



## wwPDB EM Validation Summary Report ⓘ

Nov 22, 2022 – 02:25 AM JST

PDB ID : 7DZ7  
EMDB ID : EMD-30925  
Title : State transition supercomplex PSI-LHCI-LHCII from double phosphatase mutant pph1;pbcp of green alga *Chlamydomonas reinhardtii*  
Authors : Pan, X.W.; Li, A.J.; Liu, Z.F.; Li, M.  
Deposited on : 2021-01-23  
Resolution : 2.84 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

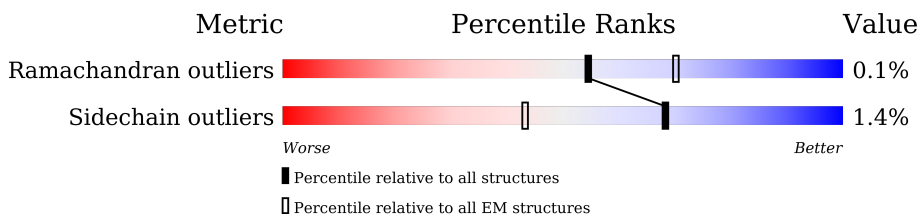
EMDB validation analysis : 0.0.1.dev43  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.9  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.31.3

# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:  
*ELECTRON MICROSCOPY*

The reported resolution of this entry is 2.84 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.



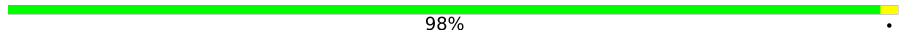







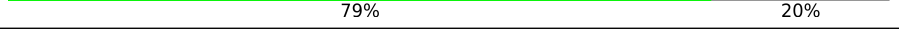

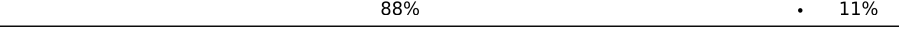
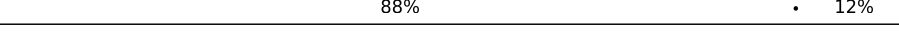

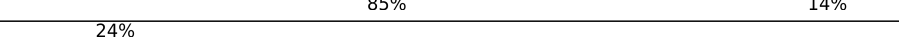




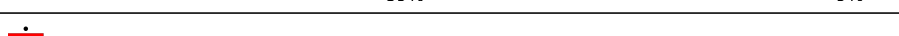

Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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

Mol	Chain	Length	Quality of chain
1	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	 98%
11	K	113	 75% 24%
12	L	196	 81% 19%
13	O	126	 76% 23%
14	1	228	 85% 15%
14	a	228	 84% 15%
15	2	246	 87% 12%
16	3	298	 73% 26%
17	4	264	 79% 20%
18	5	257	 87% 12%
19	6	257	 88% 11%
20	7	241	 88% 12%
21	8	243	 88% 11%
22	9	213	 85% 14%
23	W	249	 24% 88% 12%
23	X	249	 44% 87% 12%
24	U	257	 14% 83% 15%
24	Y	257	 33% 84% 14%
25	Z	256	 6% 89% 9%
26	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
27	CLA	1	602	X	-	-	-
27	CLA	1	603	X	-	-	-
27	CLA	1	604	X	-	-	-

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

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

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
27	CLA	7	602	X	-	-	-
27	CLA	7	603	X	-	-	-
27	CLA	7	604	X	-	-	-
27	CLA	7	607	X	-	-	-
27	CLA	7	608	X	-	-	-
27	CLA	7	609	X	-	-	-
27	CLA	7	610	X	-	-	-
27	CLA	7	611	X	-	-	-
27	CLA	7	612	X	-	-	-
27	CLA	7	613	X	-	-	-
27	CLA	7	614	X	-	-	-
27	CLA	7	615	X	-	-	-
27	CLA	7	616	X	-	-	-
27	CLA	8	601	X	-	-	-
27	CLA	8	602	X	-	-	-
27	CLA	8	603	X	-	-	-
27	CLA	8	604	X	-	-	-
27	CLA	8	606	X	-	-	-
27	CLA	8	607	X	-	-	-
27	CLA	8	608	X	-	-	-
27	CLA	8	609	X	-	-	-
27	CLA	8	610	X	-	-	-
27	CLA	8	611	X	-	-	-
27	CLA	8	612	X	-	-	-
27	CLA	8	613	X	-	-	-
27	CLA	8	614	X	-	-	-
27	CLA	8	616	X	-	-	-
27	CLA	9	601	X	-	-	-
27	CLA	9	603	X	-	-	-
27	CLA	9	604	X	-	-	-
27	CLA	9	606	X	-	-	-
27	CLA	9	609	X	-	-	-
27	CLA	9	610	X	-	-	-
27	CLA	9	611	X	-	-	-
27	CLA	9	612	X	-	-	-
27	CLA	9	613	X	-	-	-
27	CLA	9	614	X	-	-	-
27	CLA	A	801	X	-	-	-
27	CLA	A	802	X	-	-	-
27	CLA	A	803	X	-	-	-
27	CLA	A	804	X	-	-	-
27	CLA	A	806	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
27	CLA	A	807	X	-	-	-
27	CLA	A	809	X	-	-	-
27	CLA	A	810	X	-	-	-
27	CLA	A	811	X	-	-	-
27	CLA	A	812	X	-	-	-
27	CLA	A	813	X	-	-	-
27	CLA	A	814	X	-	-	-
27	CLA	A	815	X	-	-	-
27	CLA	A	816	X	-	-	-
27	CLA	A	819	X	-	-	-
27	CLA	A	820	X	-	-	-
27	CLA	A	821	X	-	-	-
27	CLA	A	822	X	-	-	-
27	CLA	A	823	X	-	-	-
27	CLA	A	824	X	-	-	-
27	CLA	A	825	X	-	-	-
27	CLA	A	826	X	-	-	-
27	CLA	A	827	X	-	-	-
27	CLA	A	828	X	-	-	-
27	CLA	A	829	X	-	-	-
27	CLA	A	830	X	-	-	-
27	CLA	A	831	X	-	-	-
27	CLA	A	832	X	-	-	-
27	CLA	A	833	X	-	-	-
27	CLA	A	834	X	-	-	-
27	CLA	A	836	X	-	-	-
27	CLA	A	838	X	-	-	-
27	CLA	A	839	X	-	-	-
27	CLA	A	841	X	-	-	-
27	CLA	A	842	X	-	-	-
27	CLA	A	843	X	-	-	-
27	CLA	A	845	X	-	-	-
27	CLA	A	854	X	-	-	-
27	CLA	B	802	X	-	-	-
27	CLA	B	803	X	-	-	-
27	CLA	B	804	X	-	-	-
27	CLA	B	805	X	-	-	-
27	CLA	B	806	X	-	-	-
27	CLA	B	808	X	-	-	-
27	CLA	B	809	X	-	-	-
27	CLA	B	810	X	-	-	-
27	CLA	B	811	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
27	CLA	B	812	X	-	-	-
27	CLA	B	813	X	-	-	-
27	CLA	B	814	X	-	-	-
27	CLA	B	815	X	-	-	-
27	CLA	B	816	X	-	-	-
27	CLA	B	817	X	-	-	-
27	CLA	B	819	X	-	-	-
27	CLA	B	820	X	-	-	-
27	CLA	B	821	X	-	-	-
27	CLA	B	823	X	-	-	-
27	CLA	B	824	X	-	-	-
27	CLA	B	826	X	-	-	-
27	CLA	B	827	X	-	-	-
27	CLA	B	828	X	-	-	-
27	CLA	B	829	X	-	-	-
27	CLA	B	830	X	-	-	-
27	CLA	B	831	X	-	-	-
27	CLA	B	833	X	-	-	-
27	CLA	B	834	X	-	-	-
27	CLA	B	835	X	-	-	-
27	CLA	B	836	X	-	-	-
27	CLA	B	839	X	-	-	-
27	CLA	B	840	X	-	-	-
27	CLA	B	841	X	-	-	-
27	CLA	F	301	X	-	-	-
27	CLA	G	203	X	-	-	-
27	CLA	G	204	X	-	-	-
27	CLA	H	202	X	-	-	-
27	CLA	J	101	X	-	-	-
27	CLA	K	201	X	-	-	-
27	CLA	K	204	X	-	-	-
27	CLA	K	206	X	-	-	-
27	CLA	L	302	X	-	-	-
27	CLA	L	304	X	-	-	-
27	CLA	L	306	X	-	-	-
27	CLA	L	307	X	-	-	-
27	CLA	O	2001	X	-	-	-
27	CLA	O	2002	X	-	-	-
27	CLA	O	2003	X	-	-	-
27	CLA	U	602	X	-	-	-
27	CLA	U	603	X	-	-	-
27	CLA	U	604	X	-	-	-

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

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

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

## 2 Entry composition [i](#)

There are 38 unique types of molecules in this entry. The entry contains 69647 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	a	194	Total	C	N	O	S	0	0
			1444	941	240	260	3		
14	1	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
			Total	C	N	O	S		
21	8	217	1649	1073	280	292	4	0	0

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
23	X	220	1675	1088	273	309	5	0	0
23	W	220	1671	1085	273	308	5	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
24	Y	220	1679	1086	273	315	5	0	0
24	U	219	1670	1080	272	313	5	0	0

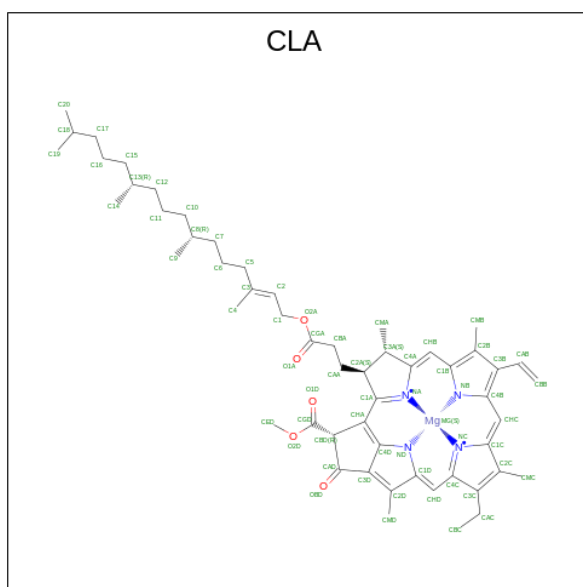
- Molecule 25 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	N	O	P	S		
25	Z	232	1780	1154	291	329	1	5	0	0

- Molecule 26 is a protein called Chlorophyll a-b binding protein, chloroplastic.

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

- Molecule 27 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
			Total	C	Mg	N	O	
27	A	1	Total 2669	C 2222	Mg 45	N 180	O 222	0
27	A	1	Total 2669	C 2222	Mg 45	N 180	O 222	0
27	A	1	Total 2669	C 2222	Mg 45	N 180	O 222	0
27	A	1	Total 2669	C 2222	Mg 45	N 180	O 222	0
27	A	1	Total 2669	C 2222	Mg 45	N 180	O 222	0
27	A	1	Total 2669	C 2222	Mg 45	N 180	O 222	0
27	A	1	Total 2669	C 2222	Mg 45	N 180	O 222	0
27	A	1	Total 2669	C 2222	Mg 45	N 180	O 222	0
27	A	1	Total 2669	C 2222	Mg 45	N 180	O 222	0
27	A	1	Total 2669	C 2222	Mg 45	N 180	O 222	0
27	A	1	Total 2669	C 2222	Mg 45	N 180	O 222	0
27	A	1	Total 2669	C 2222	Mg 45	N 180	O 222	0
27	A	1	Total 2669	C 2222	Mg 45	N 180	O 222	0
27	A	1	Total 2669	C 2222	Mg 45	N 180	O 222	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
27	A	1	Total 2669	C 2222	Mg 45	N 180	O 222	0
27	A	1	Total 2669	C 2222	Mg 45	N 180	O 222	0
27	A	1	Total 2669	C 2222	Mg 45	N 180	O 222	0
27	A	1	Total 2669	C 2222	Mg 45	N 180	O 222	0
27	A	1	Total 2669	C 2222	Mg 45	N 180	O 222	0
27	A	1	Total 2669	C 2222	Mg 45	N 180	O 222	0
27	A	1	Total 2669	C 2222	Mg 45	N 180	O 222	0
27	A	1	Total 2669	C 2222	Mg 45	N 180	O 222	0
27	A	1	Total 2669	C 2222	Mg 45	N 180	O 222	0
27	A	1	Total 2669	C 2222	Mg 45	N 180	O 222	0
27	A	1	Total 2669	C 2222	Mg 45	N 180	O 222	0
27	A	1	Total 2669	C 2222	Mg 45	N 180	O 222	0
27	A	1	Total 2669	C 2222	Mg 45	N 180	O 222	0
27	A	1	Total 2669	C 2222	Mg 45	N 180	O 222	0
27	A	1	Total 2669	C 2222	Mg 45	N 180	O 222	0
27	A	1	Total 2669	C 2222	Mg 45	N 180	O 222	0
27	A	1	Total 2669	C 2222	Mg 45	N 180	O 222	0
27	A	1	Total 2669	C 2222	Mg 45	N 180	O 222	0
27	A	1	Total 2669	C 2222	Mg 45	N 180	O 222	0
27	A	1	Total 2669	C 2222	Mg 45	N 180	O 222	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
27	A	1	Total 2669	C 2222	Mg 45	N 180	O 222	0
27	A	1	Total 2669	C 2222	Mg 45	N 180	O 222	0
27	A	1	Total 2669	C 2222	Mg 45	N 180	O 222	0
27	A	1	Total 2669	C 2222	Mg 45	N 180	O 222	0
27	A	1	Total 2669	C 2222	Mg 45	N 180	O 222	0
27	A	1	Total 2669	C 2222	Mg 45	N 180	O 222	0
27	A	1	Total 2669	C 2222	Mg 45	N 180	O 222	0
27	A	1	Total 2669	C 2222	Mg 45	N 180	O 222	0
27	A	1	Total 2669	C 2222	Mg 45	N 180	O 222	0
27	A	1	Total 2669	C 2222	Mg 45	N 180	O 222	0
27	A	1	Total 2669	C 2222	Mg 45	N 180	O 222	0
27	B	1	Total 2282	C 1895	Mg 40	N 160	O 187	0
27	B	1	Total 2282	C 1895	Mg 40	N 160	O 187	0
27	B	1	Total 2282	C 1895	Mg 40	N 160	O 187	0
27	B	1	Total 2282	C 1895	Mg 40	N 160	O 187	0
27	B	1	Total 2282	C 1895	Mg 40	N 160	O 187	0
27	B	1	Total 2282	C 1895	Mg 40	N 160	O 187	0
27	B	1	Total 2282	C 1895	Mg 40	N 160	O 187	0
27	B	1	Total 2282	C 1895	Mg 40	N 160	O 187	0
27	B	1	Total 2282	C 1895	Mg 40	N 160	O 187	0
27	B	1	Total 2282	C 1895	Mg 40	N 160	O 187	0
27	B	1	Total 2282	C 1895	Mg 40	N 160	O 187	0
27	B	1	Total 2282	C 1895	Mg 40	N 160	O 187	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
27	B	1	Total 2282	C 1895	Mg 40	N 160	O 187	0
27	B	1	Total 2282	C 1895	Mg 40	N 160	O 187	0
27	B	1	Total 2282	C 1895	Mg 40	N 160	O 187	0
27	B	1	Total 2282	C 1895	Mg 40	N 160	O 187	0
27	B	1	Total 2282	C 1895	Mg 40	N 160	O 187	0
27	B	1	Total 2282	C 1895	Mg 40	N 160	O 187	0
27	B	1	Total 2282	C 1895	Mg 40	N 160	O 187	0
27	B	1	Total 2282	C 1895	Mg 40	N 160	O 187	0
27	B	1	Total 2282	C 1895	Mg 40	N 160	O 187	0
27	B	1	Total 2282	C 1895	Mg 40	N 160	O 187	0
27	B	1	Total 2282	C 1895	Mg 40	N 160	O 187	0
27	B	1	Total 2282	C 1895	Mg 40	N 160	O 187	0
27	B	1	Total 2282	C 1895	Mg 40	N 160	O 187	0
27	B	1	Total 2282	C 1895	Mg 40	N 160	O 187	0
27	B	1	Total 2282	C 1895	Mg 40	N 160	O 187	0
27	B	1	Total 2282	C 1895	Mg 40	N 160	O 187	0
27	B	1	Total 2282	C 1895	Mg 40	N 160	O 187	0
27	B	1	Total 2282	C 1895	Mg 40	N 160	O 187	0
27	B	1	Total 2282	C 1895	Mg 40	N 160	O 187	0
27	B	1	Total 2282	C 1895	Mg 40	N 160	O 187	0
27	B	1	Total 2282	C 1895	Mg 40	N 160	O 187	0
27	B	1	Total 2282	C 1895	Mg 40	N 160	O 187	0
27	B	1	Total 2282	C 1895	Mg 40	N 160	O 187	0
27	B	1	Total 2282	C 1895	Mg 40	N 160	O 187	0
27	B	1	Total 2282	C 1895	Mg 40	N 160	O 187	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
27	B	1	Total 2282	C 1895	Mg 40	N 160	O 187	0
27	B	1	Total 2282	C 1895	Mg 40	N 160	O 187	0
27	B	1	Total 2282	C 1895	Mg 40	N 160	O 187	0
27	B	1	Total 2282	C 1895	Mg 40	N 160	O 187	0
27	B	1	Total 2282	C 1895	Mg 40	N 160	O 187	0
27	B	1	Total 2282	C 1895	Mg 40	N 160	O 187	0
27	B	1	Total 2282	C 1895	Mg 40	N 160	O 187	0
27	B	1	Total 2282	C 1895	Mg 40	N 160	O 187	0
27	F	1	Total 140	C 114	Mg 3	N 12	O 11	0
27	F	1	Total 140	C 114	Mg 3	N 12	O 11	0
27	F	1	Total 140	C 114	Mg 3	N 12	O 11	0
27	G	1	Total 87	C 69	Mg 2	N 8	O 8	0
27	G	1	Total 87	C 69	Mg 2	N 8	O 8	0
27	H	1	Total 104	C 86	Mg 2	N 8	O 8	0
27	H	1	Total 104	C 86	Mg 2	N 8	O 8	0
27	J	1	Total 42	C 34	Mg 1	N 4	O 3	0
27	K	1	Total 191	C 151	Mg 4	N 16	O 20	0
27	K	1	Total 191	C 151	Mg 4	N 16	O 20	0
27	K	1	Total 191	C 151	Mg 4	N 16	O 20	0
27	K	1	Total 191	C 151	Mg 4	N 16	O 20	0
27	L	1	Total 235	C 189	Mg 5	N 20	O 21	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
27	L	1	Total 235	C 189	Mg 5	N 20	O 21	0
27	L	1	Total 235	C 189	Mg 5	N 20	O 21	0
27	L	1	Total 235	C 189	Mg 5	N 20	O 21	0
27	L	1	Total 235	C 189	Mg 5	N 20	O 21	0
27	O	1	Total 116	C 92	Mg 3	N 12	O 9	0
27	O	1	Total 116	C 92	Mg 3	N 12	O 9	0
27	O	1	Total 116	C 92	Mg 3	N 12	O 9	0
27	a	1	Total 710	C 574	Mg 14	N 56	O 66	0
27	a	1	Total 710	C 574	Mg 14	N 56	O 66	0
27	a	1	Total 710	C 574	Mg 14	N 56	O 66	0
27	a	1	Total 710	C 574	Mg 14	N 56	O 66	0
27	a	1	Total 710	C 574	Mg 14	N 56	O 66	0
27	a	1	Total 710	C 574	Mg 14	N 56	O 66	0
27	a	1	Total 710	C 574	Mg 14	N 56	O 66	0
27	a	1	Total 710	C 574	Mg 14	N 56	O 66	0
27	a	1	Total 710	C 574	Mg 14	N 56	O 66	0
27	a	1	Total 710	C 574	Mg 14	N 56	O 66	0
27	a	1	Total 710	C 574	Mg 14	N 56	O 66	0
27	a	1	Total 710	C 574	Mg 14	N 56	O 66	0
27	a	1	Total 710	C 574	Mg 14	N 56	O 66	0
27	a	1	Total 710	C 574	Mg 14	N 56	O 66	0
27	a	1	Total 710	C 574	Mg 14	N 56	O 66	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
27	1	1	666	538	14	56	58	0
27	1	1	666	538	14	56	58	0
27	1	1	666	538	14	56	58	0
27	1	1	666	538	14	56	58	0
27	1	1	666	538	14	56	58	0
27	1	1	666	538	14	56	58	0
27	1	1	666	538	14	56	58	0
27	1	1	666	538	14	56	58	0
27	1	1	666	538	14	56	58	0
27	1	1	666	538	14	56	58	0
27	1	1	666	538	14	56	58	0
27	1	1	666	538	14	56	58	0
27	1	1	666	538	14	56	58	0
27	1	1	666	538	14	56	58	0
27	1	1	666	538	14	56	58	0
27	2	1	641	517	13	52	59	0
27	2	1	641	517	13	52	59	0
27	2	1	641	517	13	52	59	0
27	2	1	641	517	13	52	59	0
27	2	1	641	517	13	52	59	0
27	2	1	641	517	13	52	59	0
27	2	1	641	517	13	52	59	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
27	2	1	641	517	13	52	59	0
27	2	1	641	517	13	52	59	0
27	2	1	641	517	13	52	59	0
27	2	1	641	517	13	52	59	0
27	2	1	641	517	13	52	59	0
27	2	1	641	517	13	52	59	0
27	2	1	641	517	13	52	59	0
27	3	1	724	595	14	56	59	0
27	3	1	724	595	14	56	59	0
27	3	1	724	595	14	56	59	0
27	3	1	724	595	14	56	59	0
27	3	1	724	595	14	56	59	0
27	3	1	724	595	14	56	59	0
27	3	1	724	595	14	56	59	0
27	3	1	724	595	14	56	59	0
27	3	1	724	595	14	56	59	0
27	3	1	724	595	14	56	59	0
27	3	1	724	595	14	56	59	0
27	3	1	724	595	14	56	59	0
27	3	1	724	595	14	56	59	0
27	3	1	724	595	14	56	59	0
27	3	1	724	595	14	56	59	0
27	4	1	778	636	15	60	67	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
27	4	1	778	636	15	60	67	0
27	4	1	778	636	15	60	67	0
27	4	1	778	636	15	60	67	0
27	4	1	778	636	15	60	67	0
27	4	1	778	636	15	60	67	0
27	4	1	778	636	15	60	67	0
27	4	1	778	636	15	60	67	0
27	4	1	778	636	15	60	67	0
27	4	1	778	636	15	60	67	0
27	4	1	778	636	15	60	67	0
27	4	1	778	636	15	60	67	0
27	4	1	778	636	15	60	67	0
27	4	1	778	636	15	60	67	0
27	4	1	778	636	15	60	67	0
27	4	1	778	636	15	60	67	0
27	4	1	778	636	15	60	67	0
27	4	1	778	636	15	60	67	0
27	4	1	778	636	15	60	67	0
27	5	1	878	718	17	68	75	0
27	5	1	878	718	17	68	75	0
27	5	1	878	718	17	68	75	0
27	5	1	878	718	17	68	75	0
27	5	1	878	718	17	68	75	0
27	5	1	878	718	17	68	75	0
27	5	1	878	718	17	68	75	0
27	5	1	878	718	17	68	75	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
27	5	1	878	718	17	68	75	0
27	5	1	878	718	17	68	75	0
27	5	1	878	718	17	68	75	0
27	5	1	878	718	17	68	75	0
27	5	1	878	718	17	68	75	0
27	5	1	878	718	17	68	75	0
27	5	1	878	718	17	68	75	0
27	5	1	878	718	17	68	75	0
27	5	1	878	718	17	68	75	0
27	5	1	878	718	17	68	75	0
27	5	1	878	718	17	68	75	0
27	5	1	878	718	17	68	75	0
27	6	1	903	743	17	68	75	0
27	6	1	903	743	17	68	75	0
27	6	1	903	743	17	68	75	0
27	6	1	903	743	17	68	75	0
27	6	1	903	743	17	68	75	0
27	6	1	903	743	17	68	75	0
27	6	1	903	743	17	68	75	0
27	6	1	903	743	17	68	75	0
27	6	1	903	743	17	68	75	0
27	6	1	903	743	17	68	75	0
27	6	1	903	743	17	68	75	0
27	6	1	903	743	17	68	75	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
27	6	1	903	743	17	68	75	0
27	6	1	903	743	17	68	75	0
27	6	1	903	743	17	68	75	0
27	6	1	903	743	17	68	75	0
27	6	1	903	743	17	68	75	0
27	6	1	903	743	17	68	75	0
27	7	1	756	614	15	60	67	0
27	7	1	756	614	15	60	67	0
27	7	1	756	614	15	60	67	0
27	7	1	756	614	15	60	67	0
27	7	1	756	614	15	60	67	0
27	7	1	756	614	15	60	67	0
27	7	1	756	614	15	60	67	0
27	7	1	756	614	15	60	67	0
27	7	1	756	614	15	60	67	0
27	7	1	756	614	15	60	67	0
27	7	1	756	614	15	60	67	0
27	7	1	756	614	15	60	67	0
27	7	1	756	614	15	60	67	0
27	7	1	756	614	15	60	67	0
27	7	1	756	614	15	60	67	0
27	7	1	756	614	15	60	67	0
27	7	1	756	614	15	60	67	0
27	7	1	756	614	15	60	67	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
27	8	1	724	590	14	56	64	0
27	8	1	724	590	14	56	64	0
27	8	1	724	590	14	56	64	0
27	8	1	724	590	14	56	64	0
27	8	1	724	590	14	56	64	0
27	8	1	724	590	14	56	64	0
27	8	1	724	590	14	56	64	0
27	8	1	724	590	14	56	64	0
27	8	1	724	590	14	56	64	0
27	8	1	724	590	14	56	64	0
27	8	1	724	590	14	56	64	0
27	8	1	724	590	14	56	64	0
27	8	1	724	590	14	56	64	0
27	8	1	724	590	14	56	64	0
27	8	1	724	590	14	56	64	0
27	8	1	724	590	14	56	64	0
27	8	1	724	590	14	56	64	0
27	8	1	724	590	14	56	64	0
27	9	1	595	481	12	48	54	0
27	9	1	595	481	12	48	54	0
27	9	1	595	481	12	48	54	0
27	9	1	595	481	12	48	54	0
27	9	1	595	481	12	48	54	0
27	9	1	595	481	12	48	54	0
27	9	1	595	481	12	48	54	0
27	9	1	595	481	12	48	54	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
27	9	1	Total 595	C 481	Mg 12	N 48	O 54	0
27	9	1	Total 595	C 481	Mg 12	N 48	O 54	0
27	9	1	Total 595	C 481	Mg 12	N 48	O 54	0
27	9	1	Total 595	C 481	Mg 12	N 48	O 54	0
27	9	1	Total 595	C 481	Mg 12	N 48	O 54	0
27	X	1	Total 436	C 360	Mg 8	N 32	O 36	0
27	X	1	Total 436	C 360	Mg 8	N 32	O 36	0
27	X	1	Total 436	C 360	Mg 8	N 32	O 36	0
27	X	1	Total 436	C 360	Mg 8	N 32	O 36	0
27	X	1	Total 436	C 360	Mg 8	N 32	O 36	0
27	X	1	Total 436	C 360	Mg 8	N 32	O 36	0
27	X	1	Total 436	C 360	Mg 8	N 32	O 36	0
27	X	1	Total 436	C 360	Mg 8	N 32	O 36	0
27	X	1	Total 436	C 360	Mg 8	N 32	O 36	0
27	Y	1	Total 429	C 351	Mg 8	N 32	O 38	0
27	Y	1	Total 429	C 351	Mg 8	N 32	O 38	0
27	Y	1	Total 429	C 351	Mg 8	N 32	O 38	0
27	Y	1	Total 429	C 351	Mg 8	N 32	O 38	0
27	Y	1	Total 429	C 351	Mg 8	N 32	O 38	0
27	Y	1	Total 429	C 351	Mg 8	N 32	O 38	0
27	Y	1	Total 429	C 351	Mg 8	N 32	O 38	0
27	Y	1	Total 429	C 351	Mg 8	N 32	O 38	0

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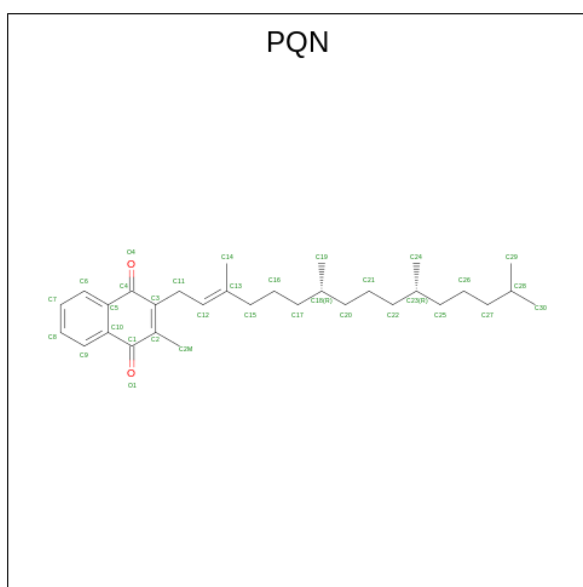
Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
27	Z	1	496	416	8	32	40	0
27	Z	1	496	416	8	32	40	0
27	Z	1	496	416	8	32	40	0
27	Z	1	496	416	8	32	40	0
27	Z	1	496	416	8	32	40	0
27	Z	1	496	416	8	32	40	0
27	Z	1	496	416	8	32	40	0
27	Z	1	496	416	8	32	40	0
27	Z	1	496	416	8	32	40	0
27	U	1	401	328	8	32	33	0
27	U	1	401	328	8	32	33	0
27	U	1	401	328	8	32	33	0
27	U	1	401	328	8	32	33	0
27	U	1	401	328	8	32	33	0
27	U	1	401	328	8	32	33	0
27	U	1	401	328	8	32	33	0
27	U	1	401	328	8	32	33	0
27	U	1	401	328	8	32	33	0
27	U	1	401	328	8	32	33	0
27	V	1	415	337	8	32	38	0
27	V	1	415	337	8	32	38	0
27	V	1	415	337	8	32	38	0
27	V	1	415	337	8	32	38	0
27	V	1	415	337	8	32	38	0

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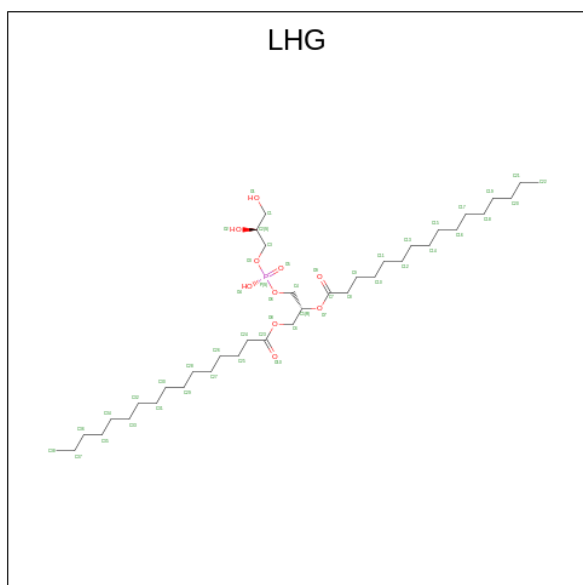
Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
27	V	1	Total 415	C 337	Mg 8	N 32	O 38	0
27	V	1	Total 415	C 337	Mg 8	N 32	O 38	0
27	V	1	Total 415	C 337	Mg 8	N 32	O 38	0
27	W	1	Total 426	C 346	Mg 8	N 32	O 40	0
27	W	1	Total 426	C 346	Mg 8	N 32	O 40	0
27	W	1	Total 426	C 346	Mg 8	N 32	O 40	0
27	W	1	Total 426	C 346	Mg 8	N 32	O 40	0
27	W	1	Total 426	C 346	Mg 8	N 32	O 40	0
27	W	1	Total 426	C 346	Mg 8	N 32	O 40	0
27	W	1	Total 426	C 346	Mg 8	N 32	O 40	0
27	W	1	Total 426	C 346	Mg 8	N 32	O 40	0
27	W	1	Total 426	C 346	Mg 8	N 32	O 40	0
27	W	1	Total 426	C 346	Mg 8	N 32	O 40	0

- Molecule 28 is PHYLLOQUINONE (three-letter code: PQN) (formula: C<sub>31</sub>H<sub>46</sub>O<sub>2</sub>).



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

- Molecule 29 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula:  $C_{38}H_{75}O_{10}P$ ).



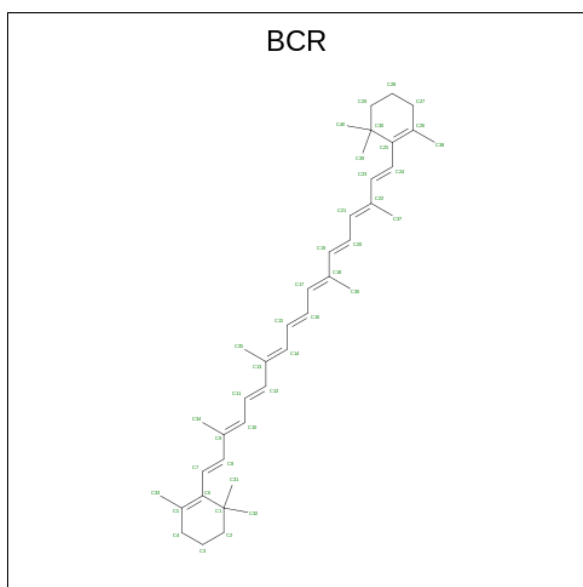
Mol	Chain	Residues	Atoms				AltConf
29	A	1	Total	C	O	P	0
			79	57	20	2	
29	A	1	Total	C	O	P	0
			79	57	20	2	
29	B	1	Total	C	O	P	0
			87	65	20	2	
29	B	1	Total	C	O	P	0
			87	65	20	2	
29	H	1	Total	C	O	P	0
			49	38	10	1	
29	O	1	Total	C	O	P	0
			36	25	10	1	
29	a	1	Total	C	O	P	0
			43	32	10	1	
29	1	1	Total	C	O	P	0
			49	38	10	1	
29	2	1	Total	C	O	P	0
			36	25	10	1	

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
29	3	1	94	72	20	2	0
29	3	1	94	72	20	2	0
29	4	1	49	38	10	1	0
29	5	1	98	76	20	2	0
29	5	1	98	76	20	2	0
29	6	1	48	37	10	1	0
29	7	1	37	26	10	1	0
29	8	1	89	67	20	2	0
29	8	1	89	67	20	2	0
29	9	1	128	95	30	3	0
29	9	1	128	95	30	3	0
29	9	1	128	95	30	3	0
29	X	1	49	38	10	1	0
29	Y	1	49	38	10	1	0
29	Z	1	49	38	10	1	0
29	U	1	49	38	10	1	0
29	V	1	48	37	10	1	0
29	W	1	44	33	10	1	0

- Molecule 30 is BETA-CAROTENE (three-letter code: BCR) (formula: C<sub>40</sub>H<sub>56</sub>).



Mol	Chain	Residues	Atoms	AltConf
30	A	1	Total C 240 240	0
30	A	1	Total C 240 240	0
30	A	1	Total C 240 240	0
30	A	1	Total C 240 240	0
30	A	1	Total C 240 240	0
30	A	1	Total C 240 240	0
30	B	1	Total C 400 400	0
30	B	1	Total C 400 400	0
30	B	1	Total C 400 400	0
30	B	1	Total C 400 400	0
30	B	1	Total C 400 400	0
30	B	1	Total C 400 400	0
30	B	1	Total C 400 400	0
30	B	1	Total C 400 400	0

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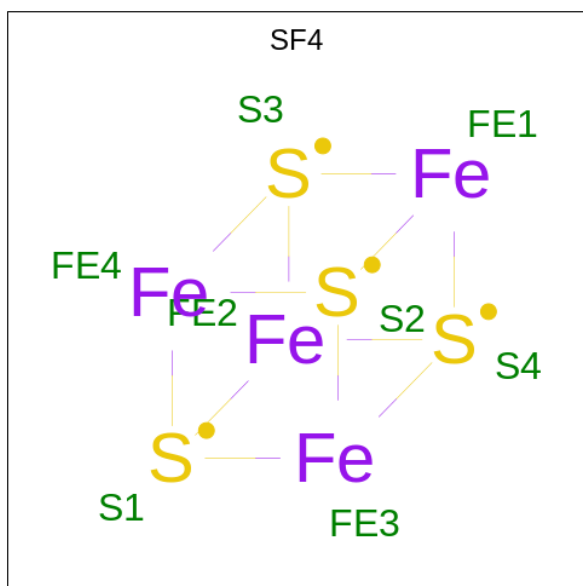
Mol	Chain	Residues	Atoms		AltConf
30	B	1	Total 400	C 400	0
30	B	1	Total 400	C 400	0
30	F	1	Total 40	C 40	0
30	G	1	Total 40	C 40	0
30	J	1	Total 40	C 40	0
30	K	1	Total 80	C 80	0
30	K	1	Total 80	C 80	0
30	L	1	Total 160	C 160	0
30	L	1	Total 160	C 160	0
30	L	1	Total 160	C 160	0
30	L	1	Total 160	C 160	0
30	O	1	Total 80	C 80	0
30	O	1	Total 80	C 80	0
30	a	1	Total 40	C 40	0
30	1	1	Total 40	C 40	0
30	2	1	Total 40	C 40	0
30	3	1	Total 120	C 120	0
30	3	1	Total 120	C 120	0
30	3	1	Total 120	C 120	0
30	4	1	Total 40	C 40	0
30	5	1	Total 40	C 40	0

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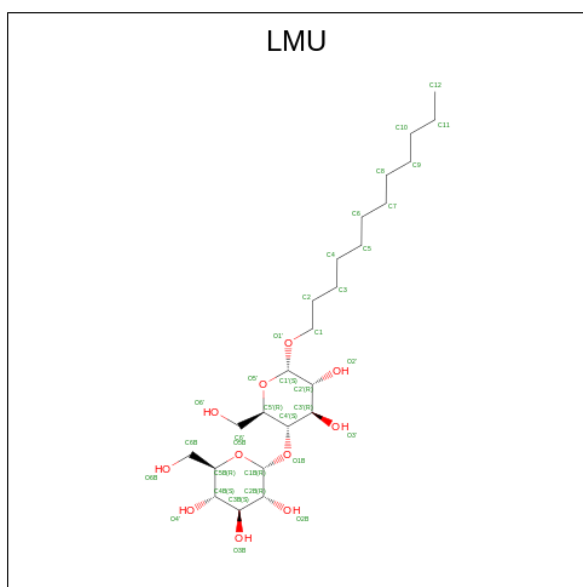
Mol	Chain	Residues	Atoms	AltConf
30	6	1	Total C 40 40	0
30	7	1	Total C 80 80	0
30	7	1	Total C 80 80	0
30	8	1	Total C 40 40	0
30	9	1	Total C 40 40	0

- Molecule 31 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe<sub>4</sub>S<sub>4</sub>).



Mol	Chain	Residues	Atoms	AltConf
31	A	1	Total Fe S 8 4 4	0
31	C	1	Total Fe S 16 8 8	0
31	C	1	Total Fe S 16 8 8	0

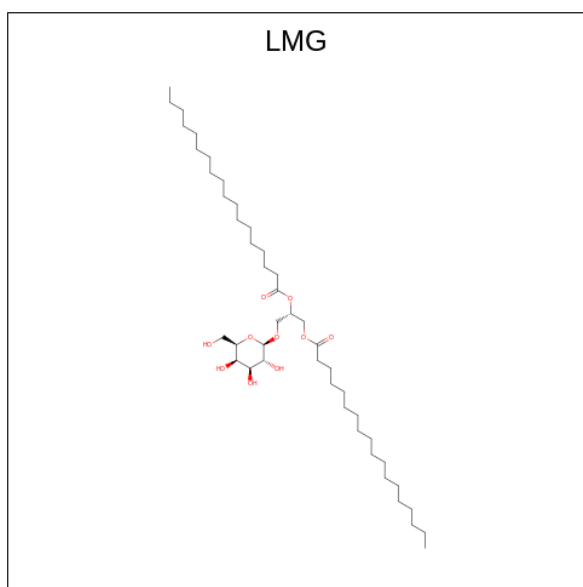
- Molecule 32 is DODECYL-ALPHA-D-MALTOSIDE (three-letter code: LMU) (formula: C<sub>24</sub>H<sub>46</sub>O<sub>11</sub>).



Mol	Chain	Residues	Atoms			AltConf
32	A	1	Total	C	O	0
			69	48	21	
32	A	1	Total	C	O	0
			69	48	21	
32	K	1	Total	C	O	0
			35	24	11	
32	1	1	Total	C	O	0
			35	24	11	
32	5	1	Total	C	O	0
			65	43	22	
32	5	1	Total	C	O	0
			65	43	22	
32	8	1	Total	C	O	0
			35	24	11	

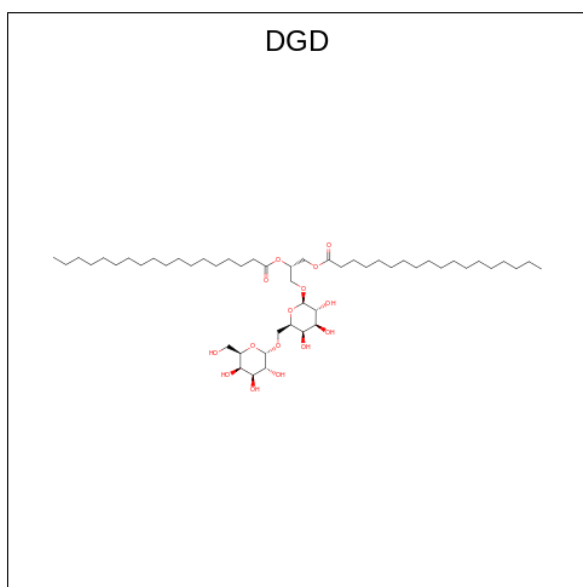
- Molecule 33 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: LMG) (formula: C<sub>45</sub>H<sub>86</sub>O<sub>10</sub>).





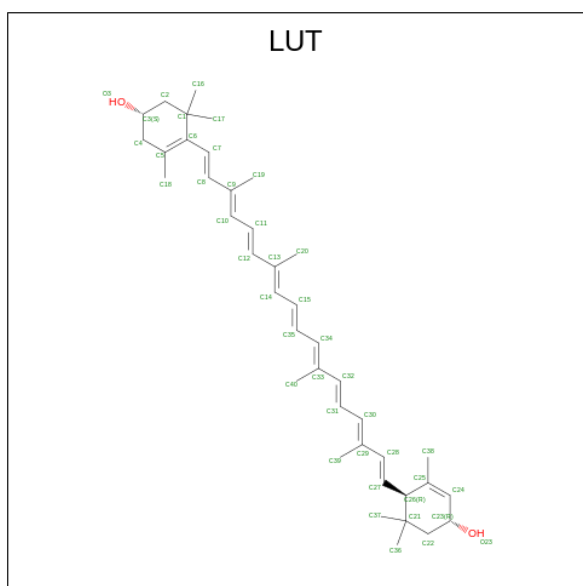
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
33	A	1	40	30	10	0
33	H	1	55	45	10	0
33	J	1	82	62	20	0
33	J	1	82	62	20	0
33	L	1	37	27	10	0
33	4	1	80	60	20	0
33	4	1	80	60	20	0
33	5	1	40	30	10	0
33	8	1	46	36	10	0
33	9	1	55	45	10	0
33	V	1	41	31	10	0

- Molecule 34 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (three-letter code: DGD) (formula:  $C_{51}H_{96}O_{15}$ ).



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

- Molecule 35 is (3R,3'R,6S)-4,5-DIDEHYDRO-5,6-DIHYDRO-BETA,BETA-CAROTENE-3,3'-DIOL (three-letter code: LUT) (formula:  $C_{40}H_{56}O_2$ ).



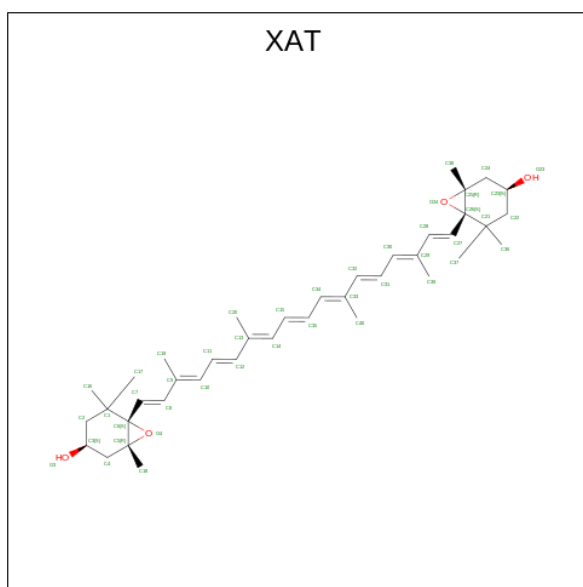
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
35	a	1	42	40	2	0
35	1	1	42	40	2	0

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Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
35	2	1	42	40	2	0
35	3	1	42	40	2	0
35	4	1	42	40	2	0
35	5	1	42	40	2	0
35	6	1	42	40	2	0
35	7	1	42	40	2	0
35	8	1	42	40	2	0
35	9	1	42	40	2	0
35	X	1	84	80	4	0
35	X	1	84	80	4	0
35	Y	1	84	80	4	0
35	Y	1	84	80	4	0
35	Z	1	84	80	4	0
35	Z	1	84	80	4	0
35	U	1	84	80	4	0
35	U	1	84	80	4	0
35	V	1	84	80	4	0
35	V	1	84	80	4	0
35	W	1	84	80	4	0
35	W	1	84	80	4	0

- Molecule 36 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: C<sub>40</sub>H<sub>56</sub>O<sub>4</sub>).



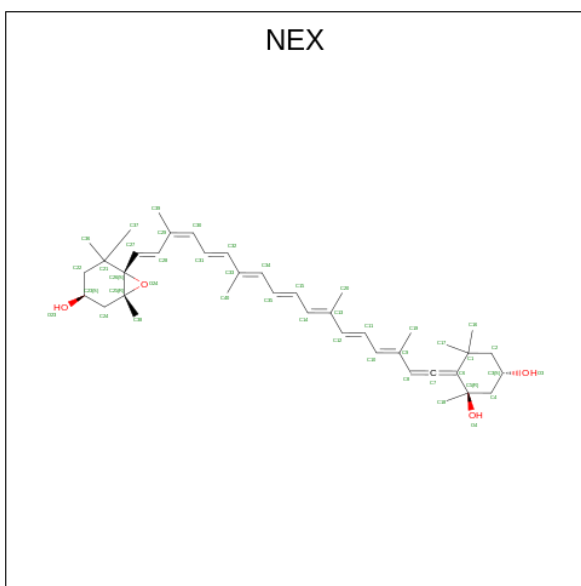
Mol	Chain	Residues	Atoms			AltConf
36	a	1	Total	C	O	0
			44	40	4	
36	1	1	Total	C	O	0
			44	40	4	
36	2	1	Total	C	O	0
			44	40	4	
36	3	1	Total	C	O	0
			44	40	4	
36	4	1	Total	C	O	0
			44	40	4	
36	5	1	Total	C	O	0
			44	40	4	
36	6	1	Total	C	O	0
			44	40	4	
36	7	1	Total	C	O	0
			44	40	4	
36	8	1	Total	C	O	0
			44	40	4	
36	9	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	

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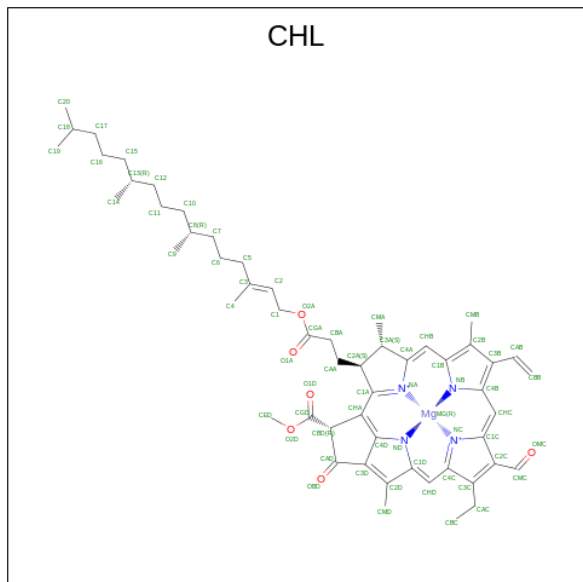
Mol	Chain	Residues	Atoms			AltConf
36	V	1	Total	C	O	0
			44	40	4	
36	W	1	Total	C	O	0
			44	40	4	

- Molecule 37 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: C<sub>40</sub>H<sub>56</sub>O<sub>4</sub>).



Mol	Chain	Residues	Atoms			AltConf
37	5	1	Total	C	O	0
			44	40	4	
37	6	1	Total	C	O	0
			44	40	4	
37	X	1	Total	C	O	0
			44	40	4	
37	Y	1	Total	C	O	0
			43	40	3	
37	Z	1	Total	C	O	0
			44	40	4	
37	U	1	Total	C	O	0
			44	40	4	
37	V	1	Total	C	O	0
			44	40	4	
37	W	1	Total	C	O	0
			44	40	4	

- Molecule 38 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
38	X	1	Total	C	Mg	N	O	0
			354	290	6	24	34	
38	X	1	Total	C	Mg	N	O	0
			354	290	6	24	34	
38	X	1	Total	C	Mg	N	O	0
			354	290	6	24	34	
38	X	1	Total	C	Mg	N	O	0
			354	290	6	24	34	
38	X	1	Total	C	Mg	N	O	0
			354	290	6	24	34	
38	X	1	Total	C	Mg	N	O	0
			354	290	6	24	34	
38	Y	1	Total	C	Mg	N	O	0
			335	271	6	24	34	
38	Y	1	Total	C	Mg	N	O	0
			335	271	6	24	34	
38	Y	1	Total	C	Mg	N	O	0
			335	271	6	24	34	
38	Y	1	Total	C	Mg	N	O	0
			335	271	6	24	34	
38	Y	1	Total	C	Mg	N	O	0
			335	271	6	24	34	
38	Y	1	Total	C	Mg	N	O	0
			335	271	6	24	34	

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
38	Z	1	Total 338	C 274	Mg 6	N 24	O 34	0
38	Z	1	Total 338	C 274	Mg 6	N 24	O 34	0
38	Z	1	Total 338	C 274	Mg 6	N 24	O 34	0
38	Z	1	Total 338	C 274	Mg 6	N 24	O 34	0
38	Z	1	Total 338	C 274	Mg 6	N 24	O 34	0
38	Z	1	Total 338	C 274	Mg 6	N 24	O 34	0
38	U	1	Total 303	C 243	Mg 6	N 24	O 30	0
38	U	1	Total 303	C 243	Mg 6	N 24	O 30	0
38	U	1	Total 303	C 243	Mg 6	N 24	O 30	0
38	U	1	Total 303	C 243	Mg 6	N 24	O 30	0
38	U	1	Total 303	C 243	Mg 6	N 24	O 30	0
38	U	1	Total 303	C 243	Mg 6	N 24	O 30	0
38	U	1	Total 303	C 243	Mg 6	N 24	O 30	0
38	V	1	Total 309	C 247	Mg 6	N 24	O 32	0
38	V	1	Total 309	C 247	Mg 6	N 24	O 32	0
38	V	1	Total 309	C 247	Mg 6	N 24	O 32	0
38	V	1	Total 309	C 247	Mg 6	N 24	O 32	0
38	V	1	Total 309	C 247	Mg 6	N 24	O 32	0
38	V	1	Total 309	C 247	Mg 6	N 24	O 32	0
38	W	1	Total 336	C 270	Mg 6	N 24	O 36	0
38	W	1	Total 336	C 270	Mg 6	N 24	O 36	0
38	W	1	Total 336	C 270	Mg 6	N 24	O 36	0

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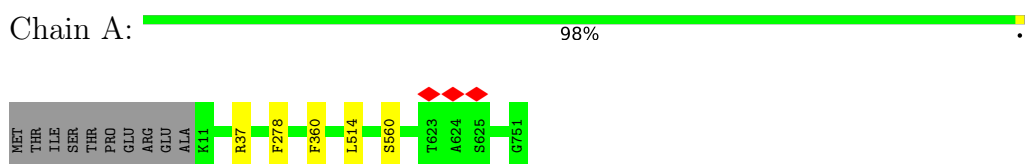
Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
38	W	1	Total 336	C 270	Mg 6	N 24	O 36	0
38	W	1	Total 336	C 270	Mg 6	N 24	O 36	0
38	W	1	Total 336	C 270	Mg 6	N 24	O 36	0



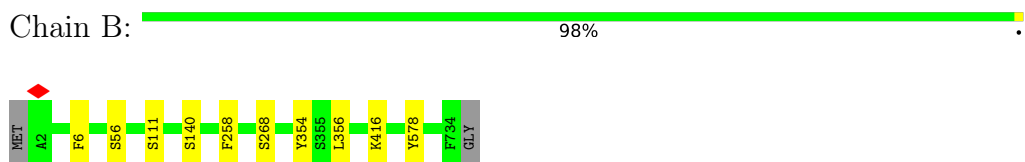
### 3 Residue-property plots [i](#)

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.

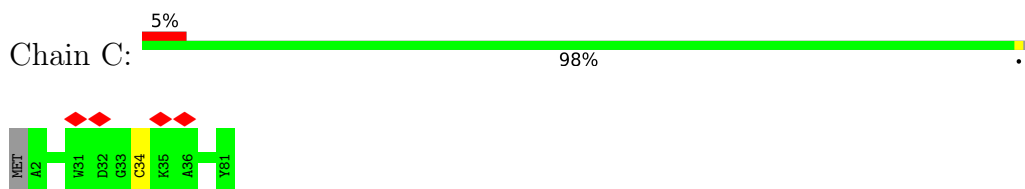
- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1



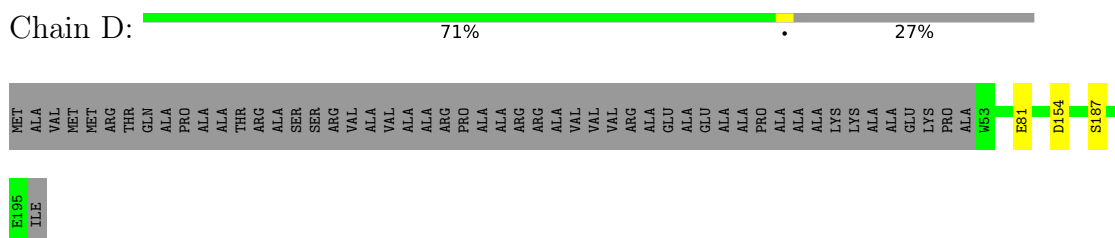
- Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2



- Molecule 3: Photosystem I iron-sulfur center

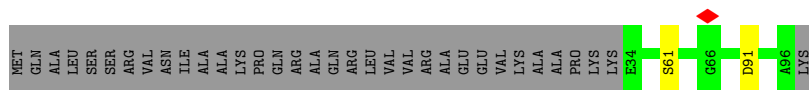


- Molecule 4: Photosystem I reaction center subunit II, chloroplastic

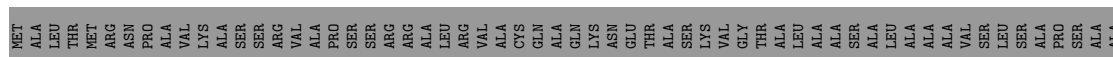


- Molecule 5: Photosystem I reaction center subunit IV, chloroplastic

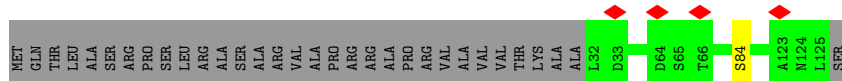
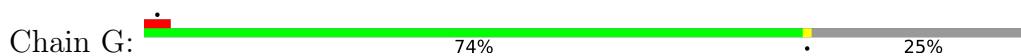




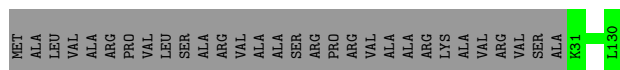
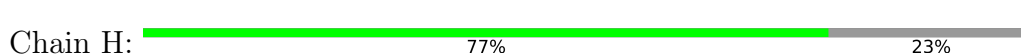
- Molecule 6: Photosystem I reaction center subunit III, chloroplastic



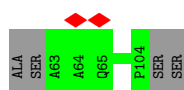
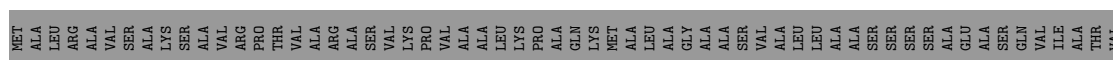
- Molecule 7: Photosystem I reaction center subunit V, chloroplastic



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



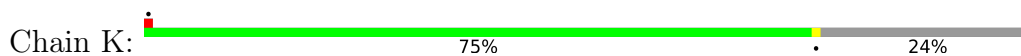
- Molecule 9: Photosystem I reaction center subunit VIII

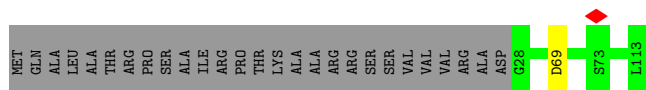


- Molecule 10: Photosystem I reaction center subunit IX

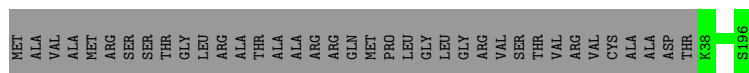
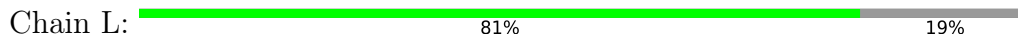


- Molecule 11: Photosystem I reaction center subunit psaK, chloroplastic

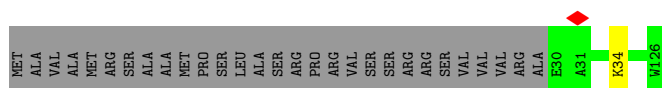




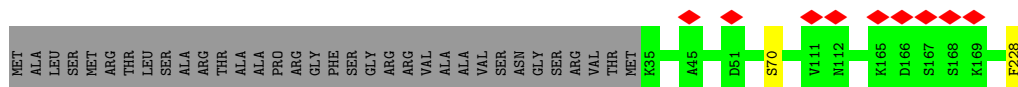
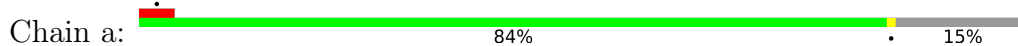
• Molecule 12: PSI subunit V



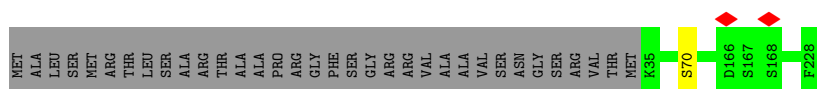
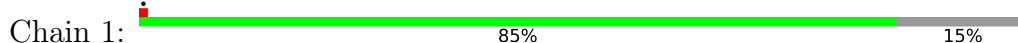
• Molecule 13: Photosystem I subunit O



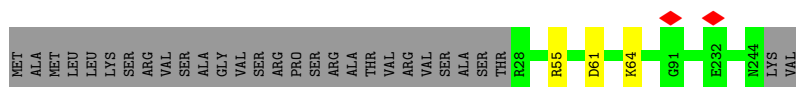
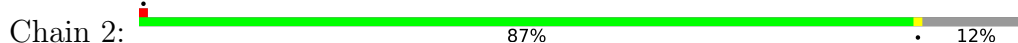
• Molecule 14: Chlorophyll a-b binding protein, chloroplastic



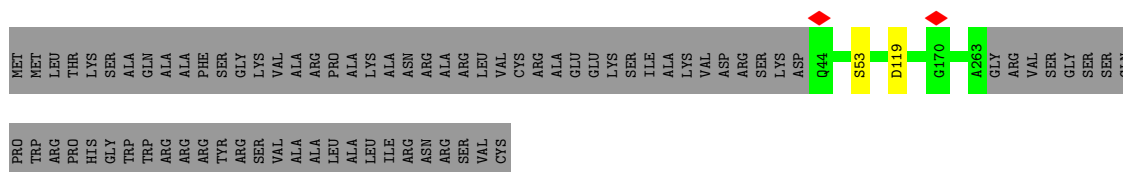
• Molecule 14: Chlorophyll a-b binding protein, chloroplastic



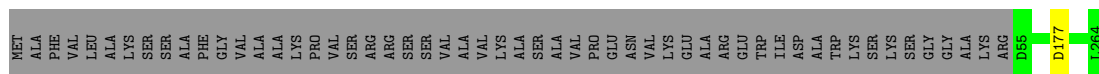
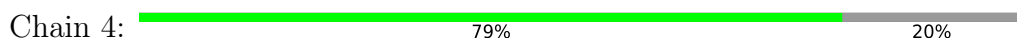
• Molecule 15: Chlorophyll a-b binding protein, chloroplastic



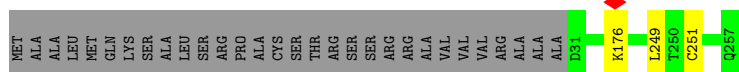
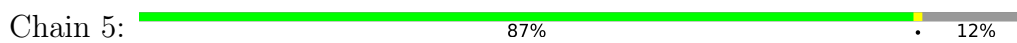
• Molecule 16: Chlorophyll a-b binding protein, chloroplastic



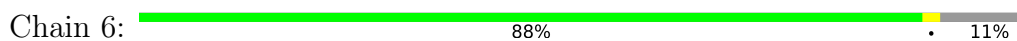
- Molecule 17: Chlorophyll a-b binding protein, chloroplastic



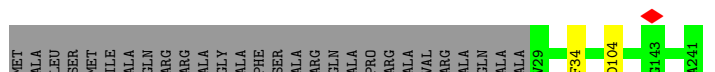
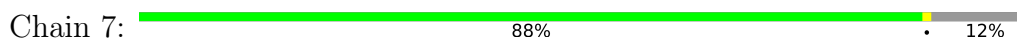
- Molecule 18: Chlorophyll a-b binding protein, chloroplastic



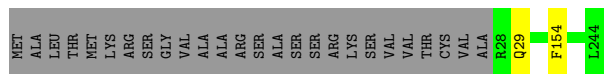
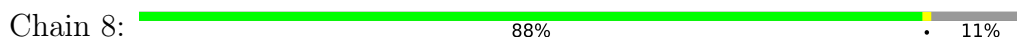
- Molecule 19: Chlorophyll a-b binding protein, chloroplastic



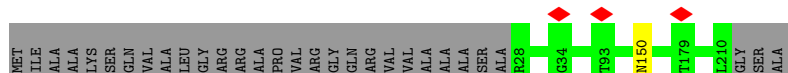
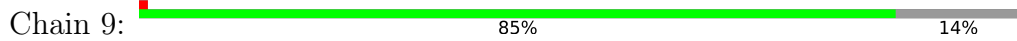
- Molecule 20: Chlorophyll a-b binding protein, chloroplastic



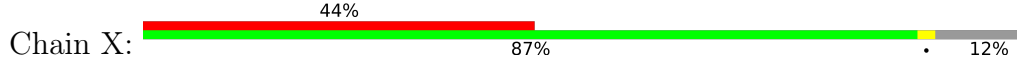
- Molecule 21: Chlorophyll a-b binding protein, chloroplastic

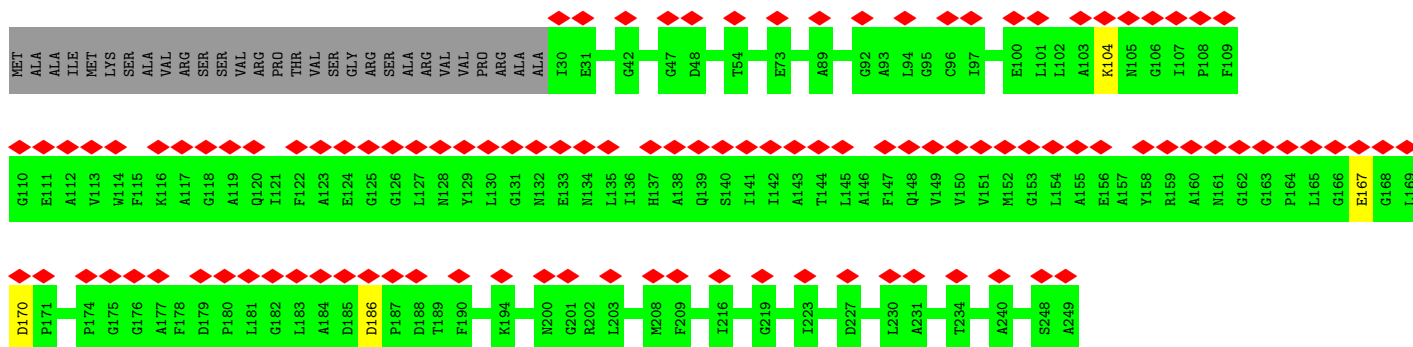


- Molecule 22: Chlorophyll a-b binding protein, chloroplastic

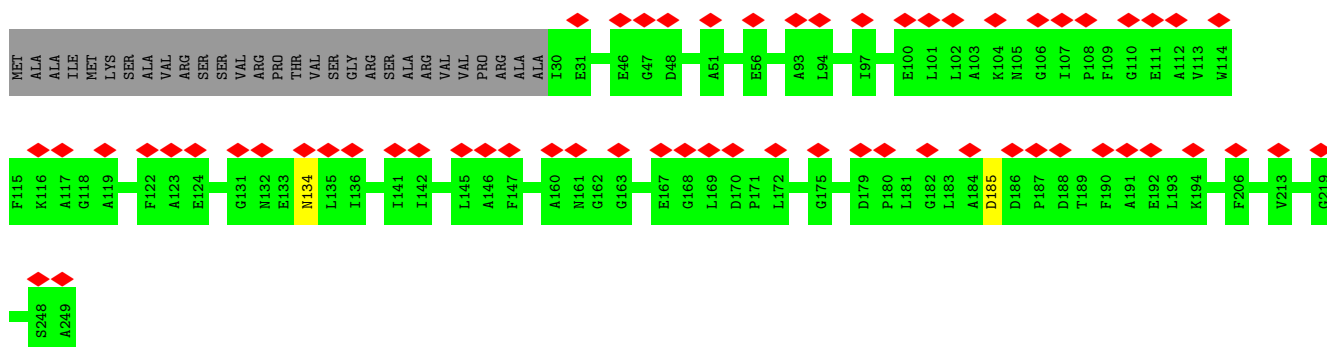
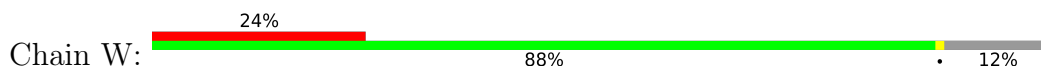


- Molecule 23: Chlorophyll a-b binding protein, chloroplastic

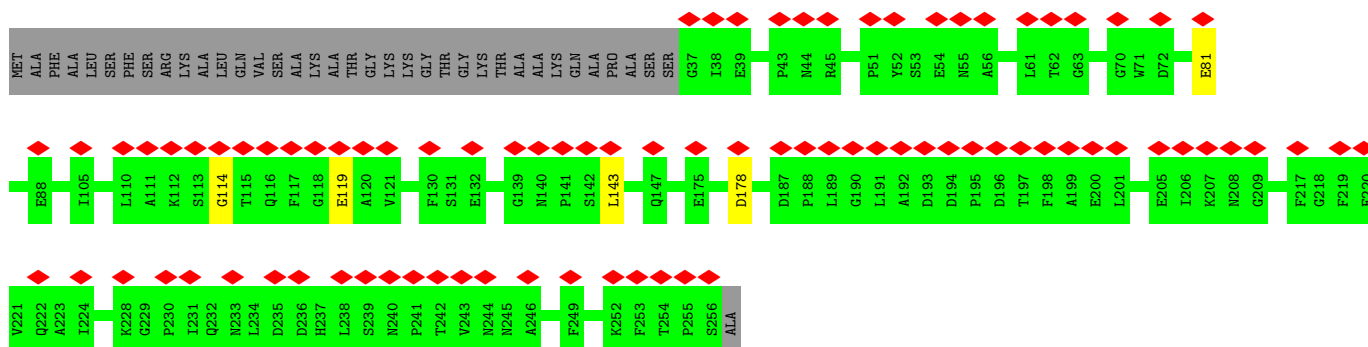
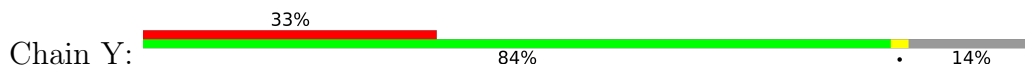




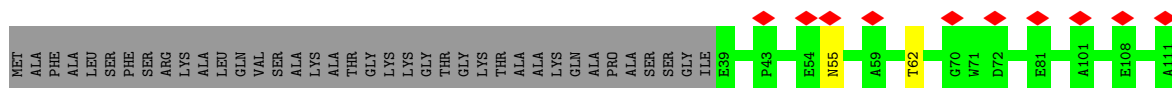
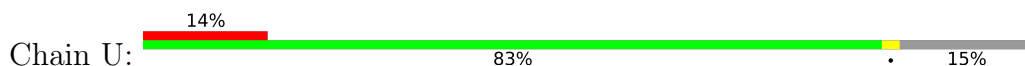
• Molecule 23: Chlorophyll a-b binding protein, chloroplastic

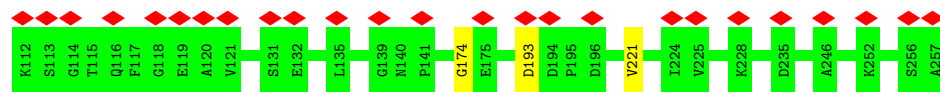


• Molecule 24: Chlorophyll a-b binding protein, chloroplastic

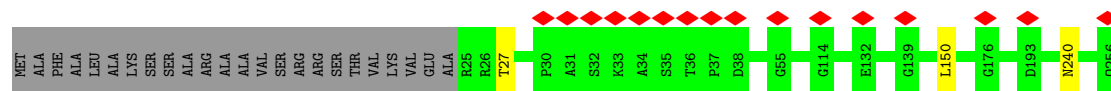
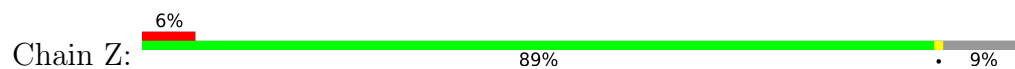


• Molecule 24: Chlorophyll a-b binding protein, chloroplastic

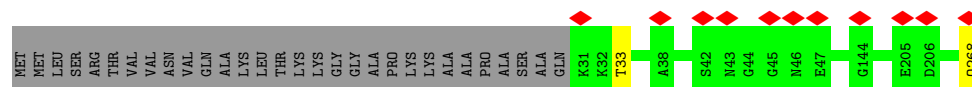
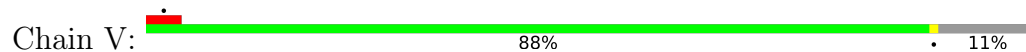




- Molecule 25: Chlorophyll a-b binding protein, chloroplastic



- Molecule 26: Chlorophyll a-b binding protein, chloroplastic



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	56601	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	0.216	Depositor
Minimum map value	-0.116	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.02	Depositor
Map size ( $\text{\AA}$ )	480.0, 480.0, 480.0	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	1.0, 1.0, 1.0	Depositor

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: TPO, BCR, LHG, CHL, LMU, LUT, CLA, SF4, DGD, XAT, PQN, NEX, 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	0.38	0/6015	0.43	0/8201
2	B	0.37	0/6036	0.44	0/8242
3	C	0.35	0/610	0.48	0/826
4	D	0.34	0/1152	0.47	0/1556
5	E	0.36	0/506	0.43	0/689
6	F	0.33	0/1291	0.43	0/1747
7	G	0.29	0/714	0.44	0/972
8	H	0.33	0/788	0.45	0/1059
9	I	0.38	0/329	0.43	0/456
10	J	0.37	0/349	0.42	0/478
11	K	0.30	0/587	0.46	0/795
12	L	0.36	0/1190	0.44	0/1628
13	O	0.33	0/784	0.45	0/1069
14	1	0.36	0/1490	0.45	0/2028
14	a	0.37	0/1490	0.46	0/2028
15	2	0.31	0/1730	0.44	0/2353
16	3	0.36	0/1726	0.42	0/2342
17	4	0.31	0/1686	0.41	0/2300
18	5	0.33	0/1829	0.43	0/2492
19	6	0.34	0/1833	0.43	0/2505
20	7	0.36	0/1701	0.41	0/2310
21	8	0.34	0/1700	0.43	0/2315
22	9	0.30	0/1444	0.45	0/1964
23	W	0.46	0/1721	0.47	0/2341
23	X	0.31	0/1725	0.50	0/2348
24	U	0.48	0/1718	0.48	0/2338
24	Y	0.31	0/1727	0.48	0/2350
25	Z	0.26	0/1822	0.42	0/2474
26	V	0.46	0/1856	0.46	0/2518
All	All	0.36	0/47549	0.44	0/64724



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%)	720 (97%)	19 (3%)	0	100	100
2	B	731/735 (100%)	714 (98%)	17 (2%)	0	100	100
3	C	78/81 (96%)	74 (95%)	4 (5%)	0	100	100
4	D	141/196 (72%)	135 (96%)	6 (4%)	0	100	100
5	E	61/97 (63%)	59 (97%)	2 (3%)	0	100	100
6	F	163/227 (72%)	155 (95%)	8 (5%)	0	100	100
7	G	92/126 (73%)	86 (94%)	6 (6%)	0	100	100
8	H	98/130 (75%)	92 (94%)	6 (6%)	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%)	79 (94%)	5 (6%)	0	100	100
12	L	157/196 (80%)	150 (96%)	7 (4%)	0	100	100
13	O	95/126 (75%)	87 (92%)	8 (8%)	0	100	100
14	1	192/228 (84%)	185 (96%)	7 (4%)	0	100	100
14	a	192/228 (84%)	185 (96%)	7 (4%)	0	100	100
15	2	215/246 (87%)	202 (94%)	13 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
16	3	218/298 (73%)	213 (98%)	5 (2%)	0	100	100
17	4	208/264 (79%)	201 (97%)	7 (3%)	0	100	100
18	5	225/257 (88%)	212 (94%)	13 (6%)	0	100	100
19	6	228/257 (89%)	206 (90%)	22 (10%)	0	100	100
20	7	211/241 (88%)	201 (95%)	10 (5%)	0	100	100
21	8	215/243 (88%)	209 (97%)	6 (3%)	0	100	100
22	9	181/213 (85%)	167 (92%)	14 (8%)	0	100	100
23	W	218/249 (88%)	204 (94%)	14 (6%)	0	100	100
23	X	218/249 (88%)	204 (94%)	13 (6%)	1 (0%)	29	51
24	U	217/257 (84%)	197 (91%)	19 (9%)	1 (0%)	29	51
24	Y	218/257 (85%)	202 (93%)	15 (7%)	1 (0%)	29	51
25	Z	229/256 (90%)	223 (97%)	6 (3%)	0	100	100
26	V	235/268 (88%)	220 (94%)	15 (6%)	0	100	100
All	All	5938/6936 (86%)	5655 (95%)	280 (5%)	3 (0%)	54	75

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
23	X	167	GLU
24	Y	114	GLY
24	U	174	GLY

### 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%)	596 (99%)	5 (1%)	81	90
2	B	596/597 (100%)	586 (98%)	10 (2%)	60	80
3	C	69/70 (99%)	68 (99%)	1 (1%)	67	83
4	D	120/152 (79%)	117 (98%)	3 (2%)	47	71

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	E	54/81 (67%)	52 (96%)	2 (4%)	34	59
6	F	127/169 (75%)	124 (98%)	3 (2%)	49	72
7	G	70/94 (74%)	69 (99%)	1 (1%)	67	83
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%)	36 (97%)	1 (3%)	44	69
11	K	59/80 (74%)	58 (98%)	1 (2%)	60	80
12	L	121/148 (82%)	121 (100%)	0	100	100
13	O	78/101 (77%)	77 (99%)	1 (1%)	69	84
14	1	137/162 (85%)	136 (99%)	1 (1%)	84	91
14	a	137/162 (85%)	135 (98%)	2 (2%)	65	82
15	2	173/198 (87%)	170 (98%)	3 (2%)	60	80
16	3	167/230 (73%)	165 (99%)	2 (1%)	71	85
17	4	165/205 (80%)	164 (99%)	1 (1%)	86	93
18	5	184/206 (89%)	181 (98%)	3 (2%)	62	81
19	6	184/203 (91%)	180 (98%)	4 (2%)	52	75
20	7	164/181 (91%)	162 (99%)	2 (1%)	71	85
21	8	163/183 (89%)	161 (99%)	2 (1%)	71	85
22	9	140/159 (88%)	139 (99%)	1 (1%)	84	91
23	W	163/187 (87%)	161 (99%)	2 (1%)	71	85
23	X	165/187 (88%)	162 (98%)	3 (2%)	59	78
24	U	168/194 (87%)	164 (98%)	4 (2%)	49	72
24	Y	170/194 (88%)	166 (98%)	4 (2%)	49	72
25	Z	178/195 (91%)	176 (99%)	2 (1%)	73	86
26	V	178/201 (89%)	177 (99%)	1 (1%)	86	93
All	All	4682/5364 (87%)	4617 (99%)	65 (1%)	68	83

5 of 65 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
25	Z	240	ASN
24	U	62	THR
7	G	84	SER

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Mol	Chain	Res	Type
6	F	182	ASP
24	U	193	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 20 such sidechains are listed below:

Mol	Chain	Res	Type
24	Y	140	ASN
24	U	169	ASN
26	V	158	GLN
26	V	156	HIS
10	J	30	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](#)

2 non-standard protein/DNA/RNA residues 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
25	TPO	Z	27	25	8,10,11	1.09	0	10,14,16	1.63	1 (10%)
26	TPO	V	33	26	8,10,11	1.54	1 (12%)	10,14,16	1.77	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. '2' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	TPO	Z	27	25	-	0/9/11/13	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	TPO	V	33	26	-	5/9/11/13	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	V	33	TPO	P-O1P	3.17	1.60	1.50

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	V	33	TPO	P-OG1-CB	-4.60	109.31	123.21
25	Z	27	TPO	P-OG1-CB	-4.57	109.42	123.21
26	V	33	TPO	CG2-CB-CA	-2.26	108.70	113.16

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
26	V	33	TPO	N-CA-CB-CG2
26	V	33	TPO	CB-OG1-P-O1P
26	V	33	TPO	CB-OG1-P-O2P
26	V	33	TPO	CB-OG1-P-O3P
26	V	33	TPO	O-C-CA-CB

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates [i](#)

There are no monosaccharides 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$
27	CLA	Z	612	25	65,73,73	1.52	5 (7%)	76,113,113	1.25	7 (9%)
35	LUT	U	1620	-	42,43,43	0.90	1 (2%)	51,60,60	1.83	10 (19%)
27	CLA	Y	614	-	48,56,73	1.80	6 (12%)	55,92,113	1.38	8 (14%)
30	BCR	B	845	-	41,41,41	0.81	0	56,56,56	2.13	22 (39%)
27	CLA	Z	613	25	65,73,73	1.54	6 (9%)	76,113,113	1.25	9 (11%)
30	BCR	8	621	-	41,41,41	0.83	0	56,56,56	2.52	17 (30%)
27	CLA	A	809	1	65,73,73	1.45	9 (13%)	76,113,113	1.34	7 (9%)
27	CLA	4	616	17	43,51,73	1.93	7 (16%)	54,87,113	1.50	8 (14%)
27	CLA	a	611	29	37,46,73	2.01	8 (21%)	46,81,113	1.57	9 (19%)
27	CLA	F	304	6	41,49,73	1.86	8 (19%)	47,84,113	1.47	7 (14%)
27	CLA	3	612	16	43,51,73	1.86	8 (18%)	49,86,113	1.48	7 (14%)
27	CLA	a	606	-	43,52,73	1.81	8 (18%)	48,87,113	1.42	6 (12%)
27	CLA	A	824	-	65,73,73	1.48	8 (12%)	76,113,113	1.34	9 (11%)
27	CLA	U	613	24	59,67,73	1.57	9 (15%)	68,105,113	1.35	9 (13%)
27	CLA	Z	603	-	65,73,73	1.48	6 (9%)	76,113,113	1.32	6 (7%)
27	CLA	4	612	17	40,49,73	1.87	8 (20%)	45,84,113	1.53	7 (15%)
27	CLA	3	607	16	56,64,73	1.63	8 (14%)	69,102,113	1.47	11 (15%)
27	CLA	V	603	-	45,53,73	1.75	9 (20%)	52,89,113	1.56	6 (11%)
29	LHG	a	620	27	42,42,48	0.98	2 (4%)	45,48,54	1.01	2 (4%)
30	BCR	O	2004	-	41,41,41	0.77	0	56,56,56	2.38	19 (33%)
27	CLA	A	803	-	65,73,73	1.49	9 (13%)	76,113,113	1.34	6 (7%)
27	CLA	A	840	-	52,60,73	1.66	8 (15%)	60,97,113	1.48	9 (15%)
27	CLA	B	810	-	64,72,73	1.51	8 (12%)	74,111,113	1.27	7 (9%)
27	CLA	B	805	-	65,73,73	1.47	8 (12%)	76,113,113	1.36	8 (10%)
27	CLA	6	601	19	65,73,73	1.50	9 (13%)	76,113,113	1.32	9 (11%)
27	CLA	Z	602	25	60,68,73	1.61	6 (10%)	70,107,113	1.25	7 (10%)
27	CLA	U	612	24	43,51,73	1.81	8 (18%)	49,86,113	1.46	6 (12%)
27	CLA	8	611	29	42,50,73	1.83	9 (21%)	48,85,113	1.39	7 (14%)
29	LHG	U	2630	27	48,48,48	0.92	2 (4%)	51,54,54	0.92	2 (3%)
27	CLA	B	821	-	43,51,73	1.91	8 (18%)	48,86,113	1.49	9 (18%)
27	CLA	A	827	-	58,66,73	1.56	9 (15%)	67,104,113	1.34	8 (11%)
27	CLA	7	616	20	43,51,73	1.90	7 (16%)	54,87,113	1.49	9 (16%)
27	CLA	A	806	-	65,73,73	1.46	8 (12%)	76,113,113	1.42	9 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
35	LUT	Y	1620	-	42,43,43	0.80	1 (2%)	51,60,60	1.94	11 (21%)
30	BCR	B	849	-	41,41,41	0.72	0	56,56,56	2.49	24 (42%)
38	CHL	X	608	-	66,74,74	1.95	16 (24%)	73,114,114	2.62	19 (26%)
27	CLA	2	606	-	45,53,73	1.78	8 (17%)	52,89,113	1.55	7 (13%)
27	CLA	Z	604	-	57,65,73	1.64	5 (8%)	66,103,113	1.33	7 (10%)
29	LHG	O	2631	-	35,35,48	1.08	2 (5%)	38,41,54	1.07	3 (7%)
30	BCR	3	621	-	41,41,41	0.81	0	56,56,56	1.79	14 (25%)
30	BCR	A	850	-	41,41,41	0.78	1 (2%)	56,56,56	2.16	22 (39%)
27	CLA	K	201	11	45,53,73	1.81	7 (15%)	52,89,113	1.37	7 (13%)
27	CLA	5	613	18	64,72,73	1.51	8 (12%)	74,111,113	1.26	7 (9%)
27	CLA	K	206	11	45,53,73	1.82	7 (15%)	52,89,113	1.47	7 (13%)
27	CLA	V	612	26	45,53,73	1.78	10 (22%)	52,89,113	1.53	9 (17%)
38	CHL	W	605	23	46,54,74	2.29	14 (30%)	49,90,114	2.91	22 (44%)
30	BCR	B	853	-	41,41,41	0.75	0	56,56,56	1.70	13 (23%)
27	CLA	7	603	-	43,52,73	1.79	9 (20%)	49,88,113	1.58	7 (14%)
30	BCR	L	308	-	41,41,41	0.82	2 (4%)	56,56,56	2.31	27 (48%)
27	CLA	B	825	-	49,57,73	1.69	8 (16%)	55,93,113	1.42	9 (16%)
27	CLA	1	609	14	40,48,73	1.93	8 (20%)	50,83,113	1.60	10 (20%)
29	LHG	A	847	27	29,29,48	1.17	2 (6%)	32,35,54	1.04	2 (6%)
35	LUT	2	619	-	42,43,43	0.82	1 (2%)	51,60,60	1.84	11 (21%)
35	LUT	1	617	-	42,43,43	0.83	1 (2%)	51,60,60	1.77	14 (27%)
27	CLA	9	610	22	57,65,73	1.61	8 (14%)	66,103,113	1.32	10 (15%)
27	CLA	2	604	-	42,50,73	1.86	8 (19%)	48,85,113	1.39	7 (14%)
27	CLA	B	816	-	54,62,73	1.62	8 (14%)	62,99,113	1.36	8 (12%)
27	CLA	3	617	16	39,48,73	1.88	9 (23%)	44,83,113	1.56	7 (15%)
27	CLA	8	608	-	51,59,73	1.68	9 (17%)	59,96,113	1.43	8 (13%)
30	BCR	F	305	-	41,41,41	0.81	0	56,56,56	2.29	26 (46%)
27	CLA	X	603	-	62,70,73	1.58	7 (11%)	72,109,113	1.29	8 (11%)
30	BCR	9	621	-	41,41,41	0.76	0	56,56,56	2.08	18 (32%)
35	LUT	W	1621	-	42,43,43	0.96	2 (4%)	51,60,60	1.70	12 (23%)
31	SF4	C	101	3	0,12,12	-	-	-	-	-
27	CLA	B	833	-	65,73,73	1.51	9 (13%)	76,113,113	1.27	11 (14%)
27	CLA	6	617	-	45,53,73	1.78	8 (17%)	52,89,113	1.42	7 (13%)
38	CHL	Z	609	25	66,74,74	2.01	15 (22%)	73,114,114	2.55	22 (30%)
27	CLA	7	614	-	42,50,73	1.85	9 (21%)	48,85,113	1.36	7 (14%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
38	CHL	V	609	26	61,69,74	2.05	15 (24%)	67,108,114	2.66	20 (29%)
30	BCR	L	309	-	41,41,41	0.68	0	56,56,56	1.97	18 (32%)
27	CLA	B	819	-	55,63,73	1.64	9 (16%)	64,101,113	1.37	8 (12%)
27	CLA	1	613	-	65,73,73	1.51	8 (12%)	76,113,113	1.23	9 (11%)
35	LUT	X	1620	-	42,43,43	0.80	0	51,60,60	1.93	10 (19%)
27	CLA	a	608	-	43,52,73	1.84	8 (18%)	49,88,113	1.42	8 (16%)
27	CLA	5	617	-	50,58,73	1.68	10 (20%)	58,95,113	1.39	9 (15%)
27	CLA	1	616	14	43,51,73	1.86	7 (16%)	54,87,113	1.60	9 (16%)
30	BCR	L	305	-	41,41,41	0.75	0	56,56,56	2.07	23 (41%)
30	BCR	K	202	-	41,41,41	0.83	0	56,56,56	2.16	18 (32%)
27	CLA	3	604	-	65,73,73	1.48	8 (12%)	76,113,113	1.29	8 (10%)
29	LHG	W	2630	27	43,43,48	0.96	2 (4%)	46,49,54	0.96	2 (4%)
30	BCR	A	851	-	41,41,41	0.88	1 (2%)	56,56,56	2.08	21 (37%)
27	CLA	4	610	17	61,69,73	1.52	8 (13%)	71,108,113	1.31	9 (12%)
27	CLA	4	618	17	39,48,73	1.94	7 (17%)	48,83,113	1.62	9 (18%)
35	LUT	a	617	-	42,43,43	0.82	1 (2%)	51,60,60	1.77	14 (27%)
27	CLA	8	613	21	65,73,73	1.53	9 (13%)	76,113,113	1.25	8 (10%)
31	SF4	C	102	3	0,12,12	-	-	-	-	-
27	CLA	8	602	21	60,68,73	1.55	9 (15%)	70,107,113	1.31	8 (11%)
30	BCR	2	623	-	41,41,41	0.78	0	56,56,56	2.33	21 (37%)
35	LUT	Z	1620	-	42,43,43	0.75	1 (2%)	51,60,60	1.78	12 (23%)
27	CLA	L	306	-	39,48,73	1.89	8 (20%)	44,83,113	1.55	7 (15%)
27	CLA	V	610	26	62,70,73	1.52	10 (16%)	72,109,113	1.33	8 (11%)
27	CLA	A	822	-	65,73,73	1.49	8 (12%)	76,113,113	1.47	10 (13%)
27	CLA	A	832	-	50,58,73	1.75	9 (18%)	58,95,113	1.38	10 (17%)
27	CLA	W	602	23	60,68,73	1.53	9 (15%)	70,107,113	1.37	6 (8%)
38	CHL	Z	601	25	66,74,74	1.91	15 (22%)	73,114,114	2.65	20 (27%)
27	CLA	A	826	-	64,72,73	1.47	7 (10%)	74,111,113	1.43	6 (8%)
38	CHL	W	606	-	46,54,74	2.25	16 (34%)	49,90,114	4.69	24 (48%)
38	CHL	X	606	-	44,52,74	2.28	14 (31%)	46,87,114	2.90	21 (45%)
28	PQN	B	842	-	34,34,34	3.39	10 (29%)	42,45,45	1.59	6 (14%)
29	LHG	5	625	-	48,48,48	0.93	2 (4%)	51,54,54	1.06	3 (5%)
27	CLA	4	607	-	45,53,73	1.78	9 (20%)	52,89,113	1.45	7 (13%)
36	XAT	9	620	-	39,47,47	0.92	1 (2%)	54,74,74	2.41	20 (37%)
35	LUT	5	620	-	42,43,43	0.84	1 (2%)	51,60,60	1.97	11 (21%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
27	CLA	U	604	-	49,56,73	1.79	10 (20%)	50,91,113	1.47	8 (16%)
27	CLA	A	818	-	60,68,73	1.52	7 (11%)	70,107,113	1.39	8 (11%)
27	CLA	9	614	-	45,53,73	1.80	8 (17%)	52,89,113	1.47	9 (17%)
38	CHL	Z	605	25	44,52,74	2.31	15 (34%)	46,87,114	2.86	23 (50%)
30	BCR	A	849	-	41,41,41	0.82	0	56,56,56	2.24	19 (33%)
27	CLA	B	828	-	65,73,73	1.48	9 (13%)	76,113,113	1.27	9 (11%)
27	CLA	2	614	-	41,50,73	1.86	8 (19%)	46,85,113	1.41	7 (15%)
27	CLA	4	611	29	42,50,73	1.84	8 (19%)	48,85,113	1.45	7 (14%)
27	CLA	6	616	19	65,73,73	1.48	8 (12%)	76,113,113	1.40	8 (10%)
36	XAT	6	621	-	39,47,47	0.87	0	54,74,74	2.39	20 (37%)
27	CLA	1	612	14	45,53,73	1.78	7 (15%)	52,89,113	1.45	7 (13%)
27	CLA	5	601	18	56,64,73	1.59	8 (14%)	65,102,113	1.46	9 (13%)
27	CLA	B	820	-	50,58,73	1.67	8 (16%)	58,95,113	1.46	9 (15%)
27	CLA	A	833	-	45,53,73	1.79	9 (20%)	52,89,113	1.51	8 (15%)
35	LUT	V	1620	-	42,43,43	0.91	1 (2%)	51,60,60	1.65	11 (21%)
27	CLA	2	603	15	43,52,73	1.87	8 (18%)	49,88,113	1.48	6 (12%)
30	BCR	4	621	-	41,41,41	0.78	1 (2%)	56,56,56	2.47	24 (42%)
34	DGD	B	850	-	63,63,67	0.84	2 (3%)	77,77,81	1.03	4 (5%)
27	CLA	B	823	-	45,53,73	1.84	9 (20%)	52,89,113	1.34	8 (15%)
27	CLA	4	606	-	39,48,73	1.92	7 (17%)	44,83,113	1.43	7 (15%)
27	CLA	5	612	18	40,49,73	1.86	7 (17%)	45,84,113	1.48	6 (13%)
27	CLA	W	610	23	55,63,73	1.65	9 (16%)	64,101,113	1.27	8 (12%)
30	BCR	G	205	-	41,41,41	0.79	0	56,56,56	1.96	15 (26%)
27	CLA	U	614	-	42,50,73	1.83	9 (21%)	48,85,113	1.45	7 (14%)
33	LMG	L	2631	-	37,37,55	1.10	2 (5%)	45,45,63	1.11	3 (6%)
27	CLA	B	831	-	65,73,73	1.45	7 (10%)	76,113,113	1.44	8 (10%)
36	XAT	Z	1622	-	39,47,47	0.90	1 (2%)	54,74,74	3.78	25 (46%)
36	XAT	1	618	-	39,47,47	0.90	0	54,74,74	2.51	22 (40%)
32	LMU	5	629	-	33,33,36	1.18	2 (6%)	44,44,47	1.09	3 (6%)
27	CLA	B	838	-	46,54,73	1.74	8 (17%)	53,90,113	1.50	8 (15%)
27	CLA	X	612	23	43,51,73	1.86	6 (13%)	49,86,113	1.45	7 (14%)
27	CLA	B	824	-	65,73,73	1.49	9 (13%)	76,113,113	1.27	6 (7%)
27	CLA	4	608	-	65,73,73	1.49	8 (12%)	76,113,113	1.28	8 (10%)
30	BCR	1	619	-	41,41,41	0.72	0	56,56,56	2.42	22 (39%)
27	CLA	a	601	14	53,62,73	1.65	9 (16%)	61,100,113	1.29	8 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
27	CLA	A	816	-	65,73,73	1.51	8 (12%)	76,113,113	1.35	8 (10%)
36	XAT	a	618	-	39,47,47	0.89	1 (2%)	54,74,74	2.51	22 (40%)
27	CLA	Z	614	-	54,62,73	1.67	6 (11%)	62,99,113	1.30	7 (11%)
27	CLA	6	602	19	65,73,73	1.51	9 (13%)	76,113,113	1.26	8 (10%)
38	CHL	W	607	-	65,73,74	1.95	16 (24%)	73,113,114	2.55	22 (30%)
27	CLA	4	609	17	57,65,73	1.59	8 (14%)	66,103,113	1.34	9 (13%)
27	CLA	B	811	-	53,60,73	1.74	9 (16%)	62,97,113	1.38	9 (14%)
29	LHG	9	623	-	48,48,48	0.92	2 (4%)	51,54,54	1.06	3 (5%)
30	BCR	7	623	-	41,41,41	0.68	0	56,56,56	2.22	26 (46%)
27	CLA	2	612	15	44,52,73	1.83	8 (18%)	51,88,113	1.43	6 (11%)
27	CLA	5	604	-	63,71,73	1.57	8 (12%)	78,111,113	1.31	11 (14%)
27	CLA	Y	612	24	45,53,73	1.85	6 (13%)	52,89,113	1.45	7 (13%)
27	CLA	a	603	-	54,62,73	1.63	8 (14%)	62,99,113	1.52	9 (14%)
29	LHG	Y	2630	27	48,48,48	0.95	2 (4%)	51,54,54	0.97	2 (3%)
30	BCR	A	852	-	41,41,41	0.85	1 (2%)	56,56,56	2.47	25 (44%)
33	LMG	8	626	-	46,46,55	0.97	2 (4%)	54,54,63	1.10	4 (7%)
27	CLA	F	301	-	57,65,73	1.64	7 (12%)	66,103,113	1.28	7 (10%)
27	CLA	2	601	15	65,73,73	1.46	6 (9%)	76,113,113	1.52	9 (11%)
35	LUT	4	619	-	42,43,43	0.78	0	51,60,60	1.76	16 (31%)
27	CLA	8	610	21	60,68,73	1.52	7 (11%)	70,107,113	1.52	8 (11%)
37	NEX	6	624	-	38,46,46	1.09	1 (2%)	50,70,70	2.10	15 (30%)
27	CLA	X	614	-	42,50,73	1.88	6 (14%)	48,85,113	1.43	7 (14%)
32	LMU	A	857	-	36,36,36	1.14	2 (5%)	47,47,47	0.98	1 (2%)
38	CHL	U	606	-	44,52,74	2.18	14 (31%)	46,87,114	2.88	21 (45%)
36	XAT	V	1622	-	39,47,47	0.97	2 (5%)	54,74,74	2.58	19 (35%)
27	CLA	5	618	18	39,48,73	1.96	7 (17%)	48,83,113	1.62	9 (18%)
27	CLA	A	812	-	65,73,73	1.49	8 (12%)	76,113,113	1.27	8 (10%)
37	NEX	Y	1623	-	40,45,46	1.03	2 (5%)	50,67,70	2.47	16 (32%)
27	CLA	A	842	-	65,73,73	1.50	8 (12%)	76,113,113	1.37	10 (13%)
27	CLA	A	854	-	65,73,73	1.51	9 (13%)	76,113,113	1.41	10 (13%)
27	CLA	B	840	-	65,73,73	1.53	8 (12%)	76,113,113	1.32	8 (10%)
27	CLA	1	614	-	37,45,73	2.12	9 (24%)	44,79,113	1.68	11 (25%)
29	LHG	H	204	-	48,48,48	0.90	2 (4%)	51,54,54	0.90	1 (1%)
27	CLA	A	817	-	45,53,73	1.76	8 (17%)	52,89,113	1.62	8 (15%)
27	CLA	a	613	-	54,62,73	1.65	8 (14%)	62,99,113	1.30	8 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
27	CLA	7	607	-	42,50,73	1.82	9 (21%)	48,85,113	1.44	7 (14%)
27	CLA	V	614	-	45,53,73	1.81	8 (17%)	52,89,113	1.45	7 (13%)
27	CLA	4	603	17	44,52,73	1.88	8 (18%)	55,88,113	1.56	8 (14%)
27	CLA	9	602	22	60,68,73	1.54	8 (13%)	70,107,113	1.38	8 (11%)
27	CLA	6	610	19	65,73,73	1.54	9 (13%)	76,113,113	1.18	8 (10%)
27	CLA	B	815	-	43,51,73	1.81	9 (20%)	49,86,113	1.43	7 (14%)
29	LHG	9	624	-	48,48,48	0.95	2 (4%)	51,54,54	1.00	2 (3%)
27	CLA	a	610	14	59,67,73	1.55	7 (11%)	69,106,113	1.42	8 (11%)
27	CLA	5	614	-	45,52,73	1.90	9 (20%)	48,87,113	1.45	8 (16%)
30	BCR	O	2005	-	41,41,41	0.80	1 (2%)	56,56,56	3.00	25 (44%)
33	LMG	J	104	-	40,40,55	1.06	2 (5%)	48,48,63	1.17	4 (8%)
27	CLA	A	811	-	65,73,73	1.48	8 (12%)	76,113,113	1.25	9 (11%)
27	CLA	1	603	-	52,61,73	1.64	7 (13%)	59,98,113	1.52	9 (15%)
27	CLA	A	828	-	65,73,73	1.48	9 (13%)	76,113,113	1.30	8 (10%)
33	LMG	4	624	-	40,40,55	1.05	2 (5%)	48,48,63	1.20	7 (14%)
37	NEX	X	1623	-	38,46,46	0.93	1 (2%)	50,70,70	2.44	16 (32%)
38	CHL	X	605	23	46,54,74	2.35	16 (34%)	49,90,114	2.88	23 (46%)
35	LUT	Z	1621	-	42,43,43	0.76	0	51,60,60	1.77	13 (25%)
27	CLA	V	602	26	60,68,73	1.54	10 (16%)	70,107,113	1.37	8 (11%)
30	BCR	6	622	-	41,41,41	0.72	1 (2%)	56,56,56	3.46	27 (48%)
38	CHL	U	609	24	60,68,74	2.04	15 (25%)	65,106,114	2.74	22 (33%)
33	LMG	A	860	-	40,40,55	1.04	2 (5%)	48,48,63	1.10	4 (8%)
29	LHG	X	2630	27	48,48,48	0.96	2 (4%)	51,54,54	0.97	2 (3%)
35	LUT	X	1621	-	42,43,43	0.79	1 (2%)	51,60,60	1.75	13 (25%)
32	LMU	A	858	-	34,35,36	1.23	3 (8%)	42,45,47	0.92	1 (2%)
27	CLA	2	610	15	55,63,73	1.59	7 (12%)	64,101,113	1.52	8 (12%)
27	CLA	7	601	20	60,68,73	1.49	7 (11%)	70,107,113	1.51	8 (11%)
38	CHL	U	607	-	46,54,74	2.21	13 (28%)	49,90,114	2.80	25 (51%)
27	CLA	J	101	10	42,50,73	1.89	9 (21%)	48,85,113	1.46	8 (16%)
27	CLA	4	613	17	65,73,73	1.51	8 (12%)	76,113,113	1.24	8 (10%)
36	XAT	5	621	-	39,47,47	0.89	1 (2%)	54,74,74	2.52	22 (40%)
30	BCR	A	848	-	41,41,41	0.82	0	56,56,56	1.97	14 (25%)
36	XAT	W	1622	-	39,47,47	1.01	3 (7%)	54,74,74	3.94	24 (44%)
36	XAT	X	1622	-	39,47,47	0.91	1 (2%)	54,74,74	3.87	25 (46%)
27	CLA	7	615	-	41,50,73	1.93	7 (17%)	50,85,113	1.50	8 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
27	CLA	3	609	16	60,68,73	1.55	9 (15%)	70,107,113	1.45	10 (14%)
29	LHG	B	854	-	48,48,48	0.94	2 (4%)	51,54,54	1.03	3 (5%)
27	CLA	B	807	-	52,60,73	1.66	10 (19%)	60,97,113	1.43	10 (16%)
27	CLA	8	616	-	43,51,73	1.94	7 (16%)	54,87,113	1.50	9 (16%)
27	CLA	B	829	-	65,73,73	1.48	9 (13%)	76,113,113	1.32	8 (10%)
37	NEX	W	1623	-	38,46,46	0.91	1 (2%)	50,70,70	2.48	16 (32%)
38	CHL	U	608	-	44,52,74	2.22	14 (31%)	46,87,114	2.80	19 (41%)
27	CLA	7	612	20	44,52,73	1.82	8 (18%)	51,88,113	1.51	6 (11%)
27	CLA	B	822	-	42,50,73	1.83	9 (21%)	48,85,113	1.42	8 (16%)
27	CLA	A	808	-	50,58,73	1.69	9 (18%)	58,95,113	1.43	8 (13%)
27	CLA	A	841	-	65,73,73	1.48	9 (13%)	76,113,113	1.29	7 (9%)
27	CLA	3	610	16	65,73,73	1.50	9 (13%)	76,113,113	1.28	7 (9%)
30	BCR	a	619	-	41,41,41	0.73	0	56,56,56	2.41	22 (39%)
27	CLA	X	602	23	65,73,73	1.56	7 (10%)	76,113,113	1.22	6 (7%)
27	CLA	3	614	-	39,48,73	1.91	8 (20%)	44,83,113	1.47	6 (13%)
27	CLA	A	845	29	50,58,73	1.69	8 (16%)	58,95,113	1.35	7 (12%)
27	CLA	1	602	14	61,69,73	1.53	9 (14%)	71,108,113	1.29	8 (11%)
27	CLA	B	837	-	65,73,73	1.52	8 (12%)	76,113,113	1.32	10 (13%)
27	CLA	7	606	-	41,49,73	1.84	9 (21%)	47,84,113	1.45	7 (14%)
36	XAT	8	620	-	39,47,47	0.95	1 (2%)	54,74,74	2.56	26 (48%)
35	LUT	Y	1621	-	42,43,43	0.78	0	51,60,60	1.75	13 (25%)
35	LUT	V	1621	-	42,43,43	0.97	2 (4%)	51,60,60	1.74	12 (23%)
27	CLA	W	603	-	52,60,73	1.65	11 (21%)	60,97,113	1.48	8 (13%)
27	CLA	O	2003	-	39,48,73	1.94	8 (20%)	44,83,113	1.45	7 (15%)
27	CLA	K	204	-	45,53,73	1.76	8 (17%)	52,89,113	1.55	8 (15%)
38	CHL	W	601	23	66,74,74	1.91	15 (22%)	73,114,114	2.68	23 (31%)
27	CLA	8	603	-	44,52,73	1.83	8 (18%)	55,88,113	1.60	9 (16%)
27	CLA	A	839	-	55,63,73	1.63	9 (16%)	64,101,113	1.34	9 (14%)
27	CLA	B	839	-	65,73,73	1.49	8 (12%)	76,113,113	1.24	7 (9%)
38	CHL	Y	606	-	46,54,74	2.32	15 (32%)	49,90,114	2.81	21 (42%)
28	PQN	A	844	-	34,34,34	3.46	11 (32%)	42,45,45	1.59	4 (9%)
30	BCR	J	102	-	41,41,41	0.76	0	56,56,56	2.18	23 (41%)
27	CLA	5	619	-	43,51,73	1.91	7 (16%)	54,87,113	1.53	10 (18%)
27	CLA	6	608	-	45,53,73	1.82	9 (20%)	52,89,113	1.43	7 (13%)
27	CLA	Y	613	24	65,73,73	1.56	6 (9%)	76,113,113	1.27	11 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
27	CLA	B	832	-	60,68,73	1.56	8 (13%)	70,107,113	1.32	10 (14%)
27	CLA	4	601	17	65,73,73	1.49	7 (10%)	76,113,113	1.34	9 (11%)
27	CLA	H	203	-	65,73,73	1.50	8 (12%)	76,113,113	1.34	8 (10%)
27	CLA	A	834	-	65,73,73	1.47	8 (12%)	76,113,113	1.33	8 (10%)
27	CLA	A	836	-	65,73,73	1.49	9 (13%)	76,113,113	1.29	9 (11%)
27	CLA	6	609	19	45,53,73	1.79	8 (17%)	52,89,113	1.47	7 (13%)
29	LHG	7	622	27	36,36,48	1.05	2 (5%)	39,42,54	0.85	2 (5%)
27	CLA	6	603	-	51,59,73	1.72	7 (13%)	63,96,113	1.45	10 (15%)
27	CLA	8	604	-	50,58,73	1.66	7 (14%)	58,95,113	1.46	9 (15%)
27	CLA	3	615	-	39,48,73	1.90	7 (17%)	44,83,113	1.70	7 (15%)
27	CLA	5	610	18	54,62,73	1.62	7 (12%)	62,99,113	1.45	8 (12%)
27	CLA	a	609	14	63,72,73	1.52	8 (12%)	73,112,113	1.25	9 (12%)
27	CLA	L	303	-	65,73,73	1.49	8 (12%)	76,113,113	1.32	9 (11%)
27	CLA	Y	611	29	43,51,73	1.87	6 (13%)	49,86,113	1.46	7 (14%)
27	CLA	W	613	23	65,73,73	1.48	9 (13%)	76,113,113	1.31	9 (11%)
27	CLA	V	611	29	43,51,73	1.81	10 (23%)	49,86,113	1.51	7 (14%)
38	CHL	U	605	24	43,51,74	2.27	12 (27%)	45,86,114	3.00	22 (48%)
27	CLA	X	610	23	65,73,73	1.58	7 (10%)	76,113,113	1.23	9 (11%)
27	CLA	5	603	-	54,62,73	1.70	8 (14%)	67,100,113	1.45	11 (16%)
27	CLA	A	821	-	53,61,73	1.66	8 (15%)	61,98,113	1.40	8 (13%)
29	LHG	6	623	27	47,47,48	0.93	2 (4%)	50,53,54	0.90	3 (6%)
27	CLA	1	610	14	38,47,73	1.87	7 (18%)	44,81,113	1.77	9 (20%)
30	BCR	L	301	-	41,41,41	0.72	0	56,56,56	2.26	27 (48%)
38	CHL	Y	605	24	42,50,74	2.45	16 (38%)	44,85,114	3.03	22 (50%)
27	CLA	B	835	-	45,53,73	1.80	7 (15%)	52,89,113	1.36	7 (13%)
27	CLA	A	837	1	45,53,73	1.79	8 (17%)	52,89,113	1.50	7 (13%)
38	CHL	X	609	23	66,74,74	1.95	15 (22%)	73,114,114	2.62	22 (30%)
30	BCR	7	621	-	41,41,41	0.75	0	56,56,56	2.34	23 (41%)
27	CLA	1	608	-	43,52,73	1.84	8 (18%)	49,88,113	1.43	8 (16%)
27	CLA	H	202	8	38,47,73	1.94	9 (23%)	43,82,113	1.43	7 (16%)
35	LUT	U	1621	-	42,43,43	0.96	2 (4%)	51,60,60	1.70	11 (21%)
27	CLA	9	601	22	45,53,73	1.81	8 (17%)	52,89,113	1.43	8 (15%)
27	CLA	a	604	-	49,57,73	1.73	8 (16%)	55,93,113	1.37	7 (12%)
27	CLA	7	608	-	50,58,73	1.69	8 (16%)	58,95,113	1.40	7 (12%)
27	CLA	6	613	-	63,72,73	1.56	8 (12%)	73,112,113	1.19	7 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
27	CLA	3	602	16	60,68,73	1.55	9 (15%)	70,107,113	1.26	8 (11%)
27	CLA	B	814	-	62,70,73	1.50	8 (12%)	72,109,113	1.27	9 (12%)
30	BCR	B	847	-	41,41,41	0.82	0	56,56,56	2.08	15 (26%)
27	CLA	V	613	26	65,73,73	1.50	10 (15%)	76,113,113	1.29	7 (9%)
35	LUT	3	618	-	42,43,43	0.82	1 (2%)	51,60,60	1.67	12 (23%)
27	CLA	a	616	14	45,53,73	1.78	6 (13%)	52,89,113	1.46	7 (13%)
27	CLA	7	611	29	59,67,73	1.55	8 (13%)	68,105,113	1.27	8 (11%)
27	CLA	9	607	-	45,53,73	1.81	9 (20%)	52,89,113	1.43	7 (13%)
27	CLA	2	607	-	45,53,73	1.78	9 (20%)	52,89,113	1.48	7 (13%)
27	CLA	9	613	22	65,73,73	1.51	8 (12%)	76,113,113	1.26	7 (9%)
30	BCR	B	846	-	41,41,41	0.76	1 (2%)	56,56,56	2.23	21 (37%)
27	CLA	A	801	-	65,73,73	1.50	9 (13%)	76,113,113	1.29	10 (13%)
27	CLA	A	805	-	52,60,73	1.67	9 (17%)	60,97,113	1.54	8 (13%)
27	CLA	X	613	23	65,73,73	1.55	6 (9%)	76,113,113	1.27	11 (14%)
38	CHL	U	601	24	66,74,74	1.91	15 (22%)	73,114,114	2.68	22 (30%)
27	CLA	a	614	-	55,62,73	1.71	9 (16%)	60,99,113	1.43	10 (16%)
29	LHG	4	622	27	48,48,48	0.92	2 (4%)	51,54,54	0.89	2 (3%)
27	CLA	A	829	-	65,73,73	1.46	7 (10%)	76,113,113	1.32	7 (9%)
27	CLA	B	804	-	41,49,73	1.83	8 (19%)	47,84,113	1.46	7 (14%)
27	CLA	X	611	29	45,53,73	1.84	6 (13%)	52,89,113	1.49	9 (17%)
30	BCR	B	848	-	41,41,41	0.78	0	56,56,56	2.20	20 (35%)
29	LHG	A	846	-	48,48,48	0.91	2 (4%)	51,54,54	0.90	2 (3%)
27	CLA	L	304	-	45,53,73	1.77	8 (17%)	52,89,113	1.42	7 (13%)
27	CLA	4	604	-	54,62,73	1.68	8 (14%)	67,100,113	1.40	10 (14%)
27	CLA	Z	610	25	65,73,73	1.51	6 (9%)	76,113,113	1.34	9 (11%)
38	CHL	X	601	23	66,74,74	1.91	15 (22%)	73,114,114	2.69	21 (28%)
36	XAT	7	620	-	39,47,47	0.91	1 (2%)	54,74,74	2.48	22 (40%)
27	CLA	5	607	-	65,73,73	1.49	9 (13%)	76,113,113	1.38	7 (9%)
29	LHG	3	624	27	48,48,48	0.92	2 (4%)	51,54,54	0.97	3 (5%)
27	CLA	A	819	-	59,67,73	1.52	10 (16%)	68,105,113	1.42	7 (10%)
27	CLA	G	204	7	45,53,73	1.81	8 (17%)	52,89,113	1.49	8 (15%)
27	CLA	B	809	2	65,73,73	1.50	9 (13%)	76,113,113	1.32	7 (9%)
27	CLA	U	602	24	59,67,73	1.55	9 (15%)	68,105,113	1.38	6 (8%)
27	CLA	Y	603	-	55,63,73	1.68	7 (12%)	64,101,113	1.35	8 (12%)
27	CLA	2	602	15	63,72,73	1.49	8 (12%)	73,112,113	1.29	6 (8%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
27	CLA	A	810	1	50,58,73	1.71	9 (18%)	58,95,113	1.47	9 (15%)
29	LHG	Z	2630	27	48,48,48	0.94	2 (4%)	51,54,54	0.85	2 (3%)
30	BCR	K	207	-	41,41,41	0.75	0	56,56,56	2.93	23 (41%)
29	LHG	B	851	27	37,37,48	1.08	2 (5%)	40,43,54	1.13	3 (7%)
27	CLA	B	836	-	50,58,73	1.67	7 (14%)	58,95,113	1.52	6 (10%)
27	CLA	4	614	-	56,64,73	1.62	7 (12%)	65,102,113	1.35	10 (15%)
27	CLA	X	604	-	49,57,73	1.77	6 (12%)	55,93,113	1.34	8 (14%)
30	BCR	B	852	-	41,41,41	0.80	0	56,56,56	3.56	24 (42%)
27	CLA	A	830	-	65,73,73	1.47	9 (13%)	76,113,113	1.33	7 (9%)
27	CLA	a	602	14	61,69,73	1.53	9 (14%)	71,108,113	1.29	8 (11%)
27	CLA	5	609	18	65,73,73	1.50	9 (13%)	76,113,113	1.27	7 (9%)
27	CLA	F	303	-	42,50,73	1.89	8 (19%)	48,85,113	1.47	7 (14%)
27	CLA	Y	610	24	65,73,73	1.57	7 (10%)	76,113,113	1.23	9 (11%)
27	CLA	A	820	-	65,73,73	1.47	7 (10%)	76,113,113	1.38	8 (10%)
27	CLA	U	611	29	42,50,73	1.79	9 (21%)	48,85,113	1.49	7 (14%)
29	LHG	9	622	27	29,29,48	1.19	2 (6%)	32,35,54	1.03	1 (3%)
27	CLA	9	606	-	39,48,73	1.94	9 (23%)	44,83,113	1.52	8 (18%)
37	NEX	Z	1623	-	38,46,46	1.14	2 (5%)	50,70,70	2.34	15 (30%)
29	LHG	2	622	27	35,35,48	1.08	2 (5%)	38,41,54	0.98	1 (2%)
36	XAT	3	619	-	39,47,47	0.89	1 (2%)	54,74,74	2.56	22 (40%)
27	CLA	8	609	21	45,53,73	1.79	9 (20%)	52,89,113	1.41	7 (13%)
27	CLA	6	607	-	41,49,73	1.87	8 (19%)	51,84,113	1.56	9 (17%)
30	BCR	B	801	-	41,41,41	0.84	0	56,56,56	2.10	20 (35%)
30	BCR	3	620	-	41,41,41	0.85	0	56,56,56	4.30	30 (53%)
27	CLA	6	612	19	40,49,73	1.85	7 (17%)	45,84,113	1.50	8 (17%)
30	BCR	A	856	-	41,41,41	0.77	0	56,56,56	2.14	19 (33%)
27	CLA	5	608	-	50,58,73	1.71	9 (18%)	58,95,113	1.37	8 (13%)
37	NEX	U	1623	-	38,46,46	0.93	2 (5%)	50,70,70	2.48	15 (30%)
27	CLA	6	618	19	39,48,73	1.93	8 (20%)	48,83,113	1.62	9 (18%)
27	CLA	1	601	14	53,62,73	1.67	9 (16%)	61,100,113	1.29	8 (13%)
27	CLA	4	602	17	60,68,73	1.54	7 (11%)	70,107,113	1.44	8 (11%)
27	CLA	8	614	-	53,61,73	1.66	8 (15%)	61,98,113	1.41	9 (14%)
36	XAT	4	620	-	39,47,47	0.88	0	54,74,74	2.49	23 (42%)
27	CLA	6	620	-	64,72,73	1.50	7 (10%)	74,111,113	1.21	6 (8%)
27	CLA	W	604	-	47,55,73	1.75	8 (17%)	54,91,113	1.41	8 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
33	LMG	4	623	-	40,40,55	1.05	2 (5%)	48,48,63	1.14	4 (8%)
27	CLA	B	802	-	65,73,73	1.47	9 (13%)	76,113,113	1.19	6 (7%)
38	CHL	V	607	-	46,54,74	2.23	16 (34%)	49,90,114	2.74	22 (44%)
29	LHG	V	2630	27	47,47,48	0.89	2 (4%)	50,53,54	1.12	3 (6%)
35	LUT	8	619	-	42,43,43	0.81	1 (2%)	51,60,60	1.66	13 (25%)
27	CLA	5	616	18	41,50,73	1.90	8 (19%)	50,85,113	1.46	9 (18%)
27	CLA	1	607	-	39,48,73	1.88	9 (23%)	44,83,113	1.51	8 (18%)
27	CLA	7	609	20	43,52,73	1.79	7 (16%)	48,87,113	1.44	6 (12%)
29	LHG	5	623	27	48,48,48	0.92	2 (4%)	51,54,54	0.83	2 (3%)
35	LUT	7	619	-	42,43,43	0.85	2 (4%)	51,60,60	1.82	11 (21%)
27	CLA	3	611	29	37,46,73	2.02	8 (21%)	46,81,113	1.56	9 (19%)
27	CLA	3	606	-	53,62,73	1.63	8 (15%)	61,100,113	1.32	7 (11%)
27	CLA	U	610	24	56,64,73	1.66	9 (16%)	65,102,113	1.27	8 (12%)
33	LMG	5	627	-	40,40,55	1.05	2 (5%)	48,48,63	1.01	2 (4%)
27	CLA	A	814	-	65,73,73	1.47	9 (13%)	76,113,113	1.40	9 (11%)
30	BCR	5	622	-	41,41,41	0.73	0	56,56,56	2.34	21 (37%)
30	BCR	3	622	-	41,41,41	0.73	0	56,56,56	2.30	19 (33%)
27	CLA	B	818	-	60,68,73	1.54	9 (15%)	70,107,113	1.48	9 (12%)
38	CHL	Y	609	24	66,74,74	1.95	15 (22%)	73,114,114	2.58	21 (28%)
33	LMG	V	2631	-	41,41,55	1.01	2 (4%)	49,49,63	1.16	4 (8%)
38	CHL	W	608	-	47,55,74	2.23	14 (29%)	50,91,114	2.73	21 (42%)
27	CLA	W	614	-	45,53,73	1.78	9 (20%)	52,89,113	1.47	8 (15%)
27	CLA	8	601	21	65,73,73	1.45	7 (10%)	76,113,113	1.36	7 (9%)
37	NEX	V	1623	-	38,46,46	0.90	2 (5%)	50,70,70	2.25	12 (24%)
29	LHG	3	623	-	44,44,48	0.96	2 (4%)	47,50,54	1.05	3 (6%)
27	CLA	6	604	-	65,73,73	1.49	8 (12%)	76,113,113	1.22	9 (11%)
27	CLA	B	826	-	62,70,73	1.52	7 (11%)	72,109,113	1.41	9 (12%)
32	LMU	K	208	-	36,36,36	1.15	2 (5%)	47,47,47	0.97	2 (4%)
27	CLA	2	609	15	45,53,73	1.81	8 (17%)	52,89,113	1.42	7 (13%)
27	CLA	6	611	29	42,50,73	1.84	8 (19%)	48,85,113	1.45	7 (14%)
38	CHL	Y	601	24	66,74,74	1.90	15 (22%)	73,114,114	2.67	22 (30%)
27	CLA	Y	604	-	50,58,73	1.76	6 (12%)	58,95,113	1.33	9 (15%)
38	CHL	Y	607	-	66,74,74	1.96	16 (24%)	73,114,114	2.66	25 (34%)
38	CHL	V	601	26	66,74,74	1.91	15 (22%)	73,114,114	2.66	21 (28%)
33	LMG	9	625	-	55,55,55	0.89	2 (3%)	63,63,63	0.95	2 (3%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
27	CLA	3	608	-	55,63,73	1.71	9 (16%)	64,101,113	1.32	7 (10%)
27	CLA	7	613	20	65,73,73	1.49	8 (12%)	76,113,113	1.22	8 (10%)
27	CLA	A	804	-	65,73,73	1.45	7 (10%)	76,113,113	1.39	8 (10%)
27	CLA	9	604	-	50,58,73	1.74	8 (16%)	62,95,113	1.42	10 (16%)
27	CLA	2	613	15	65,73,73	1.47	7 (10%)	76,113,113	1.27	8 (10%)
27	CLA	9	612	22	40,49,73	1.87	6 (15%)	45,84,113	1.54	8 (17%)
37	NEX	5	624	-	38,46,46	1.04	1 (2%)	50,70,70	2.16	13 (26%)
27	CLA	B	808	-	65,73,73	1.50	9 (13%)	76,113,113	1.22	9 (11%)
27	CLA	6	606	-	39,48,73	1.91	7 (17%)	44,83,113	1.39	7 (15%)
27	CLA	B	841	29	65,73,73	1.50	9 (13%)	76,113,113	1.28	7 (9%)
27	CLA	9	611	29	42,50,73	1.86	7 (16%)	48,85,113	1.44	7 (14%)
27	CLA	6	614	-	60,68,73	1.58	8 (13%)	70,107,113	1.28	9 (12%)
27	CLA	B	813	-	65,73,73	1.49	9 (13%)	76,113,113	1.34	8 (10%)
33	LMG	H	205	-	55,55,55	0.89	2 (3%)	63,63,63	1.12	6 (9%)
27	CLA	5	602	18	65,73,73	1.48	9 (13%)	76,113,113	1.25	7 (9%)
32	LMU	1	621	-	36,36,36	1.17	2 (5%)	47,47,47	0.95	1 (2%)
27	CLA	B	812	-	43,51,73	1.85	8 (18%)	49,86,113	1.45	8 (16%)
27	CLA	L	302	12	45,53,73	1.81	9 (20%)	52,89,113	1.49	8 (15%)
27	CLA	3	603	-	55,63,73	1.60	7 (12%)	64,101,113	1.62	9 (14%)
38	CHL	X	607	-	66,74,74	1.92	14 (21%)	73,114,114	2.72	22 (30%)
27	CLA	B	803	-	65,73,73	1.47	9 (13%)	76,113,113	1.25	6 (7%)
35	LUT	6	619	-	42,43,43	0.82	1 (2%)	51,60,60	1.83	13 (25%)
32	LMU	5	628	-	34,34,36	1.16	2 (5%)	45,45,47	1.16	6 (13%)
27	CLA	B	827	-	62,70,73	1.51	8 (12%)	72,109,113	1.35	8 (11%)
27	CLA	B	817	-	59,67,73	1.58	9 (15%)	68,105,113	1.43	10 (14%)
27	CLA	2	616	-	43,51,73	1.89	8 (18%)	54,87,113	1.49	9 (16%)
27	CLA	1	606	-	37,47,73	1.90	8 (21%)	41,80,113	1.57	8 (19%)
27	CLA	7	604	-	50,58,73	1.72	9 (18%)	58,95,113	1.35	8 (13%)
35	LUT	W	1620	-	42,43,43	0.90	1 (2%)	51,60,60	1.83	9 (17%)
27	CLA	W	612	23	45,53,73	1.78	8 (17%)	52,89,113	1.45	6 (11%)
27	CLA	3	613	16	52,61,73	1.69	8 (15%)	59,98,113	1.31	8 (13%)
27	CLA	G	203	-	42,50,73	1.83	7 (16%)	48,85,113	1.50	7 (14%)
36	XAT	2	620	-	39,47,47	0.93	0	54,74,74	2.50	21 (38%)
29	LHG	8	622	27	48,48,48	0.92	2 (4%)	51,54,54	0.85	2 (3%)
27	CLA	L	307	-	39,48,73	1.92	8 (20%)	44,83,113	1.52	6 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
27	CLA	A	835	-	61,69,73	1.54	9 (14%)	71,108,113	1.29	8 (11%)
27	CLA	A	802	-	65,73,73	1.48	9 (13%)	76,113,113	1.36	8 (10%)
27	CLA	A	813	-	54,62,73	1.61	8 (14%)	62,99,113	1.45	8 (12%)
36	XAT	U	1622	-	39,47,47	1.02	3 (7%)	54,74,74	3.93	24 (44%)
27	CLA	Y	602	24	58,66,73	1.65	6 (10%)	67,104,113	1.27	6 (8%)
30	BCR	B	844	-	41,41,41	0.87	1 (2%)	56,56,56	2.11	20 (35%)
38	CHL	Z	606	-	46,54,74	2.38	15 (32%)	49,90,114	2.83	22 (44%)
27	CLA	8	606	-	64,72,73	1.50	9 (14%)	75,112,113	1.24	8 (10%)
27	CLA	O	2001	-	36,46,73	1.97	8 (22%)	41,80,113	1.49	8 (19%)
27	CLA	A	815	-	50,58,73	1.68	9 (18%)	58,95,113	1.43	6 (10%)
27	CLA	B	834	-	60,68,73	1.54	8 (13%)	70,107,113	1.35	8 (11%)
38	CHL	W	609	23	66,74,74	1.94	15 (22%)	73,114,114	2.62	22 (30%)
27	CLA	B	806	2	65,73,73	1.48	9 (13%)	76,113,113	1.32	7 (9%)
27	CLA	7	610	20	65,73,73	1.46	7 (10%)	76,113,113	1.37	9 (11%)
38	CHL	V	606	-	44,52,74	2.17	15 (34%)	46,87,114	2.94	19 (41%)
27	CLA	8	607	-	41,49,73	1.89	8 (19%)	51,84,113	1.56	9 (17%)
27	CLA	A	823	-	42,50,73	1.86	9 (21%)	48,85,113	1.44	7 (14%)
27	CLA	A	831	-	65,73,73	1.50	10 (15%)	76,113,113	1.26	7 (9%)
27	CLA	9	609	22	61,69,73	1.54	8 (13%)	71,108,113	1.29	7 (9%)
27	CLA	9	603	22	44,52,73	1.86	9 (20%)	55,88,113	1.45	8 (14%)
27	CLA	8	612	21	40,49,73	1.87	8 (20%)	45,84,113	1.55	7 (15%)
38	CHL	Z	608	-	50,58,74	2.24	14 (28%)	52,94,114	2.73	22 (42%)
27	CLA	A	843	-	64,72,73	1.54	8 (12%)	74,111,113	1.23	8 (10%)
35	LUT	9	619	-	42,43,43	0.79	0	51,60,60	1.73	14 (27%)
38	CHL	Z	607	-	66,74,74	1.90	15 (22%)	73,114,114	2.73	20 (27%)
36	XAT	Y	1622	-	39,47,47	0.89	1 (2%)	54,74,74	3.87	25 (46%)
27	CLA	5	606	-	39,48,73	1.92	9 (23%)	44,83,113	1.35	6 (13%)
27	CLA	Z	611	29	65,73,73	1.49	5 (7%)	76,113,113	1.26	7 (9%)
29	LHG	1	620	27	48,48,48	0.91	2 (4%)	51,54,54	0.97	3 (5%)
27	CLA	A	825	-	65,73,73	1.48	9 (13%)	76,113,113	1.27	8 (10%)
31	SF4	A	853	2,1	0,12,12	-	-	-	-	-
27	CLA	W	611	29	57,65,73	1.57	8 (14%)	66,103,113	1.37	8 (12%)
38	CHL	Y	608	-	49,57,74	2.28	15 (30%)	52,93,114	2.72	23 (44%)
38	CHL	V	605	26	44,52,74	2.25	14 (31%)	46,87,114	2.85	21 (45%)
27	CLA	A	838	-	50,58,73	1.62	6 (12%)	58,95,113	1.57	9 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
32	LMU	8	625	-	36,36,36	1.15	2 (5%)	47,47,47	1.02	3 (6%)
38	CHL	V	608	-	48,56,74	2.20	16 (33%)	51,92,114	2.70	21 (41%)
27	CLA	U	603	-	52,60,73	1.64	11 (21%)	60,97,113	1.47	8 (13%)
27	CLA	a	612	14	45,53,73	1.79	8 (17%)	52,89,113	1.46	7 (13%)
27	CLA	7	602	20	65,73,73	1.47	8 (12%)	76,113,113	1.25	6 (7%)
27	CLA	5	611	29	42,50,73	1.83	8 (19%)	48,85,113	1.39	7 (14%)
27	CLA	B	830	-	43,51,73	1.85	9 (20%)	49,86,113	1.42	7 (14%)
27	CLA	1	604	-	49,57,73	1.74	8 (16%)	55,93,113	1.38	7 (12%)
27	CLA	a	607	-	45,53,73	1.80	8 (17%)	52,89,113	1.44	8 (15%)
27	CLA	O	2002	-	37,46,73	2.03	8 (21%)	46,81,113	1.53	8 (17%)
27	CLA	V	604	-	50,58,73	1.71	9 (18%)	58,95,113	1.46	7 (12%)
30	BCR	B	843	-	41,41,41	0.78	0	56,56,56	1.80	16 (28%)
27	CLA	K	203	-	56,64,73	1.62	8 (14%)	65,102,113	1.43	11 (16%)
29	LHG	8	623	-	39,39,48	1.02	2 (5%)	42,45,54	1.09	3 (7%)
27	CLA	2	611	29	42,50,73	1.85	8 (19%)	48,85,113	1.46	7 (14%)
27	CLA	A	807	1	65,73,73	1.50	9 (13%)	76,113,113	1.32	8 (10%)
33	LMG	J	103	-	42,42,55	1.01	2 (4%)	50,50,63	1.09	2 (4%)
27	CLA	1	611	29	57,65,73	1.61	8 (14%)	66,103,113	1.32	7 (10%)

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
27	CLA	Z	612	25	1/1/15/20	6/37/115/115	-
35	LUT	U	1620	-	-	2/29/67/67	0/2/2/2
27	CLA	Y	614	-	1/1/11/20	7/17/95/115	-
30	BCR	B	845	-	-	9/29/63/63	0/2/2/2
27	CLA	Z	613	25	1/1/15/20	15/37/115/115	-
30	BCR	8	621	-	-	4/29/63/63	0/2/2/2
27	CLA	A	809	1	1/1/15/20	11/37/115/115	-
27	CLA	4	616	17	1/1/11/20	9/11/87/115	-
27	CLA	a	611	29	1/1/10/20	3/4/80/115	-
27	CLA	F	304	6	-	4/8/86/115	-
27	CLA	3	612	16	1/1/10/20	1/11/89/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	CLA	a	606	-	1/1/10/20	4/10/88/115	-
27	CLA	A	824	-	1/1/15/20	10/37/115/115	-
27	CLA	U	613	24	1/1/13/20	12/30/108/115	-
27	CLA	Z	603	-	1/1/15/20	20/37/115/115	-
27	CLA	4	612	17	1/1/10/20	2/8/86/115	-
27	CLA	3	607	16	1/1/13/20	10/28/104/115	-
27	CLA	V	603	-	1/1/11/20	3/13/91/115	-
29	LHG	a	620	27	-	10/47/47/53	-
30	BCR	O	2004	-	-	3/29/63/63	0/2/2/2
27	CLA	A	803	-	1/1/15/20	3/37/115/115	-
27	CLA	A	840	-	-	5/22/100/115	-
27	CLA	B	810	-	1/1/14/20	15/35/113/115	-
27	CLA	B	805	-	1/1/15/20	15/37/115/115	-
27	CLA	6	601	19	1/1/15/20	14/37/115/115	-
27	CLA	Z	602	25	1/1/14/20	4/31/109/115	-
27	CLA	U	612	24	1/1/10/20	2/11/89/115	-
27	CLA	8	611	29	1/1/10/20	2/10/88/115	-
29	LHG	U	2630	27	-	12/53/53/53	-
27	CLA	B	821	-	1/1/11/20	2/11/89/115	-
27	CLA	A	827	-	1/1/13/20	7/29/107/115	-
27	CLA	7	616	20	1/1/11/20	2/11/87/115	-
27	CLA	A	806	-	1/1/15/20	16/37/115/115	-
35	LUT	Y	1620	-	-	2/29/67/67	0/2/2/2
30	BCR	B	849	-	-	3/29/63/63	0/2/2/2
38	CHL	X	608	-	3/3/20/26	21/39/137/137	-
27	CLA	2	606	-	1/1/11/20	5/13/91/115	-
27	CLA	Z	604	-	1/1/13/20	6/28/106/115	-
29	LHG	O	2631	-	-	17/40/40/53	-
30	BCR	3	621	-	-	0/29/63/63	0/2/2/2
30	BCR	A	850	-	-	2/29/63/63	0/2/2/2
27	CLA	K	201	11	1/1/11/20	4/13/91/115	-
27	CLA	5	613	18	1/1/14/20	16/35/113/115	-
27	CLA	K	206	11	1/1/11/20	5/13/91/115	-
27	CLA	V	612	26	1/1/11/20	2/13/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
38	CHL	W	605	23	3/3/16/26	5/15/113/137	-
30	BCR	B	853	-	-	4/29/63/63	0/2/2/2
27	CLA	7	603	-	1/1/11/20	3/11/89/115	-
30	BCR	L	308	-	-	2/29/63/63	0/2/2/2
27	CLA	B	825	-	-	4/18/96/115	-
27	CLA	1	609	14	1/1/10/20	3/8/84/115	-
29	LHG	A	847	27	-	7/34/34/53	-
35	LUT	2	619	-	-	1/29/67/67	0/2/2/2
35	LUT	1	617	-	-	0/29/67/67	0/2/2/2
27	CLA	9	610	22	1/1/13/20	5/28/106/115	-
27	CLA	2	604	-	1/1/10/20	5/9/87/115	-
27	CLA	B	816	-	1/1/12/20	12/23/101/115	-
27	CLA	3	617	16	1/1/10/20	0/6/84/115	-
27	CLA	8	608	-	1/1/12/20	7/21/99/115	-
30	BCR	F	305	-	-	6/29/63/63	0/2/2/2
27	CLA	X	603	-	1/1/14/20	7/34/112/115	-
30	BCR	9	621	-	-	4/29/63/63	0/2/2/2
35	LUT	W	1621	-	-	1/29/67/67	0/2/2/2
31	SF4	C	101	3	-	-	0/6/5/5
27	CLA	B	833	-	1/1/15/20	8/37/115/115	-
27	CLA	6	617	-	1/1/11/20	7/13/91/115	-
38	CHL	Z	609	25	3/3/20/26	18/39/137/137	-
27	CLA	7	614	-	1/1/10/20	3/10/88/115	-
38	CHL	V	609	26	3/3/19/26	16/33/131/137	-
30	BCR	L	309	-	-	1/29/63/63	0/2/2/2
27	CLA	B	819	-	1/1/13/20	7/25/103/115	-
27	CLA	1	613	-	1/1/15/20	13/37/115/115	-
35	LUT	X	1620	-	-	2/29/67/67	0/2/2/2
27	CLA	a	608	-	1/1/11/20	3/11/89/115	-
27	CLA	5	617	-	1/1/12/20	7/19/97/115	-
27	CLA	1	616	14	1/1/11/20	5/11/87/115	-
30	BCR	L	305	-	-	2/29/63/63	0/2/2/2
30	BCR	K	202	-	-	4/29/63/63	0/2/2/2
27	CLA	3	604	-	1/1/15/20	9/37/115/115	-
29	LHG	W	2630	27	-	10/48/48/53	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
30	BCR	A	851	-	-	2/29/63/63	0/2/2/2
27	CLA	4	610	17	1/1/14/20	8/33/111/115	-
27	CLA	4	618	17	1/1/10/20	2/8/84/115	-
35	LUT	a	617	-	-	0/29/67/67	0/2/2/2
27	CLA	8	613	21	1/1/15/20	14/37/115/115	-
31	SF4	C	102	3	-	-	0/6/5/5
27	CLA	8	602	21	1/1/14/20	8/31/109/115	-
30	BCR	2	623	-	-	4/29/63/63	0/2/2/2
35	LUT	Z	1620	-	-	0/29/67/67	0/2/2/2
27	CLA	L	306	-	1/1/10/20	0/6/84/115	-
27	CLA	V	610	26	1/1/14/20	7/34/112/115	-
27	CLA	A	822	-	1/1/15/20	7/37/115/115	-
27	CLA	A	832	-	1/1/12/20	6/19/97/115	-
27	CLA	W	602	23	1/1/14/20	7/31/109/115	-
38	CHL	Z	601	25	3/3/20/26	21/39/137/137	-
27	CLA	A	826	-	1/1/14/20	10/35/113/115	-
38	CHL	W	606	-	3/3/16/26	2/15/113/137	-
38	CHL	X	606	-	3/3/15/26	0/13/111/137	-
28	PQN	B	842	-	-	5/23/43/43	0/2/2/2
29	LHG	5	625	-	-	16/53/53/53	-
27	CLA	4	607	-	1/1/11/20	4/13/91/115	-
36	XAT	9	620	-	-	0/31/93/93	0/4/4/4
35	LUT	5	620	-	-	1/29/67/67	0/2/2/2
27	CLA	U	604	-	1/1/10/20	6/18/92/115	-
27	CLA	A	818	-	-	14/31/109/115	-
27	CLA	9	614	-	1/1/11/20	4/13/91/115	-
38	CHL	Z	605	25	3/3/15/26	1/13/111/137	-
30	BCR	A	849	-	-	5/29/63/63	0/2/2/2
27	CLA	B	828	-	1/1/15/20	15/37/115/115	-
27	CLA	2	614	-	1/1/10/20	0/9/87/115	-
27	CLA	4	611	29	1/1/10/20	2/10/88/115	-
27	CLA	6	616	19	1/1/15/20	22/37/115/115	-
36	XAT	6	621	-	-	0/31/93/93	0/4/4/4
27	CLA	1	612	14	1/1/11/20	5/13/91/115	-
27	CLA	5	601	18	1/1/13/20	2/27/105/115	-
27	CLA	B	820	-	1/1/12/20	1/19/97/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	CLA	A	833	-	1/1/11/20	5/13/91/115	-
35	LUT	V	1620	-	-	0/29/67/67	0/2/2/2
27	CLA	2	603	15	1/1/11/20	4/11/89/115	-
30	BCR	4	621	-	-	4/29/63/63	0/2/2/2
34	DGD	B	850	-	-	16/51/91/95	0/2/2/2
27	CLA	B	823	-	1/1/11/20	6/13/91/115	-
27	CLA	4	606	-	1/1/10/20	2/6/84/115	-
27	CLA	5	612	18	1/1/10/20	3/8/86/115	-
27	CLA	W	610	23	1/1/13/20	5/25/103/115	-
30	BCR	G	205	-	-	1/29/63/63	0/2/2/2
27	CLA	U	614	-	1/1/10/20	4/10/88/115	-
33	LMG	L	2631	-	-	8/32/52/70	0/1/1/1
27	CLA	B	831	-	1/1/15/20	15/37/115/115	-
36	XAT	Z	1622	-	-	0/31/93/93	0/4/4/4
36	XAT	1	618	-	-	0/31/93/93	0/4/4/4
32	LMU	5	629	-	-	11/18/58/61	0/2/2/2
27	CLA	B	838	-	-	3/15/93/115	-
27	CLA	X	612	23	1/1/10/20	2/11/89/115	-
27	CLA	B	824	-	1/1/15/20	12/37/115/115	-
27	CLA	4	608	-	1/1/15/20	14/37/115/115	-
30	BCR	1	619	-	-	4/29/63/63	0/2/2/2
27	CLA	a	601	14	-	2/23/101/115	-
27	CLA	A	816	-	1/1/15/20	10/37/115/115	-
36	XAT	a	618	-	-	0/31/93/93	0/4/4/4
27	CLA	Z	614	-	1/1/12/20	7/24/102/115	-
27	CLA	6	602	19	1/1/15/20	10/37/115/115	-
38	CHL	W	607	-	3/3/20/26	25/37/135/137	-
27	CLA	4	609	17	1/1/13/20	4/28/106/115	-
27	CLA	B	811	-	1/1/12/20	8/23/95/115	-
29	LHG	9	623	-	-	16/53/53/53	-
30	BCR	7	623	-	-	4/29/63/63	0/2/2/2
27	CLA	2	612	15	1/1/11/20	5/11/89/115	-
27	CLA	5	604	-	1/1/15/20	18/35/111/115	-
27	CLA	Y	612	24	1/1/11/20	4/13/91/115	-
27	CLA	a	603	-	1/1/12/20	3/23/101/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	LHG	Y	2630	27	-	11/53/53/53	-
30	BCR	A	852	-	-	8/29/63/63	0/2/2/2
33	LMG	8	626	-	-	15/41/61/70	0/1/1/1
27	CLA	F	301	-	1/1/13/20	8/28/106/115	-
27	CLA	2	601	15	1/1/15/20	14/37/115/115	-
35	LUT	4	619	-	-	4/29/67/67	0/2/2/2
27	CLA	8	610	21	1/1/14/20	8/31/109/115	-
37	NEX	6	624	-	-	2/27/83/83	0/3/3/3
27	CLA	X	614	-	1/1/10/20	4/10/88/115	-
32	LMU	A	857	-	-	3/21/61/61	0/2/2/2
38	CHL	U	606	-	3/3/15/26	0/13/111/137	-
36	XAT	V	1622	-	-	0/31/93/93	0/4/4/4
27	CLA	5	618	18	1/1/10/20	0/8/84/115	-
27	CLA	A	812	-	1/1/15/20	6/37/115/115	-
37	NEX	Y	1623	-	-	3/27/80/83	0/3/3/3
27	CLA	A	842	-	1/1/15/20	17/37/115/115	-
27	CLA	A	854	-	1/1/15/20	13/37/115/115	-
27	CLA	B	840	-	1/1/15/20	4/37/115/115	-
27	CLA	1	614	-	1/1/9/20	2/4/76/115	-
29	LHG	H	204	-	-	17/53/53/53	-
27	CLA	A	817	-	-	4/13/91/115	-
27	CLA	a	613	-	1/1/12/20	8/24/102/115	-
27	CLA	7	607	-	1/1/10/20	2/10/88/115	-
27	CLA	V	614	-	1/1/11/20	3/13/91/115	-
27	CLA	4	603	17	1/1/11/20	2/13/89/115	-
27	CLA	9	602	22	-	7/31/109/115	-
27	CLA	6	610	19	1/1/15/20	8/37/115/115	-
27	CLA	B	815	-	1/1/10/20	0/11/89/115	-
29	LHG	9	624	-	-	20/53/53/53	-
27	CLA	a	610	14	1/1/14/20	1/29/107/115	-
27	CLA	5	614	-	1/1/10/20	8/13/87/115	-
30	BCR	O	2005	-	-	5/29/63/63	0/2/2/2
33	LMG	J	104	-	-	15/35/55/70	0/1/1/1
27	CLA	A	811	-	1/1/15/20	11/37/115/115	-
27	CLA	1	603	-	1/1/12/20	4/21/99/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	CLA	A	828	-	1/1/15/20	9/37/115/115	-
33	LMG	4	624	-	-	8/35/55/70	0/1/1/1
37	NEX	X	1623	-	-	3/27/83/83	0/3/3/3
38	CHL	X	605	23	3/3/16/26	3/15/113/137	-
35	LUT	Z	1621	-	-	2/29/67/67	0/2/2/2
27	CLA	V	602	26	1/1/14/20	4/31/109/115	-
30	BCR	6	622	-	-	5/29/63/63	0/2/2/2
38	CHL	U	609	24	3/3/18/26	11/32/130/137	-
33	LMG	A	860	-	-	9/35/55/70	0/1/1/1
29	LHG	X	2630	27	-	11/53/53/53	-
35	LUT	X	1621	-	-	1/29/67/67	0/2/2/2
32	LMU	A	858	-	-	12/21/57/61	0/2/2/2
27	CLA	2	610	15	1/1/13/20	8/25/103/115	-
27	CLA	7	601	20	1/1/14/20	10/31/109/115	-
38	CHL	U	607	-	3/3/16/26	5/15/113/137	-
27	CLA	J	101	10	1/1/10/20	4/10/88/115	-
27	CLA	4	613	17	1/1/15/20	12/37/115/115	-
36	XAT	5	621	-	-	0/31/93/93	0/4/4/4
30	BCR	A	848	-	-	1/29/63/63	0/2/2/2
36	XAT	W	1622	-	-	1/31/93/93	0/4/4/4
36	XAT	X	1622	-	-	0/31/93/93	0/4/4/4
27	CLA	7	615	-	1/1/10/20	6/8/84/115	-
27	CLA	3	609	16	1/1/14/20	15/31/109/115	-
29	LHG	B	854	-	-	17/53/53/53	-
27	CLA	B	807	-	-	1/22/100/115	-
27	CLA	8	616	-	1/1/11/20	4/11/87/115	-
27	CLA	B	829	-	1/1/15/20	11/37/115/115	-
38	CHL	U	608	-	3/3/15/26	3/13/111/137	-
37	NEX	W	1623	-	-	4/27/83/83	0/3/3/3
27	CLA	7	612	20	1/1/11/20	5/11/89/115	-
27	CLA	B	822	-	-	4/10/88/115	-
27	CLA	A	808	-	-	3/19/97/115	-
27	CLA	A	841	-	1/1/15/20	16/37/115/115	-
27	CLA	3	610	16	1/1/15/20	12/37/115/115	-
30	BCR	a	619	-	-	4/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	CLA	X	602	23	1/1/15/20	10/37/115/115	-
27	CLA	3	614	-	1/1/10/20	1/6/84/115	-
27	CLA	A	845	29	1/1/12/20	4/19/97/115	-
27	CLA	1	602	14	1/1/14/20	3/33/111/115	-
27	CLA	B	837	-	-	12/37/115/115	-
27	CLA	7	606	-	-	2/8/86/115	-
36	XAT	8	620	-	-	0/31/93/93	0/4/4/4
35	LUT	Y	1621	-	-	1/29/67/67	0/2/2/2
35	LUT	V	1621	-	-	2/29/67/67	0/2/2/2
27	CLA	W	603	-	1/1/12/20	8/22/100/115	-
27	CLA	O	2003	-	1/1/10/20	3/6/84/115	-
27	CLA	K	204	-	1/1/11/20	5/13/91/115	-
38	CHL	W	601	23	3/3/20/26	18/39/137/137	-
27	CLA	8	603	-	1/1/11/20	4/13/89/115	-
27	CLA	A	839	-	1/1/13/20	6/25/103/115	-
27	CLA	B	839	-	1/1/15/20	14/37/115/115	-
38	CHL	Y	606	-	3/3/16/26	2/15/113/137	-
28	PQN	A	844	-	-	11/23/43/43	0/2/2/2
30	BCR	J	102	-	-	3/29/63/63	0/2/2/2
27	CLA	5	619	-	1/1/11/20	6/11/87/115	-
27	CLA	6	608	-	1/1/11/20	4/13/91/115	-
27	CLA	Y	613	24	1/1/15/20	16/37/115/115	-
27	CLA	B	832	-	-	9/31/109/115	-
27	CLA	4	601	17	1/1/15/20	15/37/115/115	-
27	CLA	H	203	-	-	12/37/115/115	-
27	CLA	A	834	-	1/1/15/20	13/37/115/115	-
27	CLA	A	836	-	1/1/15/20	5/37/115/115	-
27	CLA	6	609	19	1/1/11/20	2/13/91/115	-
29	LHG	7	622	27	-	21/41/41/53	-
27	CLA	6	603	-	1/1/12/20	4/22/98/115	-
27	CLA	8	604	-	1/1/12/20	4/19/97/115	-
27	CLA	3	615	-	1/1/10/20	2/6/84/115	-
27	CLA	5	610	18	1/1/12/20	4/24/102/115	-
27	CLA	a	609	14	1/1/15/20	12/35/113/115	-
27	CLA	Y	611	29	1/1/10/20	6/11/89/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	CLA	W	613	23	1/1/15/20	14/37/115/115	-
27	CLA	L	303	-	-	13/37/115/115	-
27	CLA	V	611	29	1/1/10/20	5/11/89/115	-
38	CHL	U	605	24	3/3/15/26	3/12/110/137	-
27	CLA	X	610	23	1/1/15/20	7/37/115/115	-
27	CLA	5	603	-	1/1/13/20	6/25/101/115	-
27	CLA	A	821	-	1/1/12/20	12/23/101/115	-
29	LHG	6	623	27	-	25/52/52/53	-
27	CLA	1	610	14	1/1/9/20	0/6/80/115	-
30	BCR	L	301	-	-	4/29/63/63	0/2/2/2
38	CHL	Y	605	24	3/3/15/26	2/10/108/137	-
27	CLA	B	835	-	1/1/11/20	4/13/91/115	-
27	CLA	A	837	1	-	9/13/91/115	-
38	CHL	X	609	23	3/3/20/26	17/39/137/137	-
30	BCR	7	621	-	-	5/29/63/63	0/2/2/2
27	CLA	1	608	-	1/1/11/20	3/11/89/115	-
27	CLA	H	202	8	1/1/10/20	1/4/82/115	-
35	LUT	U	1621	-	-	1/29/67/67	0/2/2/2
27	CLA	9	601	22	1/1/11/20	2/13/91/115	-
27	CLA	a	604	-	1/1/11/20	9/18/96/115	-
27	CLA	7	608	-	1/1/12/20	3/19/97/115	-
27	CLA	6	613	-	1/1/15/20	14/35/113/115	-
27	CLA	3	602	16	1/1/14/20	4/31/109/115	-
27	CLA	B	814	-	1/1/14/20	10/34/112/115	-
30	BCR	B	847	-	-	2/29/63/63	0/2/2/2
27	CLA	V	613	26	1/1/15/20	18/37/115/115	-
35	LUT	3	618	-	-	0/29/67/67	0/2/2/2
27	CLA	a	616	14	1/1/11/20	5/13/91/115	-
27	CLA	7	611	29	1/1/13/20	5/29/107/115	-
27	CLA	9	607	-	-	6/13/91/115	-
27	CLA	2	607	-	1/1/11/20	3/13/91/115	-
27	CLA	9	613	22	1/1/15/20	6/37/115/115	-
30	BCR	B	846	-	-	2/29/63/63	0/2/2/2
27	CLA	A	801	-	1/1/15/20	9/37/115/115	-
27	CLA	X	613	23	1/1/15/20	16/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
38	CHL	U	601	24	3/3/20/26	21/39/137/137	-
27	CLA	A	805	-	-	5/22/100/115	-
27	CLA	a	614	-	1/1/12/20	9/25/99/115	-
29	LHG	4	622	27	-	10/53/53/53	-
27	CLA	A	829	-	1/1/15/20	15/37/115/115	-
27	CLA	B	804	-	1/1/10/20	0/8/86/115	-
27	CLA	X	611	29	1/1/11/20	8/13/91/115	-
30	BCR	B	848	-	-	3/29/63/63	0/2/2/2
29	LHG	A	846	-	-	14/53/53/53	-
27	CLA	L	304	-	1/1/11/20	1/13/91/115	-
27	CLA	4	604	-	1/1/13/20	8/25/101/115	-
27	CLA	Z	610	25	1/1/15/20	11/37/115/115	-
38	CHL	X	601	23	3/3/20/26	22/39/137/137	-
36	XAT	7	620	-	-	0/31/93/93	0/4/4/4
27	CLA	5	607	-	1/1/15/20	14/37/115/115	-
29	LHG	3	624	27	-	23/53/53/53	-
27	CLA	A	819	-	1/1/13/20	6/30/108/115	-
27	CLA	G	204	7	1/1/11/20	5/13/91/115	-
27	CLA	B	809	2	1/1/15/20	15/37/115/115	-
27	CLA	U	602	24	1/1/13/20	7/30/108/115	-
27	CLA	Y	603	-	1/1/13/20	7/25/103/115	-
27	CLA	2	602	15	1/1/15/20	9/35/113/115	-
27	CLA	A	810	1	1/1/12/20	8/19/97/115	-
29	LHG	Z	2630	27	-	17/53/53/53	-
30	BCR	K	207	-	-	1/29/63/63	0/2/2/2
27	CLA	B	836	-	1/1/12/20	4/19/97/115	-
27	CLA	4	614	-	1/1/13/20	9/27/105/115	-
27	CLA	X	604	-	1/1/11/20	5/18/96/115	-
29	LHG	B	851	27	-	11/42/42/53	-
30	BCR	B	852	-	-	7/29/63/63	0/2/2/2
27	CLA	A	830	-	1/1/15/20	11/37/115/115	-
27	CLA	a	602	14	1/1/14/20	3/33/111/115	-
27	CLA	5	609	18	1/1/15/20	12/37/115/115	-
27	CLA	F	303	-	-	5/10/88/115	-
27	CLA	Y	610	24	1/1/15/20	7/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	CLA	A	820	-	1/1/15/20	13/37/115/115	-
27	CLA	U	611	29	1/1/10/20	6/10/88/115	-
29	LHG	9	622	27	-	12/34/34/53	-
27	CLA	9	606	-	1/1/10/20	2/6/84/115	-
37	NEX	Z	1623	-	-	3/27/83/83	0/3/3/3
29	LHG	2	622	27	-	13/40/40/53	-
36	XAT	3	619	-	-	0/31/93/93	0/4/4/4
27	CLA	8	609	21	1/1/11/20	4/13/91/115	-
27	CLA	6	607	-	1/1/10/20	5/10/86/115	-
30	BCR	B	801	-	-	4/29/63/63	0/2/2/2
30	BCR	3	620	-	-	4/29/63/63	0/2/2/2
27	CLA	6	612	19	1/1/10/20	2/8/86/115	-
30	BCR	A	856	-	-	2/29/63/63	0/2/2/2
27	CLA	5	608	-	1/1/12/20	6/19/97/115	-
37	NEX	U	1623	-	-	4/27/83/83	0/3/3/3
27	CLA	6	618	19	1/1/10/20	0/8/84/115	-
27	CLA	1	601	14	-	2/23/101/115	-
27	CLA	4	602	17	1/1/14/20	5/31/109/115	-
27	CLA	8	614	-	1/1/12/20	9/23/101/115	-
36	XAT	4	620	-	-	0/31/93/93	0/4/4/4
27	CLA	6	620	-	1/1/14/20	11/35/113/115	-
27	CLA	W	604	-	1/1/11/20	4/16/94/115	-
33	LMG	4	623	-	-	5/35/55/70	0/1/1/1
27	CLA	B	802	-	1/1/15/20	20/37/115/115	-
38	CHL	V	607	-	3/3/16/26	2/15/113/137	-
29	LHG	V	2630	27	-	9/52/52/53	-
35	LUT	8	619	-	-	1/29/67/67	0/2/2/2
27	CLA	5	616	18	1/1/10/20	3/8/84/115	-
27	CLA	1	607	-	1/1/10/20	1/6/84/115	-
27	CLA	7	609	20	1/1/10/20	4/10/88/115	-
29	LHG	5	623	27	-	14/53/53/53	-
35	LUT	7	619	-	-	1/29/67/67	0/2/2/2
27	CLA	3	611	29	1/1/10/20	2/4/80/115	-
27	CLA	3	606	-	1/1/13/20	6/23/101/115	-
27	CLA	U	610	24	1/1/13/20	5/27/105/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
33	LMG	5	627	-	-	11/35/55/70	0/1/1/1
27	CLA	A	814	-	1/1/15/20	16/37/115/115	-
30	BCR	5	622	-	-	3/29/63/63	0/2/2/2
30	BCR	3	622	-	-	2/29/63/63	0/2/2/2
38	CHL	Y	609	24	3/3/20/26	14/39/137/137	-
27	CLA	B	818	-	-	13/31/109/115	-
33	LMG	V	2631	-	-	9/36/56/70	0/1/1/1
38	CHL	W	608	-	3/3/16/26	5/17/115/137	-
27	CLA	W	614	-	1/1/11/20	3/13/91/115	-
27	CLA	8	601	21	1/1/15/20	16/37/115/115	-
37	NEX	V	1623	-	-	4/27/83/83	0/3/3/3
29	LHG	3	623	-	-	20/49/49/53	-
27	CLA	6	604	-	-	13/37/115/115	-
27	CLA	B	826	-	1/1/14/20	6/34/112/115	-
32	LMU	K	208	-	-	14/21/61/61	0/2/2/2
27	CLA	2	609	15	1/1/11/20	2/13/91/115	-
27	CLA	6	611	29	1/1/10/20	2/10/88/115	-
38	CHL	Y	601	24	3/3/20/26	22/39/137/137	-
27	CLA	Y	604	-	1/1/12/20	3/19/97/115	-
38	CHL	Y	607	-	3/3/20/26	21/39/137/137	-
38	CHL	V	601	26	3/3/20/26	14/39/137/137	-
33	LMG	9	625	-	-	16/50/70/70	0/1/1/1
27	CLA	3	608	-	1/1/13/20	2/25/103/115	-
27	CLA	7	613	20	1/1/15/20	11/37/115/115	-
27	CLA	A	804	-	1/1/15/20	16/37/115/115	-
27	CLA	9	604	-	1/1/12/20	3/20/96/115	-
27	CLA	2	613	15	1/1/15/20	7/37/115/115	-
27	CLA	9	612	22	1/1/10/20	2/8/86/115	-
37	NEX	5	624	-	-	2/27/83/83	0/3/3/3
27	CLA	B	808	-	1/1/15/20	14/37/115/115	-
27	CLA	6	606	-	1/1/10/20	0/6/84/115	-
27	CLA	B	841	29	1/1/15/20	10/37/115/115	-
27	CLA	9	611	29	1/1/10/20	3/10/88/115	-
27	CLA	6	614	-	1/1/14/20	9/31/109/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	CLA	B	813	-	1/1/15/20	19/37/115/115	-
33	LMG	H	205	-	-	8/50/70/70	0/1/1/1
27	CLA	5	602	18	-	14/37/115/115	-
32	LMU	1	621	-	-	7/21/61/61	0/2/2/2
27	CLA	B	812	-	1/1/10/20	3/11/89/115	-
27	CLA	L	302	12	1/1/11/20	4/13/91/115	-
27	CLA	3	603	-	1/1/13/20	6/25/103/115	-
38	CHL	X	607	-	3/3/20/26	17/39/137/137	-
27	CLA	B	803	-	1/1/15/20	11/37/115/115	-
35	LUT	6	619	-	-	0/29/67/67	0/2/2/2
32	LMU	5	628	-	-	9/19/59/61	0/2/2/2
27	CLA	B	827	-	1/1/14/20	17/34/112/115	-
27	CLA	B	817	-	1/1/13/20	7/30/108/115	-
27	CLA	2	616	-	1/1/11/20	4/11/87/115	-
27	CLA	1	606	-	1/1/8/20	3/5/79/115	-
27	CLA	7	604	-	1/1/12/20	7/19/97/115	-
35	LUT	W	1620	-	-	2/29/67/67	0/2/2/2
27	CLA	W	612	23	1/1/11/20	4/13/91/115	-
27	CLA	3	613	16	1/1/12/20	7/21/99/115	-
27	CLA	G	203	-	1/1/10/20	2/10/88/115	-
36	XAT	2	620	-	-	0/31/93/93	0/4/4/4
29	LHG	8	622	27	-	9/53/53/53	-
27	CLA	L	307	-	1/1/10/20	0/6/84/115	-
27	CLA	A	835	-	-	11/33/111/115	-
27	CLA	A	802	-	1/1/15/20	9/37/115/115	-
27	CLA	A	813	-	1/1/12/20	6/24/102/115	-
36	XAT	U	1622	-	-	1/31/93/93	0/4/4/4
27	CLA	Y	602	24	1/1/13/20	7/29/107/115	-
30	BCR	B	844	-	-	2/29/63/63	0/2/2/2
38	CHL	Z	606	-	3/3/16/26	4/15/113/137	-
27	CLA	8	606	-	1/1/15/20	7/35/113/115	-
27	CLA	O	2001	-	1/1/9/20	1/4/78/115	-
27	CLA	A	815	-	1/1/12/20	8/19/97/115	-
27	CLA	B	834	-	1/1/14/20	7/31/109/115	-
38	CHL	W	609	23	3/3/20/26	16/39/137/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	CLA	B	806	2	1/1/15/20	16/37/115/115	-
27	CLA	7	610	20	1/1/15/20	2/37/115/115	-
38	CHL	V	606	-	3/3/15/26	3/13/111/137	-
27	CLA	8	607	-	1/1/10/20	5/10/86/115	-
27	CLA	A	823	-	1/1/10/20	2/10/88/115	-
27	CLA	A	831	-	1/1/15/20	12/37/115/115	-
27	CLA	9	609	22	1/1/14/20	8/33/111/115	-
27	CLA	9	603	22	1/1/11/20	2/13/89/115	-
27	CLA	8	612	21	1/1/10/20	2/8/86/115	-
38	CHL	Z	608	-	3/3/16/26	6/20/118/137	-
27	CLA	A	843	-	1/1/14/20	12/35/113/115	-
35	LUT	9	619	-	-	1/29/67/67	0/2/2/2
38	CHL	Z	607	-	3/3/20/26	19/39/137/137	-
36	XAT	Y	1622	-	-	0/31/93/93	0/4/4/4
27	CLA	Z	611	29	1/1/15/20	6/37/115/115	-
27	CLA	5	606	-	-	1/6/84/115	-
29	LHG	1	620	27	-	11/53/53/53	-
27	CLA	A	825	-	1/1/15/20	19/37/115/115	-
31	SF4	A	853	2,1	-	-	0/6/5/5
27	CLA	W	611	29	1/1/13/20	12/28/106/115	-
38	CHL	Y	608	-	3/3/16/26	6/19/117/137	-
38	CHL	V	605	26	3/3/15/26	0/13/111/137	-
27	CLA	A	838	-	1/1/12/20	7/19/97/115	-
32	LMU	8	625	-	-	9/21/61/61	0/2/2/2
38	CHL	V	608	-	3/3/16/26	5/18/116/137	-
27	CLA	U	603	-	1/1/12/20	8/22/100/115	-
27	CLA	a	612	14	1/1/11/20	5/13/91/115	-
27	CLA	7	602	20	1/1/15/20	13/37/115/115	-
27	CLA	5	611	29	1/1/10/20	5/10/88/115	-
27	CLA	B	830	-	1/1/10/20	2/11/89/115	-
27	CLA	1	604	-	1/1/11/20	9/18/96/115	-
27	CLA	a	607	-	1/1/11/20	3/13/91/115	-
27	CLA	O	2002	-	1/1/10/20	0/4/80/115	-
27	CLA	V	604	-	1/1/12/20	4/19/97/115	-
30	BCR	B	843	-	-	4/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	CLA	K	203	-	-	6/27/105/115	-
29	LHG	8	623	-	-	10/44/44/53	-
27	CLA	2	611	29	1/1/10/20	3/10/88/115	-
27	CLA	A	807	1	1/1/15/20	18/37/115/115	-
33	LMG	J	103	-	-	5/37/57/70	0/1/1/1
27	CLA	1	611	29	1/1/13/20	5/28/106/115	-

The worst 5 of 3112 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	A	844	PQN	C12-C13	9.80	1.56	1.33
28	B	842	PQN	C12-C13	9.64	1.56	1.33
27	X	602	CLA	C4B-NB	8.26	1.42	1.35
27	Y	610	CLA	C4B-NB	8.25	1.42	1.35
27	X	610	CLA	C4B-NB	8.24	1.42	1.35

The worst 5 of 4865 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	W	606	CHL	O2A-CGA-O1A	-17.62	79.39	123.30
30	B	852	BCR	C32-C1-C6	-14.75	86.38	110.30
38	W	606	CHL	O2A-CGA-CBA	14.42	160.37	114.03
30	6	622	BCR	C40-C30-C25	-14.02	87.56	110.30
36	U	1622	XAT	C37-C21-C36	-14.00	86.72	107.37

5 of 379 chirality outliers are listed below:

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

5 of 3214 torsion outliers are listed below:

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

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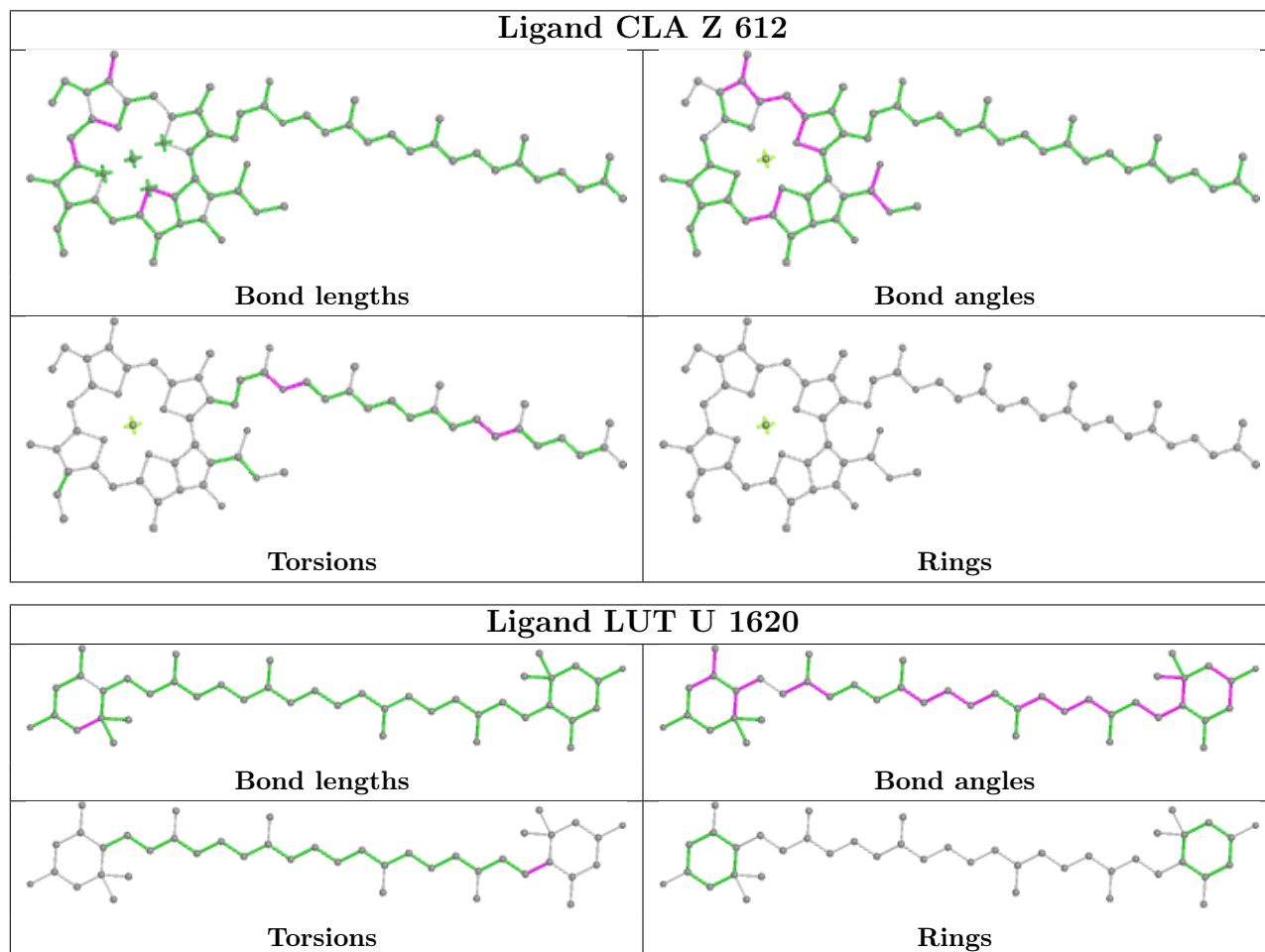
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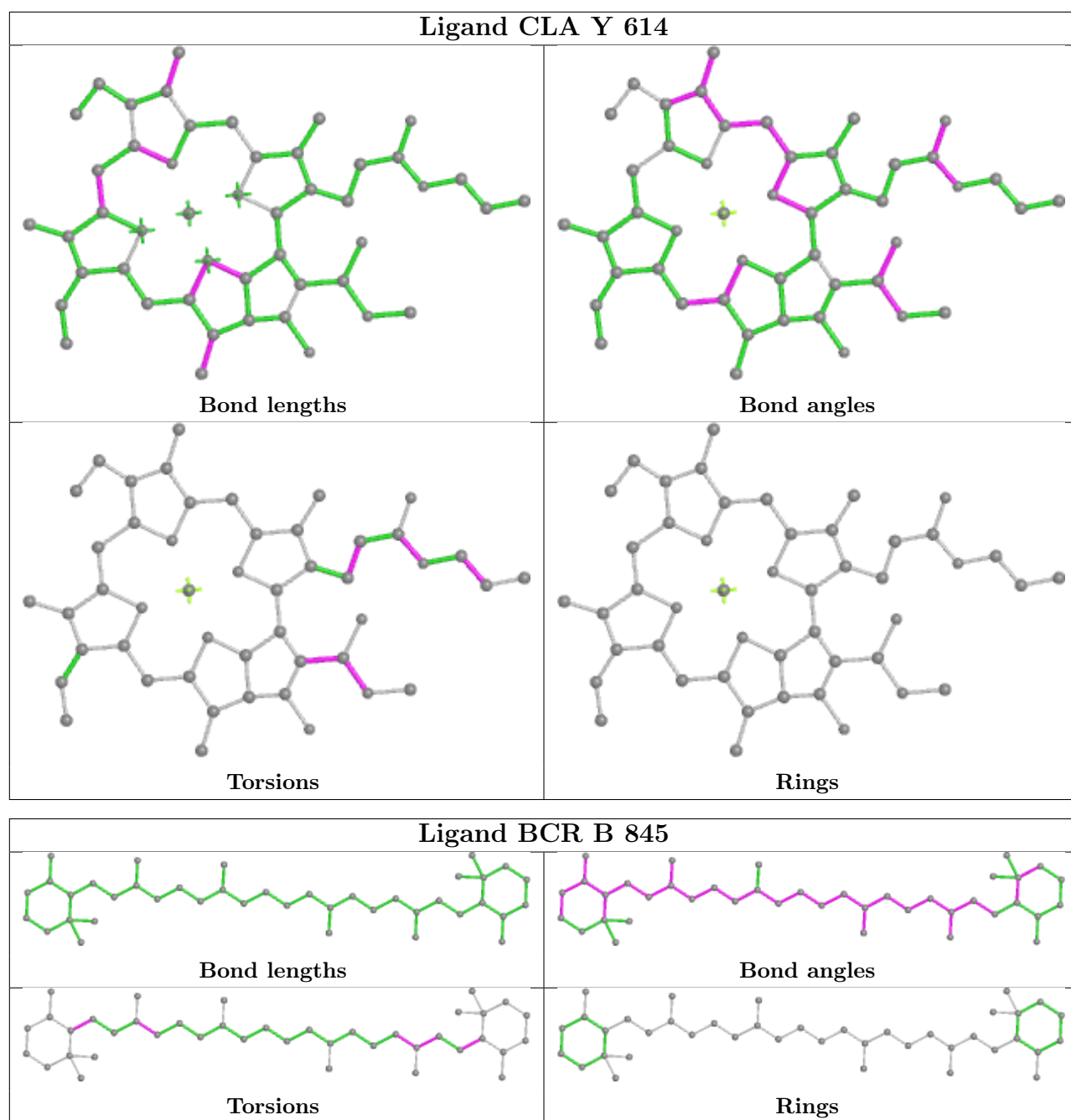
Mol	Chain	Res	Type	Atoms
27	A	804	CLA	C3A-C2A-CAA-CBA
27	A	805	CLA	C3A-C2A-CAA-CBA

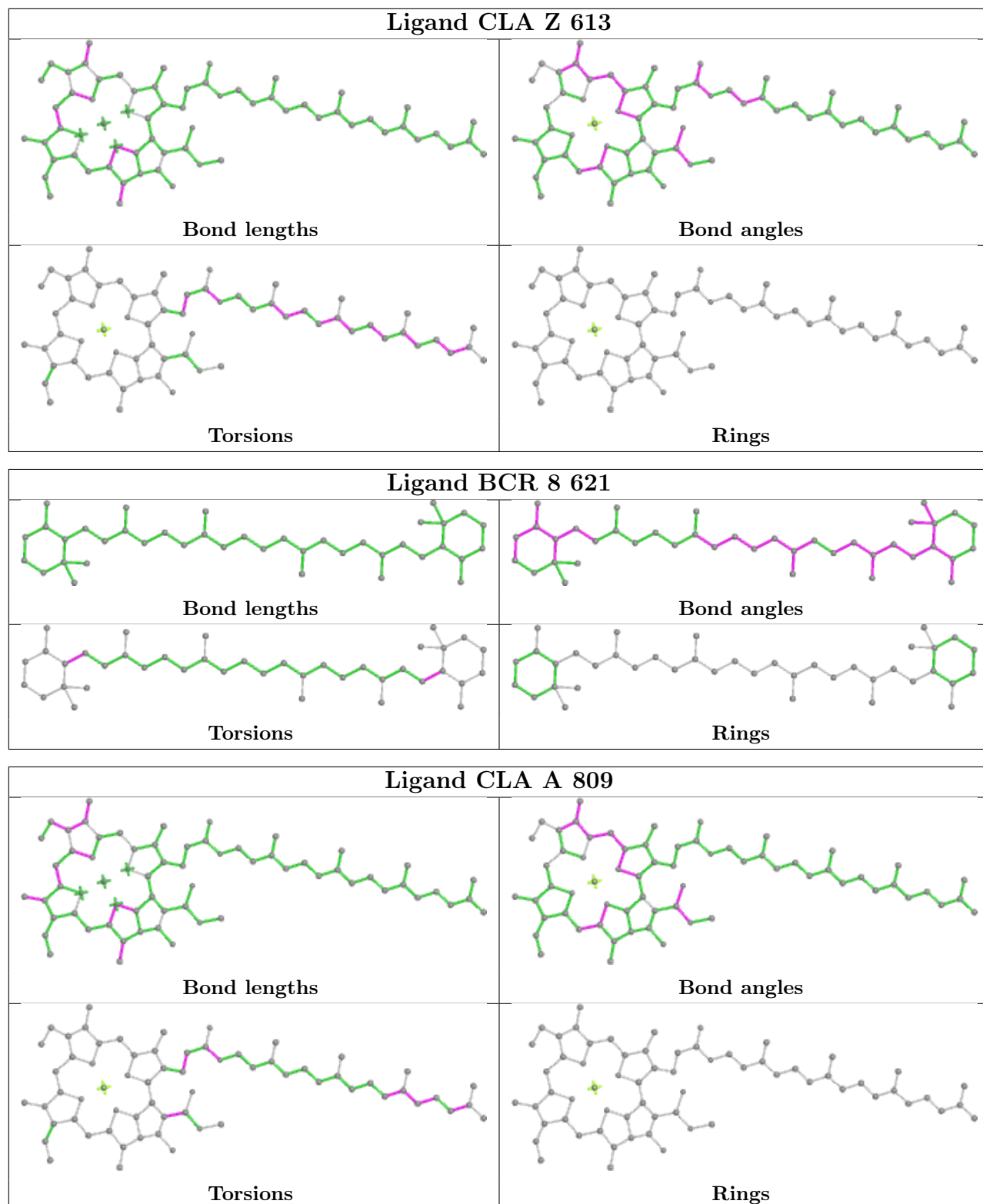
There are no ring outliers.

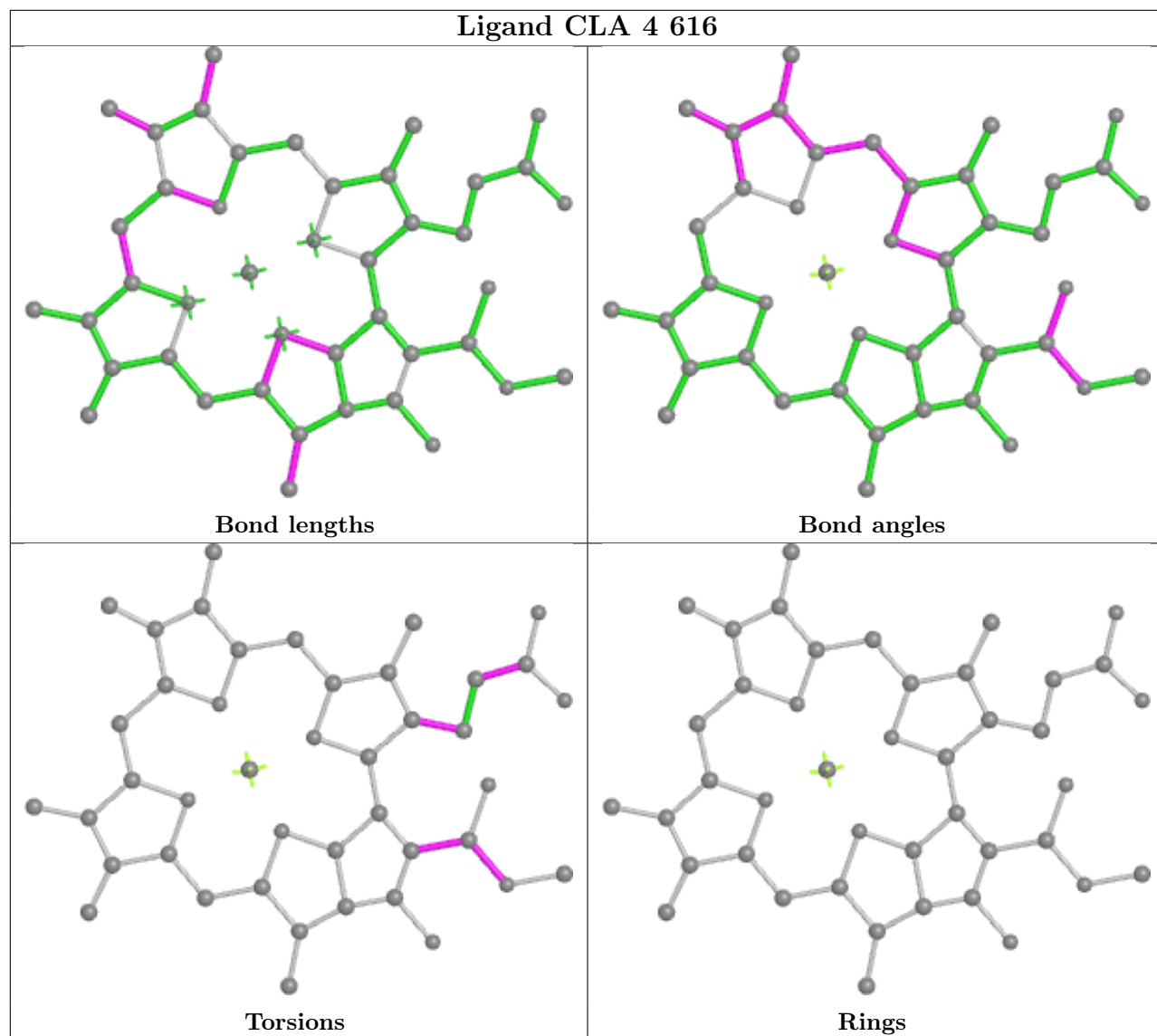
No monomer is involved in short contacts.

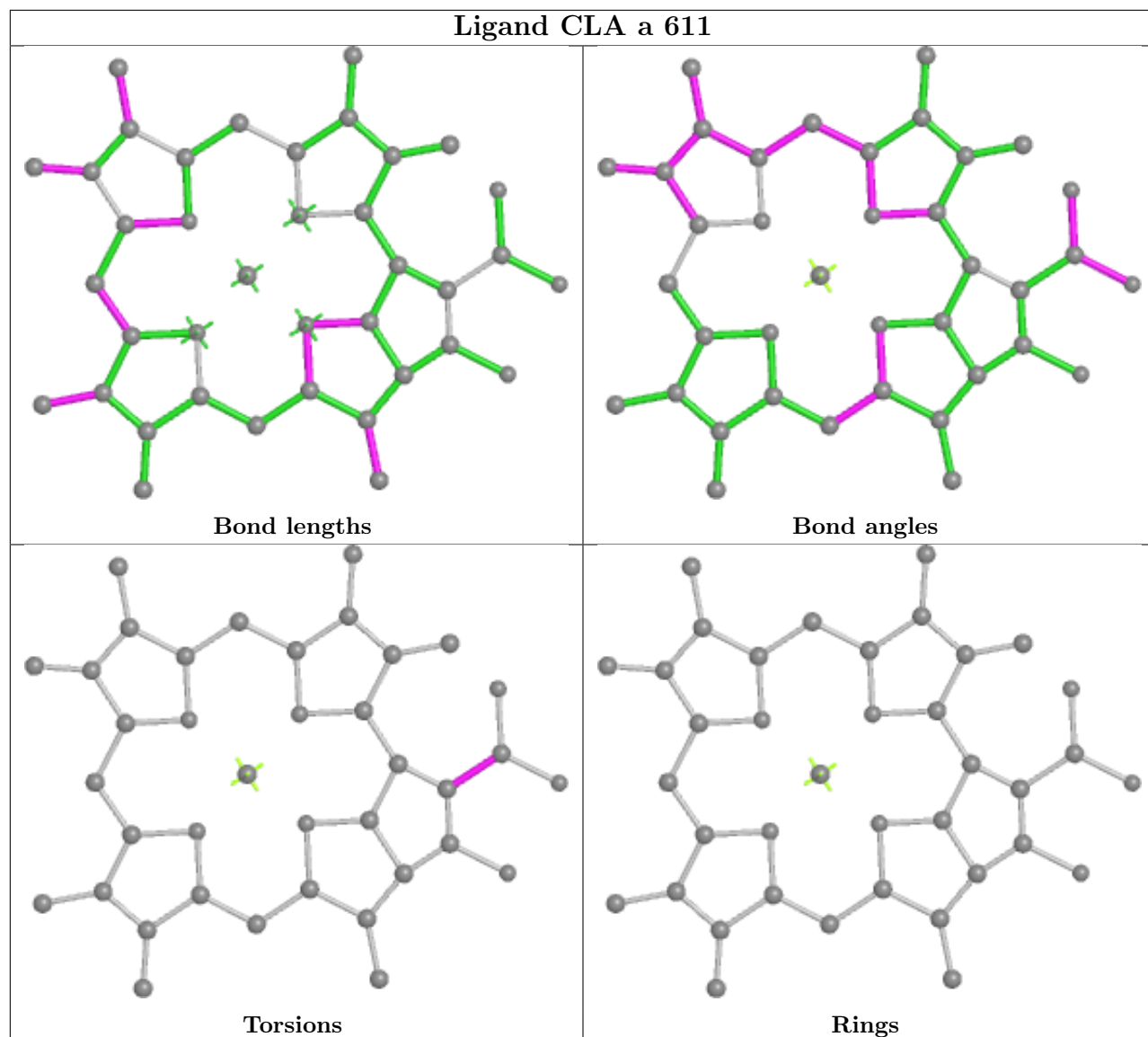
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

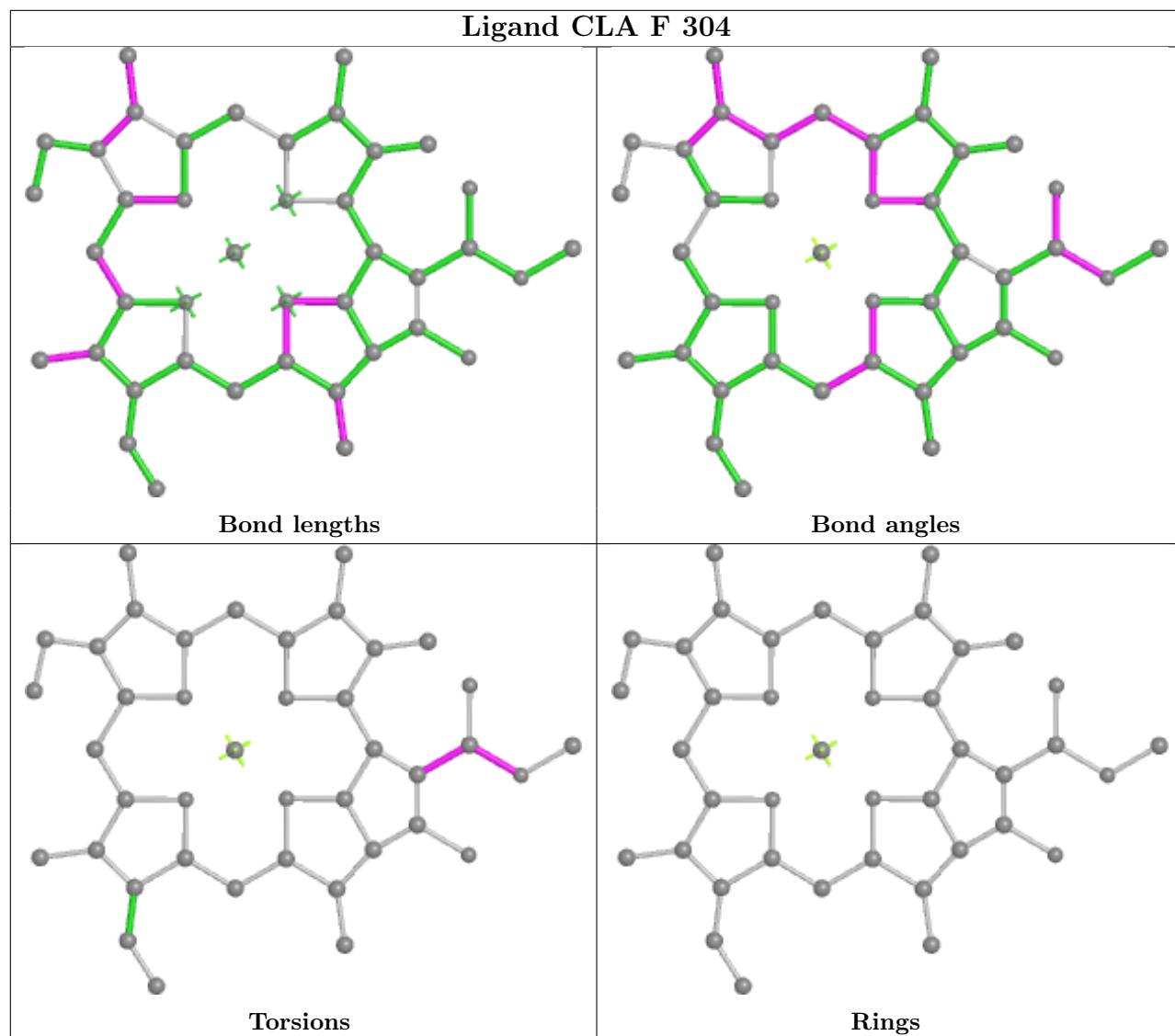


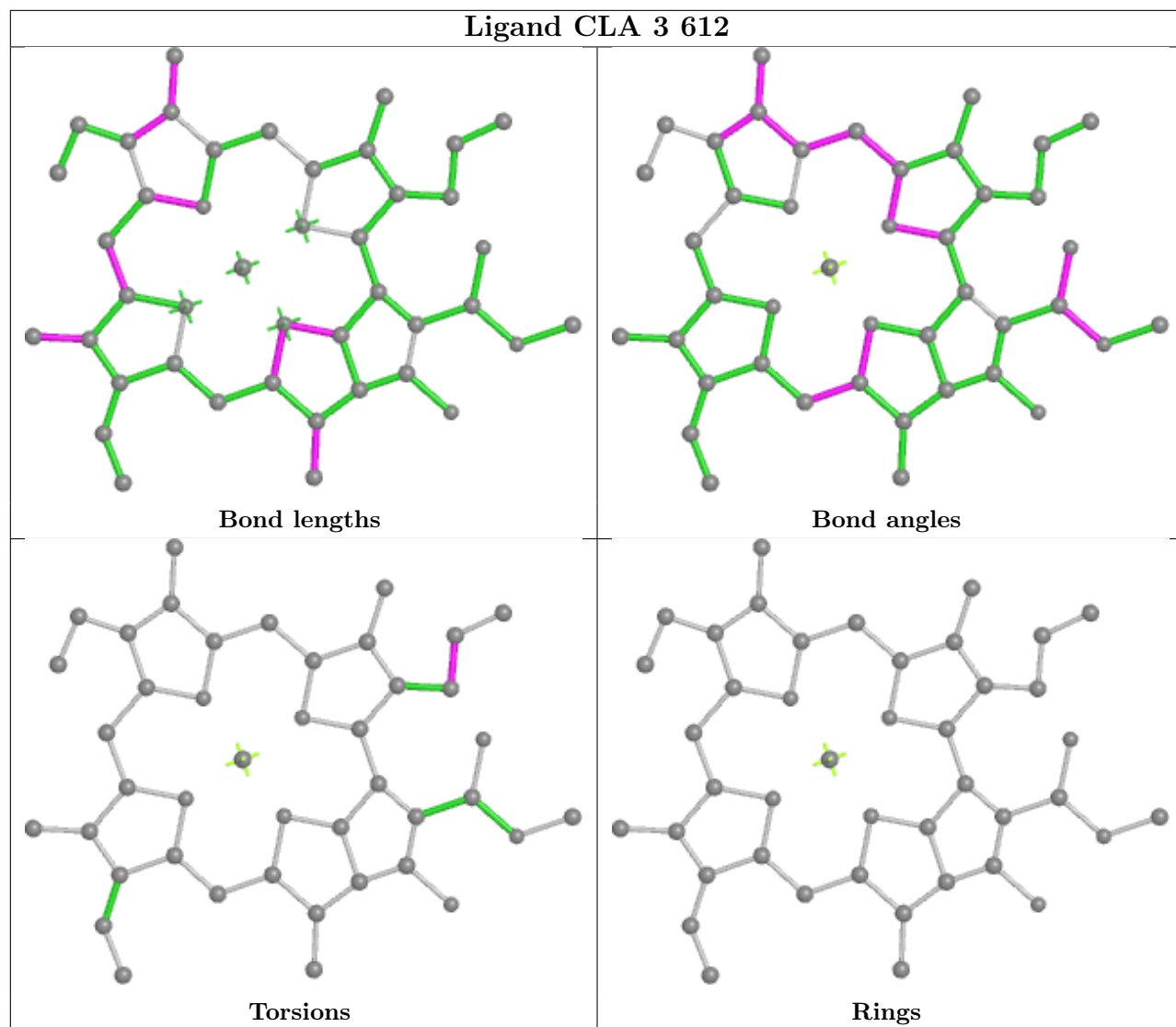




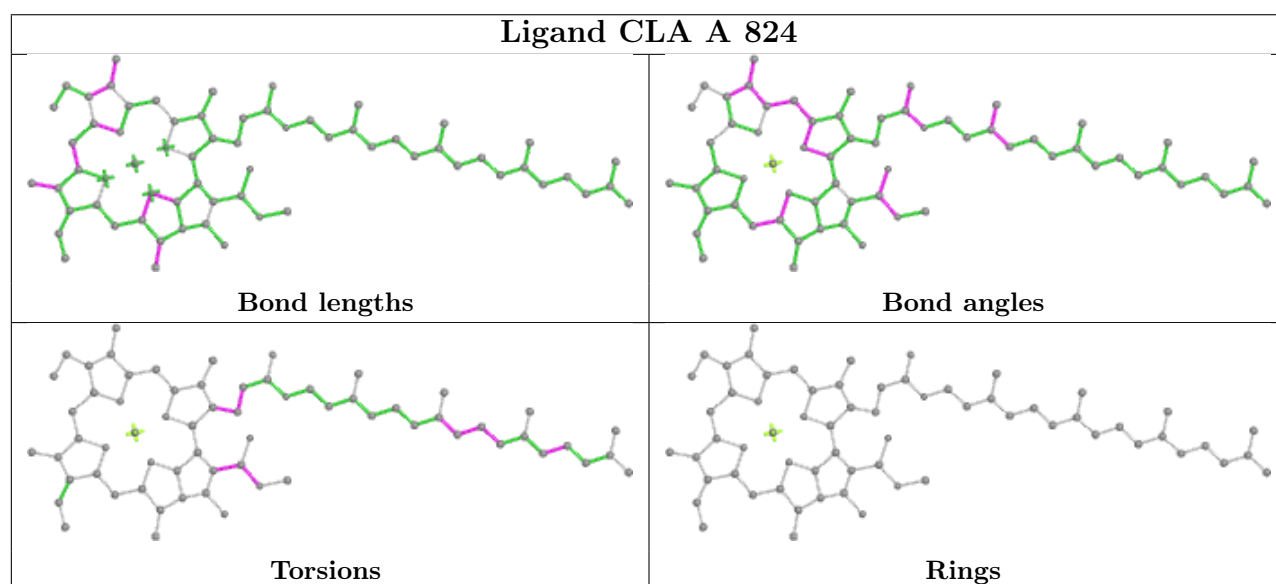
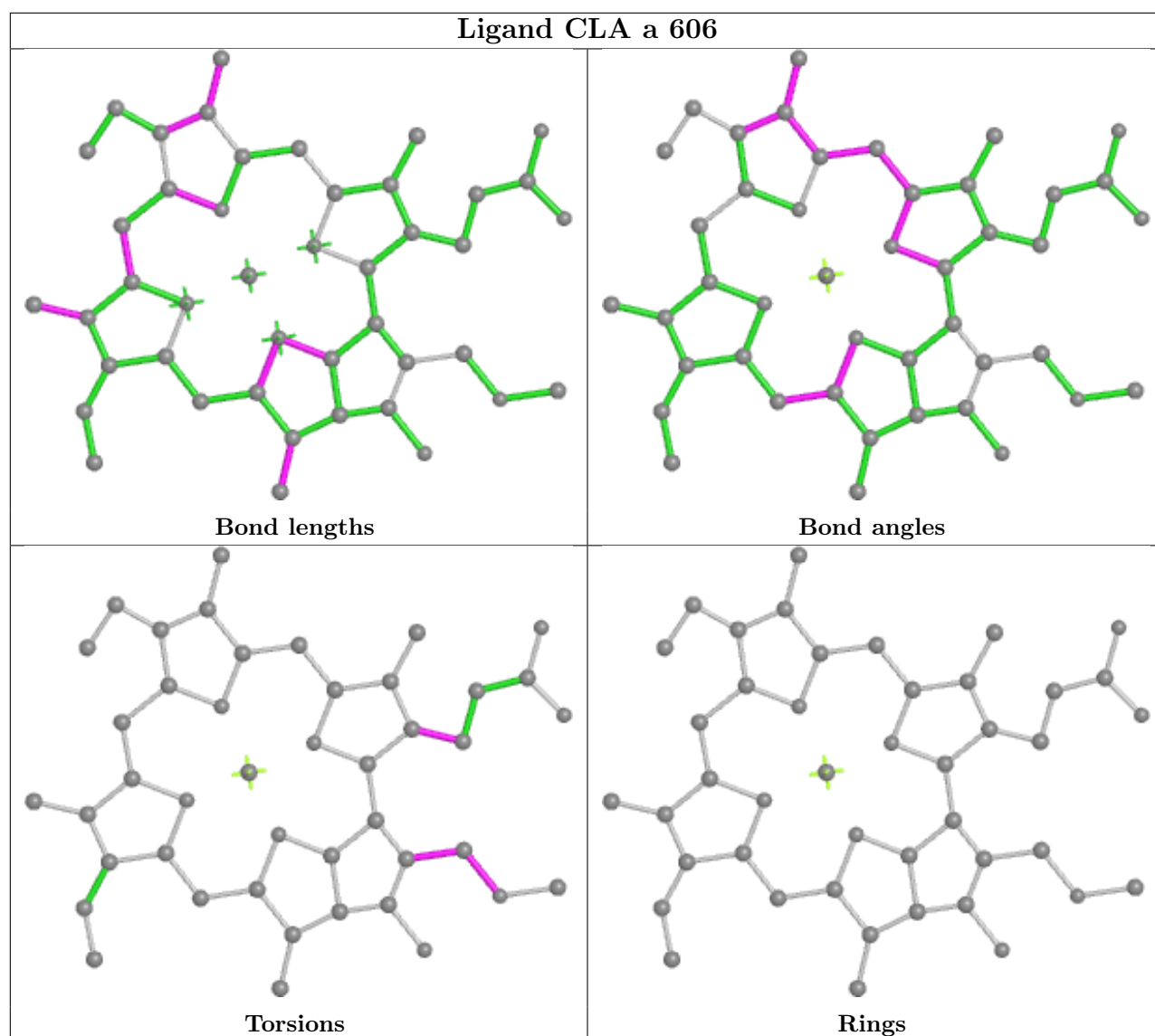


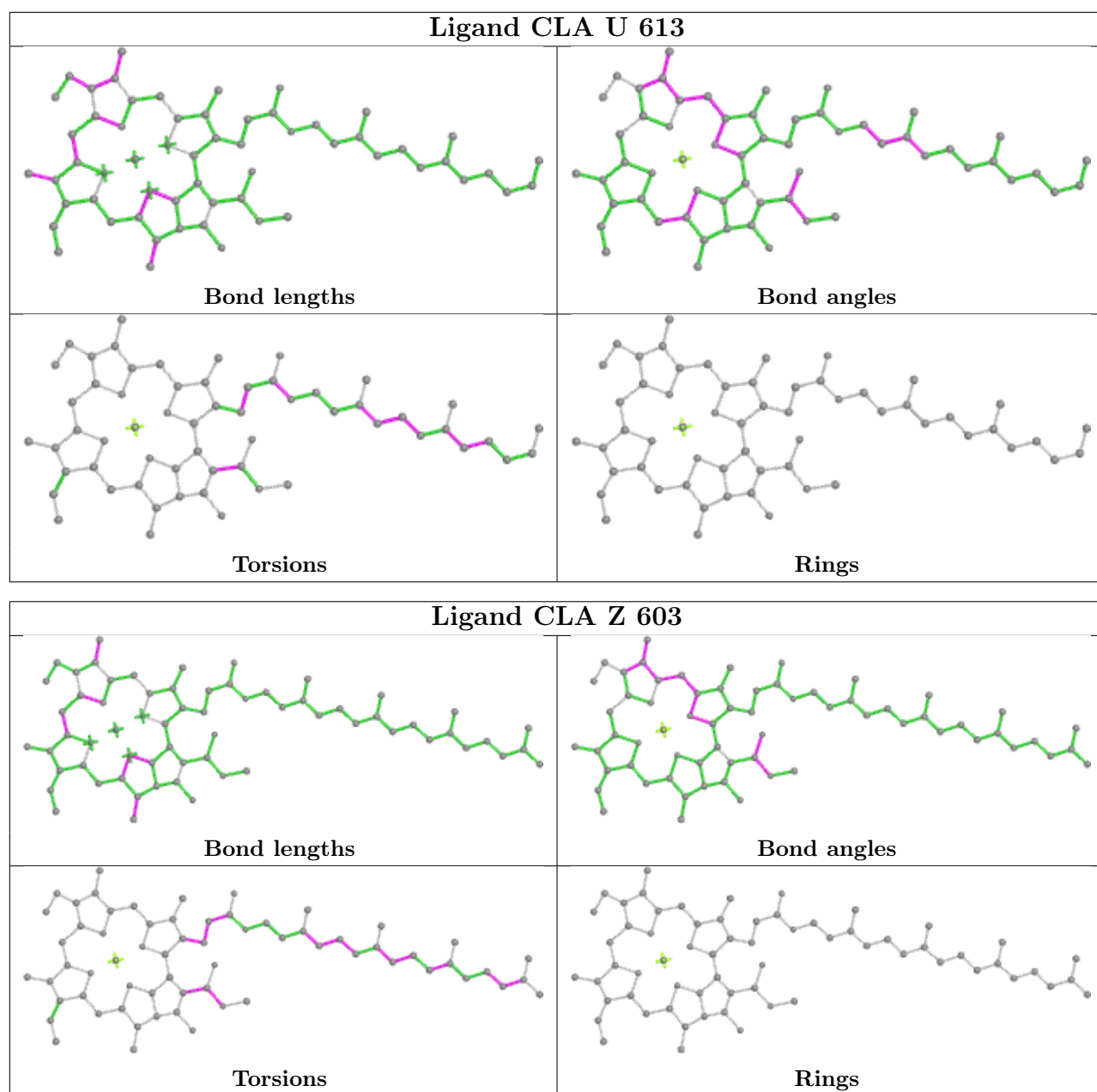


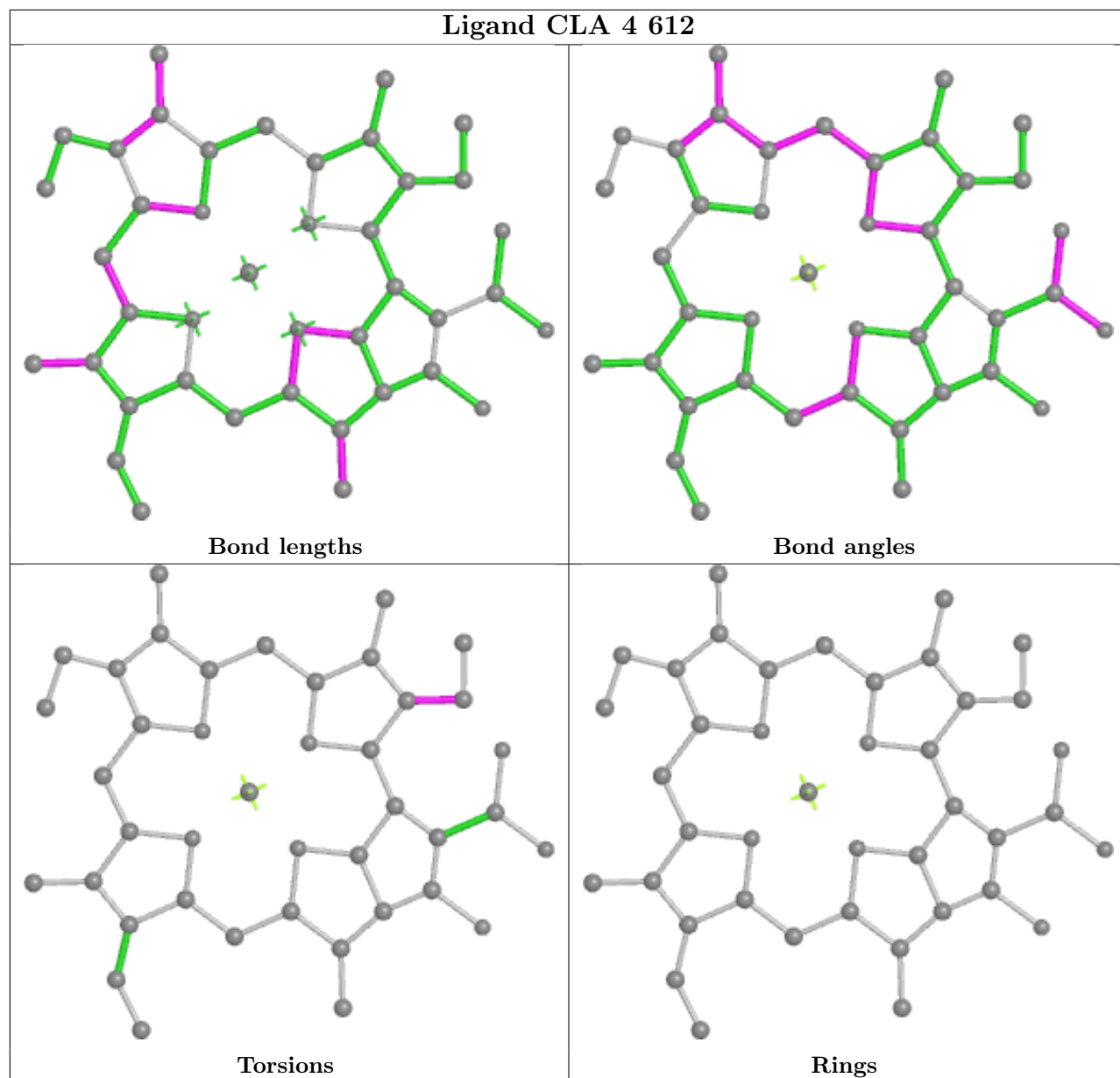


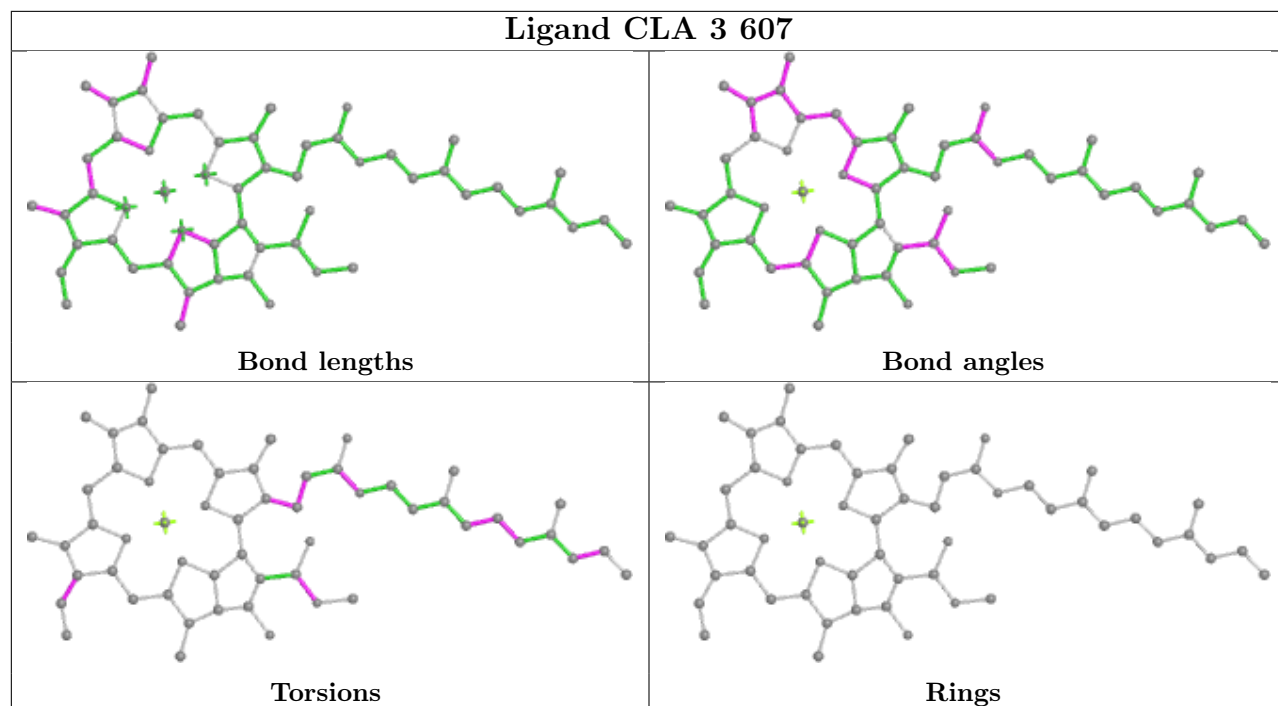


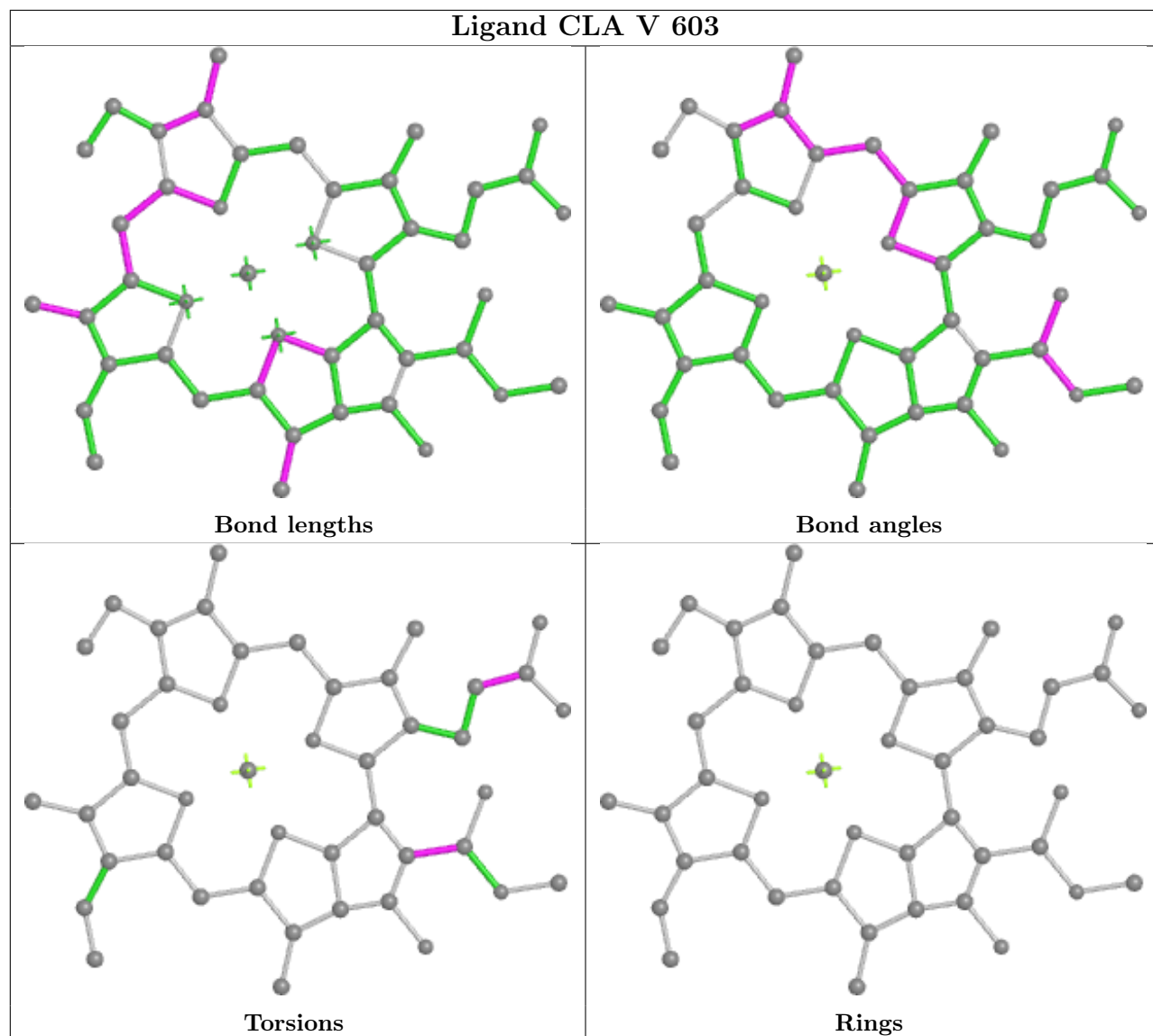


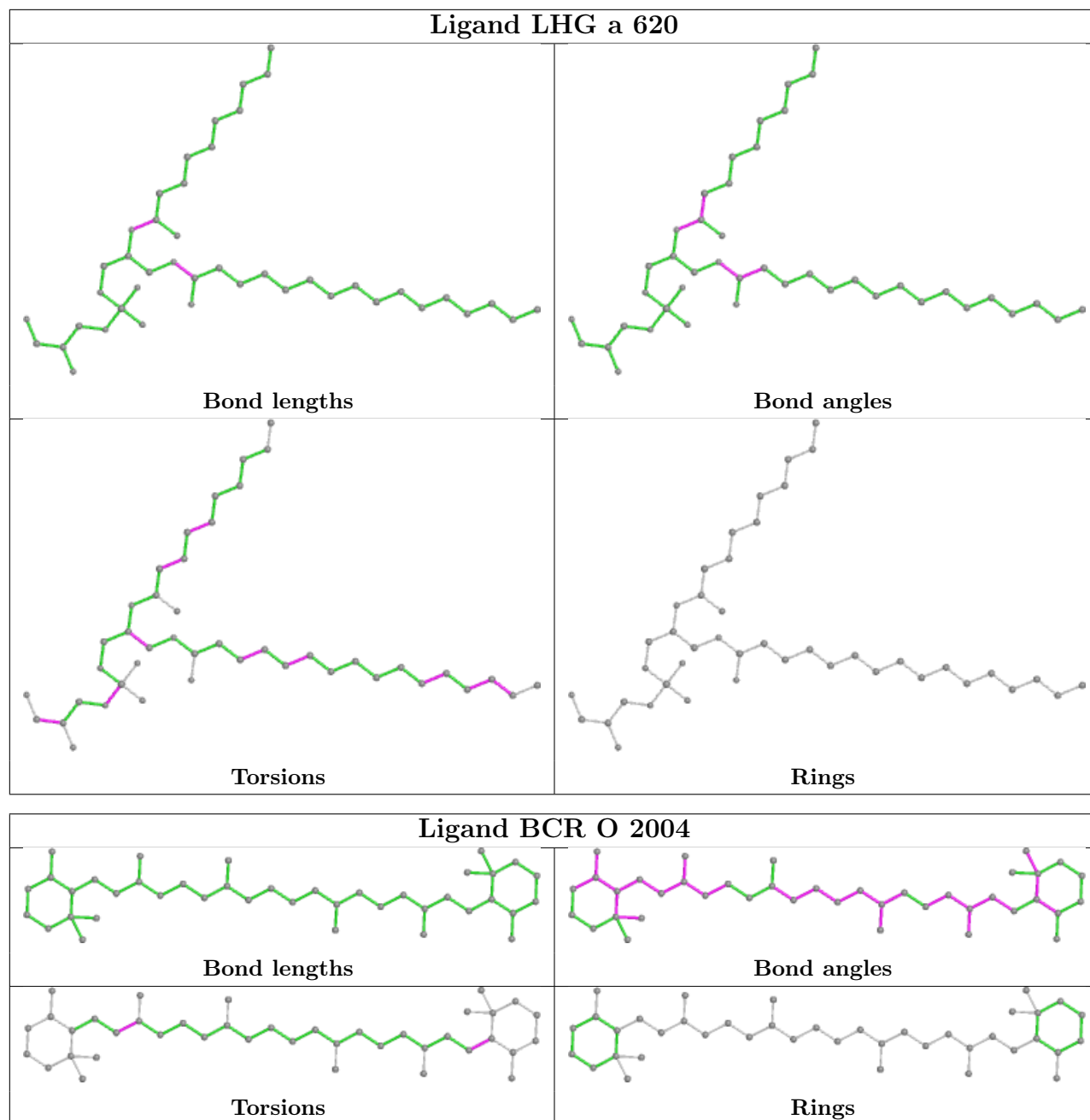


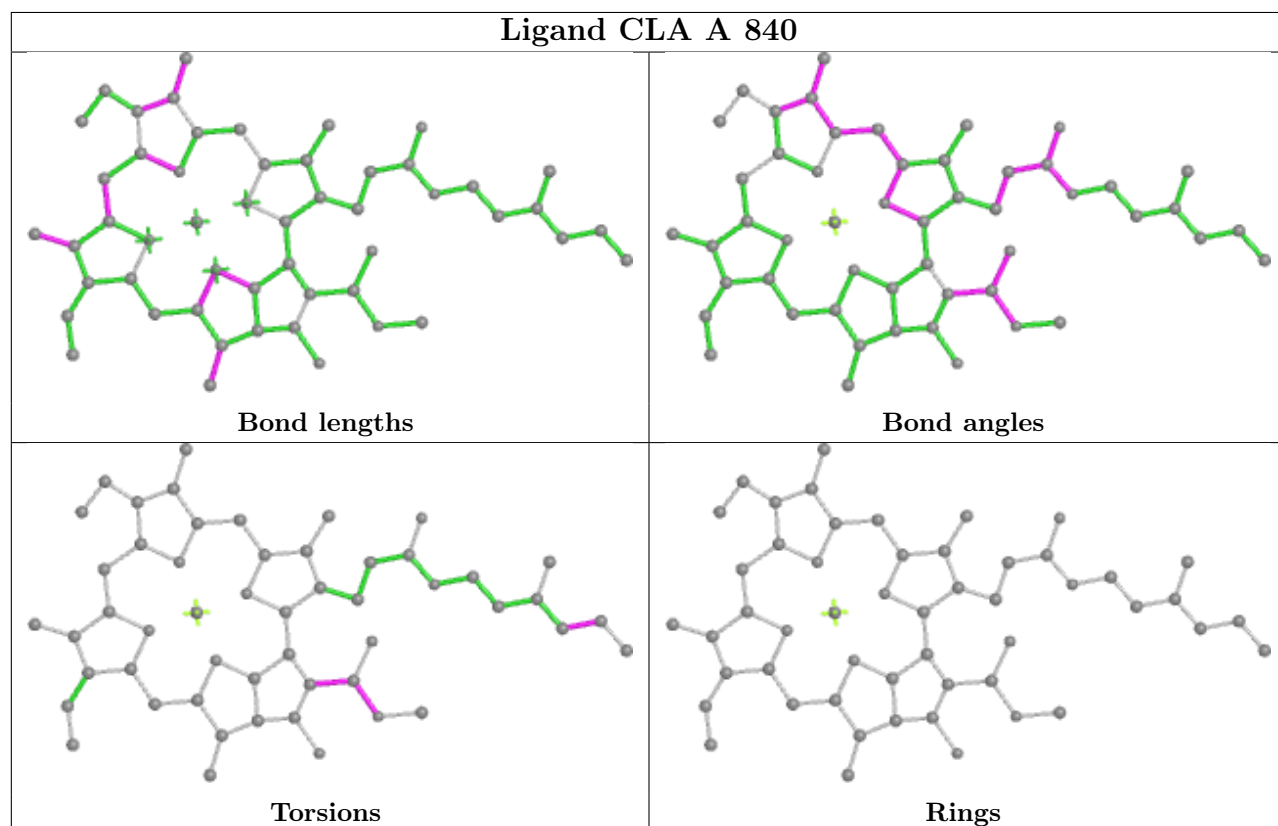
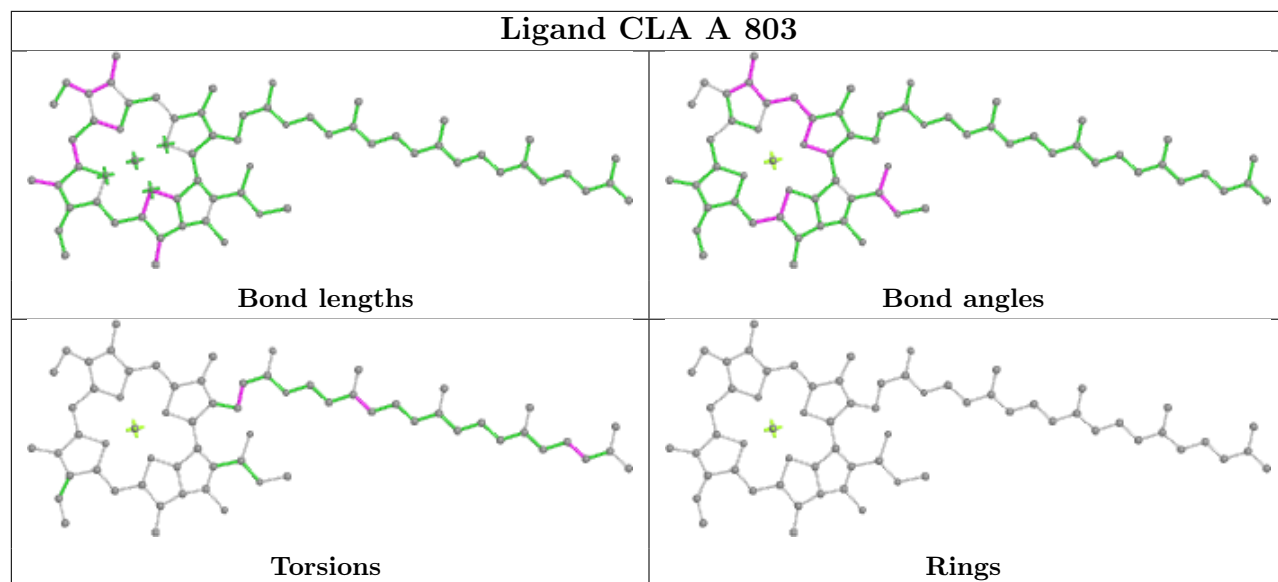


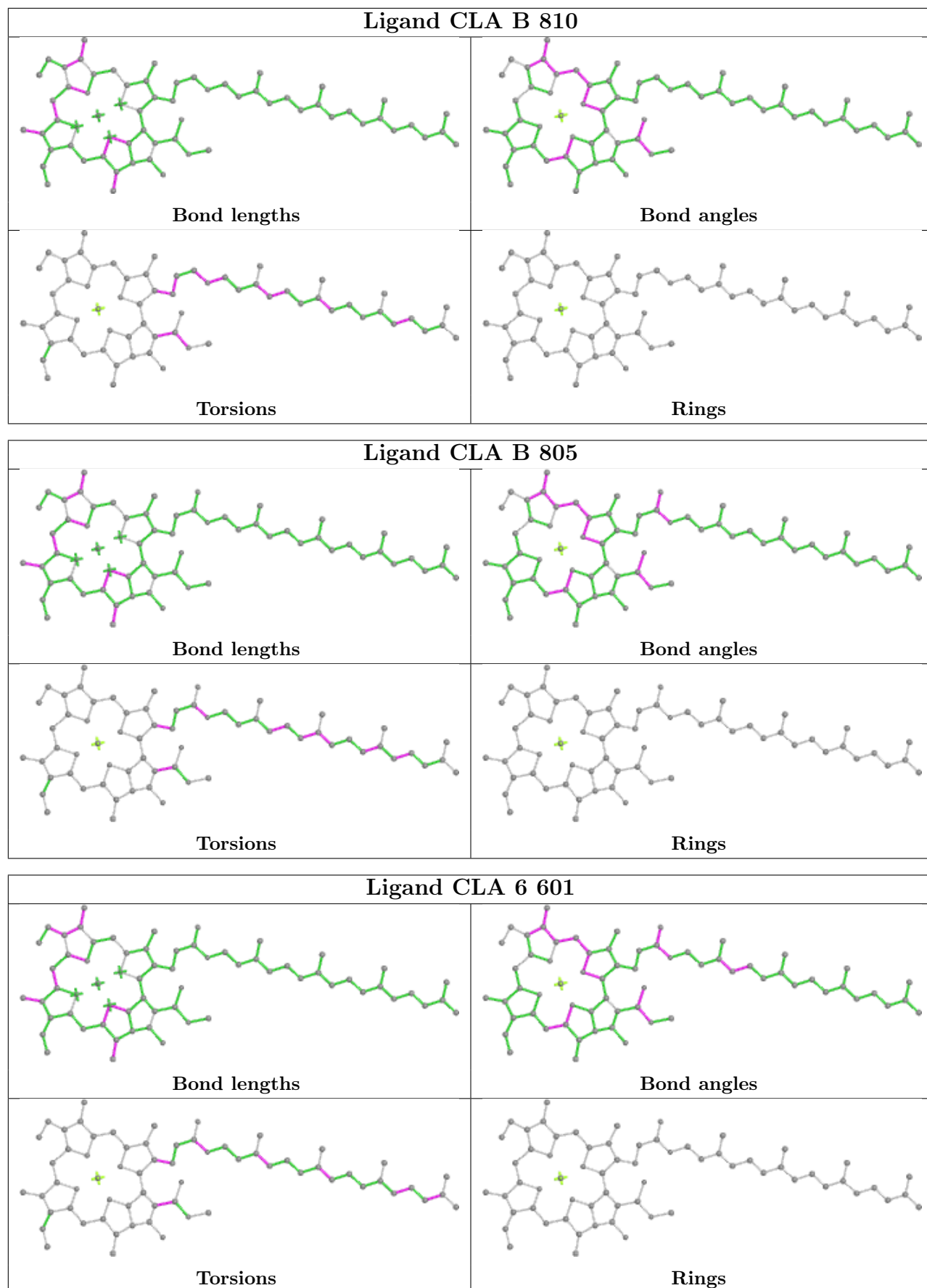




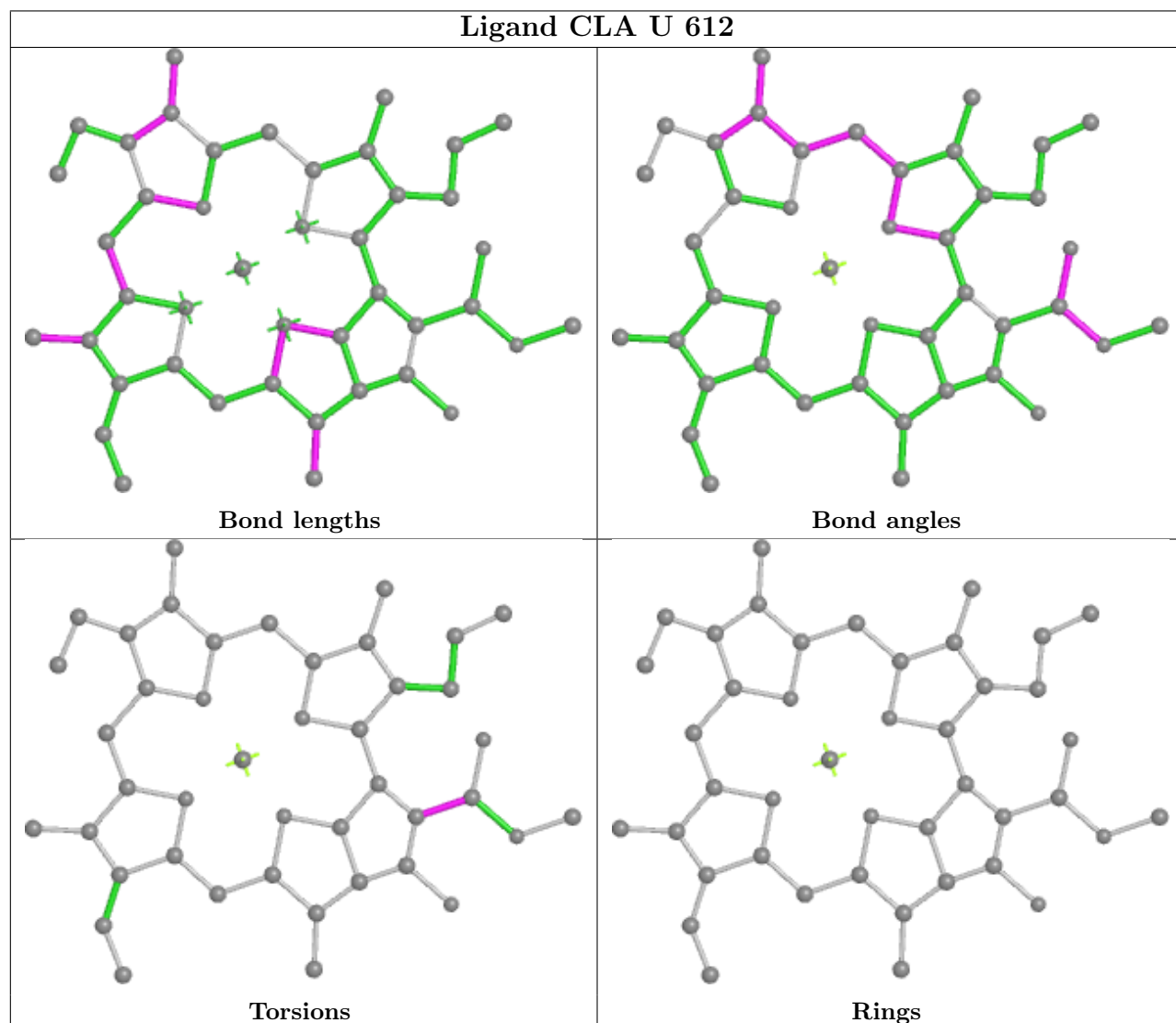
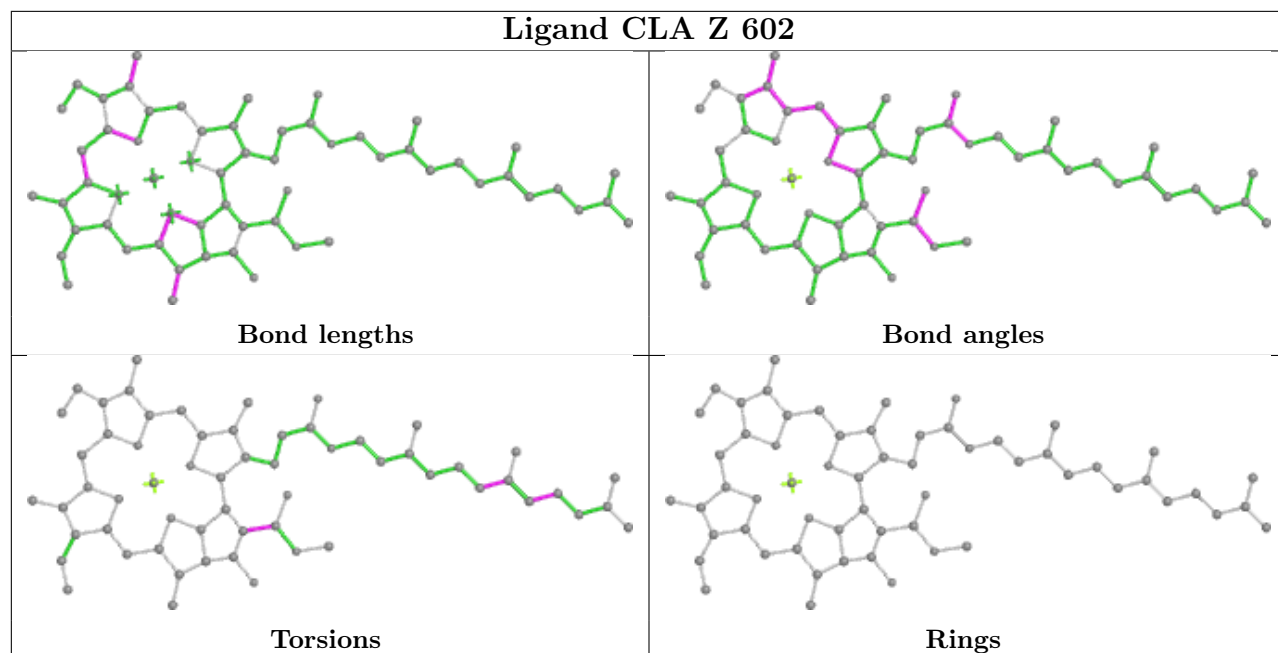


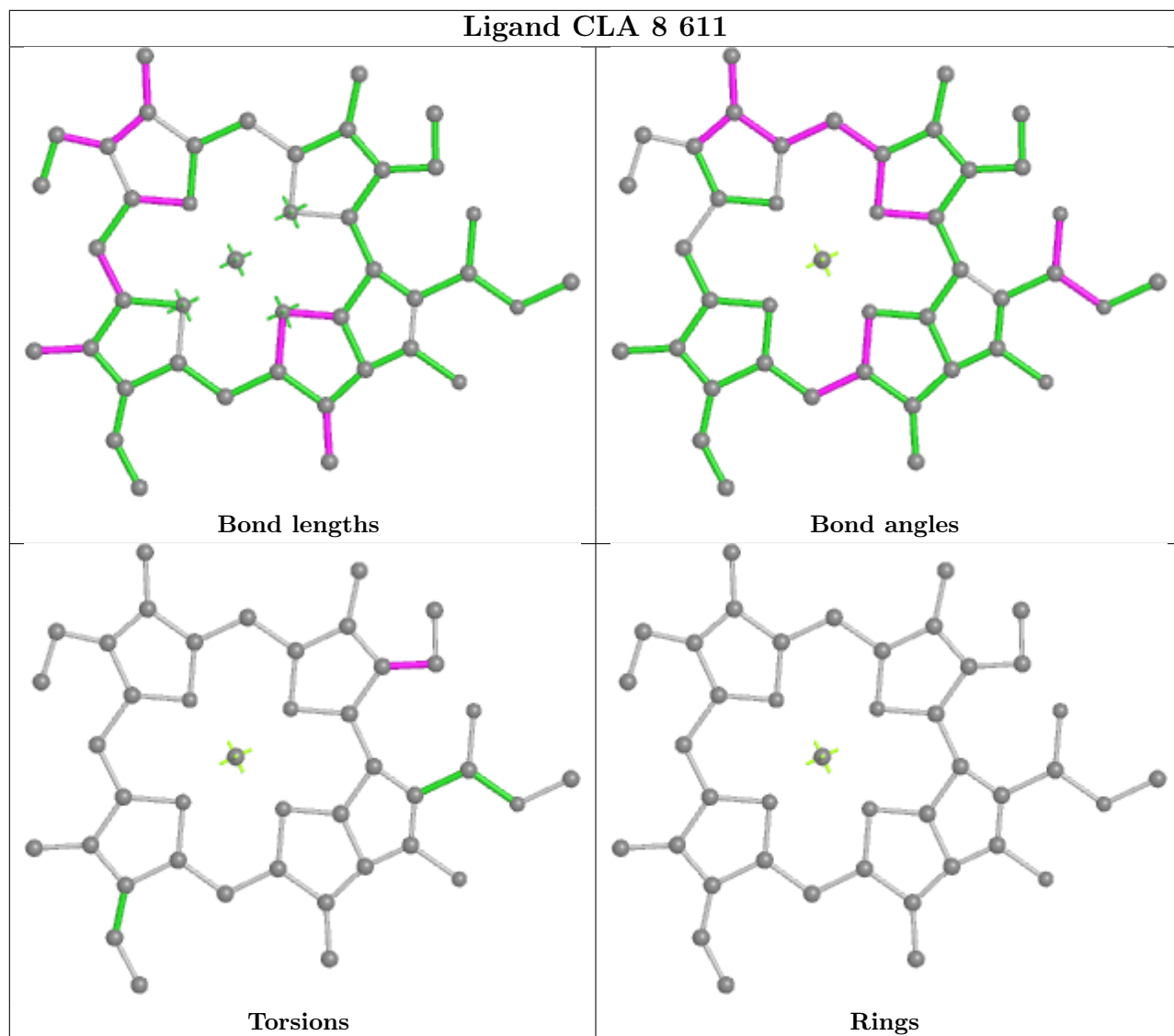


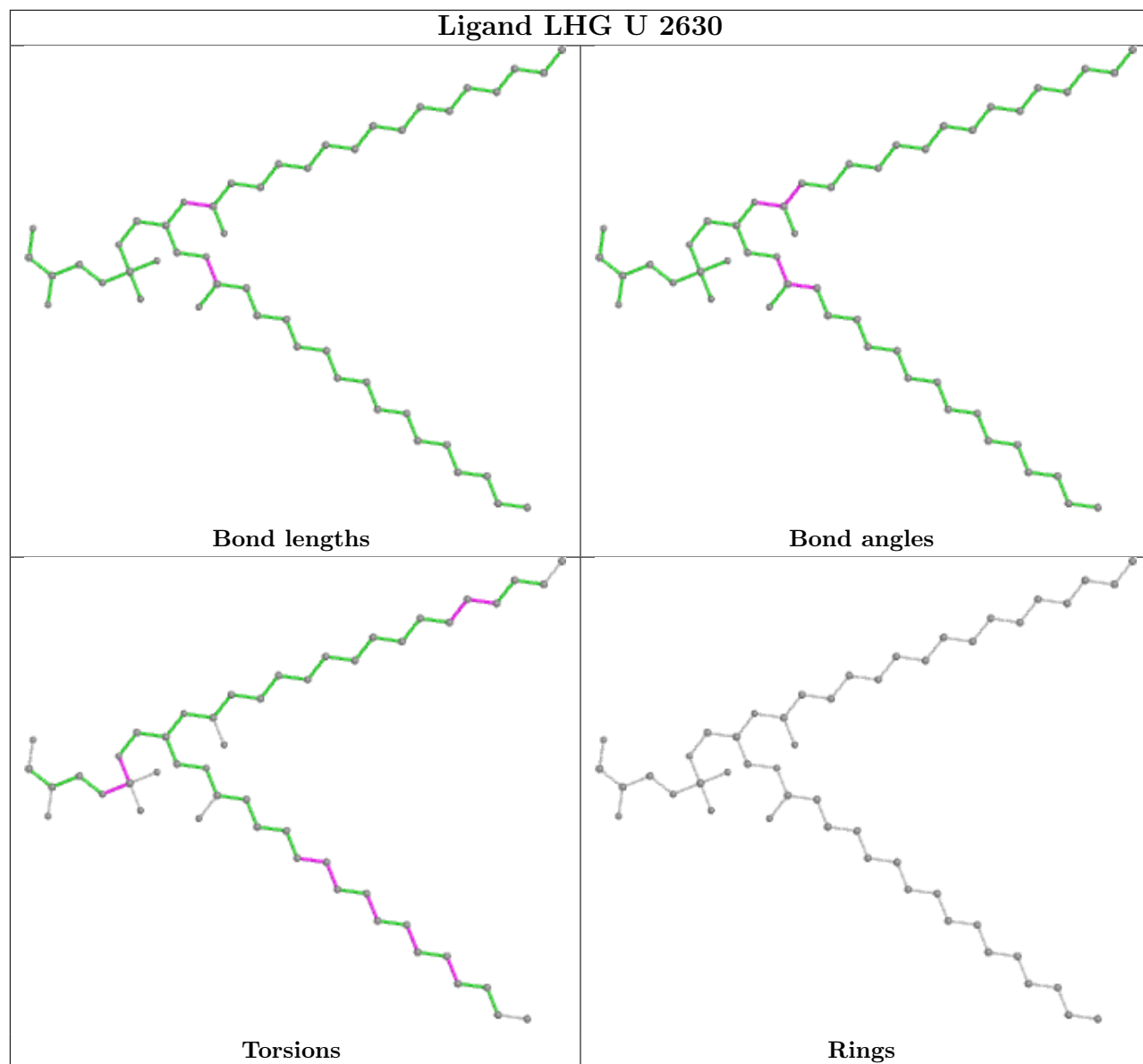


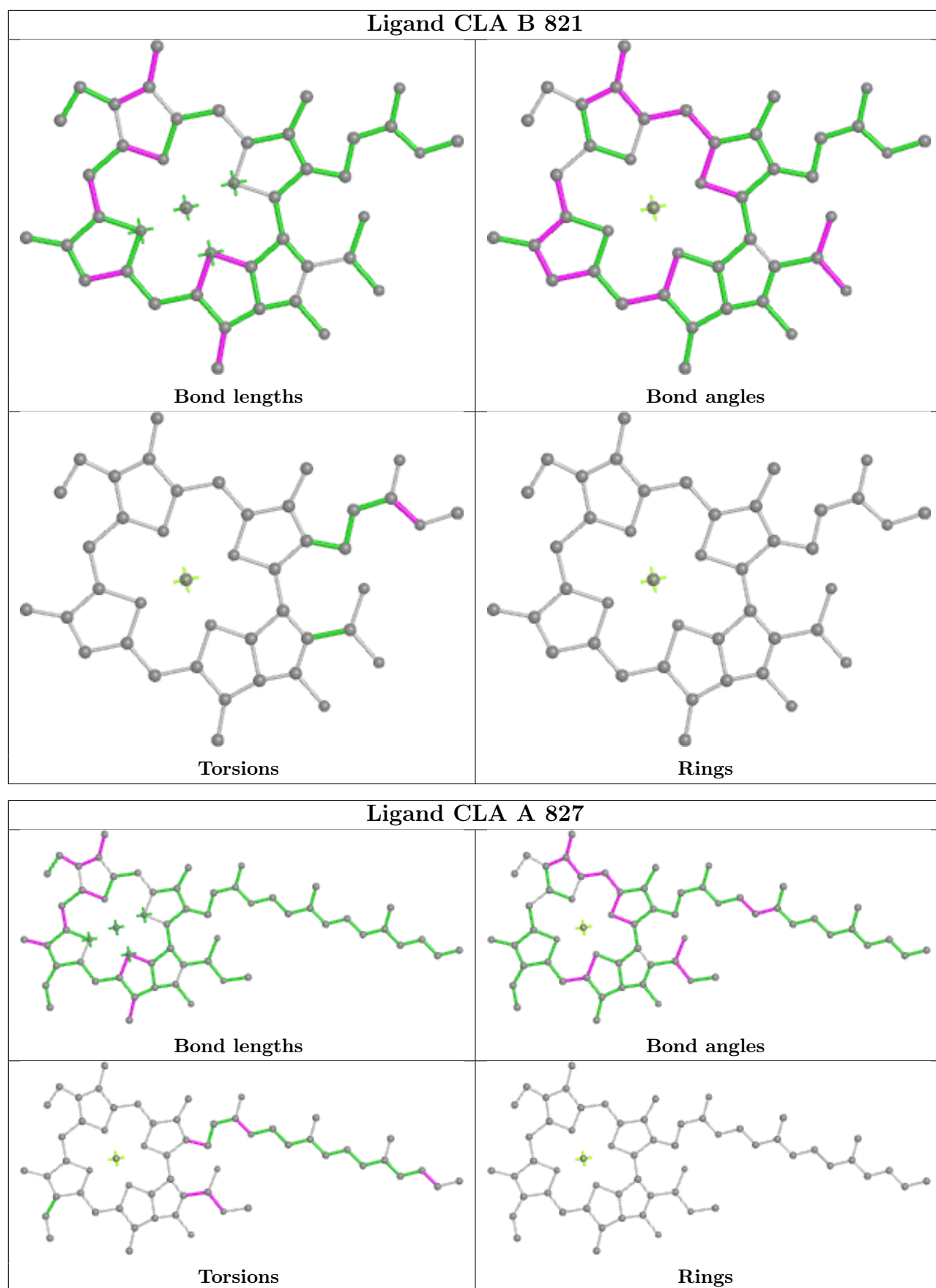


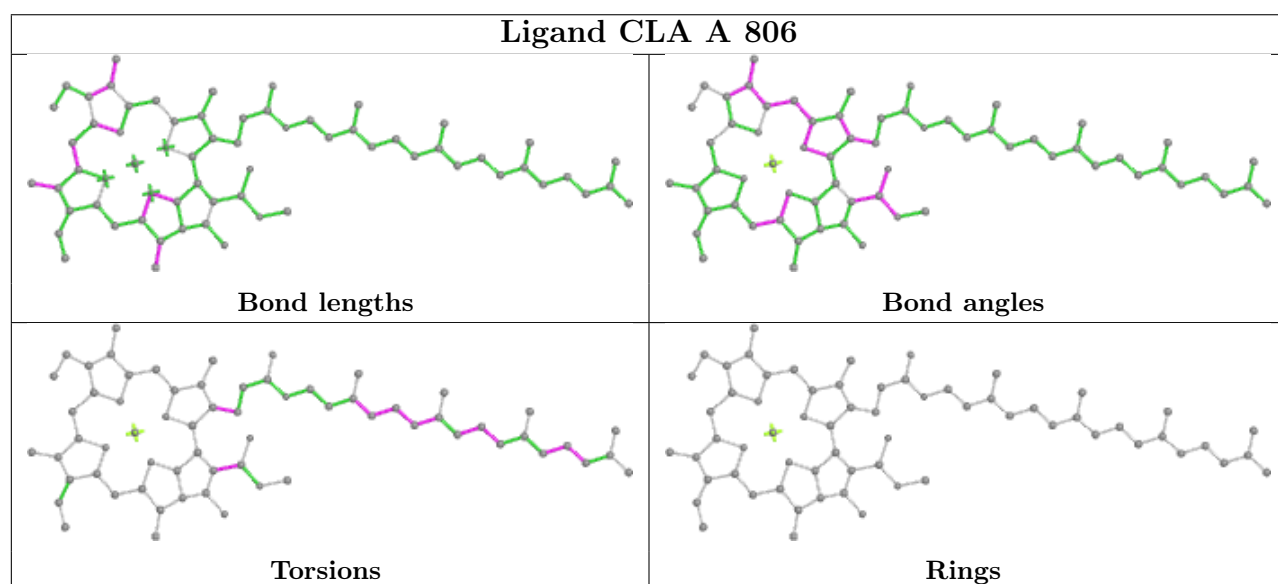
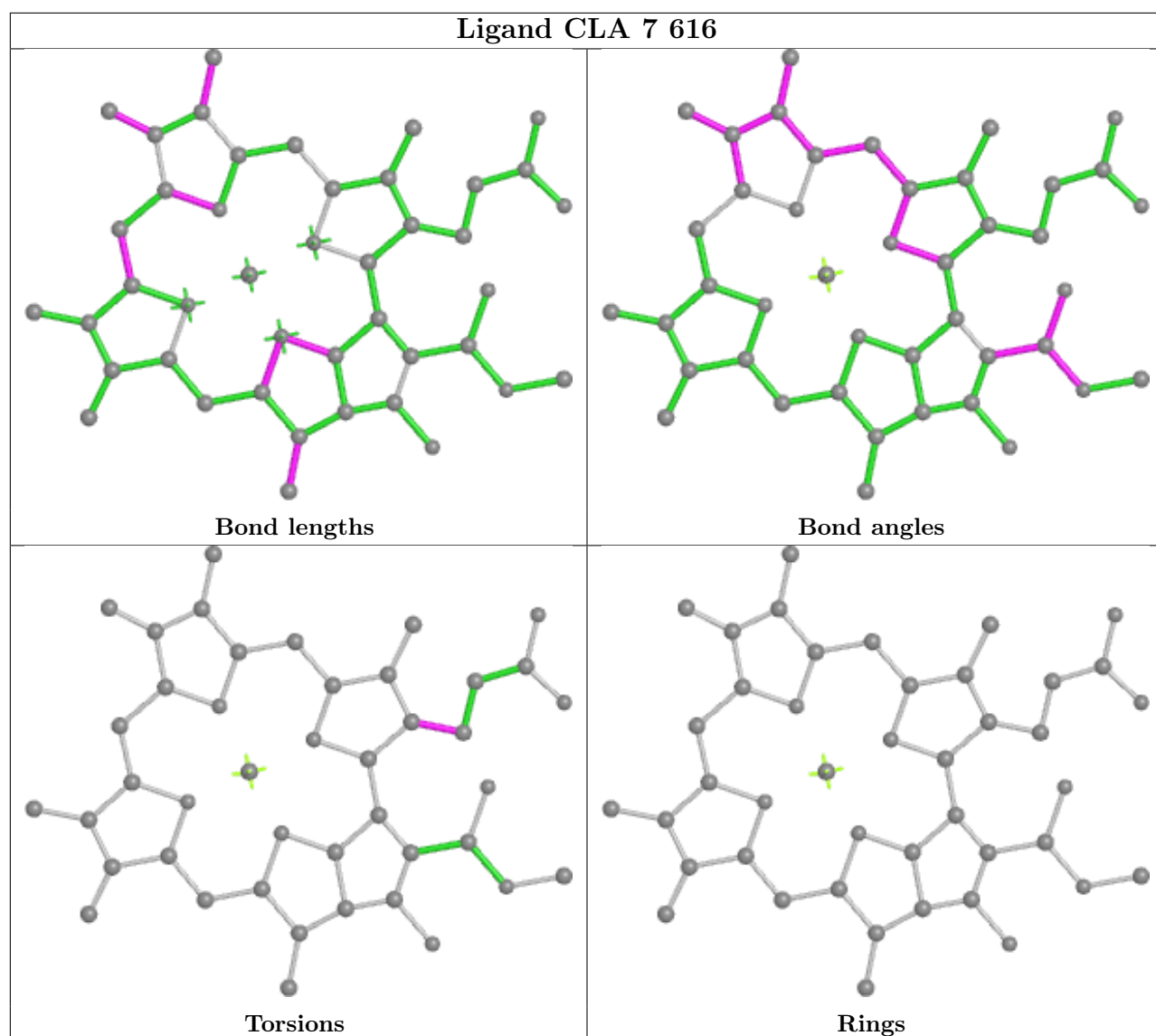


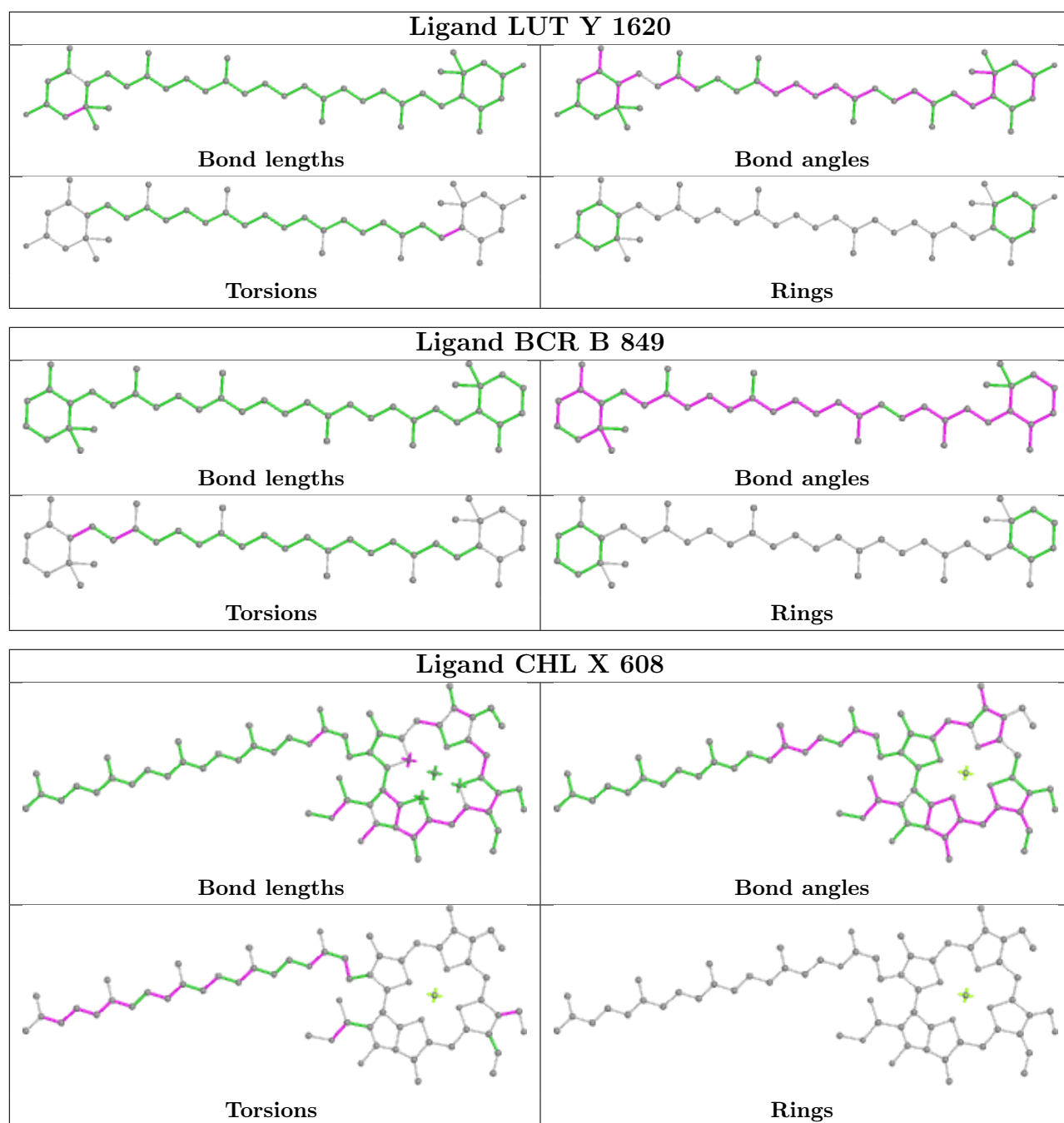


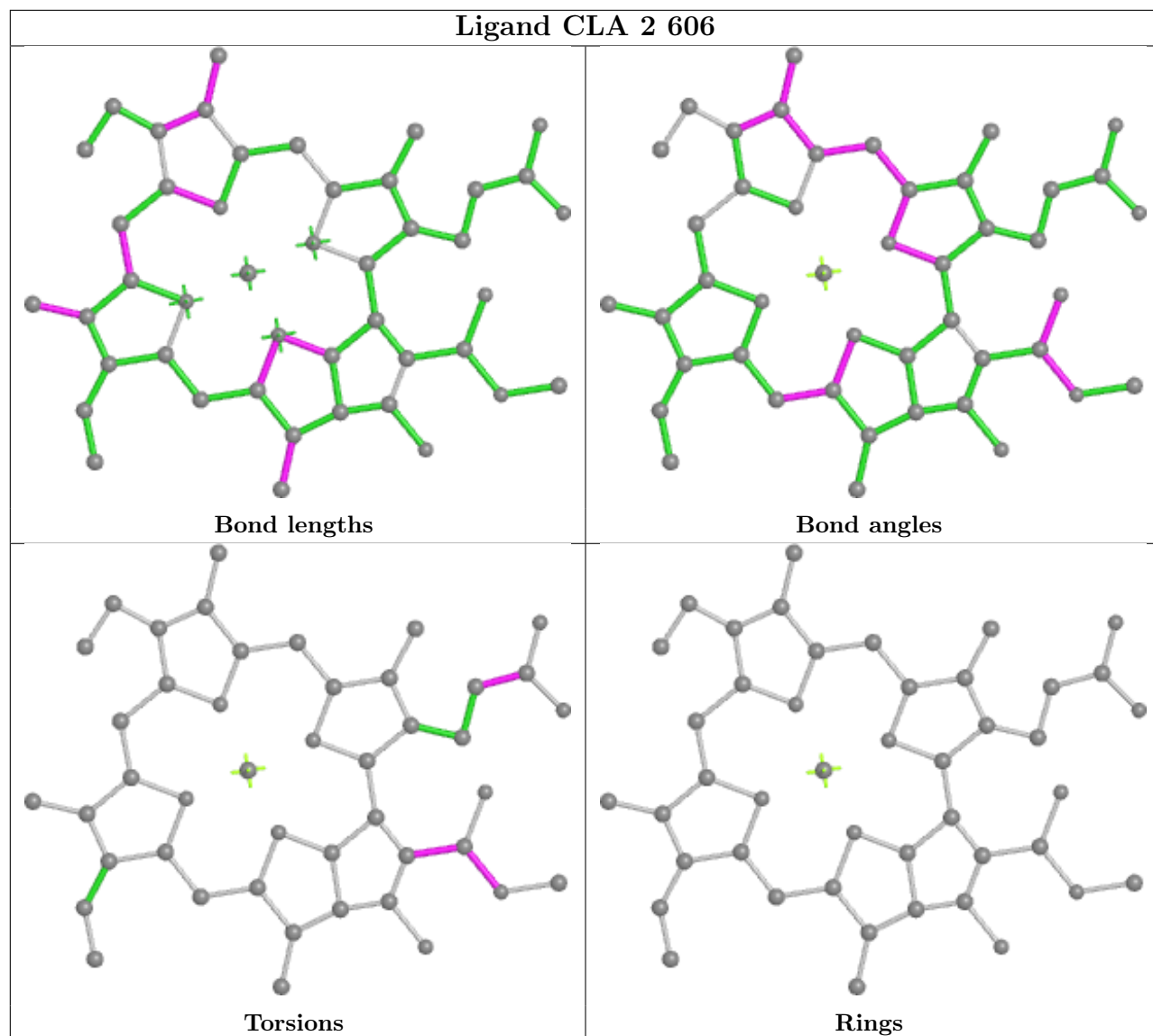


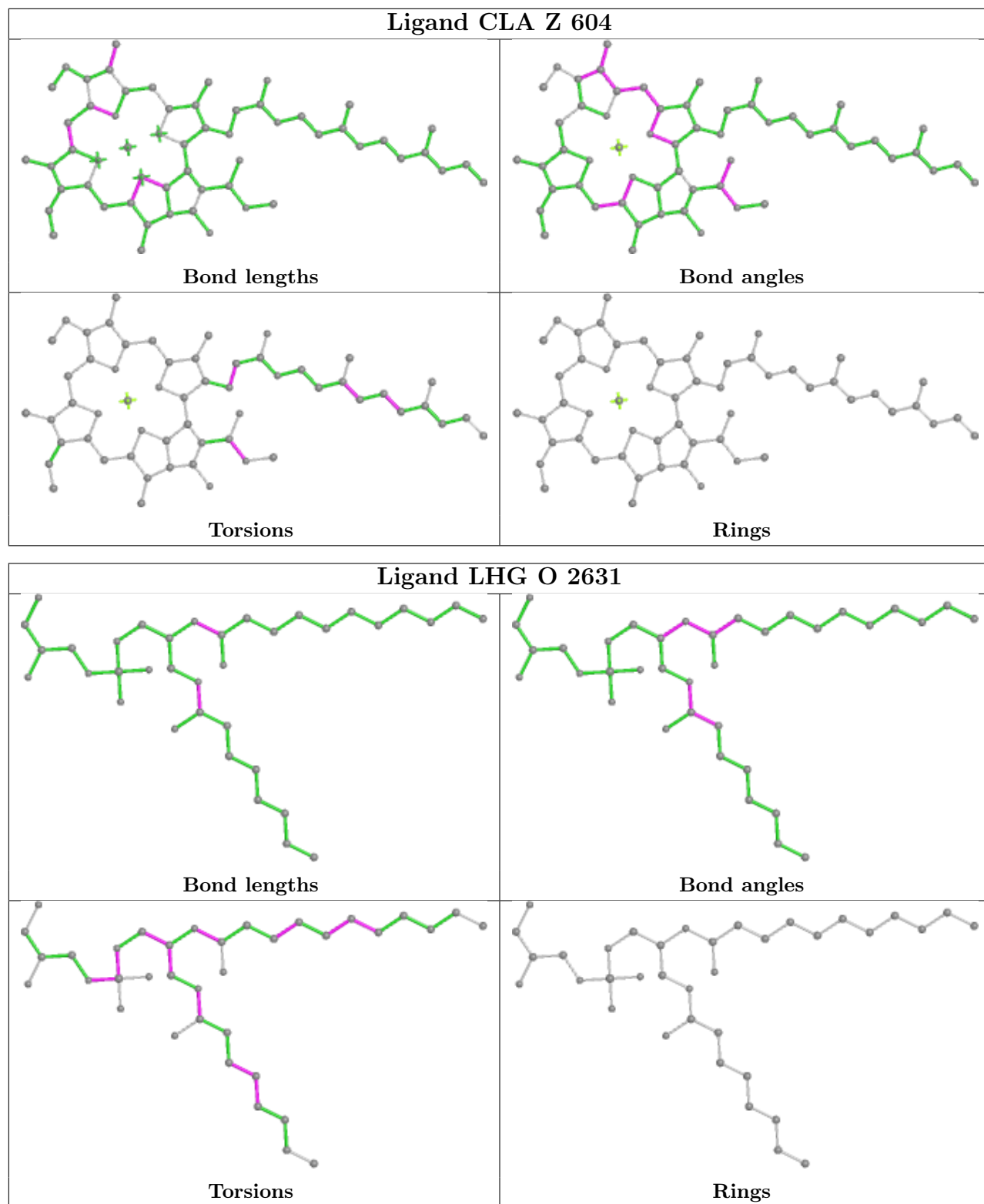




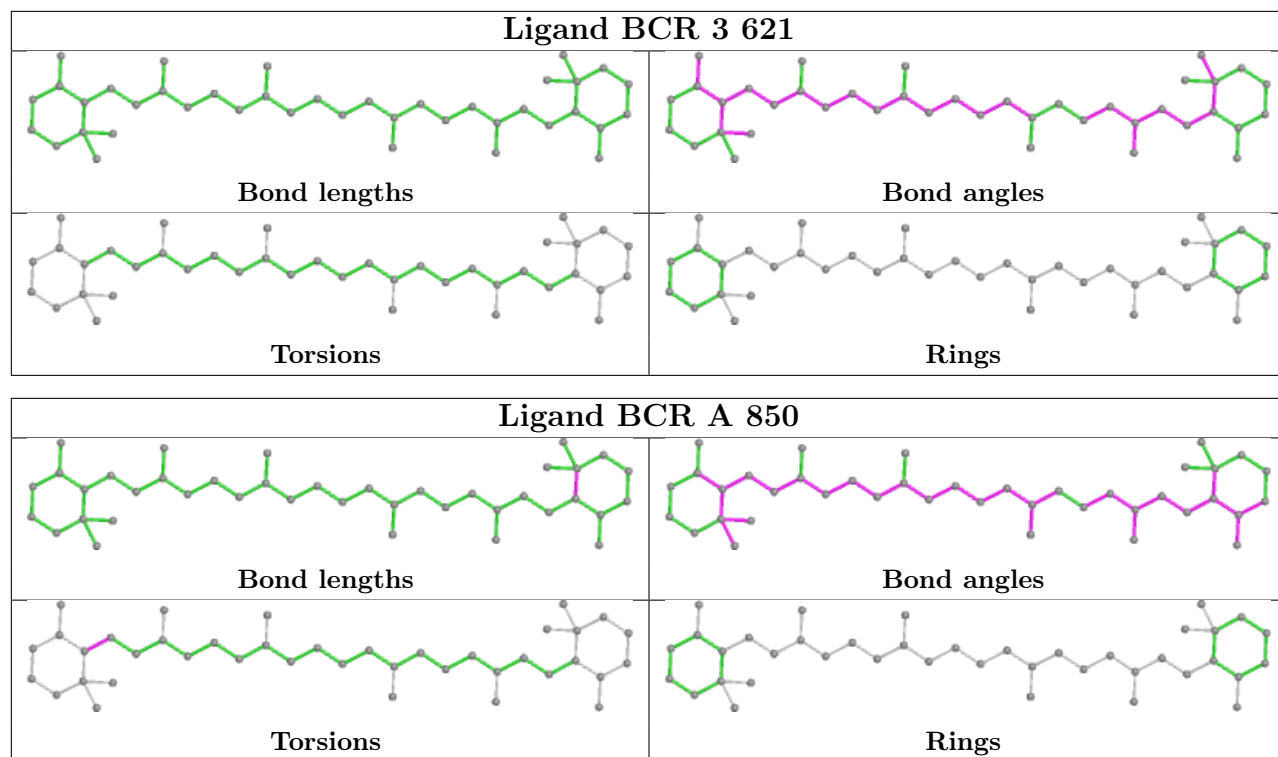


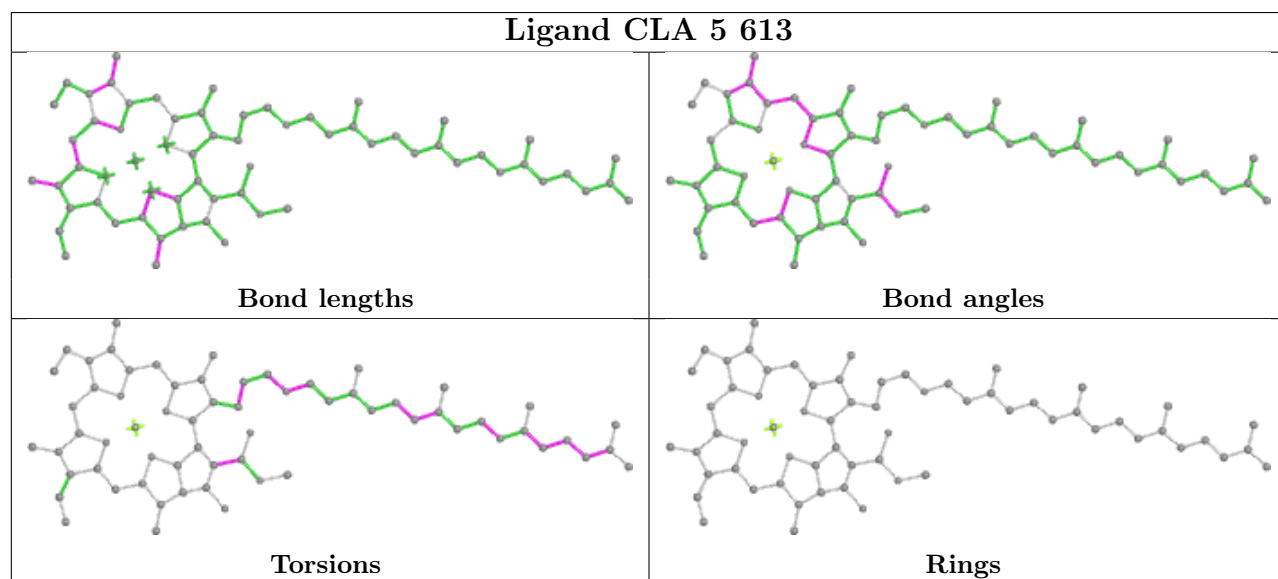
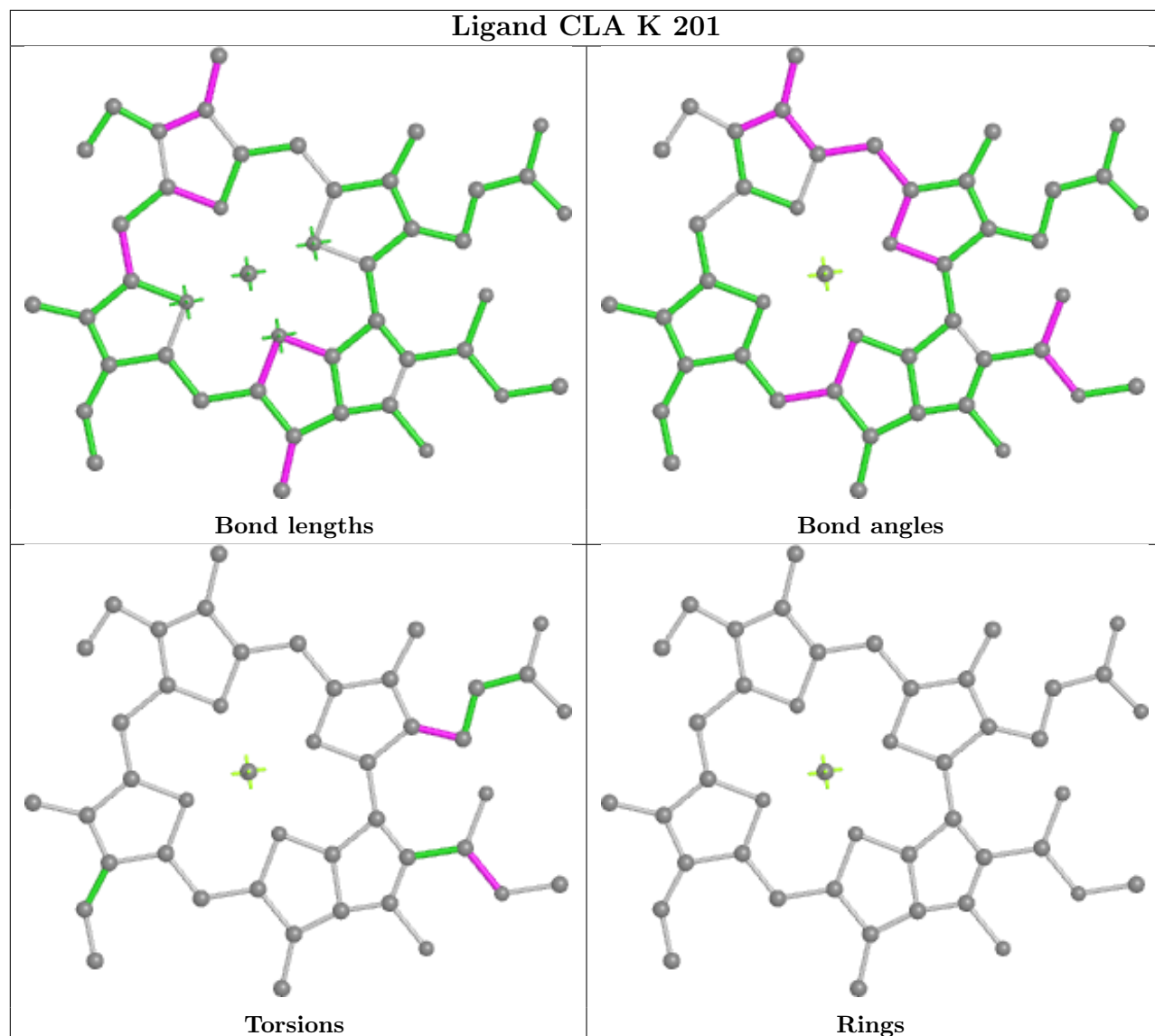


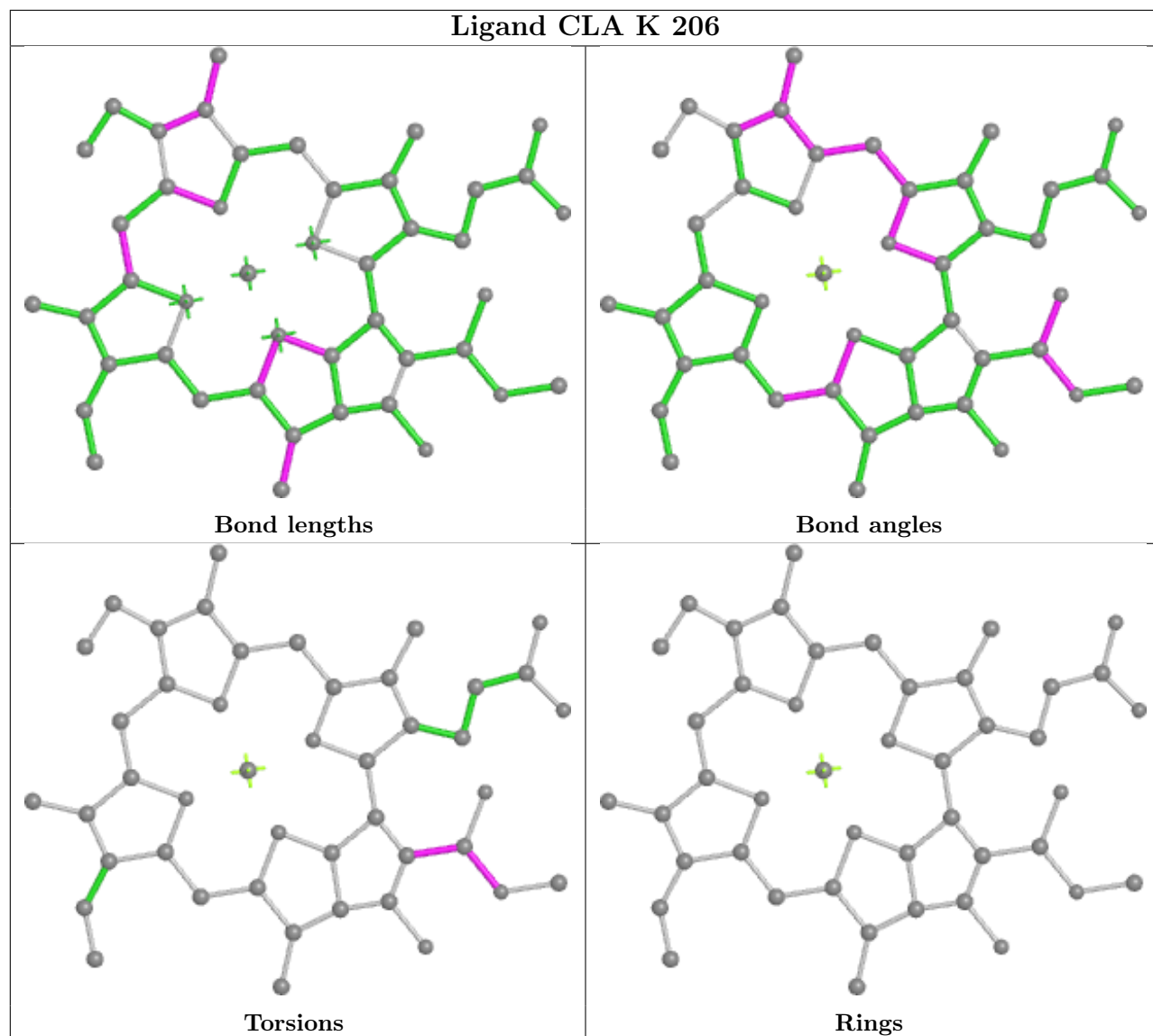


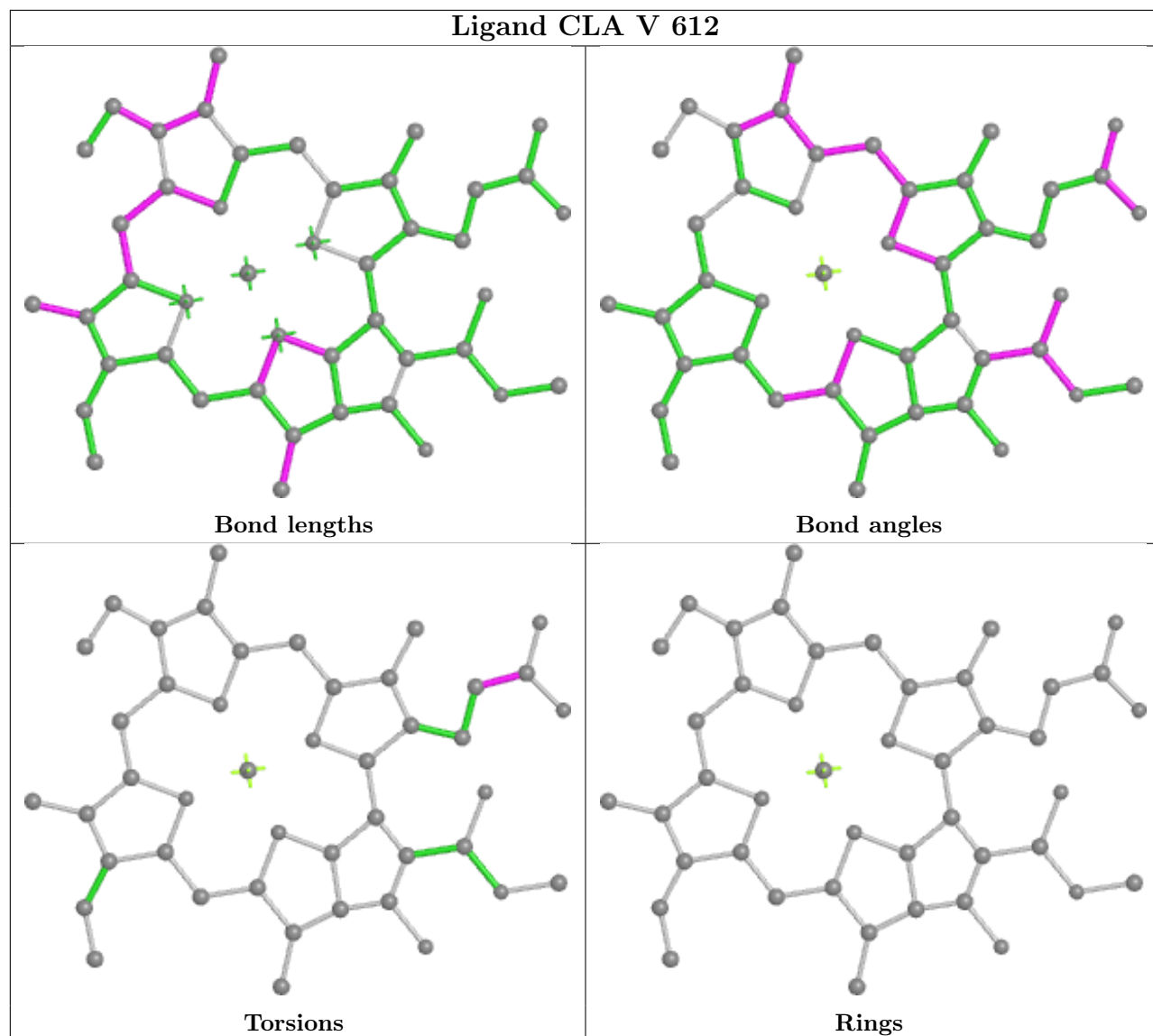


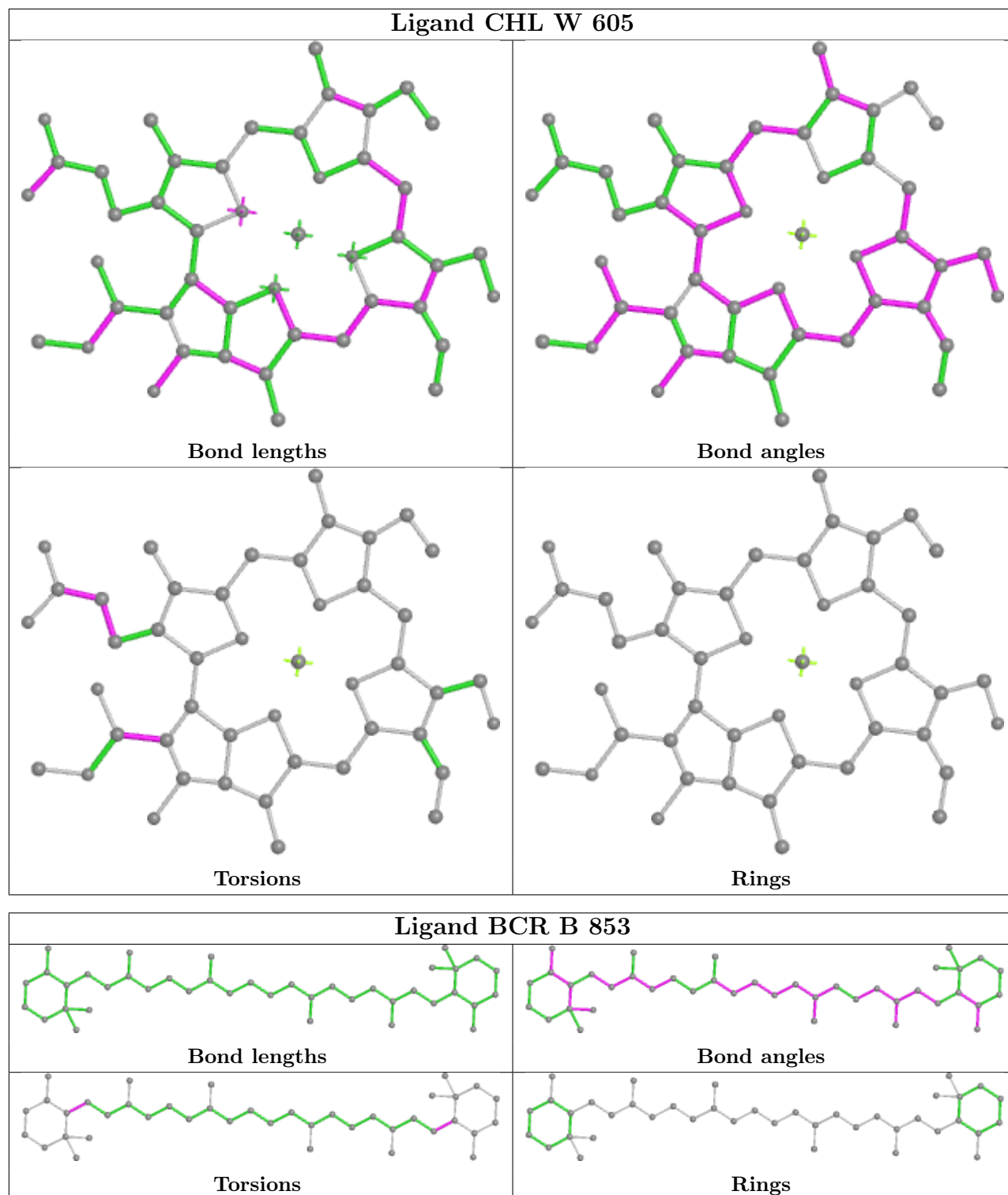


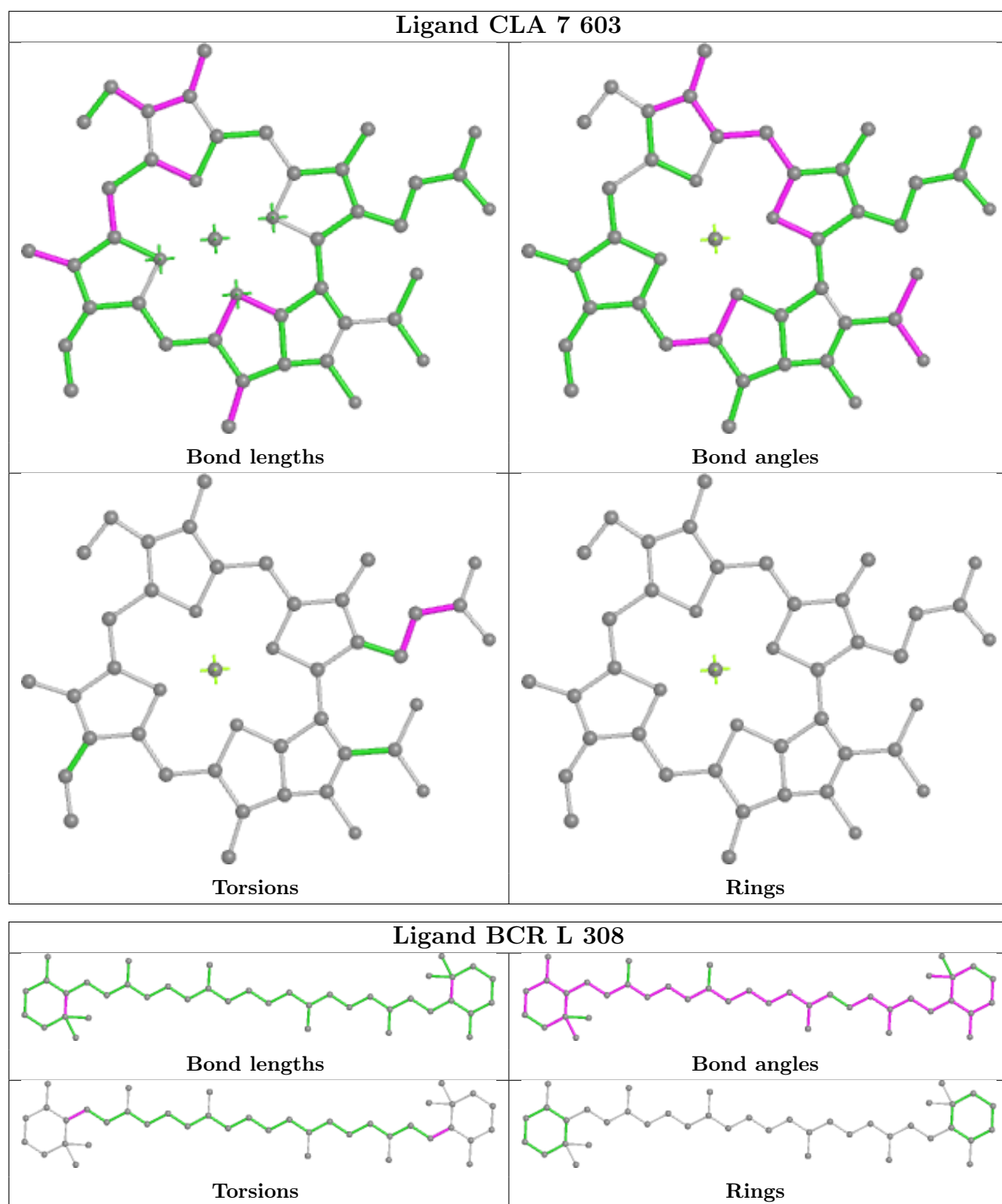


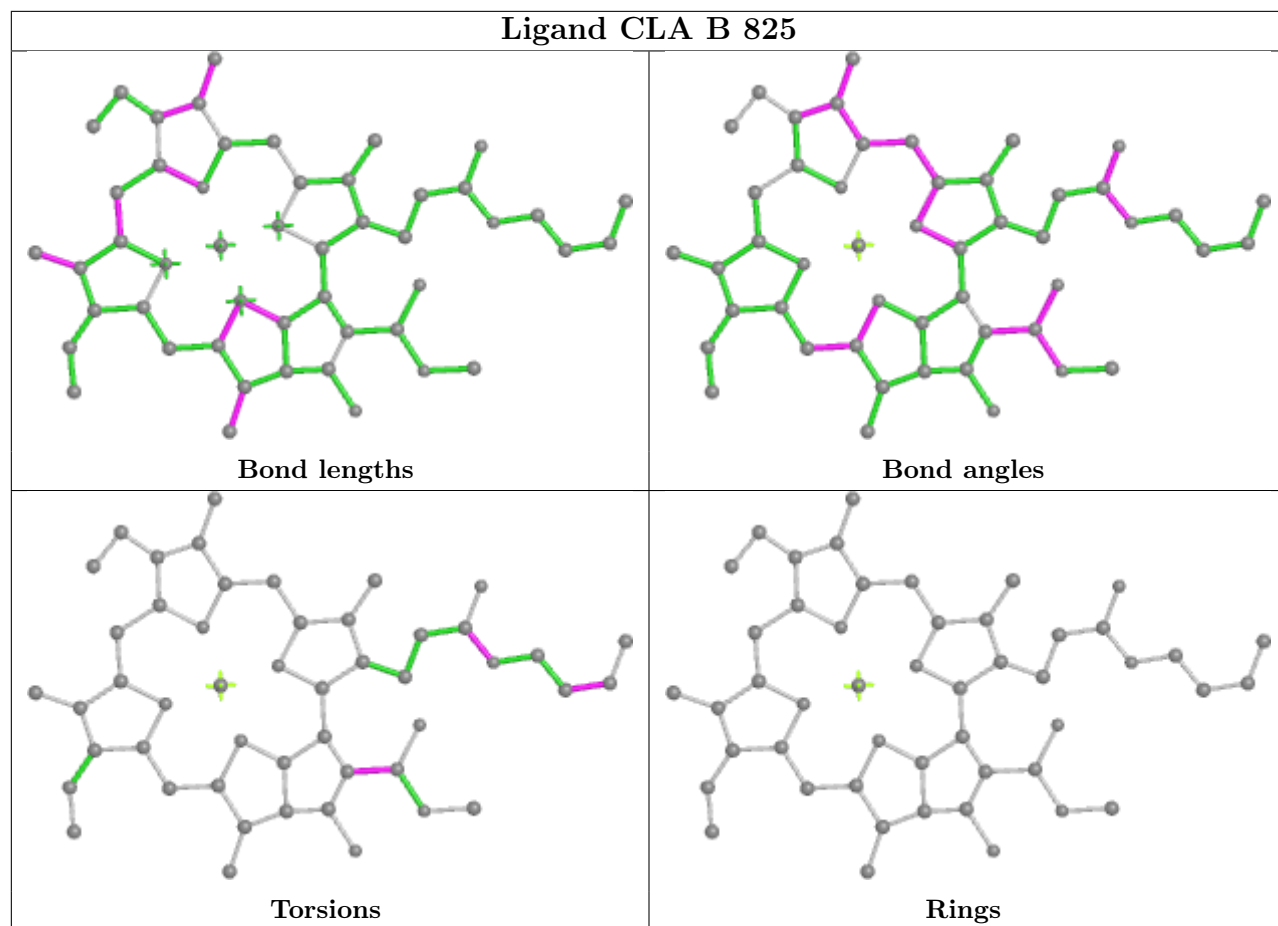


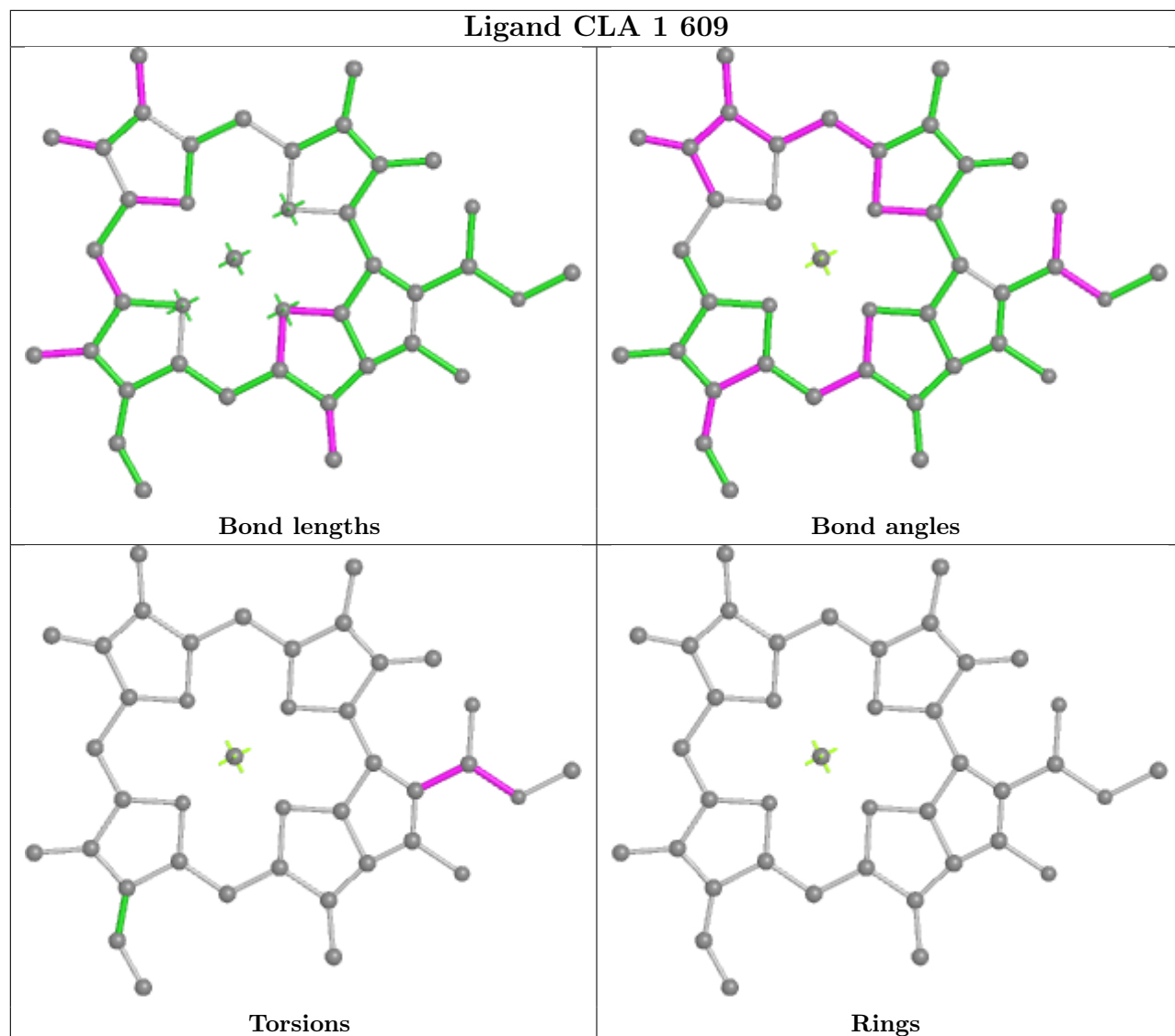




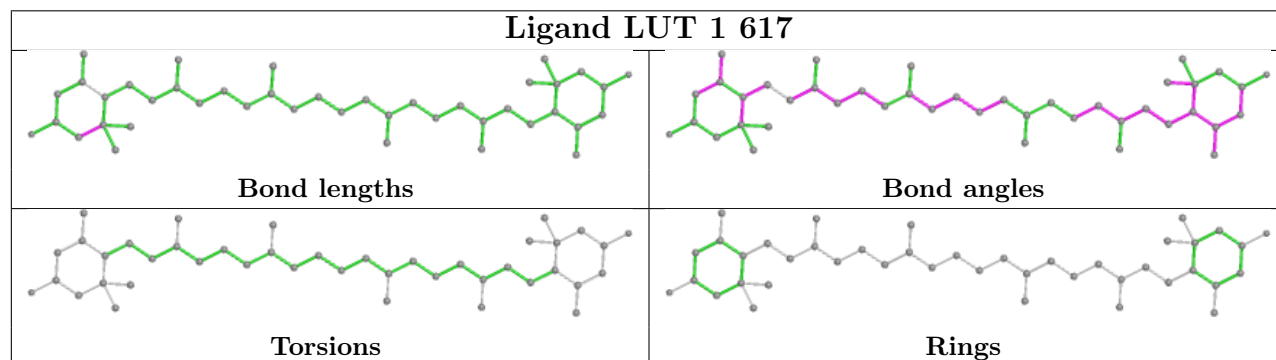
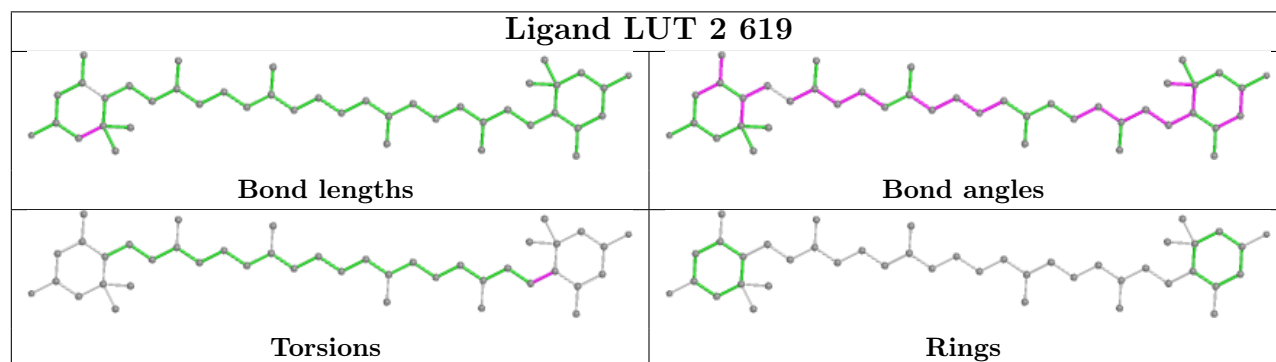
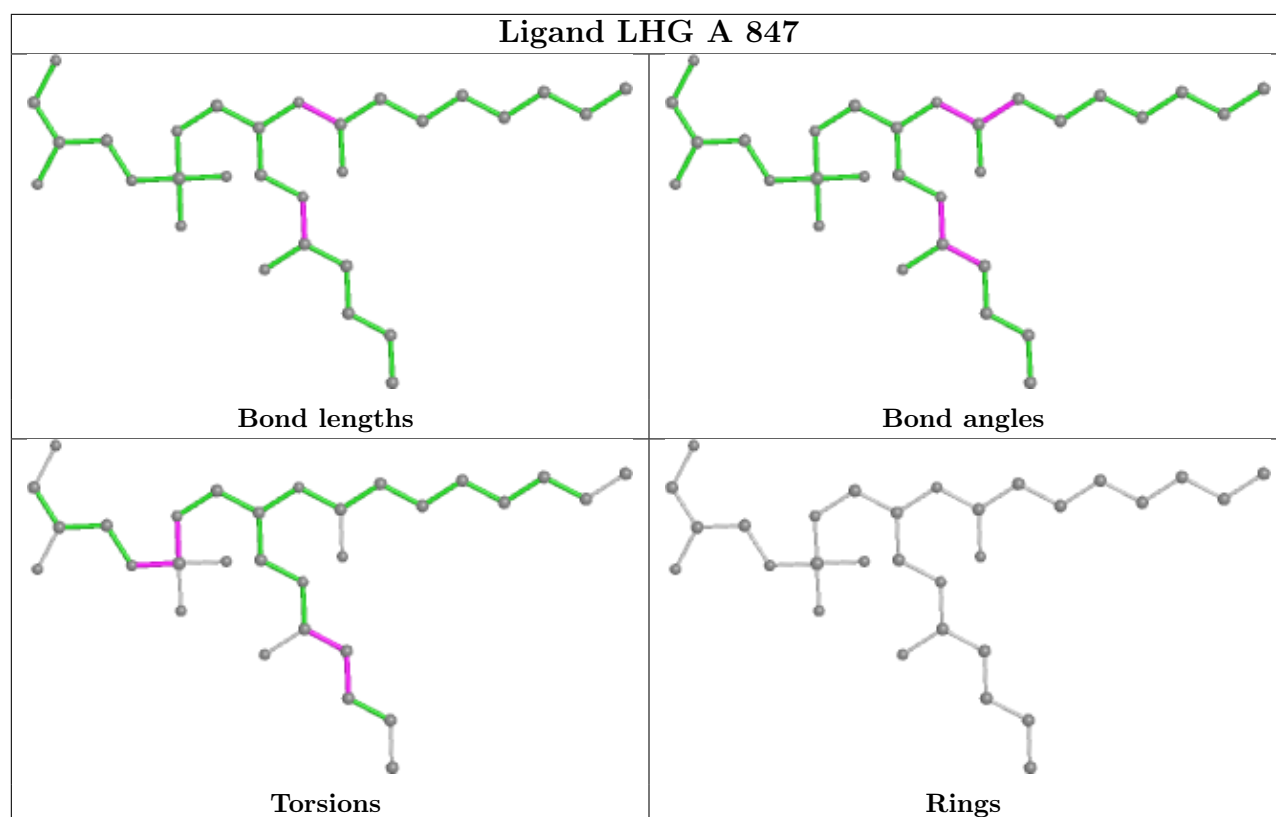


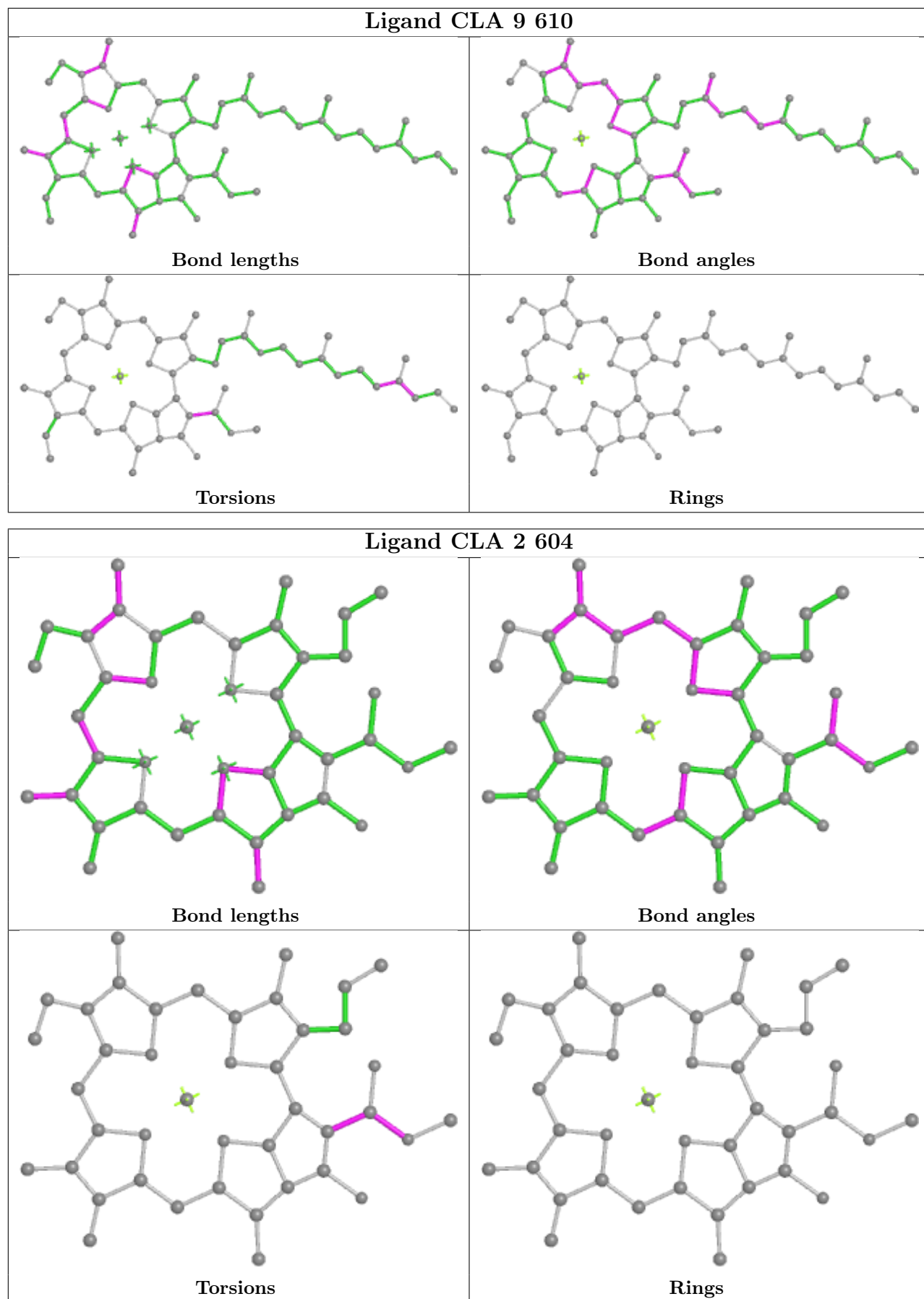


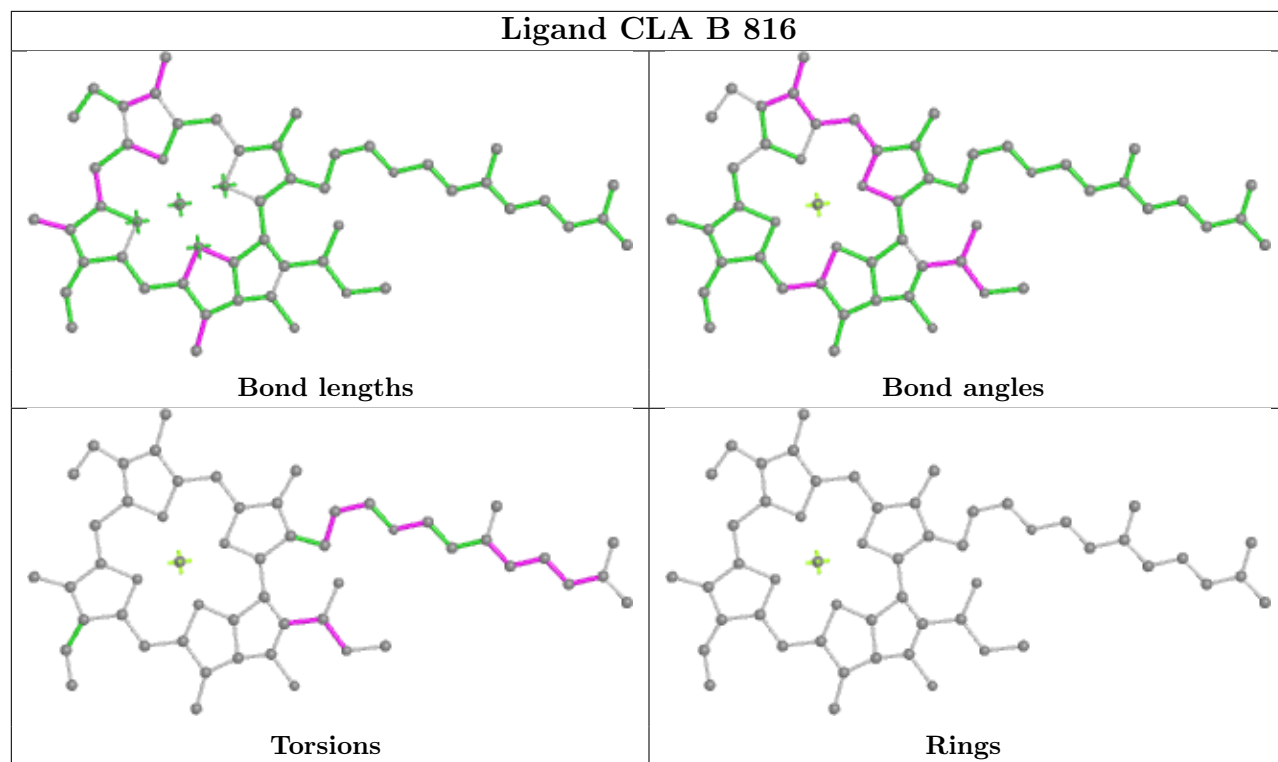


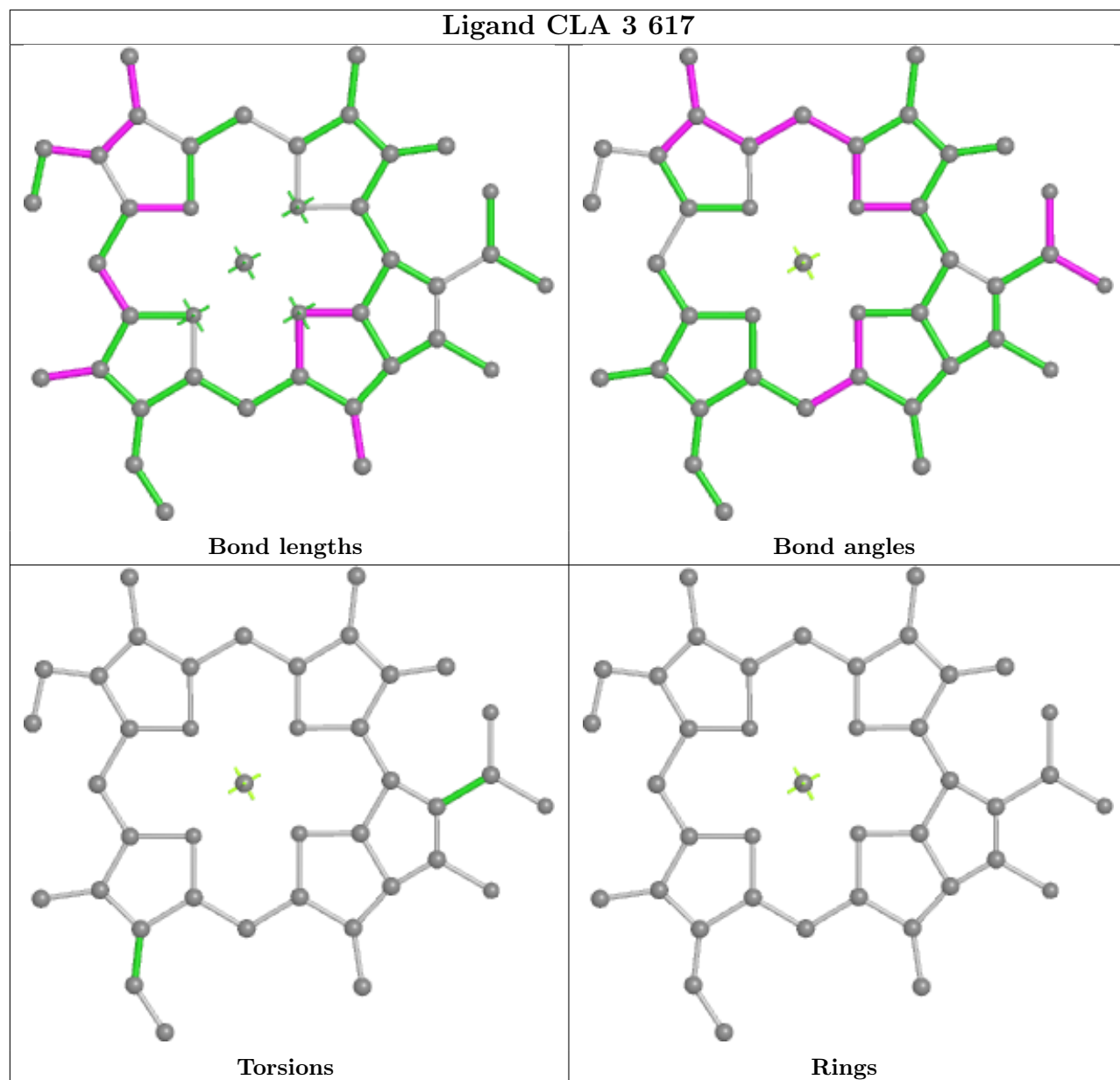


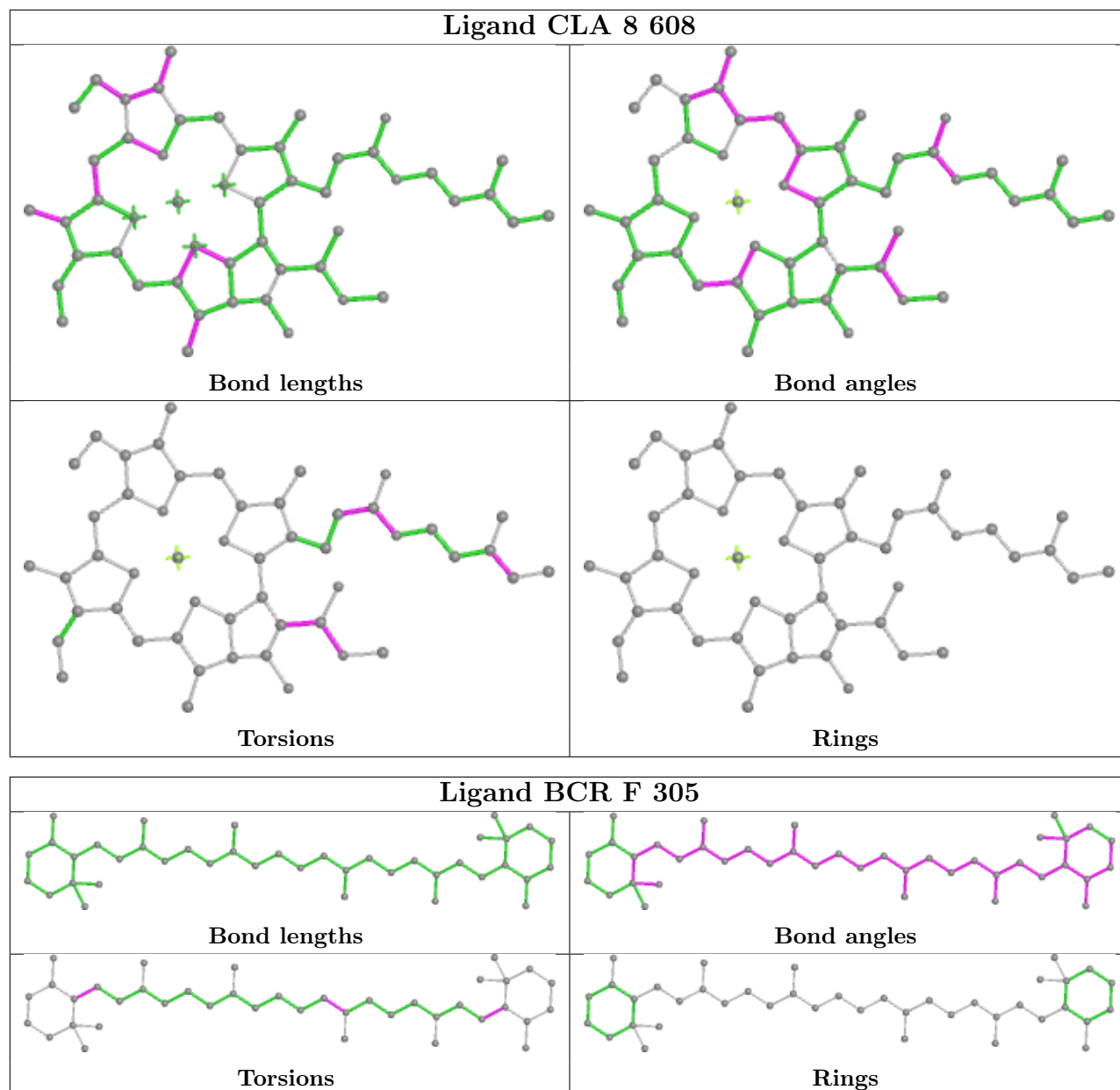


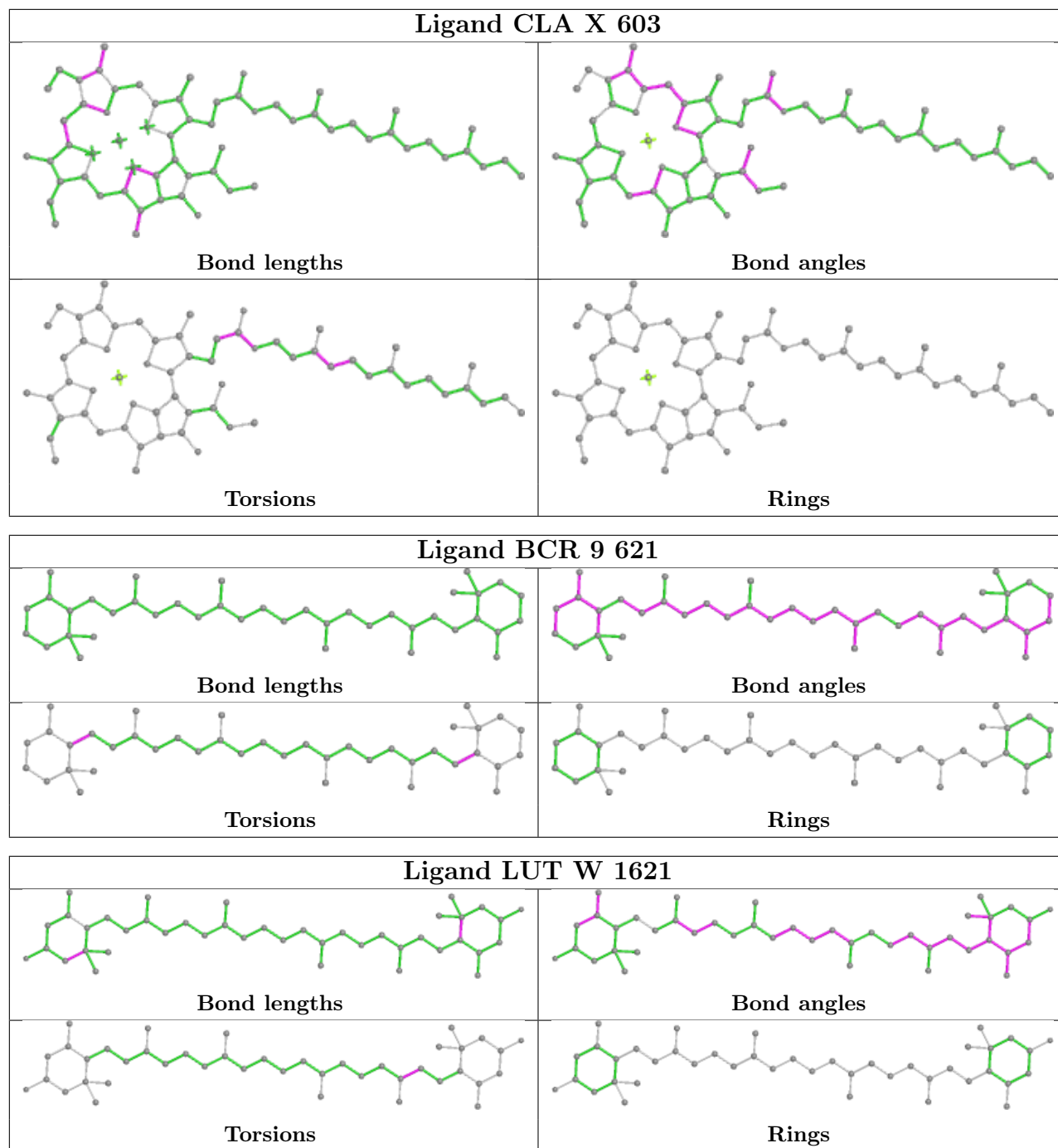


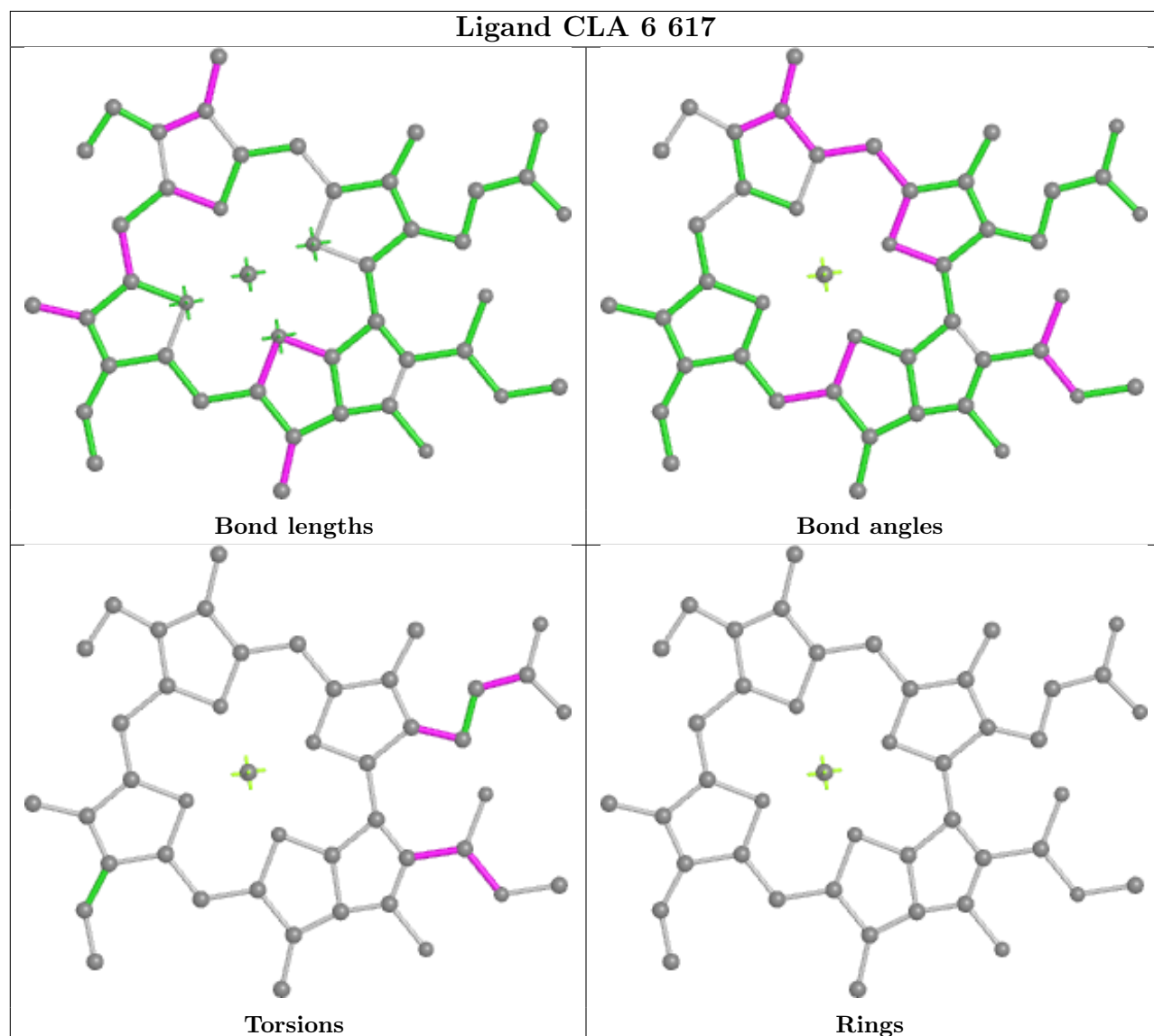
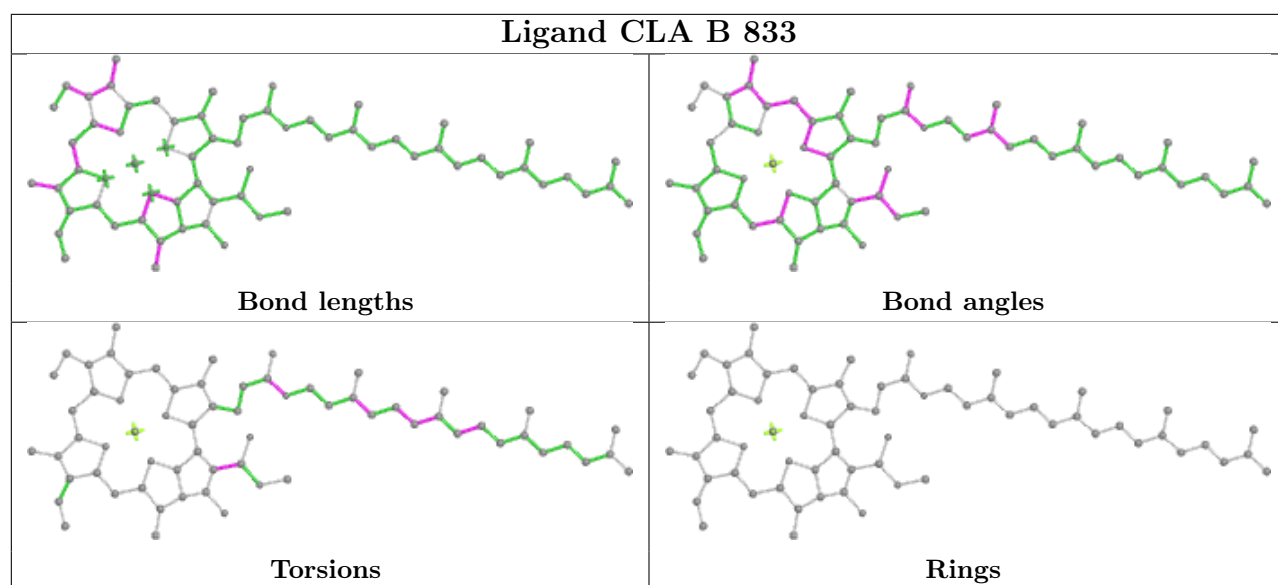


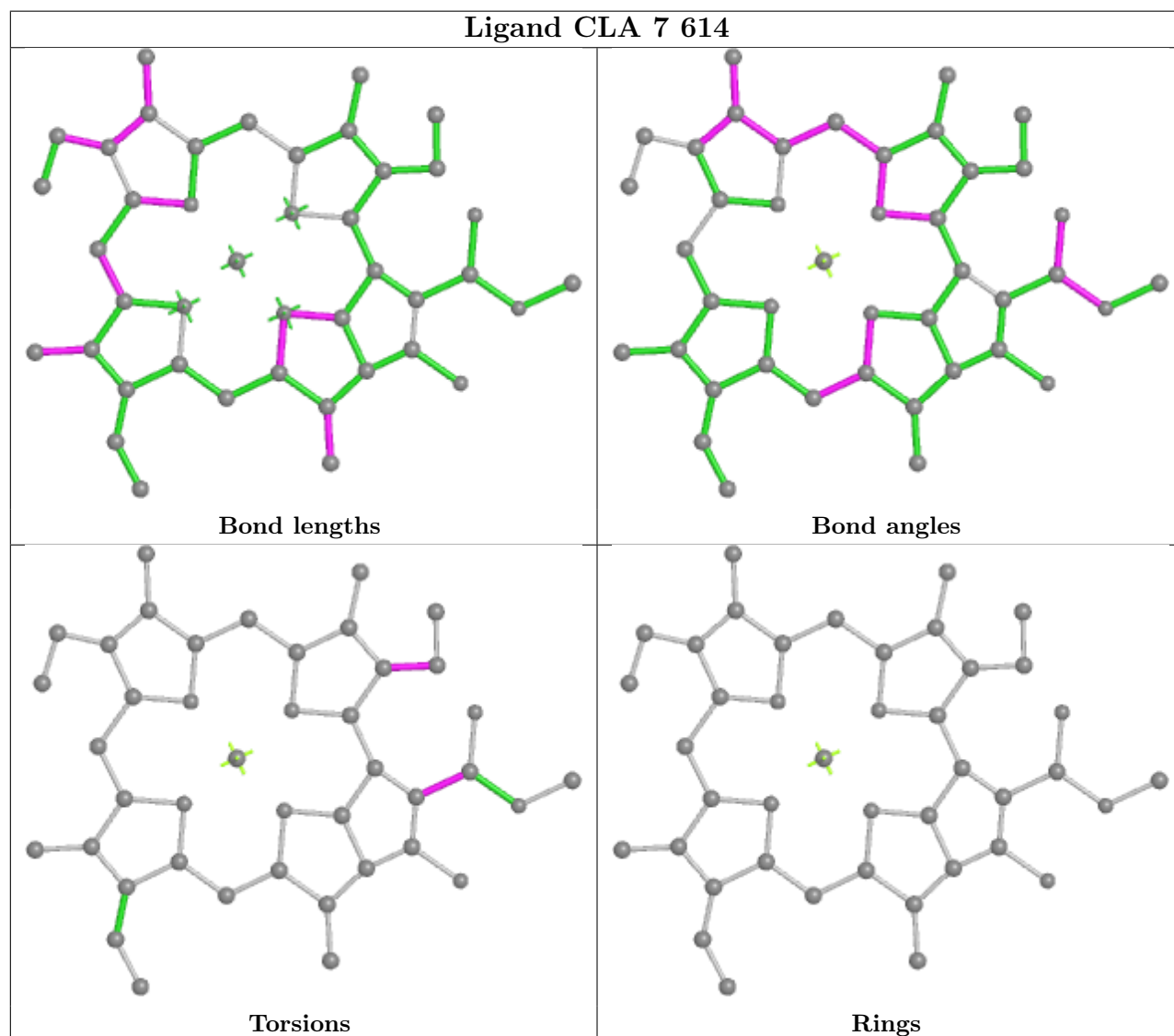
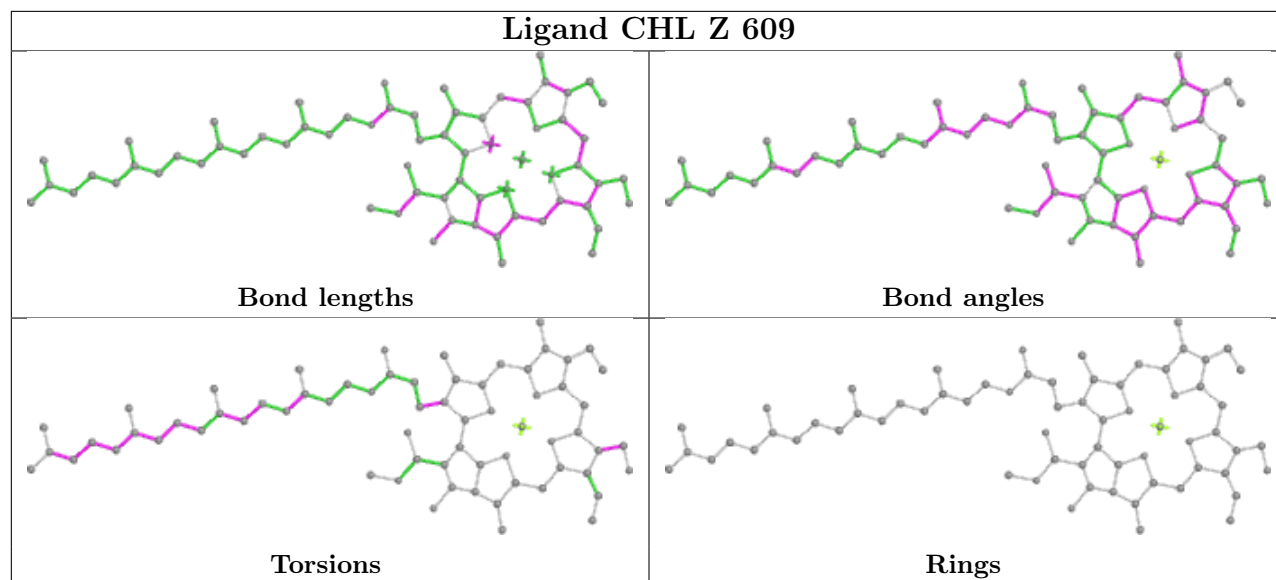




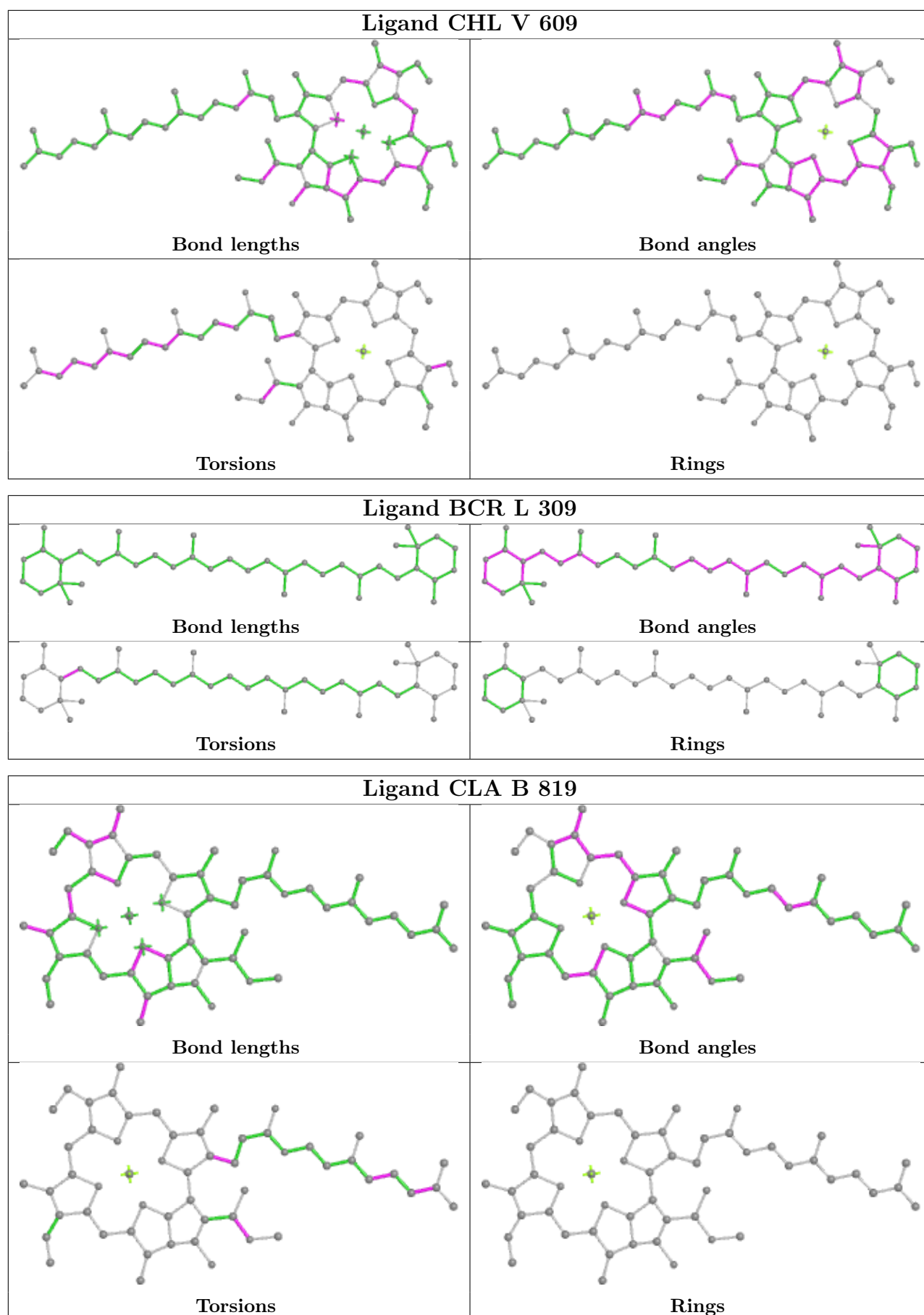


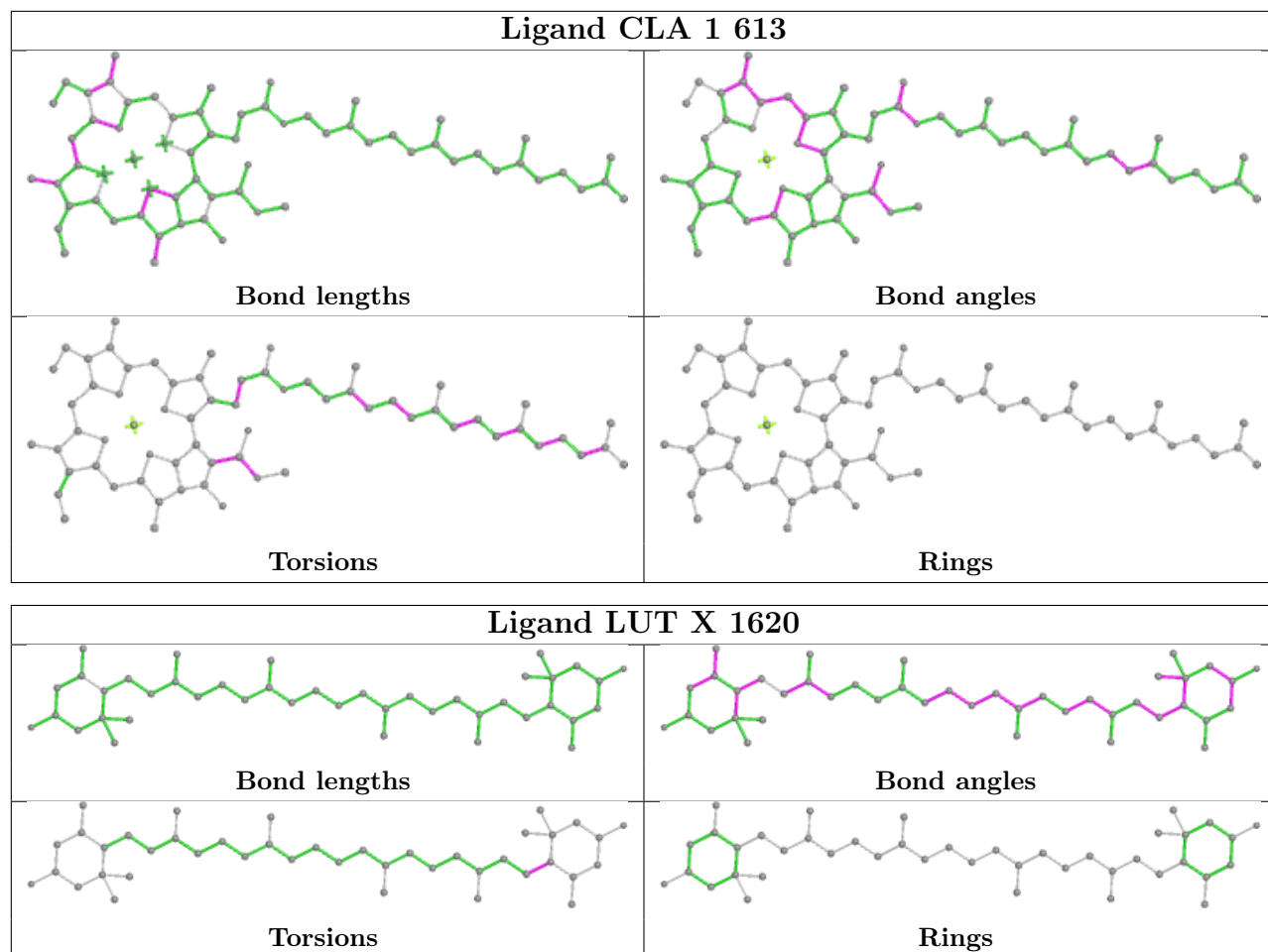


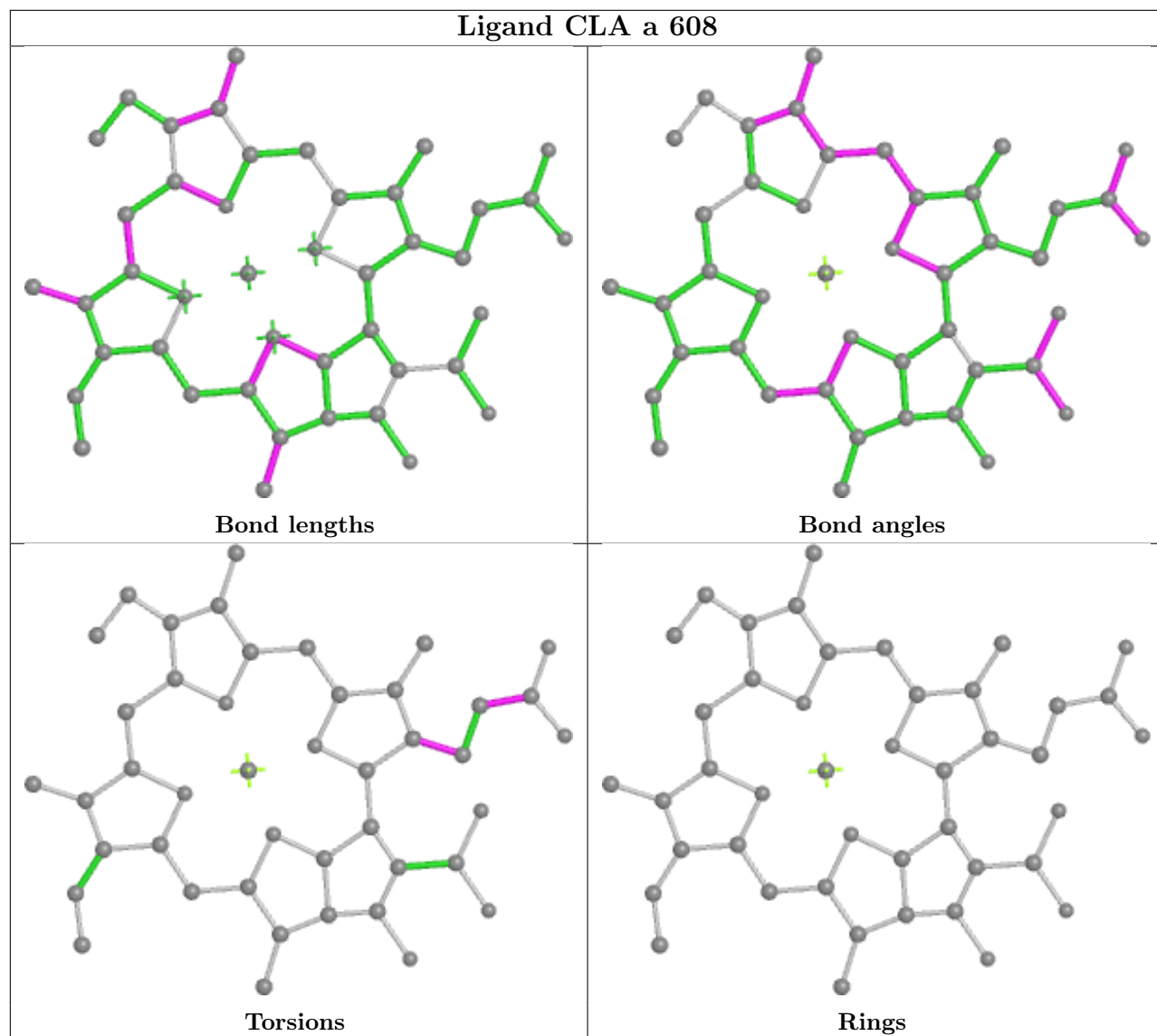


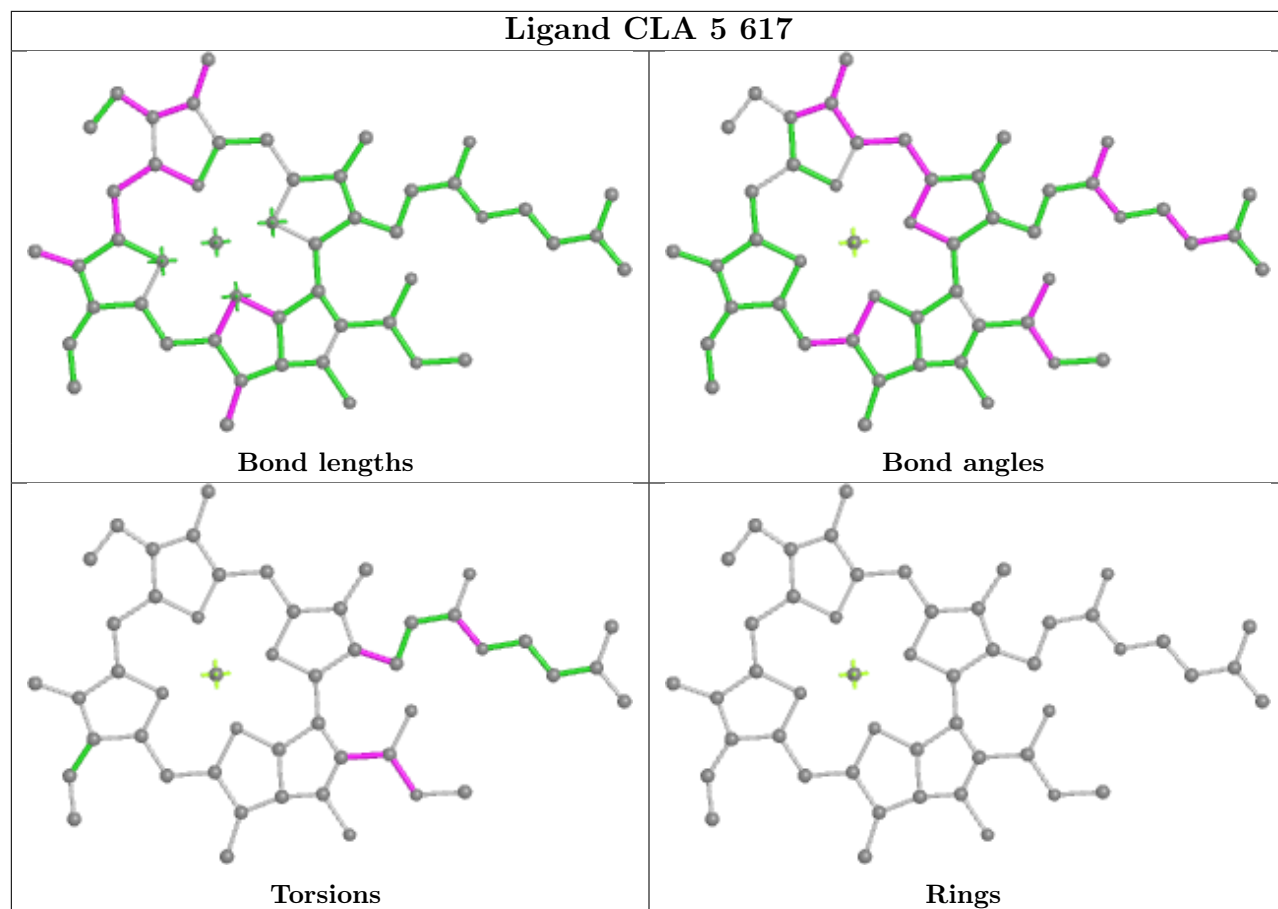


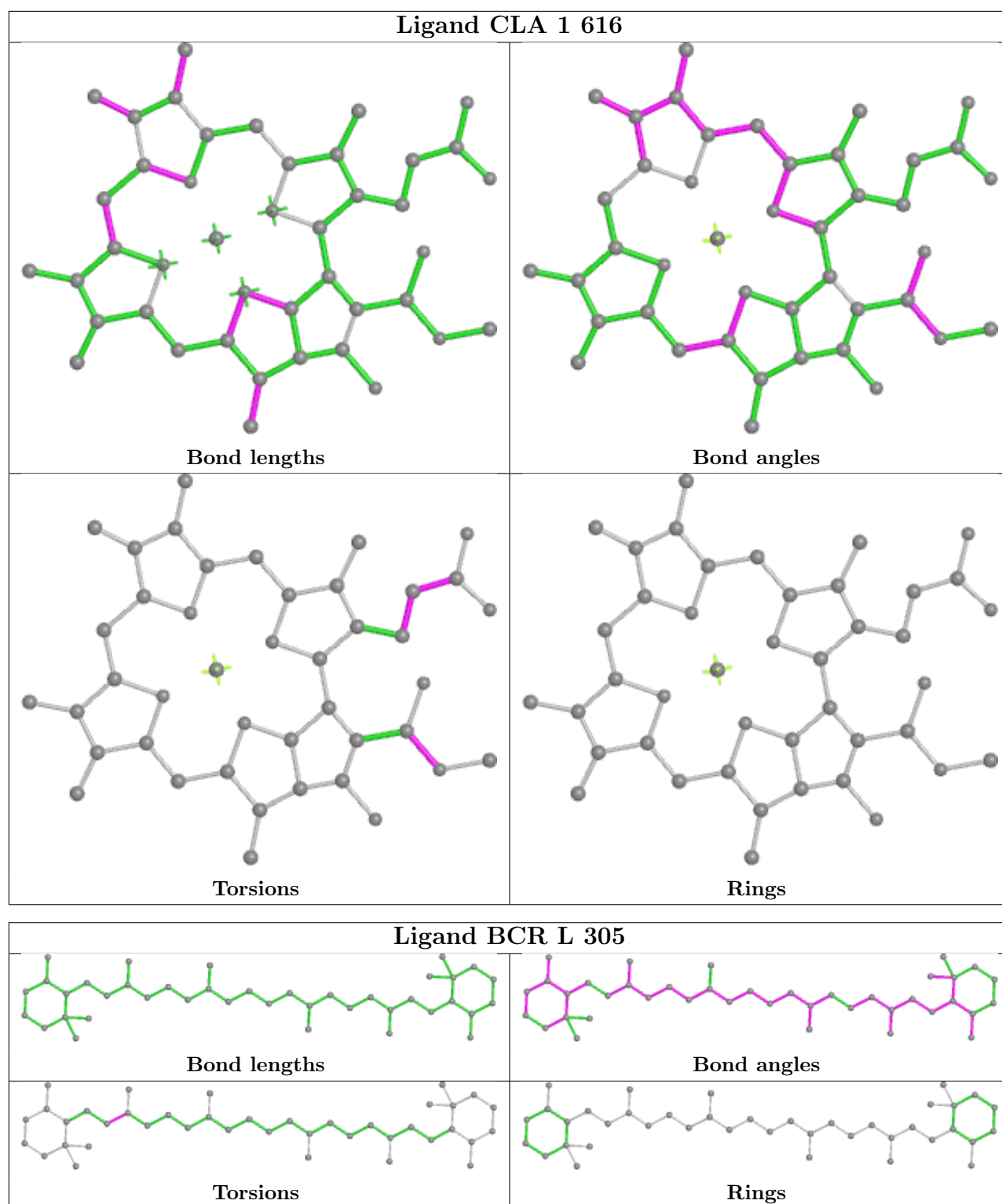


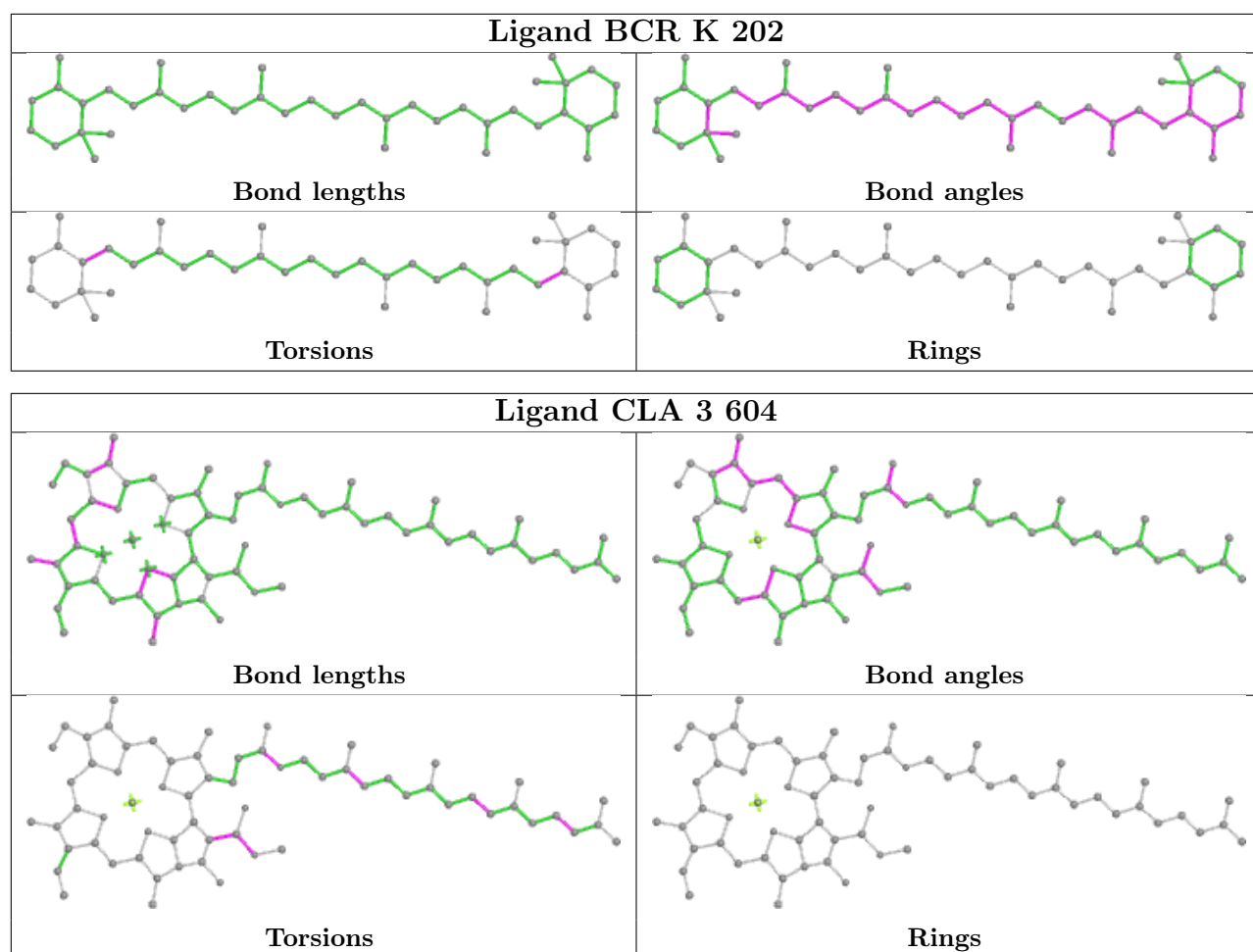


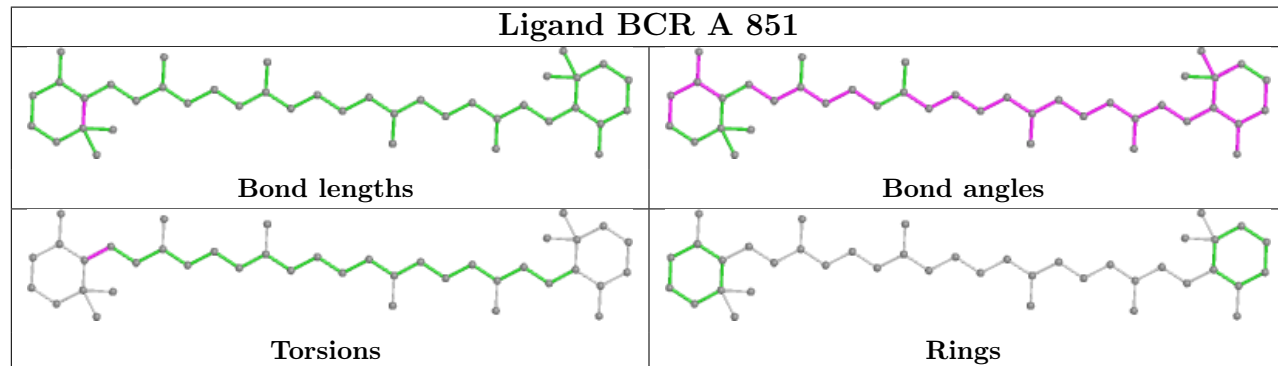
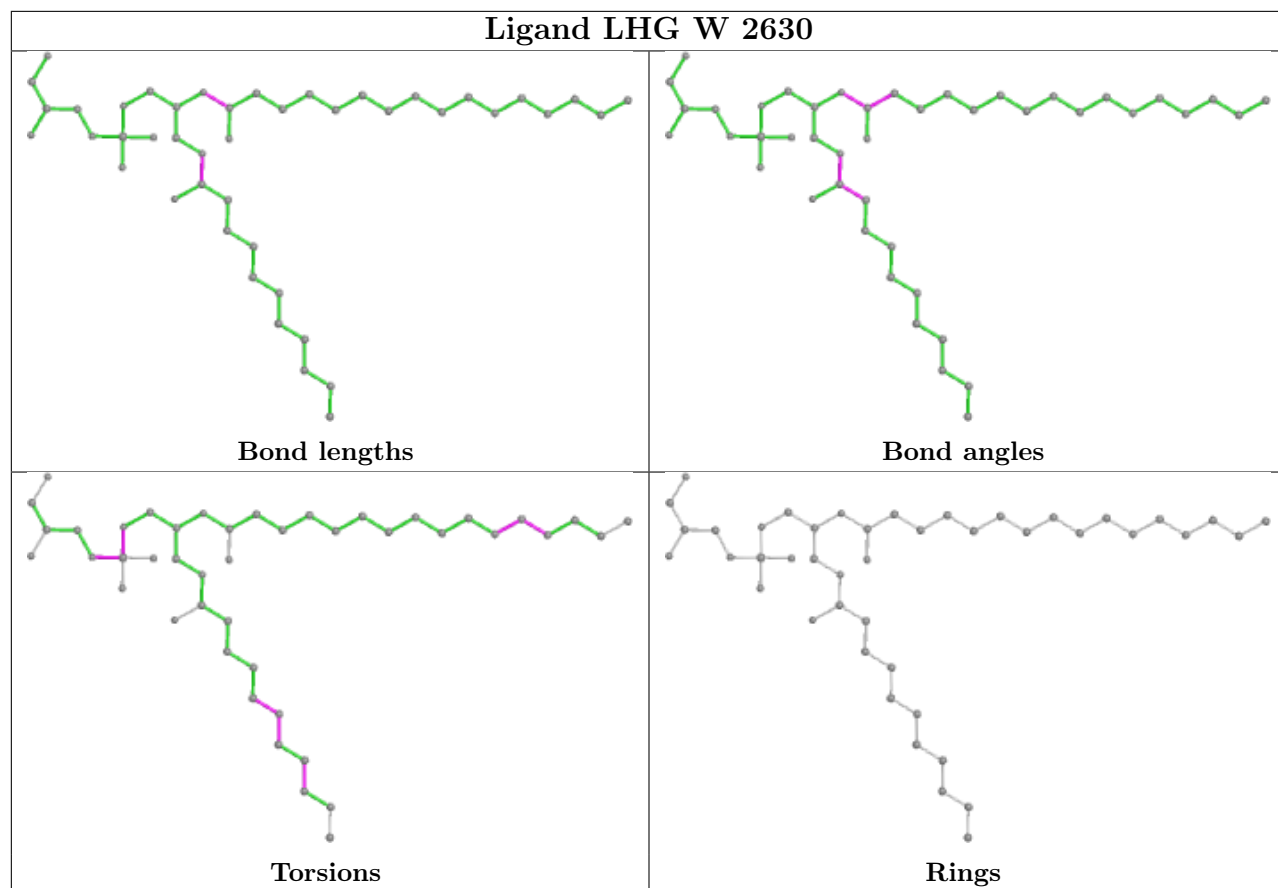


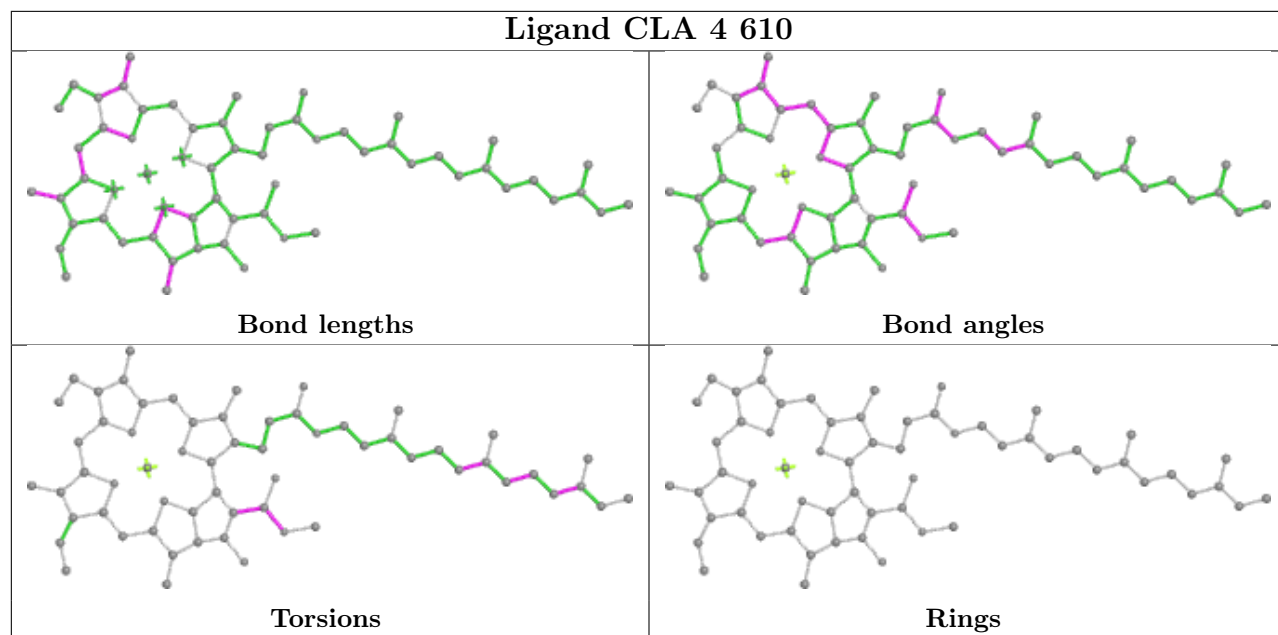




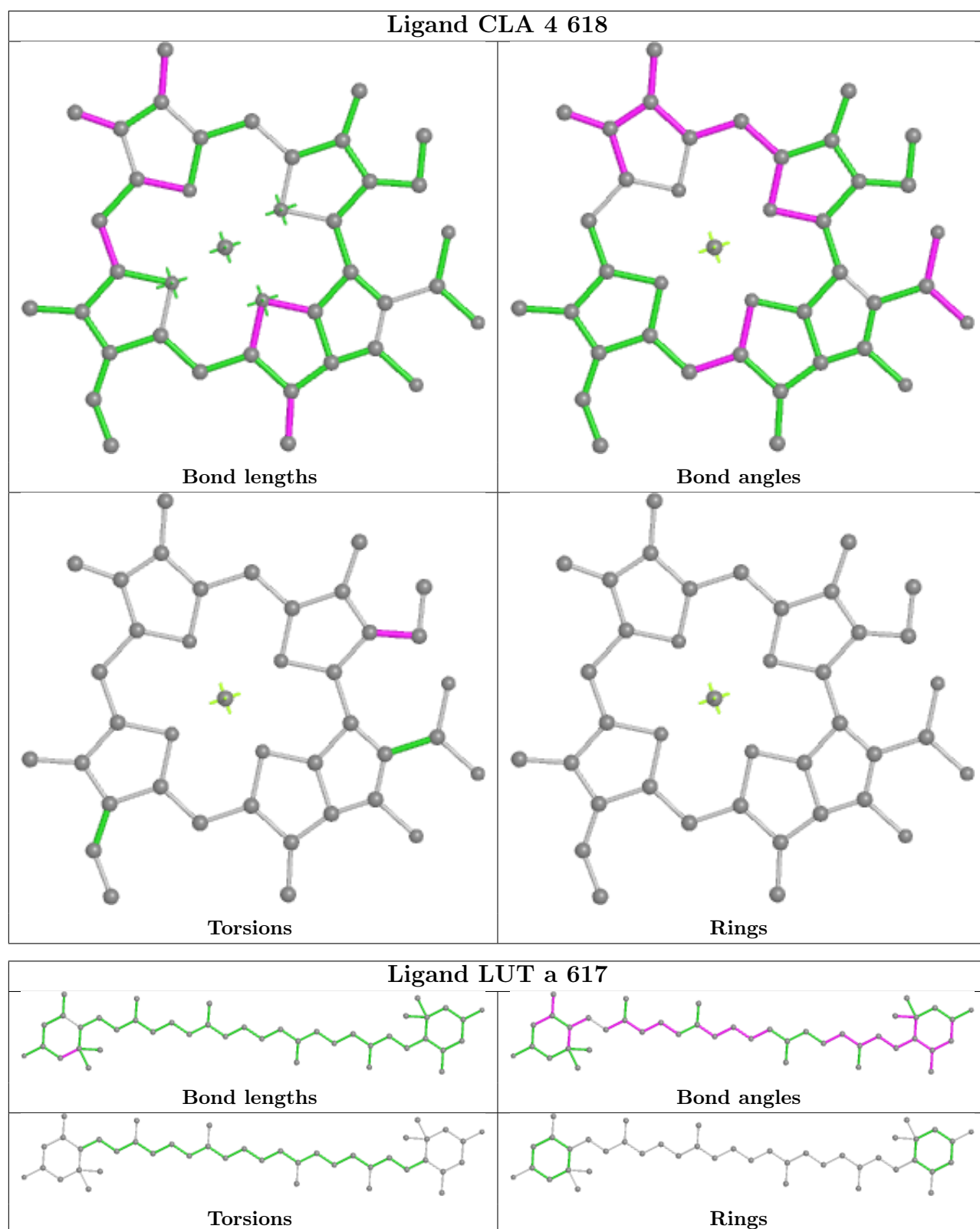


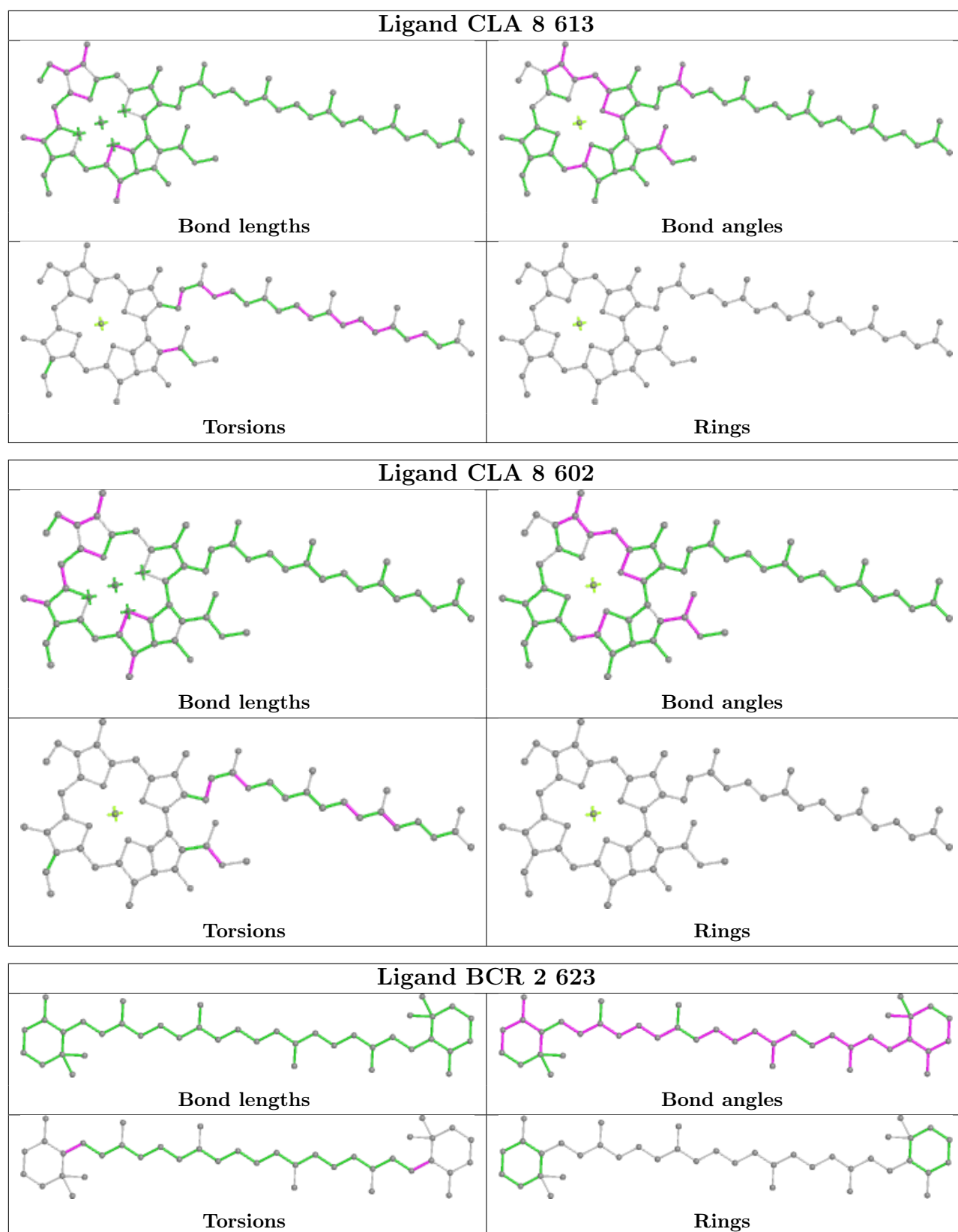


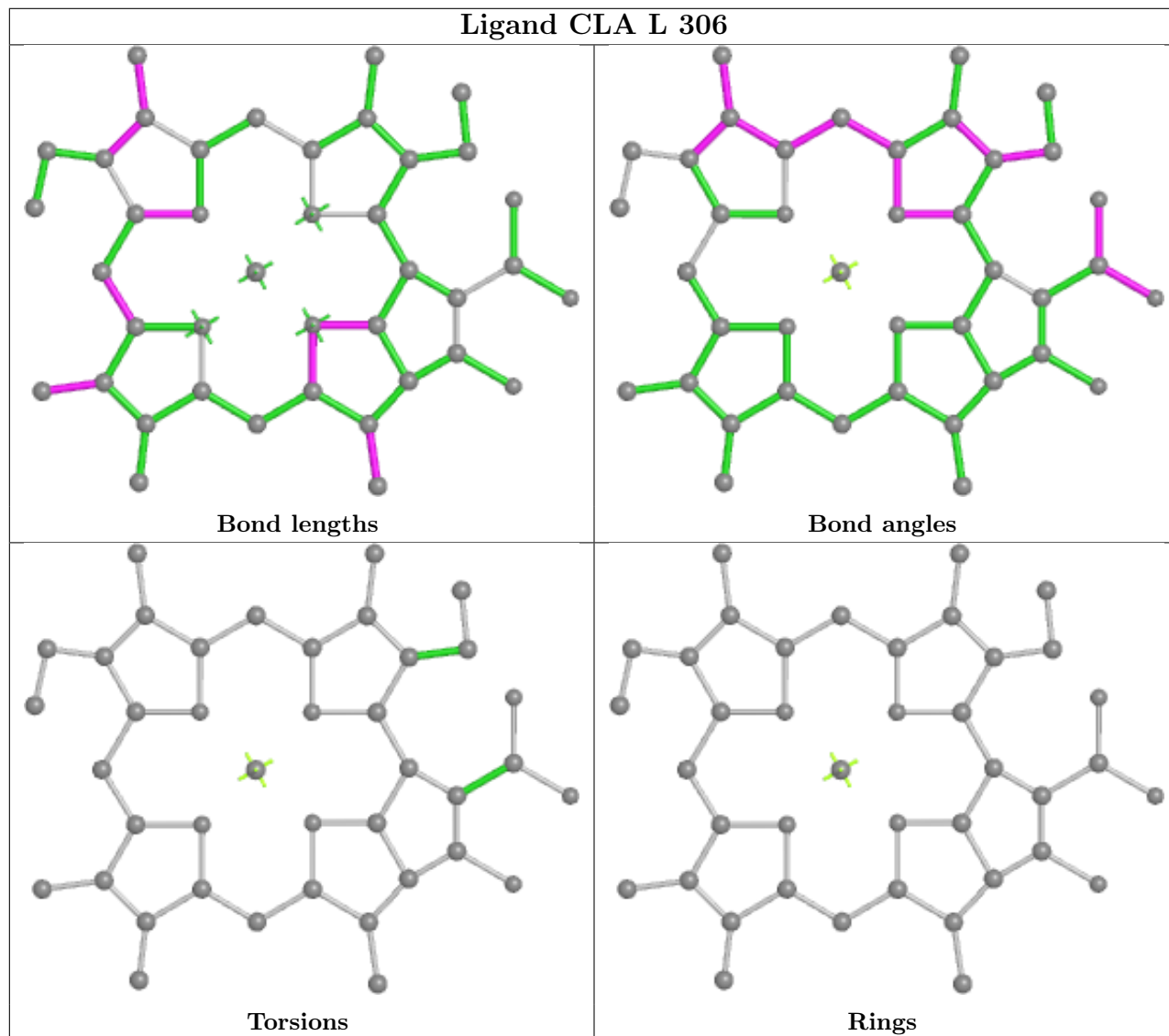
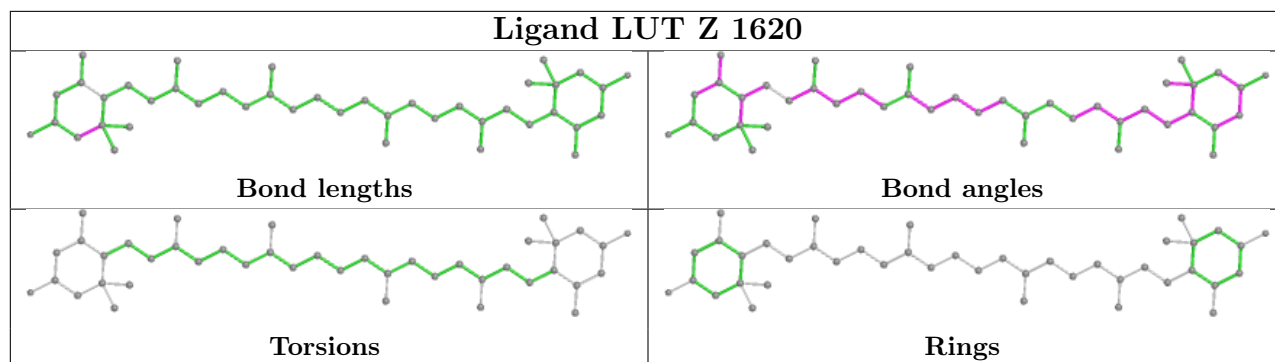


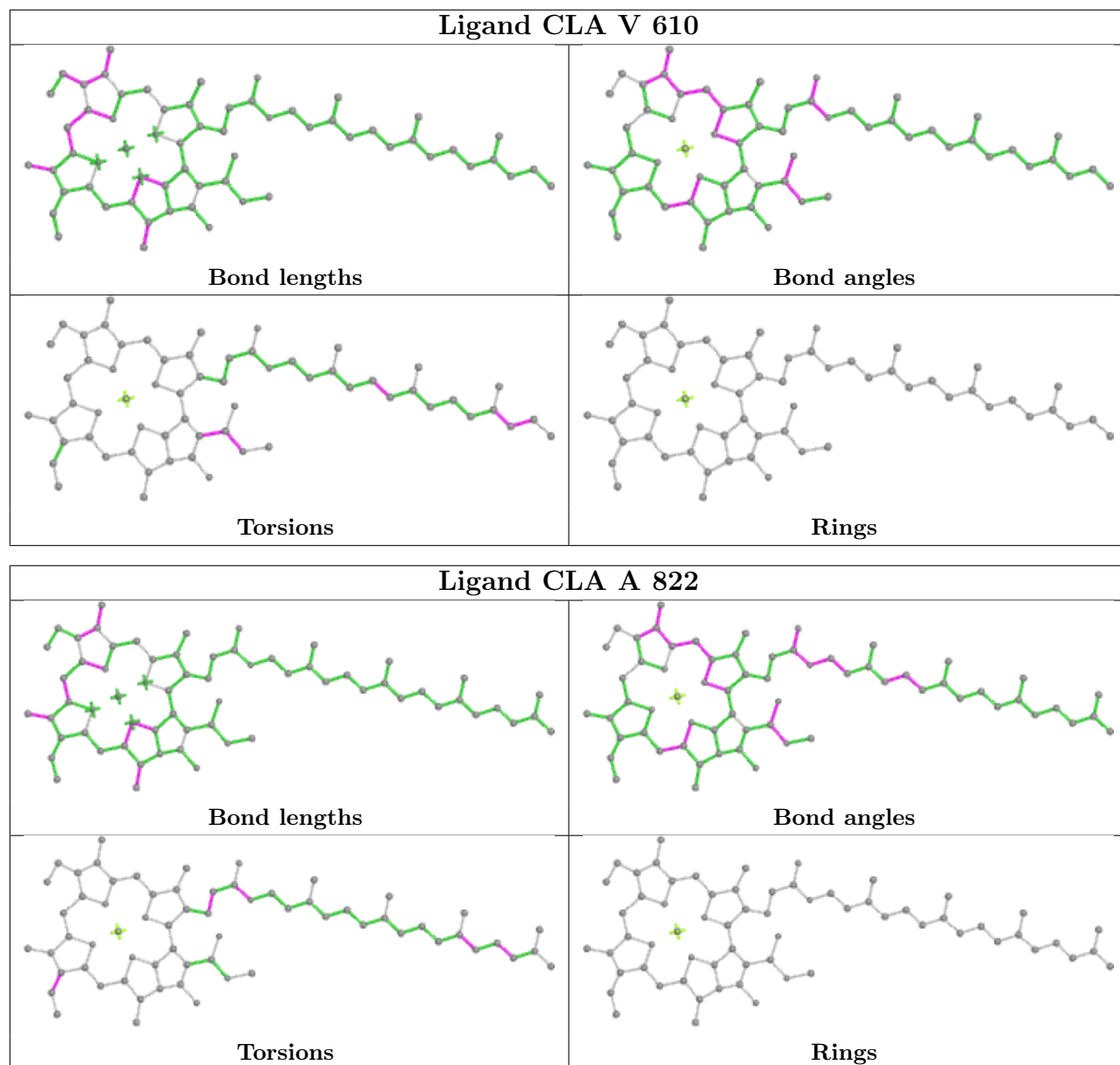


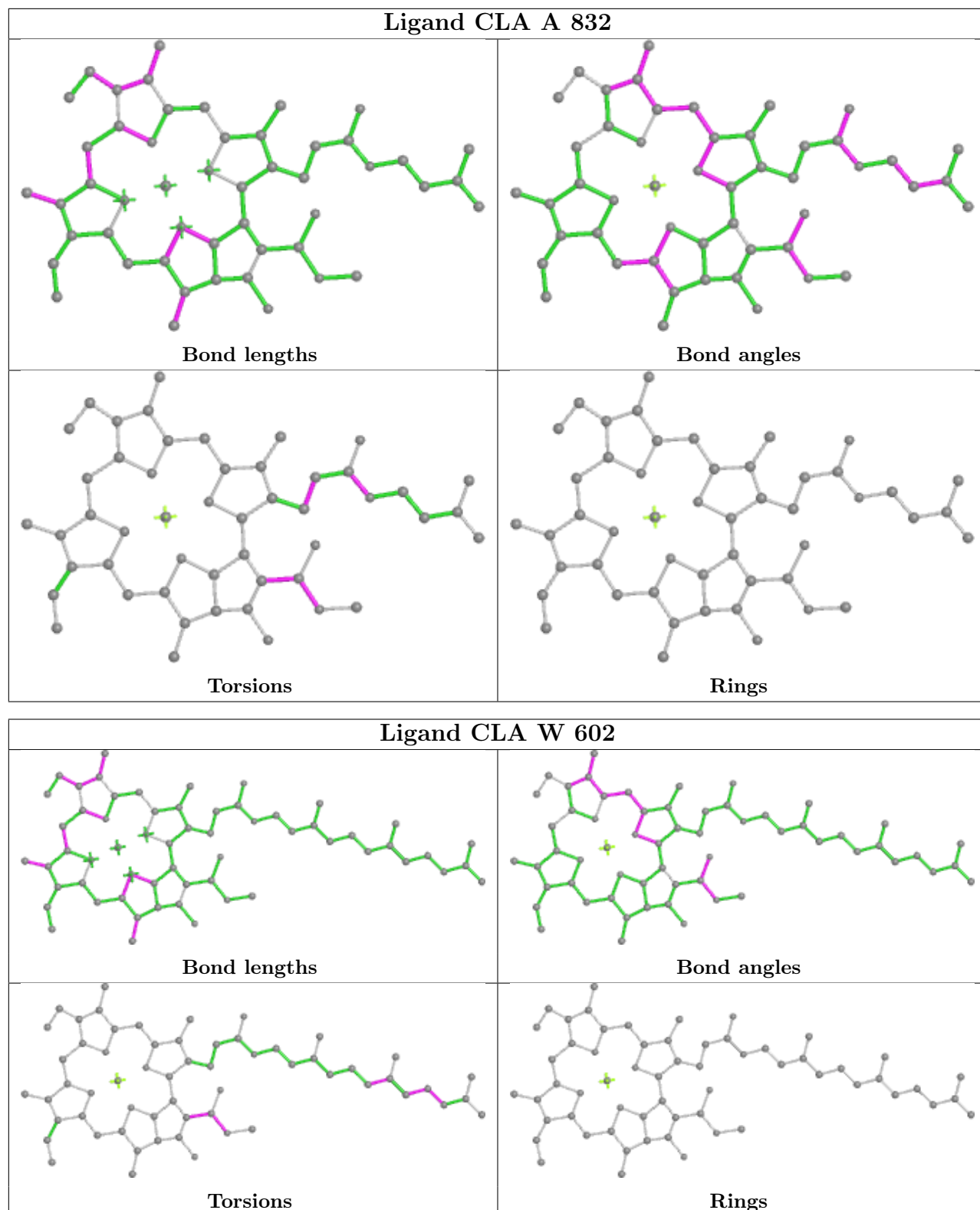


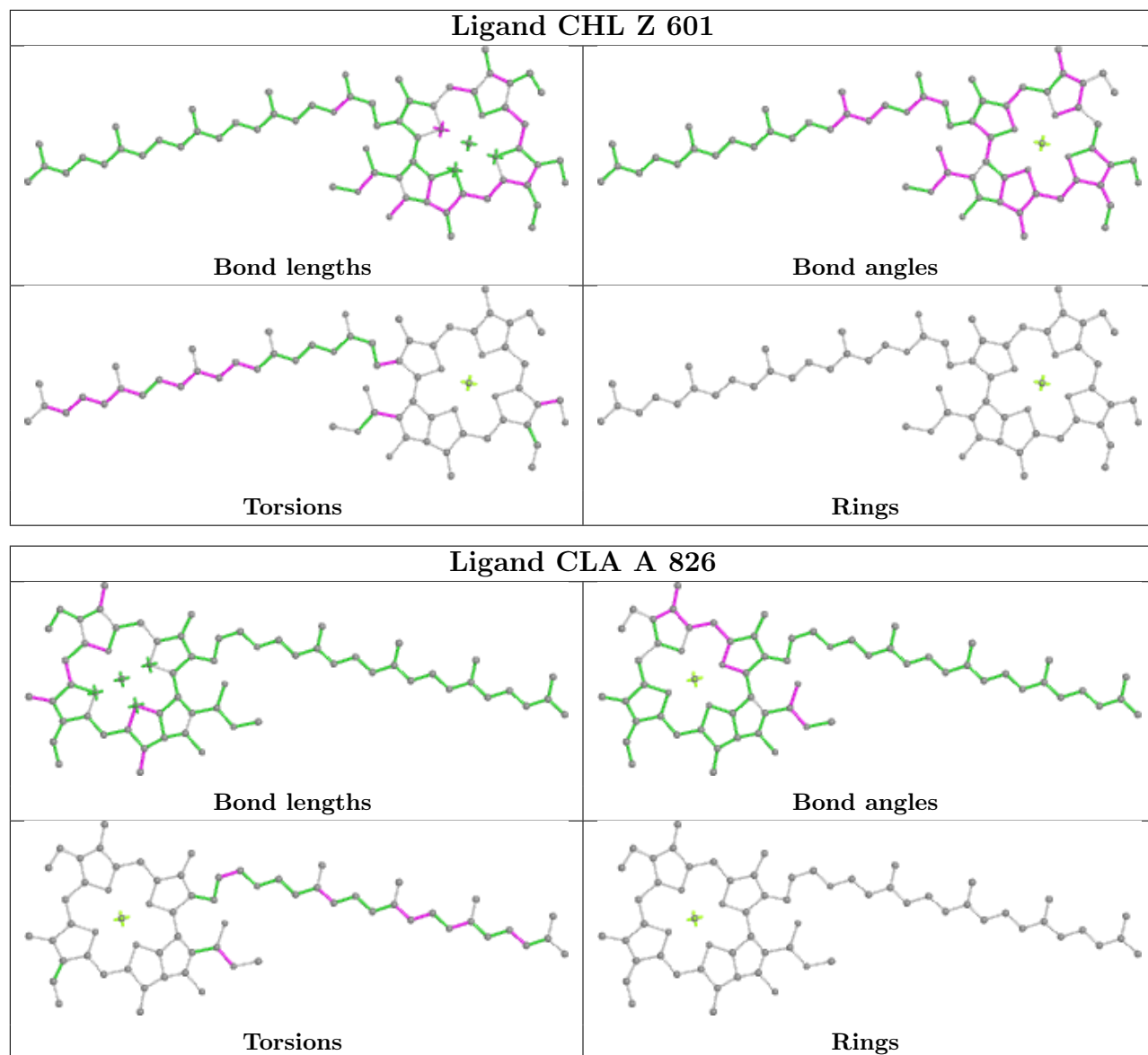


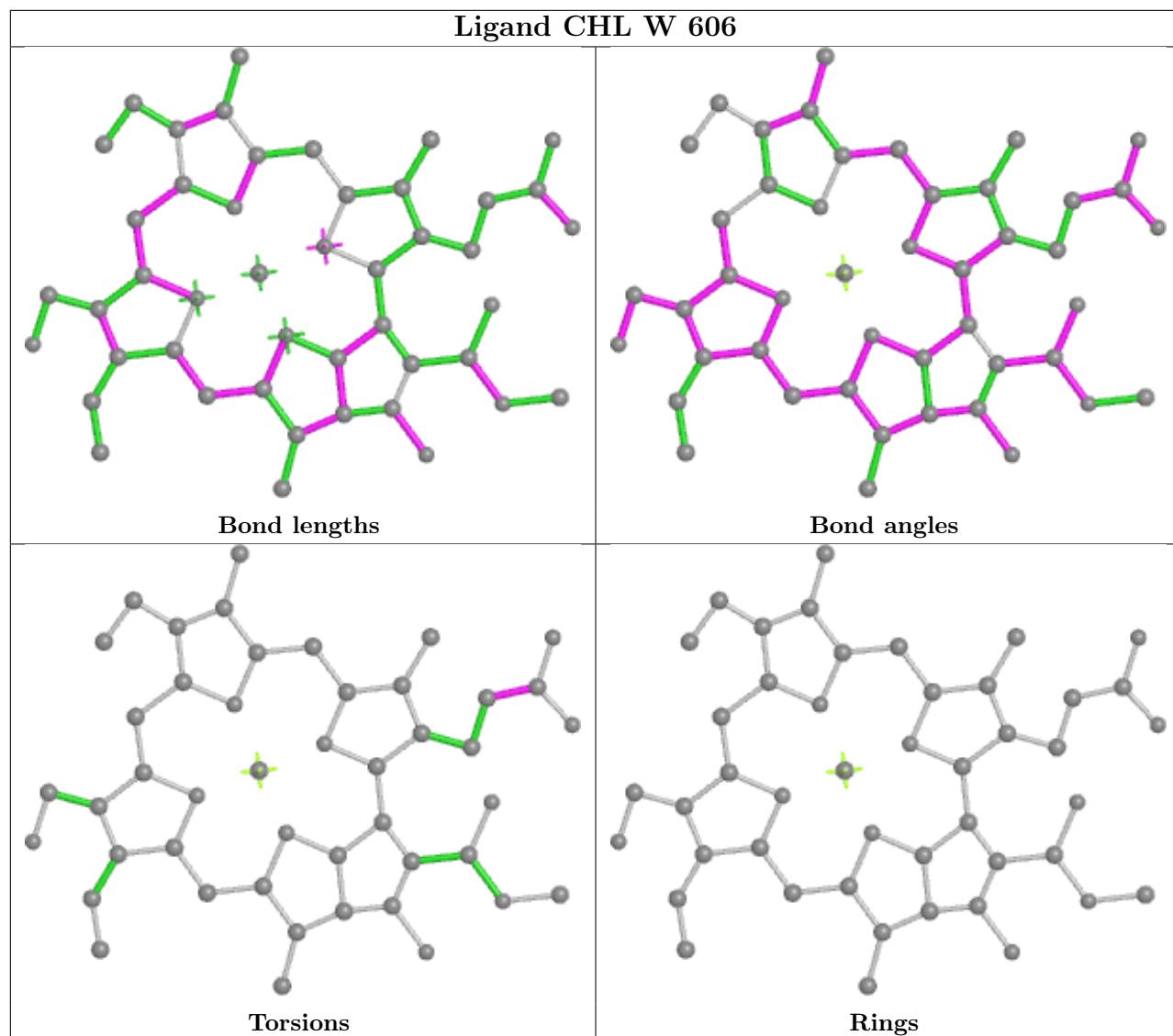


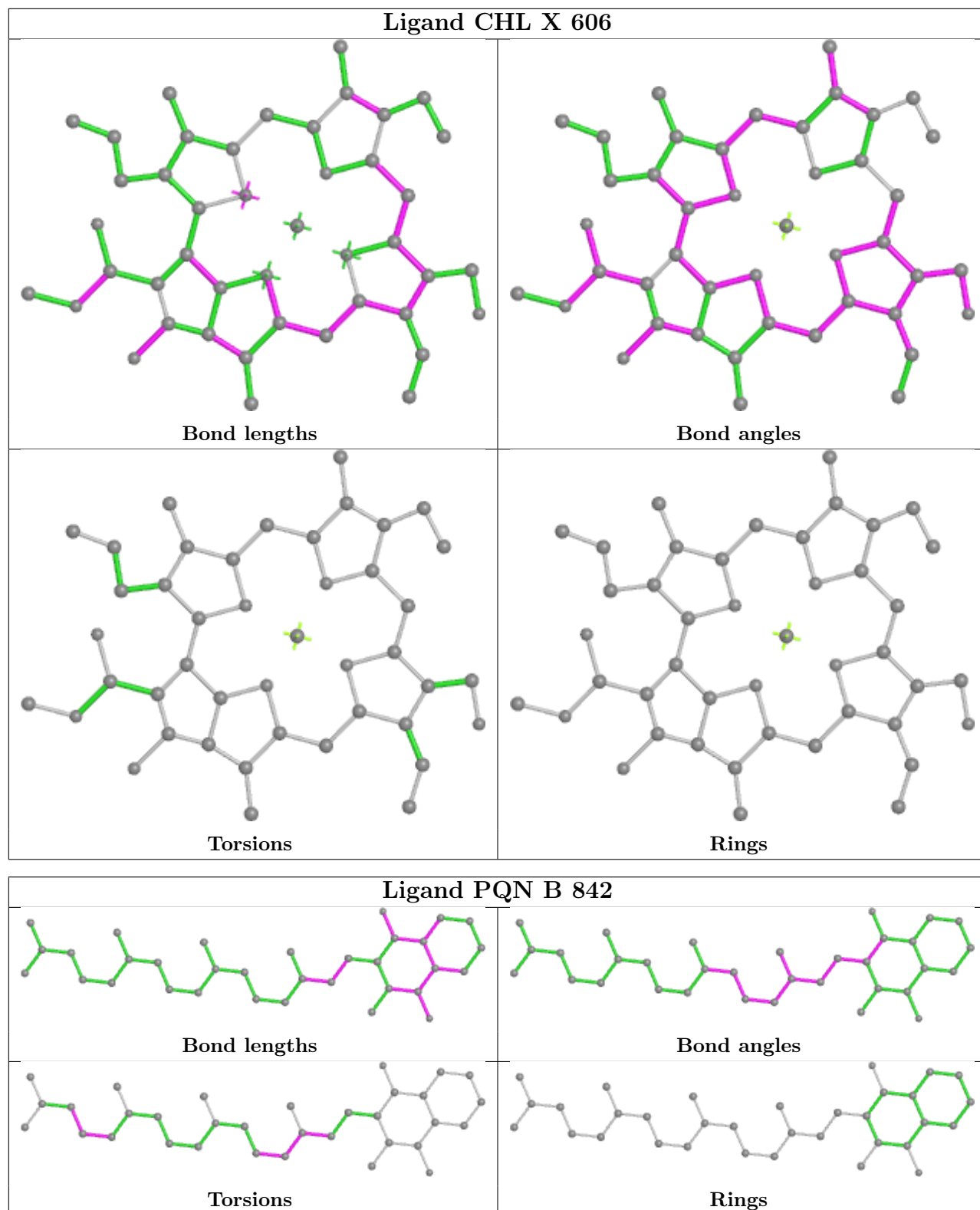




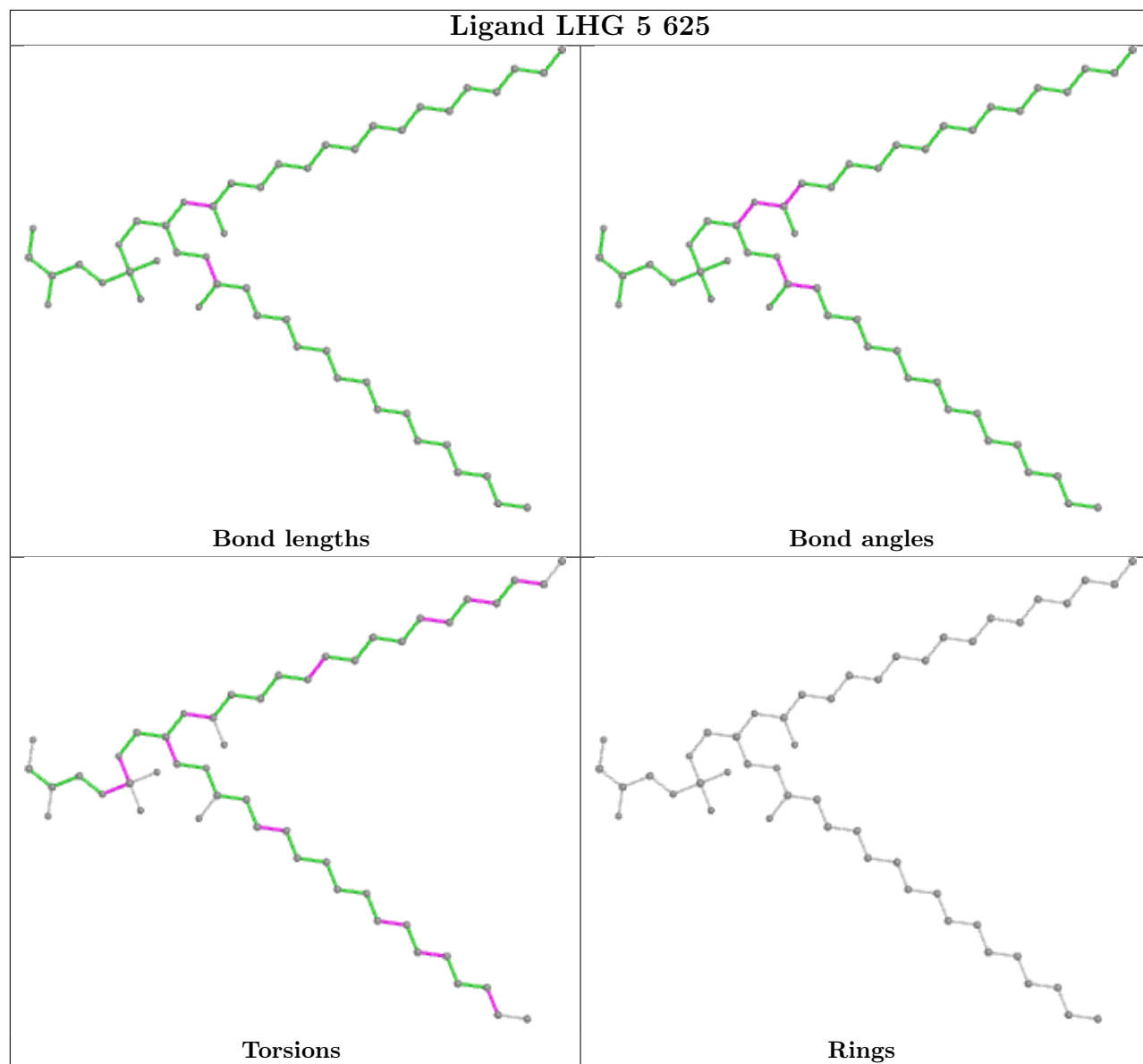


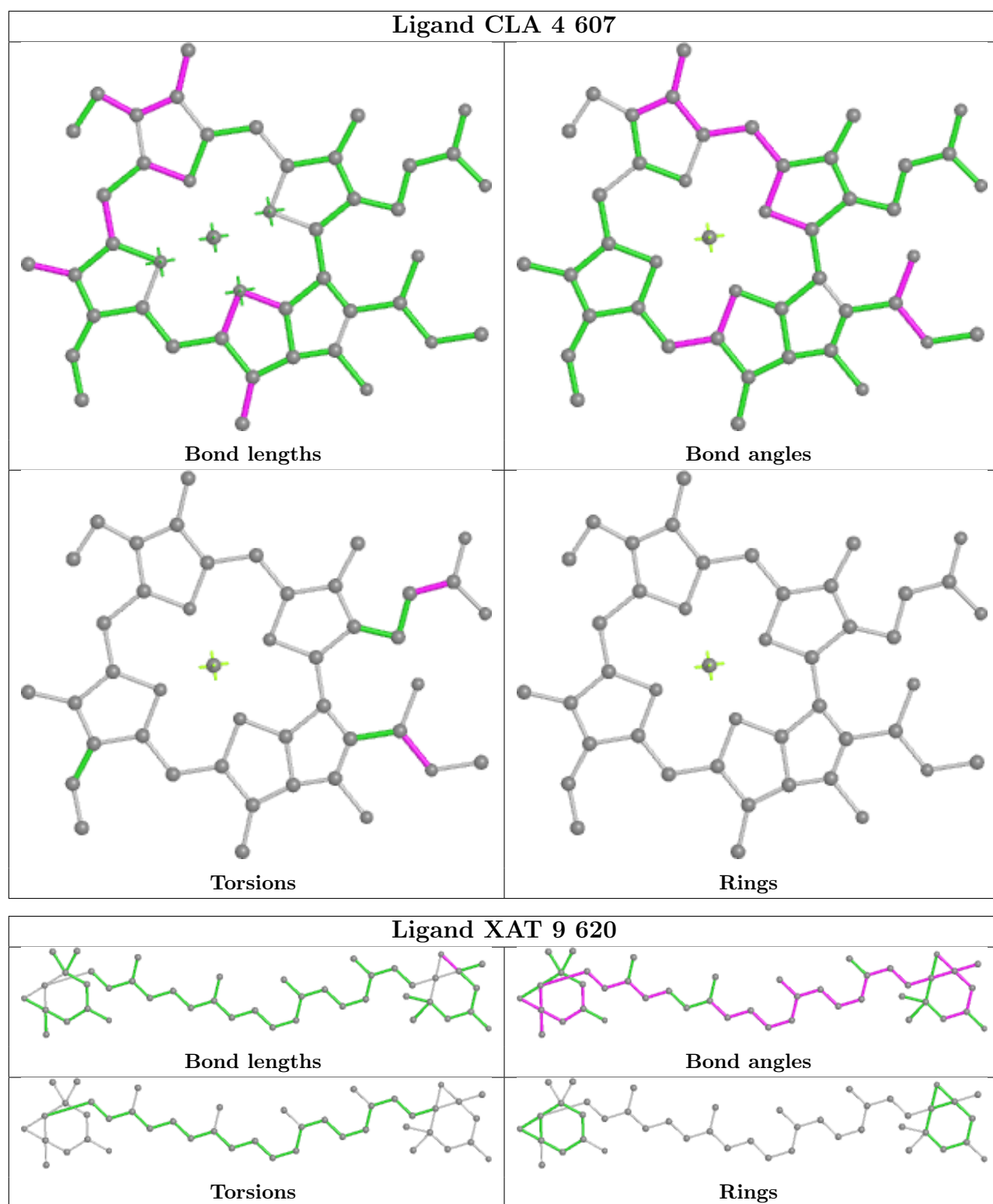


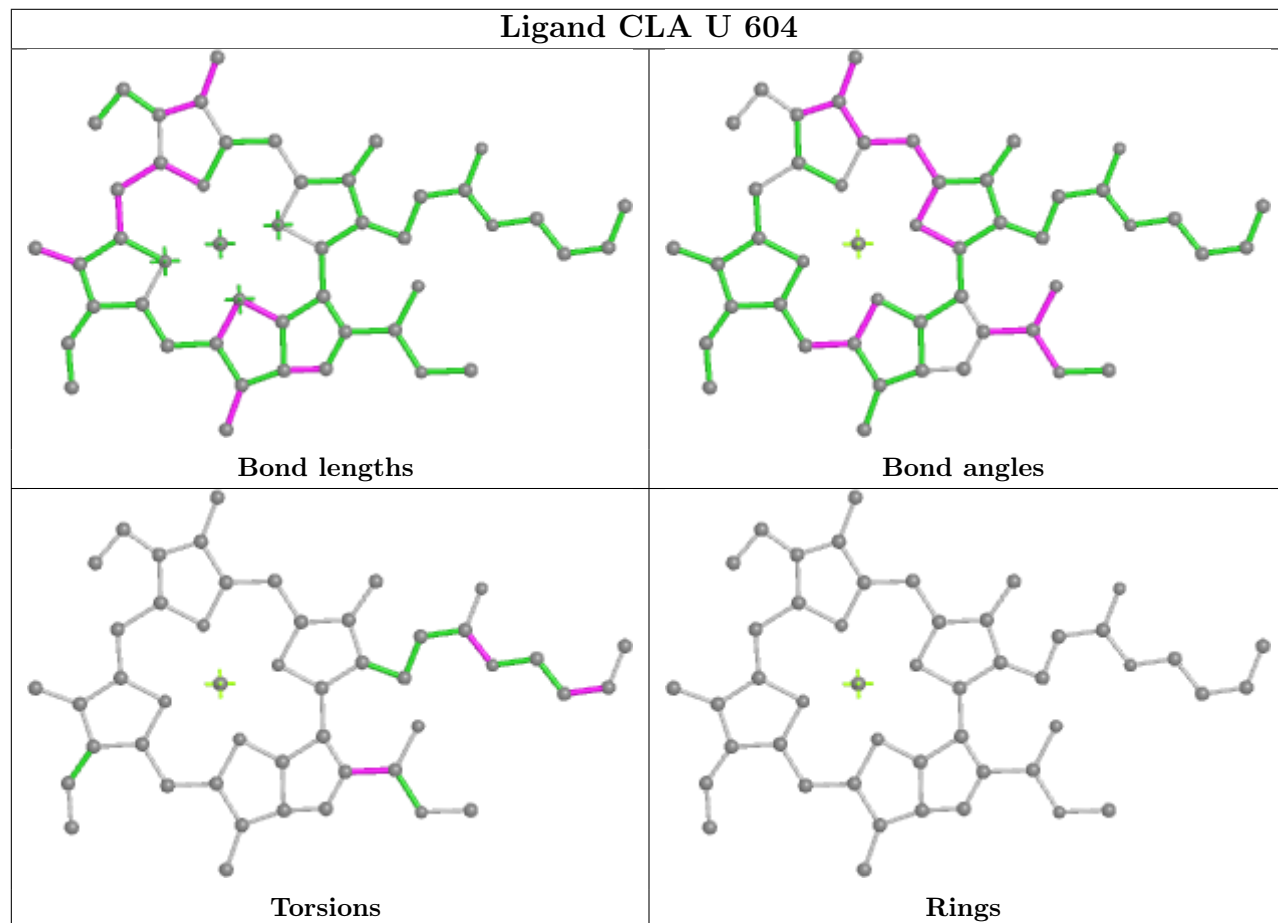
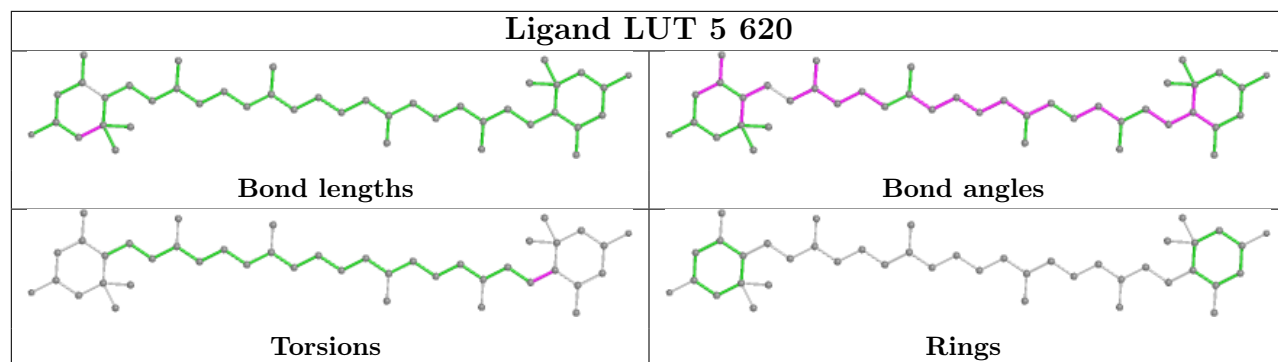


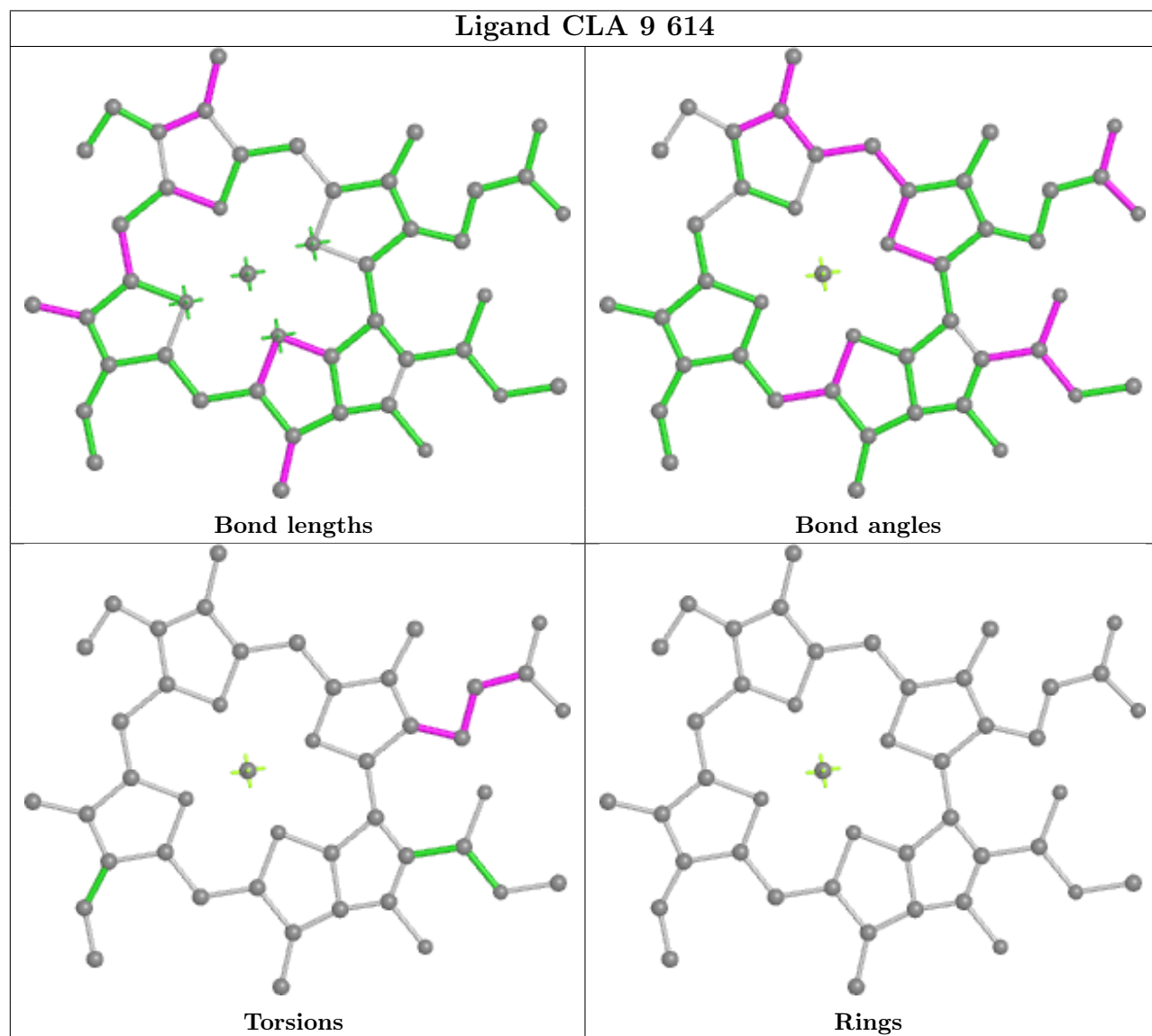
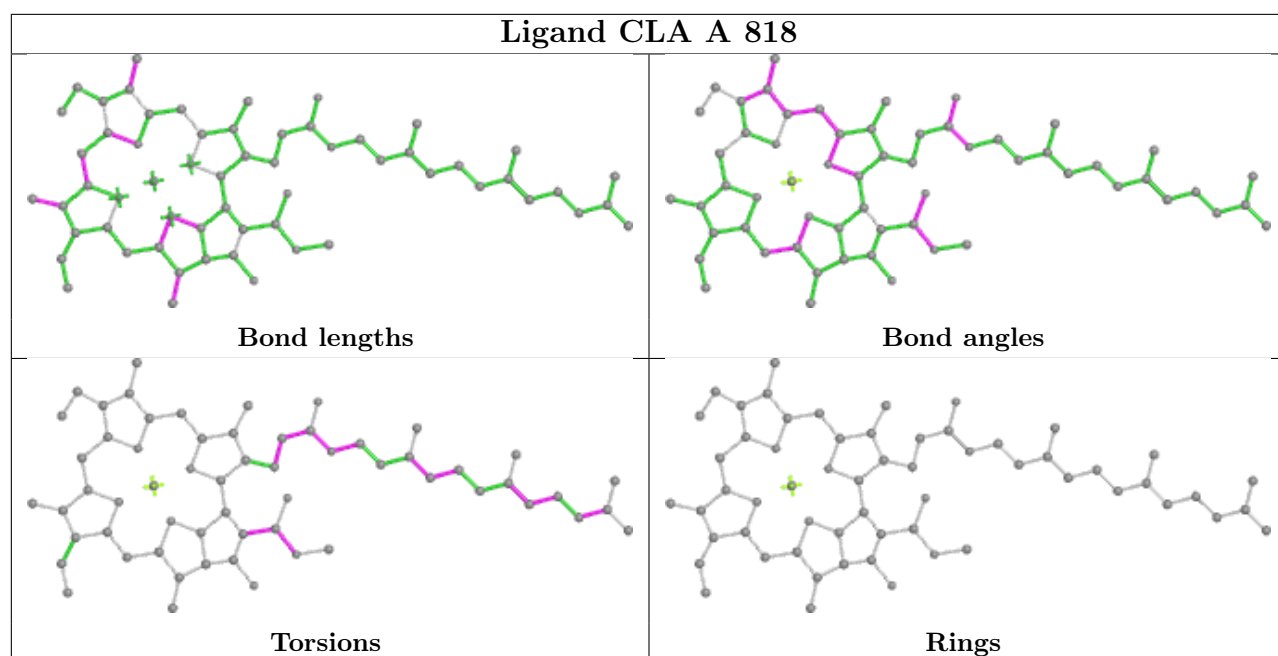


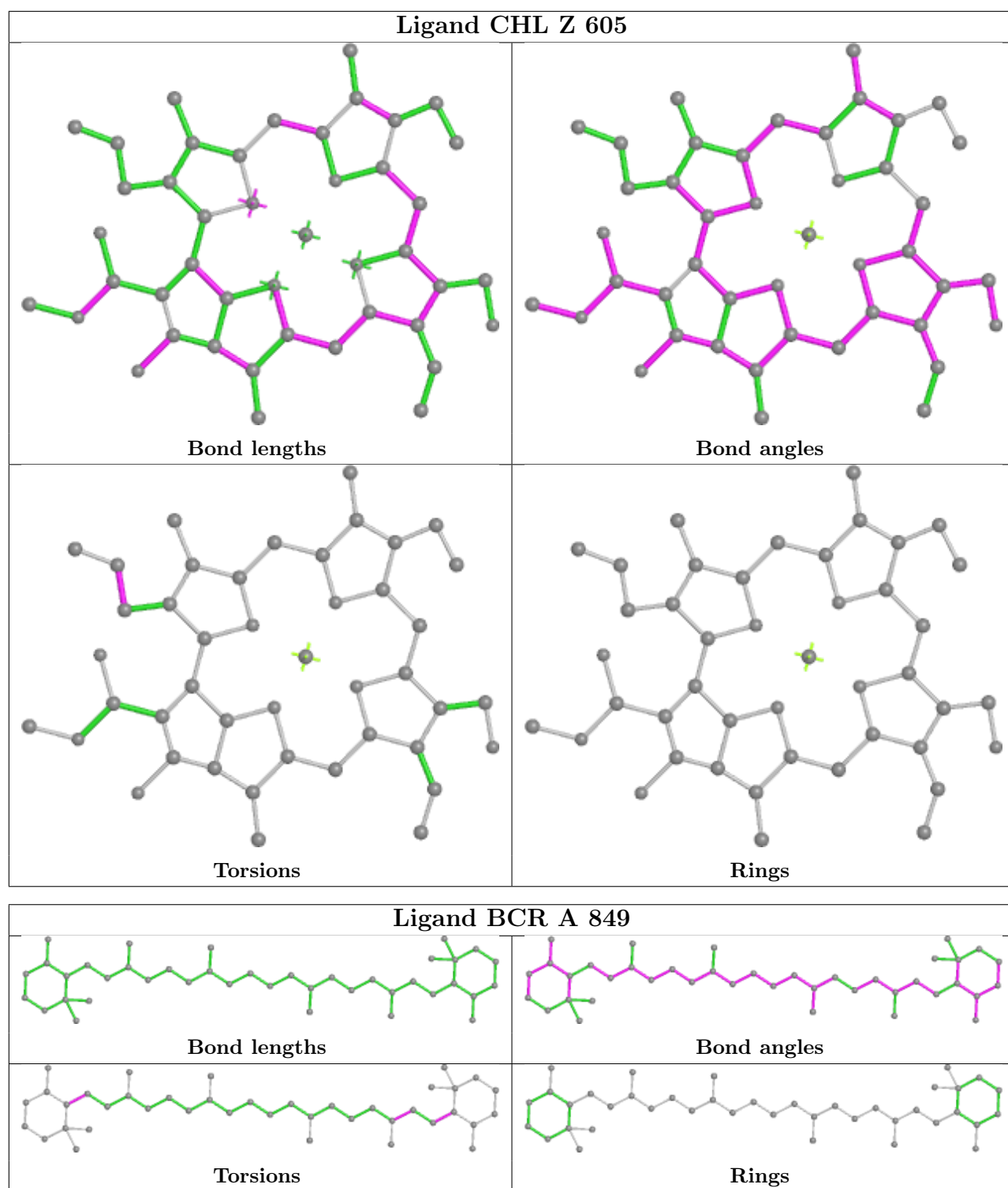


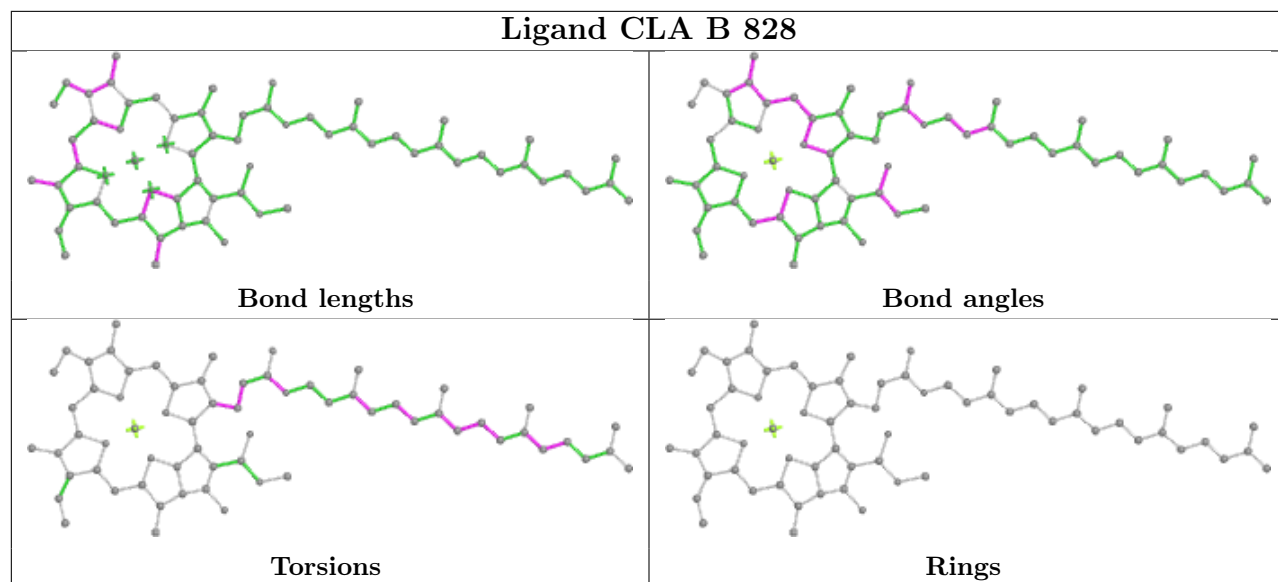


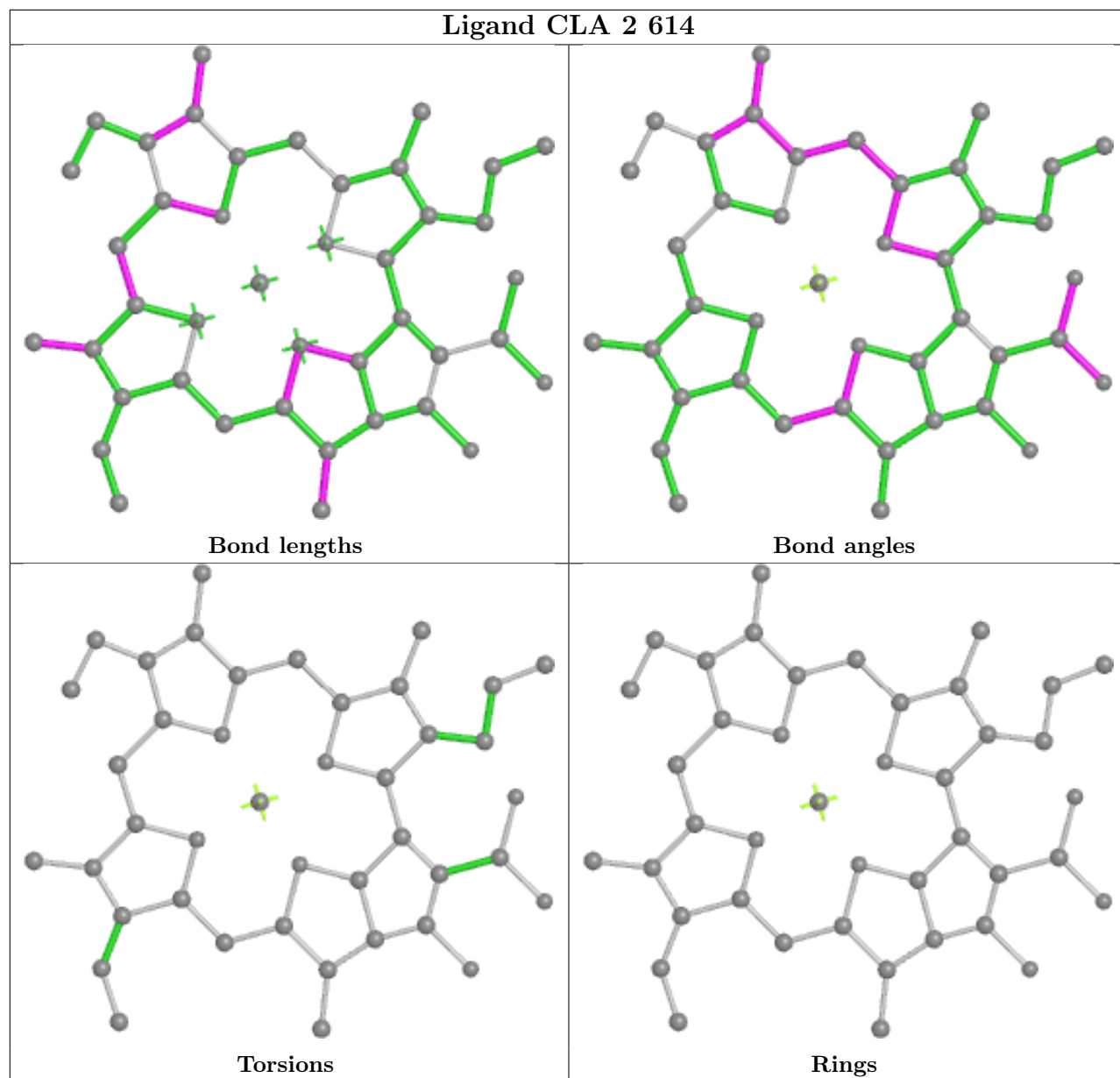


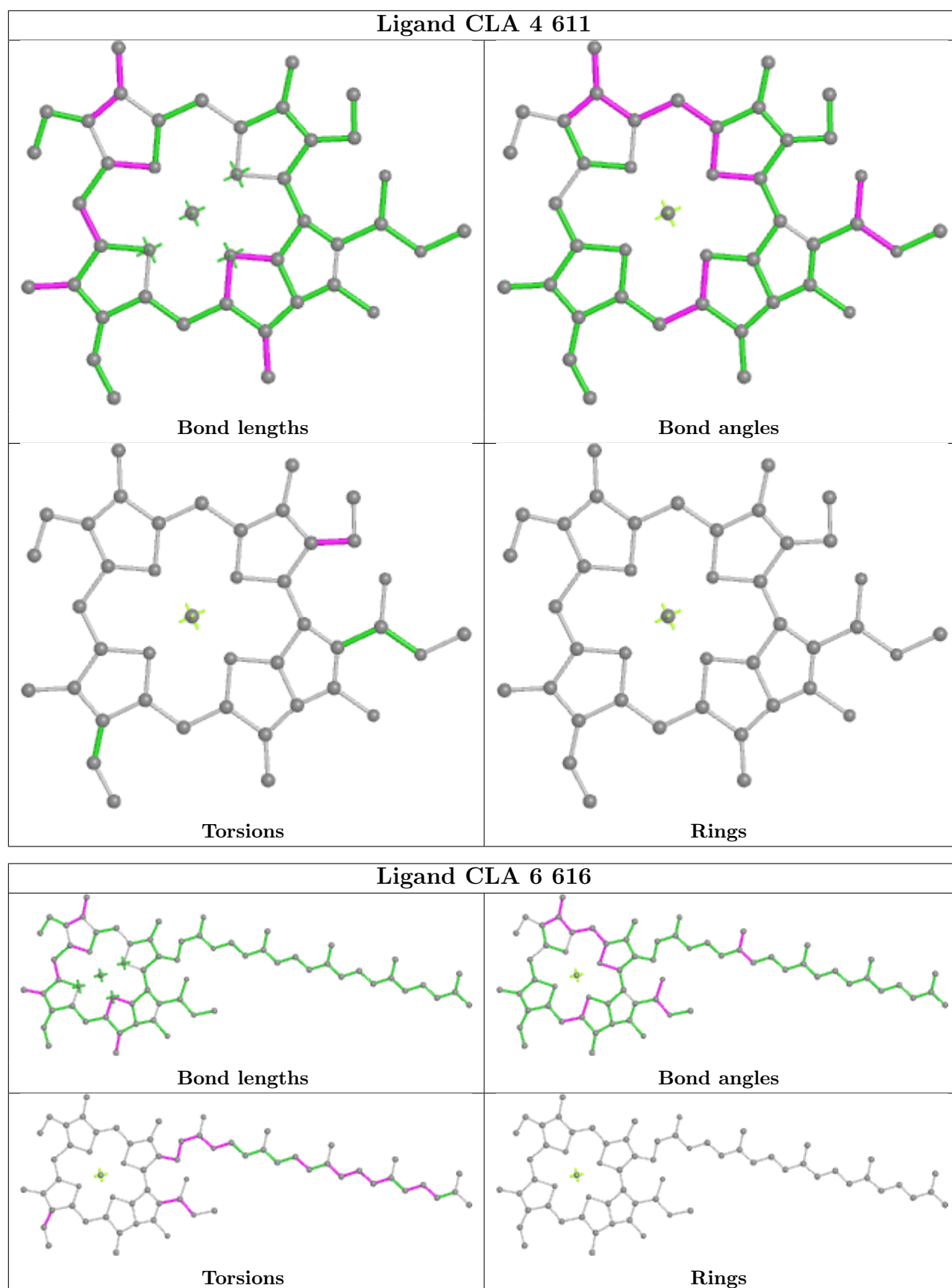




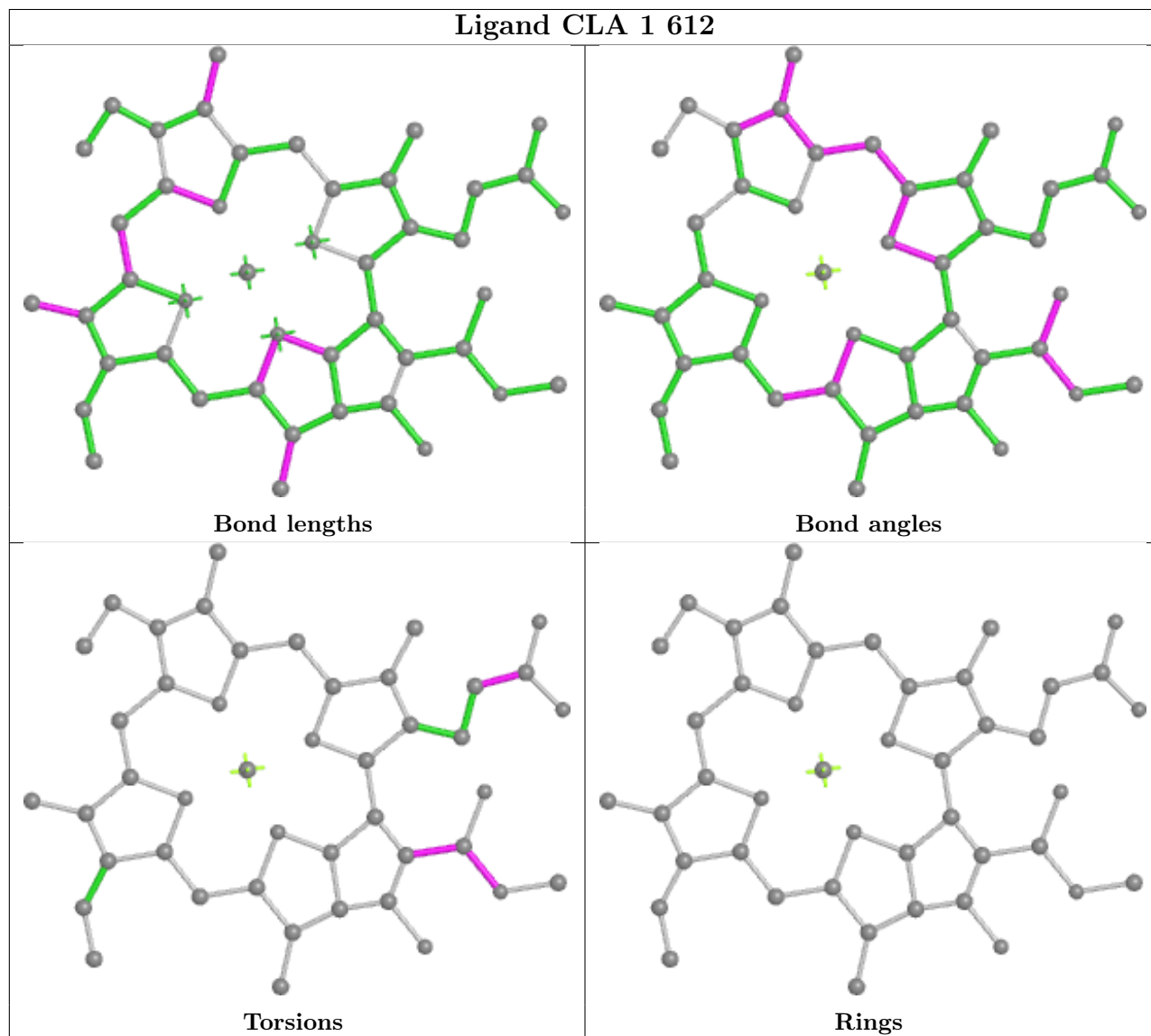
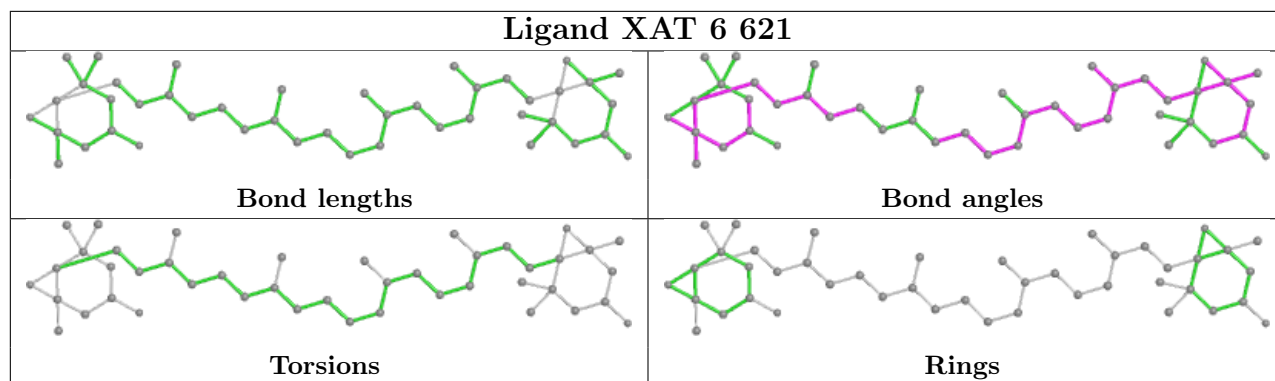


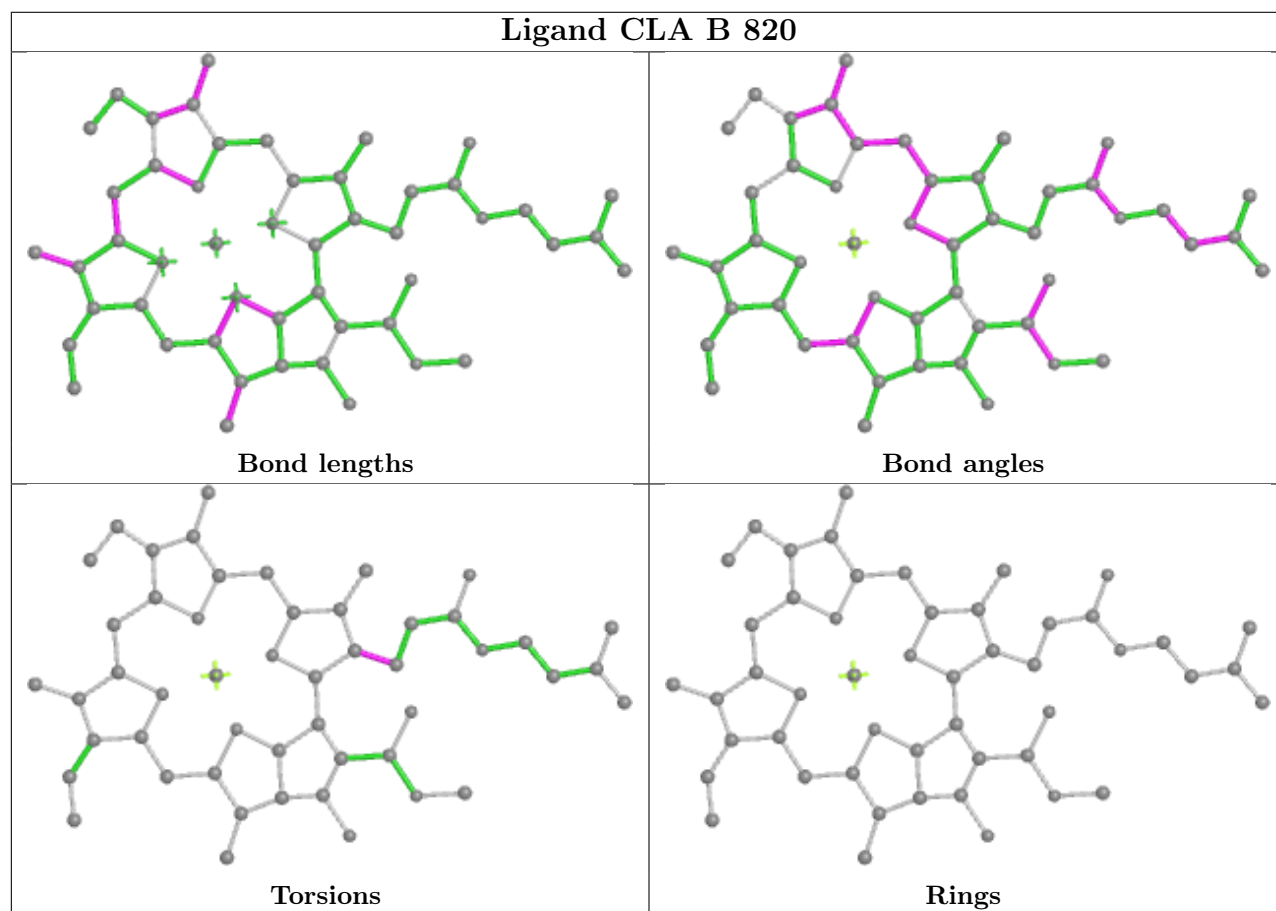
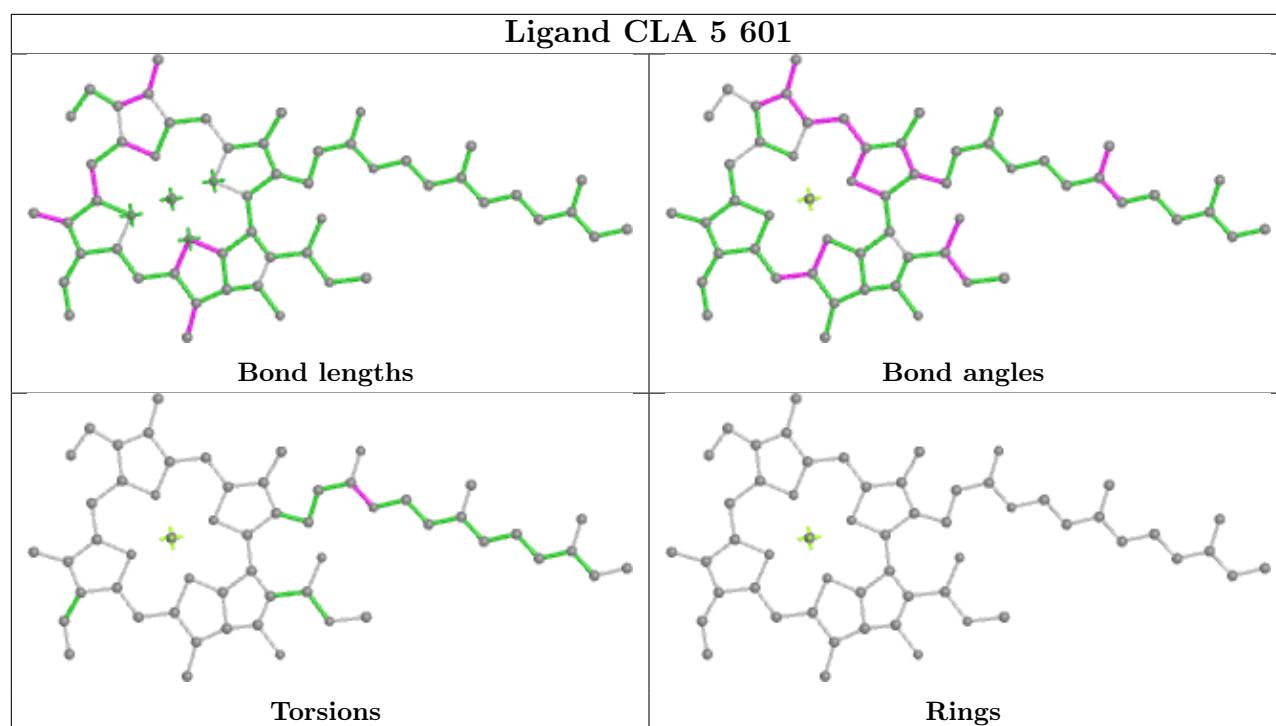


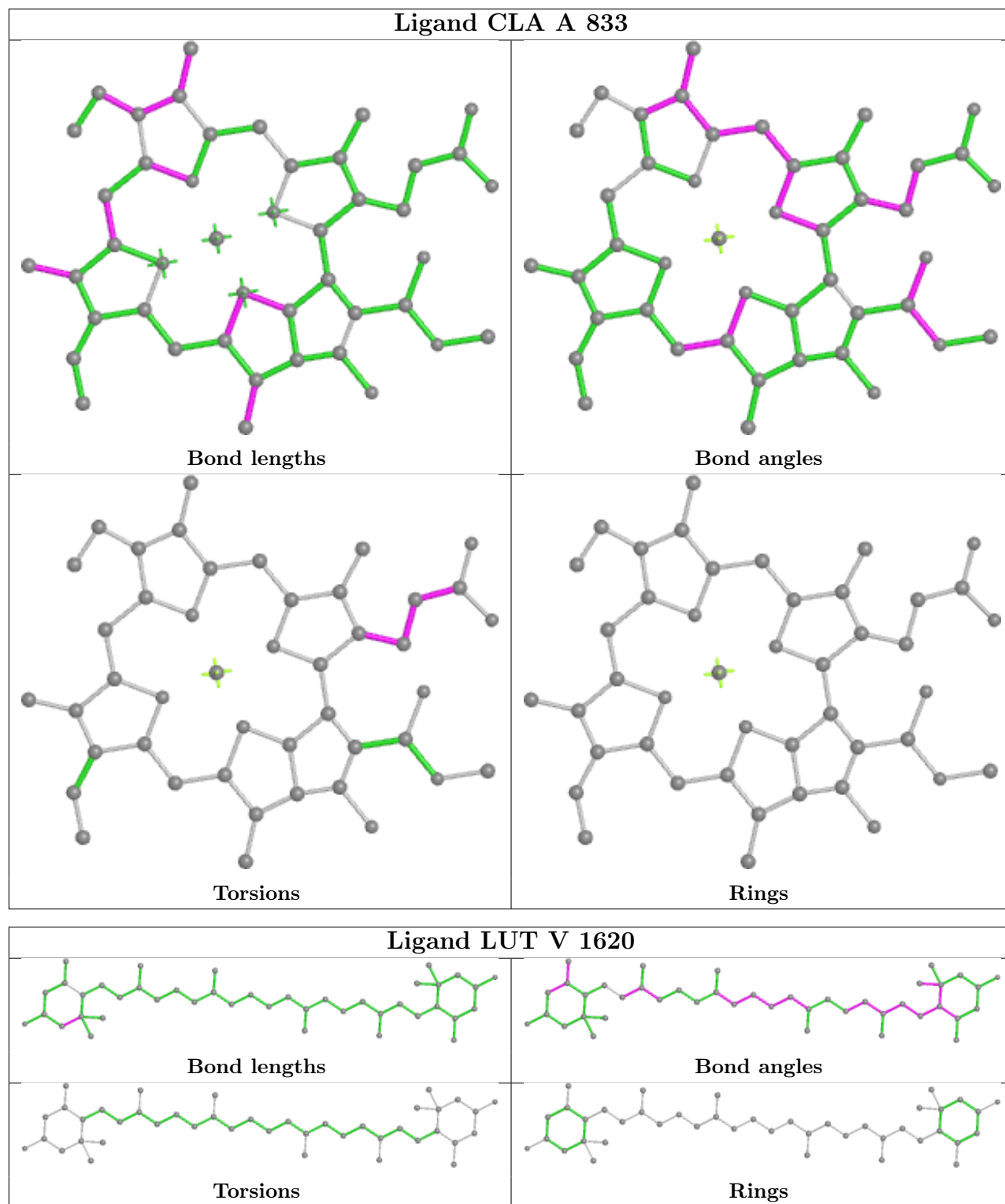


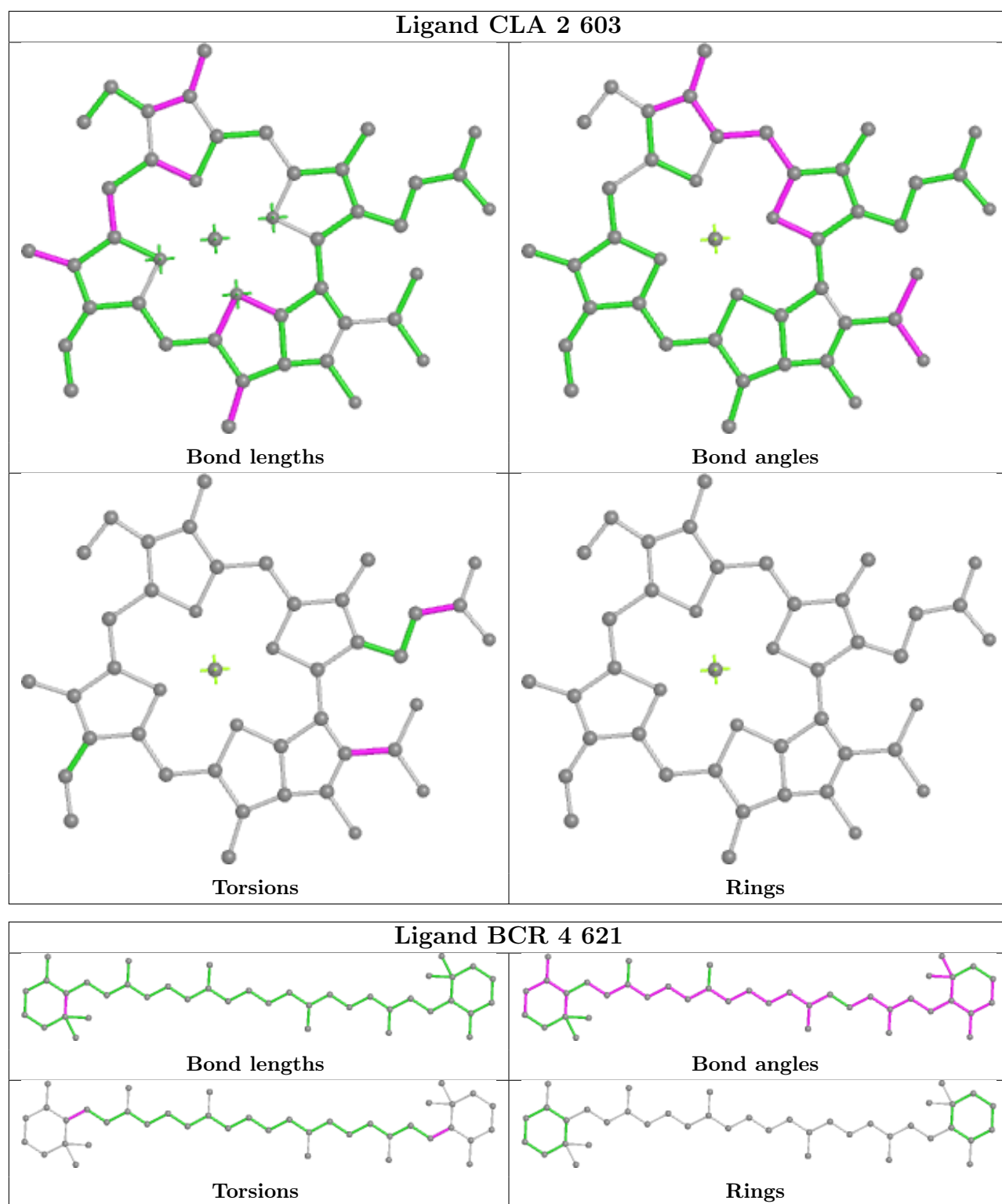


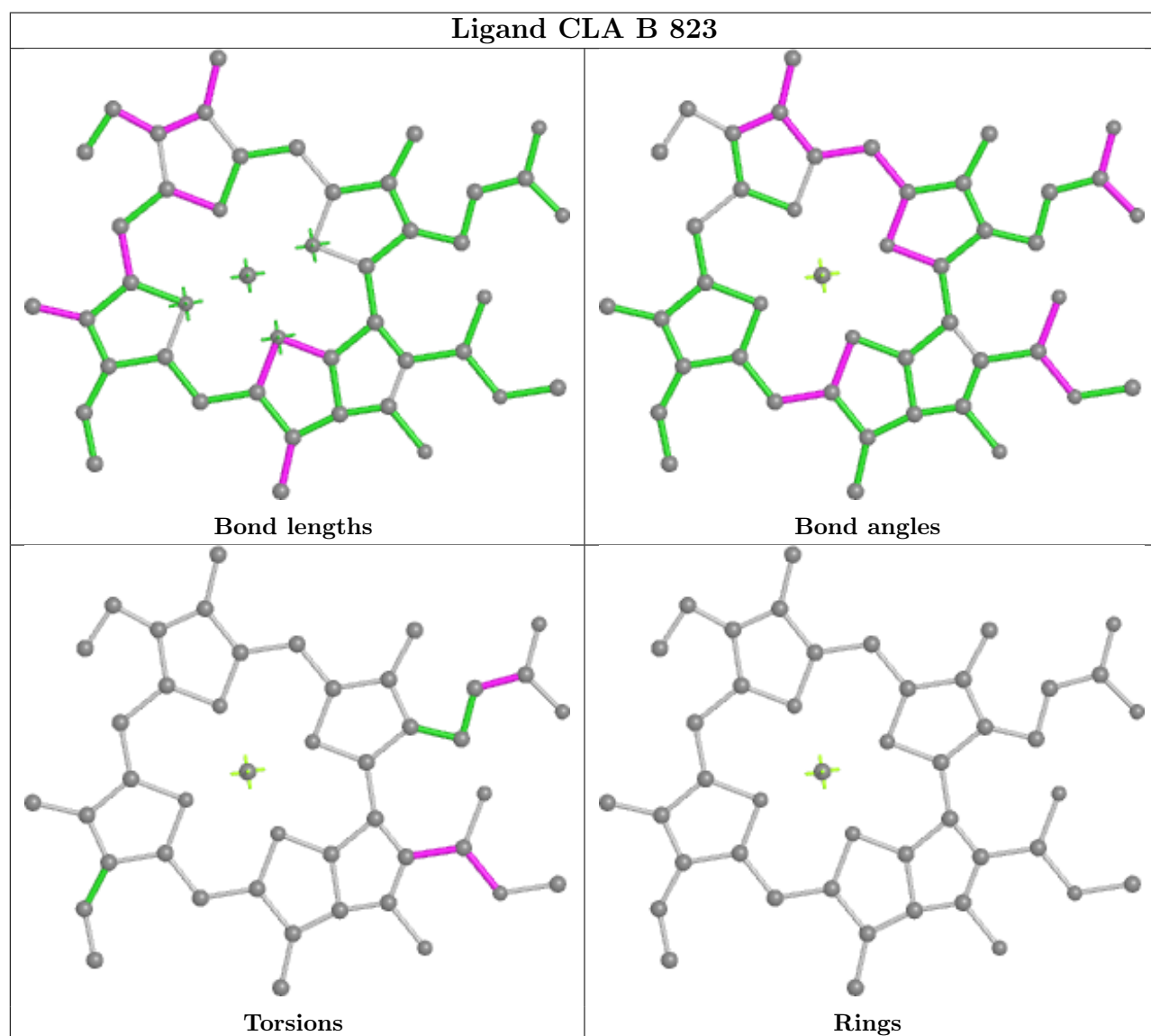
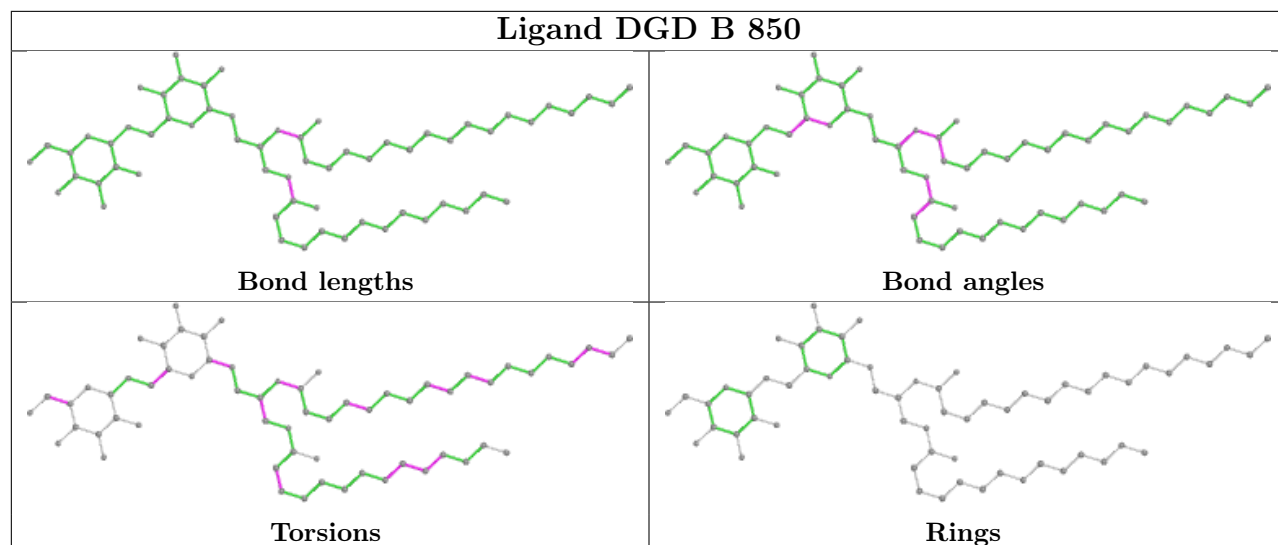


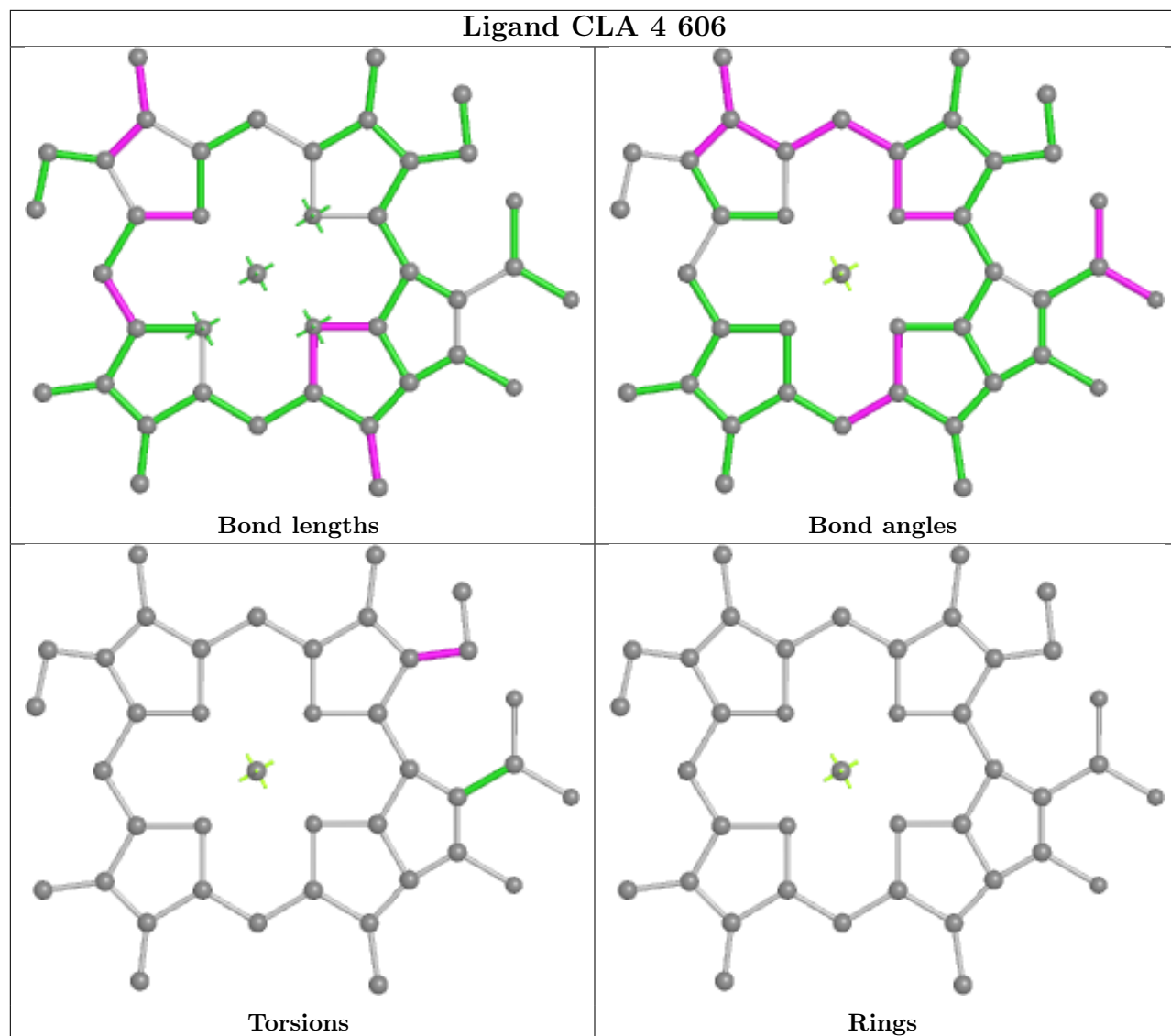


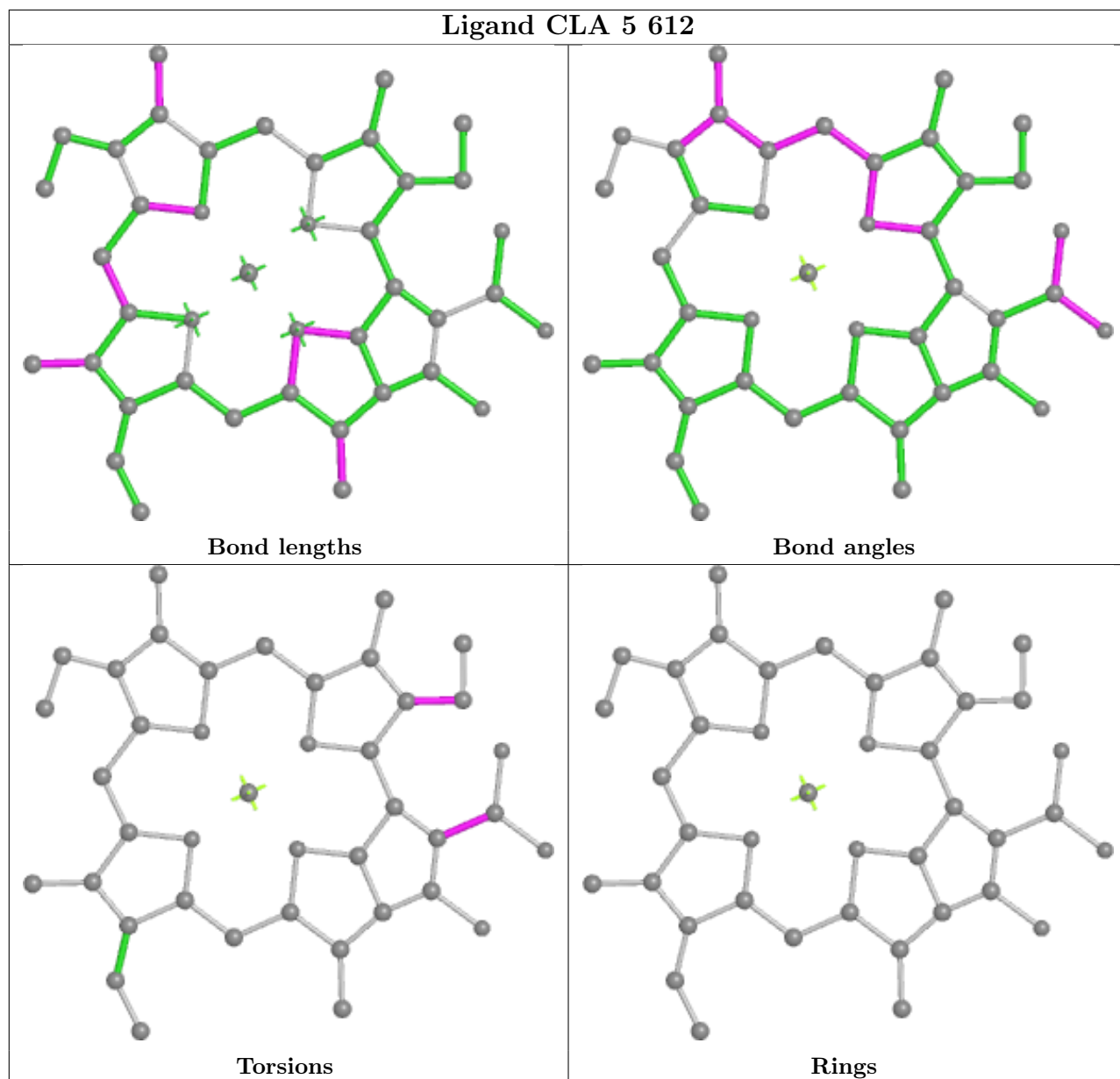


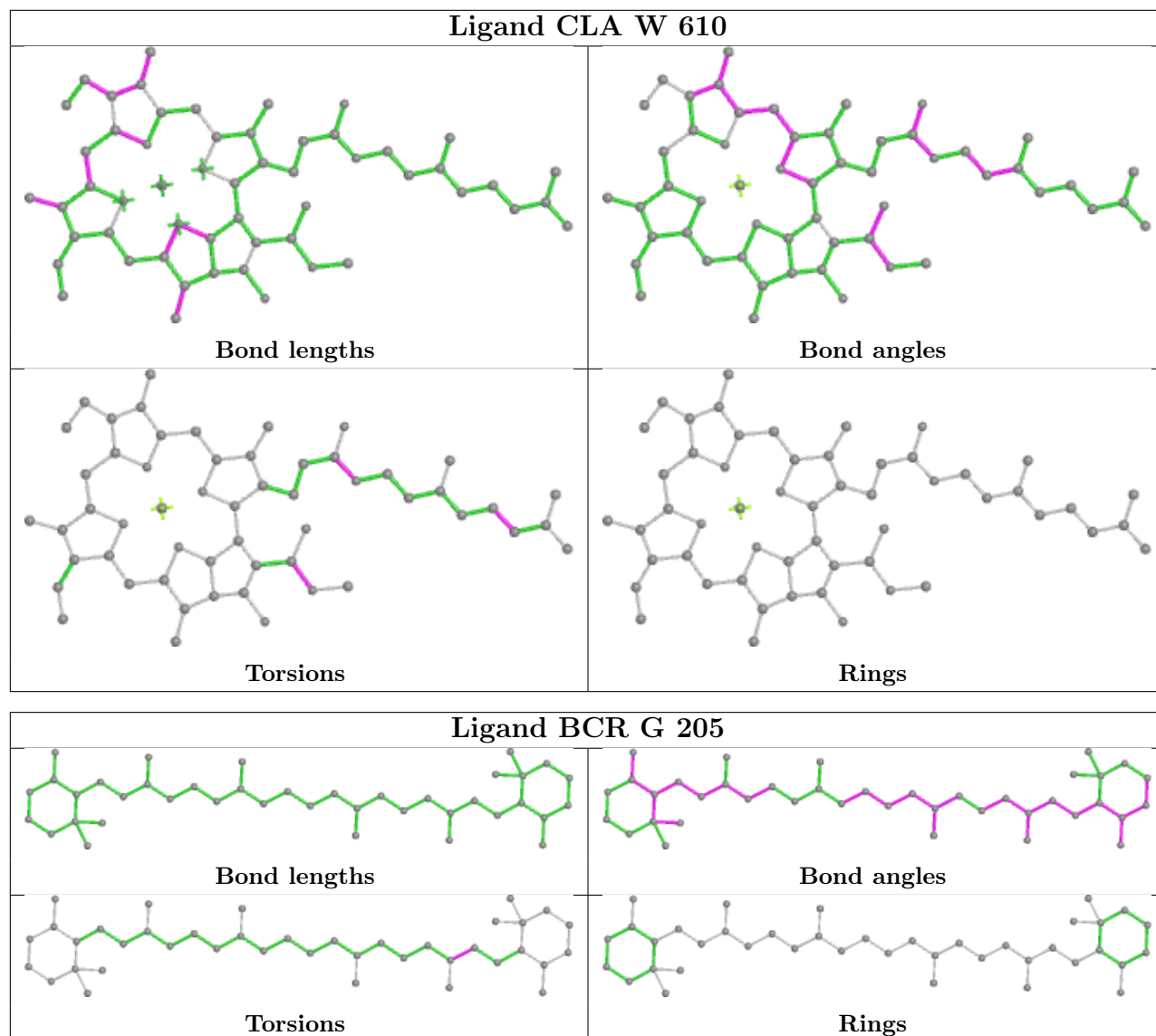




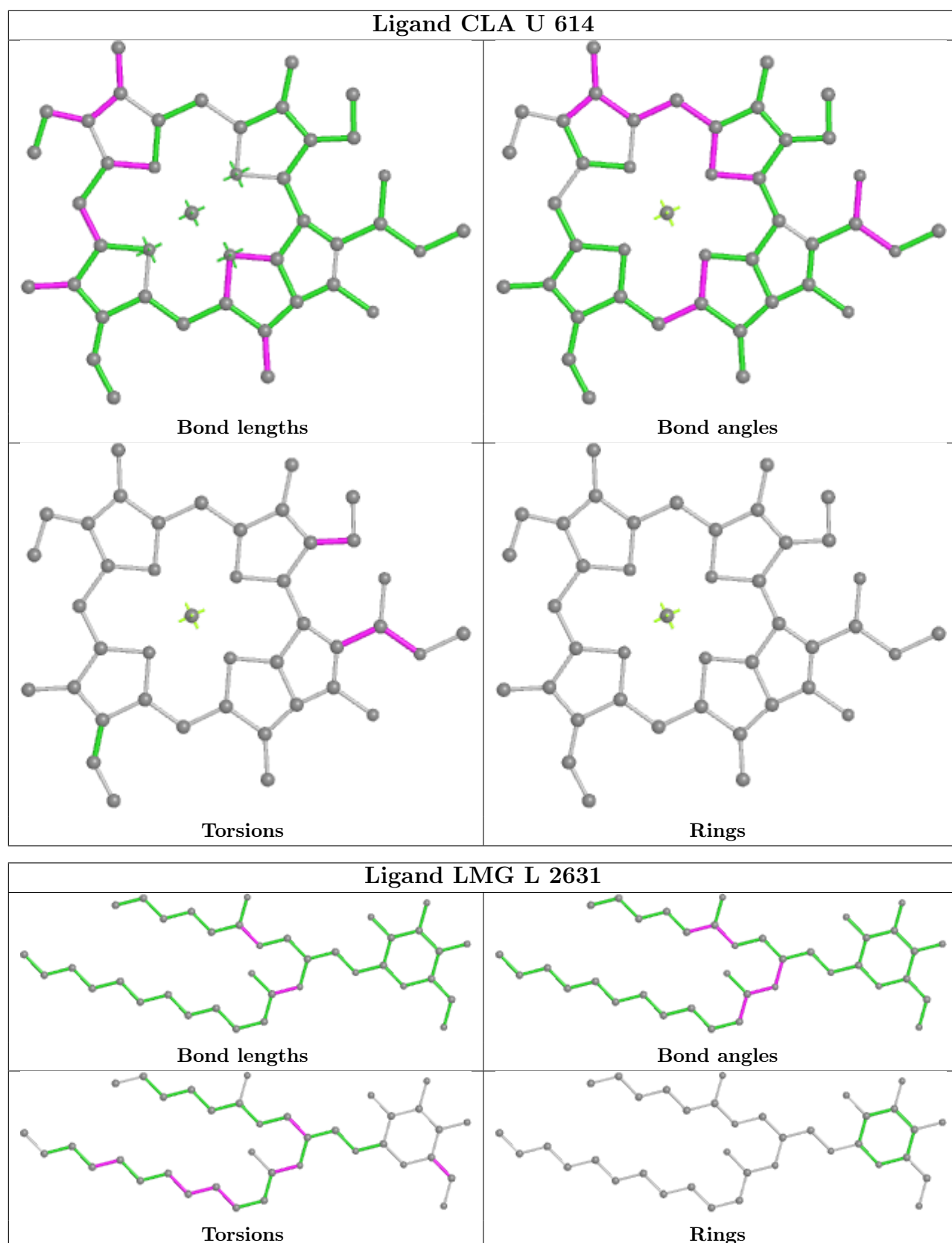


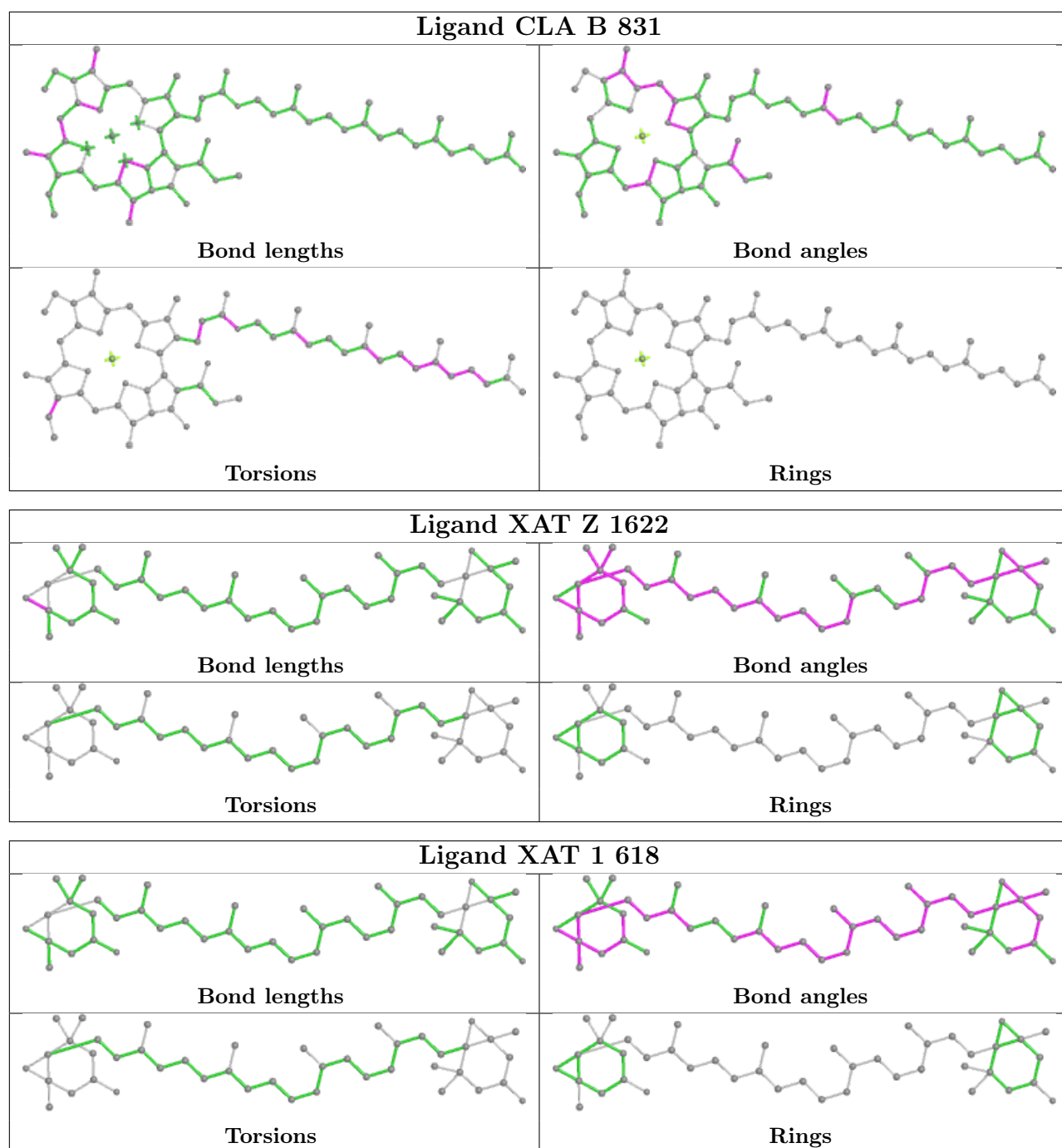


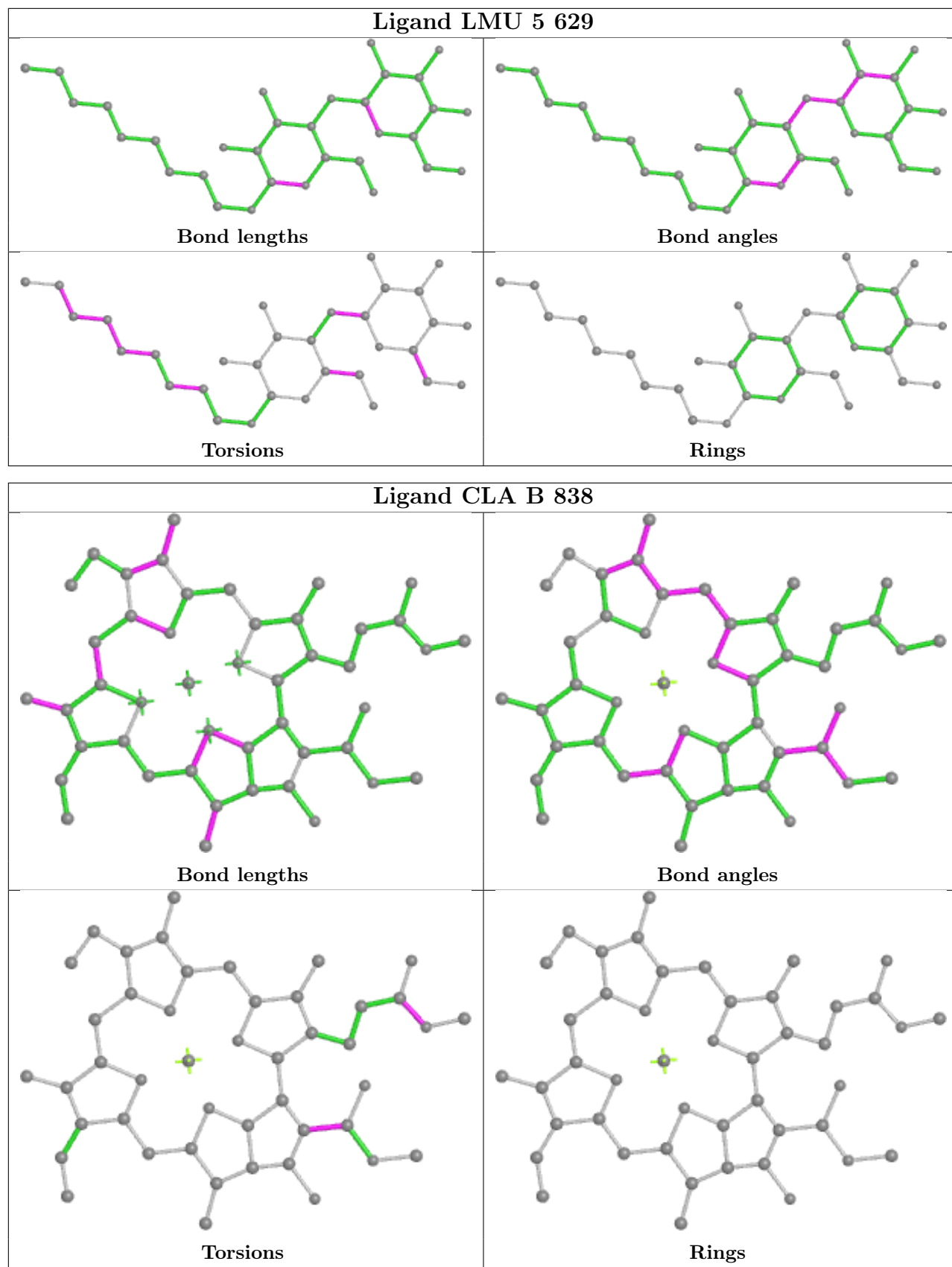


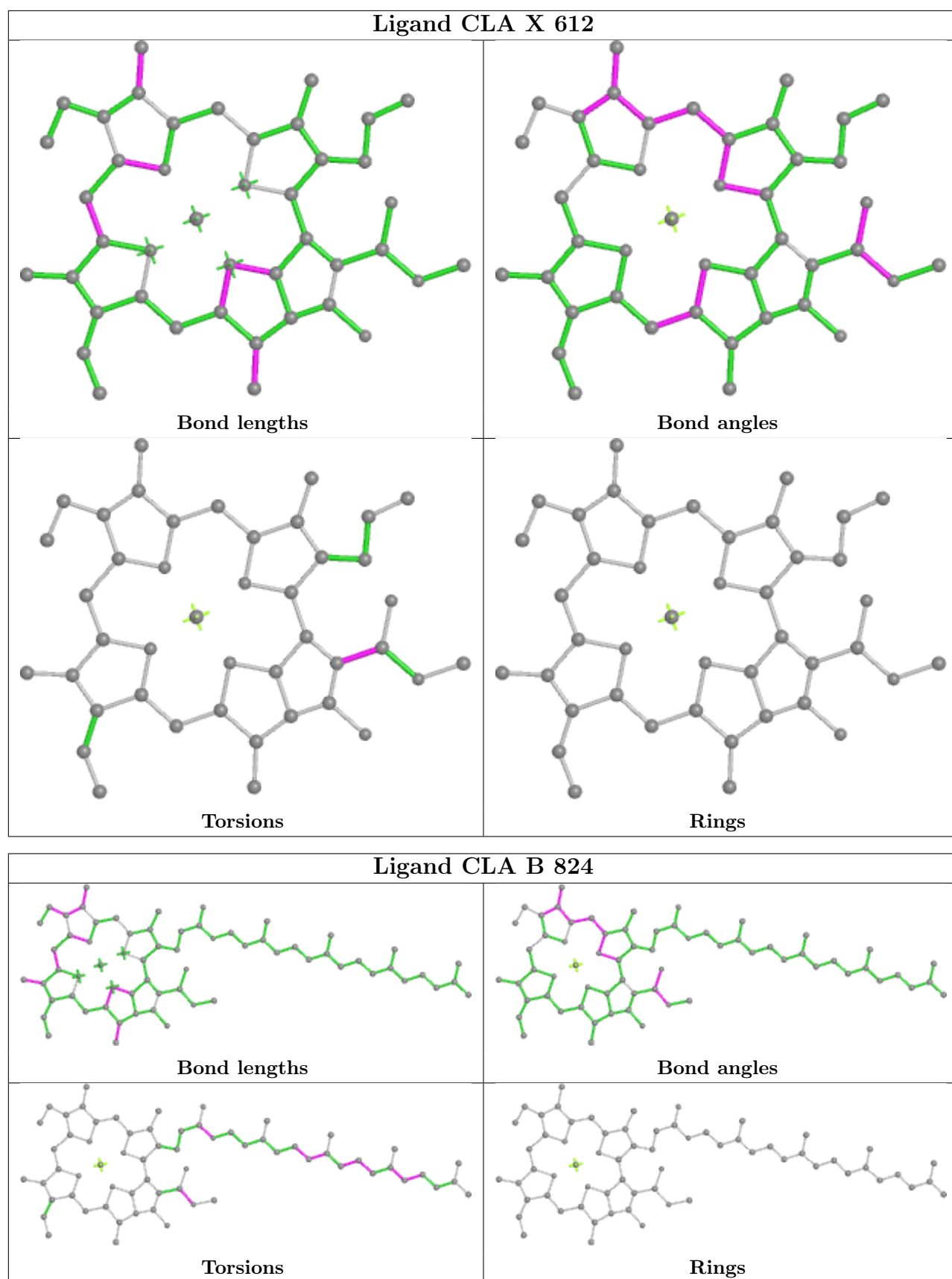


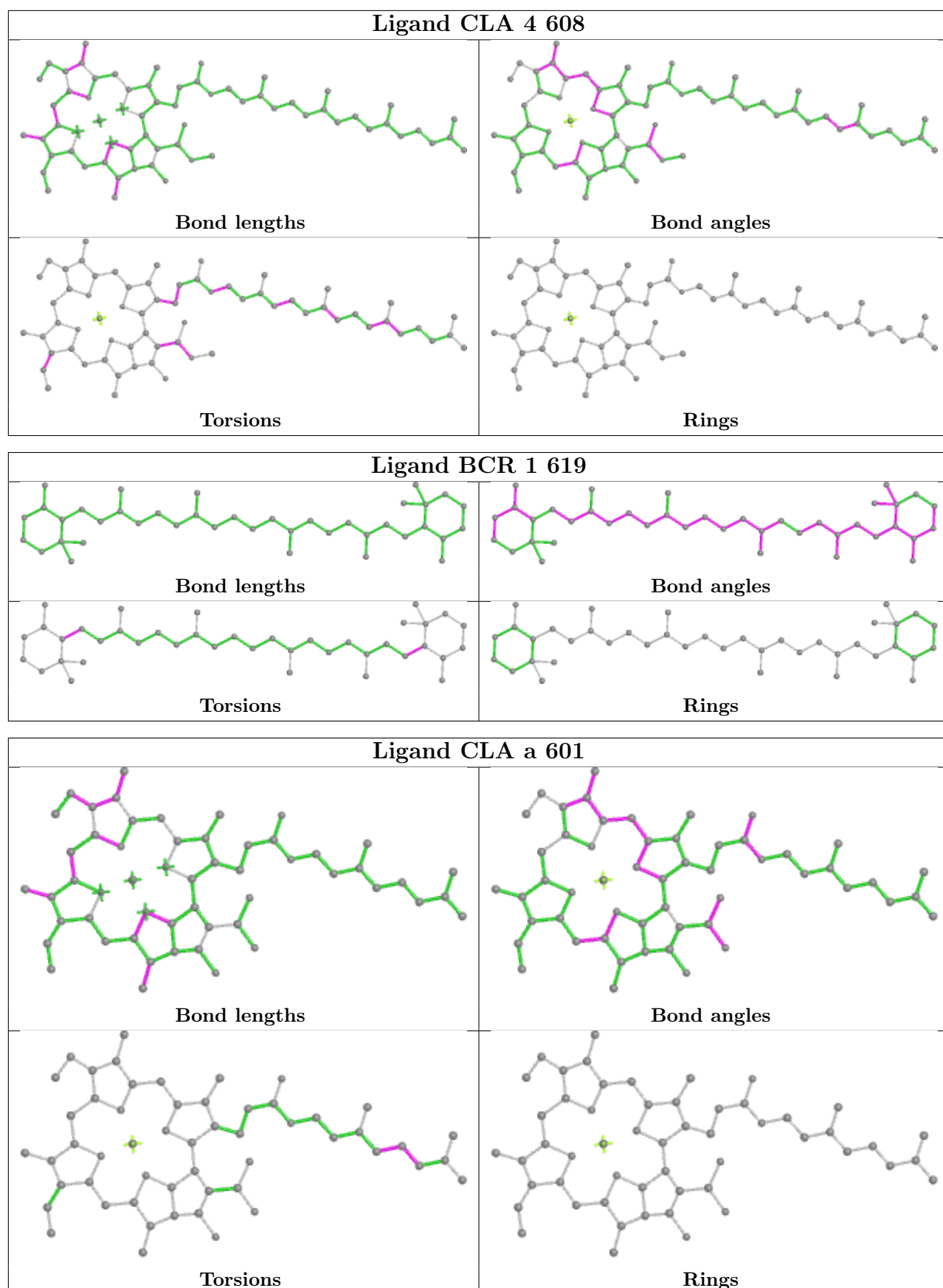


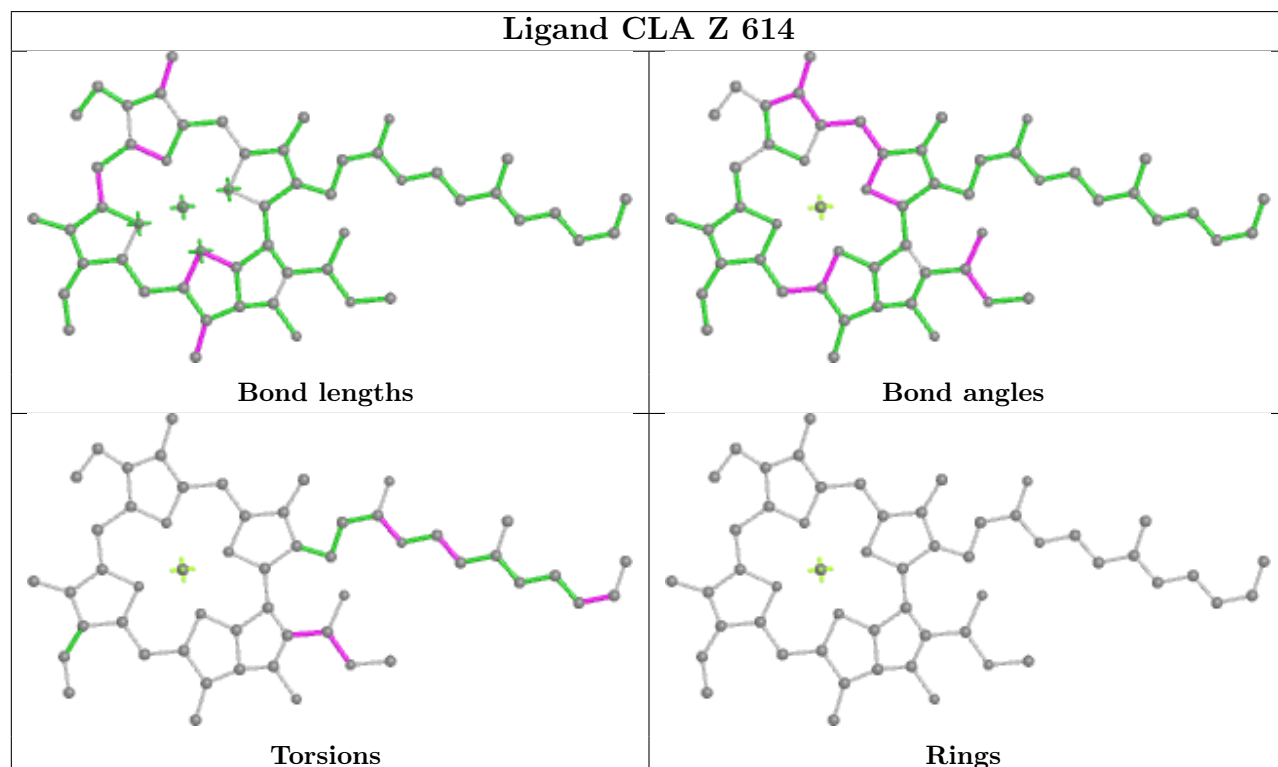
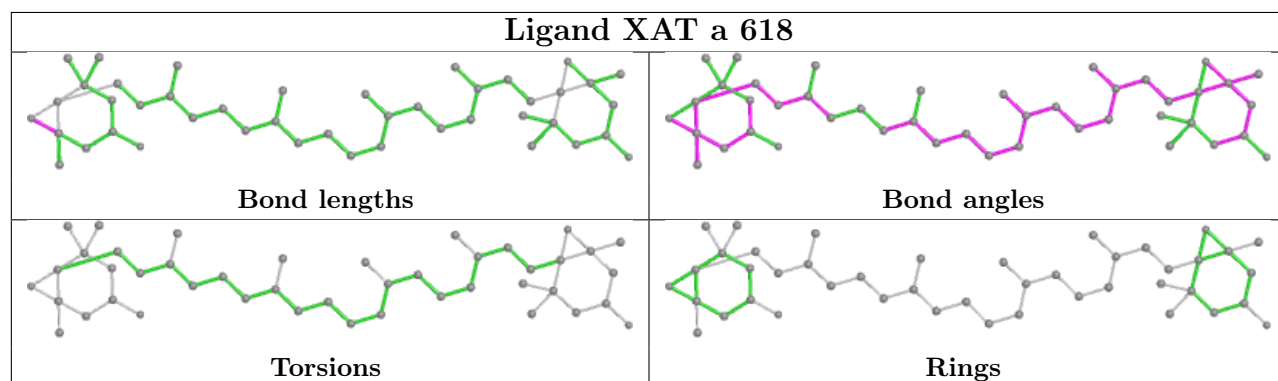
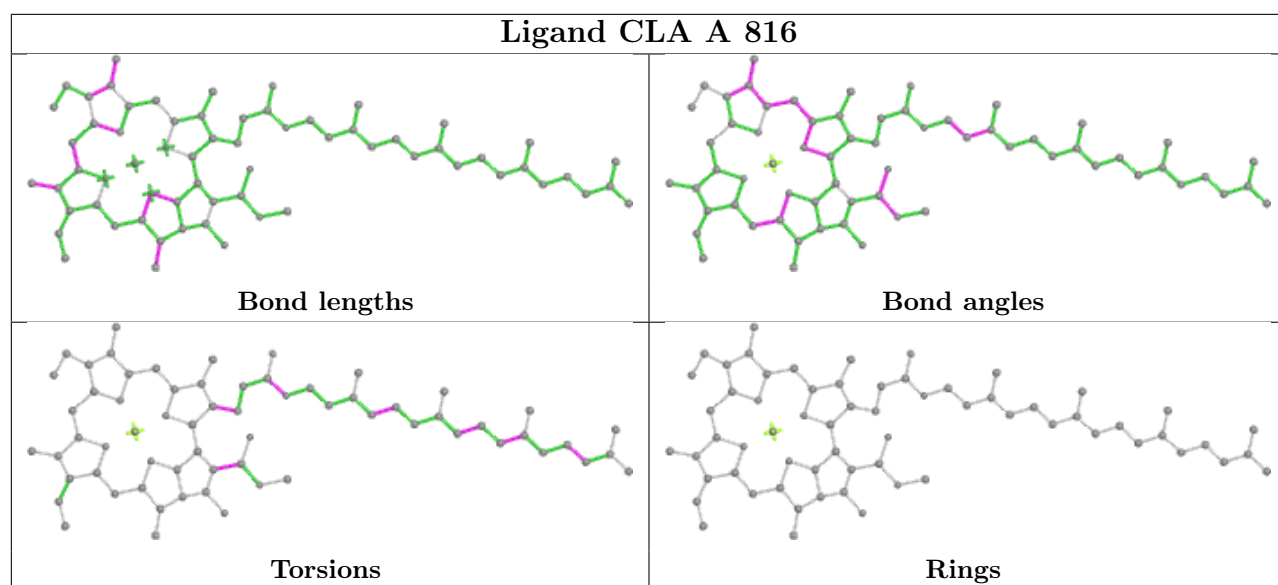


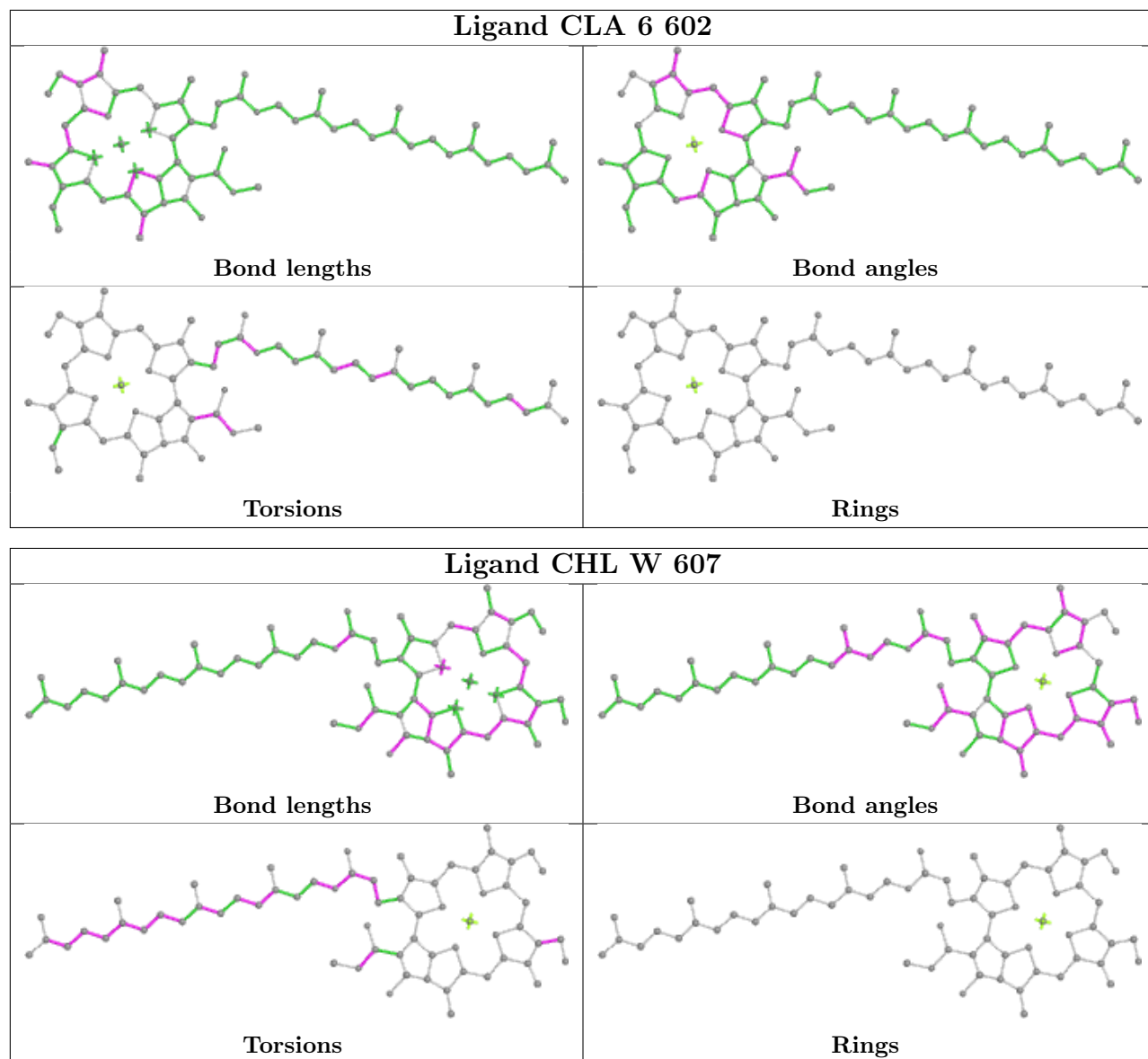


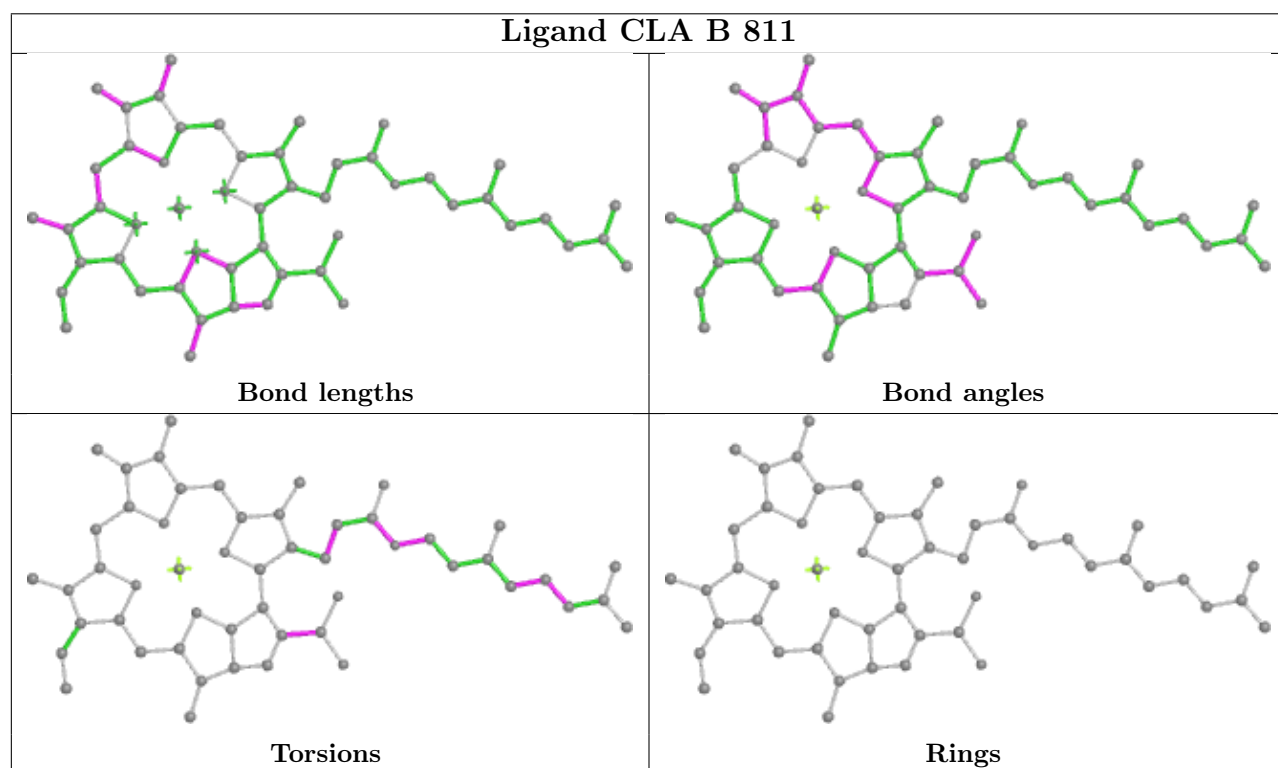
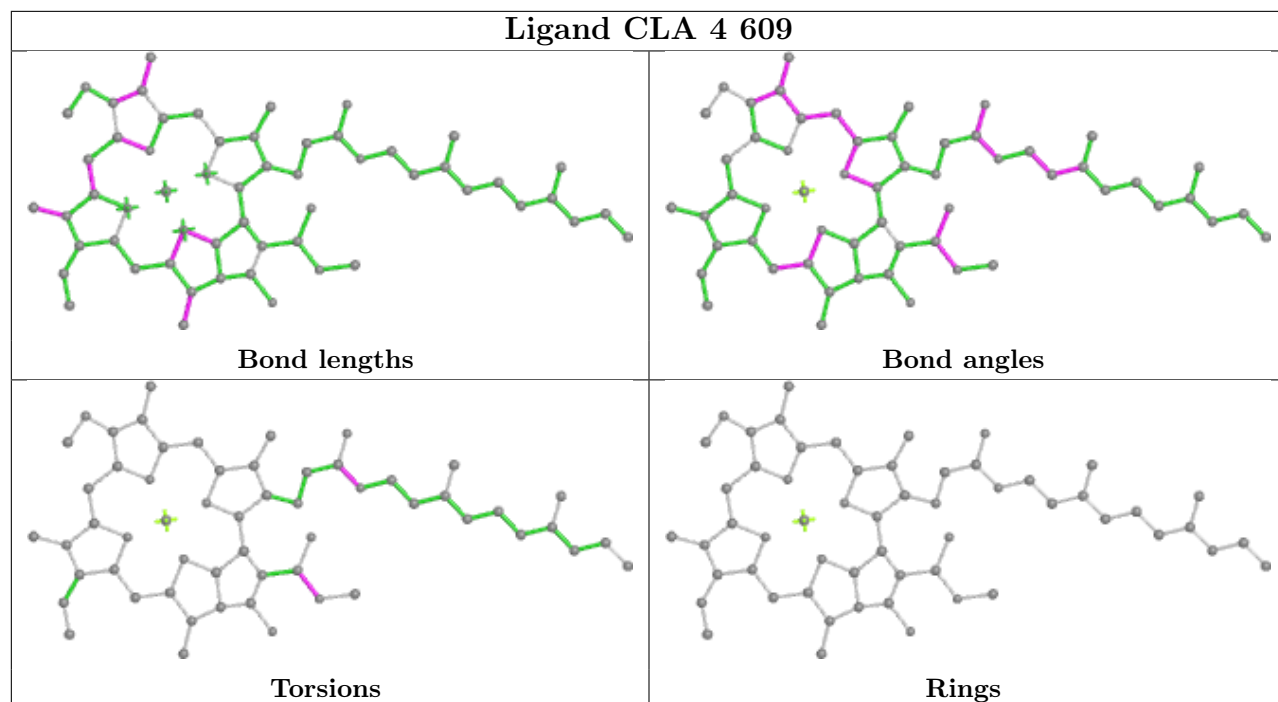




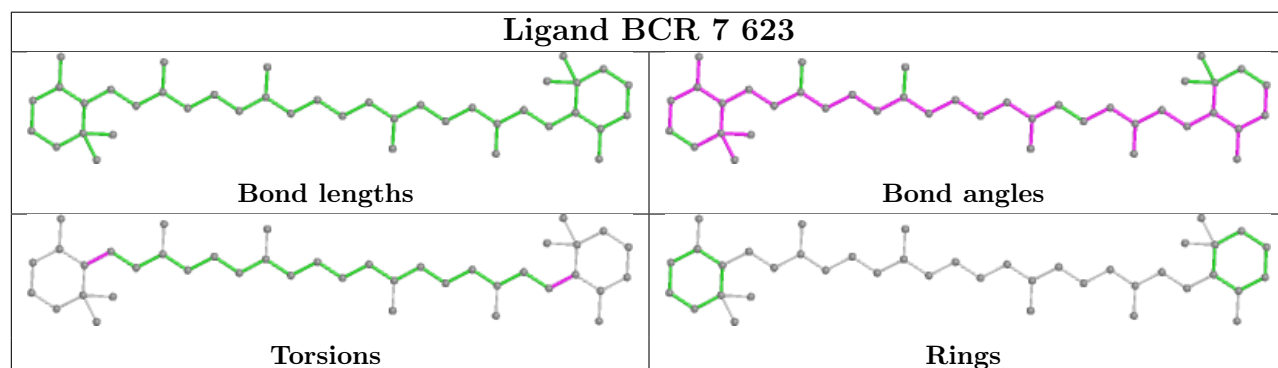
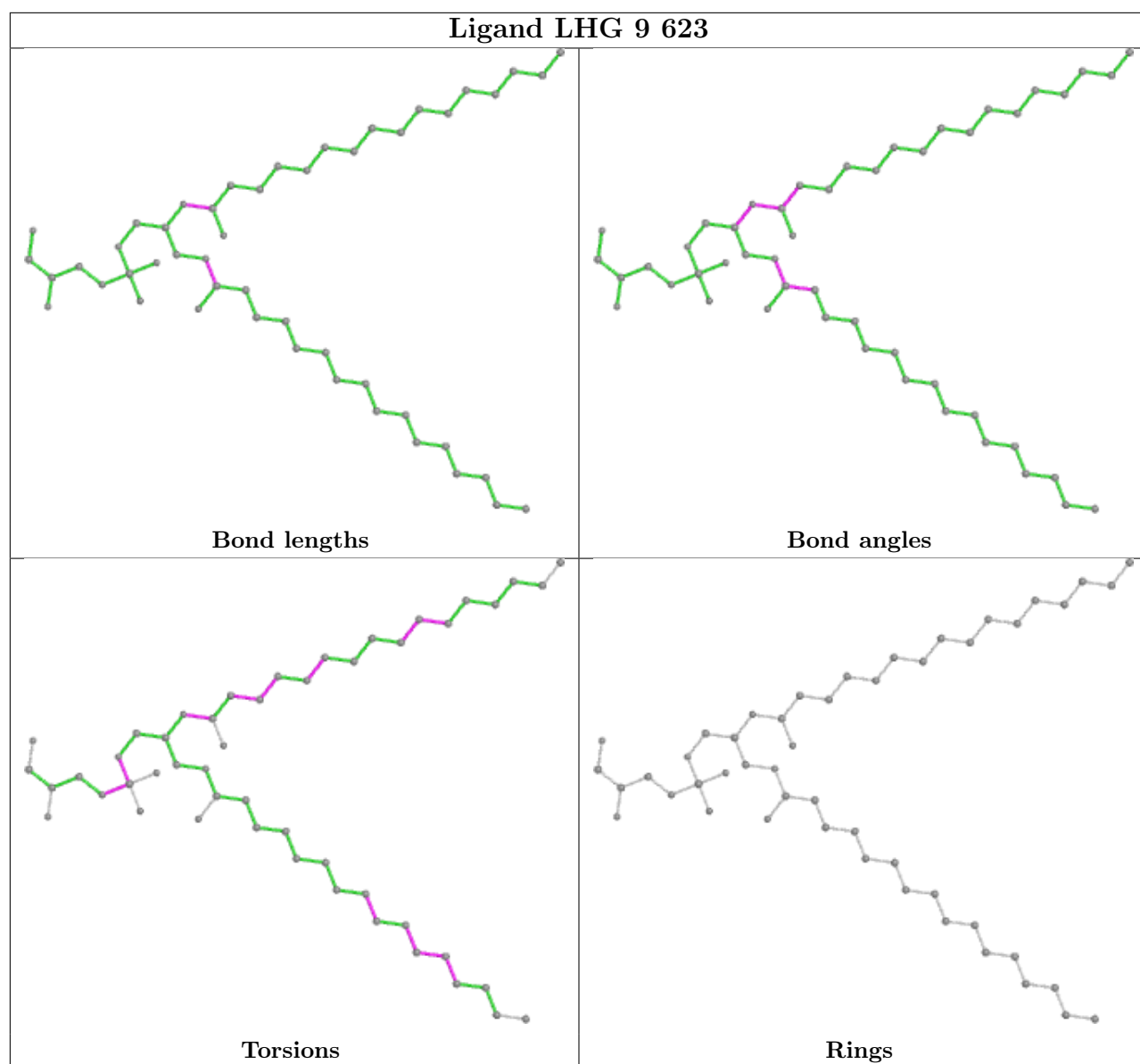


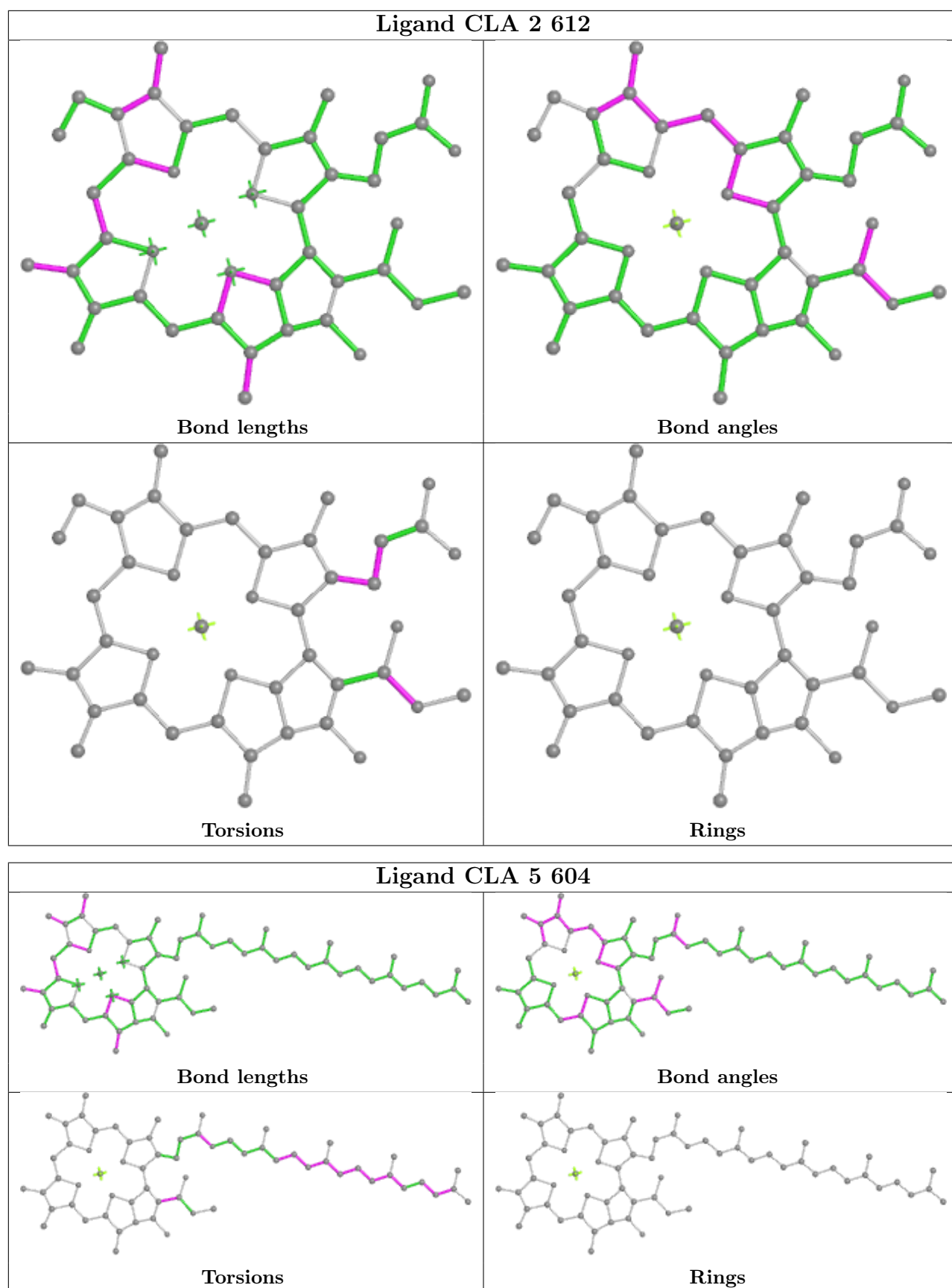


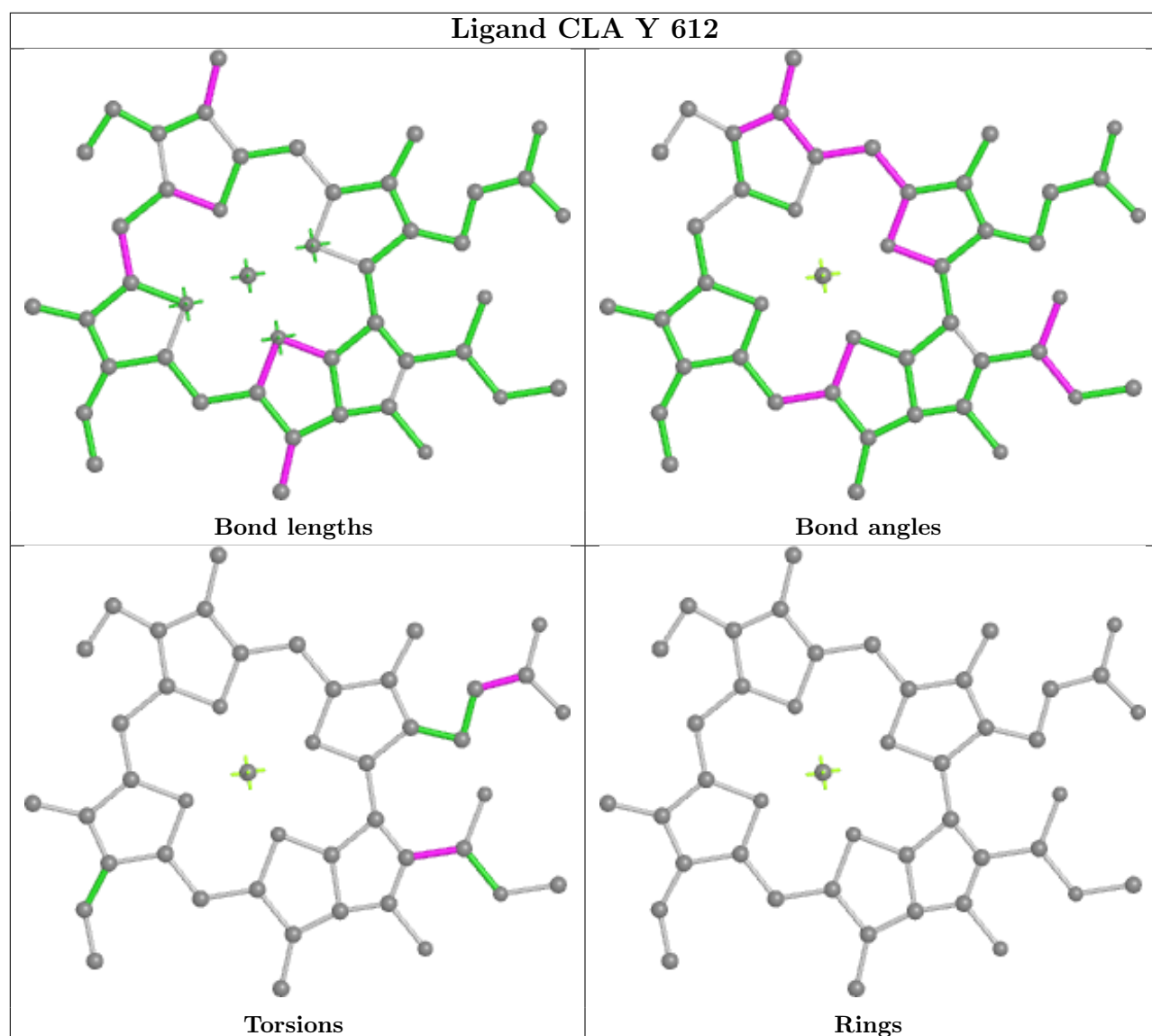


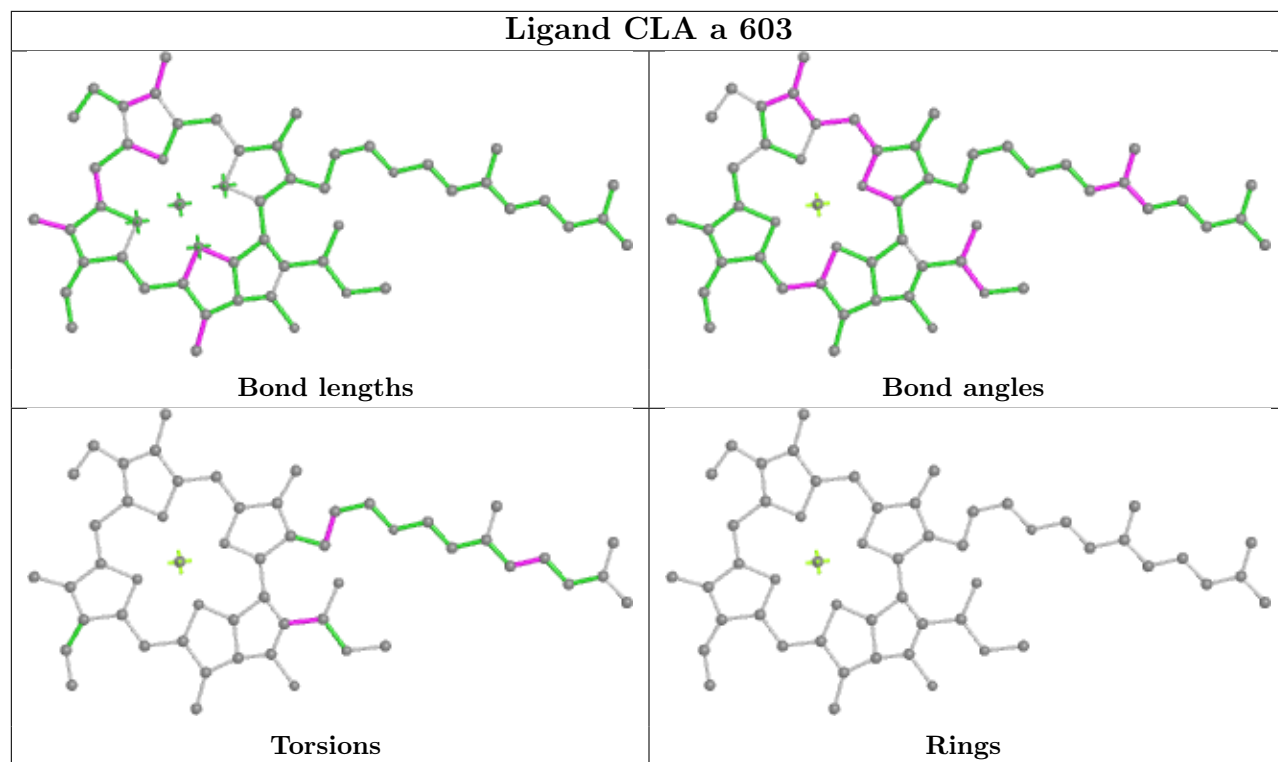


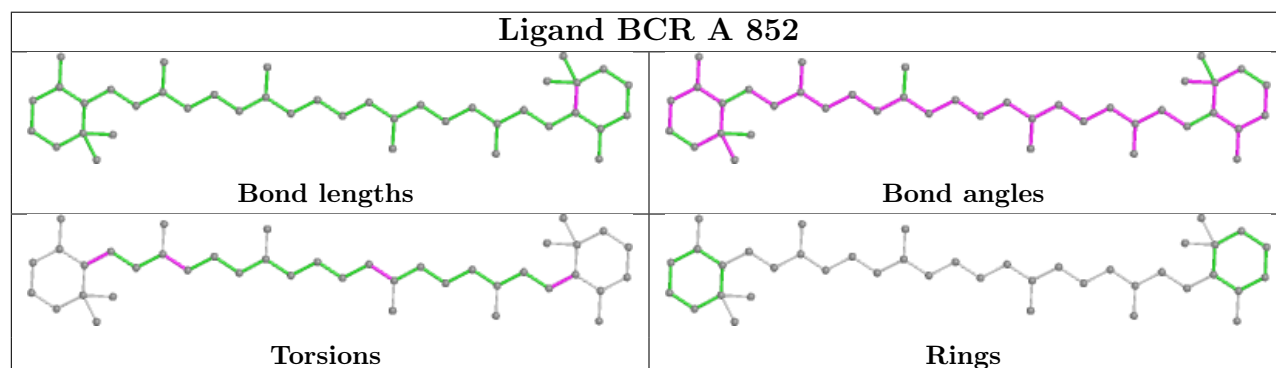
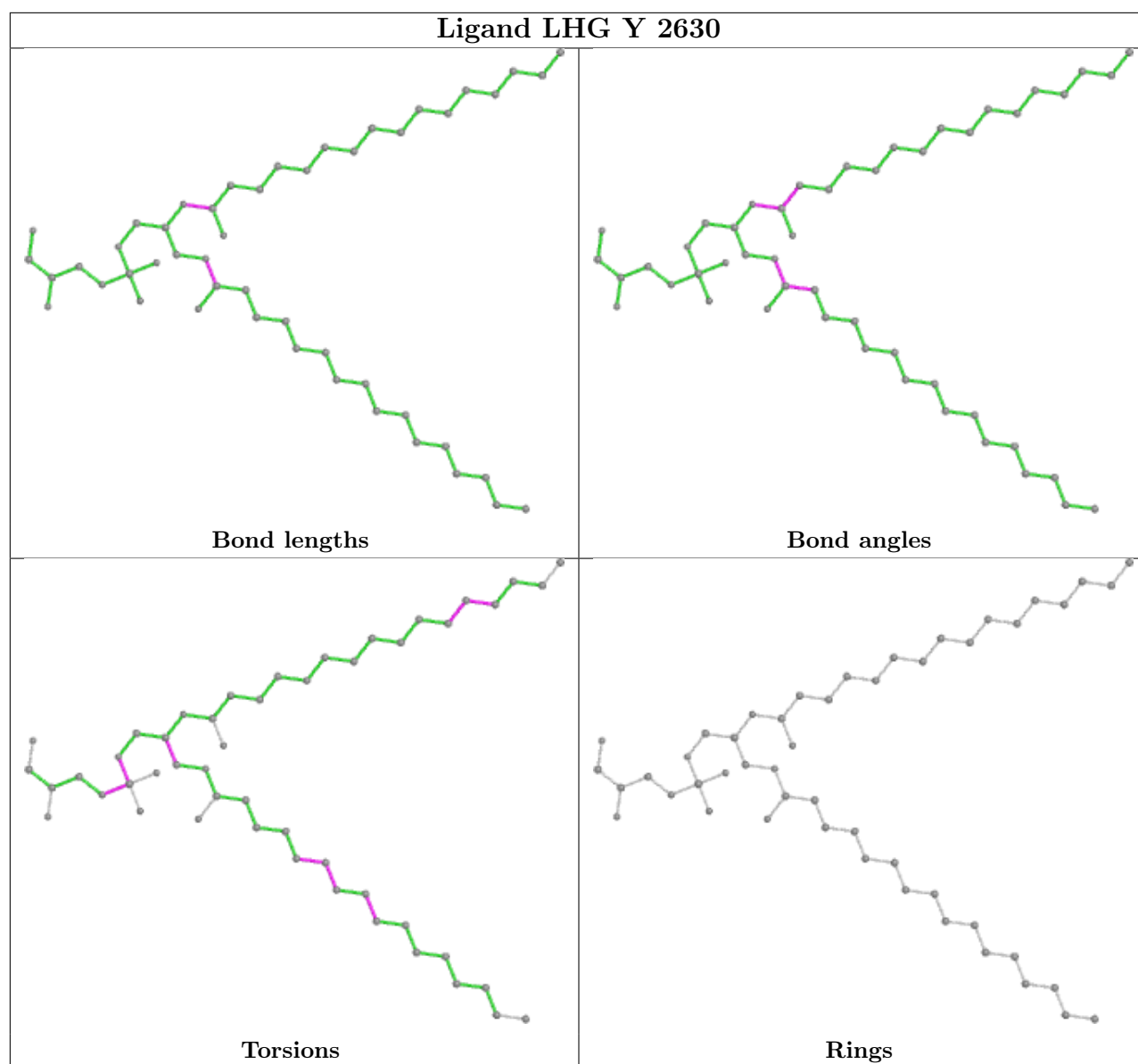


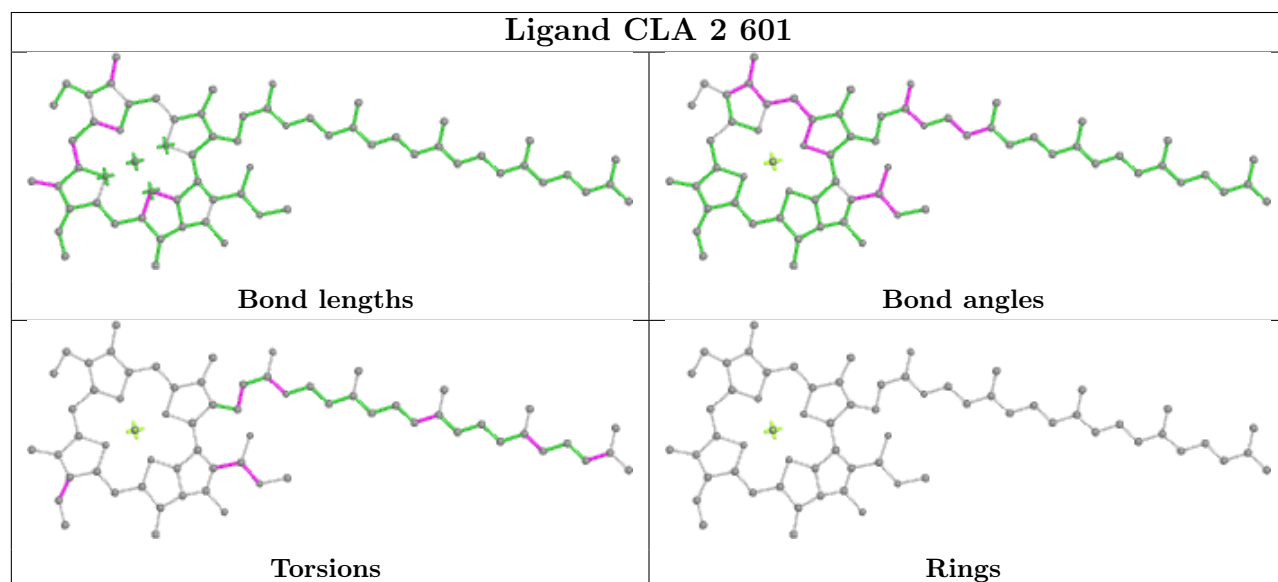
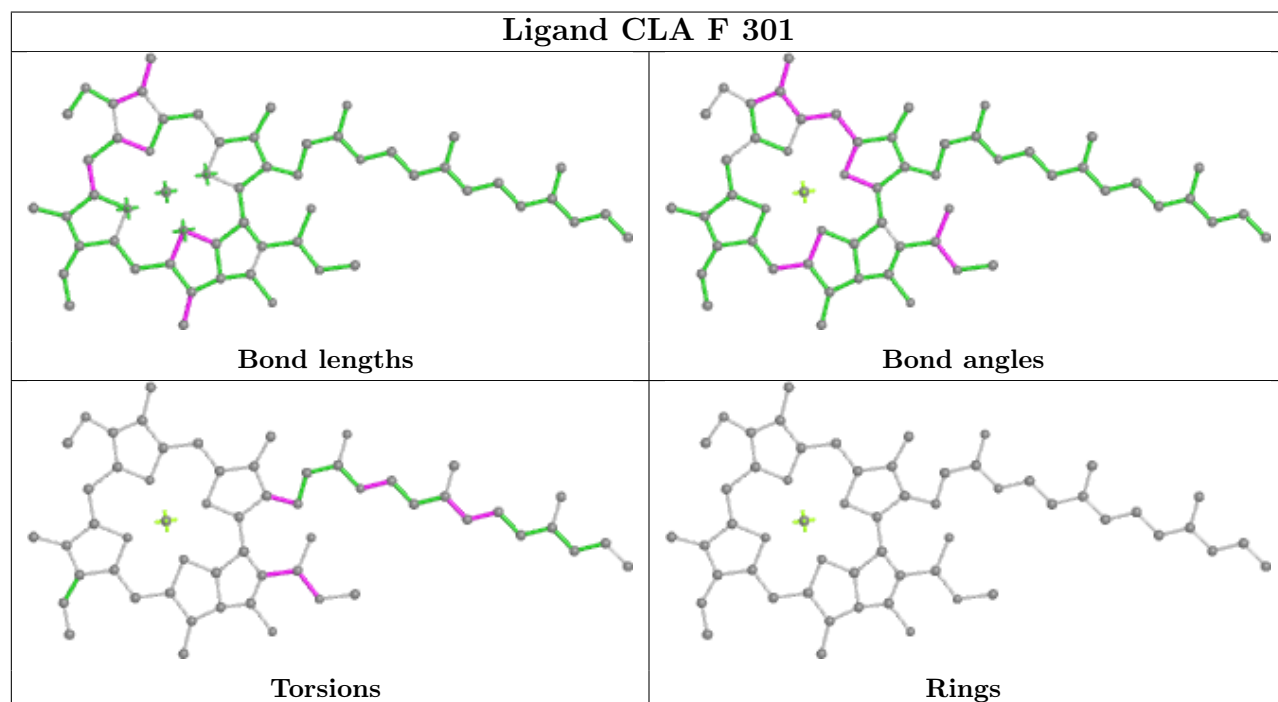
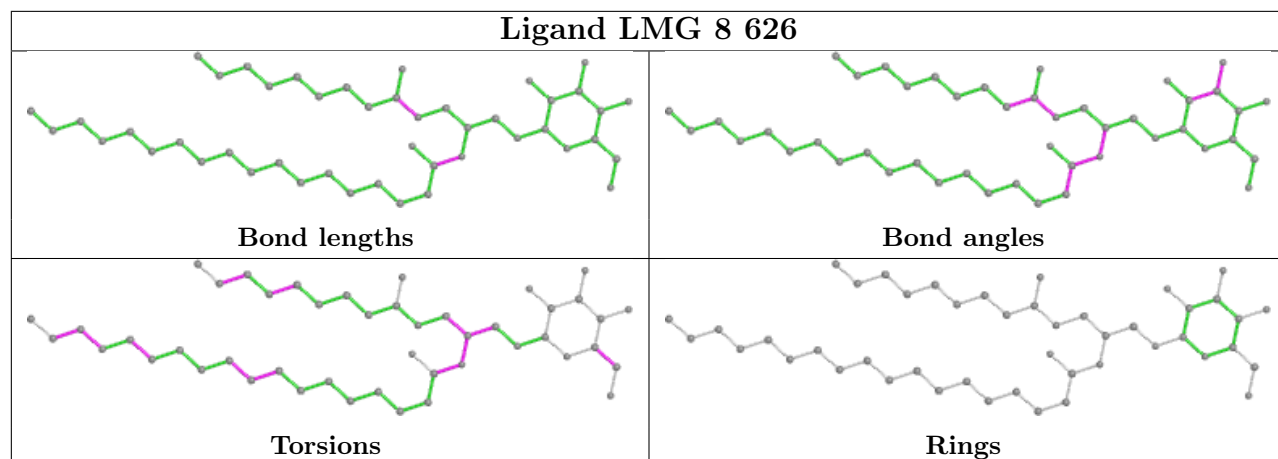


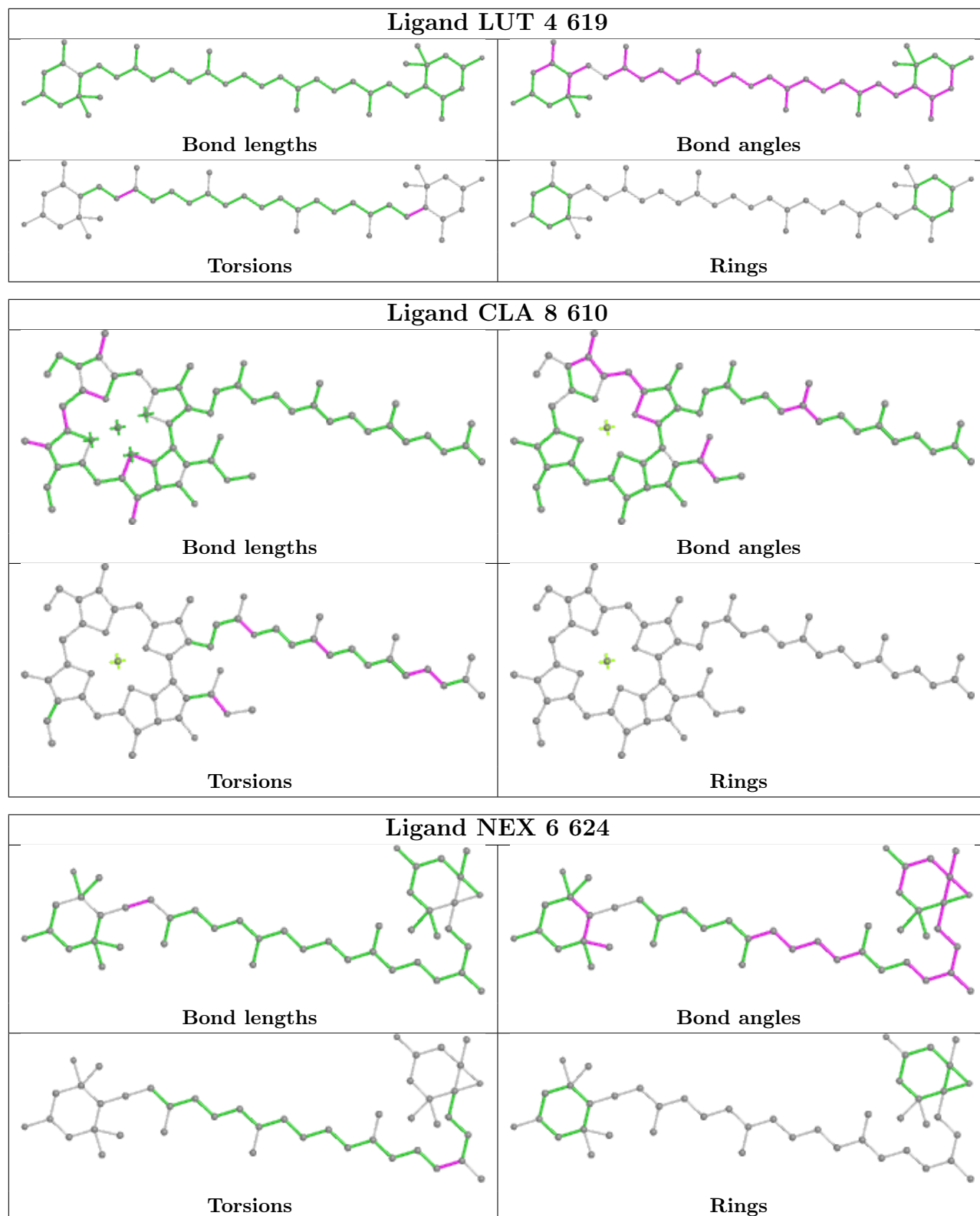


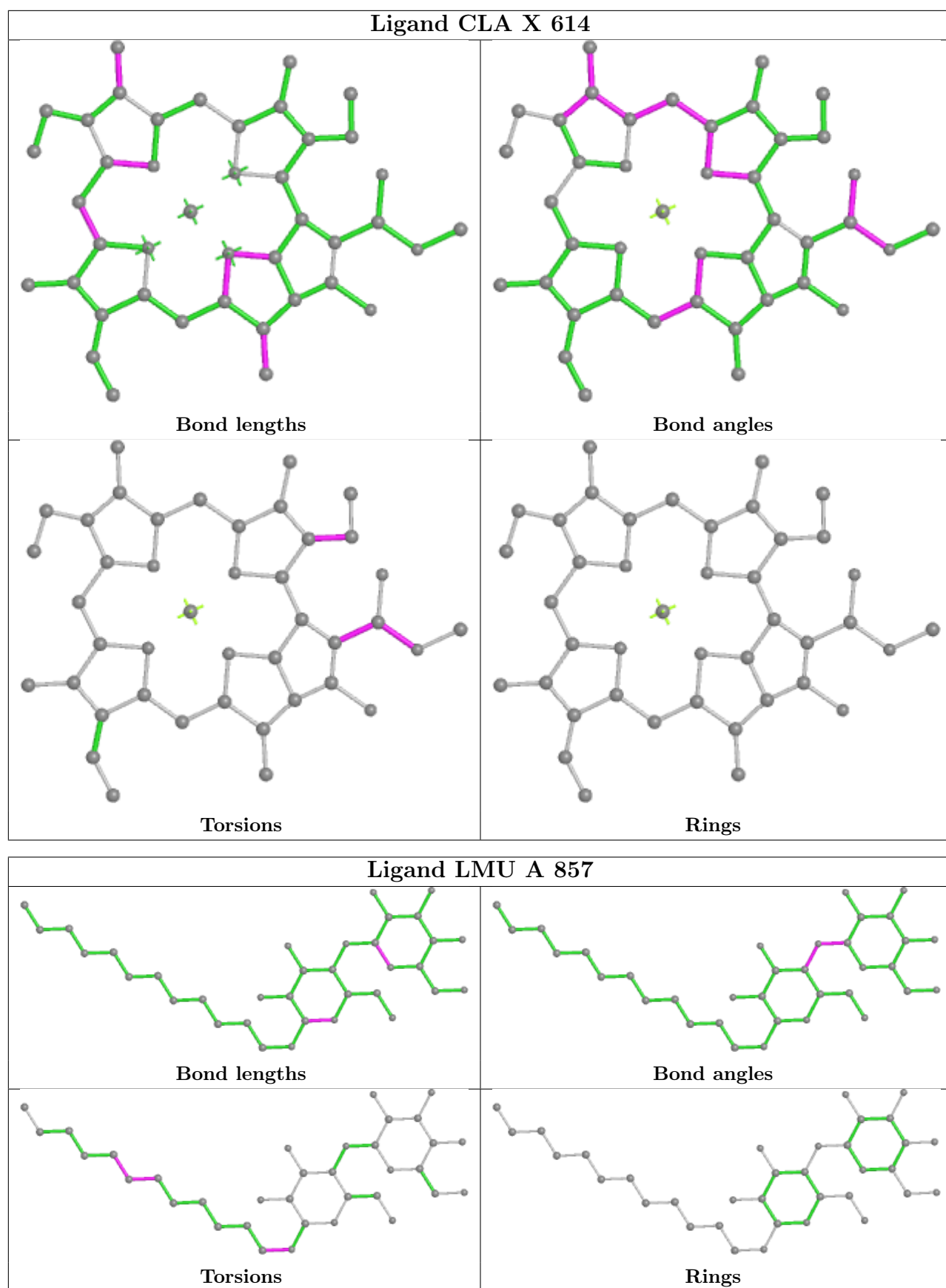




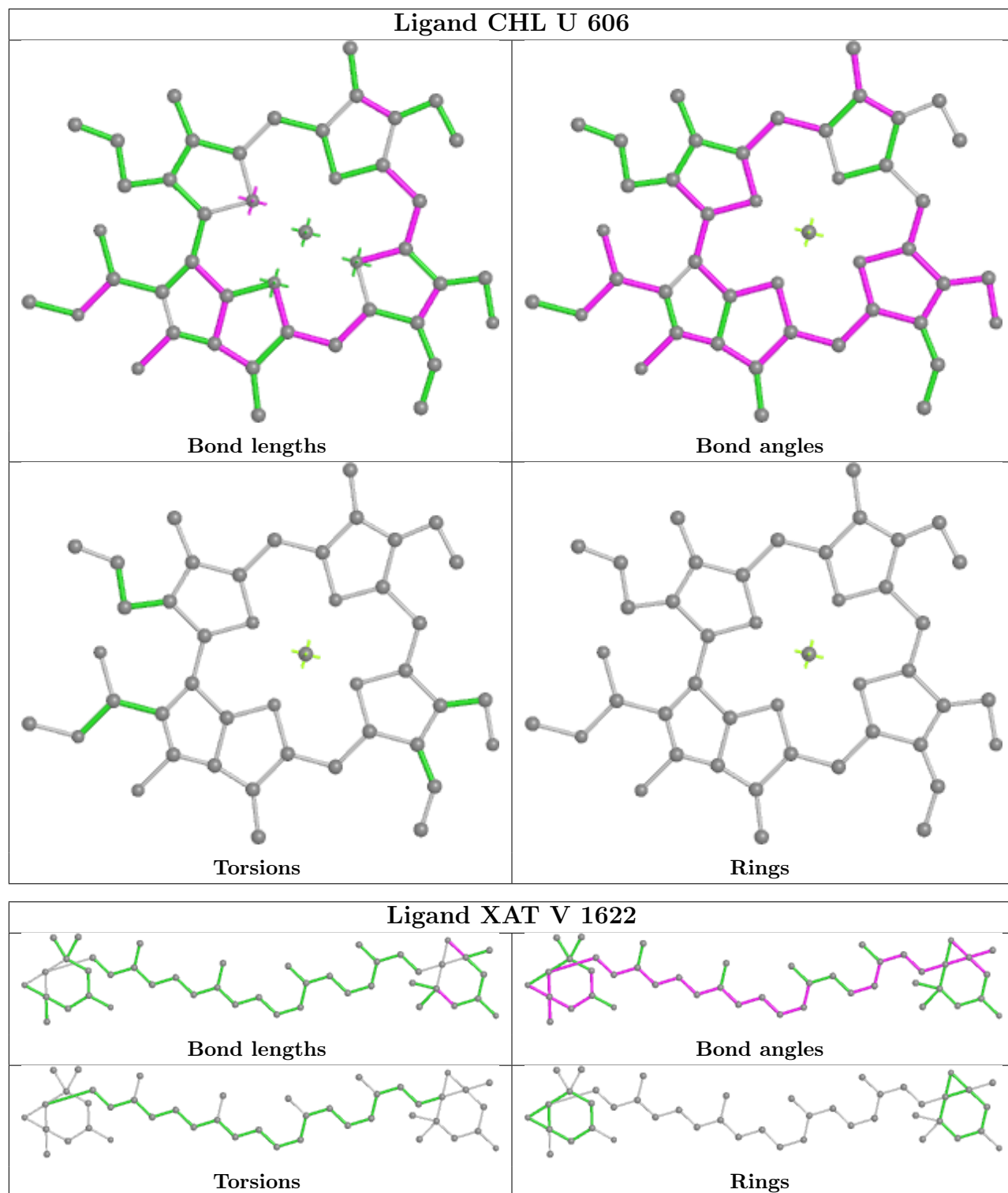


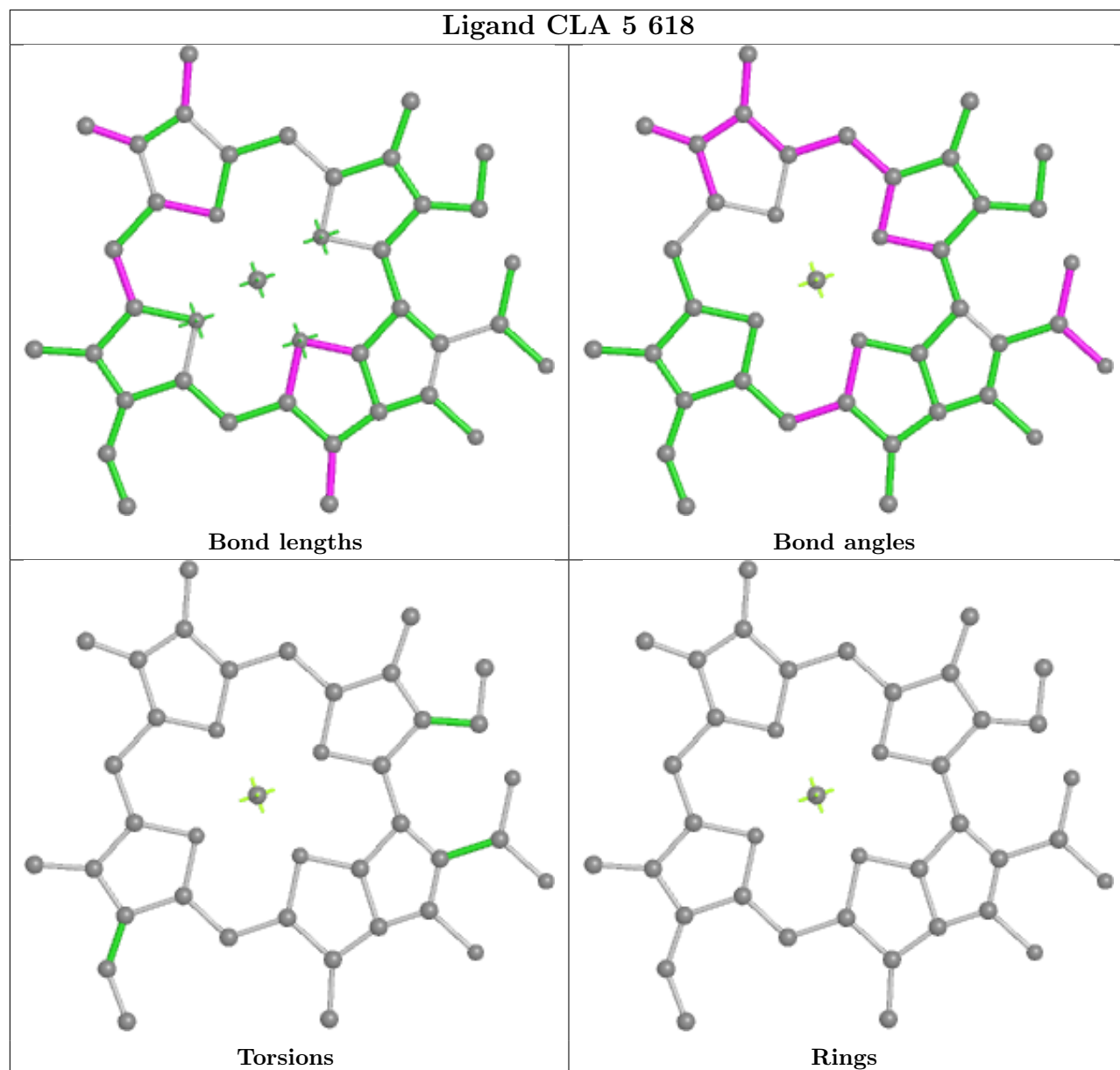


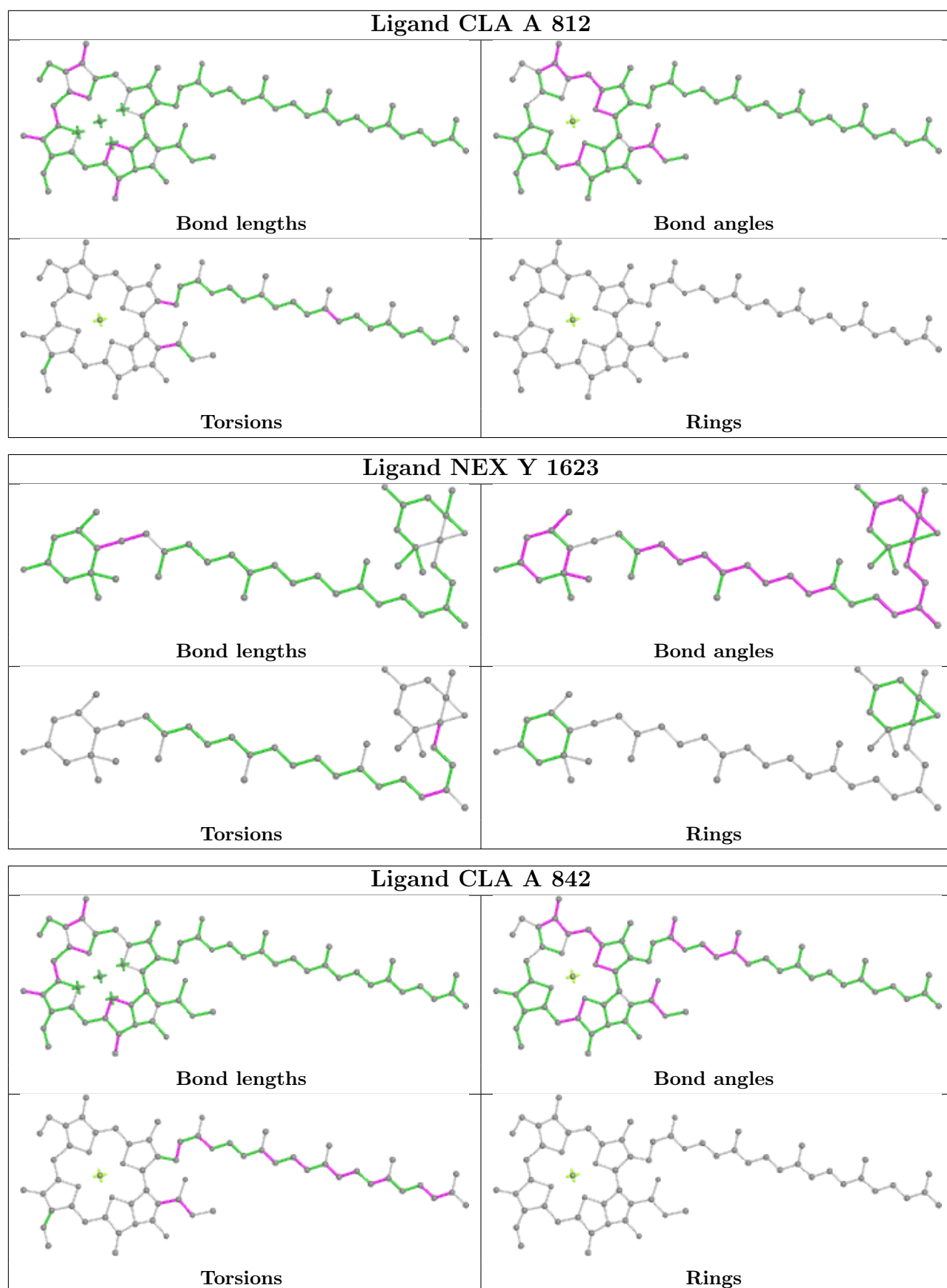


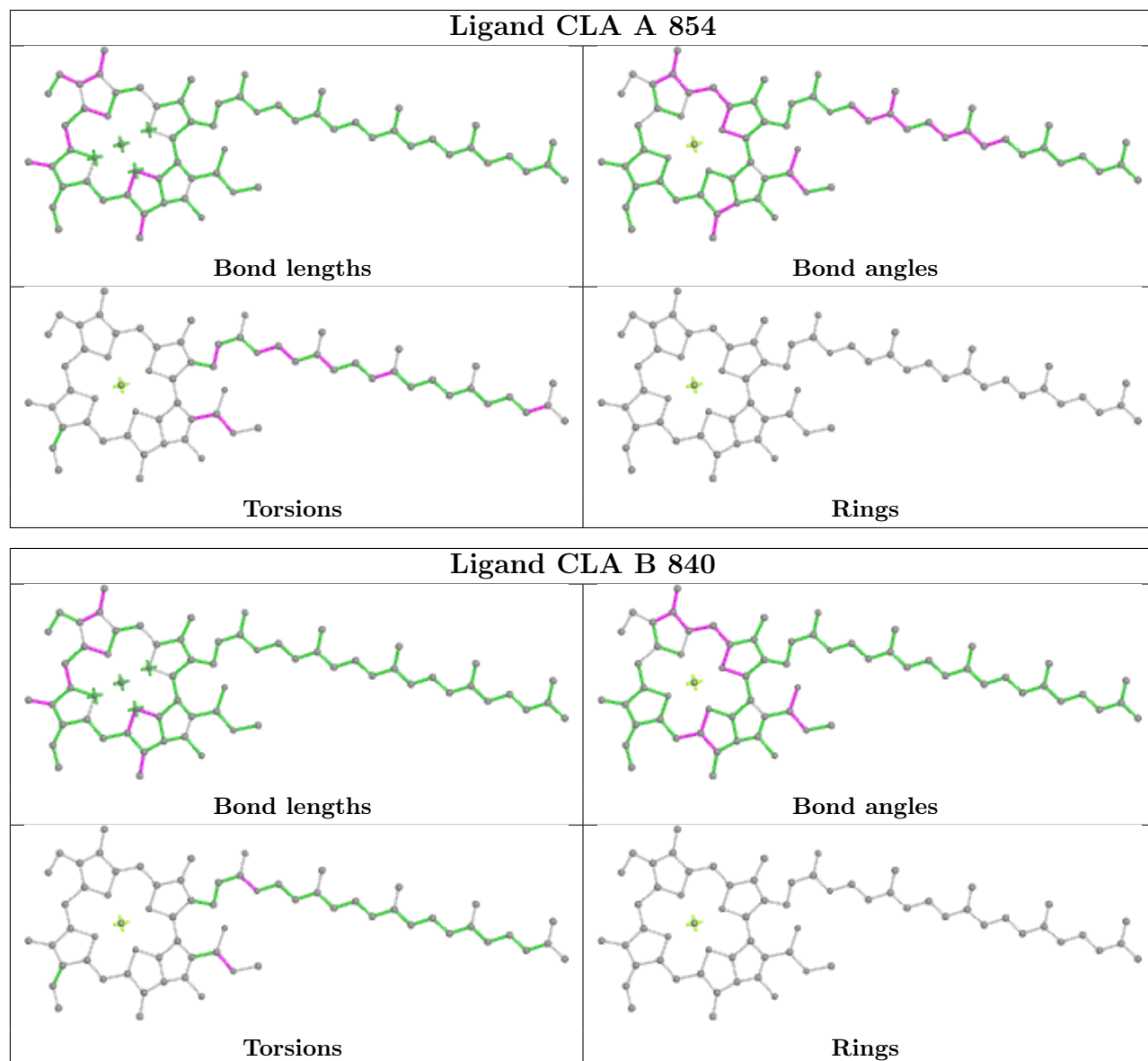


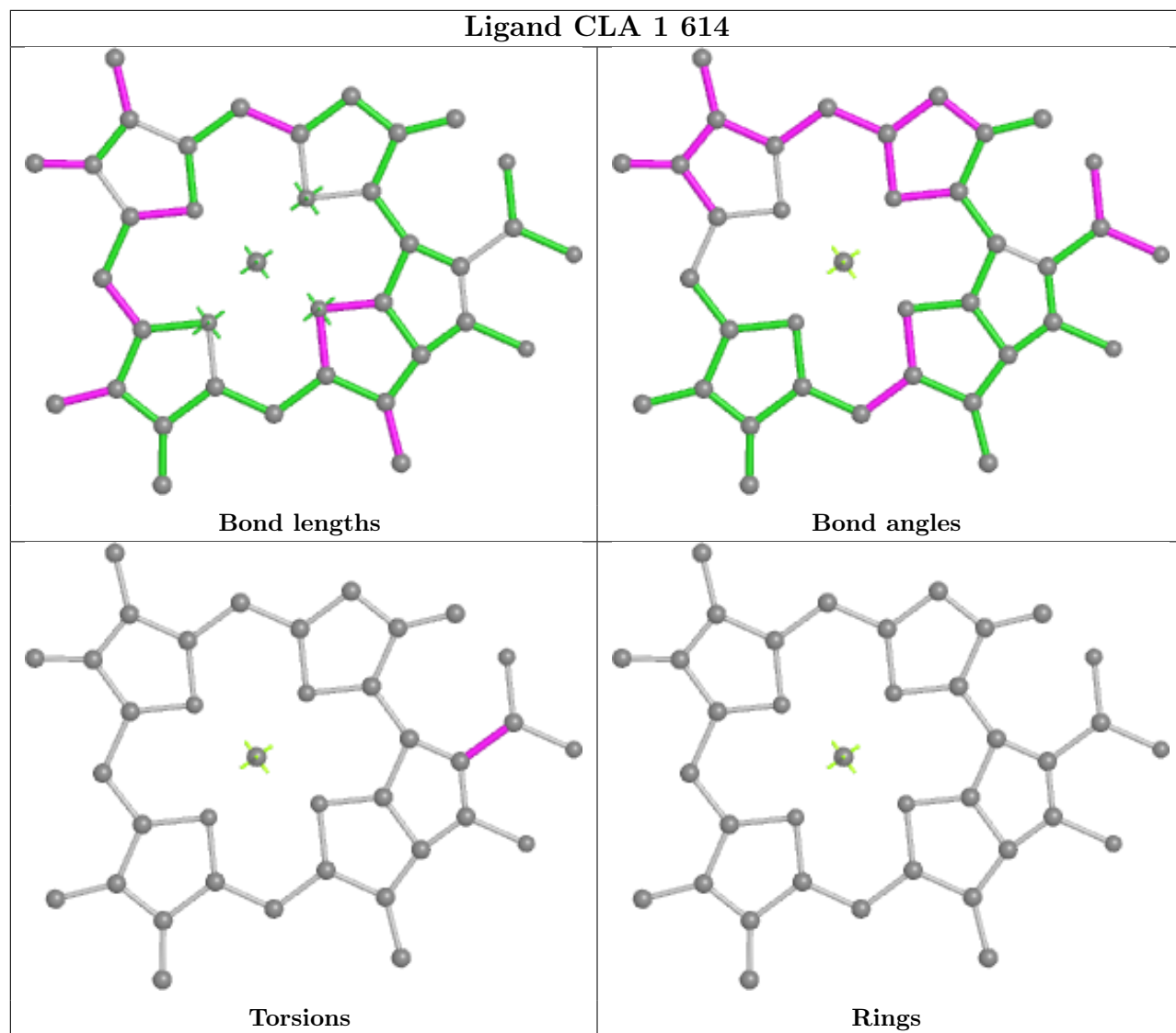


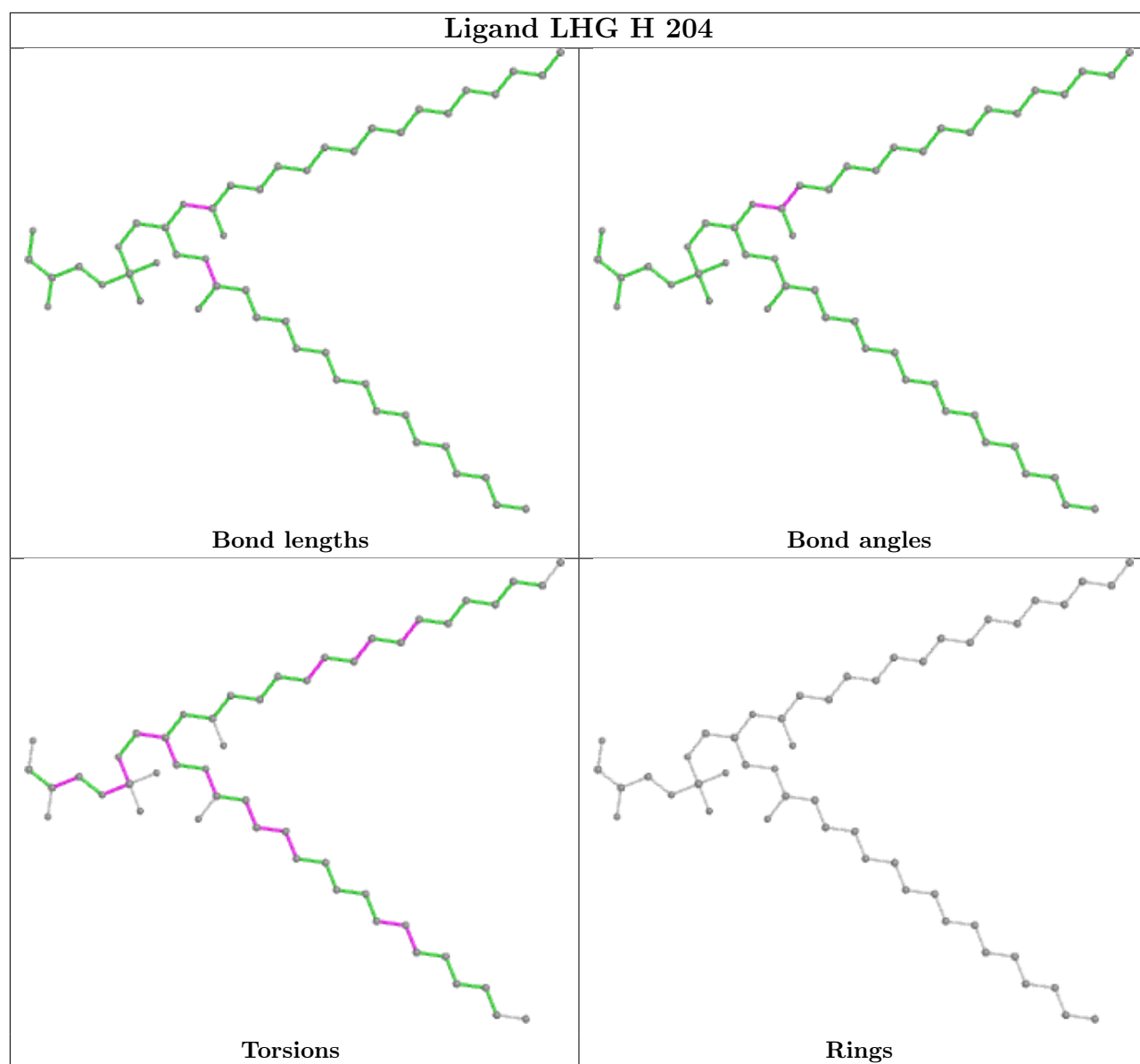


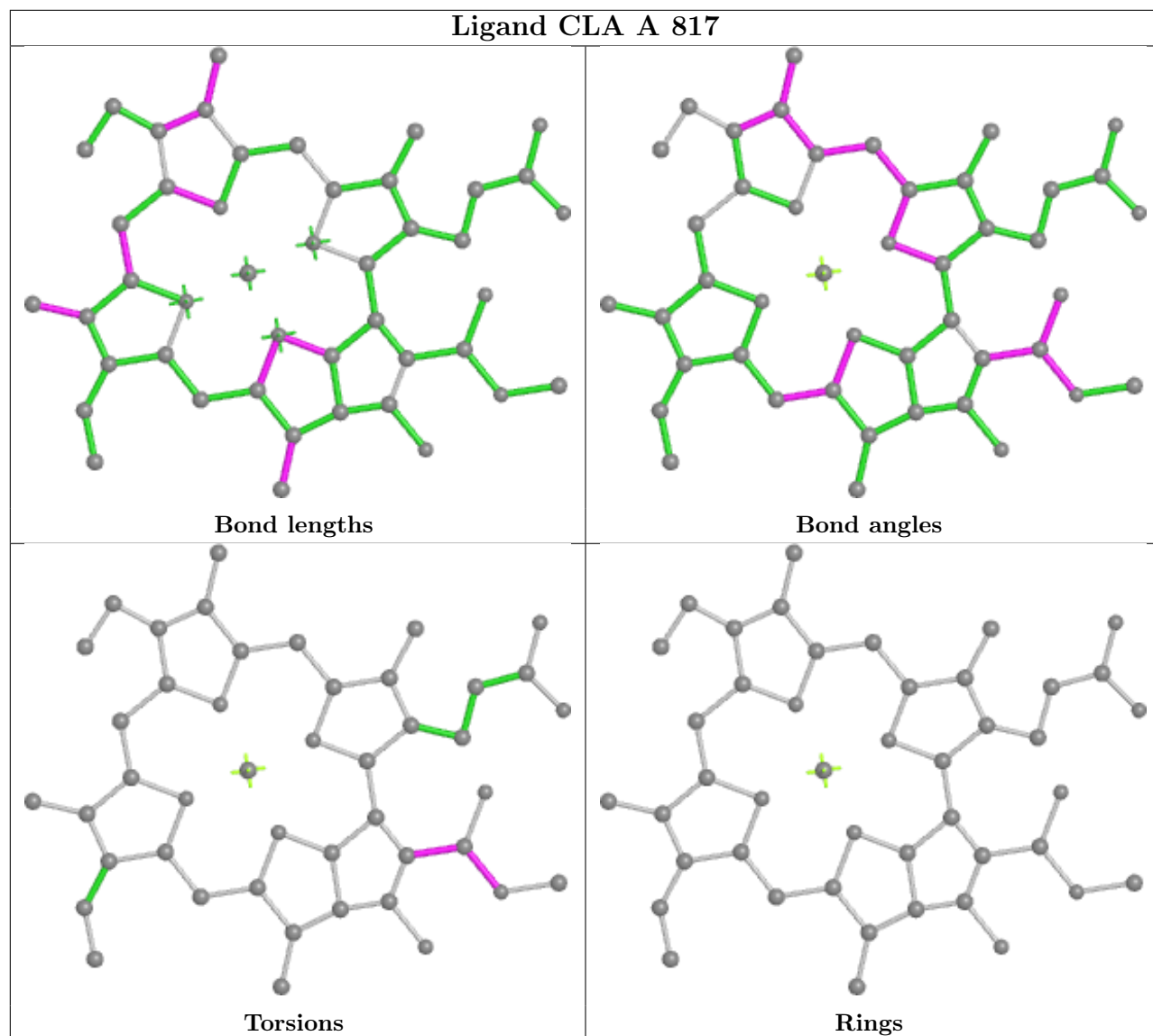


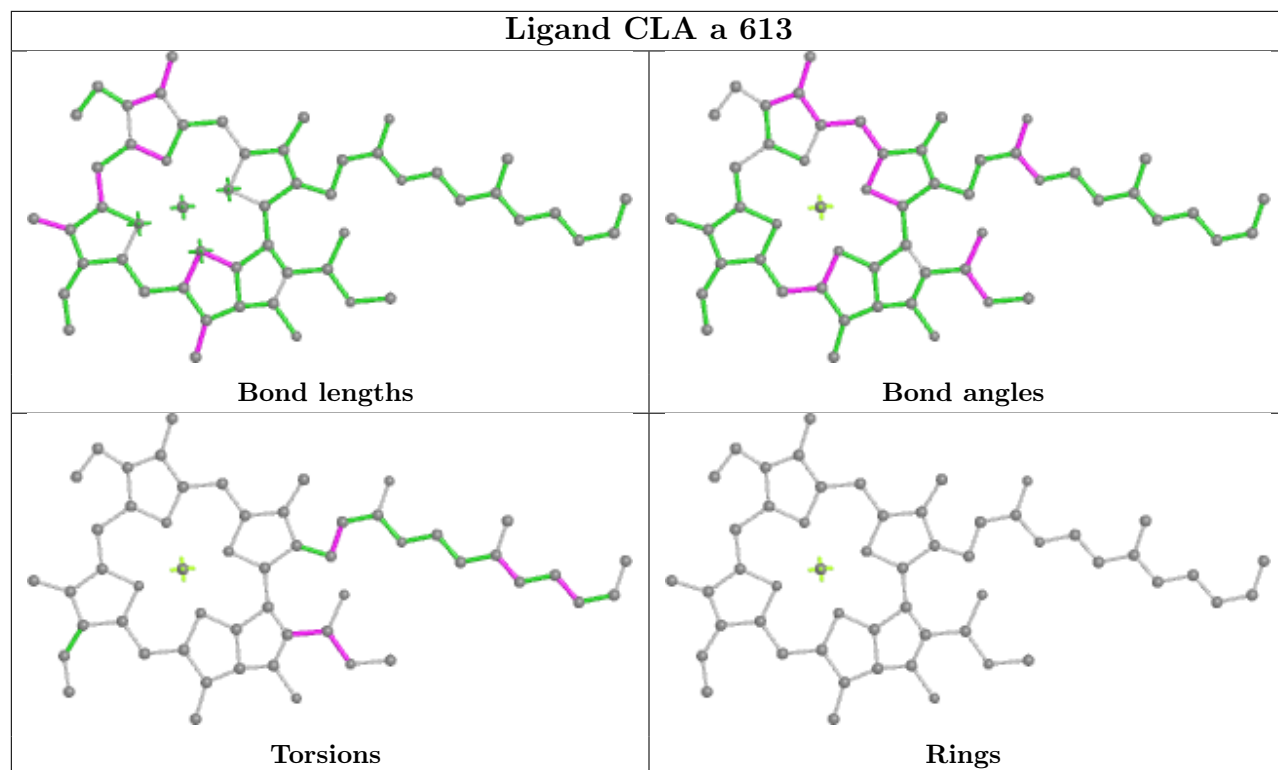




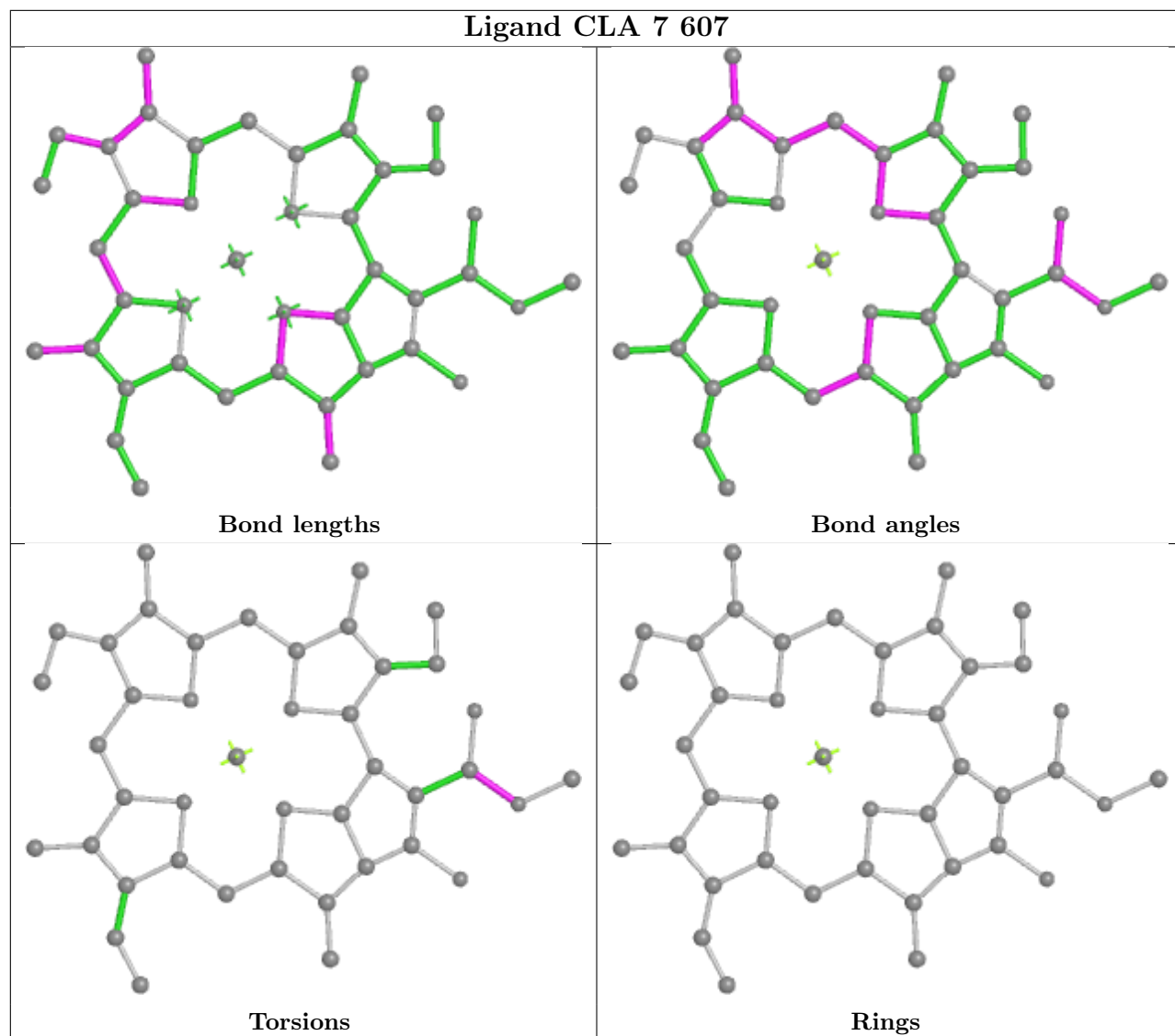


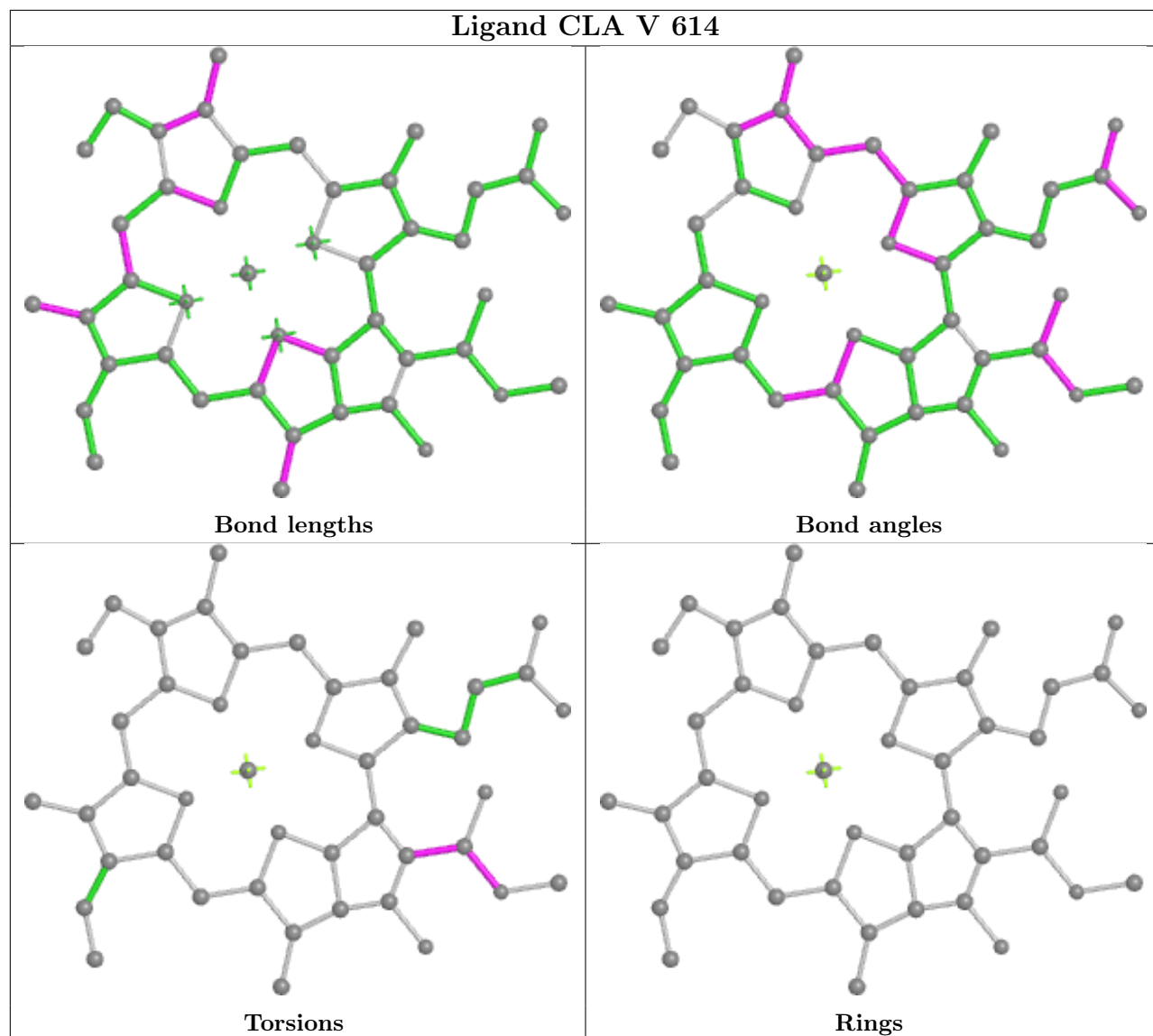


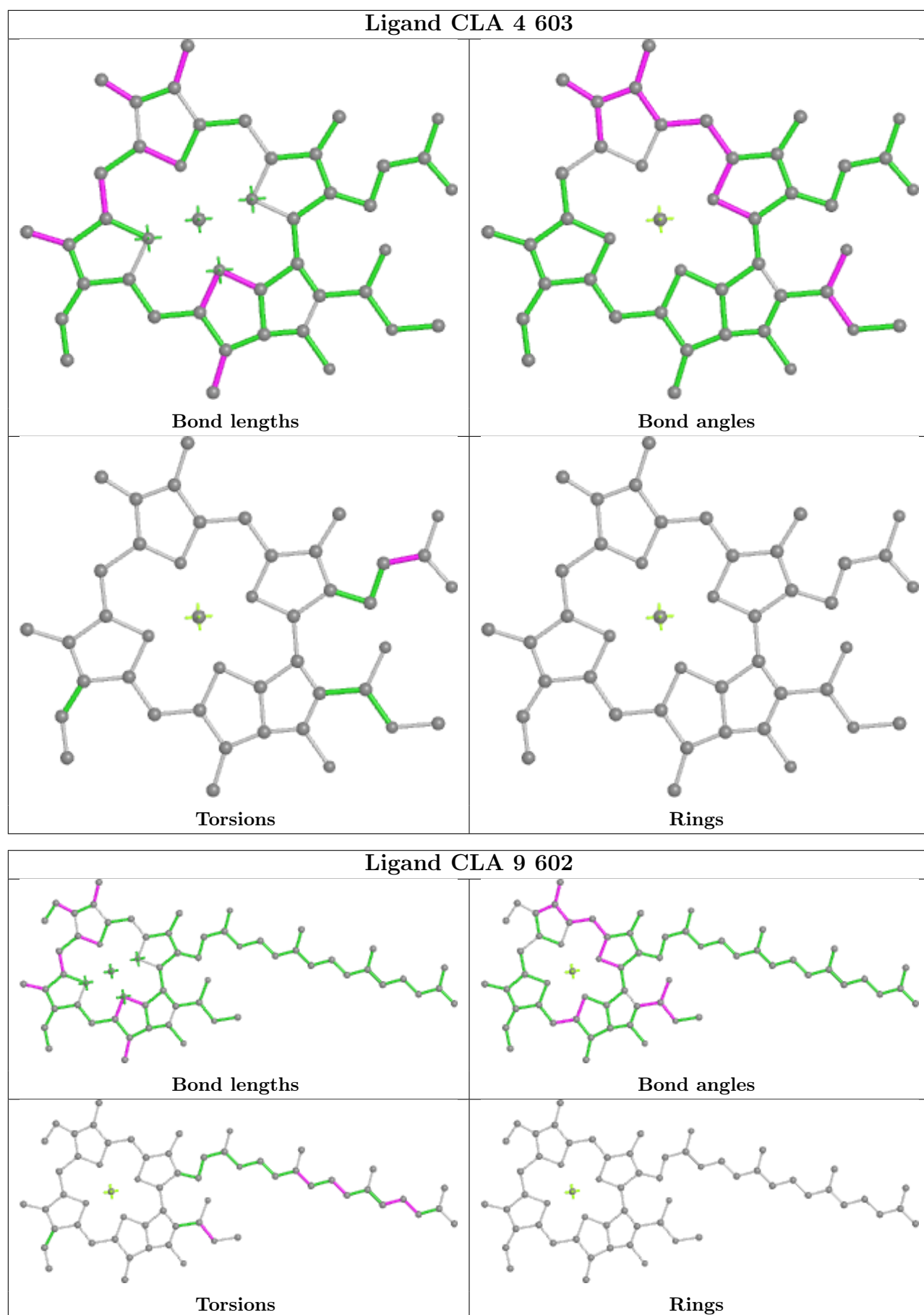


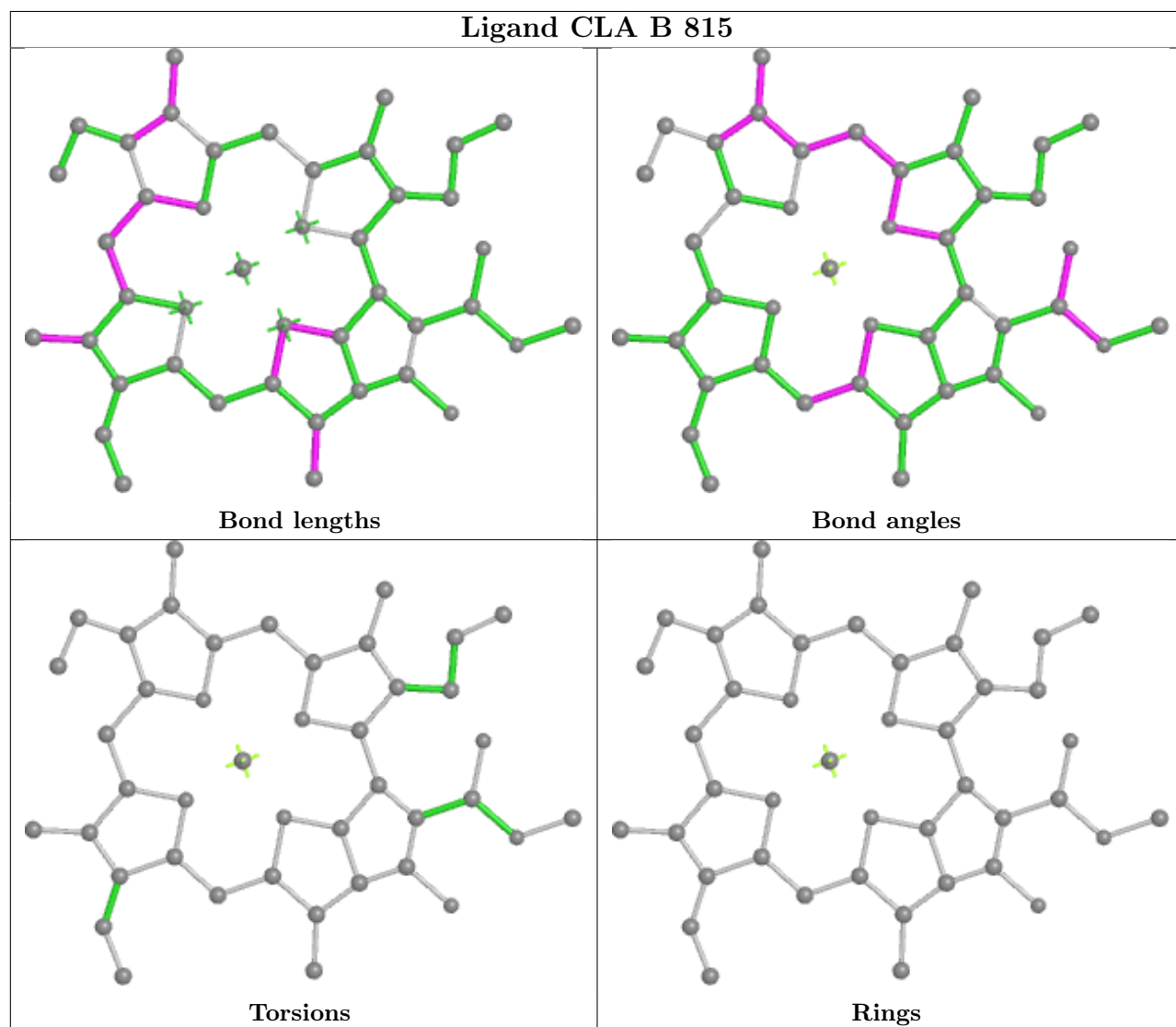
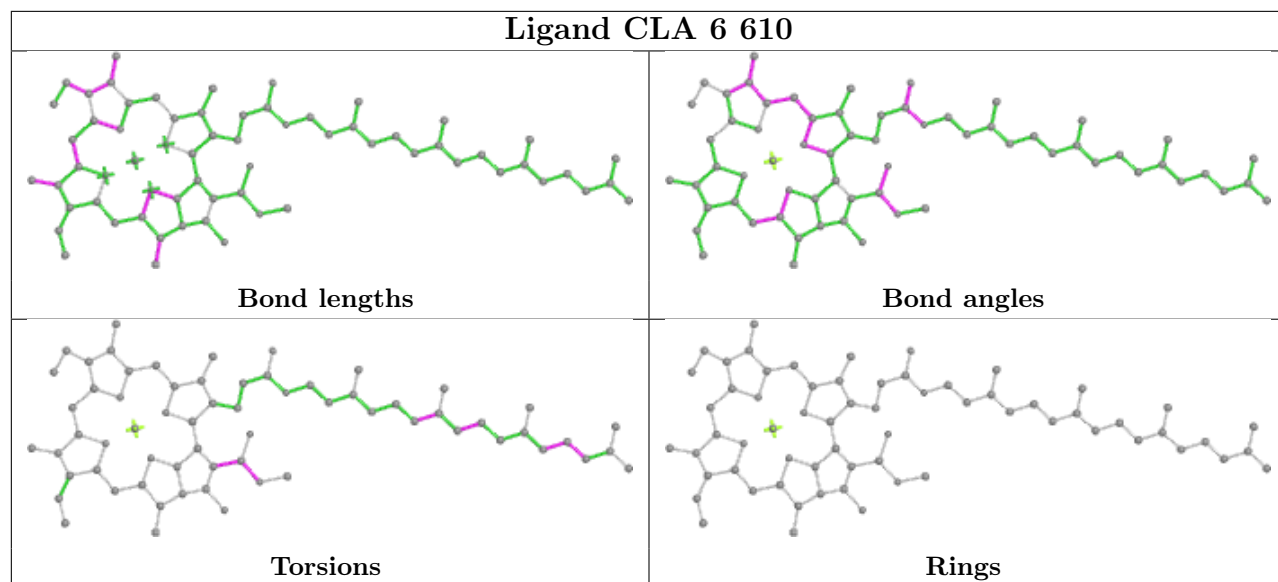


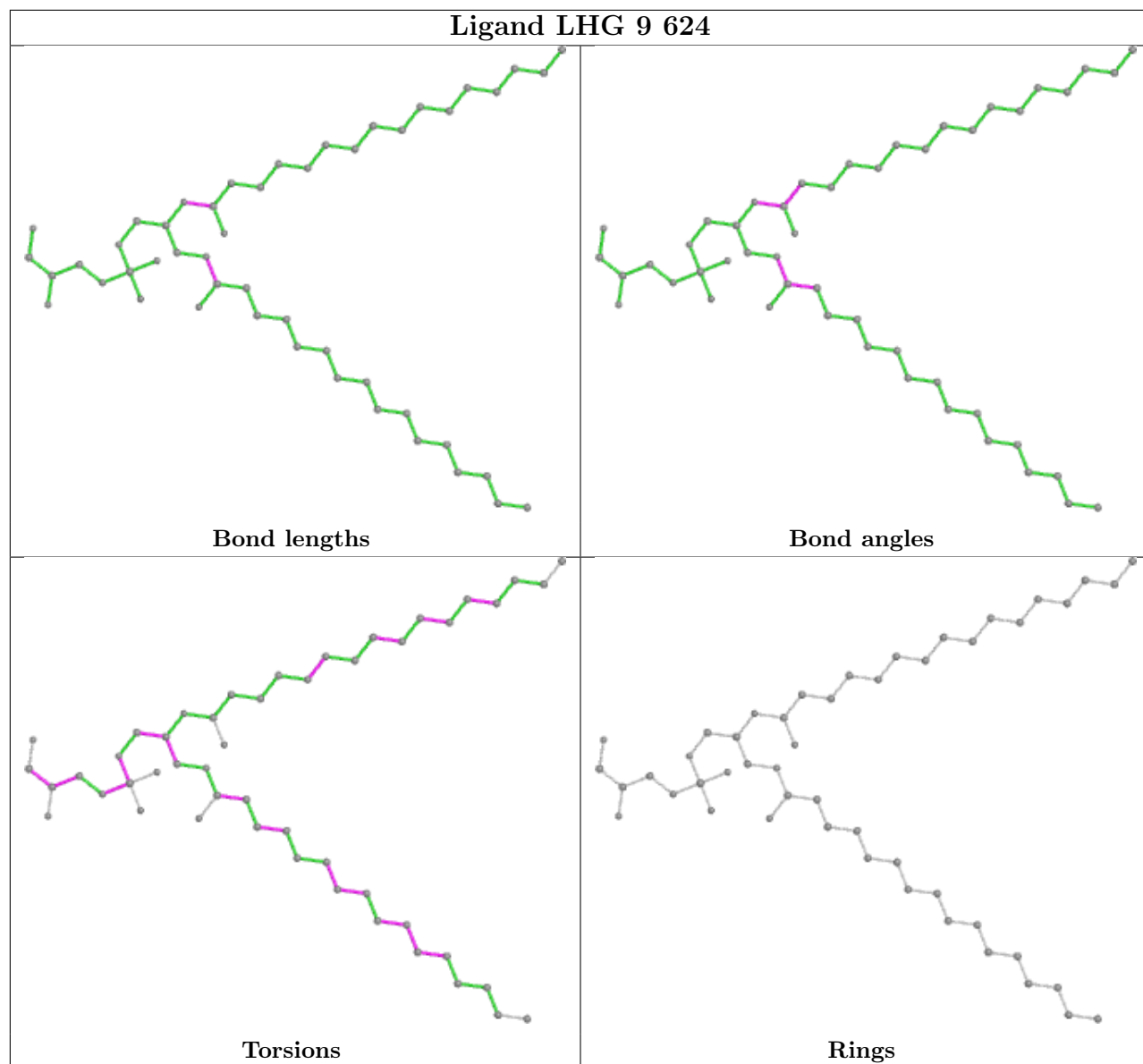


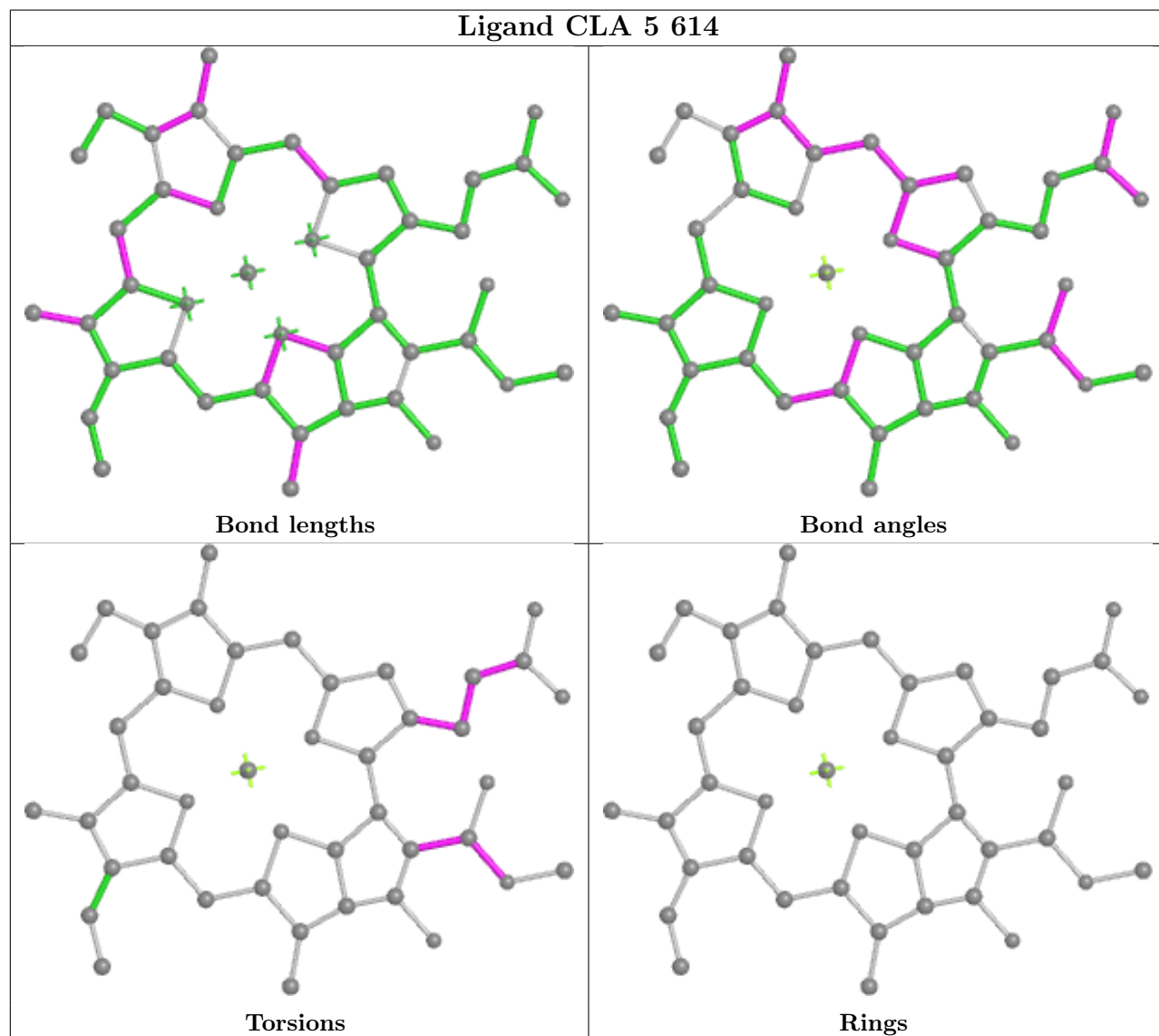
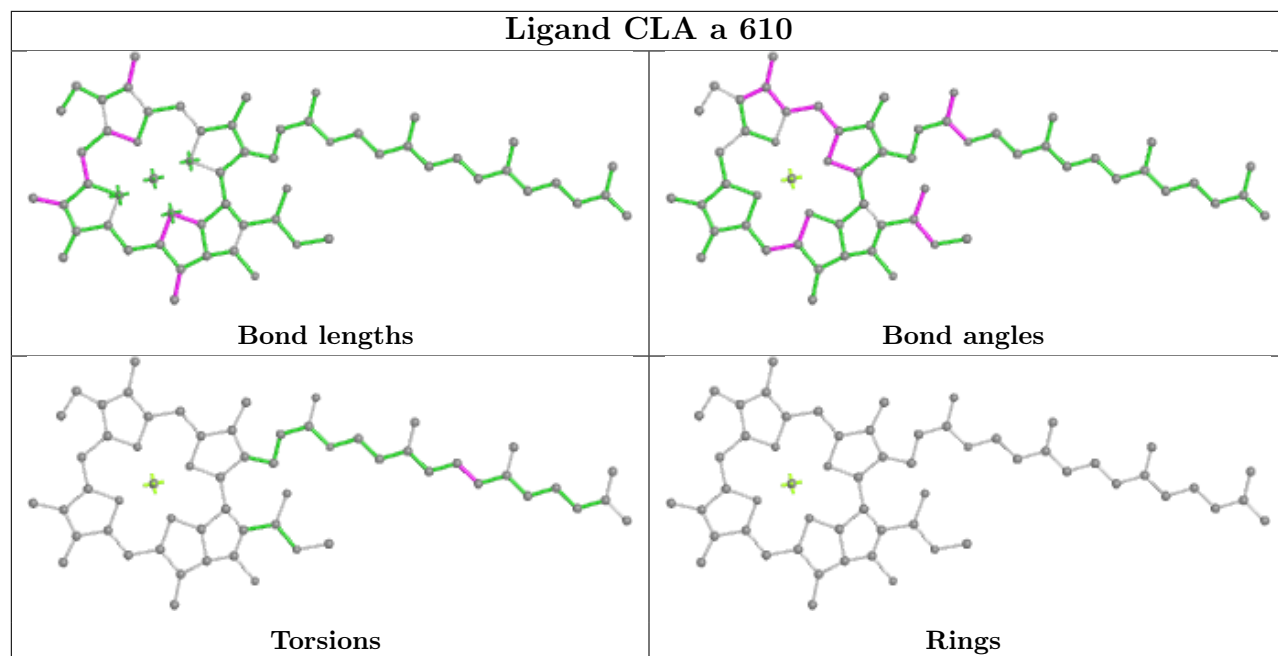


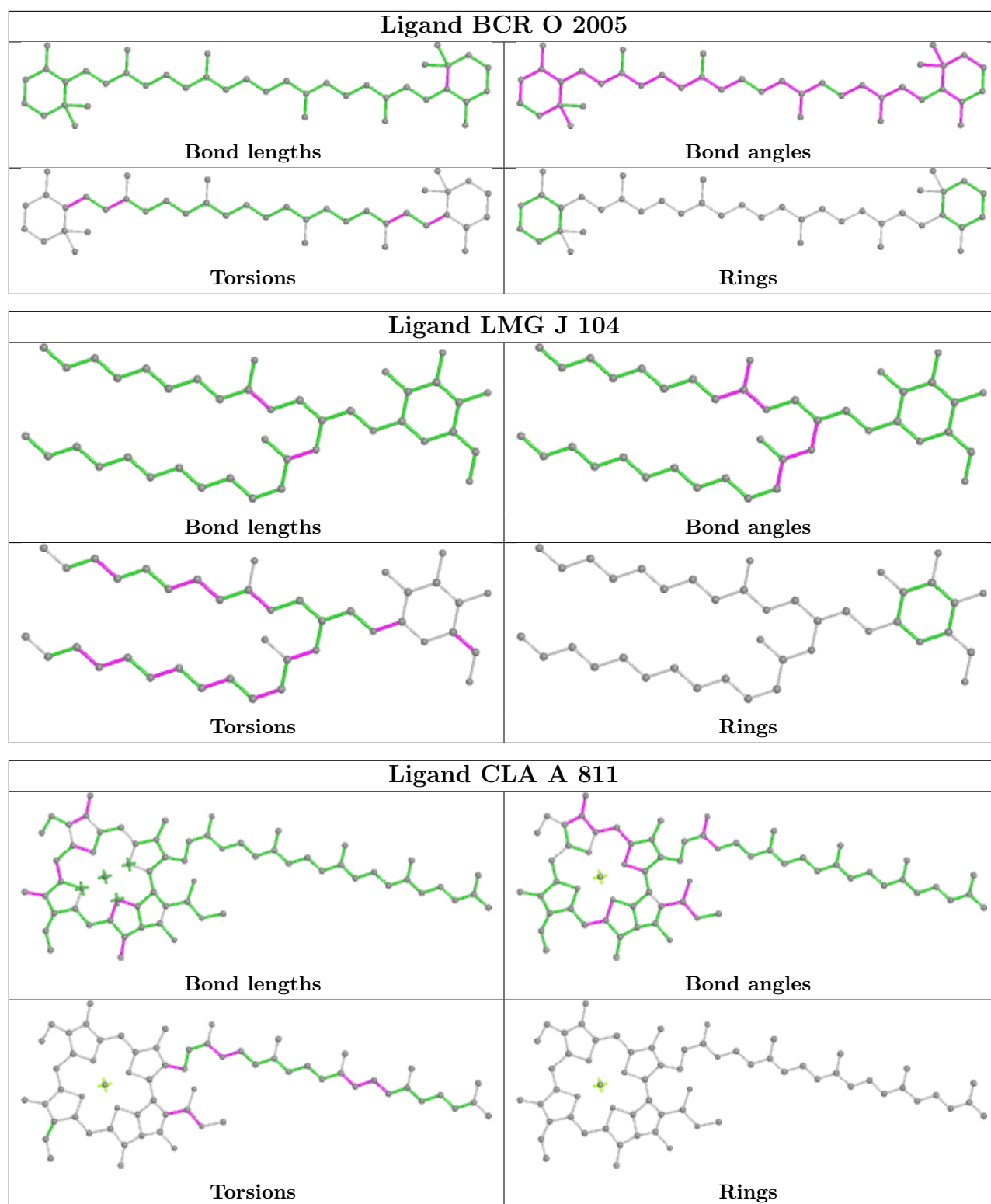


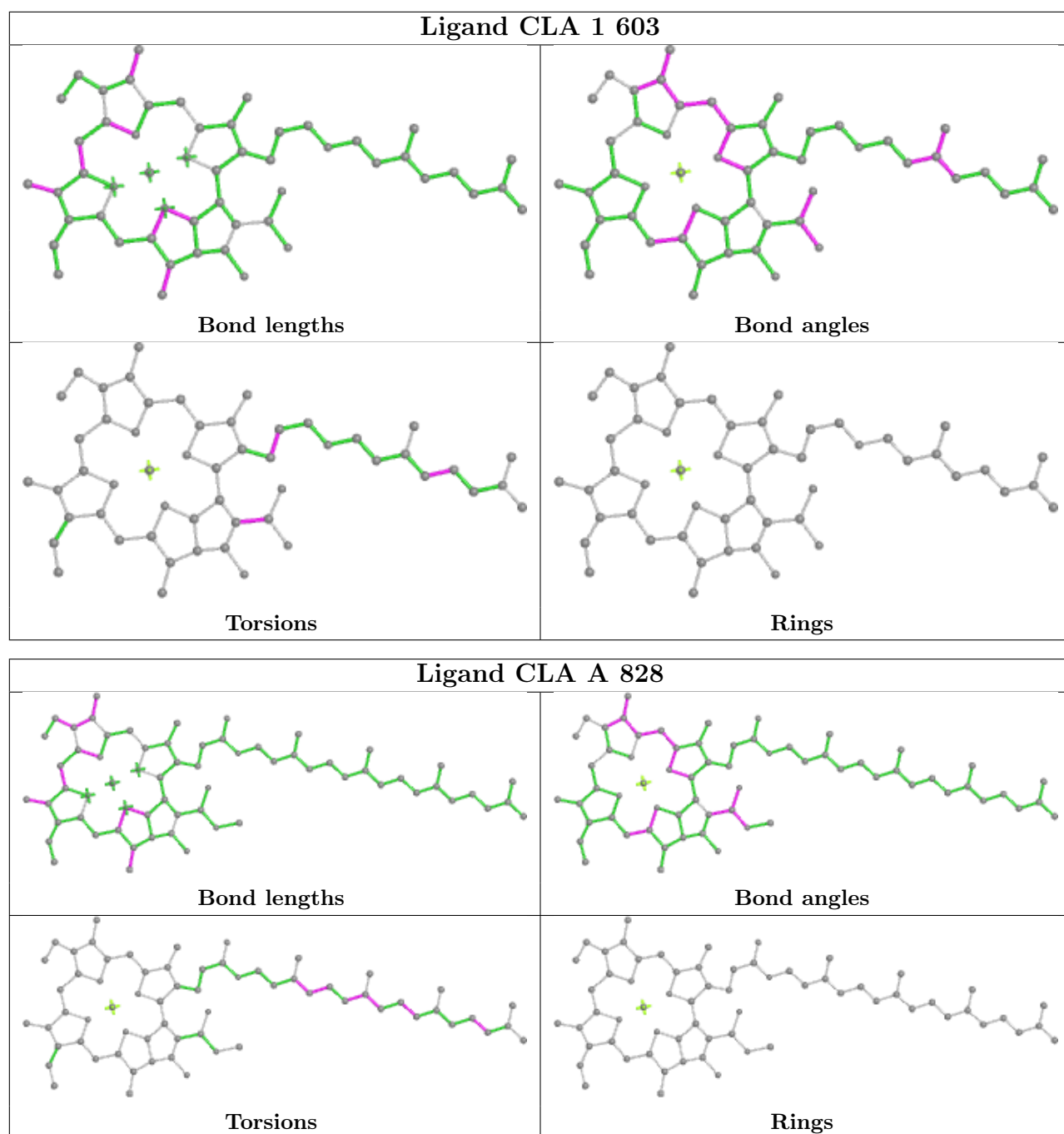




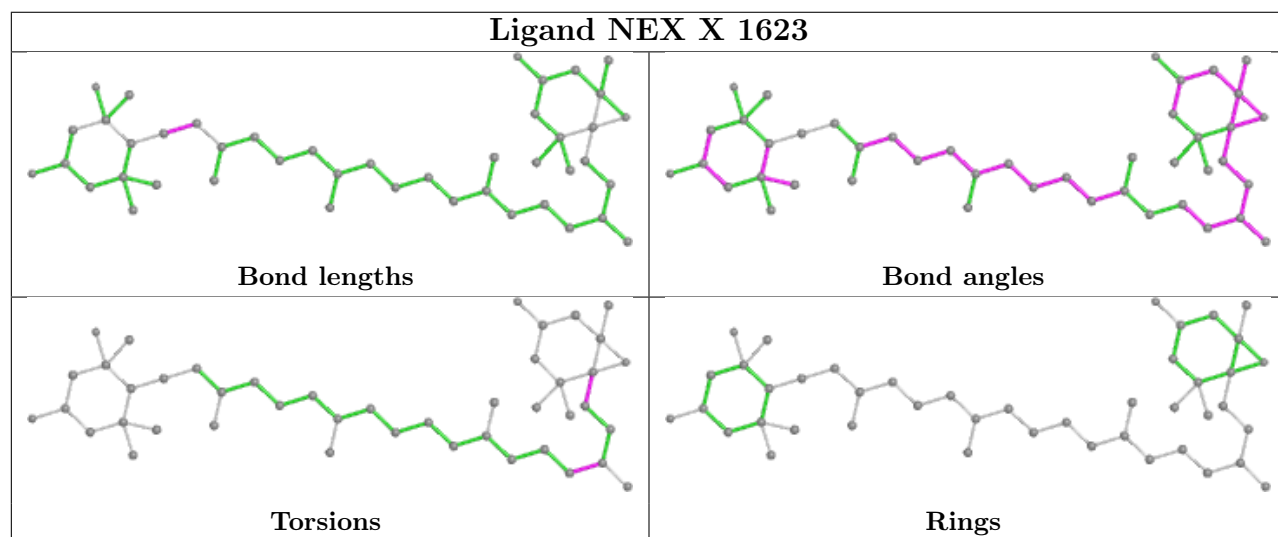
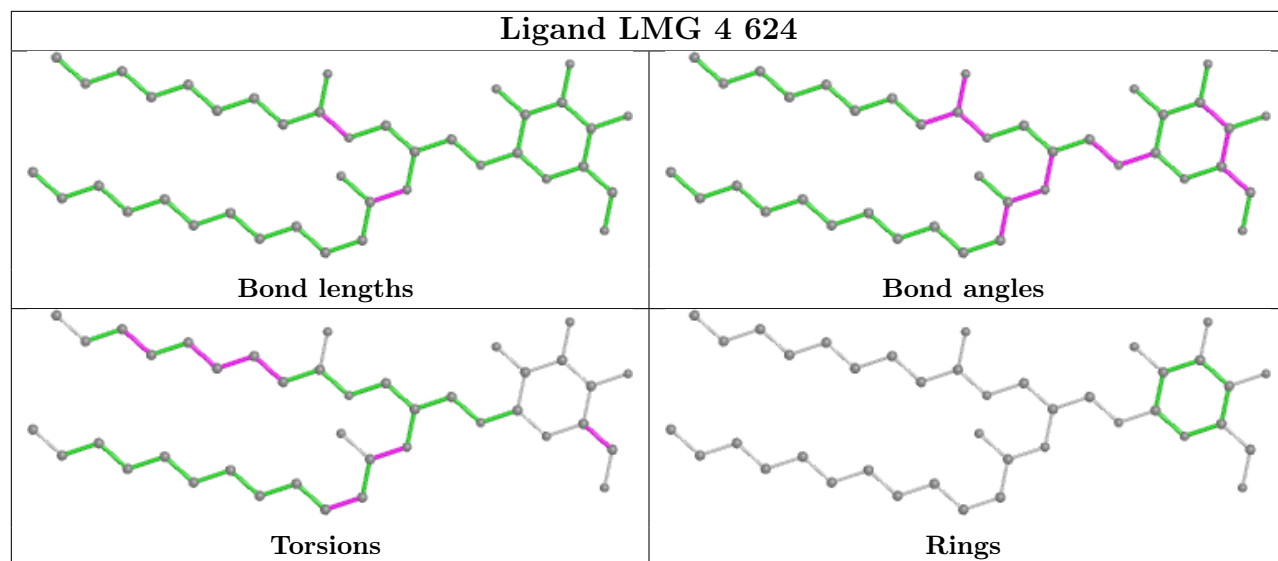


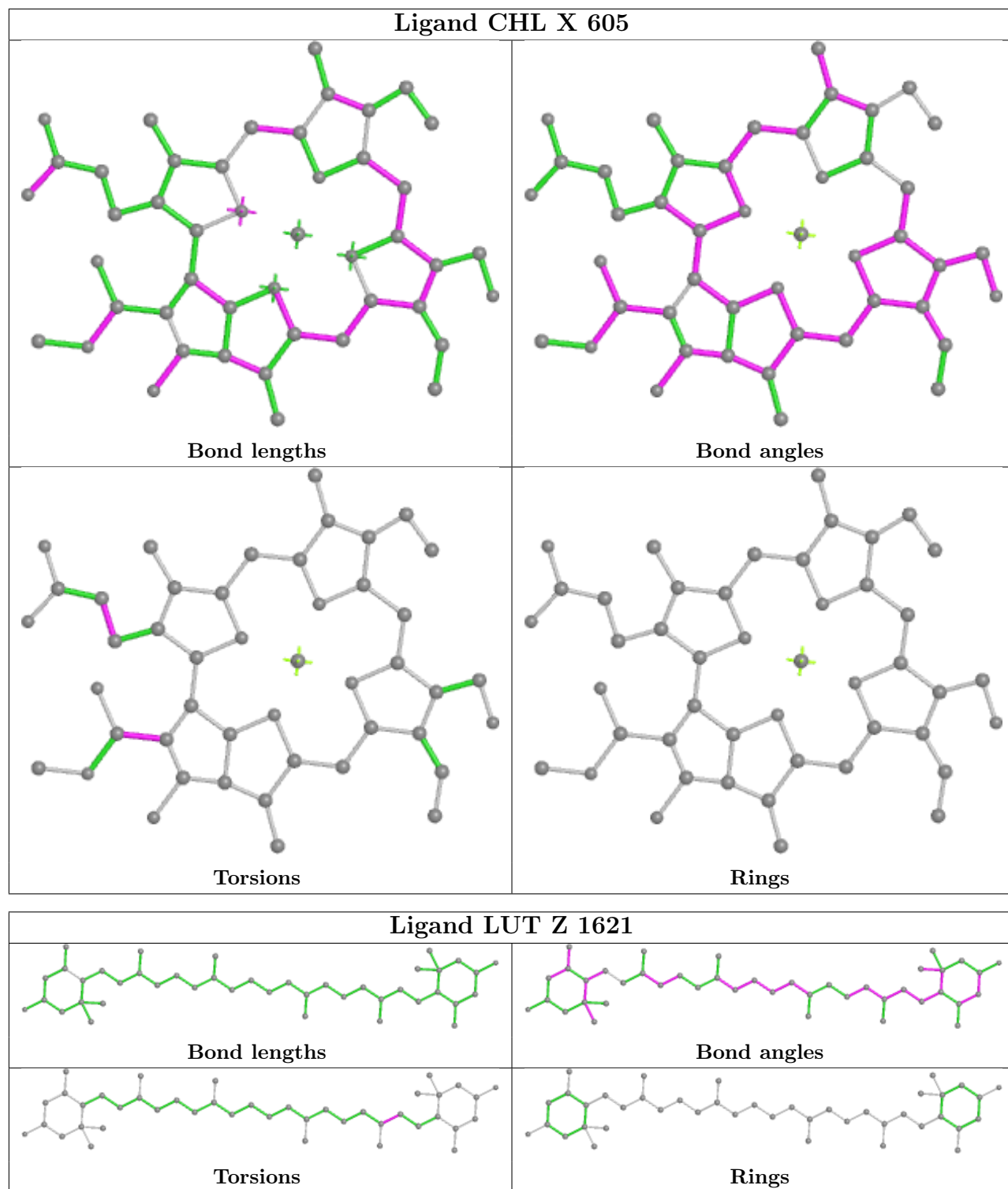


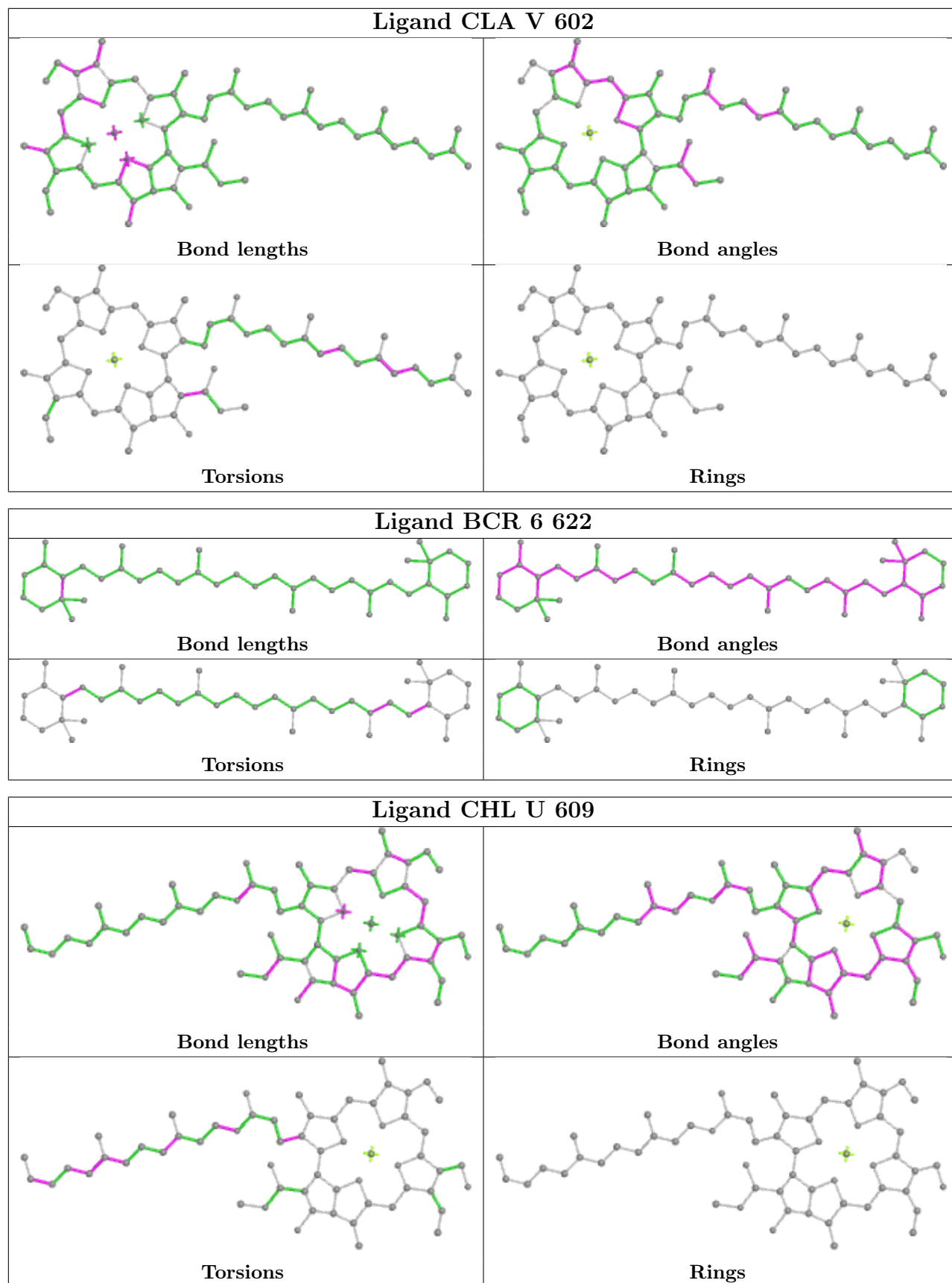


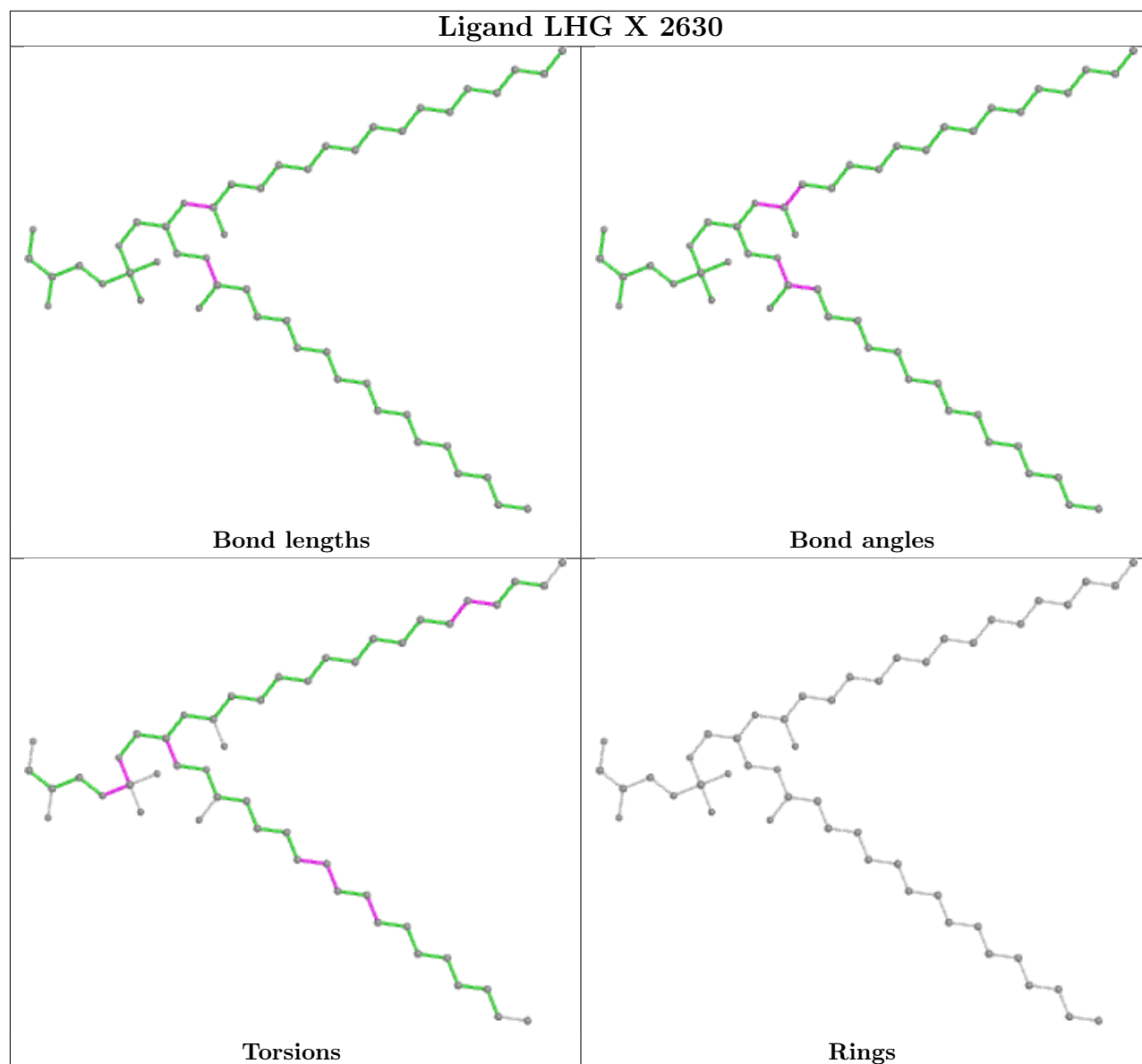
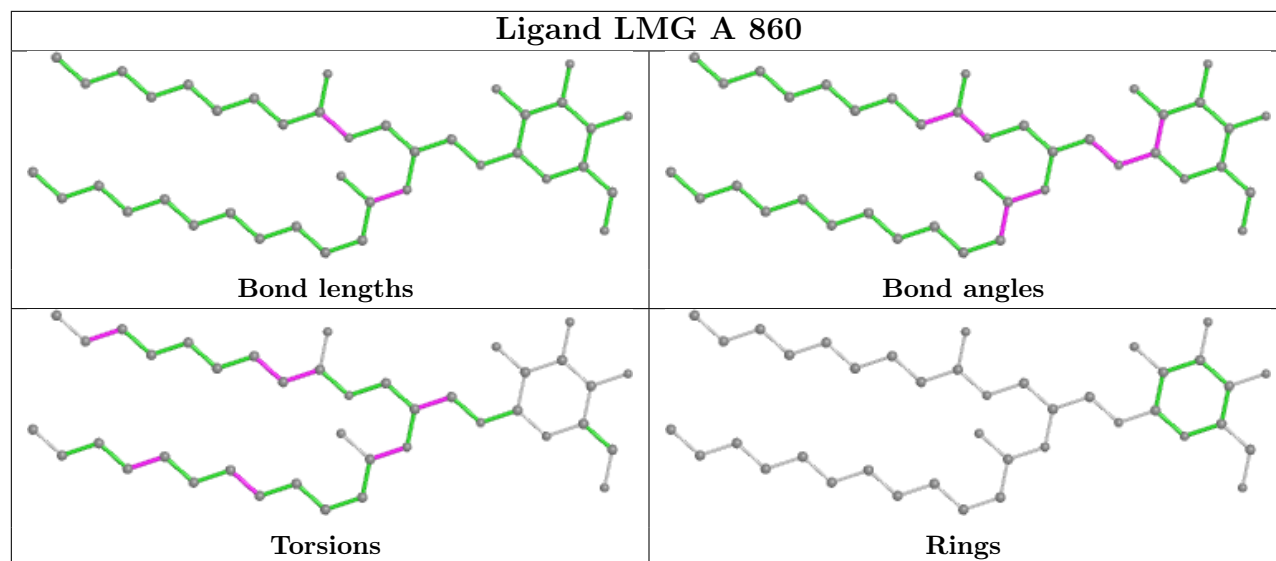


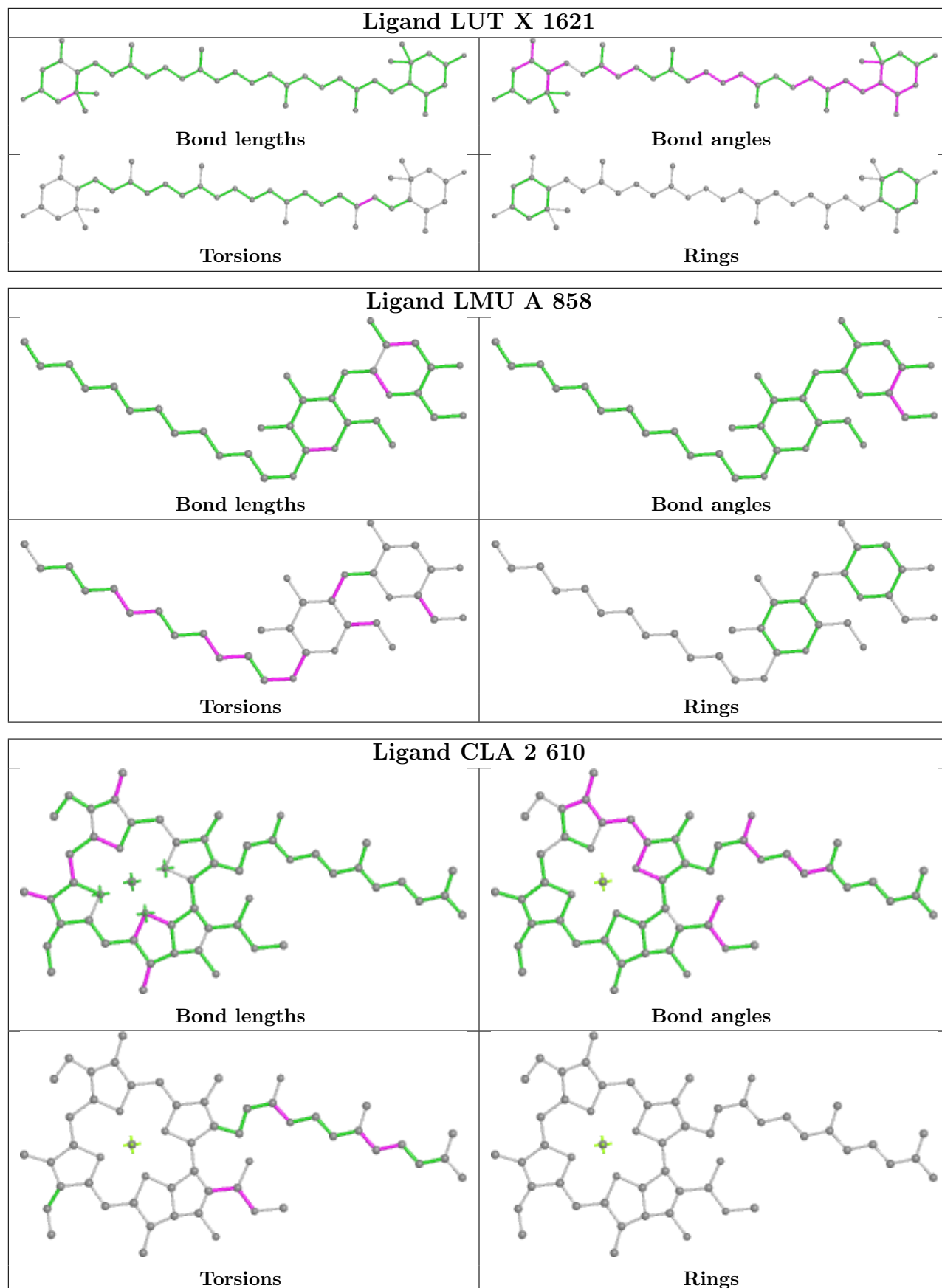


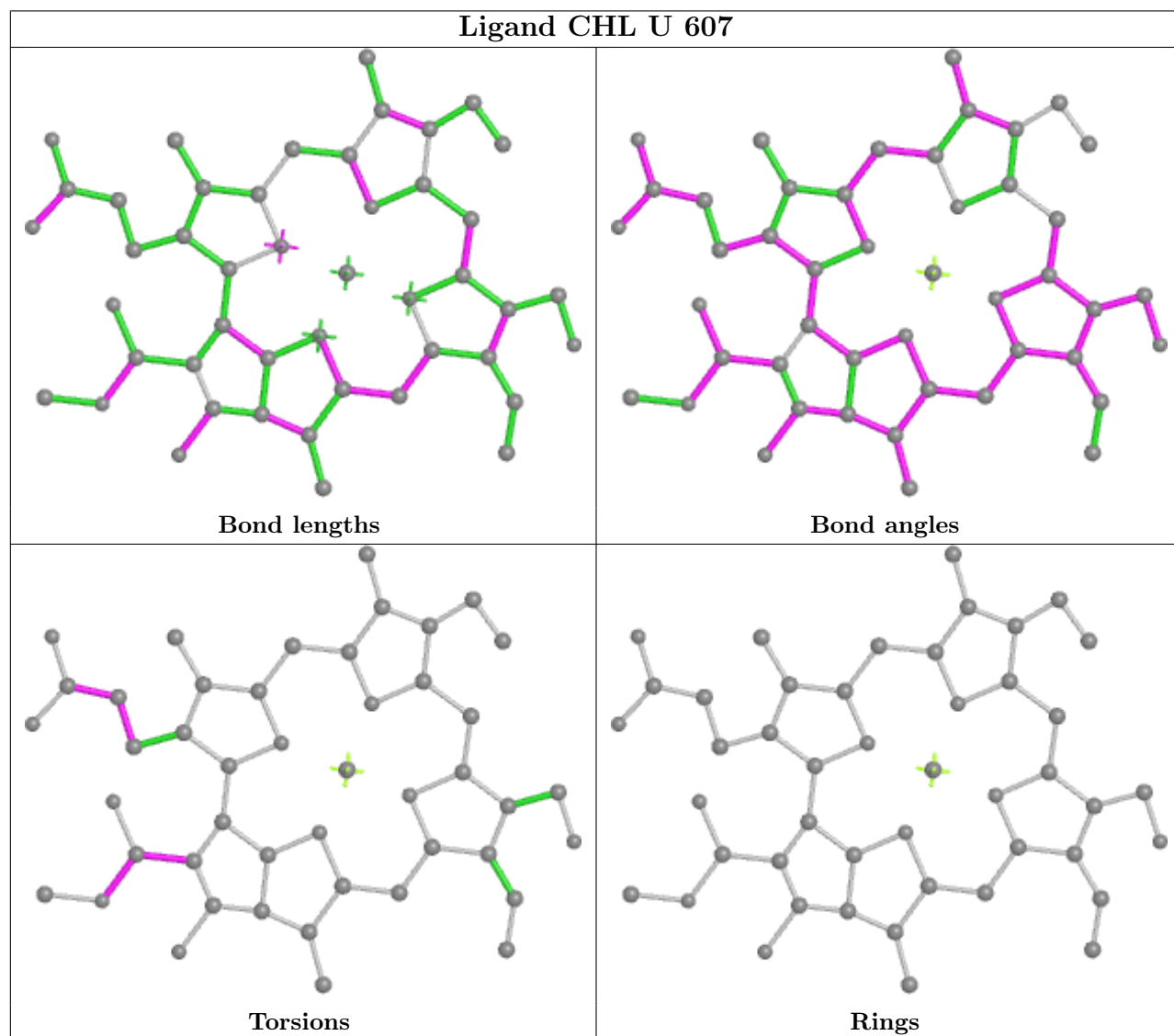
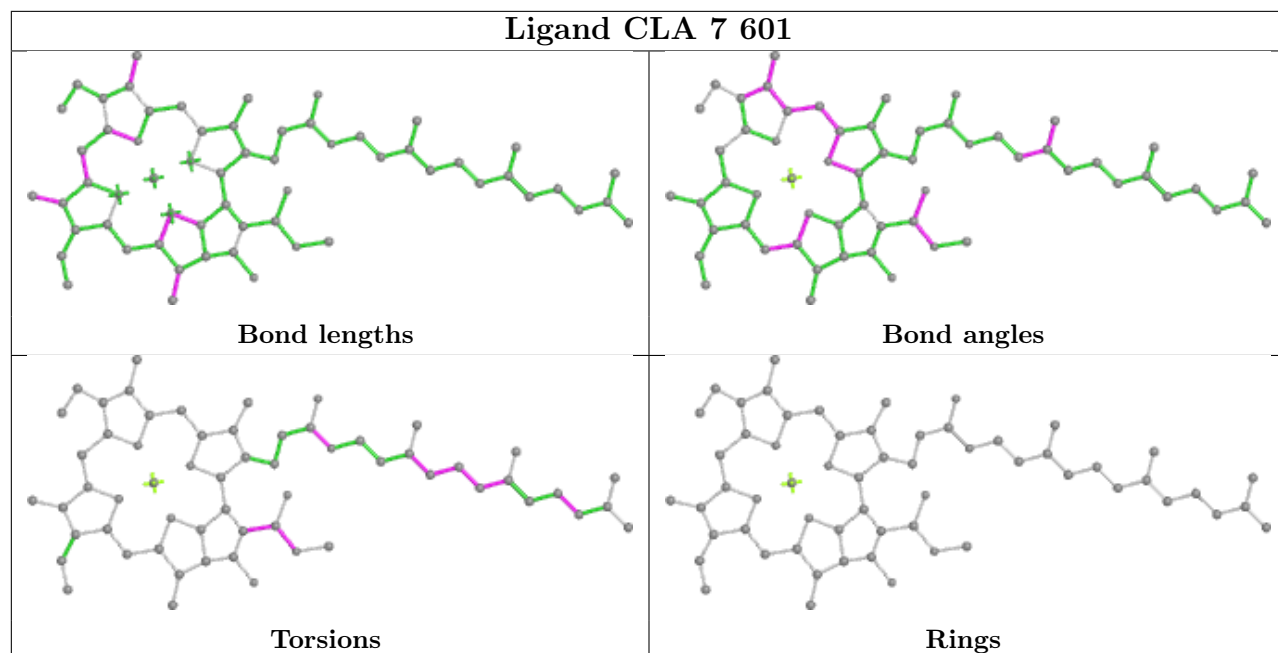


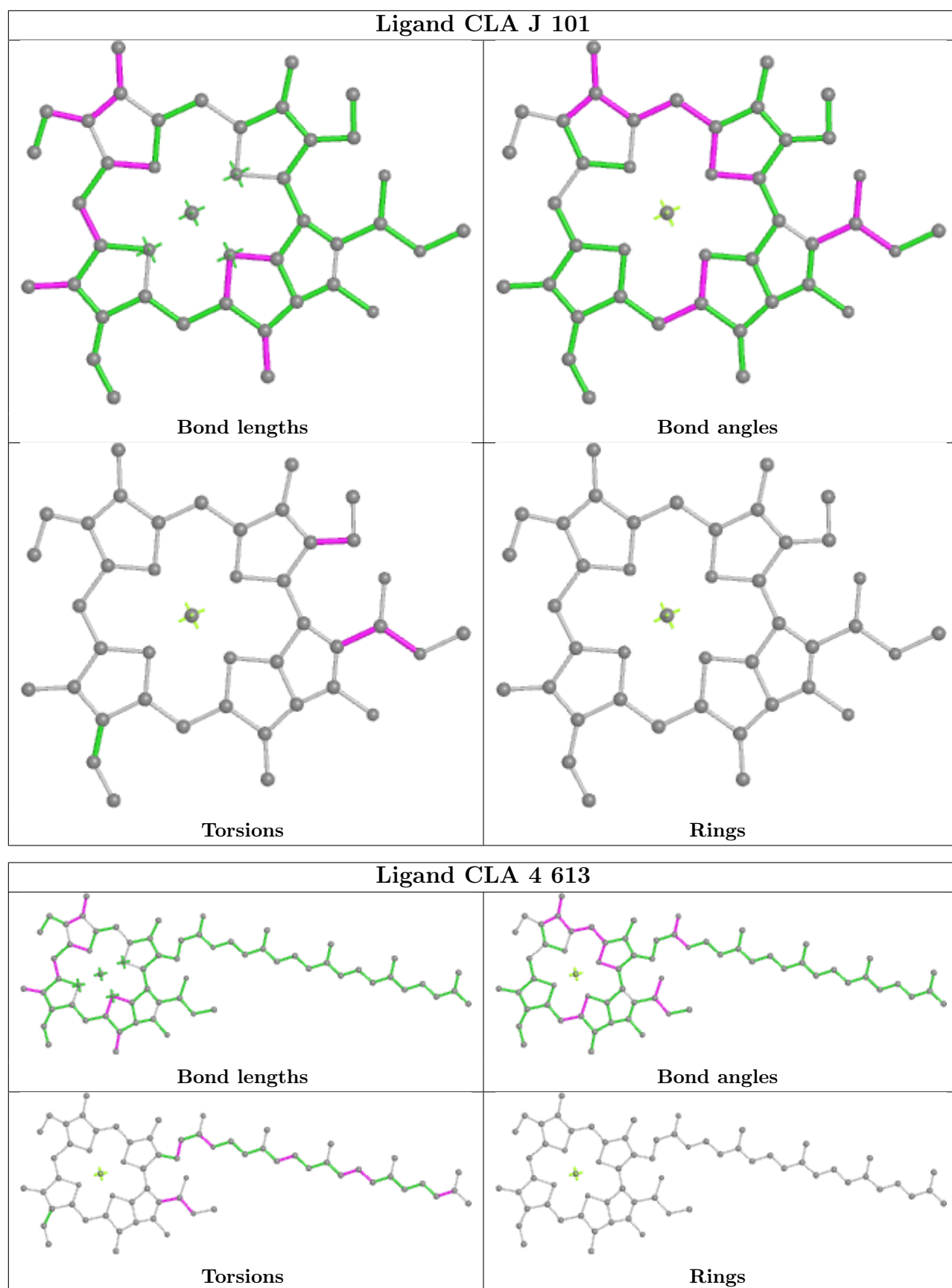


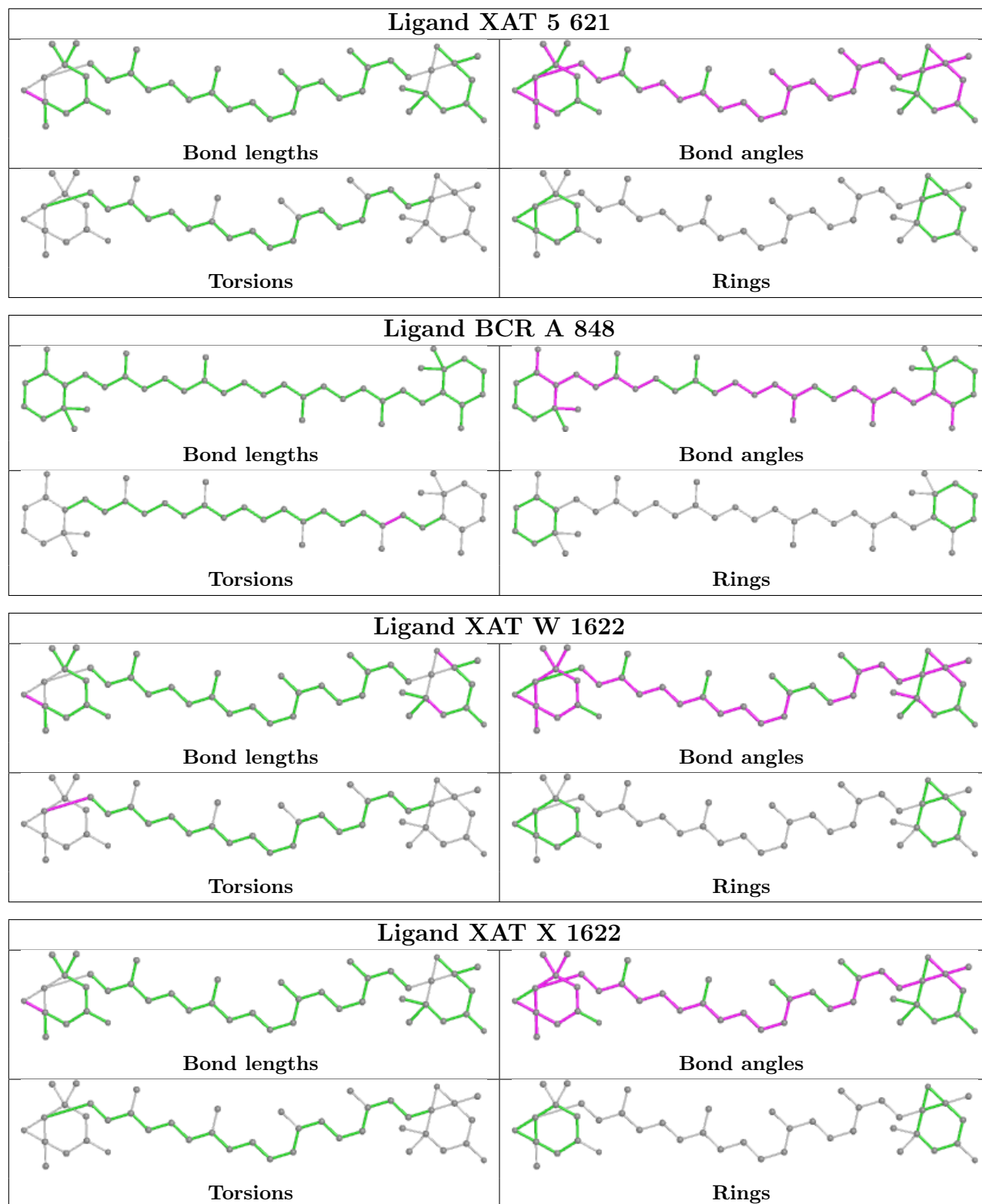






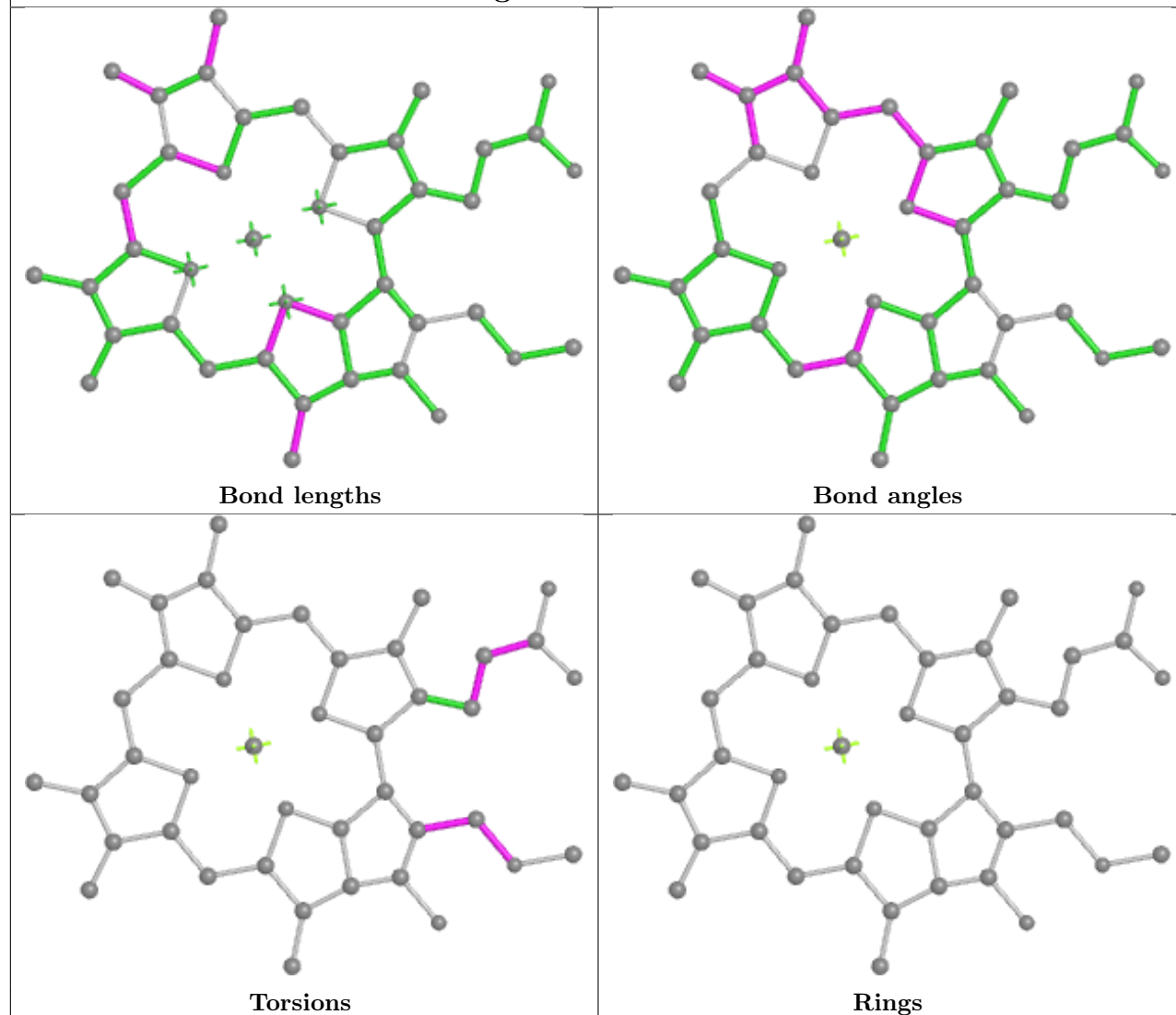




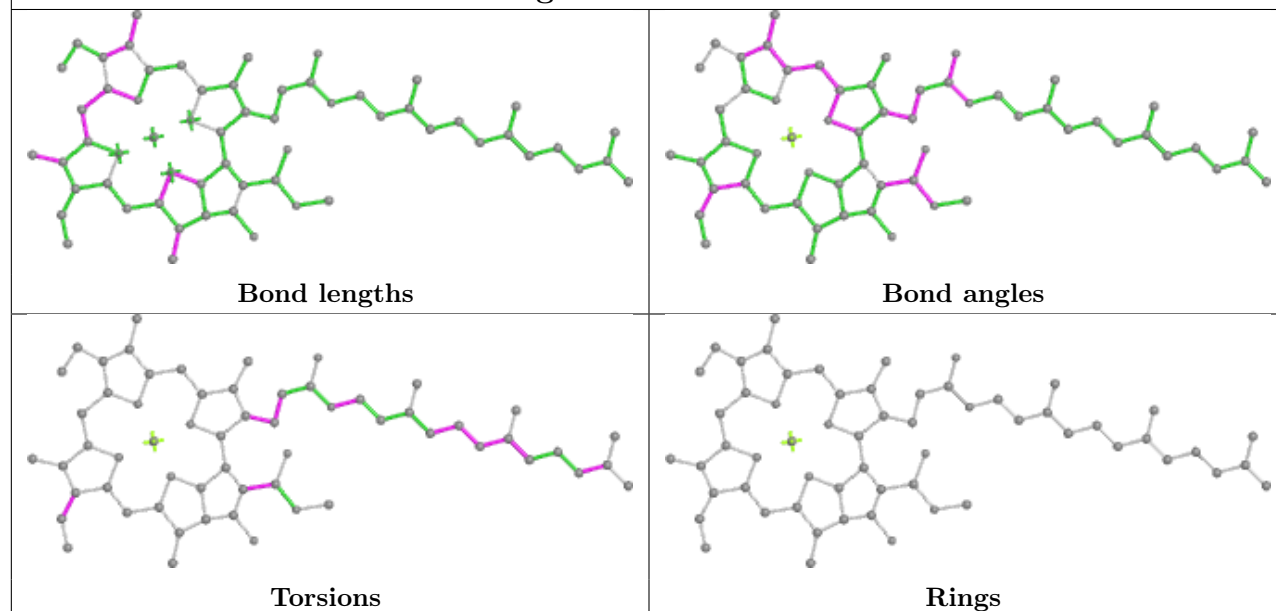


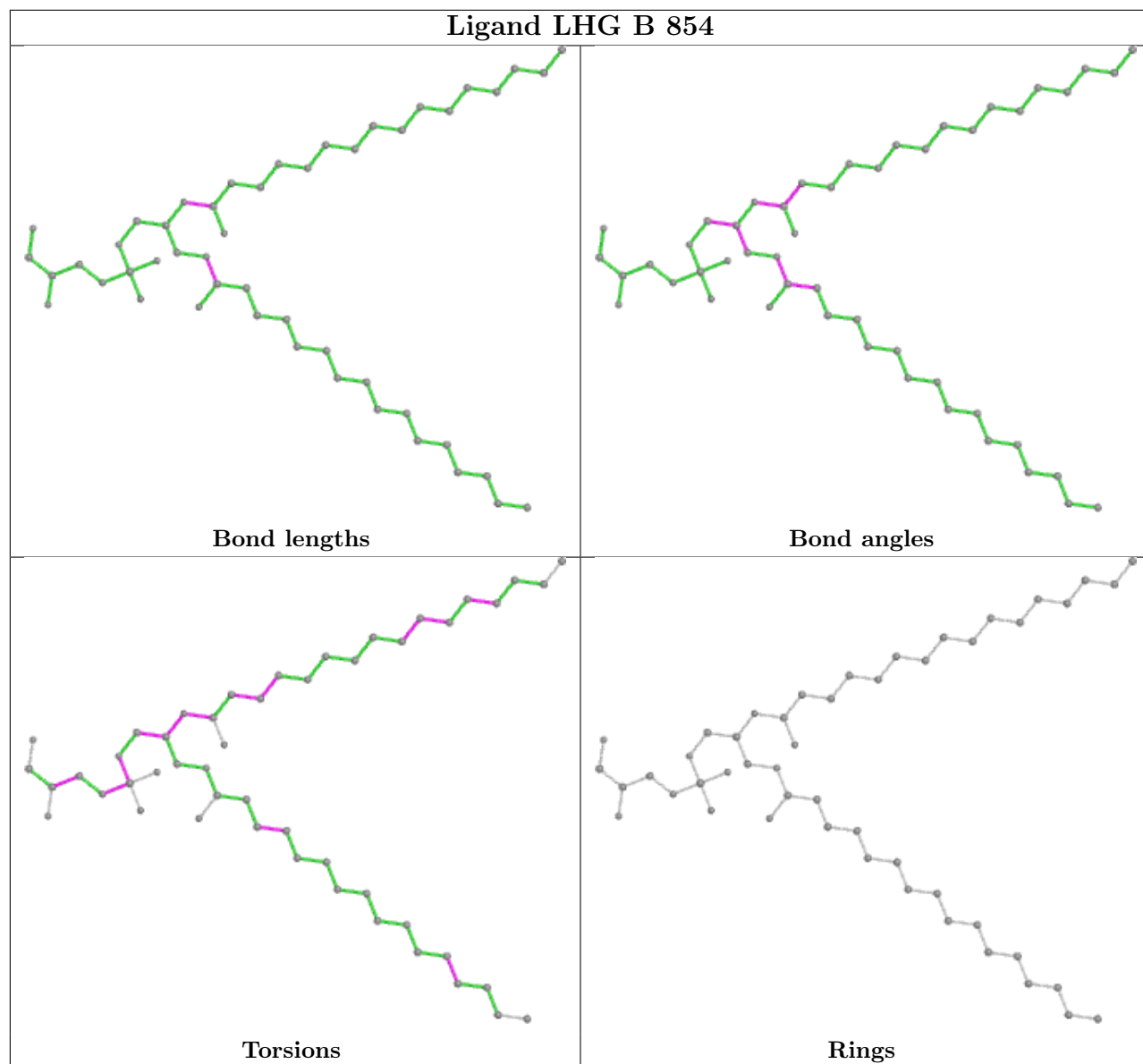


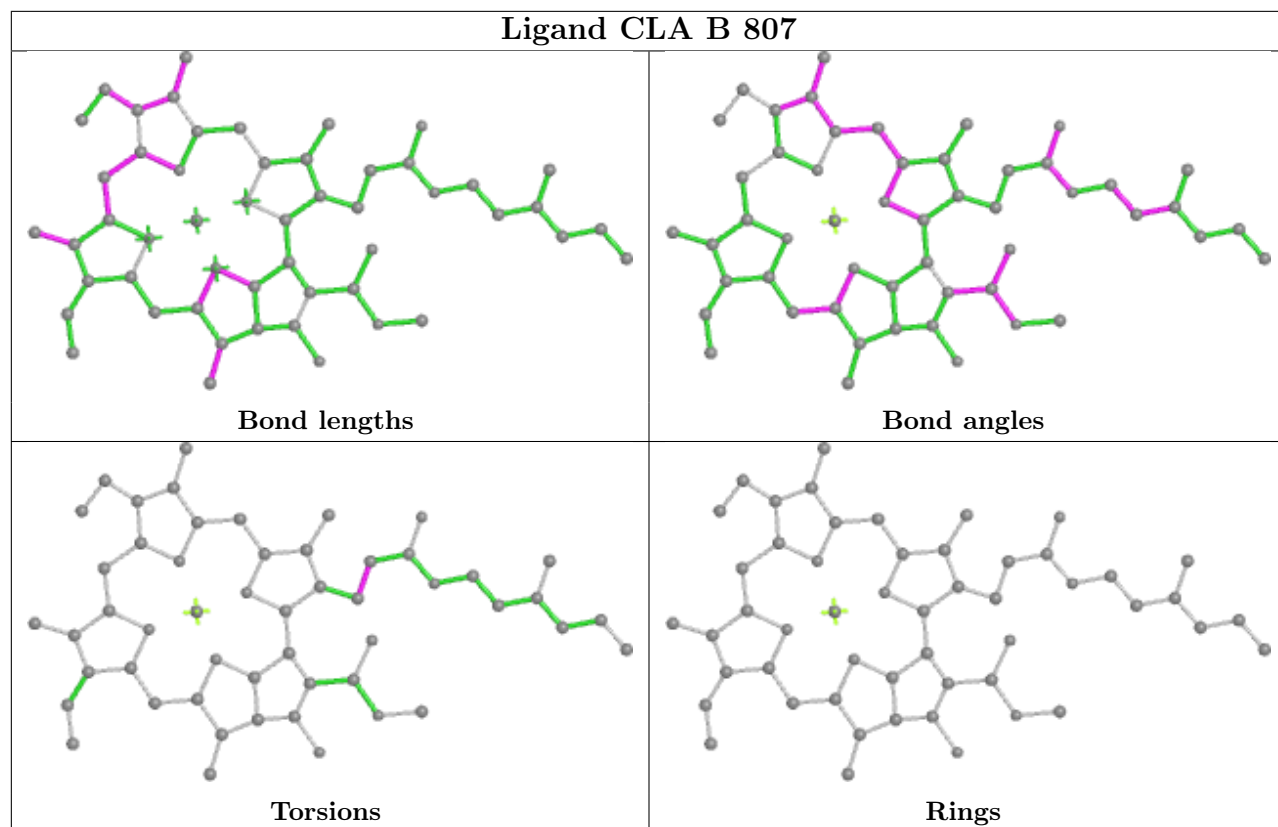
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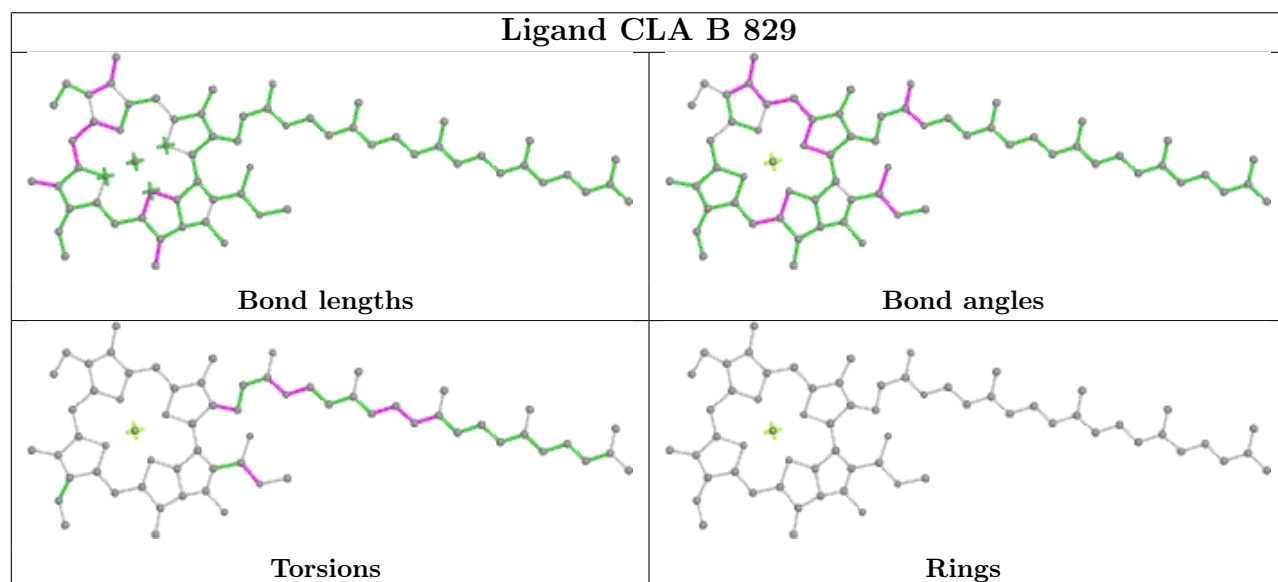
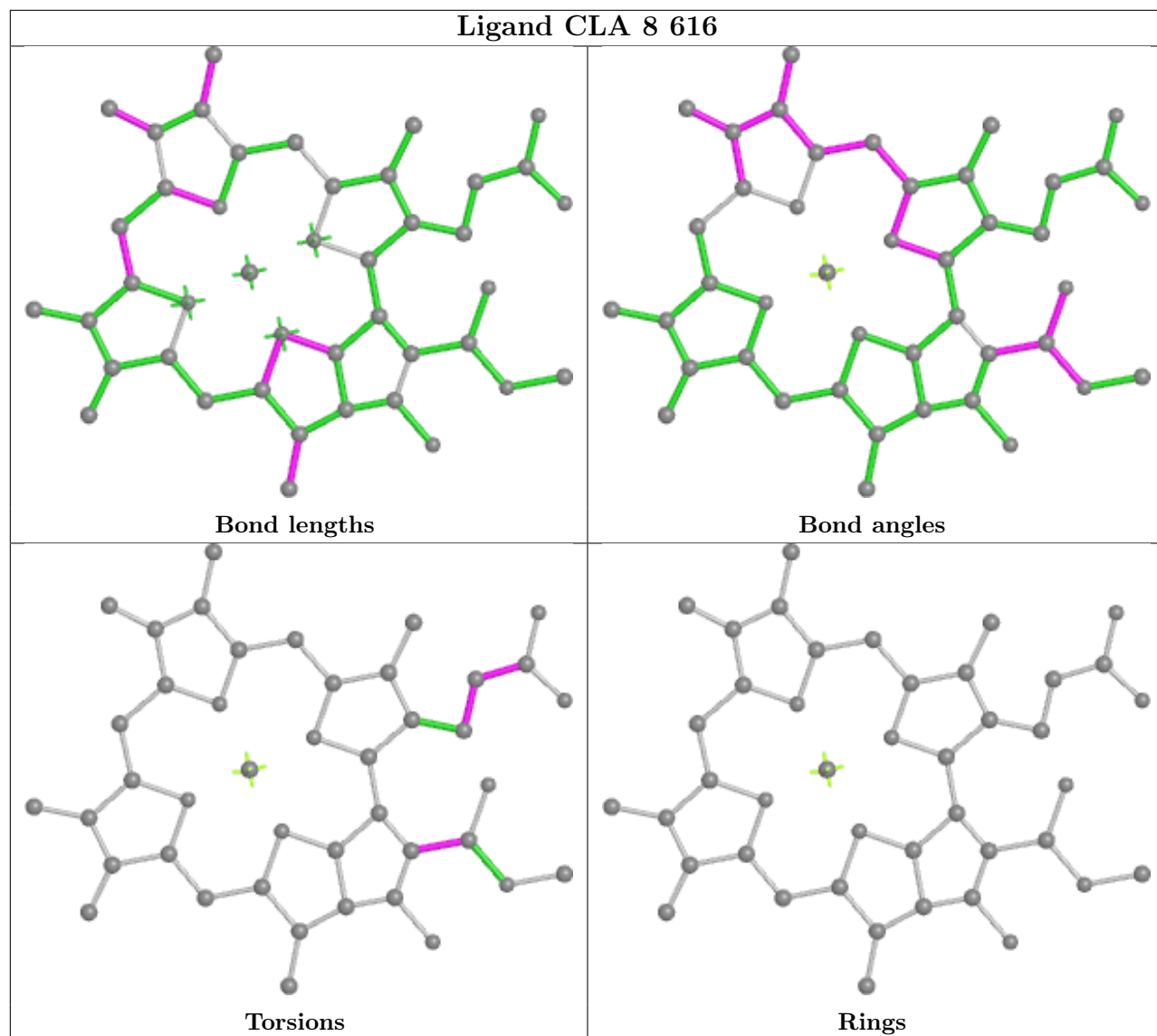


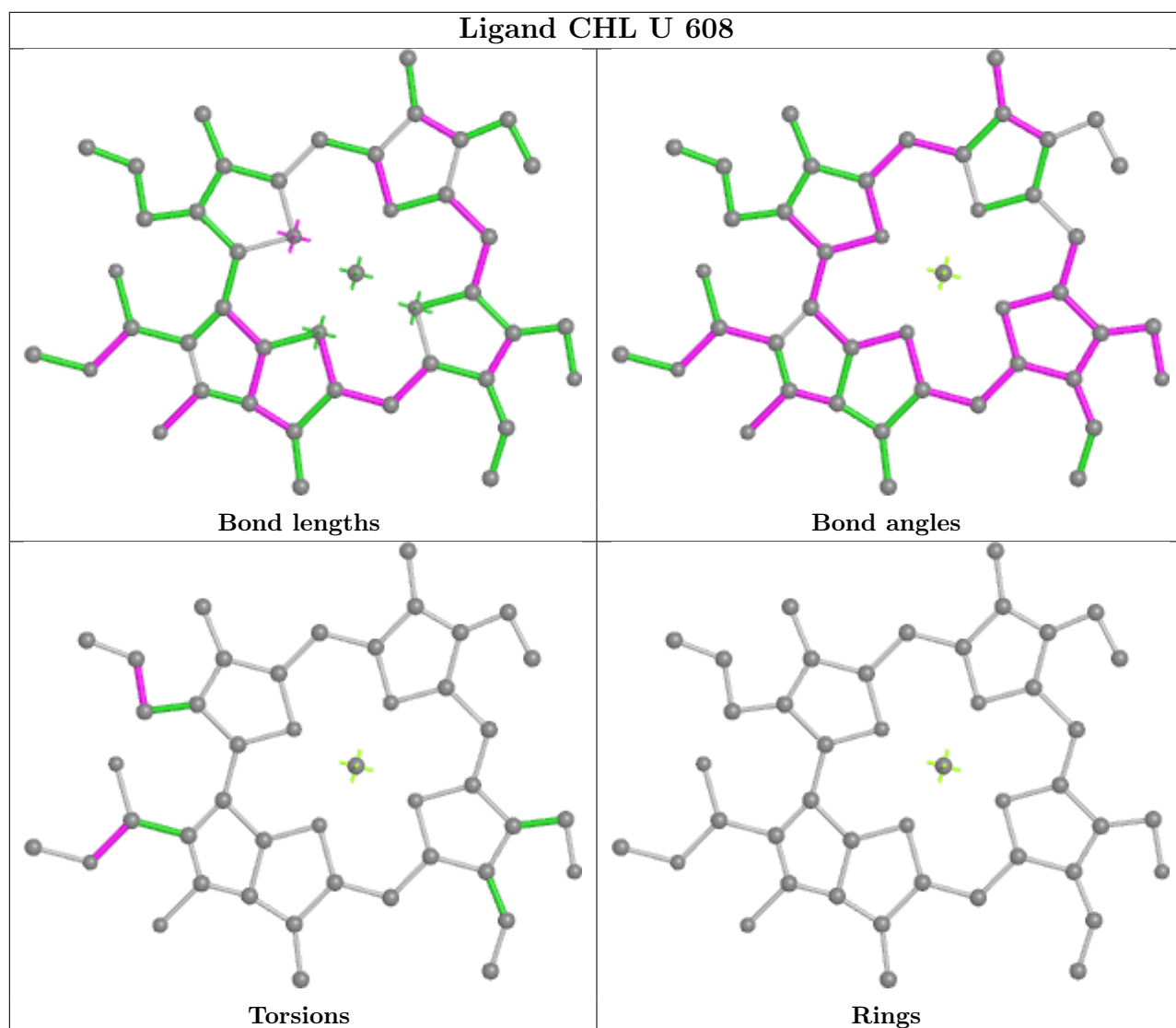
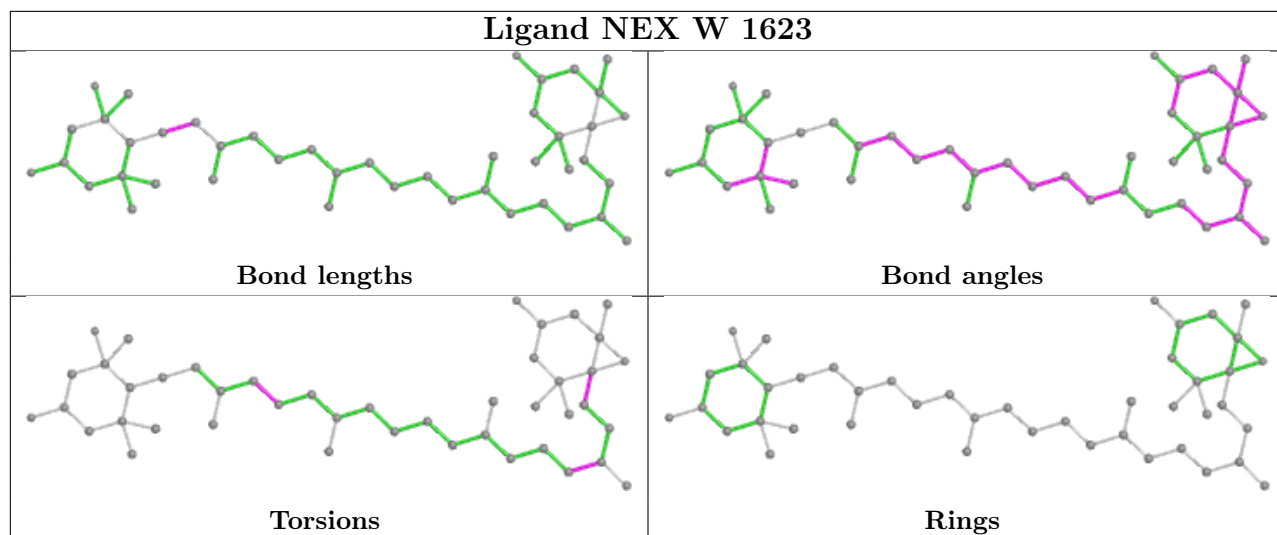
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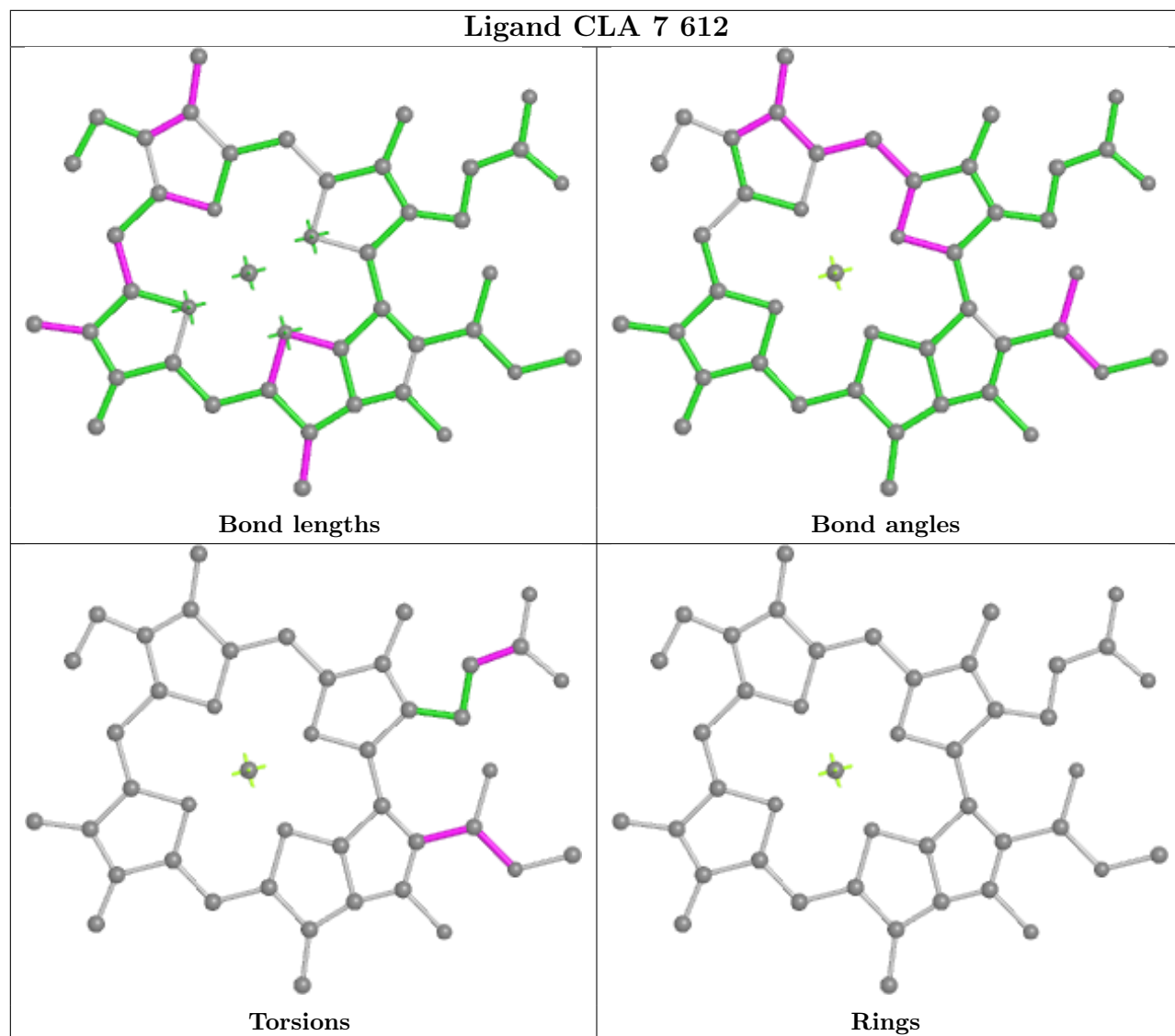


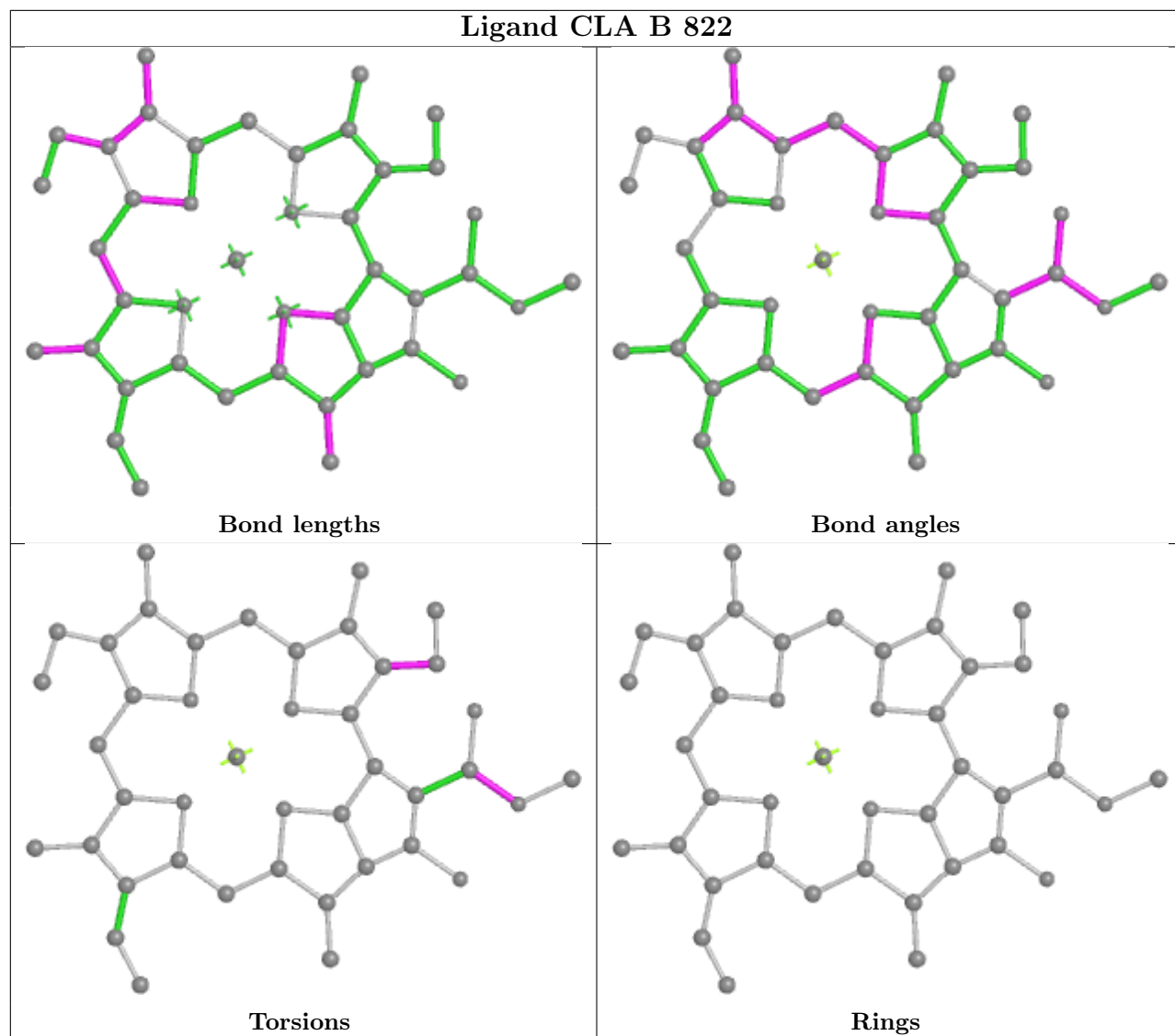


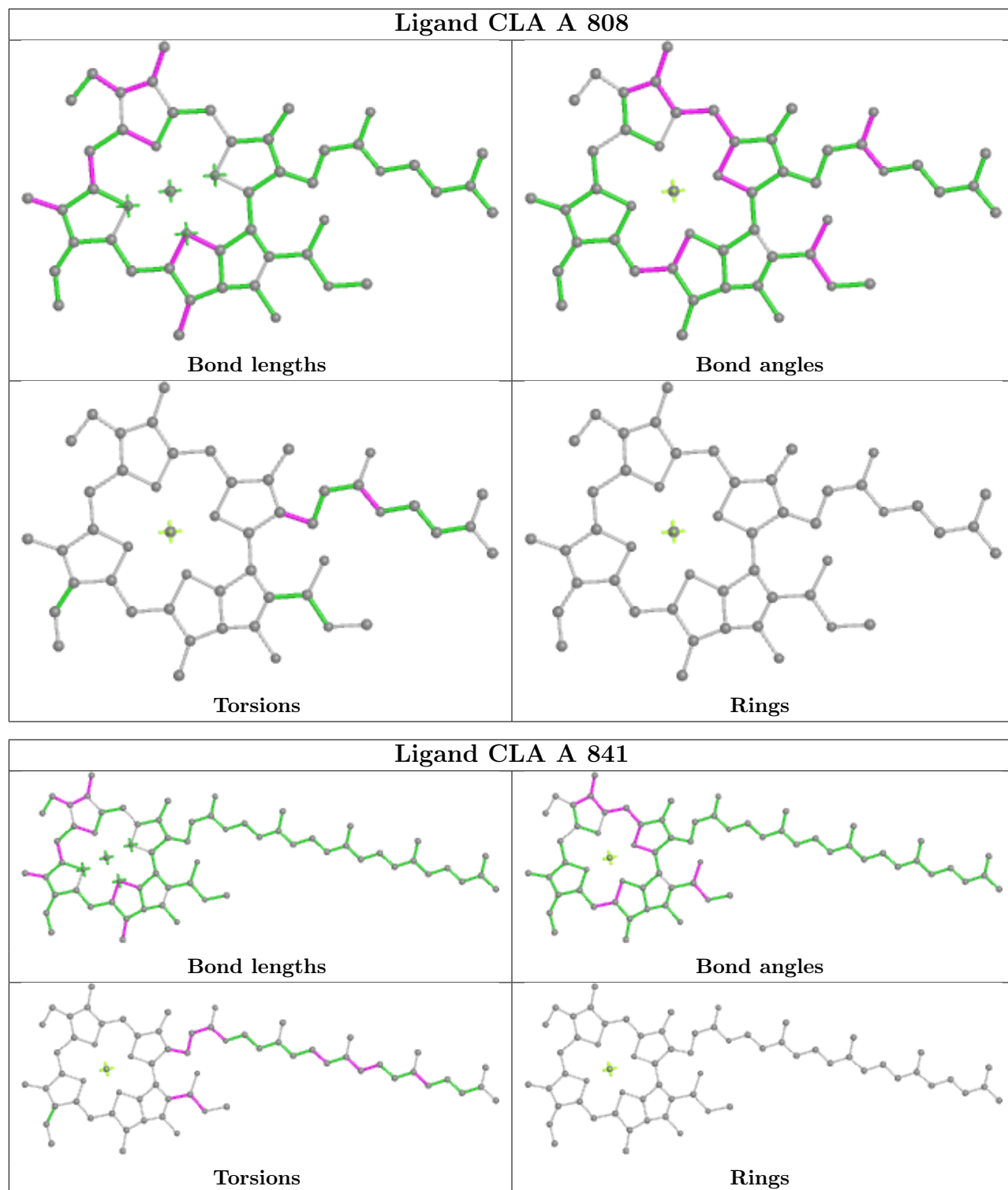




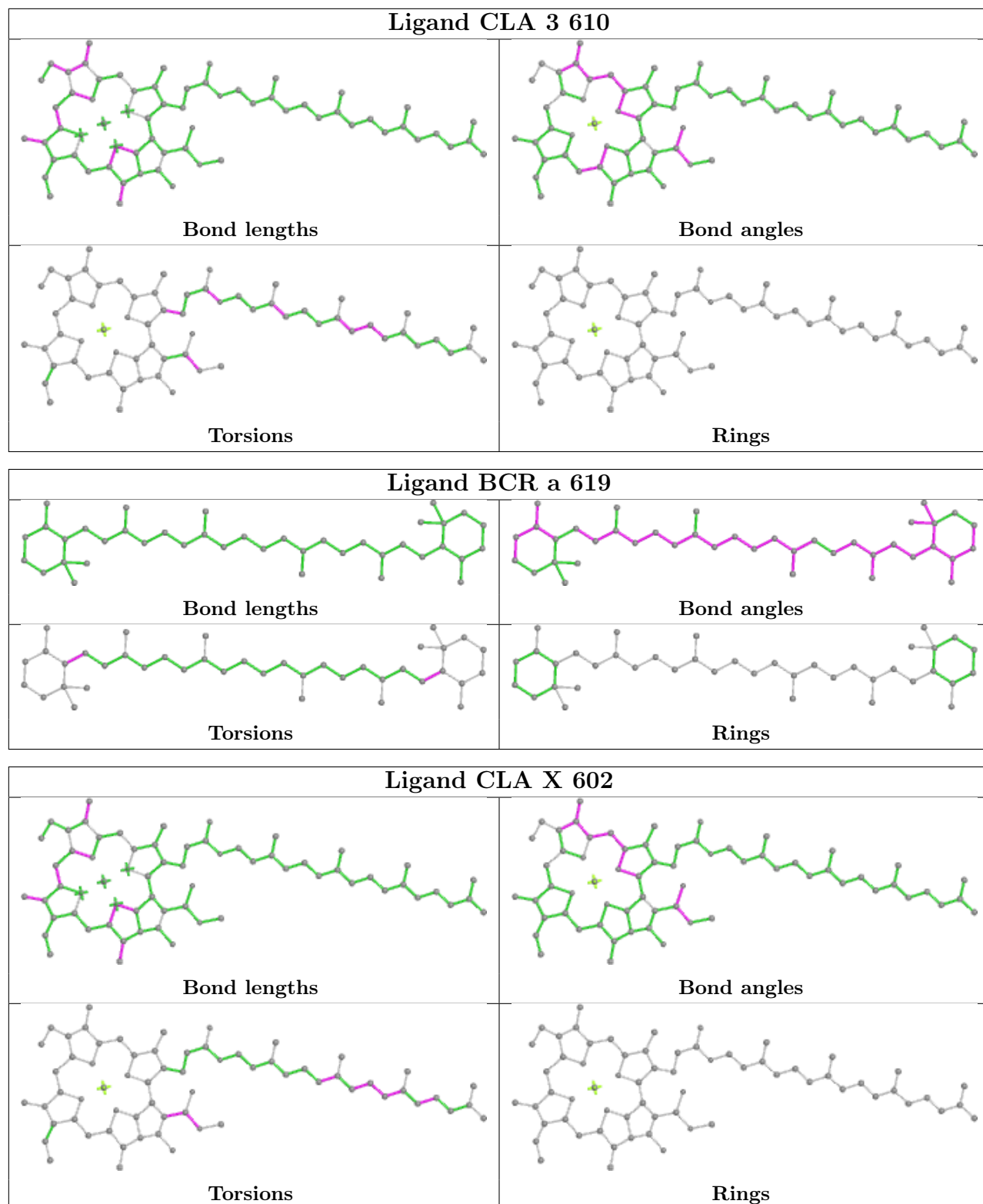


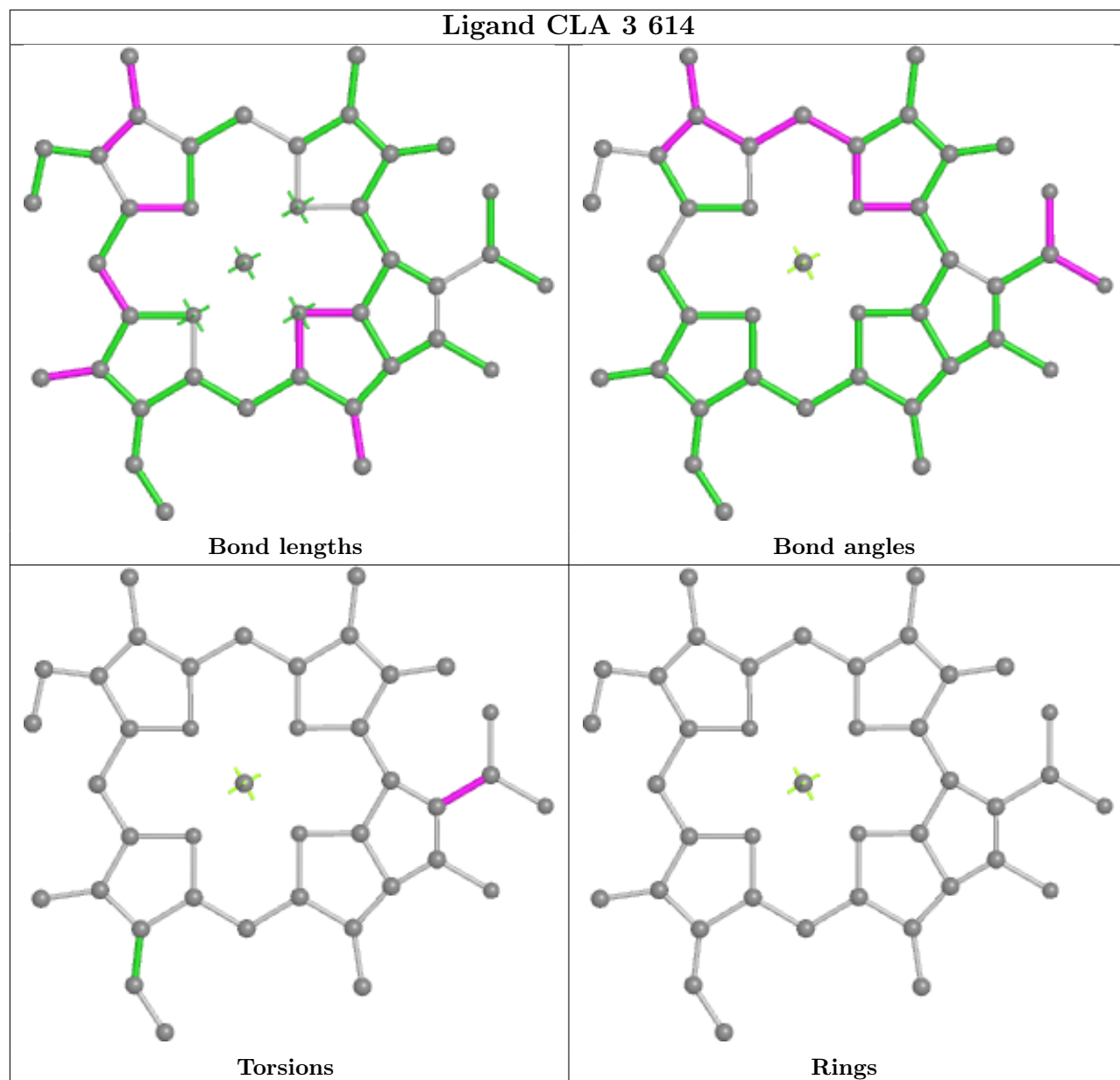


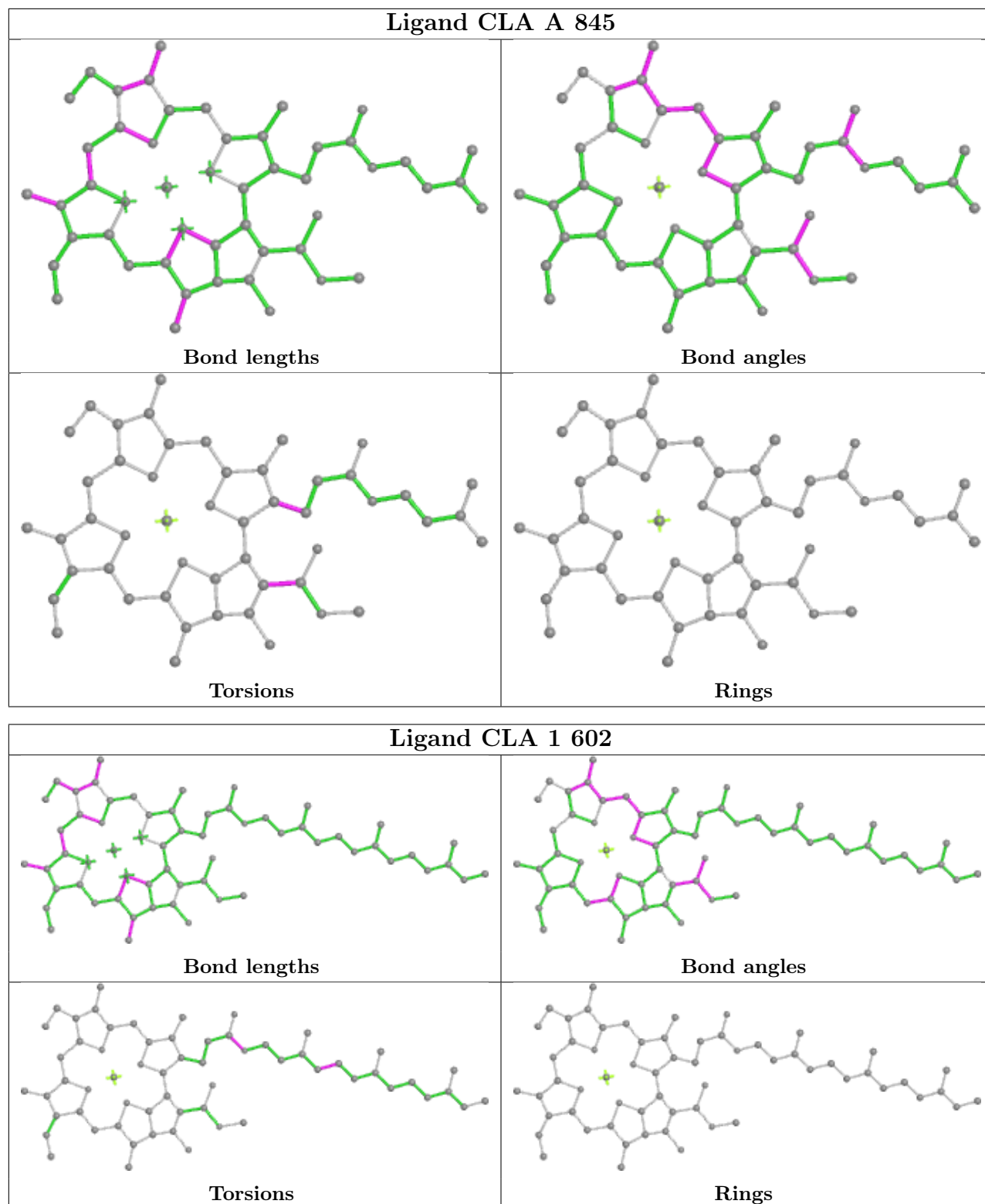


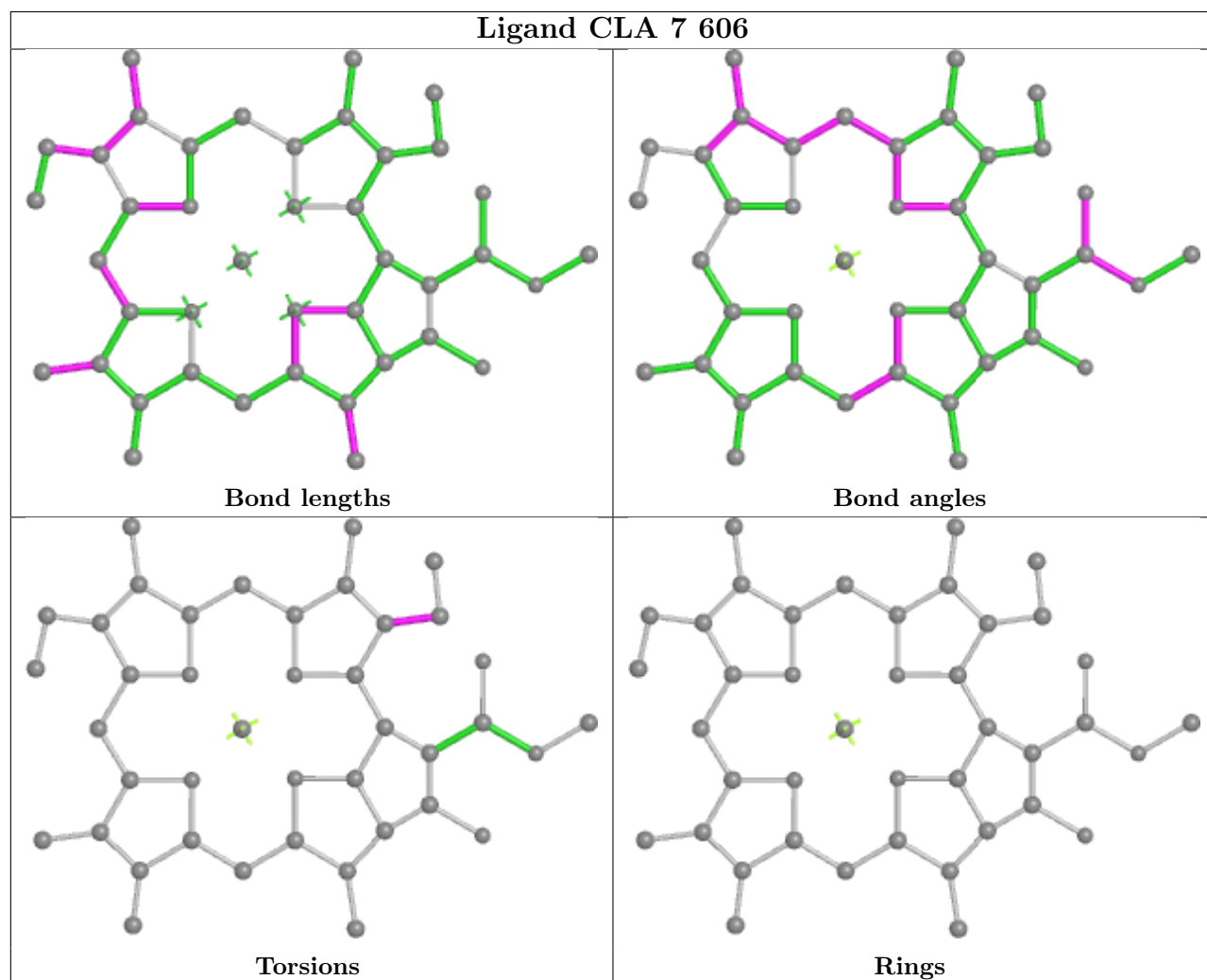
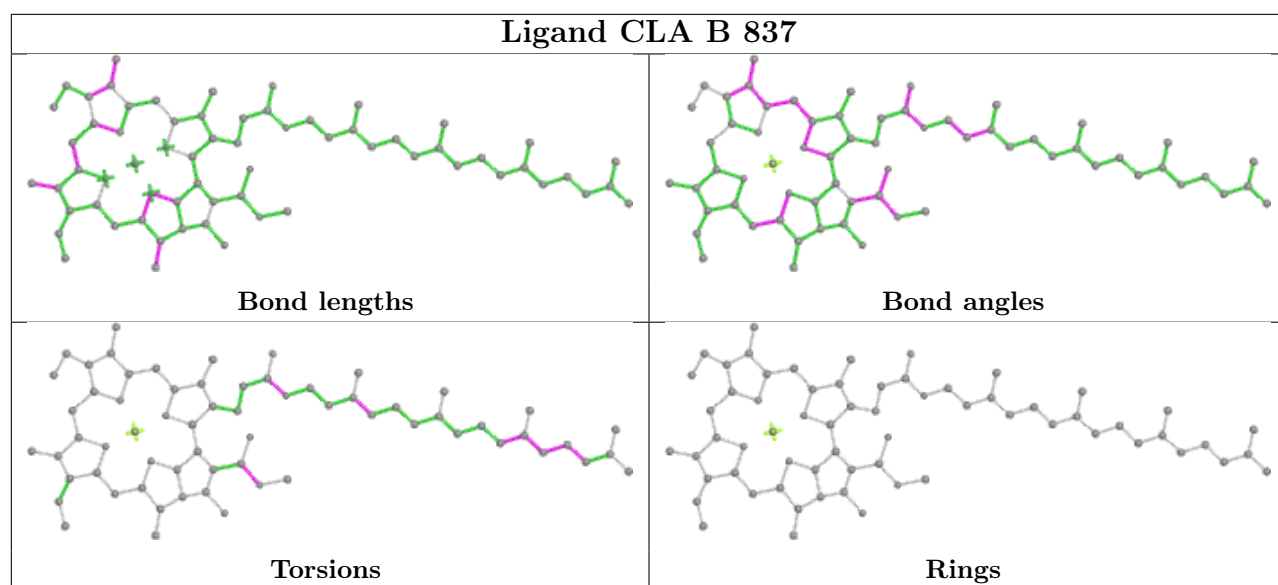


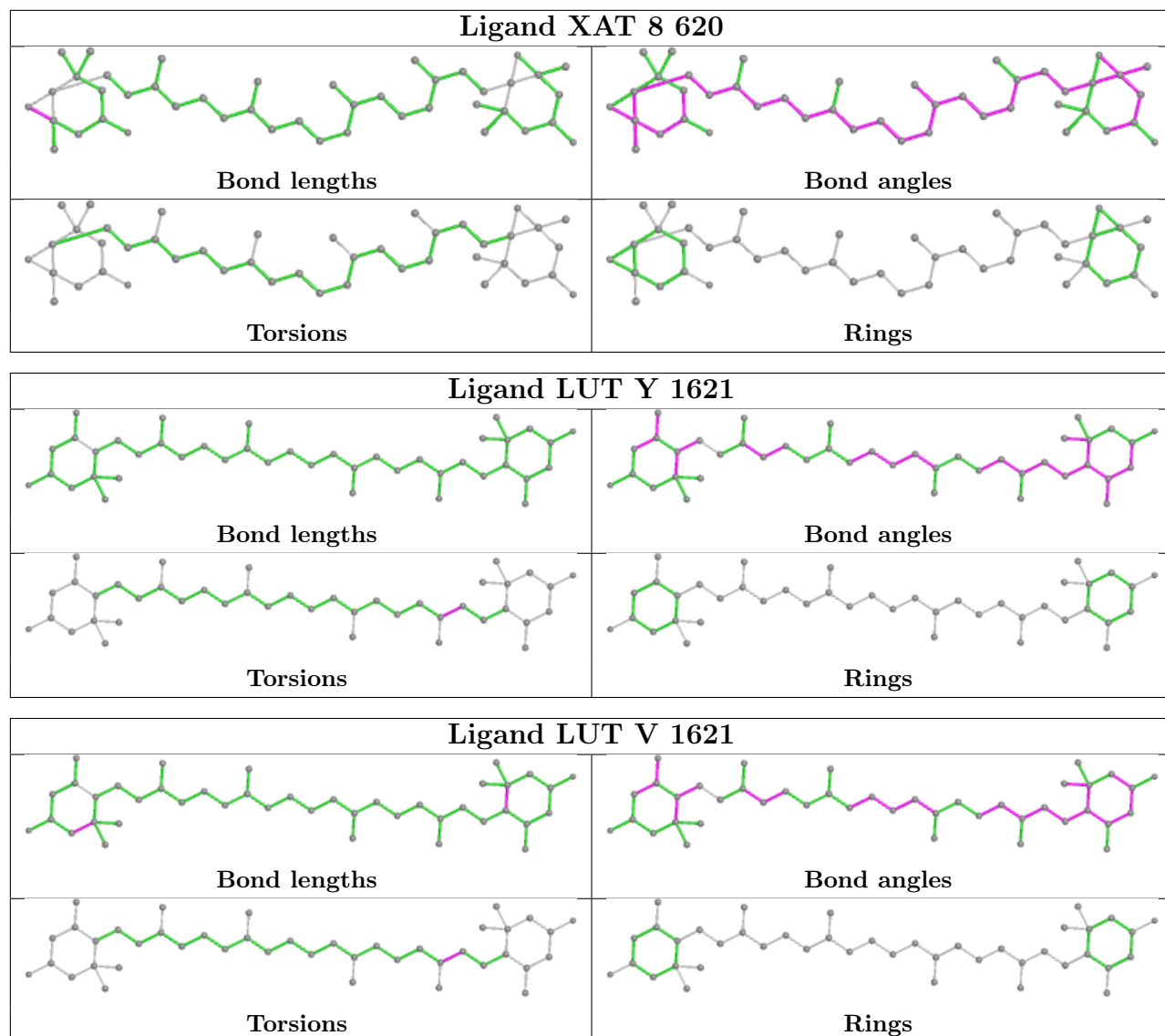


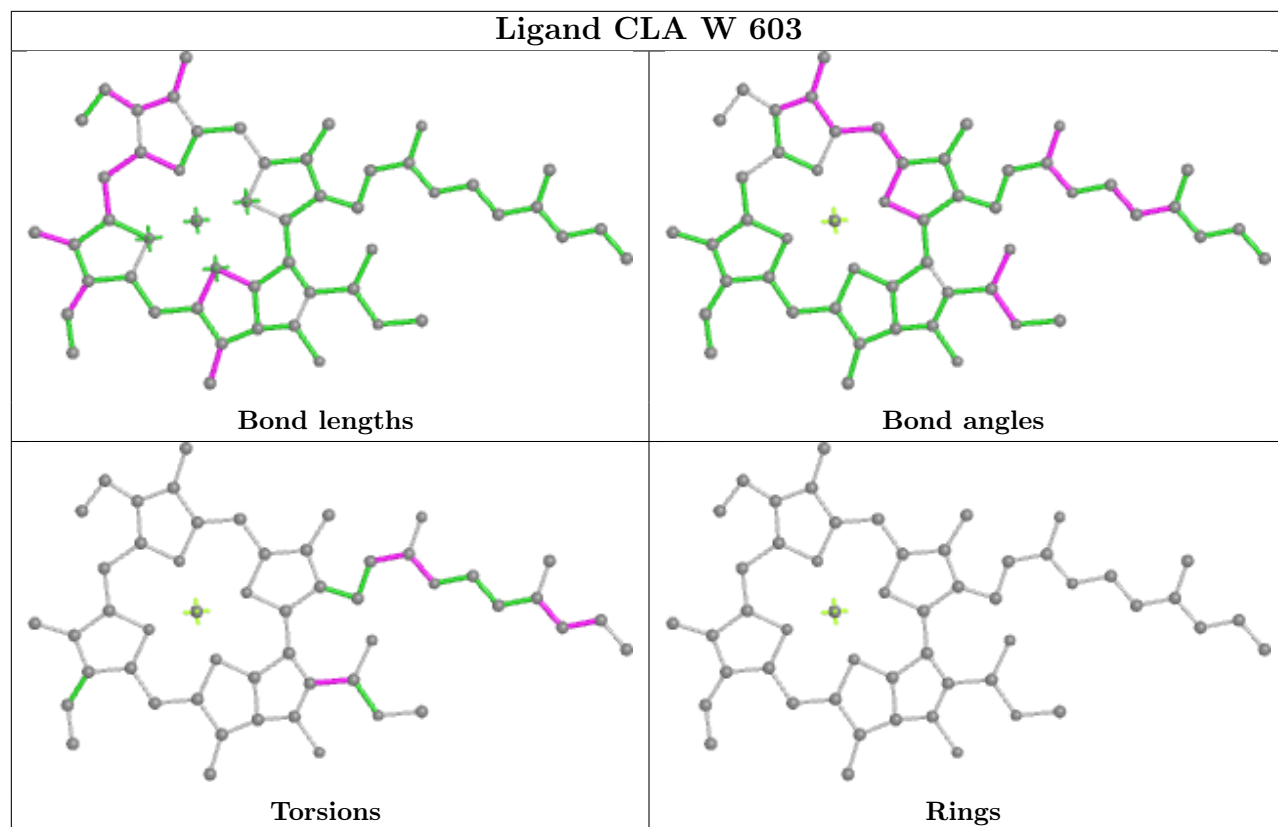


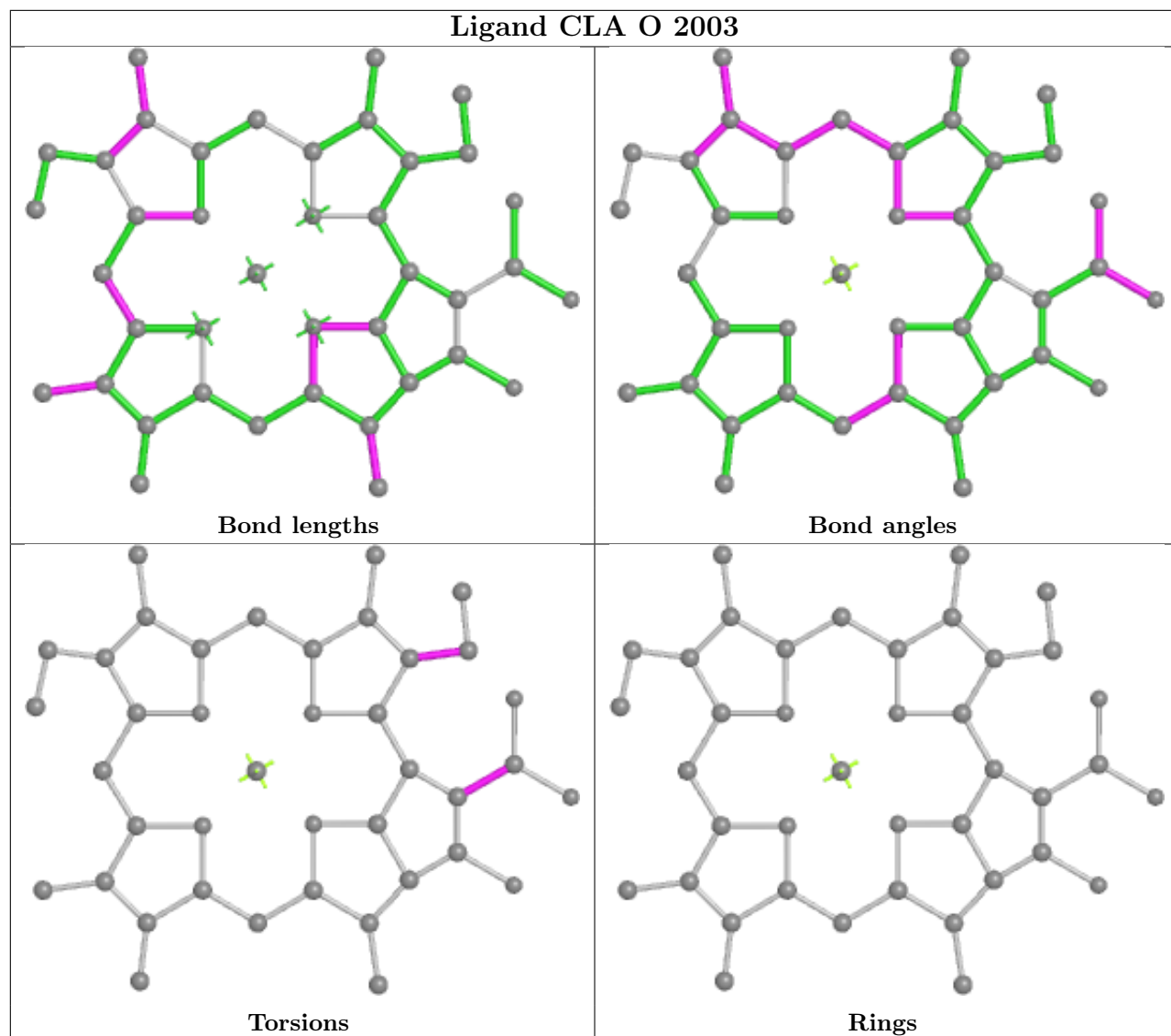


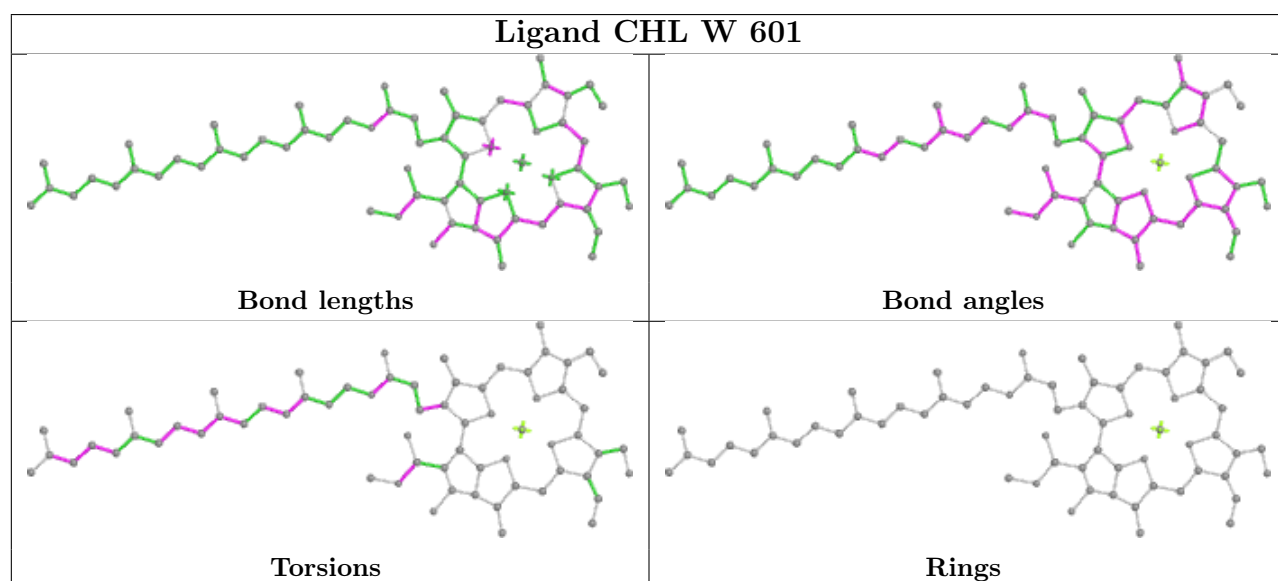
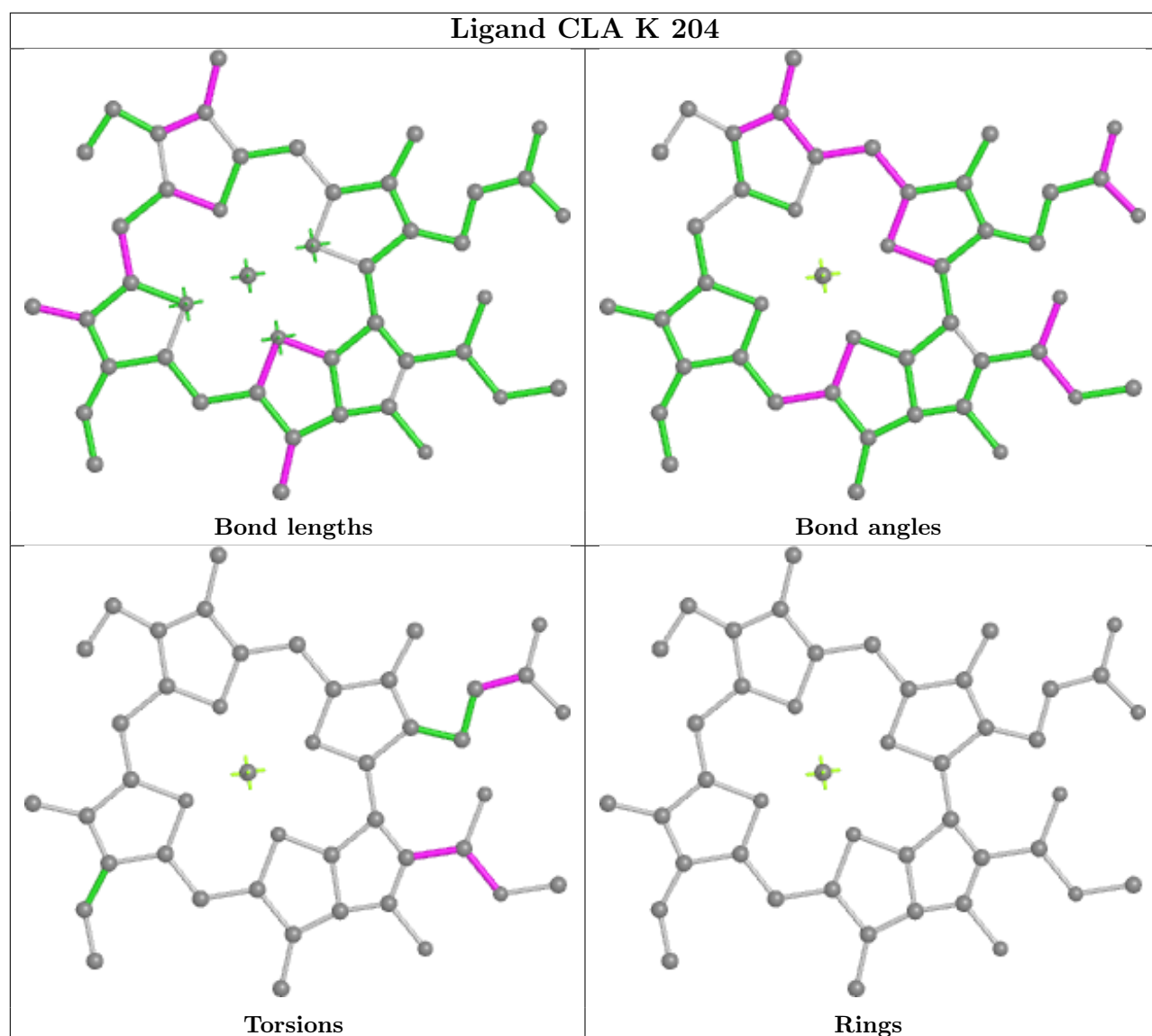




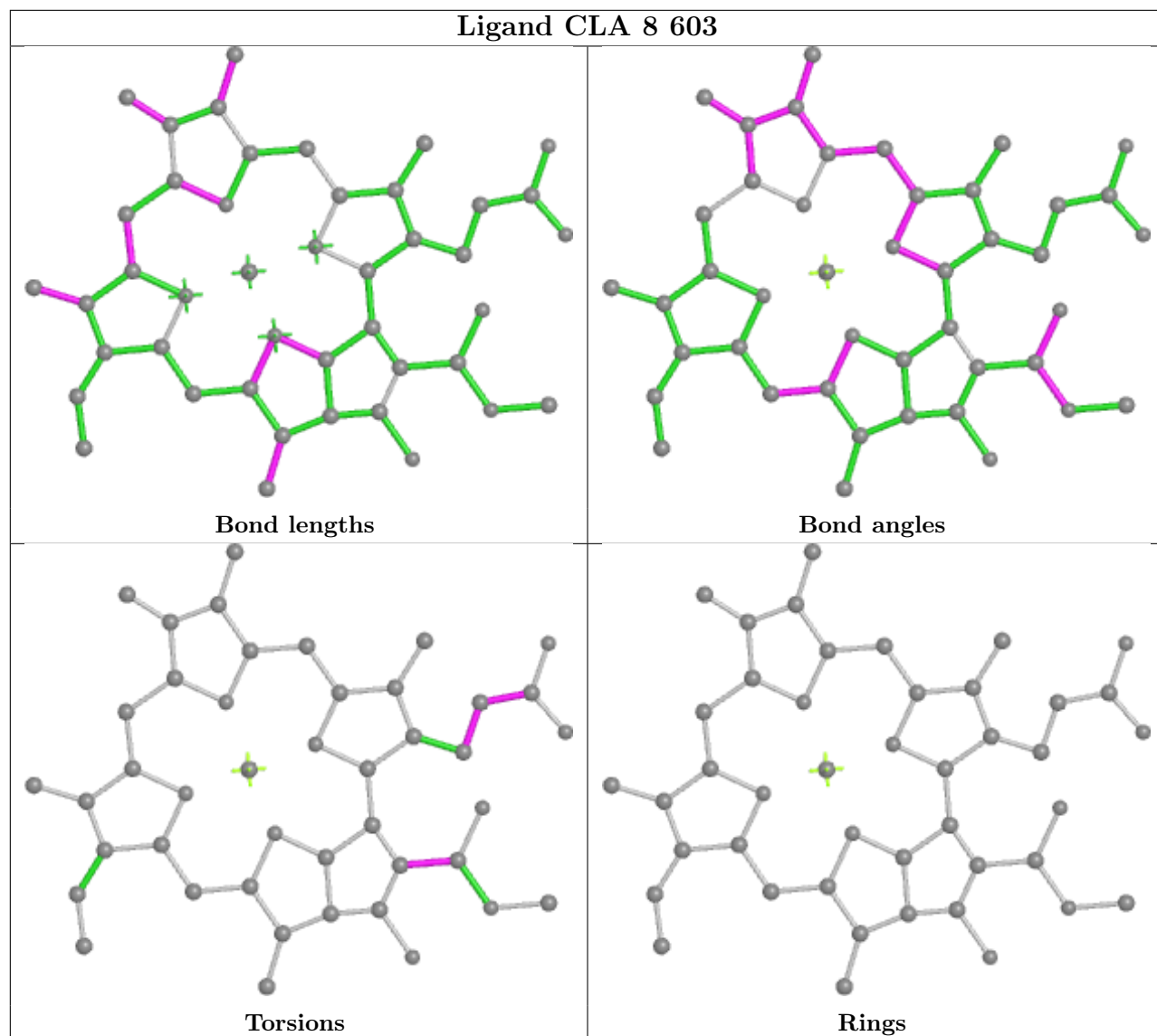


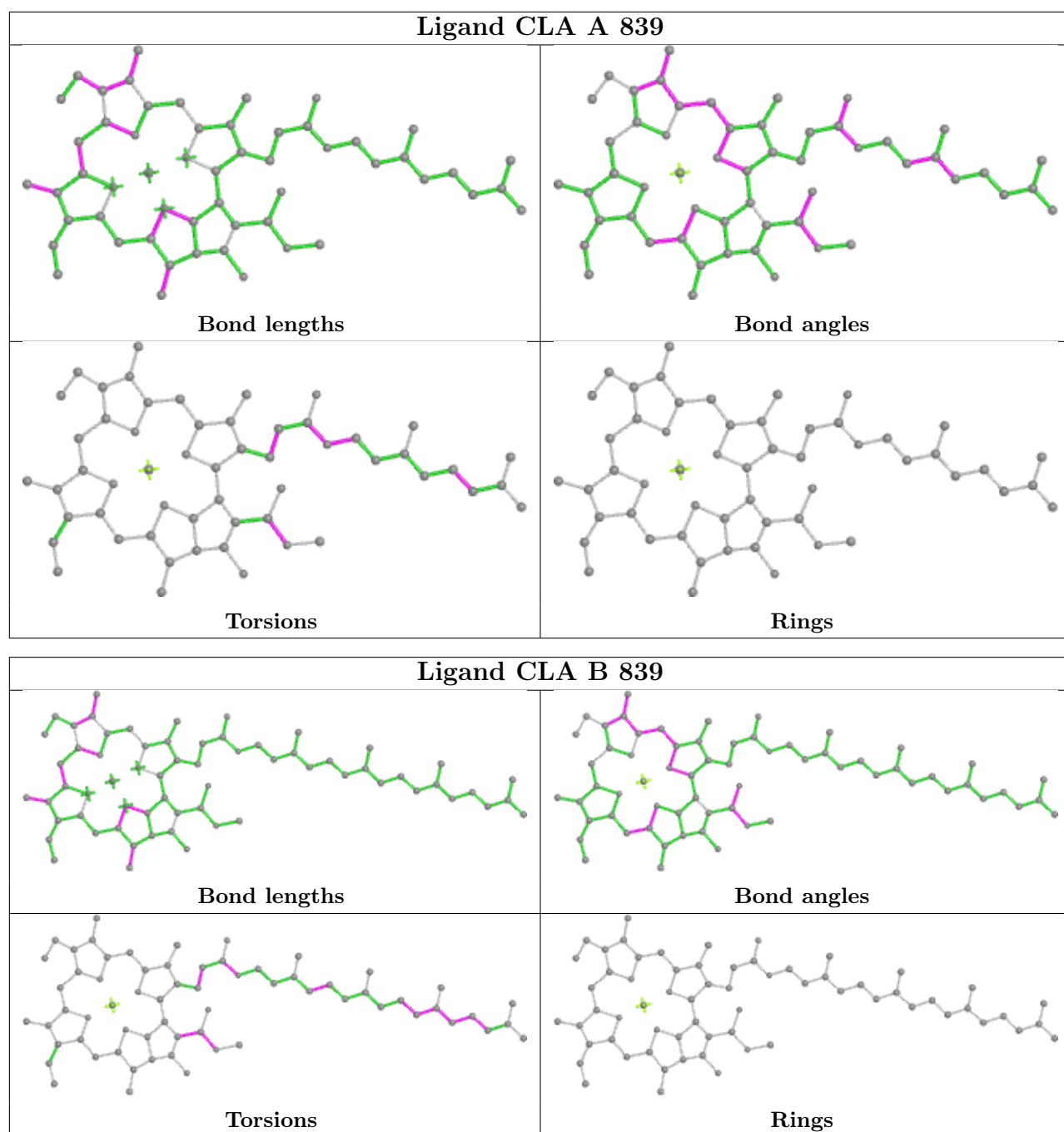


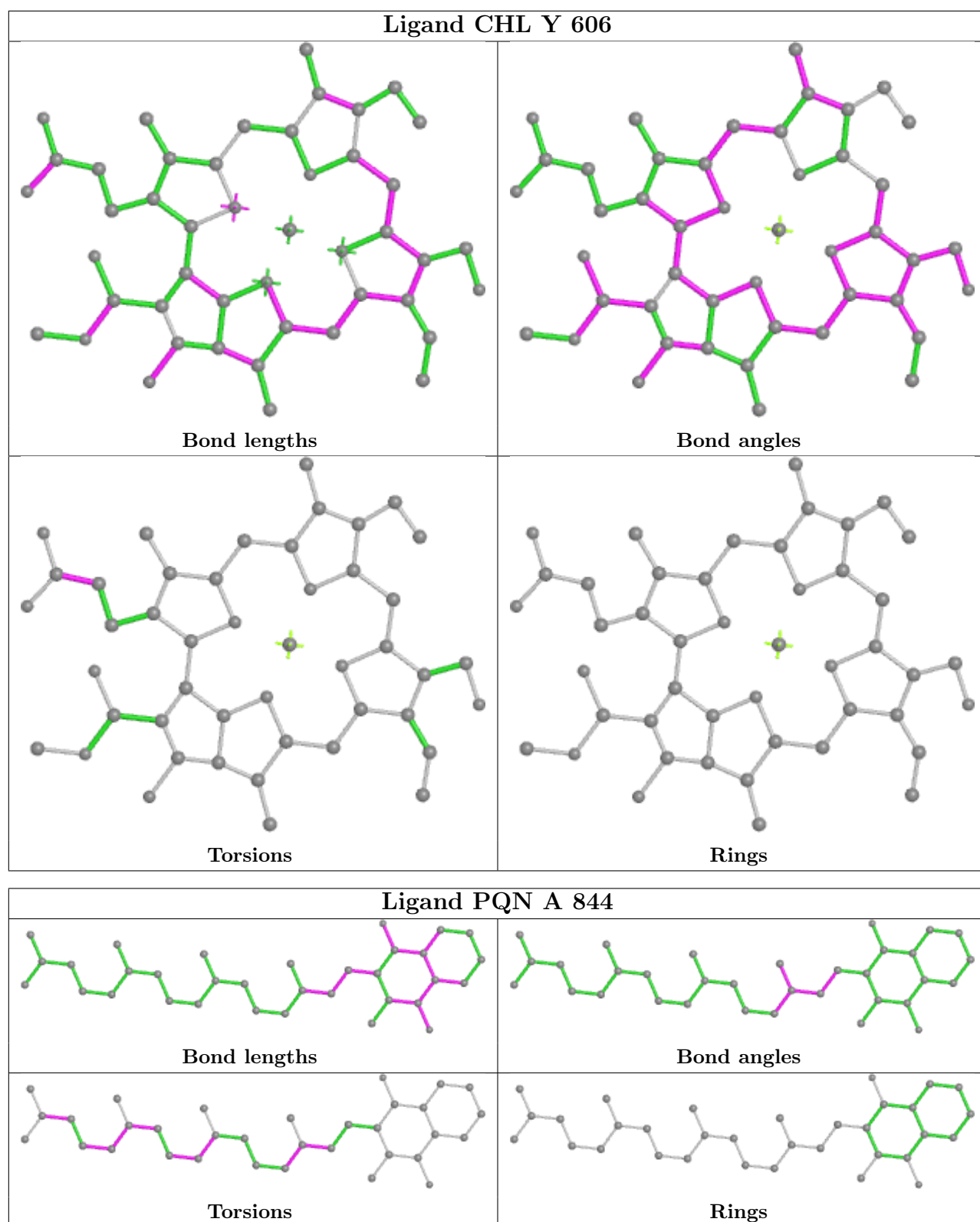


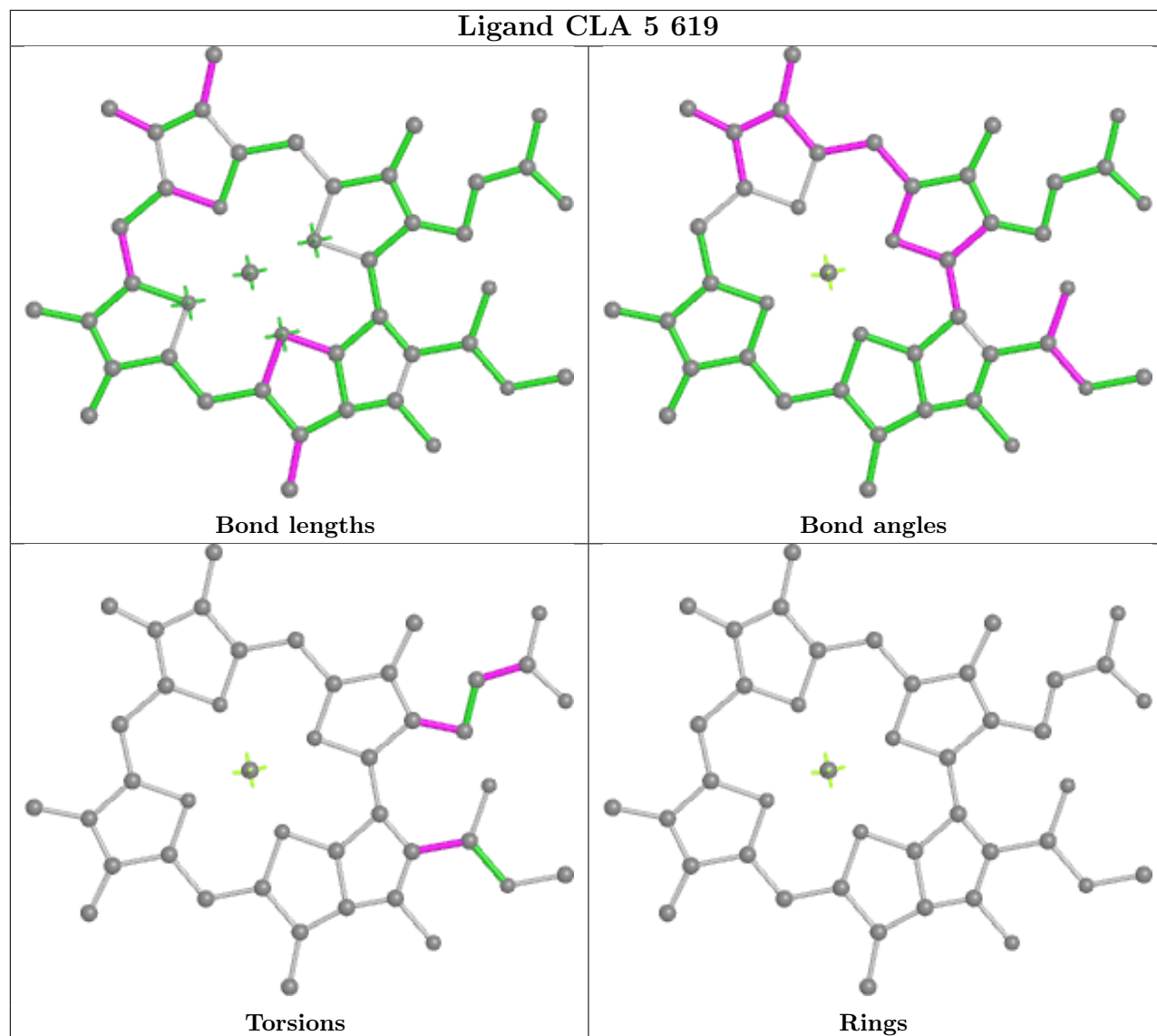
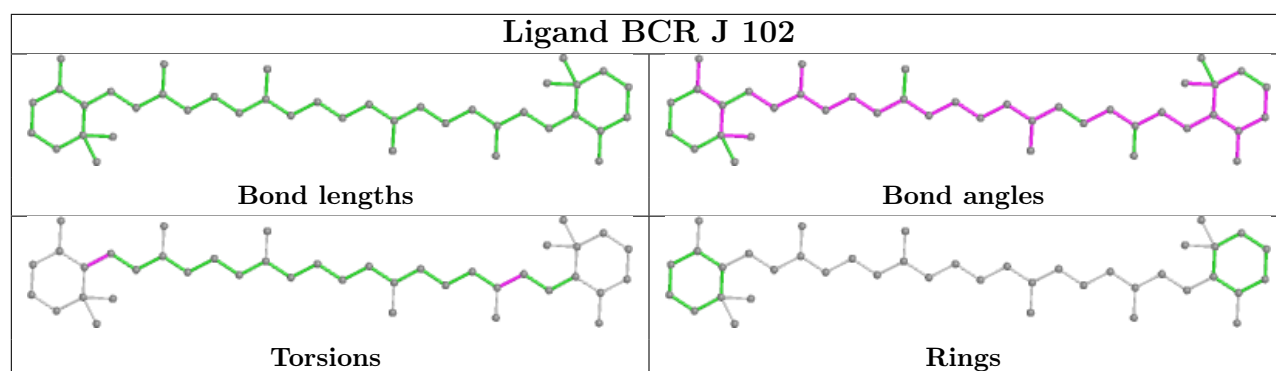


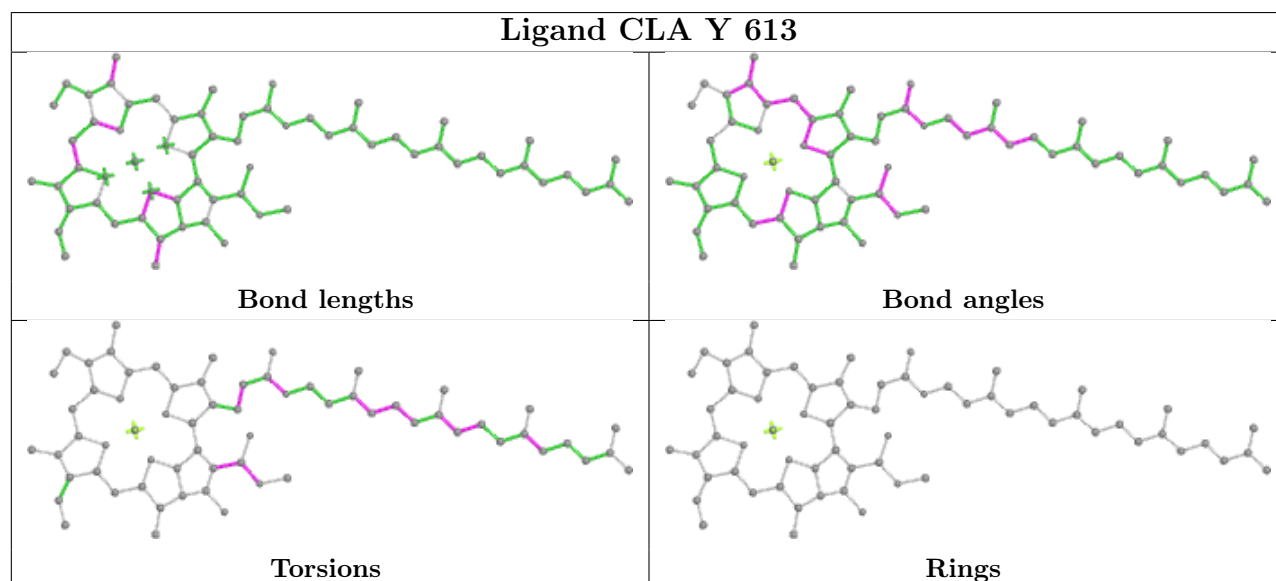
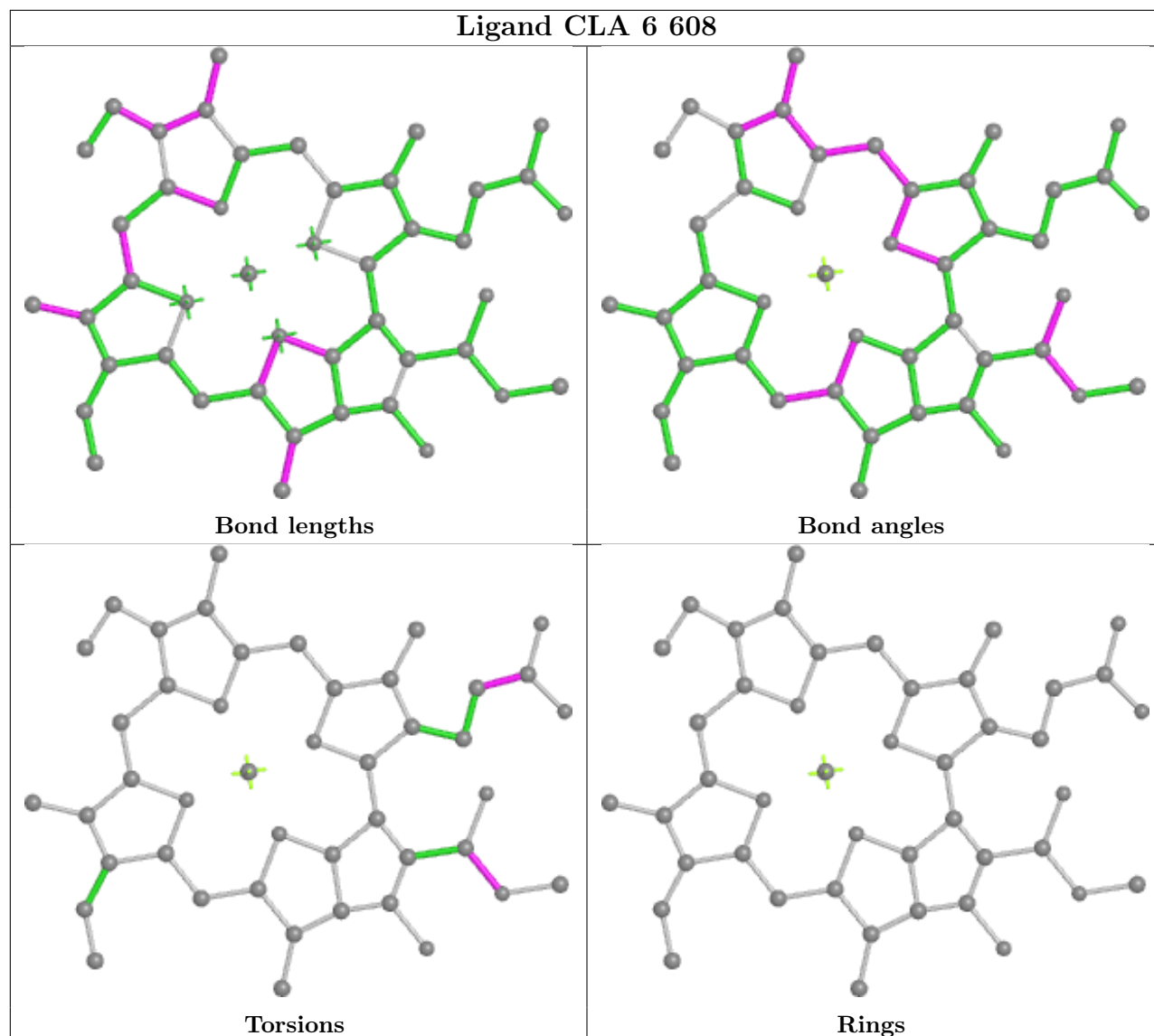


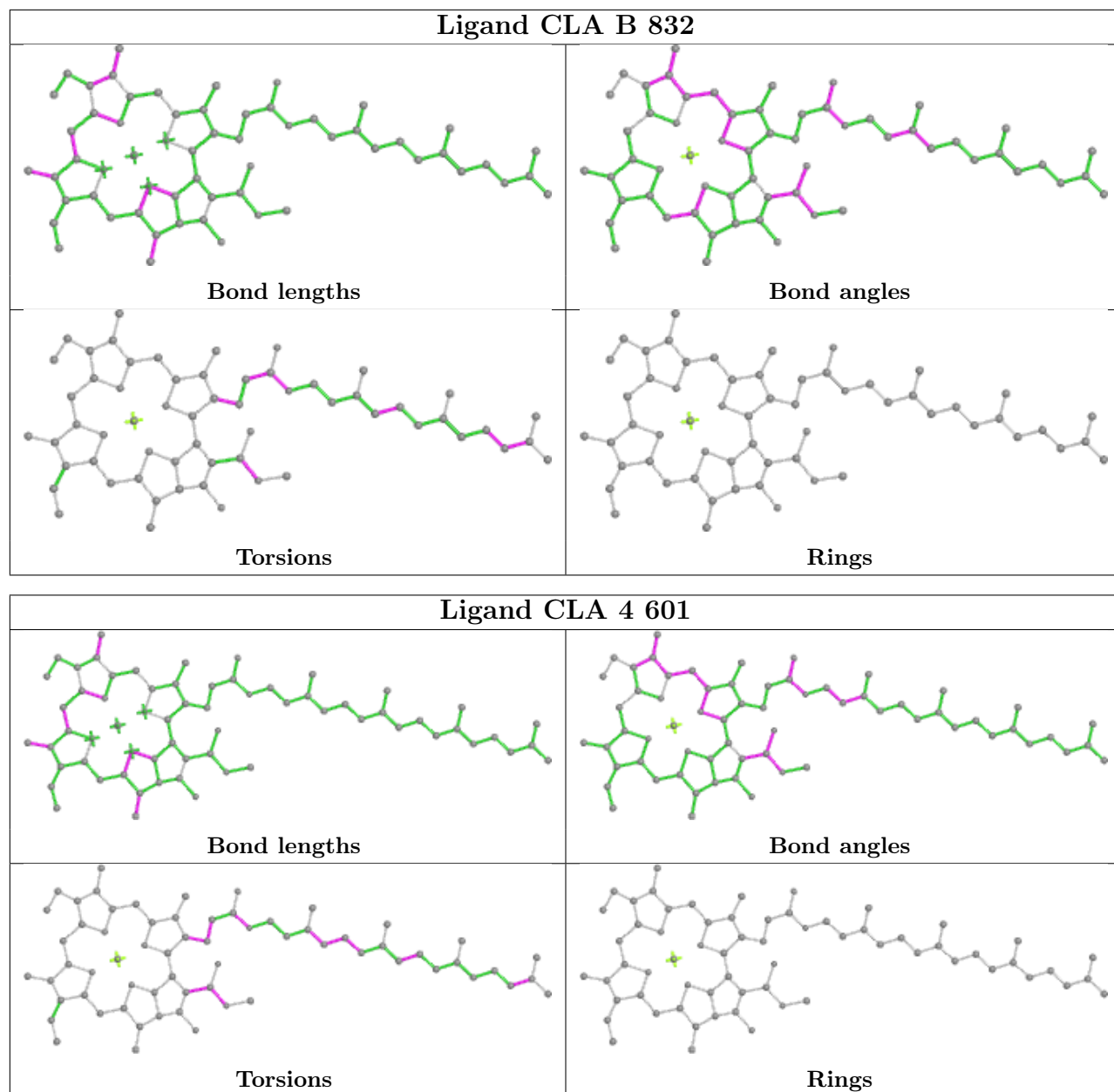


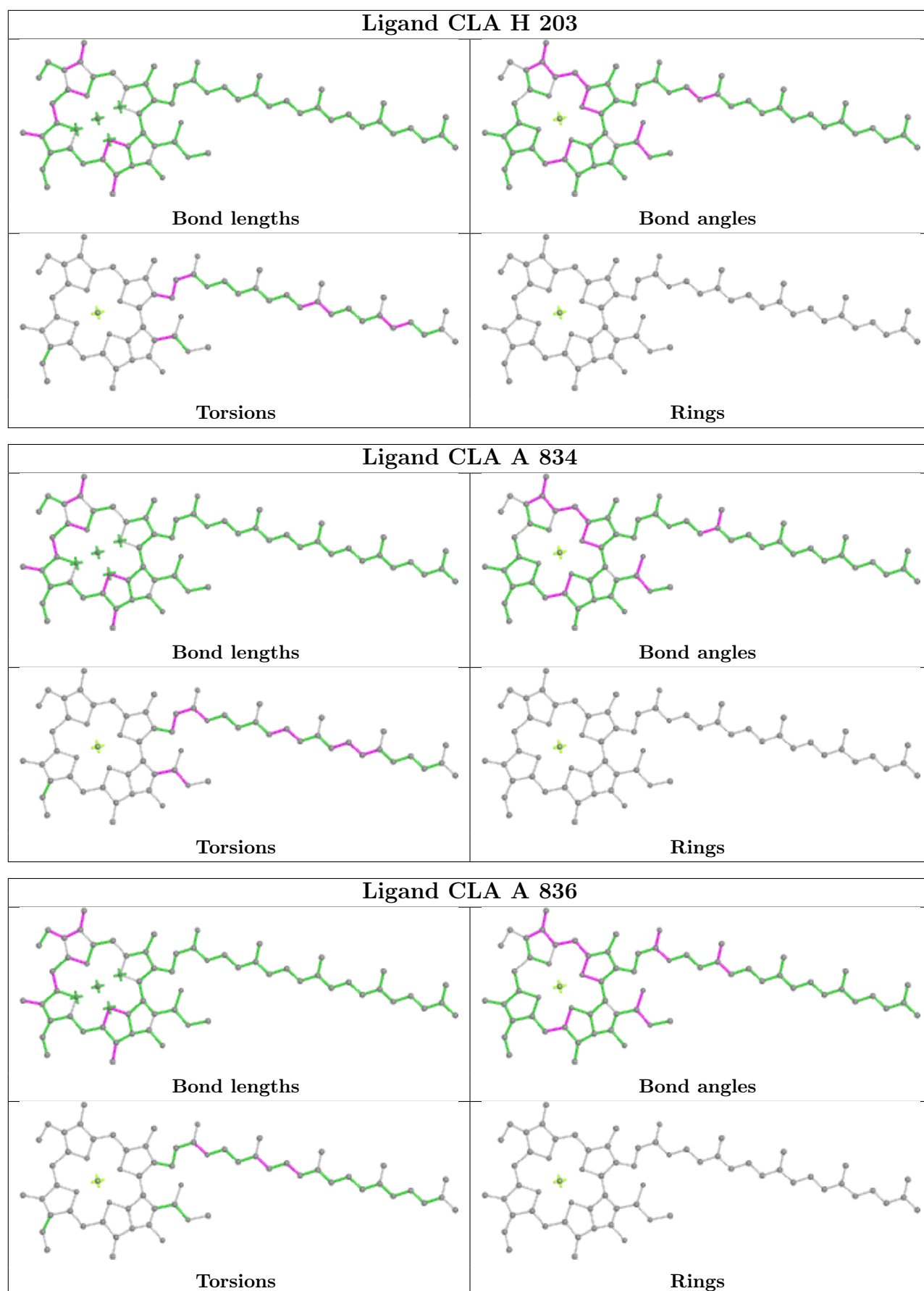


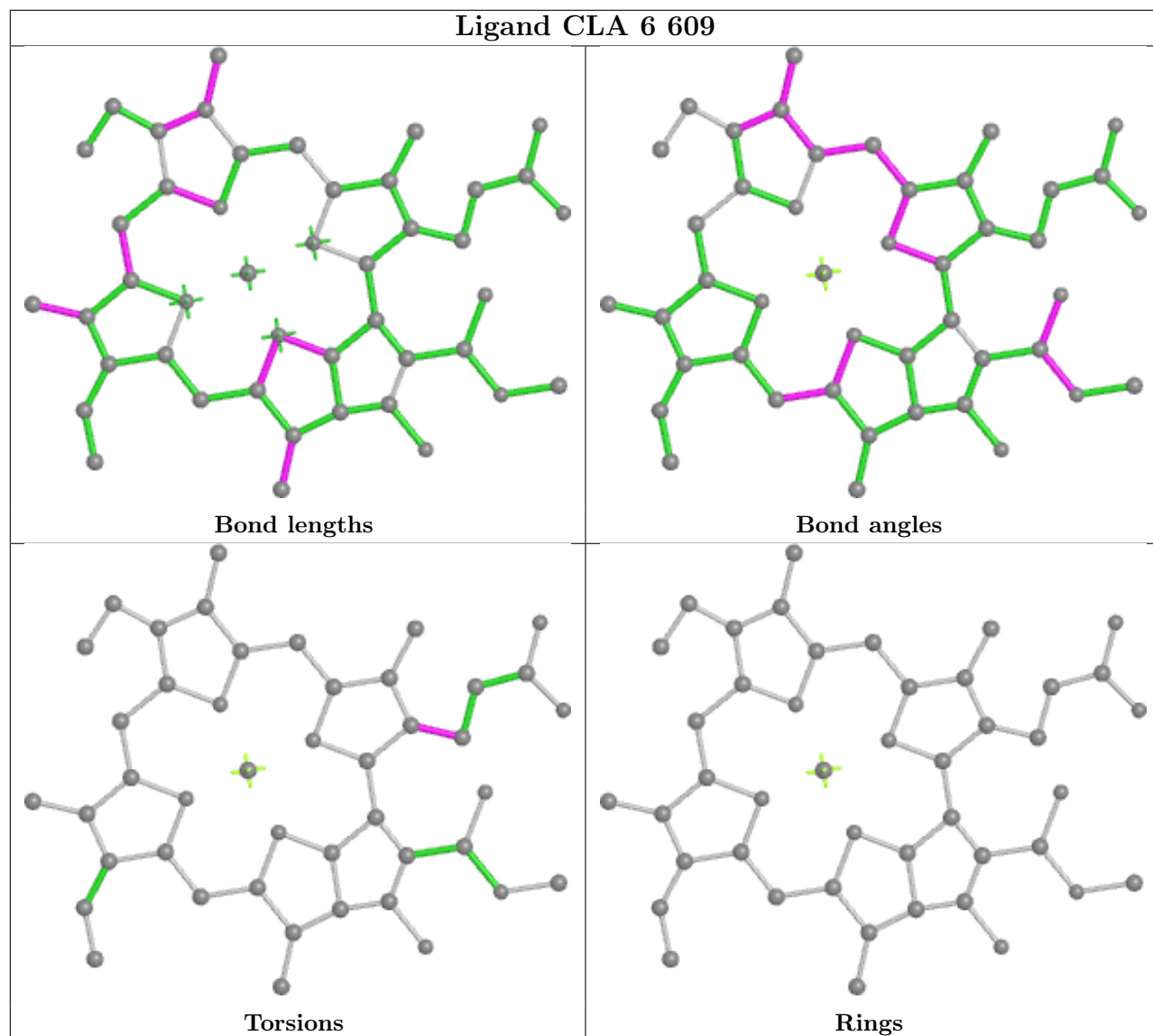




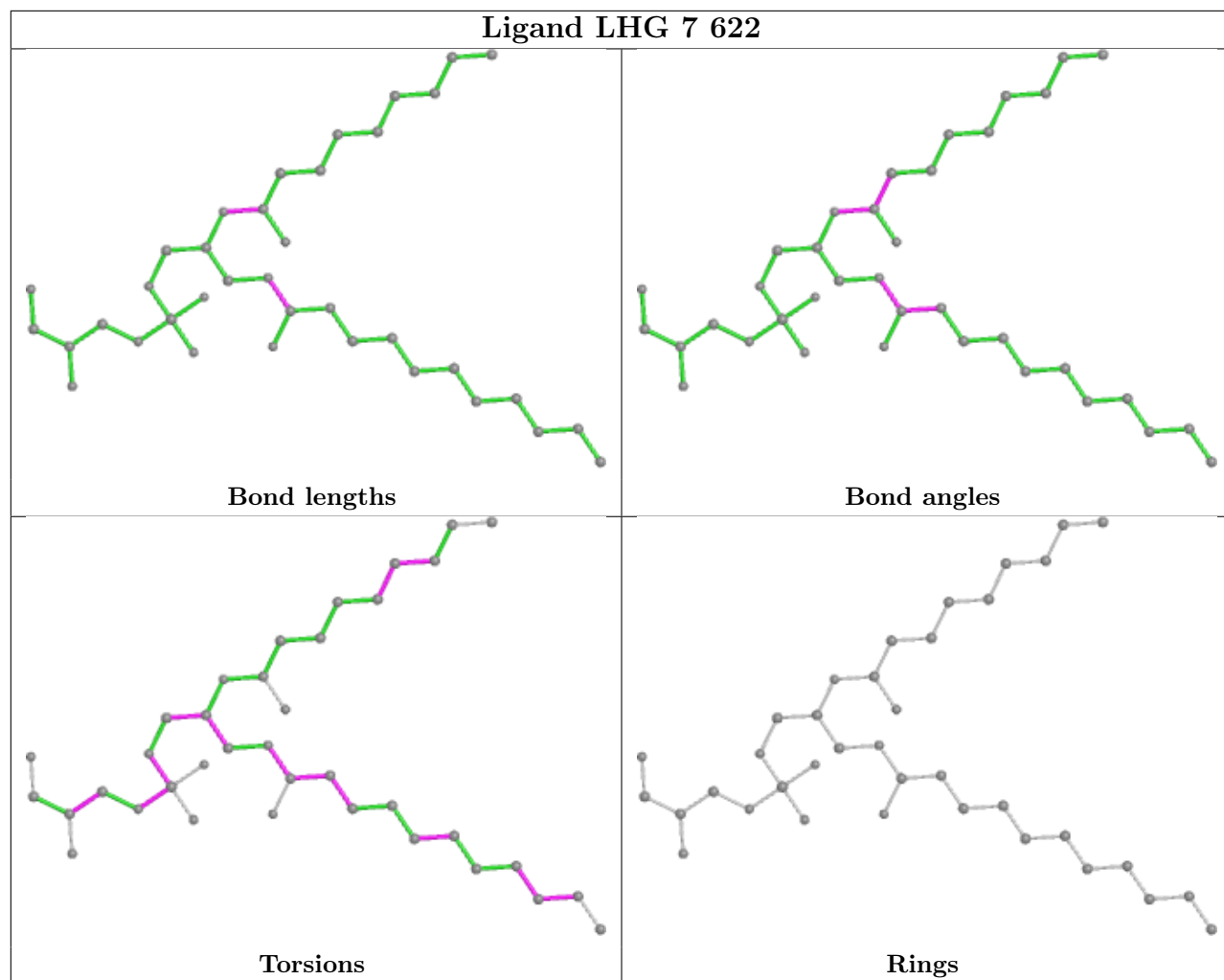


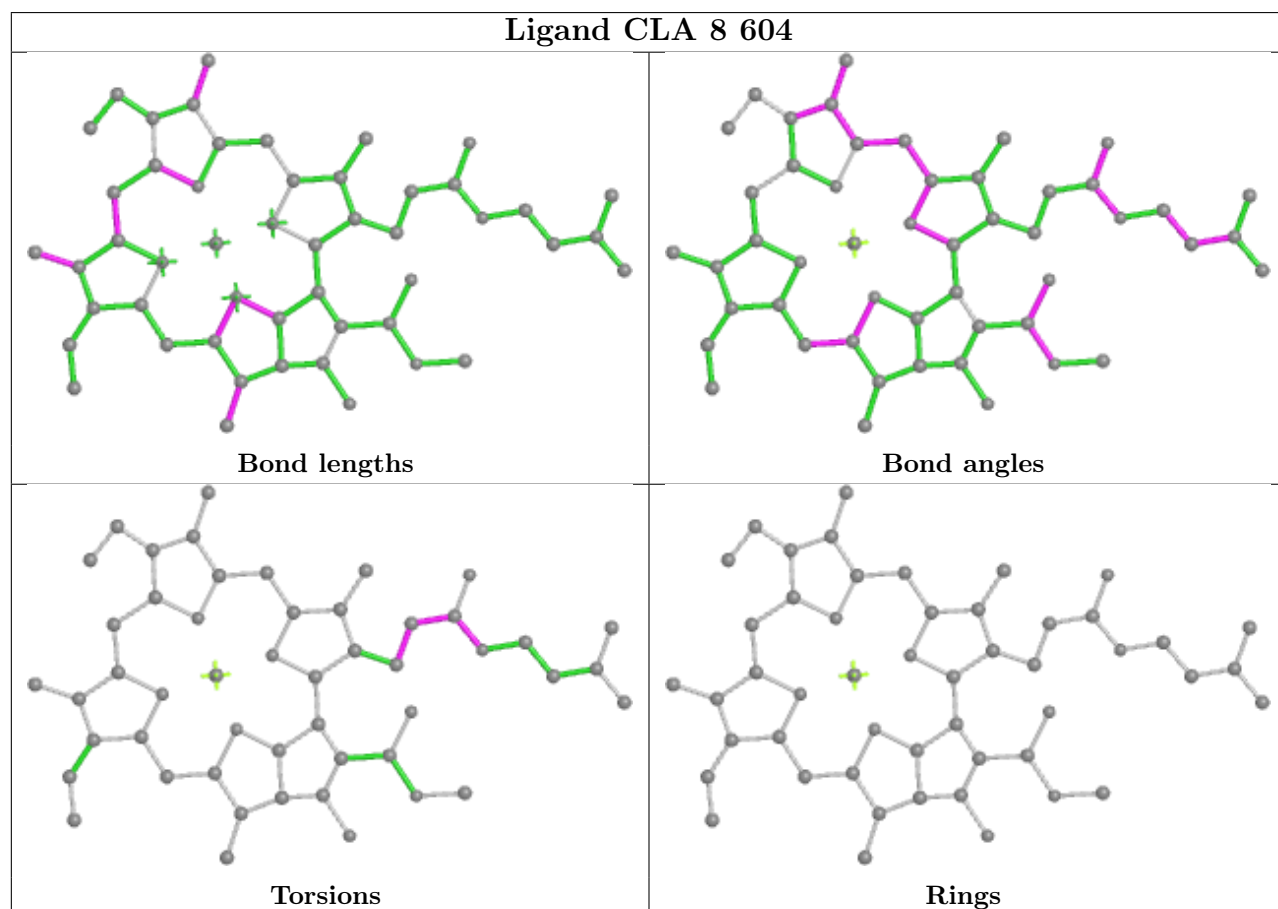
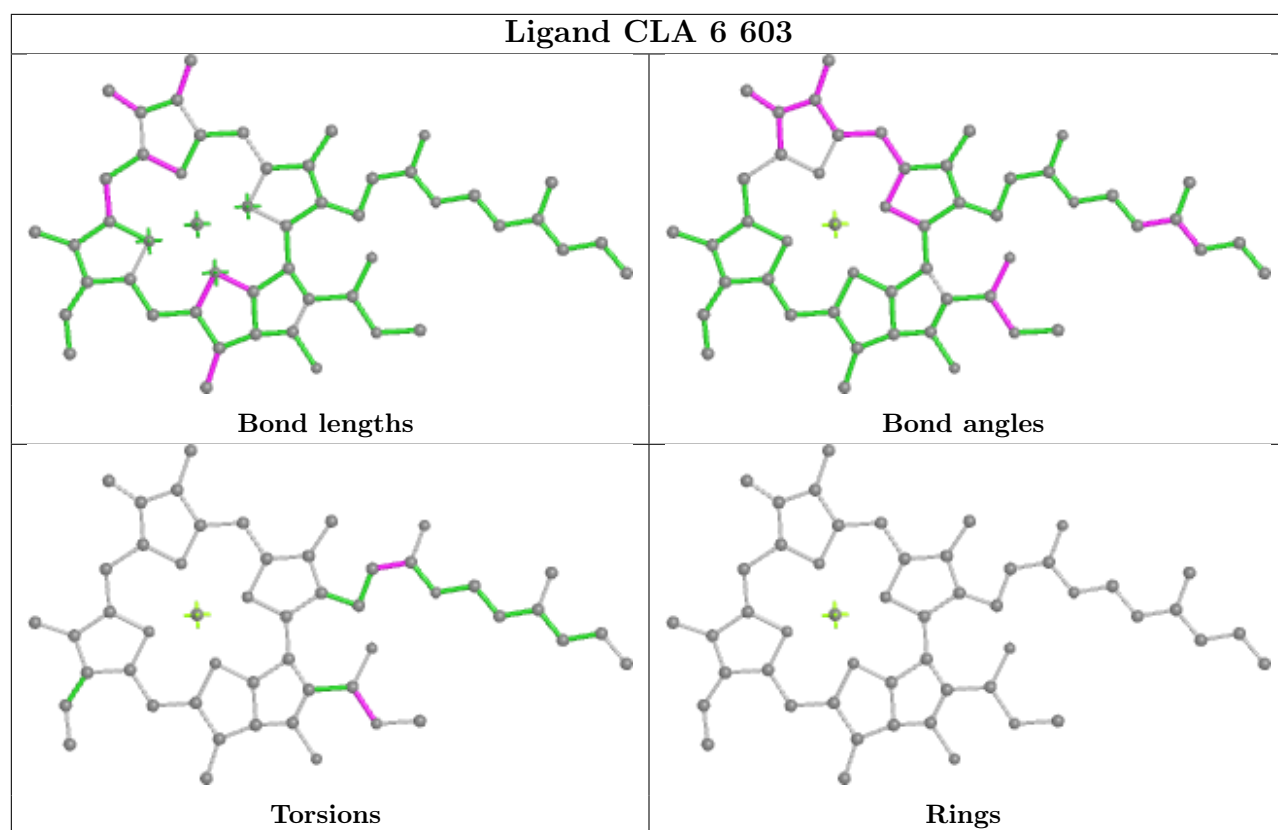


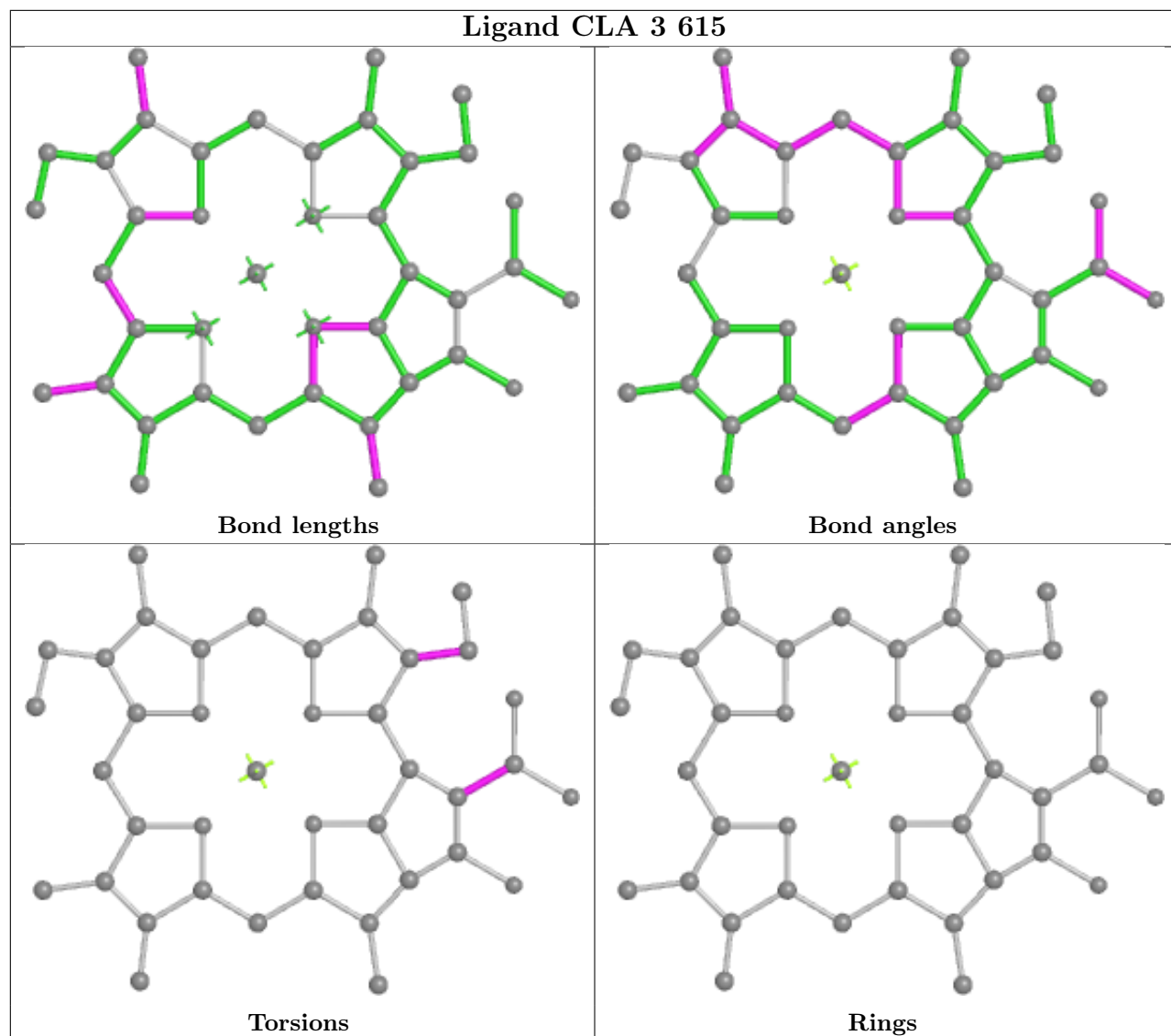


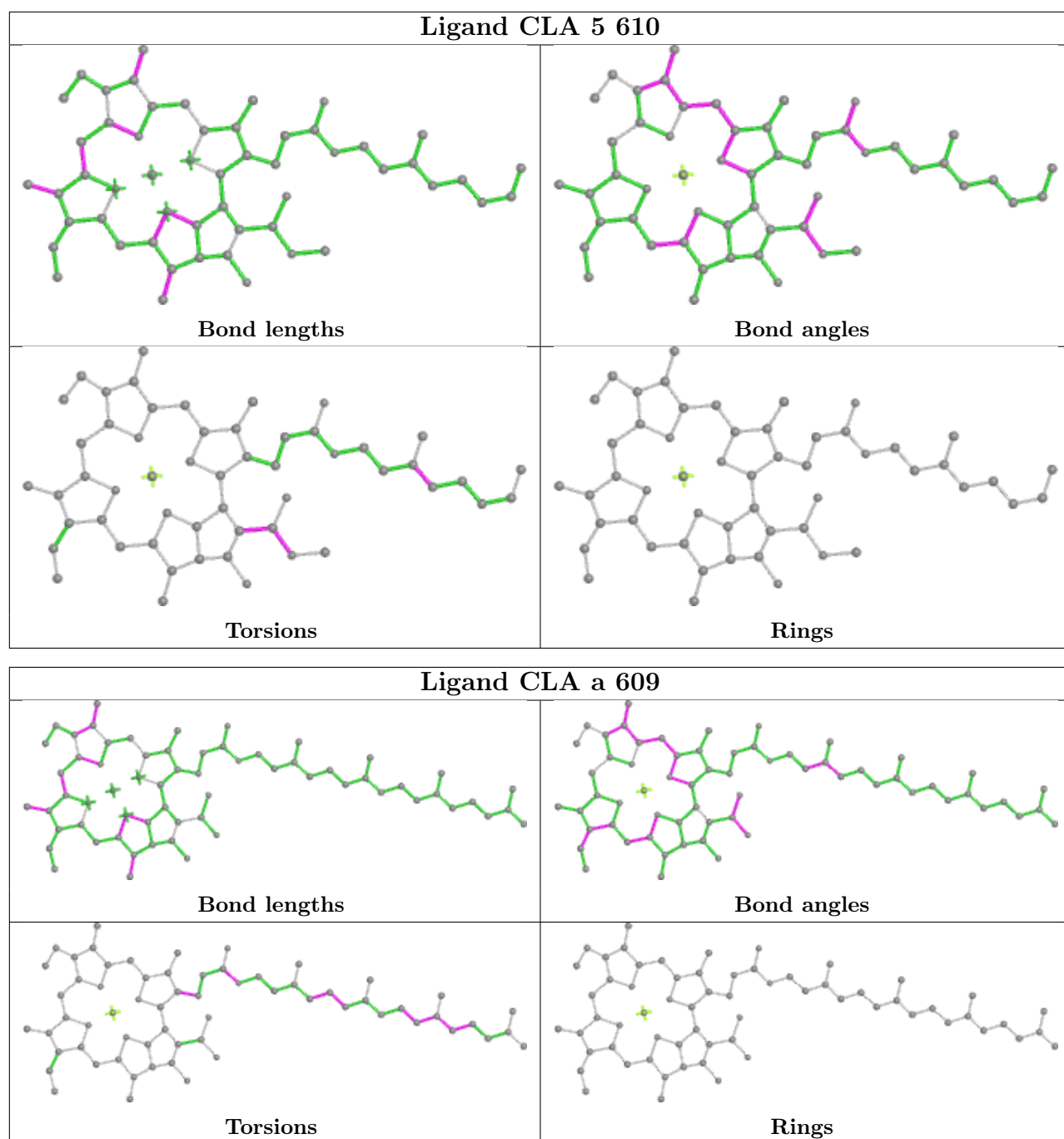


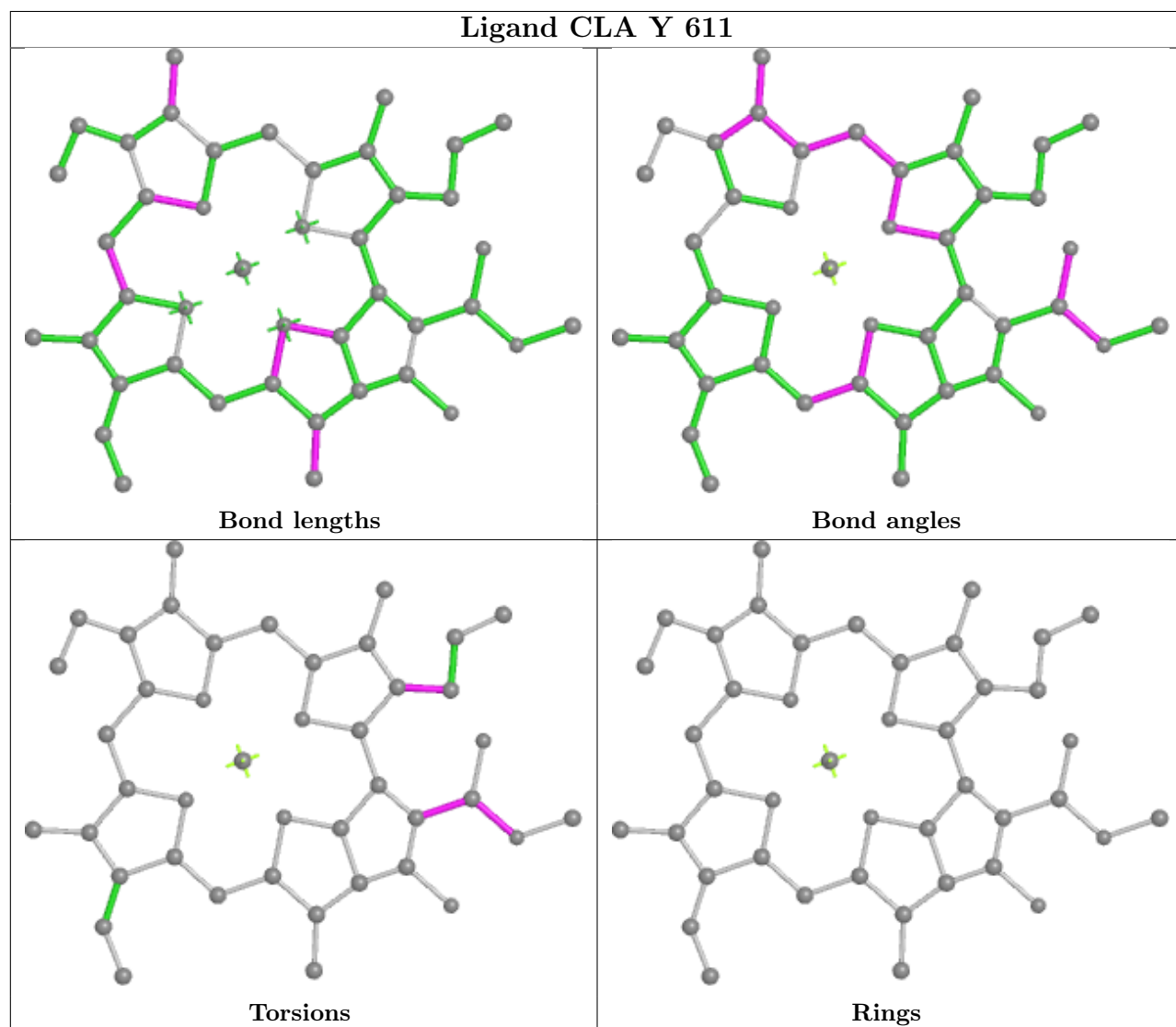
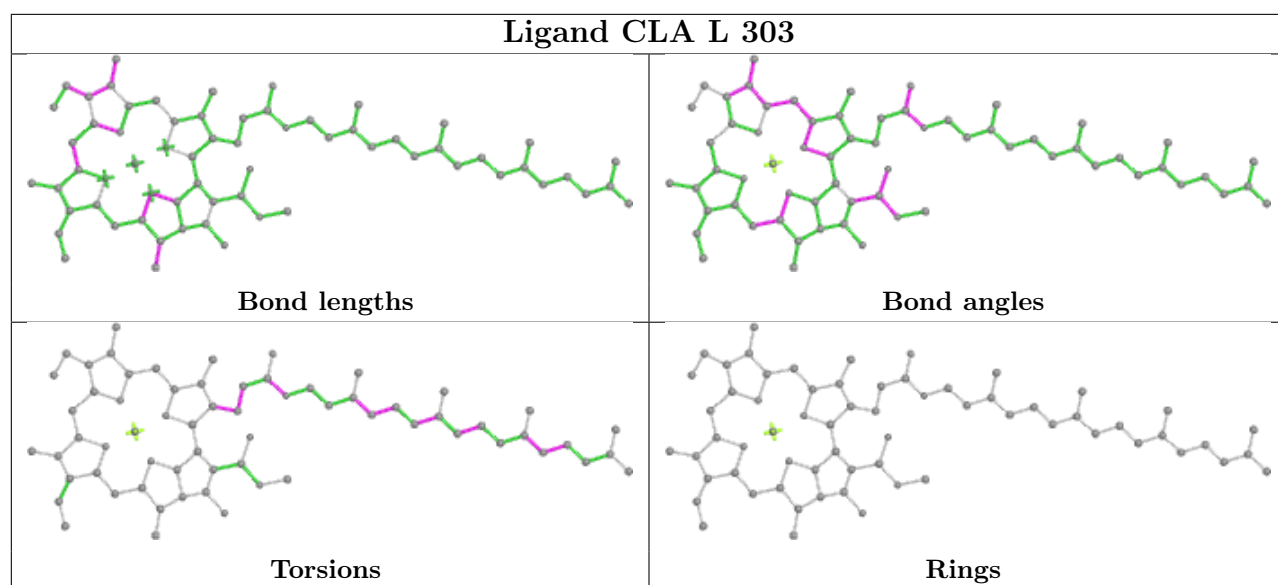


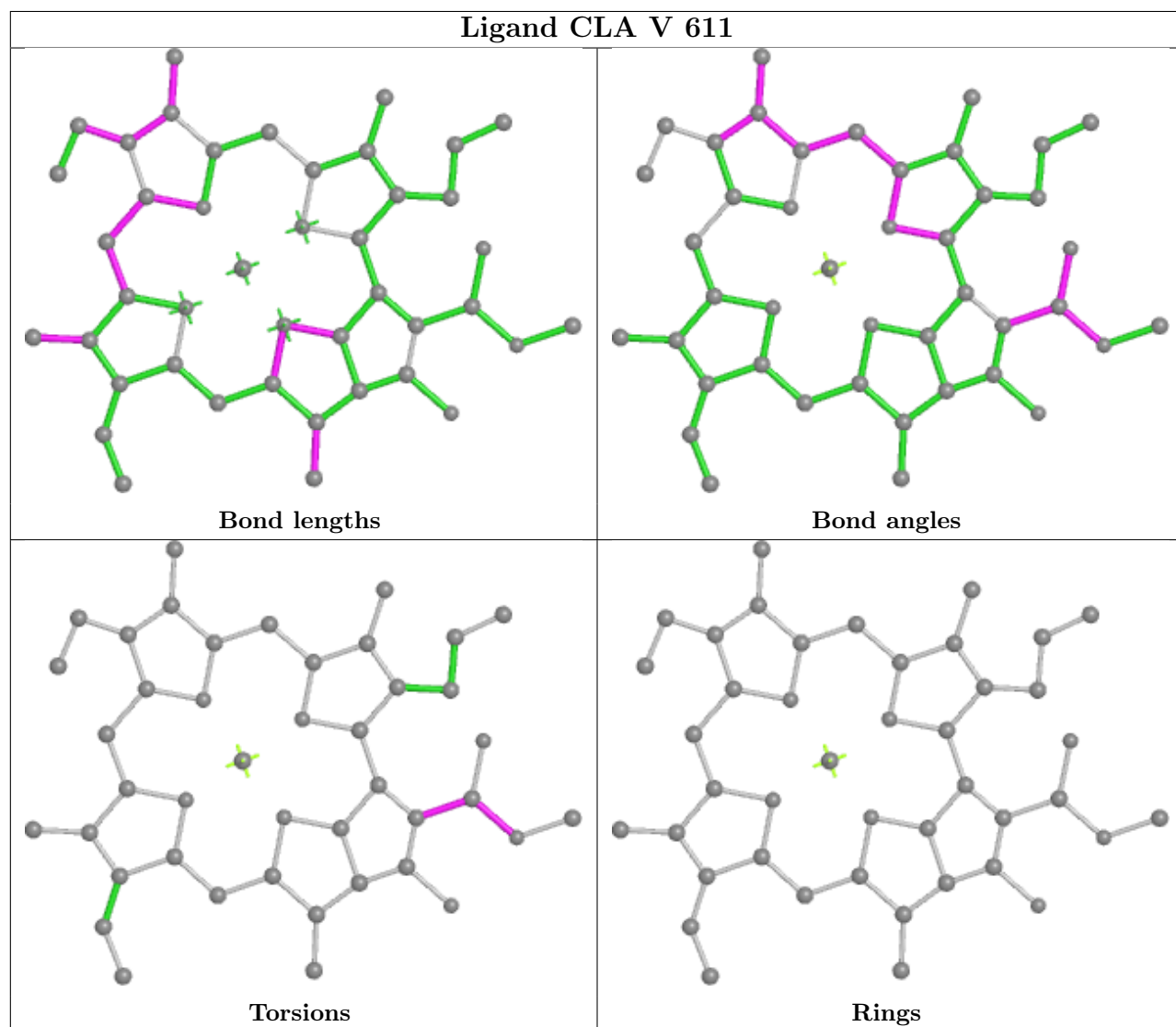
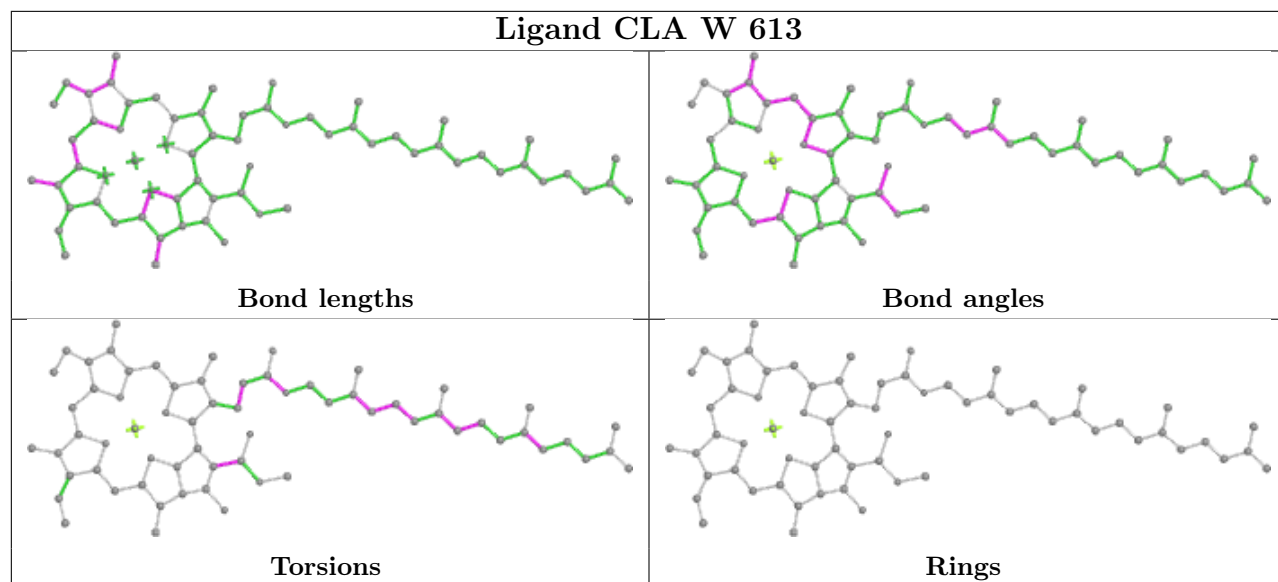


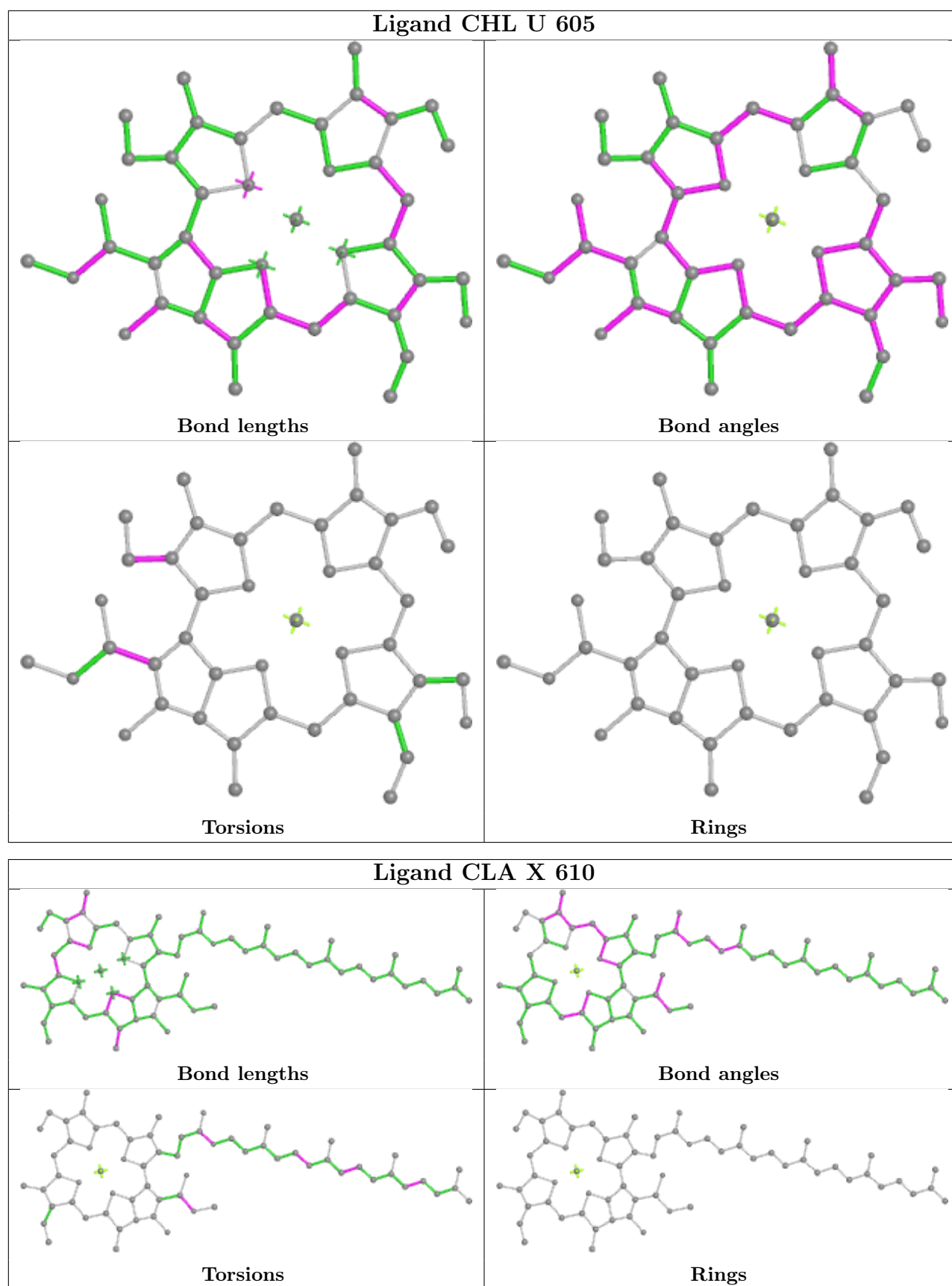


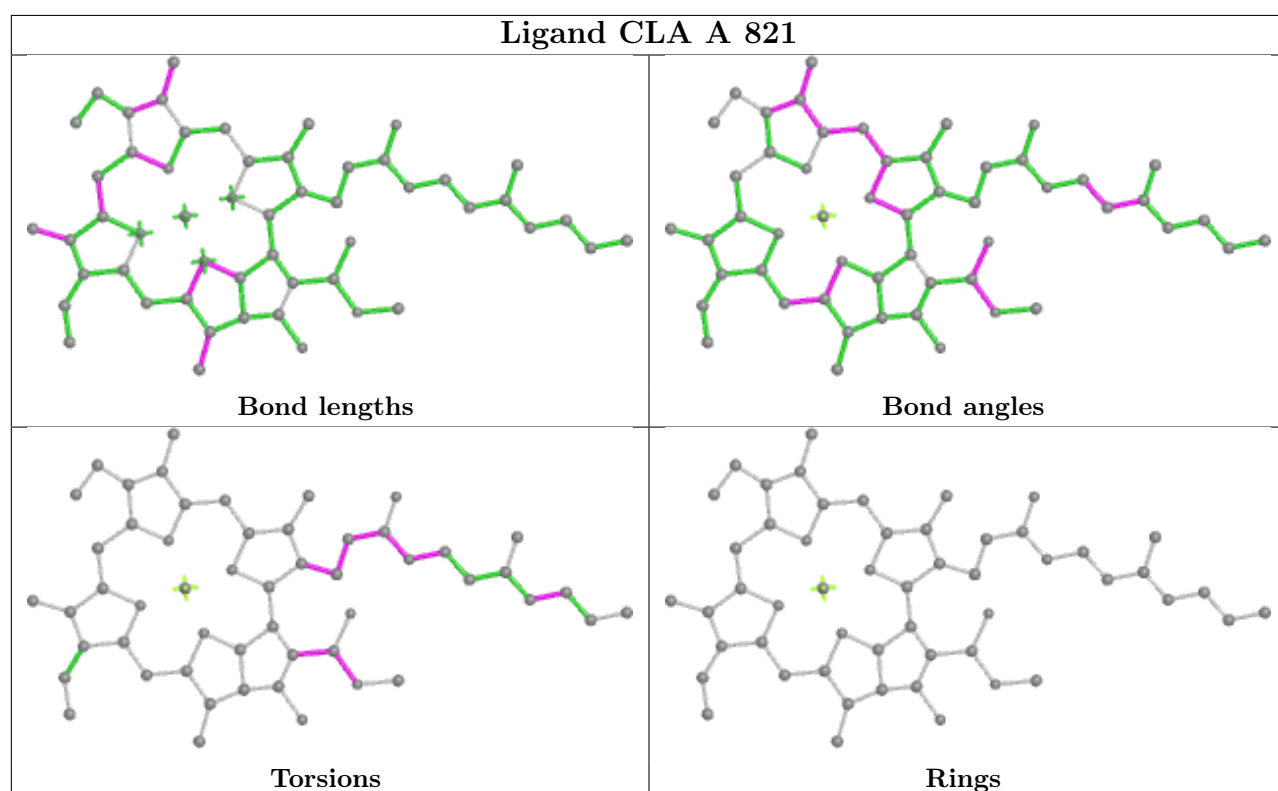
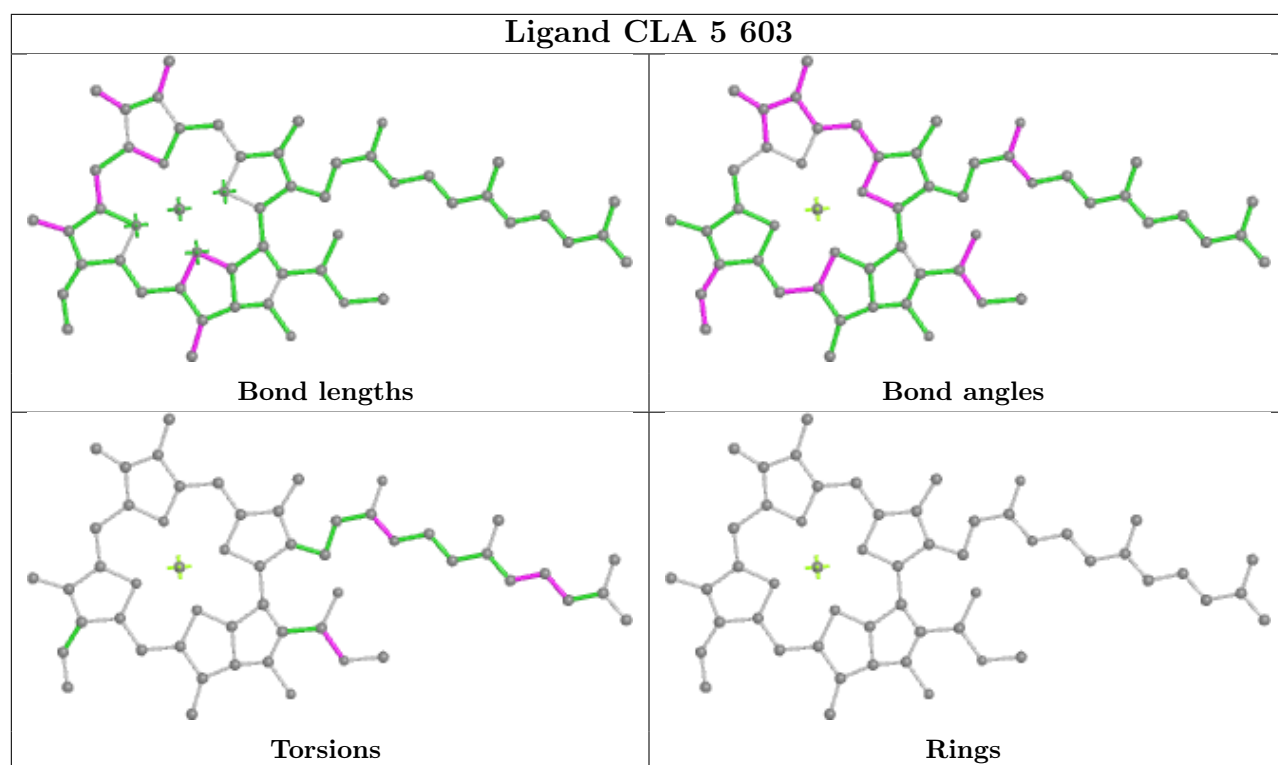




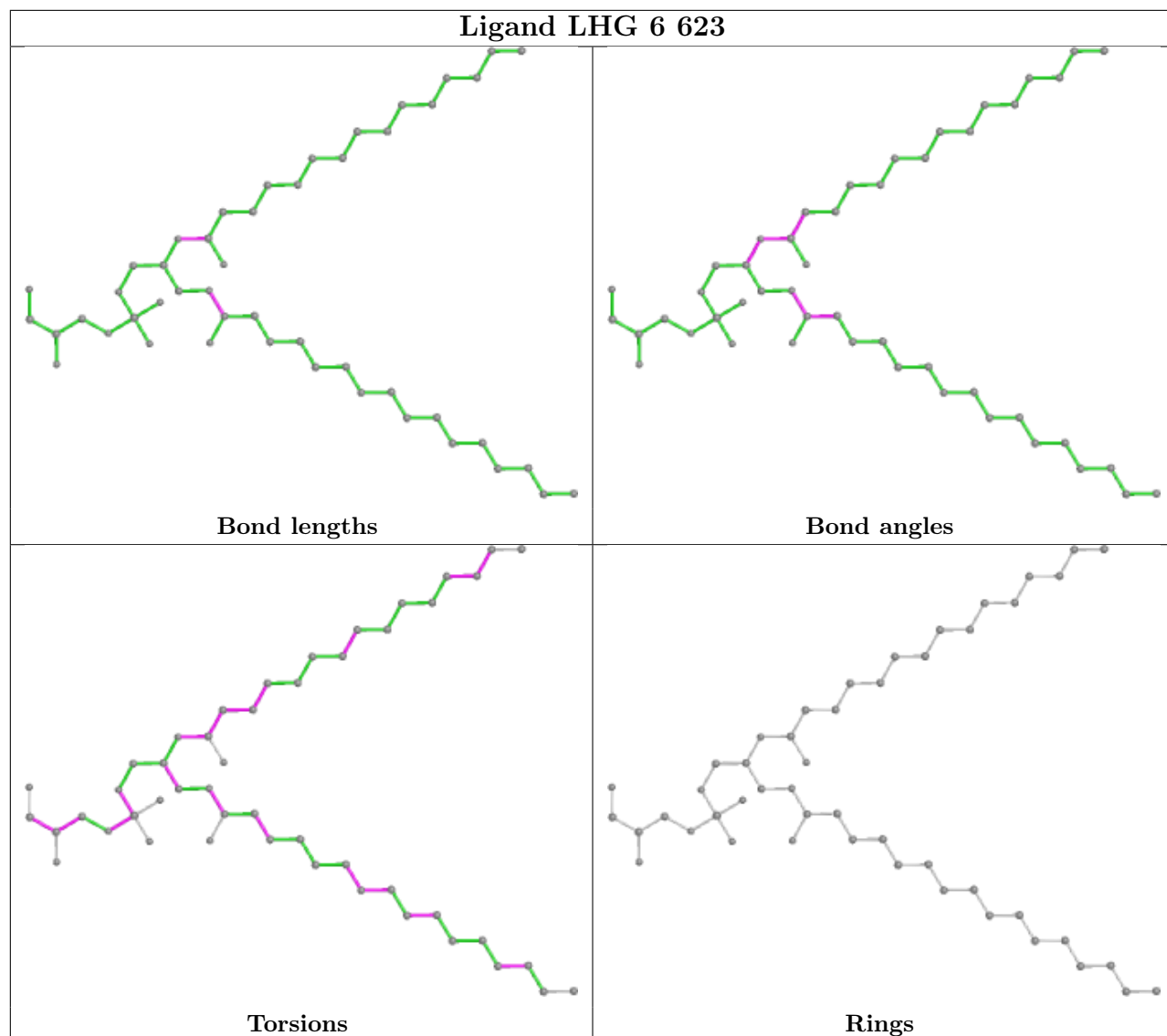


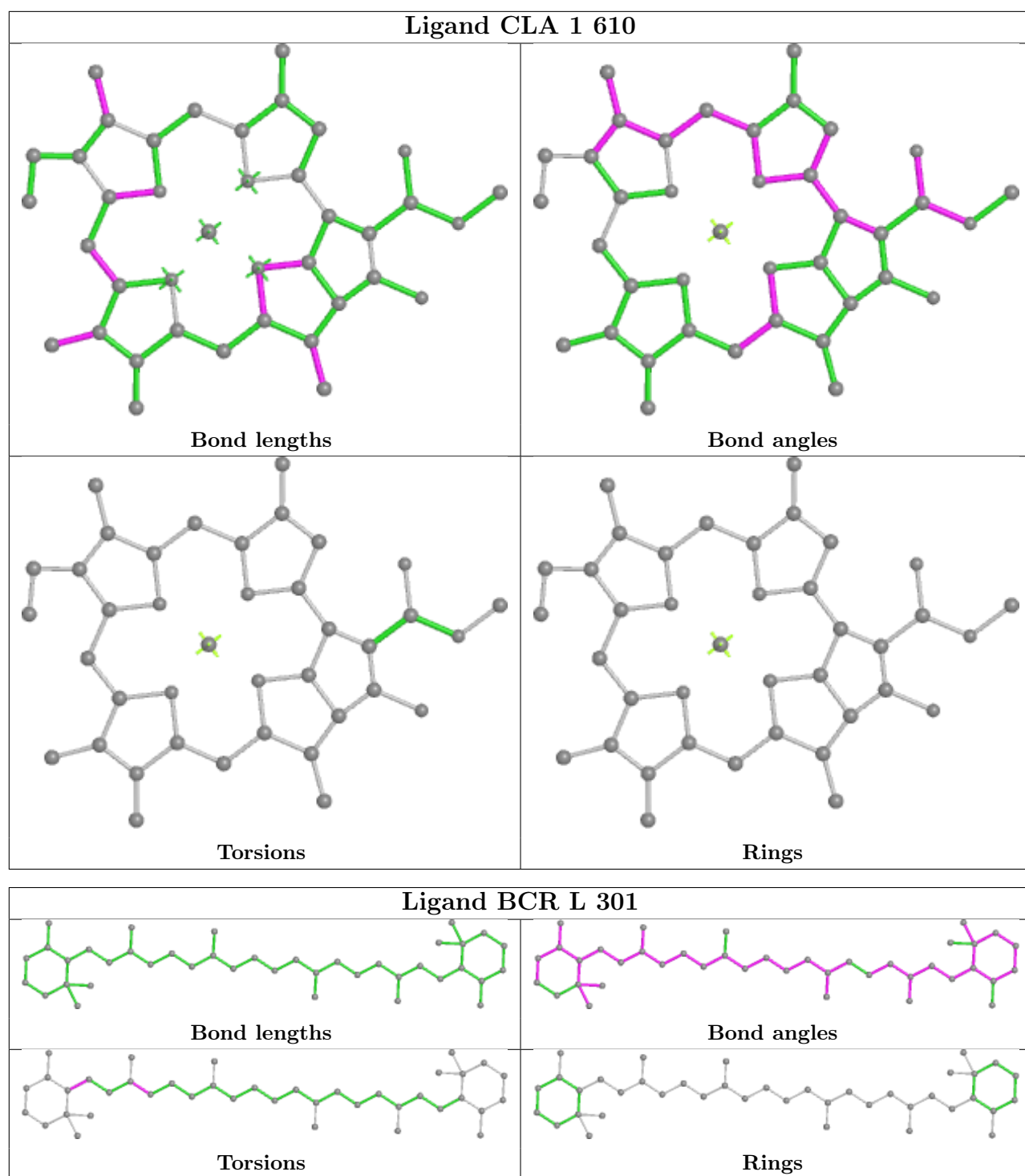


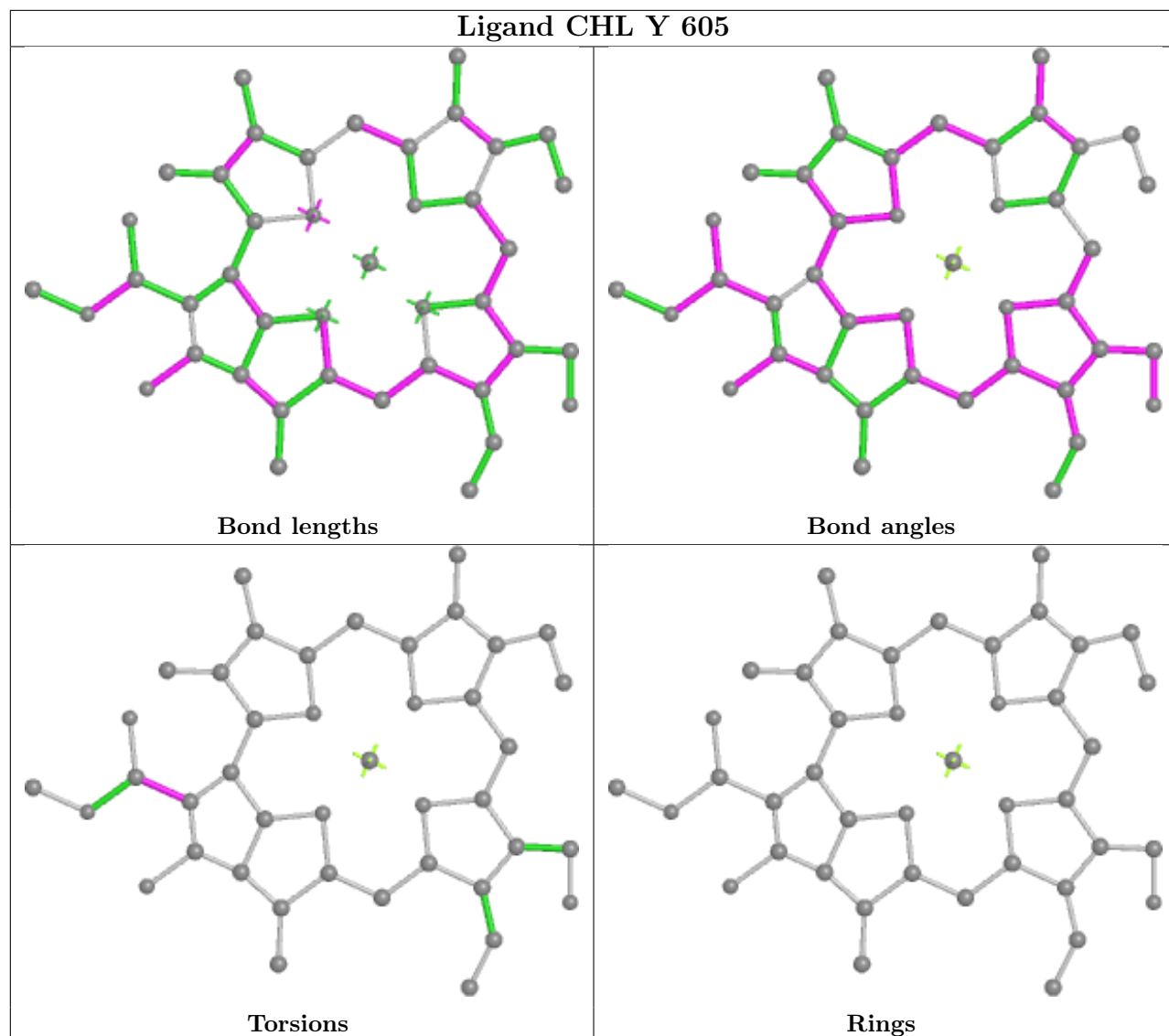


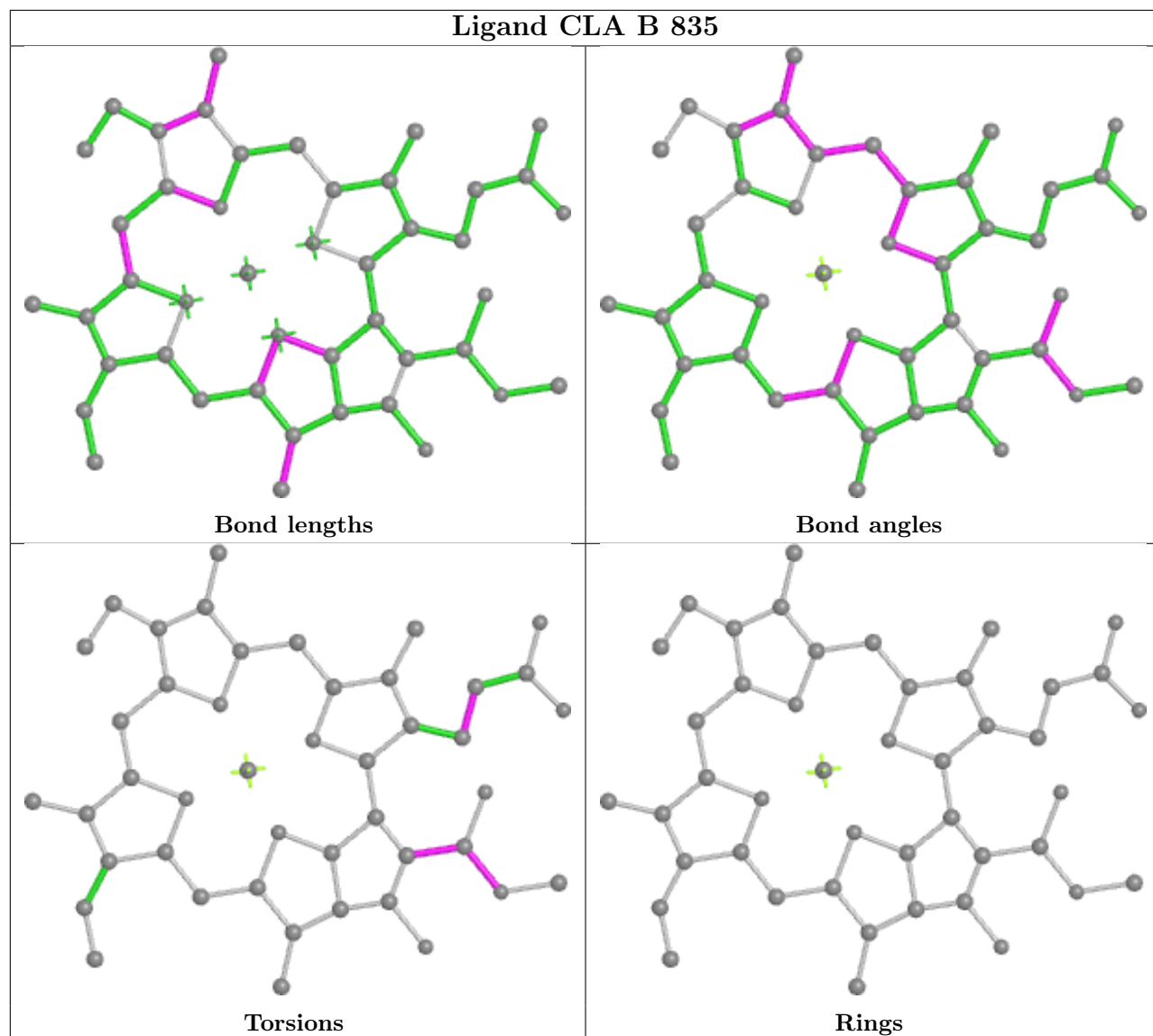


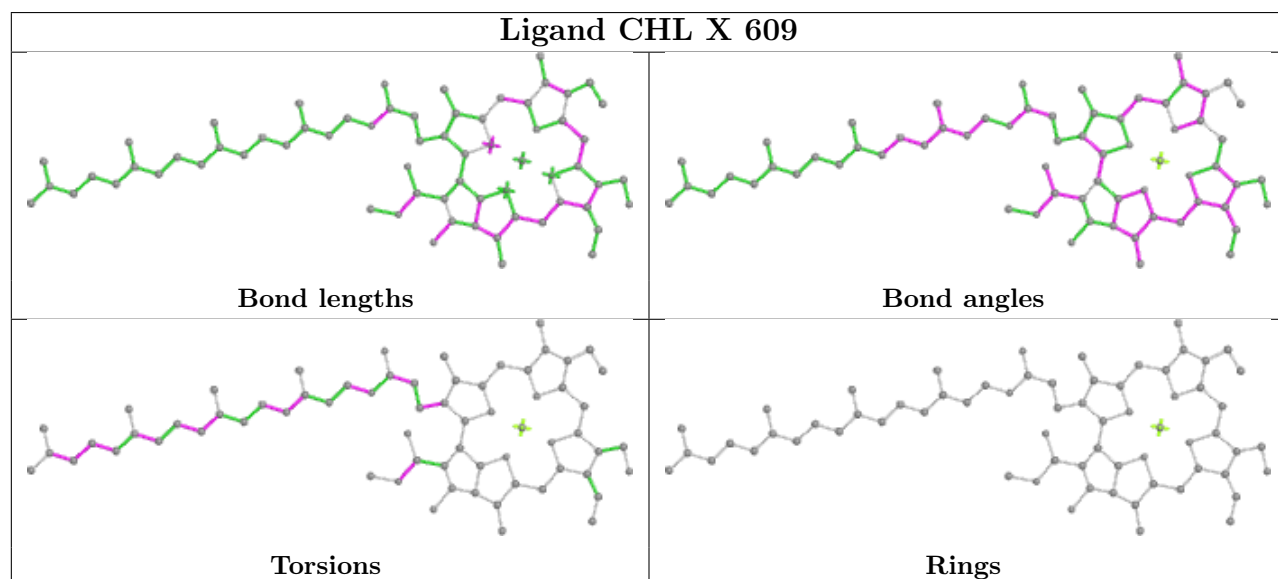
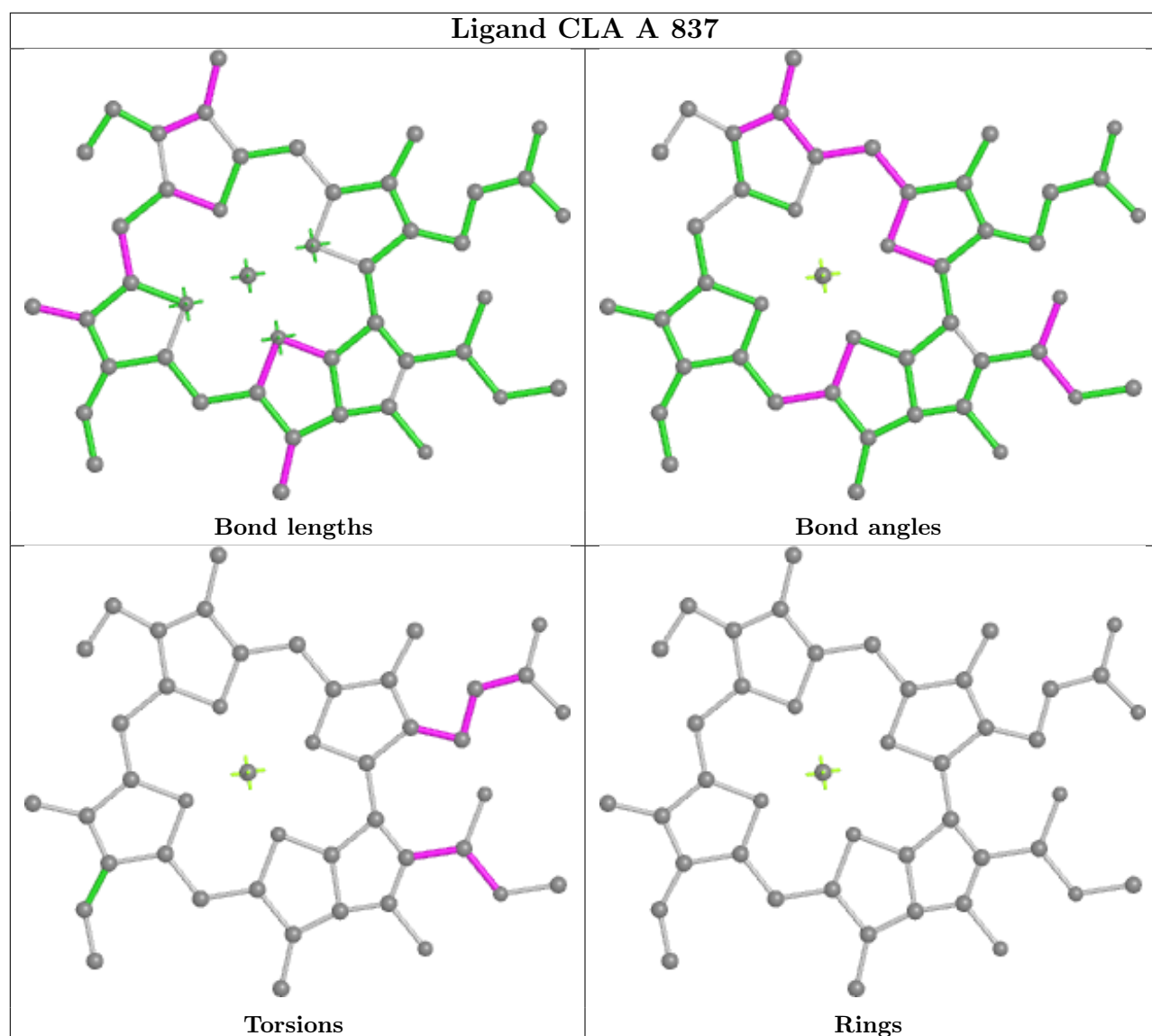


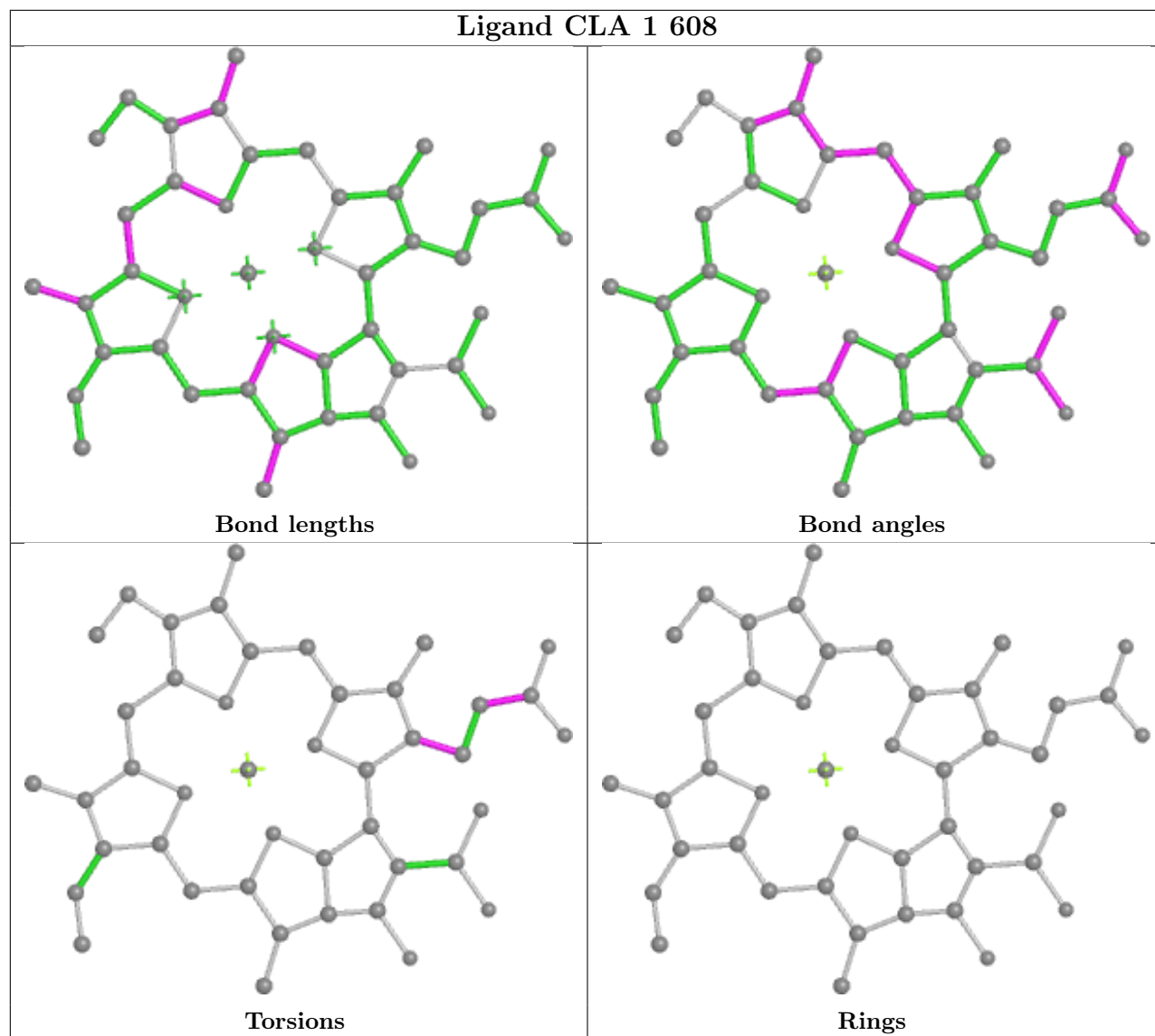
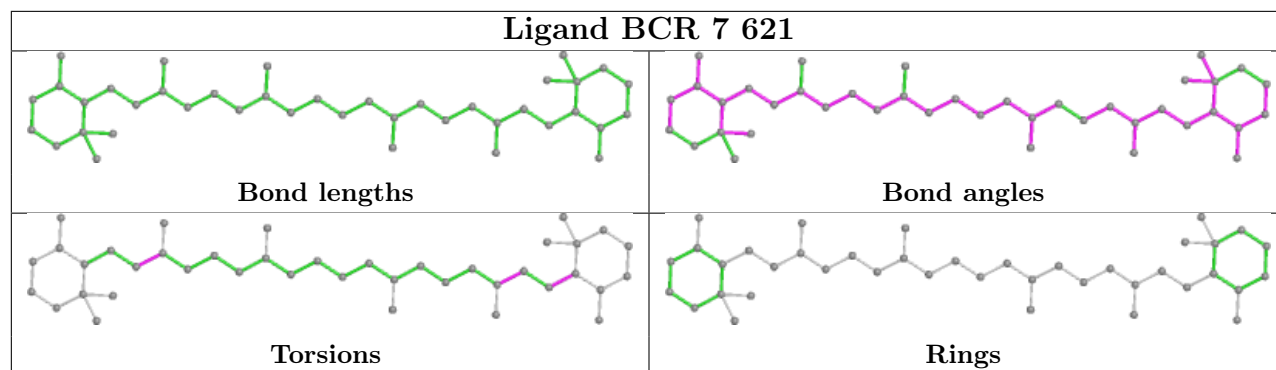


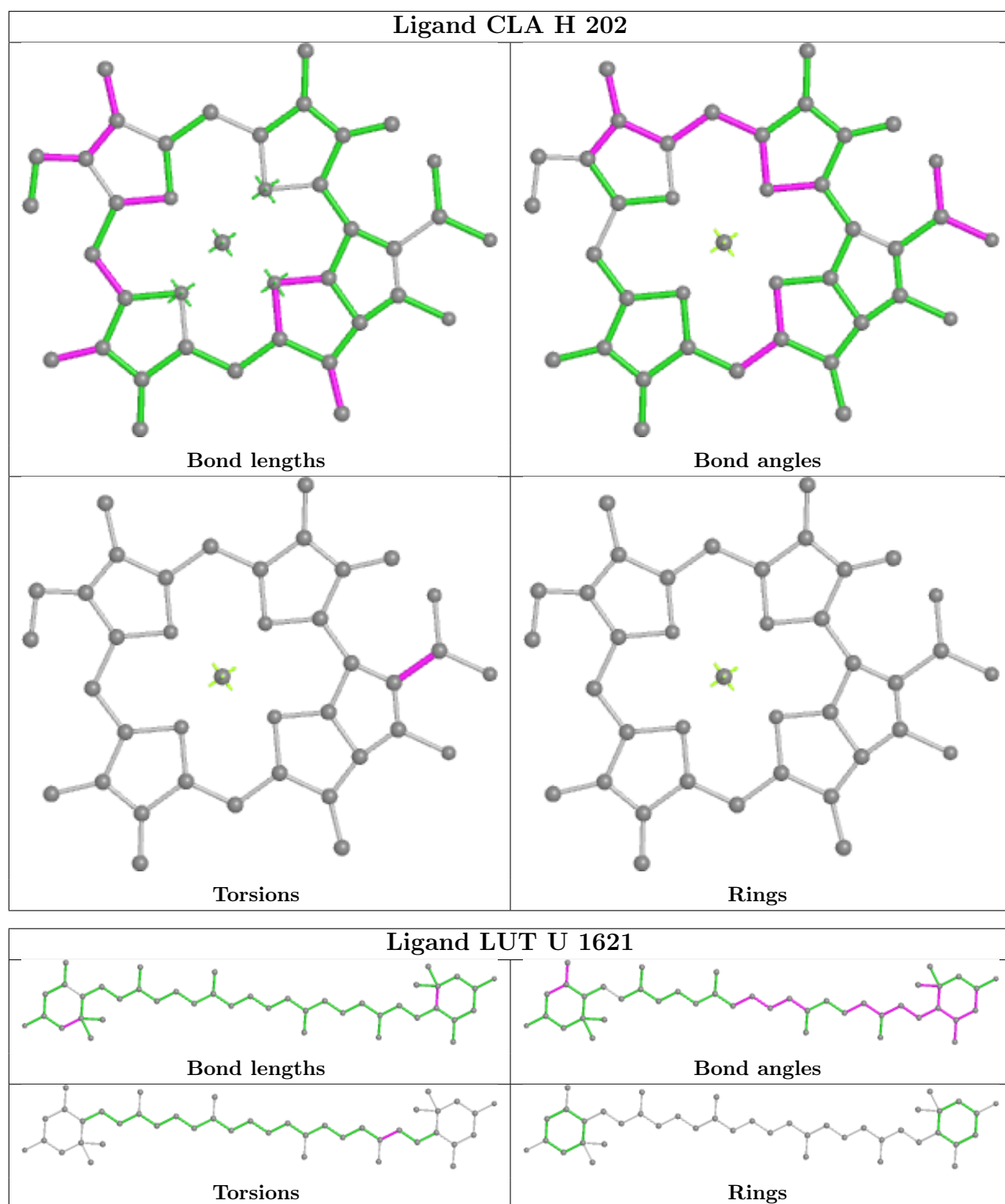


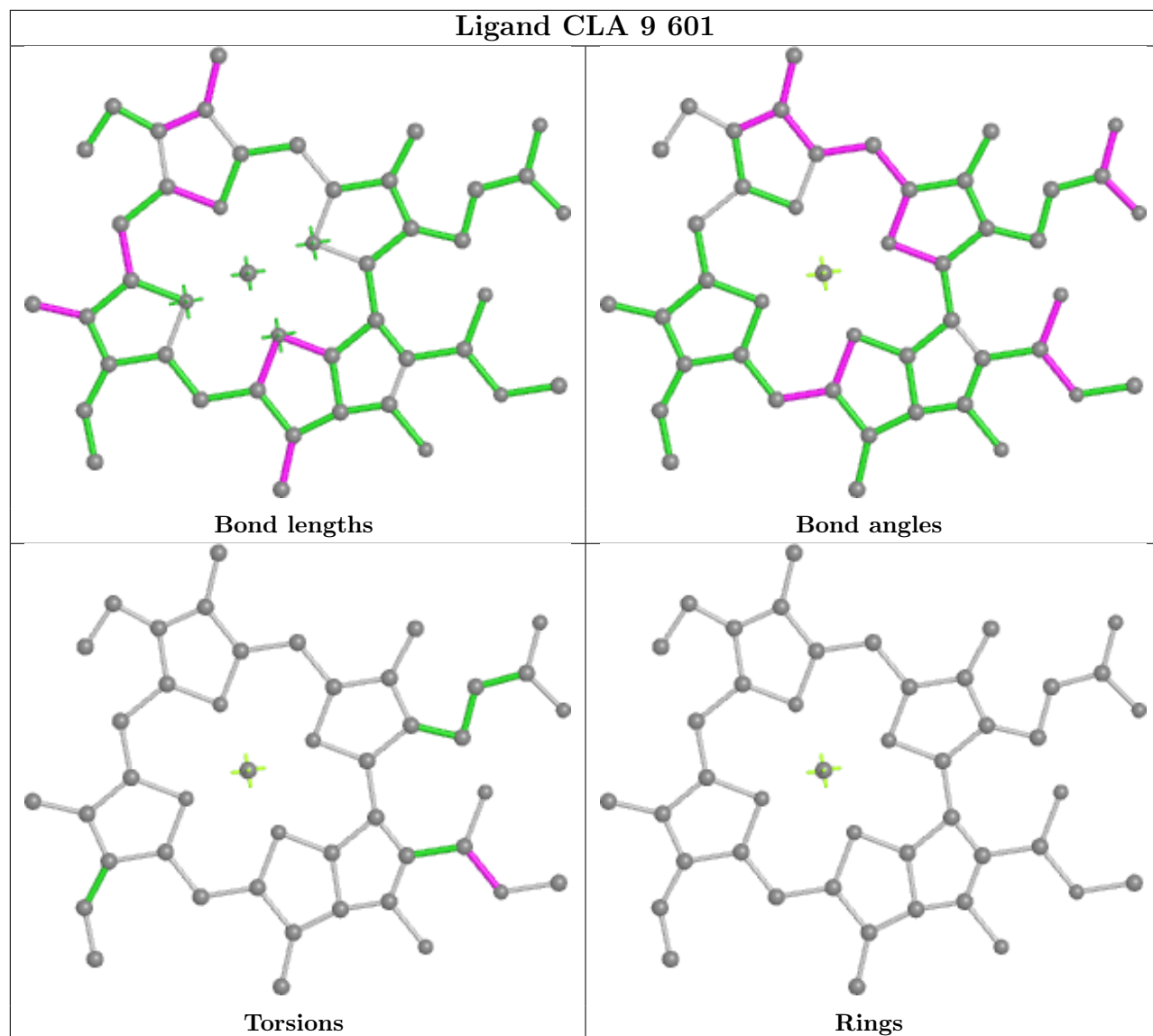




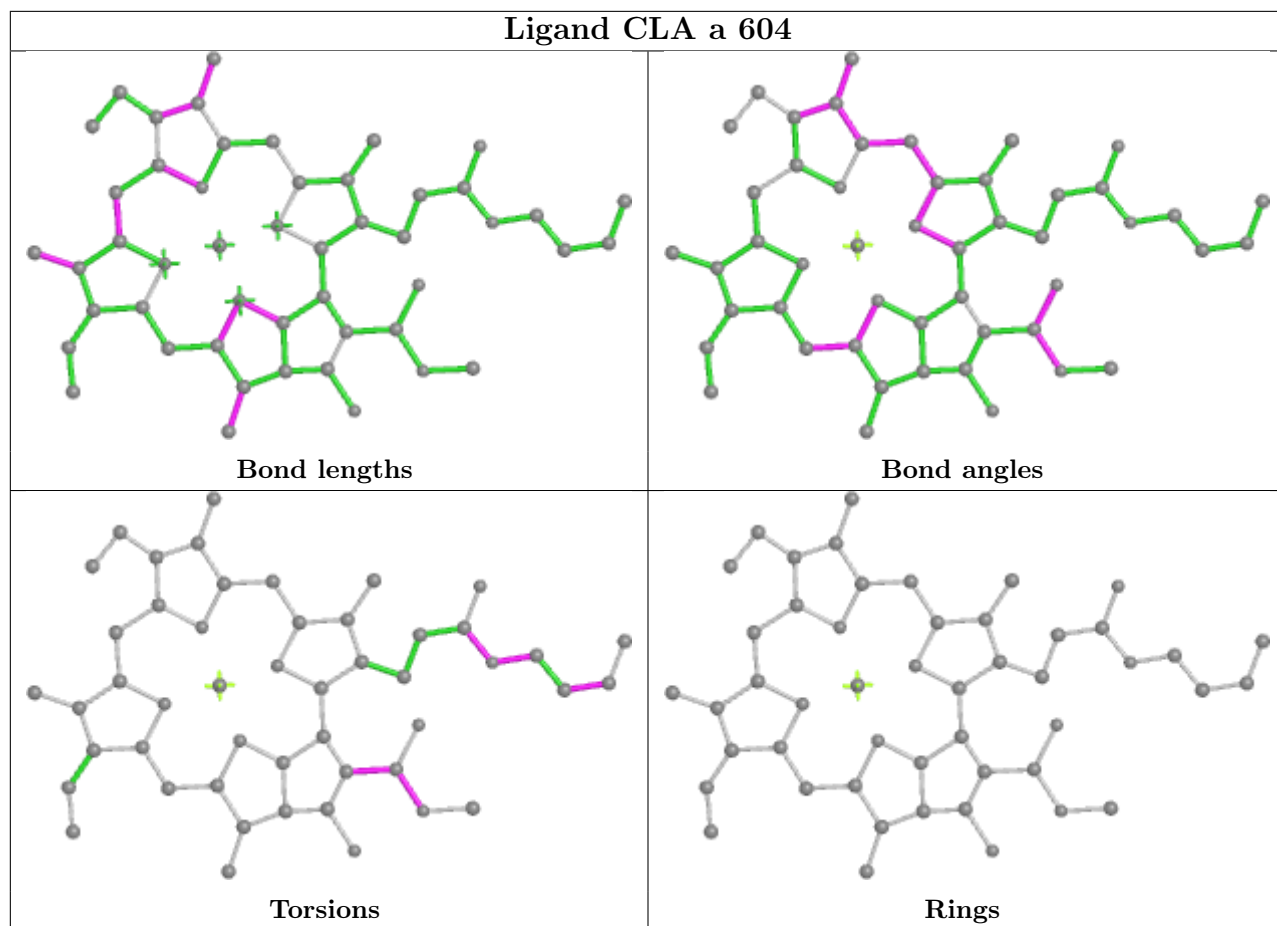


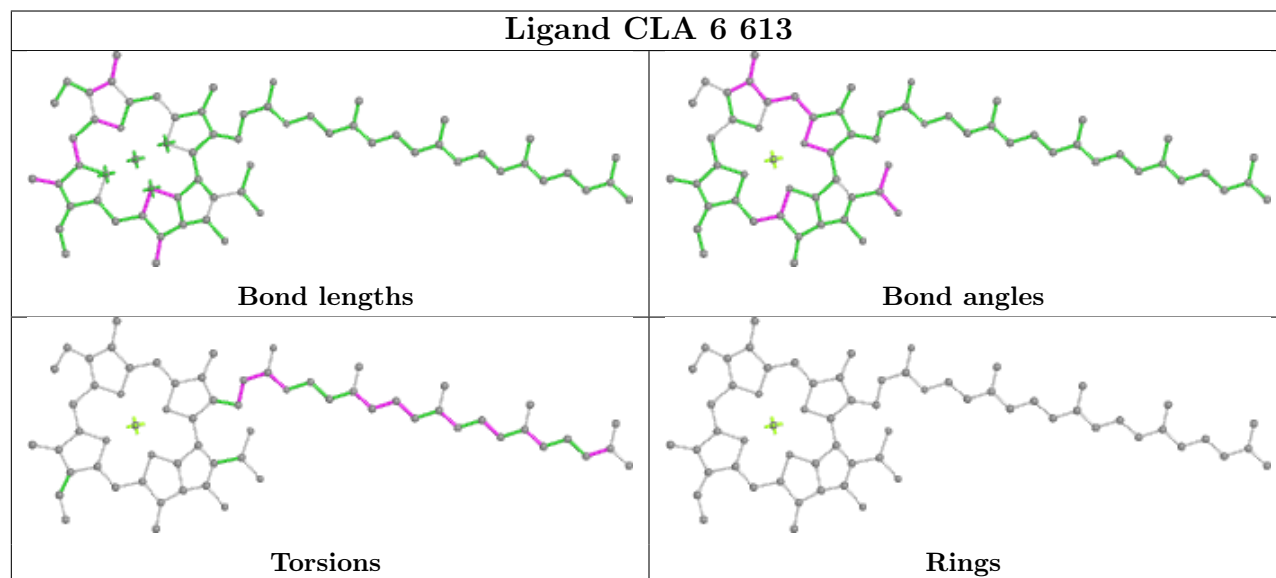
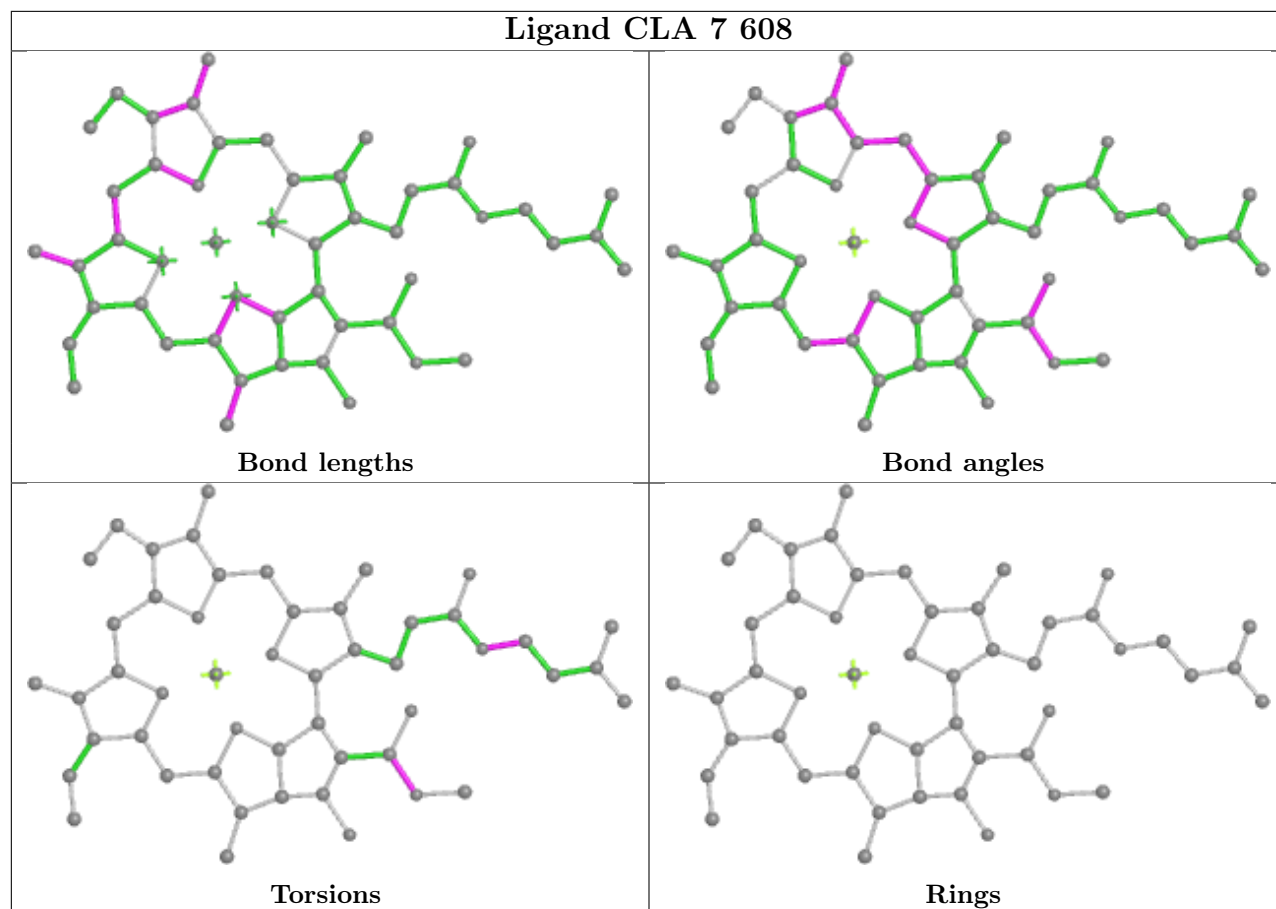


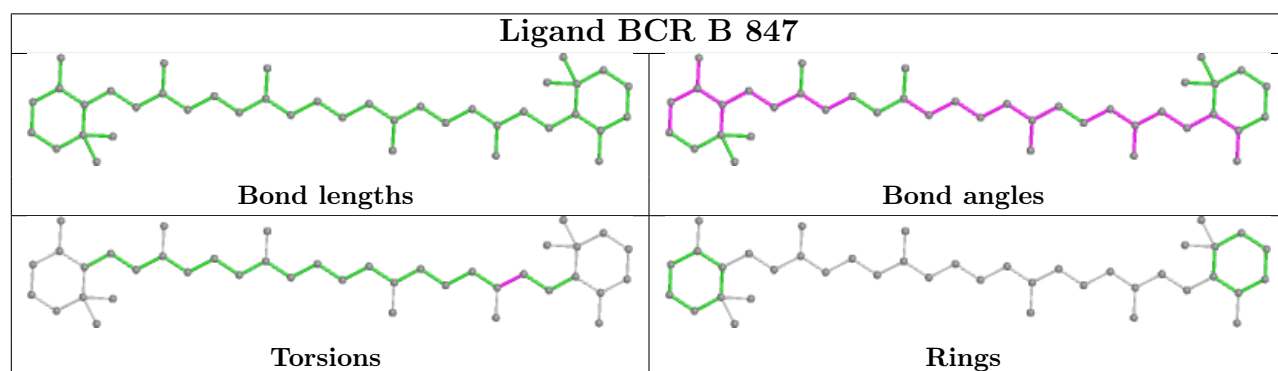
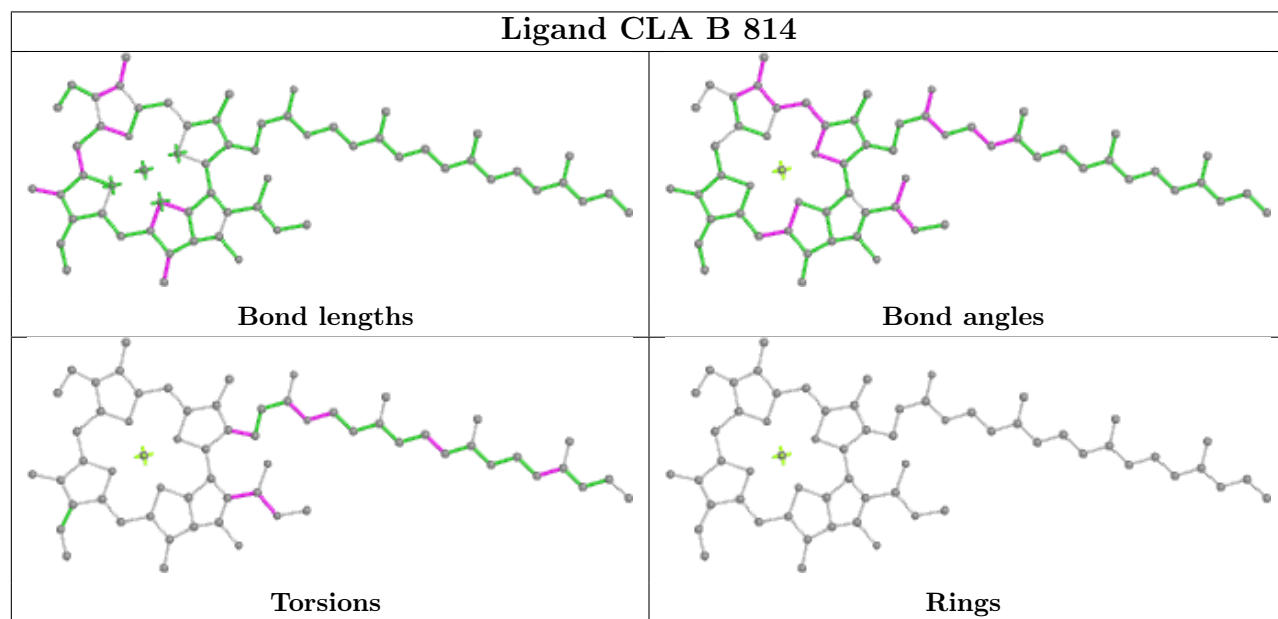
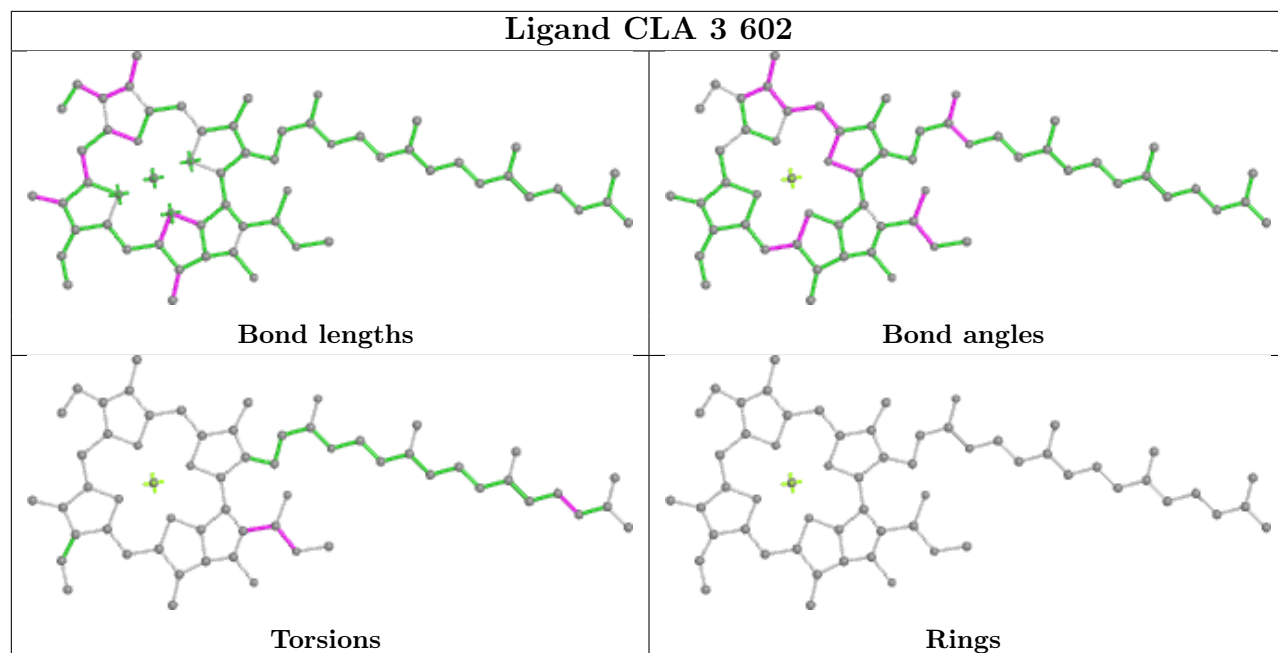


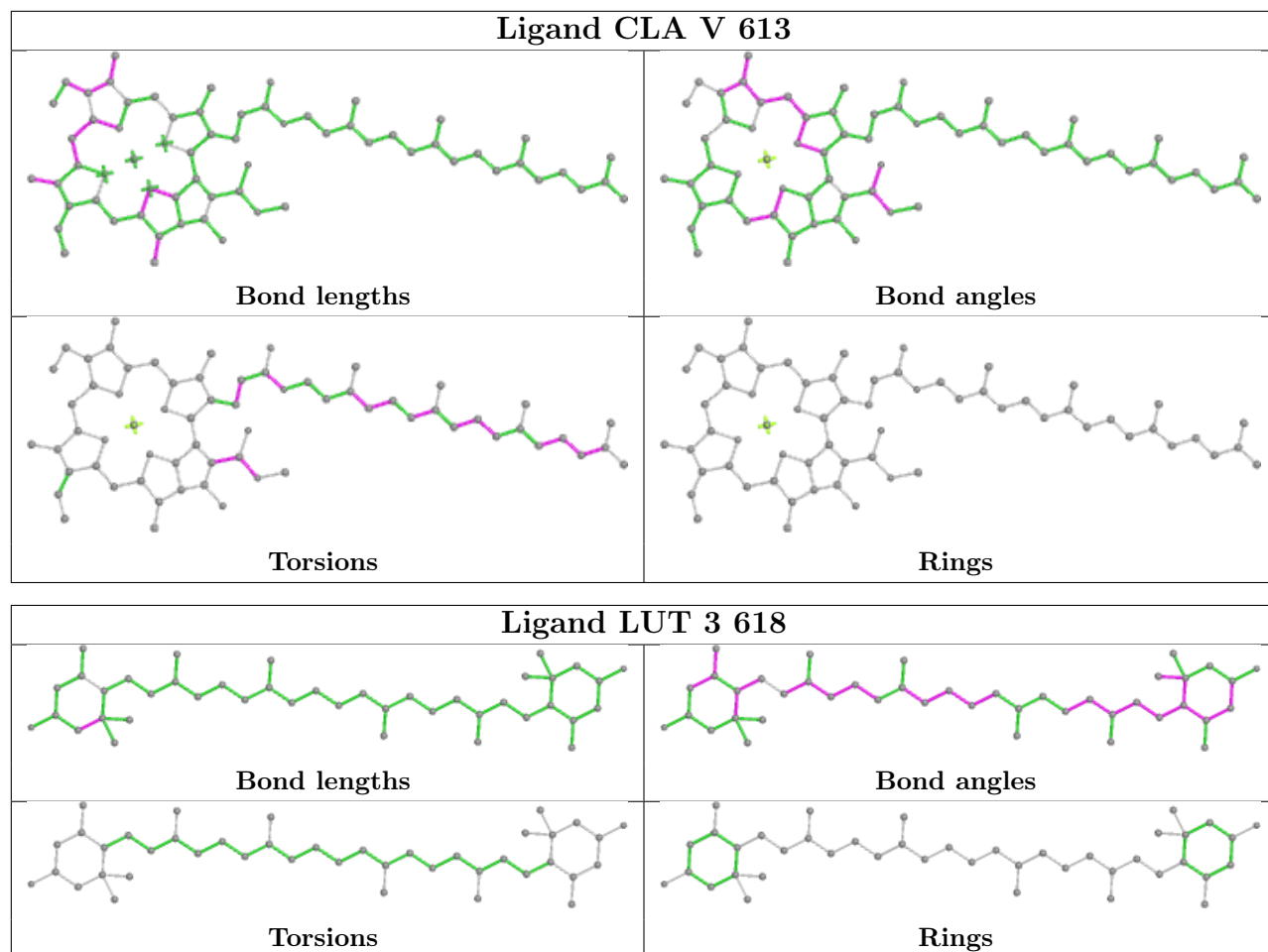


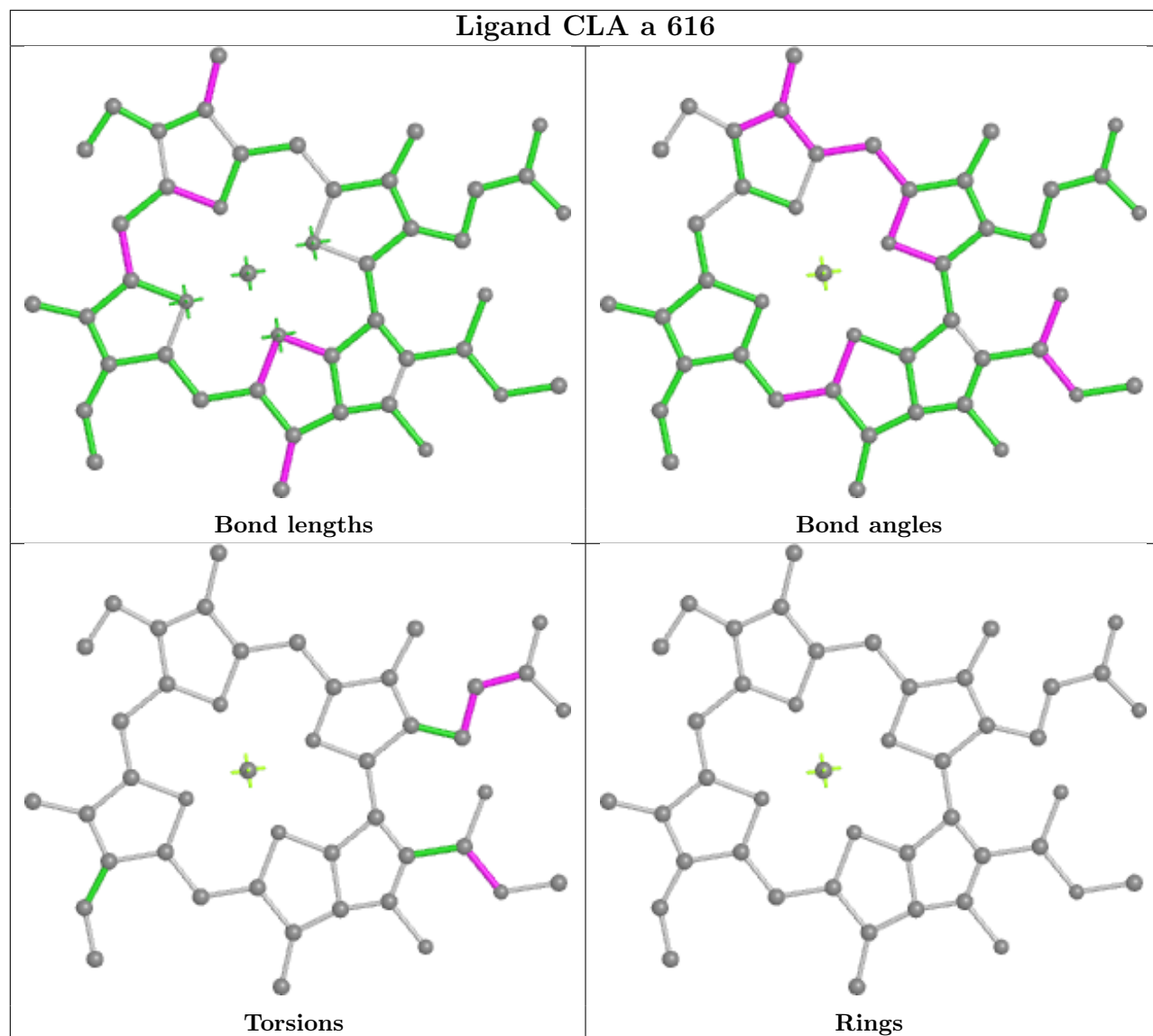


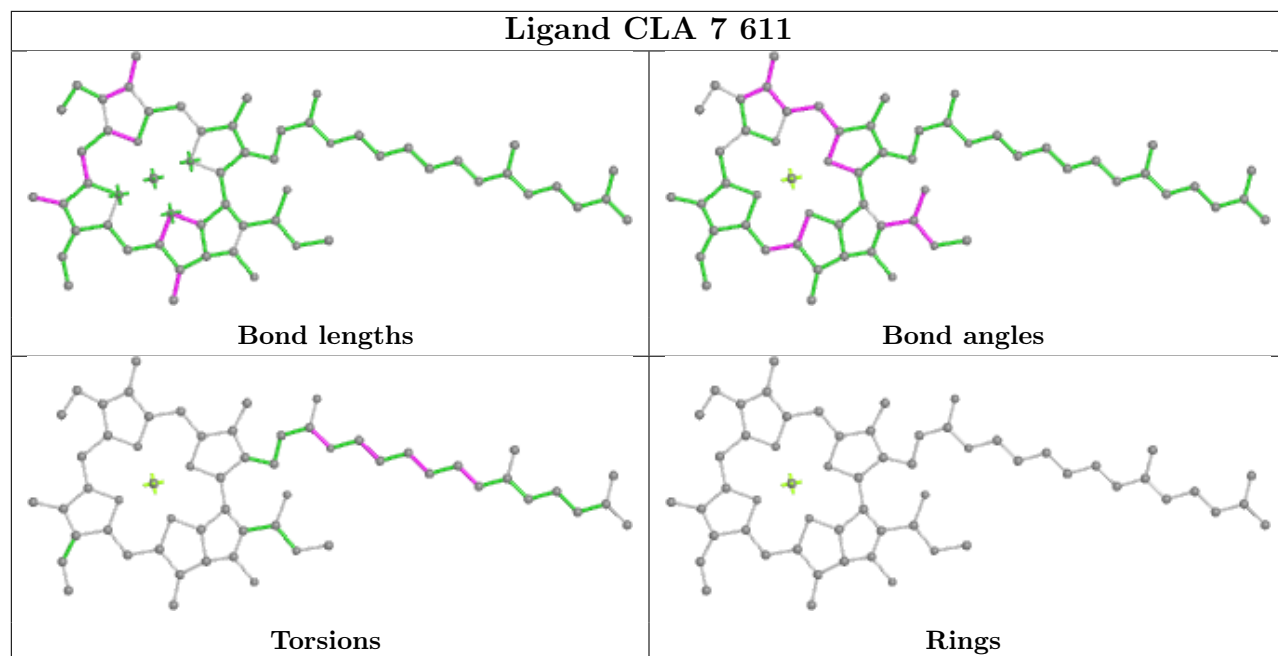


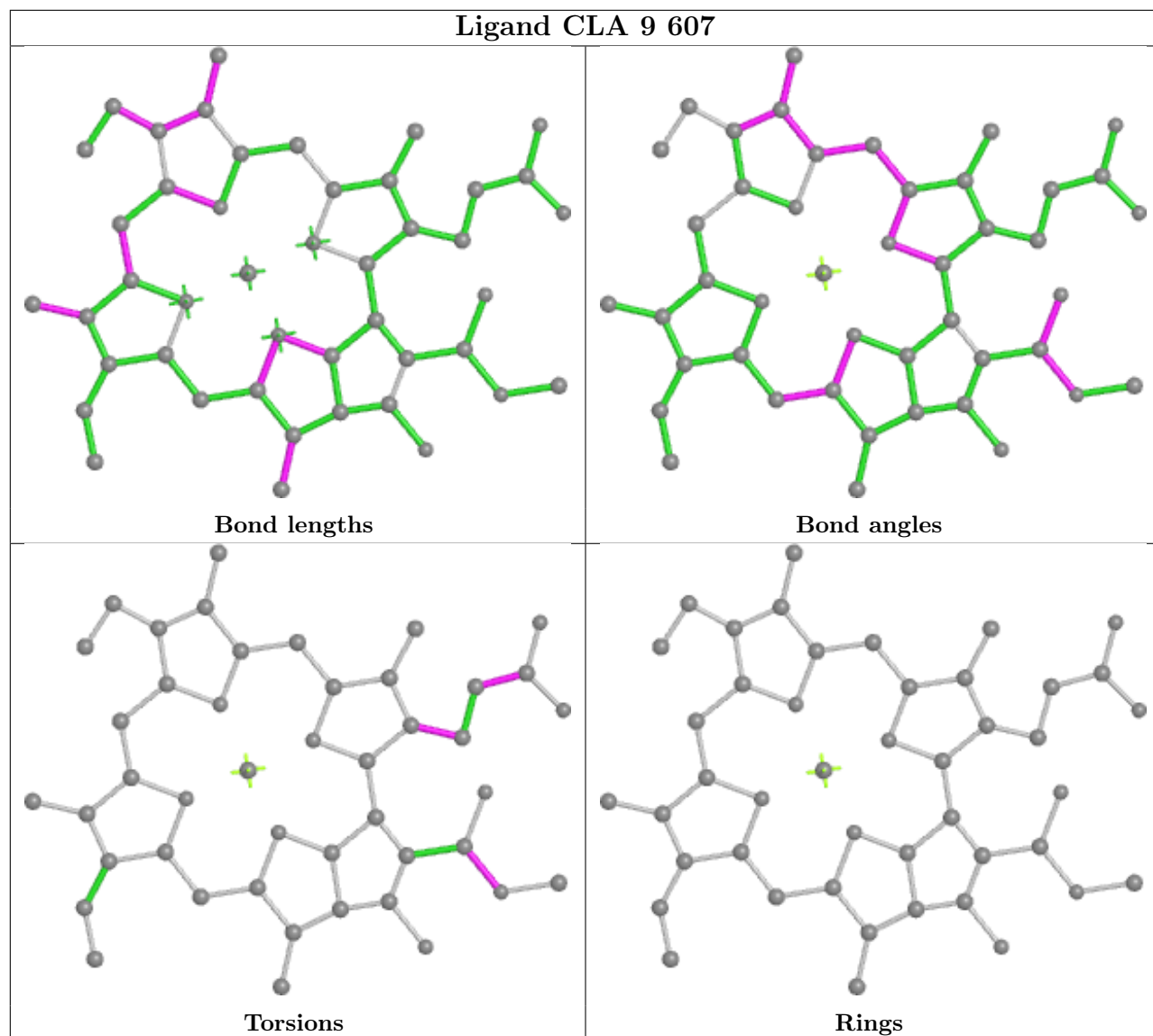


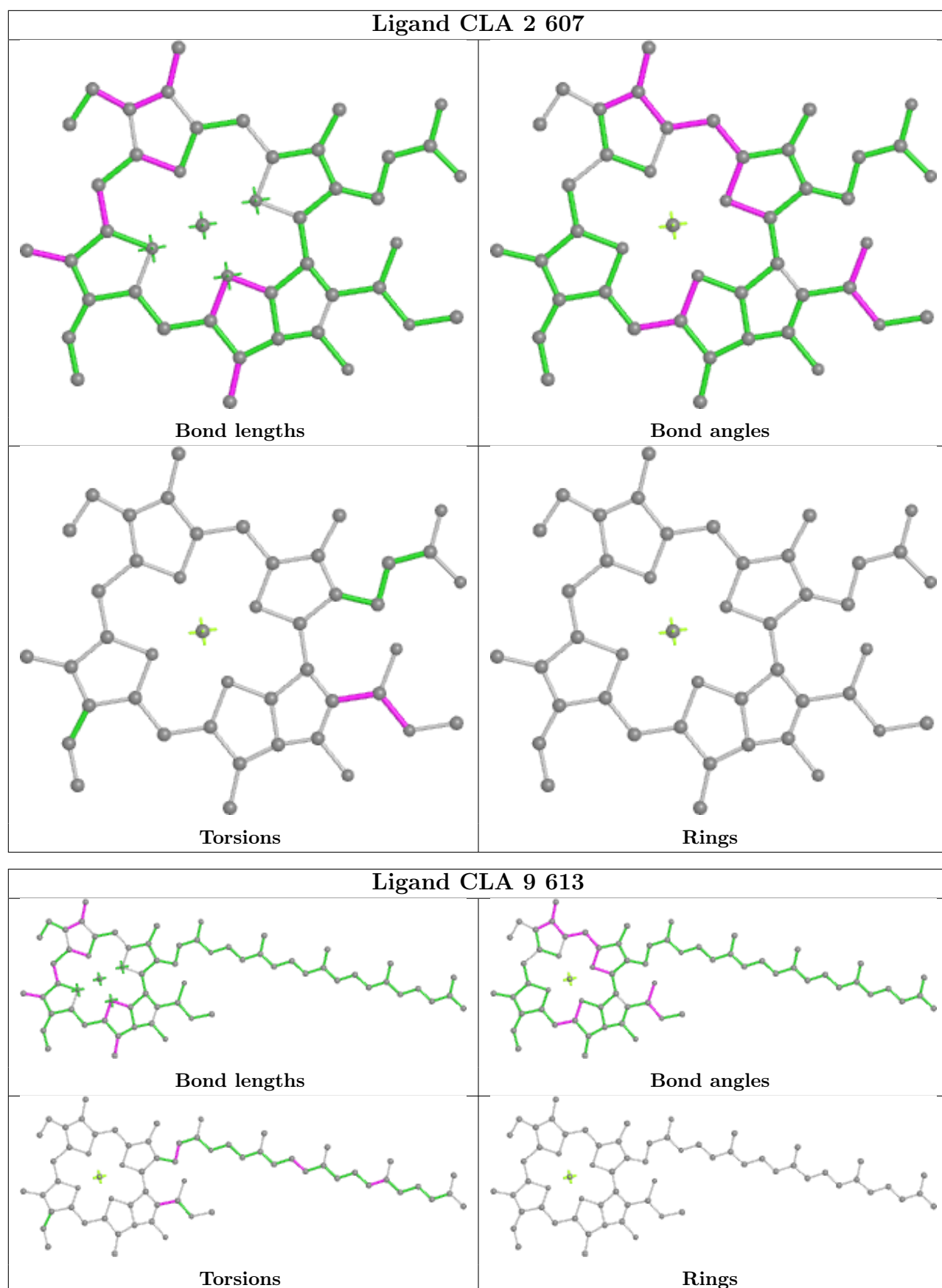




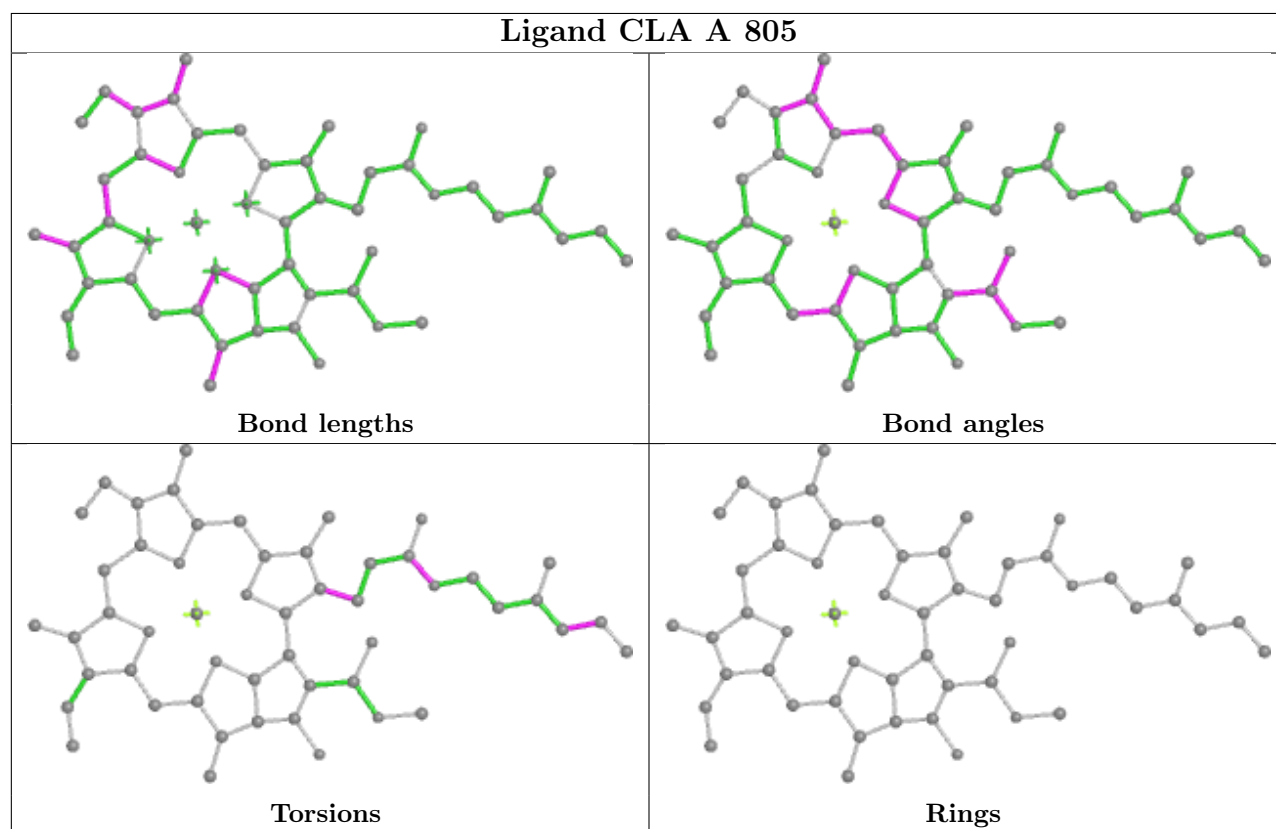
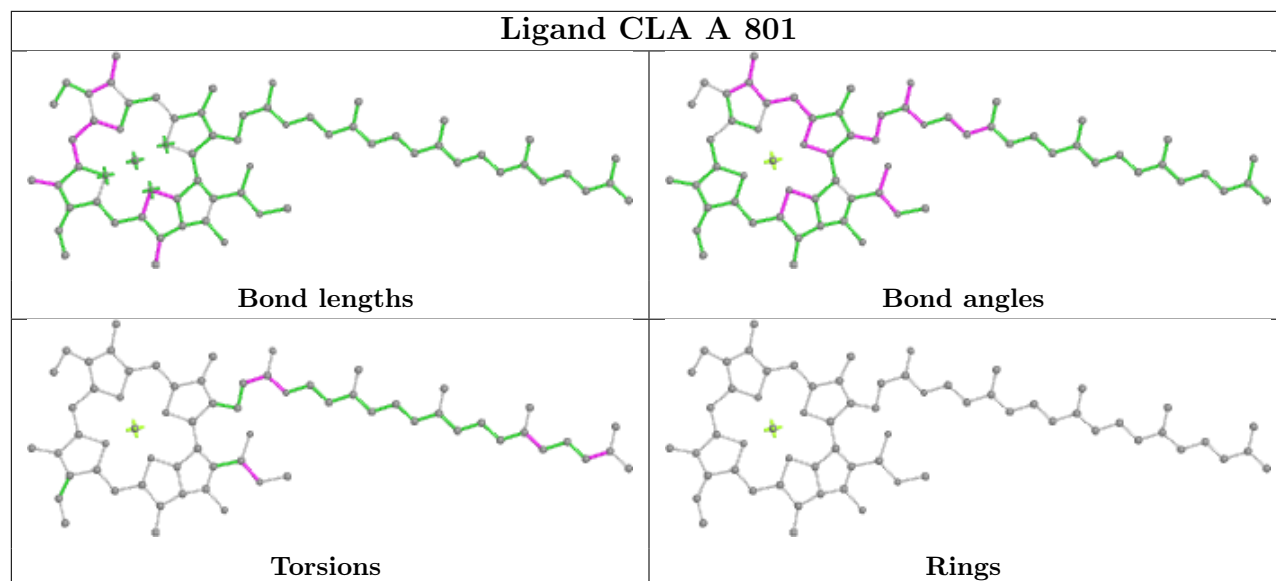
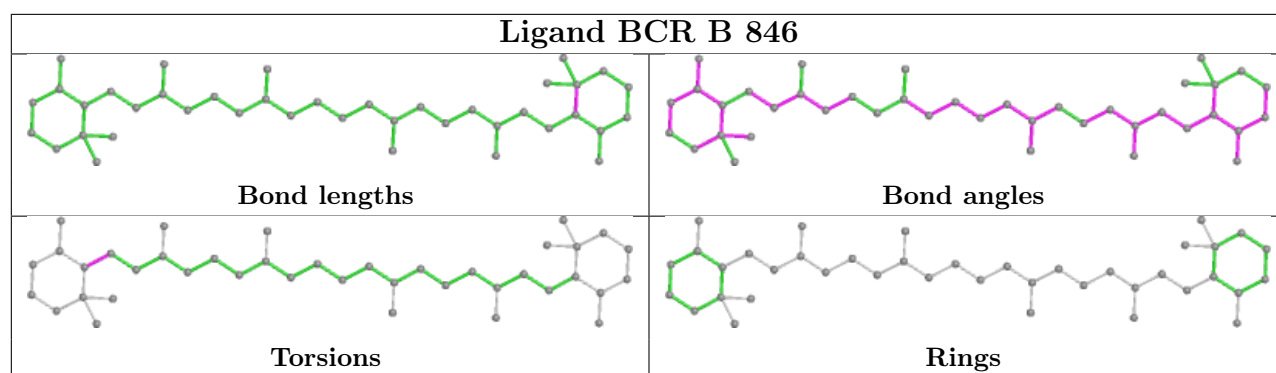


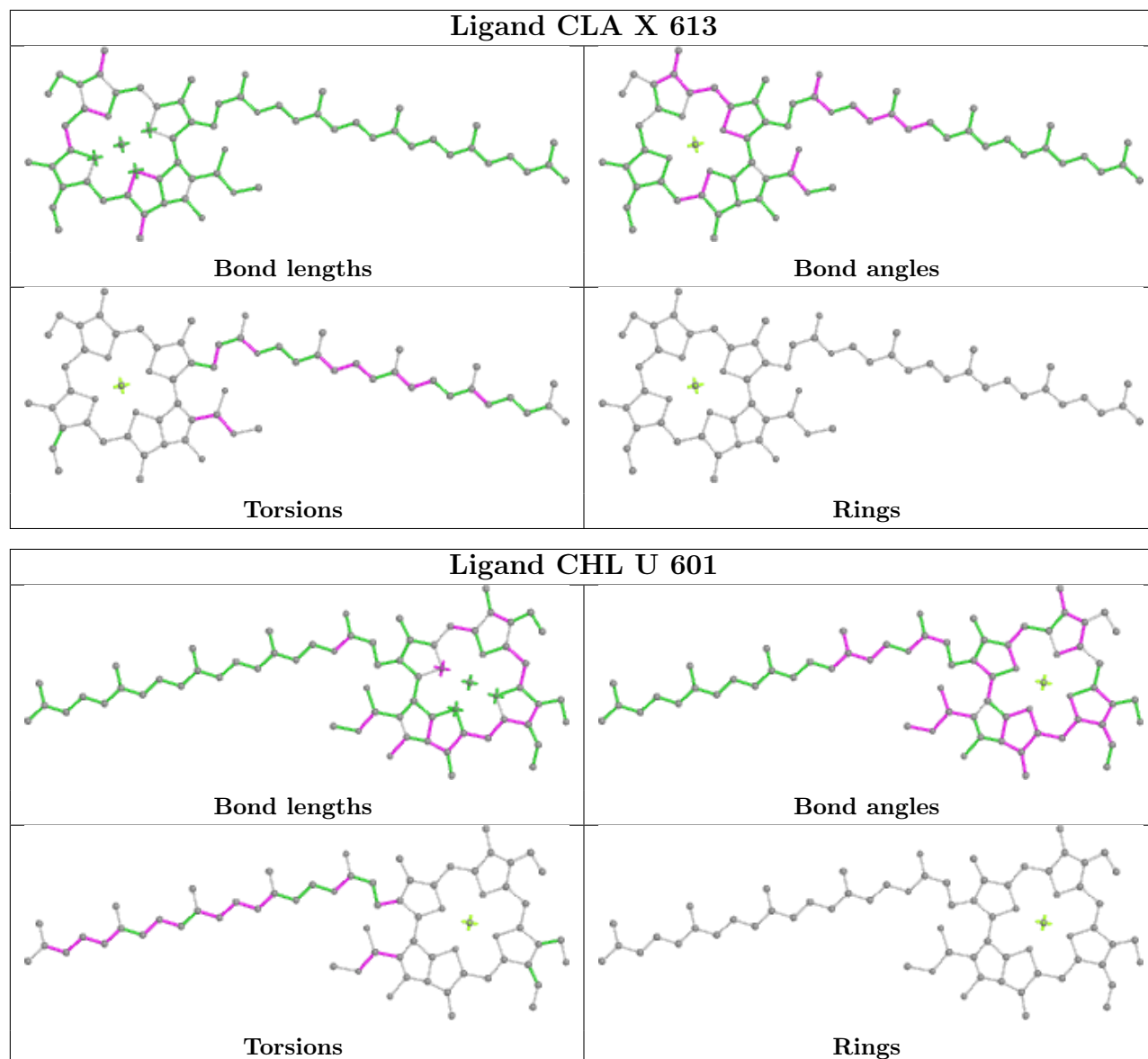


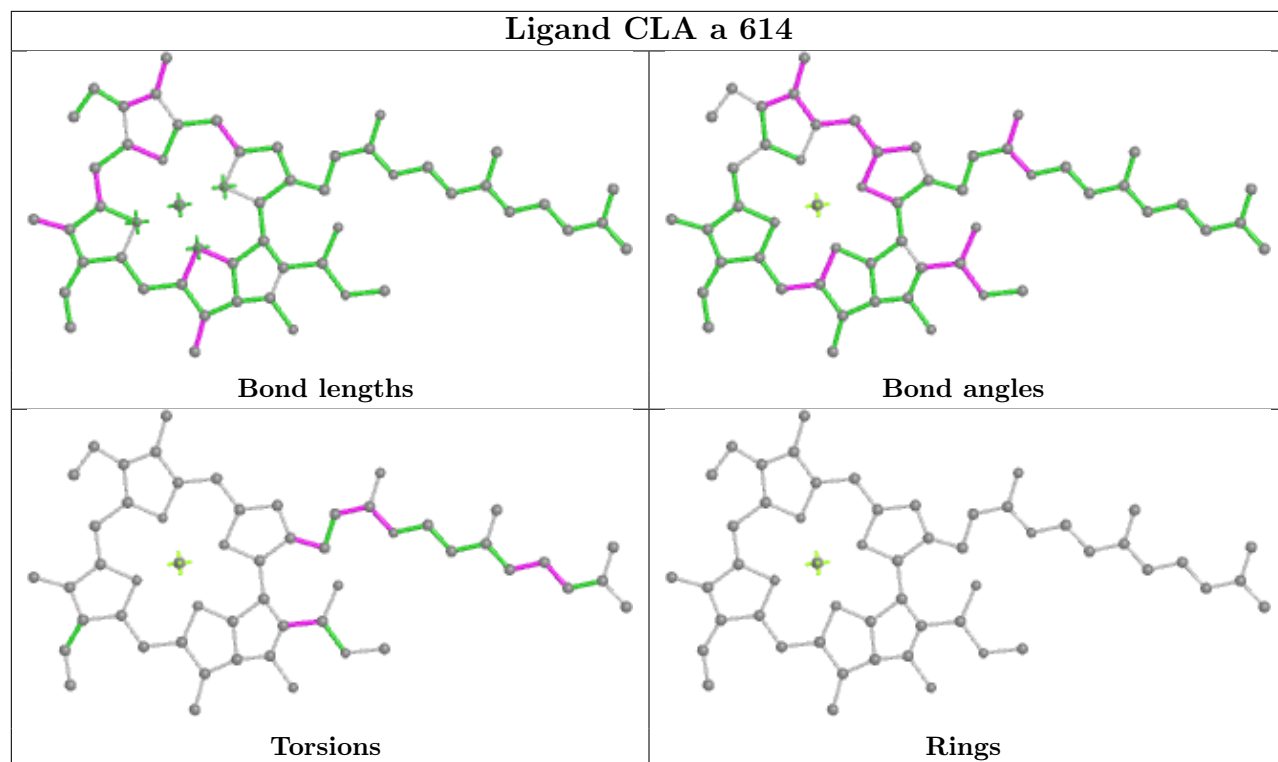


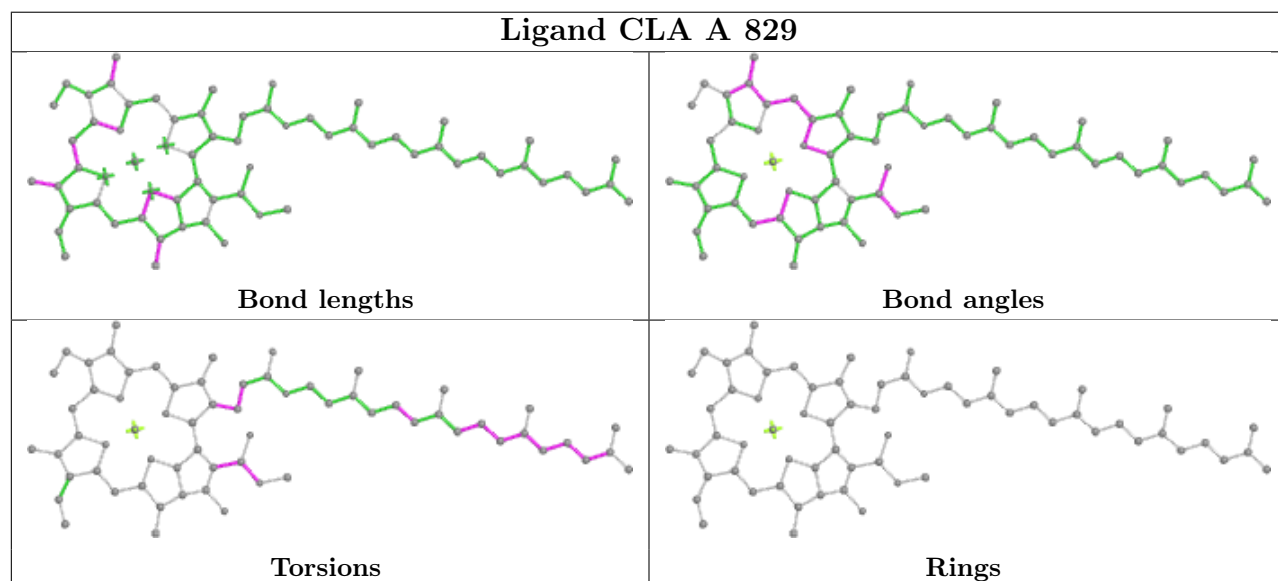
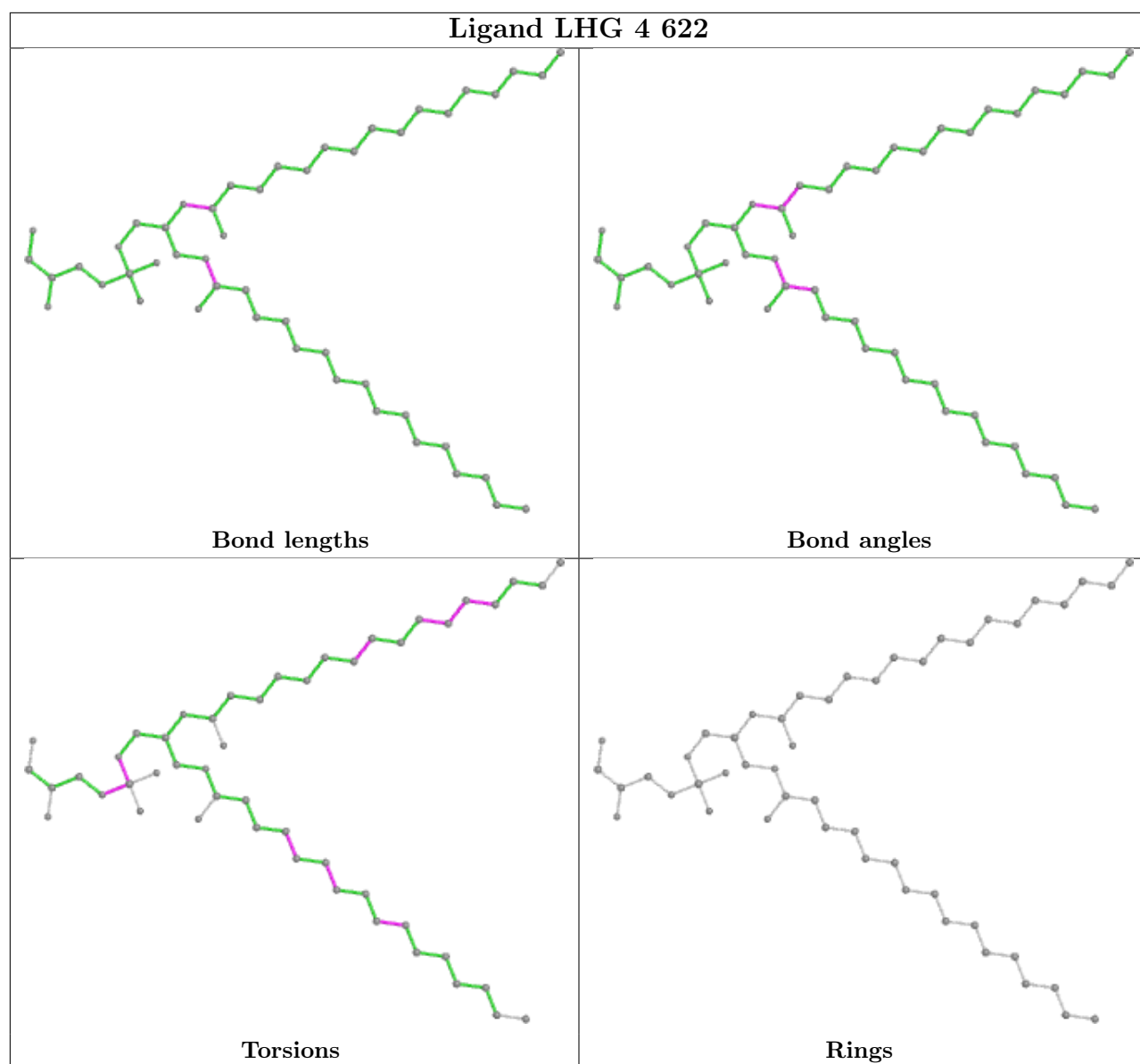


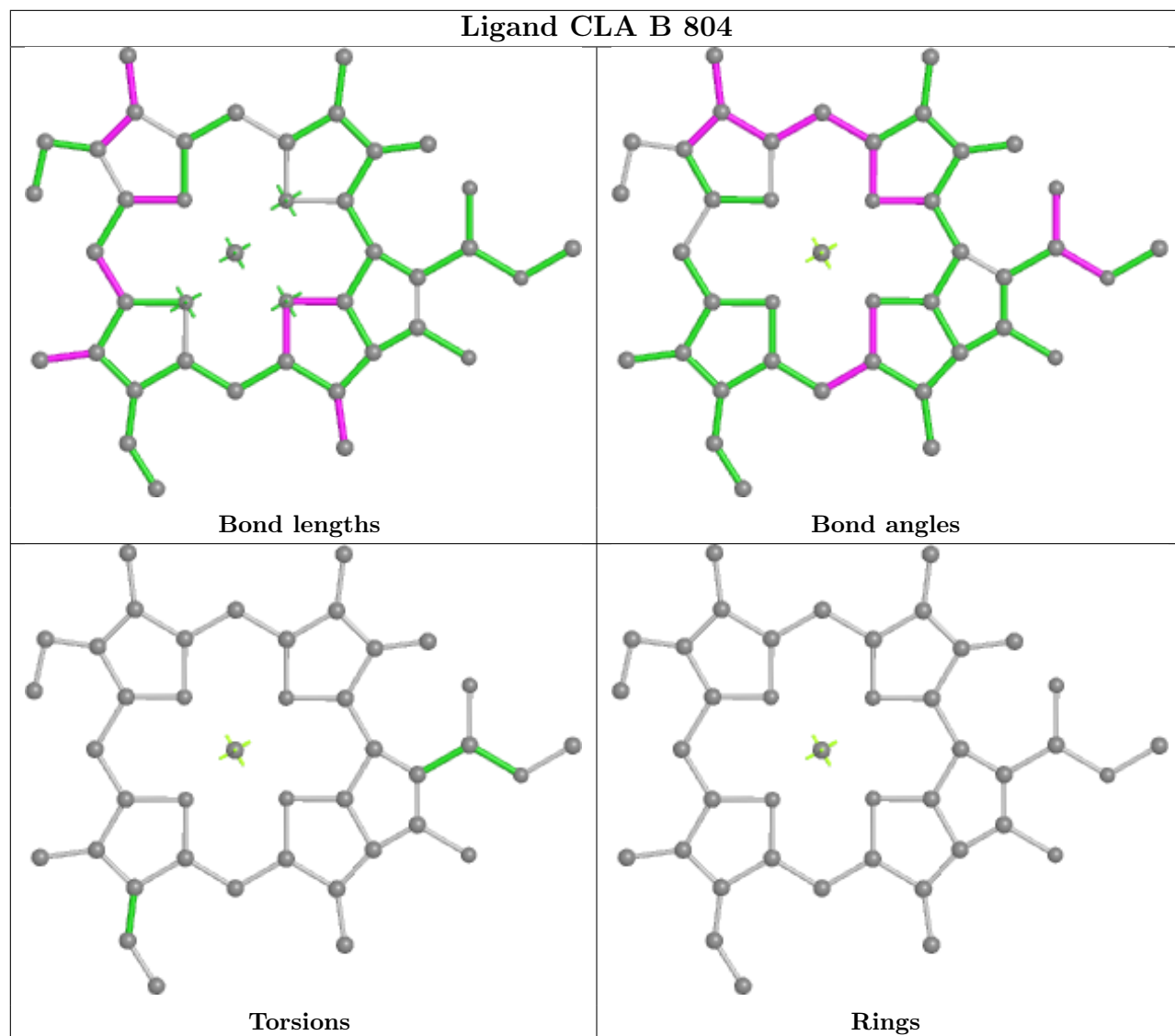


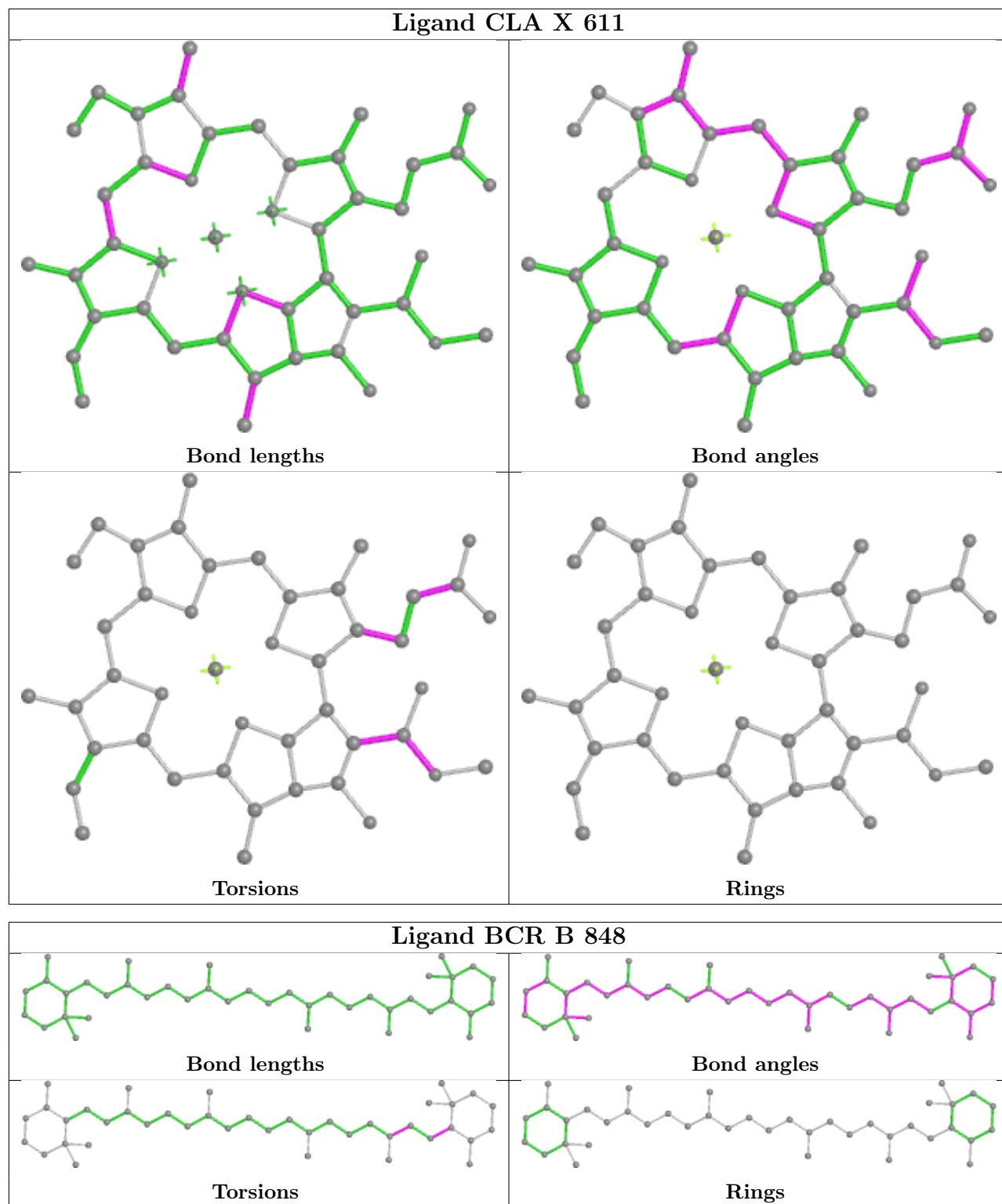


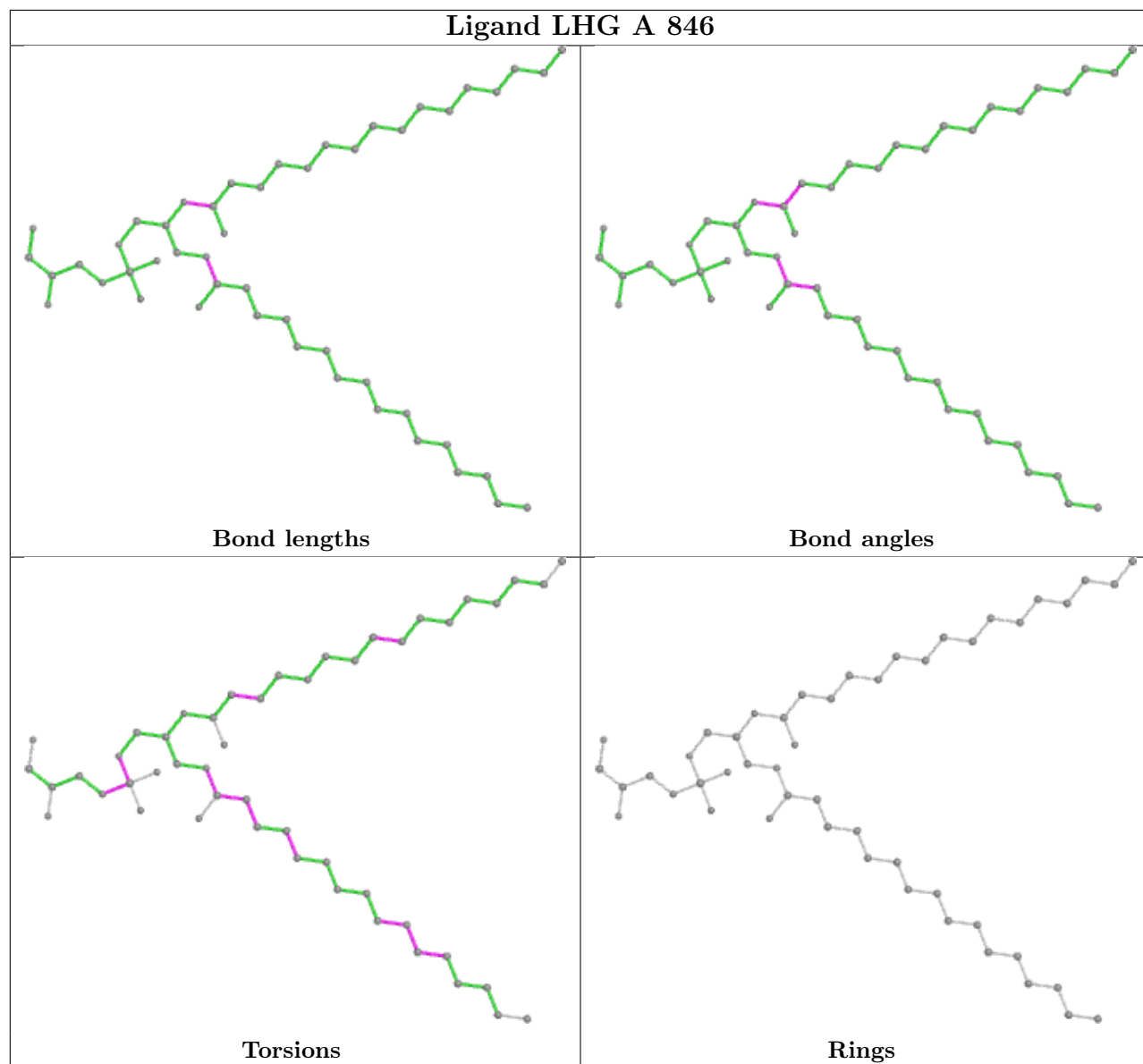


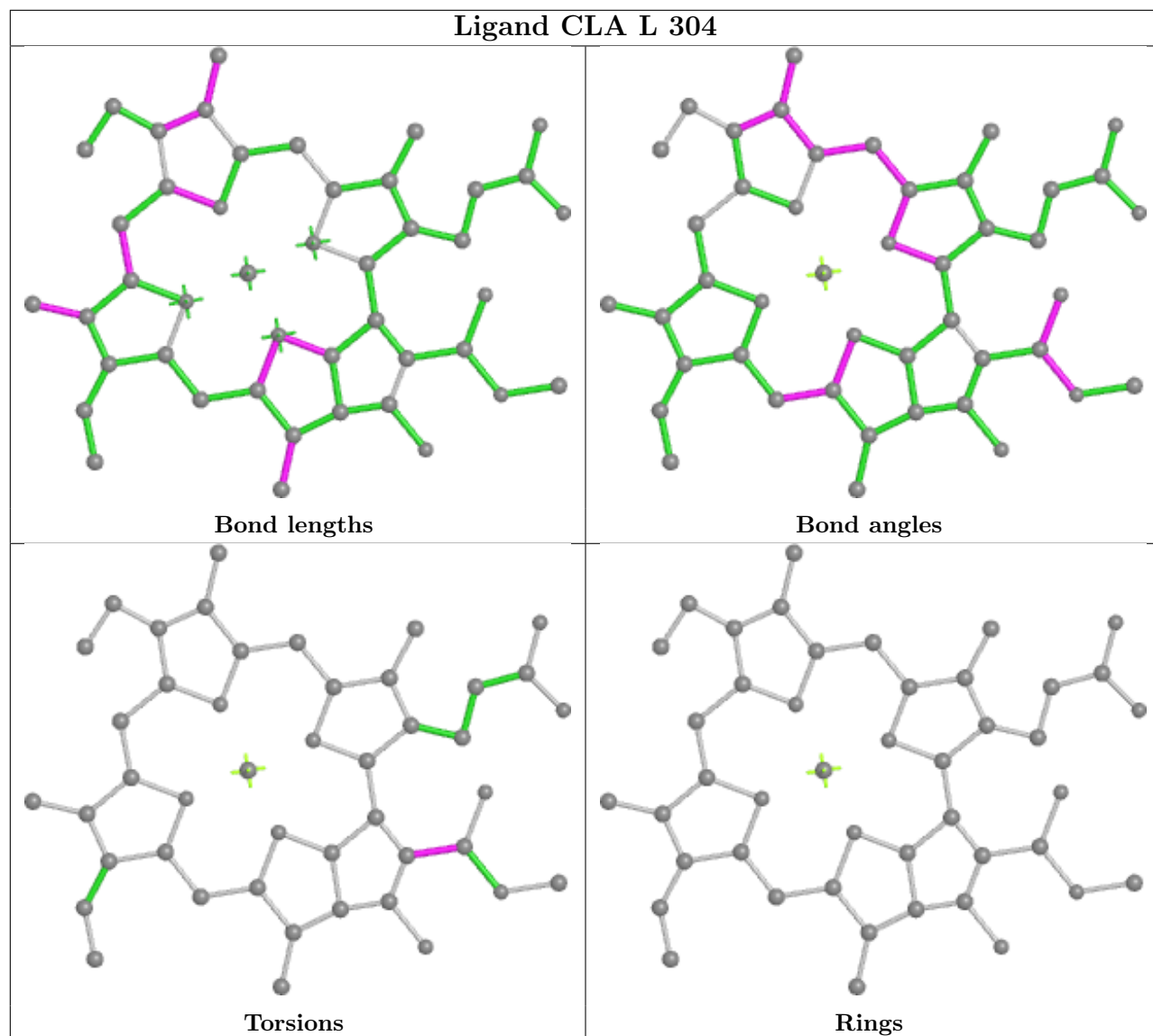




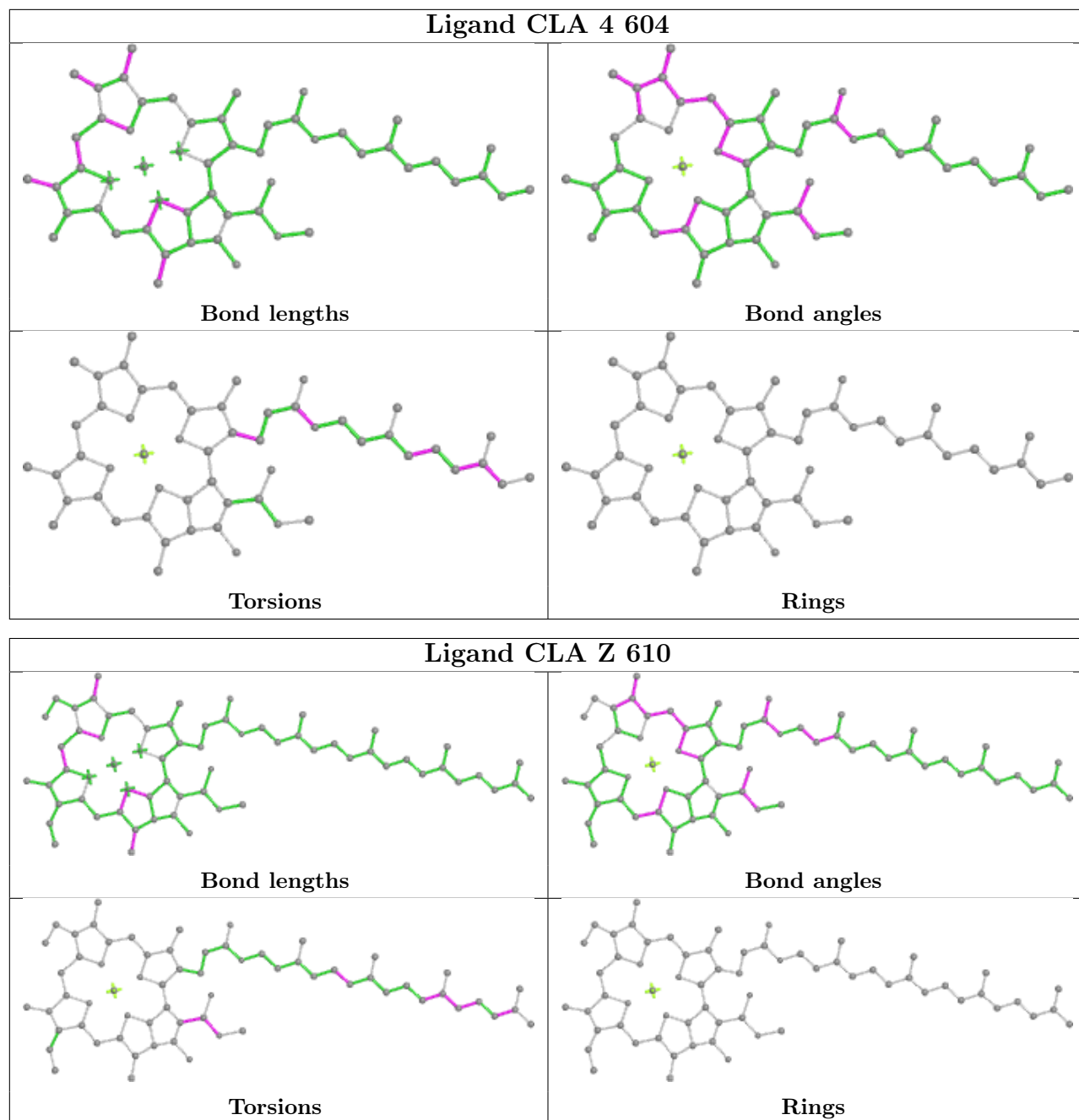


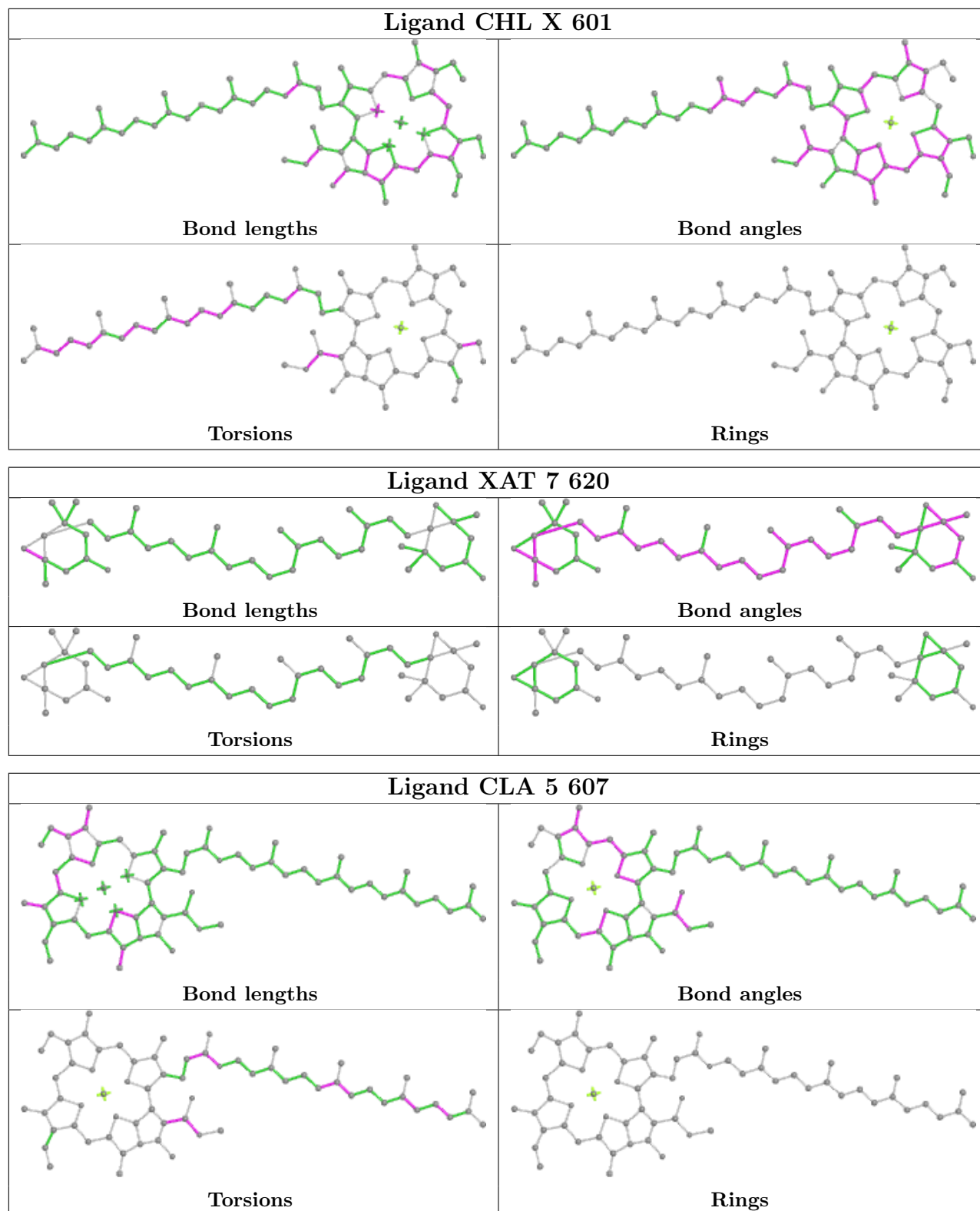


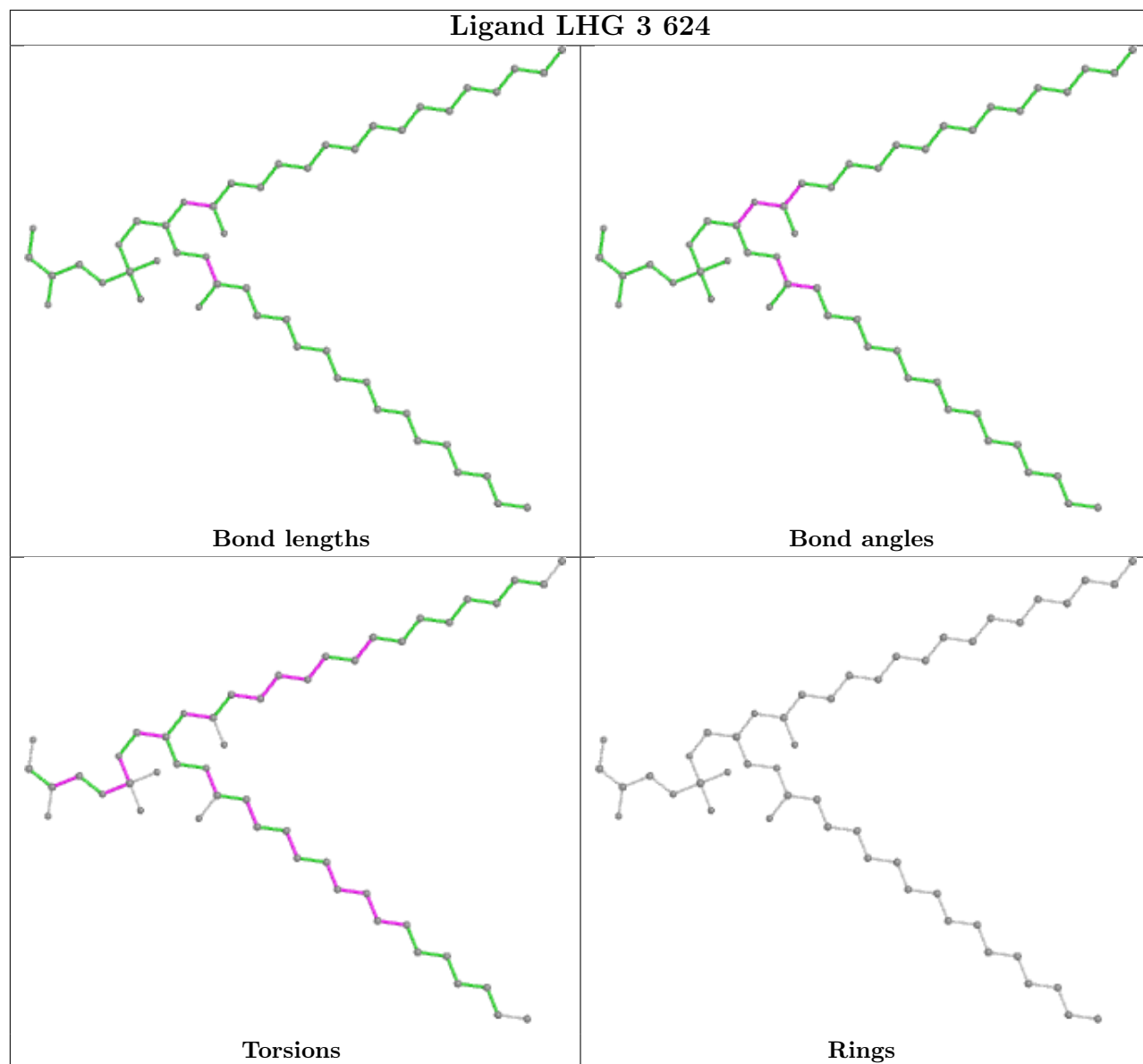


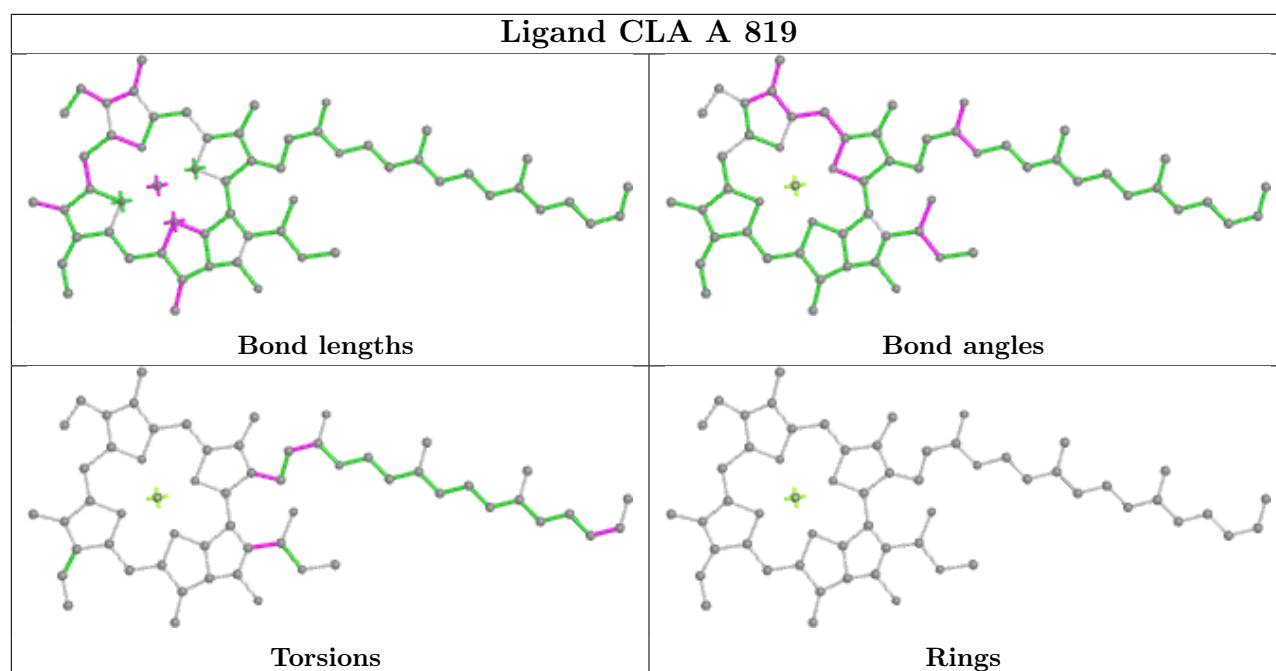


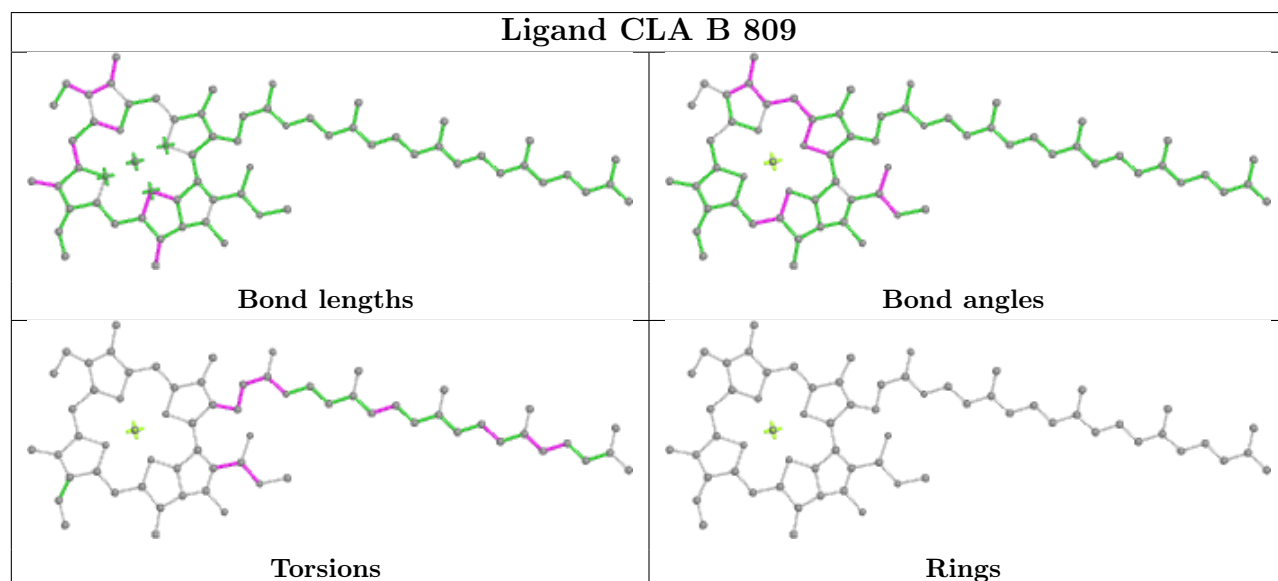
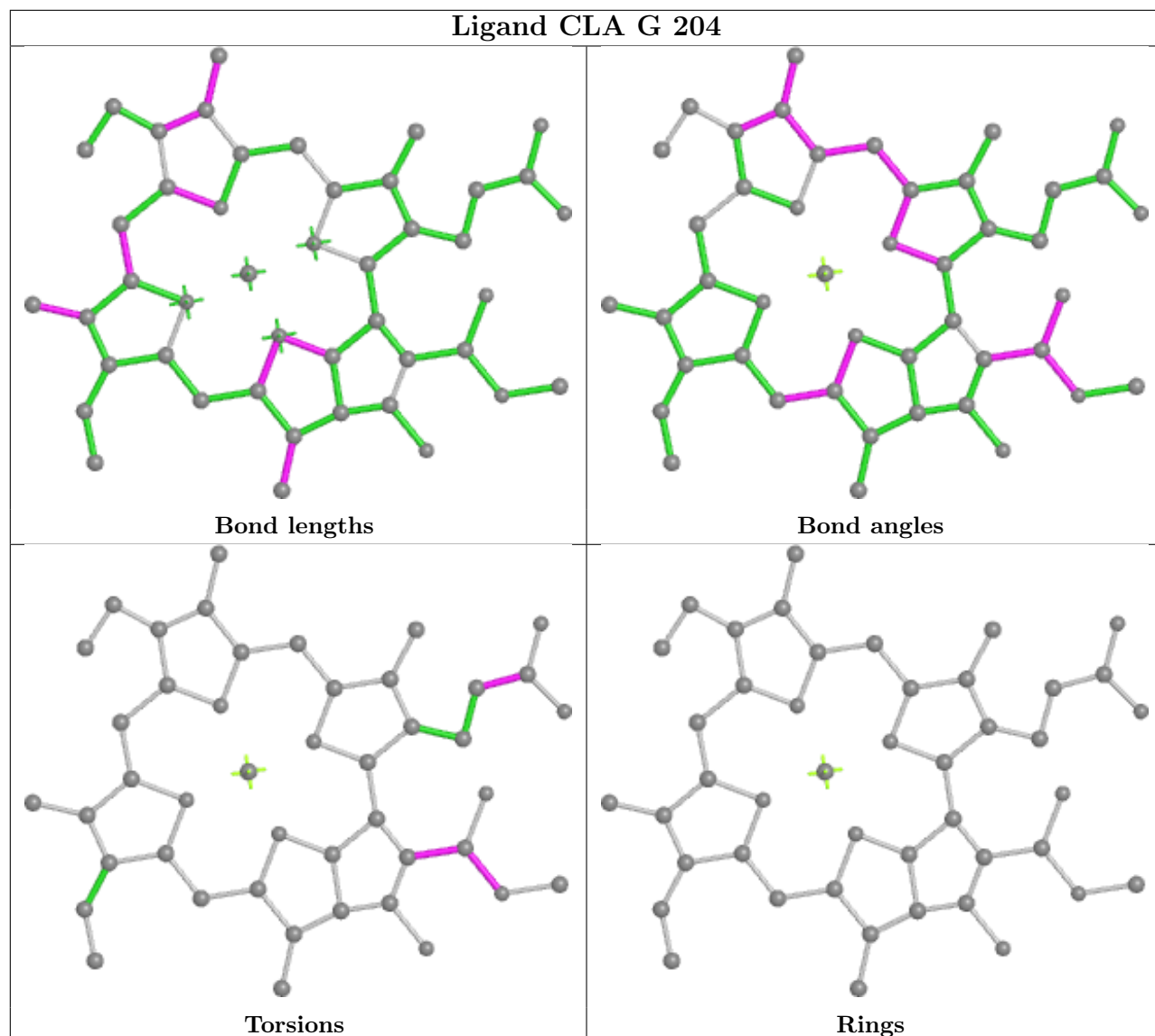


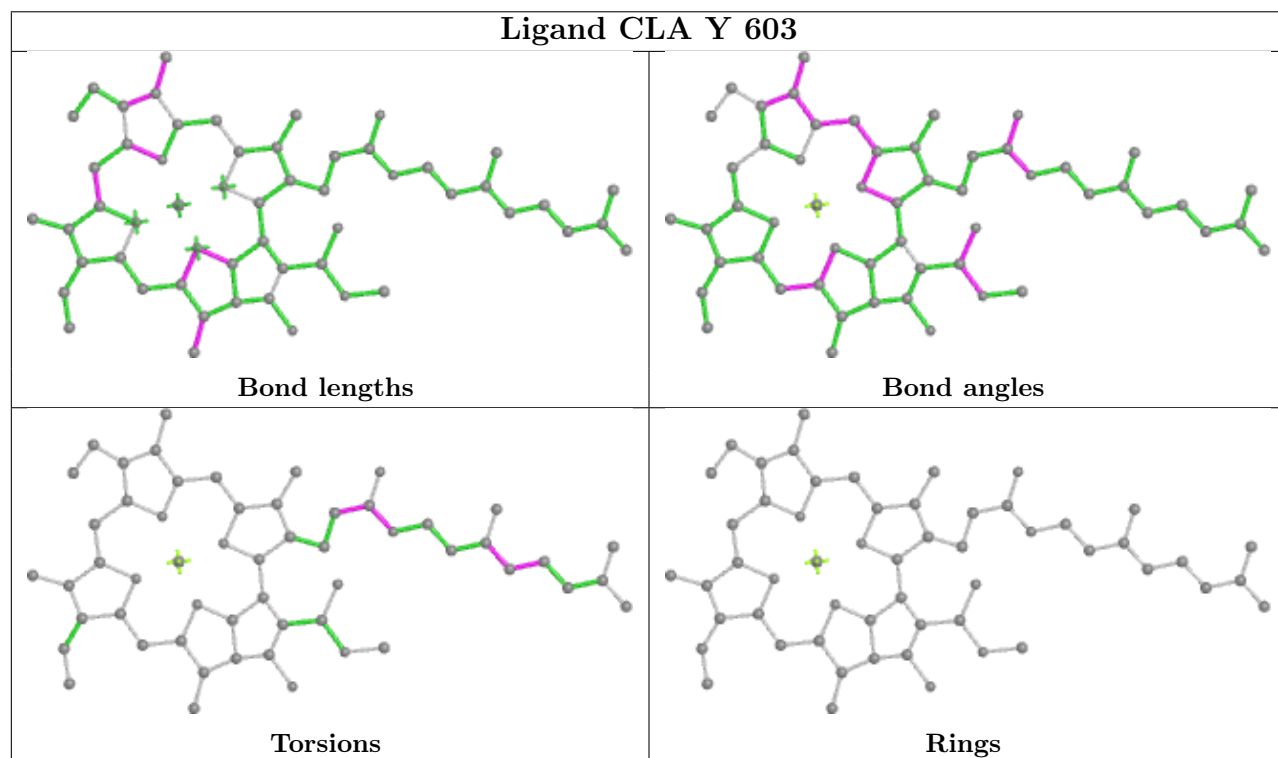
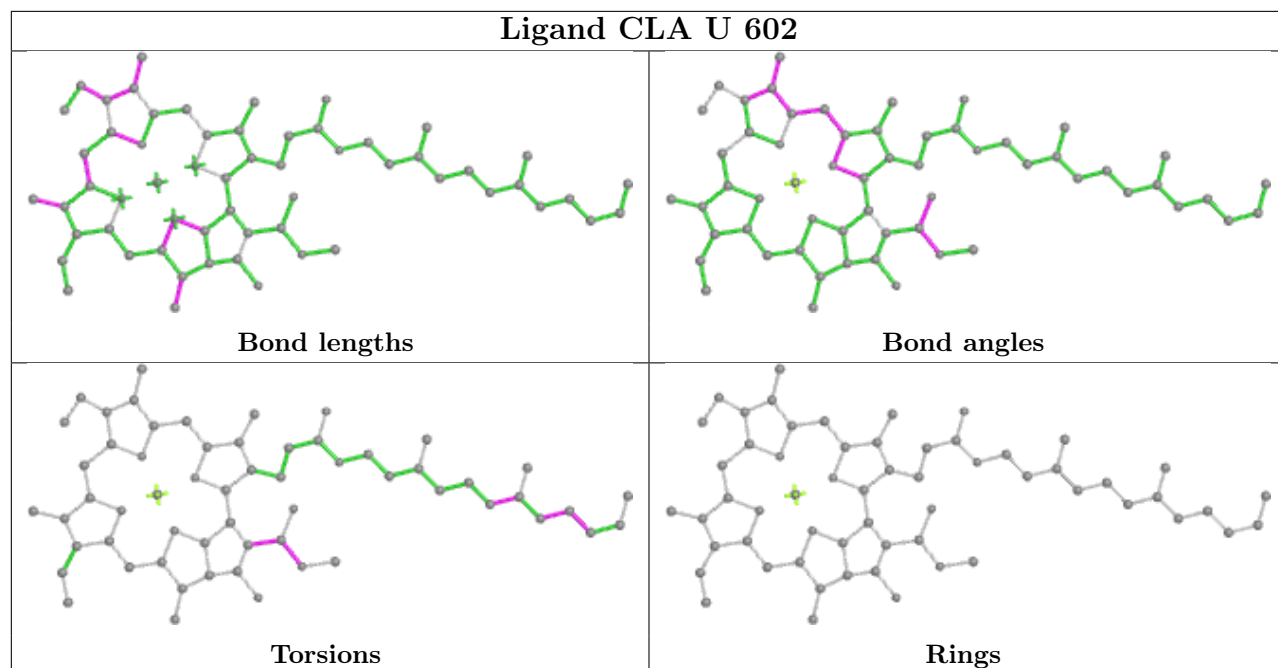


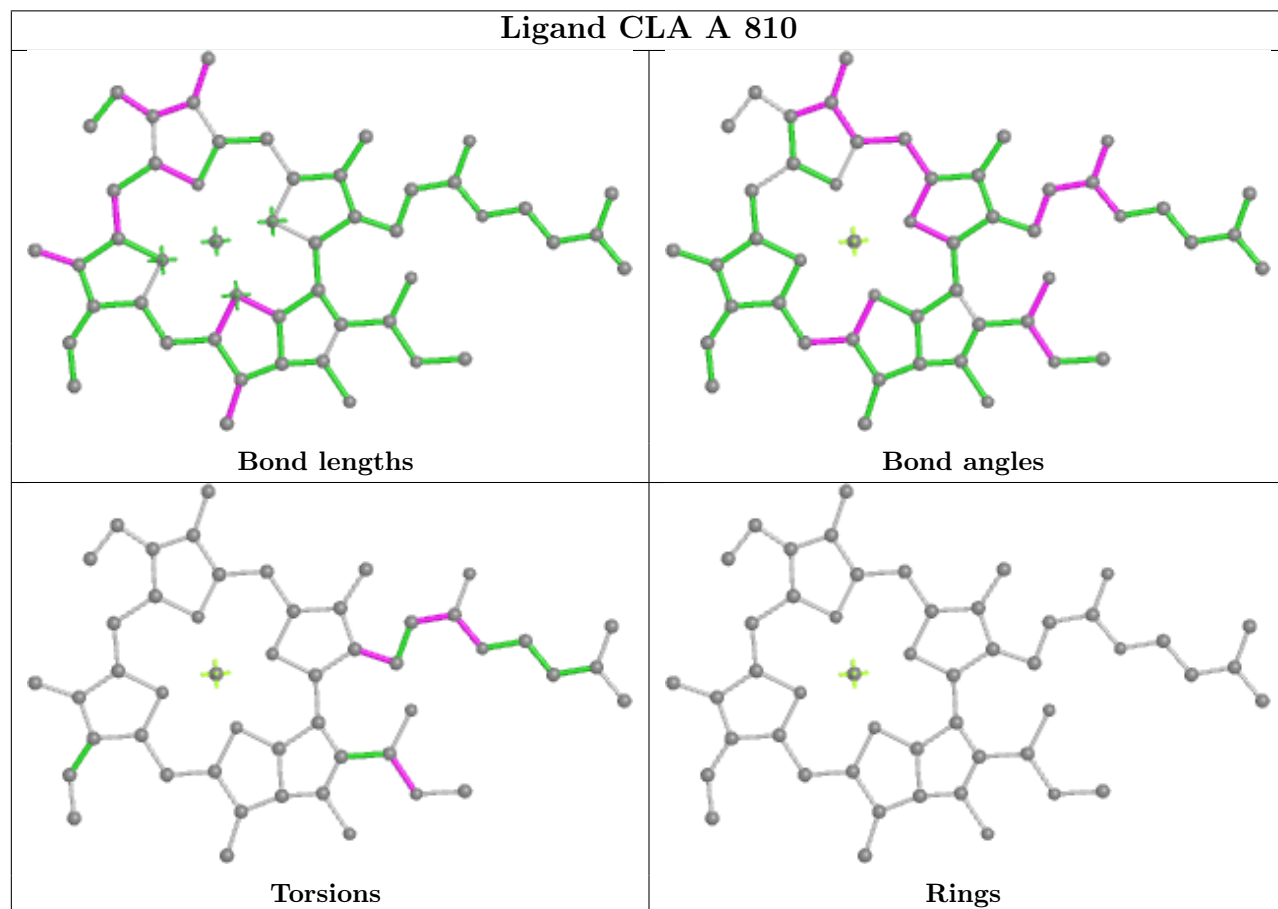
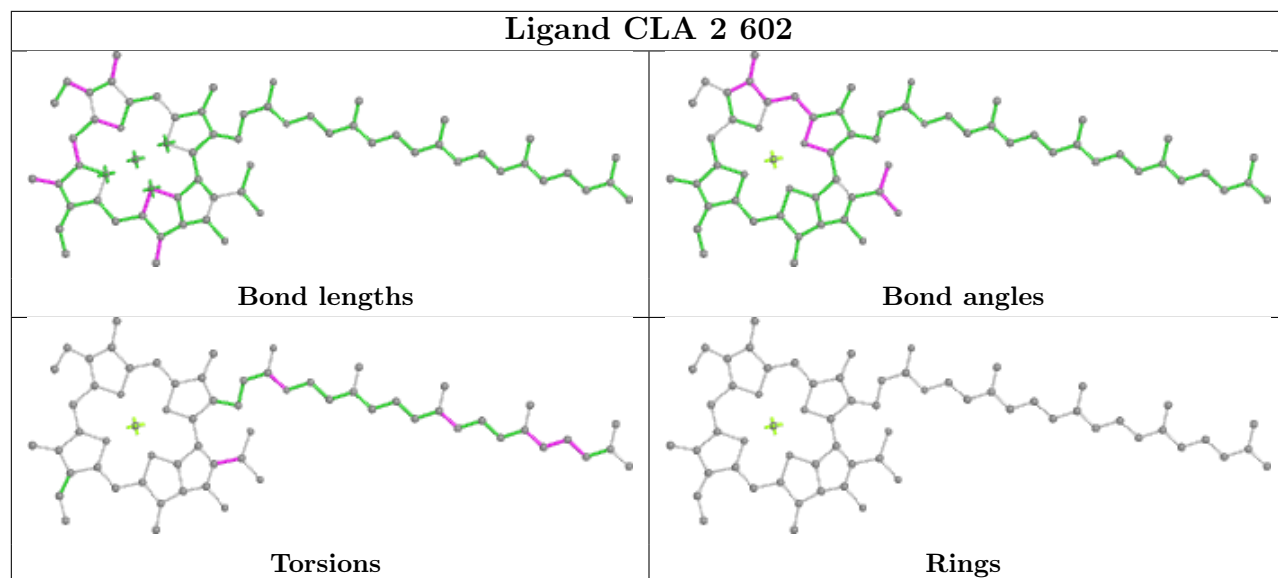


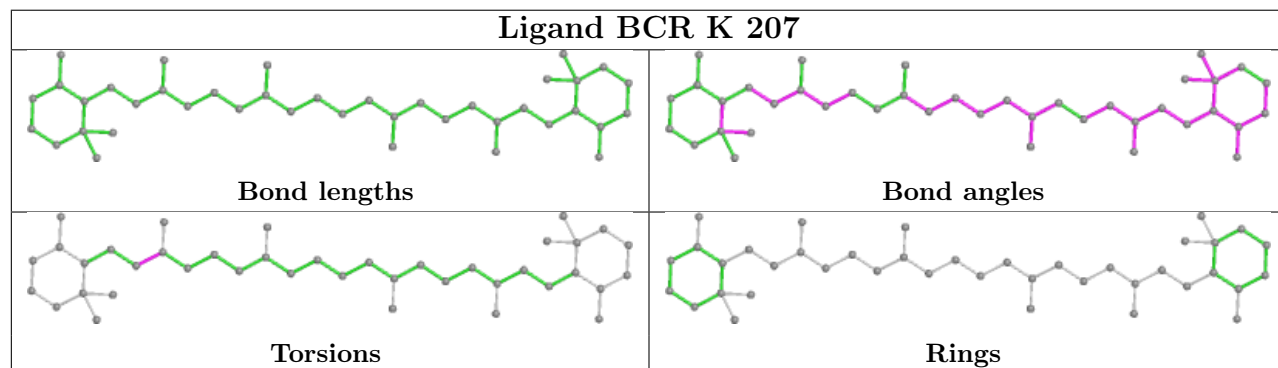
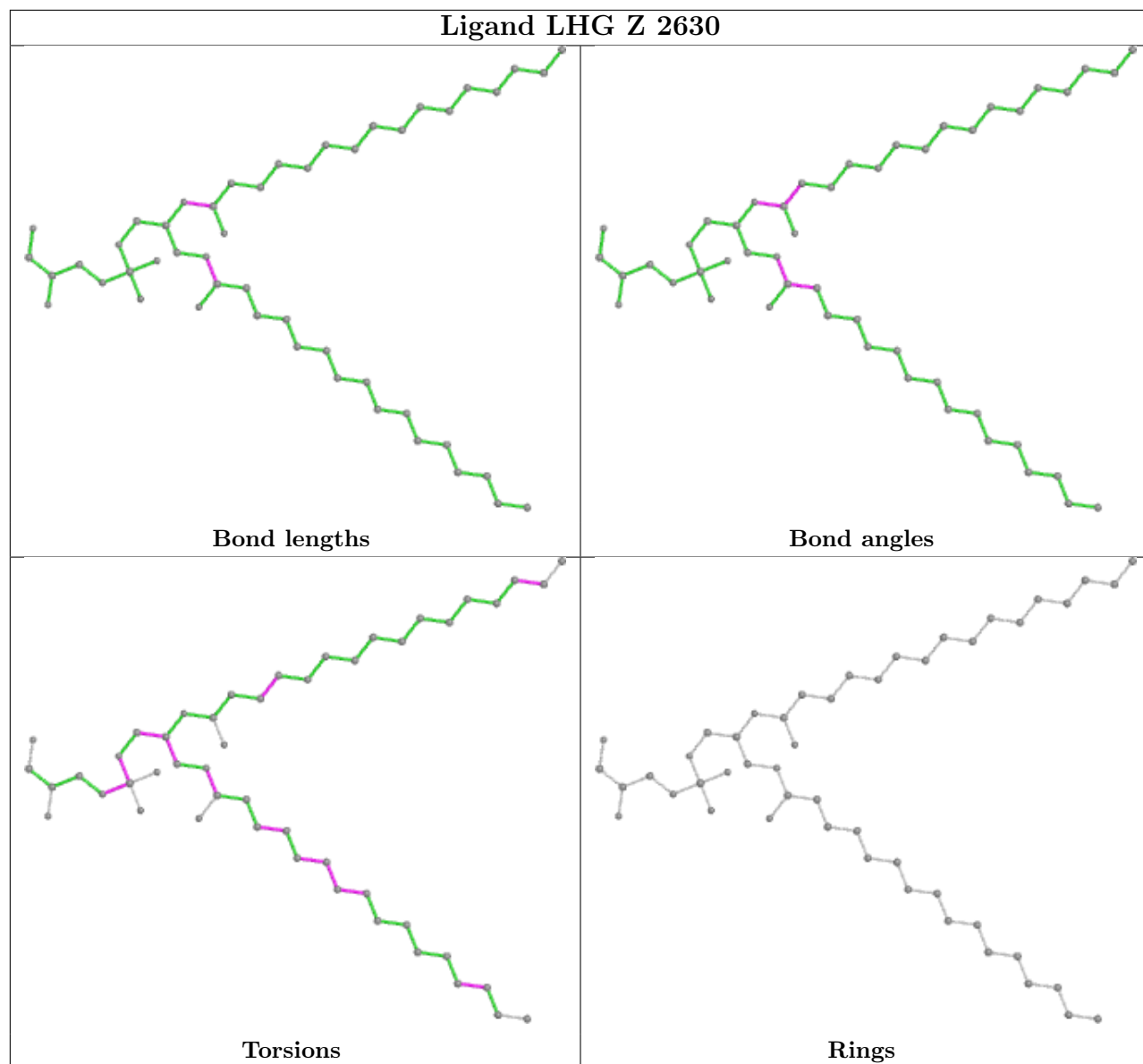




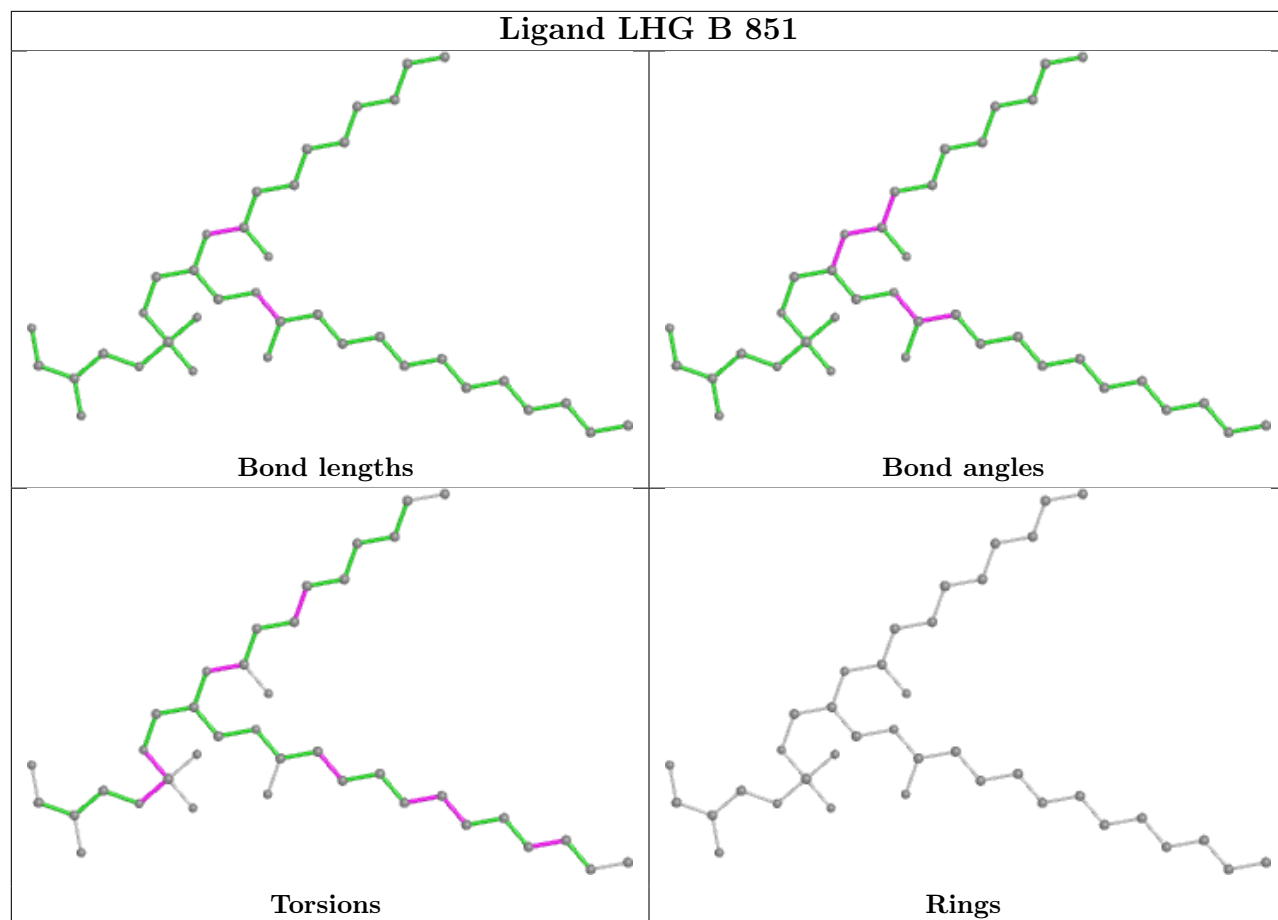


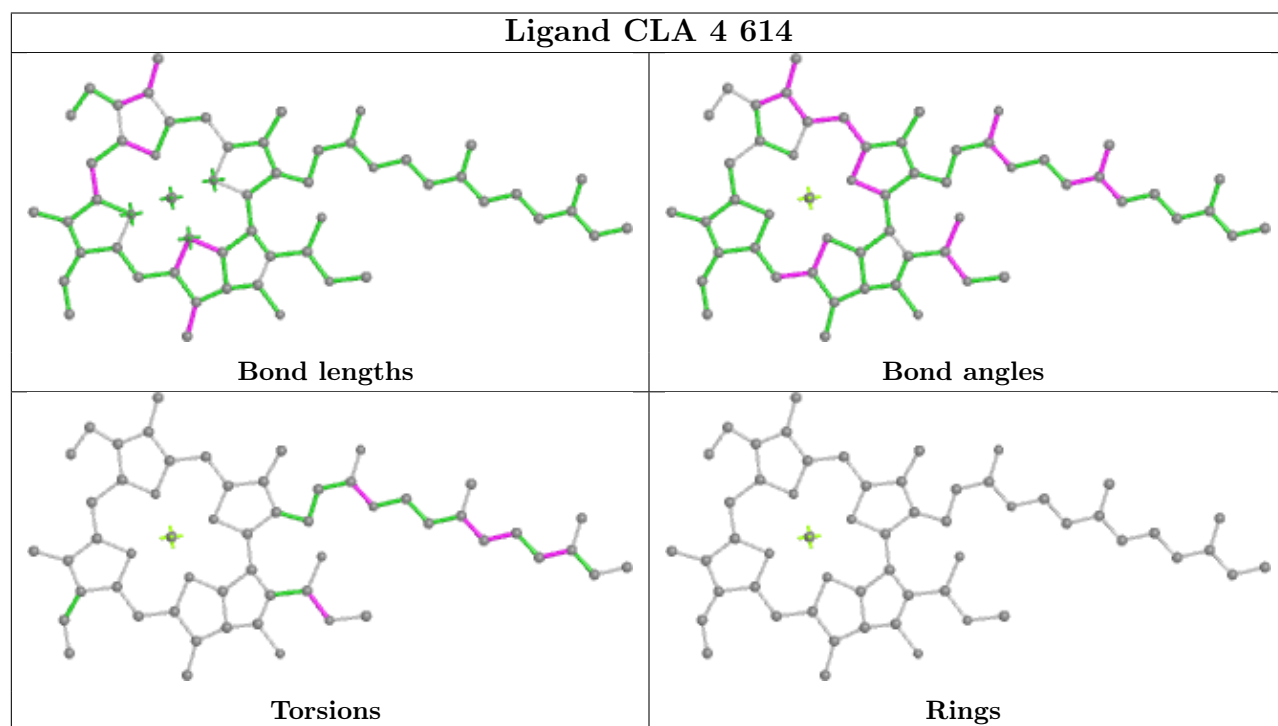
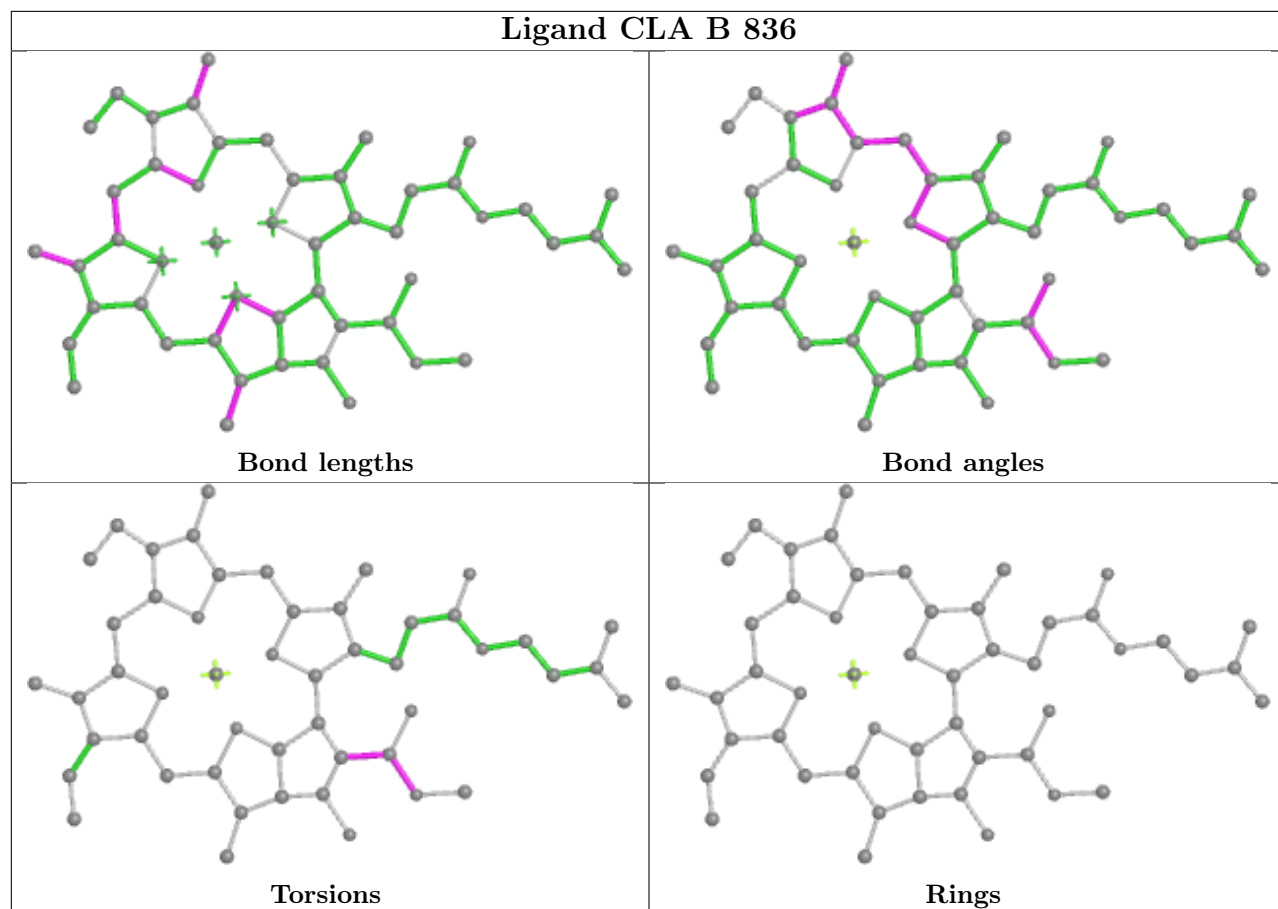


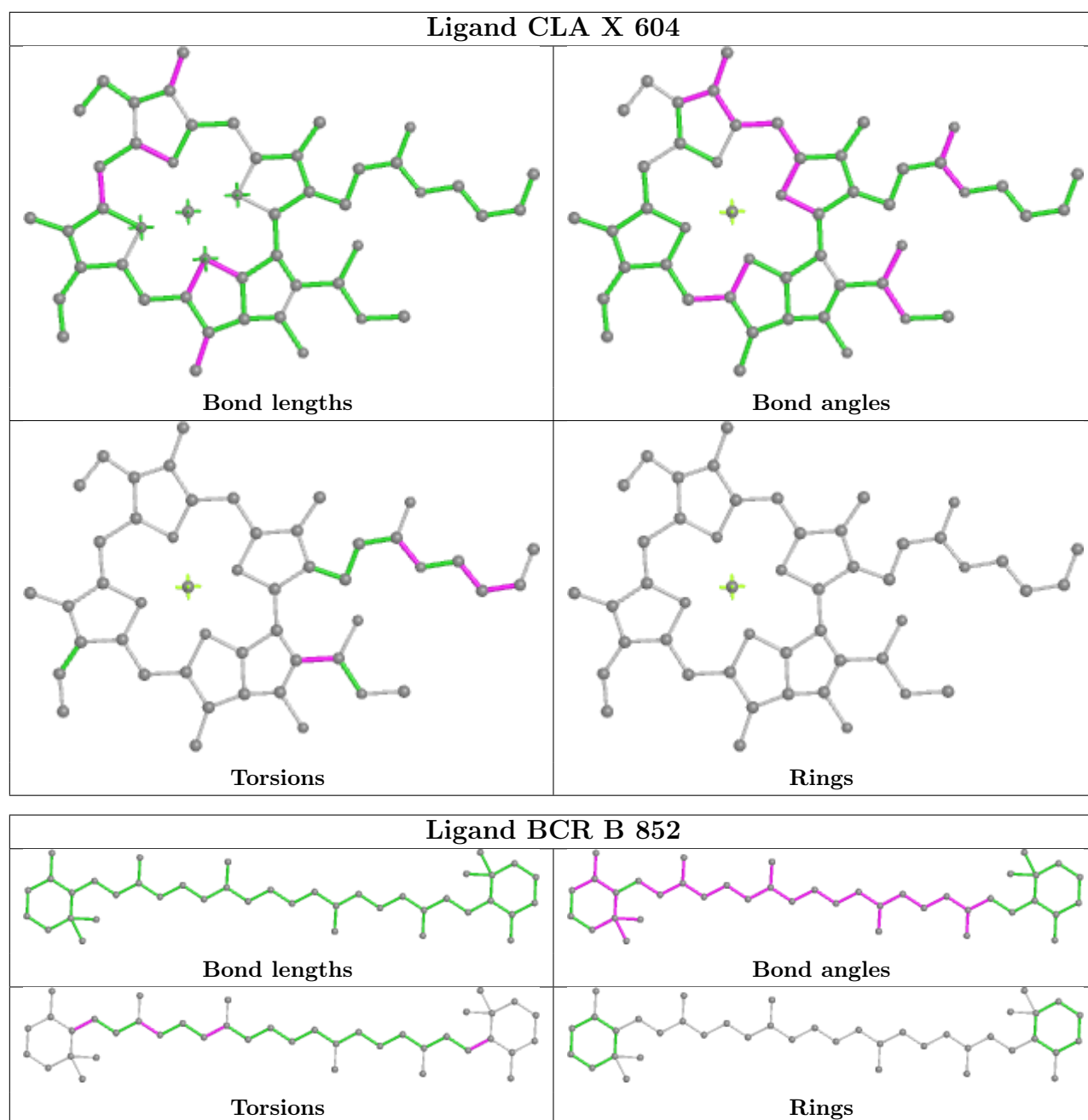


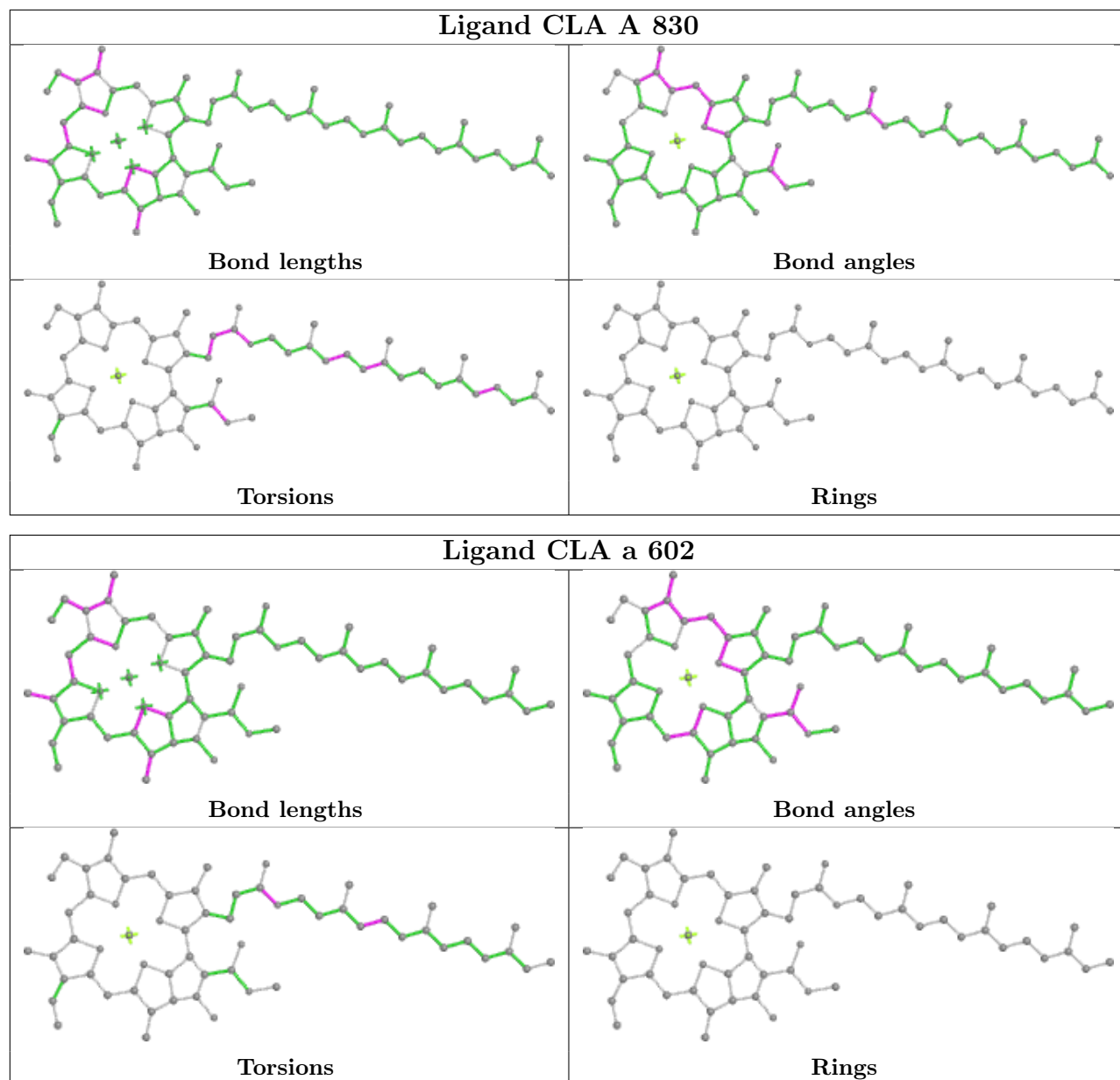


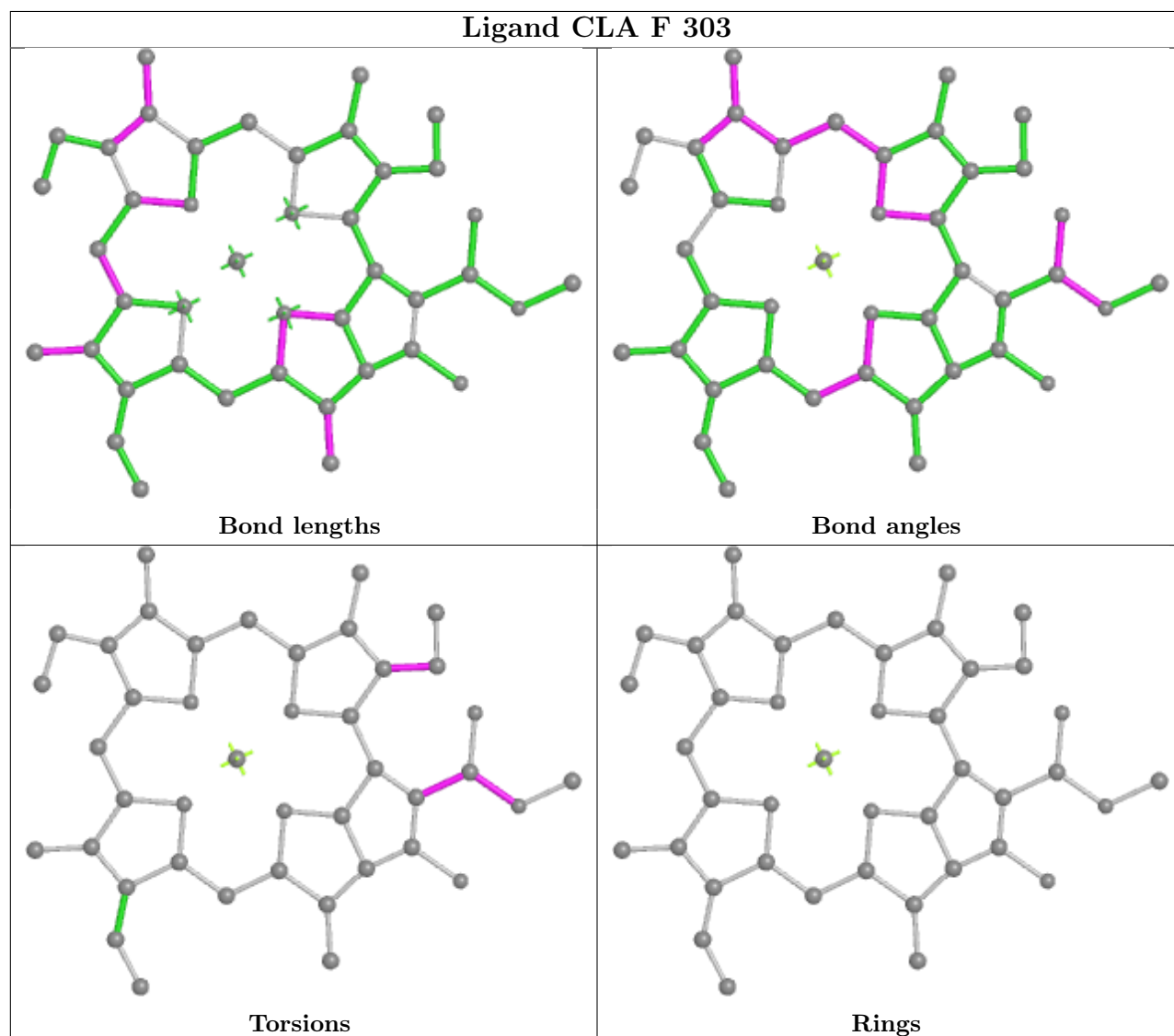
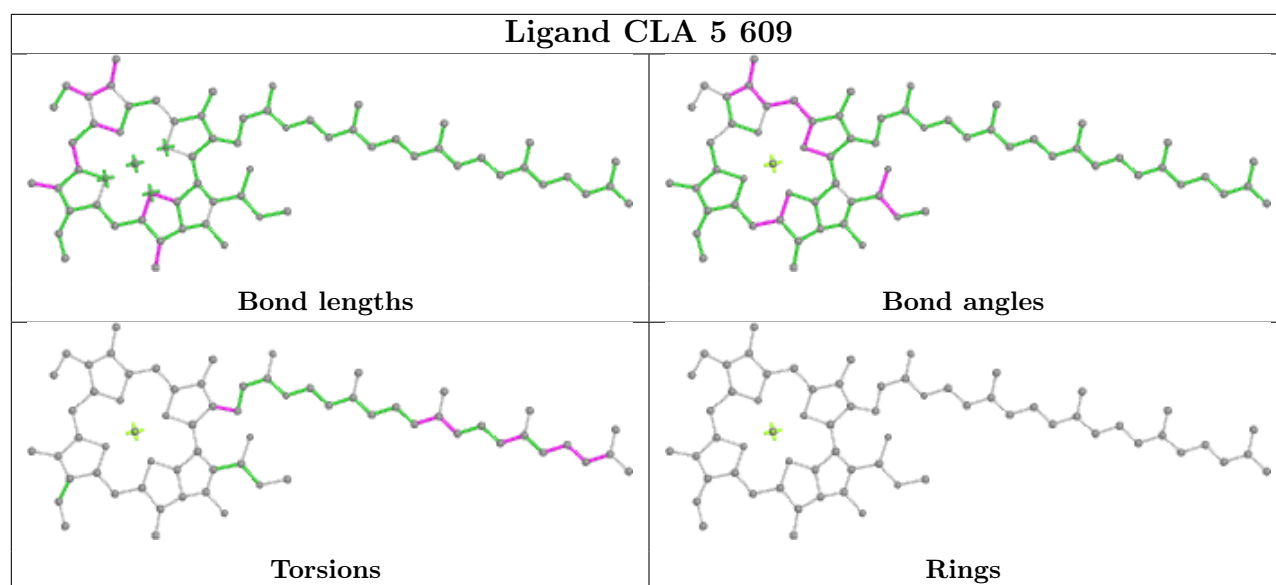


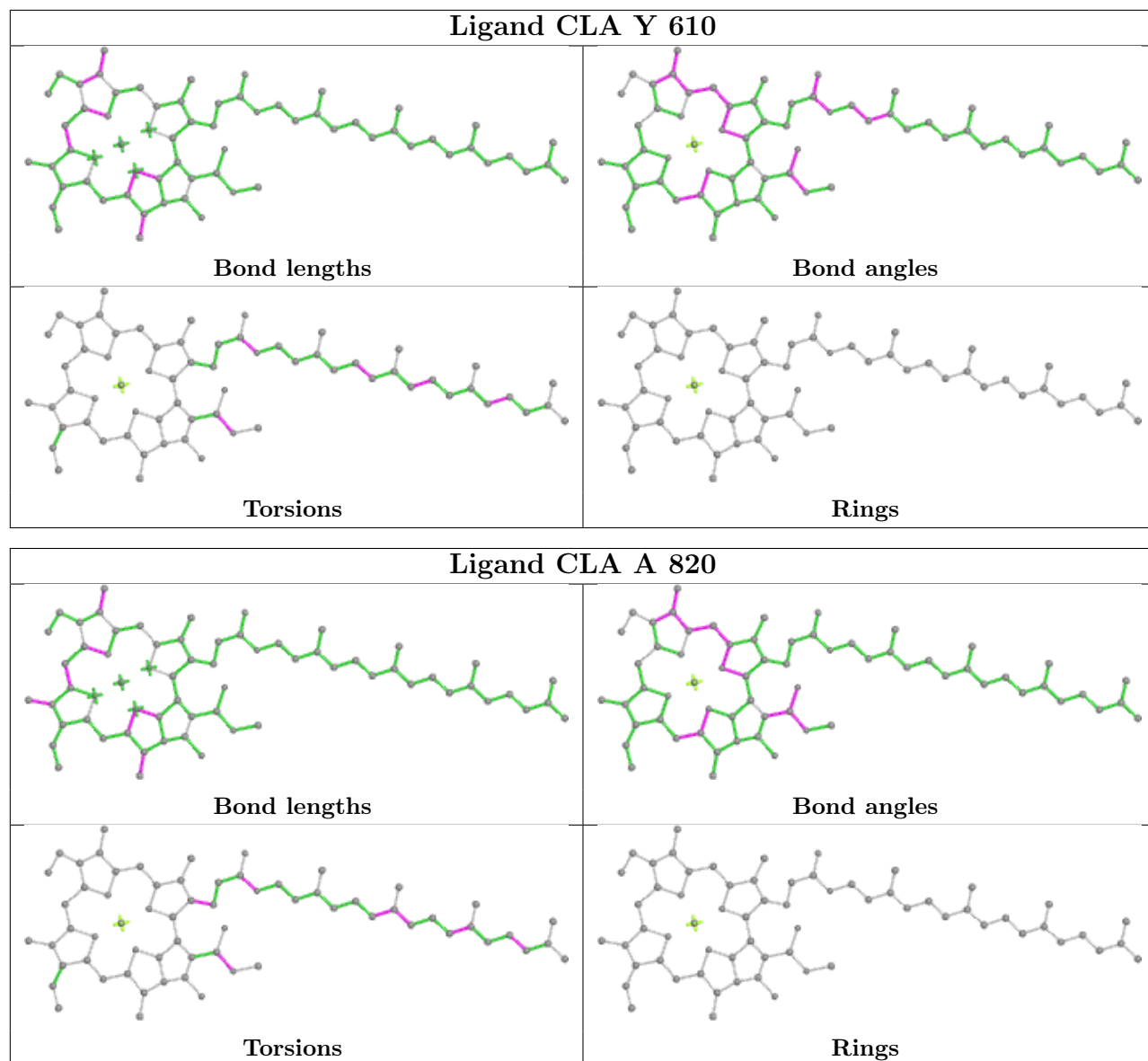


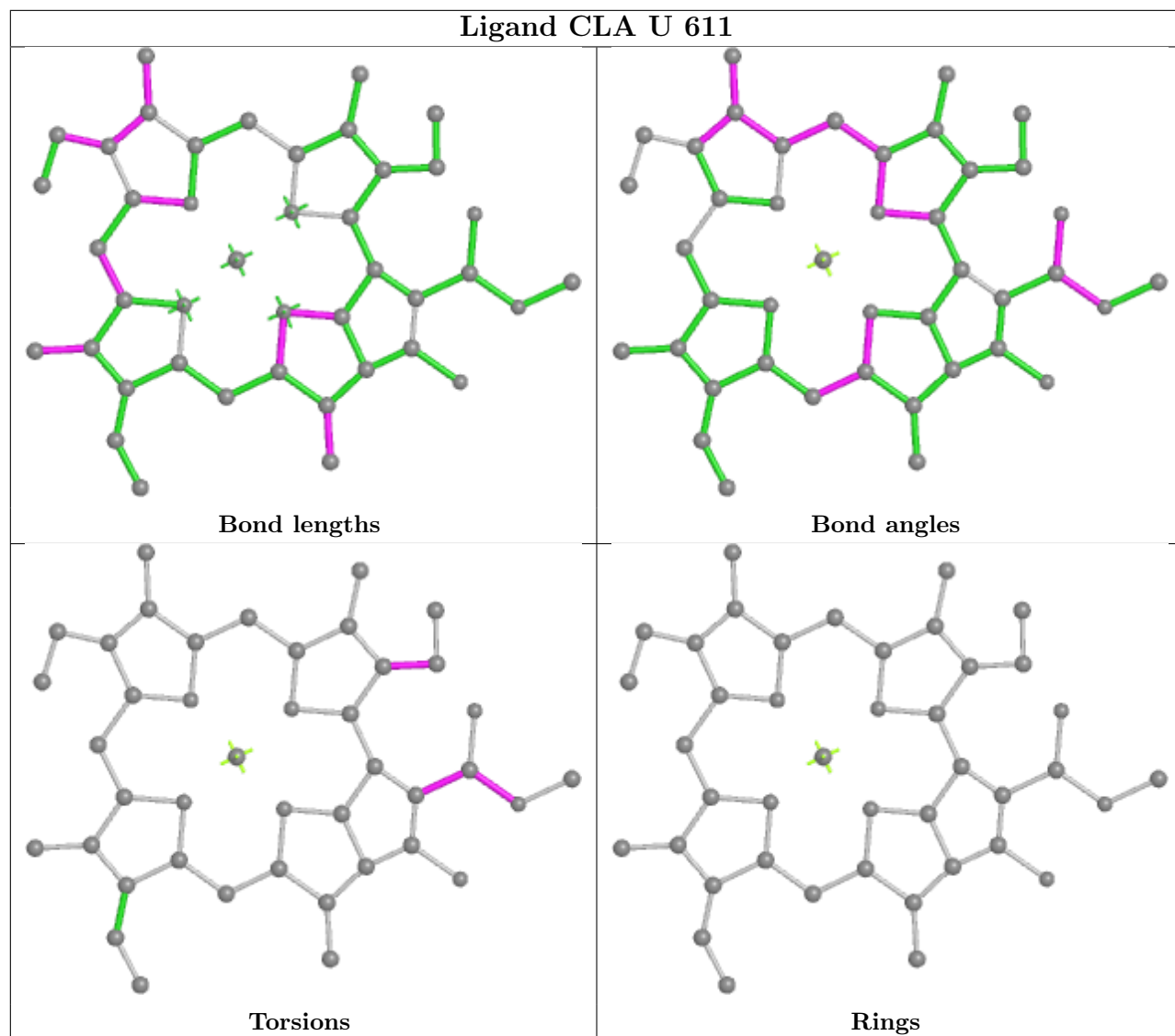


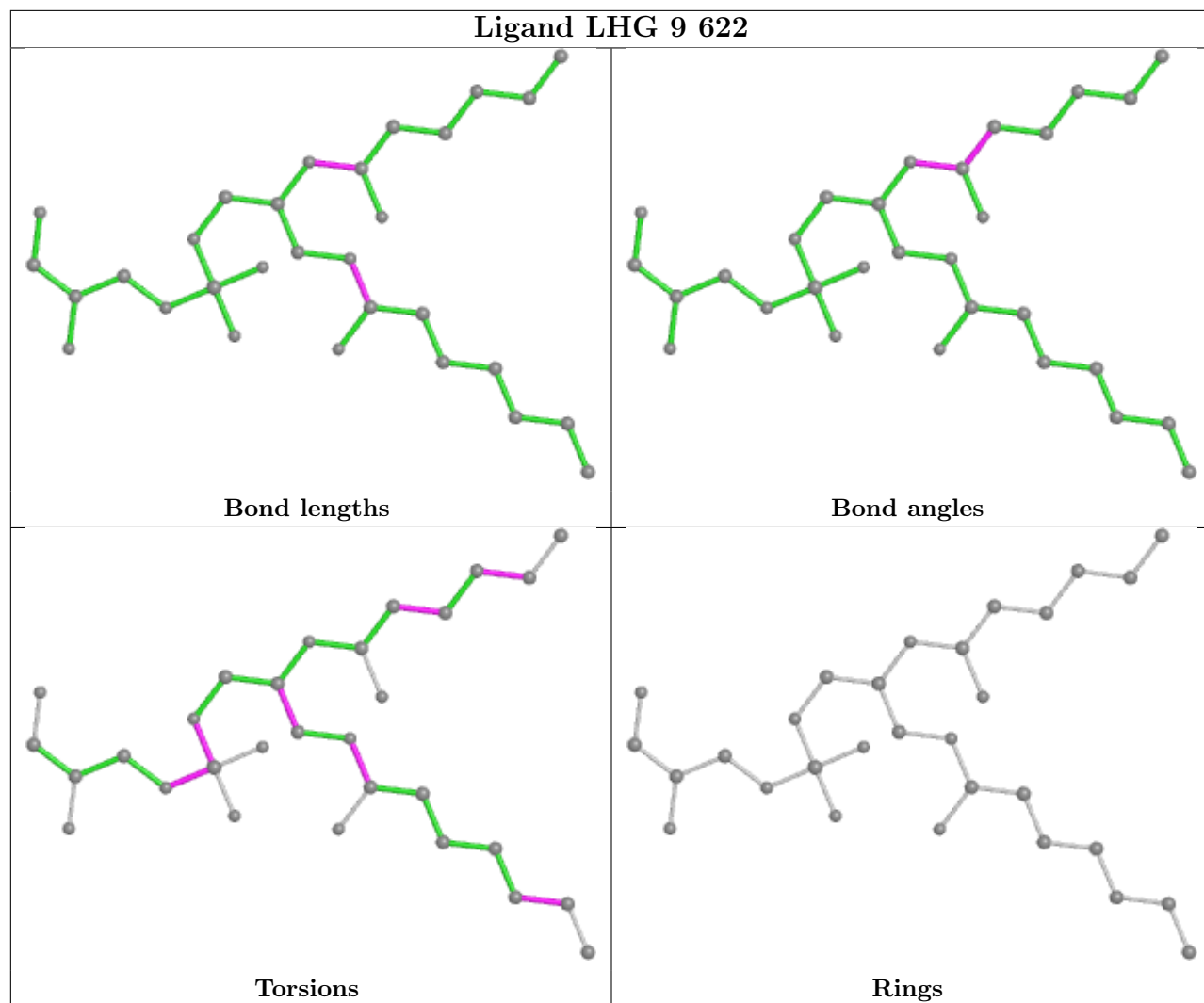




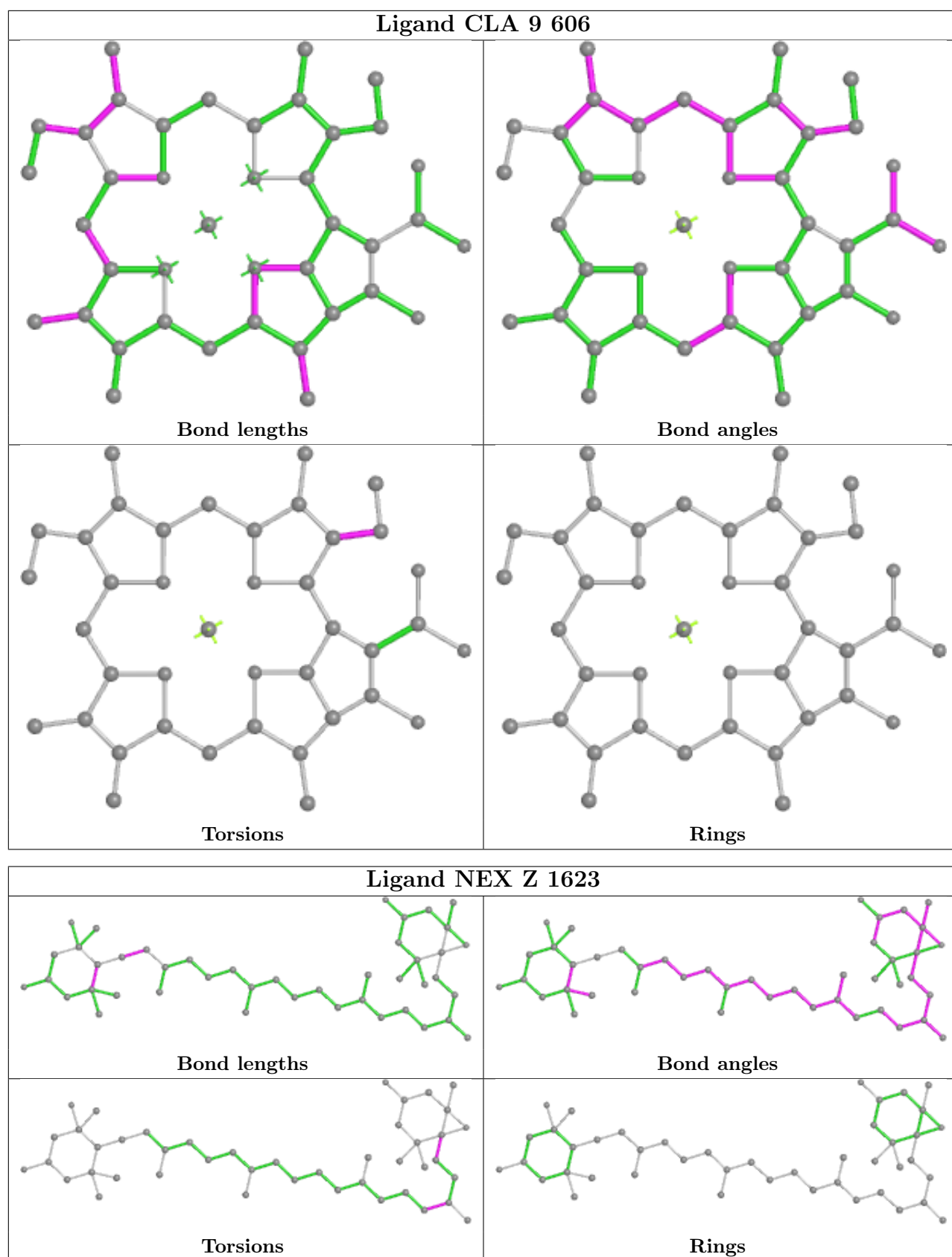


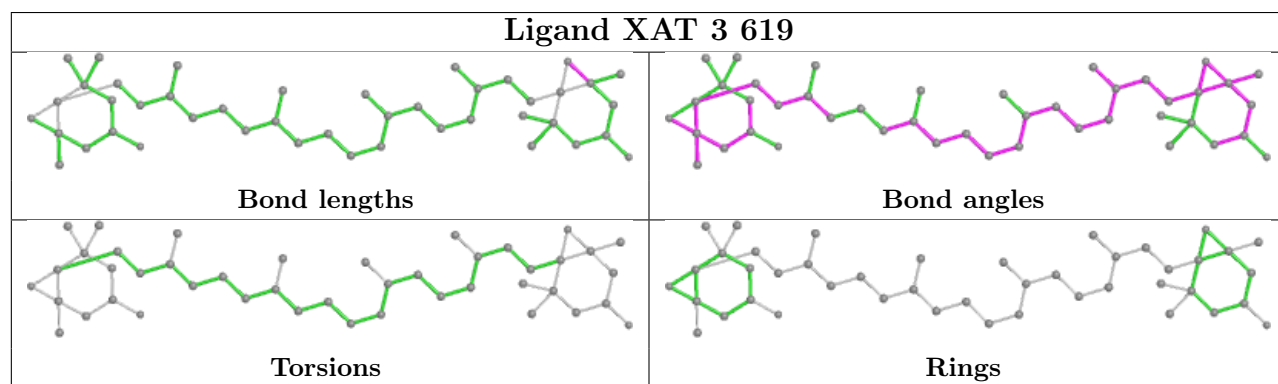
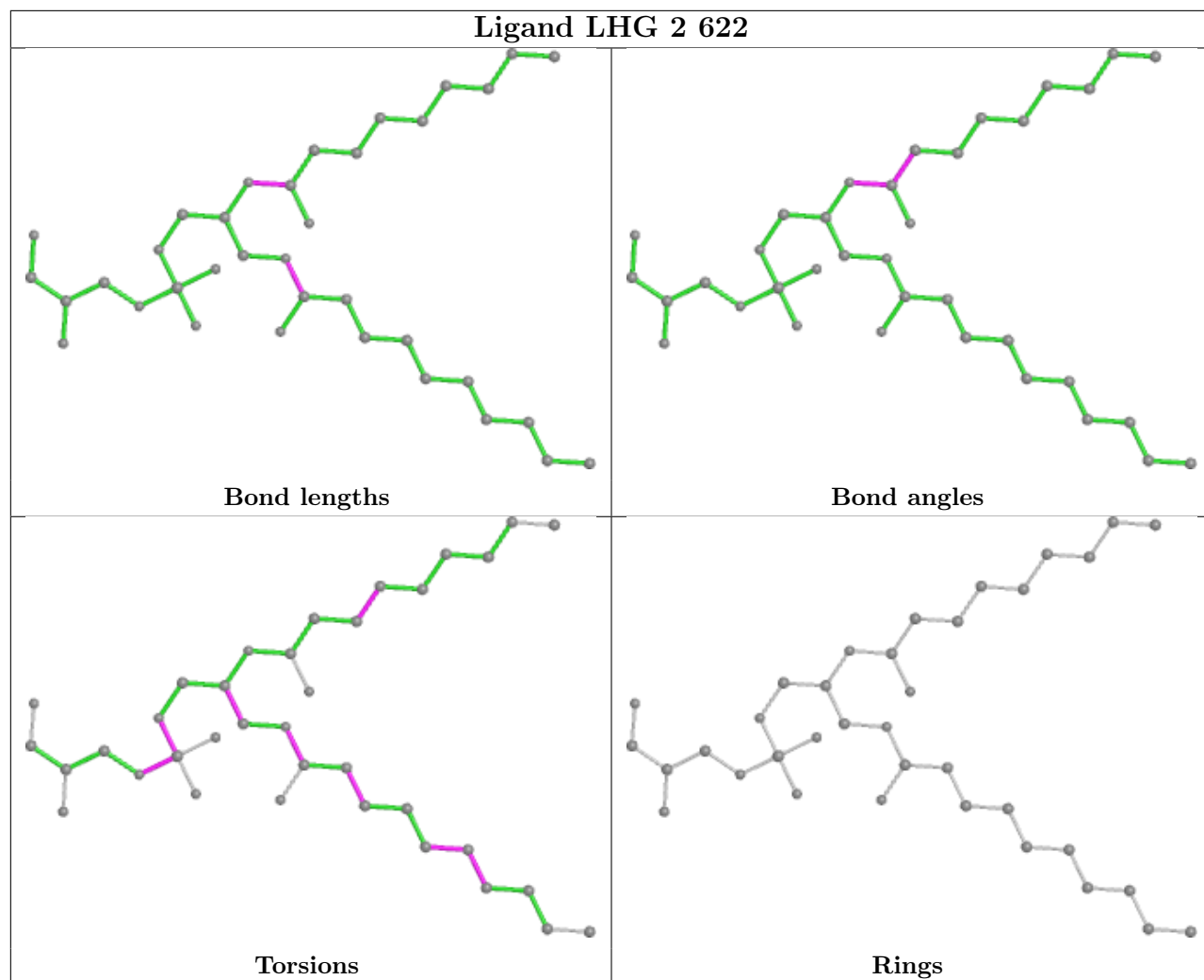


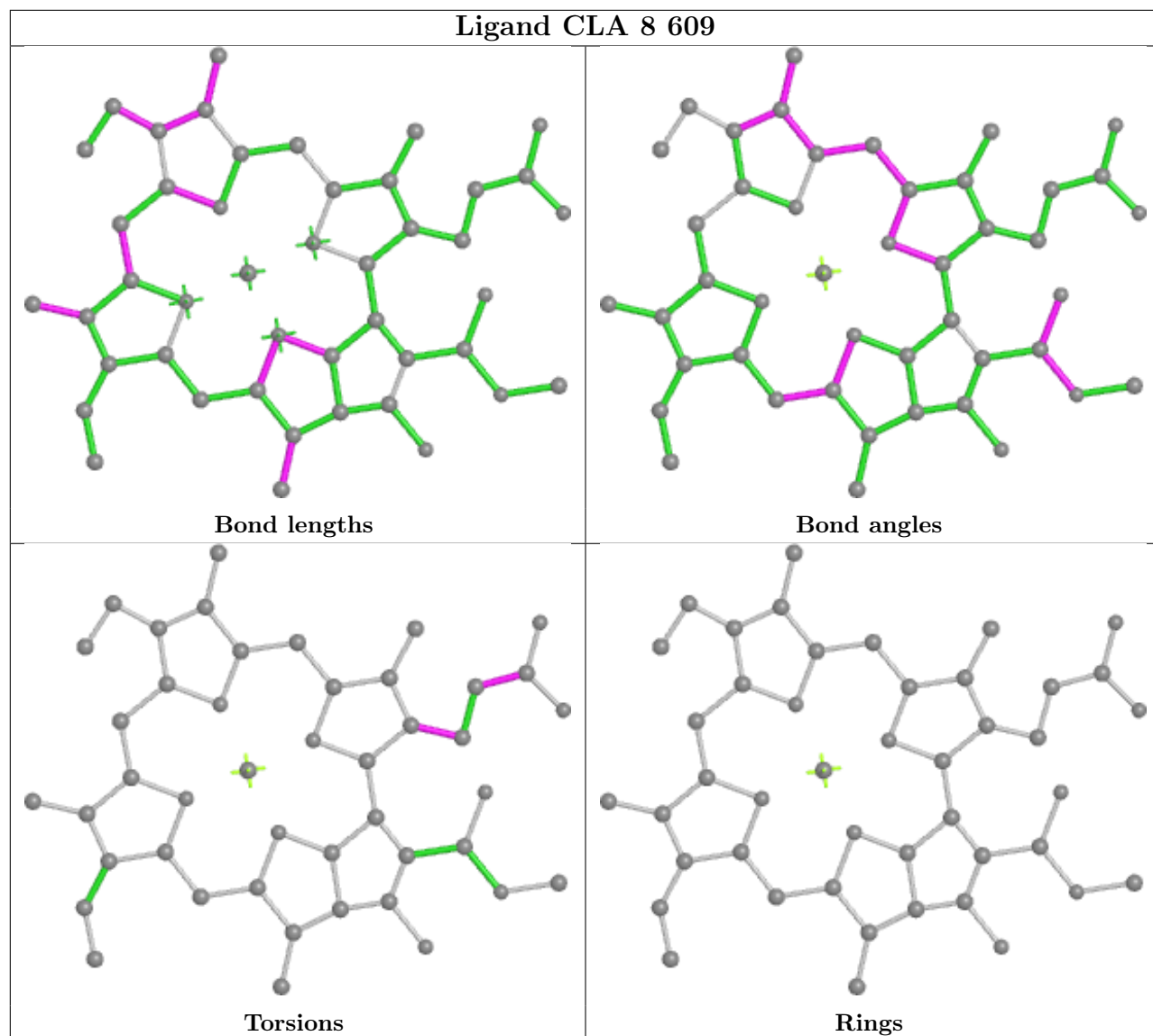


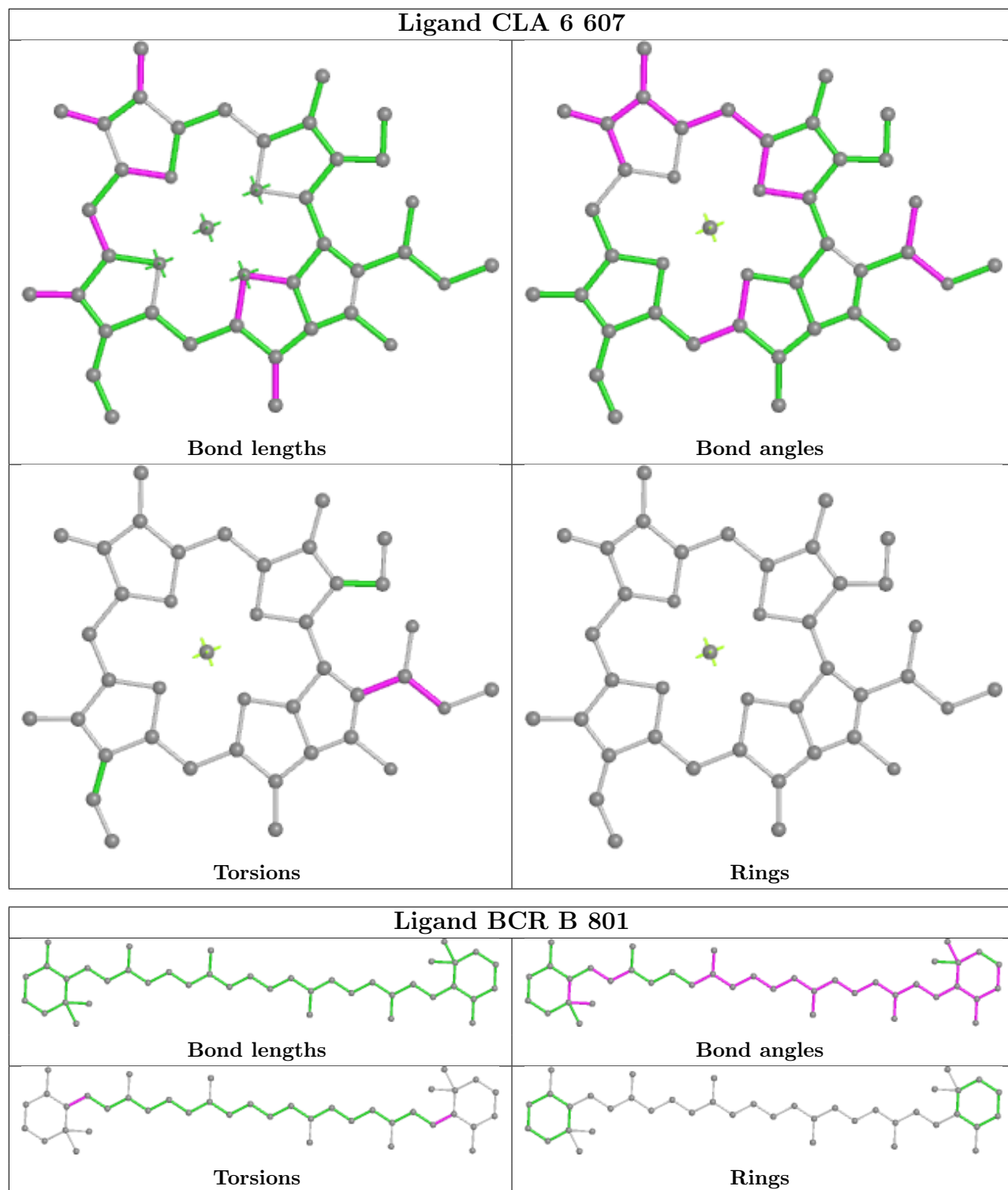


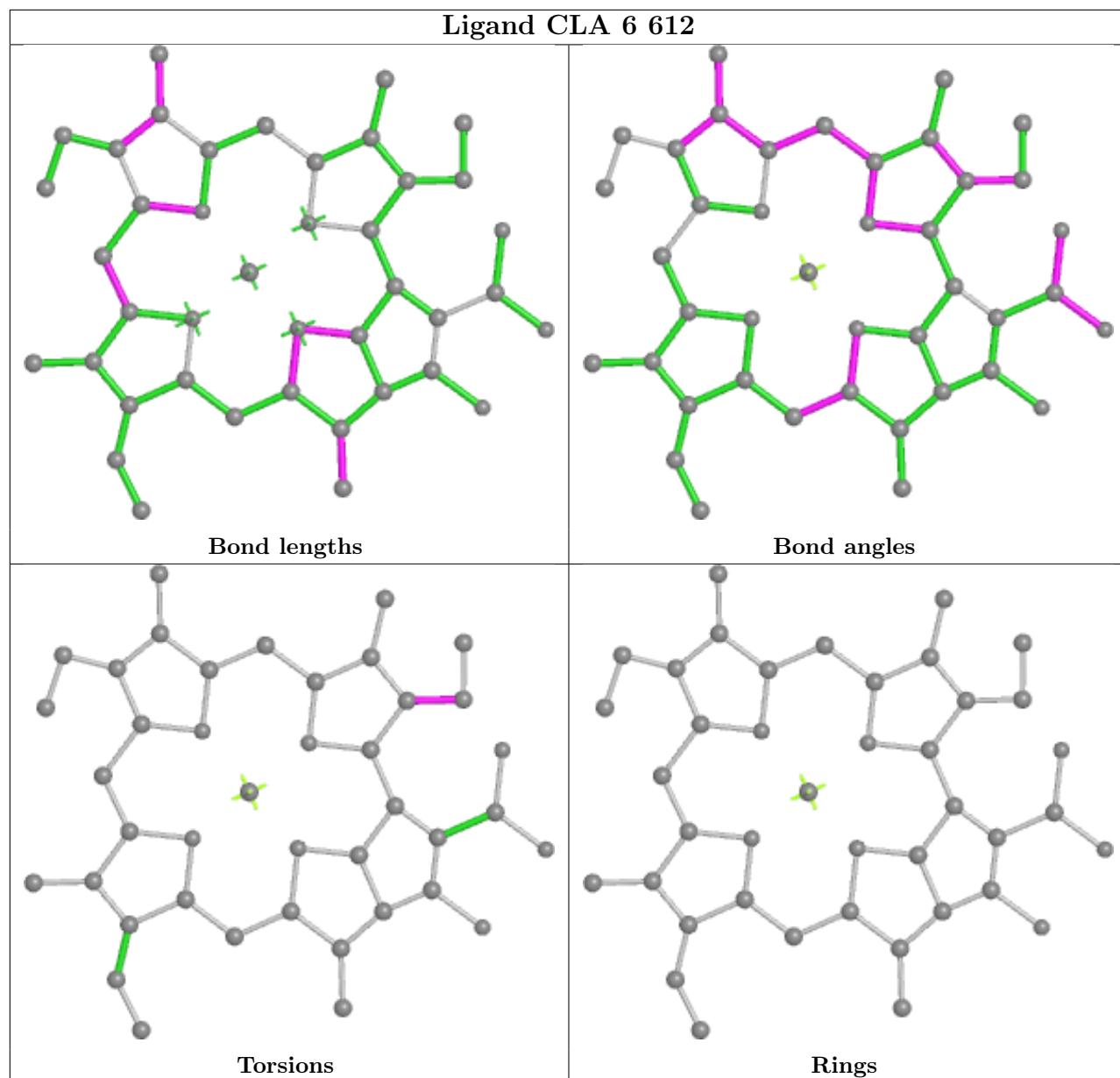
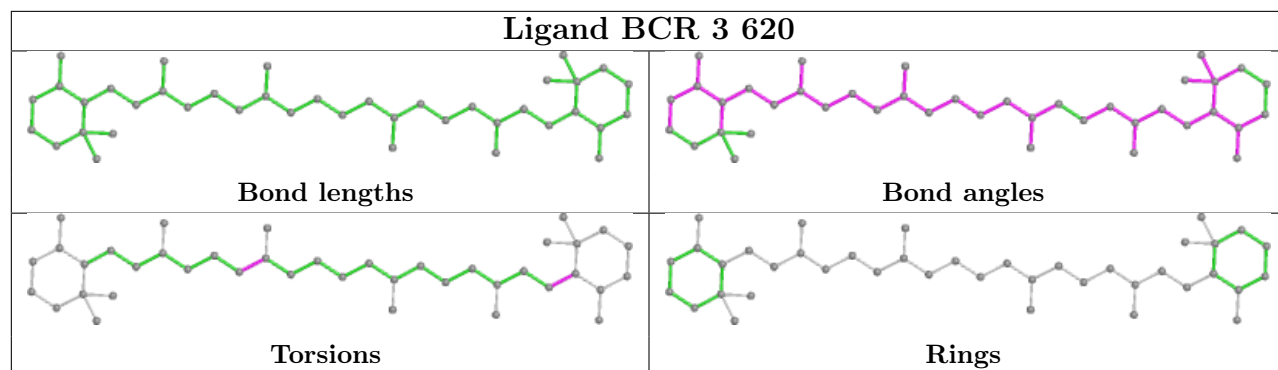


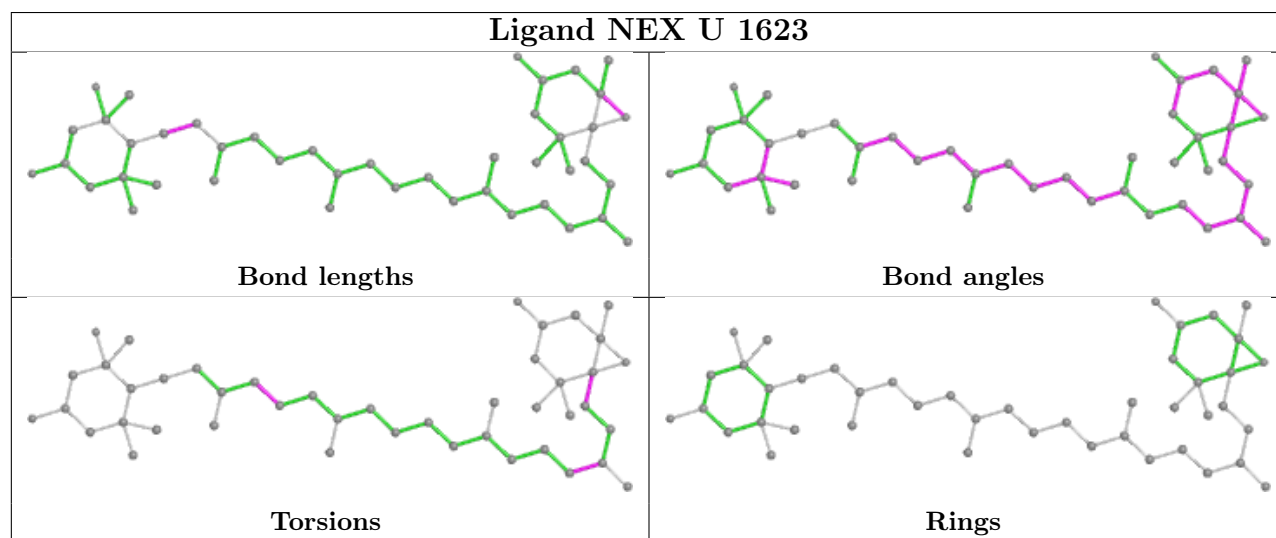
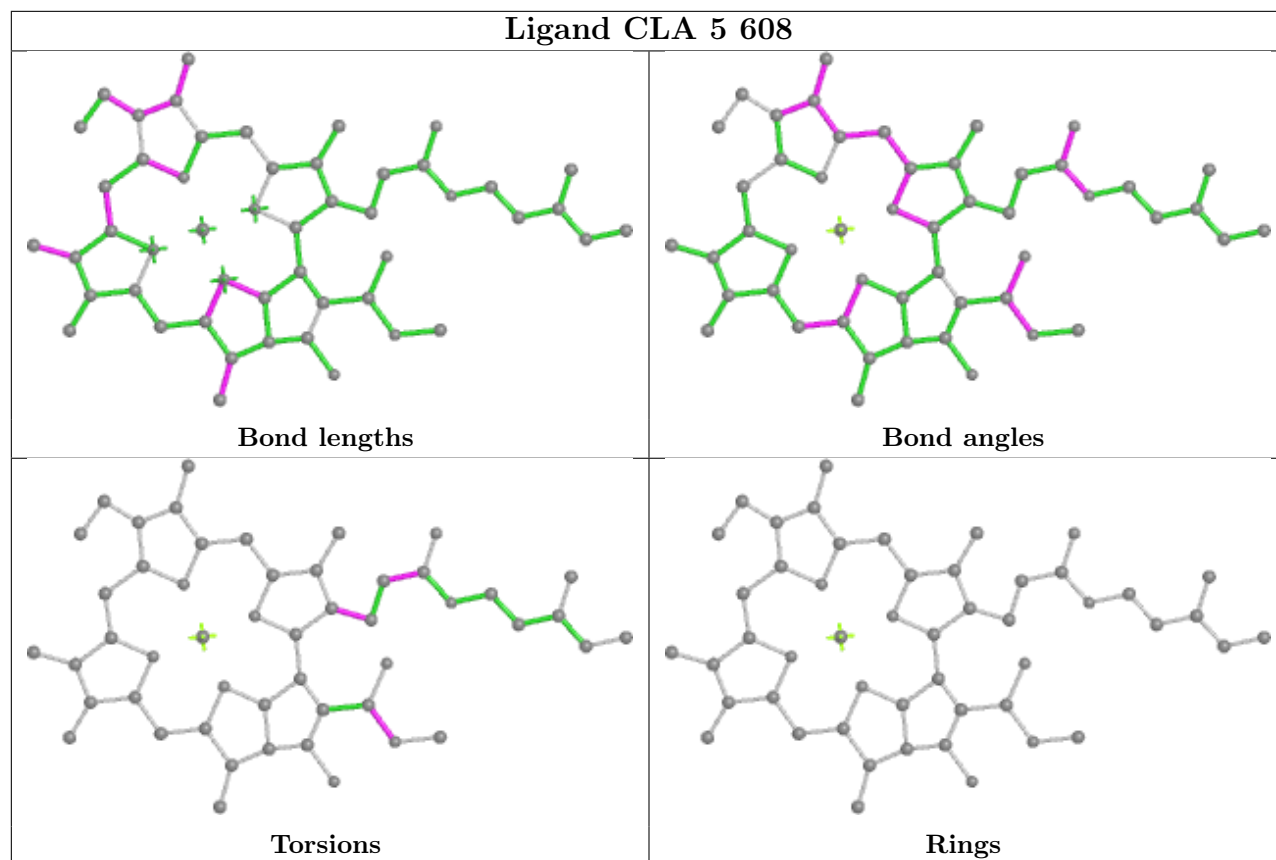
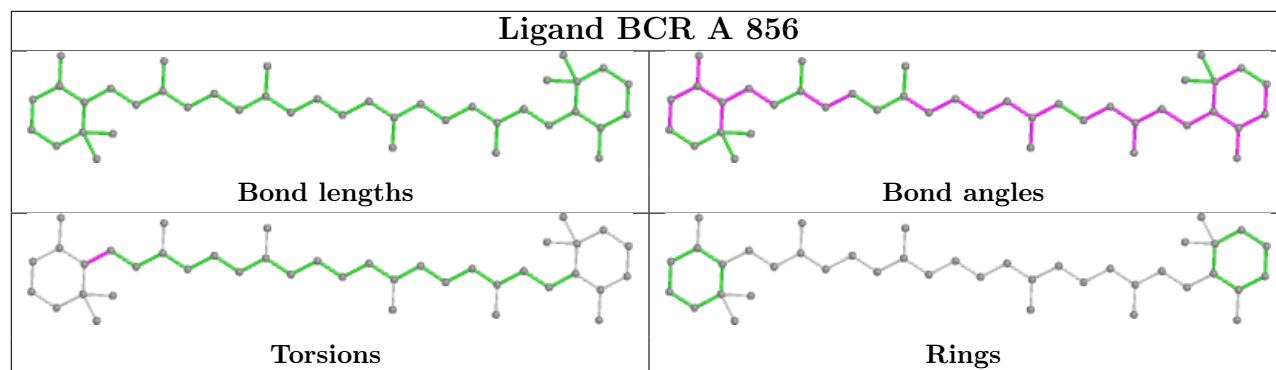


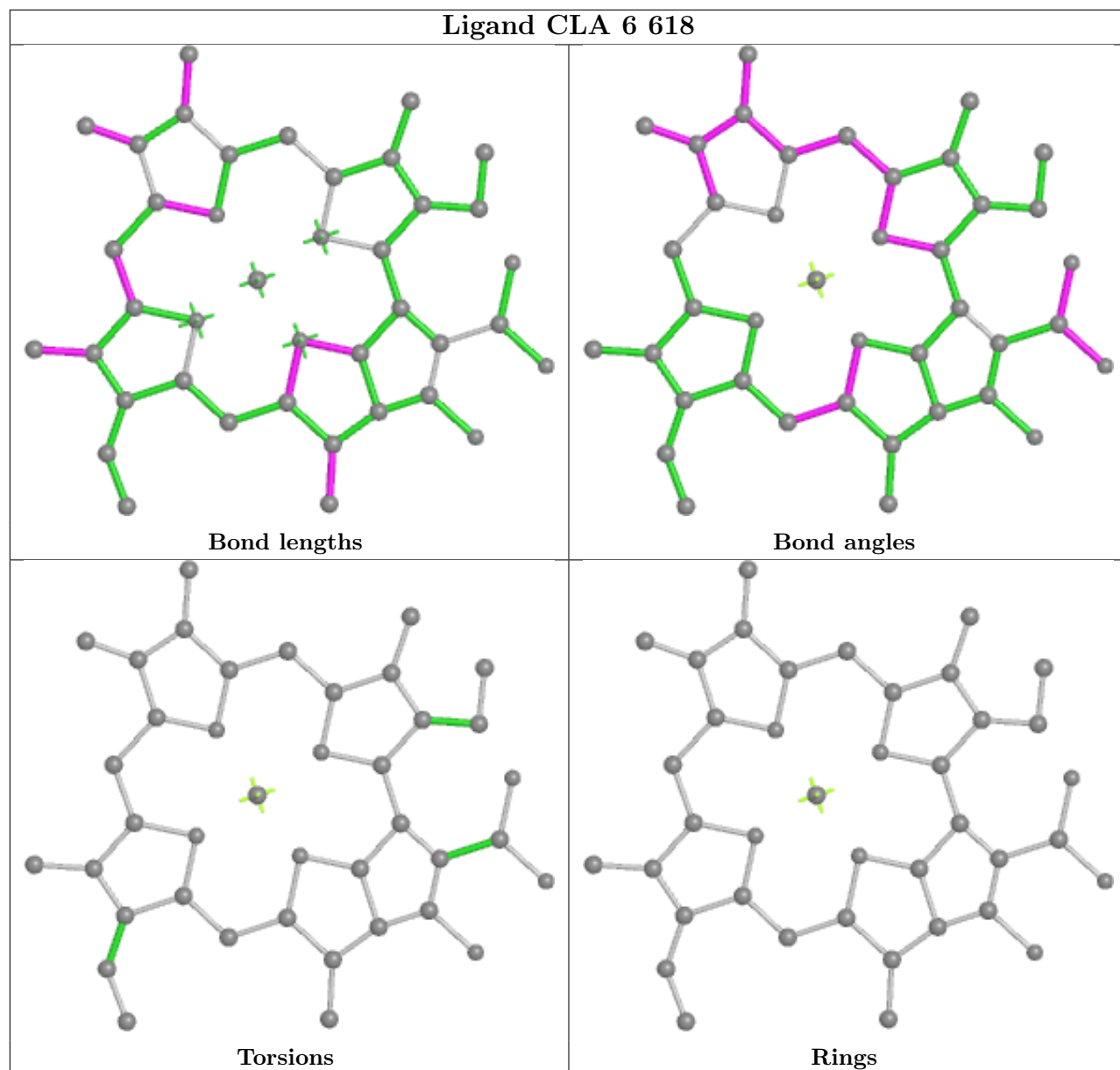


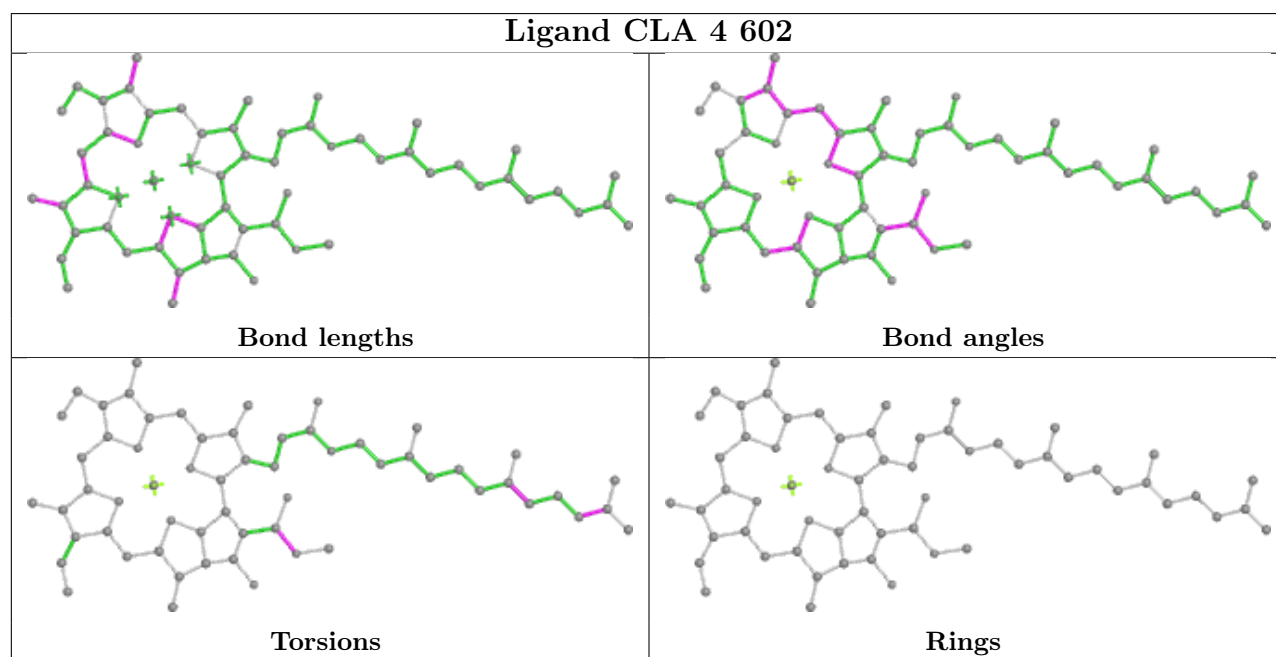
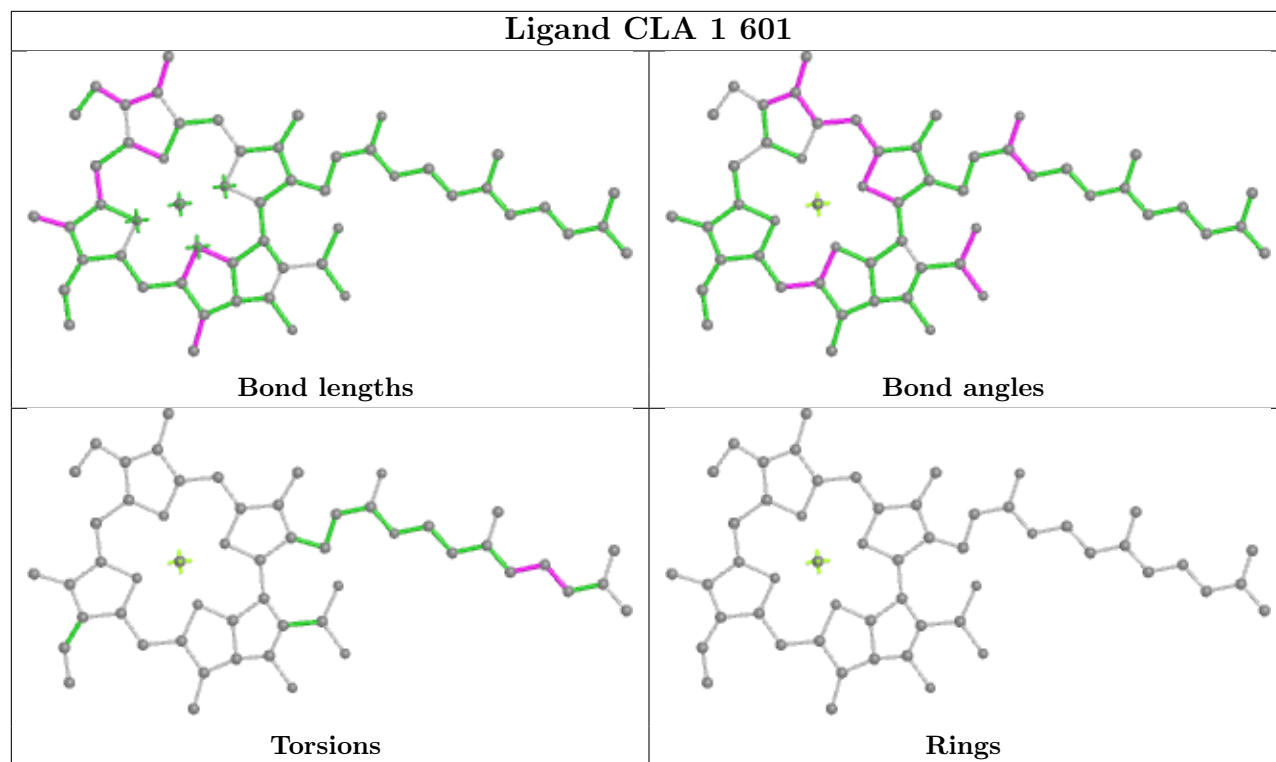




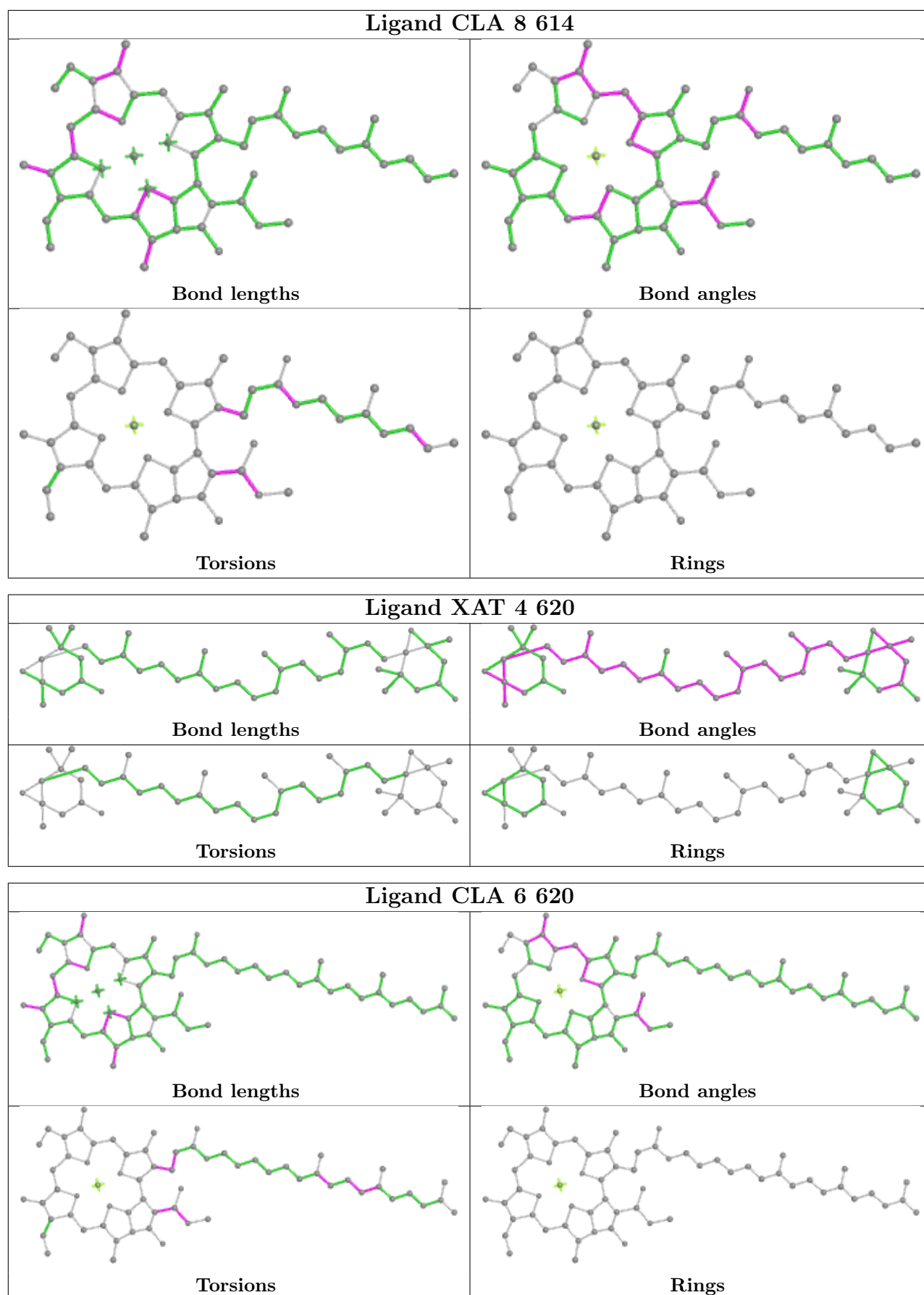


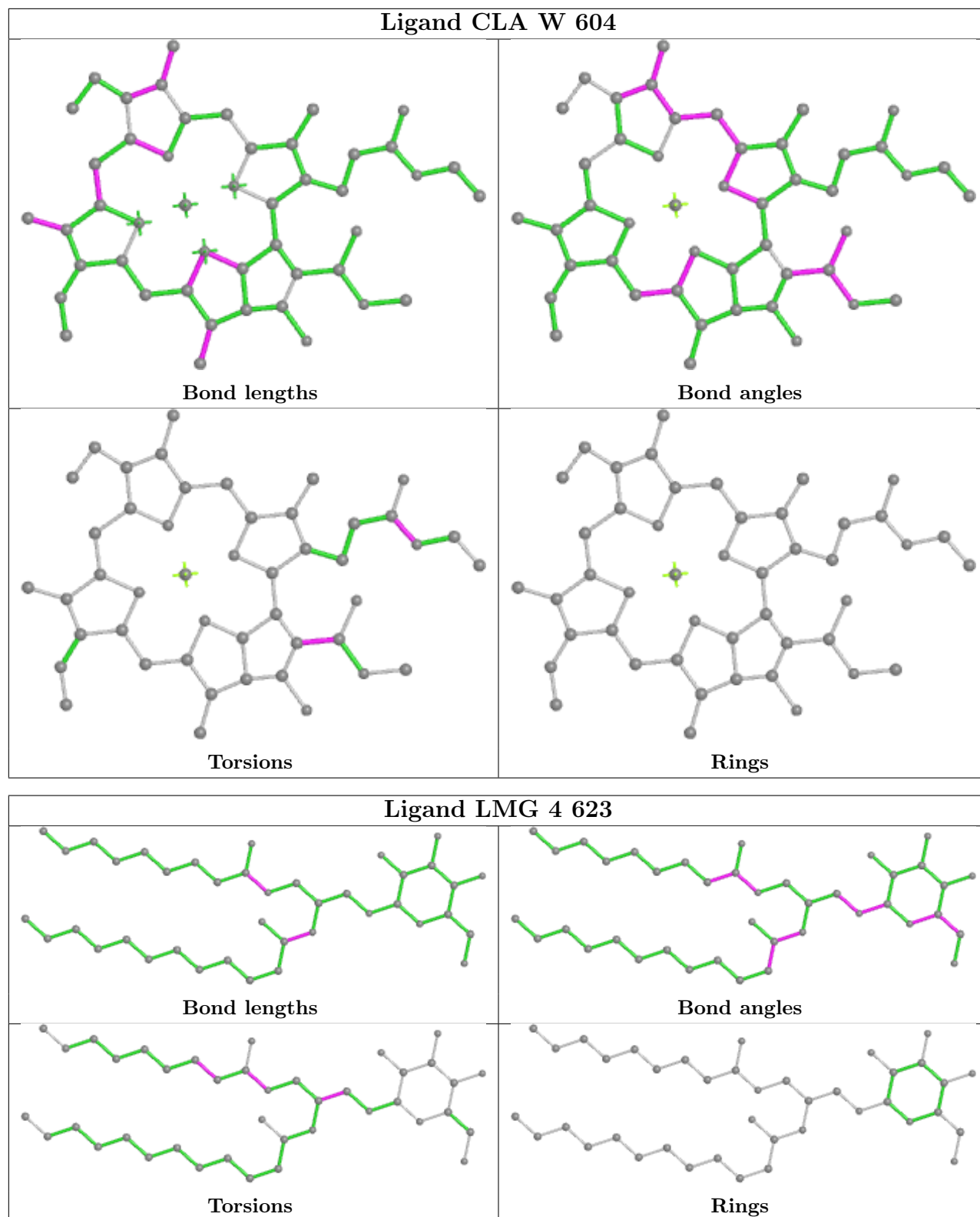


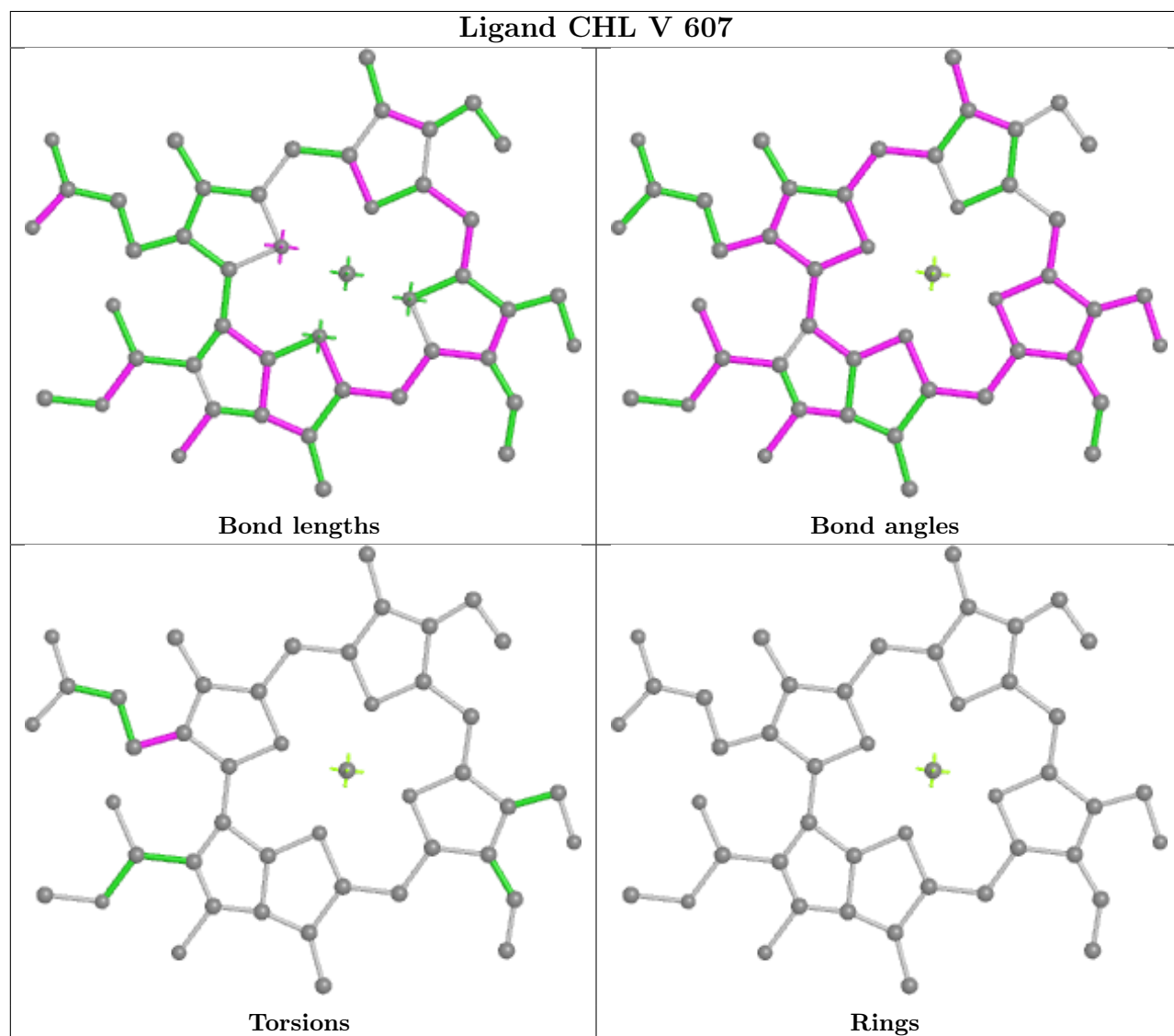
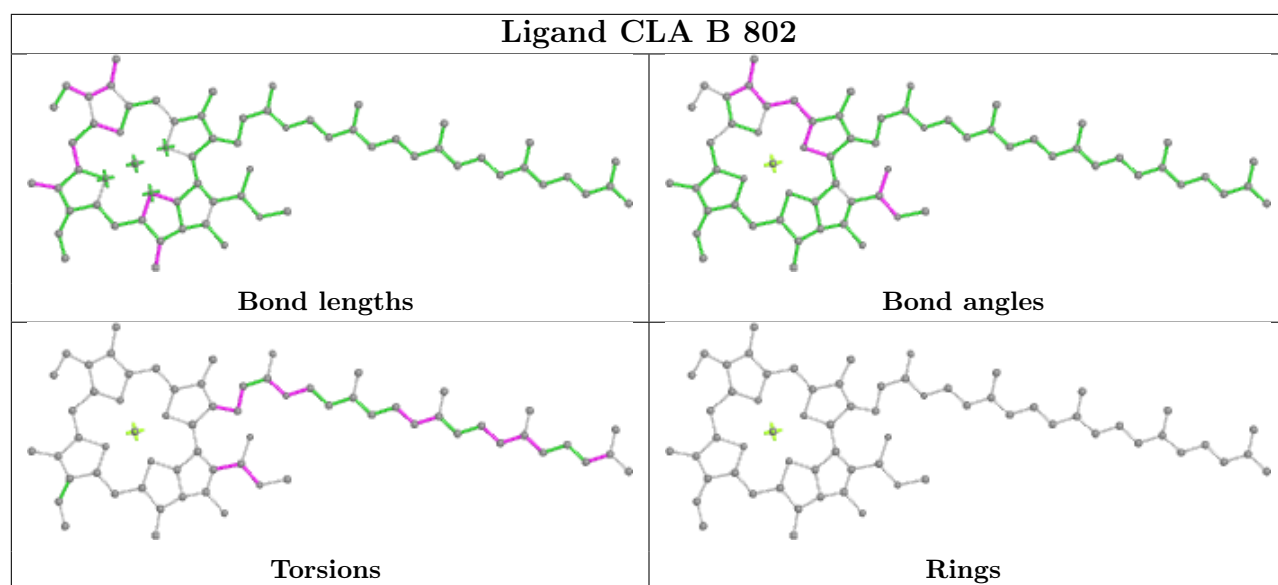


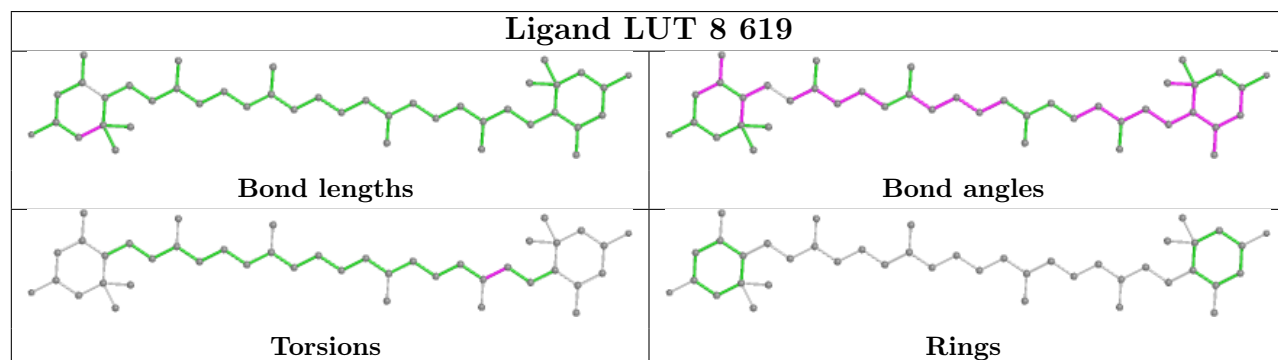
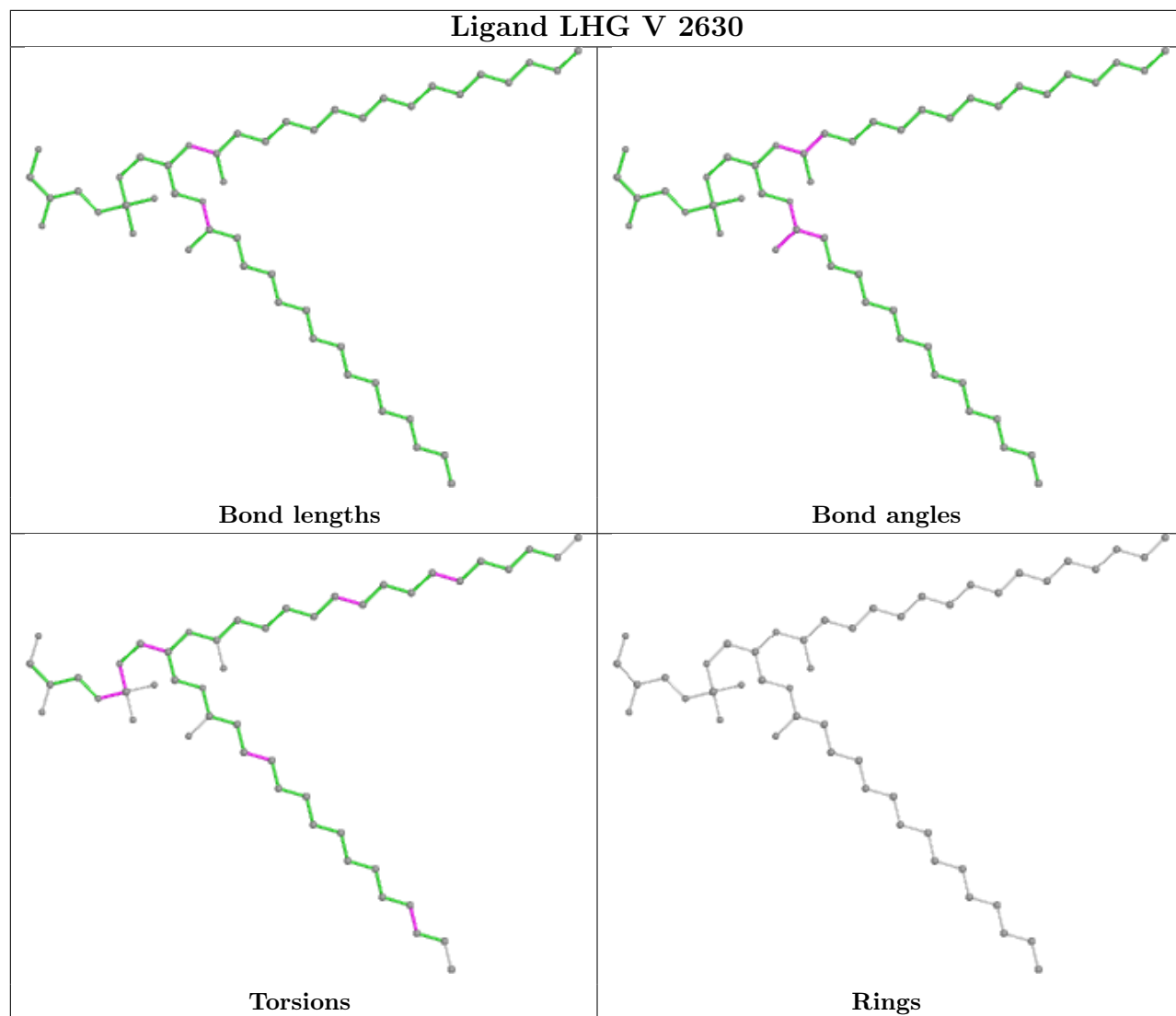


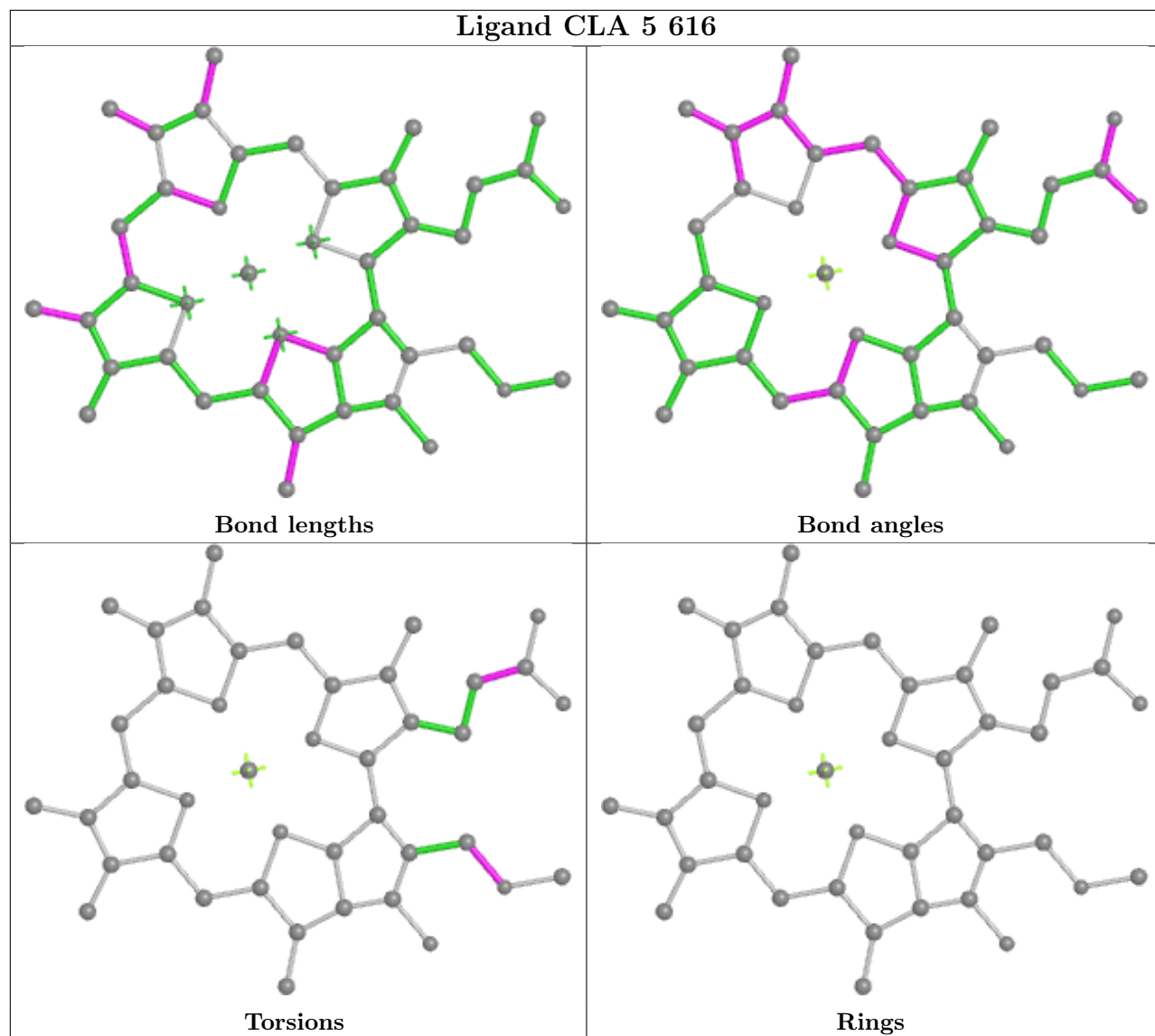


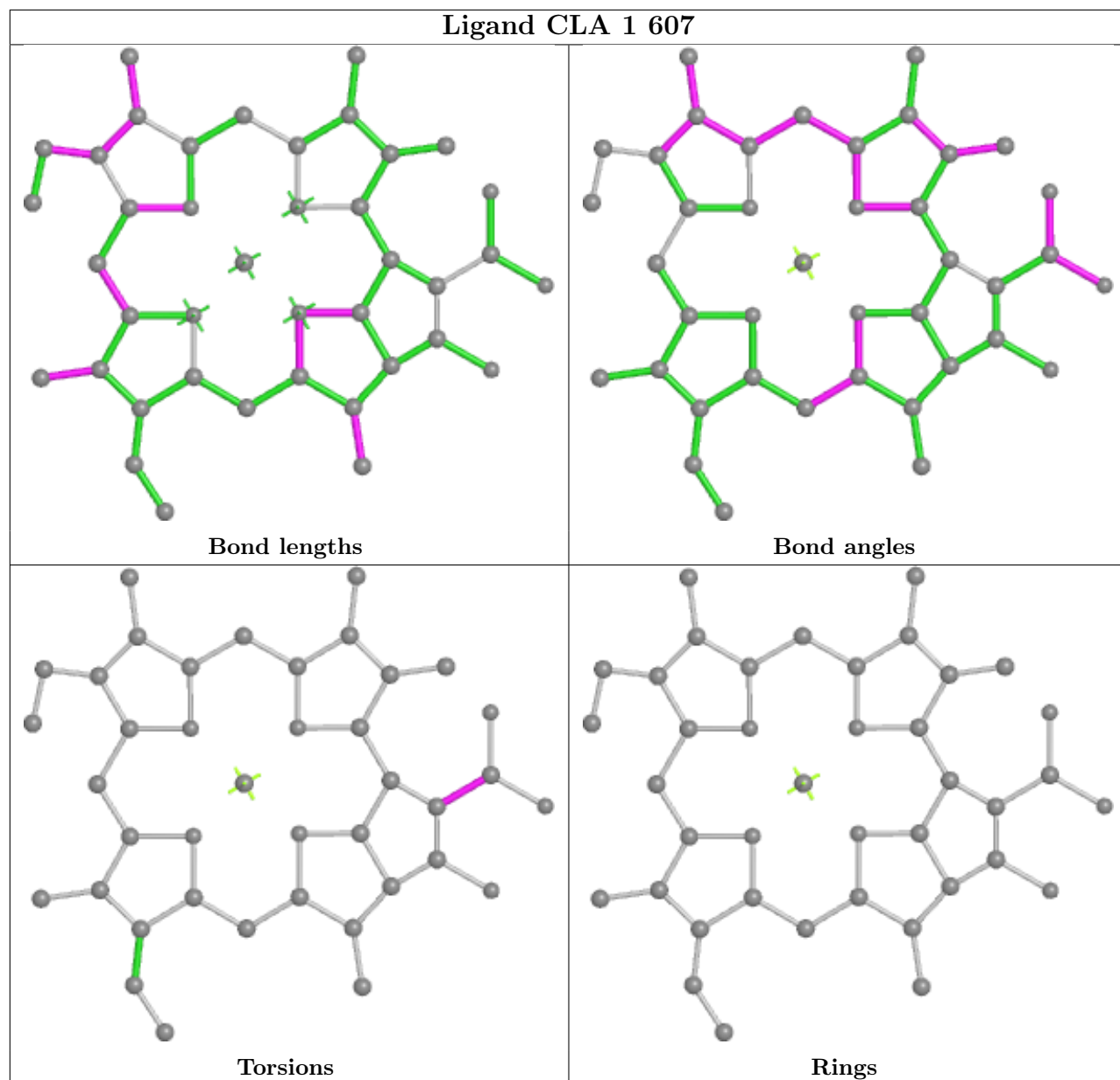


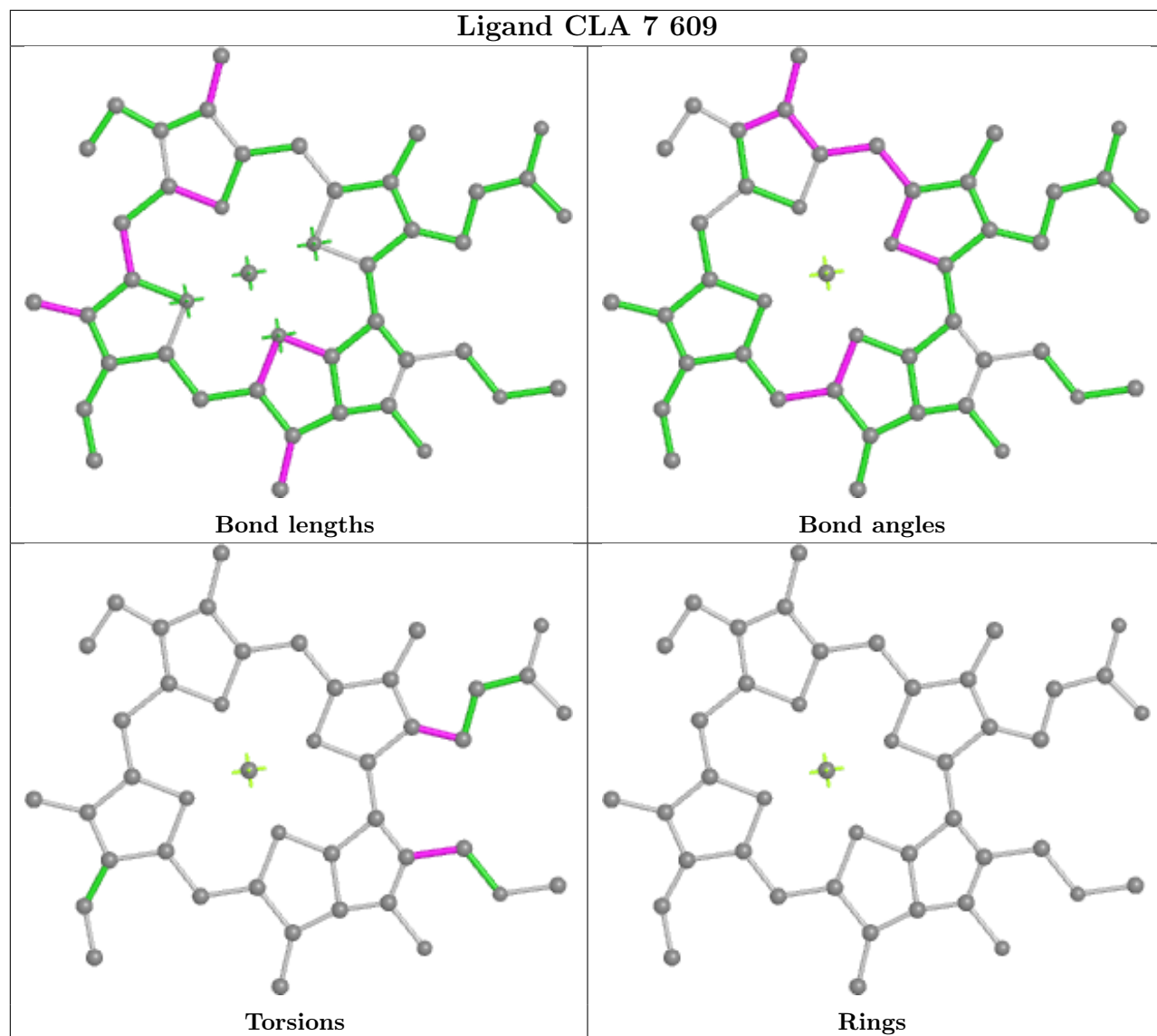


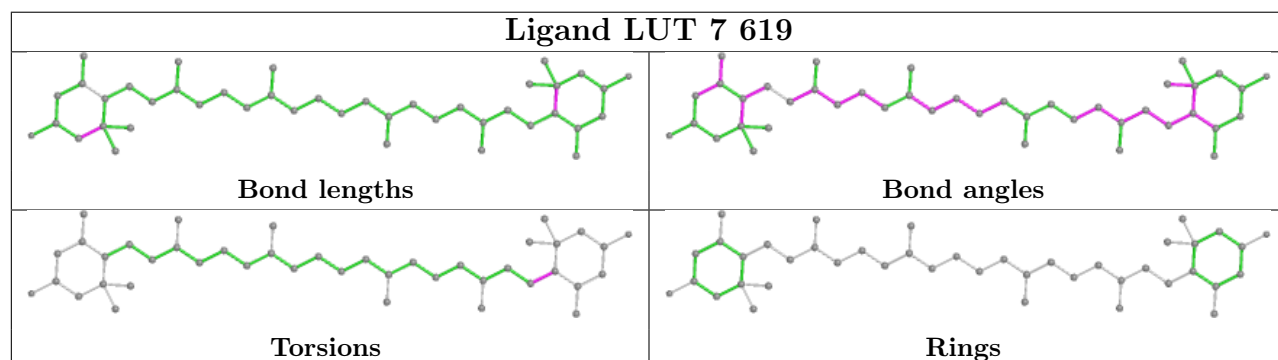
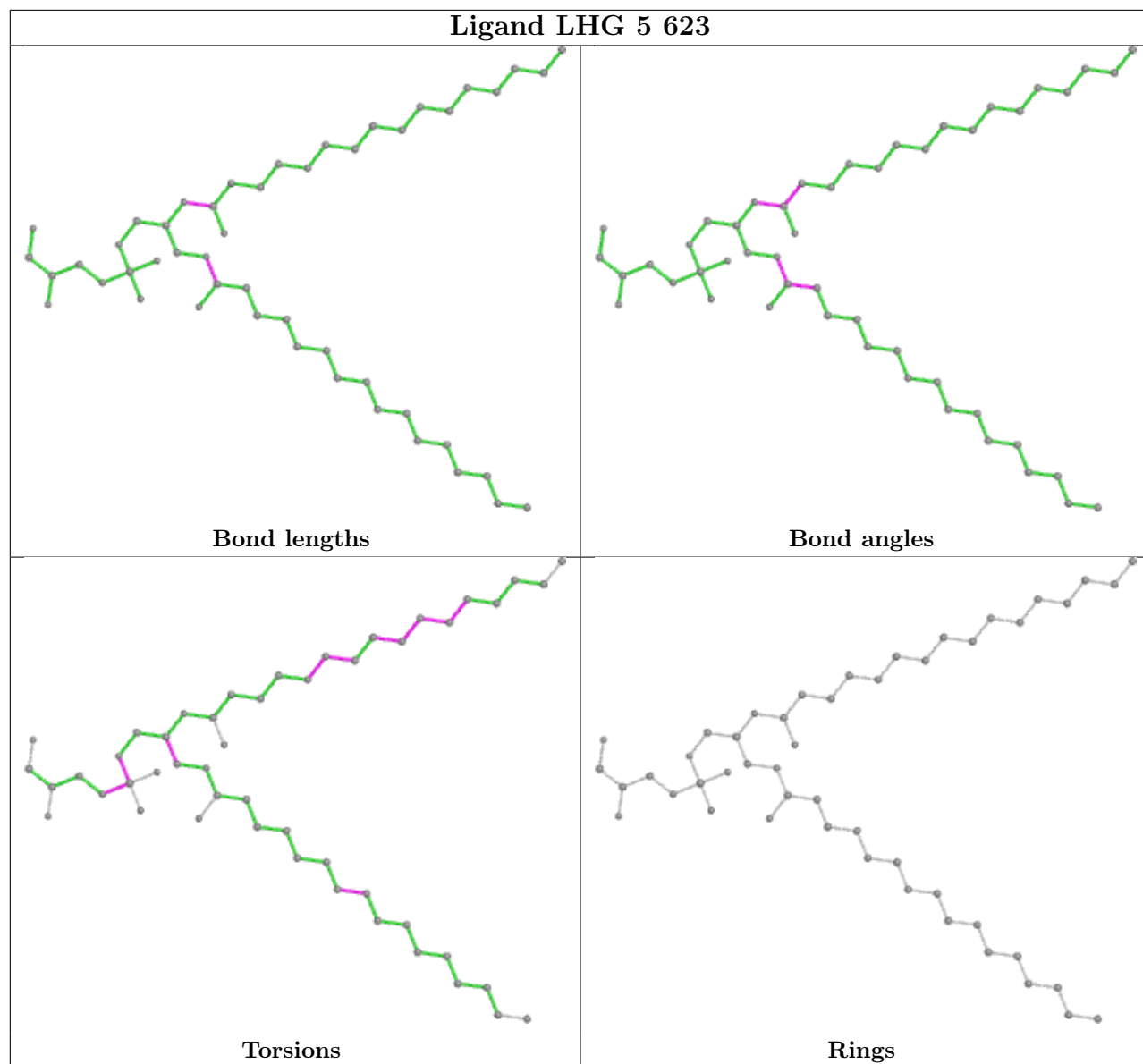




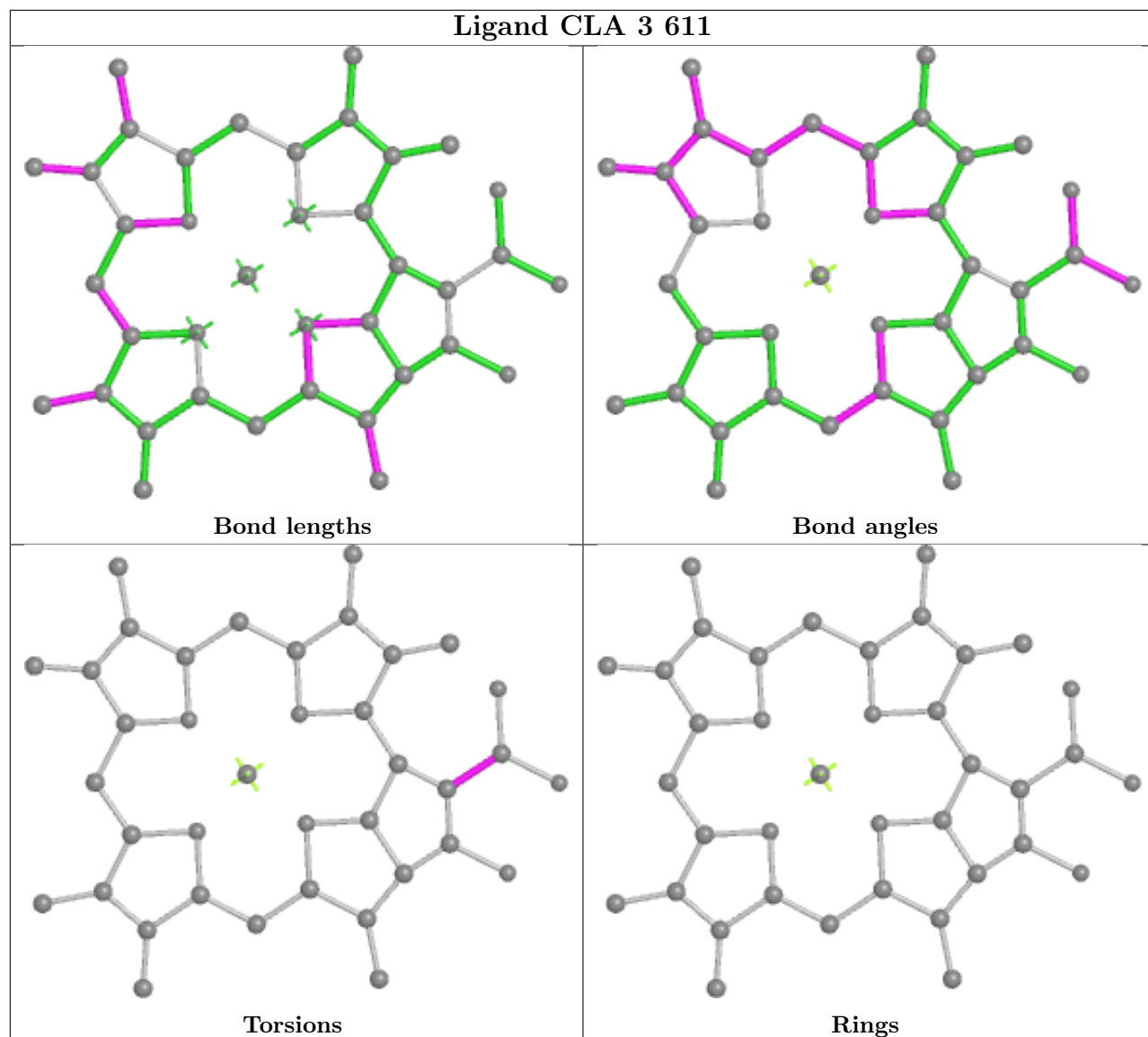


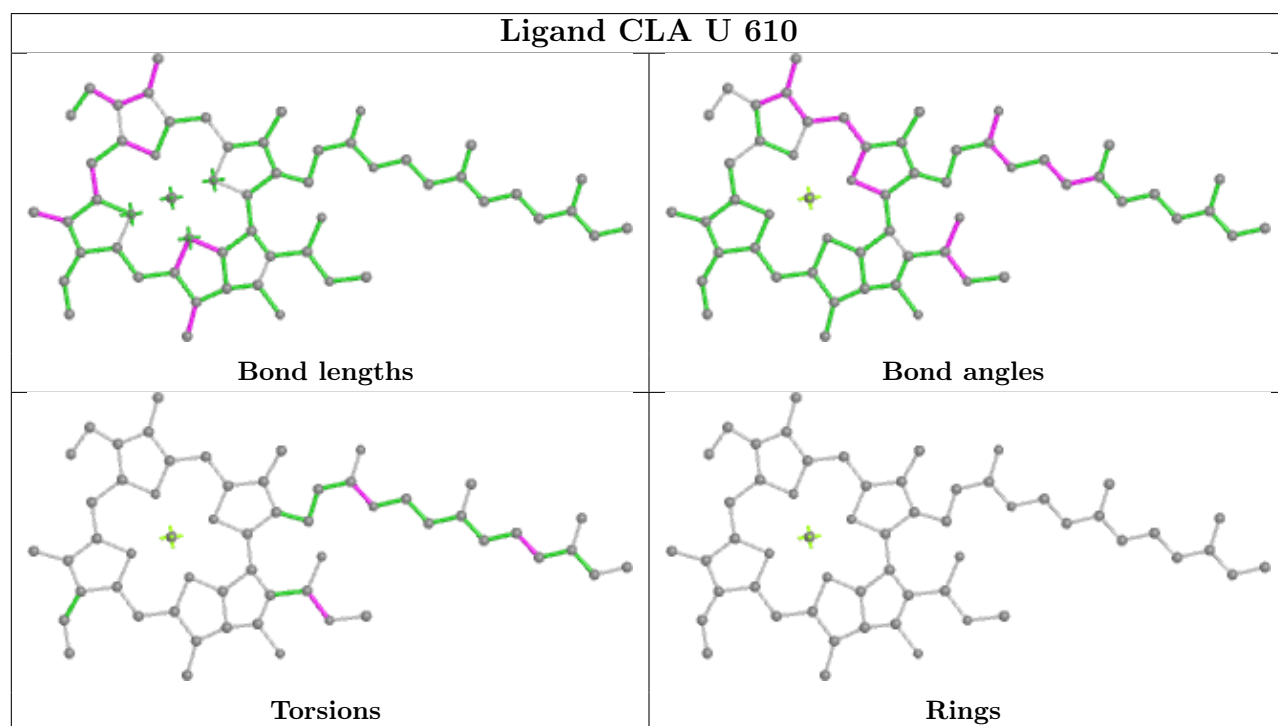
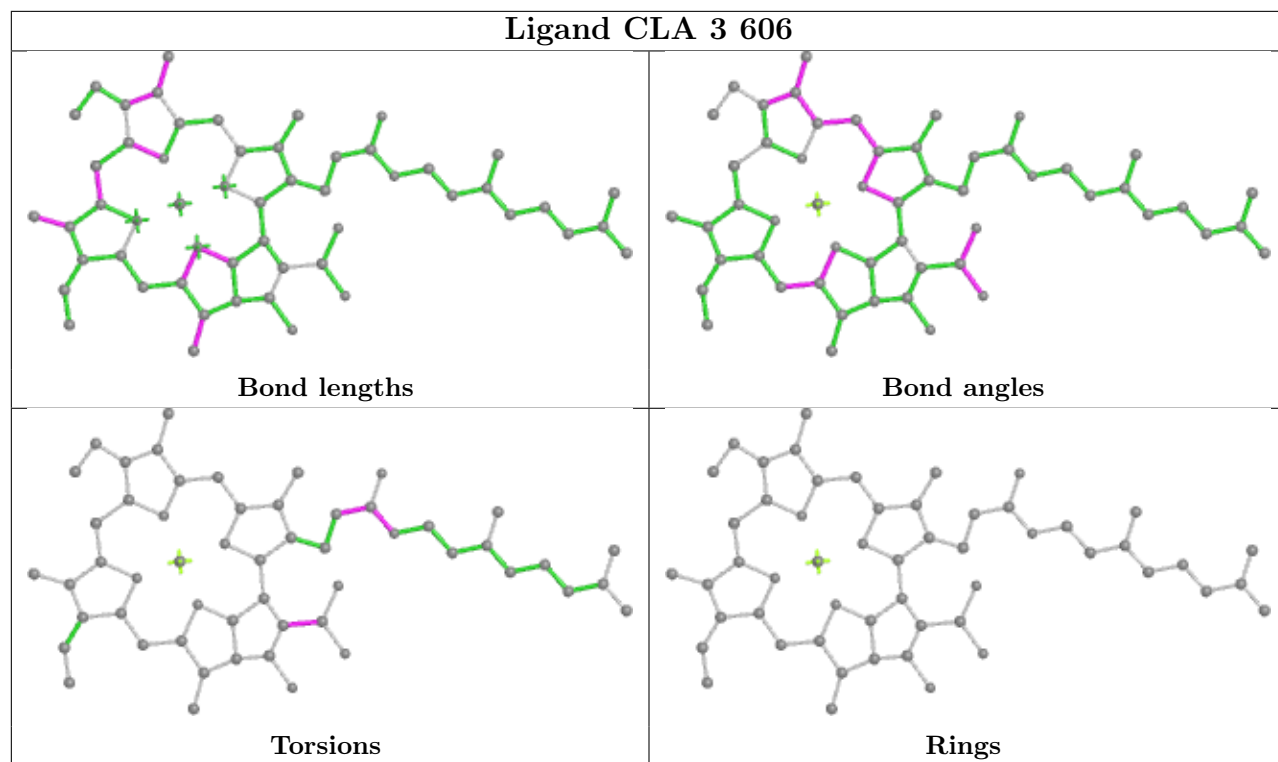


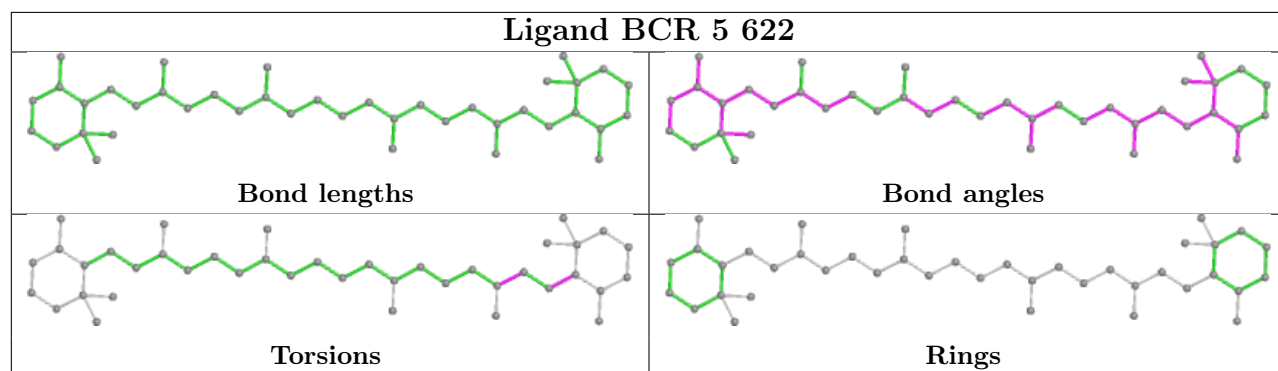
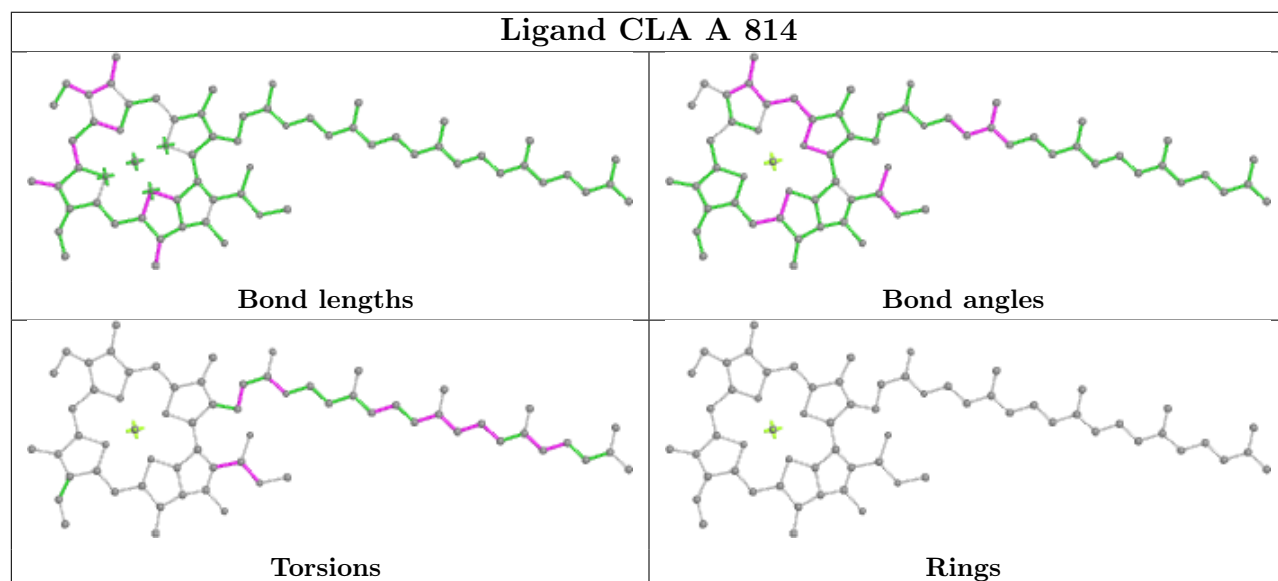
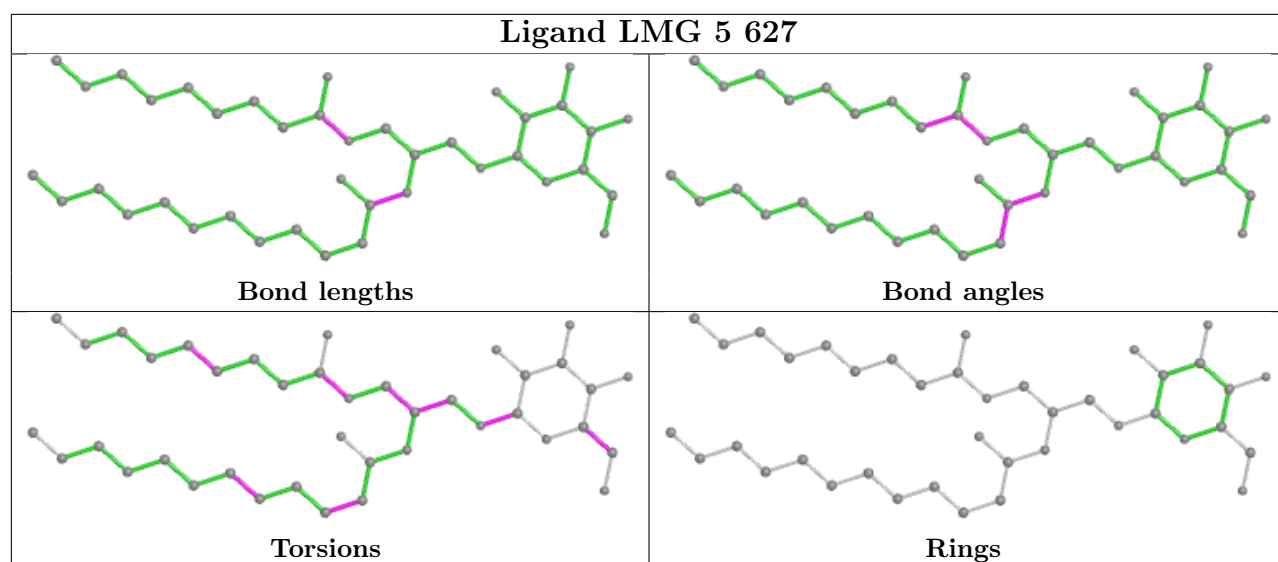


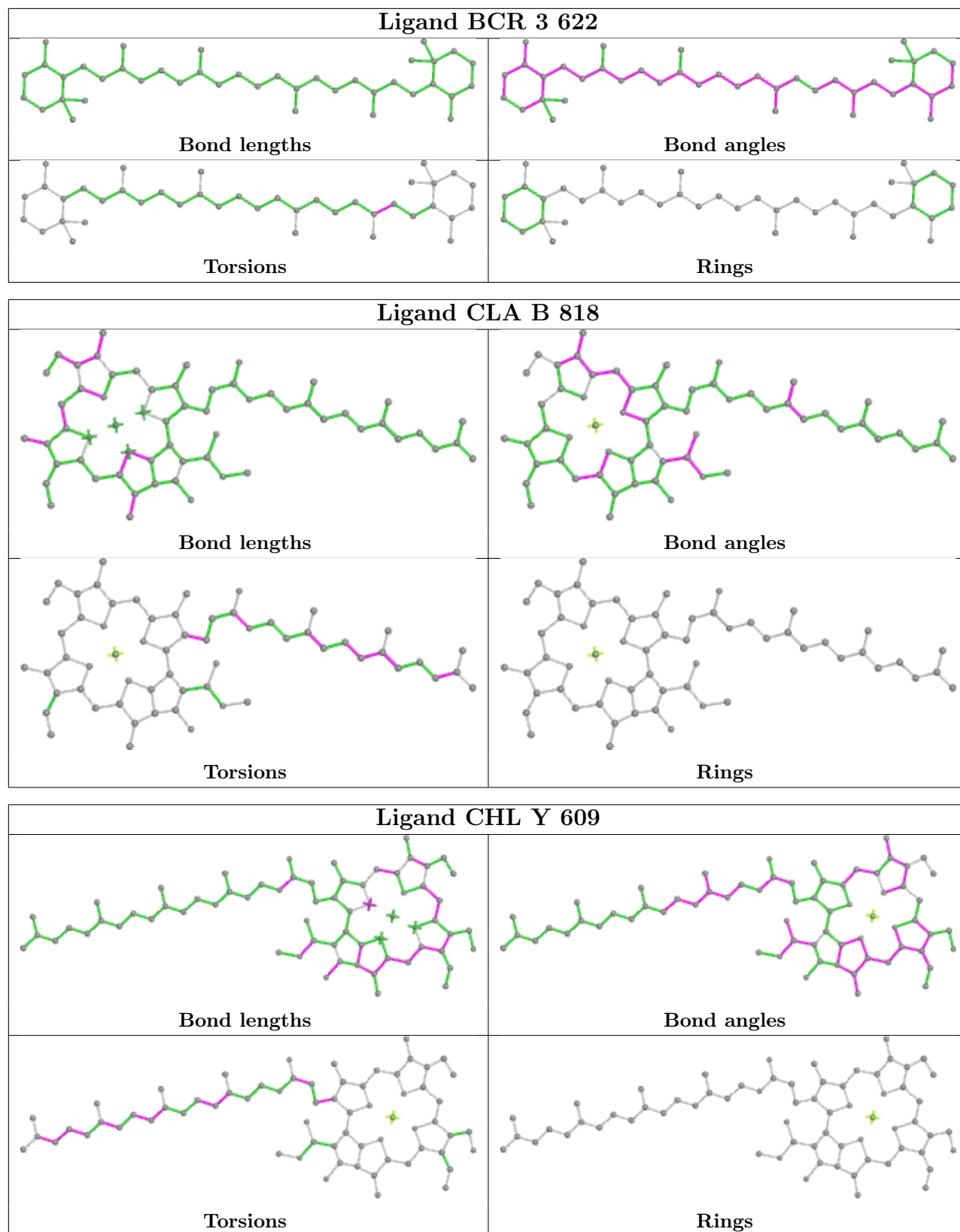


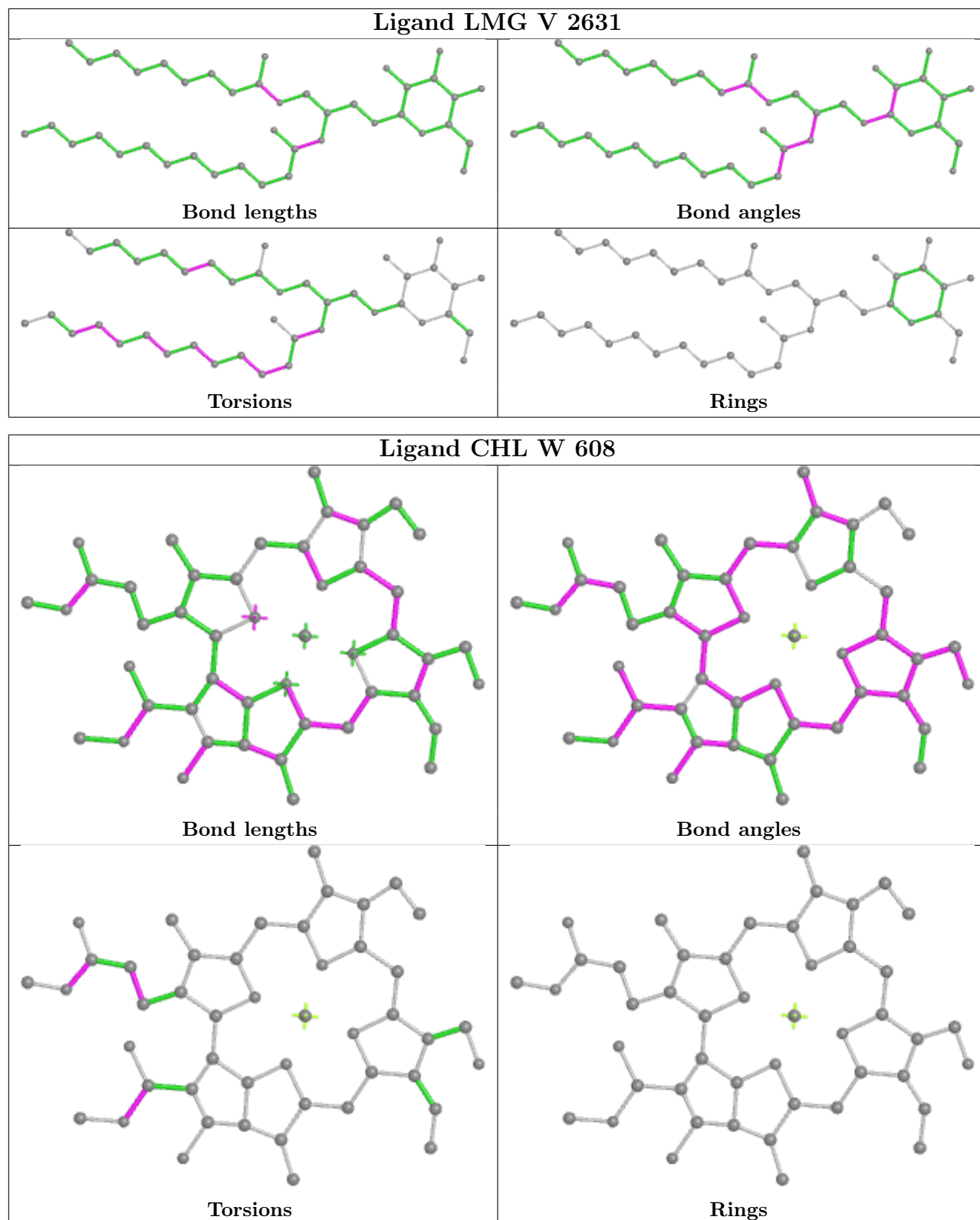


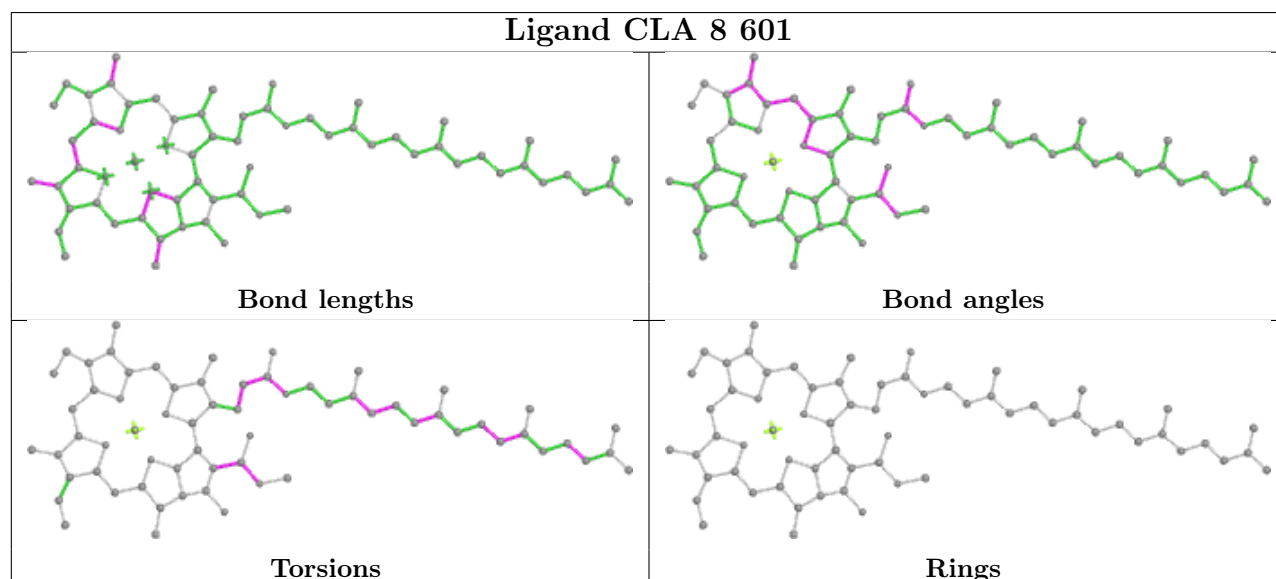
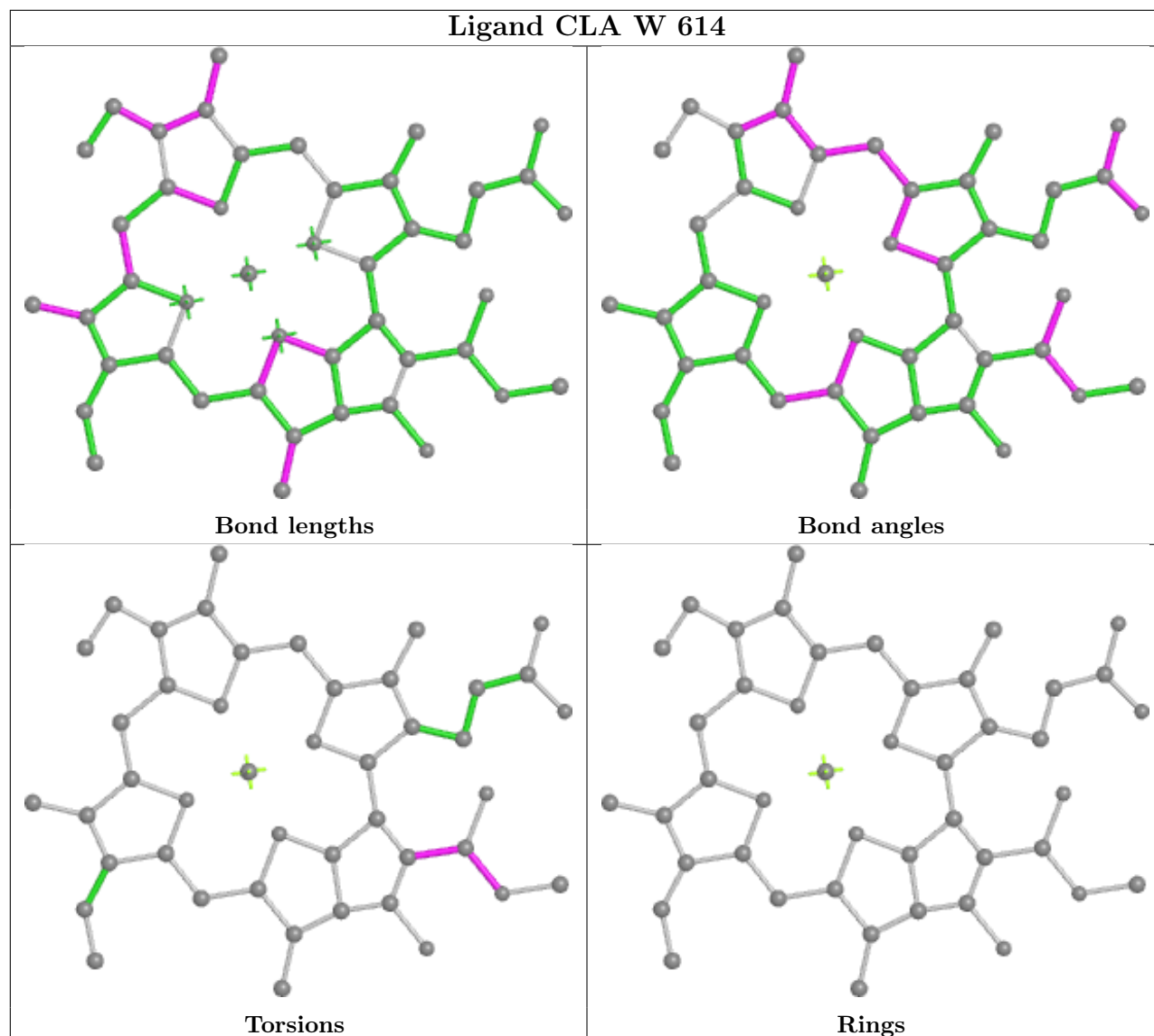


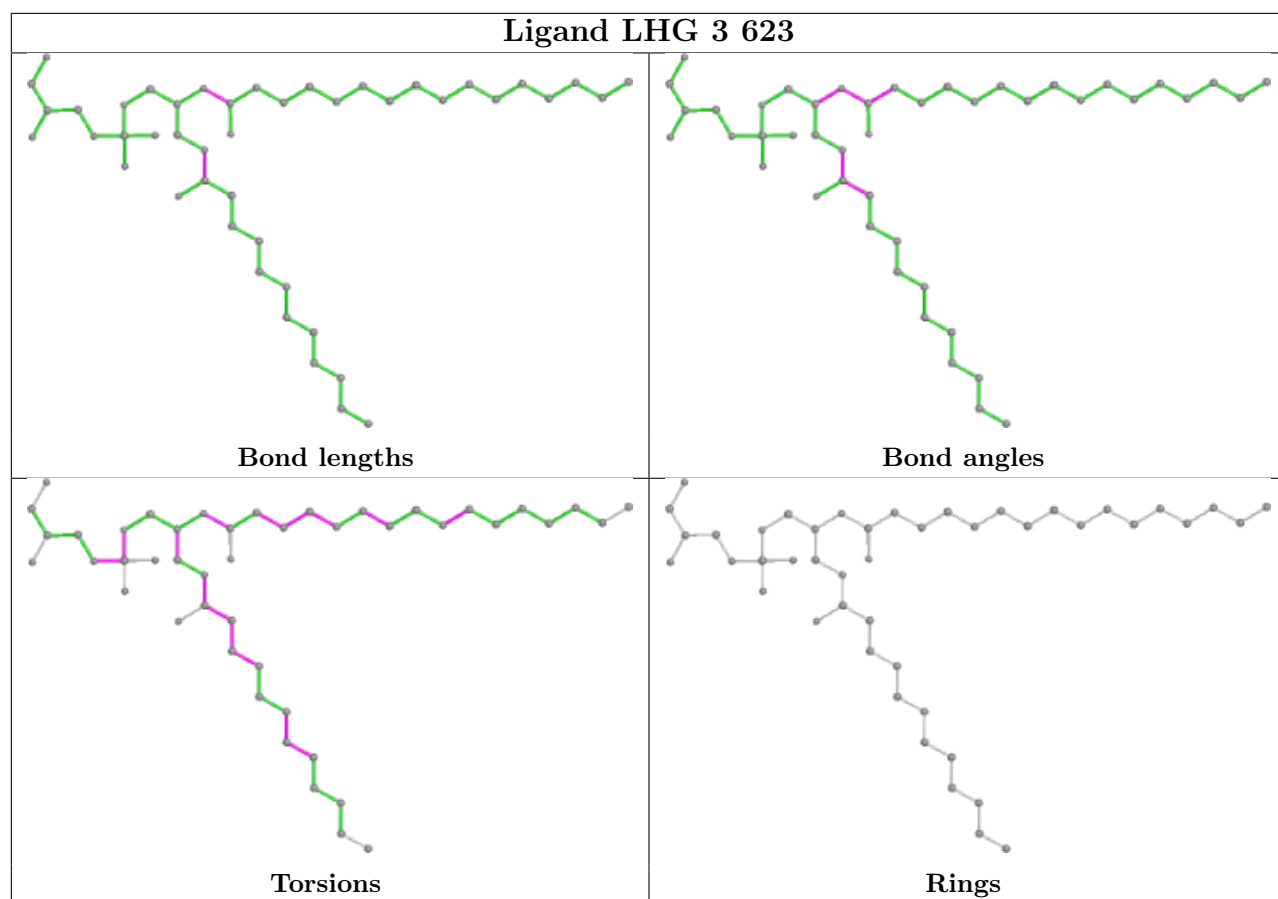
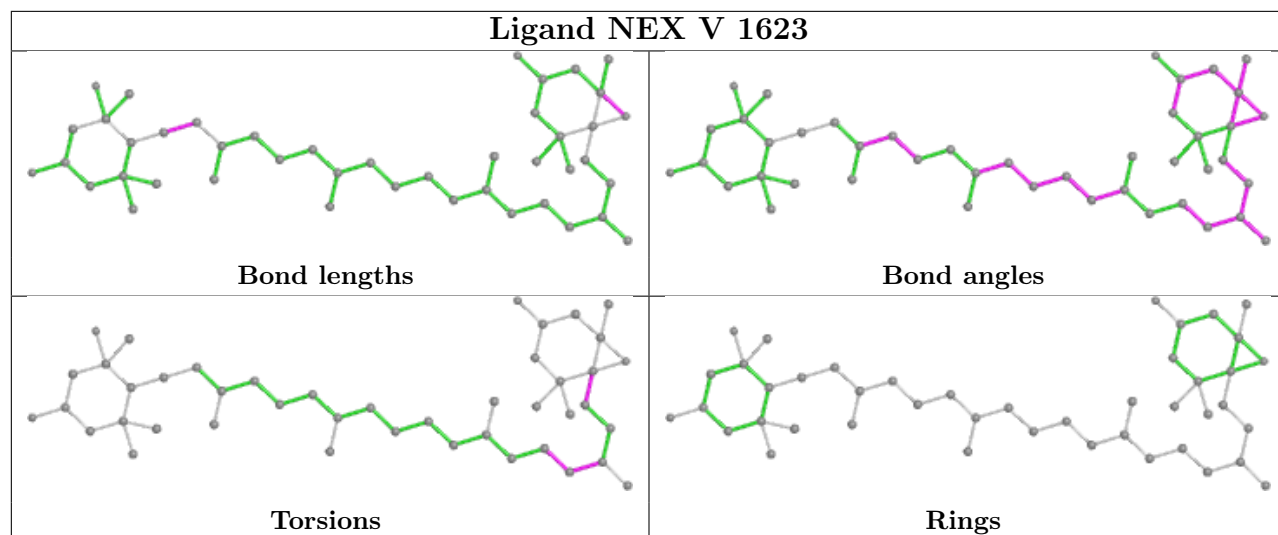


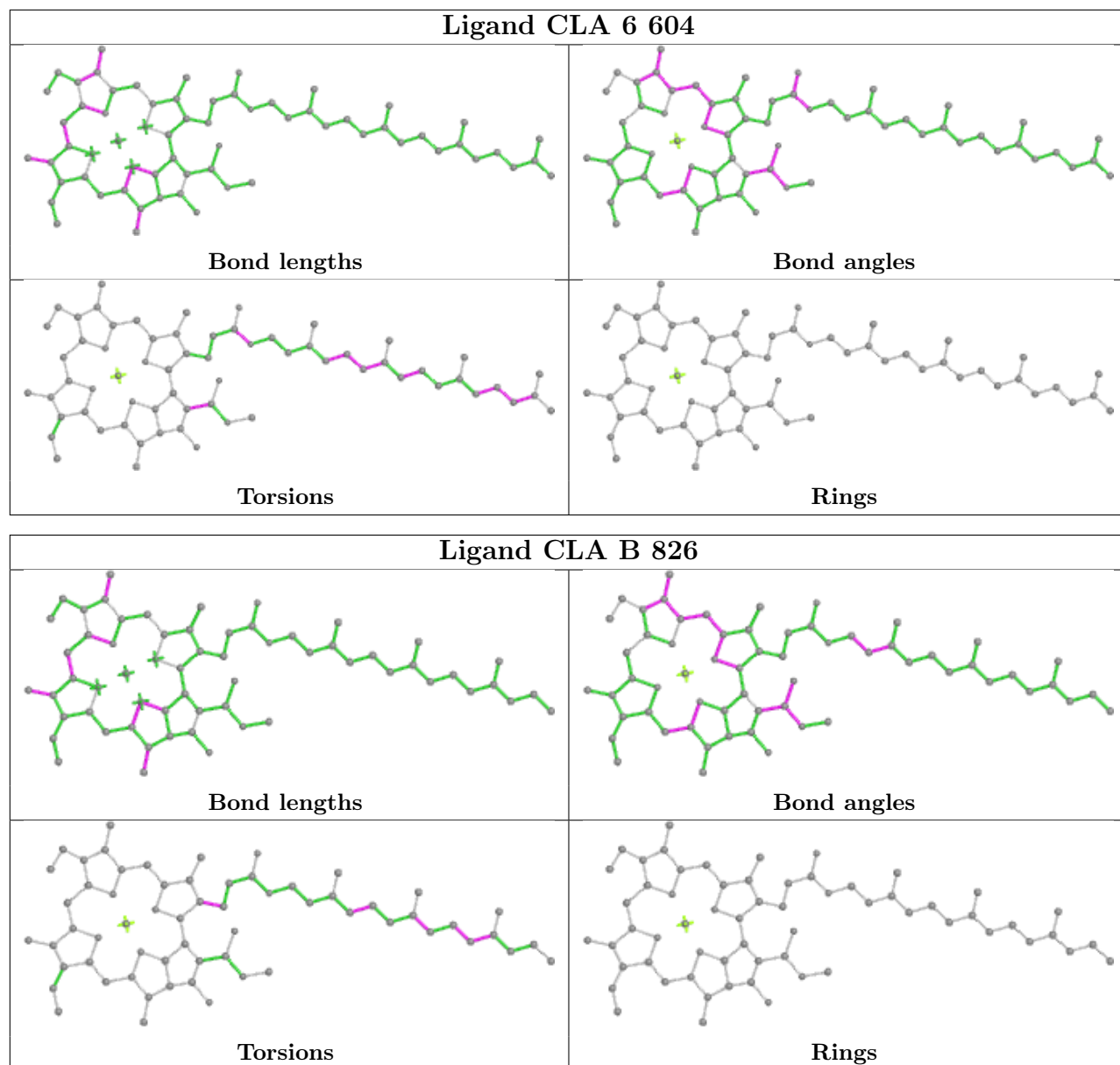




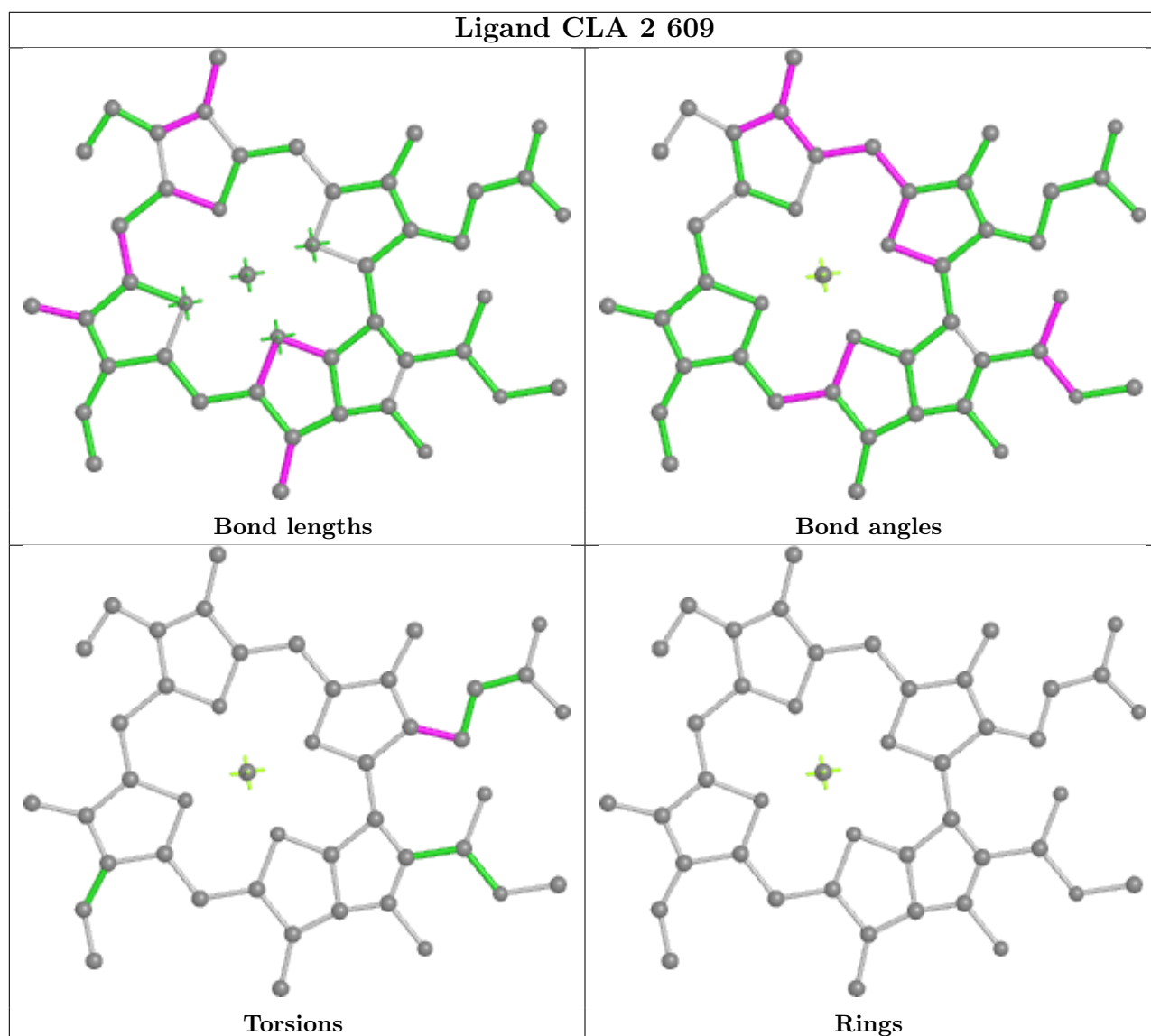
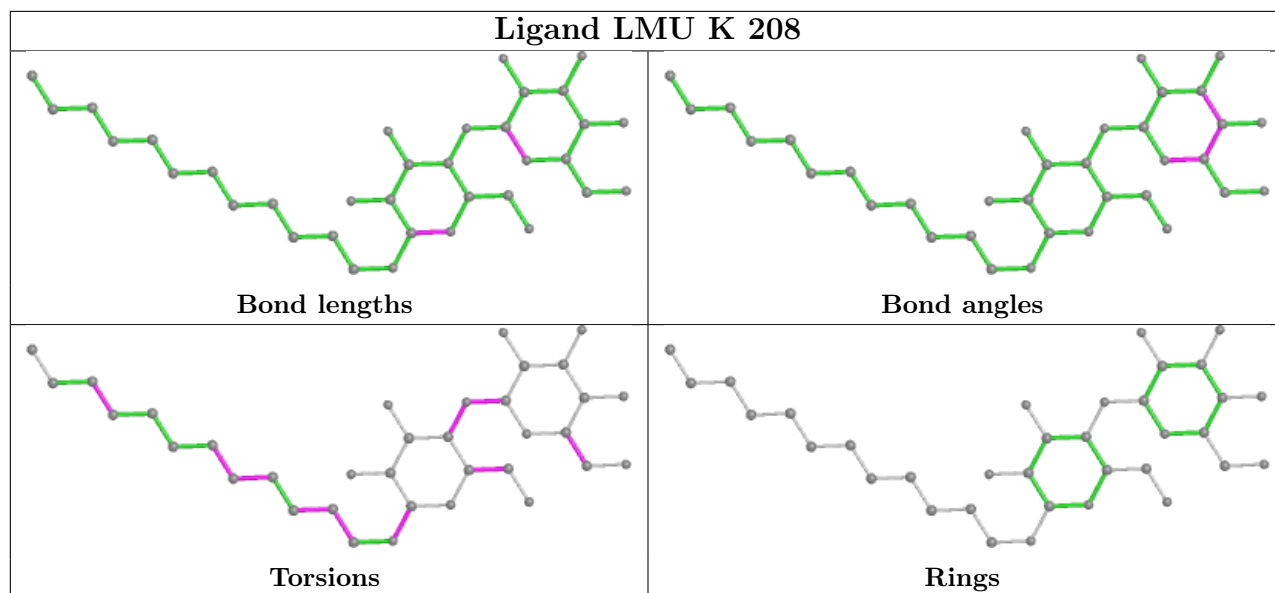


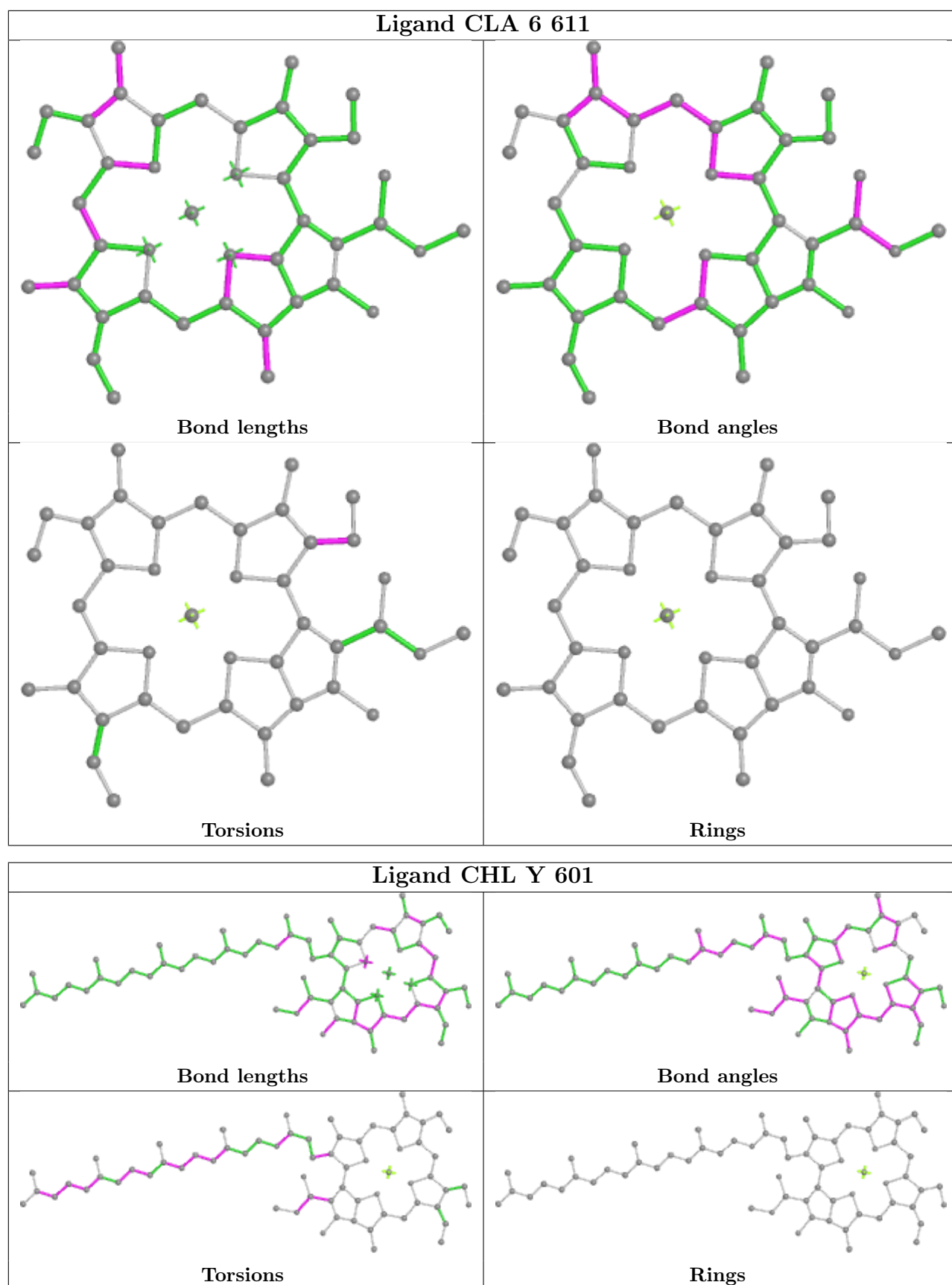


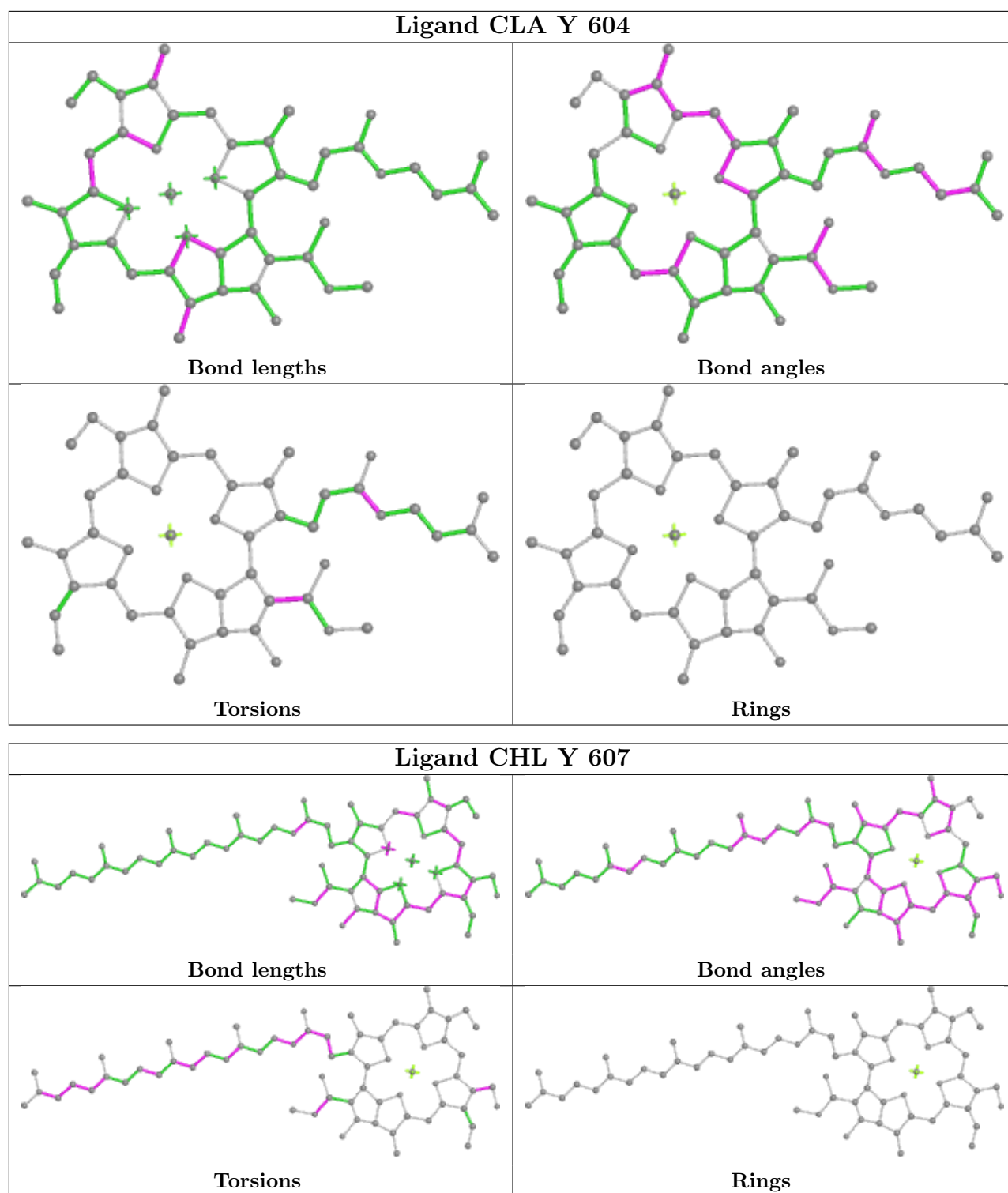


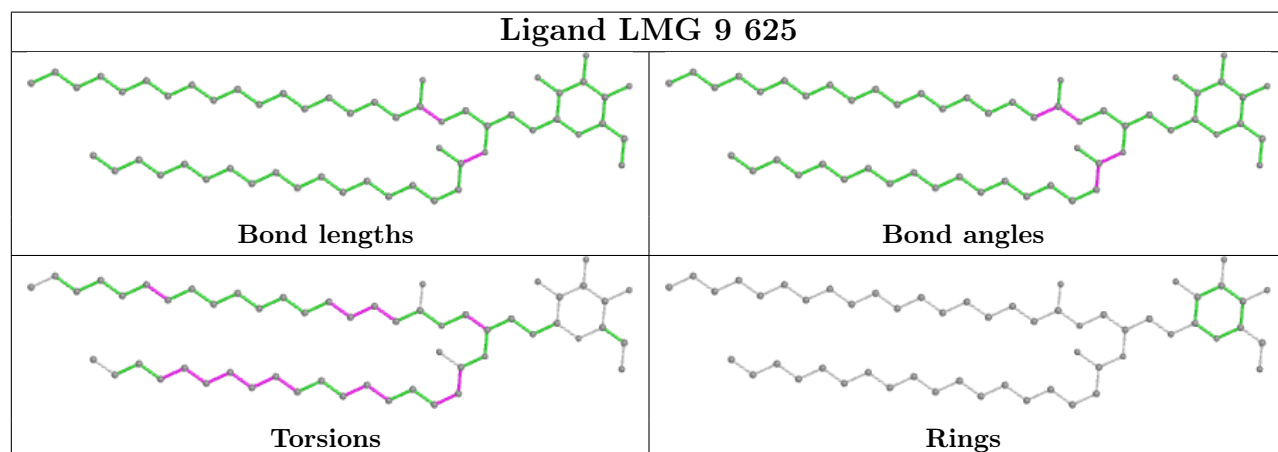
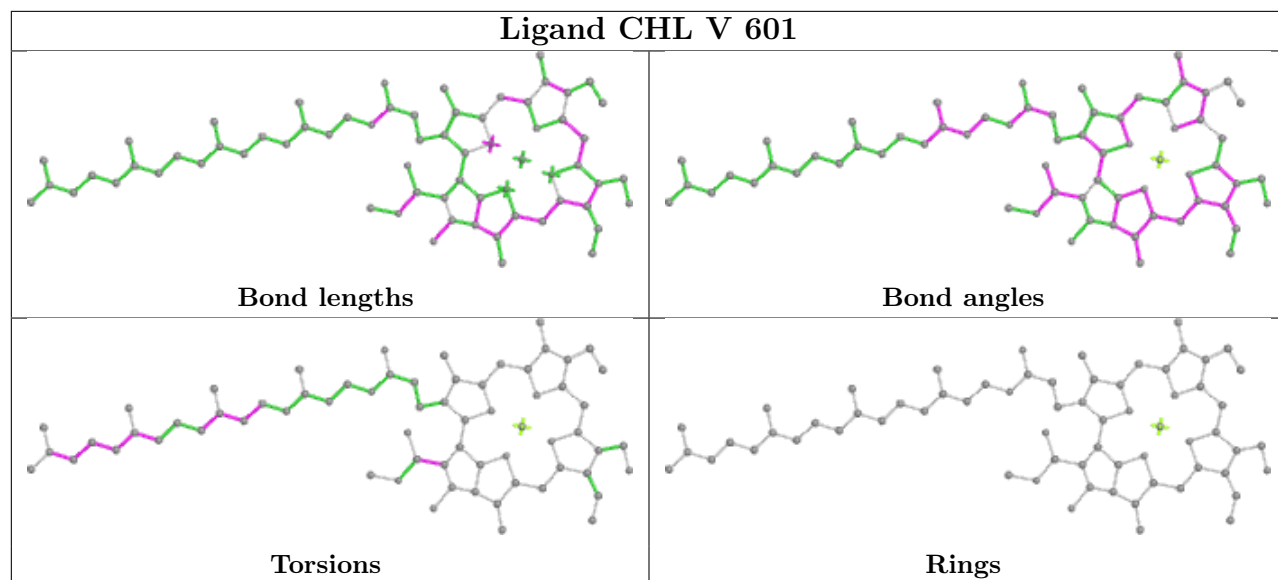


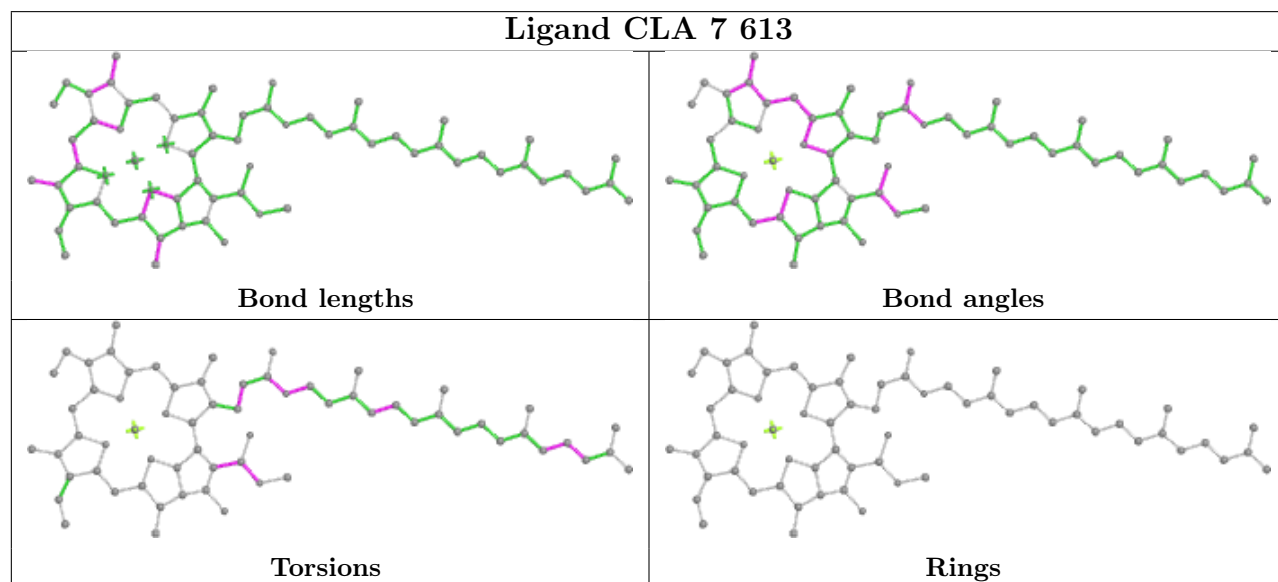
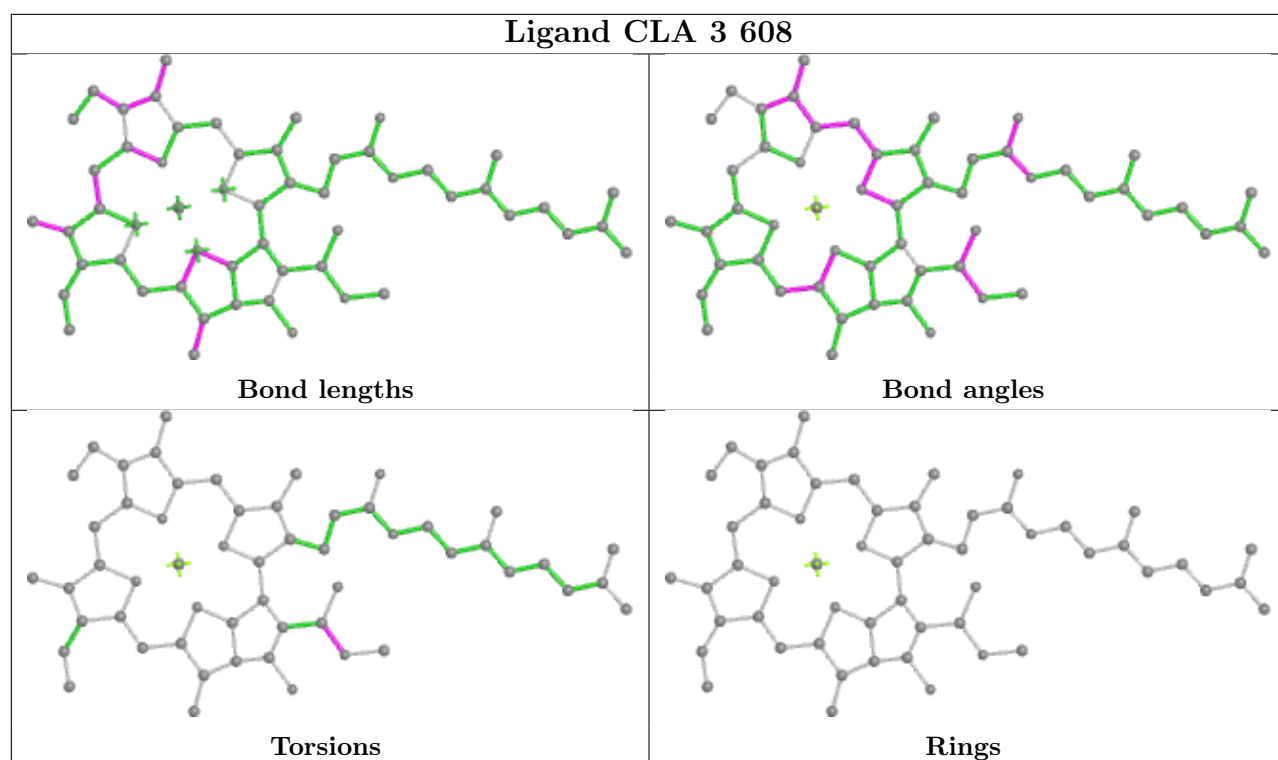


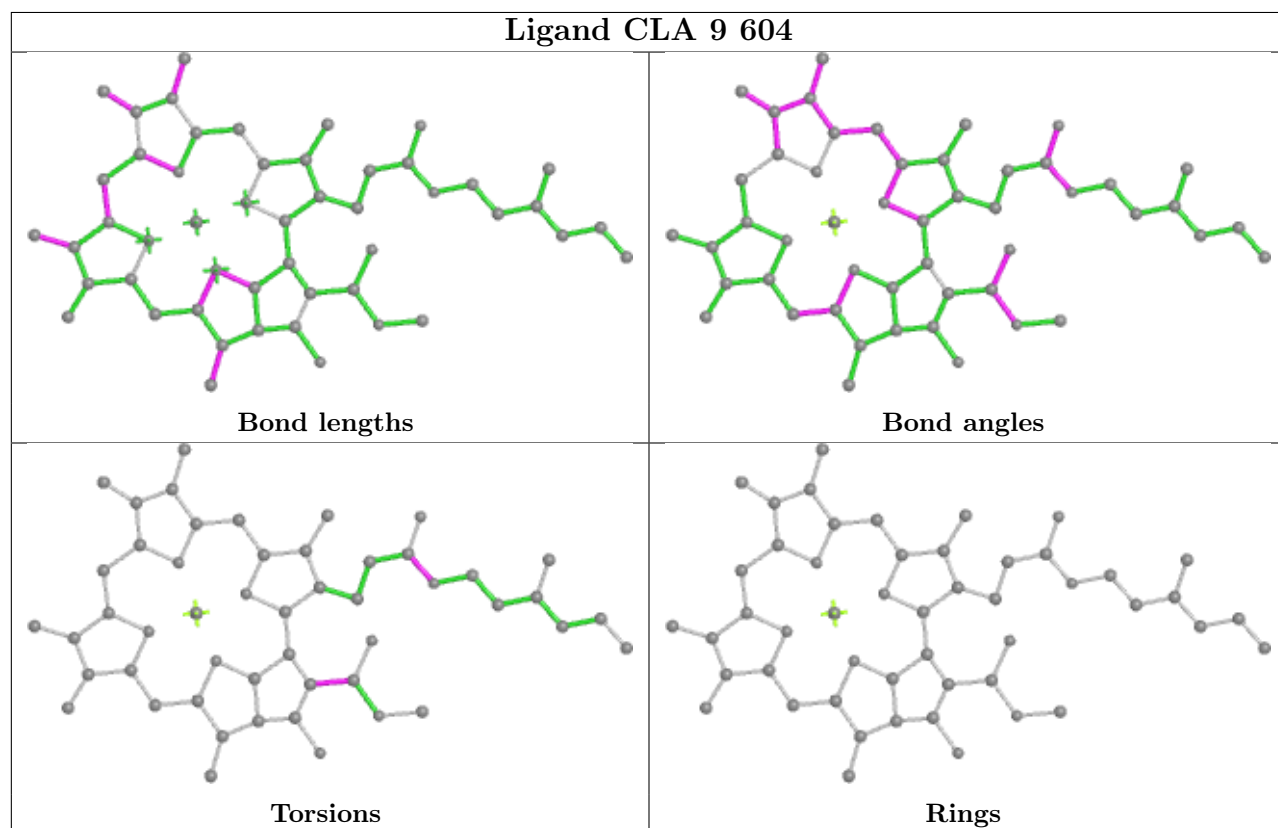
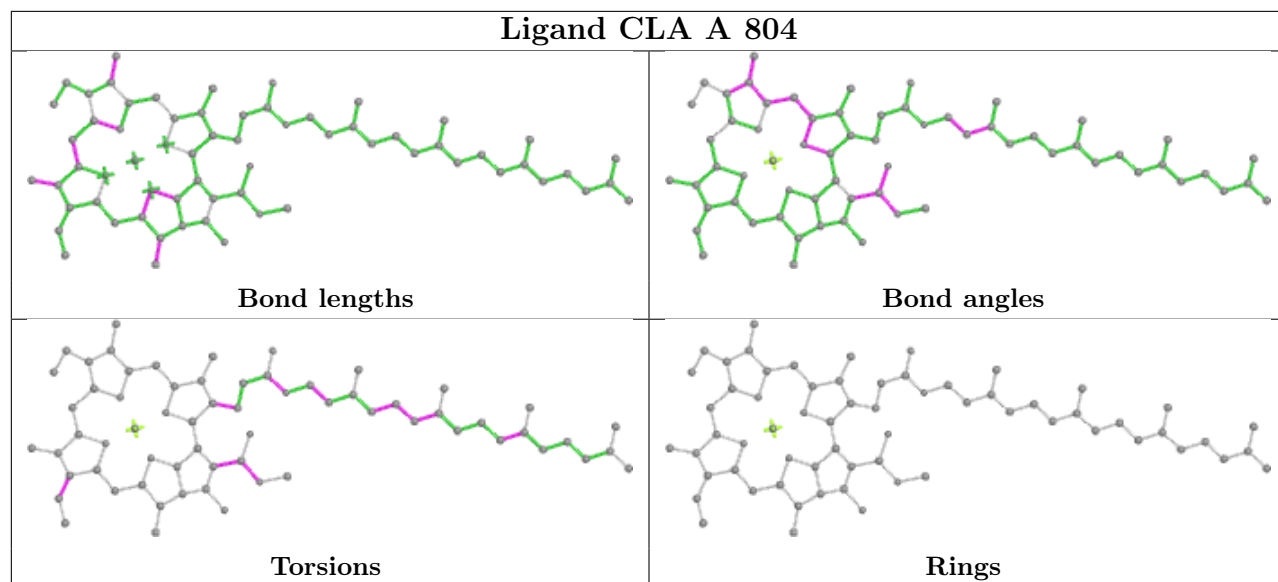


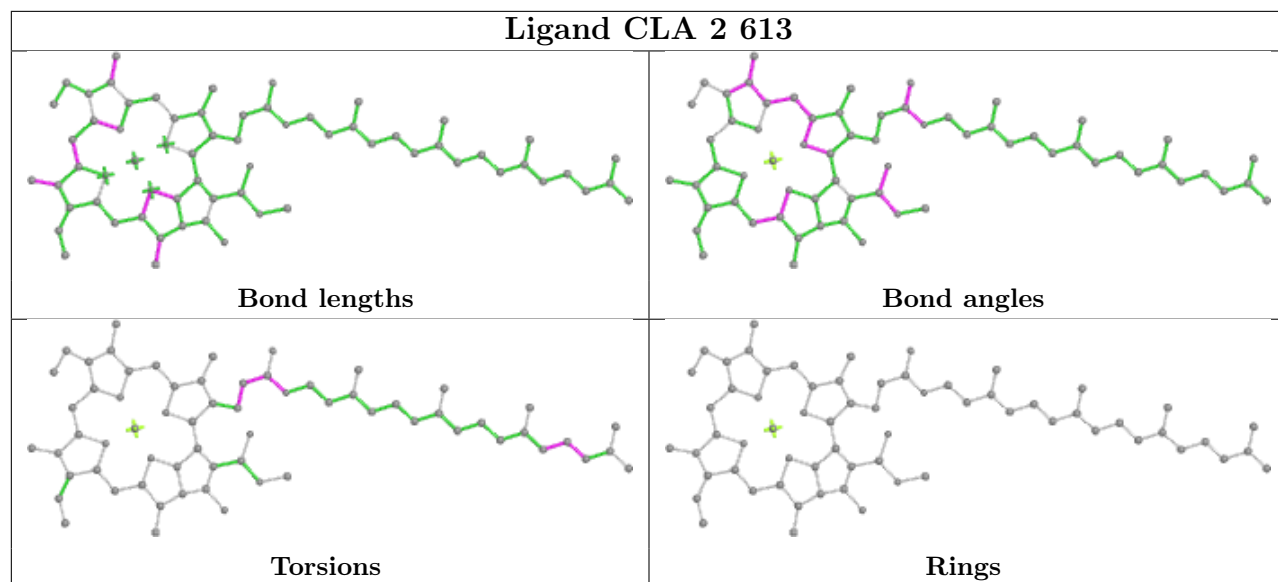


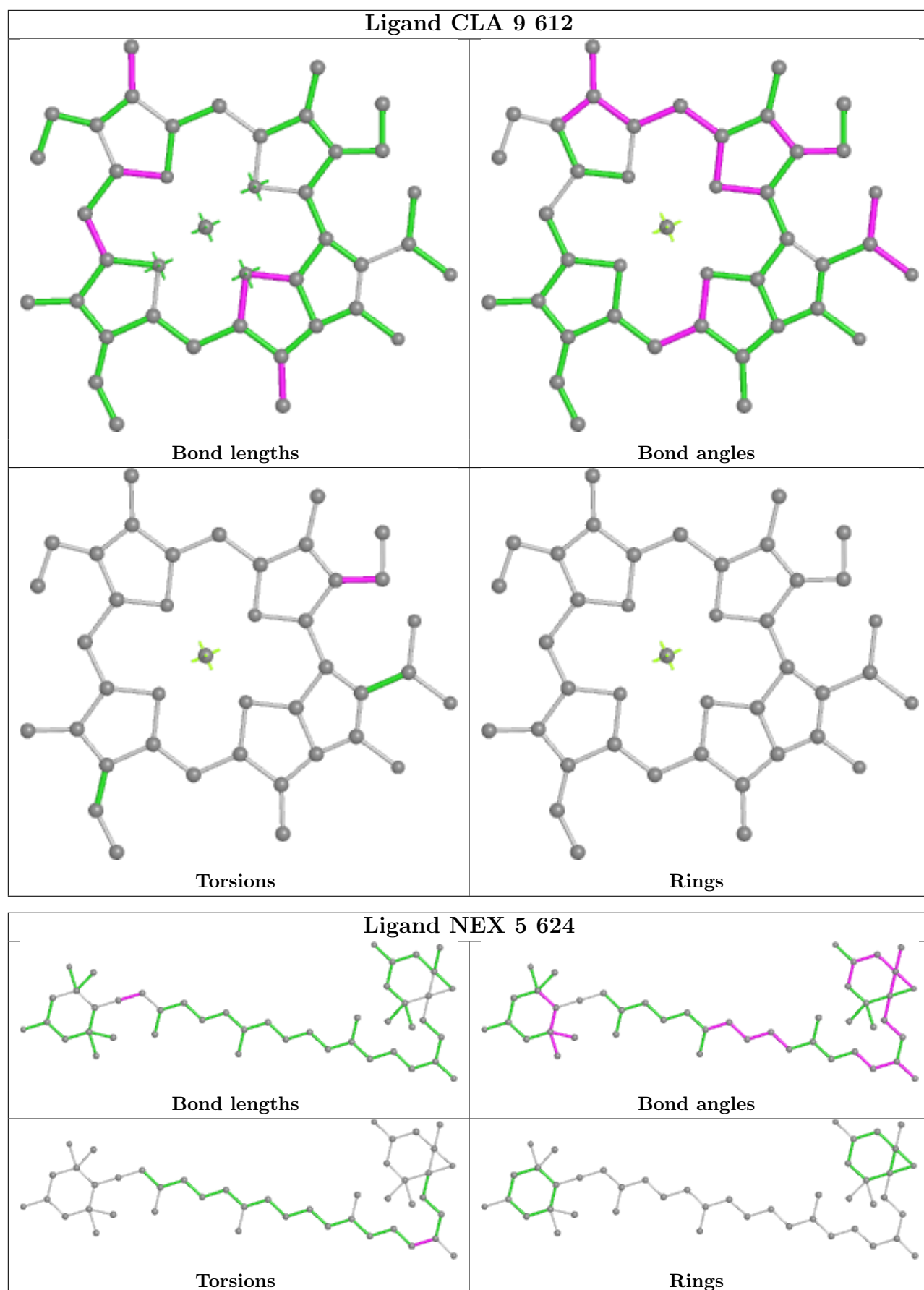




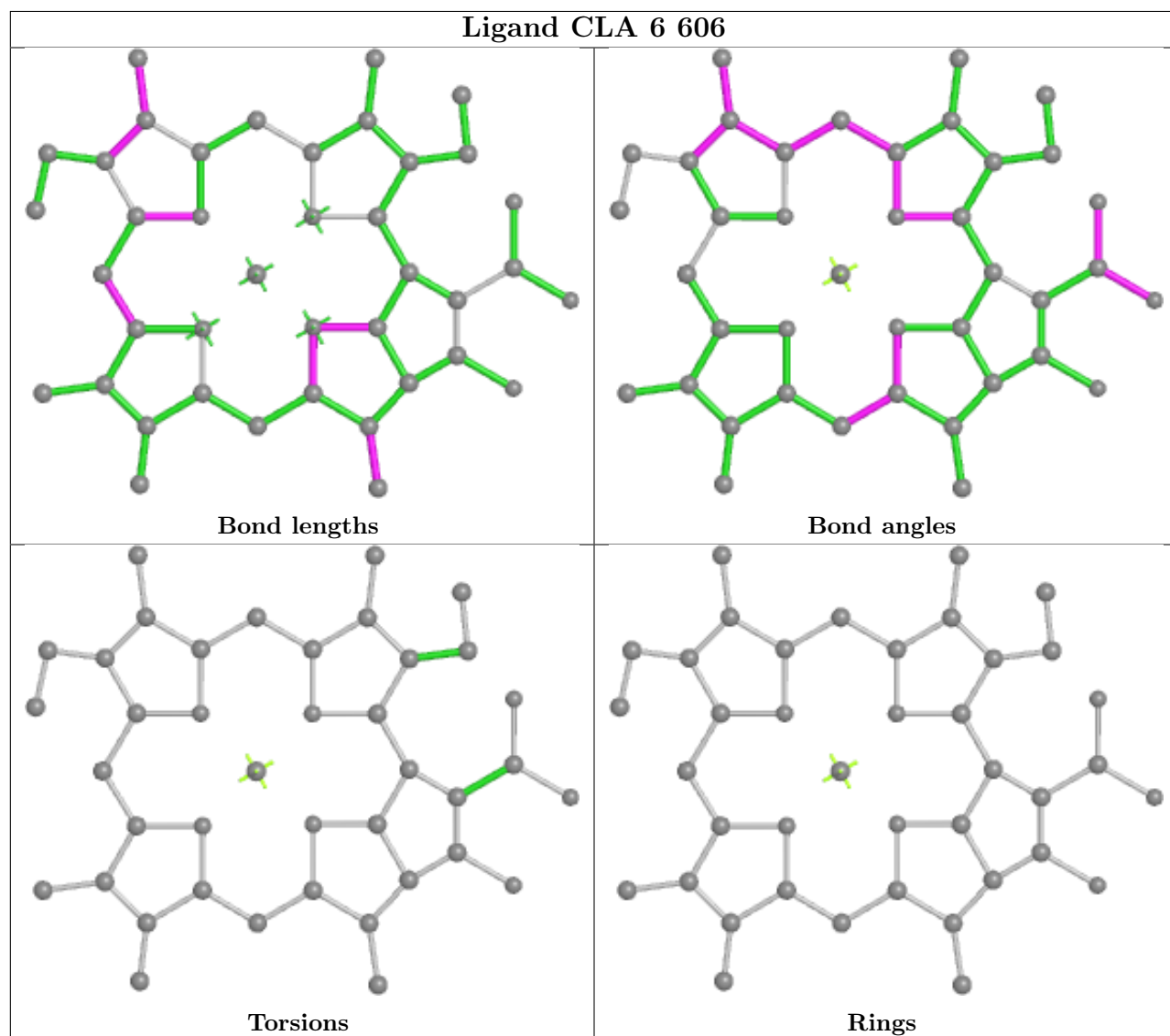
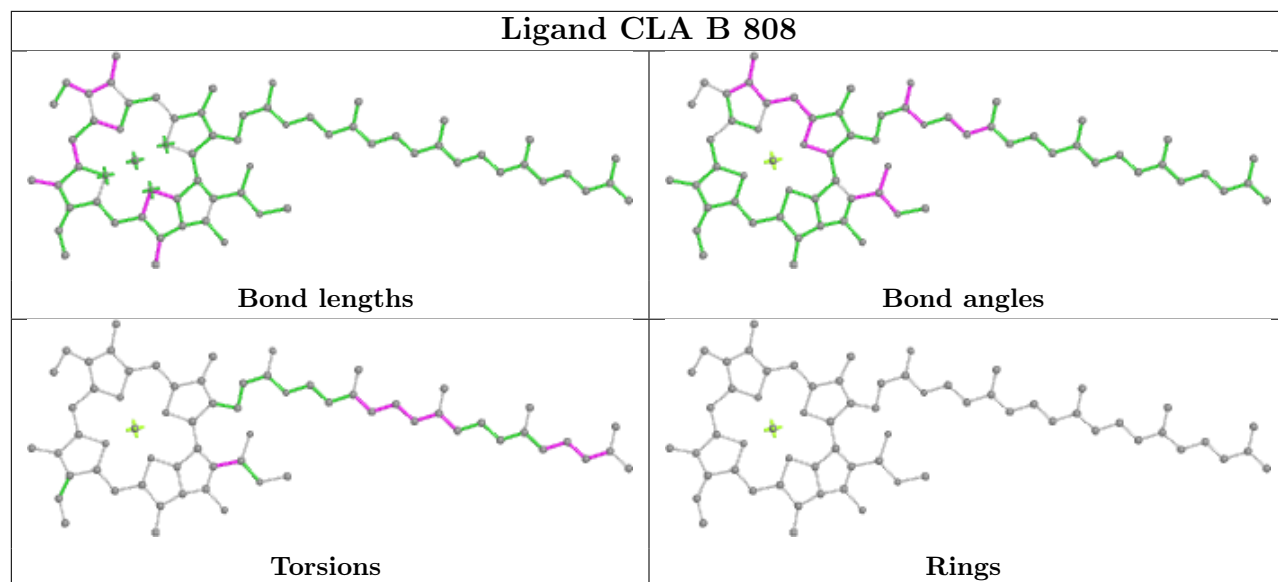


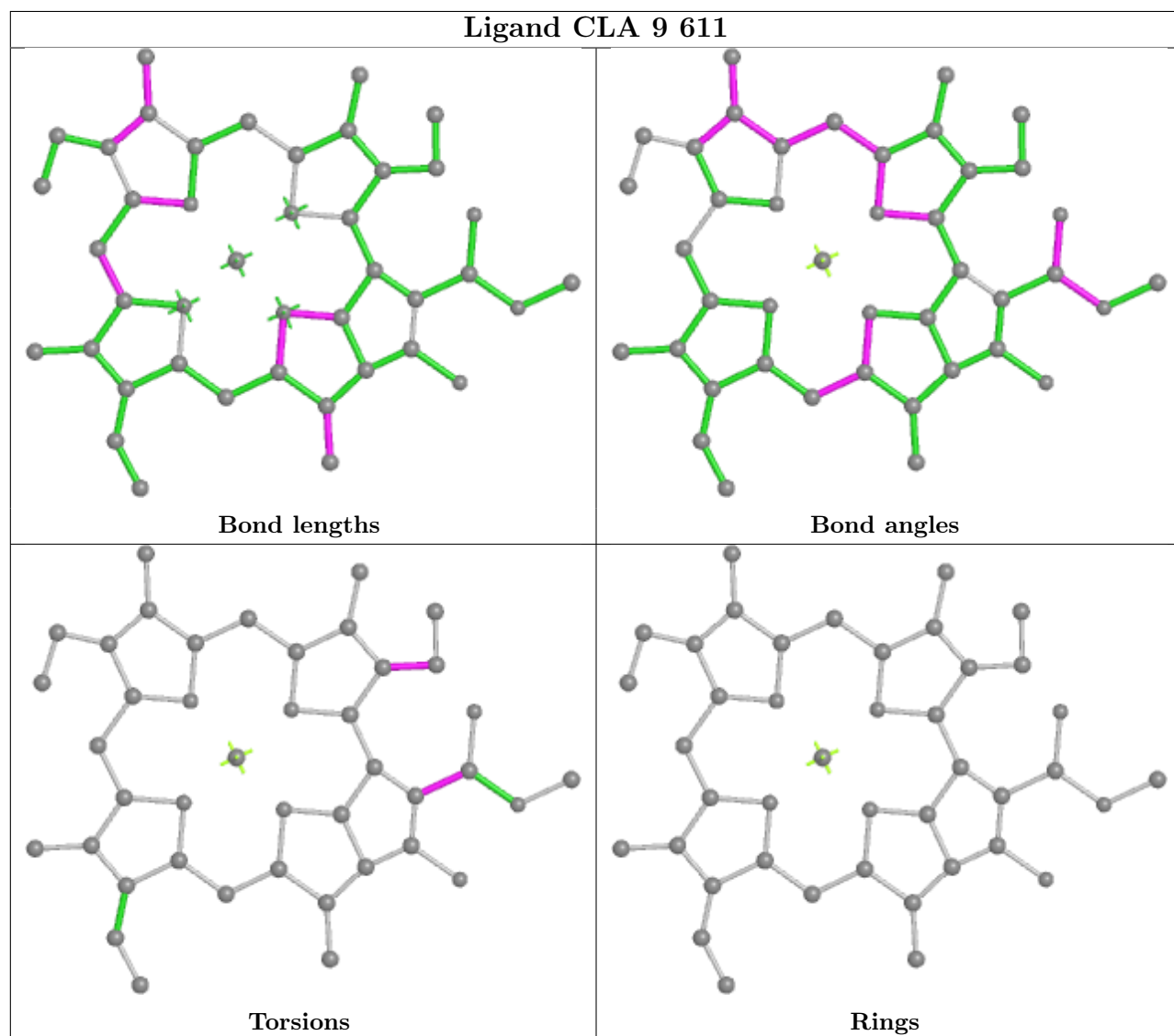
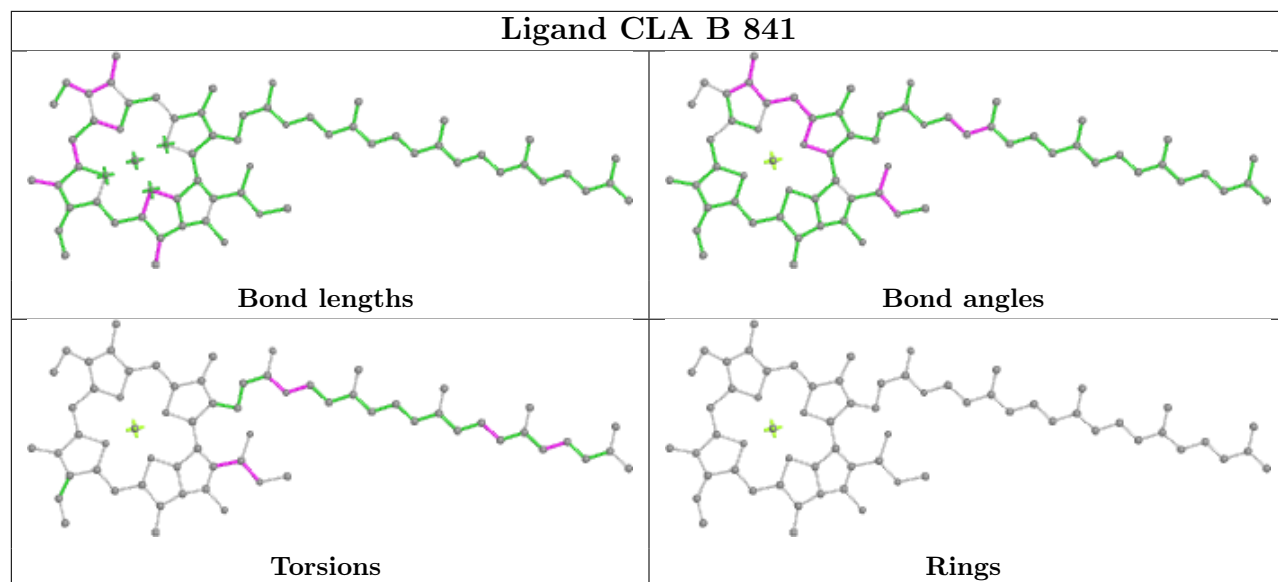


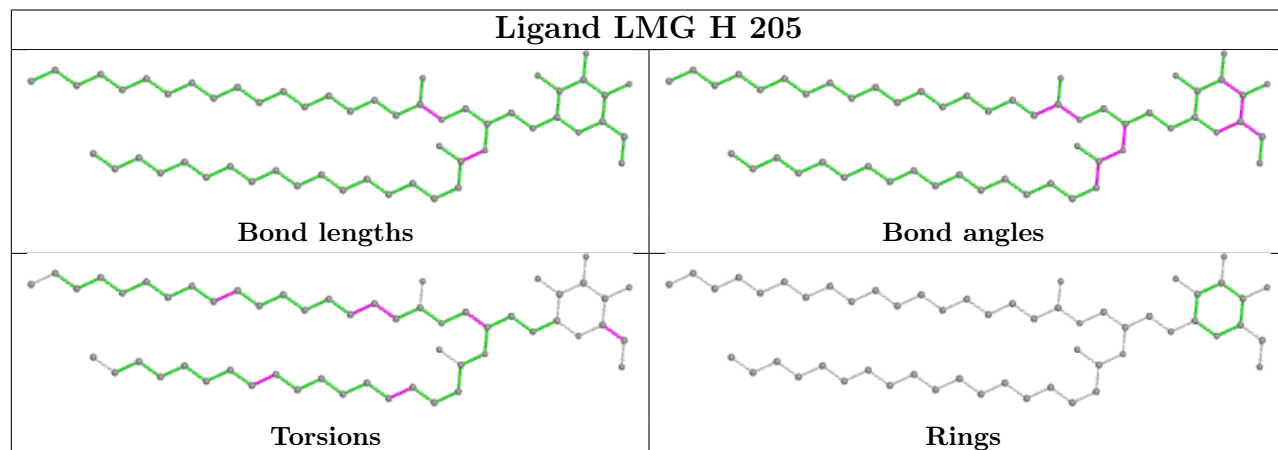
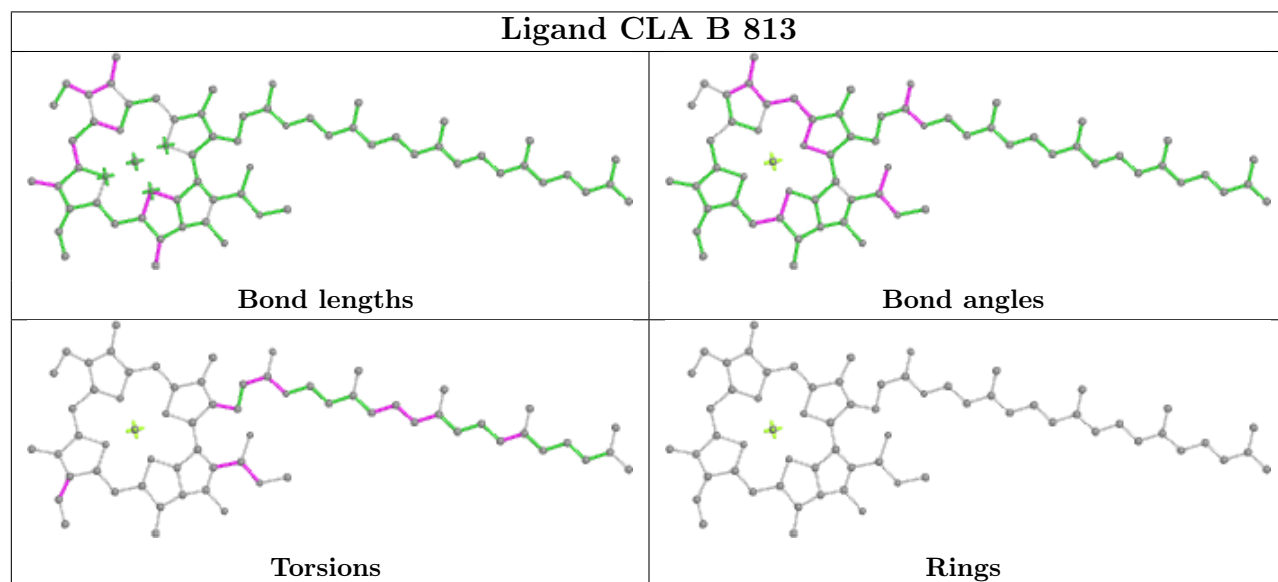
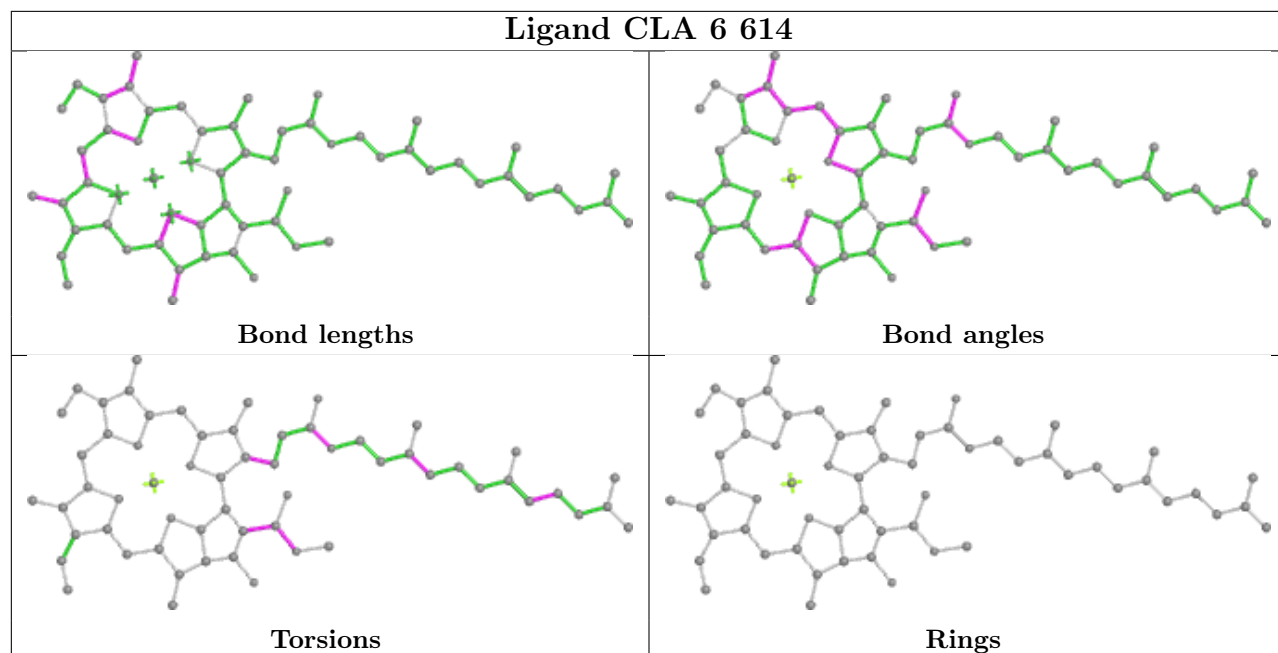


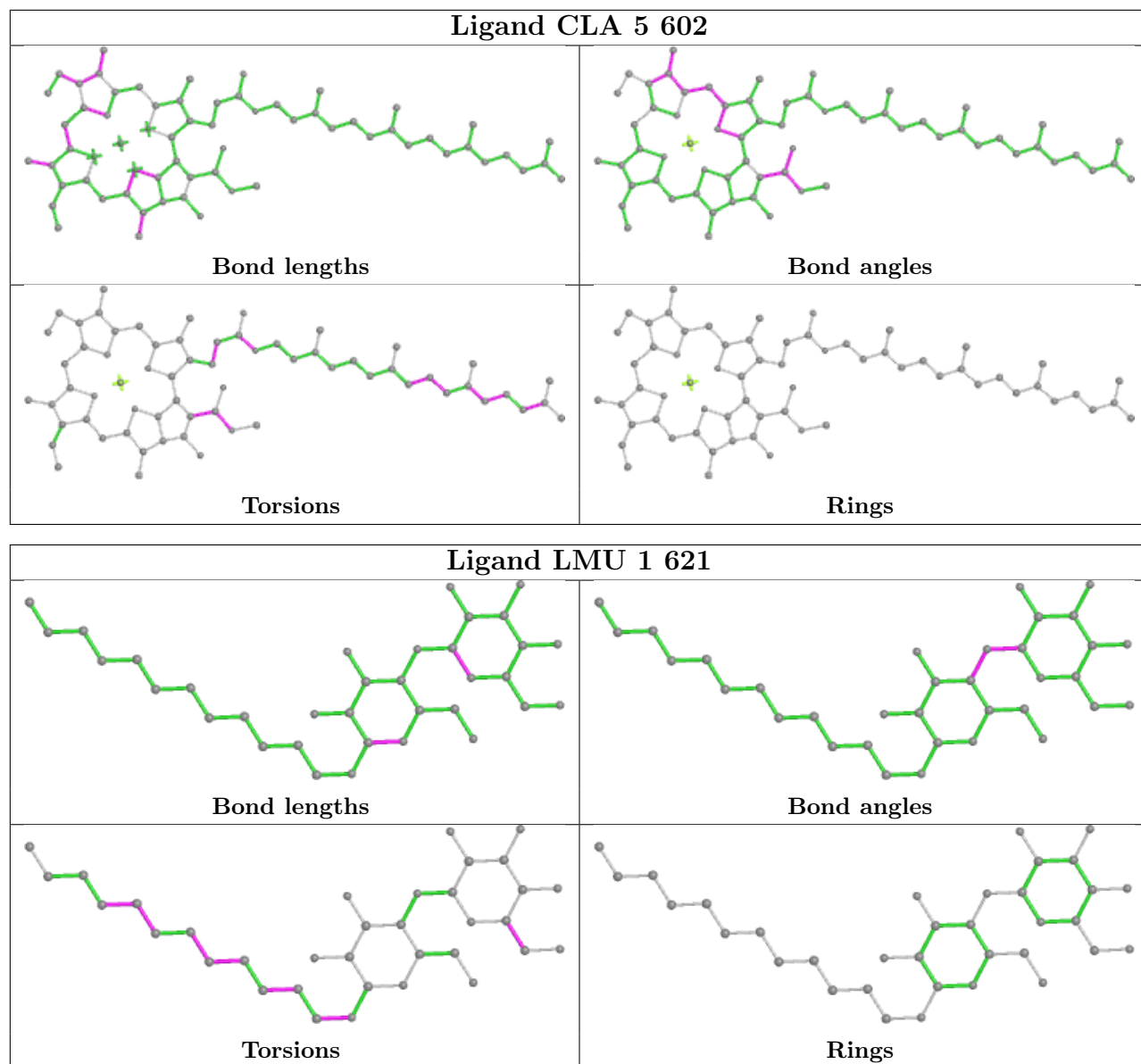


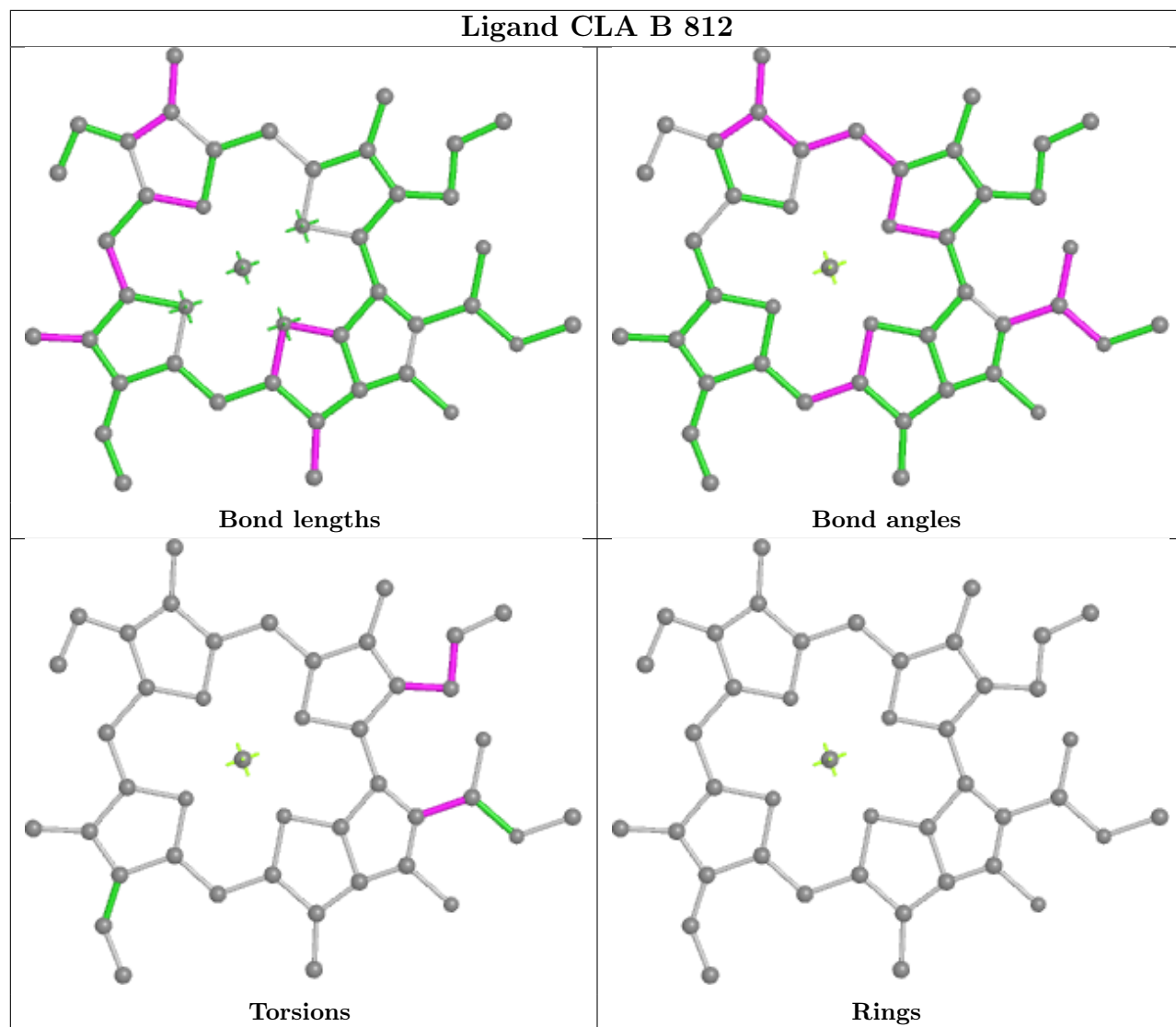


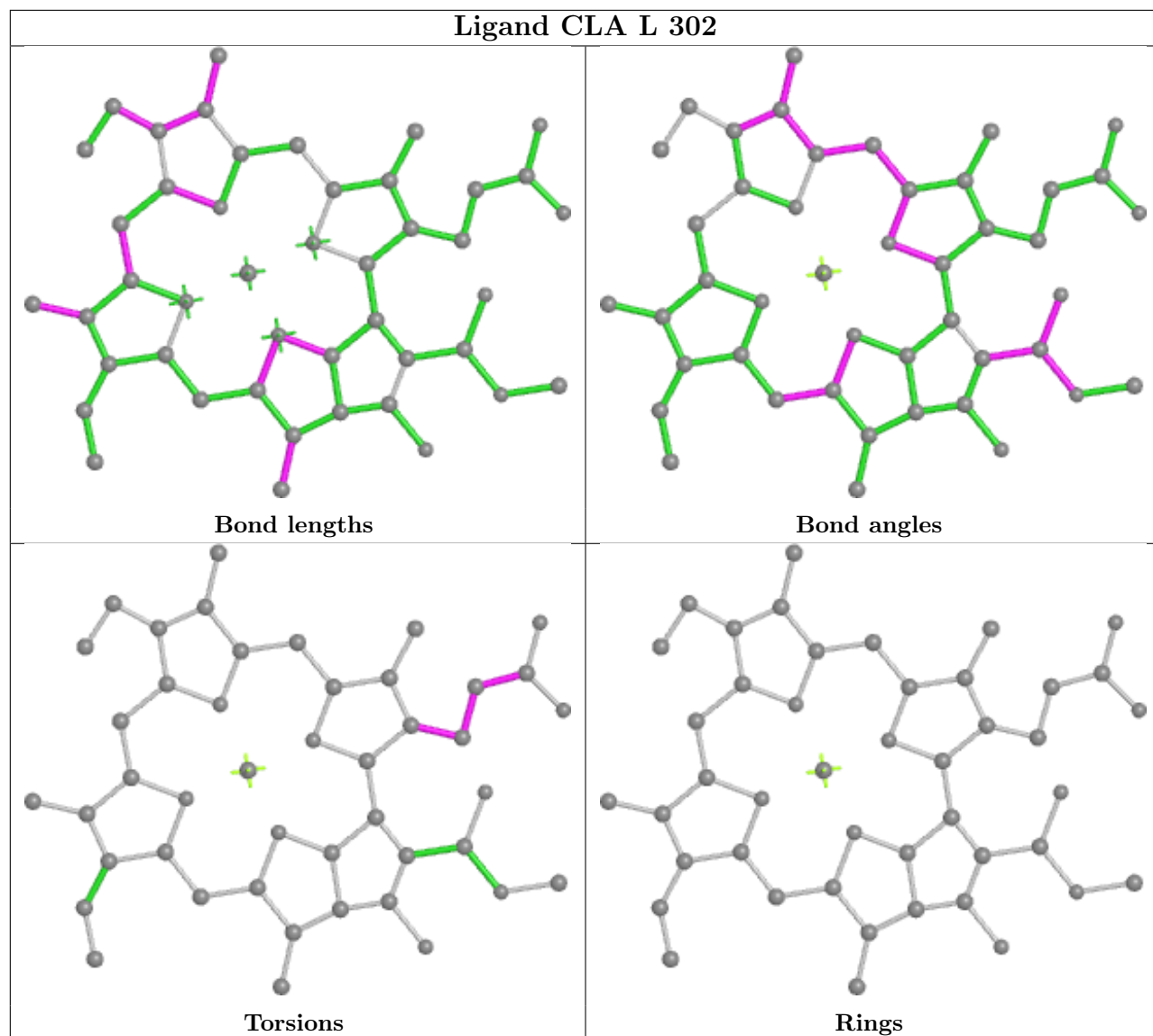


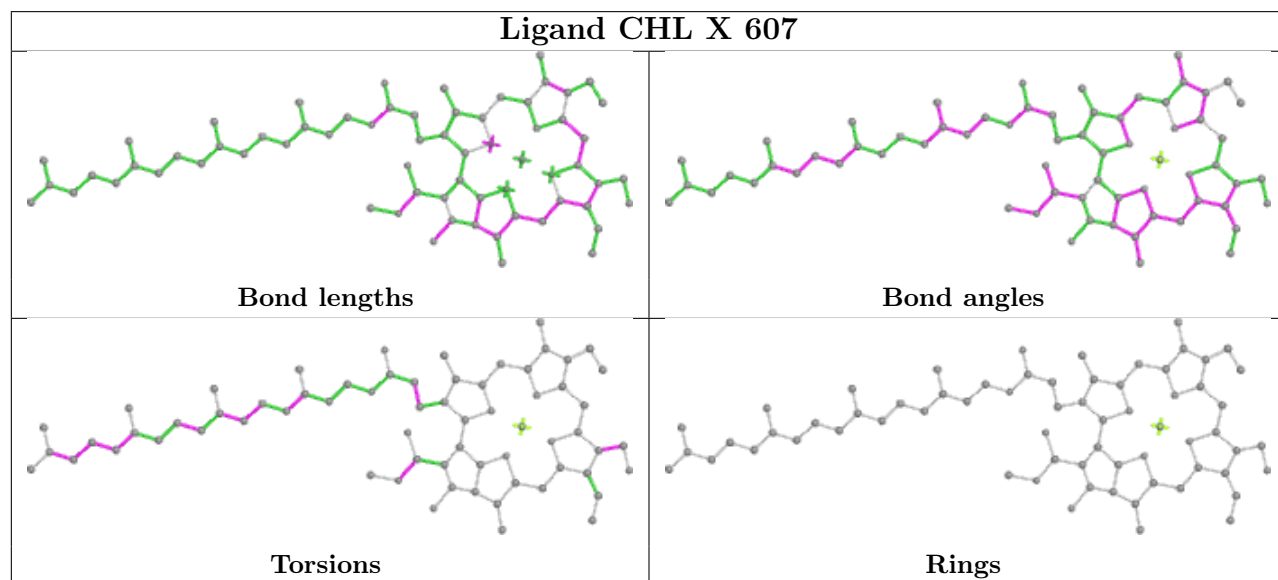
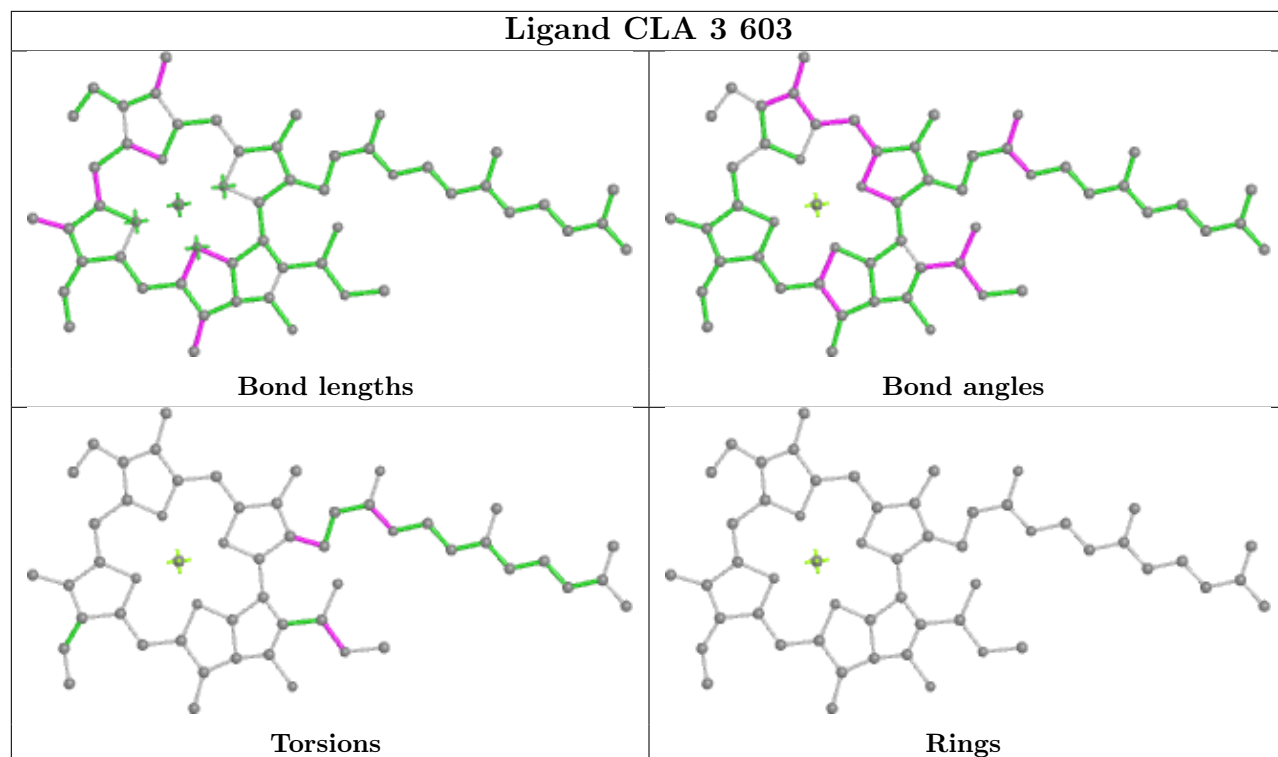


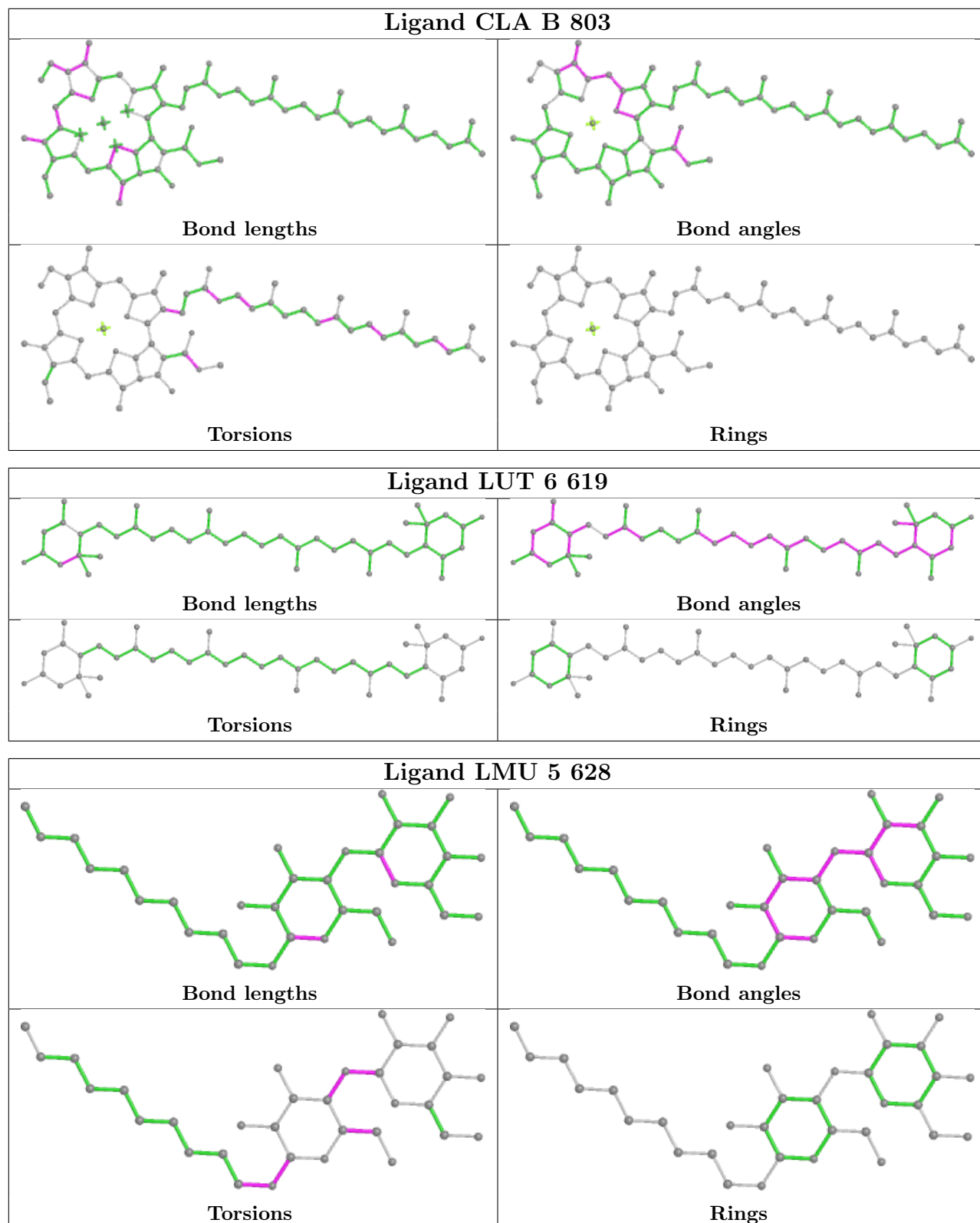




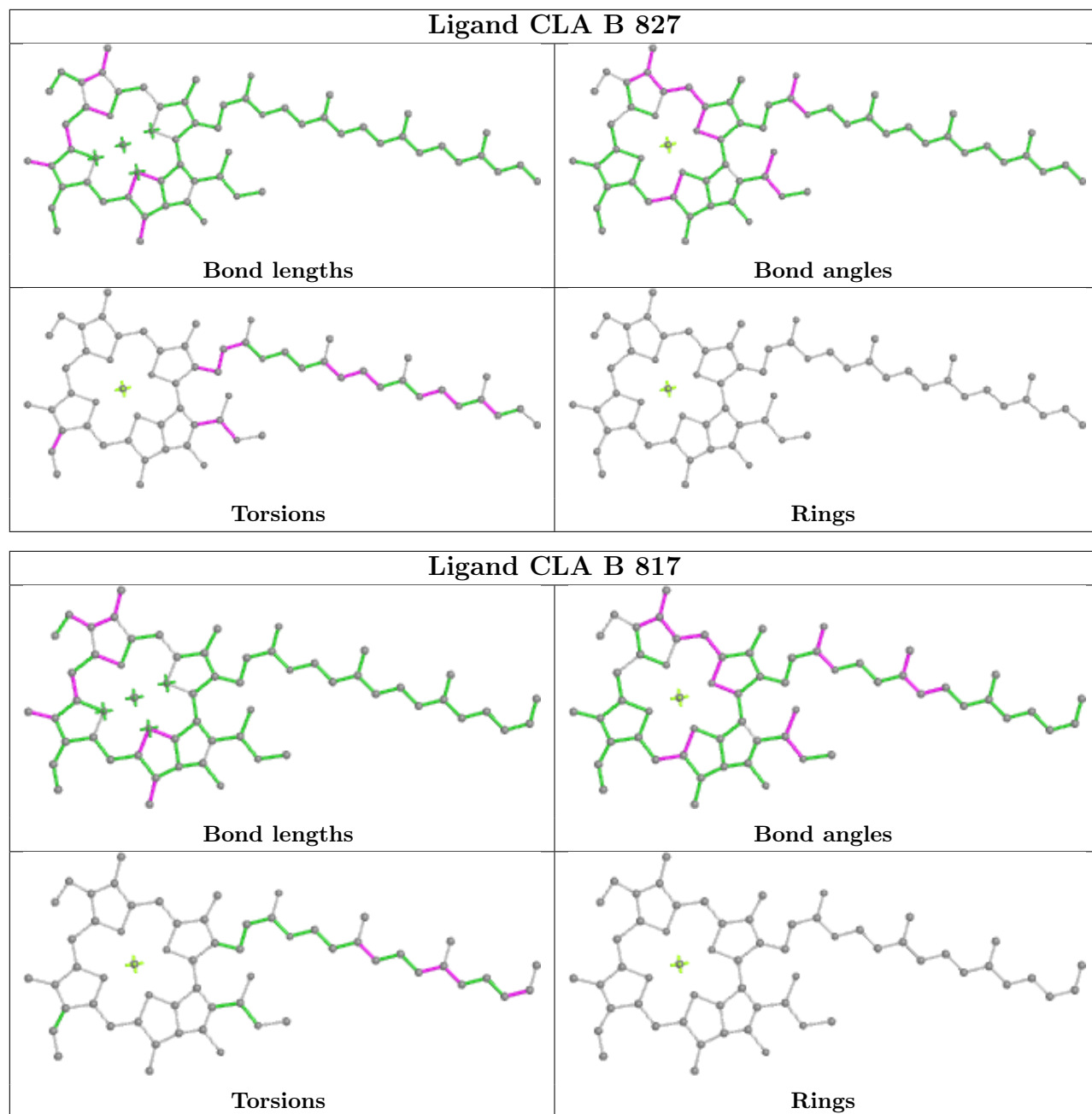


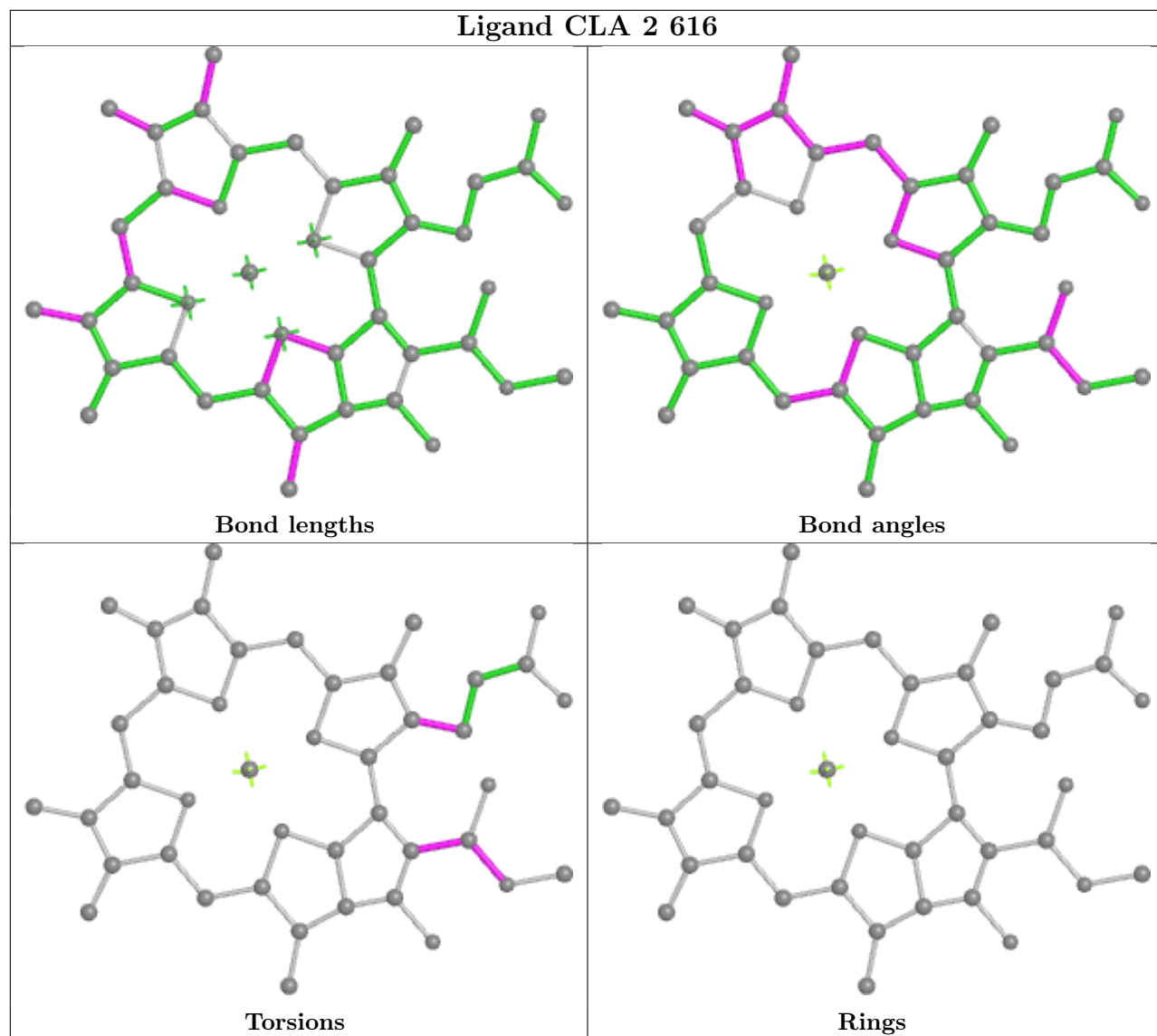


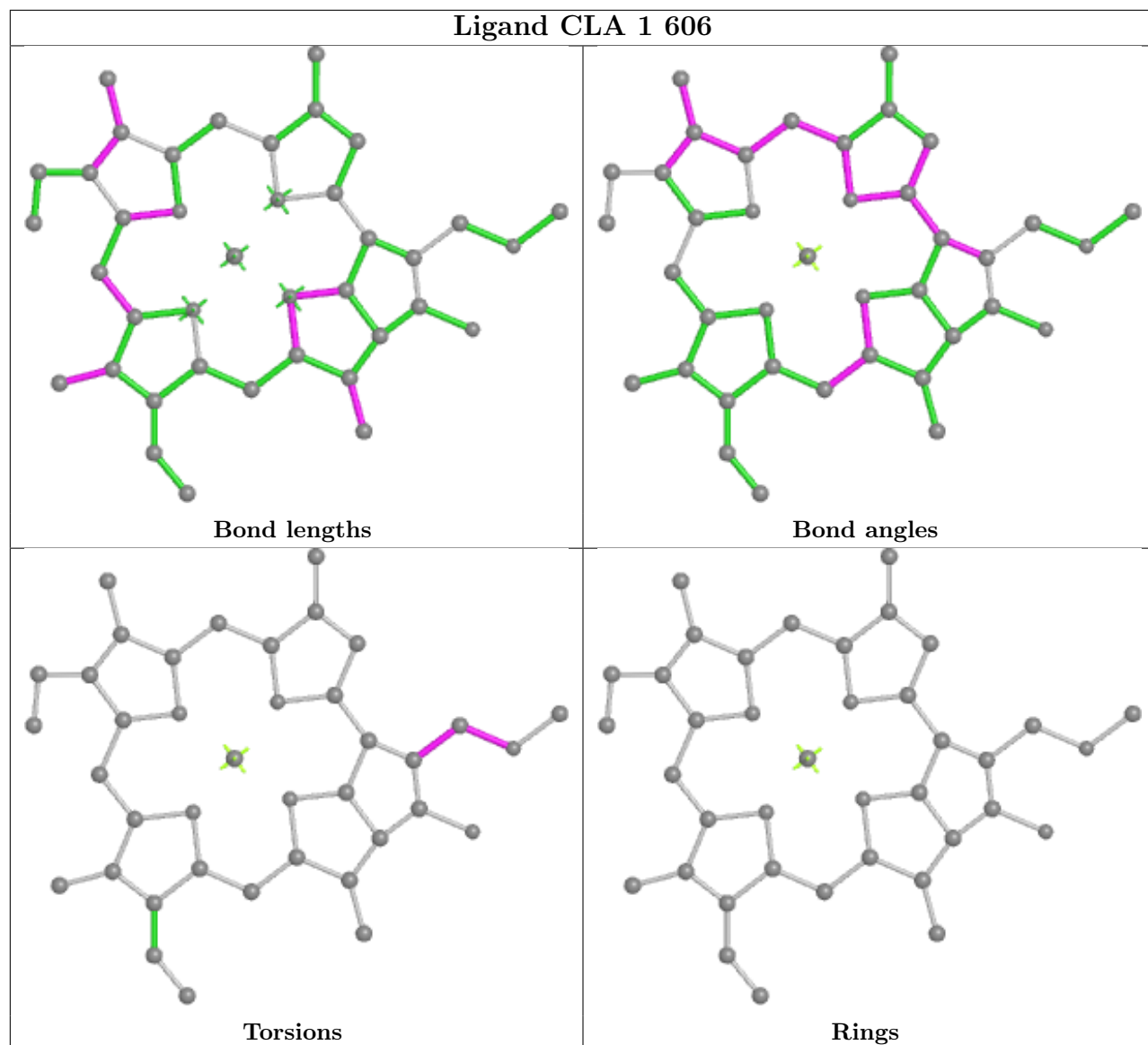


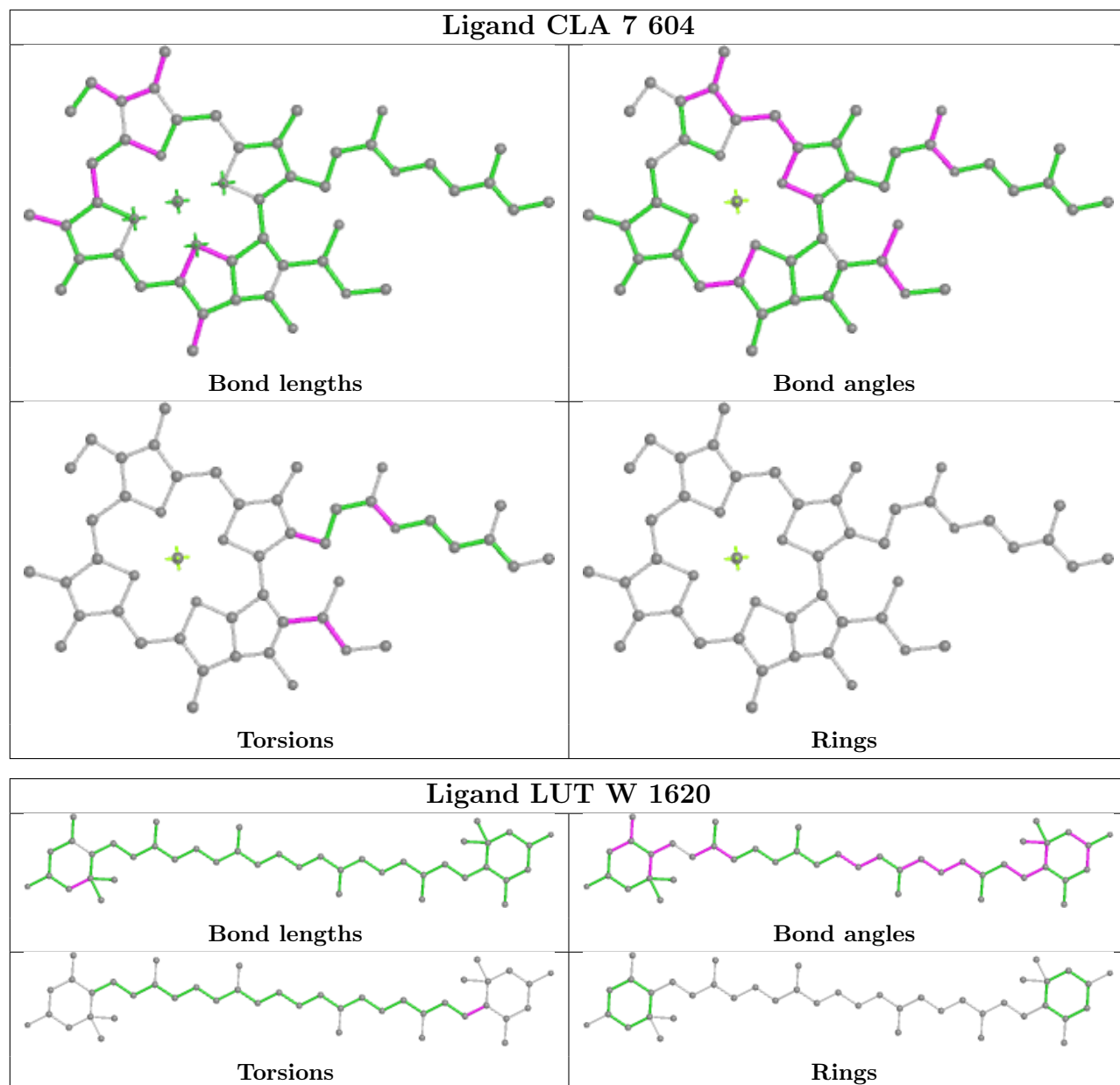


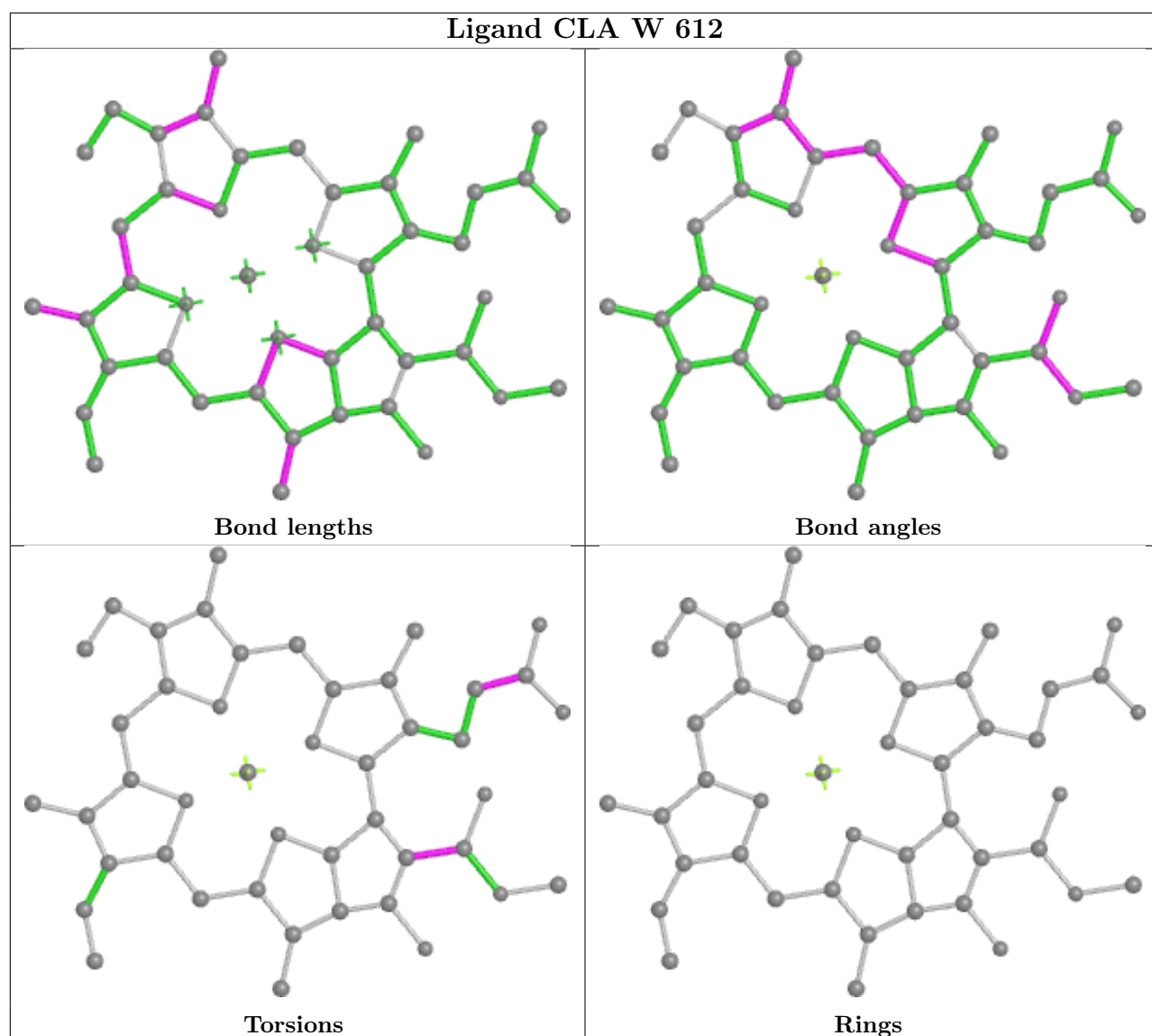


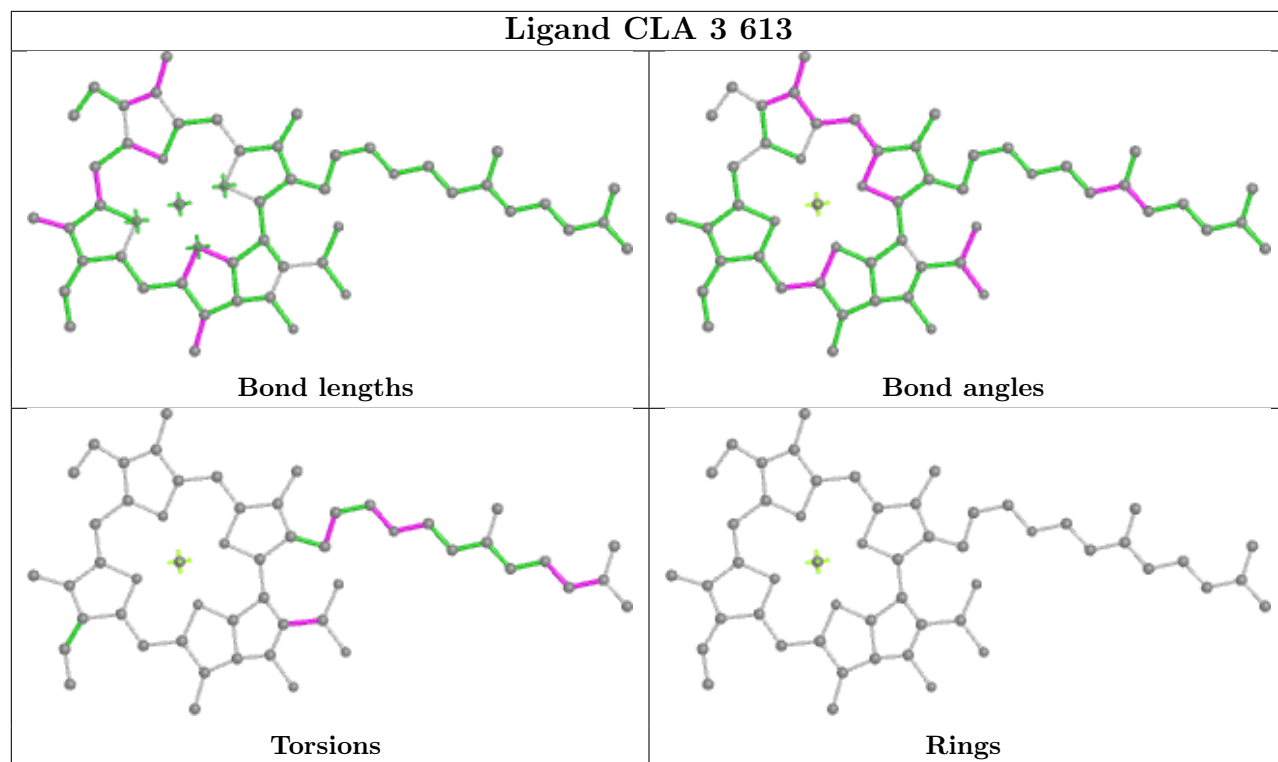


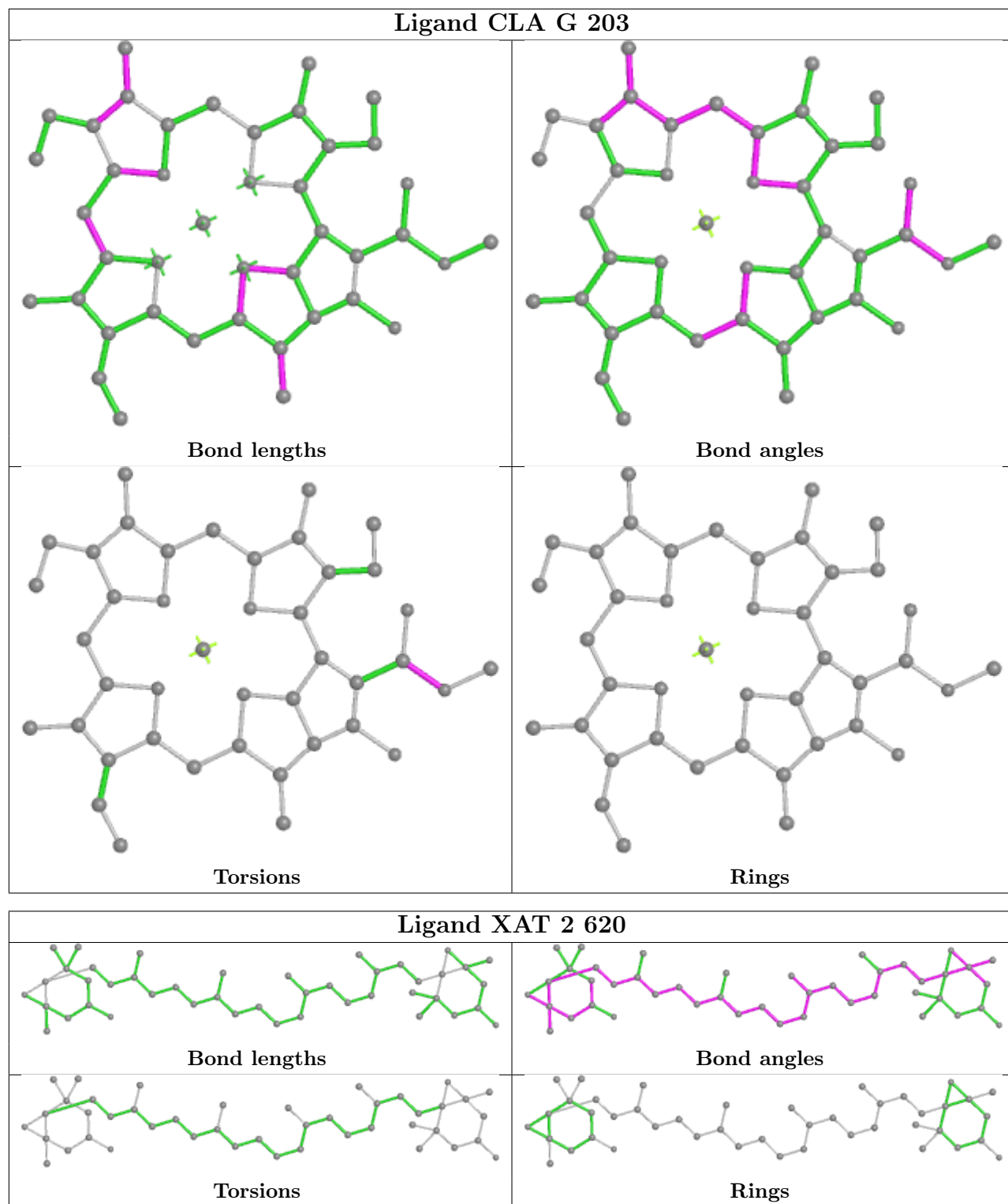


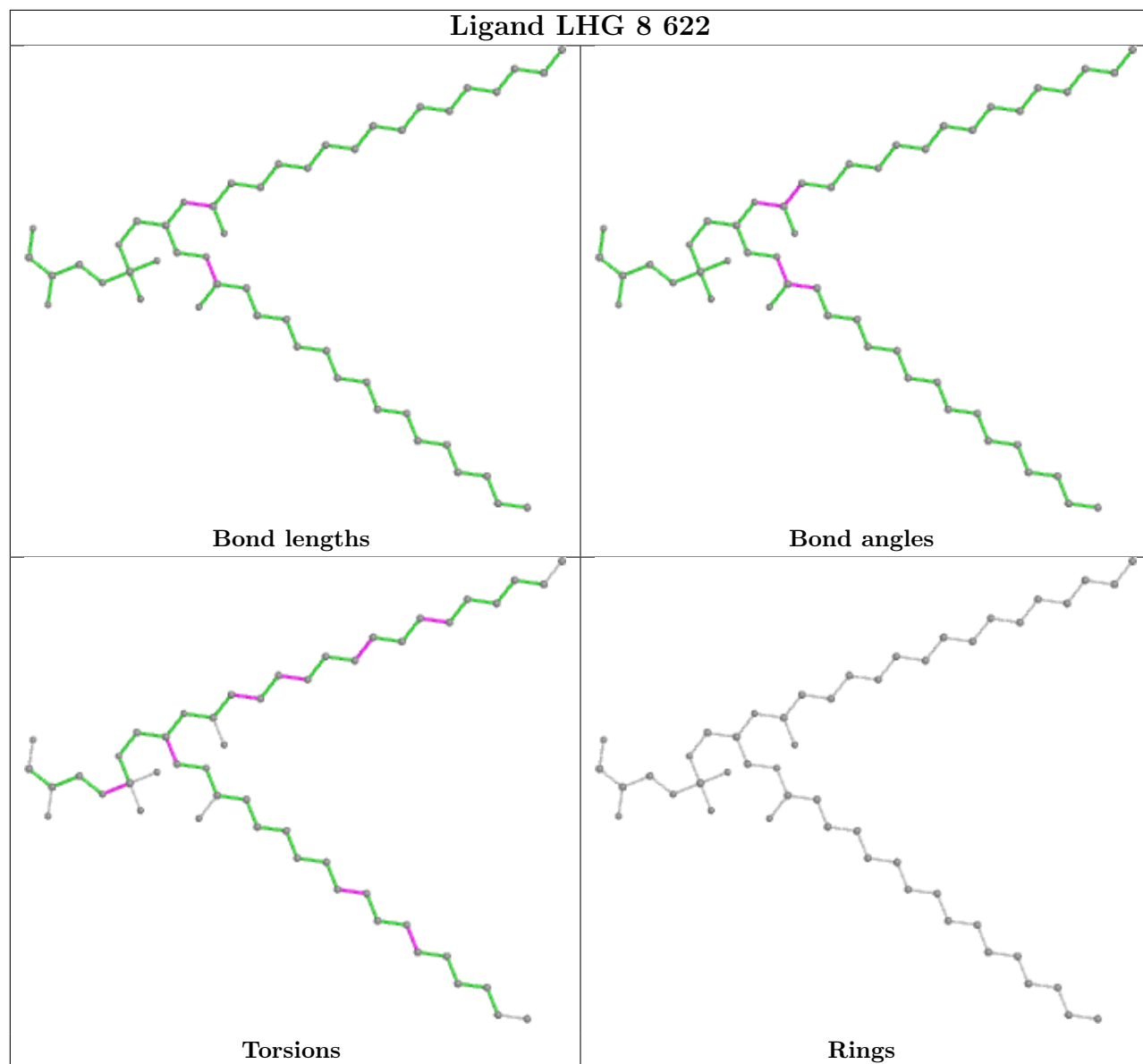




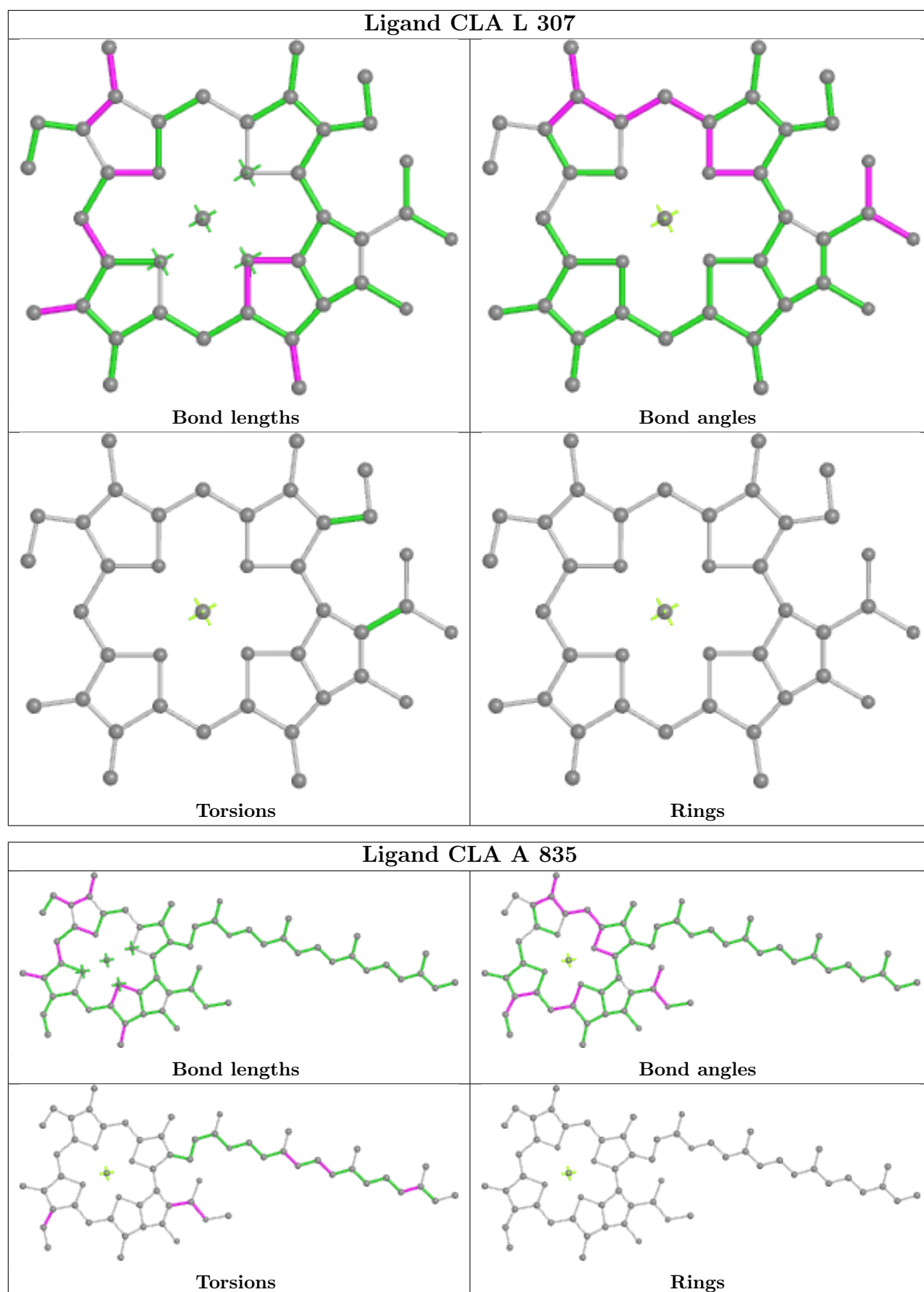


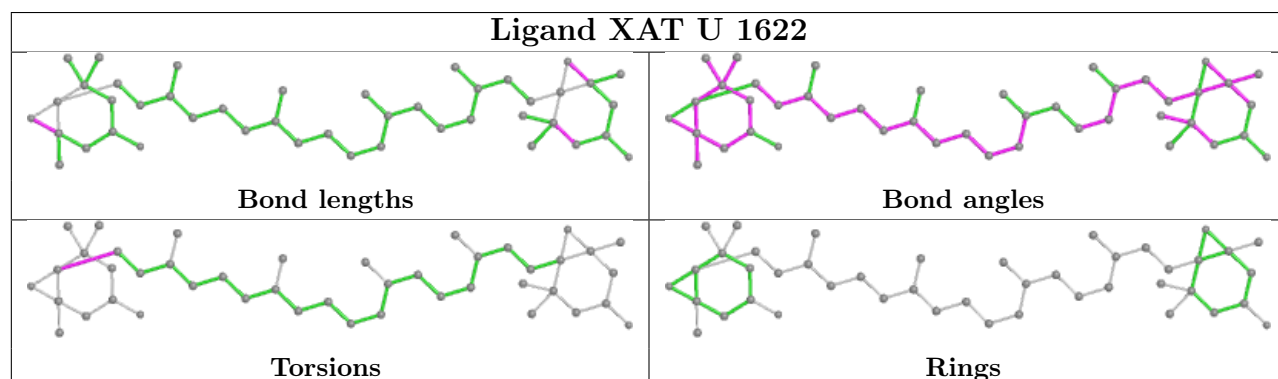
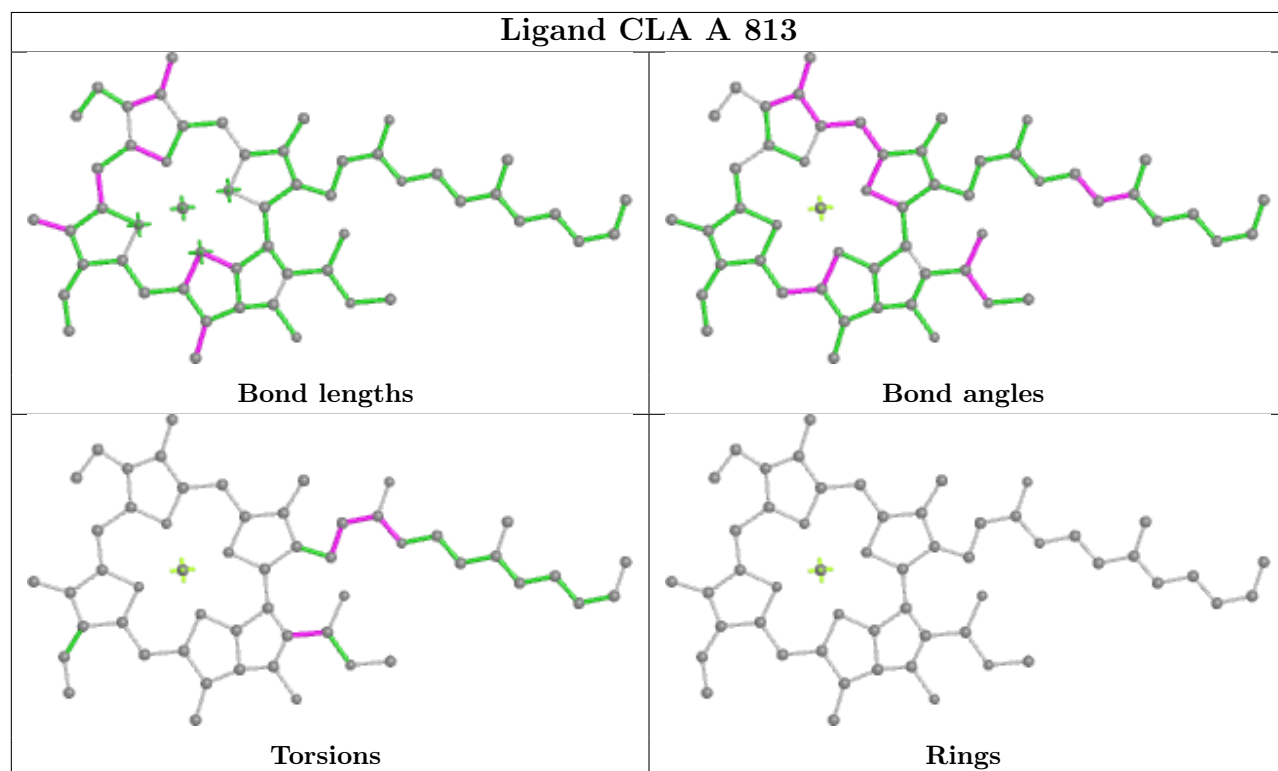
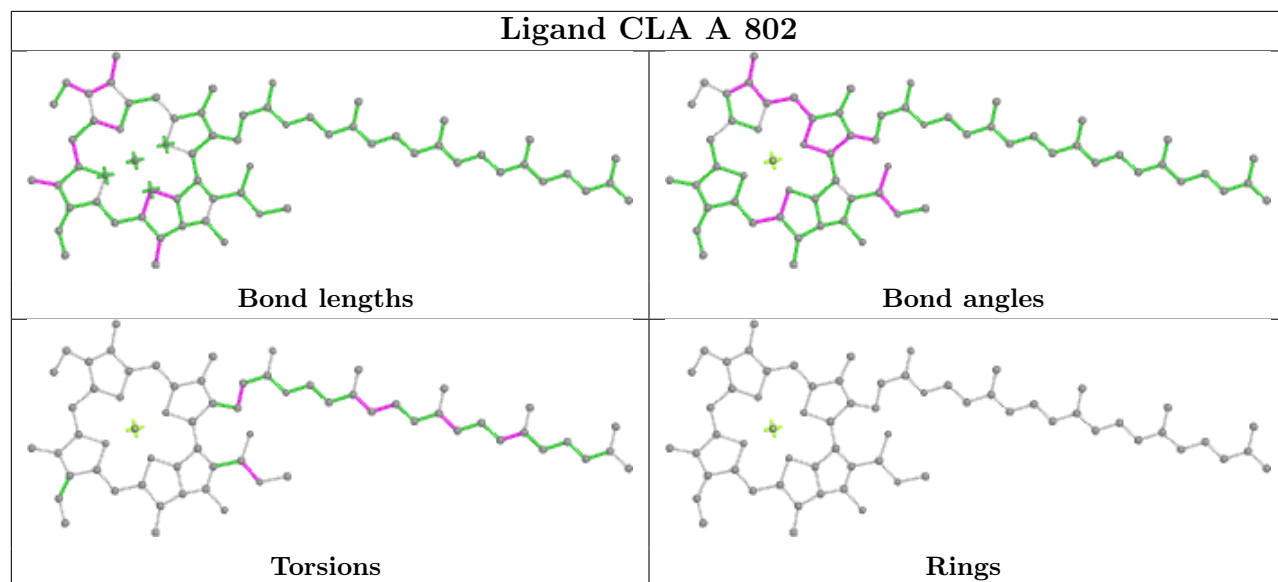


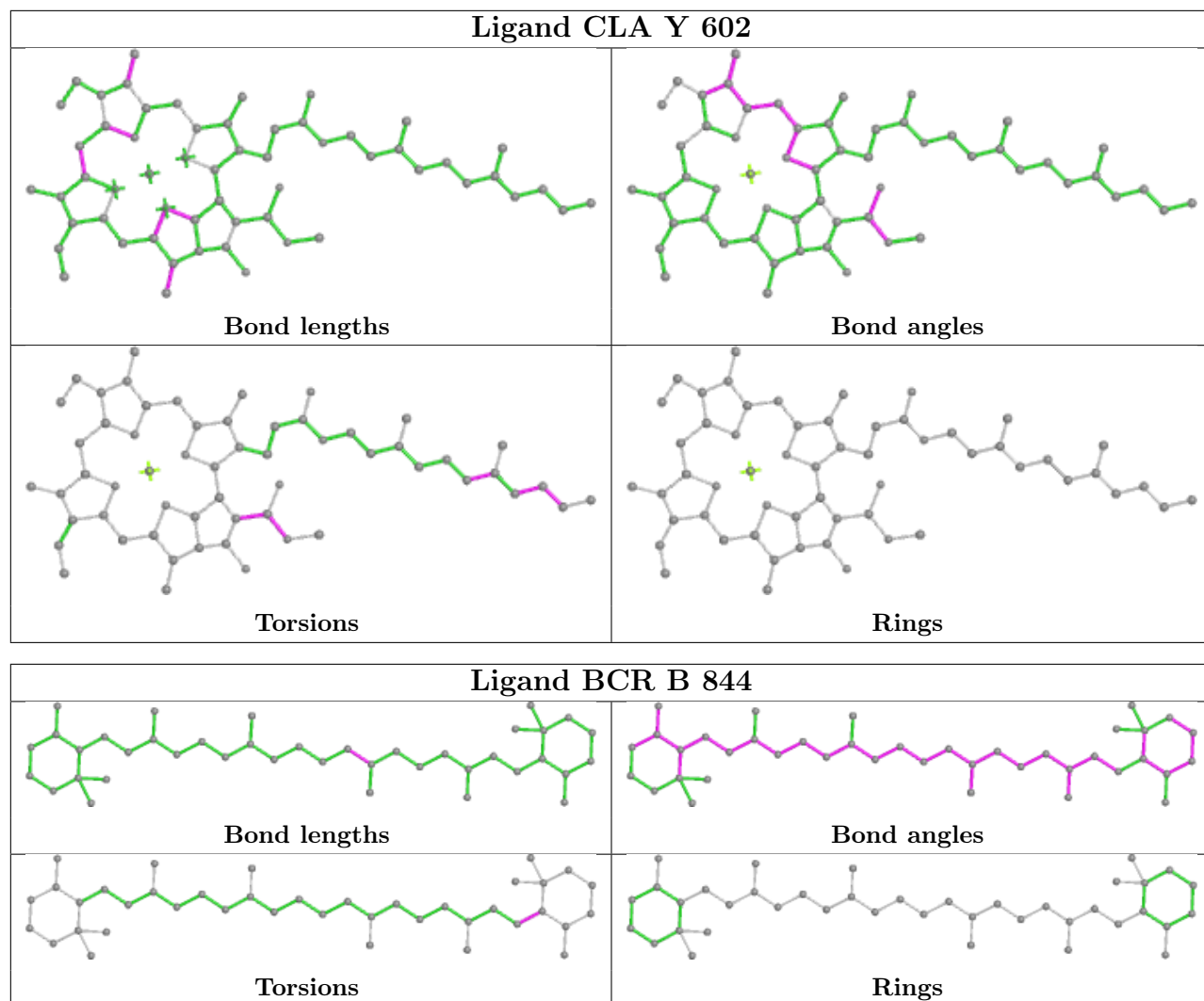


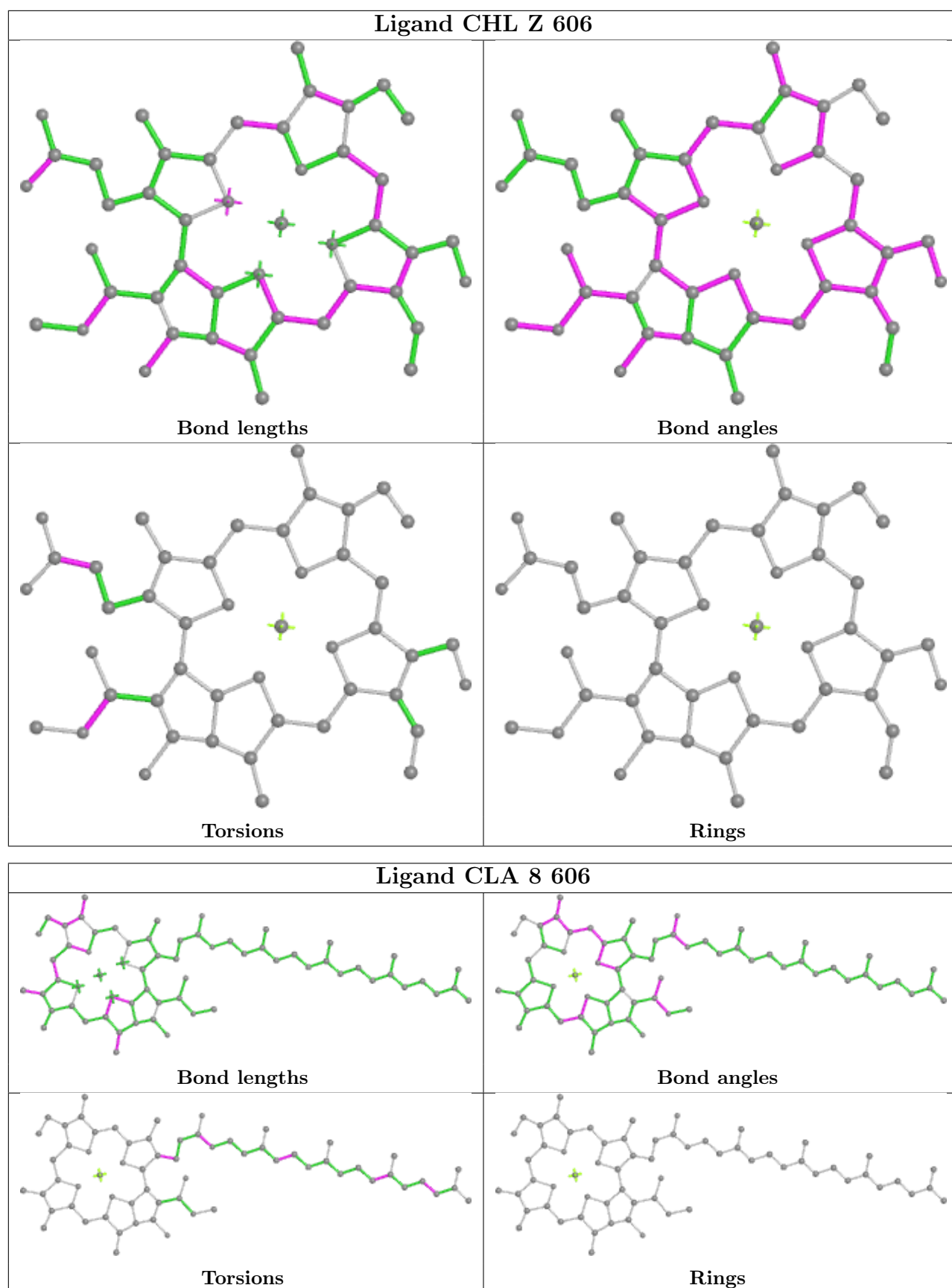


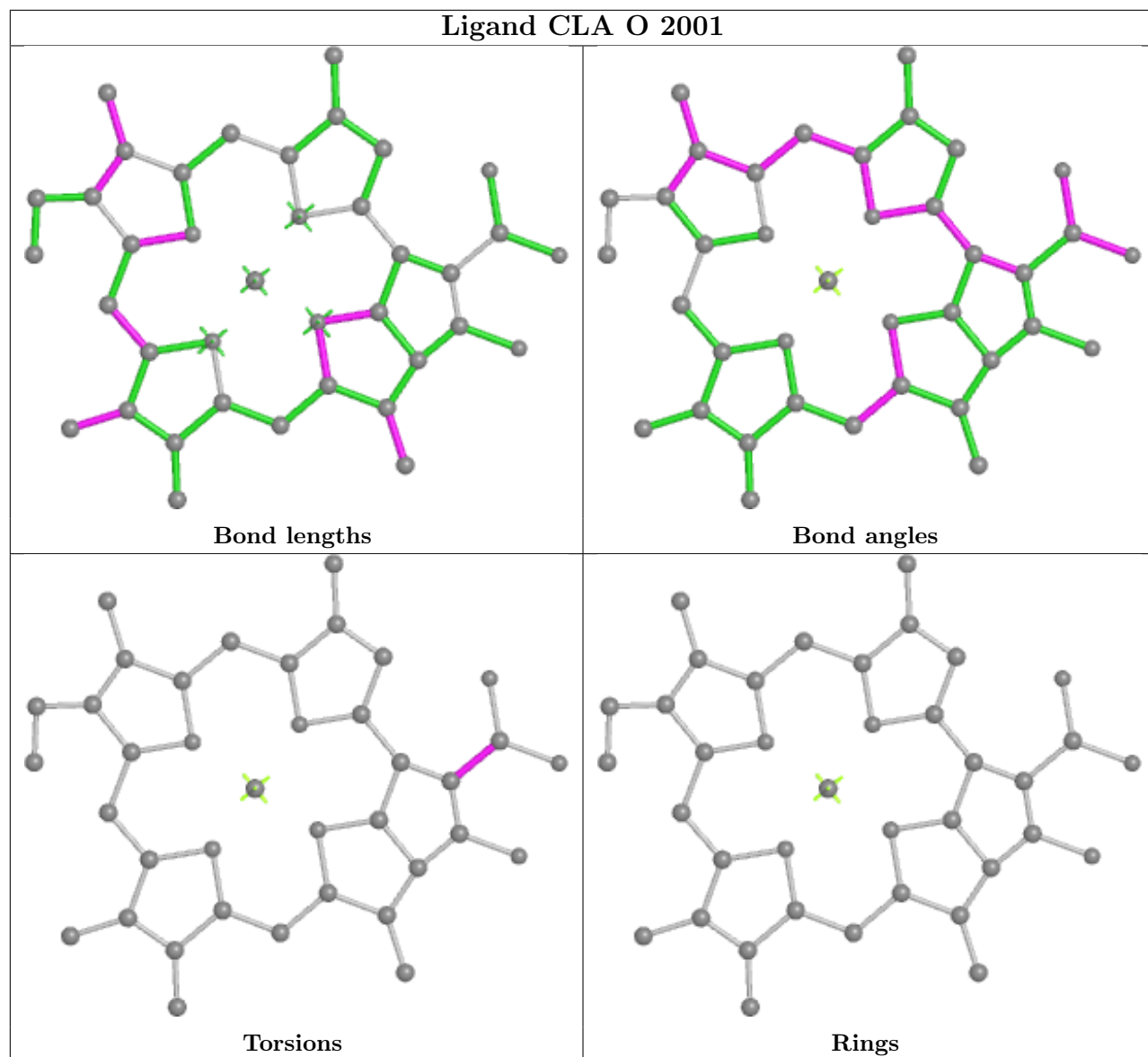


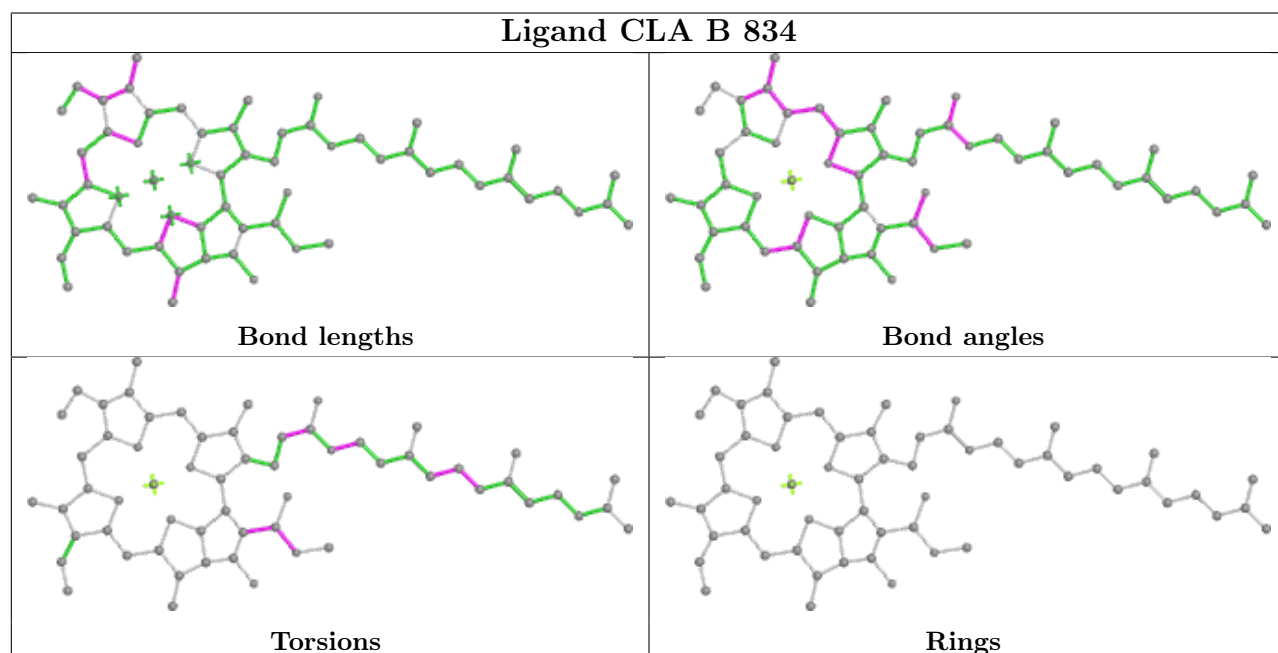
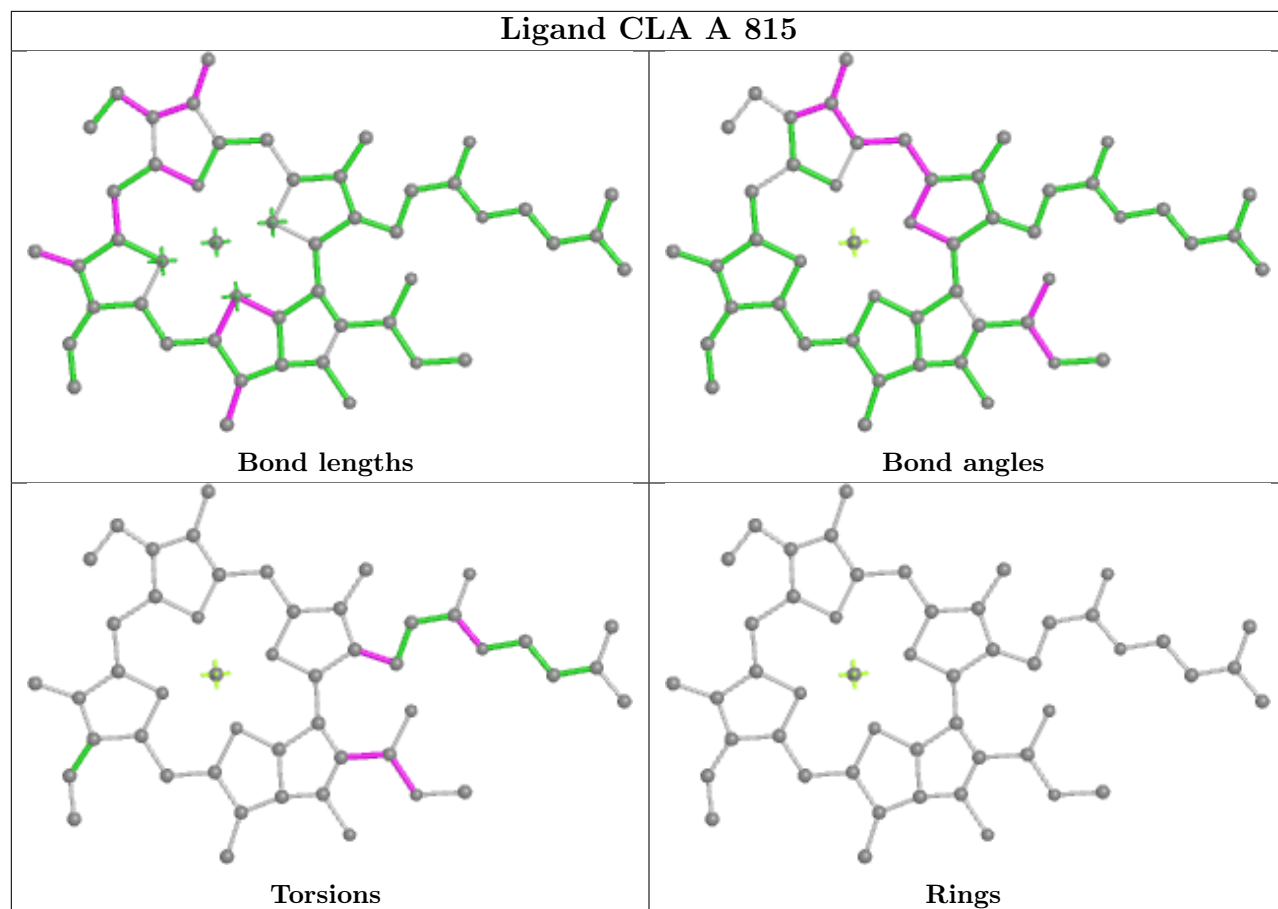


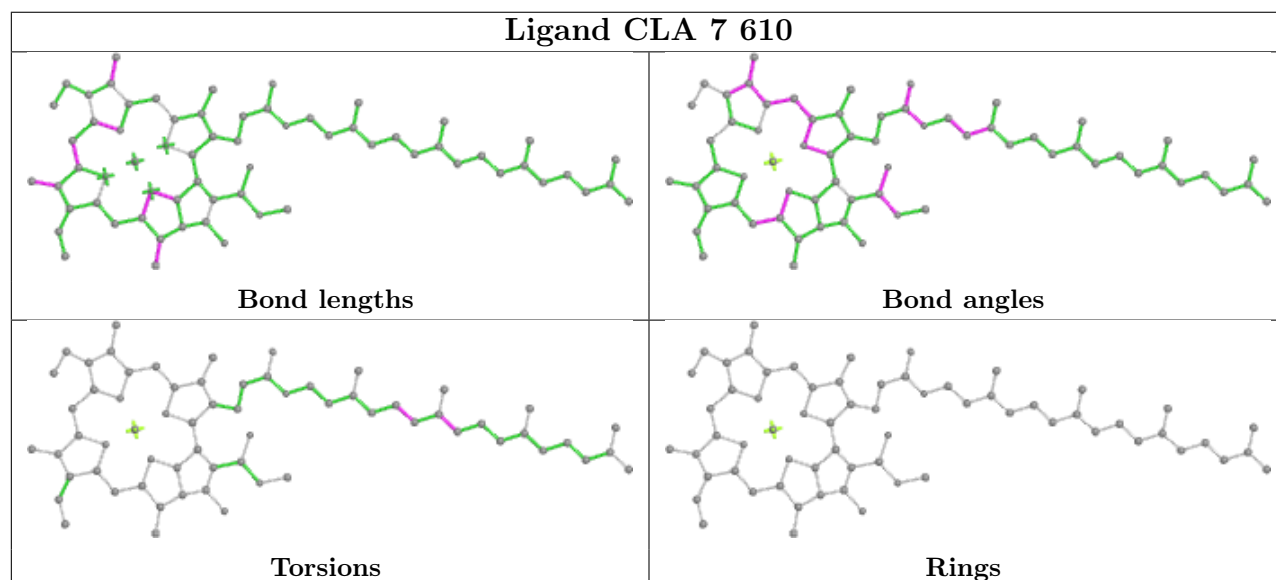
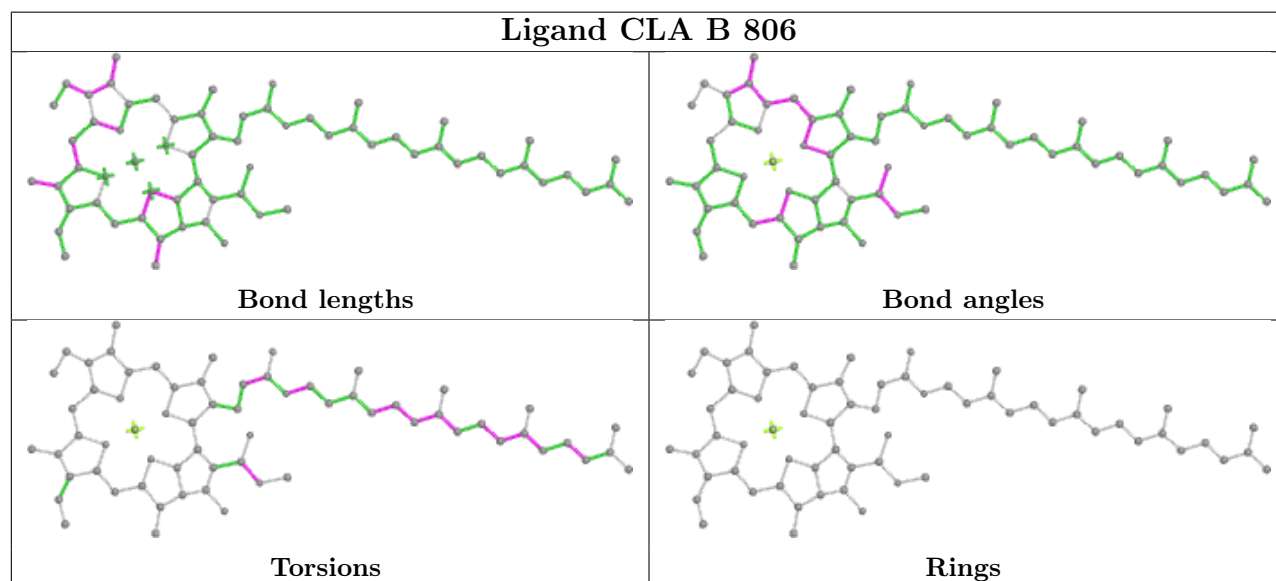
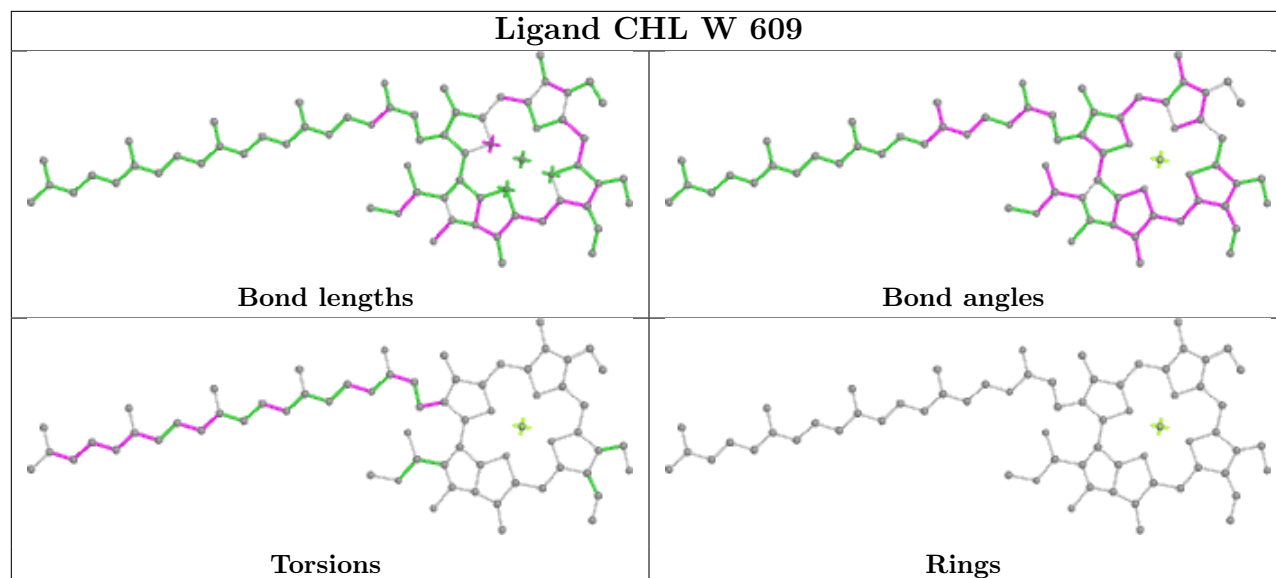


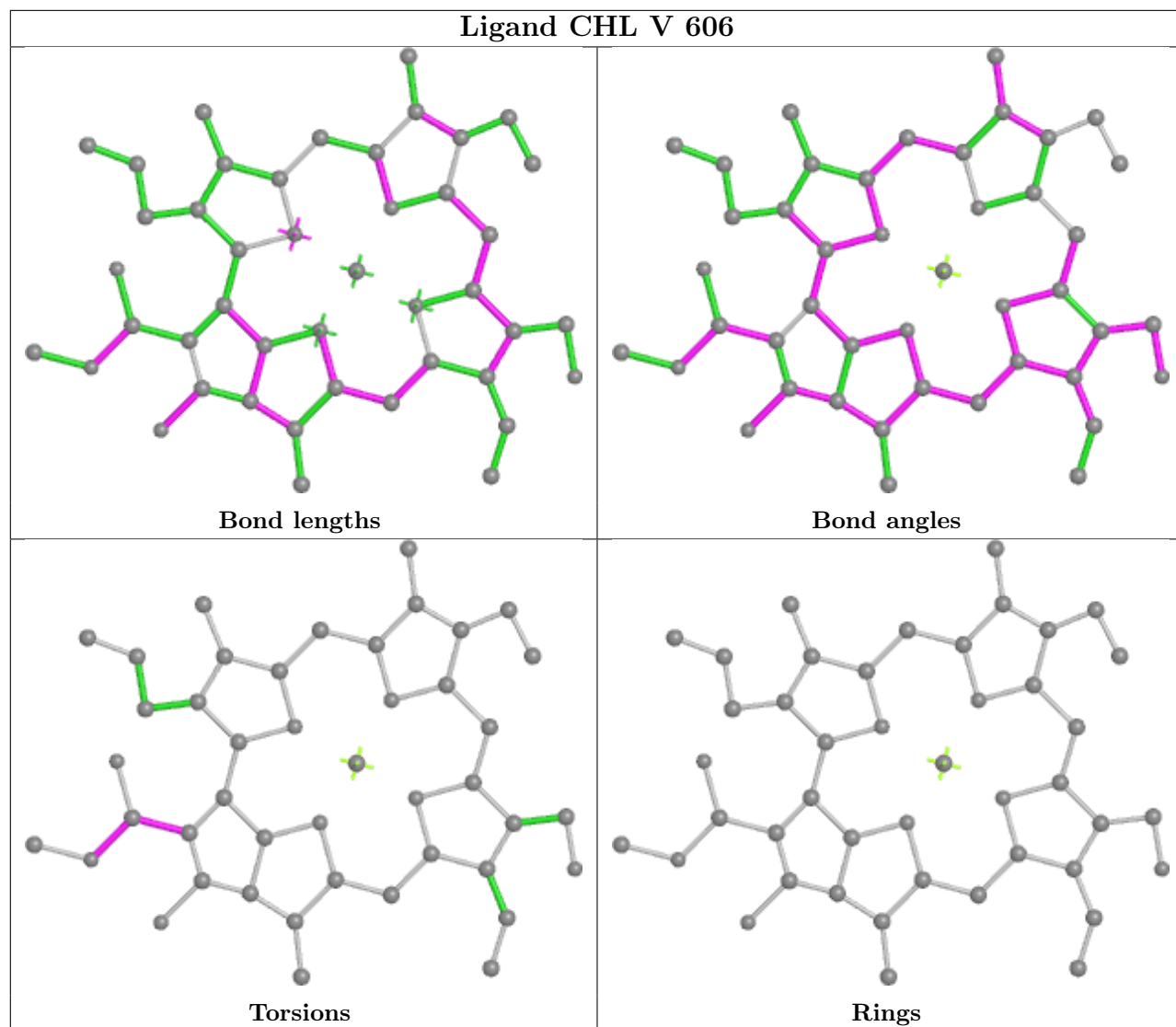




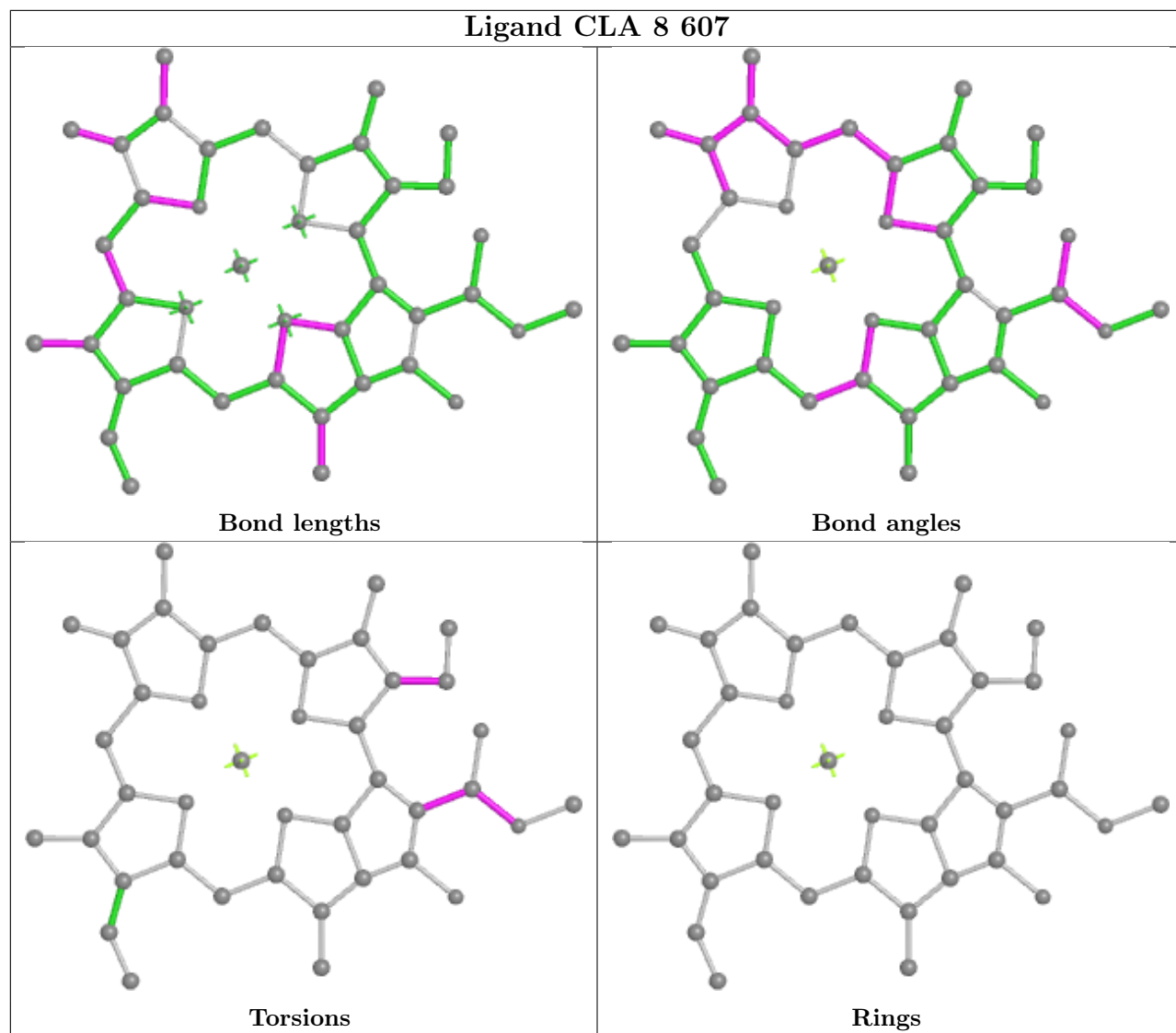


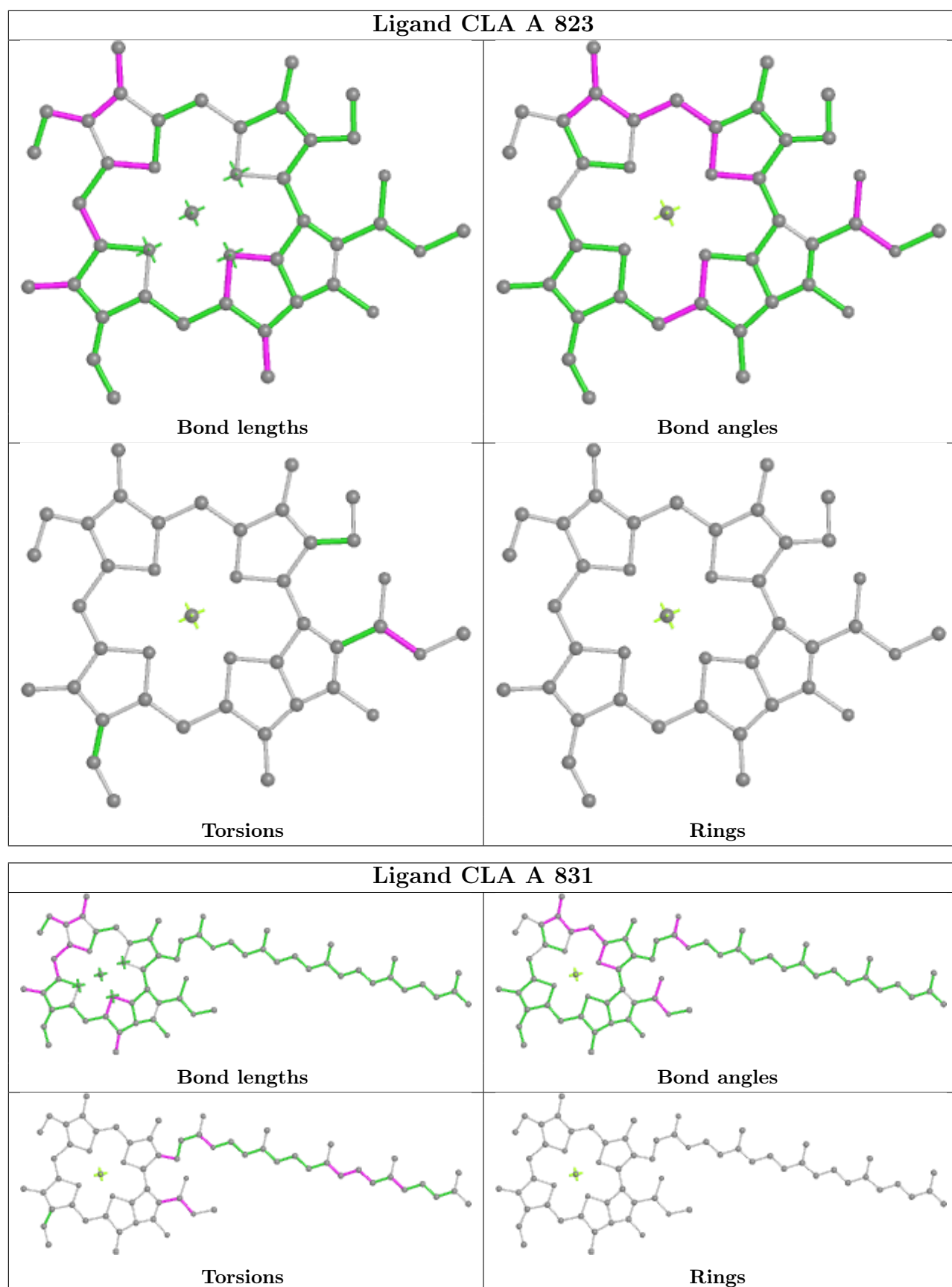


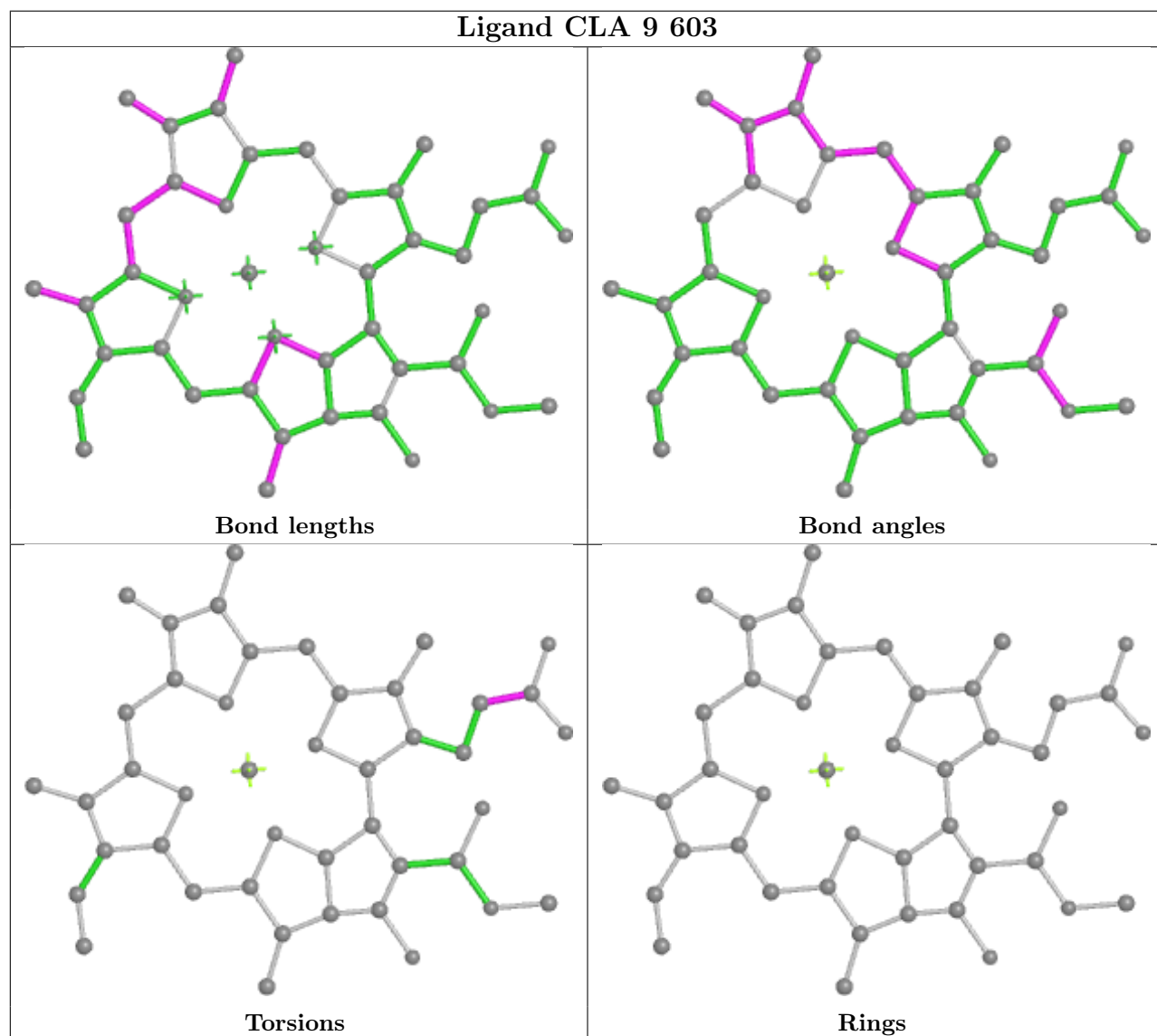
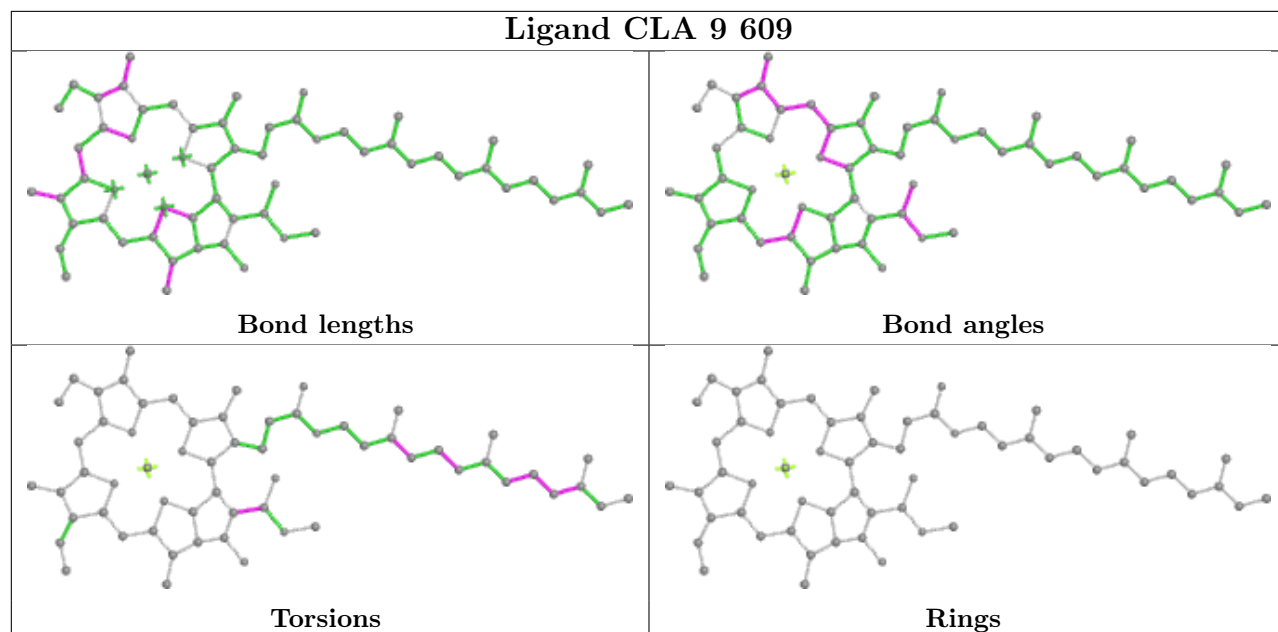


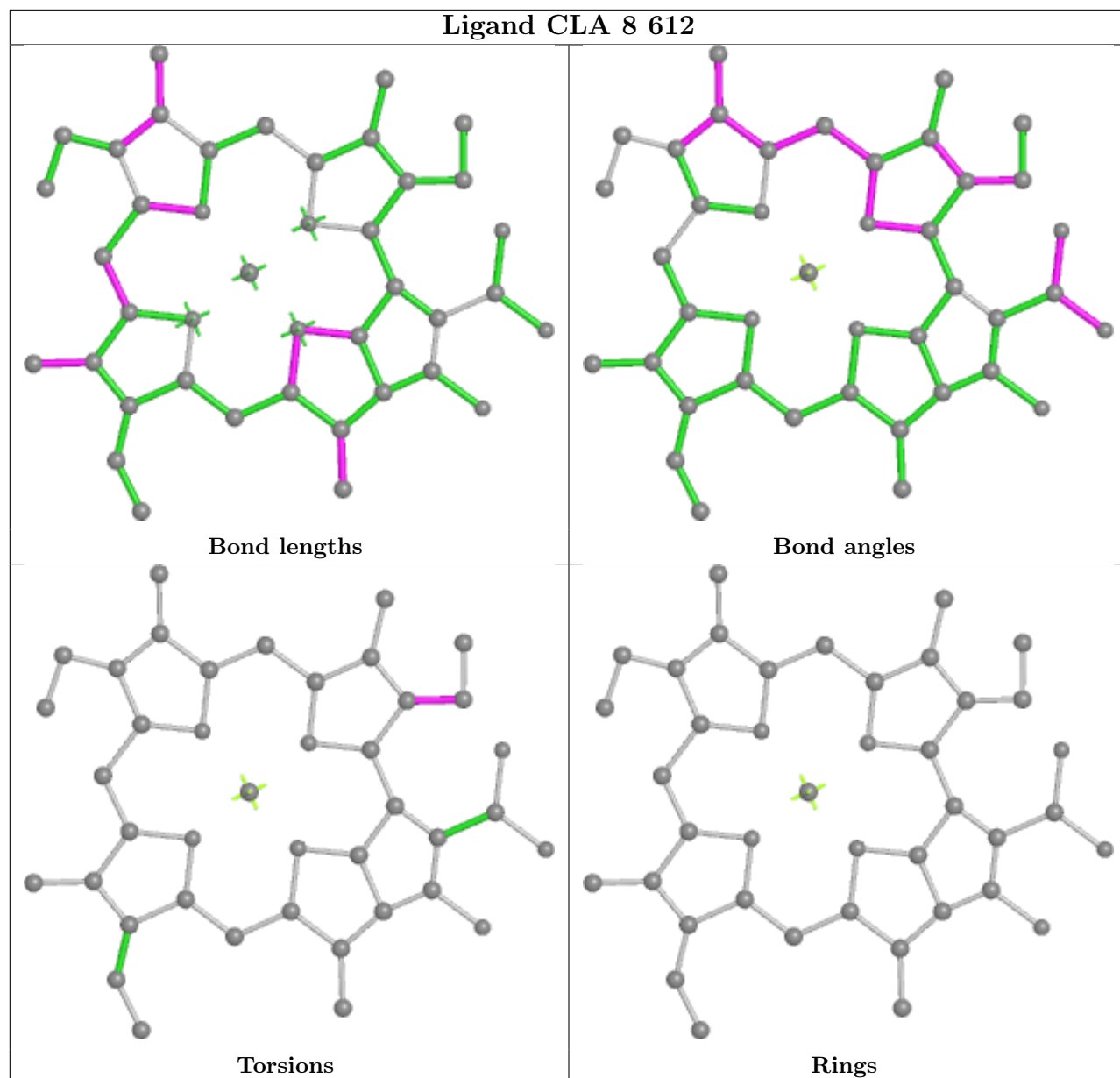


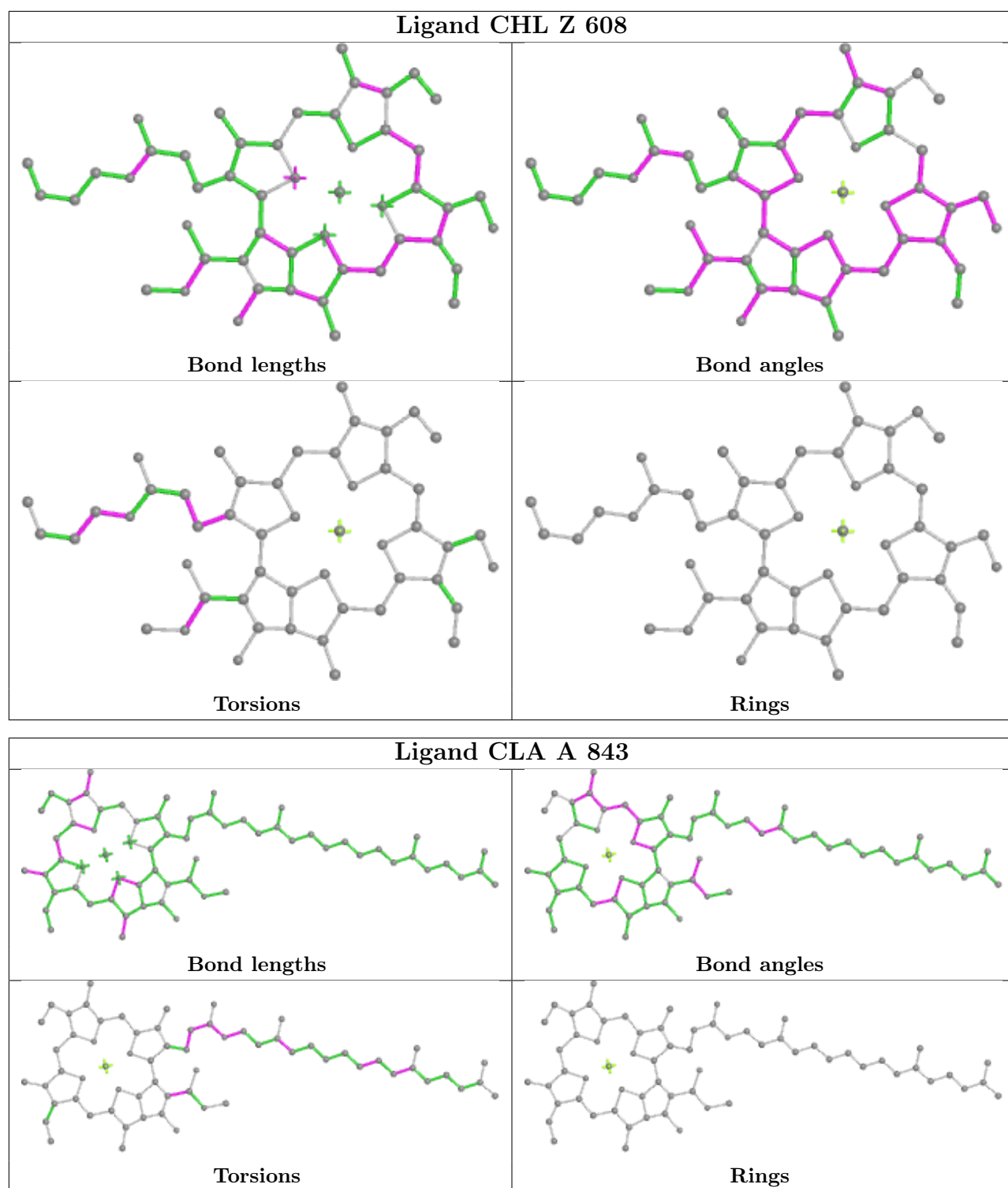


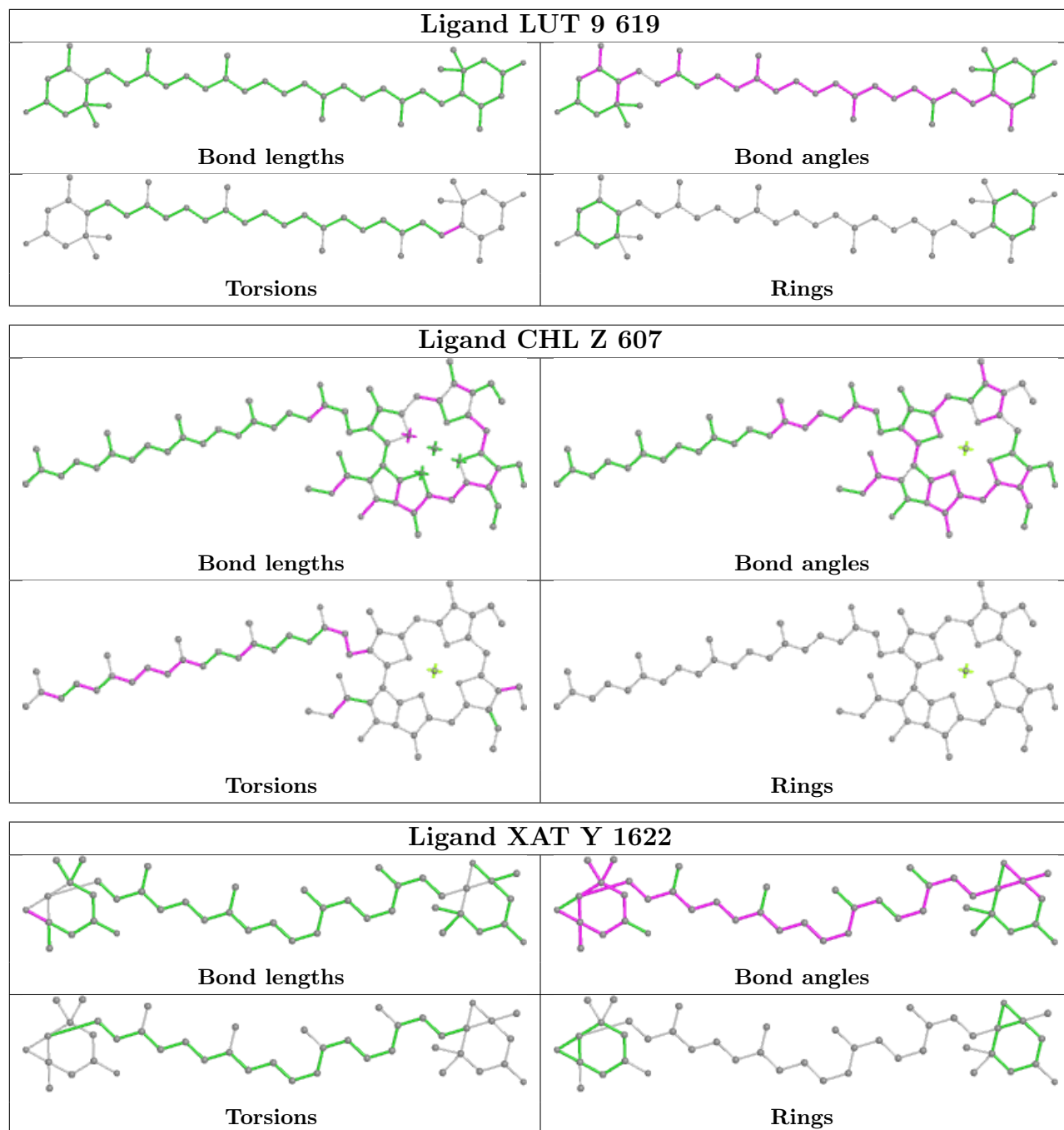


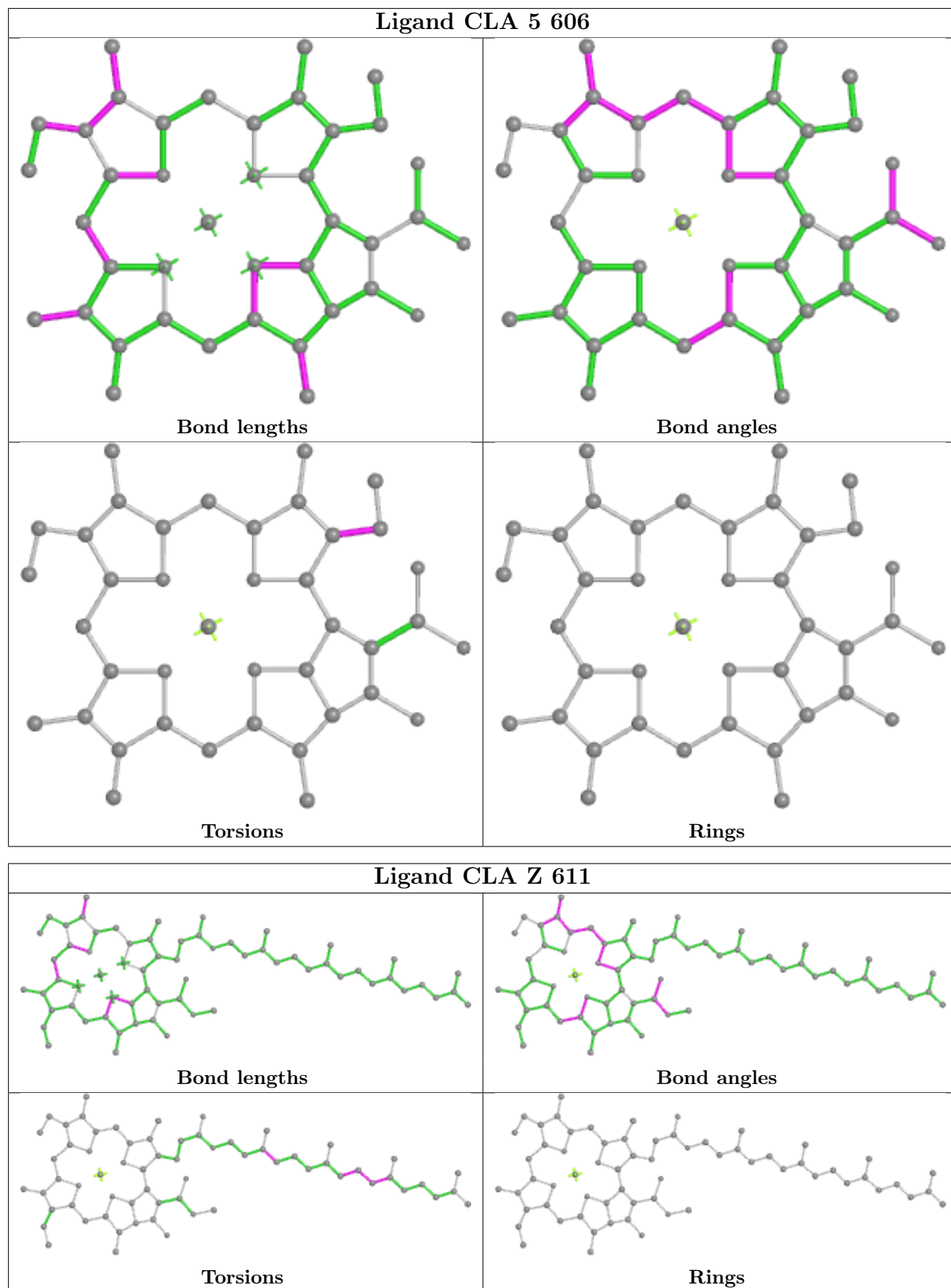


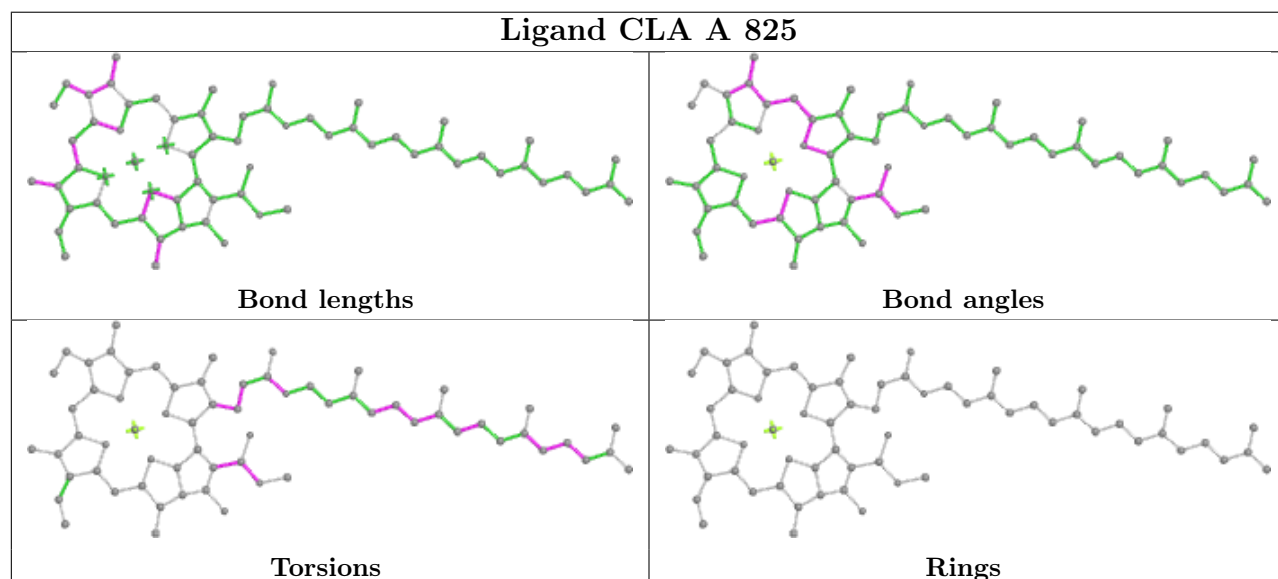
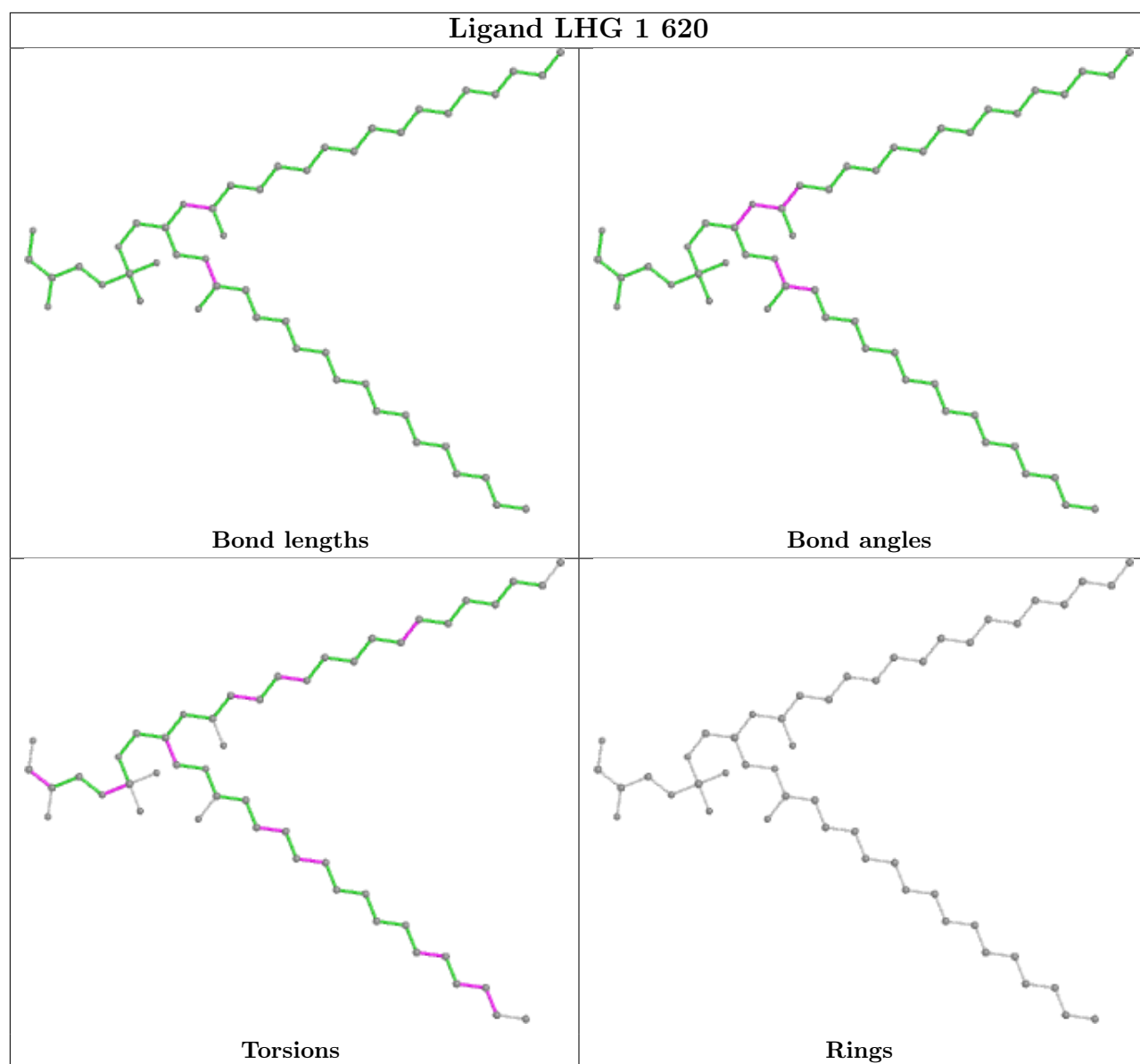




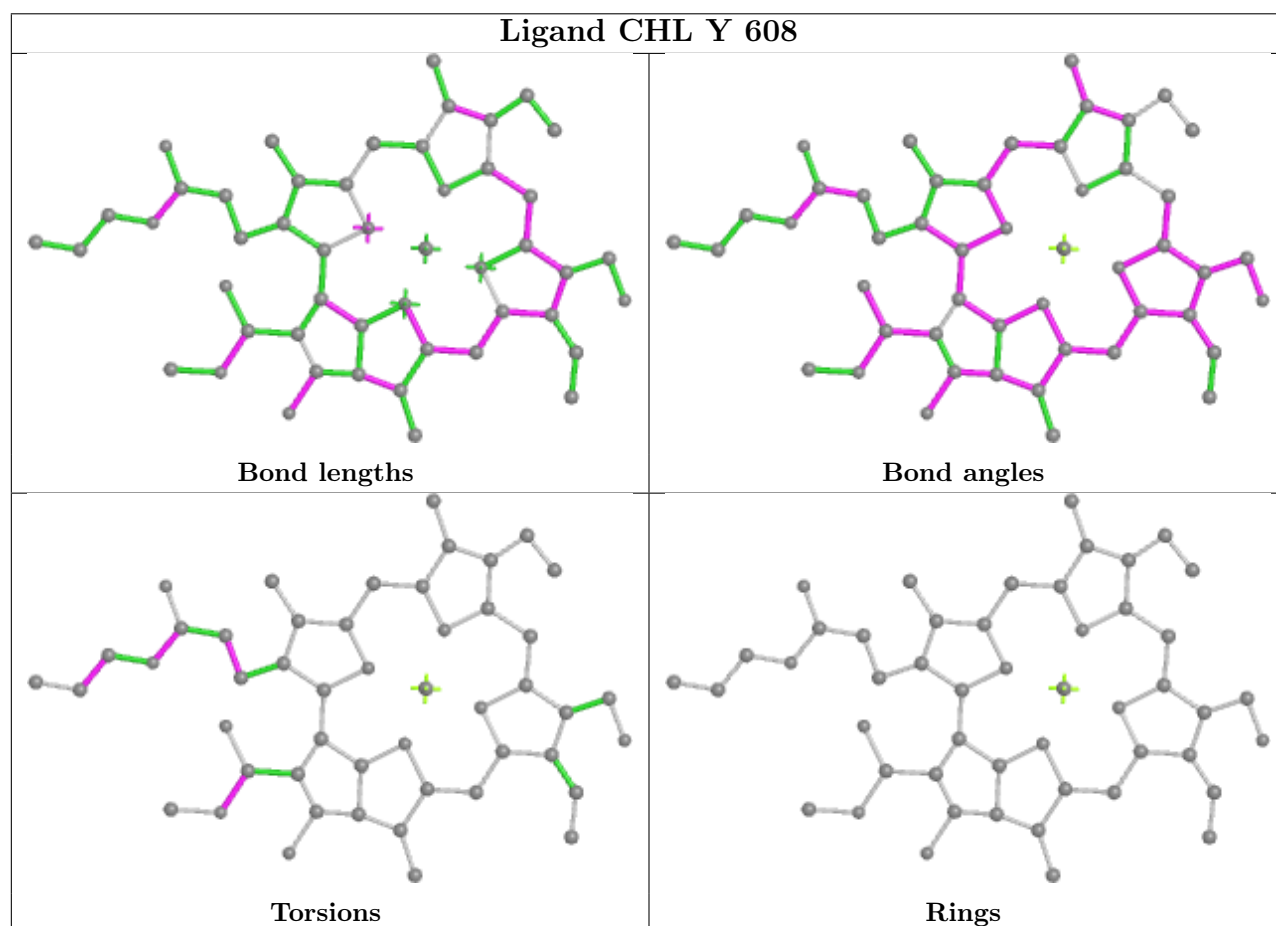
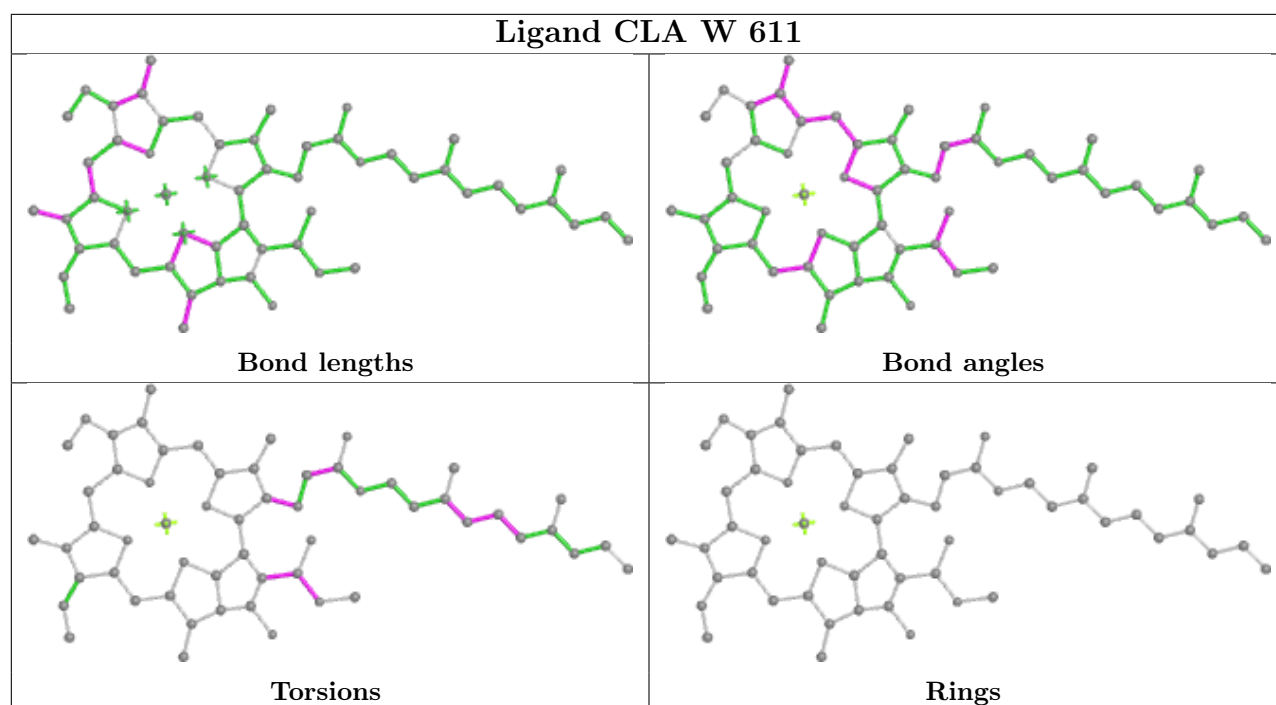


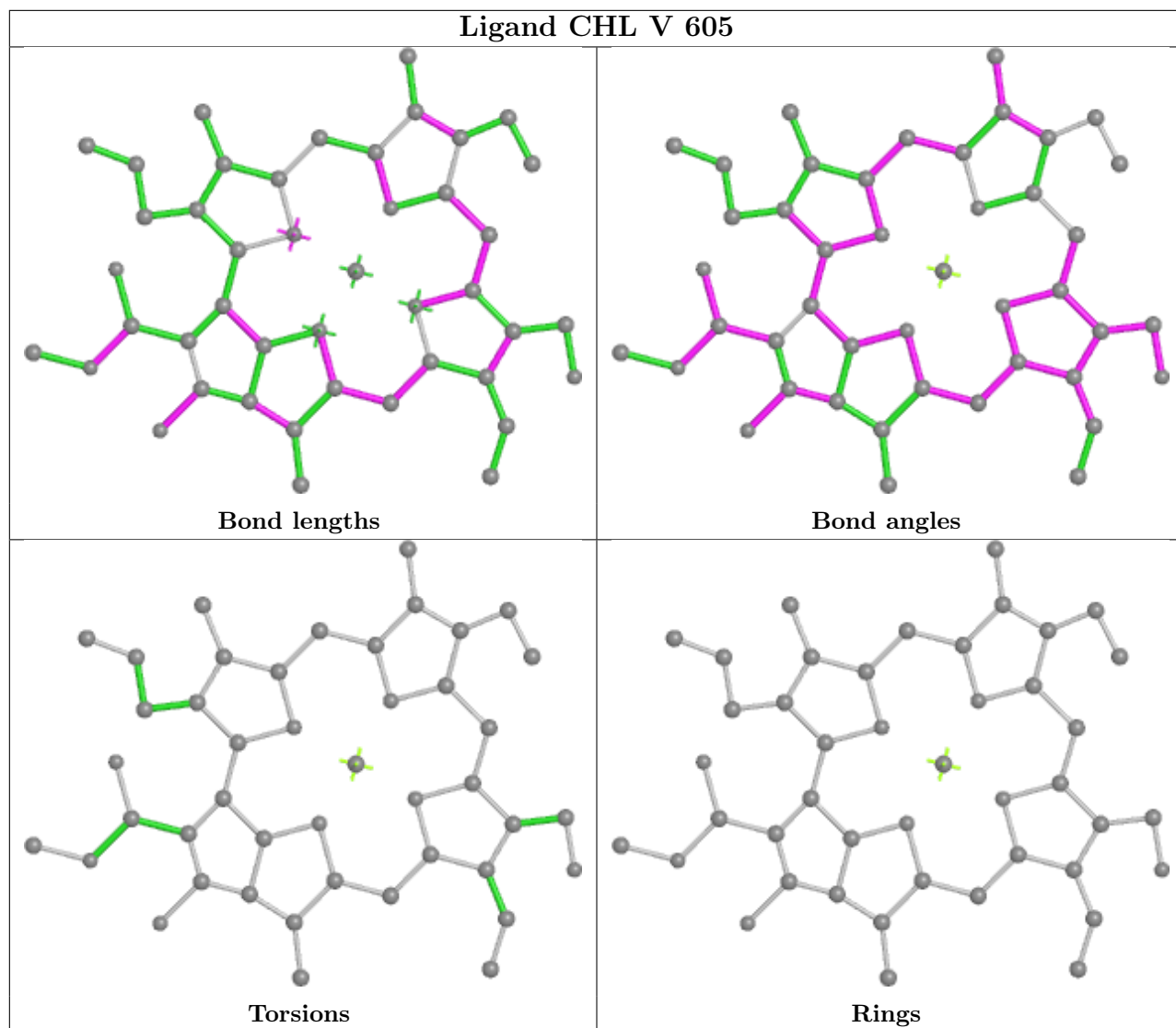


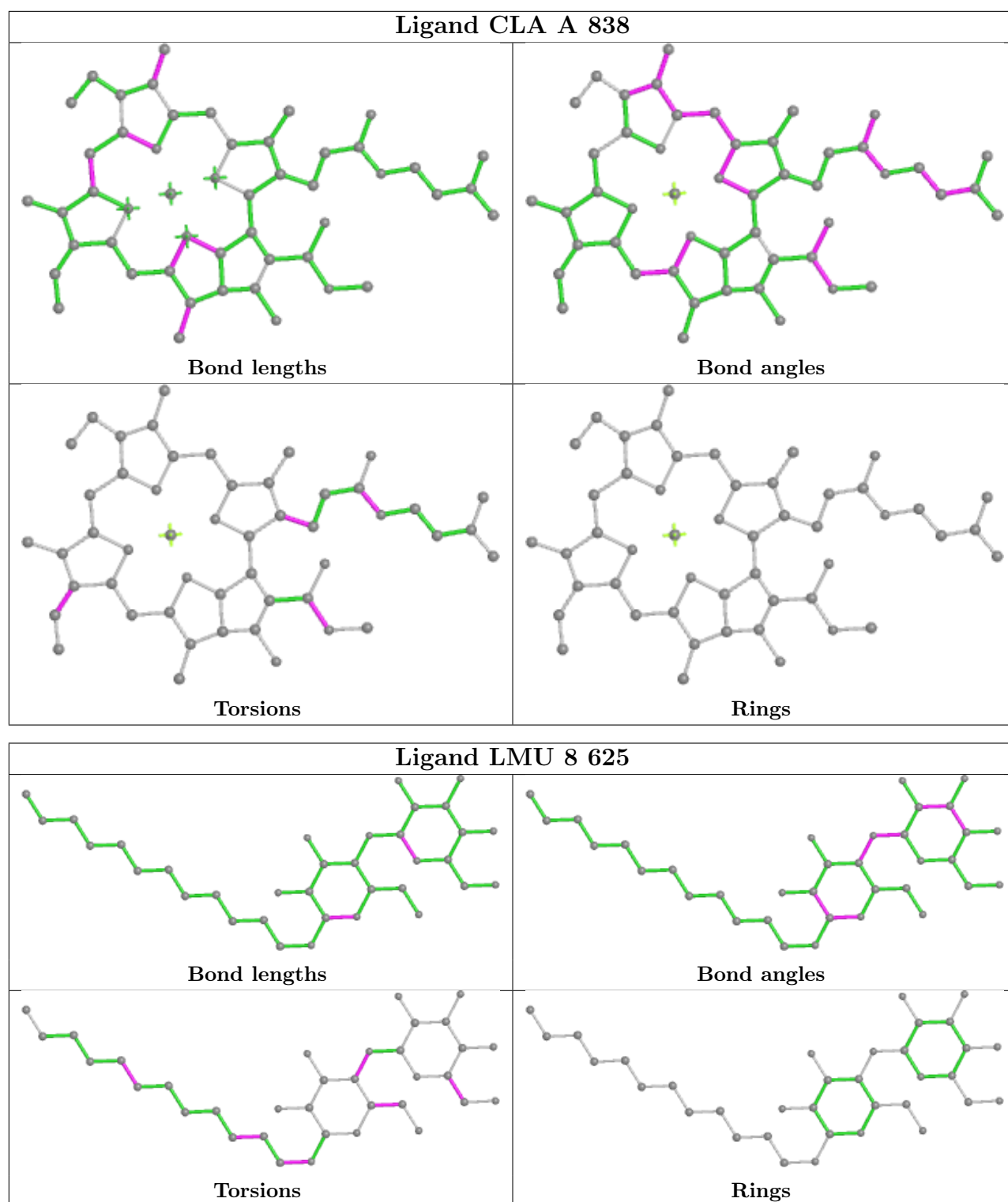


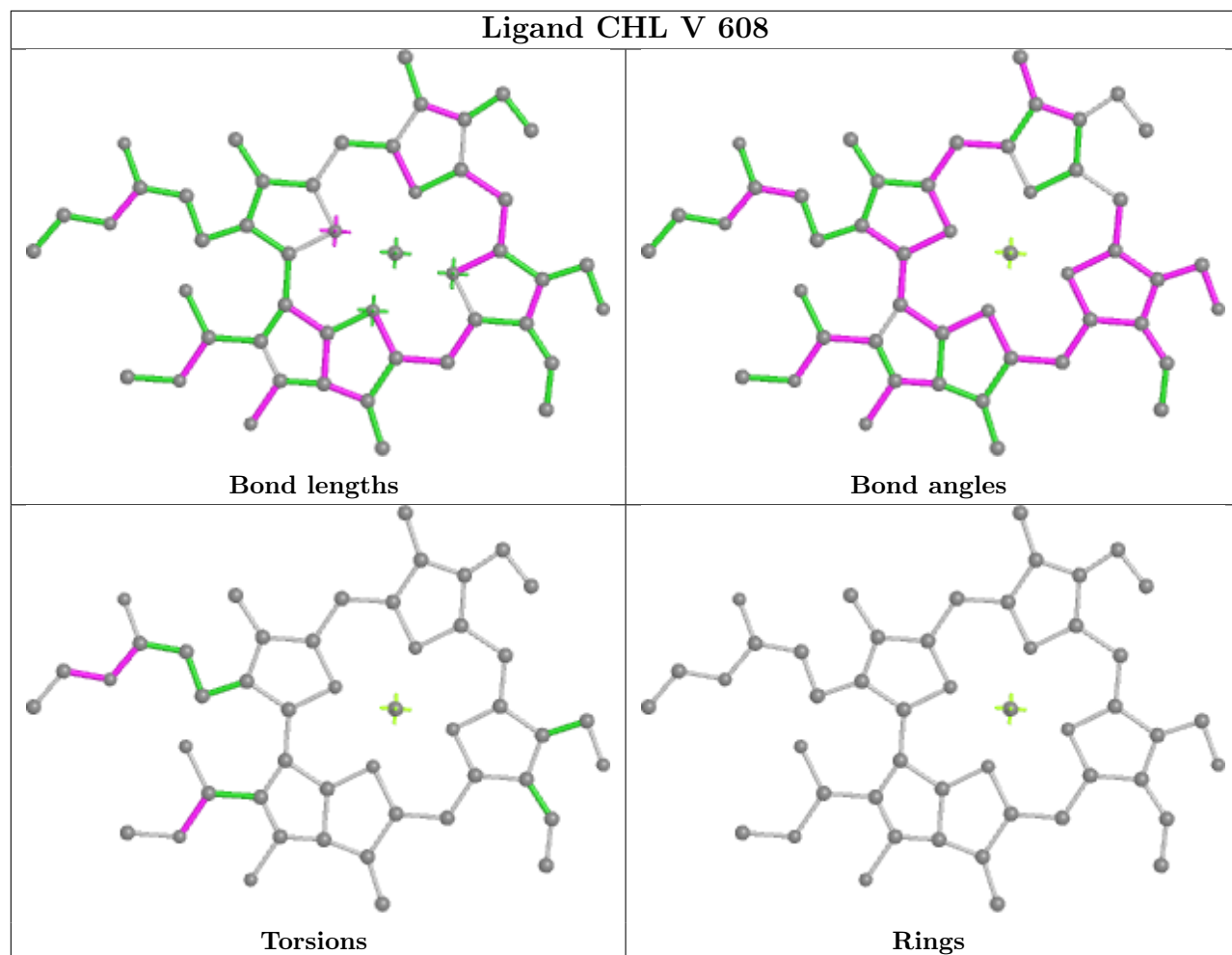


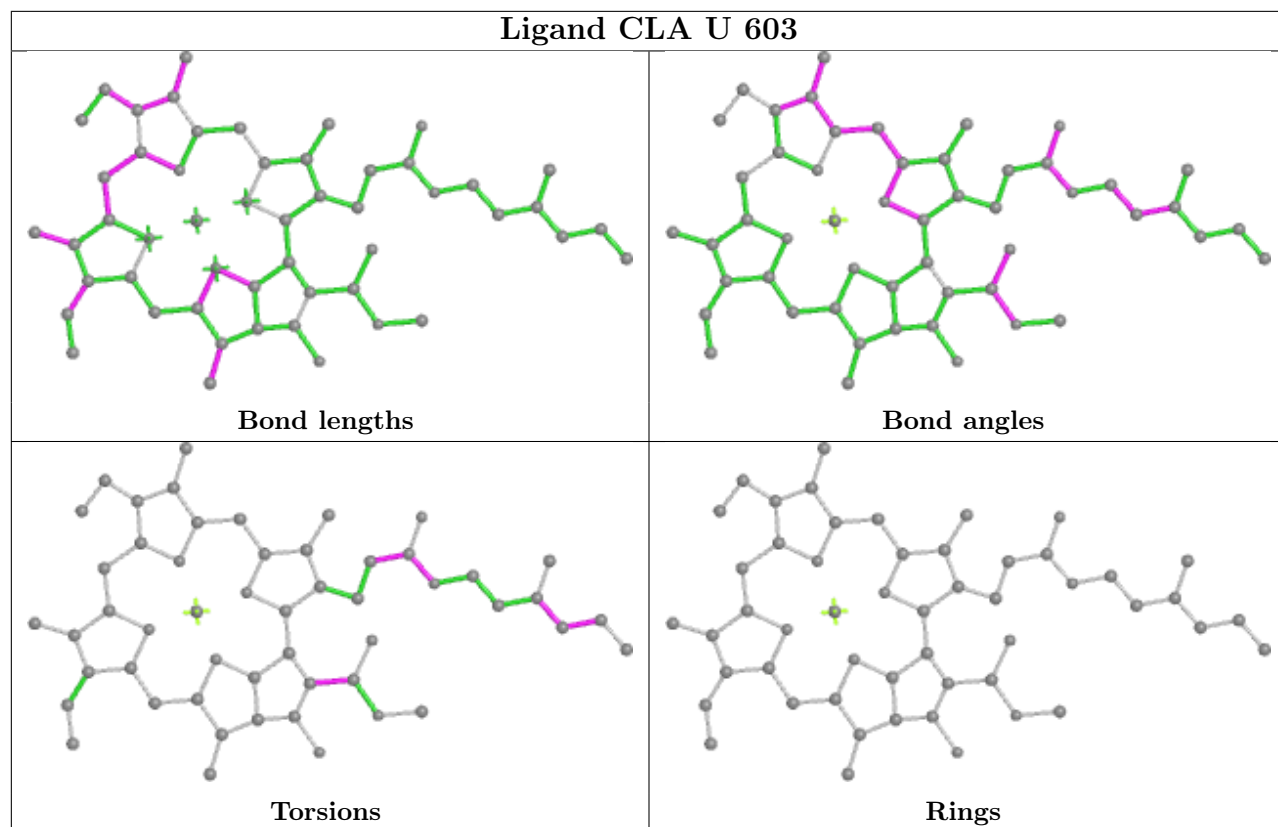


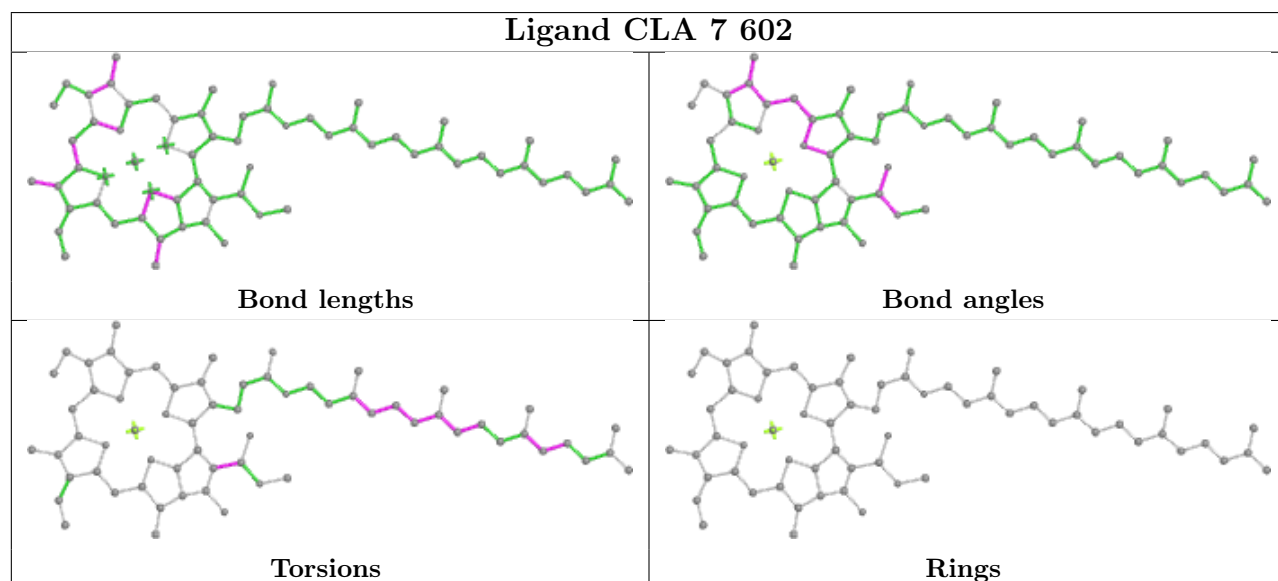
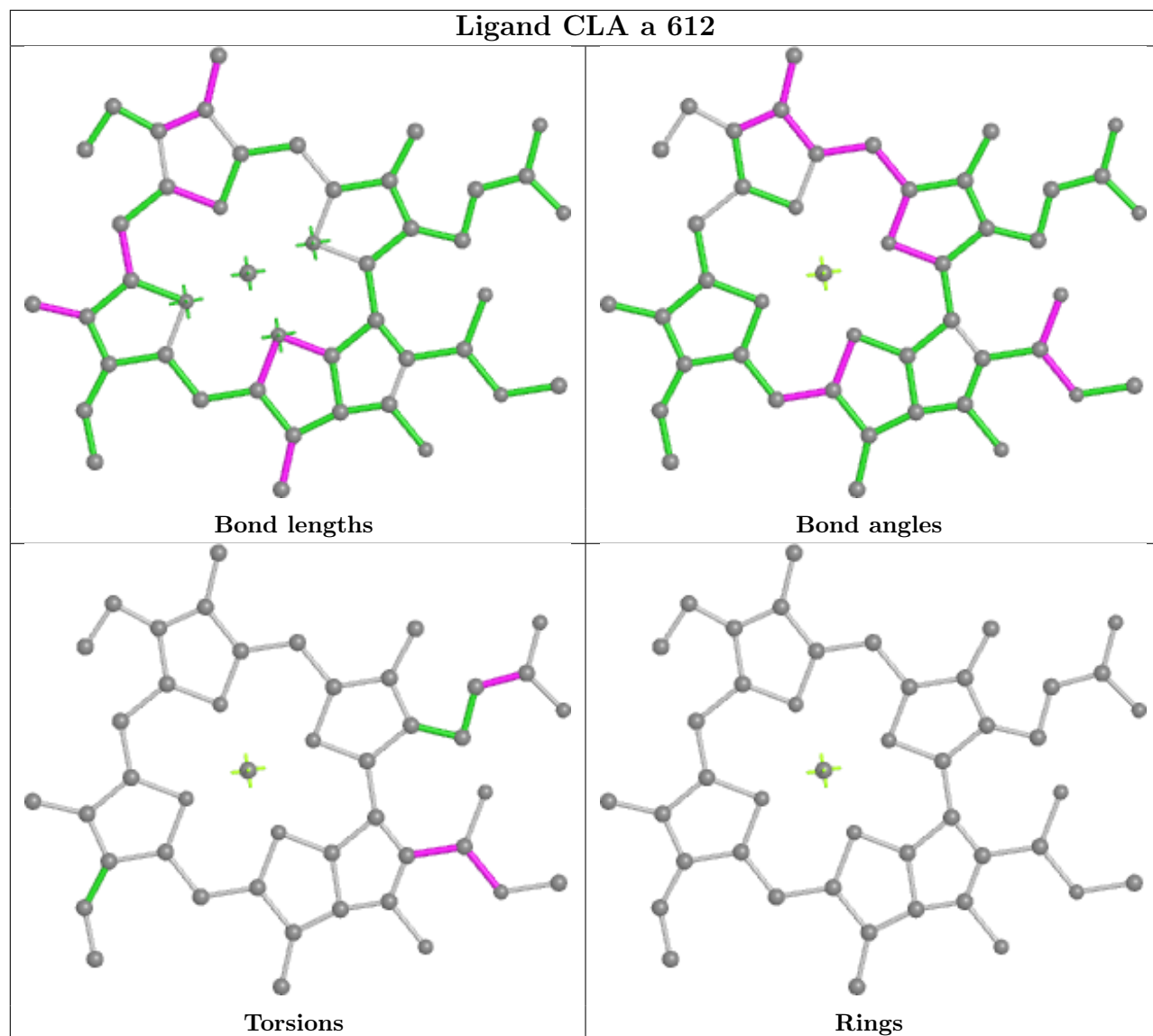




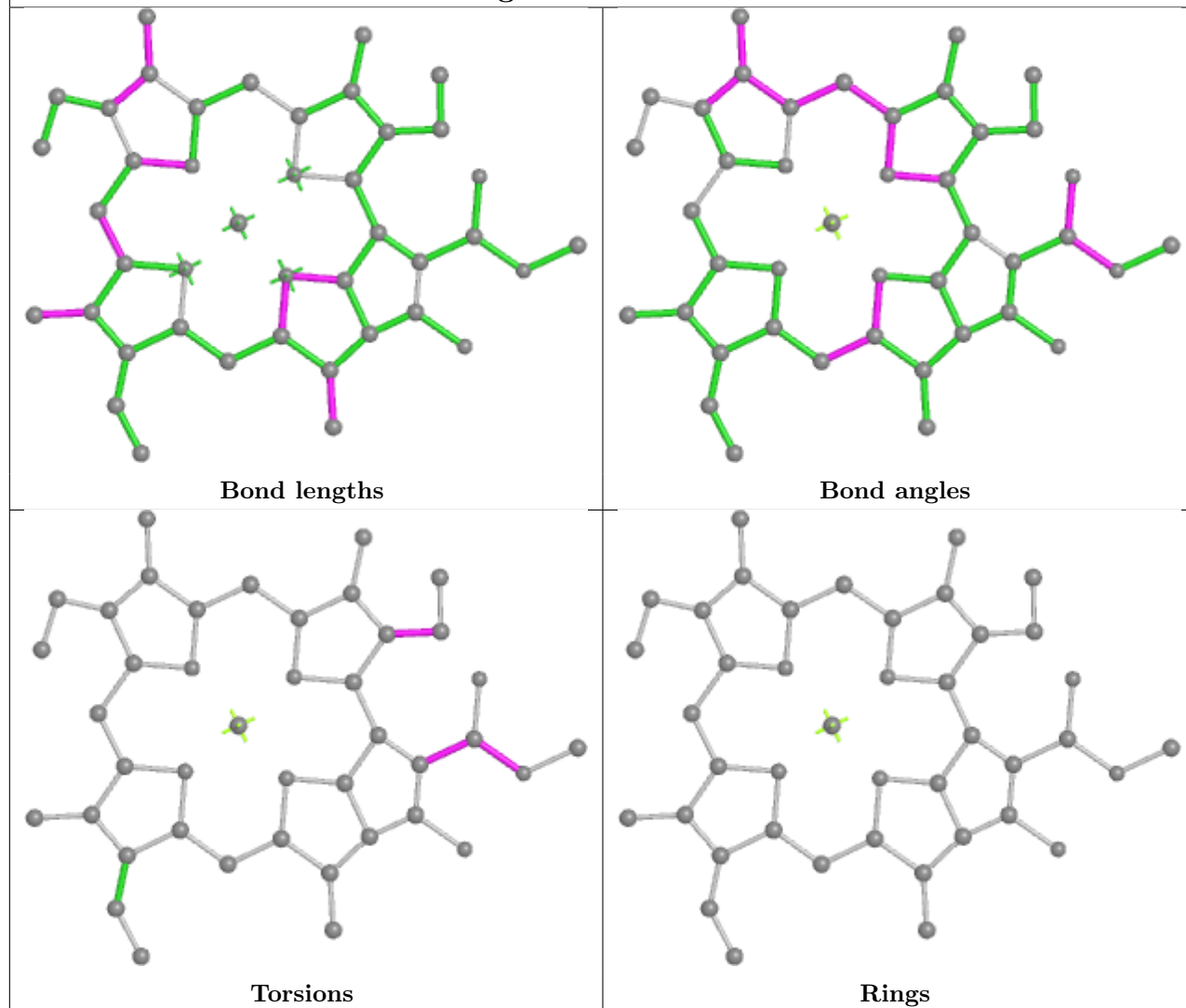


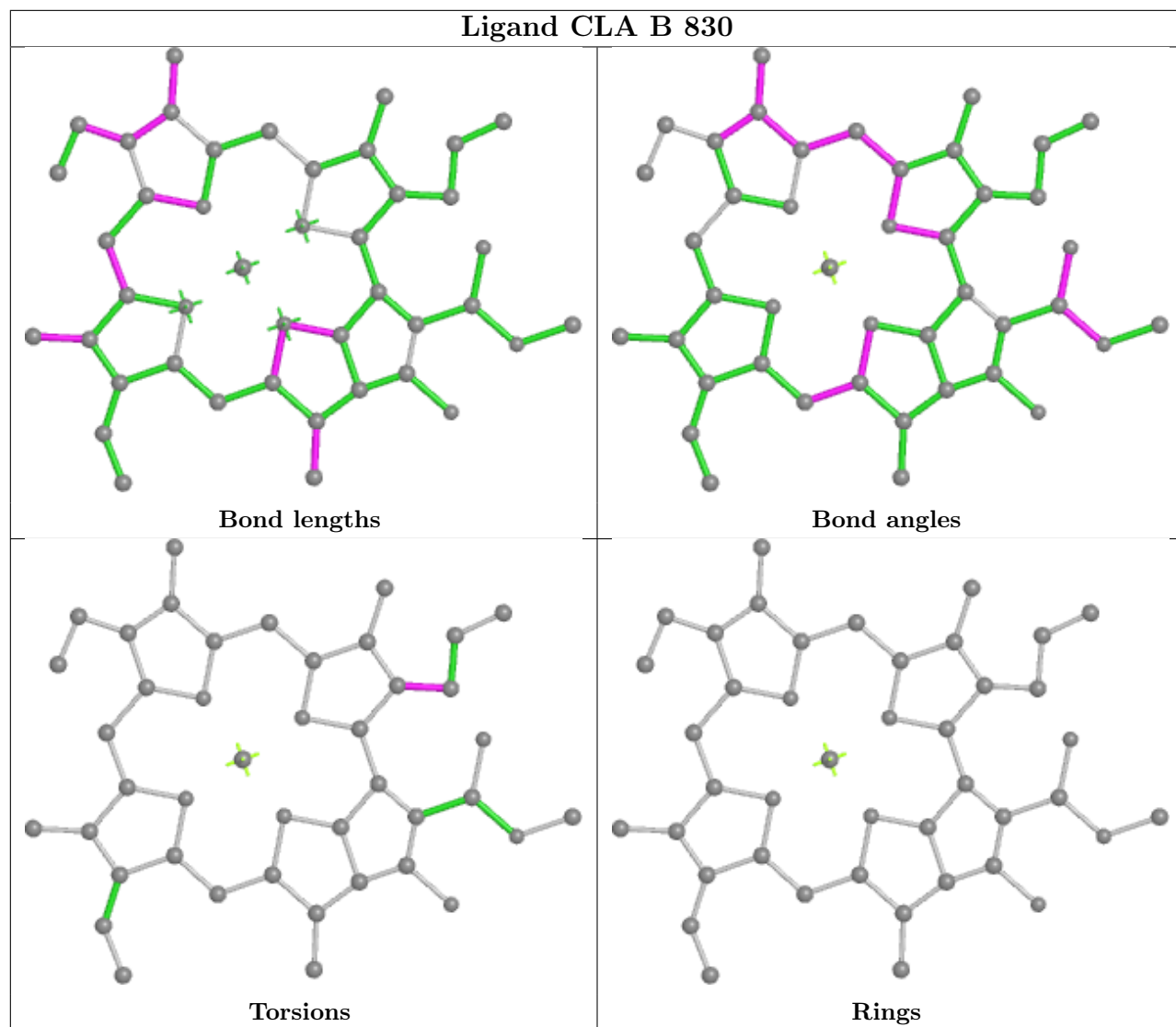




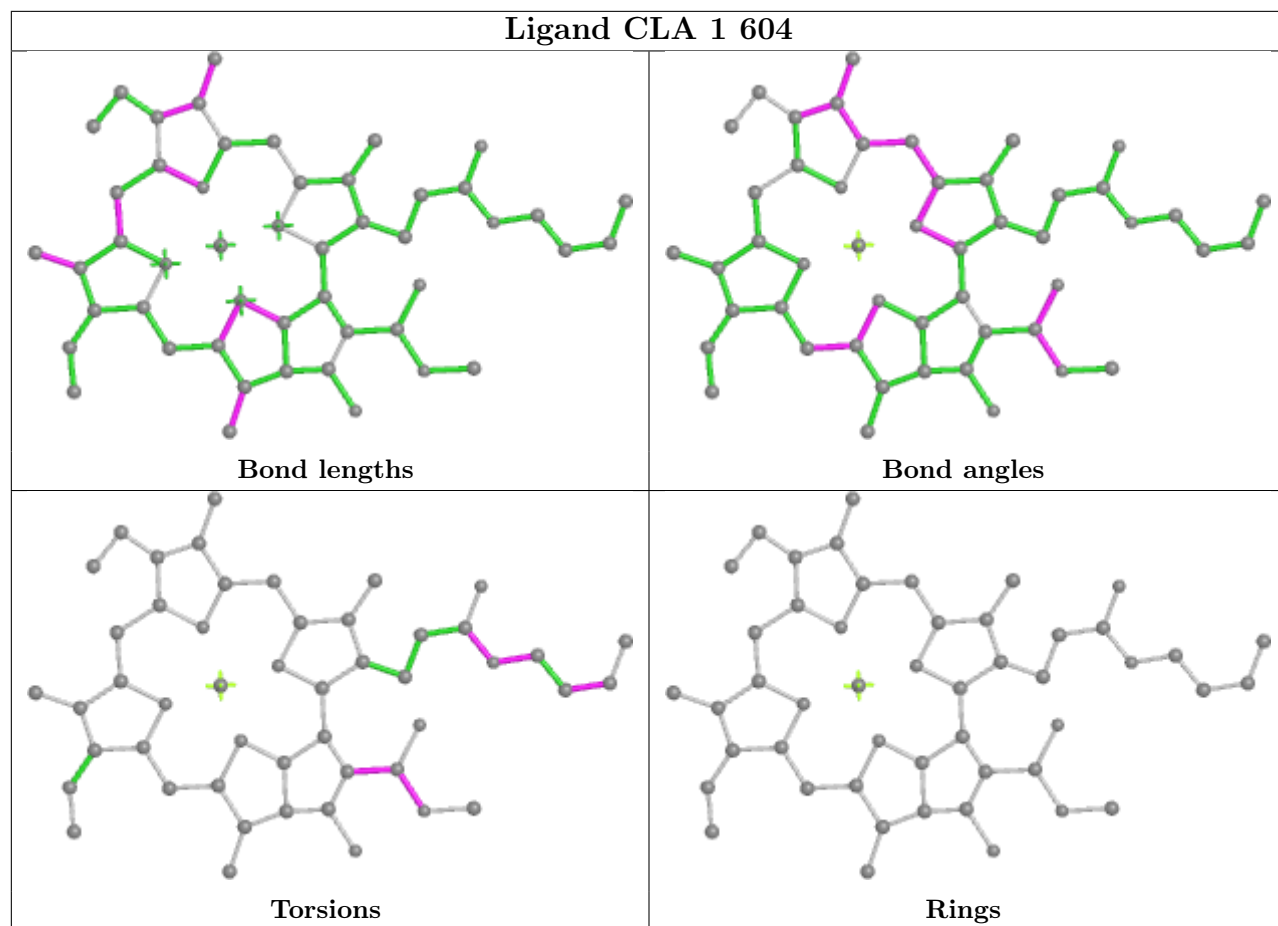


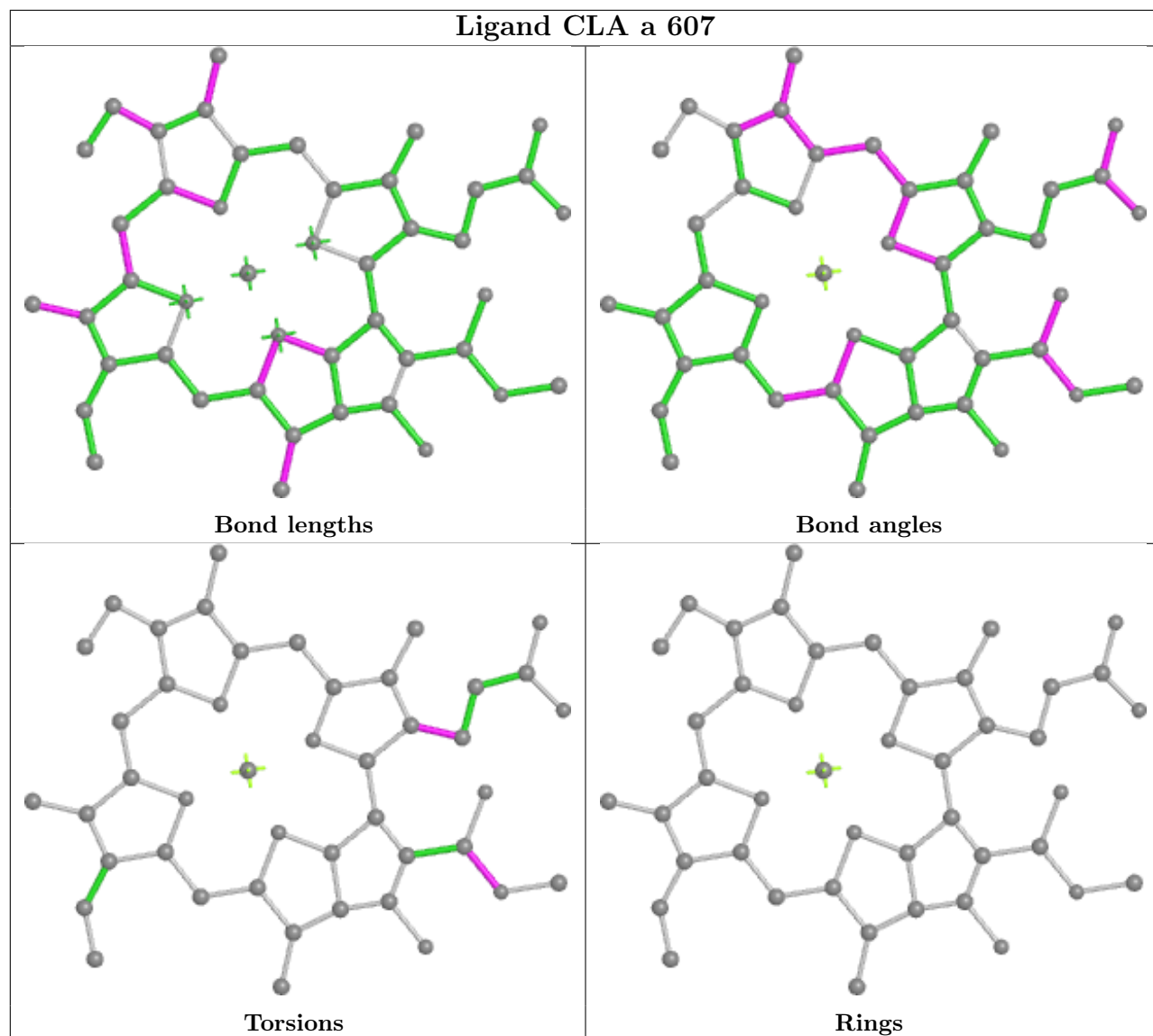
## Ligand CLA 5 611

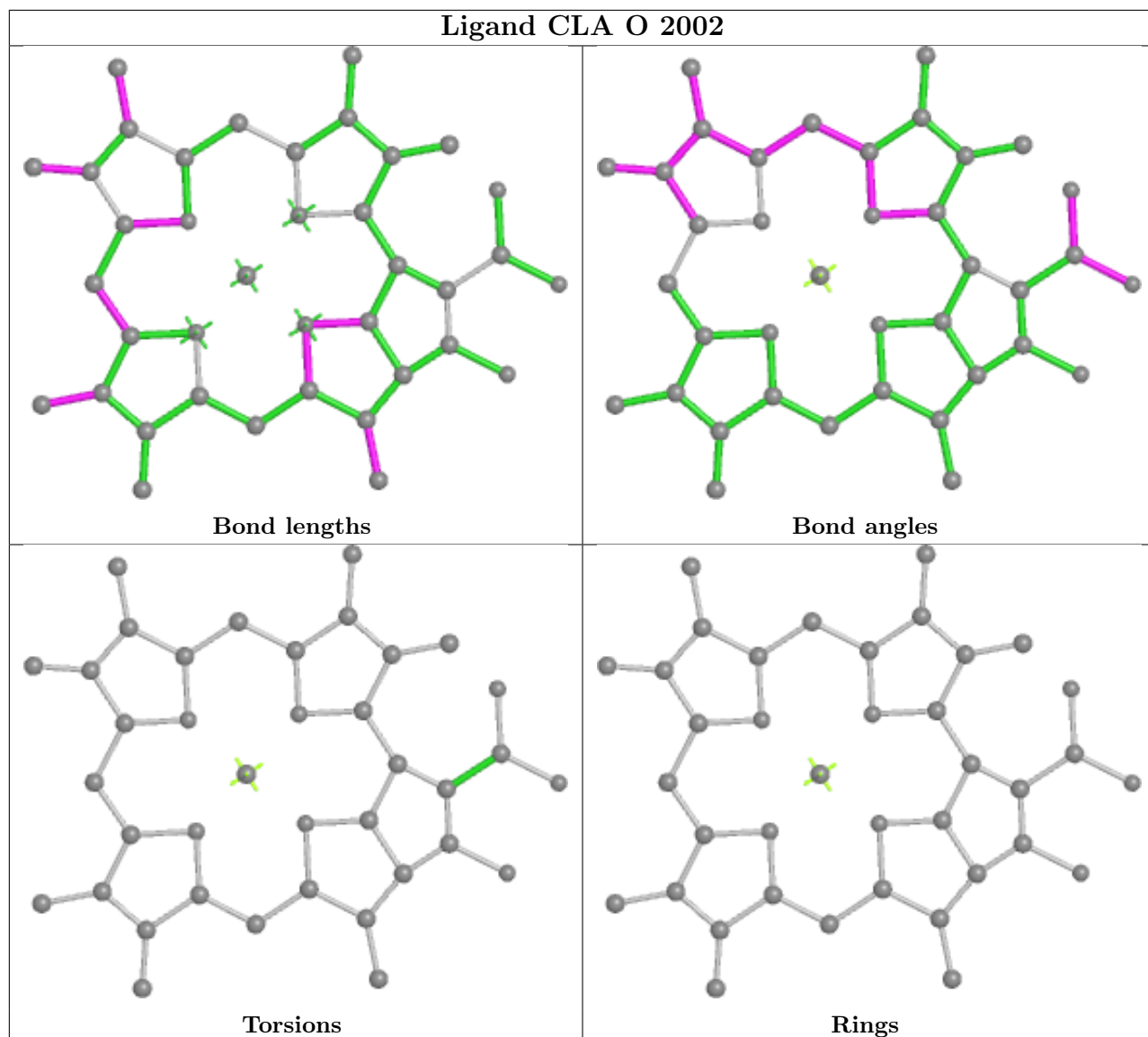


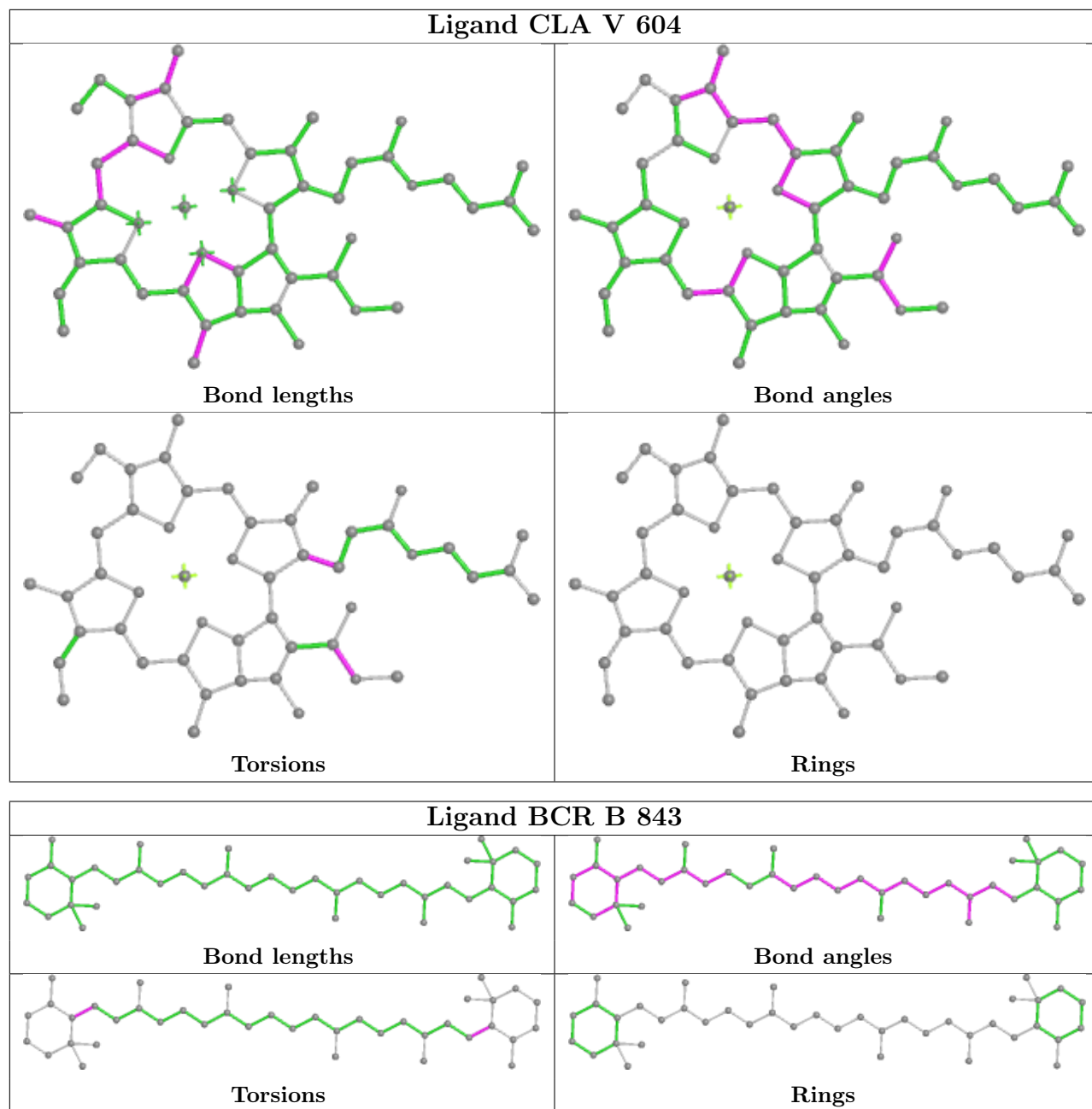


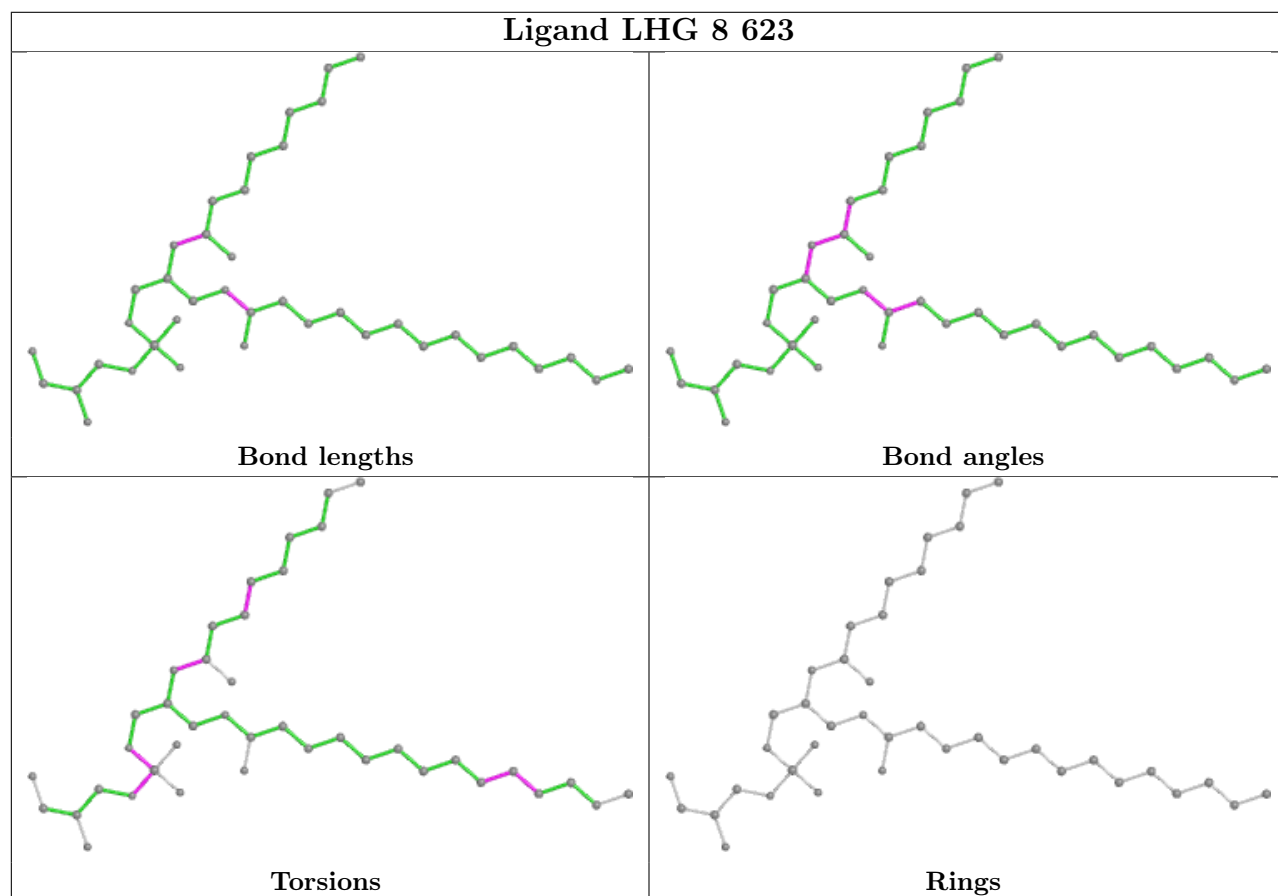
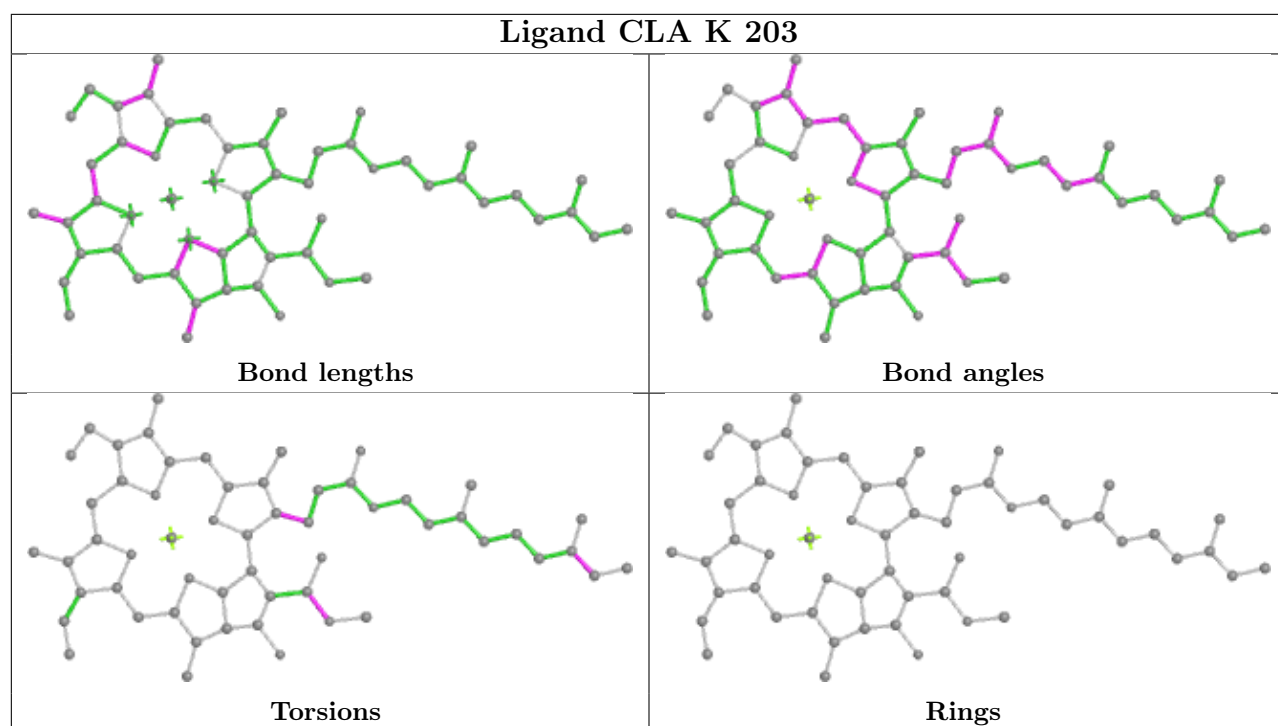


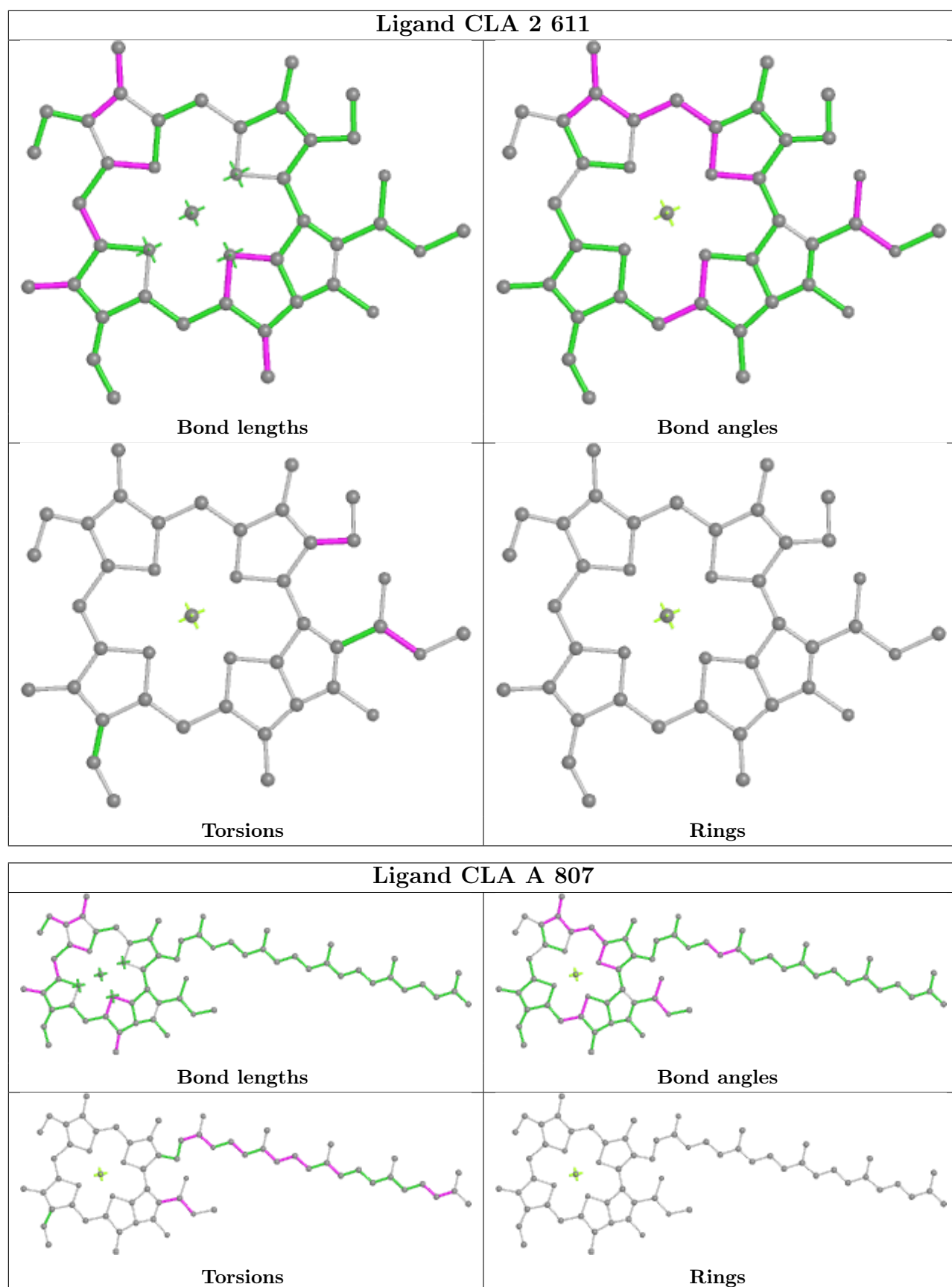


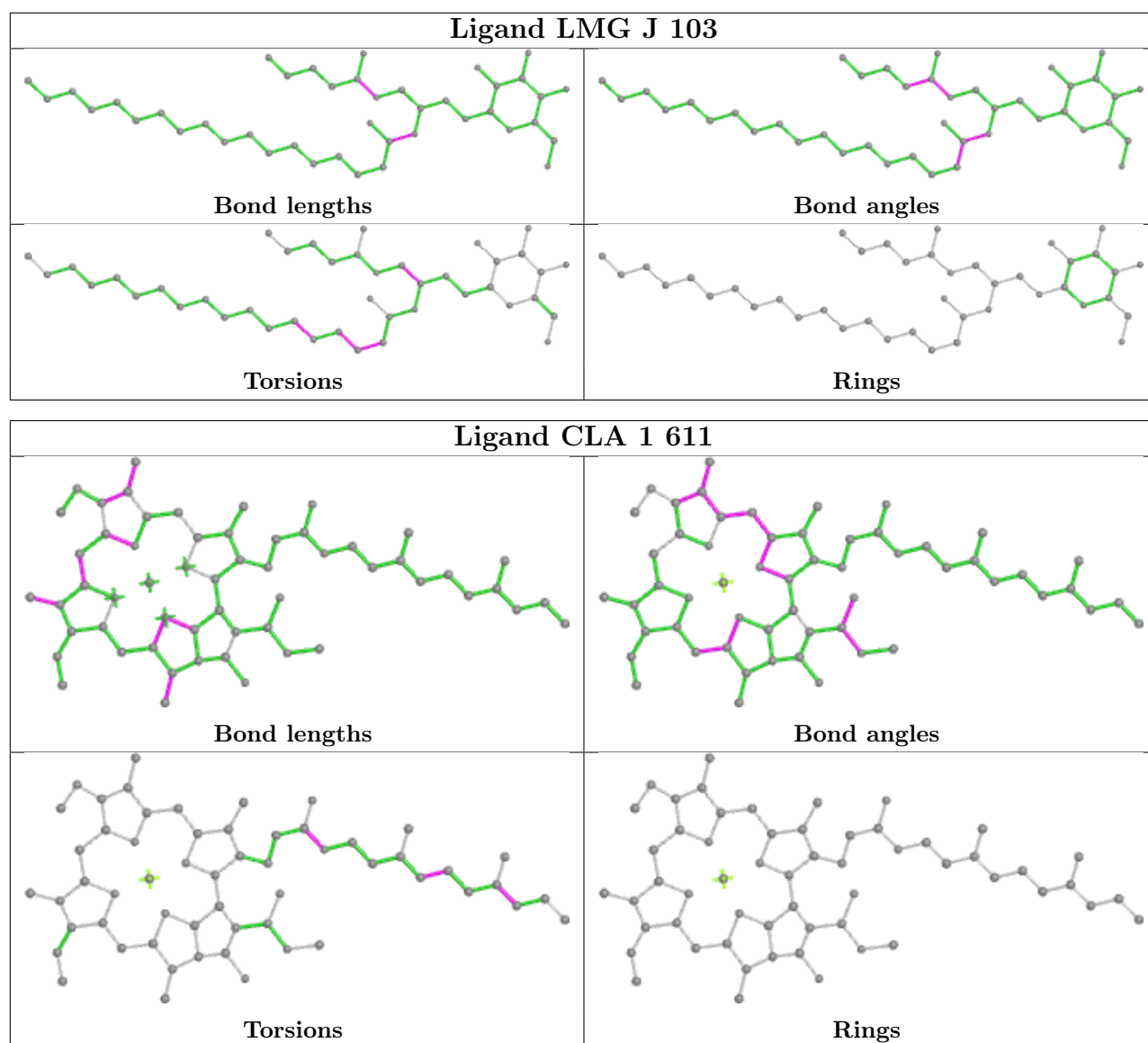












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

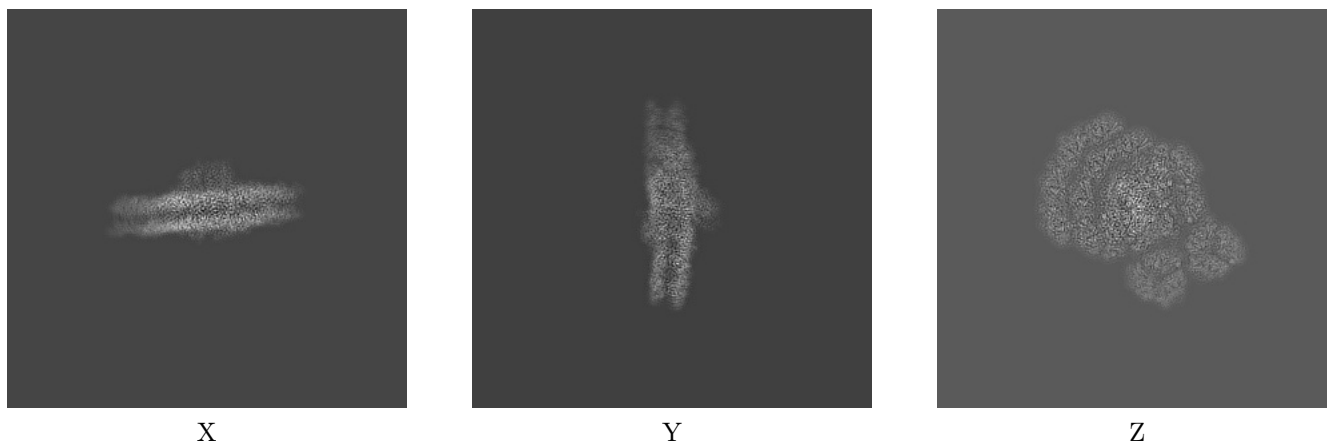
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-30925. 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](#)

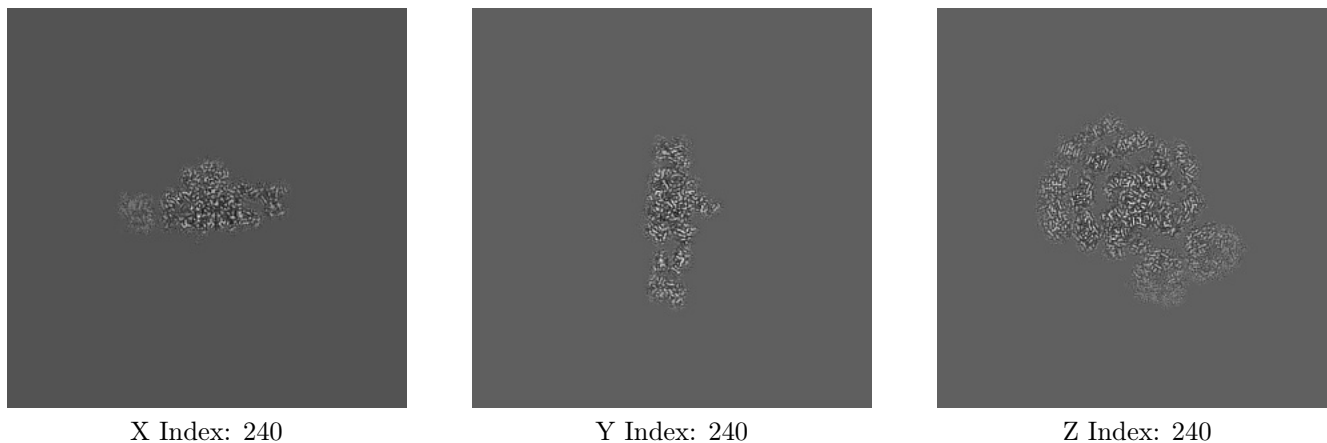
#### 6.1.1 Primary map



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

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

#### 6.2.1 Primary map

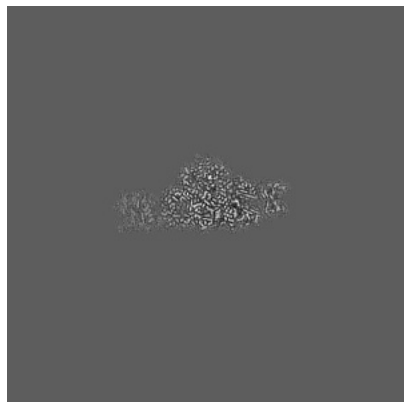




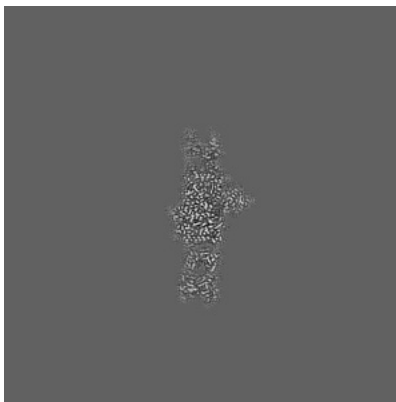
The images above show central slices of the map in three orthogonal directions.

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

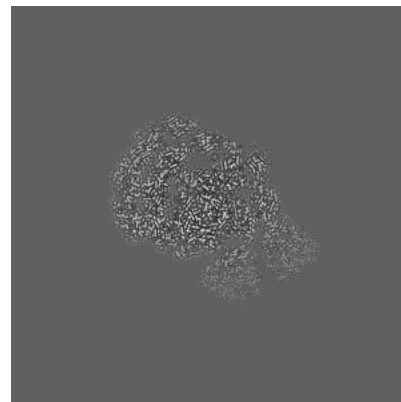
### 6.3.1 Primary map



X Index: 243



Y Index: 231



Z Index: 248

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

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

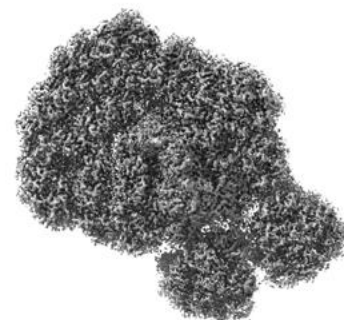
### 6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.02. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

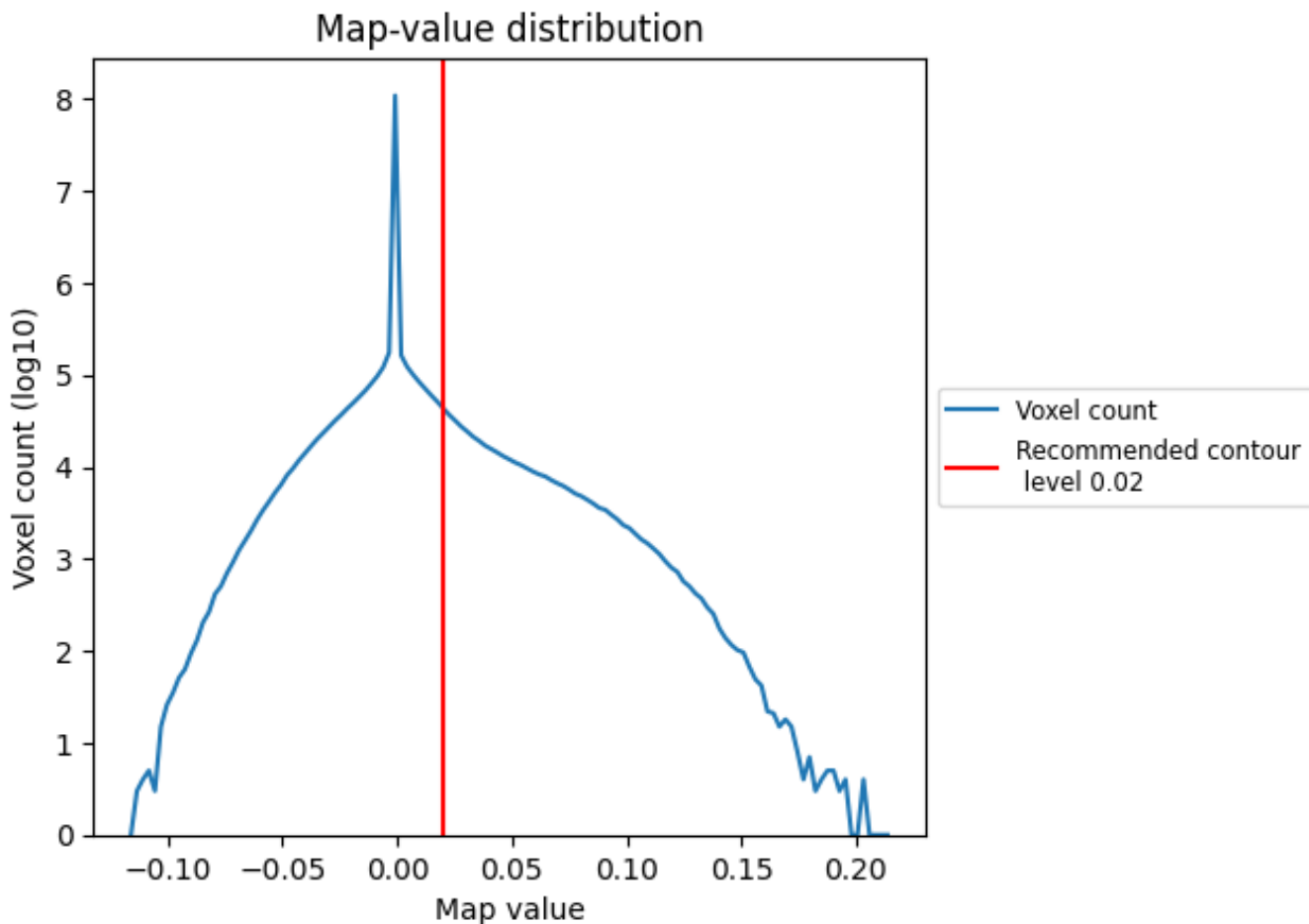
## 6.5 Mask visualisation

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

## 7 Map analysis [i](#)

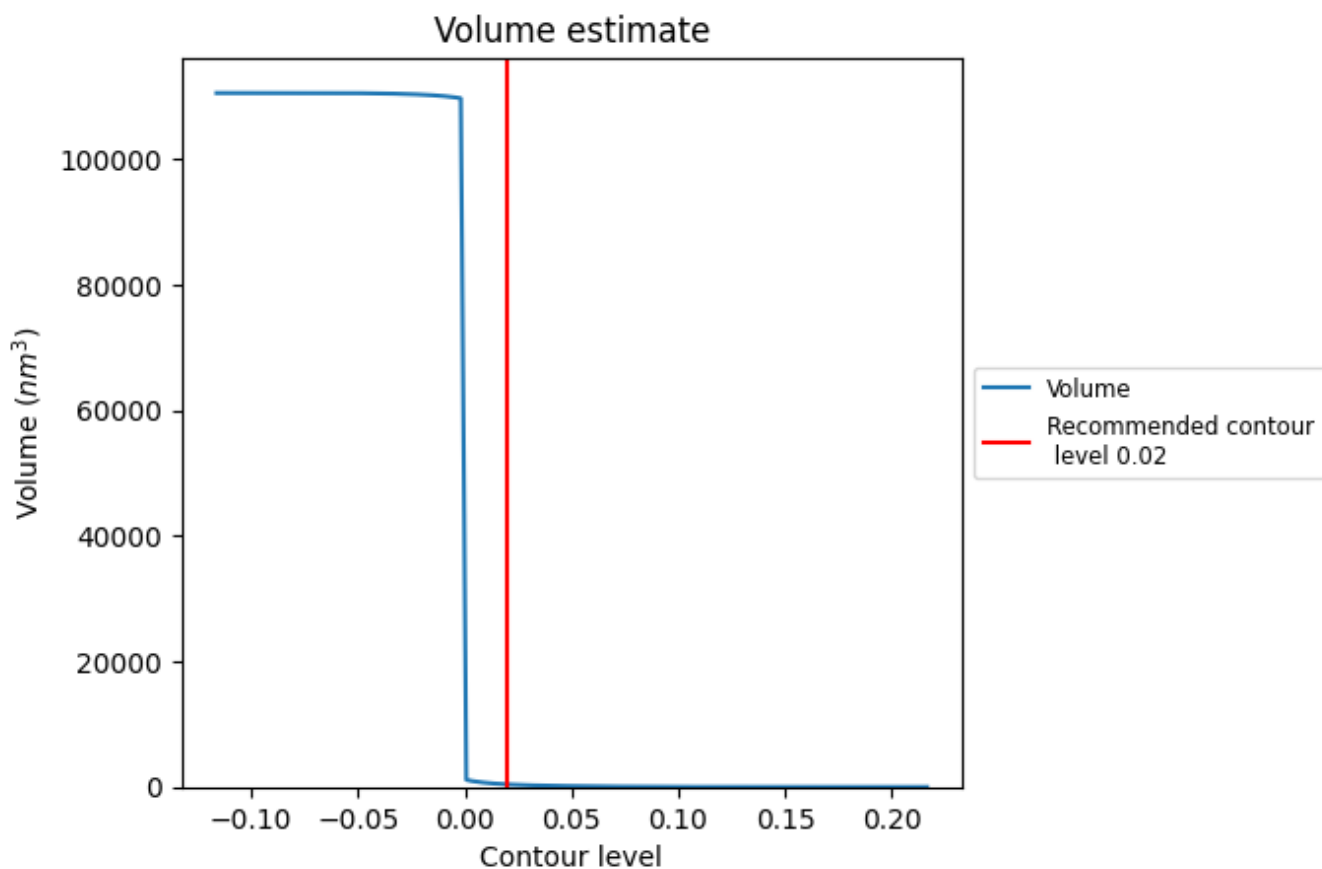
This section contains the results of statistical analysis of the map.

### 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.

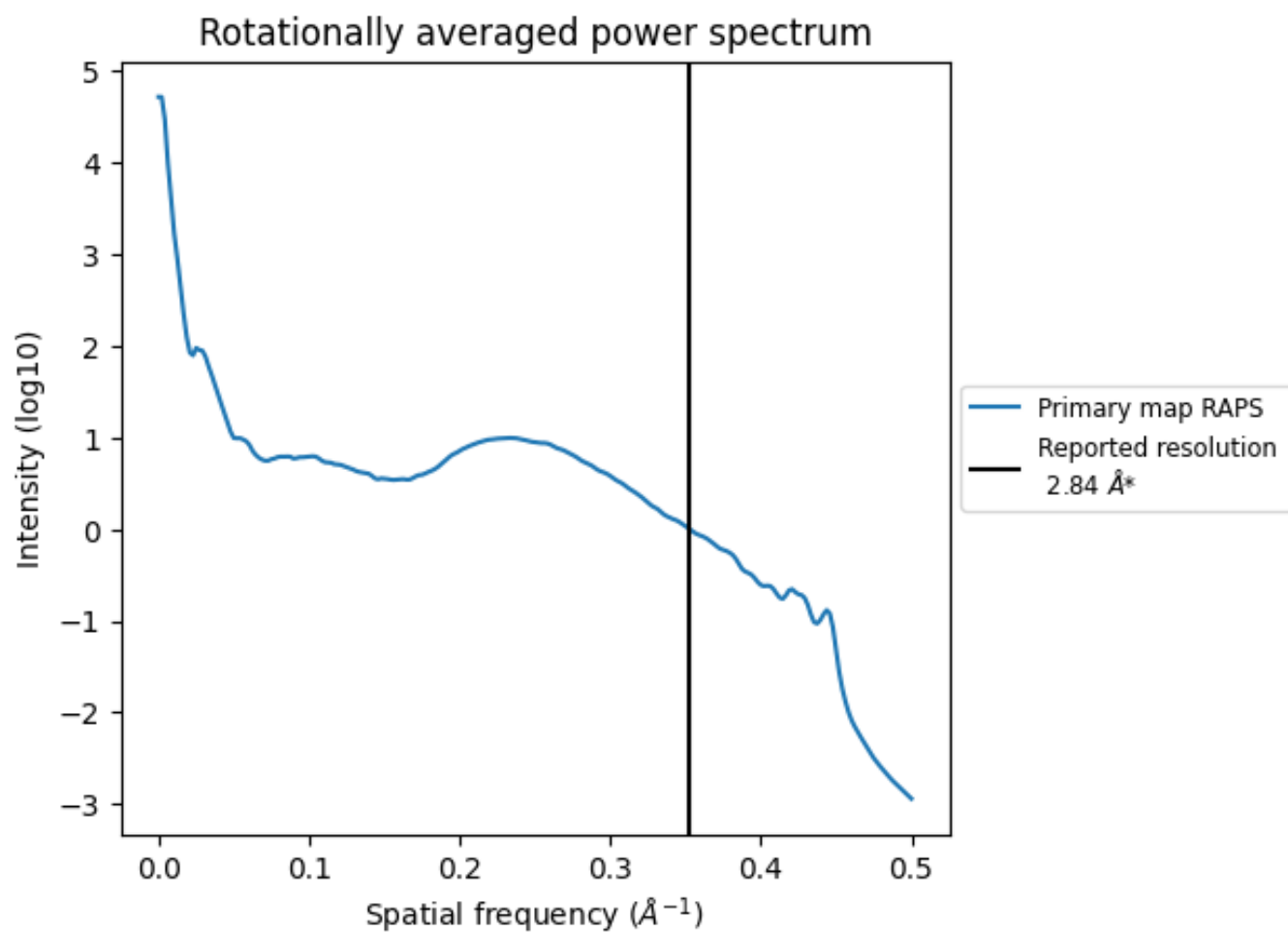
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is  $408 \text{ nm}^3$ ; this corresponds to an approximate mass of 369 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 0.352 Å<sup>-1</sup>

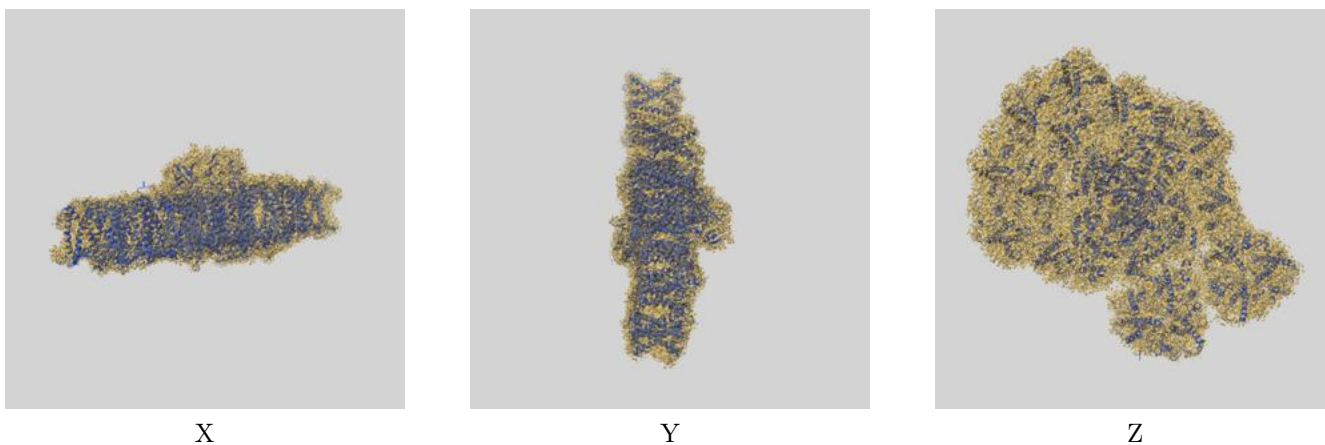
## 8 Fourier-Shell correlation

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

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

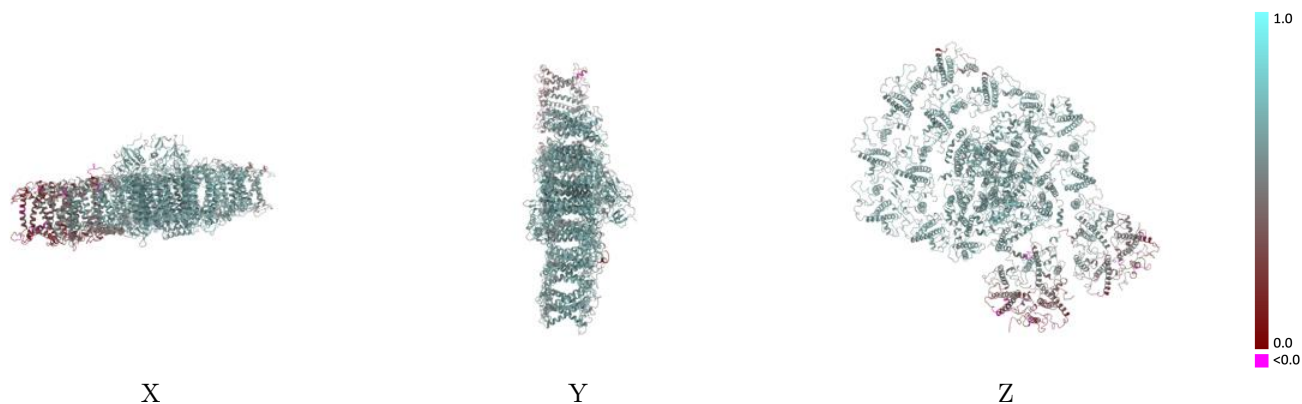
This section contains information regarding the fit between EMDB map EMD-30925 and PDB model 7DZ7. Per-residue inclusion information can be found in section 3 on page 45.

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



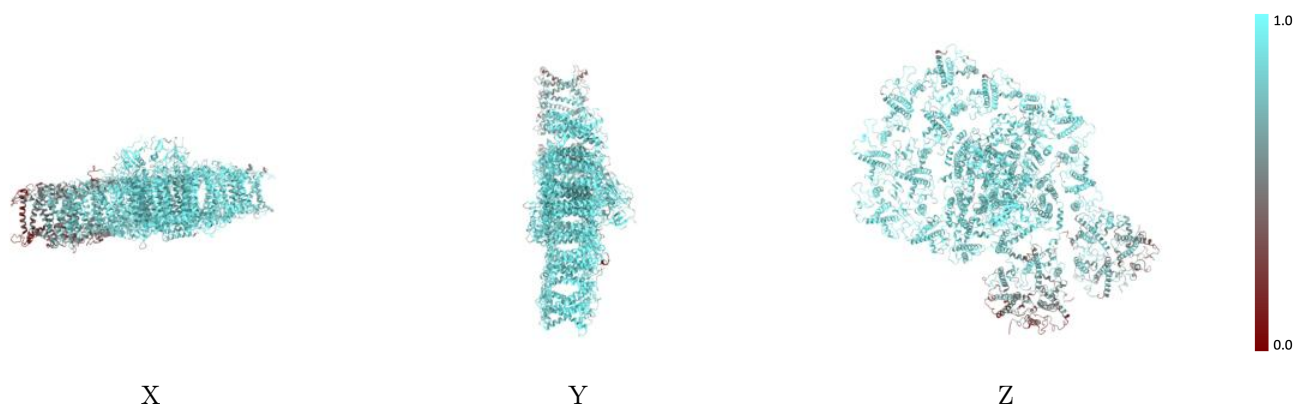
The images above show the 3D surface view of the map at the recommended contour level 0.02 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

## 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.

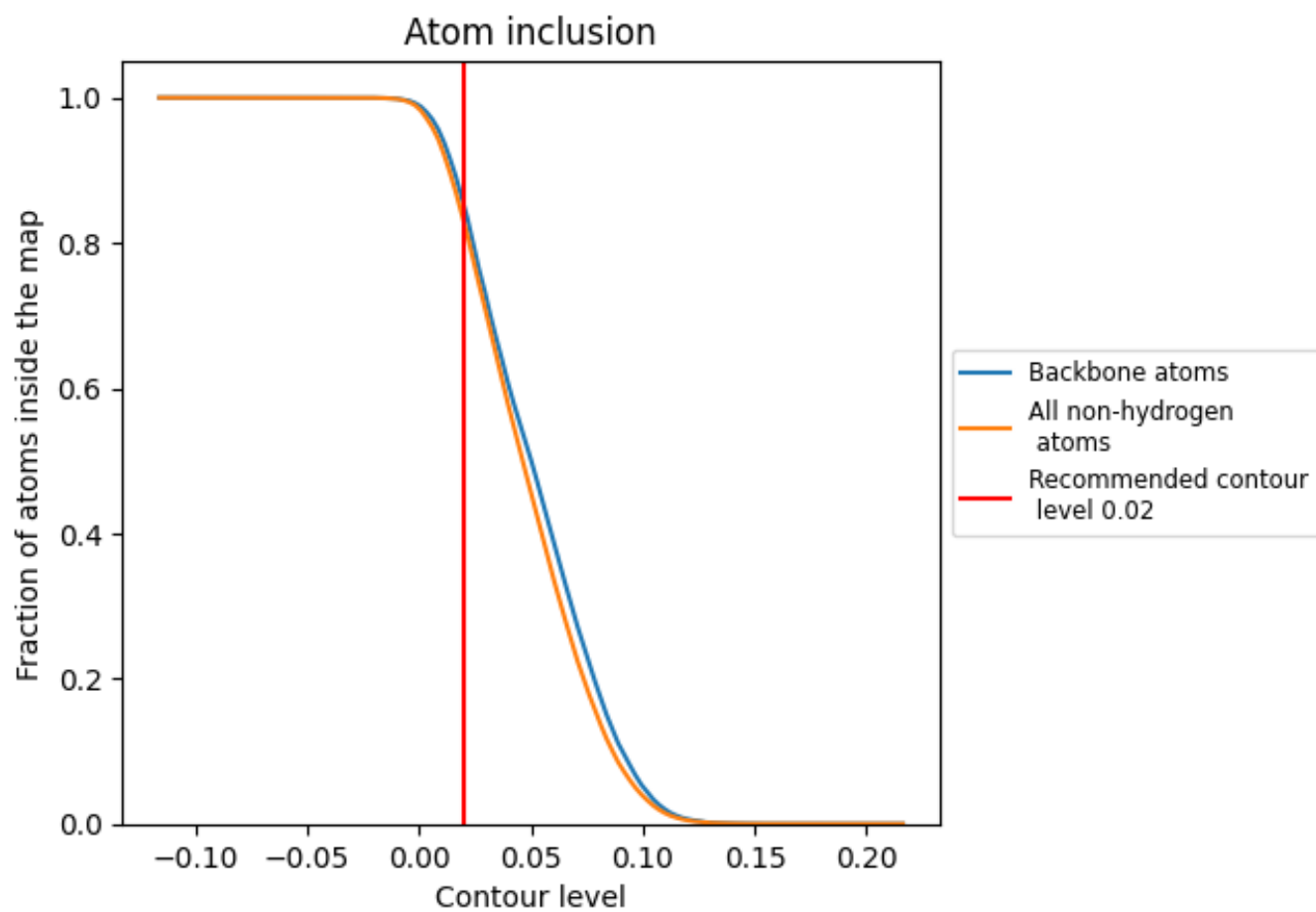
## 9.3 Atom inclusion mapped to coordinate model [i](#)



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 (0.02).































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 85% of all backbone atoms, 83% 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 (0.02) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8303	 0.5670
1	 0.8788	 0.5940
2	 0.8803	 0.5990
3	 0.9024	 0.6140
4	 0.8487	 0.5800
5	 0.8634	 0.5940
6	 0.8899	 0.5990
7	 0.9060	 0.6200
8	 0.8968	 0.6110
9	 0.8672	 0.5870
A	 0.9407	 0.6400
B	 0.9361	 0.6400
C	 0.9186	 0.6060
D	 0.9065	 0.6130
E	 0.9068	 0.6130
F	 0.8788	 0.6120
G	 0.8269	 0.5770
H	 0.8619	 0.5940
I	 0.8530	 0.5910
J	 0.8679	 0.6090
K	 0.8655	 0.5900
L	 0.9113	 0.6180
O	 0.8831	 0.5910
U	 0.6390	 0.4250
V	 0.7892	 0.5490
W	 0.5720	 0.3910
X	 0.4219	 0.2990
Y	 0.4770	 0.3310
Z	 0.7411	 0.5250
a	 0.8060	 0.5410

