



wwPDB EM Validation Summary Report ⓘ

Nov 9, 2022 – 05:13 AM JST

PDB ID : 6IJO
EMDB ID : EMD-9680
Title : Photosystem I of Chlamydomonas reinhardtii
Authors : Pan, X.; Ma, J.; Su, X.; Liu, Z.; Zhang, X.; Li, M.
Deposited on : 2018-10-10
Resolution : 3.30 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

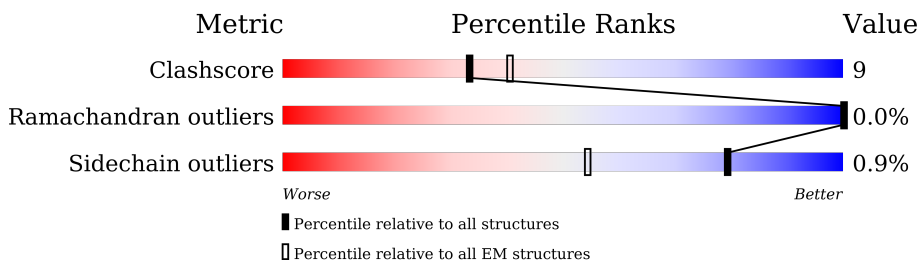
EMDB validation analysis : 0.0.1.dev43
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.2

1 Overall quality at a glance

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

The reported resolution of this entry is 3.30 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)
Clashscore	158937	4297
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 ≥ 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	247	
5	E	143	
6	F	227	
7	G	159	
8	H	155	

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Mol	Chain	Length	Quality of chain
9	I	106	
10	J	41	
11	K	160	
12	L	258	
13	1	248	
13	a	248	
14	3	298	
15	4	290	
16	5	274	
17	6	318	
18	7	241	
19	8	272	
20	2	227	
21	9	213	
22	X	26	

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
23	CLA	1	601	X	-	-	-
23	CLA	1	602	X	-	-	-
23	CLA	1	603	X	-	-	-
23	CLA	1	604	X	-	-	-
23	CLA	1	606	X	-	-	-
23	CLA	1	607	X	-	-	-
23	CLA	1	608	X	-	-	-
23	CLA	1	609	X	-	-	-
23	CLA	1	610	X	-	-	-
23	CLA	1	611	X	-	-	-
23	CLA	1	612	X	-	-	-
23	CLA	1	613	X	-	-	-

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

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

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
23	CLA	7	609	X	-	-	-
23	CLA	7	610	X	-	-	-
23	CLA	7	611	X	-	-	-
23	CLA	7	613	X	-	-	-
23	CLA	7	614	X	-	-	-
23	CLA	7	615	X	-	-	-
23	CLA	7	616	X	-	-	-
23	CLA	8	601	X	-	-	-
23	CLA	8	602	X	-	-	-
23	CLA	8	603	X	-	-	-
23	CLA	8	604	X	-	-	-
23	CLA	8	606	X	-	-	-
23	CLA	8	607	X	-	-	-
23	CLA	8	608	X	-	-	-
23	CLA	8	609	X	-	-	-
23	CLA	8	610	X	-	-	-
23	CLA	8	611	X	-	-	-
23	CLA	8	612	X	-	-	-
23	CLA	8	613	X	-	-	-
23	CLA	8	614	X	-	-	-
23	CLA	9	601	X	-	-	-
23	CLA	9	602	X	-	-	-
23	CLA	9	603	X	-	-	-
23	CLA	9	604	X	-	-	-
23	CLA	9	606	X	-	-	-
23	CLA	9	607	X	-	-	-
23	CLA	9	609	X	-	-	-
23	CLA	9	610	X	-	-	-
23	CLA	9	611	X	-	-	-
23	CLA	9	612	X	-	-	-
23	CLA	9	613	X	-	-	-
23	CLA	9	614	X	-	-	-
23	CLA	A	801	X	-	-	-
23	CLA	A	802	X	-	-	-
23	CLA	A	803	X	-	-	-
23	CLA	A	804	X	-	-	-
23	CLA	A	805	X	-	-	-
23	CLA	A	806	X	-	-	-
23	CLA	A	807	X	-	-	-
23	CLA	A	808	X	-	-	-
23	CLA	A	809	X	-	-	-
23	CLA	A	810	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
23	CLA	A	811	X	-	-	-
23	CLA	A	812	X	-	-	-
23	CLA	A	813	X	-	-	-
23	CLA	A	814	X	-	-	-
23	CLA	A	815	X	-	-	-
23	CLA	A	816	X	-	-	-
23	CLA	A	817	X	-	-	-
23	CLA	A	818	X	-	-	-
23	CLA	A	819	X	-	-	-
23	CLA	A	820	X	-	-	-
23	CLA	A	821	X	-	-	-
23	CLA	A	822	X	-	-	-
23	CLA	A	823	X	-	-	-
23	CLA	A	824	X	-	-	-
23	CLA	A	825	X	-	-	-
23	CLA	A	826	X	-	-	-
23	CLA	A	827	X	-	-	-
23	CLA	A	828	X	-	-	-
23	CLA	A	829	X	-	-	-
23	CLA	A	830	X	-	-	-
23	CLA	A	831	X	-	-	-
23	CLA	A	832	X	-	-	-
23	CLA	A	833	X	-	-	-
23	CLA	A	834	X	-	-	-
23	CLA	A	835	X	-	-	-
23	CLA	A	836	X	-	-	-
23	CLA	A	837	X	-	-	-
23	CLA	A	838	X	-	-	-
23	CLA	A	839	X	-	-	-
23	CLA	A	840	X	-	-	-
23	CLA	A	841	X	-	-	-
23	CLA	A	842	X	-	-	-
23	CLA	A	843	X	-	-	-
23	CLA	A	845	X	-	-	-
23	CLA	A	854	X	-	-	-
23	CLA	B	802	X	-	-	-
23	CLA	B	803	X	-	-	-
23	CLA	B	804	X	-	-	-
23	CLA	B	805	X	-	-	-
23	CLA	B	806	X	-	-	-
23	CLA	B	807	X	-	-	-
23	CLA	B	808	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
23	CLA	B	809	X	-	-	-
23	CLA	B	810	X	-	-	-
23	CLA	B	811	X	-	-	-
23	CLA	B	812	X	-	-	-
23	CLA	B	813	X	-	-	-
23	CLA	B	814	X	-	-	-
23	CLA	B	815	X	-	-	-
23	CLA	B	816	X	-	-	-
23	CLA	B	817	X	-	-	-
23	CLA	B	818	X	-	-	-
23	CLA	B	819	X	-	-	-
23	CLA	B	820	X	-	-	-
23	CLA	B	821	X	-	-	-
23	CLA	B	823	X	-	-	-
23	CLA	B	824	X	-	-	-
23	CLA	B	825	X	-	-	-
23	CLA	B	826	X	-	-	-
23	CLA	B	827	X	-	-	-
23	CLA	B	828	X	-	-	-
23	CLA	B	829	X	-	-	-
23	CLA	B	830	X	-	-	-
23	CLA	B	831	X	-	-	-
23	CLA	B	832	X	-	-	-
23	CLA	B	833	X	-	-	-
23	CLA	B	834	X	-	-	-
23	CLA	B	835	X	-	-	-
23	CLA	B	837	X	-	-	-
23	CLA	B	838	X	-	-	-
23	CLA	B	839	X	-	-	-
23	CLA	B	840	X	-	-	-
23	CLA	B	841	X	-	-	-
23	CLA	F	301	X	-	-	-
23	CLA	F	303	X	-	-	-
23	CLA	F	304	X	-	-	-
23	CLA	G	203	X	-	-	-
23	CLA	G	204	X	-	-	-
23	CLA	J	101	X	-	-	-
23	CLA	K	201	X	-	-	-
23	CLA	K	203	X	-	-	-
23	CLA	K	204	X	-	-	-
23	CLA	K	206	X	-	-	-
23	CLA	L	302	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
23	CLA	L	303	X	-	-	-
23	CLA	L	304	X	-	-	-
23	CLA	a	601	X	-	-	-
23	CLA	a	602	X	-	-	-
23	CLA	a	603	X	-	-	-
23	CLA	a	604	X	-	-	-
23	CLA	a	606	X	-	-	-
23	CLA	a	607	X	-	-	-
23	CLA	a	608	X	-	-	-
23	CLA	a	609	X	-	-	-
23	CLA	a	610	X	-	-	-
23	CLA	a	611	X	-	-	-
23	CLA	a	612	X	-	-	-
23	CLA	a	613	X	-	-	-
23	CLA	a	614	X	-	-	-
23	CLA	a	616	X	-	-	-

2 Entry composition [i](#)

There are 33 unique types of molecules in this entry. The entry contains 49685 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 PsaA.

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 PsaB.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	731	5812	3818	975	1001	18	0	0

- Molecule 3 is a protein called PsaC.

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 PsaD.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	D	144	1129	722	200	200	7	0	0

- Molecule 5 is a protein called PsaE.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
5	E	64	505	322	89	94	0	0

- Molecule 6 is a protein called PsaF.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	F	164	1254	811	209	231	3	0	0

- Molecule 7 is a protein called PsaG.

Mol	Chain	Residues	Atoms				AltConf	Trace
7	G	70	Total	C	N	O	0	0
			514	334	89	91		

- Molecule 8 is a protein called PsaH.

Mol	Chain	Residues	Atoms				AltConf	Trace
8	H	51	Total	C	N	O	0	0
			357	223	66	68		

- Molecule 9 is a protein called PsaI.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	32	Total	C	N	O	S	0	0
			242	166	34	41	1		

- Molecule 10 is a protein called PsaJ.

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

- Molecule 11 is a protein called PsaK.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	85	Total	C	N	O	S	0	0
			578	368	99	109	2		

- Molecule 12 is a protein called PsaL.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	106	Total	C	N	O	S	0	0
			768	507	123	136	2		

- Molecule 13 is a protein called Lhca1.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	1	193	Total	C	N	O	S	0	0
			1433	932	239	259	3		
13	a	194	Total	C	N	O	S	0	0
			1444	941	240	260	3		

- Molecule 14 is a protein called Lhca3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	3	221	1683	1099	271	305	8	0	0

- Molecule 15 is a protein called Lhca4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
15	4	210	1631	1071	263	292	5	0	0

- Molecule 16 is a protein called Lhca5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
16	5	226	1765	1149	295	313	8	0	0

- Molecule 17 is a protein called Lhca6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
17	6	230	1771	1167	293	305	6	0	0

- Molecule 18 is a protein called Lhca7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
18	7	213	1649	1072	274	297	6	0	0

- Molecule 19 is a protein called Lhca8.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
19	8	215	1630	1058	278	290	4	0	0

- Molecule 20 is a protein called Lhca2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
20	2	173	1346	874	223	241	8	0	0

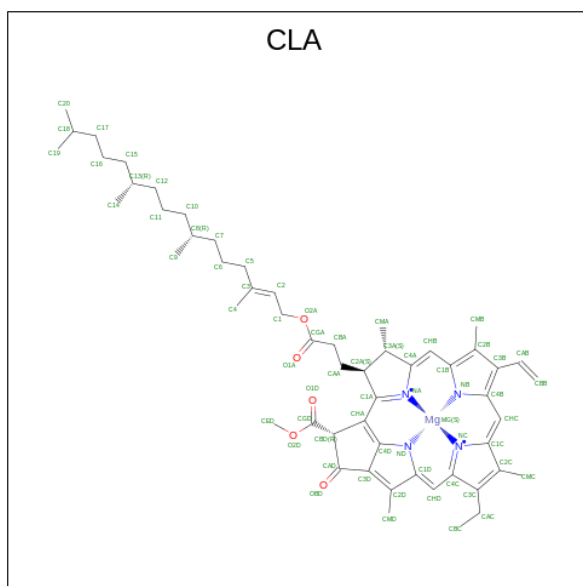
- Molecule 21 is a protein called Lhca9.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
21	9	172	1302	840	220	235	7	0	0

- Molecule 22 is a protein called ChainX.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
22	X	26	130	78	26	26	0	0

- Molecule 23 is CHLOROPHYLL A (three-letter code: CLA) (formula: $C_{55}H_{72}MgN_4O_5$).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
23	A	1	2625	2181	45	180	219	0
23	A	1	2625	2181	45	180	219	0
23	A	1	2625	2181	45	180	219	0
23	A	1	2625	2181	45	180	219	0
23	A	1	2625	2181	45	180	219	0
23	A	1	2625	2181	45	180	219	0
23	A	1	2625	2181	45	180	219	0
23	A	1	2625	2181	45	180	219	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
23	A	1	2625	2181	45	180	219	0
23	A	1	2625	2181	45	180	219	0
23	A	1	2625	2181	45	180	219	0
23	A	1	2625	2181	45	180	219	0
23	A	1	2625	2181	45	180	219	0
23	A	1	2625	2181	45	180	219	0
23	A	1	2625	2181	45	180	219	0
23	A	1	2625	2181	45	180	219	0
23	A	1	2625	2181	45	180	219	0
23	A	1	2625	2181	45	180	219	0
23	A	1	2625	2181	45	180	219	0
23	A	1	2625	2181	45	180	219	0
23	A	1	2625	2181	45	180	219	0
23	A	1	2625	2181	45	180	219	0
23	A	1	2625	2181	45	180	219	0
23	A	1	2625	2181	45	180	219	0
23	A	1	2625	2181	45	180	219	0
23	B	1	2270	1884	40	160	186	0
23	B	1	2270	1884	40	160	186	0
23	B	1	2270	1884	40	160	186	0
23	B	1	2270	1884	40	160	186	0
23	B	1	2270	1884	40	160	186	0

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Mol	Chain	Residues	Atoms					AltConf
23	B	1	Total	C	Mg	N	O	0
			2270	1884	40	160	186	
23	B	1	Total	C	Mg	N	O	0
			2270	1884	40	160	186	
23	B	1	Total	C	Mg	N	O	0
			2270	1884	40	160	186	
23	B	1	Total	C	Mg	N	O	0
			2270	1884	40	160	186	
23	B	1	Total	C	Mg	N	O	0
			2270	1884	40	160	186	
23	B	1	Total	C	Mg	N	O	0
			2270	1884	40	160	186	
23	B	1	Total	C	Mg	N	O	0
			2270	1884	40	160	186	
23	B	1	Total	C	Mg	N	O	0
			2270	1884	40	160	186	
23	B	1	Total	C	Mg	N	O	0
			2270	1884	40	160	186	
23	B	1	Total	C	Mg	N	O	0
			2270	1884	40	160	186	
23	B	1	Total	C	Mg	N	O	0
			2270	1884	40	160	186	
23	F	1	Total	C	Mg	N	O	0
			140	114	3	12	11	
23	F	1	Total	C	Mg	N	O	0
			140	114	3	12	11	
23	F	1	Total	C	Mg	N	O	0
			140	114	3	12	11	
23	G	1	Total	C	Mg	N	O	0
			87	69	2	8	8	
23	G	1	Total	C	Mg	N	O	0
			87	69	2	8	8	
23	J	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
23	K	1	Total	C	Mg	N	O	0
			201	161	4	16	20	

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
23	K	1	Total 201	C 161	Mg 4	N 16	O 20	0
23	K	1	Total 201	C 161	Mg 4	N 16	O 20	0
23	K	1	Total 201	C 161	Mg 4	N 16	O 20	0
23	L	1	Total 135	C 105	Mg 3	N 12	O 15	0
23	L	1	Total 135	C 105	Mg 3	N 12	O 15	0
23	L	1	Total 135	C 105	Mg 3	N 12	O 15	0
23	1	1	Total 674	C 546	Mg 14	N 56	O 58	0
23	1	1	Total 674	C 546	Mg 14	N 56	O 58	0
23	1	1	Total 674	C 546	Mg 14	N 56	O 58	0
23	1	1	Total 674	C 546	Mg 14	N 56	O 58	0
23	1	1	Total 674	C 546	Mg 14	N 56	O 58	0
23	1	1	Total 674	C 546	Mg 14	N 56	O 58	0
23	1	1	Total 674	C 546	Mg 14	N 56	O 58	0
23	1	1	Total 674	C 546	Mg 14	N 56	O 58	0
23	1	1	Total 674	C 546	Mg 14	N 56	O 58	0
23	1	1	Total 674	C 546	Mg 14	N 56	O 58	0
23	1	1	Total 674	C 546	Mg 14	N 56	O 58	0
23	1	1	Total 674	C 546	Mg 14	N 56	O 58	0
23	1	1	Total 674	C 546	Mg 14	N 56	O 58	0
23	a	1	Total 709	C 574	Mg 14	N 56	O 65	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
23	a	1	709	574	14	56	65	0
23	a	1	709	574	14	56	65	0
23	a	1	709	574	14	56	65	0
23	a	1	709	574	14	56	65	0
23	a	1	709	574	14	56	65	0
23	a	1	709	574	14	56	65	0
23	a	1	709	574	14	56	65	0
23	a	1	709	574	14	56	65	0
23	a	1	709	574	14	56	65	0
23	a	1	709	574	14	56	65	0
23	a	1	709	574	14	56	65	0
23	a	1	709	574	14	56	65	0
23	a	1	709	574	14	56	65	0
23	3	1	724	595	14	56	59	0
23	3	1	724	595	14	56	59	0
23	3	1	724	595	14	56	59	0
23	3	1	724	595	14	56	59	0
23	3	1	724	595	14	56	59	0
23	3	1	724	595	14	56	59	0
23	3	1	724	595	14	56	59	0
23	3	1	724	595	14	56	59	0
23	3	1	724	595	14	56	59	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
23	5	1	878	718	17	68	75	0
23	5	1	878	718	17	68	75	0
23	5	1	878	718	17	68	75	0
23	5	1	878	718	17	68	75	0
23	5	1	878	718	17	68	75	0
23	5	1	878	718	17	68	75	0
23	5	1	878	718	17	68	75	0
23	5	1	878	718	17	68	75	0
23	5	1	878	718	17	68	75	0
23	5	1	878	718	17	68	75	0
23	5	1	878	718	17	68	75	0
23	5	1	878	718	17	68	75	0
23	5	1	878	718	17	68	75	0
23	5	1	878	718	17	68	75	0
23	5	1	878	718	17	68	75	0
23	5	1	878	718	17	68	75	0
23	5	1	878	718	17	68	75	0
23	5	1	878	718	17	68	75	0
23	5	1	878	718	17	68	75	0
23	6	1	912	752	17	68	75	0
23	6	1	912	752	17	68	75	0
23	6	1	912	752	17	68	75	0
23	6	1	912	752	17	68	75	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
23	6	1	912	752	17	68	75	0
23	6	1	912	752	17	68	75	0
23	6	1	912	752	17	68	75	0
23	6	1	912	752	17	68	75	0
23	6	1	912	752	17	68	75	0
23	6	1	912	752	17	68	75	0
23	6	1	912	752	17	68	75	0
23	6	1	912	752	17	68	75	0
23	6	1	912	752	17	68	75	0
23	6	1	912	752	17	68	75	0
23	6	1	912	752	17	68	75	0
23	6	1	912	752	17	68	75	0
23	6	1	912	752	17	68	75	0
23	6	1	912	752	17	68	75	0
23	6	1	912	752	17	68	75	0
23	6	1	912	752	17	68	75	0
23	7	1	760	618	15	60	67	0
23	7	1	760	618	15	60	67	0
23	7	1	760	618	15	60	67	0
23	7	1	760	618	15	60	67	0
23	7	1	760	618	15	60	67	0
23	7	1	760	618	15	60	67	0
23	7	1	760	618	15	60	67	0
23	7	1	760	618	15	60	67	0
23	7	1	760	618	15	60	67	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
23	7	1	Total 760	C 618	Mg 15	N 60	O 67	0
23	7	1	Total 760	C 618	Mg 15	N 60	O 67	0
23	7	1	Total 760	C 618	Mg 15	N 60	O 67	0
23	7	1	Total 760	C 618	Mg 15	N 60	O 67	0
23	7	1	Total 760	C 618	Mg 15	N 60	O 67	0
23	7	1	Total 760	C 618	Mg 15	N 60	O 67	0
23	7	1	Total 760	C 618	Mg 15	N 60	O 67	0
23	8	1	Total 727	C 593	Mg 14	N 56	O 64	0
23	8	1	Total 727	C 593	Mg 14	N 56	O 64	0
23	8	1	Total 727	C 593	Mg 14	N 56	O 64	0
23	8	1	Total 727	C 593	Mg 14	N 56	O 64	0
23	8	1	Total 727	C 593	Mg 14	N 56	O 64	0
23	8	1	Total 727	C 593	Mg 14	N 56	O 64	0
23	8	1	Total 727	C 593	Mg 14	N 56	O 64	0
23	8	1	Total 727	C 593	Mg 14	N 56	O 64	0
23	8	1	Total 727	C 593	Mg 14	N 56	O 64	0
23	8	1	Total 727	C 593	Mg 14	N 56	O 64	0
23	8	1	Total 727	C 593	Mg 14	N 56	O 64	0
23	8	1	Total 727	C 593	Mg 14	N 56	O 64	0
23	8	1	Total 727	C 593	Mg 14	N 56	O 64	0
23	8	1	Total 727	C 593	Mg 14	N 56	O 64	0

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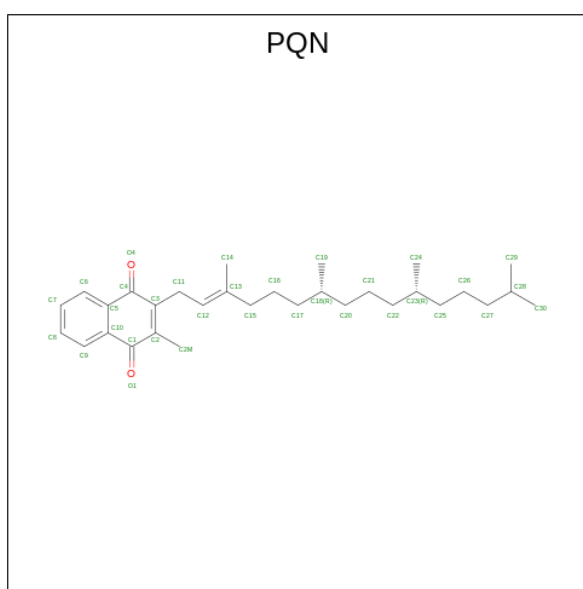
Mol	Chain	Residues	Atoms				AltConf
23	2	1	Total	C	Mg	N	0
			350	285	13	52	
23	2	1	Total	C	Mg	N	0
			350	285	13	52	
23	2	1	Total	C	Mg	N	0
			350	285	13	52	
23	2	1	Total	C	Mg	N	0
			350	285	13	52	
23	2	1	Total	C	Mg	N	0
			350	285	13	52	
23	2	1	Total	C	Mg	N	0
			350	285	13	52	
23	2	1	Total	C	Mg	N	0
			350	285	13	52	
23	2	1	Total	C	Mg	N	0
			350	285	13	52	
23	2	1	Total	C	Mg	N	0
			350	285	13	52	
23	2	1	Total	C	Mg	N	0
			350	285	13	52	
23	2	1	Total	C	Mg	N	0
			350	285	13	52	
23	2	1	Total	C	Mg	N	0
			350	285	13	52	
23	2	1	Total	C	Mg	N	0
			350	285	13	52	
23	9	1	Total	C	Mg	N	0
			324	264	12	48	
23	9	1	Total	C	Mg	N	0
			324	264	12	48	
23	9	1	Total	C	Mg	N	0
			324	264	12	48	
23	9	1	Total	C	Mg	N	0
			324	264	12	48	
23	9	1	Total	C	Mg	N	0
			324	264	12	48	
23	9	1	Total	C	Mg	N	0
			324	264	12	48	
23	9	1	Total	C	Mg	N	0
			324	264	12	48	

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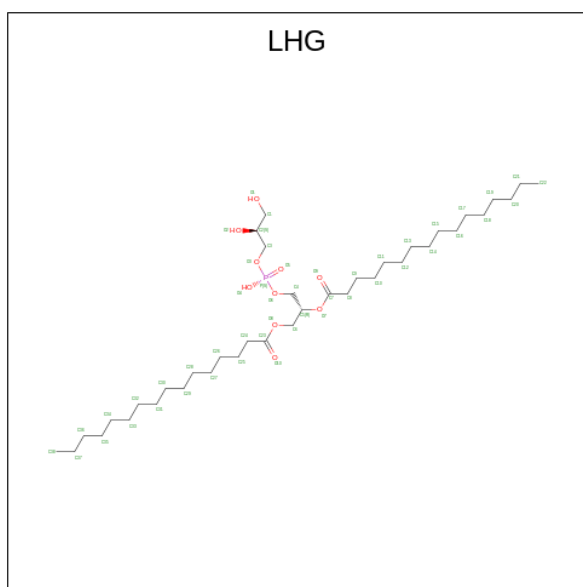
Mol	Chain	Residues	Atoms				AltConf
23	9	1	Total	C	Mg	N	0
			324	264	12	48	
23	9	1	Total	C	Mg	N	0
			324	264	12	48	
23	9	1	Total	C	Mg	N	0
			324	264	12	48	
23	9	1	Total	C	Mg	N	0
			324	264	12	48	

- Molecule 24 is PHYLLOQUINONE (three-letter code: PQN) (formula: $C_{31}H_{46}O_2$).



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

- Molecule 25 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula: $C_{38}H_{75}O_{10}P$).



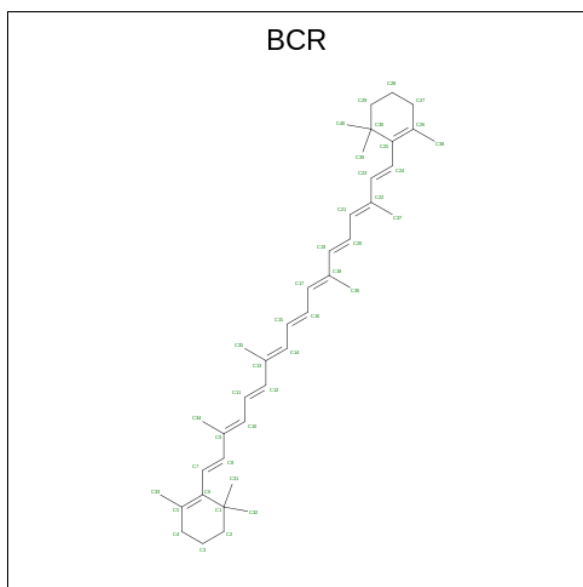
Mol	Chain	Residues	Atoms			AltConf	
			Total	C	O		P
25	A	1	79	57	20	2	0
25	A	1	79	57	20	2	0
25	B	1	38	27	10	1	0
25	1	1	49	38	10	1	0
25	a	1	49	38	10	1	0
25	3	1	94	72	20	2	0
25	3	1	94	72	20	2	0
25	4	1	49	38	10	1	0
25	5	1	98	76	20	2	0
25	5	1	98	76	20	2	0
25	6	1	48	37	10	1	0
25	7	1	37	26	10	1	0
25	8	1	96	74	20	2	0
25	8	1	96	74	20	2	0

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
25	2	1	37	26	10	1	0
25	9	1	49	38	10	1	0

- Molecule 26 is BETA-CAROTENE (three-letter code: BCR) (formula: C₄₀H₅₆).



Mol	Chain	Residues	Atoms		AltConf
26	A	1	Total	C	0
			240	240	
26	A	1	Total	C	0
			240	240	
26	A	1	Total	C	0
			240	240	
26	A	1	Total	C	0
			240	240	
26	A	1	Total	C	0
			240	240	
26	B	1	Total	C	0
			280	280	
26	B	1	Total	C	0
			280	280	
26	B	1	Total	C	0
			280	280	

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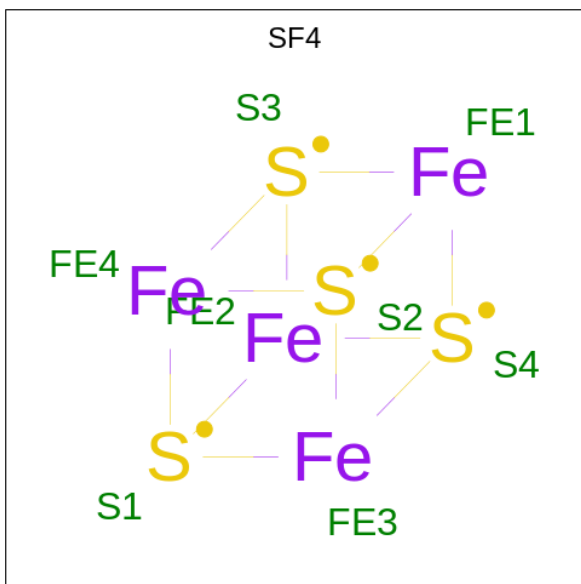
Mol	Chain	Residues	Atoms		AltConf
26	B	1	Total 280	C 280	0
26	B	1	Total 280	C 280	0
26	B	1	Total 280	C 280	0
26	B	1	Total 280	C 280	0
26	F	1	Total 40	C 40	0
26	G	1	Total 40	C 40	0
26	J	1	Total 40	C 40	0
26	K	1	Total 80	C 80	0
26	K	1	Total 80	C 80	0
26	L	1	Total 80	C 80	0
26	L	1	Total 80	C 80	0
26	1	1	Total 40	C 40	0
26	a	1	Total 40	C 40	0
26	3	1	Total 120	C 120	0
26	3	1	Total 120	C 120	0
26	3	1	Total 120	C 120	0
26	4	1	Total 40	C 40	0
26	5	1	Total 40	C 40	0
26	6	1	Total 40	C 40	0
26	7	1	Total 80	C 80	0
26	7	1	Total 80	C 80	0

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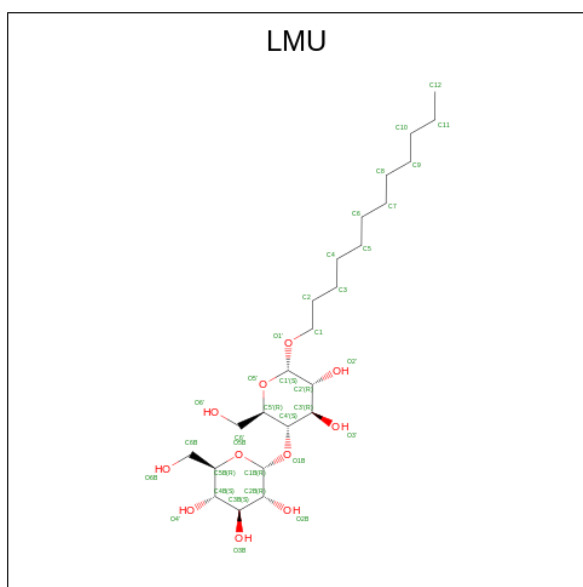
Mol	Chain	Residues	Atoms	AltConf
26	8	1	Total C 40 40	0

- Molecule 27 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe₄S₄).



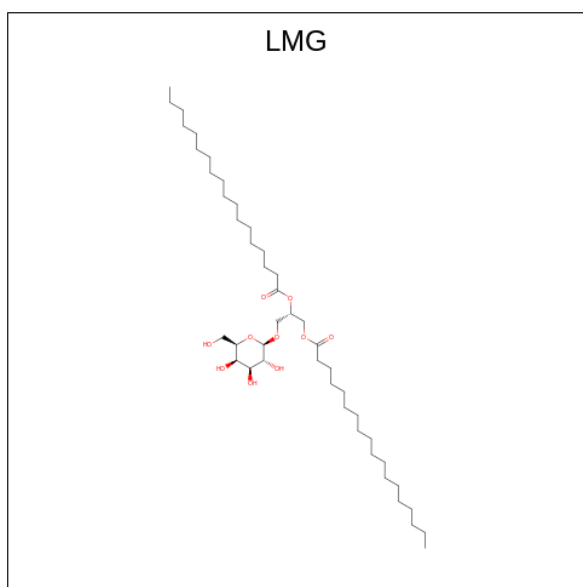
Mol	Chain	Residues	Atoms	AltConf
27	A	1	Total Fe S 8 4 4	0
27	C	1	Total Fe S 16 8 8	0
27	C	1	Total Fe S 16 8 8	0

- Molecule 28 is DODECYL-ALPHA-D-MALTOSIDE (three-letter code: LMU) (formula: C₂₄H₄₆O₁₁).



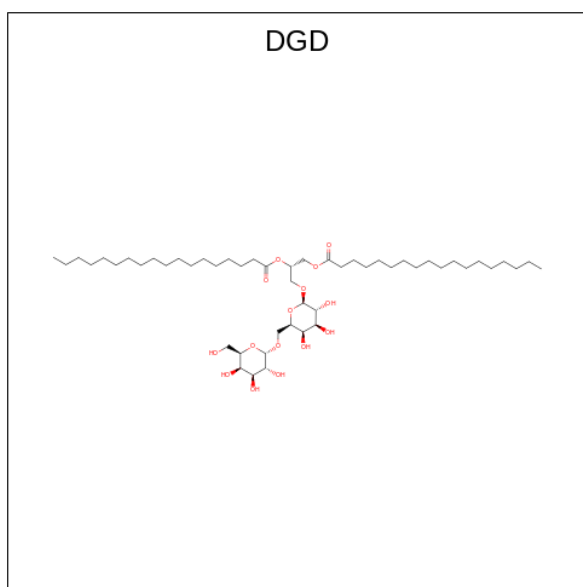
Mol	Chain	Residues	Atoms			AltConf
28	A	1	Total	C	O	0
			103	72	31	
28	A	1	Total	C	O	0
			103	72	31	
28	A	1	Total	C	O	0
			103	72	31	
28	K	1	Total	C	O	0
			35	24	11	
28	5	1	Total	C	O	0
			33	22	11	
28	8	1	Total	C	O	0
			70	48	22	
28	8	1	Total	C	O	0
			70	48	22	

- Molecule 29 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: LMG) (formula: C₄₅H₈₆O₁₀).



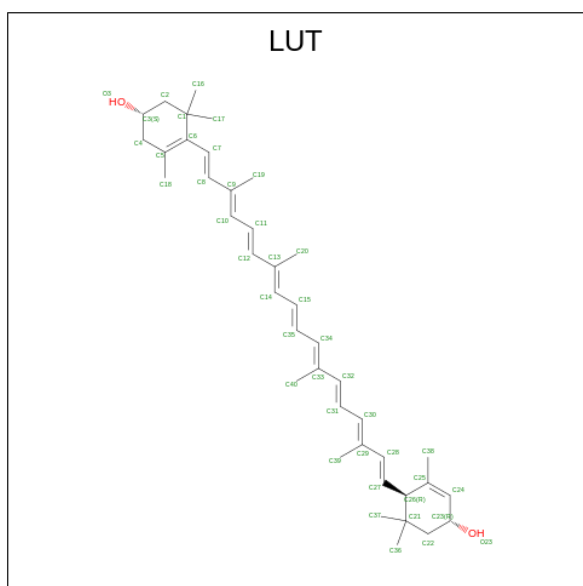
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
29	A	1	40	30	10	0
29	J	1	40	30	10	0
29	4	1	80	60	20	0
29	4	1	80	60	20	0
29	5	1	80	60	20	0
29	5	1	80	60	20	0
29	7	1	44	34	10	0

- Molecule 30 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (three-letter code: DGD) (formula: $C_{51}H_{96}O_{15}$).



Mol	Chain	Residues	Atoms			AltConf
30	B	1	Total	C	O	0
			62	47	15	
30	J	1	Total	C	O	0
			58	43	15	

- Molecule 31 is (3R,3'R,6S)-4,5-DIDEHYDRO-5,6-DIHYDRO-BETA,BETA-CAROTENE-3,3'-DIOL (three-letter code: LUT) (formula: C₄₀H₅₆O₂).



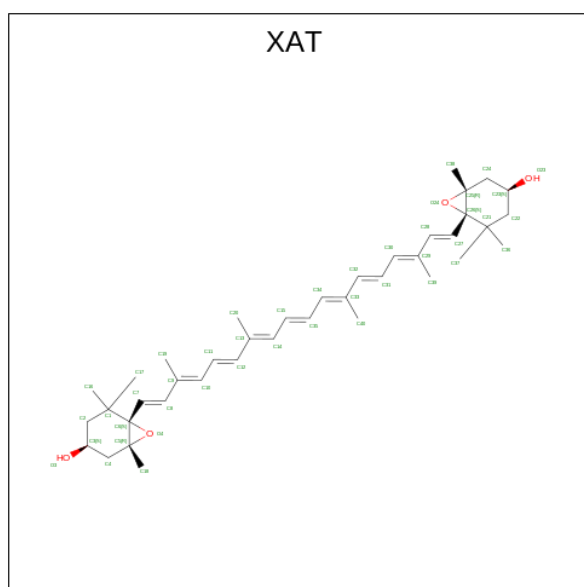
Mol	Chain	Residues	Atoms			AltConf
31	1	1	Total	C	O	0
			42	40	2	

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Mol	Chain	Residues	Atoms			AltConf
31	a	1	Total	C	O	0
			42	40	2	
31	3	1	Total	C	O	0
			42	40	2	
31	4	1	Total	C	O	0
			42	40	2	
31	5	1	Total	C	O	0
			42	40	2	
31	6	1	Total	C	O	0
			42	40	2	
31	7	1	Total	C	O	0
			42	40	2	
31	8	1	Total	C	O	0
			42	40	2	
31	2	1	Total	C	O	0
			42	40	2	
31	9	1	Total	C	O	0
			42	40	2	

- Molecule 32 is (3S,5R,6S,3'S,5'R,6'S)-5,6,5',6'-DIEPOXY-5,6,5',6'-TETRAHYDRO-BETA, BETA-CAROTENE-3,3'-DIOL (three-letter code: XAT) (formula: C₄₀H₅₆O₄).



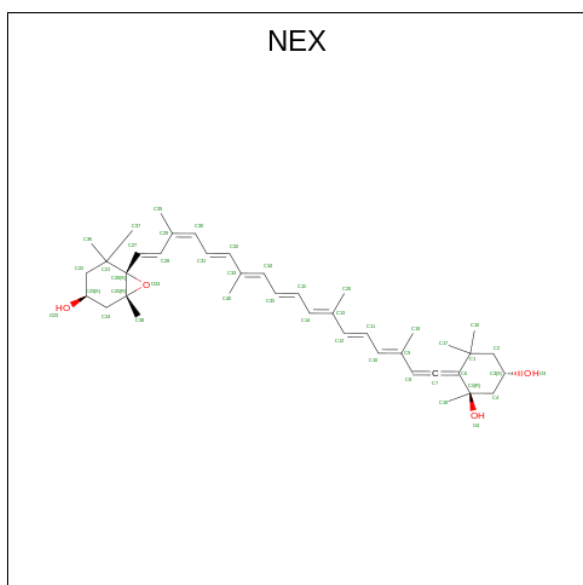
Mol	Chain	Residues	Atoms			AltConf
32	1	1	Total	C	O	0
			44	40	4	
32	a	1	Total	C	O	0
			44	40	4	

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Mol	Chain	Residues	Atoms			AltConf
32	3	1	Total	C	O	0
			44	40	4	
32	4	1	Total	C	O	0
			44	40	4	
32	5	1	Total	C	O	0
			44	40	4	
32	6	1	Total	C	O	0
			44	40	4	
32	7	1	Total	C	O	0
			44	40	4	
32	8	1	Total	C	O	0
			44	40	4	
32	2	1	Total	C	O	0
			44	40	4	
32	9	1	Total	C	O	0
			44	40	4	

- Molecule 33 is (1R,3R)-6-[(3E,5E,7E,9E,11E,13E,15E,17E)-18-[(1S,4R,6R)-4-HYDROXY-2,2,6-TRIMETHYL-7-OXABICYCLO[4.1.0]HEPT-1-YL]-3,7,12,16-TETRAMETHYLOCTADEC-1,3,5,7,9,11,13,15,17-NONAENYLIDENE]-1,5,5-TRIMETHYLCYCLOHEXANE-1,3-DIOL (three-letter code: NEX) (formula: C₄₀H₅₆O₄).

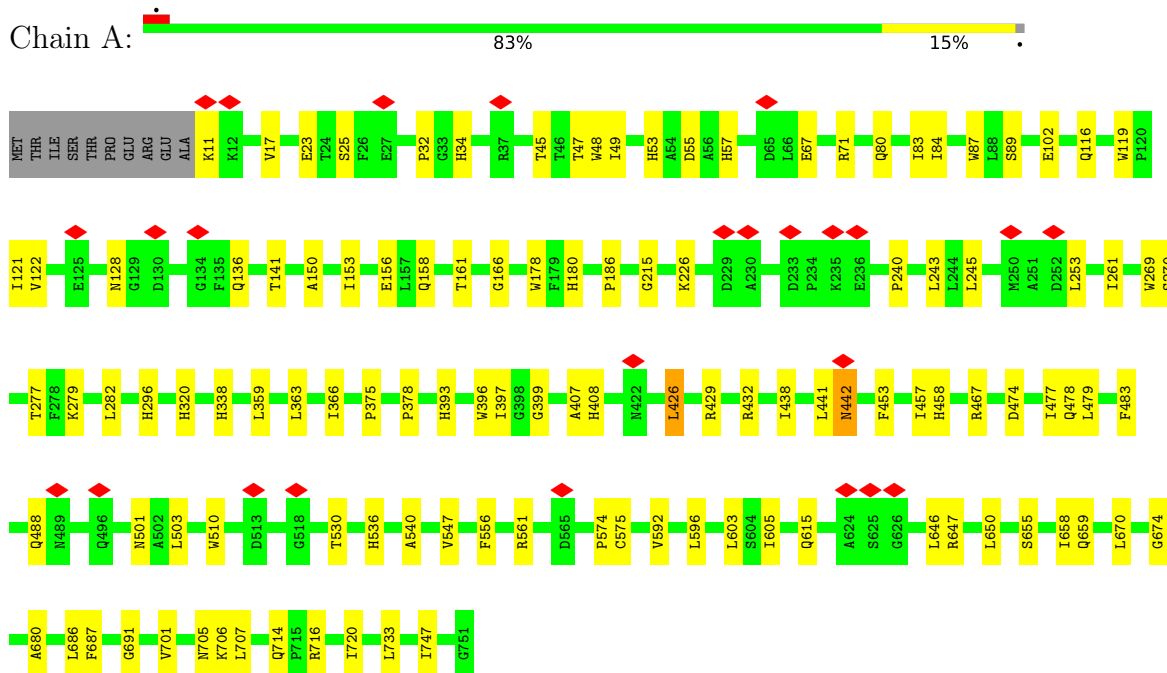


Mol	Chain	Residues	Atoms			AltConf
33	5	1	Total	C	O	0
			44	40	4	
33	6	1	Total	C	O	0
			44	40	4	

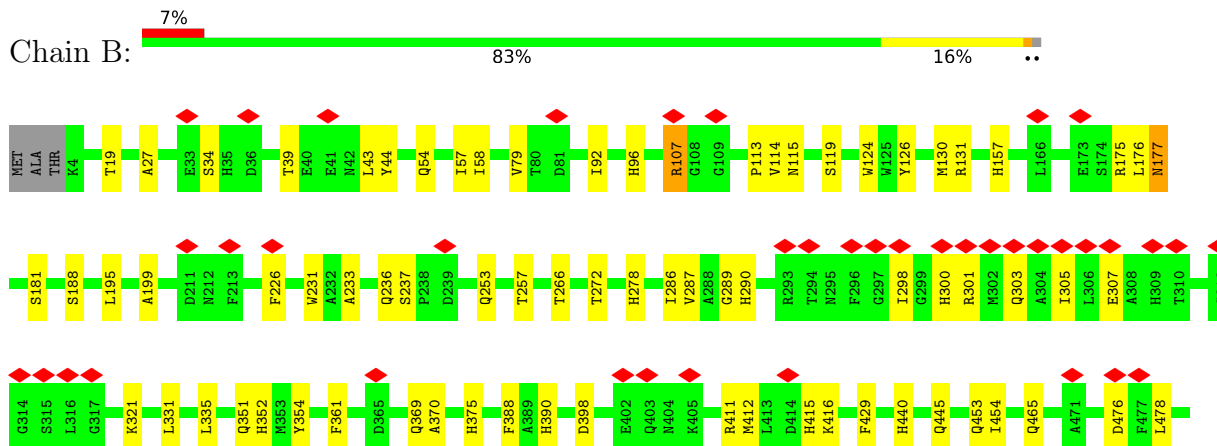
3 Residue-property plots [i](#)

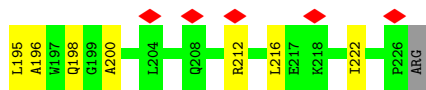
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: PsaA

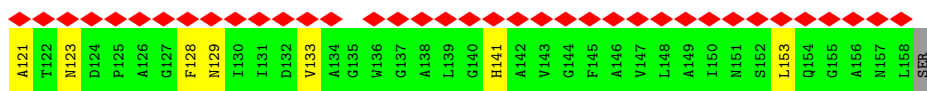
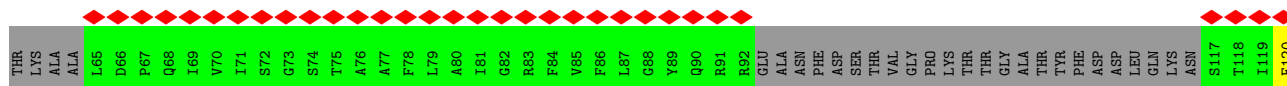
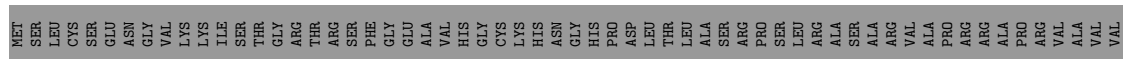
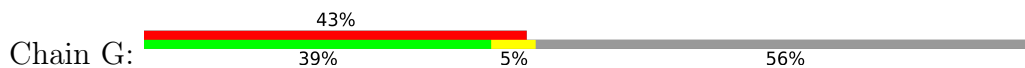


- Molecule 2: PsaB

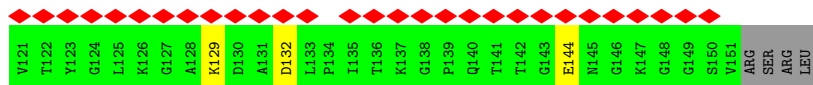
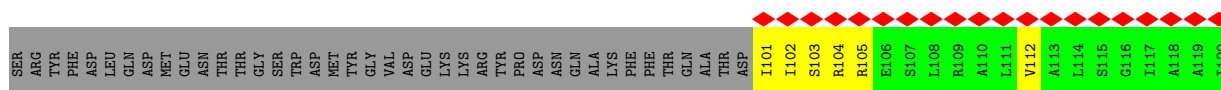
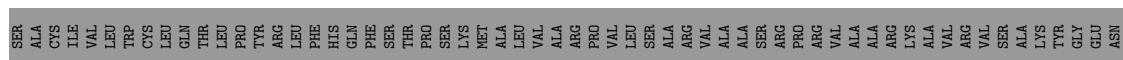




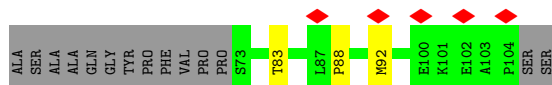
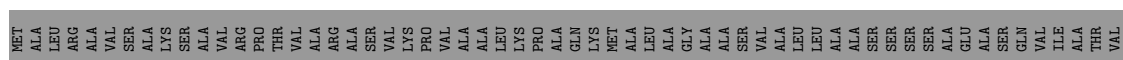
• Molecule 7: PsaG



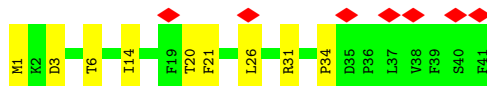
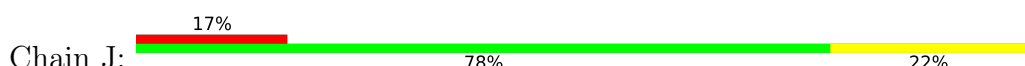
• Molecule 8: PsaH



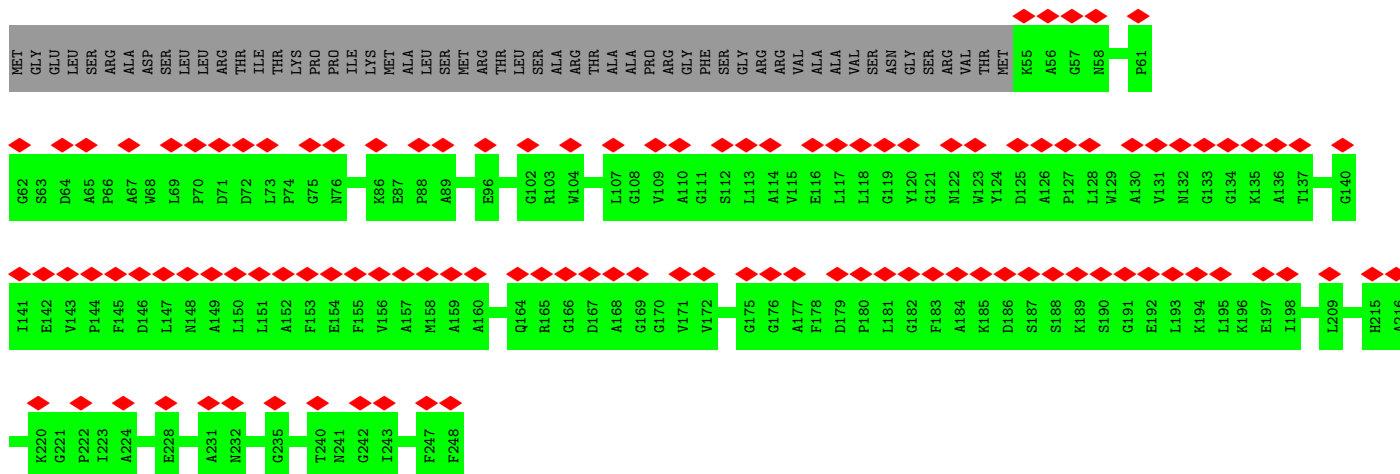
• Molecule 9: PsaI



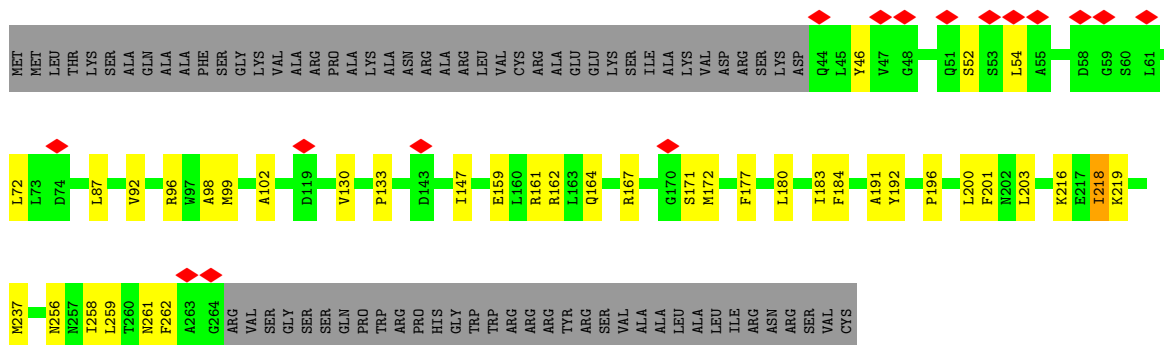
• Molecule 10: PsaJ



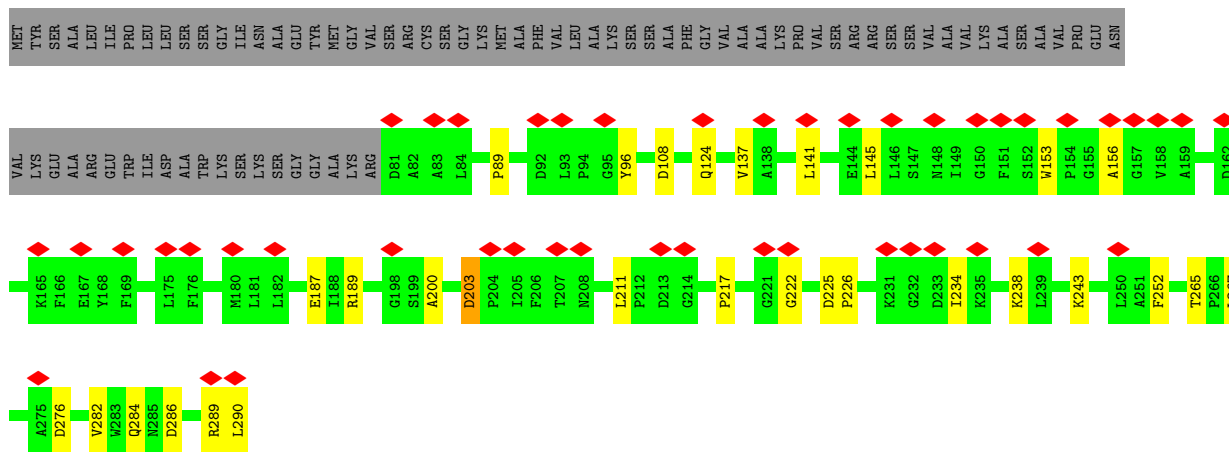
• Molecule 11: PsaK



• Molecule 14: Lhca3



• Molecule 15: Lhca4



• Molecule 16: Lhca5



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	17420	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	60.0	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	0.400	Depositor
Minimum map value	-0.135	Depositor
Average map value	0.004	Depositor
Map value standard deviation	0.022	Depositor
Recommended contour level	0.06	Depositor
Map size (Å)	208.0, 208.0, 208.0	wwPDB
Map dimensions	200, 200, 200	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.04, 1.04, 1.04	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.51	0/6015	0.57	1/8201 (0.0%)
2	B	0.49	0/6024	0.59	3/8225 (0.0%)
3	C	0.51	0/610	0.66	0/826
4	D	0.43	0/1157	0.61	0/1563
5	E	0.46	0/515	0.54	0/700
6	F	0.41	0/1280	0.55	0/1733
7	G	0.31	0/524	0.66	1/711 (0.1%)
8	H	0.31	0/359	0.61	0/483
9	I	0.43	0/250	0.63	0/345
10	J	0.43	0/349	0.58	0/478
11	K	0.32	0/583	0.69	1/790 (0.1%)
12	L	0.36	0/787	0.63	0/1074
13	1	0.38	0/1478	0.55	0/2012
13	a	0.39	0/1490	0.55	0/2028
14	3	0.49	0/1731	0.67	3/2349 (0.1%)
15	4	0.37	0/1686	0.53	0/2300
16	5	0.43	0/1820	0.62	0/2480
17	6	0.40	0/1833	0.58	0/2505
18	7	0.48	0/1701	0.61	0/2310
19	8	0.43	0/1680	0.63	1/2288 (0.0%)
20	2	0.29	0/1382	0.56	0/1870
21	9	0.32	0/1337	0.65	1/1814 (0.1%)
22	X	0.24	0/129	0.33	0/179
All	All	0.44	0/34720	0.59	11/47264 (0.0%)

There are no bond length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	3	180	LEU	CA-CB-CG	6.59	130.46	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
14	3	200	LEU	CA-CB-CG	6.43	130.10	115.30
7	G	153	LEU	CA-CB-CG	6.43	130.09	115.30
1	A	426	LEU	CA-CB-CG	6.20	129.56	115.30
11	K	114	LEU	CA-CB-CG	6.05	129.21	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5819	0	5672	96	0
2	B	5812	0	5569	94	0
3	C	600	0	589	10	0
4	D	1129	0	1144	23	0
5	E	505	0	504	4	0
6	F	1254	0	1288	14	0
7	G	514	0	509	7	0
8	H	357	0	382	6	0
9	I	242	0	252	2	0
10	J	337	0	336	10	0
11	K	578	0	617	7	0
12	L	768	0	776	20	0
13	1	1433	0	1387	29	0
13	a	1444	0	1396	0	0
14	3	1683	0	1641	28	0
15	4	1631	0	1587	26	0
16	5	1765	0	1738	45	0
17	6	1771	0	1770	30	0
18	7	1649	0	1589	30	0
19	8	1630	0	1609	26	0
20	2	1346	0	1330	17	0
21	9	1302	0	1275	30	0
22	X	130	0	132	2	0
23	1	674	0	541	19	0
23	2	350	0	39	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
23	3	724	0	628	22	0
23	4	782	0	686	24	0
23	5	878	0	758	45	0
23	6	912	0	845	37	0
23	7	760	0	643	26	0
23	8	727	0	635	16	0
23	9	324	0	36	12	0
23	A	2625	0	2614	129	0
23	B	2270	0	2210	101	0
23	F	140	0	113	8	0
23	G	87	0	64	6	0
23	J	42	0	31	2	0
23	K	201	0	171	2	0
23	L	135	0	99	5	0
23	a	709	0	597	0	0
24	A	33	0	46	5	0
24	B	33	0	46	6	0
25	1	49	0	74	6	0
25	2	37	0	44	1	0
25	3	94	0	137	3	0
25	4	49	0	74	6	0
25	5	98	0	148	7	0
25	6	48	0	69	3	0
25	7	37	0	44	2	0
25	8	96	0	141	4	0
25	9	49	0	74	5	0
25	A	79	0	104	4	0
25	B	38	0	46	2	0
25	a	49	0	74	0	0
26	1	40	0	56	2	0
26	3	120	0	168	11	0
26	4	40	0	56	2	0
26	5	40	0	56	4	0
26	6	40	0	56	4	0
26	7	80	0	112	3	0
26	8	40	0	56	4	0
26	A	240	0	336	28	0
26	B	280	0	392	15	0
26	F	40	0	56	4	0
26	G	40	0	56	6	0
26	J	40	0	56	5	0
26	K	80	0	112	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
26	L	80	0	112	5	0
26	a	40	0	56	0	0
27	A	8	0	0	0	0
27	C	16	0	0	0	0
28	5	33	0	39	3	0
28	8	70	0	92	3	0
28	A	103	0	134	3	0
28	K	35	0	46	0	0
29	4	80	0	100	1	0
29	5	80	0	100	4	0
29	7	44	0	61	1	0
29	A	40	0	50	2	0
29	J	40	0	50	1	0
30	B	62	0	84	5	0
30	J	58	0	77	1	0
31	1	42	0	56	3	0
31	2	42	0	56	3	0
31	3	42	0	56	1	0
31	4	42	0	56	5	0
31	5	42	0	56	6	0
31	6	42	0	56	4	0
31	7	42	0	56	5	0
31	8	42	0	56	6	0
31	9	42	0	56	1	0
31	a	42	0	56	0	0
32	1	44	0	56	4	0
32	2	44	0	56	3	0
32	3	44	0	56	2	0
32	4	44	0	56	3	0
32	5	44	0	56	10	0
32	6	44	0	56	1	0
32	7	44	0	56	1	0
32	8	44	0	56	1	0
32	9	44	0	56	3	0
32	a	44	0	56	0	0
33	5	44	0	56	3	0
33	6	44	0	56	4	0
All	All	49685	0	48724	855	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 9.

The worst 5 of 855 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:9:182:GLN:CB	21:9:183:PRO:HD2	1.85	1.05
1:A:11:LYS:N	14:3:52:SER:HG	1.56	1.04
12:L:223:LEU:HD12	12:L:223:LEU:O	1.78	0.82
23:9:611:CLA:NB	25:9:622:LHG:O4	2.20	0.75
23:A:830:CLA:H2	26:A:849:BCR:HC7	1.68	0.74

There are no symmetry-related clashes.

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%)	708 (96%)	31 (4%)	0	100	100
2	B	729/735 (99%)	694 (95%)	35 (5%)	0	100	100
3	C	78/81 (96%)	73 (94%)	5 (6%)	0	100	100
4	D	142/247 (58%)	131 (92%)	11 (8%)	0	100	100
5	E	62/143 (43%)	56 (90%)	6 (10%)	0	100	100
6	F	162/227 (71%)	149 (92%)	13 (8%)	0	100	100
7	G	66/159 (42%)	59 (89%)	7 (11%)	0	100	100
8	H	49/155 (32%)	41 (84%)	8 (16%)	0	100	100
9	I	30/106 (28%)	28 (93%)	2 (7%)	0	100	100
10	J	39/41 (95%)	36 (92%)	3 (8%)	0	100	100
11	K	83/160 (52%)	74 (89%)	9 (11%)	0	100	100
12	L	102/258 (40%)	94 (92%)	8 (8%)	0	100	100
13	1	191/248 (77%)	177 (93%)	14 (7%)	0	100	100
13	a	192/248 (77%)	177 (92%)	15 (8%)	0	100	100
14	3	219/298 (74%)	199 (91%)	20 (9%)	0	100	100
15	4	208/290 (72%)	195 (94%)	13 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
16	5	224/274 (82%)	198 (88%)	26 (12%)	0	100	100
17	6	228/318 (72%)	209 (92%)	19 (8%)	0	100	100
18	7	211/241 (88%)	192 (91%)	19 (9%)	0	100	100
19	8	213/272 (78%)	198 (93%)	15 (7%)	0	100	100
20	2	171/227 (75%)	145 (85%)	26 (15%)	0	100	100
21	9	168/213 (79%)	143 (85%)	23 (14%)	2 (1%)	13	42
22	X	24/26 (92%)	23 (96%)	1 (4%)	0	100	100
All	All	4330/5718 (76%)	3999 (92%)	329 (8%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
21	9	184	ILE
21	9	183	PRO

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	601/610 (98%)	600 (100%)	1 (0%)	93	97
2	B	595/597 (100%)	588 (99%)	7 (1%)	71	83
3	C	69/70 (99%)	69 (100%)	0	100	100
4	D	120/197 (61%)	119 (99%)	1 (1%)	81	89
5	E	55/123 (45%)	54 (98%)	1 (2%)	59	78
6	F	126/169 (75%)	125 (99%)	1 (1%)	81	89
7	G	50/121 (41%)	50 (100%)	0	100	100
8	H	36/126 (29%)	35 (97%)	1 (3%)	43	70
9	I	26/76 (34%)	26 (100%)	0	100	100
10	J	37/37 (100%)	37 (100%)	0	100	100
11	K	59/123 (48%)	58 (98%)	1 (2%)	60	78

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
12	L	75/198 (38%)	74 (99%)	1 (1%)	69	82
13	1	136/180 (76%)	136 (100%)	0	100	100
13	a	137/180 (76%)	137 (100%)	0	100	100
14	3	167/230 (73%)	165 (99%)	2 (1%)	71	83
15	4	165/226 (73%)	164 (99%)	1 (1%)	86	91
16	5	183/219 (84%)	181 (99%)	2 (1%)	73	85
17	6	184/260 (71%)	184 (100%)	0	100	100
18	7	164/181 (91%)	161 (98%)	3 (2%)	59	78
19	8	161/207 (78%)	159 (99%)	2 (1%)	71	83
20	2	134/183 (73%)	132 (98%)	2 (2%)	65	81
21	9	127/159 (80%)	124 (98%)	3 (2%)	49	73
All	All	3407/4472 (76%)	3378 (99%)	29 (1%)	79	87

5 of 29 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
14	3	218	ILE
21	9	149	MET
16	5	75	LEU
20	2	9	ARG
15	4	203	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 25 such sidechains are listed below:

Mol	Chain	Res	Type
6	F	132	HIS
14	3	164	GLN
21	9	49	ASN
10	J	30	ASN
15	4	284	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

333 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
23	CLA	3	606	-	53,62,73	1.62	9 (16%)	61,100,113	1.45	7 (11%)
23	CLA	3	609	14	60,68,73	1.53	7 (11%)	70,107,113	1.55	9 (12%)
23	CLA	A	854	-	65,73,73	1.42	9 (13%)	76,113,113	1.56	13 (17%)
23	CLA	B	806	2	65,73,73	1.47	11 (16%)	76,113,113	1.39	6 (7%)
23	CLA	A	832	-	50,58,73	1.65	11 (22%)	58,95,113	1.66	9 (15%)
23	CLA	B	834	-	60,68,73	1.51	8 (13%)	70,107,113	1.47	8 (11%)
29	LMG	7	624	-	44,44,55	0.83	1 (2%)	52,52,63	1.26	6 (11%)
23	CLA	A	816	-	43,52,73	1.76	7 (16%)	48,87,113	1.82	6 (12%)
23	CLA	5	617	-	50,58,73	1.67	10 (20%)	58,95,113	1.58	8 (13%)
23	CLA	5	603	-	54,62,73	1.70	10 (18%)	67,100,113	1.59	10 (14%)
23	CLA	8	606	-	64,72,73	1.45	9 (14%)	75,112,113	1.48	8 (10%)
23	CLA	A	841	-	65,73,73	1.42	10 (15%)	76,113,113	1.57	9 (11%)
32	XAT	1	618	-	39,47,47	0.93	2 (5%)	54,74,74	2.58	18 (33%)
32	XAT	7	620	-	39,47,47	1.04	2 (5%)	54,74,74	2.59	18 (33%)
32	XAT	8	620	-	39,47,47	1.00	2 (5%)	54,74,74	2.70	19 (35%)
23	CLA	B	820	-	50,58,73	1.62	7 (14%)	58,95,113	1.62	7 (12%)
24	PQN	B	842	-	34,34,34	2.91	11 (32%)	42,45,45	2.04	5 (11%)
23	CLA	9	606	21	29,35,73	2.74	8 (27%)	28,60,113	1.68	4 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	CLA	9	609	21	29,35,73	2.62	8 (27%)	28,60,113	1.76	4 (14%)
23	CLA	B	821	-	43,51,73	1.86	9 (20%)	48,86,113	1.78	9 (18%)
23	CLA	A	827	-	59,67,73	1.51	8 (13%)	68,105,113	1.59	10 (14%)
23	CLA	A	807	1	65,73,73	1.49	10 (15%)	76,113,113	1.42	9 (11%)
28	LMU	5	628	-	34,34,36	1.24	3 (8%)	45,45,47	1.50	8 (17%)
26	BCR	3	621	-	41,41,41	0.72	0	56,56,56	2.28	19 (33%)
23	CLA	6	610	17	65,73,73	1.40	7 (10%)	76,113,113	1.45	9 (11%)
29	LMG	5	626	-	40,40,55	0.94	1 (2%)	48,48,63	1.33	5 (10%)
23	CLA	B	808	-	65,73,73	1.46	10 (15%)	76,113,113	1.66	11 (14%)
26	BCR	B	845	-	41,41,41	0.84	0	56,56,56	2.06	19 (33%)
23	CLA	1	611	25	65,73,73	1.40	9 (13%)	76,113,113	1.45	8 (10%)
31	LUT	1	617	-	42,43,43	0.79	0	51,60,60	1.56	12 (23%)
23	CLA	B	816	-	54,62,73	1.55	7 (12%)	62,99,113	1.65	6 (9%)
29	LMG	4	624	-	40,40,55	1.01	4 (10%)	48,48,63	1.29	6 (12%)
23	CLA	9	610	21	29,35,73	2.63	10 (34%)	28,60,113	1.70	5 (17%)
23	CLA	a	601	13	53,62,73	1.60	9 (16%)	61,100,113	1.48	7 (11%)
23	CLA	1	612	13	45,53,73	1.73	8 (17%)	52,89,113	1.69	9 (17%)
26	BCR	8	621	-	41,41,41	0.74	0	56,56,56	1.98	18 (32%)
23	CLA	B	841	25	43,51,73	1.83	7 (16%)	49,86,113	1.72	7 (14%)
23	CLA	J	101	10	42,50,73	1.80	7 (16%)	48,85,113	1.71	8 (16%)
23	CLA	4	610	15	61,69,73	1.47	9 (14%)	71,108,113	1.44	7 (9%)
31	LUT	5	620	-	42,43,43	0.80	0	51,60,60	1.70	13 (25%)
23	CLA	3	608	-	55,63,73	1.62	10 (18%)	64,101,113	1.62	9 (14%)
23	CLA	7	602	18	65,73,73	1.48	9 (13%)	76,113,113	1.40	7 (9%)
23	CLA	8	610	19	60,68,73	1.41	8 (13%)	70,107,113	1.53	8 (11%)
23	CLA	B	802	-	65,73,73	1.47	10 (15%)	76,113,113	1.34	7 (9%)
23	CLA	B	827	-	62,70,73	1.48	8 (12%)	72,109,113	1.51	8 (11%)
23	CLA	6	614	-	60,68,73	1.50	7 (11%)	70,107,113	1.47	6 (8%)
23	CLA	A	829	-	65,73,73	1.42	10 (15%)	76,113,113	1.55	9 (11%)
23	CLA	A	803	-	65,73,73	1.52	10 (15%)	76,113,113	1.54	6 (7%)
23	CLA	5	614	-	45,52,73	1.86	8 (17%)	48,87,113	1.65	7 (14%)
27	SF4	C	101	-	0,12,12	-	-	-	-	-
23	CLA	4	613	15	65,73,73	1.45	10 (15%)	76,113,113	1.45	7 (9%)
23	CLA	A	839	-	55,63,73	1.61	9 (16%)	64,101,113	1.50	7 (10%)
23	CLA	1	604	-	49,57,73	1.68	7 (14%)	55,93,113	1.67	6 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	CLA	7	614	-	42,50,73	1.71	10 (23%)	48,85,113	1.65	8 (16%)
23	CLA	G	204	7	45,53,73	1.83	5 (11%)	52,89,113	1.78	12 (23%)
23	CLA	7	610	18	65,73,73	1.44	10 (15%)	76,113,113	1.43	8 (10%)
23	CLA	7	603	-	43,52,73	1.79	9 (20%)	49,88,113	1.66	8 (16%)
31	LUT	6	619	-	42,43,43	0.81	0	51,60,60	1.69	13 (25%)
23	CLA	A	823	-	42,50,73	1.77	9 (21%)	48,85,113	1.84	9 (18%)
26	BCR	6	622	-	41,41,41	0.69	0	56,56,56	1.94	17 (30%)
23	CLA	7	615	-	41,50,73	1.90	7 (17%)	50,85,113	1.76	9 (18%)
23	CLA	B	840	-	65,73,73	1.48	10 (15%)	76,113,113	1.46	7 (9%)
23	CLA	B	835	-	45,53,73	1.79	8 (17%)	52,89,113	1.74	11 (21%)
23	CLA	K	201	11	45,53,73	1.77	7 (15%)	52,89,113	1.79	10 (19%)
23	CLA	2	613	20	29,35,73	2.70	9 (31%)	28,60,113	1.66	5 (17%)
23	CLA	A	838	-	50,58,73	1.56	8 (16%)	58,95,113	1.77	12 (20%)
25	LHG	1	620	23	48,48,48	0.60	1 (2%)	51,54,54	1.26	6 (11%)
23	CLA	1	616	13	43,51,73	1.85	9 (20%)	54,87,113	1.61	8 (14%)
28	LMU	K	208	-	36,36,36	1.19	3 (8%)	47,47,47	1.30	5 (10%)
23	CLA	7	606	-	41,49,73	1.81	10 (24%)	47,84,113	1.74	9 (19%)
23	CLA	A	808	-	50,58,73	1.63	10 (20%)	58,95,113	1.65	9 (15%)
23	CLA	5	612	16	40,49,73	1.77	8 (20%)	45,84,113	1.81	8 (17%)
23	CLA	B	809	2	65,73,73	1.43	11 (16%)	76,113,113	1.55	7 (9%)
23	CLA	A	840	-	52,60,73	1.62	10 (19%)	60,97,113	1.69	10 (16%)
23	CLA	A	831	-	65,73,73	1.56	11 (16%)	76,113,113	1.70	12 (15%)
26	BCR	G	205	-	41,41,41	0.75	0	56,56,56	2.06	21 (37%)
23	CLA	A	828	-	65,73,73	1.43	10 (15%)	76,113,113	1.44	8 (10%)
23	CLA	5	608	-	50,58,73	1.66	11 (22%)	58,95,113	1.54	7 (12%)
31	LUT	8	619	-	42,43,43	0.87	1 (2%)	51,60,60	1.82	14 (27%)
26	BCR	A	849	-	41,41,41	0.89	1 (2%)	56,56,56	2.03	17 (30%)
32	XAT	4	620	-	39,47,47	0.91	1 (2%)	54,74,74	2.59	20 (37%)
32	XAT	9	620	-	39,47,47	0.92	0	54,74,74	2.63	16 (29%)
23	CLA	B	823	-	45,53,73	1.73	7 (15%)	52,89,113	1.76	8 (15%)
23	CLA	5	609	16	65,73,73	1.47	10 (15%)	76,113,113	1.38	10 (13%)
23	CLA	B	813	-	65,73,73	1.43	9 (13%)	76,113,113	1.46	10 (13%)
23	CLA	A	843	-	64,72,73	1.50	11 (17%)	74,111,113	1.46	7 (9%)
25	LHG	9	622	23	48,48,48	0.62	0	51,54,54	1.23	6 (11%)
23	CLA	6	616	17	65,73,73	1.42	7 (10%)	76,113,113	1.68	13 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
31	LUT	4	619	-	42,43,43	0.82	0	51,60,60	1.70	11 (21%)
32	XAT	3	619	-	39,47,47	1.02	2 (5%)	54,74,74	2.60	22 (40%)
30	DGD	B	850	-	63,63,67	1.06	5 (7%)	77,77,81	1.55	10 (12%)
23	CLA	4	606	-	39,48,73	1.84	8 (20%)	44,83,113	1.70	8 (18%)
23	CLA	9	601	21	29,35,73	2.64	9 (31%)	28,60,113	1.68	4 (14%)
23	CLA	A	837	1	45,53,73	1.76	9 (20%)	52,89,113	1.65	7 (13%)
23	CLA	A	821	-	53,61,73	1.57	10 (18%)	61,98,113	1.61	7 (11%)
26	BCR	4	621	-	41,41,41	0.73	0	56,56,56	2.10	22 (39%)
25	LHG	A	847	23	29,29,48	0.95	1 (3%)	32,35,54	1.37	3 (9%)
32	XAT	2	620	-	39,47,47	0.89	0	54,74,74	2.65	14 (25%)
23	CLA	A	824	-	41,49,73	1.75	8 (19%)	47,84,113	1.77	9 (19%)
23	CLA	B	815	-	43,51,73	1.70	10 (23%)	49,86,113	1.74	7 (14%)
29	LMG	5	627	-	40,40,55	0.91	2 (5%)	48,48,63	1.20	4 (8%)
25	LHG	6	623	23	47,47,48	0.64	1 (2%)	50,53,54	1.24	5 (10%)
23	CLA	8	601	19	65,73,73	1.44	9 (13%)	76,113,113	1.52	10 (13%)
23	CLA	1	607	-	39,48,73	1.85	7 (17%)	44,83,113	1.72	7 (15%)
29	LMG	J	104	-	40,40,55	0.89	2 (5%)	48,48,63	1.26	5 (10%)
23	CLA	2	606	20	29,35,73	2.72	8 (27%)	28,60,113	1.61	3 (10%)
23	CLA	4	616	15	43,51,73	1.84	9 (20%)	54,87,113	1.66	9 (16%)
23	CLA	4	614	-	56,64,73	1.59	8 (14%)	65,102,113	1.46	9 (13%)
29	LMG	4	623	-	40,40,55	0.90	1 (2%)	48,48,63	1.28	5 (10%)
23	CLA	a	613	-	65,73,73	1.46	9 (13%)	76,113,113	1.52	9 (11%)
23	CLA	A	833	-	45,53,73	1.72	9 (20%)	52,89,113	1.73	6 (11%)
23	CLA	5	619	-	43,51,73	1.81	10 (23%)	54,87,113	2.04	12 (22%)
23	CLA	a	607	-	45,53,73	1.74	7 (15%)	52,89,113	1.64	7 (13%)
23	CLA	4	618	15	39,48,73	1.93	9 (23%)	48,83,113	1.67	10 (20%)
23	CLA	A	845	25	50,58,73	1.63	10 (20%)	58,95,113	1.67	7 (12%)
23	CLA	B	837	-	65,73,73	1.48	10 (15%)	76,113,113	1.46	7 (9%)
31	LUT	2	619	-	42,43,43	0.75	0	51,60,60	1.77	13 (25%)
23	CLA	B	824	-	65,73,73	1.46	7 (10%)	76,113,113	1.61	11 (14%)
23	CLA	A	836	-	65,73,73	1.44	10 (15%)	76,113,113	1.53	7 (9%)
23	CLA	6	618	17	39,48,73	1.89	9 (23%)	48,83,113	1.75	10 (20%)
23	CLA	3	607	14	56,64,73	1.58	9 (16%)	69,102,113	1.54	11 (15%)
26	BCR	3	622	-	41,41,41	0.79	0	56,56,56	2.67	21 (37%)
23	CLA	B	811	-	52,61,73	1.67	9 (17%)	64,99,113	1.56	10 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	CLA	5	606	-	39,48,73	1.88	10 (25%)	44,83,113	1.60	7 (15%)
31	LUT	7	619	-	42,43,43	0.95	2 (4%)	51,60,60	1.79	16 (31%)
31	LUT	9	619	-	42,43,43	0.76	0	51,60,60	1.67	11 (21%)
23	CLA	4	608	-	65,73,73	1.42	7 (10%)	76,113,113	1.56	8 (10%)
23	CLA	1	609	13	40,48,73	1.83	7 (17%)	50,83,113	1.84	12 (24%)
23	CLA	L	303	-	45,53,73	1.71	8 (17%)	52,89,113	1.67	6 (11%)
23	CLA	7	601	18	60,68,73	1.53	11 (18%)	70,107,113	1.51	9 (12%)
25	LHG	8	622	23	48,48,48	0.63	1 (2%)	51,54,54	1.27	6 (11%)
23	CLA	9	613	21	29,35,73	2.70	8 (27%)	28,60,113	1.72	4 (14%)
23	CLA	6	608	-	51,59,73	1.67	11 (21%)	59,96,113	1.65	9 (15%)
23	CLA	3	615	-	39,48,73	1.81	8 (20%)	44,83,113	1.72	7 (15%)
23	CLA	B	818	-	60,68,73	1.49	10 (16%)	70,107,113	1.59	10 (14%)
23	CLA	a	616	13	45,53,73	1.76	9 (20%)	52,89,113	1.56	6 (11%)
23	CLA	9	607	-	29,35,73	2.60	9 (31%)	28,60,113	1.79	6 (21%)
26	BCR	A	856	-	41,41,41	0.70	0	56,56,56	1.99	19 (33%)
23	CLA	B	828	-	65,73,73	1.48	10 (15%)	76,113,113	1.48	9 (11%)
28	LMU	8	624	-	36,36,36	1.19	2 (5%)	47,47,47	0.93	1 (2%)
23	CLA	2	610	20	29,35,73	2.61	8 (27%)	28,60,113	1.79	5 (17%)
23	CLA	2	602	20	29,35,73	2.65	9 (31%)	28,60,113	1.69	3 (10%)
26	BCR	B	843	-	41,41,41	0.79	0	56,56,56	1.92	14 (25%)
23	CLA	A	805	-	52,60,73	1.66	10 (19%)	60,97,113	1.66	7 (11%)
23	CLA	8	607	-	41,49,73	1.83	9 (21%)	51,84,113	1.75	9 (17%)
23	CLA	6	620	-	64,72,73	1.43	10 (15%)	74,111,113	1.49	7 (9%)
23	CLA	B	819	-	55,63,73	1.63	9 (16%)	64,101,113	1.51	6 (9%)
23	CLA	a	612	13	45,53,73	1.73	8 (17%)	52,89,113	1.69	9 (17%)
23	CLA	1	614	-	37,45,73	2.12	10 (27%)	44,79,113	1.80	8 (18%)
23	CLA	A	835	-	61,69,73	1.51	10 (16%)	71,108,113	1.57	8 (11%)
23	CLA	A	817	-	45,53,73	1.73	9 (20%)	52,89,113	1.75	9 (17%)
23	CLA	9	602	21	29,35,73	2.64	9 (31%)	28,60,113	1.76	4 (14%)
25	LHG	B	851	23	37,37,48	0.63	0	40,43,54	1.22	4 (10%)
24	PQN	A	844	-	34,34,34	2.89	11 (32%)	42,45,45	2.11	5 (11%)
23	CLA	B	832	-	60,68,73	1.48	10 (16%)	70,107,113	1.57	10 (14%)
23	CLA	4	601	15	65,73,73	1.44	8 (12%)	76,113,113	1.49	8 (10%)
25	LHG	A	846	-	48,48,48	0.72	1 (2%)	51,54,54	1.32	6 (11%)
26	BCR	B	801	-	41,41,41	0.77	0	56,56,56	2.05	13 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	CLA	1	601	13	53,62,73	1.60	10 (18%)	61,100,113	1.47	7 (11%)
23	CLA	6	606	-	39,48,73	1.84	8 (20%)	44,83,113	1.72	7 (15%)
23	CLA	B	805	-	65,73,73	1.42	8 (12%)	76,113,113	1.66	9 (11%)
23	CLA	A	825	-	65,73,73	1.45	10 (15%)	76,113,113	1.47	11 (14%)
23	CLA	3	611	25	37,46,73	1.94	8 (21%)	46,81,113	1.82	10 (21%)
23	CLA	5	610	16	54,62,73	1.59	10 (18%)	62,99,113	1.57	9 (14%)
23	CLA	3	612	14	43,51,73	1.83	9 (20%)	49,86,113	1.65	8 (16%)
23	CLA	A	815	-	50,58,73	1.64	9 (18%)	58,95,113	1.69	11 (18%)
26	BCR	B	846	-	41,41,41	0.88	2 (4%)	56,56,56	2.17	25 (44%)
23	CLA	a	604	-	49,57,73	1.67	7 (14%)	55,93,113	1.67	6 (10%)
23	CLA	3	610	14	65,73,73	1.41	9 (13%)	76,113,113	1.57	10 (13%)
23	CLA	3	603	-	55,63,73	1.60	12 (21%)	64,101,113	1.71	10 (15%)
23	CLA	7	609	18	43,52,73	1.71	7 (16%)	48,87,113	1.87	6 (12%)
23	CLA	6	611	25	42,50,73	1.72	8 (19%)	48,85,113	1.62	7 (14%)
26	BCR	B	844	-	41,41,41	0.79	1 (2%)	56,56,56	1.95	15 (26%)
23	CLA	1	608	-	43,52,73	1.77	5 (11%)	49,88,113	1.67	7 (14%)
23	CLA	8	608	-	51,59,73	1.60	10 (19%)	59,96,113	1.62	7 (11%)
23	CLA	A	813	-	54,62,73	1.55	9 (16%)	62,99,113	1.64	7 (11%)
23	CLA	7	607	-	42,50,73	1.78	8 (19%)	48,85,113	1.86	9 (18%)
27	SF4	C	102	-	0,12,12	-	-	-	-	-
23	CLA	a	603	-	42,50,73	1.77	9 (21%)	48,85,113	1.86	9 (18%)
23	CLA	8	616	19	43,51,73	1.89	7 (16%)	54,87,113	1.85	12 (22%)
26	BCR	J	102	-	41,41,41	0.84	1 (2%)	56,56,56	2.15	16 (28%)
23	CLA	6	602	17	65,73,73	1.43	9 (13%)	76,113,113	1.46	6 (7%)
25	LHG	3	624	23	48,48,48	0.66	0	51,54,54	1.24	5 (9%)
23	CLA	K	206	11	45,53,73	1.73	7 (15%)	52,89,113	1.66	7 (13%)
23	CLA	7	613	18	65,73,73	1.46	9 (13%)	76,113,113	1.42	8 (10%)
23	CLA	2	601	20	29,35,73	2.72	9 (31%)	28,60,113	1.75	6 (21%)
23	CLA	A	804	-	65,73,73	1.40	9 (13%)	76,113,113	1.62	11 (14%)
23	CLA	B	838	-	47,55,73	1.63	10 (21%)	54,91,113	1.80	8 (14%)
23	CLA	A	826	-	64,72,73	1.43	8 (12%)	74,111,113	1.58	10 (13%)
23	CLA	6	607	-	41,49,73	1.84	9 (21%)	51,84,113	1.78	12 (23%)
23	CLA	2	611	25	30,33,73	3.40	10 (33%)	24,56,113	1.05	2 (8%)
23	CLA	8	611	25	42,50,73	1.72	9 (21%)	48,85,113	1.69	9 (18%)
26	BCR	B	847	-	41,41,41	0.89	1 (2%)	56,56,56	2.01	19 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	CLA	3	613	14	52,61,73	1.61	9 (17%)	59,98,113	1.55	7 (11%)
23	CLA	B	825	-	62,70,73	1.42	10 (16%)	72,109,113	1.46	11 (15%)
26	BCR	A	848	-	41,41,41	0.92	1 (2%)	56,56,56	2.07	17 (30%)
28	LMU	A	858	-	34,35,36	1.29	2 (5%)	42,45,47	1.28	6 (14%)
23	CLA	a	614	-	55,62,73	1.72	9 (16%)	60,99,113	1.47	7 (11%)
23	CLA	3	602	14	60,68,73	1.47	10 (16%)	70,107,113	1.48	8 (11%)
23	CLA	a	611	25	37,46,73	1.88	9 (24%)	46,81,113	1.87	10 (21%)
23	CLA	A	811	-	65,73,73	1.43	10 (15%)	76,113,113	1.52	10 (13%)
26	BCR	A	850	-	41,41,41	0.82	1 (2%)	56,56,56	2.02	18 (32%)
23	CLA	4	607	-	45,53,73	1.77	9 (20%)	52,89,113	1.60	6 (11%)
26	BCR	K	207	-	41,41,41	0.75	0	56,56,56	1.86	16 (28%)
23	CLA	4	611	25	42,50,73	1.76	7 (16%)	48,85,113	1.64	7 (14%)
23	CLA	B	803	-	65,73,73	1.43	9 (13%)	76,113,113	1.80	13 (17%)
23	CLA	A	814	-	65,73,73	1.44	10 (15%)	76,113,113	1.56	12 (15%)
23	CLA	4	604	-	54,62,73	1.63	9 (16%)	67,100,113	1.46	7 (10%)
23	CLA	7	608	-	50,58,73	1.63	10 (20%)	58,95,113	1.53	7 (12%)
23	CLA	9	603	21	29,35,73	2.66	9 (31%)	28,60,113	1.63	4 (14%)
23	CLA	3	604	-	65,73,73	1.47	10 (15%)	76,113,113	1.44	7 (9%)
26	BCR	A	851	-	41,41,41	0.88	2 (4%)	56,56,56	1.97	16 (28%)
23	CLA	B	804	-	41,49,73	1.81	10 (24%)	47,84,113	1.85	8 (17%)
25	LHG	2	622	23	36,36,48	0.78	1 (2%)	39,42,54	1.29	5 (12%)
23	CLA	B	826	-	55,63,73	1.58	8 (14%)	64,101,113	1.56	8 (12%)
29	LMG	A	860	-	40,40,55	0.95	3 (7%)	48,48,63	1.32	5 (10%)
23	CLA	A	834	-	65,73,73	1.45	10 (15%)	76,113,113	1.47	7 (9%)
23	CLA	7	616	18	43,51,73	1.80	9 (20%)	54,87,113	1.70	10 (18%)
26	BCR	B	848	-	41,41,41	0.87	0	56,56,56	1.79	12 (21%)
23	CLA	3	614	-	39,48,73	1.85	9 (23%)	44,83,113	1.66	8 (18%)
23	CLA	8	604	-	50,58,73	1.64	7 (14%)	58,95,113	1.63	8 (13%)
25	LHG	5	625	-	48,48,48	0.62	1 (2%)	51,54,54	1.24	6 (11%)
23	CLA	F	304	-	41,49,73	1.78	7 (17%)	47,84,113	1.78	7 (14%)
23	CLA	4	609	15	61,69,73	1.57	7 (11%)	71,108,113	1.49	7 (9%)
26	BCR	K	202	-	41,41,41	0.79	0	56,56,56	2.26	20 (35%)
33	NEX	6	624	-	38,46,46	1.01	2 (5%)	50,70,70	2.27	17 (34%)
23	CLA	2	612	20	29,35,73	2.72	8 (27%)	28,60,113	1.68	3 (10%)
23	CLA	8	612	19	40,49,73	1.78	8 (20%)	45,84,113	1.82	8 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	LHG	5	623	23	48,48,48	0.62	1 (2%)	51,54,54	1.21	5 (9%)
23	CLA	a	610	13	59,67,73	1.57	9 (15%)	69,106,113	1.42	7 (10%)
23	CLA	A	806	-	65,73,73	1.47	13 (20%)	76,113,113	1.69	12 (15%)
23	CLA	A	809	1	65,73,73	1.43	10 (15%)	76,113,113	1.50	8 (10%)
23	CLA	B	833	-	65,73,73	1.46	10 (15%)	76,113,113	1.54	10 (13%)
23	CLA	2	604	-	29,35,73	2.68	8 (27%)	28,60,113	1.80	6 (21%)
25	LHG	3	623	-	44,44,48	0.66	2 (4%)	47,50,54	1.26	6 (12%)
23	CLA	6	601	17	65,73,73	1.42	9 (13%)	76,113,113	1.52	9 (11%)
23	CLA	A	822	-	65,73,73	1.45	10 (15%)	76,113,113	1.49	8 (10%)
23	CLA	B	812	-	43,51,73	1.78	7 (16%)	49,86,113	1.72	7 (14%)
23	CLA	B	810	-	64,72,73	1.44	10 (15%)	74,111,113	1.41	8 (10%)
23	CLA	1	603	-	52,61,73	1.63	9 (17%)	59,98,113	1.68	9 (15%)
26	BCR	1	619	-	41,41,41	0.68	0	56,56,56	2.01	16 (28%)
23	CLA	8	614	-	56,64,73	1.54	9 (16%)	65,102,113	1.53	10 (15%)
32	XAT	a	618	-	39,47,47	0.94	2 (5%)	54,74,74	2.57	18 (33%)
23	CLA	A	820	-	65,73,73	1.52	11 (16%)	76,113,113	1.68	15 (19%)
23	CLA	A	842	-	65,73,73	1.45	10 (15%)	76,113,113	1.43	7 (9%)
23	CLA	A	810	1	50,58,73	1.63	10 (20%)	58,95,113	1.58	7 (12%)
23	CLA	7	611	25	59,67,73	1.47	9 (15%)	68,105,113	1.56	8 (11%)
23	CLA	9	614	-	29,35,73	2.65	9 (31%)	28,60,113	1.76	5 (17%)
23	CLA	9	611	25	29,35,73	2.73	9 (31%)	28,60,113	1.75	6 (21%)
23	CLA	7	604	-	54,62,73	1.56	8 (14%)	63,100,113	1.66	10 (15%)
23	CLA	B	817	-	59,67,73	1.54	10 (16%)	68,105,113	1.57	9 (13%)
23	CLA	A	818	-	60,68,73	1.45	8 (13%)	70,107,113	1.60	7 (10%)
23	CLA	7	612	18	44,52,73	1.83	9 (20%)	51,88,113	1.63	9 (17%)
26	BCR	F	305	-	41,41,41	0.83	1 (2%)	56,56,56	2.26	23 (41%)
23	CLA	1	606	13	37,47,73	1.90	6 (16%)	41,80,113	1.77	7 (17%)
26	BCR	a	619	-	41,41,41	0.69	0	56,56,56	2.01	16 (28%)
23	CLA	B	822	-	42,50,73	1.81	7 (16%)	48,85,113	1.66	7 (14%)
23	CLA	6	603	-	54,62,73	1.67	9 (16%)	67,100,113	1.54	8 (11%)
23	CLA	8	613	19	65,73,73	1.48	9 (13%)	76,113,113	1.64	10 (13%)
28	LMU	8	625	-	36,36,36	1.16	2 (5%)	47,47,47	1.41	7 (14%)
23	CLA	K	203	-	65,73,73	1.47	8 (12%)	76,113,113	1.43	7 (9%)
23	CLA	A	819	-	59,67,73	1.57	10 (16%)	68,105,113	1.52	8 (11%)
25	LHG	4	622	23	48,48,48	0.60	0	51,54,54	1.29	6 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
26	BCR	L	305	-	41,41,41	0.80	0	56,56,56	1.88	14 (25%)
26	BCR	A	852	-	41,41,41	0.73	0	56,56,56	1.90	12 (21%)
23	CLA	B	829	-	65,73,73	1.55	10 (15%)	76,113,113	1.69	10 (13%)
23	CLA	3	617	14	39,48,73	1.86	9 (23%)	44,83,113	1.78	8 (18%)
33	NEX	5	624	-	38,46,46	0.93	0	50,70,70	2.49	19 (38%)
23	CLA	1	610	13	38,47,73	1.90	9 (23%)	44,81,113	1.76	8 (18%)
23	CLA	5	613	16	64,72,73	1.56	9 (14%)	74,111,113	1.54	7 (9%)
23	CLA	1	613	-	65,73,73	1.46	9 (13%)	76,113,113	1.52	9 (11%)
31	LUT	3	618	-	42,43,43	0.88	0	51,60,60	1.73	13 (25%)
23	CLA	2	616	-	29,35,73	2.65	9 (31%)	28,60,113	1.78	6 (21%)
23	CLA	a	602	13	61,69,73	1.47	8 (13%)	71,108,113	1.51	7 (9%)
23	CLA	9	604	-	29,35,73	2.63	9 (31%)	28,60,113	1.73	5 (17%)
23	CLA	G	203	-	42,50,73	1.82	6 (14%)	48,85,113	1.74	7 (14%)
23	CLA	L	302	12	45,53,73	1.79	5 (11%)	52,89,113	1.67	8 (15%)
32	XAT	5	621	-	39,47,47	1.02	2 (5%)	54,74,74	2.89	23 (42%)
23	CLA	B	814	-	64,72,73	1.43	9 (14%)	74,111,113	1.52	8 (10%)
25	LHG	7	622	23	36,36,48	0.70	0	39,42,54	1.23	4 (10%)
23	CLA	F	303	-	42,50,73	1.83	8 (19%)	48,85,113	1.71	10 (20%)
26	BCR	7	621	-	41,41,41	0.80	0	56,56,56	2.04	18 (32%)
23	CLA	A	802	-	65,73,73	1.48	10 (15%)	76,113,113	1.71	10 (13%)
23	CLA	B	807	-	52,60,73	1.61	10 (19%)	60,97,113	1.53	7 (11%)
23	CLA	5	604	-	63,71,73	1.54	9 (14%)	78,111,113	1.45	9 (11%)
23	CLA	2	607	-	29,35,73	2.63	9 (31%)	28,60,113	1.72	4 (14%)
28	LMU	A	859	-	35,35,36	1.33	3 (8%)	43,45,47	1.27	6 (13%)
26	BCR	L	301	-	41,41,41	0.84	0	56,56,56	1.78	16 (28%)
23	CLA	5	602	16	65,73,73	1.44	7 (10%)	76,113,113	1.57	8 (10%)
23	CLA	B	831	-	65,73,73	1.38	7 (10%)	76,113,113	1.61	6 (7%)
32	XAT	6	621	-	39,47,47	0.93	2 (5%)	54,74,74	2.61	20 (37%)
23	CLA	1	602	13	61,69,73	1.46	8 (13%)	71,108,113	1.51	7 (9%)
23	CLA	A	830	-	65,73,73	1.46	11 (16%)	76,113,113	1.59	11 (14%)
23	CLA	6	609	17	45,53,73	1.78	9 (20%)	52,89,113	1.69	8 (15%)
23	CLA	5	616	16	41,50,73	1.89	9 (21%)	50,85,113	1.61	9 (18%)
23	CLA	B	836	-	50,58,73	1.61	8 (16%)	58,95,113	1.73	11 (18%)
23	CLA	6	604	-	65,73,73	1.42	10 (15%)	76,113,113	1.42	8 (10%)
23	CLA	a	606	13	43,52,73	1.78	7 (16%)	48,87,113	1.60	6 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	LHG	8	623	-	46,46,48	0.66	1 (2%)	49,52,54	1.24	5 (10%)
23	CLA	a	609	13	63,72,73	1.45	7 (11%)	73,112,113	1.39	8 (10%)
23	CLA	L	304	-	45,53,73	1.76	5 (11%)	52,89,113	1.66	7 (13%)
30	DGD	J	103	-	59,59,67	0.99	3 (5%)	73,73,81	1.48	8 (10%)
23	CLA	5	618	16	39,48,73	1.91	8 (20%)	48,83,113	1.74	9 (18%)
26	BCR	5	622	-	41,41,41	0.71	0	56,56,56	2.17	19 (33%)
26	BCR	7	623	-	41,41,41	0.68	0	56,56,56	1.81	13 (23%)
23	CLA	6	613	-	63,72,73	1.45	10 (15%)	73,112,113	1.43	9 (12%)
23	CLA	4	603	15	44,52,73	1.83	9 (20%)	55,88,113	1.69	10 (18%)
27	SF4	A	853	-	0,12,12	-	-	-	-	-
23	CLA	5	611	25	42,50,73	1.76	9 (21%)	48,85,113	1.62	8 (16%)
23	CLA	2	609	20	29,35,73	2.76	9 (31%)	28,60,113	1.75	6 (21%)
23	CLA	B	839	-	65,73,73	1.44	10 (15%)	76,113,113	1.51	9 (11%)
23	CLA	8	609	19	45,53,73	1.68	8 (17%)	52,89,113	1.74	8 (15%)
23	CLA	B	830	-	43,51,73	1.78	11 (25%)	49,86,113	1.71	6 (12%)
23	CLA	2	614	-	29,35,73	2.64	9 (31%)	28,60,113	1.72	5 (17%)
23	CLA	6	617	-	45,53,73	1.73	9 (20%)	52,89,113	1.49	7 (13%)
23	CLA	9	612	21	29,35,73	2.71	9 (31%)	28,60,113	1.67	4 (14%)
23	CLA	2	603	20	29,35,73	2.70	9 (31%)	28,60,113	1.77	6 (21%)
23	CLA	8	602	19	60,68,73	1.52	9 (15%)	70,107,113	1.58	10 (14%)
23	CLA	4	612	15	40,49,73	1.80	7 (17%)	45,84,113	1.78	8 (17%)
28	LMU	A	857	-	36,36,36	1.20	3 (8%)	47,47,47	1.33	4 (8%)
23	CLA	5	607	-	65,73,73	1.47	10 (15%)	76,113,113	1.58	8 (10%)
25	LHG	a	620	23	48,48,48	0.60	1 (2%)	51,54,54	1.26	6 (11%)
31	LUT	a	617	-	42,43,43	0.79	0	51,60,60	1.56	12 (23%)
23	CLA	A	812	-	65,73,73	1.44	10 (15%)	76,113,113	1.52	10 (13%)
23	CLA	A	801	-	65,73,73	1.48	10 (15%)	76,113,113	1.41	7 (9%)
23	CLA	4	602	15	60,68,73	1.46	7 (11%)	70,107,113	1.62	8 (11%)
23	CLA	6	612	17	40,49,73	1.83	7 (17%)	45,84,113	1.78	9 (20%)
23	CLA	5	601	16	56,64,73	1.55	8 (14%)	65,102,113	1.42	8 (12%)
23	CLA	8	603	-	44,52,73	1.87	9 (20%)	55,88,113	1.65	12 (21%)
23	CLA	F	301	-	57,65,73	1.57	10 (17%)	66,103,113	1.44	5 (7%)
23	CLA	K	204	-	46,54,73	1.72	7 (15%)	53,90,113	1.60	8 (15%)
23	CLA	a	608	-	43,52,73	1.77	6 (13%)	49,88,113	1.66	7 (14%)
26	BCR	3	620	-	41,41,41	0.83	0	56,56,56	2.17	20 (35%)

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
23	CLA	3	606	-	1/1/13/20	10/23/101/115	-
23	CLA	3	609	14	1/1/14/20	16/31/109/115	-
23	CLA	A	854	-	1/1/15/20	13/37/115/115	-
23	CLA	B	806	2	1/1/15/20	13/37/115/115	-
23	CLA	A	832	-	1/1/12/20	7/19/97/115	-
23	CLA	B	834	-	1/1/14/20	13/31/109/115	-
29	LMG	7	624	-	-	19/39/59/70	0/1/1/1
23	CLA	A	816	-	1/1/10/20	2/10/88/115	-
23	CLA	5	617	-	1/1/12/20	6/19/97/115	-
23	CLA	5	603	-	1/1/13/20	10/25/101/115	-
23	CLA	8	606	-	1/1/15/20	14/35/113/115	-
23	CLA	A	841	-	1/1/15/20	18/37/115/115	-
32	XAT	1	618	-	-	1/31/93/93	0/4/4/4
32	XAT	7	620	-	-	1/31/93/93	0/4/4/4
32	XAT	8	620	-	-	2/31/93/93	0/4/4/4
23	CLA	B	820	-	1/1/12/20	7/19/97/115	-
24	PQN	B	842	-	-	7/23/43/43	0/2/2/2
23	CLA	9	606	21	1/1/5/20	-	-
23	CLA	9	609	21	1/1/5/20	-	-
23	CLA	B	821	-	1/1/11/20	3/11/89/115	-
23	CLA	A	827	-	1/1/13/20	5/30/108/115	-
23	CLA	A	807	1	1/1/15/20	13/37/115/115	-
28	LMU	5	628	-	-	11/19/59/61	0/2/2/2
26	BCR	3	621	-	-	6/29/63/63	0/2/2/2
23	CLA	6	610	17	1/1/15/20	10/37/115/115	-
29	LMG	5	626	-	-	23/35/55/70	0/1/1/1
23	CLA	B	808	-	1/1/15/20	14/37/115/115	-
26	BCR	B	845	-	-	5/29/63/63	0/2/2/2
23	CLA	1	611	25	1/1/15/20	11/37/115/115	-
31	LUT	1	617	-	-	2/29/67/67	0/2/2/2
23	CLA	B	816	-	1/1/12/20	10/23/101/115	-
29	LMG	4	624	-	-	15/35/55/70	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	9	610	21	1/1/5/20	-	-
23	CLA	a	601	13	1/1/13/20	5/23/101/115	-
23	CLA	1	612	13	1/1/11/20	6/13/91/115	-
26	BCR	8	621	-	-	6/29/63/63	0/2/2/2
23	CLA	B	841	25	1/1/10/20	1/11/89/115	-
23	CLA	J	101	10	1/1/10/20	5/10/88/115	-
23	CLA	4	610	15	1/1/14/20	12/33/111/115	-
31	LUT	5	620	-	-	2/29/67/67	0/2/2/2
23	CLA	3	608	-	1/1/13/20	9/25/103/115	-
23	CLA	7	602	18	1/1/15/20	16/37/115/115	-
23	CLA	8	610	19	1/1/14/20	7/31/109/115	-
23	CLA	B	802	-	1/1/15/20	19/37/115/115	-
23	CLA	B	827	-	1/1/14/20	14/34/112/115	-
23	CLA	6	614	-	1/1/14/20	7/31/109/115	-
23	CLA	A	829	-	1/1/15/20	11/37/115/115	-
23	CLA	A	803	-	1/1/15/20	9/37/115/115	-
23	CLA	5	614	-	1/1/10/20	7/13/87/115	-
27	SF4	C	101	-	-	-	0/6/5/5
23	CLA	4	613	15	1/1/15/20	12/37/115/115	-
23	CLA	A	839	-	1/1/13/20	5/25/103/115	-
23	CLA	1	604	-	1/1/11/20	10/18/96/115	-
23	CLA	7	614	-	1/1/10/20	3/10/88/115	-
23	CLA	G	204	7	1/1/11/20	6/13/91/115	-
23	CLA	7	610	18	1/1/15/20	6/37/115/115	-
23	CLA	7	603	-	1/1/11/20	2/11/89/115	-
31	LUT	6	619	-	-	2/29/67/67	0/2/2/2
23	CLA	A	823	-	1/1/10/20	5/10/88/115	-
26	BCR	6	622	-	-	7/29/63/63	0/2/2/2
23	CLA	7	615	-	1/1/10/20	4/8/84/115	-
23	CLA	B	840	-	1/1/15/20	9/37/115/115	-
23	CLA	B	835	-	1/1/11/20	8/13/91/115	-
23	CLA	K	201	11	1/1/11/20	6/13/91/115	-
23	CLA	2	613	20	1/1/5/20	-	-
23	CLA	A	838	-	1/1/12/20	7/19/97/115	-
25	LHG	1	620	23	-	24/53/53/53	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	1	616	13	1/1/11/20	4/11/87/115	-
28	LMU	K	208	-	-	10/21/61/61	0/2/2/2
23	CLA	7	606	-	1/1/10/20	2/8/86/115	-
23	CLA	A	808	-	1/1/12/20	0/19/97/115	-
23	CLA	5	612	16	1/1/10/20	3/8/86/115	-
23	CLA	B	809	2	1/1/15/20	15/37/115/115	-
23	CLA	A	840	-	1/1/12/20	5/22/100/115	-
23	CLA	A	831	-	1/1/15/20	14/37/115/115	-
26	BCR	G	205	-	-	0/29/63/63	0/2/2/2
23	CLA	A	828	-	1/1/15/20	9/37/115/115	-
23	CLA	5	608	-	1/1/12/20	7/19/97/115	-
31	LUT	8	619	-	-	2/29/67/67	0/2/2/2
26	BCR	A	849	-	-	5/29/63/63	0/2/2/2
32	XAT	4	620	-	-	1/31/93/93	0/4/4/4
32	XAT	9	620	-	-	0/31/93/93	0/4/4/4
23	CLA	B	823	-	1/1/11/20	4/13/91/115	-
23	CLA	5	609	16	1/1/15/20	13/37/115/115	-
23	CLA	B	813	-	1/1/15/20	20/37/115/115	-
23	CLA	A	843	-	1/1/14/20	16/35/113/115	-
25	LHG	9	622	23	-	23/53/53/53	-
23	CLA	6	616	17	1/1/15/20	18/37/115/115	-
31	LUT	4	619	-	-	4/29/67/67	0/2/2/2
32	XAT	3	619	-	-	1/31/93/93	0/4/4/4
30	DGD	B	850	-	-	22/51/91/95	0/2/2/2
23	CLA	4	606	-	1/1/10/20	3/6/84/115	-
23	CLA	9	601	21	1/1/5/20	-	-
23	CLA	A	837	1	1/1/11/20	7/13/91/115	-
23	CLA	A	821	-	1/1/12/20	12/23/101/115	-
26	BCR	4	621	-	-	1/29/63/63	0/2/2/2
25	LHG	A	847	23	-	11/34/34/53	-
32	XAT	2	620	-	-	0/31/93/93	0/4/4/4
23	CLA	A	824	-	1/1/10/20	0/8/86/115	-
23	CLA	B	815	-	1/1/10/20	2/11/89/115	-
29	LMG	5	627	-	-	13/35/55/70	0/1/1/1
25	LHG	6	623	23	-	23/52/52/53	-
23	CLA	8	601	19	1/1/15/20	20/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	1	607	-	1/1/10/20	3/6/84/115	-
29	LMG	J	104	-	-	19/35/55/70	0/1/1/1
23	CLA	2	606	20	1/1/5/20	-	-
23	CLA	4	616	15	1/1/11/20	6/11/87/115	-
23	CLA	4	614	-	1/1/13/20	7/27/105/115	-
29	LMG	4	623	-	-	11/35/55/70	0/1/1/1
23	CLA	a	613	-	1/1/15/20	12/37/115/115	-
23	CLA	A	833	-	1/1/11/20	2/13/91/115	-
23	CLA	5	619	-	1/1/11/20	7/11/87/115	-
23	CLA	a	607	-	1/1/11/20	6/13/91/115	-
23	CLA	4	618	15	1/1/10/20	0/8/84/115	-
23	CLA	A	845	25	1/1/12/20	9/19/97/115	-
23	CLA	B	837	-	1/1/15/20	15/37/115/115	-
31	LUT	2	619	-	-	2/29/67/67	0/2/2/2
23	CLA	B	824	-	1/1/15/20	9/37/115/115	-
23	CLA	A	836	-	1/1/15/20	11/37/115/115	-
23	CLA	6	618	17	1/1/10/20	2/8/84/115	-
23	CLA	3	607	14	1/1/13/20	9/28/104/115	-
26	BCR	3	622	-	-	8/29/63/63	0/2/2/2
23	CLA	B	811	-	1/1/13/20	8/23/99/115	-
23	CLA	5	606	-	1/1/10/20	2/6/84/115	-
31	LUT	7	619	-	-	5/29/67/67	0/2/2/2
31	LUT	9	619	-	-	3/29/67/67	0/2/2/2
23	CLA	4	608	-	1/1/15/20	11/37/115/115	-
23	CLA	1	609	13	1/1/10/20	5/8/84/115	-
23	CLA	L	303	-	1/1/11/20	5/13/91/115	-
23	CLA	7	601	18	1/1/14/20	13/31/109/115	-
25	LHG	8	622	23	-	26/53/53/53	-
23	CLA	9	613	21	1/1/5/20	-	-
23	CLA	6	608	-	1/1/12/20	8/21/99/115	-
23	CLA	3	615	-	1/1/10/20	1/6/84/115	-
23	CLA	B	818	-	1/1/14/20	14/31/109/115	-
23	CLA	a	616	13	1/1/11/20	4/13/91/115	-
23	CLA	9	607	-	1/1/5/20	-	-
26	BCR	A	856	-	-	8/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	B	828	-	1/1/15/20	16/37/115/115	-
28	LMU	8	624	-	-	6/21/61/61	0/2/2/2
23	CLA	2	610	20	1/1/5/20	-	-
23	CLA	2	602	20	1/1/5/20	-	-
26	BCR	B	843	-	-	8/29/63/63	0/2/2/2
23	CLA	A	805	-	1/1/12/20	5/22/100/115	-
23	CLA	8	607	-	1/1/10/20	3/10/86/115	-
23	CLA	6	620	-	1/1/14/20	14/35/113/115	-
23	CLA	B	819	-	1/1/13/20	11/25/103/115	-
23	CLA	a	612	13	1/1/11/20	6/13/91/115	-
23	CLA	1	614	-	1/1/9/20	0/4/76/115	-
23	CLA	A	835	-	1/1/14/20	13/33/111/115	-
23	CLA	A	817	-	1/1/11/20	5/13/91/115	-
23	CLA	9	602	21	1/1/5/20	-	-
25	LHG	B	851	23	-	22/42/42/53	-
24	PQN	A	844	-	-	8/23/43/43	0/2/2/2
23	CLA	B	832	-	1/1/14/20	7/31/109/115	-
23	CLA	4	601	15	1/1/15/20	16/37/115/115	-
25	LHG	A	846	-	-	25/53/53/53	-
26	BCR	B	801	-	-	4/29/63/63	0/2/2/2
23	CLA	1	601	13	1/1/13/20	5/23/101/115	-
23	CLA	6	606	-	1/1/10/20	0/6/84/115	-
23	CLA	B	805	-	1/1/15/20	16/37/115/115	-
23	CLA	A	825	-	1/1/15/20	18/37/115/115	-
23	CLA	3	611	25	1/1/10/20	2/4/80/115	-
23	CLA	5	610	16	1/1/12/20	5/24/102/115	-
23	CLA	3	612	14	1/1/10/20	3/11/89/115	-
23	CLA	A	815	-	1/1/12/20	7/19/97/115	-
26	BCR	B	846	-	-	5/29/63/63	0/2/2/2
23	CLA	a	604	-	1/1/11/20	10/18/96/115	-
23	CLA	3	610	14	1/1/15/20	16/37/115/115	-
23	CLA	3	603	-	1/1/13/20	11/25/103/115	-
23	CLA	7	609	18	1/1/10/20	4/10/88/115	-
23	CLA	6	611	25	1/1/10/20	3/10/88/115	-
26	BCR	B	844	-	-	9/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	1	608	-	1/1/11/20	4/11/89/115	-
23	CLA	8	608	-	1/1/12/20	4/21/99/115	-
23	CLA	A	813	-	1/1/12/20	5/24/102/115	-
23	CLA	7	607	-	1/1/10/20	6/10/88/115	-
27	SF4	C	102	-	-	-	0/6/5/5
23	CLA	a	603	-	1/1/10/20	3/10/88/115	-
23	CLA	8	616	19	-	7/11/87/115	-
26	BCR	J	102	-	-	5/29/63/63	0/2/2/2
23	CLA	6	602	17	1/1/15/20	8/37/115/115	-
25	LHG	3	624	23	-	26/53/53/53	-
23	CLA	K	206	11	1/1/11/20	5/13/91/115	-
23	CLA	7	613	18	1/1/15/20	17/37/115/115	-
23	CLA	2	601	20	1/1/5/20	-	-
23	CLA	A	804	-	1/1/15/20	11/37/115/115	-
23	CLA	B	838	-	1/1/11/20	5/16/94/115	-
23	CLA	A	826	-	1/1/14/20	12/35/113/115	-
23	CLA	6	607	-	1/1/10/20	6/10/86/115	-
23	CLA	2	611	25	1/1/4/20	-	-
23	CLA	8	611	25	1/1/10/20	4/10/88/115	-
26	BCR	B	847	-	-	1/29/63/63	0/2/2/2
23	CLA	3	613	14	1/1/12/20	5/21/99/115	-
23	CLA	B	825	-	1/1/14/20	9/34/112/115	-
26	BCR	A	848	-	-	4/29/63/63	0/2/2/2
28	LMU	A	858	-	-	6/21/57/61	0/2/2/2
23	CLA	a	614	-	1/1/12/20	10/25/99/115	-
23	CLA	3	602	14	1/1/14/20	8/31/109/115	-
23	CLA	a	611	25	1/1/10/20	0/4/80/115	-
23	CLA	A	811	-	1/1/15/20	16/37/115/115	-
26	BCR	A	850	-	-	1/29/63/63	0/2/2/2
23	CLA	4	607	-	1/1/11/20	5/13/91/115	-
26	BCR	K	207	-	-	3/29/63/63	0/2/2/2
23	CLA	4	611	25	1/1/10/20	4/10/88/115	-
23	CLA	B	803	-	1/1/15/20	15/37/115/115	-
23	CLA	A	814	-	1/1/15/20	20/37/115/115	-
23	CLA	4	604	-	1/1/13/20	6/25/101/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	7	608	-	1/1/12/20	4/19/97/115	-
23	CLA	9	603	21	1/1/5/20	-	-
23	CLA	3	604	-	1/1/15/20	11/37/115/115	-
26	BCR	A	851	-	-	4/29/63/63	0/2/2/2
23	CLA	B	804	-	1/1/10/20	3/8/86/115	-
25	LHG	2	622	23	-	19/41/41/53	-
23	CLA	B	826	-	1/1/13/20	8/25/103/115	-
29	LMG	A	860	-	-	18/35/55/70	0/1/1/1
23	CLA	A	834	-	1/1/15/20	17/37/115/115	-
23	CLA	7	616	18	1/1/11/20	7/11/87/115	-
26	BCR	B	848	-	-	4/29/63/63	0/2/2/2
23	CLA	3	614	-	1/1/10/20	0/6/84/115	-
23	CLA	8	604	-	1/1/12/20	5/19/97/115	-
25	LHG	5	625	-	-	23/53/53/53	-
23	CLA	F	304	-	1/1/10/20	4/8/86/115	-
23	CLA	4	609	15	1/1/14/20	13/33/111/115	-
26	BCR	K	202	-	-	4/29/63/63	0/2/2/2
33	NEX	6	624	-	-	4/27/83/83	0/3/3/3
23	CLA	2	612	20	1/1/5/20	-	-
23	CLA	8	612	19	1/1/10/20	2/8/86/115	-
25	LHG	5	623	23	-	23/53/53/53	-
23	CLA	a	610	13	1/1/14/20	5/29/107/115	-
23	CLA	A	806	-	1/1/15/20	15/37/115/115	-
23	CLA	A	809	1	1/1/15/20	12/37/115/115	-
23	CLA	B	833	-	1/1/15/20	19/37/115/115	-
23	CLA	2	604	-	1/1/5/20	-	-
25	LHG	3	623	-	-	26/49/49/53	-
23	CLA	6	601	17	1/1/15/20	14/37/115/115	-
23	CLA	A	822	-	1/1/15/20	13/37/115/115	-
23	CLA	B	812	-	1/1/10/20	6/11/89/115	-
23	CLA	B	810	-	1/1/14/20	15/35/113/115	-
23	CLA	1	603	-	1/1/12/20	11/21/99/115	-
26	BCR	1	619	-	-	4/29/63/63	0/2/2/2
23	CLA	8	614	-	1/1/13/20	10/27/105/115	-
32	XAT	a	618	-	-	1/31/93/93	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	A	820	-	1/1/15/20	15/37/115/115	-
23	CLA	A	842	-	1/1/15/20	10/37/115/115	-
23	CLA	A	810	1	1/1/12/20	5/19/97/115	-
23	CLA	7	611	25	1/1/13/20	10/29/107/115	-
23	CLA	9	614	-	1/1/5/20	-	-
23	CLA	9	611	25	1/1/5/20	-	-
23	CLA	7	604	-	1/1/13/20	8/23/101/115	-
23	CLA	B	817	-	1/1/13/20	10/30/108/115	-
23	CLA	A	818	-	1/1/14/20	12/31/109/115	-
23	CLA	7	612	18	-	6/11/89/115	-
26	BCR	F	305	-	-	2/29/63/63	0/2/2/2
23	CLA	1	606	13	1/1/8/20	1/5/79/115	-
26	BCR	a	619	-	-	4/29/63/63	0/2/2/2
23	CLA	B	822	-	-	4/10/88/115	-
23	CLA	6	603	-	1/1/13/20	4/25/101/115	-
23	CLA	8	613	19	1/1/15/20	16/37/115/115	-
28	LMU	8	625	-	-	10/21/61/61	0/2/2/2
23	CLA	K	203	-	1/1/15/20	10/37/115/115	-
23	CLA	A	819	-	1/1/13/20	8/30/108/115	-
25	LHG	4	622	23	-	21/53/53/53	-
26	BCR	L	305	-	-	10/29/63/63	0/2/2/2
26	BCR	A	852	-	-	11/29/63/63	0/2/2/2
23	CLA	B	829	-	1/1/15/20	7/37/115/115	-
23	CLA	3	617	14	1/1/10/20	0/6/84/115	-
33	NEX	5	624	-	-	2/27/83/83	0/3/3/3
23	CLA	1	610	13	1/1/9/20	1/6/80/115	-
23	CLA	5	613	16	1/1/14/20	19/35/113/115	-
23	CLA	1	613	-	1/1/15/20	12/37/115/115	-
31	LUT	3	618	-	-	2/29/67/67	0/2/2/2
23	CLA	2	616	-	1/1/5/20	-	-
23	CLA	a	602	13	1/1/14/20	6/33/111/115	-
23	CLA	9	604	-	1/1/5/20	-	-
23	CLA	G	203	-	1/1/10/20	3/10/88/115	-
23	CLA	L	302	12	1/1/11/20	3/13/91/115	-
32	XAT	5	621	-	-	2/31/93/93	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	B	814	-	1/1/14/20	12/36/114/115	-
25	LHG	7	622	23	-	24/41/41/53	-
23	CLA	F	303	-	1/1/10/20	5/10/88/115	-
26	BCR	7	621	-	-	6/29/63/63	0/2/2/2
23	CLA	A	802	-	1/1/15/20	9/37/115/115	-
23	CLA	B	807	-	1/1/12/20	4/22/100/115	-
23	CLA	5	604	-	1/1/15/20	13/35/111/115	-
23	CLA	2	607	-	1/1/5/20	-	-
28	LMU	A	859	-	-	13/21/57/61	0/2/2/2
26	BCR	L	301	-	-	6/29/63/63	0/2/2/2
23	CLA	5	602	16	1/1/15/20	11/37/115/115	-
23	CLA	B	831	-	1/1/15/20	12/37/115/115	-
32	XAT	6	621	-	-	2/31/93/93	0/4/4/4
23	CLA	1	602	13	1/1/14/20	6/33/111/115	-
23	CLA	A	830	-	1/1/15/20	14/37/115/115	-
23	CLA	6	609	17	1/1/11/20	4/13/91/115	-
23	CLA	5	616	16	1/1/10/20	4/8/84/115	-
23	CLA	B	836	-	-	6/19/97/115	-
23	CLA	6	604	-	1/1/15/20	22/37/115/115	-
23	CLA	a	606	13	1/1/10/20	3/10/88/115	-
25	LHG	8	623	-	-	24/51/51/53	-
23	CLA	a	609	13	1/1/15/20	19/35/113/115	-
23	CLA	L	304	-	1/1/11/20	6/13/91/115	-
30	DGD	J	103	-	-	25/47/87/95	0/2/2/2
23	CLA	5	618	16	1/1/10/20	2/8/84/115	-
26	BCR	5	622	-	-	3/29/63/63	0/2/2/2
26	BCR	7	623	-	-	0/29/63/63	0/2/2/2
23	CLA	6	613	-	1/1/15/20	13/35/113/115	-
23	CLA	4	603	15	1/1/11/20	7/13/89/115	-
27	SF4	A	853	-	-	-	0/6/5/5
23	CLA	5	611	25	1/1/10/20	3/10/88/115	-
23	CLA	2	609	20	1/1/5/20	-	-
23	CLA	B	839	-	1/1/15/20	12/37/115/115	-
23	CLA	8	609	19	1/1/11/20	4/13/91/115	-
23	CLA	B	830	-	1/1/10/20	2/11/89/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	2	614	-	1/1/5/20	-	-
23	CLA	6	617	-	1/1/11/20	7/13/91/115	-
23	CLA	9	612	21	1/1/5/20	-	-
23	CLA	2	603	20	1/1/5/20	-	-
23	CLA	8	602	19	1/1/14/20	8/31/109/115	-
23	CLA	4	612	15	-	2/8/86/115	-
28	LMU	A	857	-	-	11/21/61/61	0/2/2/2
23	CLA	5	607	-	1/1/15/20	15/37/115/115	-
25	LHG	a	620	23	-	24/53/53/53	-
31	LUT	a	617	-	-	2/29/67/67	0/2/2/2
23	CLA	A	812	-	1/1/15/20	11/37/115/115	-
23	CLA	A	801	-	1/1/15/20	10/37/115/115	-
23	CLA	4	602	15	1/1/14/20	10/31/109/115	-
23	CLA	6	612	17	1/1/10/20	2/8/86/115	-
23	CLA	5	601	16	1/1/13/20	6/27/105/115	-
23	CLA	8	603	-	1/1/11/20	8/13/89/115	-
23	CLA	F	301	-	1/1/13/20	9/28/106/115	-
23	CLA	K	204	-	1/1/11/20	7/15/93/115	-
23	CLA	a	608	-	1/1/11/20	4/11/89/115	-
26	BCR	3	620	-	-	4/29/63/63	0/2/2/2

The worst 5 of 2248 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	2	611	CLA	C1A-NA	12.76	1.40	1.29
24	A	844	PQN	C12-C13	8.62	1.53	1.33
24	B	842	PQN	C12-C13	8.55	1.53	1.33
23	4	609	CLA	C4B-NB	8.10	1.42	1.35
23	5	613	CLA	C4B-NB	7.97	1.42	1.35

The worst 5 of 3030 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	5	621	XAT	O24-C25-C24	10.95	121.61	113.38
32	2	620	XAT	O24-C25-C24	10.87	121.55	113.38
32	9	620	XAT	O4-C5-C4	10.55	121.31	113.38
23	B	803	CLA	C4A-NA-C1A	9.04	110.77	106.71
23	8	613	CLA	C4A-NA-C1A	8.99	110.75	106.71

5 of 238 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
23	A	801	CLA	ND
23	A	802	CLA	ND
23	A	803	CLA	ND
23	A	804	CLA	ND
23	A	805	CLA	ND

5 of 2598 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
23	A	801	CLA	CBD-CGD-O2D-CED
23	A	804	CLA	C1A-C2A-CAA-CBA
23	A	804	CLA	CHA-CBD-CGD-O1D
23	A	804	CLA	CHA-CBD-CGD-O2D
23	A	805	CLA	C3A-C2A-CAA-CBA

There are no ring outliers.

257 monomers are involved in 596 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	3	606	CLA	2	0
23	3	609	CLA	6	0
23	A	854	CLA	5	0
23	B	806	CLA	3	0
23	A	832	CLA	2	0
23	B	834	CLA	3	0
29	7	624	LMG	1	0
23	A	816	CLA	1	0
23	5	603	CLA	1	0
23	A	841	CLA	6	0
32	1	618	XAT	4	0
32	7	620	XAT	1	0
32	8	620	XAT	1	0
23	B	820	CLA	1	0
24	B	842	PQN	6	0
23	9	606	CLA	1	0
23	9	609	CLA	1	0
23	B	821	CLA	3	0
23	A	827	CLA	2	0
23	A	807	CLA	2	0
28	5	628	LMU	3	0
26	3	621	BCR	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	6	610	CLA	4	0
29	5	626	LMG	1	0
23	B	808	CLA	2	0
26	B	845	BCR	2	0
23	1	611	CLA	5	0
31	1	617	LUT	3	0
29	4	624	LMG	1	0
23	1	612	CLA	1	0
26	8	621	BCR	4	0
23	B	841	CLA	3	0
23	J	101	CLA	2	0
23	4	610	CLA	1	0
31	5	620	LUT	6	0
23	3	608	CLA	3	0
23	7	602	CLA	2	0
23	8	610	CLA	3	0
23	B	802	CLA	2	0
23	B	827	CLA	6	0
23	6	614	CLA	3	0
23	A	829	CLA	10	0
23	A	803	CLA	5	0
23	5	614	CLA	2	0
23	4	613	CLA	5	0
23	A	839	CLA	3	0
23	7	614	CLA	2	0
23	G	204	CLA	3	0
23	7	610	CLA	5	0
23	7	603	CLA	2	0
31	6	619	LUT	4	0
23	A	823	CLA	2	0
26	6	622	BCR	4	0
23	B	840	CLA	3	0
23	B	835	CLA	2	0
23	K	201	CLA	1	0
23	2	613	CLA	1	0
23	A	838	CLA	1	0
25	1	620	LHG	6	0
23	A	808	CLA	1	0
23	B	809	CLA	3	0
23	A	840	CLA	5	0
23	A	831	CLA	4	0
26	G	205	BCR	6	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	A	828	CLA	1	0
23	5	608	CLA	4	0
31	8	619	LUT	6	0
26	A	849	BCR	4	0
32	4	620	XAT	3	0
32	9	620	XAT	3	0
23	B	823	CLA	1	0
23	5	609	CLA	6	0
23	B	813	CLA	5	0
23	A	843	CLA	5	0
25	9	622	LHG	5	0
23	6	616	CLA	6	0
31	4	619	LUT	5	0
32	3	619	XAT	2	0
30	B	850	DGD	5	0
23	4	606	CLA	1	0
23	9	601	CLA	1	0
23	A	837	CLA	2	0
23	A	821	CLA	1	0
26	4	621	BCR	2	0
25	A	847	LHG	1	0
32	2	620	XAT	3	0
23	A	824	CLA	1	0
23	B	815	CLA	1	0
29	5	627	LMG	3	0
25	6	623	LHG	3	0
23	8	601	CLA	3	0
23	1	607	CLA	1	0
29	J	104	LMG	1	0
23	4	616	CLA	1	0
23	4	614	CLA	1	0
23	5	619	CLA	2	0
23	4	618	CLA	1	0
23	A	845	CLA	1	0
23	B	837	CLA	5	0
31	2	619	LUT	3	0
23	B	824	CLA	5	0
23	A	836	CLA	4	0
23	3	607	CLA	2	0
26	3	622	BCR	4	0
23	B	811	CLA	2	0
23	5	606	CLA	6	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
31	7	619	LUT	5	0
31	9	619	LUT	1	0
23	4	608	CLA	4	0
23	1	609	CLA	2	0
23	L	303	CLA	2	0
23	7	601	CLA	5	0
25	8	622	LHG	1	0
23	9	613	CLA	1	0
23	6	608	CLA	2	0
23	B	818	CLA	2	0
26	A	856	BCR	7	0
23	B	828	CLA	1	0
28	8	624	LMU	3	0
23	2	610	CLA	1	0
26	B	843	BCR	2	0
23	A	805	CLA	4	0
23	8	607	CLA	2	0
23	6	620	CLA	5	0
23	B	819	CLA	2	0
23	A	835	CLA	3	0
23	A	817	CLA	2	0
25	B	851	LHG	2	0
24	A	844	PQN	5	0
23	B	832	CLA	6	0
23	4	601	CLA	6	0
25	A	846	LHG	3	0
26	B	801	BCR	5	0
23	1	601	CLA	6	0
23	6	606	CLA	1	0
23	B	805	CLA	4	0
23	A	825	CLA	5	0
23	5	610	CLA	5	0
23	3	612	CLA	1	0
26	B	846	BCR	1	0
23	3	610	CLA	3	0
23	3	603	CLA	2	0
26	B	844	BCR	3	0
23	1	608	CLA	2	0
23	8	608	CLA	3	0
23	A	813	CLA	2	0
23	7	607	CLA	2	0
23	8	616	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
26	J	102	BCR	5	0
23	6	602	CLA	6	0
25	3	624	LHG	2	0
23	7	613	CLA	4	0
23	A	804	CLA	3	0
23	B	838	CLA	4	0
23	A	826	CLA	1	0
26	B	847	BCR	2	0
23	3	613	CLA	1	0
23	B	825	CLA	4	0
26	A	848	BCR	5	0
23	3	602	CLA	1	0
23	A	811	CLA	5	0
26	A	850	BCR	3	0
23	4	607	CLA	1	0
26	K	207	BCR	3	0
23	B	803	CLA	3	0
23	A	814	CLA	4	0
23	4	604	CLA	1	0
23	7	608	CLA	5	0
23	3	604	CLA	1	0
26	A	851	BCR	3	0
25	2	622	LHG	1	0
23	B	826	CLA	3	0
29	A	860	LMG	2	0
23	A	834	CLA	2	0
23	7	616	CLA	2	0
26	B	848	BCR	1	0
23	3	614	CLA	1	0
25	5	625	LHG	5	0
23	F	304	CLA	1	0
23	4	609	CLA	3	0
26	K	202	BCR	3	0
33	6	624	NEX	4	0
23	8	612	CLA	1	0
25	5	623	LHG	2	0
23	A	806	CLA	3	0
23	A	809	CLA	6	0
23	B	833	CLA	4	0
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23	6	601	CLA	5	0
23	A	822	CLA	4	0

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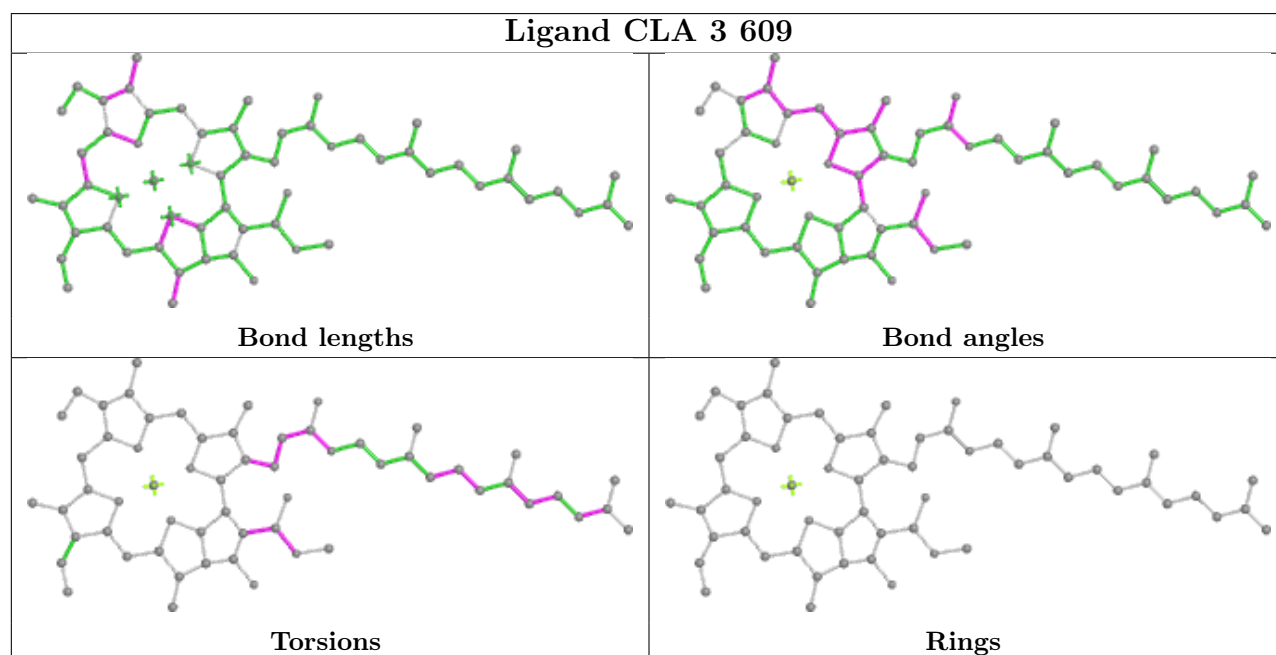
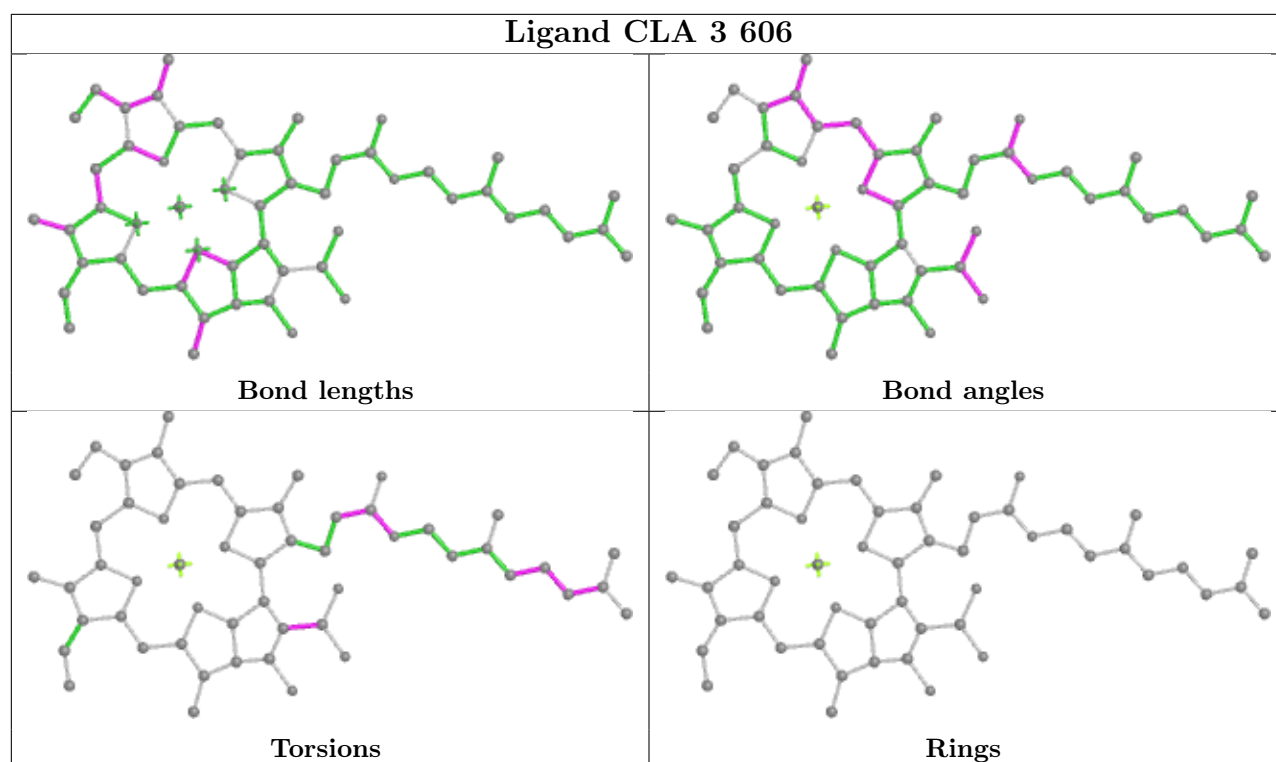
Mol	Chain	Res	Type	Clashes	Symm-Clashes
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23	1	603	CLA	1	0
26	1	619	BCR	2	0
23	8	614	CLA	2	0
23	A	820	CLA	4	0
23	A	842	CLA	8	0
23	A	810	CLA	3	0
23	7	611	CLA	3	0
23	9	614	CLA	1	0
23	9	611	CLA	7	0
23	B	817	CLA	2	0
23	A	818	CLA	4	0
26	F	305	BCR	4	0
23	1	606	CLA	2	0
23	B	822	CLA	1	0
23	6	603	CLA	1	0
23	8	613	CLA	1	0
23	A	819	CLA	2	0
25	4	622	LHG	6	0
26	L	305	BCR	4	0
26	A	852	BCR	7	0
23	B	829	CLA	9	0
23	3	617	CLA	2	0
33	5	624	NEX	3	0
23	5	613	CLA	7	0
31	3	618	LUT	1	0
23	G	203	CLA	3	0
23	L	302	CLA	1	0
32	5	621	XAT	10	0
23	B	814	CLA	3	0
25	7	622	LHG	2	0
23	F	303	CLA	3	0
26	7	621	BCR	3	0
23	A	802	CLA	7	0
23	B	807	CLA	2	0
23	5	604	CLA	5	0
28	A	859	LMU	2	0
26	L	301	BCR	1	0
23	5	602	CLA	5	0
23	B	831	CLA	3	0
32	6	621	XAT	1	0
23	A	830	CLA	5	0

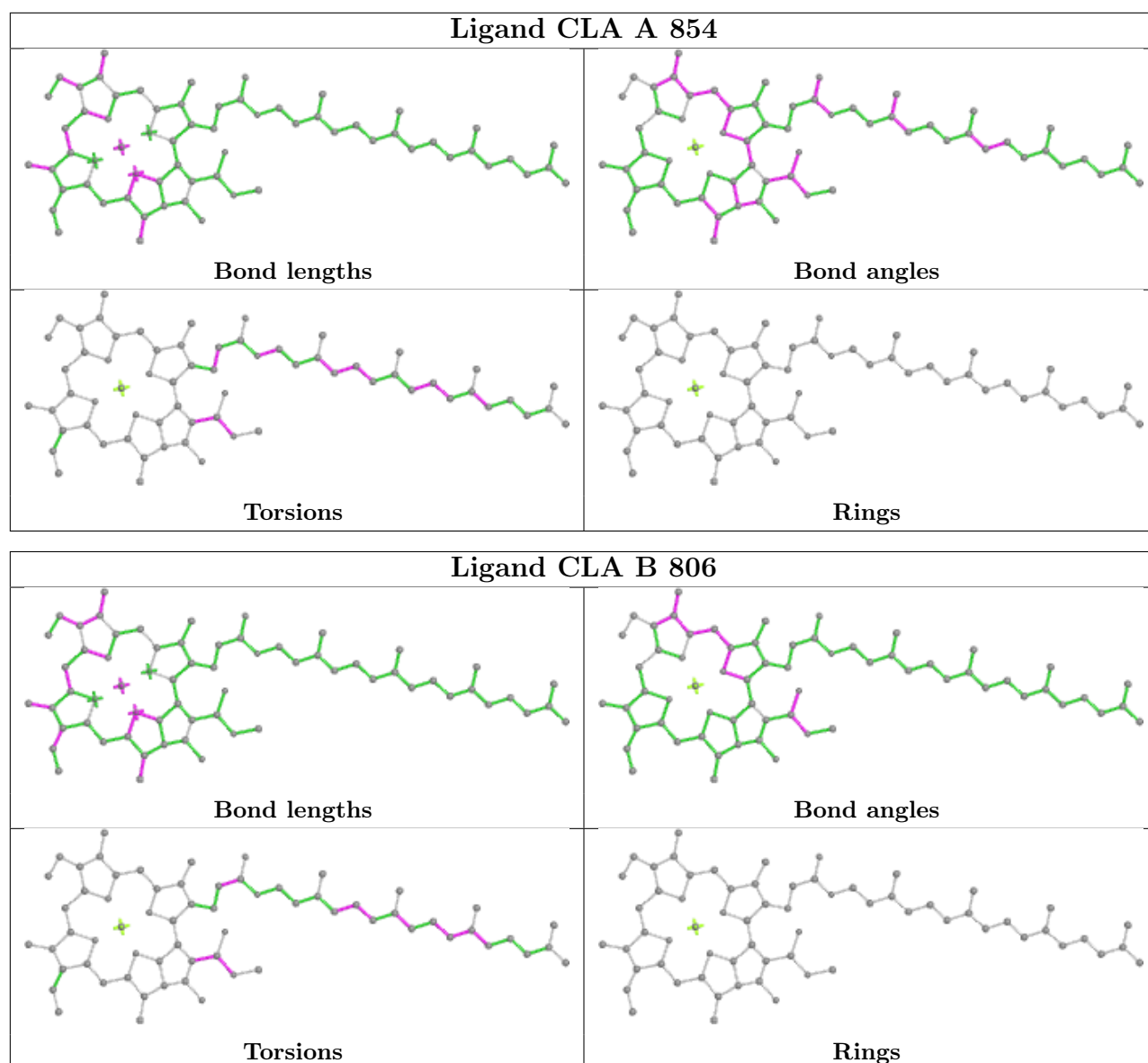
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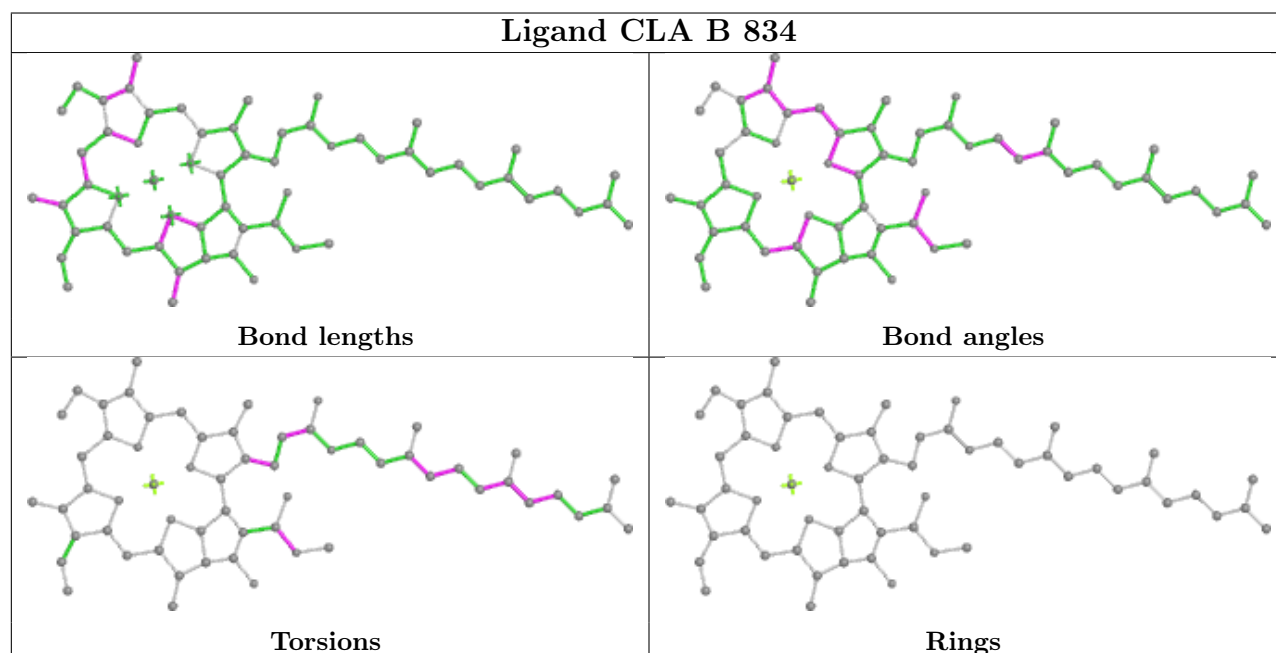
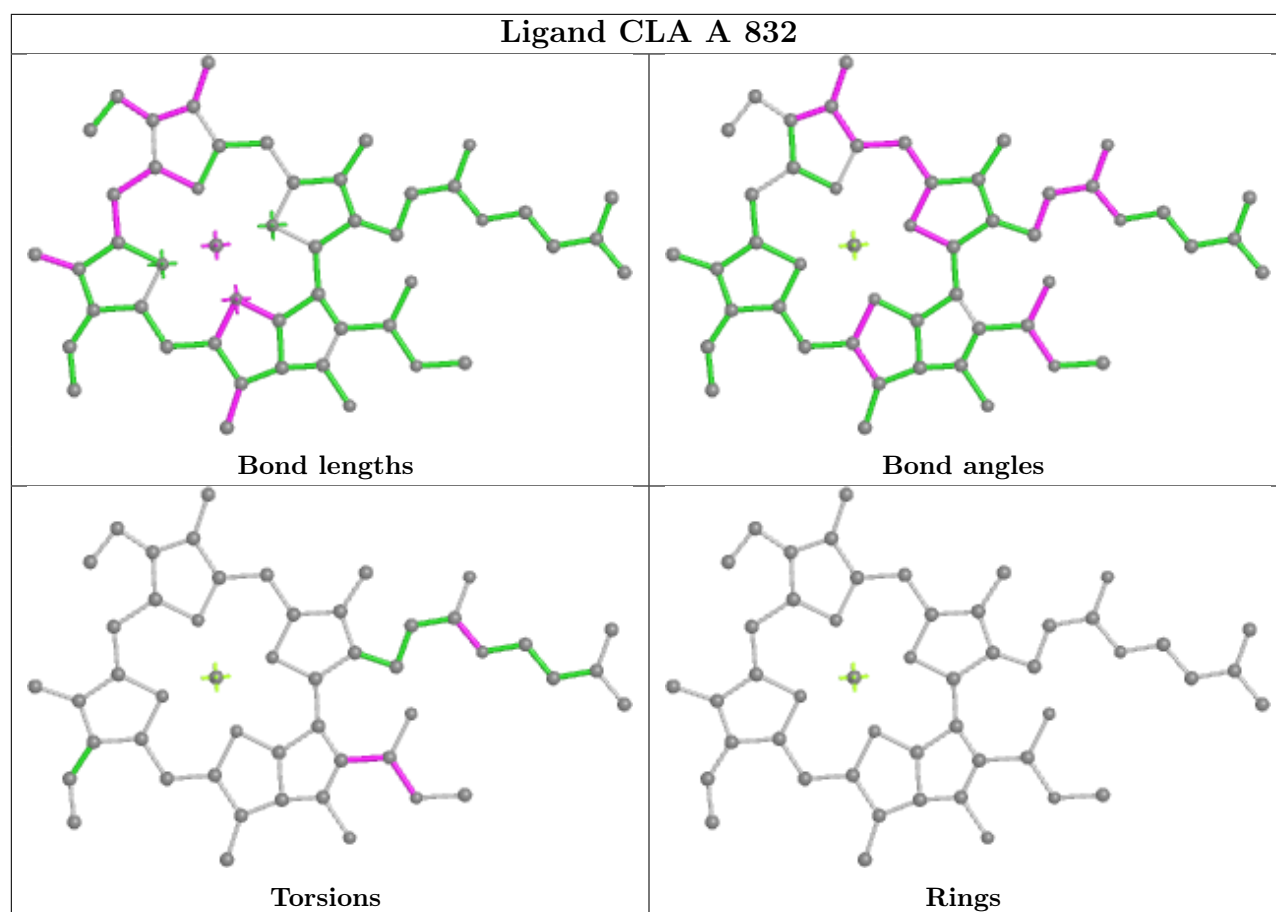
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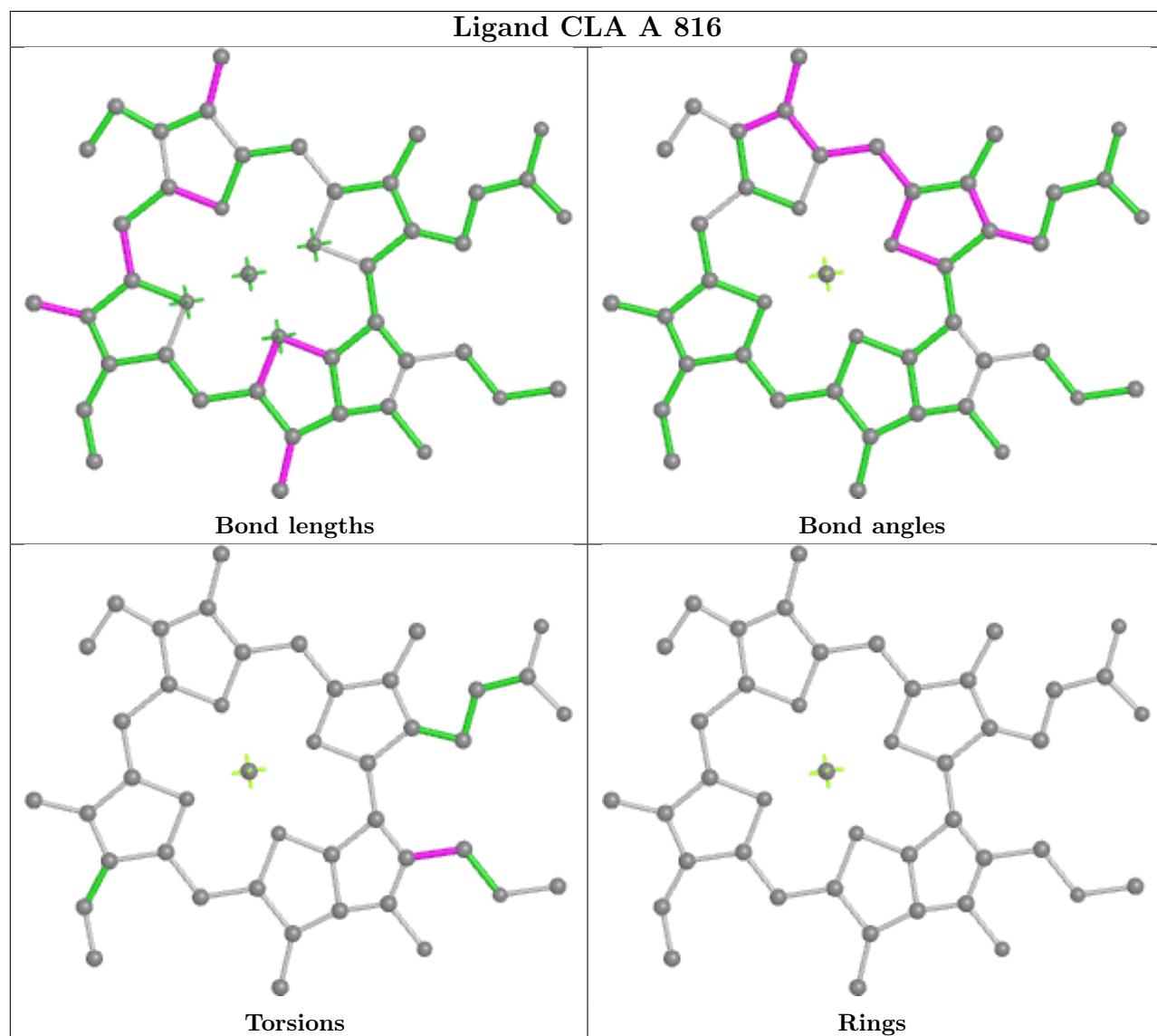
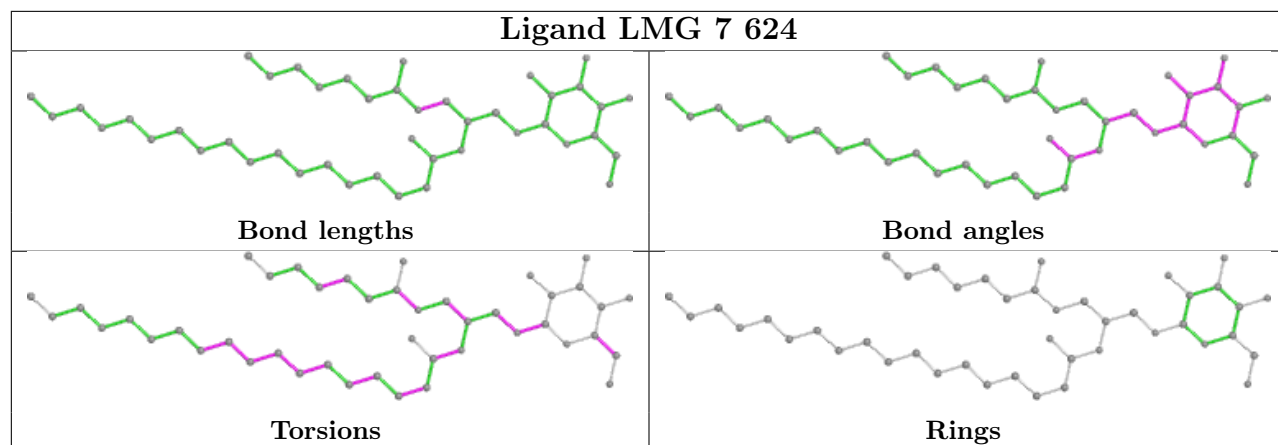
Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	6	609	CLA	2	0
23	5	616	CLA	2	0
23	B	836	CLA	2	0
23	6	604	CLA	3	0
25	8	623	LHG	3	0
23	L	304	CLA	2	0
30	J	103	DGD	1	0
26	5	622	BCR	4	0
23	6	613	CLA	5	0
23	2	609	CLA	1	0
23	B	839	CLA	4	0
23	8	609	CLA	1	0
23	B	830	CLA	5	0
23	2	614	CLA	1	0
28	A	857	LMU	1	0
23	5	607	CLA	5	0
23	A	812	CLA	4	0
23	A	801	CLA	5	0
23	4	602	CLA	1	0
23	6	612	CLA	1	0
23	5	601	CLA	1	0
23	8	603	CLA	1	0
23	F	301	CLA	4	0
23	K	204	CLA	1	0
26	3	620	BCR	5	0

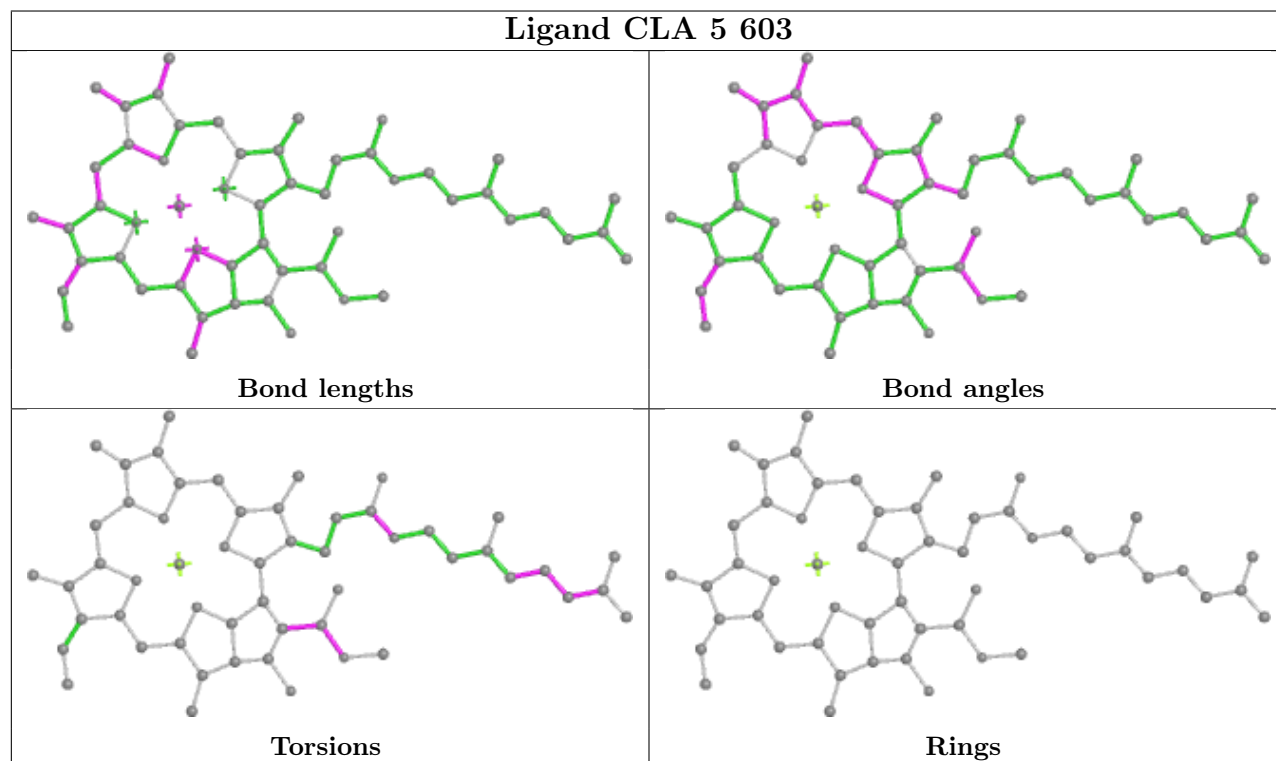
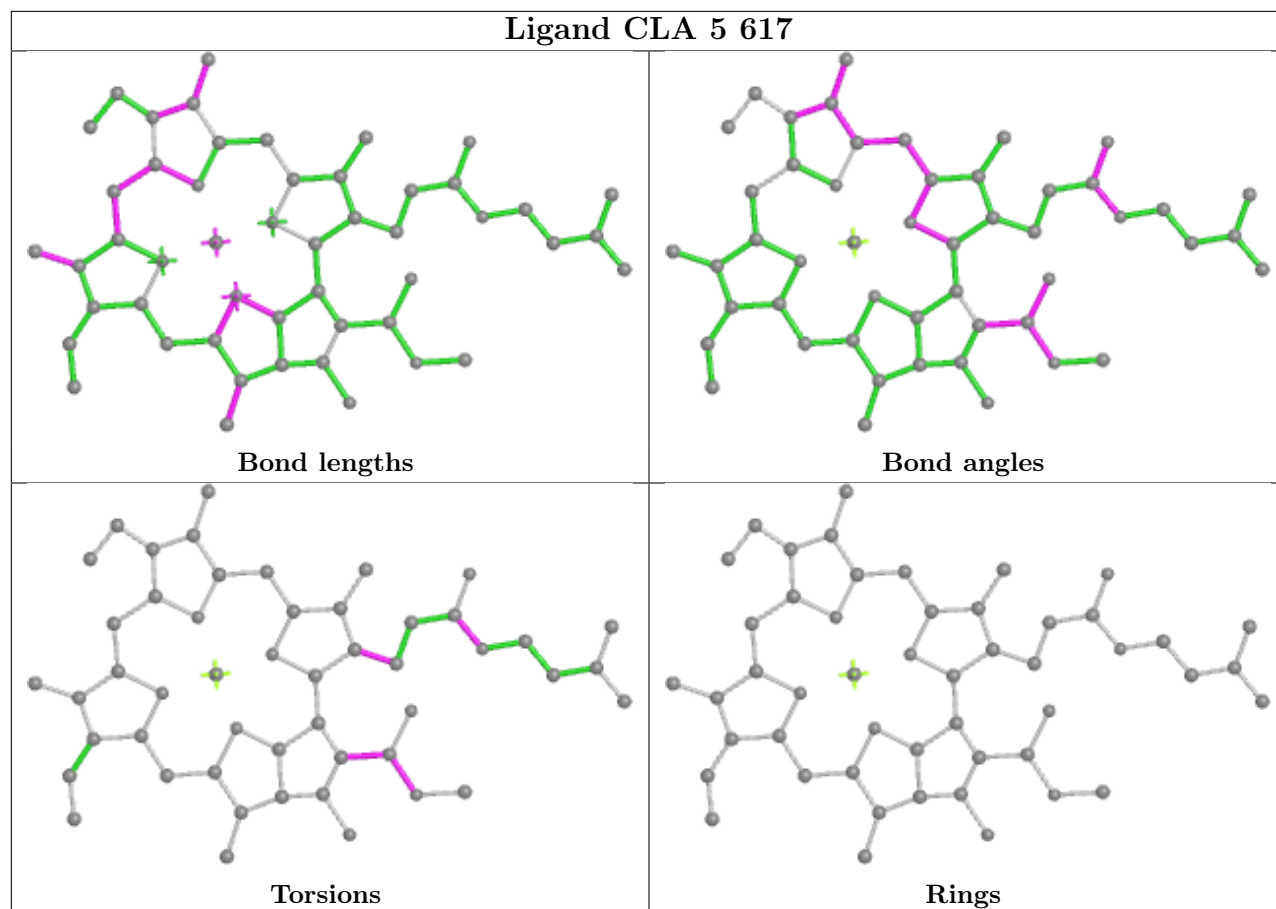
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

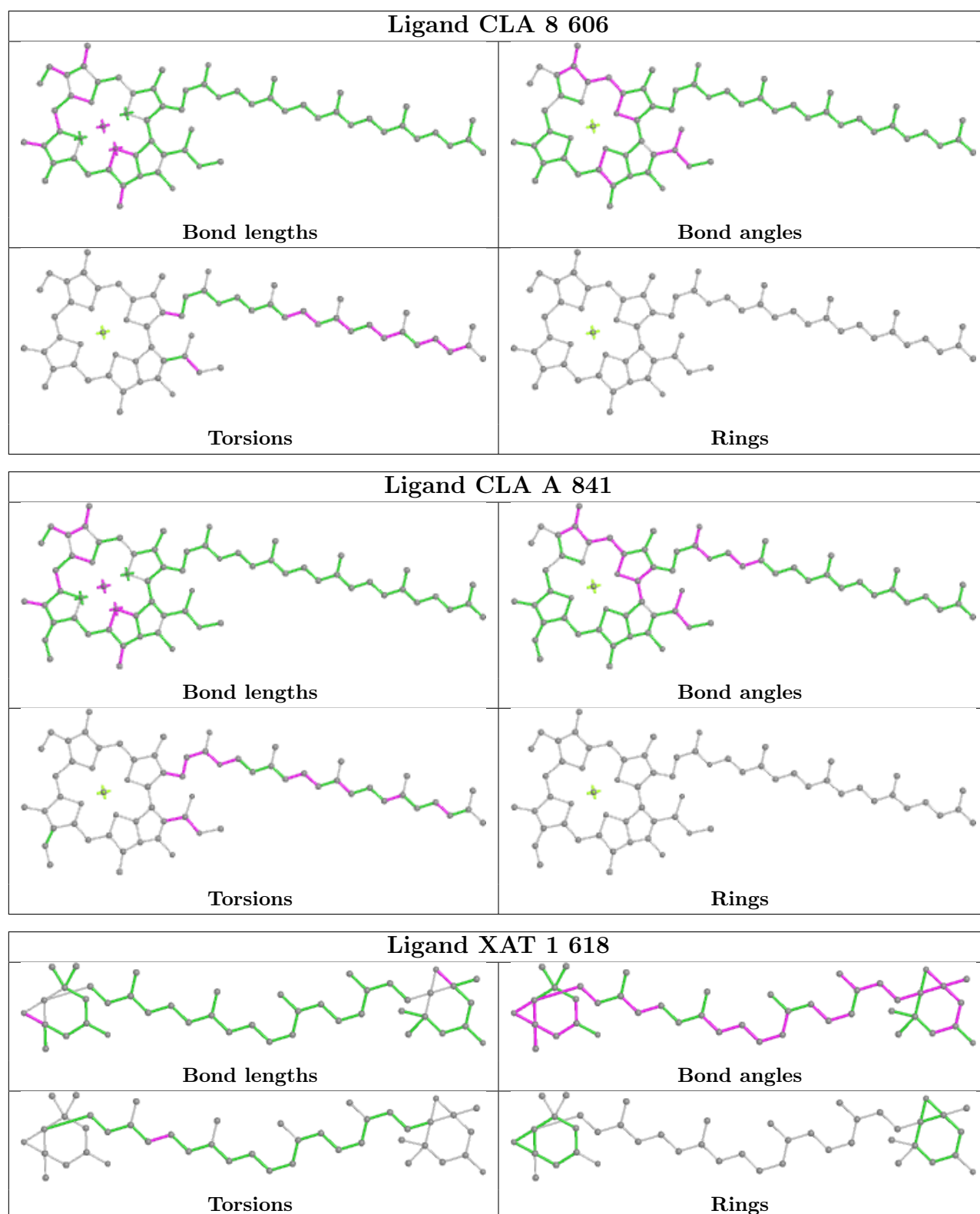


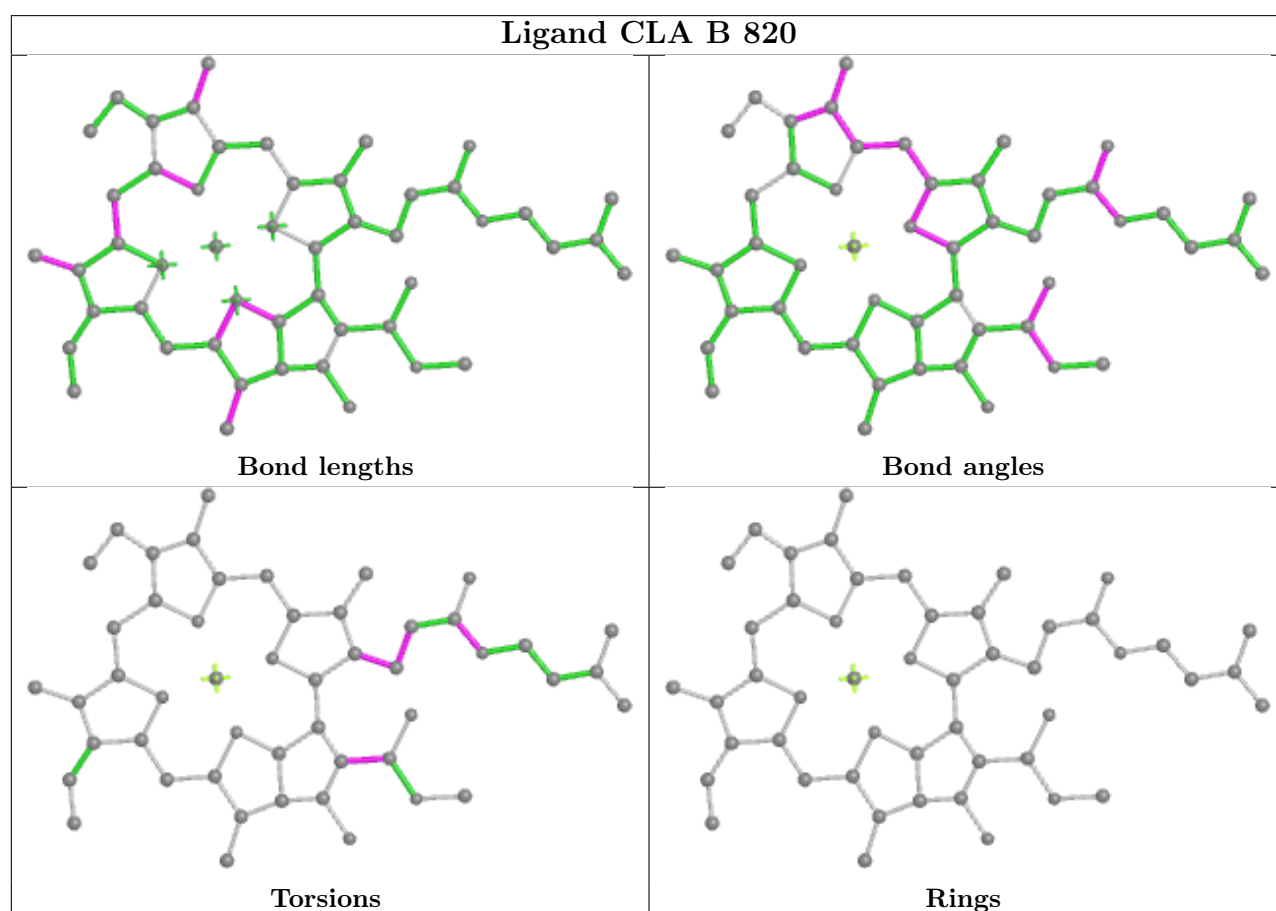
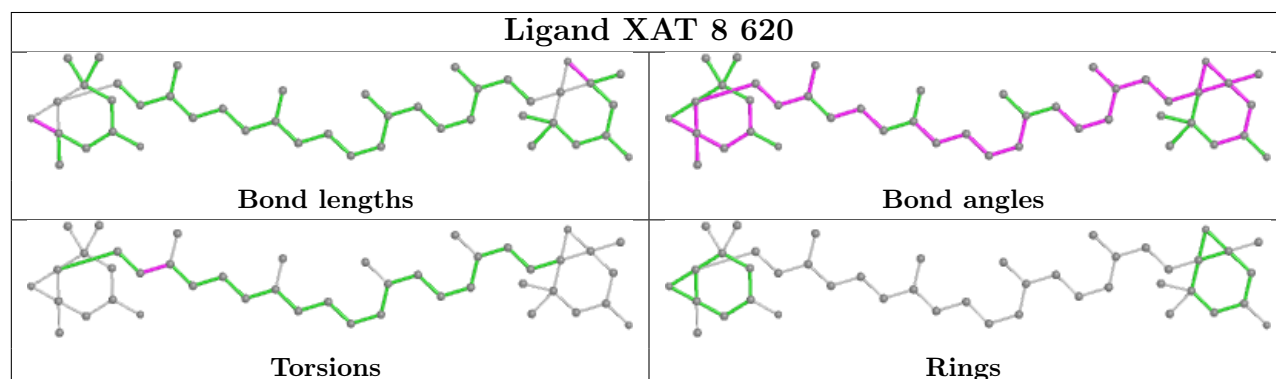
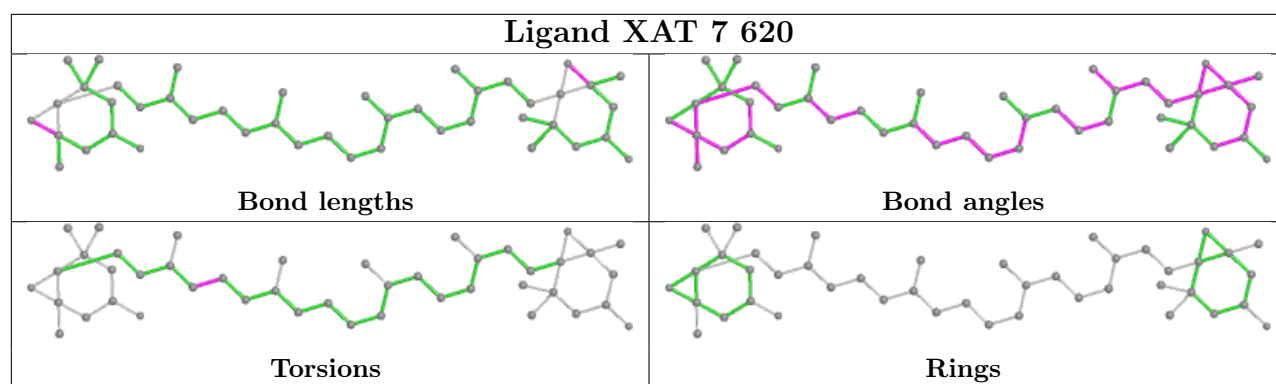


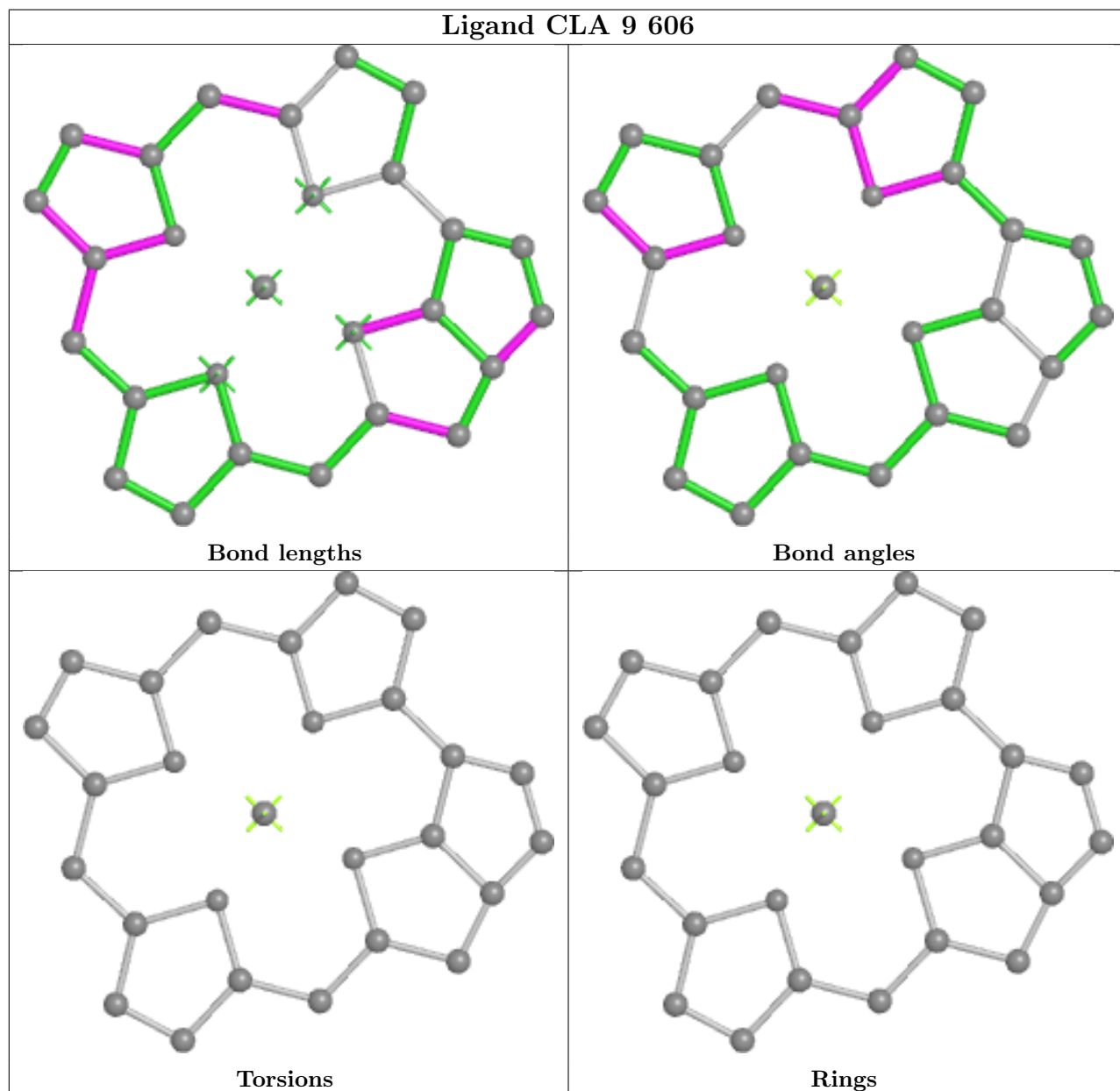
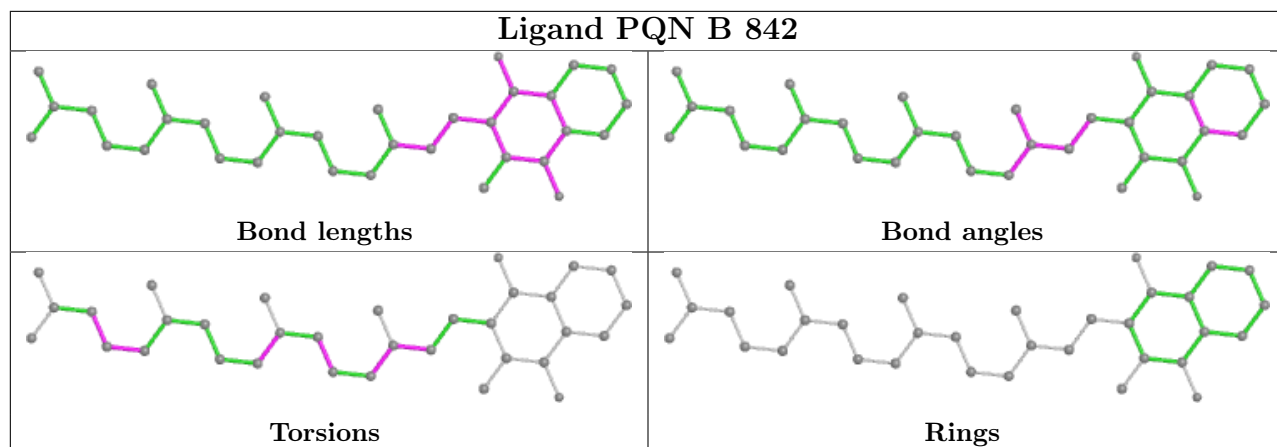


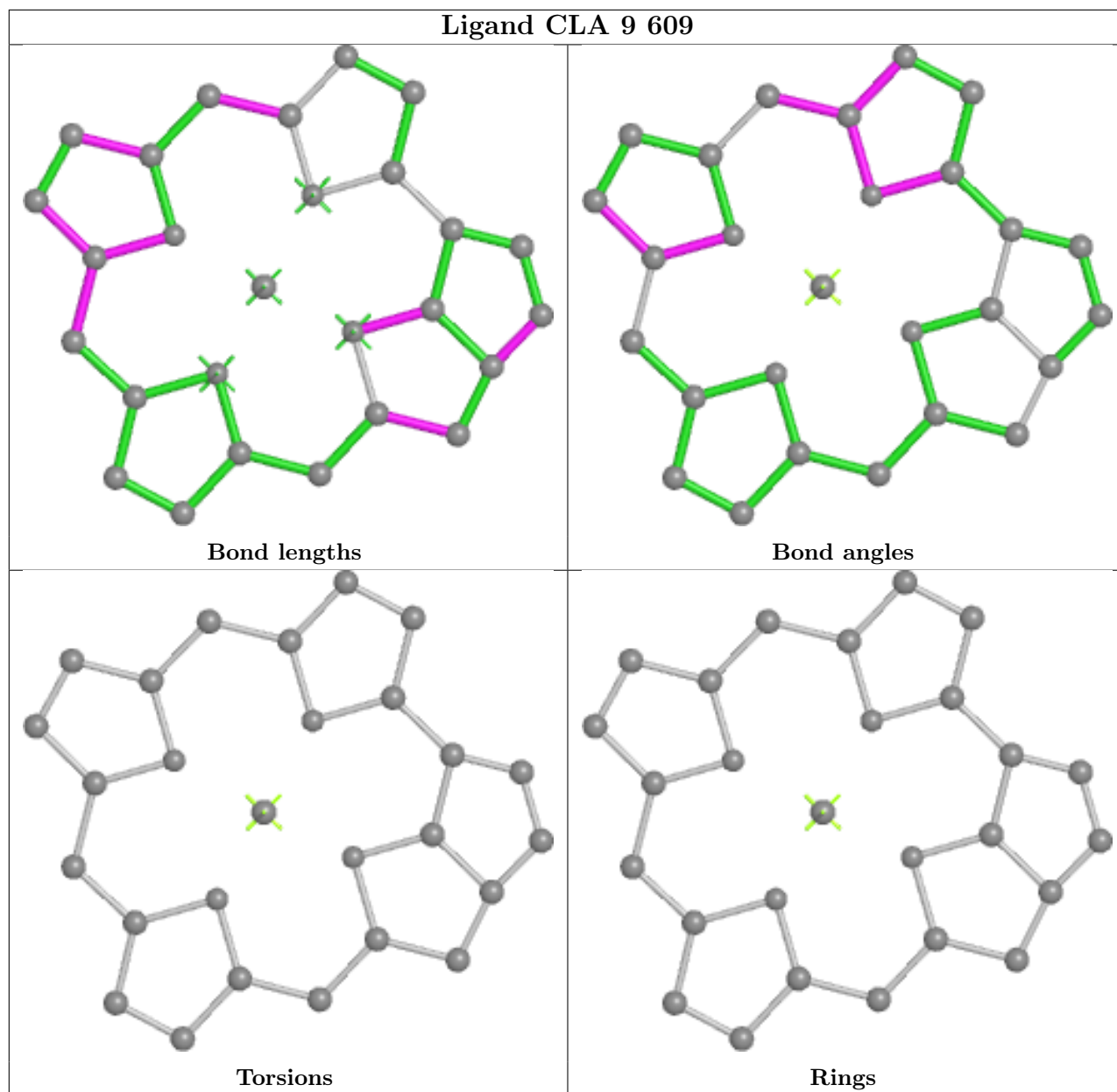


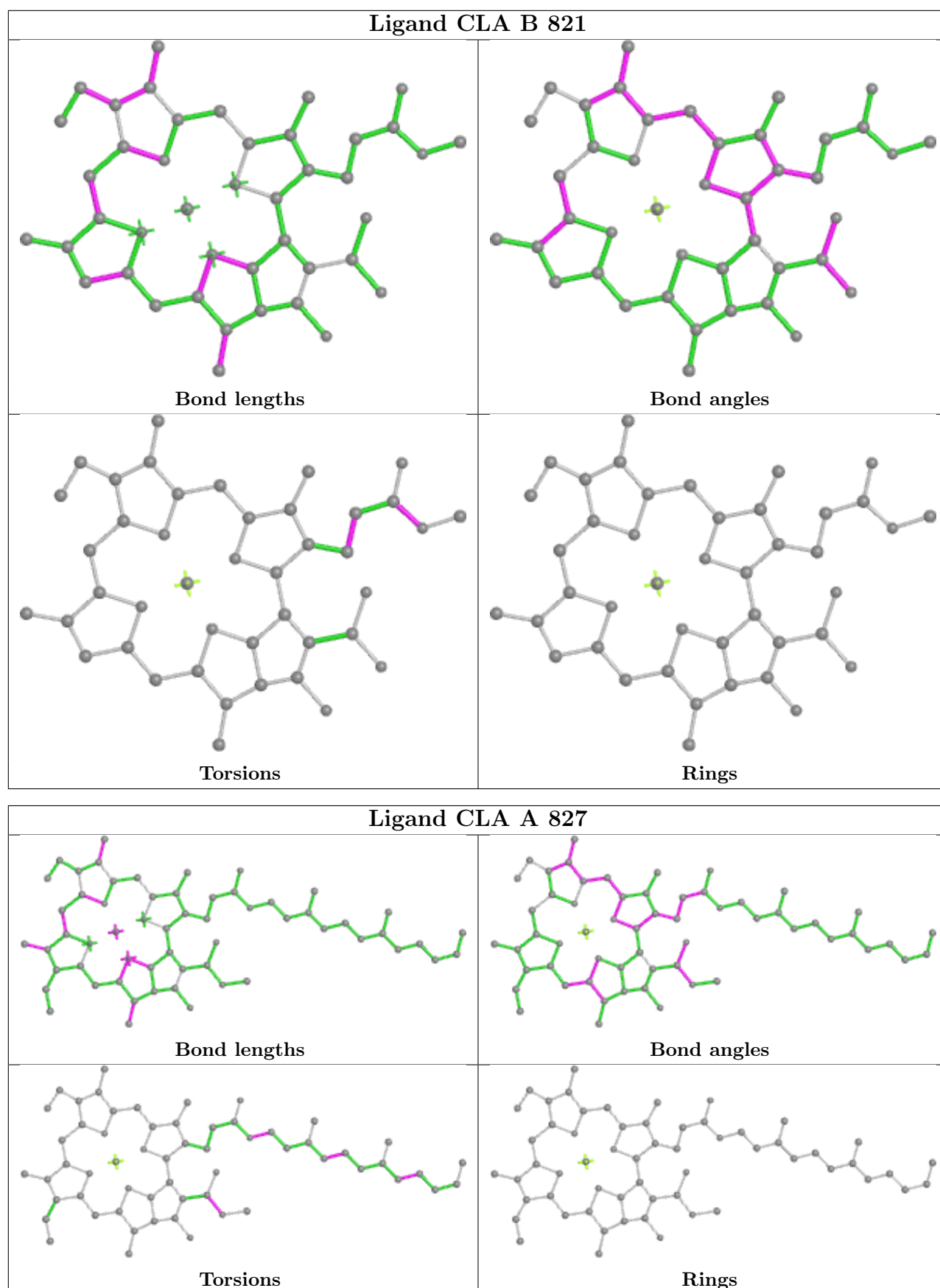


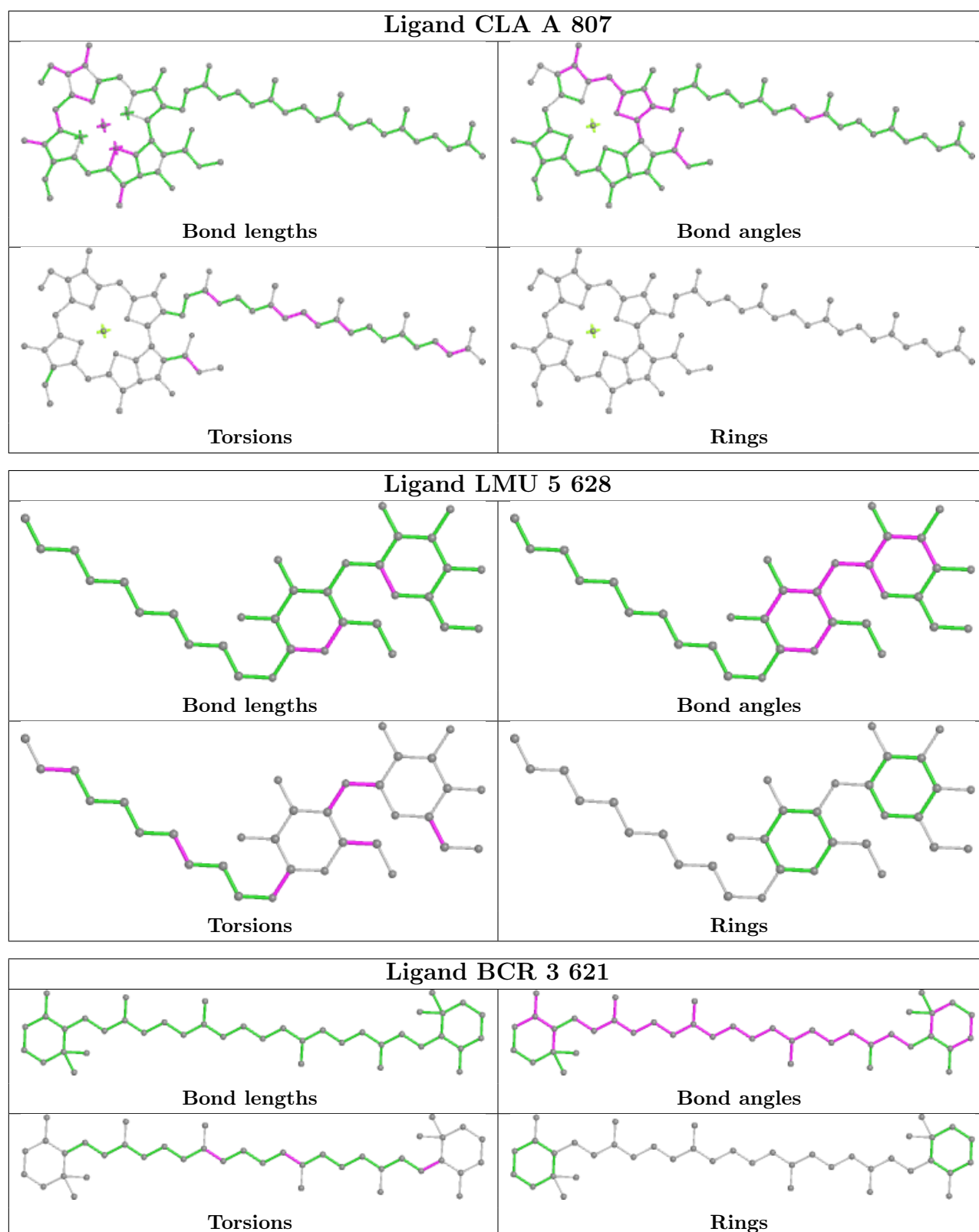


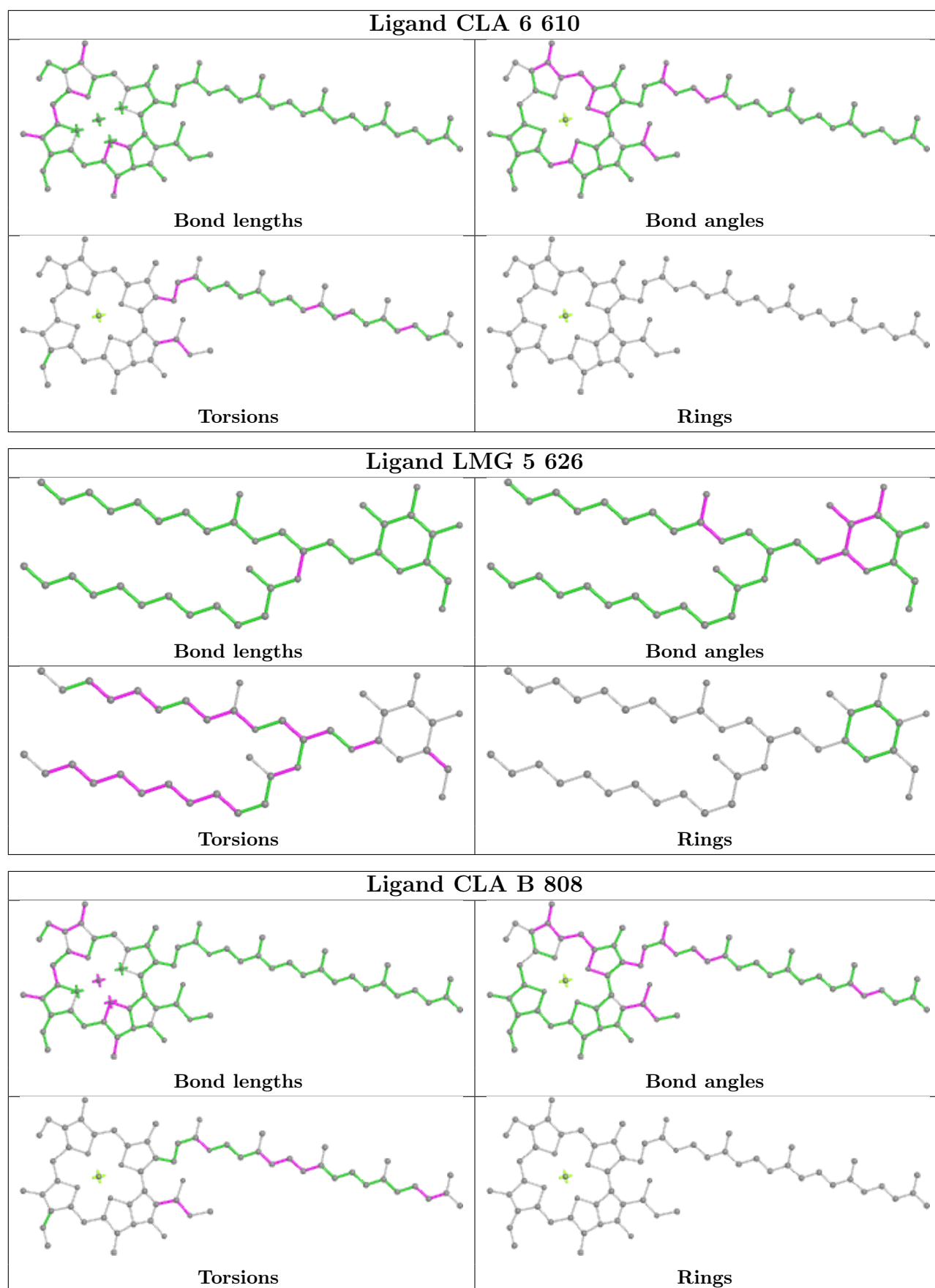


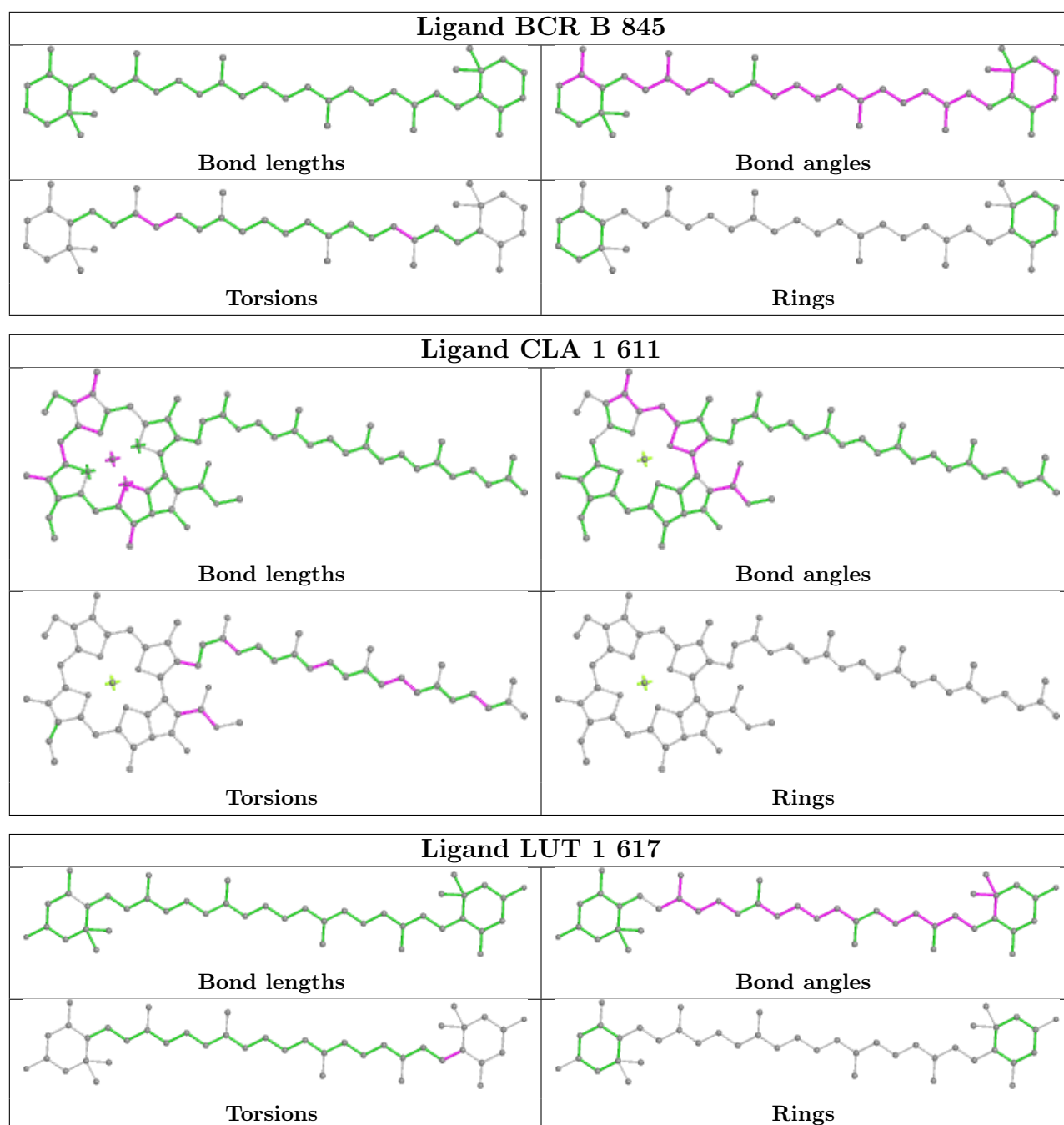


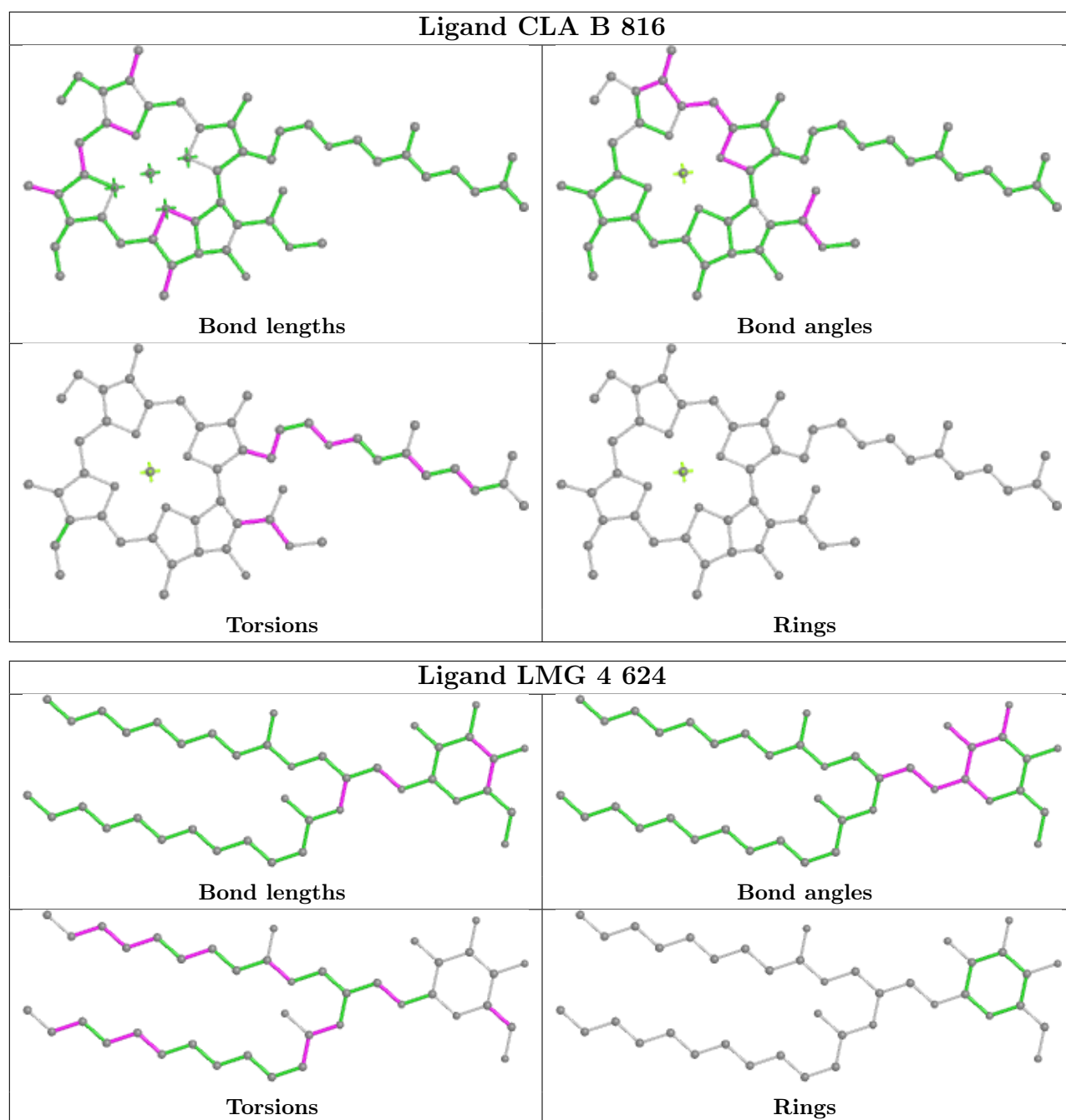


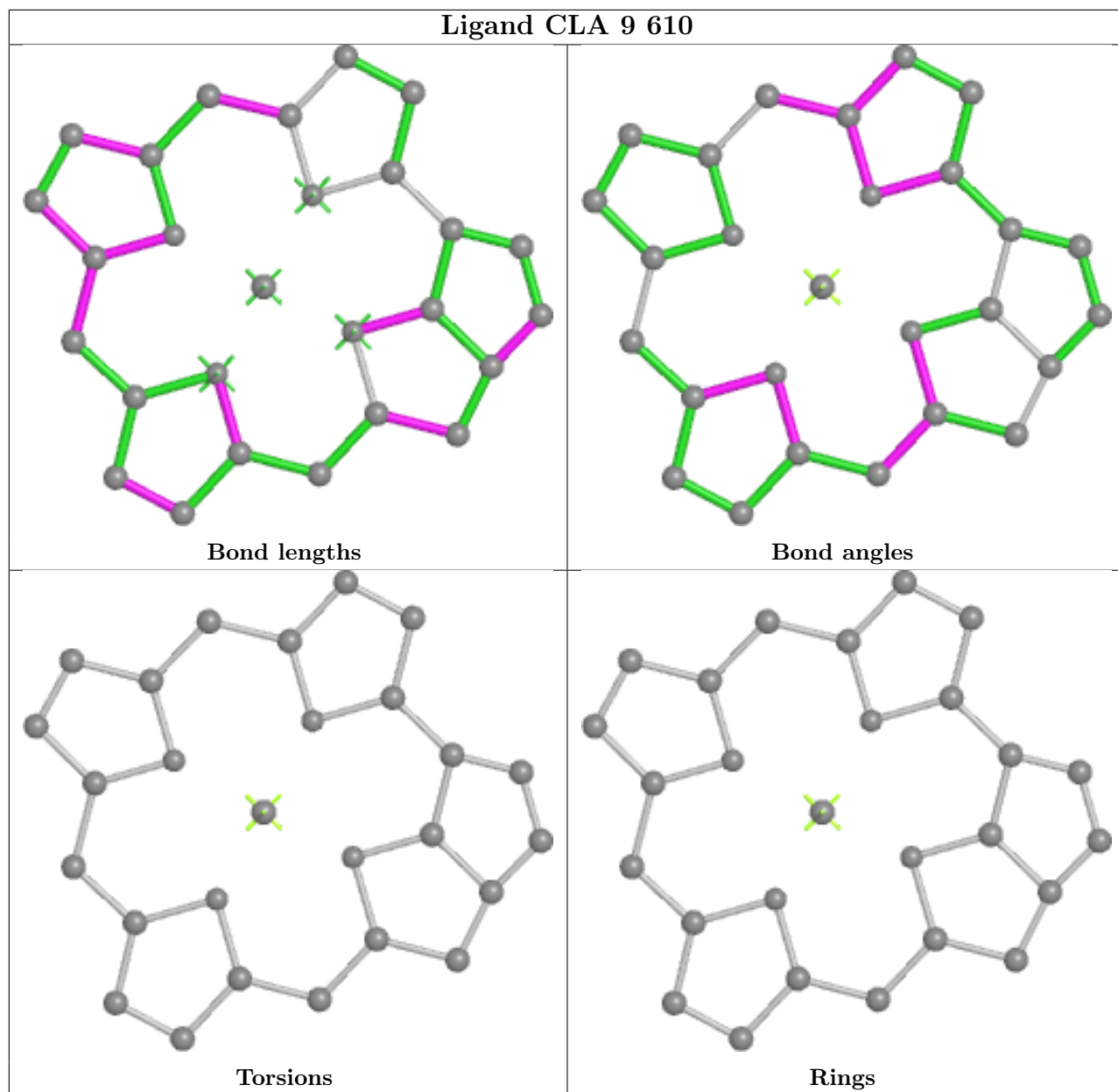


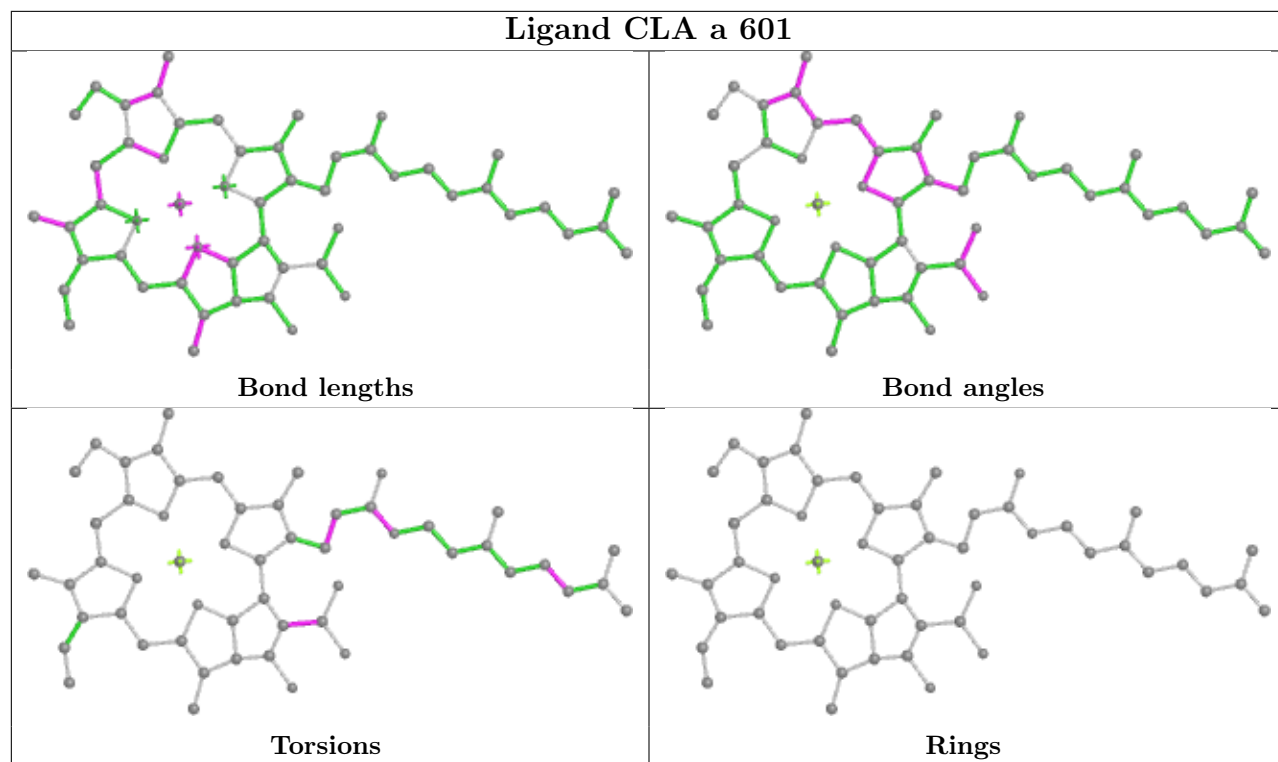


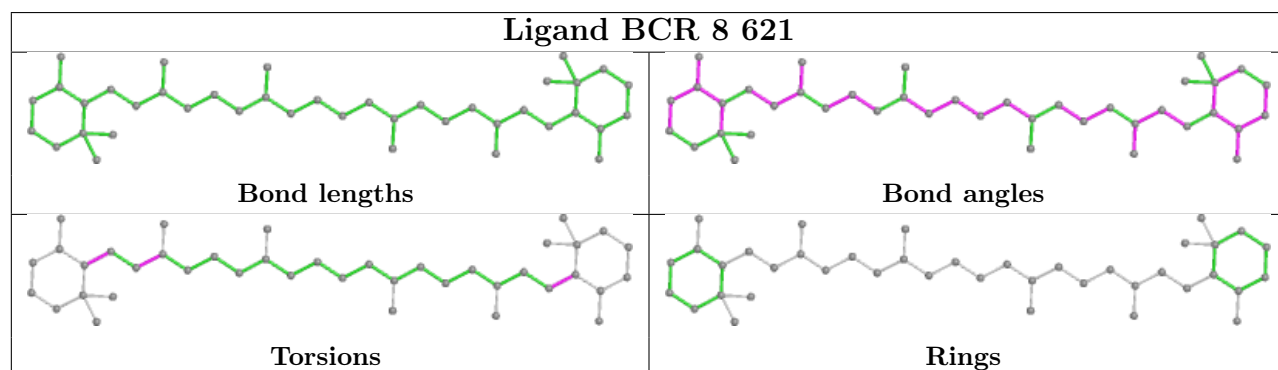
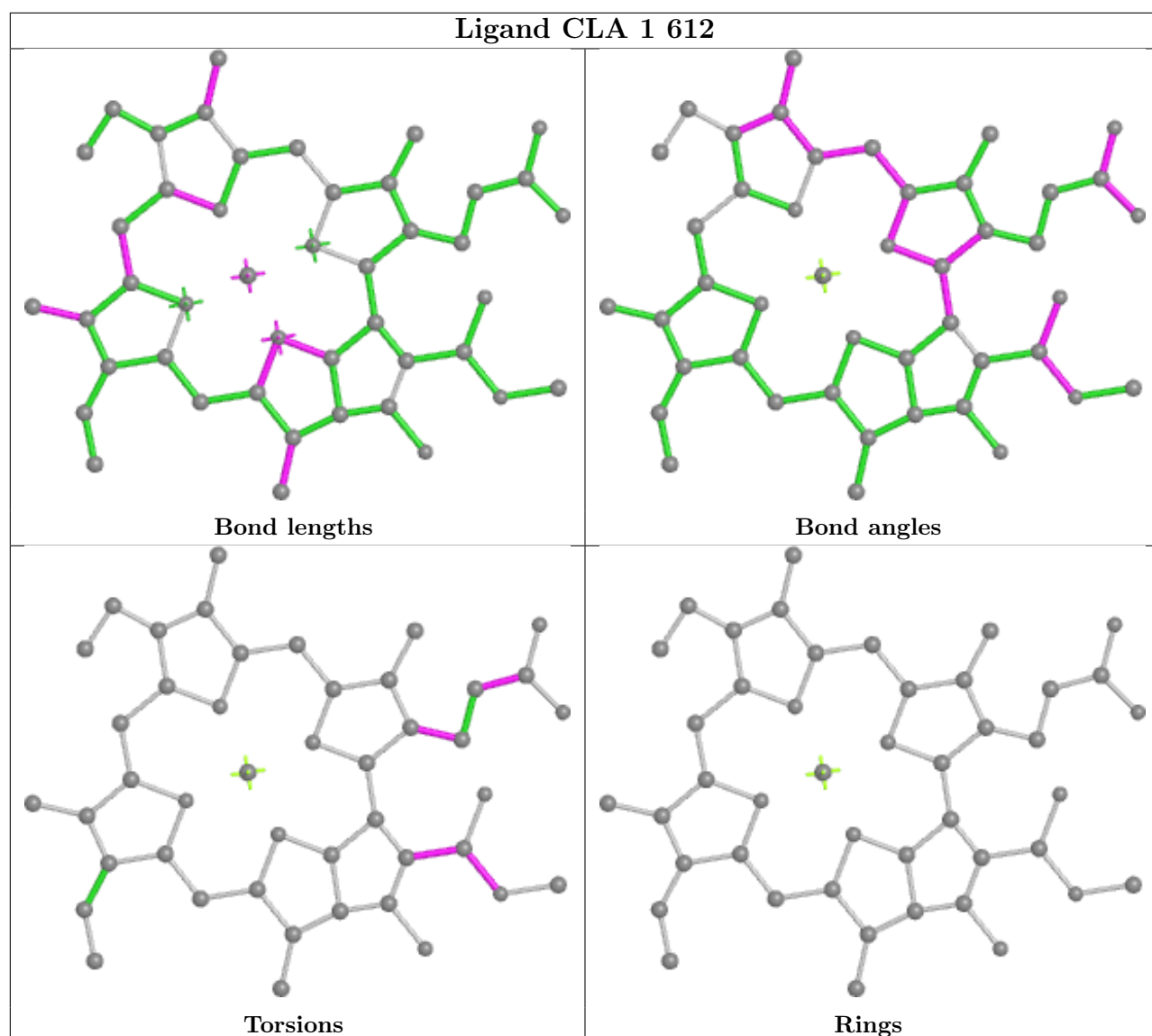


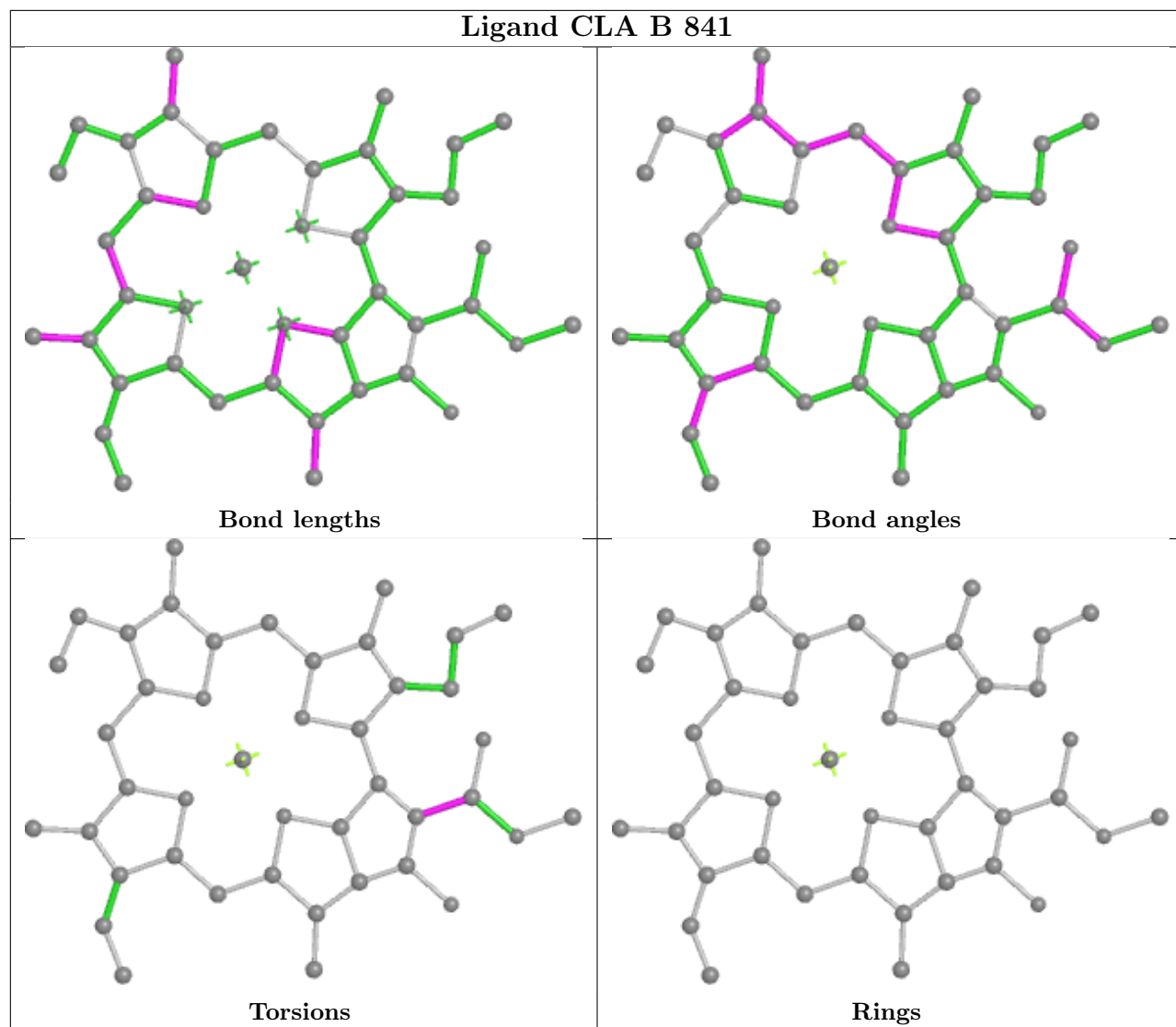


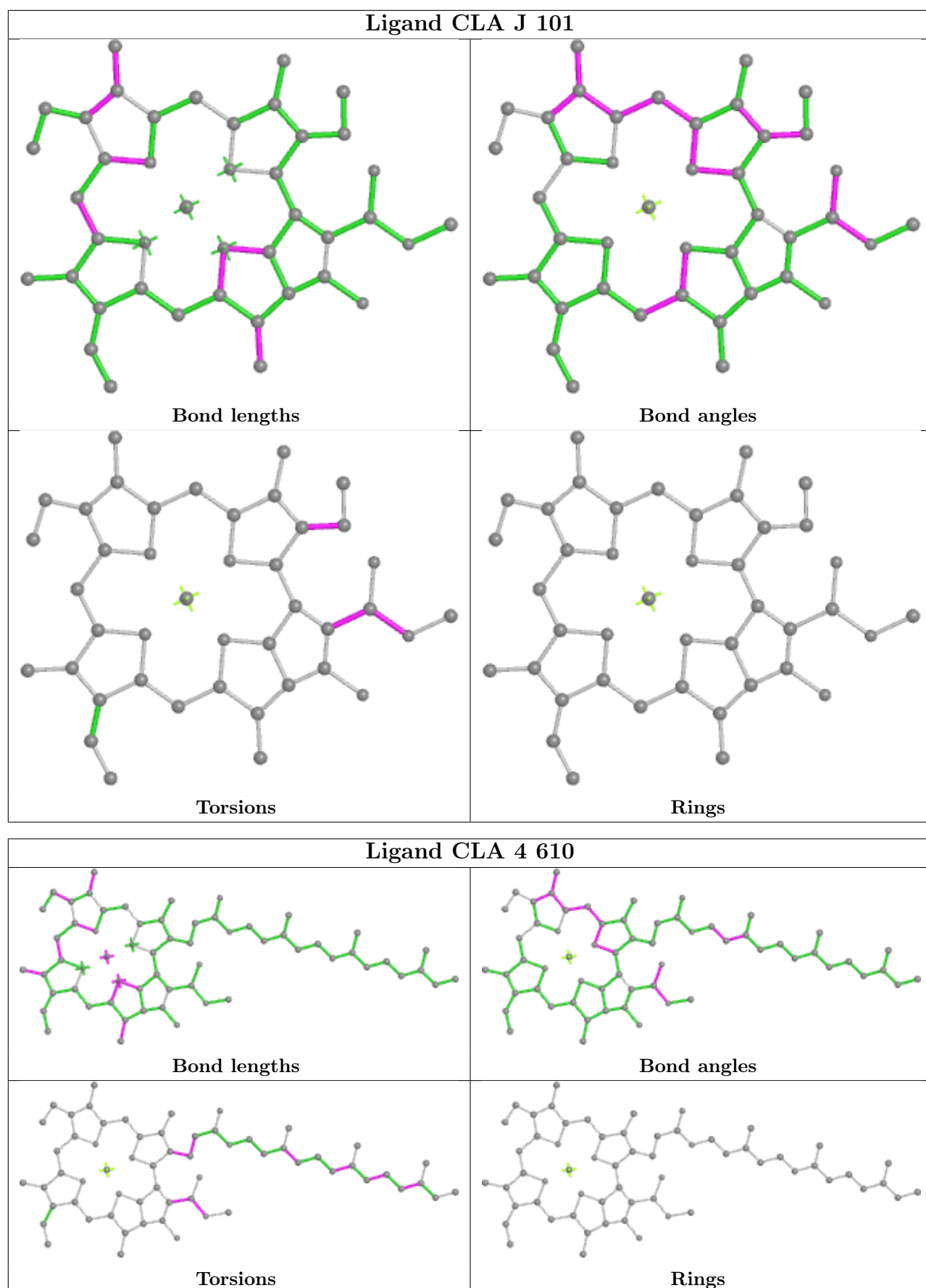


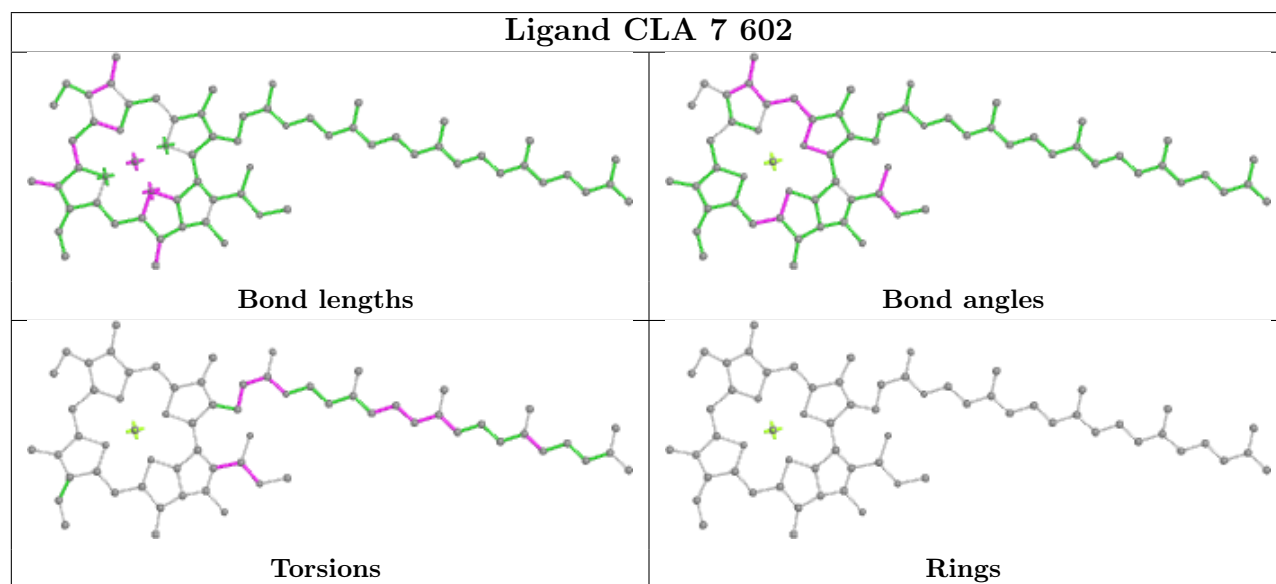
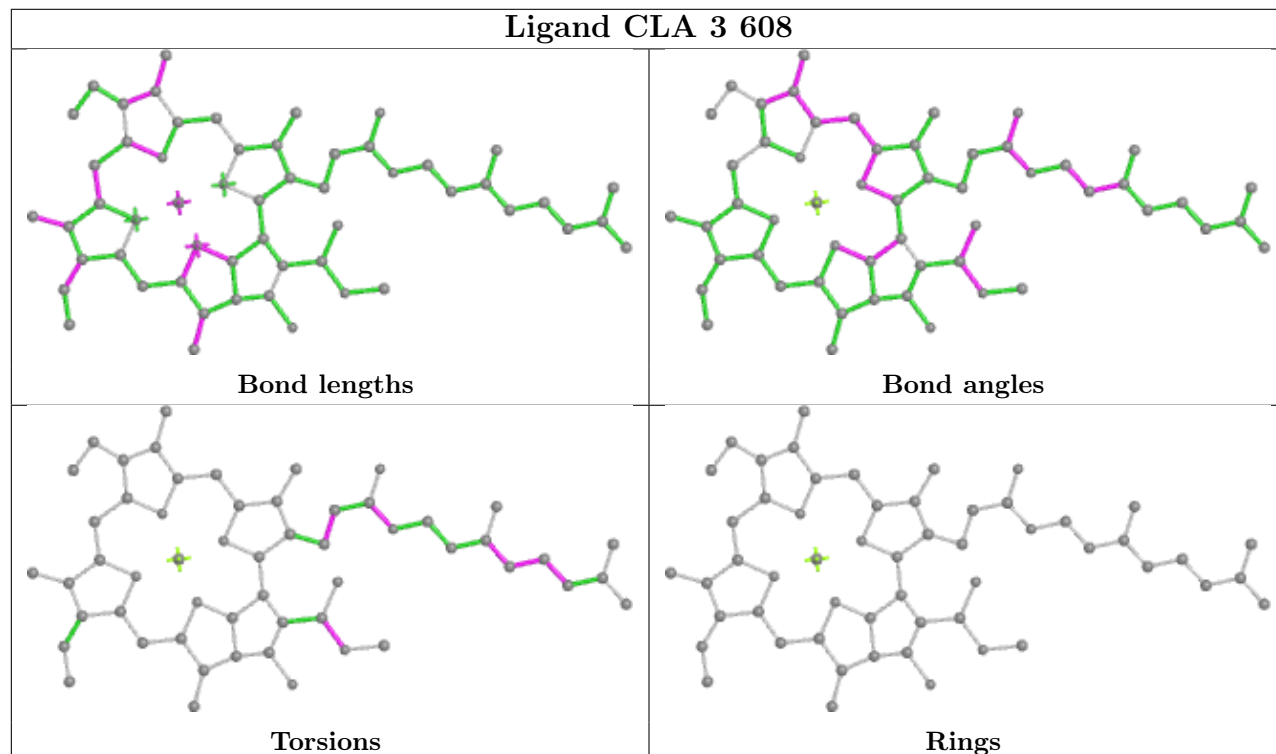
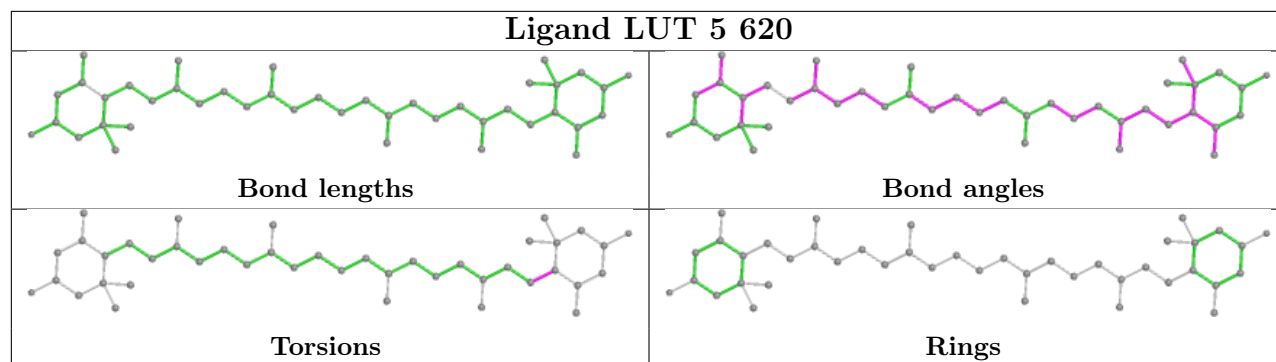


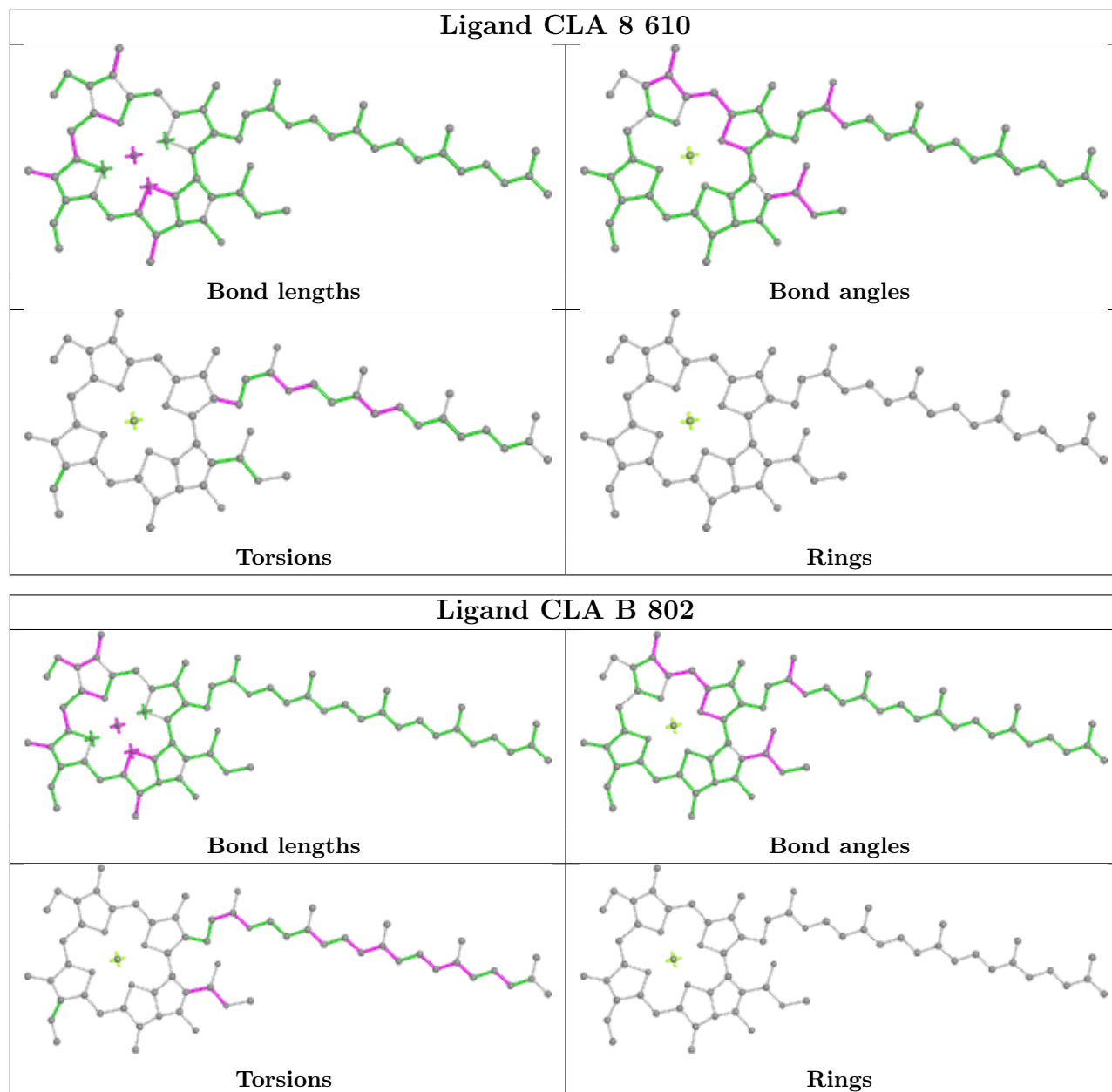


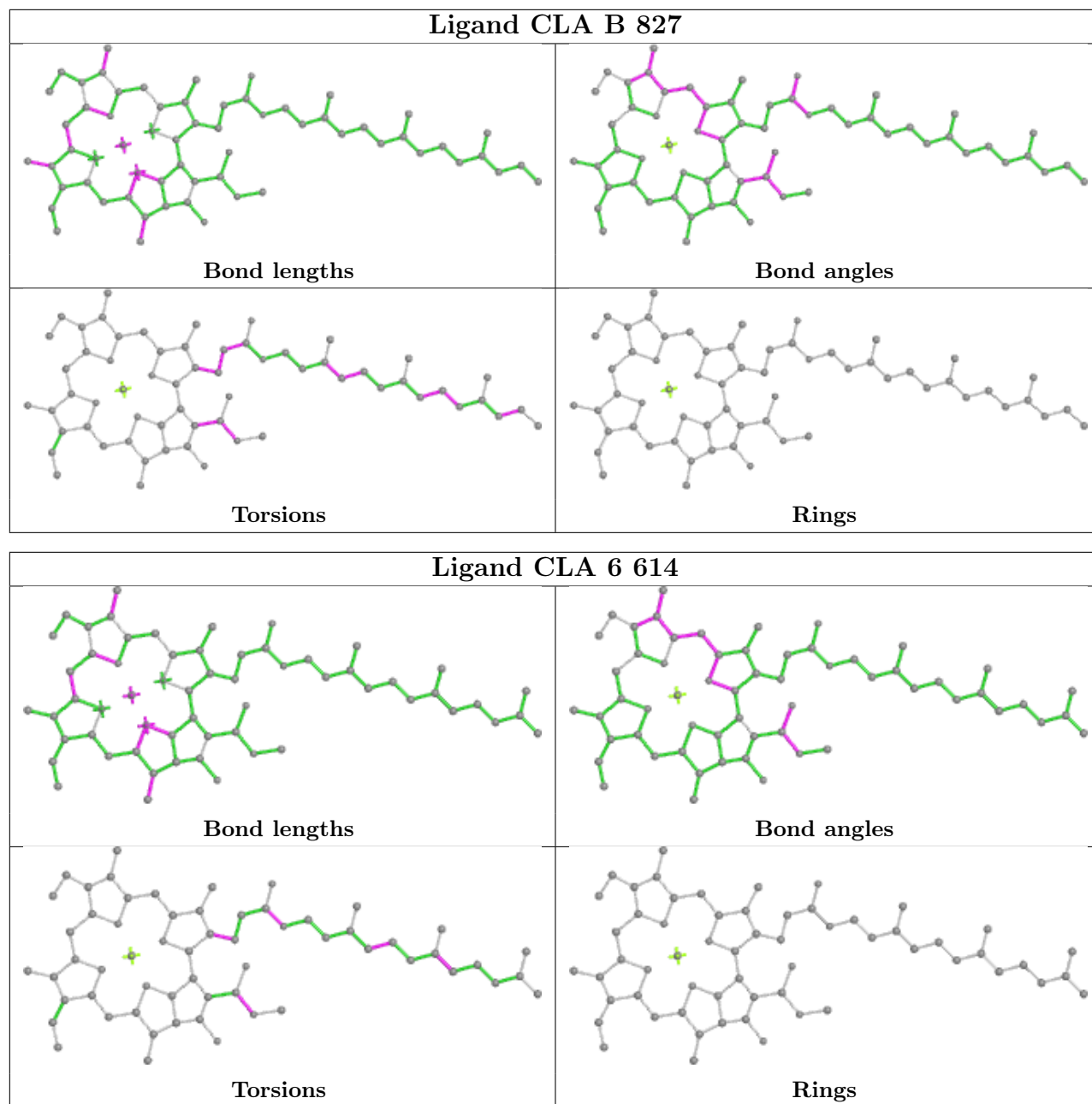


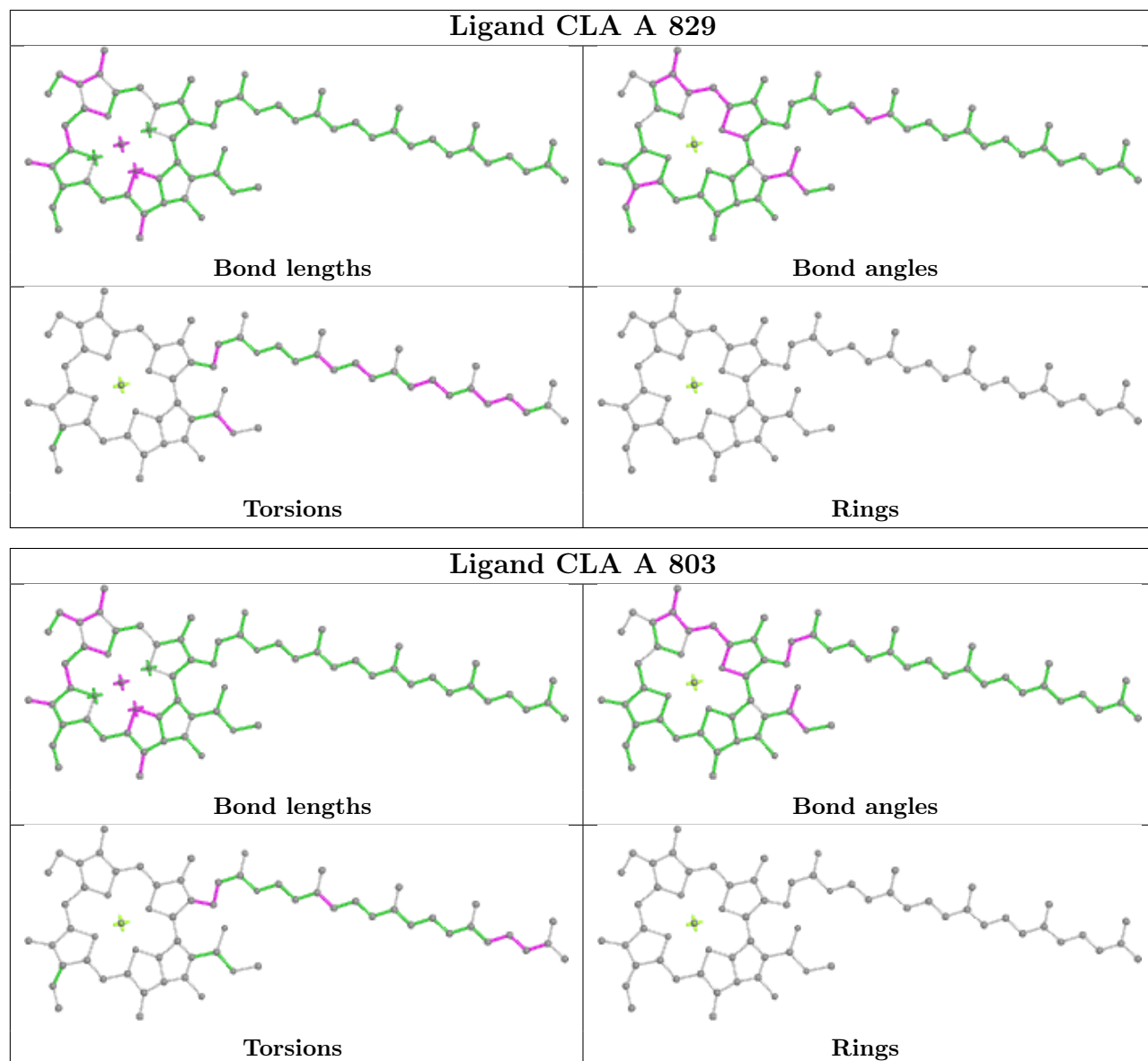




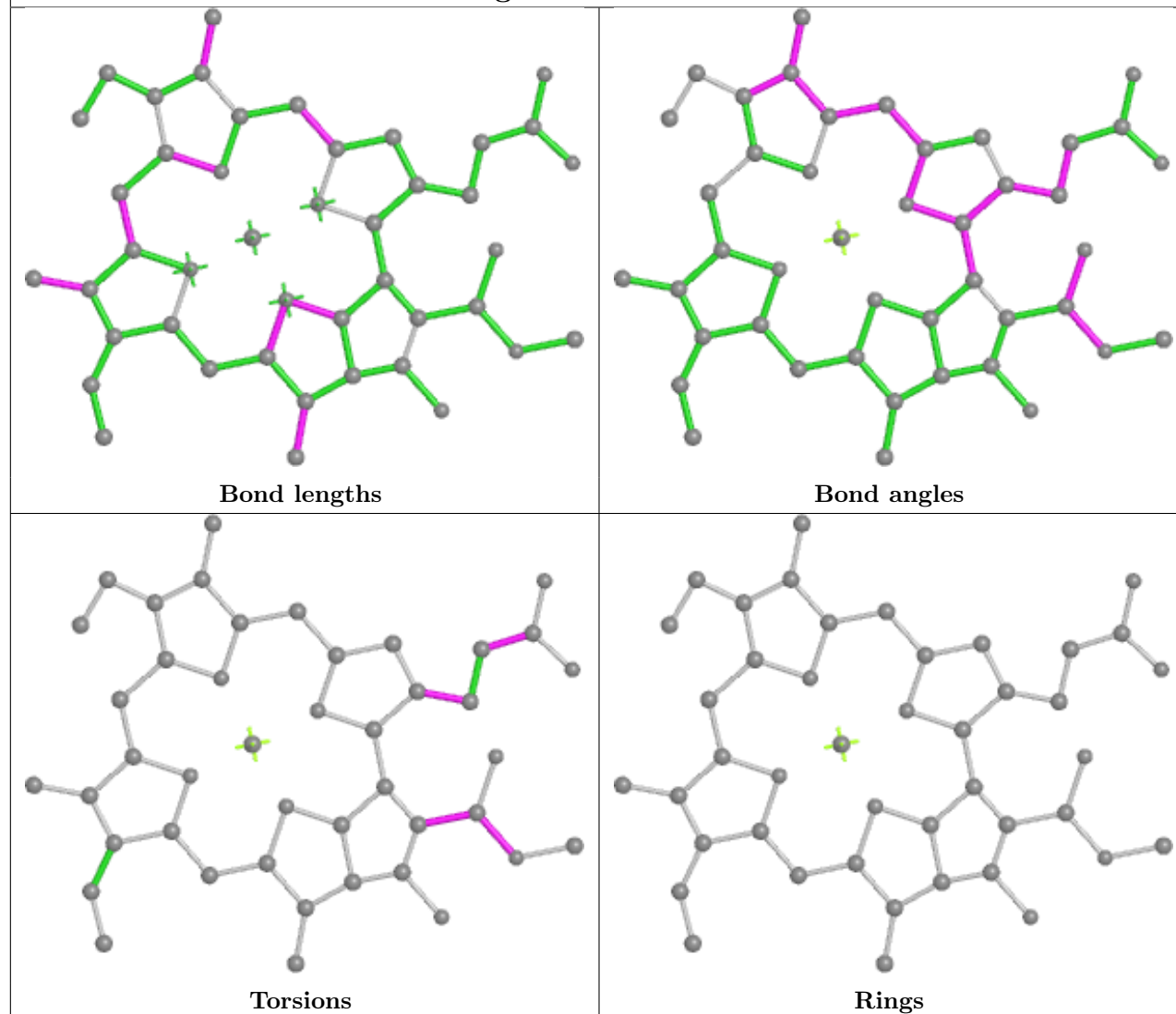




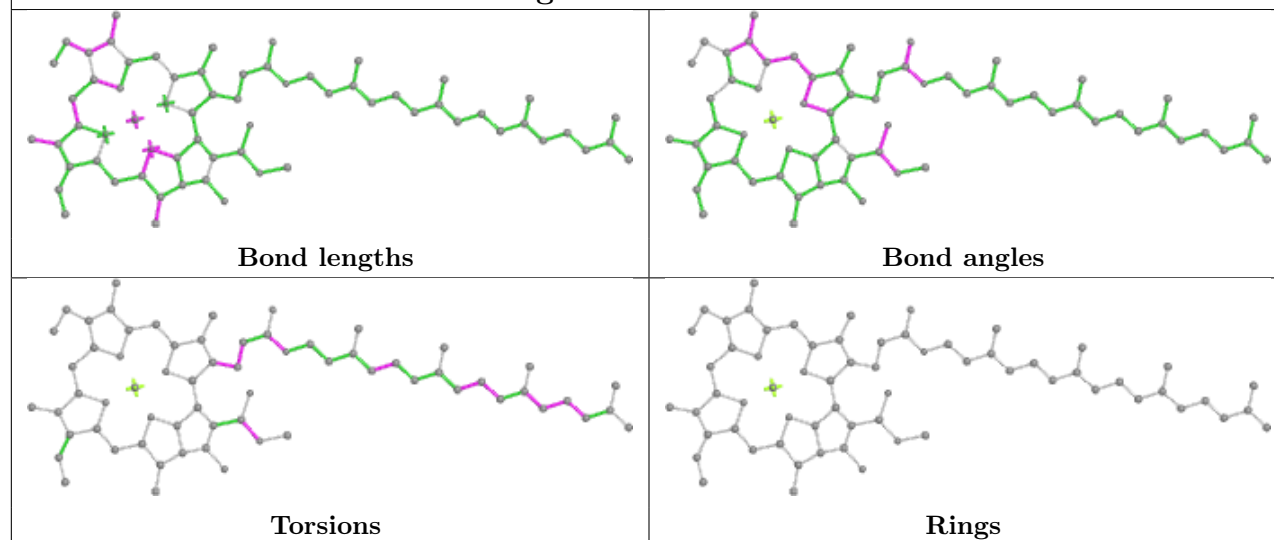


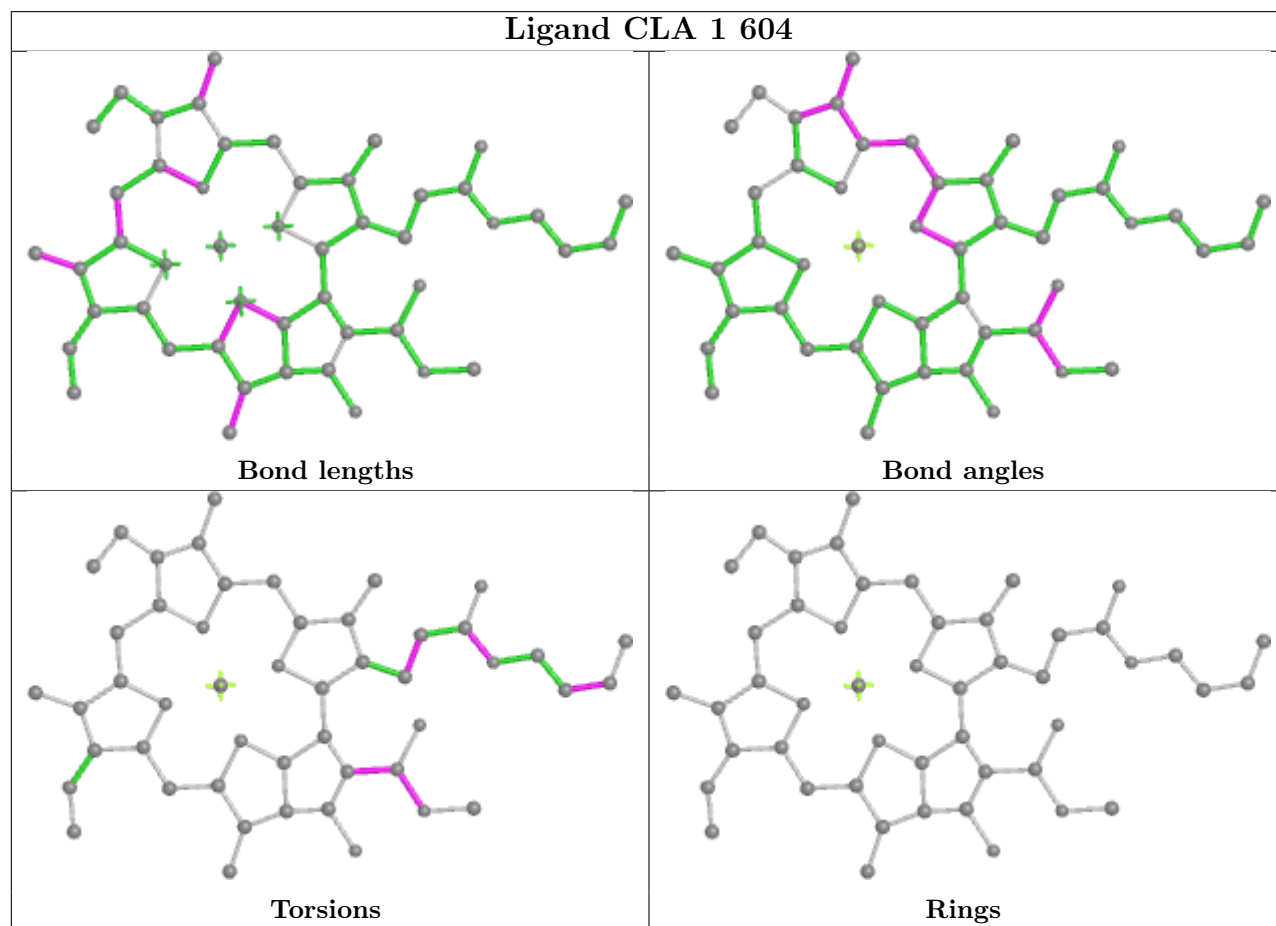
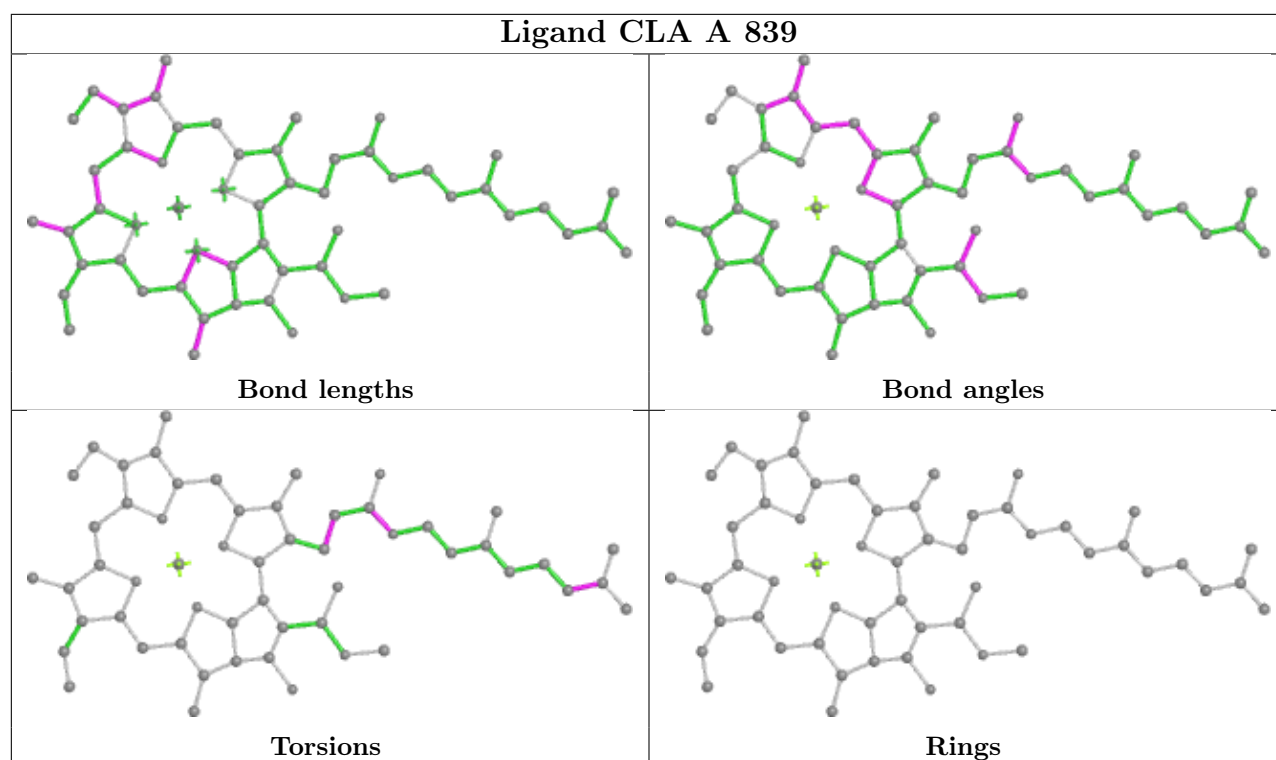


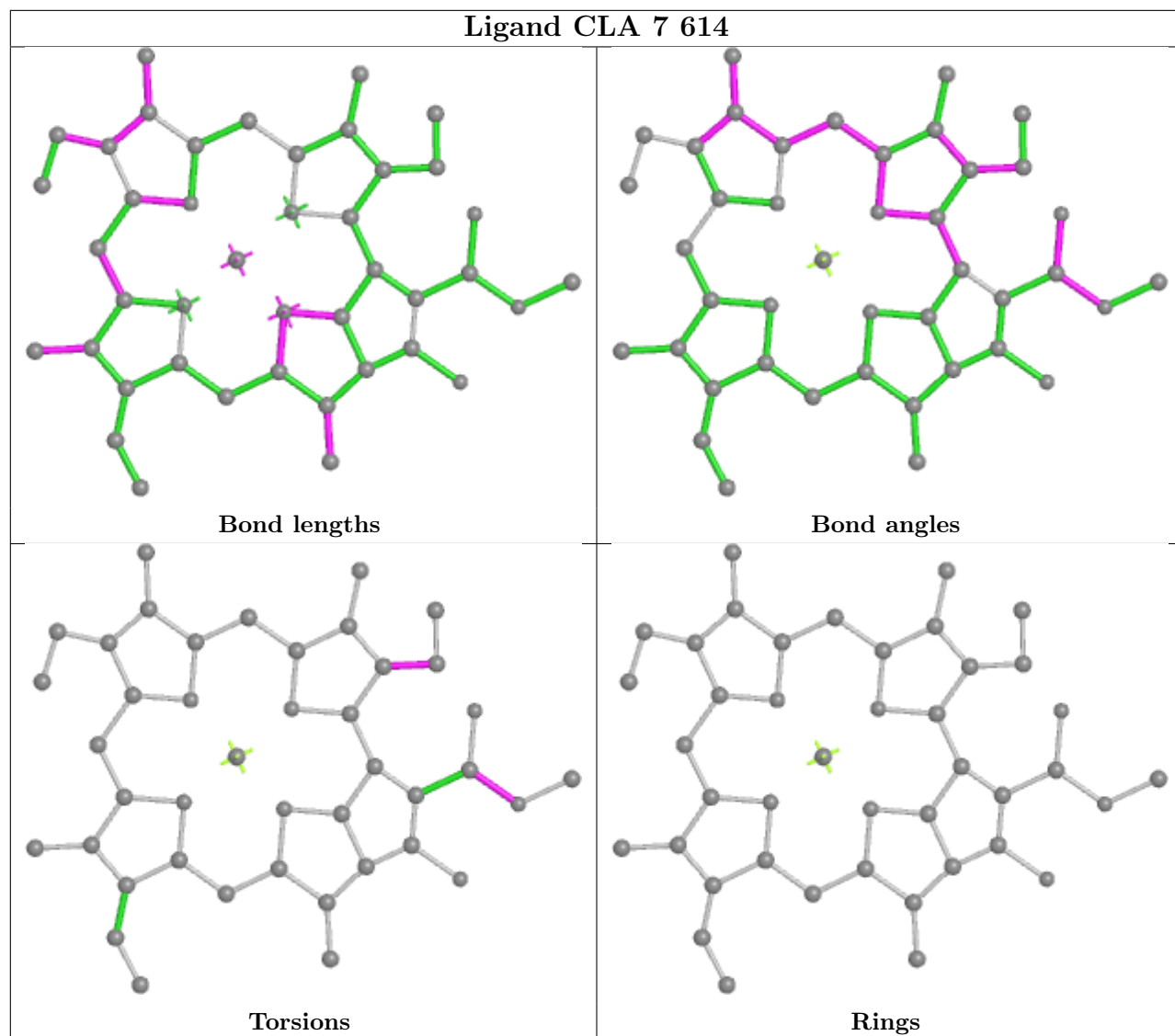
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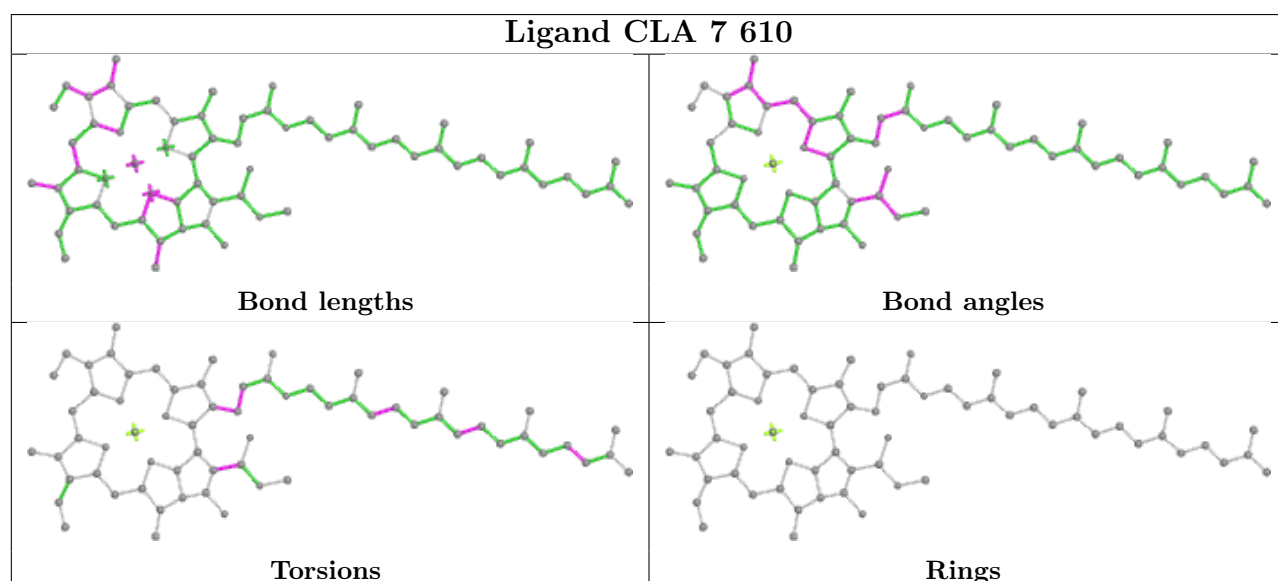
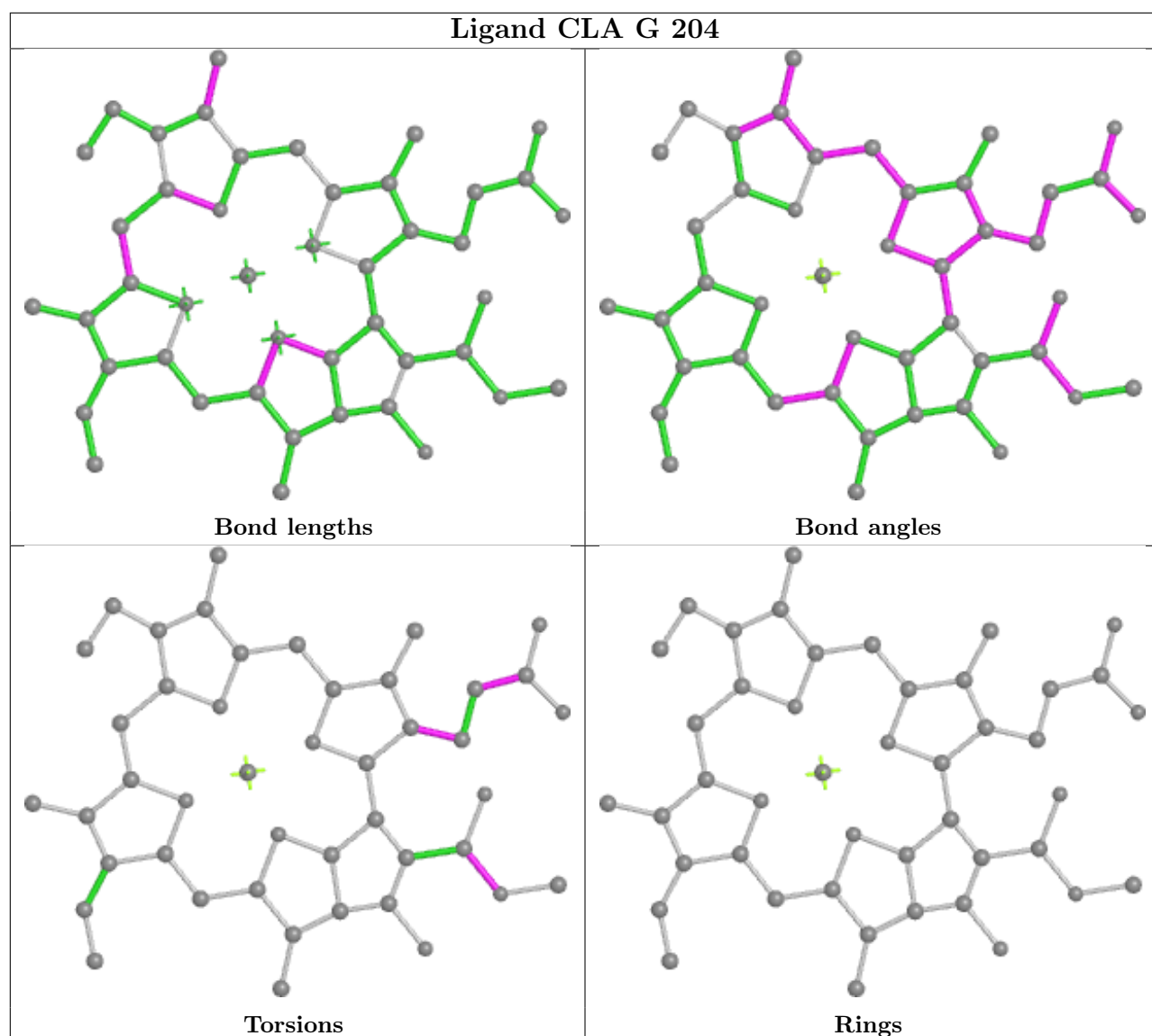


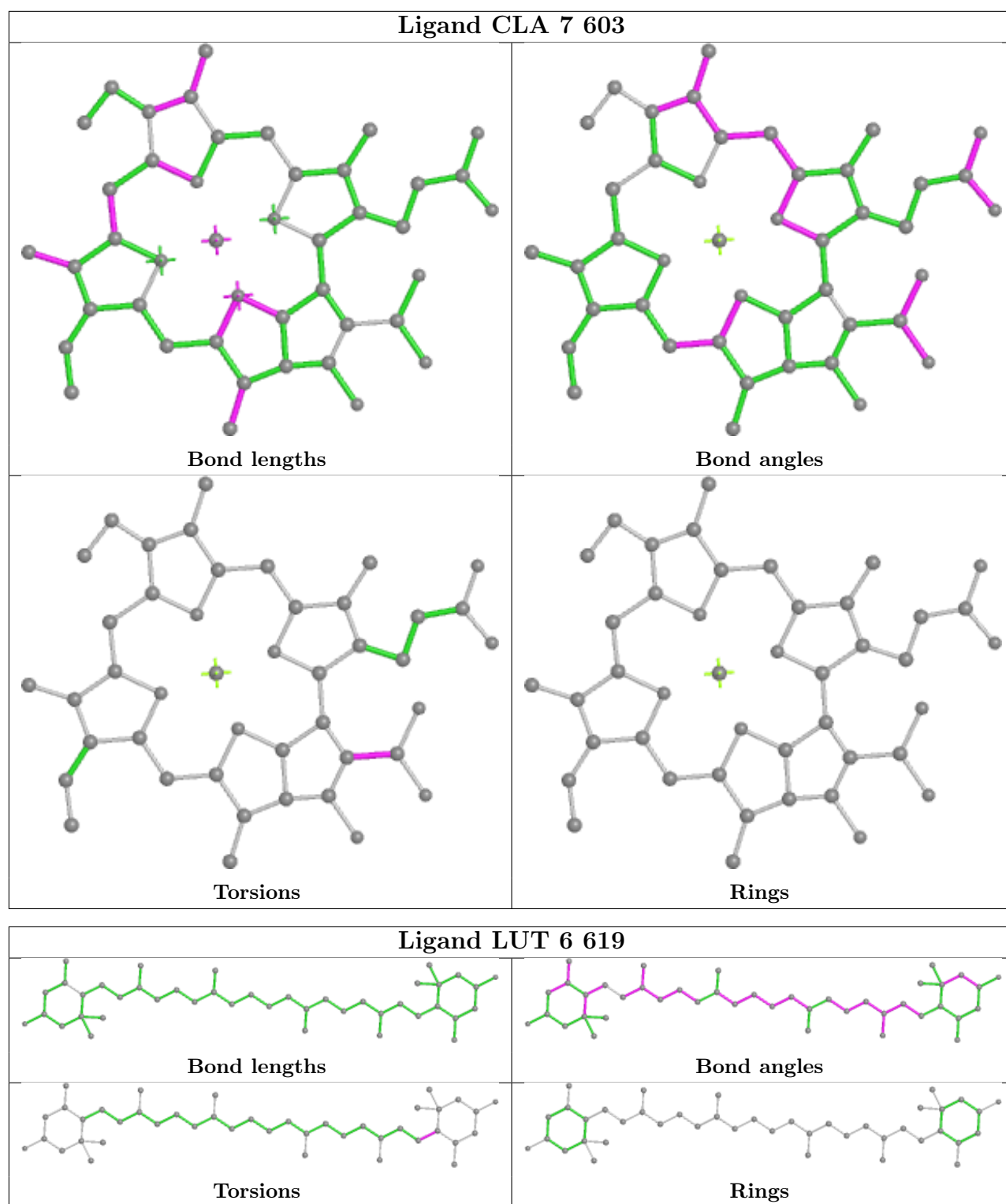
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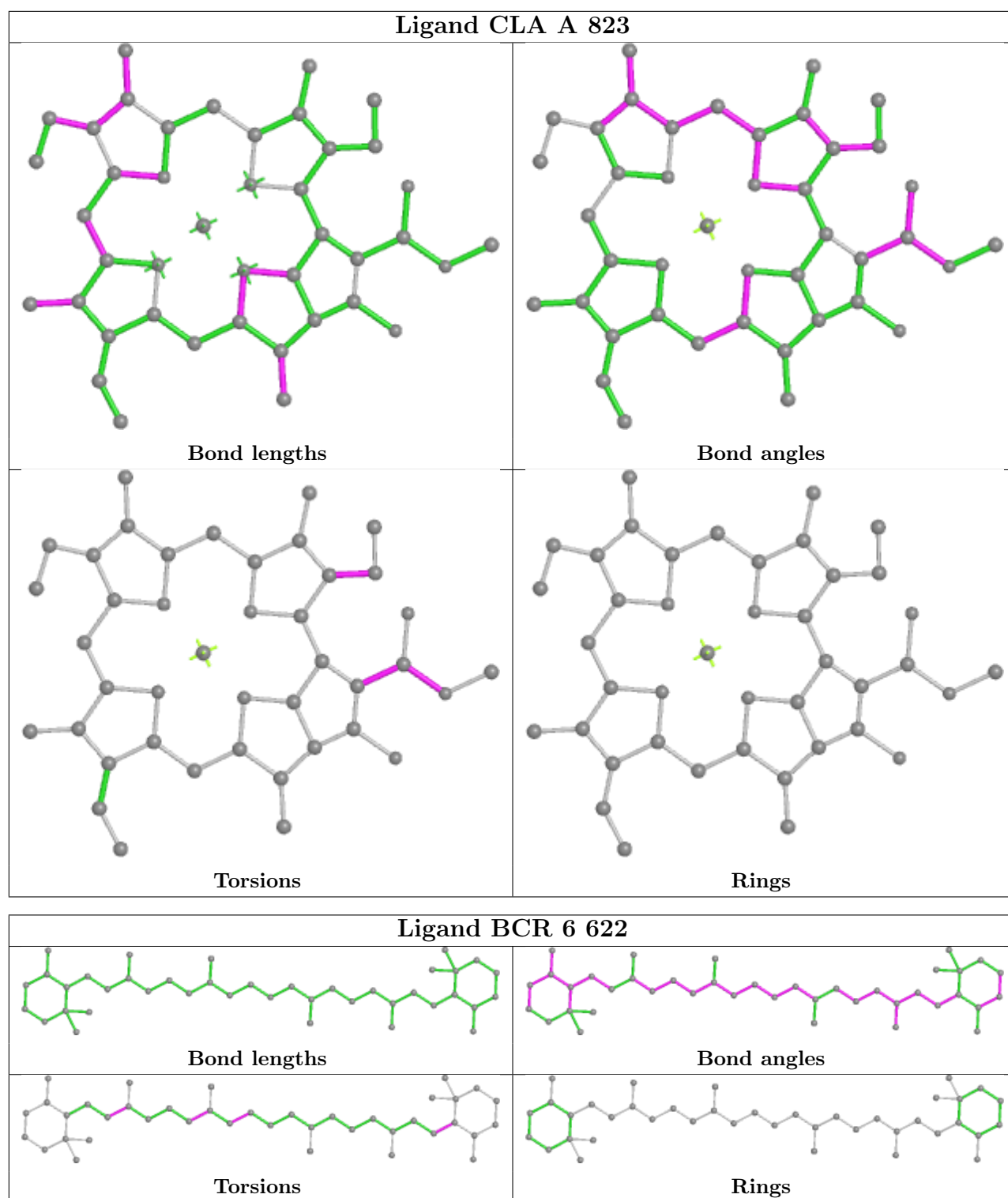


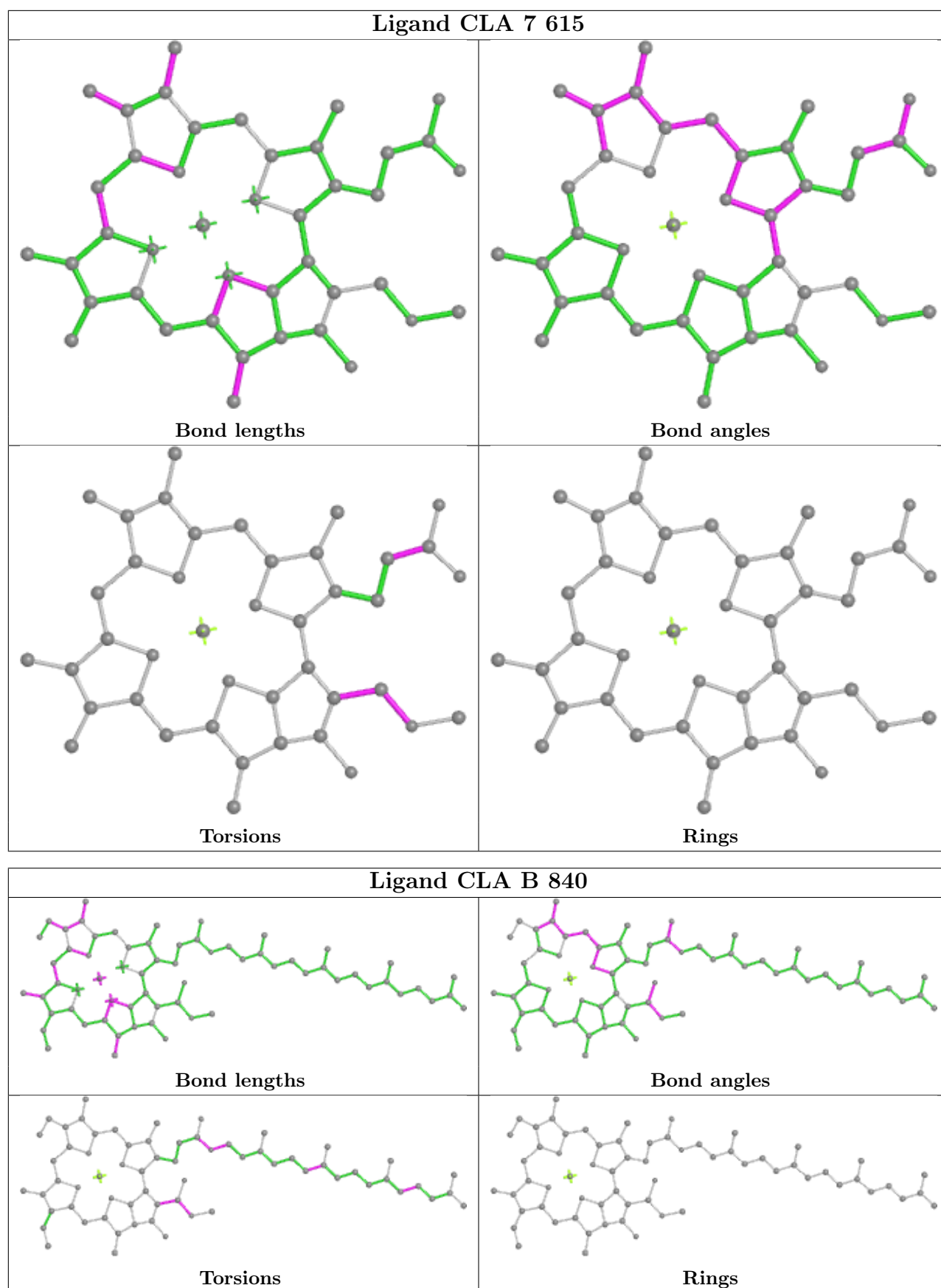


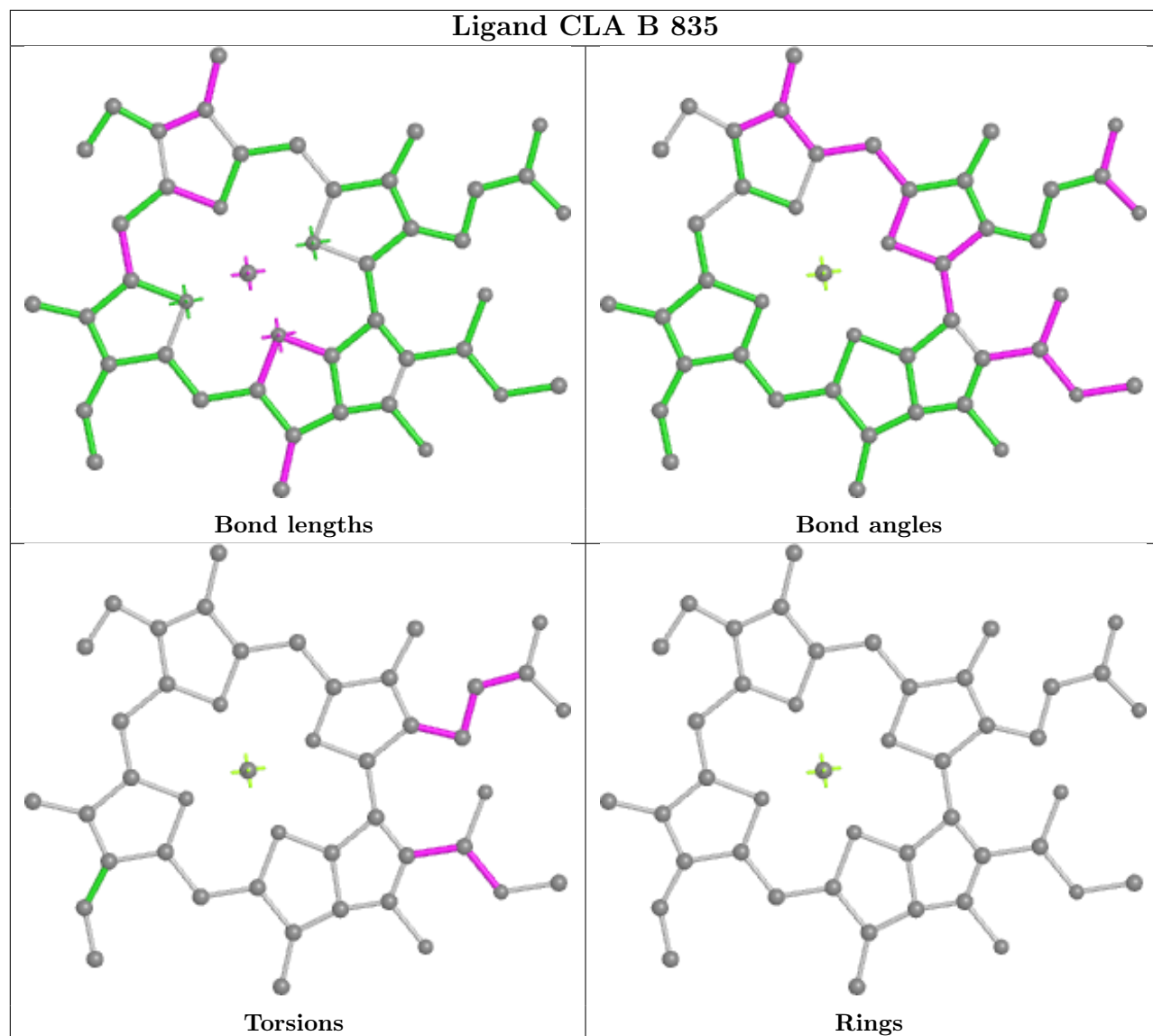


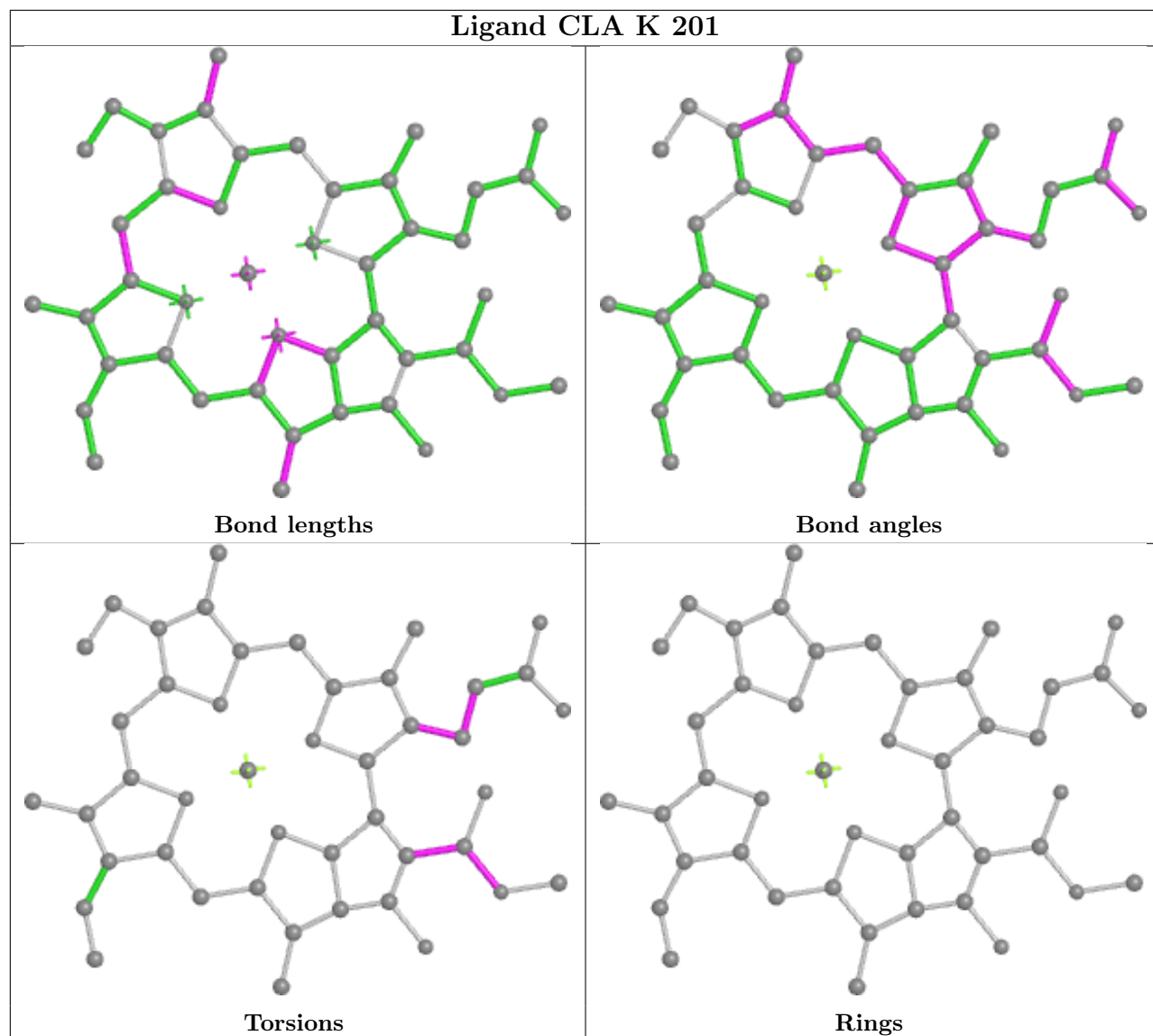


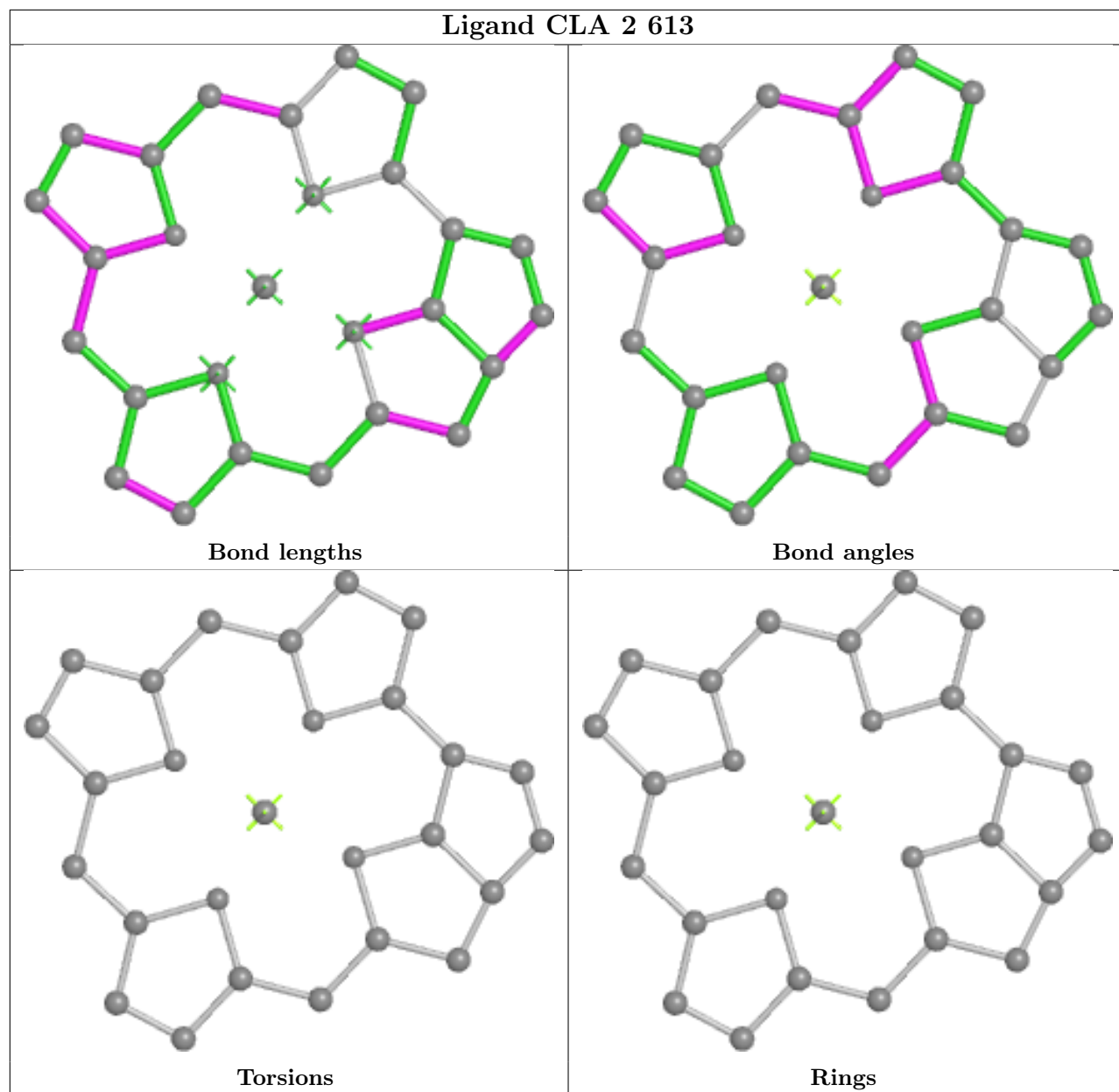


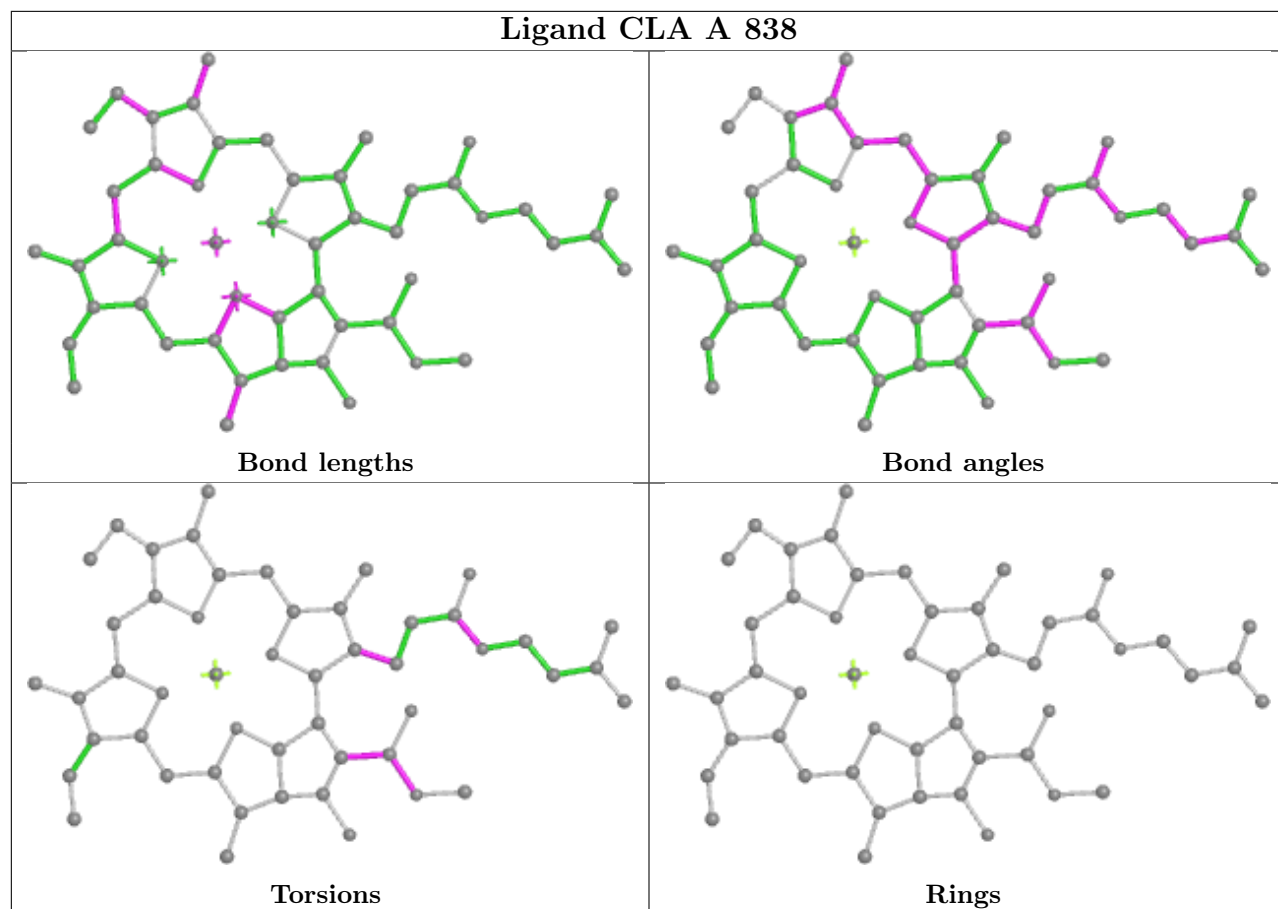


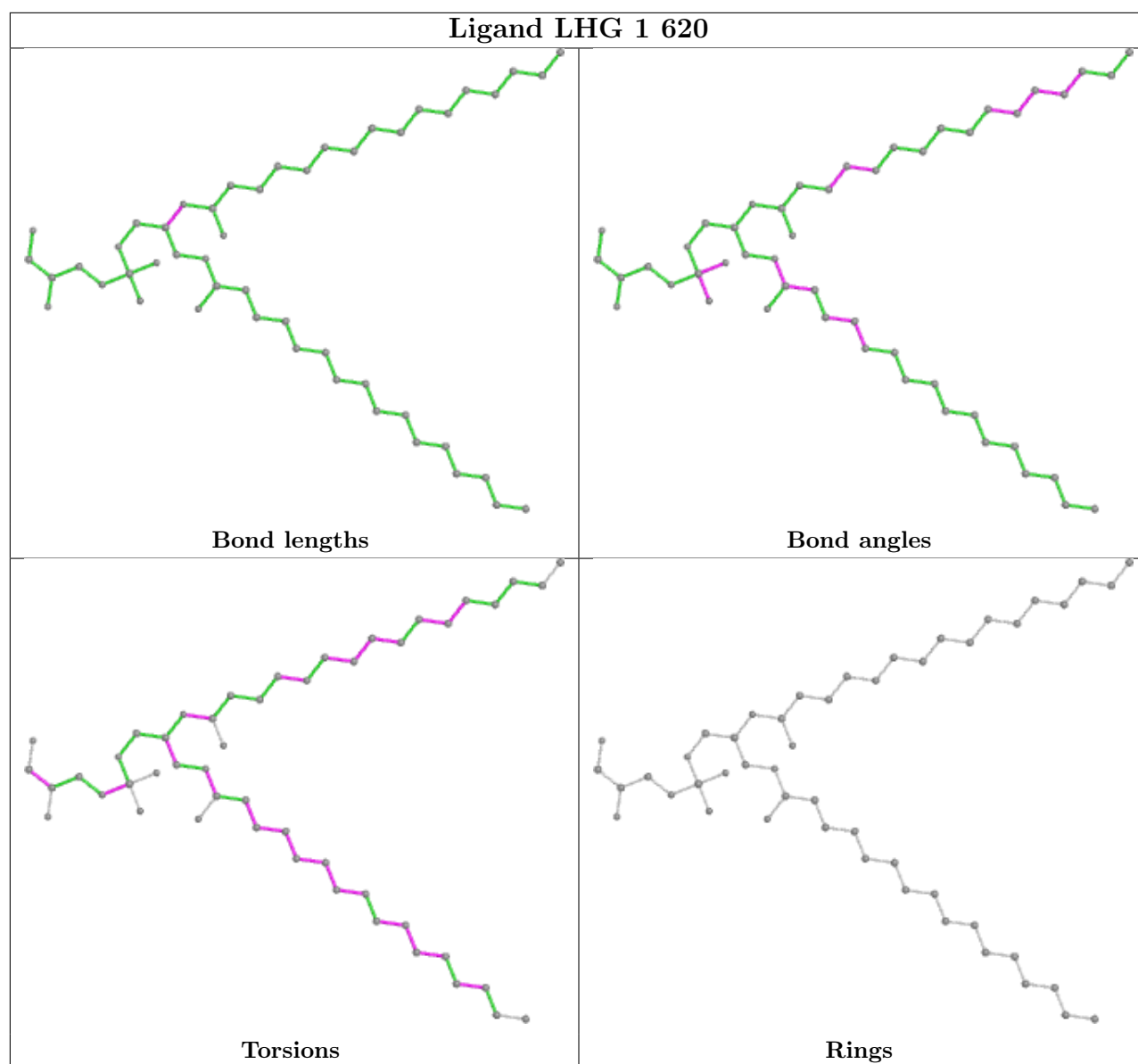


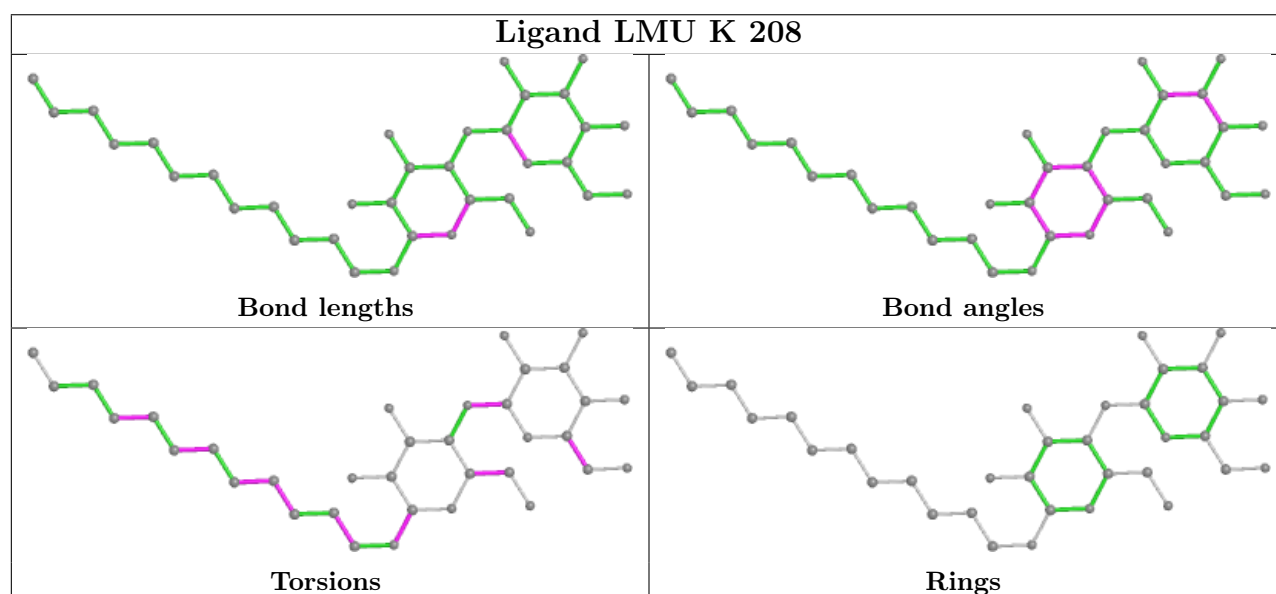
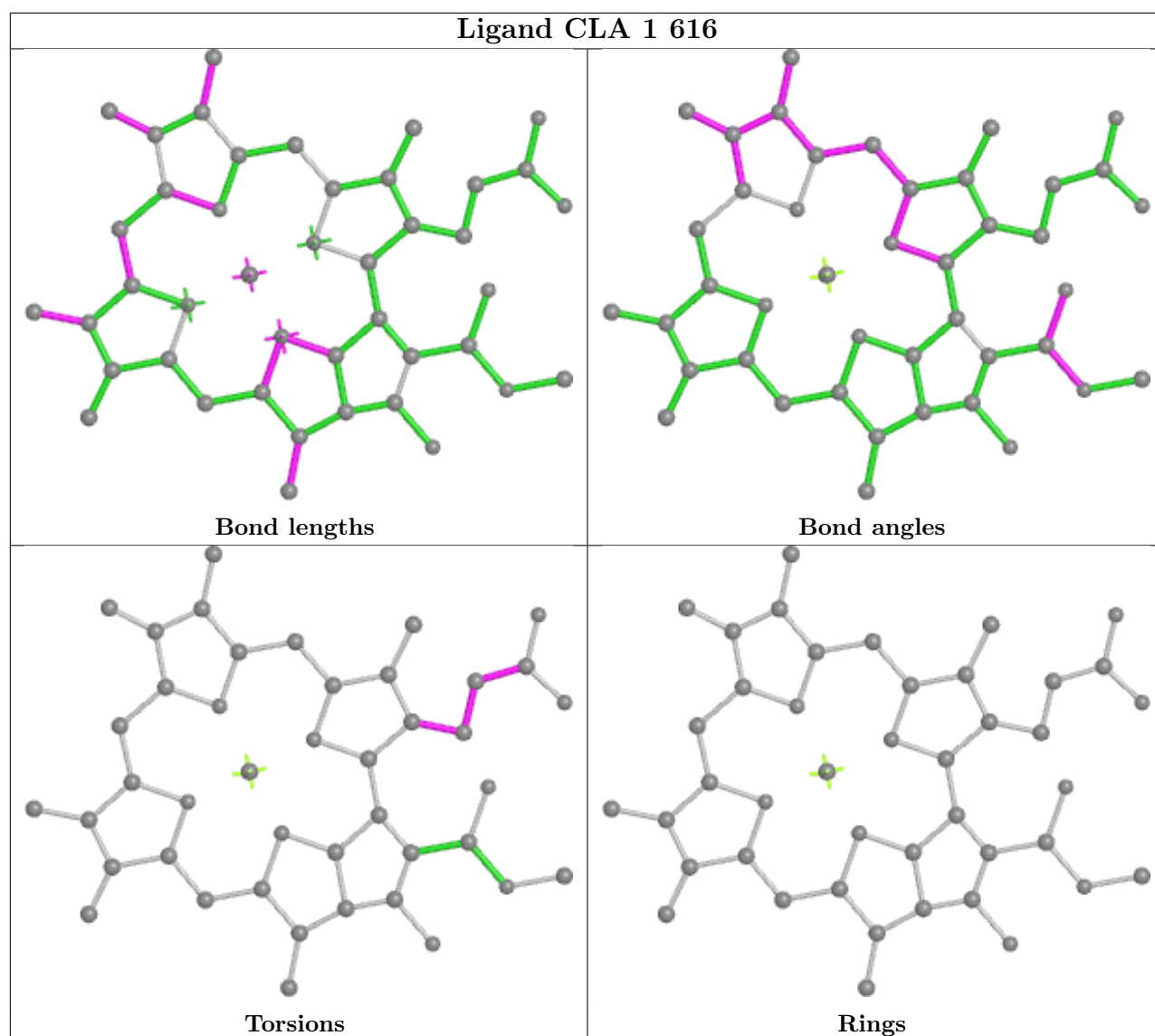


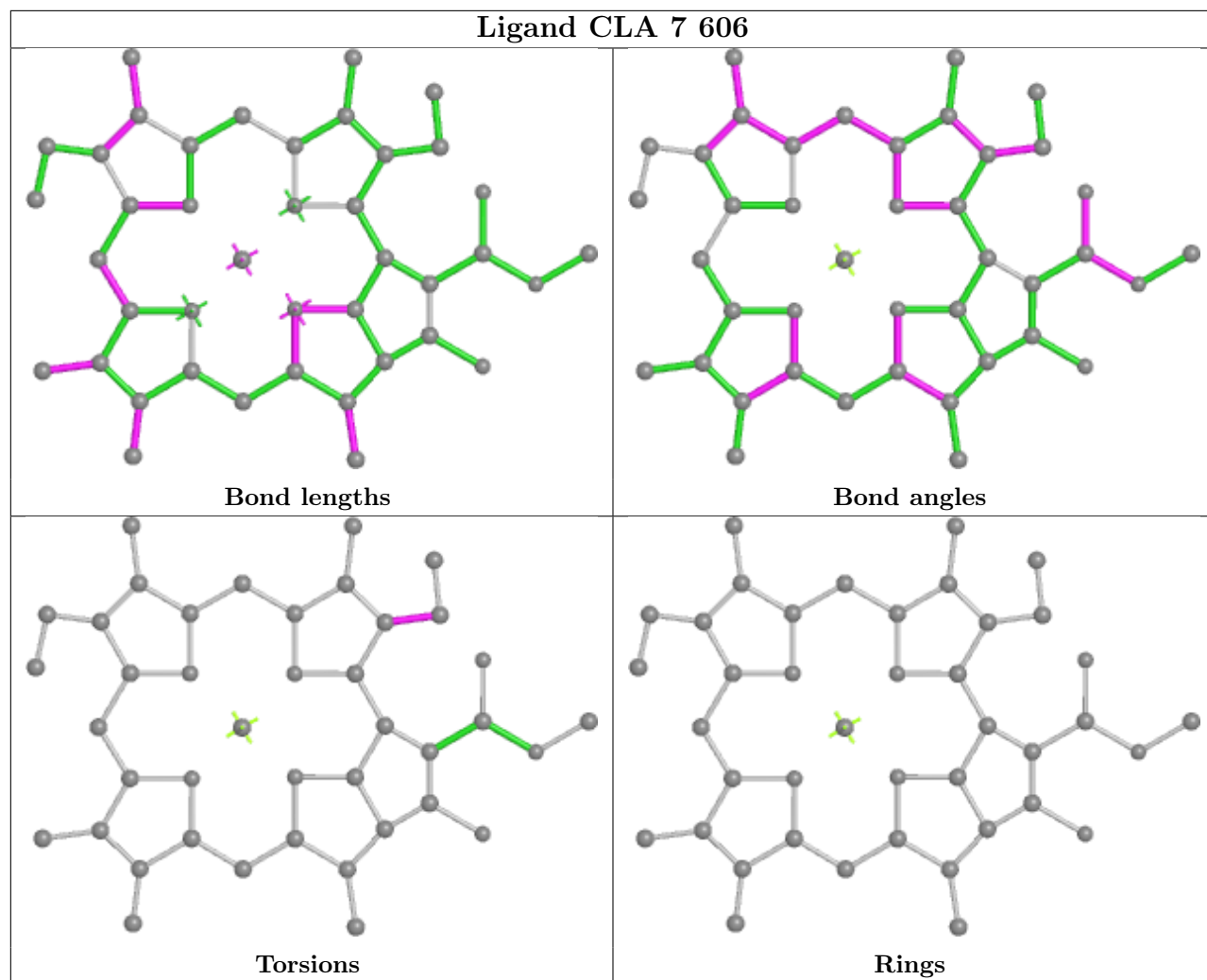


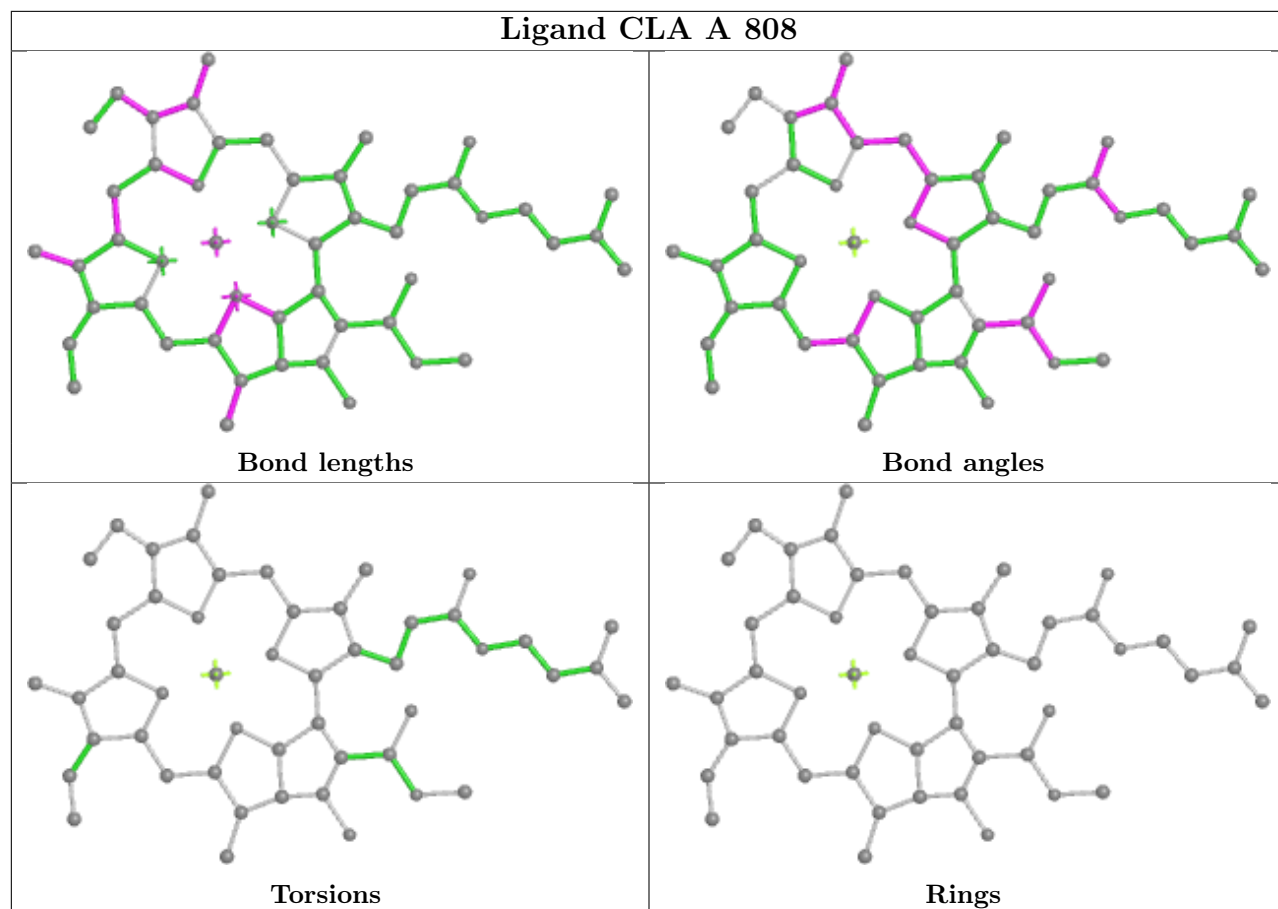


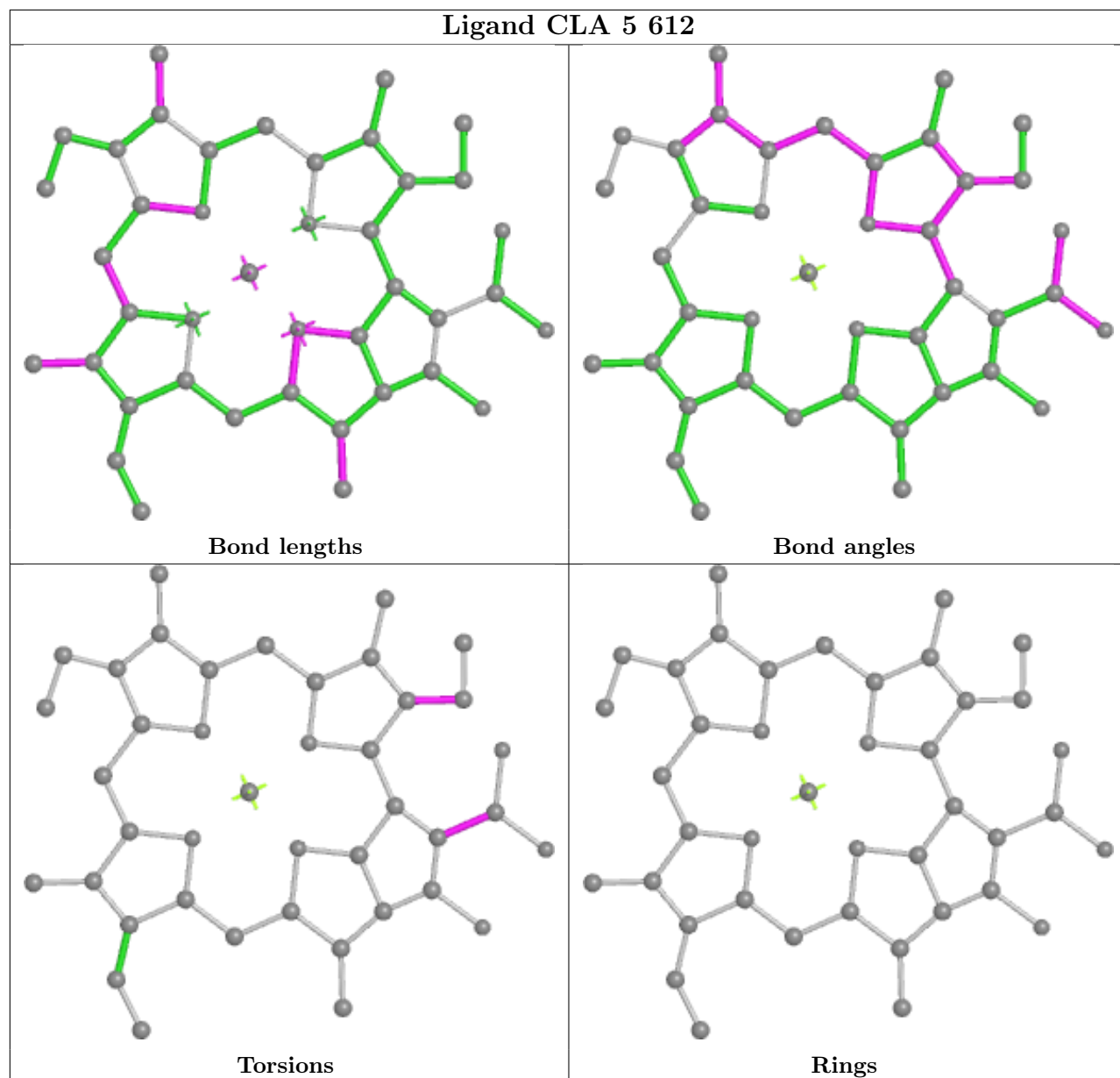


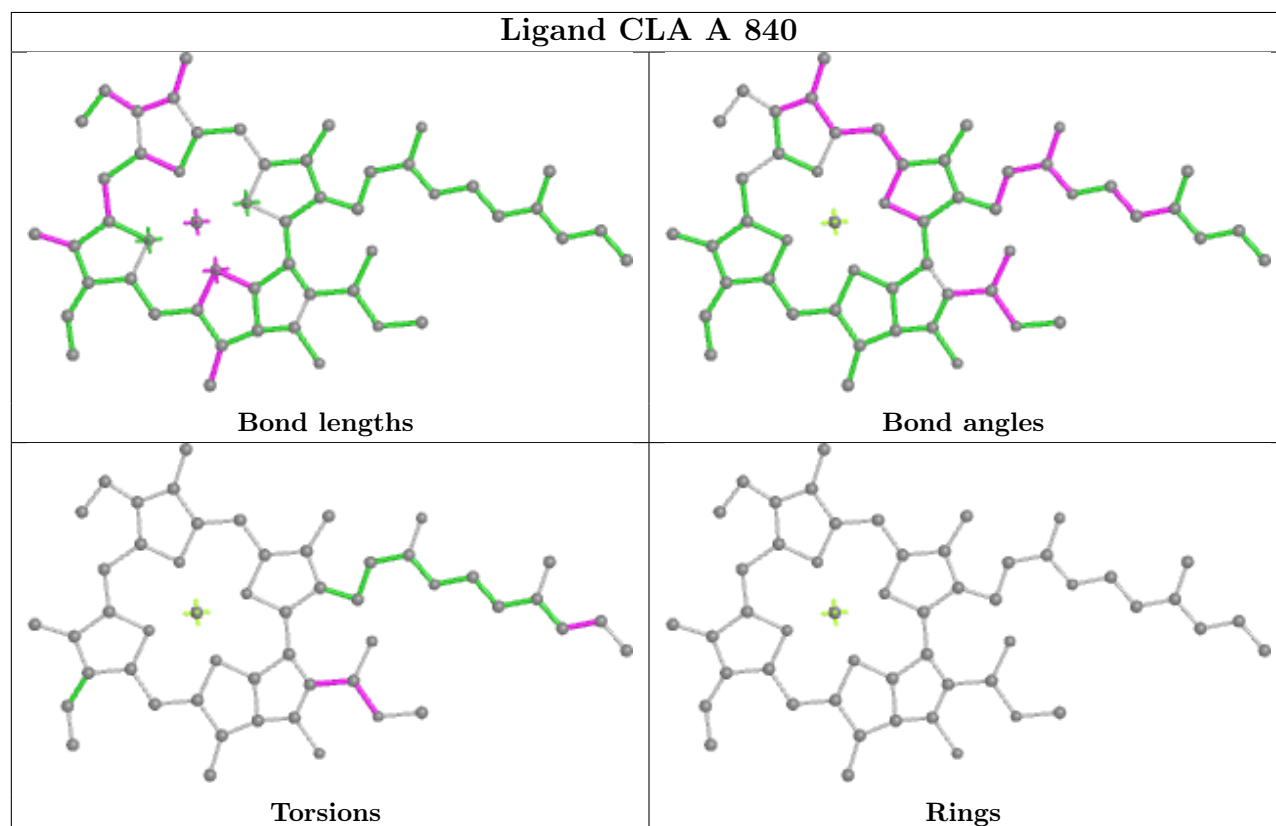
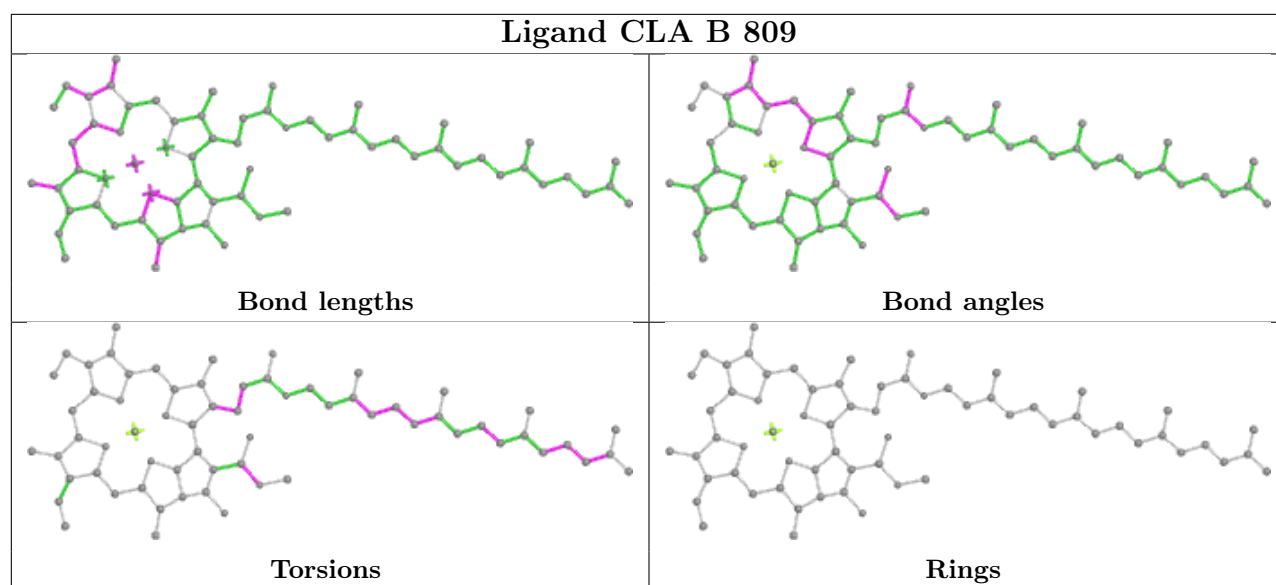


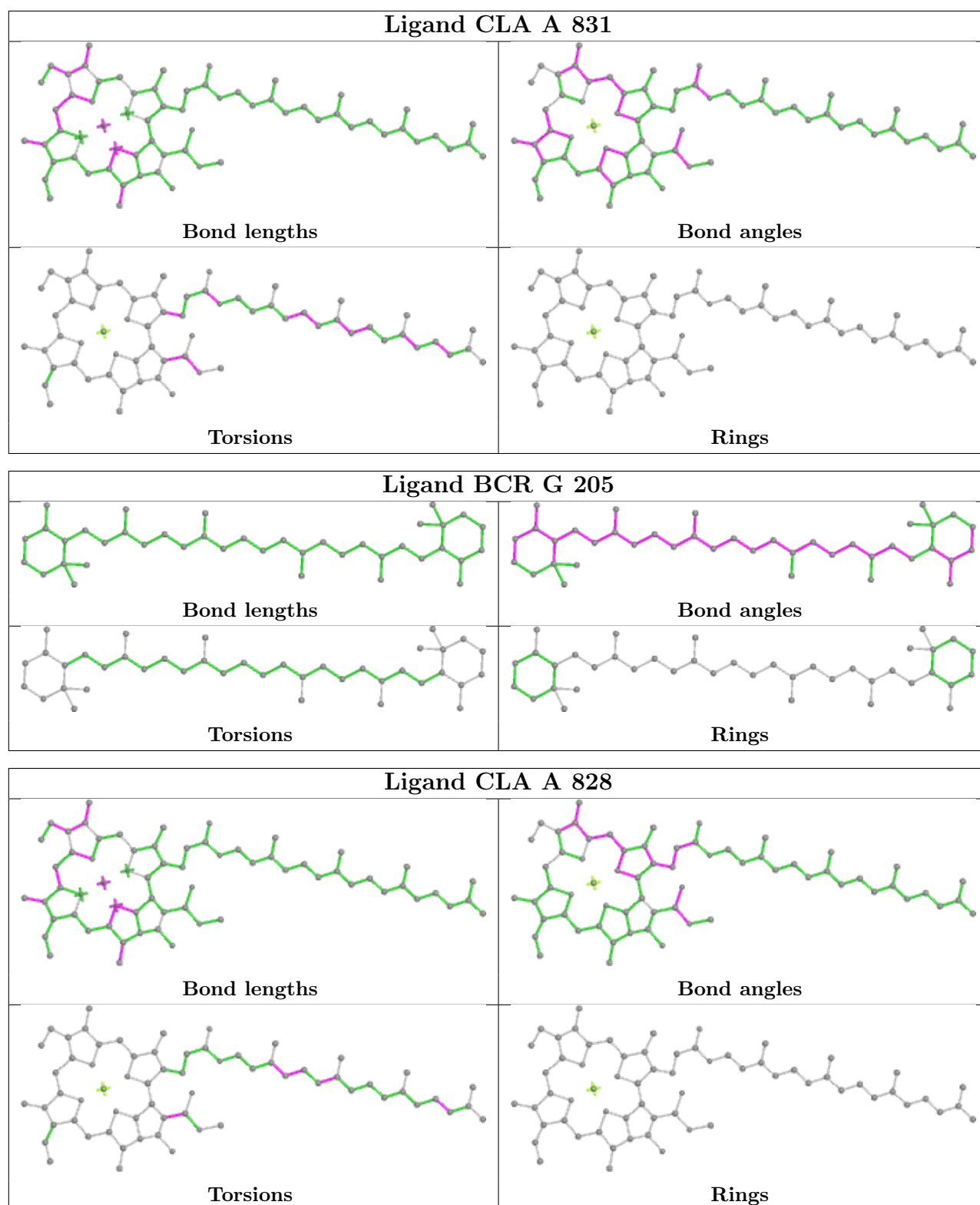


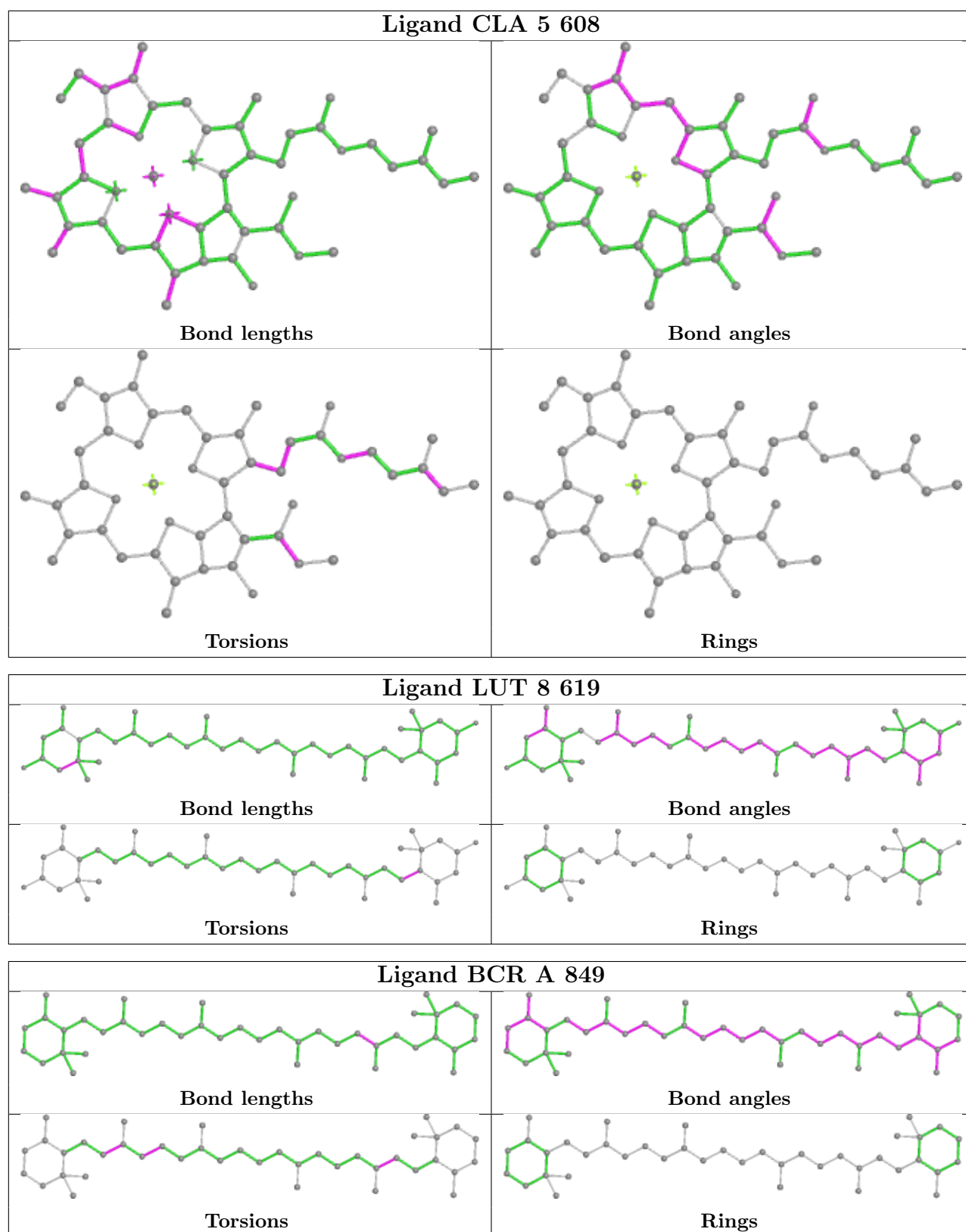


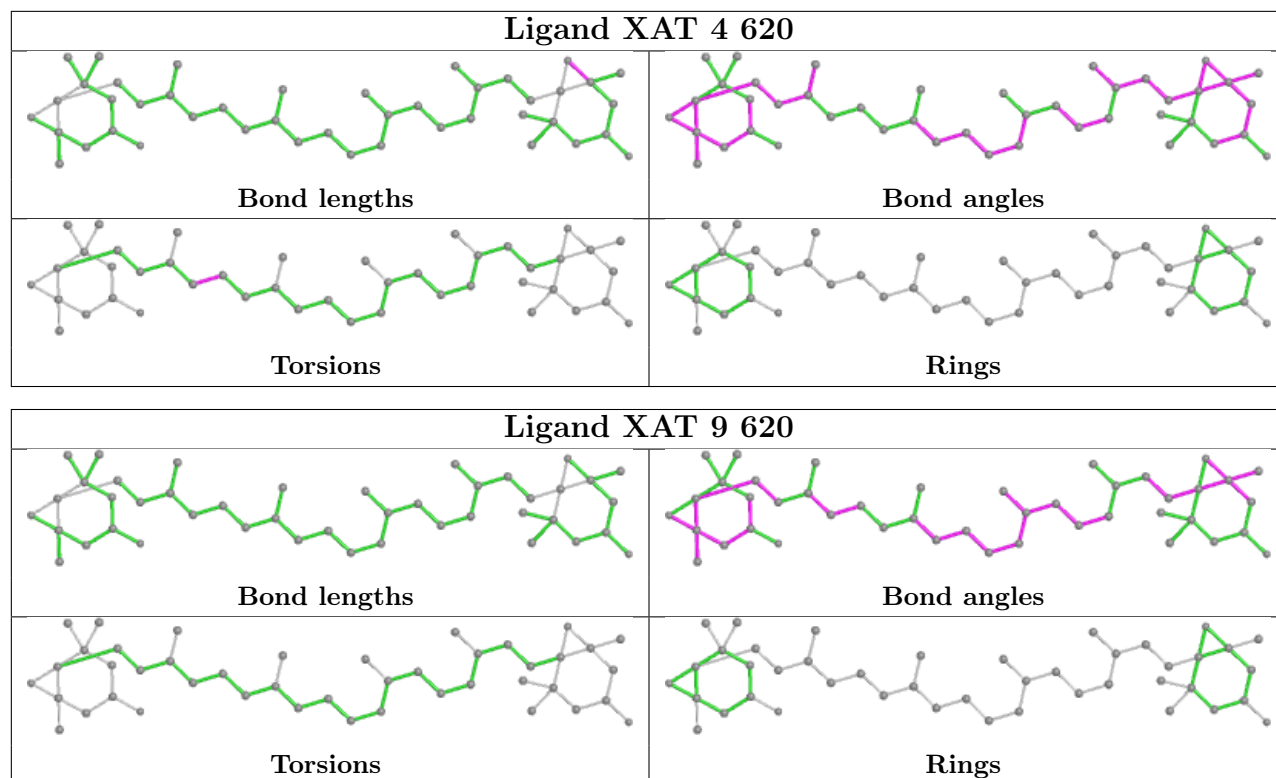


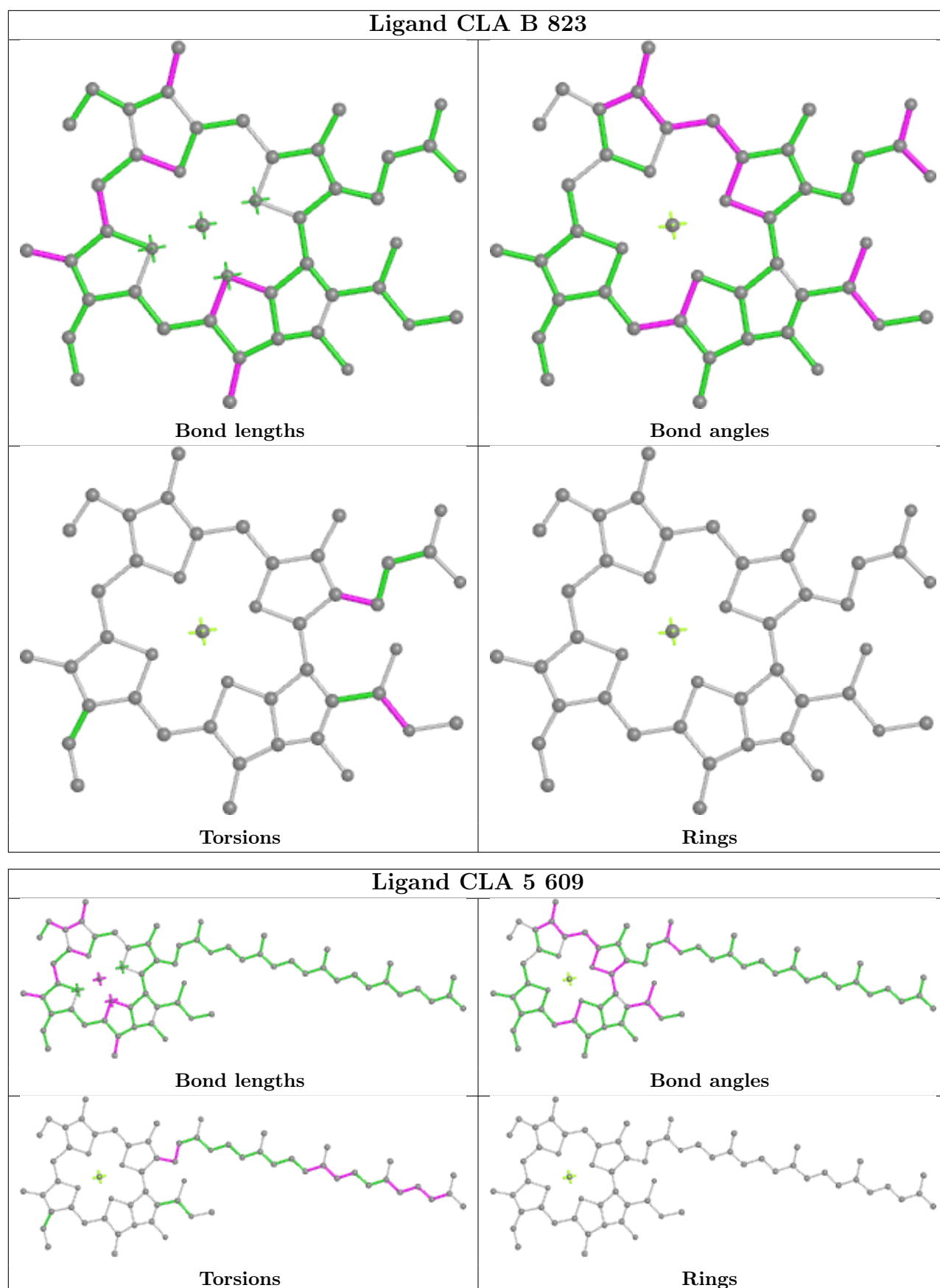


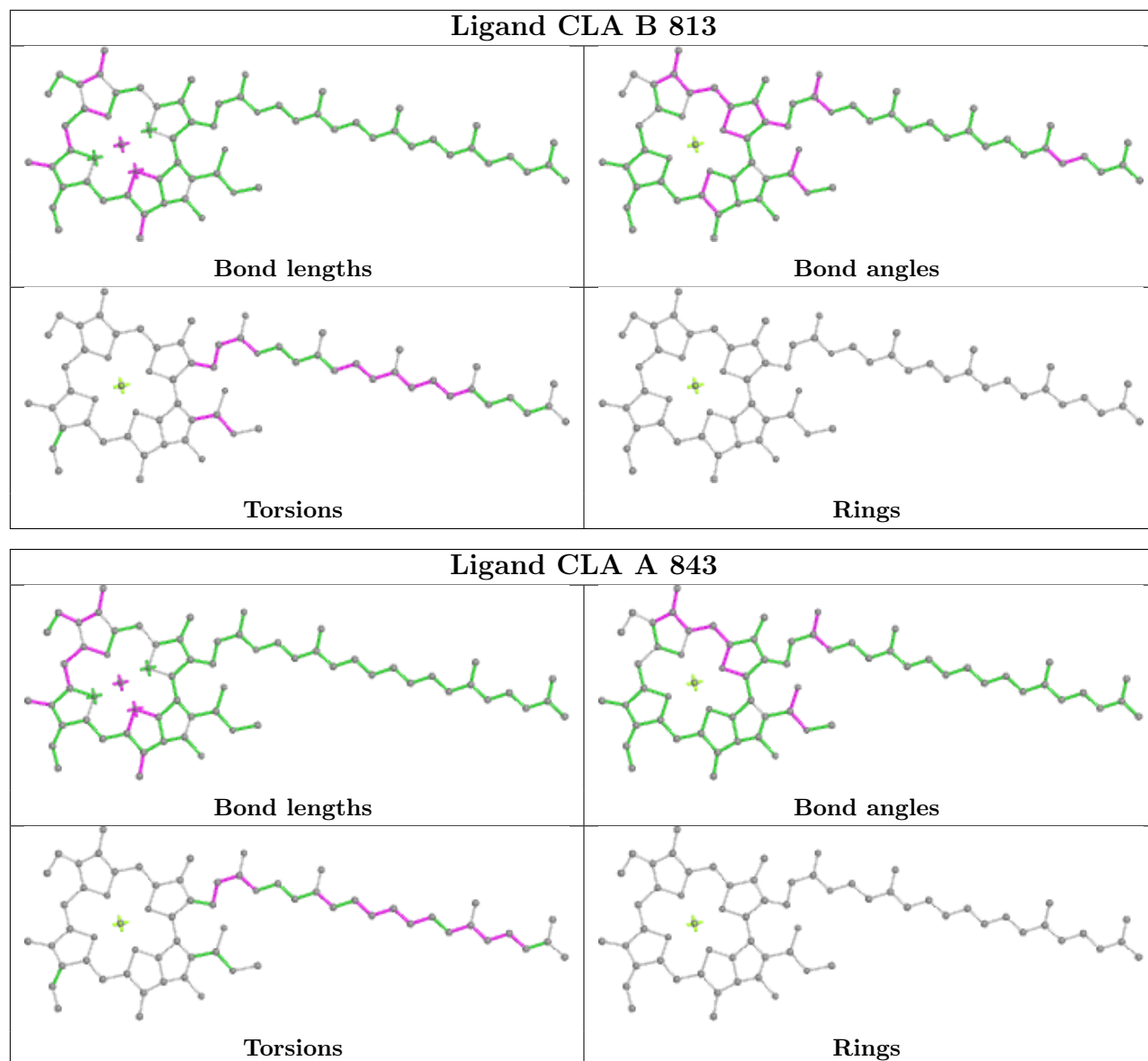


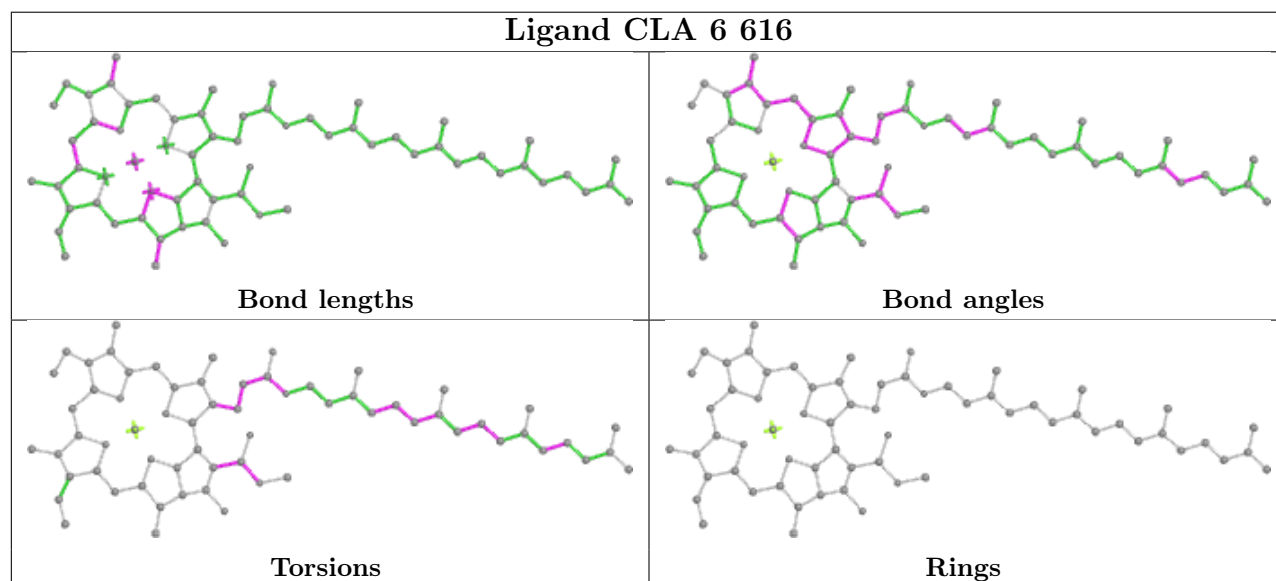
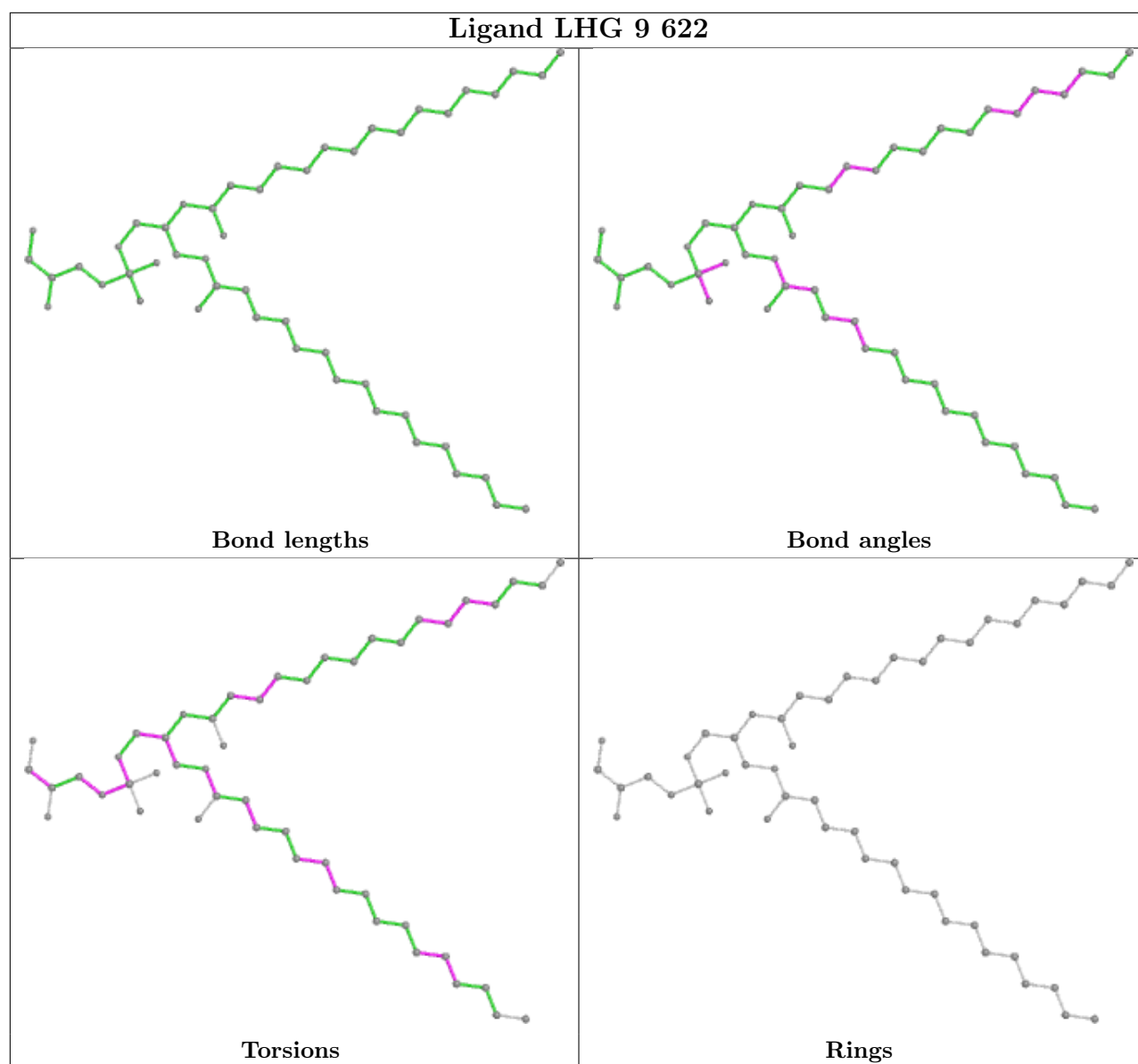


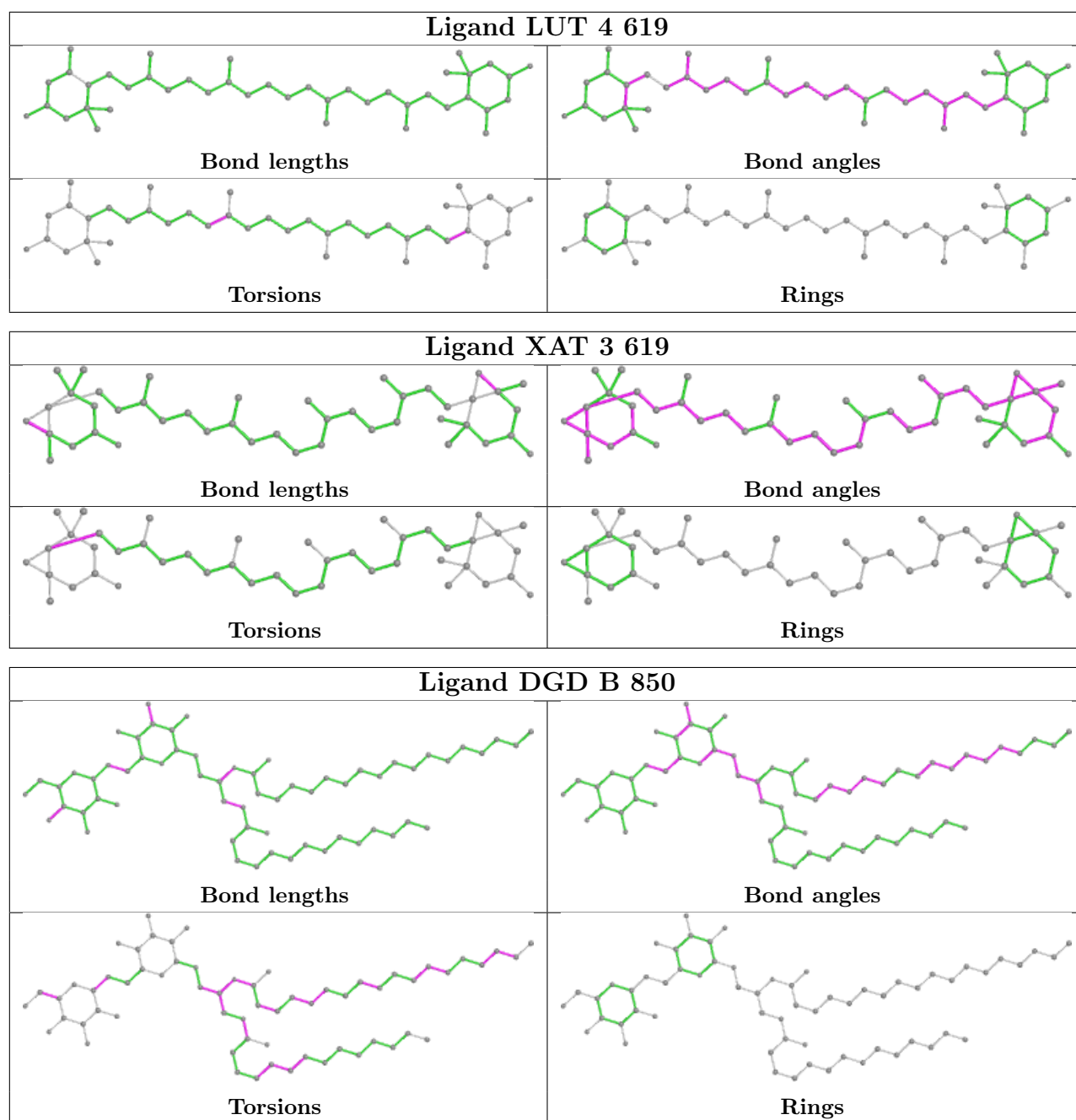


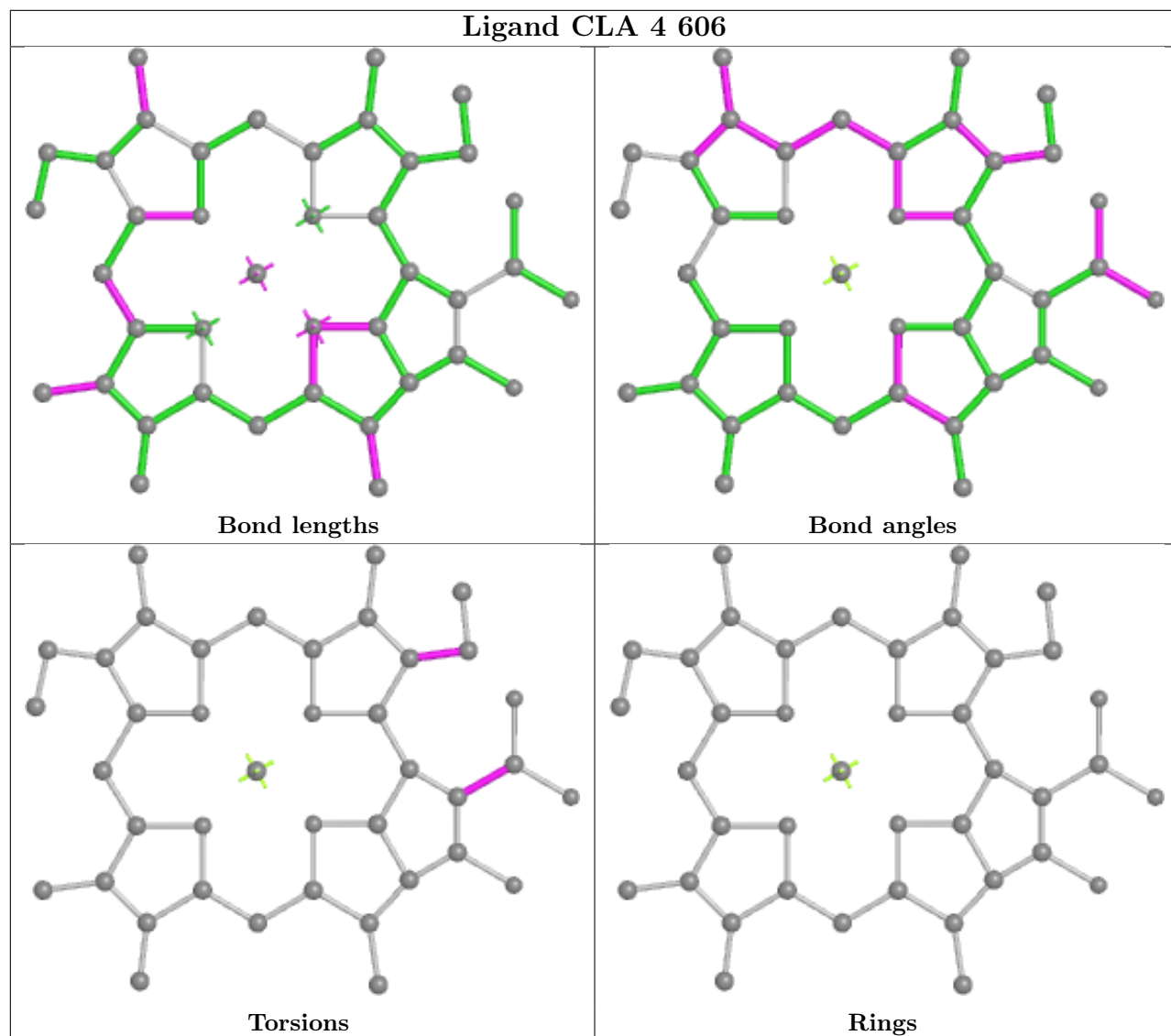


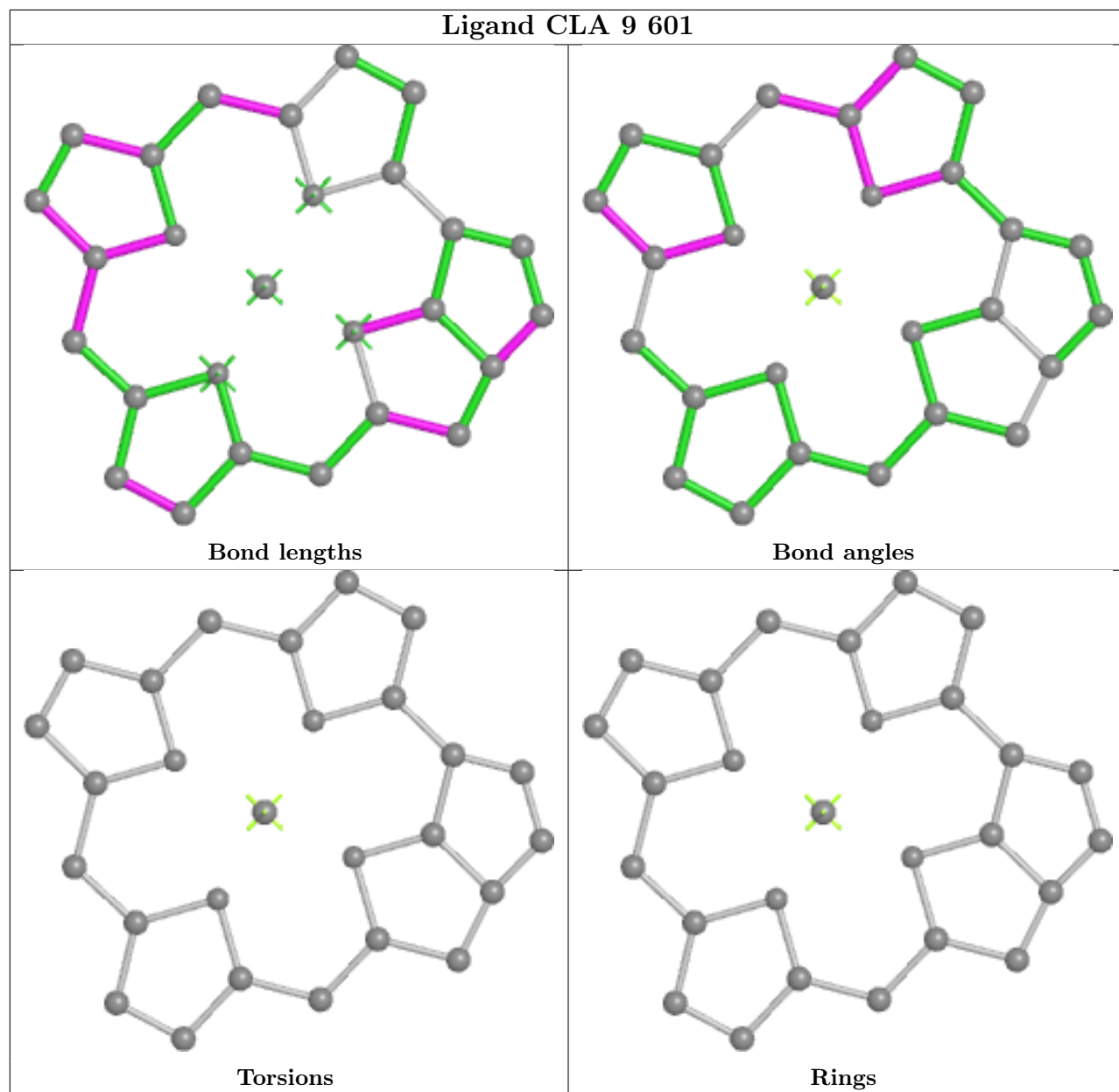


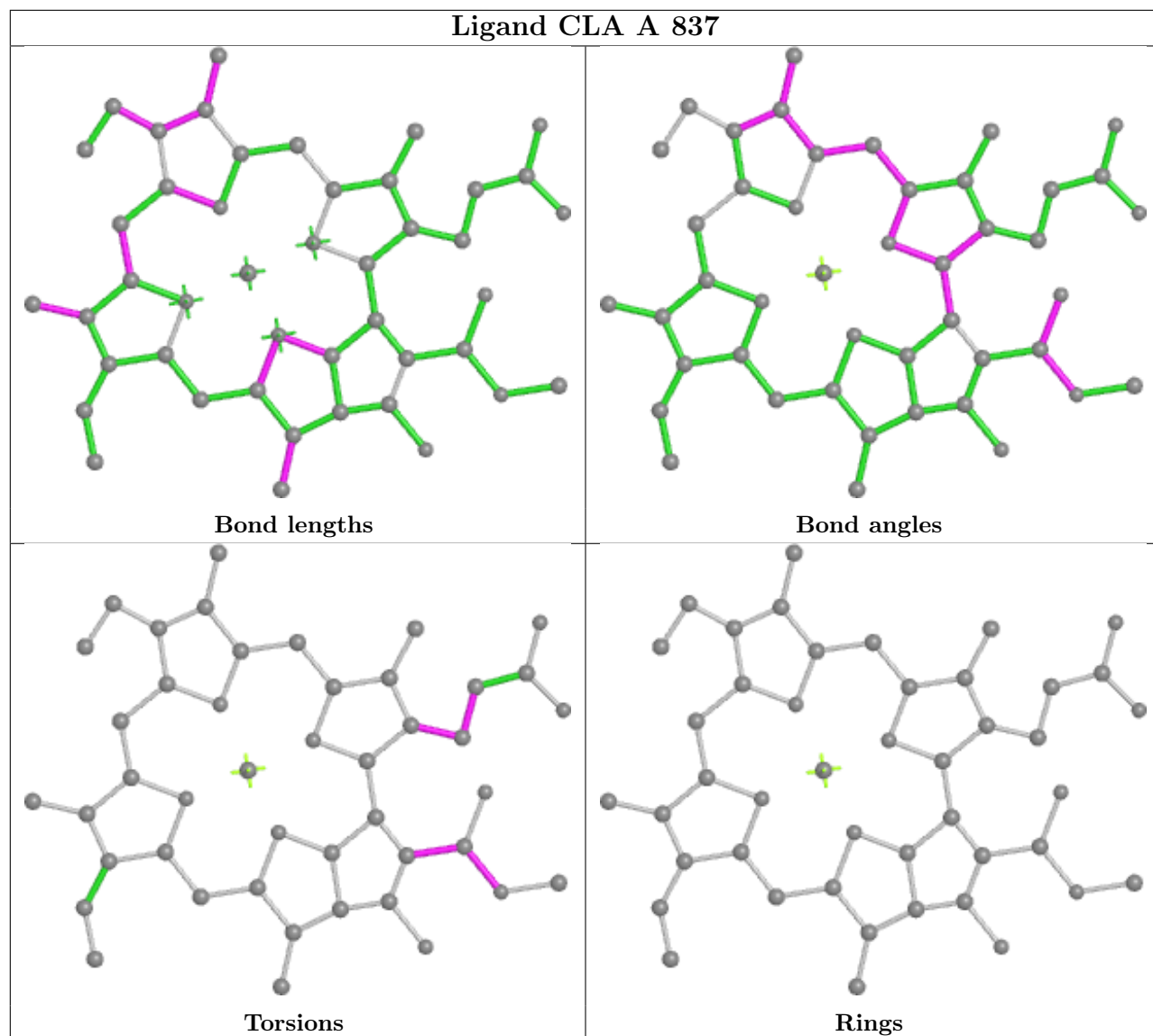


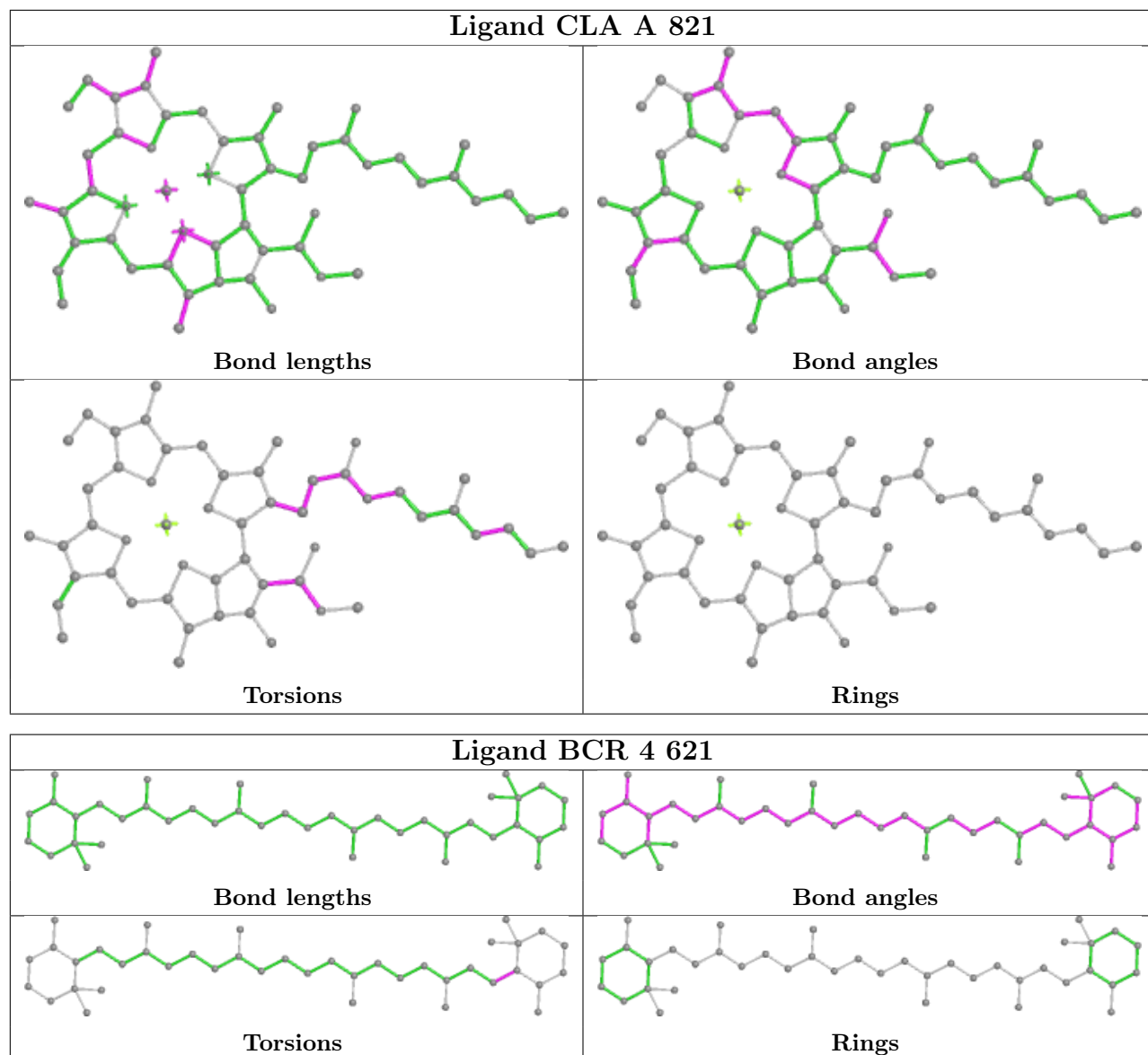


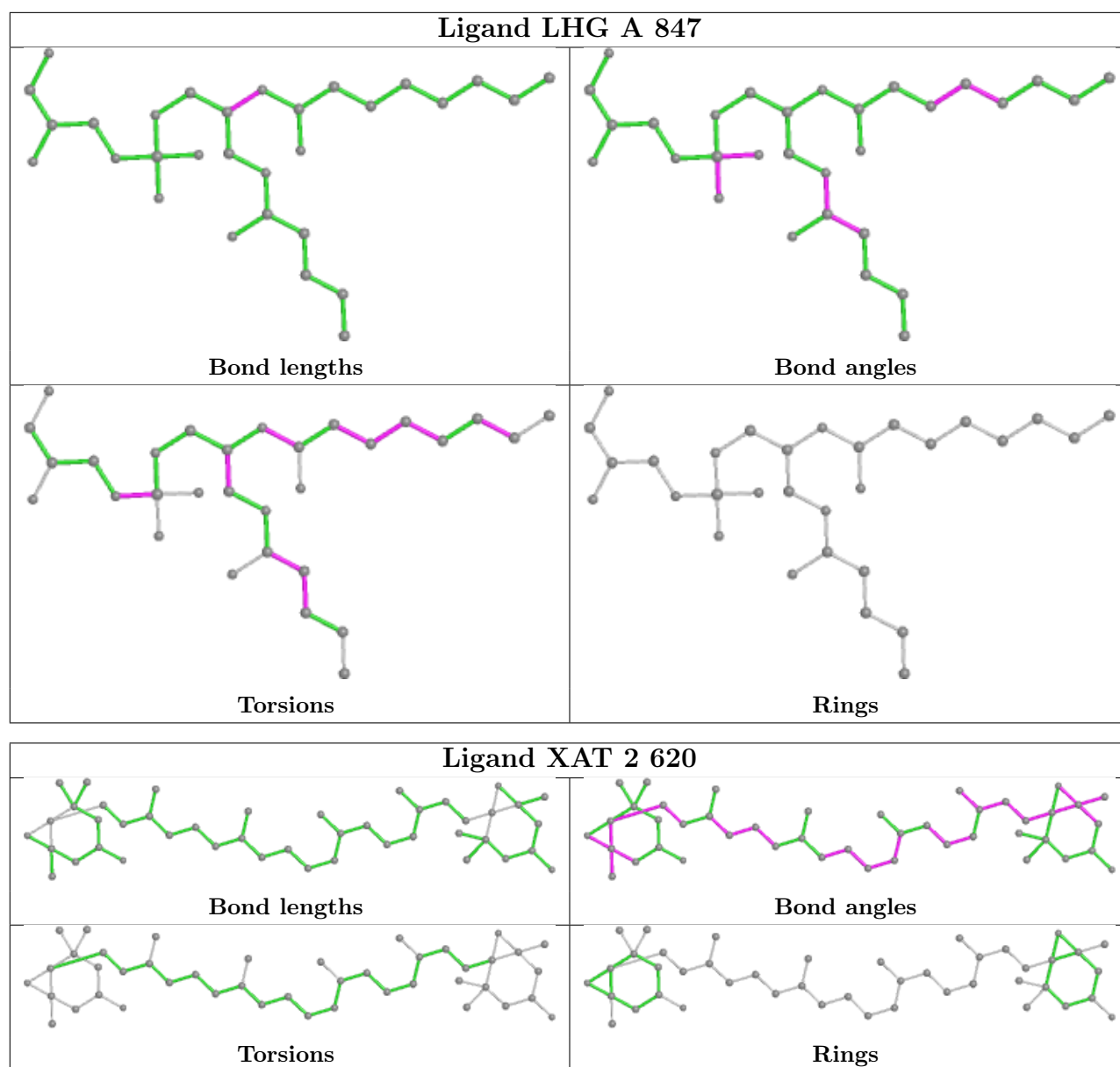


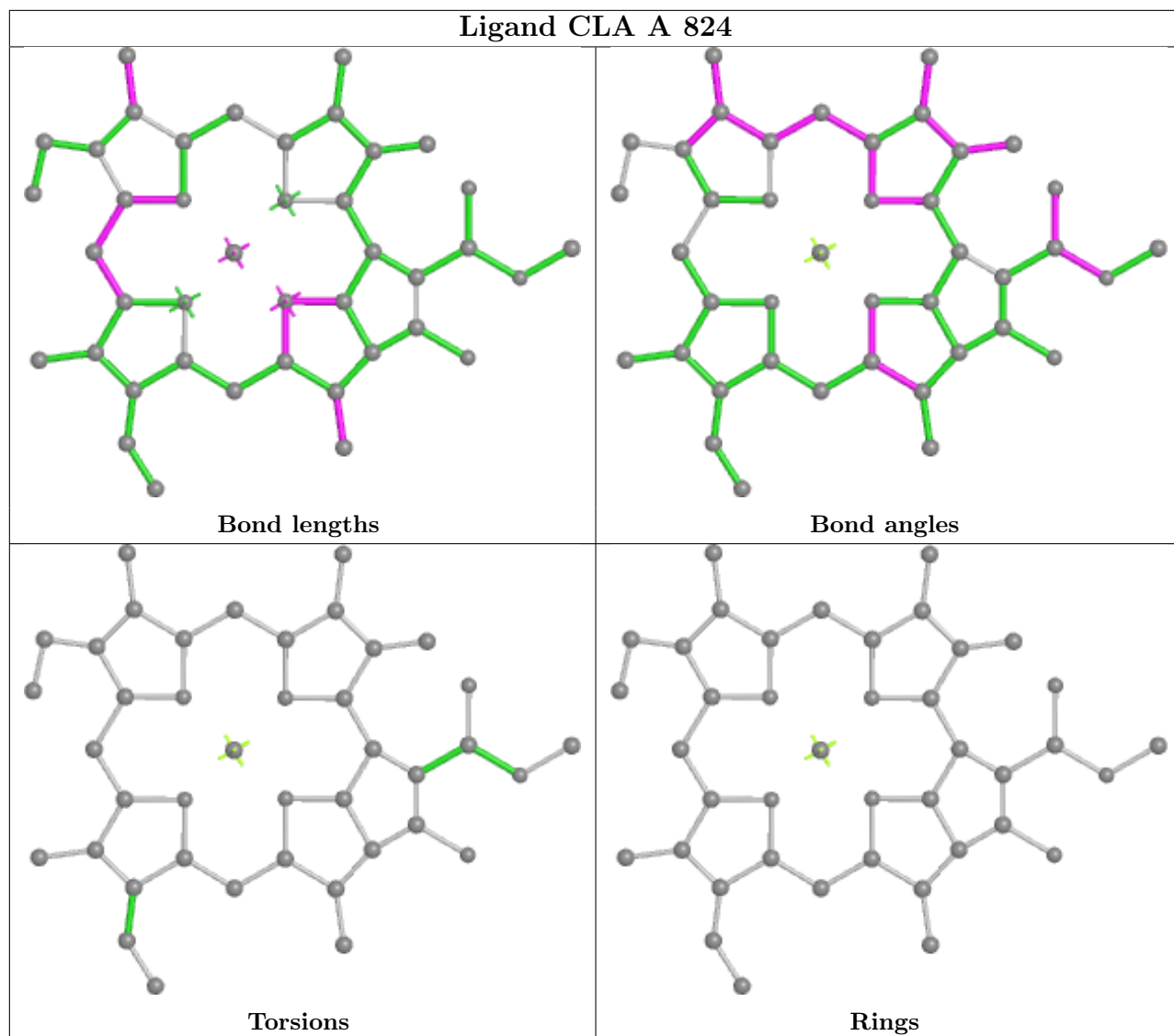


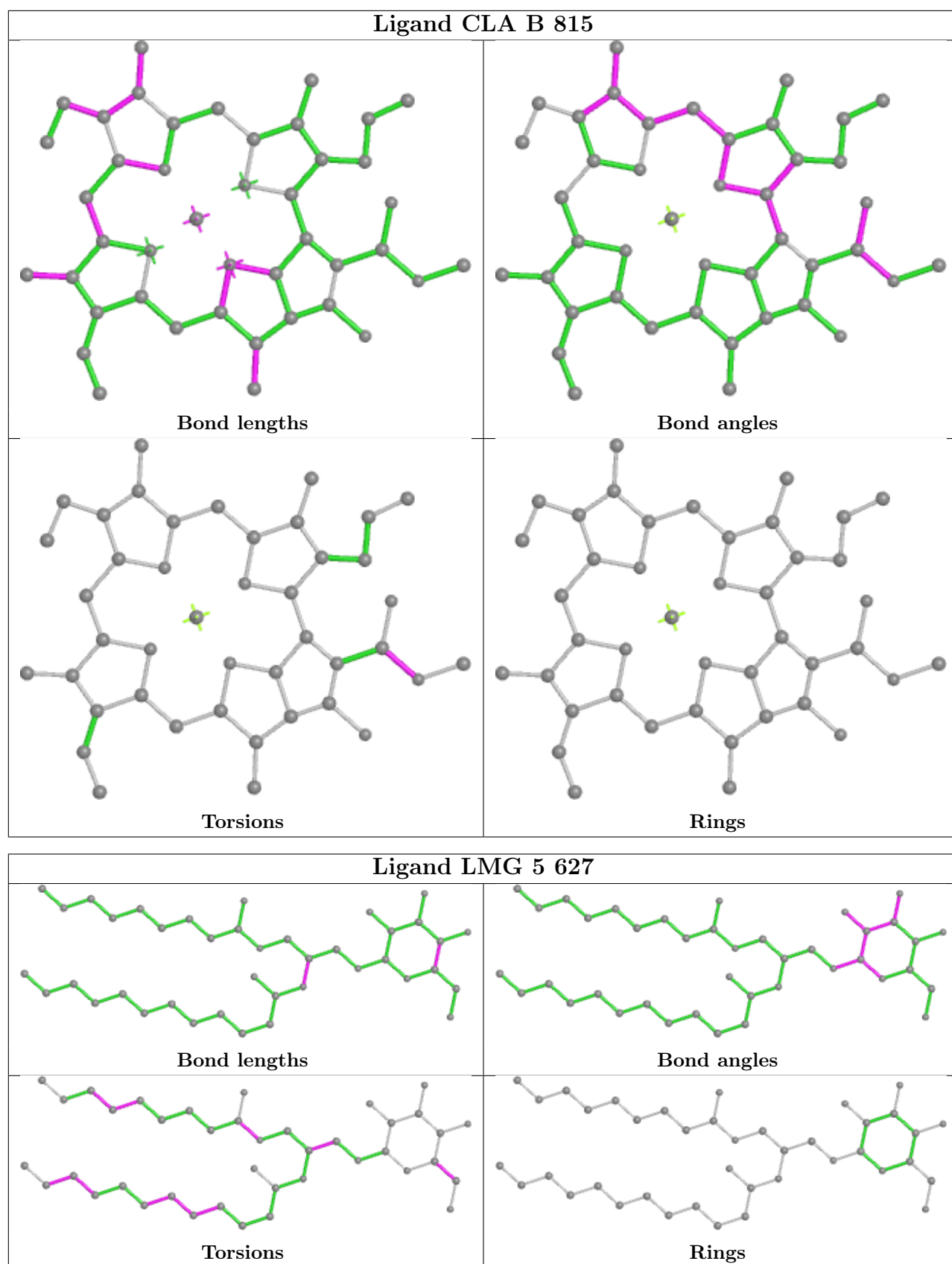


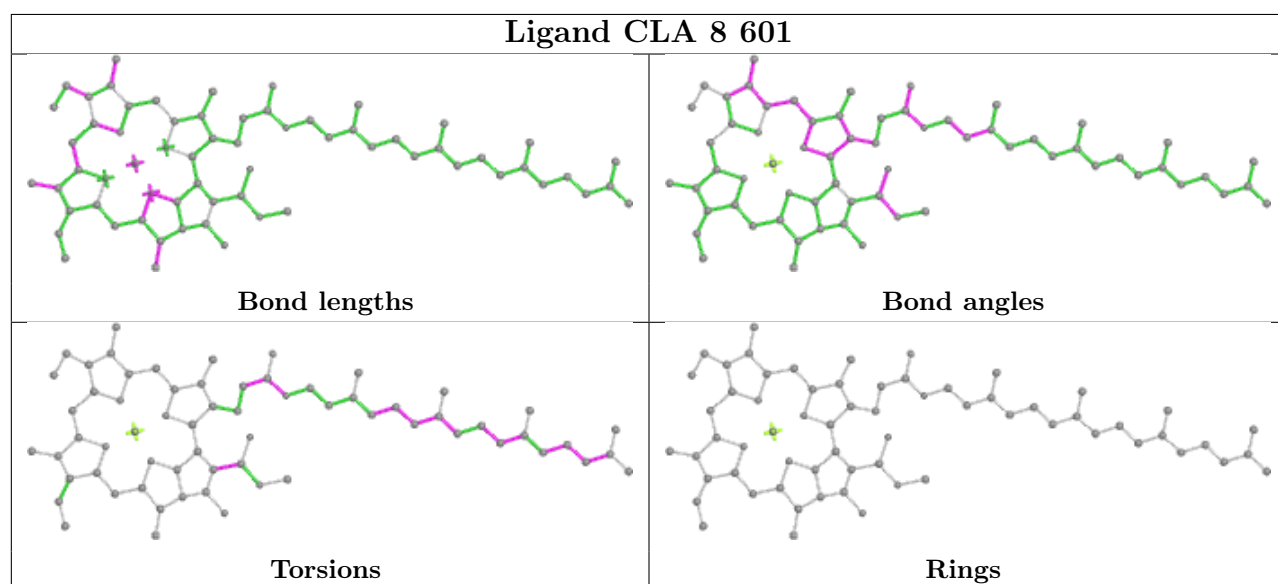
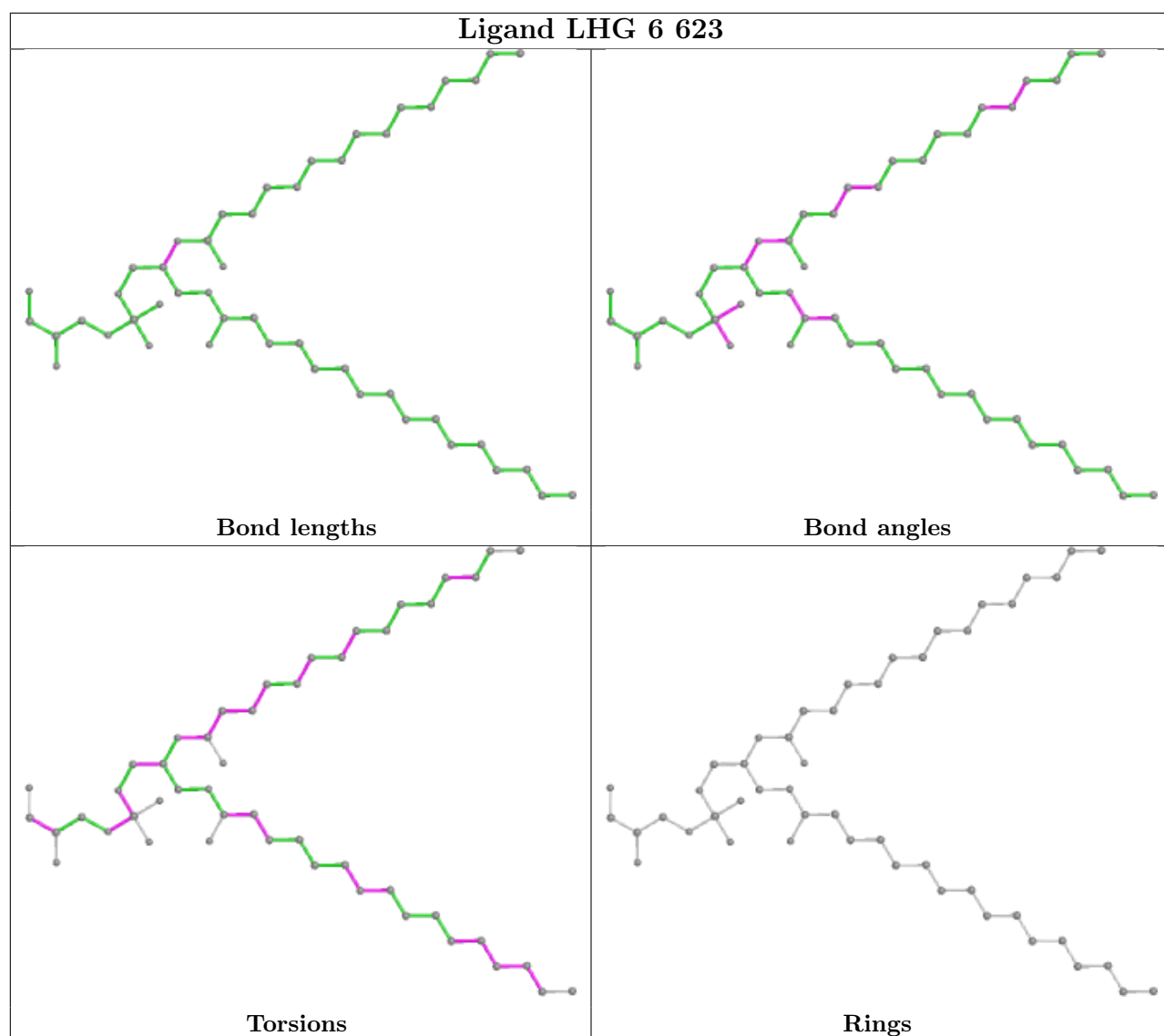


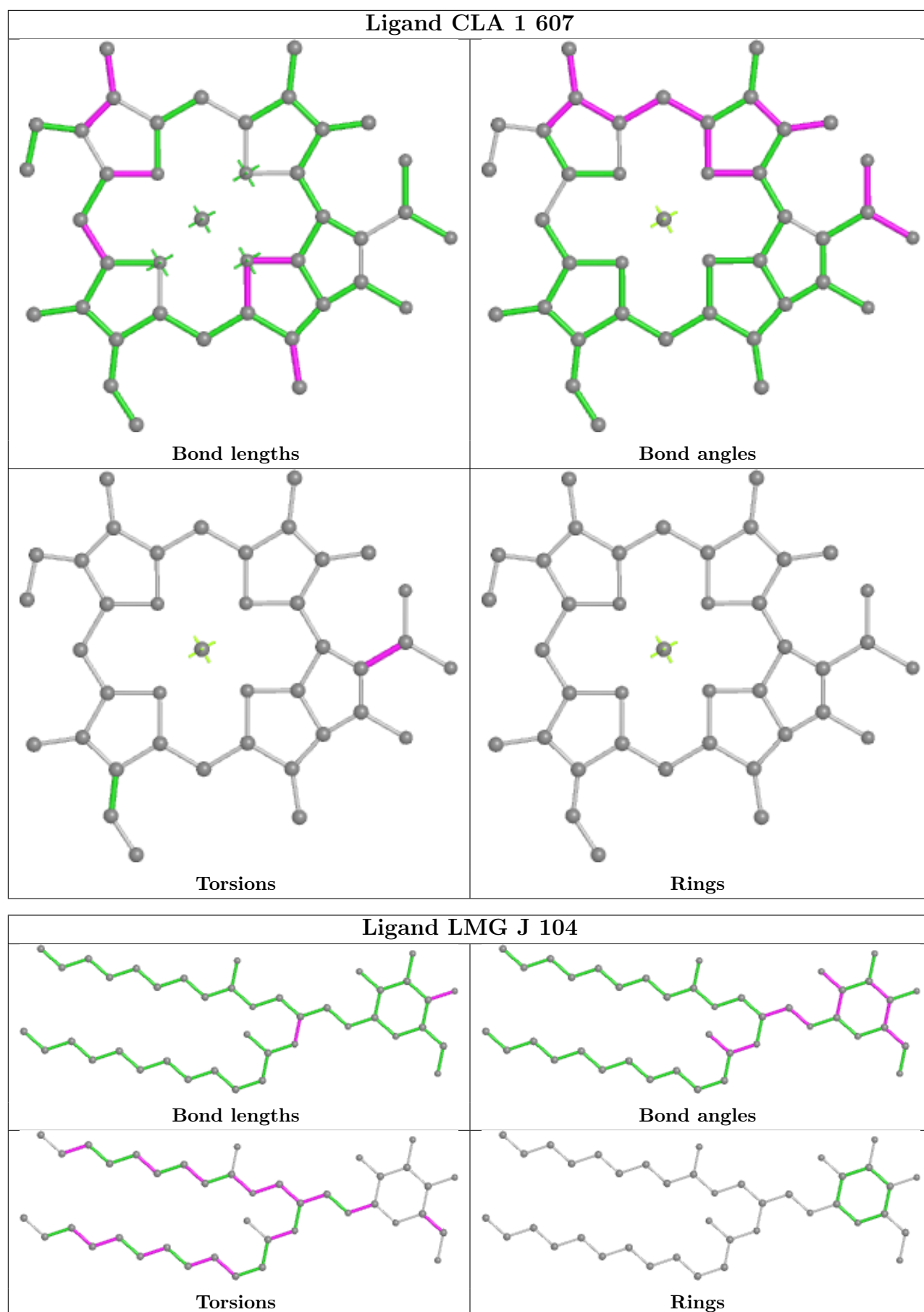


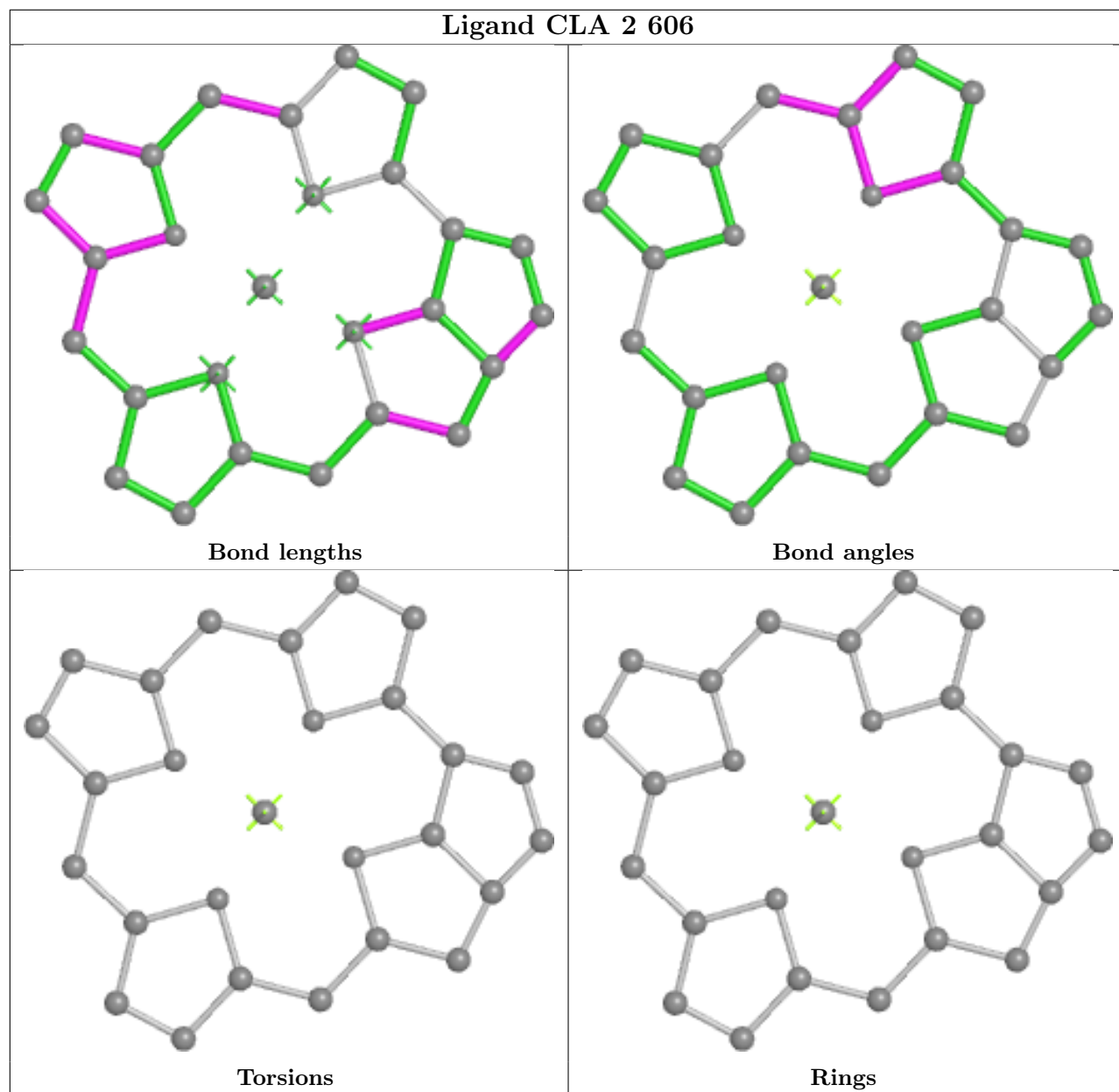


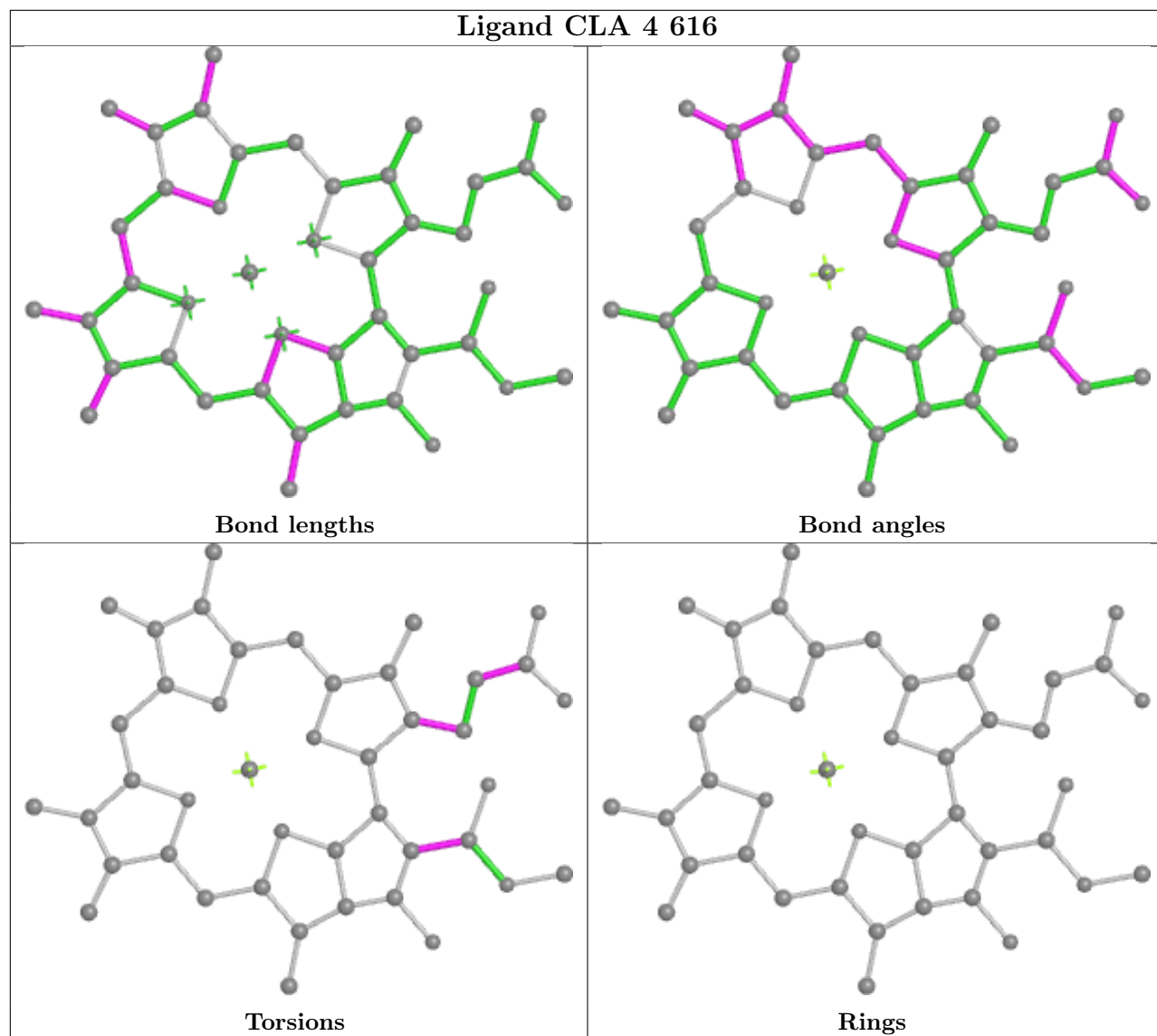


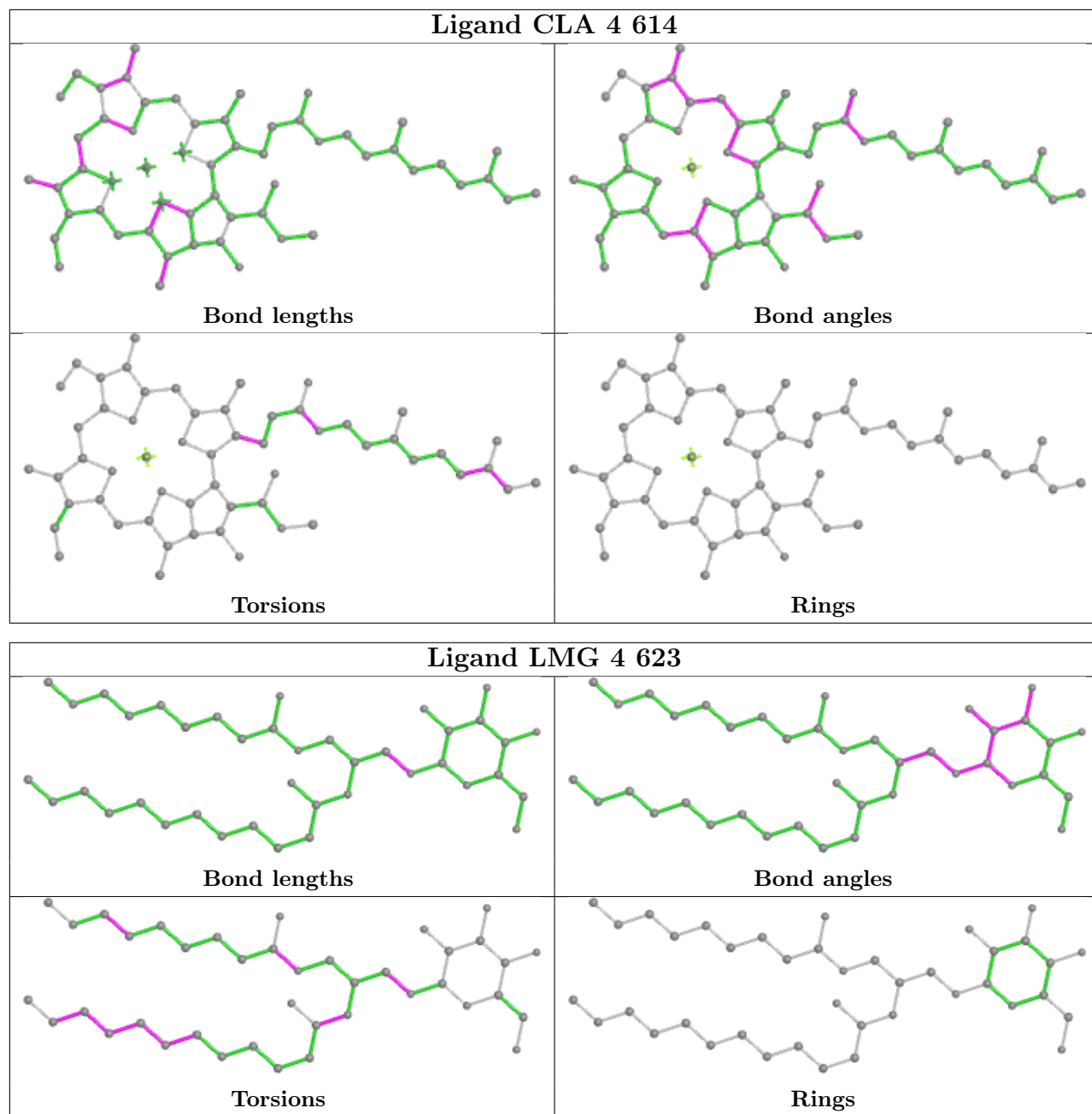


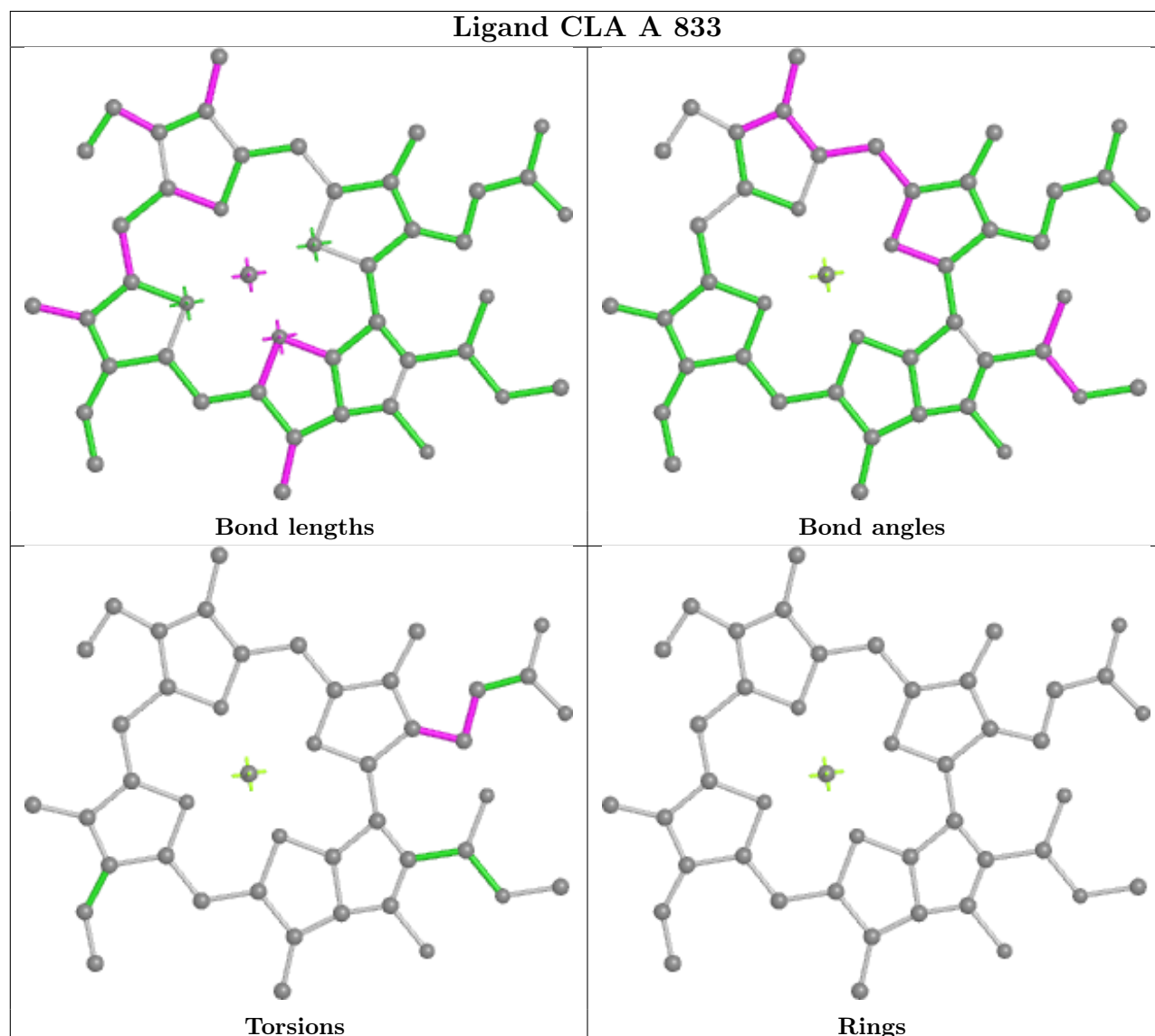
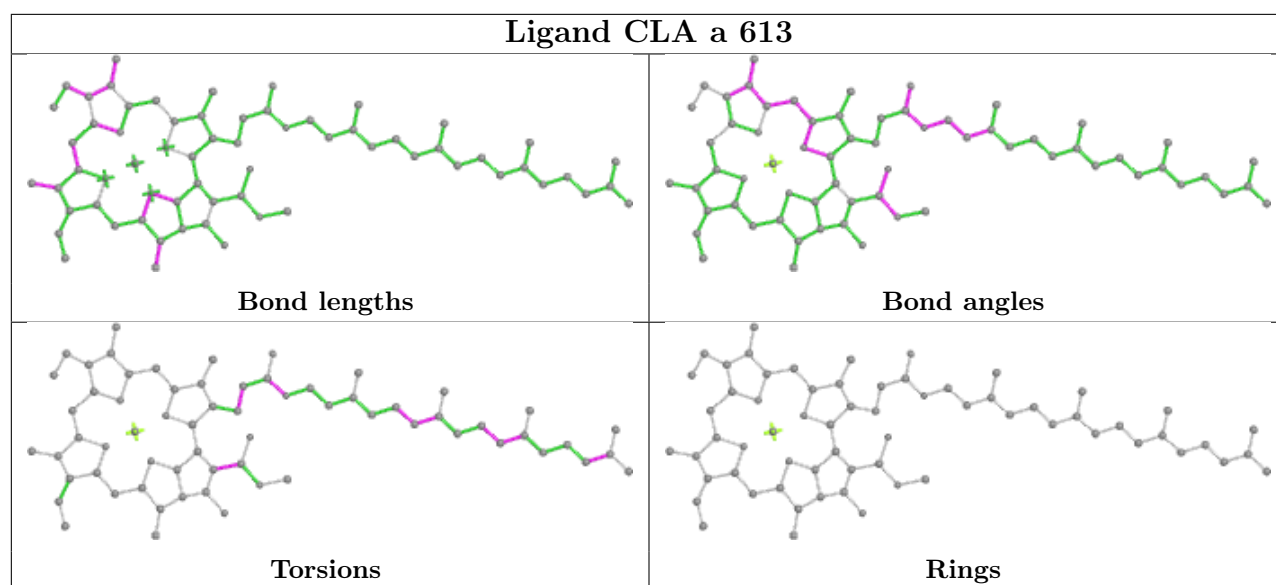


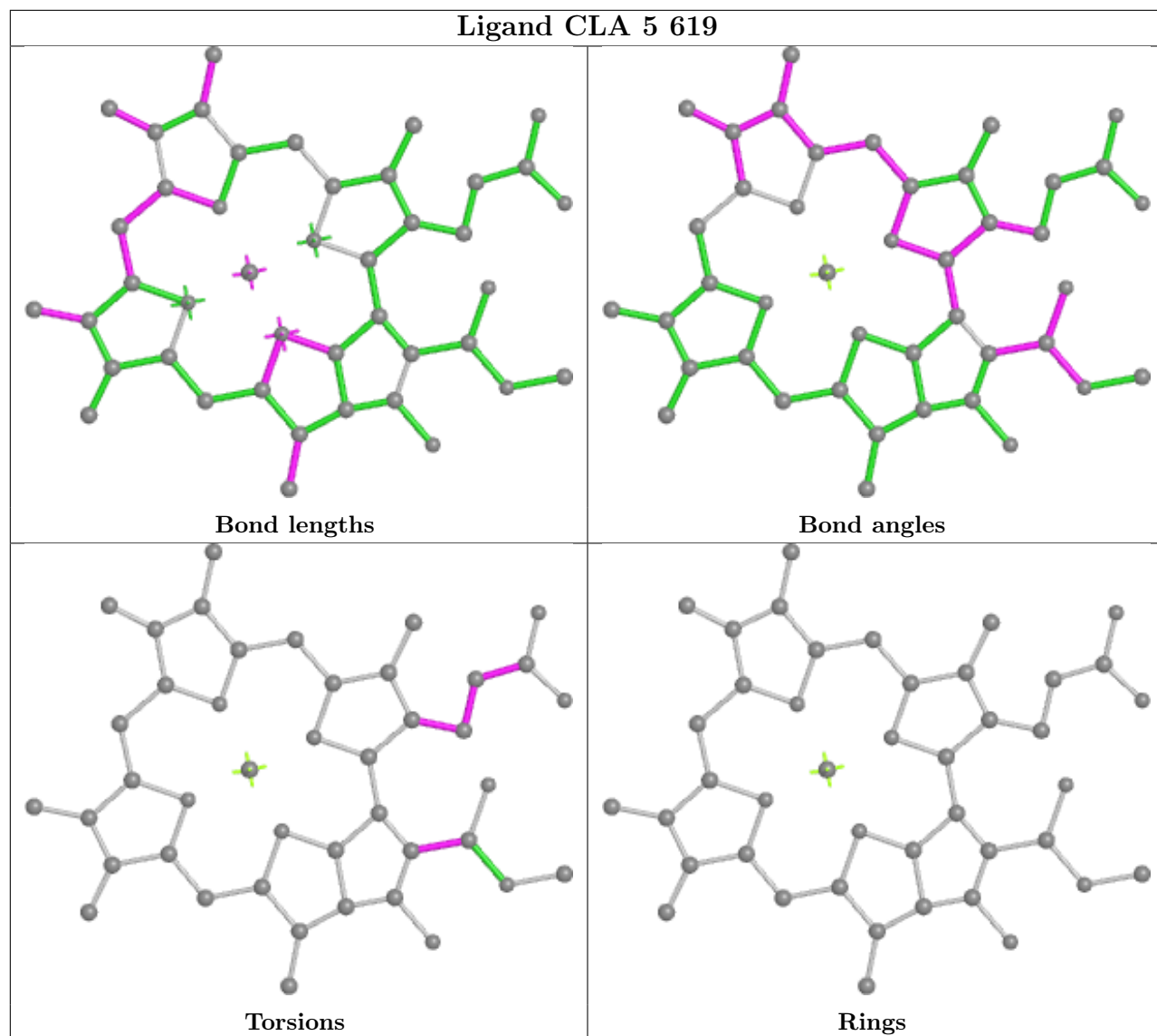


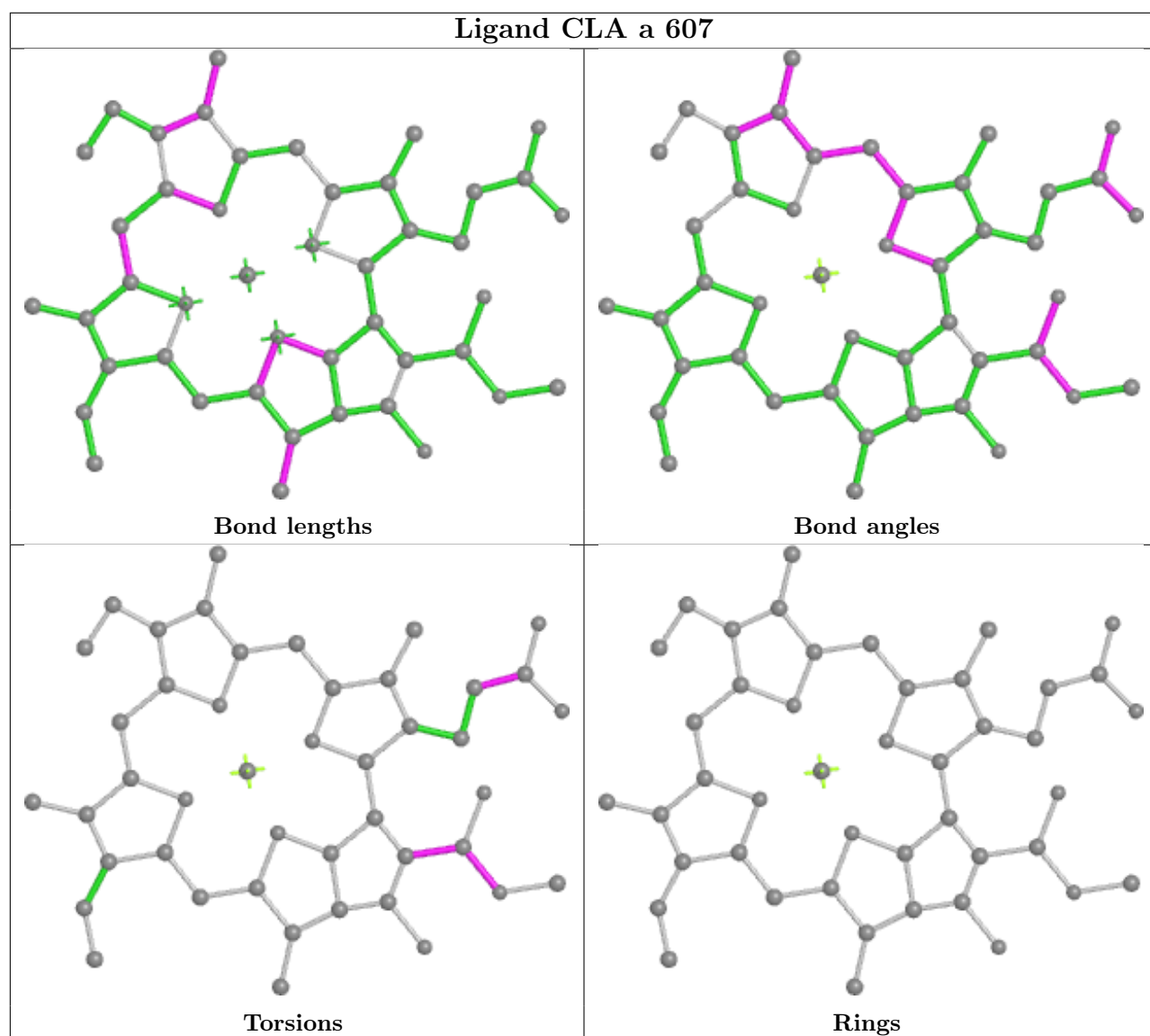


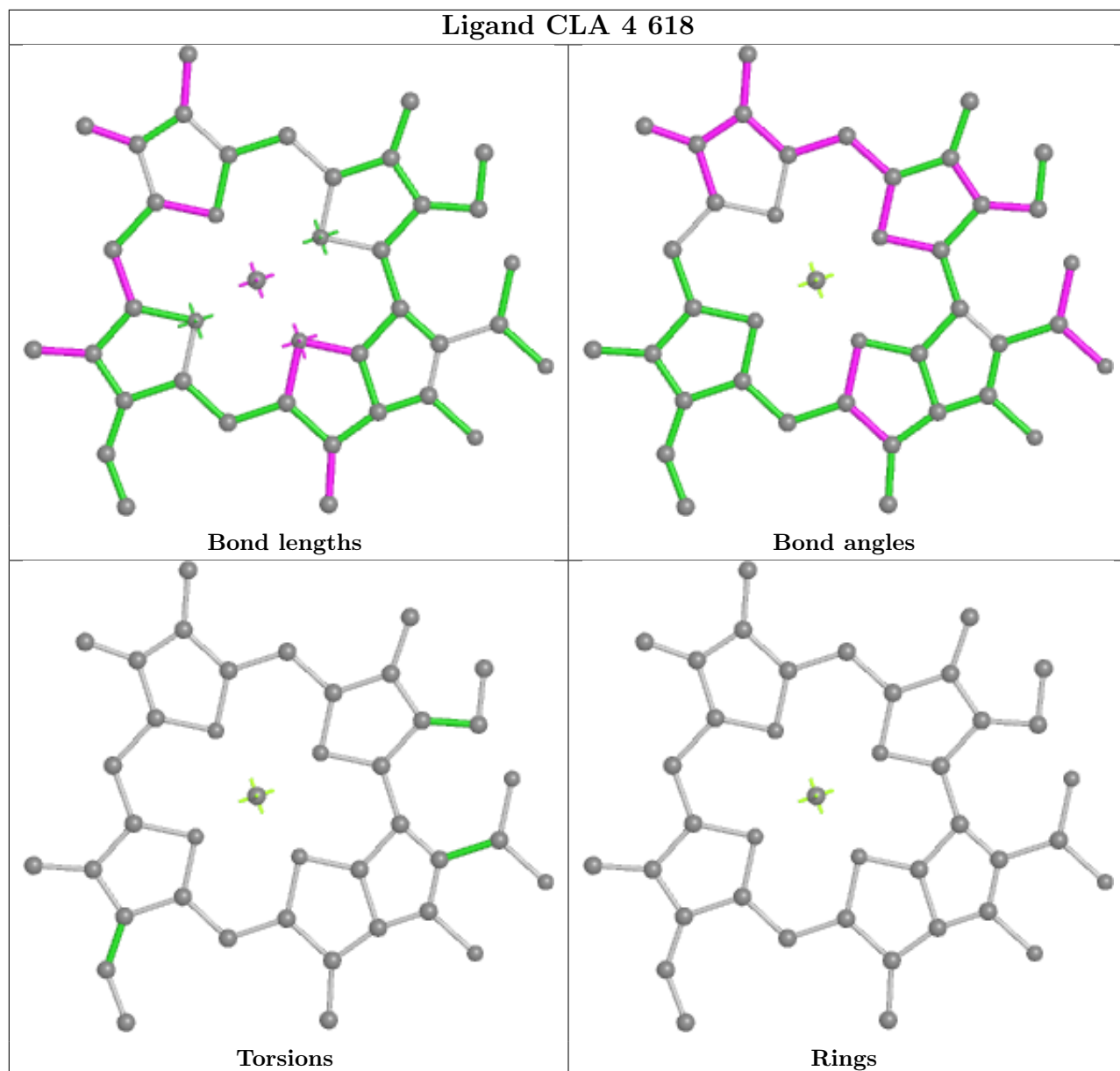


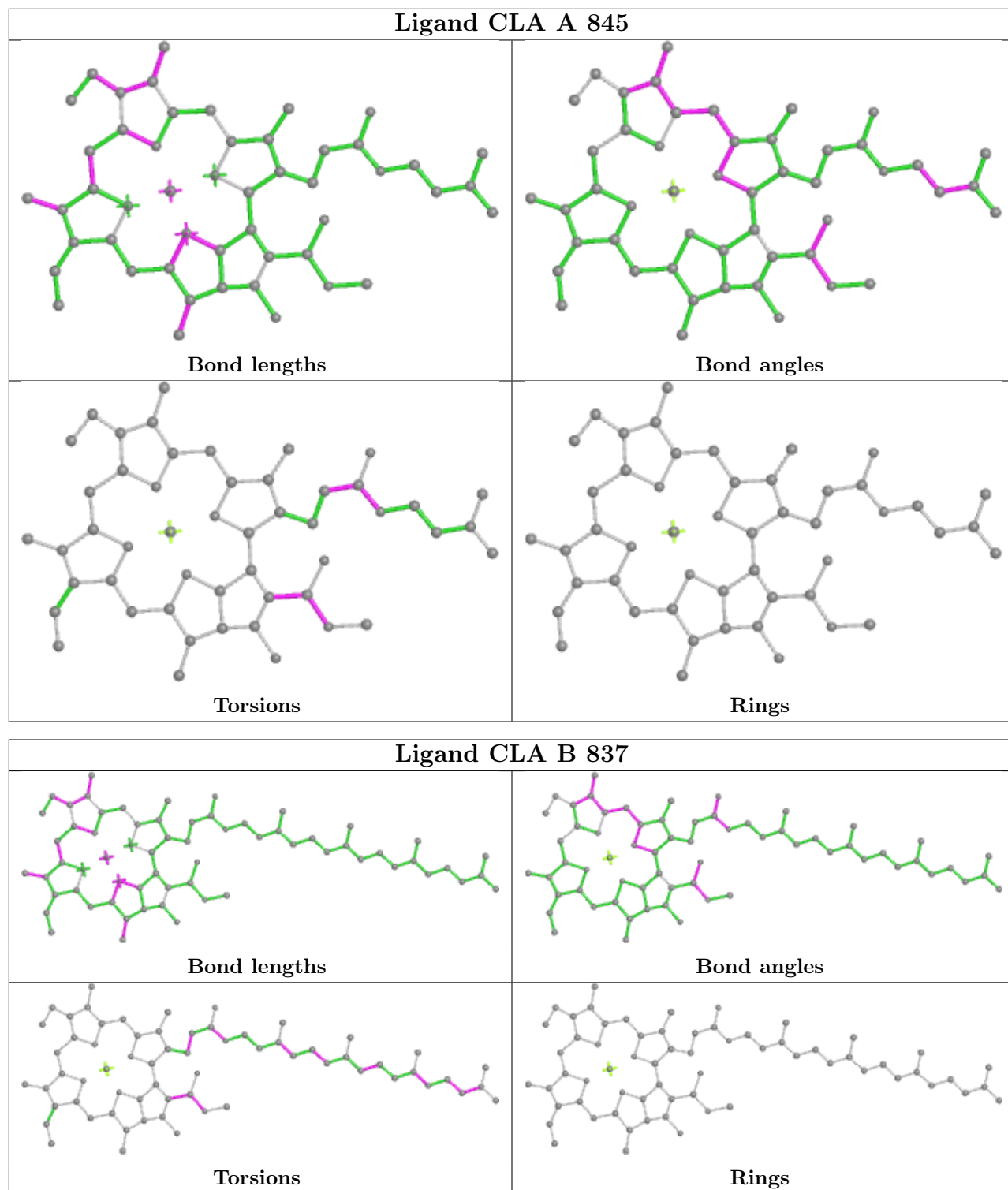


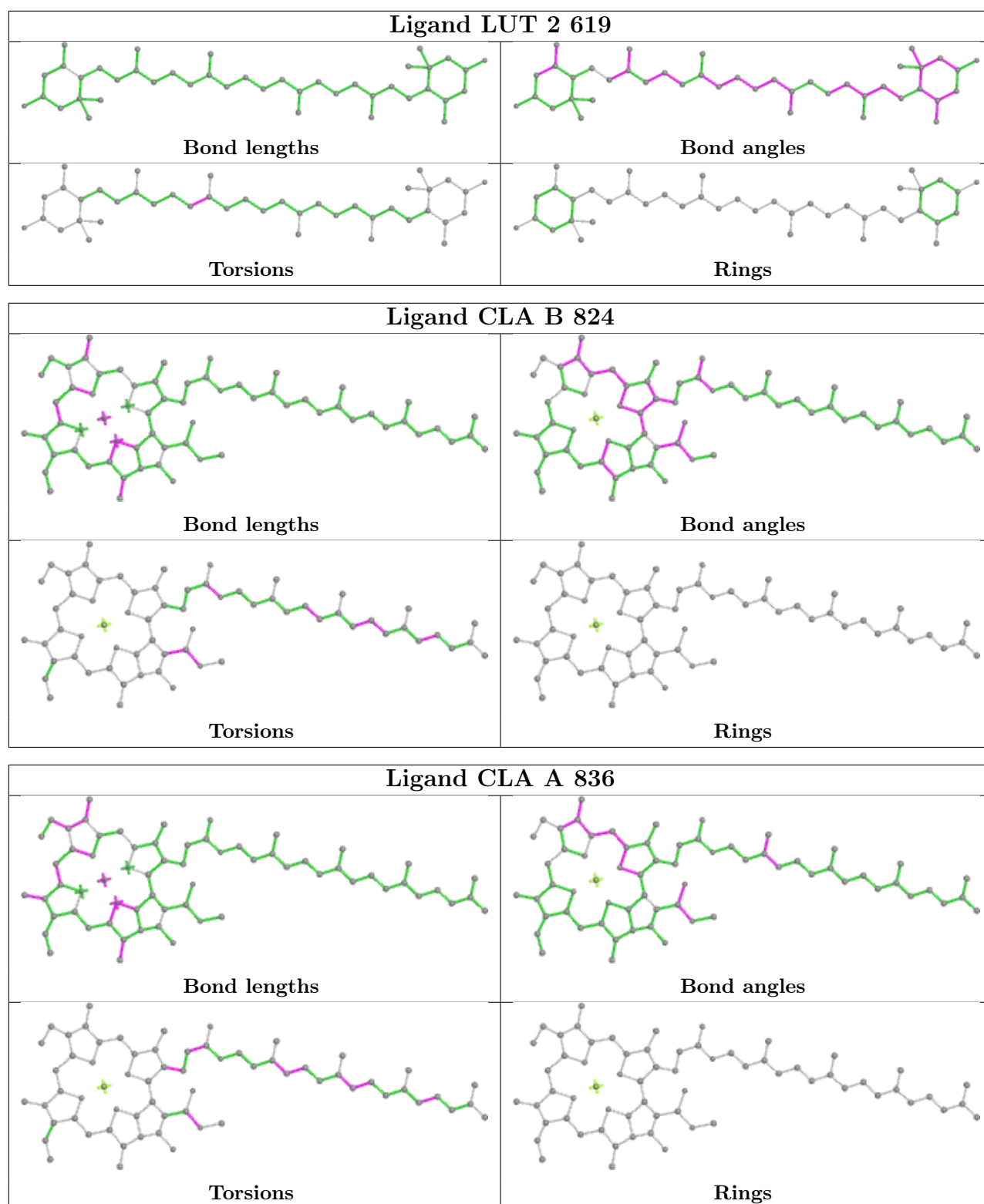


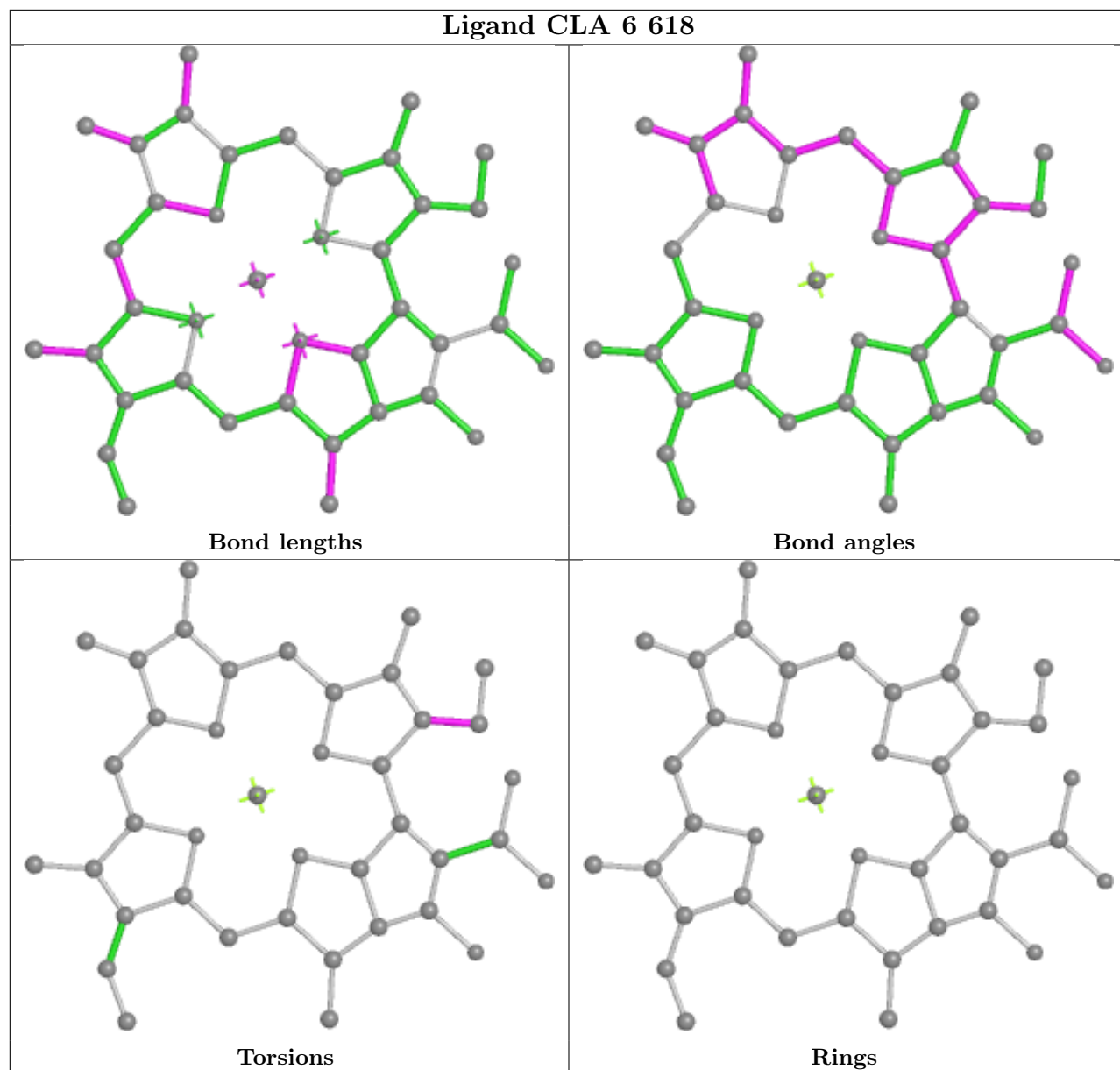


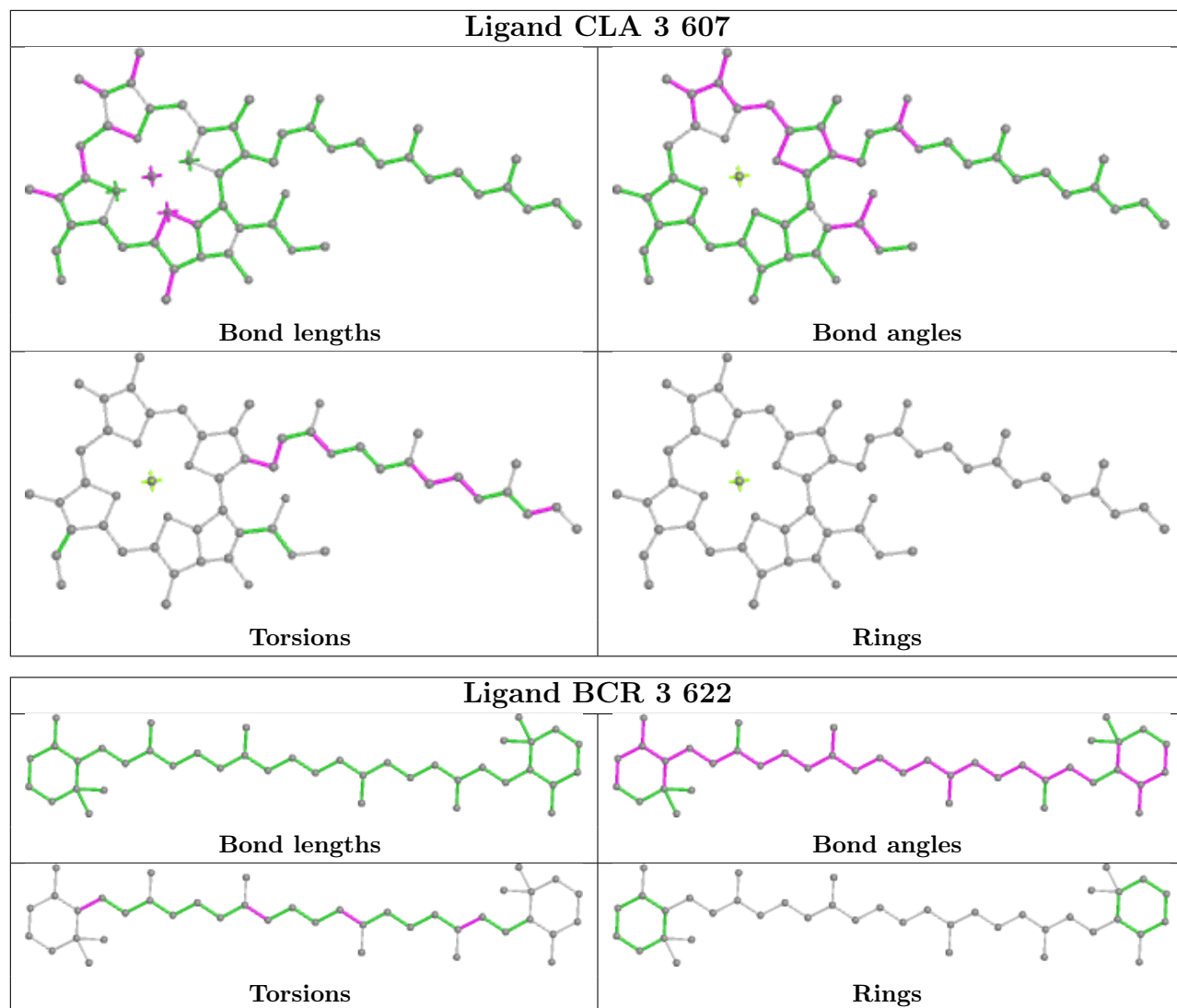


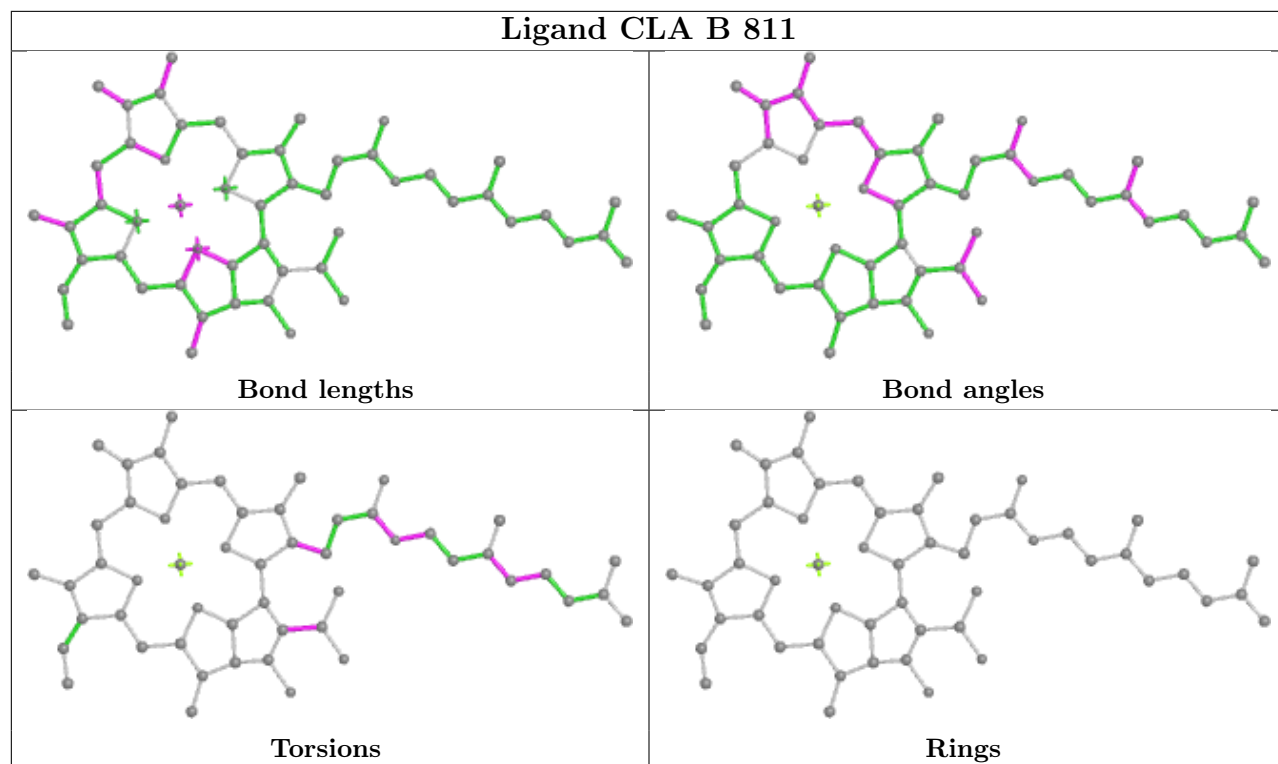


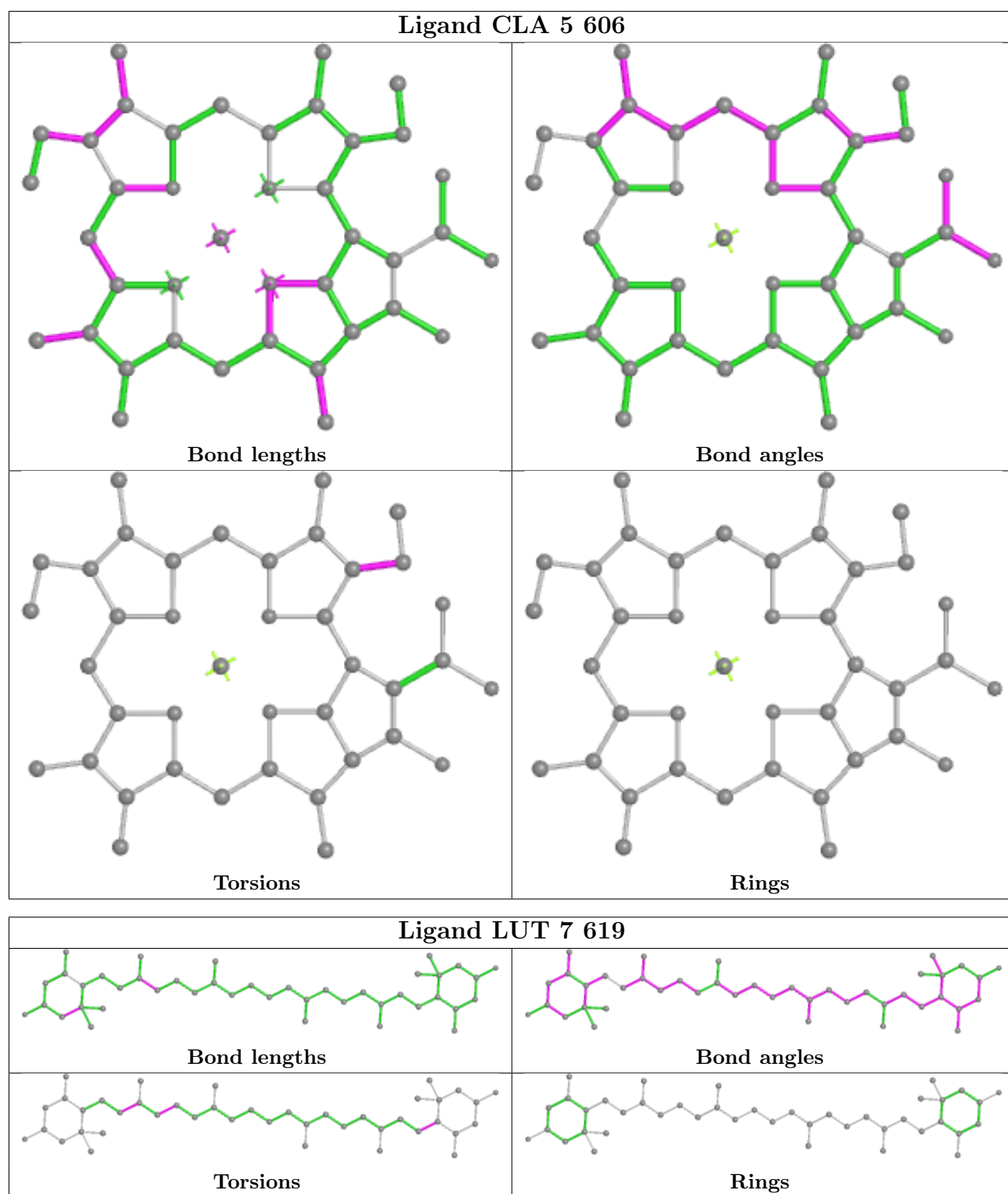


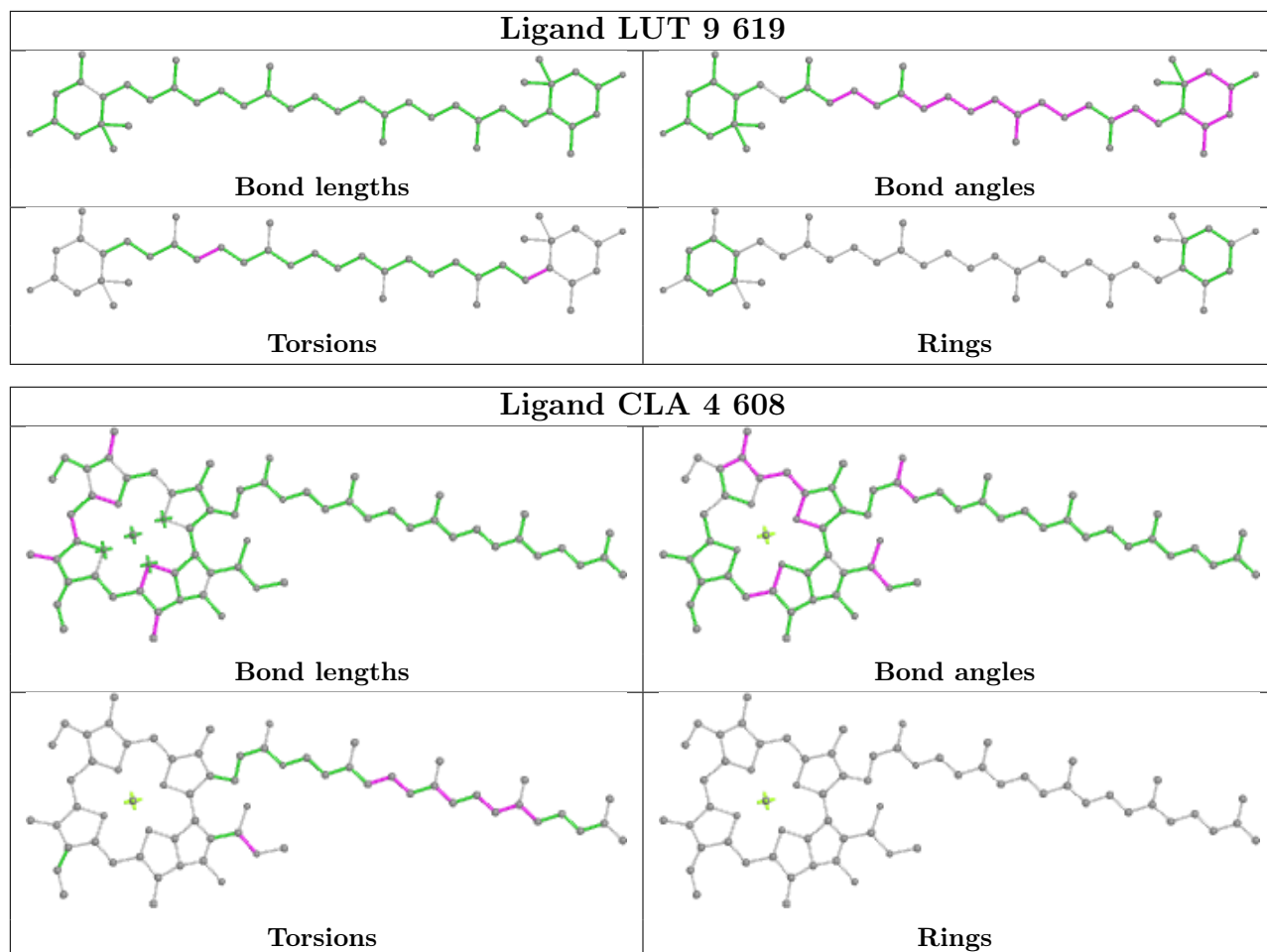


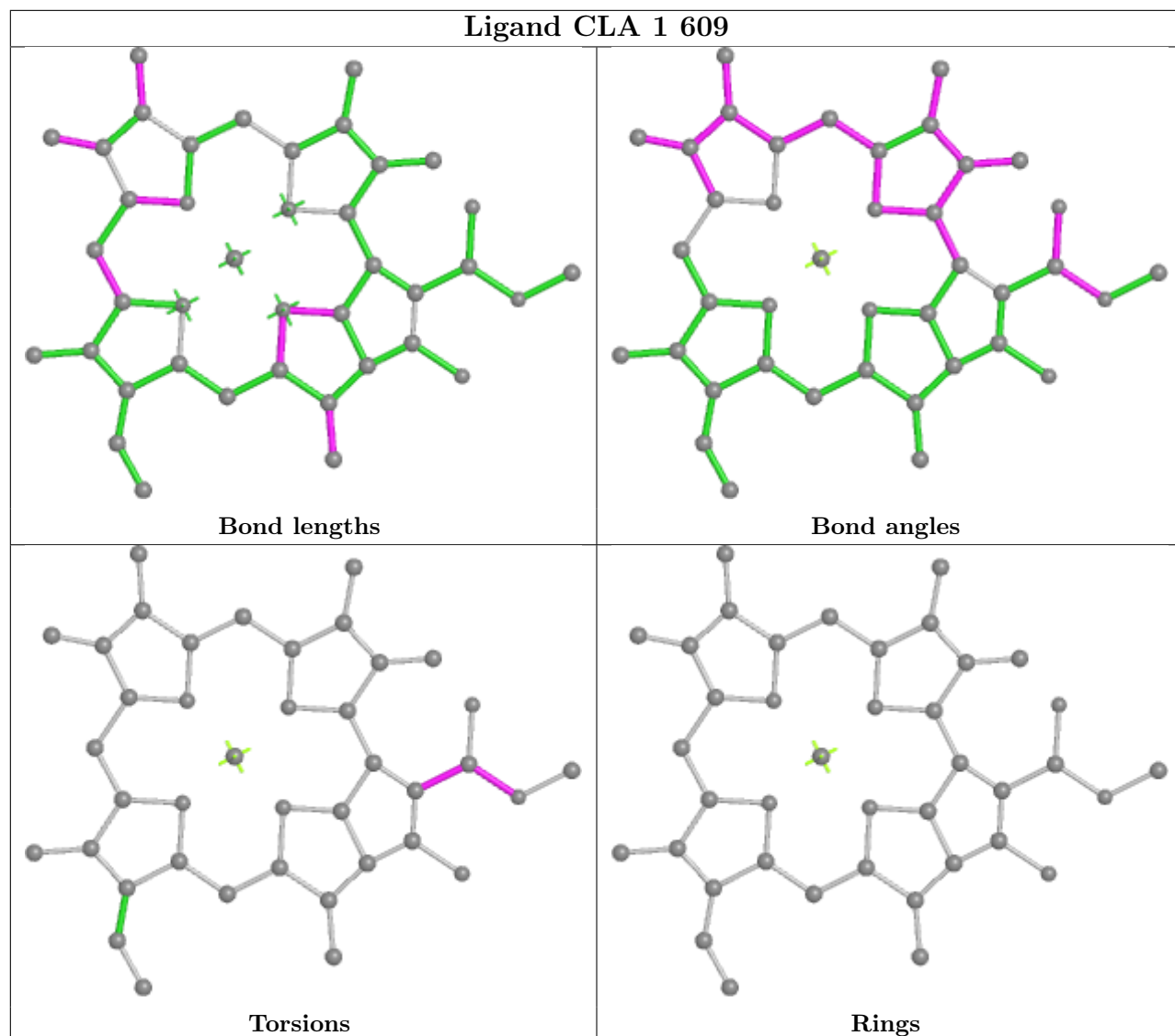


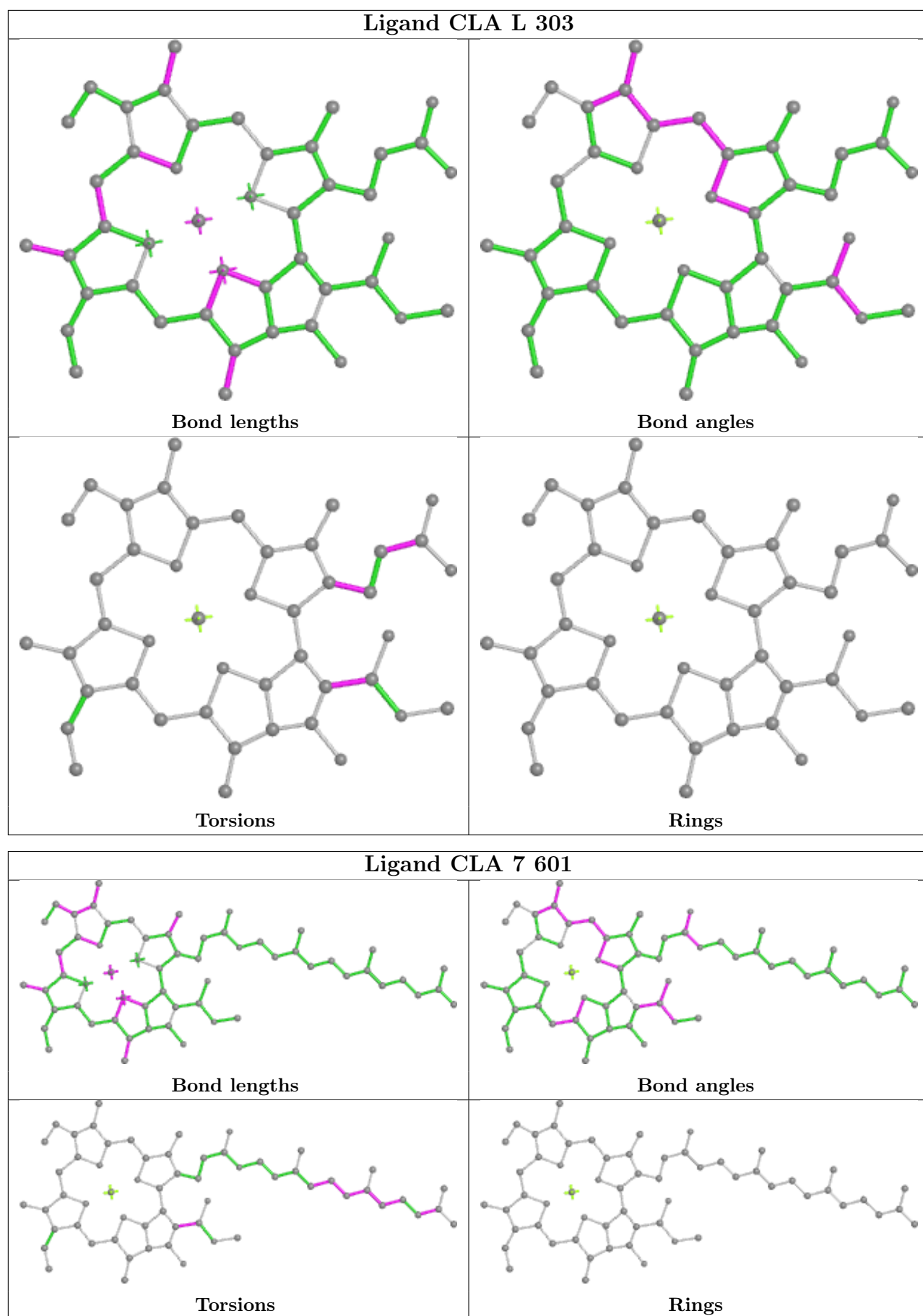


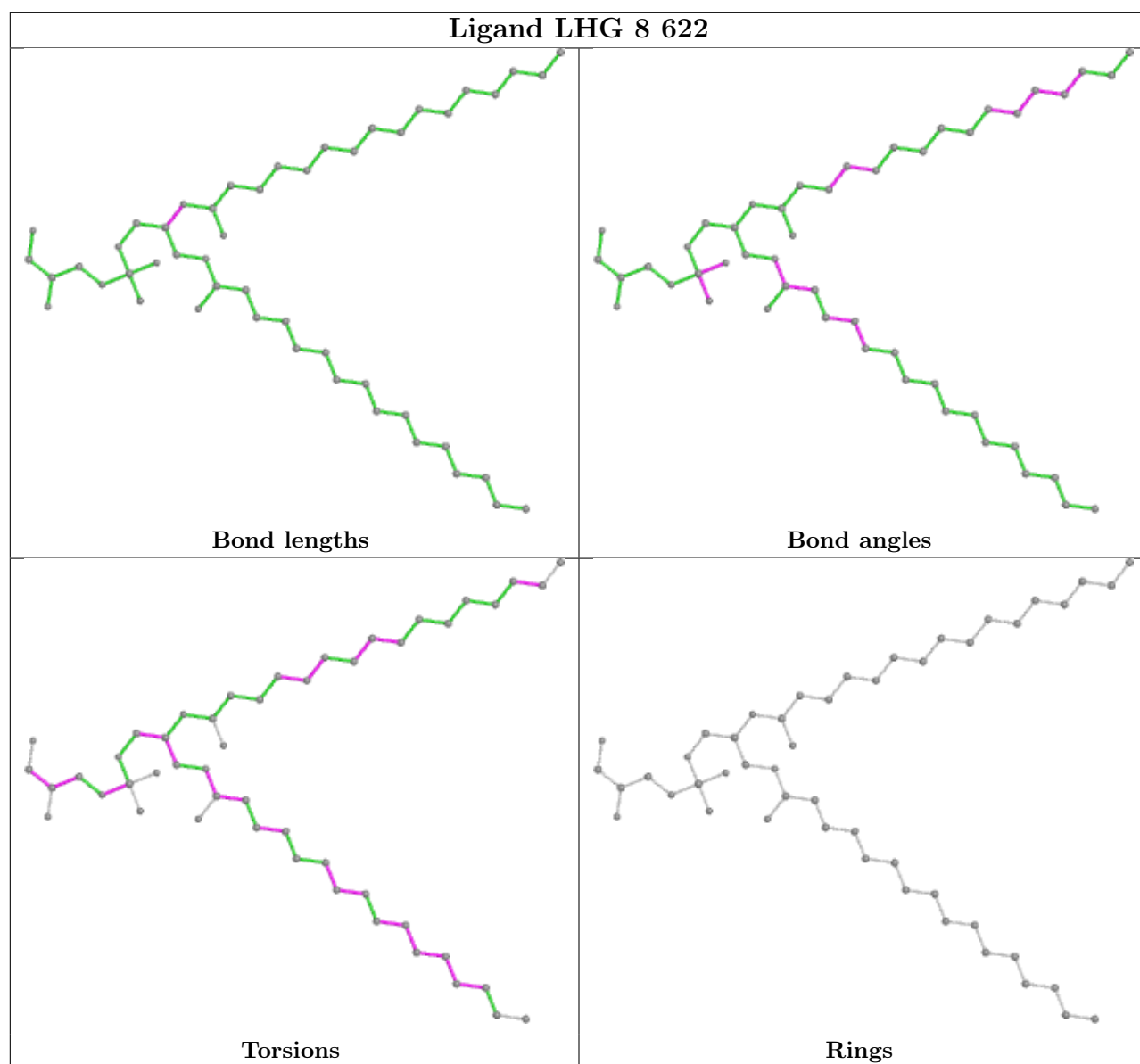




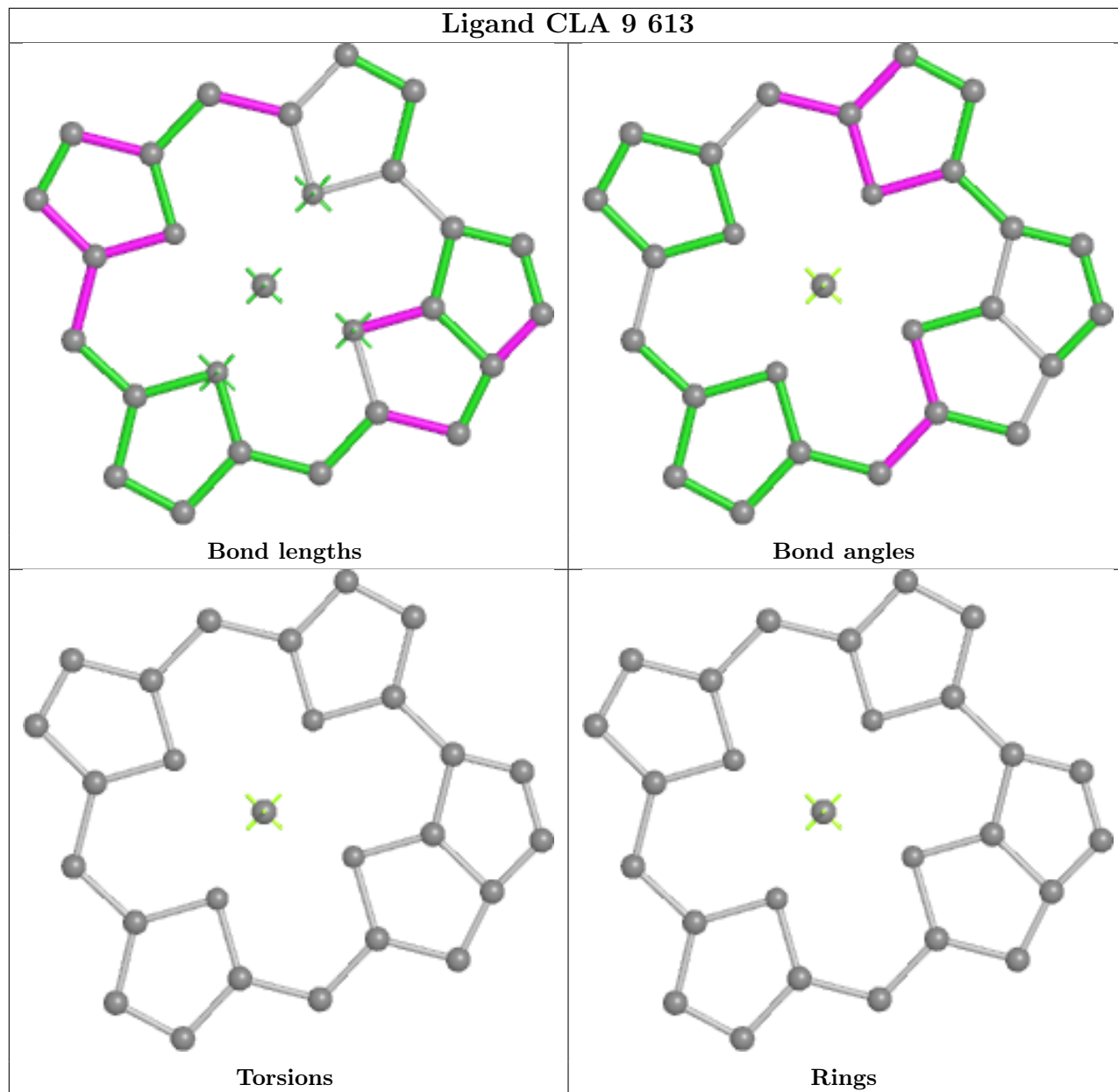


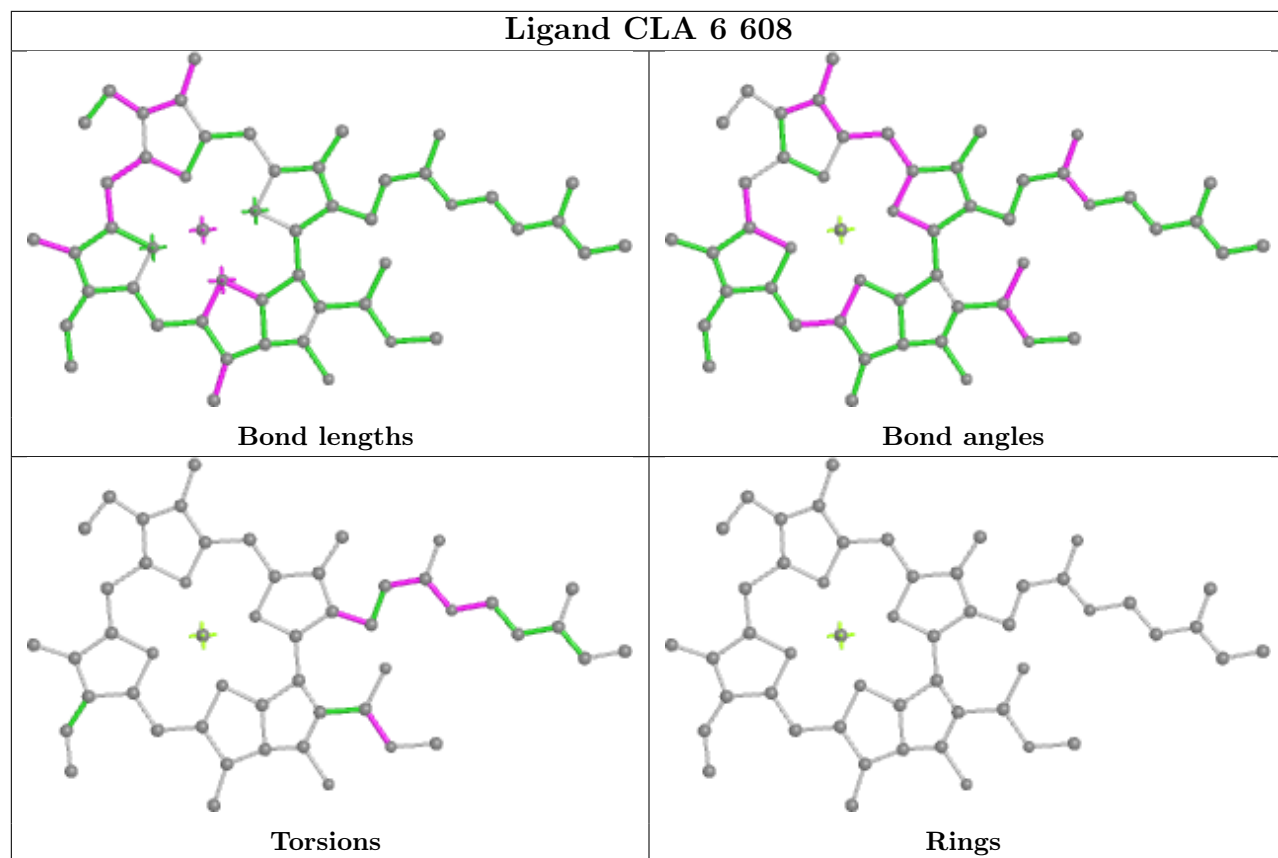


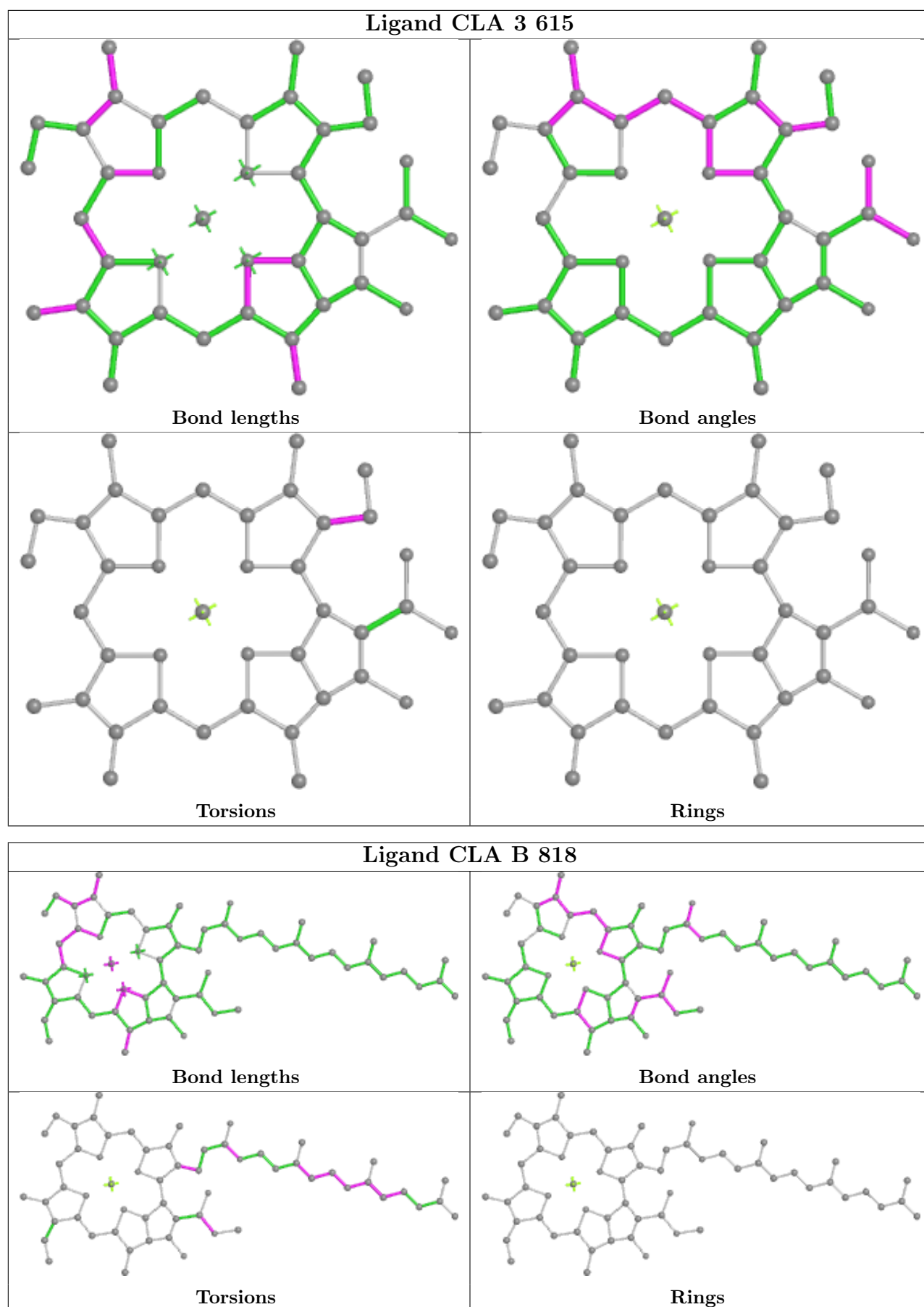


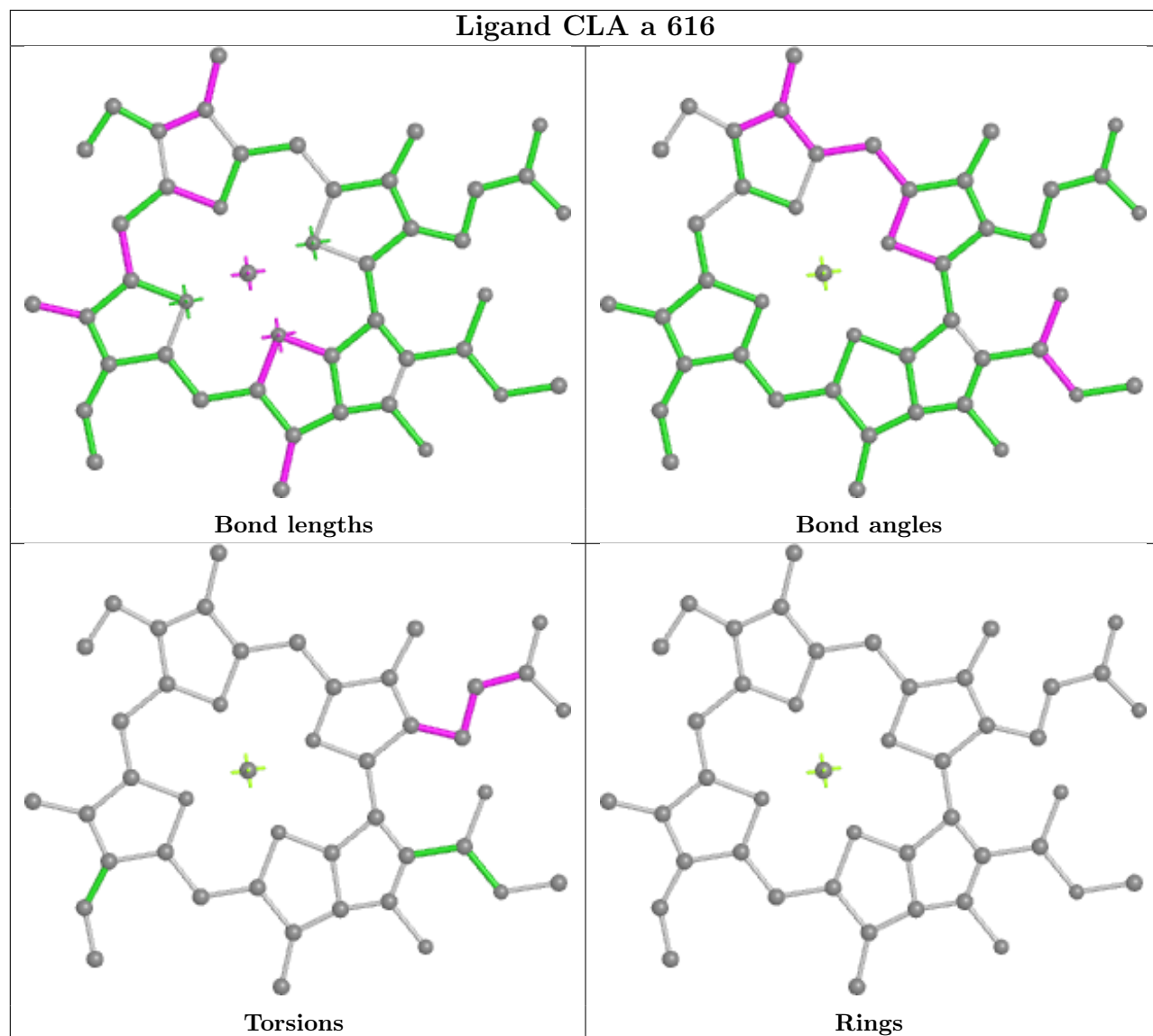


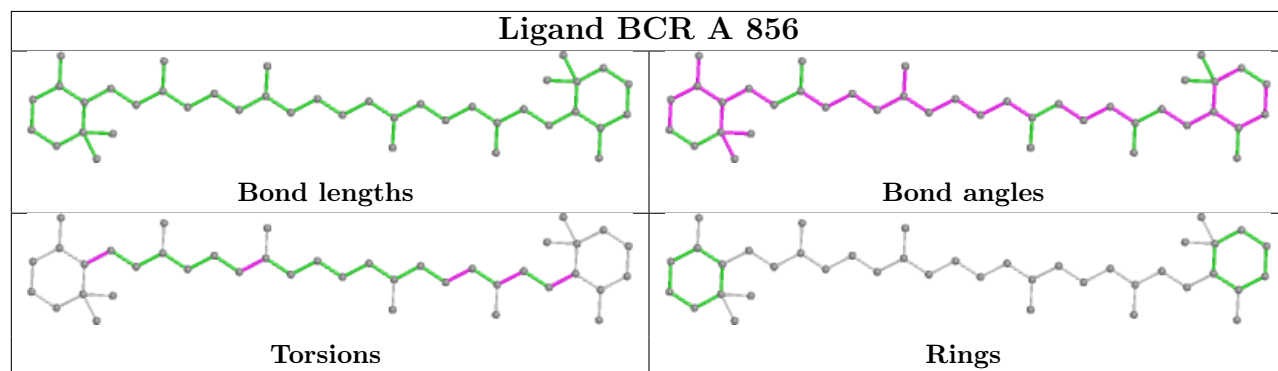
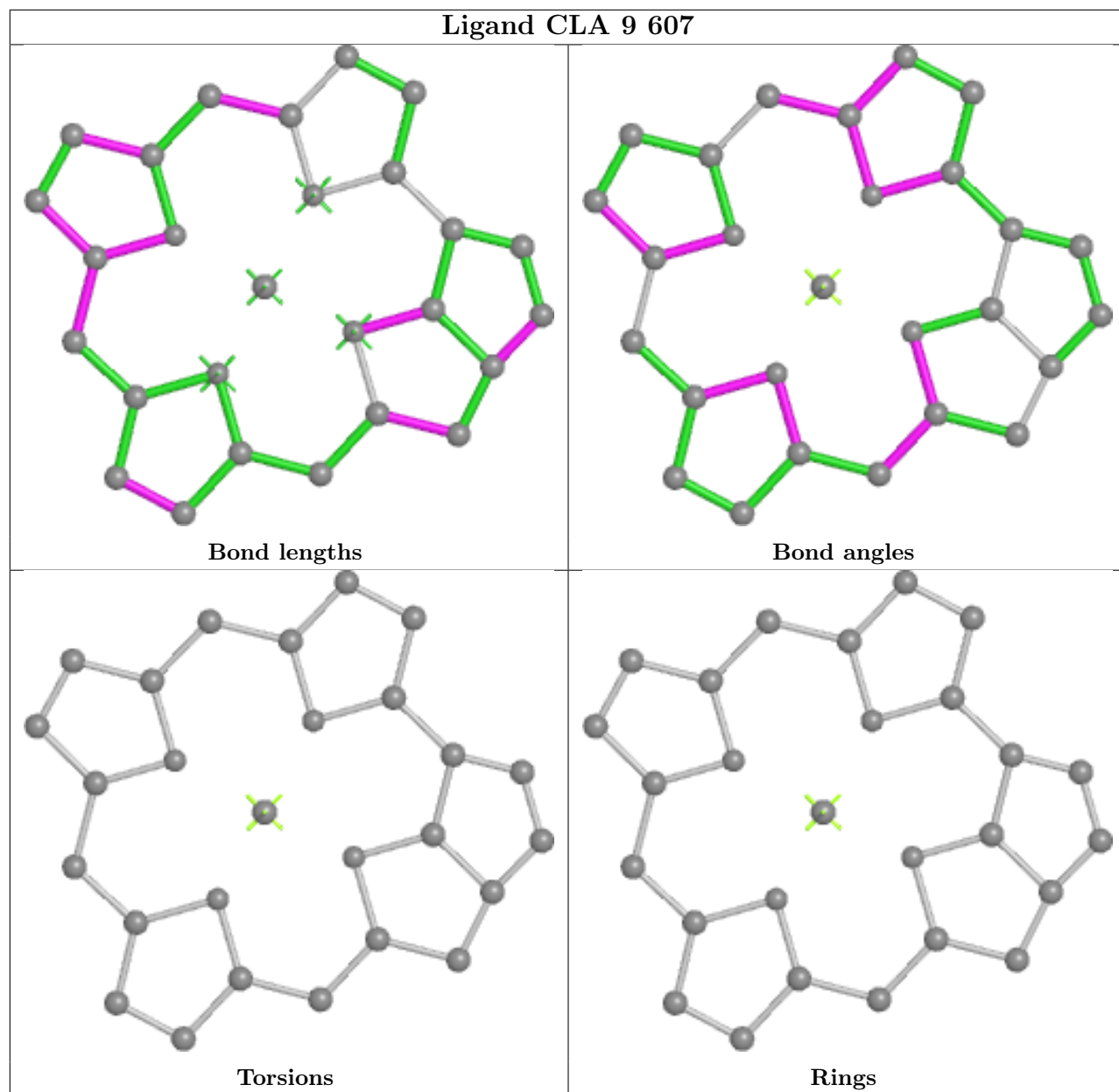
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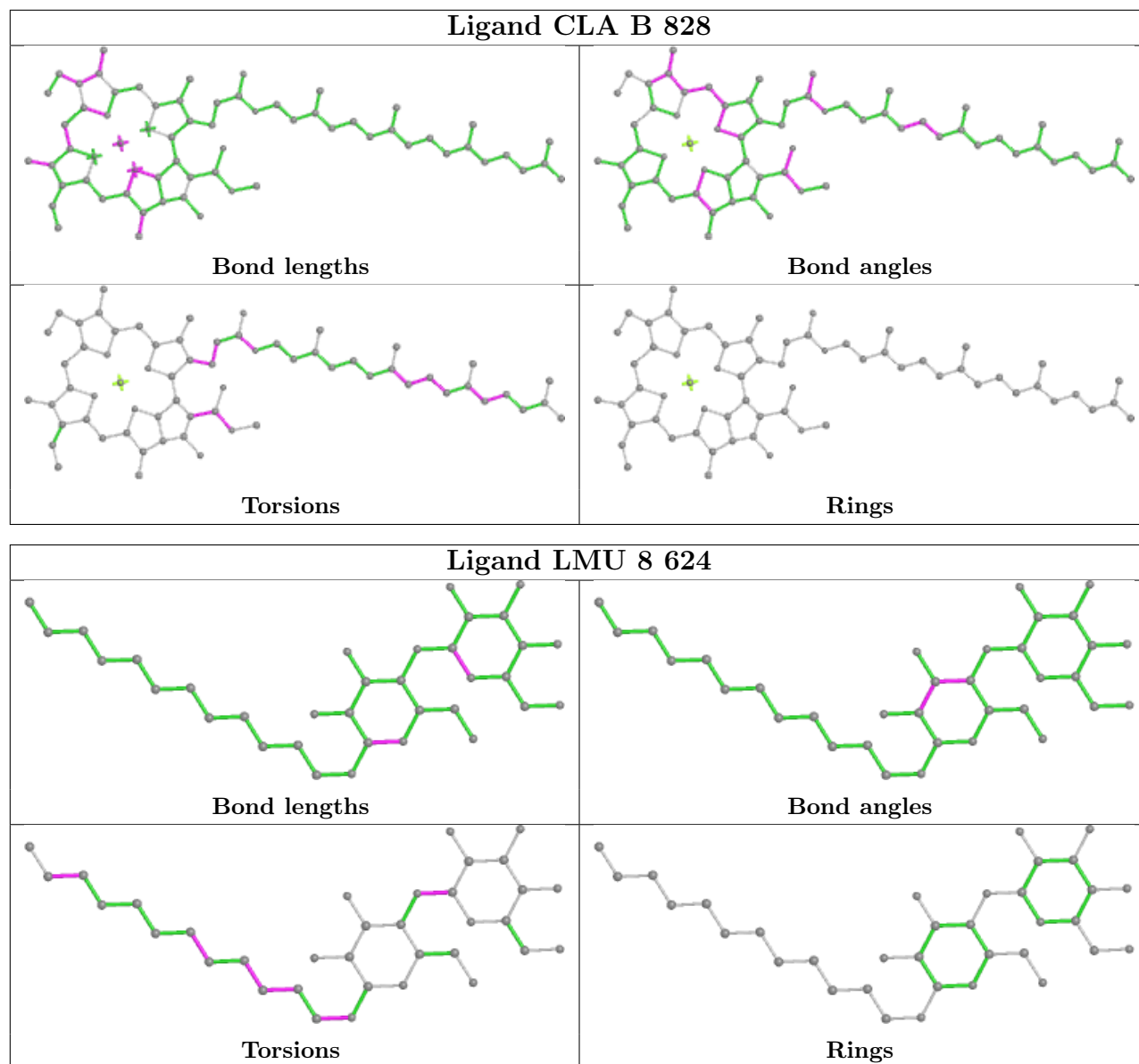


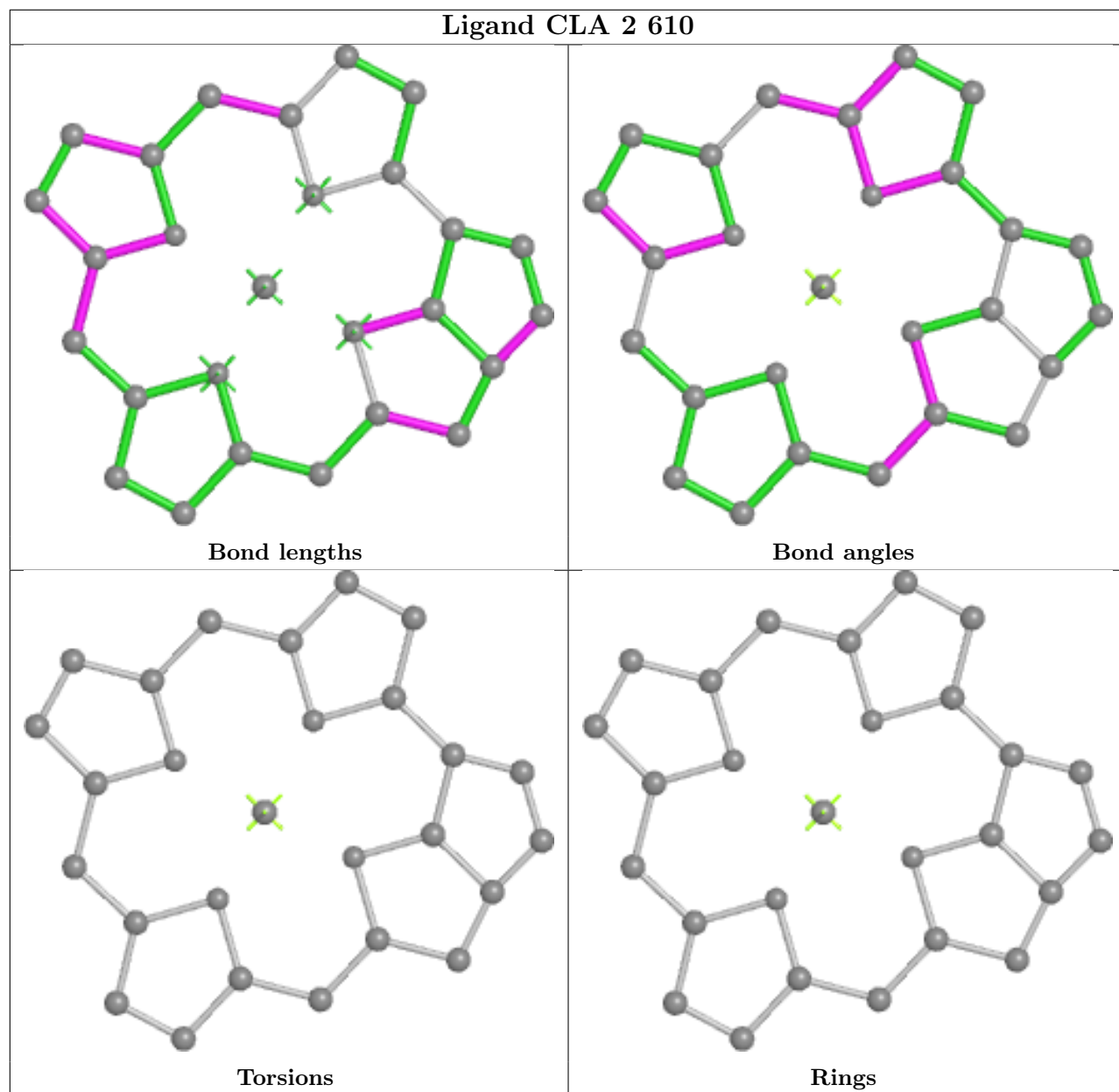


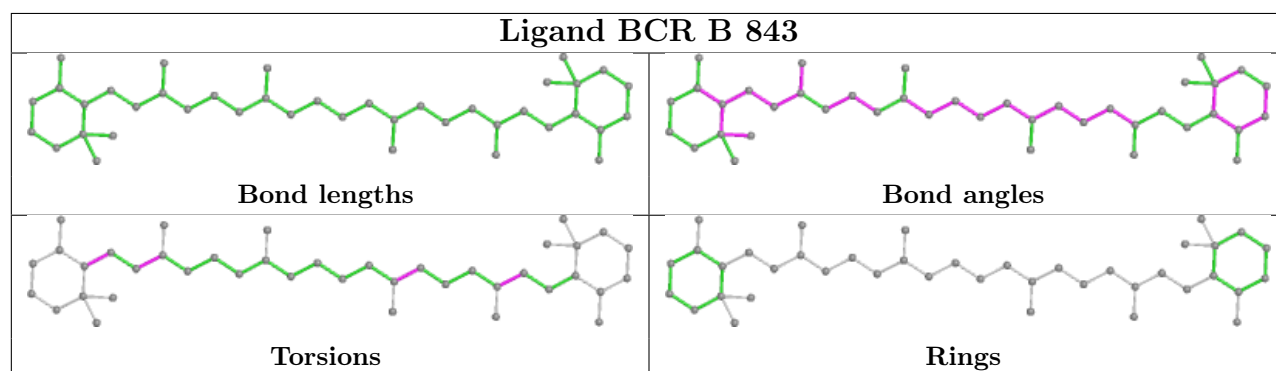
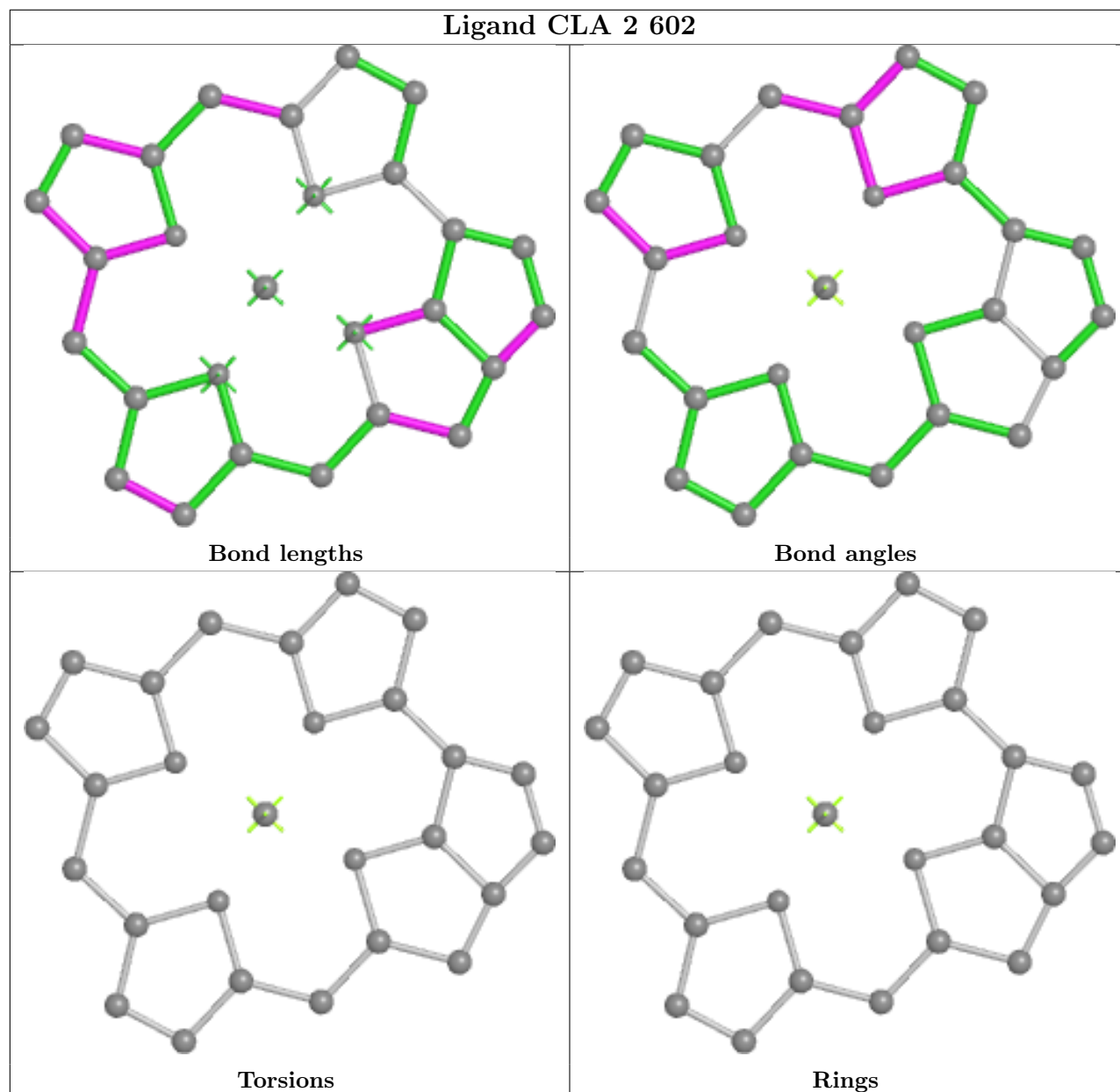


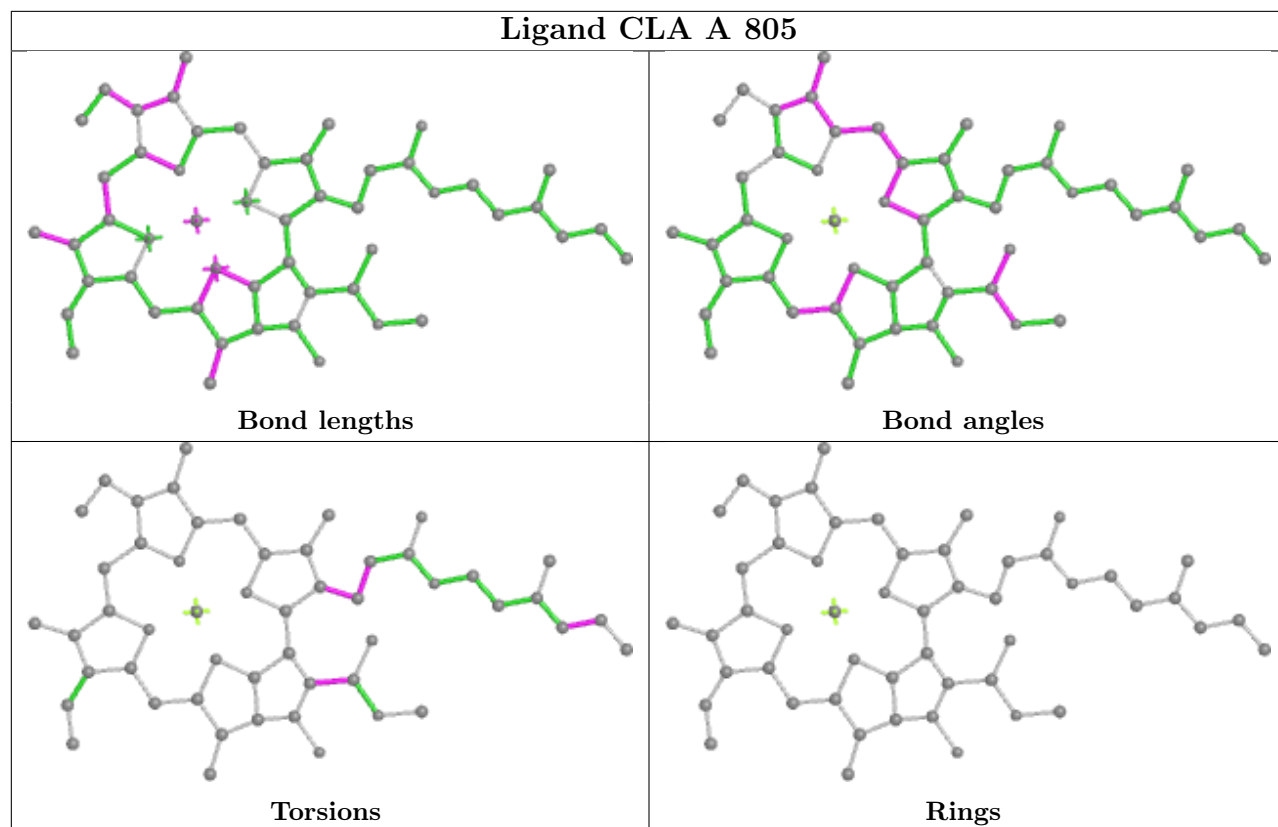


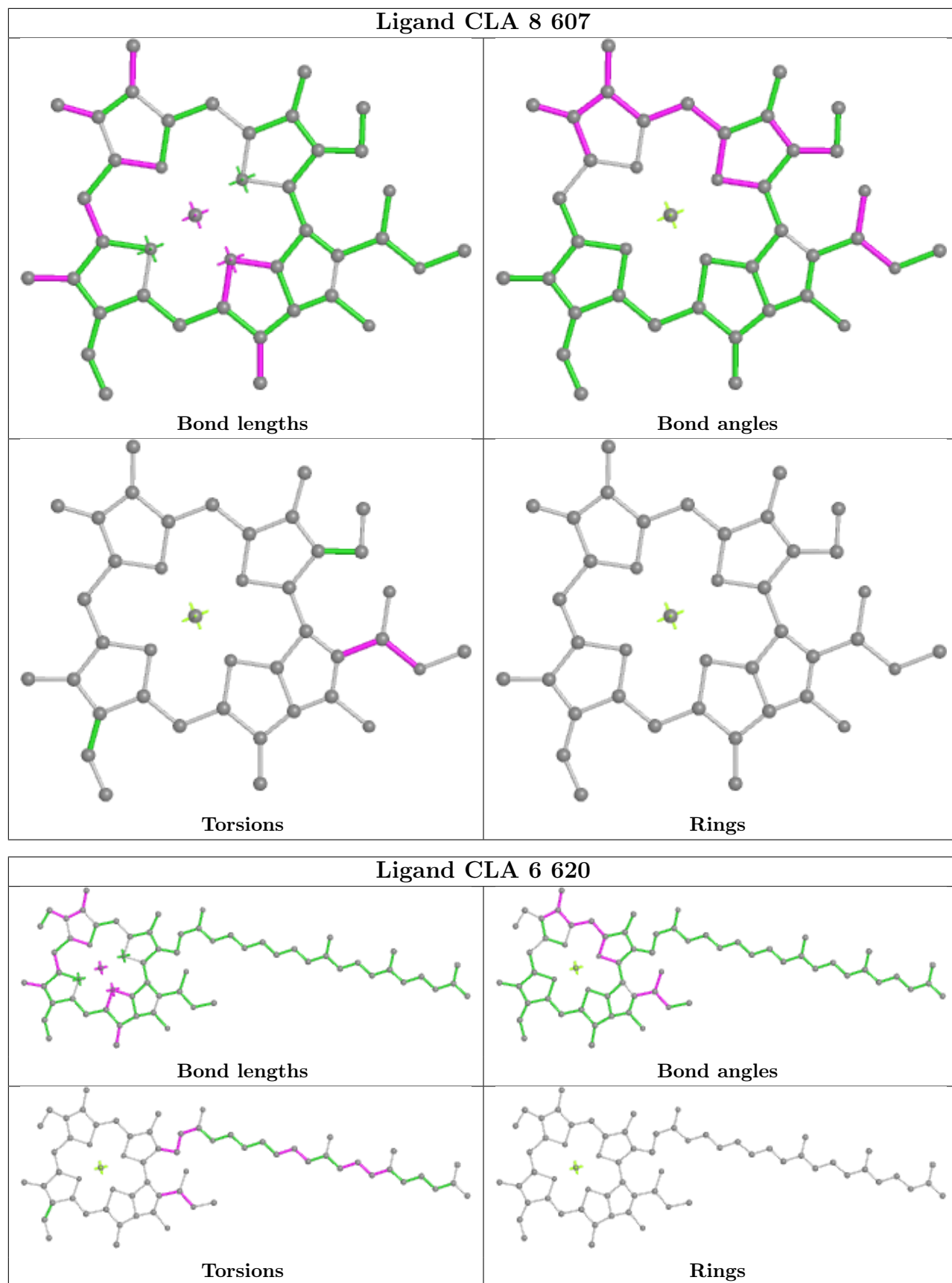


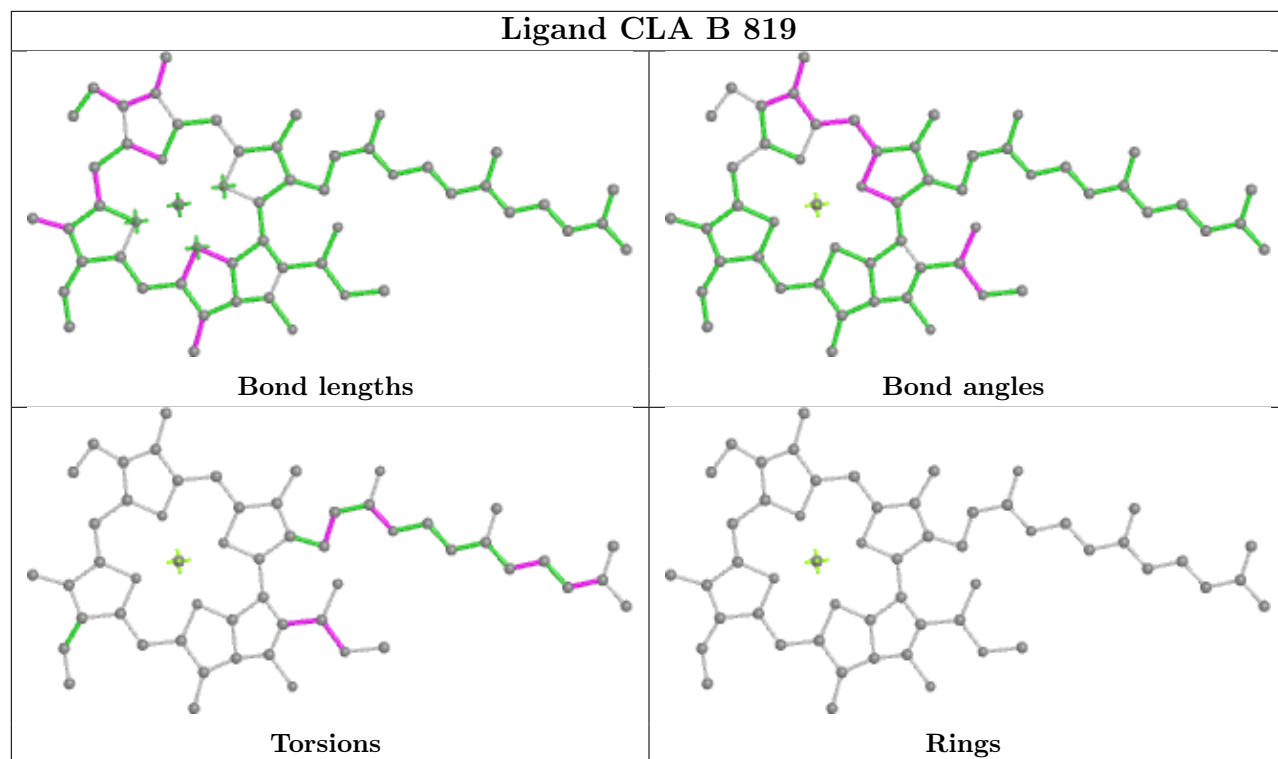


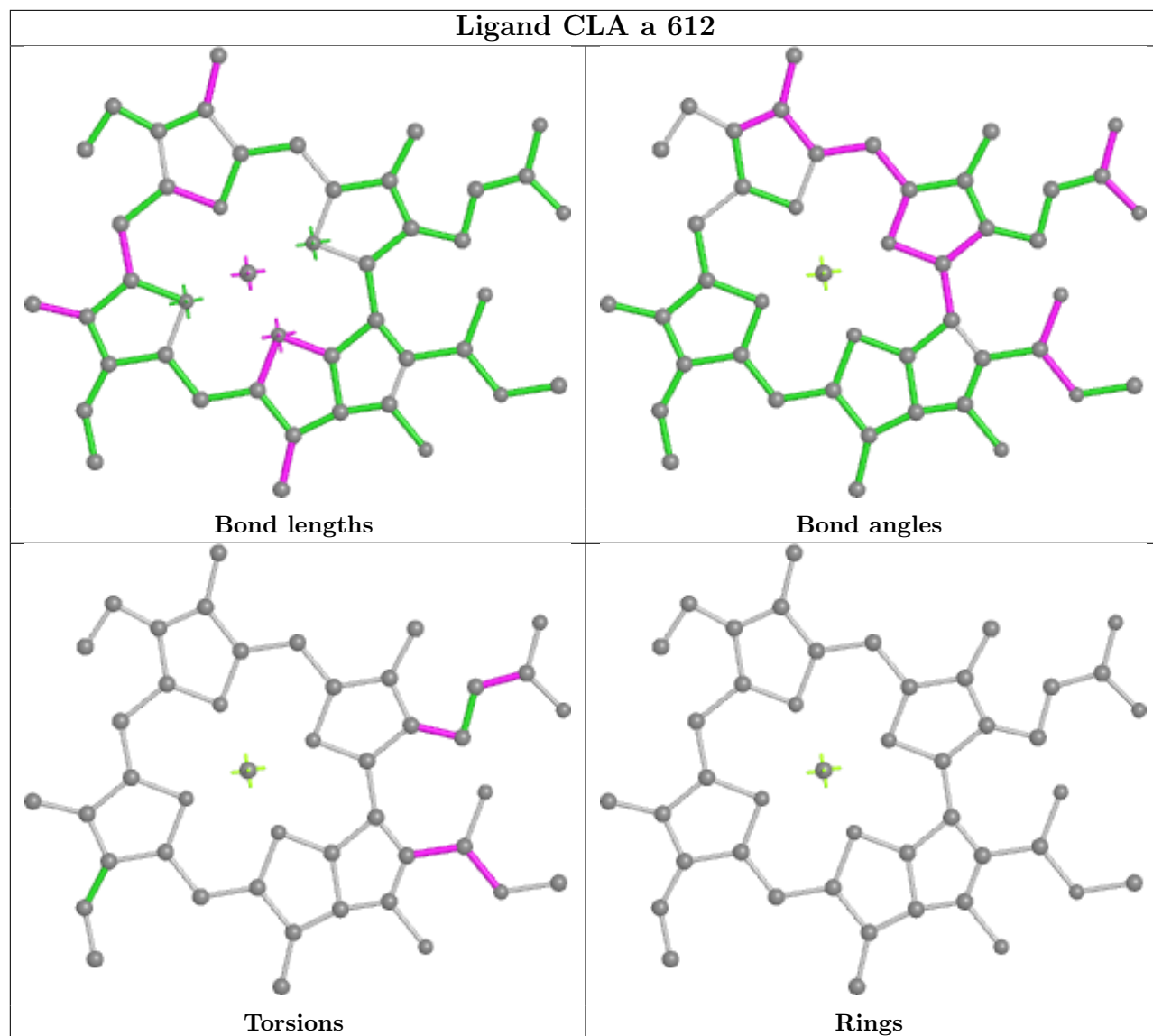


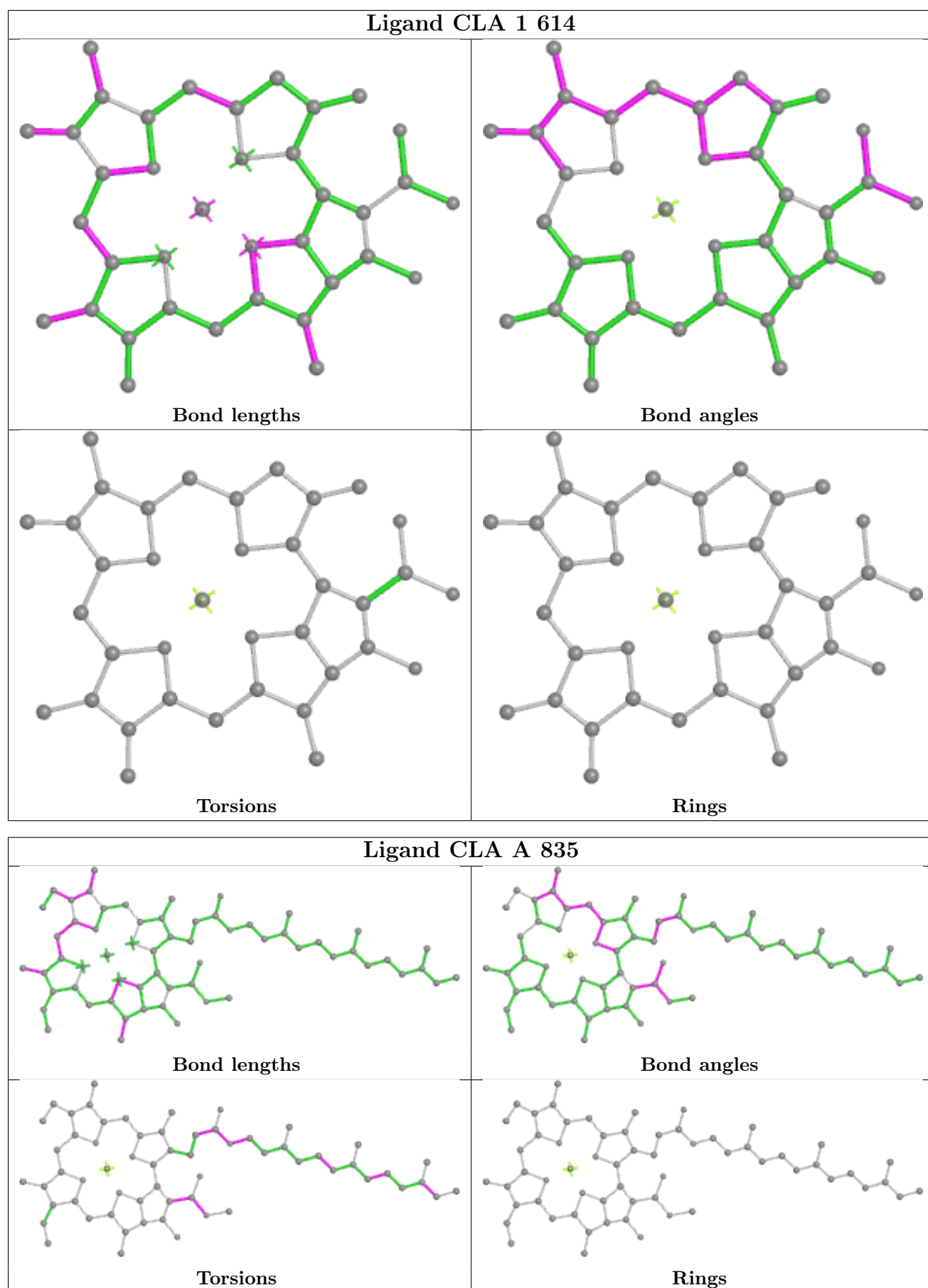


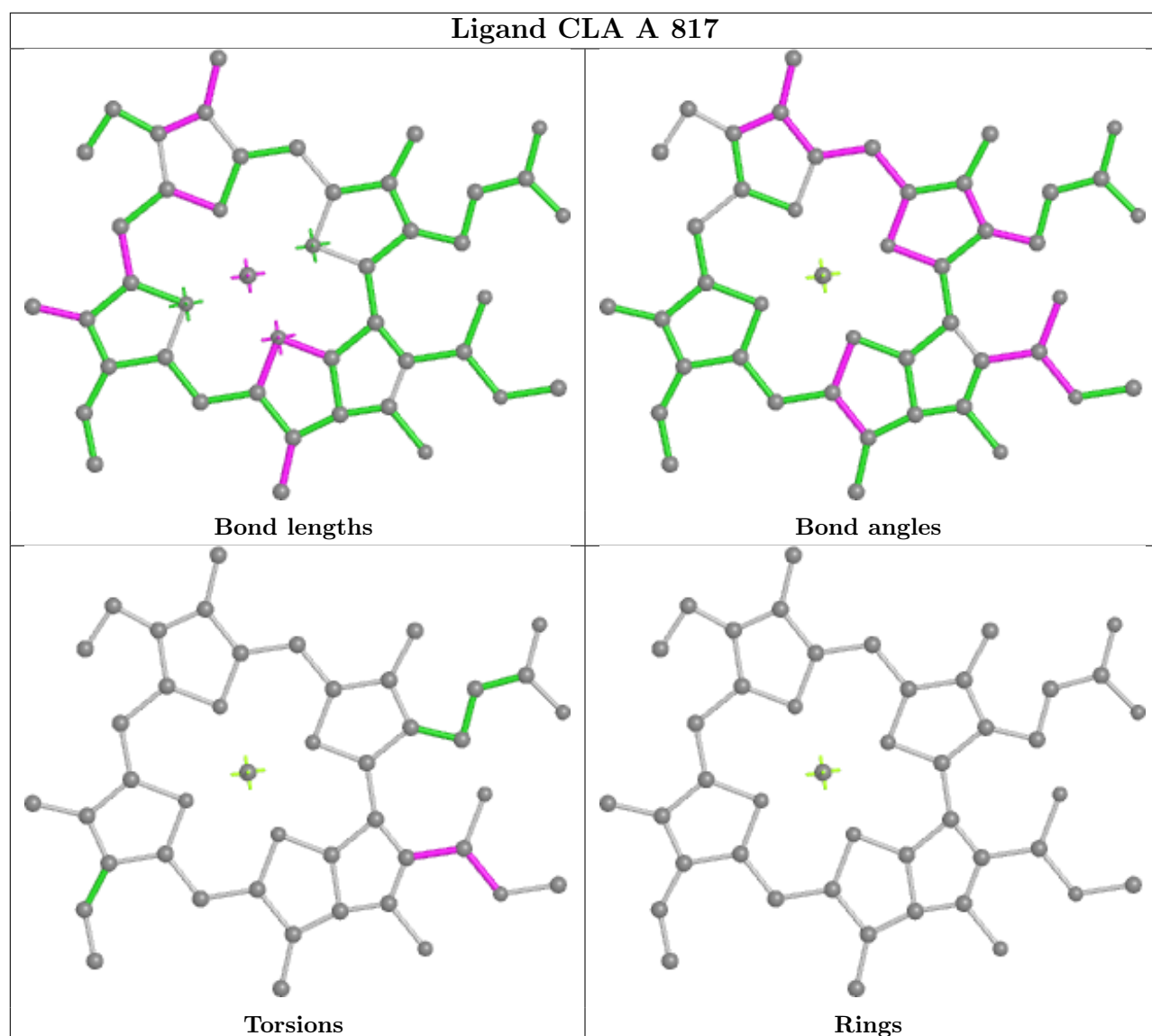


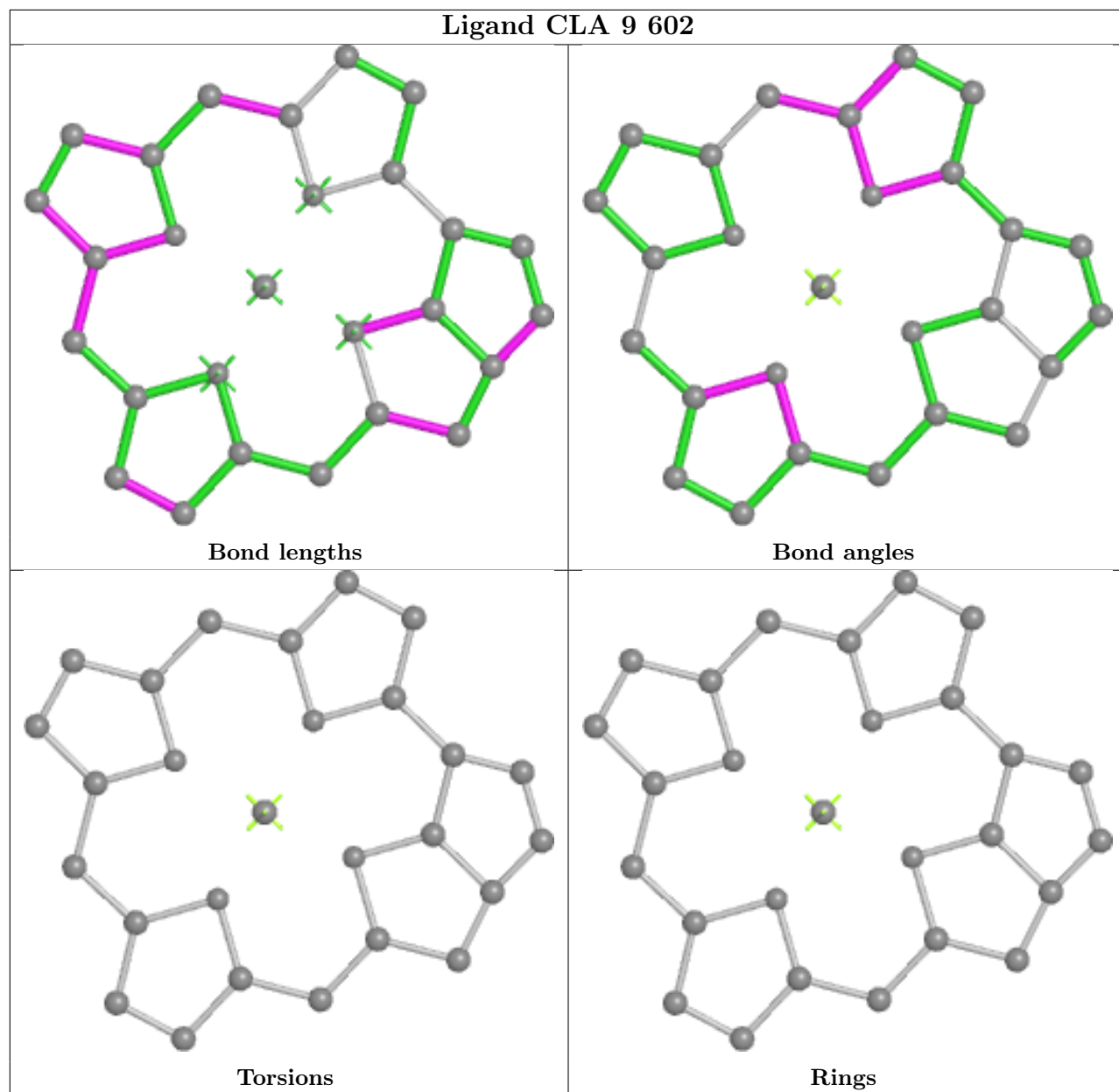


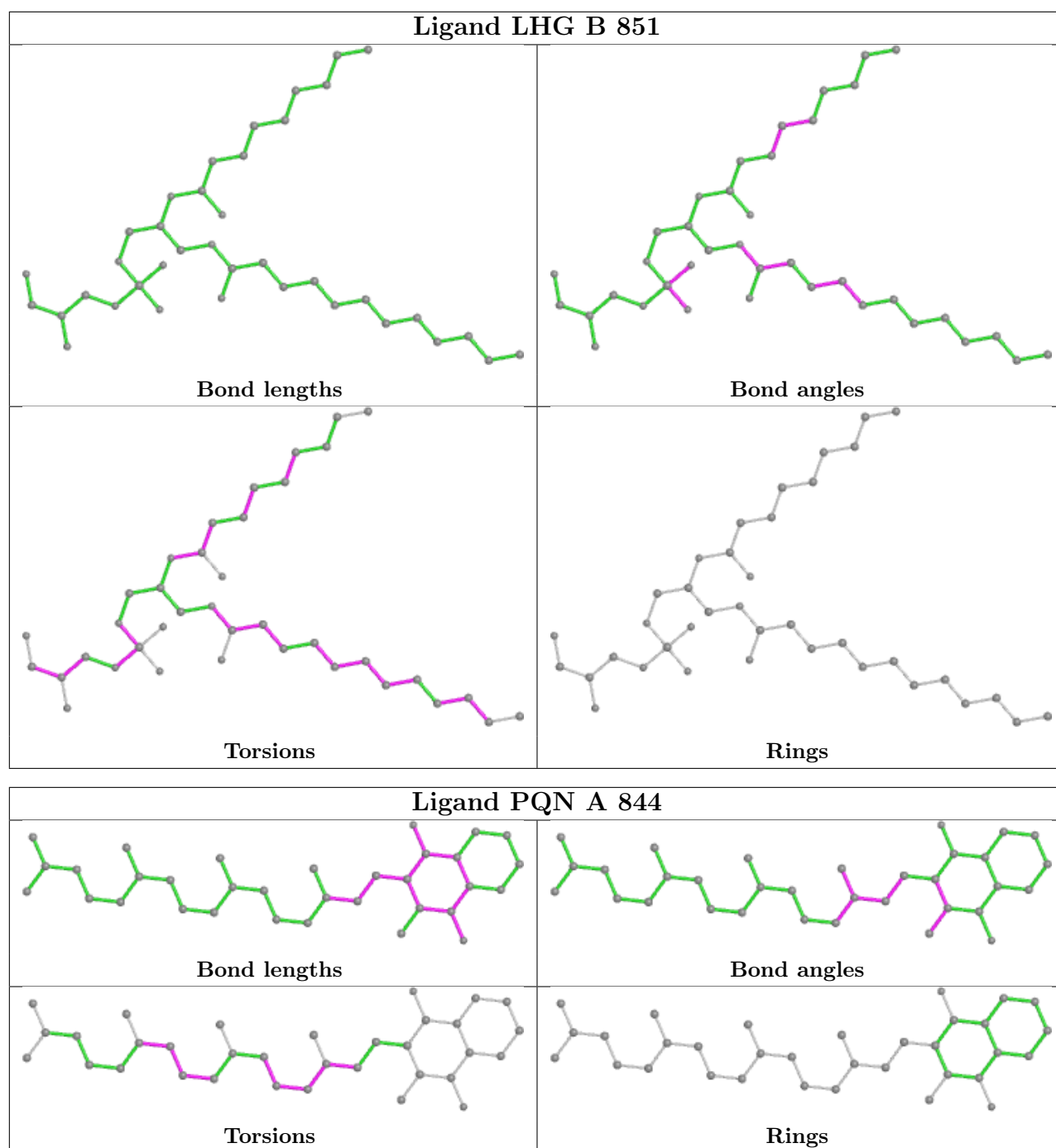


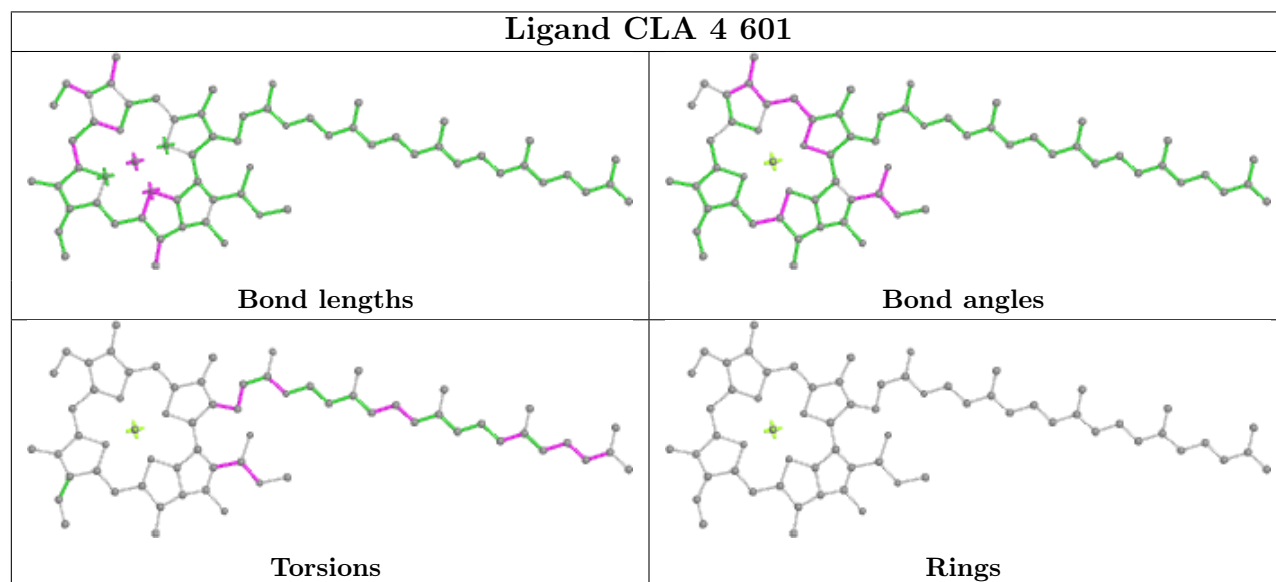
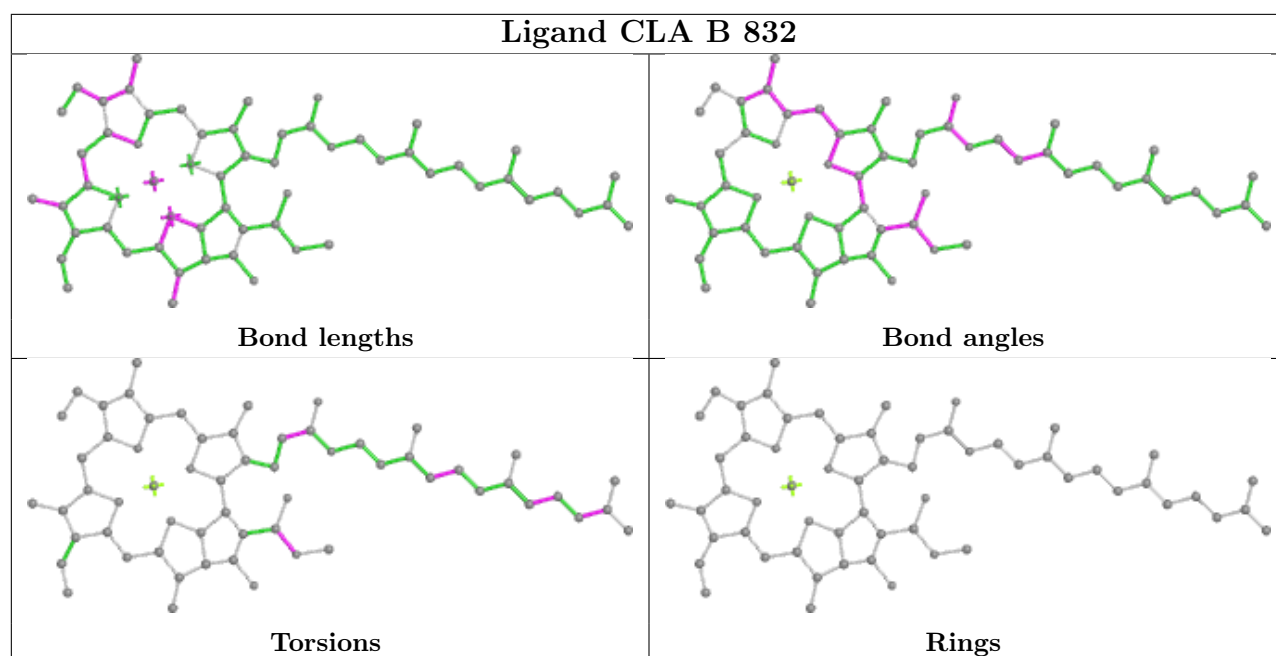


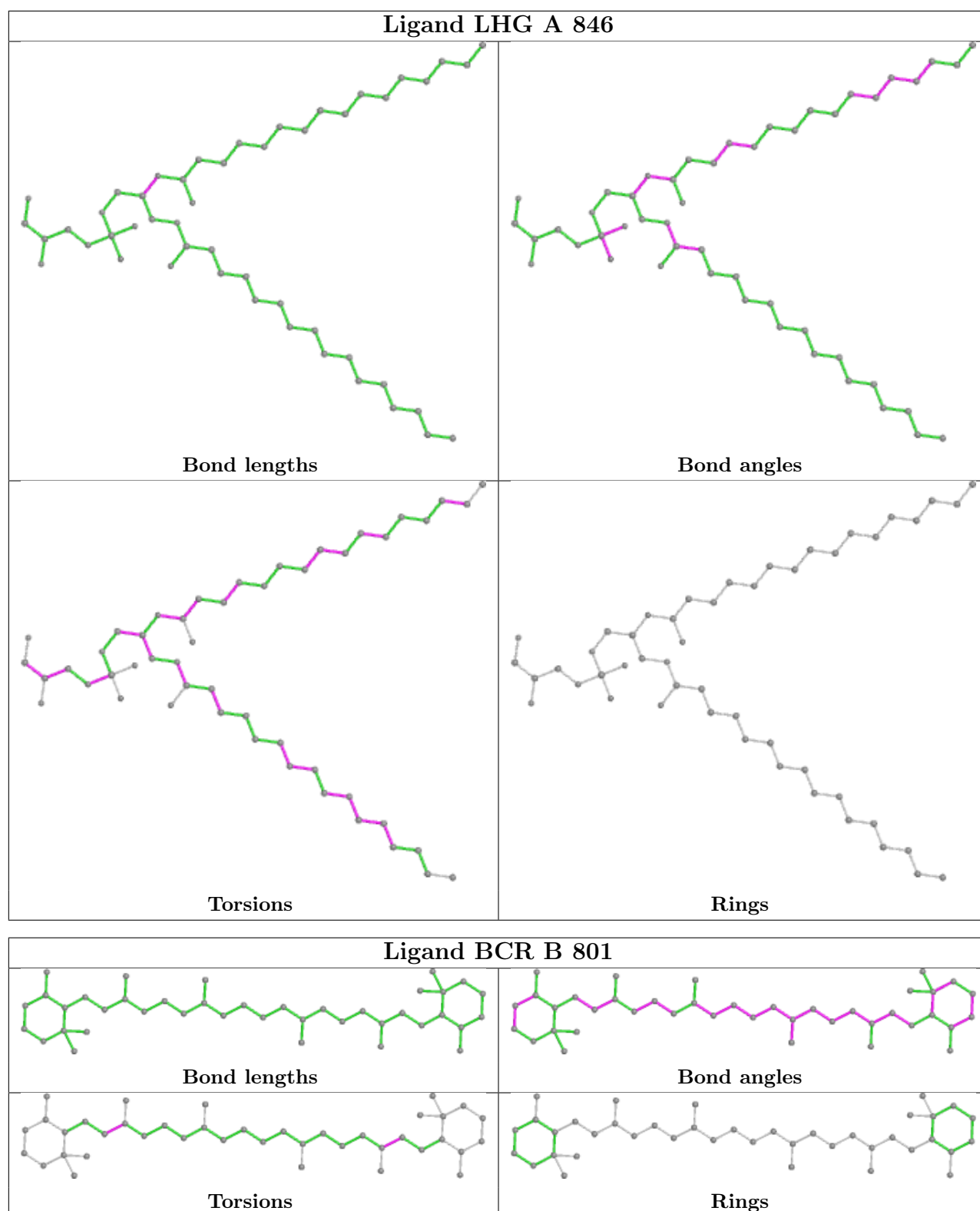


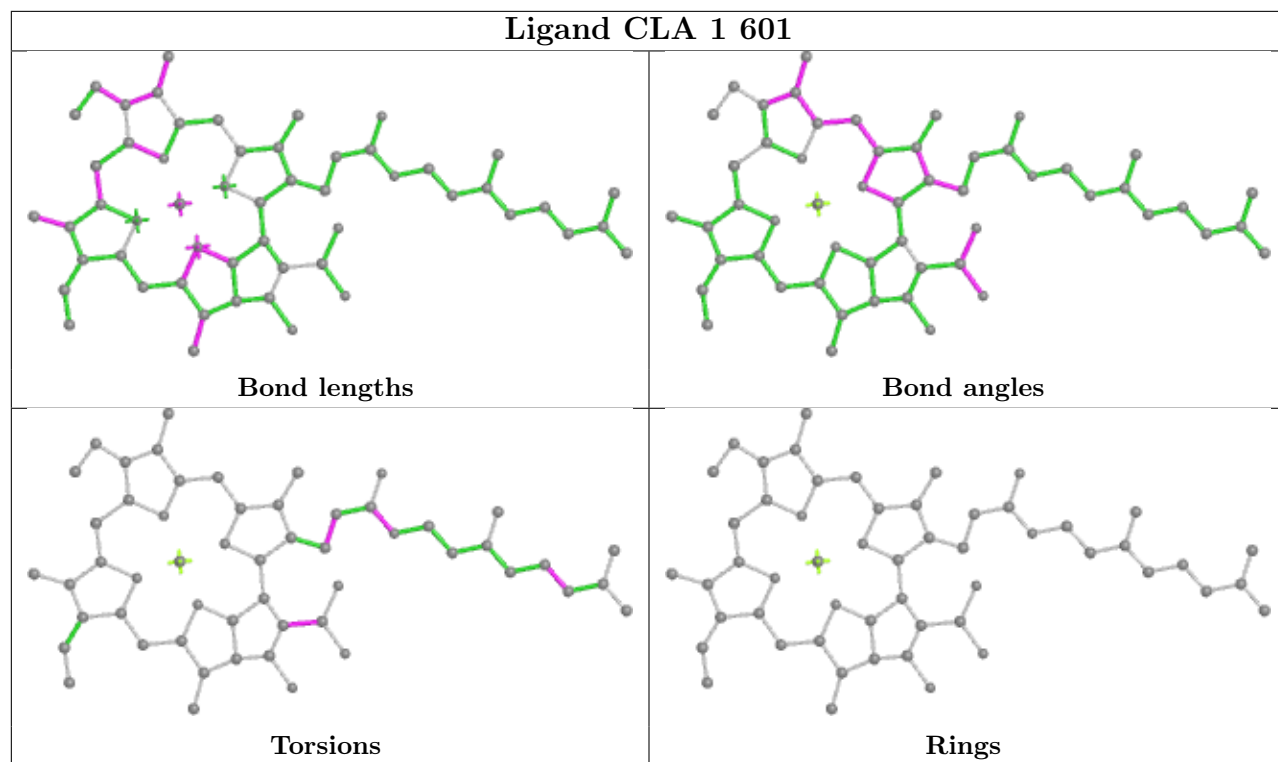


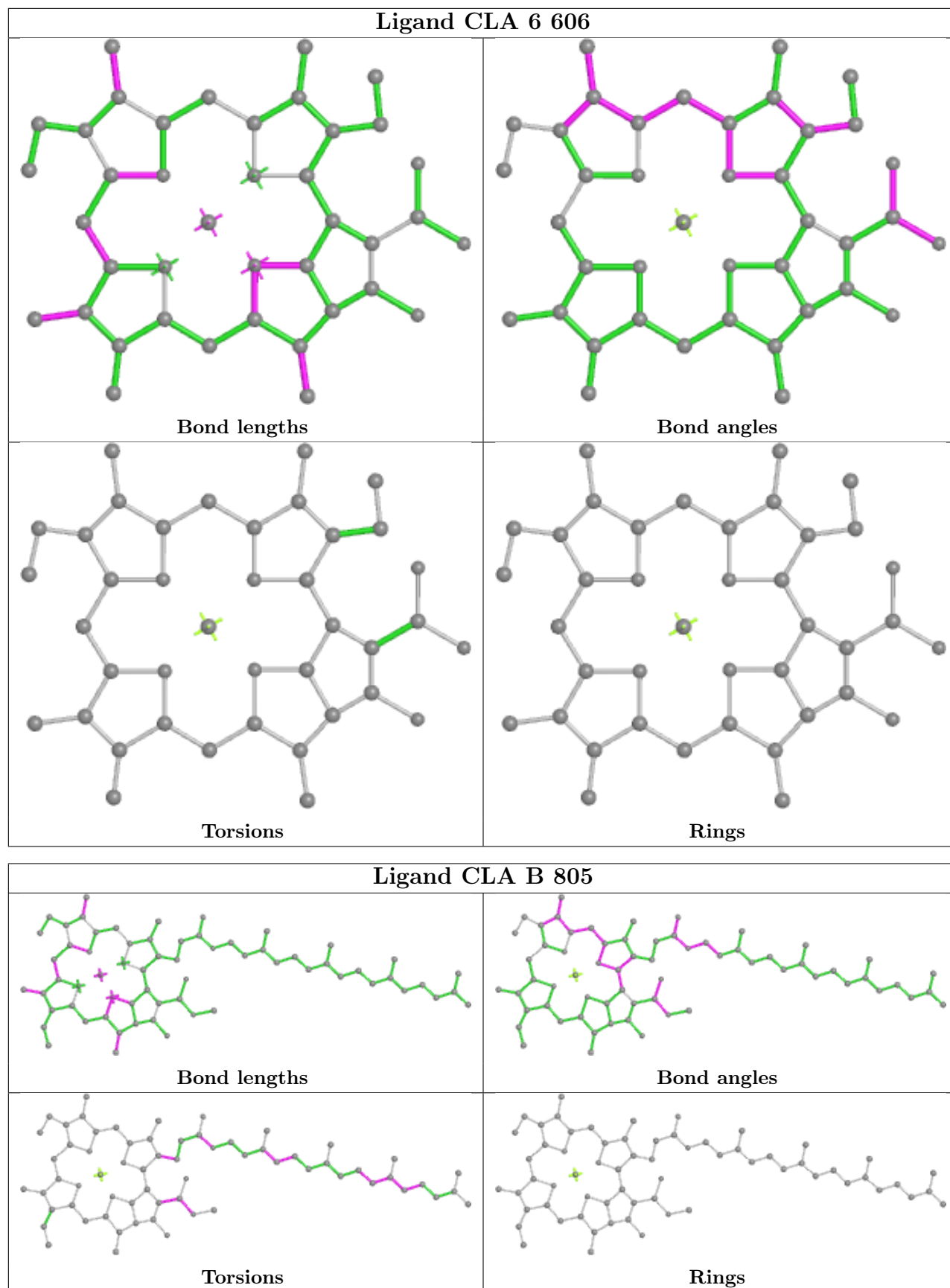


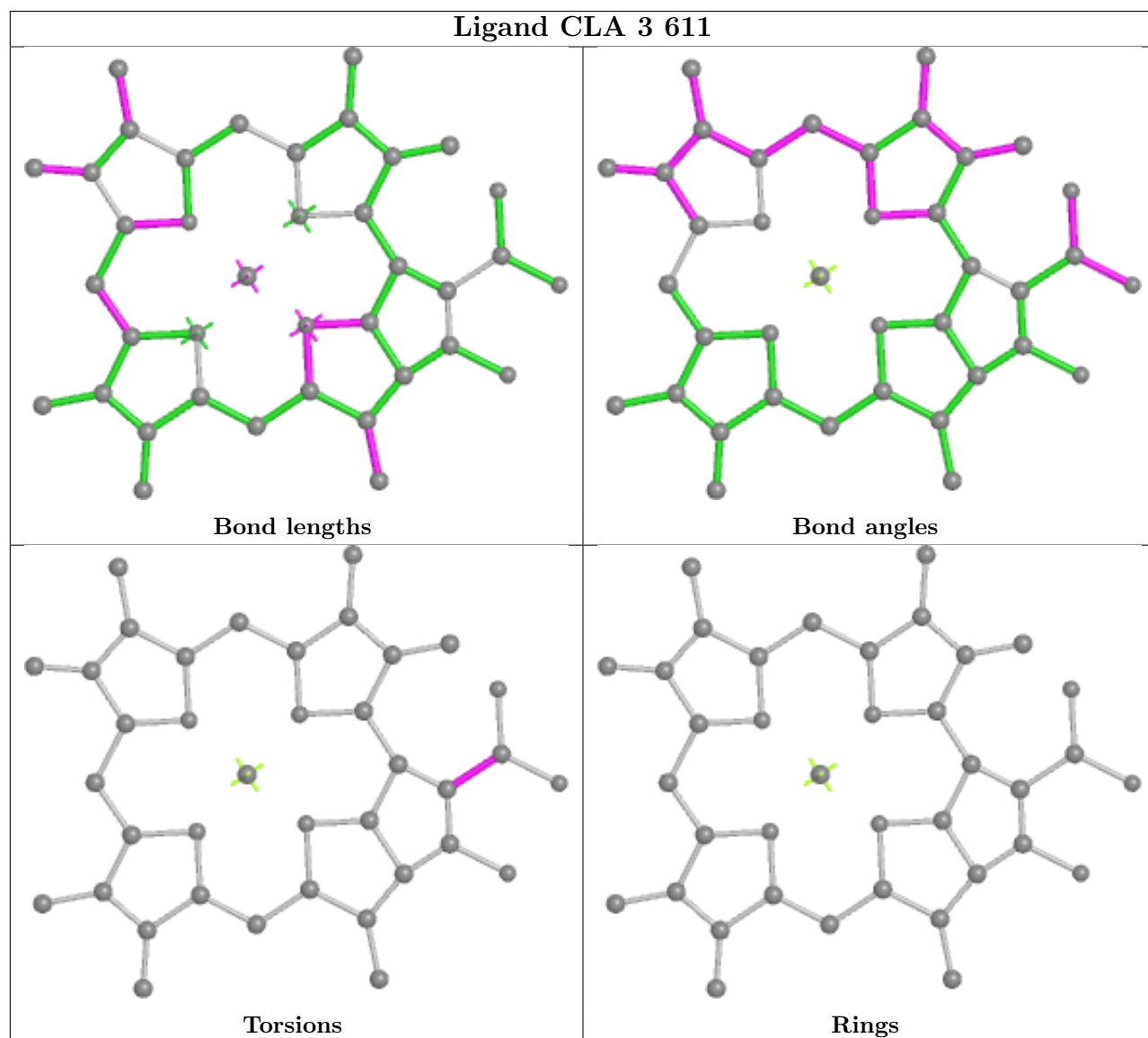
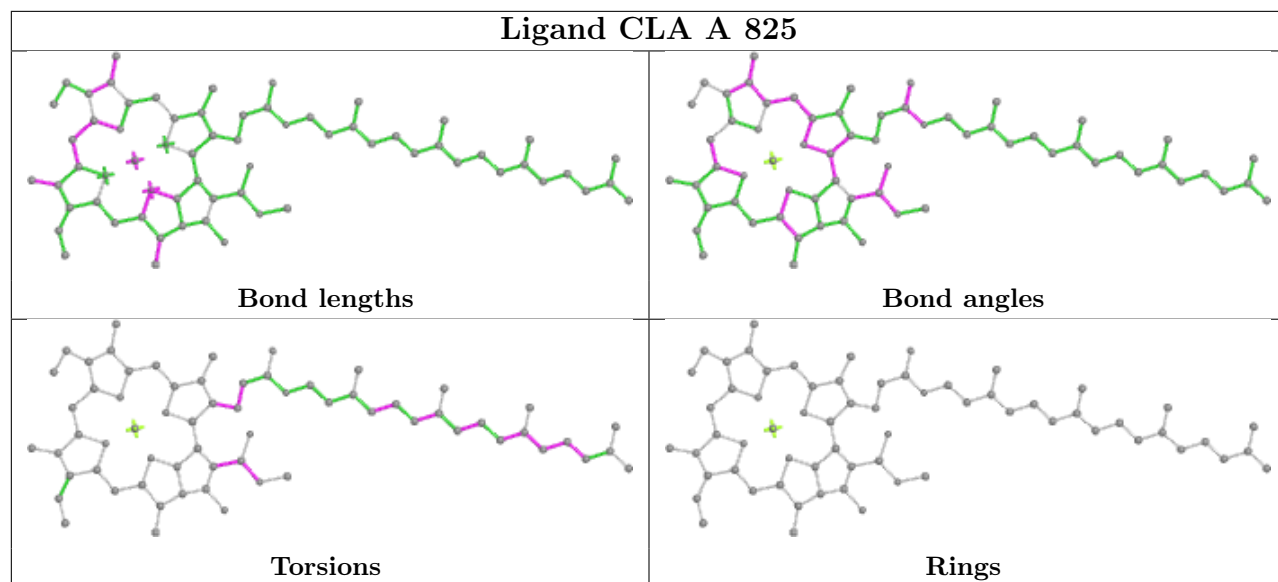


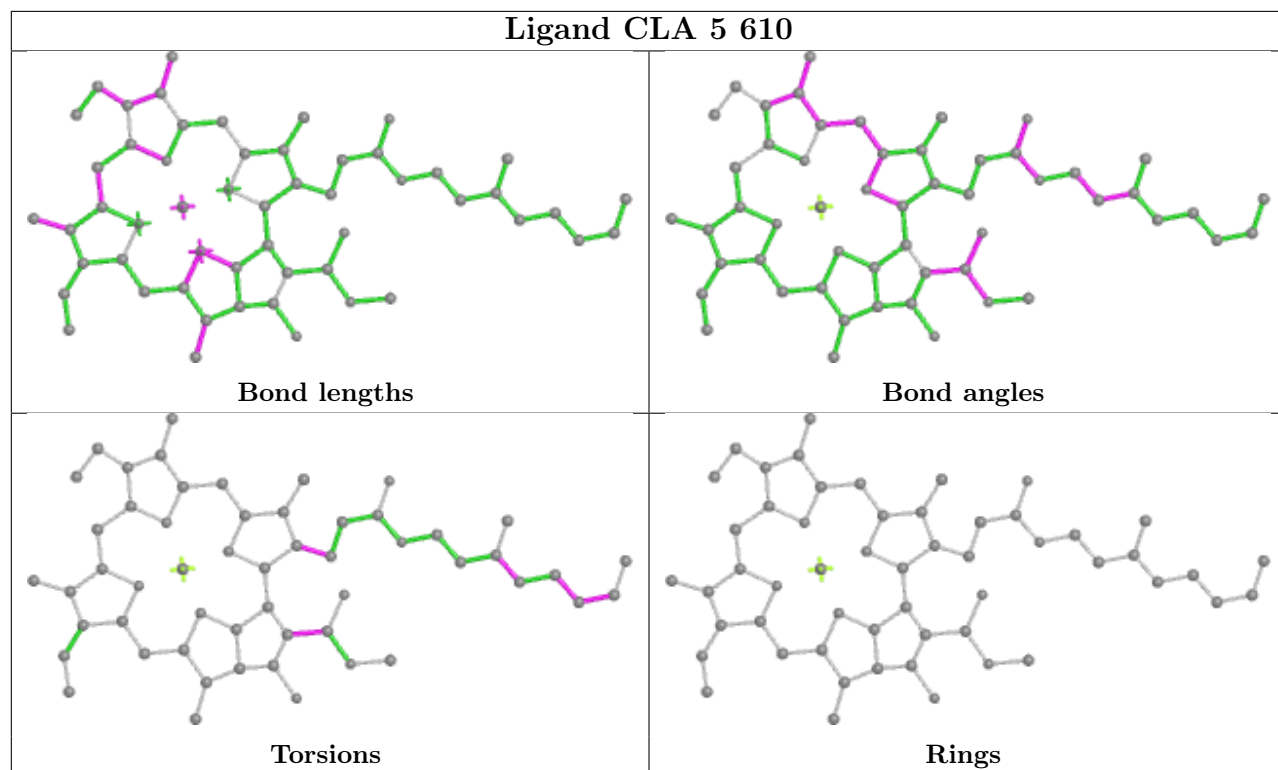


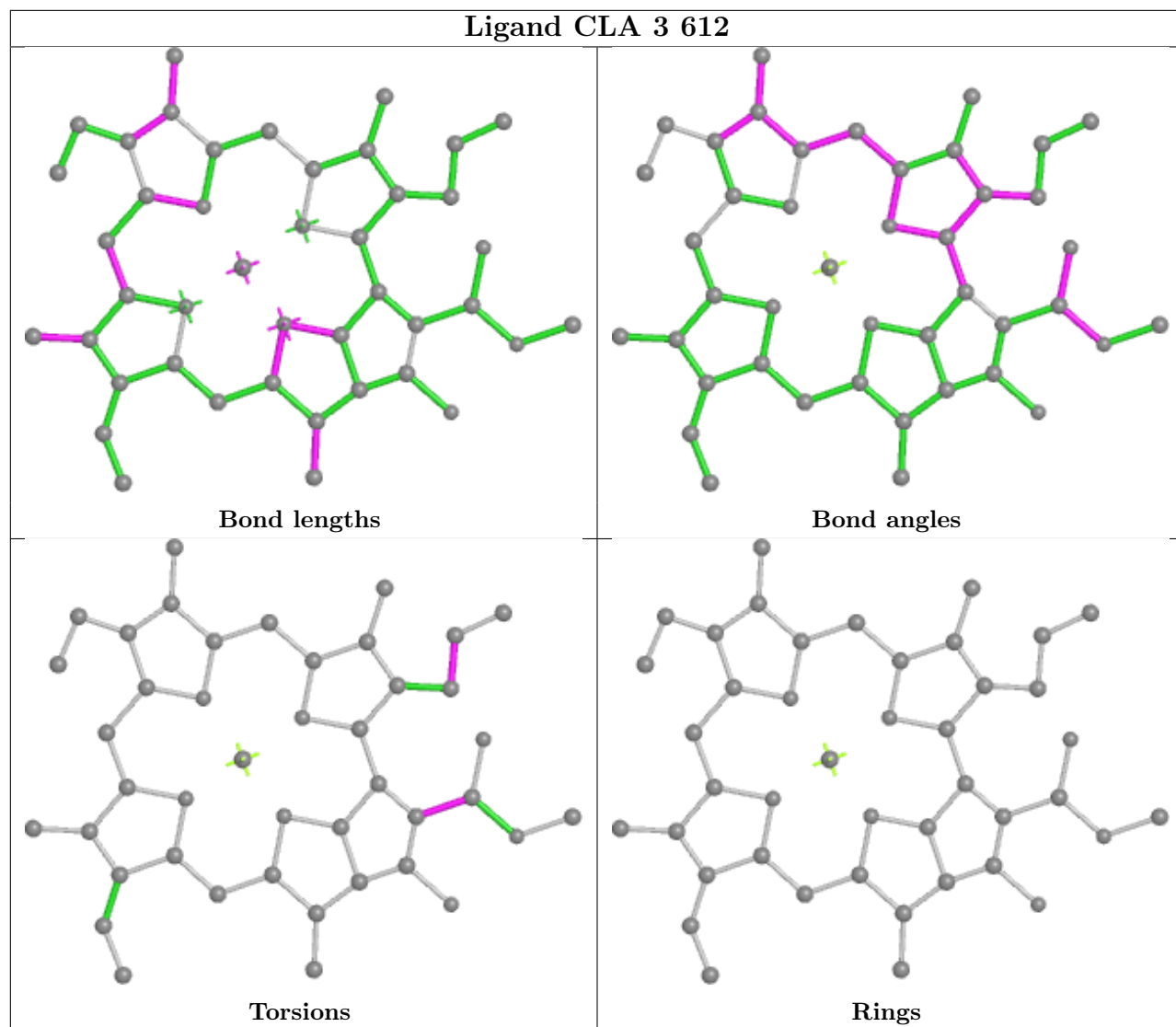


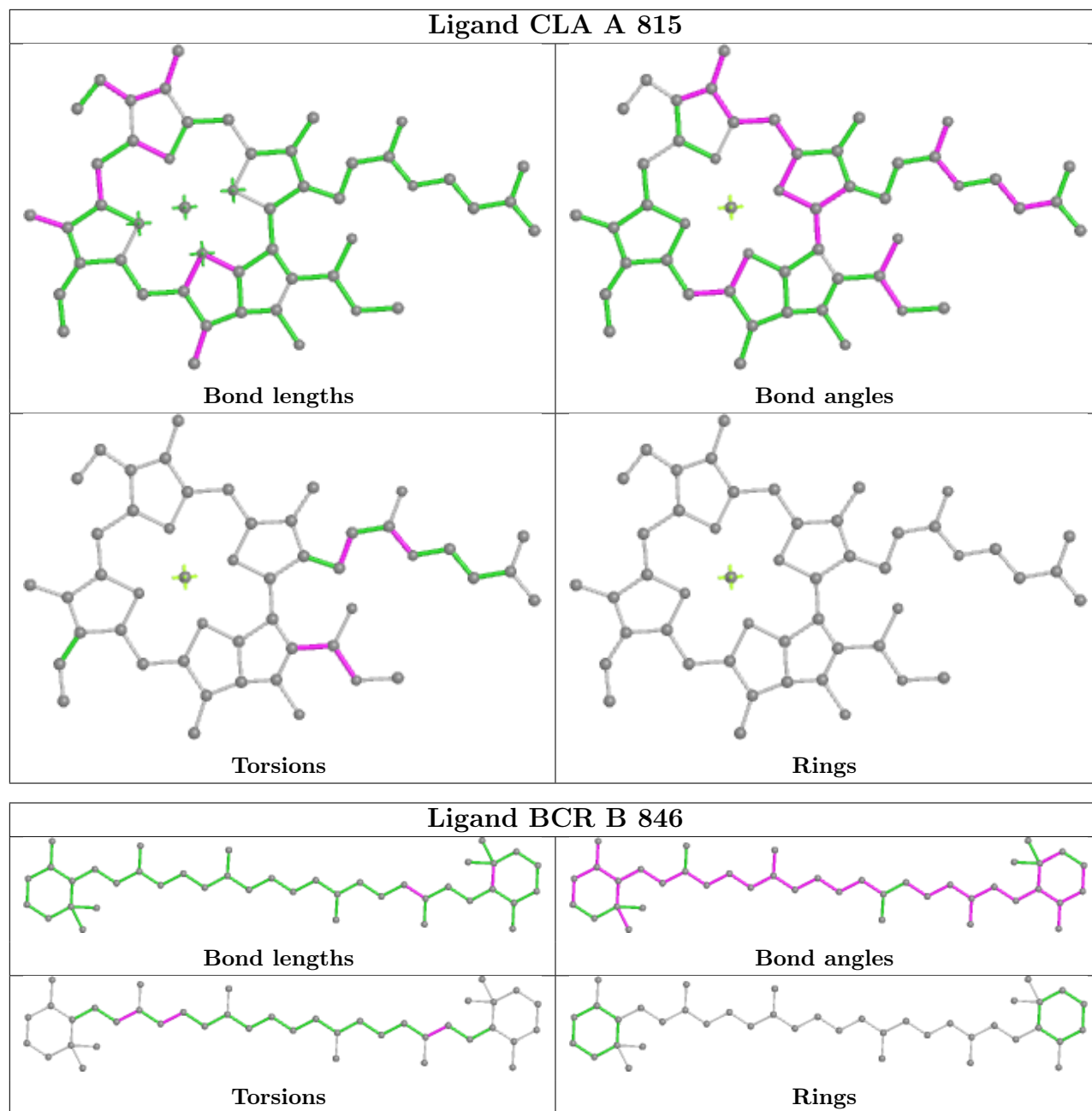


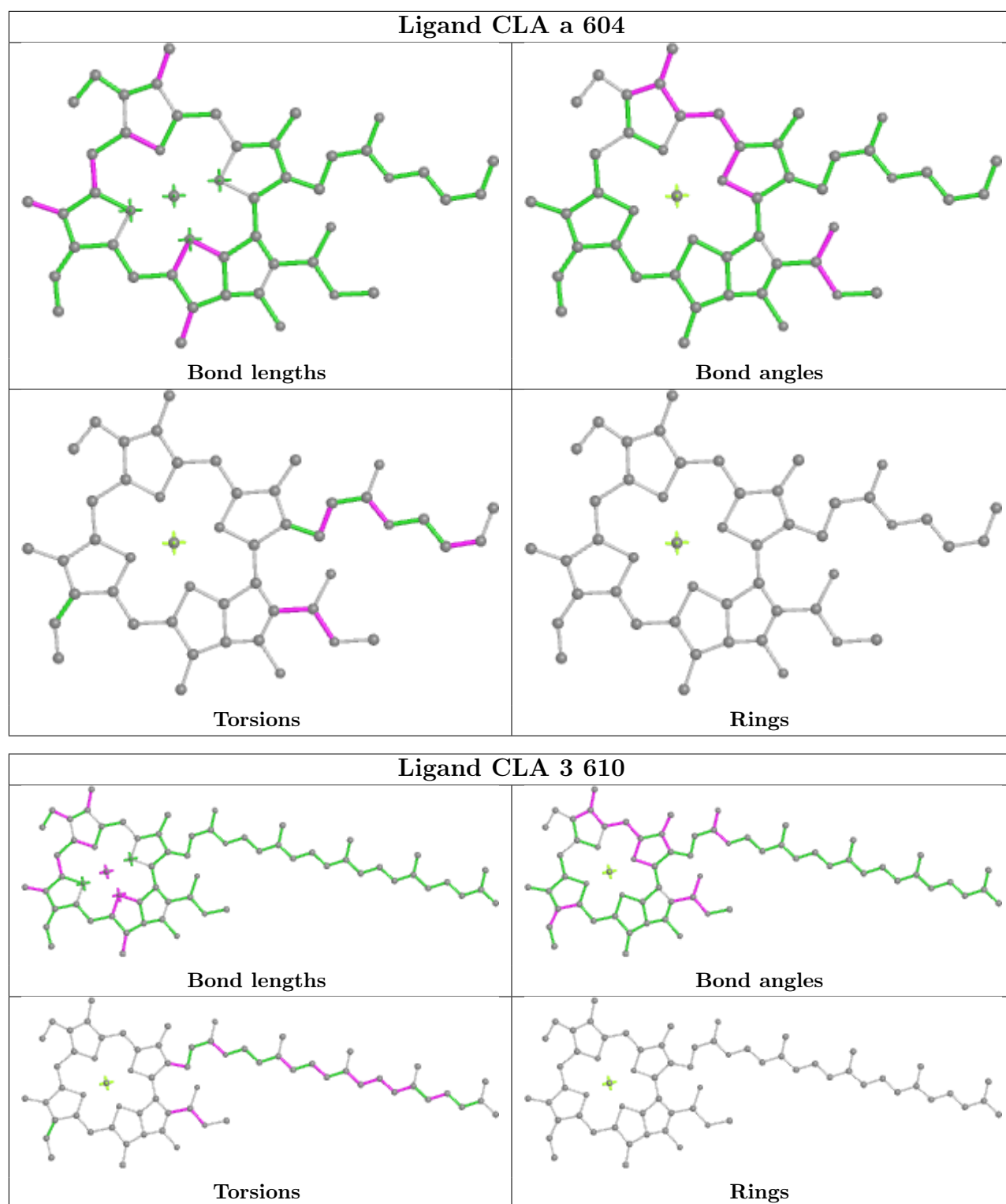


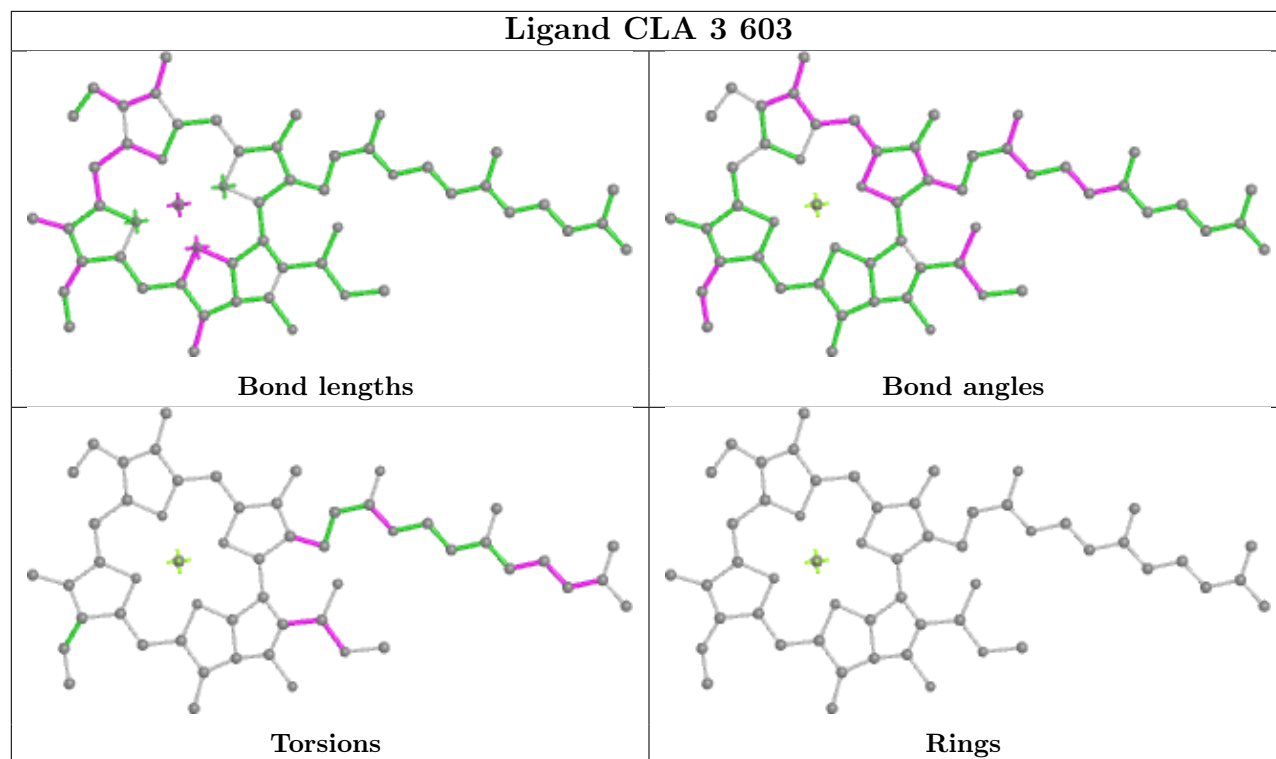


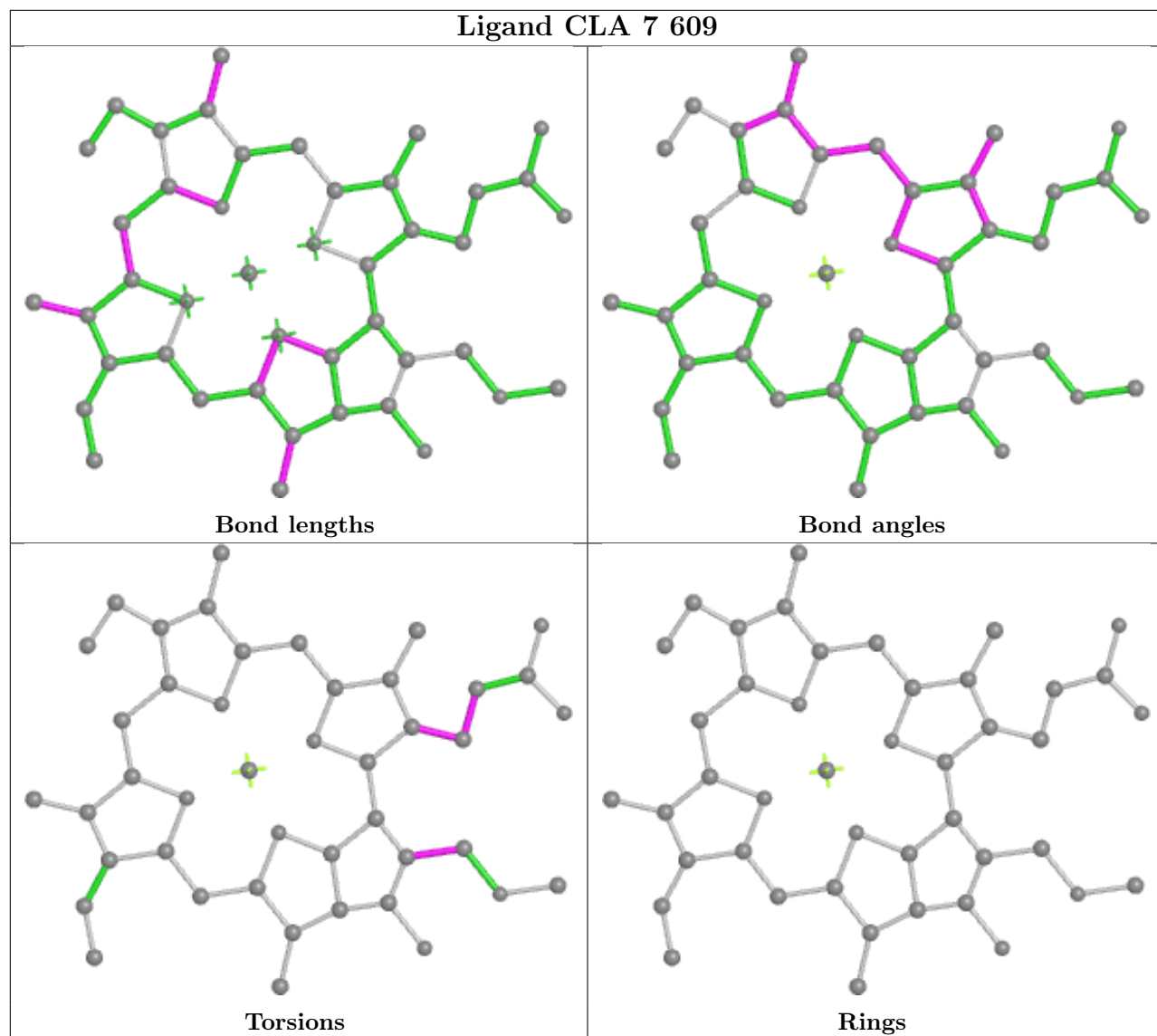


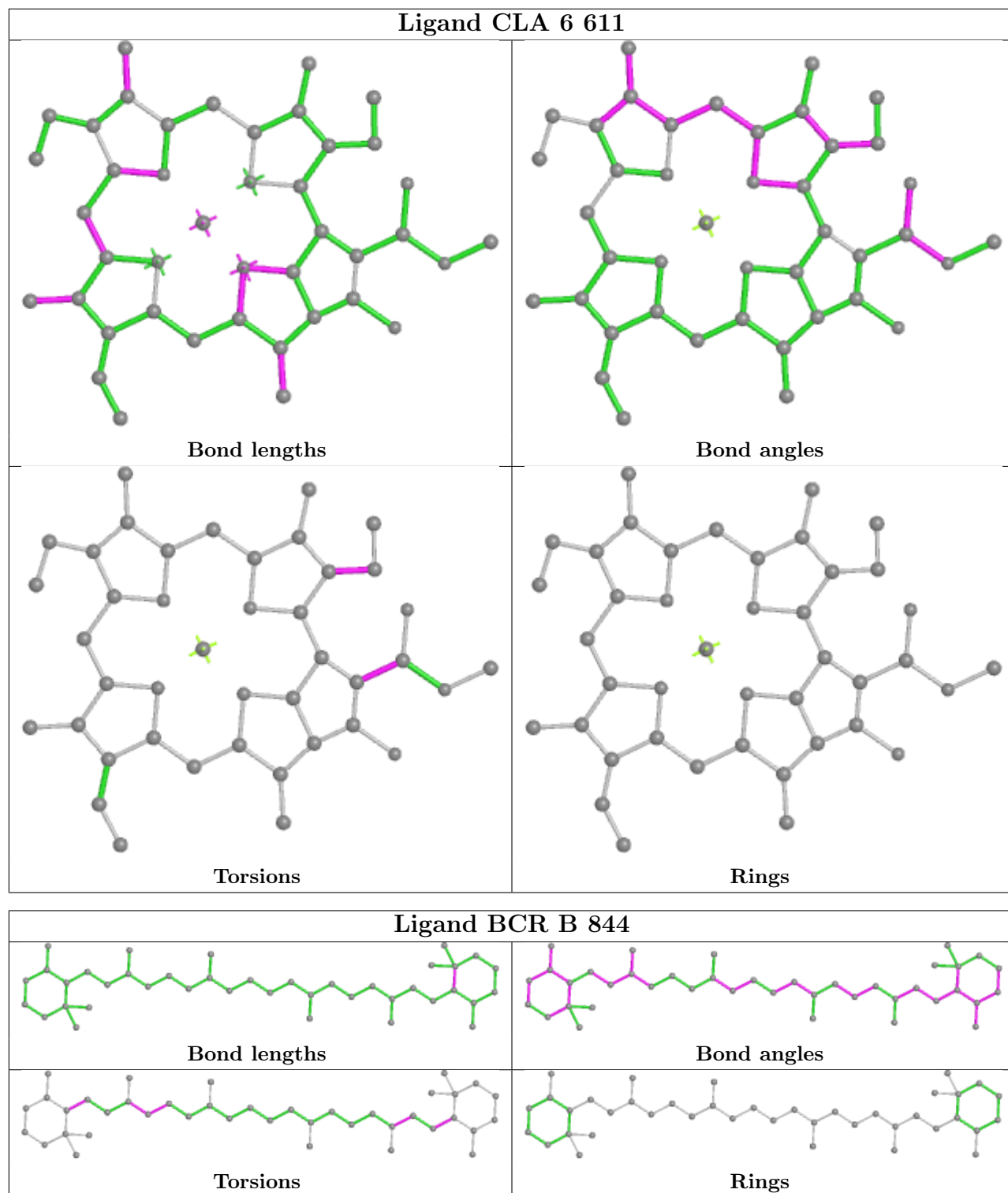


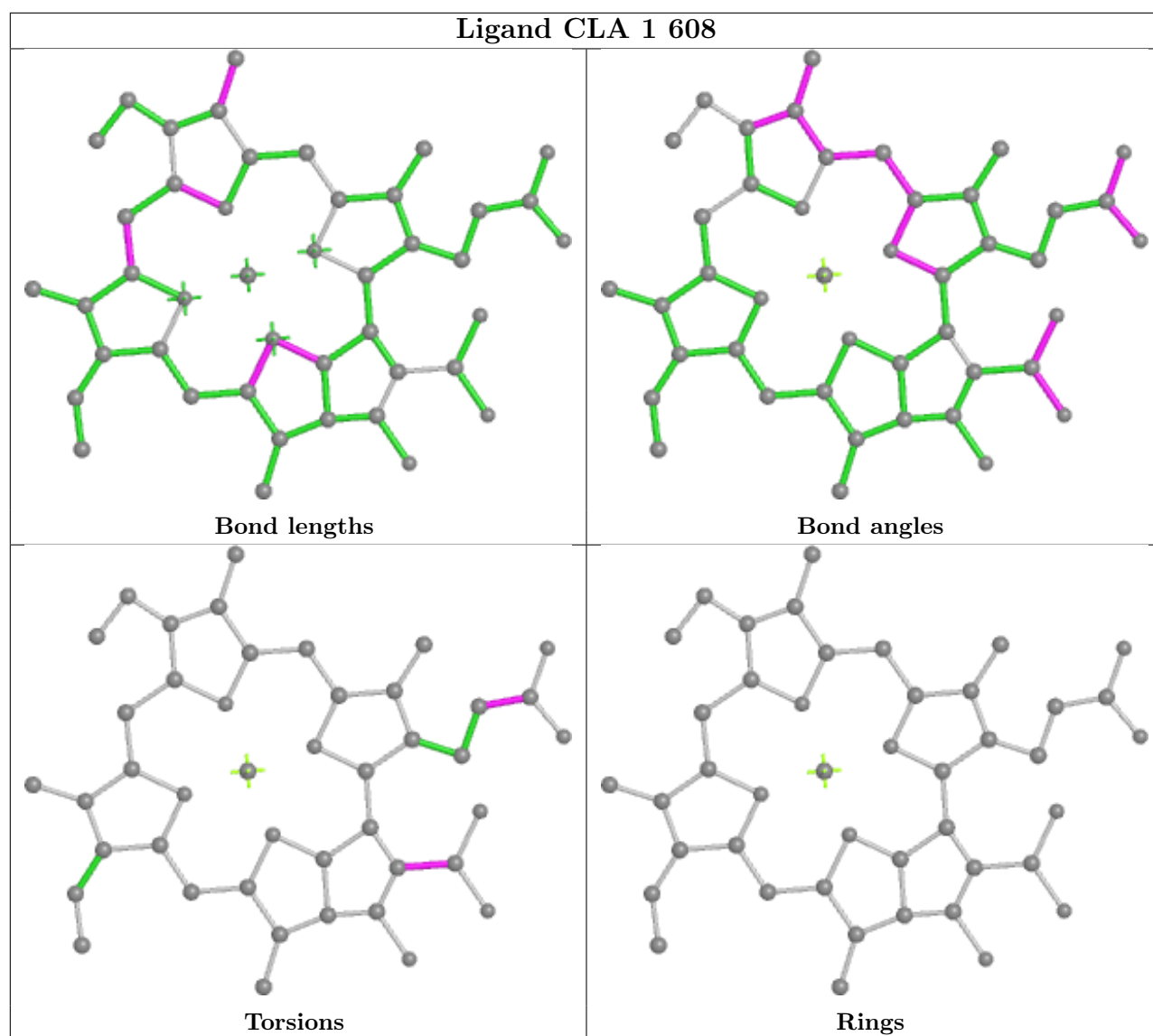


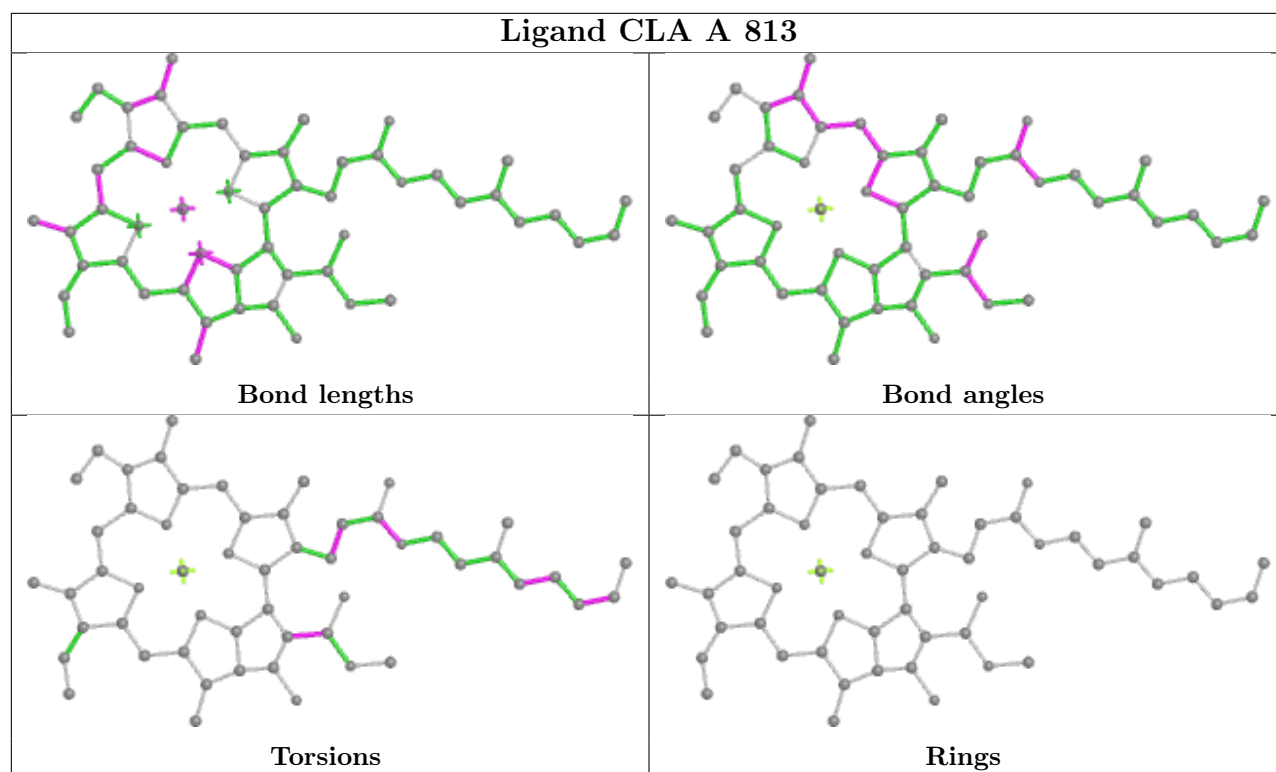
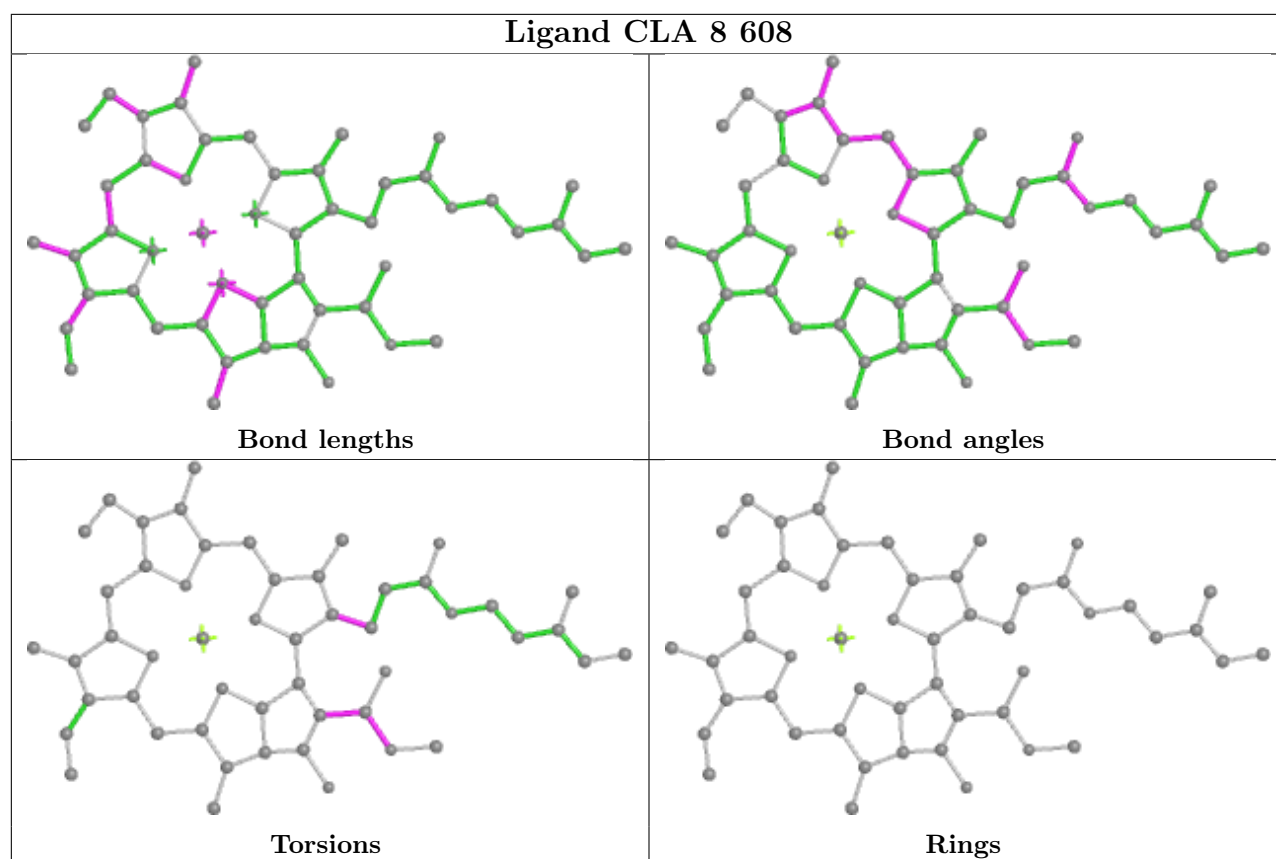




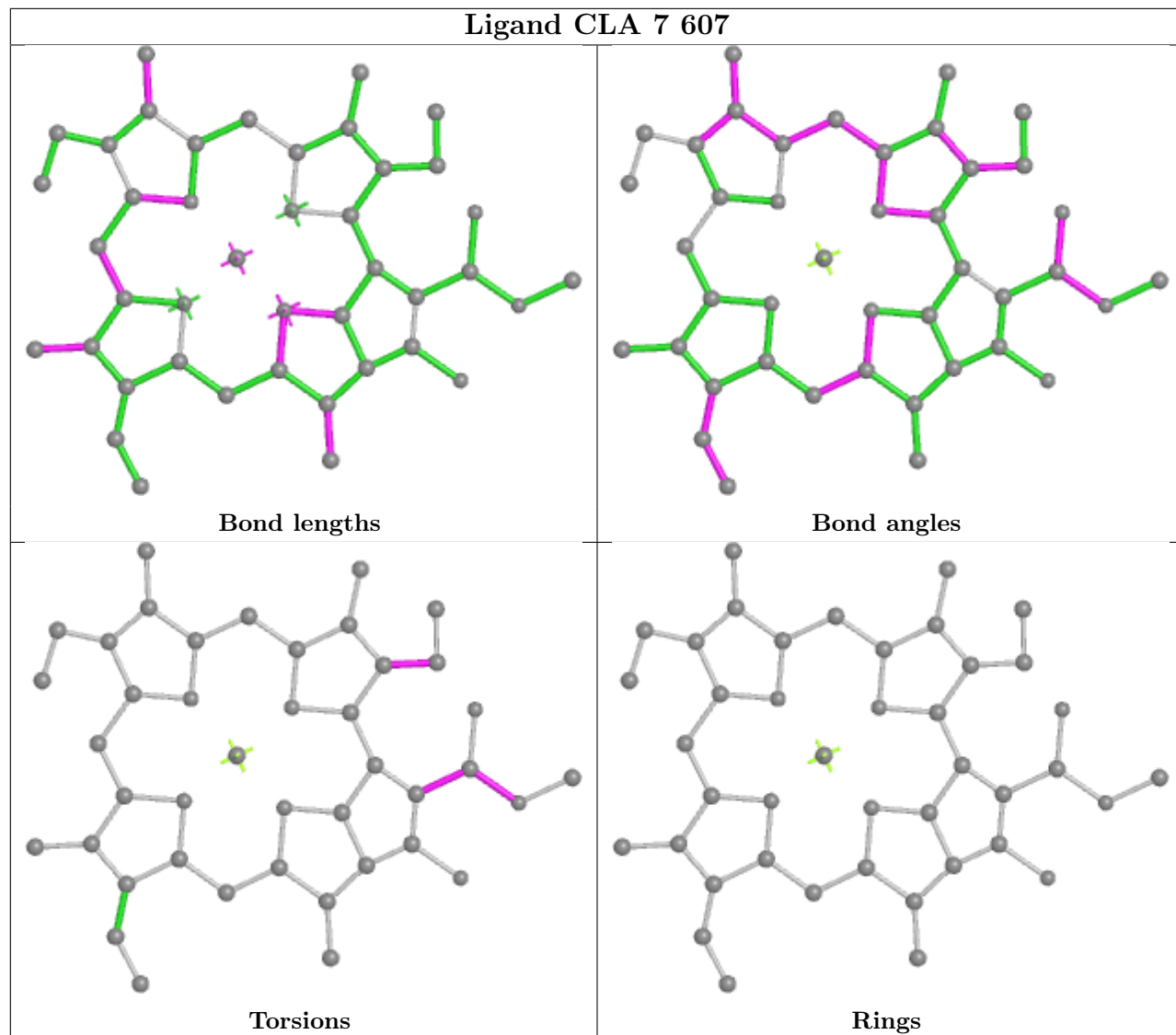


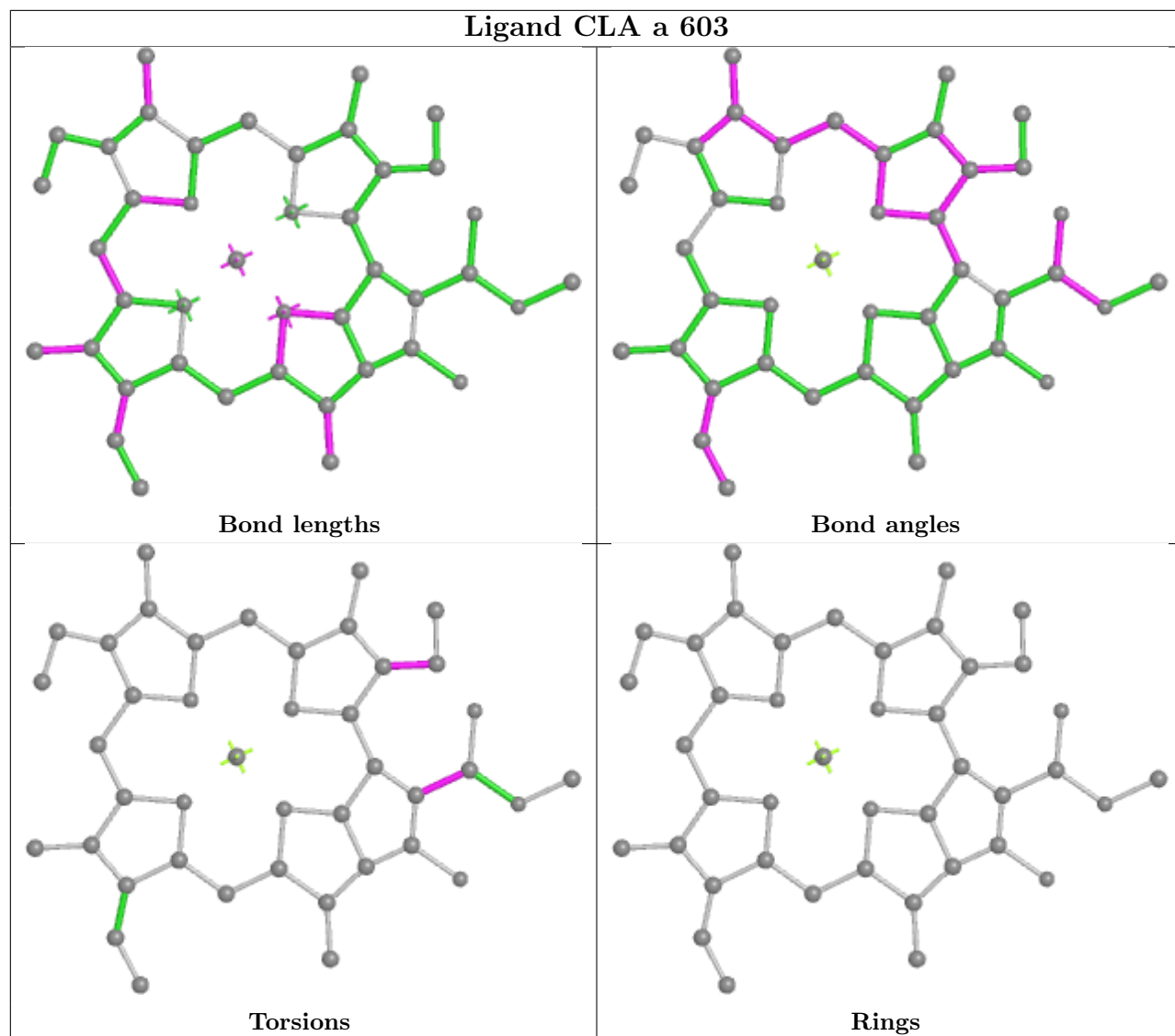


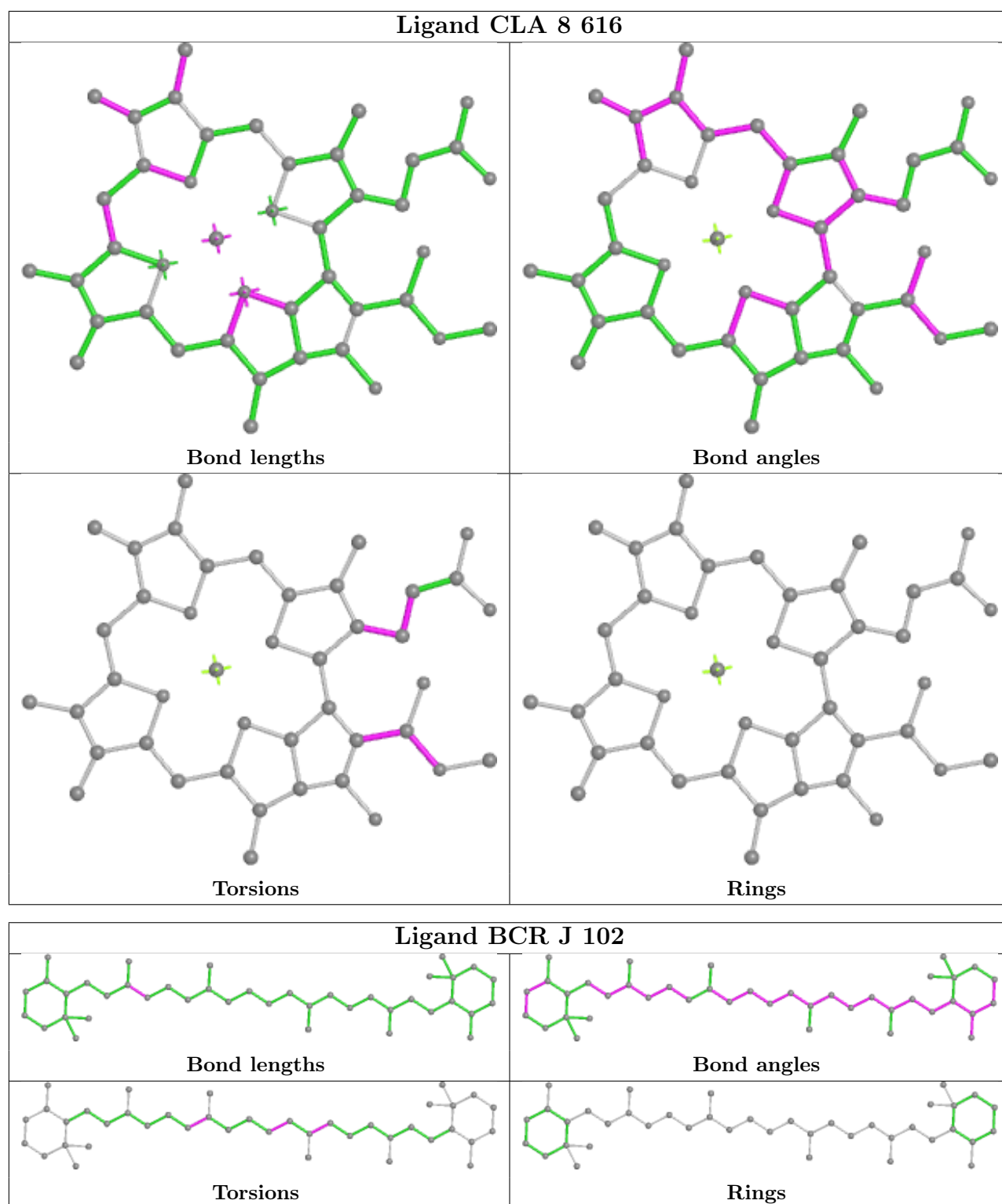


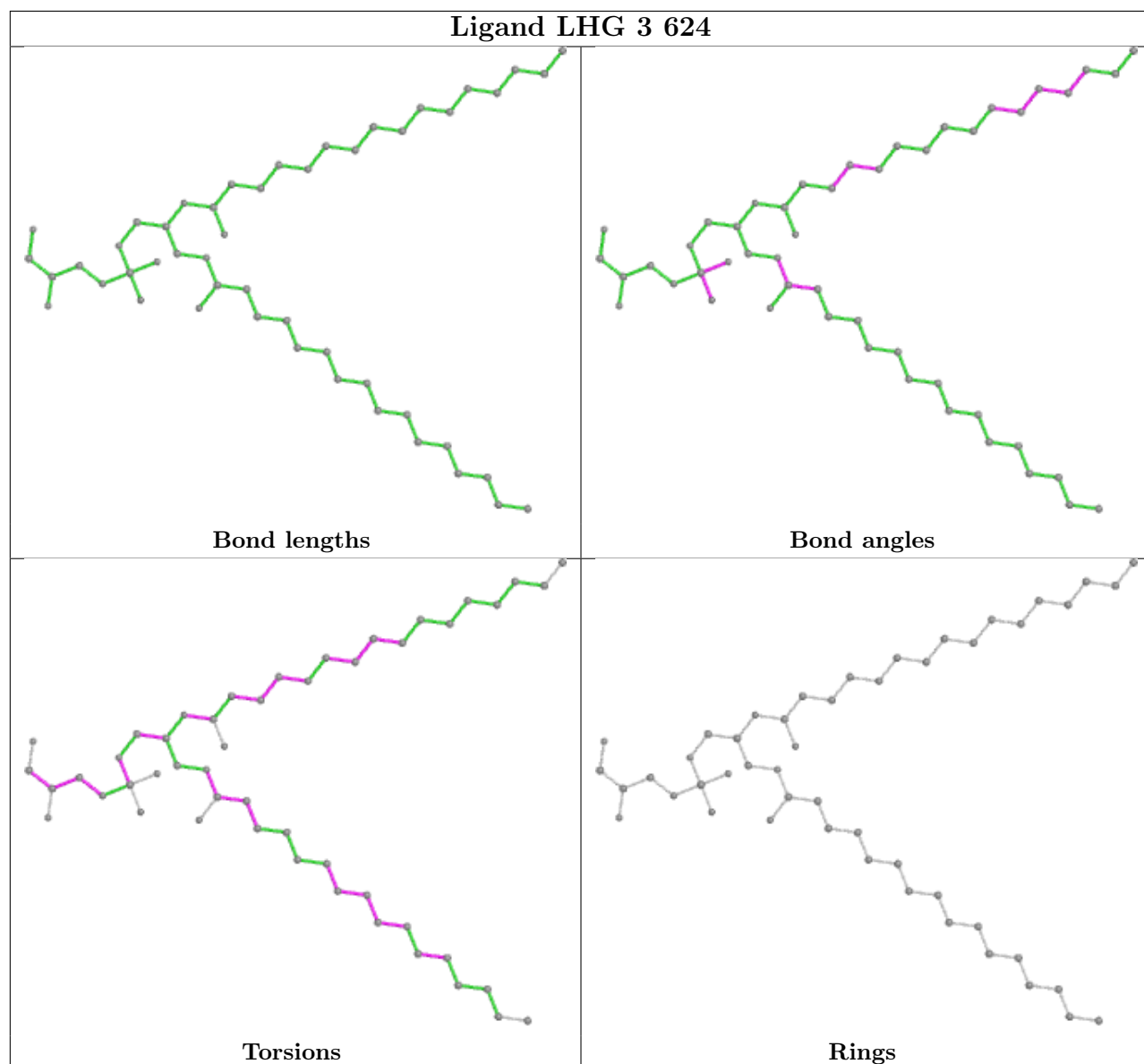
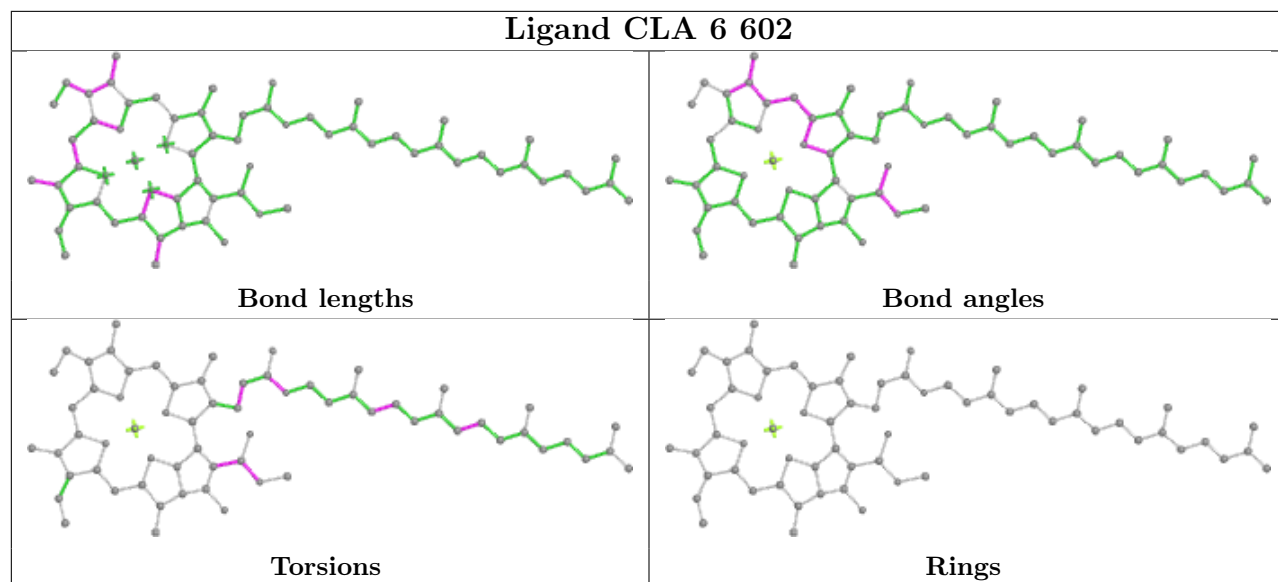


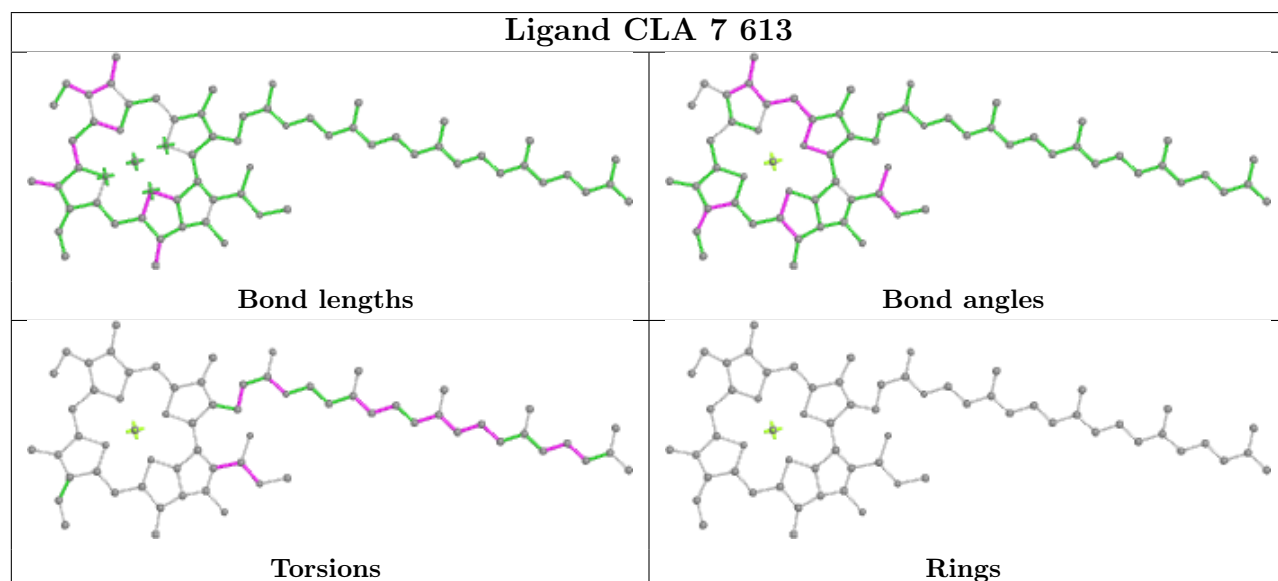
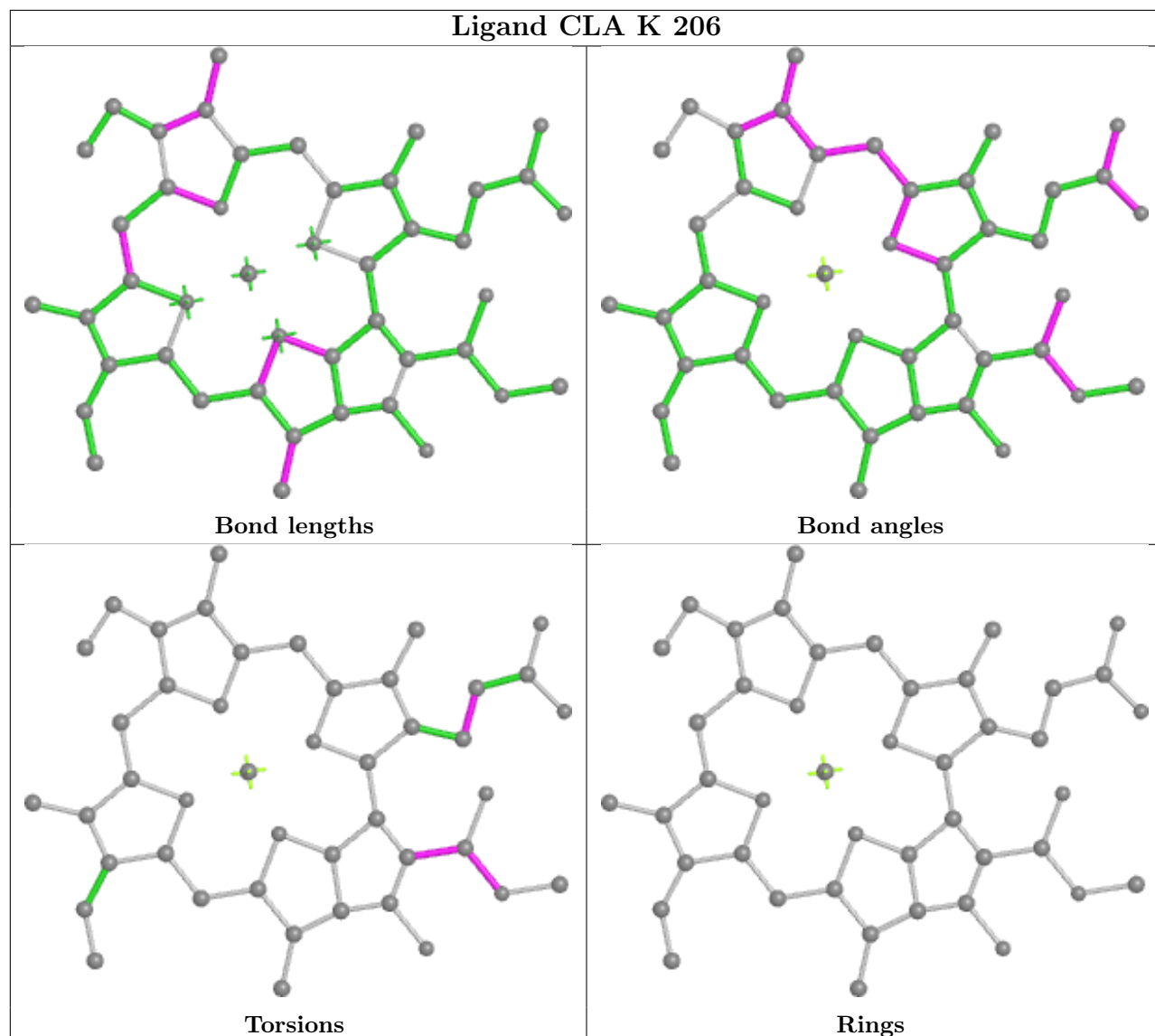
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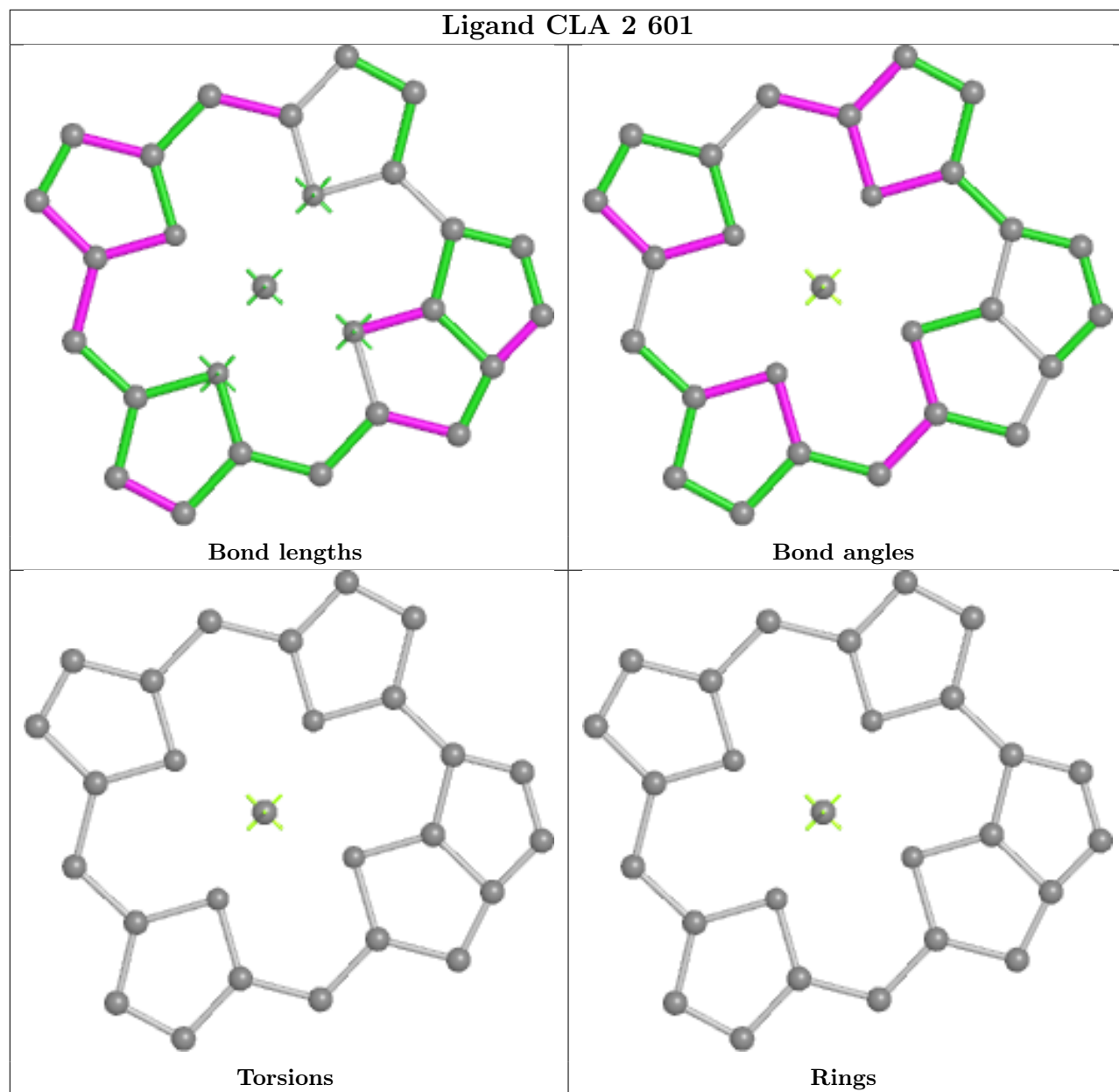


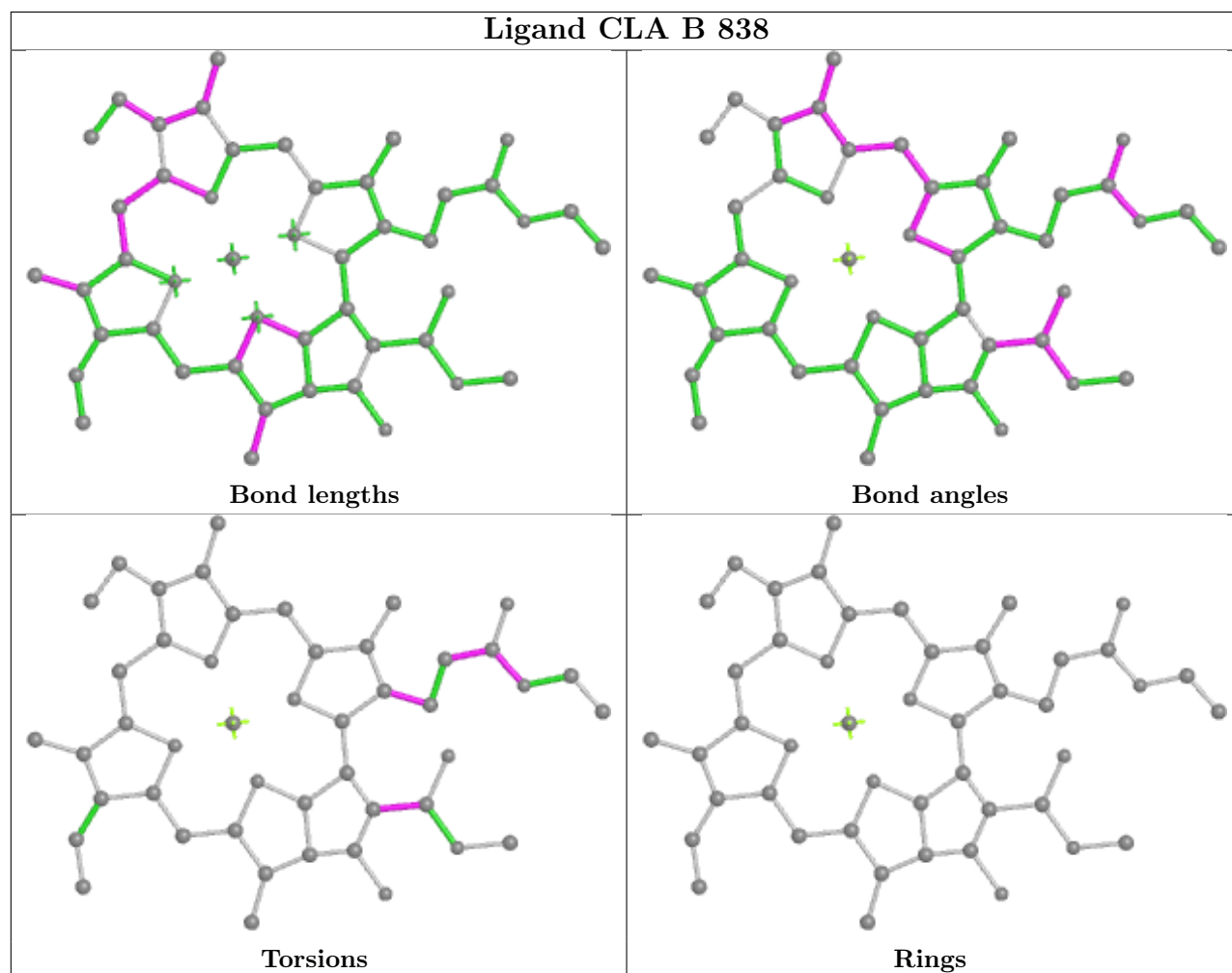
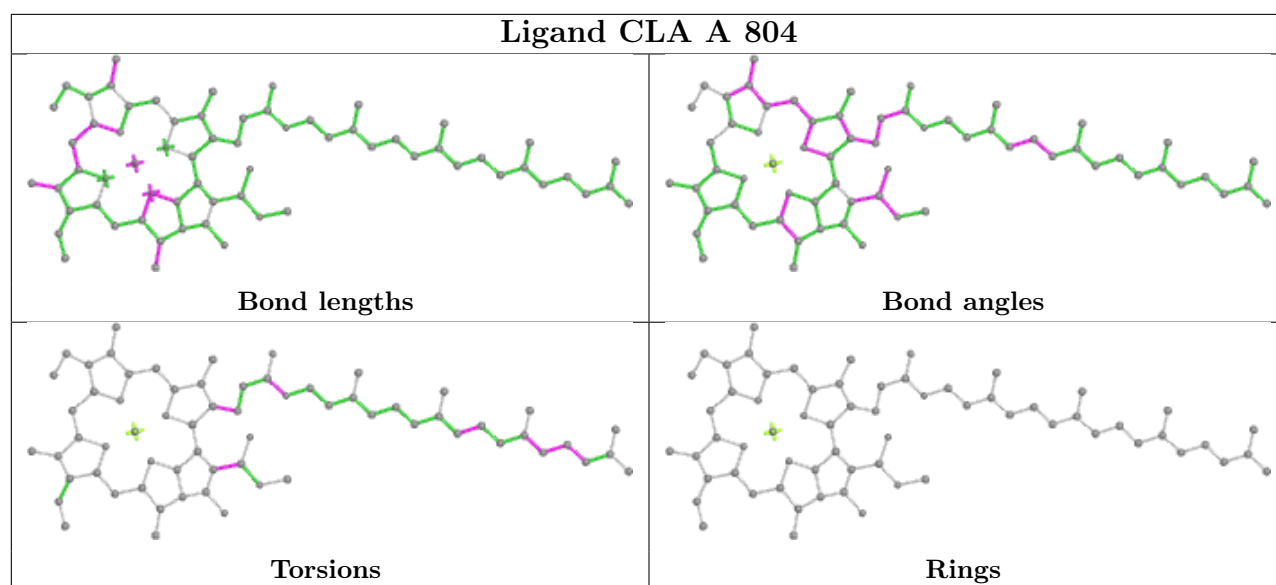


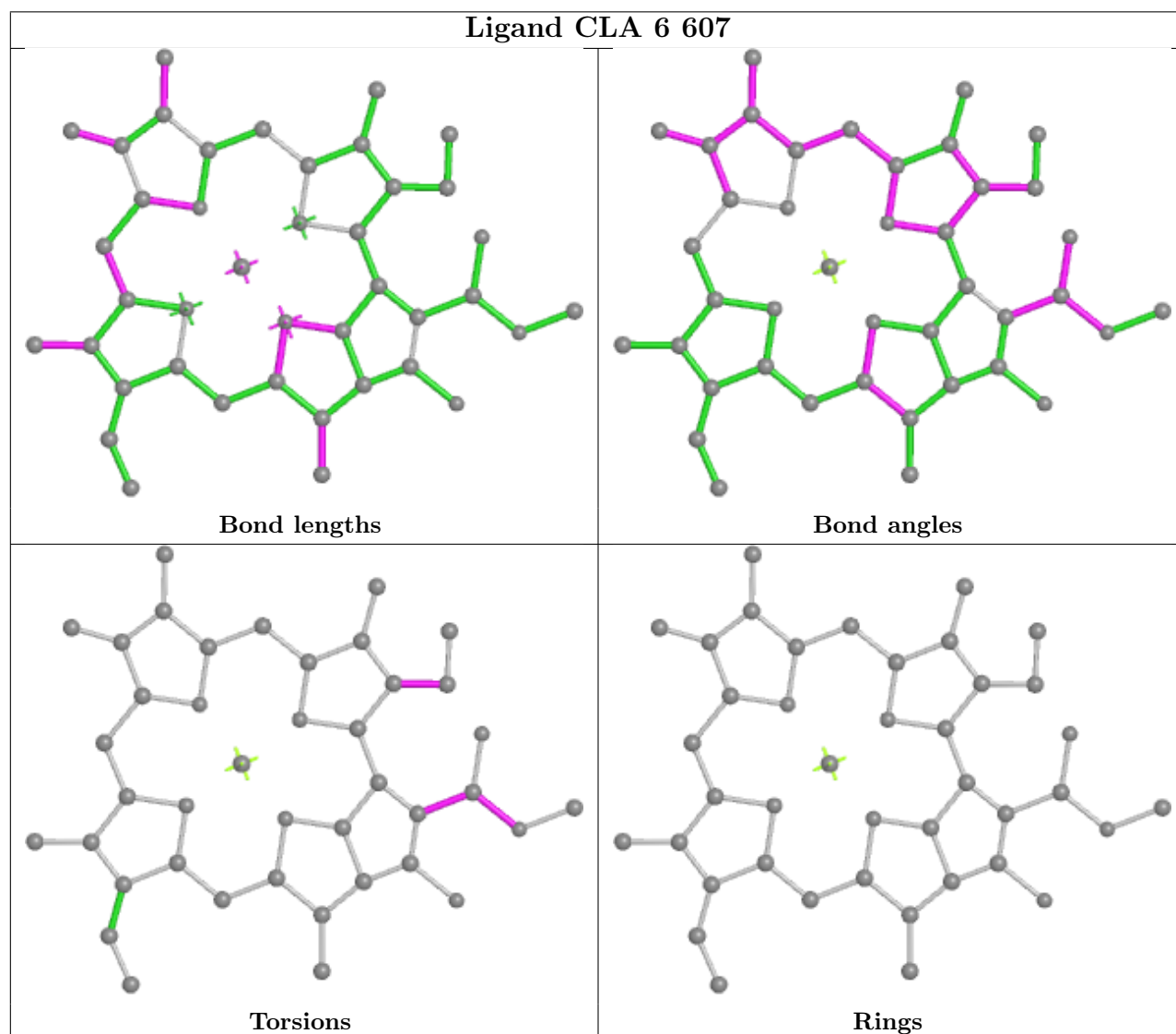
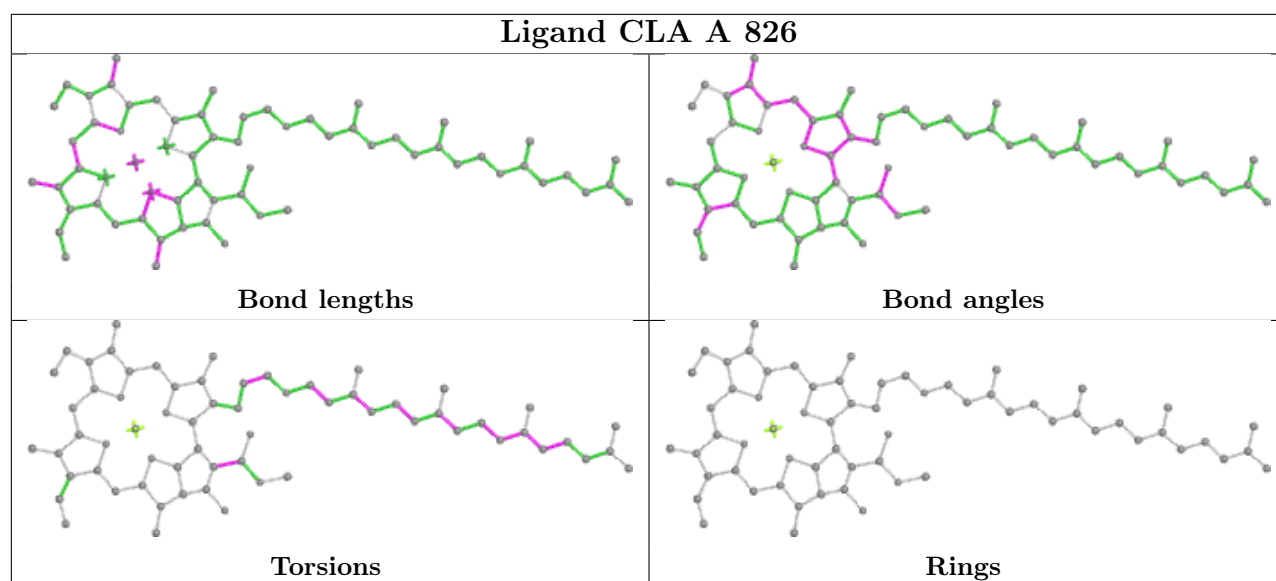


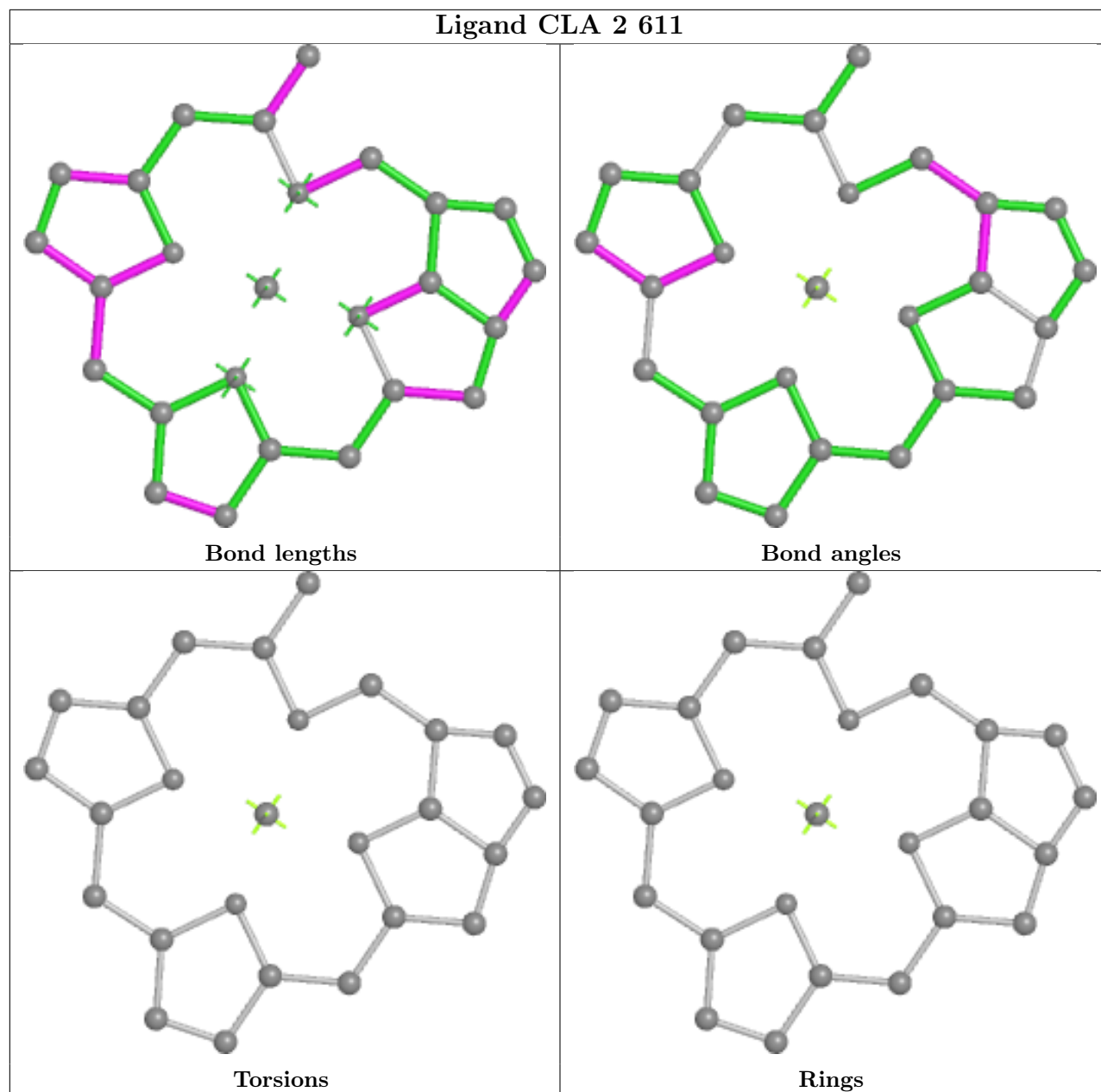


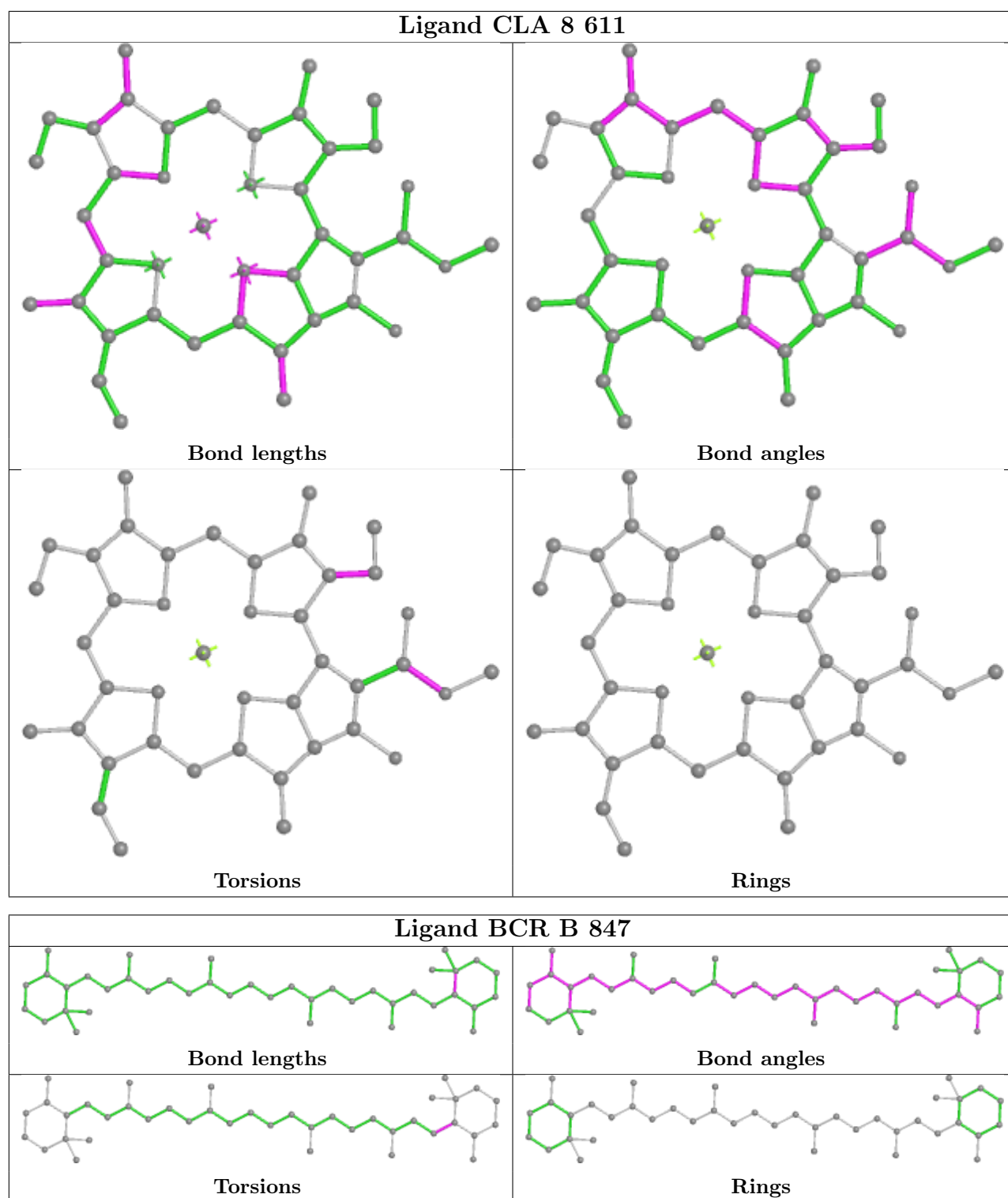


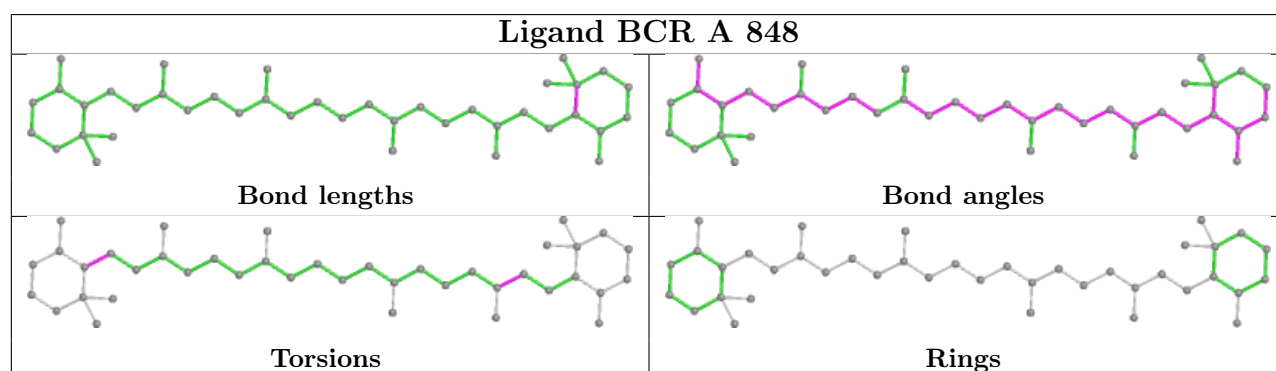
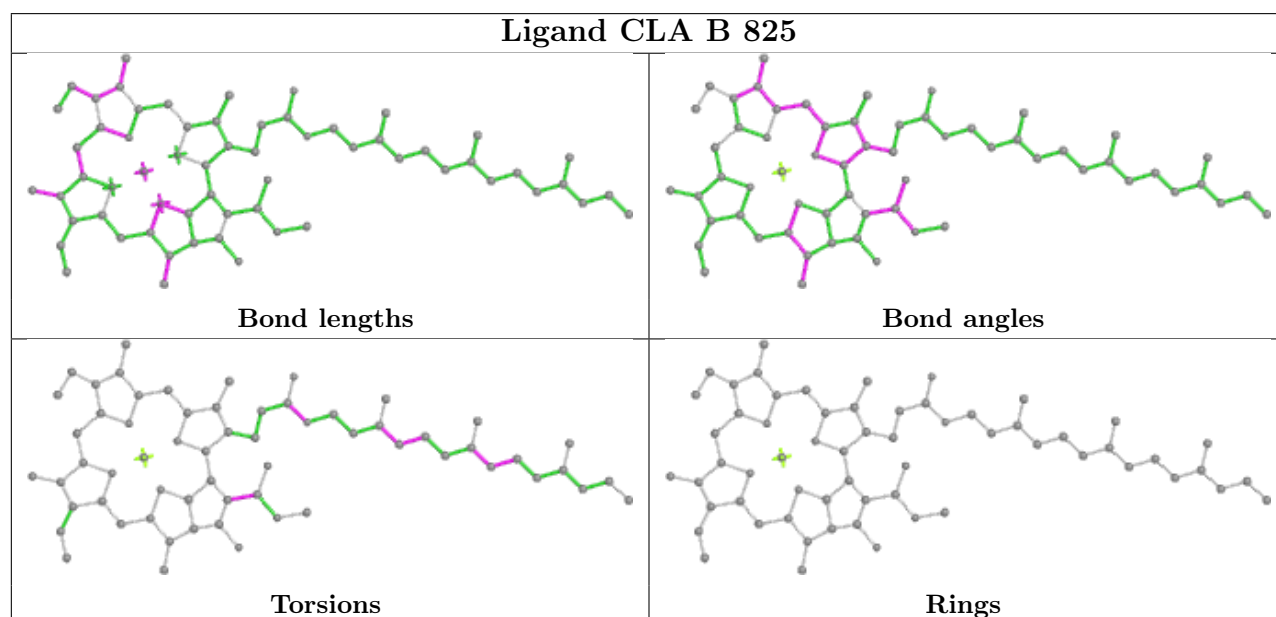
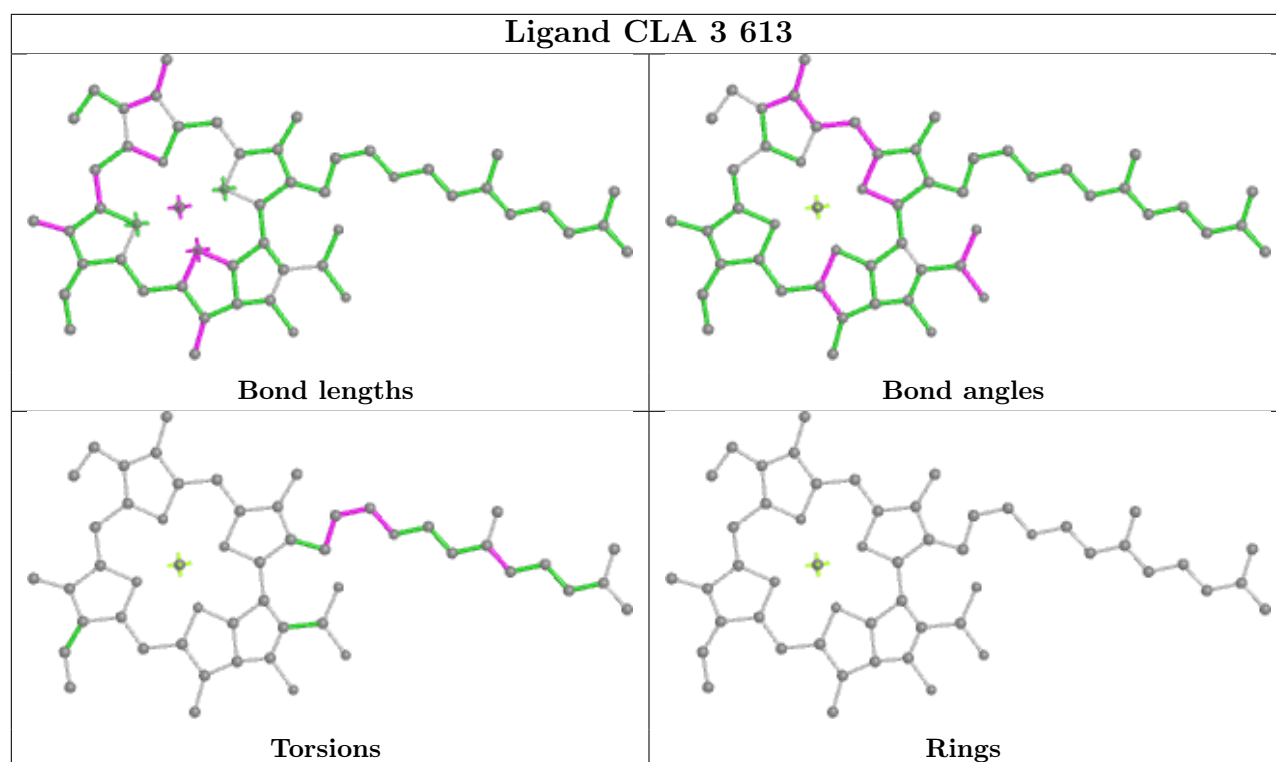


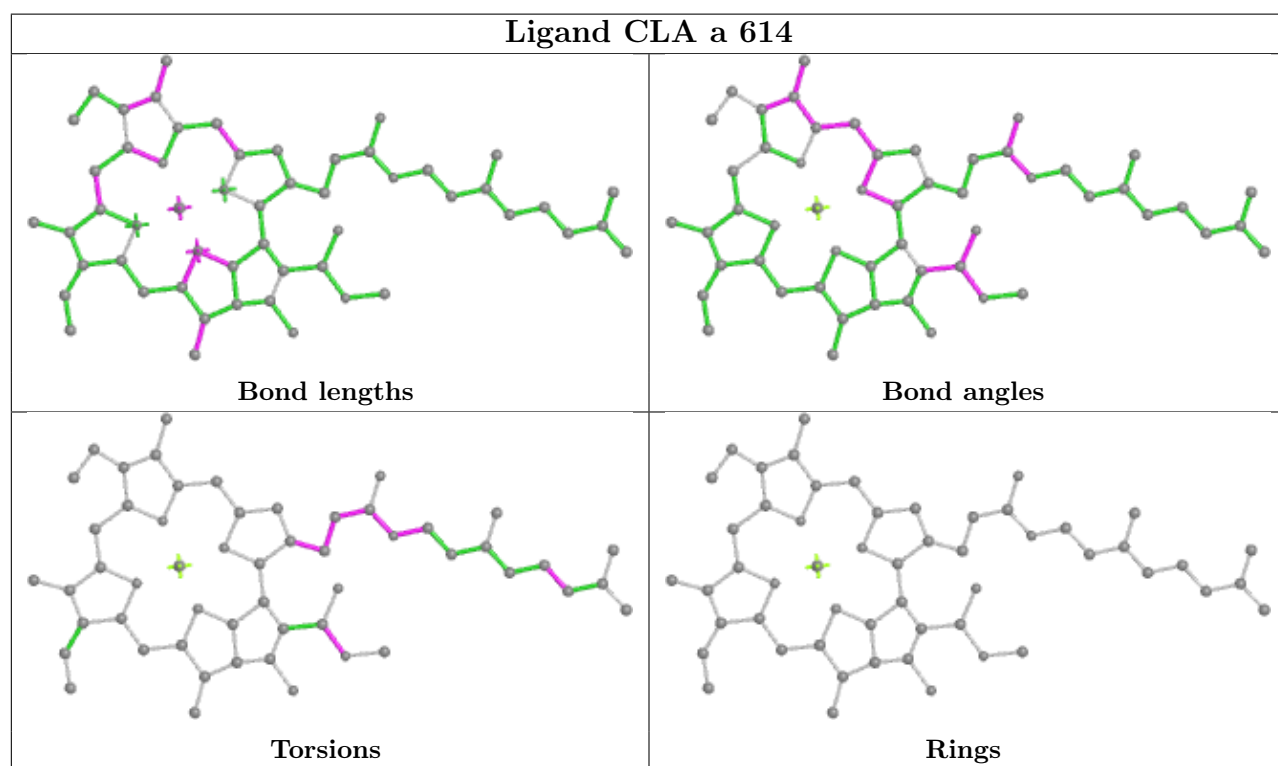
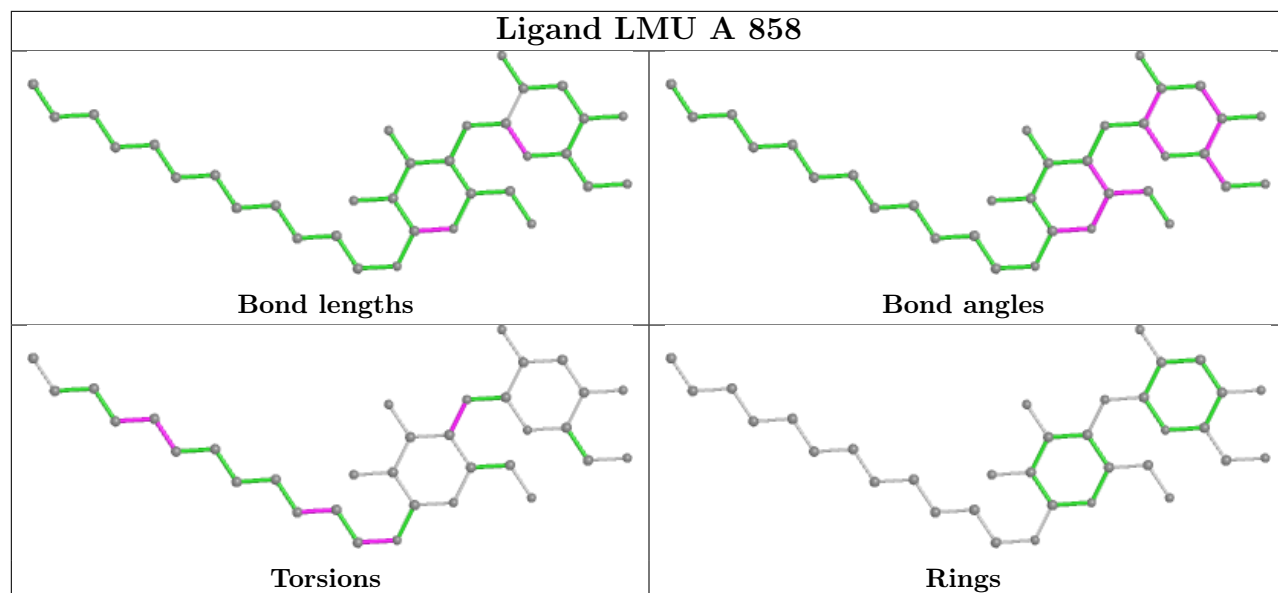


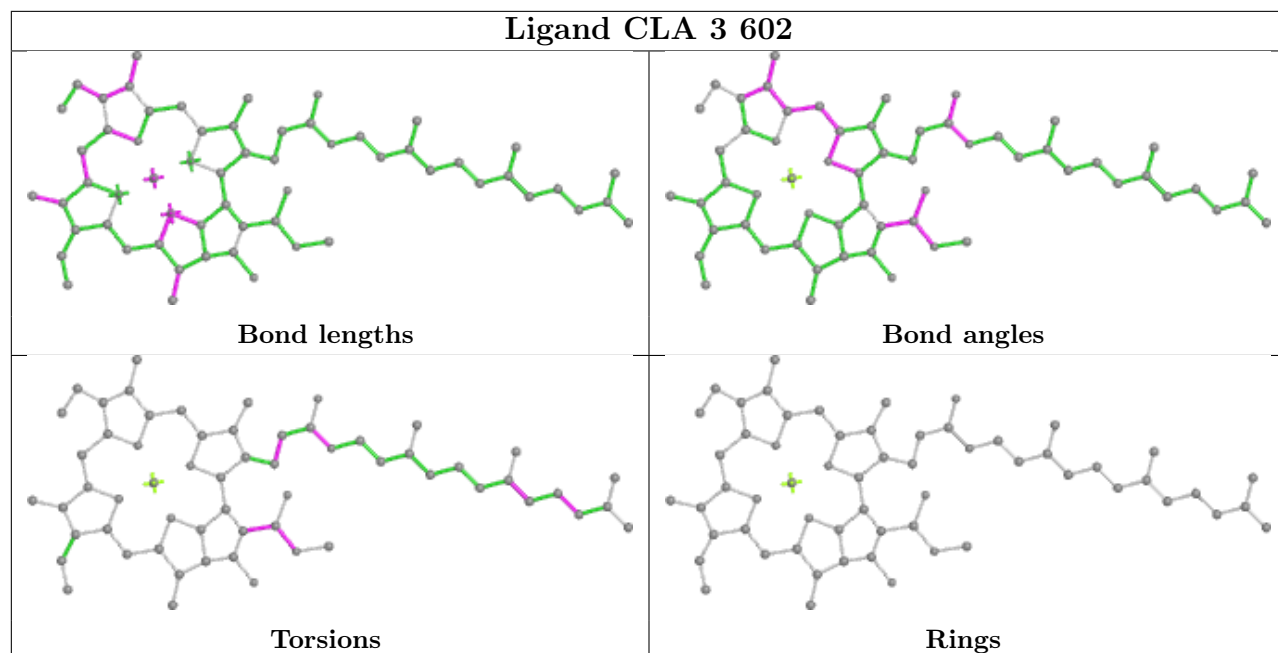


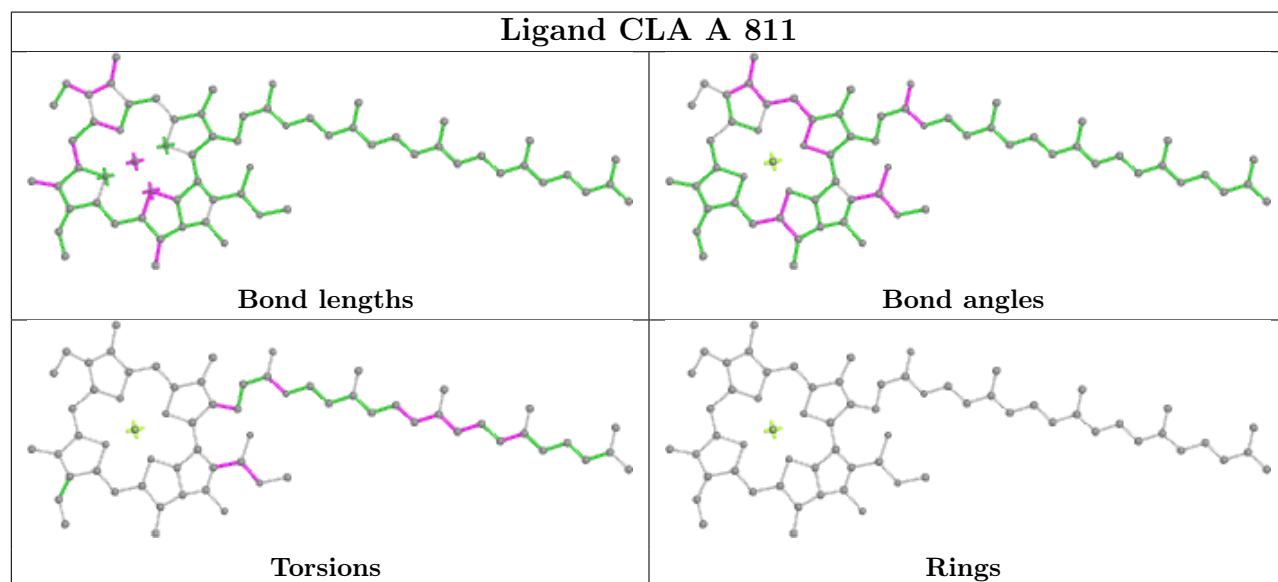
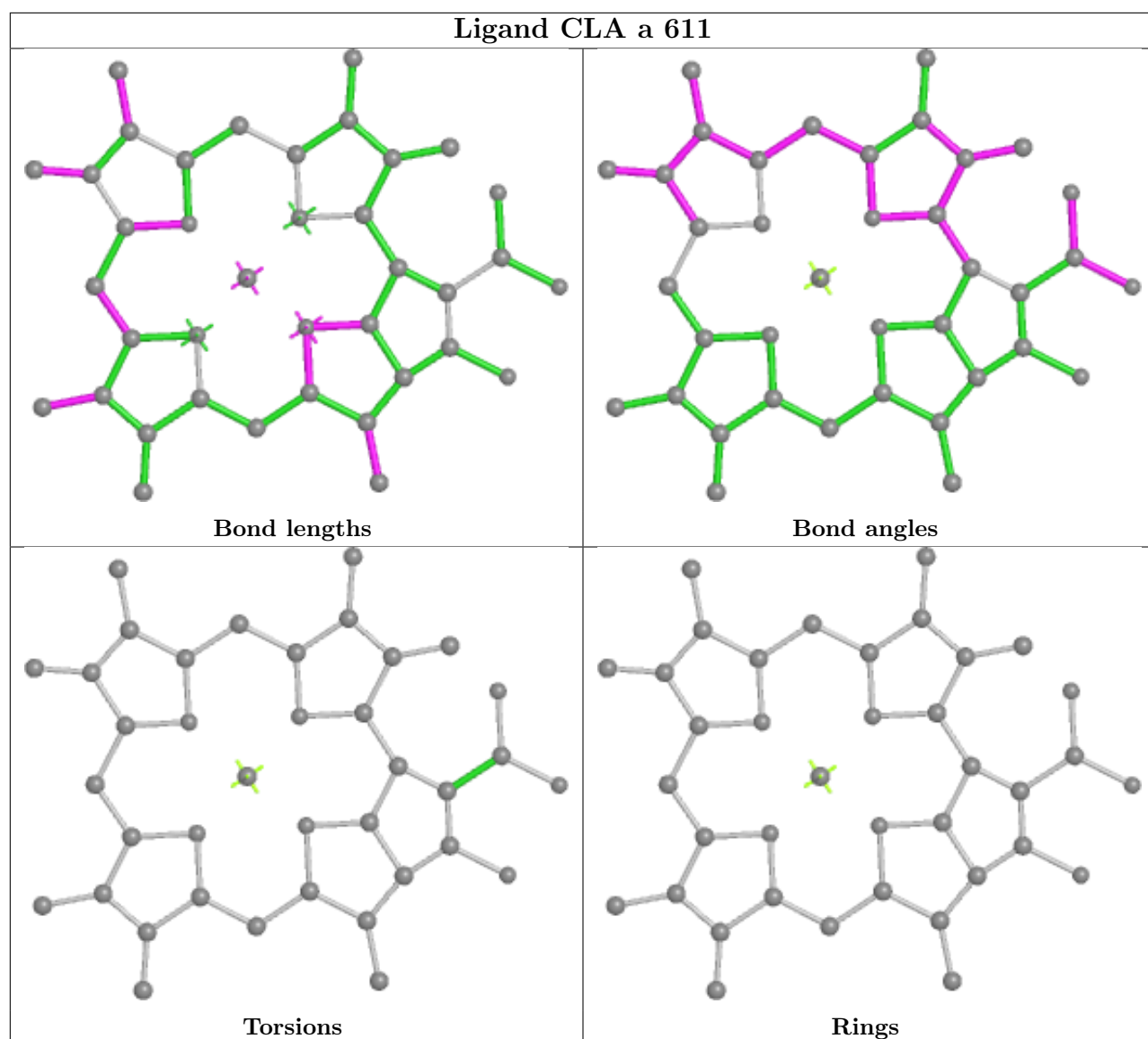


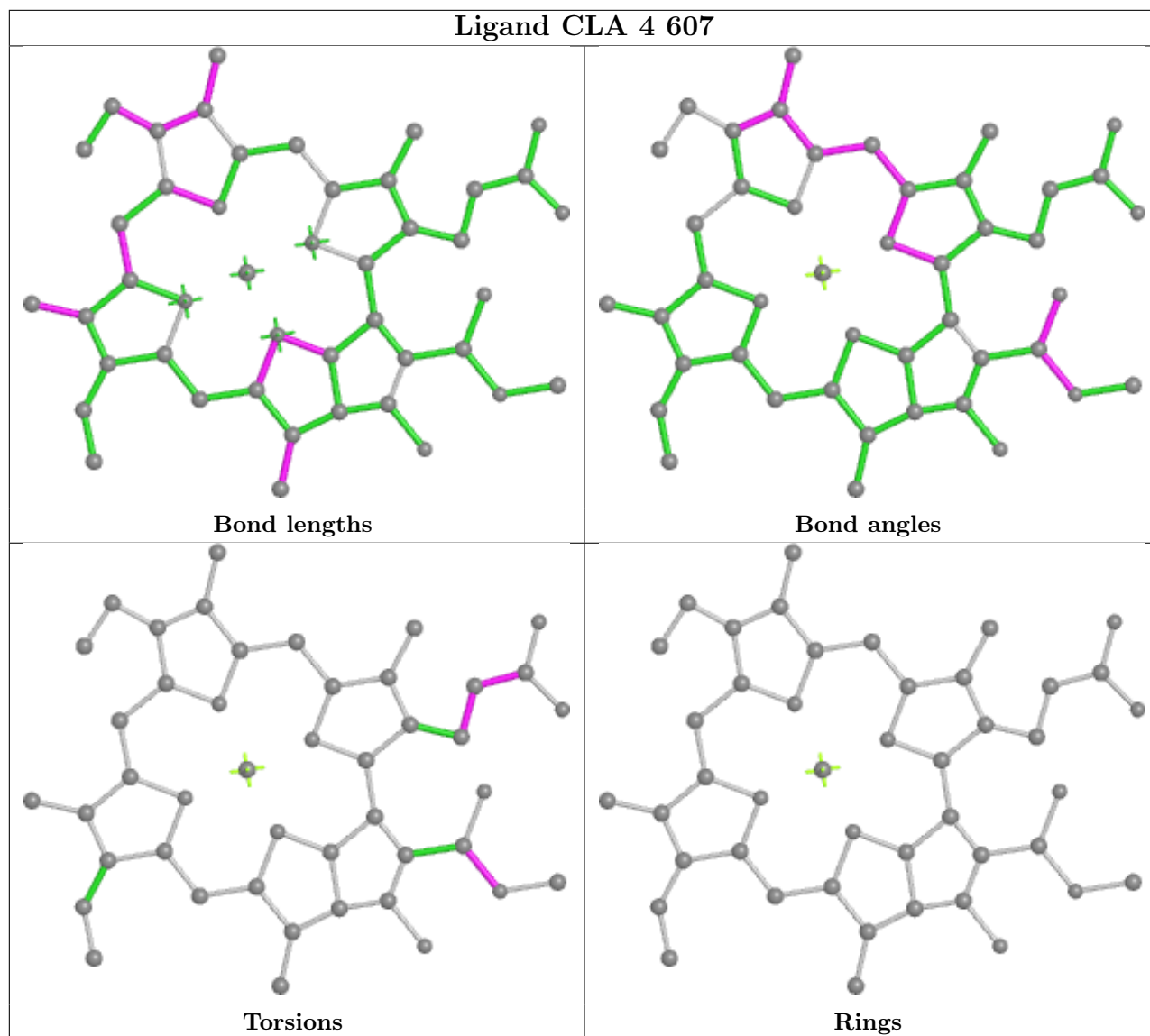
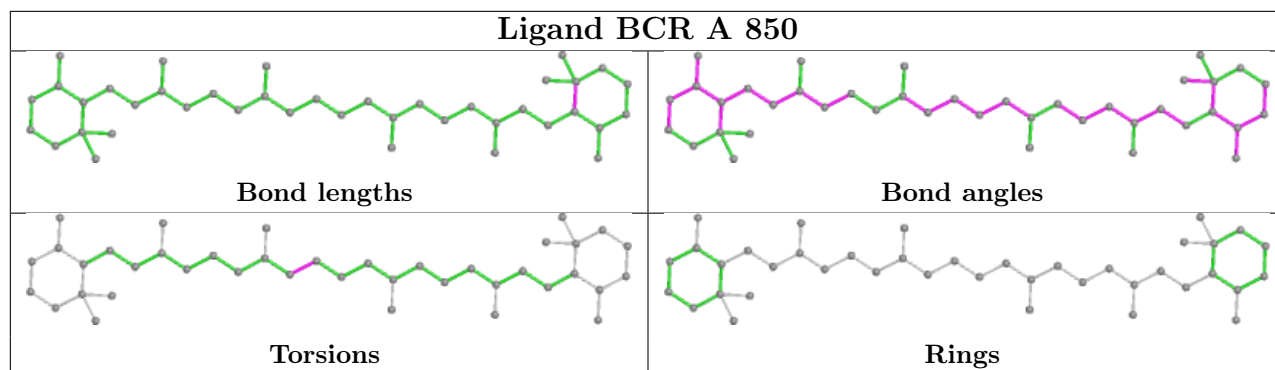


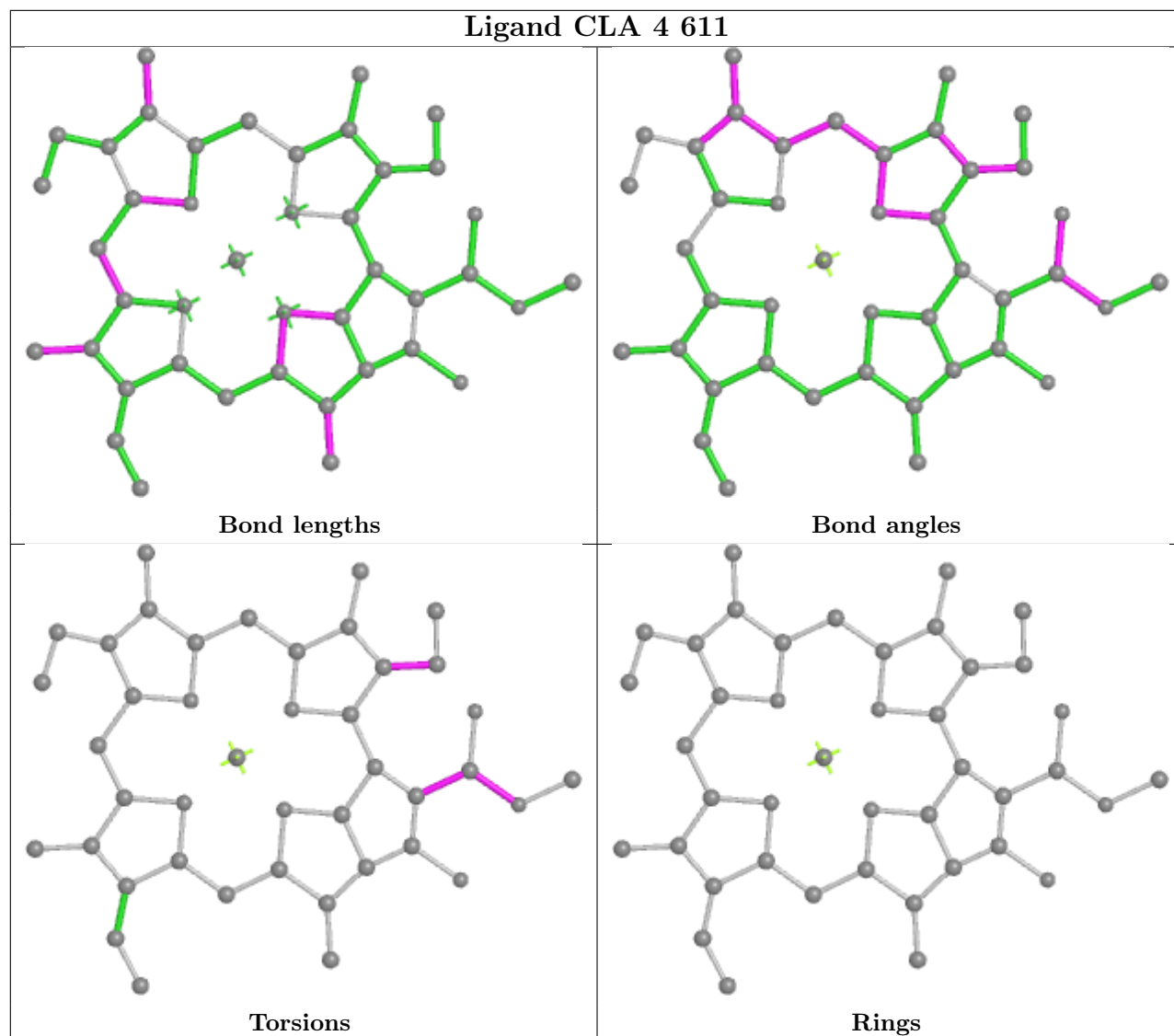
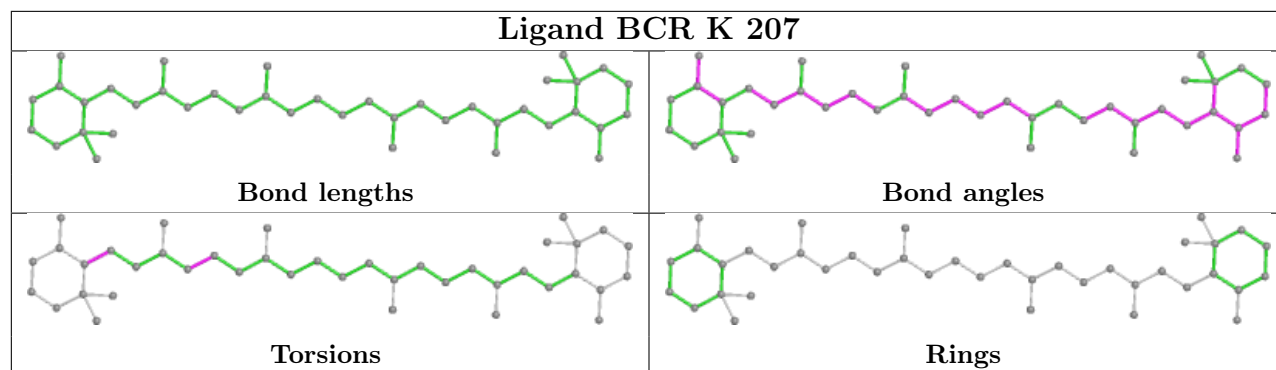


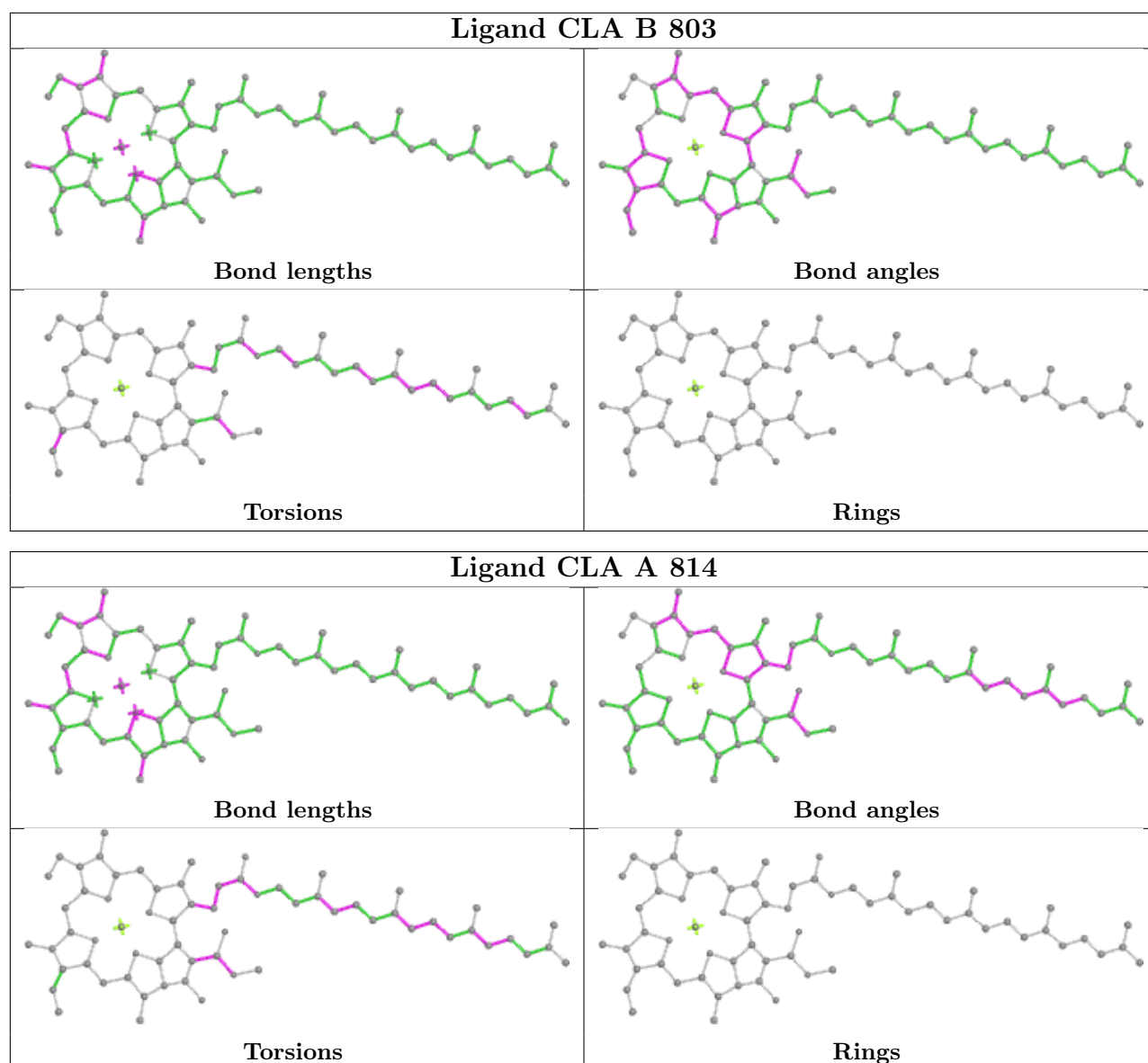


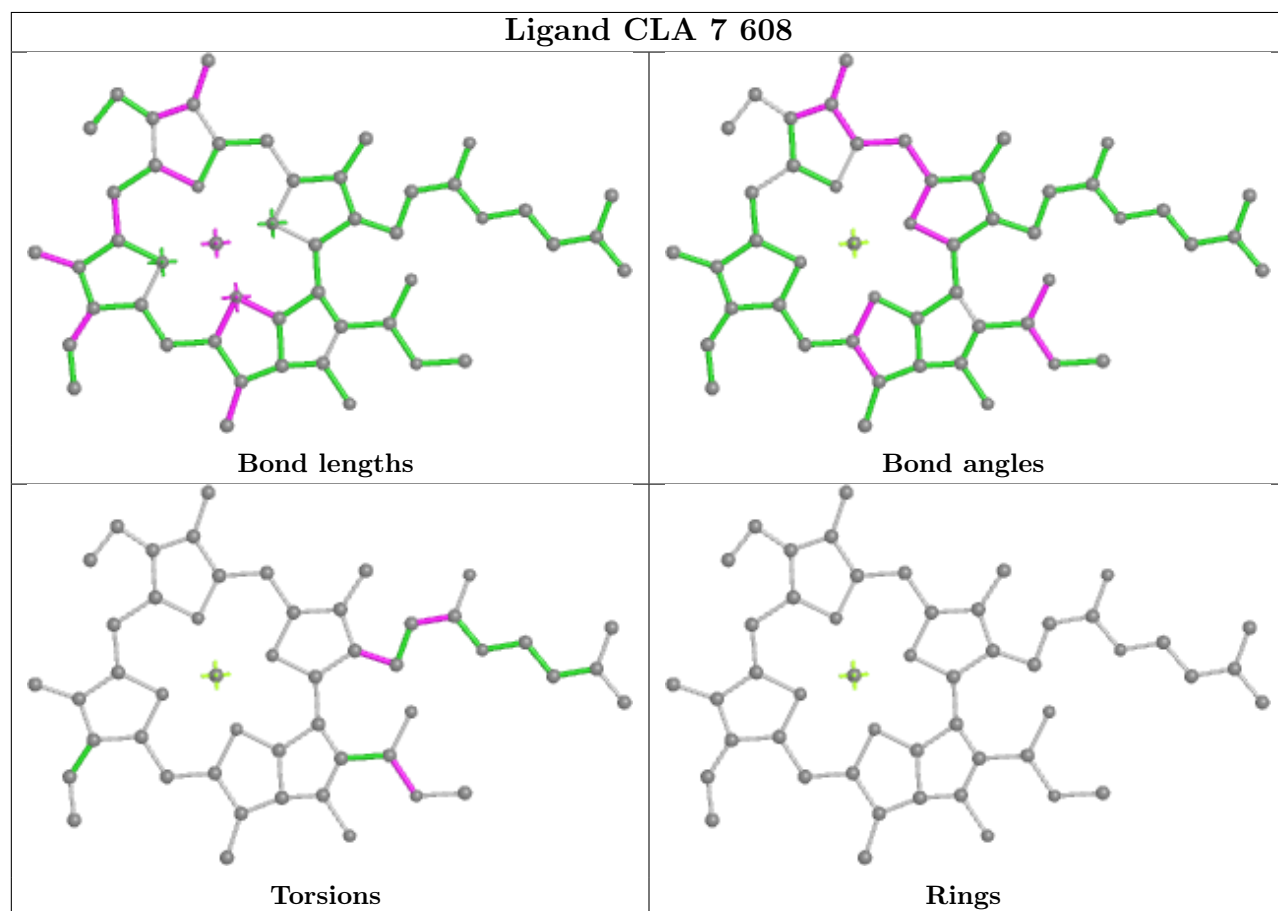
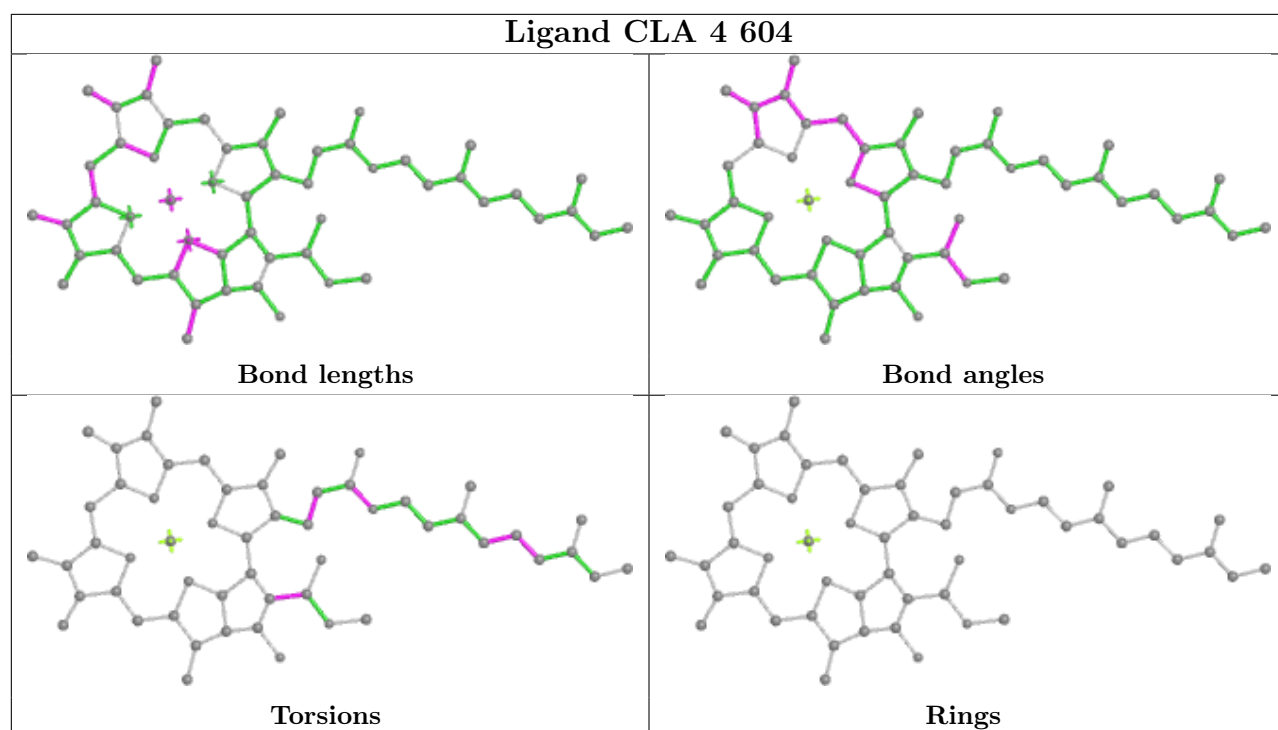


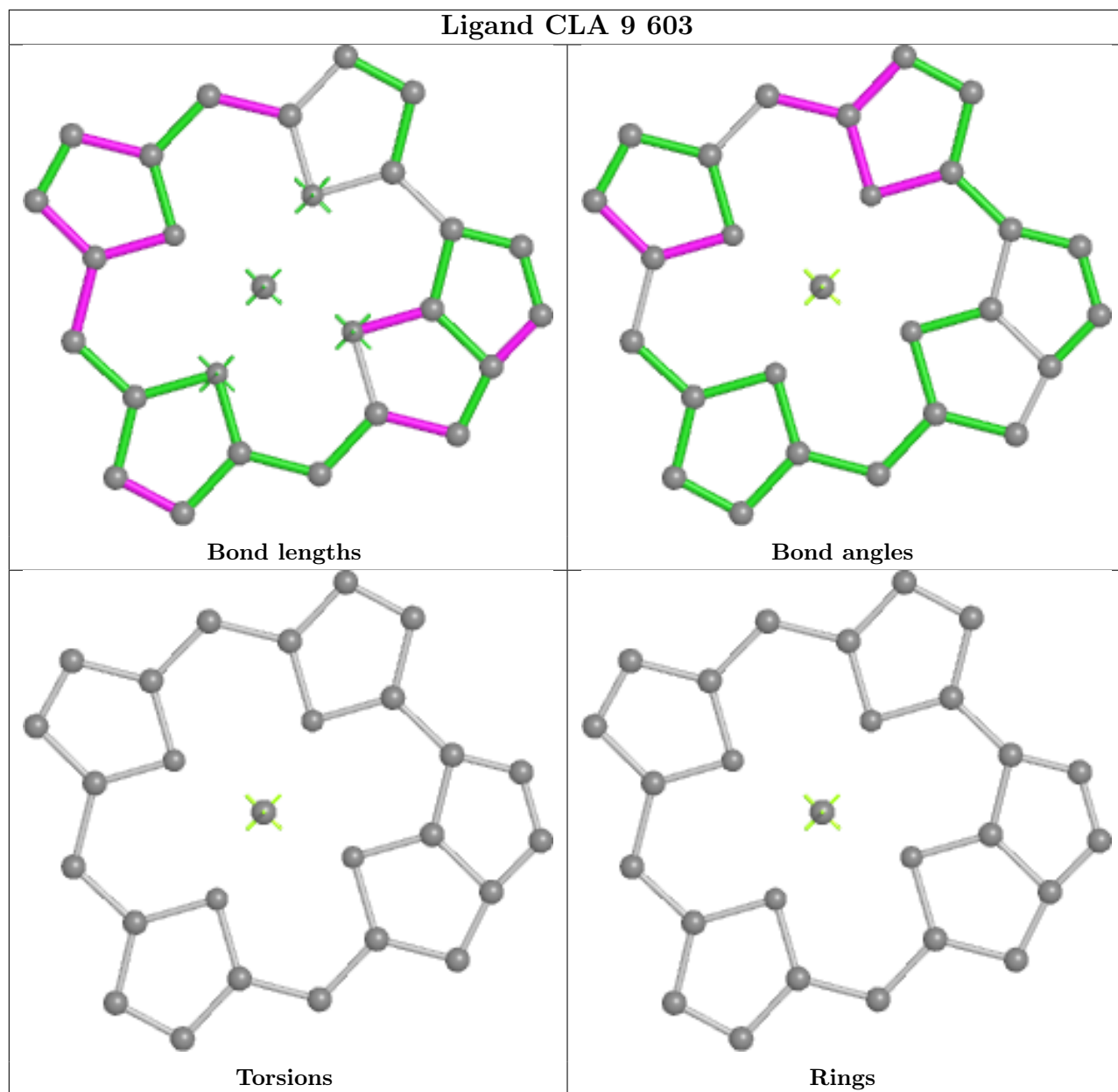


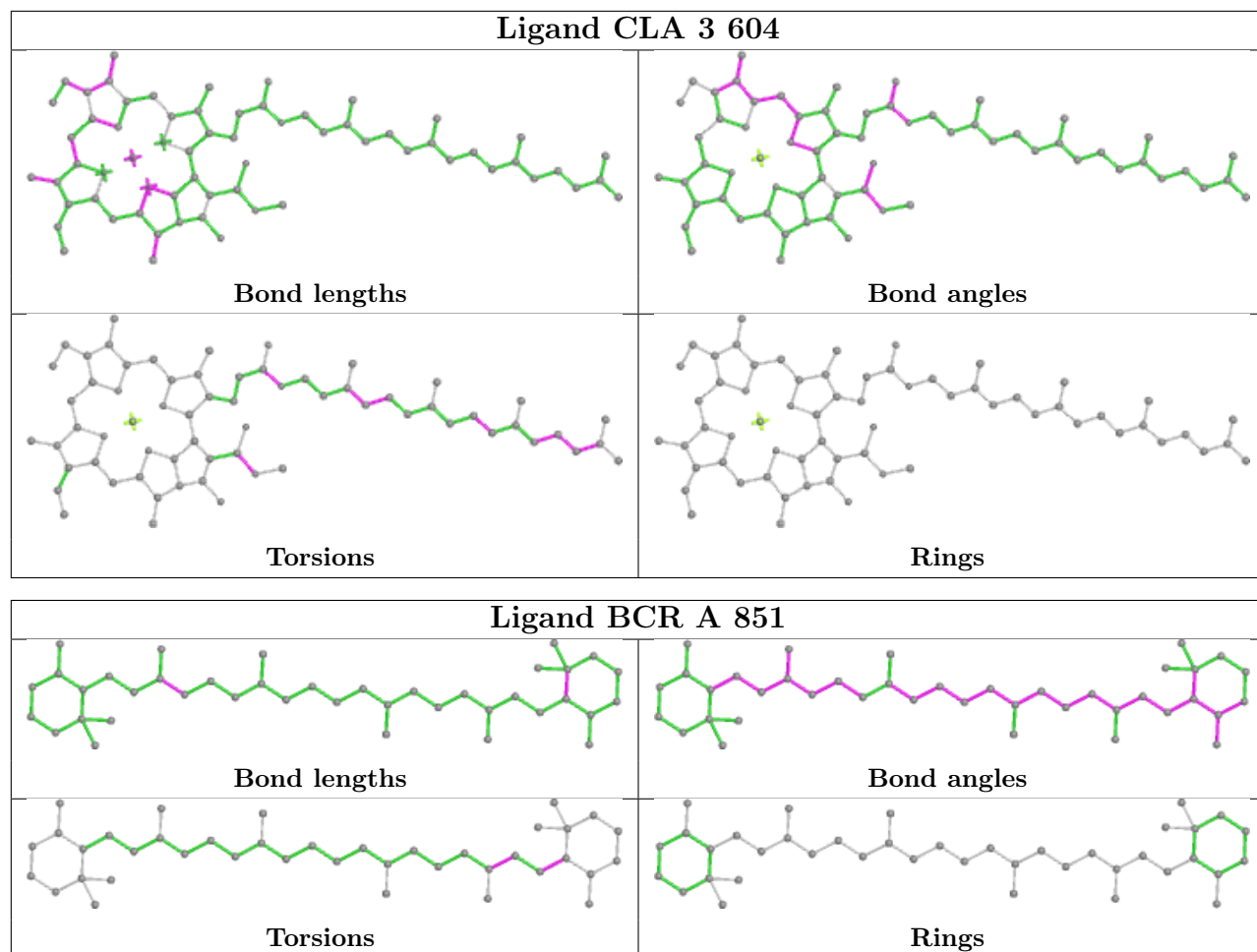


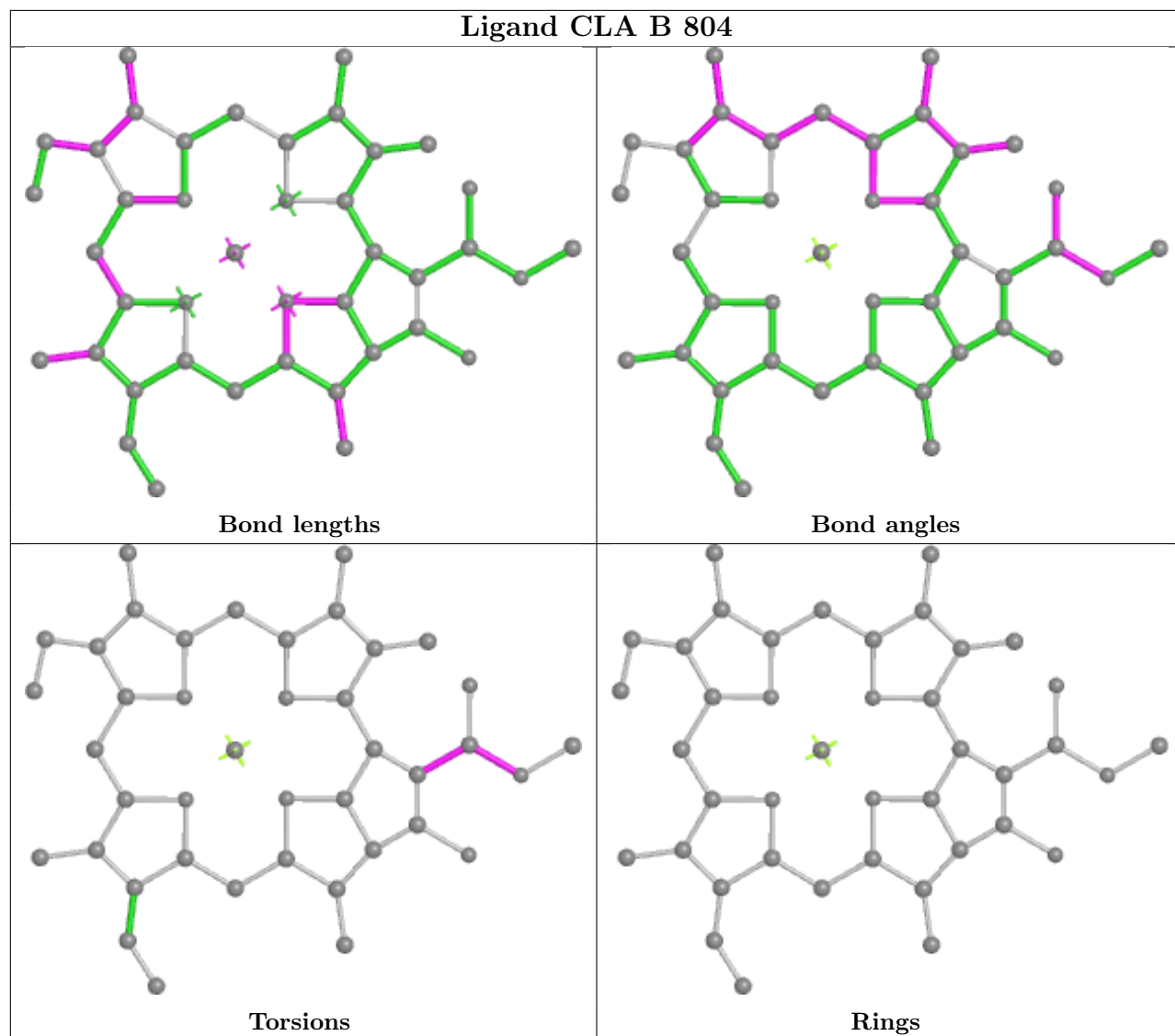


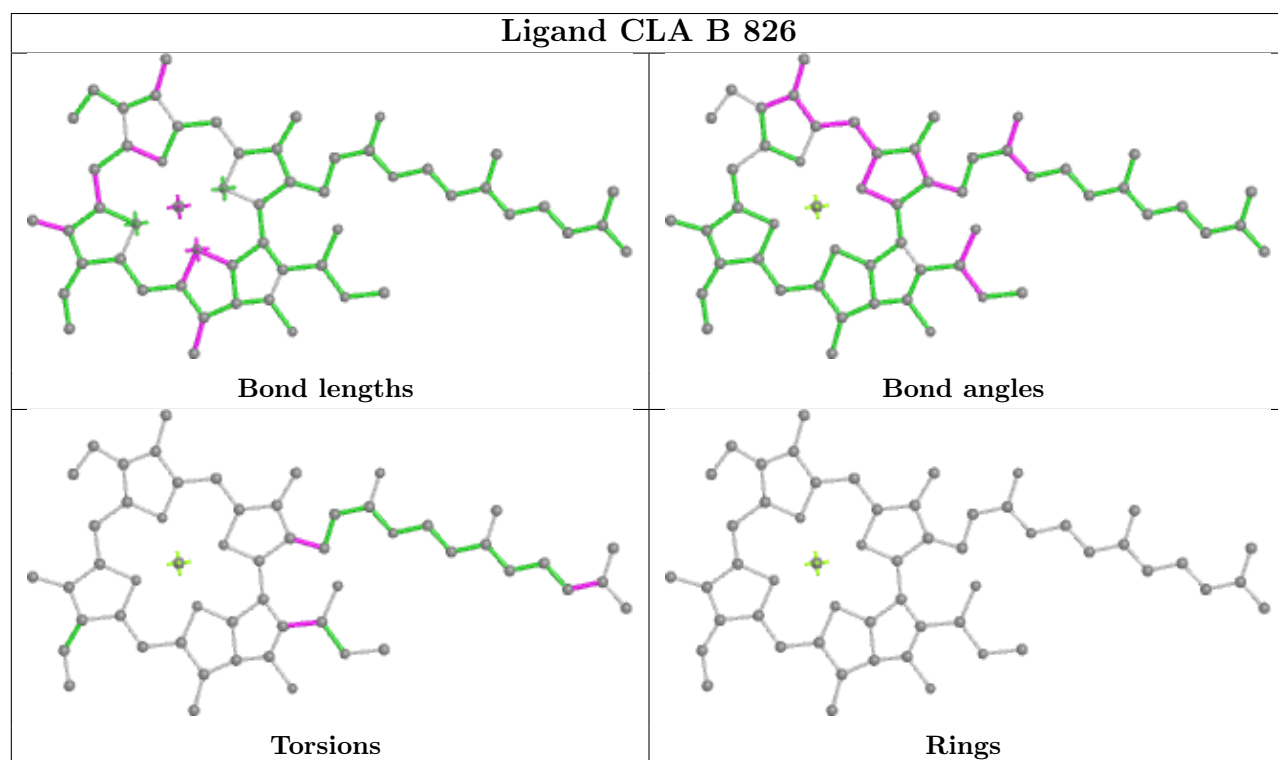
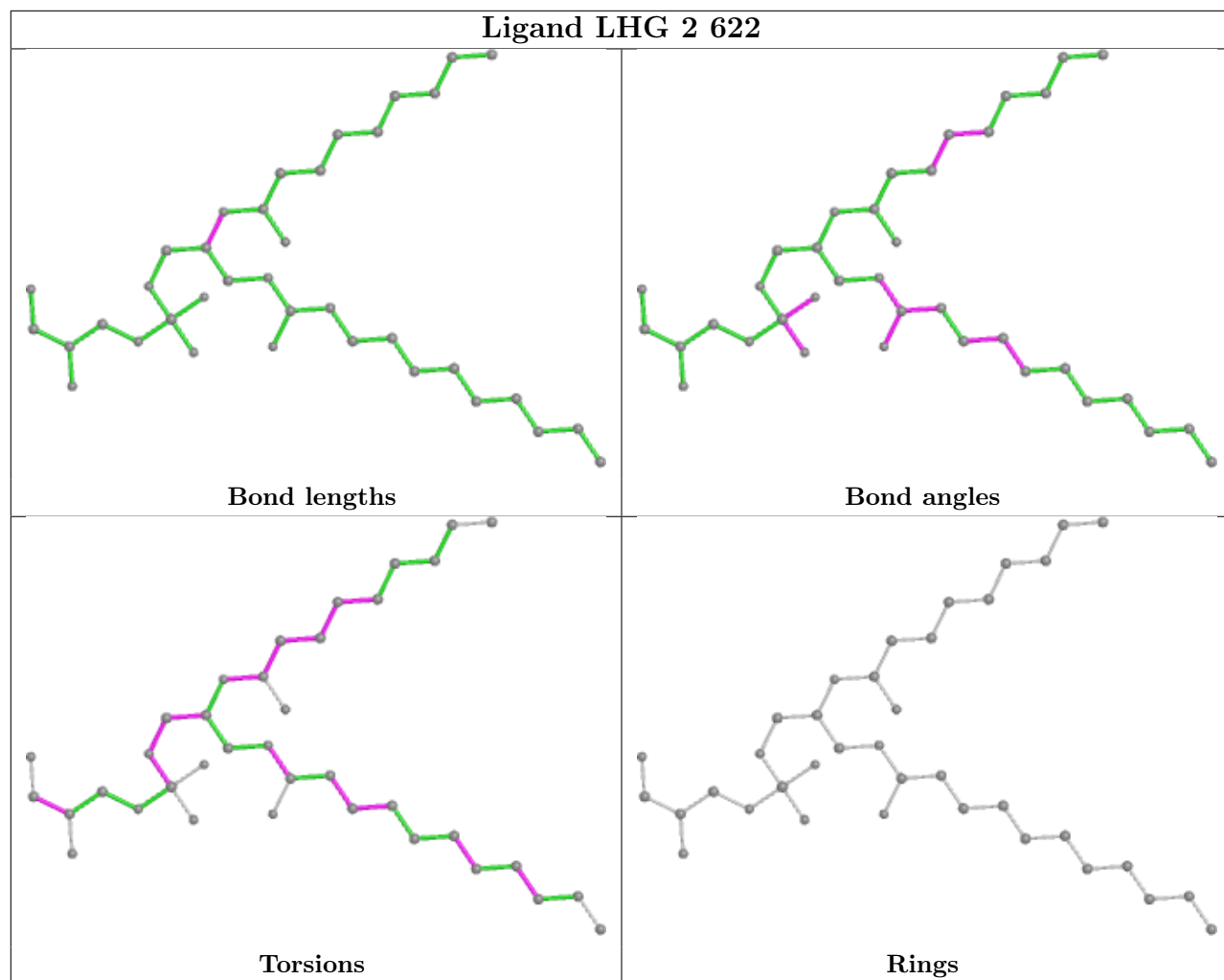


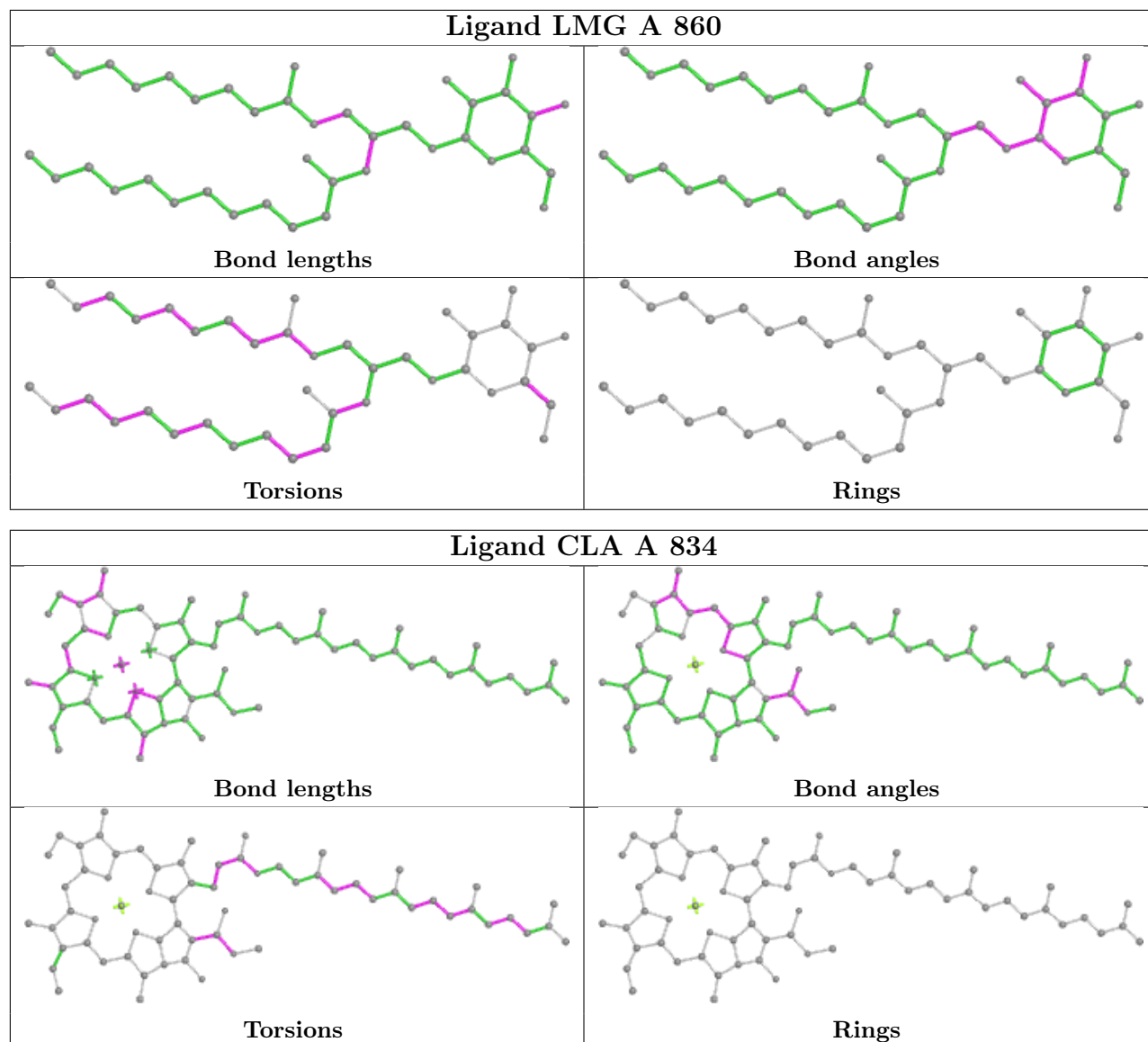


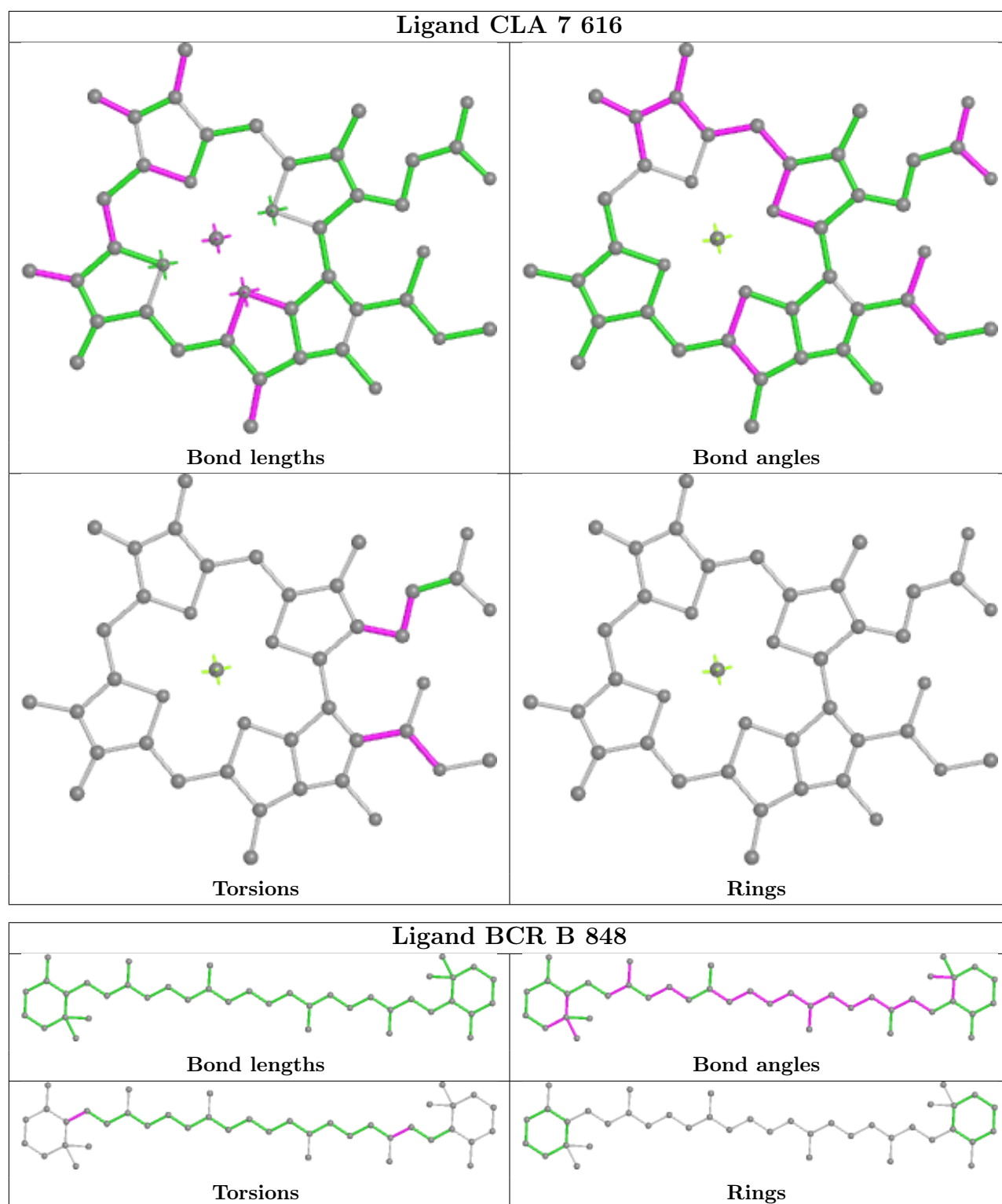


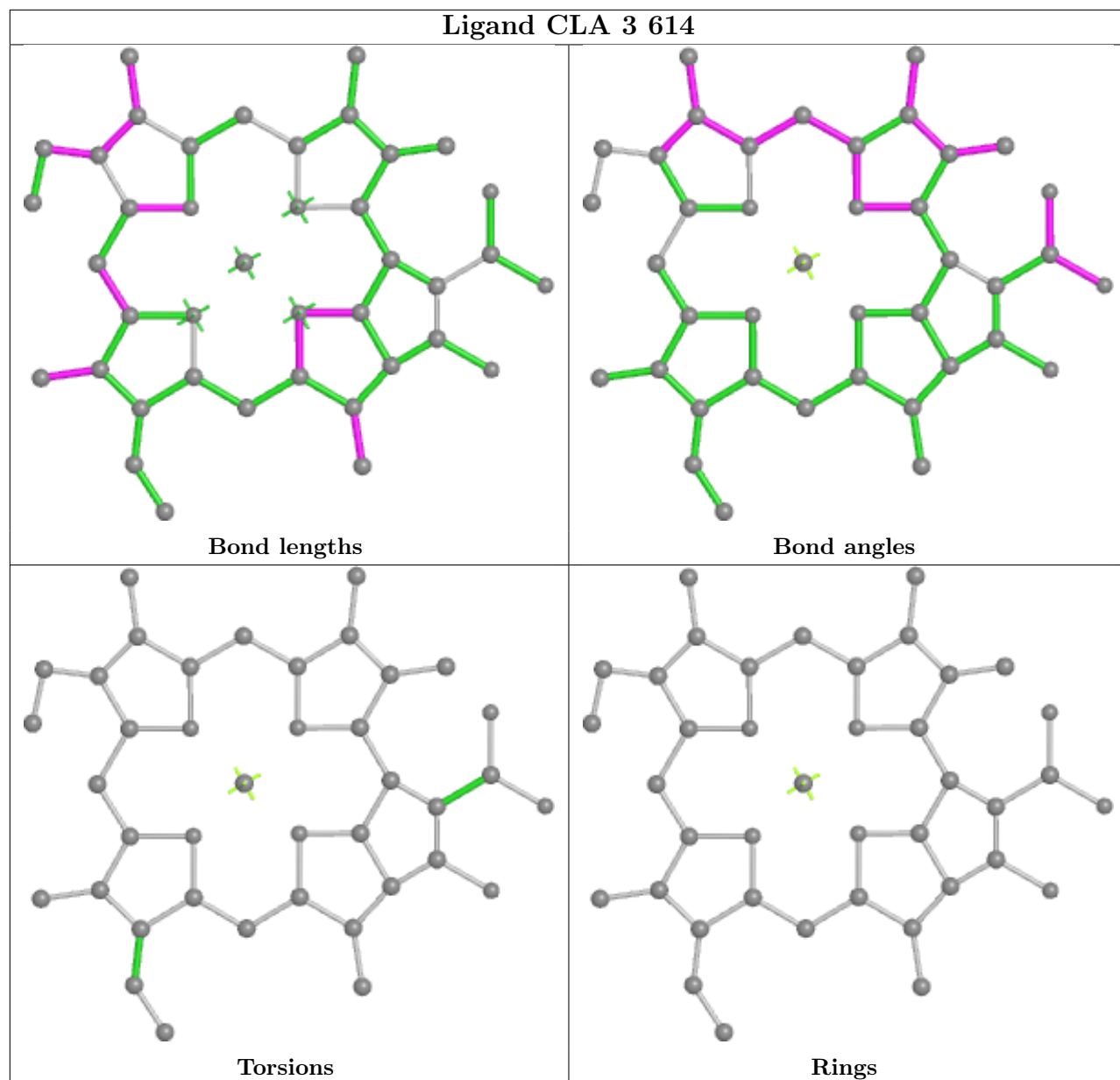


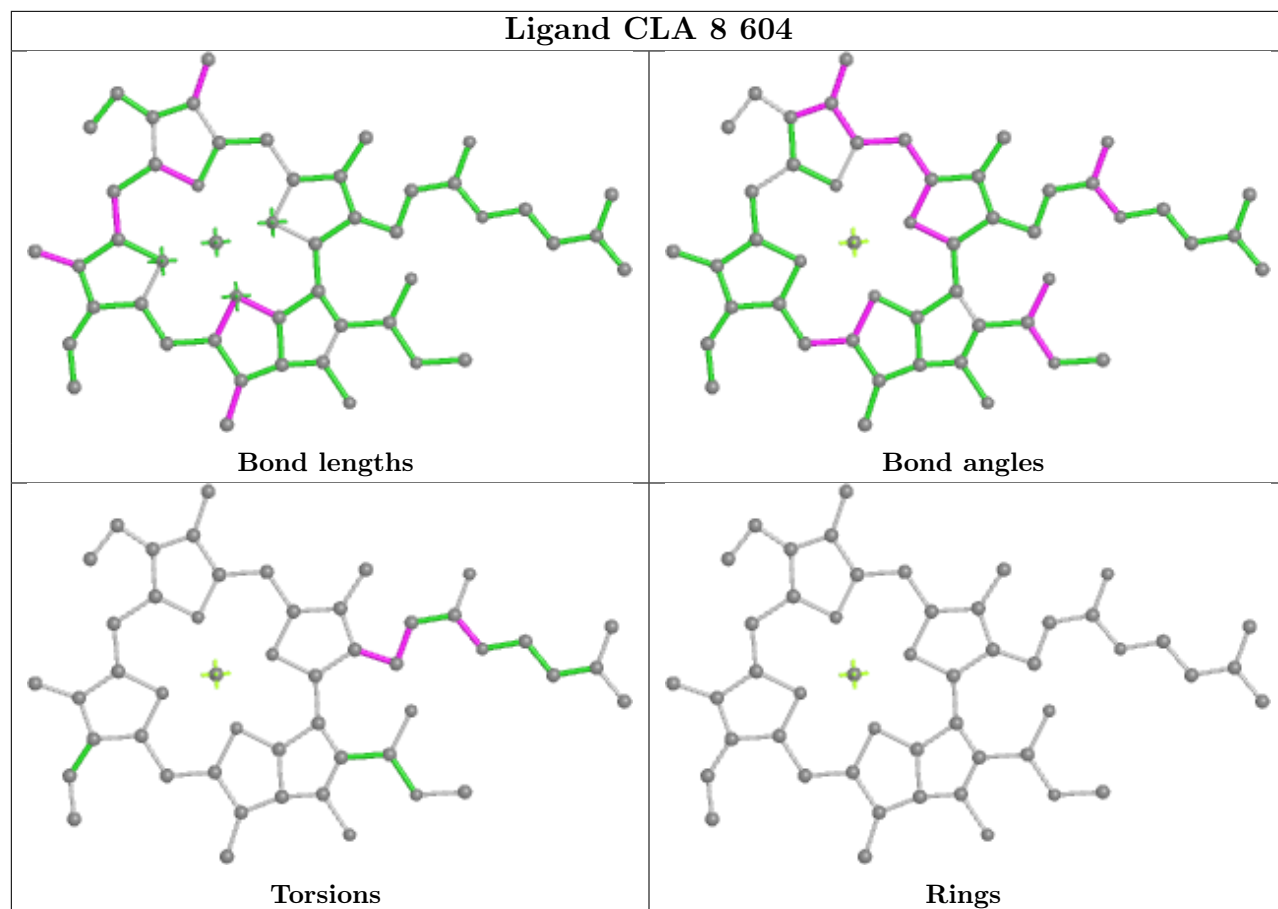


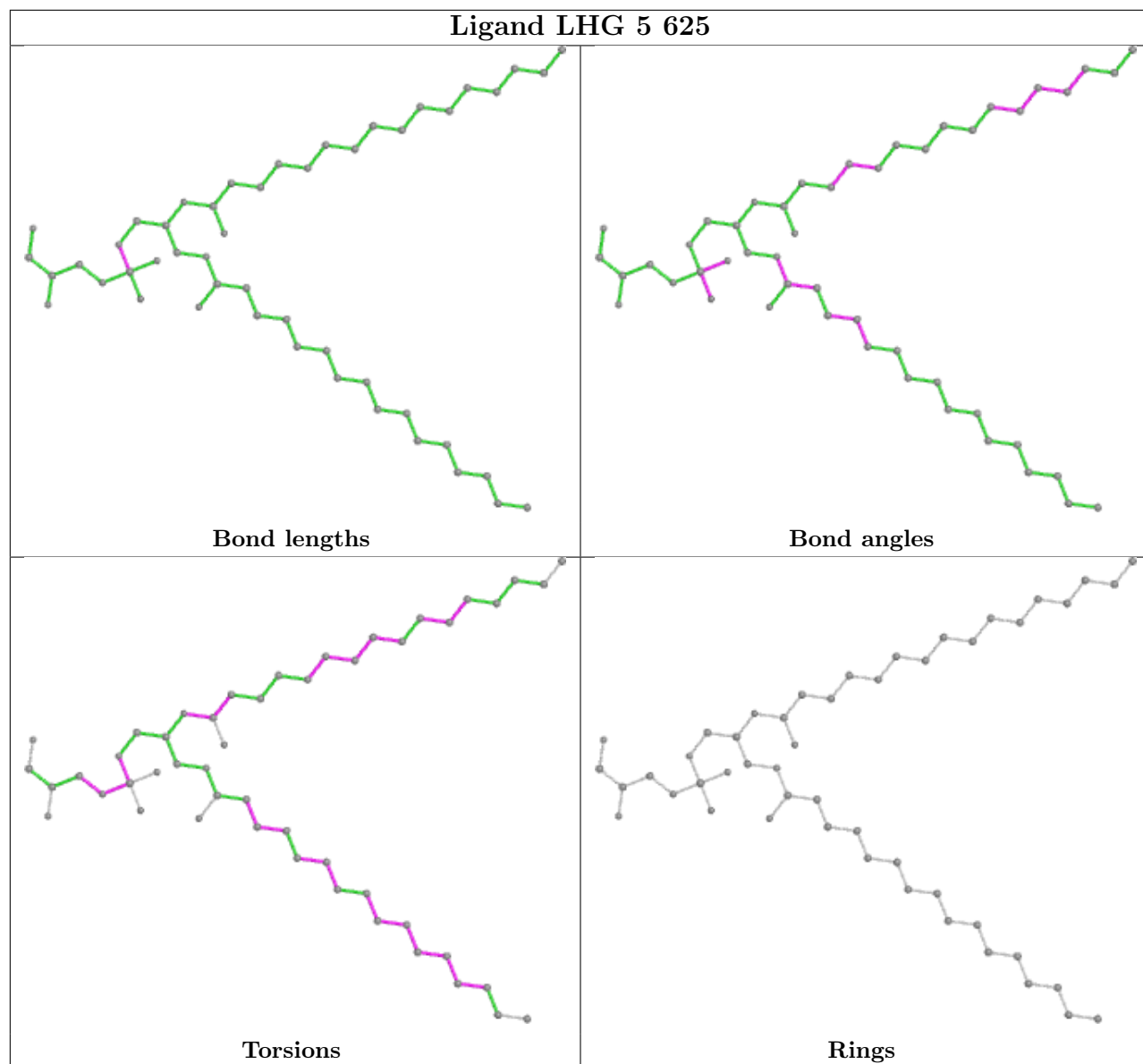


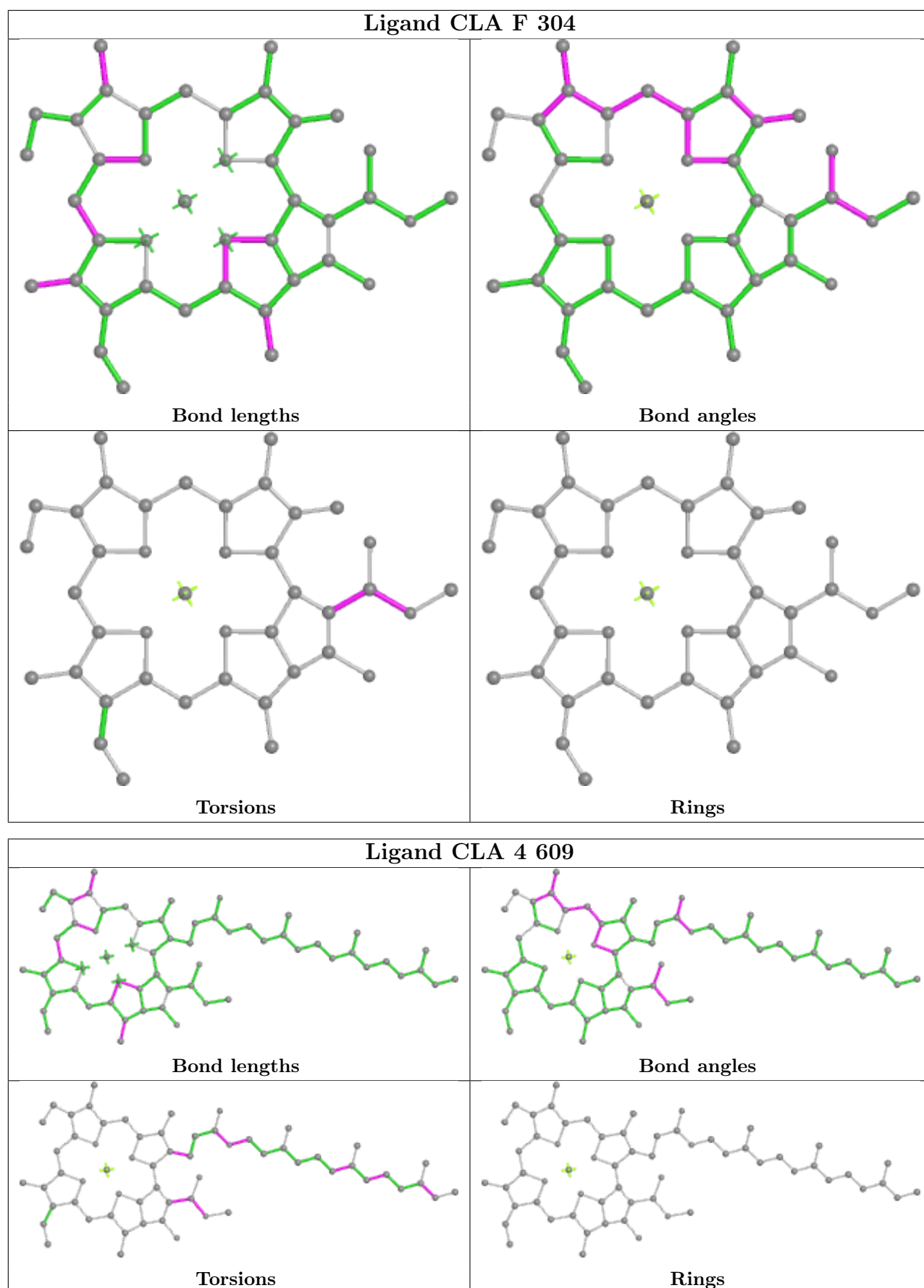


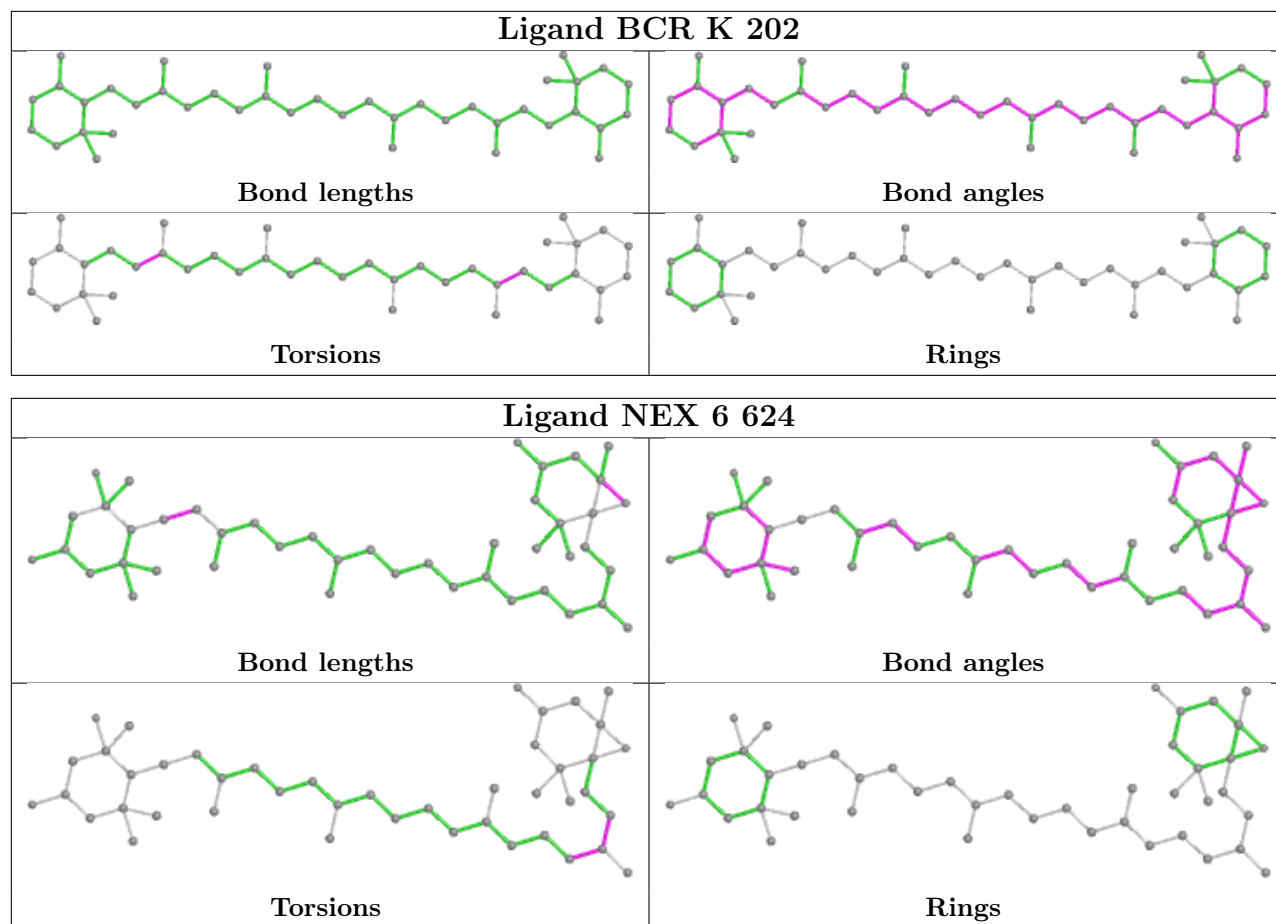


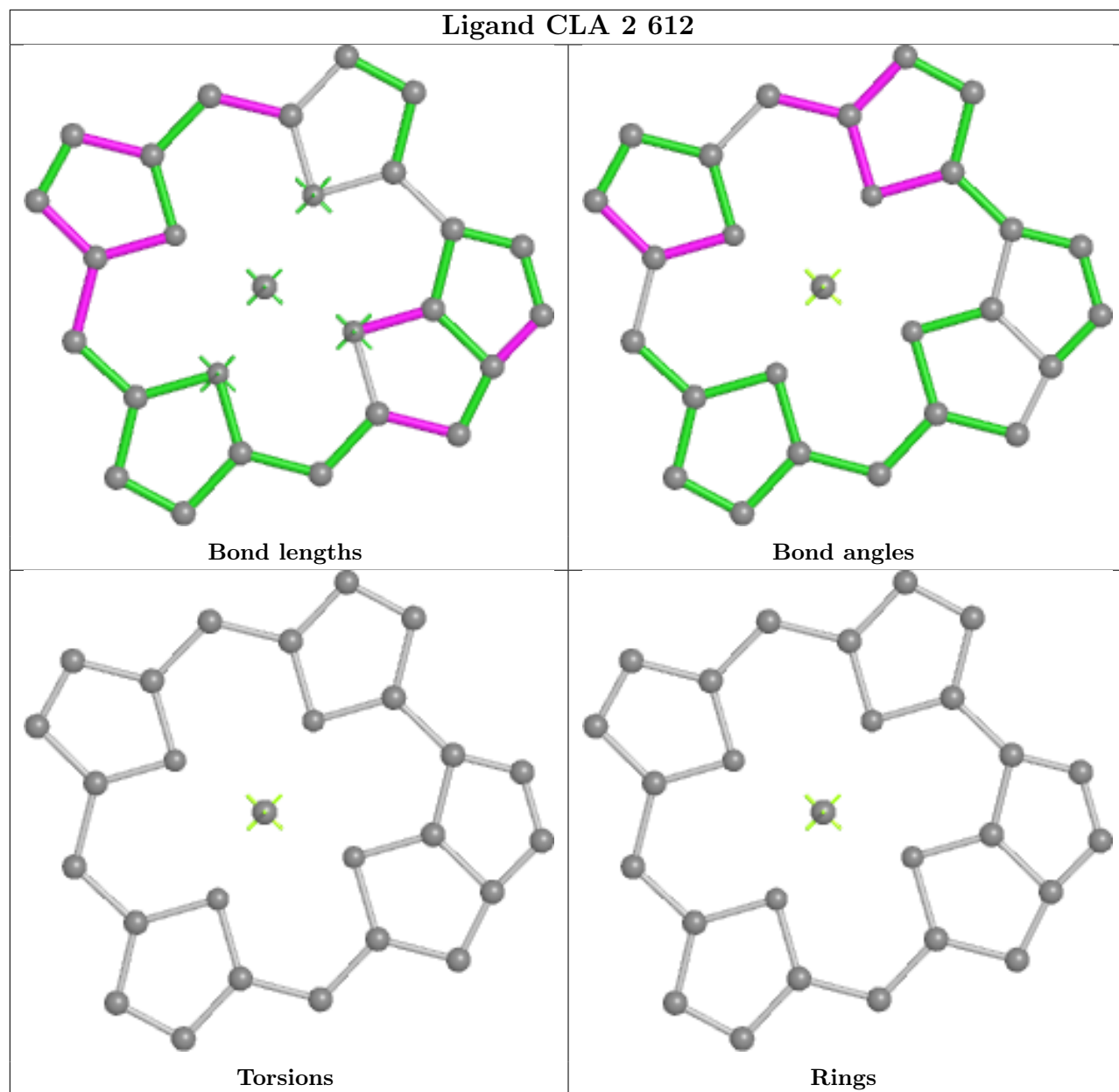


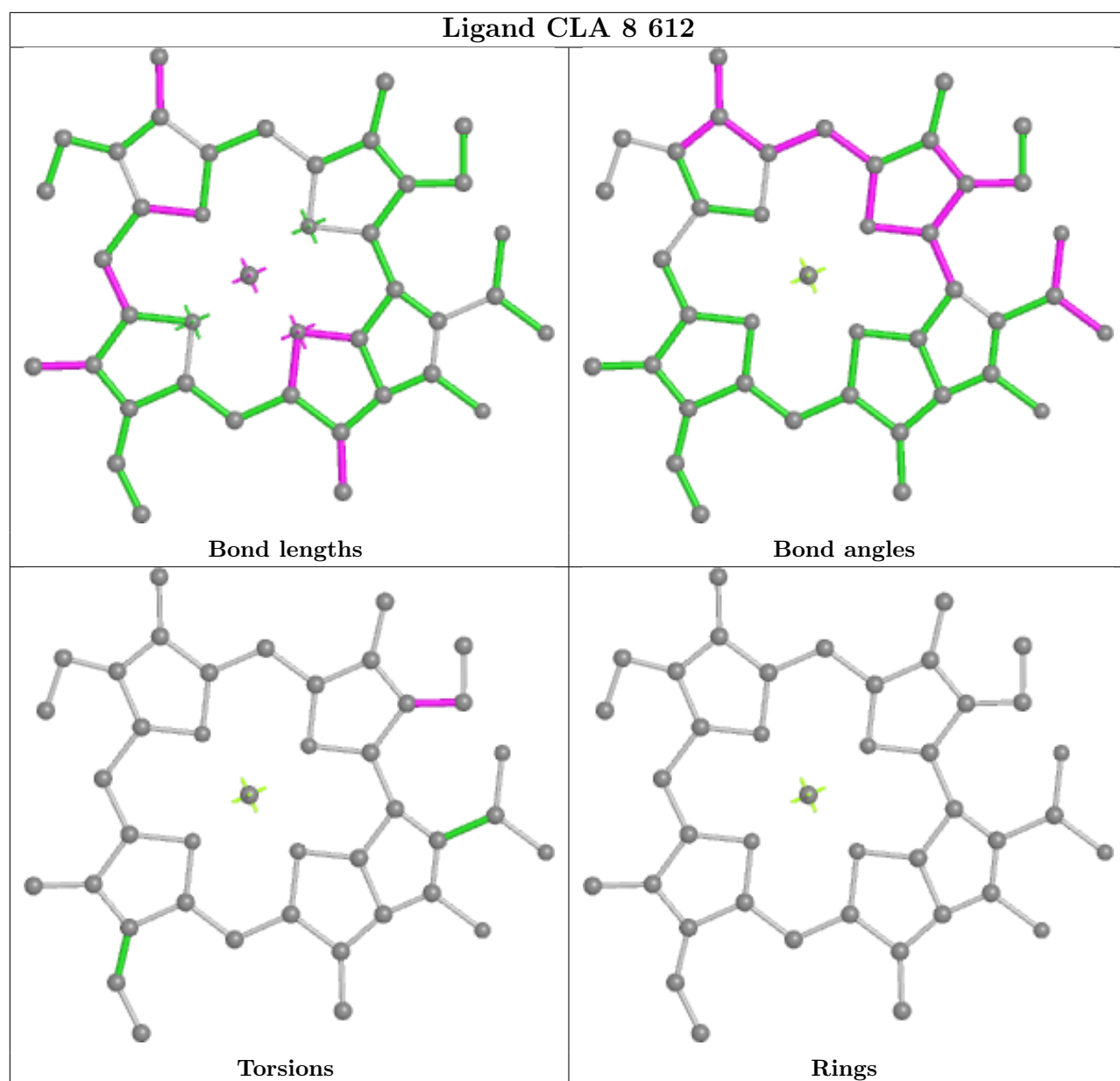


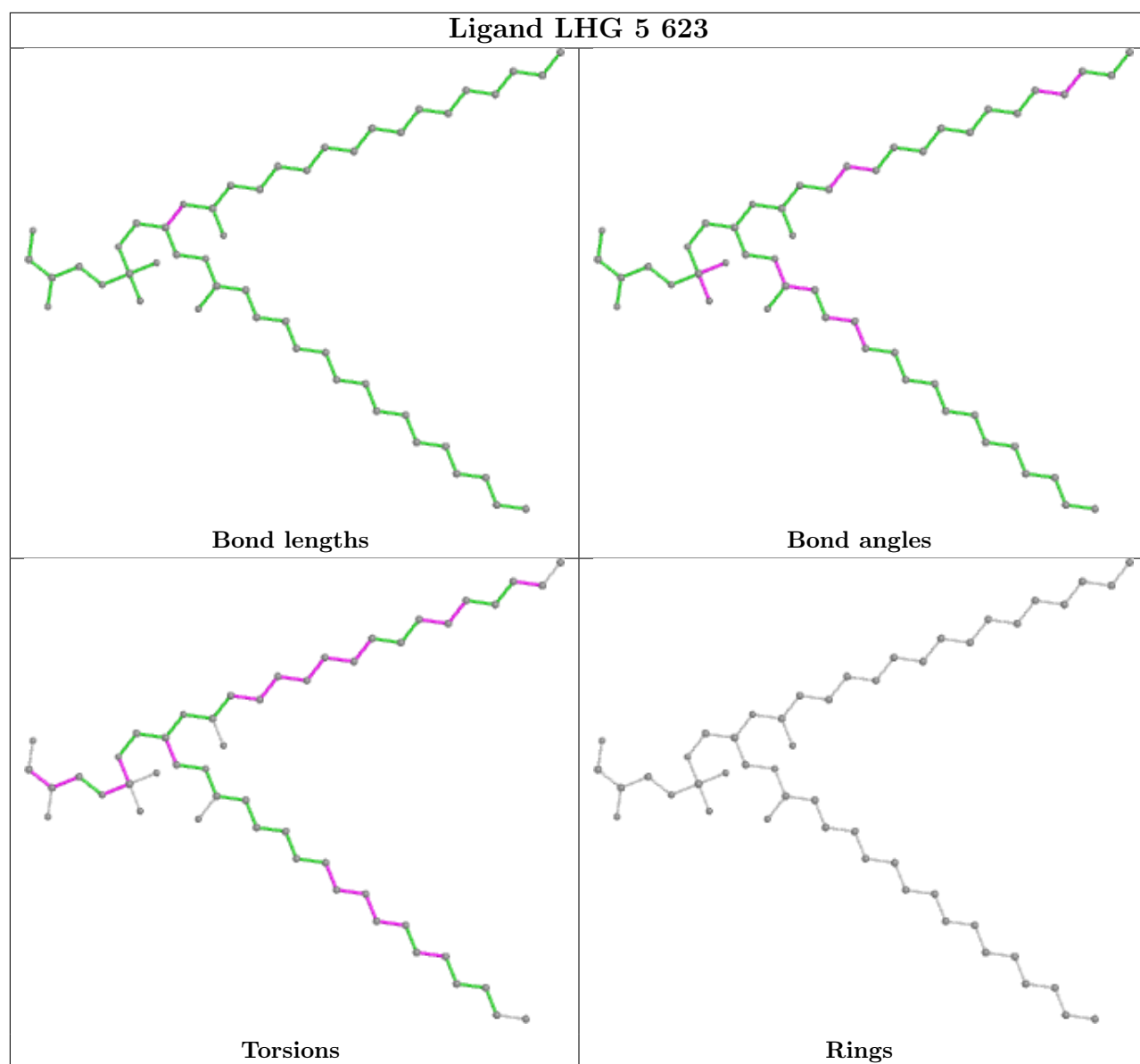


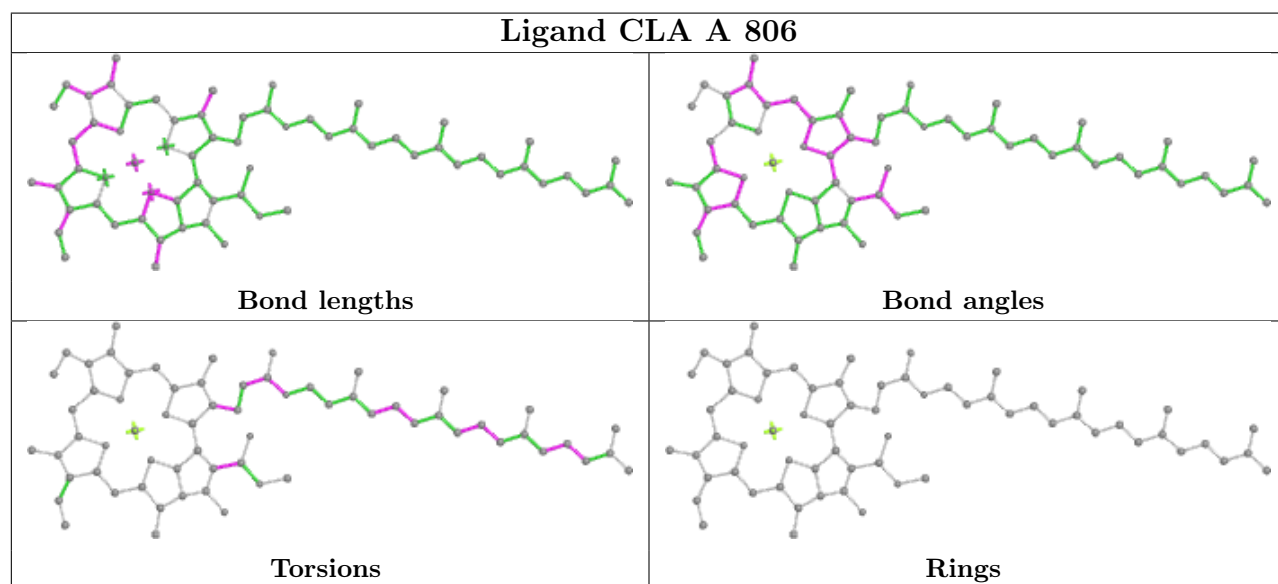
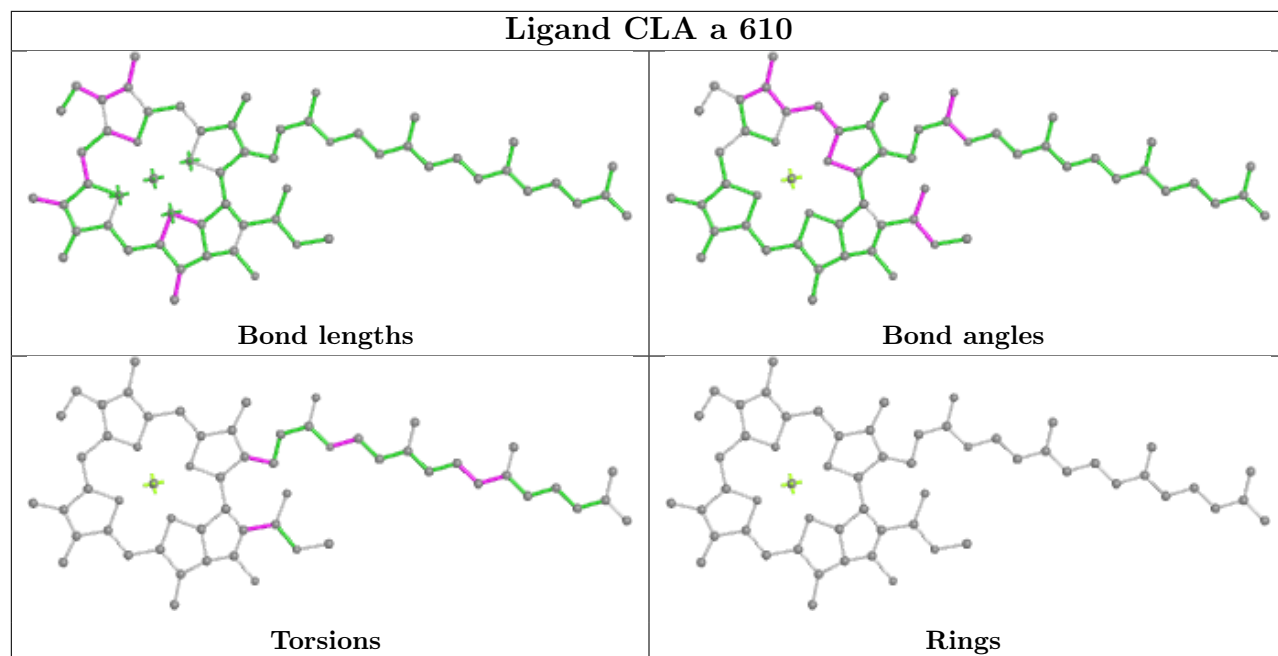


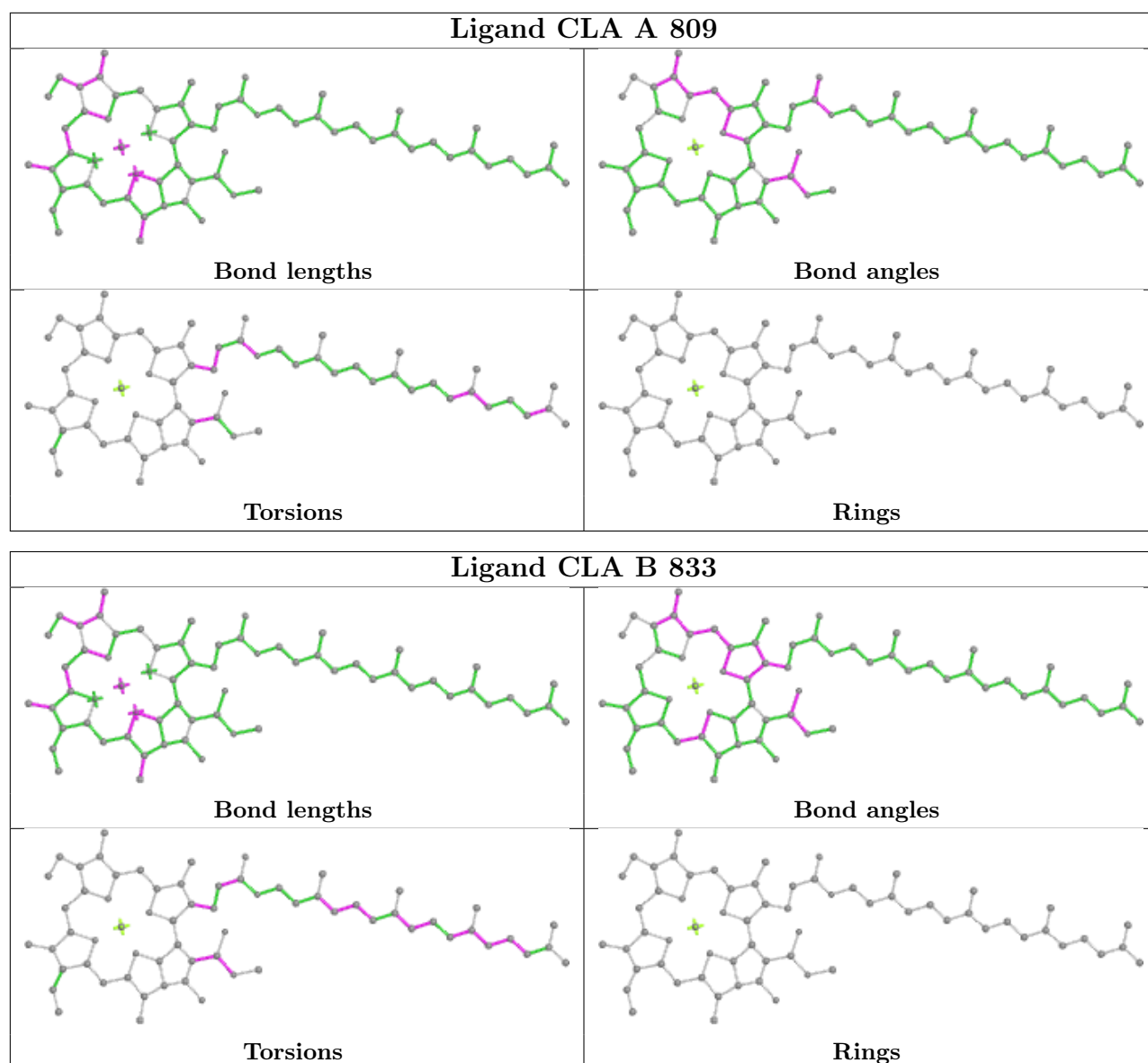


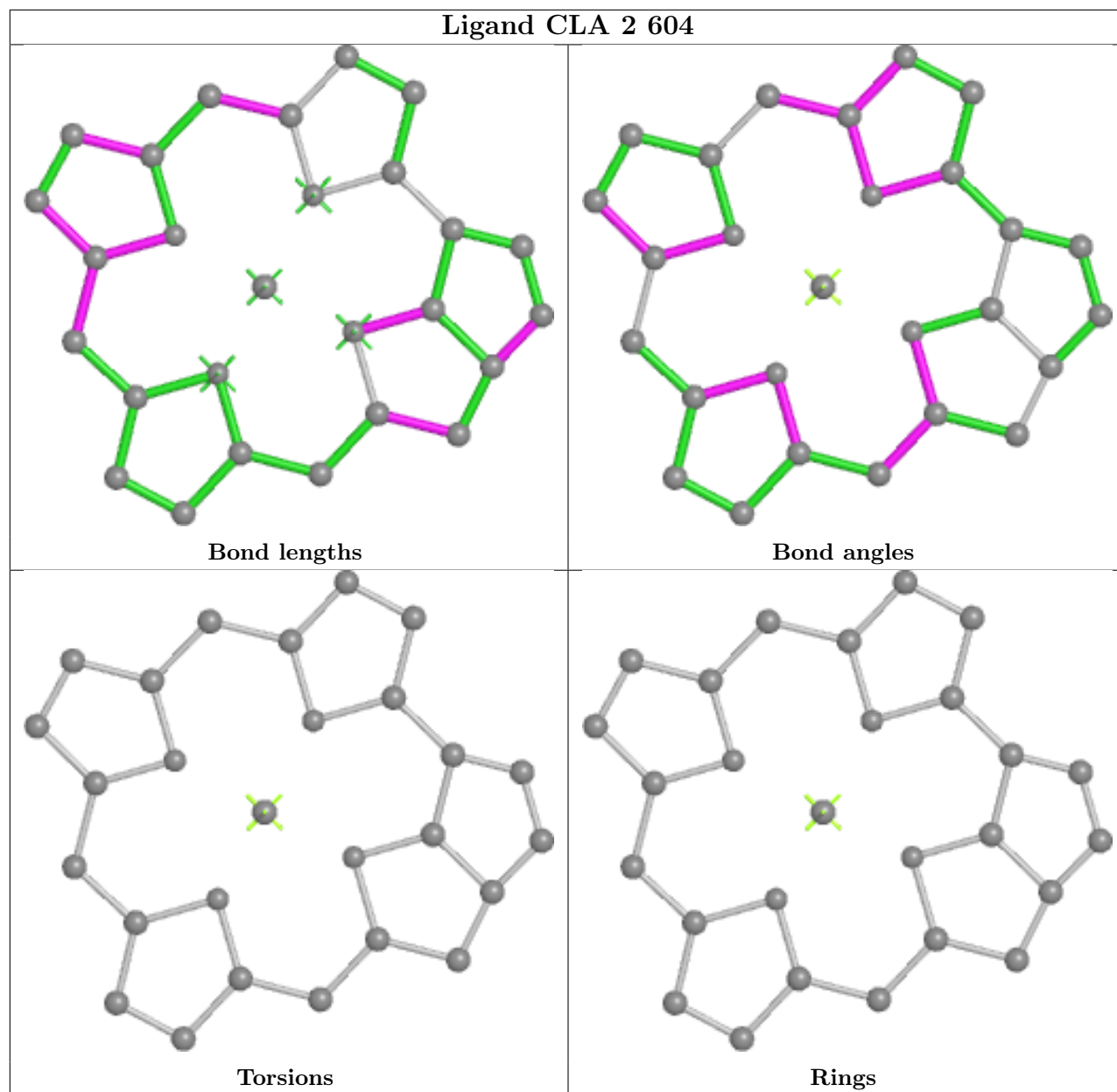


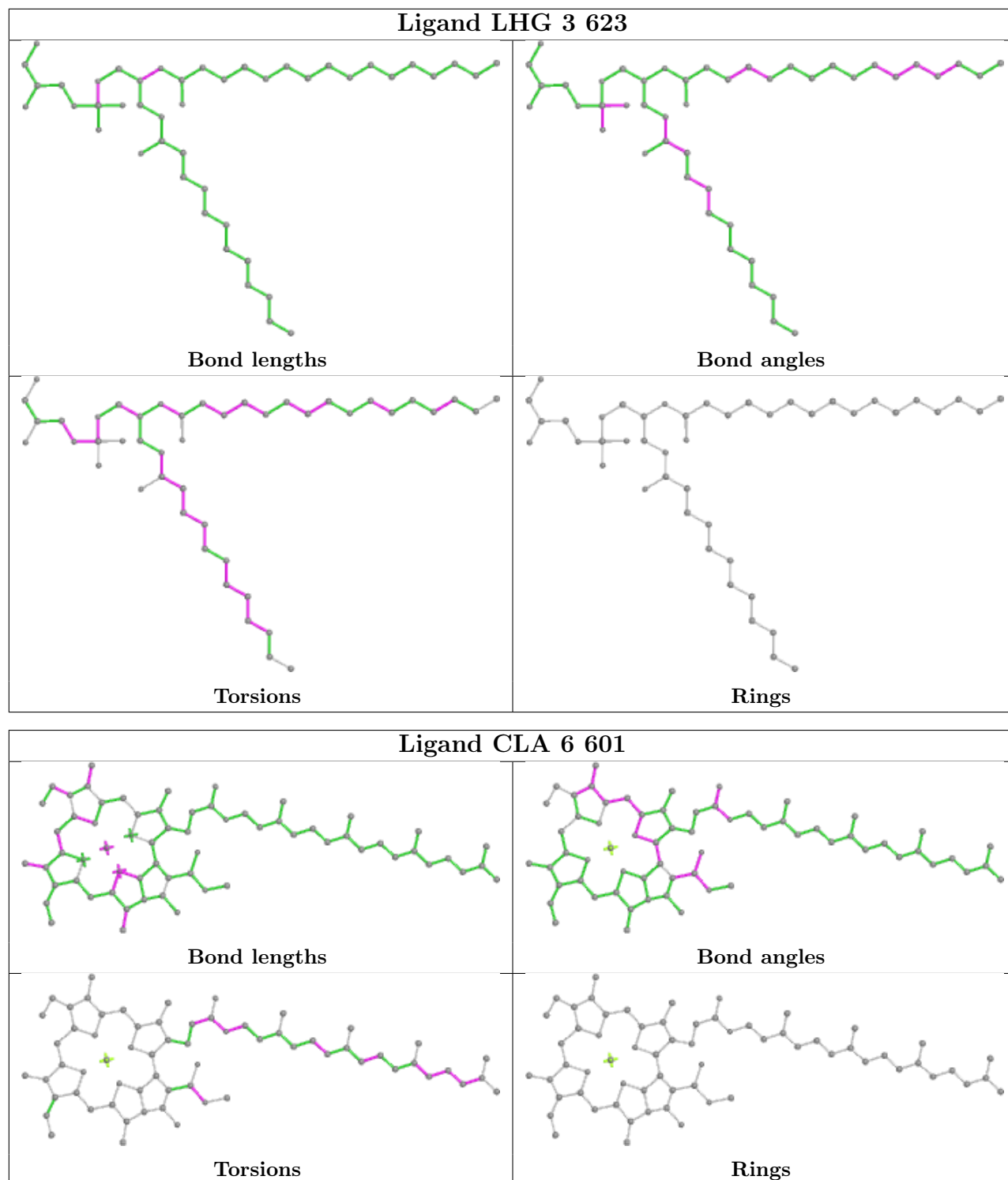


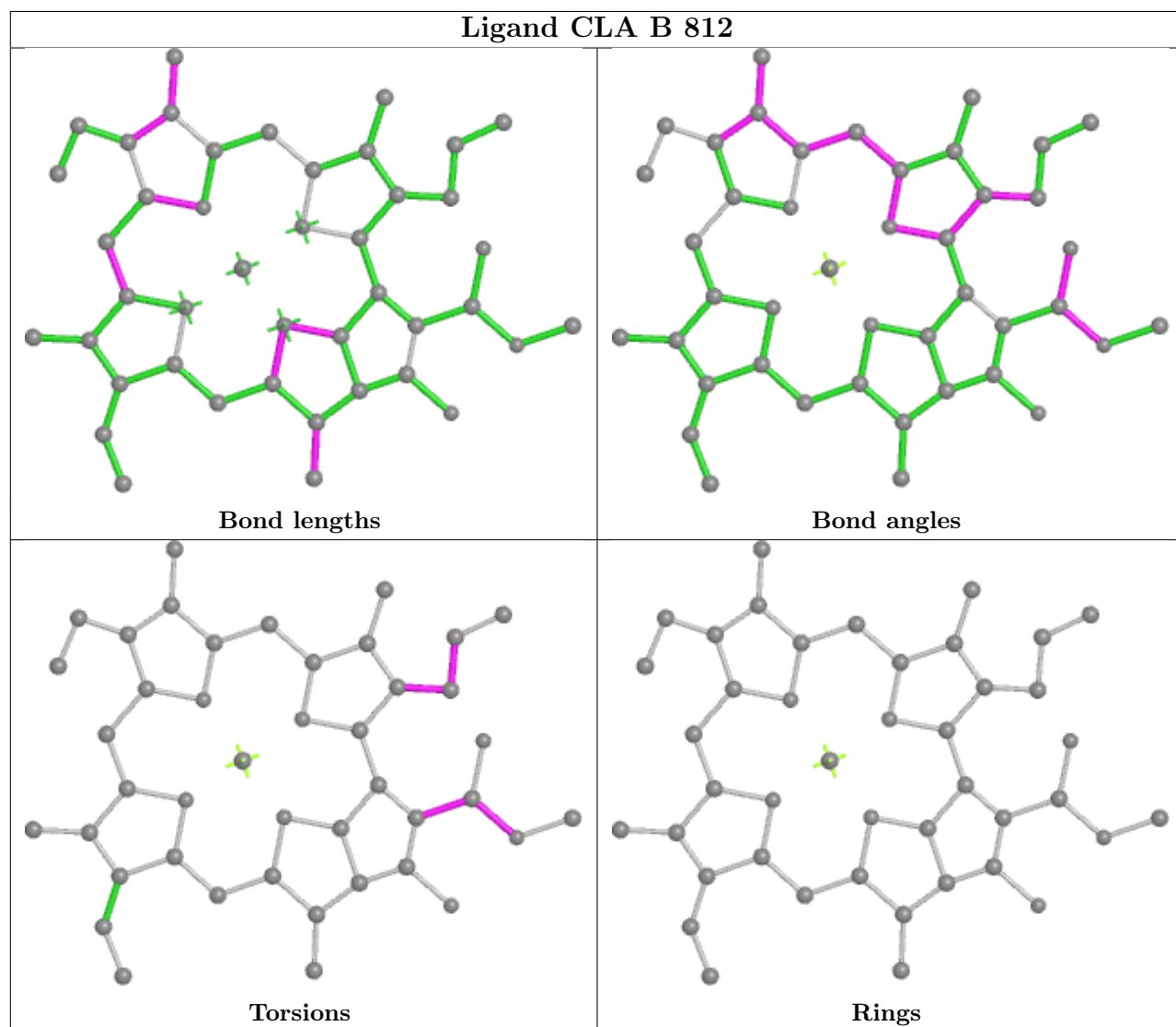
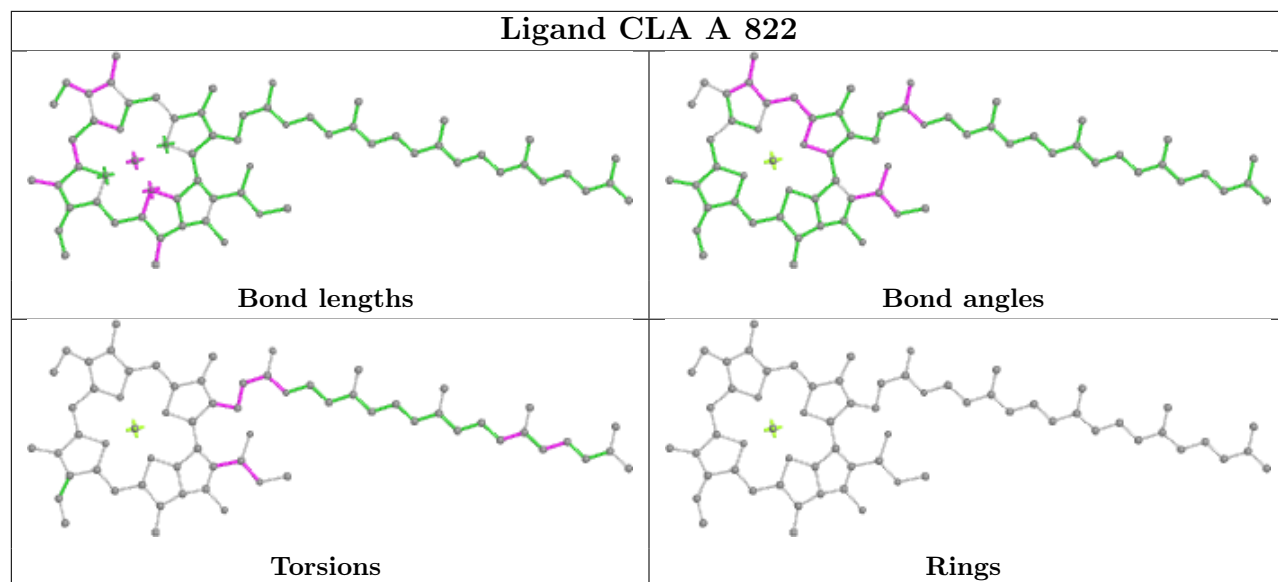


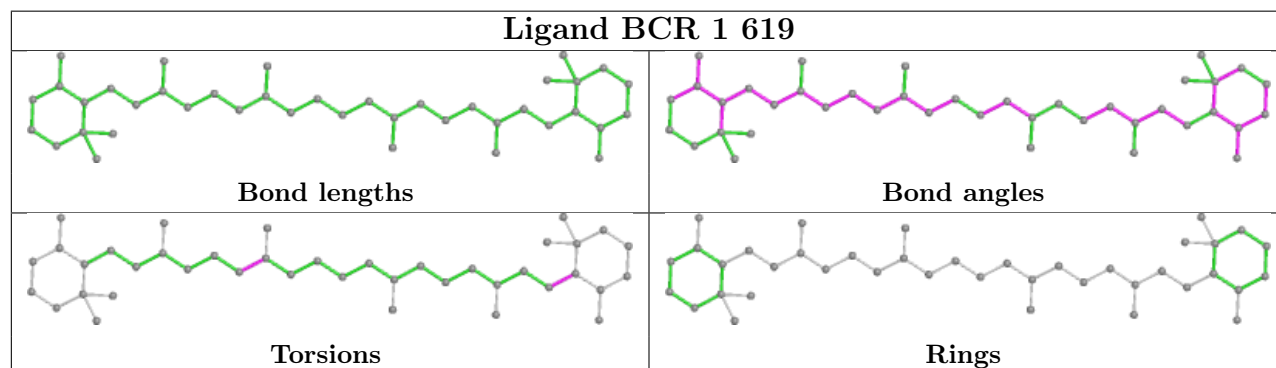
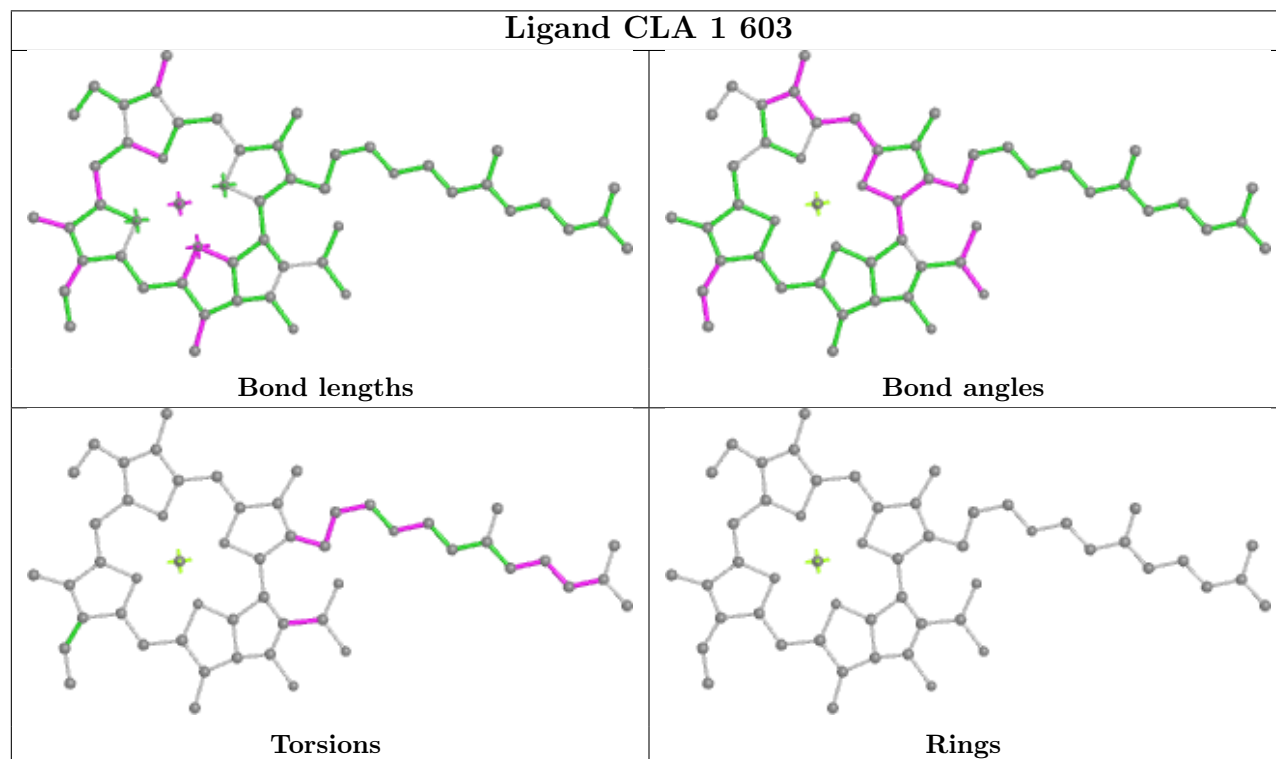
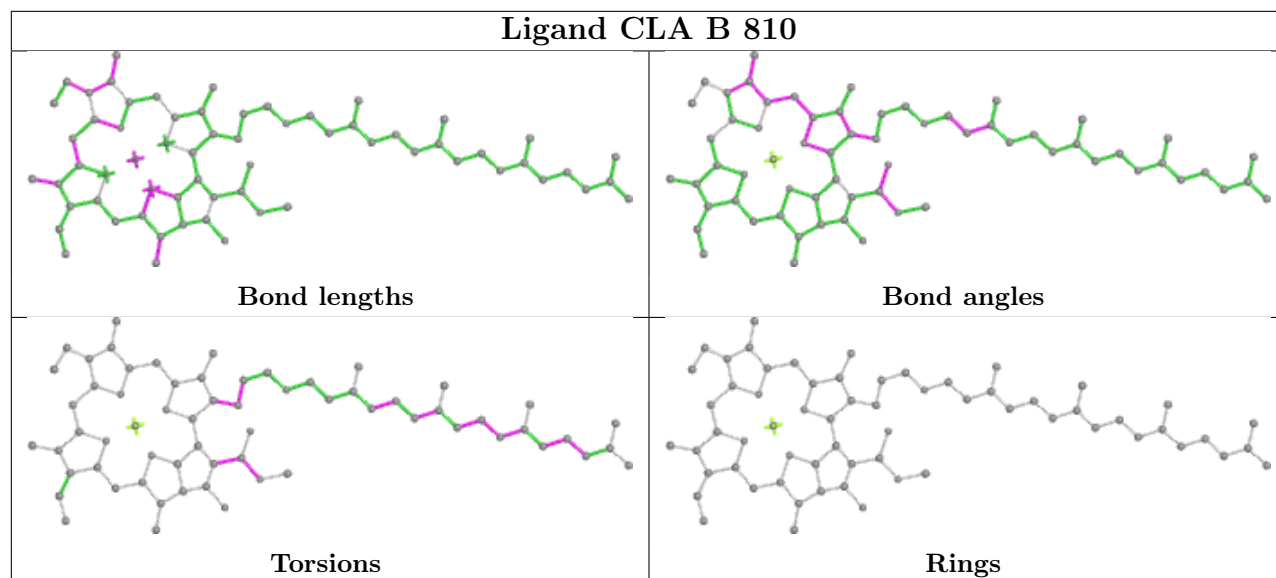


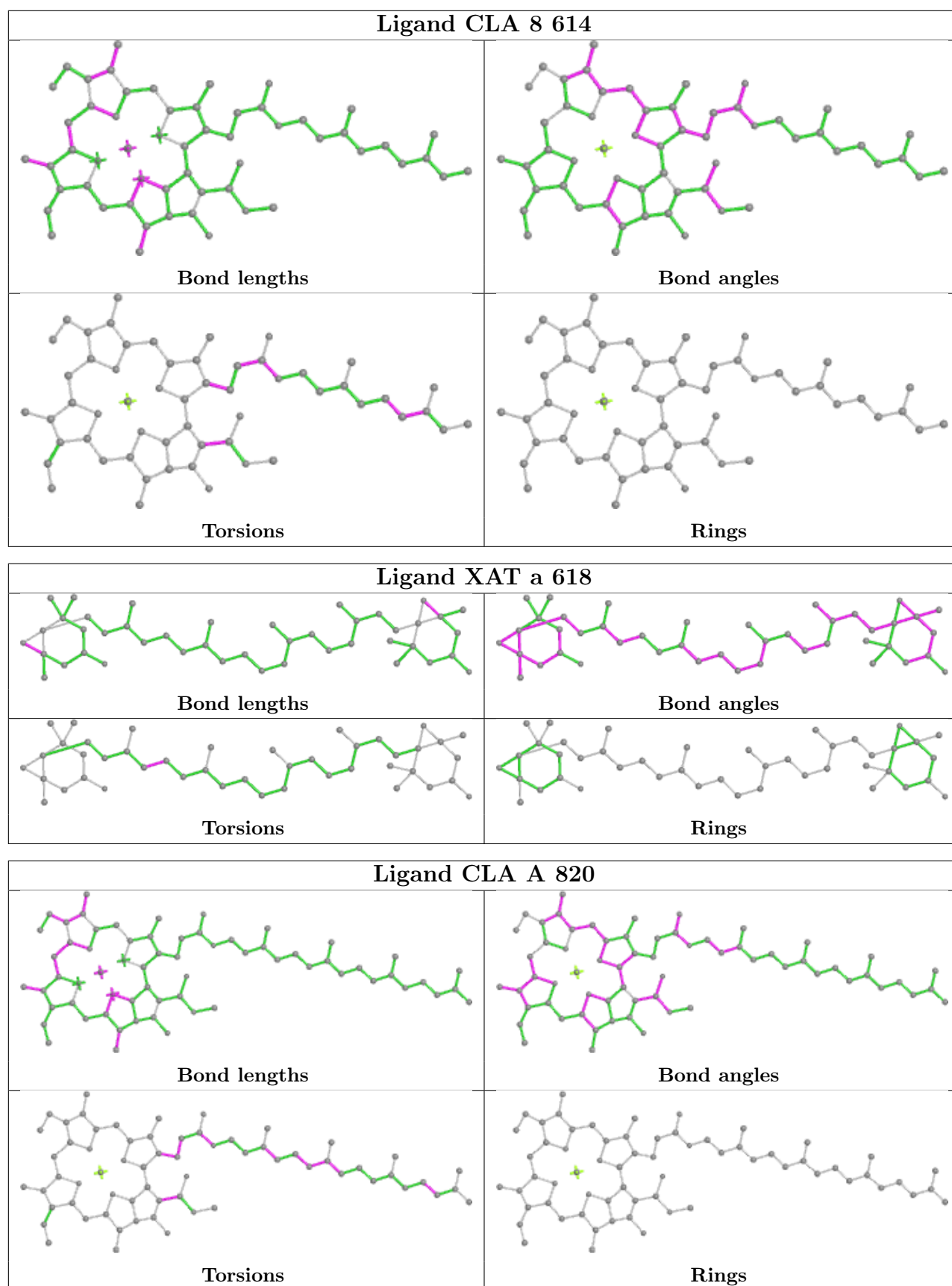


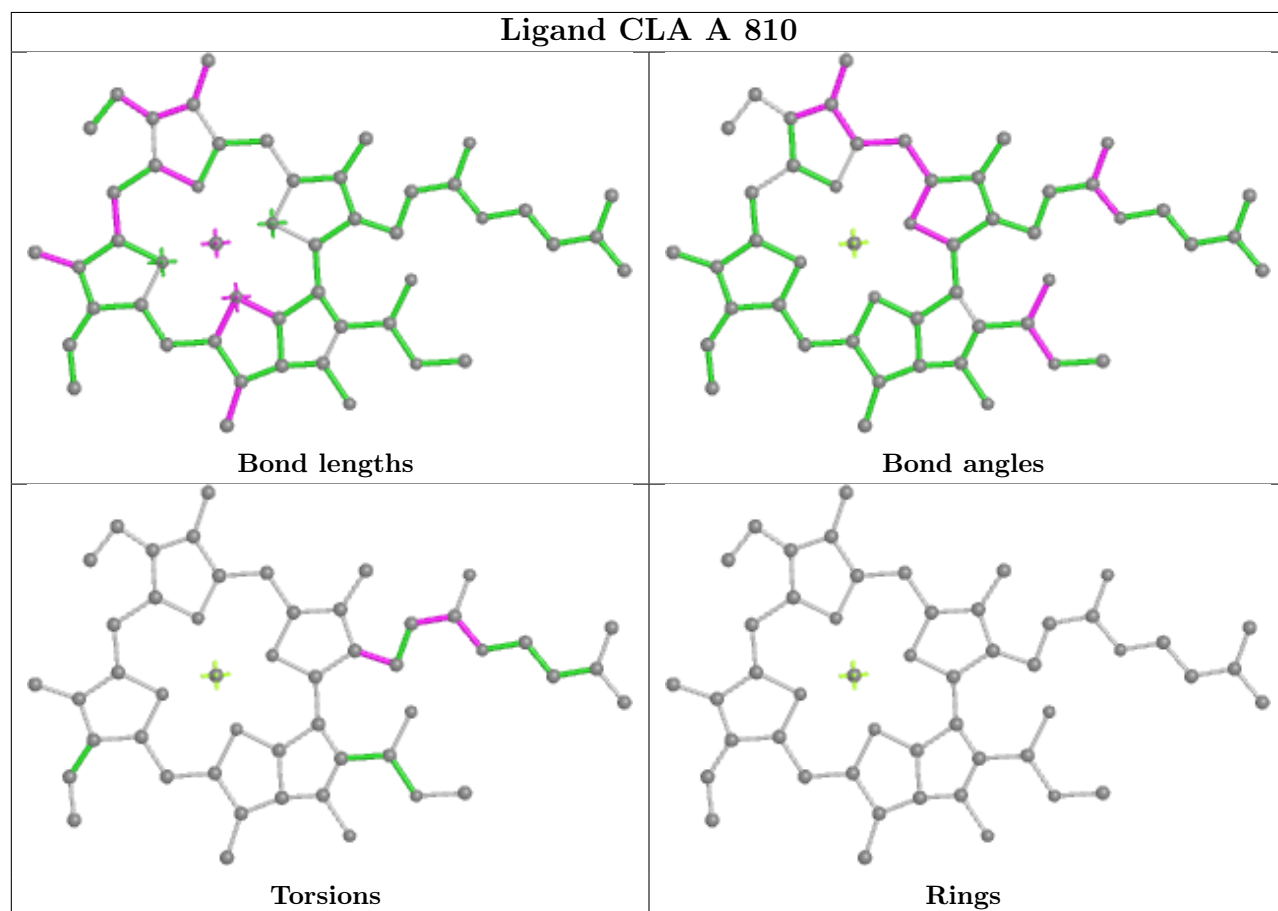
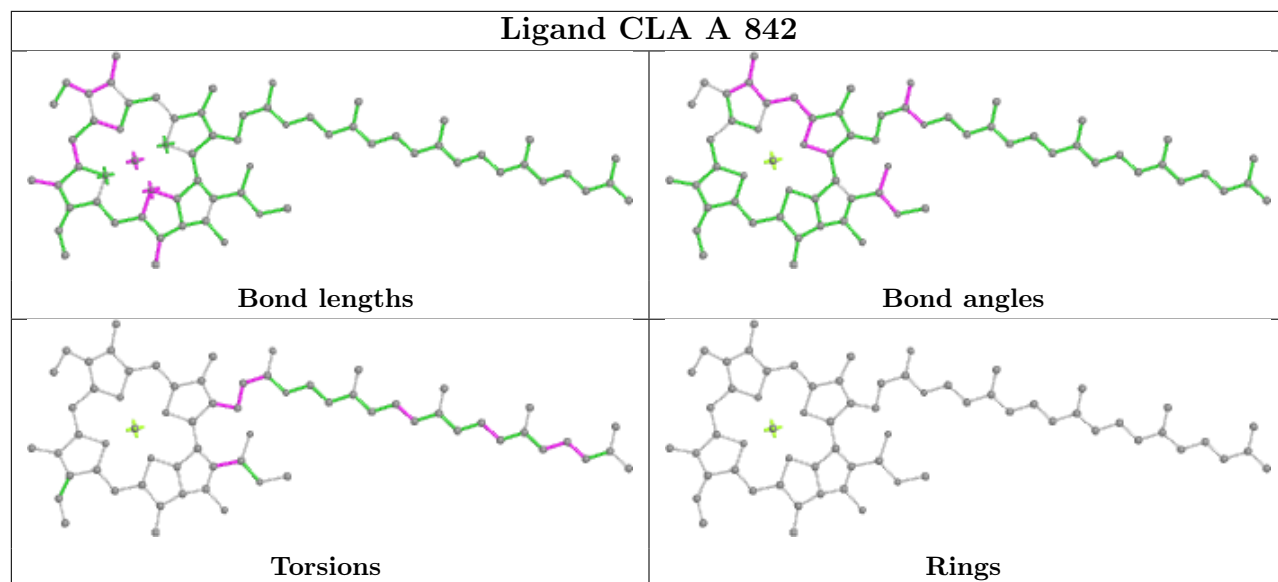


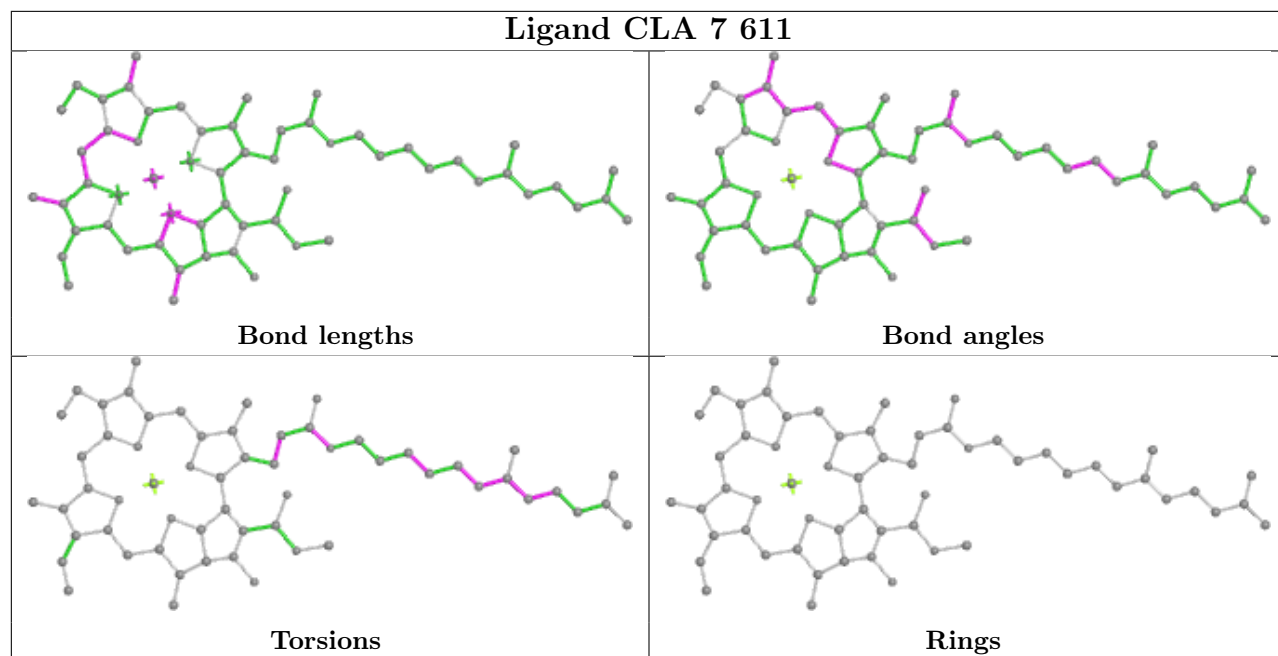


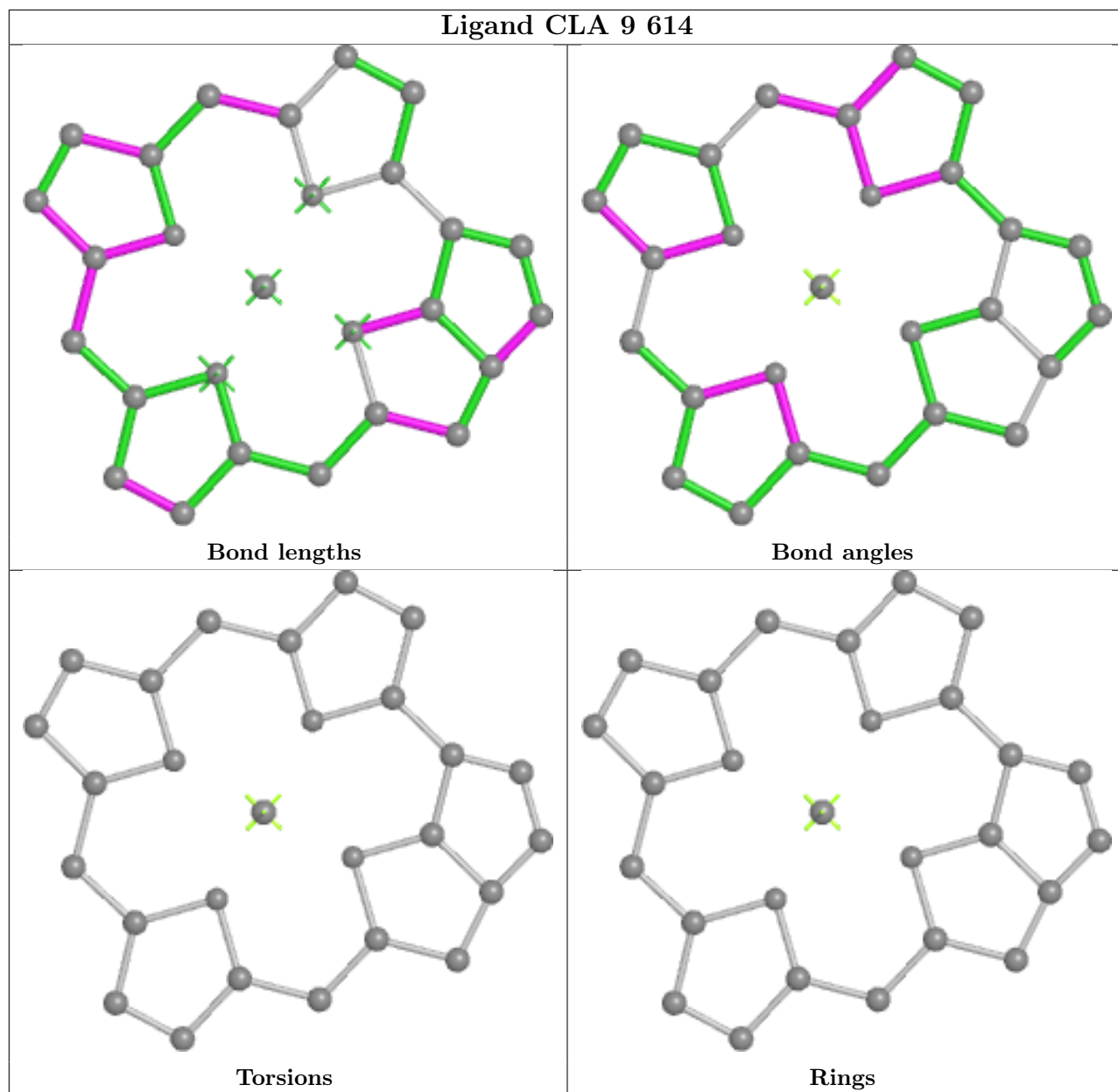


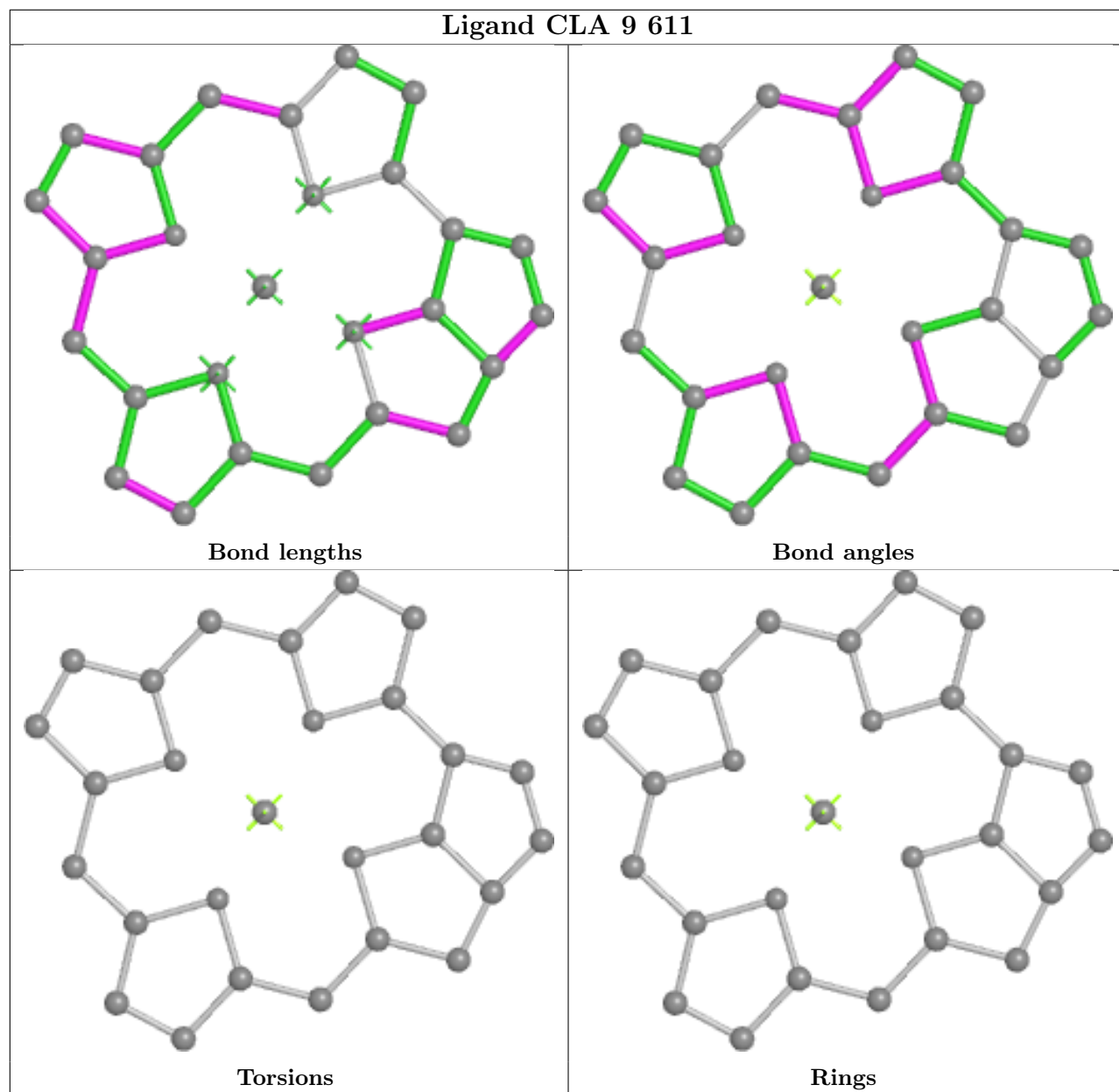


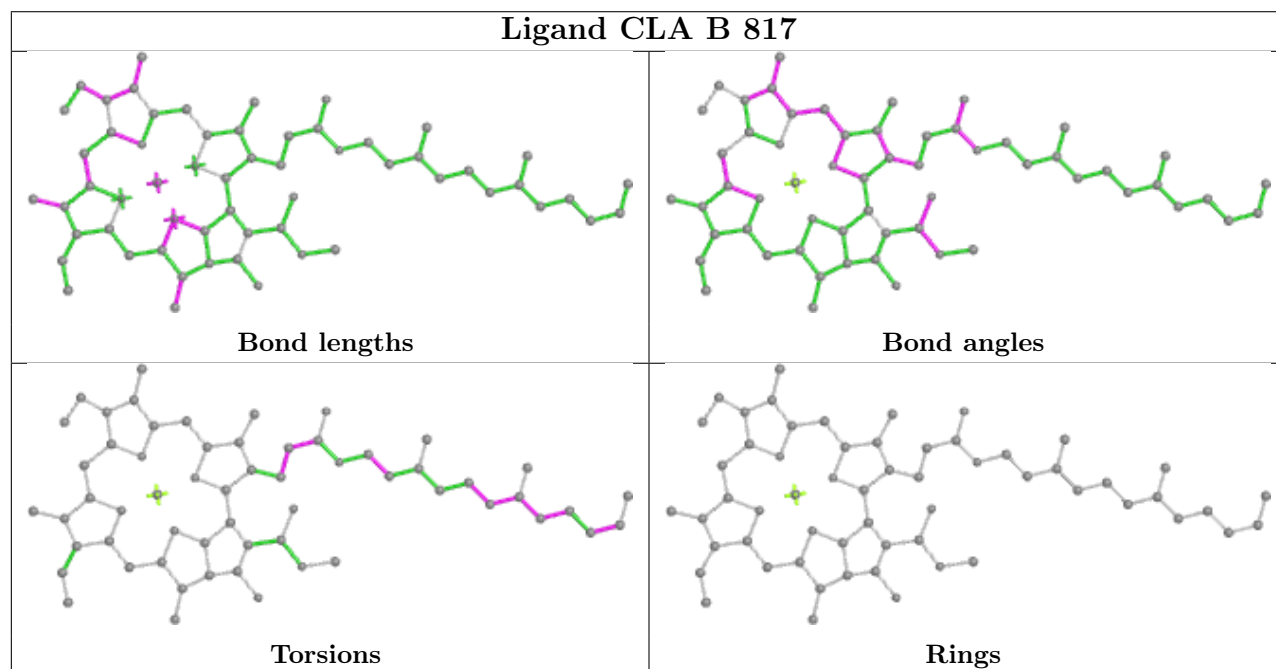
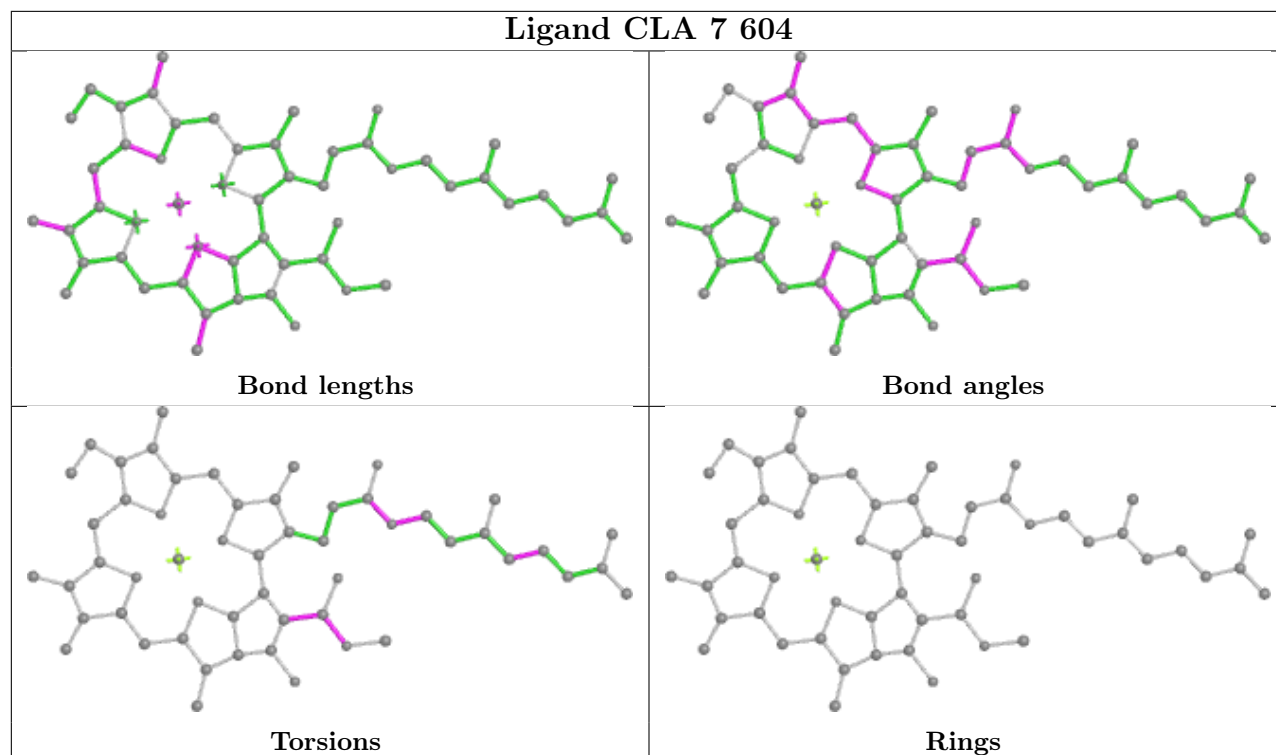


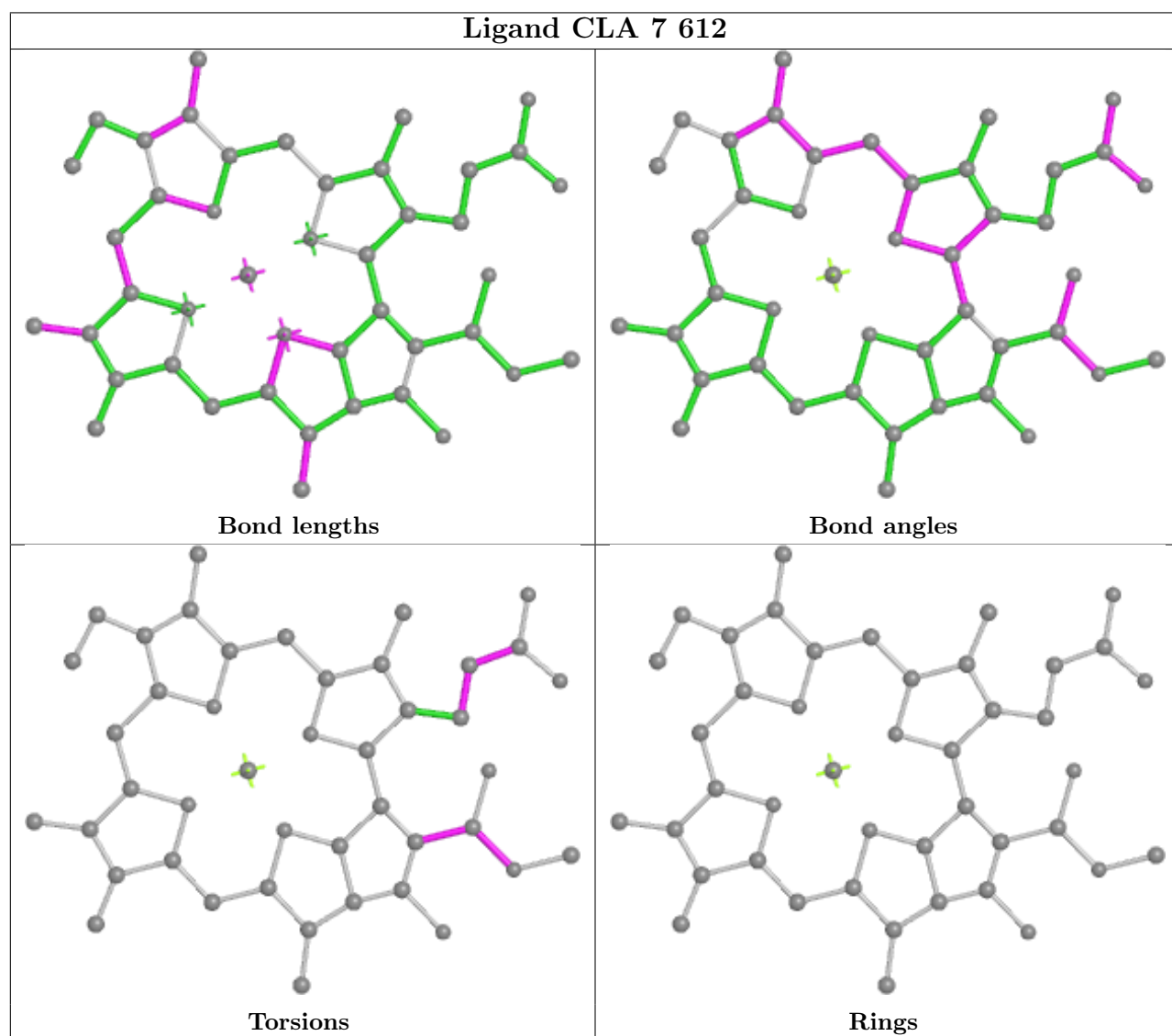
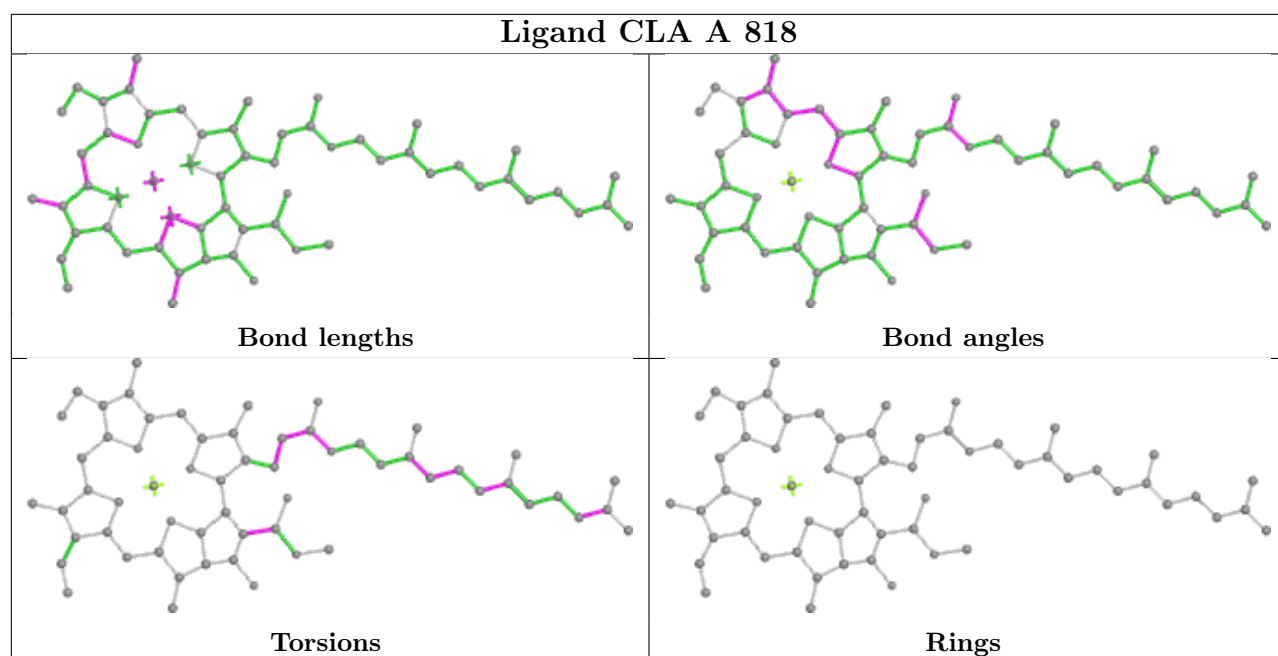


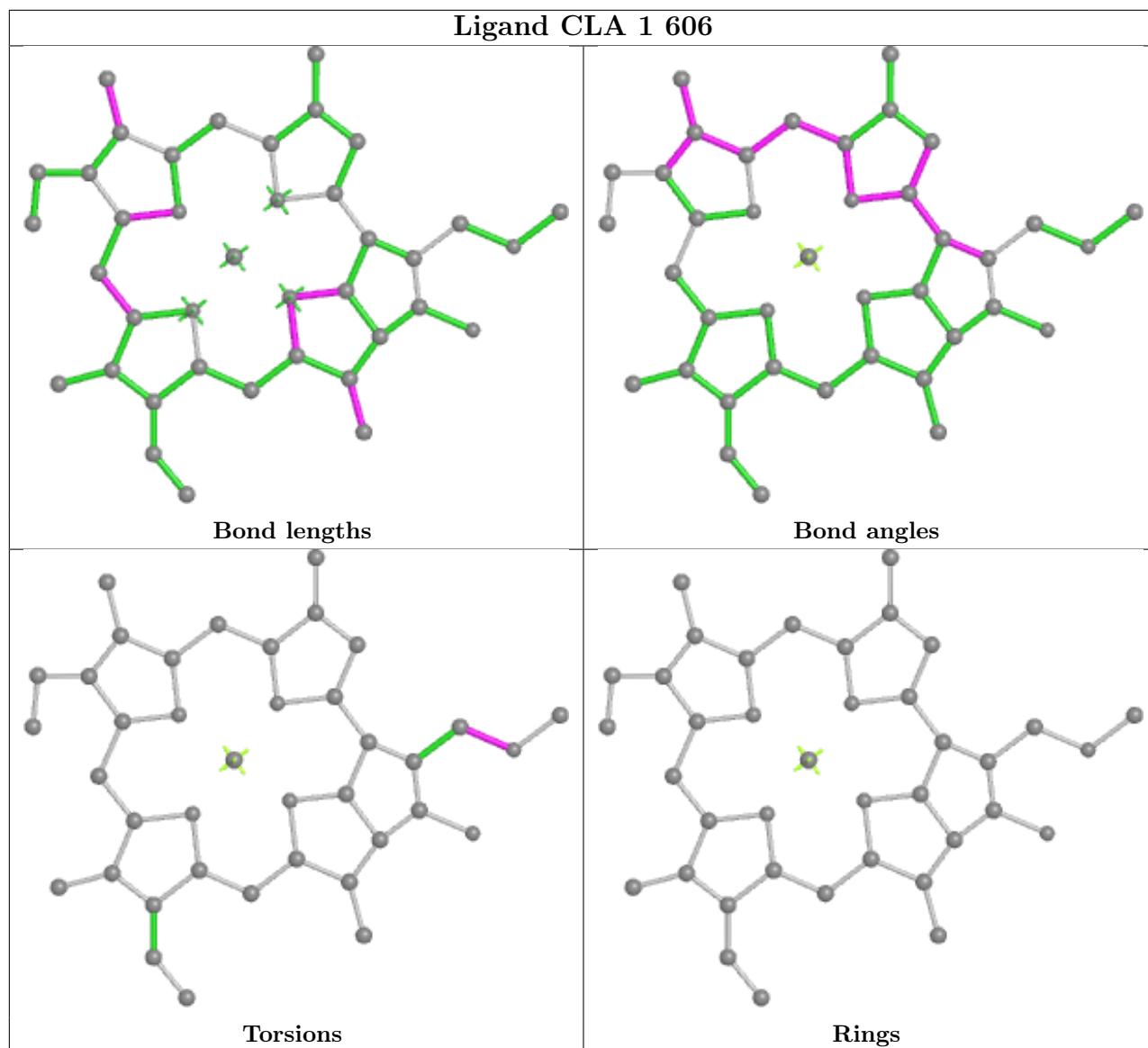
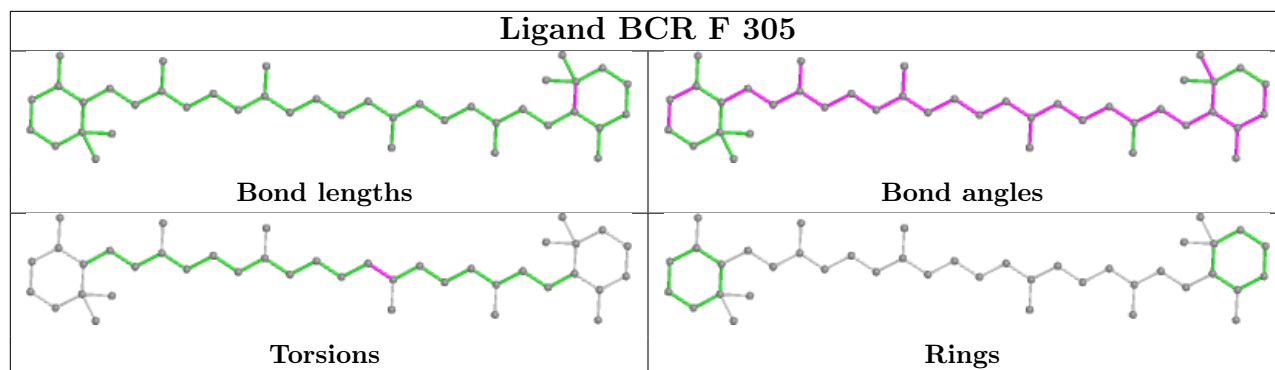


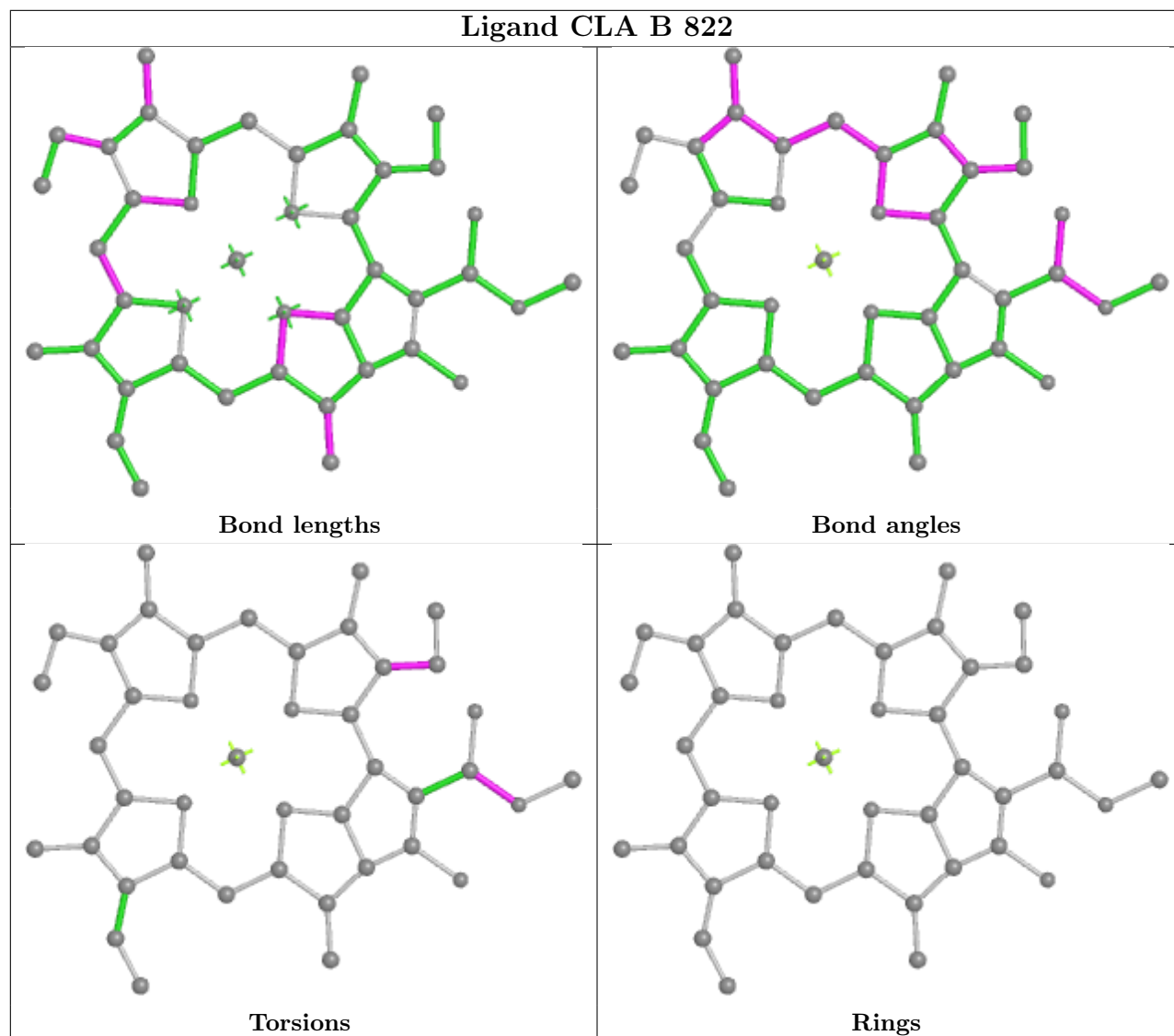
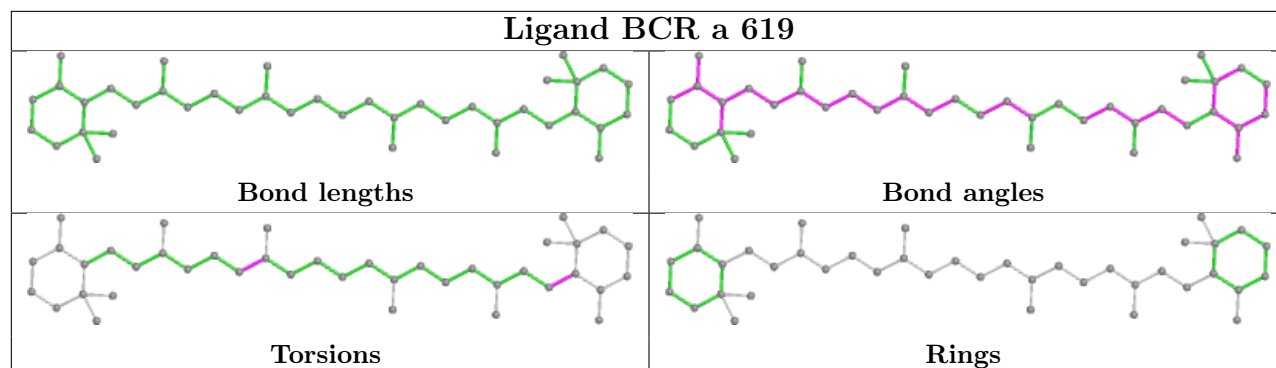


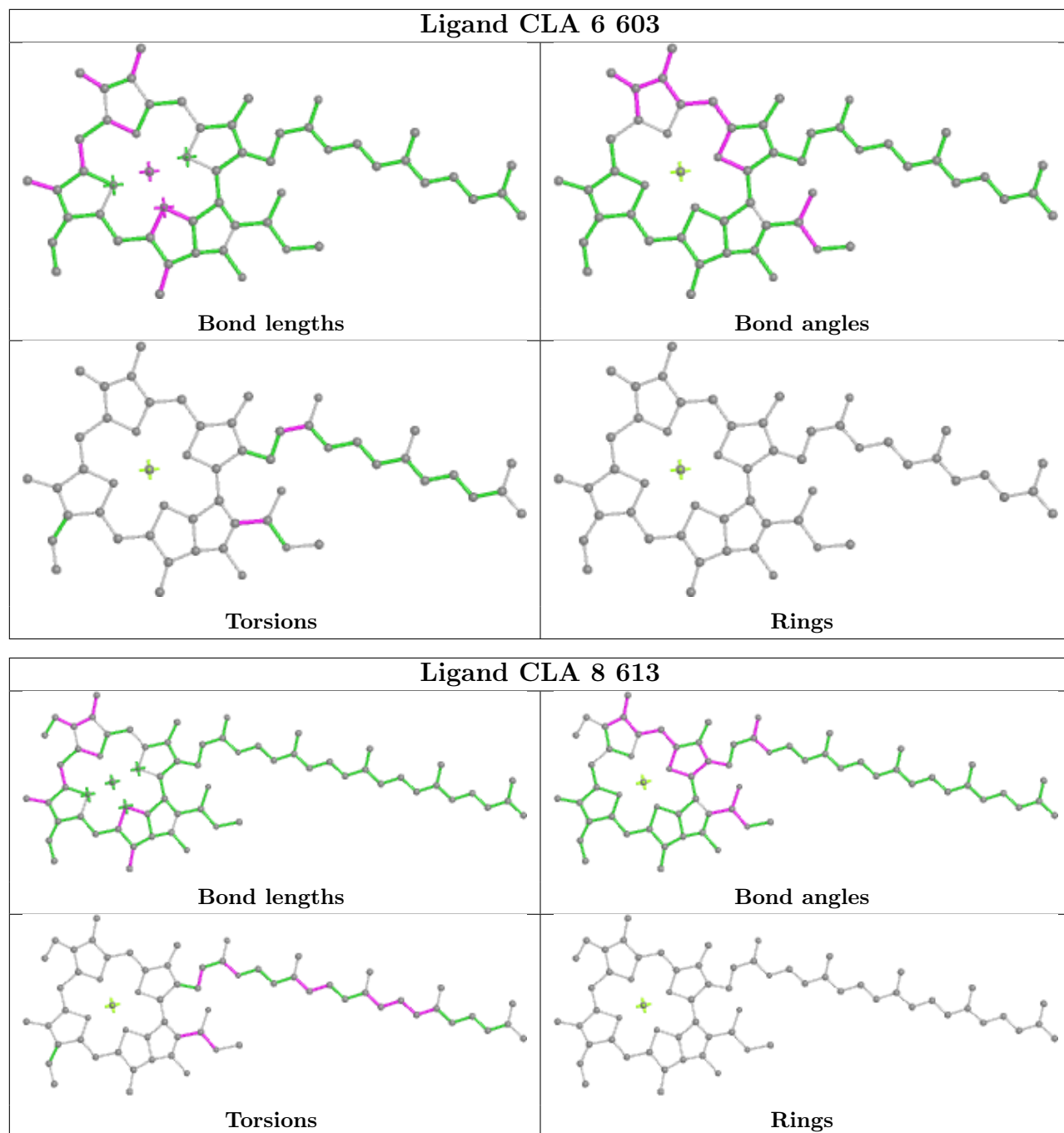


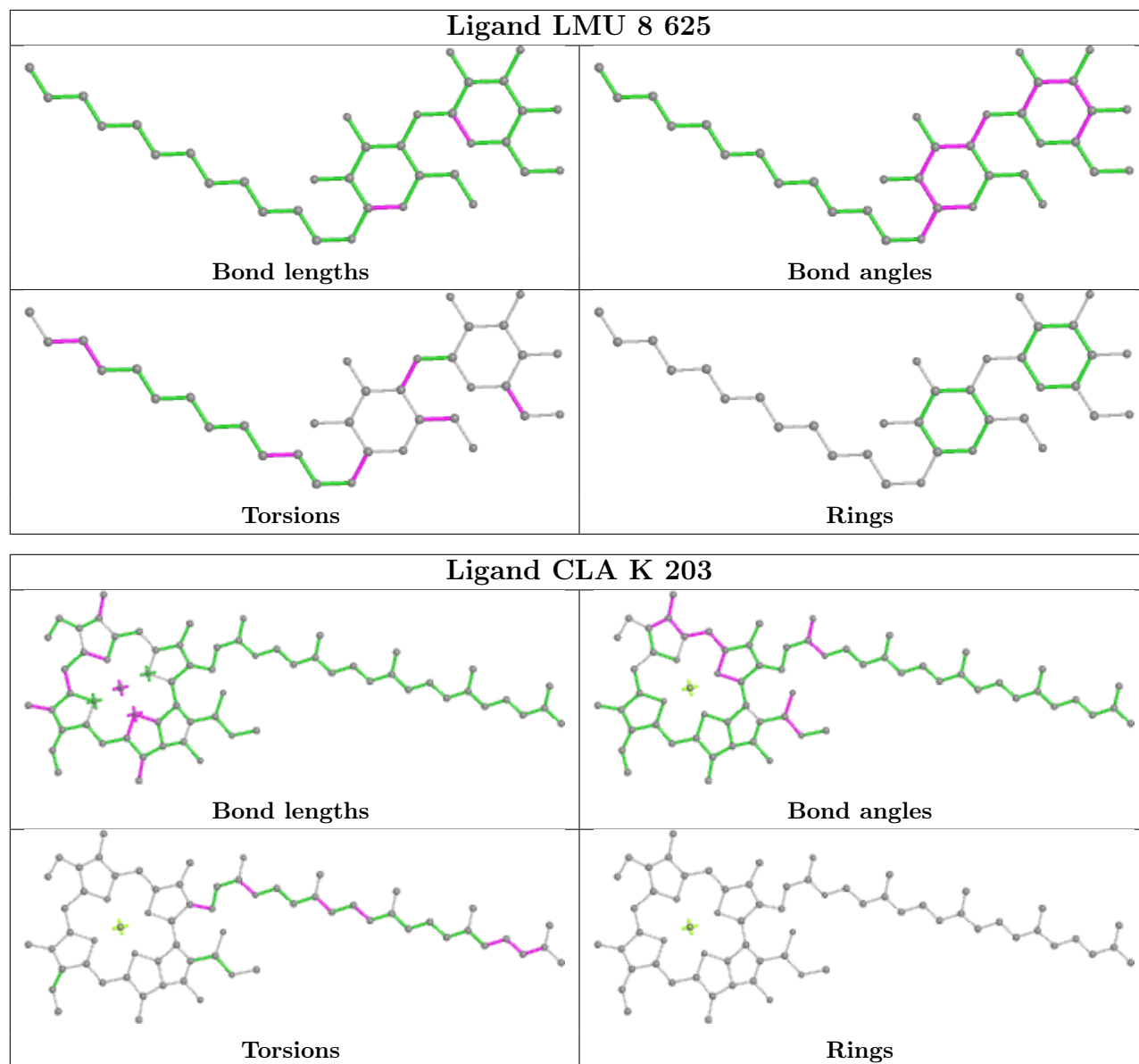


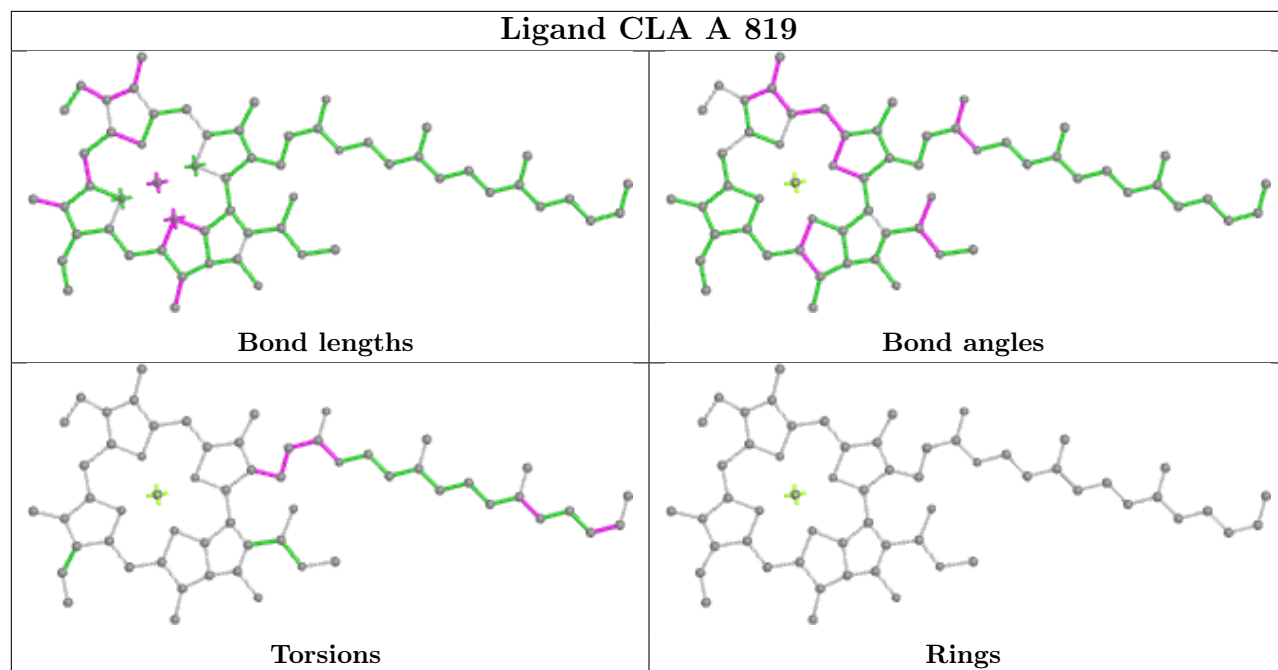


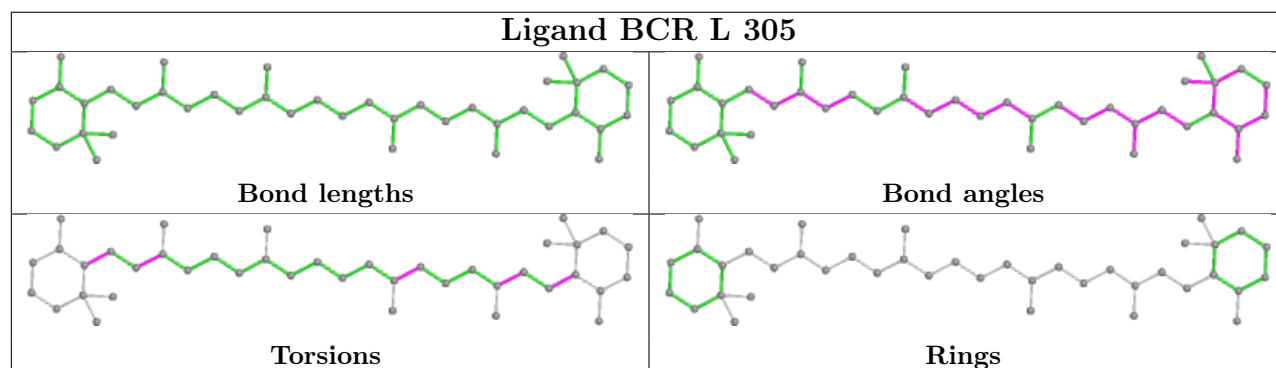
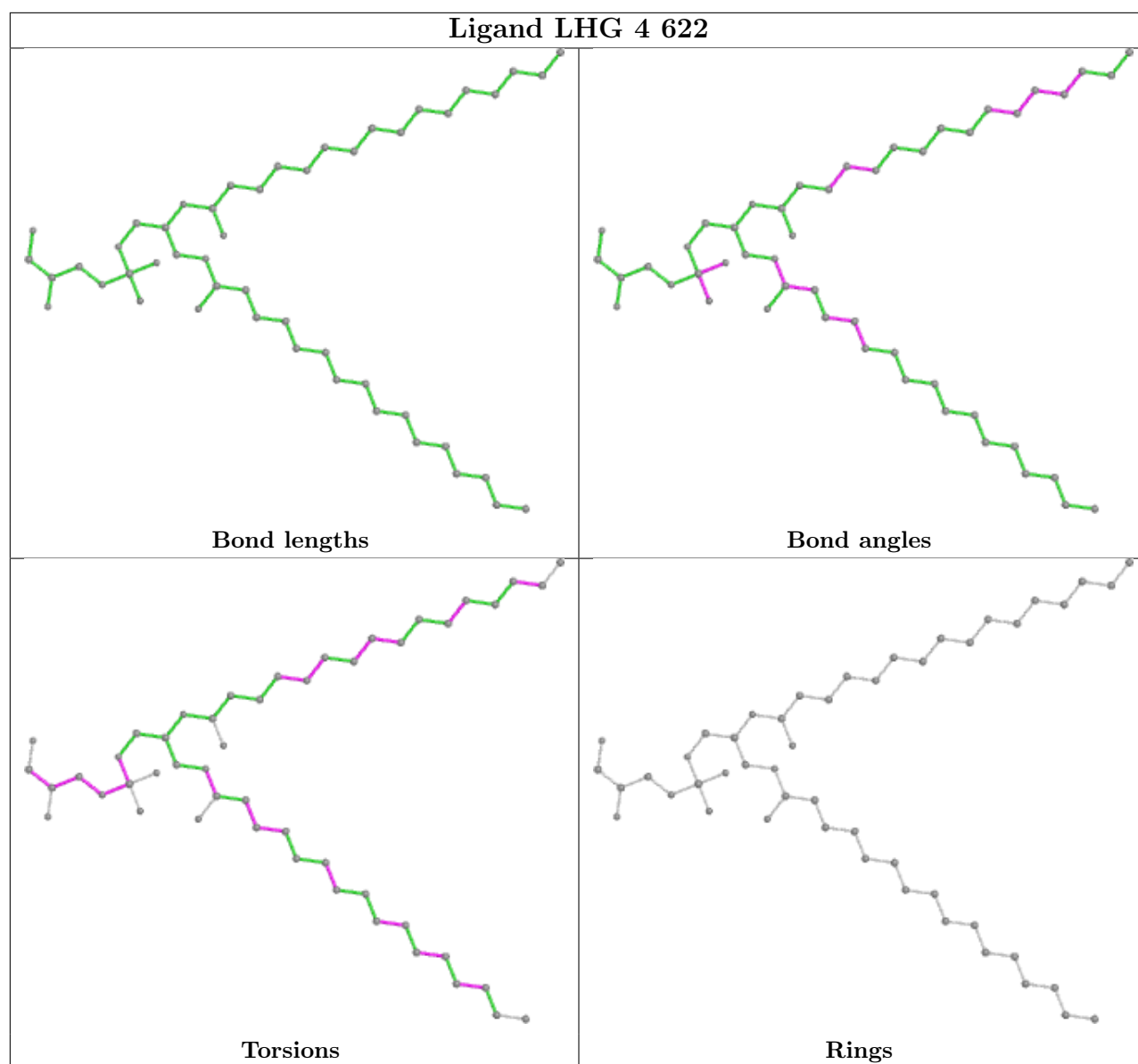


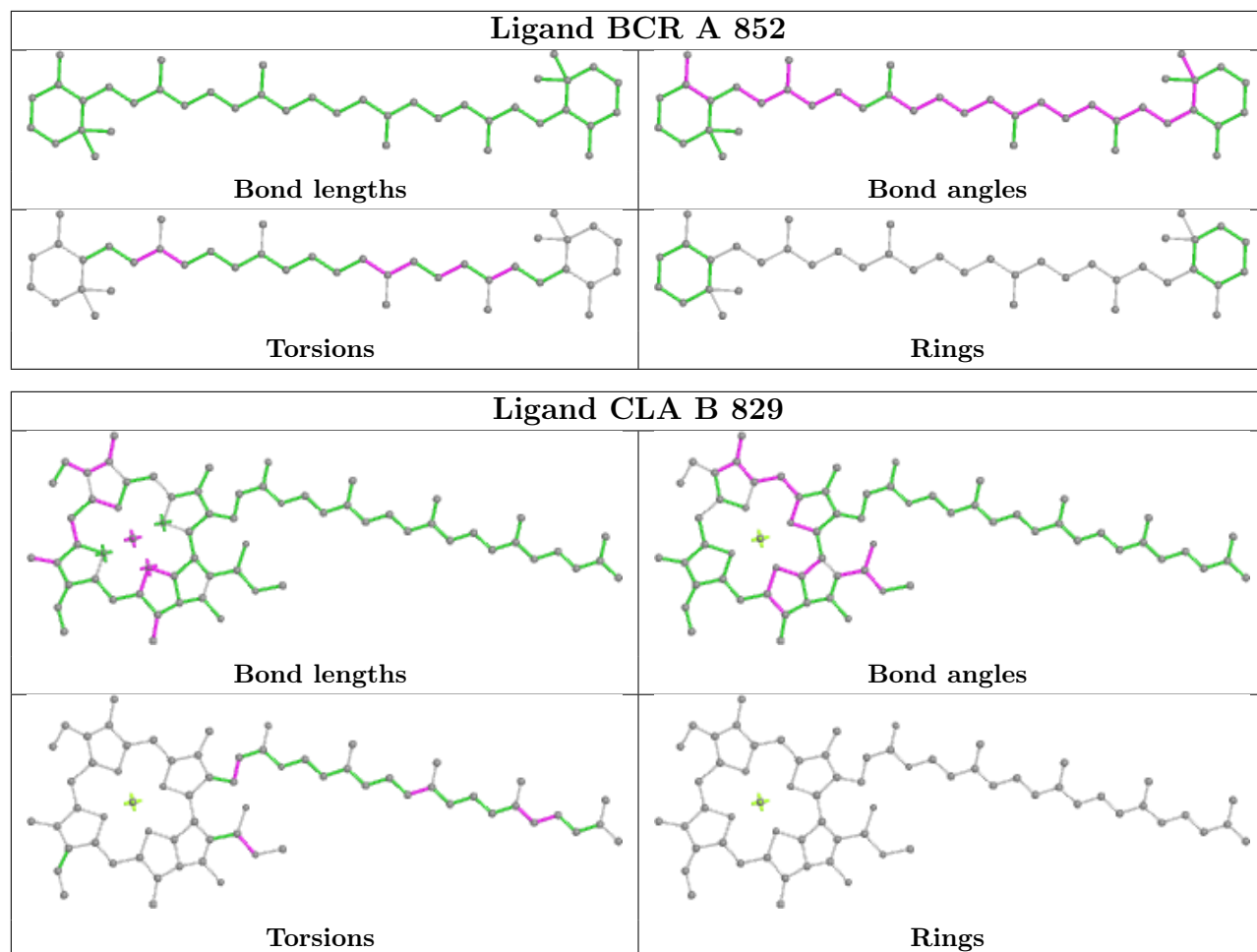


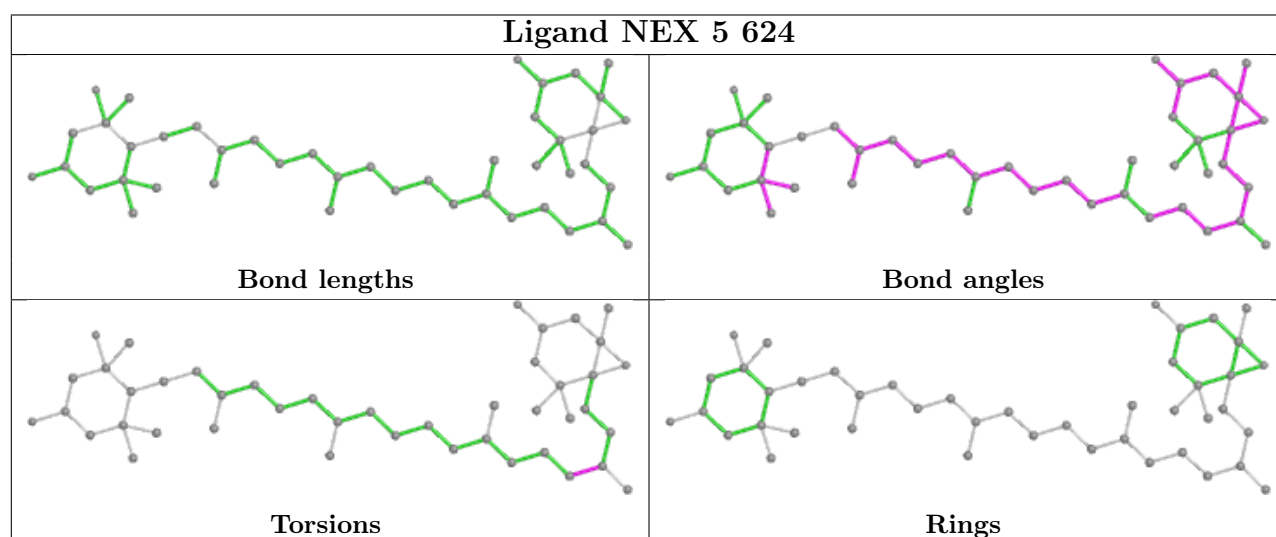
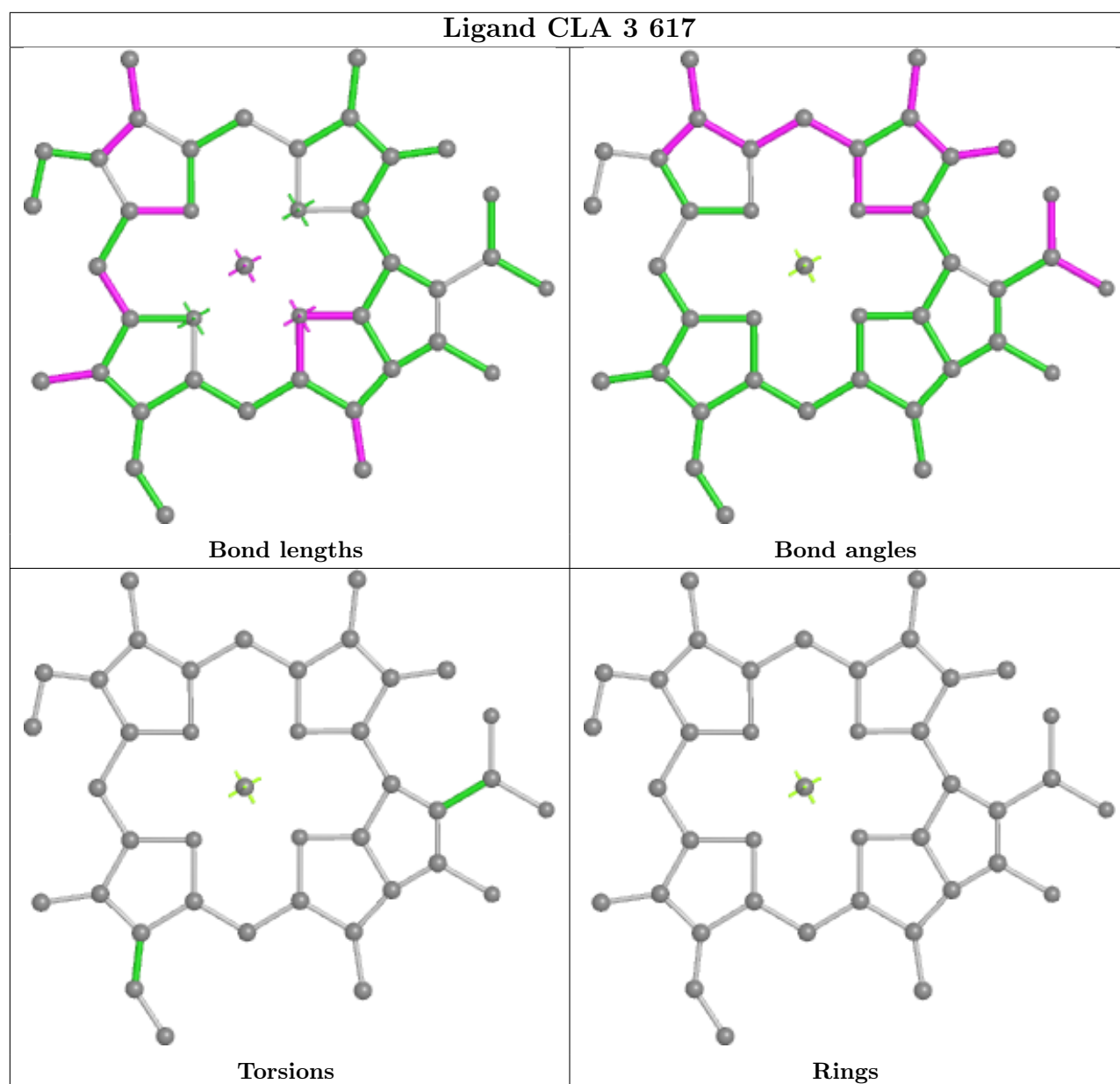


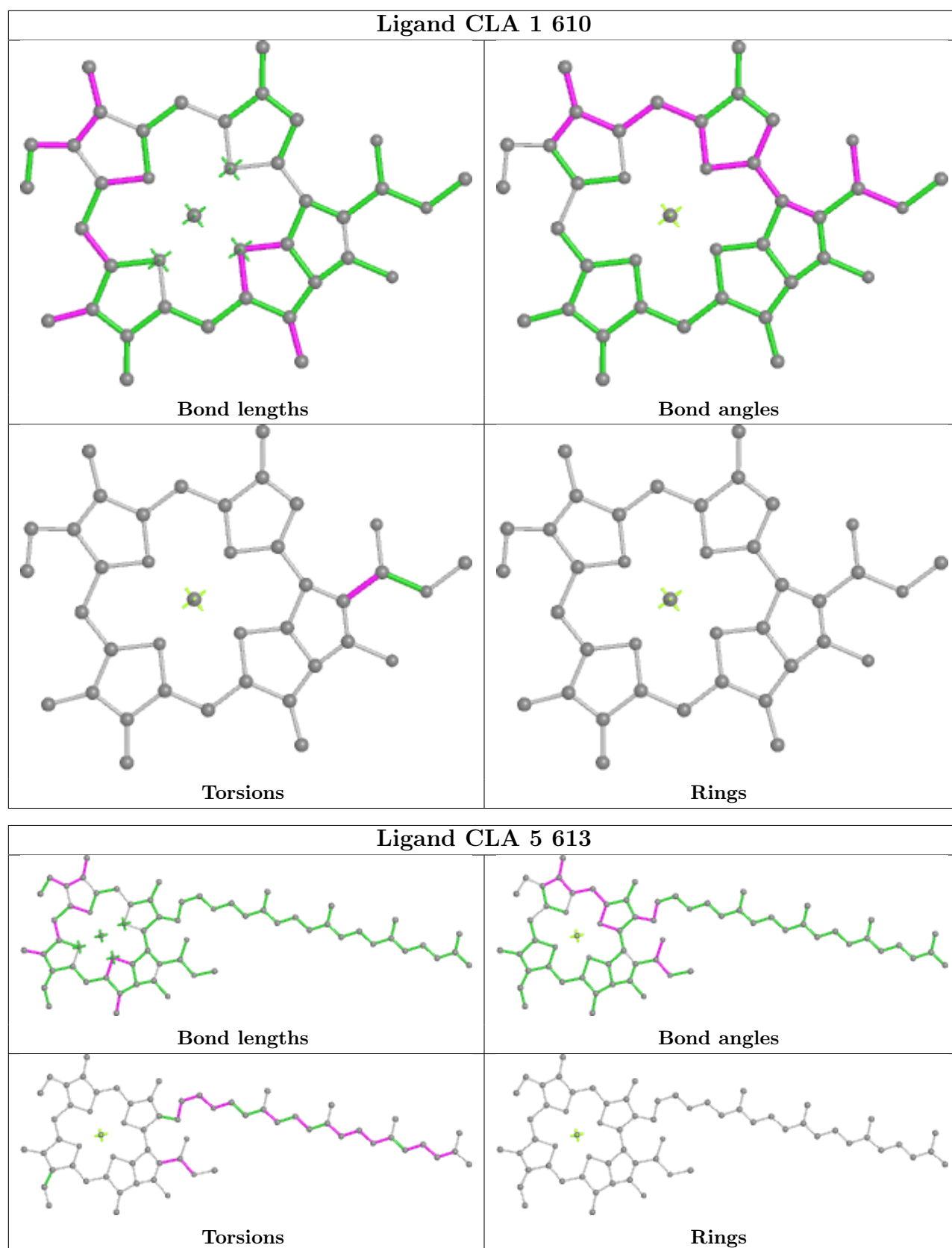


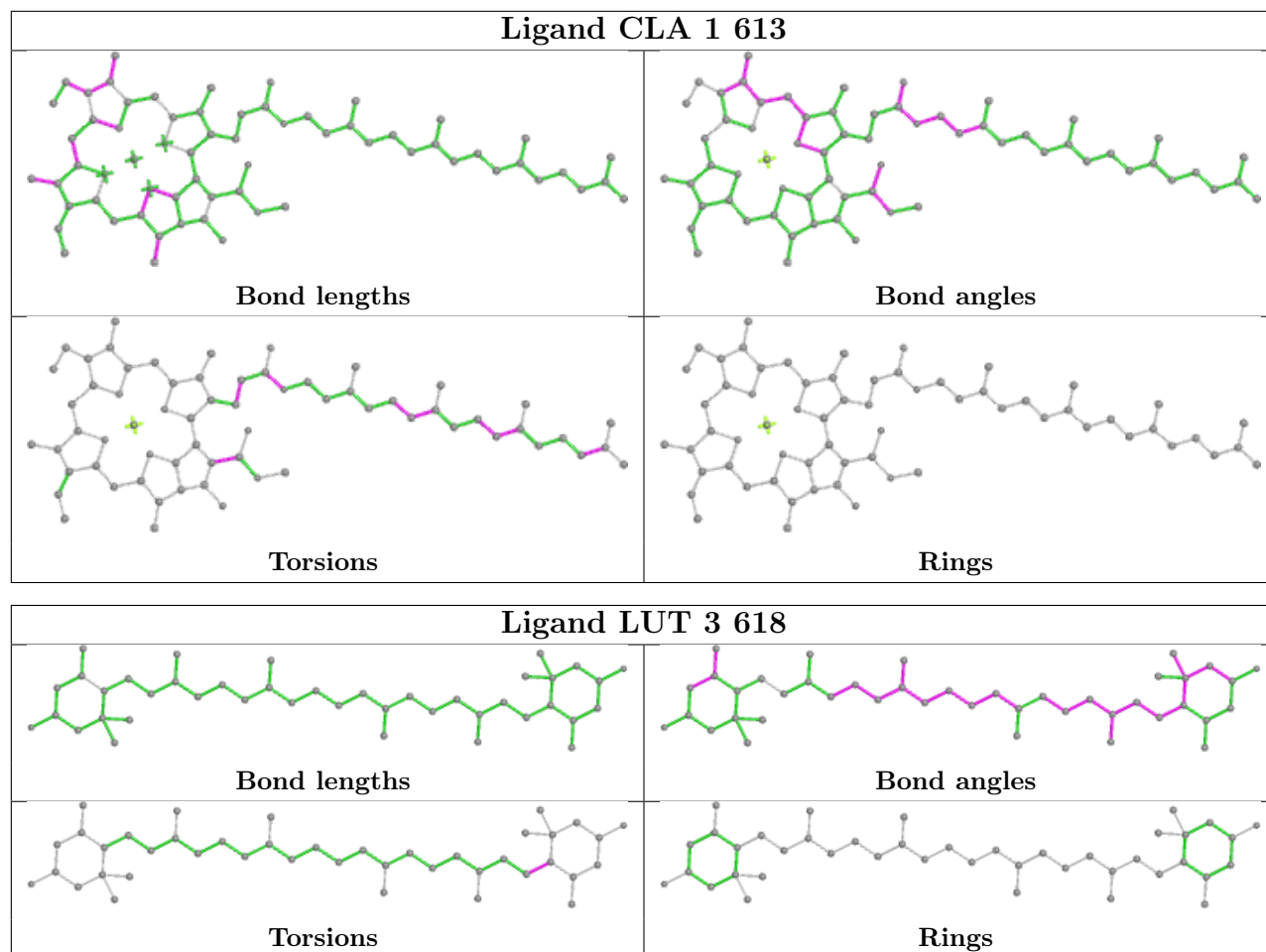


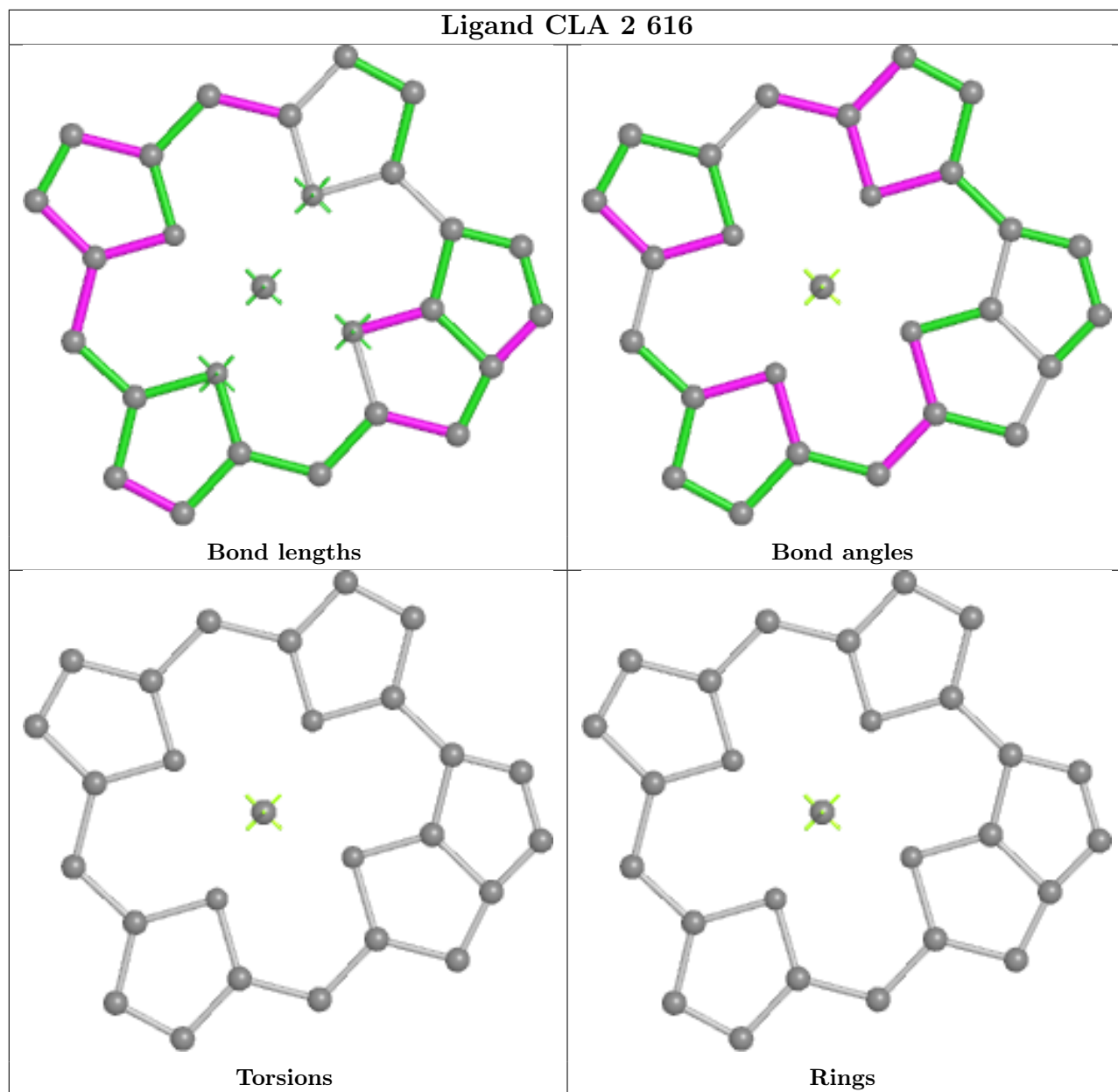


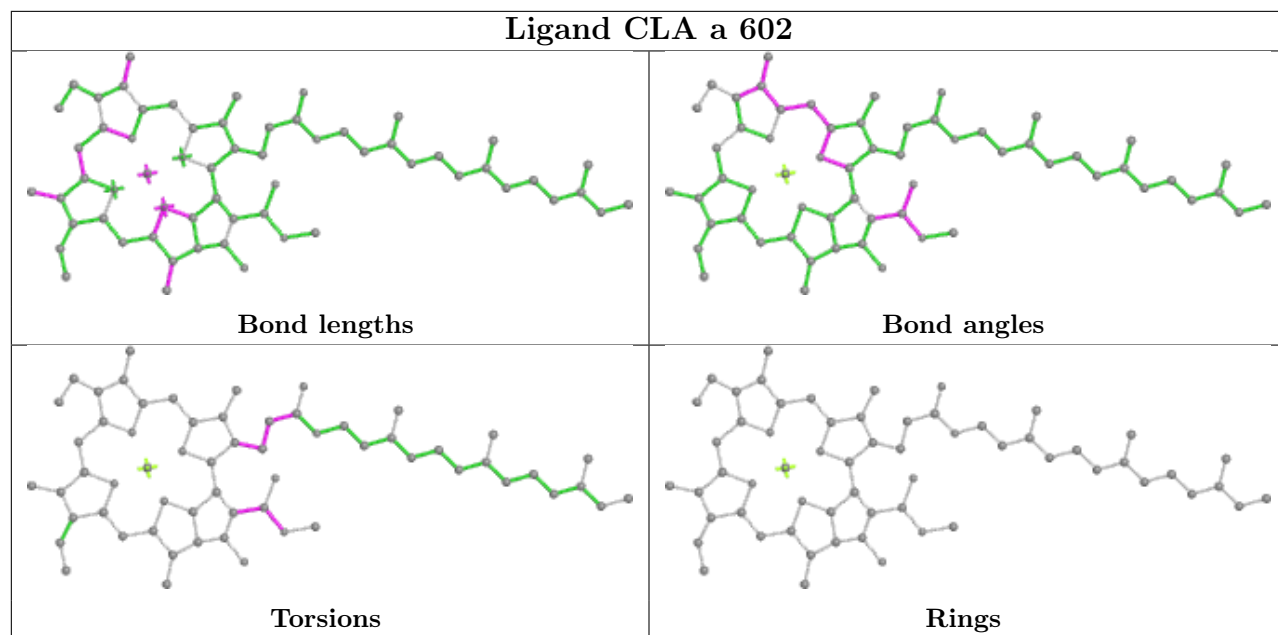


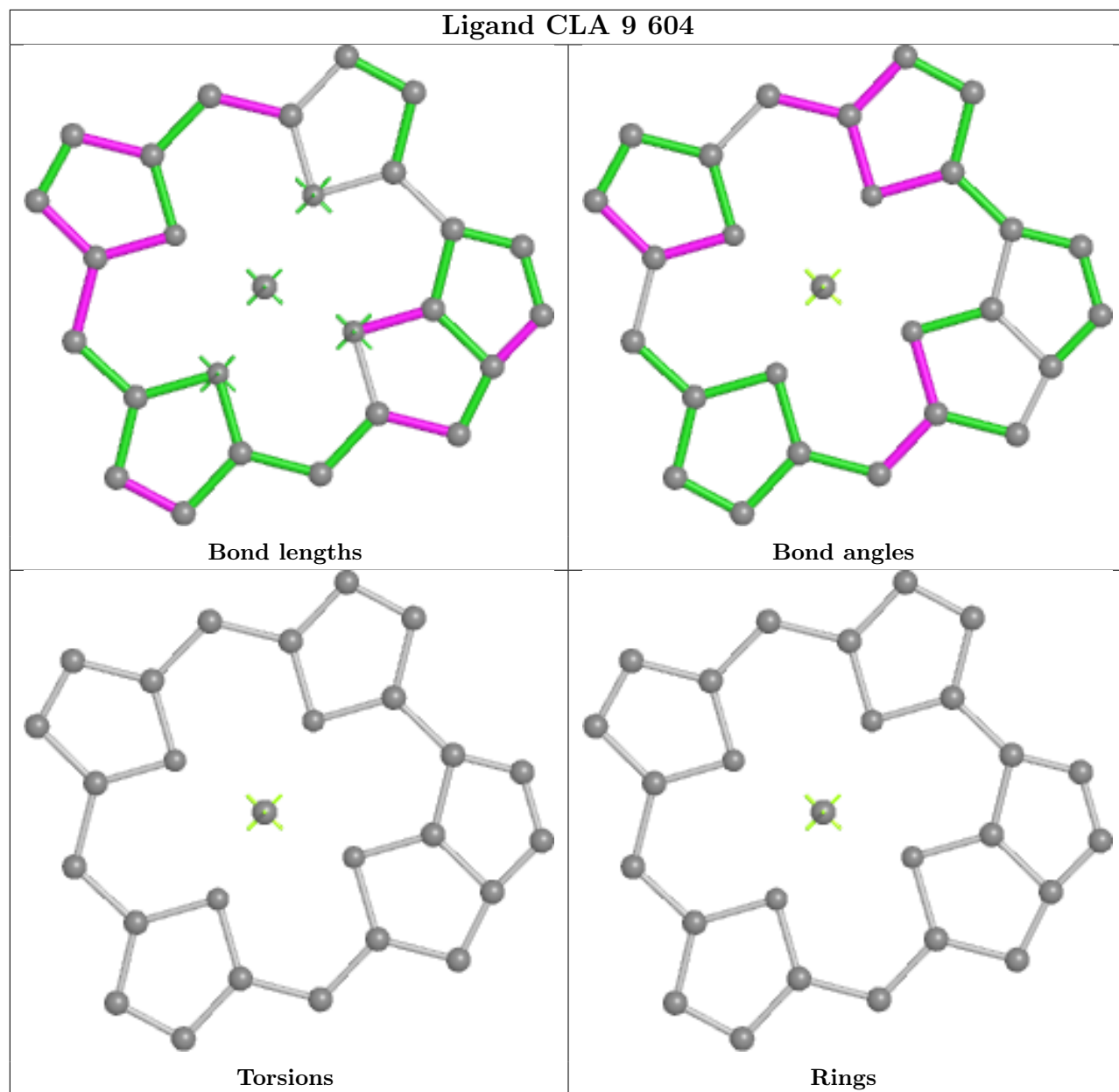


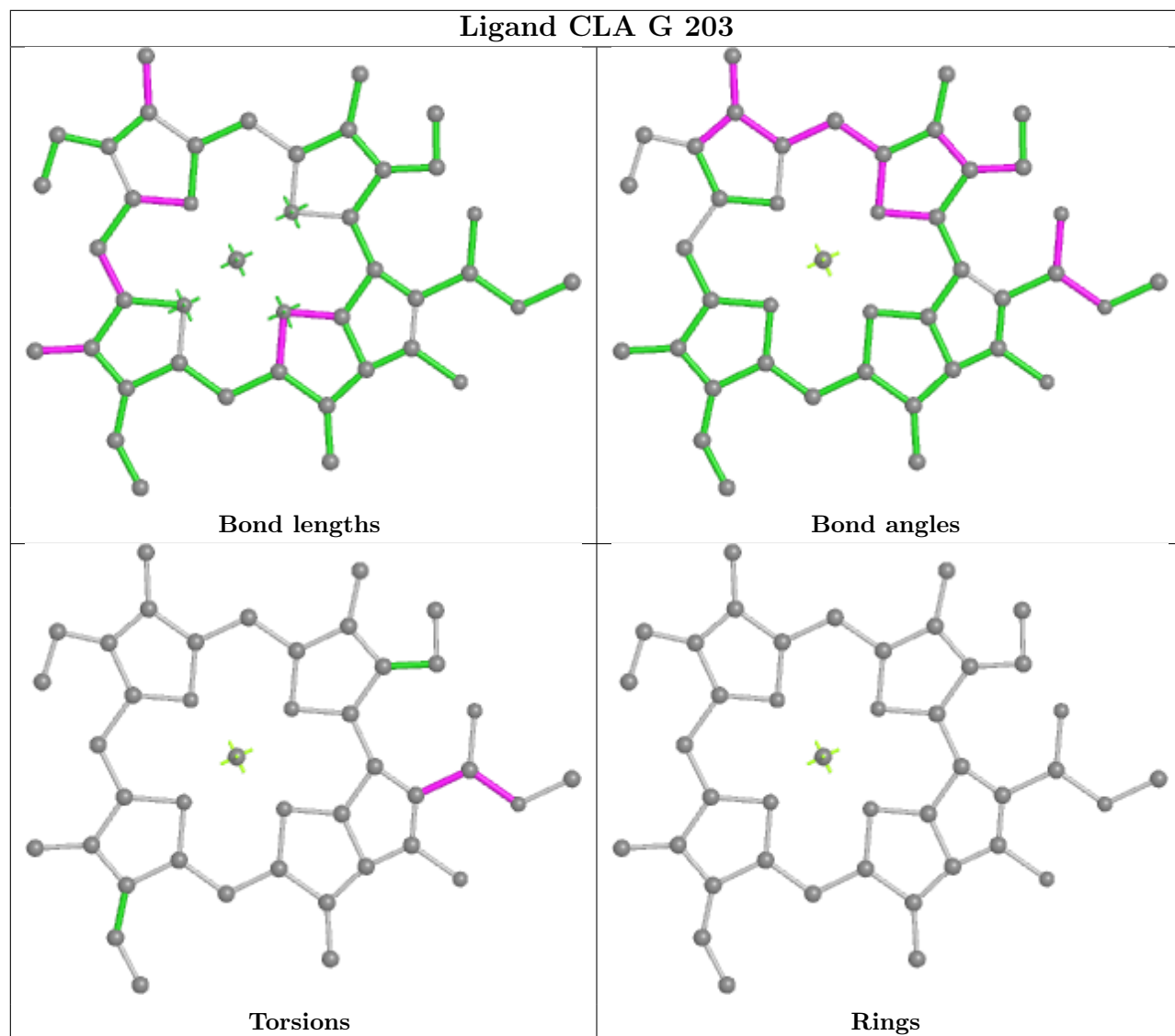


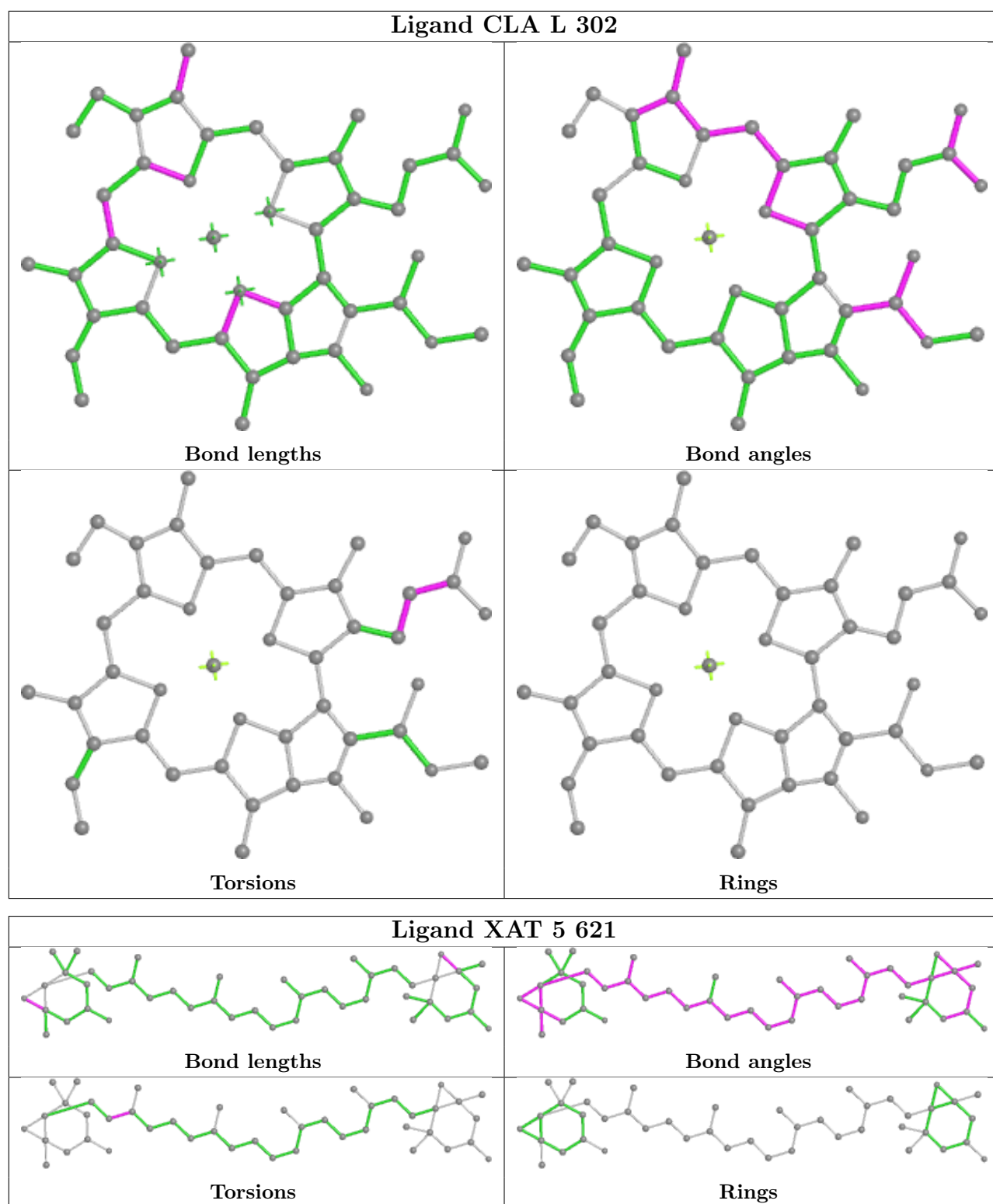


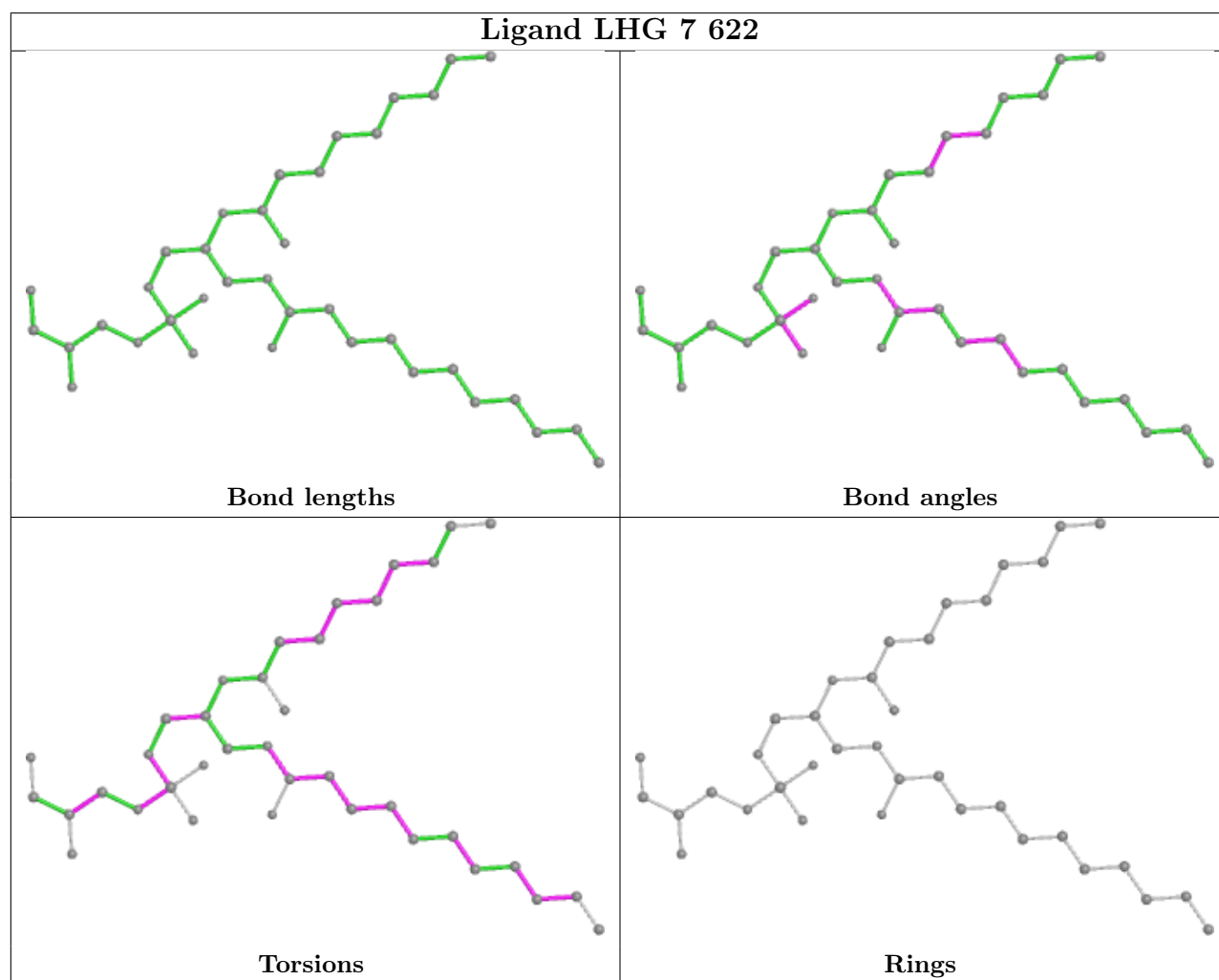
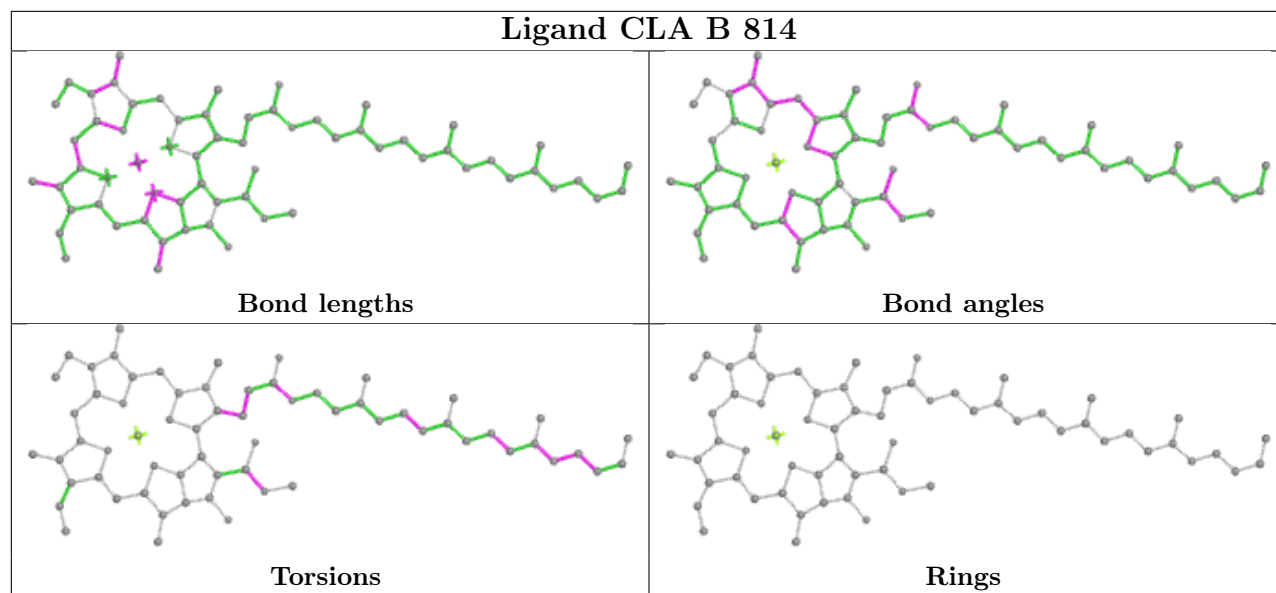


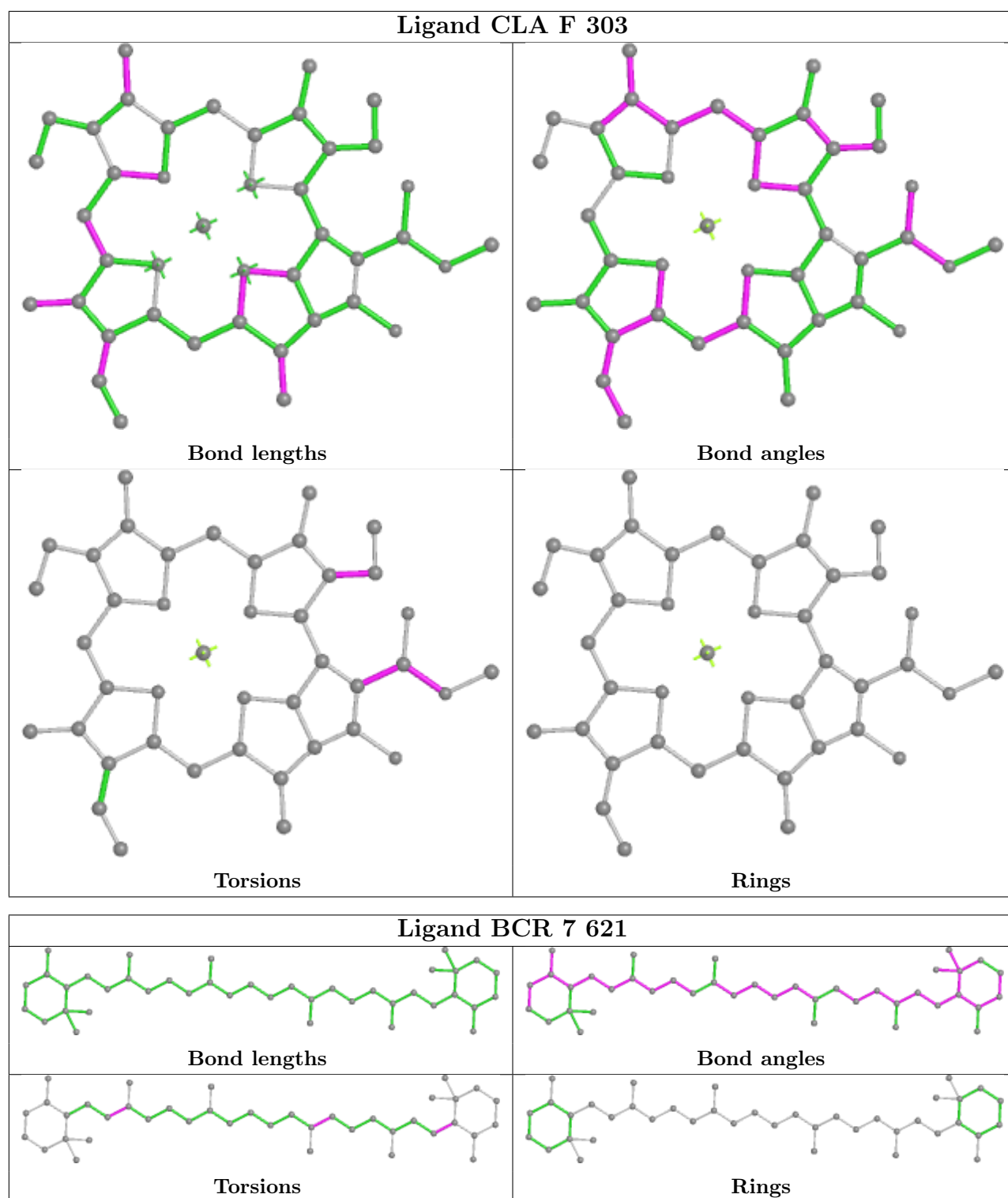


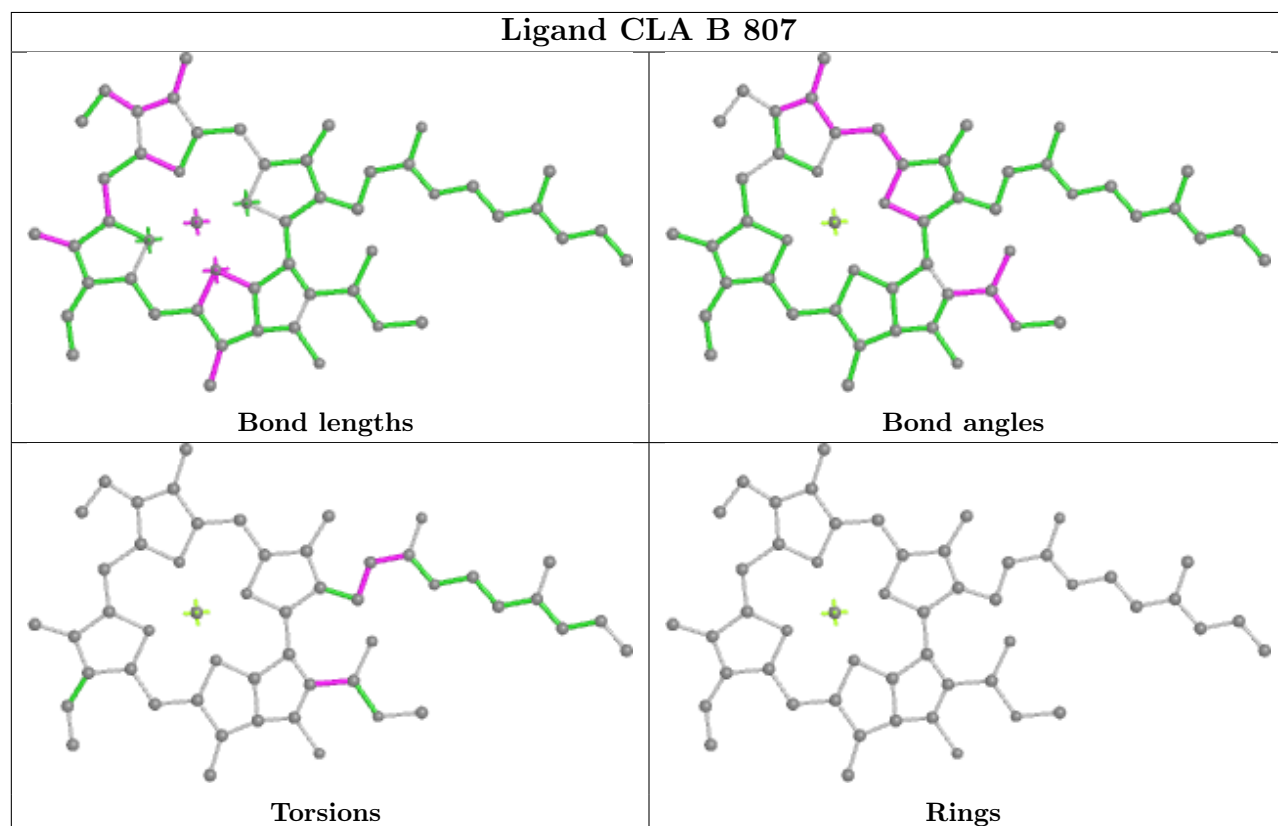
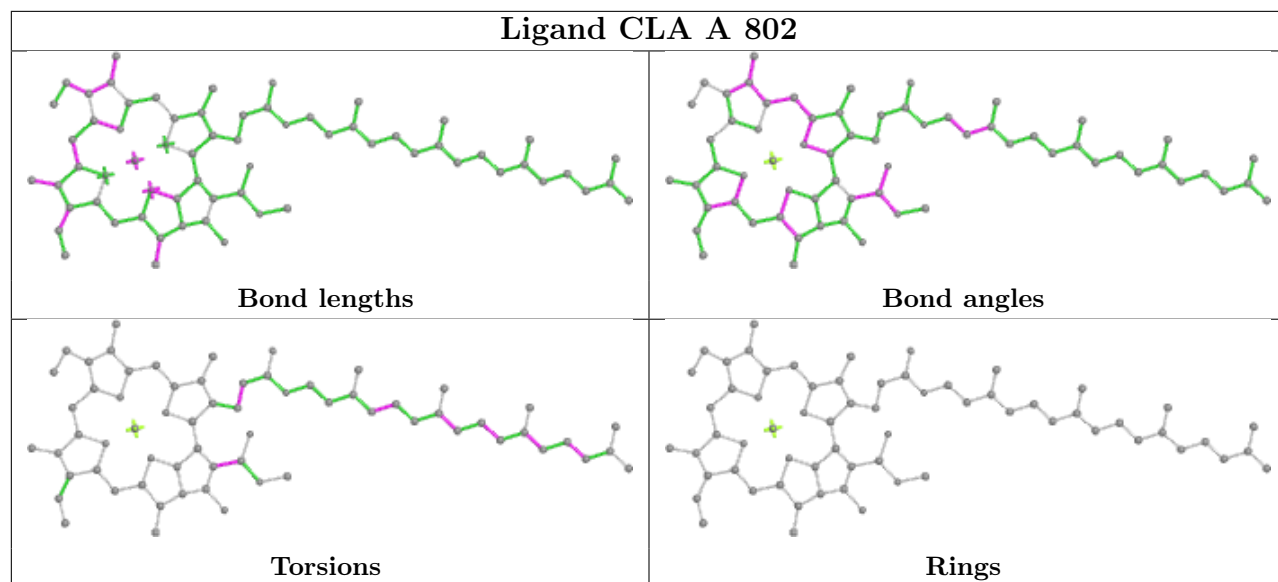


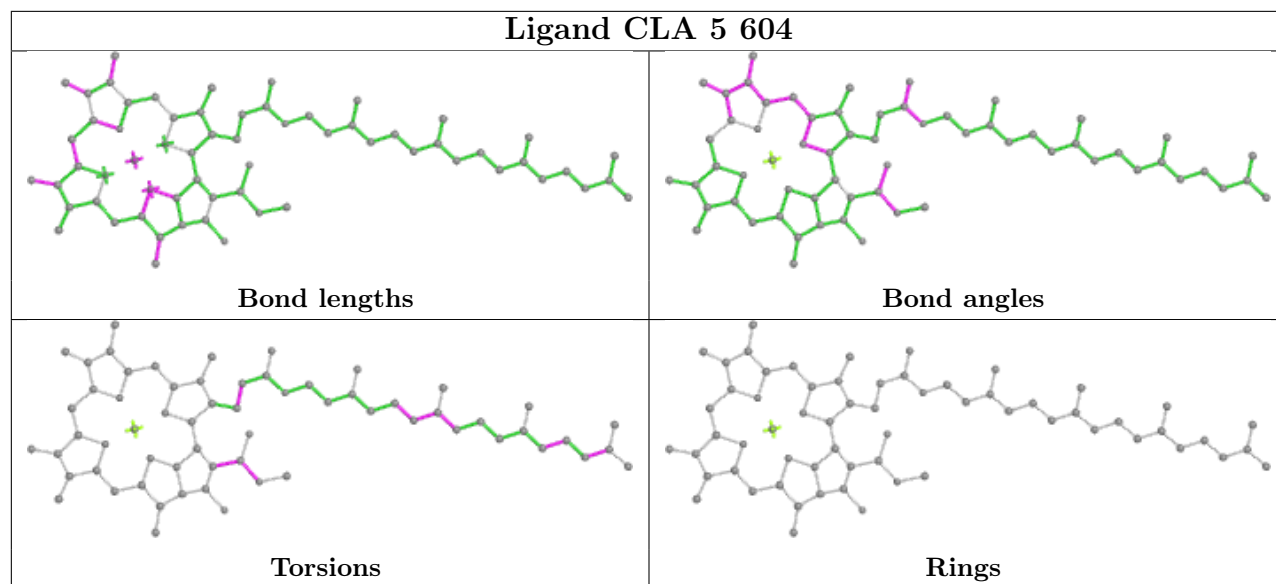


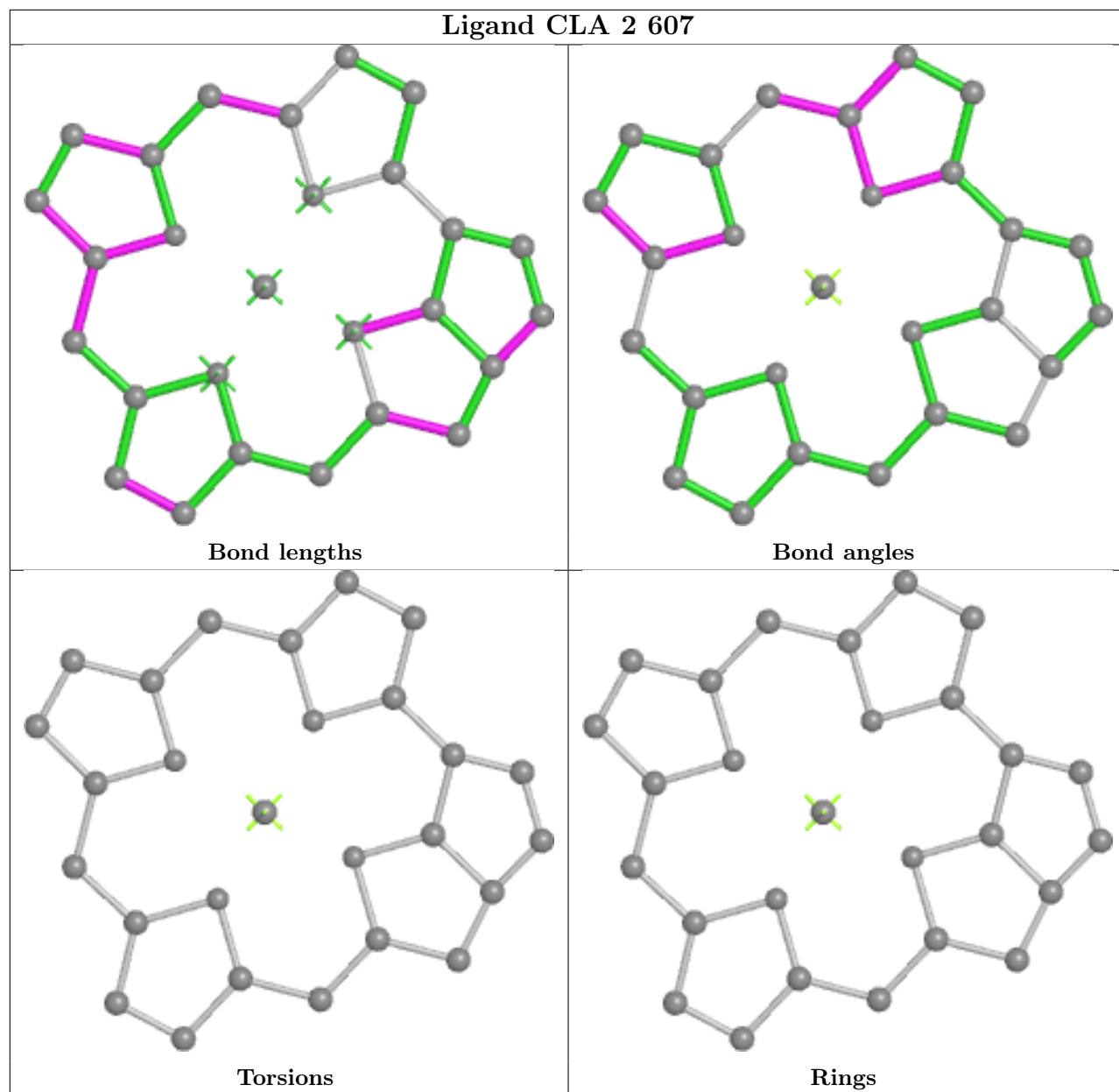


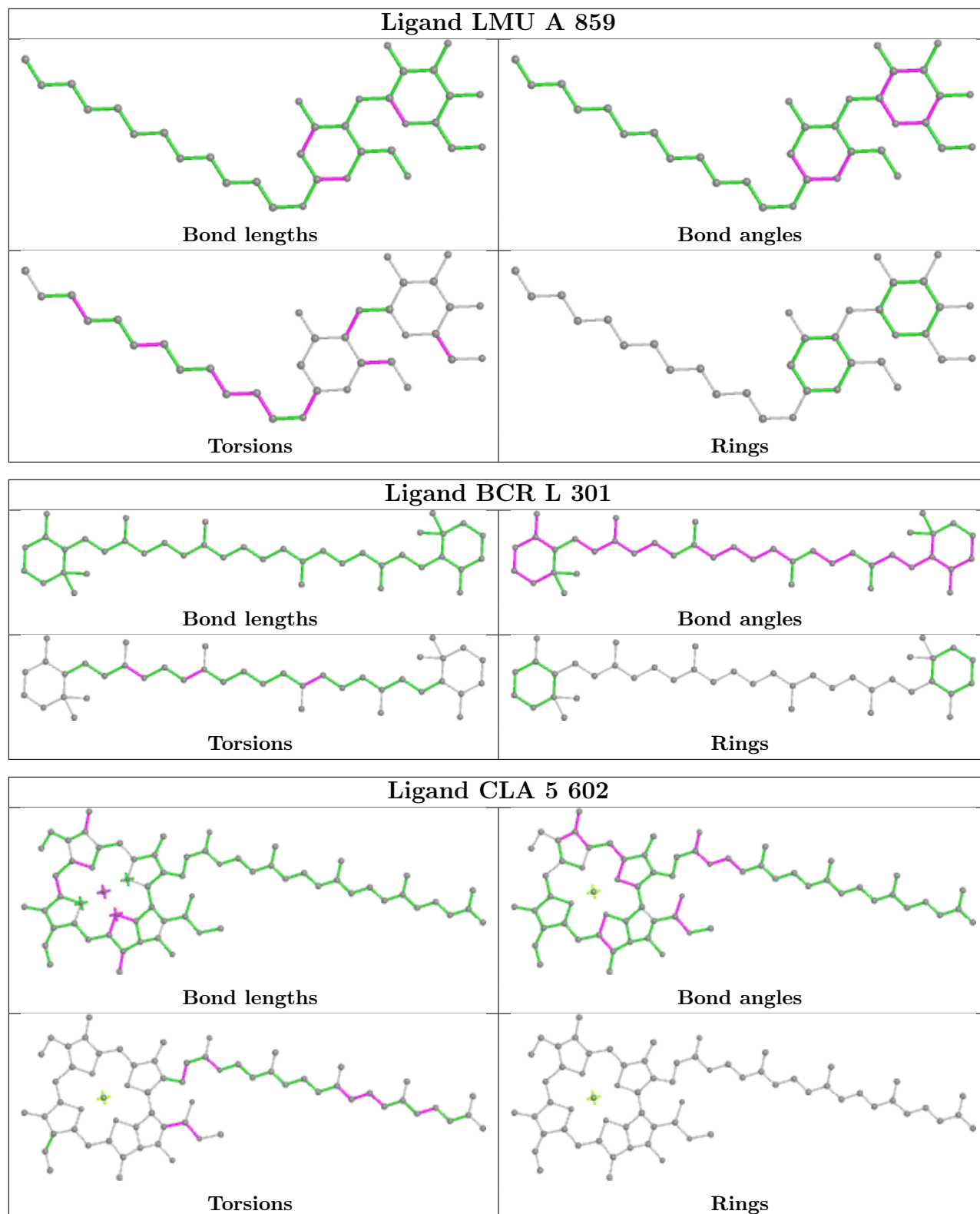


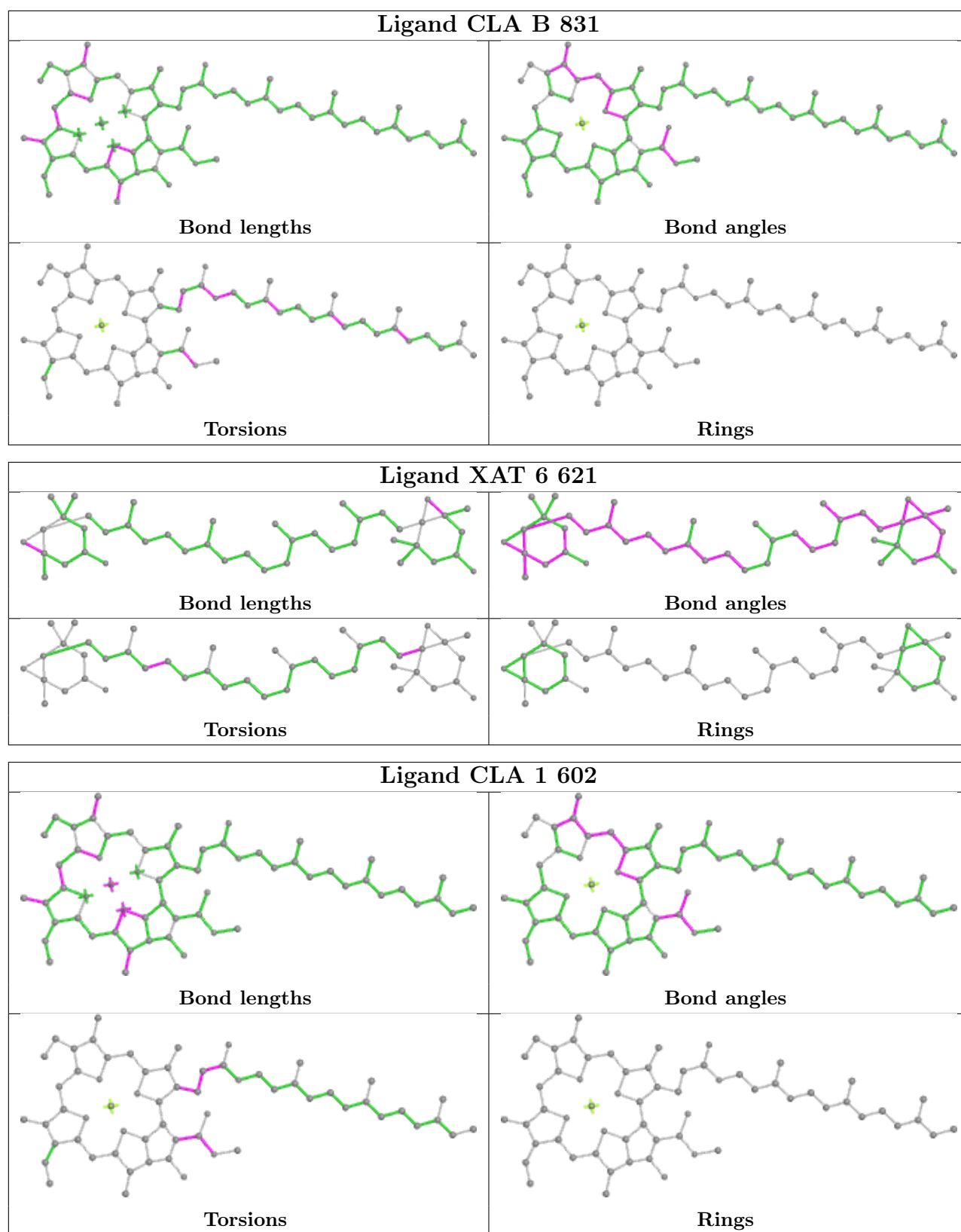


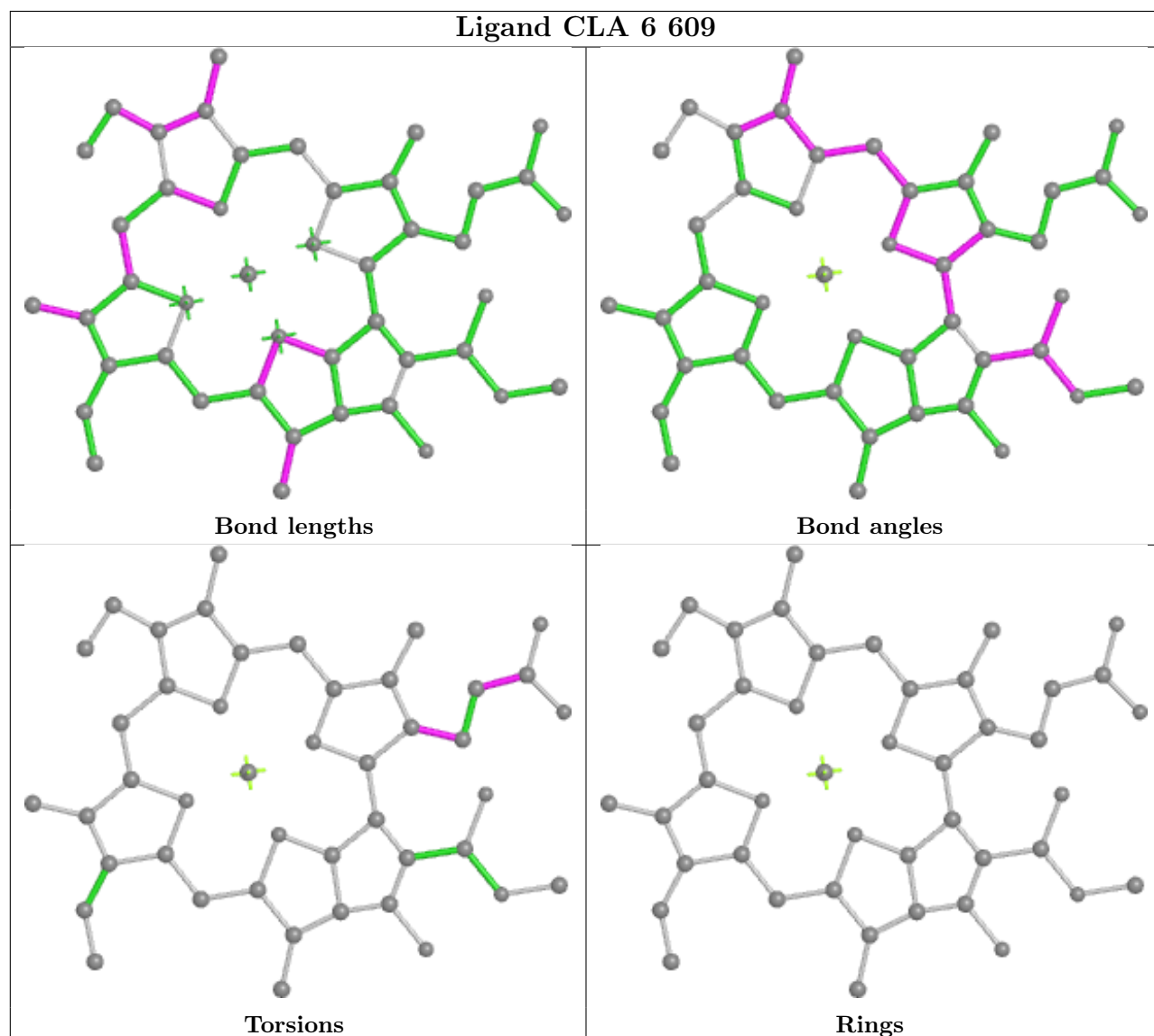
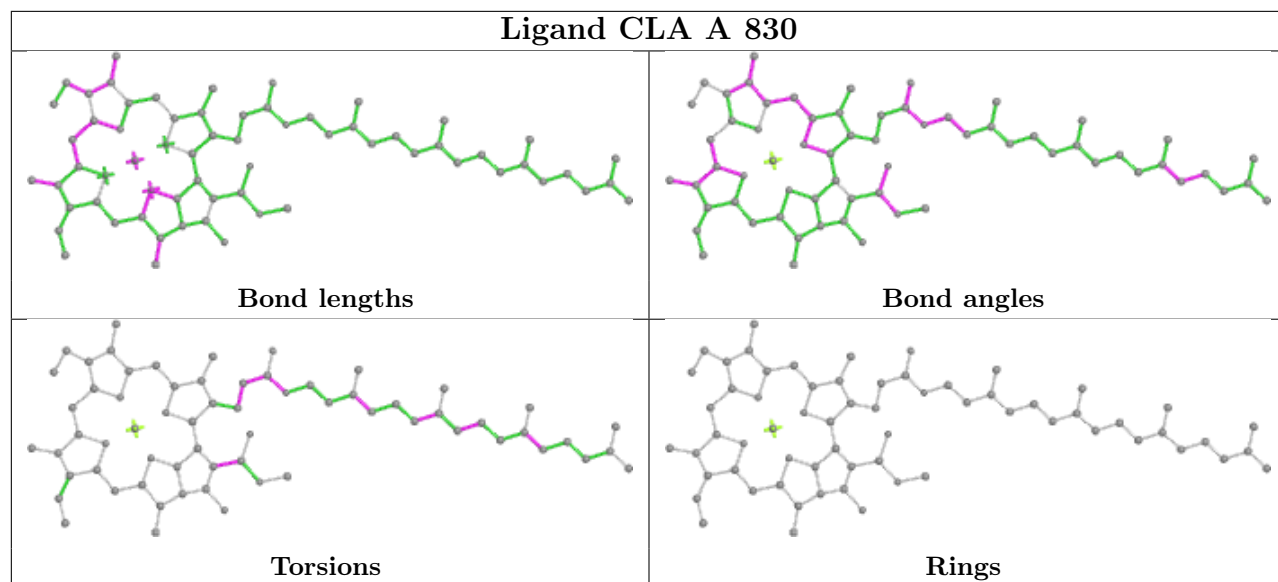


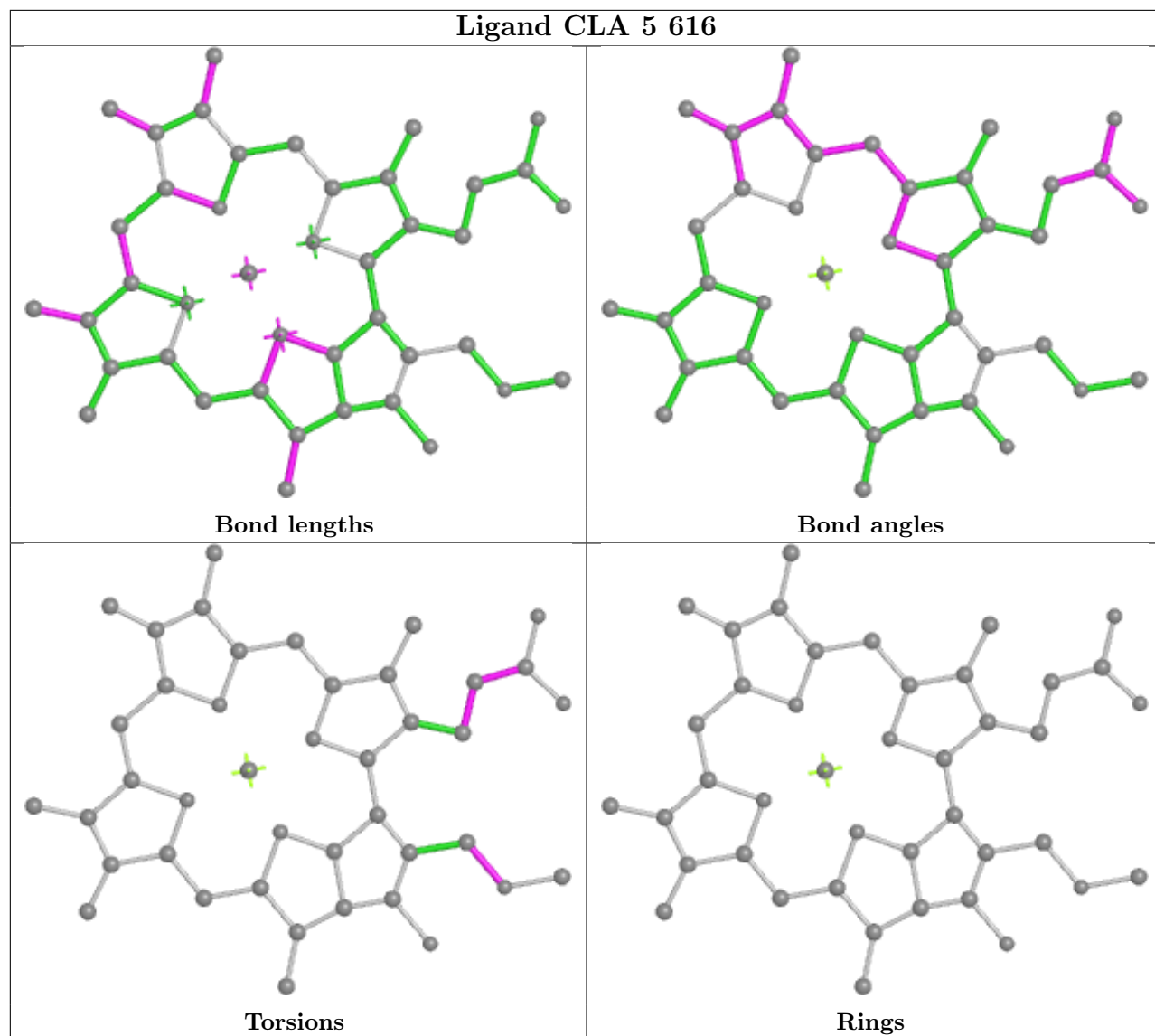


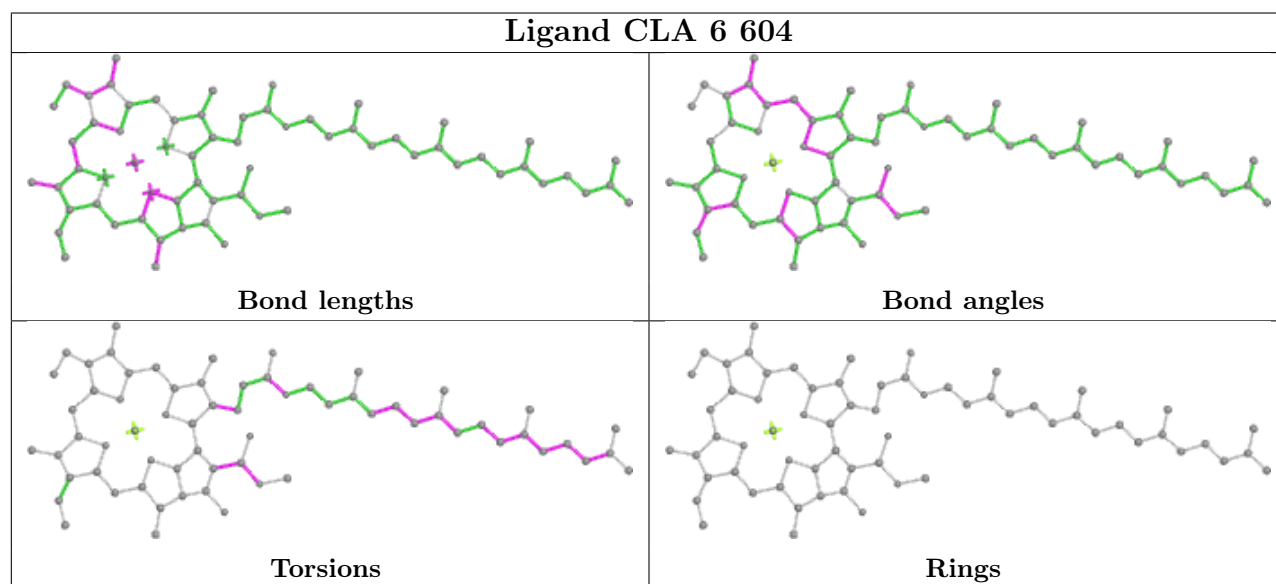
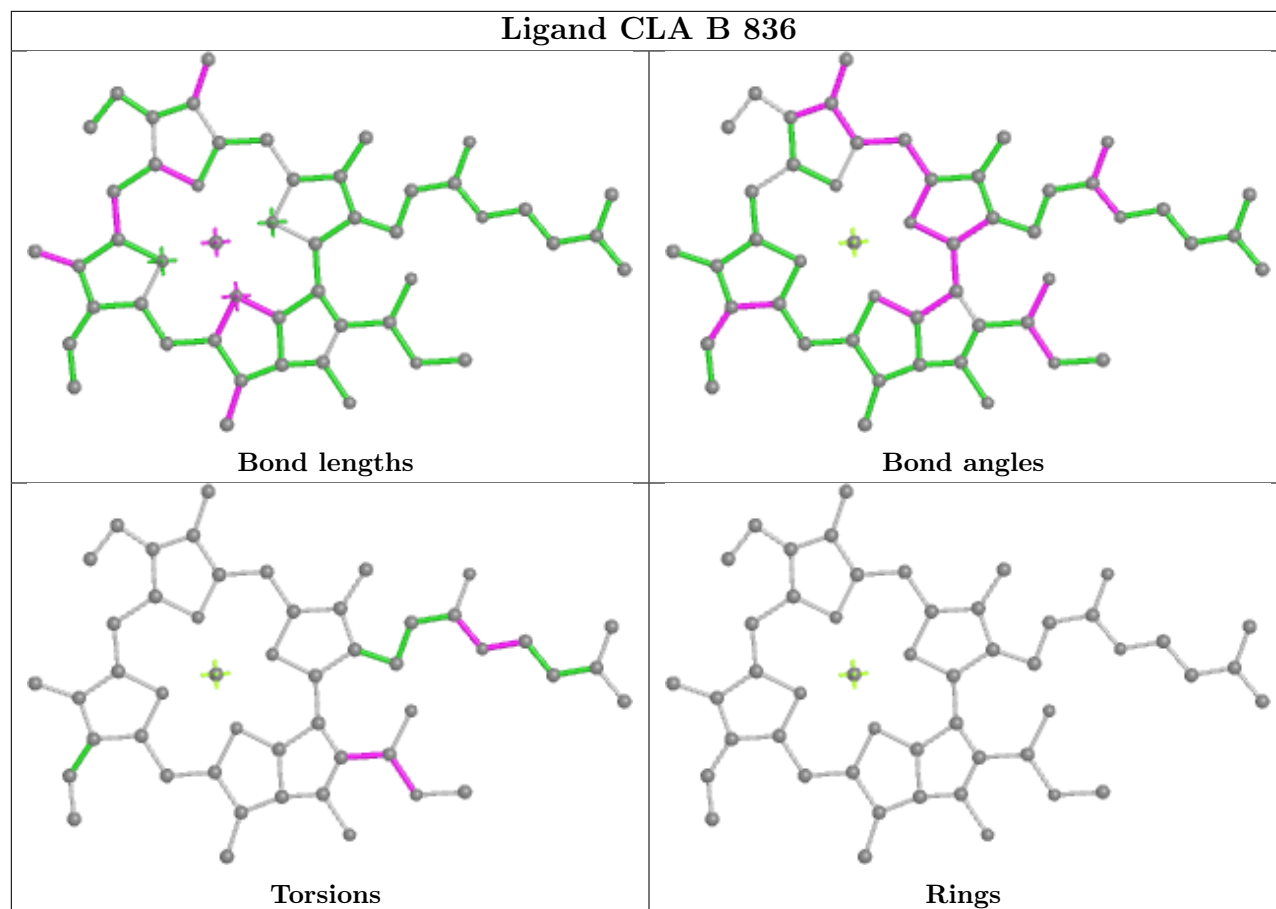


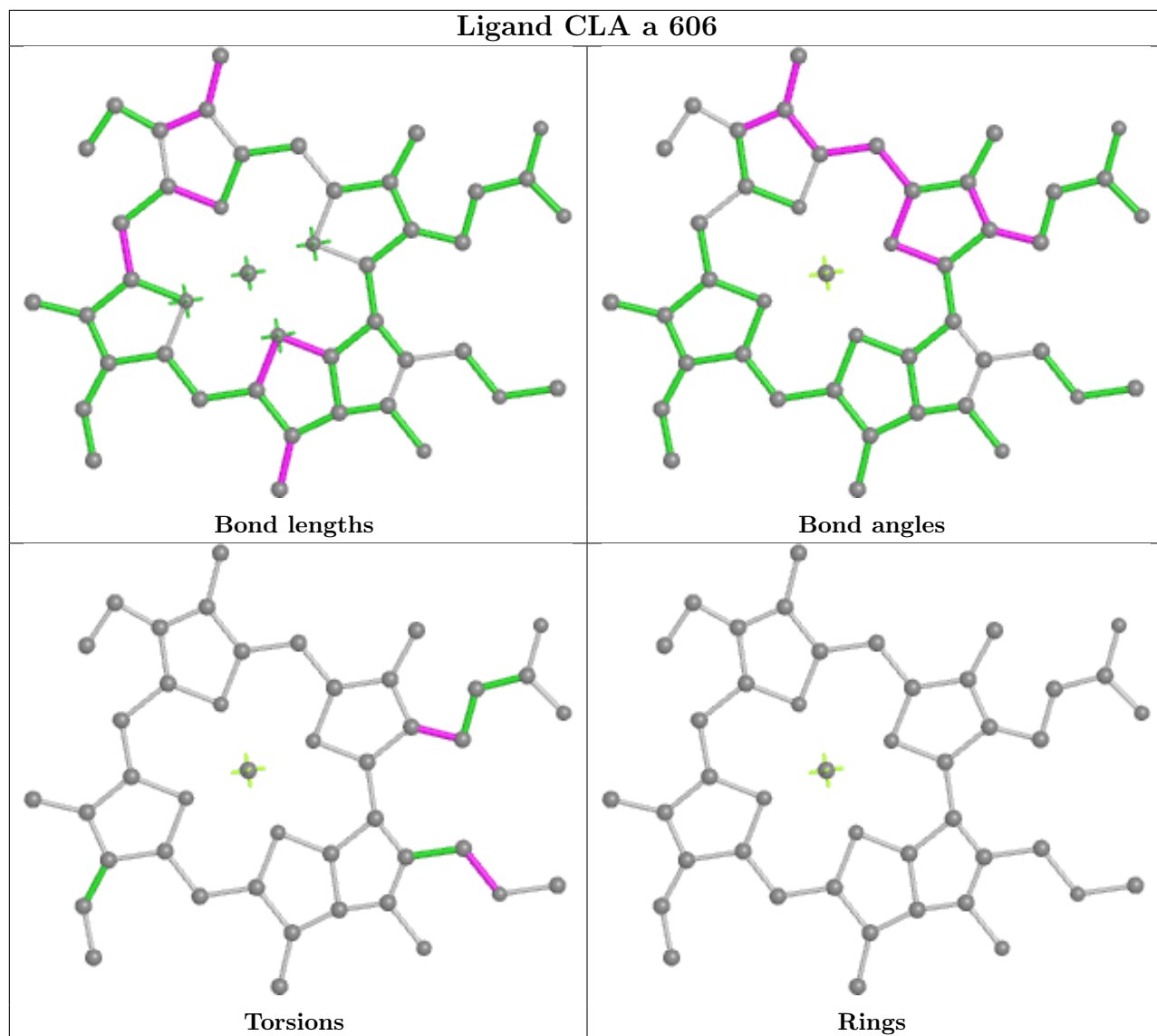


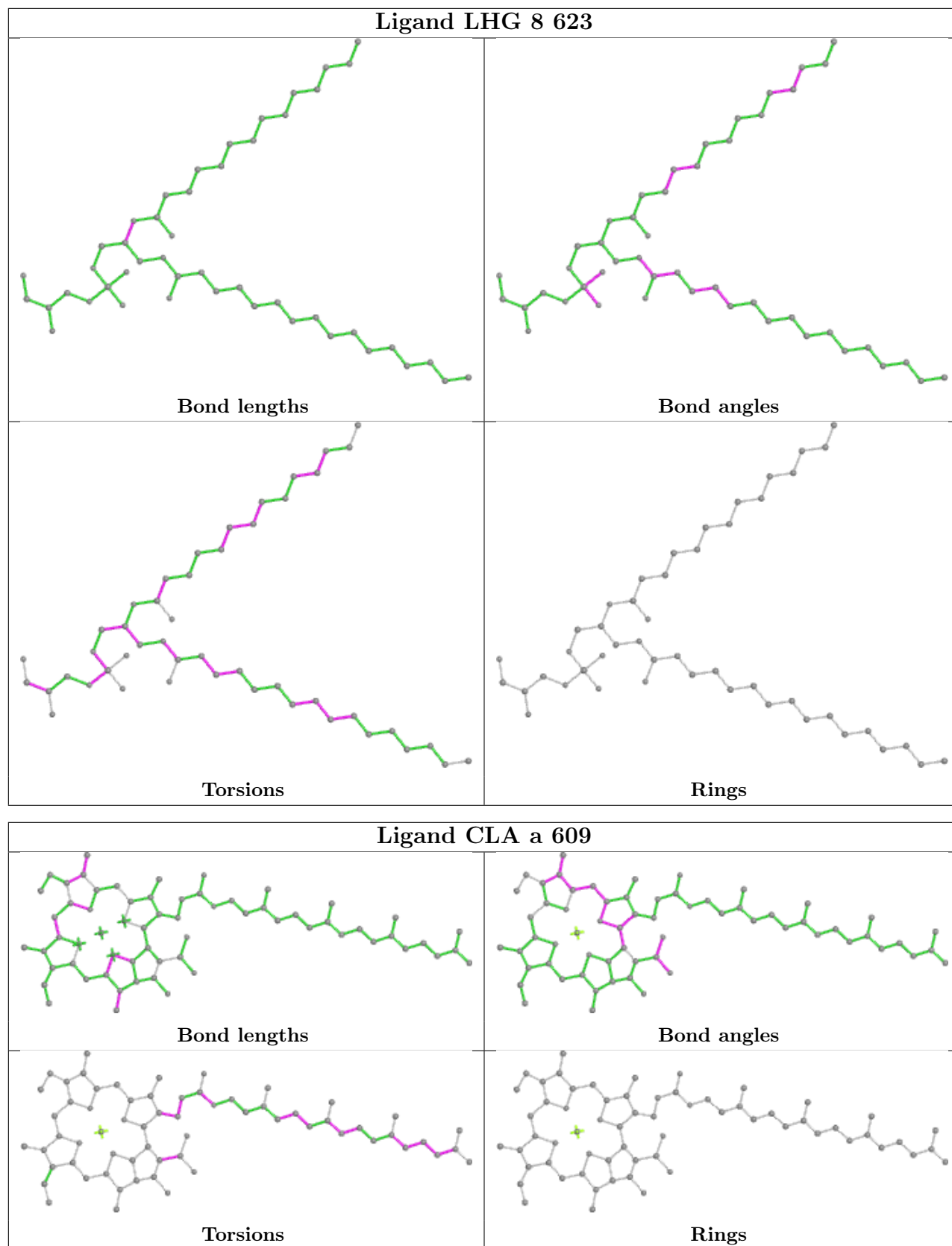


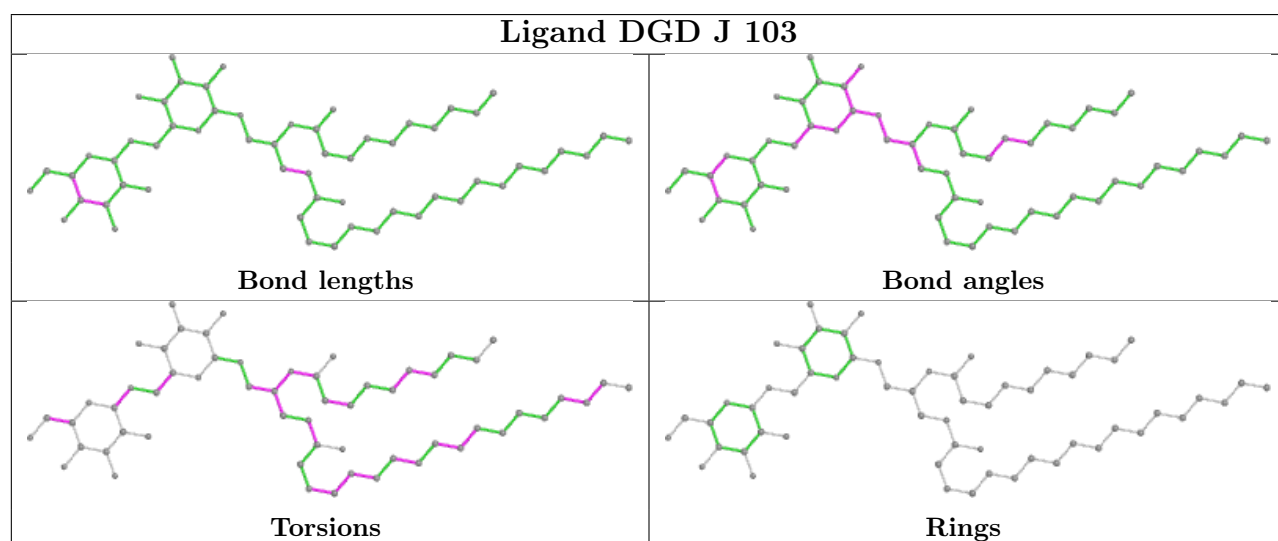
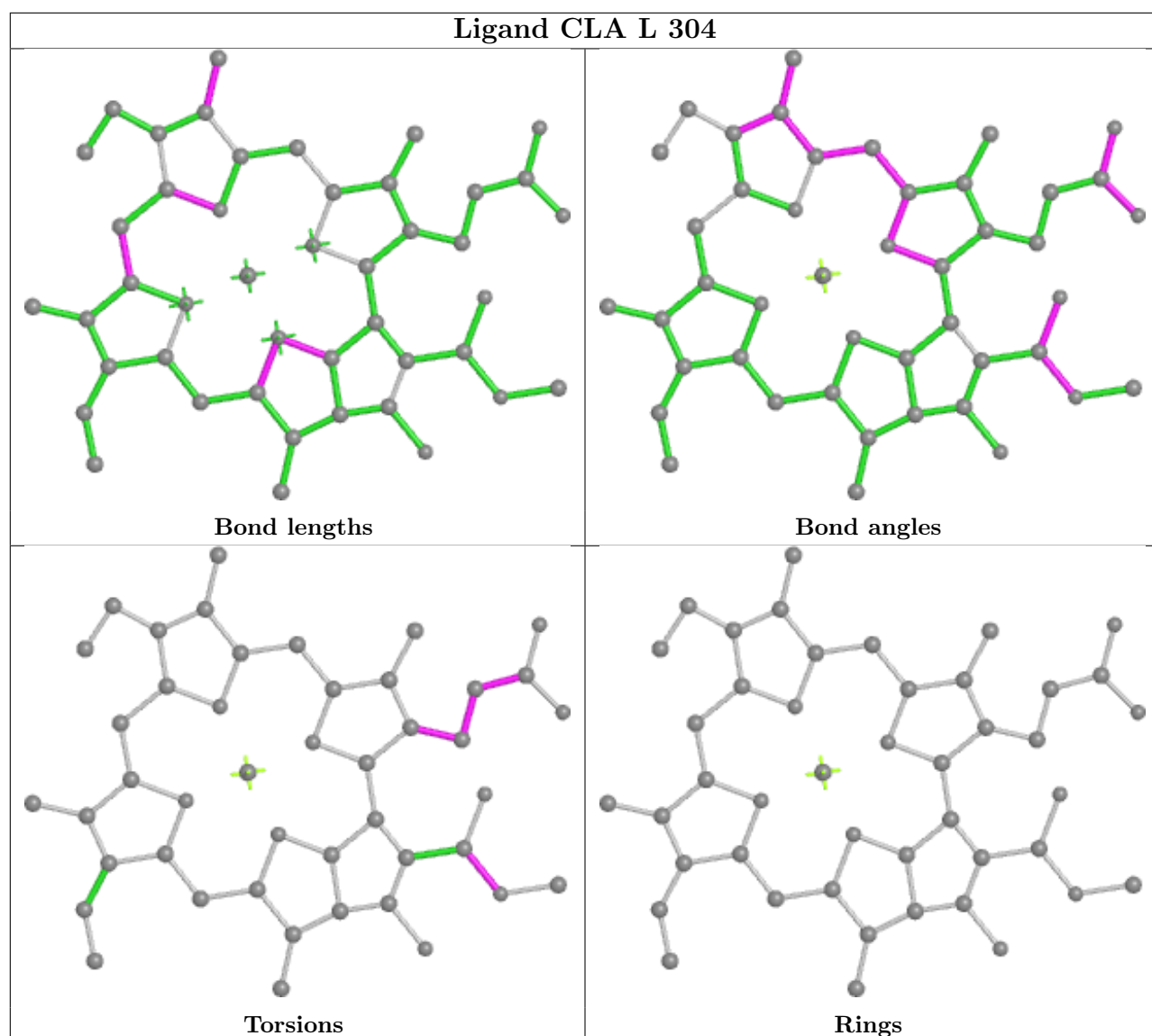


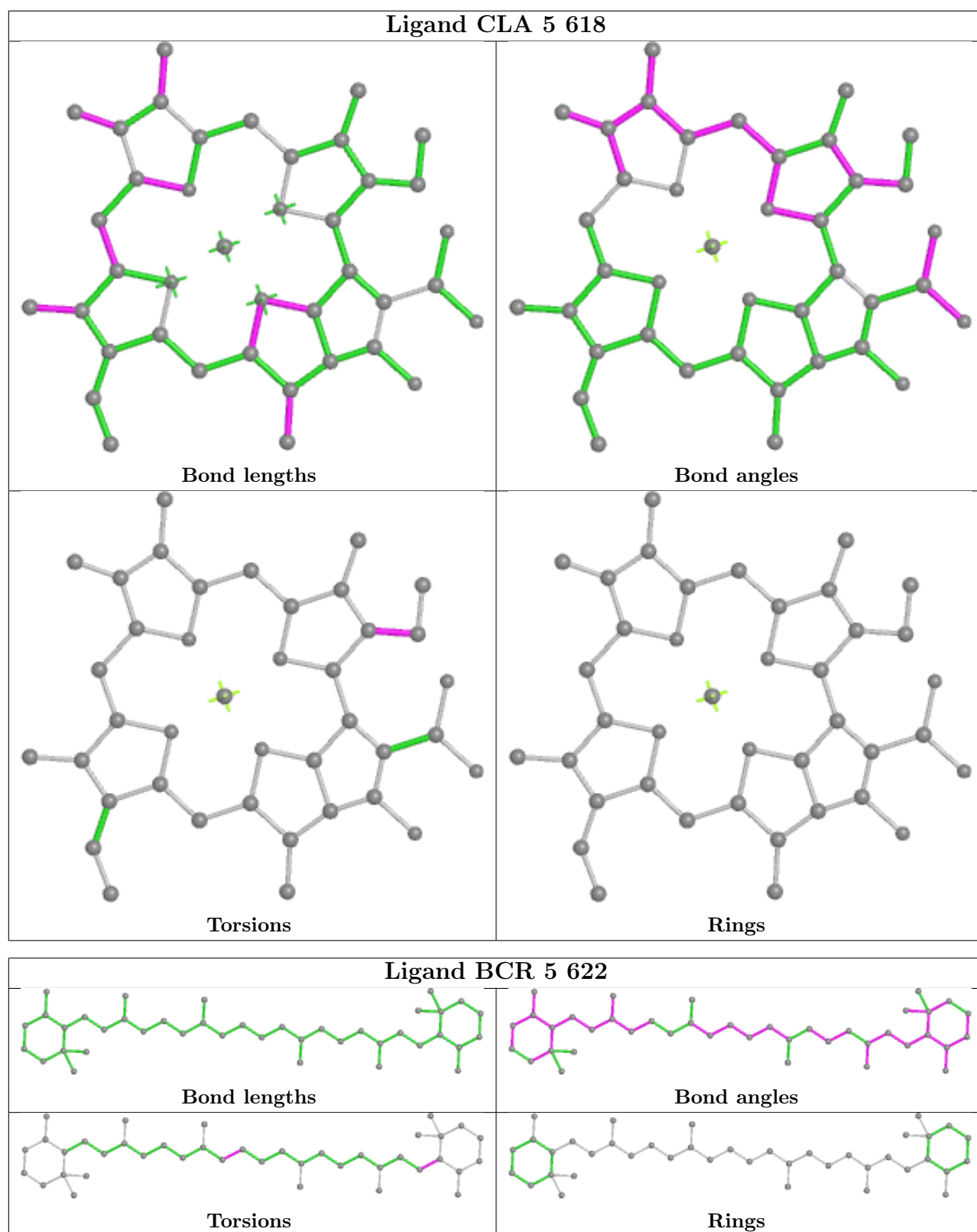


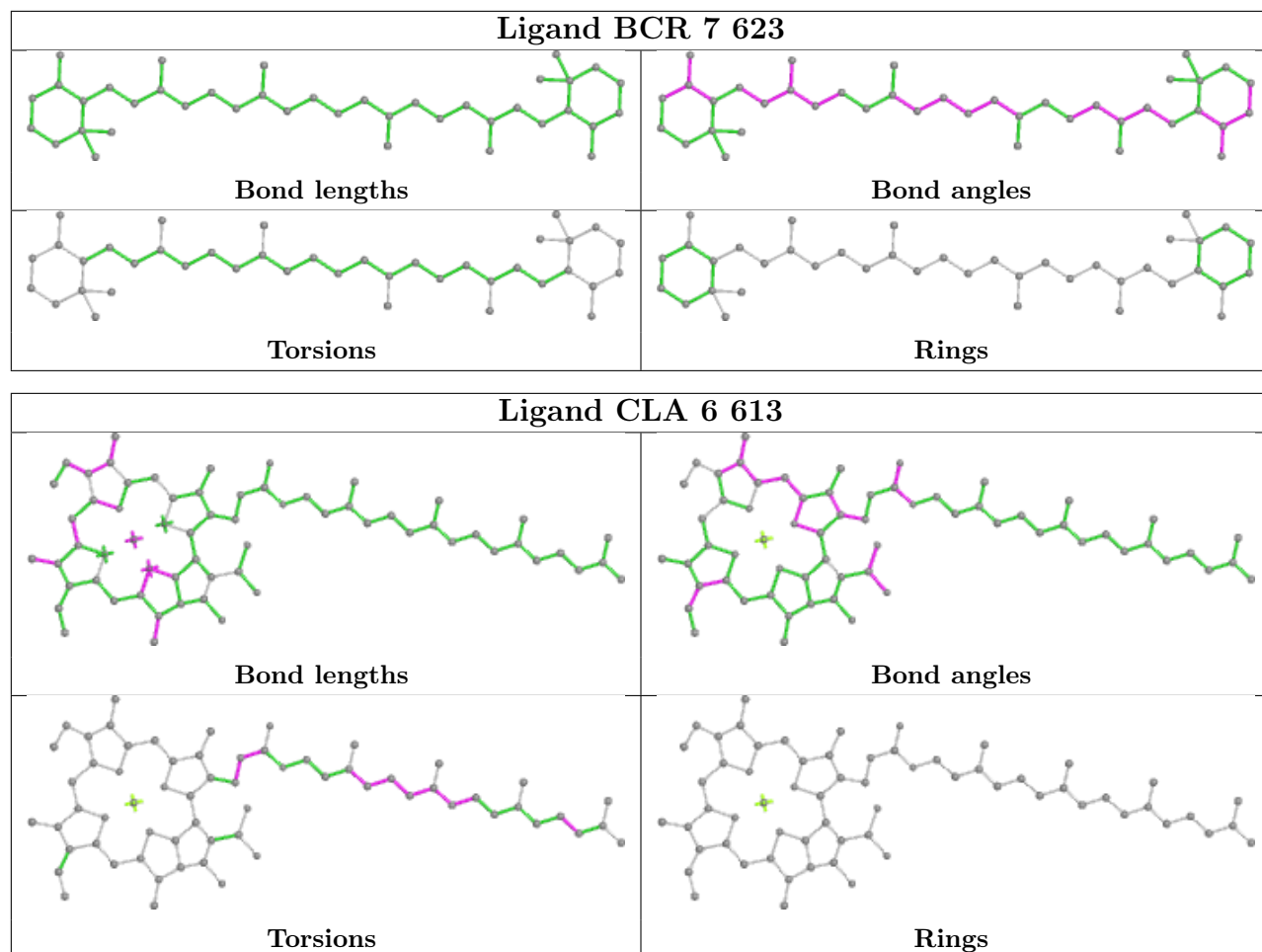


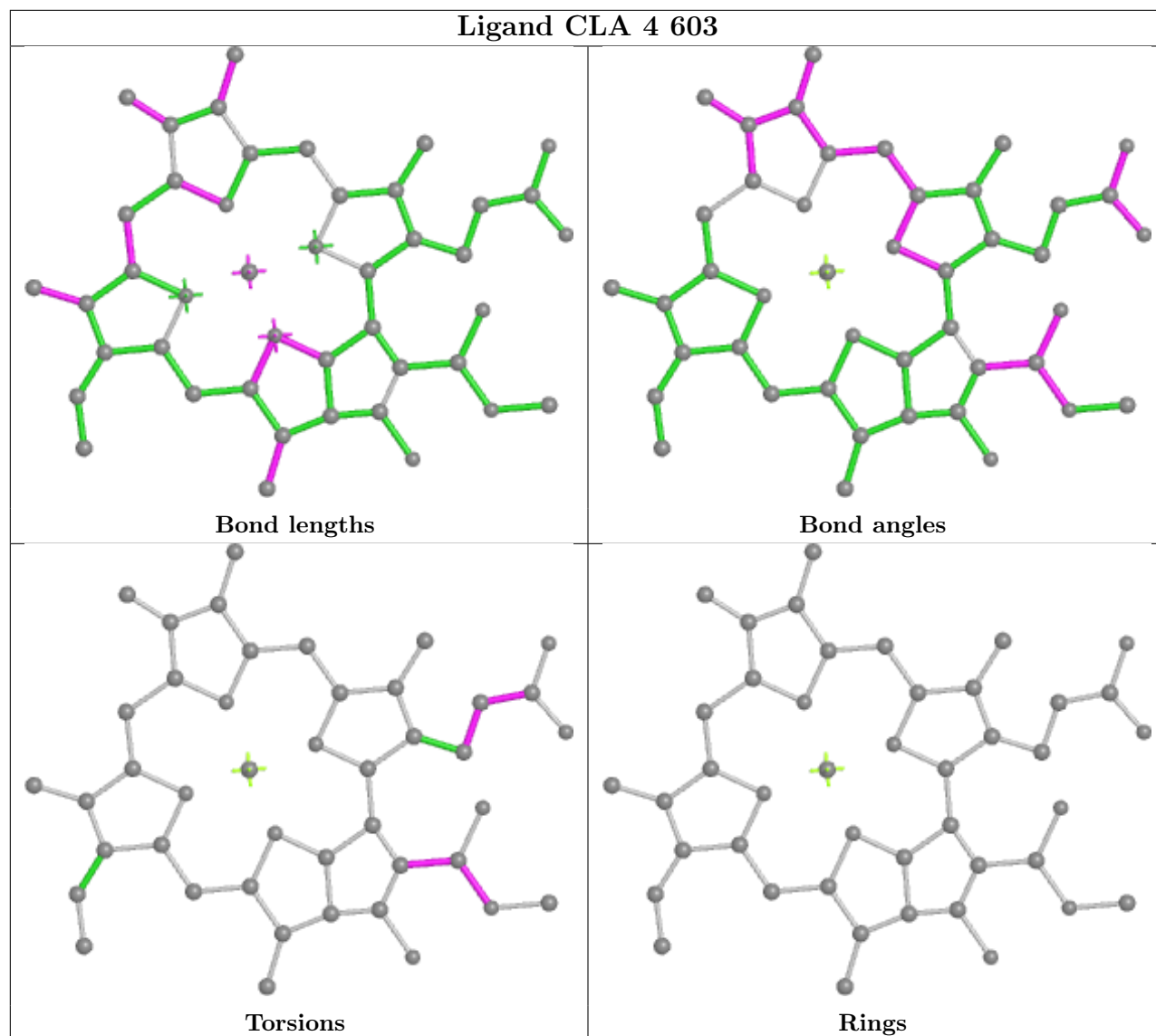




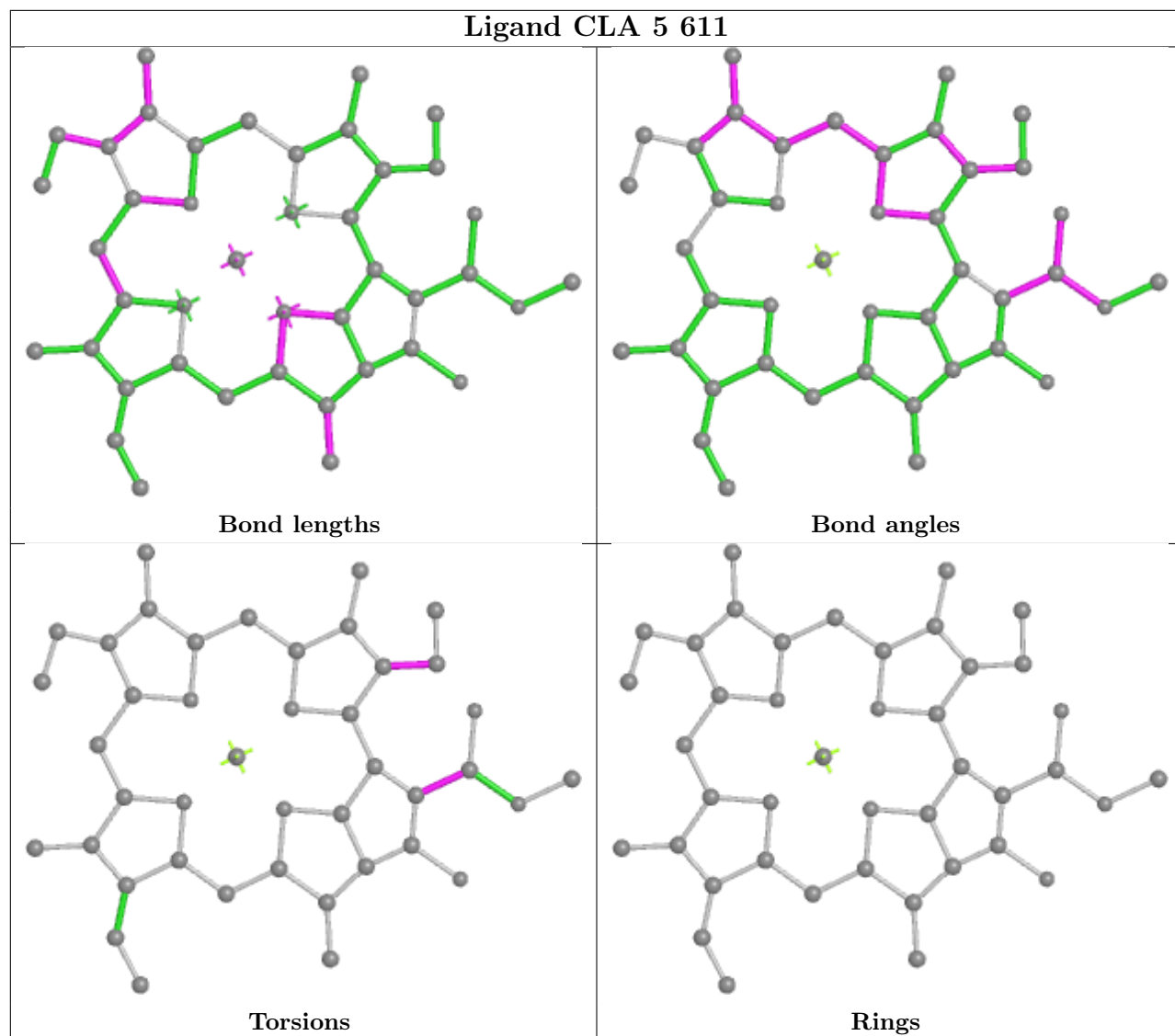


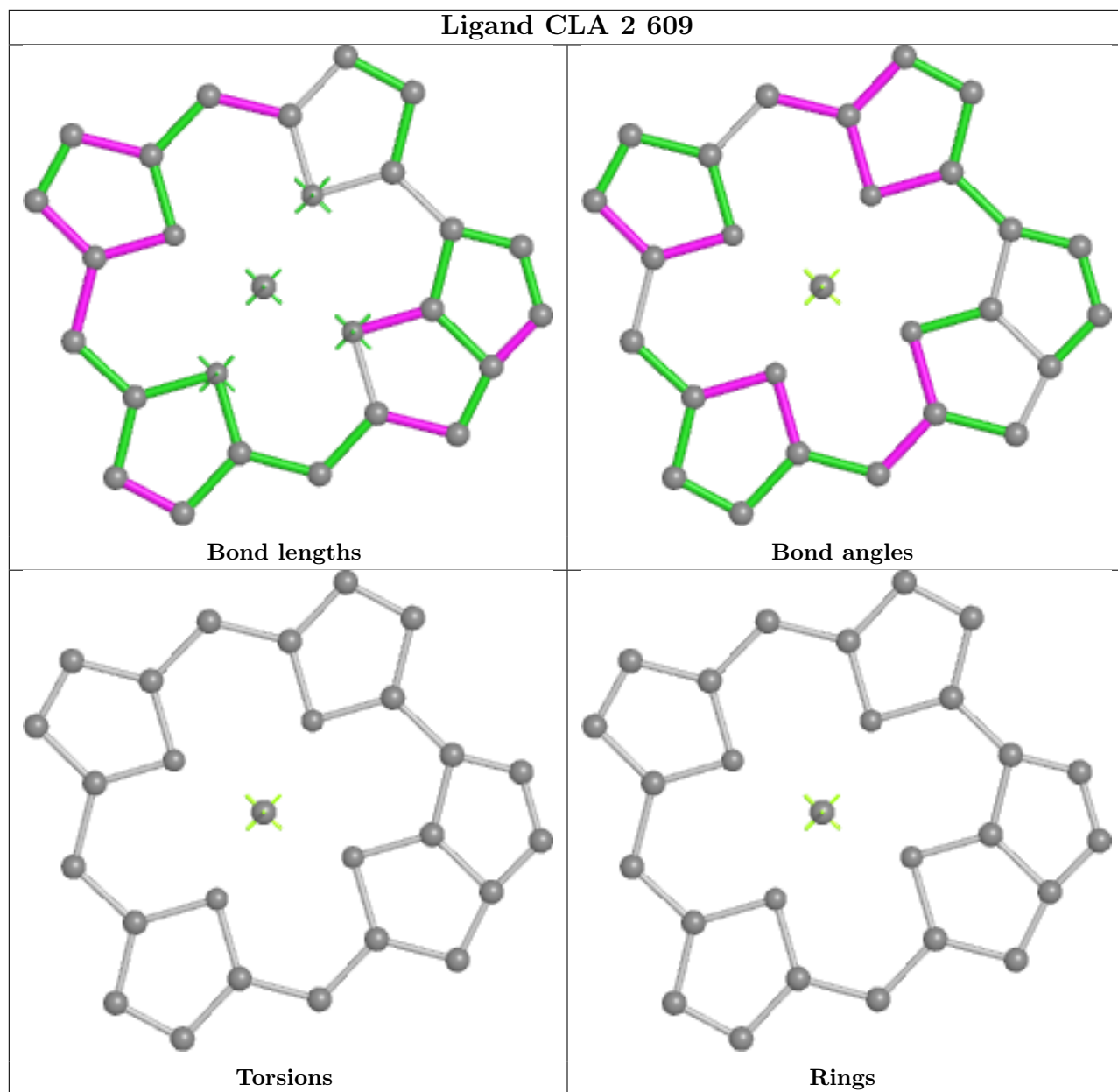


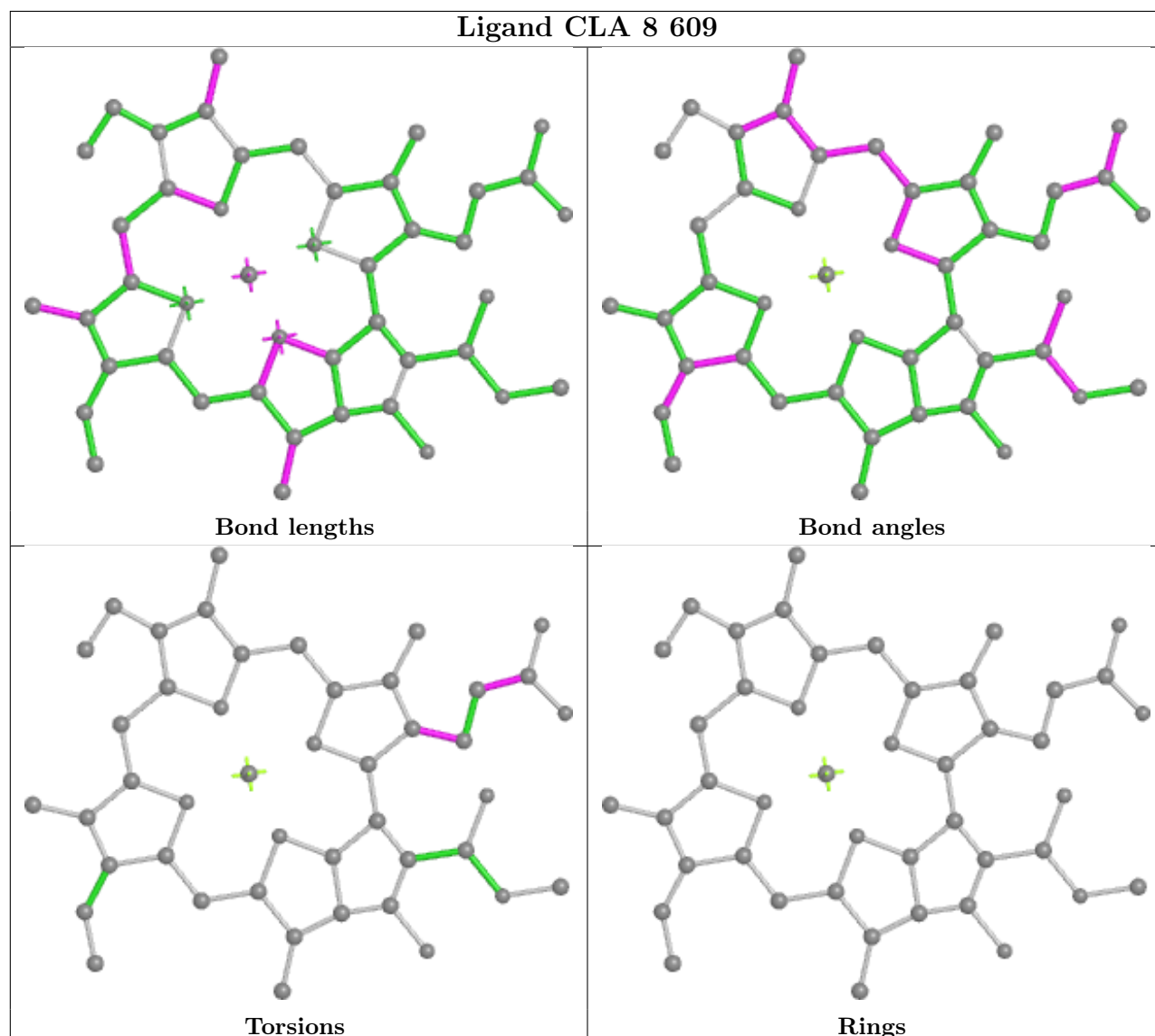
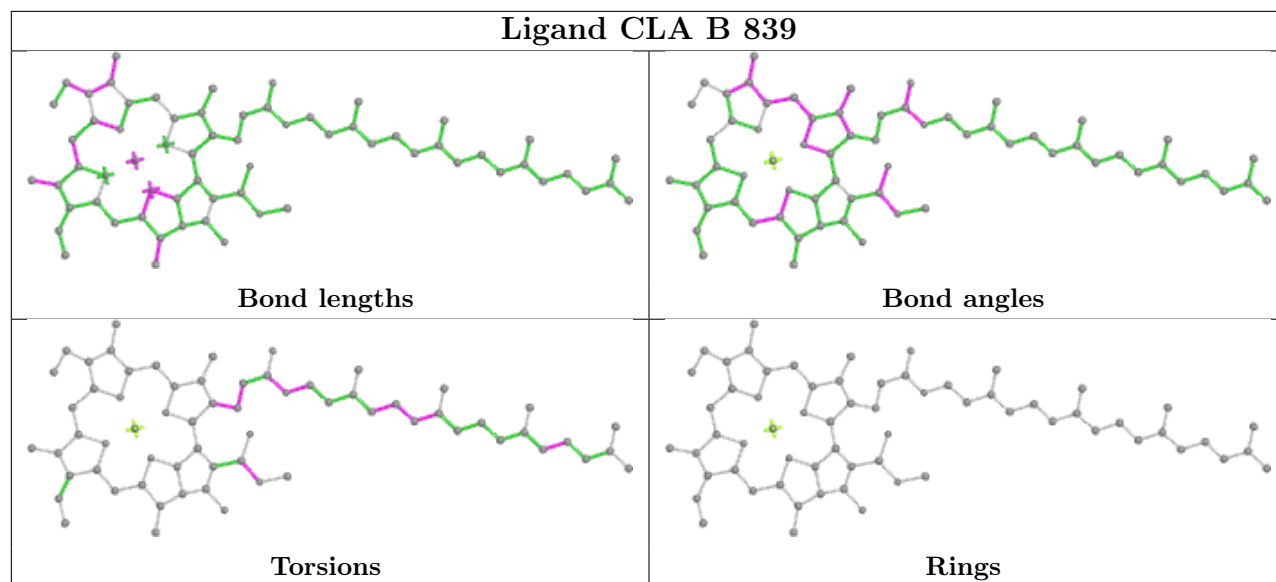


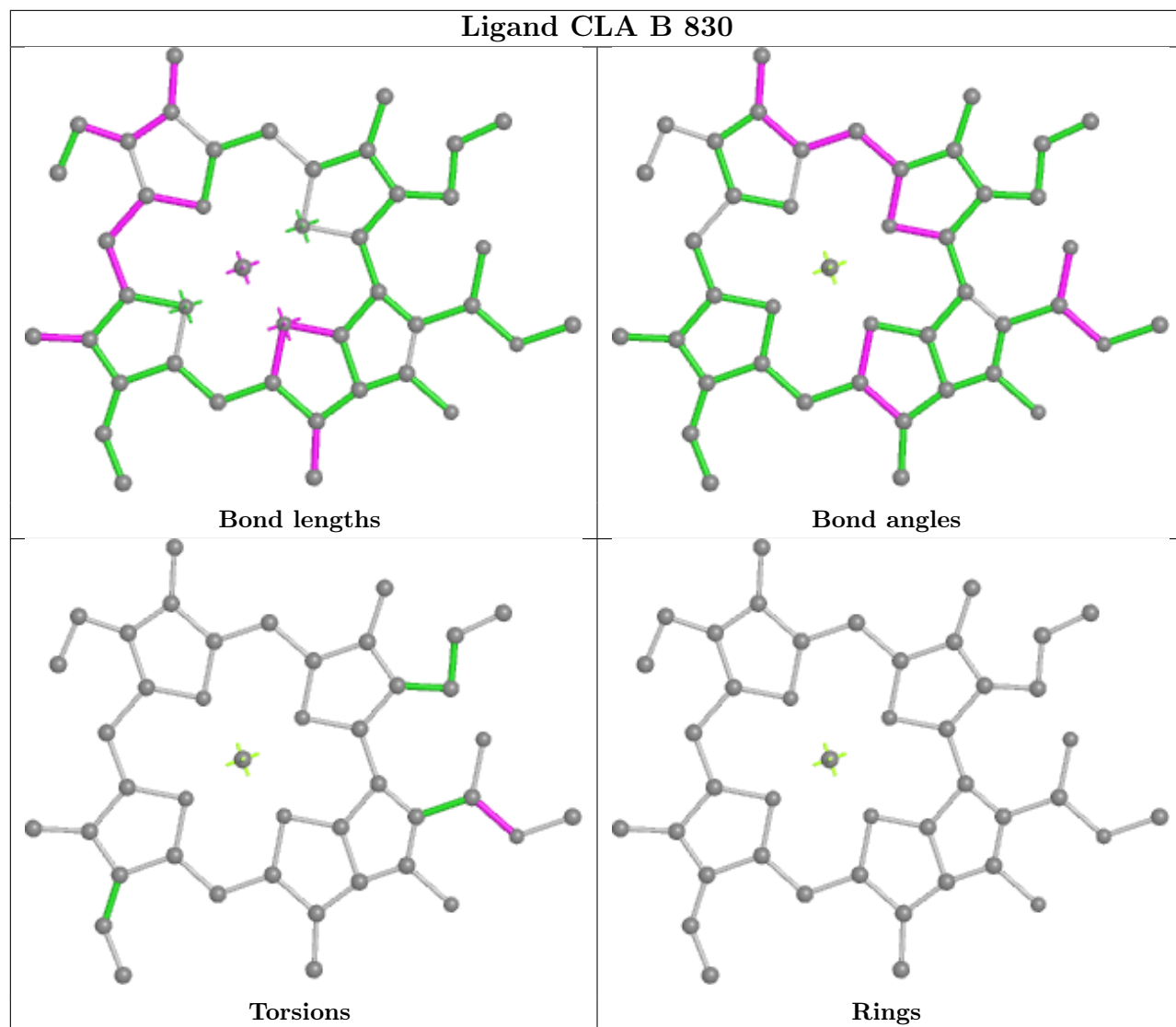


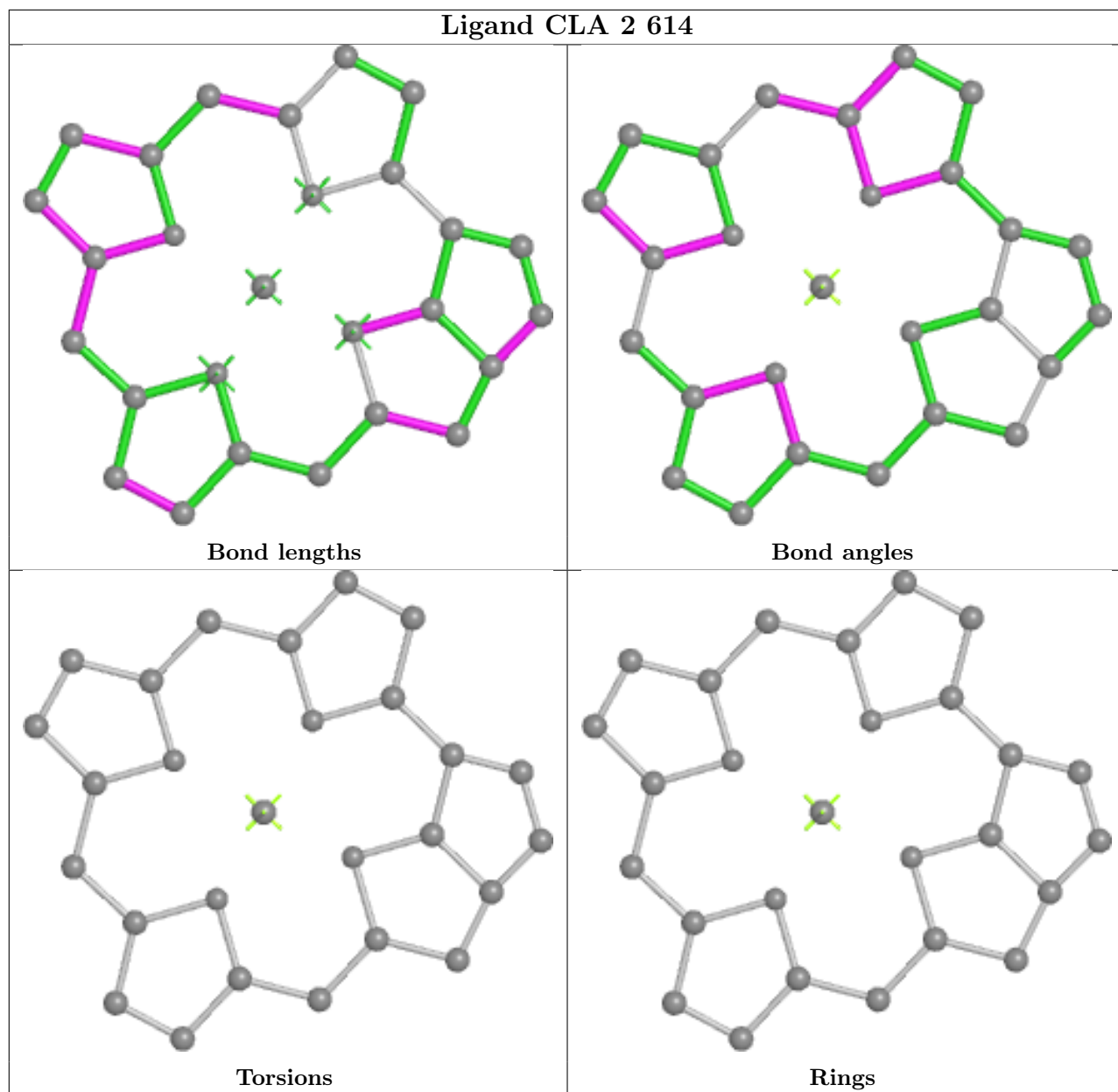
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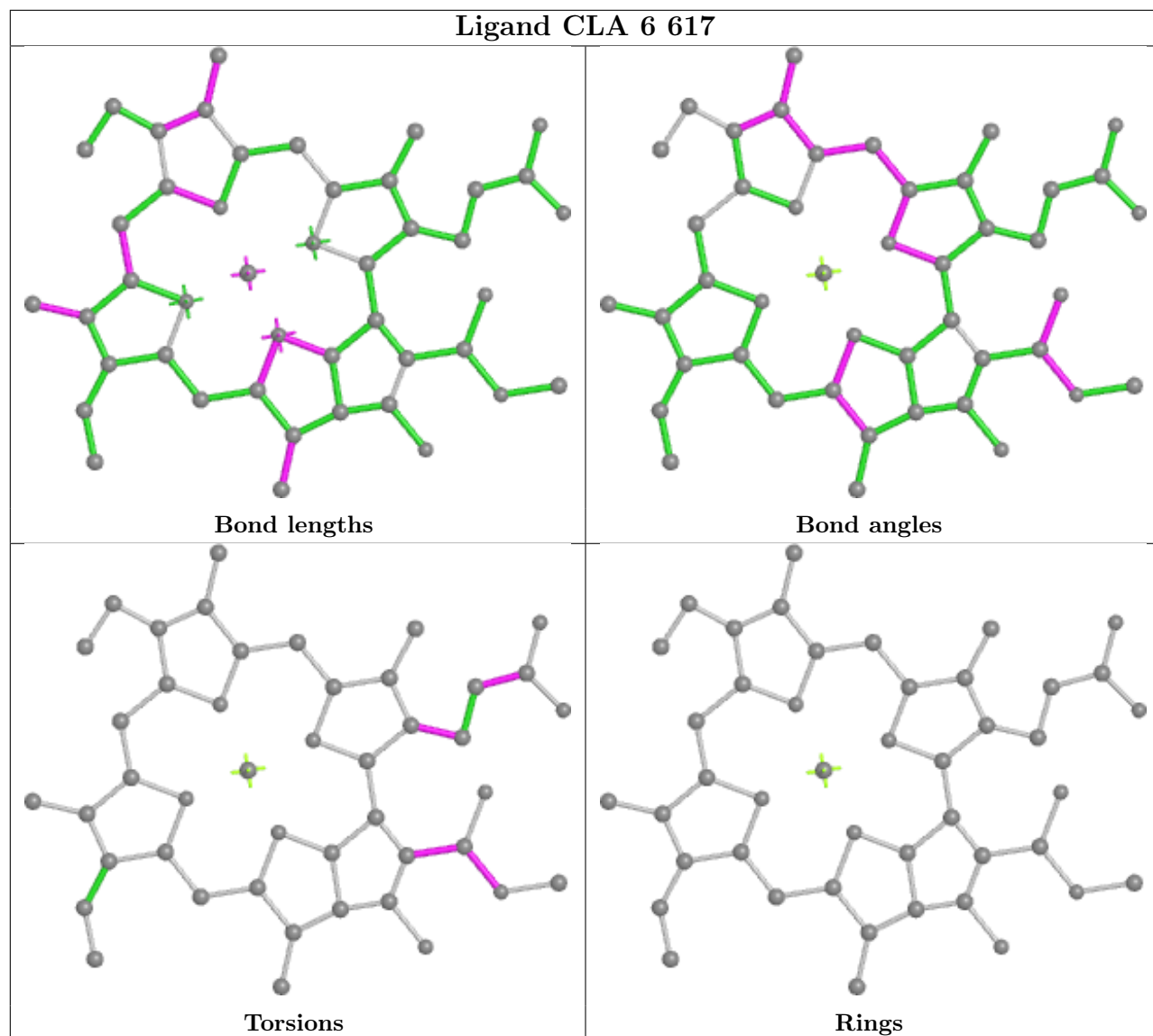


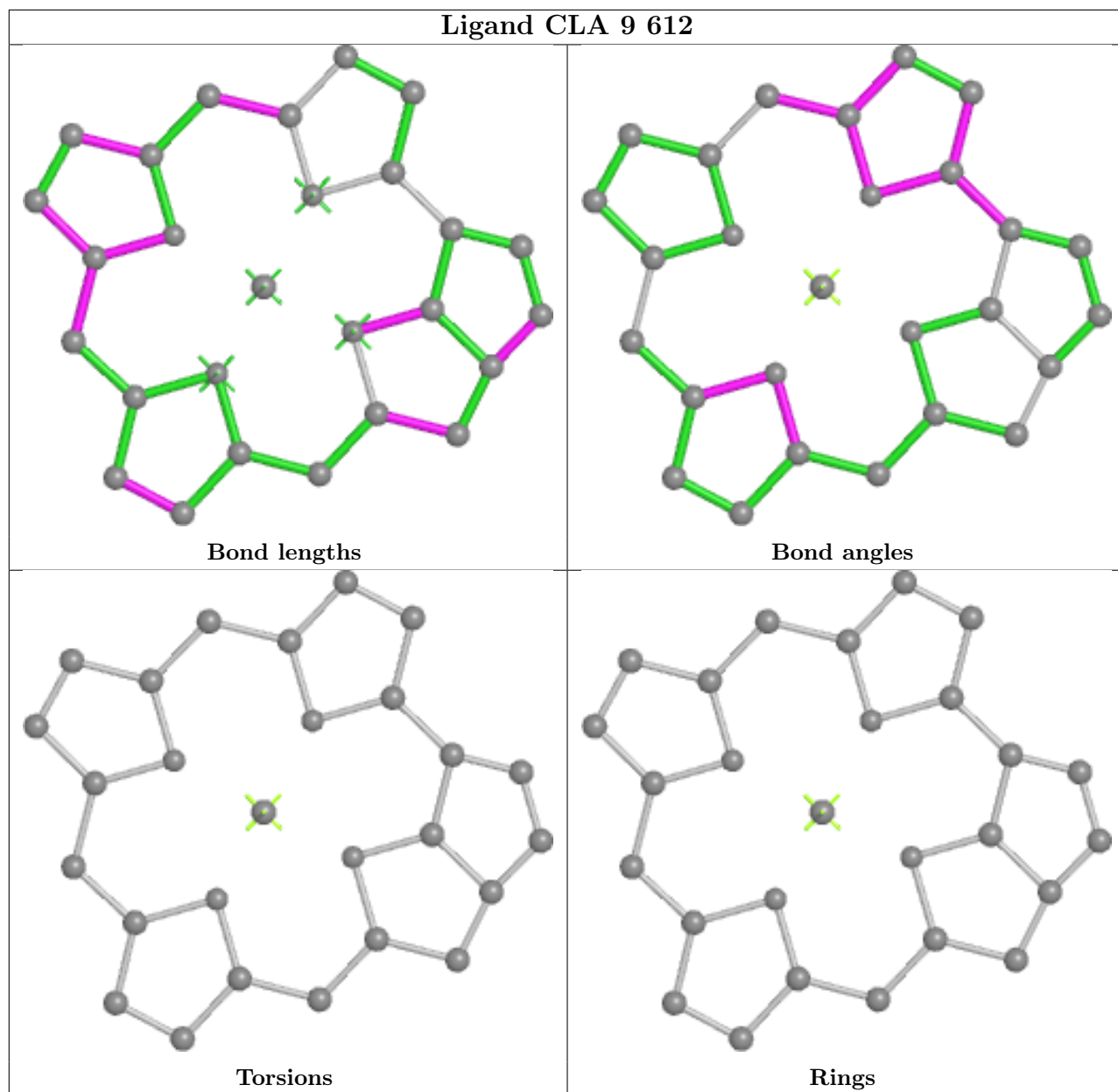


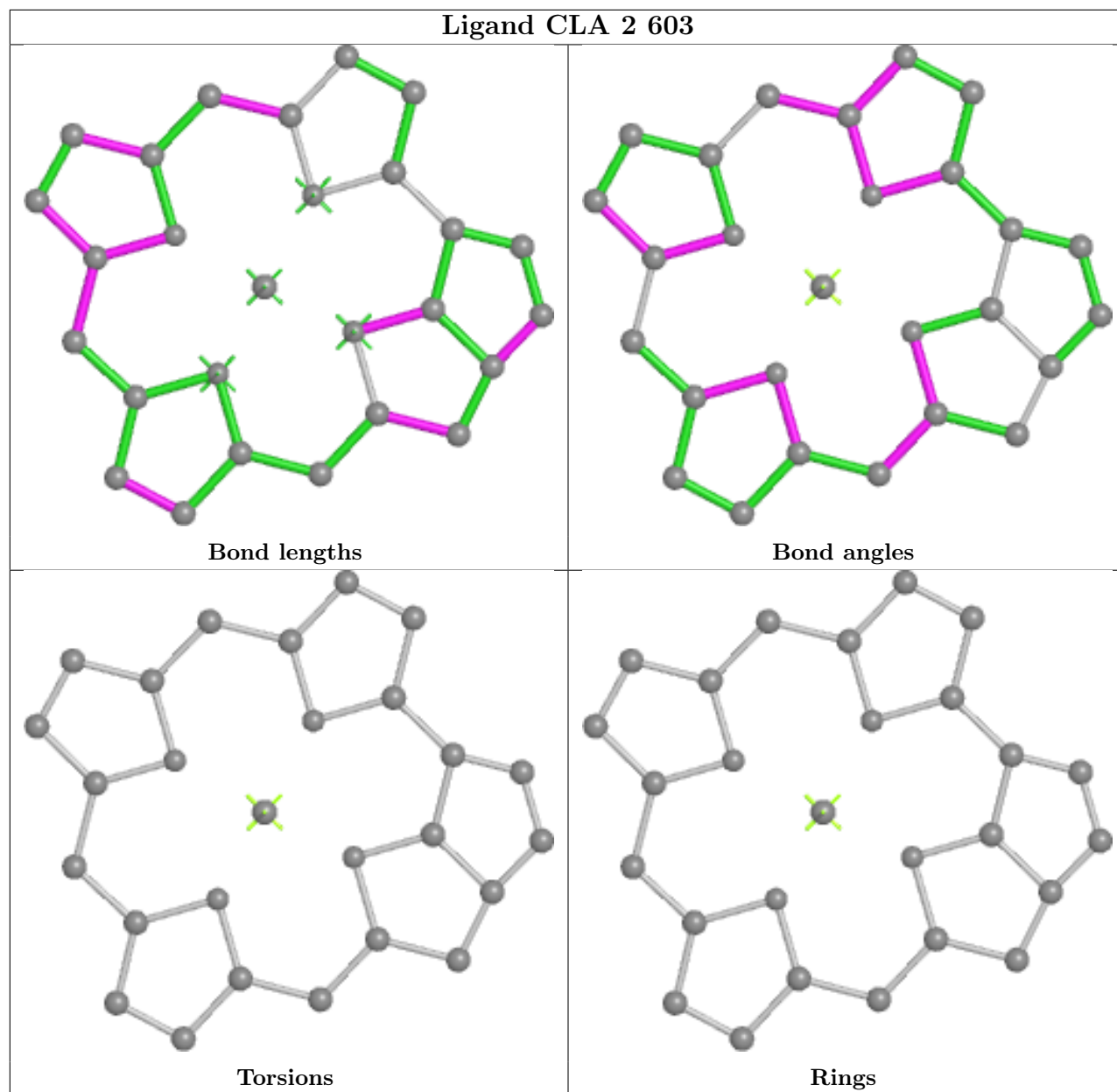


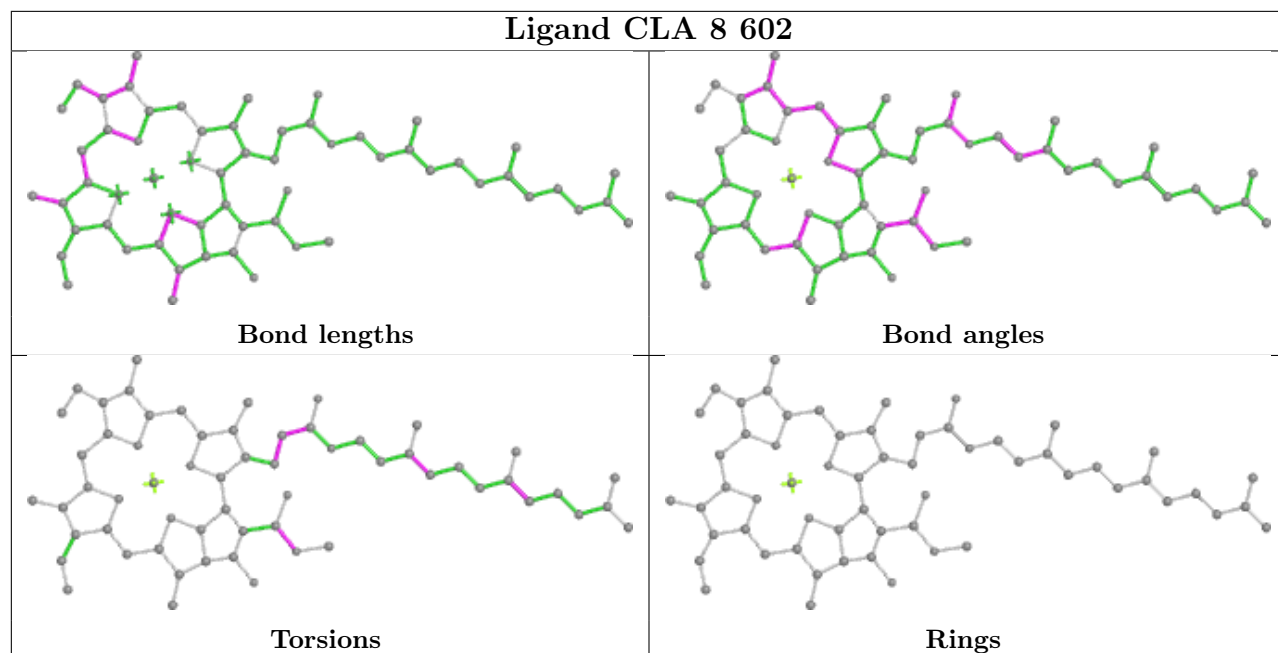


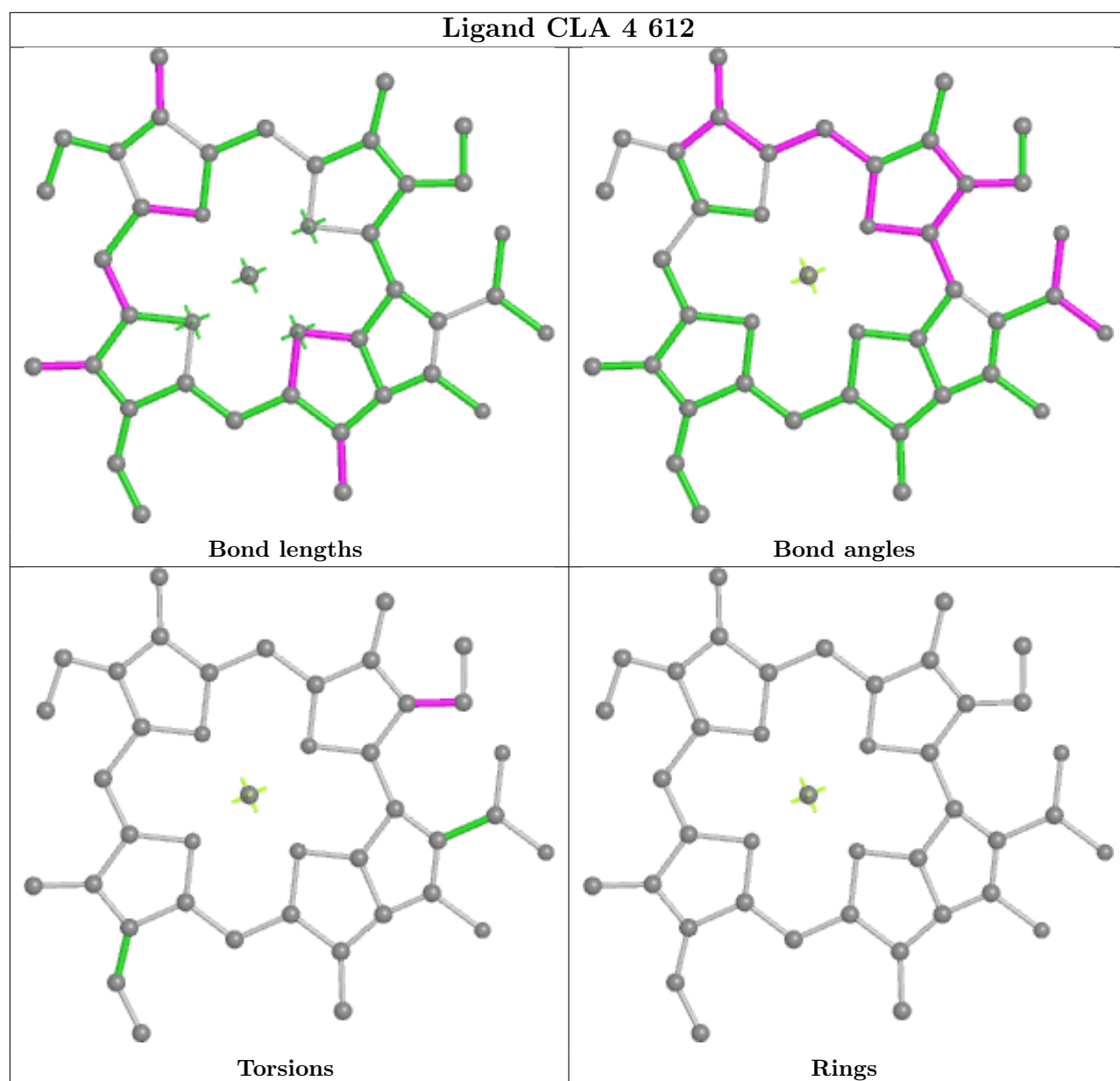


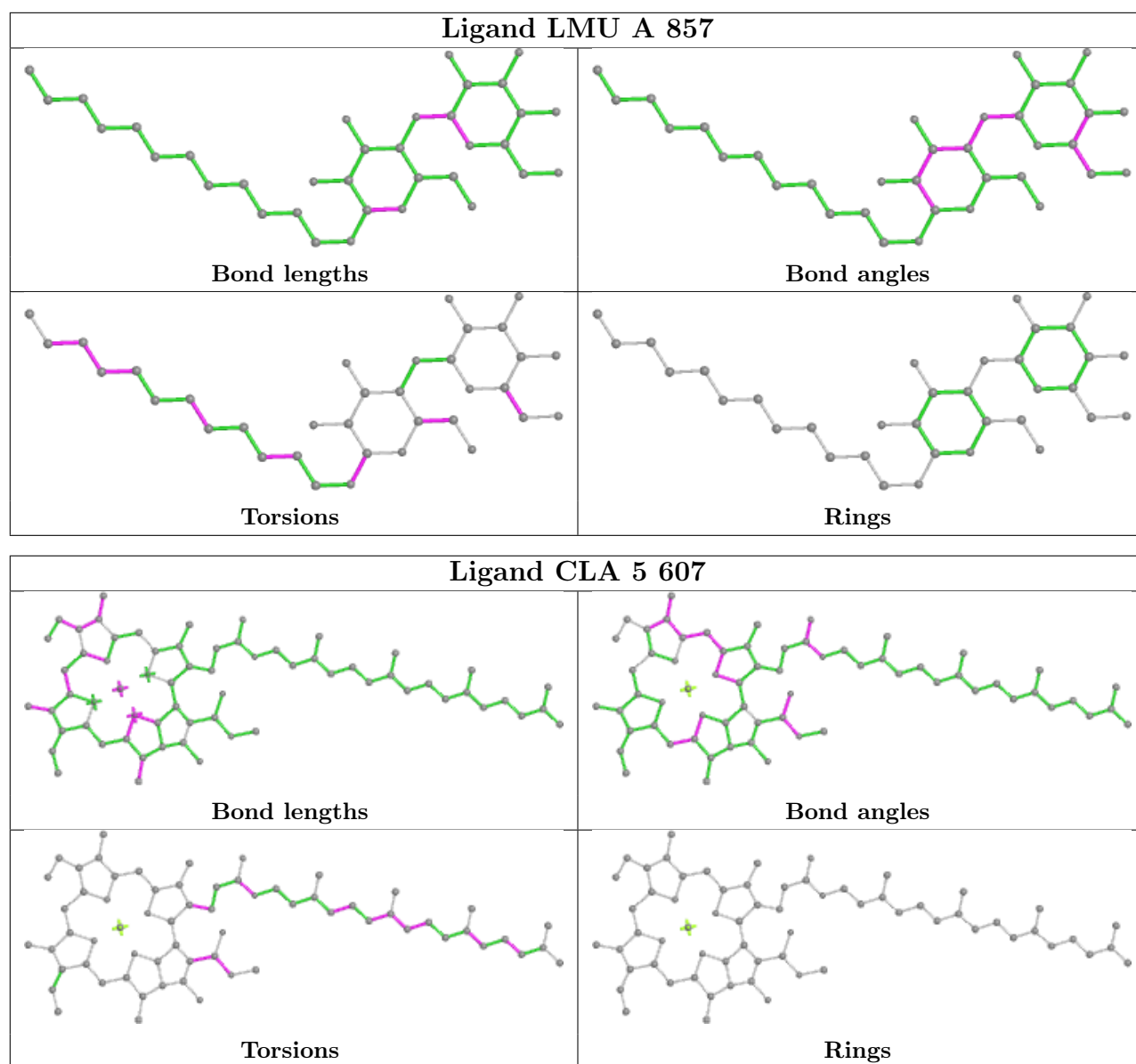


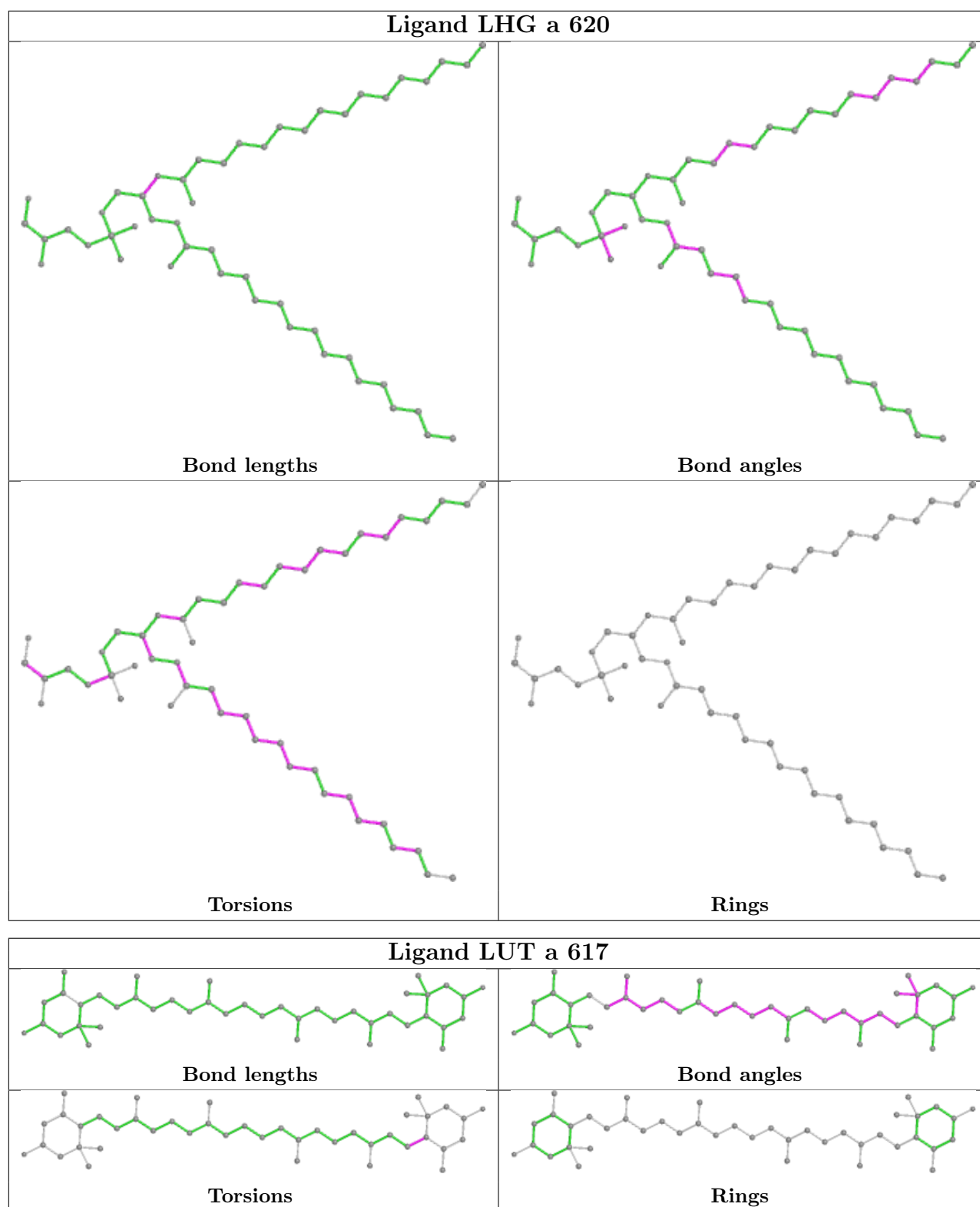


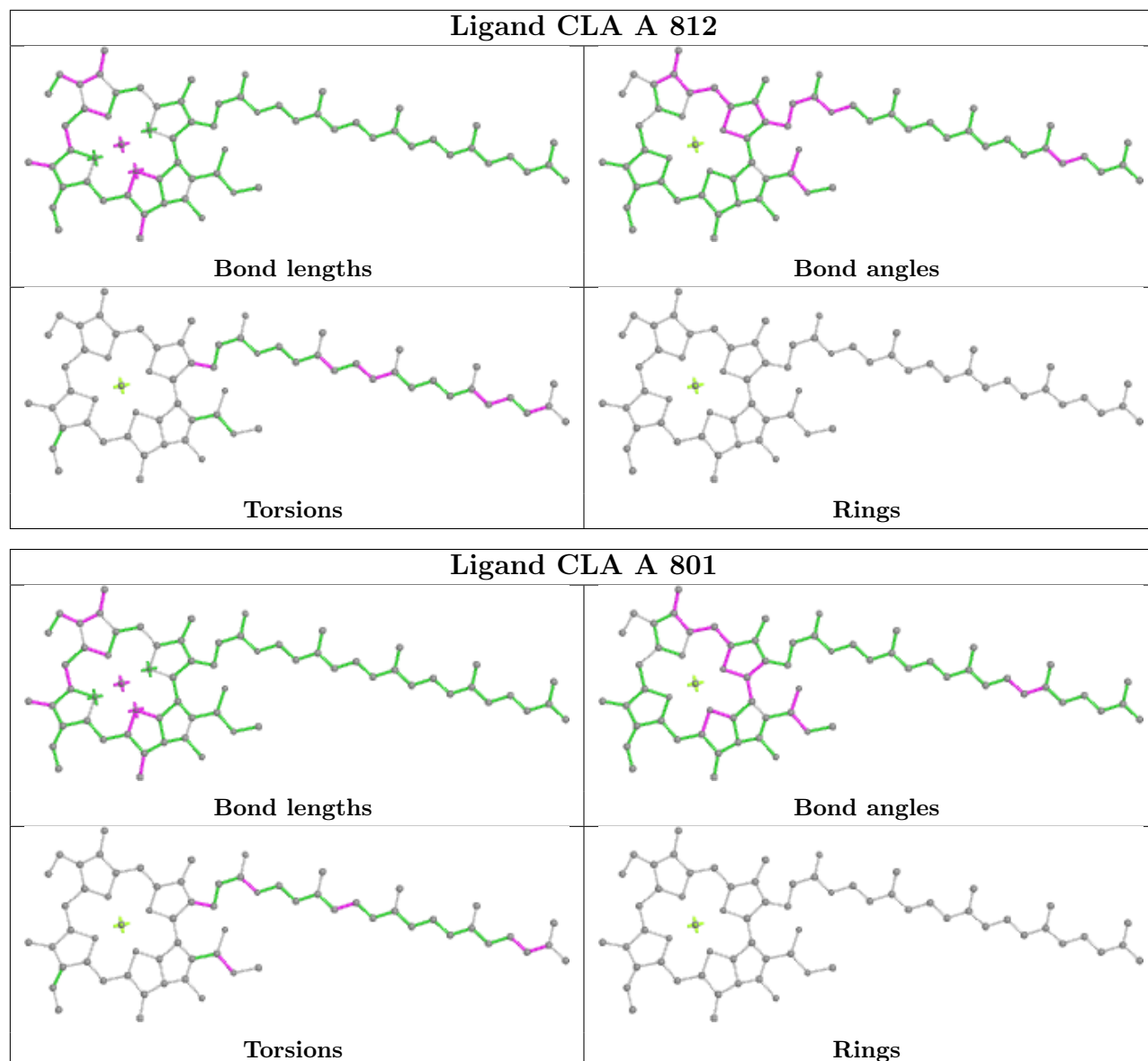


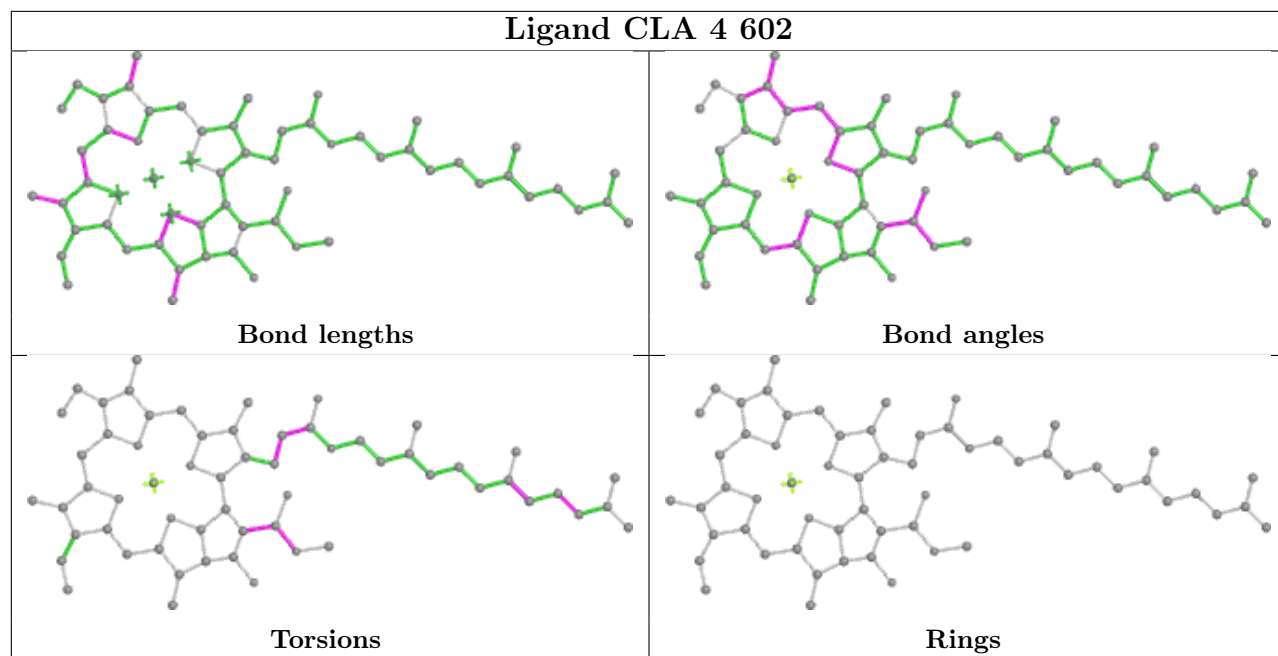


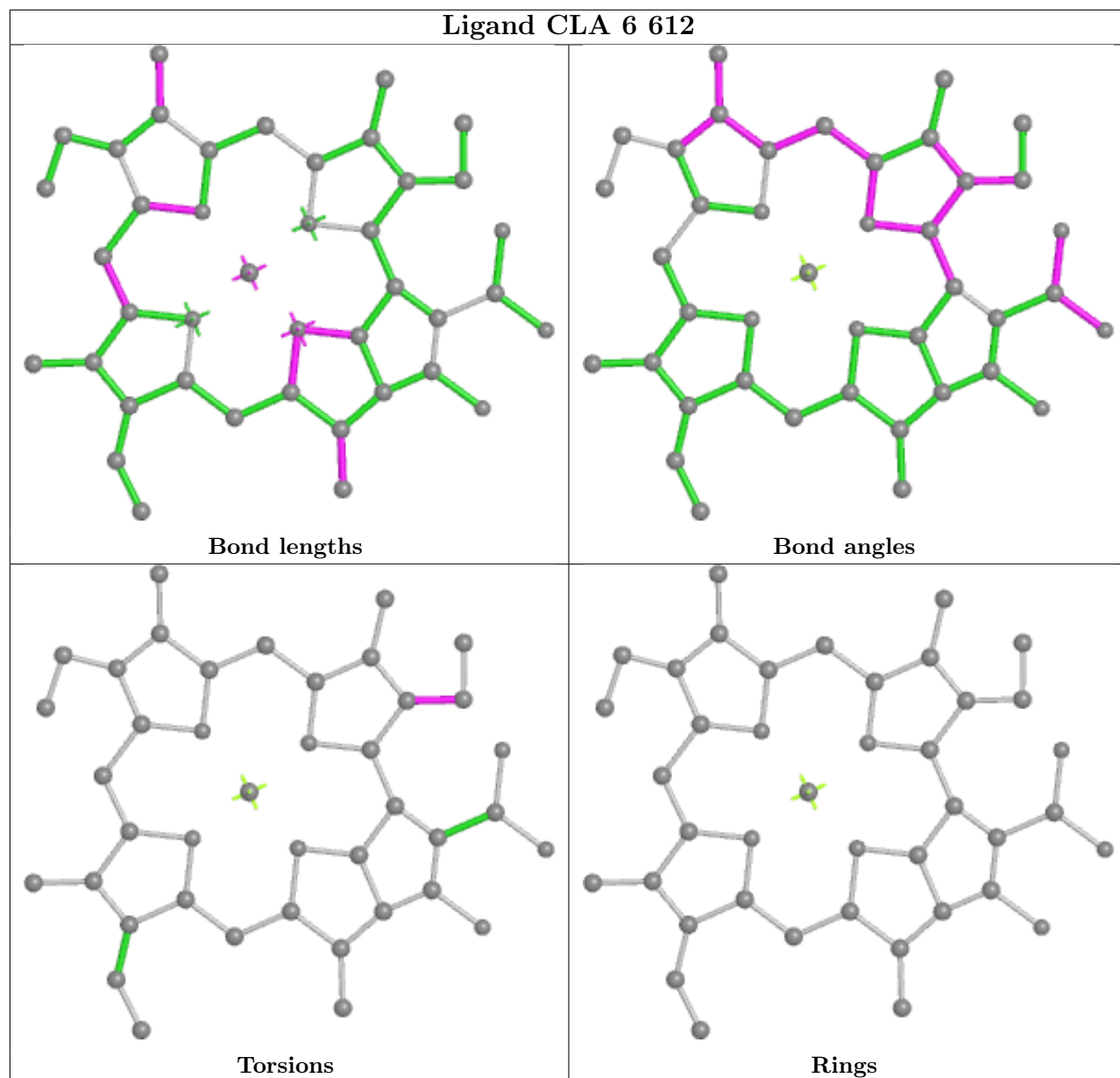


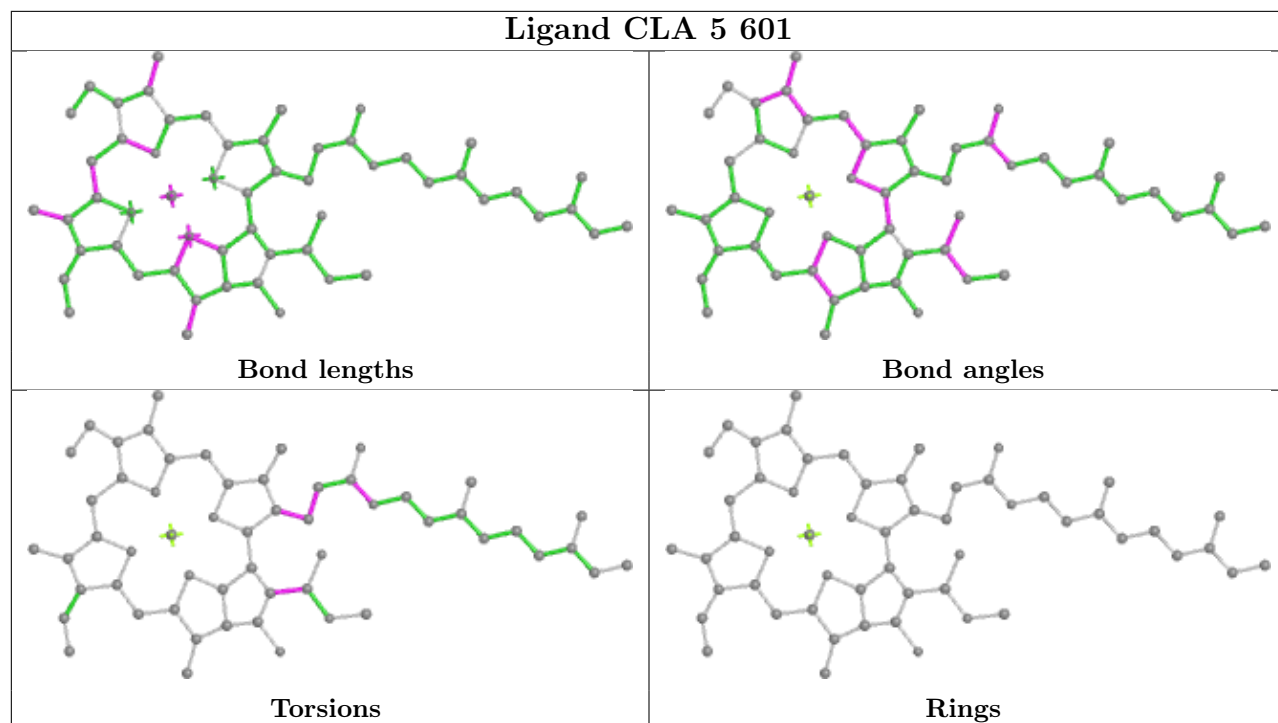


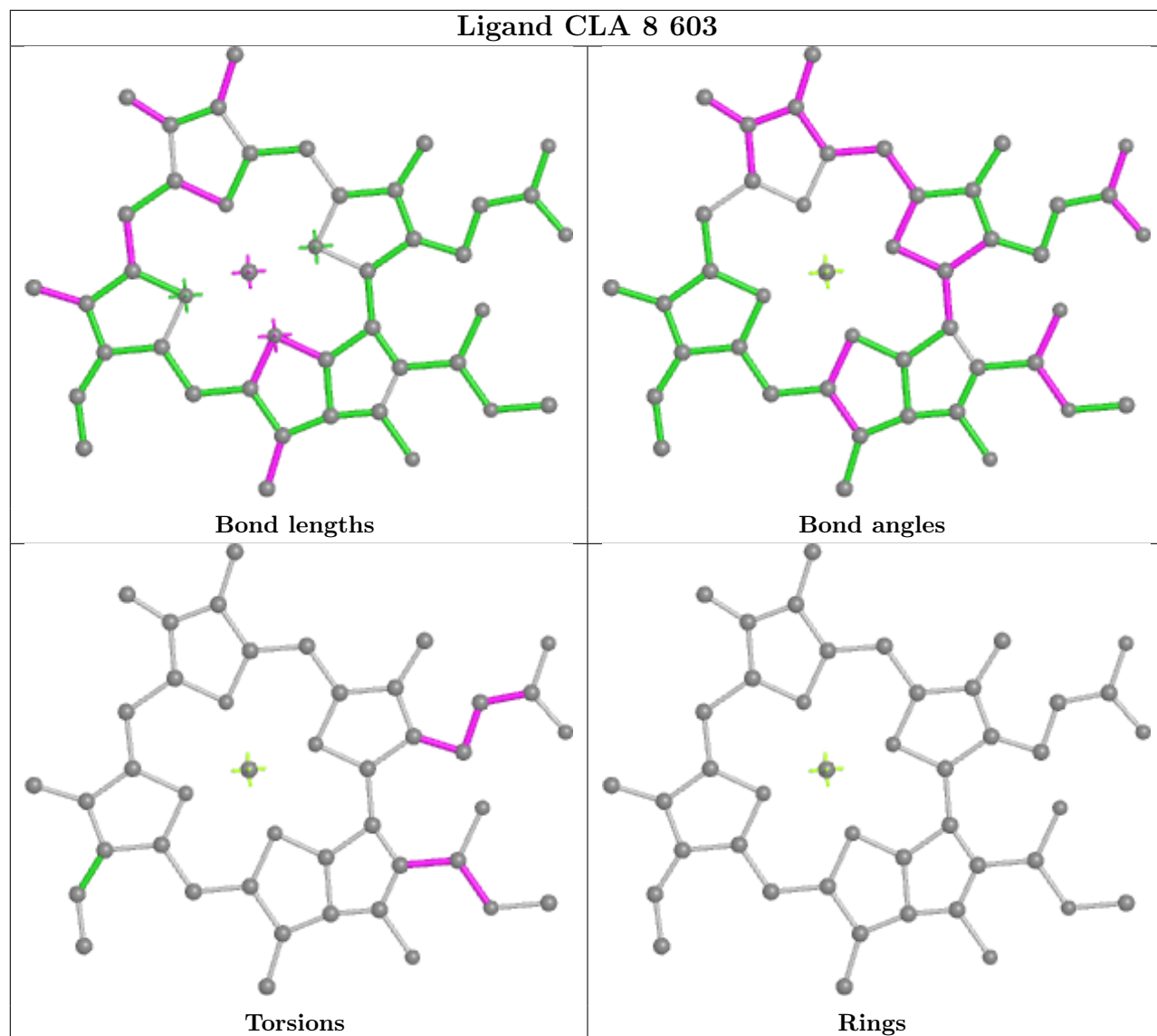


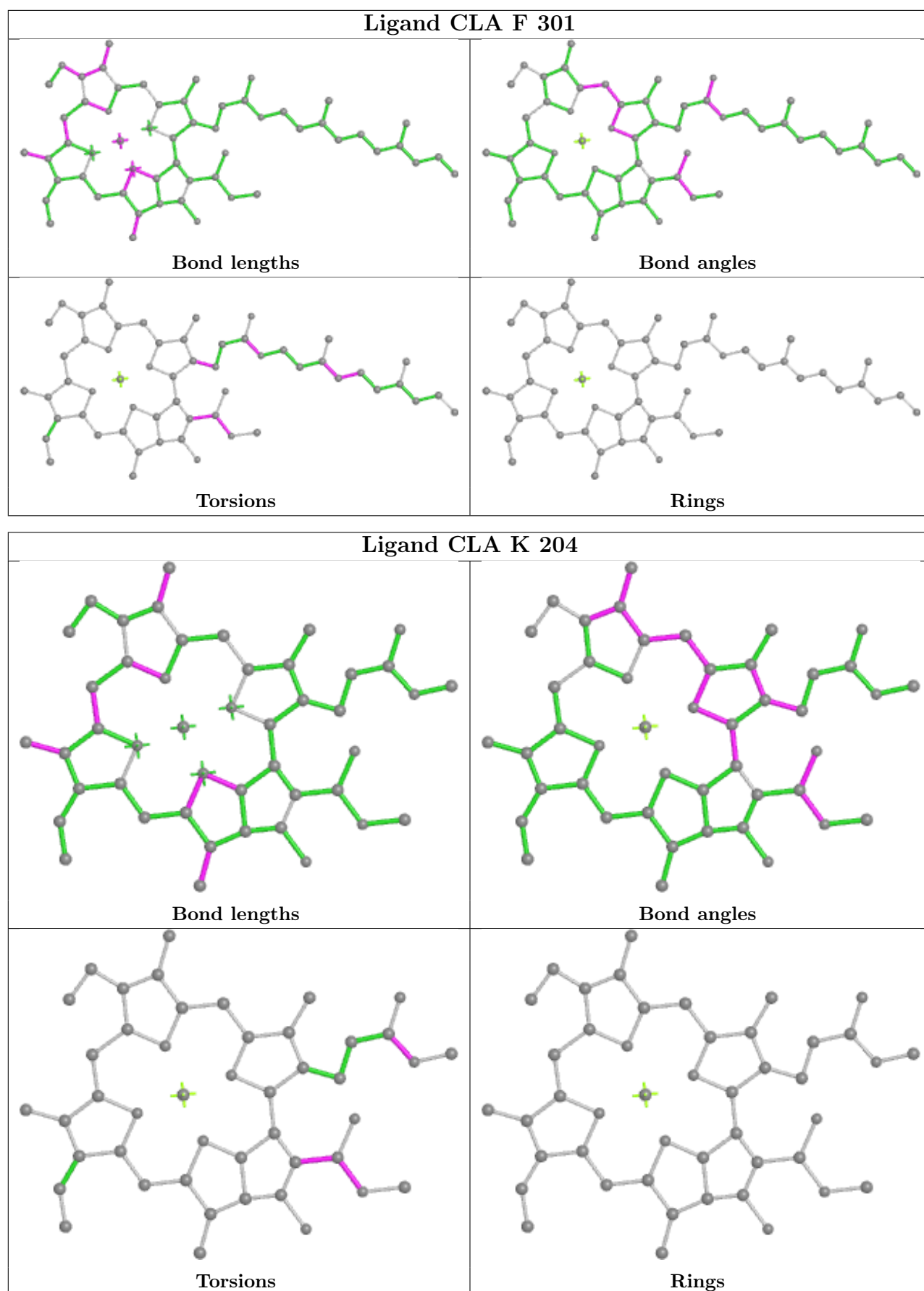


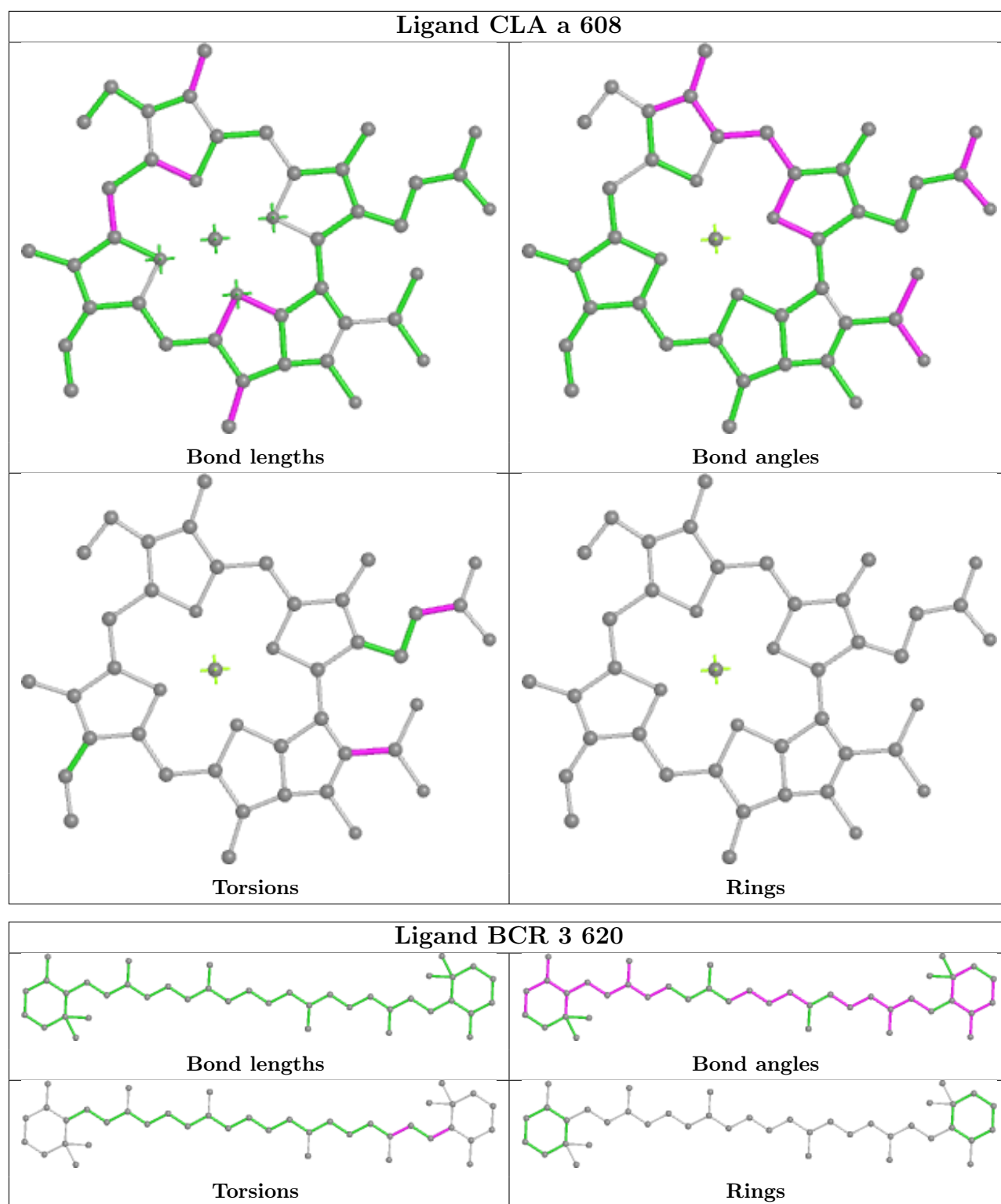












5.7 Other polymers [\(i\)](#)

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

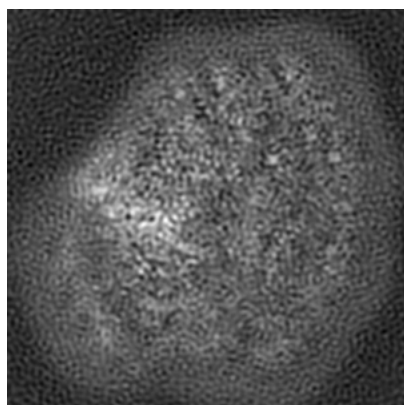
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-9680. These allow visual inspection of the internal detail of the map and identification of artifacts.

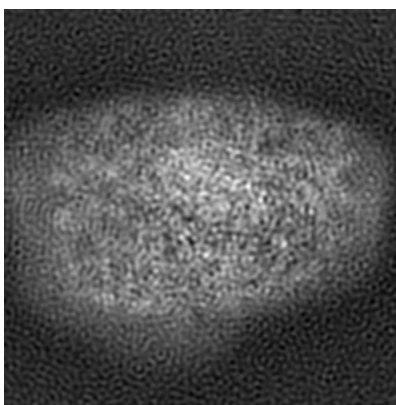
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

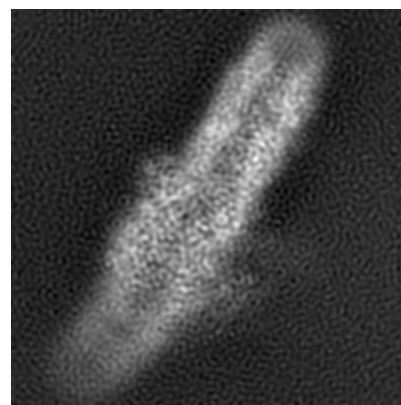
6.1.1 Primary map



X



Y

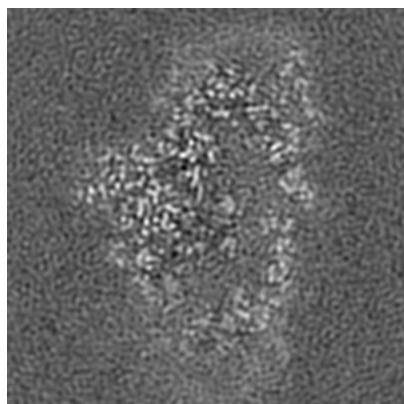


Z

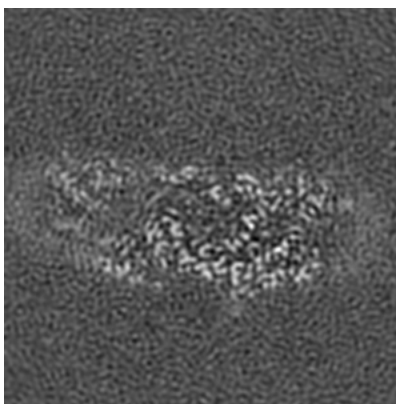
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

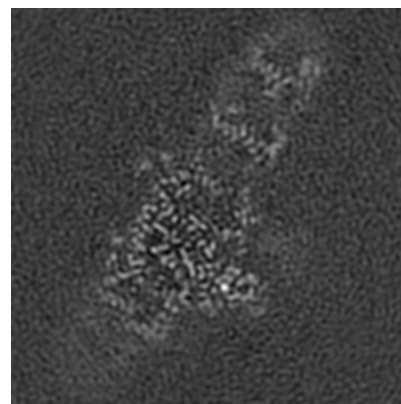
6.2.1 Primary map



X Index: 100



Y Index: 100

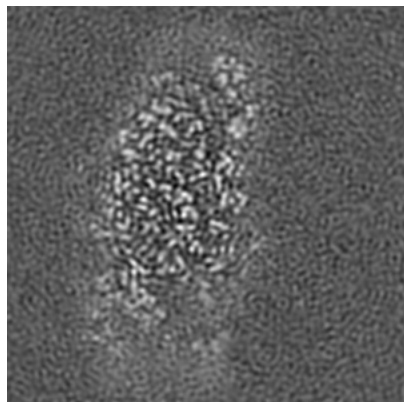


Z Index: 100

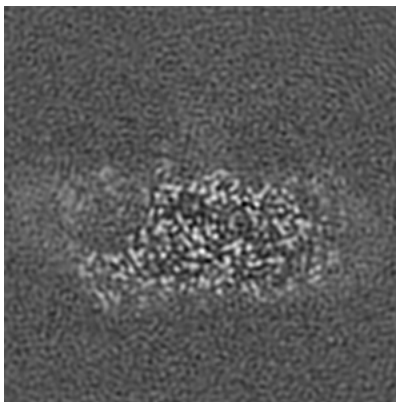
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

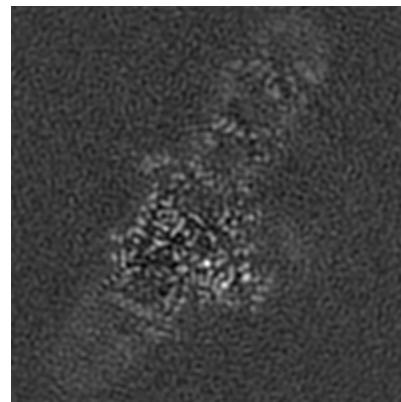
6.3.1 Primary map



X Index: 84



Y Index: 88



Z Index: 98

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 0.06. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

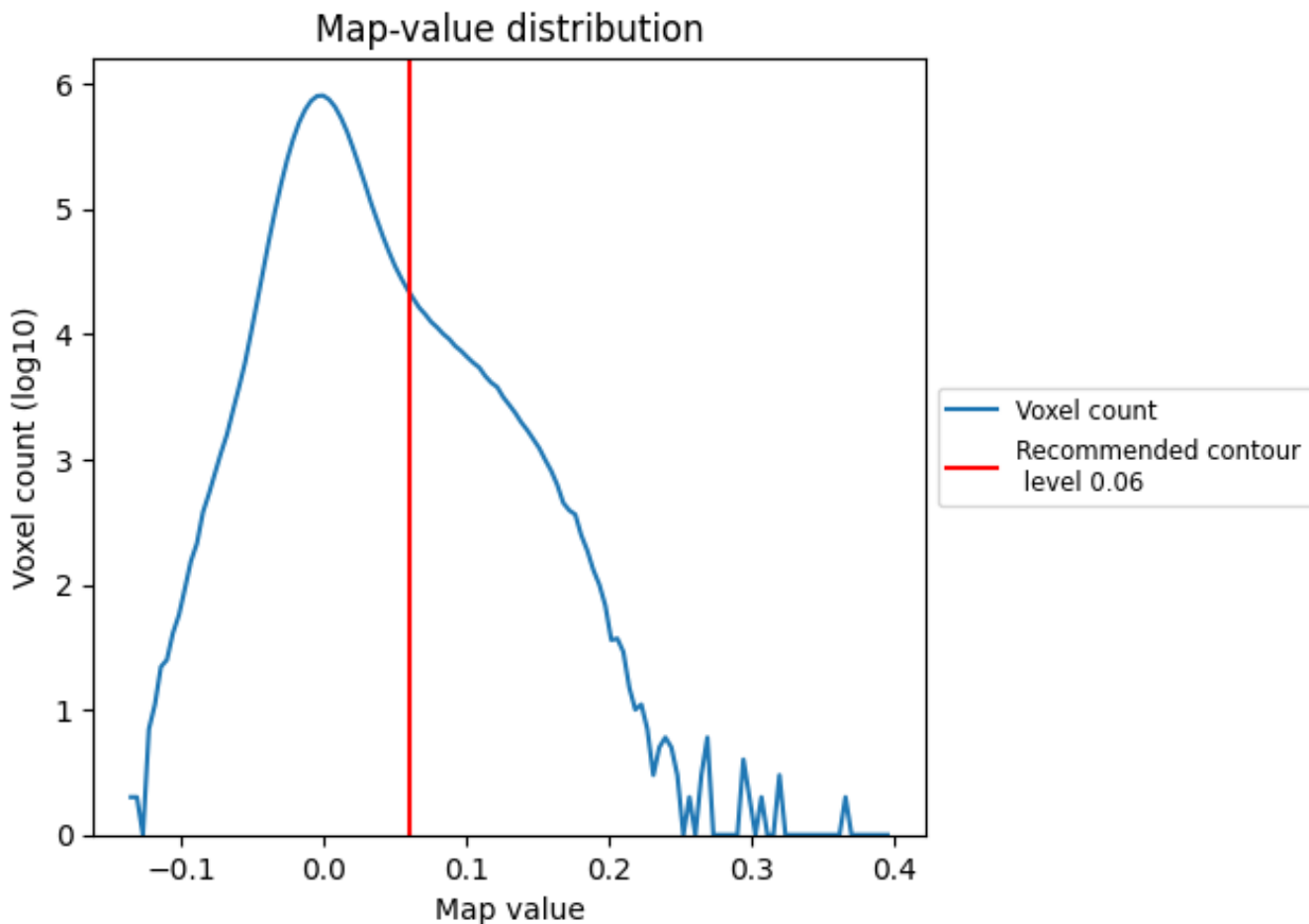
6.5 Mask visualisation

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

7 Map analysis [i](#)

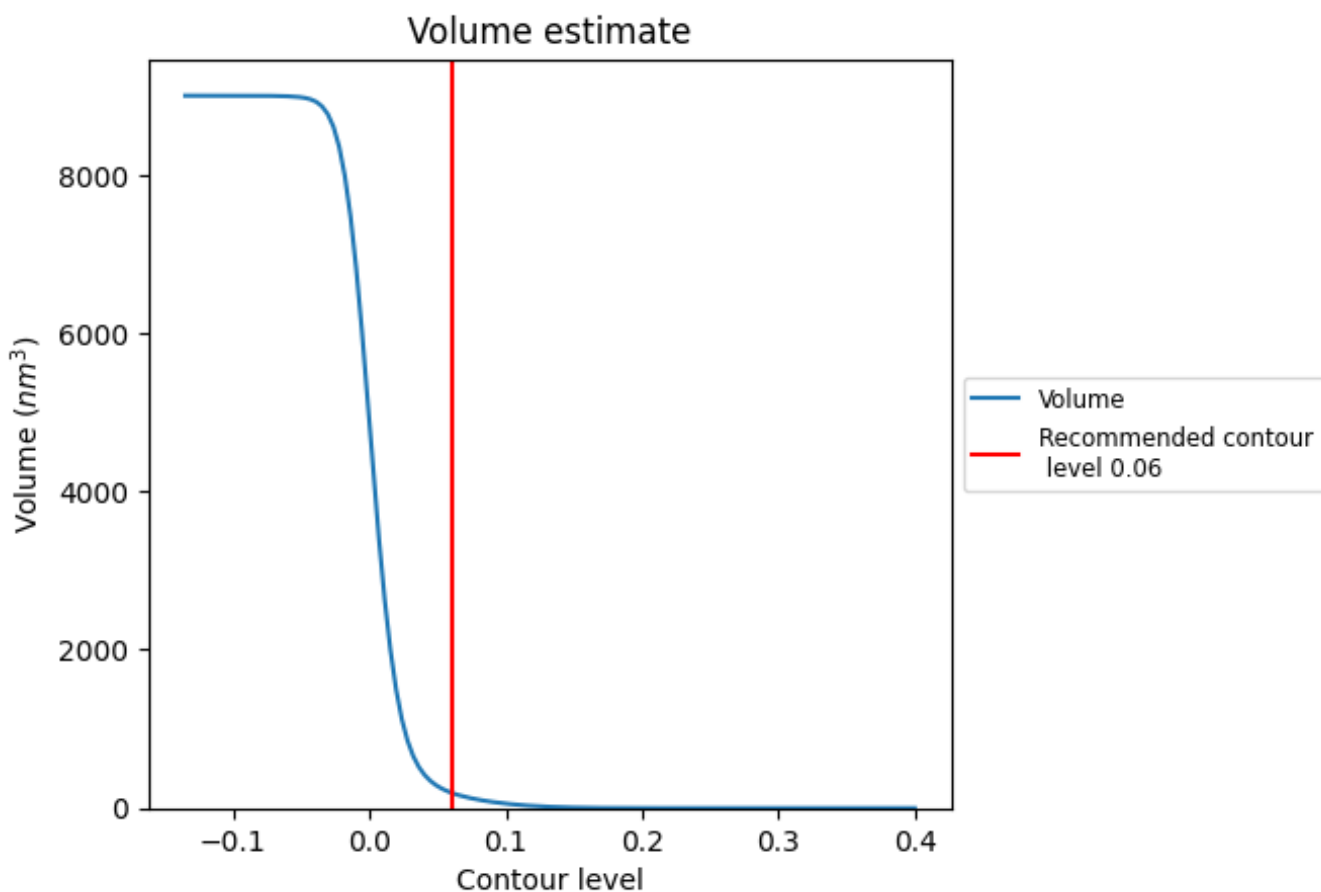
This section contains the results of statistical analysis of the map.

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.

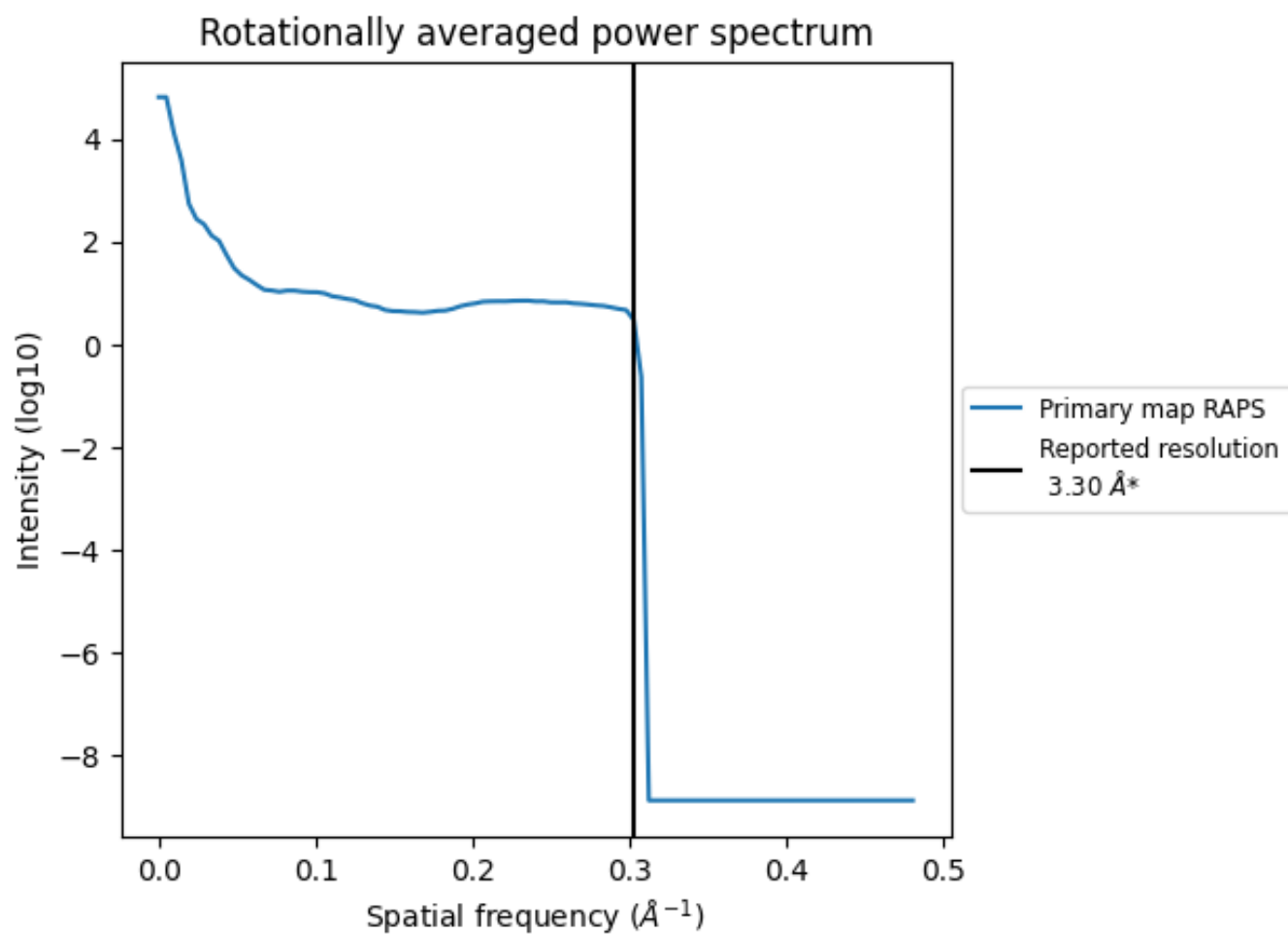
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 196 nm^3 ; this corresponds to an approximate mass of 177 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 0.303 Å⁻¹

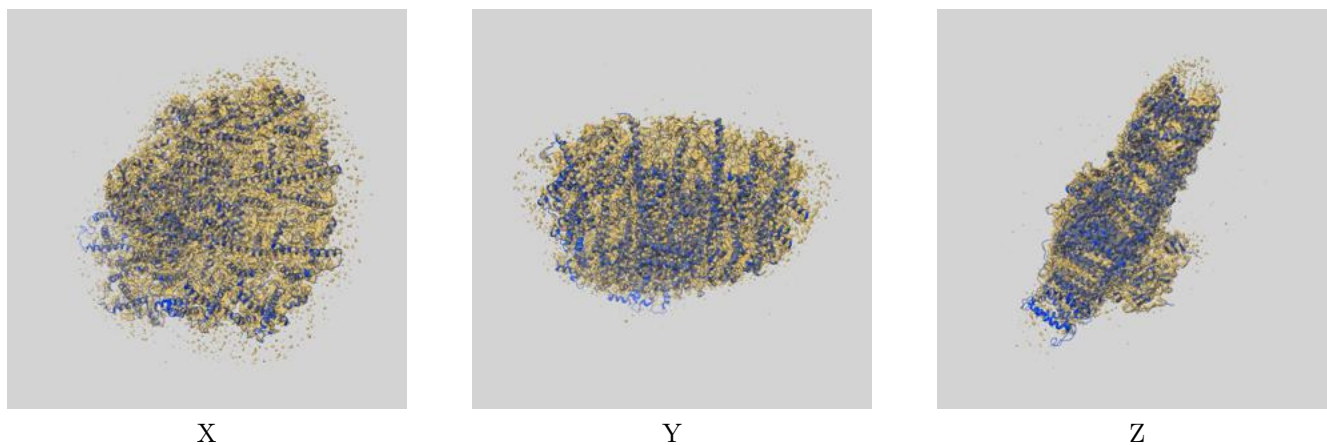
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

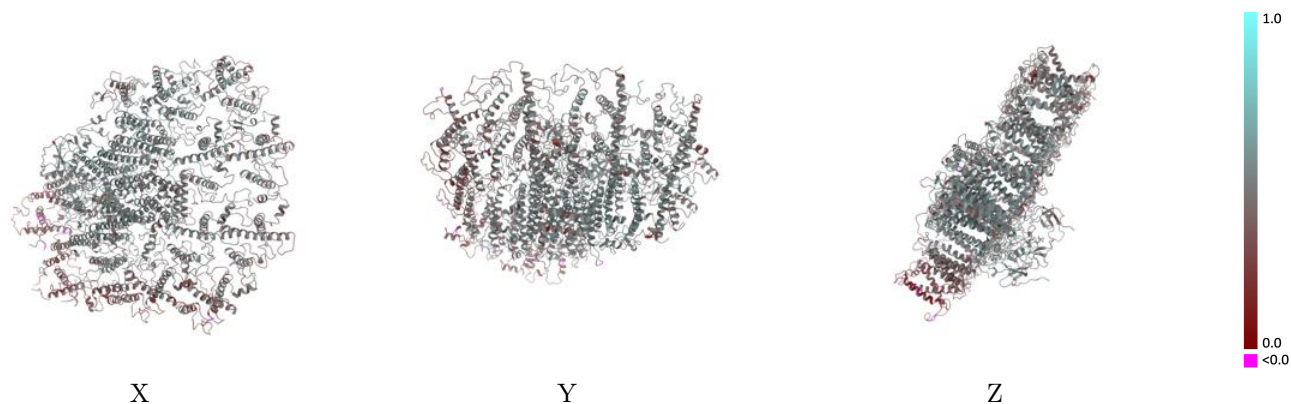
This section contains information regarding the fit between EMDB map EMD-9680 and PDB model 6IJO. Per-residue inclusion information can be found in section 3 on page 35.

9.1 Map-model overlay [i](#)



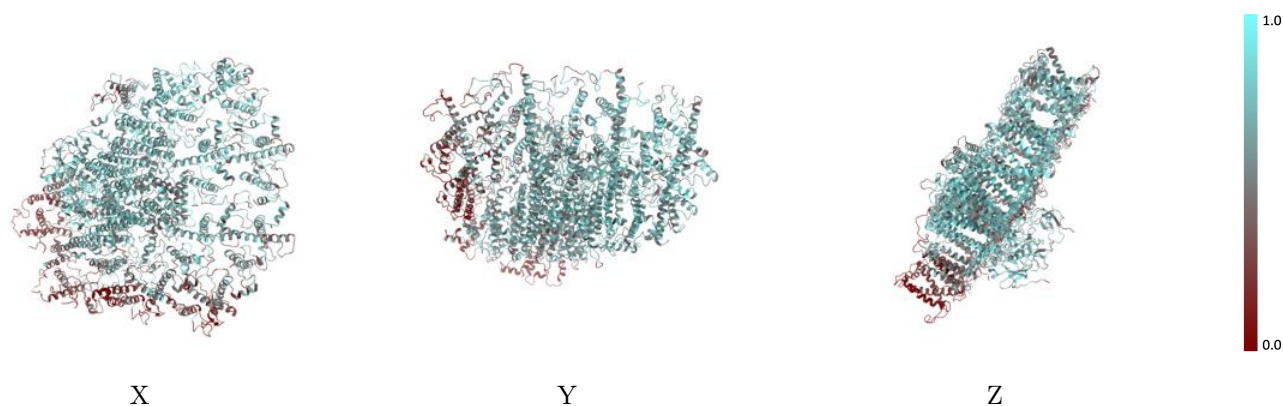
The images above show the 3D surface view of the map at the recommended contour level 0.06 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



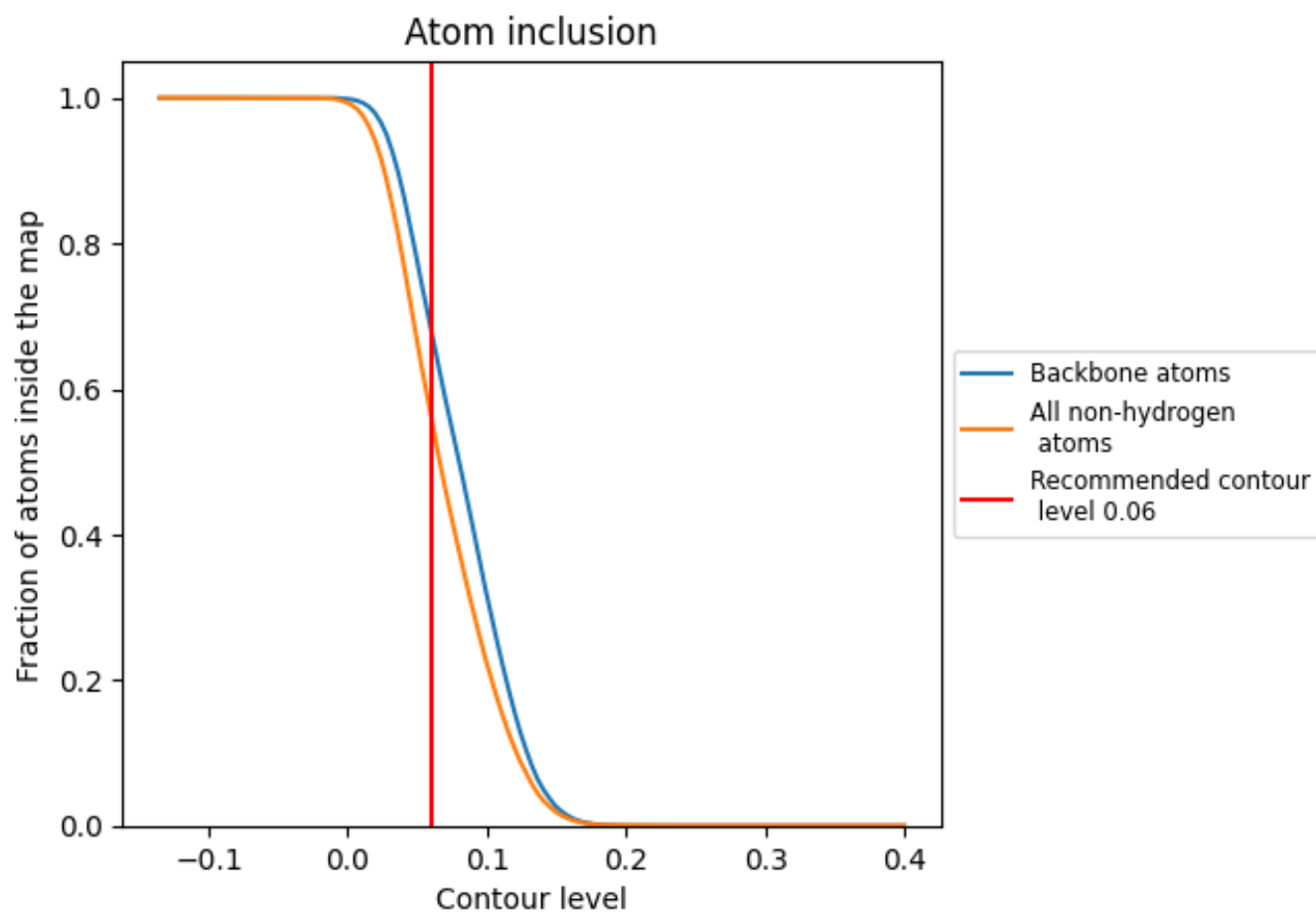
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.06).

















































9.4 Atom inclusion [i](#)



At the recommended contour level, 68% of all backbone atoms, 56% 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 (0.06) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5616	 0.4690
1	 0.4304	 0.3900
2	 0.0935	 0.2380
3	 0.6631	 0.5120
4	 0.5194	 0.4540
5	 0.5823	 0.4790
6	 0.5810	 0.4770
7	 0.6370	 0.4970
8	 0.5962	 0.4870
9	 0.2723	 0.2900
A	 0.7079	 0.5400
B	 0.6437	 0.5150
C	 0.7143	 0.4870
D	 0.6486	 0.4900
E	 0.6159	 0.4570
F	 0.5685	 0.4590
G	 0.0736	 0.3300
H	 0.0914	 0.3340
I	 0.5667	 0.4660
J	 0.4221	 0.4370
K	 0.4795	 0.4470
L	 0.4380	 0.4150
X	 0.2615	 0.2840
a	 0.3999	 0.4140

