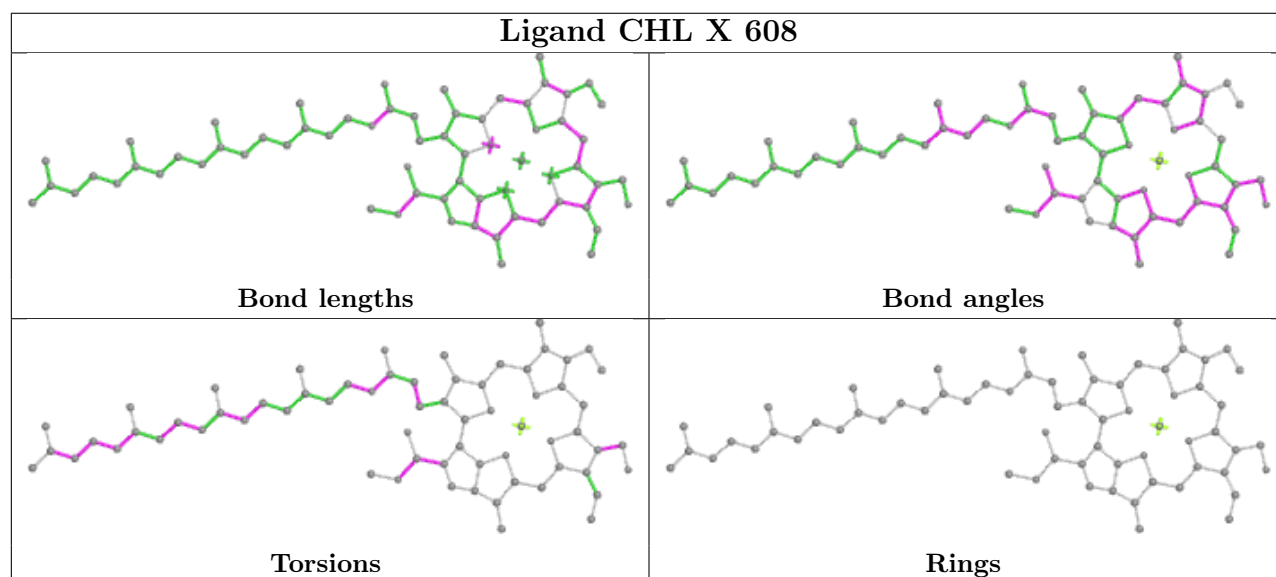
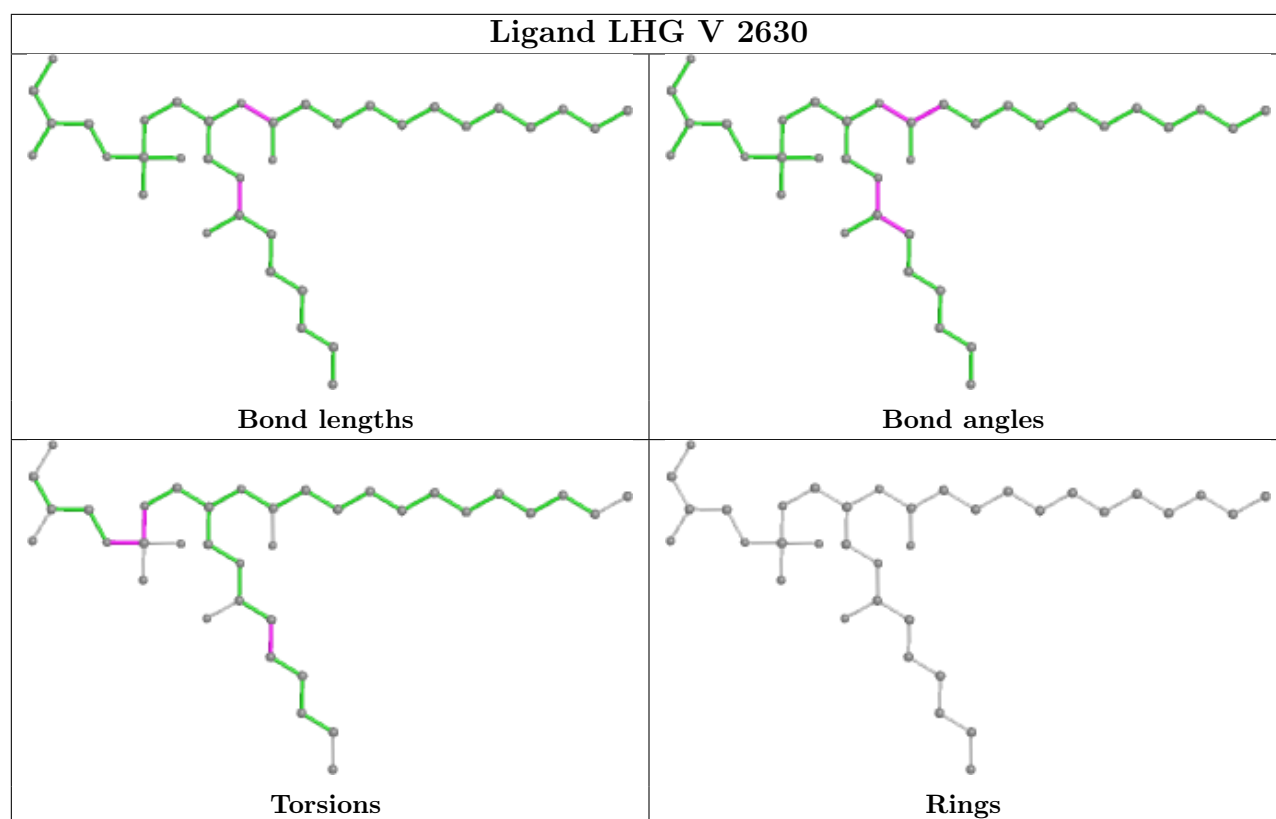


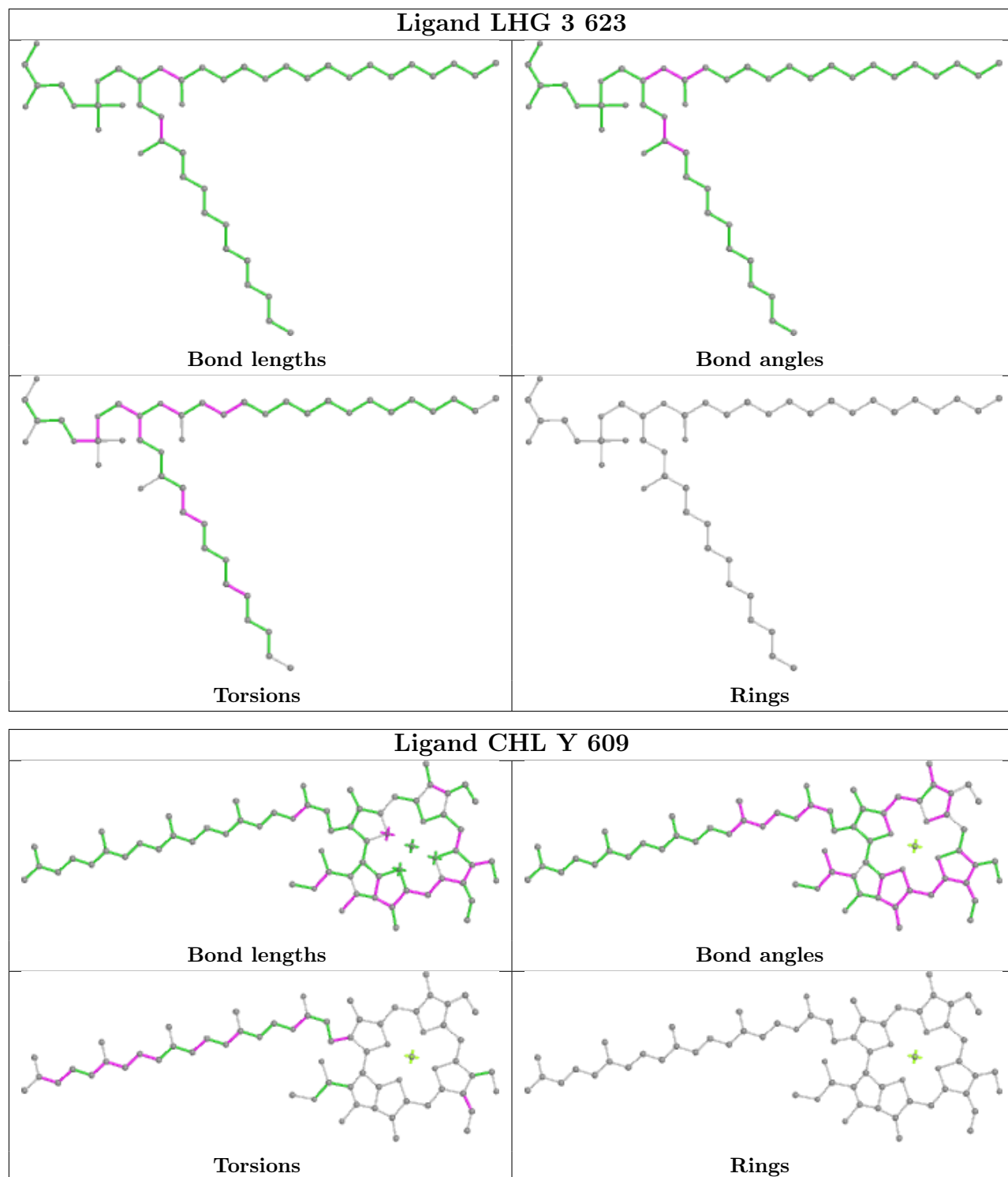


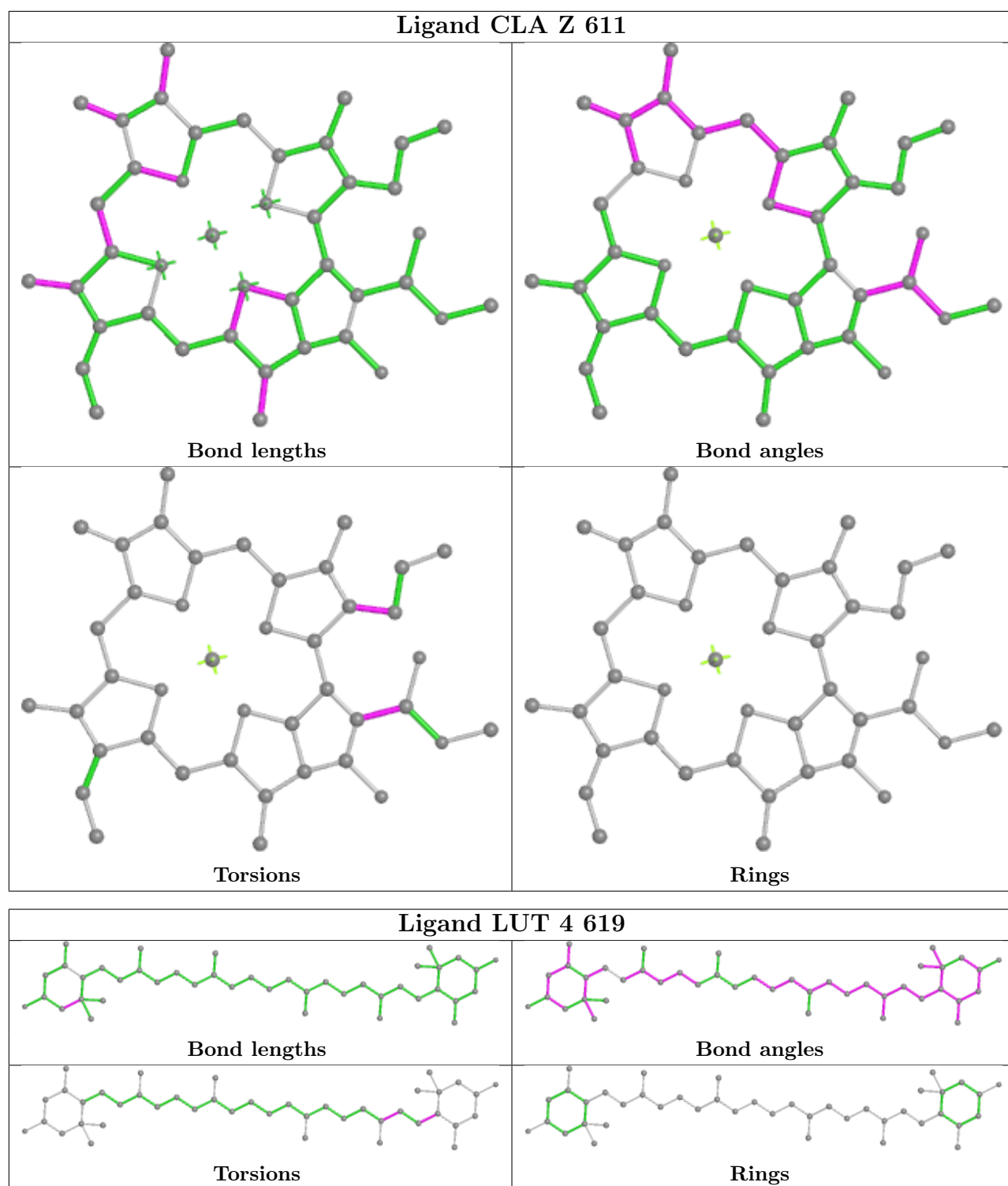


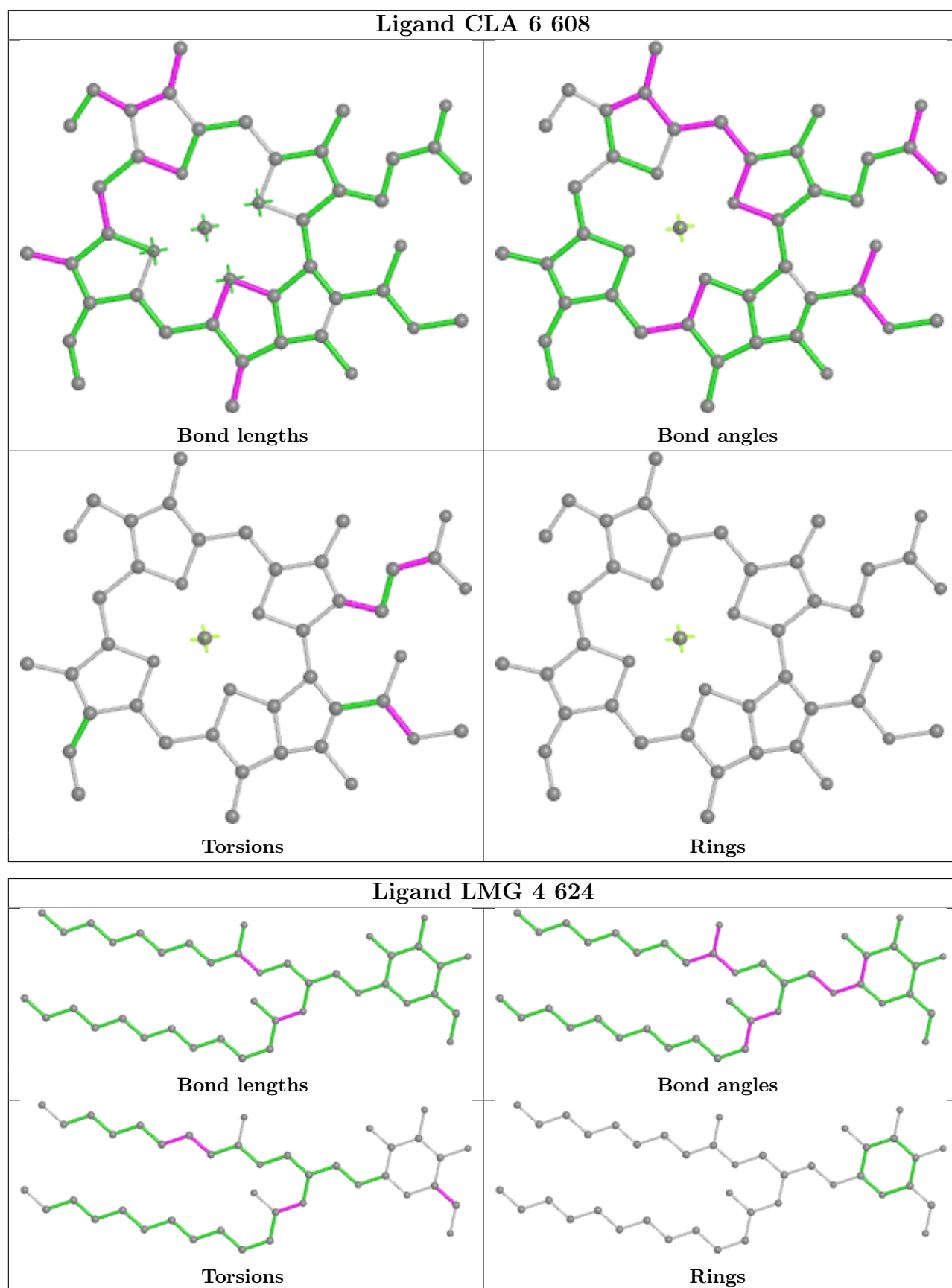


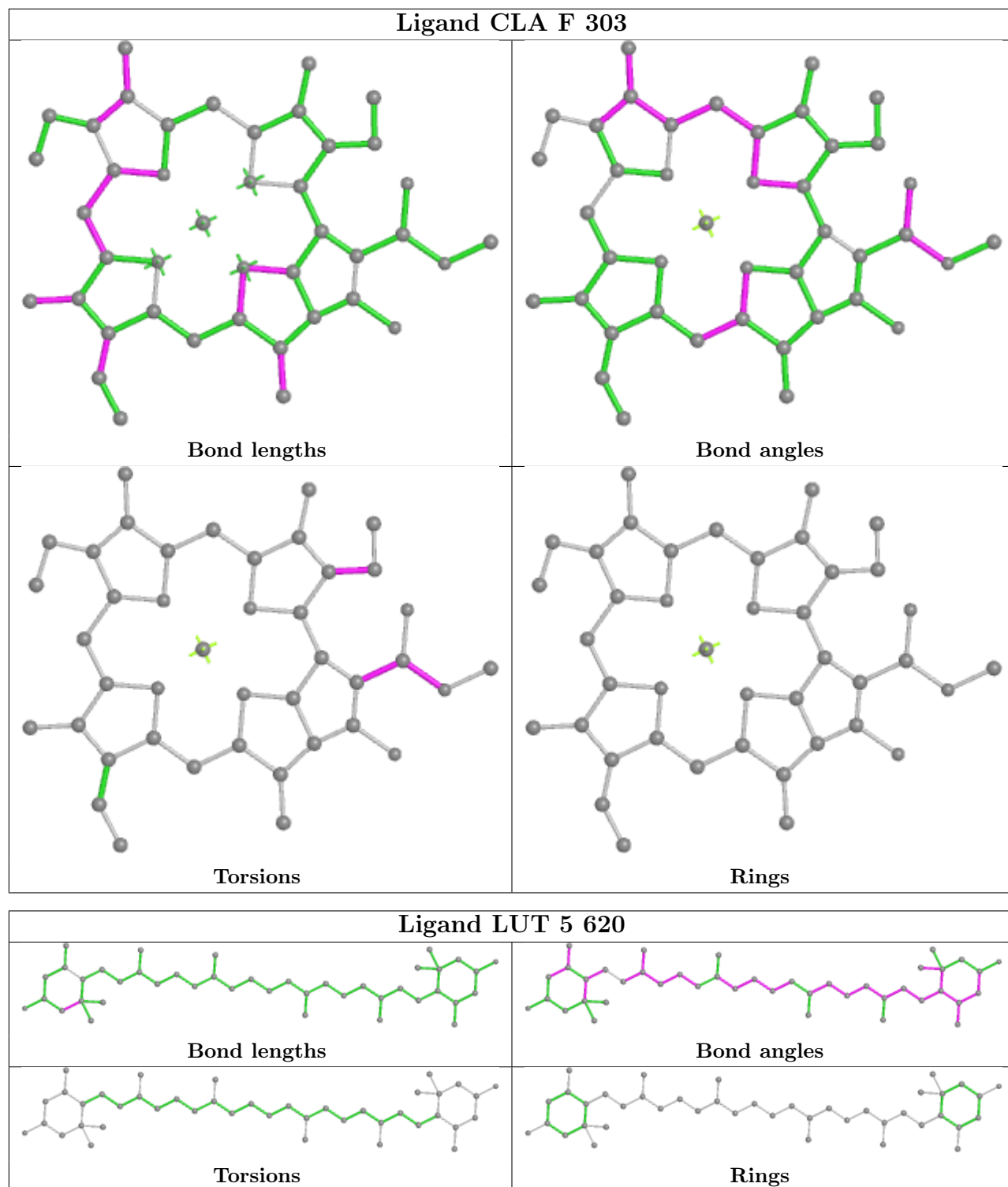


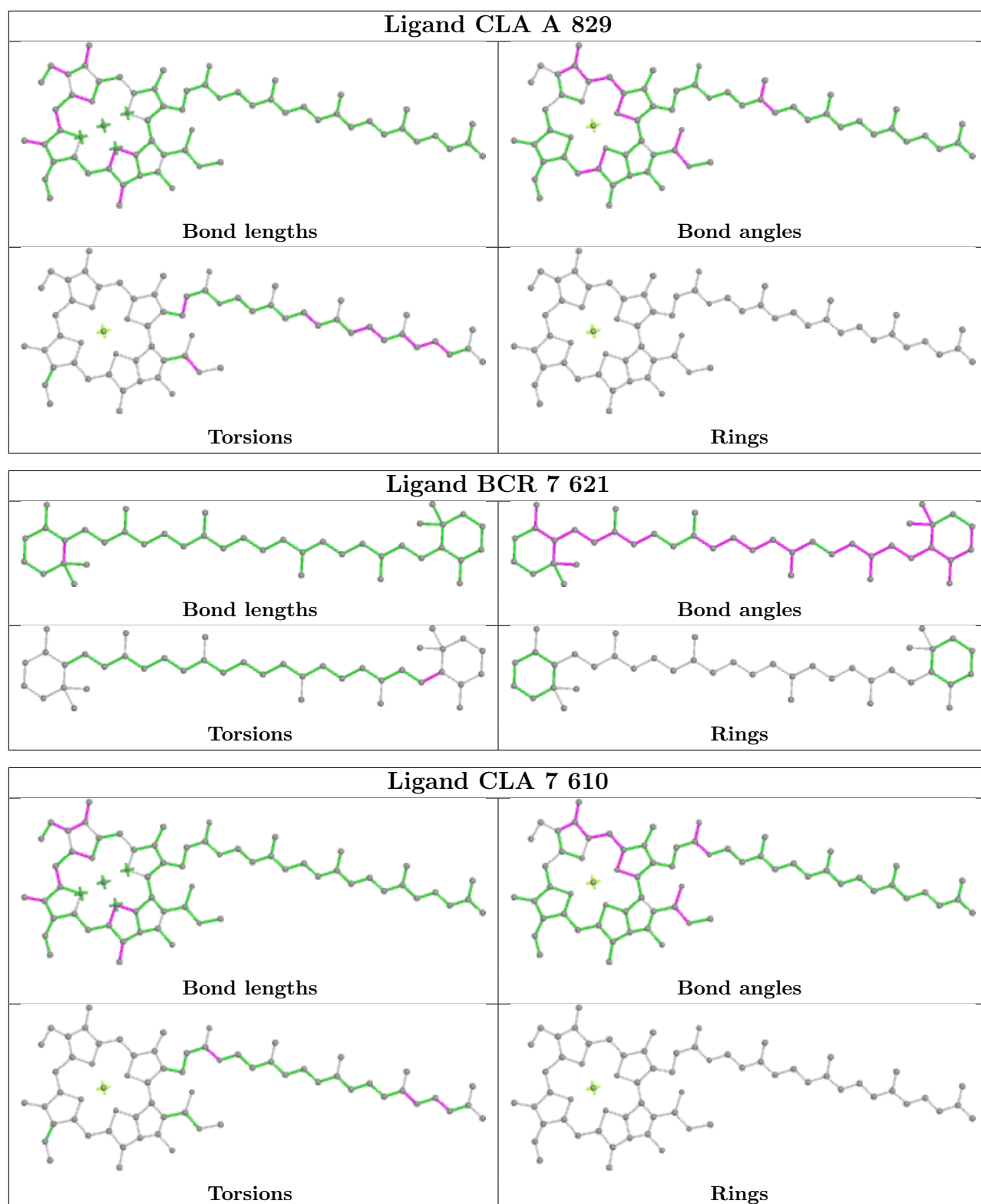


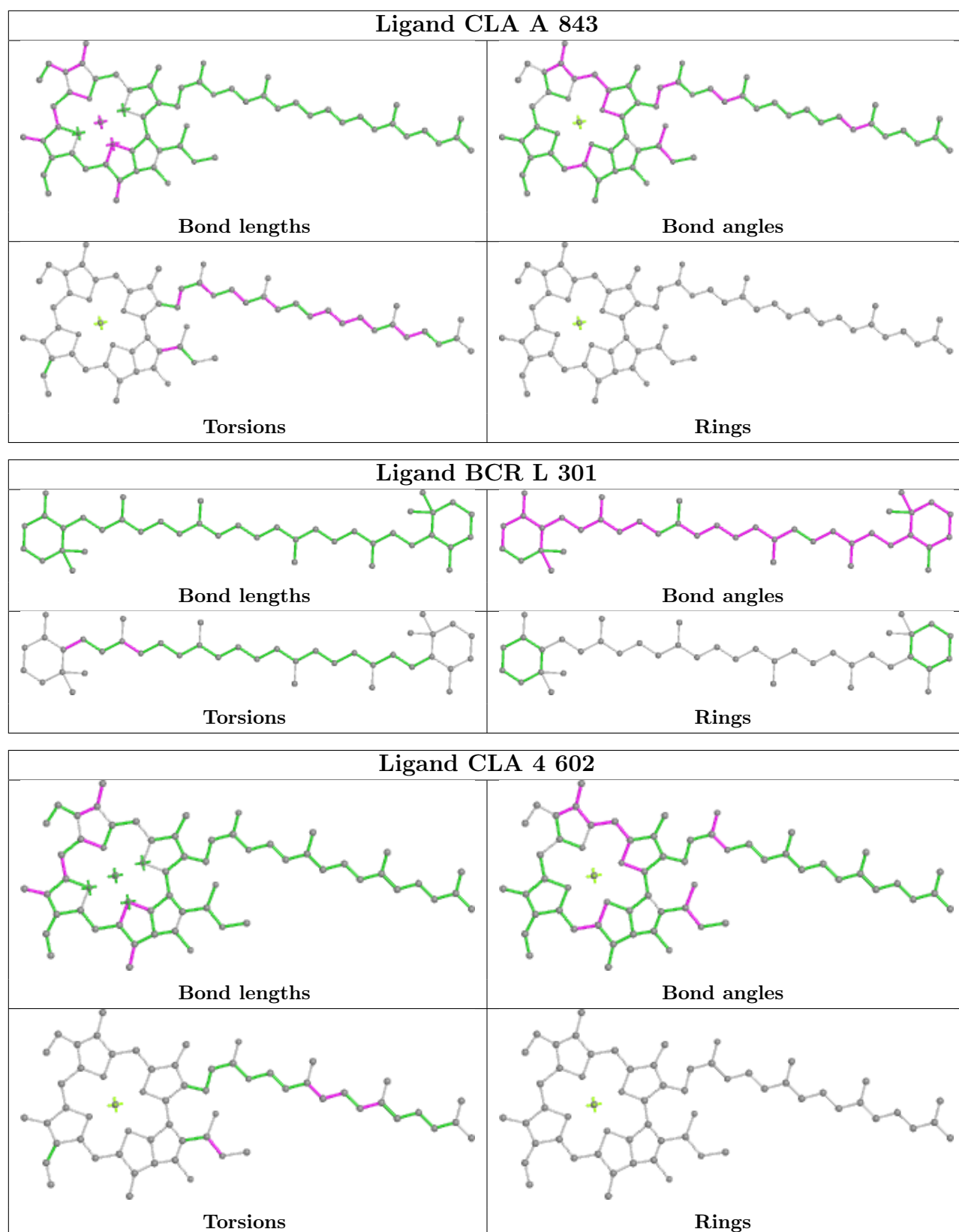


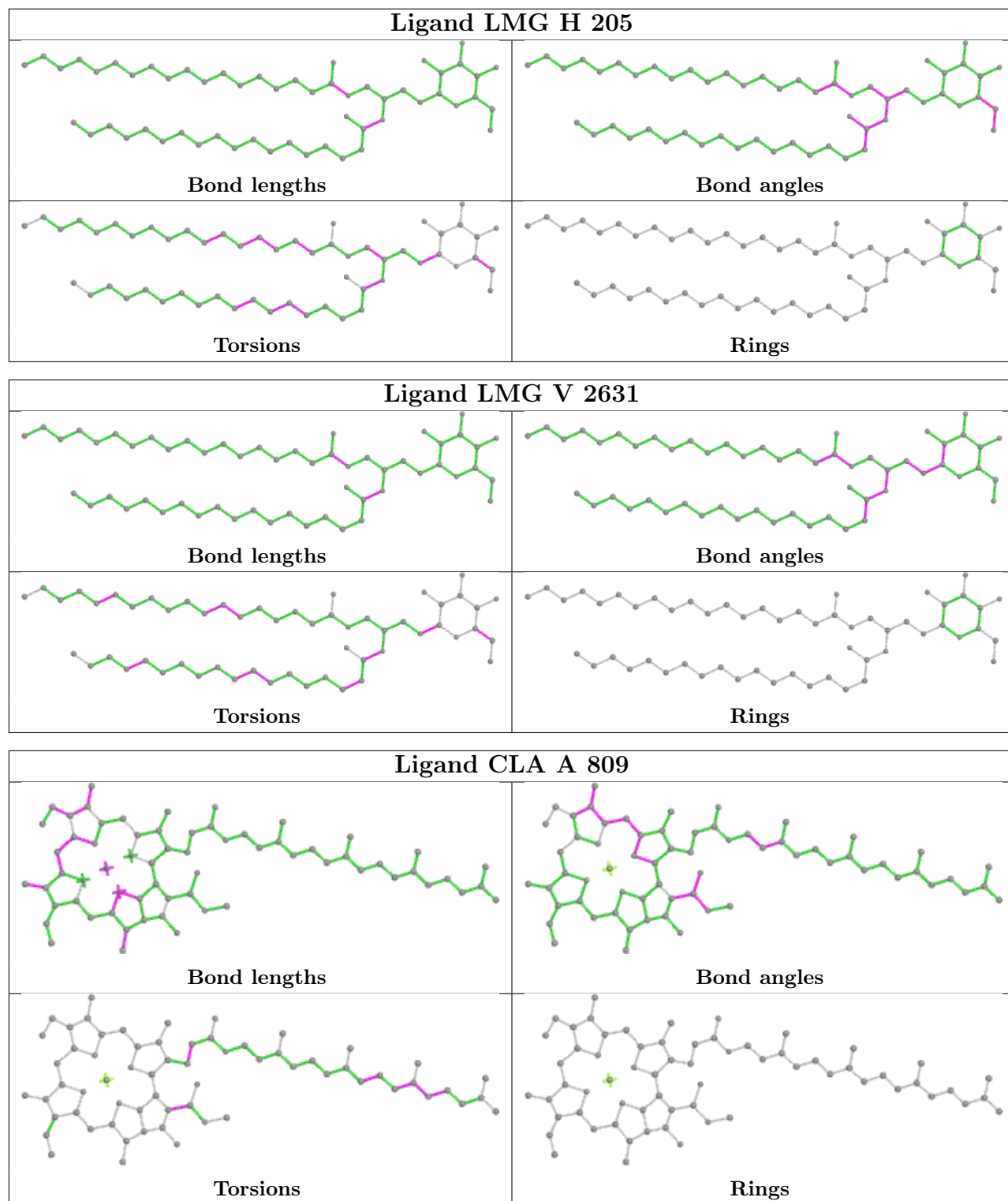


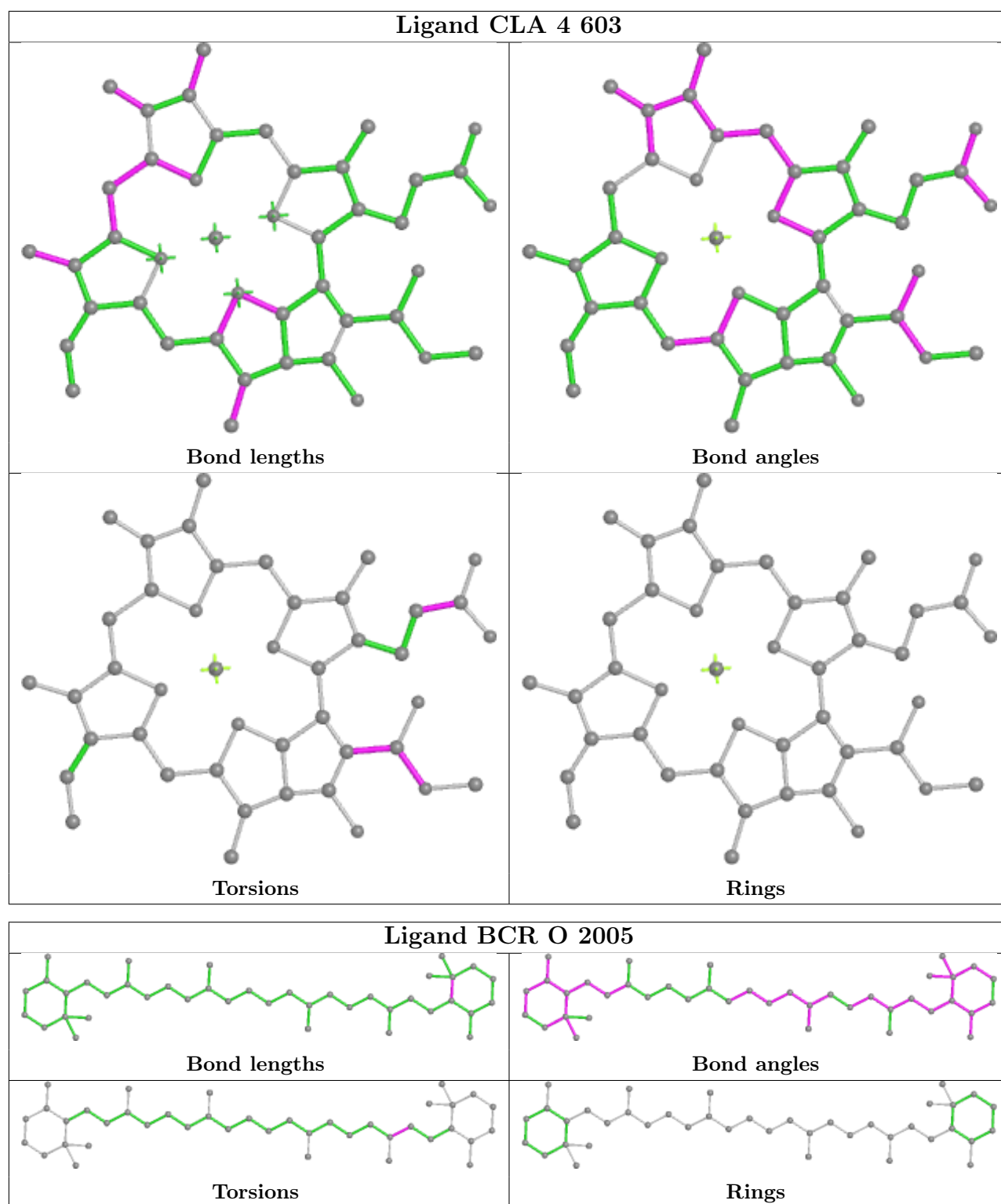


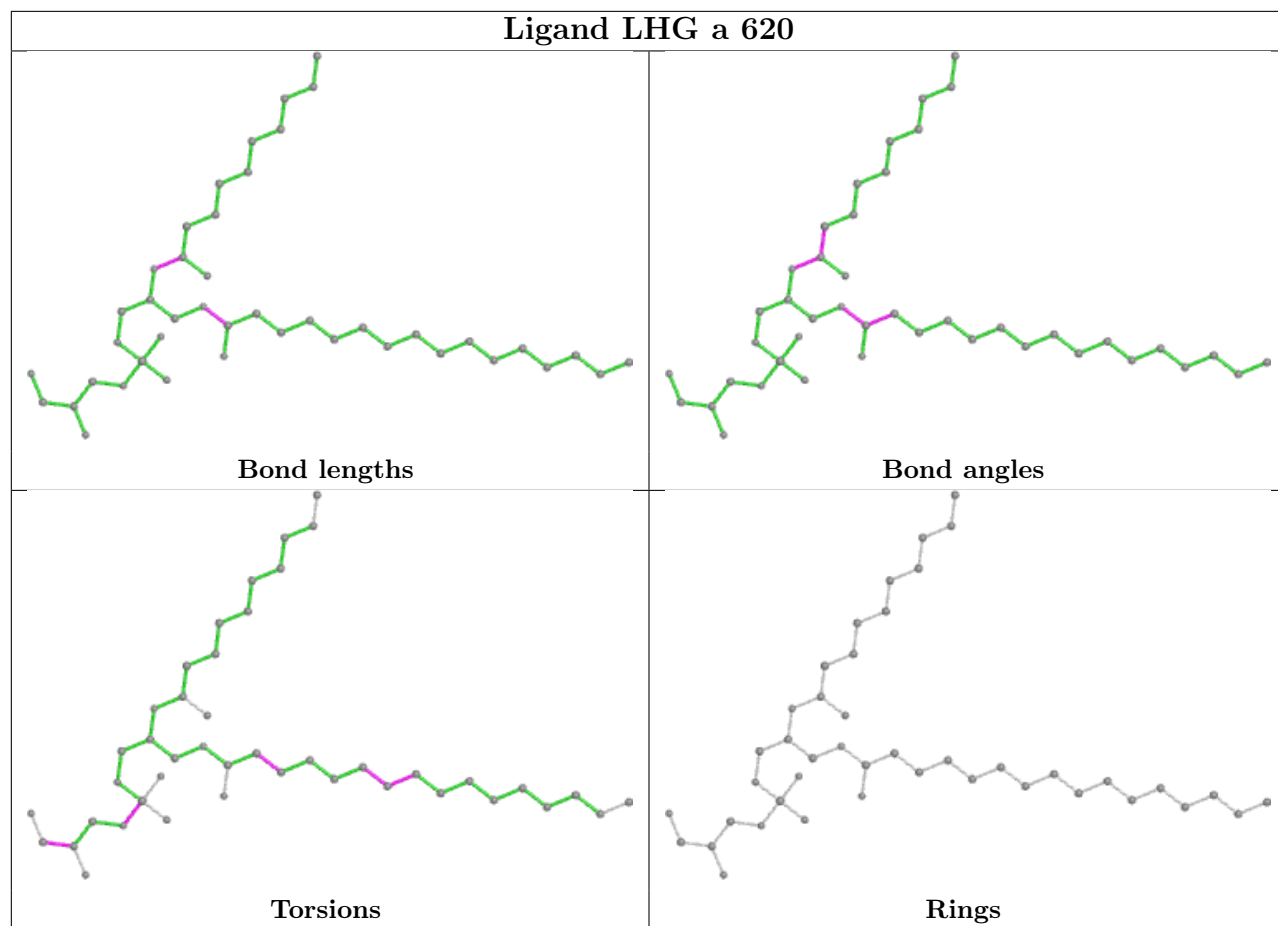


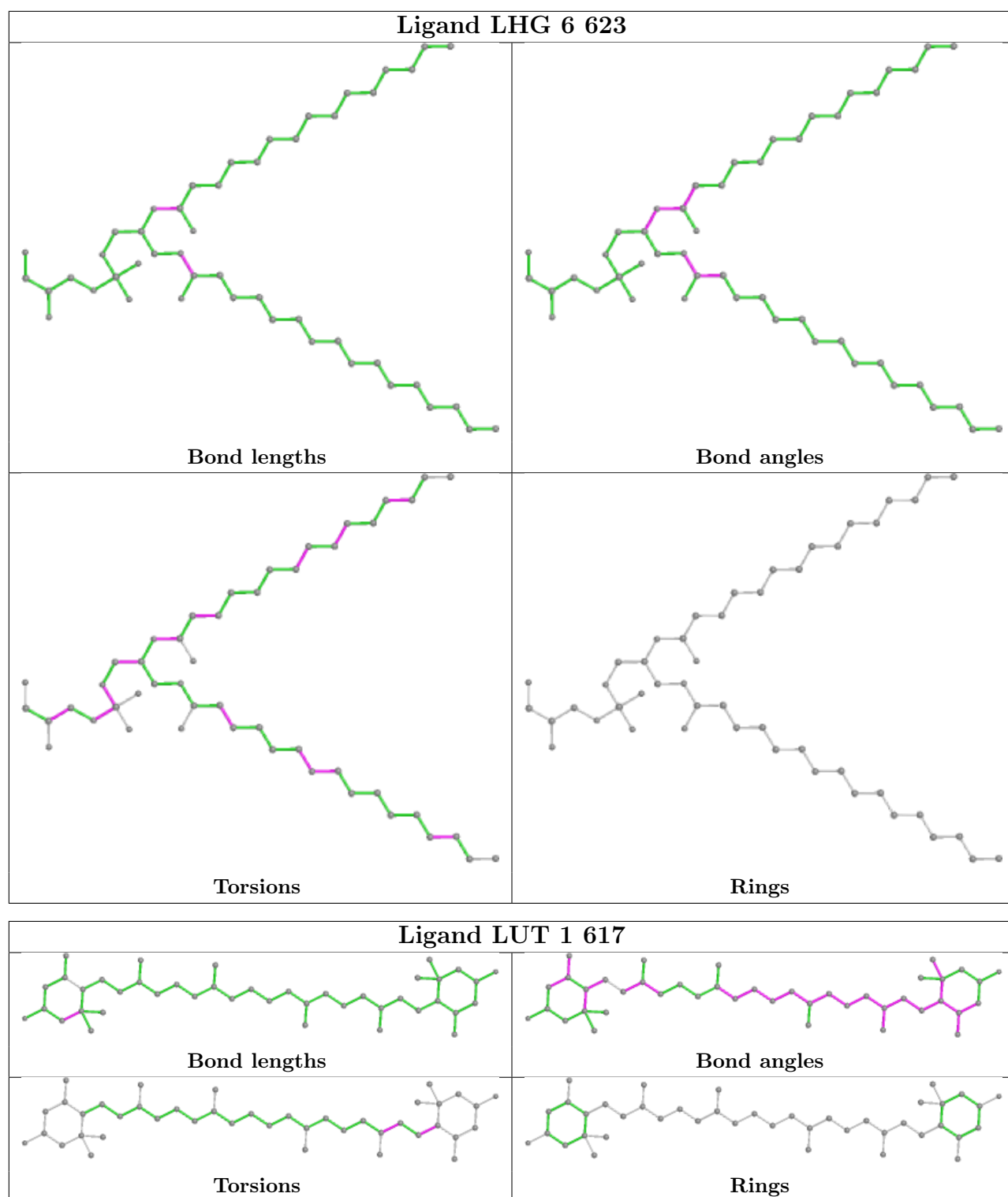


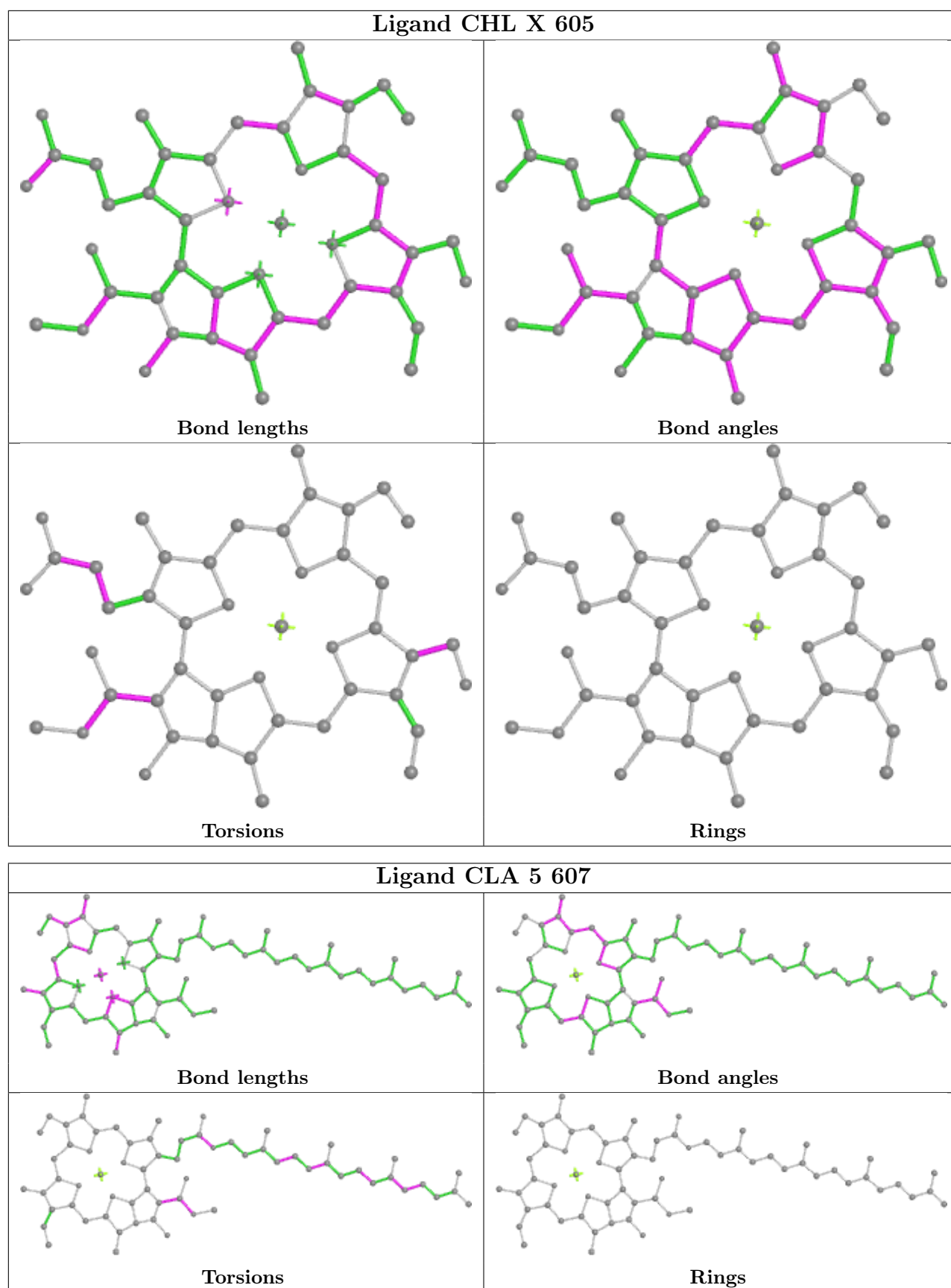


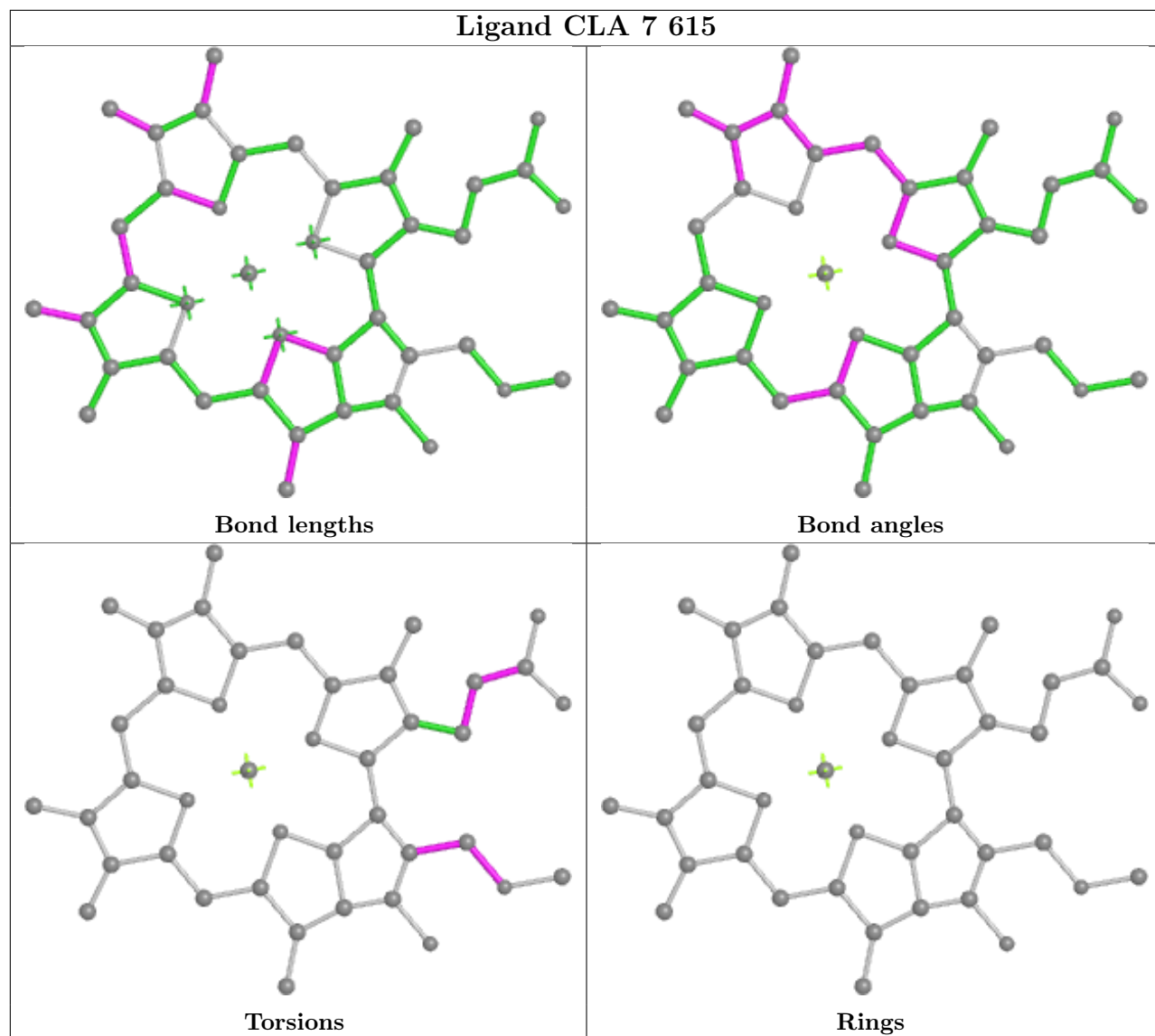


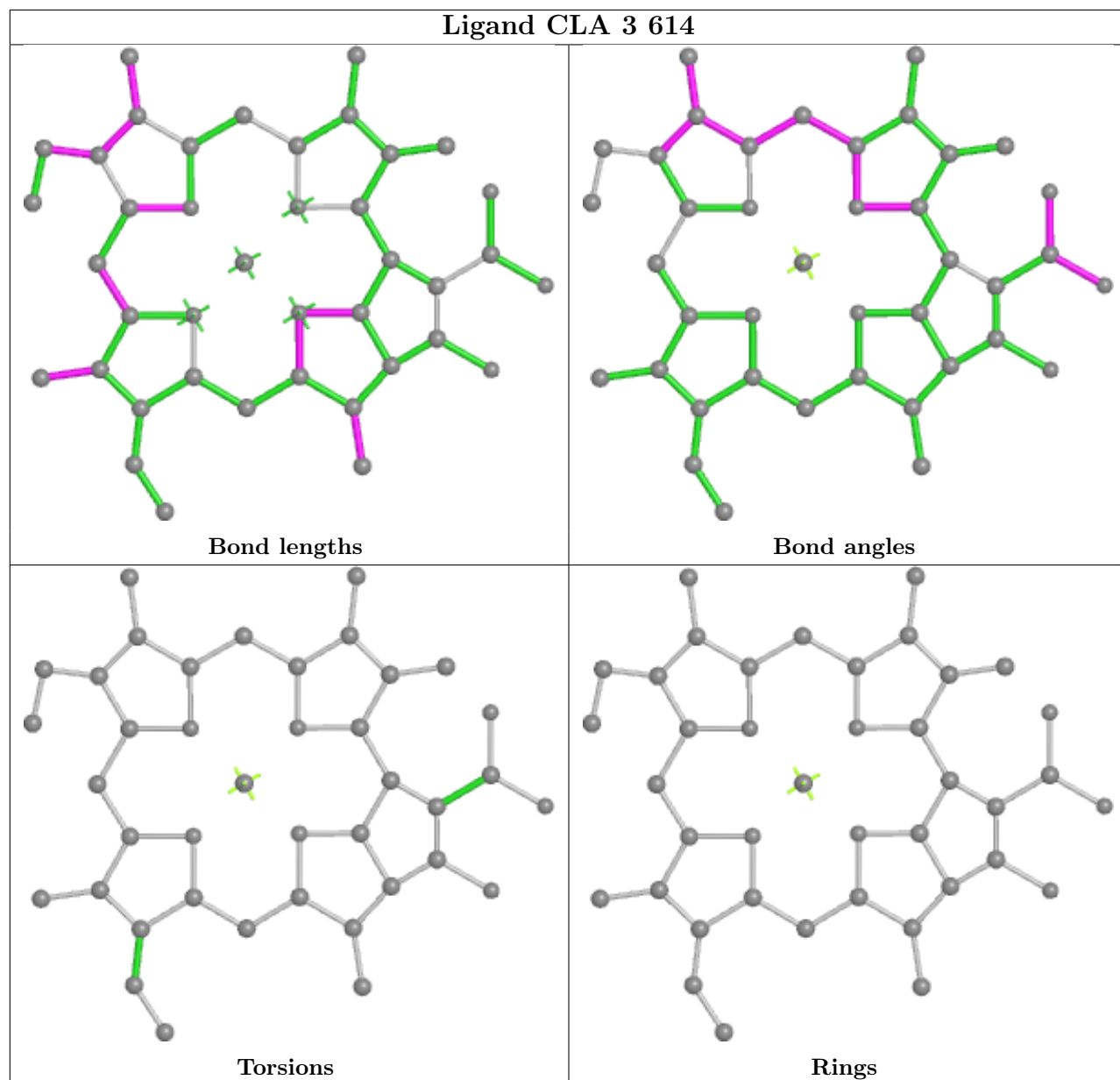


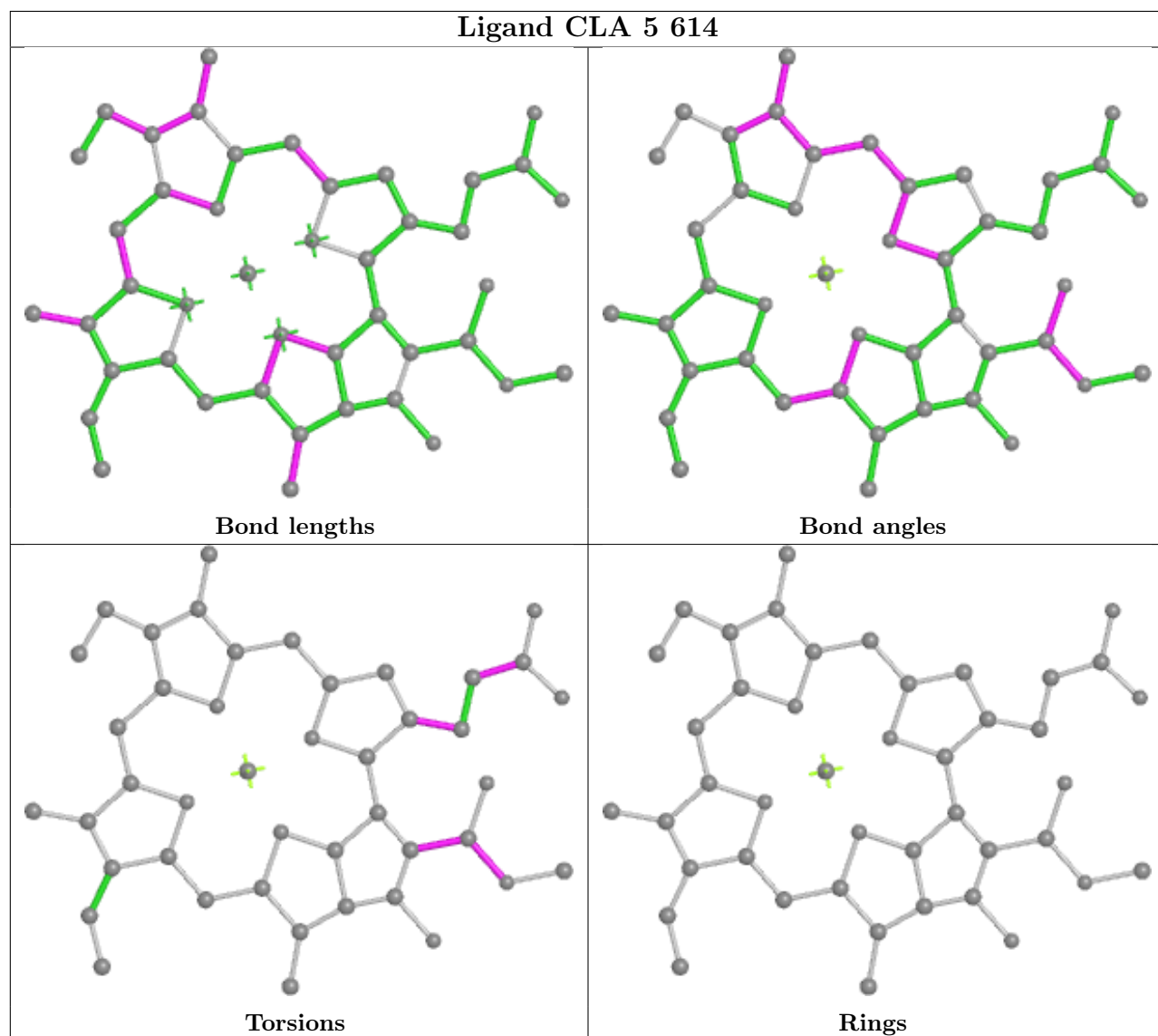
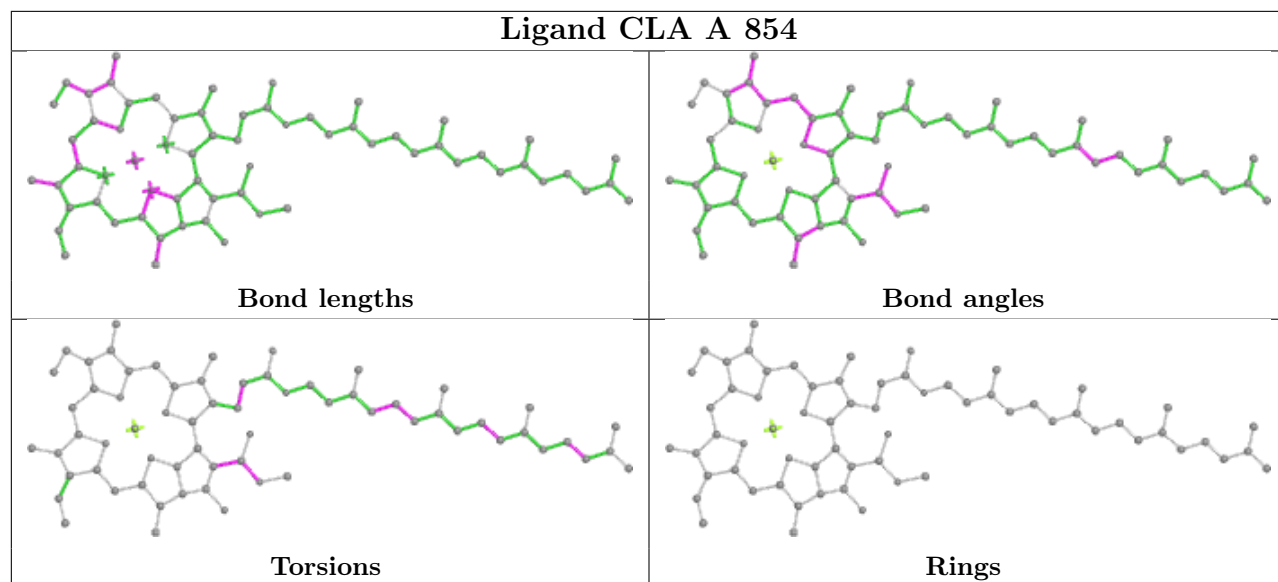


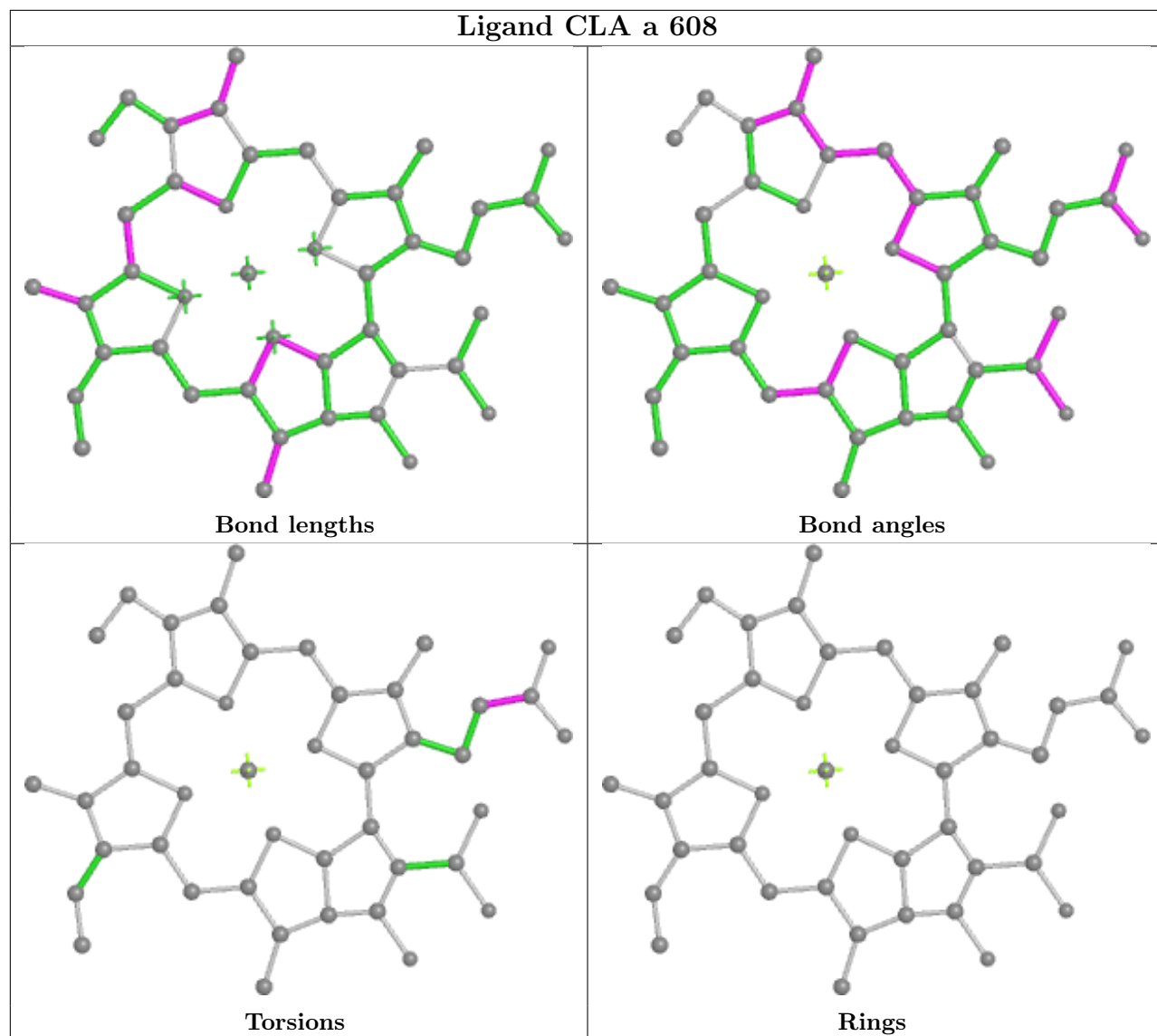


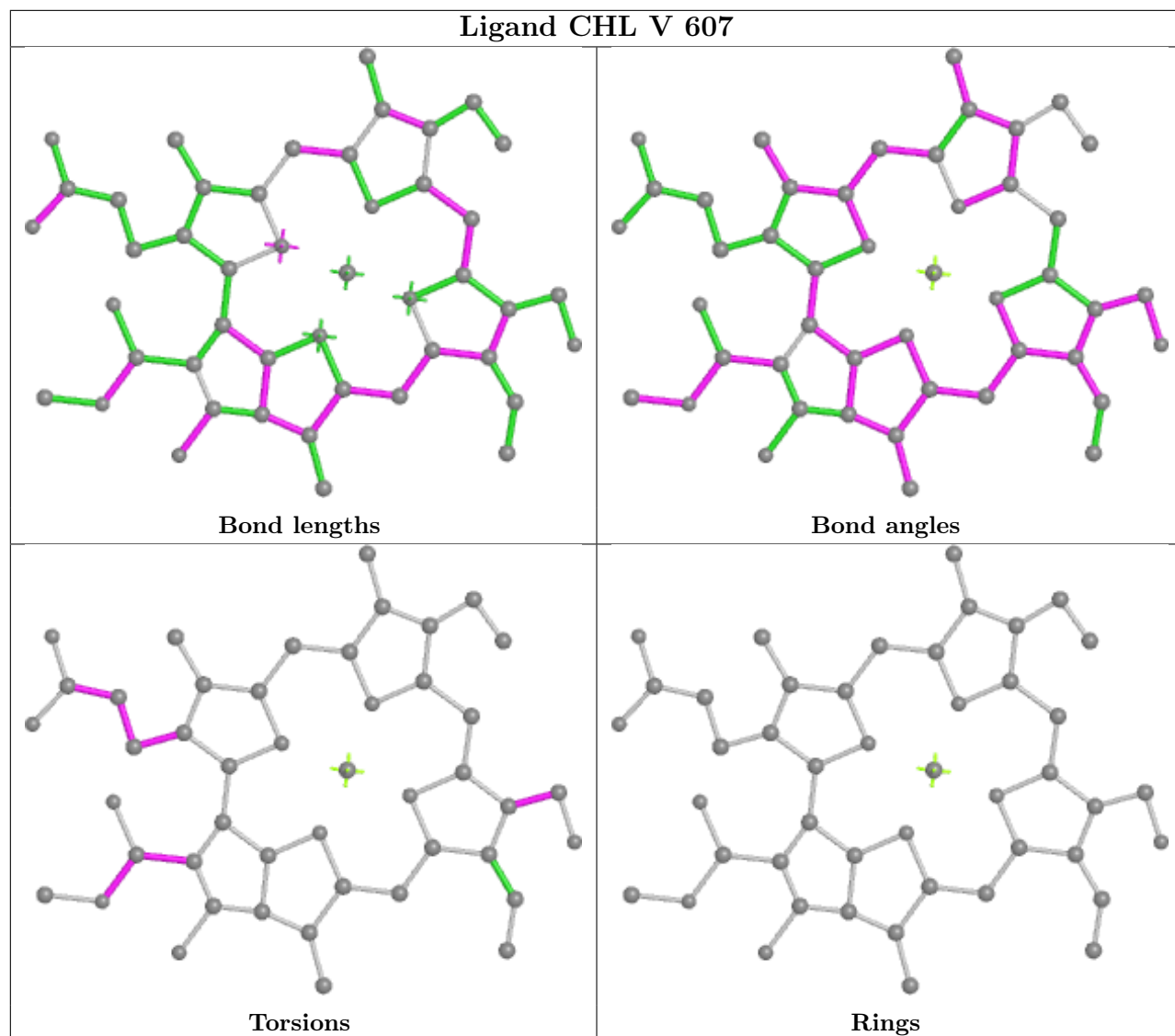


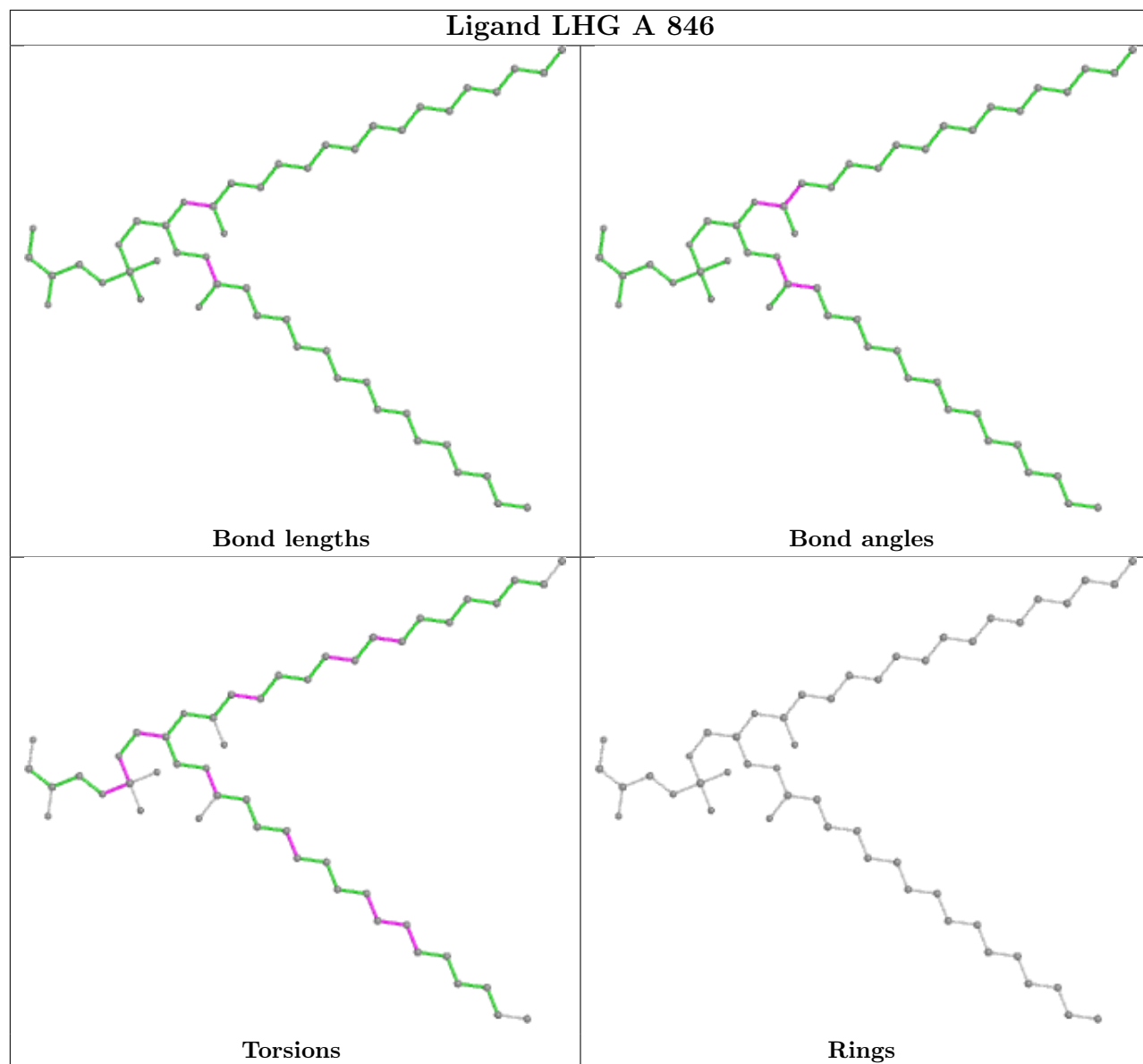


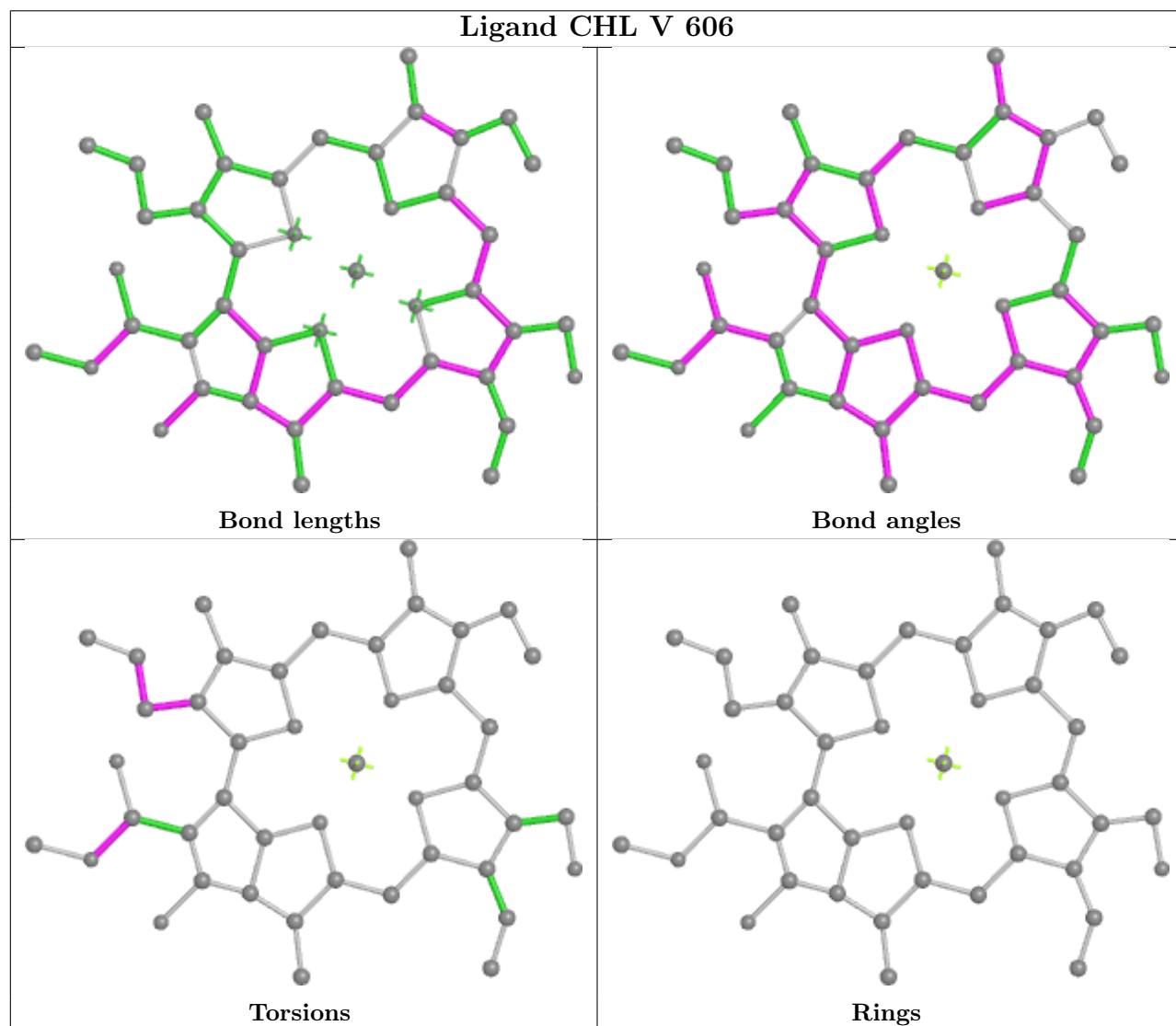
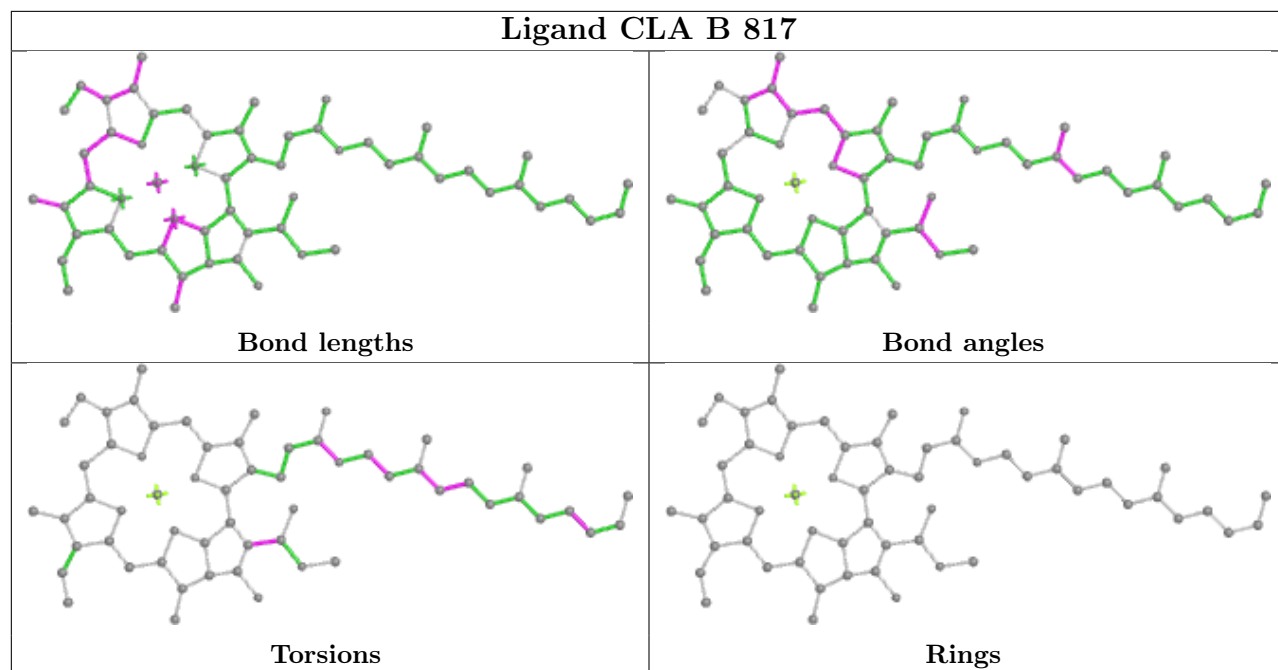


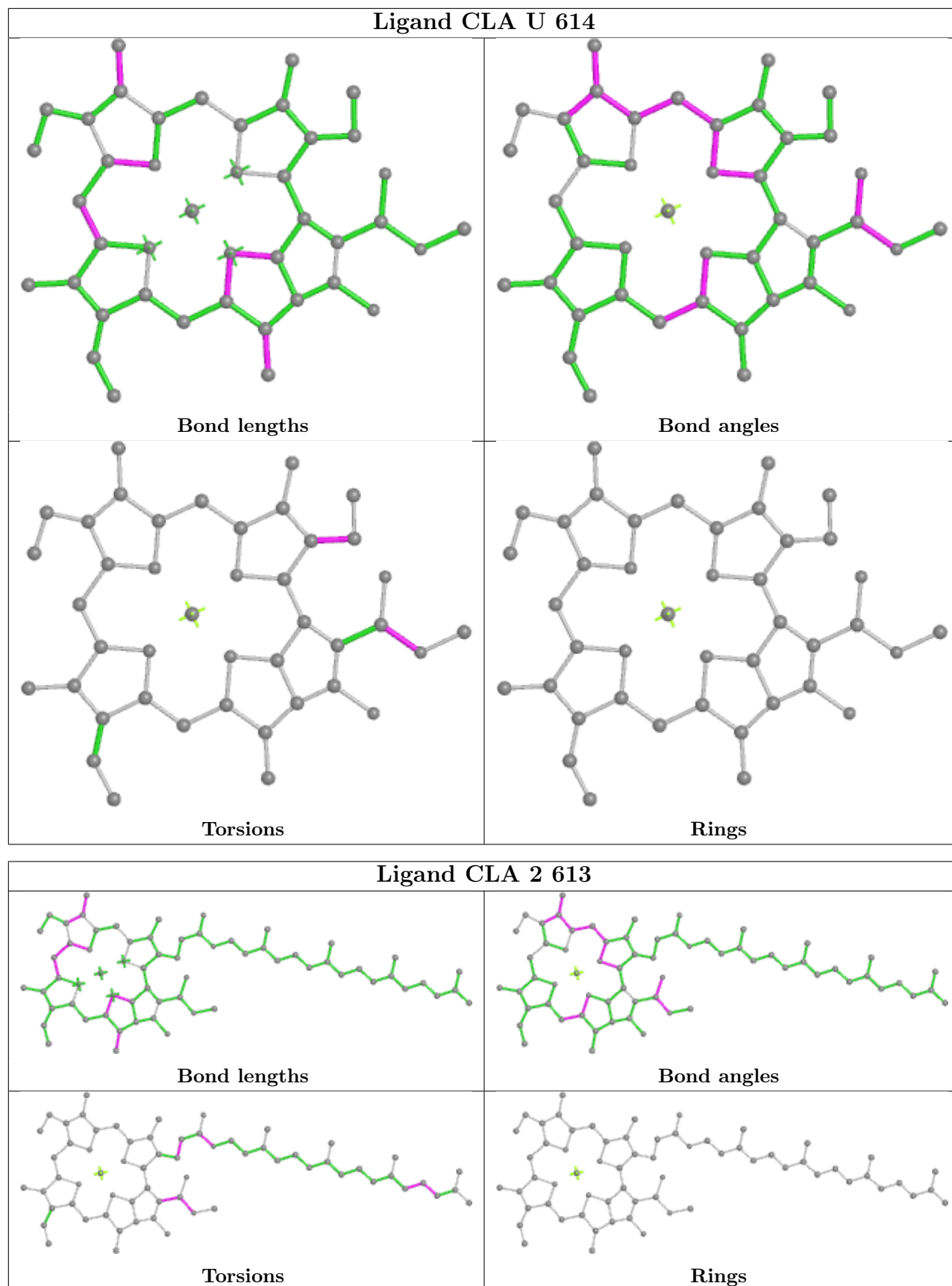


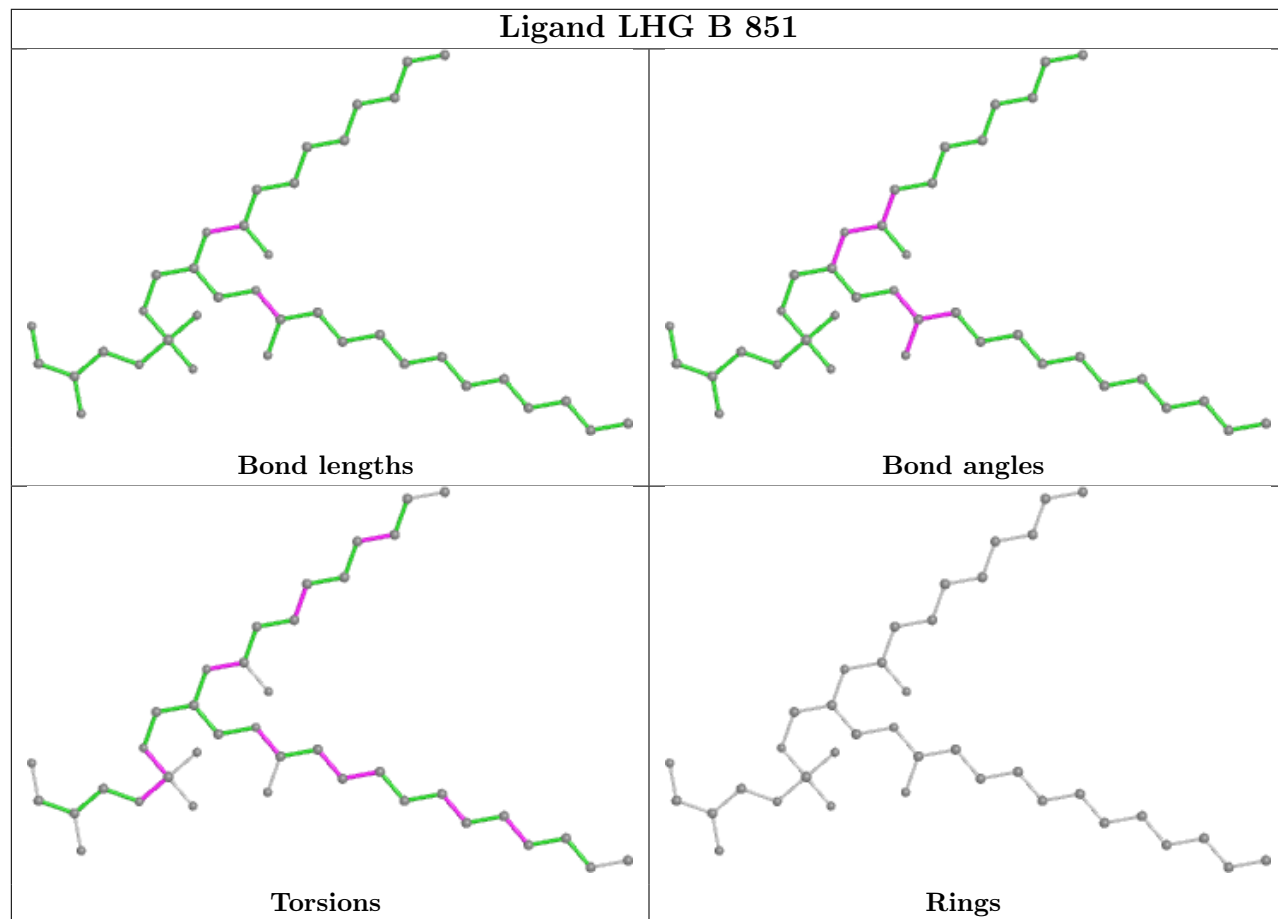
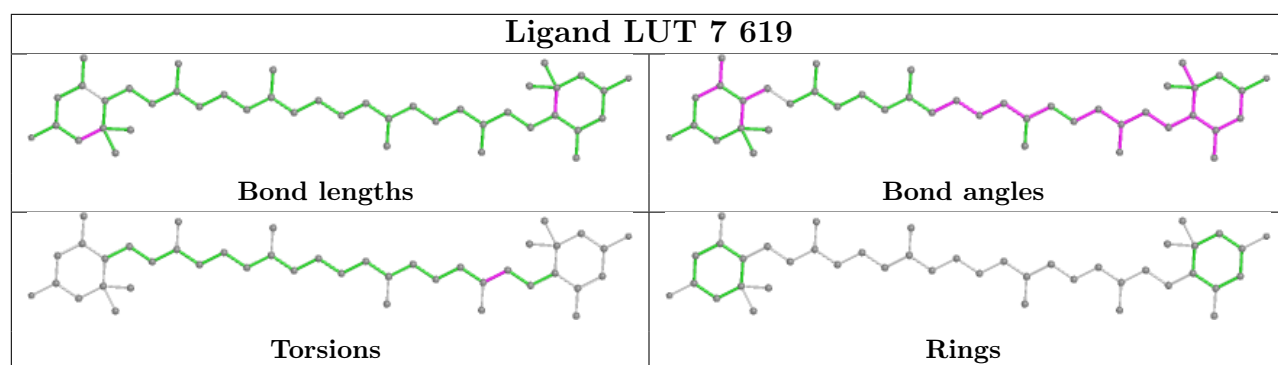


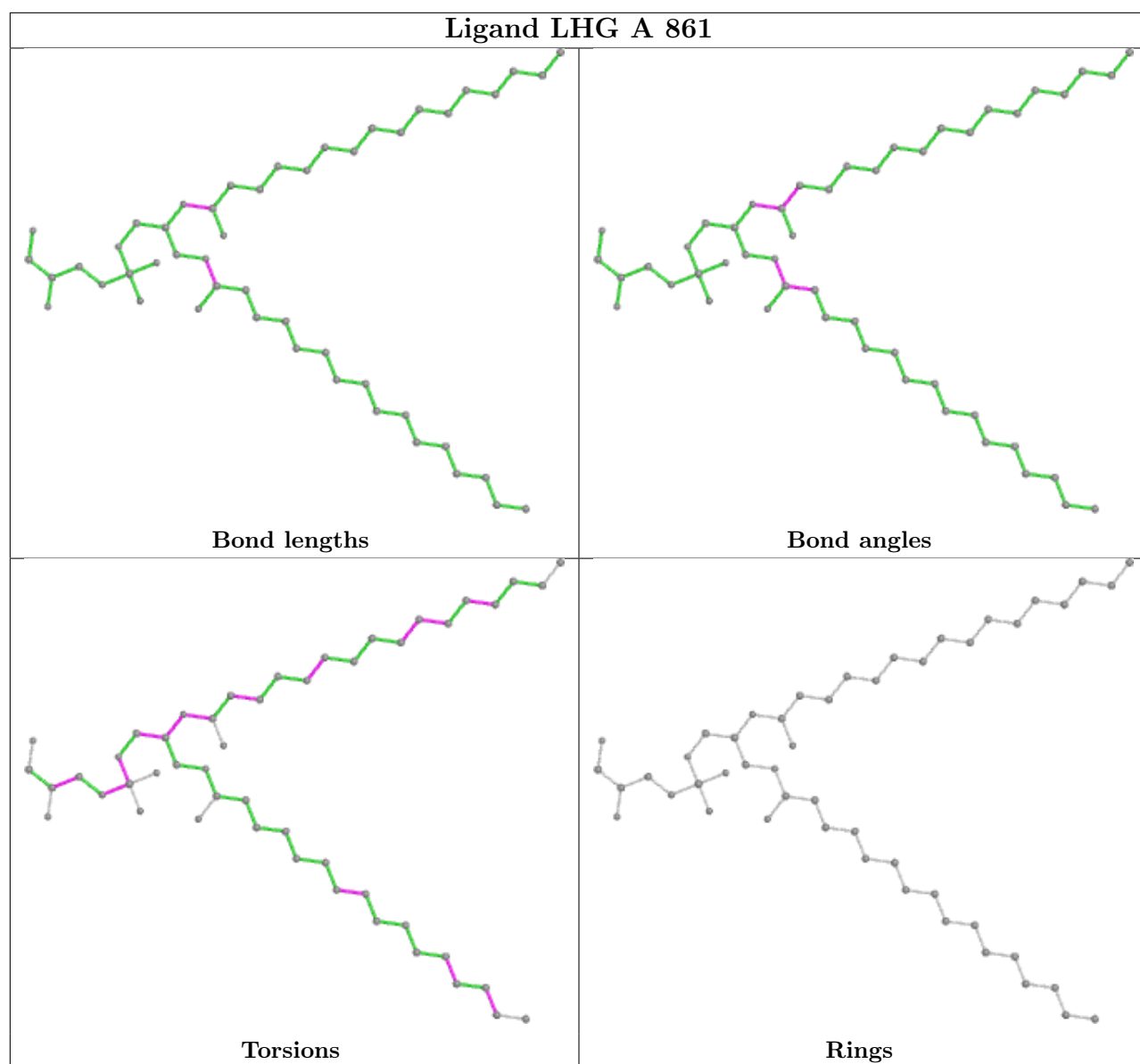


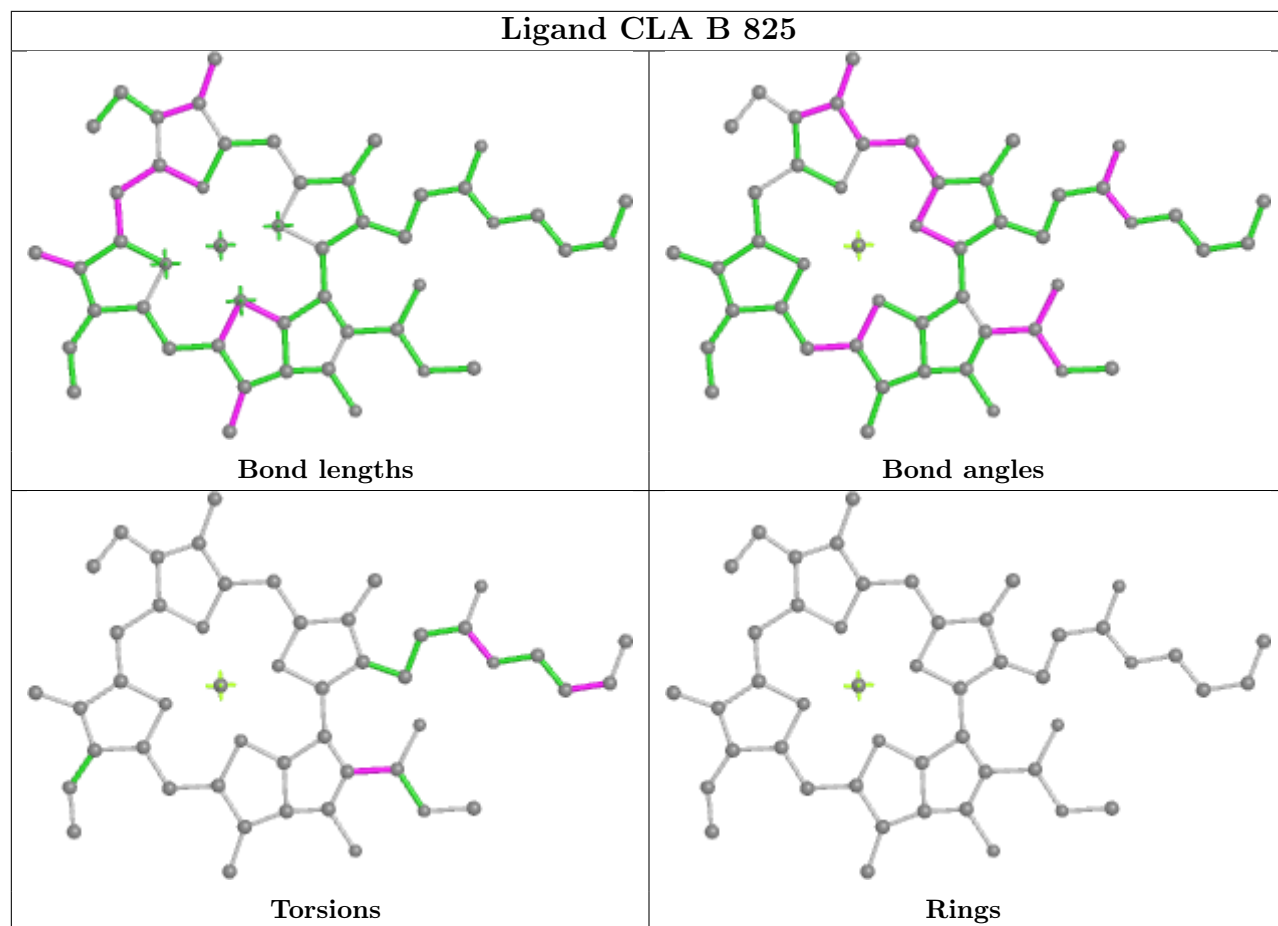


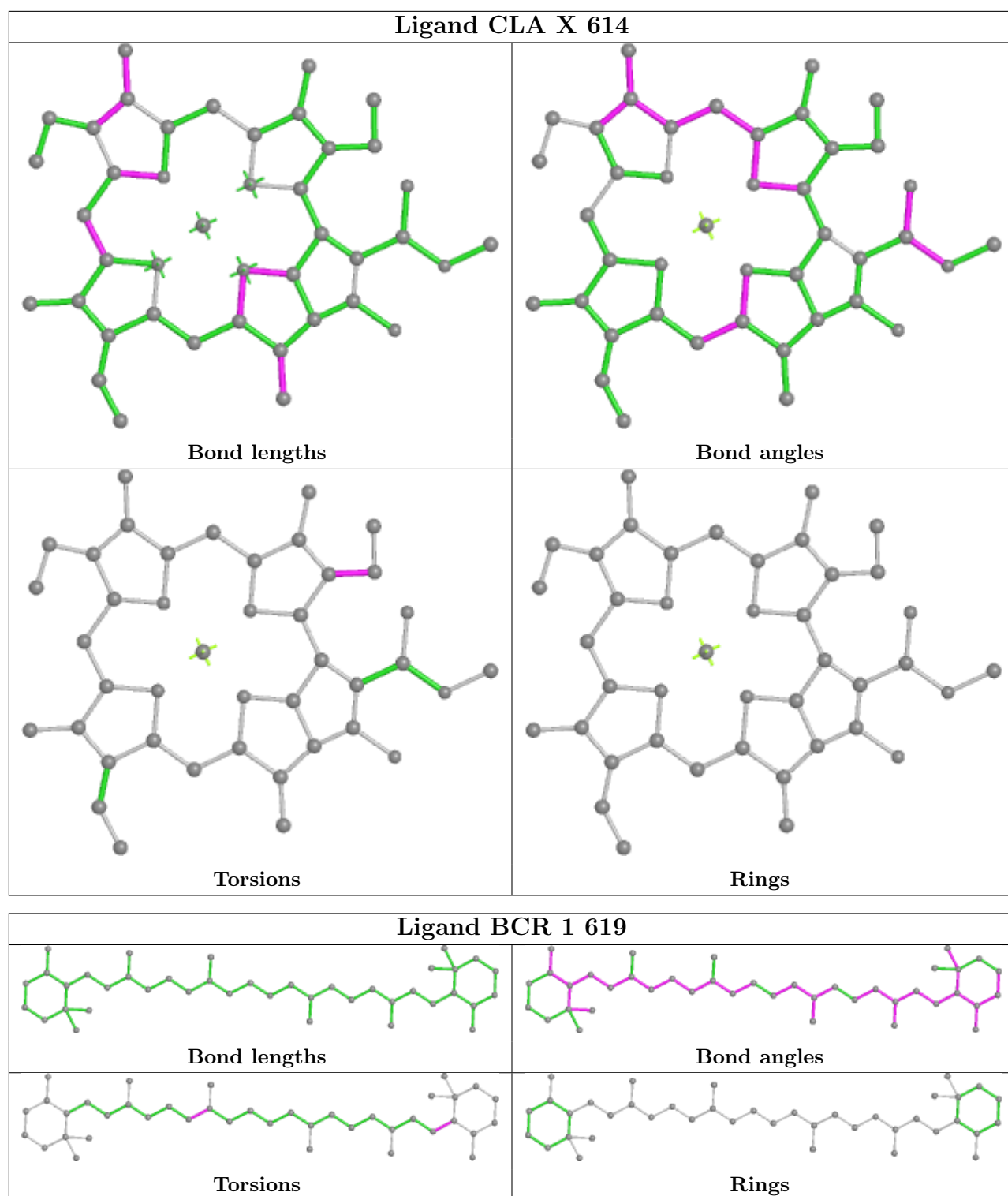


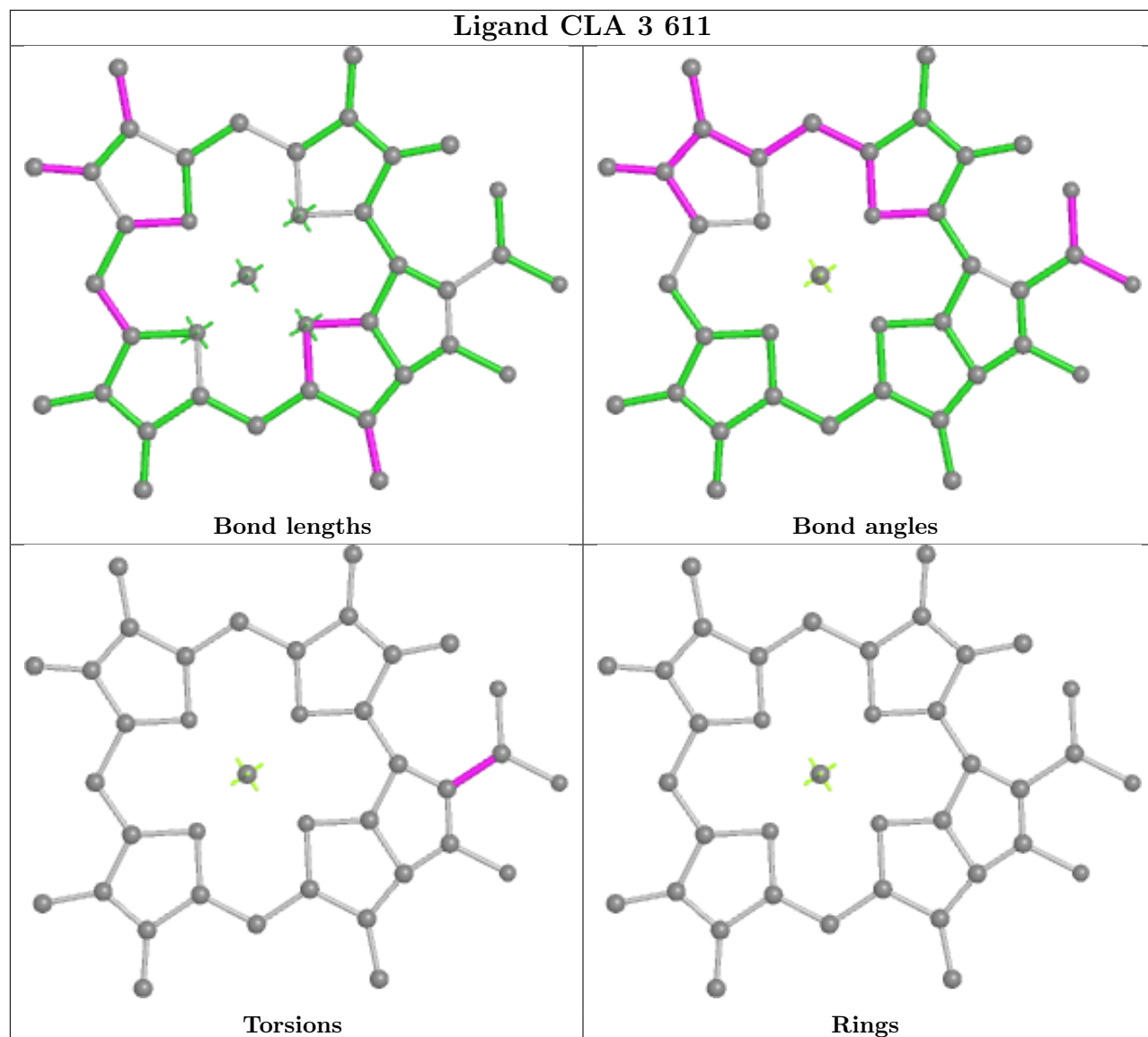


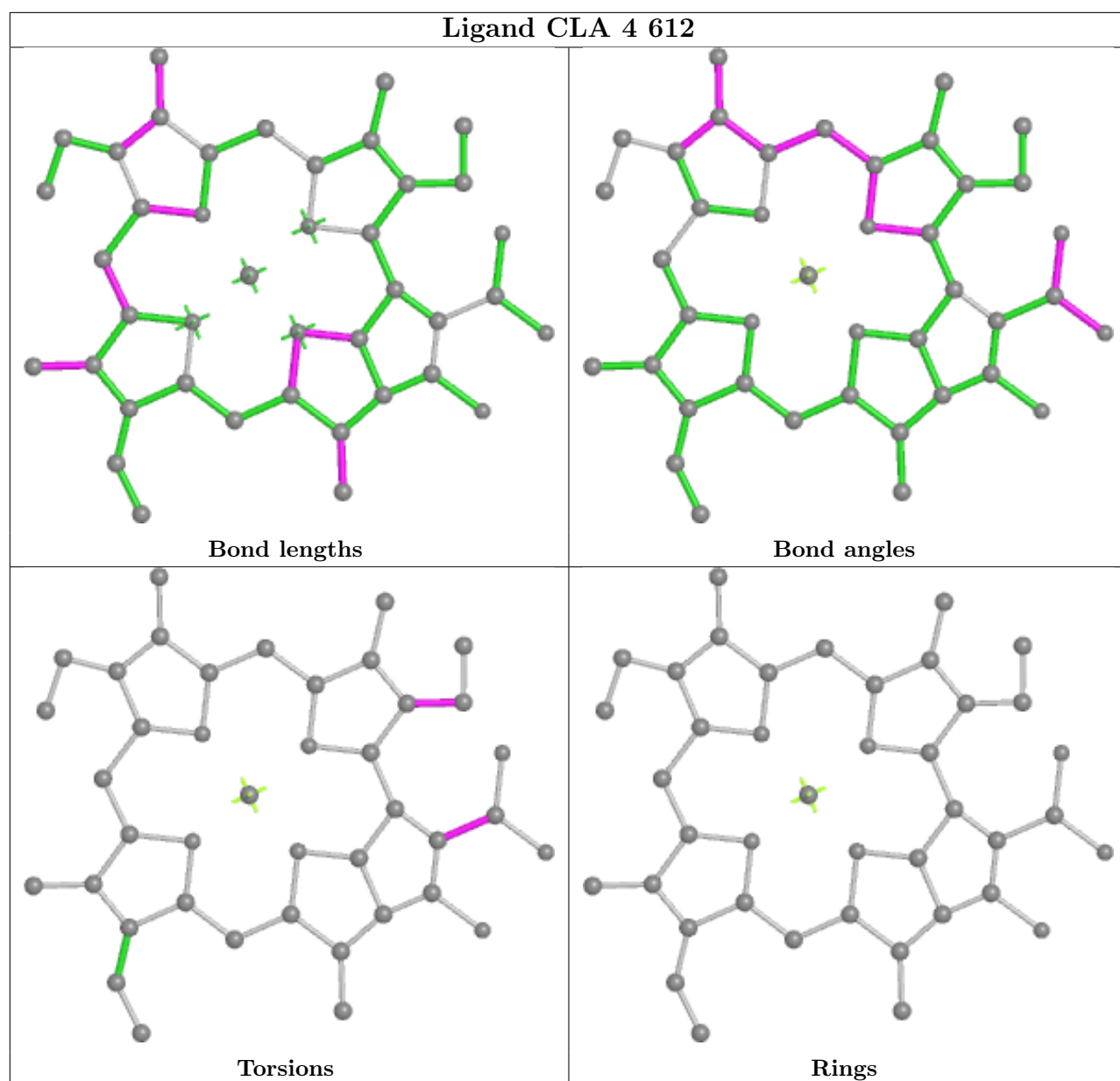


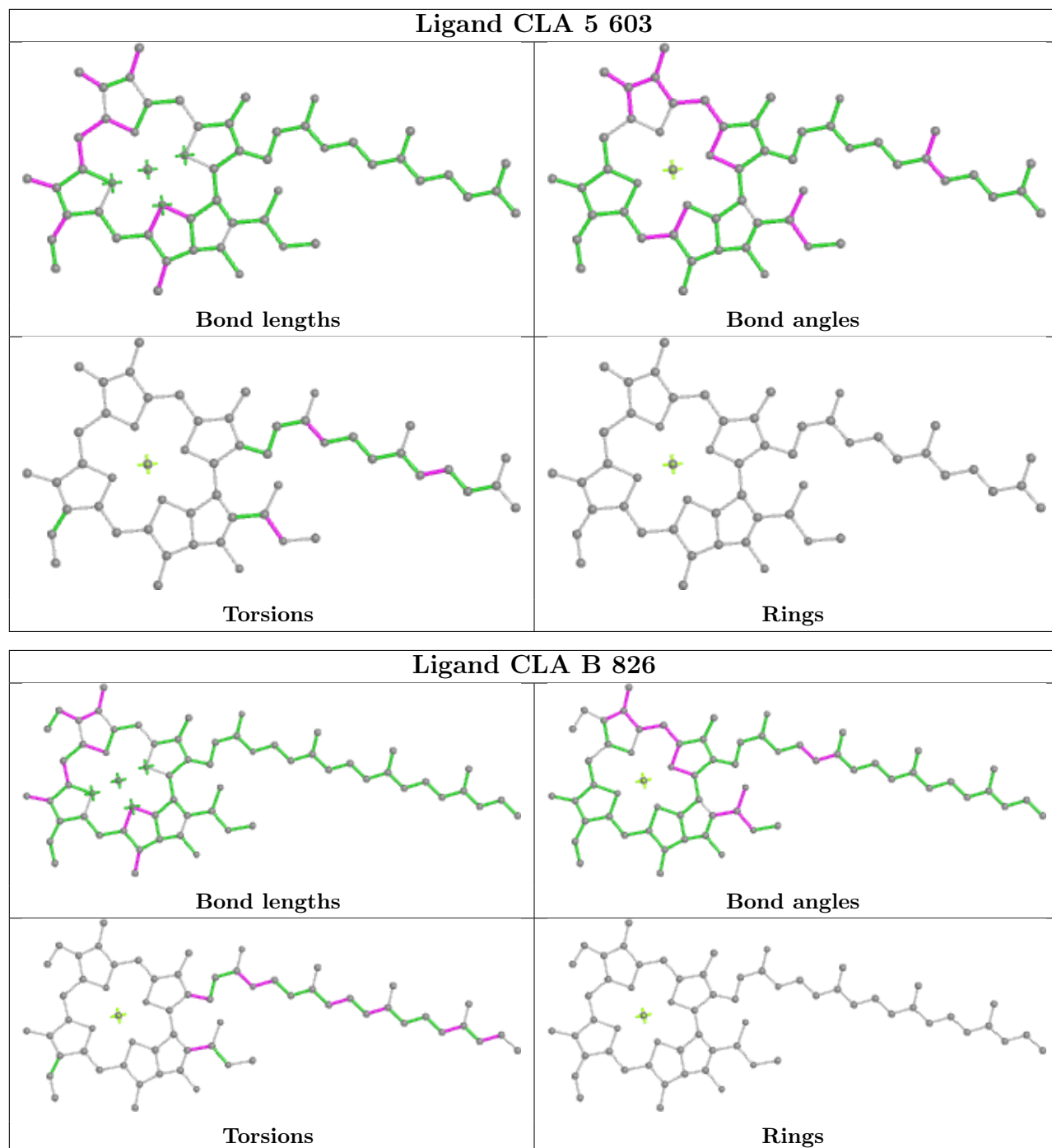


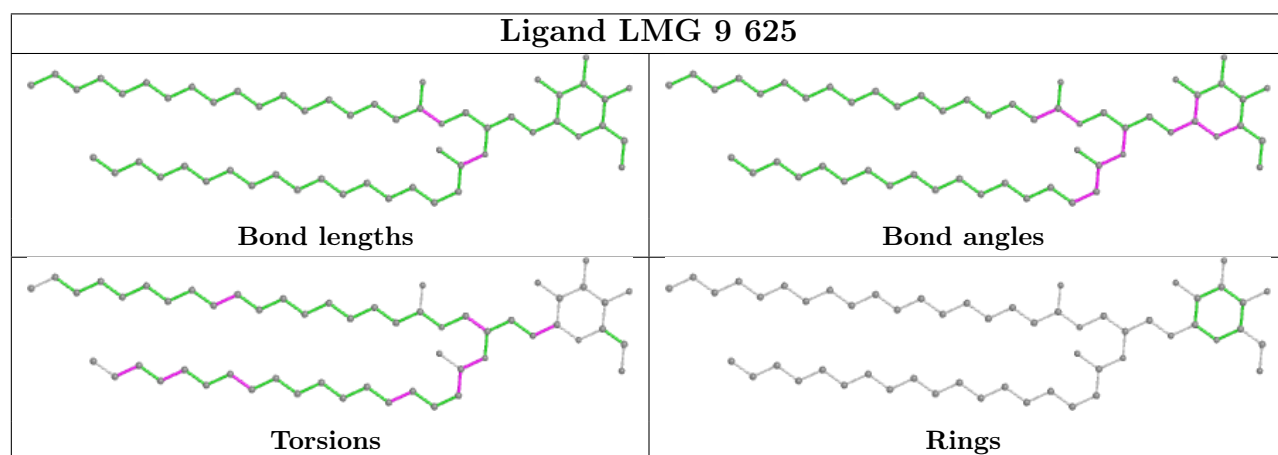
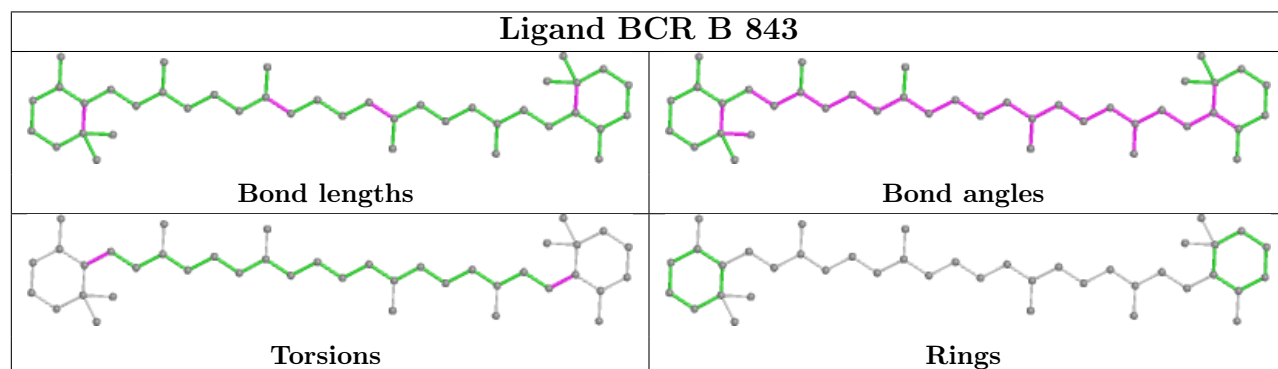
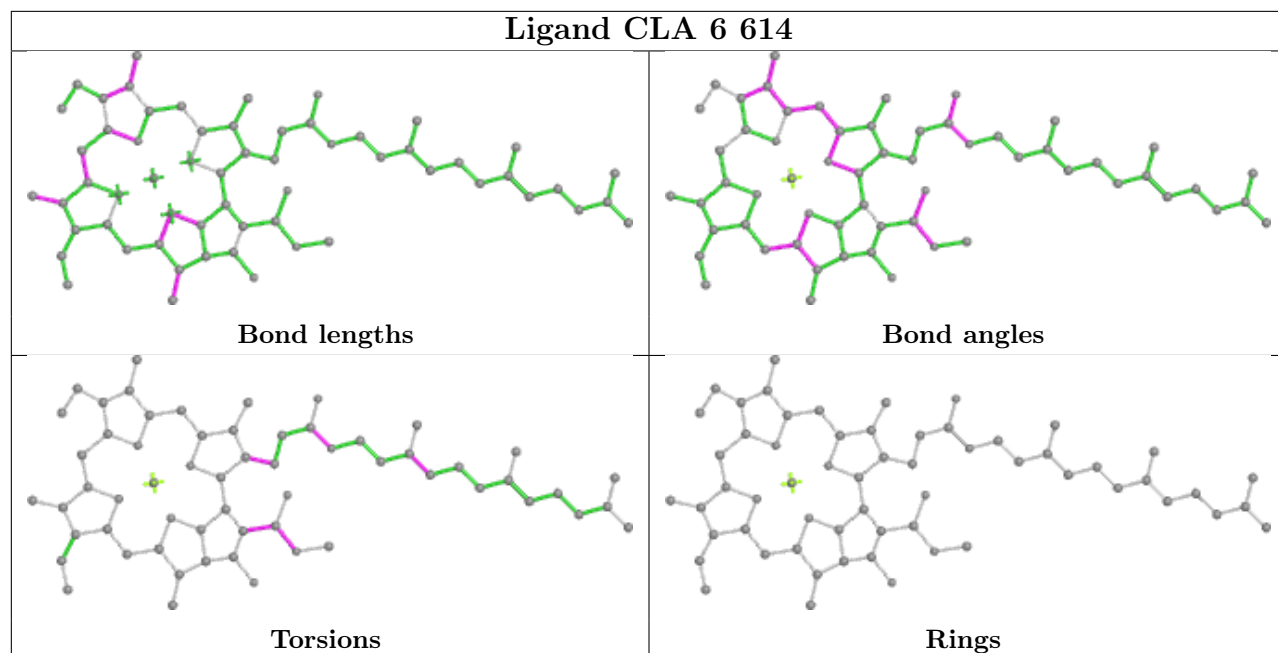


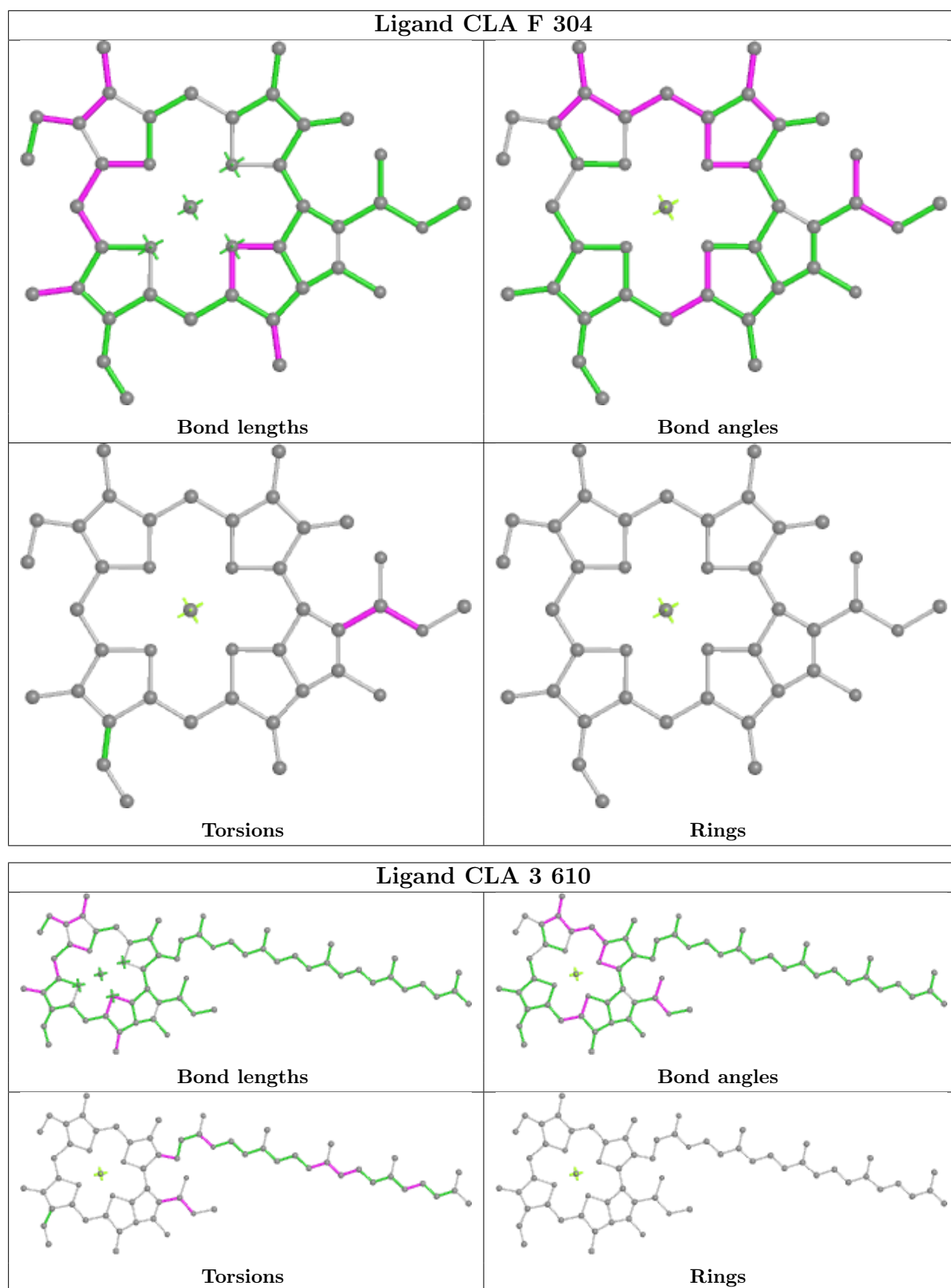


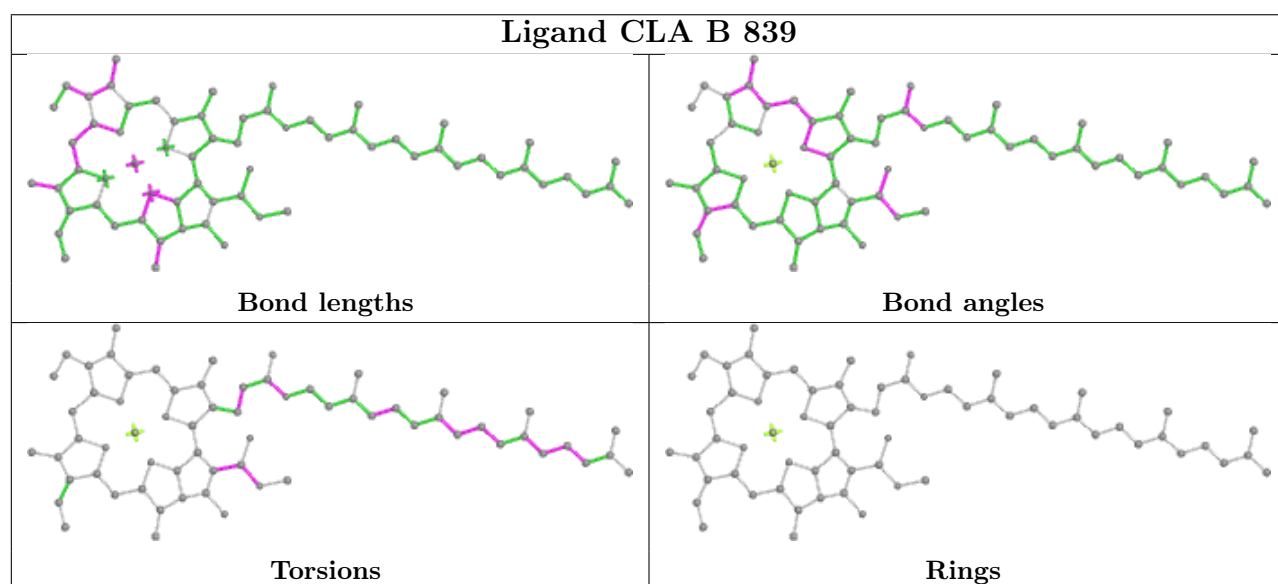
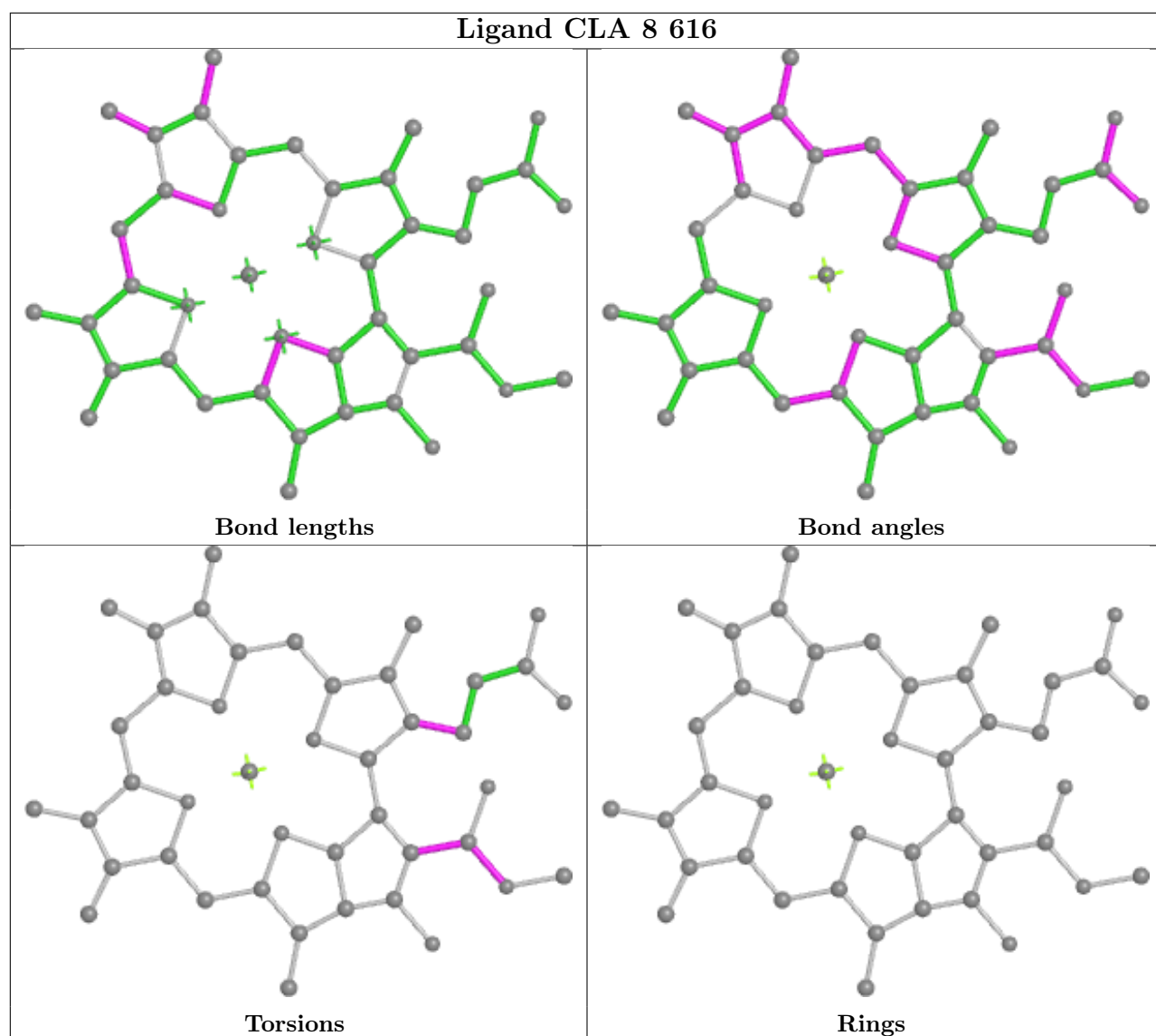


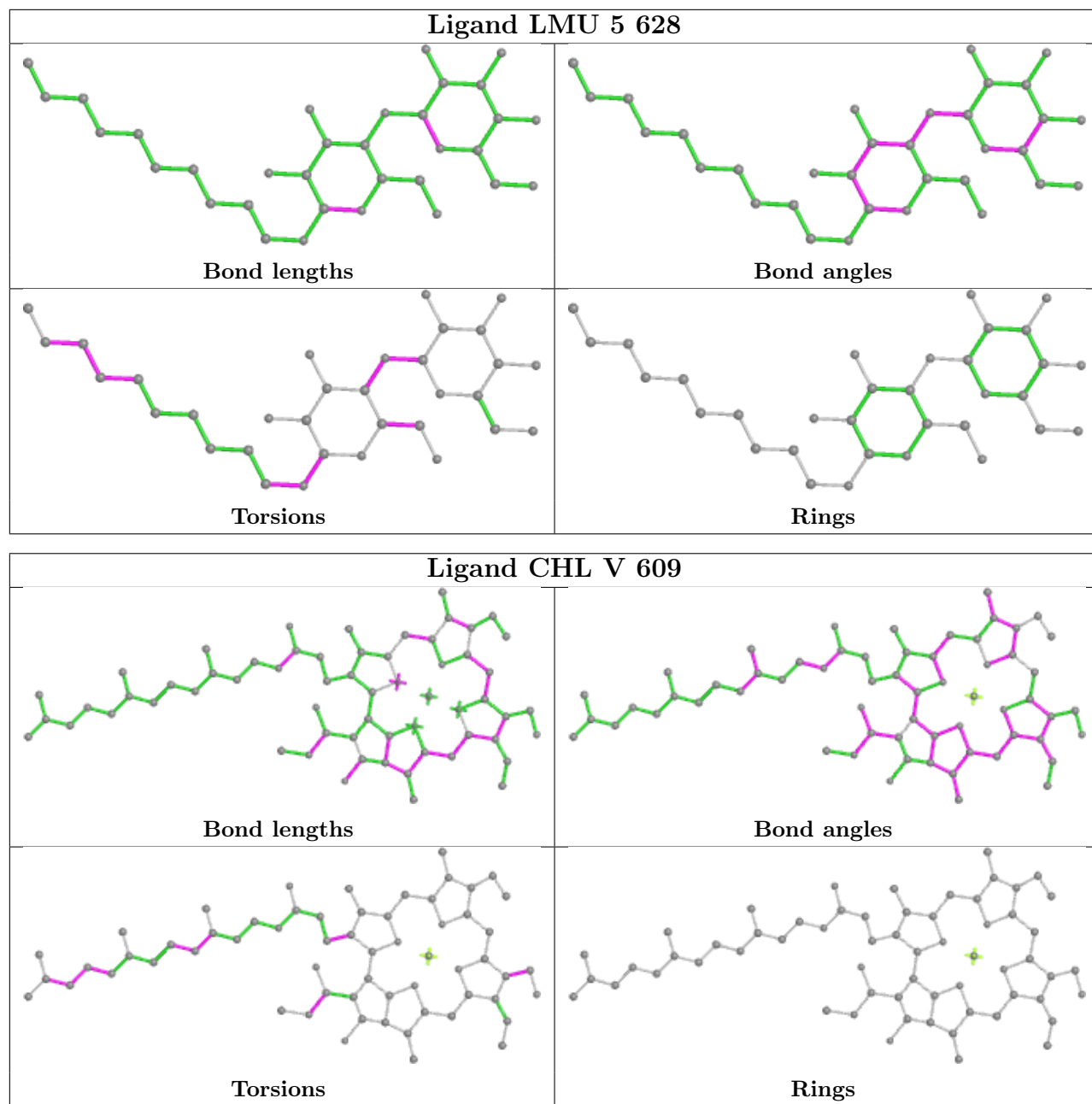


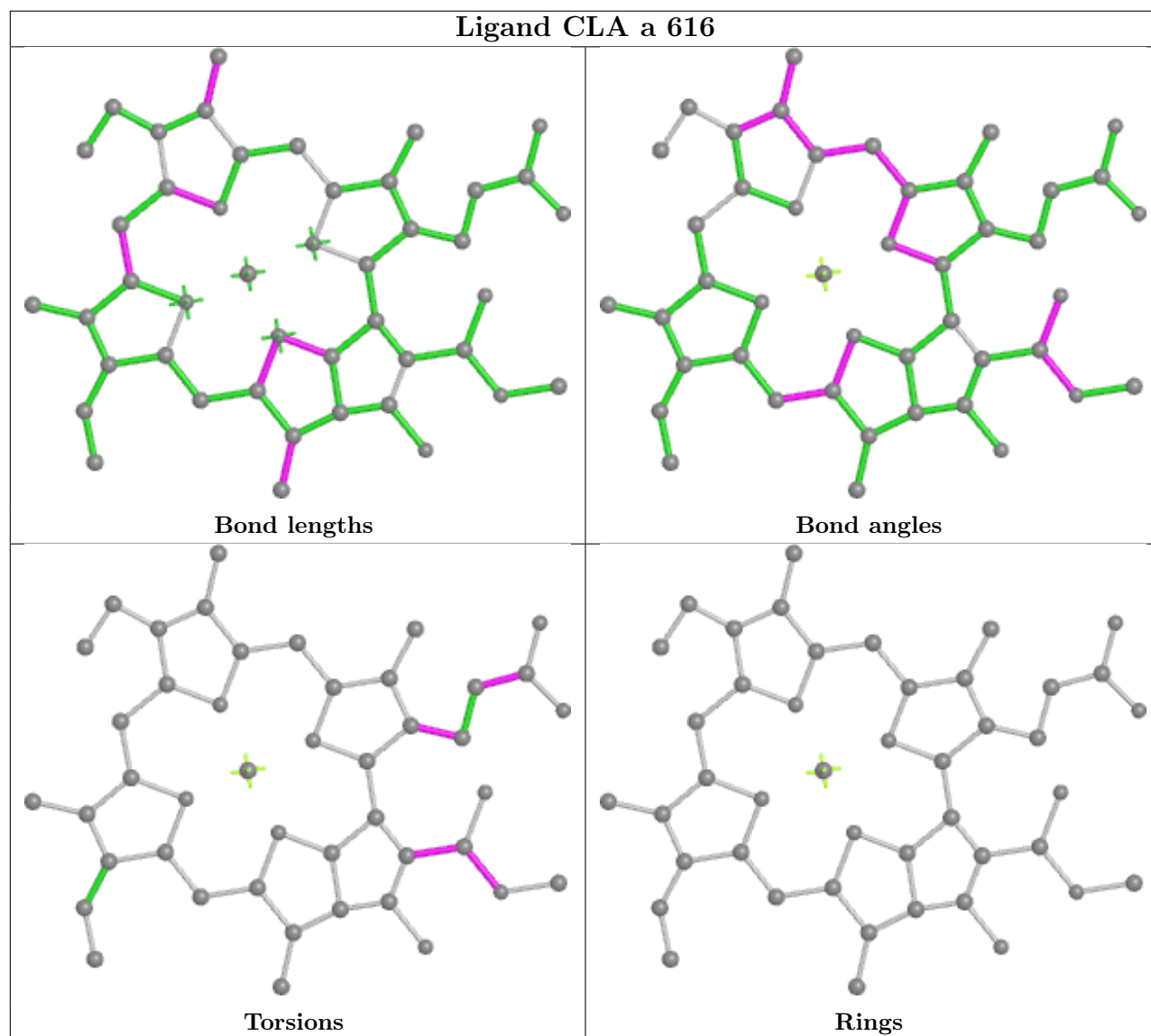
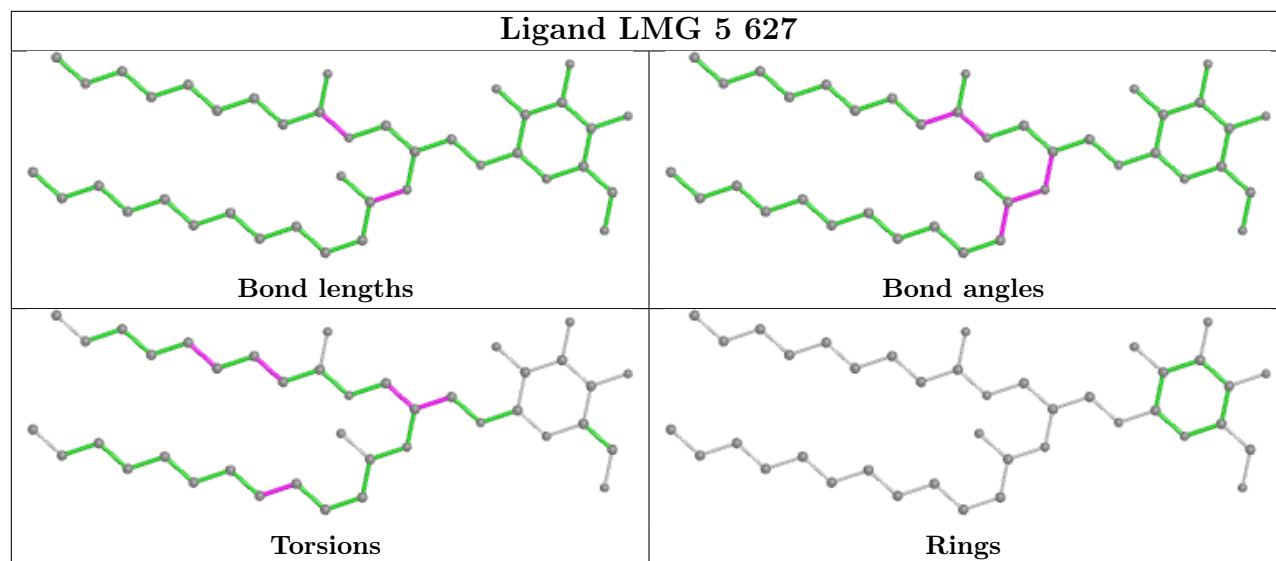


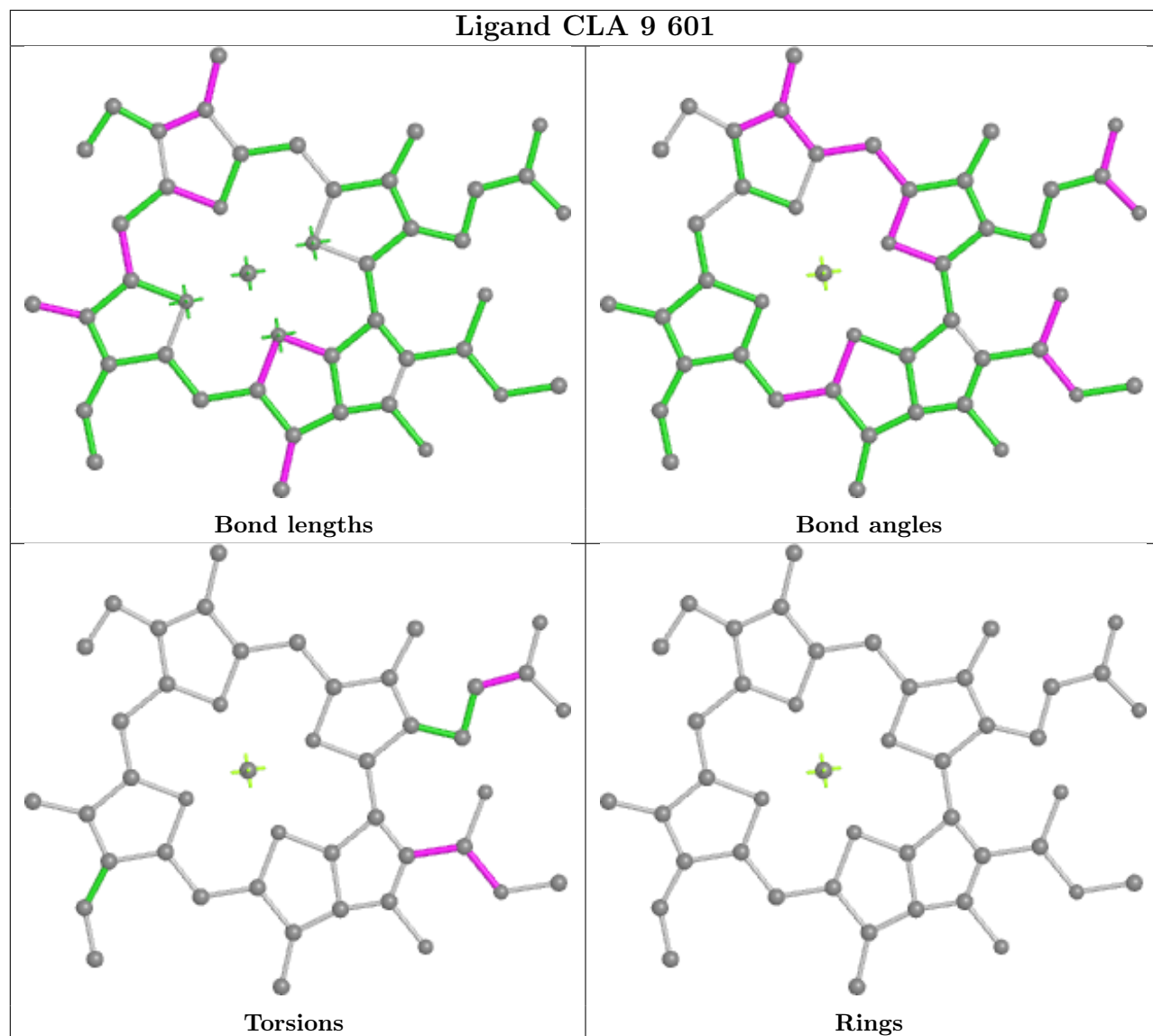


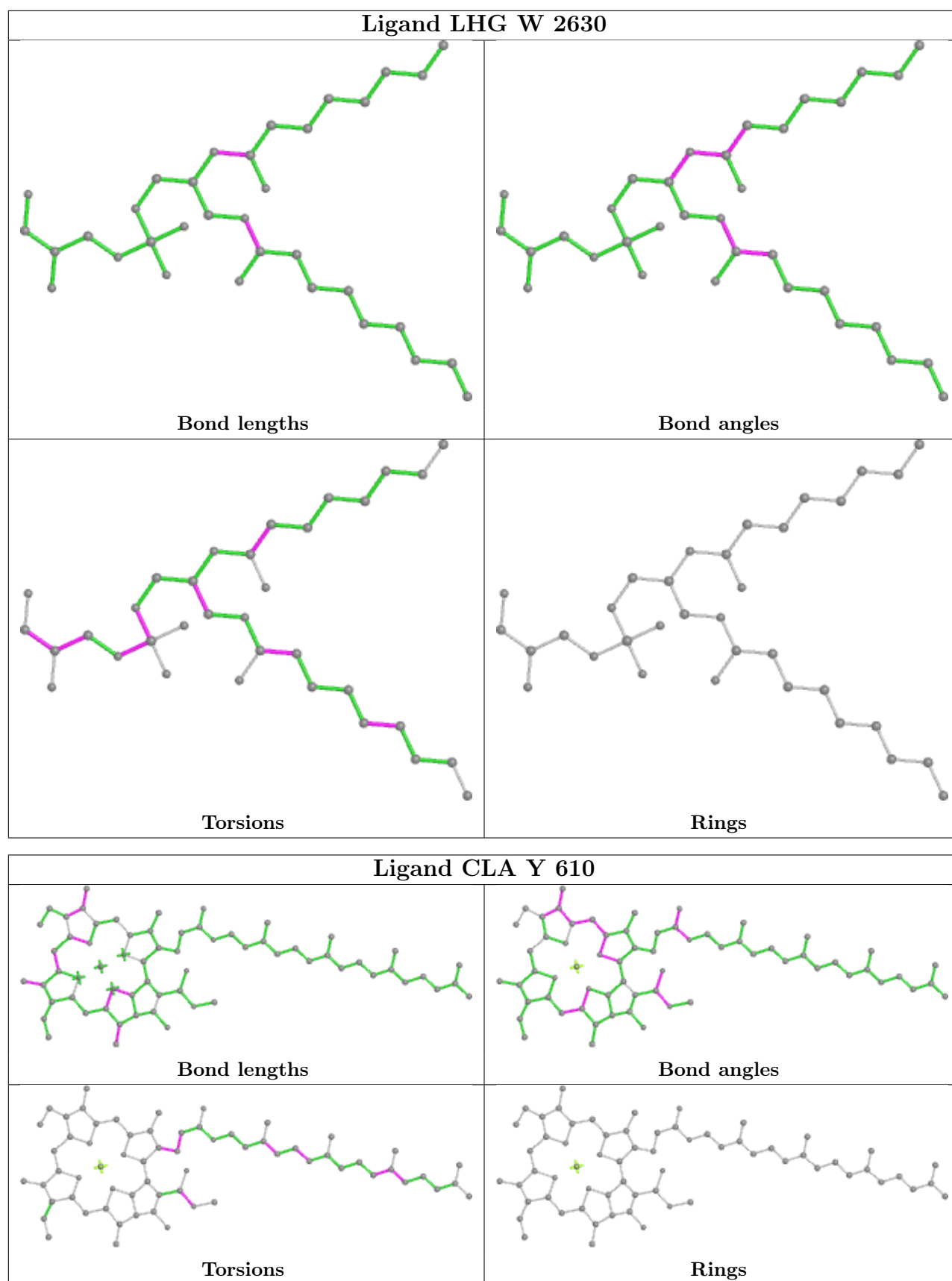


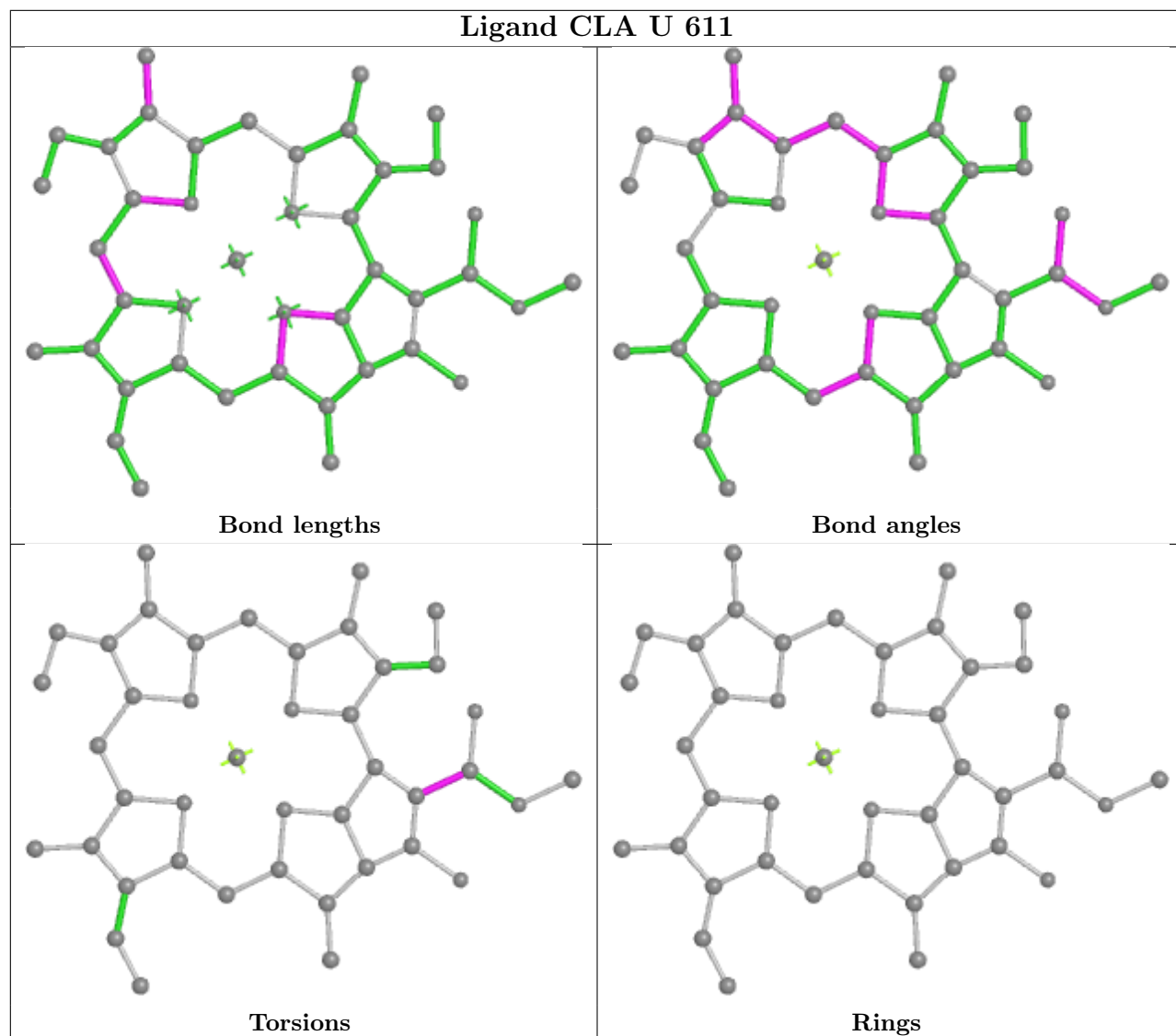
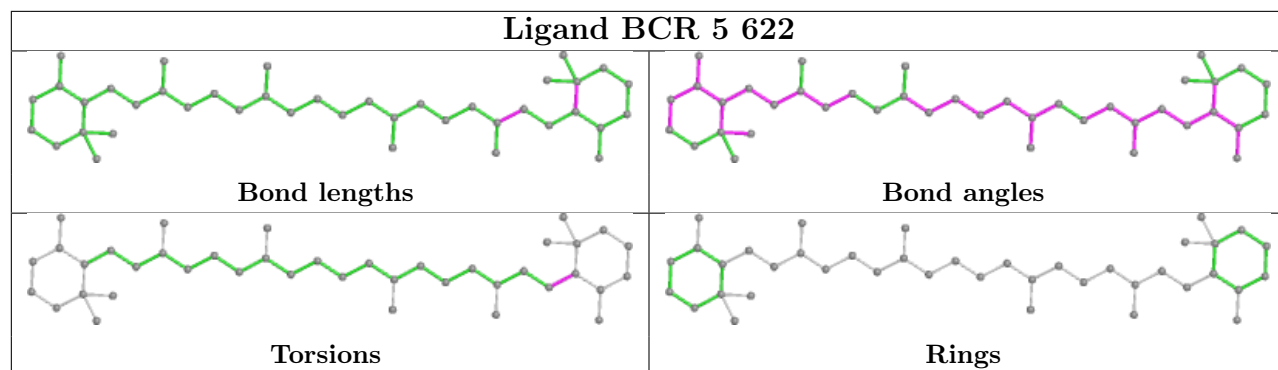


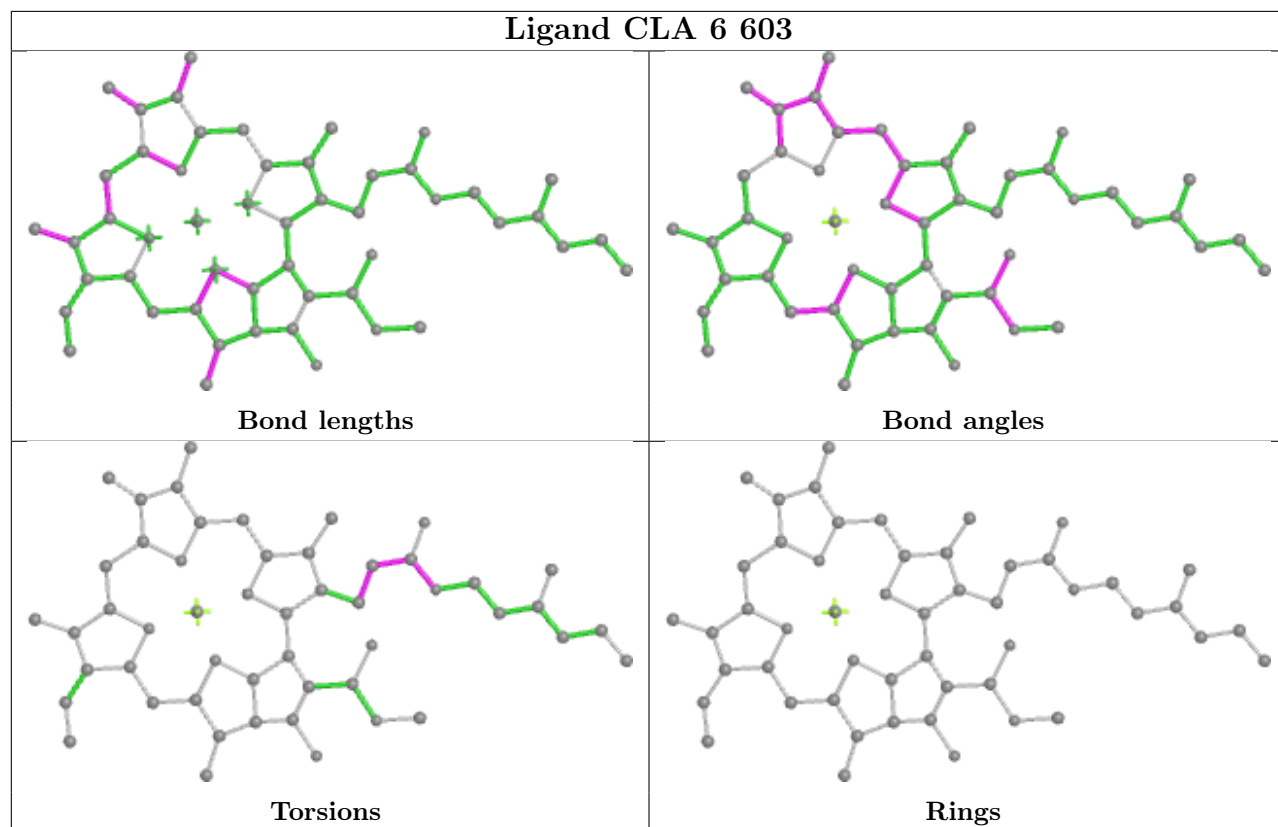


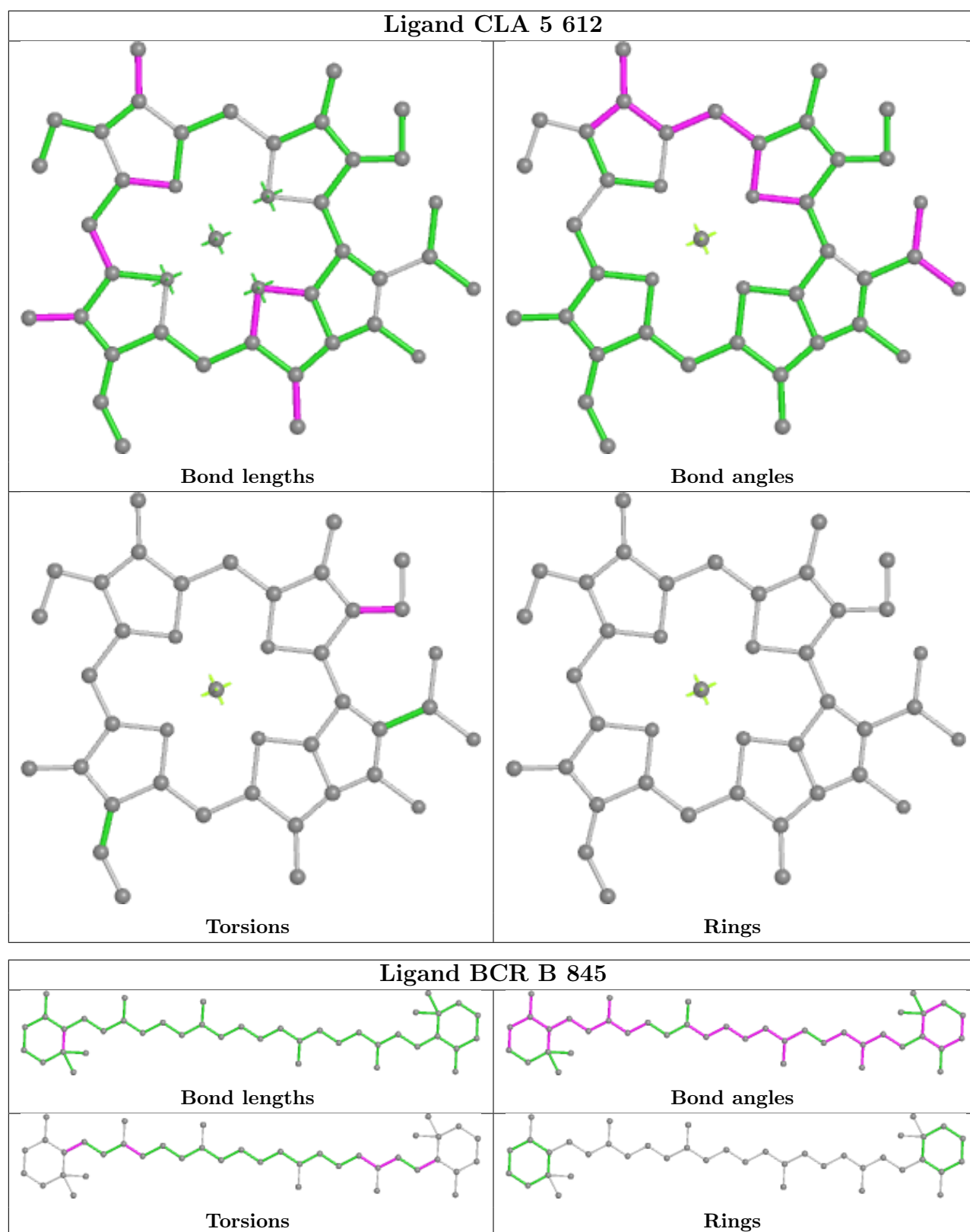


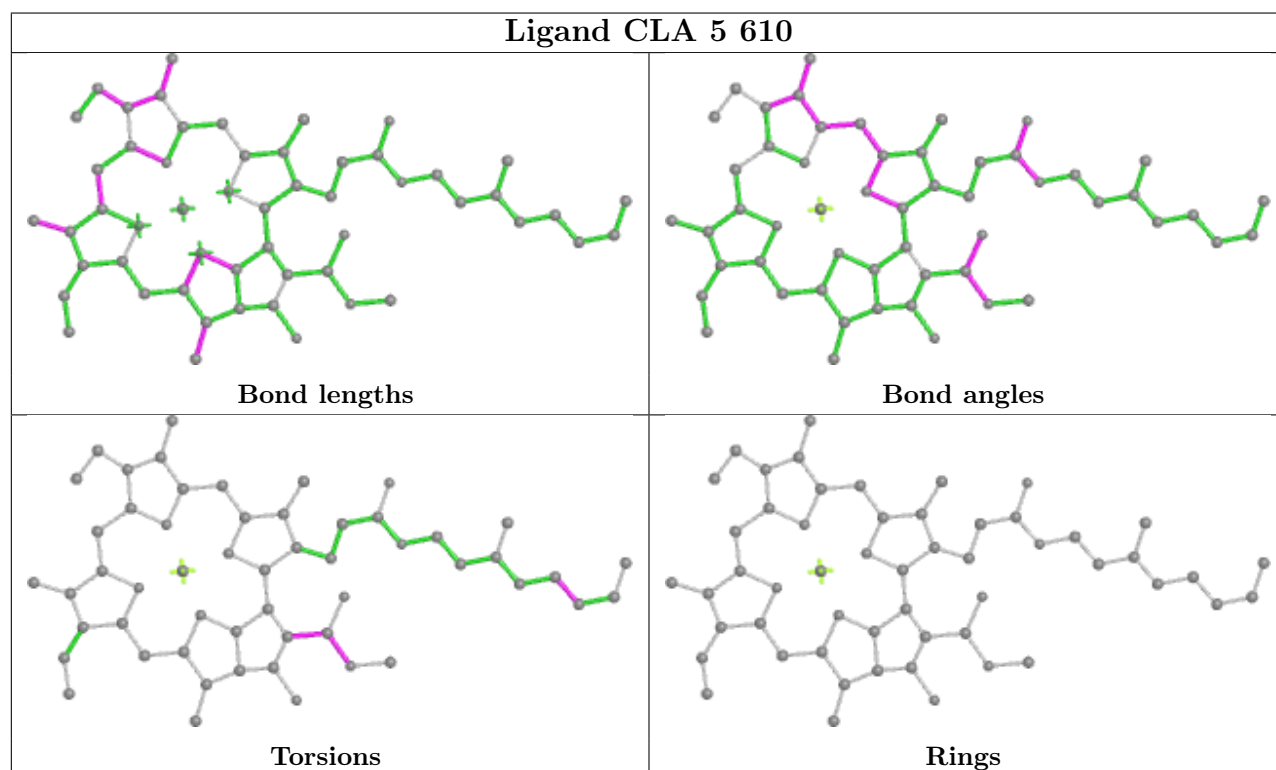
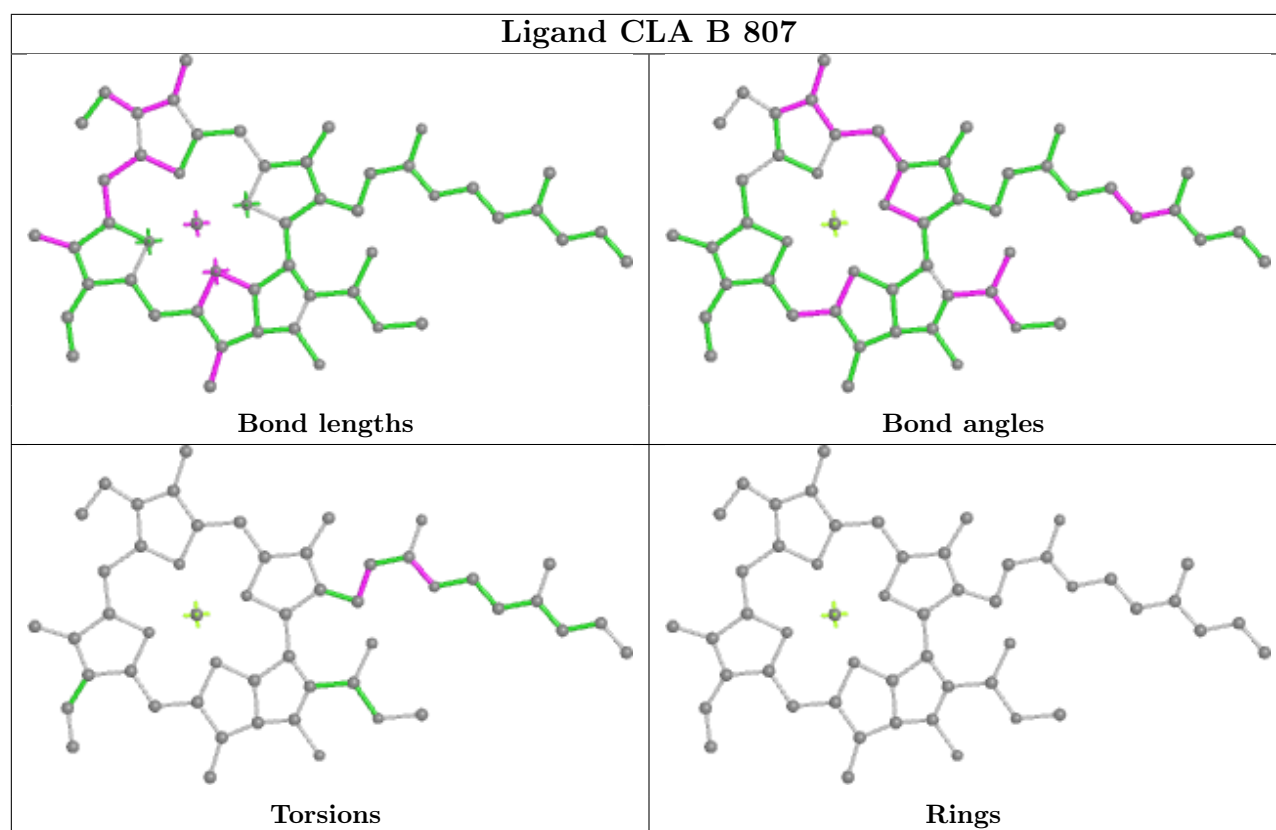


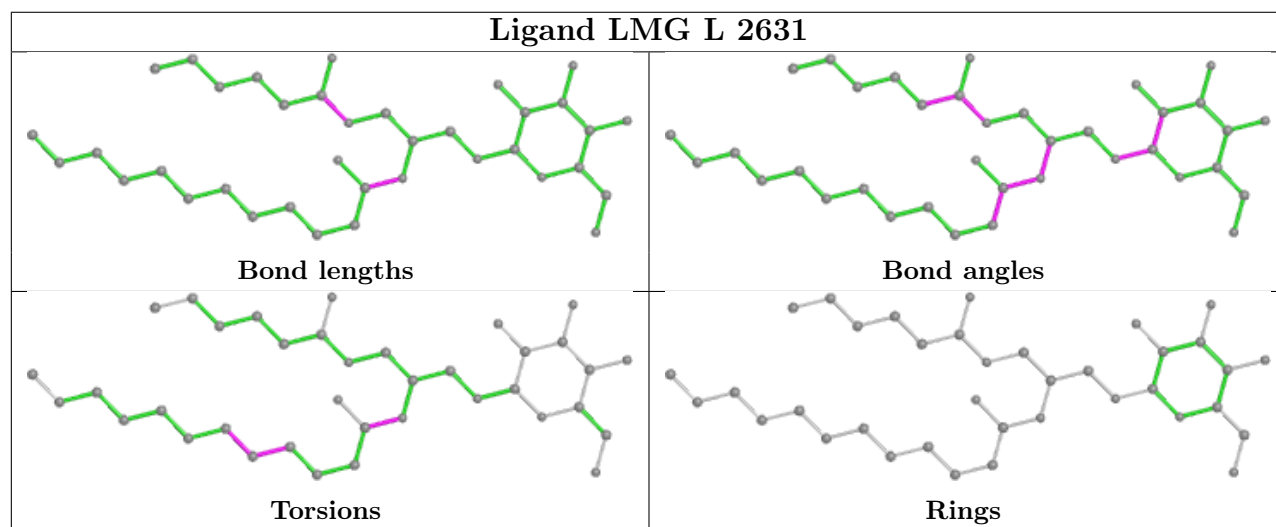
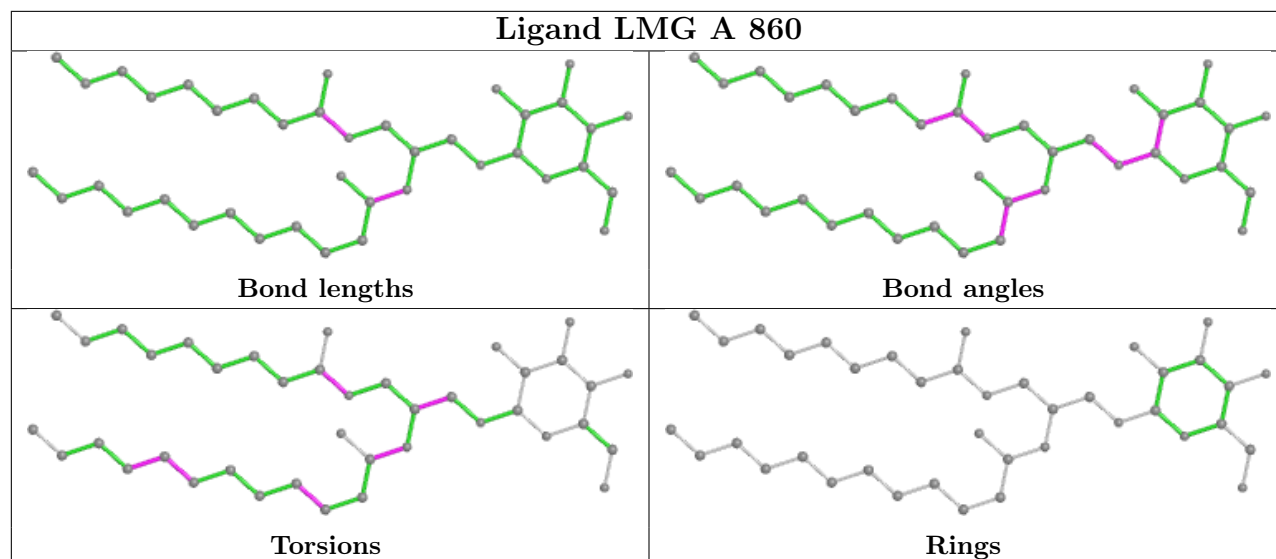


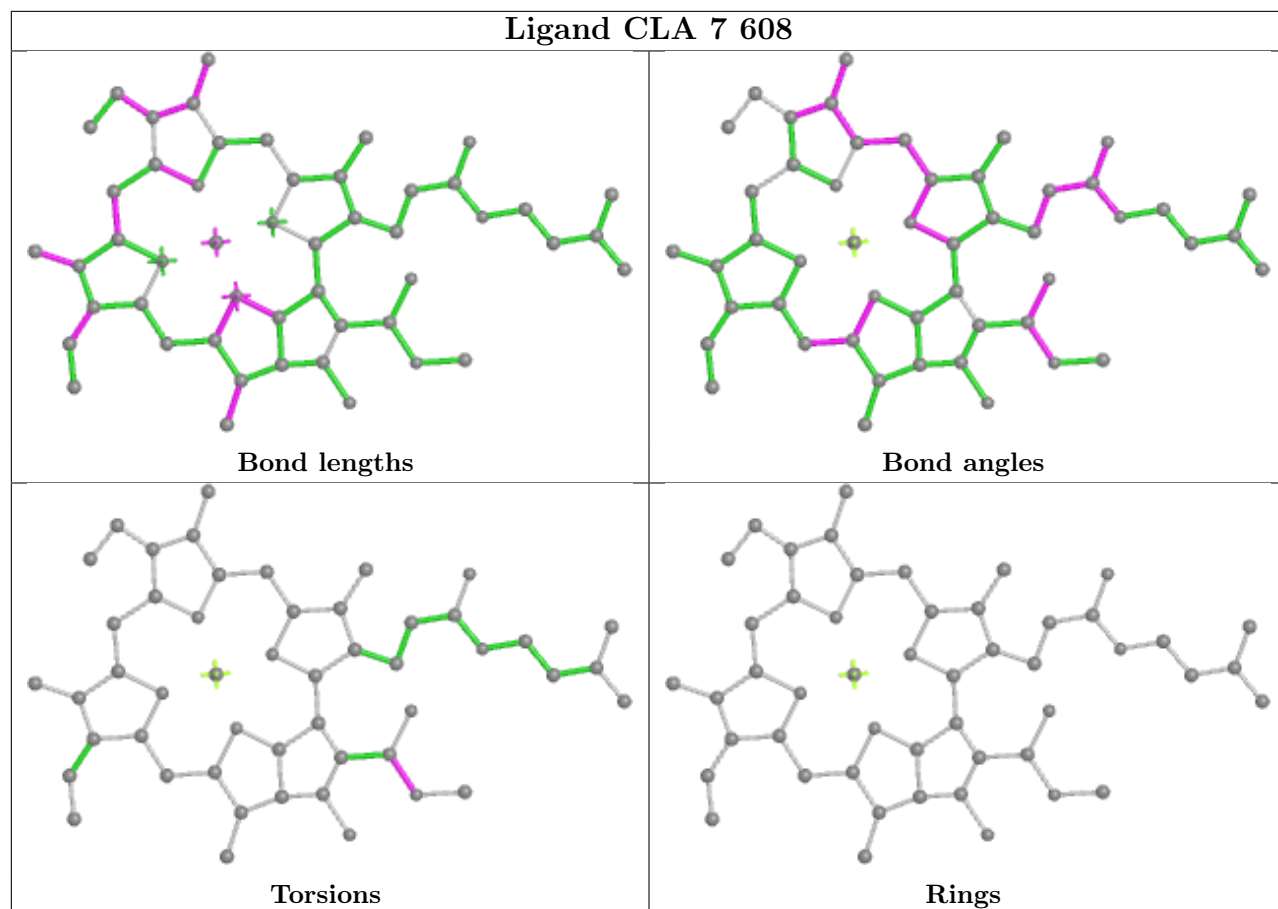


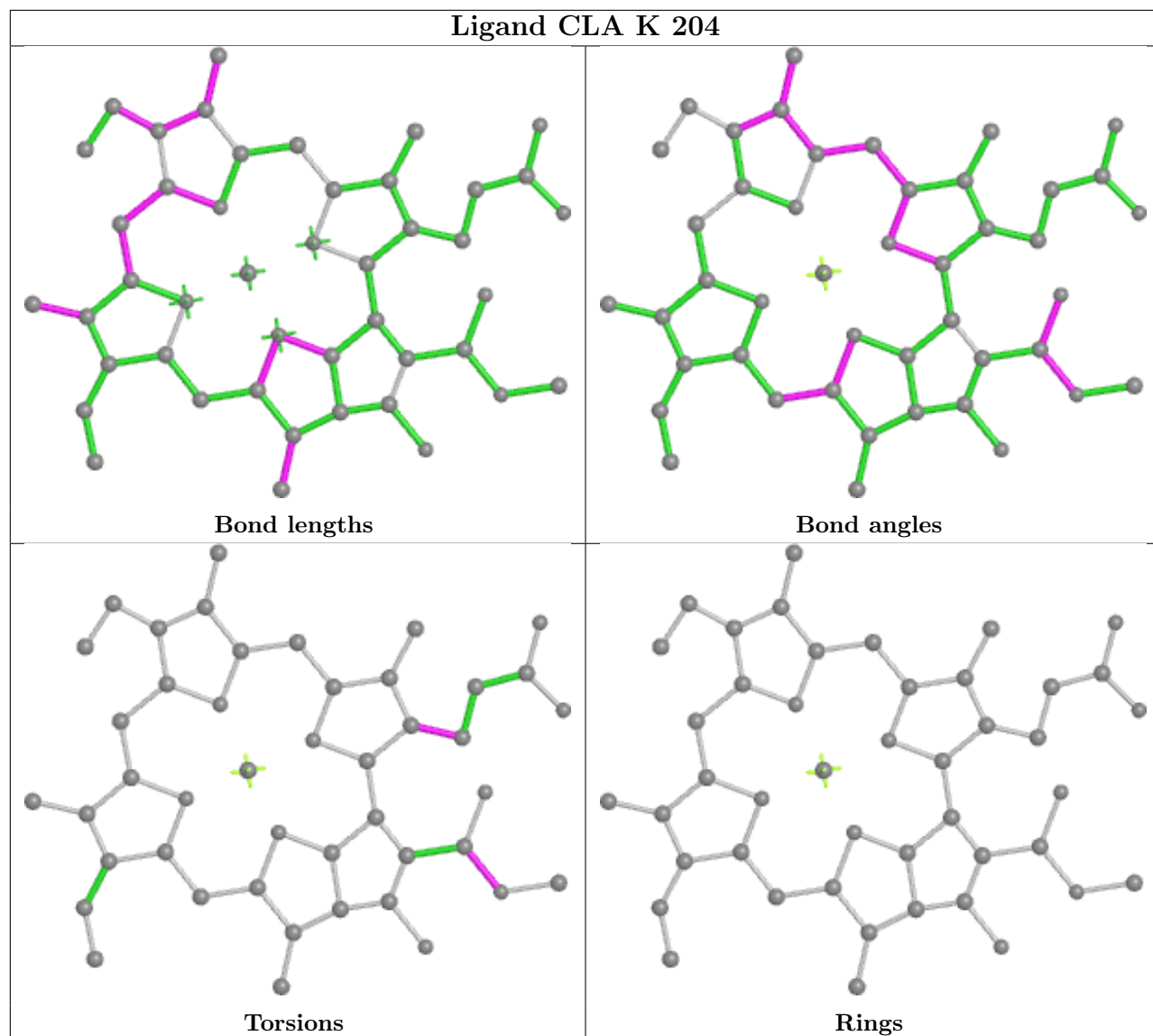


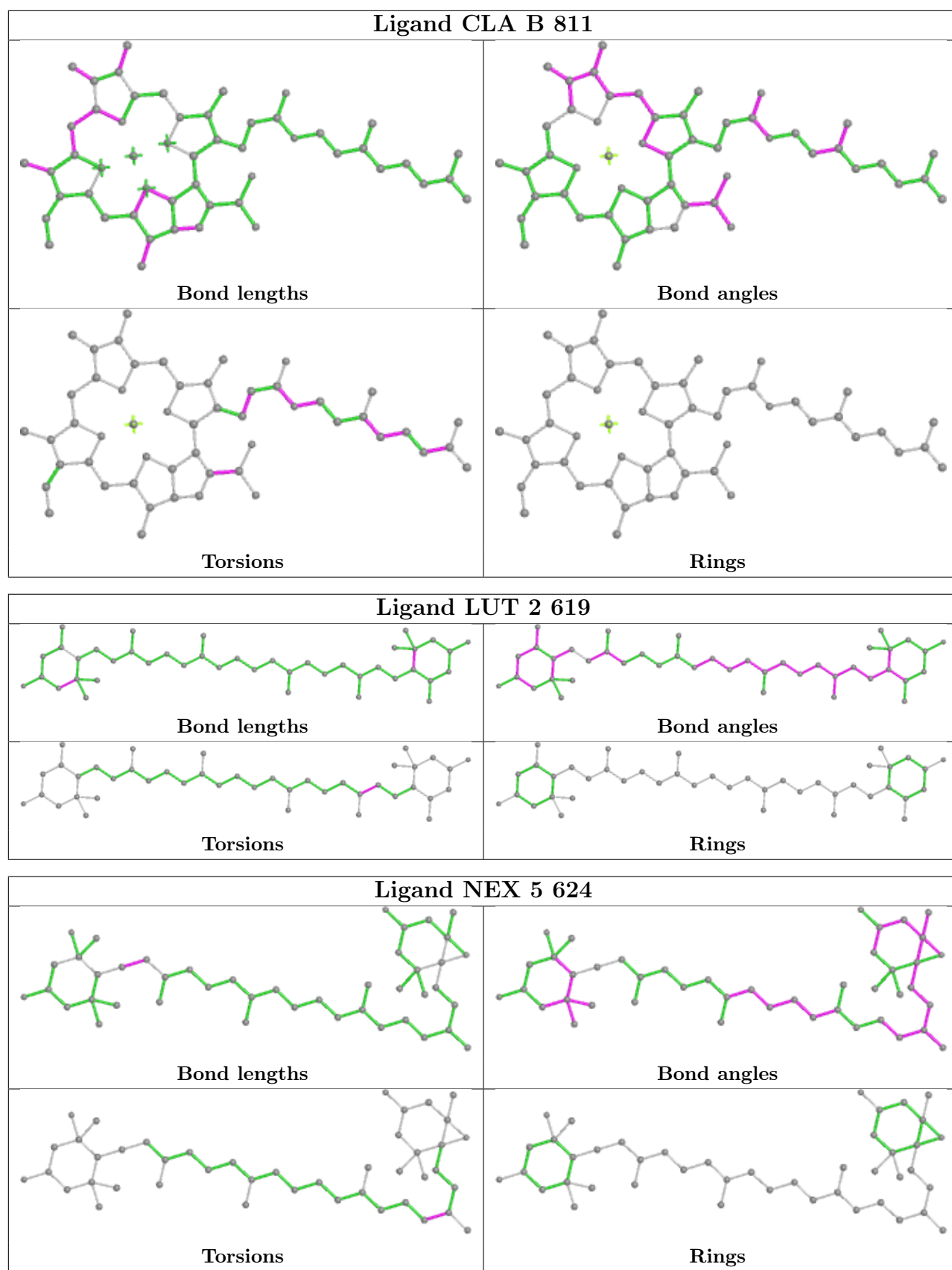


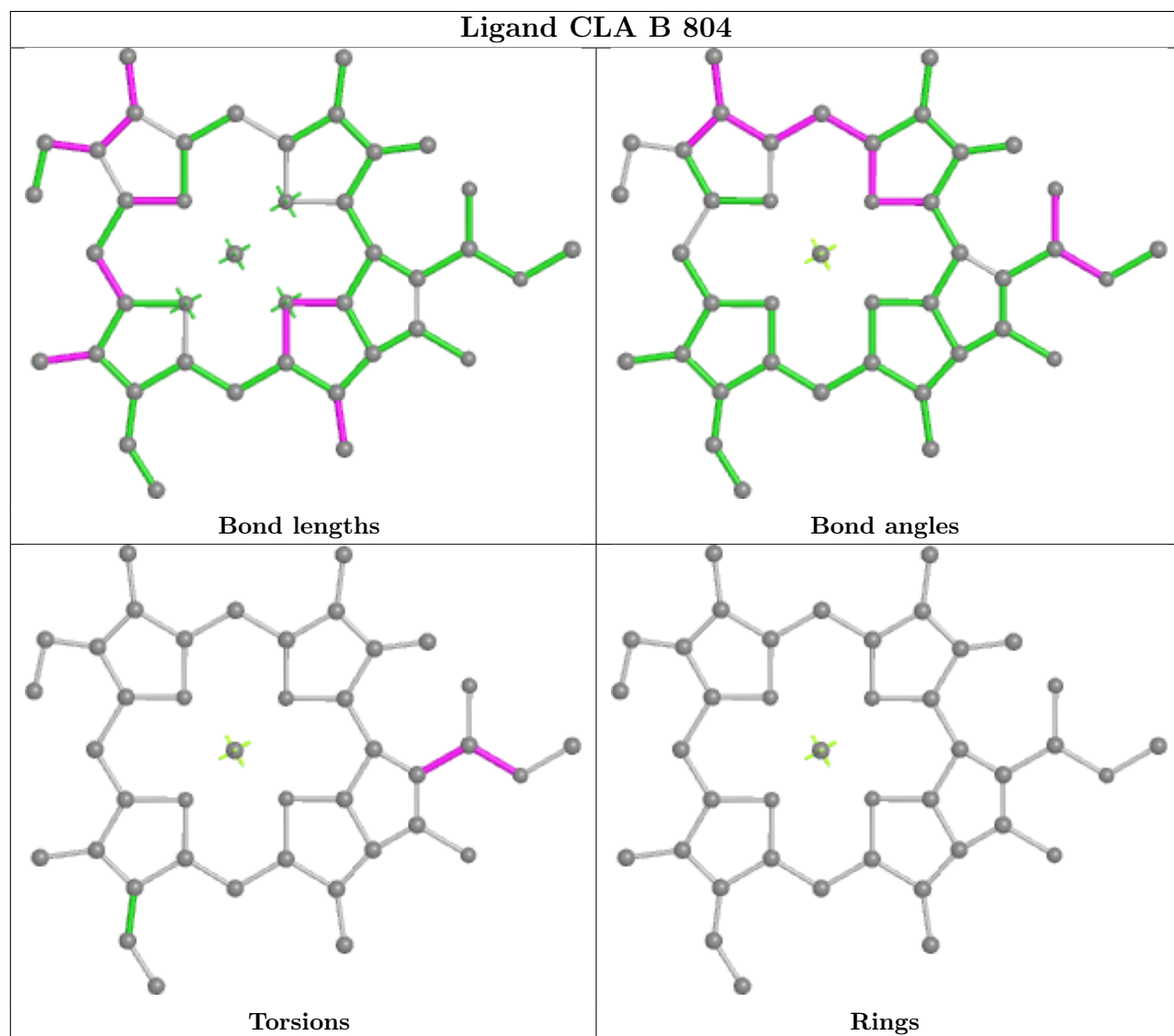
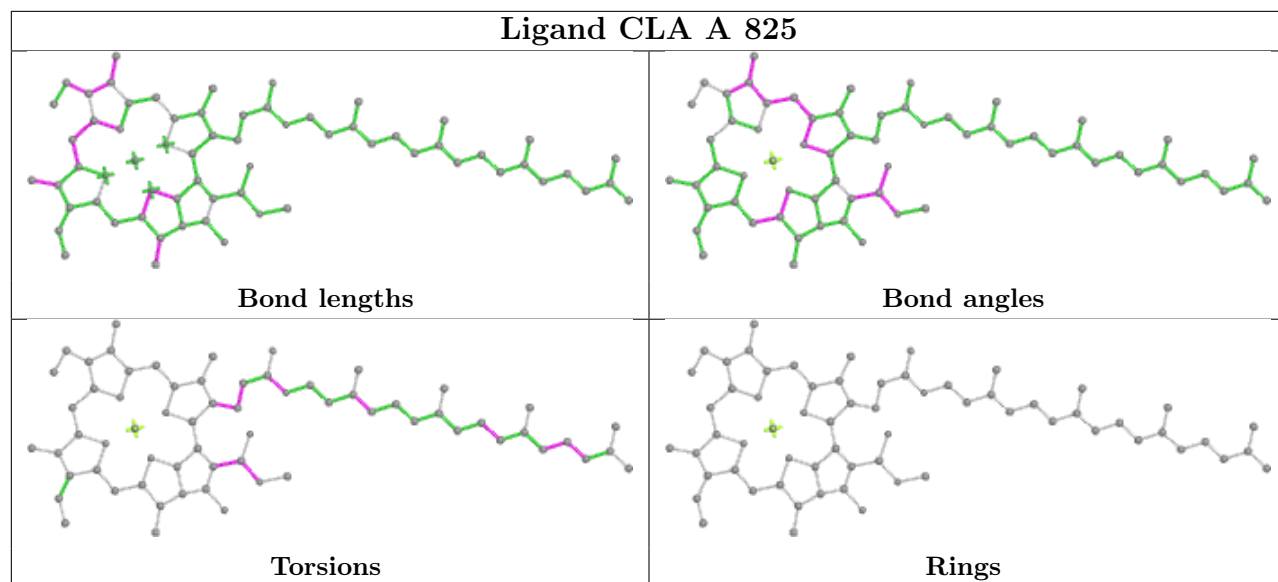


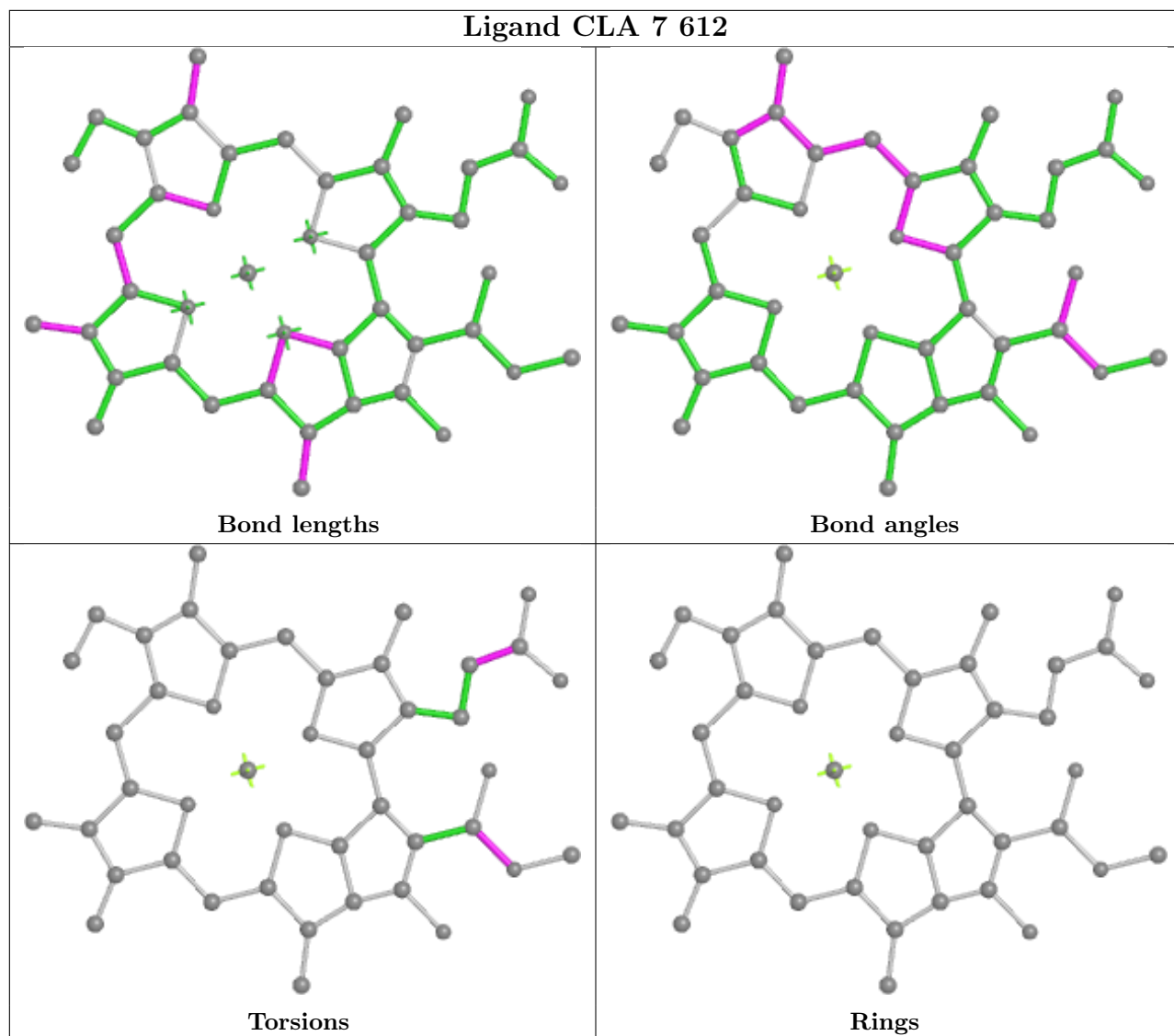


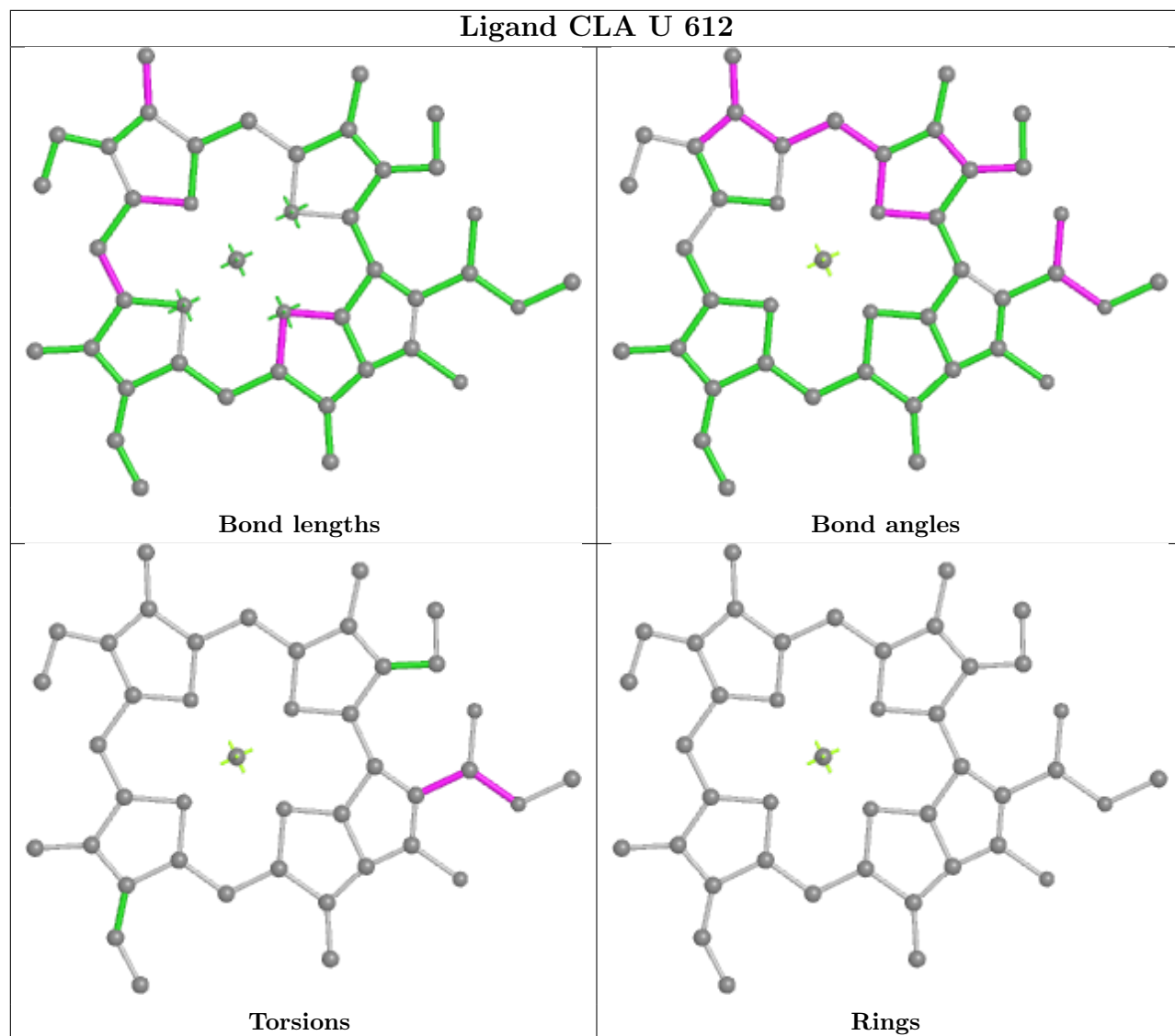


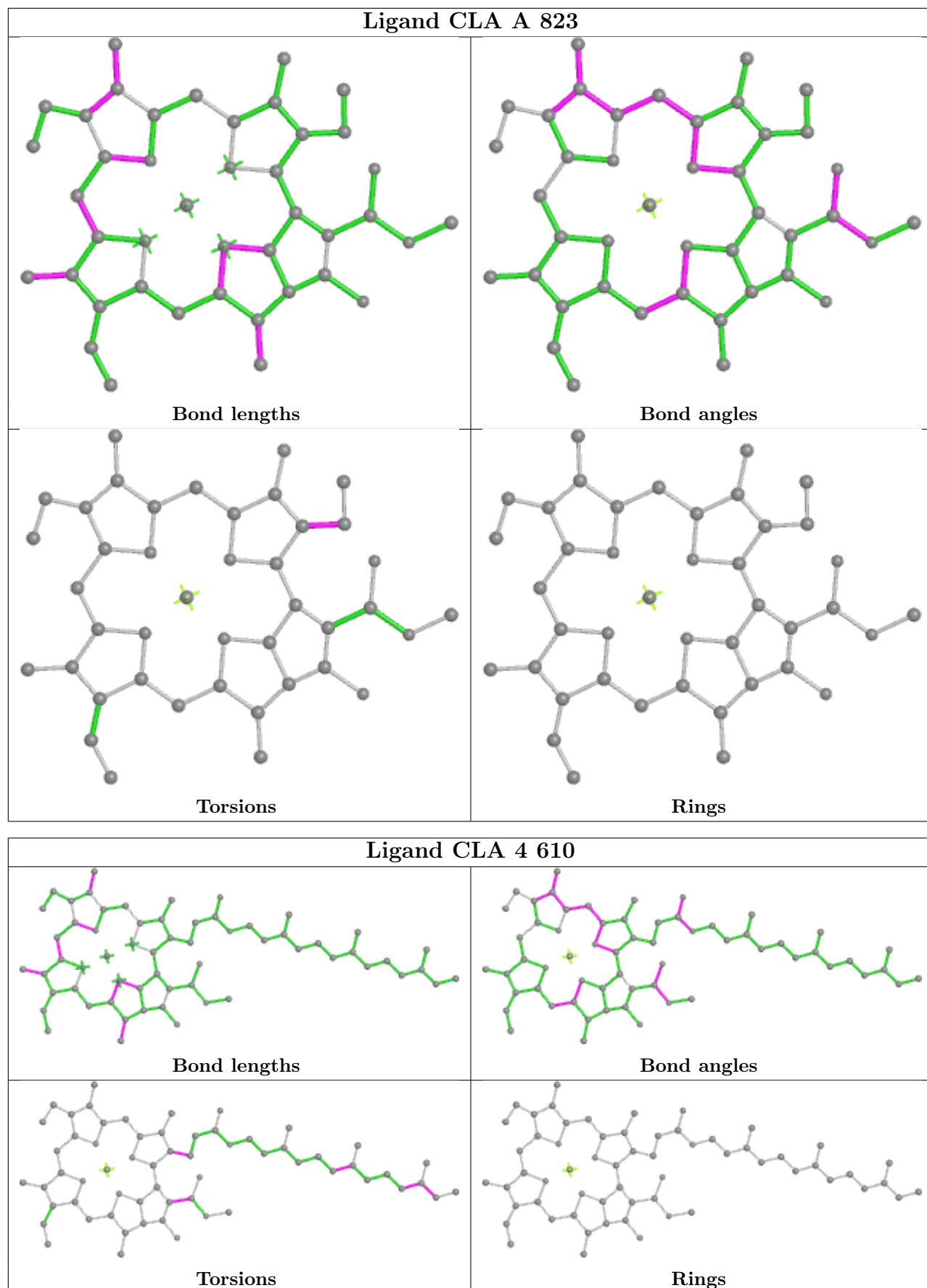


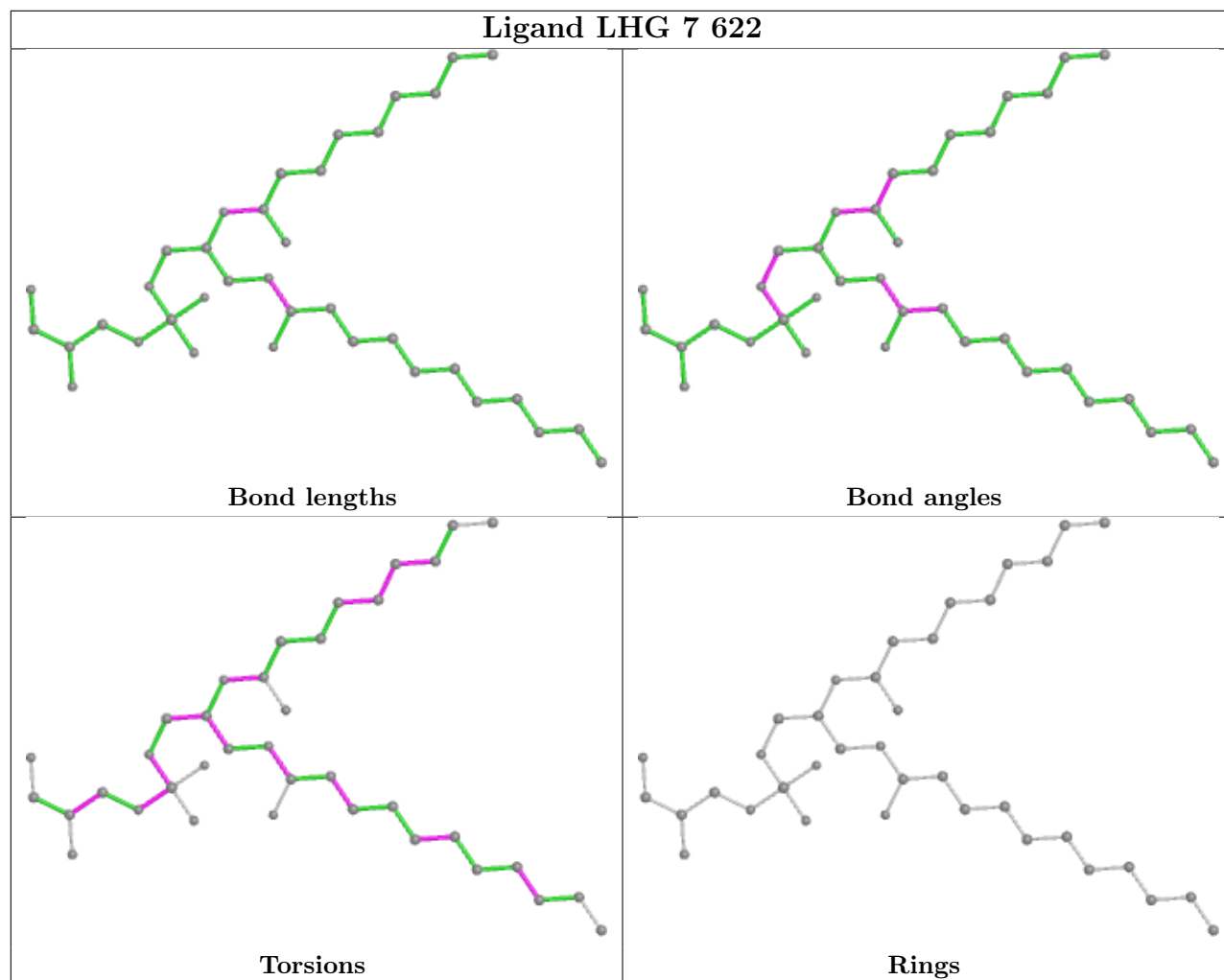
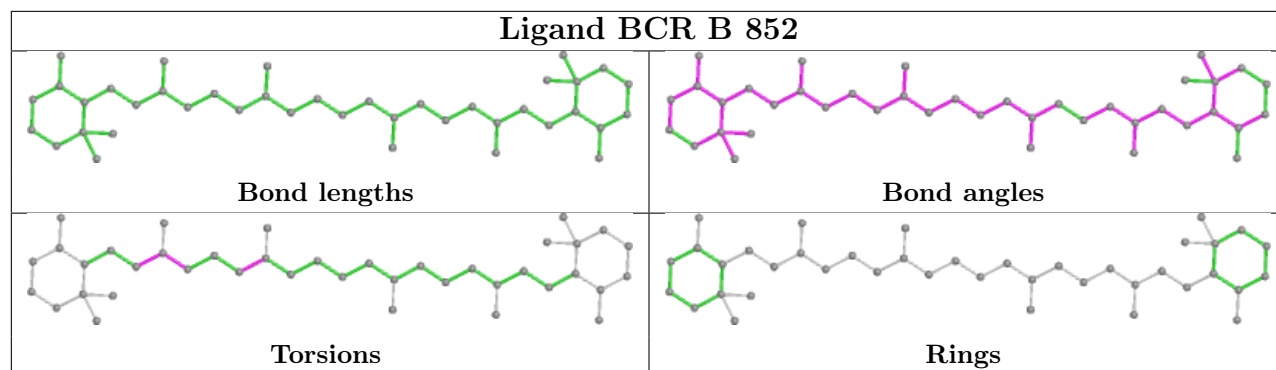


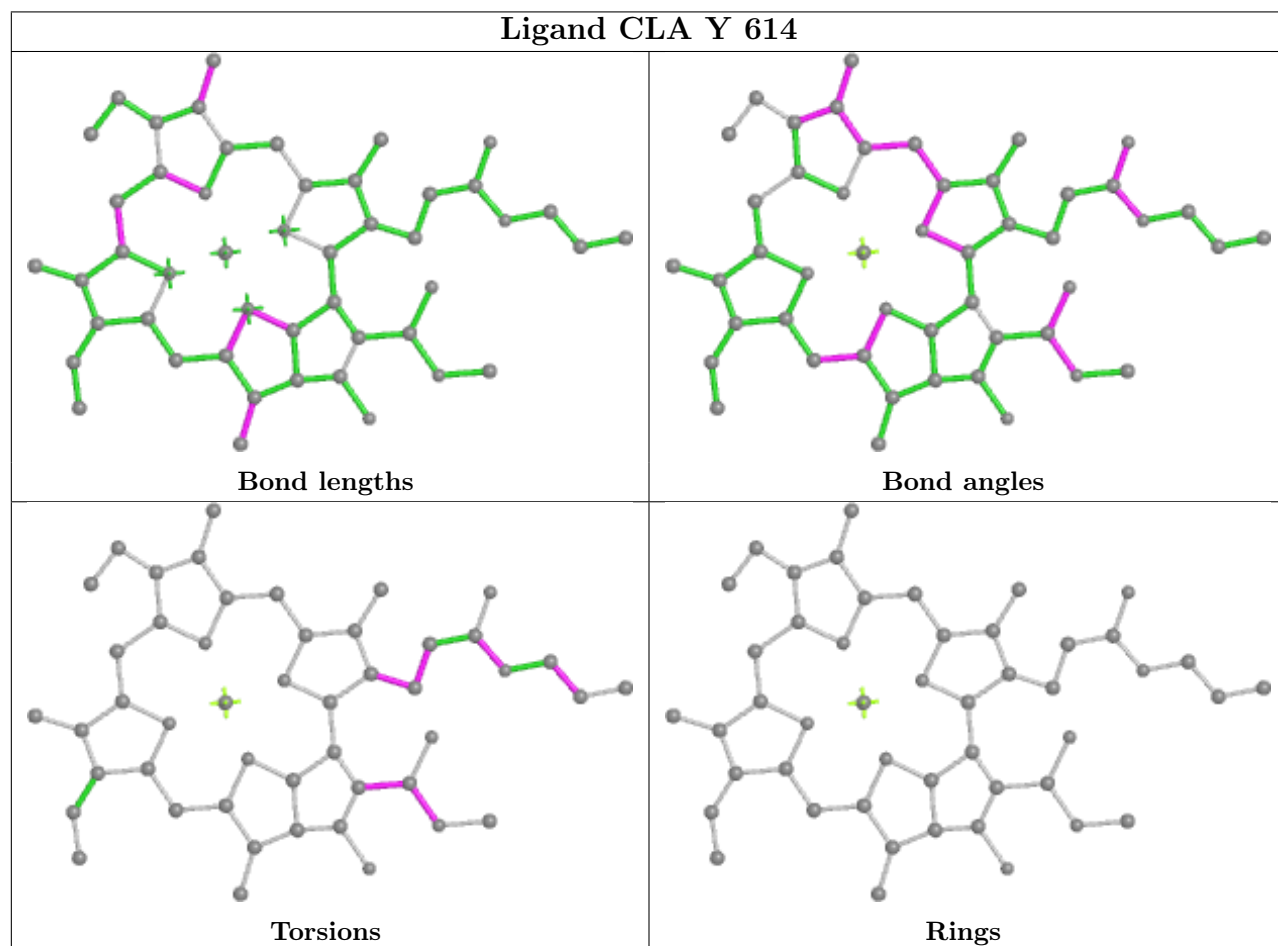
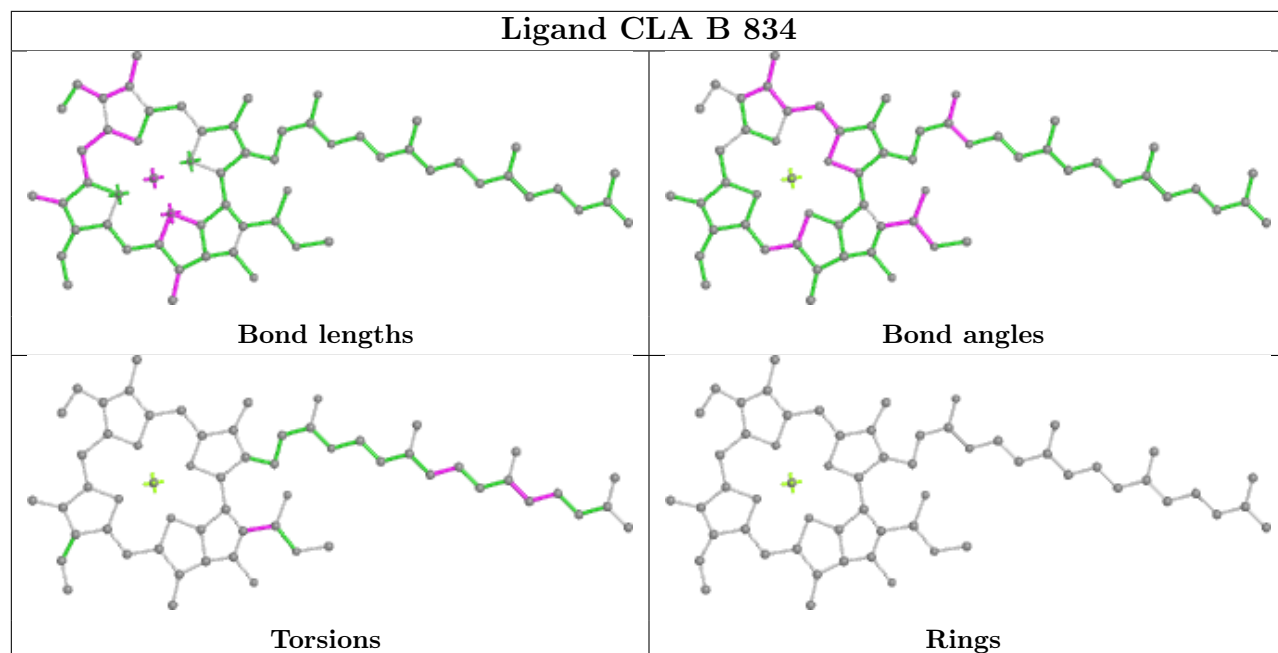


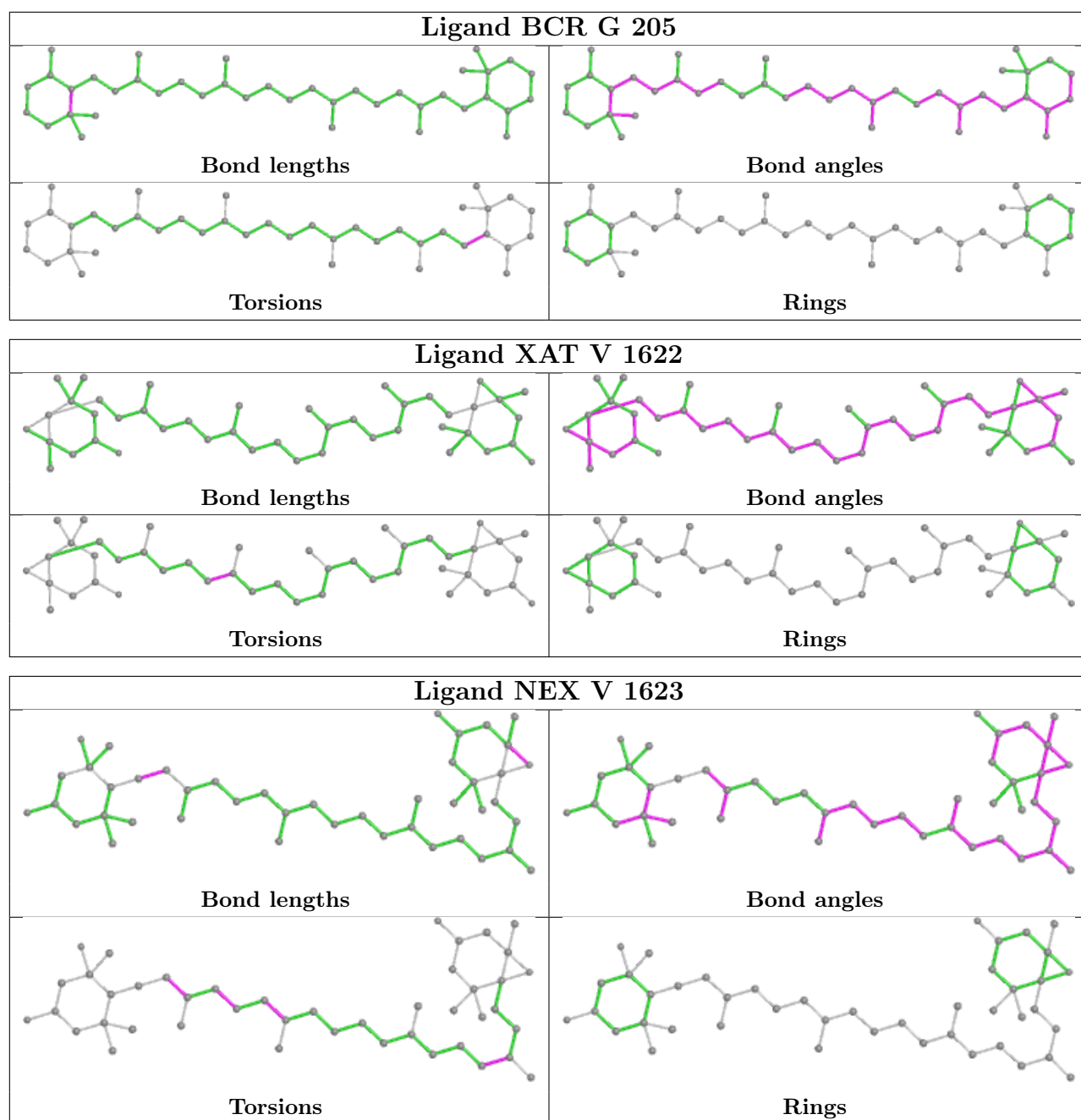


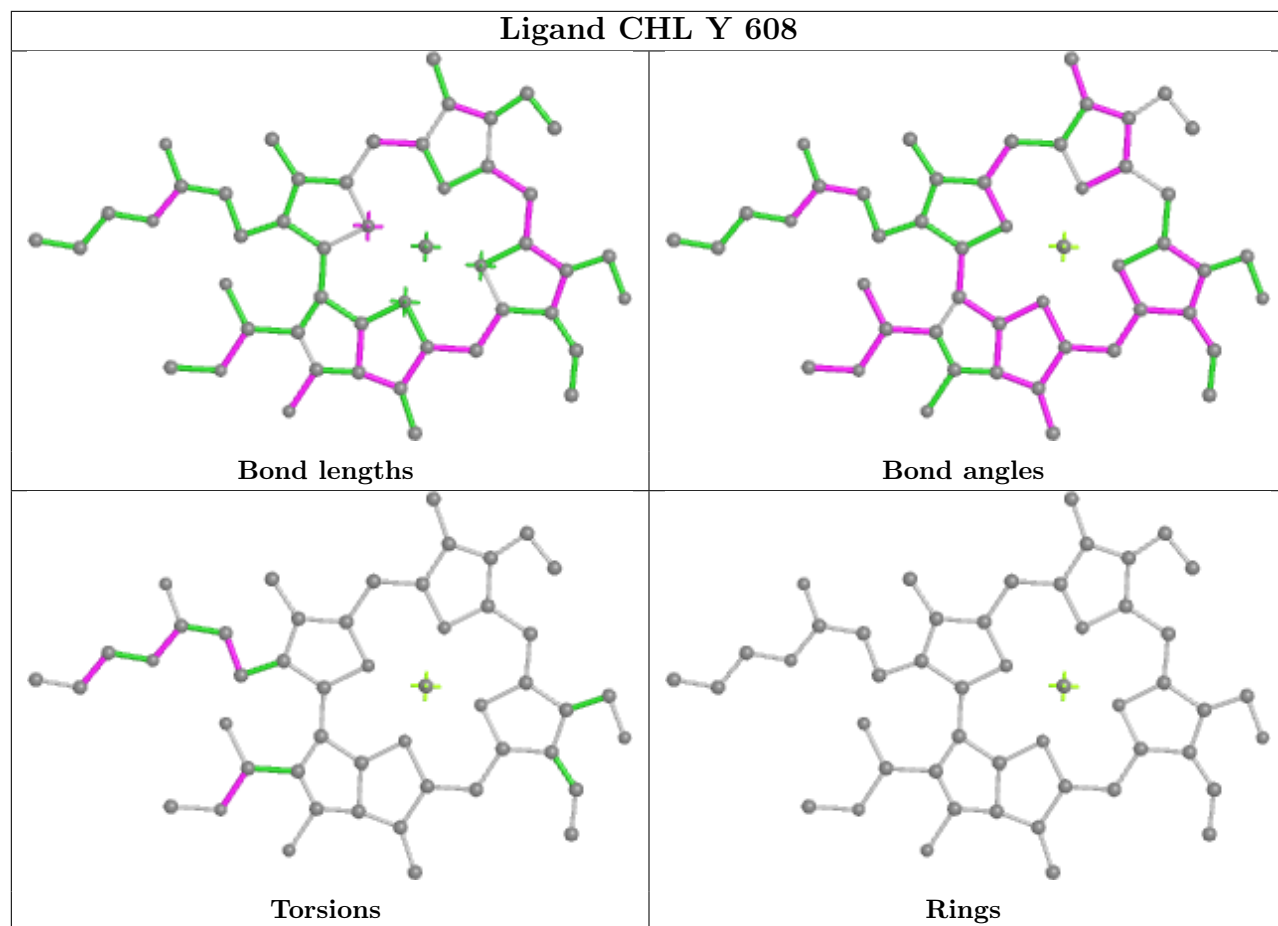


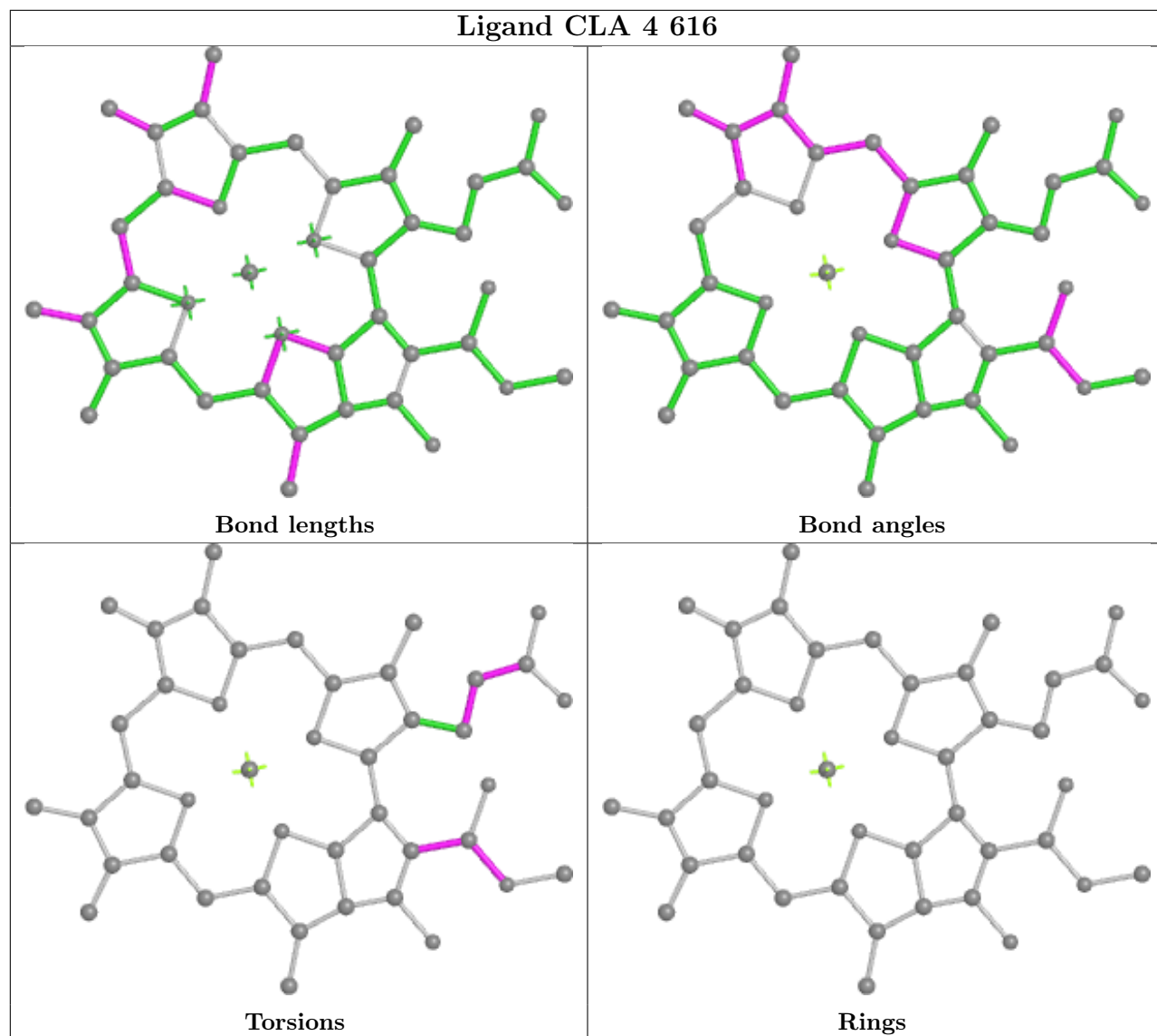


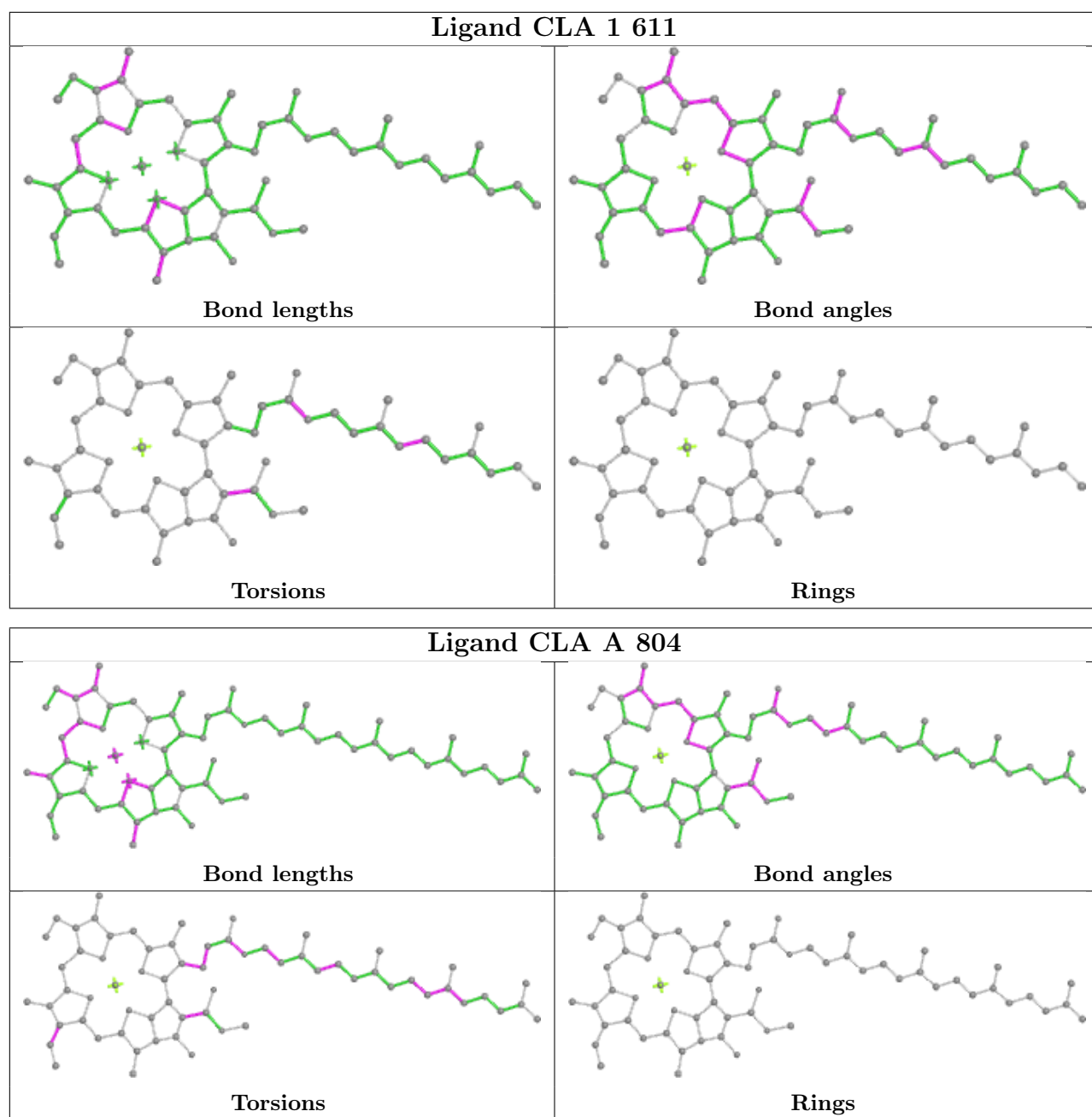


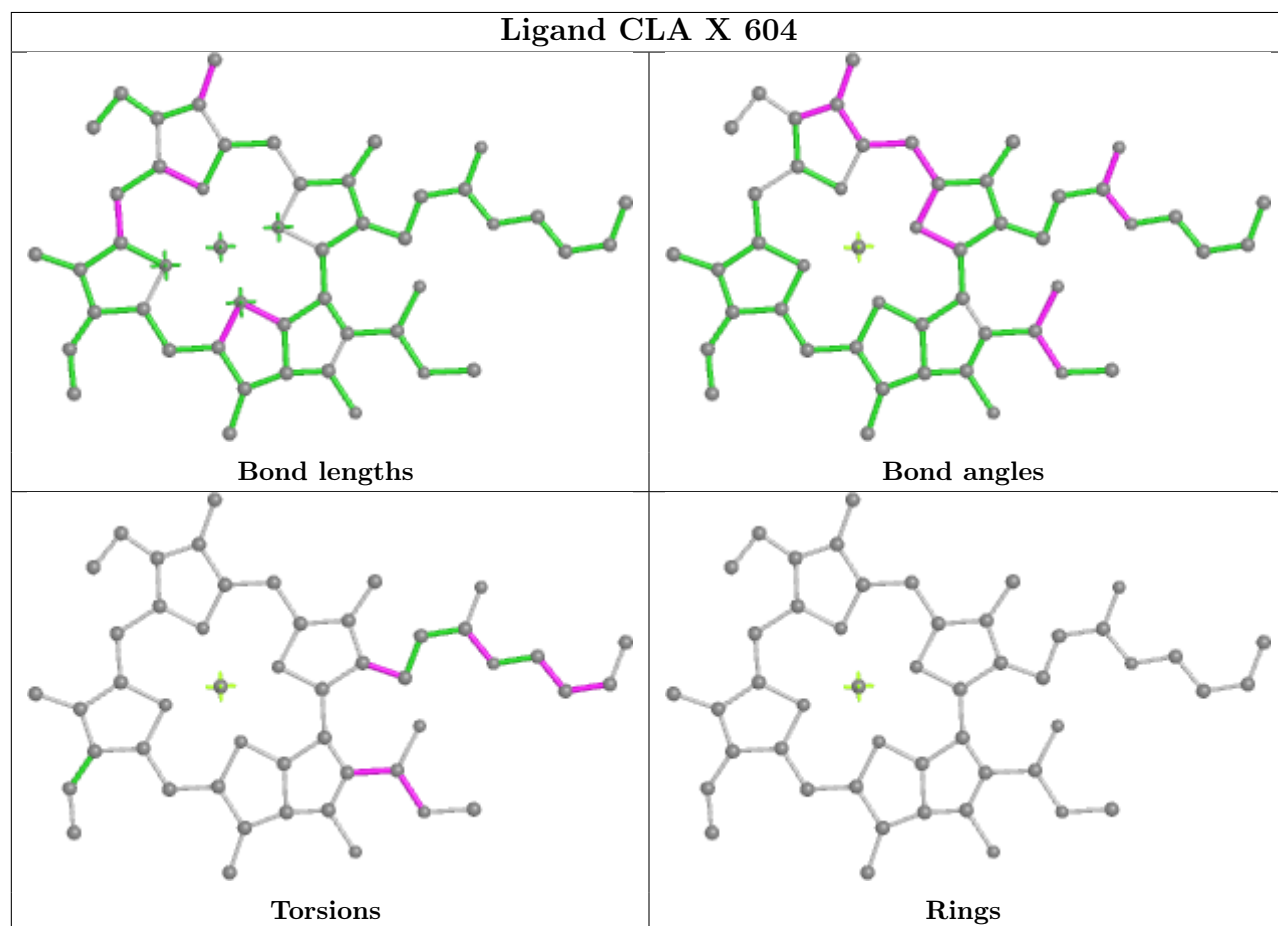
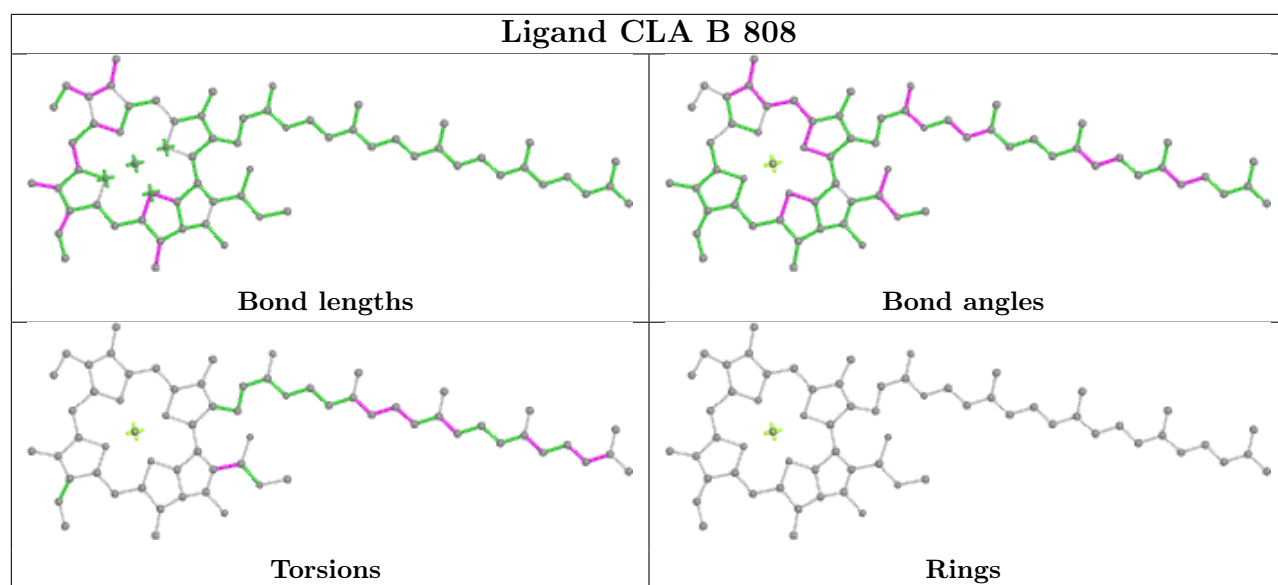


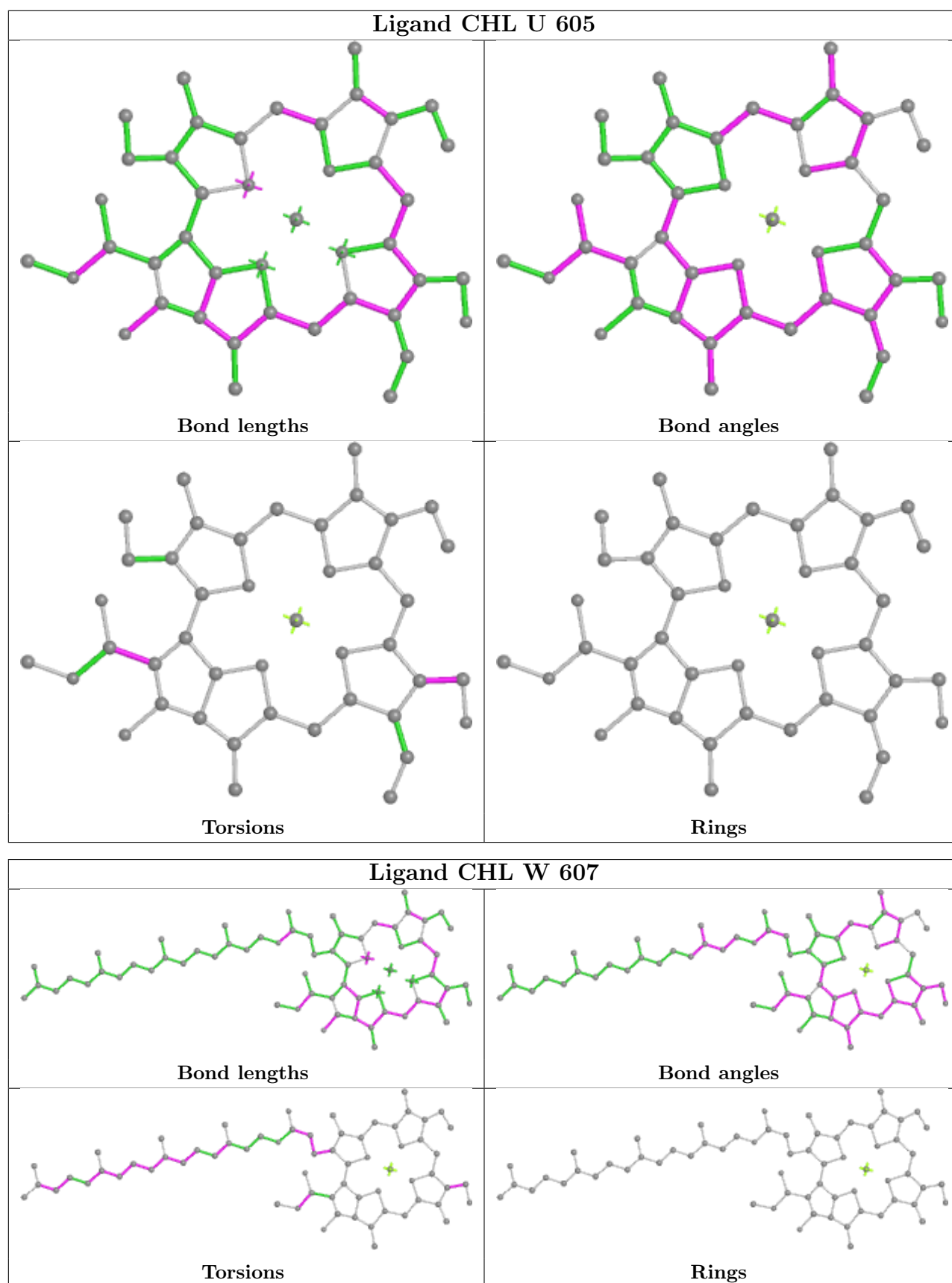


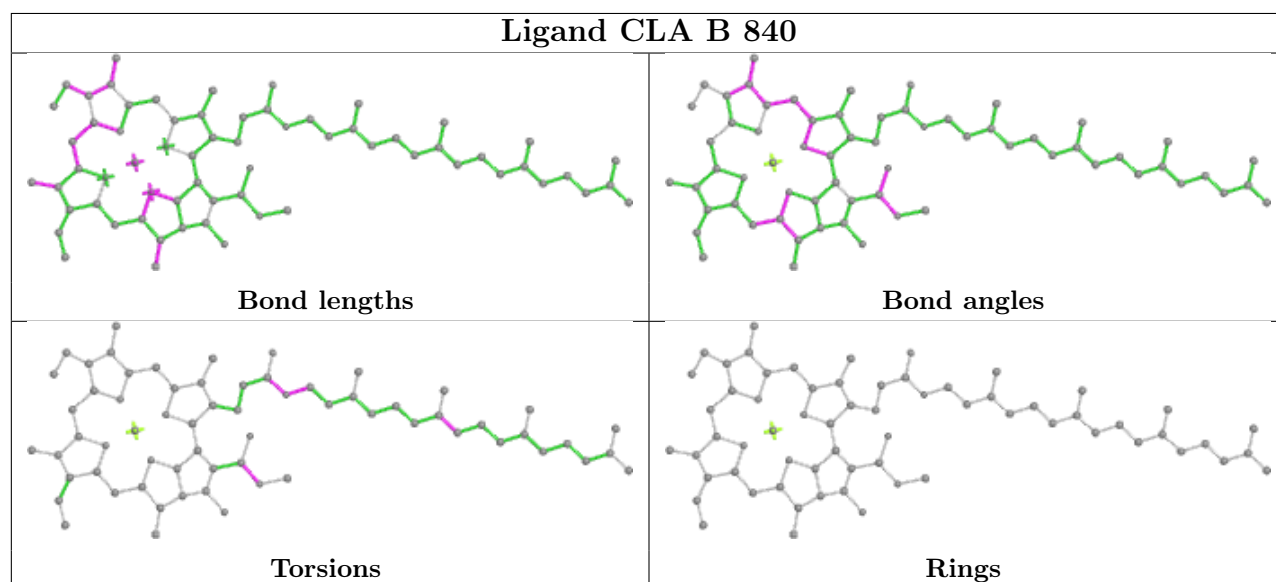
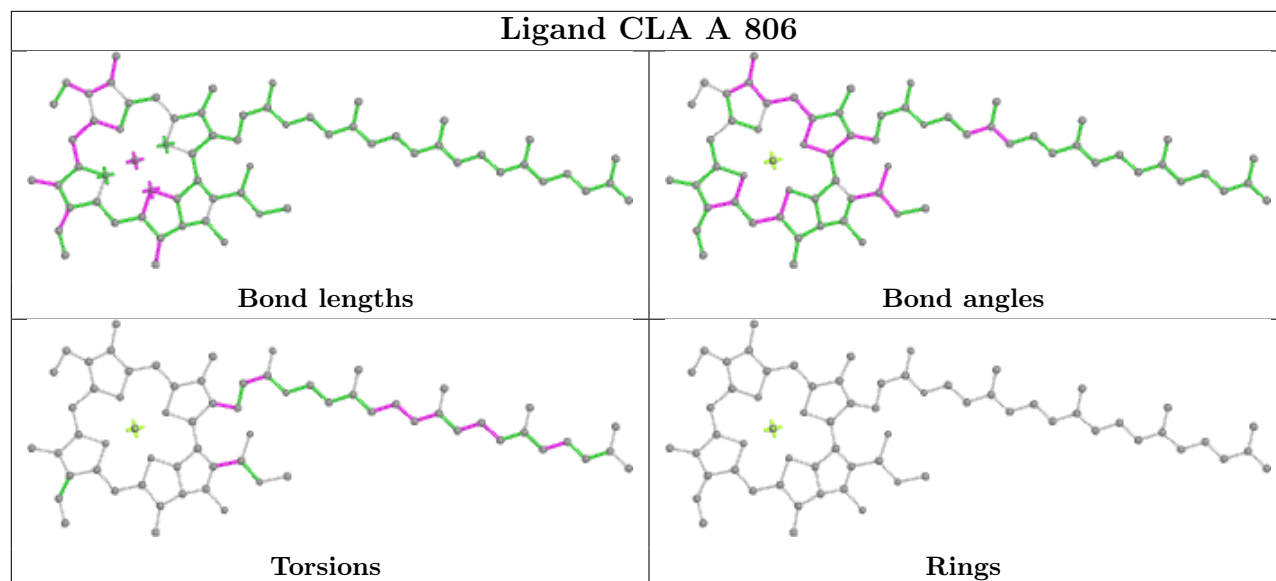
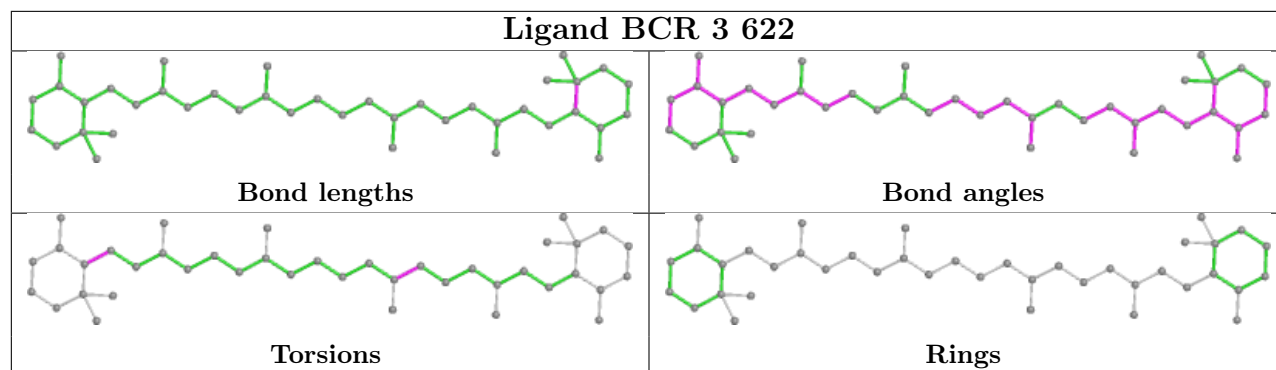


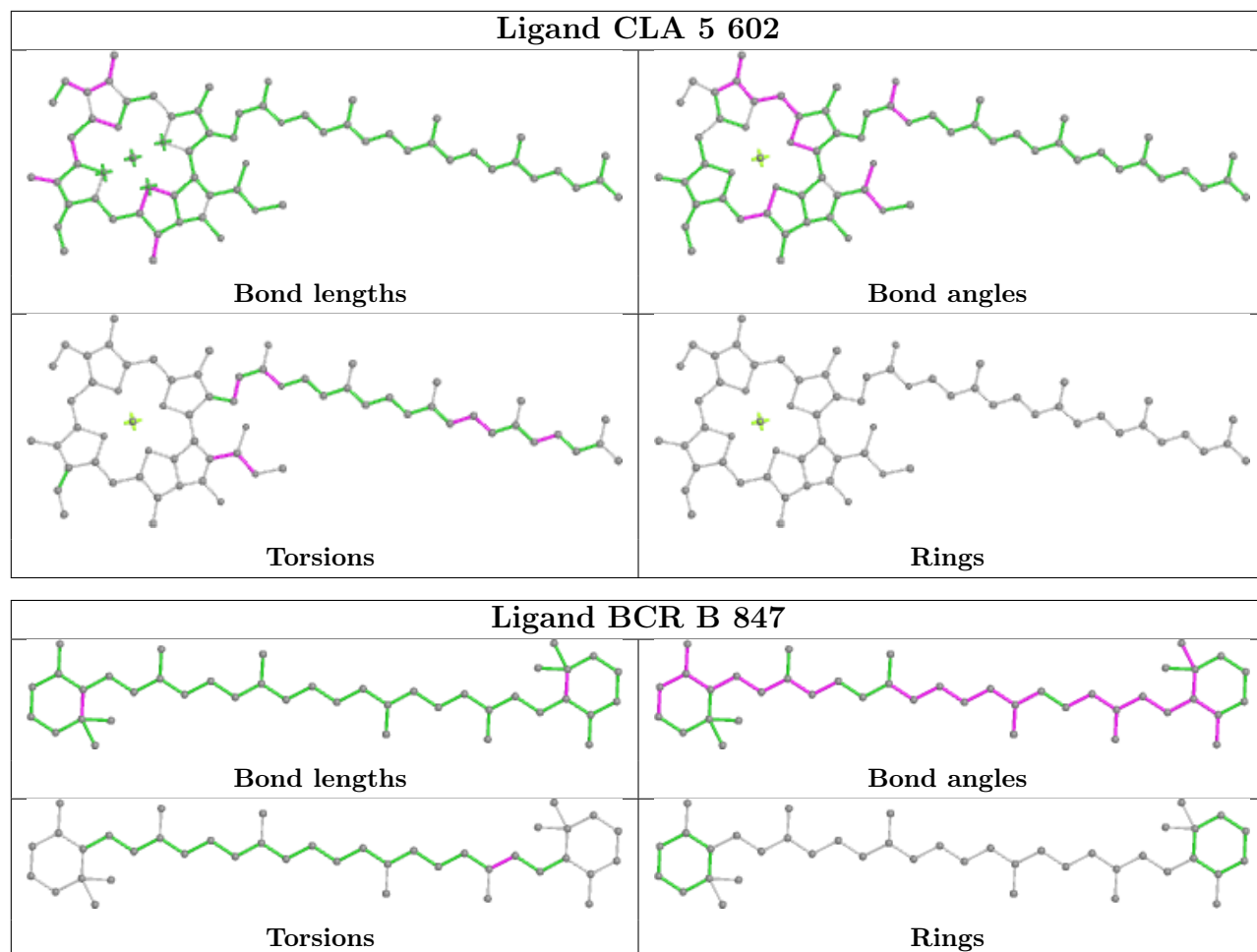


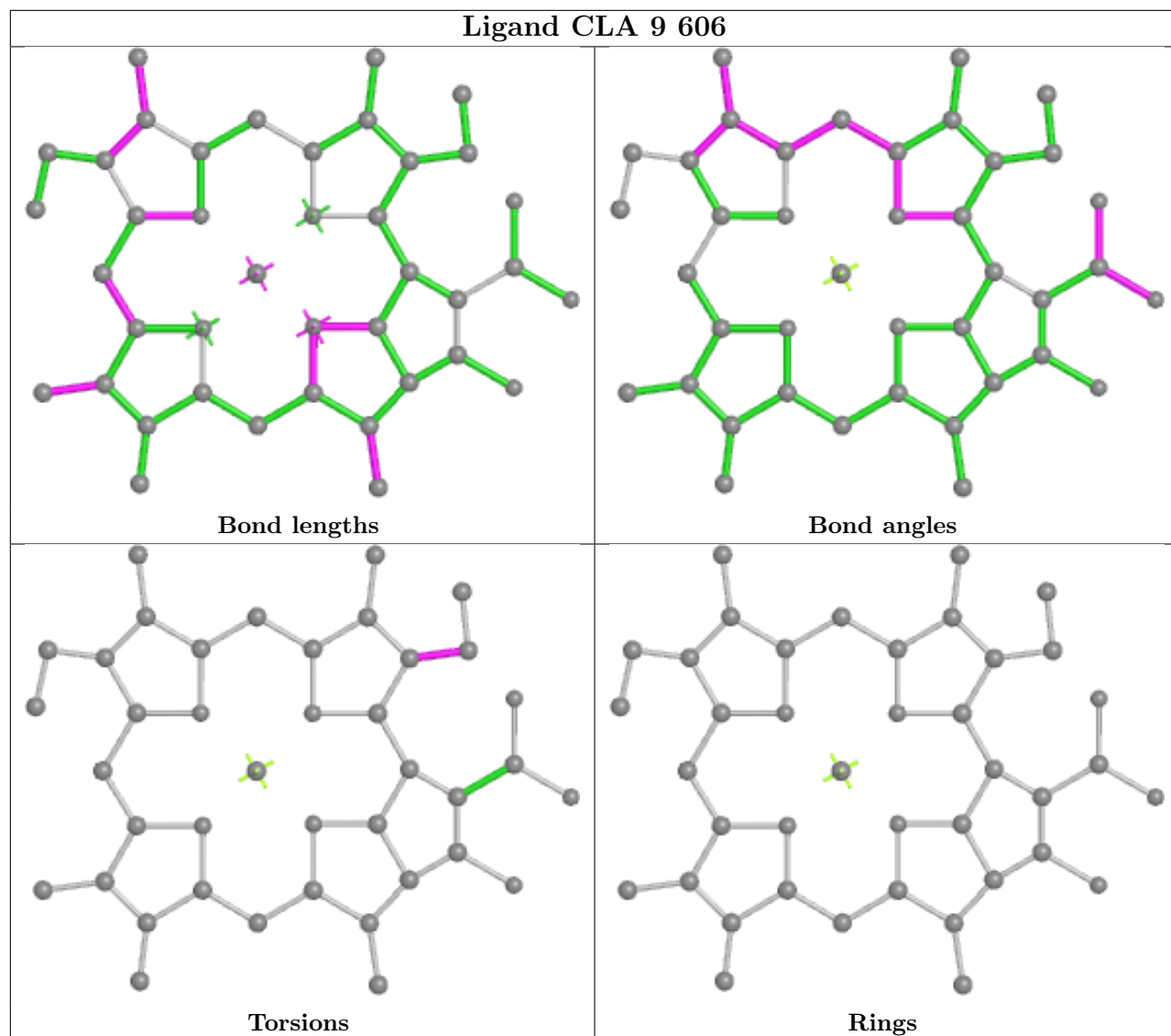


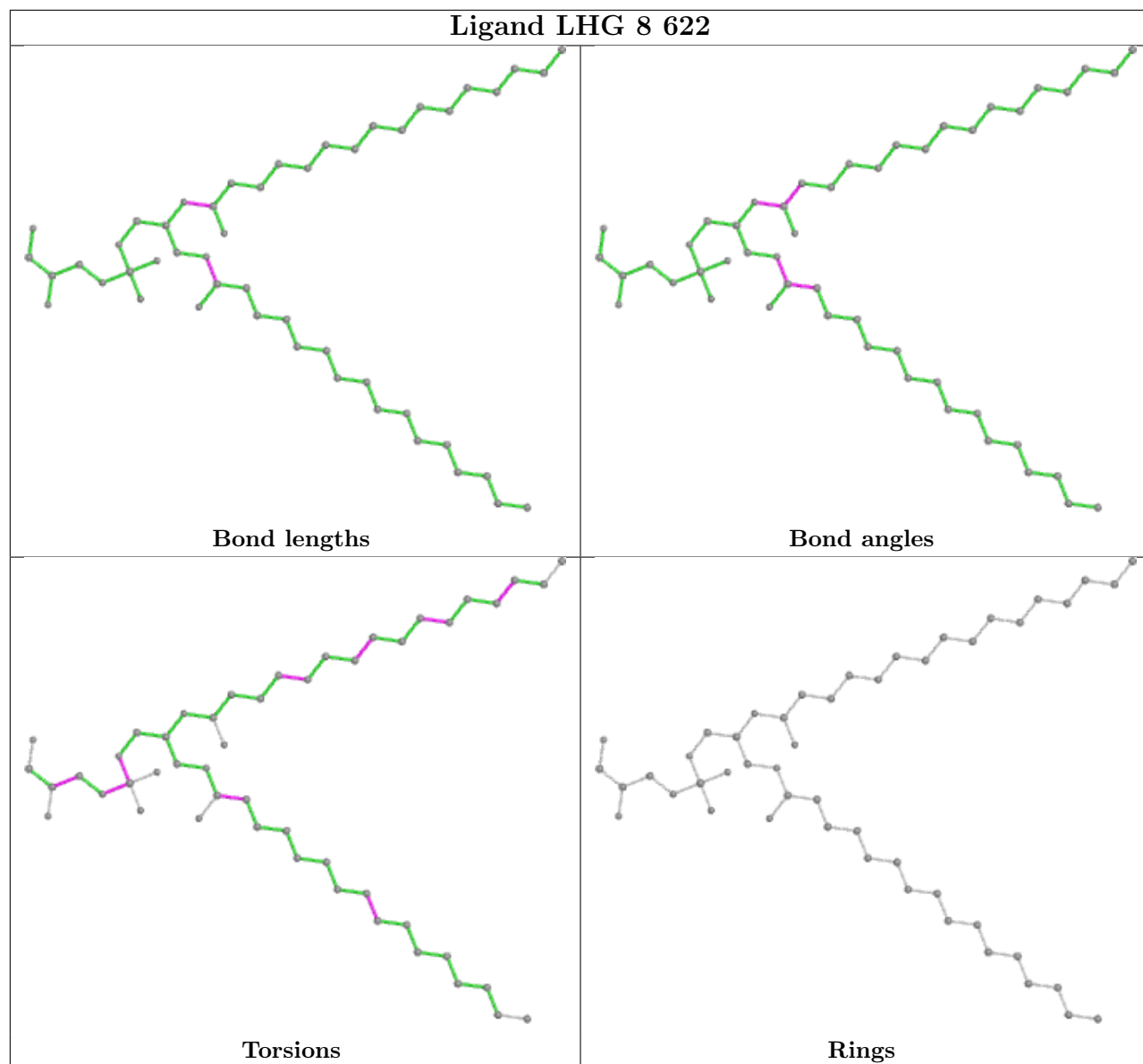


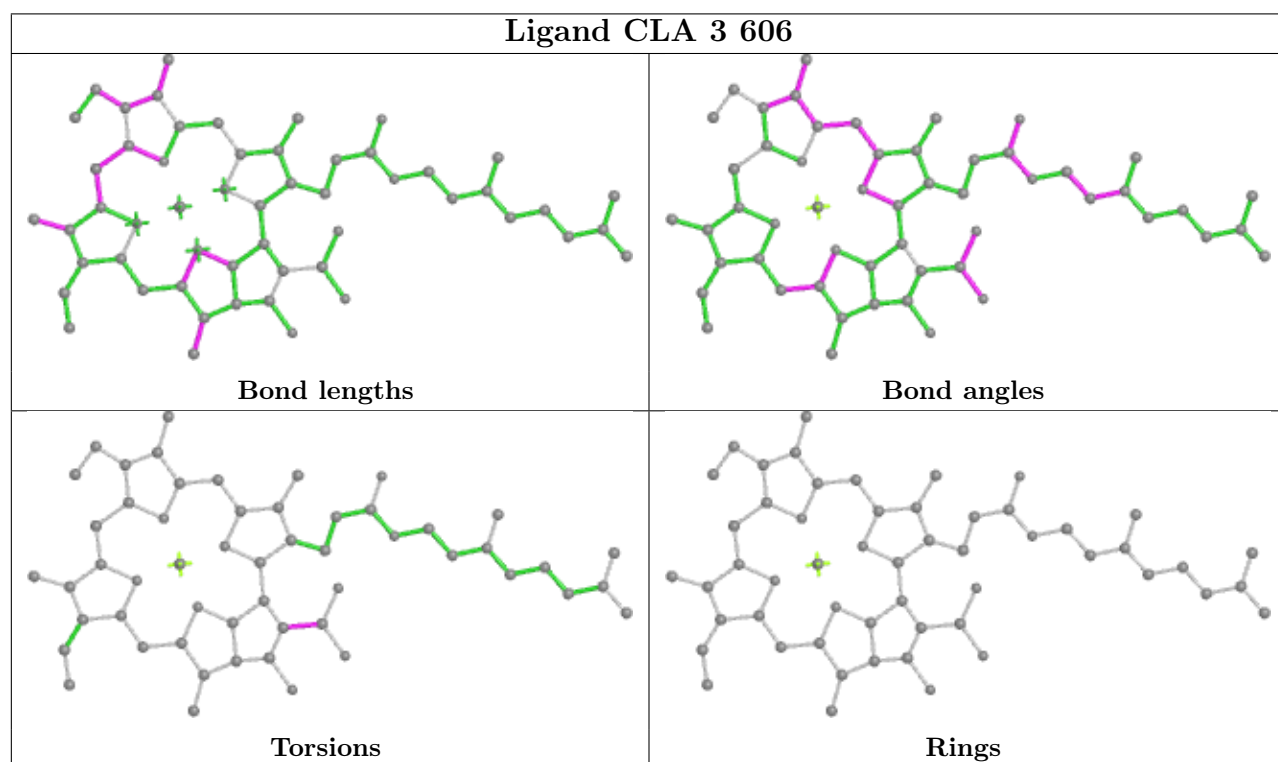
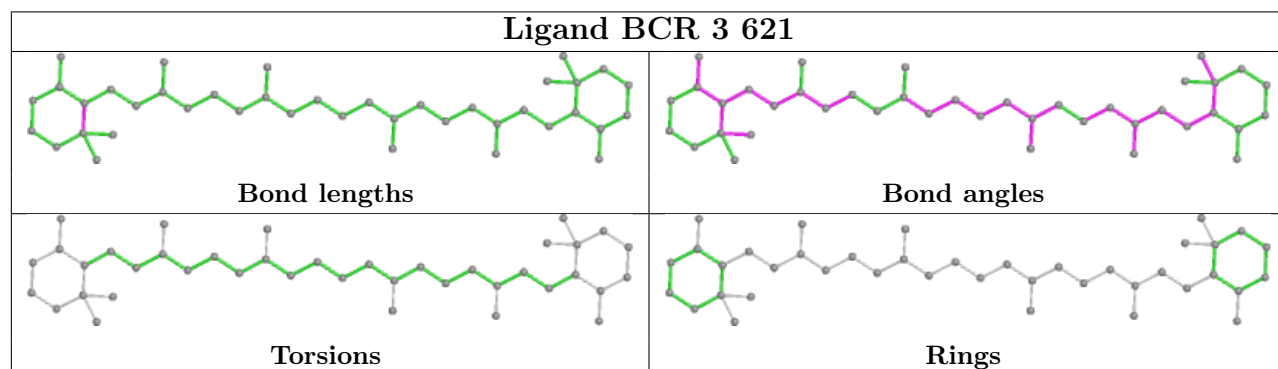
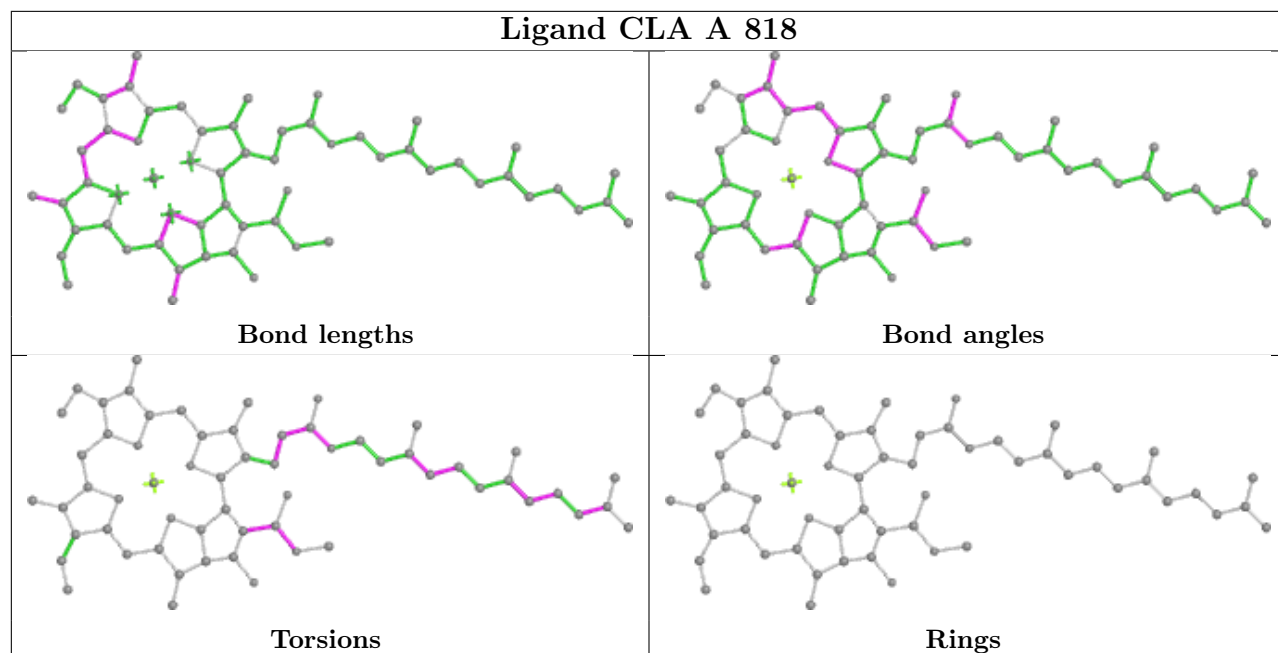


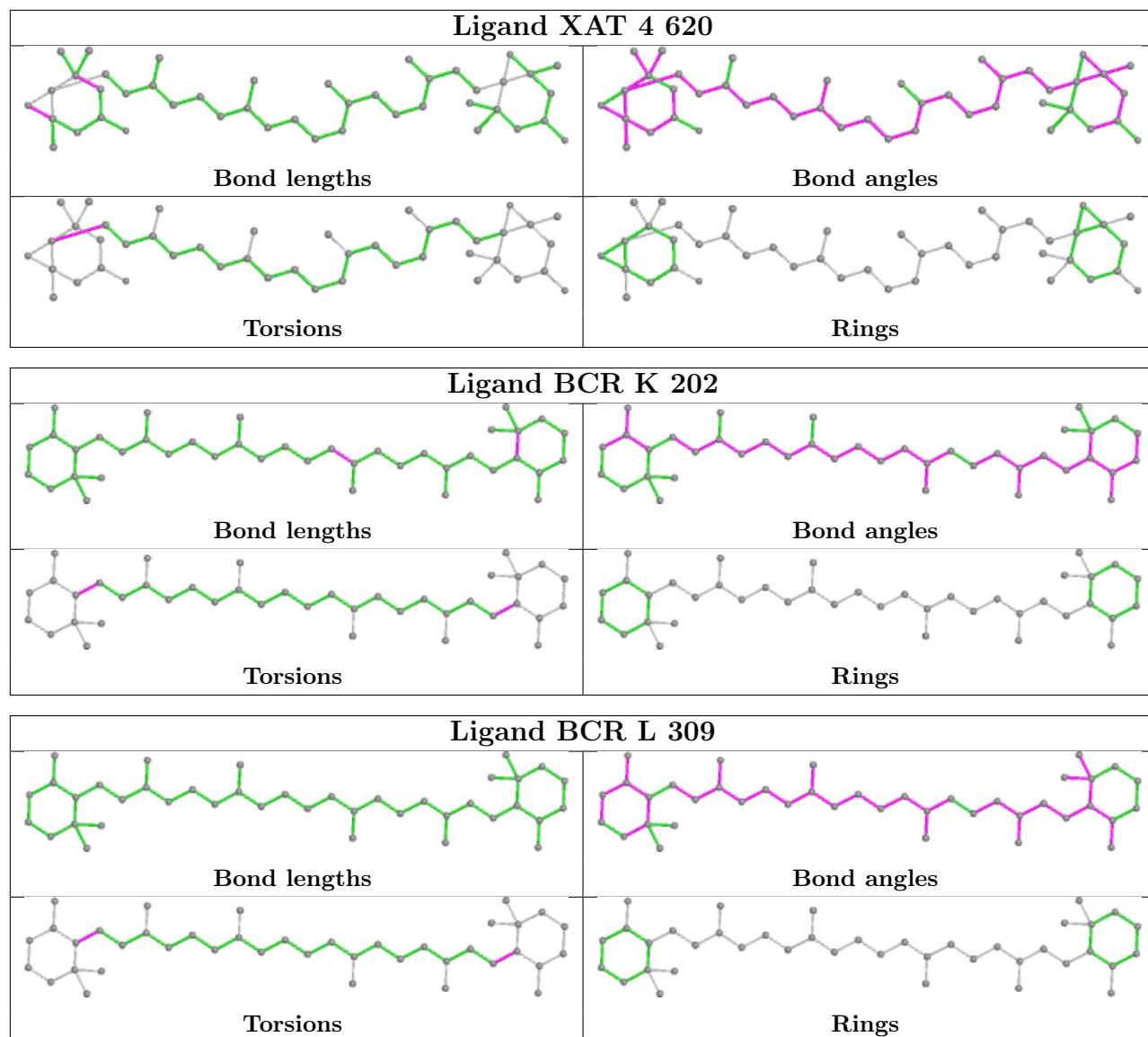


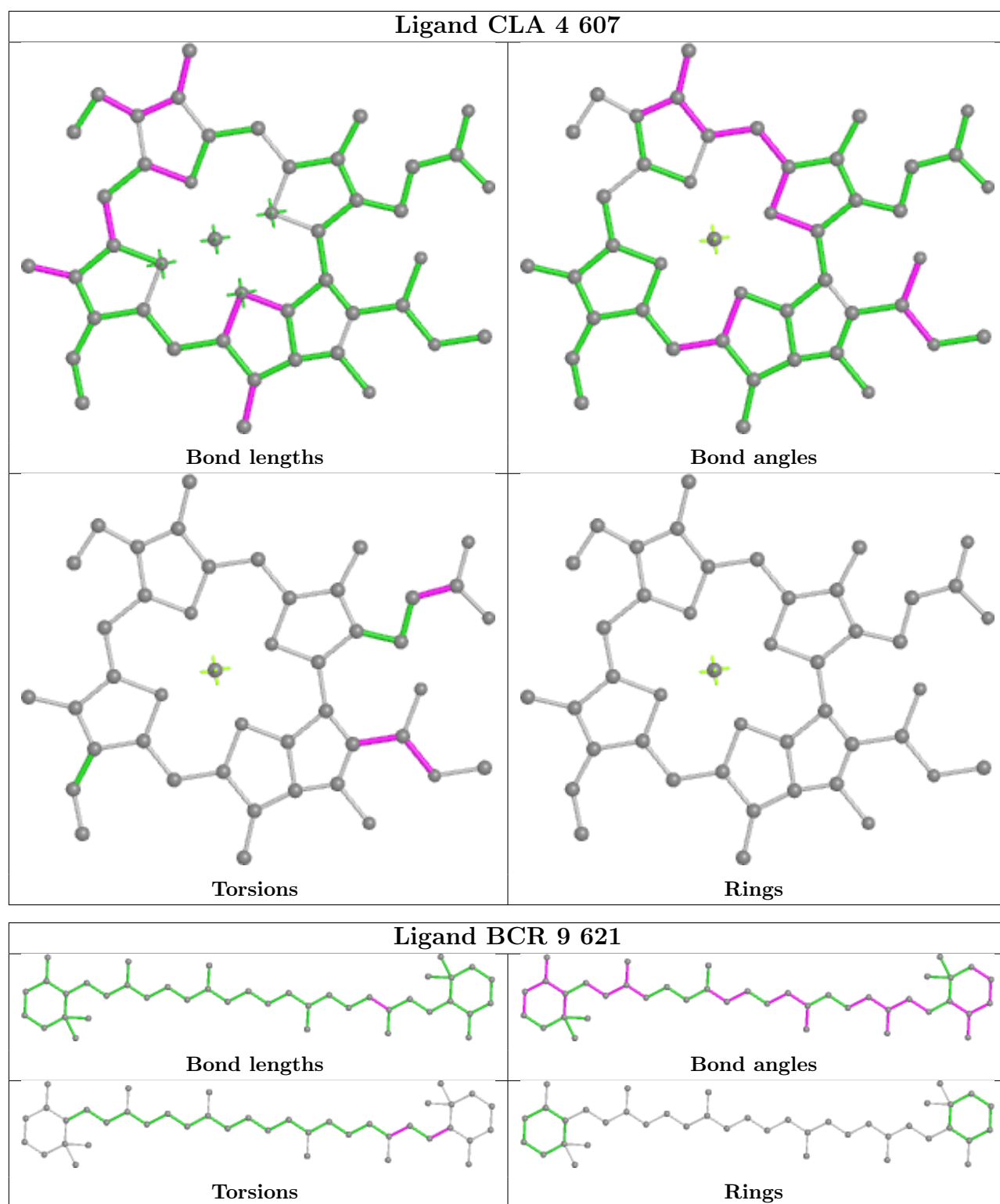


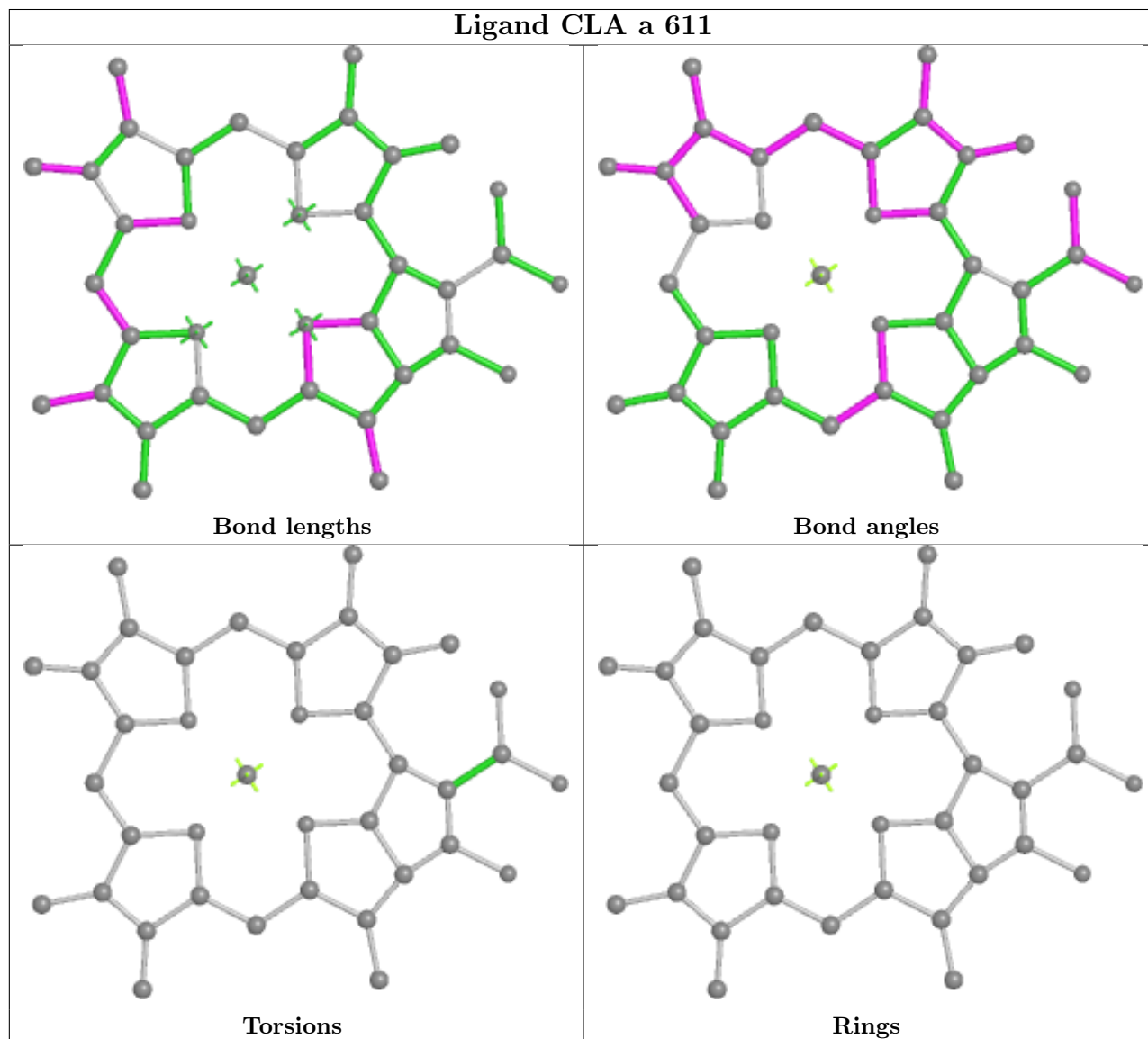
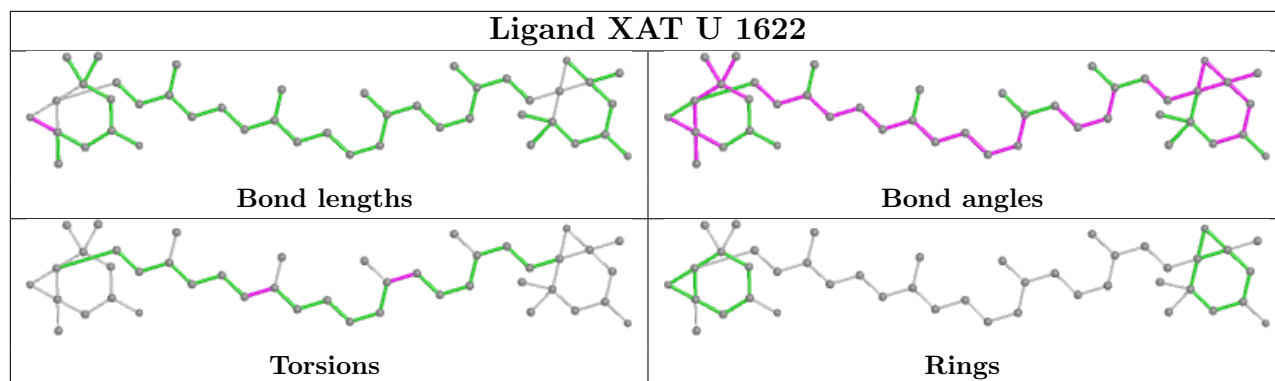


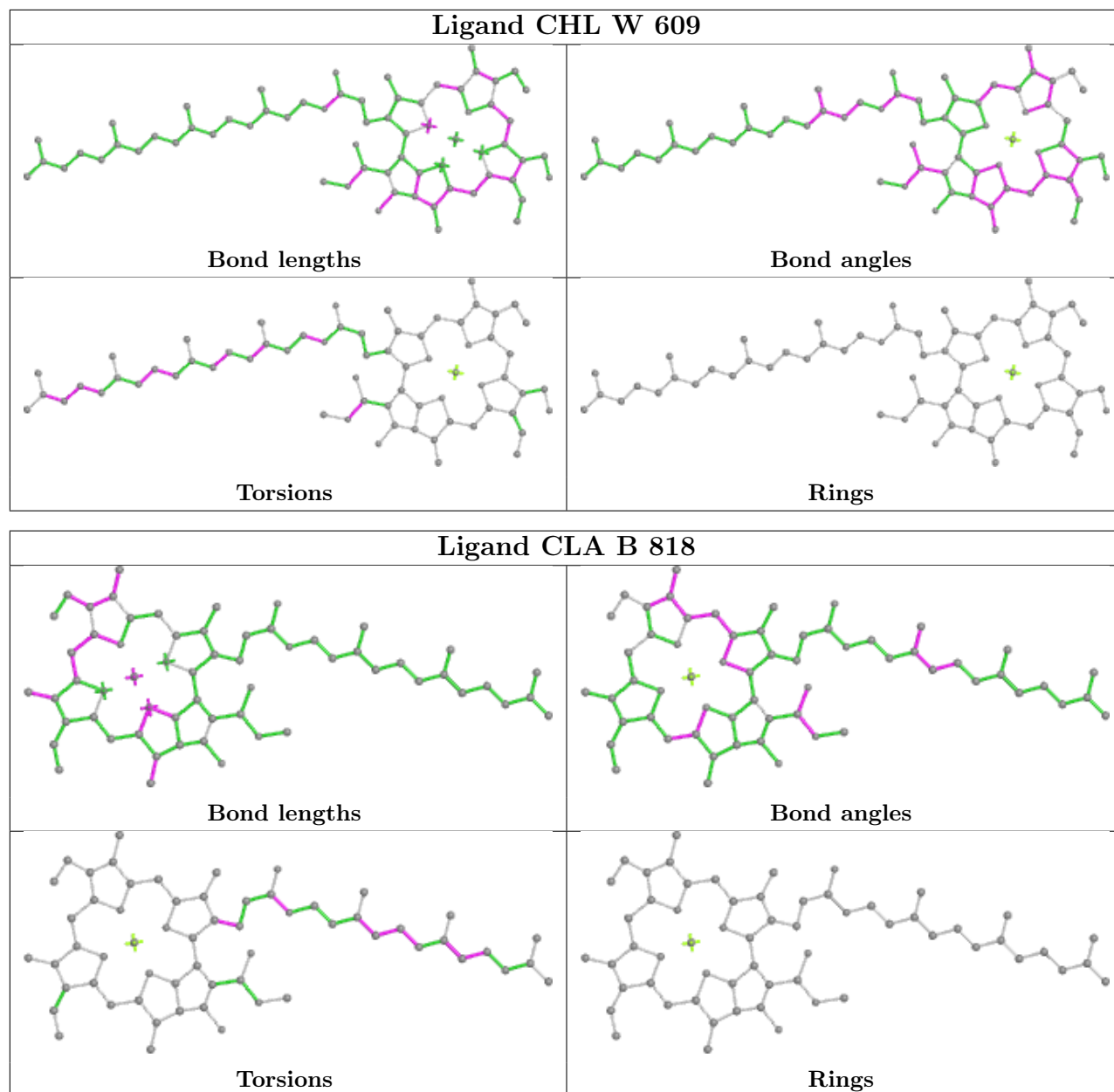


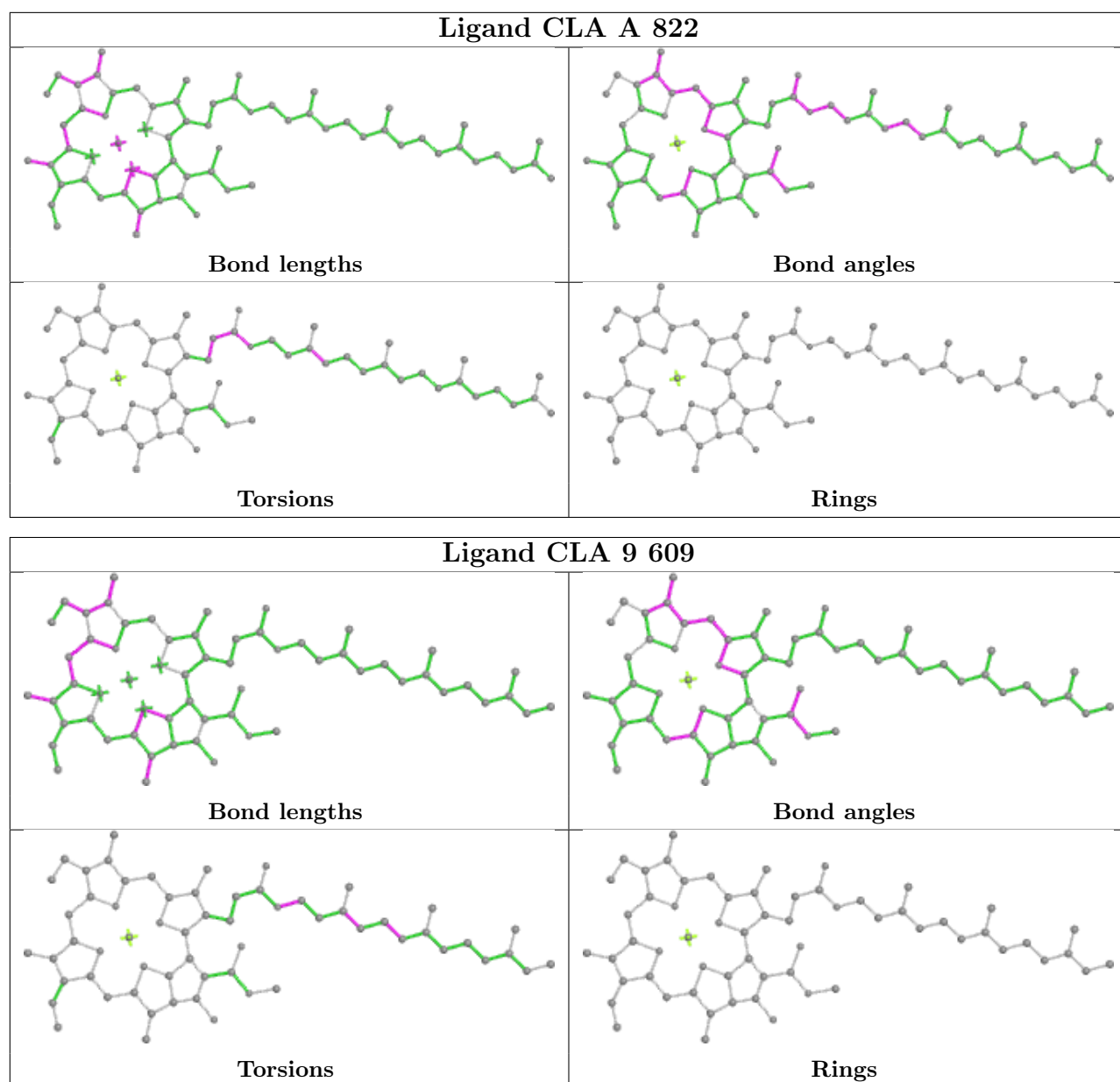


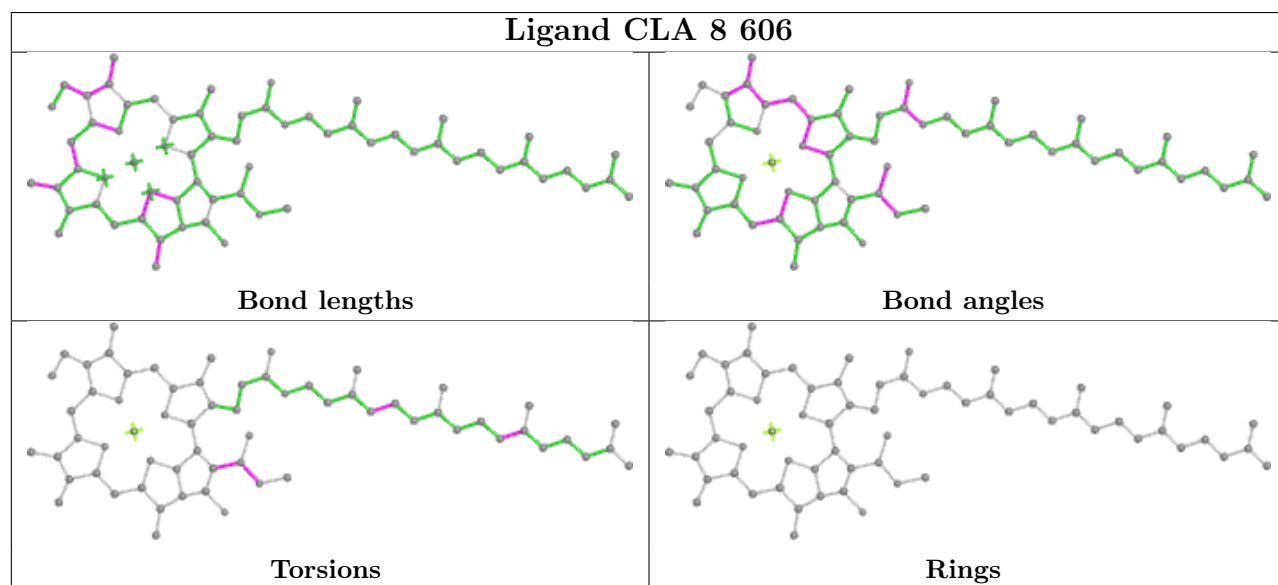
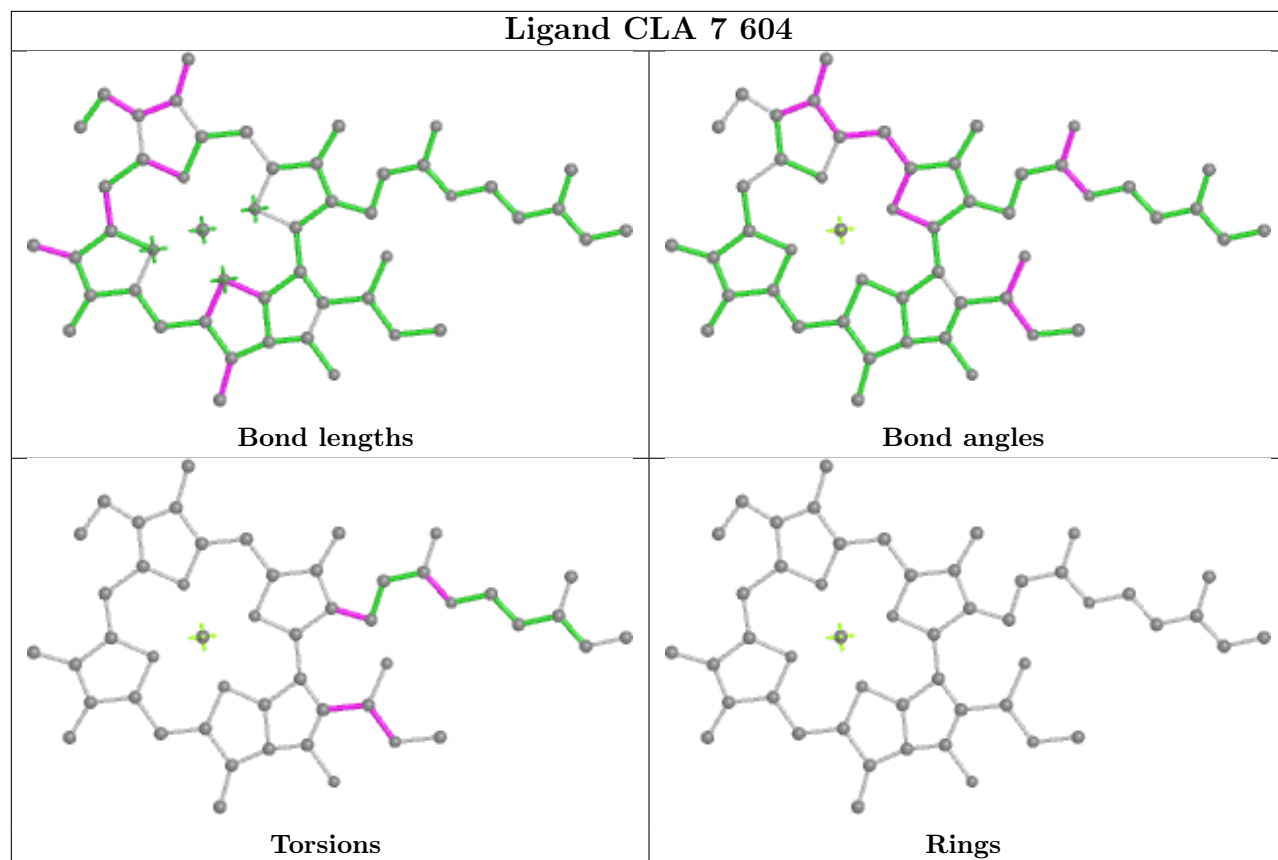


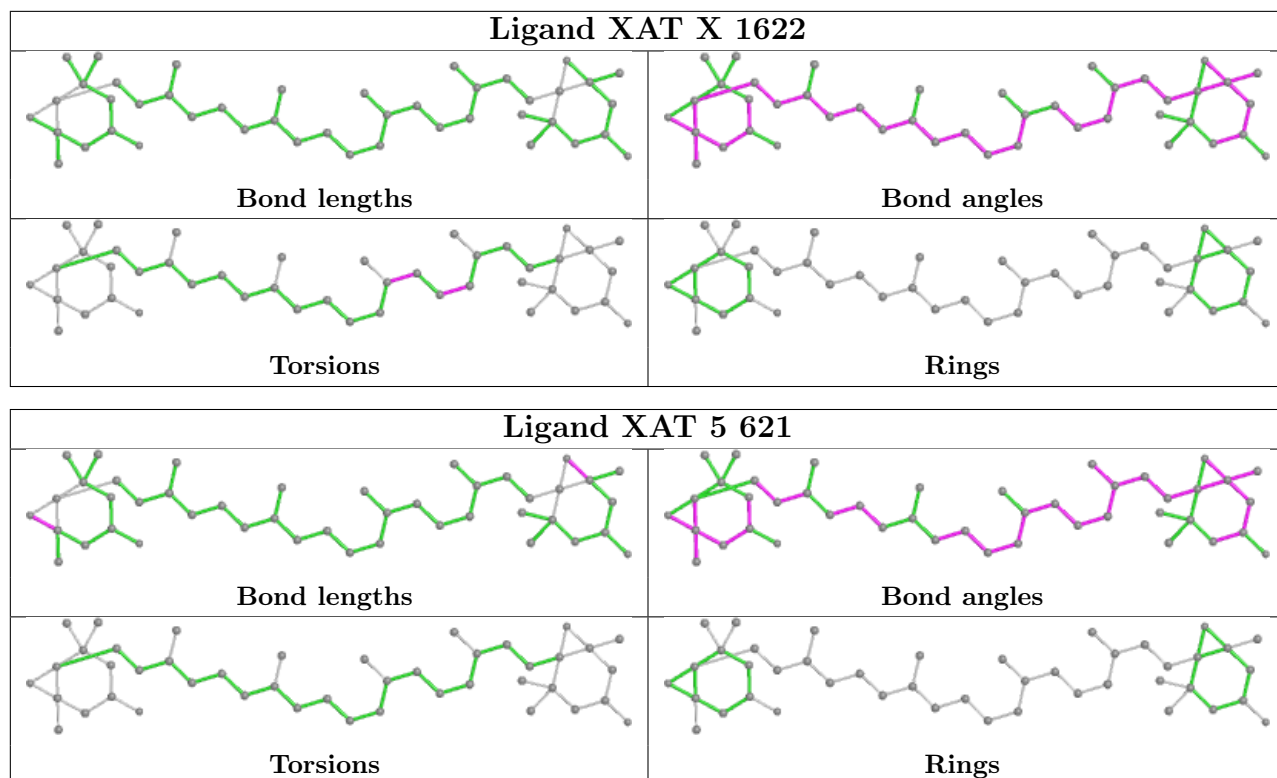


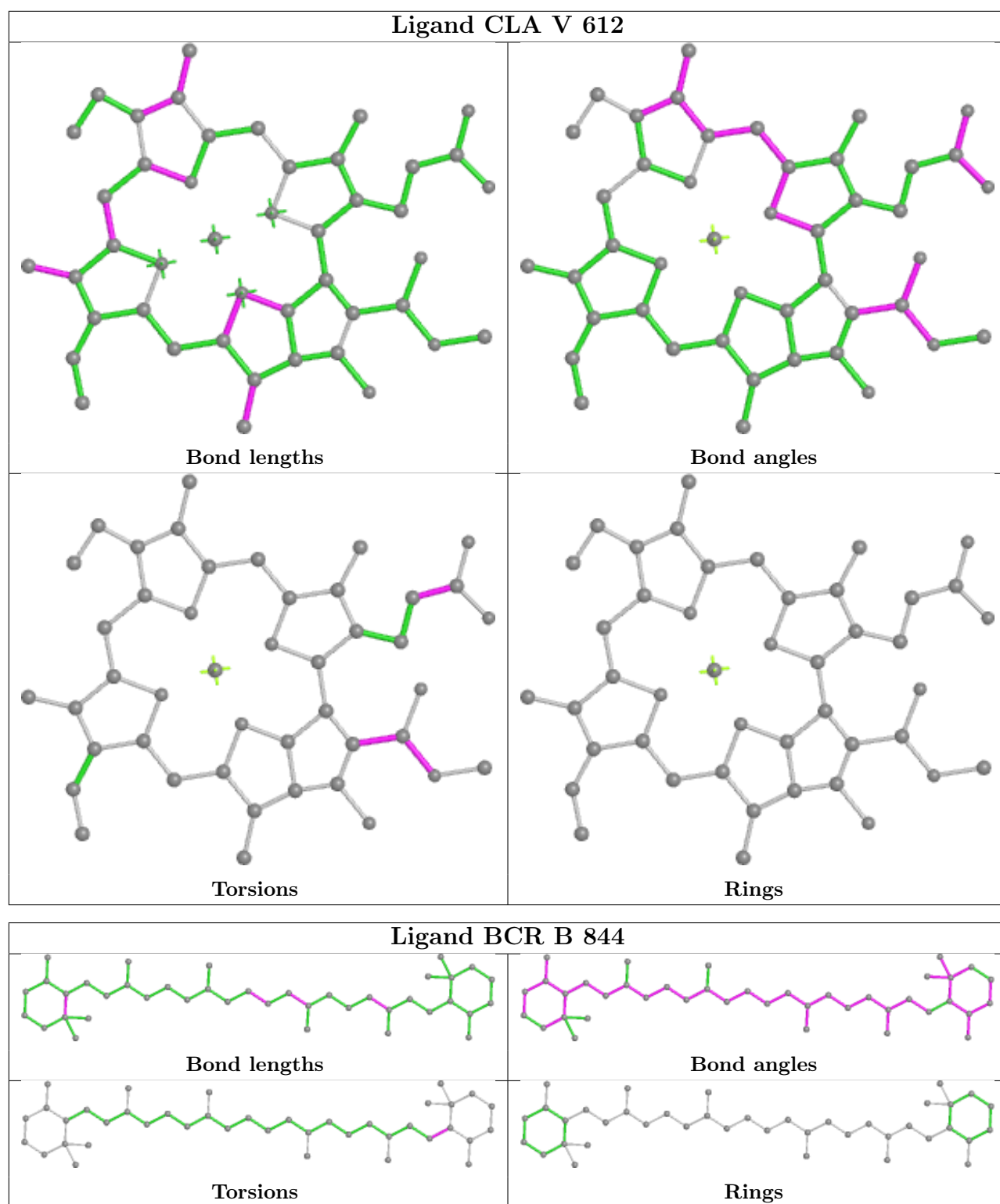


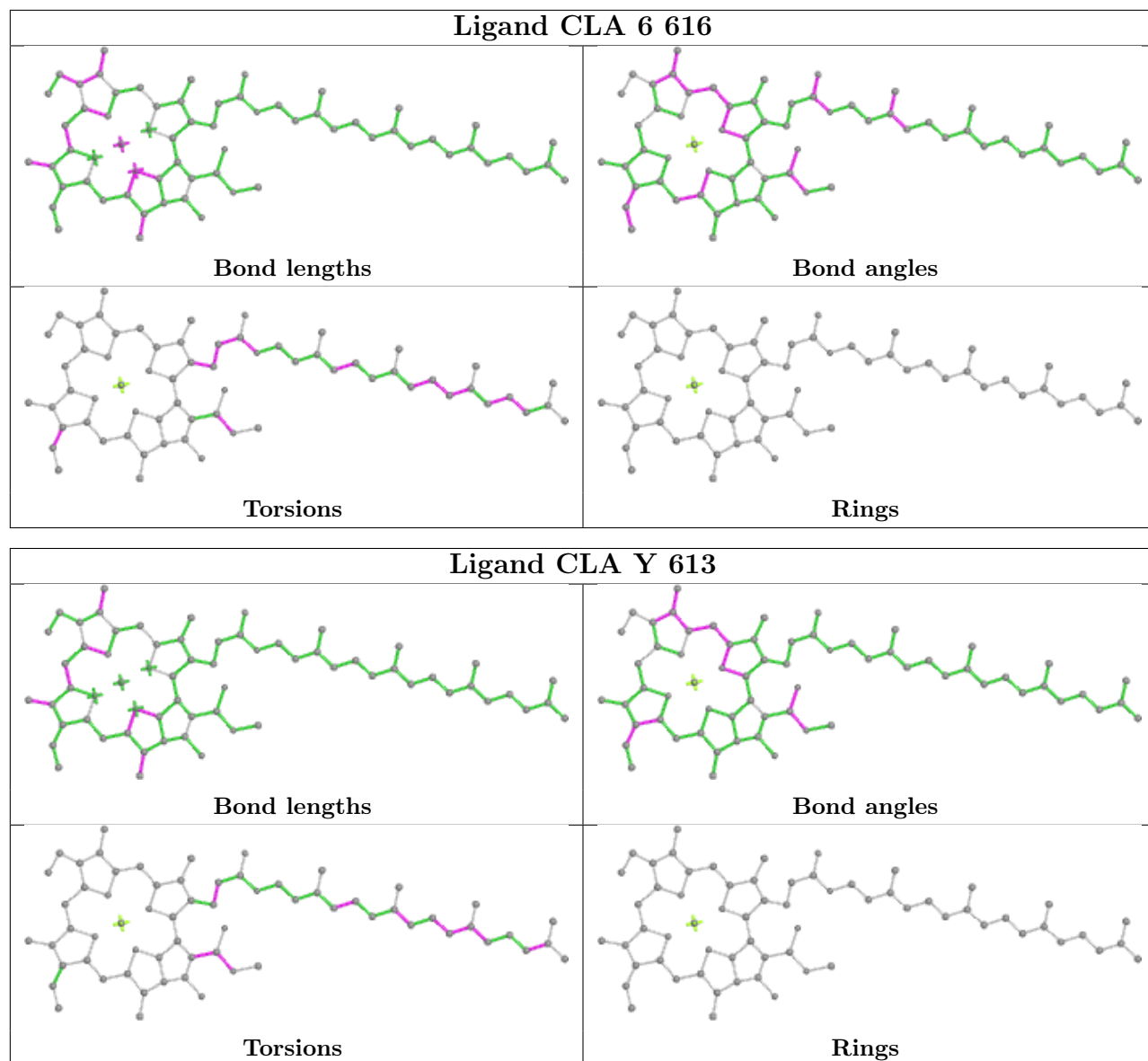


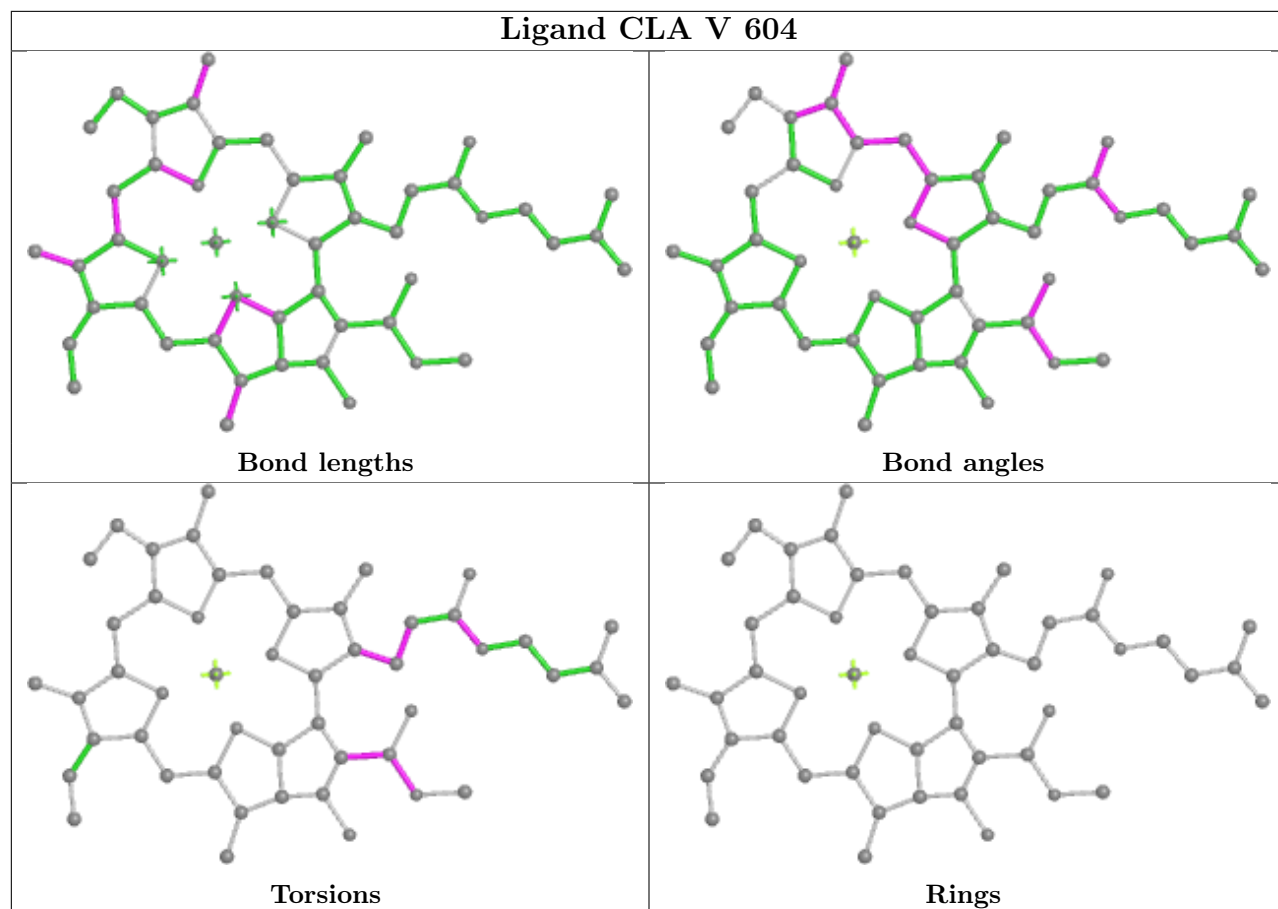


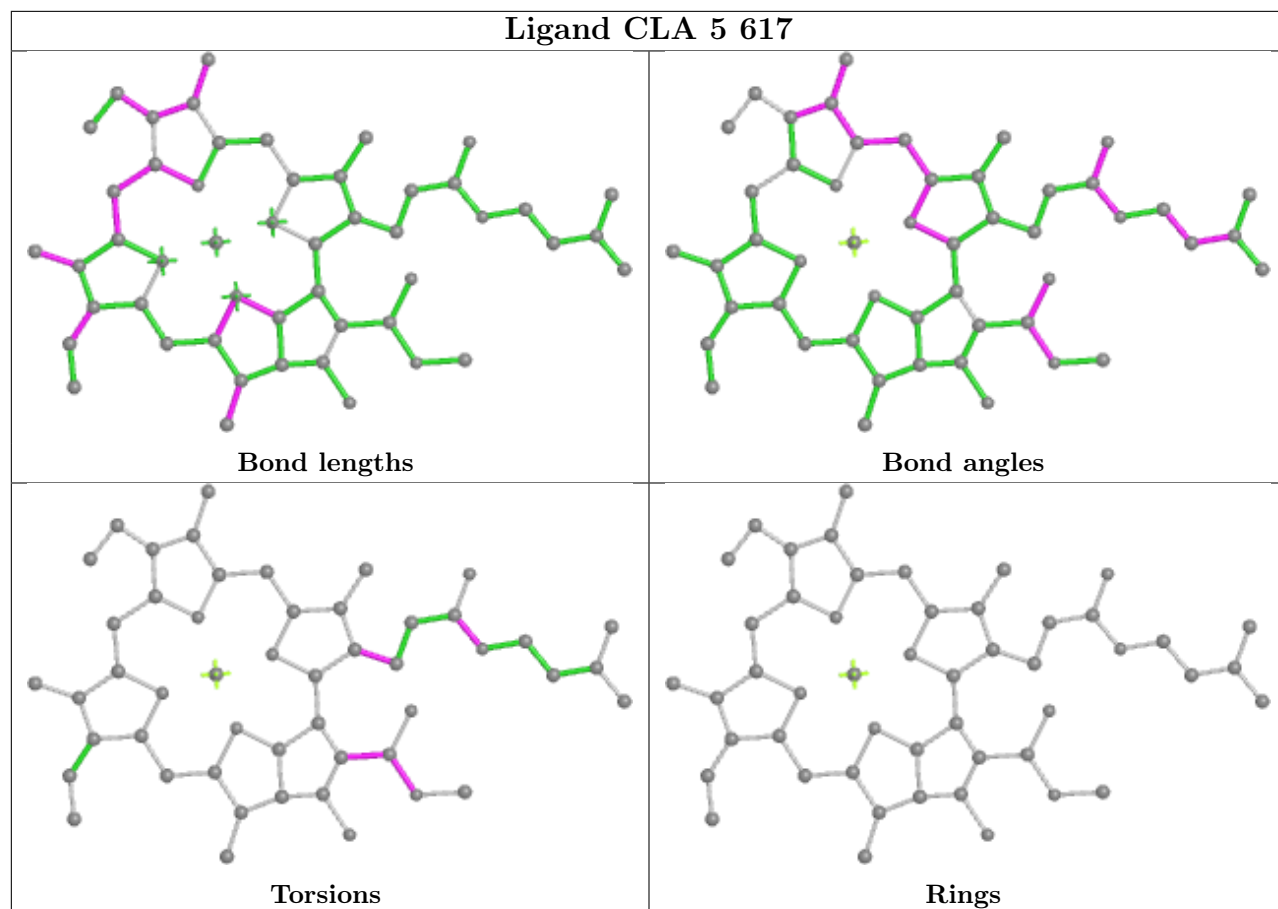


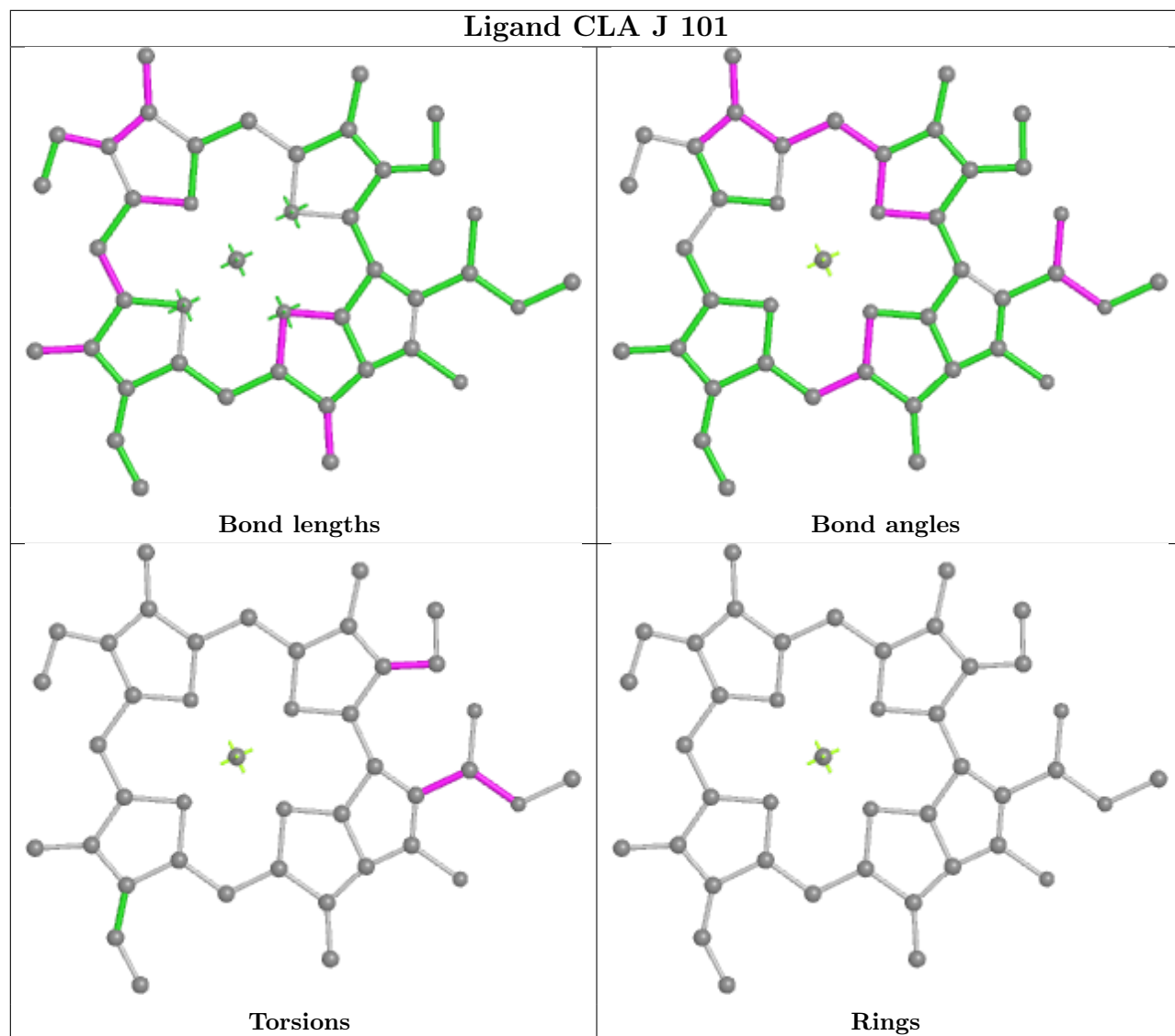


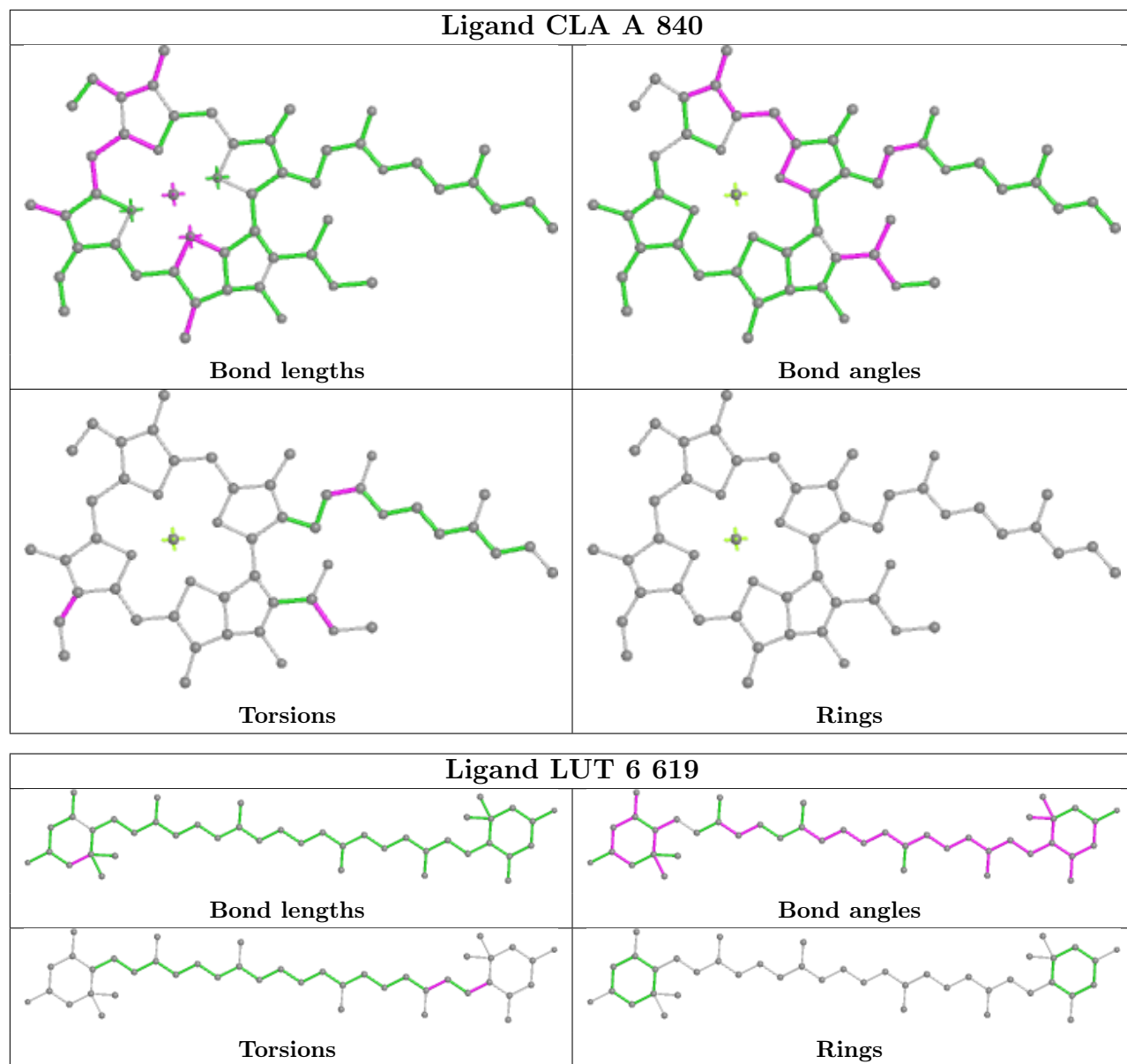


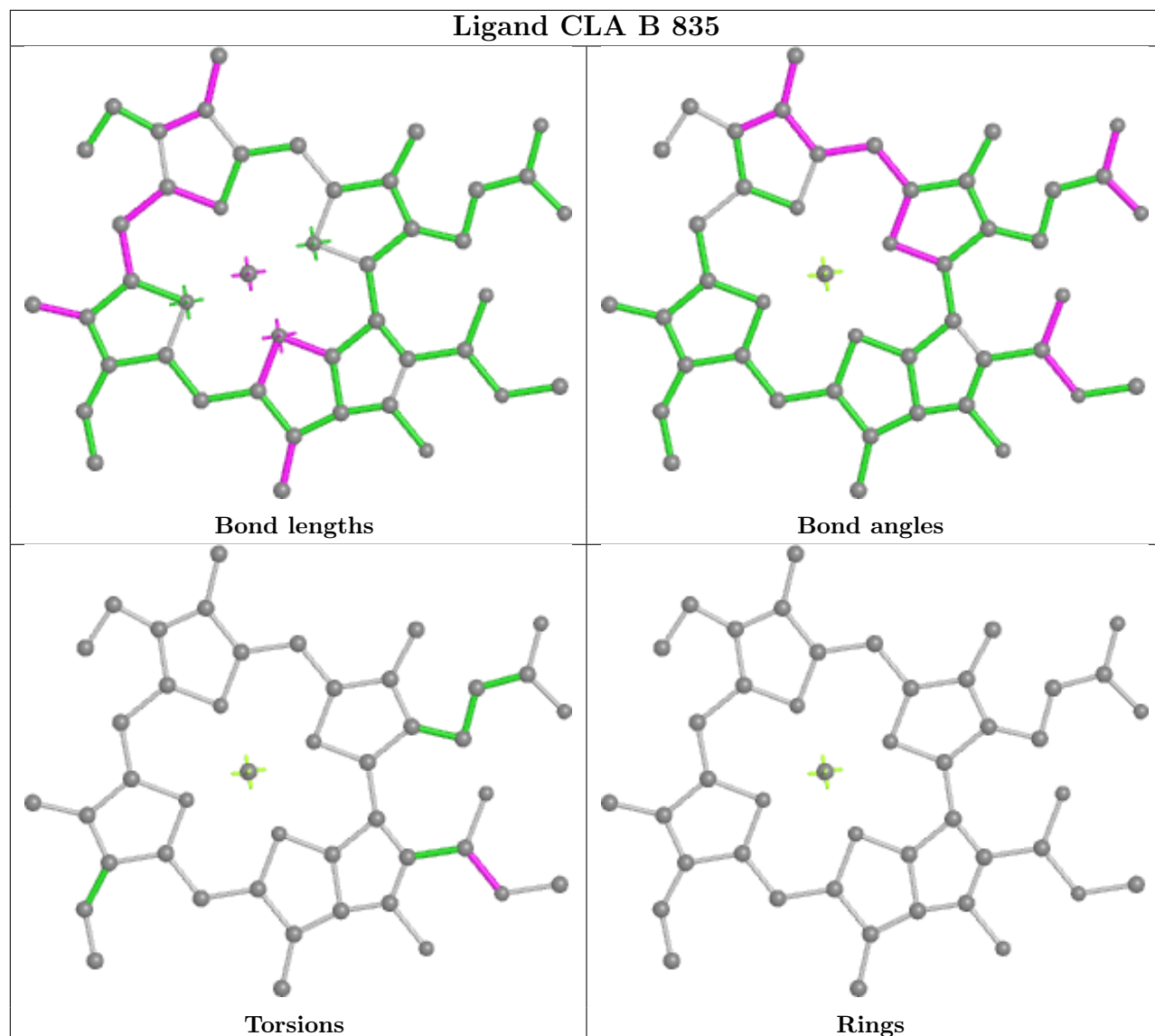


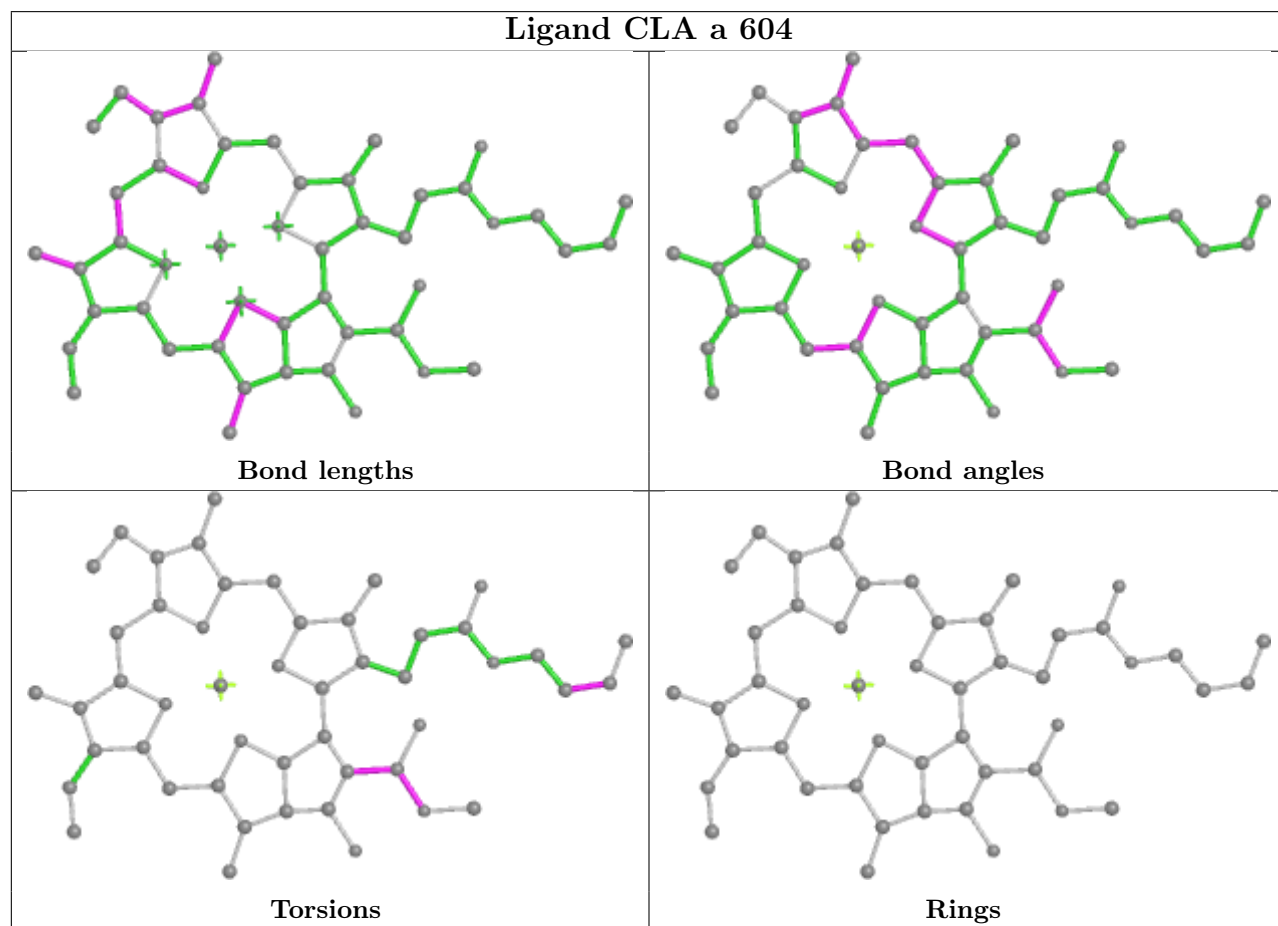
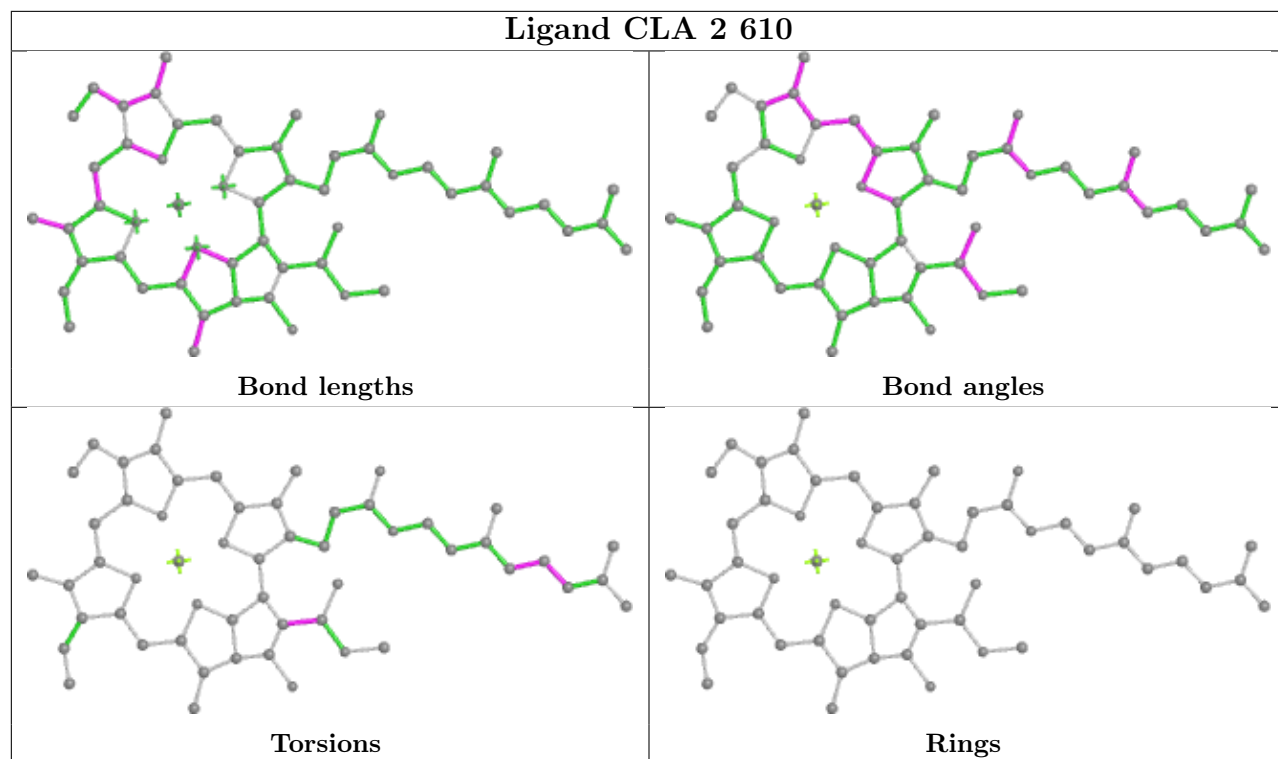


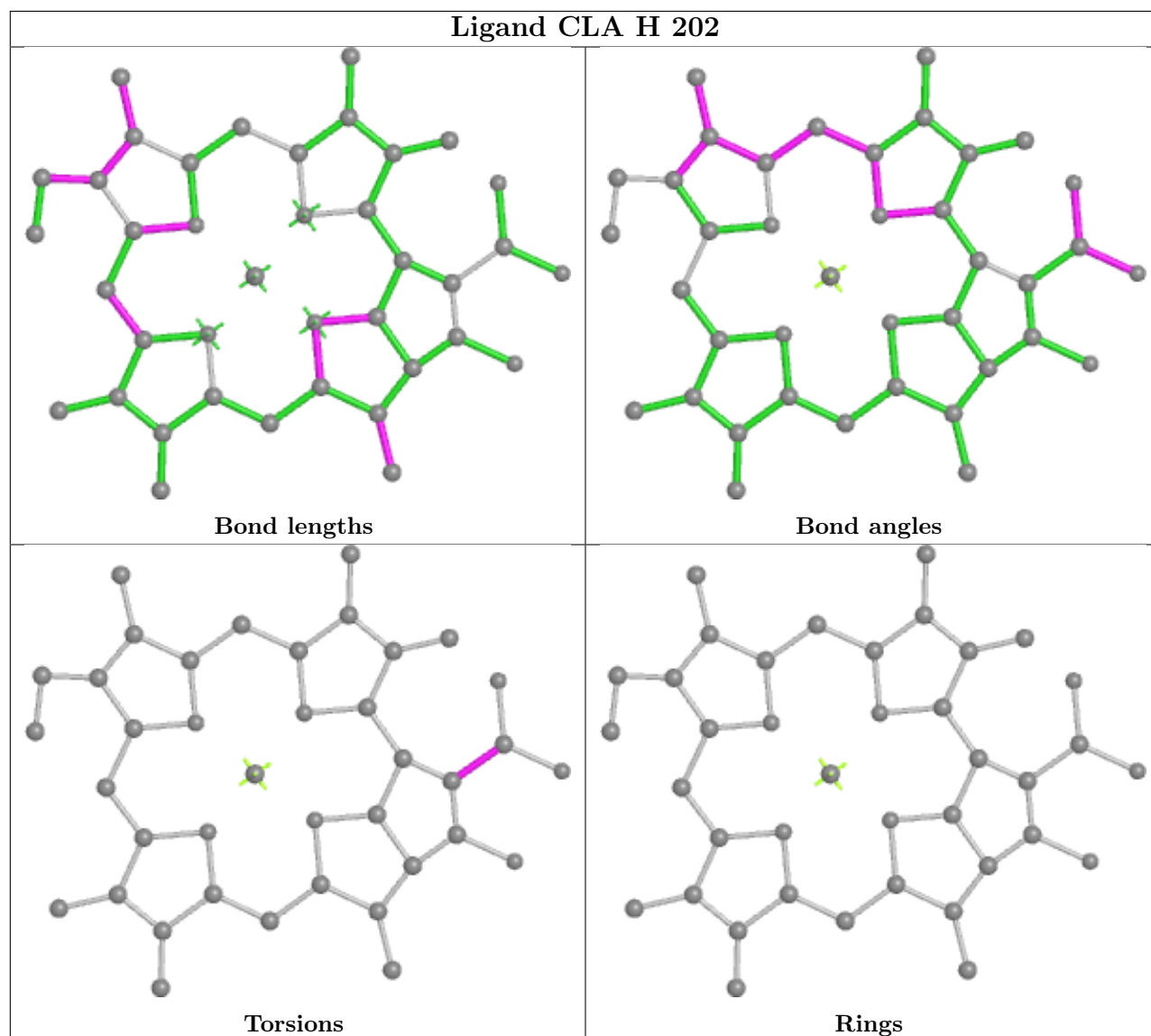
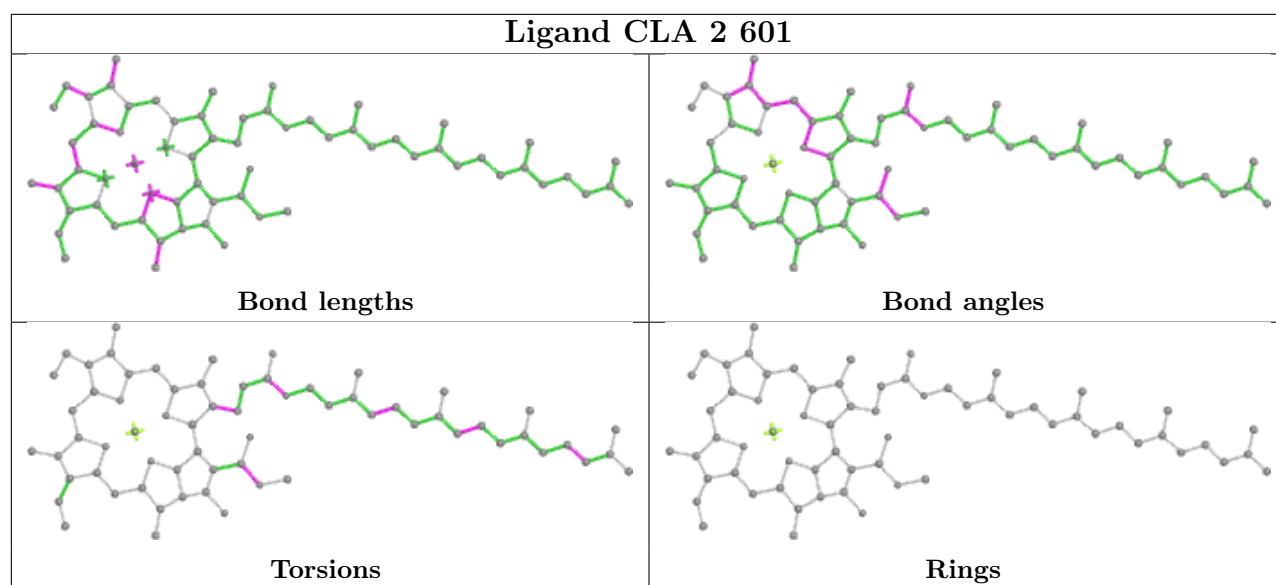


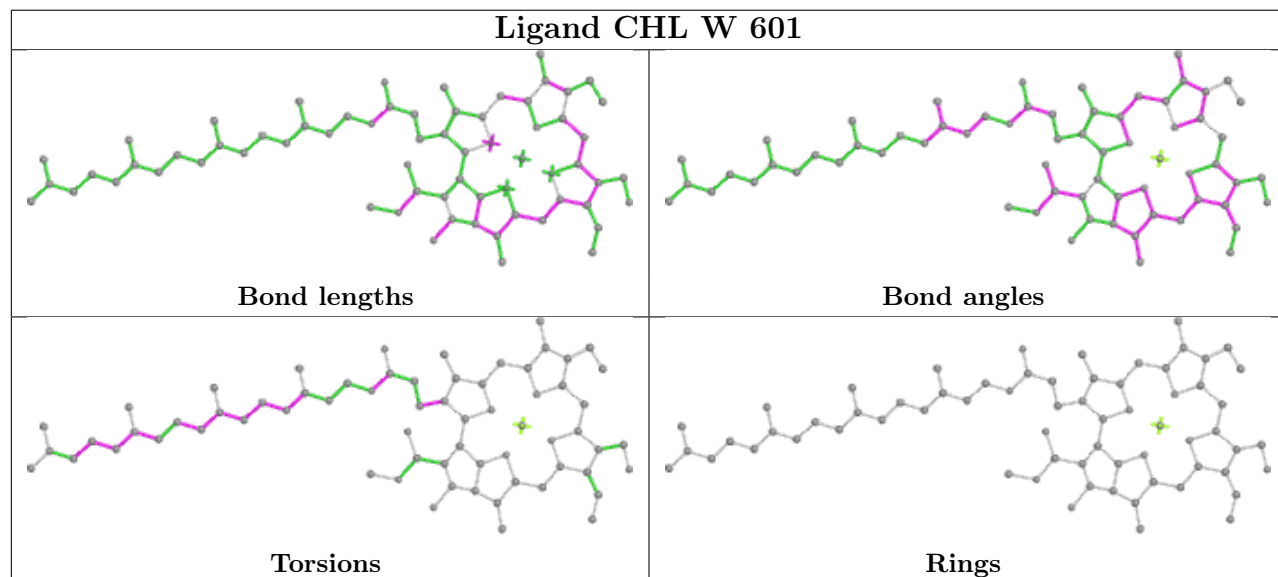
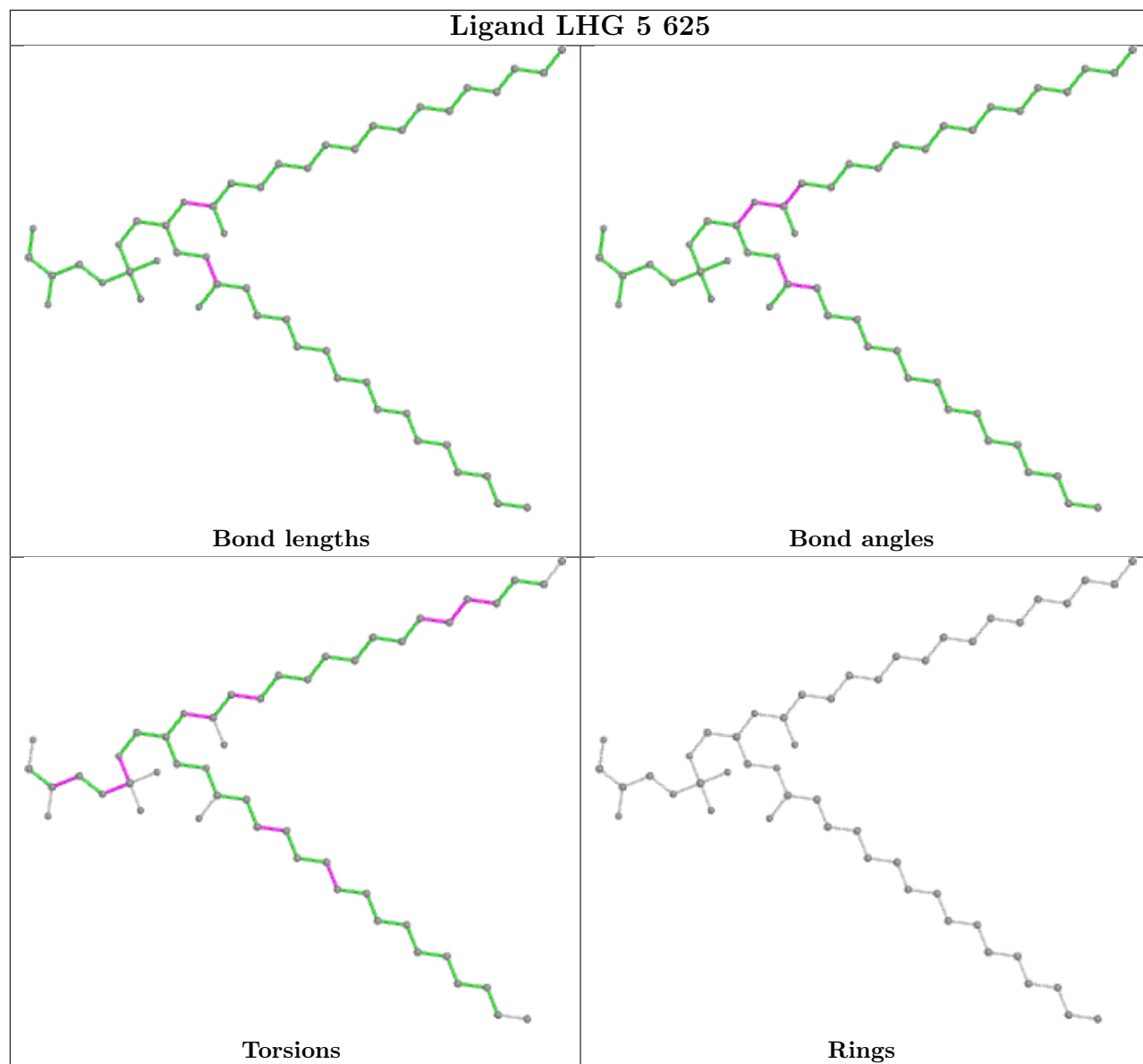


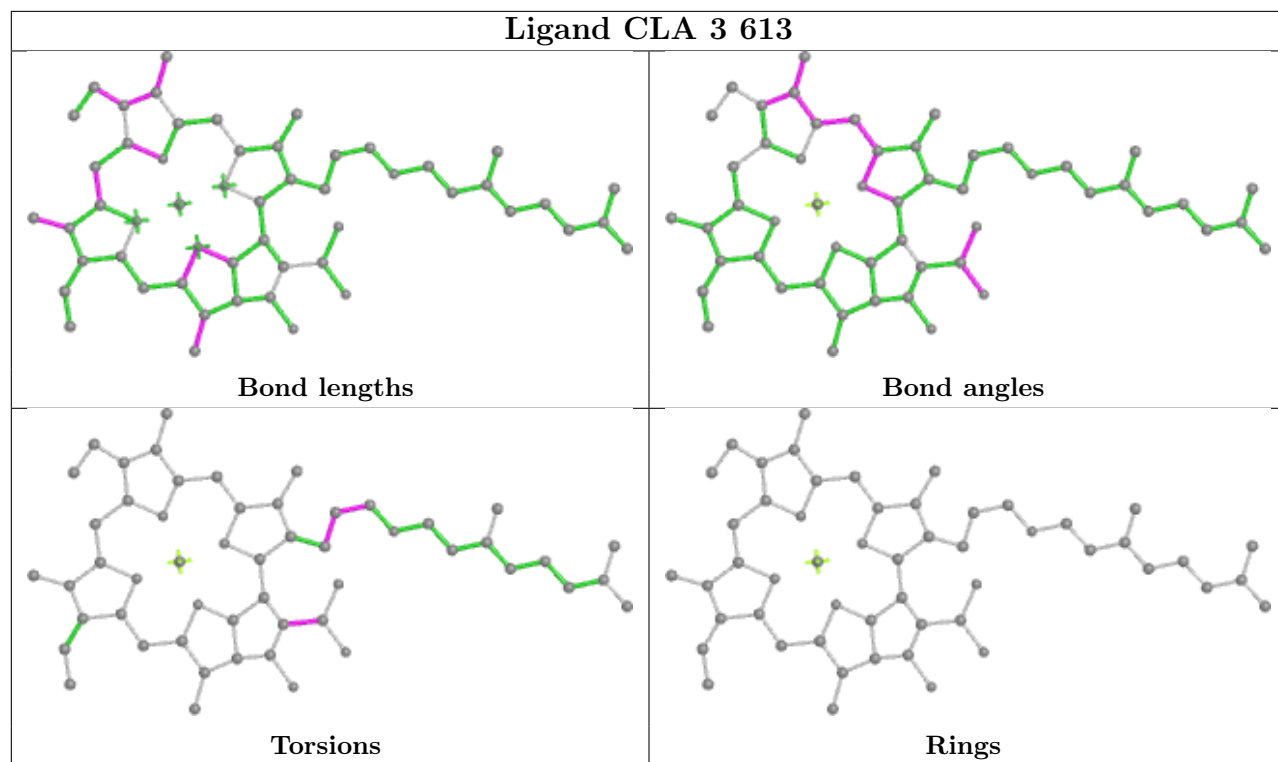


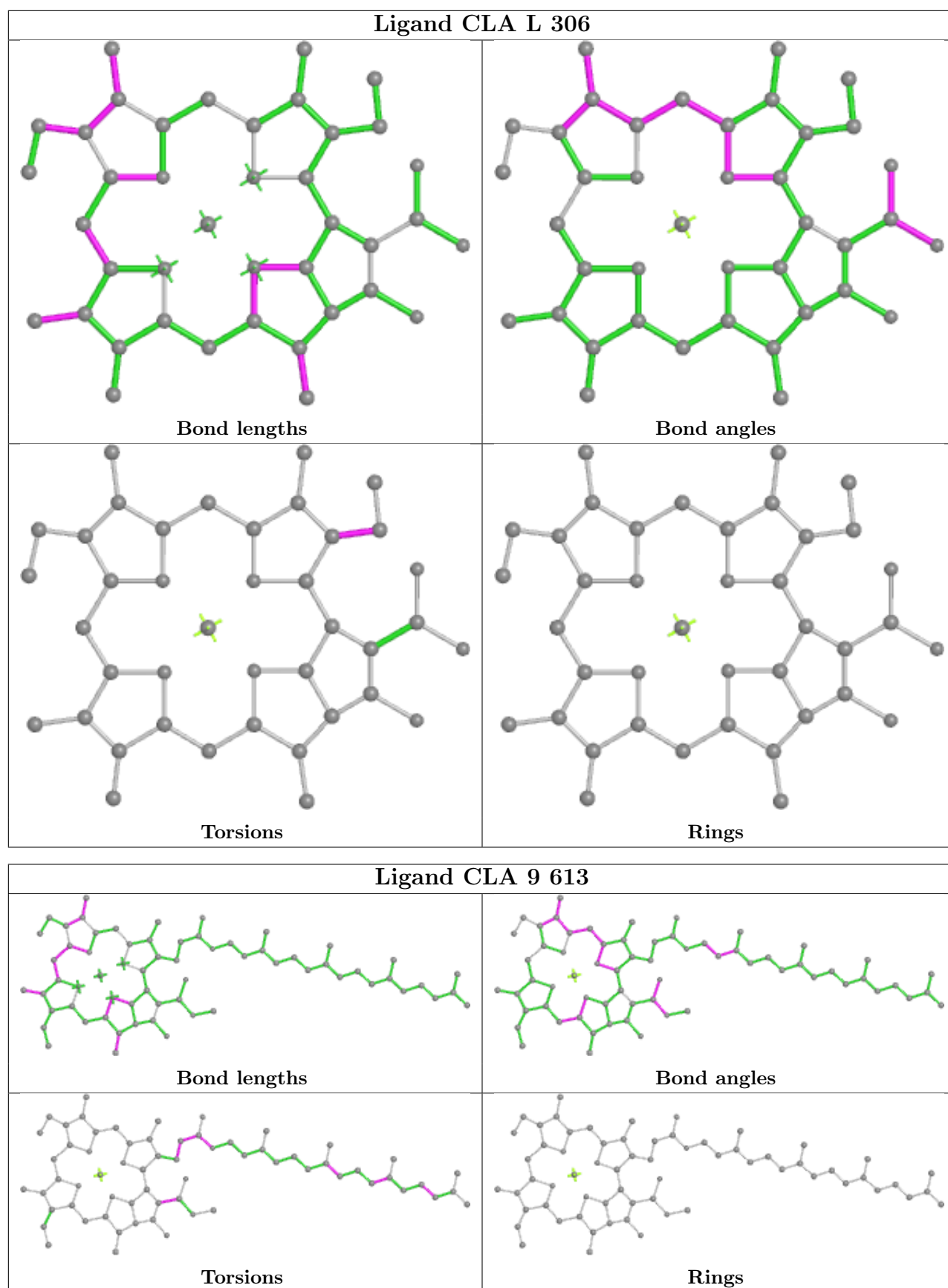




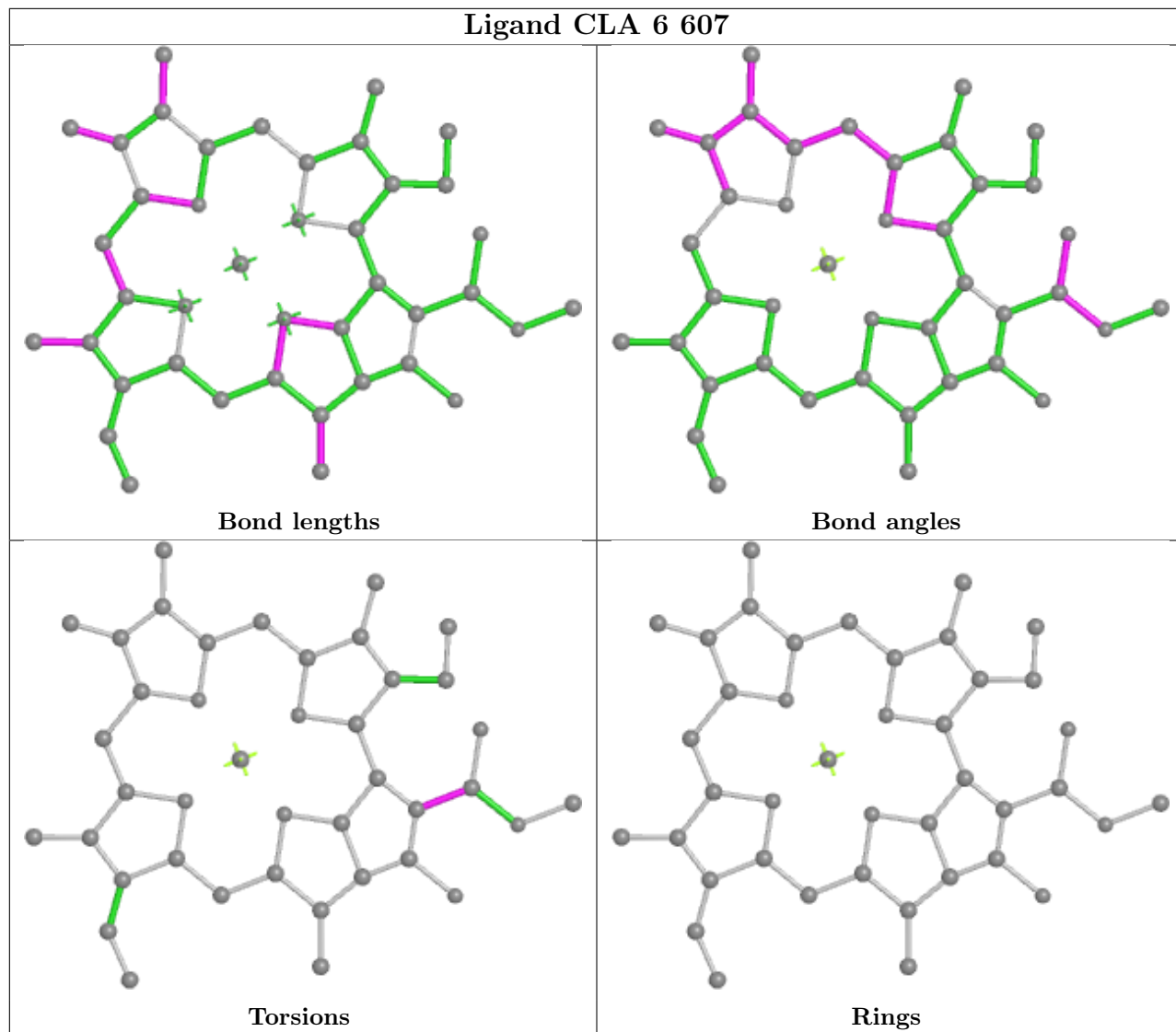


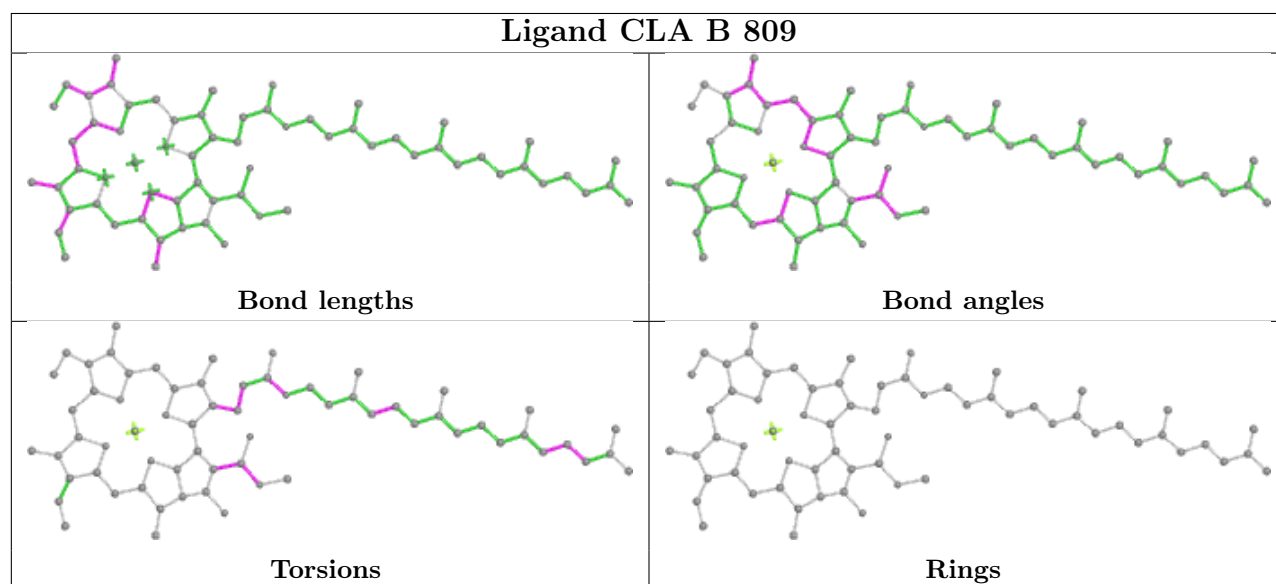
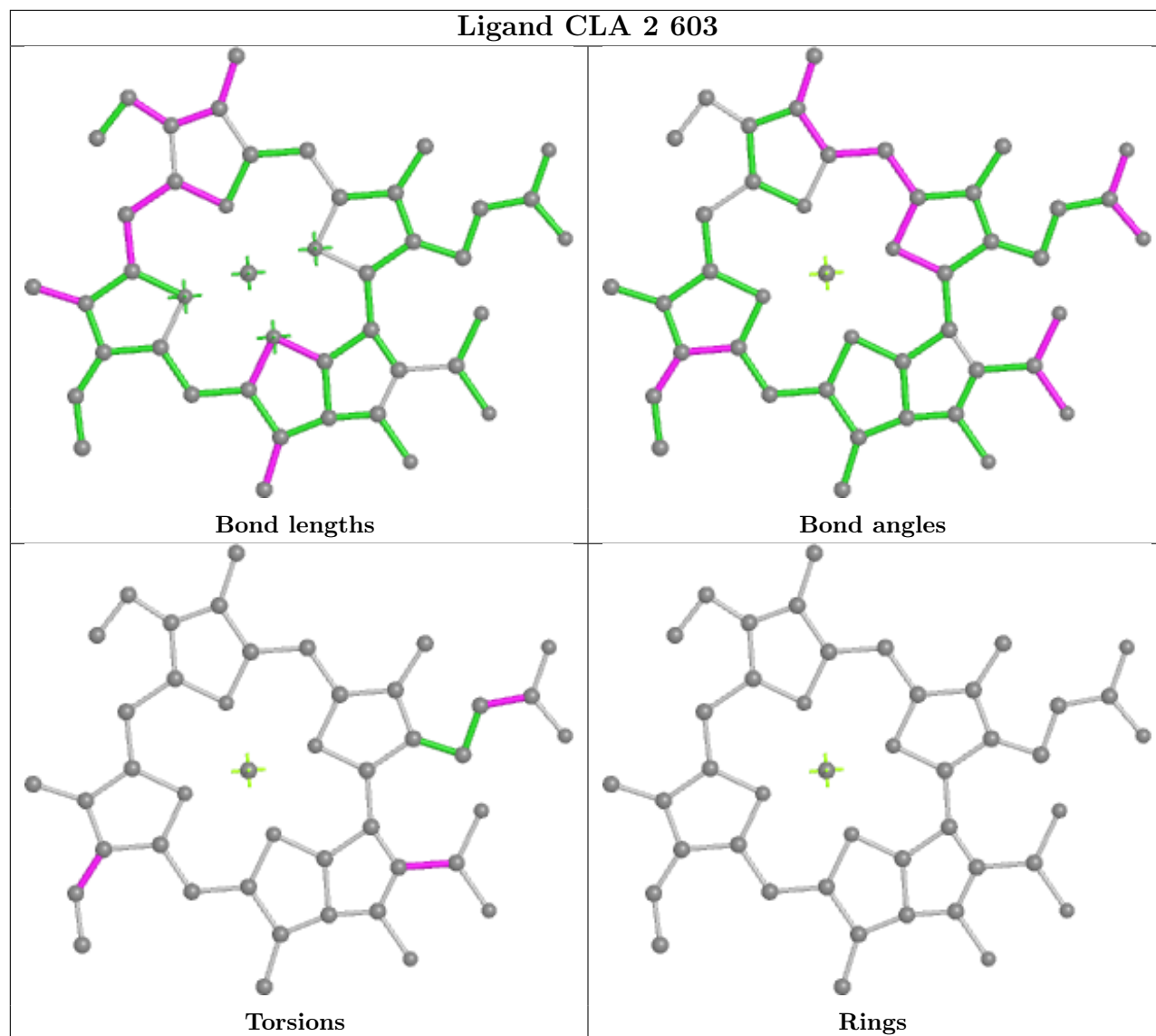


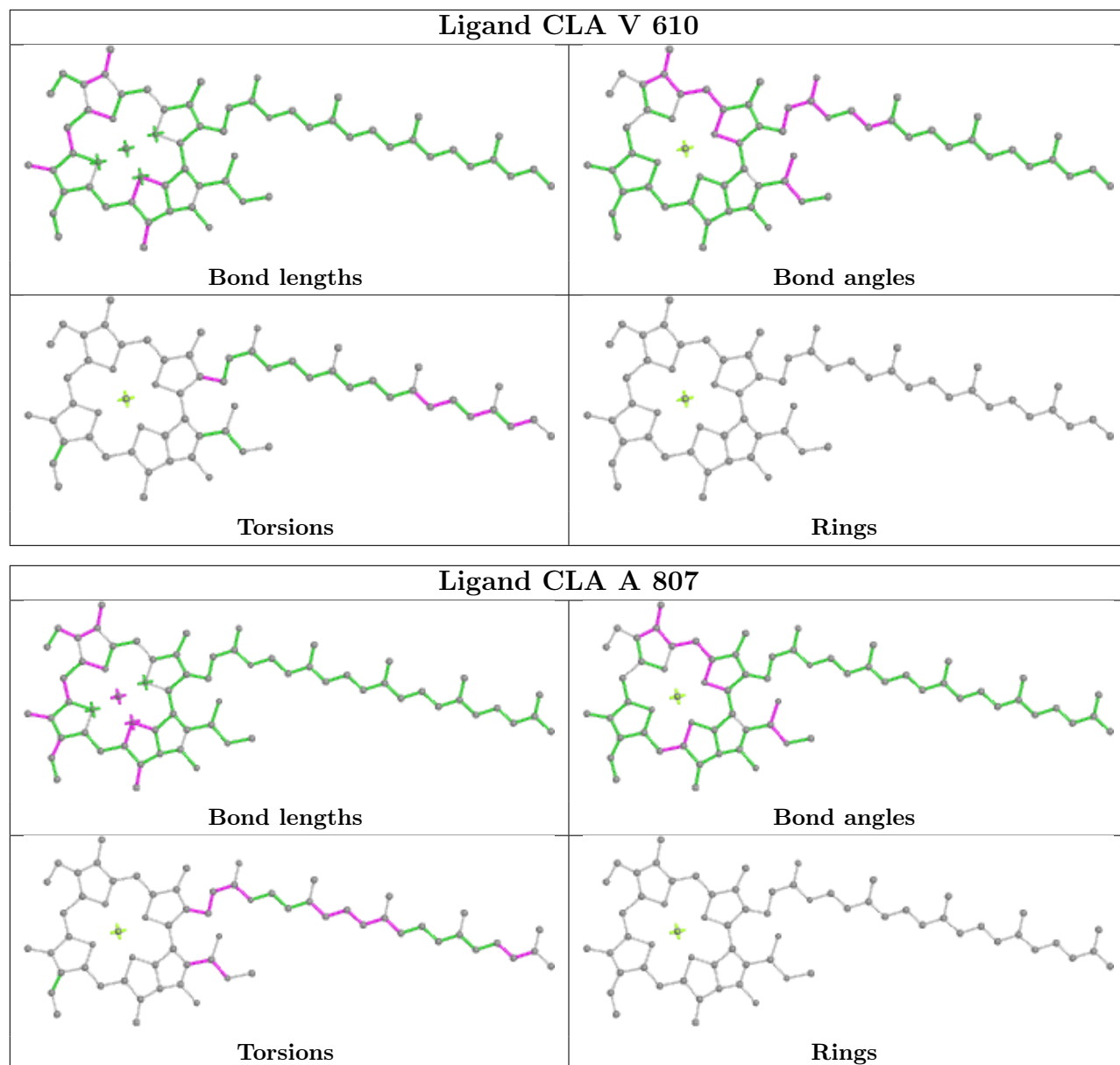


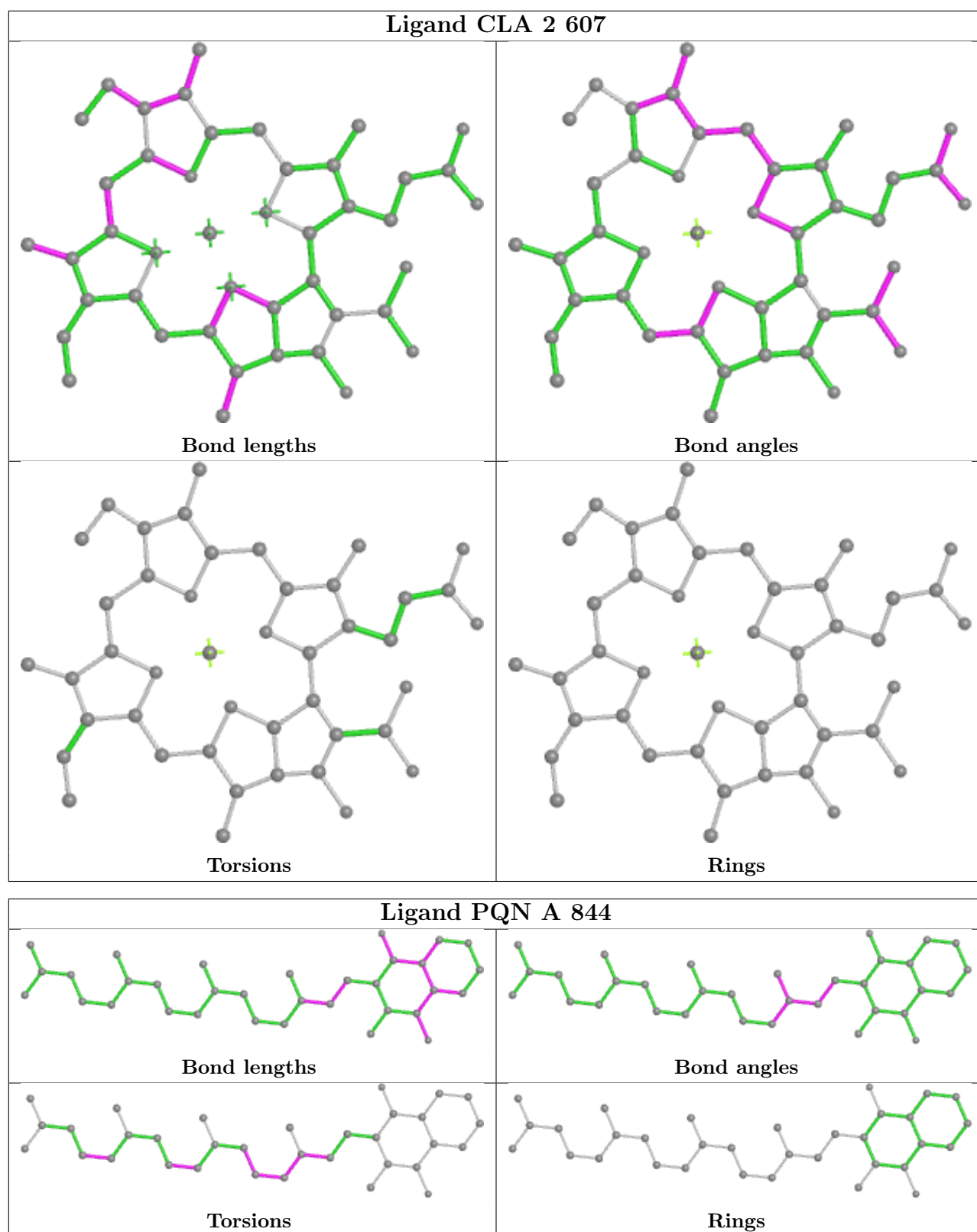


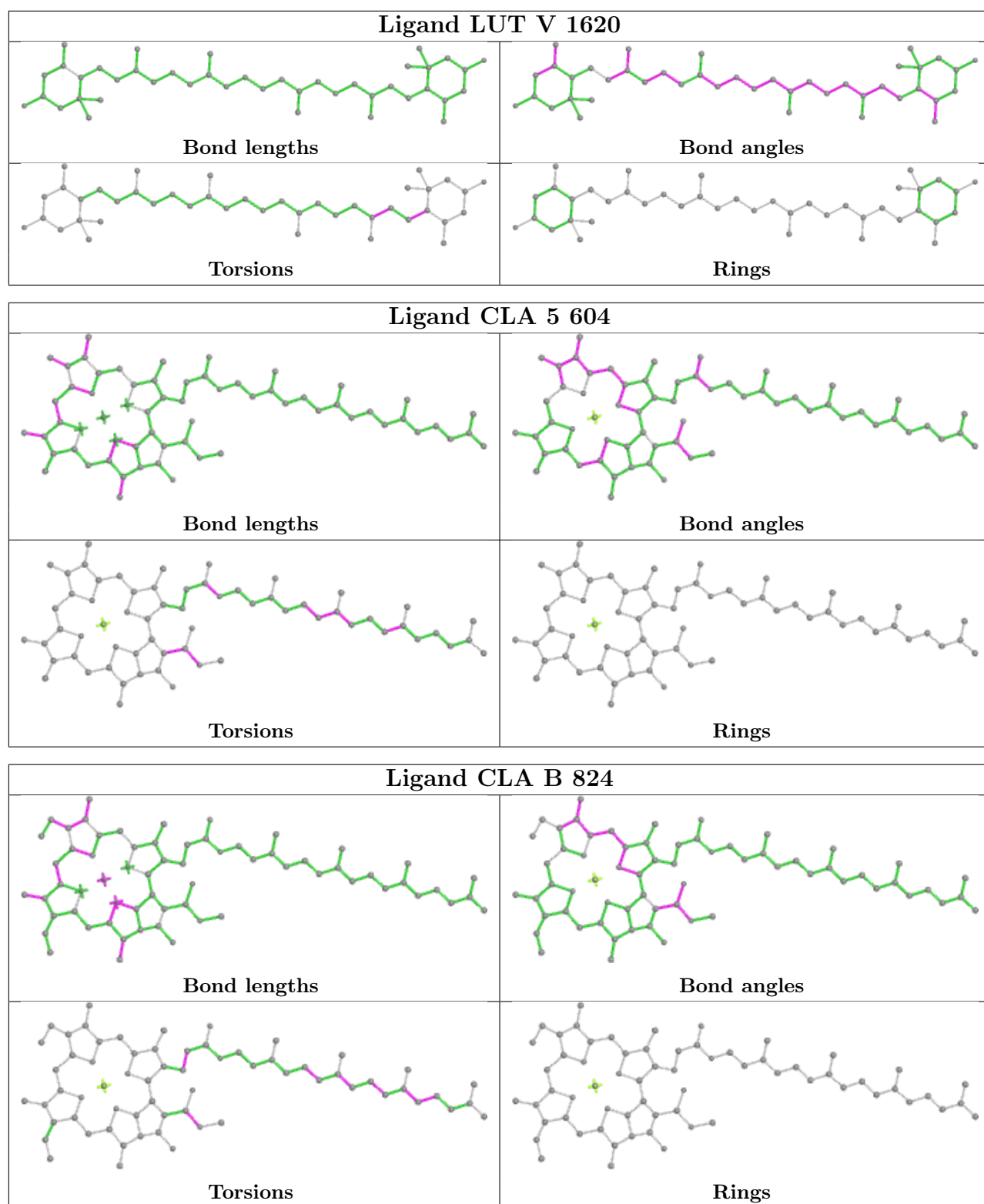
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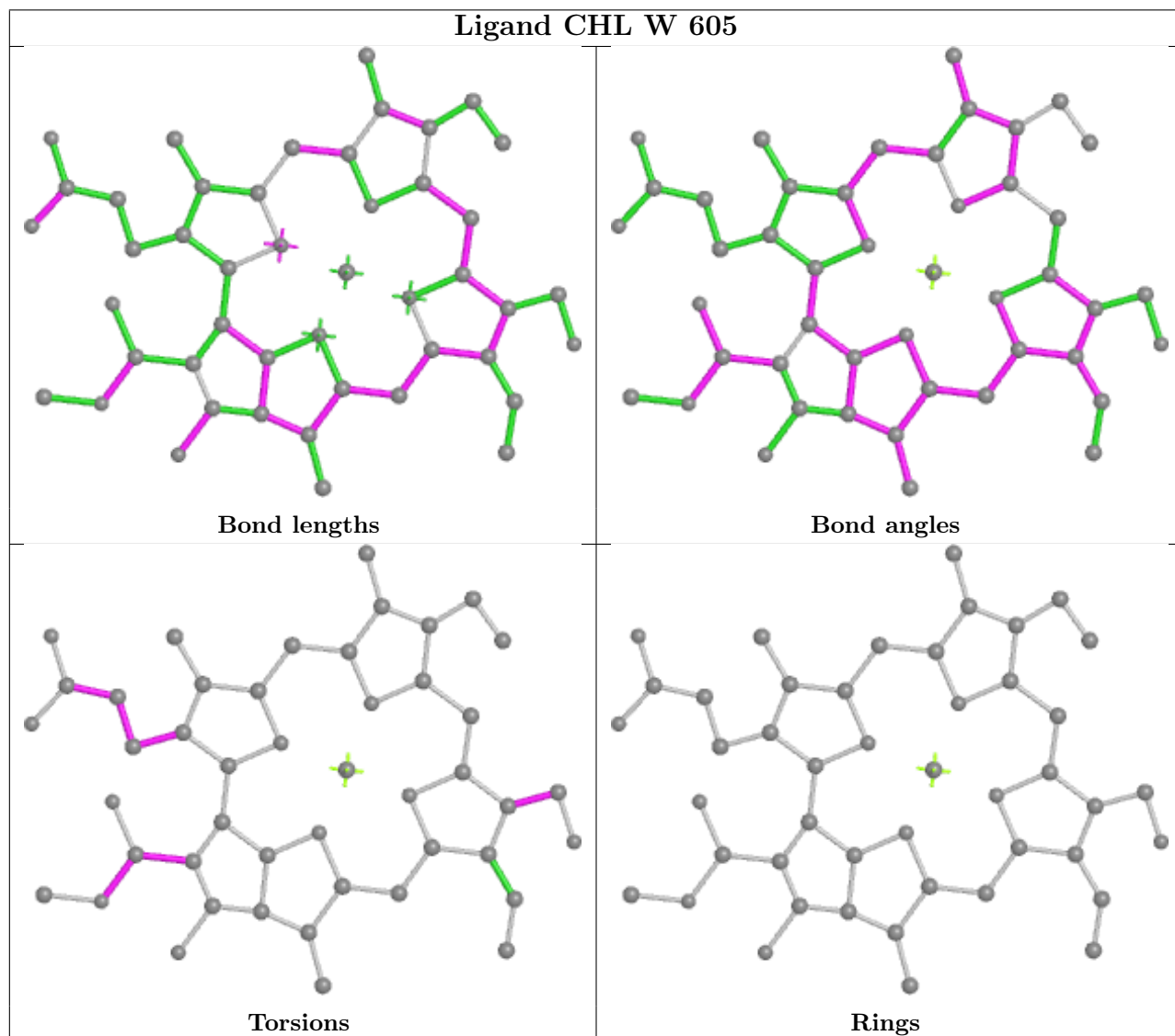
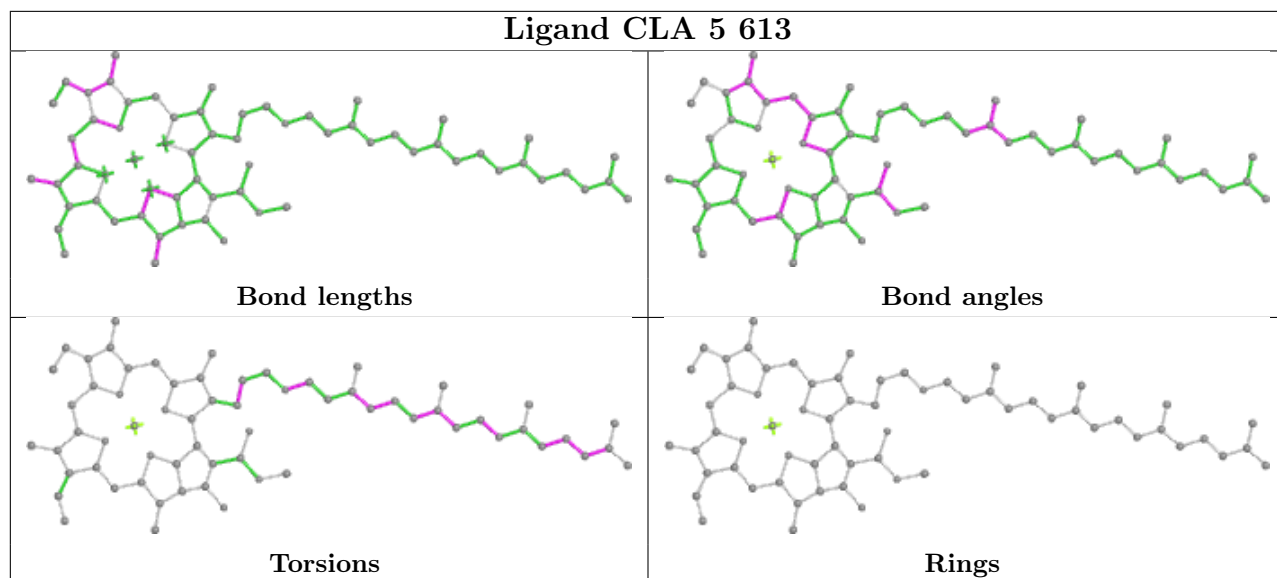


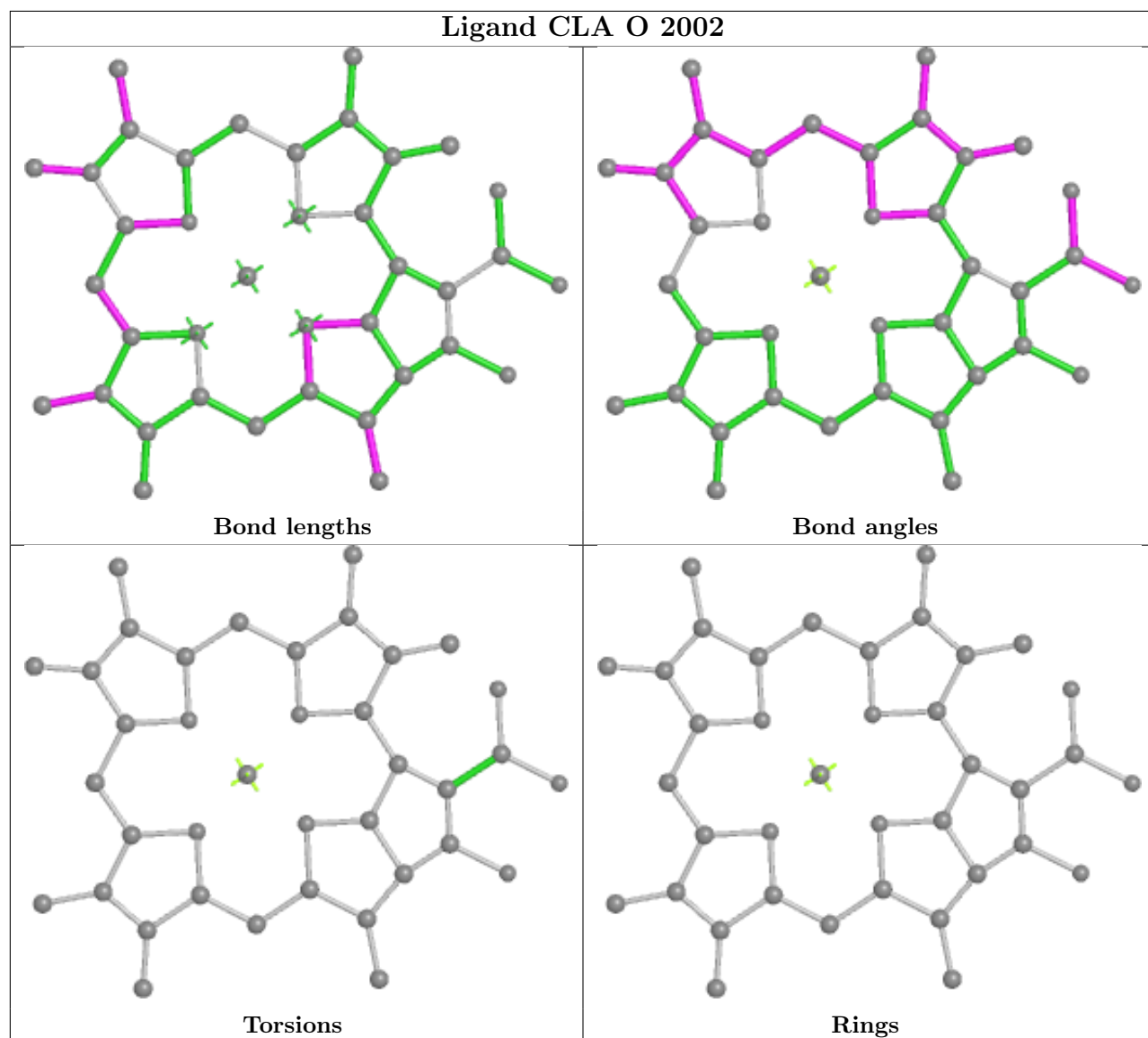
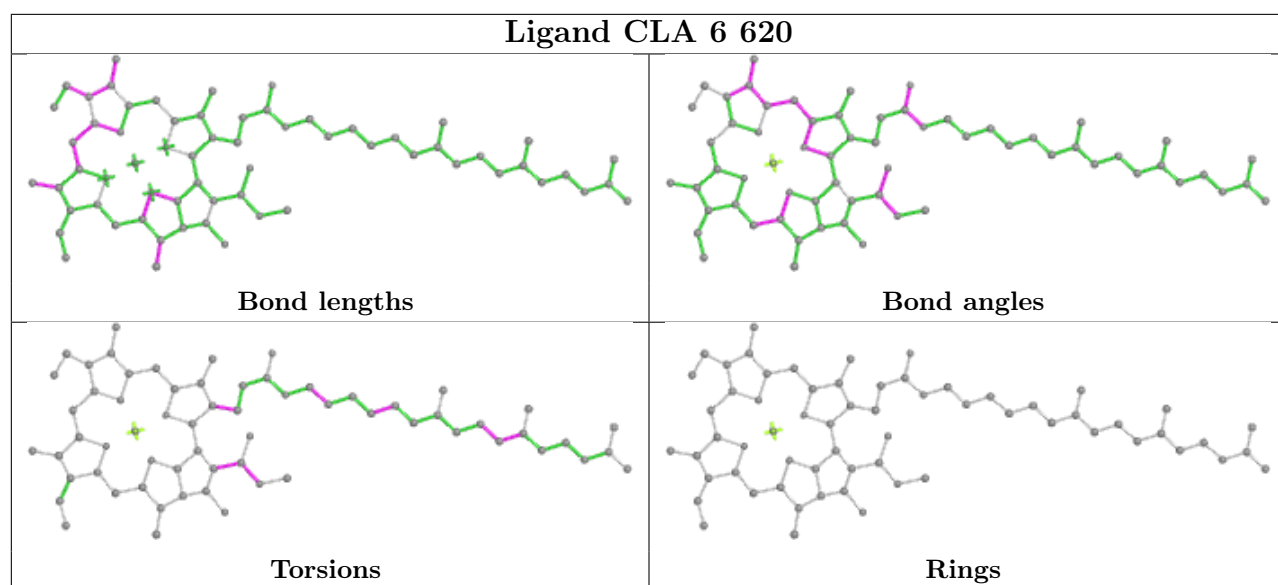


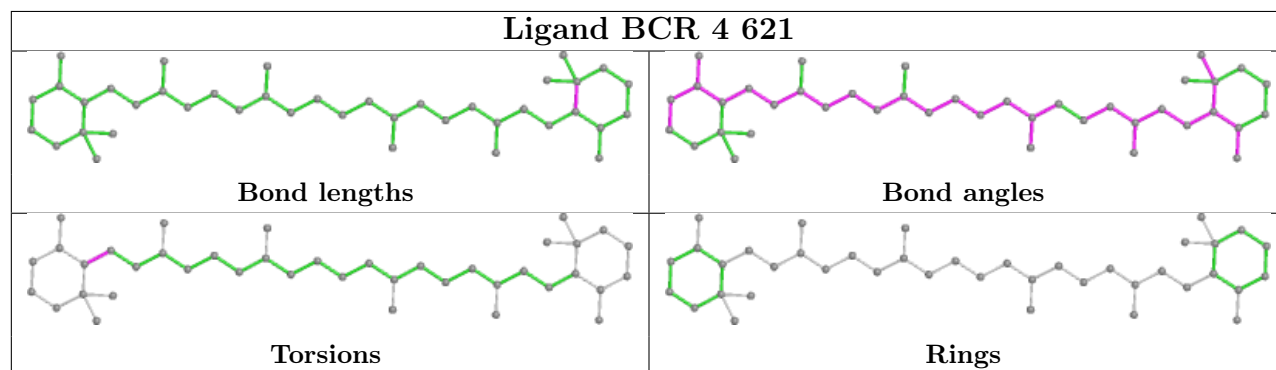
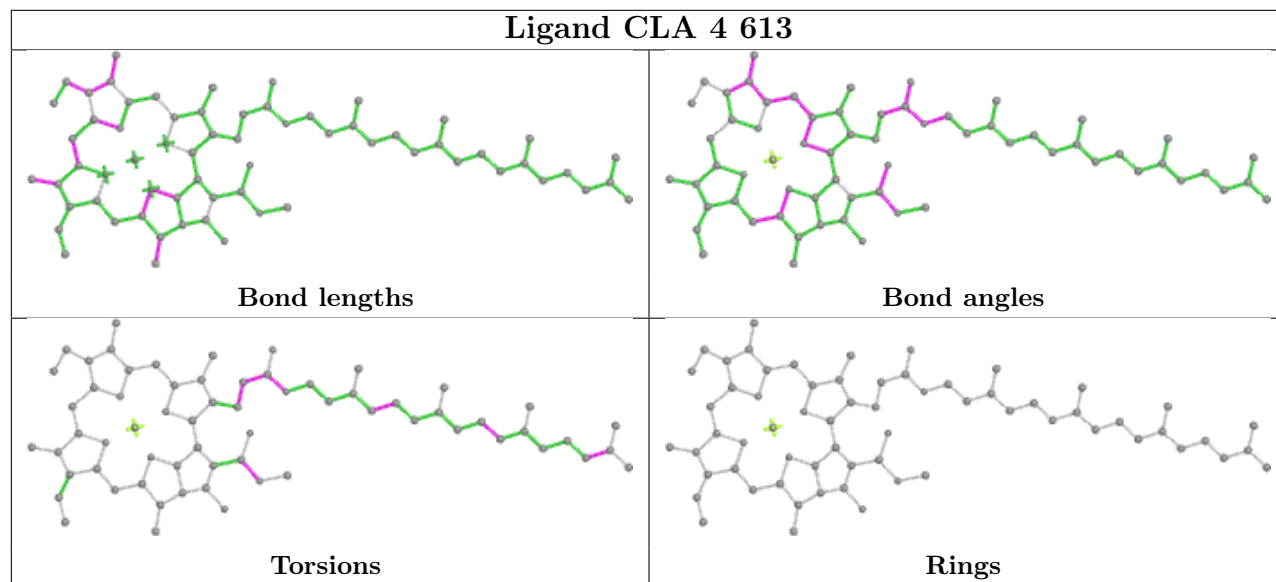
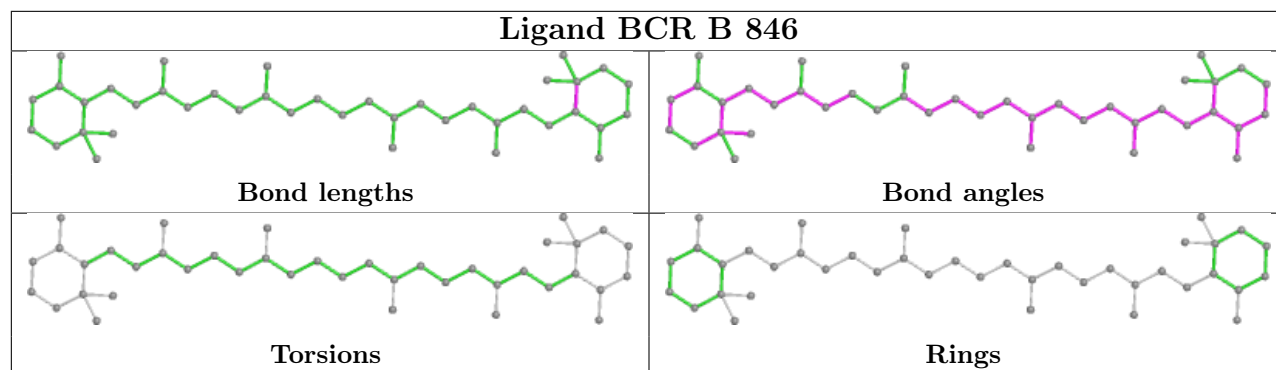
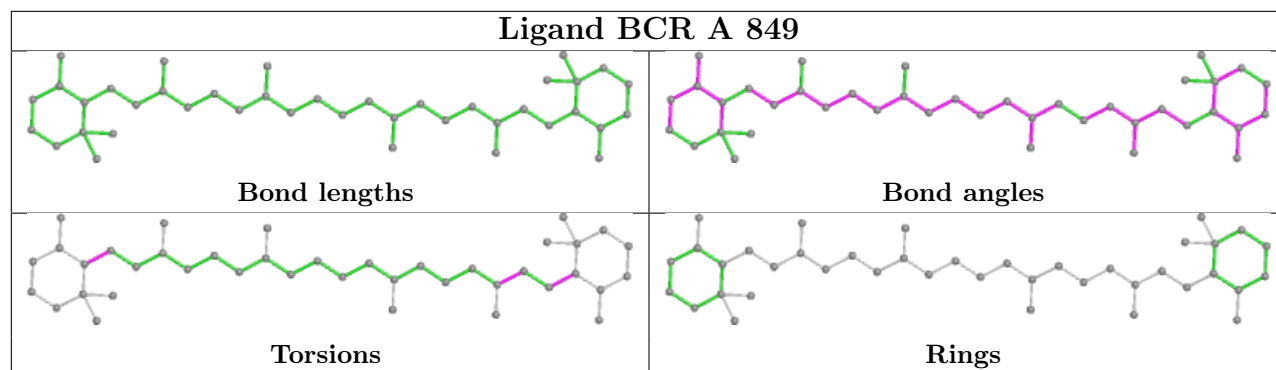


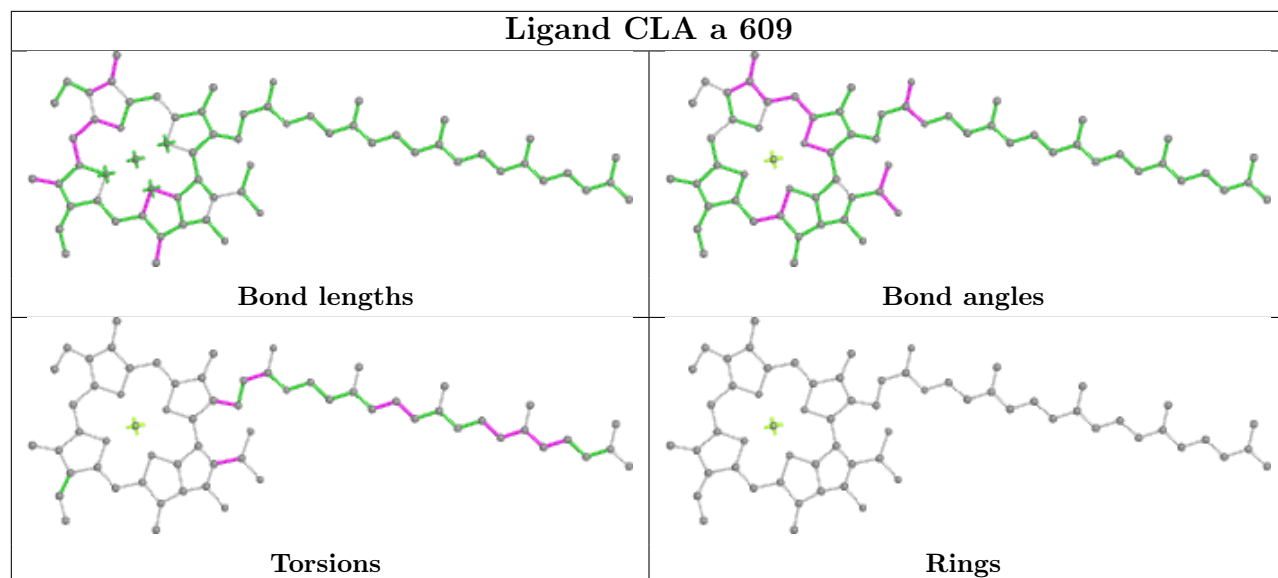


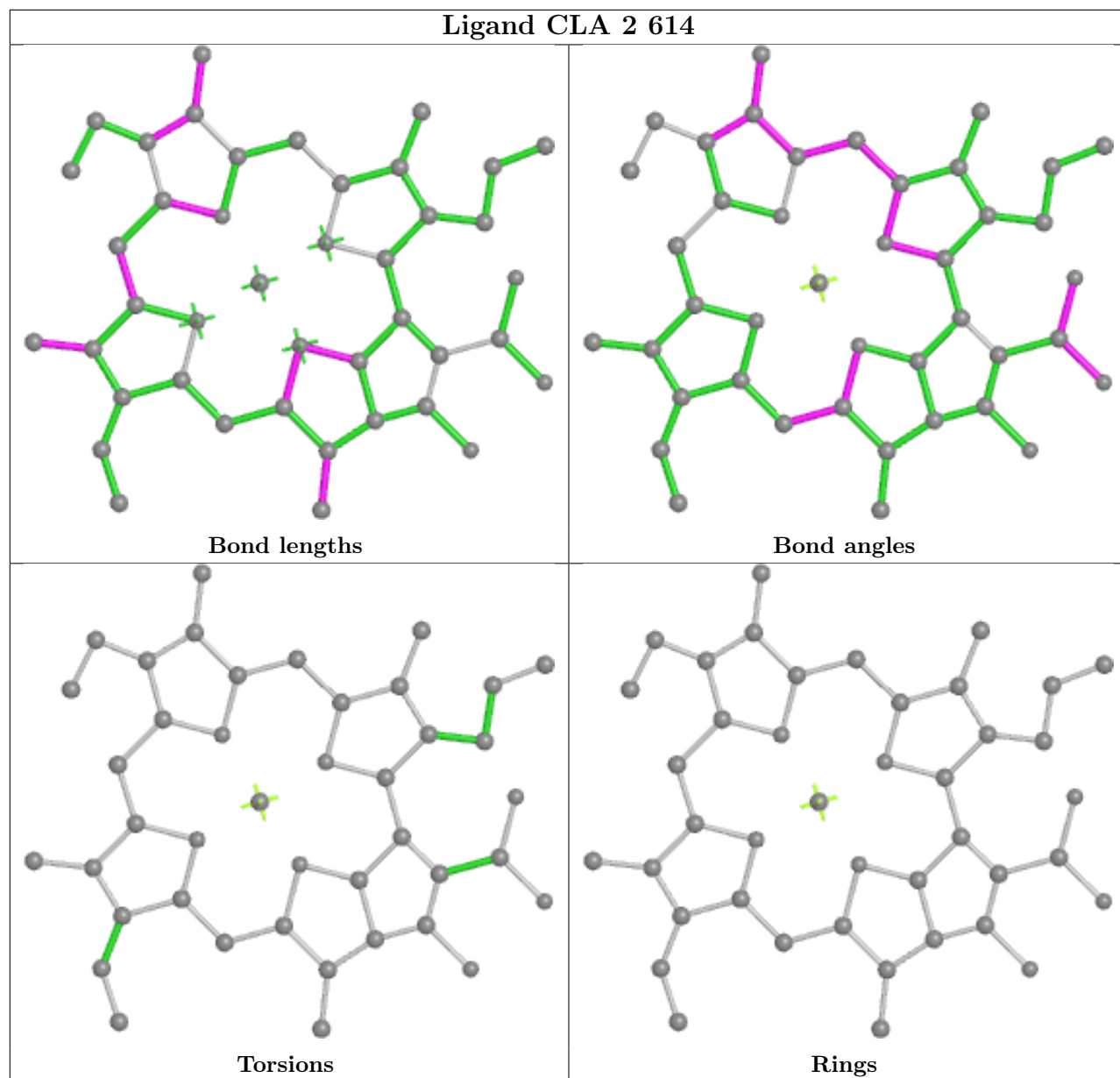


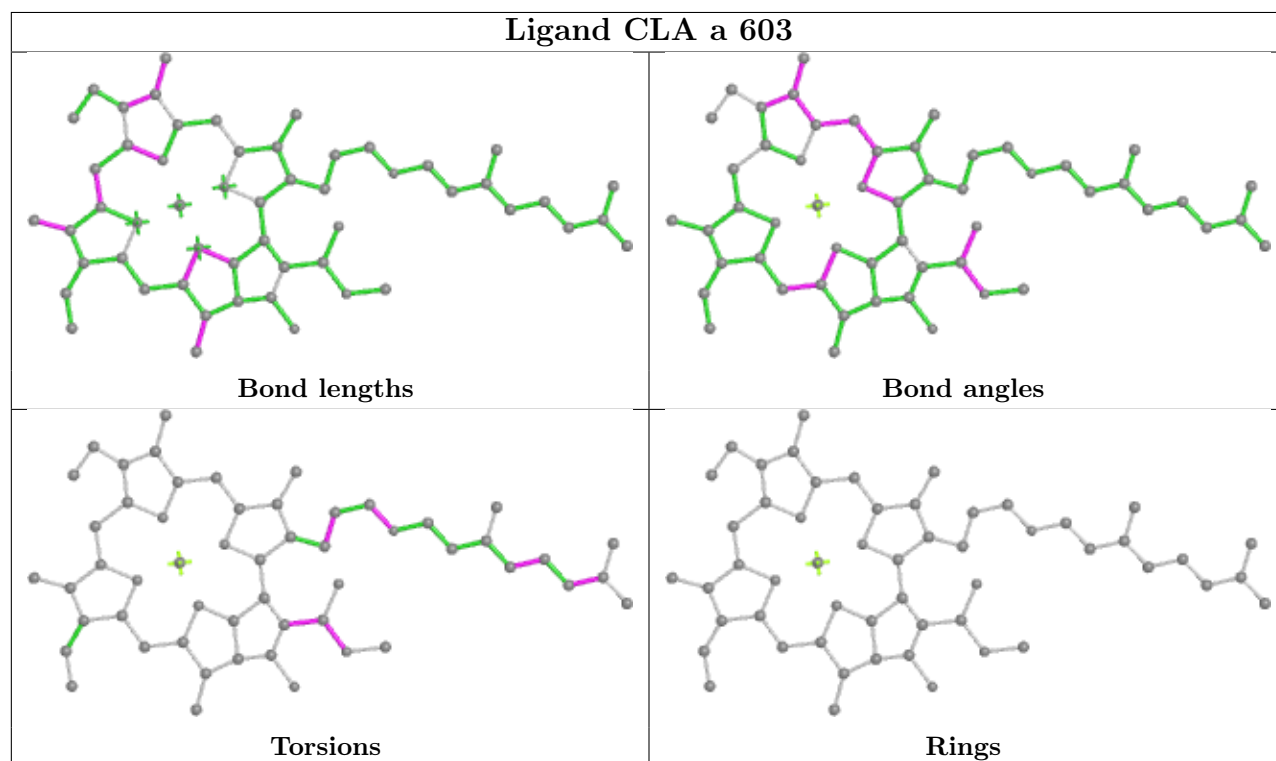
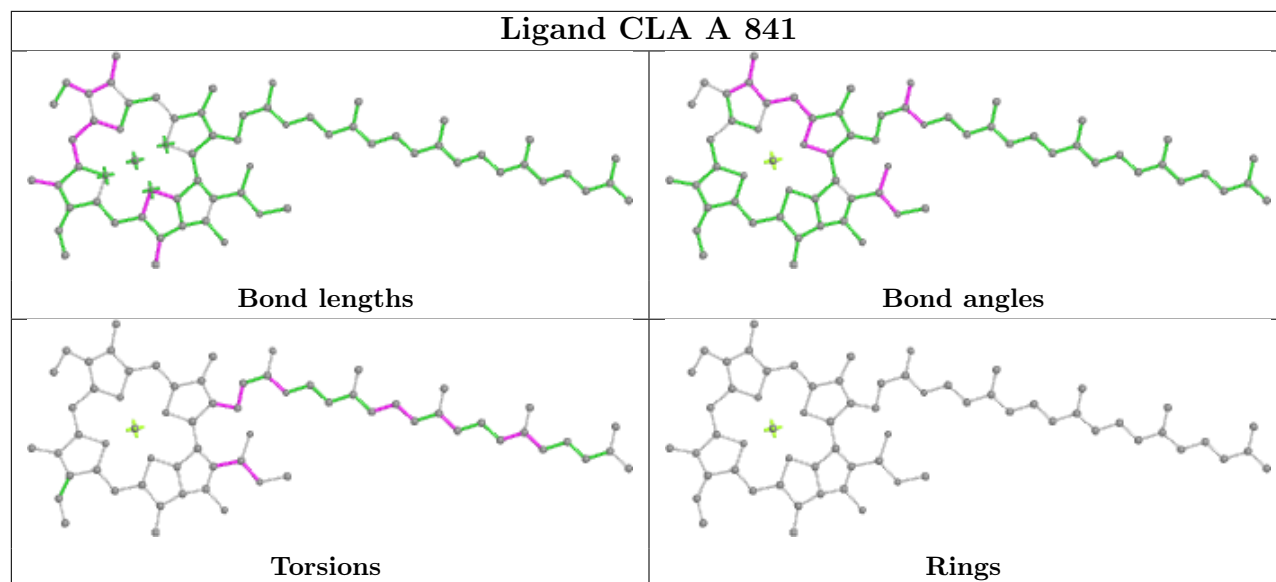


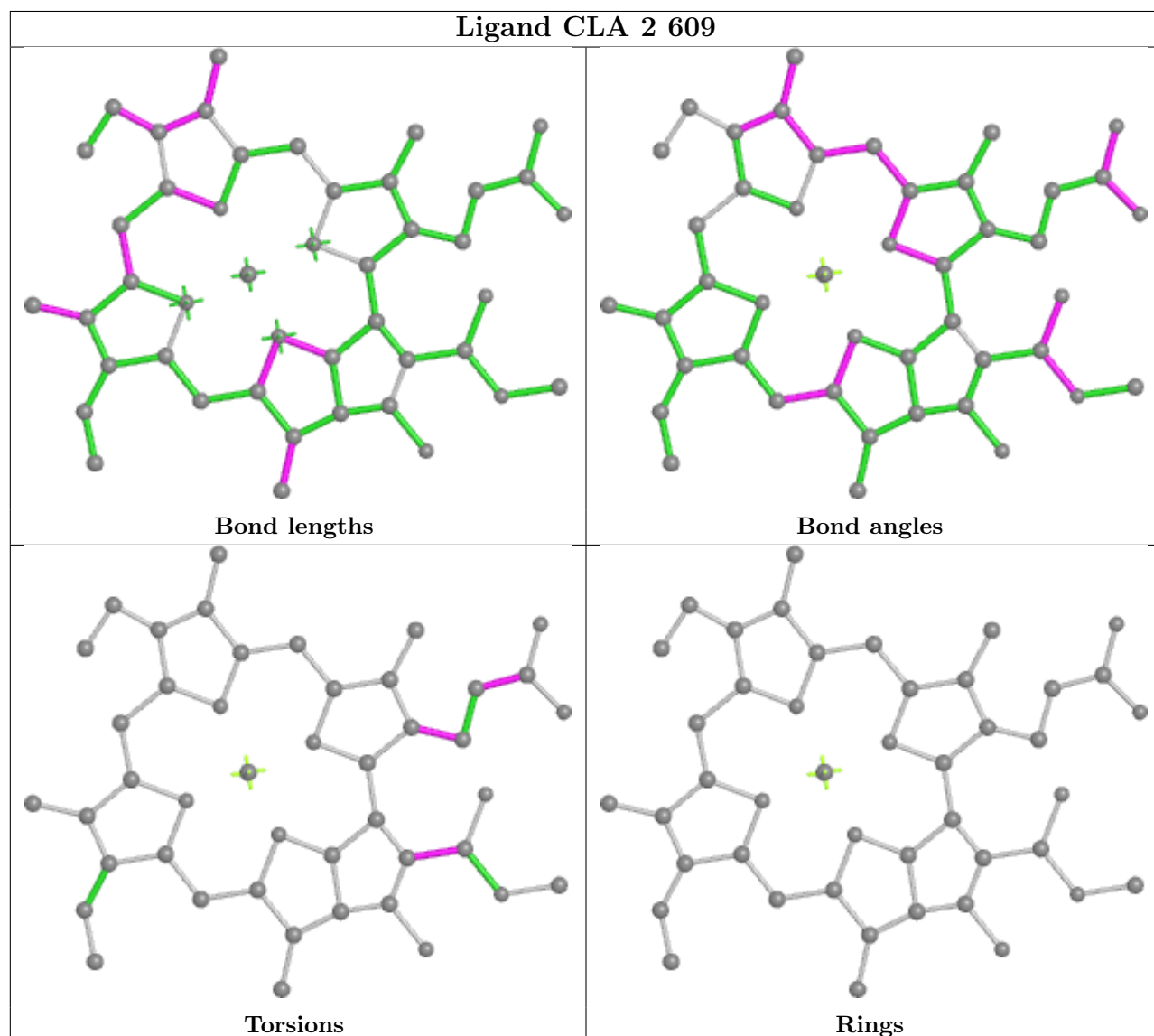
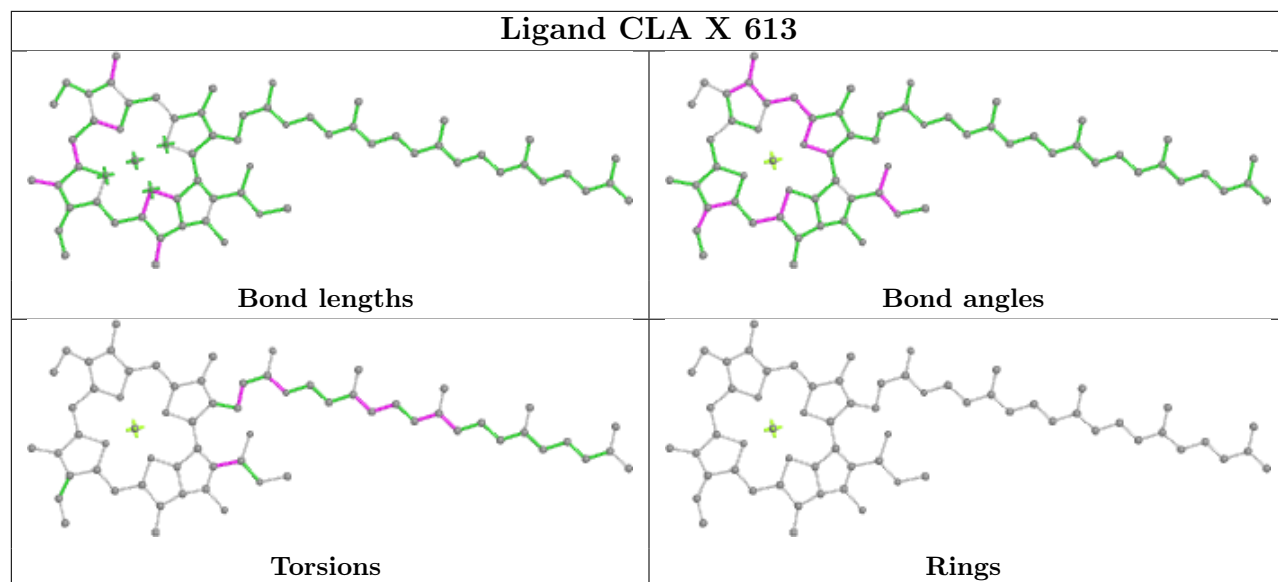


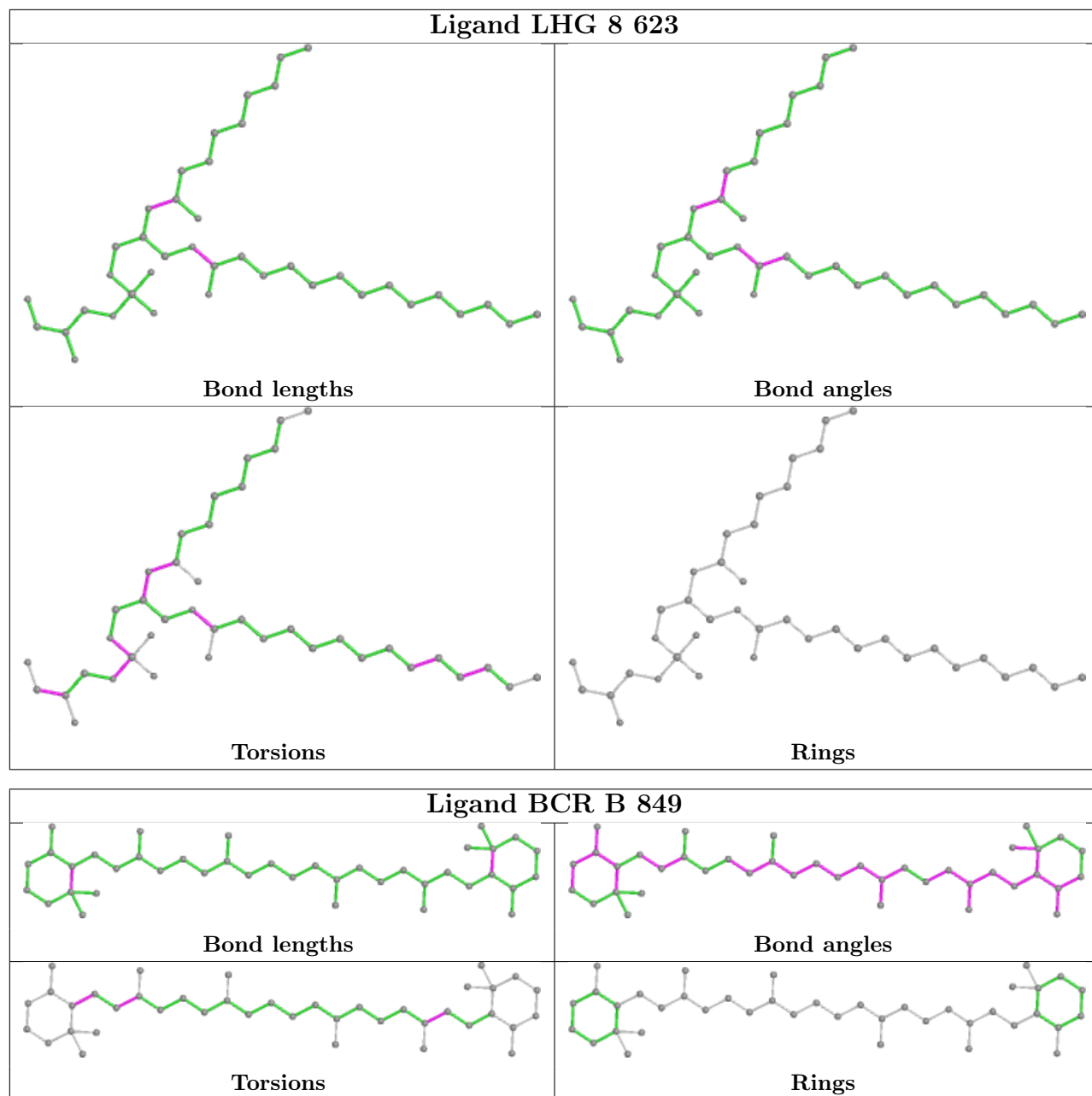


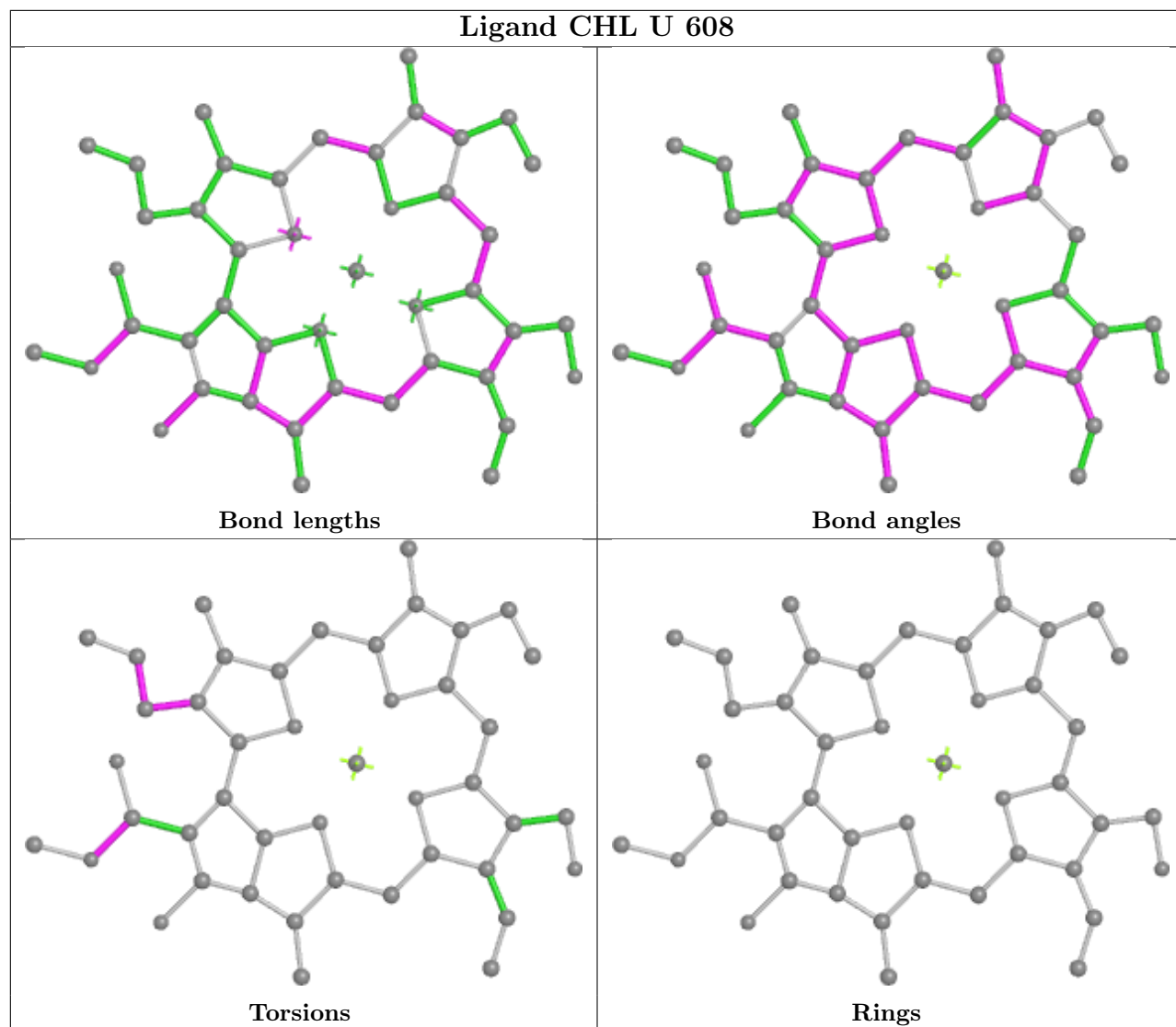


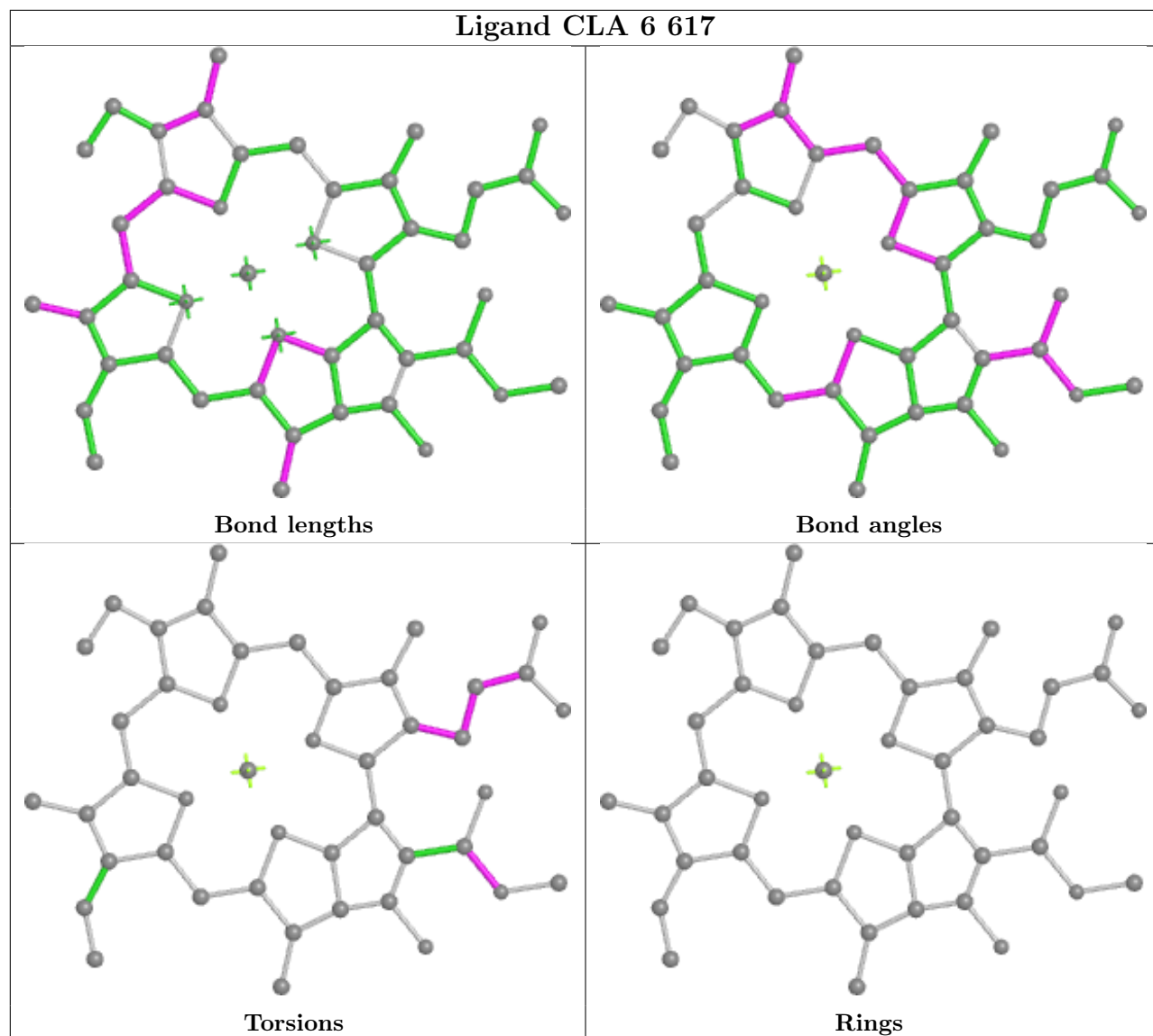


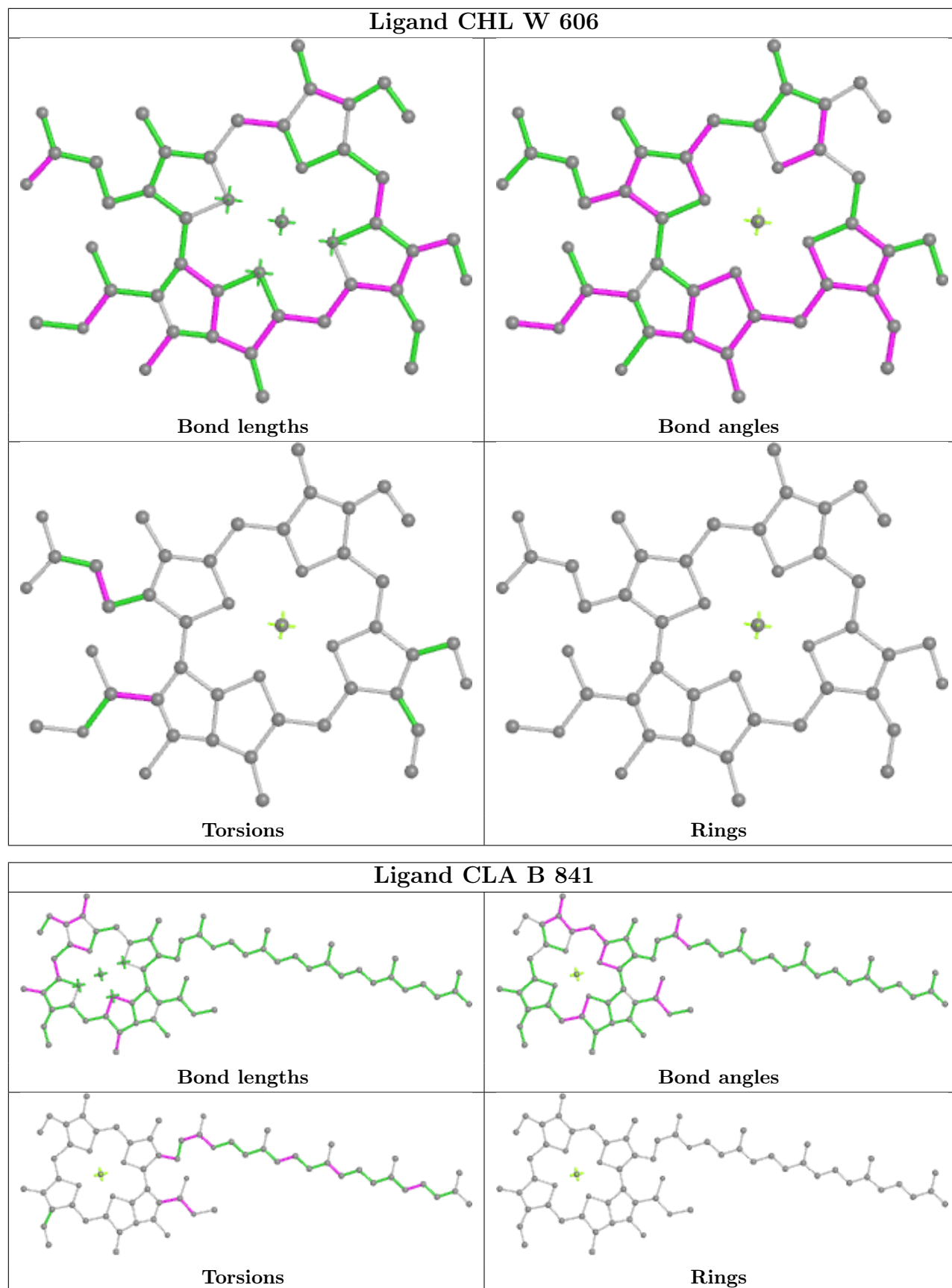


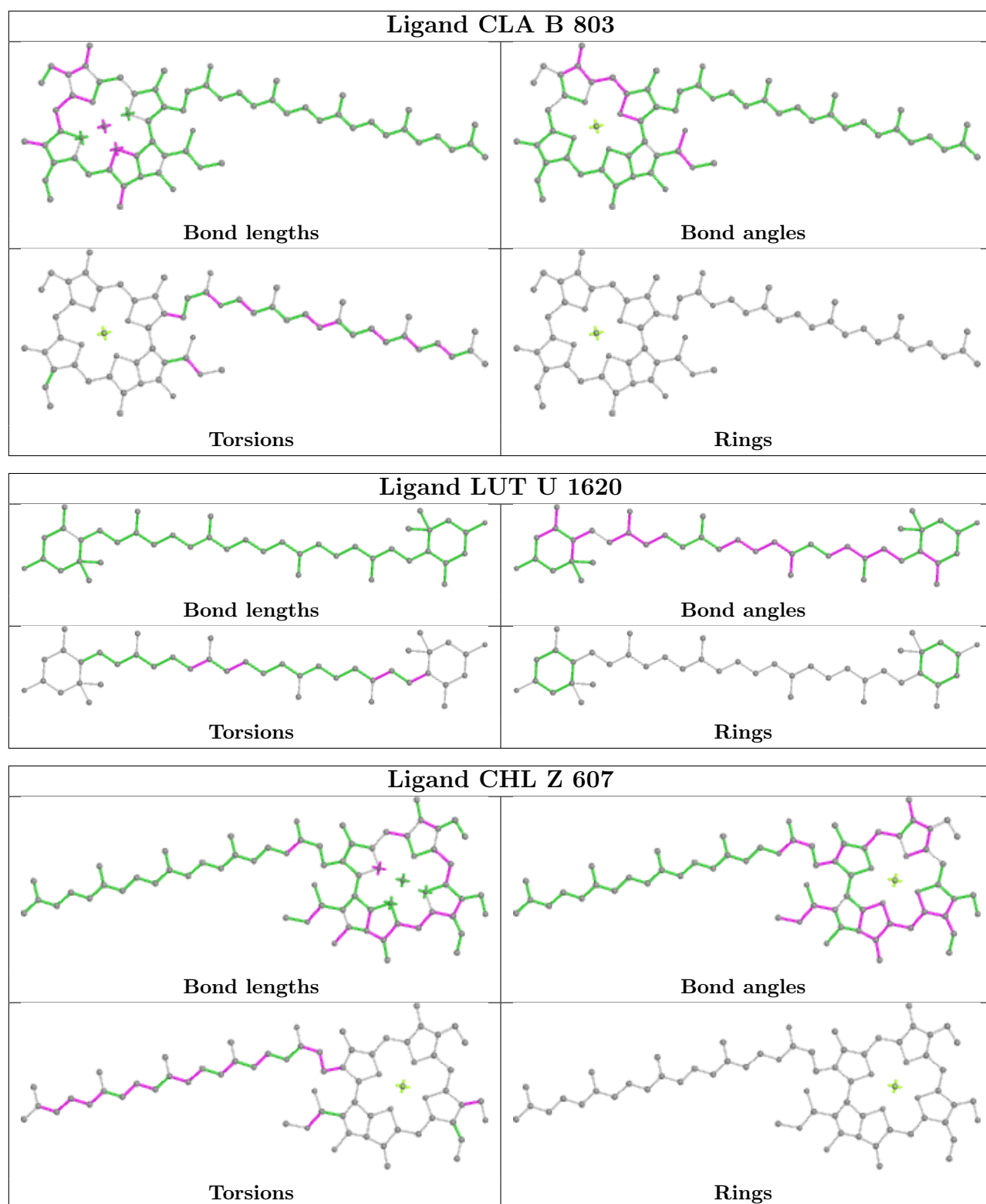


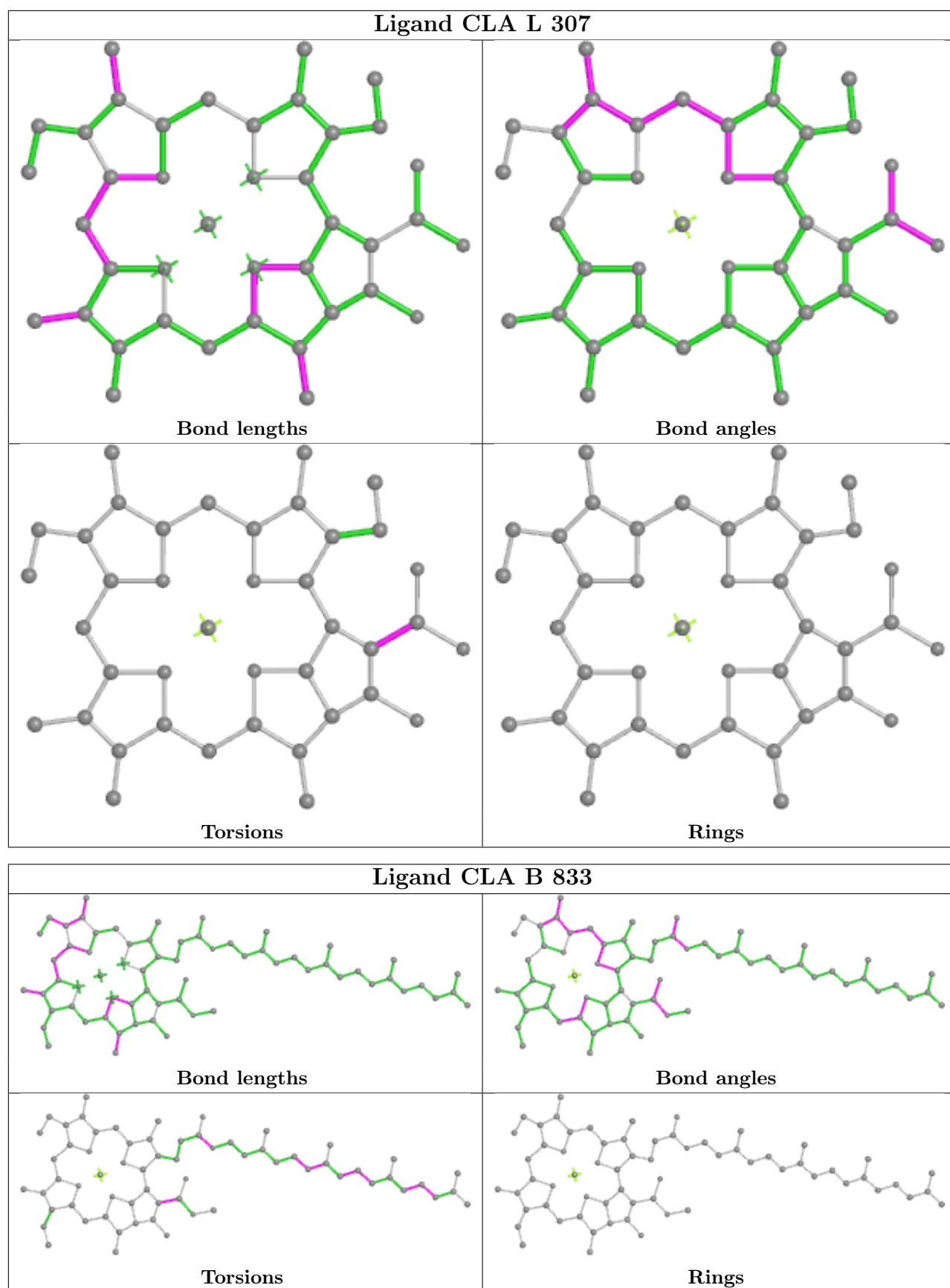


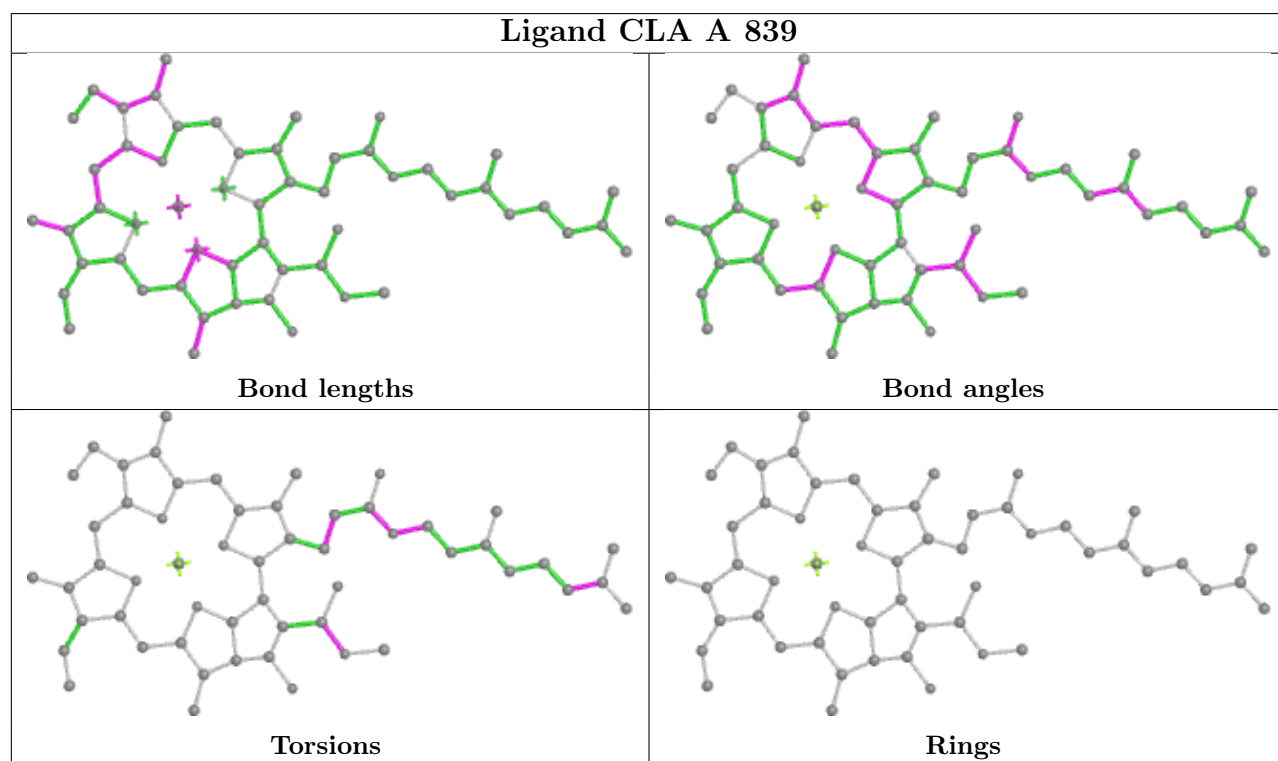
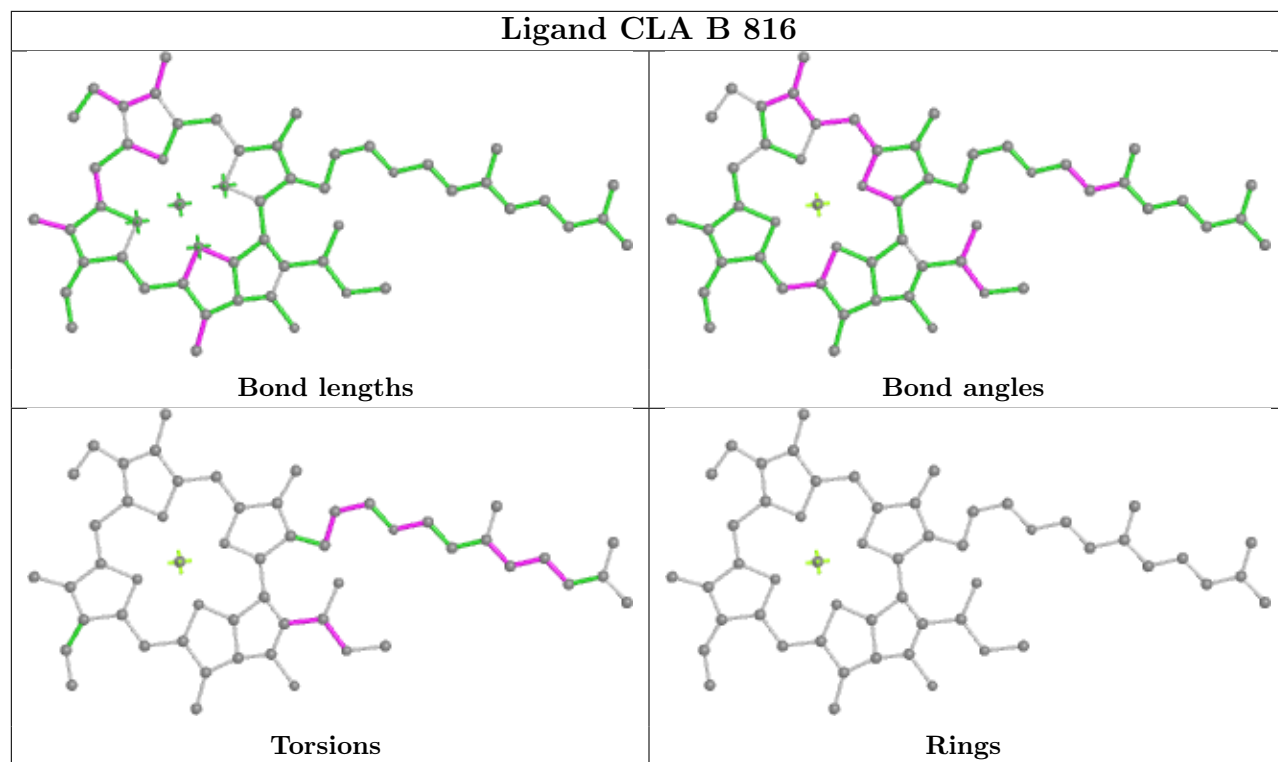


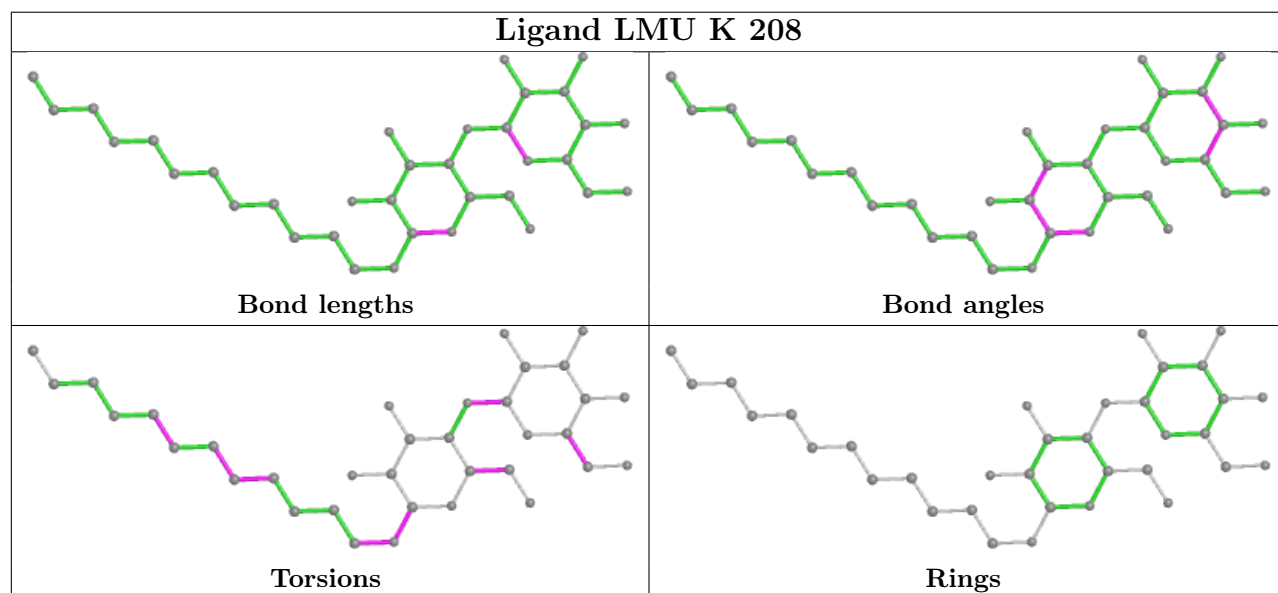
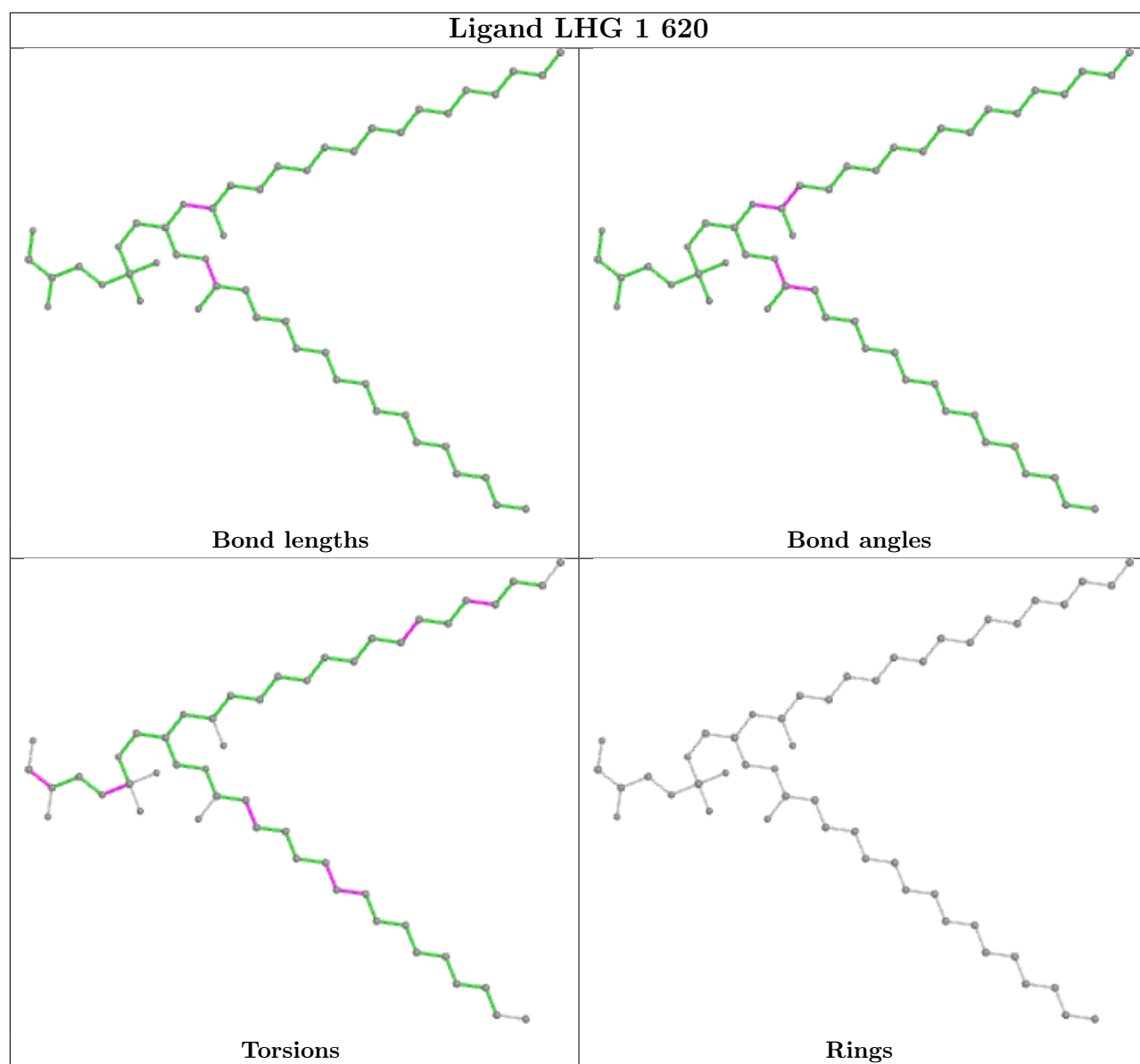


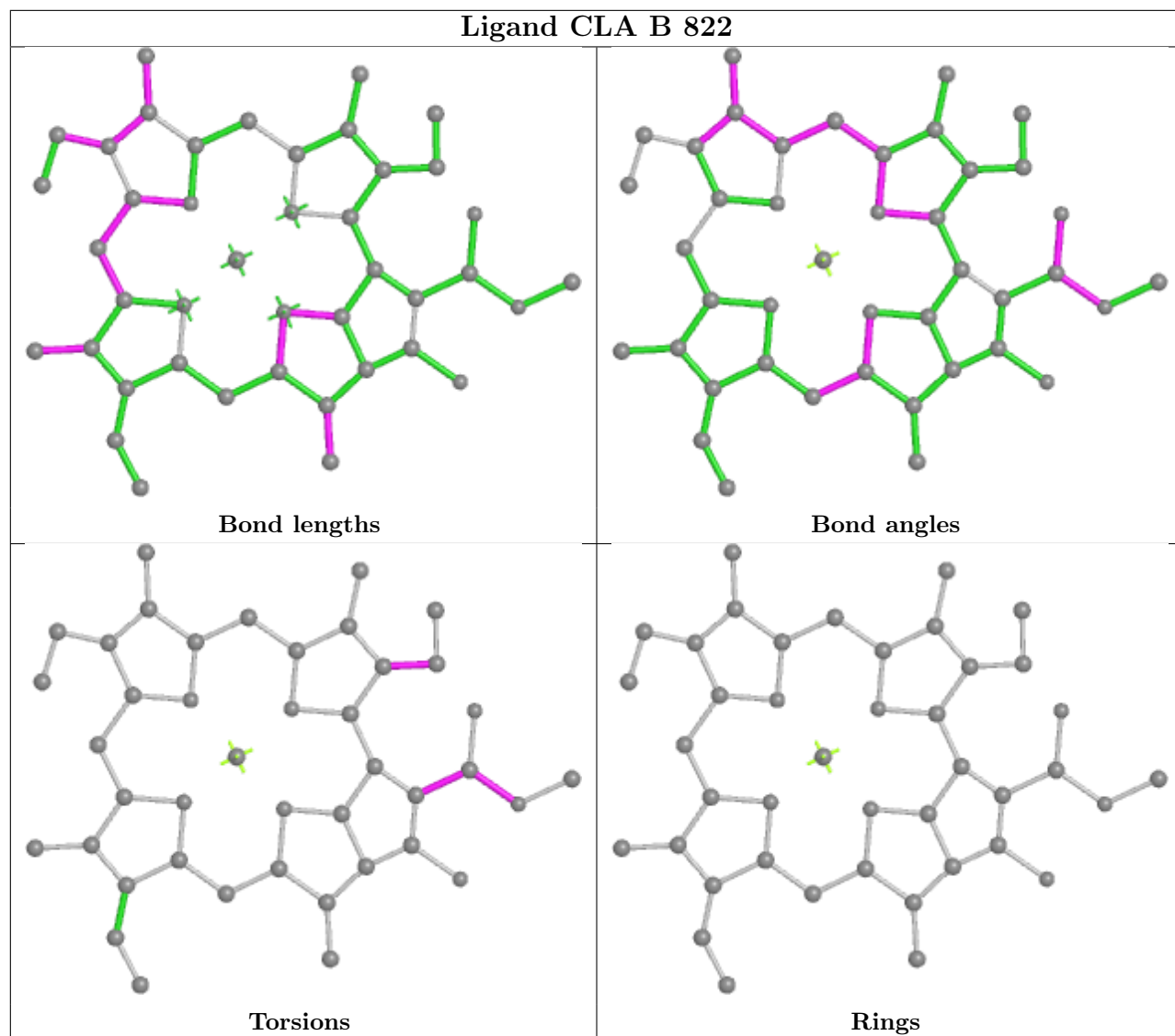


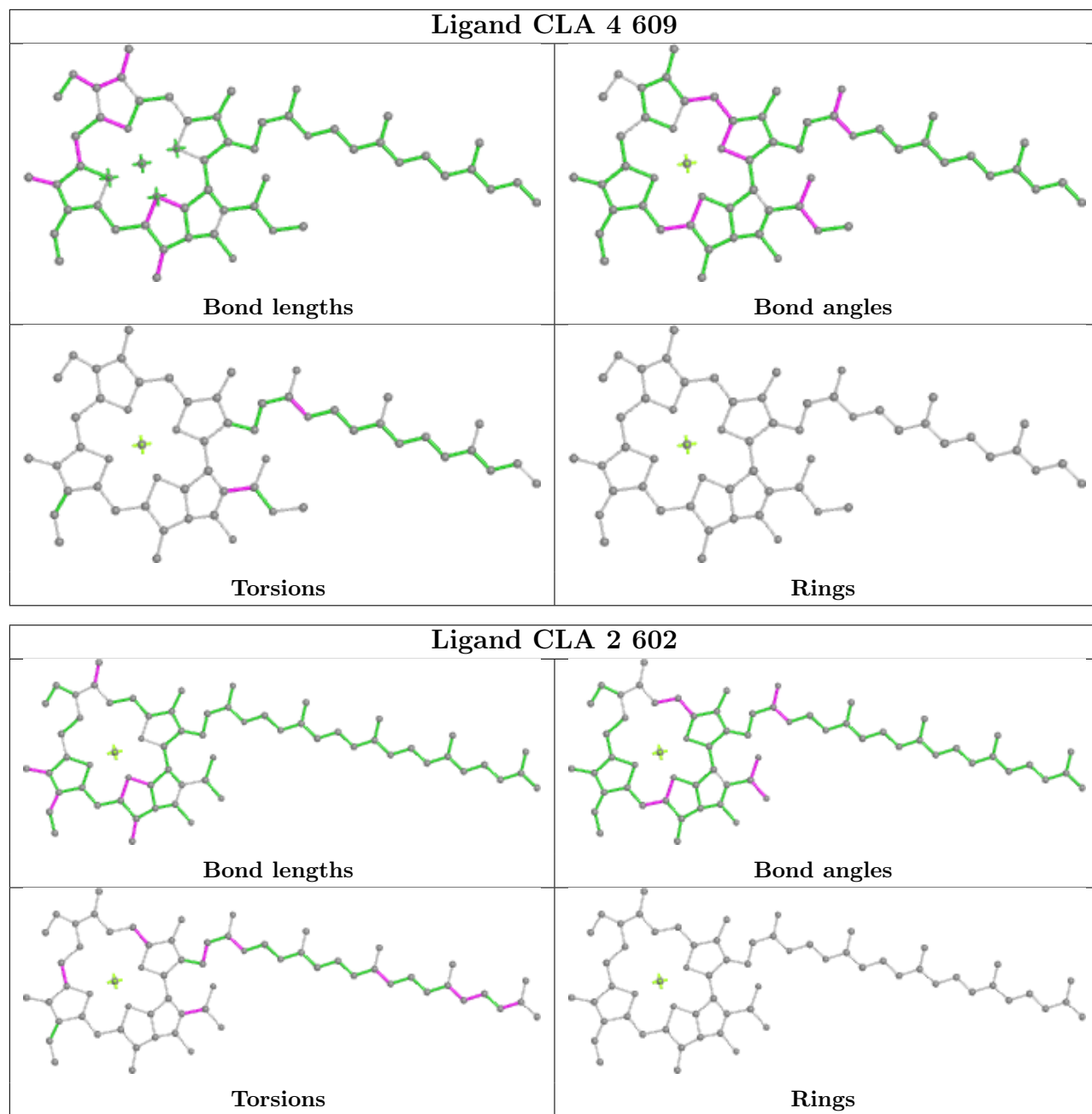


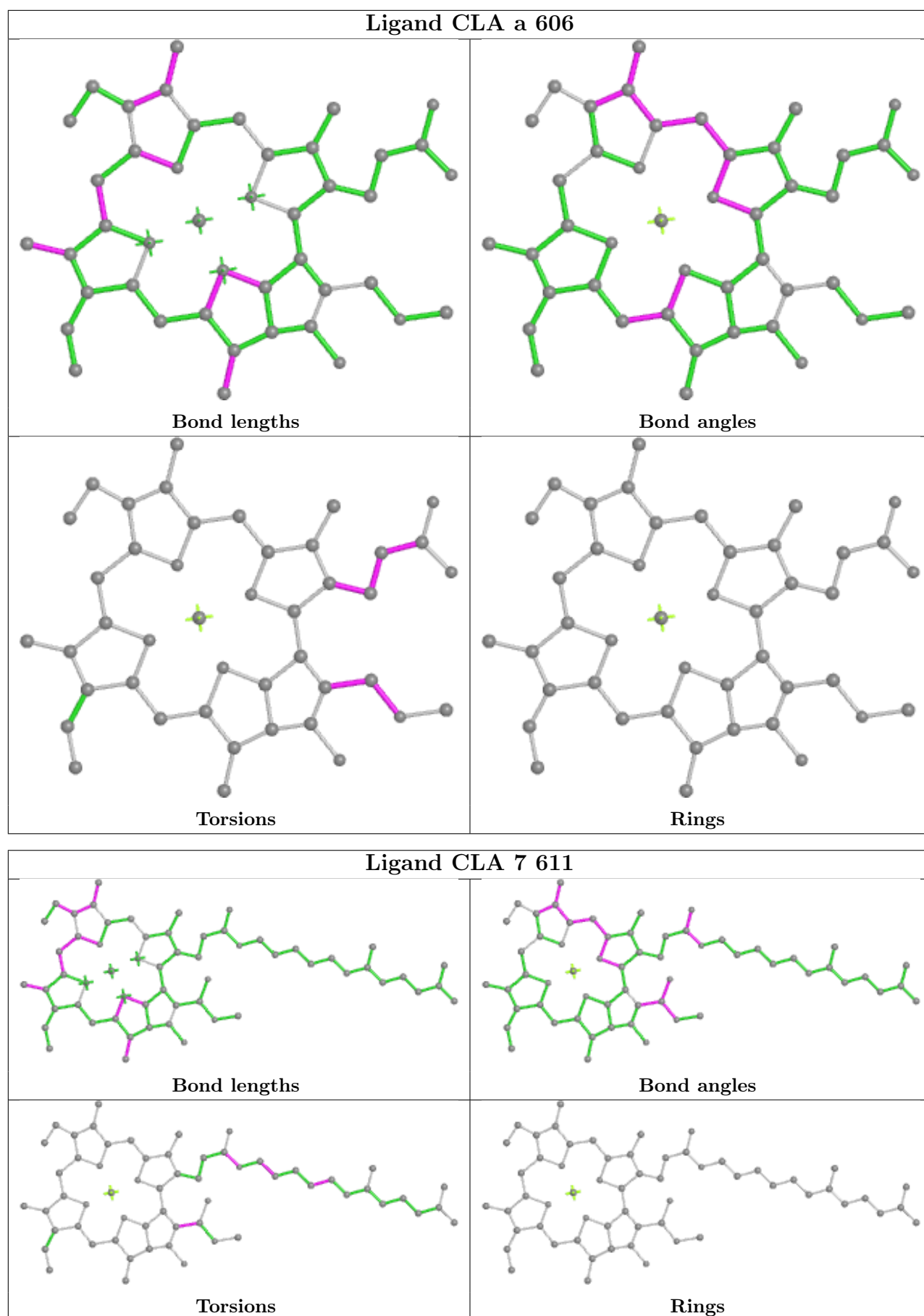


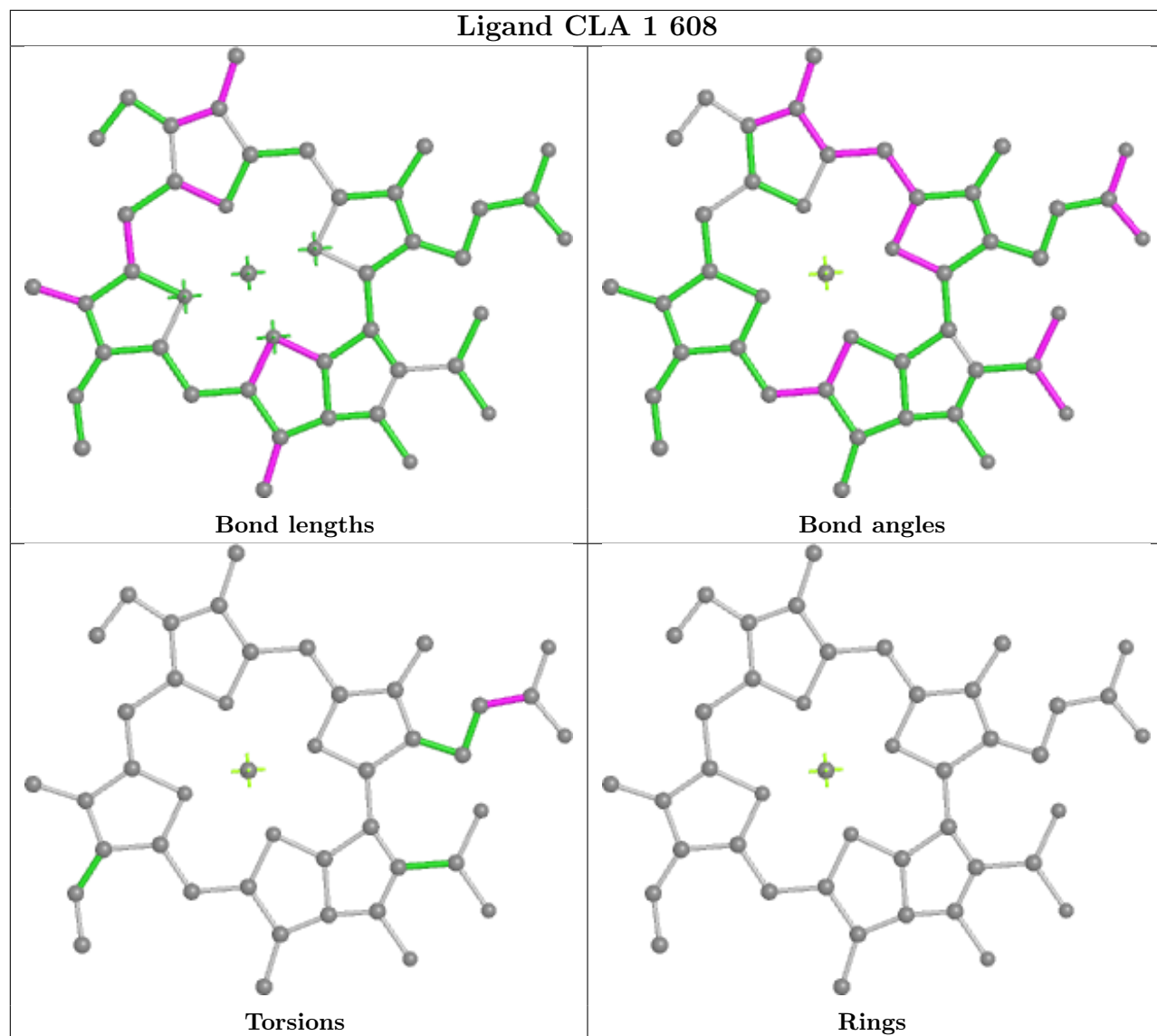


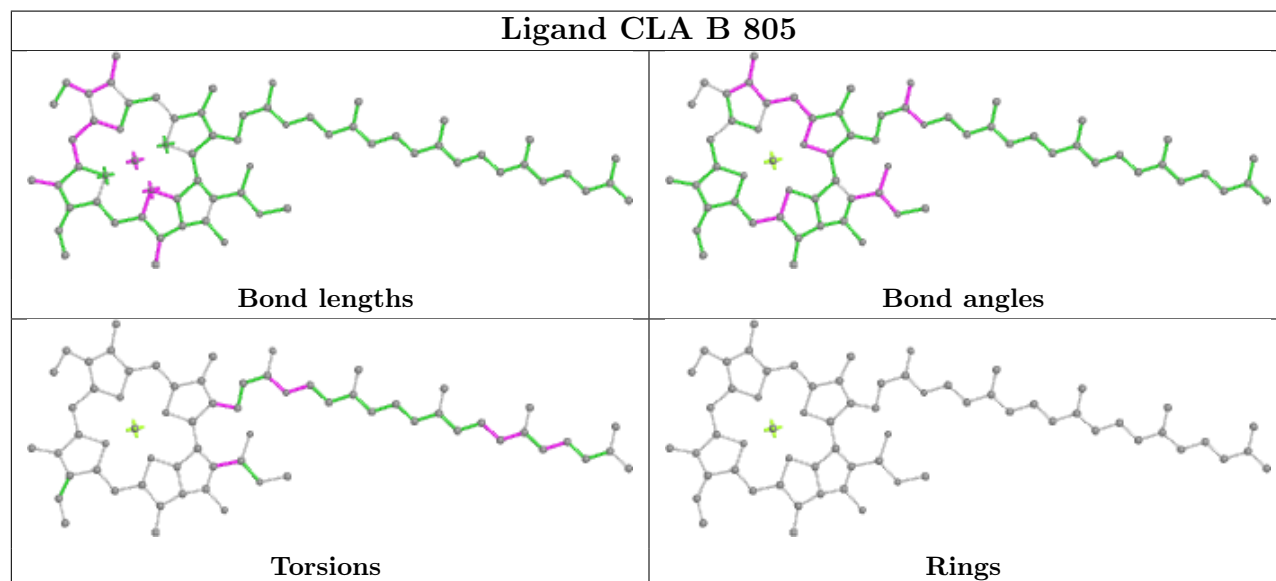
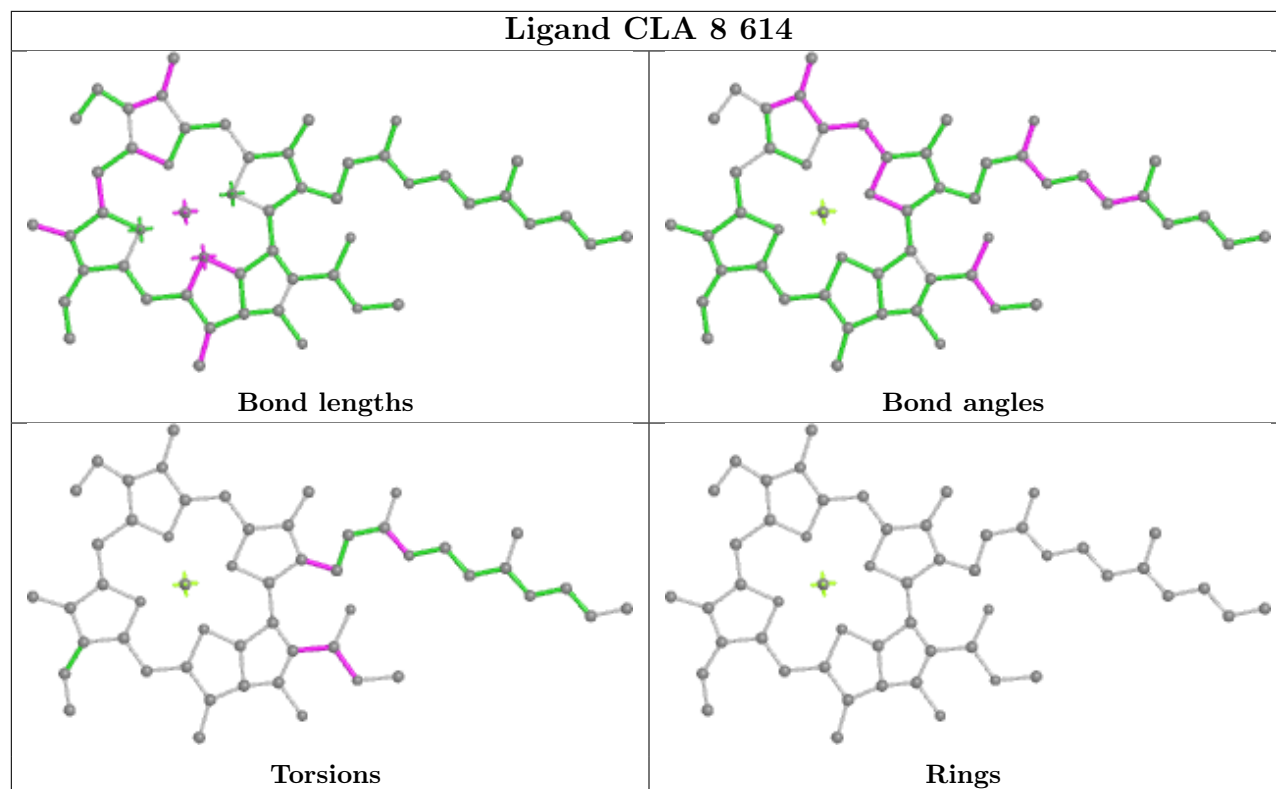


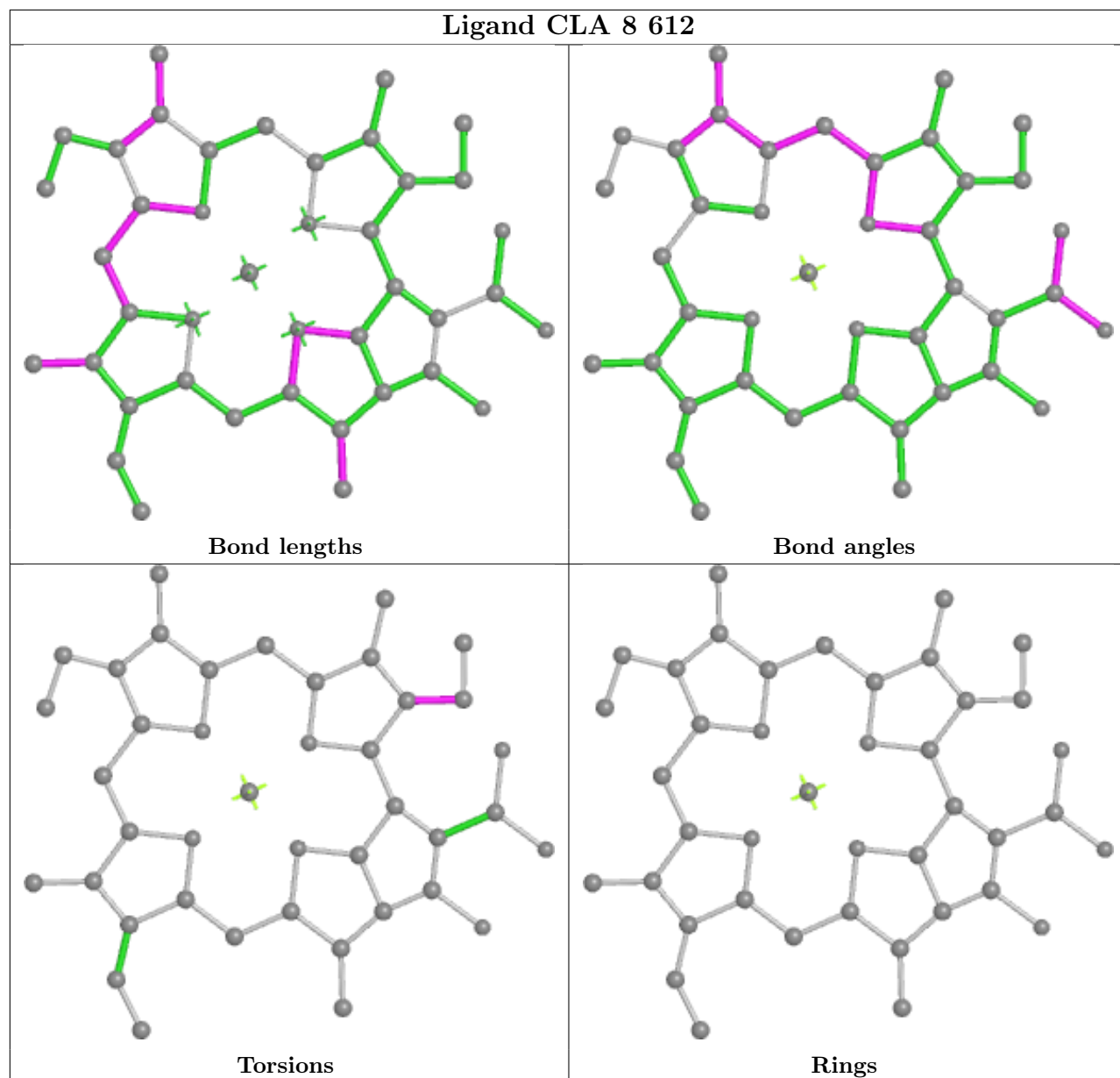


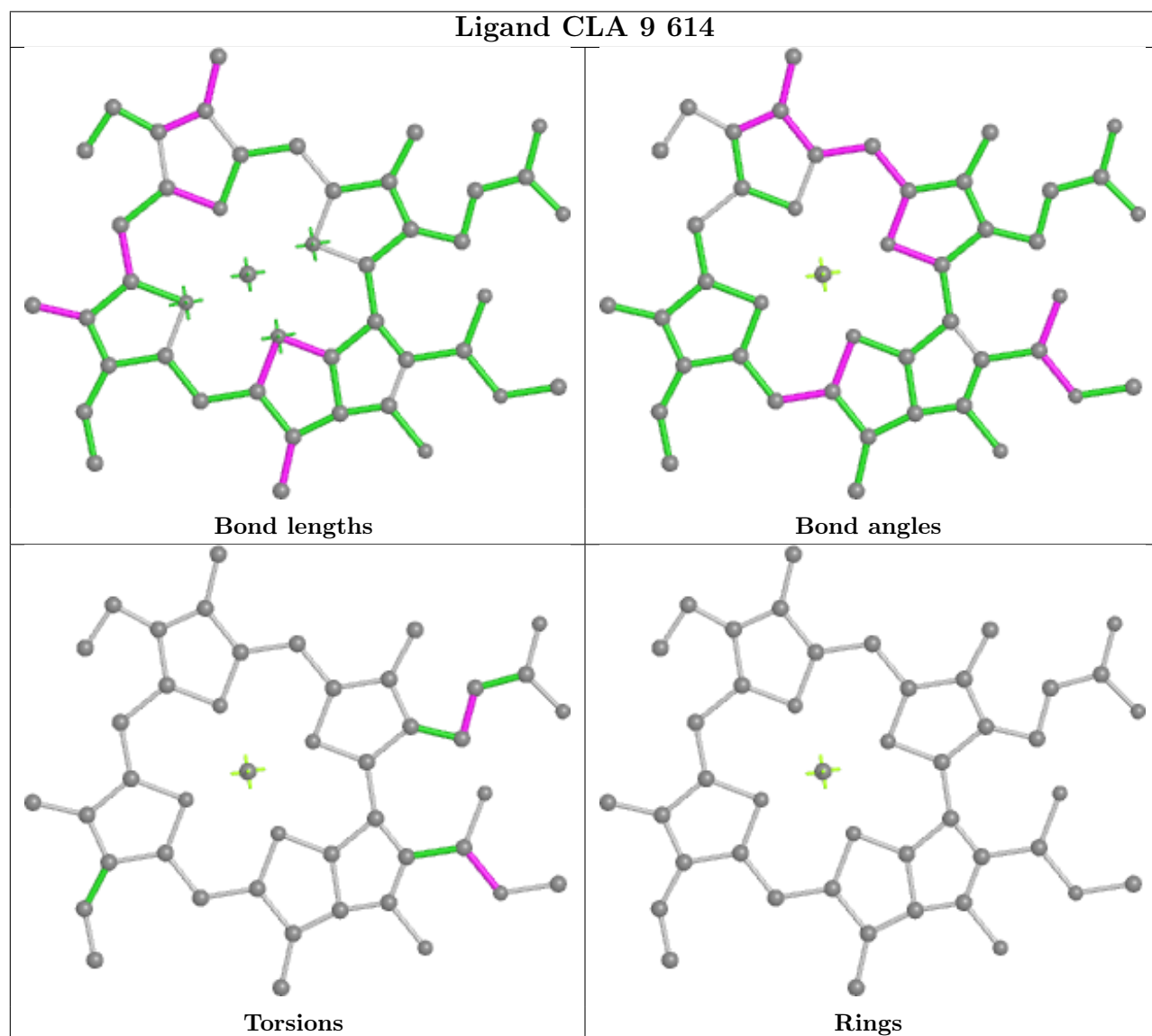
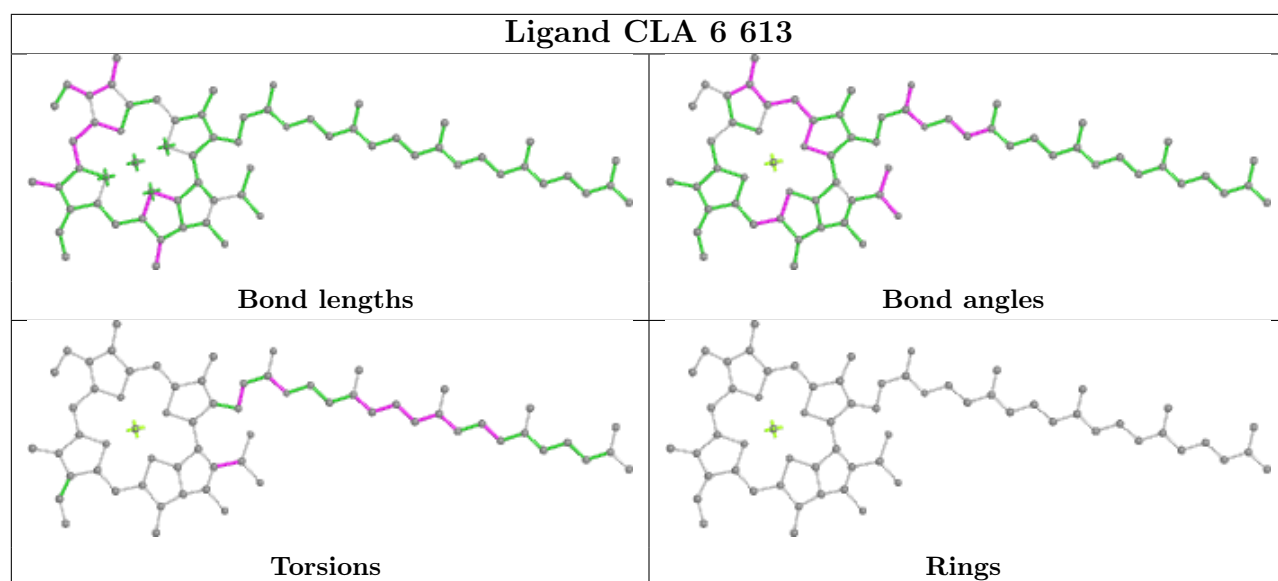


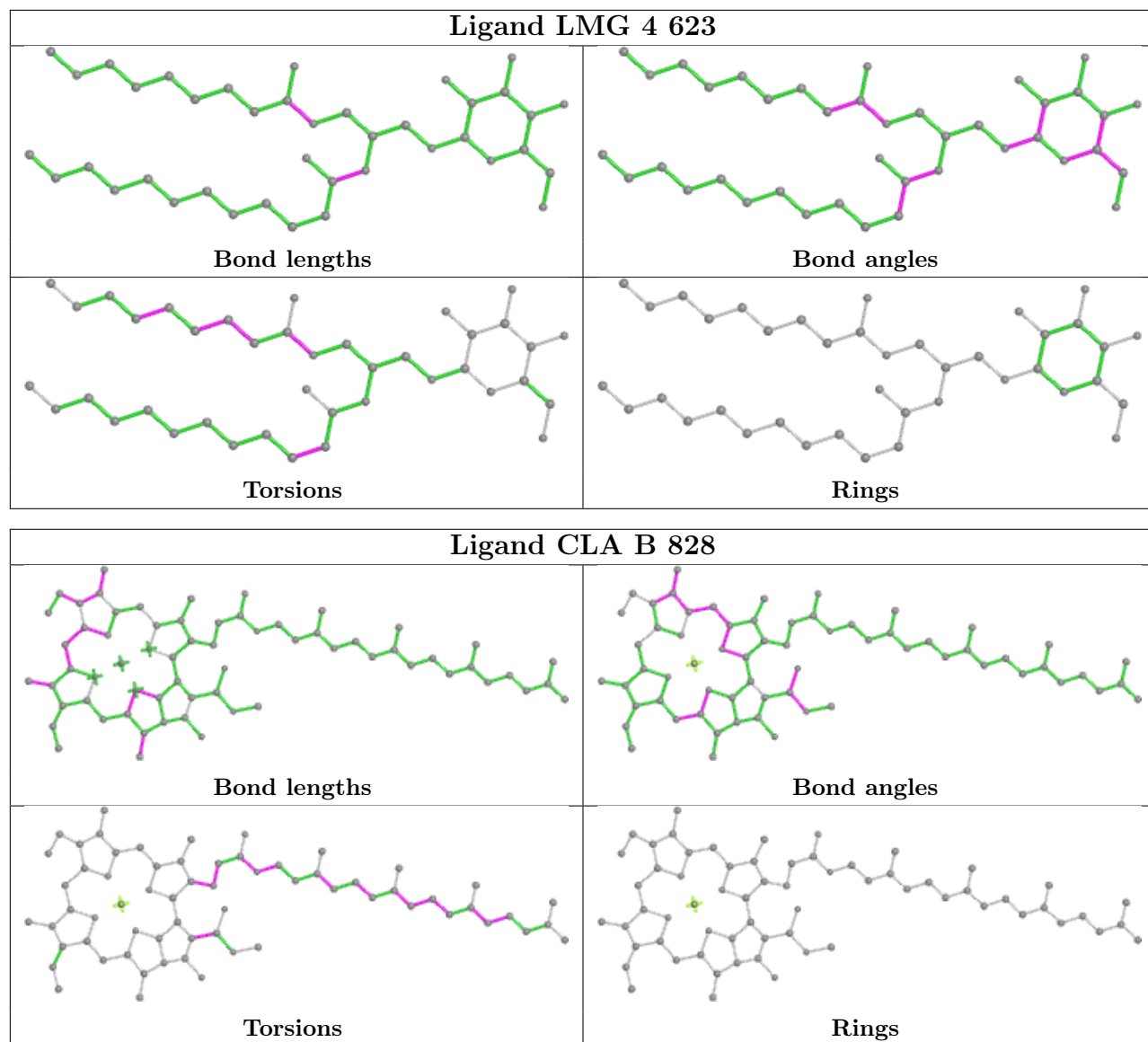


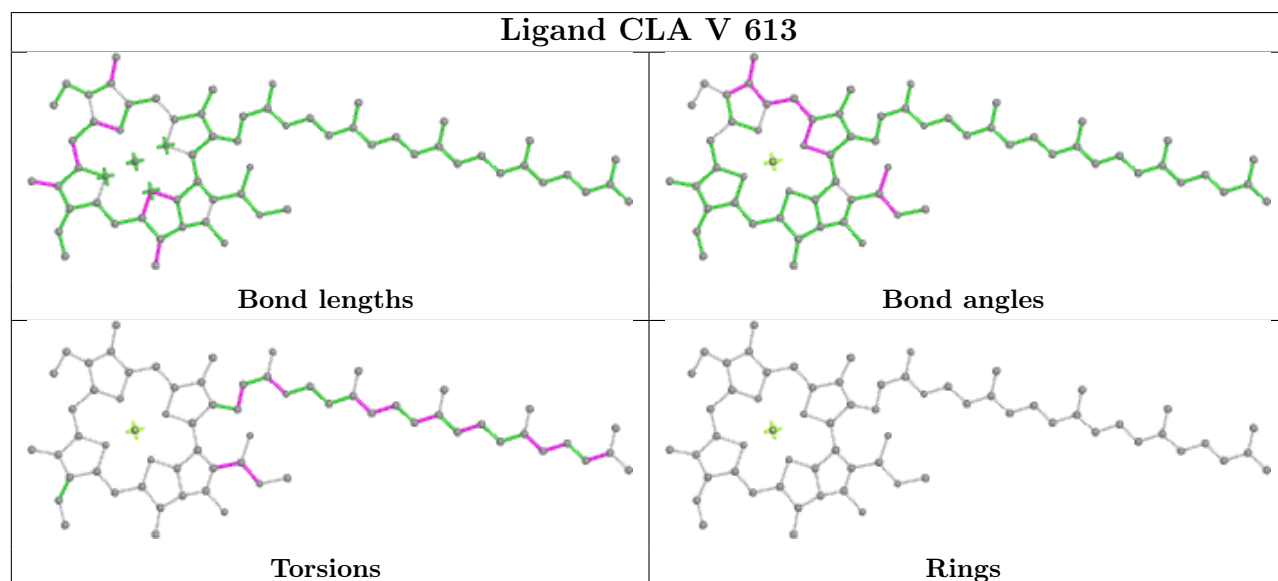
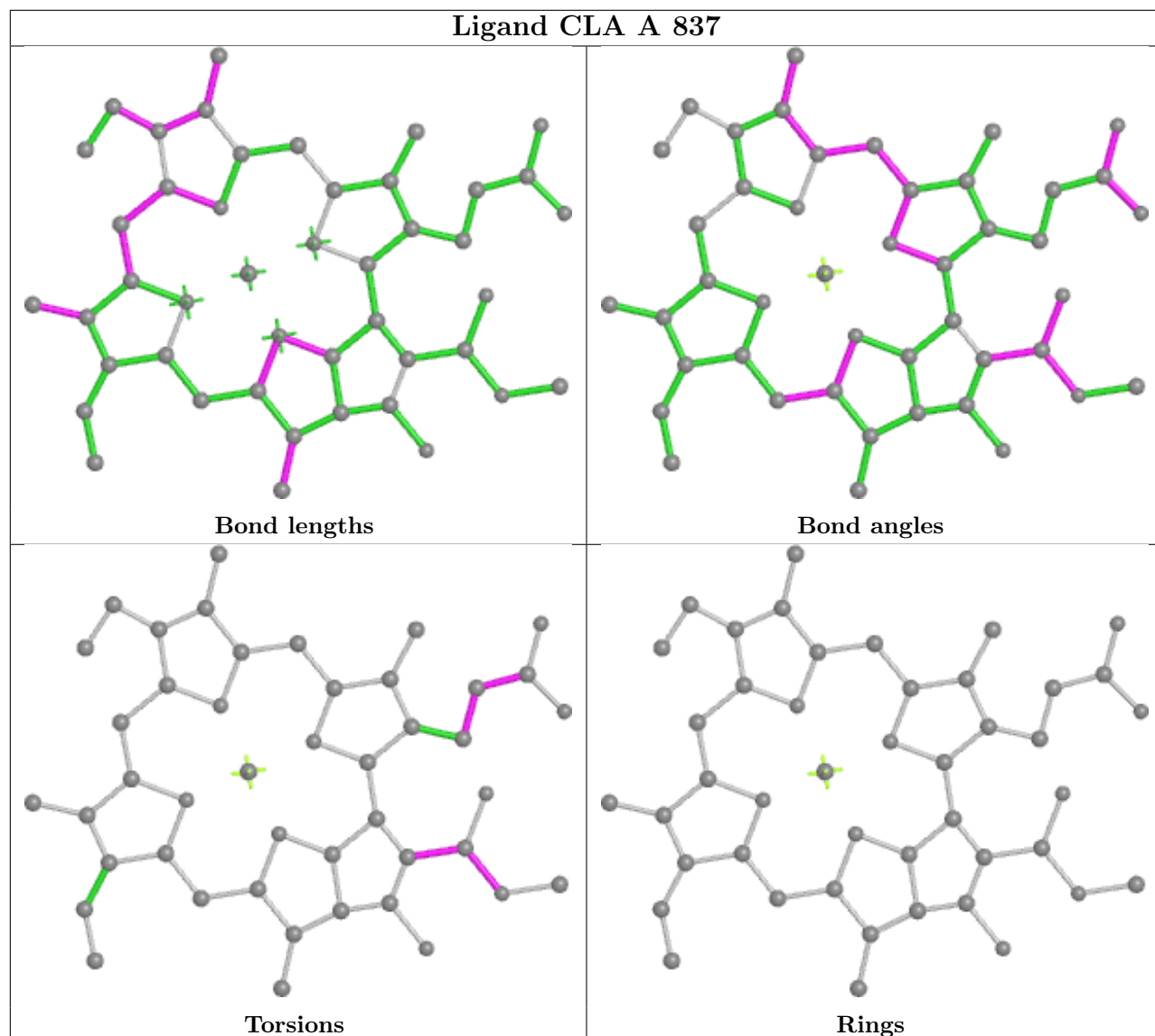


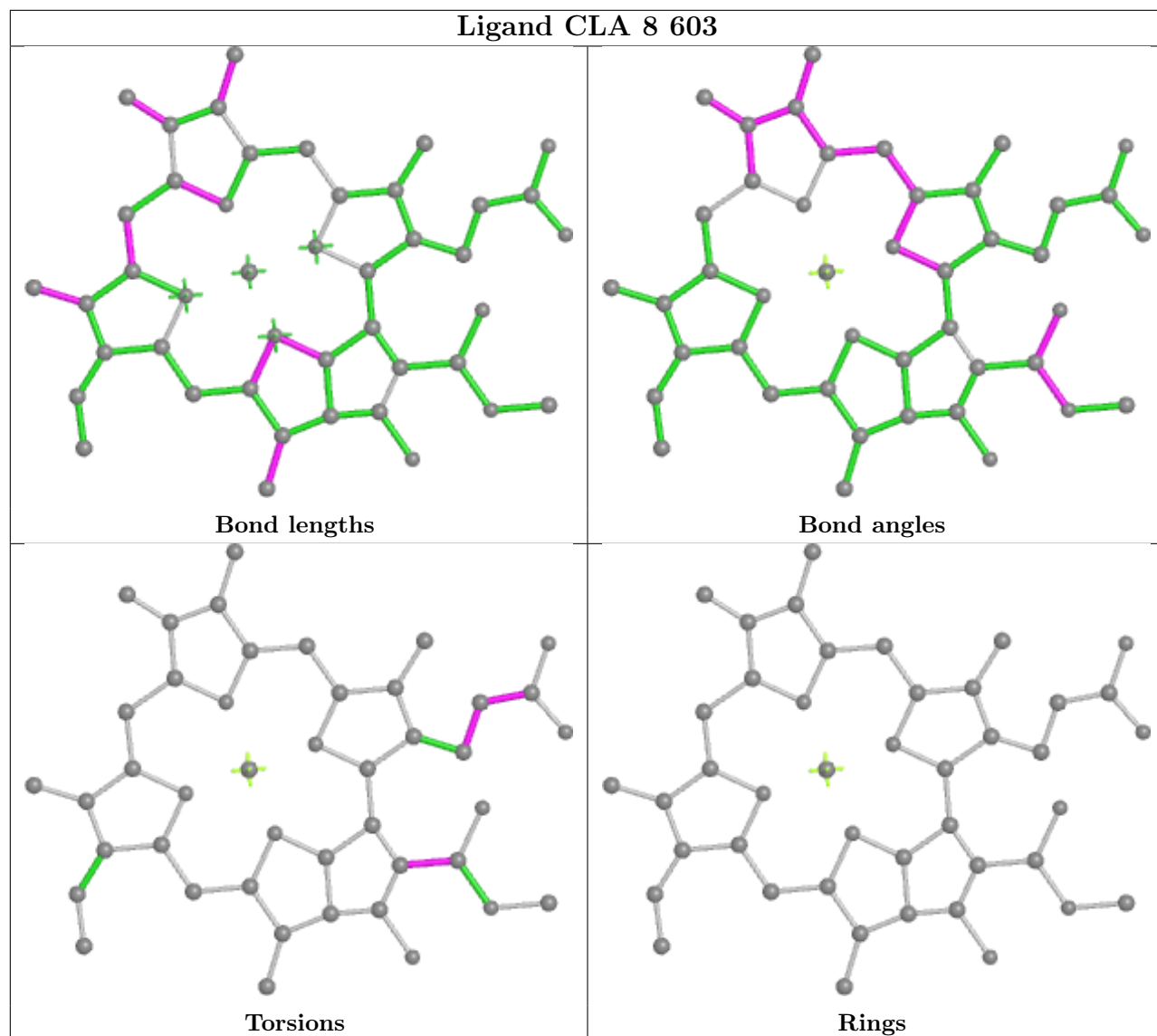


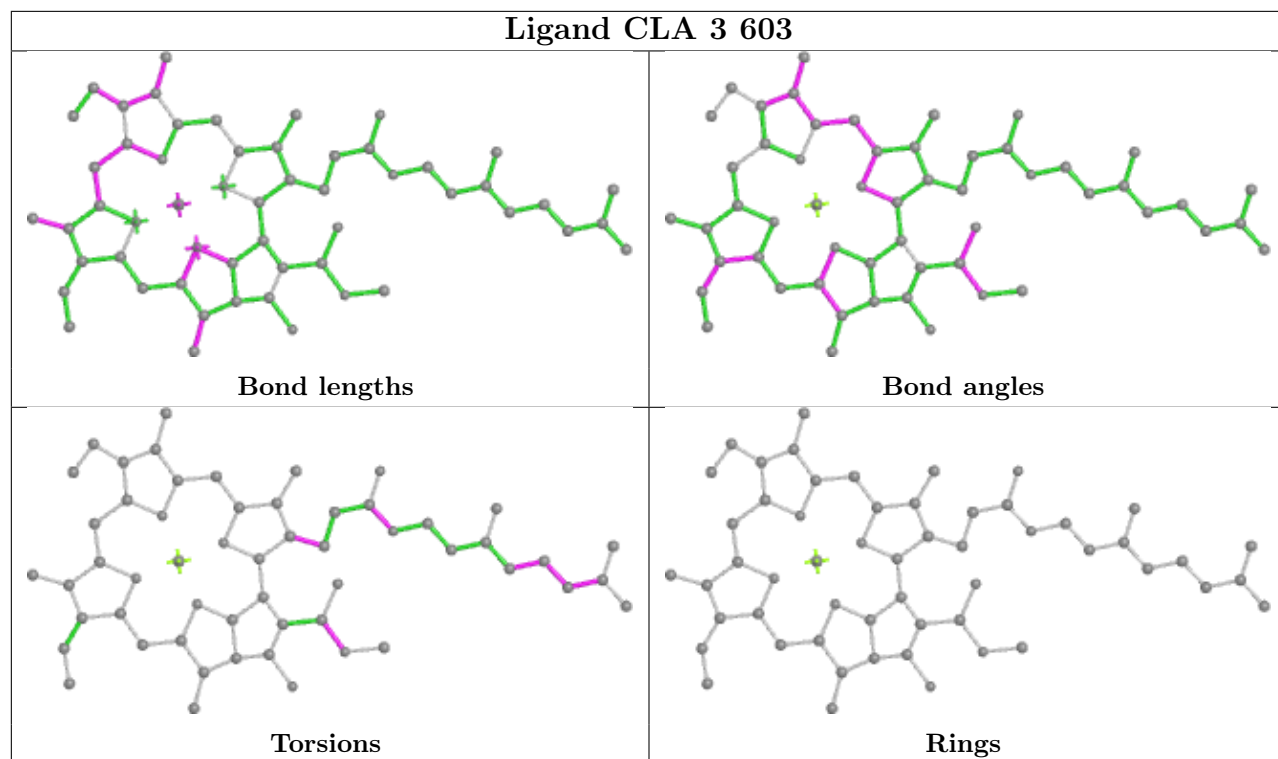


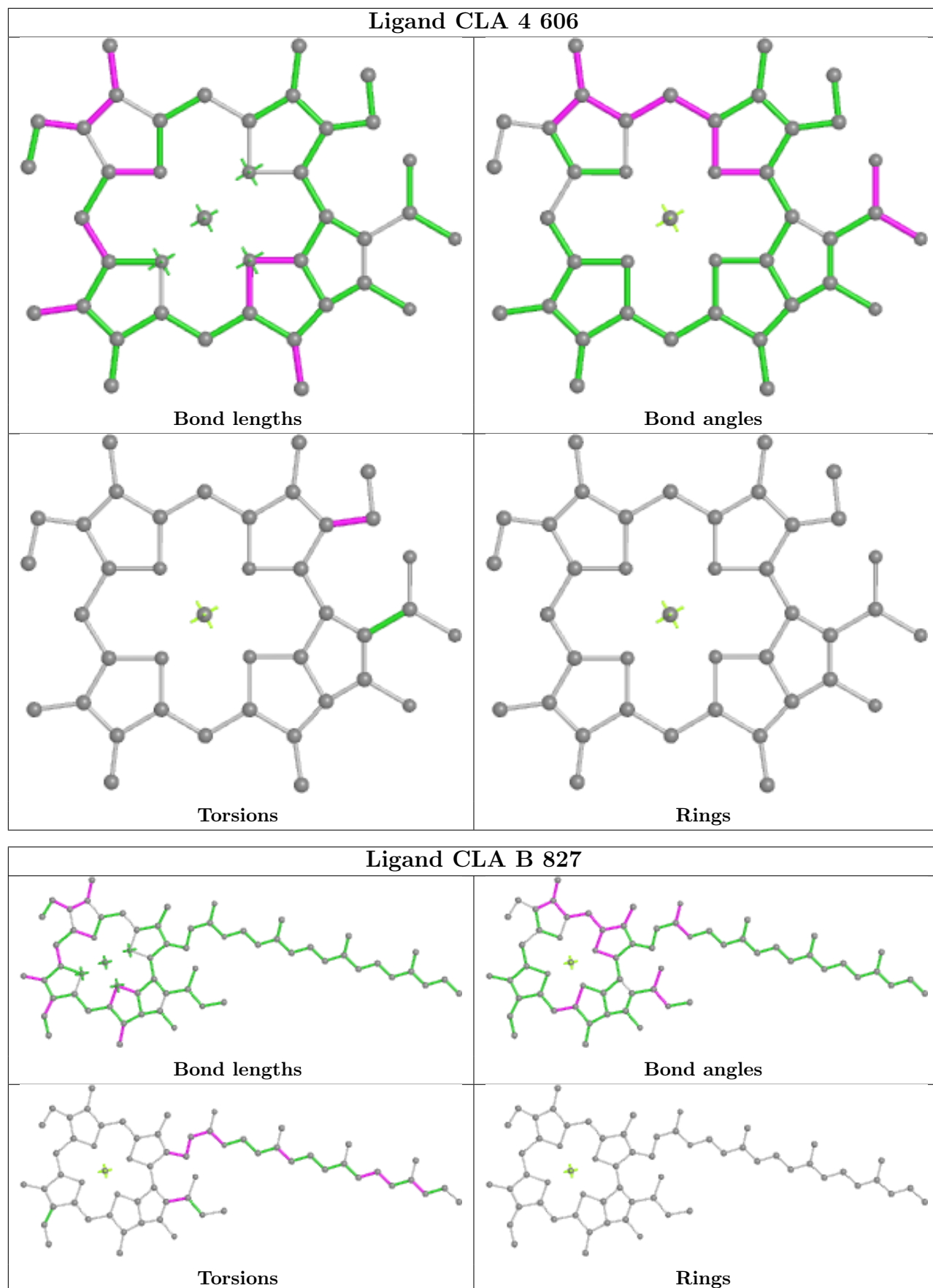


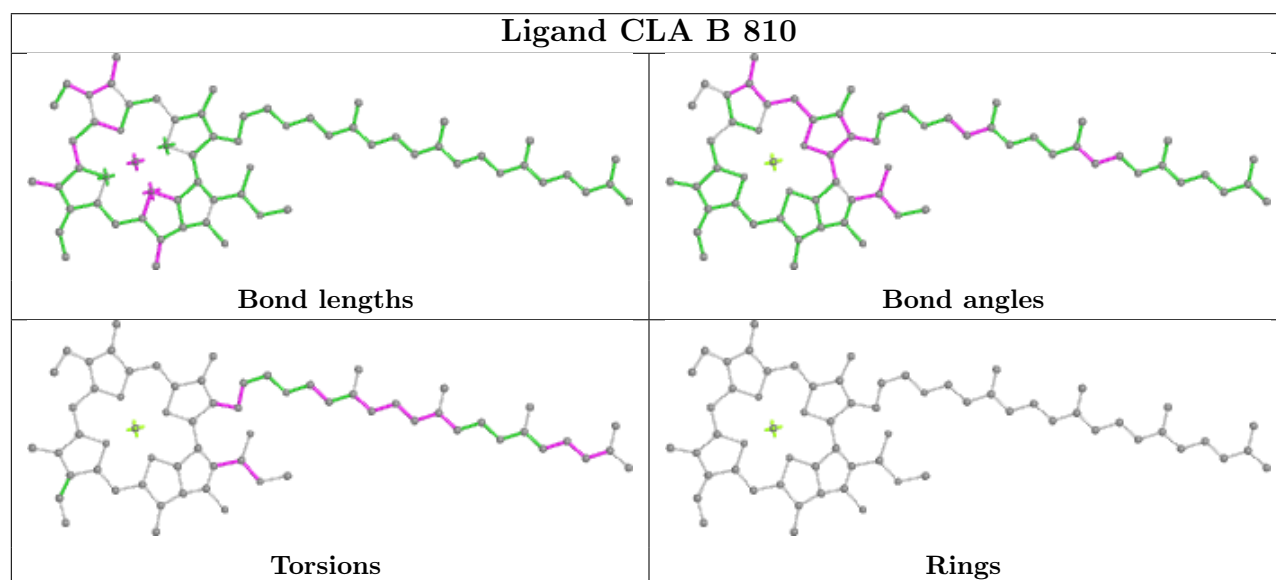
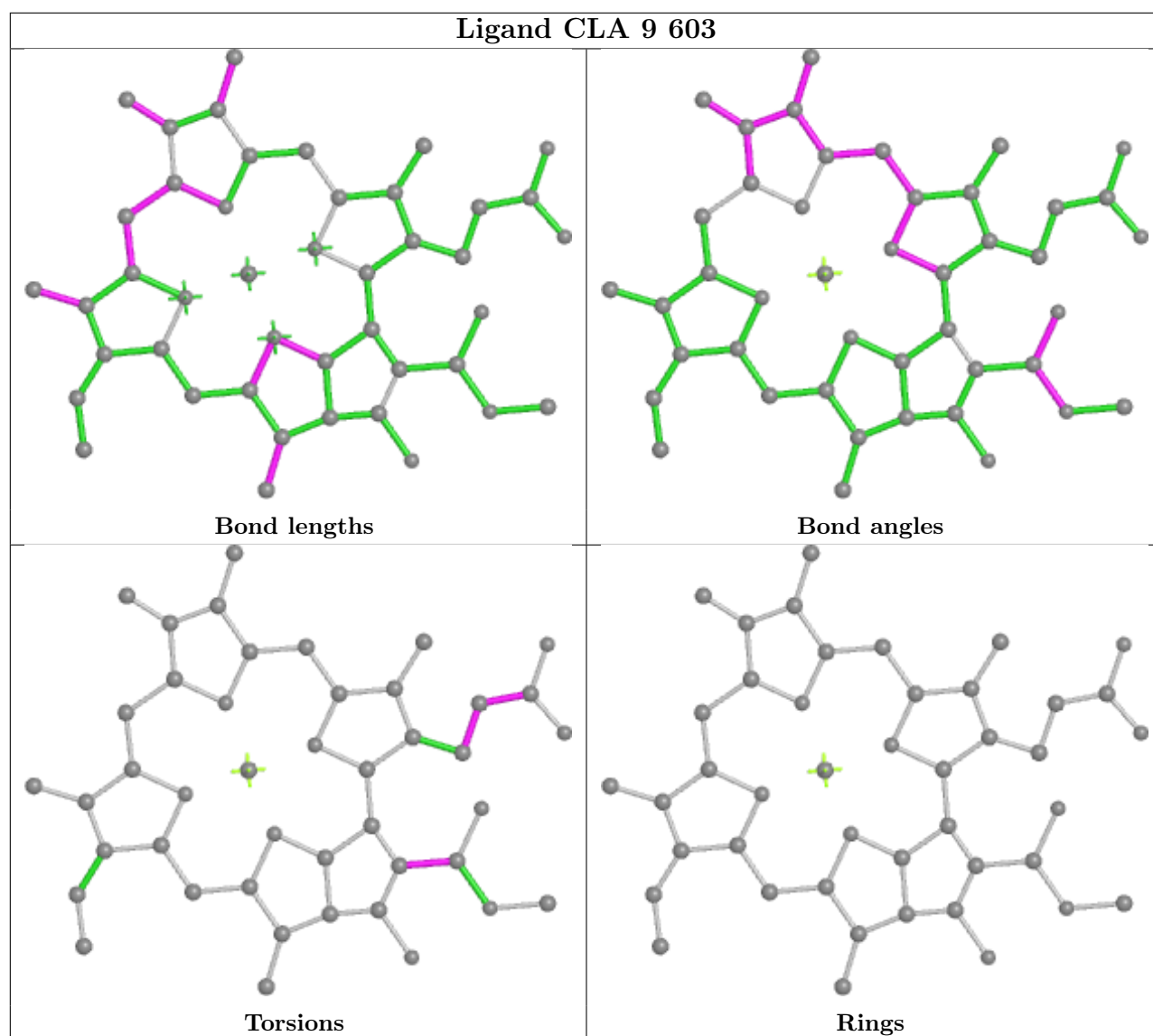


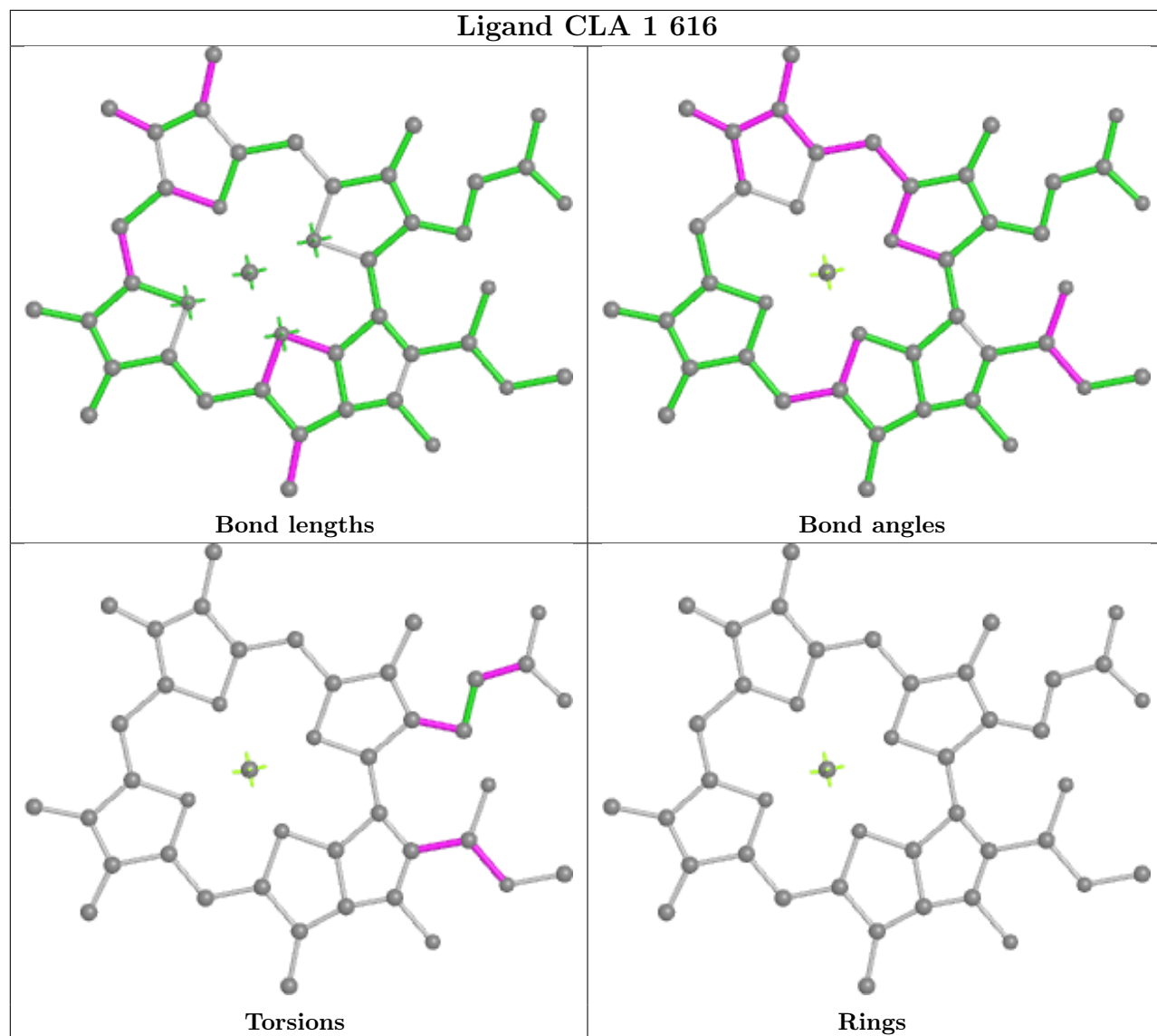


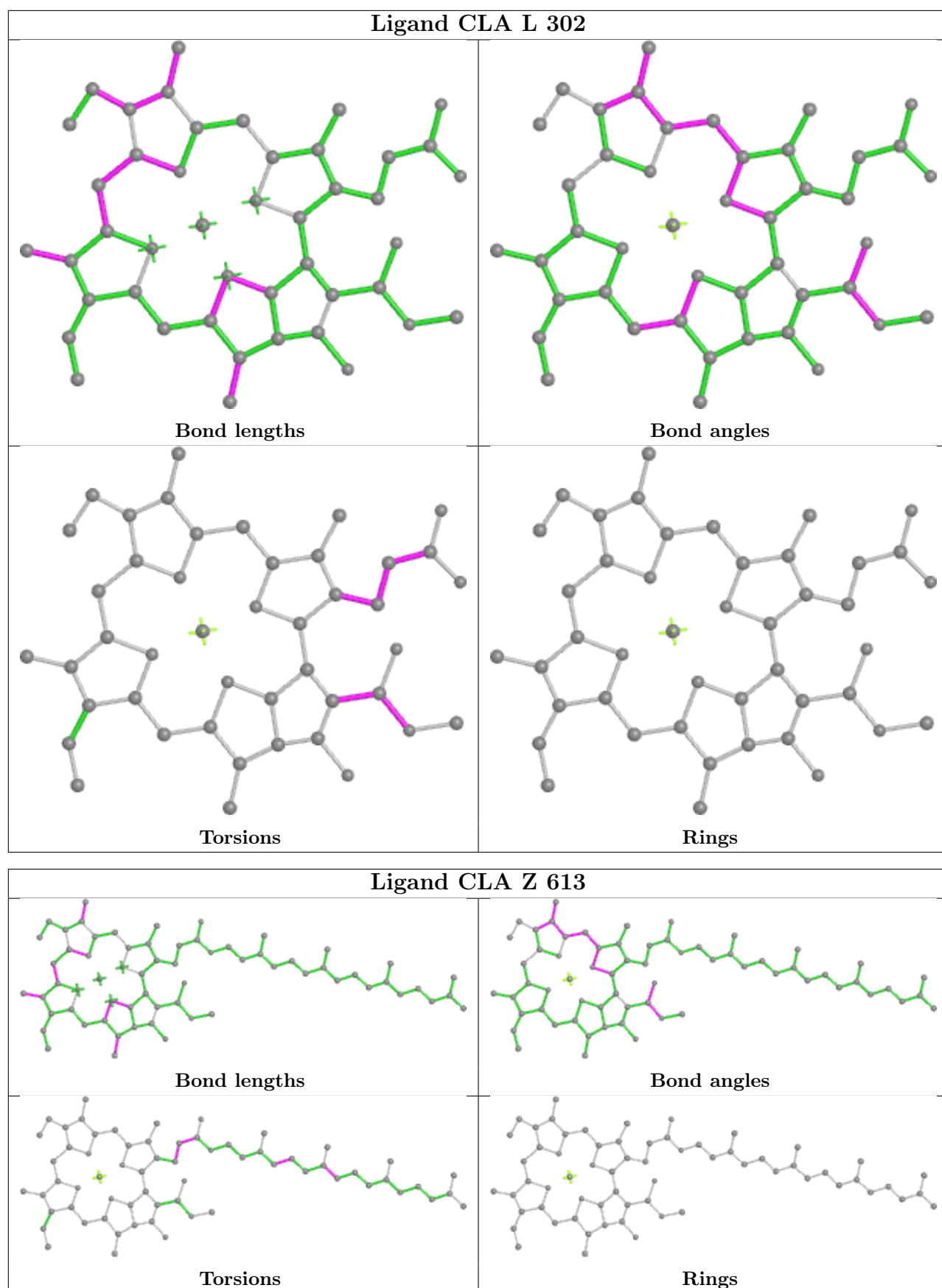


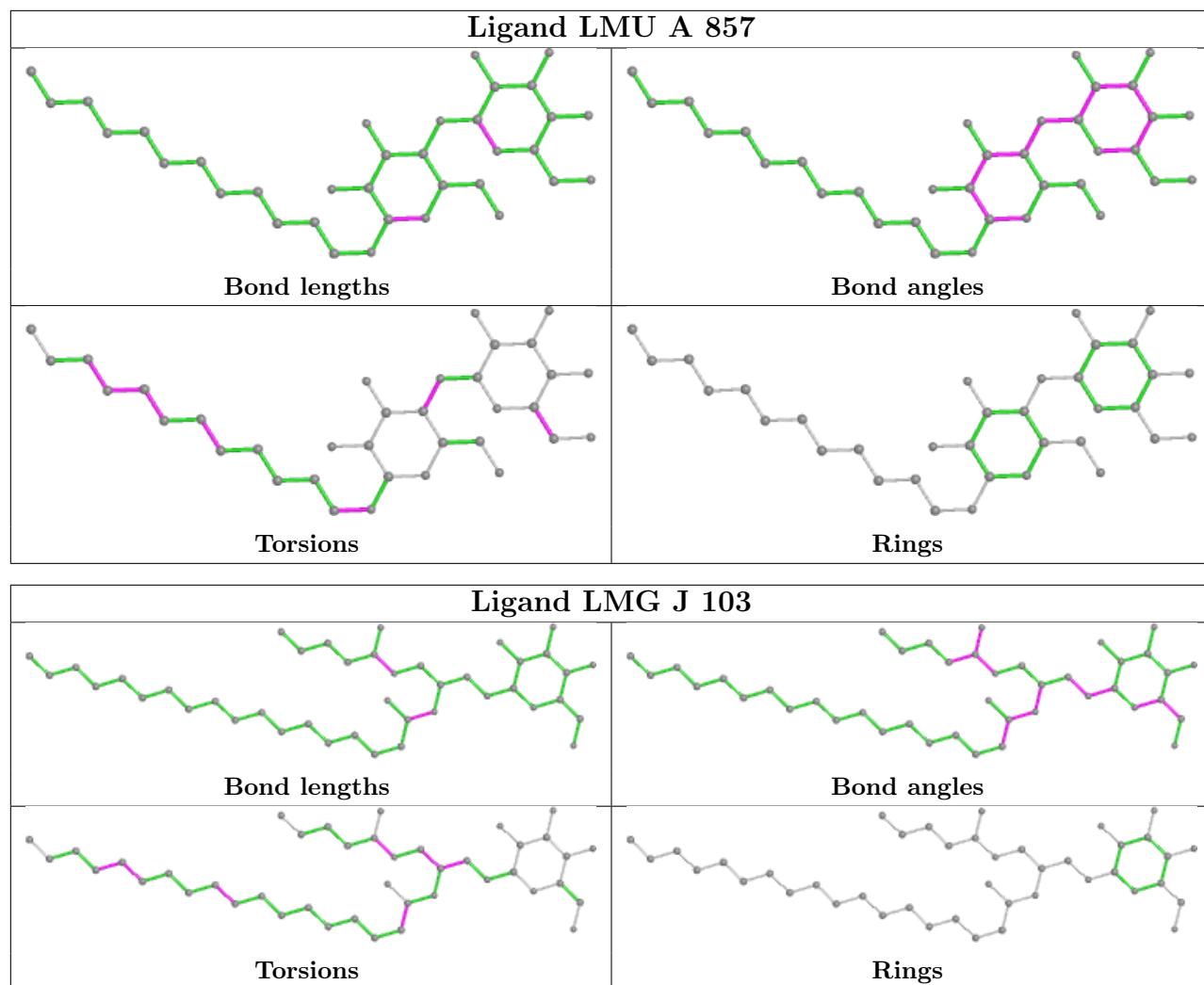


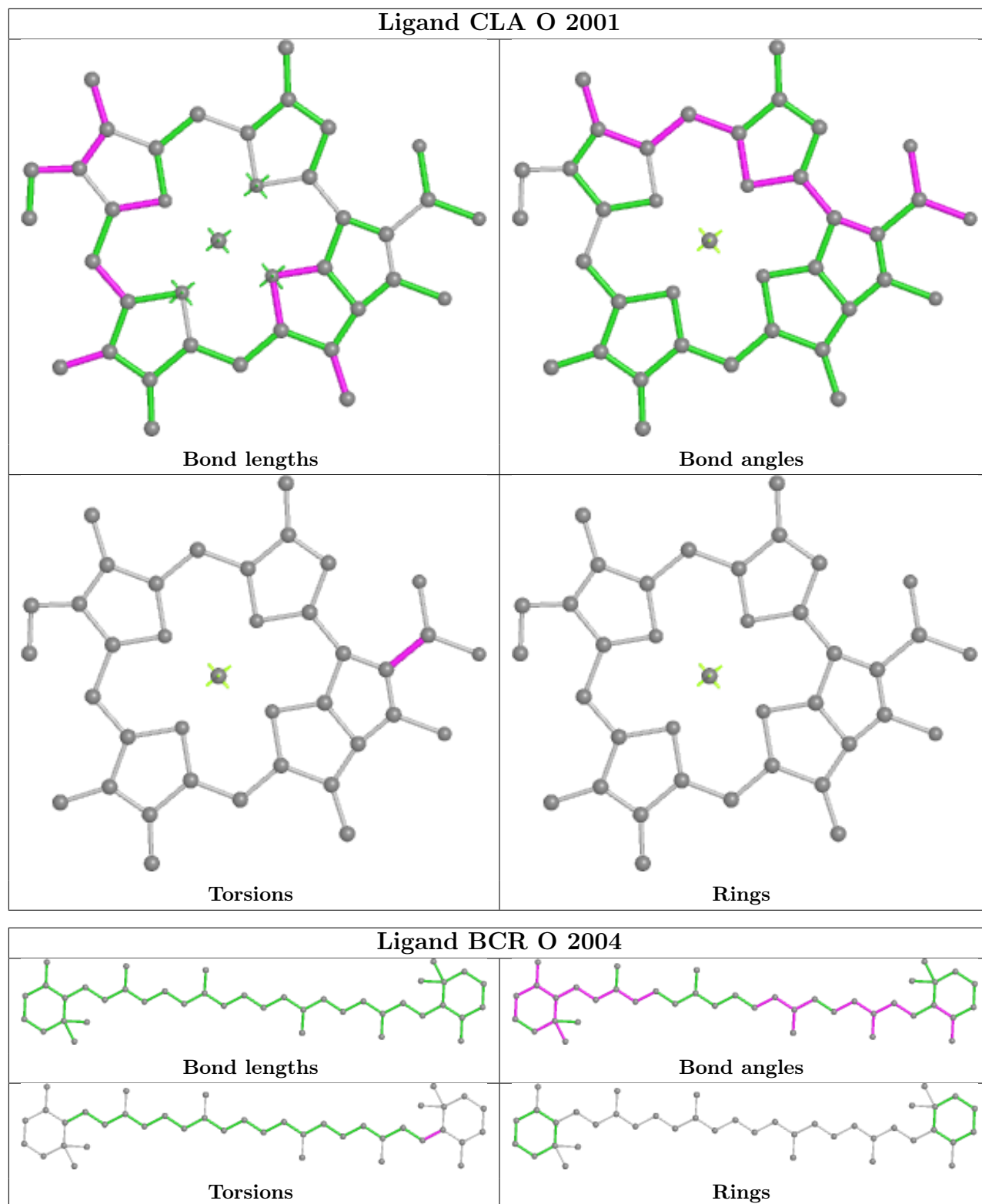


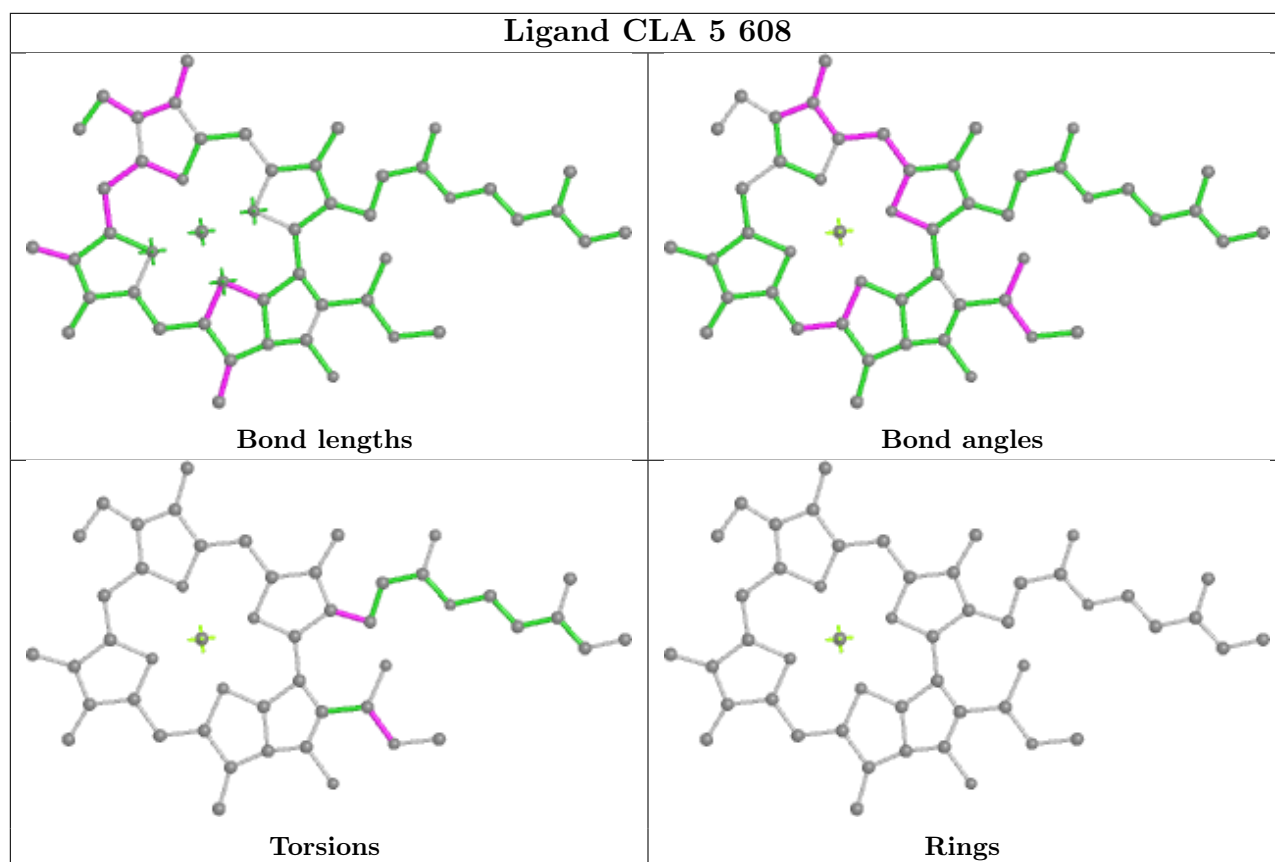
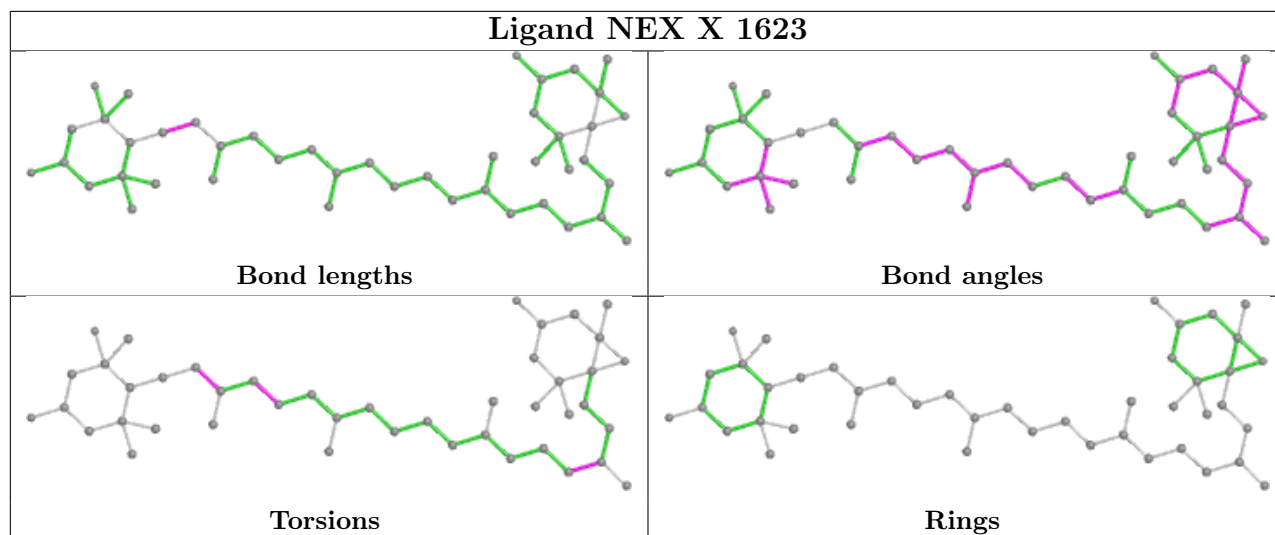


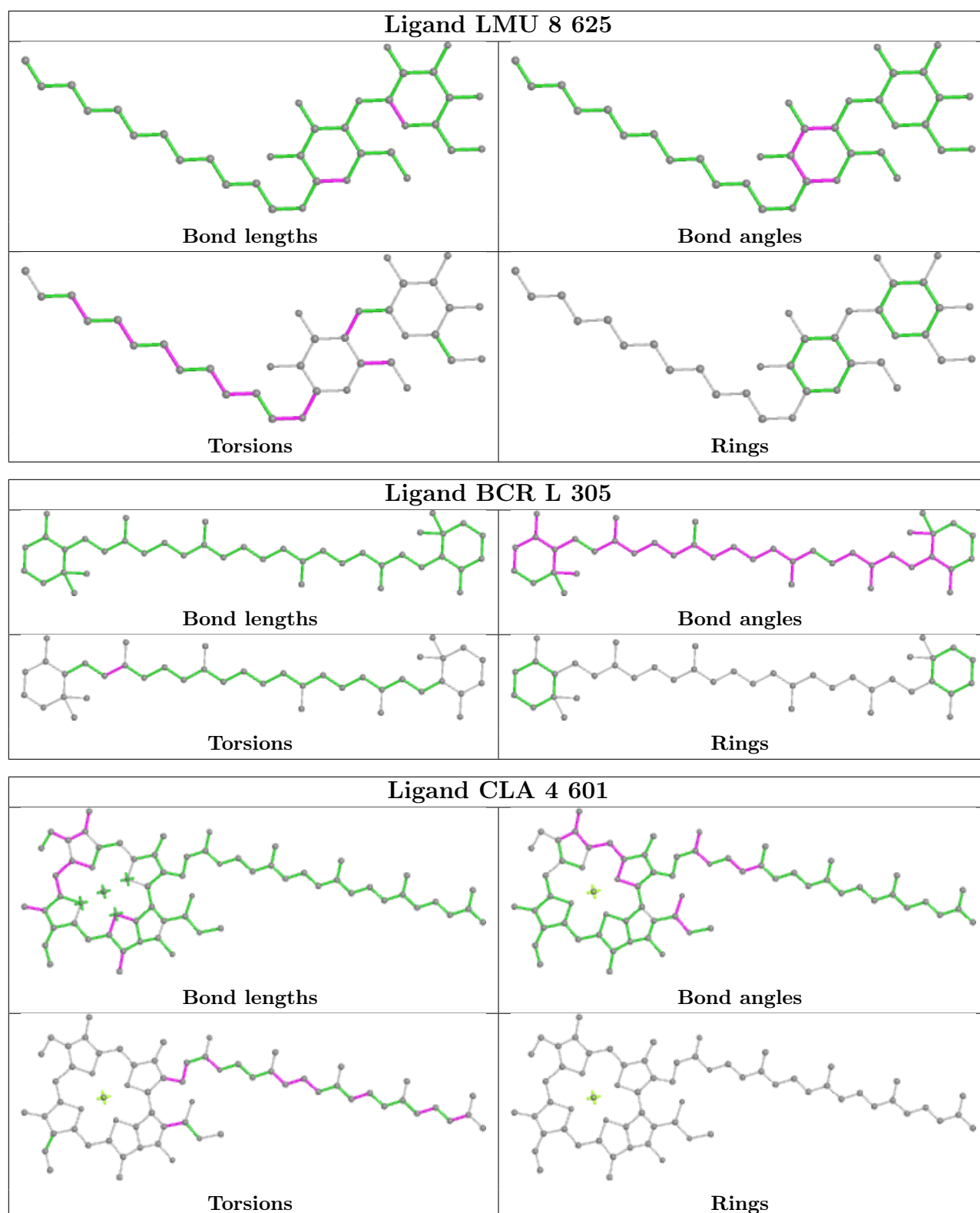


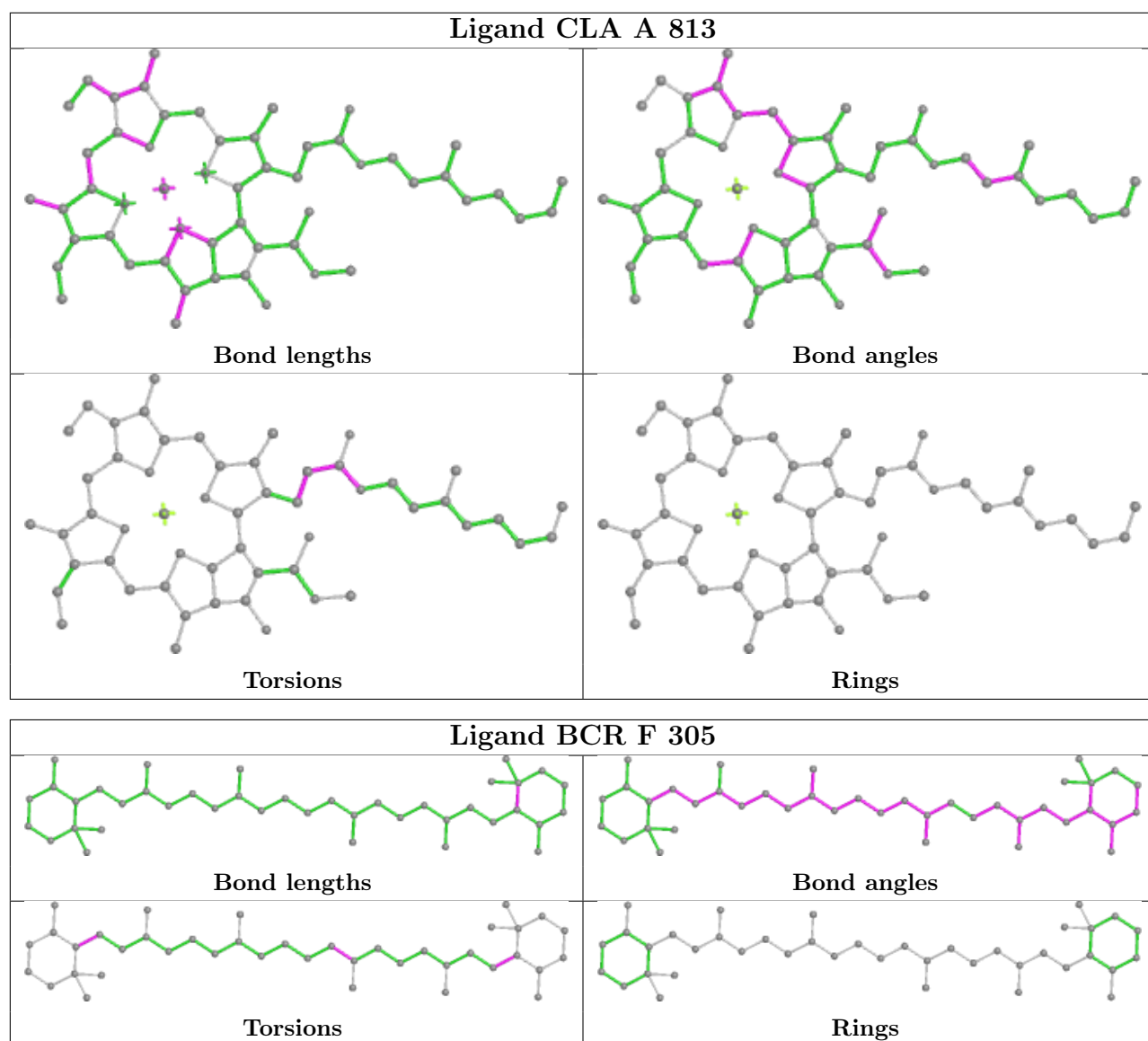


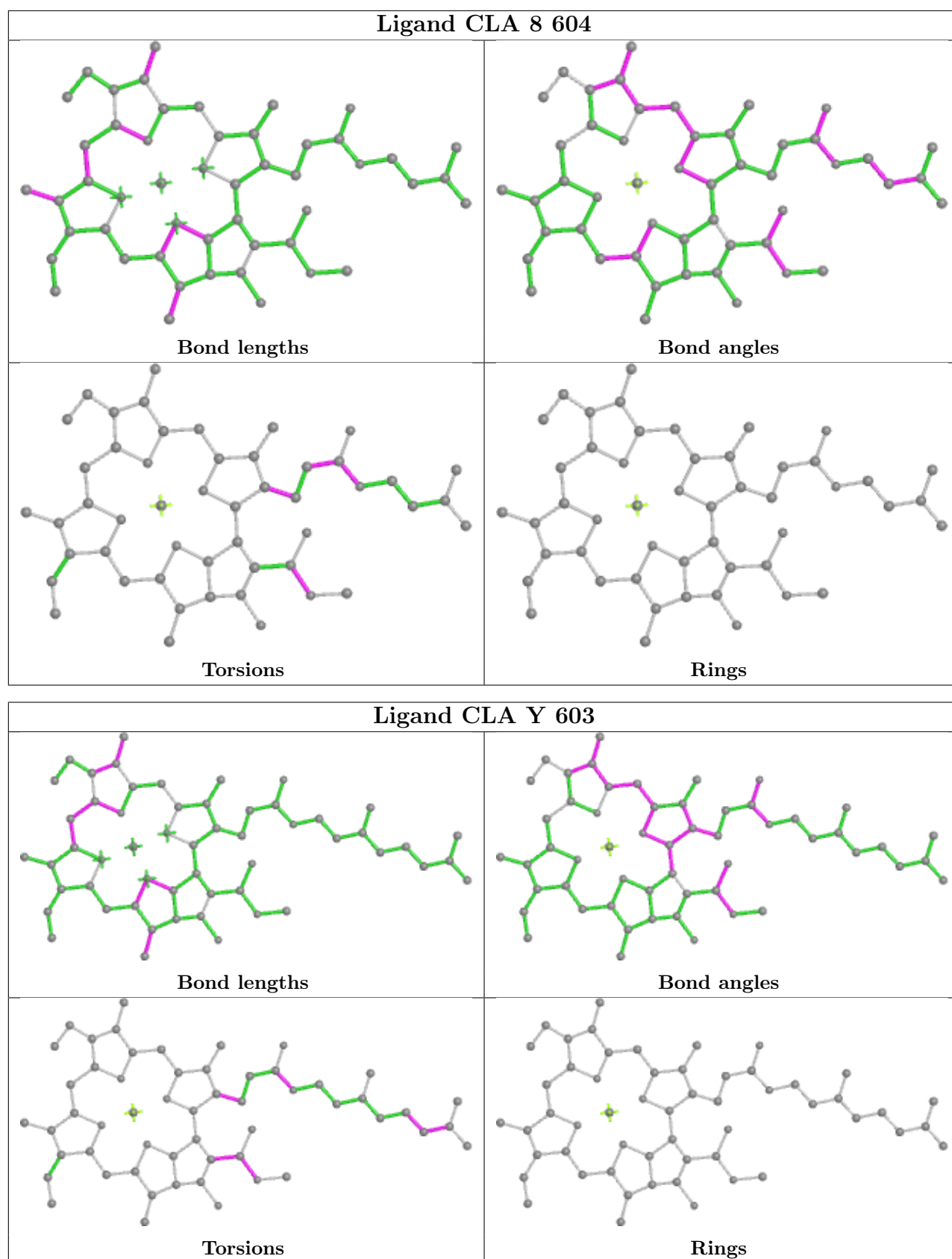


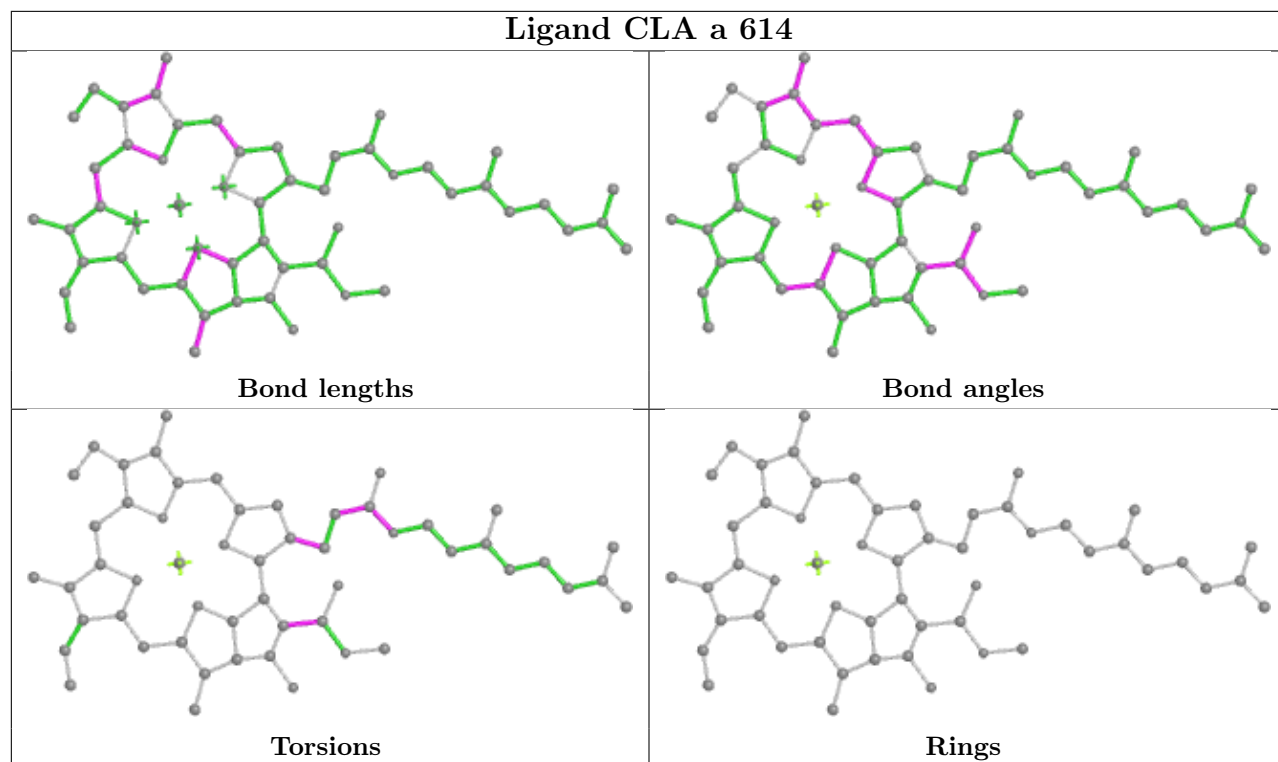


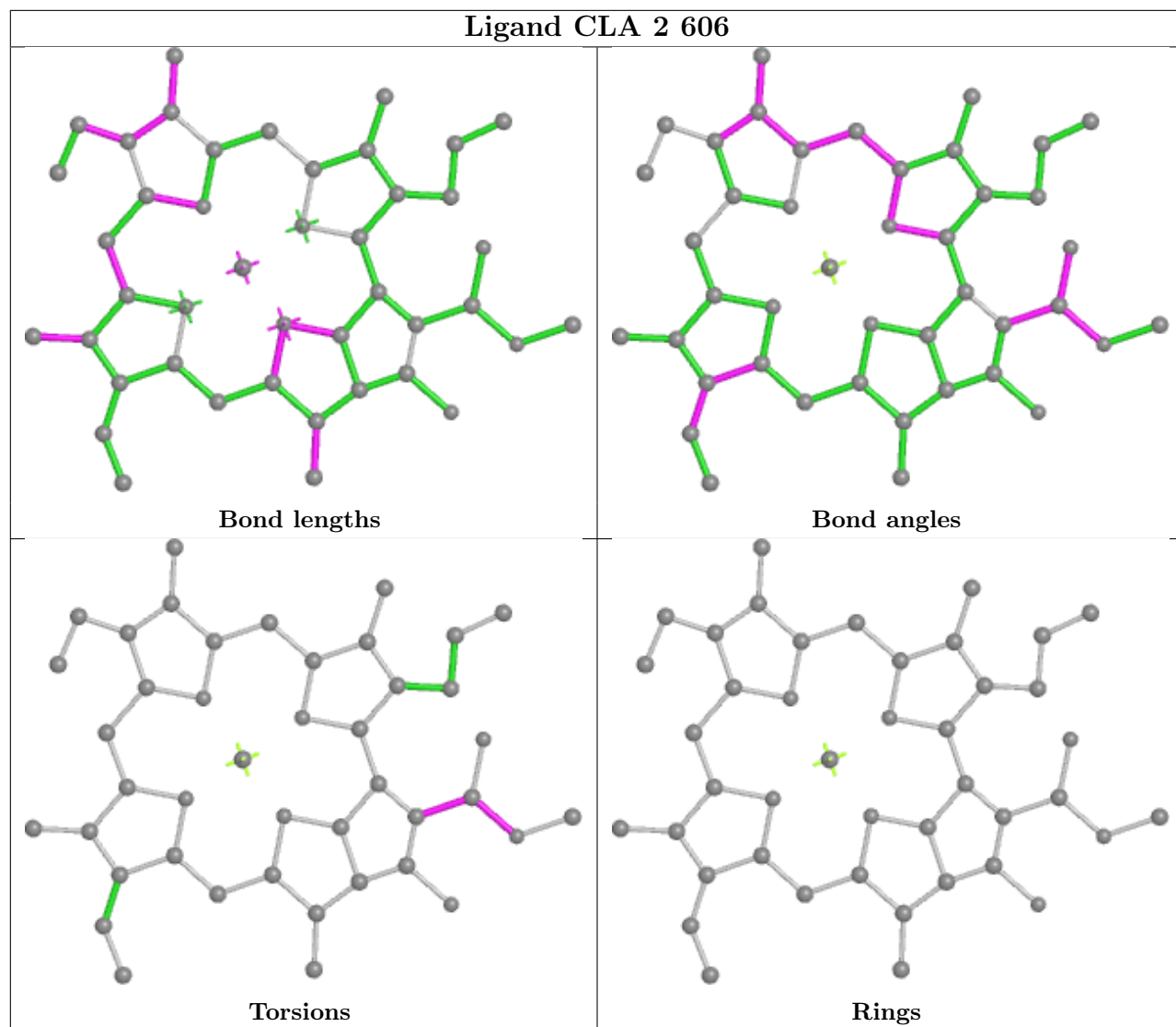


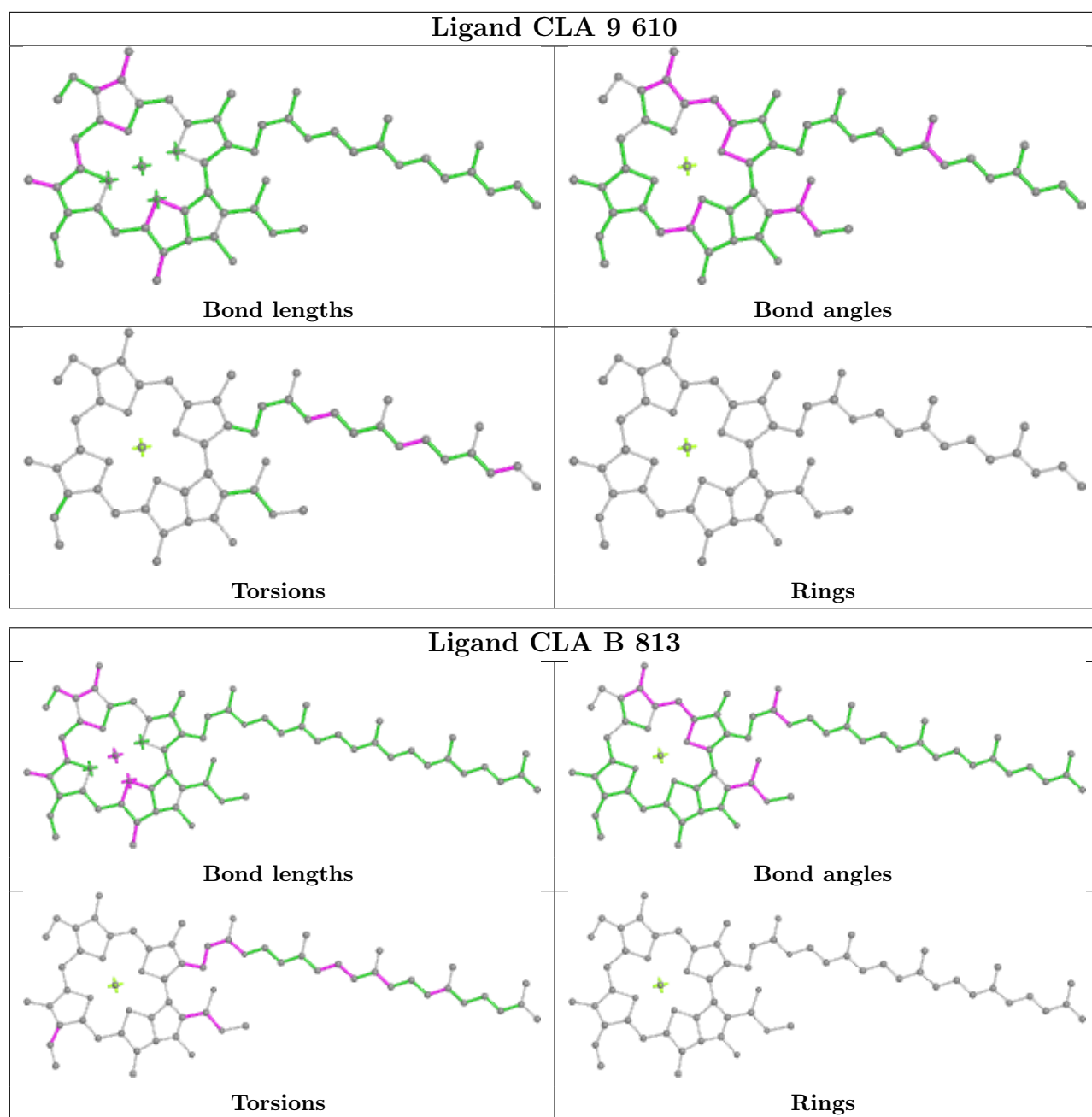


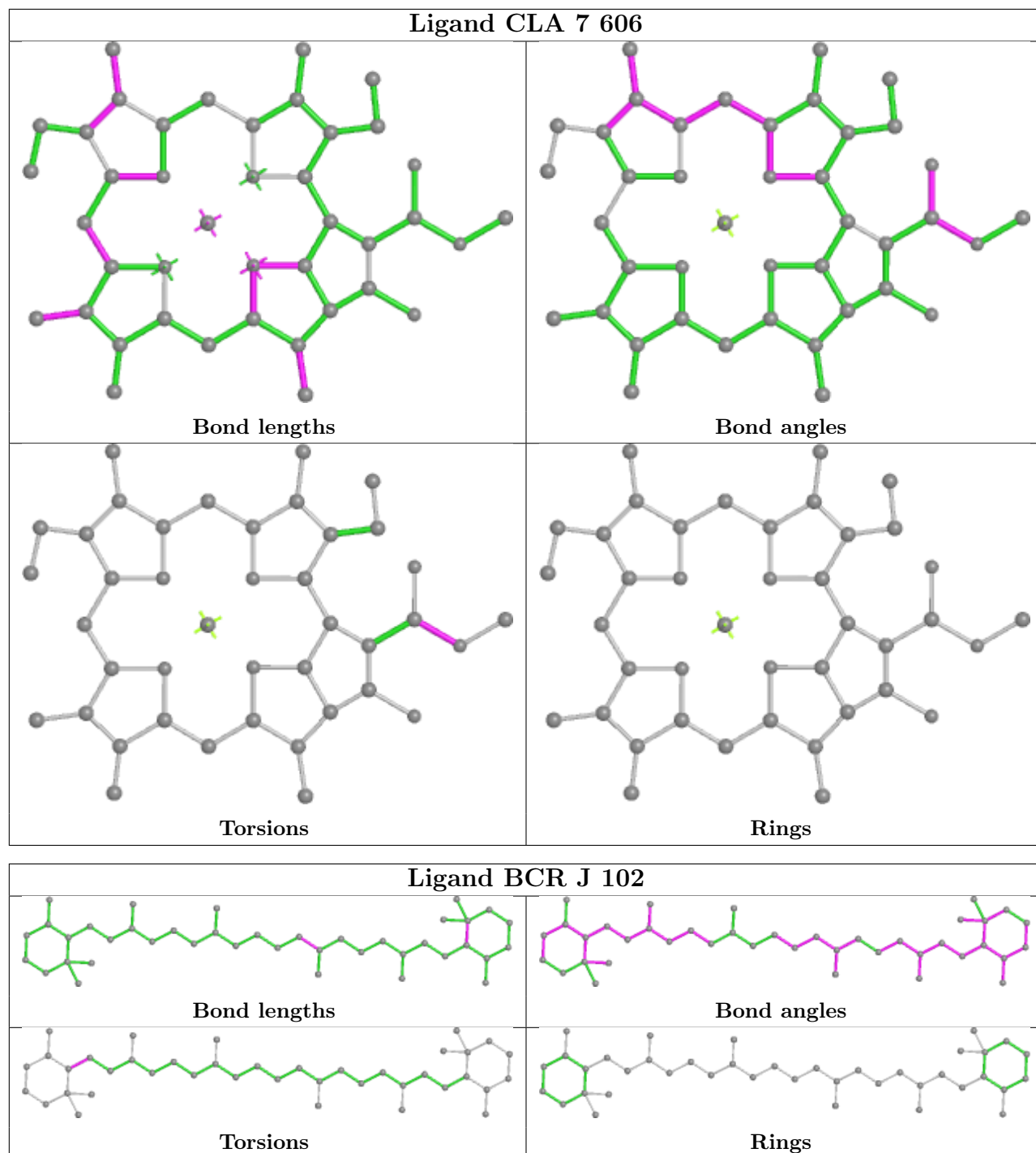


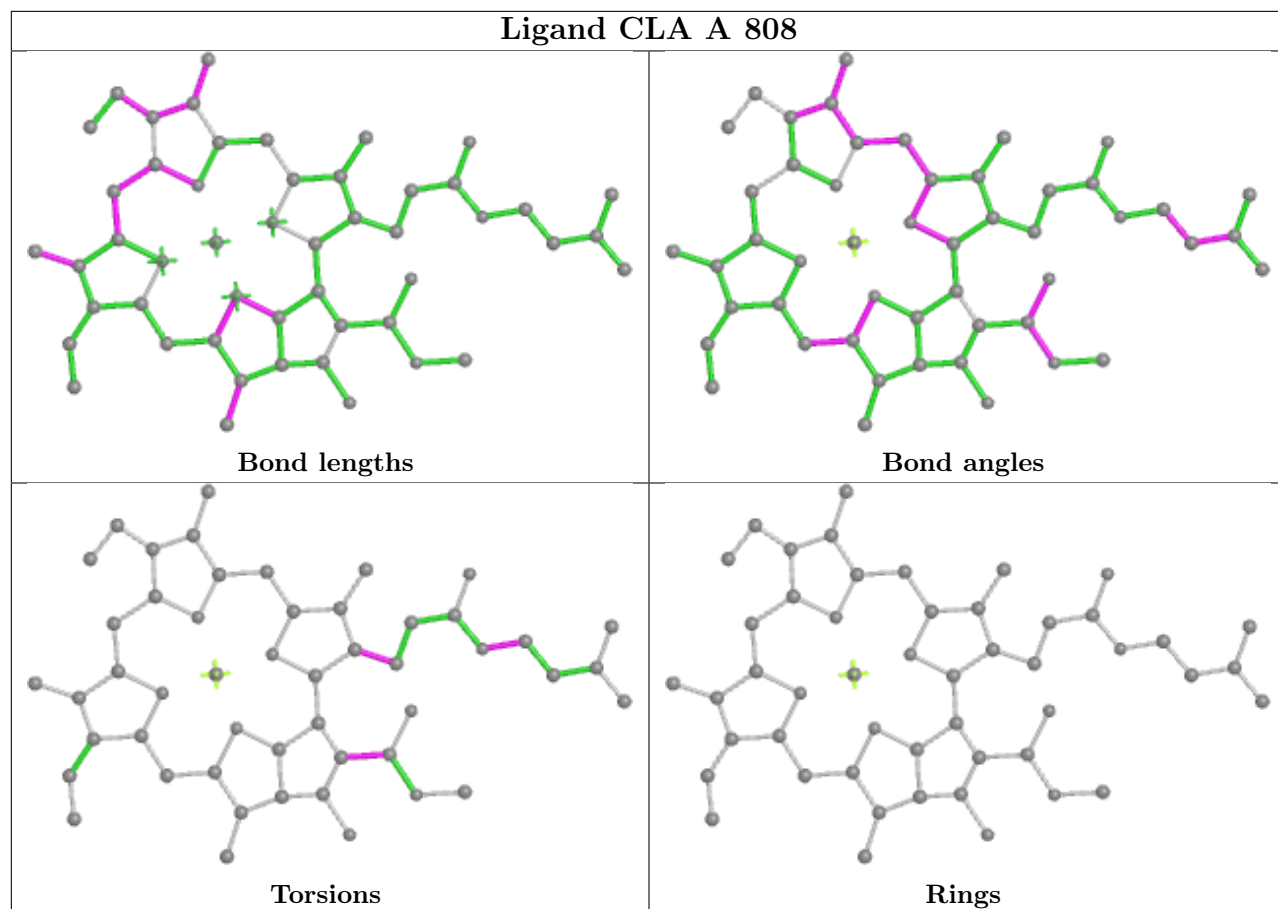


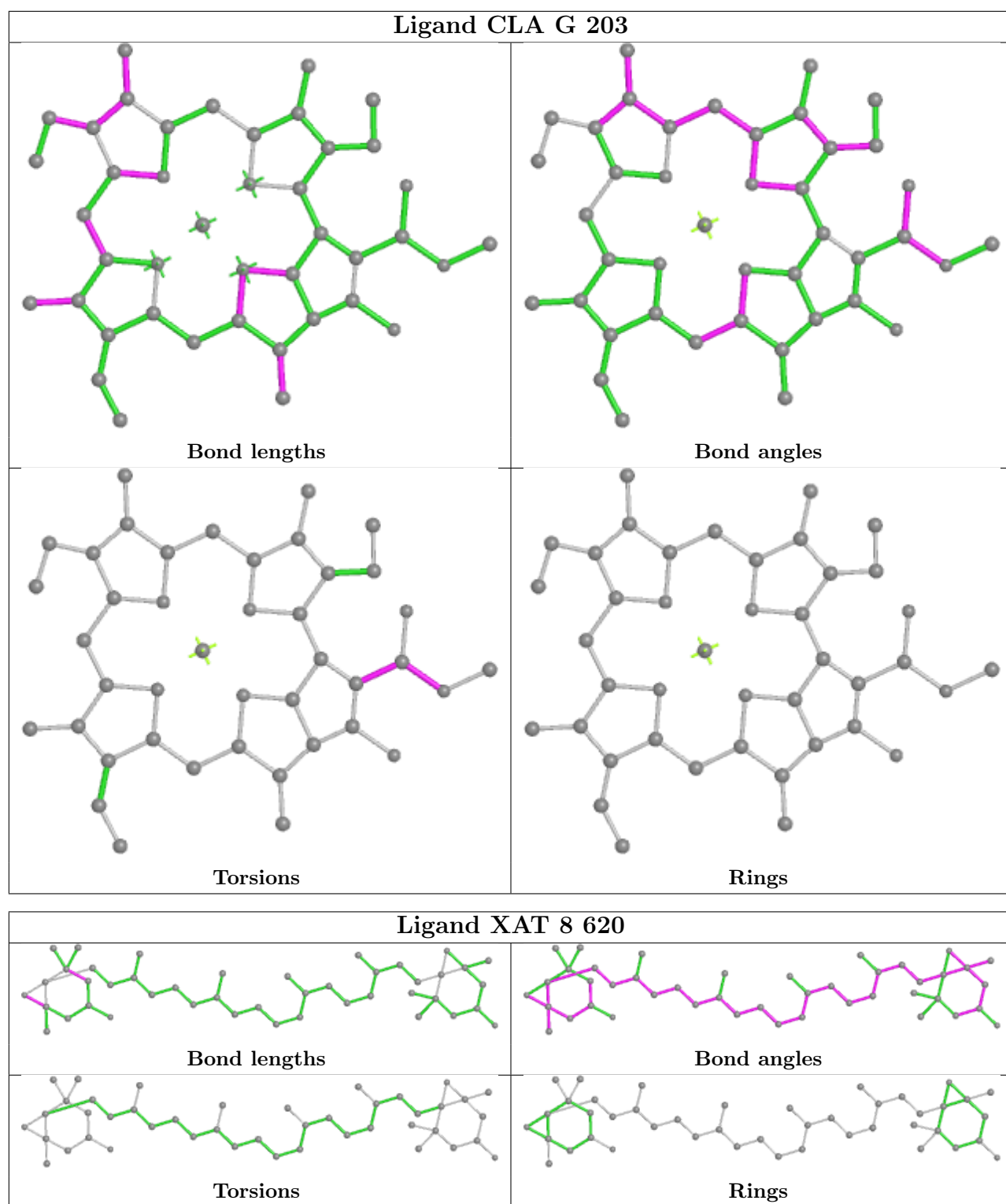


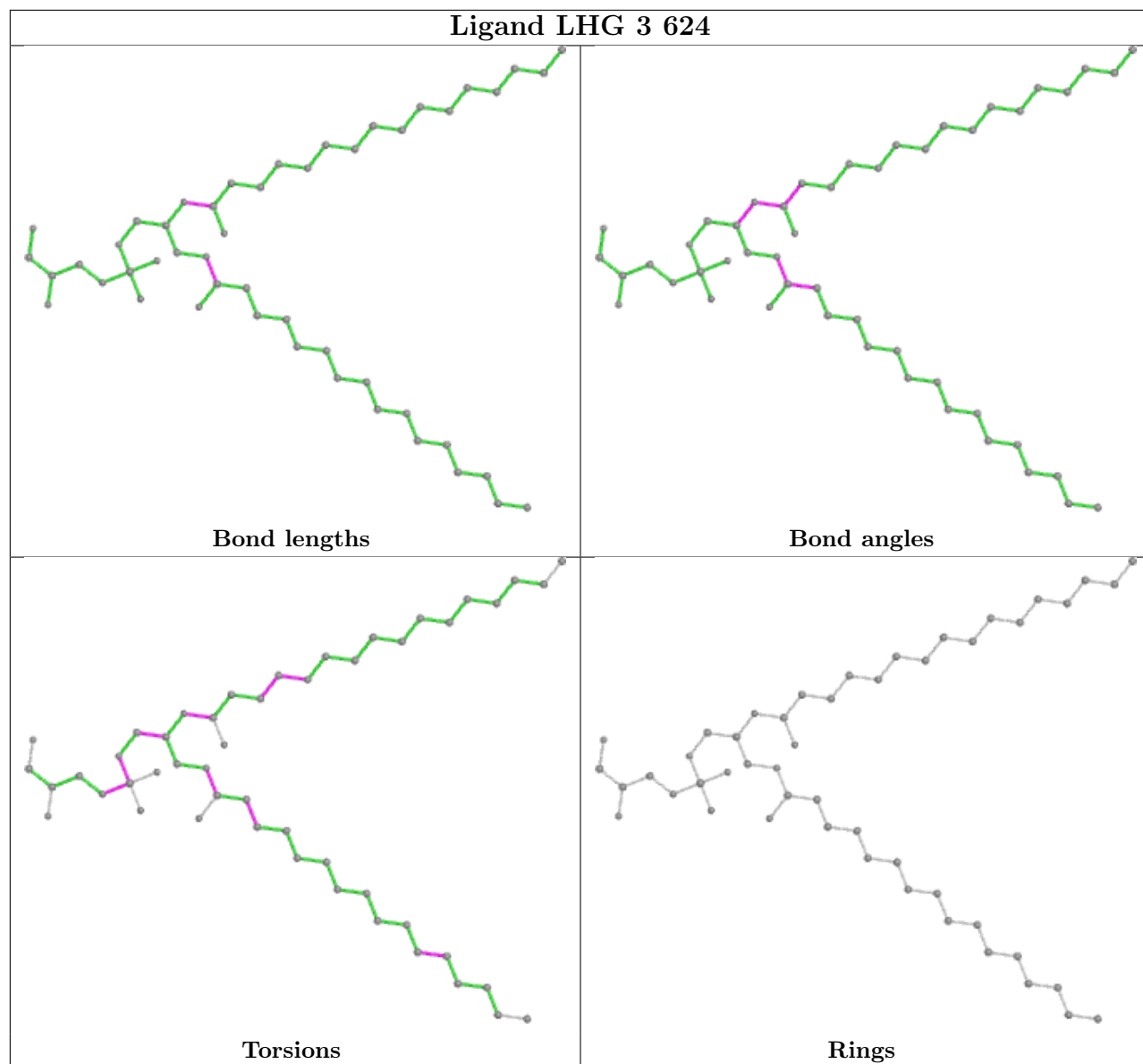


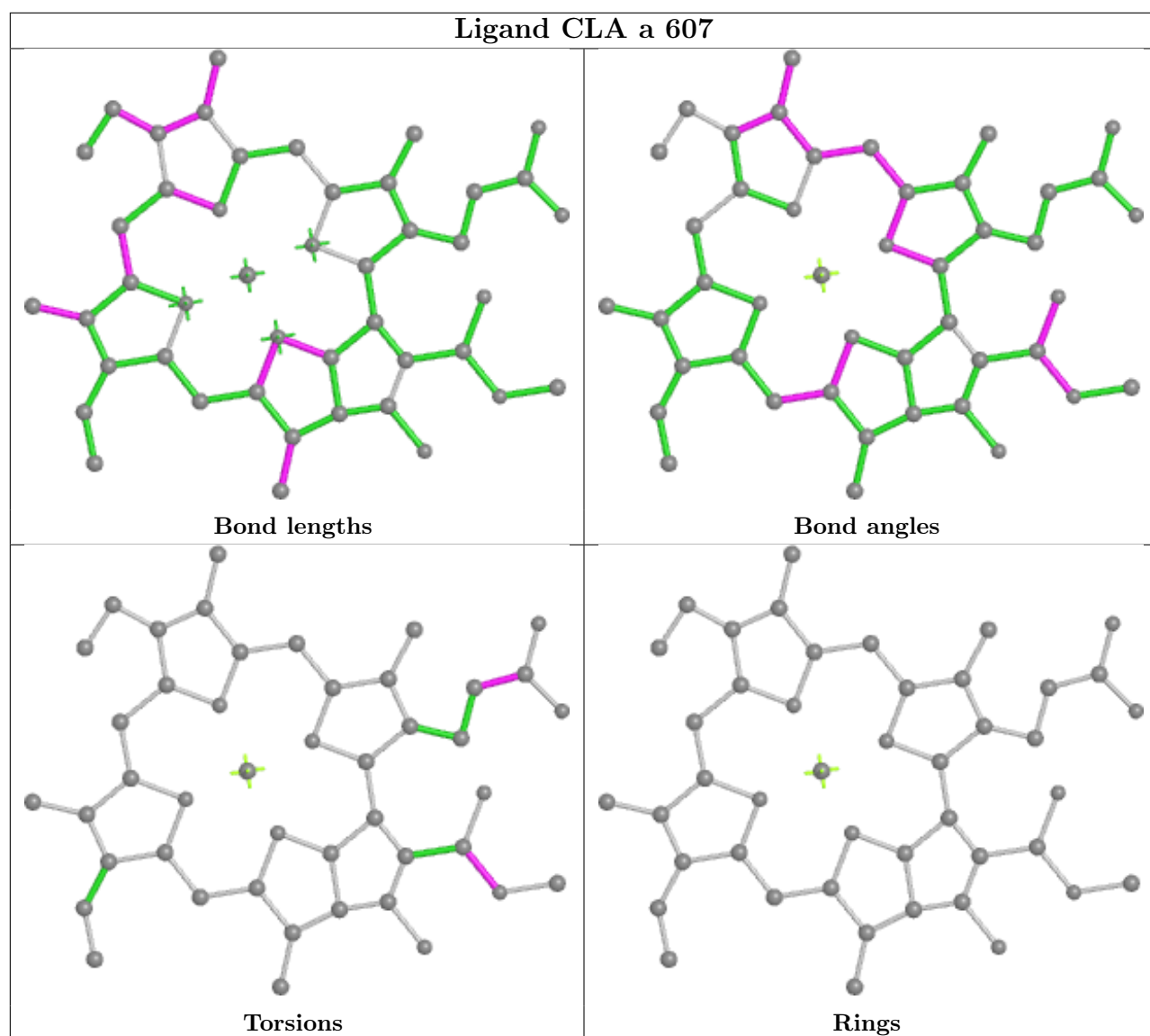


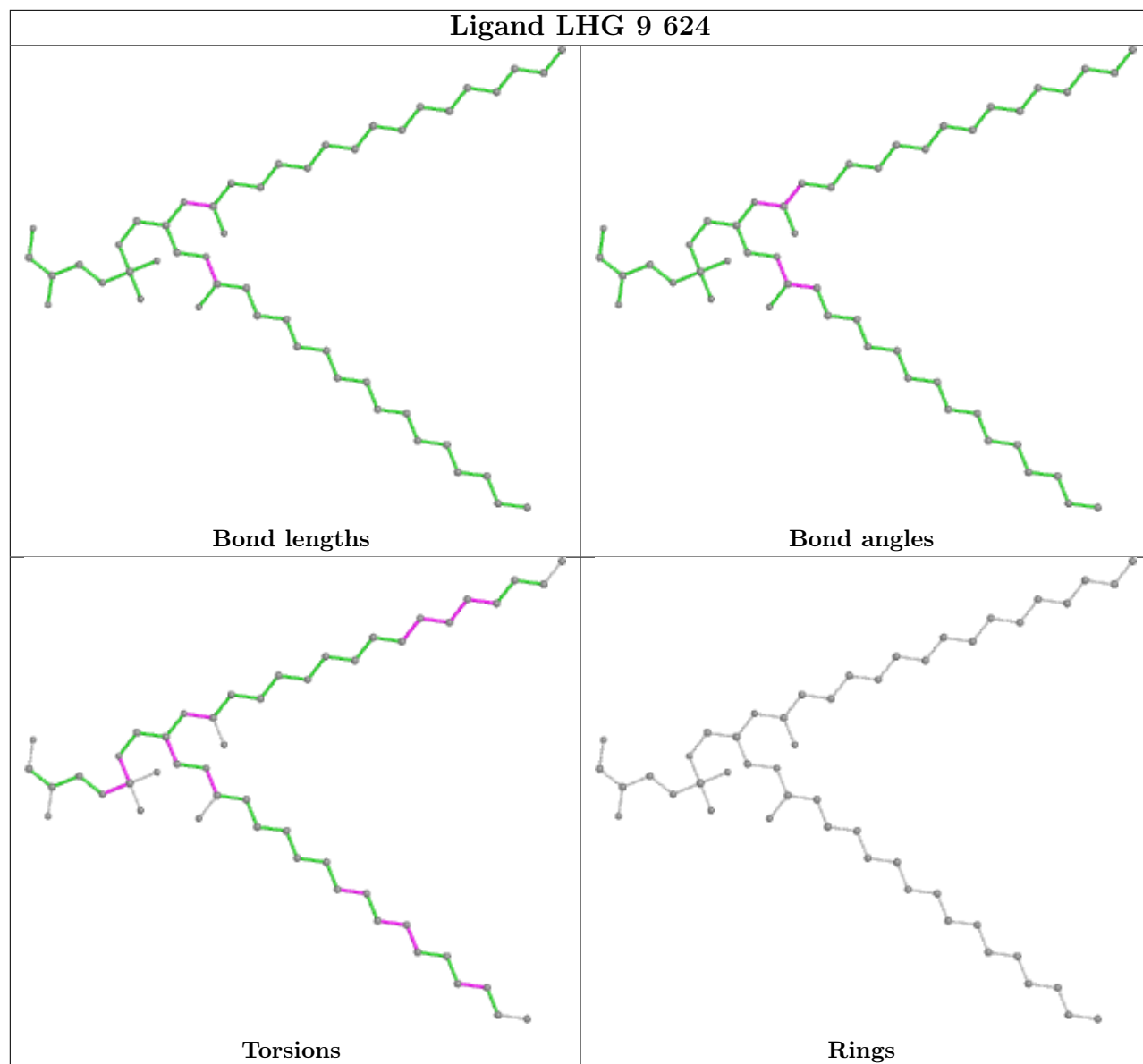


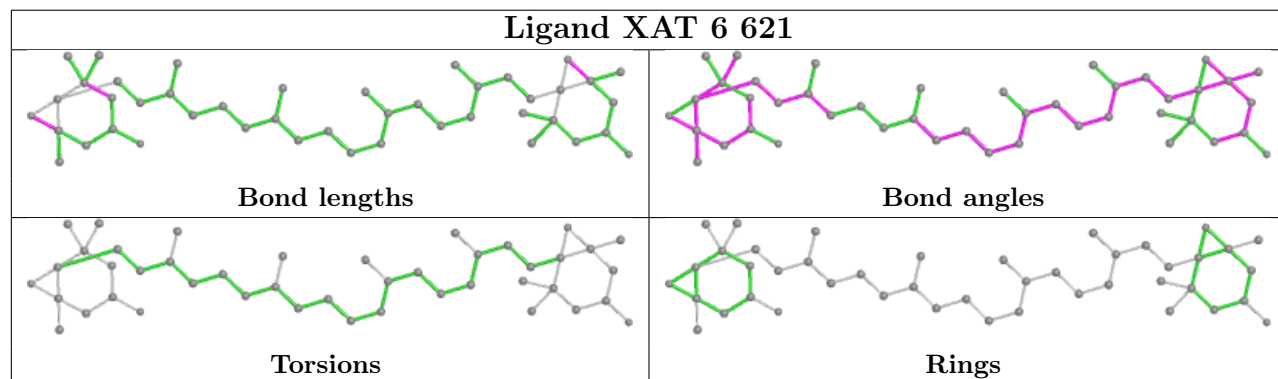
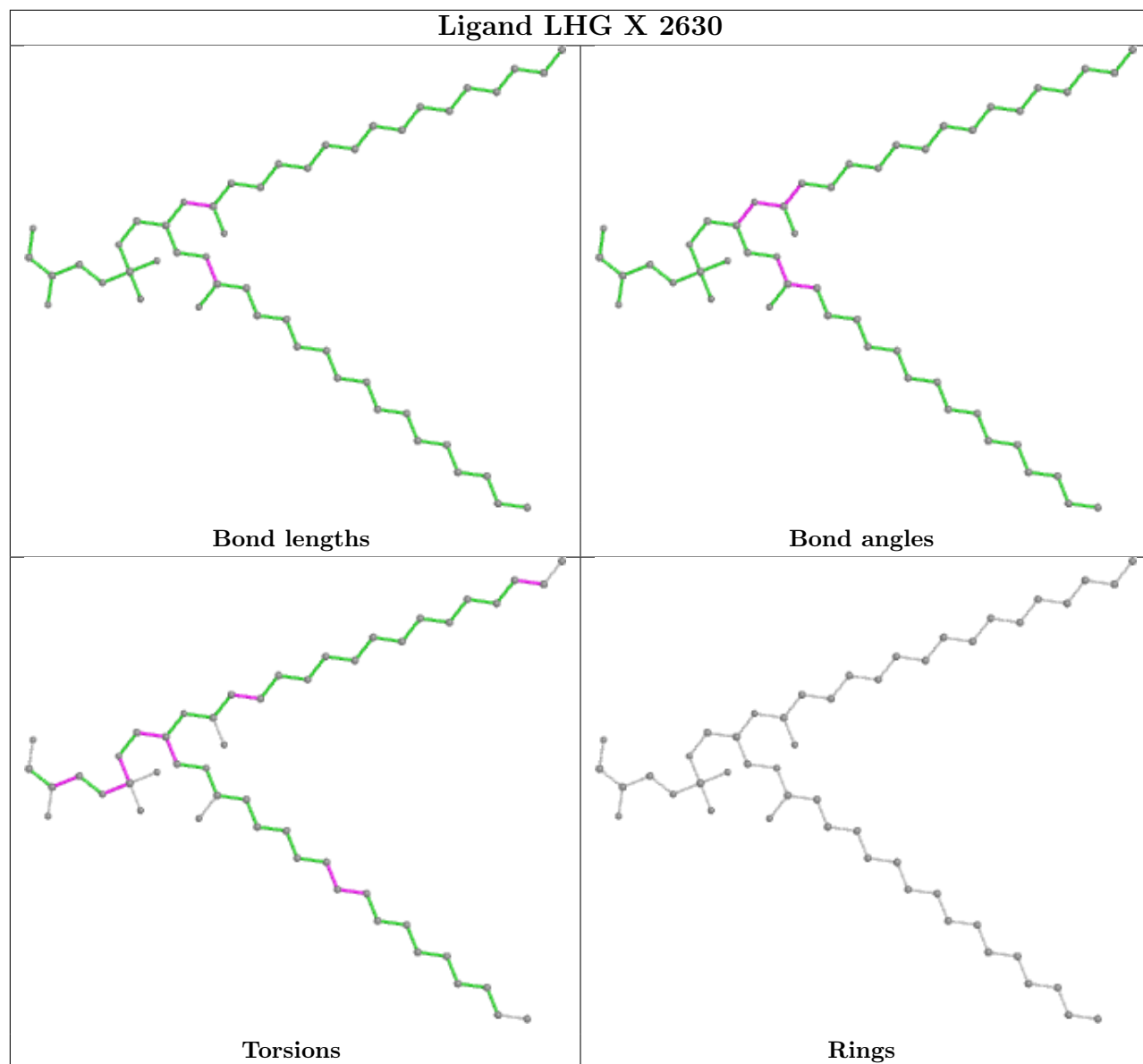


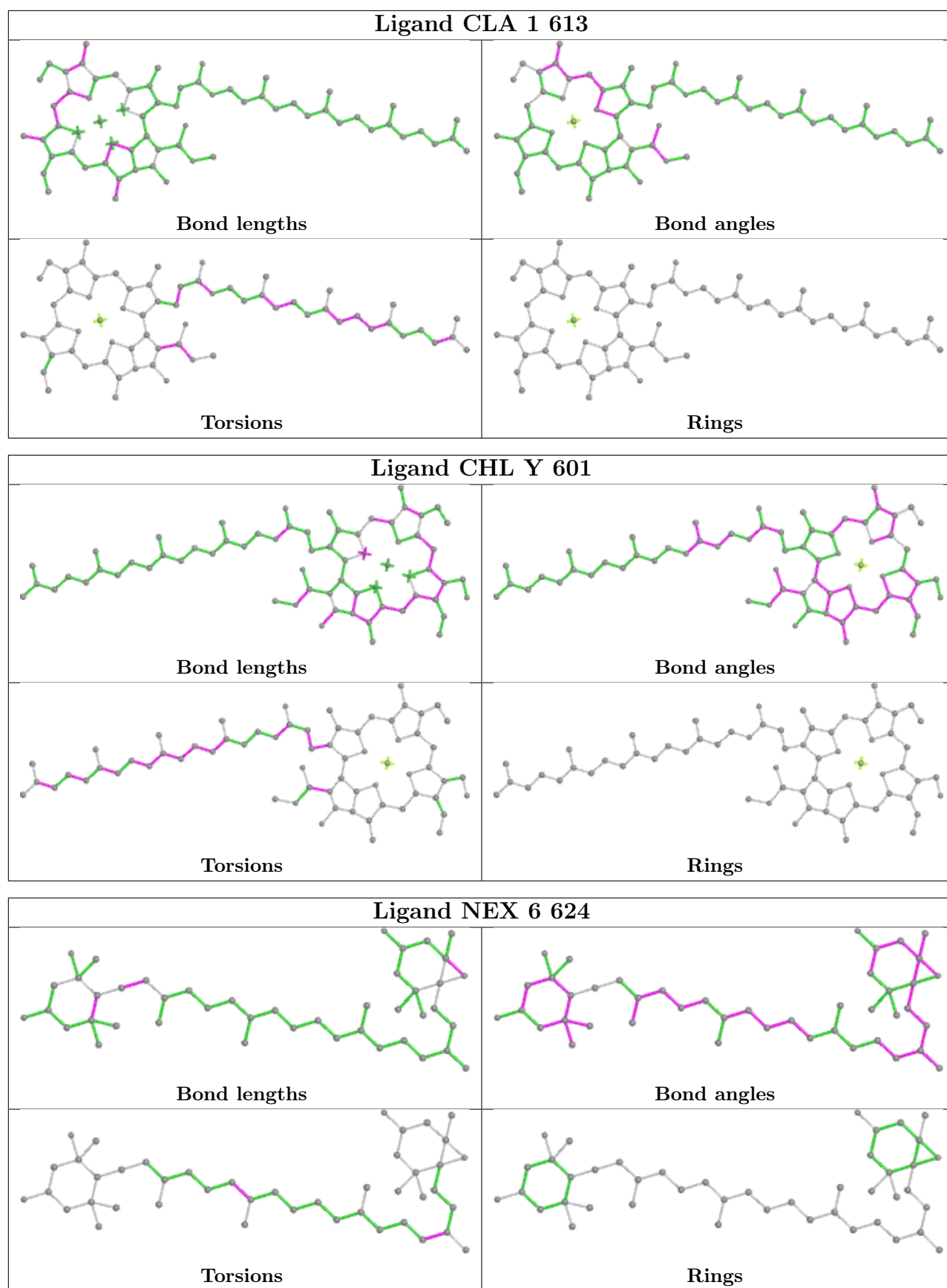


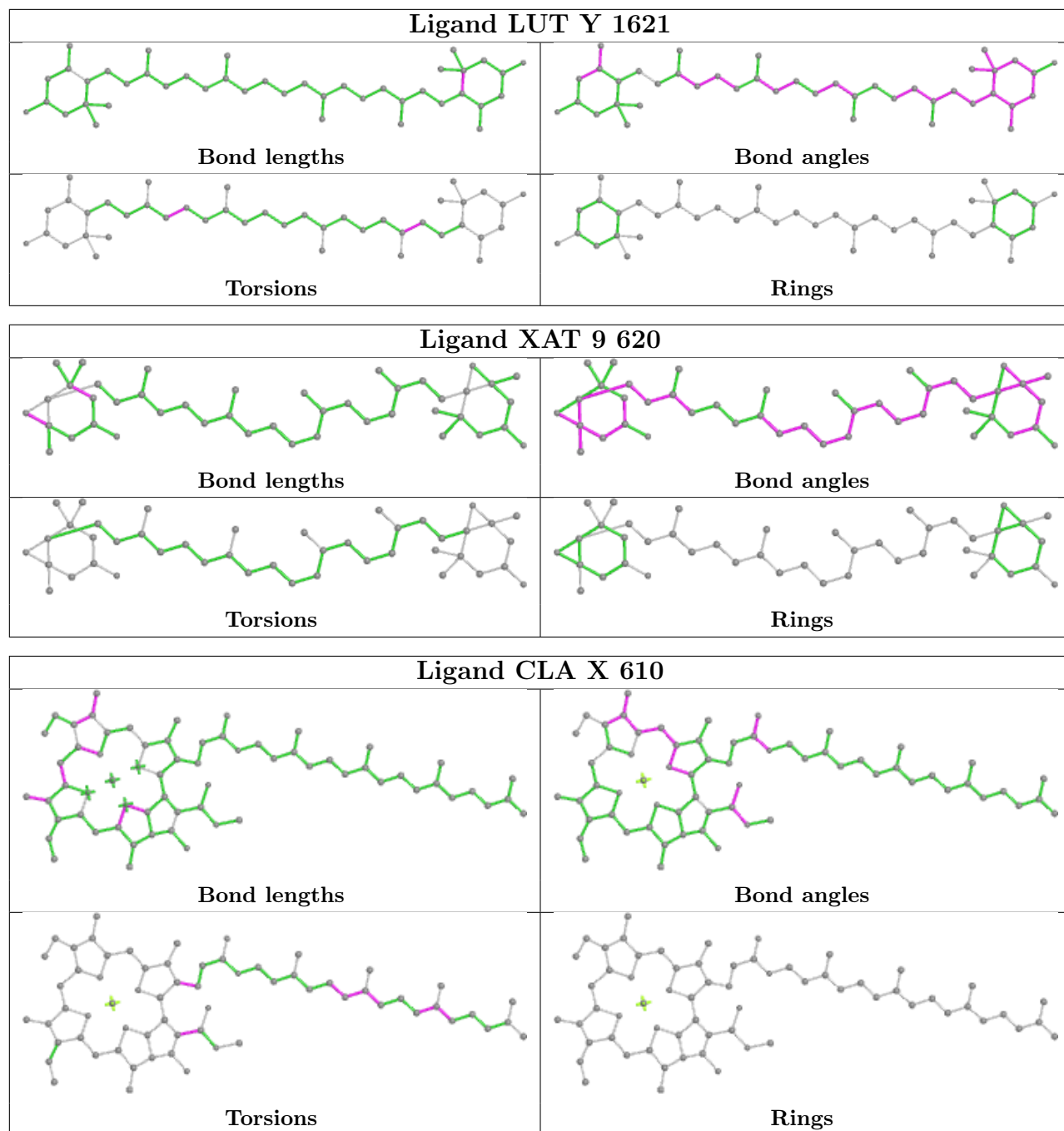


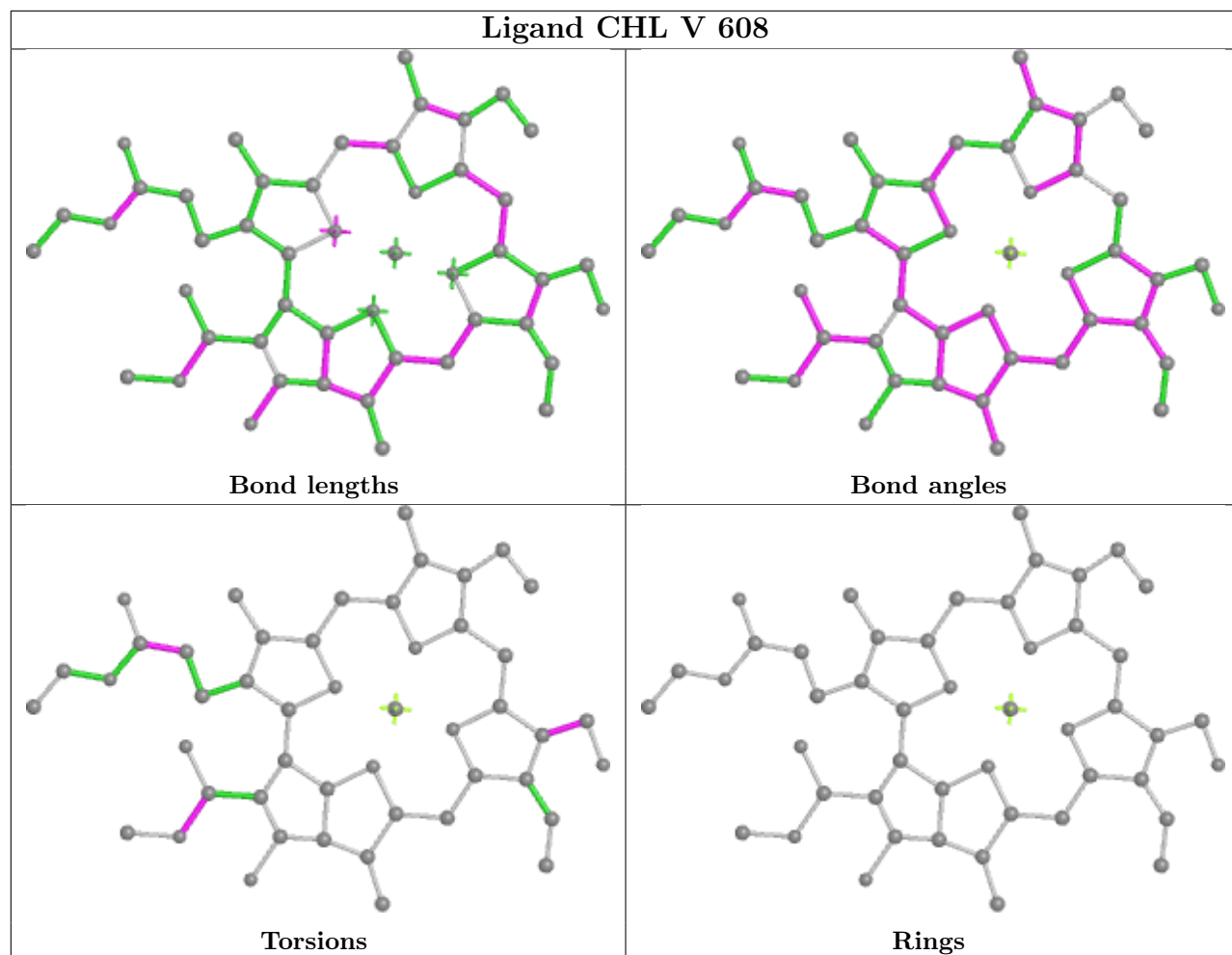


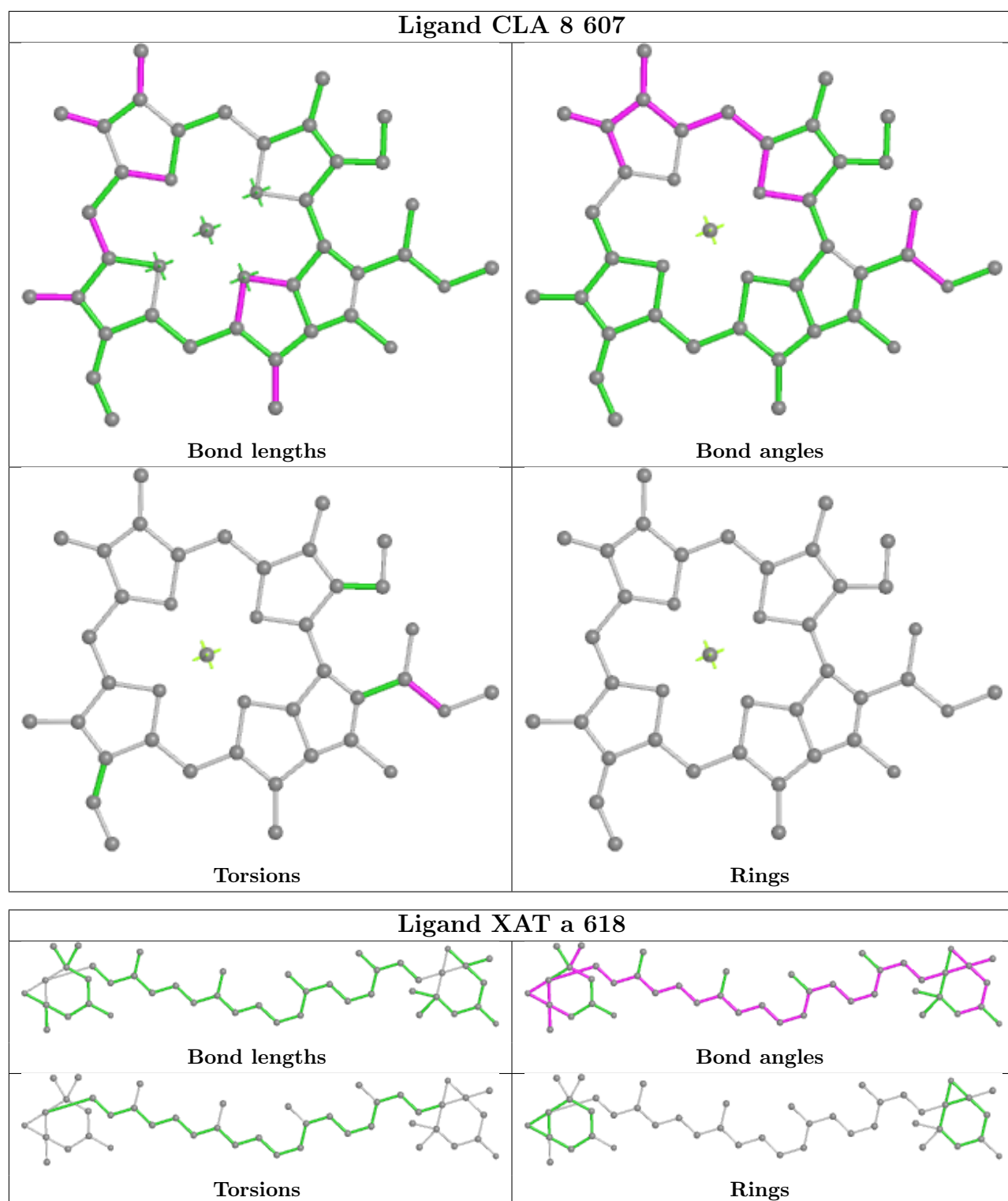


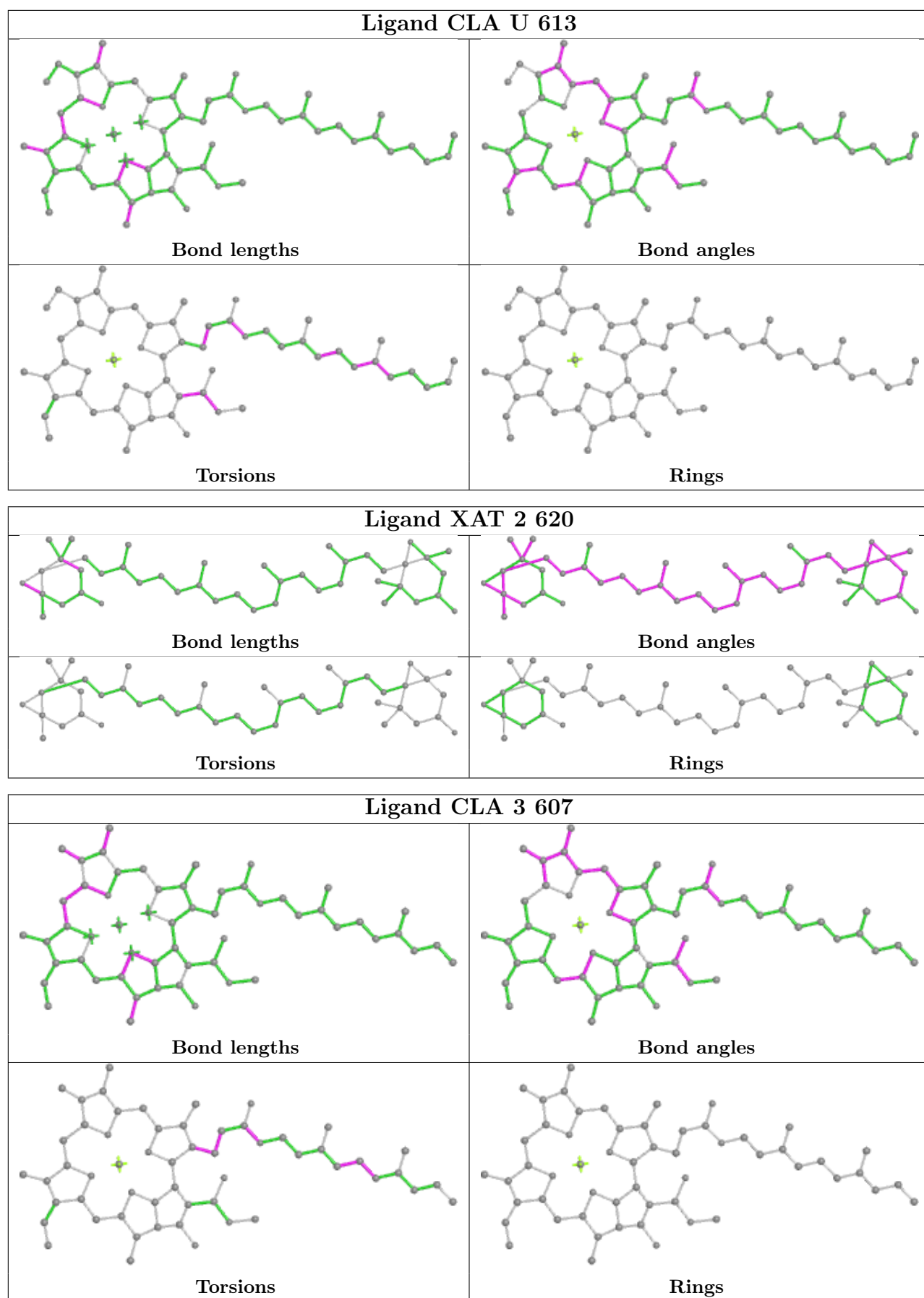


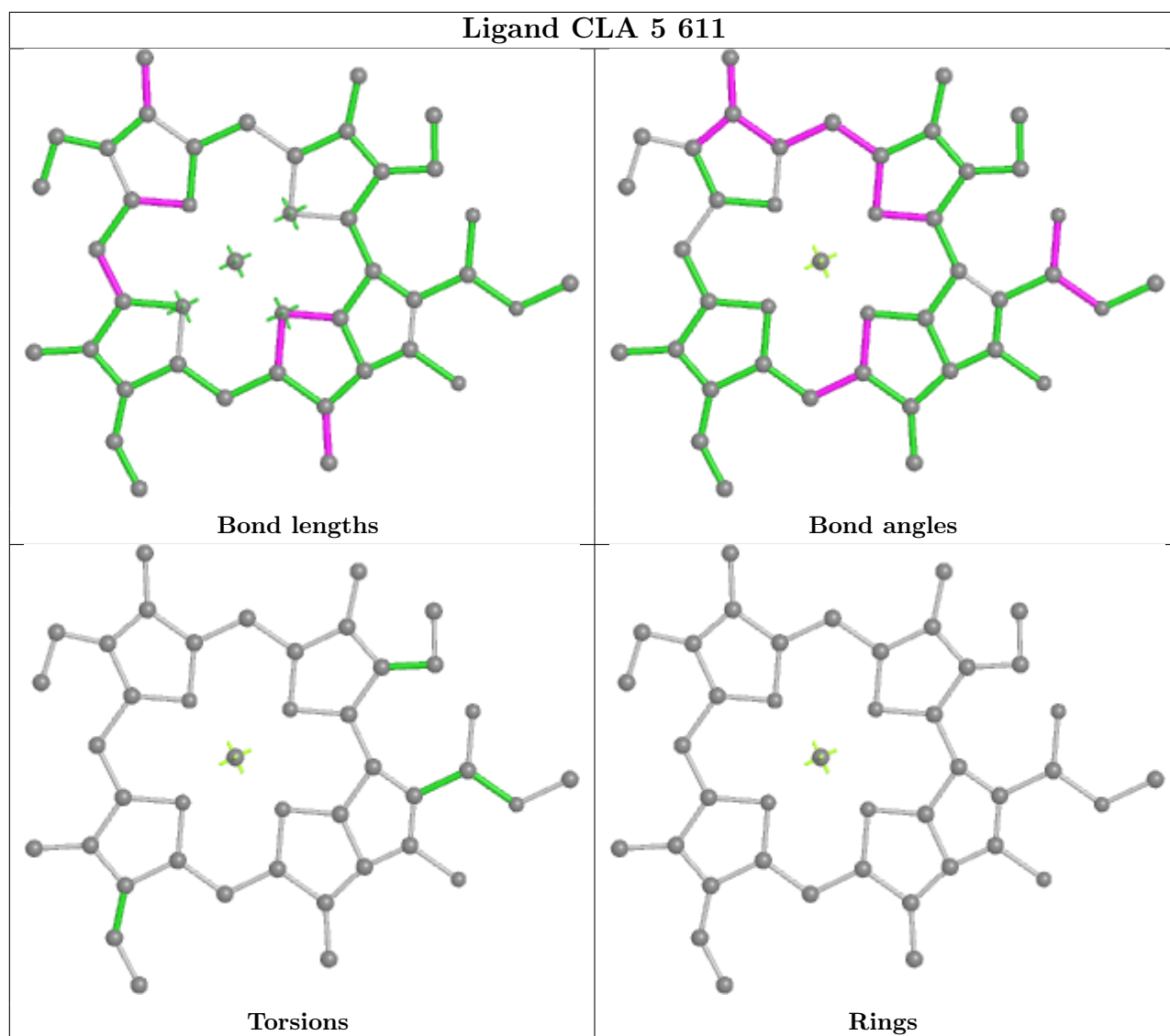
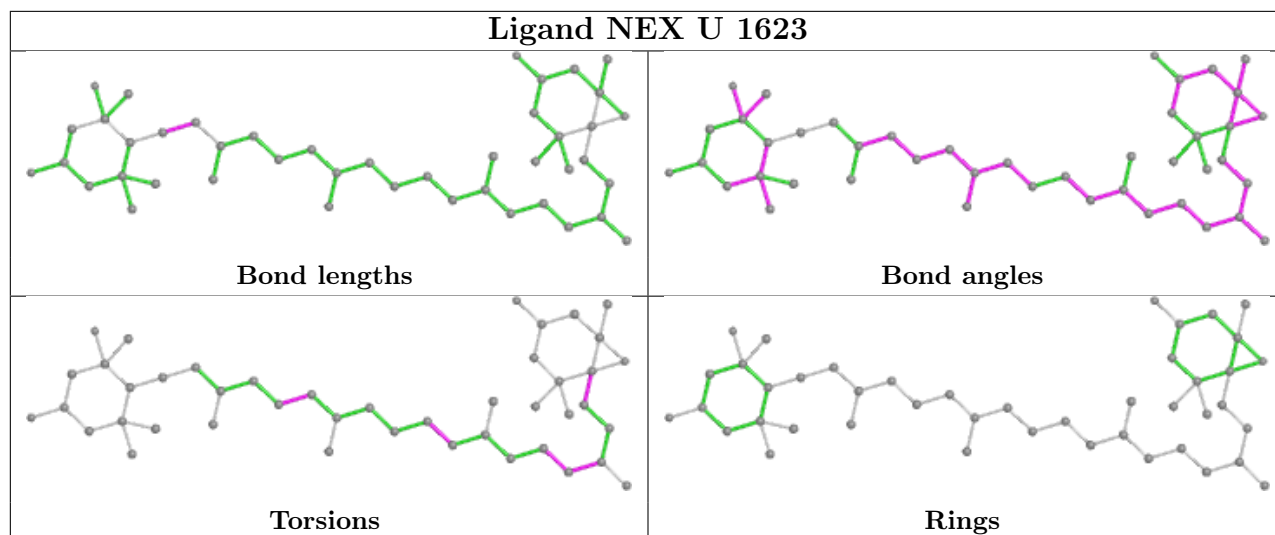












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

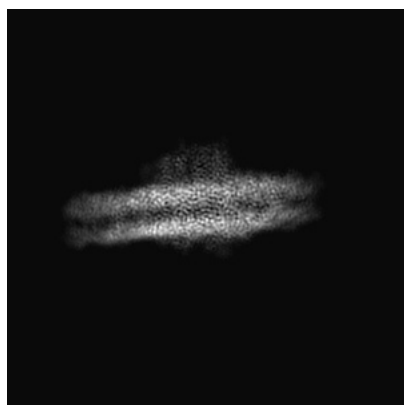
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-30926. 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](#)

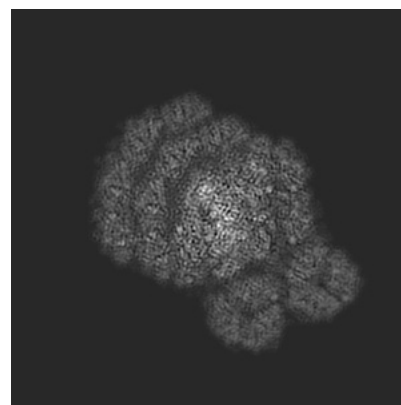
6.1.1 Primary map



X



Y

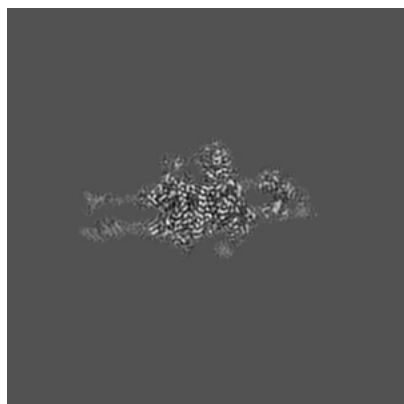


Z

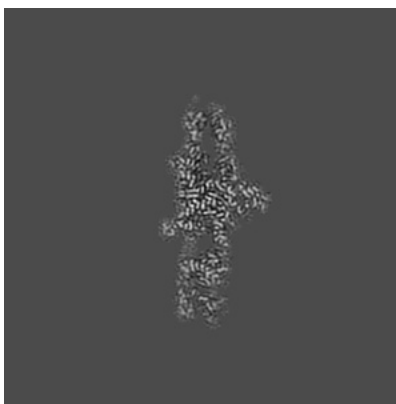
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

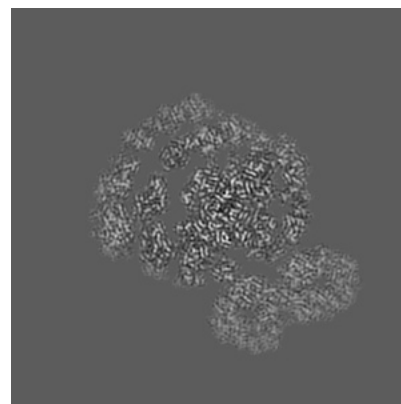
6.2.1 Primary map



X Index: 180



Y Index: 180

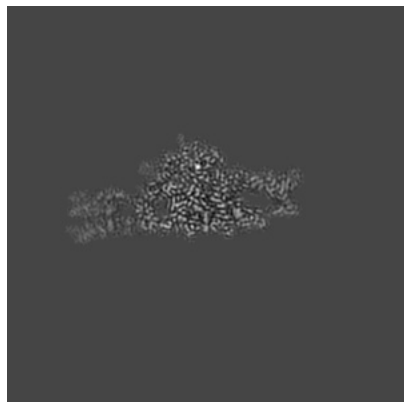


Z Index: 180

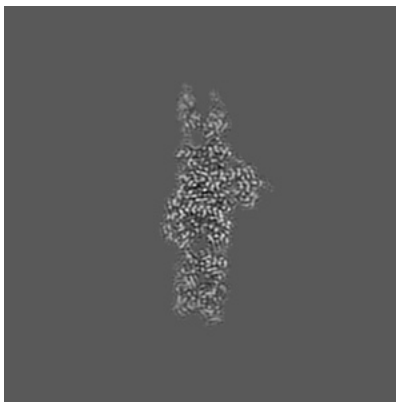
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

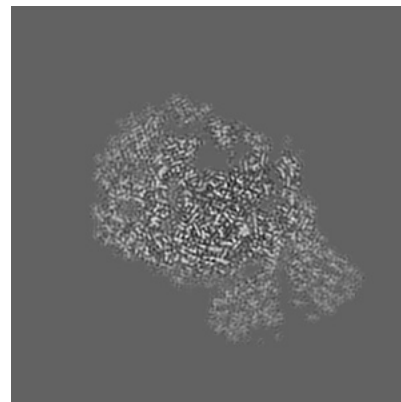
6.3.1 Primary map



X Index: 194



Y Index: 153

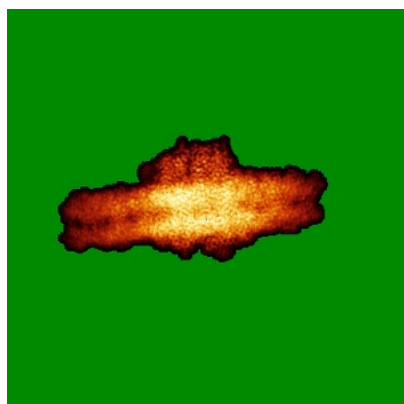


Z Index: 190

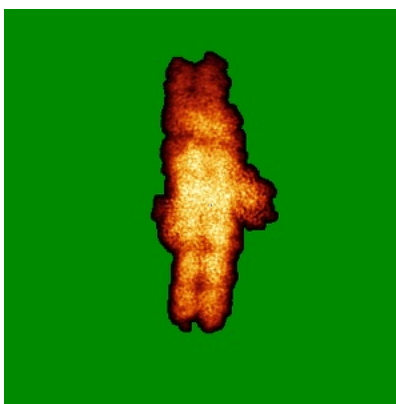
The images above show the largest variance slices of the map in three orthogonal directions.

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

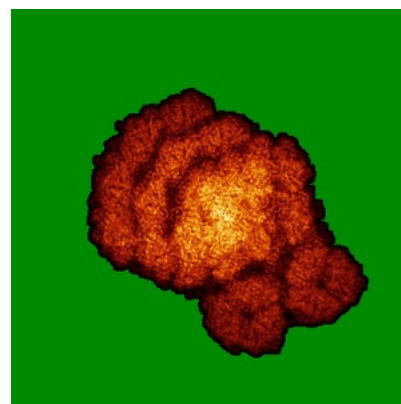
6.4.1 Primary map



X



Y

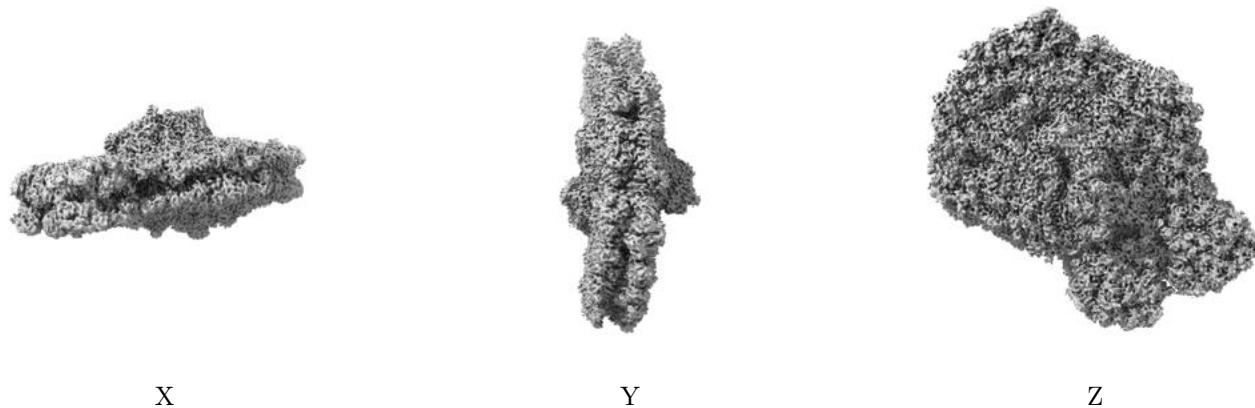


Z

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



The images above show the 3D surface view of the map at the recommended contour level 0.005. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

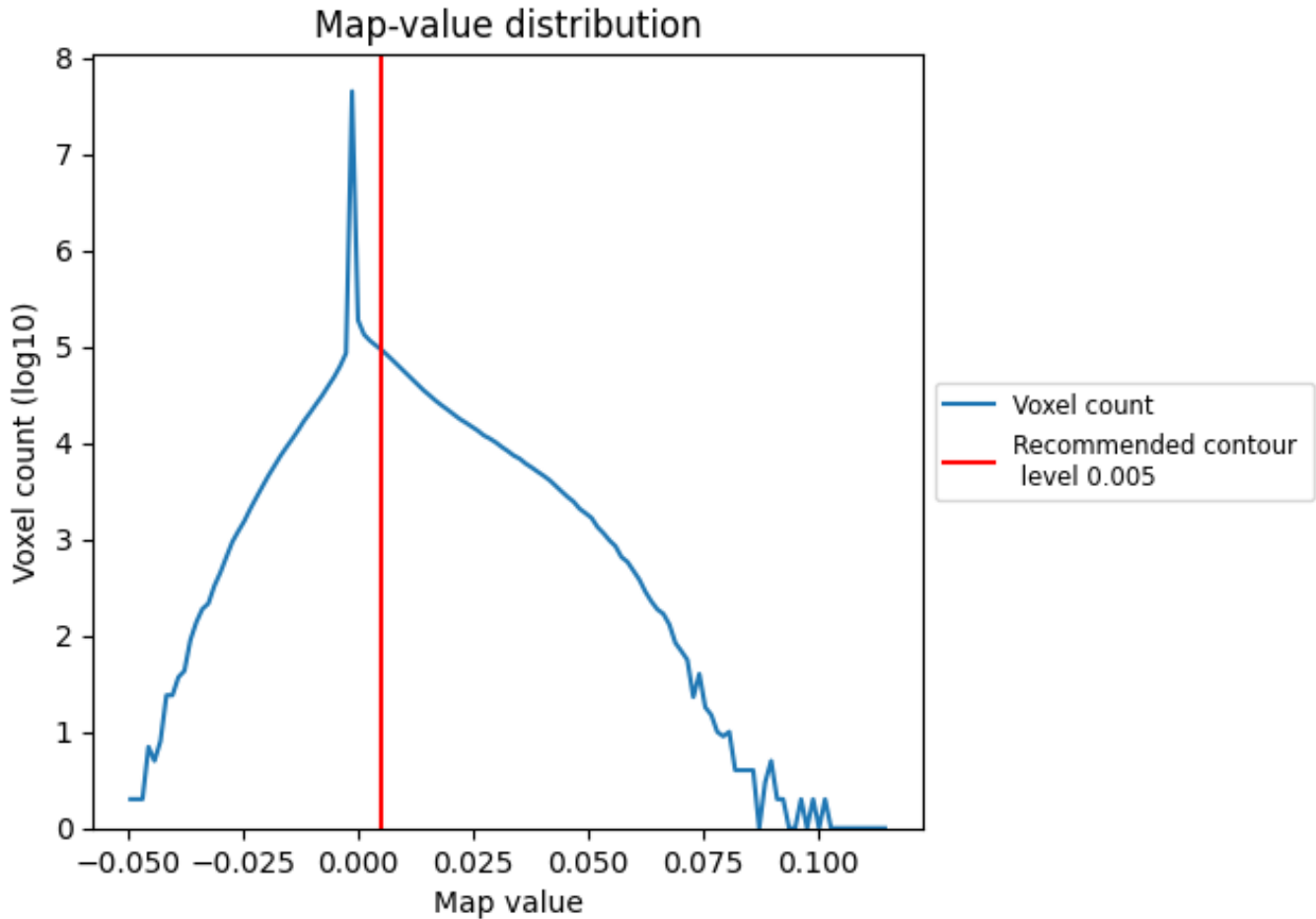
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

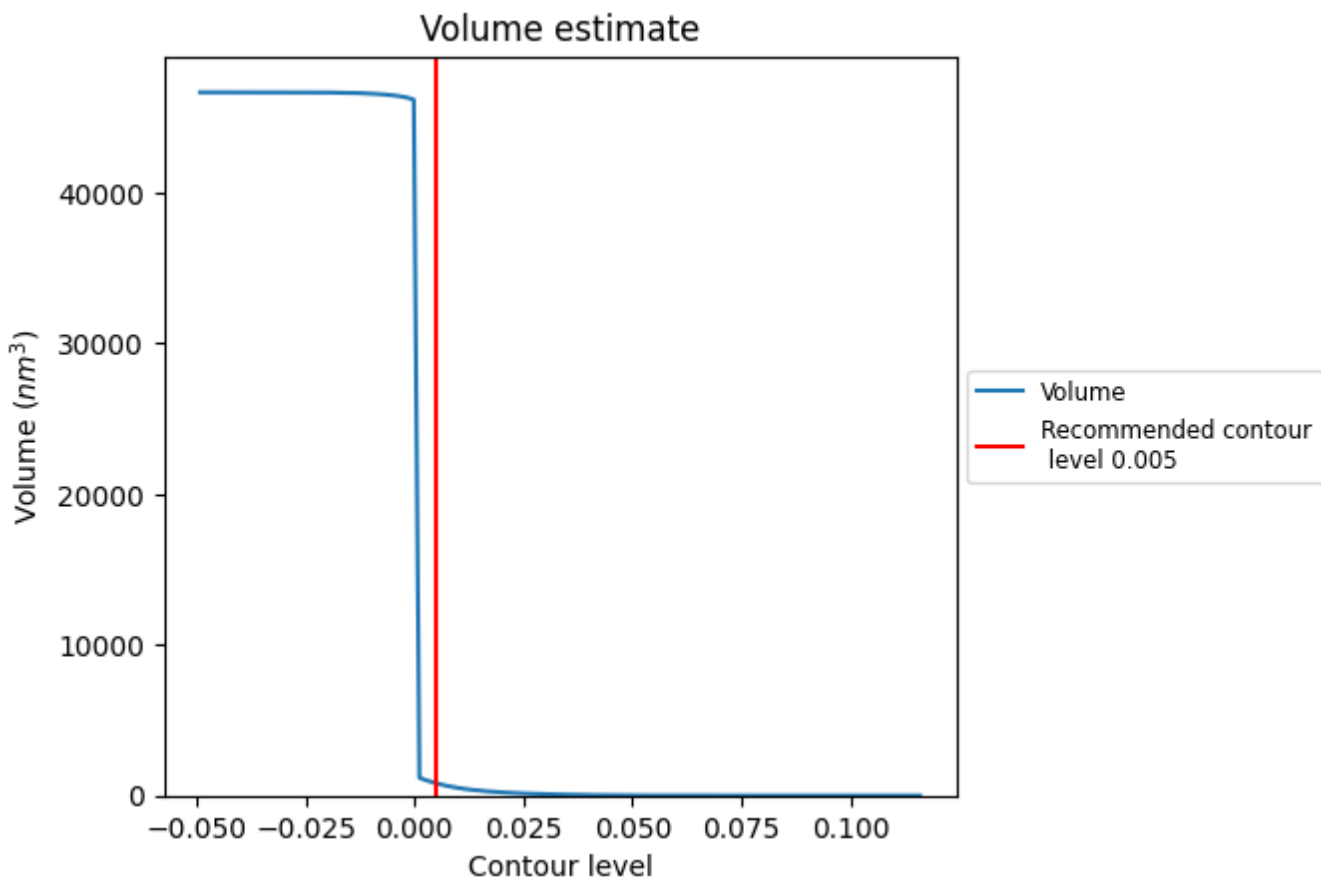
This section contains the results of statistical analysis of the map.

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.

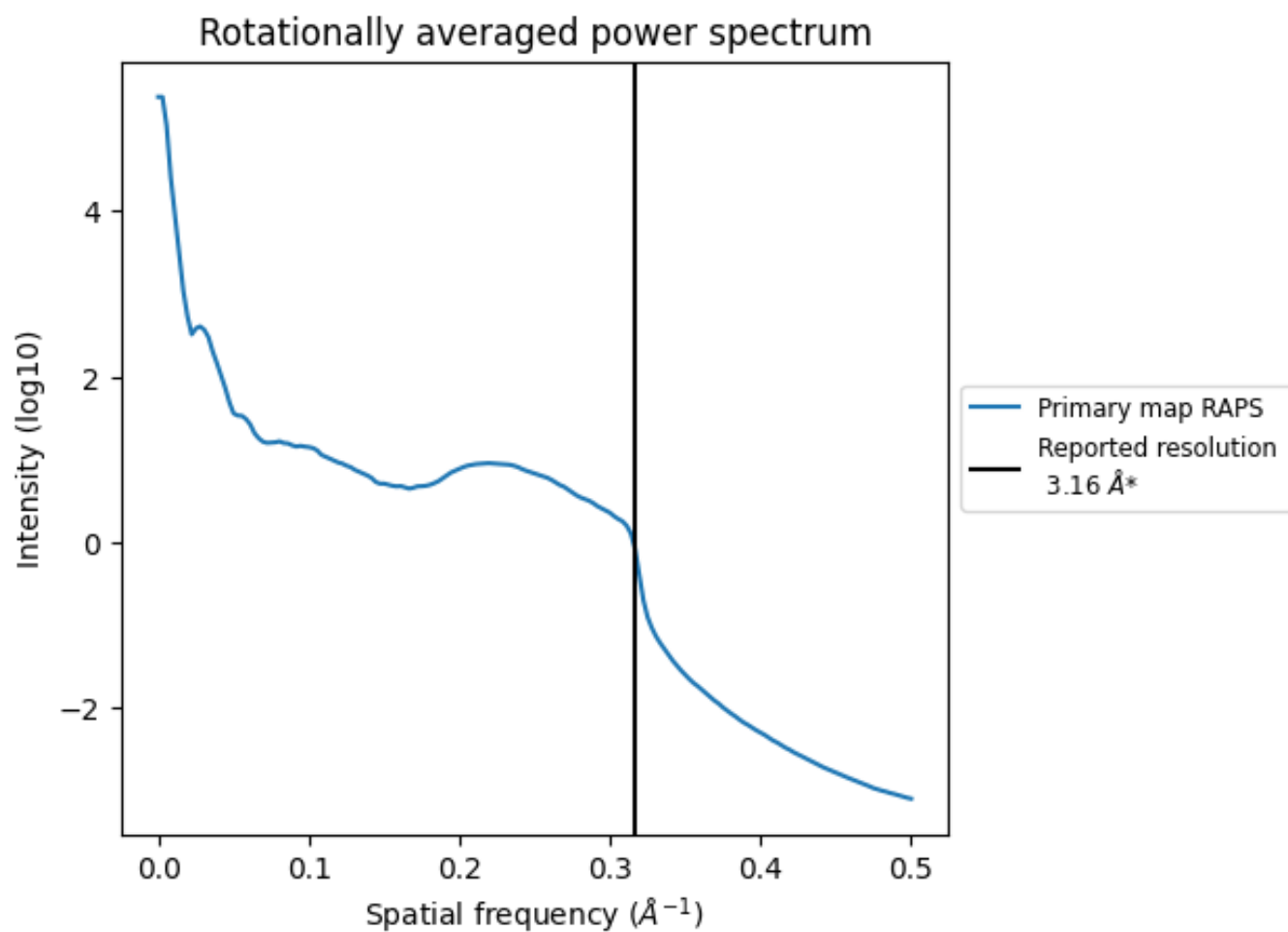
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 811 nm^3 ; this corresponds to an approximate mass of 733 kDa.

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

7.3 Rotationally averaged power spectrum [i](#)



*Reported resolution corresponds to spatial frequency of 0.316 Å⁻¹

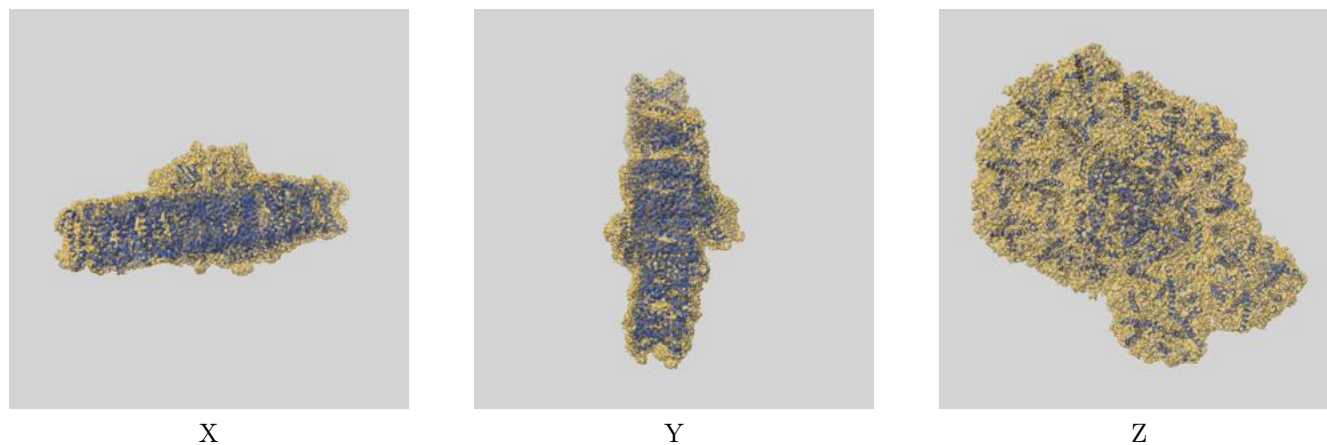
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

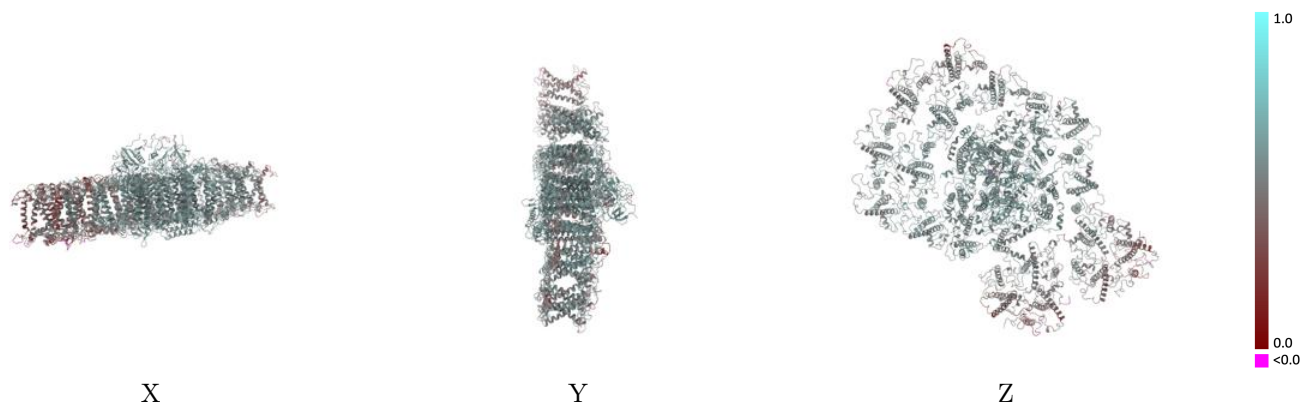
This section contains information regarding the fit between EMDB map EMD-30926 and PDB model 7DZ8. Per-residue inclusion information can be found in section [3](#) on page [45](#).

9.1 Map-model overlay [i](#)



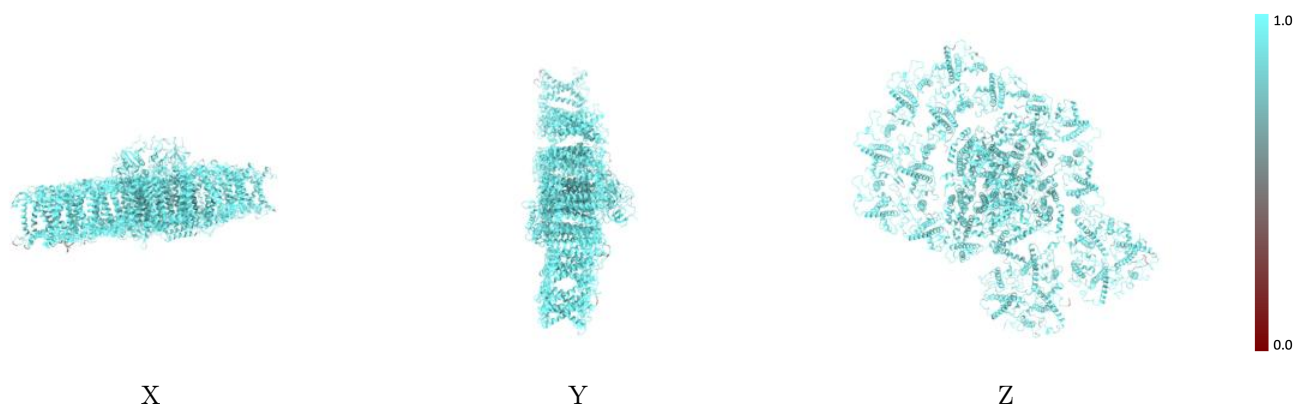
The images above show the 3D surface view of the map at the recommended contour level 0.005 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



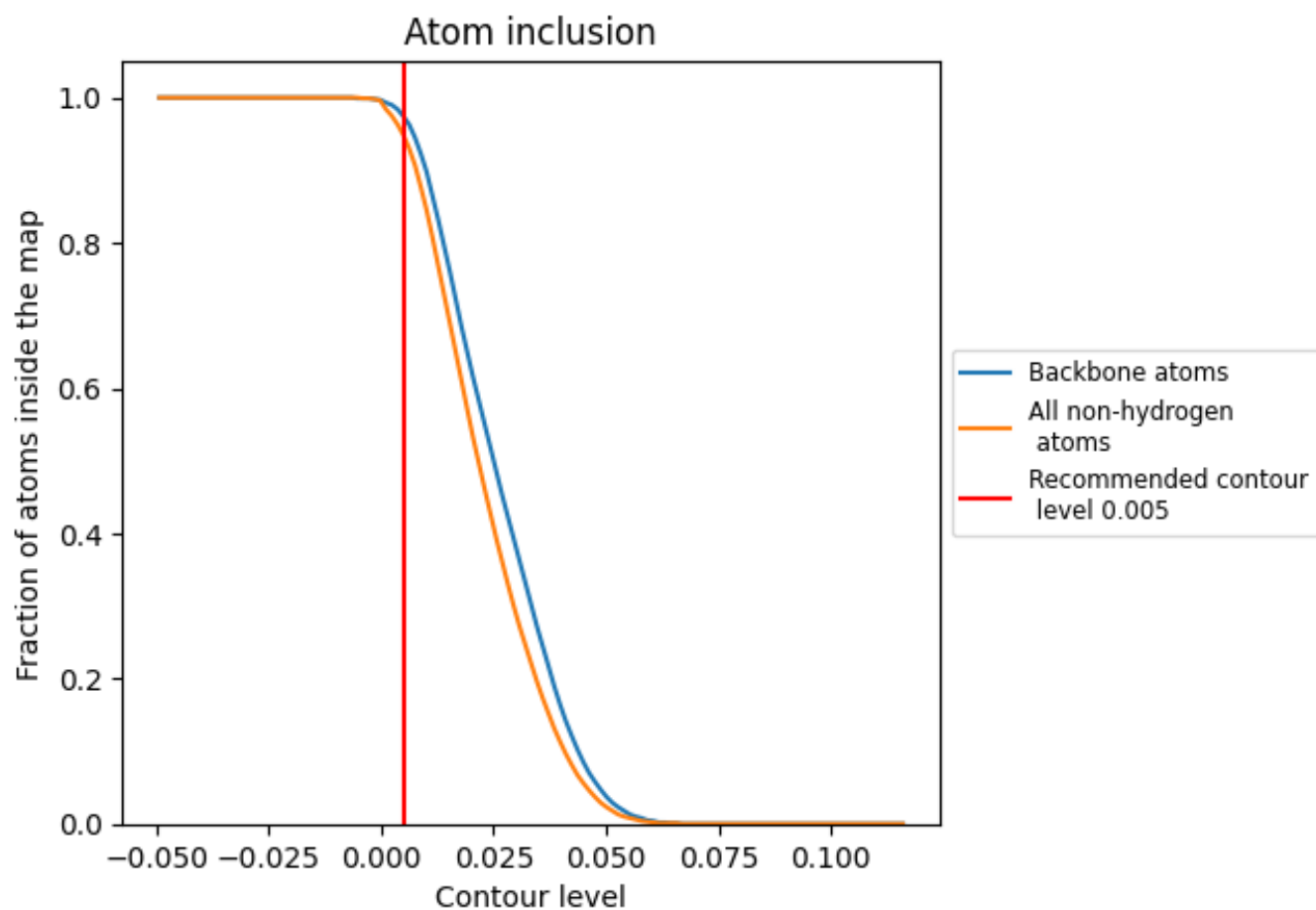
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.005).





























































9.4 Atom inclusion [i](#)



At the recommended contour level, 97% of all backbone atoms, 95% 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 (0.005) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9480	 0.5180
1	 0.9450	 0.5180
2	 0.9720	 0.5370
3	 0.9620	 0.5530
4	 0.9300	 0.4740
5	 0.9380	 0.5160
6	 0.9480	 0.5130
7	 0.9750	 0.5640
8	 0.9680	 0.5530
9	 0.9410	 0.5060
A	 0.9810	 0.5850
B	 0.9750	 0.5810
C	 0.9700	 0.5390
D	 0.9900	 0.5690
E	 0.9900	 0.5660
F	 0.9890	 0.5650
G	 0.9410	 0.5040
H	 0.9700	 0.5480
I	 0.9430	 0.5380
J	 0.9610	 0.5550
K	 0.9690	 0.5310
L	 0.9740	 0.5570
O	 0.9750	 0.5400
U	 0.9200	 0.4270
V	 0.9480	 0.4950
W	 0.8530	 0.3620
X	 0.8550	 0.3700
Y	 0.8830	 0.4070
Z	 0.9350	 0.4990
a	 0.8970	 0.4270

