



wwPDB EM Validation Summary Report ⓘ

Nov 16, 2022 – 05:02 PM JST

PDB ID : 7D0J
EMDB ID : EMD-30536
Title : Photosystem I-LHCI-LHCII of Chlamydomonas reinhardtii
Authors : Wang, W.D.; Shen, L.L.; Huang, Z.H.; Han, G.Y.; Zhang, X.; Shen, J.R.
Deposited on : 2020-09-10
Resolution : 3.42 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:

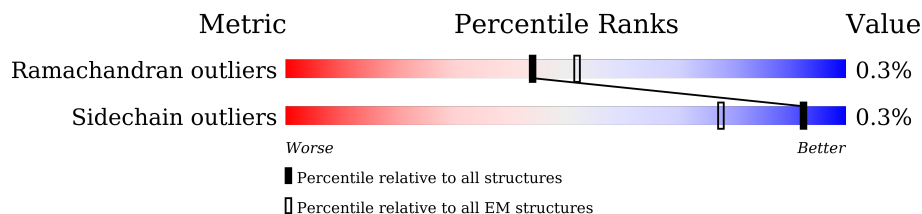
EMDB validation analysis : 0.0.1.dev43
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (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 3.42 Å.

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



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 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	740	
2	B	734	
3	C	80	
4	D	144	
5	E	63	
6	F	165	
7	G	91	
8	H	100	
9	I	37	

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Mol	Chain	Length	Quality of chain
10	J	41	51% 98%
11	K	85	95% 98%
12	L	159	36% 99%
13	O	93	70% 99%
14	P	219	100%
14	Q	219	99%
14	R	219	100%
14	T	219	99%
14	U	219	100%
15	S	234	100%
16	1	194	97%
16	a	194	69% 100%
17	2	201	98% 99%
18	3	203	80% 97%
19	4	205	41% 100%
20	5	225	95% 99%
21	6	230	56% 100%
22	7	213	76% 98%
23	8	217	44% 99%
24	9	182	62% 100%
			87% 99%

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
25	CLA	1	602	X	-	-	-
25	CLA	1	603	X	-	-	-
25	CLA	1	604	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
25	CLA	1	605	X	-	-	-
25	CLA	1	607	X	-	-	-
25	CLA	1	608	X	-	-	-
25	CLA	1	609	X	-	-	-
25	CLA	1	610	X	-	-	-
25	CLA	1	611	X	-	-	-
25	CLA	1	612	X	-	-	-
25	CLA	1	613	X	-	-	-
25	CLA	1	614	X	-	-	-
25	CLA	2	302	X	-	-	-
25	CLA	2	303	X	-	-	-
25	CLA	2	304	X	-	-	-
25	CLA	2	305	X	-	-	-
25	CLA	2	306	X	-	-	-
25	CLA	2	307	X	-	-	-
25	CLA	2	308	X	-	-	-
25	CLA	2	309	X	-	-	-
25	CLA	2	310	X	-	-	-
25	CLA	2	311	X	-	-	-
25	CLA	2	312	X	-	-	-
25	CLA	2	313	X	-	-	-
25	CLA	2	314	X	-	-	-
25	CLA	3	301	X	-	-	-
25	CLA	3	302	X	-	-	-
25	CLA	3	303	X	-	-	-
25	CLA	3	304	X	-	-	-
25	CLA	3	305	X	-	-	-
25	CLA	3	307	X	-	-	-
25	CLA	3	308	X	-	-	-
25	CLA	3	309	X	-	-	-
25	CLA	3	310	X	-	-	-
25	CLA	3	311	X	-	-	-
25	CLA	3	312	X	-	-	-
25	CLA	3	313	X	-	-	-
25	CLA	3	314	X	-	-	-
25	CLA	3	320	X	-	-	-
25	CLA	4	301	X	-	-	-
25	CLA	4	302	X	-	-	-
25	CLA	4	303	X	-	-	-
25	CLA	4	307	X	-	-	-
25	CLA	4	308	X	-	-	-
25	CLA	4	309	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
25	CLA	4	310	X	-	-	-
25	CLA	4	311	X	-	-	-
25	CLA	4	312	X	-	-	-
25	CLA	4	313	X	-	-	-
25	CLA	5	302	X	-	-	-
25	CLA	5	304	X	-	-	-
25	CLA	5	305	X	-	-	-
25	CLA	5	306	X	-	-	-
25	CLA	5	309	X	-	-	-
25	CLA	5	310	X	-	-	-
25	CLA	5	311	X	-	-	-
25	CLA	5	312	X	-	-	-
25	CLA	5	313	X	-	-	-
25	CLA	5	314	X	-	-	-
25	CLA	5	315	X	-	-	-
25	CLA	5	316	X	-	-	-
25	CLA	5	324	X	-	-	-
25	CLA	6	601	X	-	-	-
25	CLA	6	603	X	-	-	-
25	CLA	6	604	X	-	-	-
25	CLA	6	605	X	-	-	-
25	CLA	6	609	X	-	-	-
25	CLA	6	610	X	-	-	-
25	CLA	6	611	X	-	-	-
25	CLA	6	612	X	-	-	-
25	CLA	6	613	X	-	-	-
25	CLA	6	614	X	-	-	-
25	CLA	6	615	X	-	-	-
25	CLA	6	616	X	-	-	-
25	CLA	6	620	X	-	-	-
25	CLA	6	623	X	-	-	-
25	CLA	7	301	X	-	-	-
25	CLA	7	302	X	-	-	-
25	CLA	7	303	X	-	-	-
25	CLA	7	304	X	-	-	-
25	CLA	7	306	X	-	-	-
25	CLA	7	307	X	-	-	-
25	CLA	7	308	X	-	-	-
25	CLA	7	309	X	-	-	-
25	CLA	7	310	X	-	-	-
25	CLA	7	311	X	-	-	-
25	CLA	7	312	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
25	CLA	7	313	X	-	-	-
25	CLA	8	302	X	-	-	-
25	CLA	8	303	X	-	-	-
25	CLA	8	304	X	-	-	-
25	CLA	8	305	X	-	-	-
25	CLA	8	306	X	-	-	-
25	CLA	8	308	X	-	-	-
25	CLA	8	309	X	-	-	-
25	CLA	8	310	X	-	-	-
25	CLA	8	311	X	-	-	-
25	CLA	8	312	X	-	-	-
25	CLA	8	313	X	-	-	-
25	CLA	8	314	X	-	-	-
25	CLA	8	315	X	-	-	-
25	CLA	9	301	X	-	-	-
25	CLA	9	302	X	-	-	-
25	CLA	9	303	X	-	-	-
25	CLA	9	304	X	-	-	-
25	CLA	9	305	X	-	-	-
25	CLA	9	308	X	-	-	-
25	CLA	9	309	X	-	-	-
25	CLA	9	310	X	-	-	-
25	CLA	9	311	X	-	-	-
25	CLA	A	801	X	-	-	-
25	CLA	A	802	X	-	-	-
25	CLA	A	803	X	-	-	-
25	CLA	A	804	X	-	-	-
25	CLA	A	805	X	-	-	-
25	CLA	A	806	X	-	-	-
25	CLA	A	807	X	-	-	-
25	CLA	A	808	X	-	-	-
25	CLA	A	809	X	-	-	-
25	CLA	A	810	X	-	-	-
25	CLA	A	811	X	-	-	-
25	CLA	A	812	X	-	-	-
25	CLA	A	813	X	-	-	-
25	CLA	A	814	X	-	-	-
25	CLA	A	815	X	-	-	-
25	CLA	A	816	X	-	-	-
25	CLA	A	817	X	-	-	-
25	CLA	A	818	X	-	-	-
25	CLA	A	819	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
25	CLA	A	820	X	-	-	-
25	CLA	A	821	X	-	-	-
25	CLA	A	822	X	-	-	-
25	CLA	A	823	X	-	-	-
25	CLA	A	824	X	-	-	-
25	CLA	A	825	X	-	-	-
25	CLA	A	826	X	-	-	-
25	CLA	A	827	X	-	-	-
25	CLA	A	828	X	-	-	-
25	CLA	A	829	X	-	-	-
25	CLA	A	830	X	-	-	-
25	CLA	A	831	X	-	-	-
25	CLA	A	832	X	-	-	-
25	CLA	A	833	X	-	-	-
25	CLA	A	834	X	-	-	-
25	CLA	A	835	X	-	-	-
25	CLA	A	836	X	-	-	-
25	CLA	A	837	X	-	-	-
25	CLA	A	838	X	-	-	-
25	CLA	A	839	X	-	-	-
25	CLA	A	840	X	-	-	-
25	CLA	A	842	X	-	-	-
25	CLA	A	851	X	-	-	-
25	CLA	A	853	X	-	-	-
25	CLA	B	801	X	-	-	-
25	CLA	B	802	X	-	-	-
25	CLA	B	803	X	-	-	-
25	CLA	B	804	X	-	-	-
25	CLA	B	805	X	-	-	-
25	CLA	B	806	X	-	-	-
25	CLA	B	807	X	-	-	-
25	CLA	B	808	X	-	-	-
25	CLA	B	809	X	-	-	-
25	CLA	B	810	X	-	-	-
25	CLA	B	811	X	-	-	-
25	CLA	B	812	X	-	-	-
25	CLA	B	813	X	-	-	-
25	CLA	B	814	X	-	-	-
25	CLA	B	815	X	-	-	-
25	CLA	B	816	X	-	-	-
25	CLA	B	817	X	-	-	-
25	CLA	B	818	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
25	CLA	B	819	X	-	-	-
25	CLA	B	820	X	-	-	-
25	CLA	B	821	X	-	-	-
25	CLA	B	822	X	-	-	-
25	CLA	B	823	X	-	-	-
25	CLA	B	824	X	-	-	-
25	CLA	B	825	X	-	-	-
25	CLA	B	826	X	-	-	-
25	CLA	B	827	X	-	-	-
25	CLA	B	828	X	-	-	-
25	CLA	B	829	X	-	-	-
25	CLA	B	830	X	-	-	-
25	CLA	B	831	X	-	-	-
25	CLA	B	832	X	-	-	-
25	CLA	B	833	X	-	-	-
25	CLA	B	834	X	-	-	-
25	CLA	B	835	X	-	-	-
25	CLA	B	836	X	-	-	-
25	CLA	B	837	X	-	-	-
25	CLA	B	838	X	-	-	-
25	CLA	B	849	X	-	-	-
25	CLA	F	802	X	-	-	-
25	CLA	G	201	X	-	-	-
25	CLA	G	202	X	-	-	-
25	CLA	H	201	X	-	-	-
25	CLA	H	202	X	-	-	-
25	CLA	H	203	X	-	-	-
25	CLA	H	205	X	-	-	-
25	CLA	J	103	X	-	-	-
25	CLA	J	105	X	-	-	-
25	CLA	K	201	X	-	-	-
25	CLA	K	202	X	-	-	-
25	CLA	K	203	X	-	-	-
25	CLA	K	204	X	-	-	-
25	CLA	K	205	X	-	-	-
25	CLA	L	201	X	-	-	-
25	CLA	L	202	X	-	-	-
25	CLA	L	205	X	-	-	-
25	CLA	L	206	X	-	-	-
25	CLA	L	209	X	-	-	-
25	CLA	O	201	X	-	-	-
25	CLA	O	202	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
25	CLA	O	203	X	-	-	-
25	CLA	P	602	X	-	-	-
25	CLA	P	603	X	-	-	-
25	CLA	P	604	X	-	-	-
25	CLA	P	610	X	-	-	-
25	CLA	P	611	X	-	-	-
25	CLA	P	612	X	-	-	-
25	CLA	P	613	X	-	-	-
25	CLA	Q	602	X	-	-	-
25	CLA	Q	603	X	-	-	-
25	CLA	Q	604	X	-	-	-
25	CLA	Q	609	X	-	-	-
25	CLA	Q	610	X	-	-	-
25	CLA	Q	611	X	-	-	-
25	CLA	Q	612	X	-	-	-
25	CLA	Q	613	X	-	-	-
25	CLA	R	602	X	-	-	-
25	CLA	R	603	X	-	-	-
25	CLA	R	604	X	-	-	-
25	CLA	R	610	X	-	-	-
25	CLA	R	611	X	-	-	-
25	CLA	R	612	X	-	-	-
25	CLA	R	613	X	-	-	-
25	CLA	R	614	X	-	-	-
25	CLA	S	301	X	-	-	-
25	CLA	S	303	X	-	-	-
25	CLA	S	304	X	-	-	-
25	CLA	S	305	X	-	-	-
25	CLA	S	311	X	-	-	-
25	CLA	S	312	X	-	-	-
25	CLA	S	313	X	-	-	-
25	CLA	S	315	X	-	-	-
25	CLA	S	320	X	-	-	-
25	CLA	T	602	X	-	-	-
25	CLA	T	603	X	-	-	-
25	CLA	T	608	X	-	-	-
25	CLA	T	610	X	-	-	-
25	CLA	T	611	X	-	-	-
25	CLA	T	612	X	-	-	-
25	CLA	U	302	X	-	-	-
25	CLA	U	303	X	-	-	-
25	CLA	U	304	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
25	CLA	U	310	X	-	-	-
25	CLA	U	311	X	-	-	-
25	CLA	U	312	X	-	-	-
25	CLA	U	313	X	-	-	-
25	CLA	a	301	X	-	-	-
25	CLA	a	302	X	-	-	-
25	CLA	a	303	X	-	-	-
25	CLA	a	304	X	-	-	-
25	CLA	a	306	X	-	-	-
25	CLA	a	307	X	-	-	-
25	CLA	a	308	X	-	-	-
25	CLA	a	309	X	-	-	-
25	CLA	a	310	X	-	-	-
25	CLA	a	311	X	-	-	-
25	CLA	a	312	X	-	-	-
25	CLA	a	313	X	-	-	-
33	CHL	1	601	X	-	-	-
33	CHL	1	606	X	-	-	-
33	CHL	3	306	X	-	-	-
33	CHL	4	304	X	-	-	-
33	CHL	4	305	X	-	-	-
33	CHL	4	306	X	-	-	-
33	CHL	4	314	X	-	-	-
33	CHL	4	322	X	-	-	-
33	CHL	5	307	X	-	-	-
33	CHL	5	308	X	-	-	-
33	CHL	5	317	X	-	-	-
33	CHL	6	606	X	-	-	-
33	CHL	6	607	X	-	-	-
33	CHL	6	608	X	-	-	-
33	CHL	6	617	X	-	-	-
33	CHL	7	305	X	-	-	-
33	CHL	8	307	X	-	-	-
33	CHL	9	306	X	-	-	-
33	CHL	9	307	X	-	-	-
33	CHL	P	601	X	-	-	-
33	CHL	P	605	X	-	-	-
33	CHL	P	606	X	-	-	-
33	CHL	P	607	X	-	-	-
33	CHL	P	608	X	-	-	-
33	CHL	P	609	X	-	-	-
33	CHL	P	619	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
33	CHL	P	622	X	-	-	-
33	CHL	Q	601	X	-	-	-
33	CHL	Q	605	X	-	-	-
33	CHL	Q	606	X	-	-	-
33	CHL	Q	607	X	-	-	-
33	CHL	Q	608	X	-	-	-
33	CHL	R	601	X	-	-	-
33	CHL	R	605	X	-	-	-
33	CHL	R	606	X	-	-	-
33	CHL	R	607	X	-	-	-
33	CHL	R	608	X	-	-	-
33	CHL	R	609	X	-	-	-
33	CHL	S	302	X	-	-	-
33	CHL	S	306	X	-	-	-
33	CHL	S	307	X	-	-	-
33	CHL	S	308	X	-	-	-
33	CHL	S	309	X	-	-	-
33	CHL	S	310	X	-	-	-
33	CHL	S	321	X	-	-	-
33	CHL	T	601	X	-	-	-
33	CHL	T	604	X	-	-	-
33	CHL	T	605	X	-	-	-
33	CHL	T	606	X	-	-	-
33	CHL	T	607	X	-	-	-
33	CHL	U	305	X	-	-	-
33	CHL	U	306	X	-	-	-
33	CHL	U	307	X	-	-	-
33	CHL	U	308	X	-	-	-
33	CHL	U	309	X	-	-	-
33	CHL	a	305	X	-	-	-

2 Entry composition

There are 36 unique types of molecules in this entry. The entry contains 68860 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Photosystem I P700 chlorophyll a apoprotein A1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	740	5811	3799	991	999	22	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	734	5828	3827	978	1005	18	0	0

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	D	144	1132	725	200	200	7	0	0

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

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

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

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

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

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
7	G	91	678	436	114	128	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	H	100	773	479	138	154	2	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	I	37	281	195	39	46	1	0	0

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

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

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

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

- Molecule 12 is a protein called PSI subunit V.

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

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

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
13	O	93	720	477	118	125	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
14	P	219	Total	C	N	O	S	0	0
			1669	1080	272	314	3		
14	Q	219	Total	C	N	O	S	0	0
			1669	1080	272	314	3		
14	R	219	Total	C	N	O	S	0	0
			1669	1080	272	314	3		
14	T	219	Total	C	N	O	S	0	0
			1669	1080	272	314	3		
14	U	219	Total	C	N	O	S	0	0
			1669	1080	272	314	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace	
15	S	233	Total	C	N	O	P	S	0	0
			1717	1098	285	328	1	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
16	1	194	Total	C	N	O	S	0	0
			1444	941	240	260	3		
16	a	194	Total	C	N	O	S	0	0
			1444	941	240	260	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
17	2	201	Total	C	N	O	S	0	0
			1545	1002	253	280	10		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
18	3	203	Total	C	N	O	S	0	0
			1560	1021	253	278	8		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
19	4	205	Total	C	N	O	S	0	0
			1590	1046	254	285	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
20	5	225	1757	1145	294	310	8	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
21	6	230	1771	1167	293	305	6	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
22	7	212	1644	1067	274	297	6	0	0

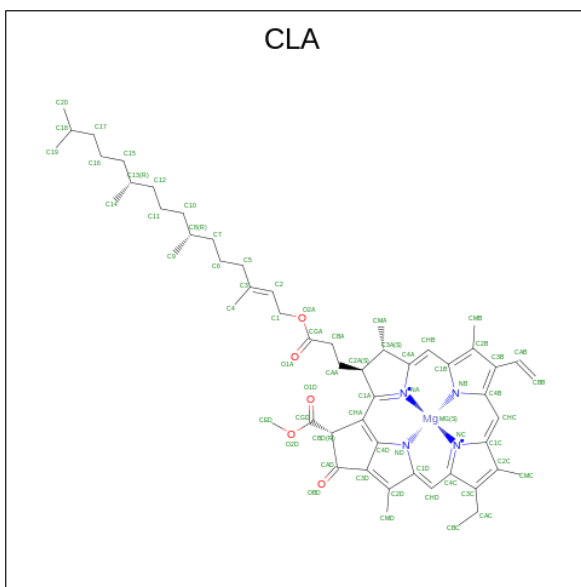
- Molecule 23 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
23	8	217	1649	1073	280	292	4	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
24	9	182	1392	903	231	251	7	0	0

- Molecule 25 is CHLOROPHYLL A (three-letter code: CLA) (formula: C₅₅H₇₂MgN₄O₅).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
25	A	1	Total 2638	C 2208	Mg 43	N 172	O 215	0
25	A	1	Total 2638	C 2208	Mg 43	N 172	O 215	0
25	A	1	Total 2638	C 2208	Mg 43	N 172	O 215	0
25	A	1	Total 2638	C 2208	Mg 43	N 172	O 215	0
25	A	1	Total 2638	C 2208	Mg 43	N 172	O 215	0
25	A	1	Total 2638	C 2208	Mg 43	N 172	O 215	0
25	A	1	Total 2638	C 2208	Mg 43	N 172	O 215	0
25	A	1	Total 2638	C 2208	Mg 43	N 172	O 215	0
25	A	1	Total 2638	C 2208	Mg 43	N 172	O 215	0
25	A	1	Total 2638	C 2208	Mg 43	N 172	O 215	0
25	A	1	Total 2638	C 2208	Mg 43	N 172	O 215	0
25	A	1	Total 2638	C 2208	Mg 43	N 172	O 215	0
25	A	1	Total 2638	C 2208	Mg 43	N 172	O 215	0
25	A	1	Total 2638	C 2208	Mg 43	N 172	O 215	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
25	A	1	Total 2638	C 2208	Mg 43	N 172	O 215	0
25	A	1	Total 2638	C 2208	Mg 43	N 172	O 215	0
25	A	1	Total 2638	C 2208	Mg 43	N 172	O 215	0
25	A	1	Total 2638	C 2208	Mg 43	N 172	O 215	0
25	A	1	Total 2638	C 2208	Mg 43	N 172	O 215	0
25	A	1	Total 2638	C 2208	Mg 43	N 172	O 215	0
25	A	1	Total 2638	C 2208	Mg 43	N 172	O 215	0
25	A	1	Total 2638	C 2208	Mg 43	N 172	O 215	0
25	B	1	Total 2368	C 1978	Mg 39	N 156	O 195	0
25	B	1	Total 2368	C 1978	Mg 39	N 156	O 195	0
25	B	1	Total 2368	C 1978	Mg 39	N 156	O 195	0
25	B	1	Total 2368	C 1978	Mg 39	N 156	O 195	0
25	B	1	Total 2368	C 1978	Mg 39	N 156	O 195	0
25	B	1	Total 2368	C 1978	Mg 39	N 156	O 195	0
25	B	1	Total 2368	C 1978	Mg 39	N 156	O 195	0
25	B	1	Total 2368	C 1978	Mg 39	N 156	O 195	0
25	B	1	Total 2368	C 1978	Mg 39	N 156	O 195	0
25	B	1	Total 2368	C 1978	Mg 39	N 156	O 195	0
25	B	1	Total 2368	C 1978	Mg 39	N 156	O 195	0
25	B	1	Total 2368	C 1978	Mg 39	N 156	O 195	0
25	B	1	Total 2368	C 1978	Mg 39	N 156	O 195	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
25	B	1	Total 2368	C 1978	Mg 39	N 156	O 195	0
25	B	1	Total 2368	C 1978	Mg 39	N 156	O 195	0
25	B	1	Total 2368	C 1978	Mg 39	N 156	O 195	0
25	B	1	Total 2368	C 1978	Mg 39	N 156	O 195	0
25	B	1	Total 2368	C 1978	Mg 39	N 156	O 195	0
25	F	1	Total 45	C 35	Mg 1	N 4	O 5	0
25	G	1	Total 96	C 76	Mg 2	N 8	O 10	0
25	G	1	Total 96	C 76	Mg 2	N 8	O 10	0
25	H	1	Total 175	C 139	Mg 4	N 16	O 16	0
25	H	1	Total 175	C 139	Mg 4	N 16	O 16	0
25	H	1	Total 175	C 139	Mg 4	N 16	O 16	0
25	H	1	Total 175	C 139	Mg 4	N 16	O 16	0
25	J	1	Total 100	C 82	Mg 2	N 8	O 8	0
25	J	1	Total 100	C 82	Mg 2	N 8	O 8	0
25	K	1	Total 232	C 182	Mg 5	N 20	O 25	0
25	K	1	Total 232	C 182	Mg 5	N 20	O 25	0
25	K	1	Total 232	C 182	Mg 5	N 20	O 25	0
25	K	1	Total 232	C 182	Mg 5	N 20	O 25	0
25	K	1	Total 232	C 182	Mg 5	N 20	O 25	0
25	L	1	Total 278	C 232	Mg 5	N 20	O 21	0
25	L	1	Total 278	C 232	Mg 5	N 20	O 21	0

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Mol	Chain	Residues	Atoms					AltConf
25	L	1	Total	C	Mg	N	O	0
			278	232	5	20	21	
25	L	1	Total	C	Mg	N	O	0
			278	232	5	20	21	
25	L	1	Total	C	Mg	N	O	0
			278	232	5	20	21	
25	O	1	Total	C	Mg	N	O	0
			117	93	3	12	9	
25	O	1	Total	C	Mg	N	O	0
			117	93	3	12	9	
25	O	1	Total	C	Mg	N	O	0
			117	93	3	12	9	
25	P	1	Total	C	Mg	N	O	0
			399	331	7	28	33	
25	P	1	Total	C	Mg	N	O	0
			399	331	7	28	33	
25	P	1	Total	C	Mg	N	O	0
			399	331	7	28	33	
25	P	1	Total	C	Mg	N	O	0
			399	331	7	28	33	
25	P	1	Total	C	Mg	N	O	0
			399	331	7	28	33	
25	P	1	Total	C	Mg	N	O	0
			399	331	7	28	33	
25	P	1	Total	C	Mg	N	O	0
			399	331	7	28	33	
25	P	1	Total	C	Mg	N	O	0
			399	331	7	28	33	
25	Q	1	Total	C	Mg	N	O	0
			493	407	9	36	41	
25	Q	1	Total	C	Mg	N	O	0
			493	407	9	36	41	
25	Q	1	Total	C	Mg	N	O	0
			493	407	9	36	41	
25	Q	1	Total	C	Mg	N	O	0
			493	407	9	36	41	
25	Q	1	Total	C	Mg	N	O	0
			493	407	9	36	41	
25	Q	1	Total	C	Mg	N	O	0
			493	407	9	36	41	
25	Q	1	Total	C	Mg	N	O	0
			493	407	9	36	41	

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Mol	Chain	Residues	Atoms					AltConf
25	Q	1	Total	C	Mg	N	O	0
			493	407	9	36	41	
25	R	1	Total	C	Mg	N	O	0
			477	397	8	32	40	
25	R	1	Total	C	Mg	N	O	0
			477	397	8	32	40	
25	R	1	Total	C	Mg	N	O	0
			477	397	8	32	40	
25	R	1	Total	C	Mg	N	O	0
			477	397	8	32	40	
25	R	1	Total	C	Mg	N	O	0
			477	397	8	32	40	
25	R	1	Total	C	Mg	N	O	0
			477	397	8	32	40	
25	R	1	Total	C	Mg	N	O	0
			477	397	8	32	40	
25	S	1	Total	C	Mg	N	O	0
			585	485	10	40	50	
25	S	1	Total	C	Mg	N	O	0
			585	485	10	40	50	
25	S	1	Total	C	Mg	N	O	0
			585	485	10	40	50	
25	S	1	Total	C	Mg	N	O	0
			585	485	10	40	50	
25	S	1	Total	C	Mg	N	O	0
			585	485	10	40	50	
25	S	1	Total	C	Mg	N	O	0
			585	485	10	40	50	
25	S	1	Total	C	Mg	N	O	0
			585	485	10	40	50	
25	S	1	Total	C	Mg	N	O	0
			585	485	10	40	50	
25	S	1	Total	C	Mg	N	O	0
			585	485	10	40	50	
25	T	1	Total	C	Mg	N	O	0
			408	338	7	28	35	
25	T	1	Total	C	Mg	N	O	0
			408	338	7	28	35	

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
25	T	1	408	338	7	28	35	0
25	T	1	408	338	7	28	35	0
25	T	1	408	338	7	28	35	0
25	T	1	408	338	7	28	35	0
25	T	1	408	338	7	28	35	0
25	U	1	408	341	7	28	32	0
25	U	1	408	341	7	28	32	0
25	U	1	408	341	7	28	32	0
25	U	1	408	341	7	28	32	0
25	U	1	408	341	7	28	32	0
25	U	1	408	341	7	28	32	0
25	U	1	408	341	7	28	32	0
25	U	1	408	341	7	28	32	0
25	1	1	722	602	12	48	60	0
25	1	1	722	602	12	48	60	0
25	1	1	722	602	12	48	60	0
25	1	1	722	602	12	48	60	0
25	1	1	722	602	12	48	60	0
25	1	1	722	602	12	48	60	0
25	1	1	722	602	12	48	60	0
25	1	1	722	602	12	48	60	0
25	1	1	722	602	12	48	60	0
25	1	1	722	602	12	48	60	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
25	1	1	722	602	12	48	60	0
25	1	1	722	602	12	48	60	0
25	1	1	722	602	12	48	60	0
25	2	1	681	557	13	52	59	0
25	2	1	681	557	13	52	59	0
25	2	1	681	557	13	52	59	0
25	2	1	681	557	13	52	59	0
25	2	1	681	557	13	52	59	0
25	2	1	681	557	13	52	59	0
25	2	1	681	557	13	52	59	0
25	2	1	681	557	13	52	59	0
25	2	1	681	557	13	52	59	0
25	2	1	681	557	13	52	59	0
25	2	1	681	557	13	52	59	0
25	2	1	681	557	13	52	59	0
25	2	1	681	557	13	52	59	0
25	2	1	681	557	13	52	59	0
25	2	1	681	557	13	52	59	0
25	3	1	761	625	14	56	66	0
25	3	1	761	625	14	56	66	0
25	3	1	761	625	14	56	66	0
25	3	1	761	625	14	56	66	0
25	3	1	761	625	14	56	66	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
25	3	1	761	625	14	56	66	0
25	3	1	761	625	14	56	66	0
25	3	1	761	625	14	56	66	0
25	3	1	761	625	14	56	66	0
25	3	1	761	625	14	56	66	0
25	3	1	761	625	14	56	66	0
25	3	1	761	625	14	56	66	0
25	3	1	761	625	14	56	66	0
25	3	1	761	625	14	56	66	0
25	3	1	761	625	14	56	66	0
25	4	1	515	417	10	40	48	0
25	4	1	515	417	10	40	48	0
25	4	1	515	417	10	40	48	0
25	4	1	515	417	10	40	48	0
25	4	1	515	417	10	40	48	0
25	4	1	515	417	10	40	48	0
25	4	1	515	417	10	40	48	0
25	4	1	515	417	10	40	48	0
25	4	1	515	417	10	40	48	0
25	4	1	515	417	10	40	48	0
25	4	1	515	417	10	40	48	0
25	5	1	799	651	15	60	73	0
25	5	1	799	651	15	60	73	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
25	5	1	799	651	15	60	73	0
25	5	1	799	651	15	60	73	0
25	5	1	799	651	15	60	73	0
25	5	1	799	651	15	60	73	0
25	5	1	799	651	15	60	73	0
25	5	1	799	651	15	60	73	0
25	5	1	799	651	15	60	73	0
25	5	1	799	651	15	60	73	0
25	5	1	799	651	15	60	73	0
25	5	1	799	651	15	60	73	0
25	5	1	799	651	15	60	73	0
25	5	1	799	651	15	60	73	0
25	5	1	799	651	15	60	73	0
25	5	1	799	651	15	60	73	0
25	5	1	799	651	15	60	73	0
25	5	1	799	651	15	60	73	0
25	5	1	799	651	15	60	73	0
25	6	1	752	612	14	56	70	0
25	6	1	752	612	14	56	70	0
25	6	1	752	612	14	56	70	0
25	6	1	752	612	14	56	70	0
25	6	1	752	612	14	56	70	0
25	6	1	752	612	14	56	70	0
25	6	1	752	612	14	56	70	0
25	6	1	752	612	14	56	70	0
25	6	1	752	612	14	56	70	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
25	6	1	752	612	14	56	70	0
25	6	1	752	612	14	56	70	0
25	6	1	752	612	14	56	70	0
25	6	1	752	612	14	56	70	0
25	6	1	752	612	14	56	70	0
25	6	1	752	612	14	56	70	0
25	7	1	616	502	12	48	54	0
25	7	1	616	502	12	48	54	0
25	7	1	616	502	12	48	54	0
25	7	1	616	502	12	48	54	0
25	7	1	616	502	12	48	54	0
25	7	1	616	502	12	48	54	0
25	7	1	616	502	12	48	54	0
25	7	1	616	502	12	48	54	0
25	7	1	616	502	12	48	54	0
25	7	1	616	502	12	48	54	0
25	7	1	616	502	12	48	54	0
25	7	1	616	502	12	48	54	0
25	7	1	616	502	12	48	54	0
25	8	1	680	552	13	52	63	0
25	8	1	680	552	13	52	63	0
25	8	1	680	552	13	52	63	0

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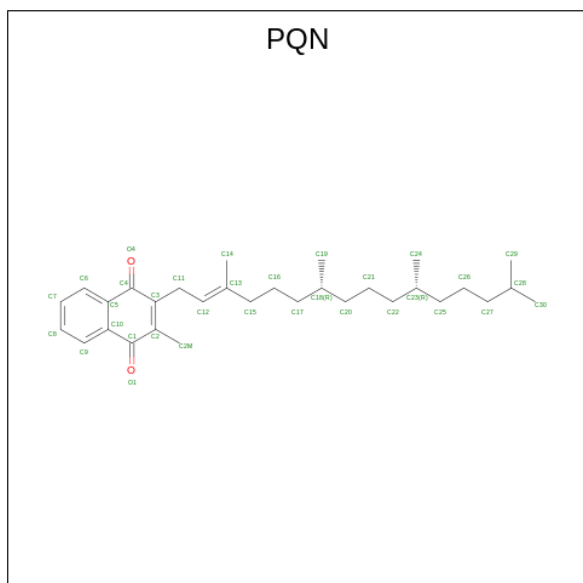
Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
25	8	1	680	552	13	52	63	0
25	8	1	680	552	13	52	63	0
25	8	1	680	552	13	52	63	0
25	8	1	680	552	13	52	63	0
25	8	1	680	552	13	52	63	0
25	8	1	680	552	13	52	63	0
25	8	1	680	552	13	52	63	0
25	8	1	680	552	13	52	63	0
25	8	1	680	552	13	52	63	0
25	8	1	680	552	13	52	63	0
25	8	1	680	552	13	52	63	0
25	9	1	461	371	9	36	45	0
25	9	1	461	371	9	36	45	0
25	9	1	461	371	9	36	45	0
25	9	1	461	371	9	36	45	0
25	9	1	461	371	9	36	45	0
25	9	1	461	371	9	36	45	0
25	9	1	461	371	9	36	45	0
25	9	1	461	371	9	36	45	0
25	9	1	461	371	9	36	45	0
25	9	1	461	371	9	36	45	0
25	a	1	714	594	12	48	60	0
25	a	1	714	594	12	48	60	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
25	a	1	Total 714	C 594	Mg 12	N 48	O 60	0
25	a	1	Total 714	C 594	Mg 12	N 48	O 60	0
25	a	1	Total 714	C 594	Mg 12	N 48	O 60	0
25	a	1	Total 714	C 594	Mg 12	N 48	O 60	0
25	a	1	Total 714	C 594	Mg 12	N 48	O 60	0
25	a	1	Total 714	C 594	Mg 12	N 48	O 60	0
25	a	1	Total 714	C 594	Mg 12	N 48	O 60	0
25	a	1	Total 714	C 594	Mg 12	N 48	O 60	0
25	a	1	Total 714	C 594	Mg 12	N 48	O 60	0
25	a	1	Total 714	C 594	Mg 12	N 48	O 60	0

- Molecule 26 is PHYLLOQUINONE (three-letter code: PQN) (formula: C₃₁H₄₆O₂).



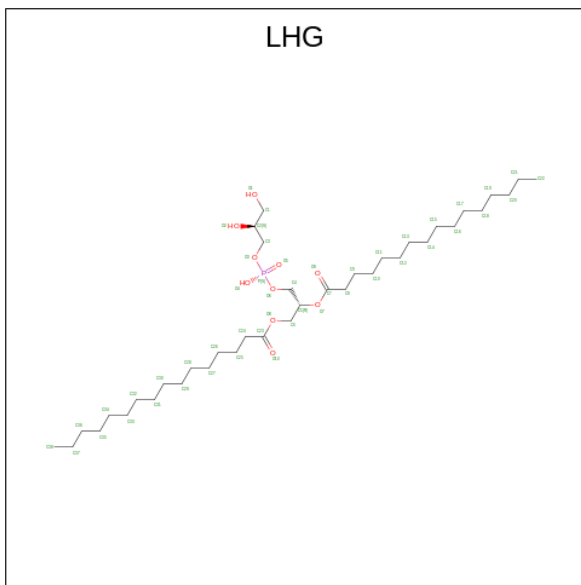
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
26	A	1	Total 33	C 31	O 2	0

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

- Molecule 27 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula: $C_{38}H_{75}O_{10}P$).



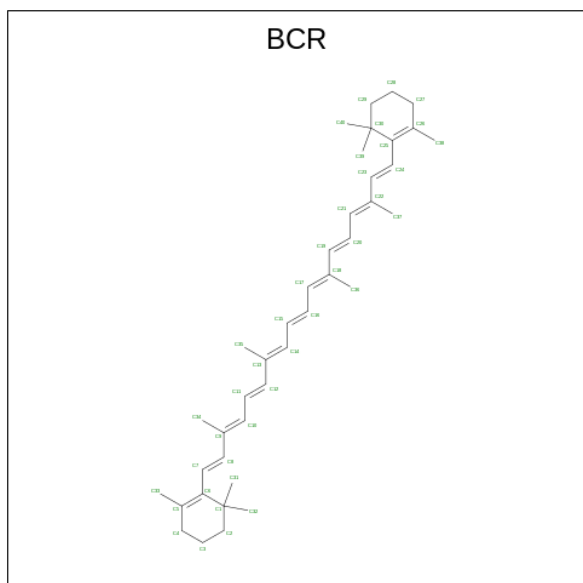
Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
27	A	1	135	102	30	3	0
27	A	1	135	102	30	3	0
27	A	1	135	102	30	3	0
27	B	1	38	27	10	1	0
27	P	1	98	76	20	2	0
27	P	1	98	76	20	2	0
27	Q	1	49	38	10	1	0
27	R	1	49	38	10	1	0
27	S	1	49	38	10	1	0
27	T	1	49	38	10	1	0

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
27	1	1	Total 43	C 32	O 10	P 1	0
27	2	1	Total 49	C 38	O 10	P 1	0
27	4	1	Total 81	C 59	O 20	P 2	0
27	4	1	Total 81	C 59	O 20	P 2	0
27	5	1	Total 82	C 60	O 20	P 2	0
27	5	1	Total 82	C 60	O 20	P 2	0
27	6	1	Total 49	C 38	O 10	P 1	0
27	7	1	Total 37	C 26	O 10	P 1	0
27	8	1	Total 49	C 38	O 10	P 1	0
27	a	1	Total 43	C 32	O 10	P 1	0

- Molecule 28 is BETA-CAROTENE (three-letter code: BCR) (formula: $C_{40}H_{56}$).



Mol	Chain	Residues	Atoms		AltConf
28	A	1	Total 240	C 240	0

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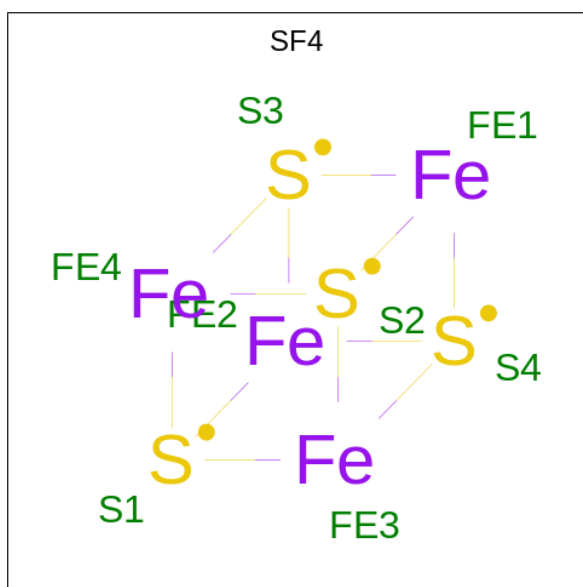
Mol	Chain	Residues	Atoms		AltConf
28	A	1	Total 240	C 240	0
28	A	1	Total 240	C 240	0
28	A	1	Total 240	C 240	0
28	A	1	Total 240	C 240	0
28	A	1	Total 240	C 240	0
28	B	1	Total 280	C 280	0
28	B	1	Total 280	C 280	0
28	B	1	Total 280	C 280	0
28	B	1	Total 280	C 280	0
28	B	1	Total 280	C 280	0
28	B	1	Total 280	C 280	0
28	B	1	Total 280	C 280	0
28	B	1	Total 280	C 280	0
28	F	1	Total 80	C 80	0
28	F	1	Total 80	C 80	0
28	G	1	Total 40	C 40	0
28	I	1	Total 40	C 40	0
28	J	1	Total 80	C 80	0
28	J	1	Total 80	C 80	0
28	K	1	Total 40	C 40	0
28	L	1	Total 160	C 160	0
28	L	1	Total 160	C 160	0

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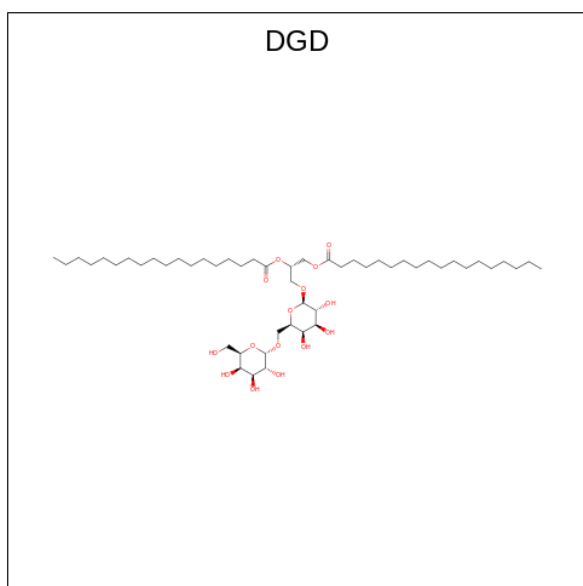
Mol	Chain	Residues	Atoms		AltConf
28	L	1	Total 160	C 160	0
28	L	1	Total 160	C 160	0
28	O	1	Total 80	C 80	0
28	O	1	Total 80	C 80	0
28	3	1	Total 120	C 120	0
28	3	1	Total 120	C 120	0
28	3	1	Total 120	C 120	0
28	4	1	Total 80	C 80	0
28	4	1	Total 80	C 80	0
28	5	1	Total 80	C 80	0
28	5	1	Total 80	C 80	0
28	6	1	Total 40	C 40	0
28	7	1	Total 40	C 40	0
28	8	1	Total 80	C 80	0
28	8	1	Total 80	C 80	0

- Molecule 29 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe₄S₄).



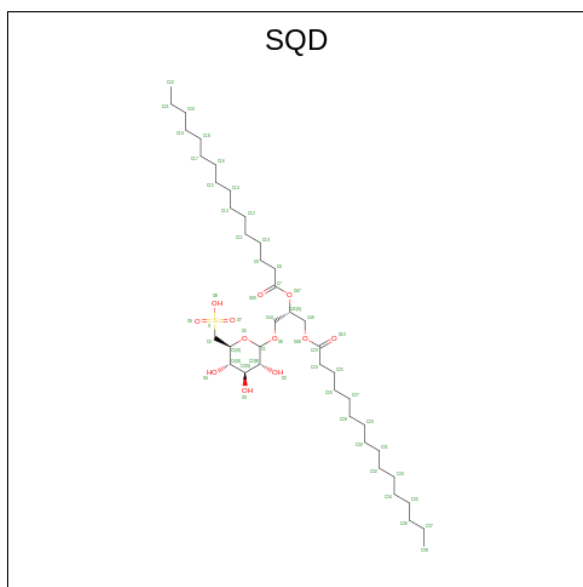
Mol	Chain	Residues	Atoms			AltConf
29	A	1	Total	Fe	S	0
			8	4	4	
29	C	1	Total	Fe	S	0
			16	8	8	
29	C	1	Total	Fe	S	0
			16	8	8	

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



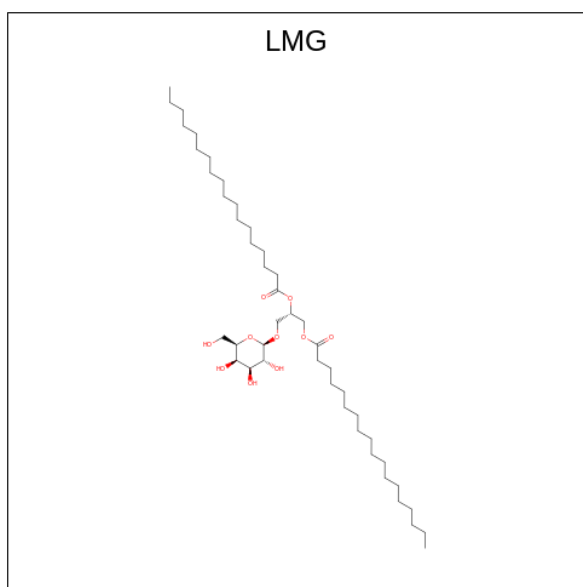
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
30	B	1	123	93	30	0
30	B	1	123	93	30	0

- Molecule 31 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (three-letter code: SQD) (formula: $C_{41}H_{78}O_{12}S$).



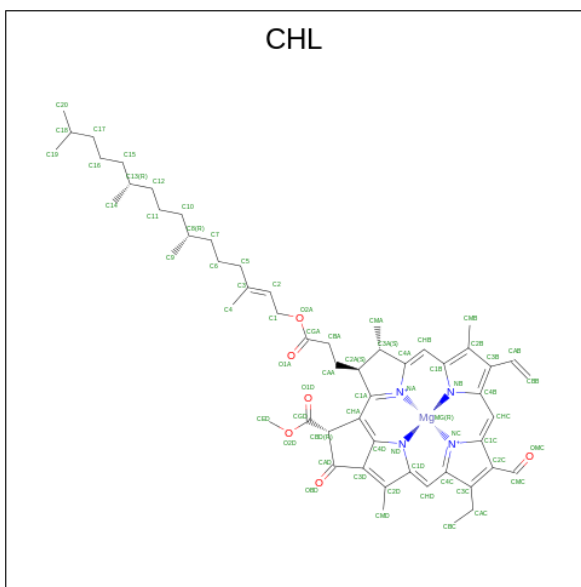
Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	S	
31	B	1	51	38	12	1	0

- Molecule 32 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: LMG) (formula: $C_{45}H_{86}O_{10}$).



Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
32	H	1	47	37	10	0
32	J	1	130	100	30	0
32	J	1	130	100	30	0
32	J	1	130	100	30	0
32	1	1	46	36	10	0
32	2	1	41	31	10	0
32	4	1	40	30	10	0
32	6	1	40	30	10	0
32	7	1	71	51	20	0
32	7	1	71	51	20	0

- Molecule 33 is CHLOROPHYLL B (three-letter code: CHL) (formula: $C_{55}H_{70}MgN_4O_6$).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
33	P	1	416	330	8	32	46	0
33	P	1	416	330	8	32	46	0
33	P	1	416	330	8	32	46	0
33	P	1	416	330	8	32	46	0
33	P	1	416	330	8	32	46	0
33	P	1	416	330	8	32	46	0
33	P	1	416	330	8	32	46	0
33	P	1	416	330	8	32	46	0
33	Q	1	253	202	5	20	26	0
33	Q	1	253	202	5	20	26	0
33	Q	1	253	202	5	20	26	0
33	Q	1	253	202	5	20	26	0
33	Q	1	253	202	5	20	26	0
33	R	1	309	245	6	24	34	0

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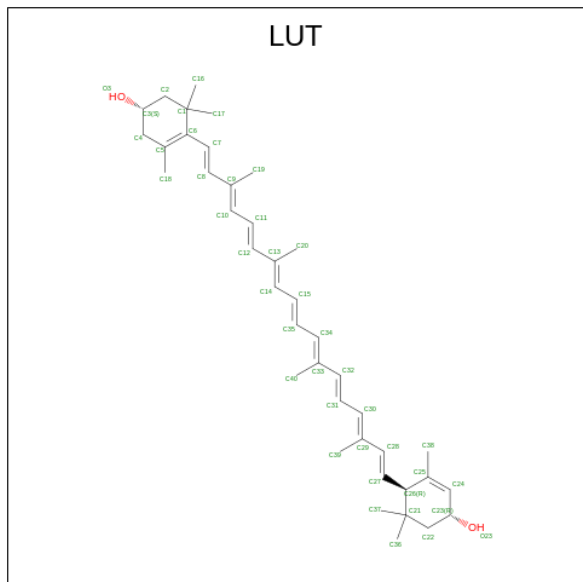
Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
33	R	1	Total 309	C 245	Mg 6	N 24	O 34	0
33	R	1	Total 309	C 245	Mg 6	N 24	O 34	0
33	R	1	Total 309	C 245	Mg 6	N 24	O 34	0
33	R	1	Total 309	C 245	Mg 6	N 24	O 34	0
33	R	1	Total 309	C 245	Mg 6	N 24	O 34	0
33	S	1	Total 358	C 281	Mg 7	N 28	O 42	0
33	S	1	Total 358	C 281	Mg 7	N 28	O 42	0
33	S	1	Total 358	C 281	Mg 7	N 28	O 42	0
33	S	1	Total 358	C 281	Mg 7	N 28	O 42	0
33	S	1	Total 358	C 281	Mg 7	N 28	O 42	0
33	S	1	Total 358	C 281	Mg 7	N 28	O 42	0
33	S	1	Total 358	C 281	Mg 7	N 28	O 42	0
33	S	1	Total 358	C 281	Mg 7	N 28	O 42	0
33	T	1	Total 244	C 191	Mg 5	N 20	O 28	0
33	T	1	Total 244	C 191	Mg 5	N 20	O 28	0
33	T	1	Total 244	C 191	Mg 5	N 20	O 28	0
33	T	1	Total 244	C 191	Mg 5	N 20	O 28	0
33	T	1	Total 244	C 191	Mg 5	N 20	O 28	0
33	T	1	Total 244	C 191	Mg 5	N 20	O 28	0
33	U	1	Total 241	C 188	Mg 5	N 20	O 28	0
33	U	1	Total 241	C 188	Mg 5	N 20	O 28	0
33	U	1	Total 241	C 188	Mg 5	N 20	O 28	0
33	U	1	Total 241	C 188	Mg 5	N 20	O 28	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
33	U	1	Total 241	C 188	Mg 5	N 20	O 28	0
33	1	1	Total 101	C 79	Mg 2	N 8	O 12	0
33	1	1	Total 101	C 79	Mg 2	N 8	O 12	0
33	3	1	Total 53	C 42	Mg 1	N 4	O 6	0
33	4	1	Total 240	C 189	Mg 5	N 20	O 26	0
33	4	1	Total 240	C 189	Mg 5	N 20	O 26	0
33	4	1	Total 240	C 189	Mg 5	N 20	O 26	0
33	4	1	Total 240	C 189	Mg 5	N 20	O 26	0
33	4	1	Total 240	C 189	Mg 5	N 20	O 26	0
33	4	1	Total 240	C 189	Mg 5	N 20	O 26	0
33	5	1	Total 145	C 114	Mg 3	N 12	O 16	0
33	5	1	Total 145	C 114	Mg 3	N 12	O 16	0
33	5	1	Total 145	C 114	Mg 3	N 12	O 16	0
33	6	1	Total 200	C 158	Mg 4	N 16	O 22	0
33	6	1	Total 200	C 158	Mg 4	N 16	O 22	0
33	6	1	Total 200	C 158	Mg 4	N 16	O 22	0
33	6	1	Total 200	C 158	Mg 4	N 16	O 22	0
33	7	1	Total 54	C 43	Mg 1	N 4	O 6	0
33	8	1	Total 53	C 42	Mg 1	N 4	O 6	0
33	9	1	Total 93	C 73	Mg 2	N 8	O 10	0
33	9	1	Total 93	C 73	Mg 2	N 8	O 10	0
33	a	1	Total 48	C 37	Mg 1	N 4	O 6	0

- Molecule 34 is (3R,3'R,6S)-4,5-DIDEHYDRO-5,6-DIHYDRO-BETA,BETA-CAROTENE-3,3'-DIOL (three-letter code: LUT) (formula: C₄₀H₅₆O₂).



Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
34	P	1	84	80	4	0
34	P	1	84	80	4	0
34	Q	1	84	80	4	0
34	Q	1	84	80	4	0
34	R	1	84	80	4	0
34	R	1	84	80	4	0
34	S	1	84	80	4	0
34	S	1	84	80	4	0
34	T	1	84	80	4	0
34	T	1	84	80	4	0
34	U	1	84	80	4	0
34	U	1	84	80	4	0

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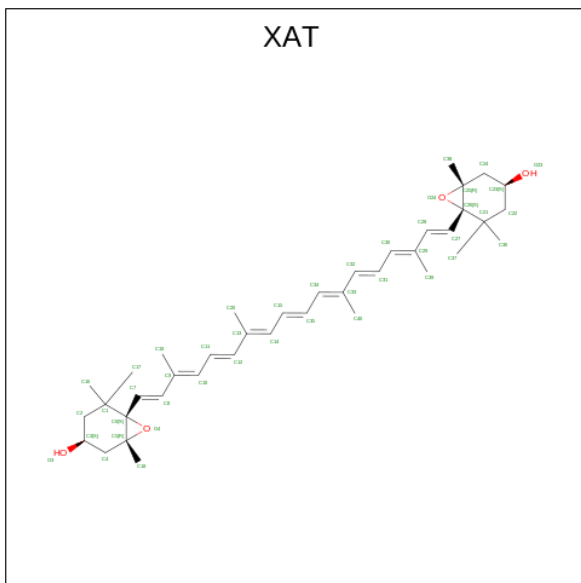
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
34	1	1	126	120	6	0
34	1	1	126	120	6	0
34	1	1	126	120	6	0
34	2	1	84	80	4	0
34	2	1	84	80	4	0
34	3	1	84	80	4	0
34	3	1	84	80	4	0
34	4	1	84	80	4	0
34	4	1	84	80	4	0
34	5	1	84	80	4	0
34	5	1	84	80	4	0
34	6	1	84	80	4	0
34	6	1	84	80	4	0
34	7	1	84	80	4	0
34	7	1	84	80	4	0
34	8	1	84	80	4	0
34	8	1	84	80	4	0
34	9	1	84	80	4	0
34	9	1	84	80	4	0
34	a	1	126	120	6	0
34	a	1	126	120	6	0

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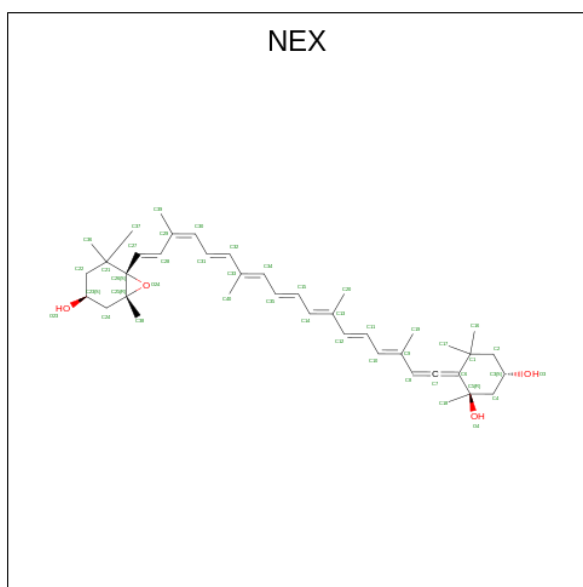
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
34	a	1	126	120	6	0

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



Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
35	P	1	131	119	12	0
35	P	1	131	119	12	0
35	P	1	131	119	12	0
35	Q	1	44	40	4	0
35	S	1	44	40	4	0
35	T	1	44	40	4	0

- Molecule 36 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-TETRAMETHYLOCTA DECA-1,3,5,7,9,11,13,15,17-NONAENYLIDENE]-1,5,5-TRIMETHYLCYCLOHEXANE-1,3-DIOL (three-letter code: NEX) (formula: C₄₀H₅₆O₄).

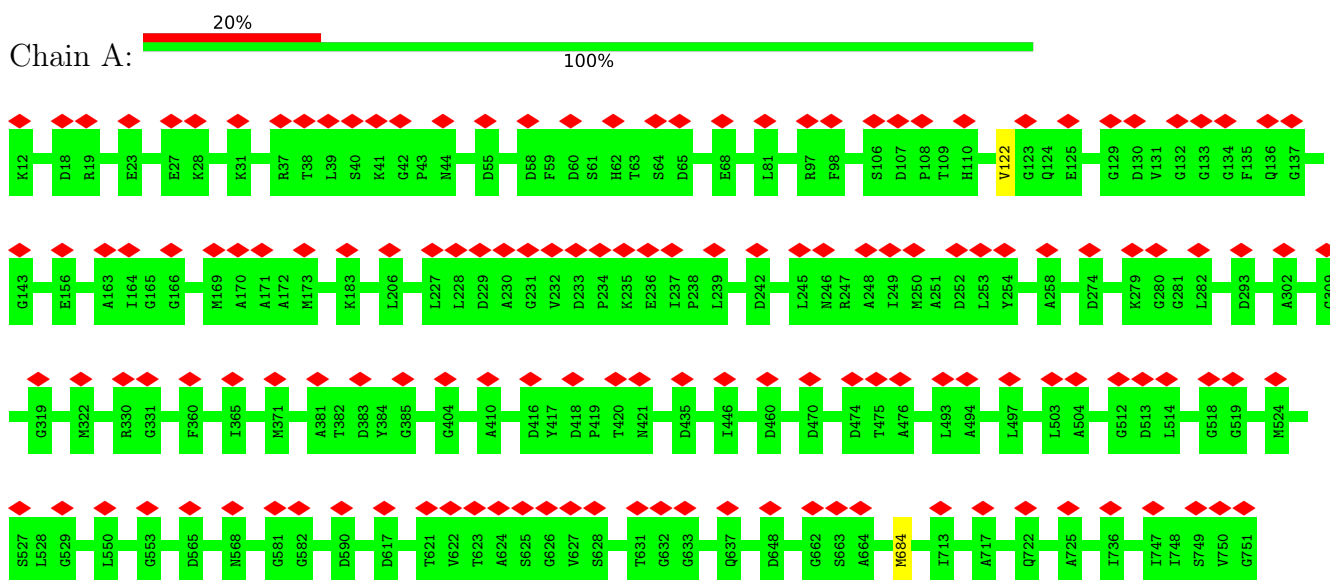


Mol	Chain	Residues	Atoms			AltConf
36	P	1	Total	C	O	0
			88	80	8	
36	P	1	Total	C	O	0
			88	80	8	
36	R	1	Total	C	O	0
			44	40	4	
36	T	1	Total	C	O	0
			44	40	4	
36	U	1	Total	C	O	0
			88	80	8	
36	U	1	Total	C	O	0
			88	80	8	

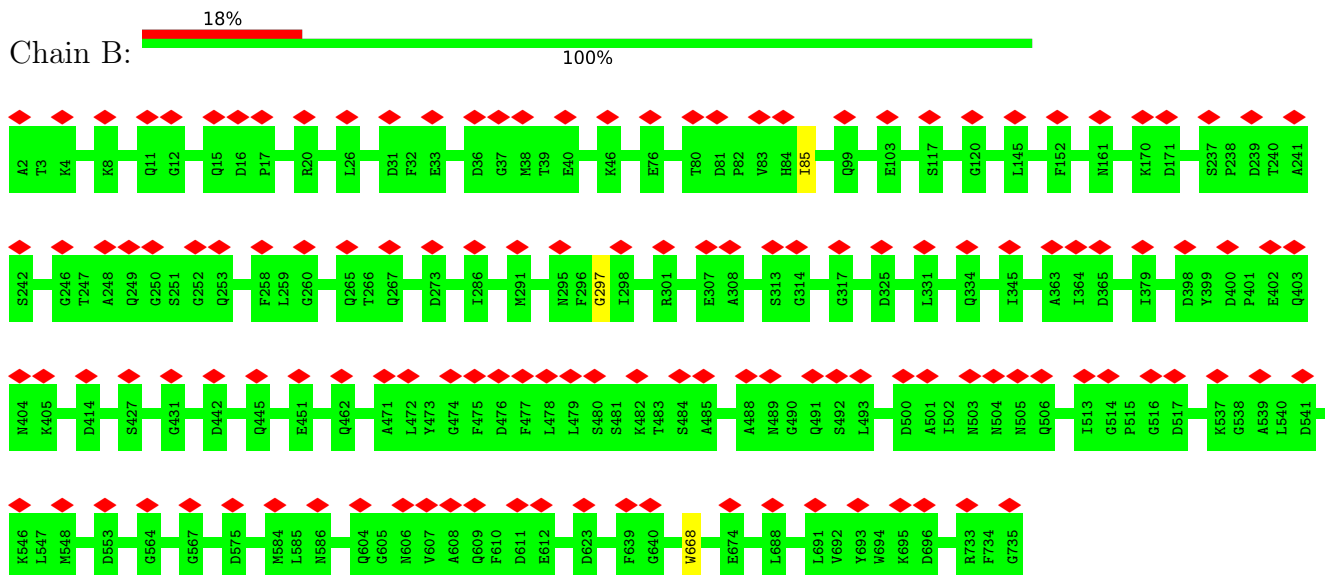
3 Residue-property plots

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

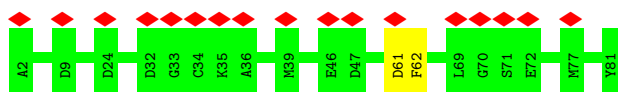
- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1



- Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2



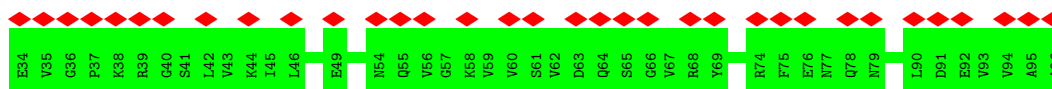
- Molecule 3: Photosystem I iron-sulfur center



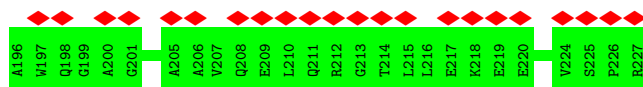
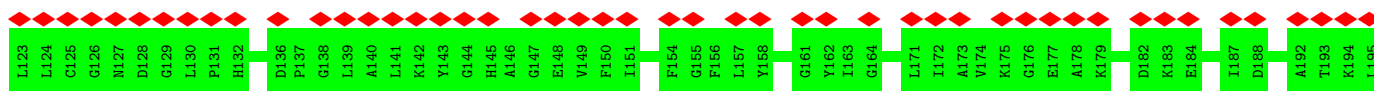
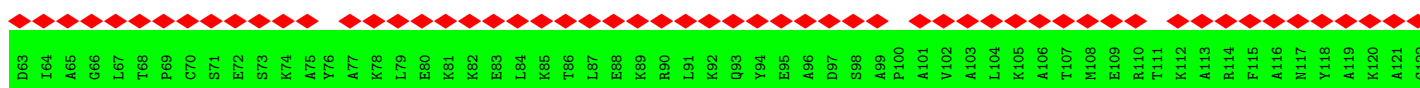
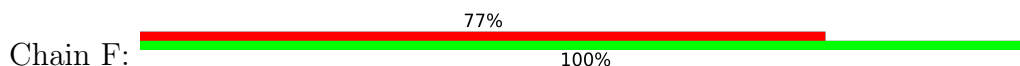
- Molecule 4: Photosystem I reaction center subunit II, chloroplastic



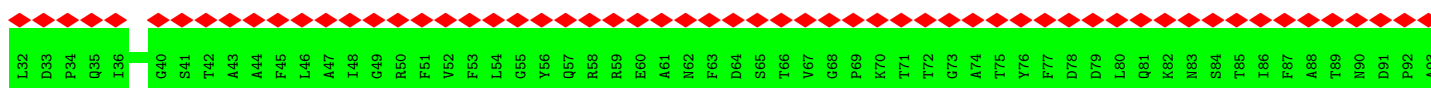
- Molecule 5: Photosystem I reaction center subunit IV, chloroplastic



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

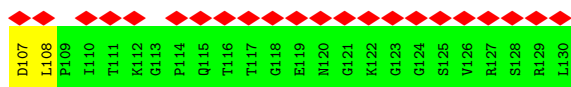
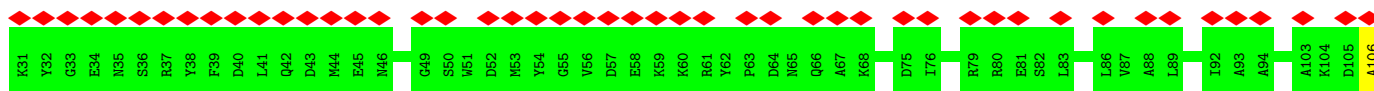


- Molecule 7: Photosystem I reaction center subunit V, chloroplastic

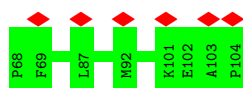




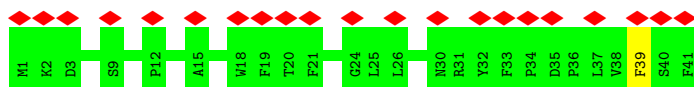
- Molecule 8: Photosystem I reaction center subunit VI, chloroplastic



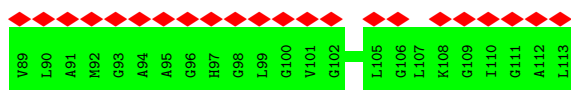
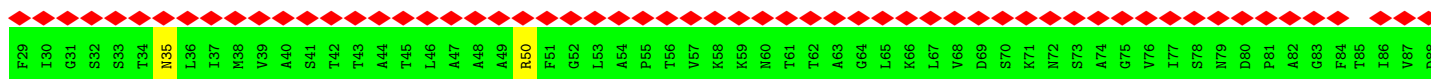
- Molecule 9: Photosystem I reaction center subunit VIII



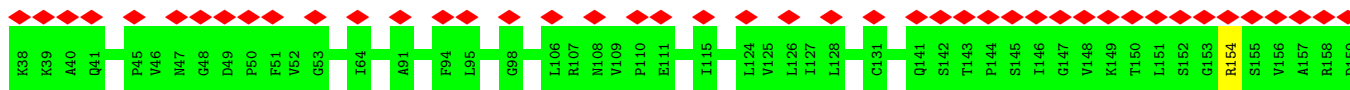
- Molecule 10: Photosystem I reaction center subunit IX

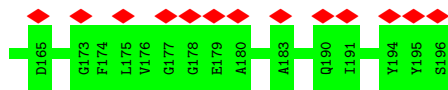


- Molecule 11: Photosystem I reaction center subunit psaK, chloroplastic

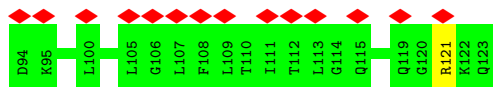
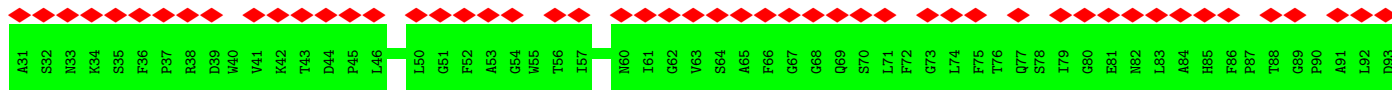


- Molecule 12: PSI subunit V

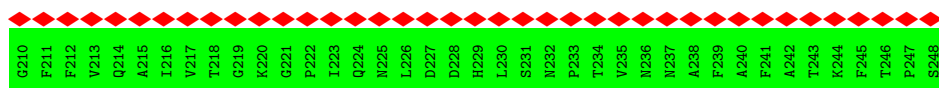
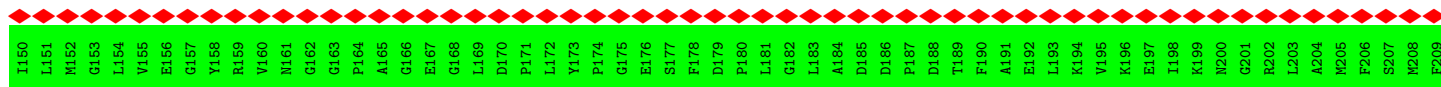
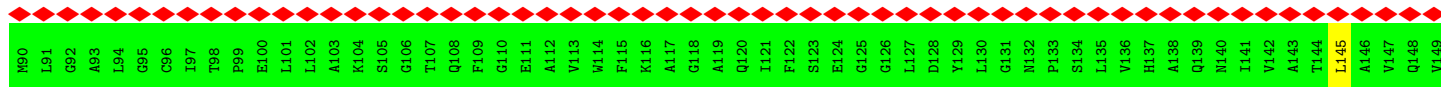
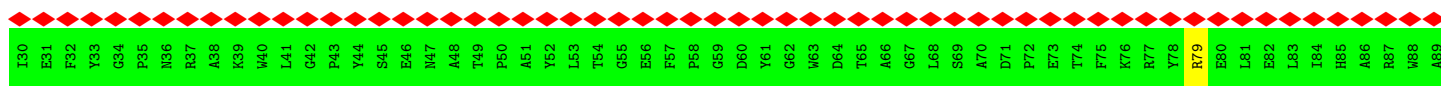




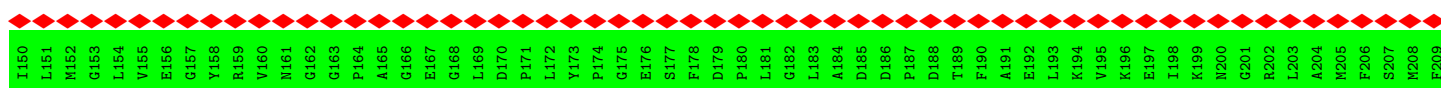
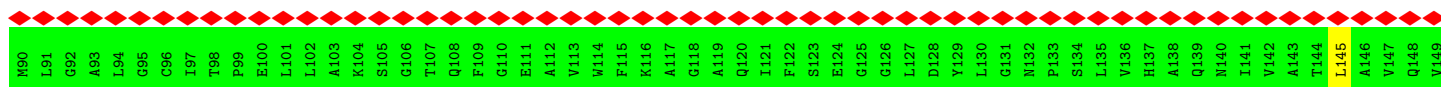
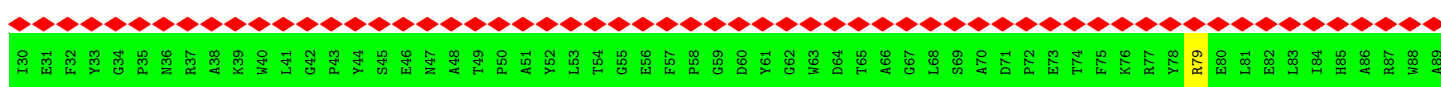
• Molecule 13: Photosystem I subunit O

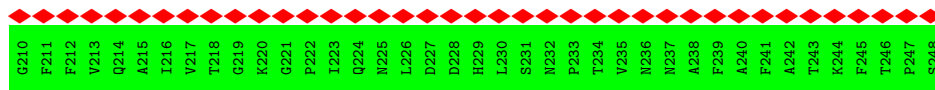


• Molecule 14: Chlorophyll a-b binding protein, chloroplastic

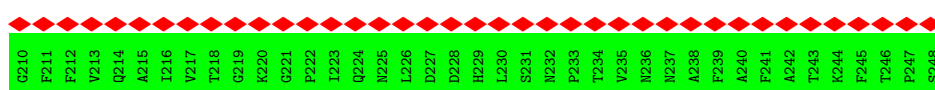
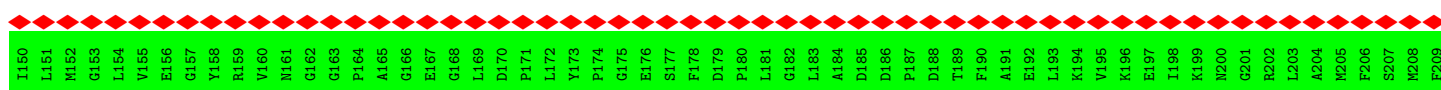
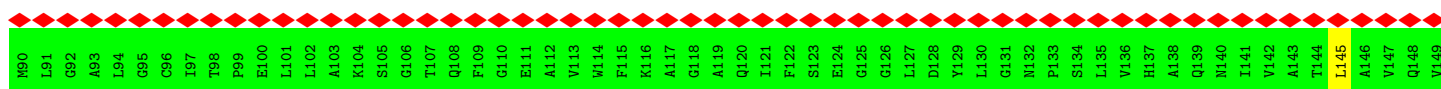


• Molecule 14: Chlorophyll a-b binding protein, chloroplastic

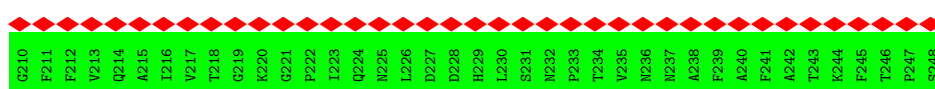
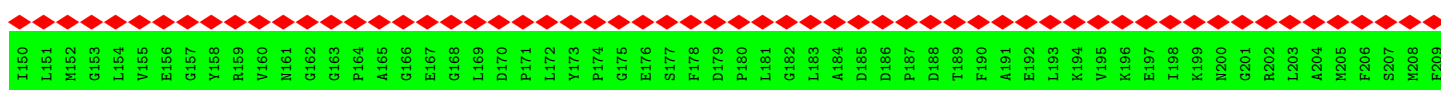
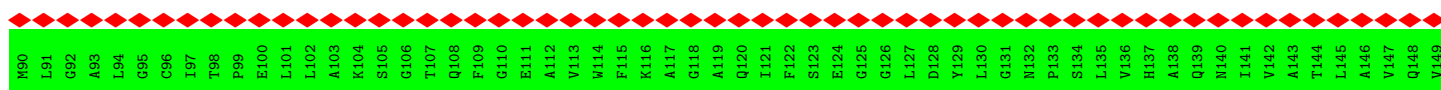




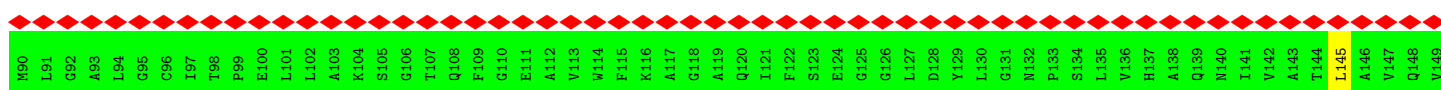
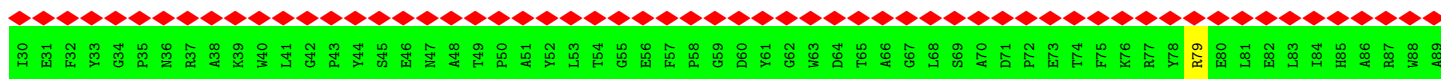
• Molecule 14: Chlorophyll a-b binding protein, chloroplastic

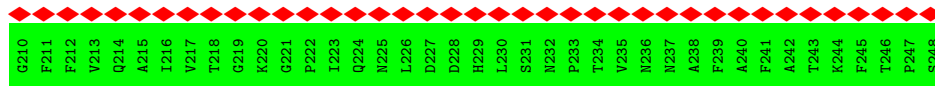
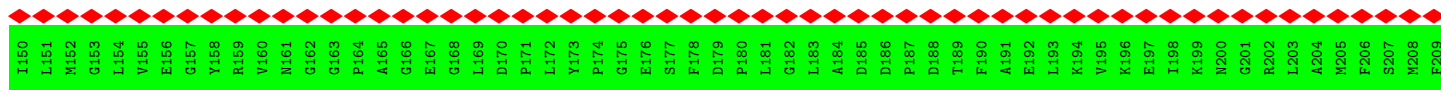


• Molecule 14: Chlorophyll a-b binding protein, chloroplastic

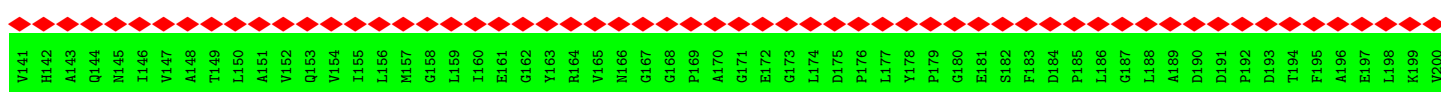
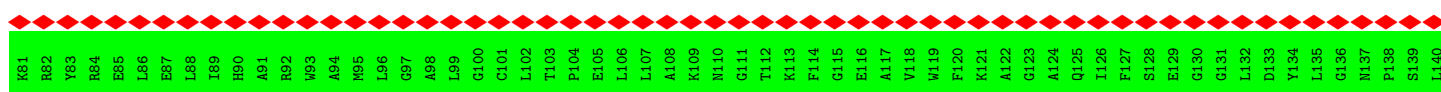
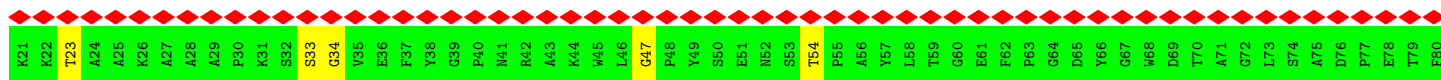


• Molecule 14: Chlorophyll a-b binding protein, chloroplastic

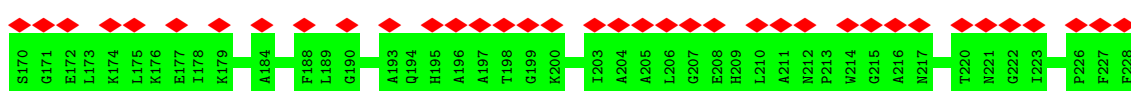
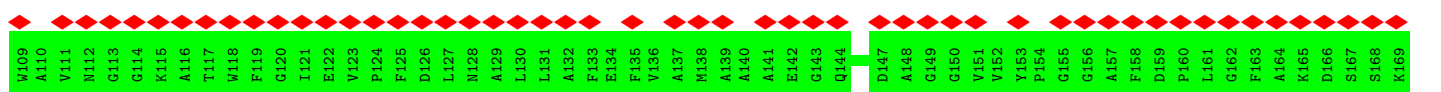
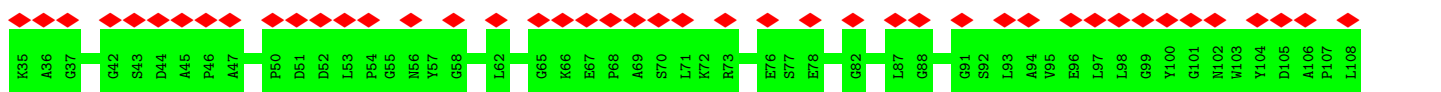




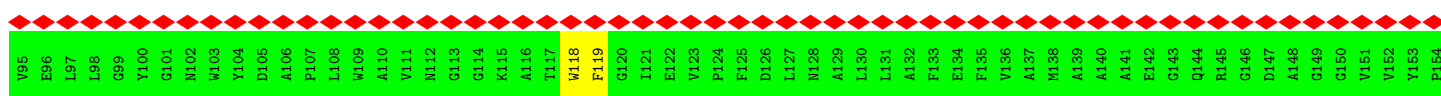
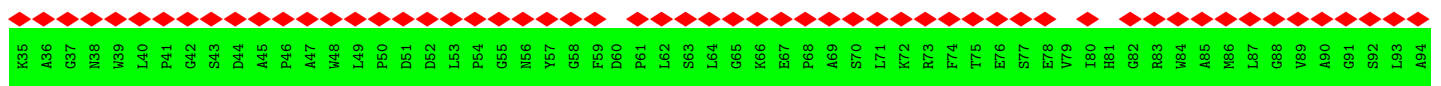
• Molecule 15: Chlorophyll a-b binding protein, chloroplastic

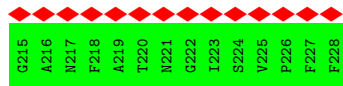
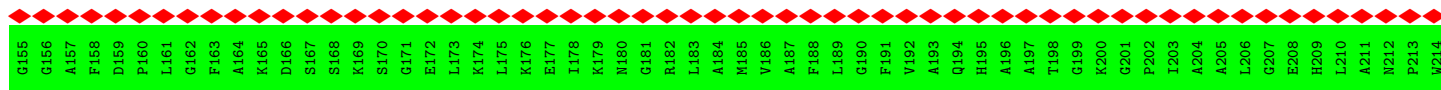


• Molecule 16: Chlorophyll a-b binding protein, chloroplastic

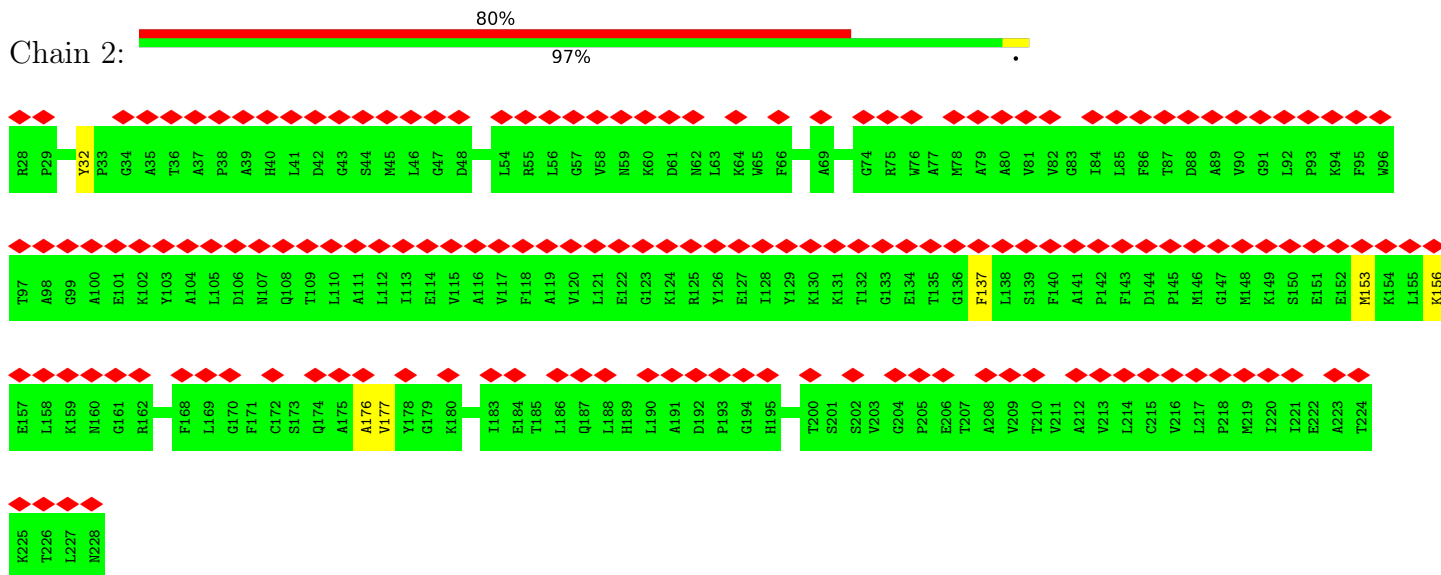


• Molecule 16: Chlorophyll a-b binding protein, chloroplastic

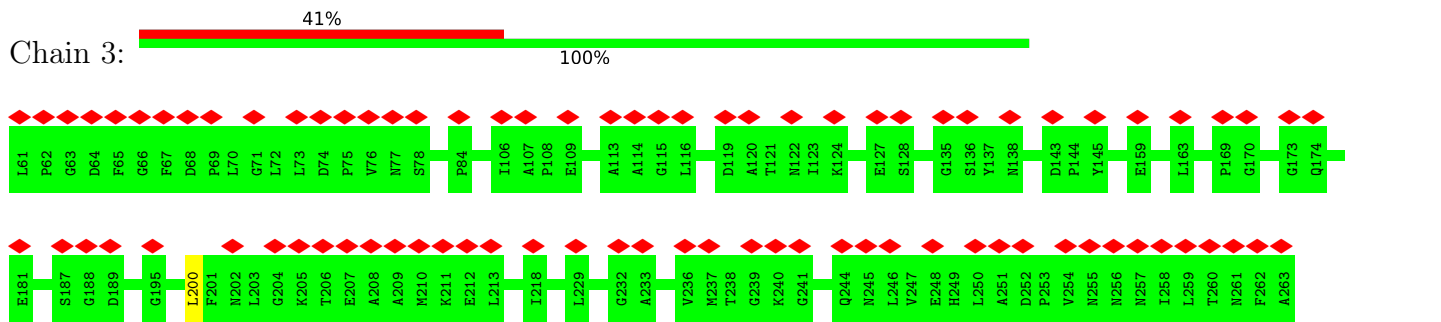




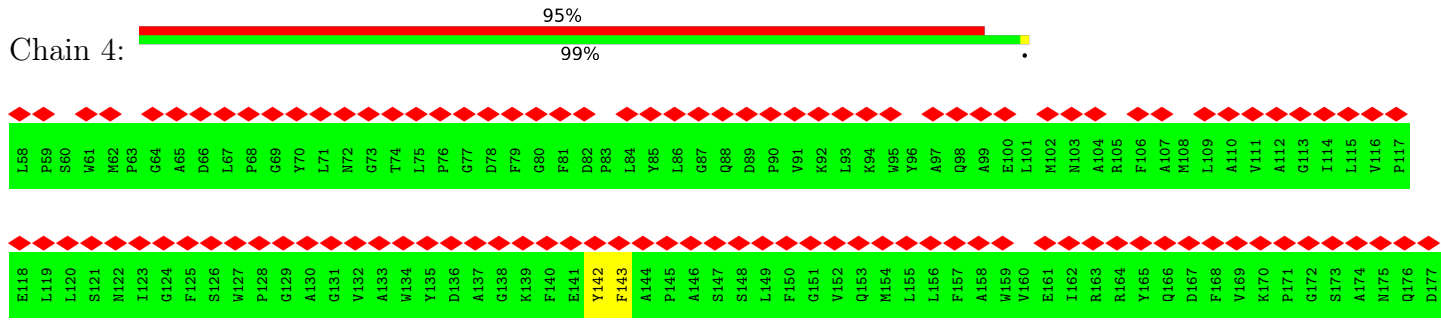
• Molecule 17: Chlorophyll a-b binding protein, chloroplastic

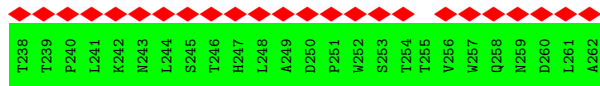
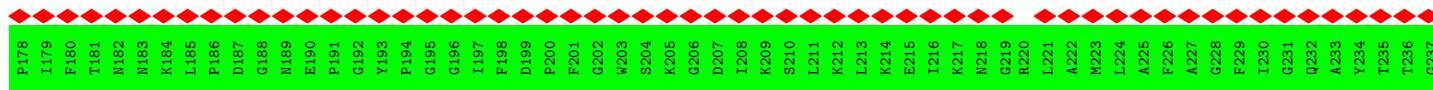


• Molecule 18: Chlorophyll a-b binding protein, chloroplastic

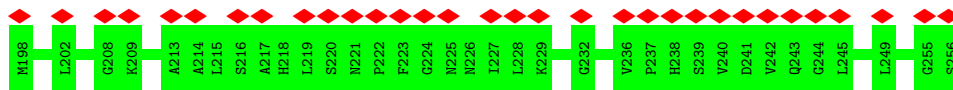
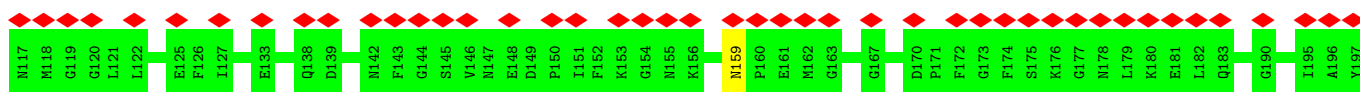
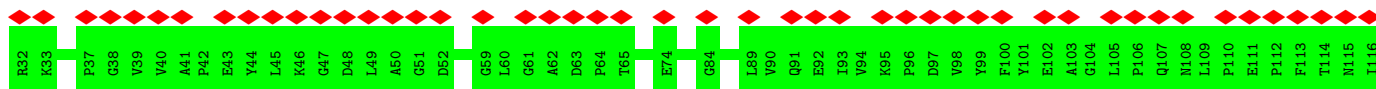


• Molecule 19: Chlorophyll a-b binding protein, chloroplastic

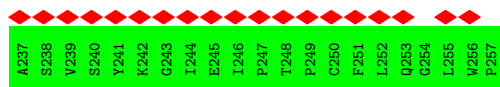
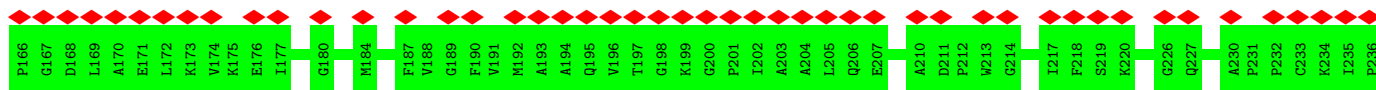
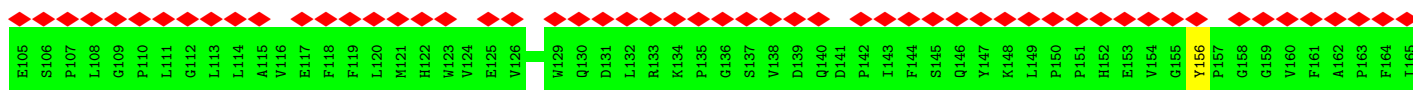
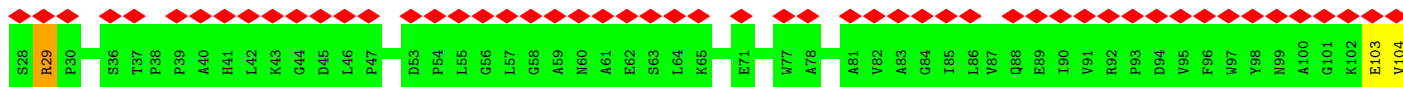
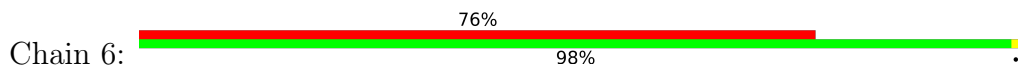




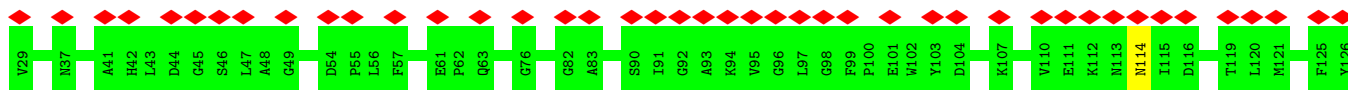
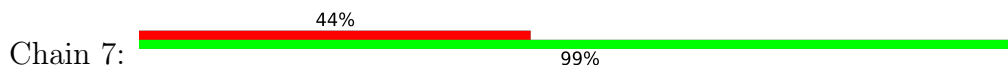
- Molecule 20: Chlorophyll a-b binding protein, chloroplastic

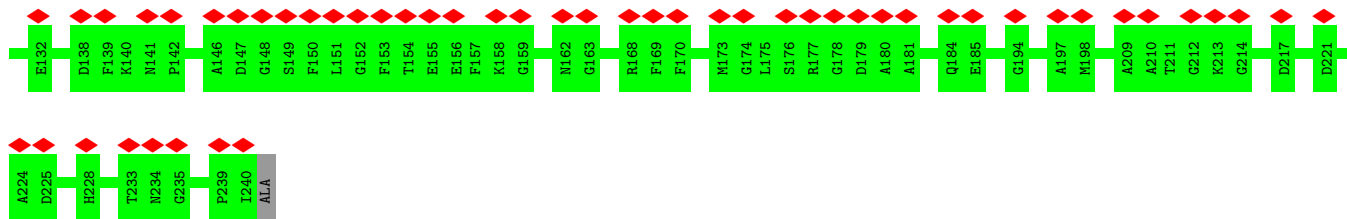


- Molecule 21: Chlorophyll a-b binding protein, chloroplastic

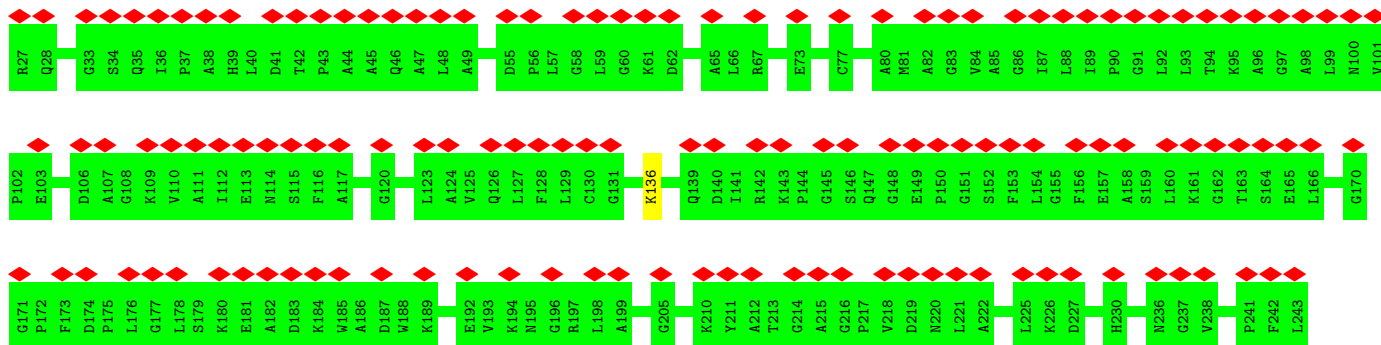


- Molecule 22: Chlorophyll a-b binding protein, chloroplastic

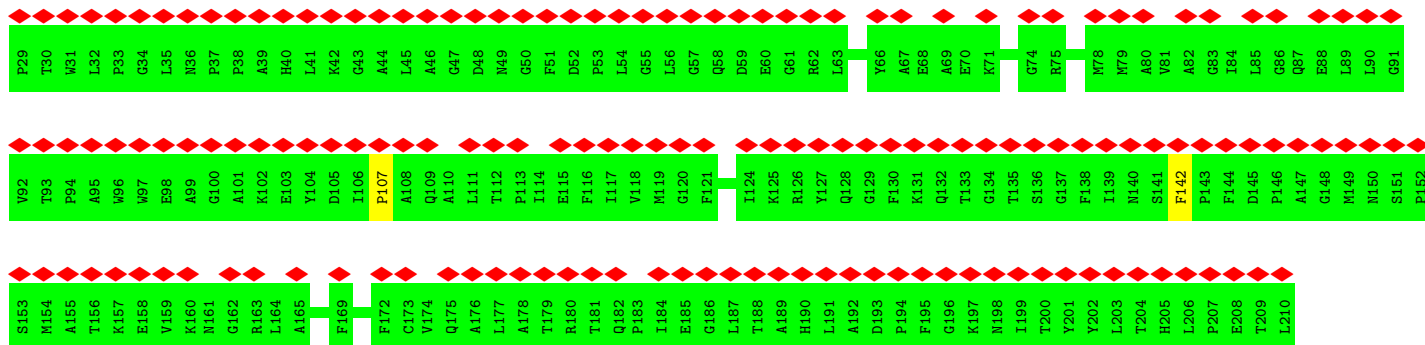




• Molecule 23: Chlorophyll a-b binding protein, chloroplastic



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



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	283763	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 ($e^-/\text{\AA}^2$)	50	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	5.004	Depositor
Minimum map value	-1.725	Depositor
Average map value	-0.002	Depositor
Map value standard deviation	0.085	Depositor
Recommended contour level	1.0	Depositor
Map size (Å)	470.52002, 470.52002, 470.52002	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.307, 1.307, 1.307	Depositor

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.57	0/6007	0.57	1/8190 (0.0%)
2	B	0.59	0/6040	0.57	0/8247
3	C	0.62	0/610	0.60	0/826
4	D	0.51	0/1160	0.60	2/1567 (0.1%)
5	E	0.52	0/506	0.48	0/689
6	F	0.46	0/1291	0.55	0/1747
7	G	0.43	0/693	0.58	1/943 (0.1%)
8	H	0.47	0/785	0.63	0/1055
9	I	0.58	0/293	0.56	0/406
10	J	0.48	0/349	0.53	0/478
11	K	0.38	0/583	0.60	0/790
12	L	0.53	0/1190	0.61	0/1628
13	O	0.49	0/743	0.65	0/1013
14	P	0.33	0/1717	0.54	1/2339 (0.0%)
14	Q	0.32	0/1717	0.52	1/2339 (0.0%)
14	R	0.31	0/1717	0.52	1/2339 (0.0%)
14	T	0.28	0/1717	0.50	0/2339
14	U	0.30	0/1717	0.51	1/2339 (0.0%)
15	S	0.40	0/1748	0.63	1/2376 (0.0%)
16	1	0.43	0/1490	0.51	0/2028
16	a	0.68	6/1490 (0.4%)	0.63	5/2028 (0.2%)
17	2	0.49	0/1583	0.72	2/2148 (0.1%)
18	3	0.52	0/1606	0.59	1/2180 (0.0%)
19	4	0.41	0/1645	0.54	0/2246
20	5	0.51	0/1812	0.56	0/2469
21	6	0.50	1/1833 (0.1%)	0.56	0/2505
22	7	0.52	0/1696	0.54	0/2303
23	8	0.51	0/1700	0.57	1/2315 (0.0%)
24	9	0.41	0/1433	0.56	0/1949
All	All	0.49	7/46871 (0.0%)	0.57	18/63821 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	2
3	C	0	2
10	J	0	1
15	S	0	1
17	2	0	2
19	4	0	2
21	6	0	1
22	7	0	1
24	9	0	1
All	All	0	13

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	a	118	TRP	CB-CG	-11.53	1.29	1.50
16	a	118	TRP	CE2-CZ2	-9.35	1.23	1.39
16	a	118	TRP	NE1-CE2	8.79	1.49	1.37
16	a	118	TRP	CE3-CZ3	-8.03	1.24	1.38
16	a	118	TRP	CG-CD2	-6.54	1.32	1.43

The worst 5 of 18 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	2	153	MET	CG-SD-CE	-10.21	83.86	100.20
23	8	136	LYS	CD-CE-NZ	-9.85	89.04	111.70
16	a	118	TRP	CD1-NE1-CE2	-9.59	100.37	109.00
1	A	684	MET	CG-SD-CE	-9.56	84.90	100.20
4	D	76	ARG	NE-CZ-NH1	-7.66	116.47	120.30

There are no chirality outliers.

5 of 13 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	297	GLY	Peptide
2	B	668	TRP	Peptide
3	C	61	ASP	Peptide
3	C	62	PHE	Peptide
10	J	39	PHE	Peptide

5.2 Too-close contacts [i](#)

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

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	738/740 (100%)	698 (95%)	39 (5%)	1 (0%)	51	83
2	B	732/734 (100%)	675 (92%)	56 (8%)	1 (0%)	51	83
3	C	78/80 (98%)	73 (94%)	5 (6%)	0	100	100
4	D	142/144 (99%)	127 (89%)	15 (11%)	0	100	100
5	E	61/63 (97%)	56 (92%)	5 (8%)	0	100	100
6	F	163/165 (99%)	152 (93%)	11 (7%)	0	100	100
7	G	89/91 (98%)	83 (93%)	6 (7%)	0	100	100
8	H	98/100 (98%)	77 (79%)	18 (18%)	3 (3%)	4	28
9	I	35/37 (95%)	33 (94%)	2 (6%)	0	100	100
10	J	39/41 (95%)	37 (95%)	2 (5%)	0	100	100
11	K	83/85 (98%)	77 (93%)	6 (7%)	0	100	100
12	L	157/159 (99%)	145 (92%)	12 (8%)	0	100	100
13	O	91/93 (98%)	76 (84%)	15 (16%)	0	100	100
14	P	217/219 (99%)	189 (87%)	28 (13%)	0	100	100
14	Q	217/219 (99%)	189 (87%)	28 (13%)	0	100	100
14	R	217/219 (99%)	189 (87%)	28 (13%)	0	100	100
14	T	217/219 (99%)	190 (88%)	27 (12%)	0	100	100
14	U	217/219 (99%)	190 (88%)	27 (12%)	0	100	100
15	S	230/234 (98%)	192 (84%)	36 (16%)	2 (1%)	17	53
16	1	192/194 (99%)	176 (92%)	16 (8%)	0	100	100
16	a	192/194 (99%)	175 (91%)	16 (8%)	1 (0%)	29	65

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
17	2	199/201 (99%)	169 (85%)	28 (14%)	2 (1%)	15	51
18	3	201/203 (99%)	181 (90%)	20 (10%)	0	100	100
19	4	203/205 (99%)	186 (92%)	16 (8%)	1 (0%)	29	65
20	5	223/225 (99%)	200 (90%)	23 (10%)	0	100	100
21	6	228/230 (99%)	209 (92%)	16 (7%)	3 (1%)	12	45
22	7	210/213 (99%)	195 (93%)	15 (7%)	0	100	100
23	8	215/217 (99%)	204 (95%)	11 (5%)	0	100	100
24	9	180/182 (99%)	154 (86%)	25 (14%)	1 (1%)	25	61
All	All	5864/5925 (99%)	5297 (90%)	552 (9%)	15 (0%)	44	74

5 of 15 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	122	VAL
21	6	104	VAL
8	H	106	ALA
19	4	143	PHE
15	S	54	THR

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	600/600 (100%)	600 (100%)	0	100	100
2	B	596/596 (100%)	596 (100%)	0	100	100
3	C	69/69 (100%)	69 (100%)	0	100	100
4	D	121/121 (100%)	120 (99%)	1 (1%)	81	92
5	E	54/54 (100%)	54 (100%)	0	100	100
6	F	127/127 (100%)	127 (100%)	0	100	100
7	G	68/68 (100%)	67 (98%)	1 (2%)	65	83
8	H	80/81 (99%)	80 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
9	I	31/31 (100%)	31 (100%)	0	100	100
10	J	37/37 (100%)	37 (100%)	0	100	100
11	K	59/59 (100%)	57 (97%)	2 (3%)	37	68
12	L	121/121 (100%)	120 (99%)	1 (1%)	81	92
13	O	75/75 (100%)	74 (99%)	1 (1%)	69	86
14	P	168/170 (99%)	167 (99%)	1 (1%)	86	94
14	Q	168/170 (99%)	167 (99%)	1 (1%)	86	94
14	R	168/170 (99%)	167 (99%)	1 (1%)	86	94
14	T	168/170 (99%)	167 (99%)	1 (1%)	86	94
14	U	168/170 (99%)	167 (99%)	1 (1%)	86	94
15	S	164/177 (93%)	164 (100%)	0	100	100
16	1	137/137 (100%)	137 (100%)	0	100	100
16	a	137/137 (100%)	137 (100%)	0	100	100
17	2	159/159 (100%)	159 (100%)	0	100	100
18	3	155/155 (100%)	155 (100%)	0	100	100
19	4	161/162 (99%)	161 (100%)	0	100	100
20	5	182/182 (100%)	181 (100%)	1 (0%)	88	95
21	6	184/184 (100%)	184 (100%)	0	100	100
22	7	164/164 (100%)	164 (100%)	0	100	100
23	8	163/163 (100%)	163 (100%)	0	100	100
24	9	139/140 (99%)	139 (100%)	0	100	100
All	All	4623/4649 (99%)	4611 (100%)	12 (0%)	92	97

5 of 12 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
14	Q	79	ARG
14	R	79	ARG
20	5	159	ASN
14	T	79	ARG
11	K	50	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 12 such sidechains are listed below:

Mol	Chain	Res	Type
15	S	153	GLN
17	2	62	ASN
24	9	128	GLN
20	5	117	ASN
4	D	170	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
15	TPO	S	23	15	8,10,11	0.88	0	10,14,16	1.70	1 (10%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	TPO	S	23	15	-	3/9/11/13	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	S	23	TPO	P-OG1-CB	-4.90	108.41	123.21

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
15	S	23	TPO	N-CA-CB-OG1
15	S	23	TPO	C-CA-CB-CG2
15	S	23	TPO	CB-OG1-P-O1P

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

453 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
34	LUT	Q	615	-	42,43,43	0.83	1 (2%)	51,60,60	1.85	16 (31%)
34	LUT	6	622	-	42,43,43	0.88	1 (2%)	51,60,60	1.50	11 (21%)
28	BCR	3	318	-	41,41,41	0.84	1 (2%)	56,56,56	2.79	24 (42%)
25	CLA	8	311	27	46,54,73	1.72	10 (21%)	53,90,113	1.51	7 (13%)
28	BCR	L	203	-	41,41,41	0.90	1 (2%)	56,56,56	2.03	15 (26%)
25	CLA	3	314	-	56,64,73	1.58	10 (17%)	65,102,113	1.49	6 (9%)
28	BCR	A	854	-	41,41,41	0.88	1 (2%)	56,56,56	1.96	16 (28%)
28	BCR	L	208	-	41,41,41	0.87	2 (4%)	56,56,56	1.98	18 (32%)
25	CLA	a	301	-	65,73,73	1.53	9 (13%)	76,113,113	1.36	8 (10%)
25	CLA	8	304	-	45,53,73	1.75	10 (22%)	52,89,113	1.61	7 (13%)
29	SF4	C	101	3	0,12,12	-	-	-	-	-
25	CLA	7	303	-	56,64,73	1.60	10 (17%)	65,102,113	1.47	7 (10%)
28	BCR	4	317	-	41,41,41	0.88	0	56,56,56	2.30	19 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	CLA	A	819	-	65,73,73	1.50	10 (15%)	76,113,113	1.49	8 (10%)
34	LUT	a	315	-	42,43,43	0.87	0	51,60,60	1.83	15 (29%)
33	CHL	S	302	-	53,61,74	2.04	17 (32%)	57,98,114	2.87	27 (47%)
25	CLA	1	608	-	65,73,73	1.44	8 (12%)	76,113,113	1.30	7 (9%)
25	CLA	6	605	-	65,73,73	1.42	8 (12%)	76,113,113	1.41	7 (9%)
25	CLA	A	853	-	65,73,73	1.48	10 (15%)	76,113,113	1.41	8 (10%)
32	LMG	H	204	-	47,47,55	0.95	2 (4%)	55,55,63	1.16	5 (9%)
25	CLA	a	308	16	60,68,73	1.41	8 (13%)	70,107,113	1.79	14 (20%)
25	CLA	1	610	27	65,73,73	1.48	10 (15%)	76,113,113	1.31	8 (10%)
27	LHG	4	319	-	31,31,48	1.13	2 (6%)	34,37,54	1.23	4 (11%)
25	CLA	6	609	-	50,58,73	1.64	9 (18%)	58,95,113	1.56	7 (12%)
25	CLA	6	614	-	45,53,73	1.73	10 (22%)	52,89,113	1.64	9 (17%)
25	CLA	S	311	-	60,68,73	1.53	6 (10%)	70,107,113	1.37	8 (11%)
25	CLA	B	807	-	65,73,73	1.46	10 (15%)	76,113,113	1.59	10 (13%)
25	CLA	1	602	-	65,73,73	1.48	10 (15%)	76,113,113	1.32	8 (10%)
25	CLA	A	822	-	65,73,73	1.45	10 (15%)	76,113,113	1.48	8 (10%)
25	CLA	3	308	-	65,73,73	1.43	10 (15%)	76,113,113	1.40	7 (9%)
33	CHL	P	622	-	53,61,74	2.20	16 (30%)	57,98,114	3.02	29 (50%)
25	CLA	3	301	-	60,68,73	1.53	10 (16%)	70,107,113	1.47	8 (11%)
25	CLA	a	310	-	52,60,73	1.68	8 (15%)	60,97,113	1.51	6 (10%)
35	XAT	Q	616	-	39,47,47	0.96	1 (2%)	54,74,74	3.04	24 (44%)
34	LUT	a	314	-	42,43,43	0.88	2 (4%)	51,60,60	1.87	16 (31%)
25	CLA	O	203	-	37,46,73	1.94	8 (21%)	46,81,113	1.79	9 (19%)
32	LMG	7	318	-	35,35,55	1.10	2 (5%)	43,43,63	1.11	2 (4%)
32	LMG	J	104	-	35,35,55	1.06	2 (5%)	43,43,63	1.25	5 (11%)
25	CLA	A	809	1	65,73,73	1.46	10 (15%)	76,113,113	1.42	8 (10%)
25	CLA	2	305	-	52,60,73	1.65	8 (15%)	60,97,113	1.51	7 (11%)
25	CLA	T	612	-	48,56,73	1.73	5 (10%)	55,92,113	1.59	7 (12%)
25	CLA	B	811	-	65,73,73	1.51	11 (16%)	76,113,113	1.50	9 (11%)
25	CLA	U	303	-	65,73,73	1.48	6 (9%)	76,113,113	1.44	7 (9%)
25	CLA	9	308	-	50,58,73	1.68	9 (18%)	58,95,113	1.59	10 (17%)
25	CLA	4	311	-	56,64,73	1.56	9 (16%)	65,102,113	1.52	8 (12%)
29	SF4	A	850	2,1	0,12,12	-	-	-	-	-
25	CLA	A	835	-	51,59,73	1.66	10 (19%)	59,96,113	1.58	9 (15%)
28	BCR	L	207	-	41,41,41	0.93	2 (4%)	56,56,56	2.00	13 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	CLA	a	313	-	46,54,73	1.72	7 (15%)	53,90,113	1.54	6 (11%)
25	CLA	6	615	21	46,54,73	1.70	9 (19%)	53,90,113	1.67	9 (16%)
25	CLA	2	302	17	46,54,73	1.78	10 (21%)	53,90,113	1.63	8 (15%)
25	CLA	B	837	-	65,73,73	1.48	10 (15%)	76,113,113	1.54	7 (9%)
25	CLA	P	613	-	58,66,73	1.58	5 (8%)	67,104,113	1.44	8 (11%)
33	CHL	P	606	-	50,58,74	2.17	16 (32%)	52,94,114	2.84	23 (44%)
25	CLA	S	304	-	65,73,73	1.49	6 (9%)	76,113,113	1.37	7 (9%)
34	LUT	1	616	-	42,43,43	0.95	2 (4%)	51,60,60	1.84	18 (35%)
25	CLA	8	310	-	60,68,73	1.50	10 (16%)	70,107,113	1.40	8 (11%)
25	CLA	K	201	-	51,59,73	1.63	10 (19%)	59,96,113	1.63	10 (16%)
25	CLA	2	310	-	41,49,73	1.83	9 (21%)	47,84,113	1.60	7 (14%)
36	NEX	P	621	-	38,46,46	0.86	0	50,70,70	3.27	27 (54%)
25	CLA	A	834	1	45,53,73	1.76	10 (22%)	52,89,113	1.67	5 (9%)
25	CLA	3	302	-	65,73,73	1.51	9 (13%)	76,113,113	1.42	9 (11%)
33	CHL	T	605	-	50,58,74	2.18	17 (34%)	52,94,114	2.85	22 (42%)
34	LUT	U	315	-	42,43,43	0.78	0	51,60,60	1.81	17 (33%)
34	LUT	8	316	-	42,43,43	0.90	1 (2%)	51,60,60	1.78	14 (27%)
32	LMG	7	319	-	36,36,55	1.12	3 (8%)	44,44,63	1.25	5 (11%)
25	CLA	B	822	-	65,73,73	1.46	10 (15%)	76,113,113	1.43	10 (13%)
34	LUT	5	318	-	42,43,43	0.92	2 (4%)	51,60,60	1.68	13 (25%)
25	CLA	T	608	-	65,73,73	1.46	6 (9%)	76,113,113	1.38	8 (10%)
25	CLA	A	831	-	50,58,73	1.66	10 (20%)	58,95,113	1.61	9 (15%)
25	CLA	P	611	-	41,49,73	1.73	8 (19%)	47,84,113	2.11	18 (38%)
25	CLA	S	315	-	48,56,73	1.67	9 (18%)	55,92,113	1.52	8 (14%)
25	CLA	3	312	-	45,53,73	1.77	9 (20%)	52,89,113	1.59	8 (15%)
25	CLA	5	304	-	46,54,73	1.69	8 (17%)	53,90,113	1.68	6 (11%)
25	CLA	B	834	-	65,73,73	1.47	10 (15%)	76,113,113	1.44	8 (10%)
25	CLA	1	612	-	65,73,73	1.51	11 (16%)	76,113,113	2.07	15 (19%)
25	CLA	B	805	-	65,73,73	1.47	11 (16%)	76,113,113	1.47	7 (9%)
25	CLA	9	310	24	50,58,73	1.68	9 (18%)	58,95,113	1.61	7 (12%)
25	CLA	R	604	-	50,58,73	1.69	6 (12%)	58,95,113	1.70	10 (17%)
25	CLA	B	825	-	65,73,73	1.46	11 (16%)	76,113,113	1.49	9 (11%)
34	LUT	Q	614	-	42,43,43	0.73	0	51,60,60	1.84	12 (23%)
25	CLA	a	312	-	65,73,73	1.48	7 (10%)	76,113,113	1.38	9 (11%)
33	CHL	Q	608	-	66,74,74	1.51	12 (18%)	73,114,114	1.84	11 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	CLA	Q	611	-	60,68,73	1.60	7 (11%)	70,107,113	1.43	11 (15%)
34	LUT	S	316	-	42,43,43	0.79	0	51,60,60	1.82	16 (31%)
32	LMG	1	619	-	46,46,55	0.98	2 (4%)	54,54,63	1.17	3 (5%)
25	CLA	R	603	-	65,73,73	1.53	5 (7%)	76,113,113	1.39	8 (10%)
25	CLA	B	835	-	47,55,73	1.78	10 (21%)	54,91,113	1.50	7 (12%)
33	CHL	S	310	15	52,60,74	2.16	16 (30%)	56,97,114	2.76	24 (42%)
25	CLA	5	315	20	46,54,73	1.70	9 (19%)	53,90,113	1.58	6 (11%)
28	BCR	A	845	-	41,41,41	0.83	1 (2%)	56,56,56	2.08	21 (37%)
25	CLA	A	804	-	65,73,73	1.45	10 (15%)	76,113,113	1.47	9 (11%)
25	CLA	O	201	-	41,49,73	1.78	9 (21%)	47,84,113	1.71	8 (17%)
25	CLA	H	205	12	42,50,73	1.75	9 (21%)	48,85,113	1.99	9 (18%)
25	CLA	1	609	16	60,68,73	1.42	11 (18%)	70,107,113	1.75	12 (17%)
25	CLA	1	614	-	46,54,73	1.73	10 (21%)	53,90,113	1.58	6 (11%)
25	CLA	A	817	-	57,65,73	1.59	9 (15%)	66,103,113	1.39	4 (6%)
25	CLA	3	310	-	46,54,73	1.74	10 (21%)	53,90,113	1.57	7 (13%)
34	LUT	T	613	-	42,43,43	0.72	0	51,60,60	1.91	13 (25%)
25	CLA	A	820	-	65,73,73	1.45	12 (18%)	76,113,113	1.45	9 (11%)
28	BCR	8	301	-	41,41,41	0.78	0	56,56,56	1.88	15 (26%)
25	CLA	A	814	-	65,73,73	1.51	11 (16%)	76,113,113	1.52	10 (13%)
25	CLA	8	302	23	65,73,73	1.46	10 (15%)	76,113,113	1.33	9 (11%)
34	LUT	1	617	-	42,43,43	0.79	0	51,60,60	2.17	18 (35%)
25	CLA	U	302	-	65,73,73	1.51	6 (9%)	76,113,113	1.41	9 (11%)
34	LUT	6	619	-	42,43,43	0.89	1 (2%)	51,60,60	1.82	14 (27%)
34	LUT	5	322	-	42,43,43	1.01	2 (4%)	51,60,60	1.64	13 (25%)
25	CLA	5	314	-	45,53,73	1.78	9 (20%)	52,89,113	1.58	8 (15%)
25	CLA	2	311	-	52,60,73	1.63	10 (19%)	60,97,113	1.50	8 (13%)
25	CLA	9	302	-	46,54,73	1.74	7 (15%)	53,90,113	1.53	5 (9%)
25	CLA	5	324	-	65,73,73	1.48	9 (13%)	76,113,113	1.33	6 (7%)
25	CLA	A	832	-	65,73,73	1.45	10 (15%)	76,113,113	1.43	7 (9%)
25	CLA	B	817	-	65,73,73	1.47	10 (15%)	76,113,113	1.40	8 (10%)
25	CLA	Q	603	-	65,73,73	1.51	6 (9%)	76,113,113	1.48	8 (10%)
25	CLA	5	303	-	65,73,73	1.46	11 (16%)	76,113,113	1.51	8 (10%)
34	LUT	1	615	-	42,43,43	0.96	2 (4%)	51,60,60	1.87	16 (31%)
34	LUT	3	316	-	42,43,43	0.97	2 (4%)	51,60,60	1.65	15 (29%)
25	CLA	B	803	-	45,53,73	1.75	10 (22%)	52,89,113	1.75	7 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
27	LHG	Q	617	-	48,48,48	0.93	2 (4%)	51,54,54	0.99	2 (3%)
25	CLA	K	203	-	46,54,73	1.73	10 (21%)	53,90,113	1.57	7 (13%)
35	XAT	T	615	-	39,47,47	0.92	0	54,74,74	3.00	21 (38%)
25	CLA	B	813	-	57,65,73	1.56	10 (17%)	66,103,113	1.46	8 (12%)
25	CLA	5	309	-	50,58,73	1.68	10 (20%)	58,95,113	1.49	9 (15%)
27	LHG	4	318	25	48,48,48	0.92	2 (4%)	51,54,54	1.09	3 (5%)
25	CLA	O	202	-	36,46,73	1.96	10 (27%)	41,80,113	1.72	8 (19%)
25	CLA	A	837	-	65,73,73	1.46	10 (15%)	76,113,113	1.45	9 (11%)
33	CHL	6	608	-	51,59,74	2.03	16 (31%)	55,96,114	3.09	30 (54%)
34	LUT	7	315	-	42,43,43	0.93	2 (4%)	51,60,60	1.56	12 (23%)
25	CLA	A	830	-	65,73,73	1.48	10 (15%)	76,113,113	1.52	10 (13%)
25	CLA	B	832	-	45,53,73	1.78	10 (22%)	52,89,113	1.58	6 (11%)
25	CLA	A	807	-	65,73,73	1.50	11 (16%)	76,113,113	1.48	8 (10%)
27	LHG	R	618	-	48,48,48	0.93	2 (4%)	51,54,54	0.96	2 (3%)
25	CLA	Q	609	-	65,73,73	1.50	5 (7%)	76,113,113	1.38	8 (10%)
25	CLA	2	303	17	65,73,73	1.47	10 (15%)	76,113,113	1.38	8 (10%)
25	CLA	Q	618	-	39,48,73	1.93	8 (20%)	45,82,113	1.89	11 (24%)
34	LUT	9	313	-	42,43,43	0.90	1 (2%)	51,60,60	1.61	14 (27%)
25	CLA	4	309	27	55,63,73	1.56	7 (12%)	64,101,113	1.41	8 (12%)
27	LHG	2	317	-	48,48,48	0.90	2 (4%)	51,54,54	0.99	2 (3%)
25	CLA	T	609	-	60,68,73	1.55	7 (11%)	70,107,113	1.52	11 (15%)
34	LUT	8	317	-	42,43,43	0.92	2 (4%)	51,60,60	1.56	12 (23%)
25	CLA	T	611	-	60,68,73	1.55	5 (8%)	70,107,113	1.41	7 (10%)
25	CLA	7	304	-	42,50,73	1.82	10 (23%)	48,85,113	1.46	6 (12%)
32	LMG	2	301	-	41,41,55	1.03	2 (4%)	49,49,63	1.19	4 (8%)
25	CLA	A	806	-	65,73,73	1.47	10 (15%)	76,113,113	1.51	9 (11%)
25	CLA	7	310	-	52,60,73	1.64	10 (19%)	60,97,113	1.52	7 (11%)
25	CLA	B	814	-	55,63,73	1.57	10 (18%)	64,101,113	1.52	8 (12%)
25	CLA	R	602	-	65,73,73	1.52	5 (7%)	76,113,113	1.40	9 (11%)
25	CLA	9	311	-	45,53,73	1.84	9 (20%)	52,89,113	1.52	9 (17%)
33	CHL	4	306	-	51,59,74	2.04	15 (29%)	55,96,114	2.75	24 (43%)
25	CLA	H	201	-	46,54,73	1.71	10 (21%)	53,90,113	1.55	6 (11%)
34	LUT	4	316	-	42,43,43	0.88	2 (4%)	51,60,60	1.53	11 (21%)
25	CLA	K	204	-	45,53,73	1.81	7 (15%)	52,89,113	1.72	9 (17%)
25	CLA	8	305	-	46,54,73	1.73	10 (21%)	53,90,113	1.54	7 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
28	BCR	3	317	-	41,41,41	0.94	2 (4%)	56,56,56	2.33	17 (30%)
28	BCR	7	316	-	41,41,41	0.89	1 (2%)	56,56,56	2.00	16 (28%)
25	CLA	A	840	-	65,73,73	1.50	10 (15%)	76,113,113	1.45	10 (13%)
34	LUT	2	316	-	42,43,43	0.86	1 (2%)	51,60,60	1.66	13 (25%)
25	CLA	A	815	-	60,68,73	1.51	10 (16%)	70,107,113	1.45	8 (11%)
25	CLA	2	312	-	65,73,73	1.48	9 (13%)	76,113,113	1.50	10 (13%)
25	CLA	L	209	-	41,49,73	1.79	8 (19%)	47,84,113	1.81	9 (19%)
25	CLA	B	833	-	60,68,73	1.49	10 (16%)	70,107,113	1.42	8 (11%)
33	CHL	S	307	-	50,58,74	2.24	16 (32%)	52,94,114	2.84	22 (42%)
36	NEX	T	616	-	38,46,46	0.98	1 (2%)	50,70,70	2.76	16 (32%)
25	CLA	B	838	-	65,73,73	1.48	10 (15%)	76,113,113	1.39	6 (7%)
25	CLA	5	302	20	65,73,73	1.49	10 (15%)	76,113,113	1.39	8 (10%)
27	LHG	P	624	-	48,48,48	0.94	2 (4%)	51,54,54	0.96	2 (3%)
25	CLA	R	612	-	60,68,73	1.39	9 (15%)	70,107,113	1.62	9 (12%)
27	LHG	8	319	25	48,48,48	0.92	2 (4%)	51,54,54	1.07	4 (7%)
25	CLA	7	308	-	60,68,73	1.56	10 (16%)	70,107,113	1.44	9 (12%)
25	CLA	J	105	-	42,50,73	1.75	10 (23%)	48,85,113	1.61	7 (14%)
25	CLA	B	812	-	60,68,73	1.52	10 (16%)	70,107,113	1.42	7 (10%)
25	CLA	7	302	-	46,54,73	1.71	10 (21%)	53,90,113	1.60	8 (15%)
33	CHL	S	321	-	51,59,74	2.16	17 (33%)	55,96,114	2.86	25 (45%)
25	CLA	2	306	17	41,49,73	1.85	9 (21%)	47,84,113	1.78	10 (21%)
25	CLA	6	610	-	60,68,73	1.57	9 (15%)	70,107,113	1.41	7 (10%)
34	LUT	9	312	-	42,43,43	0.84	2 (4%)	51,60,60	1.60	13 (25%)
25	CLA	1	611	-	52,60,73	1.66	10 (19%)	60,97,113	1.49	8 (13%)
25	CLA	3	307	-	50,58,73	1.65	10 (20%)	58,95,113	1.49	8 (13%)
25	CLA	a	303	-	57,65,73	1.88	15 (26%)	66,103,113	3.65	19 (28%)
28	BCR	5	323	-	41,41,41	0.96	2 (4%)	56,56,56	3.15	22 (39%)
25	CLA	A	826	-	65,73,73	1.44	10 (15%)	76,113,113	1.34	8 (10%)
33	CHL	5	307	-	51,59,74	2.09	16 (31%)	55,96,114	2.94	26 (47%)
28	BCR	O	205	-	41,41,41	0.82	1 (2%)	56,56,56	2.18	16 (28%)
25	CLA	9	301	-	54,62,73	1.64	9 (16%)	67,100,113	1.55	11 (16%)
36	NEX	U	316	-	38,46,46	0.99	1 (2%)	50,70,70	2.72	18 (36%)
28	BCR	J	106	-	41,41,41	0.86	2 (4%)	56,56,56	2.25	18 (32%)
25	CLA	A	828	-	65,73,73	1.45	10 (15%)	76,113,113	1.49	8 (10%)
27	LHG	1	618	25	42,42,48	0.96	2 (4%)	45,48,54	1.22	4 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
28	BCR	O	204	-	41,41,41	0.86	2 (4%)	56,56,56	2.34	21 (37%)
25	CLA	a	309	27	65,73,73	1.48	7 (10%)	76,113,113	1.32	8 (10%)
34	LUT	7	314	-	42,43,43	0.96	2 (4%)	51,60,60	1.74	14 (27%)
34	LUT	3	315	-	42,43,43	0.92	2 (4%)	51,60,60	1.65	13 (25%)
27	LHG	P	618	-	48,48,48	0.93	2 (4%)	51,54,54	0.96	2 (3%)
25	CLA	B	806	-	65,73,73	1.49	10 (15%)	76,113,113	1.40	8 (10%)
25	CLA	9	304	-	46,54,73	1.75	10 (21%)	53,90,113	1.55	6 (11%)
33	CHL	R	605	14	46,54,74	2.33	16 (34%)	49,90,114	2.95	24 (48%)
36	NEX	P	617	-	38,46,46	1.01	1 (2%)	50,70,70	2.80	18 (36%)
36	NEX	R	617	-	38,46,46	0.98	1 (2%)	50,70,70	2.79	19 (38%)
25	CLA	U	310	-	64,72,73	1.51	5 (7%)	74,111,113	1.40	8 (10%)
27	LHG	S	319	-	48,48,48	0.93	2 (4%)	51,54,54	1.02	3 (5%)
34	LUT	4	315	-	42,43,43	0.89	1 (2%)	51,60,60	1.94	17 (33%)
25	CLA	B	818	-	56,64,73	1.58	10 (17%)	65,102,113	1.58	8 (12%)
25	CLA	B	827	-	65,73,73	1.51	10 (15%)	76,113,113	1.39	9 (11%)
25	CLA	8	313	-	65,73,73	1.48	10 (15%)	76,113,113	1.41	7 (9%)
25	CLA	6	613	-	56,64,73	1.62	8 (14%)	65,102,113	1.58	9 (13%)
28	BCR	4	321	-	41,41,41	0.94	2 (4%)	56,56,56	2.73	24 (42%)
25	CLA	L	206	-	42,50,73	1.78	10 (23%)	48,85,113	1.64	6 (12%)
25	CLA	8	315	23	46,54,73	1.71	10 (21%)	53,90,113	1.56	6 (11%)
33	CHL	T	607	-	52,60,74	2.22	17 (32%)	56,97,114	2.82	26 (46%)
25	CLA	3	304	-	42,50,73	1.84	10 (23%)	48,85,113	1.57	7 (14%)
25	CLA	A	825	-	65,73,73	1.50	10 (15%)	76,113,113	1.47	12 (15%)
25	CLA	6	620	-	45,53,73	1.73	10 (22%)	52,89,113	1.58	7 (13%)
25	CLA	S	301	-	47,55,73	1.77	9 (19%)	54,91,113	1.68	10 (18%)
25	CLA	B	823	-	65,73,73	1.45	10 (15%)	76,113,113	1.36	7 (9%)
25	CLA	K	202	-	45,53,73	1.73	10 (22%)	52,89,113	1.61	7 (13%)
25	CLA	4	301	-	60,68,73	1.51	10 (16%)	70,107,113	1.44	7 (10%)
25	CLA	5	311	-	55,63,73	1.58	10 (18%)	64,101,113	1.41	7 (10%)
33	CHL	Q	606	-	50,58,74	2.19	16 (32%)	52,94,114	2.85	20 (38%)
25	CLA	2	307	-	50,58,73	1.64	9 (18%)	58,95,113	1.49	8 (13%)
25	CLA	H	202	-	41,49,73	1.83	9 (21%)	47,84,113	1.78	8 (17%)
26	PQN	A	841	-	34,34,34	1.37	2 (5%)	42,45,45	1.33	6 (14%)
25	CLA	A	802	-	65,73,73	1.47	10 (15%)	76,113,113	1.51	11 (14%)
25	CLA	F	802	-	45,53,73	1.77	10 (22%)	52,89,113	1.55	7 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
28	BCR	F	803	-	41,41,41	0.91	2 (4%)	56,56,56	2.20	20 (35%)
28	BCR	A	846	-	41,41,41	1.00	2 (4%)	56,56,56	2.10	20 (35%)
28	BCR	I	201	-	41,41,41	0.93	2 (4%)	56,56,56	2.42	22 (39%)
35	XAT	P	620	-	39,47,47	0.89	0	54,74,74	2.97	23 (42%)
25	CLA	P	612	-	60,68,73	1.39	9 (15%)	70,107,113	1.64	9 (12%)
25	CLA	1	613	-	65,73,73	1.48	10 (15%)	76,113,113	1.39	9 (11%)
28	BCR	K	206	-	41,41,41	0.81	0	56,56,56	2.35	20 (35%)
25	CLA	7	301	-	65,73,73	1.49	10 (15%)	76,113,113	1.37	8 (10%)
25	CLA	6	604	-	46,54,73	1.74	9 (19%)	53,90,113	1.55	7 (13%)
25	CLA	L	202	-	65,73,73	1.44	10 (15%)	76,113,113	1.37	7 (9%)
25	CLA	A	827	-	65,73,73	1.50	10 (15%)	76,113,113	1.42	10 (13%)
28	BCR	5	320	-	41,41,41	0.82	1 (2%)	56,56,56	1.92	16 (28%)
28	BCR	B	851	-	41,41,41	0.83	2 (4%)	56,56,56	2.12	19 (33%)
33	CHL	1	601	16	53,61,74	1.98	14 (26%)	57,98,114	2.80	25 (43%)
25	CLA	T	610	-	60,68,73	1.60	6 (10%)	70,107,113	1.48	8 (11%)
25	CLA	4	313	19	41,49,73	1.82	8 (19%)	47,84,113	1.71	9 (19%)
25	CLA	G	201	-	50,58,73	1.67	9 (18%)	58,95,113	1.54	9 (15%)
25	CLA	3	303	-	65,73,73	1.44	10 (15%)	76,113,113	1.47	8 (10%)
33	CHL	7	305	-	54,62,74	1.99	17 (31%)	58,99,114	2.78	22 (37%)
25	CLA	B	821	-	60,68,73	1.52	10 (16%)	70,107,113	1.42	8 (11%)
25	CLA	U	304	-	50,58,73	1.67	6 (12%)	58,95,113	1.61	10 (17%)
35	XAT	S	318	-	39,47,47	0.98	1 (2%)	54,74,74	2.87	22 (40%)
25	CLA	J	103	-	58,66,73	1.56	10 (17%)	67,104,113	1.51	8 (11%)
25	CLA	Q	613	-	48,56,73	1.81	7 (14%)	55,92,113	1.57	8 (14%)
33	CHL	6	607	-	53,61,74	2.02	15 (28%)	57,98,114	2.80	25 (43%)
33	CHL	Q	601	-	51,59,74	2.29	17 (33%)	55,96,114	2.77	24 (43%)
33	CHL	1	606	-	48,56,74	2.20	17 (35%)	51,92,114	2.77	21 (41%)
33	CHL	U	305	14	46,54,74	2.29	15 (32%)	49,90,114	2.88	25 (51%)
25	CLA	5	306	-	55,63,73	1.59	10 (18%)	64,101,113	1.43	6 (9%)
25	CLA	8	306	-	42,50,73	1.80	9 (21%)	48,85,113	1.59	8 (16%)
33	CHL	9	306	-	42,50,74	2.24	17 (40%)	44,85,114	3.18	21 (47%)
25	CLA	A	838	-	65,73,73	1.47	10 (15%)	76,113,113	1.49	9 (11%)
25	CLA	H	203	-	46,54,73	1.71	10 (21%)	53,90,113	1.60	7 (13%)
25	CLA	6	611	27	55,63,73	1.56	9 (16%)	64,101,113	1.41	7 (10%)
32	LMG	J	102	-	40,40,55	0.99	2 (5%)	48,48,63	1.11	5 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	CLA	9	305	-	50,58,73	1.70	9 (18%)	58,95,113	1.57	8 (13%)
33	CHL	8	307	-	53,61,74	2.06	16 (30%)	57,98,114	3.17	28 (49%)
25	CLA	R	613	-	65,73,73	1.46	5 (7%)	76,113,113	1.42	9 (11%)
25	CLA	S	305	-	50,58,73	1.67	6 (12%)	58,95,113	1.56	8 (13%)
25	CLA	B	802	-	65,73,73	1.46	10 (15%)	76,113,113	1.52	9 (11%)
25	CLA	R	614	-	48,56,73	1.73	5 (10%)	55,92,113	1.64	8 (14%)
33	CHL	Q	607	-	44,52,74	2.20	15 (34%)	46,87,114	2.91	22 (47%)
25	CLA	A	801	-	65,73,73	1.44	10 (15%)	76,113,113	1.38	7 (9%)
27	LHG	7	317	25	36,36,48	1.00	2 (5%)	39,42,54	1.31	4 (10%)
33	CHL	4	322	16	53,61,74	2.03	15 (28%)	57,98,114	2.95	26 (45%)
34	LUT	T	614	-	42,43,43	0.76	0	51,60,60	1.73	14 (27%)
28	BCR	B	842	-	41,41,41	1.02	2 (4%)	56,56,56	2.27	20 (35%)
33	CHL	P	608	-	44,52,74	2.20	16 (36%)	46,87,114	2.91	22 (47%)
34	LUT	U	314	-	42,43,43	0.73	0	51,60,60	1.91	14 (27%)
25	CLA	7	313	22	46,54,73	1.70	10 (21%)	53,90,113	1.54	6 (11%)
25	CLA	5	319	-	46,54,73	1.77	9 (19%)	53,90,113	1.60	8 (15%)
33	CHL	P	605	14	48,56,74	2.25	17 (35%)	51,92,114	2.97	24 (47%)
25	CLA	4	302	-	46,54,73	1.78	8 (17%)	53,90,113	1.54	6 (11%)
25	CLA	A	816	-	65,73,73	1.48	9 (13%)	76,113,113	1.45	8 (10%)
33	CHL	P	607	-	52,60,74	2.14	17 (32%)	56,97,114	2.83	27 (48%)
34	LUT	a	316	-	42,43,43	0.74	0	51,60,60	2.13	15 (29%)
25	CLA	2	308	-	43,51,73	1.77	10 (23%)	49,86,113	1.60	9 (18%)
25	CLA	3	320	22	65,73,73	1.43	11 (16%)	76,113,113	1.44	8 (10%)
33	CHL	R	609	-	66,74,74	1.50	11 (16%)	73,114,114	1.84	11 (15%)
34	LUT	P	615	-	42,43,43	0.81	0	51,60,60	1.78	18 (35%)
33	CHL	5	317	-	43,51,74	2.12	14 (32%)	45,86,114	3.06	21 (46%)
33	CHL	U	308	-	44,52,74	2.22	15 (34%)	46,87,114	2.90	21 (45%)
25	CLA	a	311	-	65,73,73	1.46	9 (13%)	76,113,113	1.60	9 (11%)
25	CLA	P	610	-	60,68,73	1.54	6 (10%)	70,107,113	1.39	8 (11%)
25	CLA	A	851	-	65,73,73	1.46	10 (15%)	76,113,113	1.37	8 (10%)
25	CLA	8	309	-	46,54,73	1.72	9 (19%)	53,90,113	1.59	6 (11%)
25	CLA	7	311	-	65,73,73	1.46	10 (15%)	76,113,113	1.43	8 (10%)
25	CLA	B	831	-	65,73,73	1.48	10 (15%)	76,113,113	1.43	8 (10%)
28	BCR	6	621	-	41,41,41	0.83	1 (2%)	56,56,56	2.23	18 (32%)
27	LHG	a	317	25	42,42,48	0.95	2 (4%)	45,48,54	1.21	4 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	CLA	B	820	-	59,67,73	1.51	10 (16%)	68,105,113	1.52	8 (11%)
25	CLA	2	309	-	60,68,73	1.52	9 (15%)	70,107,113	1.45	6 (8%)
27	LHG	A	844	25	37,37,48	1.05	3 (8%)	40,43,54	1.20	3 (7%)
27	LHG	5	301	-	44,44,48	0.96	2 (4%)	47,50,54	1.05	3 (6%)
25	CLA	2	313	-	55,63,73	1.61	8 (14%)	64,101,113	1.56	12 (18%)
25	CLA	U	311	-	54,62,73	1.66	8 (14%)	57,97,113	1.40	7 (12%)
33	CHL	S	306	-	48,56,74	2.20	15 (31%)	51,92,114	2.80	25 (49%)
25	CLA	Q	610	-	39,48,73	1.84	7 (17%)	45,82,113	1.86	10 (22%)
25	CLA	A	823	-	49,57,73	1.66	10 (20%)	55,93,113	1.67	9 (16%)
33	CHL	T	606	-	44,52,74	2.23	14 (31%)	46,87,114	2.93	23 (50%)
35	XAT	P	616	-	39,47,47	0.93	0	54,74,74	3.03	20 (37%)
25	CLA	T	603	-	50,58,73	1.69	5 (10%)	58,95,113	1.60	8 (13%)
28	BCR	A	849	-	41,41,41	0.91	2 (4%)	56,56,56	2.08	17 (30%)
25	CLA	B	849	-	65,73,73	1.46	10 (15%)	76,113,113	1.40	8 (10%)
28	BCR	B	845	-	41,41,41	1.03	3 (7%)	56,56,56	2.16	18 (32%)
25	CLA	B	801	-	65,73,73	1.47	10 (15%)	76,113,113	1.42	8 (10%)
25	CLA	a	307	-	65,73,73	1.48	8 (12%)	76,113,113	1.33	7 (9%)
33	CHL	3	306	-	53,61,74	1.93	15 (28%)	57,98,114	2.84	25 (43%)
33	CHL	U	307	-	53,61,74	2.13	16 (30%)	57,98,114	2.79	25 (43%)
30	DGD	B	846	-	67,67,67	0.80	3 (4%)	81,81,81	1.18	5 (6%)
33	CHL	6	606	-	53,61,74	1.98	15 (28%)	57,98,114	2.78	24 (42%)
26	PQN	B	839	-	34,34,34	1.35	2 (5%)	42,45,45	1.33	4 (9%)
25	CLA	L	201	-	65,73,73	1.45	10 (15%)	76,113,113	1.40	6 (7%)
32	LMG	J	107	-	55,55,55	0.90	2 (3%)	63,63,63	1.23	8 (12%)
25	CLA	B	830	-	65,73,73	1.52	10 (15%)	76,113,113	1.42	10 (13%)
28	BCR	B	844	-	41,41,41	0.96	2 (4%)	56,56,56	2.11	16 (28%)
25	CLA	1	607	-	65,73,73	1.47	9 (13%)	76,113,113	1.41	9 (11%)
33	CHL	S	308	-	52,60,74	2.11	16 (30%)	56,97,114	2.79	25 (44%)
25	CLA	P	604	-	50,58,73	1.69	7 (14%)	58,95,113	1.62	9 (15%)
25	CLA	S	313	-	60,68,73	1.57	6 (10%)	70,107,113	1.41	7 (10%)
25	CLA	A	842	27	52,60,73	1.65	10 (19%)	60,97,113	1.79	14 (23%)
28	BCR	3	319	-	41,41,41	0.80	1 (2%)	56,56,56	2.42	16 (28%)
25	CLA	3	311	-	55,63,73	1.57	9 (16%)	64,101,113	1.55	8 (12%)
33	CHL	S	309	-	52,60,74	2.10	16 (30%)	56,97,114	2.83	25 (44%)
25	CLA	B	816	-	60,68,73	1.53	11 (18%)	70,107,113	1.55	9 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	CLA	A	805	-	55,63,73	1.62	10 (18%)	64,101,113	1.50	6 (9%)
34	LUT	P	614	-	42,43,43	0.74	0	51,60,60	1.92	15 (29%)
25	CLA	U	313	-	45,53,73	1.71	7 (15%)	52,89,113	1.68	7 (13%)
25	CLA	3	309	-	41,49,73	1.80	10 (24%)	47,84,113	1.67	9 (19%)
34	LUT	R	616	-	42,43,43	0.78	0	51,60,60	1.83	18 (35%)
25	CLA	Q	604	-	50,58,73	1.71	6 (12%)	58,95,113	1.64	9 (15%)
33	CHL	4	304	-	42,50,74	2.25	15 (35%)	44,85,114	2.98	21 (47%)
25	CLA	3	313	-	46,54,73	1.68	10 (21%)	53,90,113	1.58	6 (11%)
25	CLA	8	303	-	62,70,73	1.53	11 (17%)	72,109,113	1.44	6 (8%)
25	CLA	B	810	-	65,73,73	1.49	10 (15%)	76,113,113	1.41	8 (10%)
27	LHG	T	617	-	48,48,48	0.94	2 (4%)	51,54,54	0.93	2 (3%)
28	BCR	B	841	-	41,41,41	0.95	2 (4%)	56,56,56	2.24	18 (32%)
25	CLA	9	303	-	60,68,73	1.51	10 (16%)	70,107,113	1.42	7 (10%)
28	BCR	A	847	-	41,41,41	0.92	2 (4%)	56,56,56	2.00	18 (32%)
33	CHL	5	308	-	51,59,74	2.00	16 (31%)	55,96,114	2.96	27 (49%)
32	LMG	6	602	-	40,40,55	1.03	2 (5%)	48,48,63	1.41	6 (12%)
25	CLA	A	821	-	45,53,73	1.75	10 (22%)	52,89,113	1.76	10 (19%)
25	CLA	G	202	-	46,54,73	1.74	9 (19%)	53,90,113	1.69	9 (16%)
25	CLA	8	312	-	52,60,73	1.61	9 (17%)	60,97,113	1.49	6 (10%)
33	CHL	9	307	-	51,59,74	2.11	16 (31%)	55,96,114	2.81	24 (43%)
25	CLA	S	314	-	65,73,73	1.49	6 (9%)	76,113,113	1.40	8 (10%)
33	CHL	P	609	-	66,74,74	1.50	11 (16%)	73,114,114	1.84	12 (16%)
28	BCR	J	101	-	41,41,41	0.90	1 (2%)	56,56,56	2.08	19 (33%)
25	CLA	5	316	-	43,51,73	1.76	10 (23%)	49,86,113	1.68	7 (14%)
25	CLA	7	312	-	43,51,73	1.78	10 (23%)	49,86,113	1.64	7 (14%)
25	CLA	B	829	-	49,57,73	1.64	10 (20%)	55,93,113	1.57	7 (12%)
25	CLA	A	836	-	65,73,73	1.51	10 (15%)	76,113,113	1.44	7 (9%)
25	CLA	8	314	-	55,63,73	1.59	10 (18%)	64,101,113	1.47	11 (17%)
25	CLA	R	610	-	64,72,73	1.55	6 (9%)	74,111,113	1.42	10 (13%)
25	CLA	6	603	-	65,73,73	1.48	10 (15%)	76,113,113	1.39	7 (9%)
27	LHG	A	852	-	46,46,48	0.95	2 (4%)	48,51,54	1.20	5 (10%)
25	CLA	S	312	-	60,68,73	1.52	6 (10%)	70,107,113	1.41	7 (10%)
25	CLA	A	813	-	54,62,73	1.63	10 (18%)	62,99,113	1.54	8 (12%)
25	CLA	S	303	15	65,73,73	1.53	7 (10%)	76,113,113	1.48	10 (13%)
25	CLA	4	307	-	50,58,73	1.71	9 (18%)	58,95,113	1.42	7 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	CLA	a	302	-	57,65,73	1.60	9 (15%)	66,103,113	1.44	6 (9%)
35	XAT	P	623	-	38,46,47	0.97	1 (2%)	52,72,74	3.12	22 (42%)
27	LHG	5	321	-	36,36,48	1.03	2 (5%)	39,42,54	1.29	5 (12%)
25	CLA	B	815	-	59,67,73	1.59	11 (18%)	68,105,113	1.60	11 (16%)
25	CLA	4	308	19	60,68,73	1.46	10 (16%)	70,107,113	1.47	8 (11%)
25	CLA	T	602	-	65,73,73	1.48	6 (9%)	76,113,113	1.38	9 (11%)
25	CLA	4	303	-	50,58,73	1.62	10 (20%)	58,95,113	1.57	8 (13%)
25	CLA	9	309	-	60,68,73	1.53	9 (15%)	70,107,113	1.47	9 (12%)
34	LUT	2	315	-	42,43,43	0.83	1 (2%)	51,60,60	1.84	13 (25%)
25	CLA	B	826	-	65,73,73	1.51	10 (15%)	76,113,113	1.44	10 (13%)
25	CLA	L	205	-	65,73,73	1.42	11 (16%)	76,113,113	1.47	9 (11%)
33	CHL	R	608	-	44,52,74	2.21	14 (31%)	46,87,114	2.91	22 (47%)
33	CHL	4	314	19	43,51,74	2.18	14 (32%)	45,86,114	2.99	21 (46%)
25	CLA	4	310	-	52,60,73	1.73	10 (19%)	60,97,113	1.76	10 (16%)
28	BCR	G	203	-	41,41,41	0.84	1 (2%)	56,56,56	2.09	16 (28%)
30	DGD	B	848	-	58,58,67	0.96	4 (6%)	72,72,81	1.37	11 (15%)
25	CLA	B	836	-	65,73,73	1.46	10 (15%)	76,113,113	1.40	8 (10%)
25	CLA	a	304	-	52,60,73	1.66	7 (13%)	60,97,113	1.39	6 (10%)
25	CLA	7	307	-	50,58,73	1.64	10 (20%)	58,95,113	1.53	6 (10%)
25	CLA	B	824	-	65,73,73	1.46	10 (15%)	76,113,113	1.45	11 (14%)
33	CHL	P	601	-	51,59,74	2.30	17 (33%)	55,96,114	2.78	24 (43%)
36	NEX	U	301	-	38,46,46	1.08	2 (5%)	50,70,70	2.95	18 (36%)
25	CLA	a	306	-	65,73,73	1.45	7 (10%)	76,113,113	1.43	10 (13%)
25	CLA	P	603	-	65,73,73	1.49	6 (9%)	76,113,113	1.47	9 (11%)
25	CLA	R	611	-	60,68,73	1.53	5 (8%)	70,107,113	1.68	11 (15%)
25	CLA	7	309	27	41,49,73	1.82	10 (24%)	47,84,113	1.65	9 (19%)
25	CLA	7	306	-	50,58,73	1.69	10 (20%)	58,95,113	1.56	9 (15%)
25	CLA	B	809	-	65,73,73	1.47	10 (15%)	76,113,113	1.41	7 (9%)
25	CLA	K	205	-	45,53,73	1.76	7 (15%)	52,89,113	1.64	6 (11%)
25	CLA	6	616	-	46,54,73	1.74	9 (19%)	53,90,113	1.59	8 (15%)
25	CLA	B	808	2	65,73,73	1.47	10 (15%)	76,113,113	1.41	9 (11%)
33	CHL	T	601	-	50,58,74	2.33	17 (34%)	52,94,114	2.79	22 (42%)
25	CLA	Q	612	-	60,68,73	1.58	6 (10%)	70,107,113	1.46	10 (14%)
28	BCR	B	840	-	41,41,41	0.93	1 (2%)	56,56,56	2.11	15 (26%)
25	CLA	B	819	-	46,54,73	1.70	10 (21%)	53,90,113	1.64	9 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	CLA	U	312	-	65,73,73	1.49	6 (9%)	76,113,113	1.37	7 (9%)
25	CLA	A	808	-	65,73,73	1.49	9 (13%)	76,113,113	1.40	9 (11%)
25	CLA	1	605	-	52,60,73	1.69	8 (15%)	60,97,113	1.46	8 (13%)
33	CHL	a	305	-	48,56,74	2.23	17 (35%)	51,92,114	2.76	21 (41%)
28	BCR	F	801	-	41,41,41	0.90	2 (4%)	56,56,56	2.10	17 (30%)
25	CLA	5	310	-	60,68,73	1.44	9 (15%)	70,107,113	1.45	8 (11%)
25	CLA	B	828	-	50,58,73	1.66	10 (20%)	58,95,113	1.56	6 (10%)
29	SF4	C	102	3	0,12,12	-	-	-	-	-
33	CHL	T	604	14	48,56,74	2.23	16 (33%)	51,92,114	2.91	25 (49%)
25	CLA	A	833	-	50,58,73	1.66	10 (20%)	58,95,113	1.64	8 (13%)
25	CLA	P	602	-	65,73,73	1.47	5 (7%)	76,113,113	1.39	8 (10%)
25	CLA	5	312	-	52,60,73	1.68	9 (17%)	60,97,113	1.52	8 (13%)
28	BCR	8	318	-	41,41,41	0.82	1 (2%)	56,56,56	2.16	20 (35%)
33	CHL	P	619	-	52,60,74	2.14	17 (32%)	56,97,114	2.84	27 (48%)
33	CHL	U	306	-	50,58,74	2.18	16 (32%)	52,94,114	2.82	23 (44%)
33	CHL	R	601	-	51,59,74	2.29	17 (33%)	55,96,114	2.78	24 (43%)
25	CLA	6	601	19	61,69,73	1.48	9 (14%)	71,108,113	1.44	7 (9%)
25	CLA	2	314	-	46,54,73	1.76	10 (21%)	53,90,113	1.54	7 (13%)
25	CLA	1	603	-	65,73,73	1.45	10 (15%)	76,113,113	1.34	8 (10%)
25	CLA	6	623	-	60,68,73	1.50	9 (15%)	70,107,113	1.58	9 (12%)
25	CLA	5	313	-	56,64,73	1.60	11 (19%)	65,102,113	1.79	14 (21%)
25	CLA	Q	602	-	65,73,73	1.51	6 (9%)	76,113,113	1.39	7 (9%)
25	CLA	A	829	-	65,73,73	1.49	11 (16%)	76,113,113	1.47	9 (11%)
27	LHG	A	843	-	48,48,48	0.90	2 (4%)	51,54,54	1.13	3 (5%)
28	BCR	L	204	-	41,41,41	1.01	2 (4%)	56,56,56	2.21	23 (41%)
25	CLA	A	839	-	65,73,73	1.47	10 (15%)	76,113,113	1.50	8 (10%)
25	CLA	4	312	-	45,53,73	1.76	8 (17%)	52,89,113	1.52	8 (15%)
33	CHL	R	607	-	52,60,74	2.13	17 (32%)	56,97,114	2.83	27 (48%)
32	LMG	4	320	-	40,40,55	1.06	3 (7%)	48,48,63	1.30	6 (12%)
25	CLA	2	304	-	65,73,73	1.49	10 (15%)	76,113,113	1.42	7 (9%)
28	BCR	A	848	-	41,41,41	0.91	1 (2%)	56,56,56	1.97	16 (28%)
25	CLA	1	604	-	57,65,73	1.59	10 (17%)	66,103,113	1.43	8 (12%)
25	CLA	A	810	1	65,73,73	1.47	10 (15%)	76,113,113	1.41	9 (11%)
25	CLA	8	308	-	50,58,73	1.63	12 (24%)	58,95,113	1.68	8 (13%)
27	LHG	6	618	25	48,48,48	0.87	2 (4%)	51,54,54	1.22	4 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	CLA	6	612	-	52,60,73	1.73	8 (15%)	60,97,113	1.46	6 (10%)
34	LUT	R	615	-	42,43,43	0.76	0	51,60,60	1.93	14 (27%)
33	CHL	R	606	-	50,58,74	2.16	17 (34%)	52,94,114	2.82	24 (46%)
31	SQD	B	850	-	50,51,54	1.21	4 (8%)	59,62,65	1.21	7 (11%)
25	CLA	S	320	-	65,73,73	1.48	6 (9%)	76,113,113	1.43	8 (10%)
25	CLA	A	812	-	65,73,73	1.49	10 (15%)	76,113,113	1.44	9 (11%)
25	CLA	3	305	18	60,68,73	1.51	10 (16%)	70,107,113	1.46	8 (11%)
27	LHG	B	847	-	37,37,48	1.03	2 (5%)	40,43,54	1.20	5 (12%)
33	CHL	4	305	-	51,59,74	2.22	17 (33%)	55,96,114	2.77	23 (41%)
25	CLA	A	811	-	65,73,73	1.48	10 (15%)	76,113,113	1.49	8 (10%)
25	CLA	A	818	-	65,73,73	1.45	9 (13%)	76,113,113	1.38	8 (10%)
33	CHL	6	617	21	43,51,74	2.18	14 (32%)	45,86,114	3.01	22 (48%)
25	CLA	A	803	-	65,73,73	1.46	10 (15%)	76,113,113	1.37	7 (9%)
25	CLA	B	804	-	65,73,73	1.50	10 (15%)	76,113,113	1.45	9 (11%)
33	CHL	Q	605	14	42,50,74	2.39	16 (38%)	44,85,114	3.11	22 (50%)
33	CHL	U	309	-	48,56,74	2.34	17 (35%)	51,92,114	2.92	22 (43%)
25	CLA	A	824	-	55,63,73	1.59	10 (18%)	64,101,113	1.53	8 (12%)
28	BCR	B	843	-	41,41,41	0.86	2 (4%)	56,56,56	1.86	18 (32%)
34	LUT	S	317	-	42,43,43	0.77	0	51,60,60	1.65	9 (17%)
25	CLA	5	305	-	50,58,73	1.66	11 (22%)	58,95,113	1.56	8 (13%)

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
34	LUT	Q	615	-	-	2/29/67/67	0/2/2/2
34	LUT	6	622	-	-	1/29/67/67	0/2/2/2
28	BCR	3	318	-	-	8/29/63/63	0/2/2/2
25	CLA	8	311	27	1/1/11/20	5/15/93/115	-
28	BCR	L	203	-	-	4/29/63/63	0/2/2/2
25	CLA	3	314	-	1/1/13/20	13/27/105/115	-
28	BCR	A	854	-	-	2/29/63/63	0/2/2/2
28	BCR	L	208	-	-	2/29/63/63	0/2/2/2
25	CLA	a	301	-	1/1/15/20	10/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CLA	8	304	-	1/1/11/20	8/13/91/115	-
29	SF4	C	101	3	-	-	0/6/5/5
25	CLA	7	303	-	1/1/13/20	9/27/105/115	-
28	BCR	4	317	-	-	8/29/63/63	0/2/2/2
25	CLA	A	819	-	1/1/15/20	12/37/115/115	-
34	LUT	a	315	-	-	4/29/67/67	0/2/2/2
33	CHL	S	302	-	3/3/17/26	13/24/122/137	-
25	CLA	1	608	-	1/1/15/20	11/37/115/115	-
25	CLA	6	605	-	1/1/15/20	11/37/115/115	-
25	CLA	A	853	-	1/1/15/20	15/37/115/115	-
32	LMG	H	204	-	-	14/42/62/70	0/1/1/1
25	CLA	a	308	16	1/1/14/20	7/31/109/115	-
25	CLA	1	610	27	1/1/15/20	10/37/115/115	-
27	LHG	4	319	-	-	7/36/36/53	-
25	CLA	6	609	-	1/1/12/20	8/19/97/115	-
25	CLA	6	614	-	1/1/11/20	3/13/91/115	-
25	CLA	S	311	-	1/1/14/20	7/31/109/115	-
25	CLA	B	807	-	1/1/15/20	11/37/115/115	-
25	CLA	1	602	-	1/1/15/20	9/37/115/115	-
25	CLA	A	822	-	1/1/15/20	14/37/115/115	-
25	CLA	3	308	-	1/1/15/20	12/37/115/115	-
33	CHL	P	622	-	3/3/17/26	9/24/122/137	-
25	CLA	3	301	-	1/1/14/20	3/31/109/115	-
25	CLA	a	310	-	1/1/12/20	8/22/100/115	-
35	XAT	Q	616	-	-	4/31/93/93	0/4/4/4
34	LUT	a	314	-	-	2/29/67/67	0/2/2/2
25	CLA	O	203	-	1/1/10/20	0/4/80/115	-
32	LMG	7	318	-	-	11/30/50/70	0/1/1/1
32	LMG	J	104	-	-	13/30/50/70	0/1/1/1
25	CLA	A	809	1	1/1/15/20	13/37/115/115	-
25	CLA	2	305	-	1/1/12/20	7/22/100/115	-
25	CLA	T	612	-	1/1/11/20	9/17/95/115	-
25	CLA	B	811	-	1/1/15/20	15/37/115/115	-
25	CLA	U	303	-	1/1/15/20	11/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CLA	9	308	-	1/1/12/20	4/19/97/115	-
25	CLA	4	311	-	1/1/13/20	14/27/105/115	-
29	SF4	A	850	2,1	-	-	0/6/5/5
25	CLA	A	835	-	1/1/12/20	6/21/99/115	-
28	BCR	L	207	-	-	8/29/63/63	0/2/2/2
25	CLA	a	313	-	1/1/11/20	4/15/93/115	-
25	CLA	6	615	21	1/1/11/20	4/15/93/115	-
25	CLA	2	302	17	1/1/11/20	11/15/93/115	-
25	CLA	B	837	-	1/1/15/20	15/37/115/115	-
25	CLA	P	613	-	1/1/13/20	9/29/107/115	-
33	CHL	P	606	-	3/3/16/26	7/20/118/137	-
25	CLA	S	304	-	1/1/15/20	12/37/115/115	-
34	LUT	1	616	-	-	4/29/67/67	0/2/2/2
25	CLA	8	310	-	1/1/14/20	8/31/109/115	-
25	CLA	K	201	-	1/1/12/20	8/21/99/115	-
25	CLA	2	310	-	1/1/10/20	2/8/86/115	-
36	NEX	P	621	-	-	10/27/83/83	0/3/3/3
25	CLA	A	834	1	1/1/11/20	9/13/91/115	-
25	CLA	3	302	-	1/1/15/20	8/37/115/115	-
33	CHL	T	605	-	3/3/16/26	7/20/118/137	-
34	LUT	U	315	-	-	2/29/67/67	0/2/2/2
34	LUT	8	316	-	-	1/29/67/67	0/2/2/2
32	LMG	7	319	-	-	13/31/51/70	0/1/1/1
25	CLA	B	822	-	1/1/15/20	14/37/115/115	-
34	LUT	5	318	-	-	0/29/67/67	0/2/2/2
25	CLA	T	608	-	1/1/15/20	12/37/115/115	-
25	CLA	A	831	-	1/1/12/20	8/19/97/115	-
25	CLA	P	611	-	1/1/10/20	4/8/86/115	-
25	CLA	S	315	-	1/1/11/20	6/17/95/115	-
25	CLA	3	312	-	1/1/11/20	4/13/91/115	-
25	CLA	5	304	-	1/1/11/20	5/15/93/115	-
25	CLA	B	834	-	1/1/15/20	20/37/115/115	-
25	CLA	1	612	-	1/1/15/20	14/37/115/115	-
25	CLA	B	805	-	1/1/15/20	16/37/115/115	-
25	CLA	9	310	24	1/1/12/20	10/19/97/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CLA	R	604	-	1/1/12/20	6/19/97/115	-
25	CLA	B	825	-	1/1/15/20	13/37/115/115	-
34	LUT	Q	614	-	-	0/29/67/67	0/2/2/2
25	CLA	a	312	-	1/1/15/20	9/37/115/115	-
33	CHL	Q	608	-	3/3/20/26	16/39/137/137	-
25	CLA	Q	611	-	1/1/14/20	7/31/109/115	-
34	LUT	S	316	-	-	5/29/67/67	0/2/2/2
32	LMG	1	619	-	-	15/41/61/70	0/1/1/1
25	CLA	R	603	-	1/1/15/20	11/37/115/115	-
25	CLA	B	835	-	1/1/11/20	4/16/94/115	-
33	CHL	S	310	15	3/3/17/26	7/23/121/137	-
25	CLA	5	315	20	1/1/11/20	6/15/93/115	-
28	BCR	A	845	-	-	3/29/63/63	0/2/2/2
25	CLA	A	804	-	1/1/15/20	9/37/115/115	-
25	CLA	O	201	-	1/1/10/20	6/8/86/115	-
25	CLA	H	205	12	1/1/10/20	2/10/88/115	-
25	CLA	1	609	16	1/1/14/20	7/31/109/115	-
25	CLA	1	614	-	1/1/11/20	4/15/93/115	-
25	CLA	A	817	-	1/1/13/20	3/28/106/115	-
25	CLA	3	310	-	1/1/11/20	5/15/93/115	-
34	LUT	T	613	-	-	0/29/67/67	0/2/2/2
25	CLA	A	820	-	1/1/15/20	12/37/115/115	-
28	BCR	8	301	-	-	3/29/63/63	0/2/2/2
25	CLA	A	814	-	1/1/15/20	19/37/115/115	-
25	CLA	8	302	23	1/1/15/20	13/37/115/115	-
34	LUT	1	617	-	-	6/29/67/67	0/2/2/2
25	CLA	U	302	-	1/1/15/20	8/37/115/115	-
34	LUT	6	619	-	-	1/29/67/67	0/2/2/2
34	LUT	5	322	-	-	0/29/67/67	0/2/2/2
25	CLA	5	314	-	1/1/11/20	5/13/91/115	-
25	CLA	2	311	-	1/1/12/20	8/22/100/115	-
25	CLA	9	302	-	1/1/11/20	9/15/93/115	-
25	CLA	5	324	-	1/1/15/20	17/37/115/115	-
25	CLA	A	832	-	1/1/15/20	13/37/115/115	-
25	CLA	B	817	-	1/1/15/20	5/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CLA	Q	603	-	1/1/15/20	11/37/115/115	-
25	CLA	5	303	-	-	13/37/115/115	-
34	LUT	1	615	-	-	2/29/67/67	0/2/2/2
34	LUT	3	316	-	-	0/29/67/67	0/2/2/2
25	CLA	B	803	-	1/1/11/20	5/13/91/115	-
27	LHG	Q	617	-	-	13/53/53/53	-
25	CLA	K	203	-	1/1/11/20	6/15/93/115	-
35	XAT	T	615	-	-	4/31/93/93	0/4/4/4
25	CLA	B	813	-	1/1/13/20	8/28/106/115	-
25	CLA	5	309	-	1/1/12/20	10/19/97/115	-
27	LHG	4	318	25	-	20/53/53/53	-
25	CLA	O	202	-	1/1/9/20	0/4/78/115	-
25	CLA	A	837	-	1/1/15/20	10/37/115/115	-
33	CHL	6	608	-	3/3/17/26	10/21/119/137	-
34	LUT	7	315	-	-	2/29/67/67	0/2/2/2
25	CLA	A	830	-	1/1/15/20	14/37/115/115	-
25	CLA	B	832	-	1/1/11/20	5/13/91/115	-
25	CLA	A	807	-	1/1/15/20	21/37/115/115	-
27	LHG	R	618	-	-	13/53/53/53	-
25	CLA	Q	609	-	1/1/15/20	11/37/115/115	-
25	CLA	2	303	17	1/1/15/20	13/37/115/115	-
25	CLA	Q	618	-	-	0/8/82/115	-
34	LUT	9	313	-	-	2/29/67/67	0/2/2/2
25	CLA	4	309	27	1/1/13/20	8/25/103/115	-
27	LHG	2	317	-	-	24/53/53/53	-
25	CLA	T	609	-	-	12/31/109/115	-
34	LUT	8	317	-	-	1/29/67/67	0/2/2/2
25	CLA	T	611	-	1/1/14/20	11/31/109/115	-
25	CLA	7	304	-	1/1/10/20	8/10/88/115	-
32	LMG	2	301	-	-	12/36/56/70	0/1/1/1
25	CLA	A	806	-	1/1/15/20	17/37/115/115	-
25	CLA	7	310	-	1/1/12/20	7/22/100/115	-
25	CLA	B	814	-	1/1/13/20	7/25/103/115	-
25	CLA	R	602	-	1/1/15/20	8/37/115/115	-
25	CLA	9	311	-	1/1/11/20	0/13/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
33	CHL	4	306	-	3/3/17/26	4/21/119/137	-
25	CLA	H	201	-	1/1/11/20	8/15/93/115	-
34	LUT	4	316	-	-	4/29/67/67	0/2/2/2
25	CLA	K	204	-	1/1/11/20	7/13/91/115	-
25	CLA	8	305	-	1/1/11/20	4/15/93/115	-
28	BCR	3	317	-	-	6/29/63/63	0/2/2/2
28	BCR	7	316	-	-	2/29/63/63	0/2/2/2
25	CLA	A	840	-	1/1/15/20	15/37/115/115	-
34	LUT	2	316	-	-	0/29/67/67	0/2/2/2
25	CLA	A	815	-	1/1/14/20	15/31/109/115	-
25	CLA	2	312	-	1/1/15/20	12/37/115/115	-
25	CLA	L	209	-	1/1/10/20	4/8/86/115	-
25	CLA	B	833	-	1/1/14/20	5/31/109/115	-
33	CHL	S	307	-	3/3/16/26	4/20/118/137	-
36	NEX	T	616	-	-	7/27/83/83	0/3/3/3
25	CLA	B	838	-	1/1/15/20	9/37/115/115	-
25	CLA	5	302	20	1/1/15/20	10/37/115/115	-
27	LHG	P	624	-	-	12/53/53/53	-
25	CLA	R	612	-	1/1/14/20	13/31/109/115	-
27	LHG	8	319	25	-	17/53/53/53	-
25	CLA	7	308	-	1/1/14/20	10/31/109/115	-
25	CLA	J	105	-	1/1/10/20	6/10/88/115	-
25	CLA	B	812	-	1/1/14/20	10/31/109/115	-
25	CLA	7	302	-	1/1/11/20	3/15/93/115	-
33	CHL	S	321	-	3/3/17/26	9/21/119/137	-
25	CLA	2	306	17	1/1/10/20	2/8/86/115	-
25	CLA	6	610	-	1/1/14/20	8/31/109/115	-
34	LUT	9	312	-	-	2/29/67/67	0/2/2/2
25	CLA	1	611	-	1/1/12/20	8/22/100/115	-
25	CLA	3	307	-	1/1/12/20	7/19/97/115	-
25	CLA	a	303	-	1/1/13/20	10/28/106/115	-
28	BCR	5	323	-	-	8/29/63/63	0/2/2/2
25	CLA	A	826	-	1/1/15/20	6/37/115/115	-
33	CHL	5	307	-	3/3/17/26	9/21/119/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	BCR	O	205	-	-	4/29/63/63	0/2/2/2
25	CLA	9	301	-	1/1/13/20	5/25/101/115	-
36	NEX	U	316	-	-	7/27/83/83	0/3/3/3
28	BCR	J	106	-	-	6/29/63/63	0/2/2/2
25	CLA	A	828	-	1/1/15/20	15/37/115/115	-
27	LHG	1	618	25	-	15/47/47/53	-
28	BCR	O	204	-	-	5/29/63/63	0/2/2/2
25	CLA	a	309	27	1/1/15/20	10/37/115/115	-
34	LUT	7	314	-	-	2/29/67/67	0/2/2/2
34	LUT	3	315	-	-	0/29/67/67	0/2/2/2
27	LHG	P	618	-	-	12/53/53/53	-
25	CLA	B	806	-	1/1/15/20	10/37/115/115	-
25	CLA	9	304	-	1/1/11/20	6/15/93/115	-
33	CHL	R	605	14	3/3/16/26	4/15/113/137	-
36	NEX	P	617	-	-	7/27/83/83	0/3/3/3
36	NEX	R	617	-	-	6/27/83/83	0/3/3/3
25	CLA	U	310	-	1/1/14/20	10/36/114/115	-
27	LHG	S	319	-	-	10/53/53/53	-
34	LUT	4	315	-	-	1/29/67/67	0/2/2/2
25	CLA	B	818	-	1/1/13/20	9/27/105/115	-
25	CLA	B	827	-	1/1/15/20	7/37/115/115	-
25	CLA	8	313	-	1/1/15/20	11/37/115/115	-
25	CLA	6	613	-	1/1/13/20	9/27/105/115	-
28	BCR	4	321	-	-	7/29/63/63	0/2/2/2
25	CLA	L	206	-	1/1/10/20	4/10/88/115	-
25	CLA	8	315	23	1/1/11/20	5/15/93/115	-
33	CHL	T	607	-	3/3/17/26	6/23/121/137	-
25	CLA	3	304	-	1/1/10/20	0/10/88/115	-
25	CLA	A	825	-	1/1/15/20	20/37/115/115	-
25	CLA	6	620	-	1/1/11/20	6/13/91/115	-
25	CLA	S	301	-	1/1/11/20	7/16/94/115	-
25	CLA	B	823	-	1/1/15/20	5/37/115/115	-
25	CLA	K	202	-	1/1/11/20	4/13/91/115	-
25	CLA	4	301	-	1/1/14/20	11/31/109/115	-
25	CLA	5	311	-	1/1/13/20	8/25/103/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
33	CHL	Q	606	-	3/3/16/26	7/20/118/137	-
25	CLA	2	307	-	1/1/12/20	6/19/97/115	-
25	CLA	H	202	-	1/1/10/20	2/8/86/115	-
26	PQN	A	841	-	-	6/23/43/43	0/2/2/2
25	CLA	A	802	-	1/1/15/20	8/37/115/115	-
25	CLA	F	802	-	1/1/11/20	3/13/91/115	-
28	BCR	F	803	-	-	2/29/63/63	0/2/2/2
28	BCR	A	846	-	-	2/29/63/63	0/2/2/2
28	BCR	I	201	-	-	7/29/63/63	0/2/2/2
35	XAT	P	620	-	-	4/31/93/93	0/4/4/4
25	CLA	P	612	-	1/1/14/20	13/31/109/115	-
25	CLA	1	613	-	1/1/15/20	9/37/115/115	-
28	BCR	K	206	-	-	10/29/63/63	0/2/2/2
25	CLA	7	301	-	1/1/15/20	14/37/115/115	-
25	CLA	6	604	-	1/1/11/20	3/15/93/115	-
25	CLA	L	202	-	1/1/15/20	12/37/115/115	-
25	CLA	A	827	-	1/1/15/20	7/37/115/115	-
28	BCR	5	320	-	-	9/29/63/63	0/2/2/2
28	BCR	B	851	-	-	3/29/63/63	0/2/2/2
33	CHL	1	601	16	3/3/17/26	5/24/122/137	-
25	CLA	T	610	-	1/1/14/20	10/31/109/115	-
25	CLA	4	313	19	1/1/10/20	0/8/86/115	-
25	CLA	G	201	-	1/1/12/20	3/19/97/115	-
25	CLA	3	303	-	1/1/15/20	10/37/115/115	-
33	CHL	7	305	-	3/3/17/26	10/25/123/137	-
25	CLA	B	821	-	1/1/14/20	6/31/109/115	-
25	CLA	U	304	-	1/1/12/20	6/19/97/115	-
35	XAT	S	318	-	-	4/31/93/93	0/4/4/4
25	CLA	J	103	-	1/1/13/20	11/29/107/115	-
25	CLA	Q	613	-	1/1/11/20	9/17/95/115	-
33	CHL	6	607	-	3/3/17/26	9/24/122/137	-
33	CHL	Q	601	-	3/3/17/26	8/21/119/137	-
33	CHL	1	606	-	3/3/16/26	6/18/116/137	-
33	CHL	U	305	14	3/3/16/26	7/15/113/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CLA	5	306	-	1/1/13/20	2/25/103/115	-
25	CLA	8	306	-	1/1/10/20	3/10/88/115	-
33	CHL	9	306	-	3/3/15/26	5/10/108/137	-
25	CLA	A	838	-	1/1/15/20	12/37/115/115	-
25	CLA	H	203	-	1/1/11/20	8/15/93/115	-
25	CLA	6	611	27	1/1/13/20	6/25/103/115	-
32	LMG	J	102	-	-	8/35/55/70	0/1/1/1
25	CLA	9	305	-	1/1/12/20	7/19/97/115	-
33	CHL	8	307	-	3/3/17/26	11/24/122/137	-
25	CLA	R	613	-	1/1/15/20	15/37/115/115	-
25	CLA	S	305	-	1/1/12/20	6/19/97/115	-
25	CLA	B	802	-	1/1/15/20	13/37/115/115	-
25	CLA	R	614	-	1/1/11/20	9/17/95/115	-
33	CHL	Q	607	-	3/3/15/26	5/13/111/137	-
25	CLA	A	801	-	1/1/15/20	11/37/115/115	-
27	LHG	7	317	25	-	14/41/41/53	-
33	CHL	4	322	16	3/3/17/26	5/24/122/137	-
34	LUT	T	614	-	-	2/29/67/67	0/2/2/2
28	BCR	B	842	-	-	6/29/63/63	0/2/2/2
33	CHL	P	608	-	3/3/15/26	5/13/111/137	-
34	LUT	U	314	-	-	0/29/67/67	0/2/2/2
25	CLA	7	313	22	1/1/11/20	8/15/93/115	-
33	CHL	P	605	14	3/3/16/26	6/18/116/137	-
25	CLA	5	319	-	-	8/15/93/115	-
25	CLA	4	302	-	1/1/11/20	3/15/93/115	-
25	CLA	A	816	-	1/1/15/20	12/37/115/115	-
33	CHL	P	607	-	3/3/17/26	10/23/121/137	-
34	LUT	a	316	-	-	6/29/67/67	0/2/2/2
25	CLA	2	308	-	1/1/10/20	4/11/89/115	-
25	CLA	3	320	22	1/1/15/20	16/37/115/115	-
33	CHL	R	609	-	3/3/20/26	16/39/137/137	-
34	LUT	P	615	-	-	2/29/67/67	0/2/2/2
33	CHL	5	317	-	3/3/15/26	2/12/110/137	-
33	CHL	U	308	-	3/3/15/26	5/13/111/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CLA	a	311	-	1/1/15/20	13/37/115/115	-
25	CLA	P	610	-	1/1/14/20	9/31/109/115	-
25	CLA	A	851	-	1/1/15/20	14/37/115/115	-
25	CLA	8	309	-	1/1/11/20	6/15/93/115	-
25	CLA	7	311	-	1/1/15/20	13/37/115/115	-
25	CLA	B	831	-	1/1/15/20	10/37/115/115	-
28	BCR	6	621	-	-	8/29/63/63	0/2/2/2
27	LHG	a	317	25	-	17/47/47/53	-
25	CLA	B	820	-	1/1/13/20	4/30/108/115	-
25	CLA	2	309	-	1/1/14/20	13/31/109/115	-
27	LHG	A	844	25	-	14/42/42/53	-
27	LHG	5	301	-	-	19/49/49/53	-
25	CLA	2	313	-	1/1/13/20	5/25/103/115	-
25	CLA	U	311	-	1/1/11/20	7/25/96/115	-
33	CHL	S	306	-	3/3/16/26	9/18/116/137	-
25	CLA	Q	610	-	1/1/9/20	0/8/82/115	-
25	CLA	A	823	-	1/1/11/20	10/18/96/115	-
33	CHL	T	606	-	3/3/15/26	5/13/111/137	-
35	XAT	P	616	-	-	4/31/93/93	0/4/4/4
25	CLA	T	603	-	1/1/12/20	6/19/97/115	-
28	BCR	A	849	-	-	6/29/63/63	0/2/2/2
25	CLA	B	849	-	1/1/15/20	13/37/115/115	-
28	BCR	B	845	-	-	4/29/63/63	0/2/2/2
25	CLA	B	801	-	1/1/15/20	12/37/115/115	-
25	CLA	a	307	-	1/1/15/20	10/37/115/115	-
33	CHL	3	306	-	3/3/17/26	9/24/122/137	-
33	CHL	U	307	-	3/3/17/26	11/24/122/137	-
33	CHL	6	606	-	3/3/17/26	7/24/122/137	-
30	DGD	B	846	-	-	15/55/95/95	0/2/2/2
26	PQN	B	839	-	-	3/23/43/43	0/2/2/2
25	CLA	L	201	-	1/1/15/20	10/37/115/115	-
32	LMG	J	107	-	-	18/50/70/70	0/1/1/1
25	CLA	B	830	-	1/1/15/20	16/37/115/115	-
28	BCR	B	844	-	-	2/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CLA	1	607	-	1/1/15/20	6/37/115/115	-
33	CHL	S	308	-	3/3/17/26	6/23/121/137	-
25	CLA	P	604	-	1/1/12/20	6/19/97/115	-
25	CLA	S	313	-	1/1/14/20	13/31/109/115	-
25	CLA	A	842	27	1/1/12/20	11/22/100/115	-
28	BCR	3	319	-	-	6/29/63/63	0/2/2/2
25	CLA	3	311	-	1/1/13/20	9/25/103/115	-
33	CHL	S	309	-	3/3/17/26	6/23/121/137	-
25	CLA	B	816	-	1/1/14/20	11/31/109/115	-
25	CLA	A	805	-	1/1/13/20	8/25/103/115	-
34	LUT	P	614	-	-	0/29/67/67	0/2/2/2
25	CLA	U	313	-	1/1/11/20	7/13/91/115	-
25	CLA	3	309	-	1/1/10/20	4/8/86/115	-
34	LUT	R	616	-	-	2/29/67/67	0/2/2/2
25	CLA	Q	604	-	1/1/12/20	6/19/97/115	-
33	CHL	4	304	-	3/3/15/26	3/10/108/137	-
25	CLA	3	313	-	1/1/11/20	4/15/93/115	-
25	CLA	8	303	-	1/1/14/20	8/34/112/115	-
25	CLA	B	810	-	1/1/15/20	12/37/115/115	-
27	LHG	T	617	-	-	12/53/53/53	-
28	BCR	B	841	-	-	4/29/63/63	0/2/2/2
25	CLA	9	303	-	1/1/14/20	12/31/109/115	-
28	BCR	A	847	-	-	2/29/63/63	0/2/2/2
33	CHL	5	308	-	3/3/17/26	6/21/119/137	-
32	LMG	6	602	-	-	12/35/55/70	0/1/1/1
25	CLA	A	821	-	1/1/11/20	1/13/91/115	-
25	CLA	G	202	-	1/1/11/20	3/15/93/115	-
25	CLA	8	312	-	1/1/12/20	7/22/100/115	-
33	CHL	9	307	-	3/3/17/26	6/21/119/137	-
25	CLA	S	314	-	-	20/37/115/115	-
33	CHL	P	609	-	3/3/20/26	16/39/137/137	-
28	BCR	J	101	-	-	6/29/63/63	0/2/2/2
25	CLA	5	316	-	1/1/10/20	2/11/89/115	-
25	CLA	7	312	-	1/1/10/20	1/11/89/115	-
25	CLA	B	829	-	1/1/11/20	5/18/96/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CLA	A	836	-	1/1/15/20	14/37/115/115	-
25	CLA	8	314	-	1/1/13/20	7/25/103/115	-
25	CLA	R	610	-	1/1/14/20	12/36/114/115	-
25	CLA	6	603	-	1/1/15/20	11/37/115/115	-
27	LHG	A	852	-	-	24/49/49/53	-
25	CLA	S	312	-	1/1/14/20	9/31/109/115	-
25	CLA	A	813	-	1/1/12/20	2/24/102/115	-
25	CLA	S	303	15	1/1/15/20	11/37/115/115	-
25	CLA	4	307	-	1/1/12/20	7/19/97/115	-
25	CLA	a	302	-	1/1/13/20	8/28/106/115	-
35	XAT	P	623	-	-	3/29/91/93	0/4/4/4
27	LHG	5	321	-	-	13/41/41/53	-
25	CLA	B	815	-	1/1/13/20	15/30/108/115	-
25	CLA	4	308	19	1/1/14/20	12/31/109/115	-
25	CLA	T	602	-	1/1/15/20	7/37/115/115	-
25	CLA	4	303	-	1/1/12/20	7/19/97/115	-
25	CLA	9	309	-	1/1/14/20	10/31/109/115	-
34	LUT	2	315	-	-	6/29/67/67	0/2/2/2
25	CLA	B	826	-	1/1/15/20	17/37/115/115	-
25	CLA	L	205	-	1/1/15/20	11/37/115/115	-
33	CHL	R	608	-	3/3/15/26	5/13/111/137	-
33	CHL	4	314	19	3/3/15/26	4/12/110/137	-
25	CLA	4	310	-	1/1/12/20	8/22/100/115	-
28	BCR	G	203	-	-	1/29/63/63	0/2/2/2
30	DGD	B	848	-	-	16/46/86/95	0/2/2/2
25	CLA	B	836	-	1/1/15/20	15/37/115/115	-
25	CLA	a	304	-	1/1/12/20	2/22/100/115	-
25	CLA	7	307	-	1/1/12/20	4/19/97/115	-
25	CLA	B	824	-	1/1/15/20	17/37/115/115	-
33	CHL	P	601	-	3/3/17/26	8/21/119/137	-
36	NEX	U	301	-	-	6/27/83/83	0/3/3/3
25	CLA	a	306	-	1/1/15/20	6/37/115/115	-
25	CLA	P	603	-	1/1/15/20	11/37/115/115	-
25	CLA	R	611	-	1/1/14/20	9/31/109/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CLA	7	309	27	1/1/10/20	2/8/86/115	-
25	CLA	7	306	-	1/1/12/20	2/19/97/115	-
25	CLA	B	809	-	1/1/15/20	14/37/115/115	-
25	CLA	K	205	-	1/1/11/20	6/13/91/115	-
25	CLA	6	616	-	1/1/11/20	4/15/93/115	-
25	CLA	B	808	2	1/1/15/20	8/37/115/115	-
33	CHL	T	601	-	3/3/16/26	9/20/118/137	-
25	CLA	Q	612	-	1/1/14/20	11/31/109/115	-
28	BCR	B	840	-	-	7/29/63/63	0/2/2/2
25	CLA	B	819	-	1/1/11/20	6/15/93/115	-
25	CLA	U	312	-	1/1/15/20	15/37/115/115	-
25	CLA	A	808	-	1/1/15/20	11/37/115/115	-
25	CLA	1	605	-	1/1/12/20	2/22/100/115	-
33	CHL	a	305	-	3/3/16/26	6/18/116/137	-
28	BCR	F	801	-	-	4/29/63/63	0/2/2/2
25	CLA	5	310	-	1/1/14/20	5/31/109/115	-
25	CLA	B	828	-	1/1/12/20	3/19/97/115	-
29	SF4	C	102	3	-	-	0/6/5/5
33	CHL	T	604	14	3/3/16/26	3/18/116/137	-
25	CLA	A	833	-	1/1/12/20	0/19/97/115	-
25	CLA	P	602	-	1/1/15/20	7/37/115/115	-
25	CLA	5	312	-	1/1/12/20	5/22/100/115	-
33	CHL	P	619	-	3/3/17/26	10/23/121/137	-
28	BCR	8	318	-	-	5/29/63/63	0/2/2/2
33	CHL	U	306	-	3/3/16/26	7/20/118/137	-
33	CHL	R	601	-	3/3/17/26	8/21/119/137	-
25	CLA	6	601	19	1/1/14/20	13/33/111/115	-
25	CLA	2	314	-	1/1/11/20	5/15/93/115	-
25	CLA	1	603	-	1/1/15/20	10/37/115/115	-
25	CLA	6	623	-	1/1/14/20	13/31/109/115	-
25	CLA	5	313	-	1/1/13/20	6/27/105/115	-
25	CLA	Q	602	-	1/1/15/20	7/37/115/115	-
25	CLA	A	829	-	1/1/15/20	10/37/115/115	-
27	LHG	A	843	-	-	18/53/53/53	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	BCR	L	204	-	-	7/29/63/63	0/2/2/2
25	CLA	A	839	-	1/1/15/20	11/37/115/115	-
25	CLA	4	312	-	1/1/11/20	2/13/91/115	-
33	CHL	R	607	-	3/3/17/26	10/23/121/137	-
32	LMG	4	320	-	-	6/35/55/70	0/1/1/1
25	CLA	2	304	-	1/1/15/20	16/37/115/115	-
25	CLA	1	604	-	1/1/13/20	8/28/106/115	-
28	BCR	A	848	-	-	6/29/63/63	0/2/2/2
25	CLA	A	810	1	1/1/15/20	11/37/115/115	-
25	CLA	8	308	-	1/1/12/20	4/19/97/115	-
27	LHG	6	618	25	-	23/53/53/53	-
25	CLA	6	612	-	1/1/12/20	3/22/100/115	-
34	LUT	R	615	-	-	2/29/67/67	0/2/2/2
33	CHL	R	606	-	3/3/16/26	8/20/118/137	-
31	SQD	B	850	-	-	16/46/66/69	0/1/1/1
25	CLA	S	320	-	1/1/15/20	11/37/115/115	-
25	CLA	A	812	-	1/1/15/20	14/37/115/115	-
25	CLA	3	305	18	1/1/14/20	12/31/109/115	-
27	LHG	B	847	-	-	17/42/42/53	-
33	CHL	4	305	-	3/3/17/26	5/21/119/137	-
25	CLA	A	811	-	1/1/15/20	6/37/115/115	-
25	CLA	A	818	-	1/1/15/20	15/37/115/115	-
33	CHL	6	617	21	3/3/15/26	4/12/110/137	-
25	CLA	A	803	-	1/1/15/20	5/37/115/115	-
25	CLA	B	804	-	1/1/15/20	13/37/115/115	-
33	CHL	Q	605	14	3/3/15/26	1/10/108/137	-
33	CHL	U	309	-	3/3/16/26	3/18/116/137	-
25	CLA	A	824	-	1/1/13/20	8/25/103/115	-
28	BCR	B	843	-	-	5/29/63/63	0/2/2/2
34	LUT	S	317	-	-	6/29/67/67	0/2/2/2
25	CLA	5	305	-	1/1/12/20	2/19/97/115	-

The worst 5 of 3554 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	S	303	CLA	C4B-NB	7.98	1.42	1.35
25	Q	613	CLA	C4B-NB	7.93	1.42	1.35
25	R	610	CLA	C4B-NB	7.83	1.42	1.35
25	R	603	CLA	C4B-NB	7.79	1.42	1.35
25	Q	612	CLA	C4B-NB	7.77	1.42	1.35

The worst 5 of 5126 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	a	303	CLA	C1-C2-C3	16.98	155.41	126.04
25	1	612	CLA	C4A-NA-C1A	13.26	112.67	106.71
36	P	621	NEX	C16-C1-C6	12.24	121.42	110.47
25	a	303	CLA	C4-C3-C5	-10.98	96.79	115.27
33	R	609	CHL	C4A-NA-C1A	10.42	111.39	106.71

5 of 439 chirality outliers are listed below:

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

5 of 3566 torsion outliers are listed below:

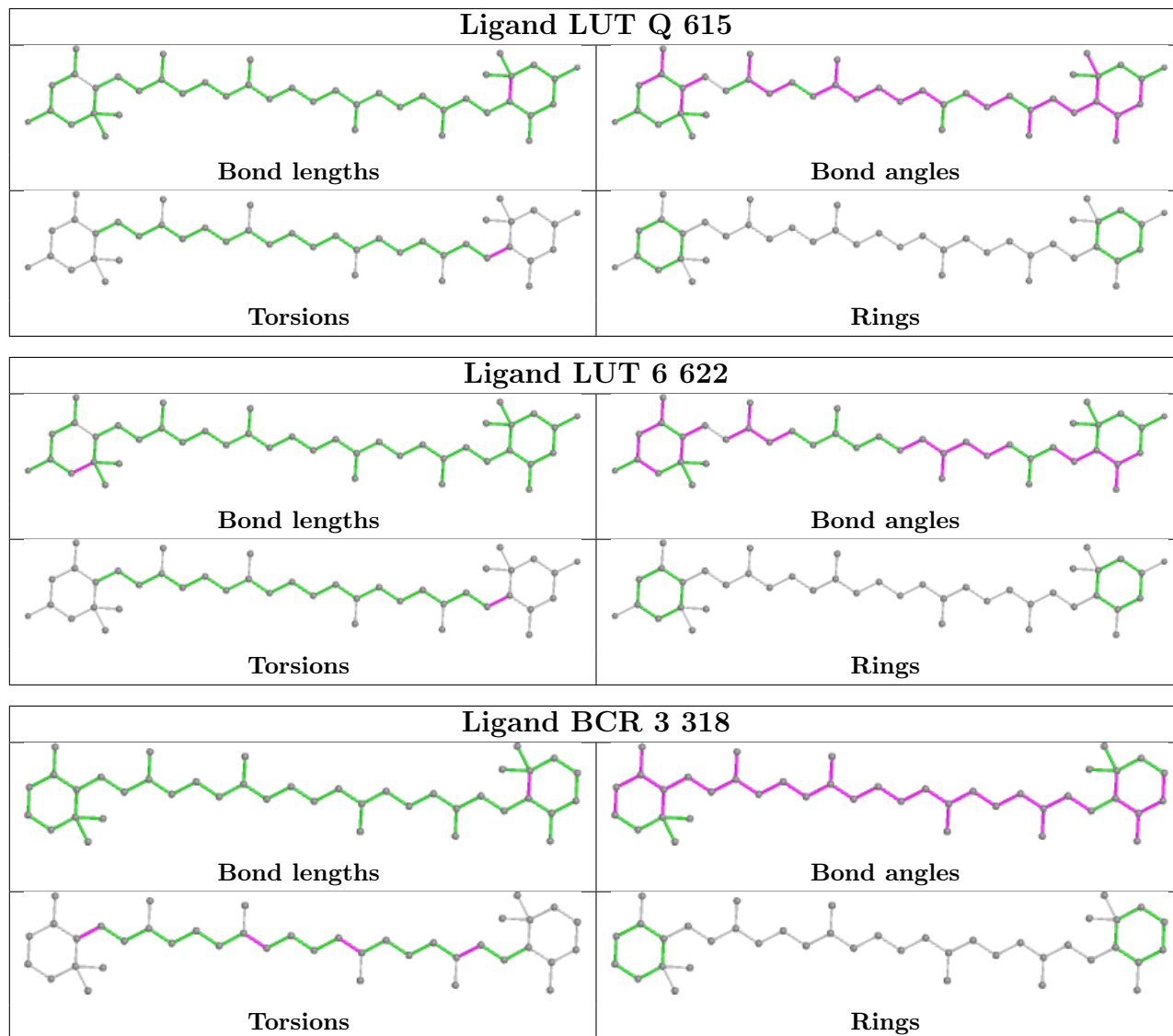
Mol	Chain	Res	Type	Atoms
25	A	801	CLA	CBD-CGD-O2D-CED
25	A	804	CLA	CAD-CBD-CGD-O1D
25	A	804	CLA	CAD-CBD-CGD-O2D
25	A	806	CLA	CHA-CBD-CGD-O1D
25	A	806	CLA	CHA-CBD-CGD-O2D

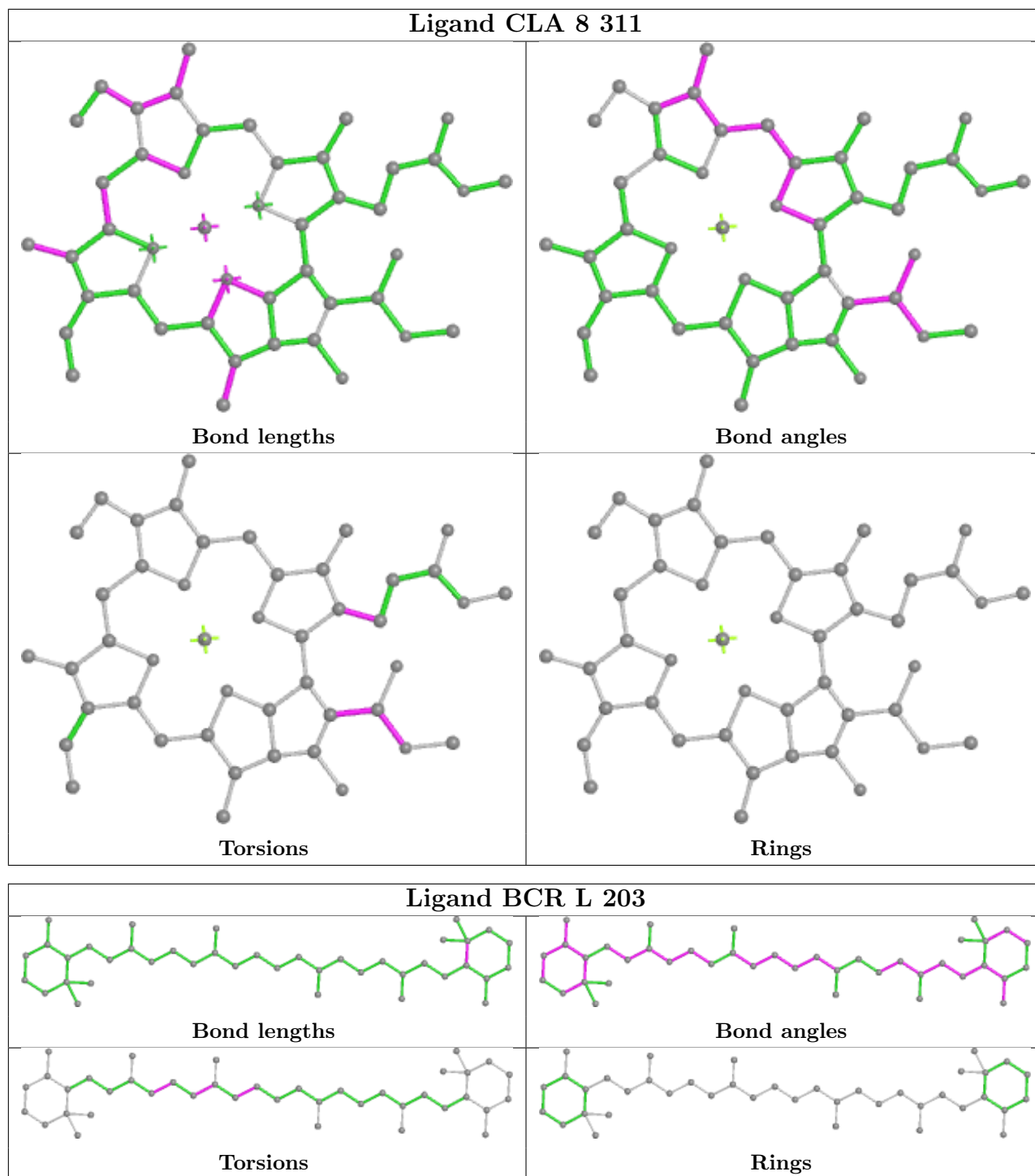
There are no ring outliers.

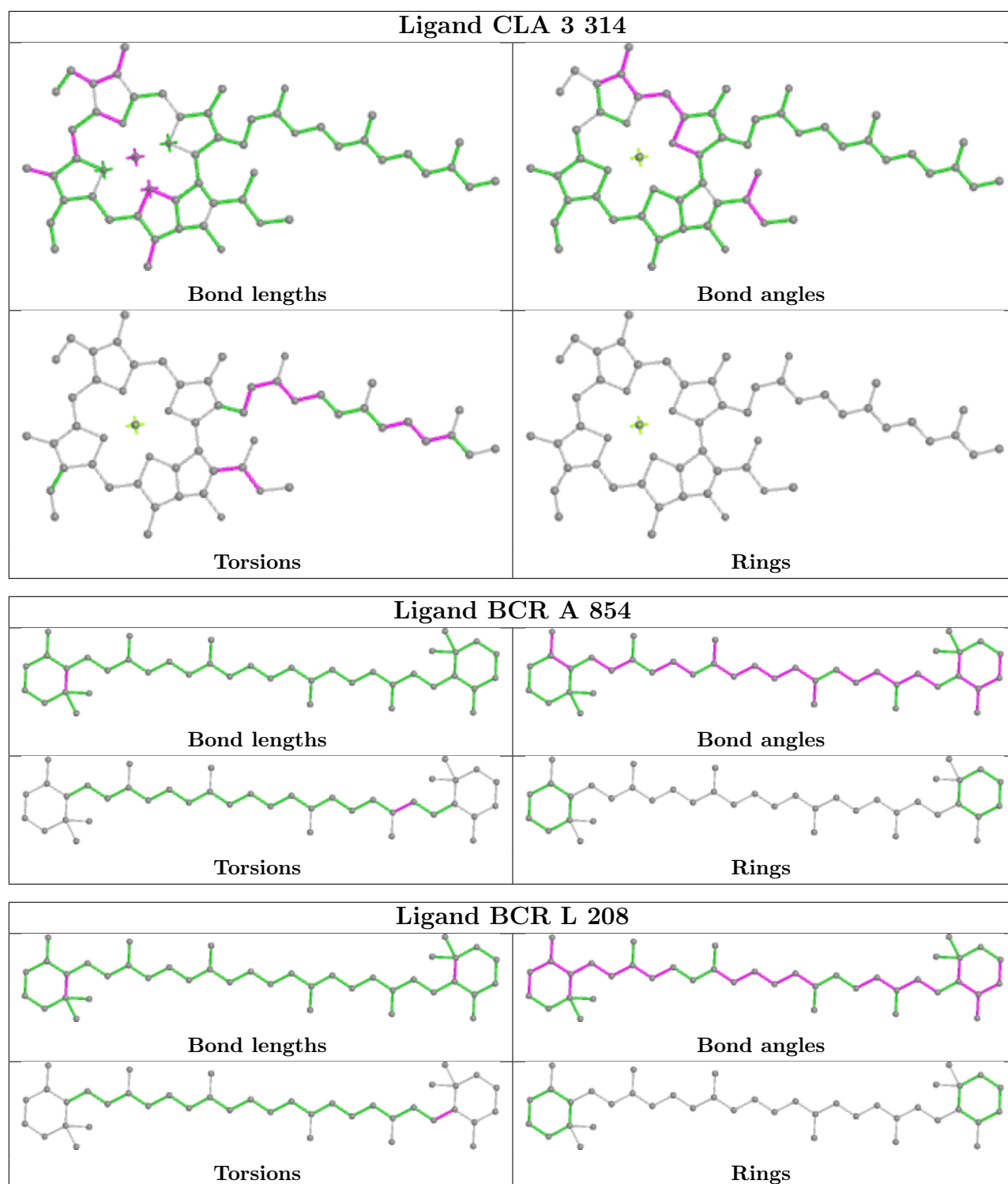
No monomer is involved in short contacts.

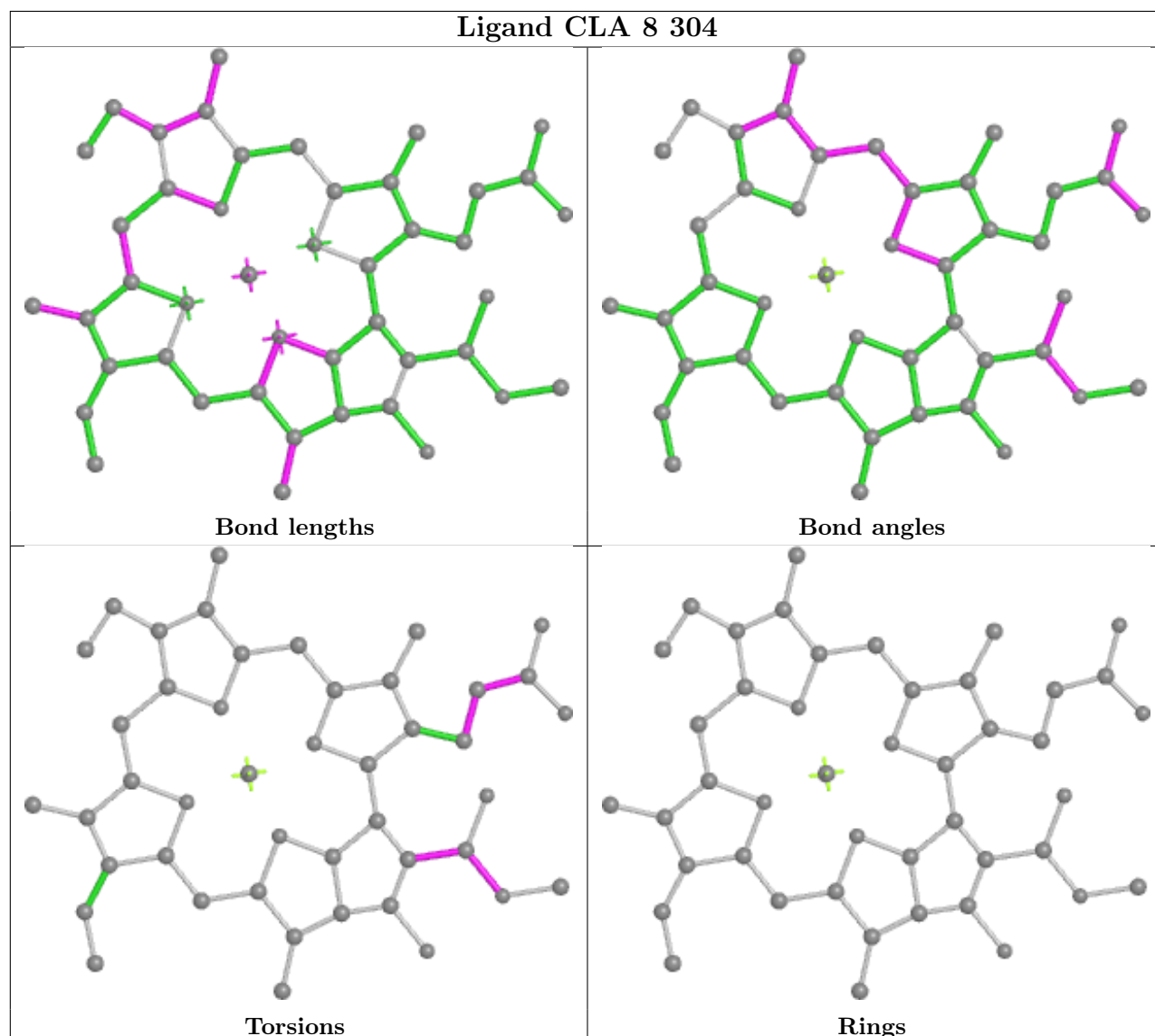
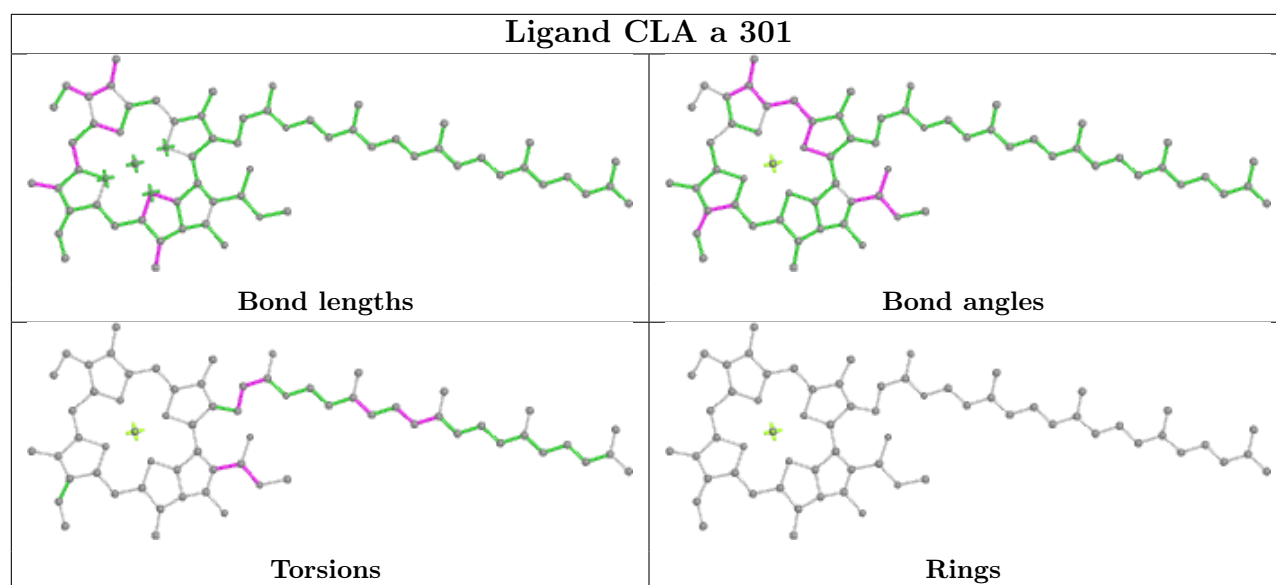
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring

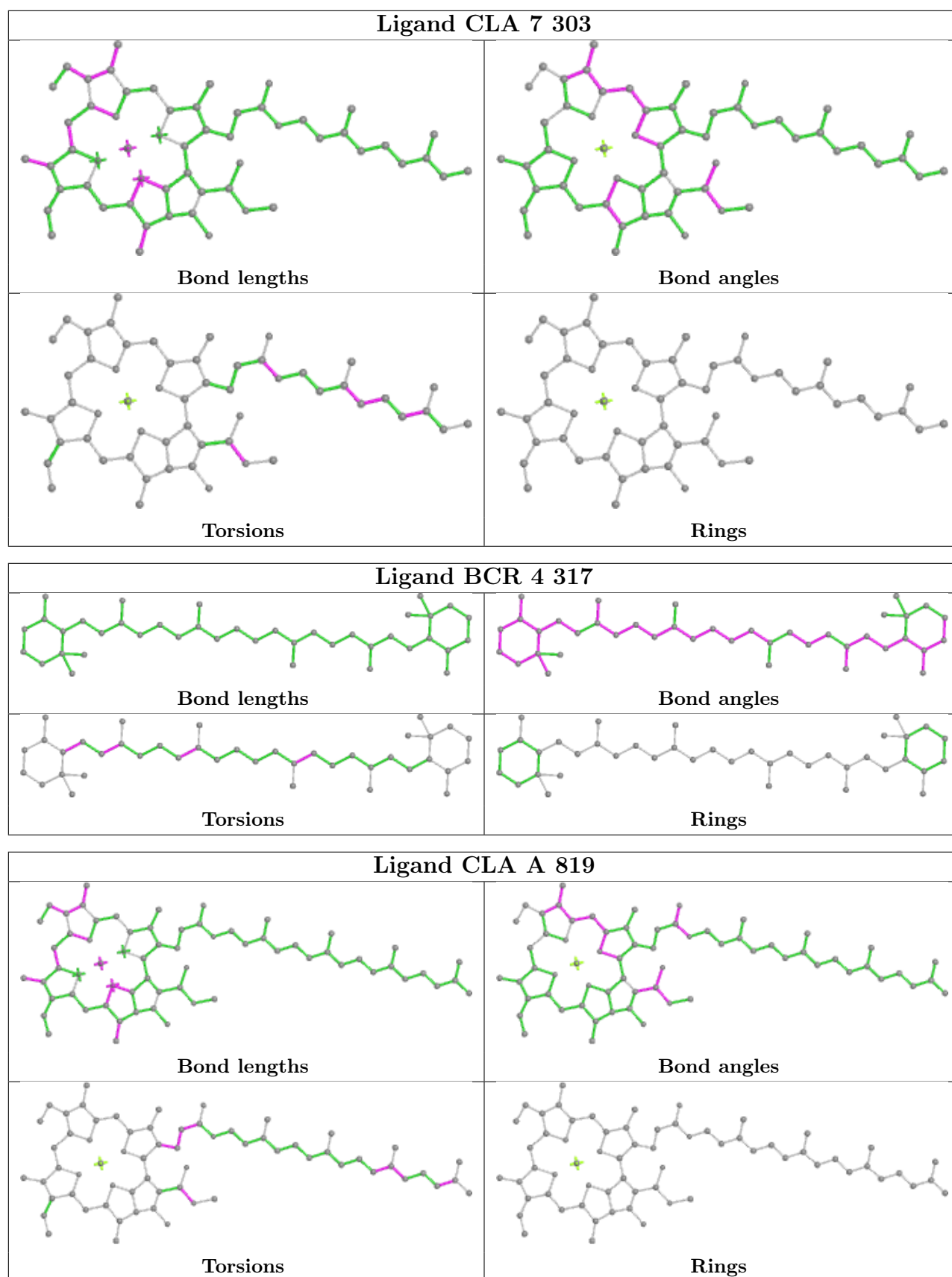
in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

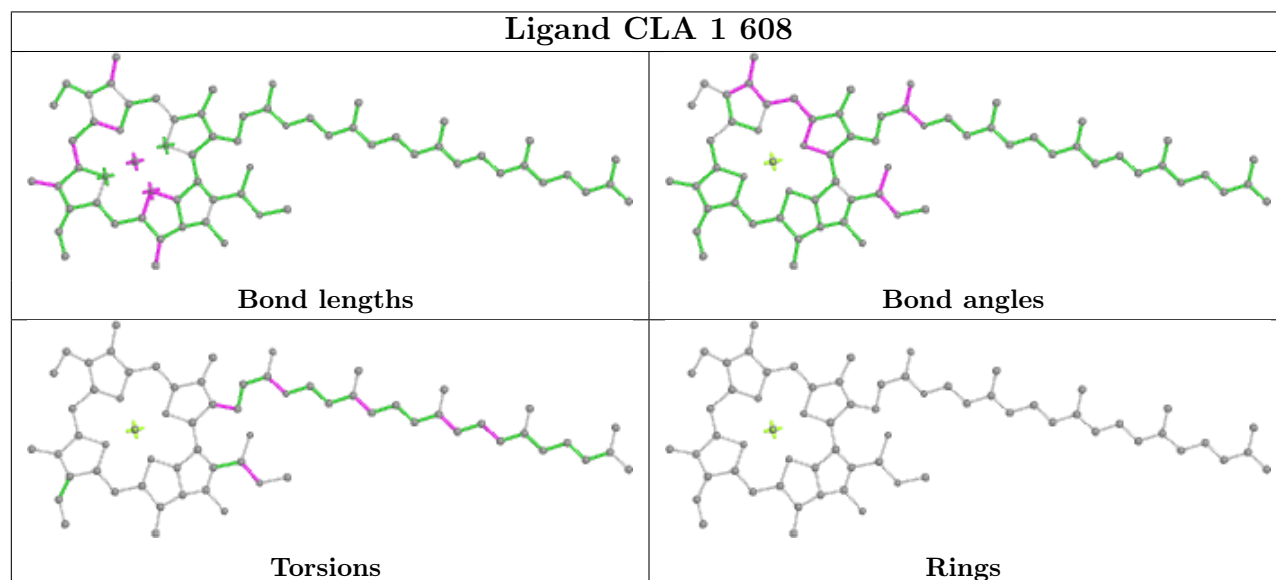
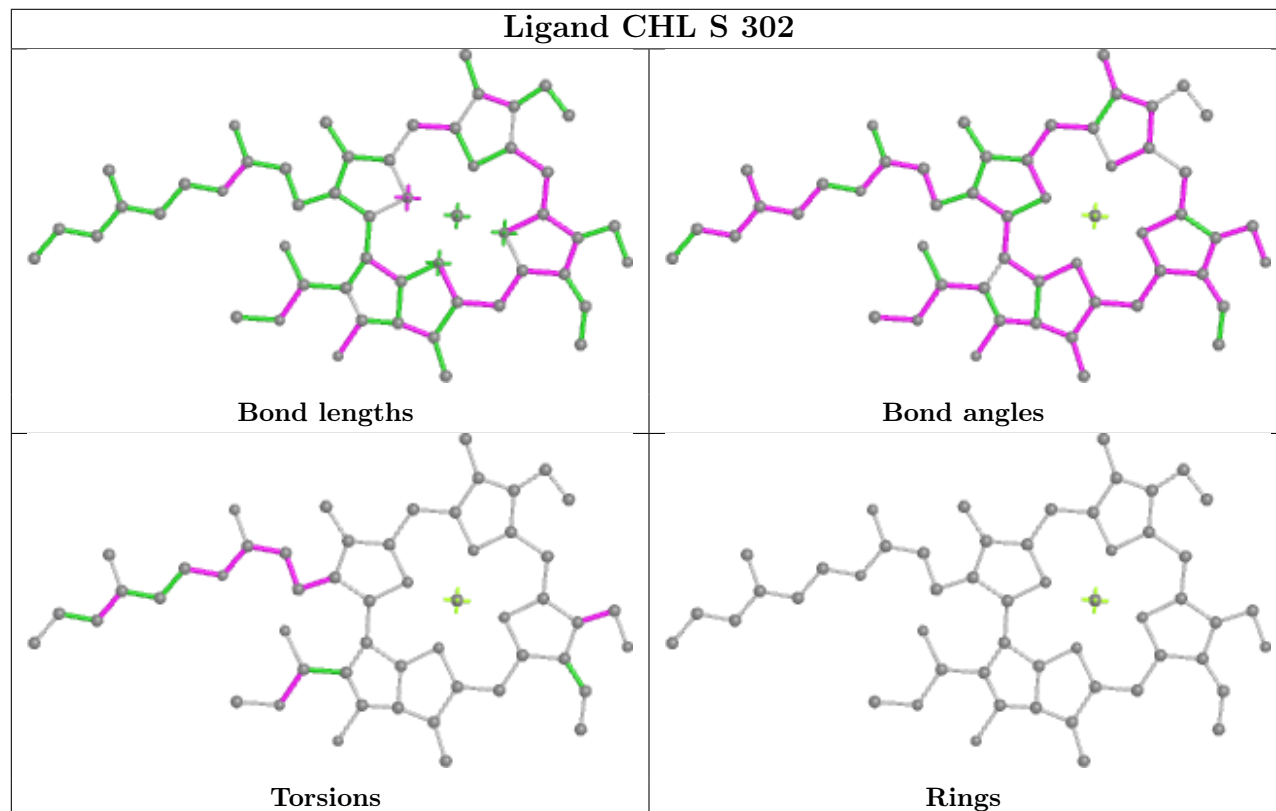
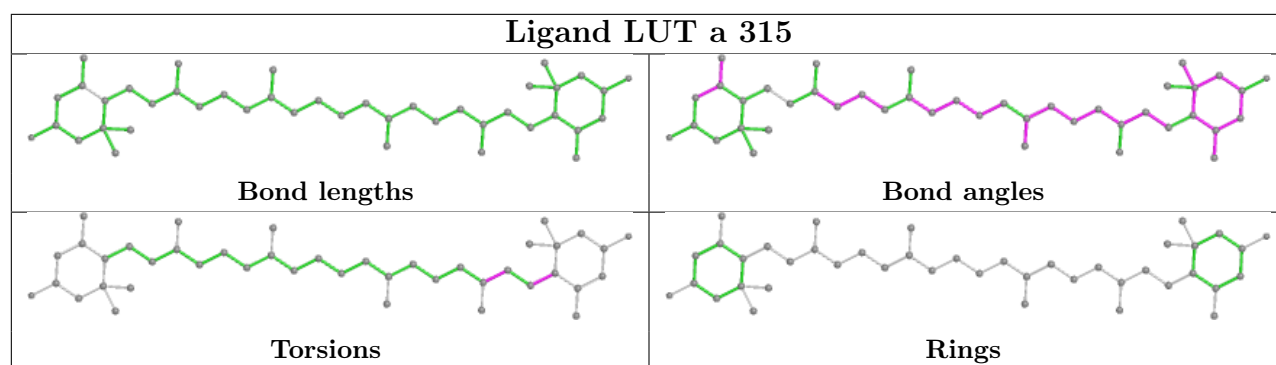


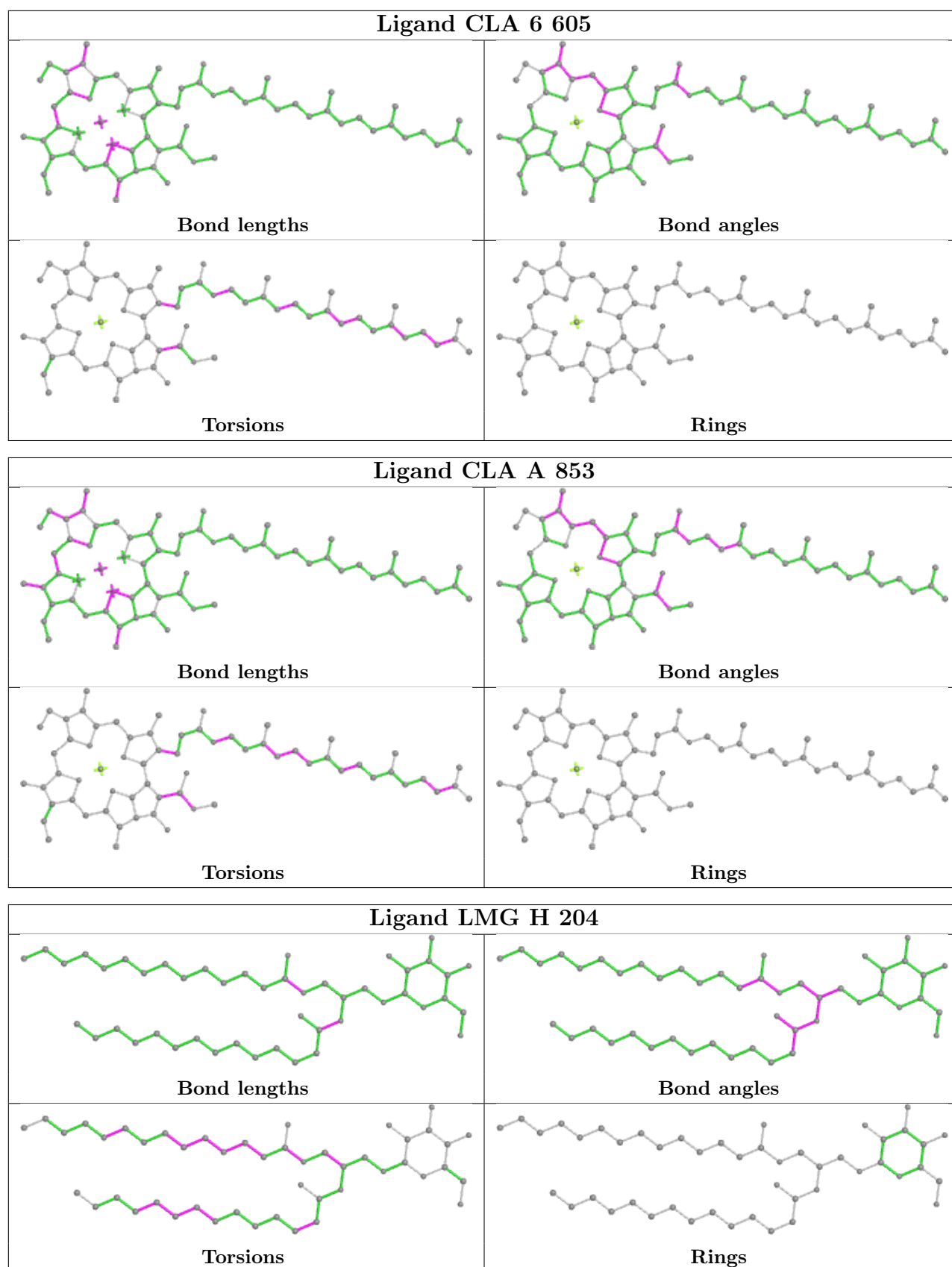


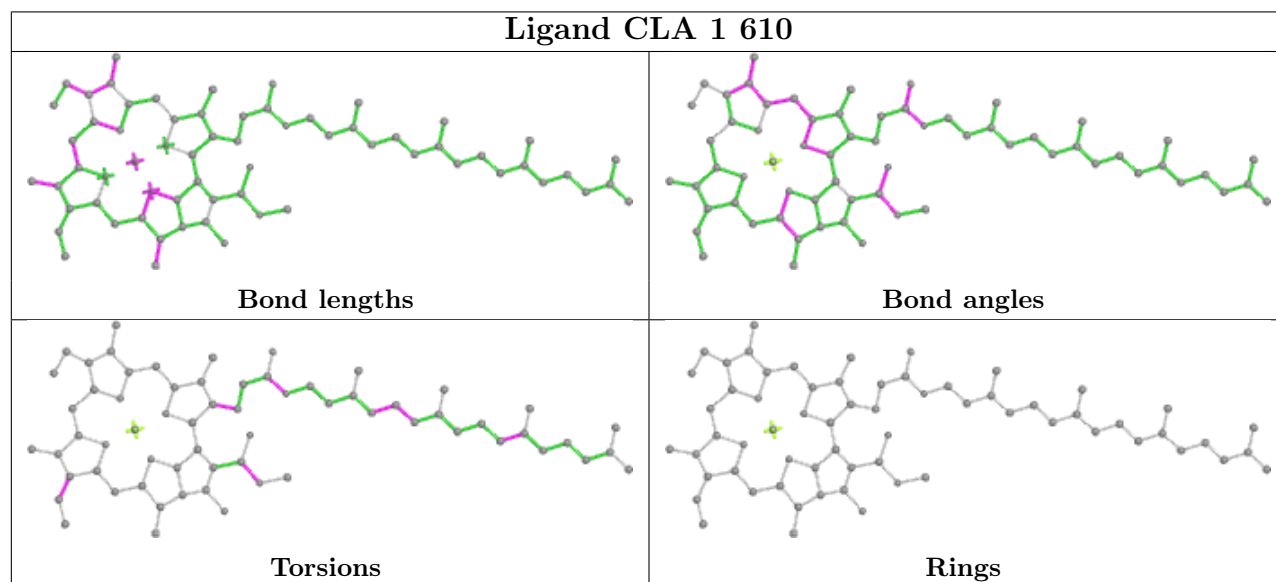
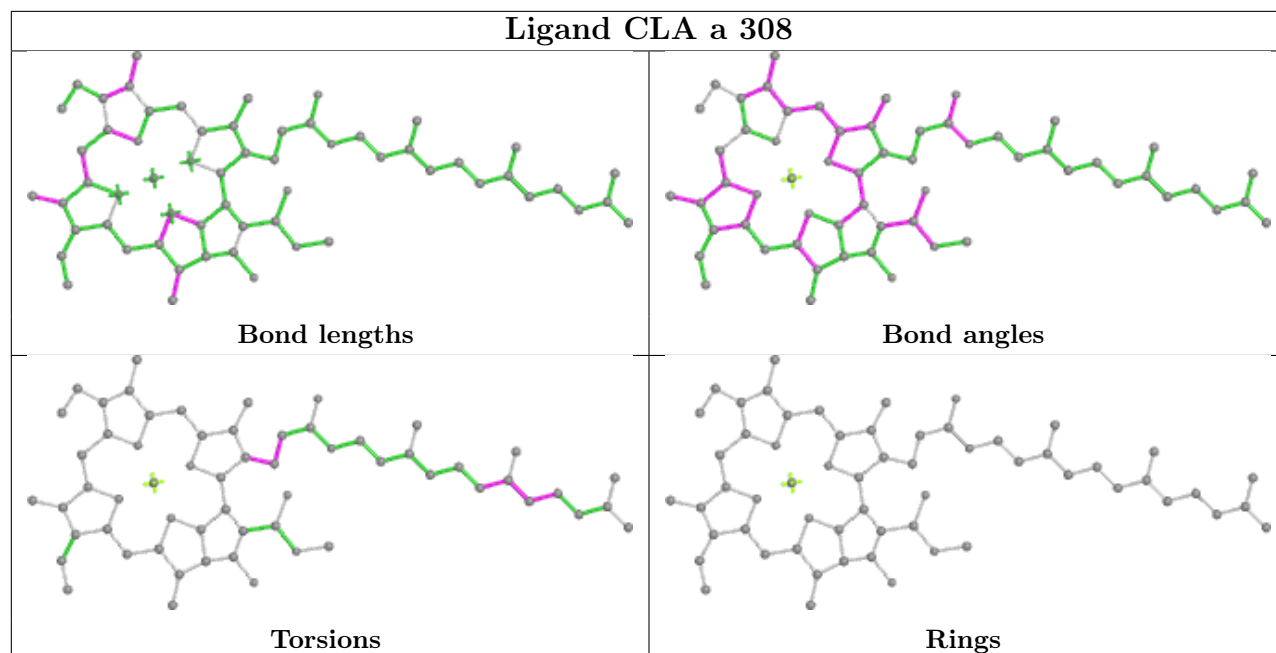


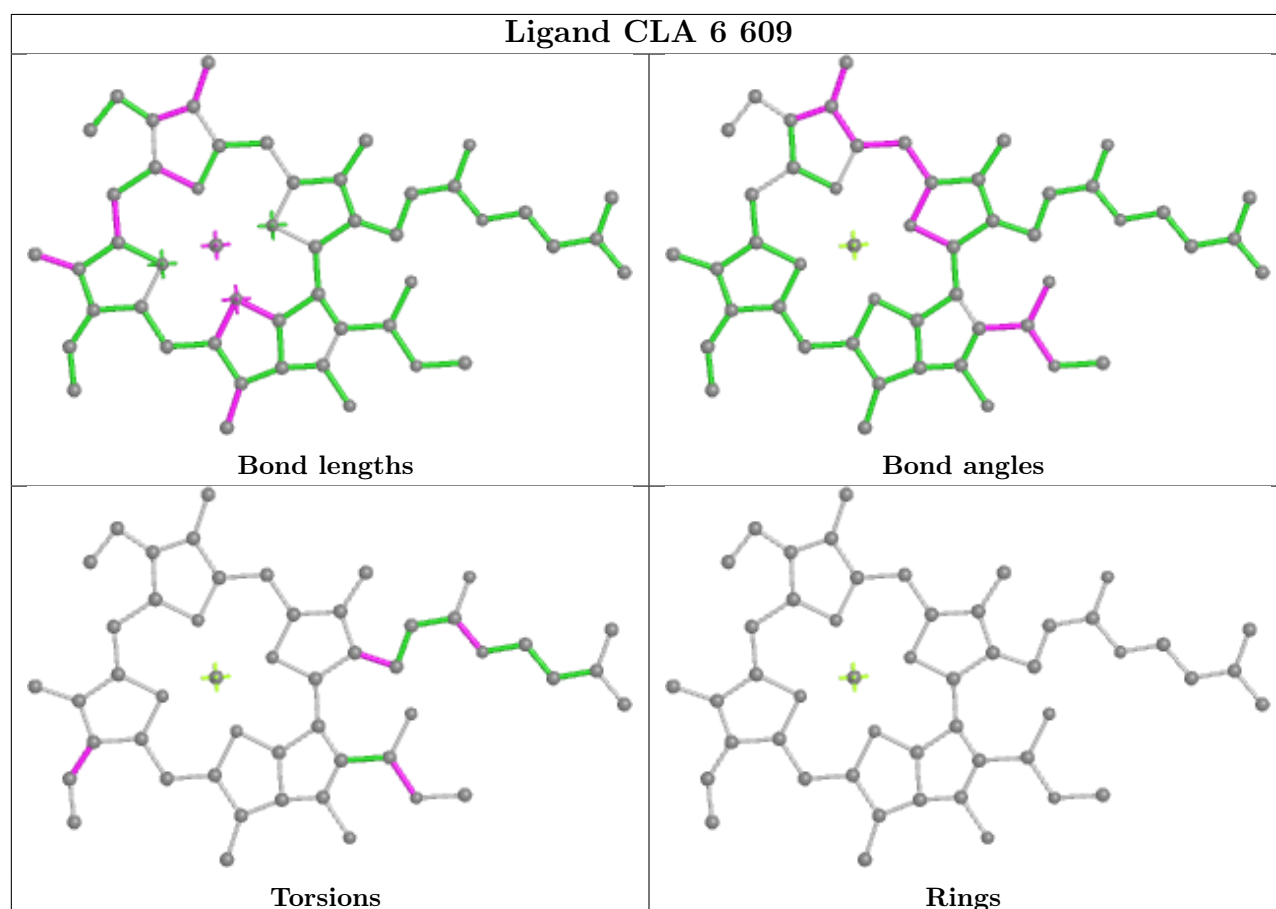
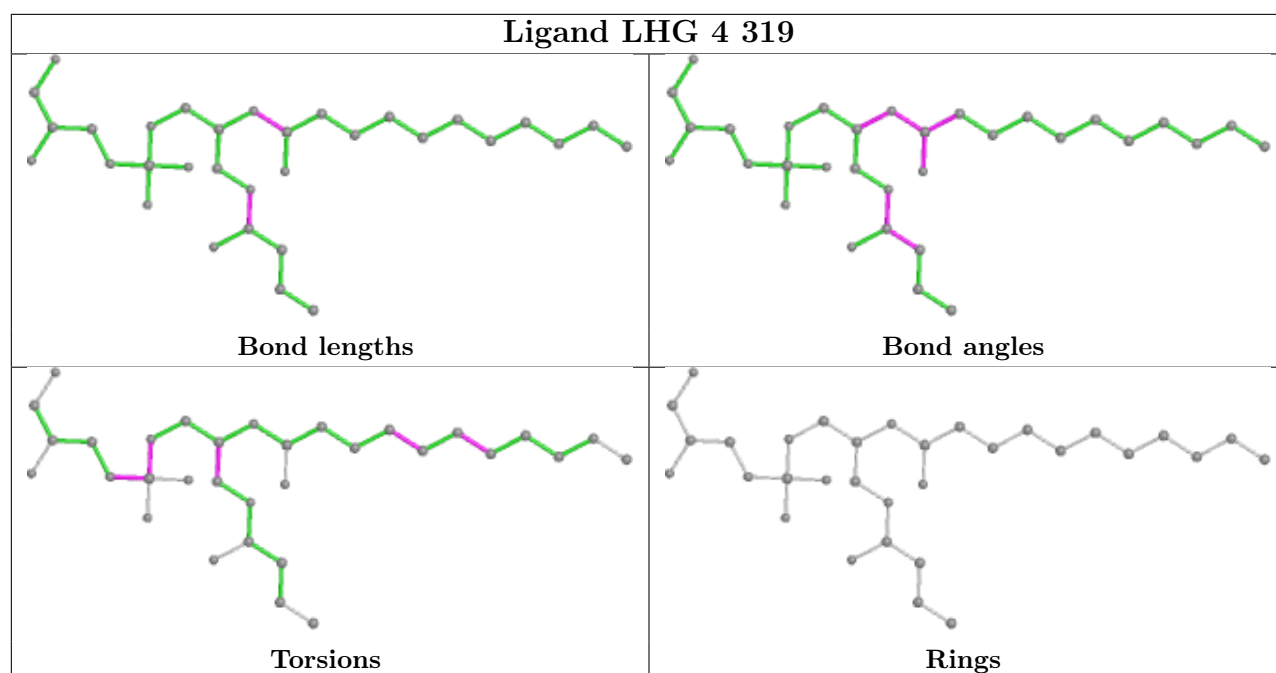




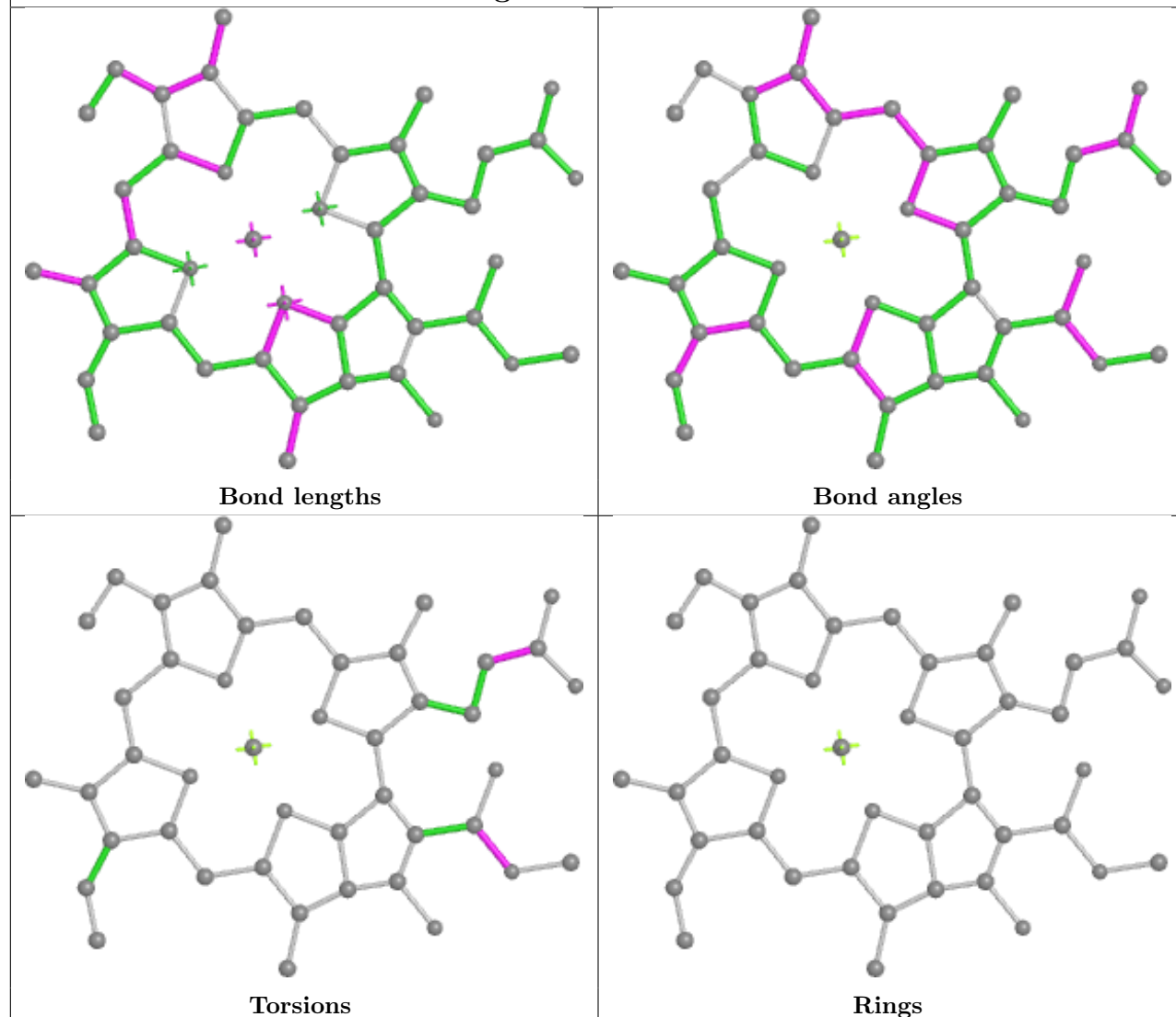




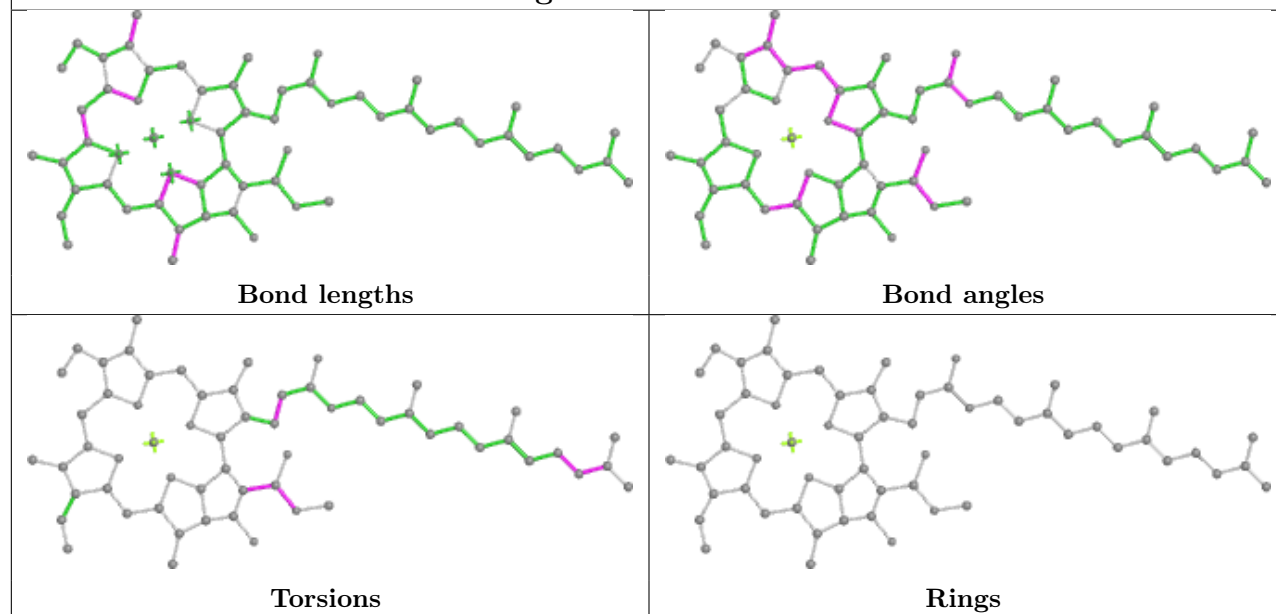


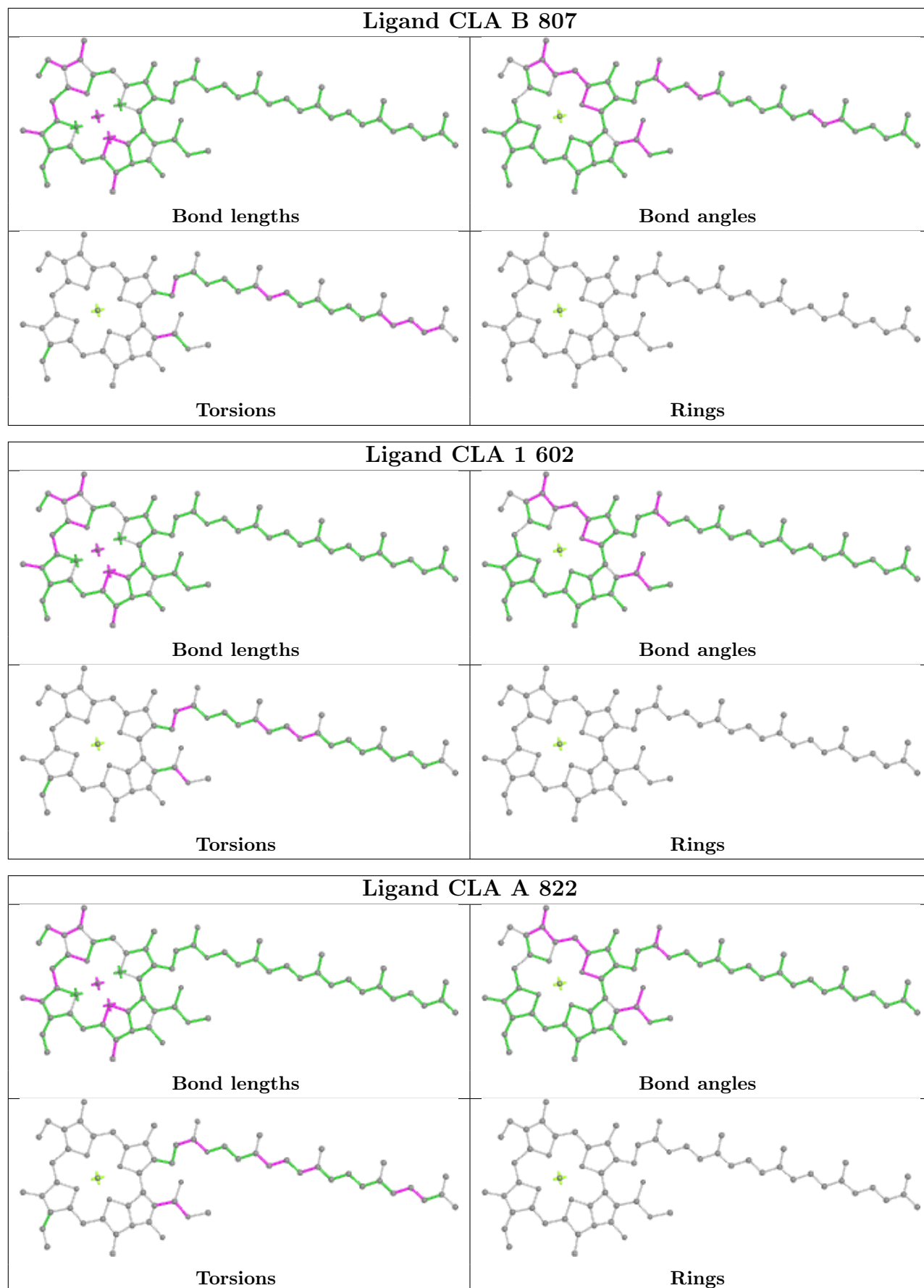


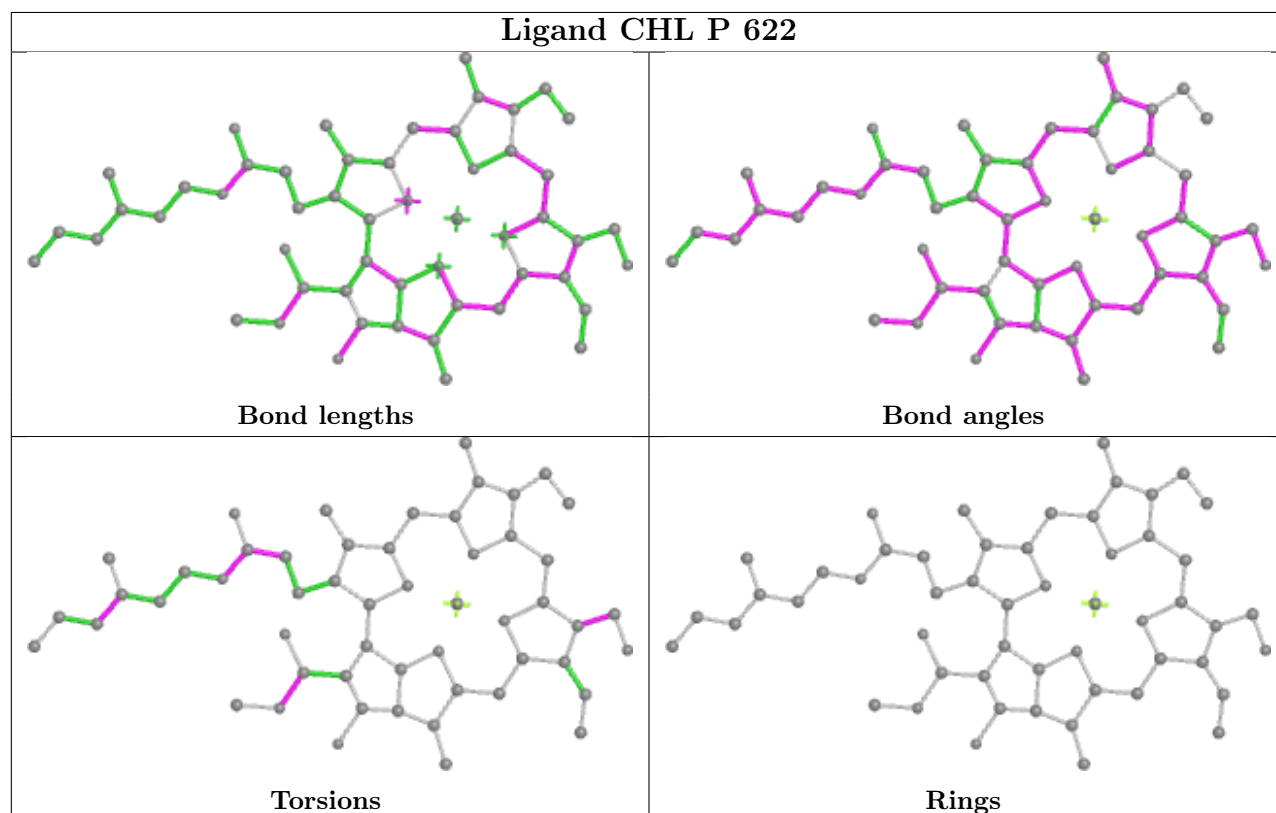
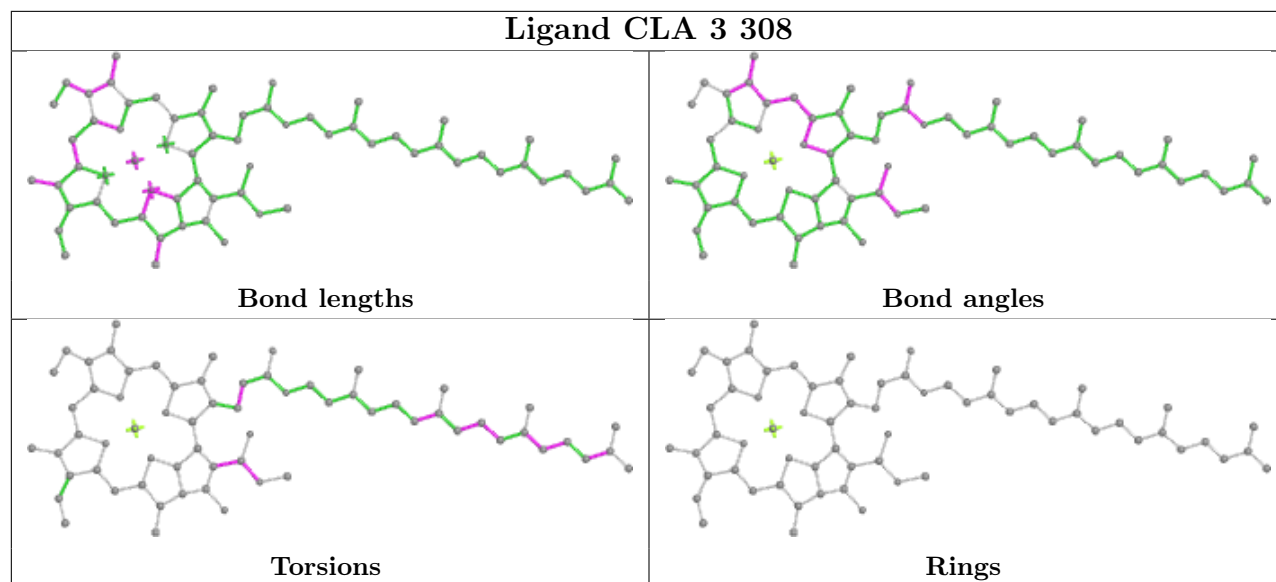
Ligand CLA 6 614

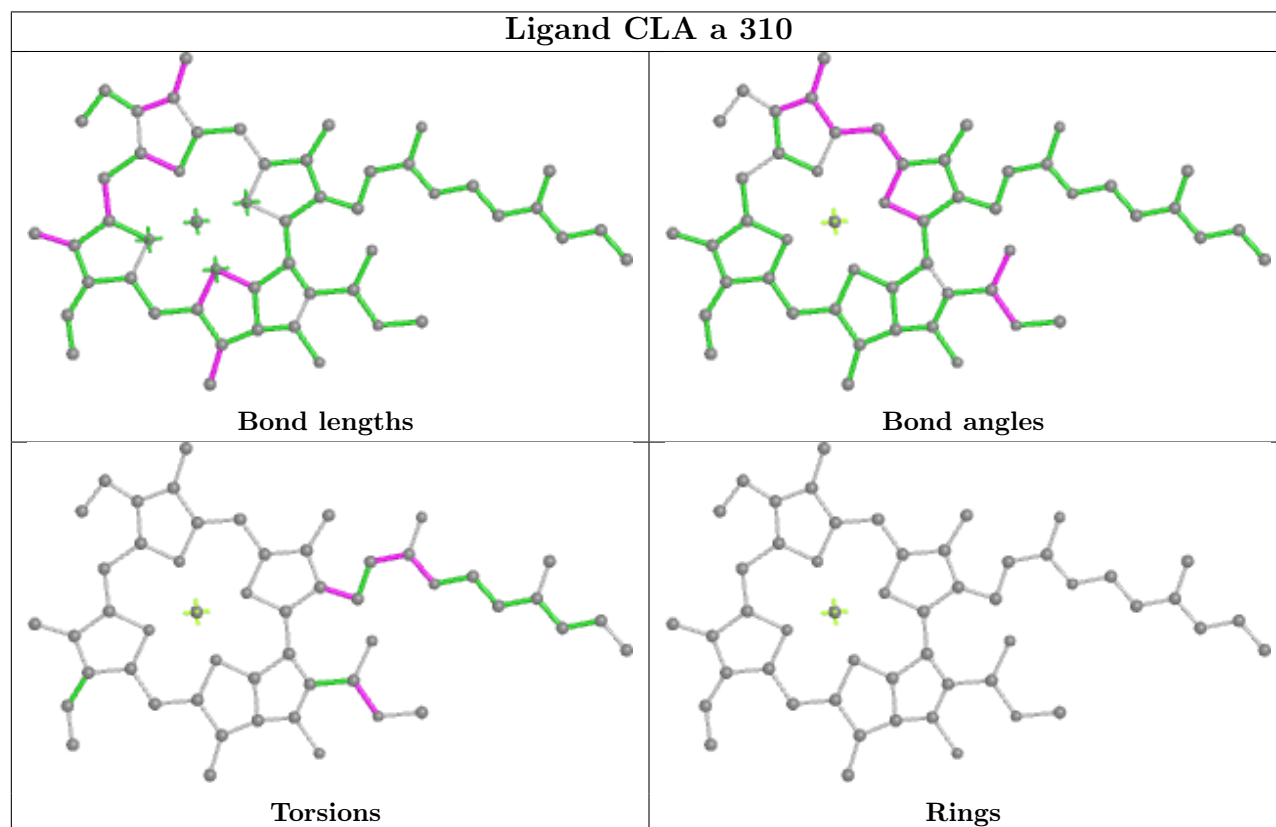
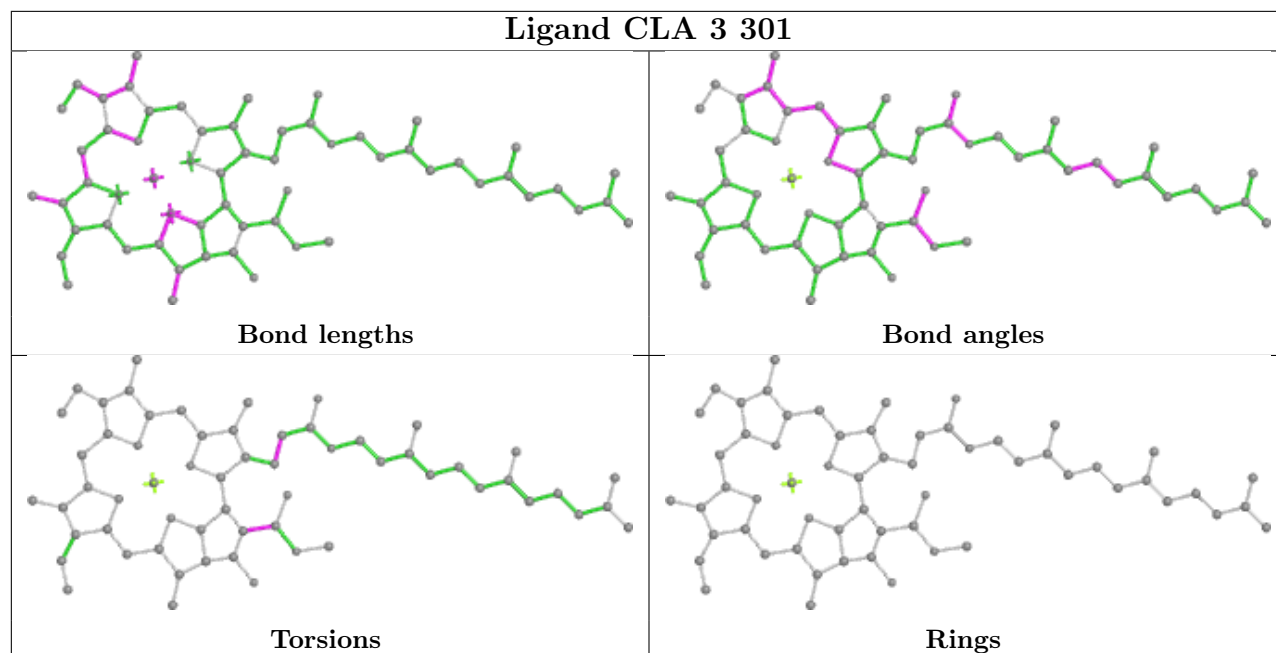


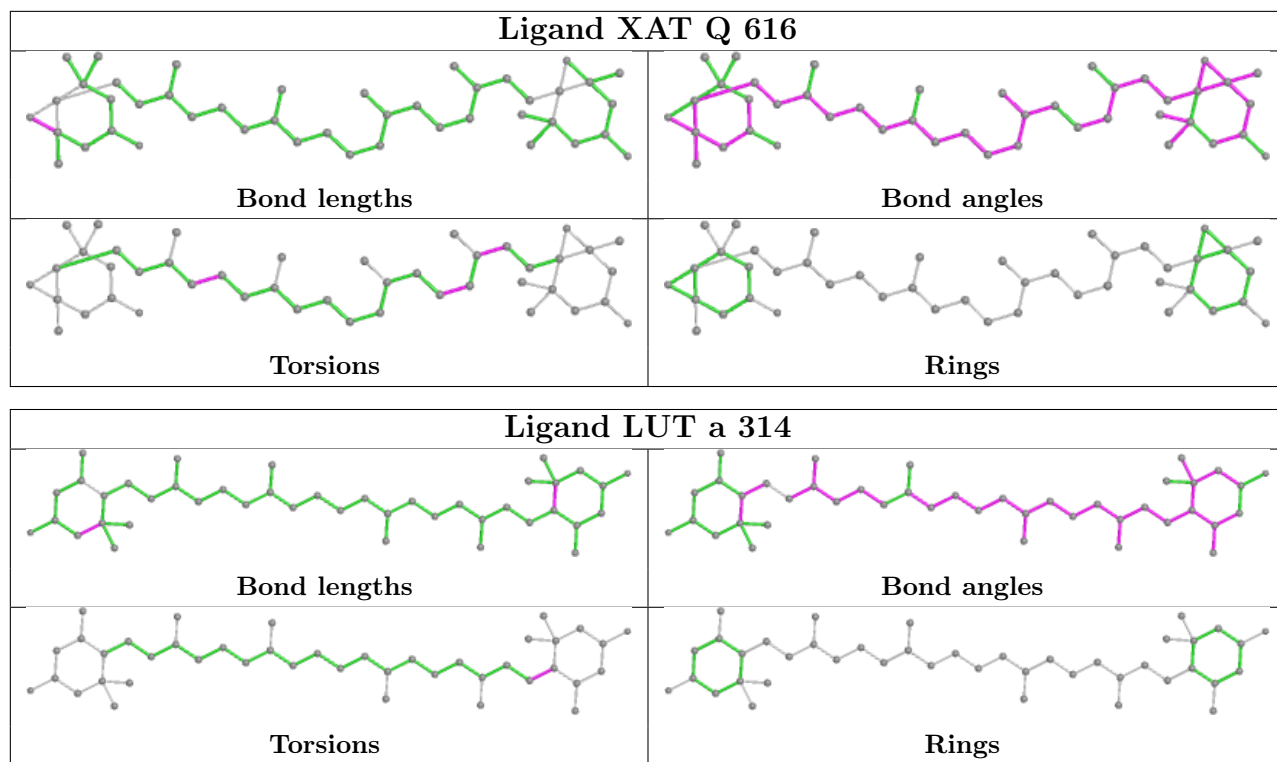
Ligand CLA S 311

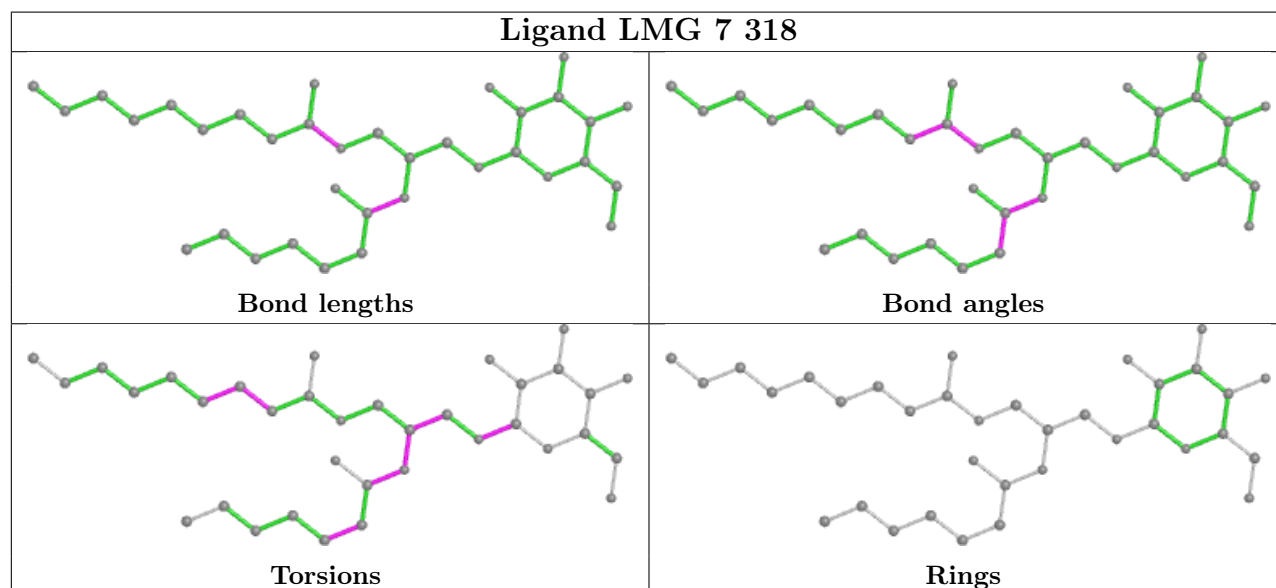
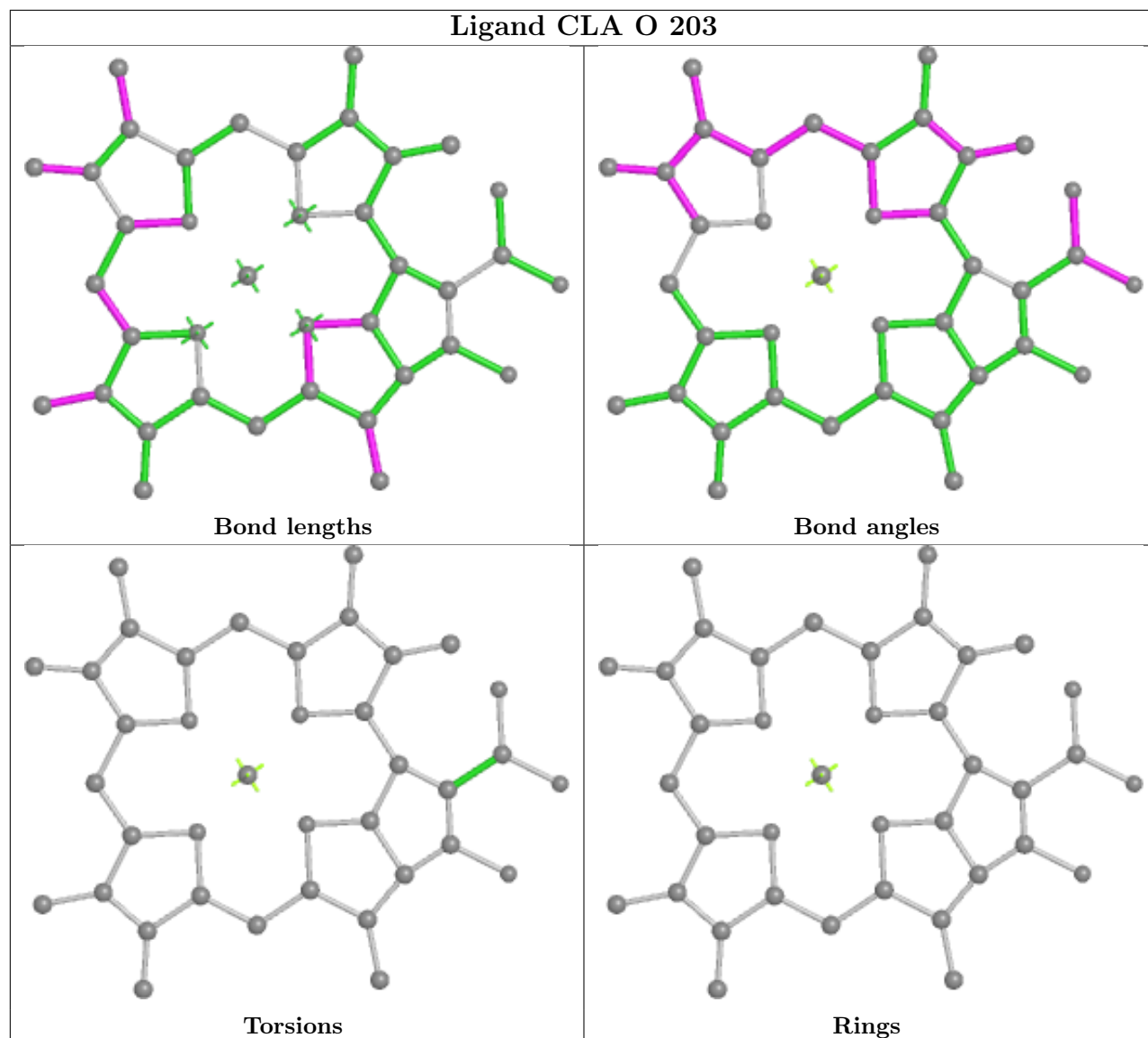


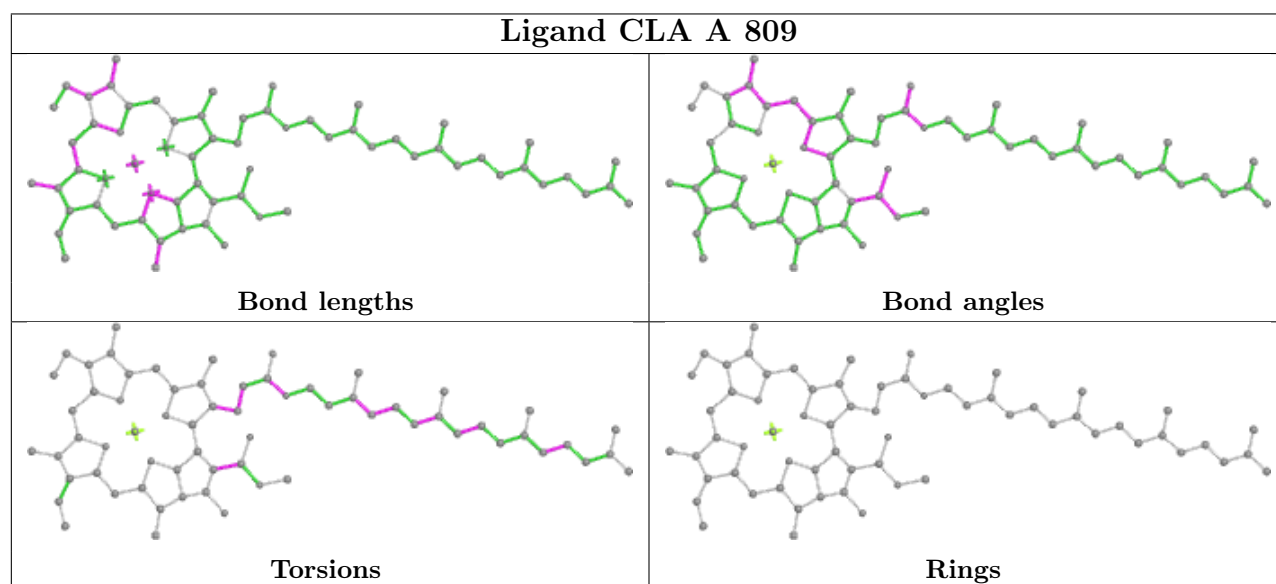
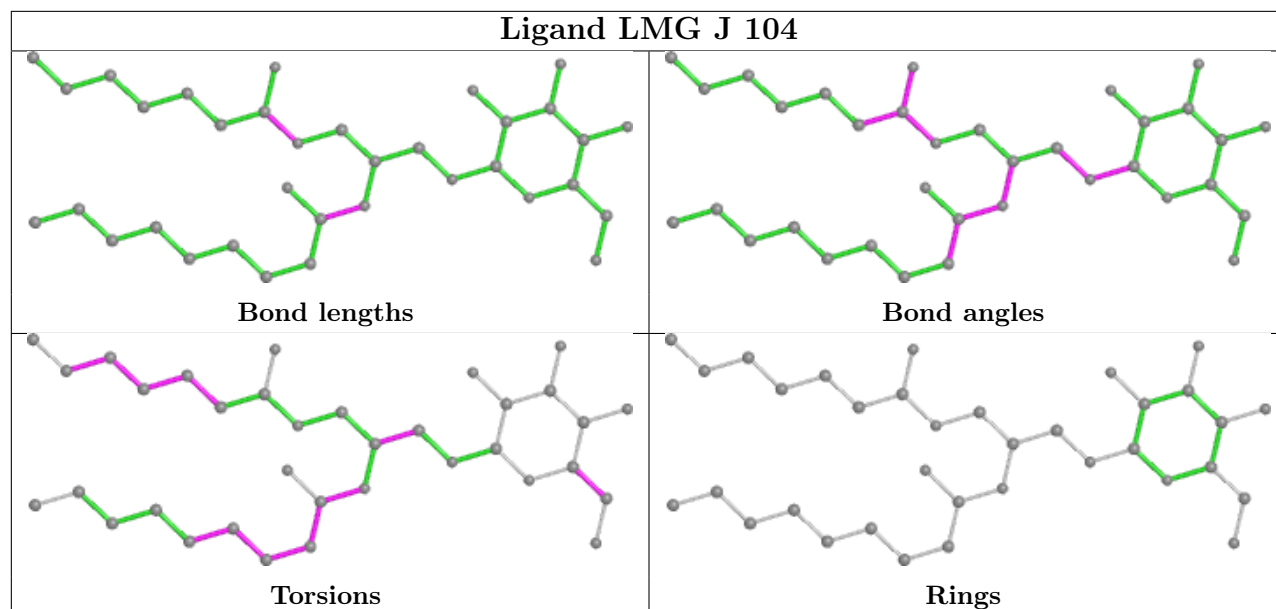


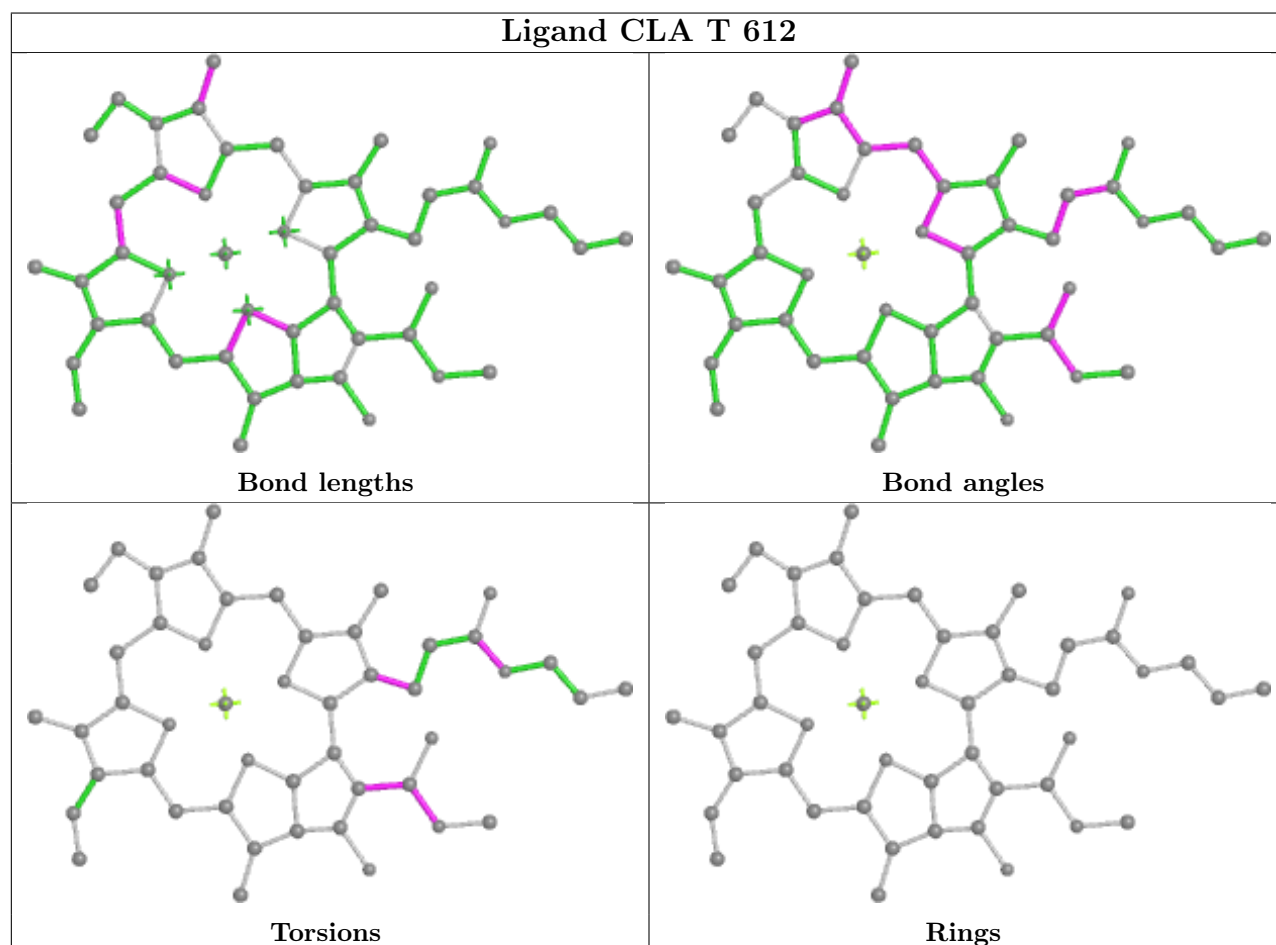
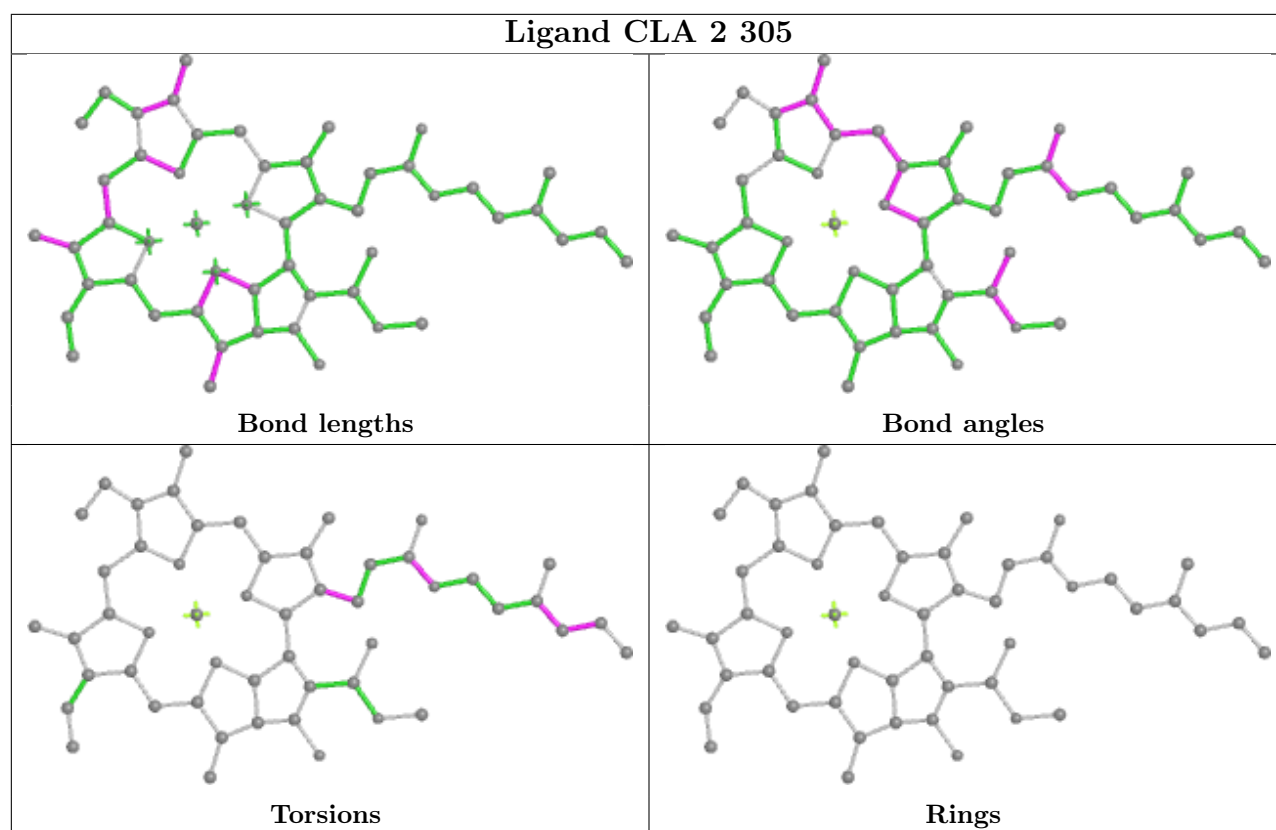


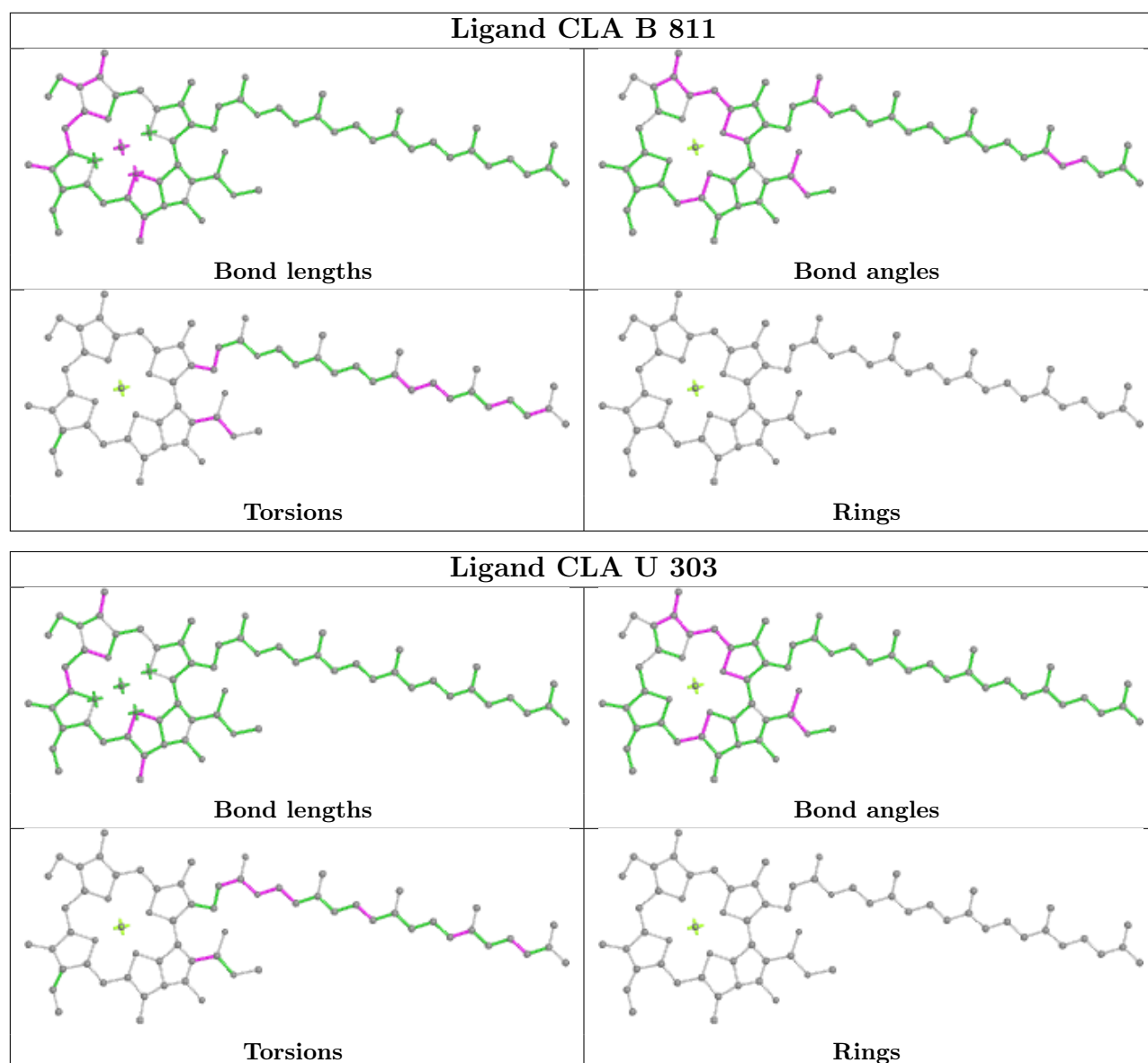


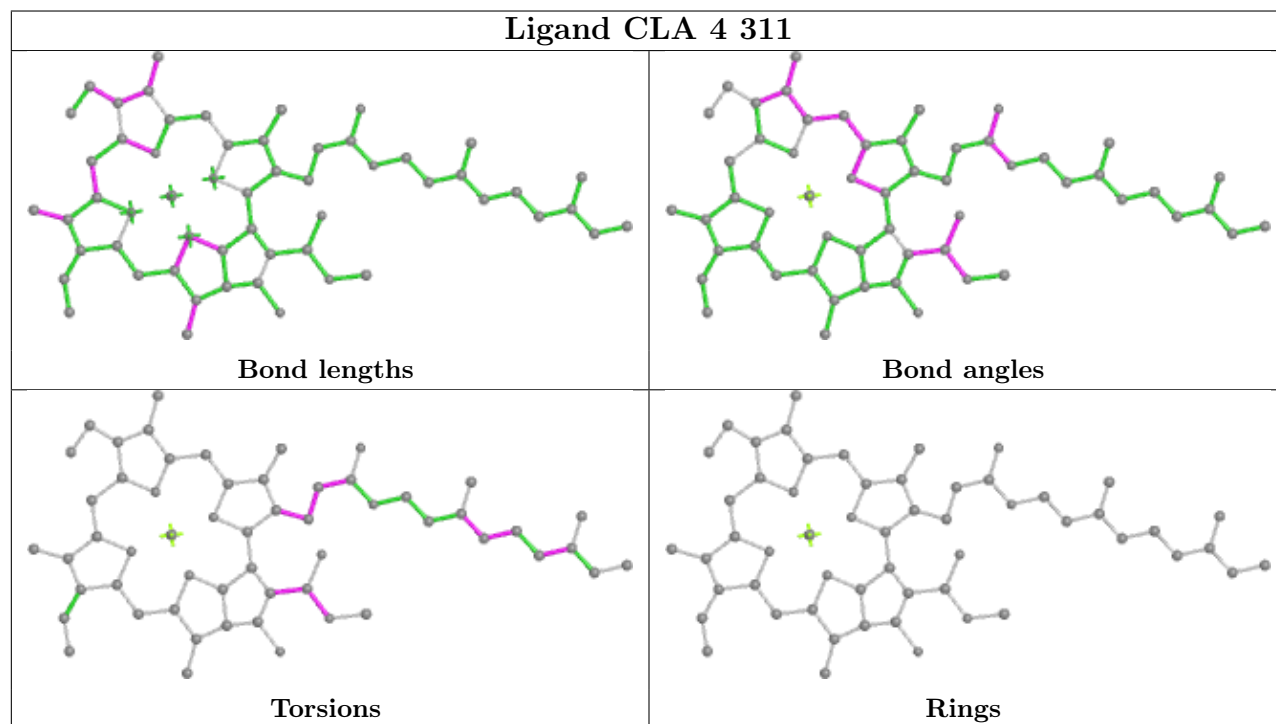
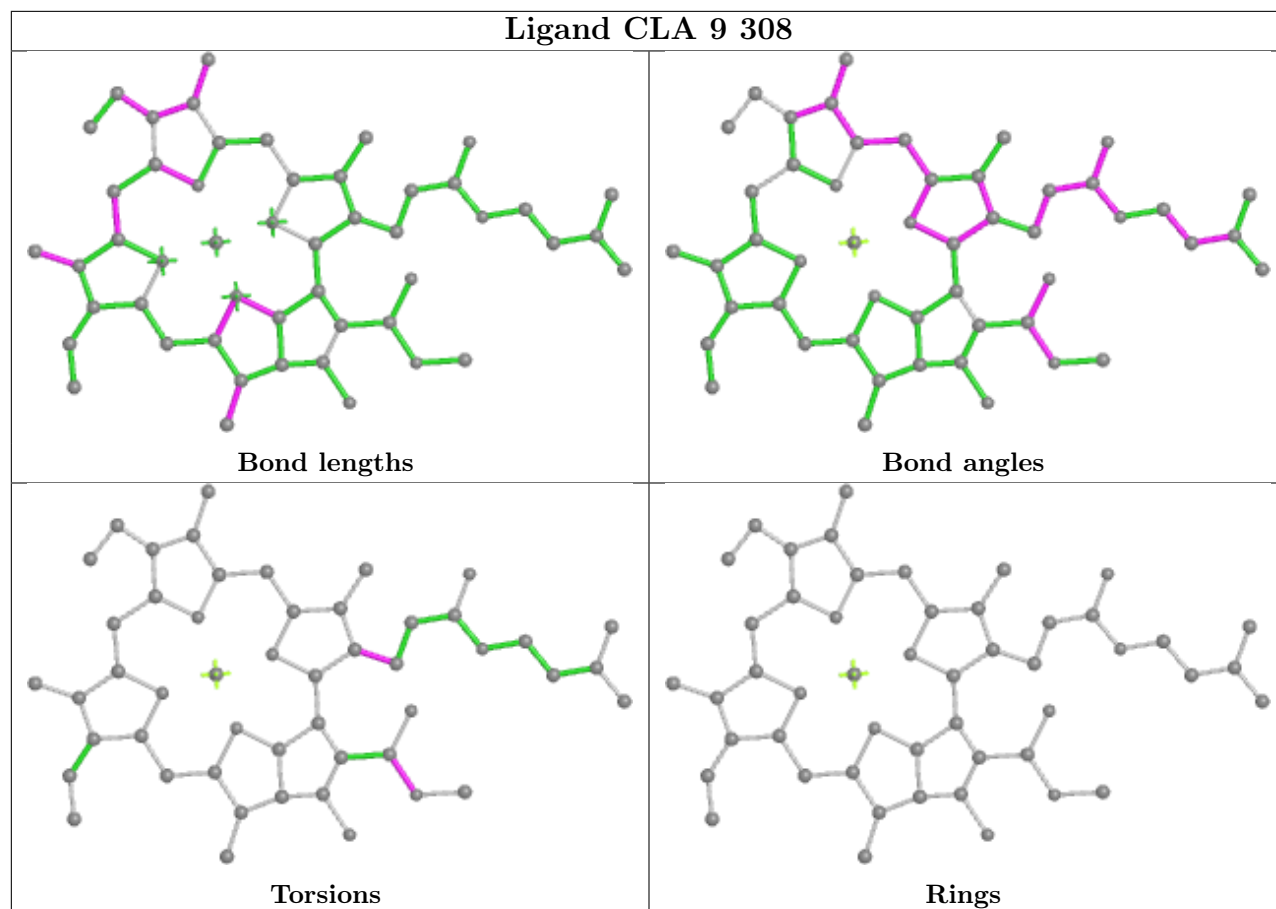


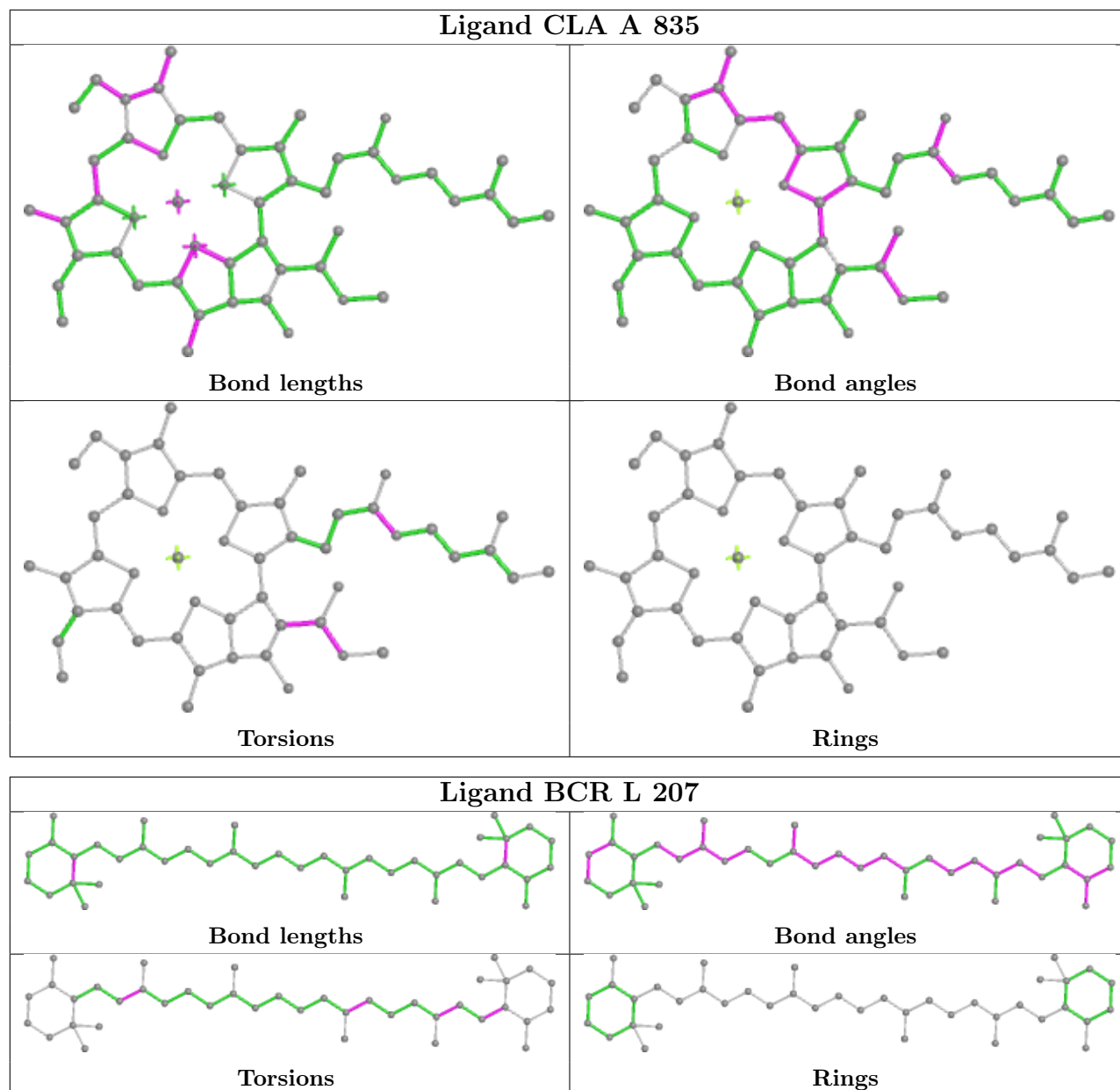


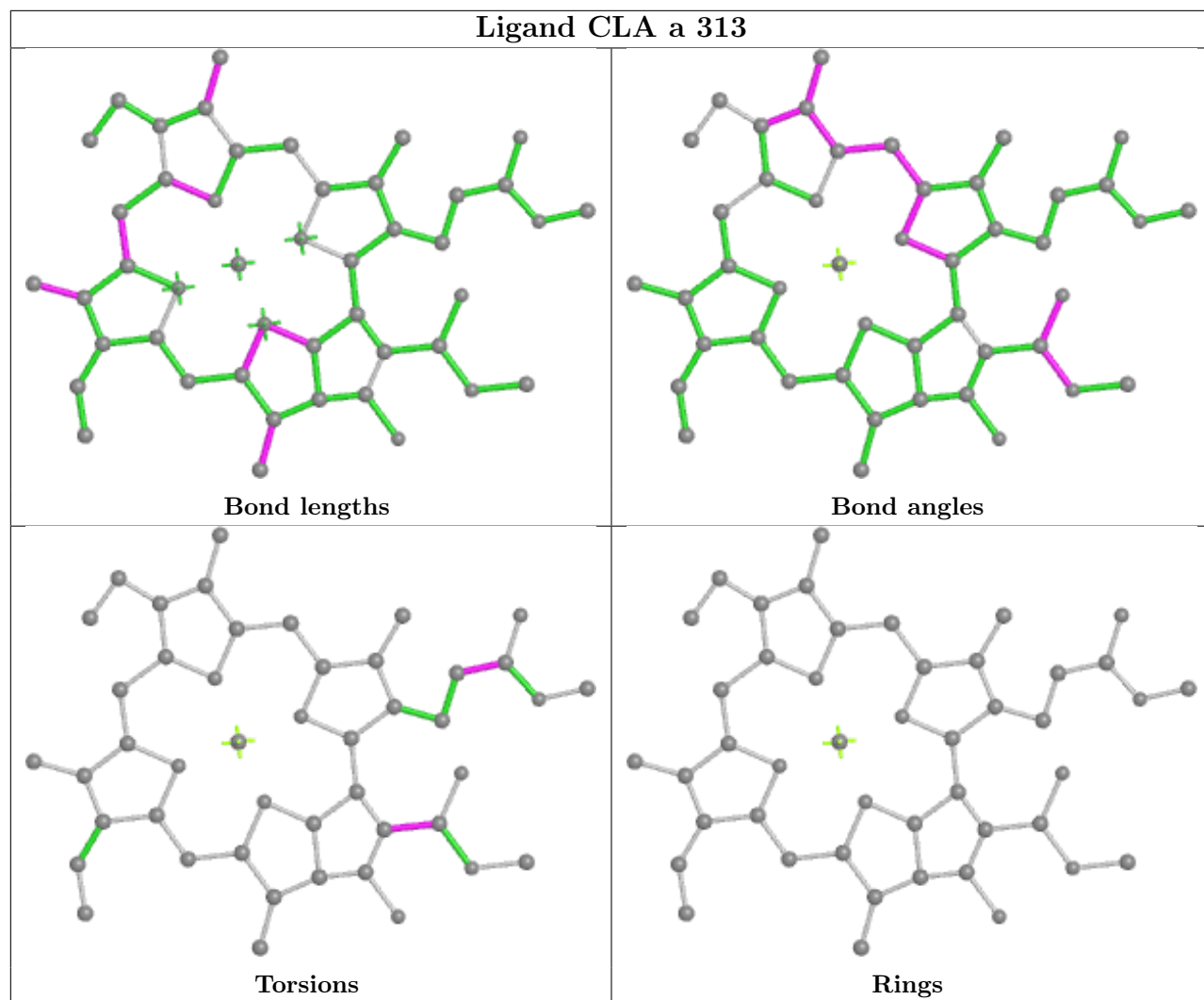


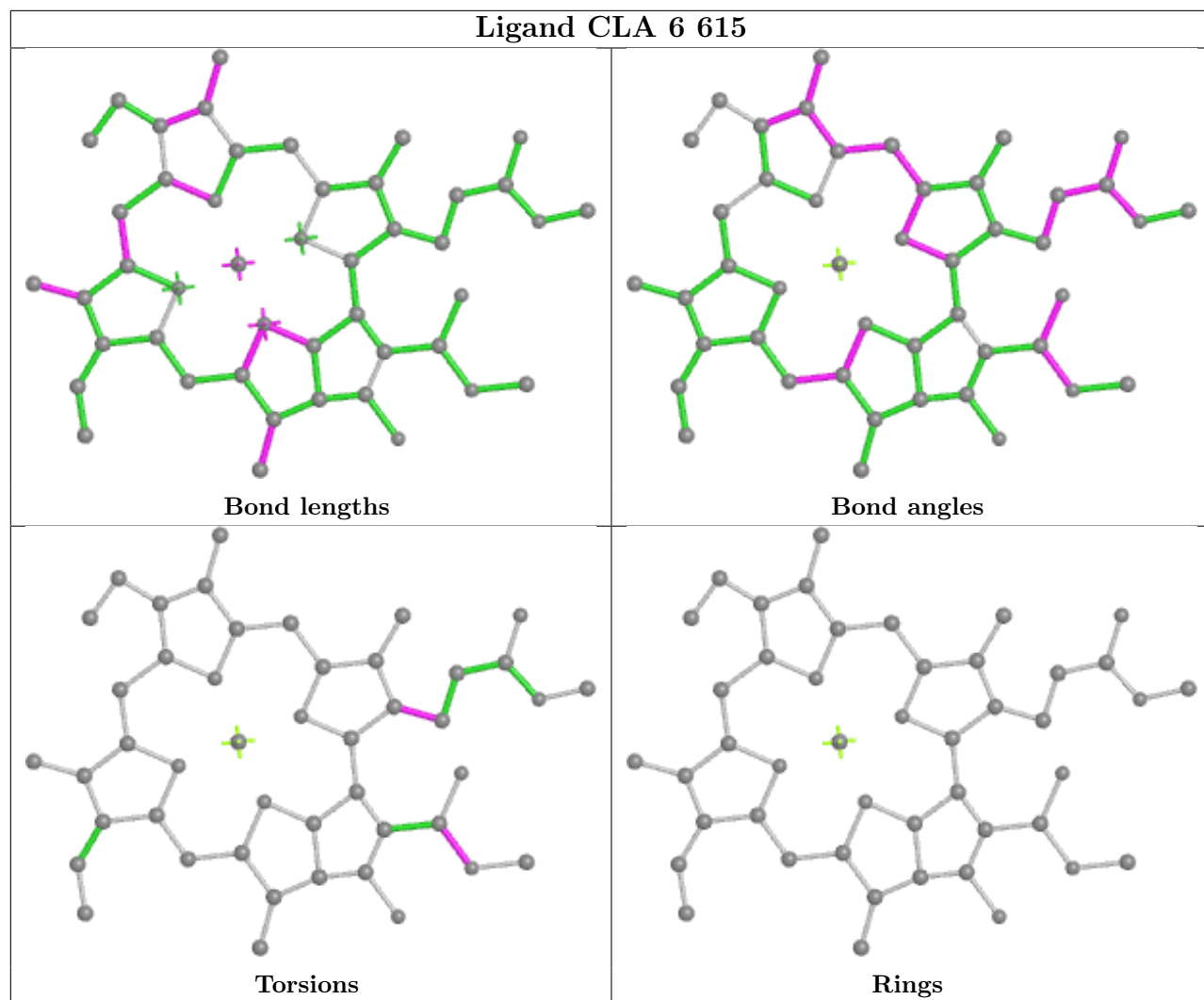


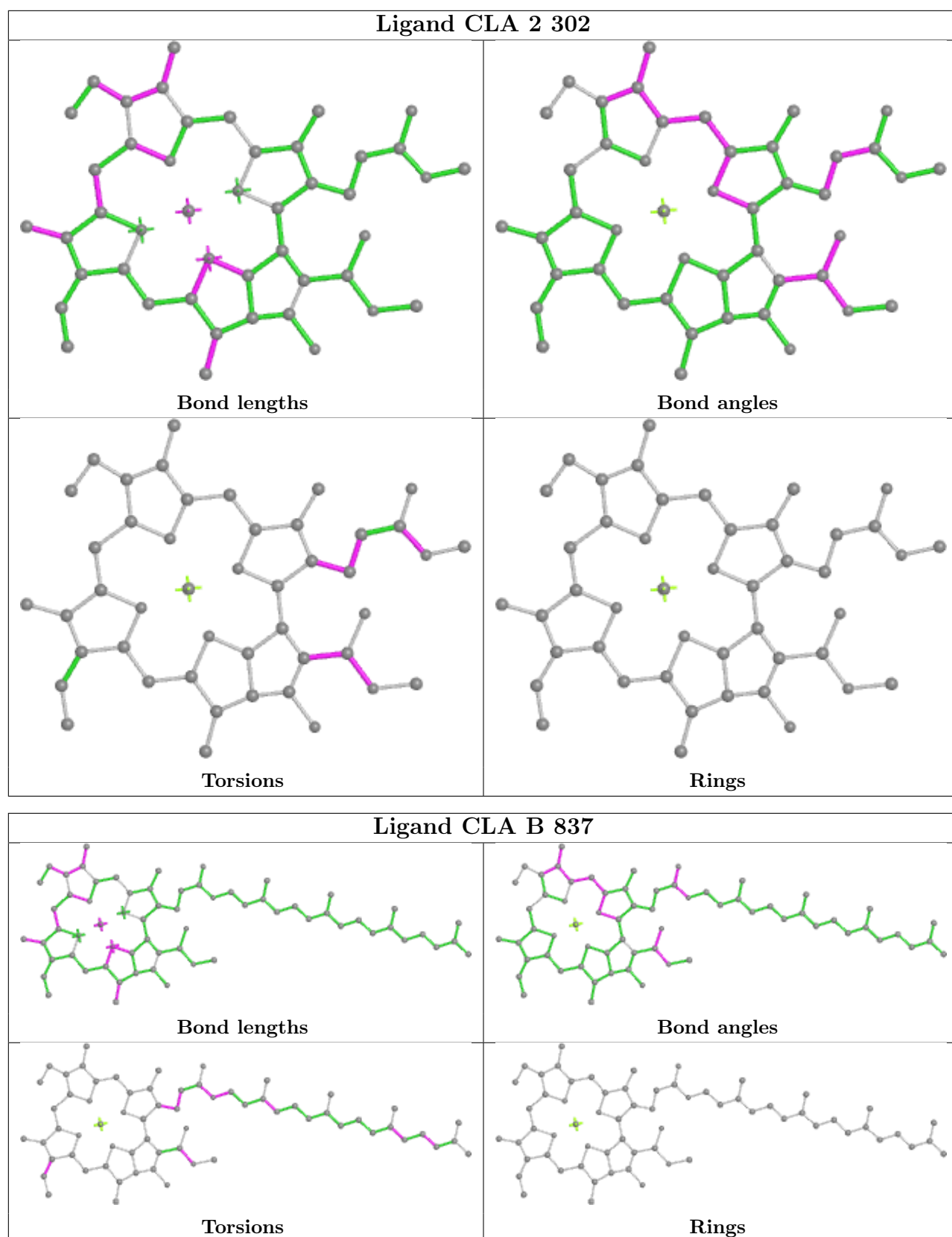


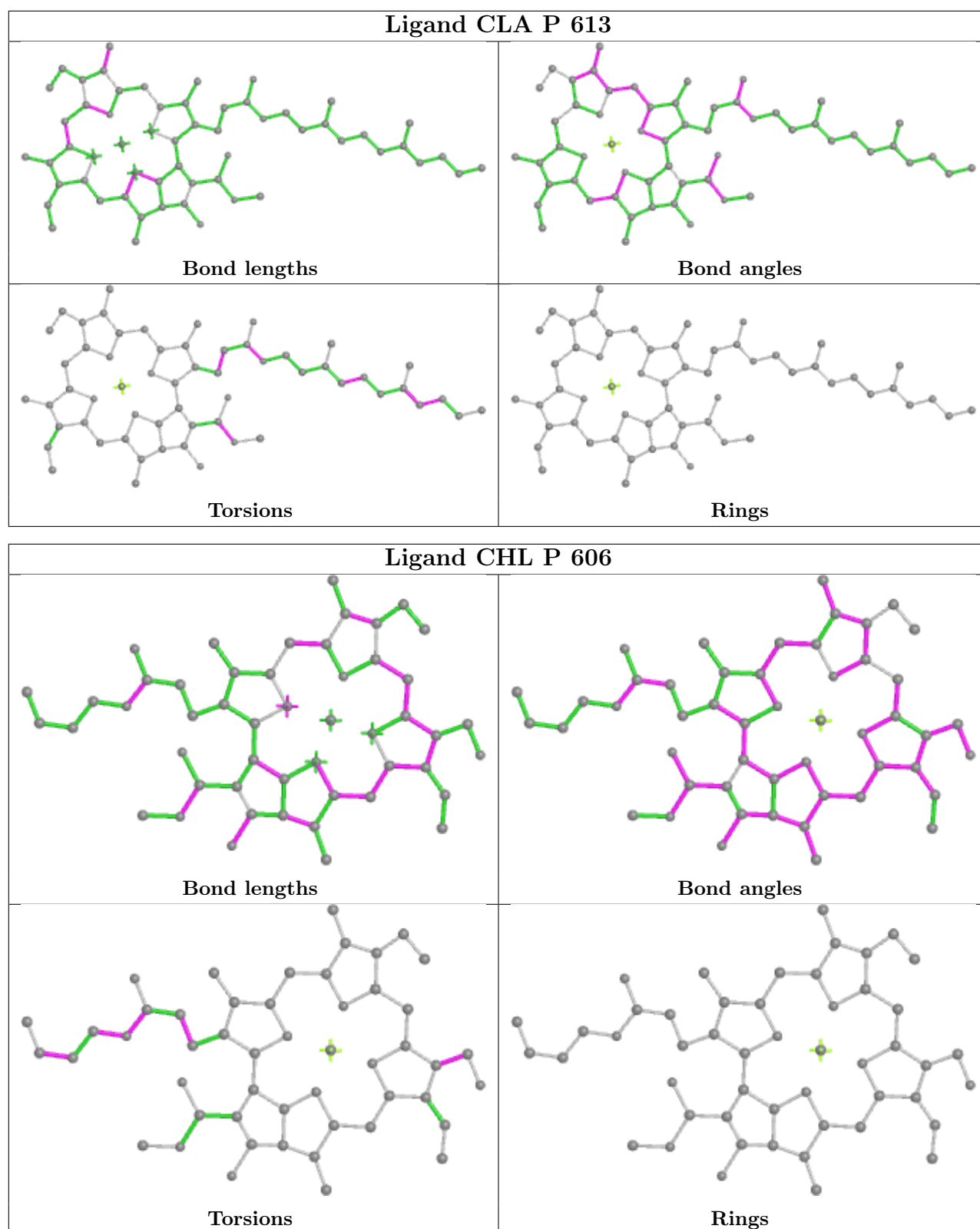


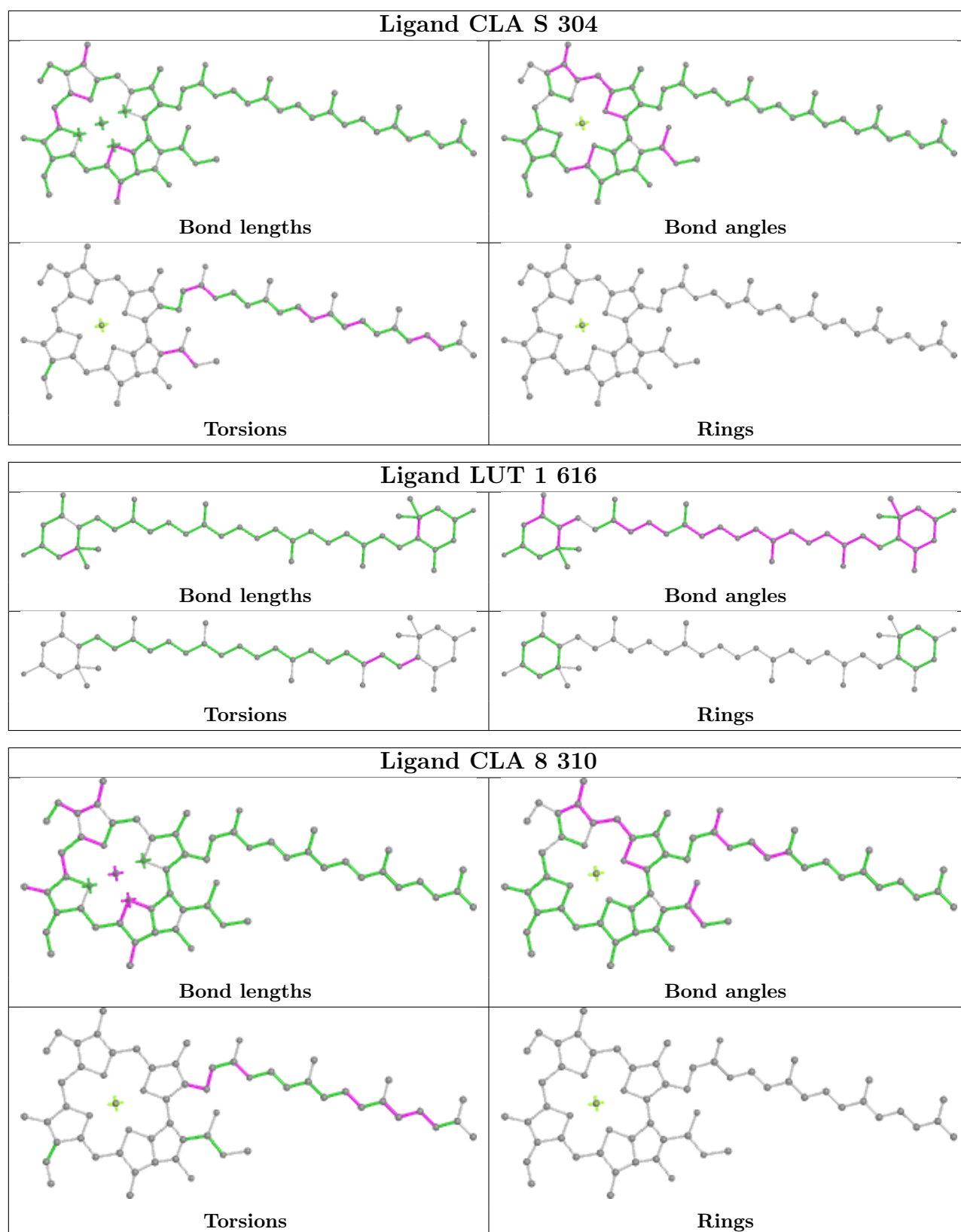


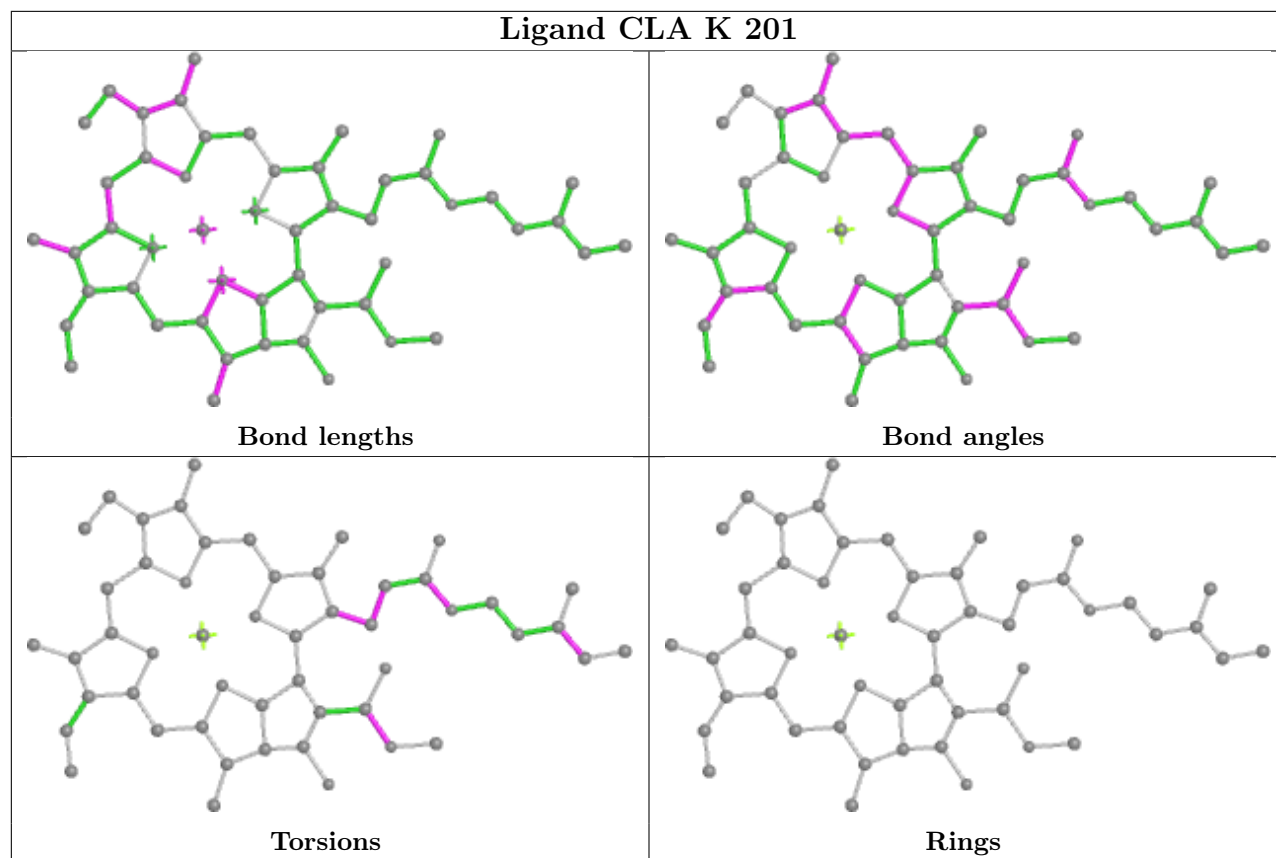


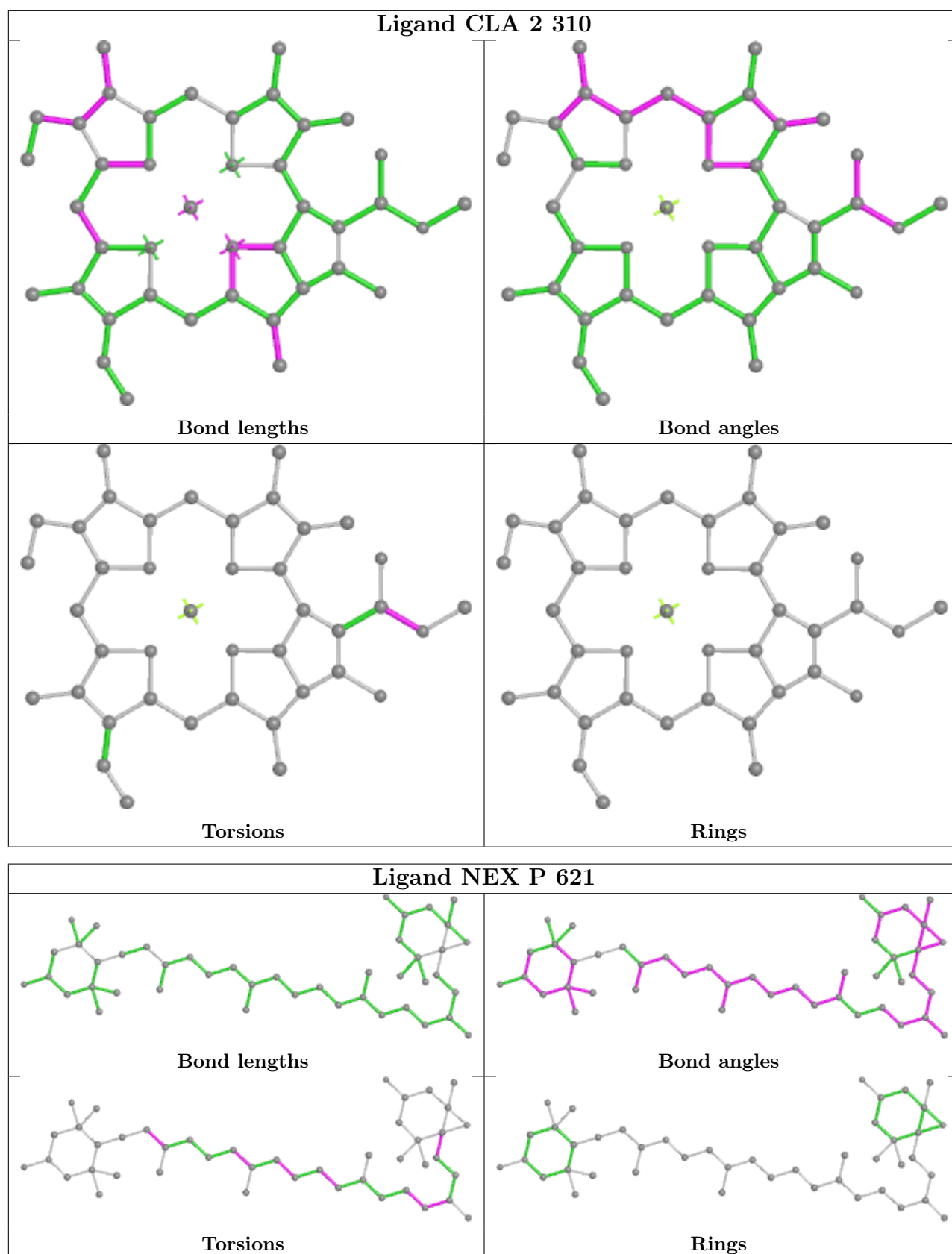


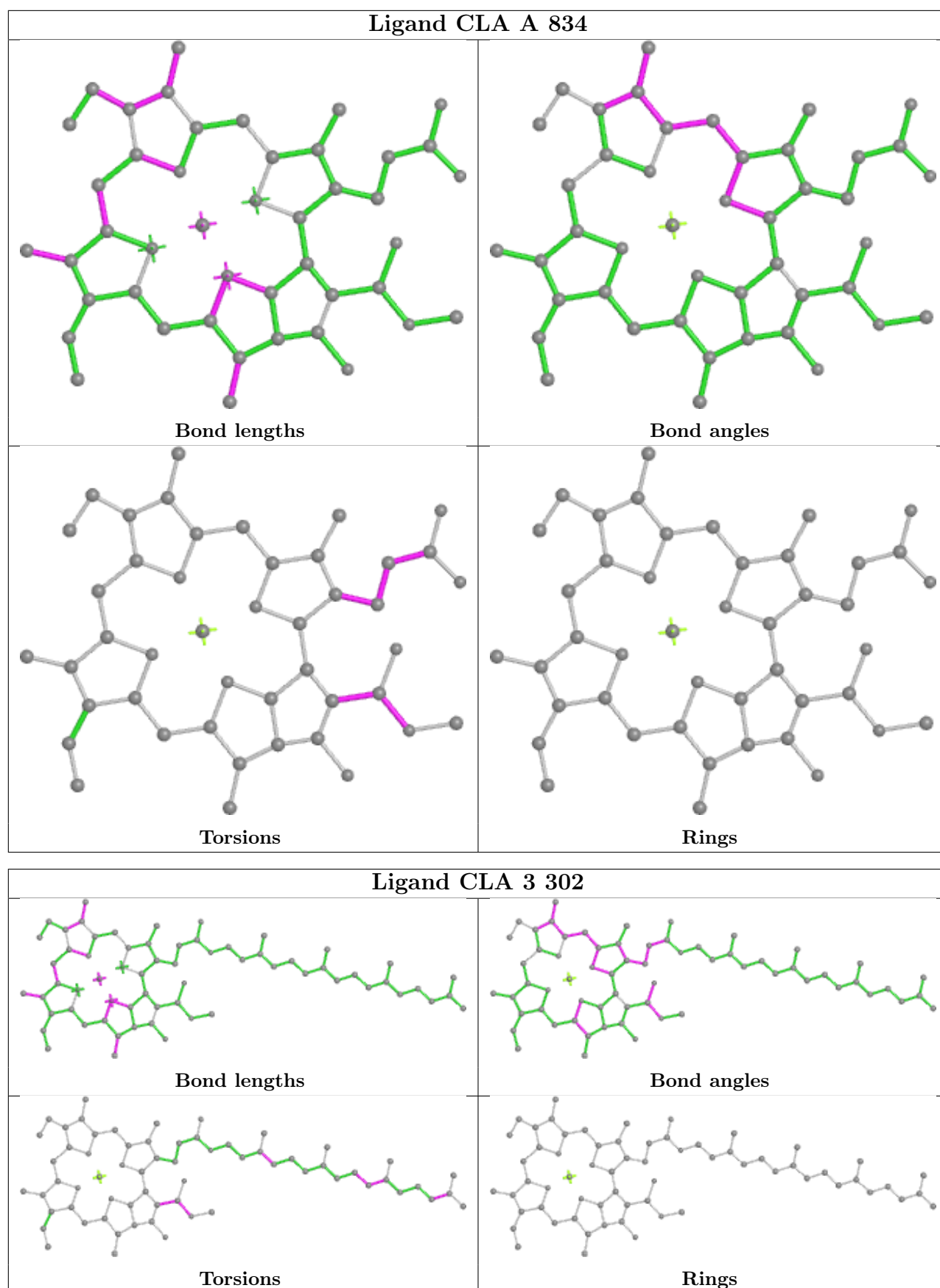


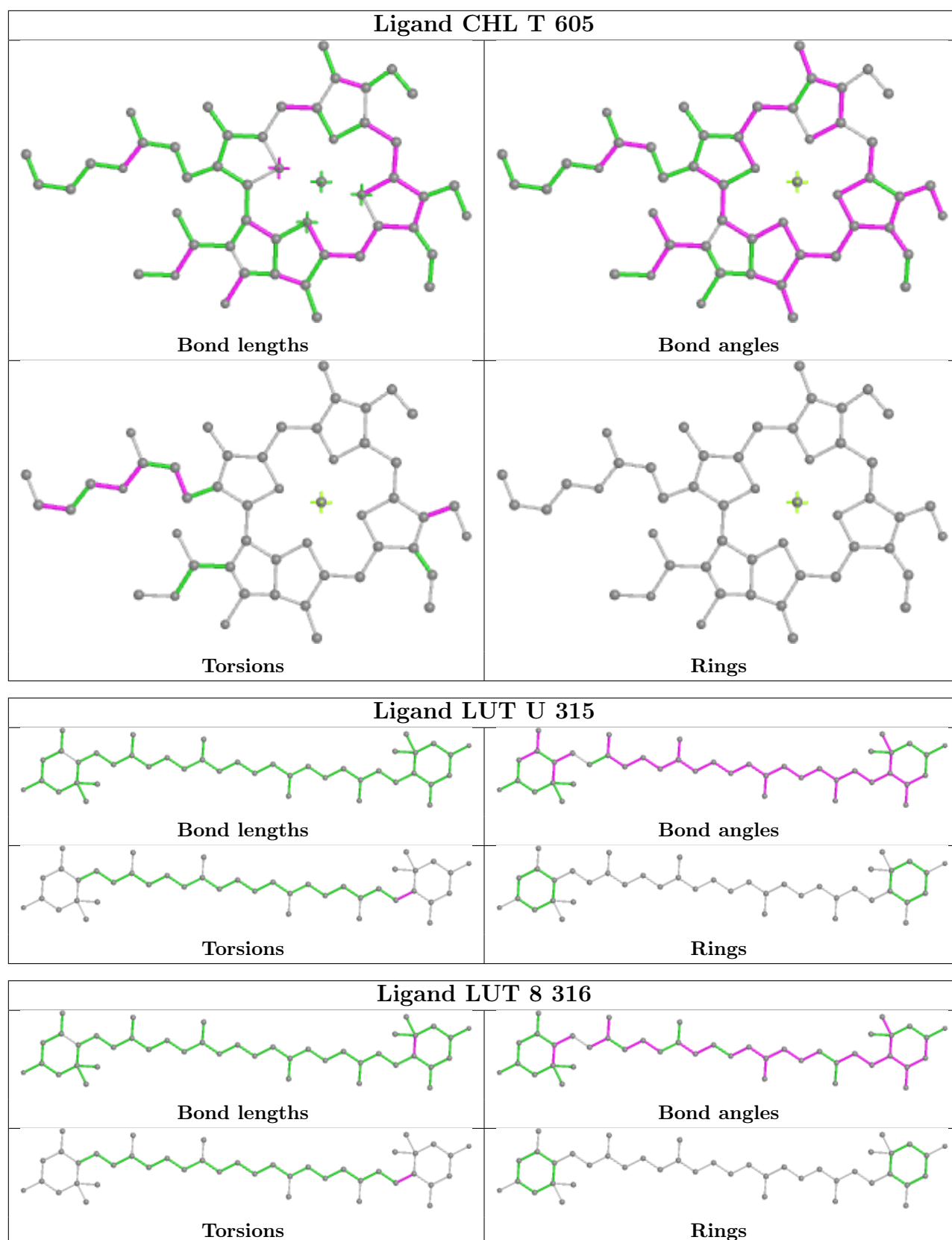


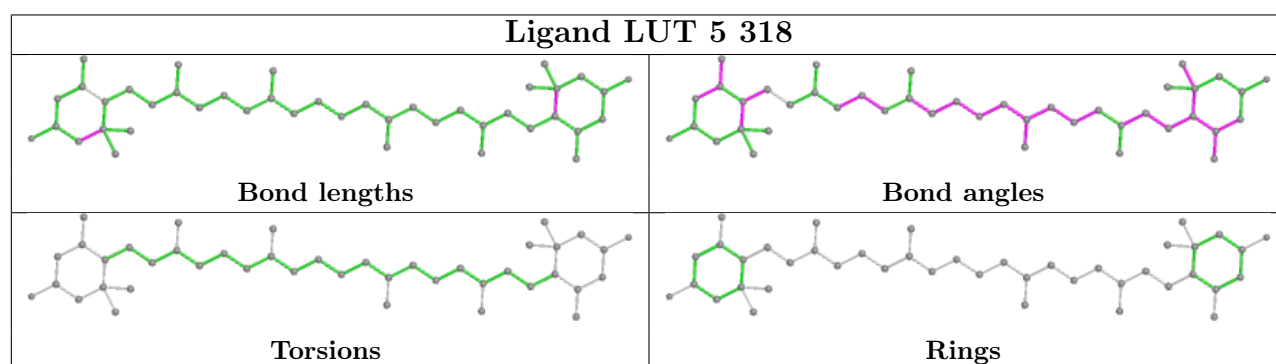
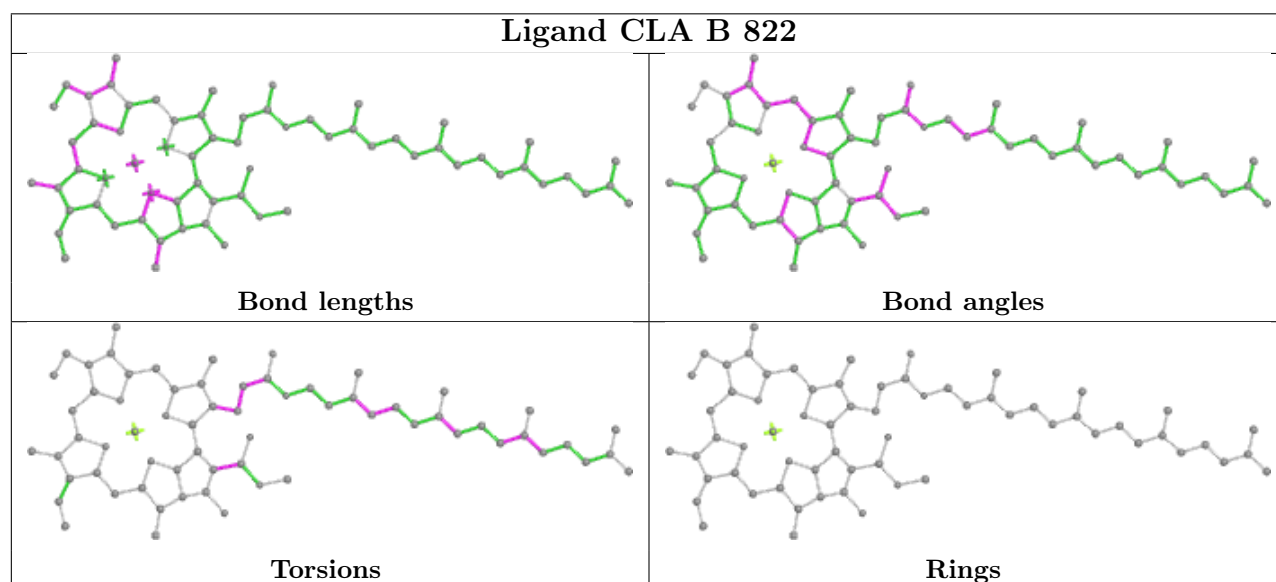
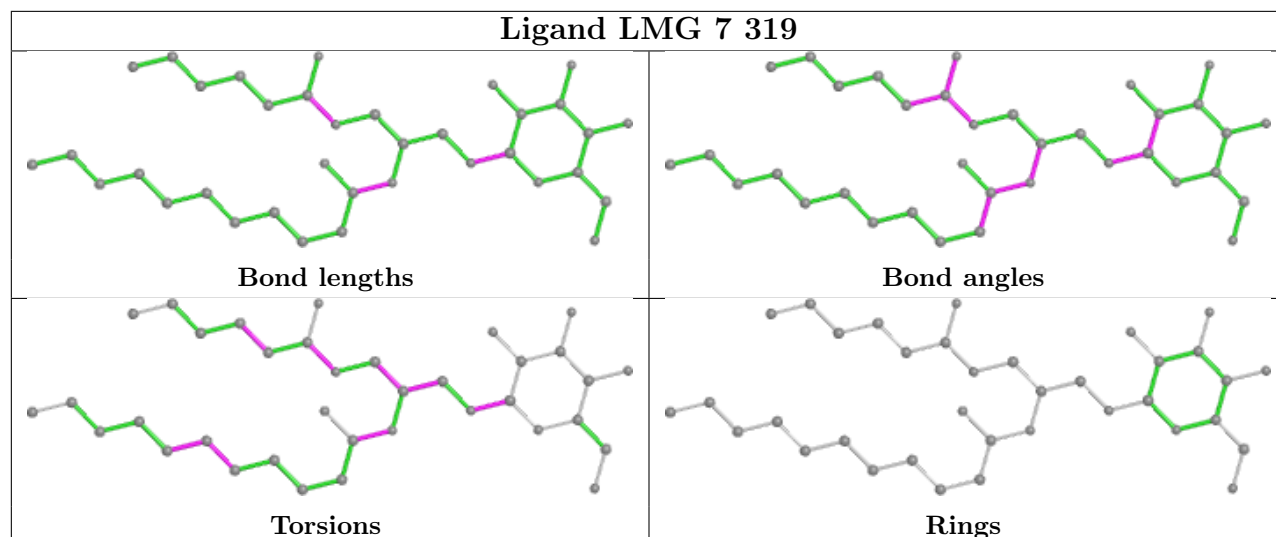


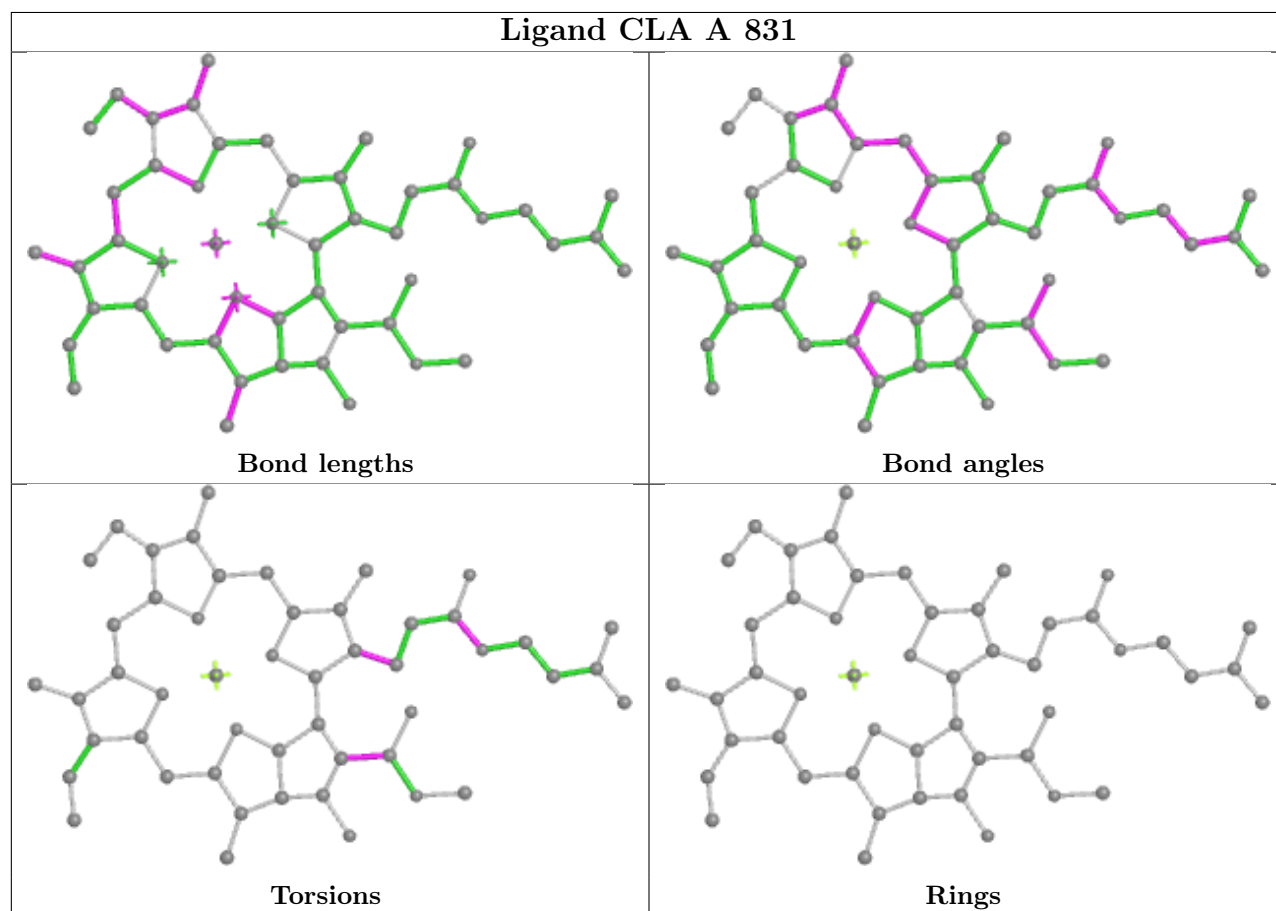
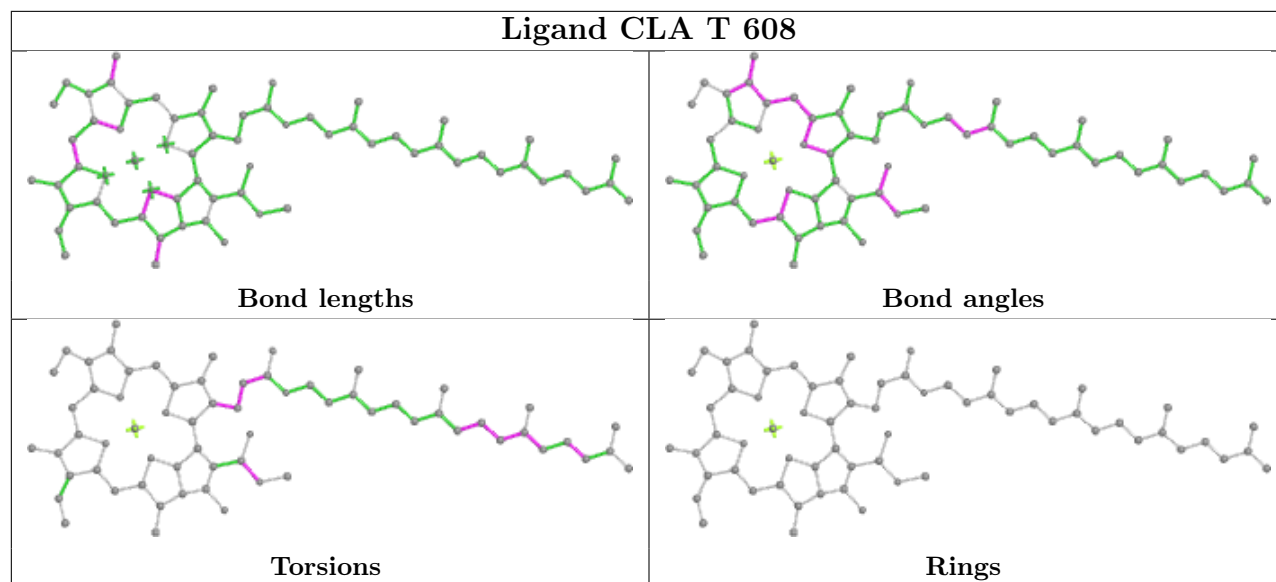


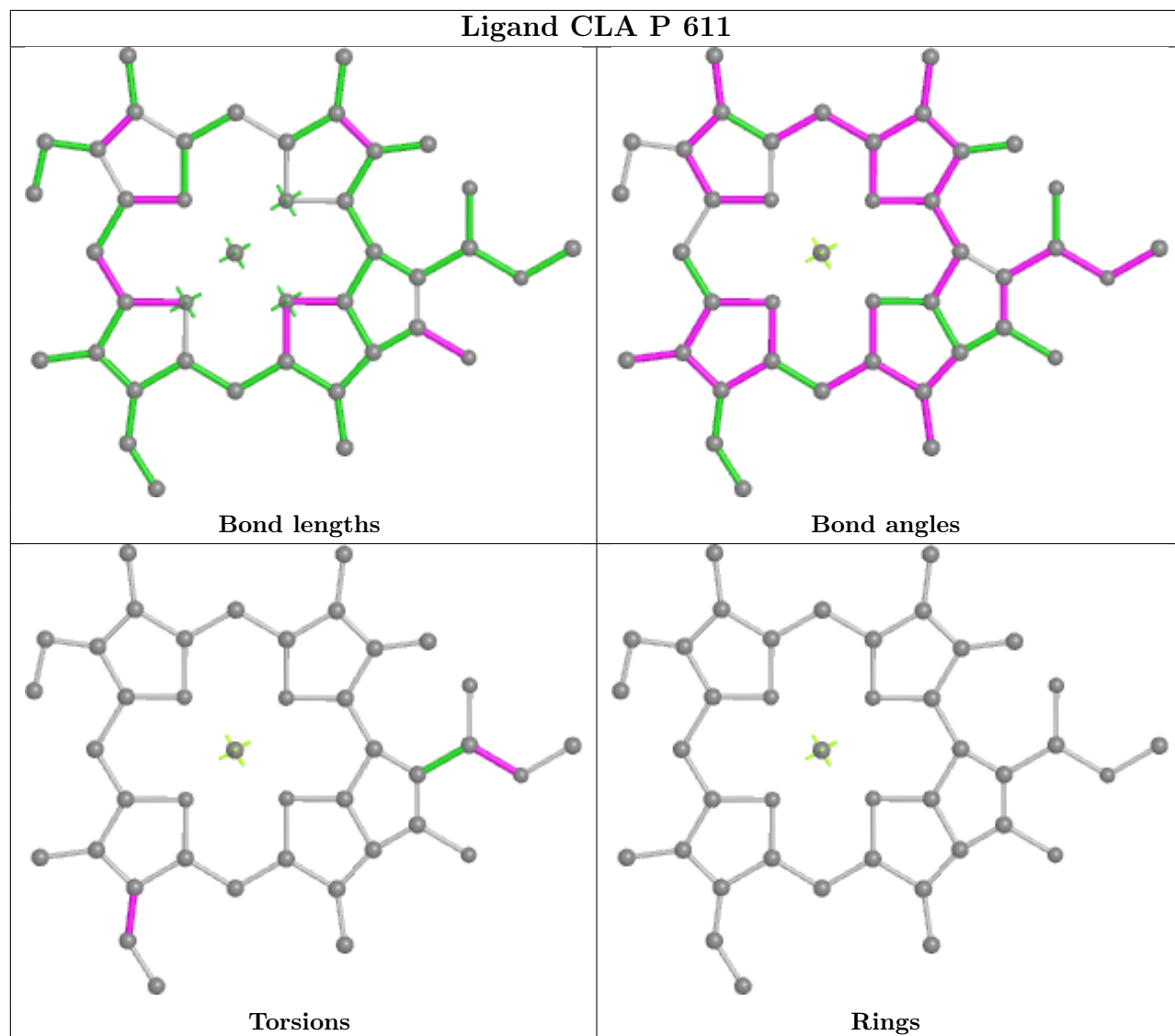


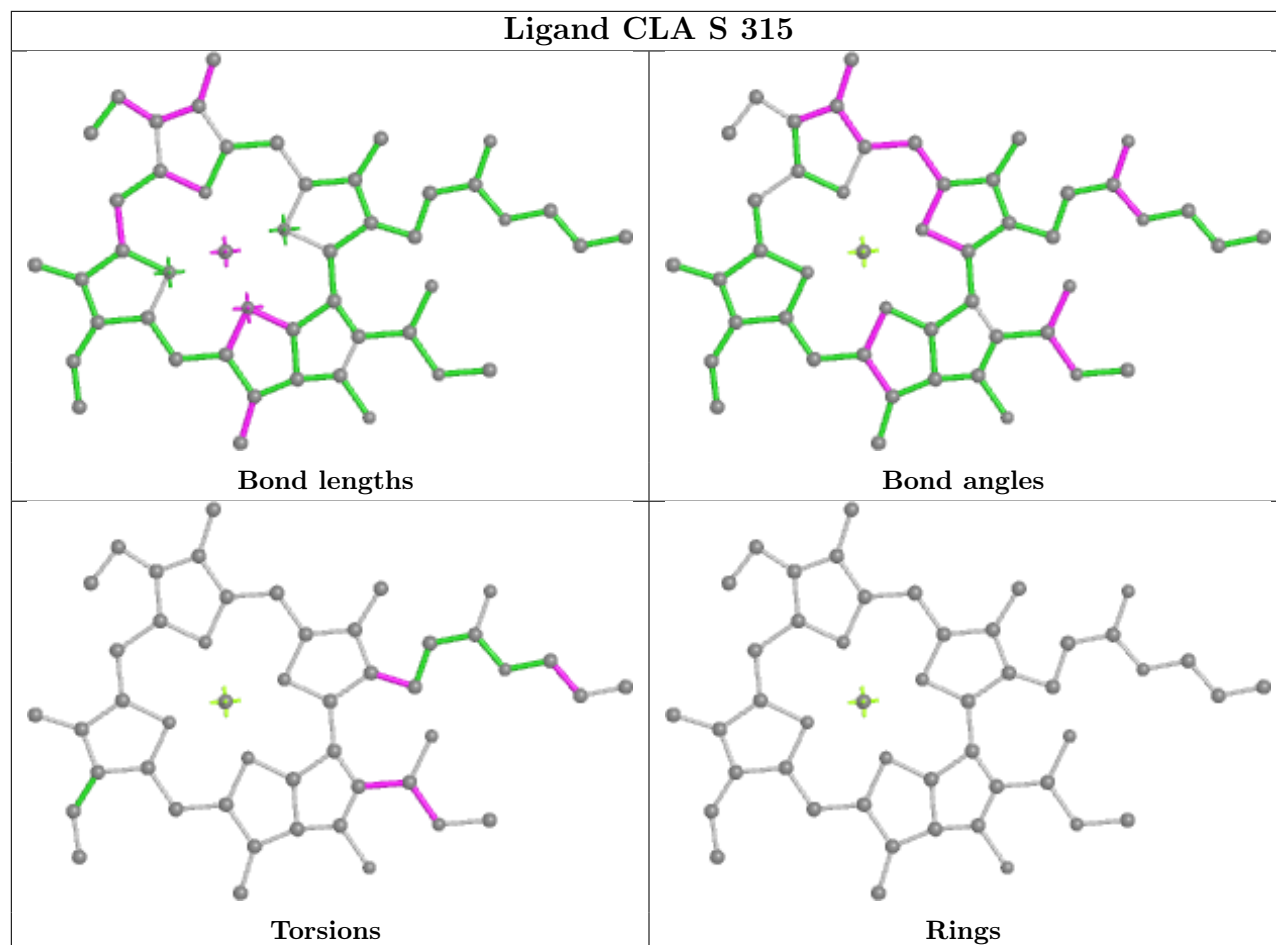


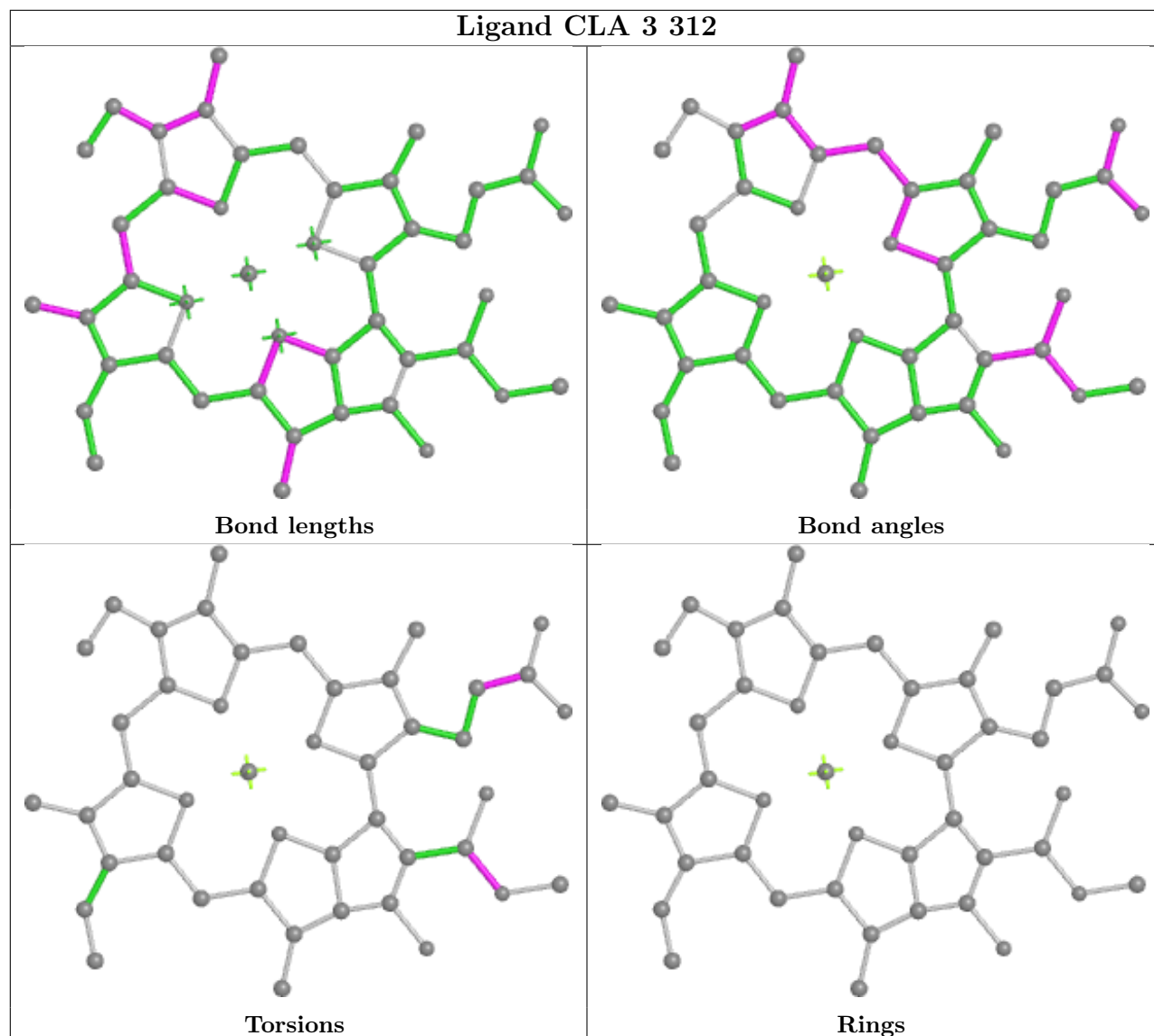


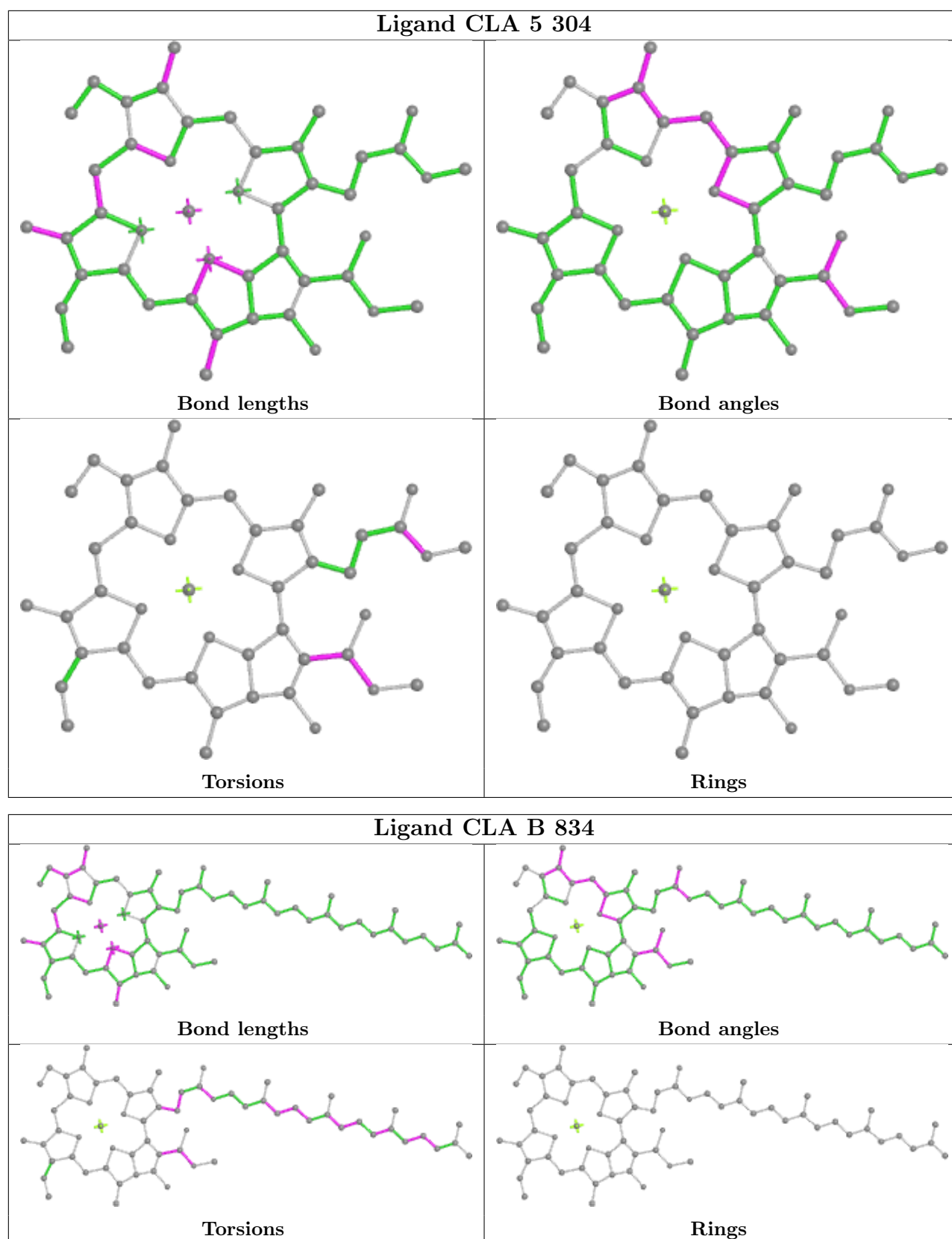


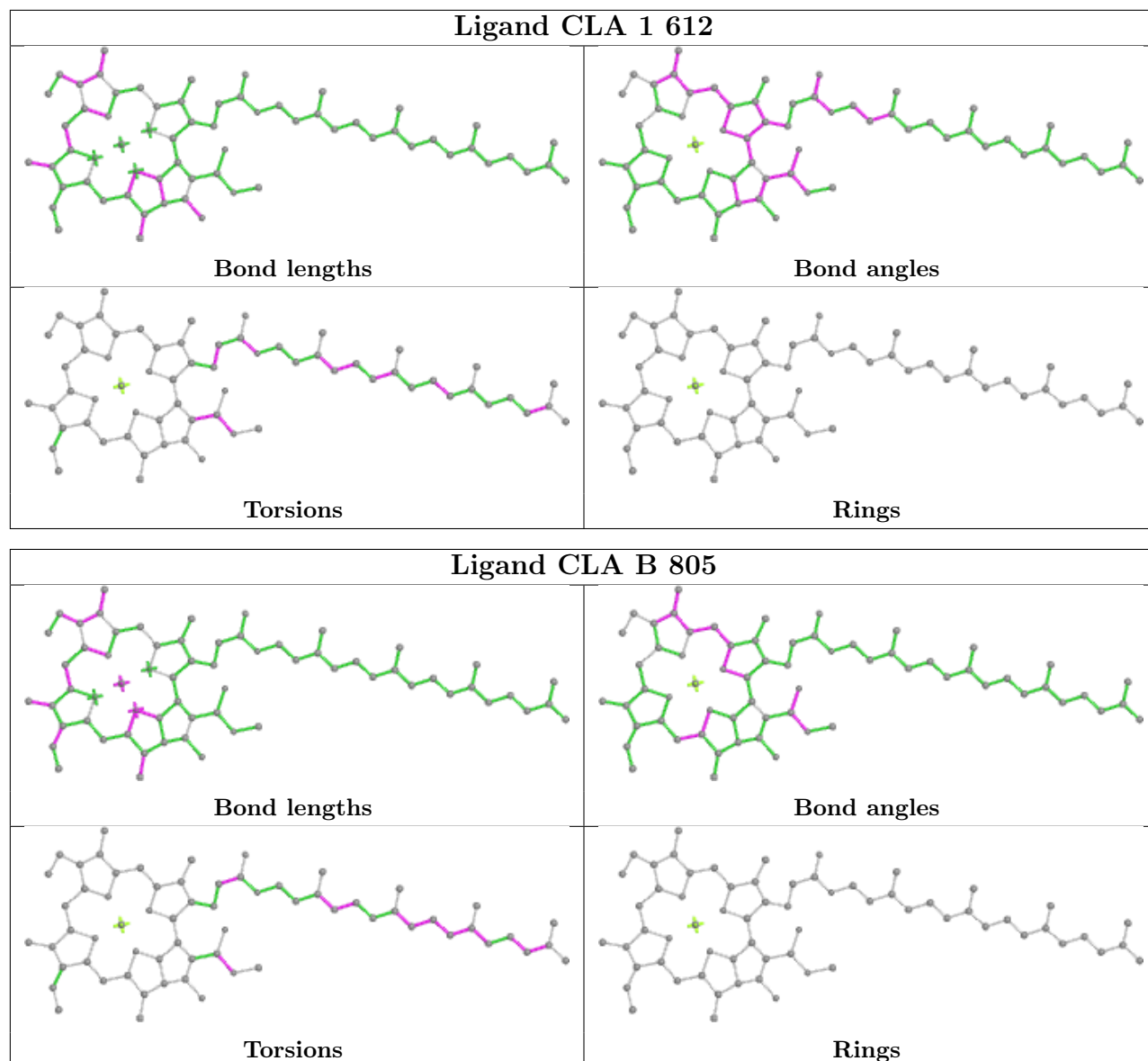


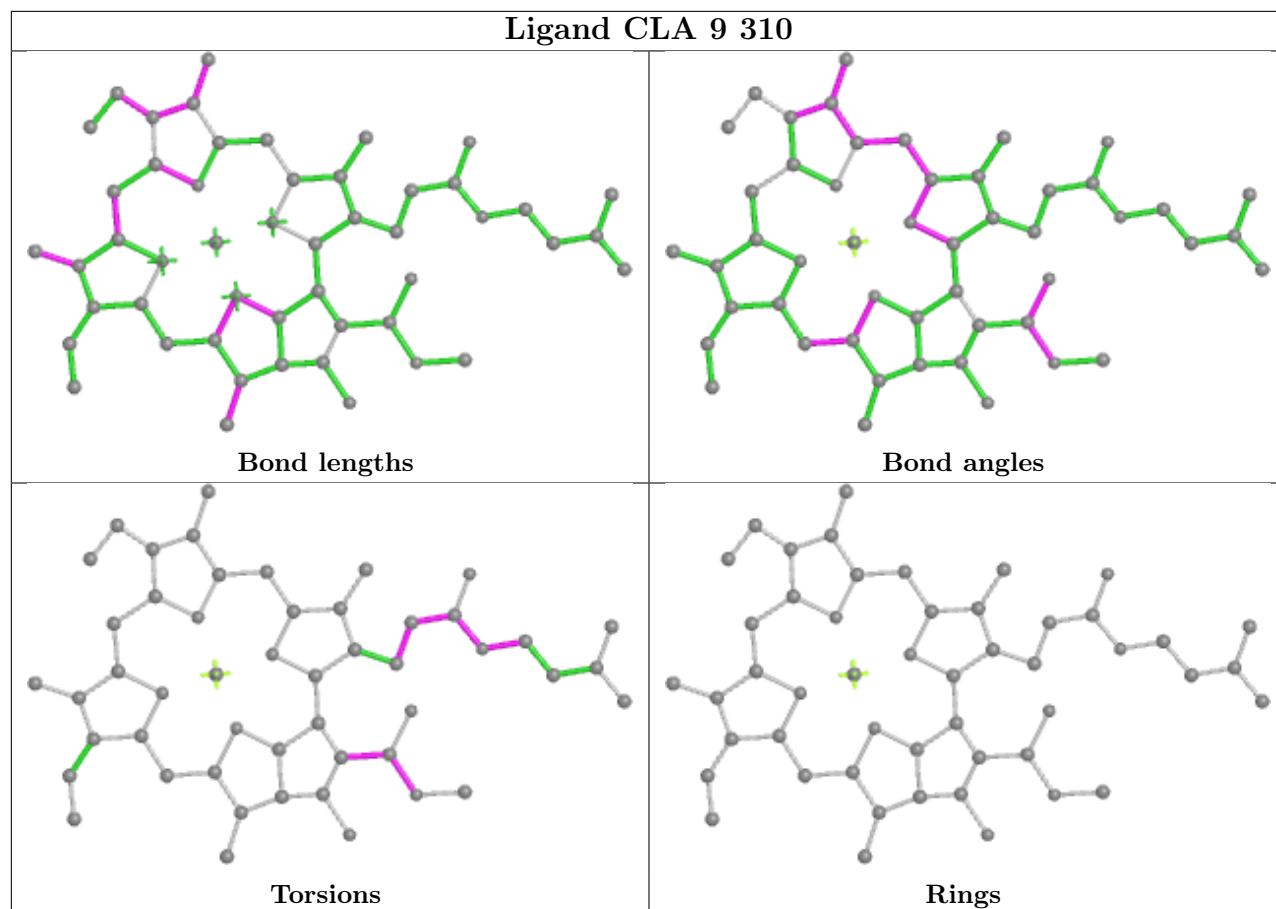


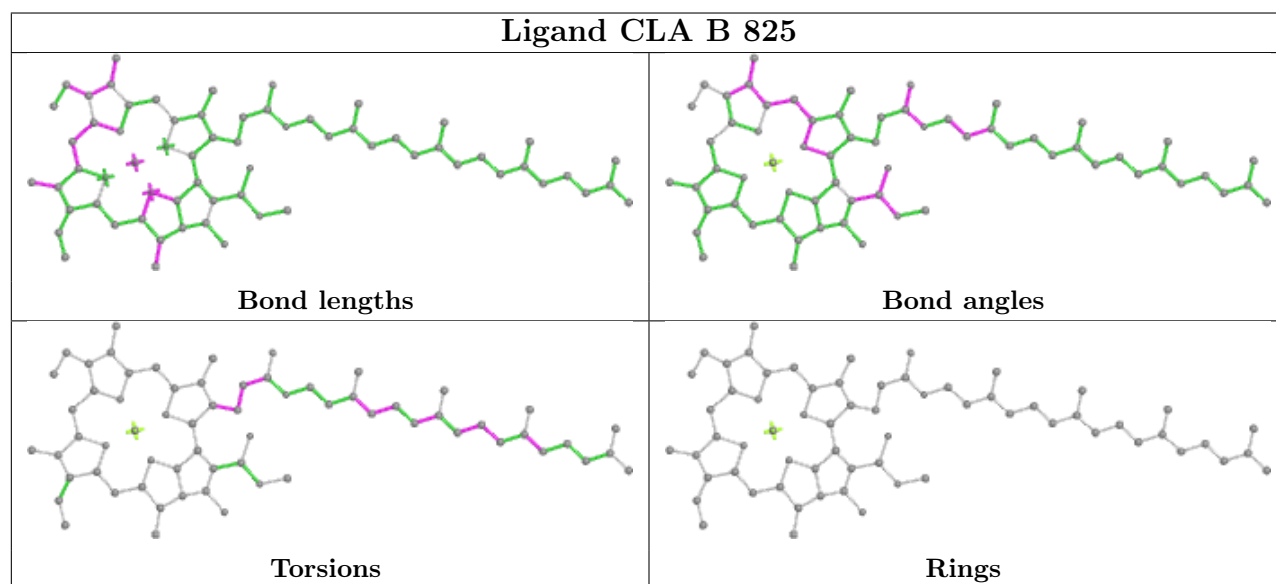
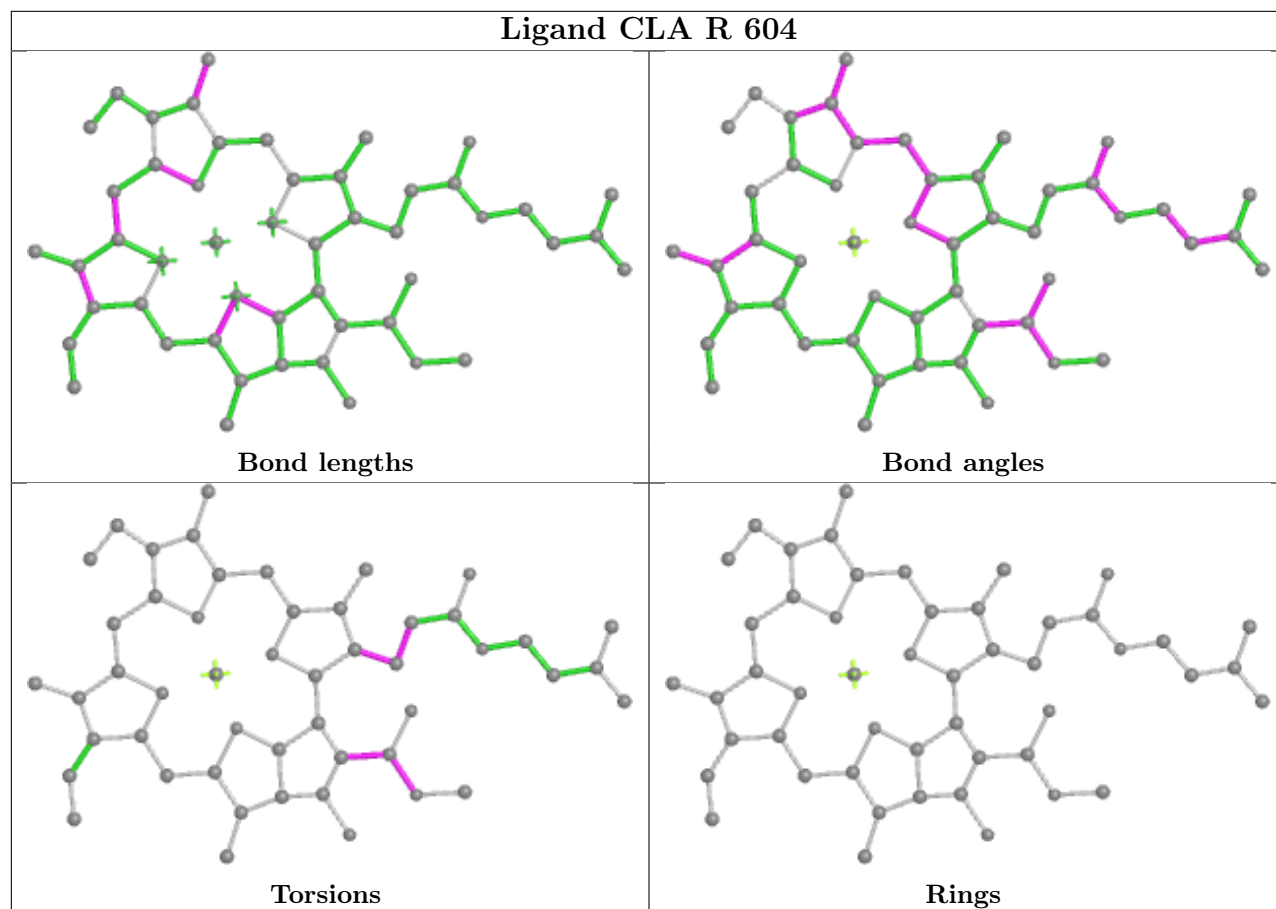


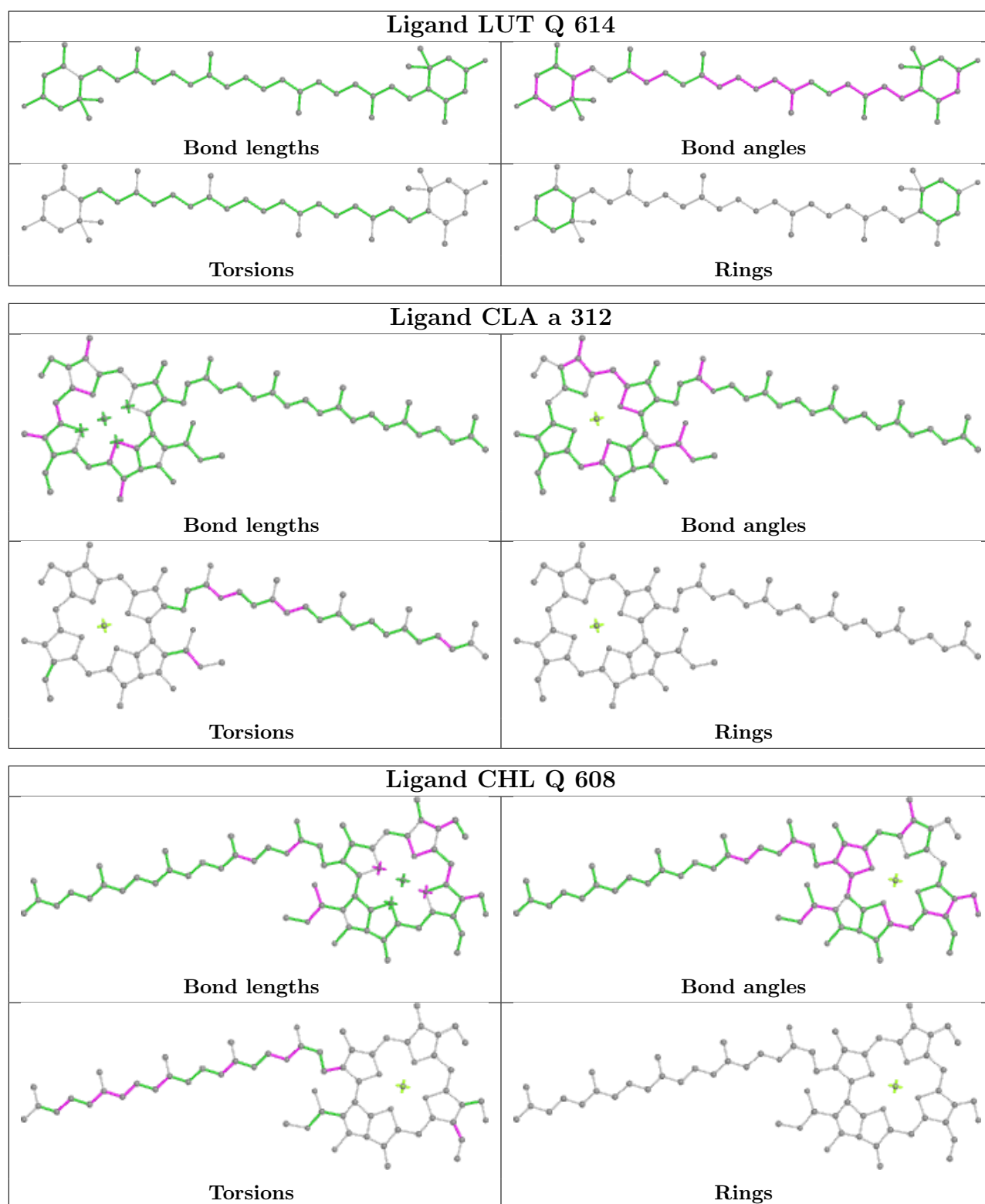


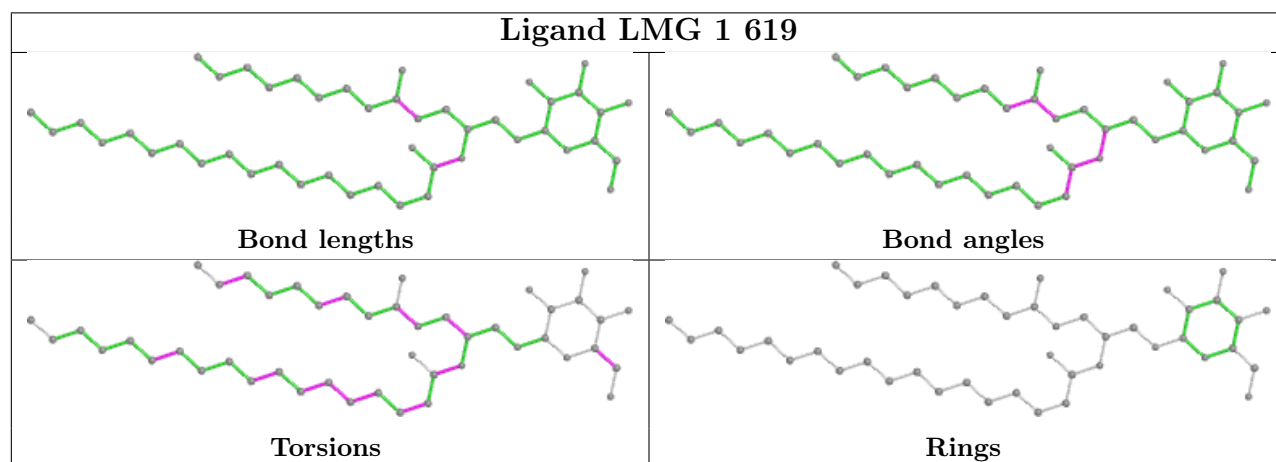
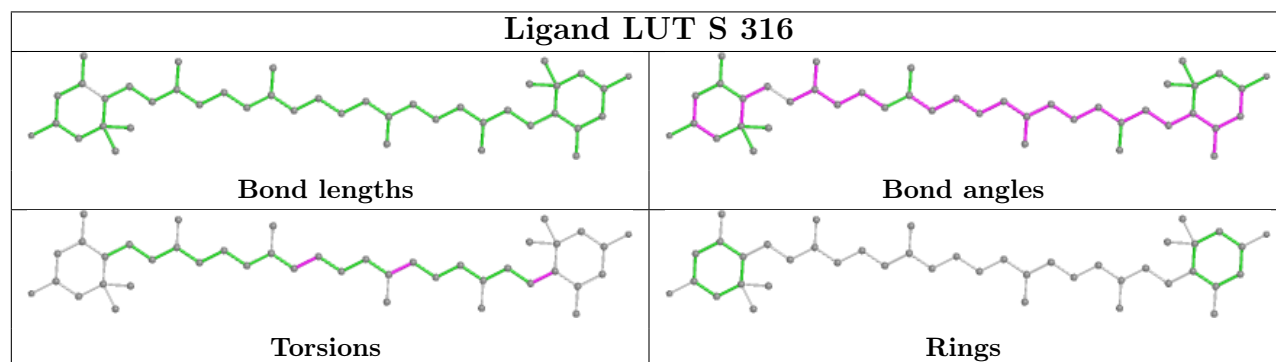
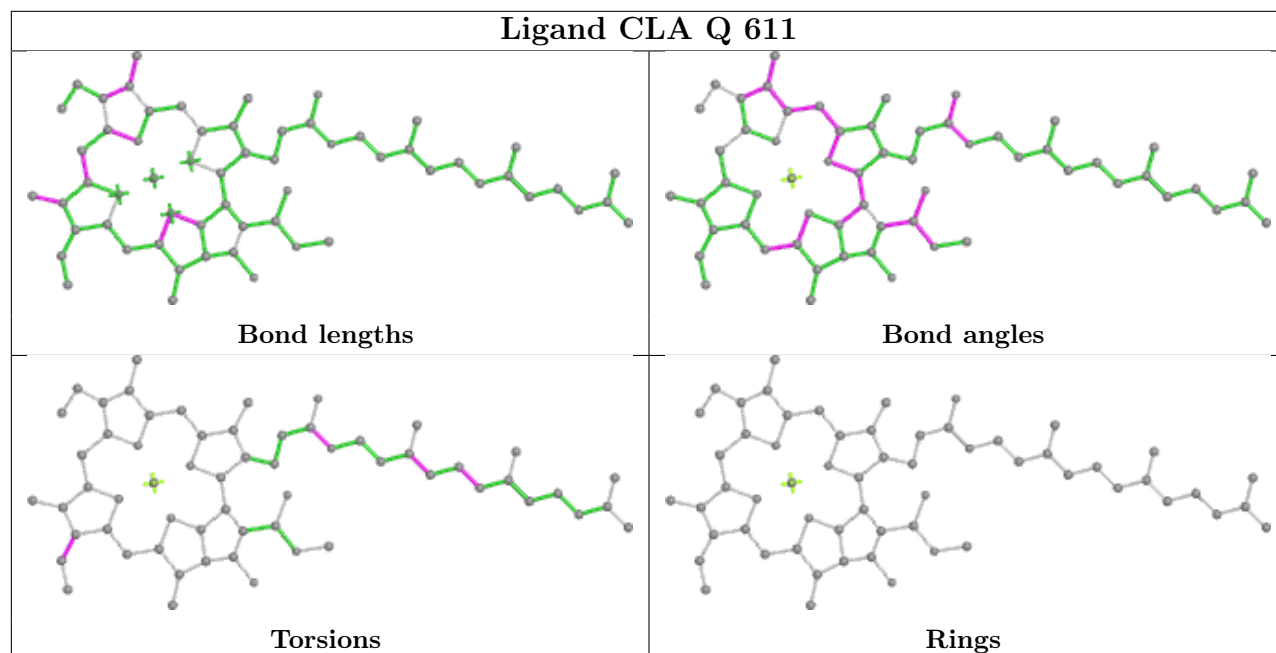


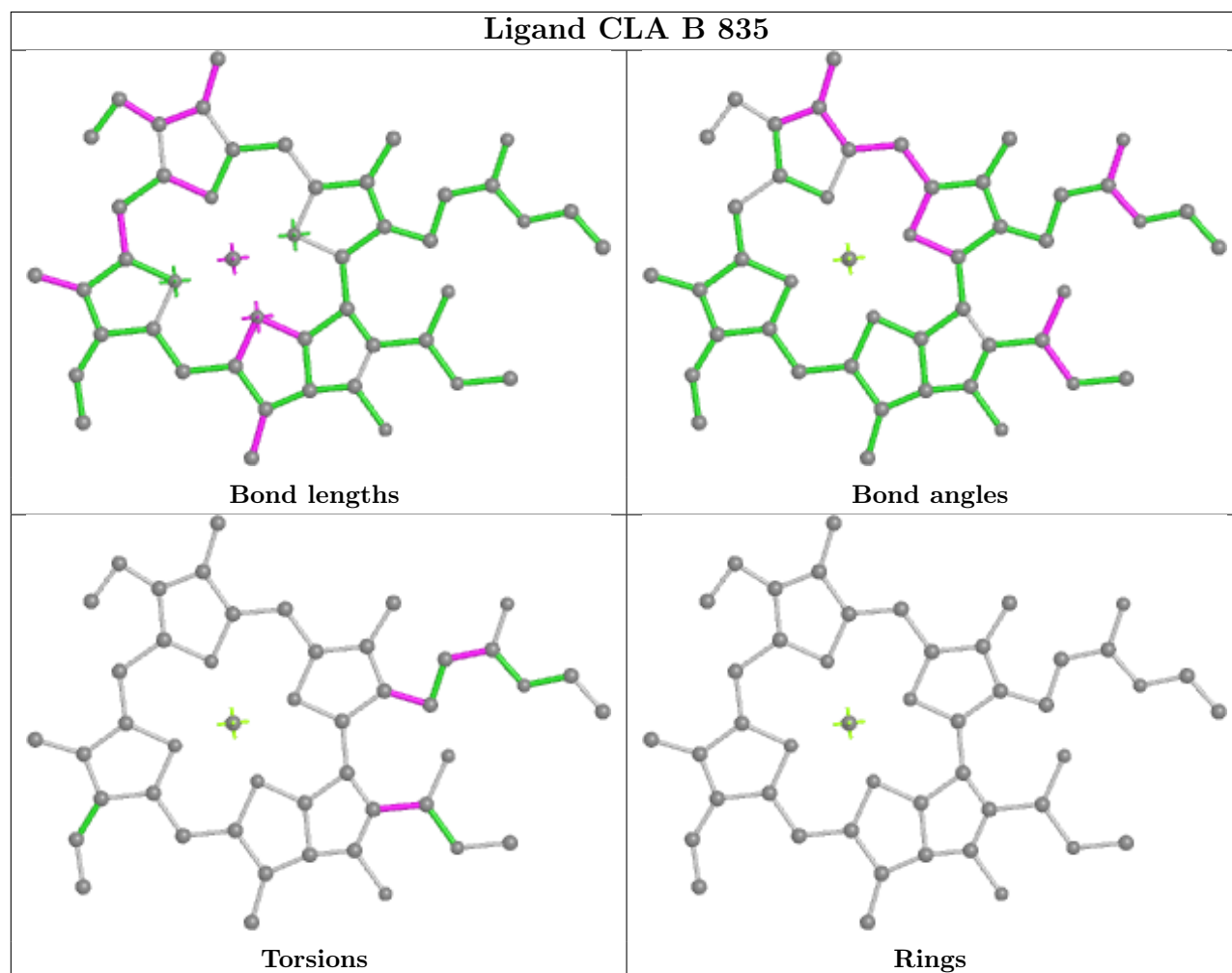
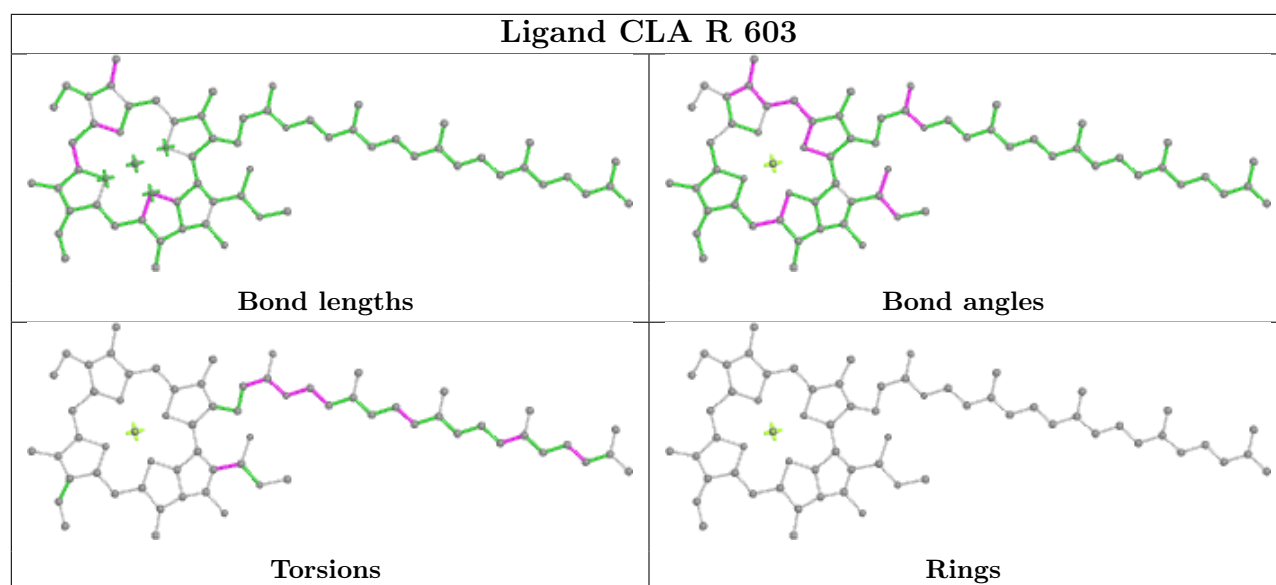


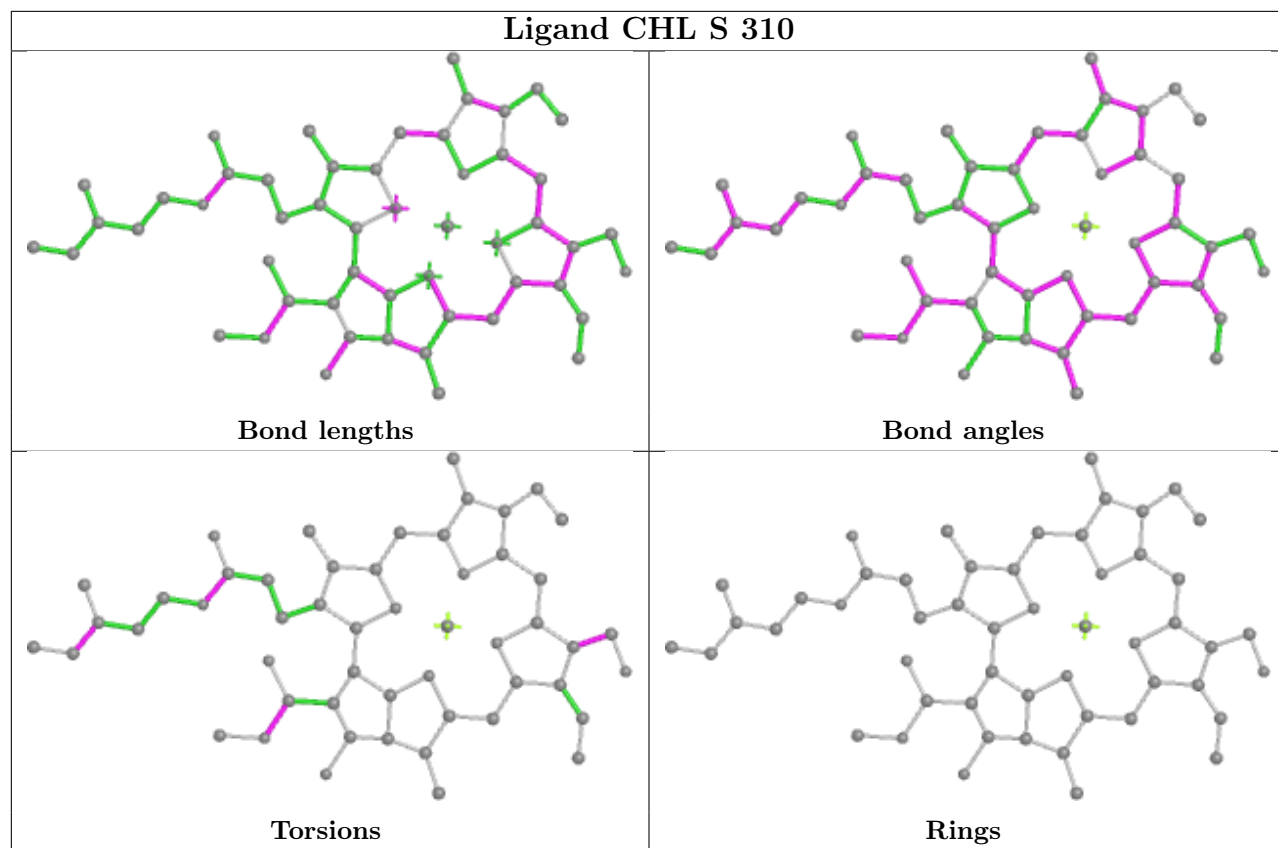


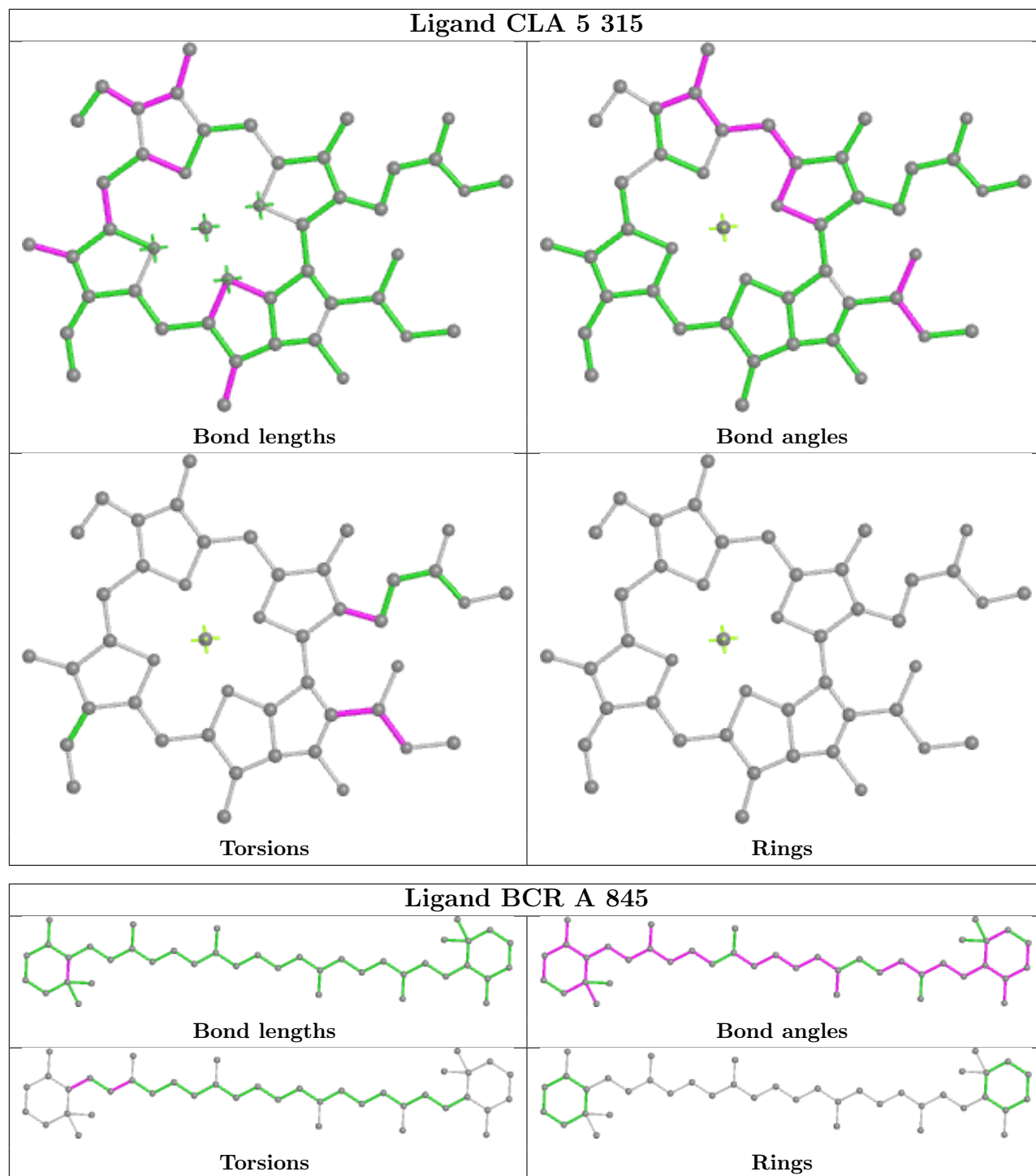


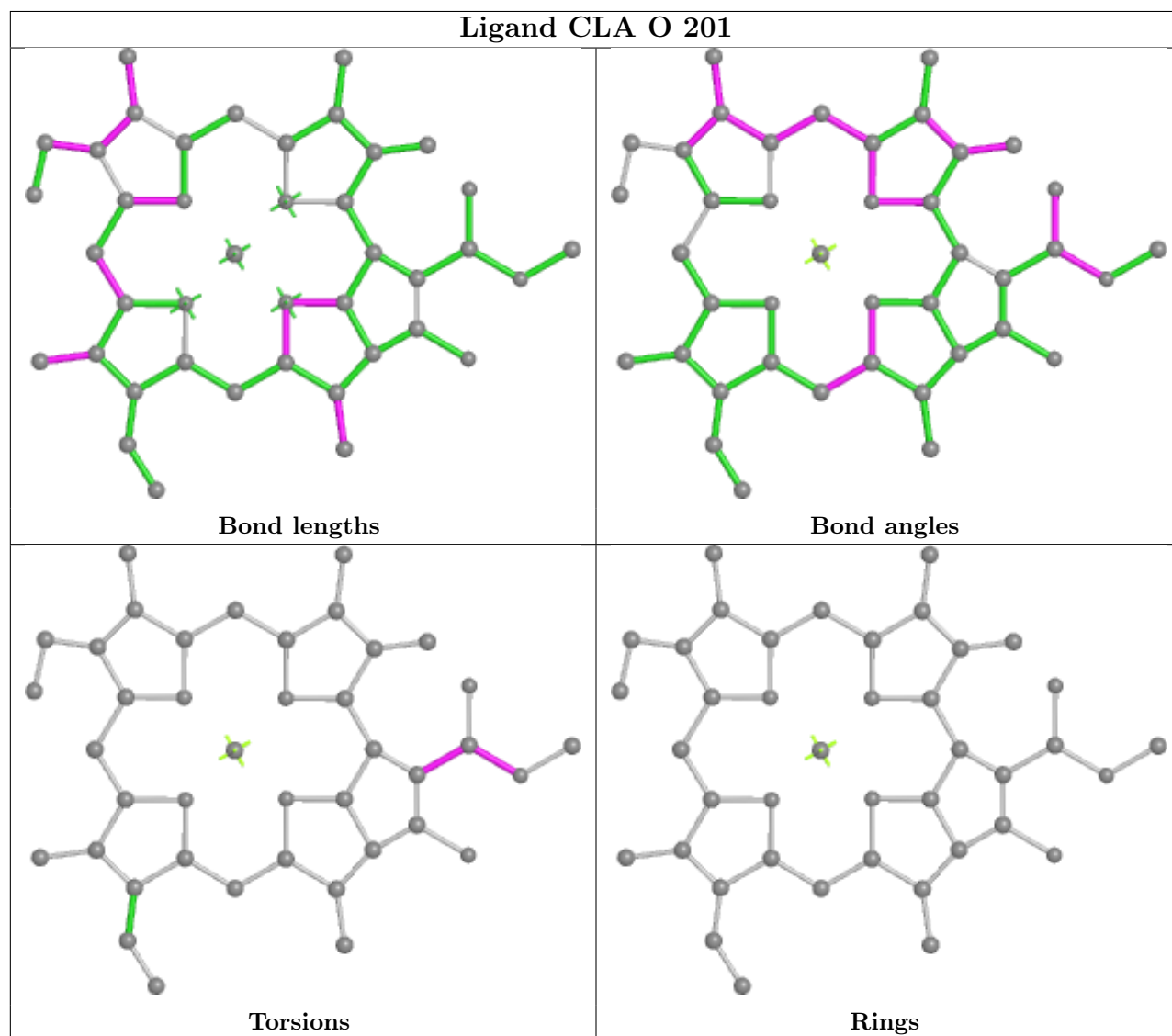
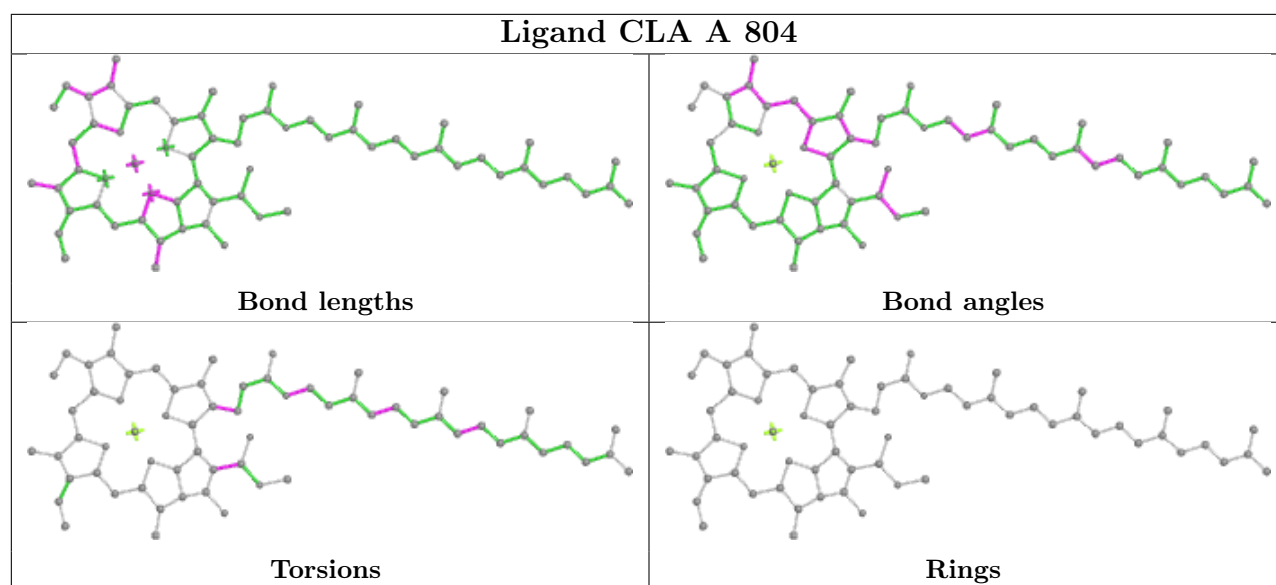


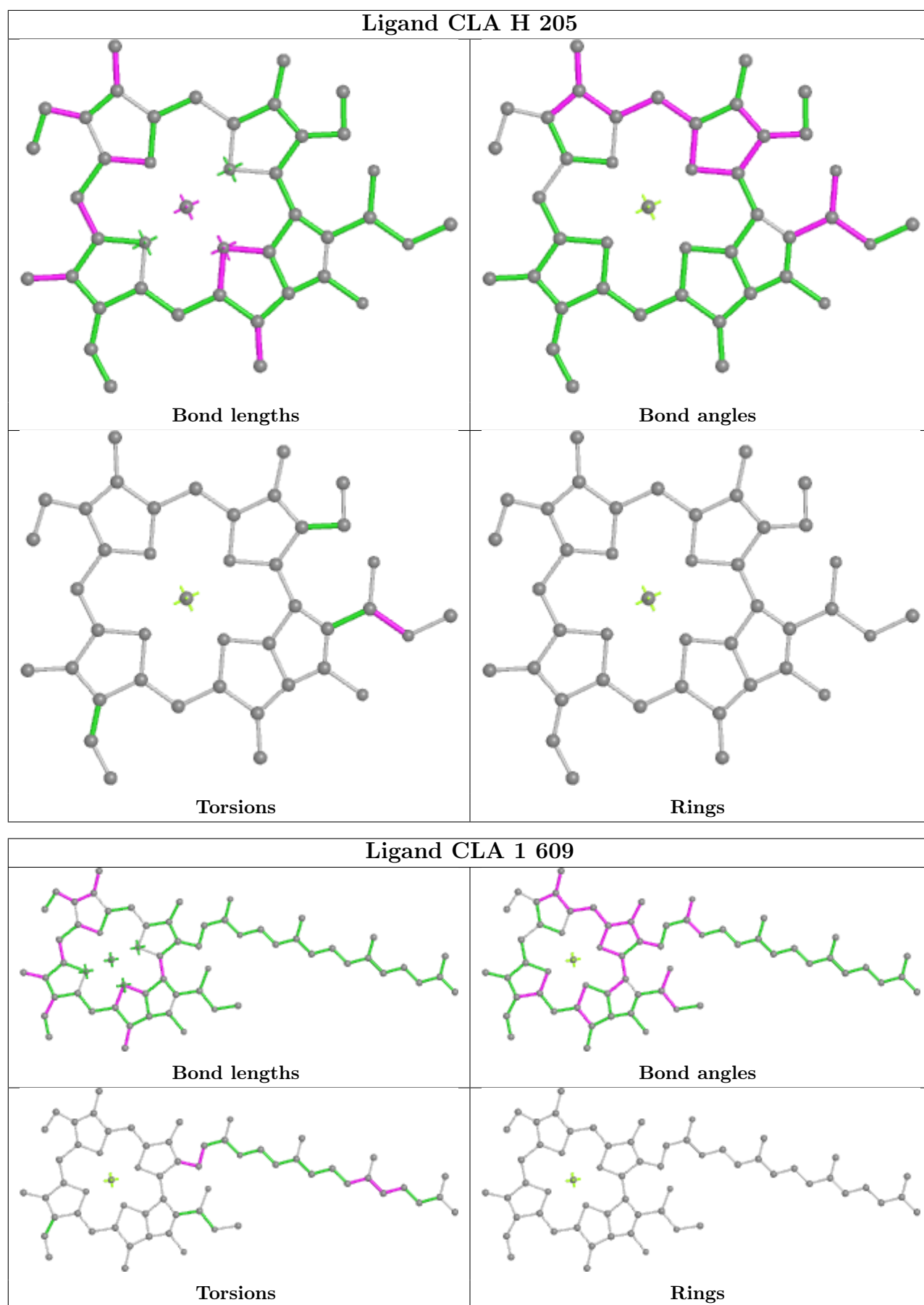


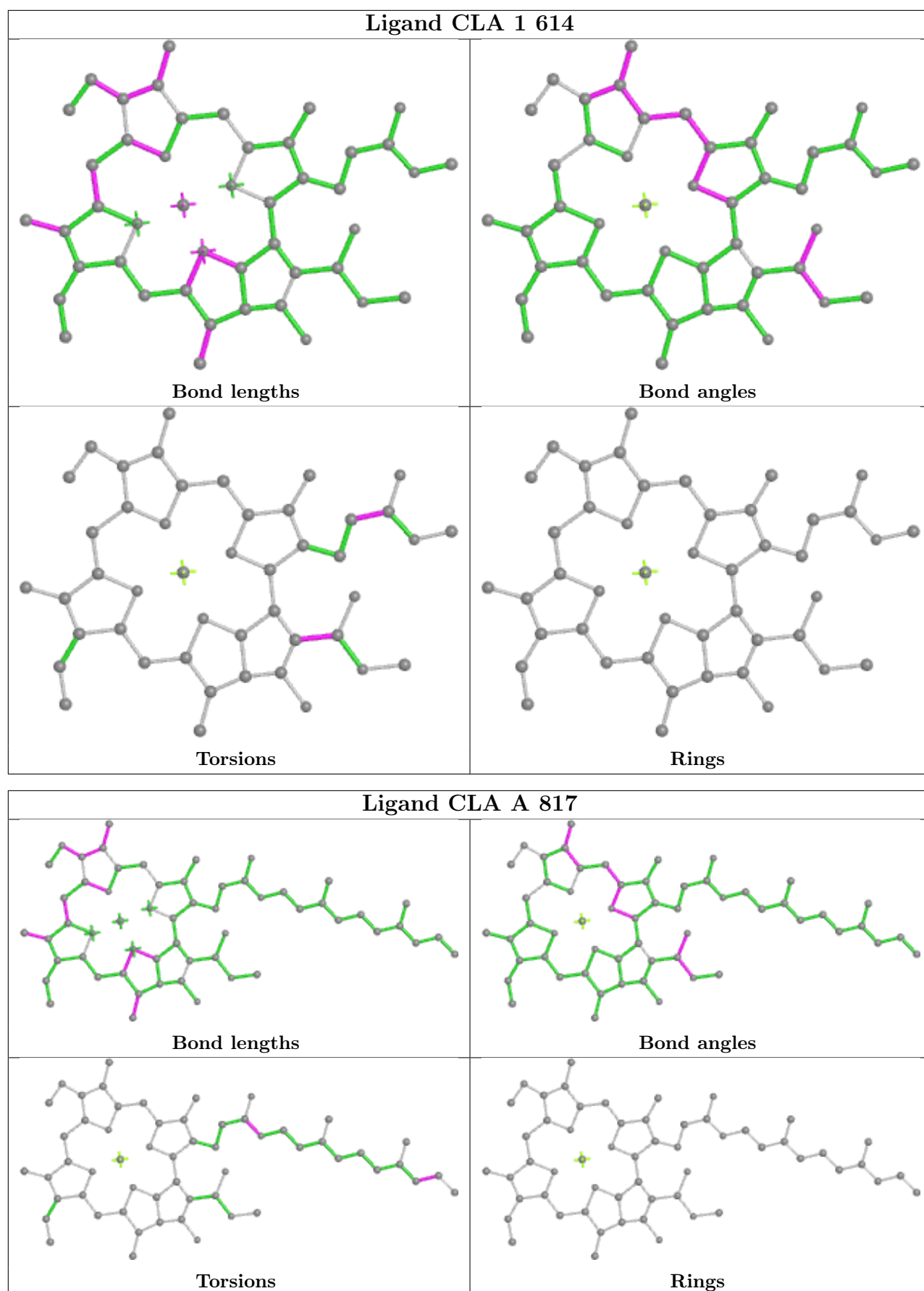


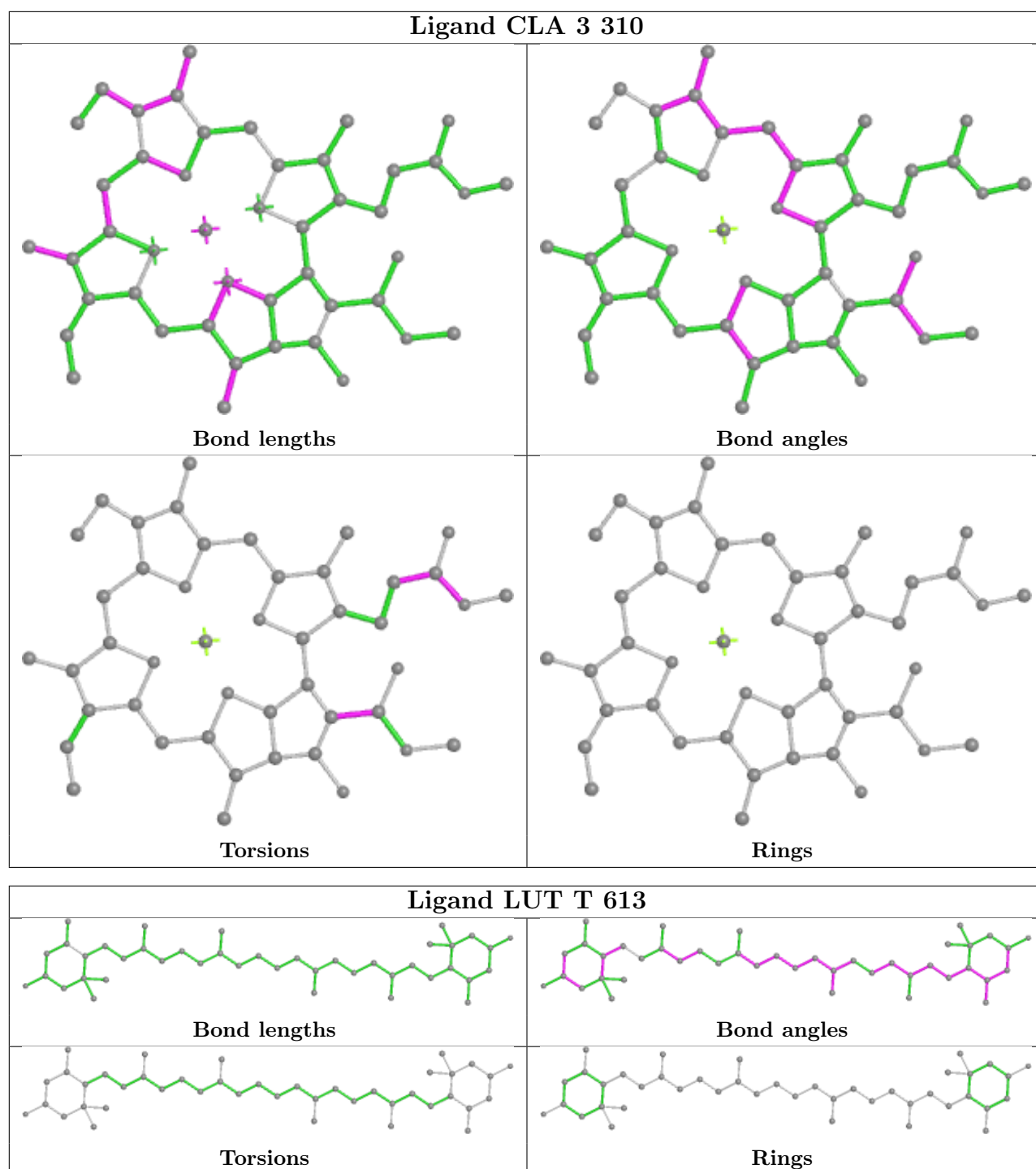


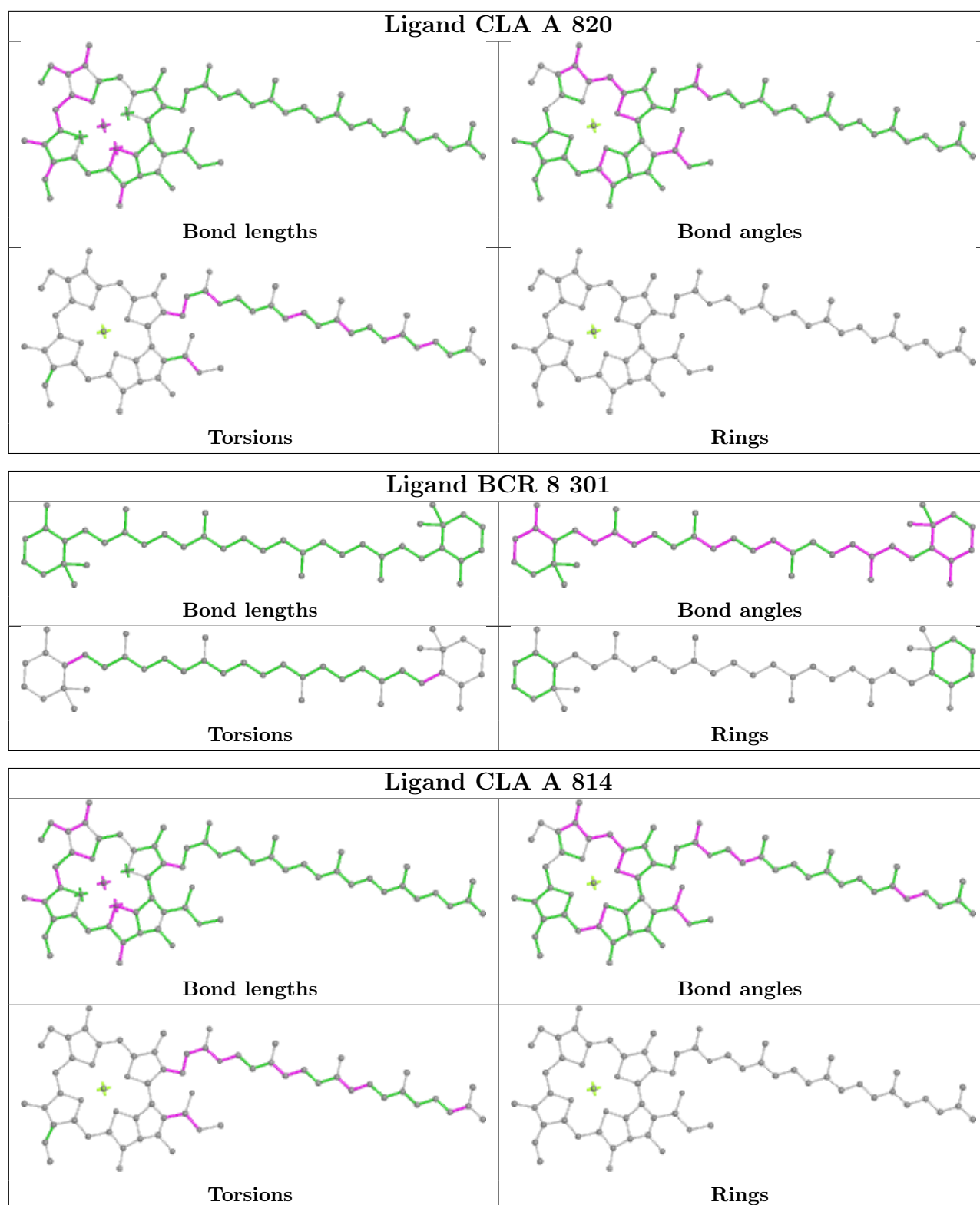


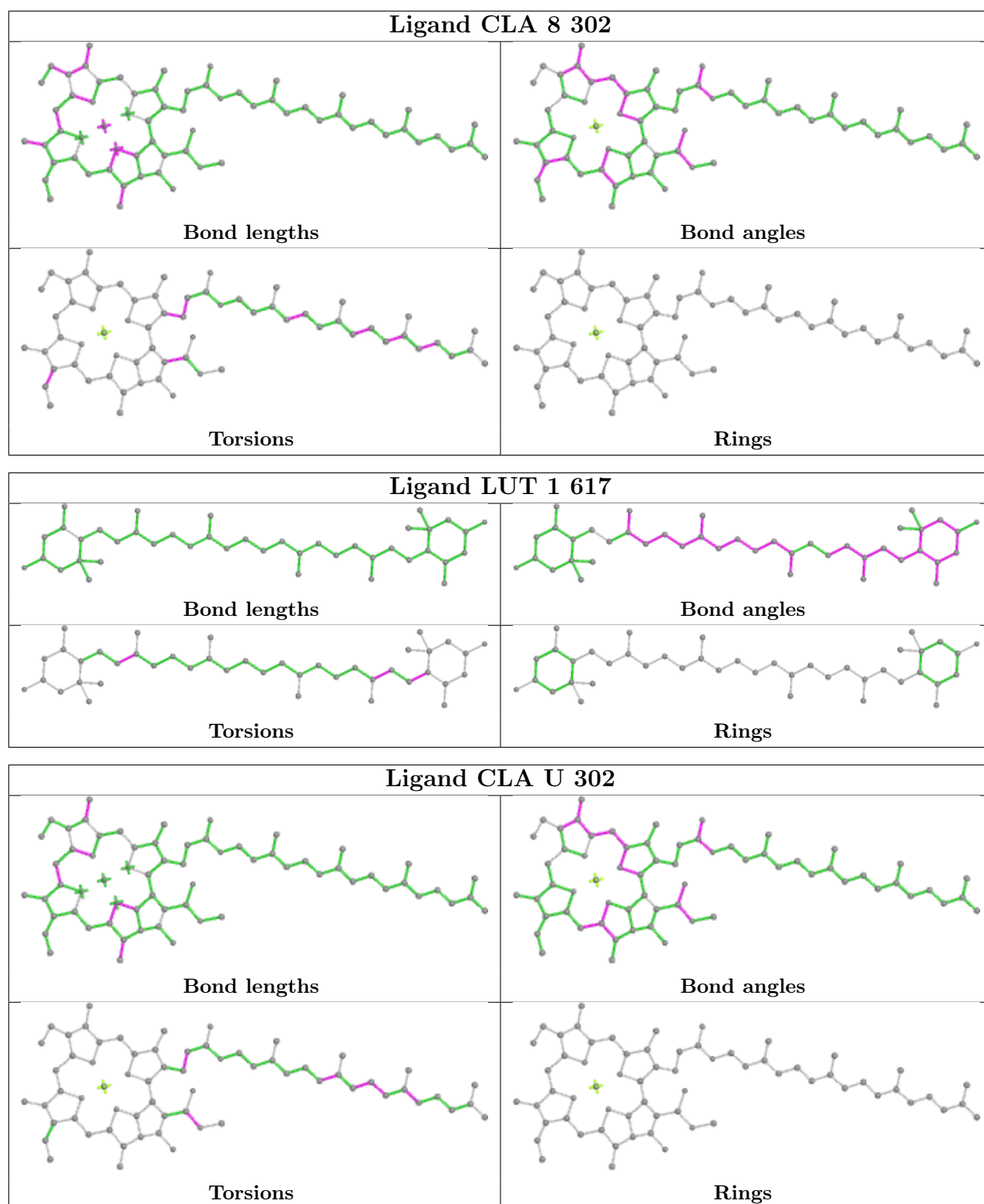


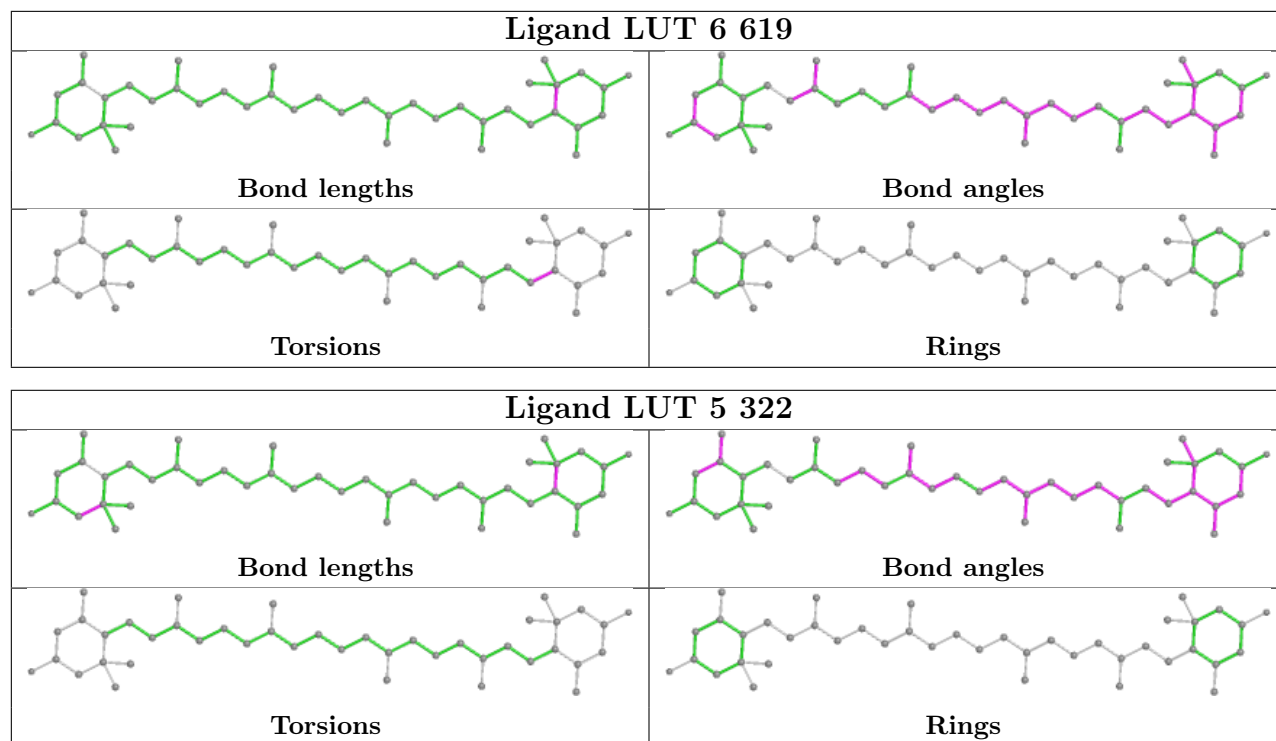


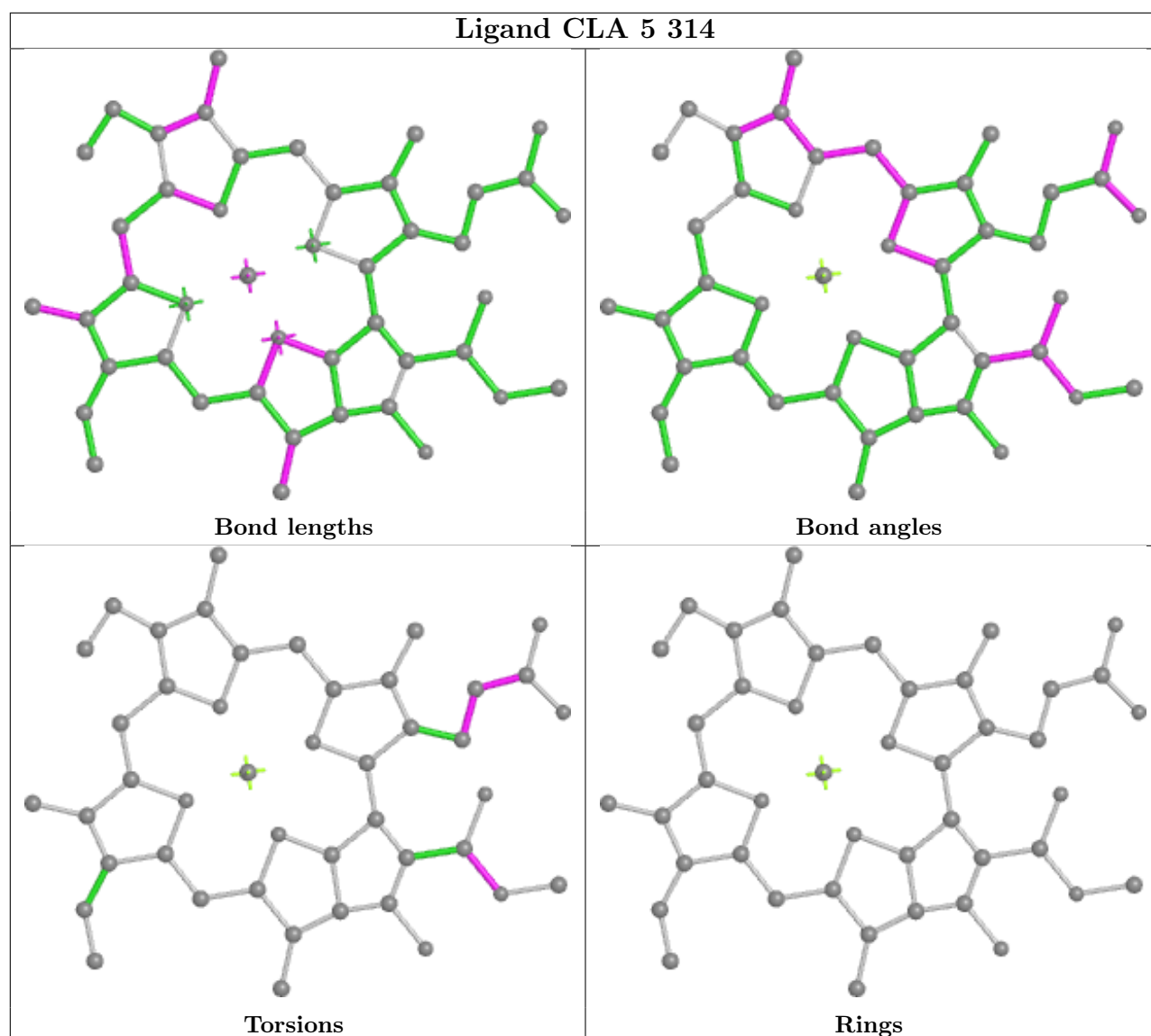


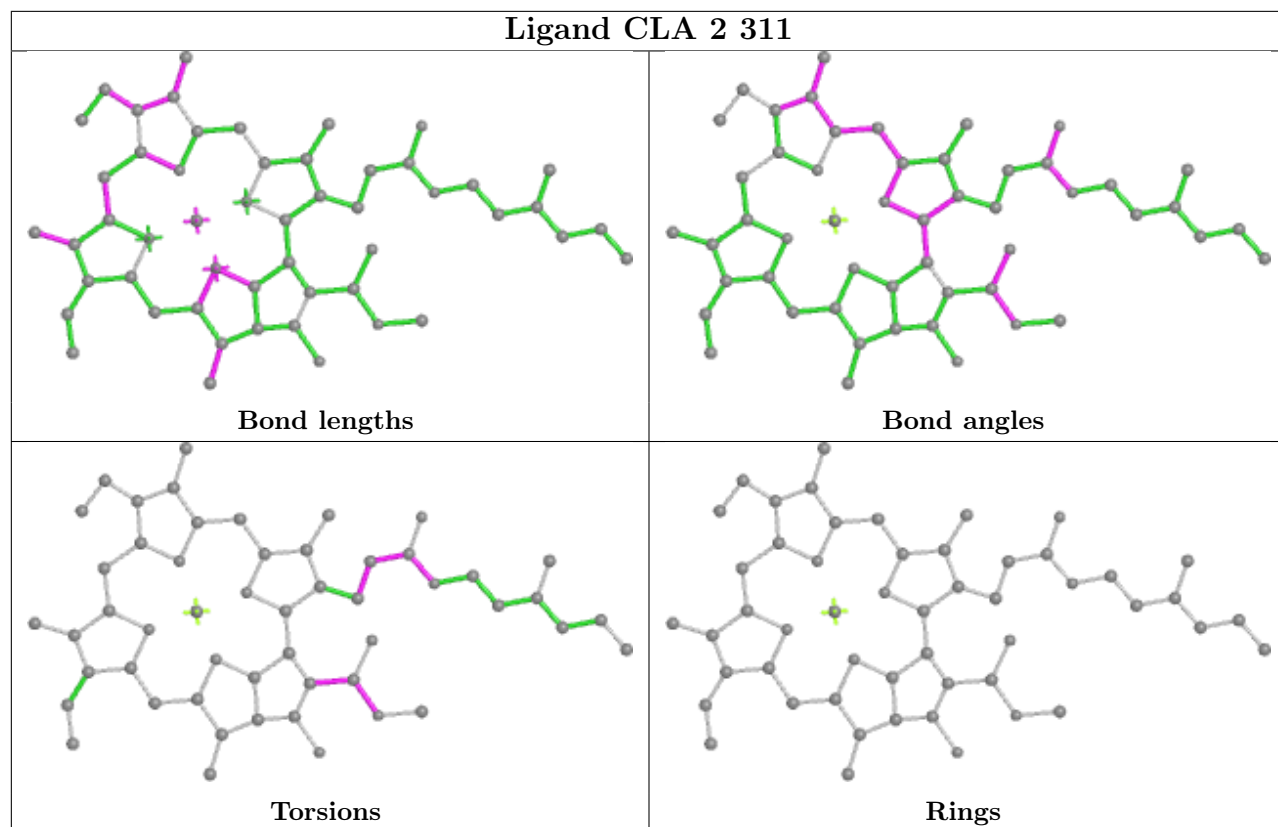


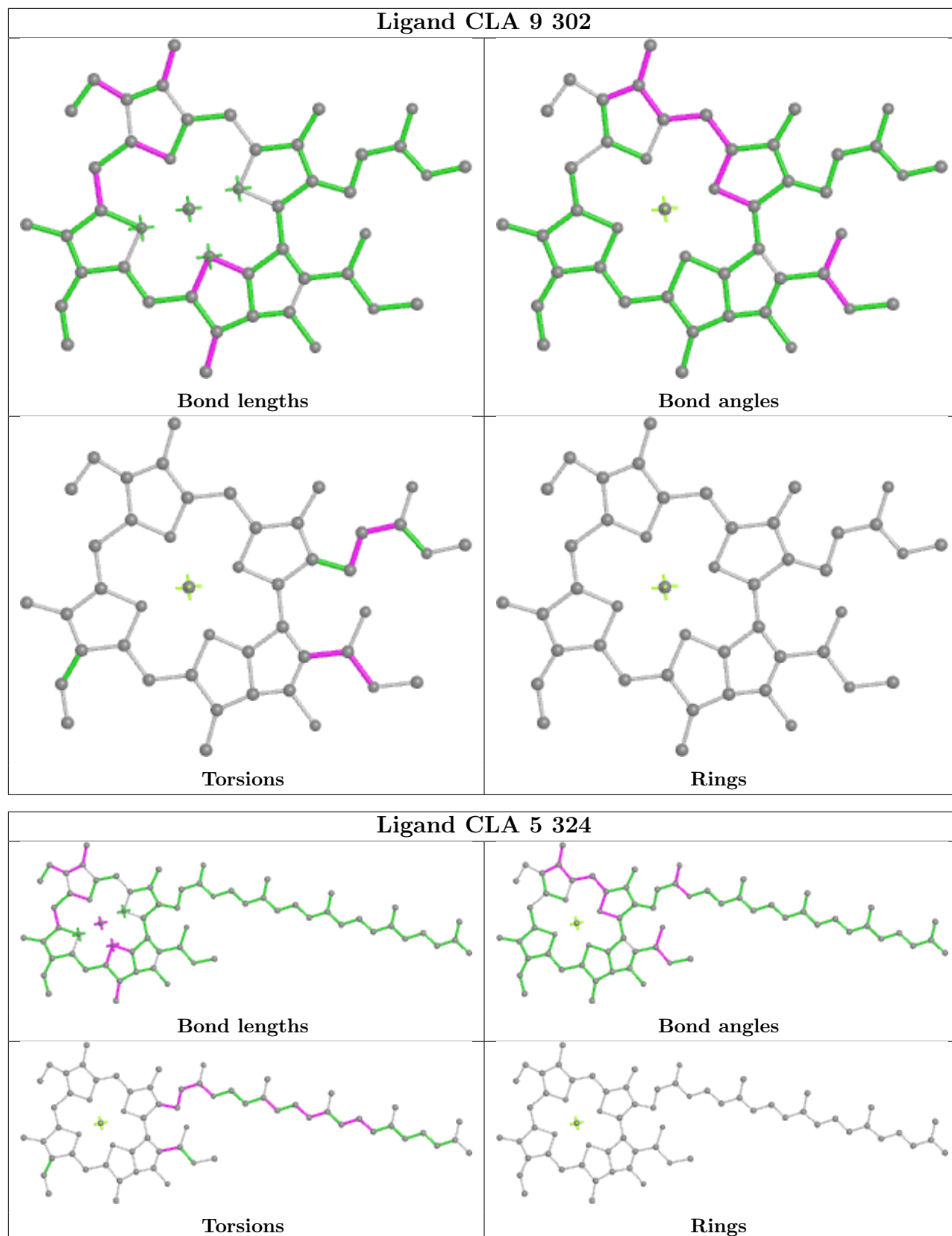


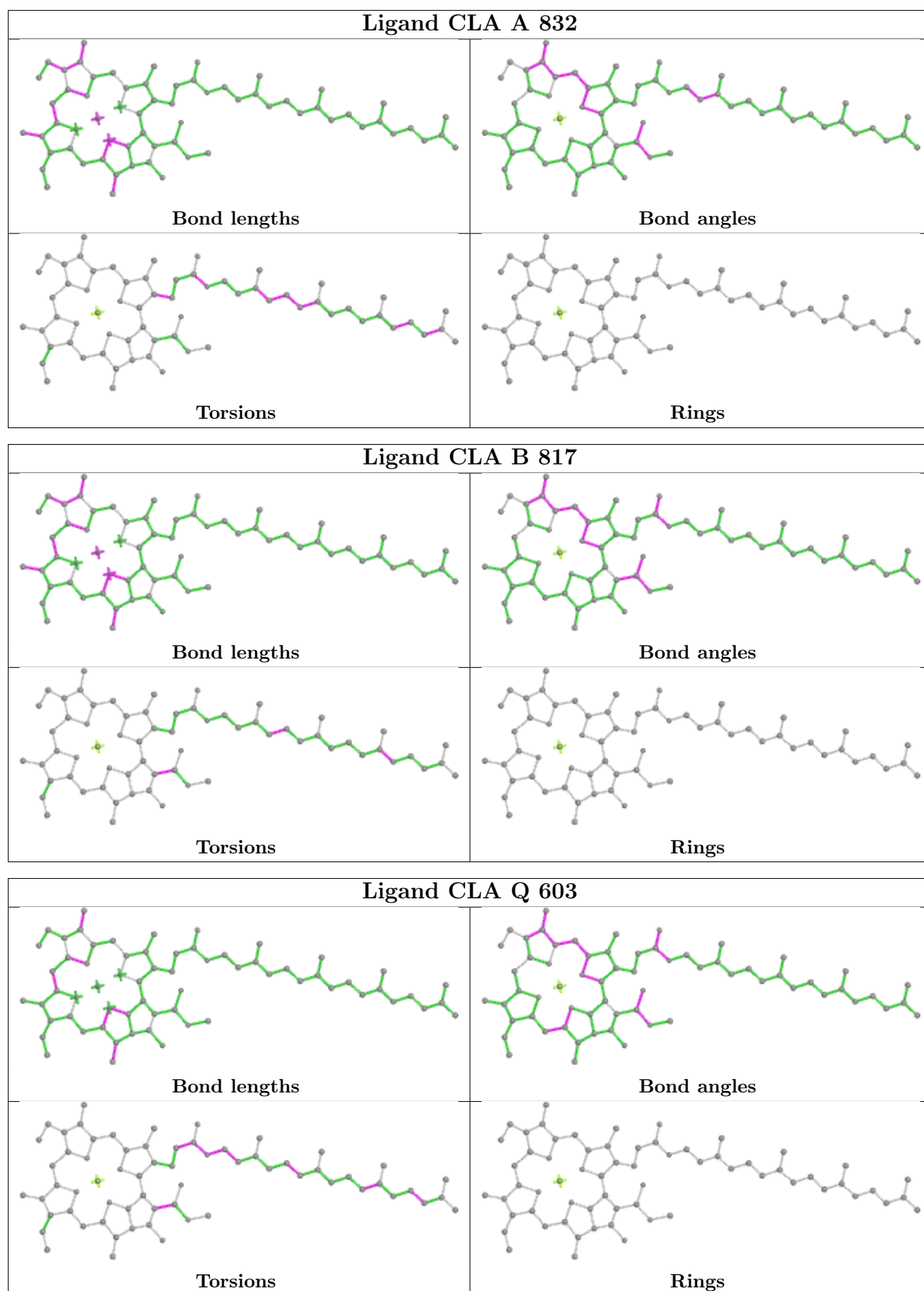


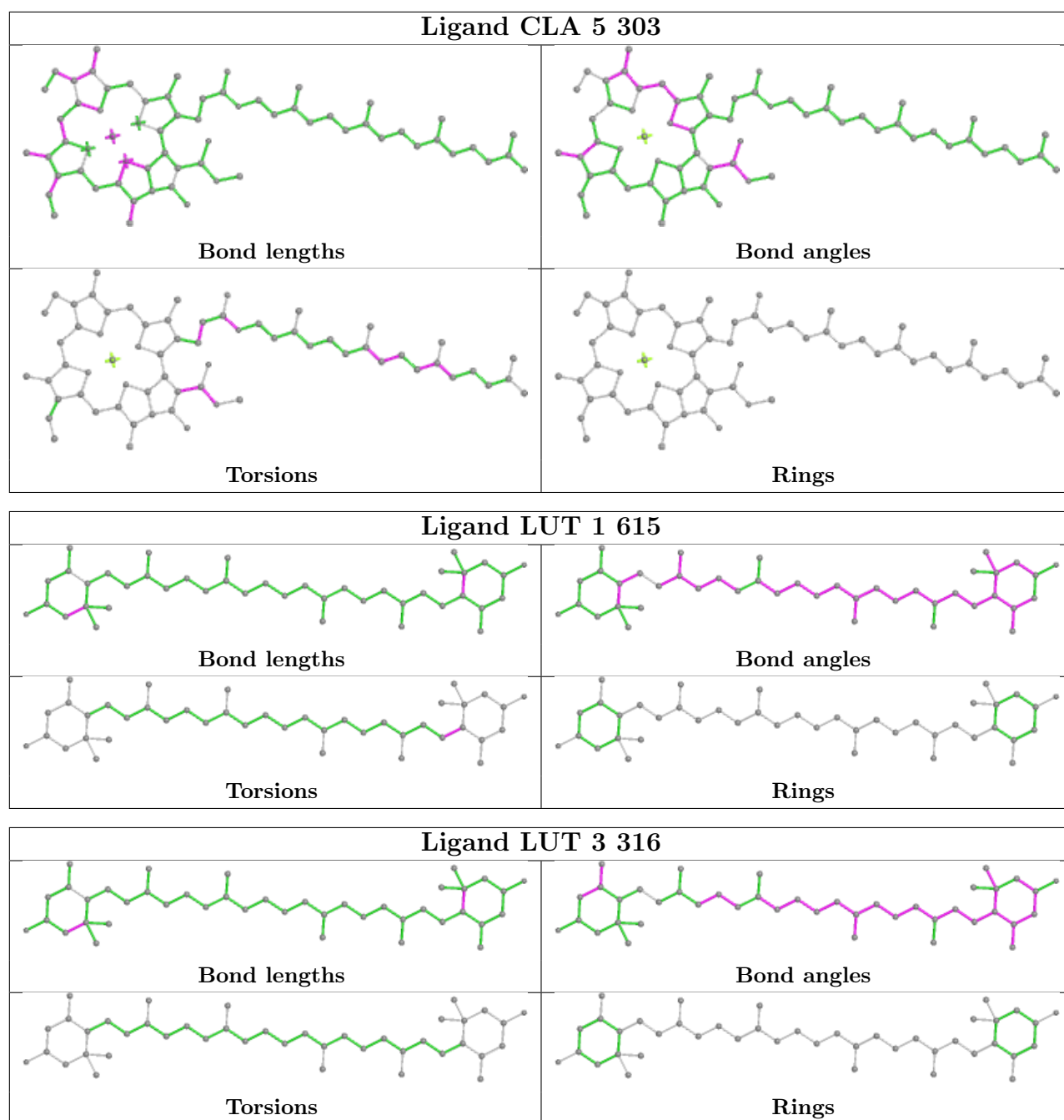


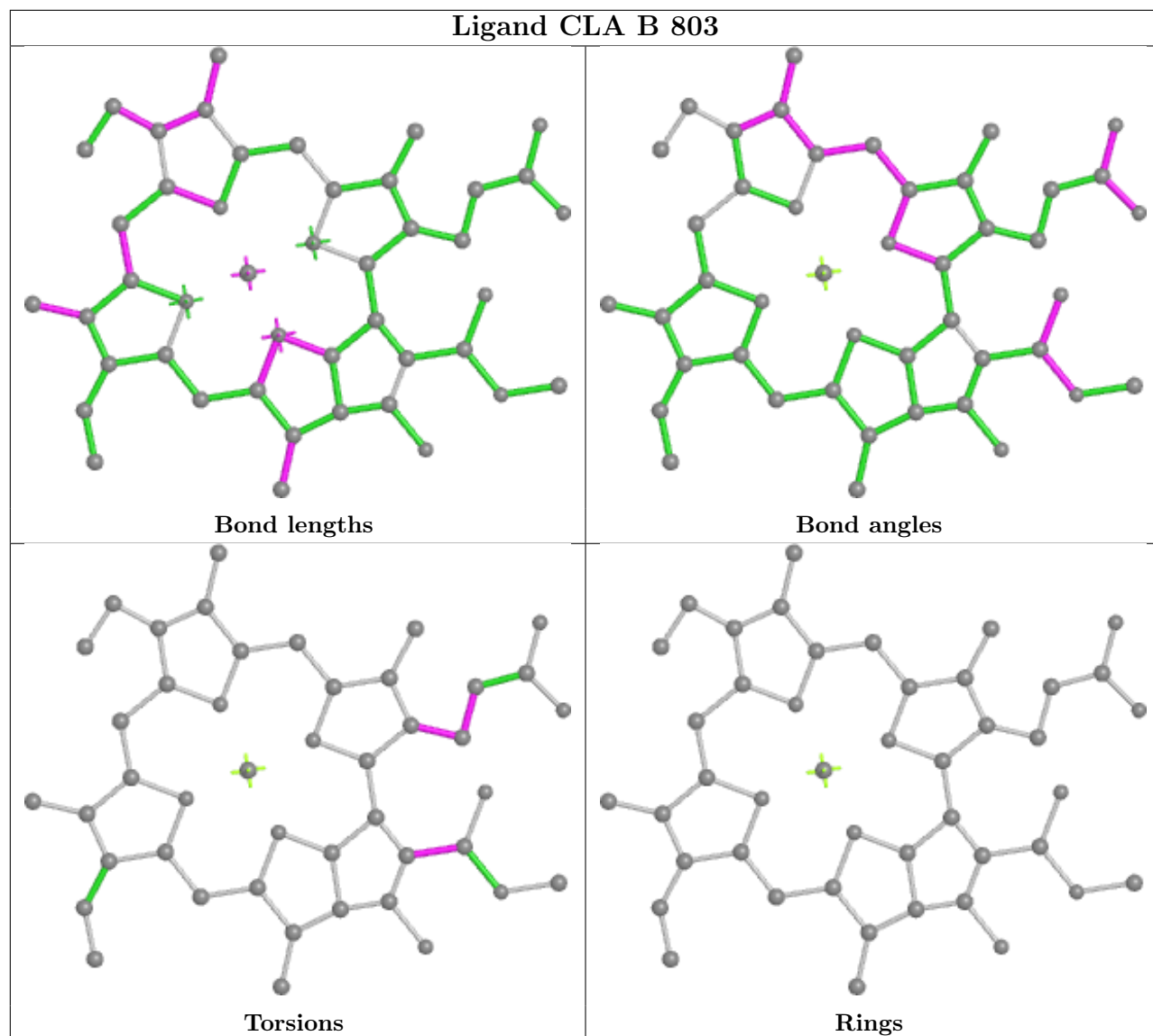


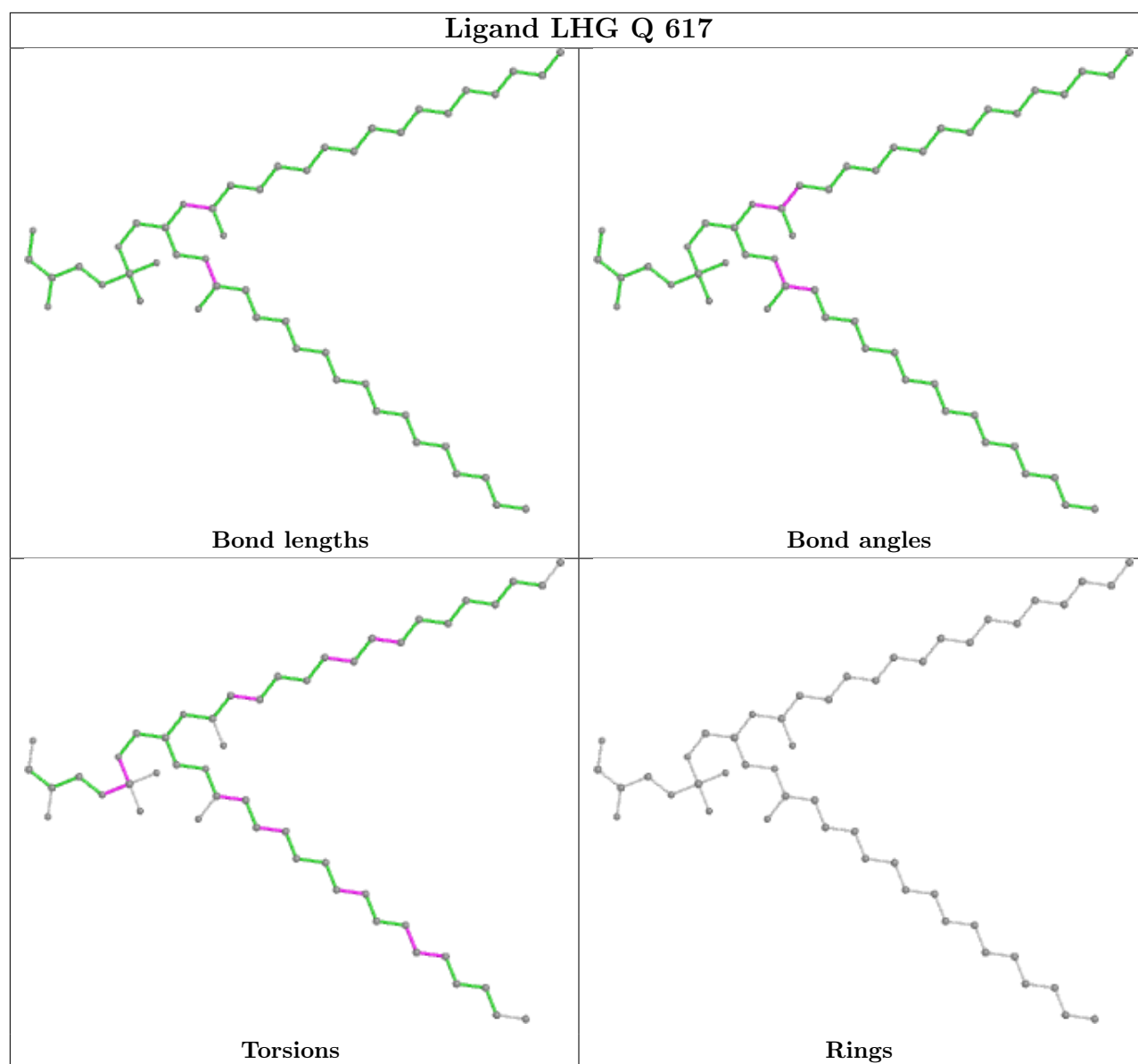


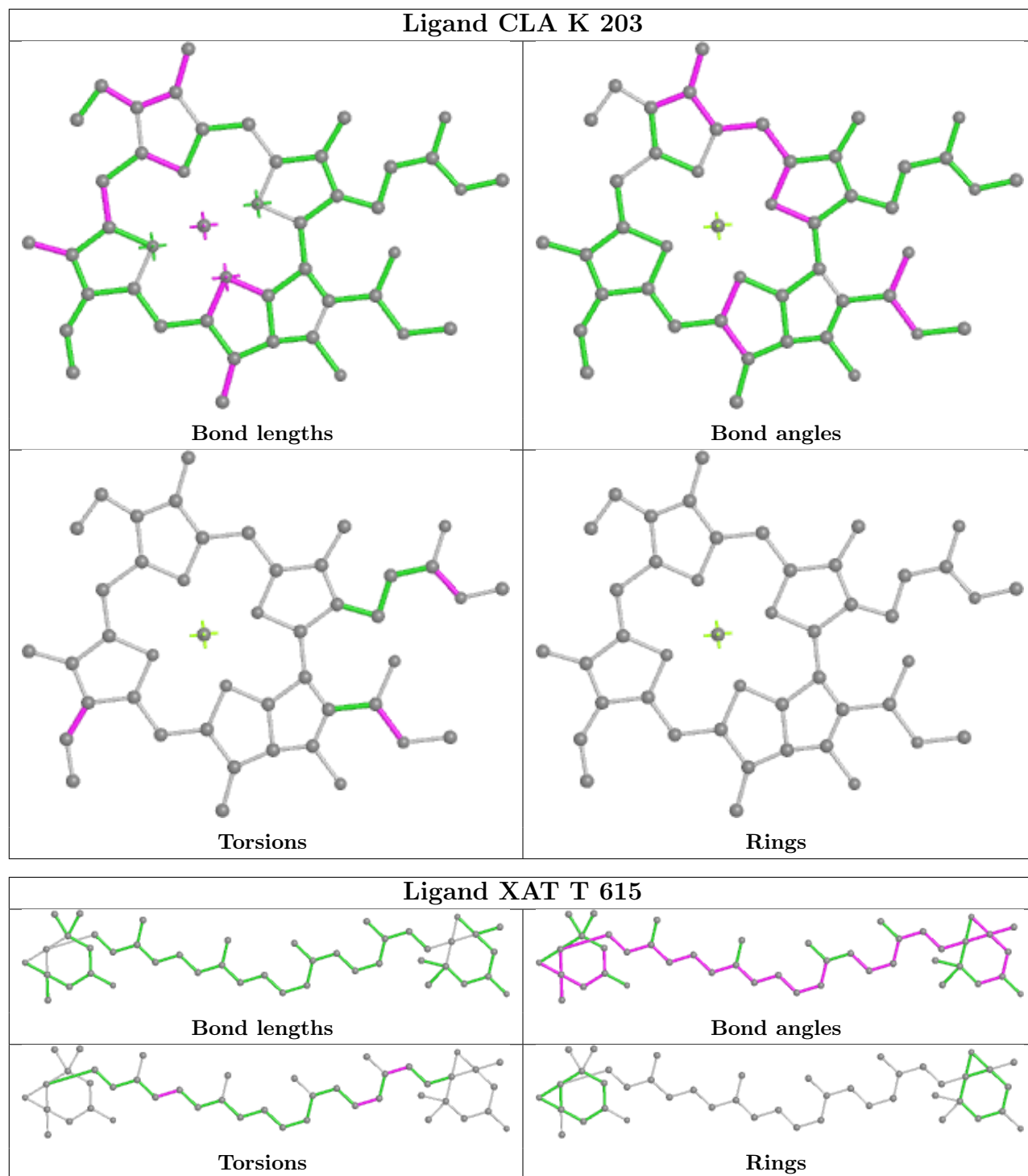


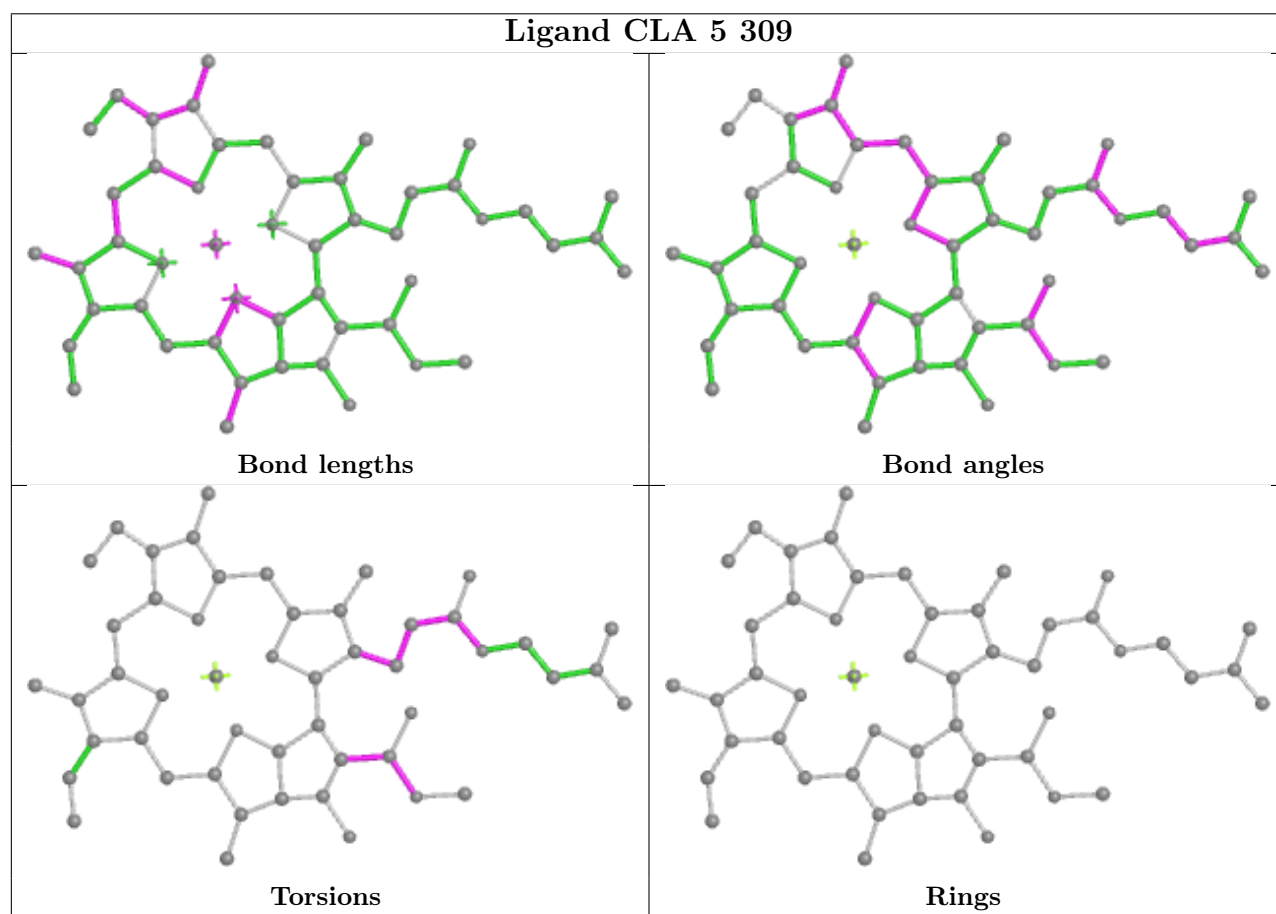
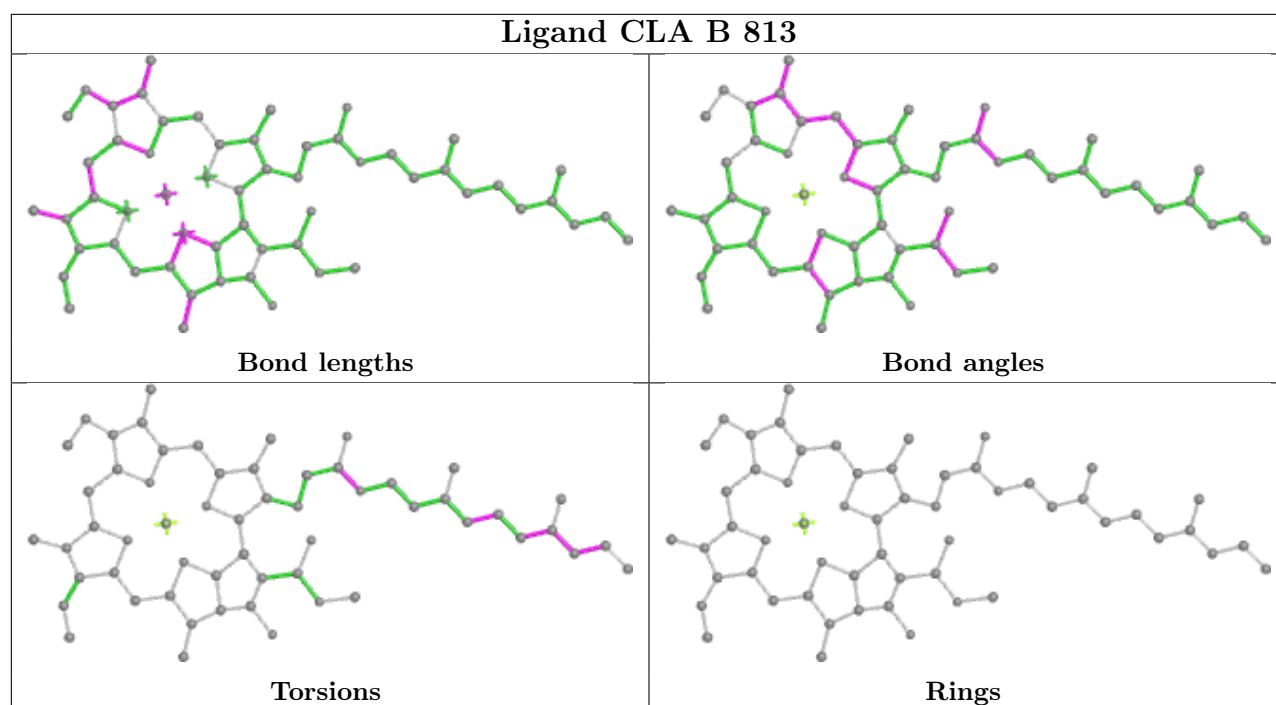


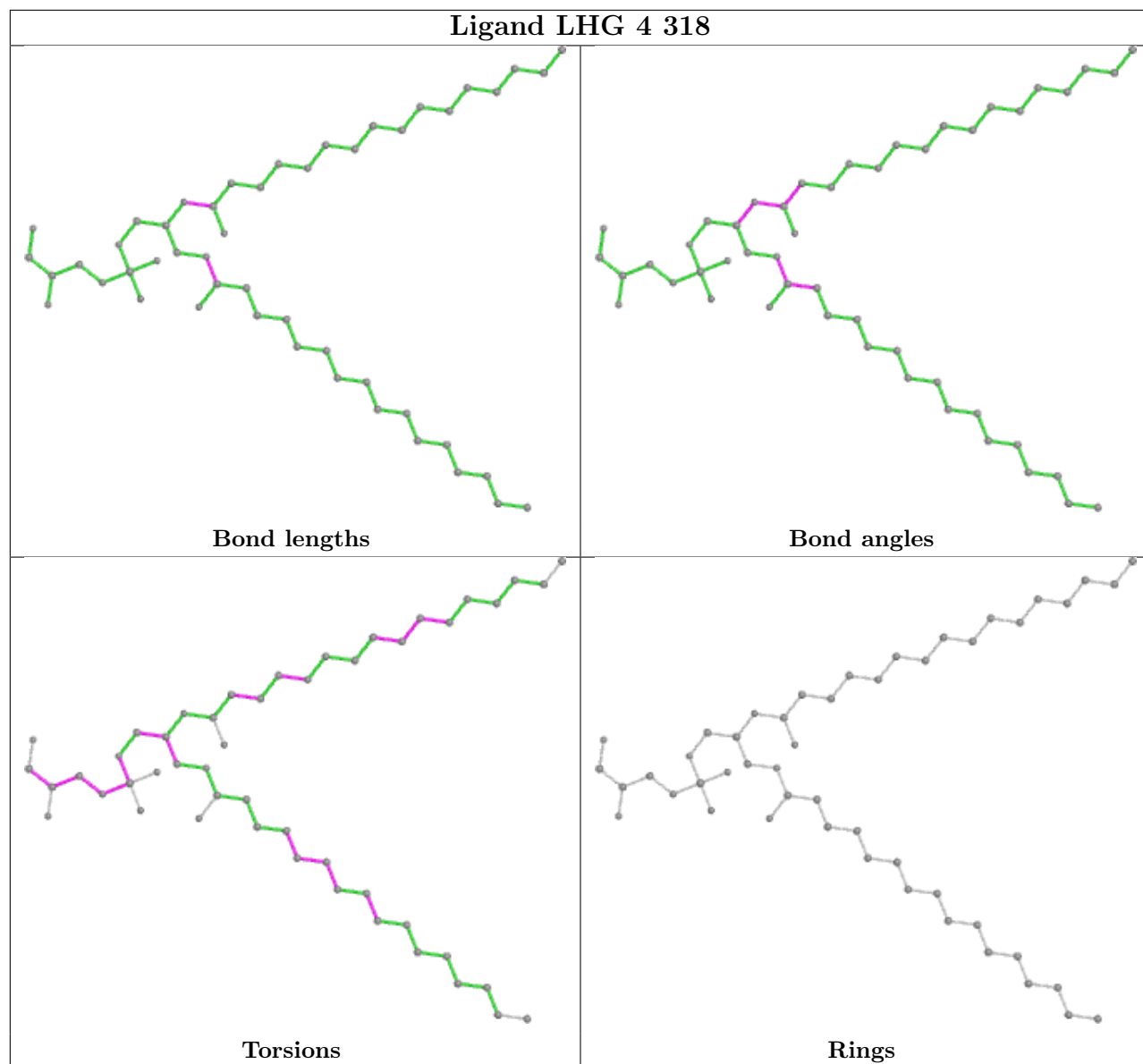


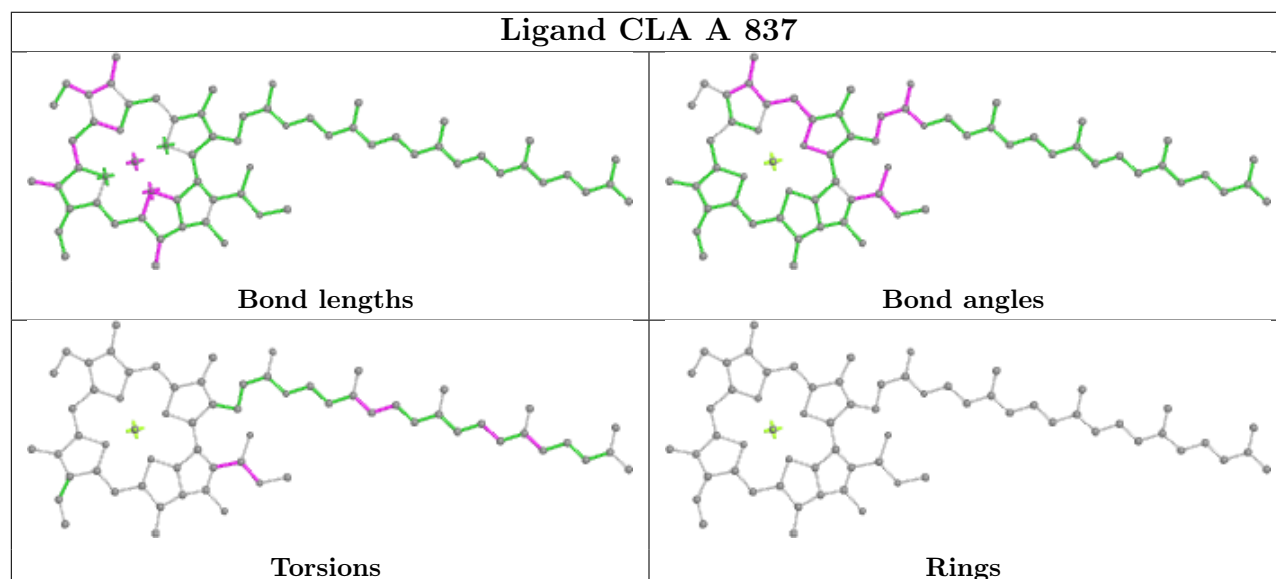
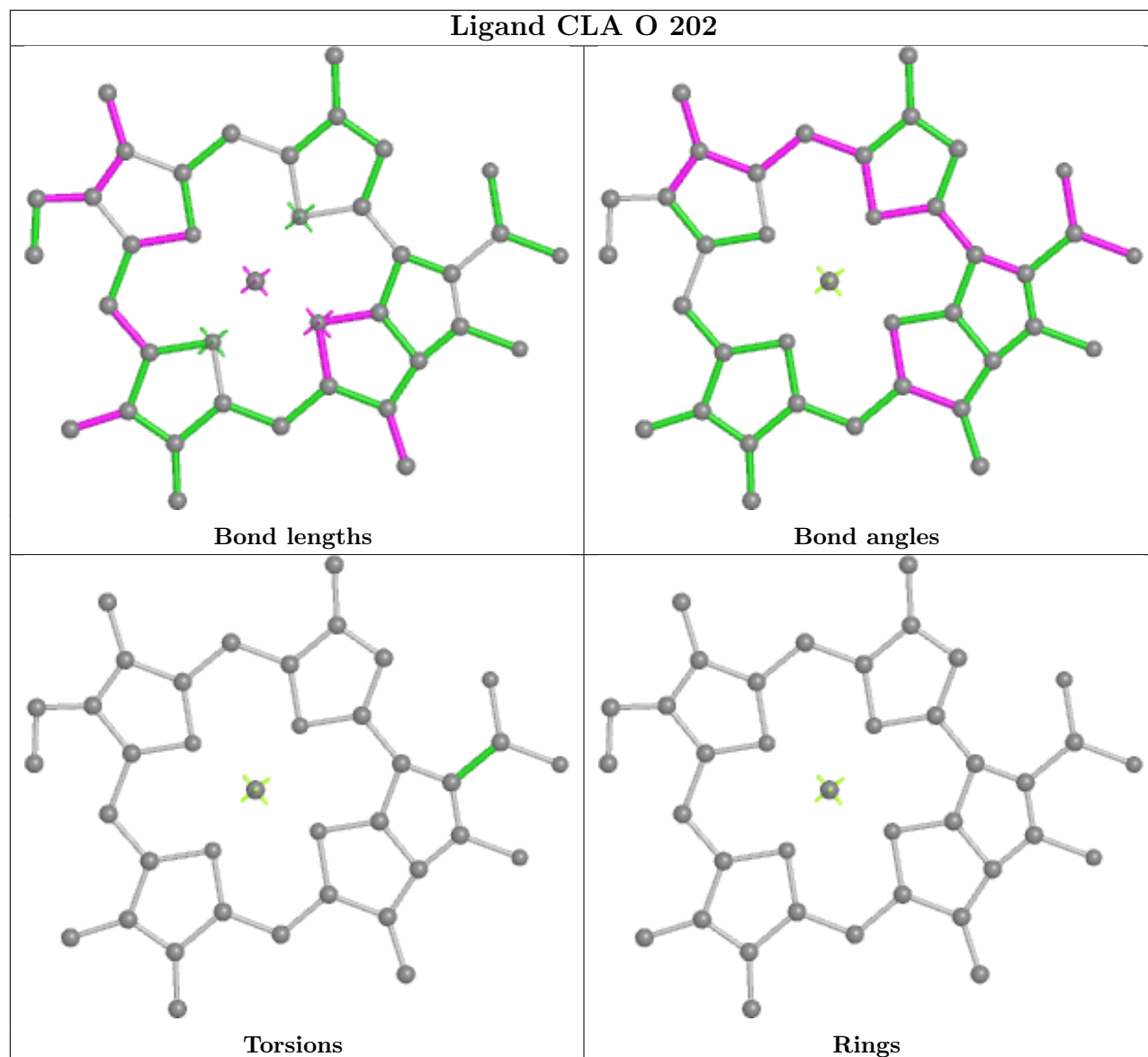


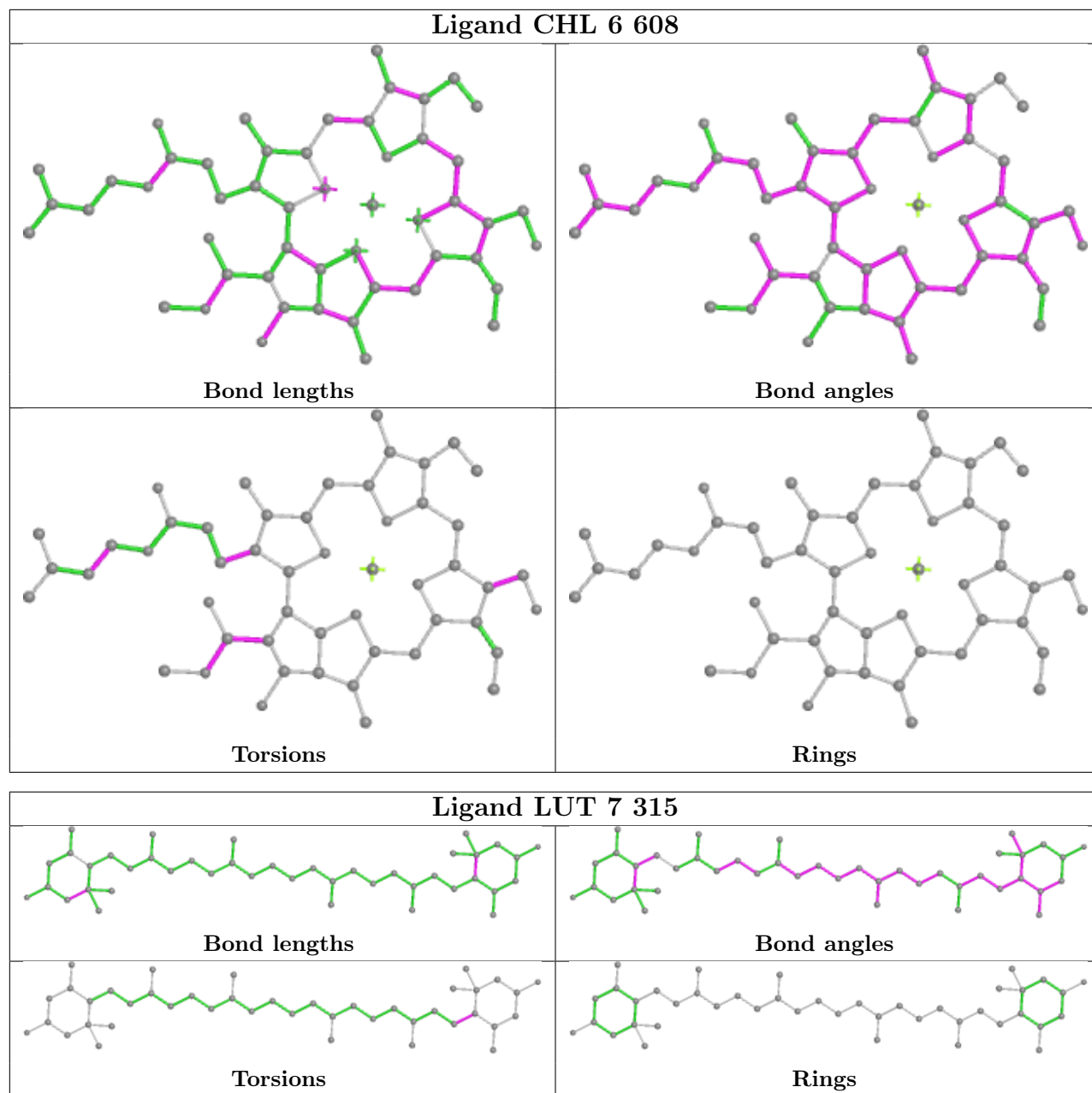


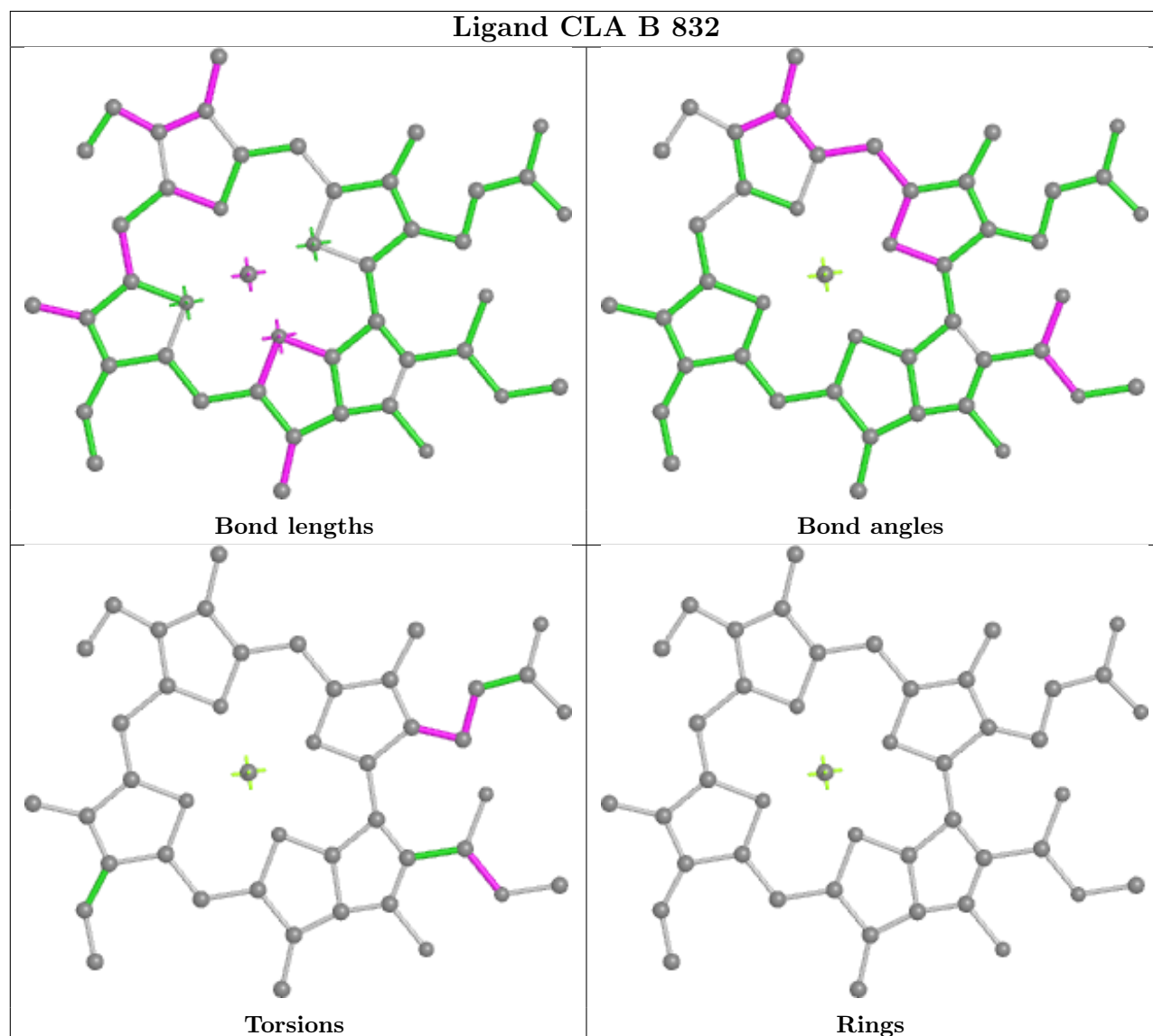
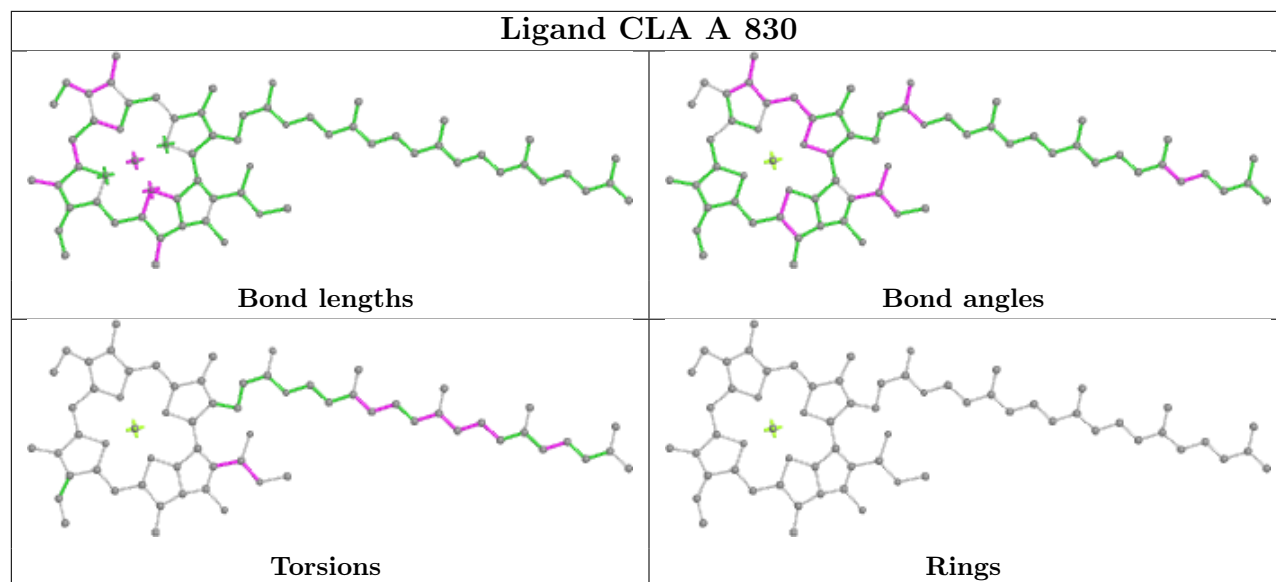


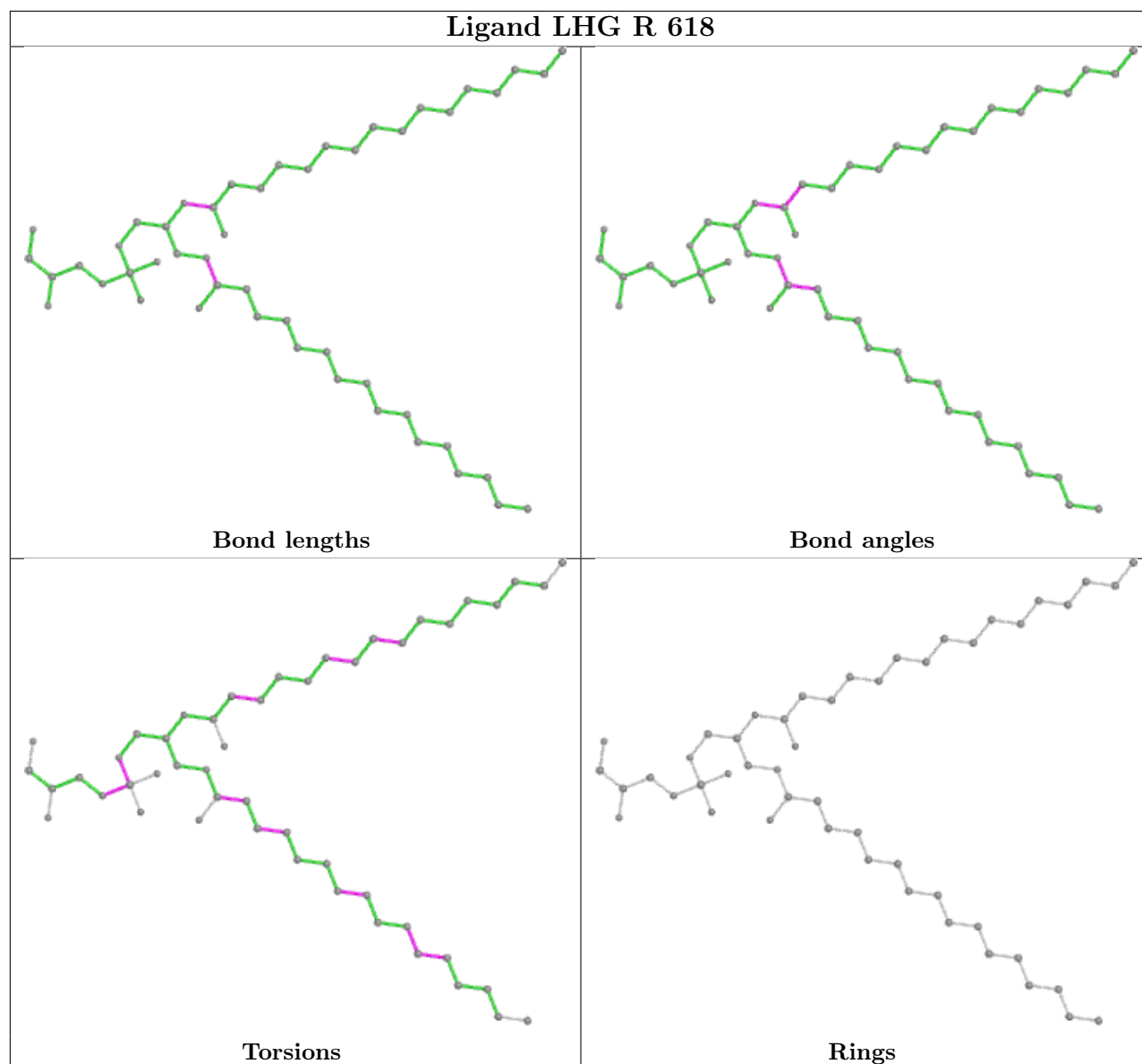
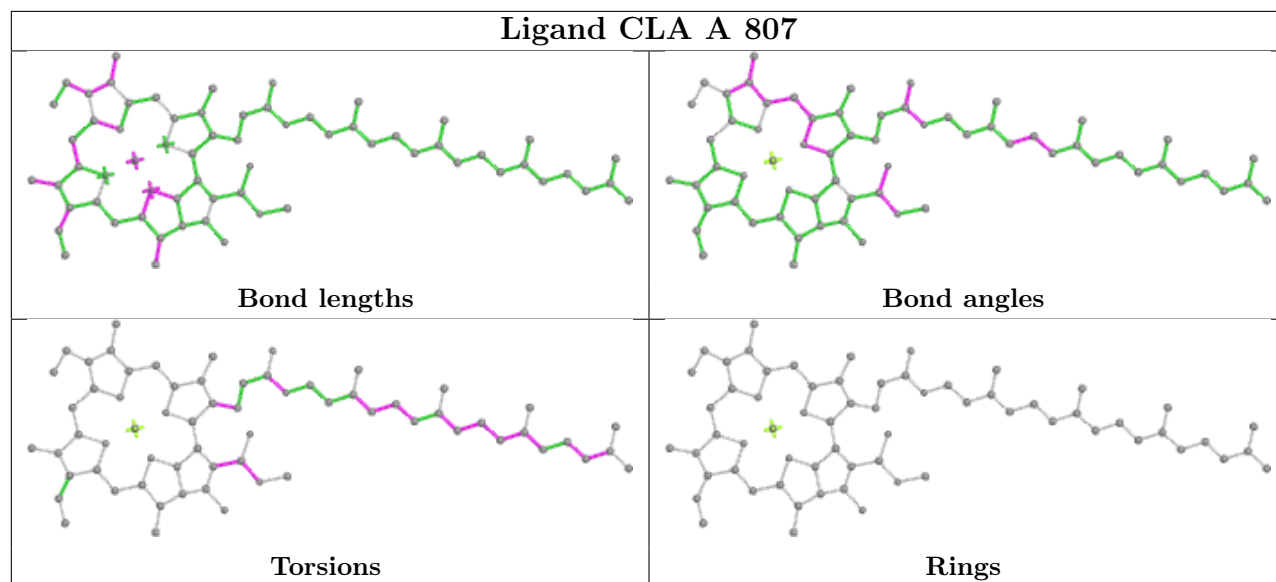


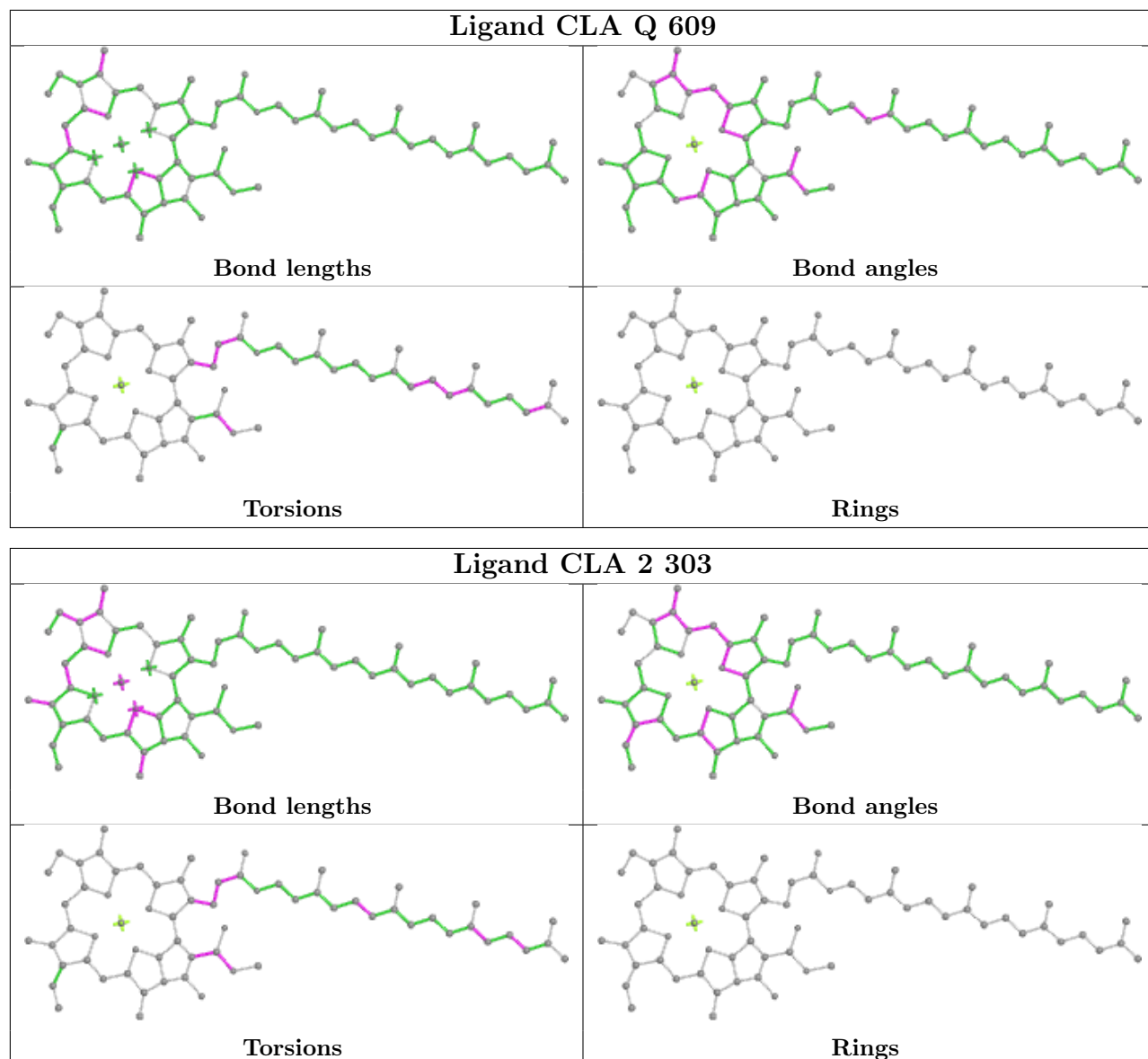


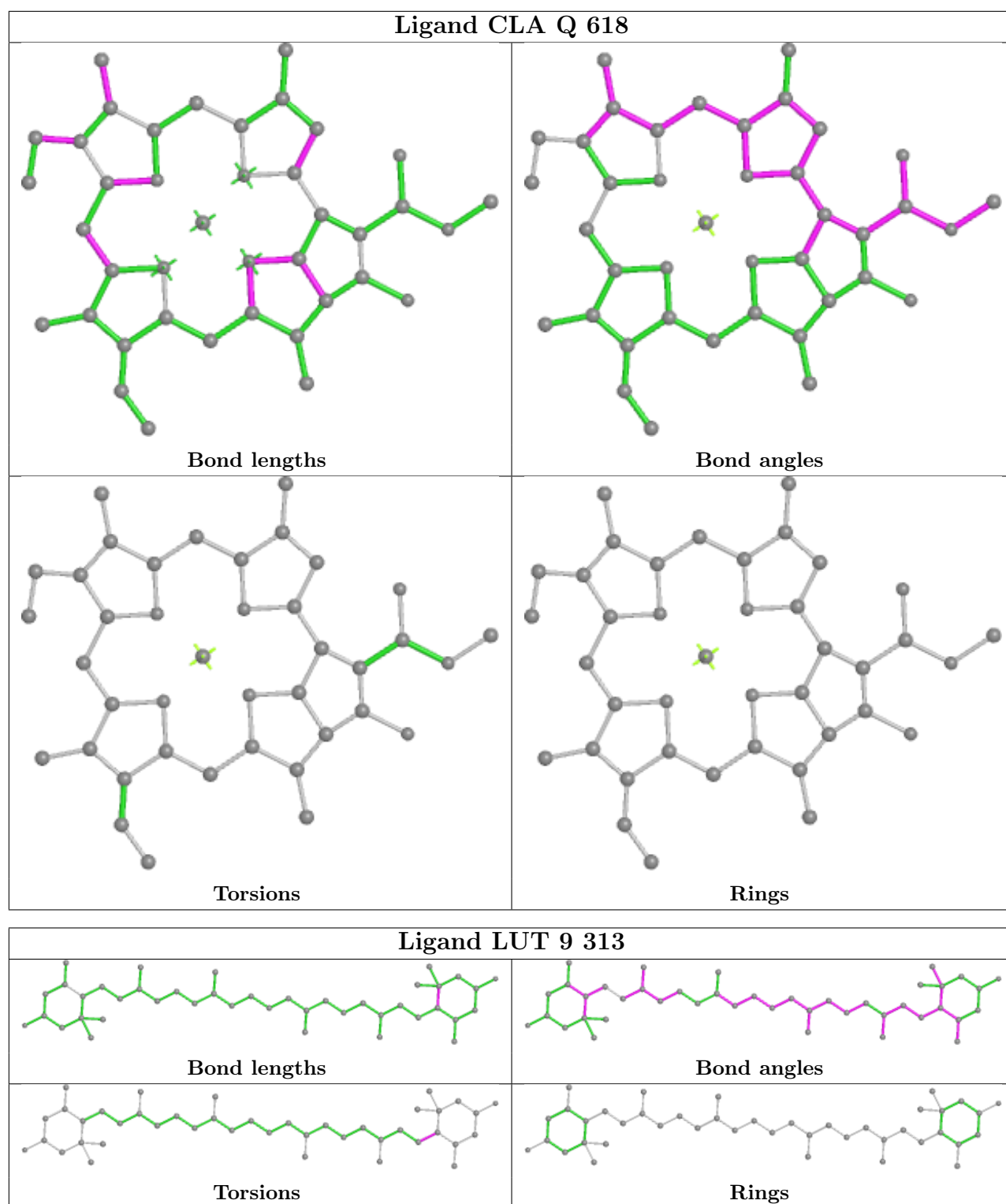


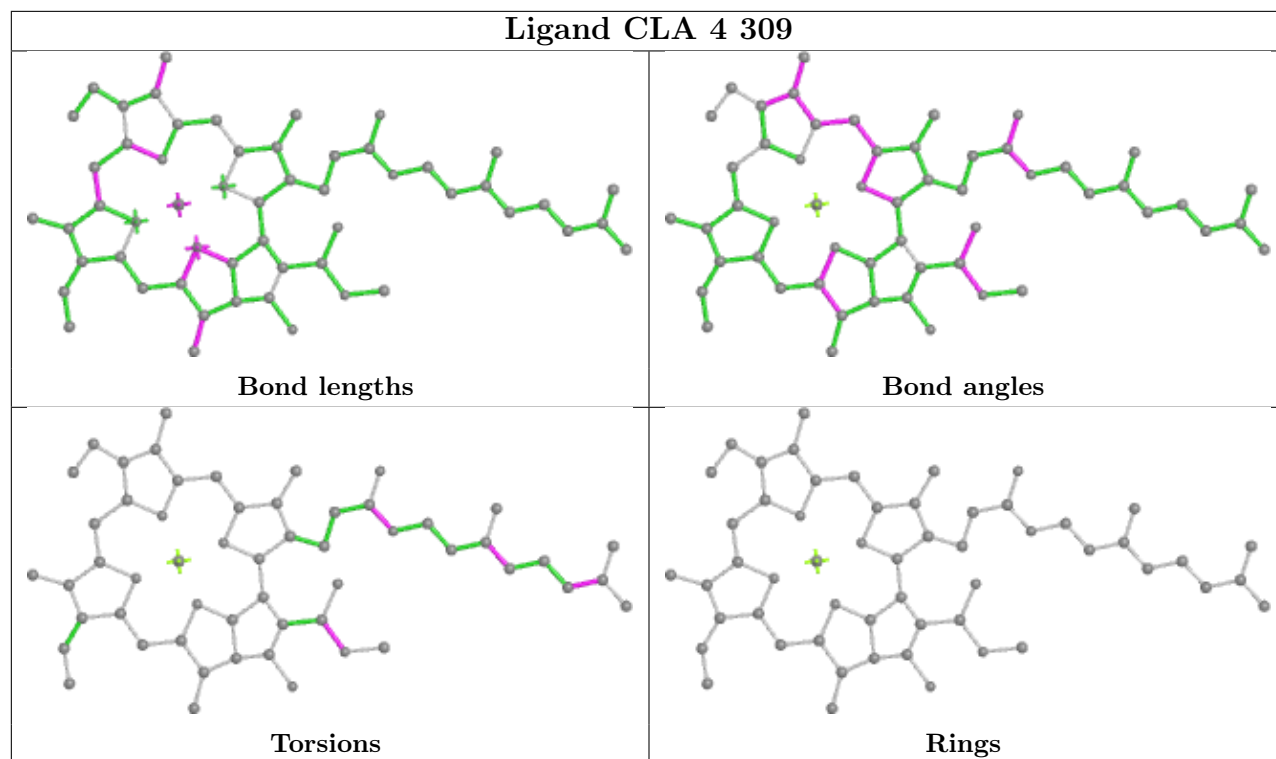


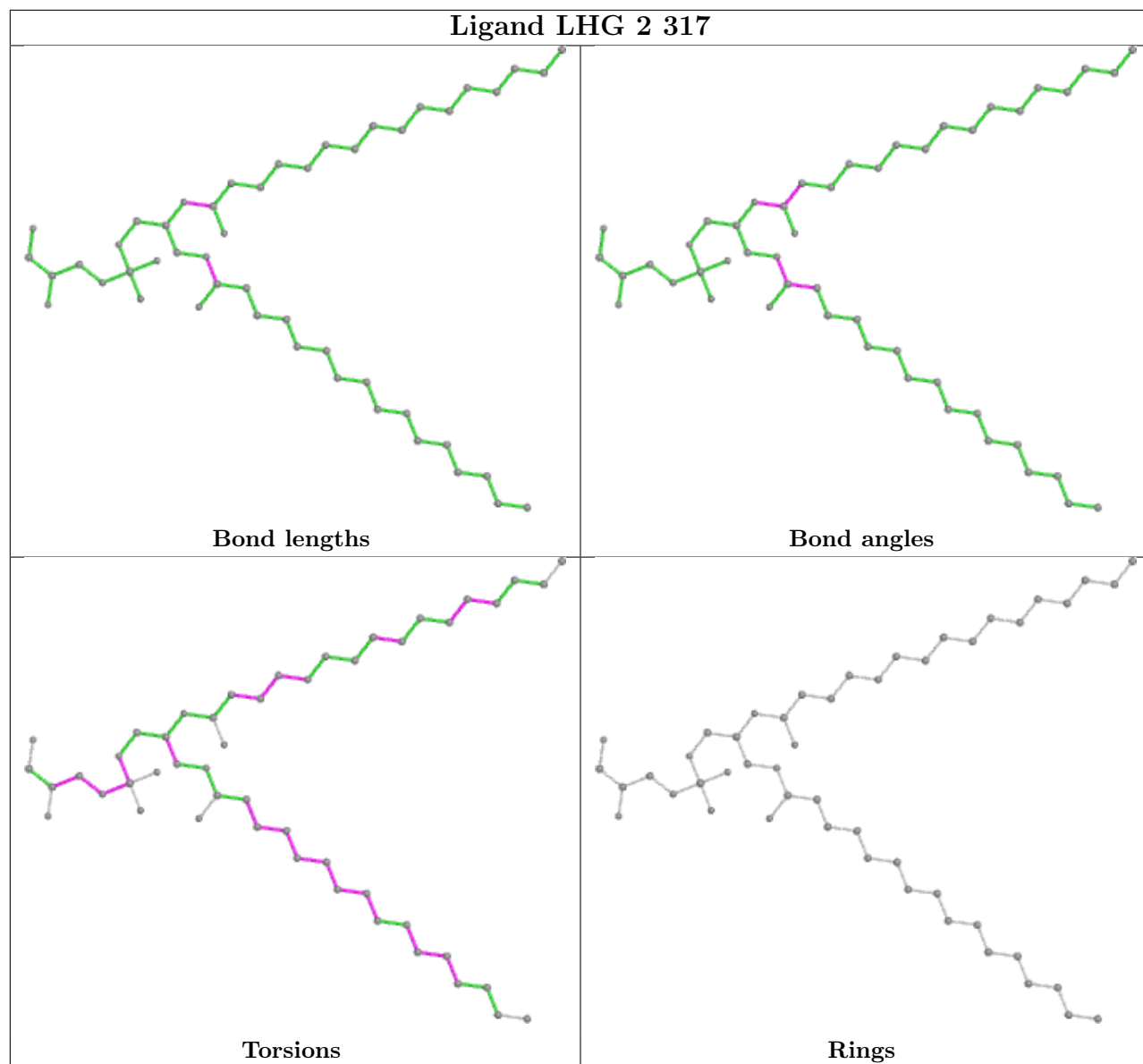


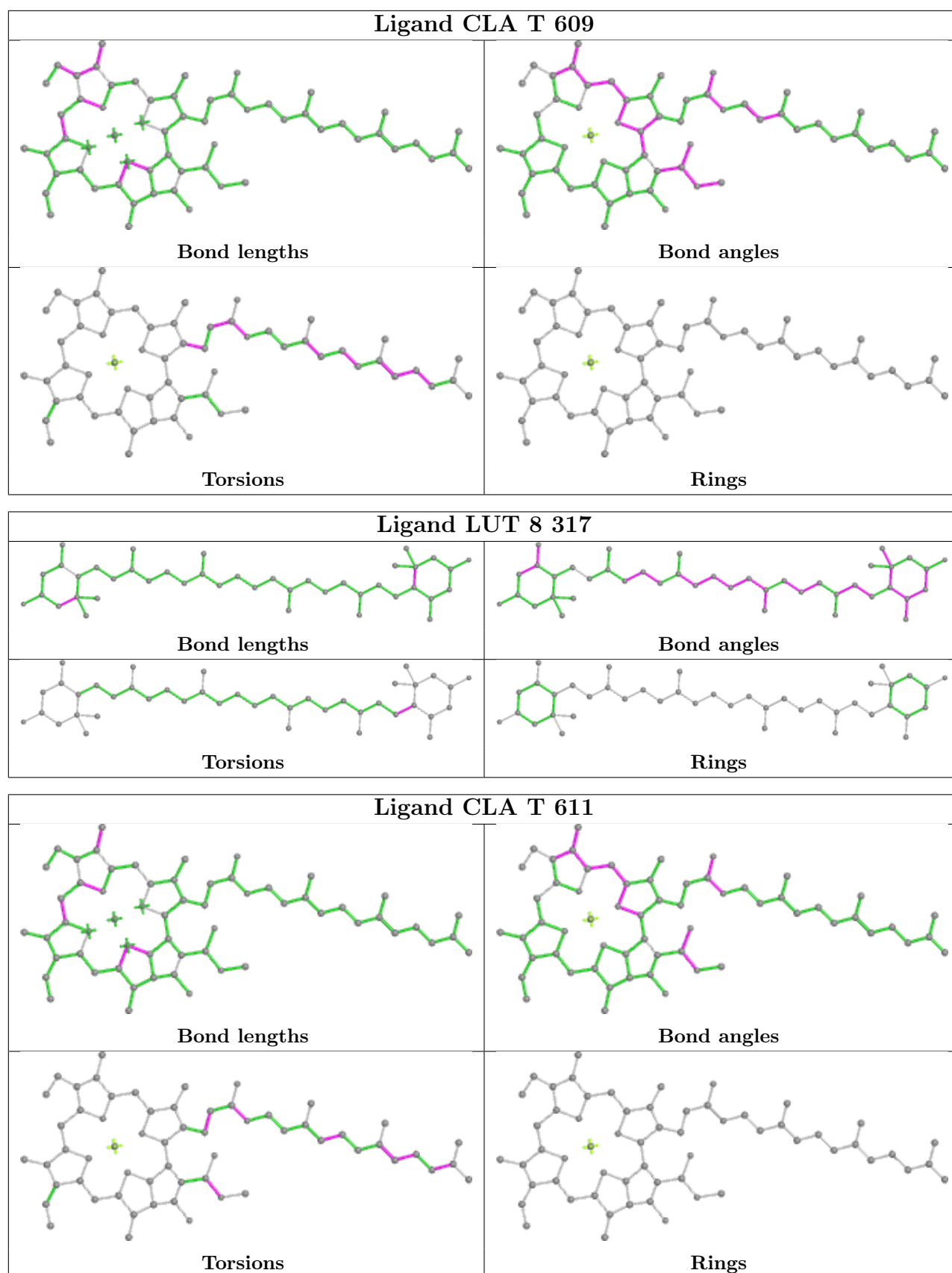


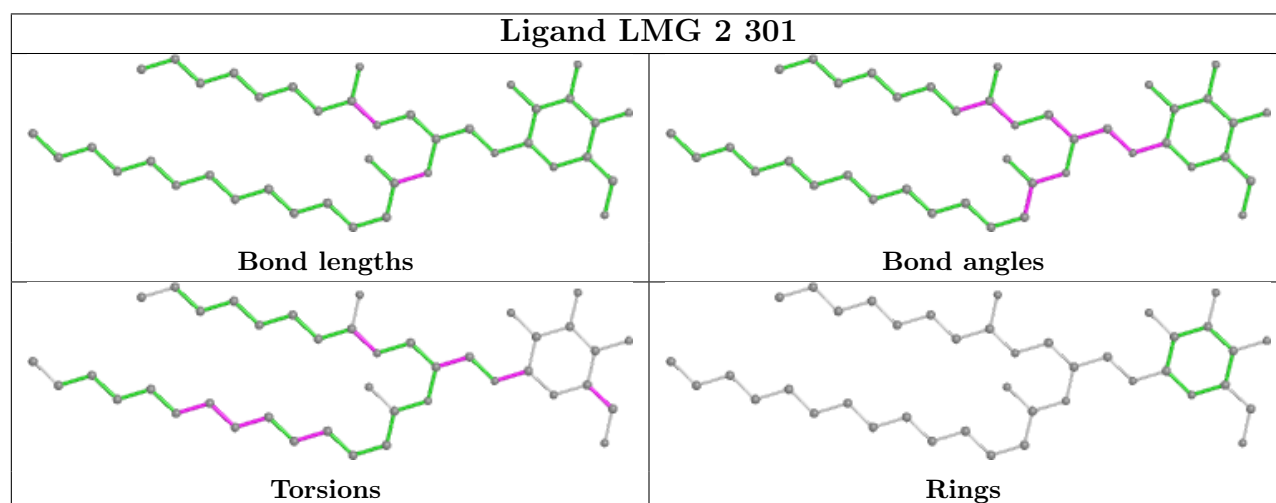
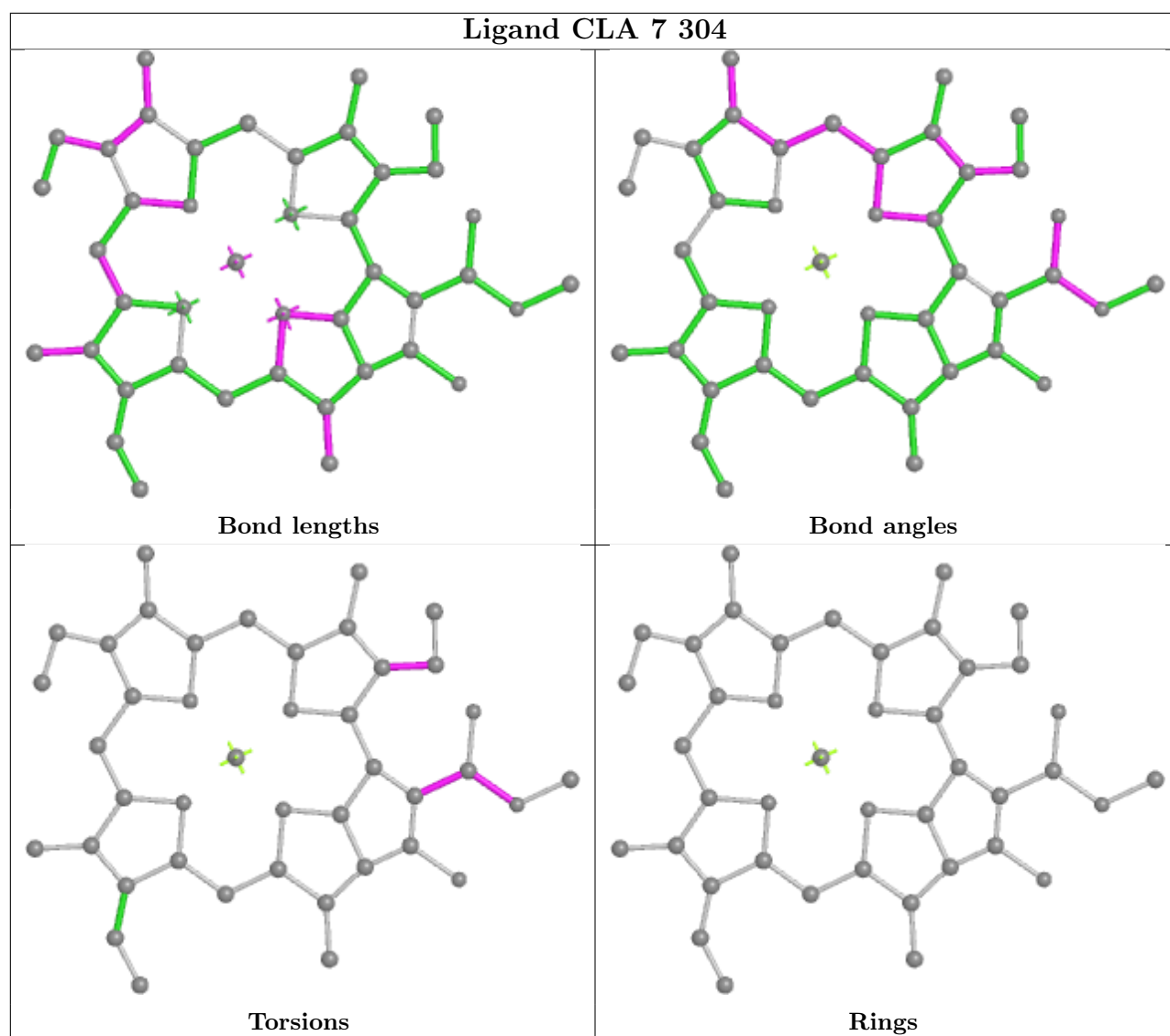


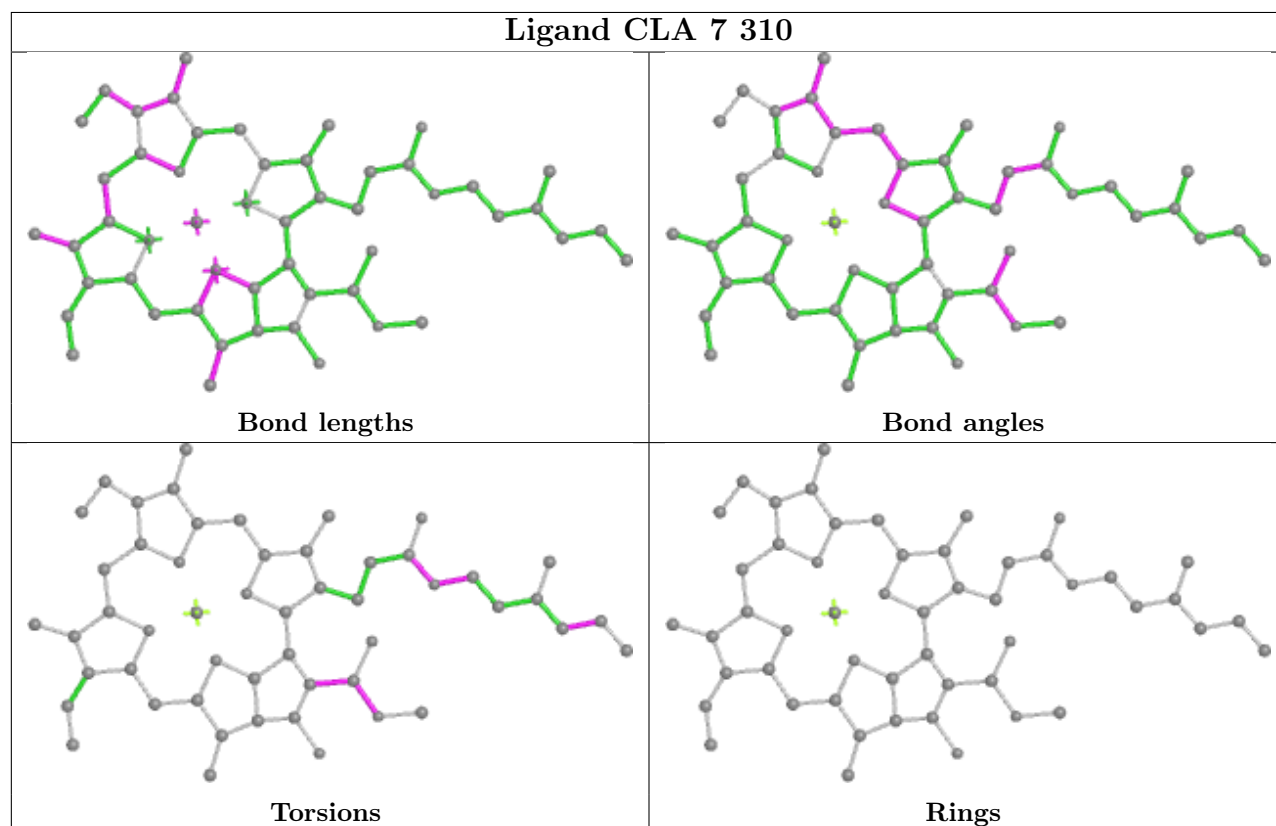
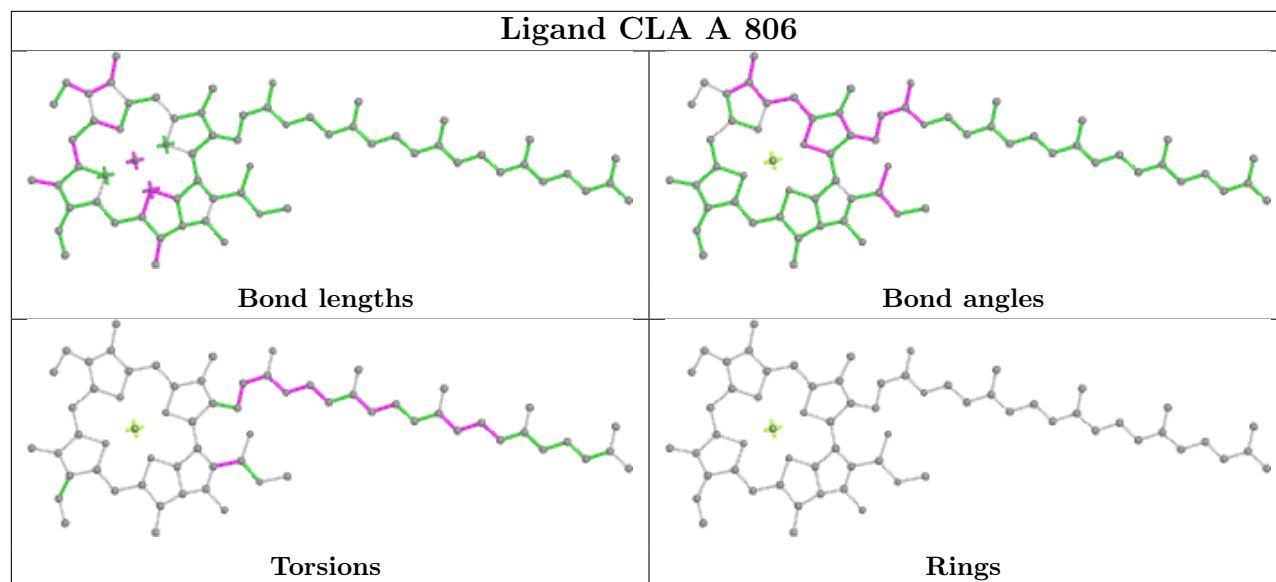


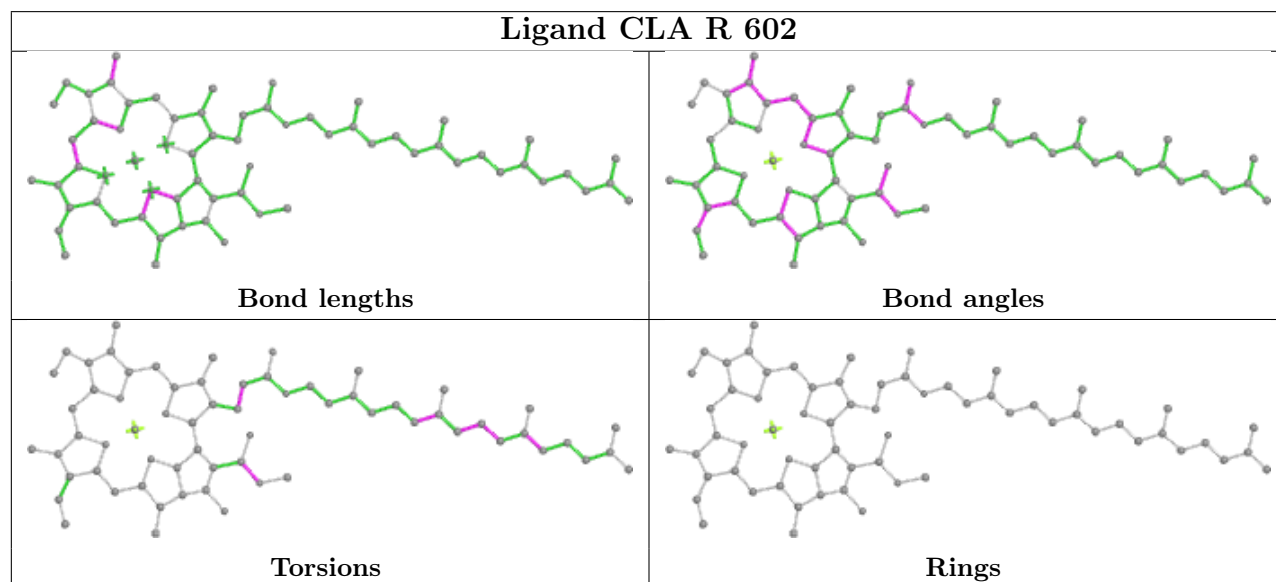
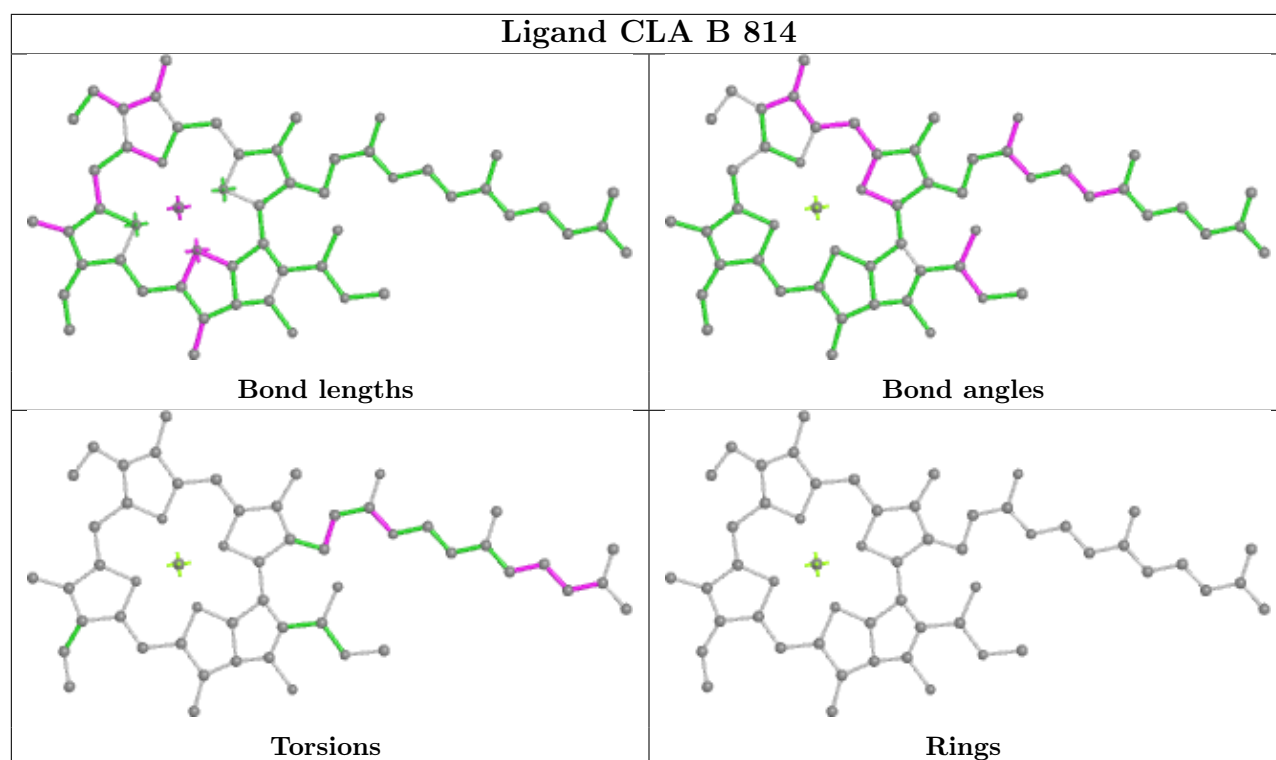


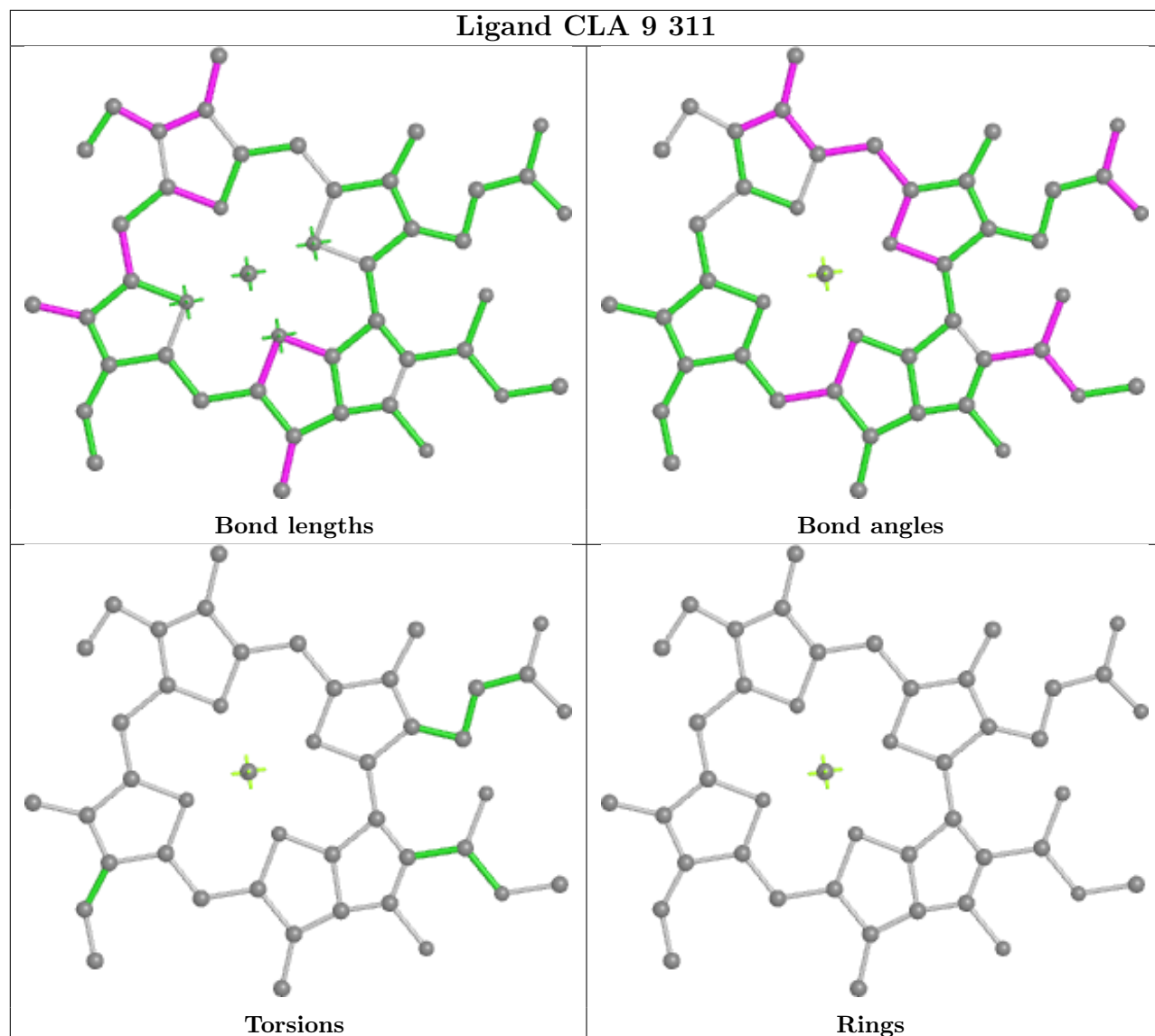


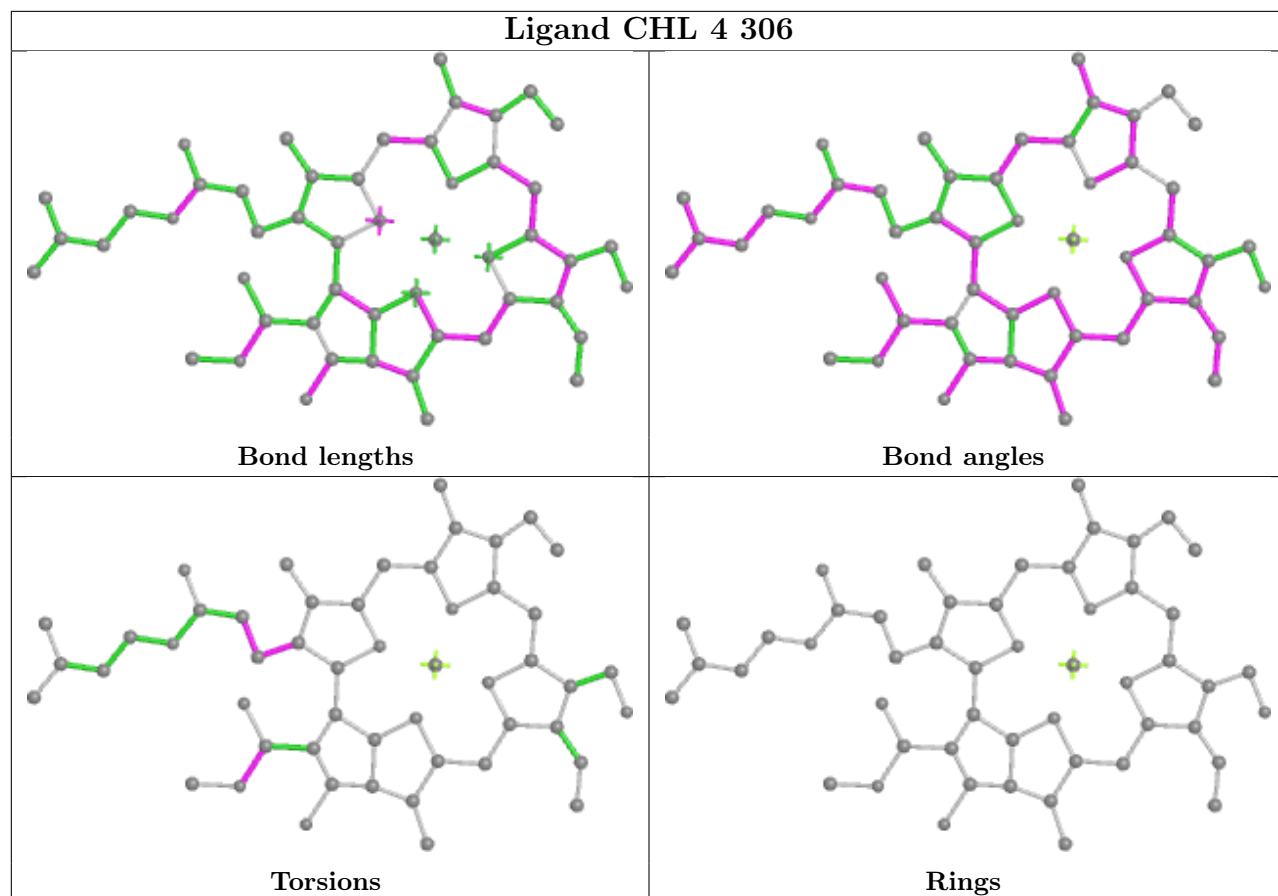


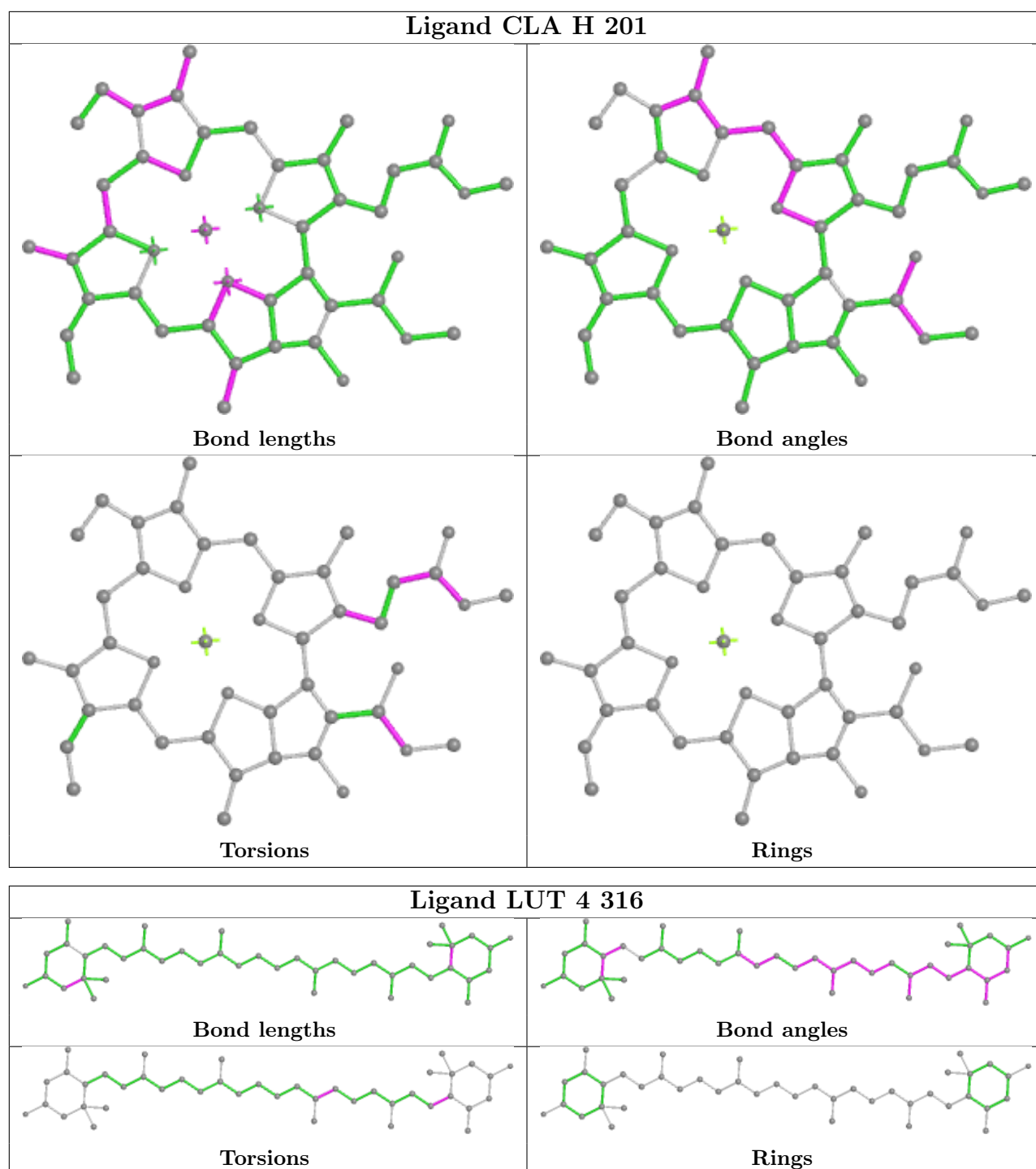


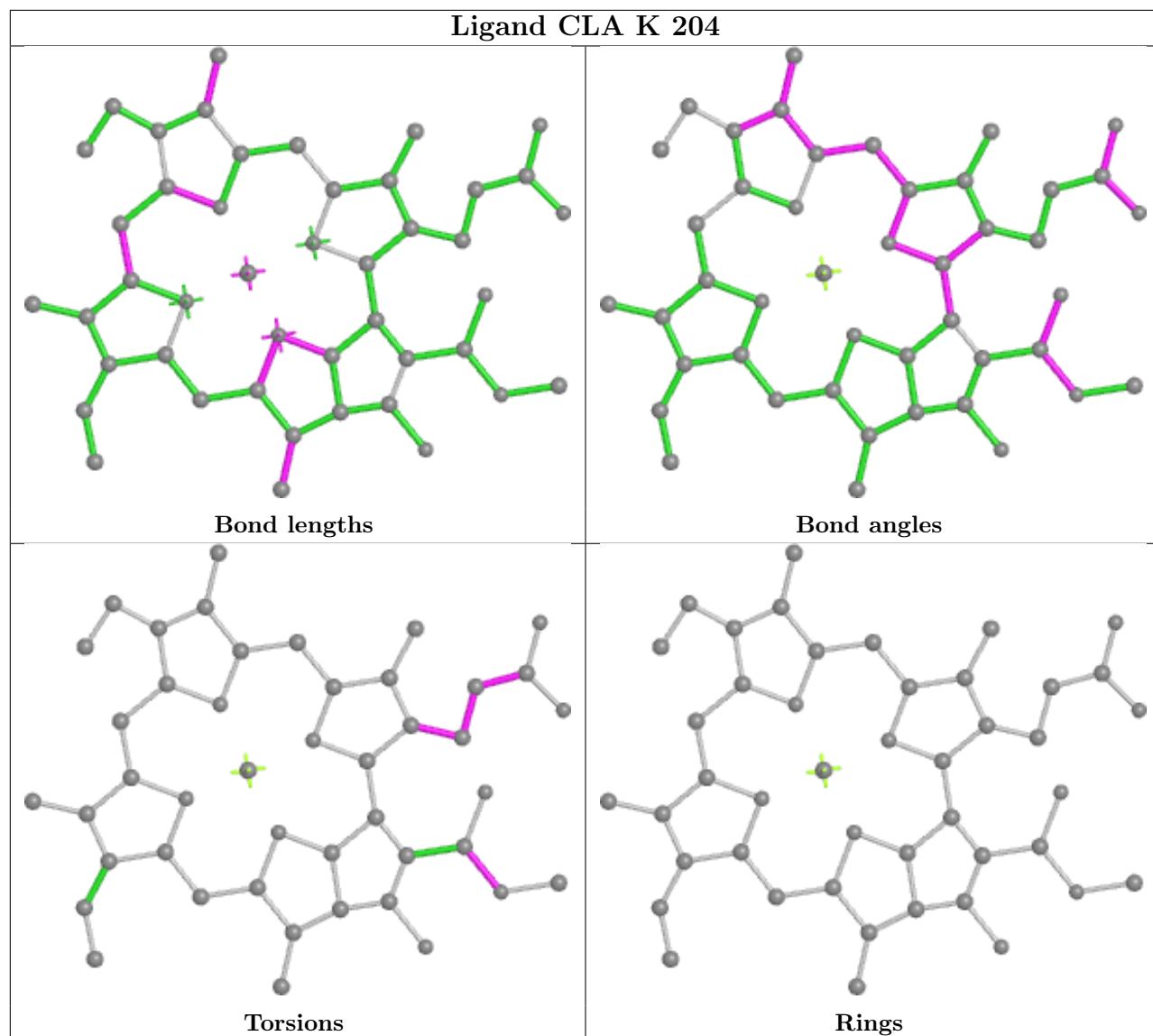


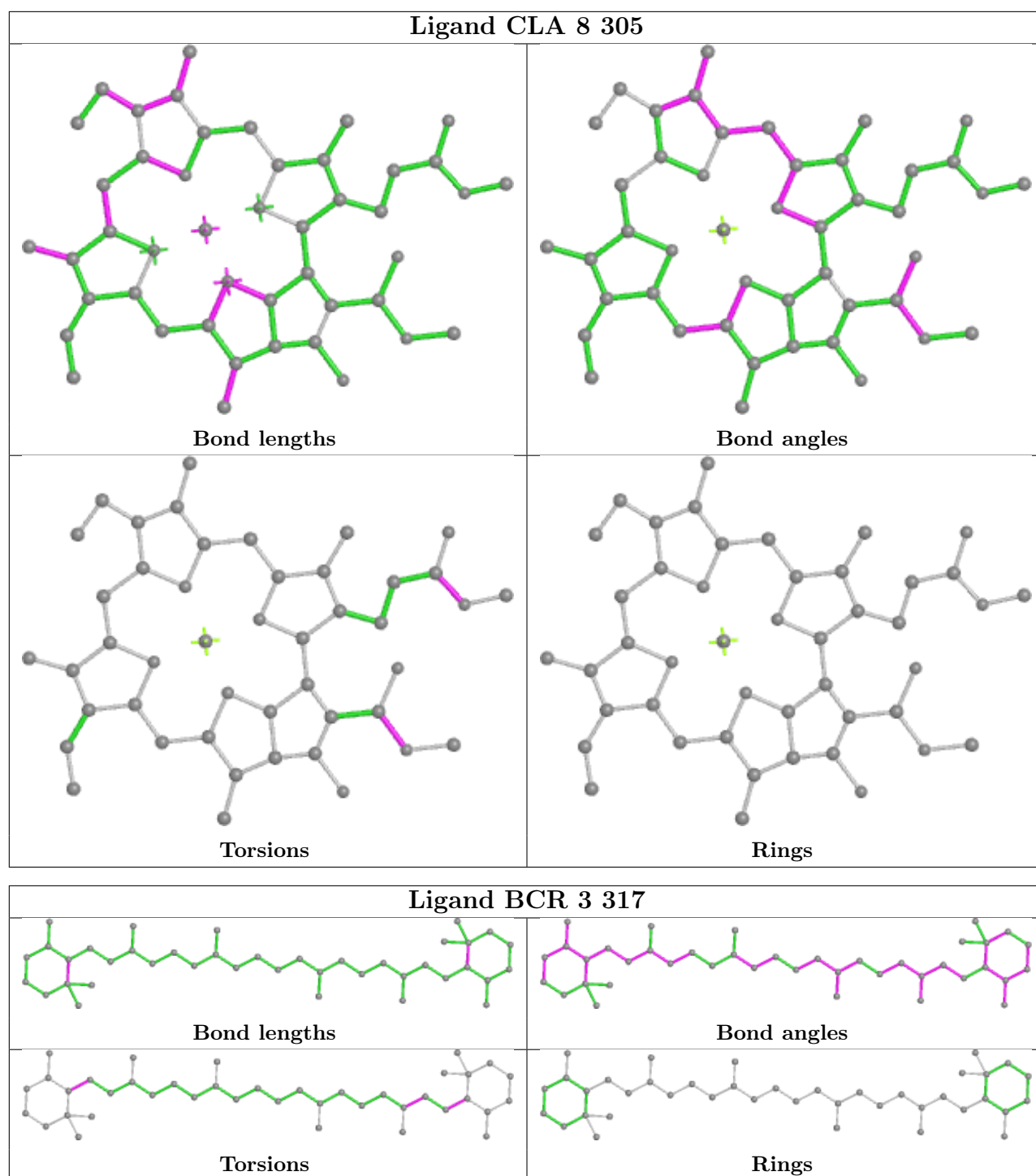


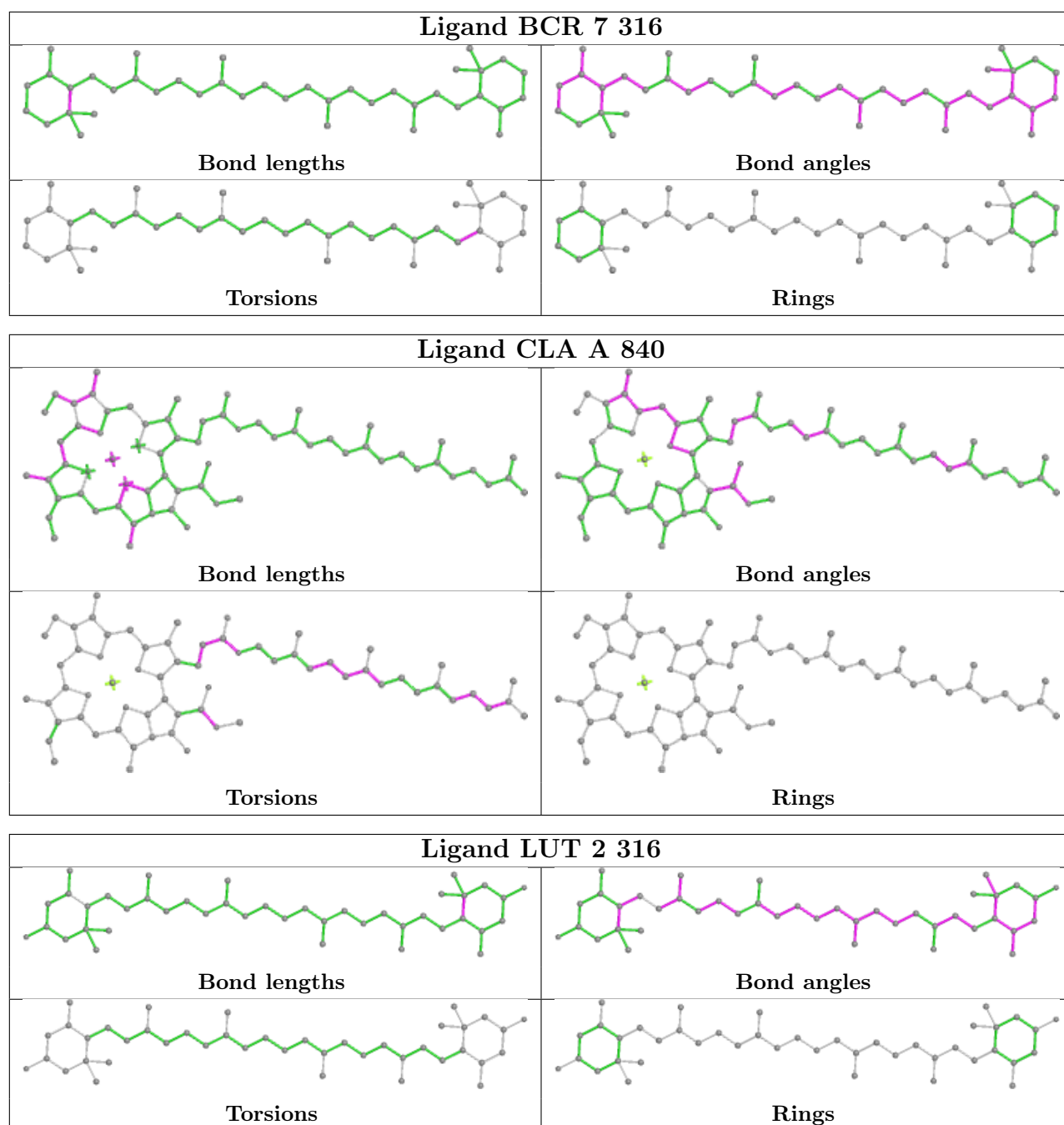


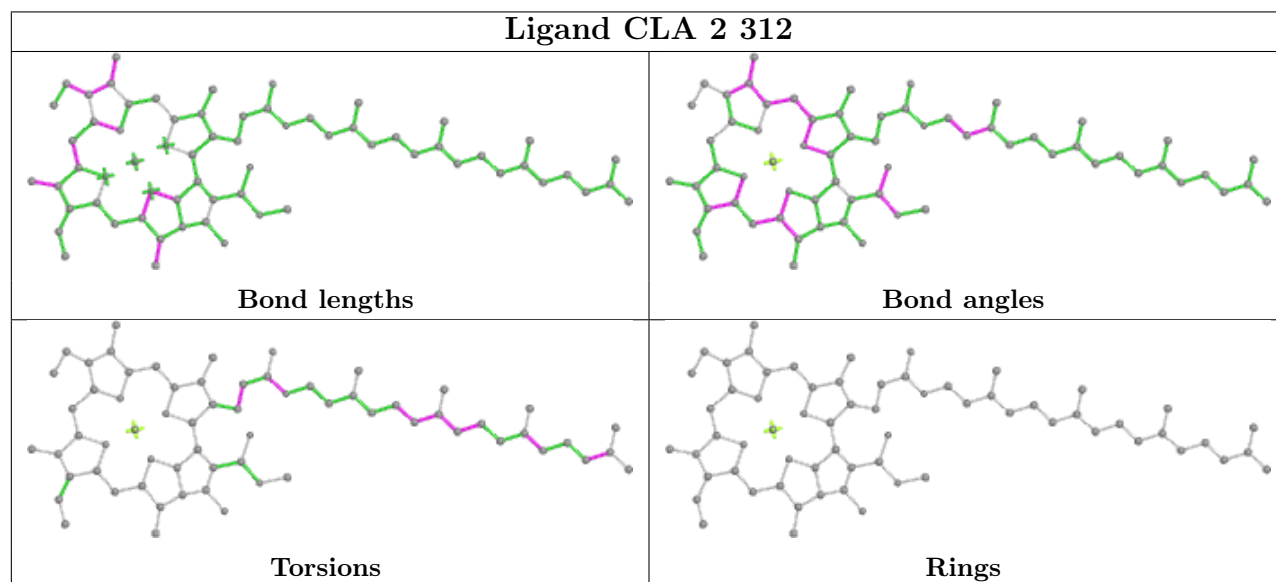
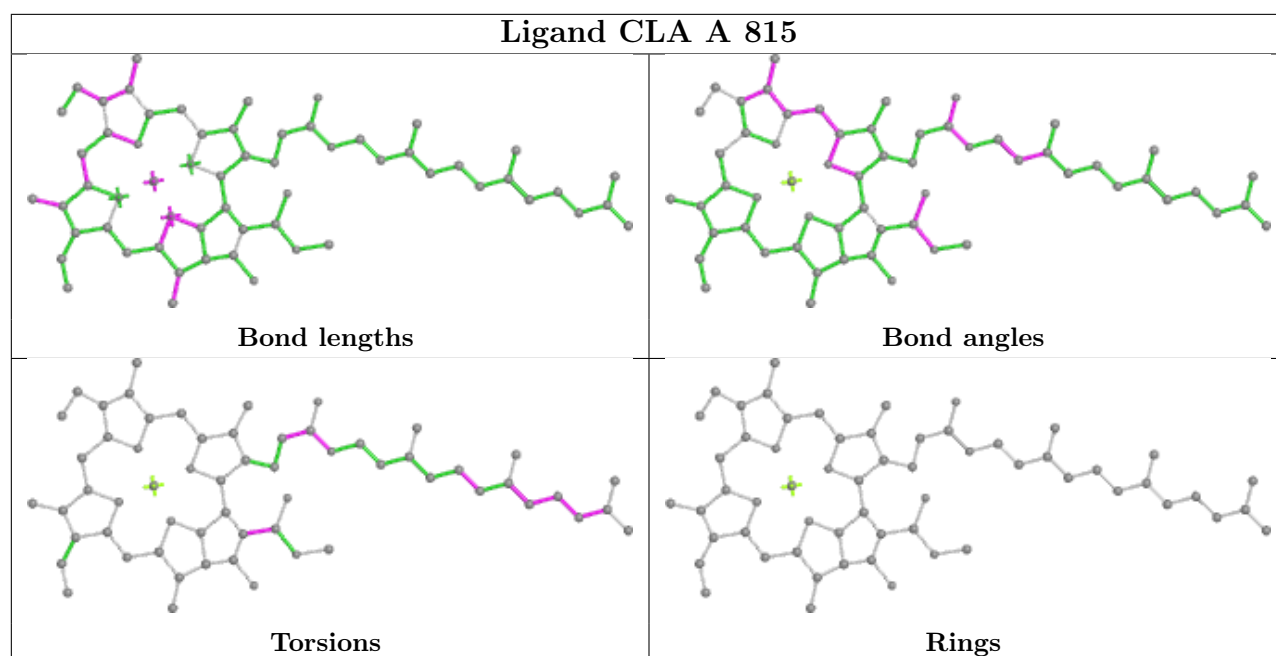


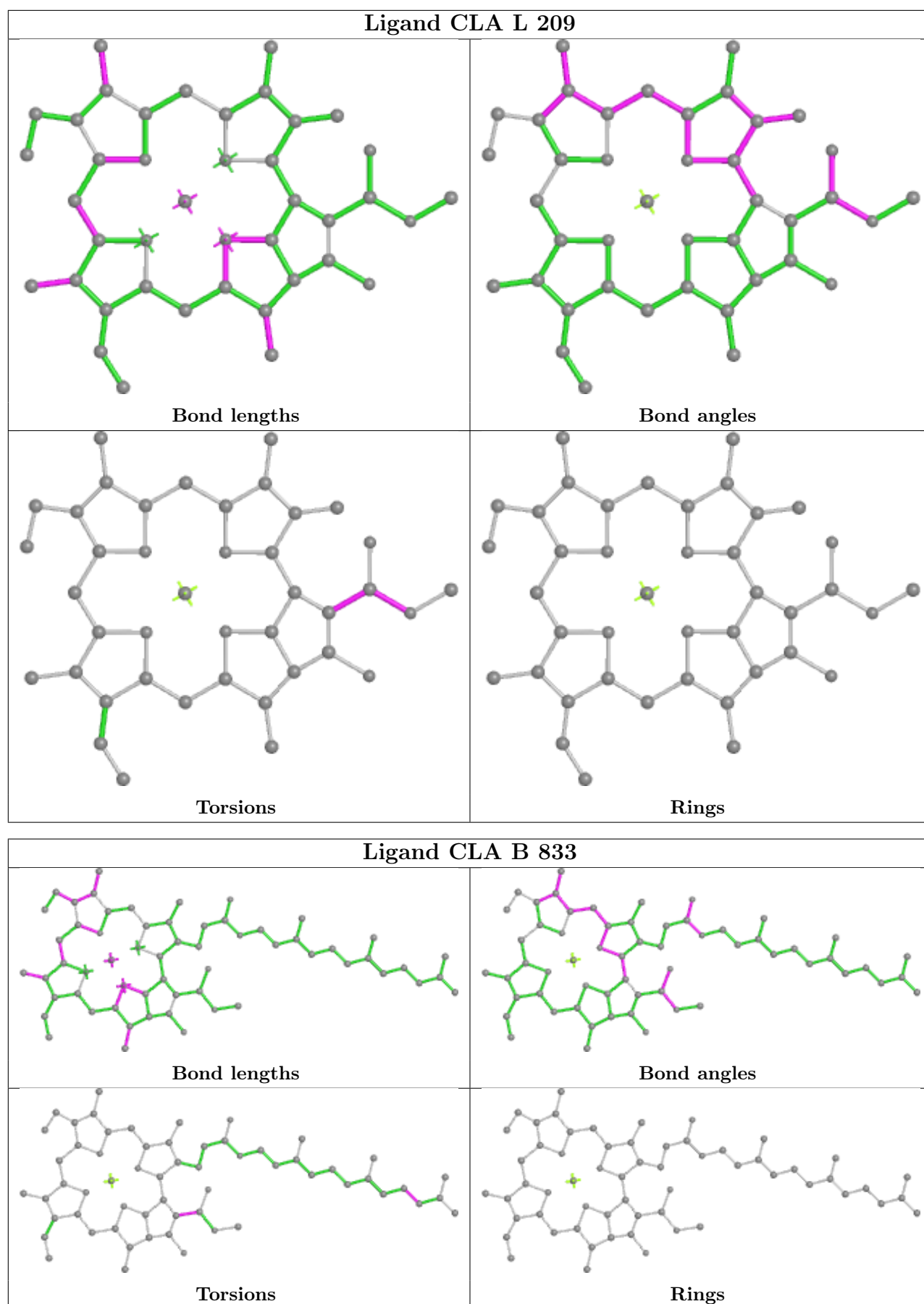


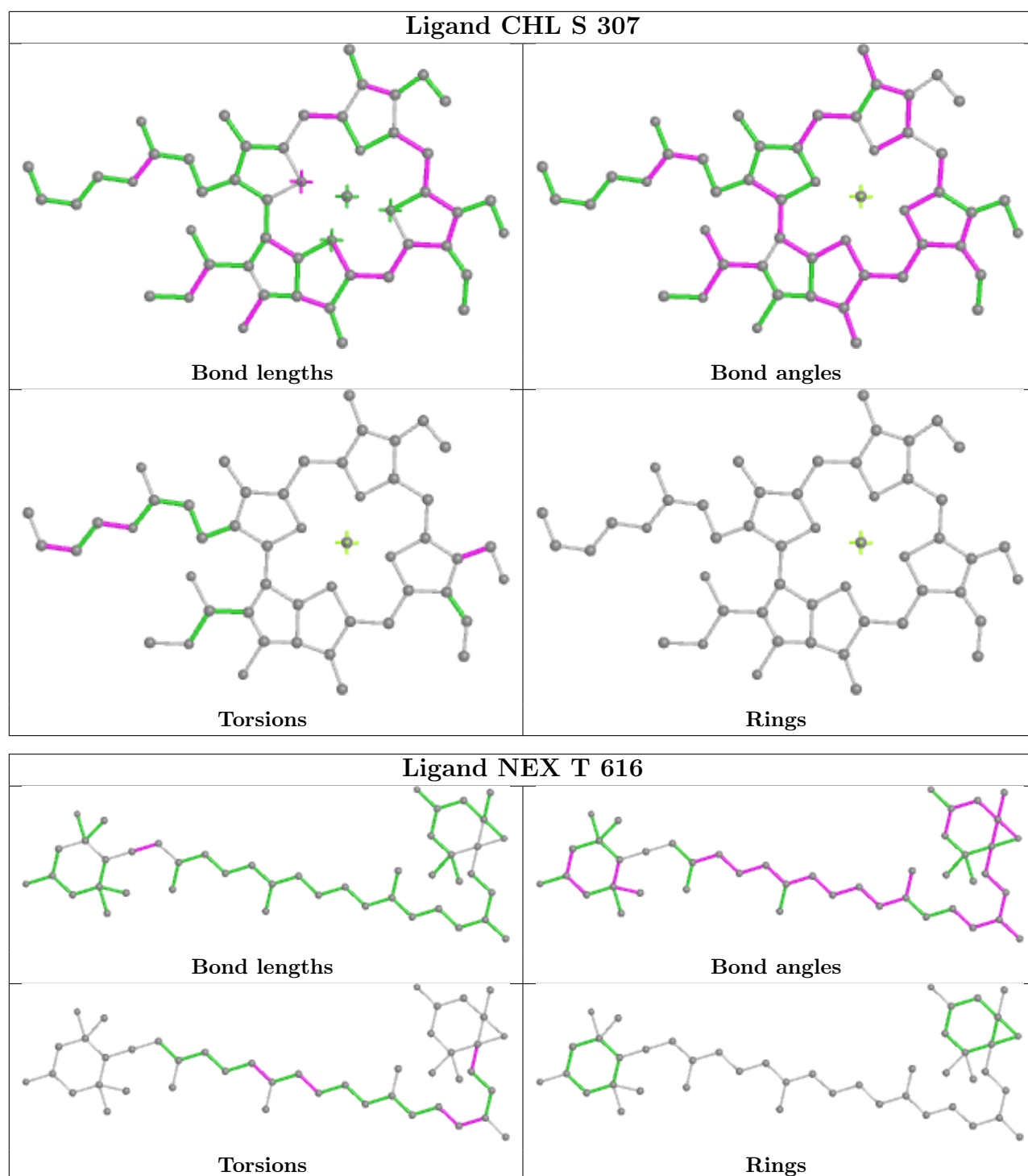


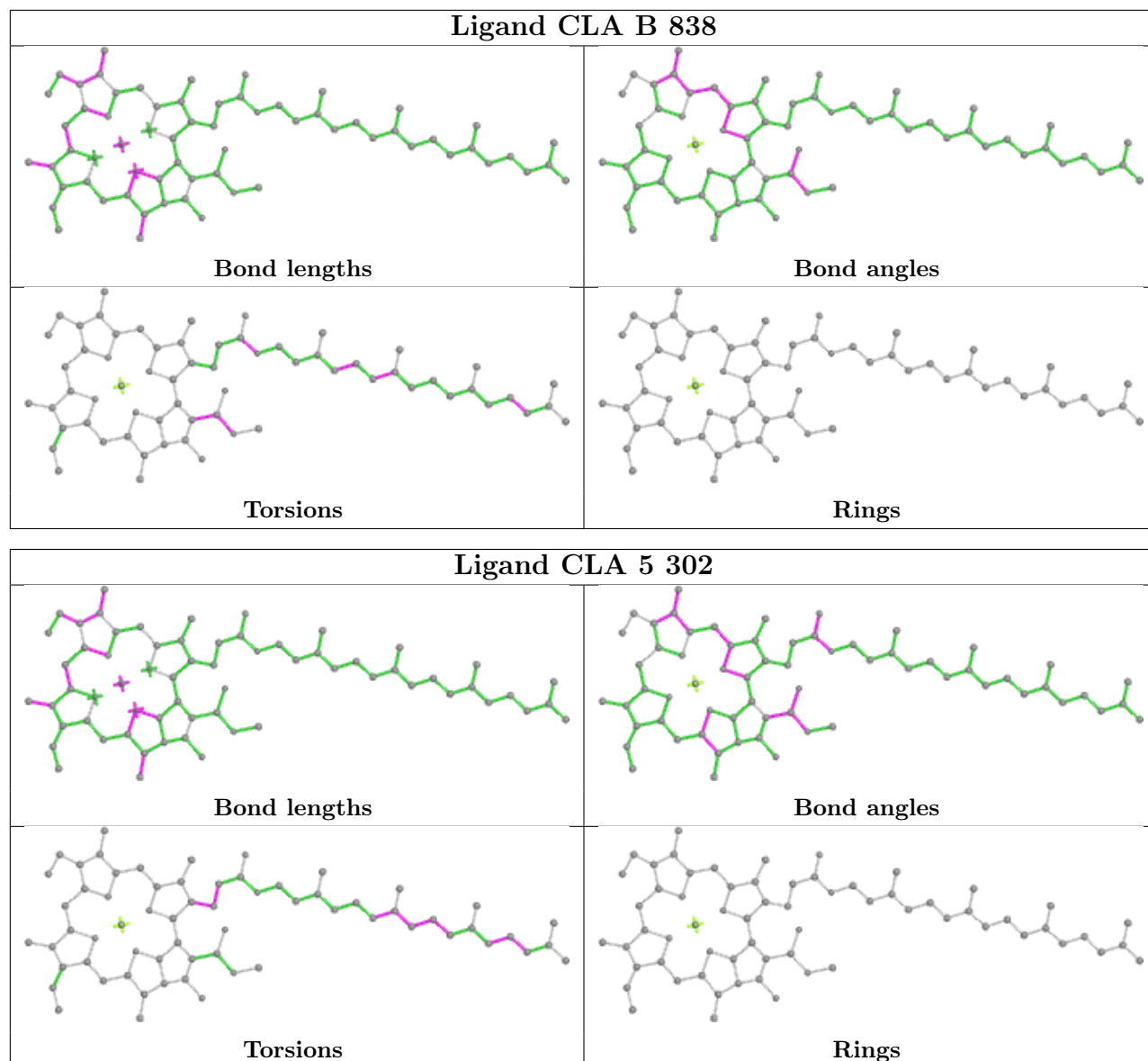


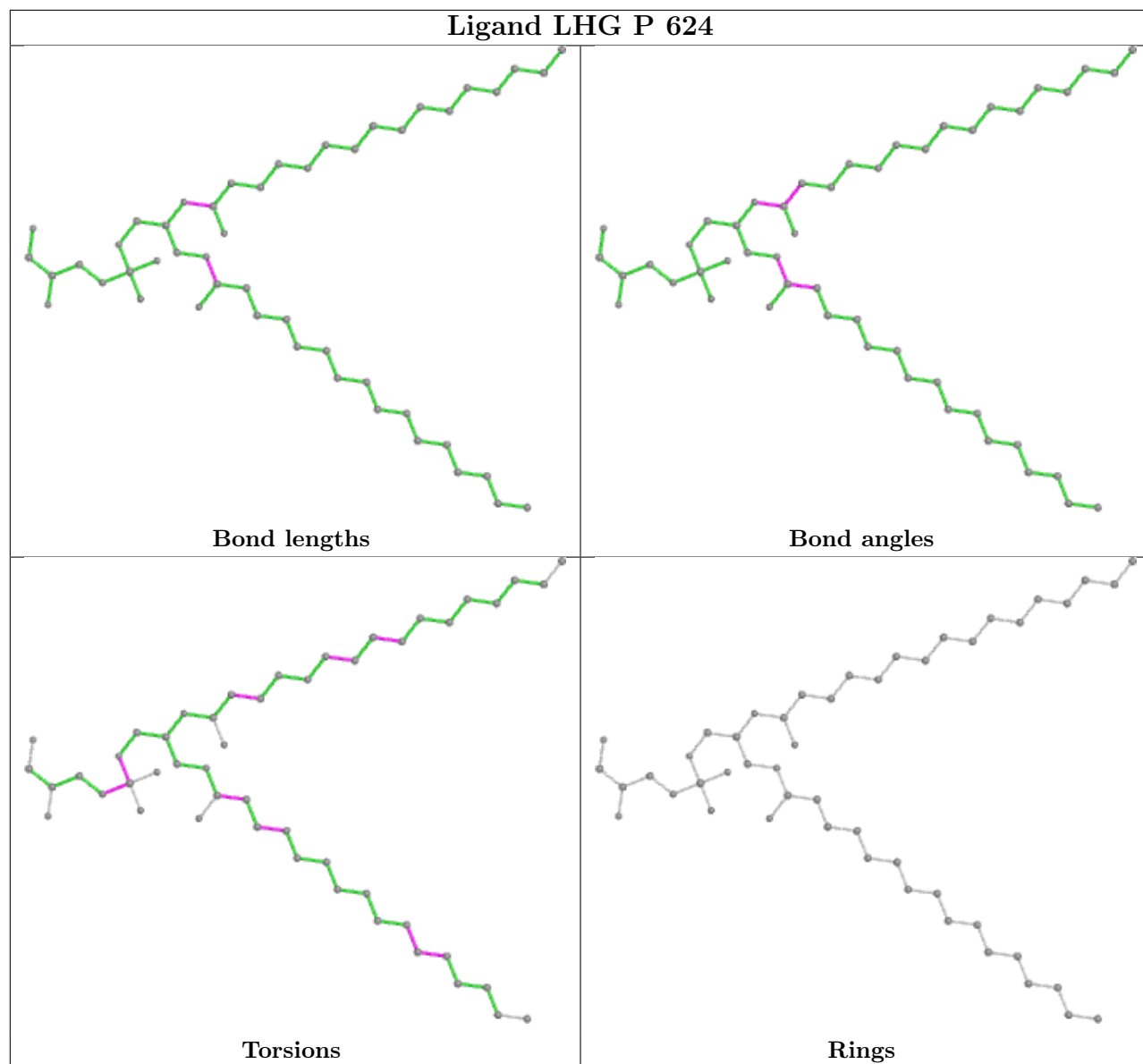


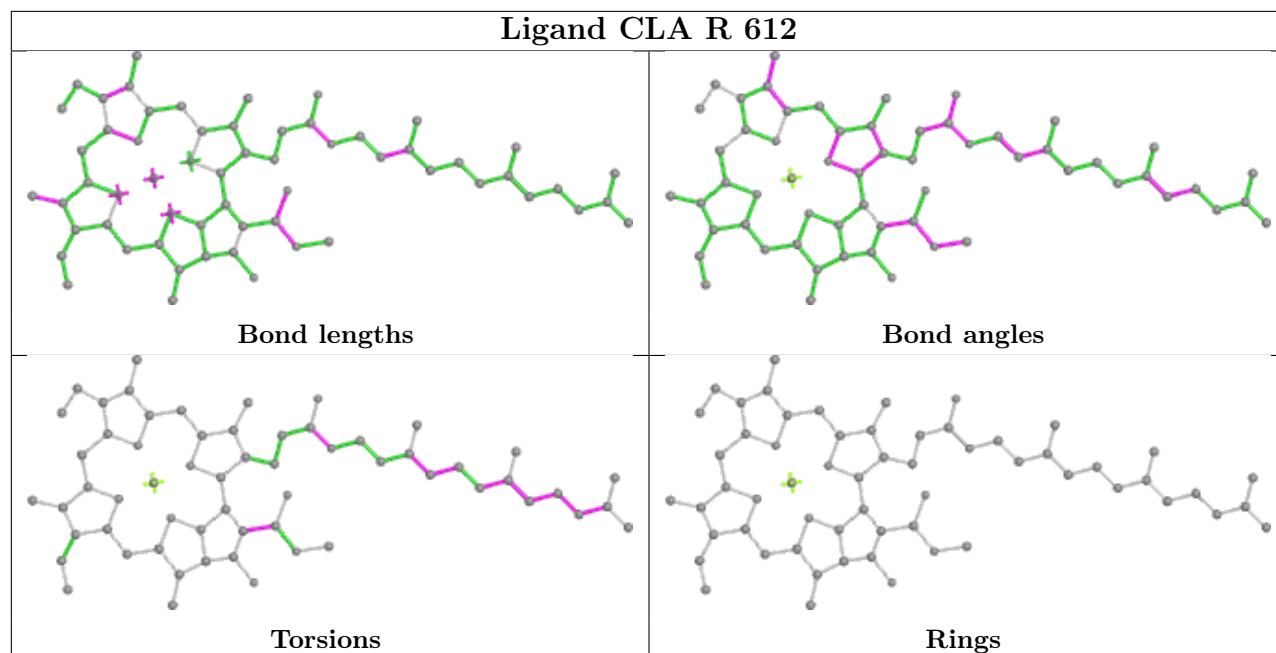


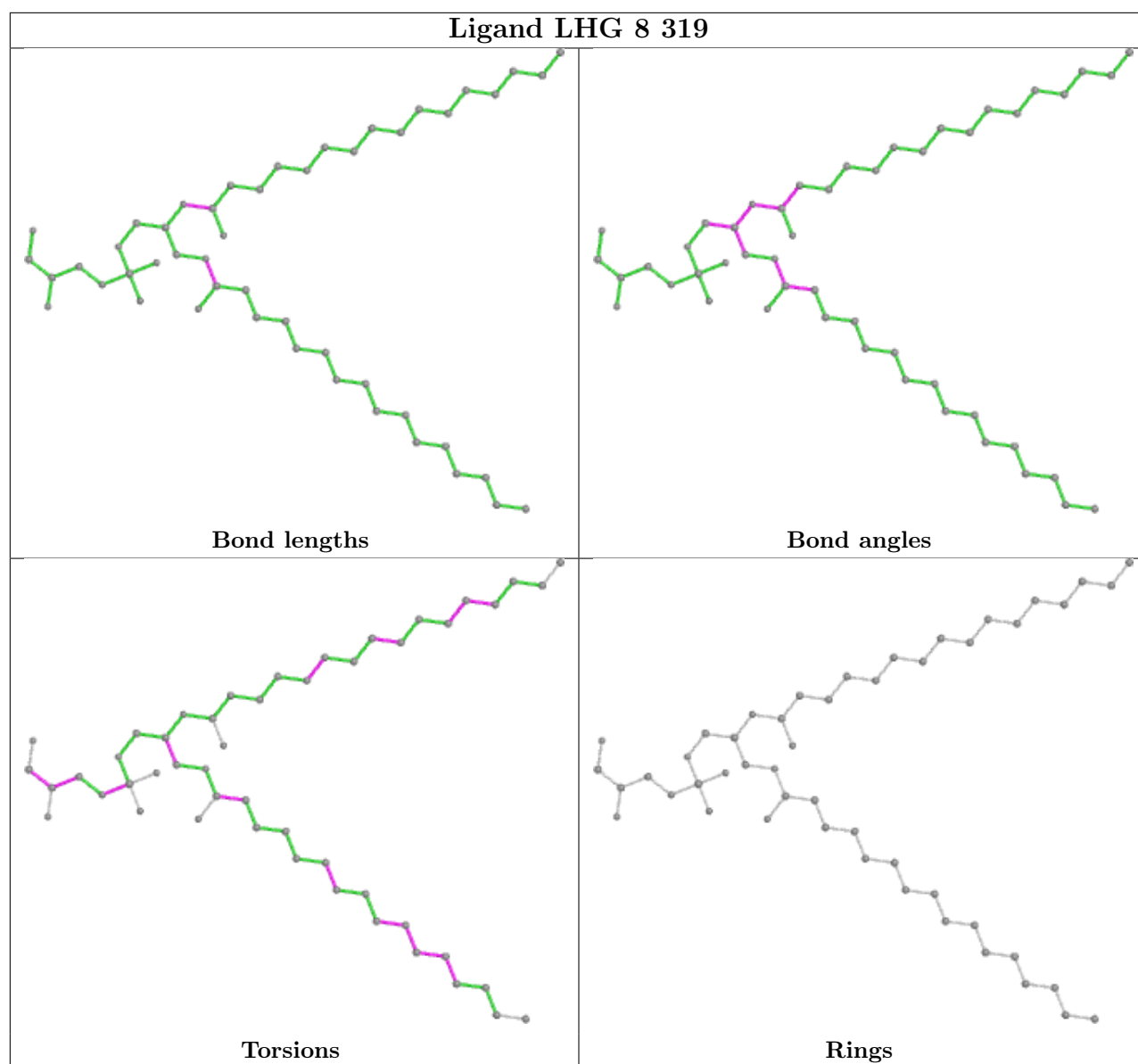


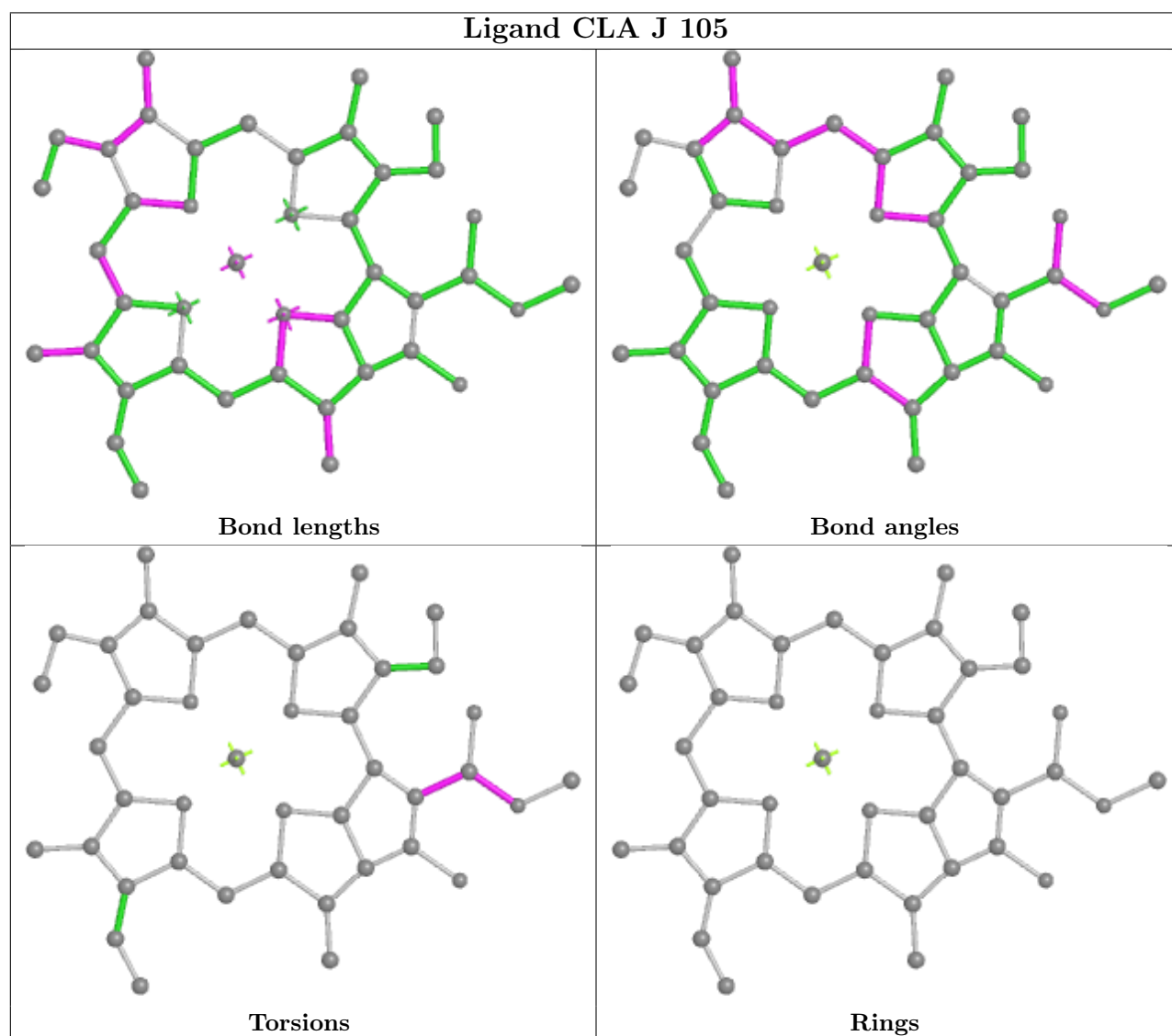
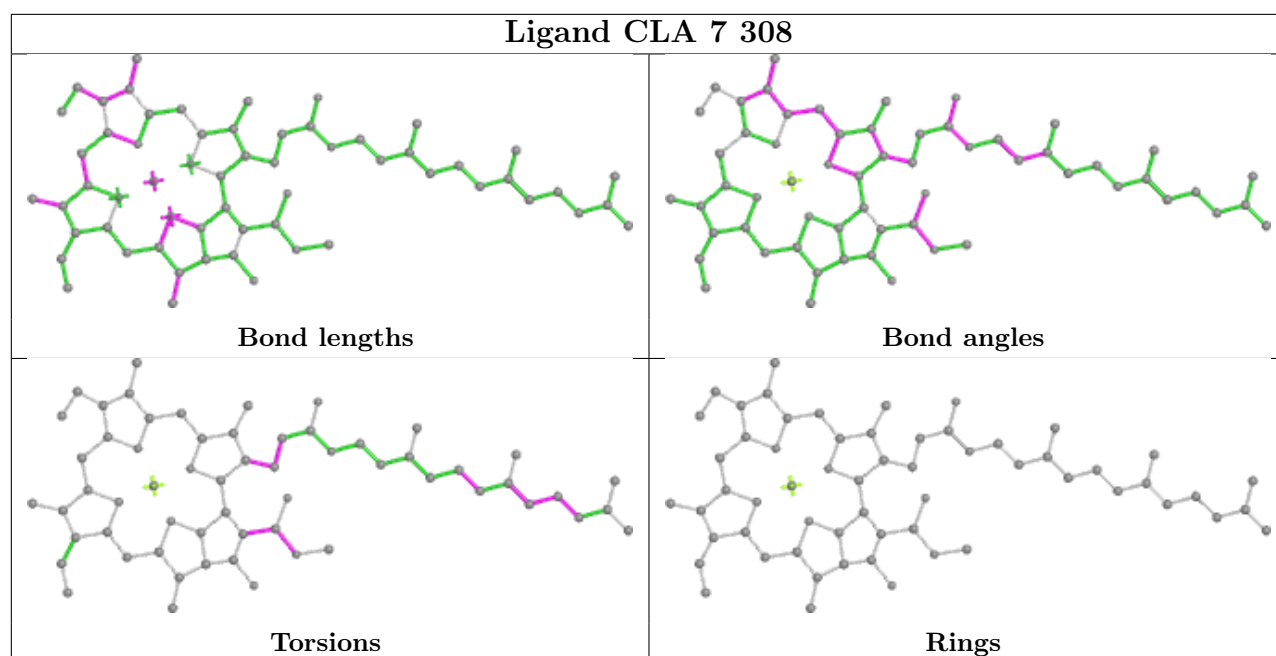


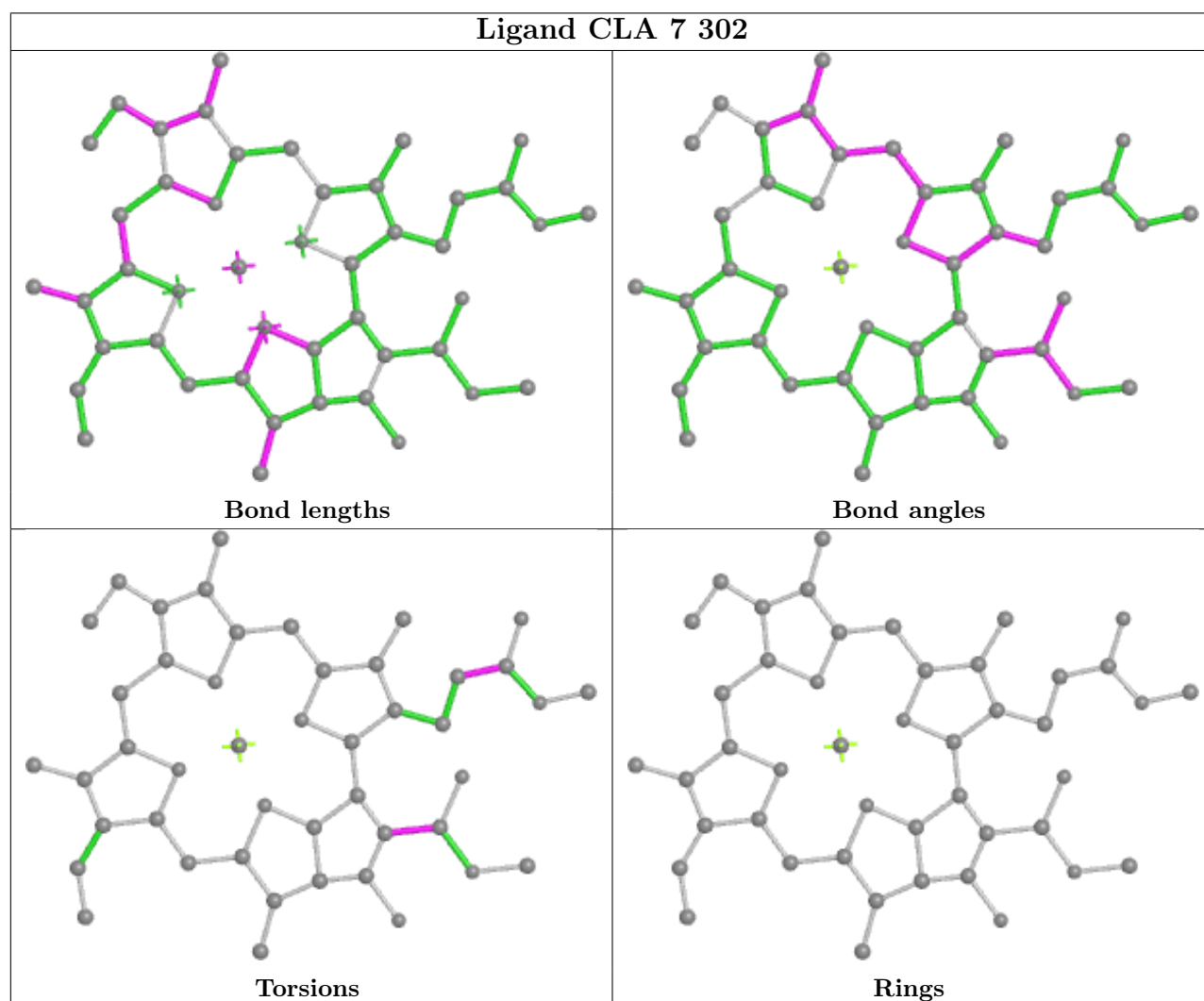
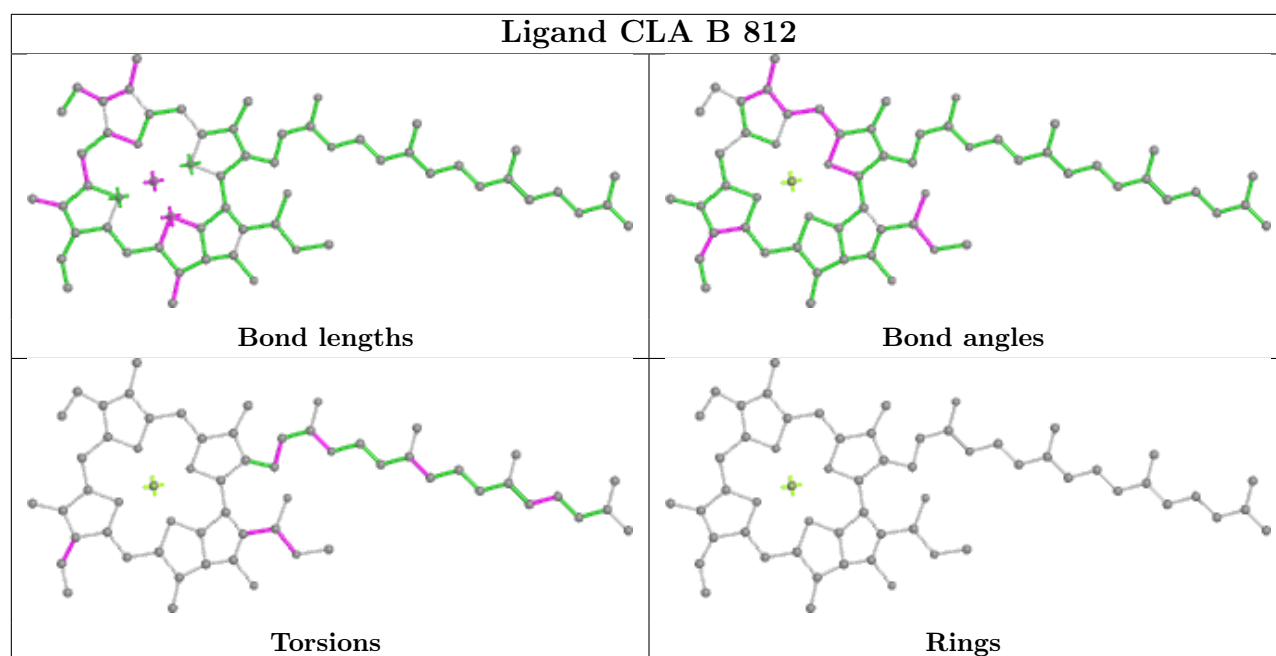


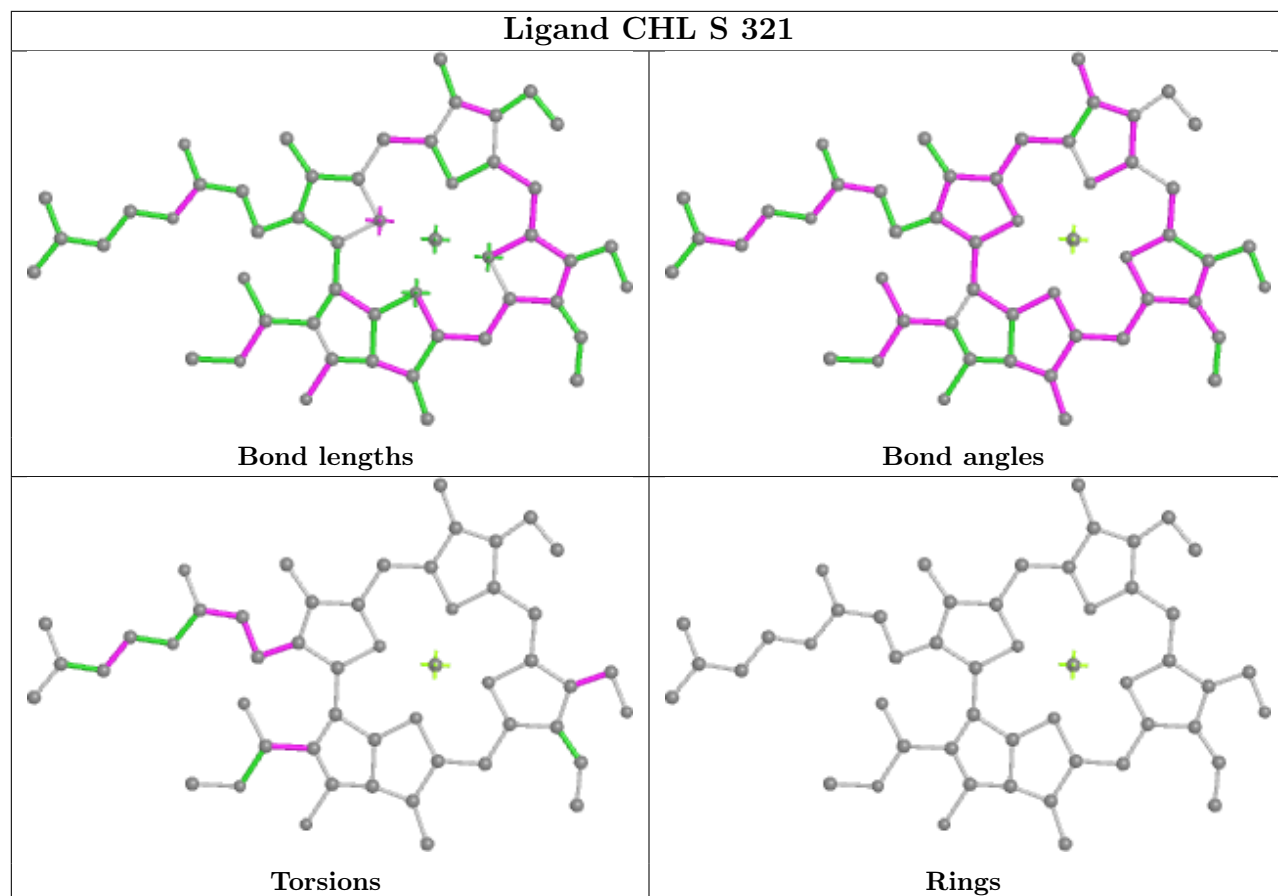


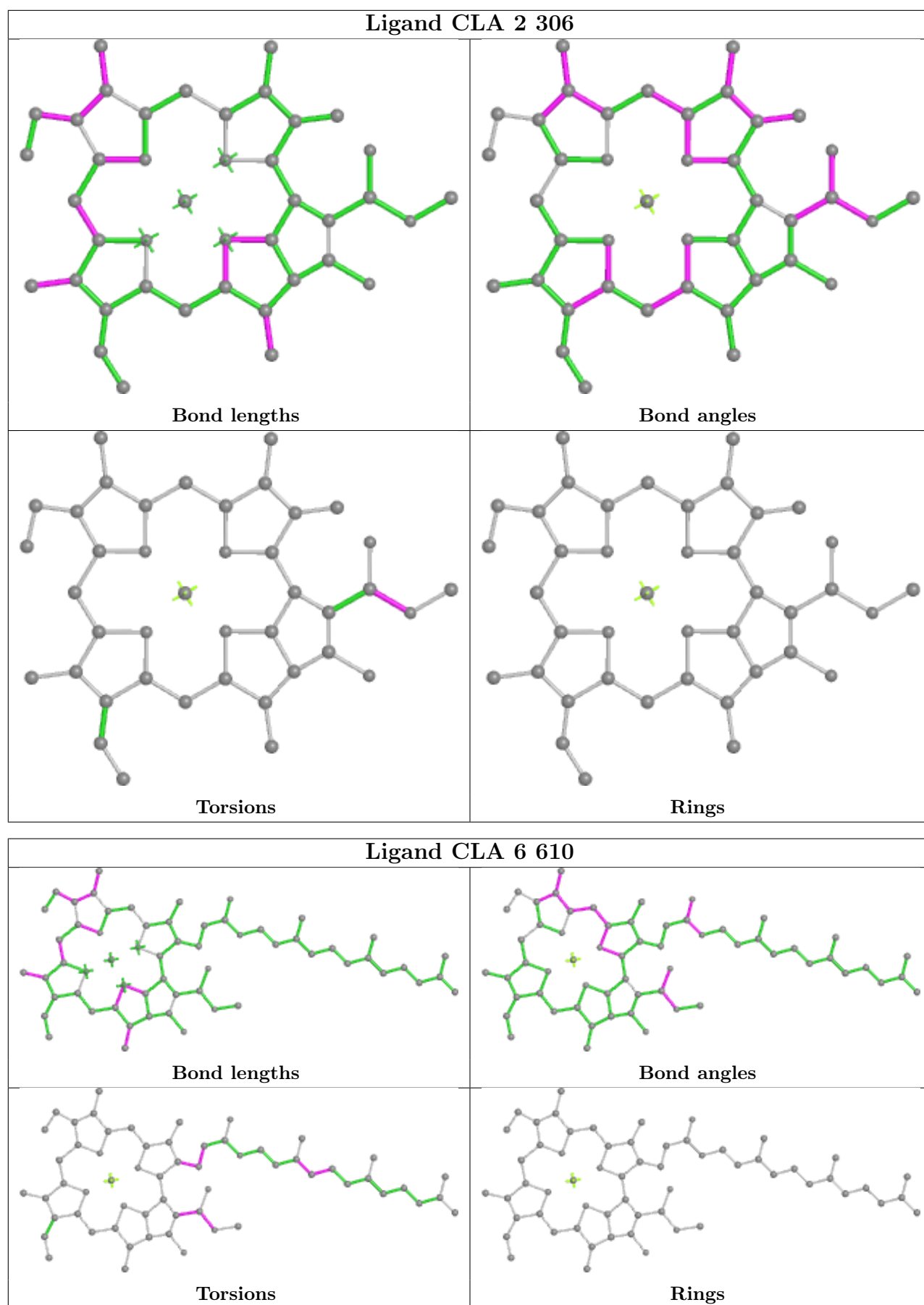


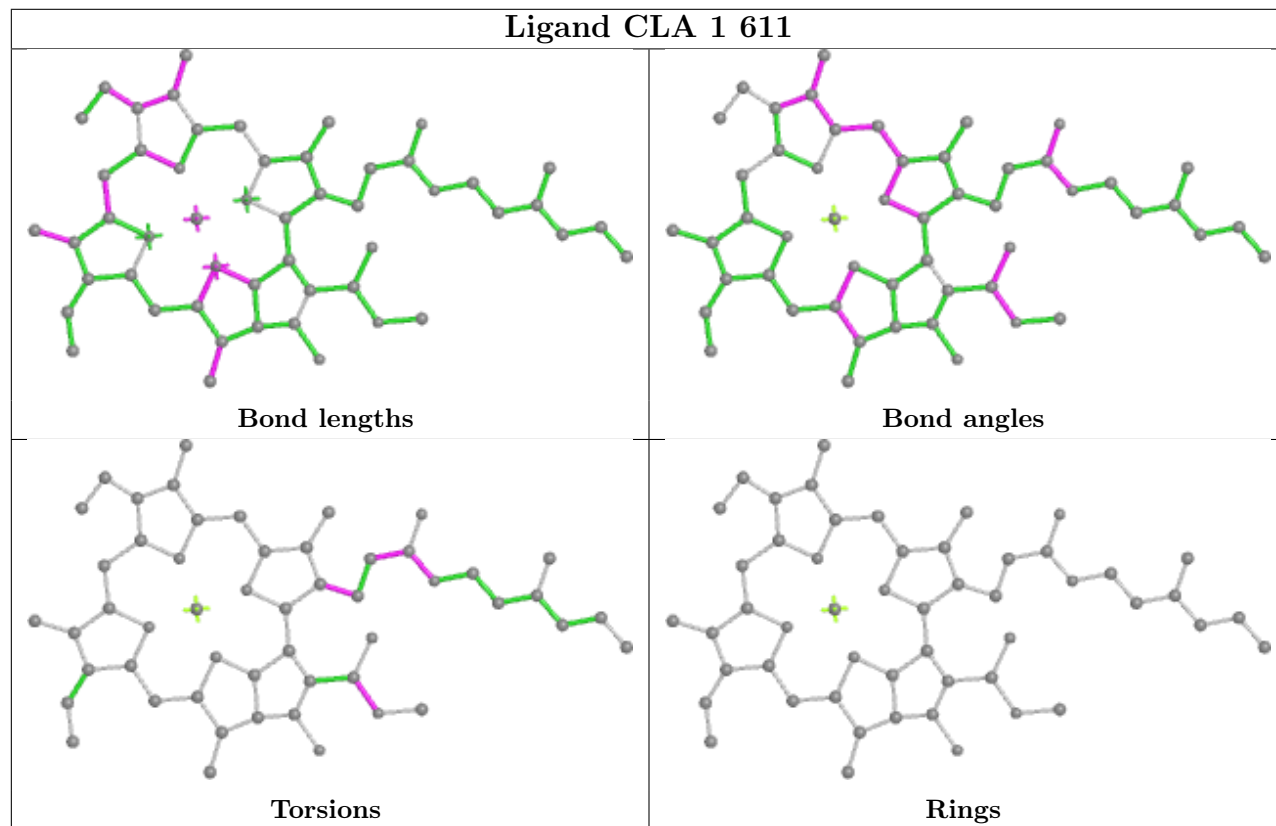
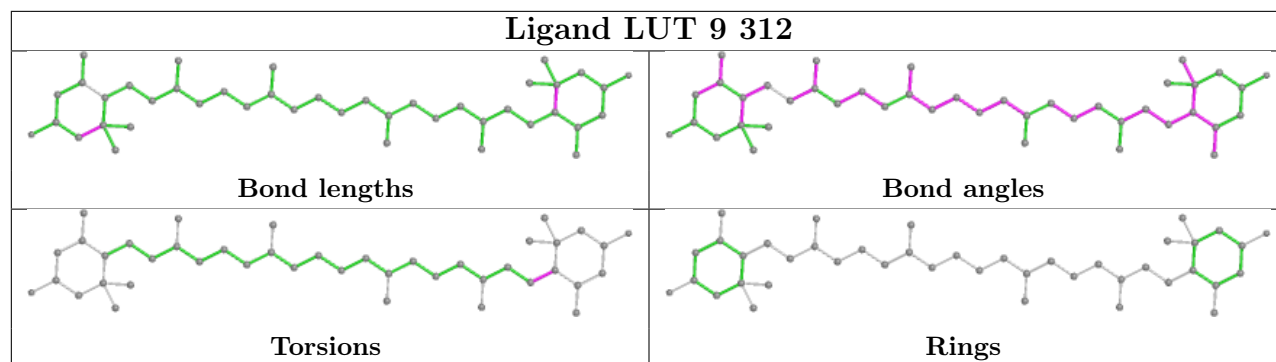


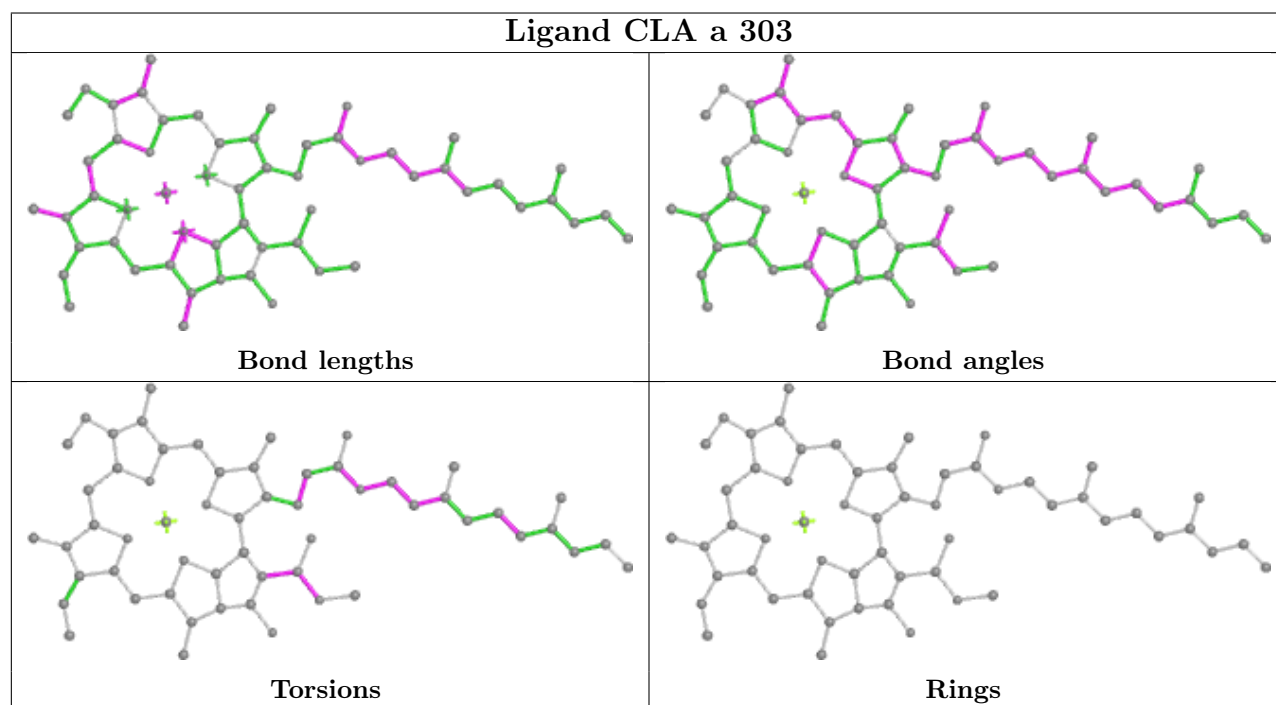
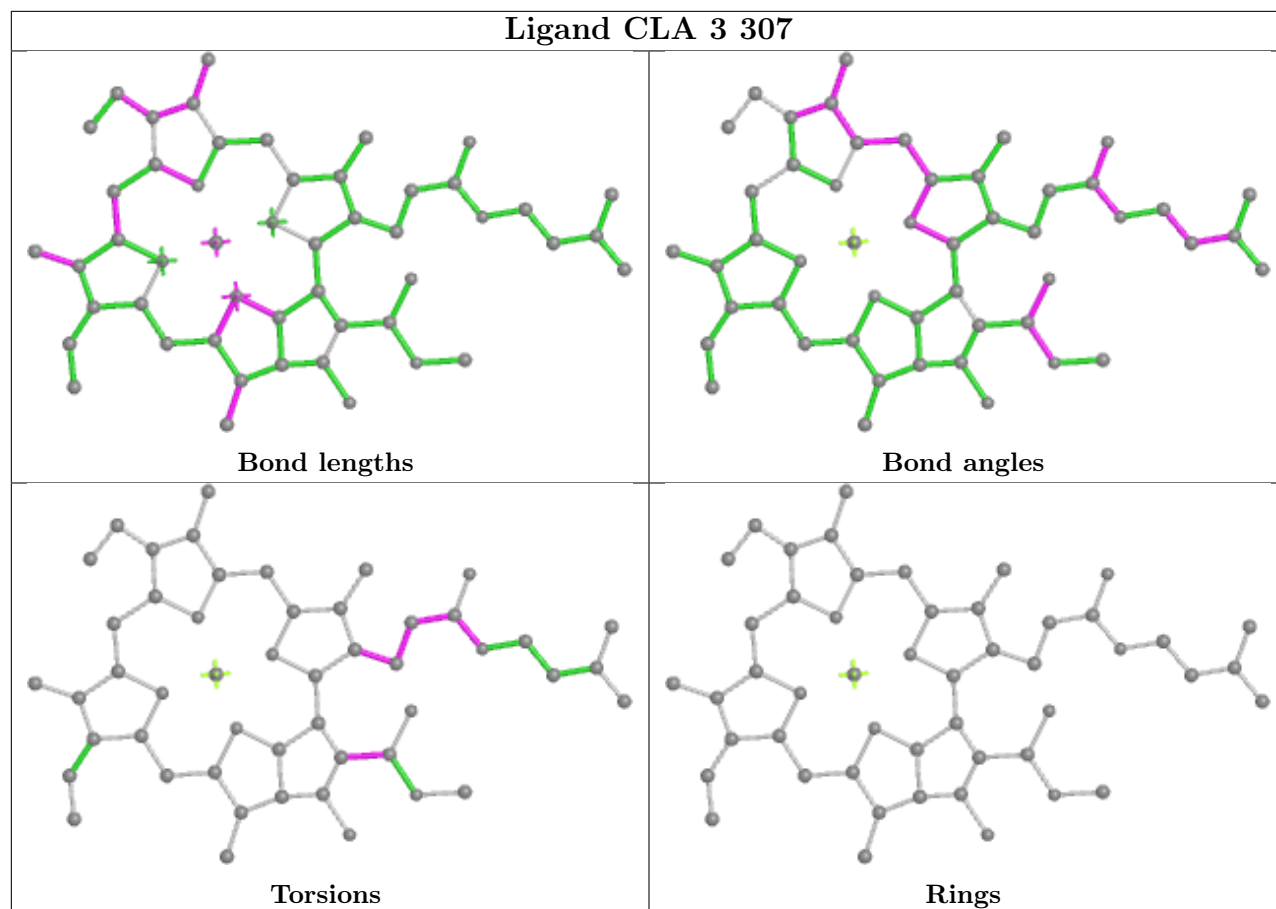


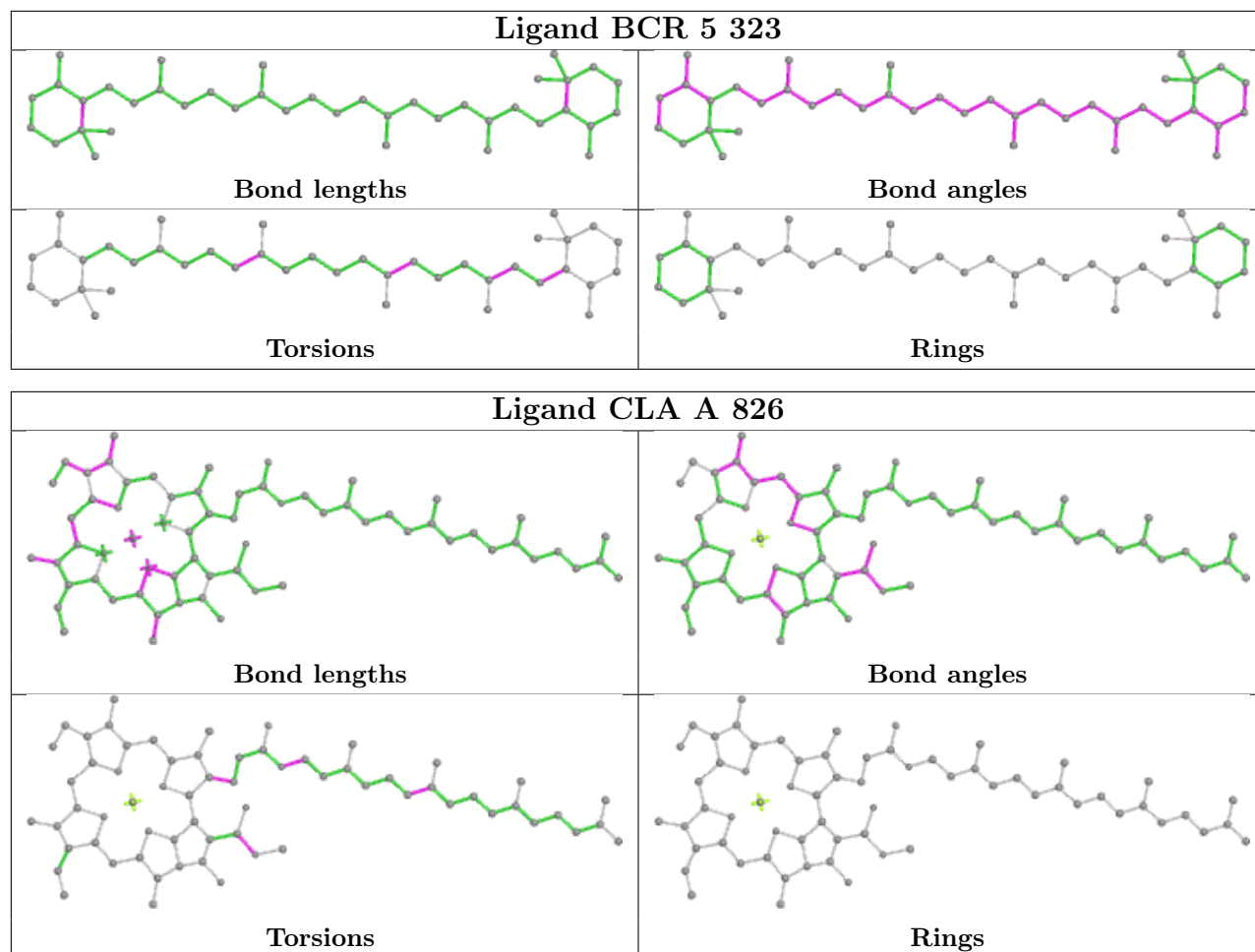


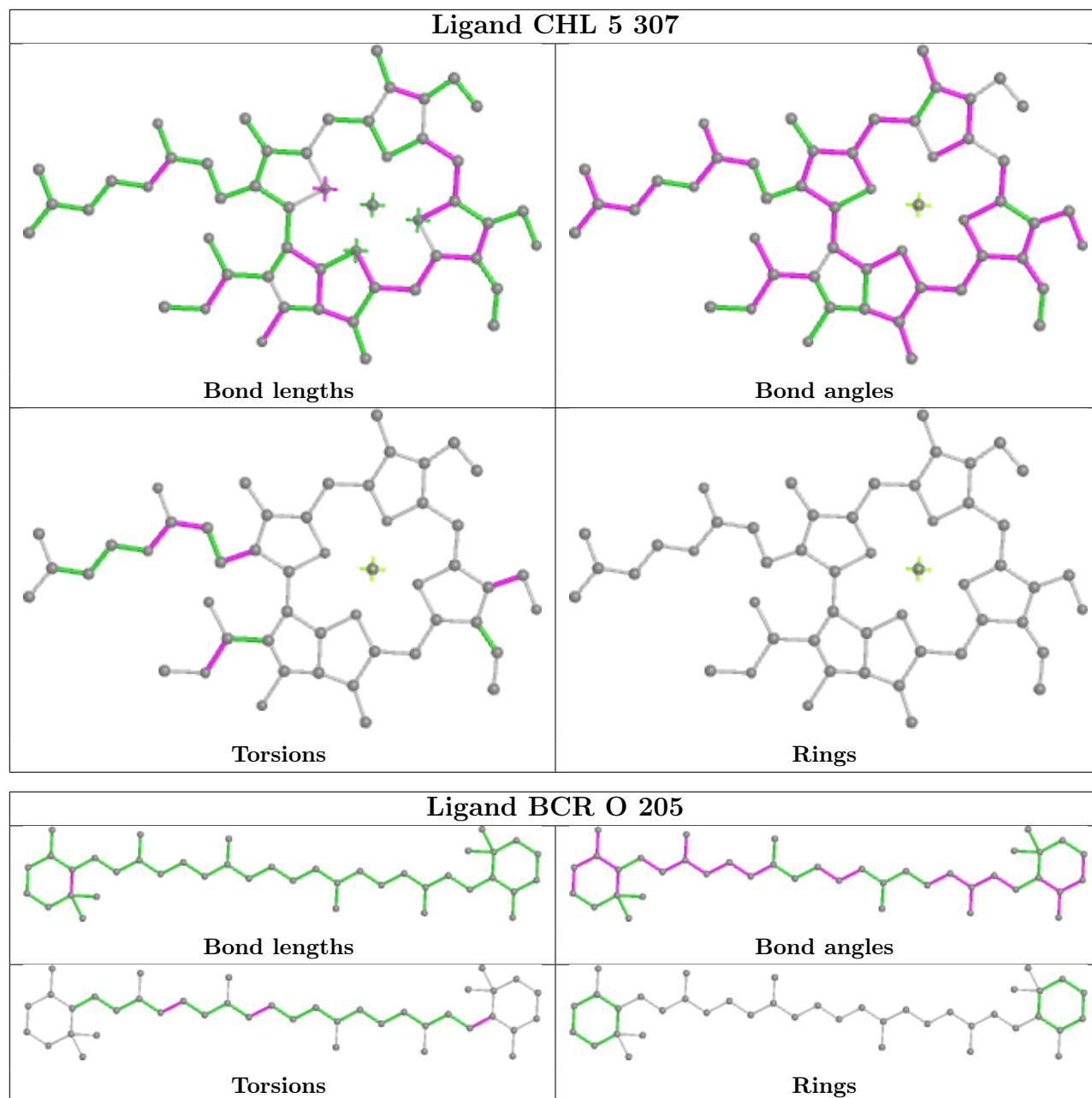


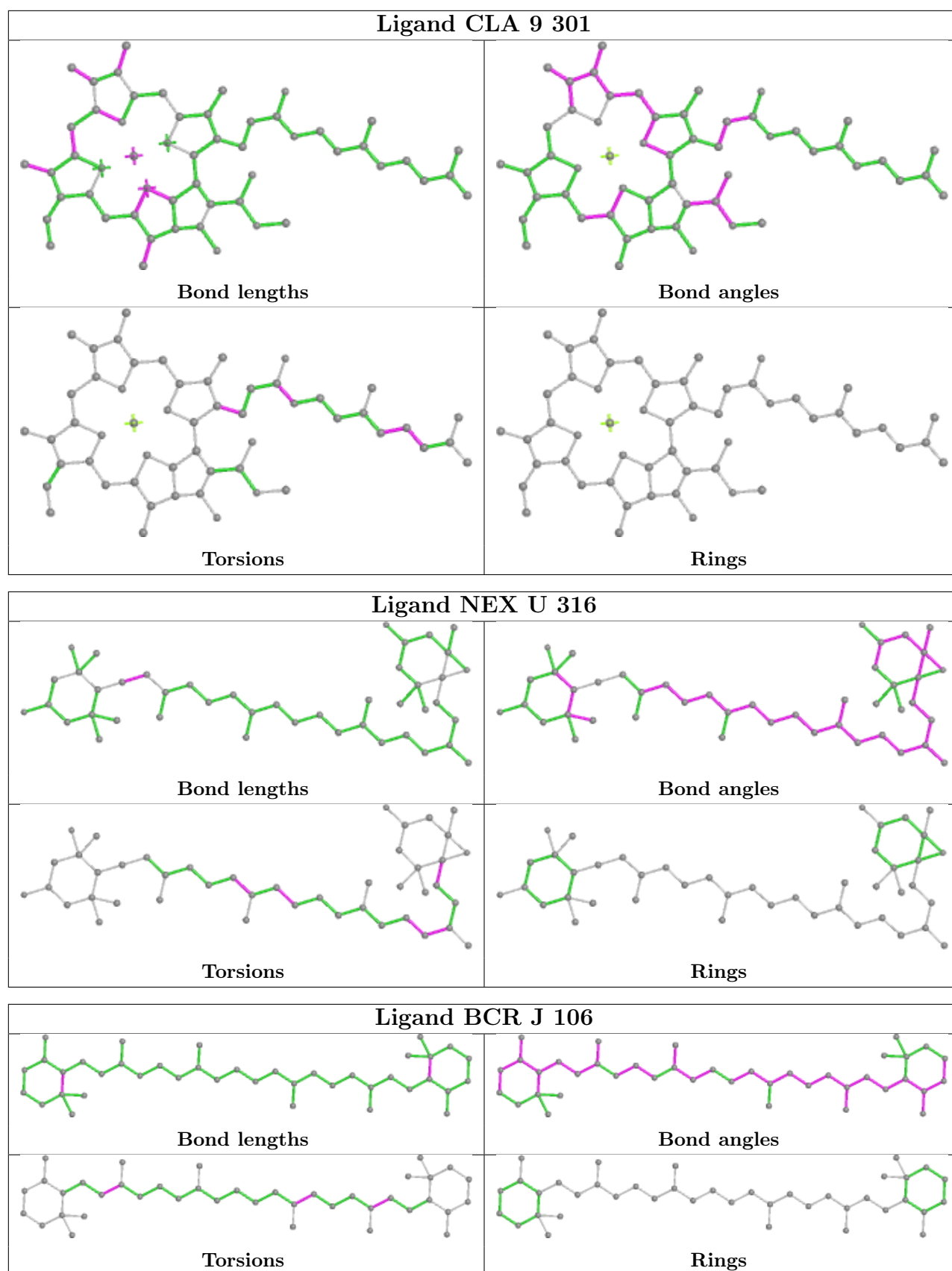


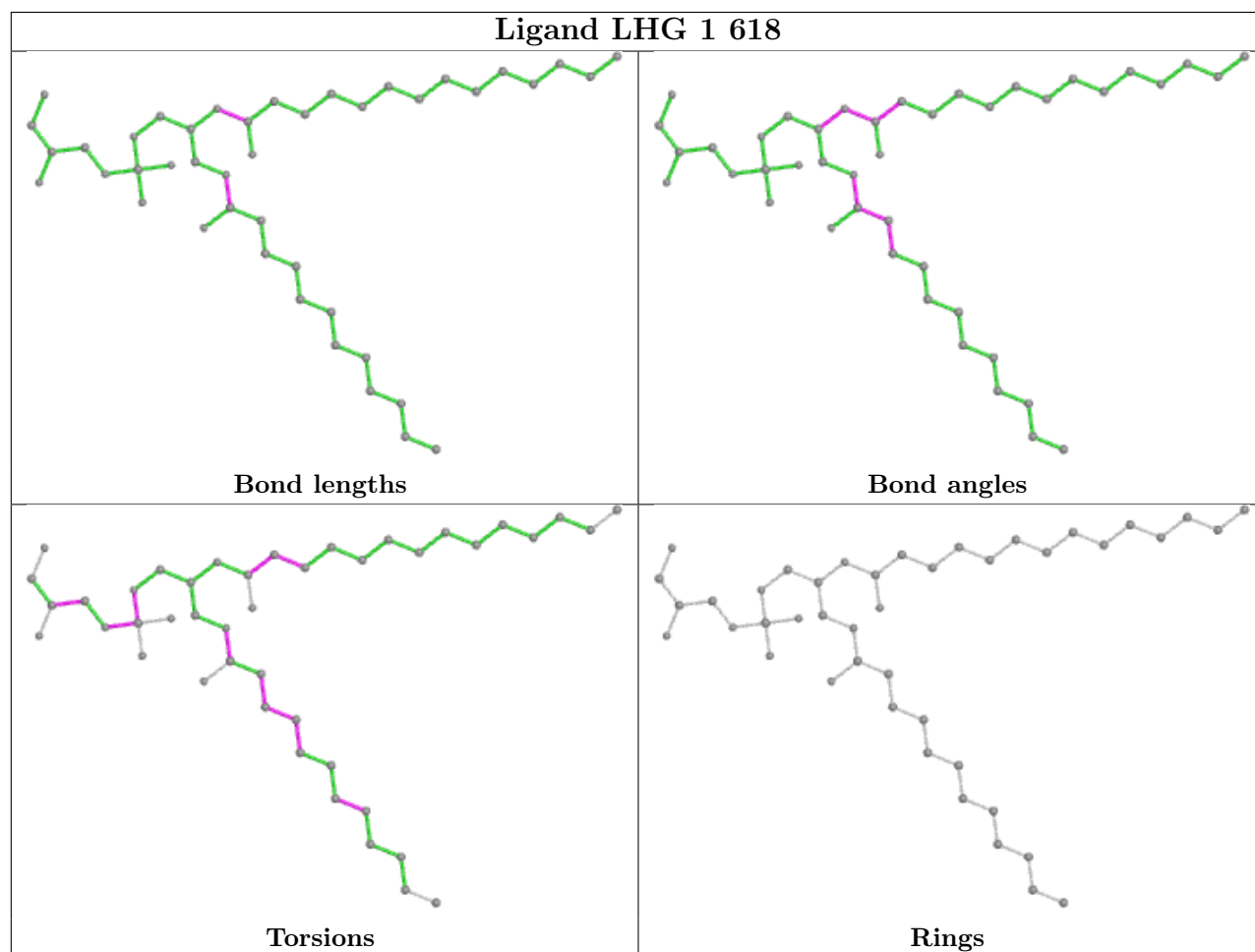
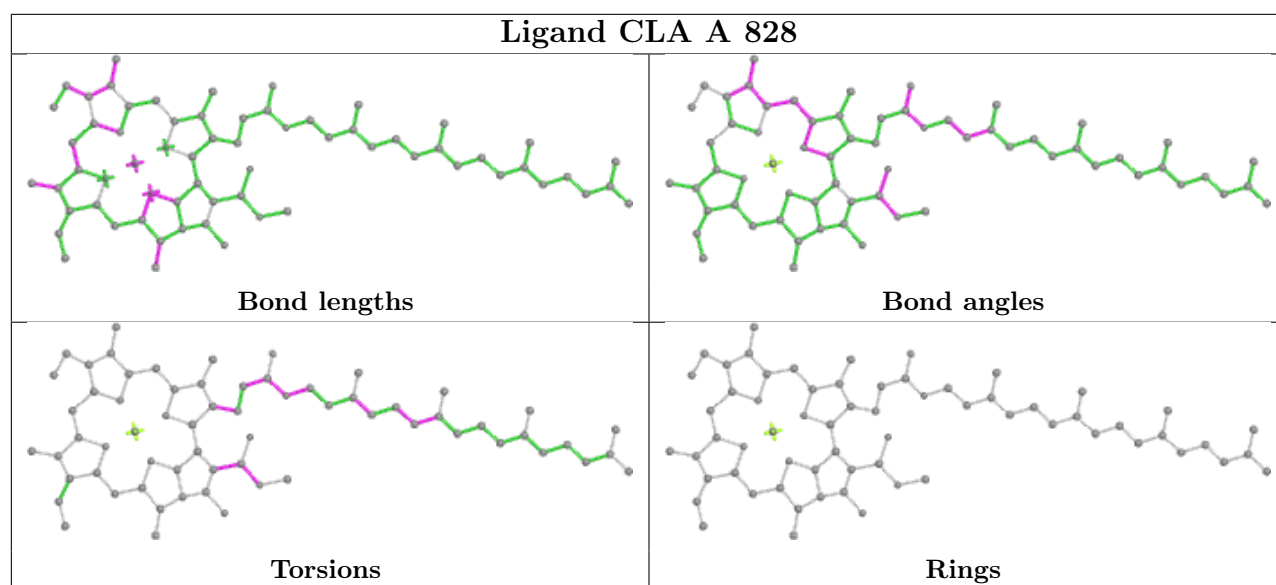


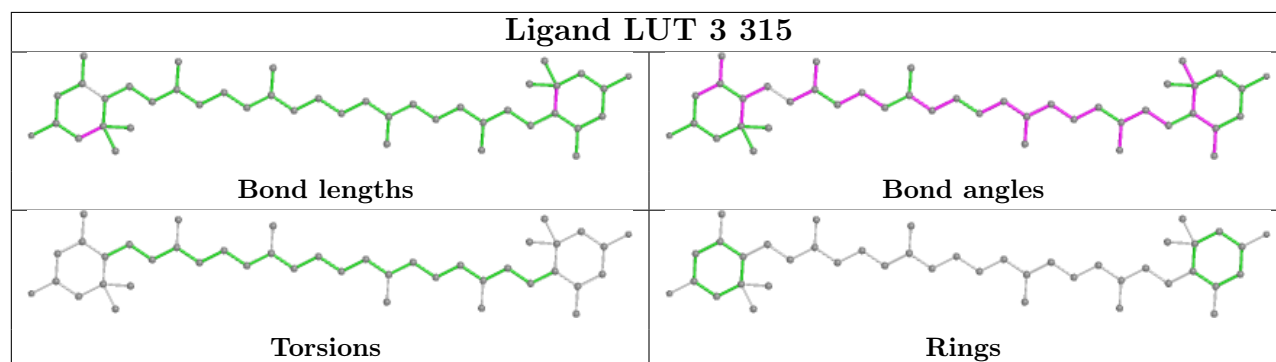
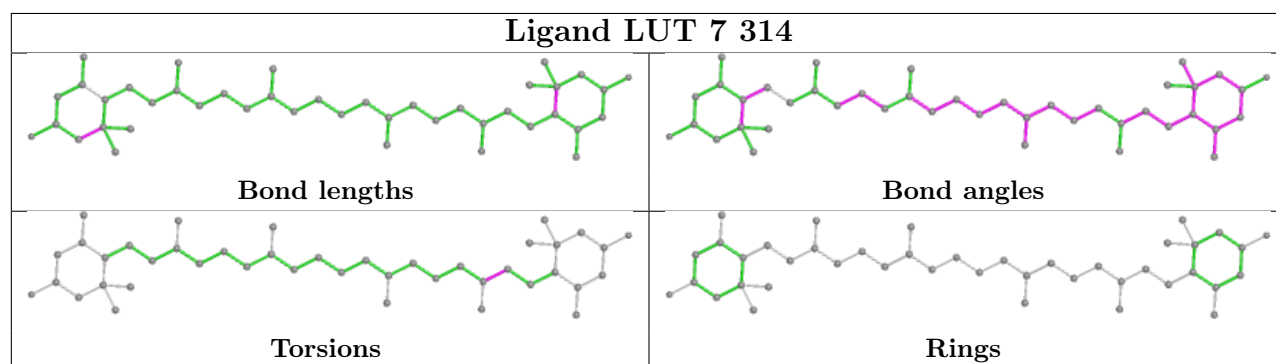
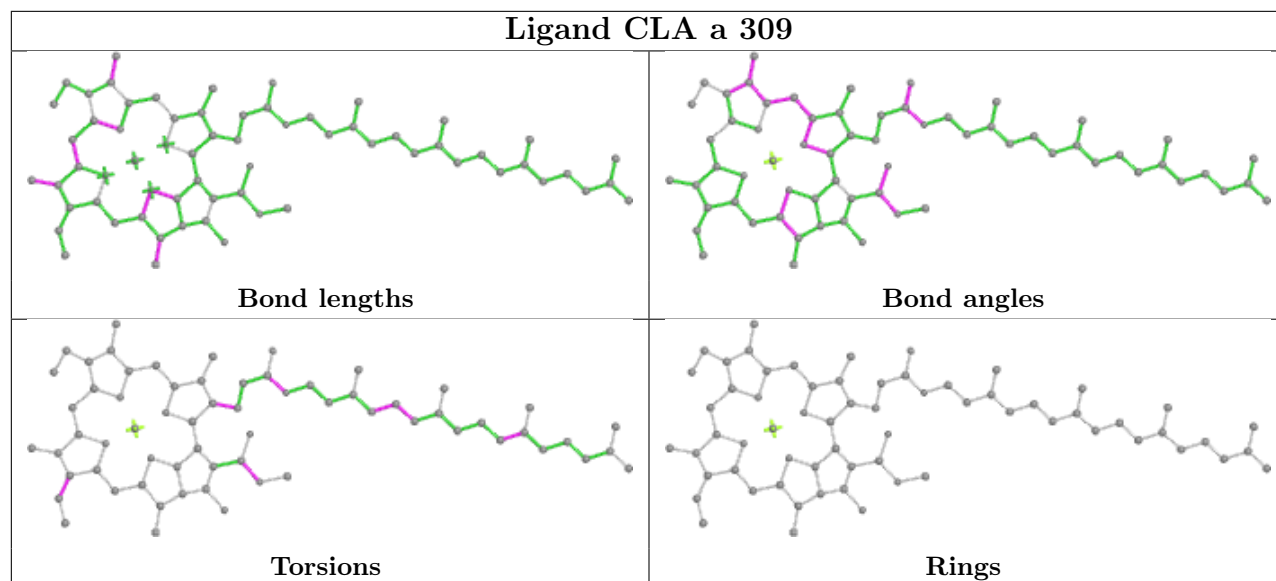
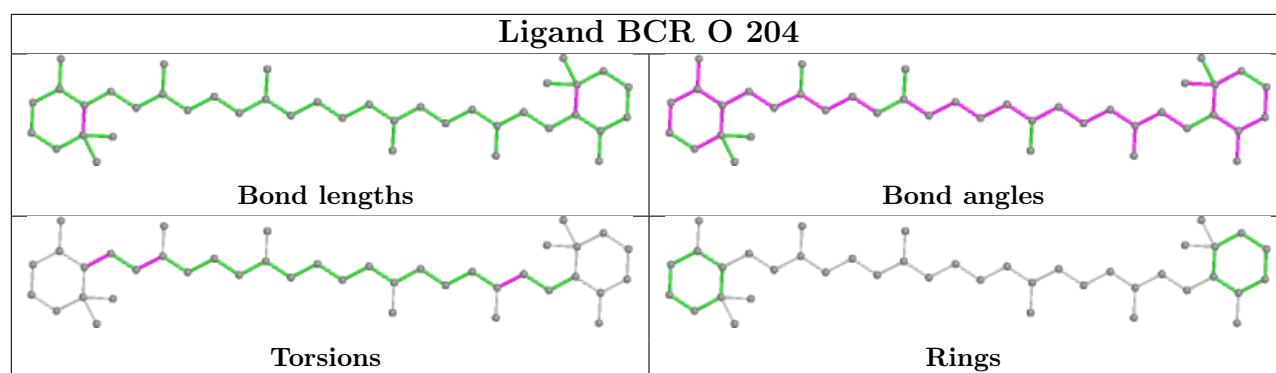


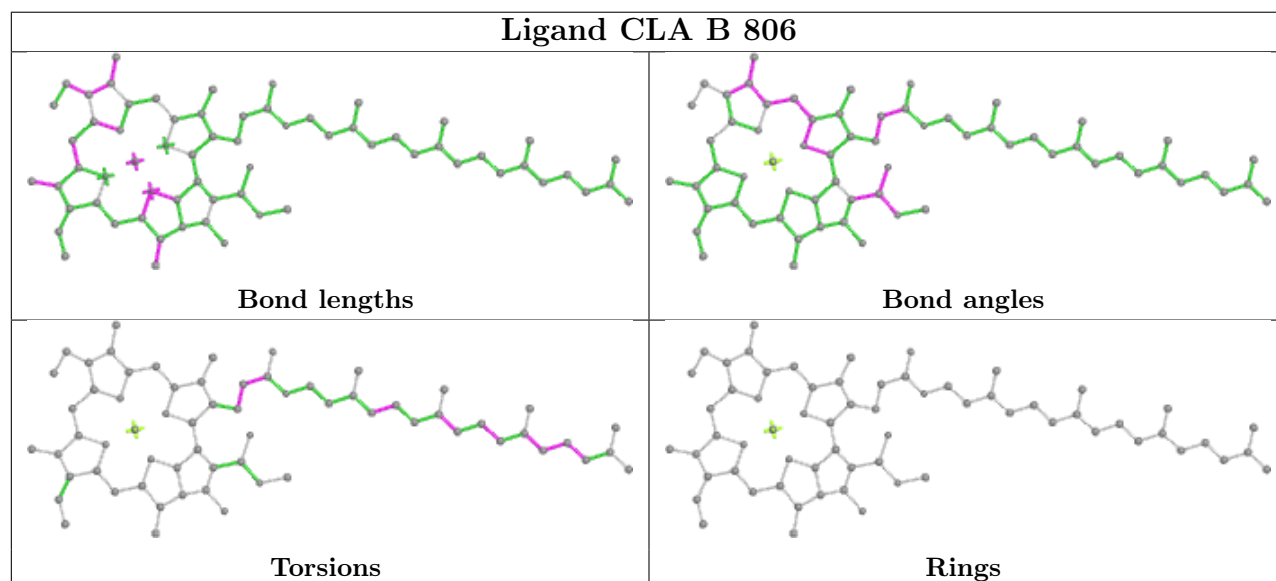
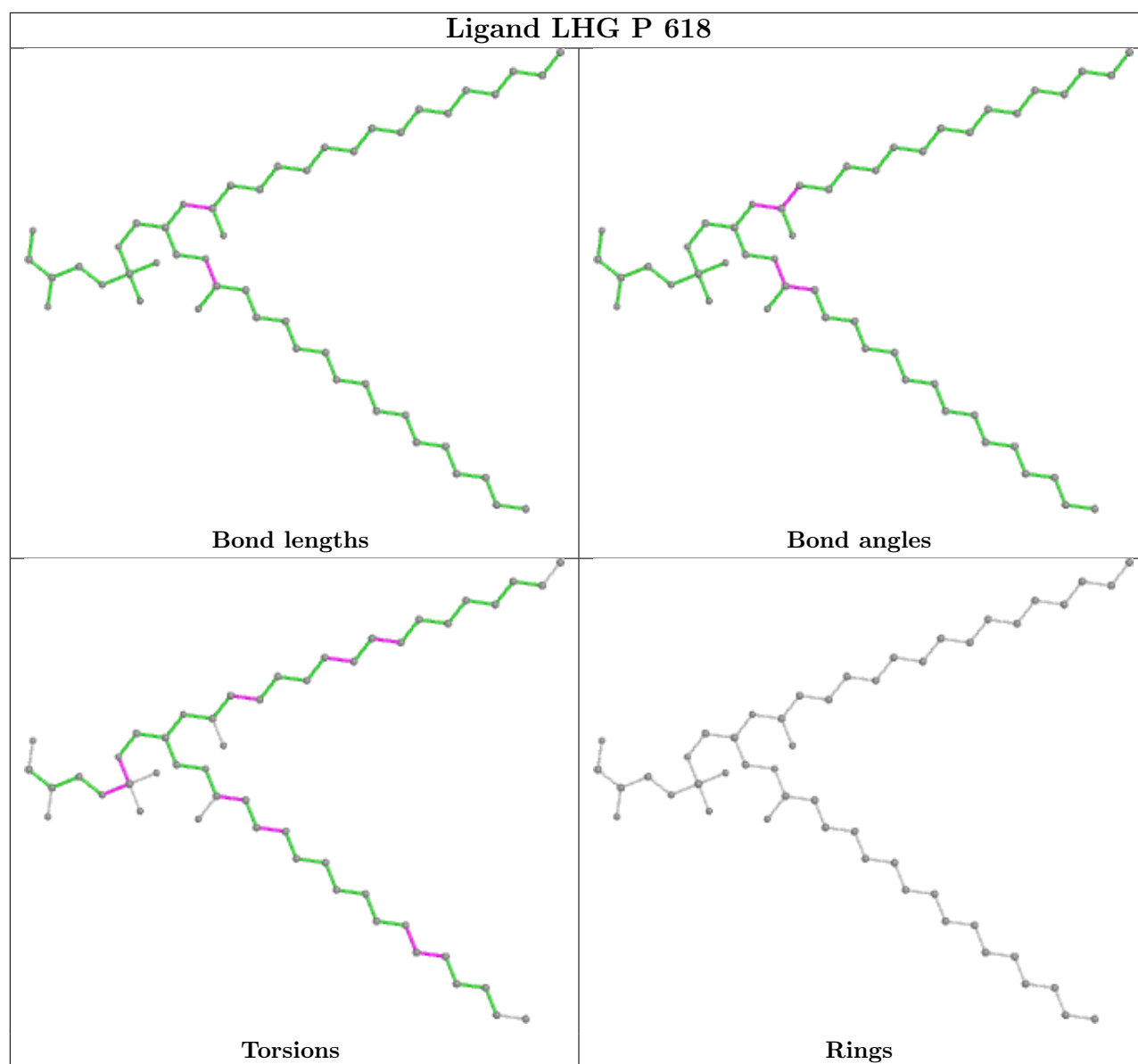


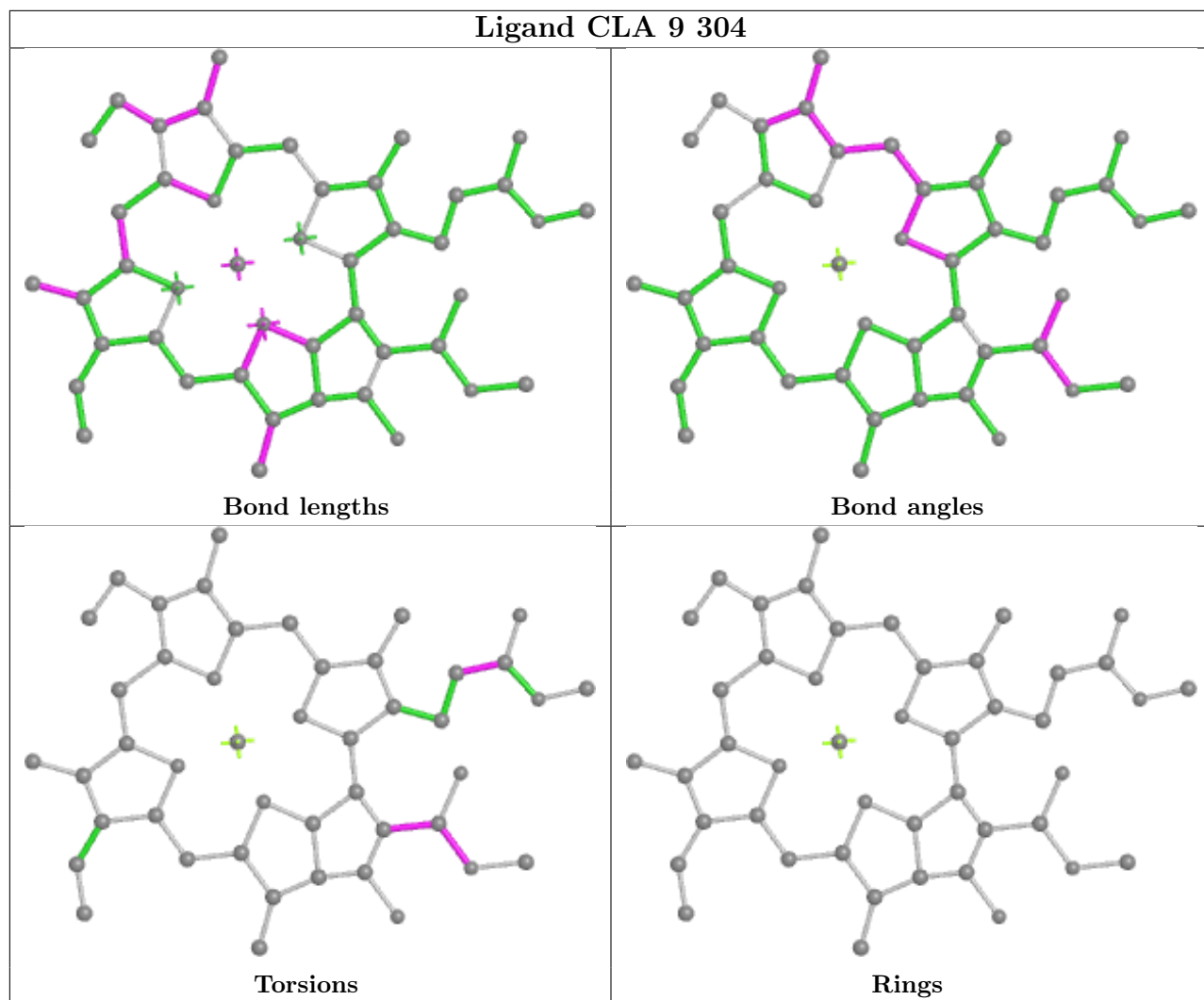


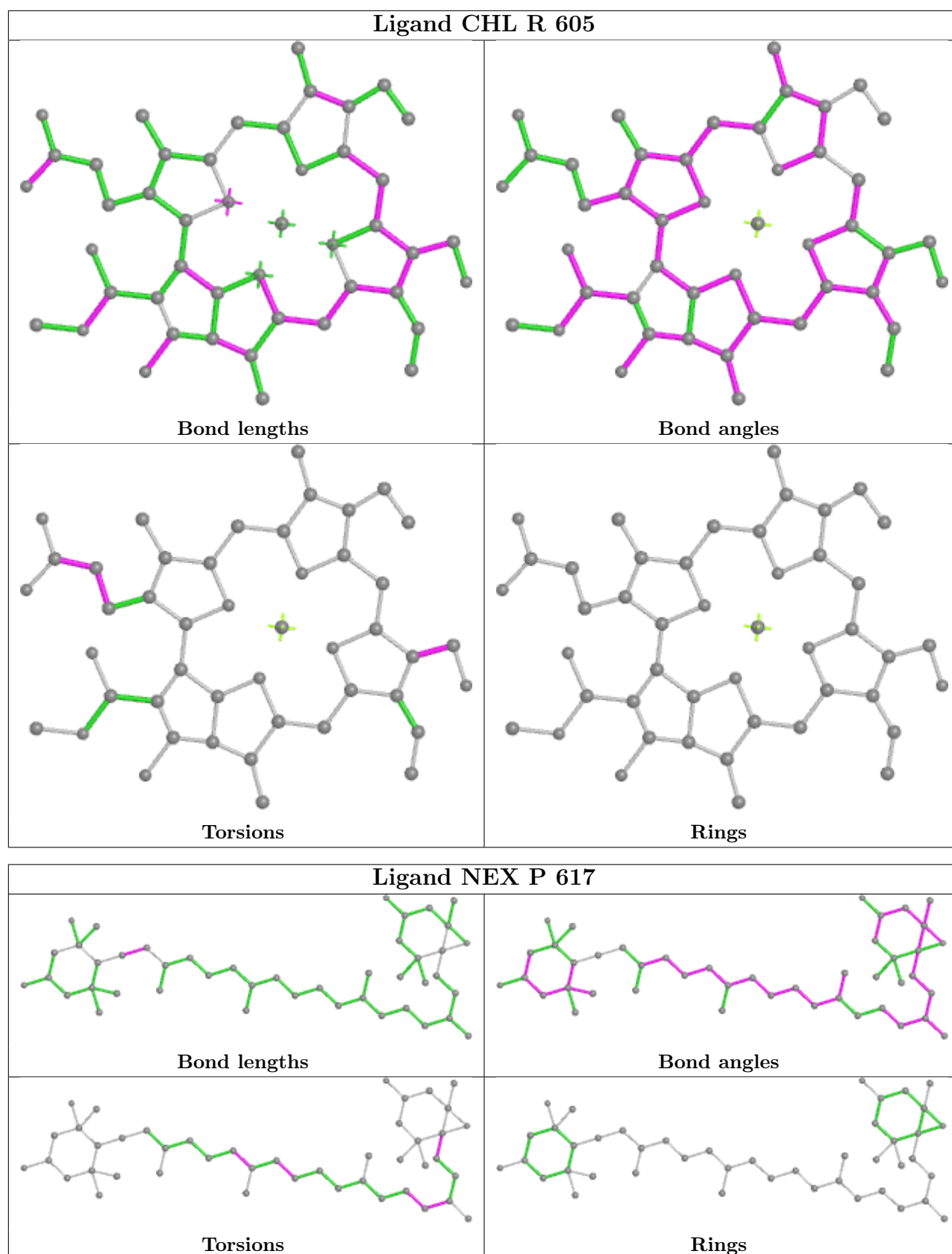


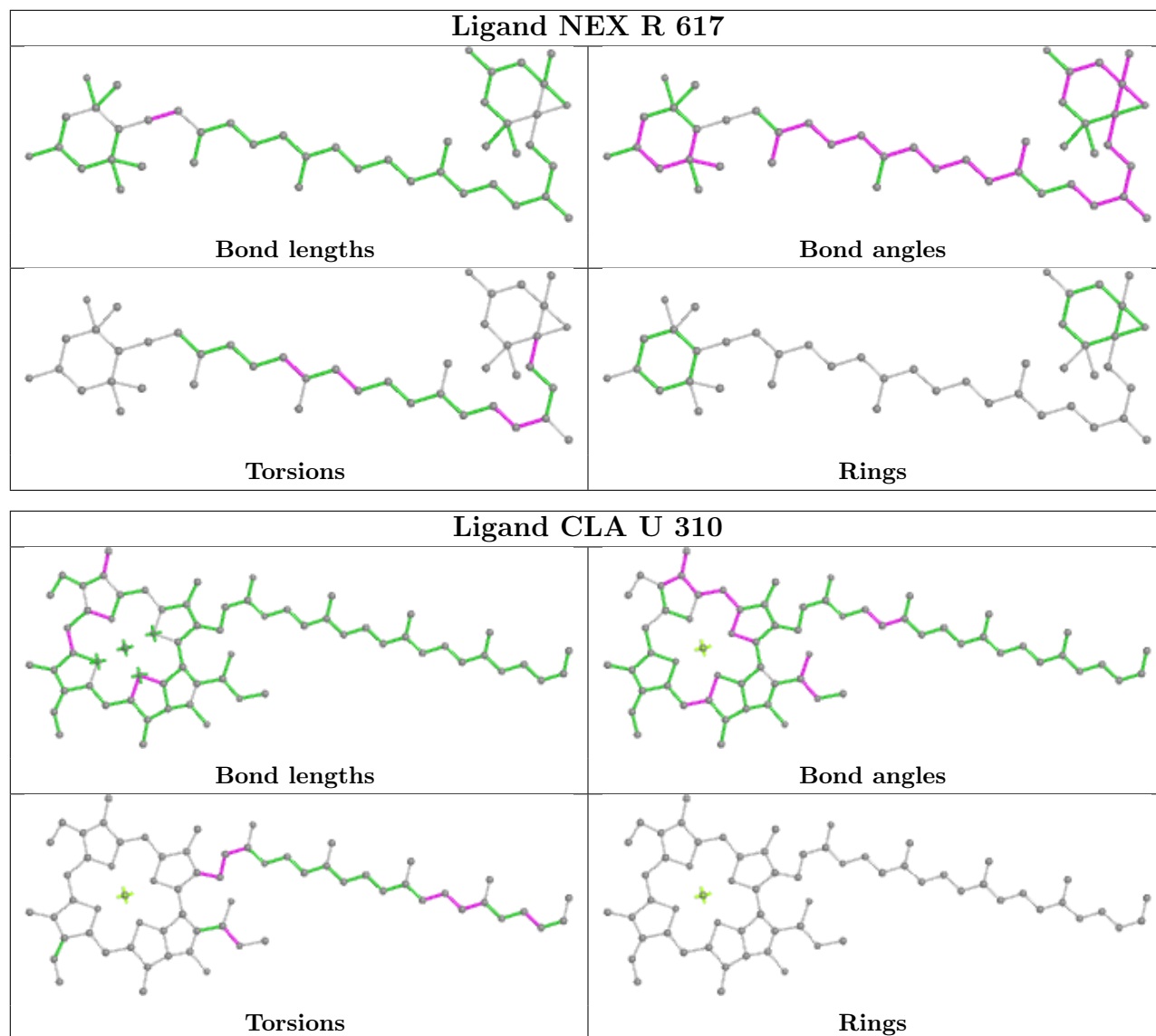


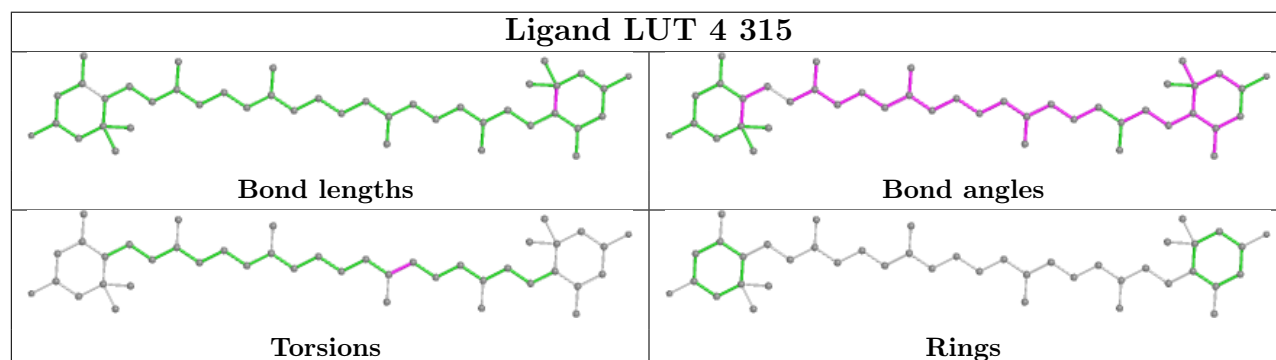
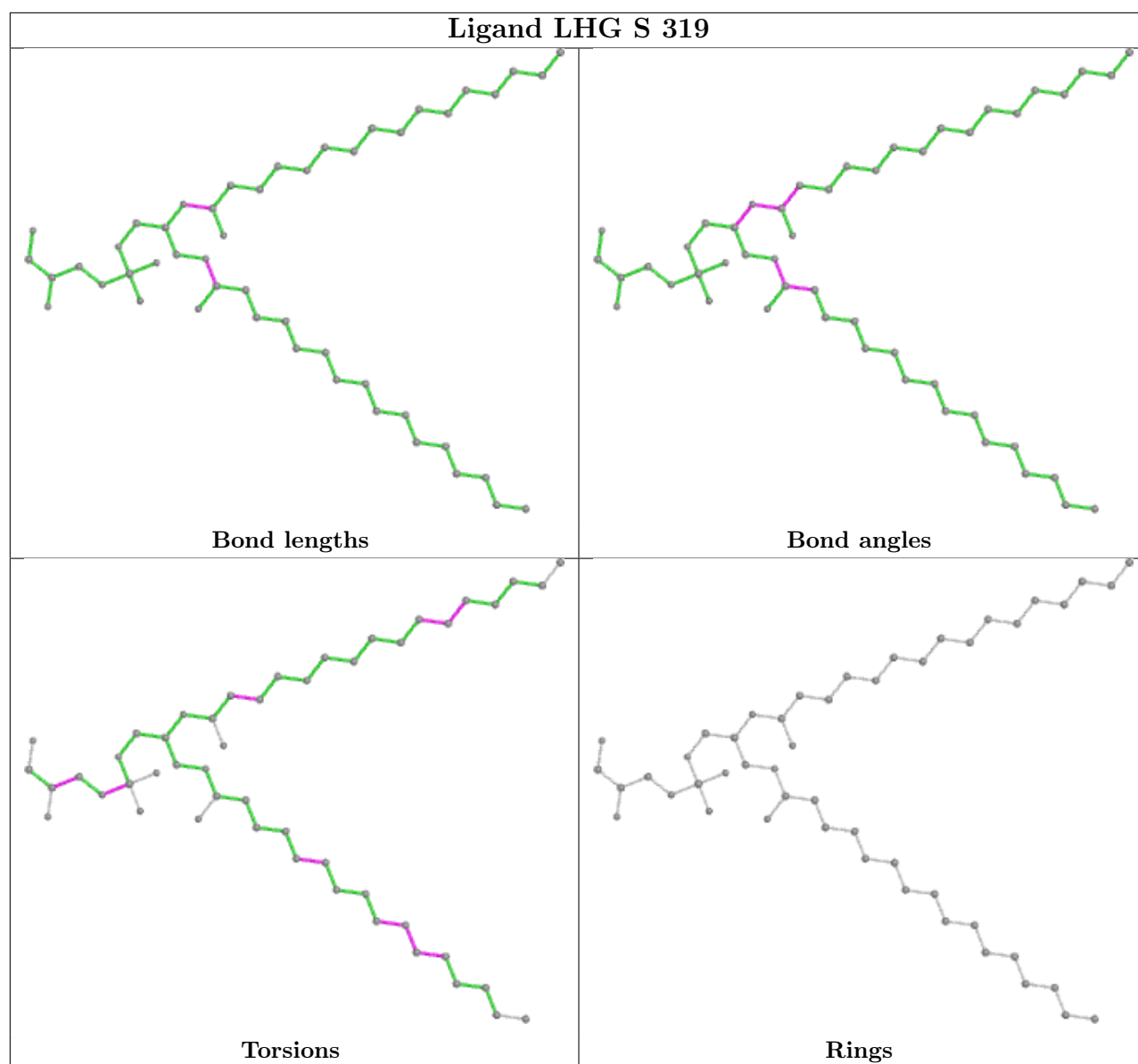


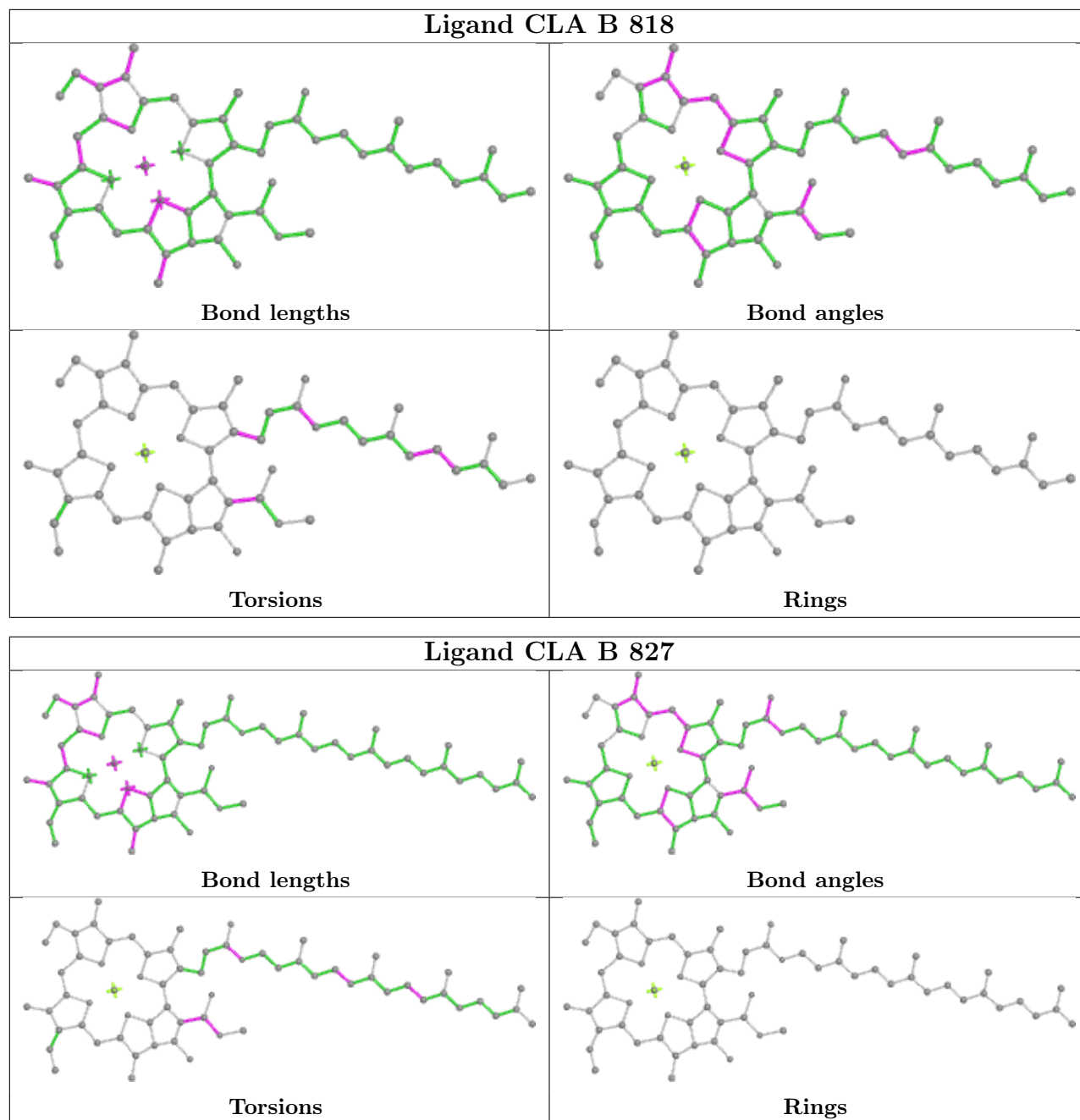


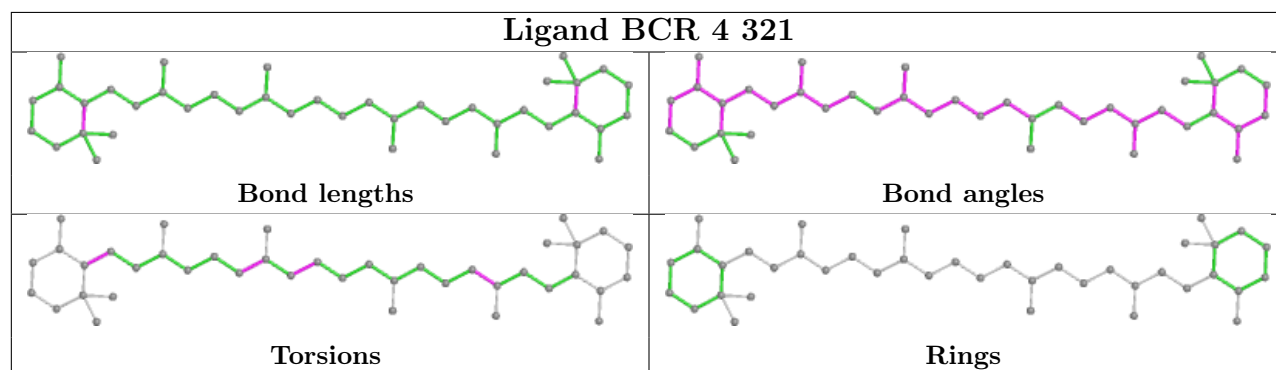
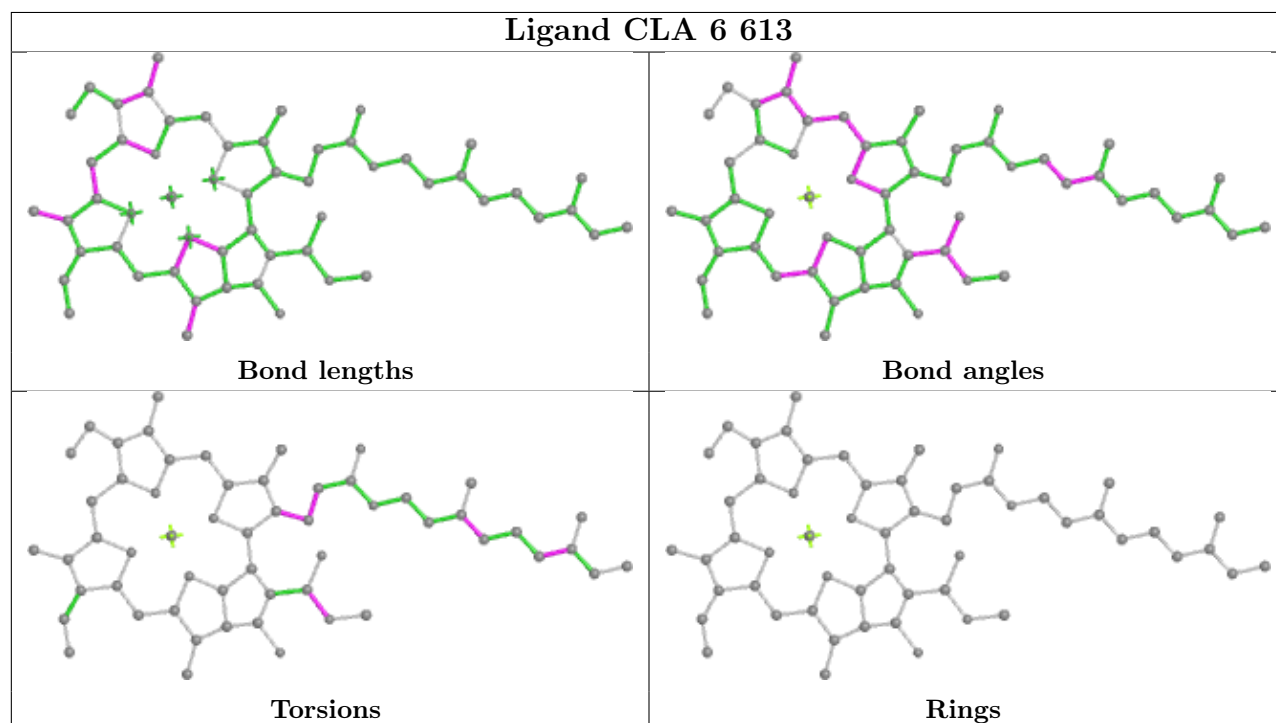
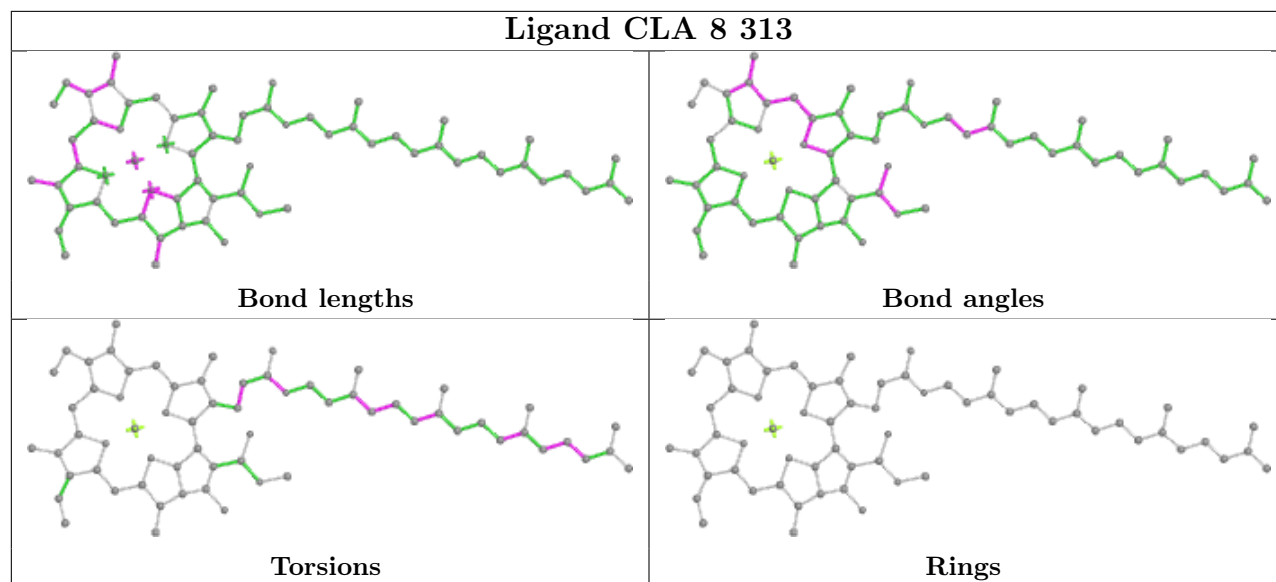




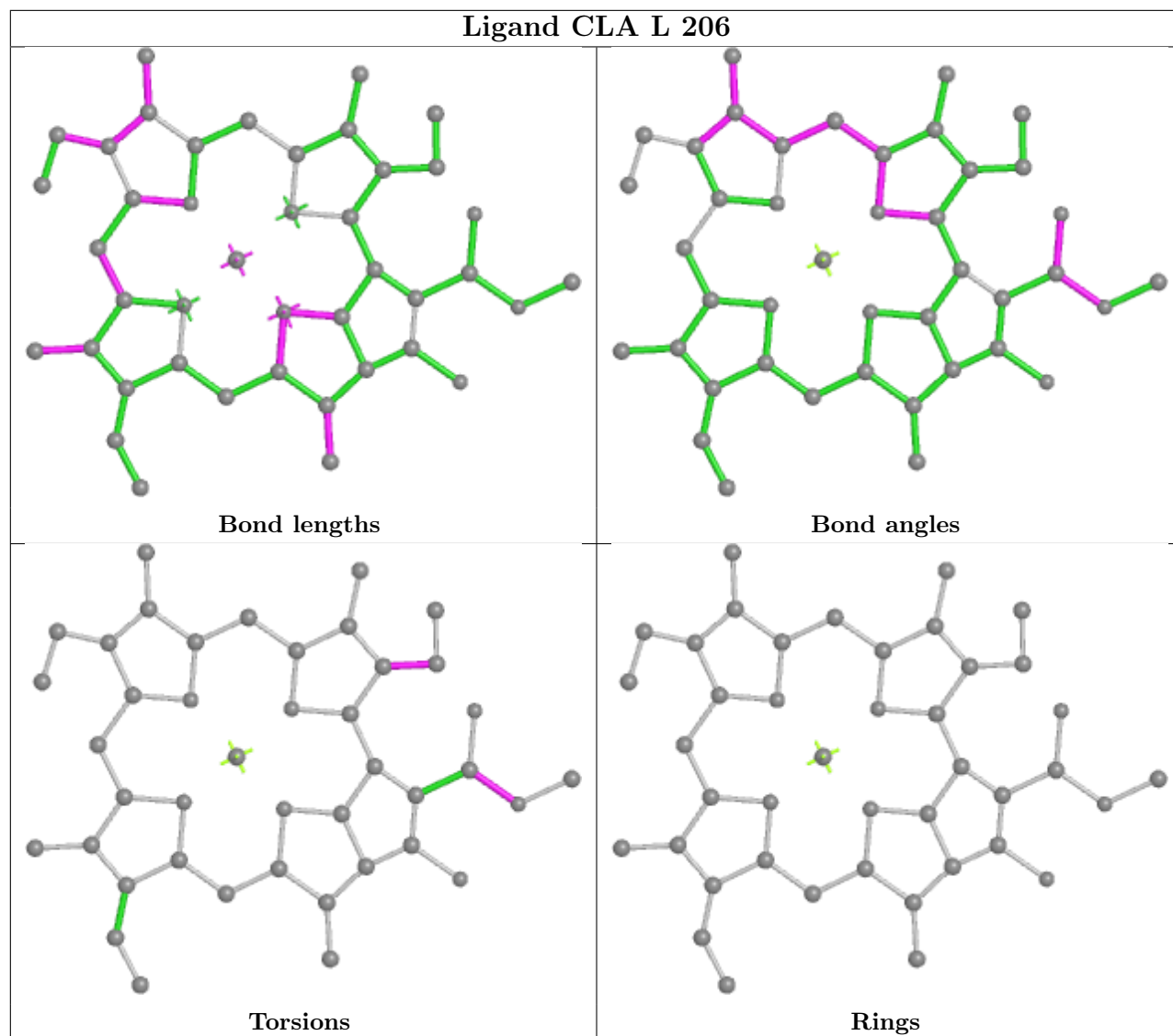


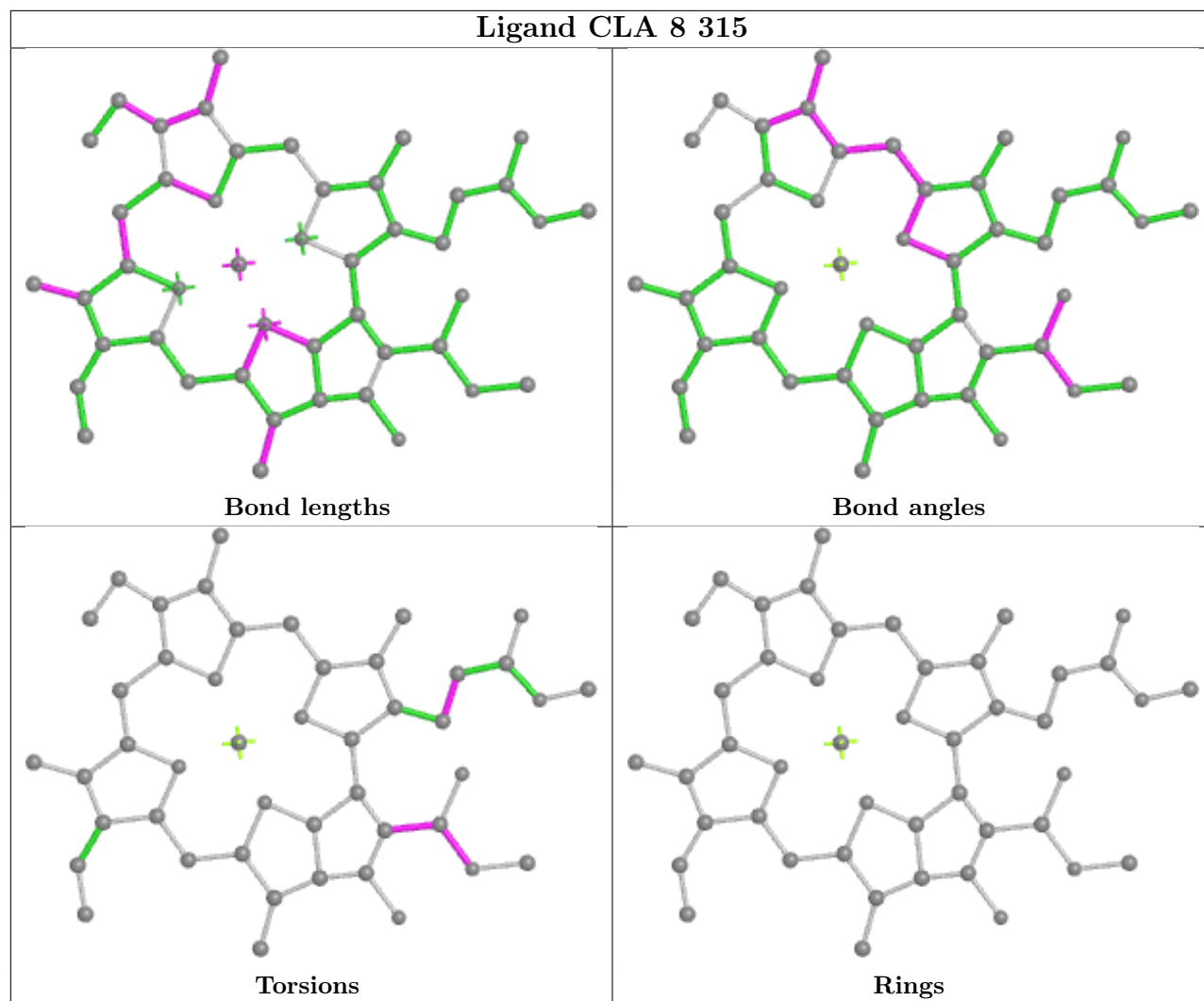


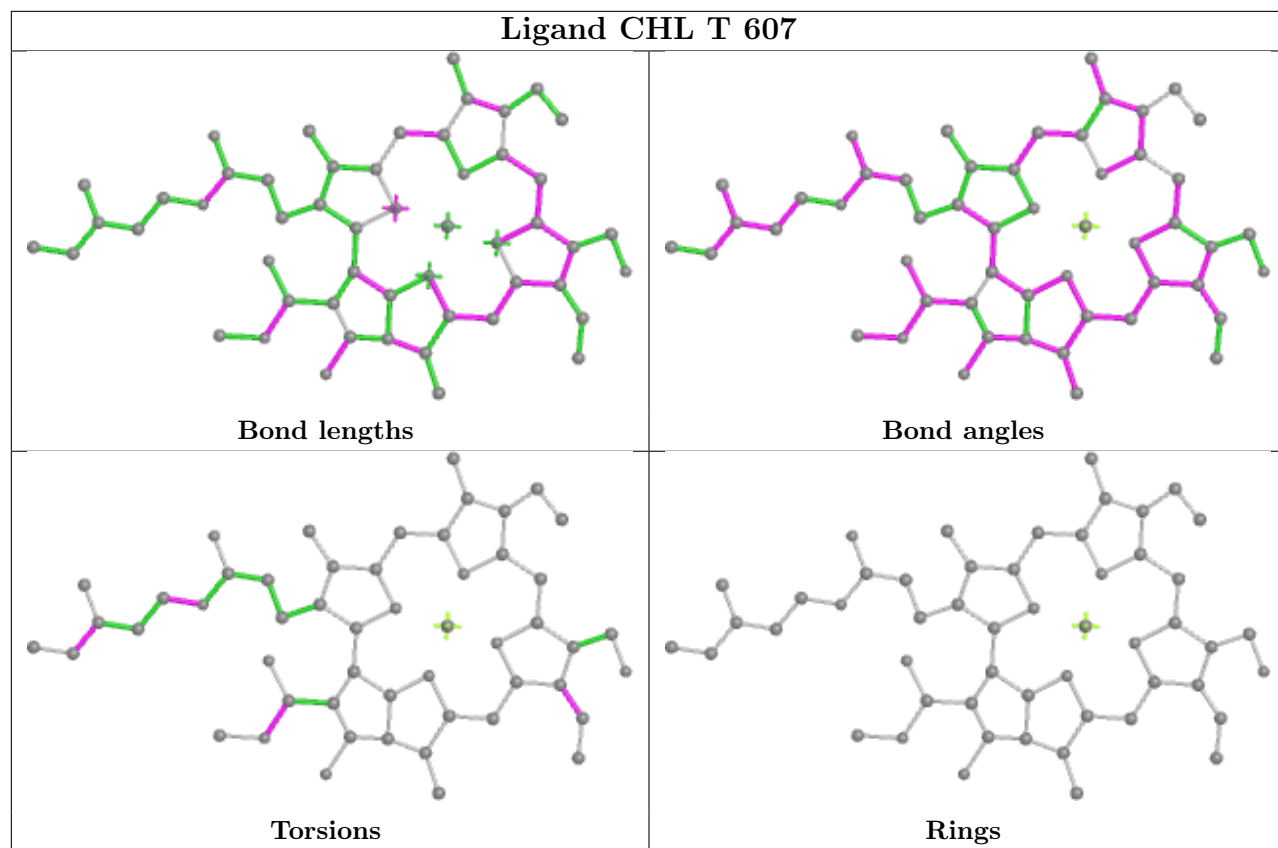


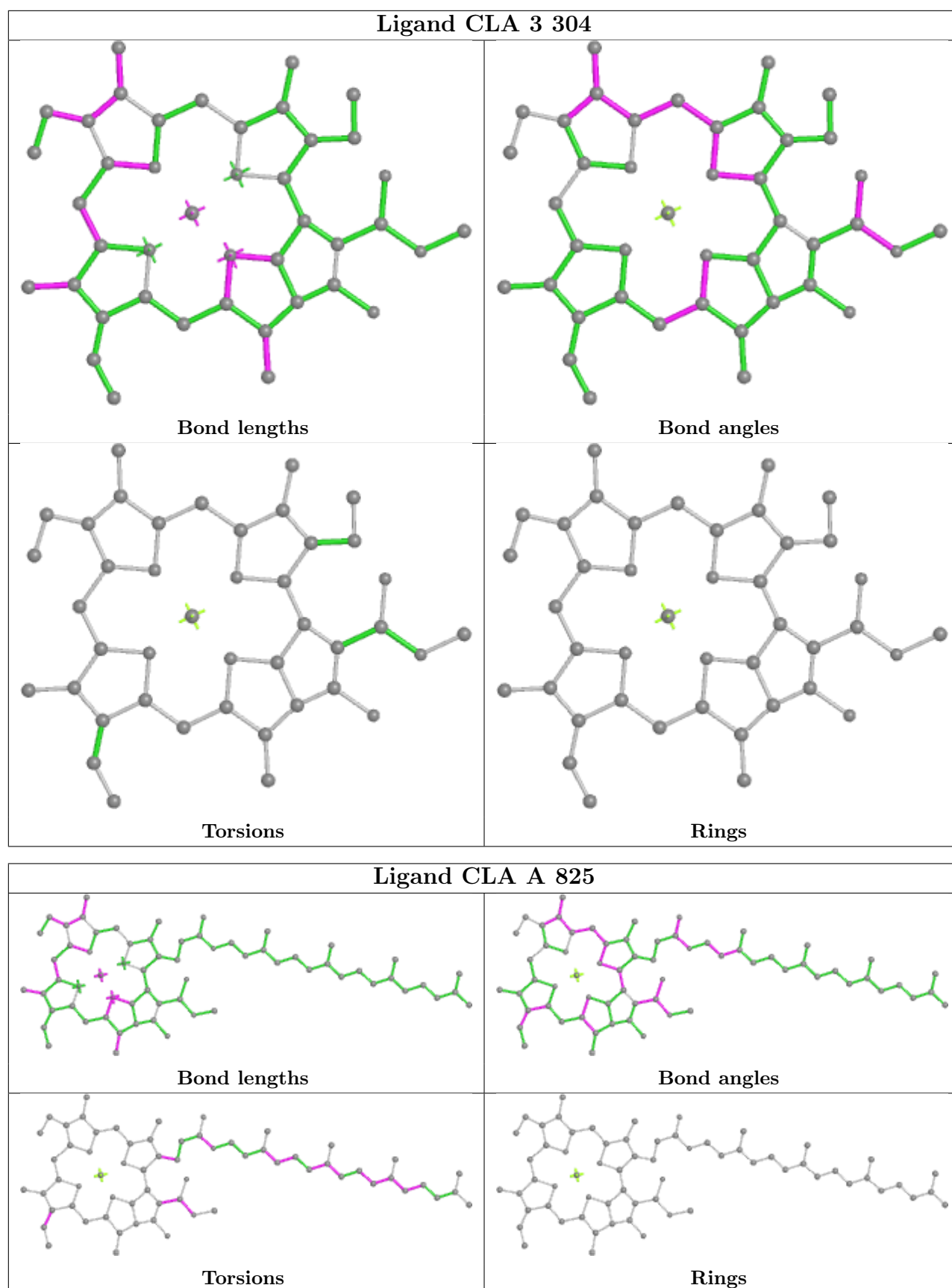


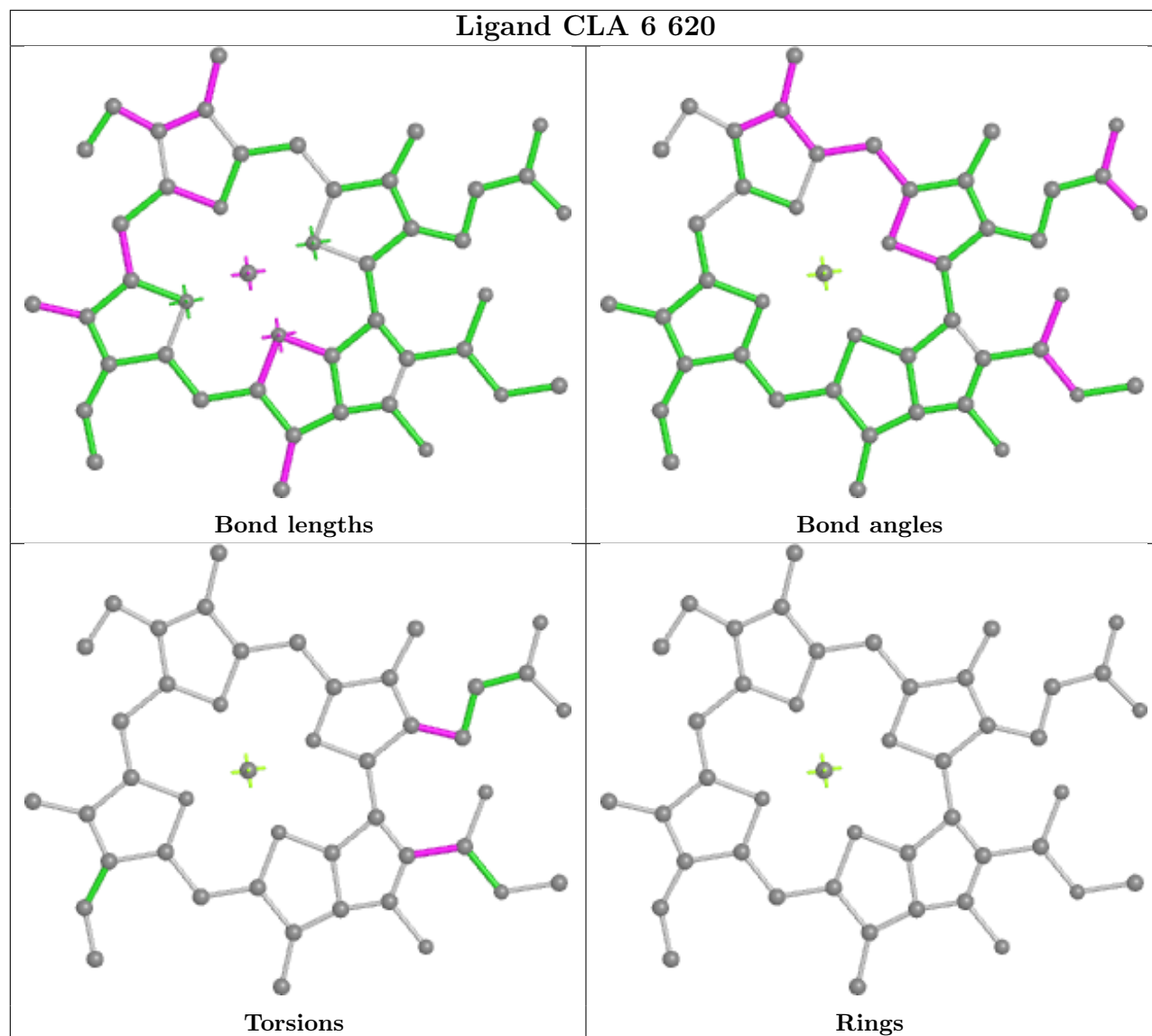
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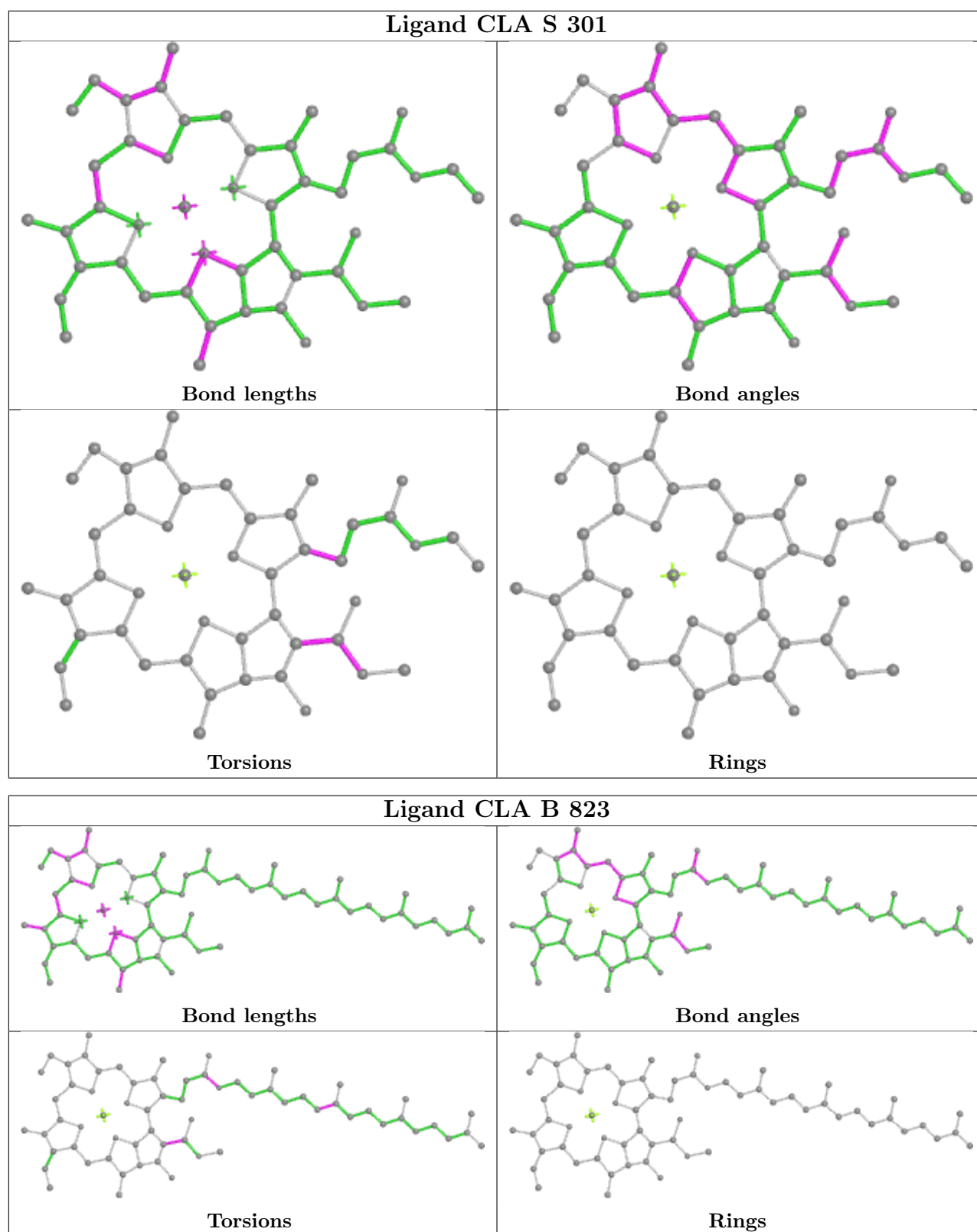


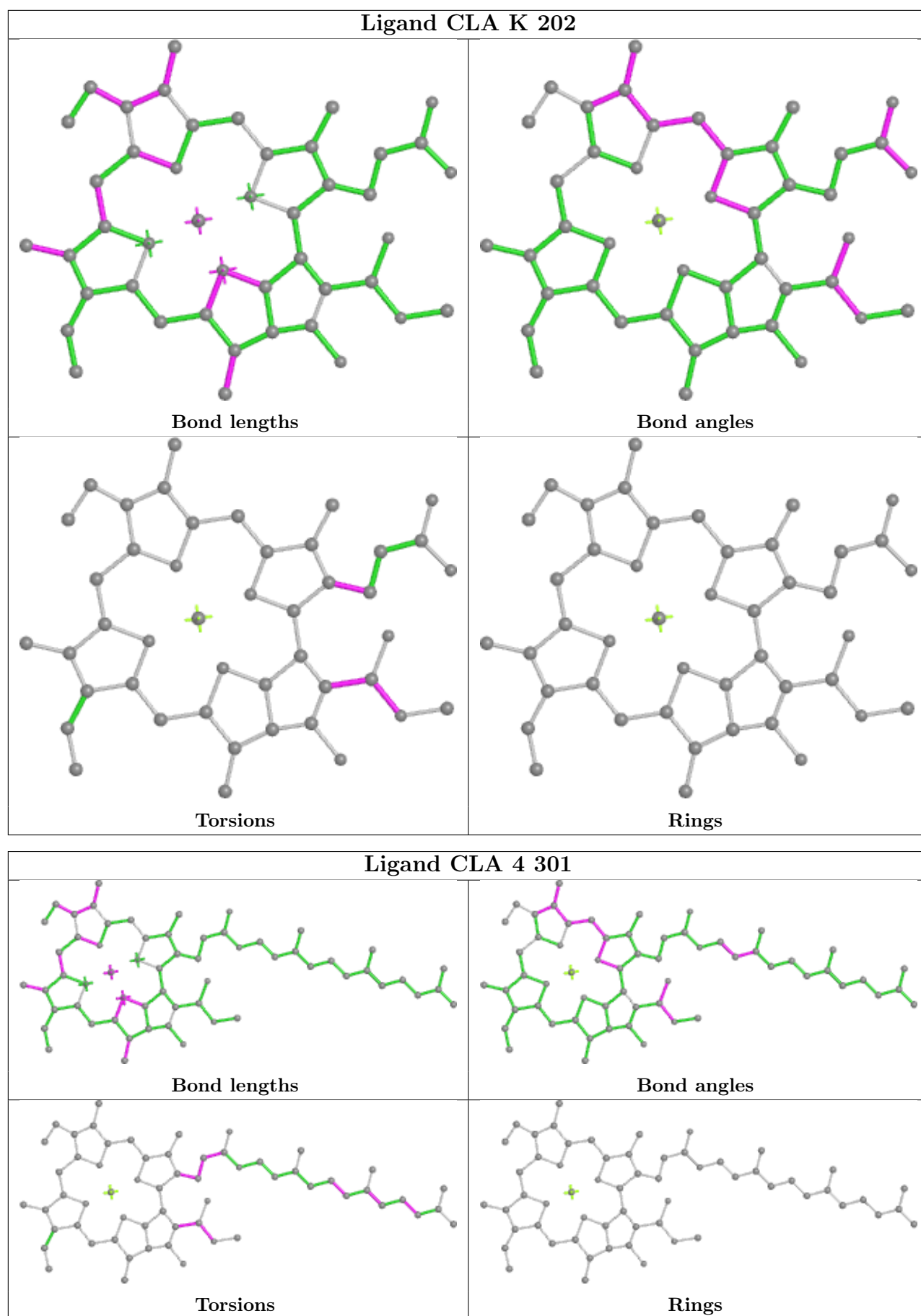


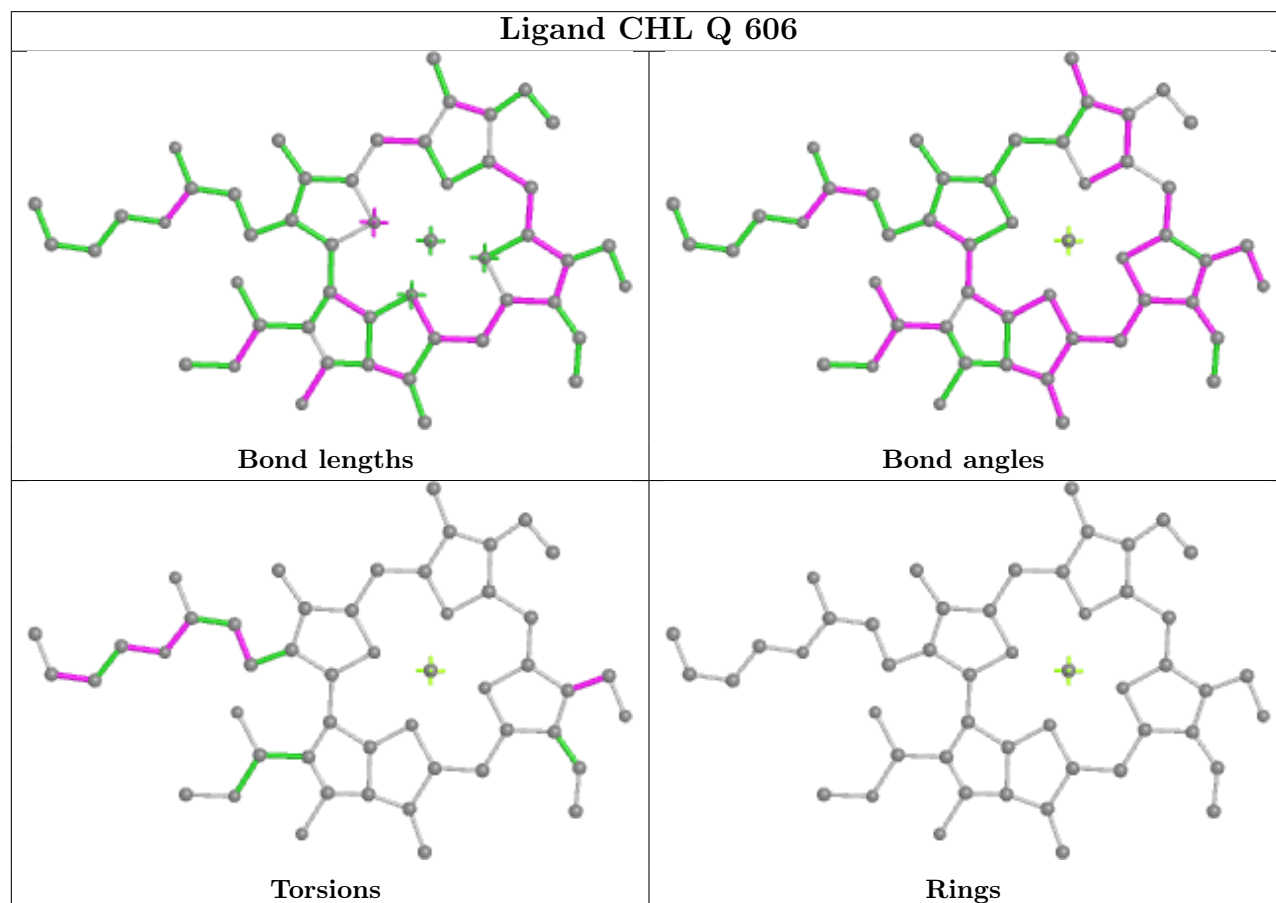
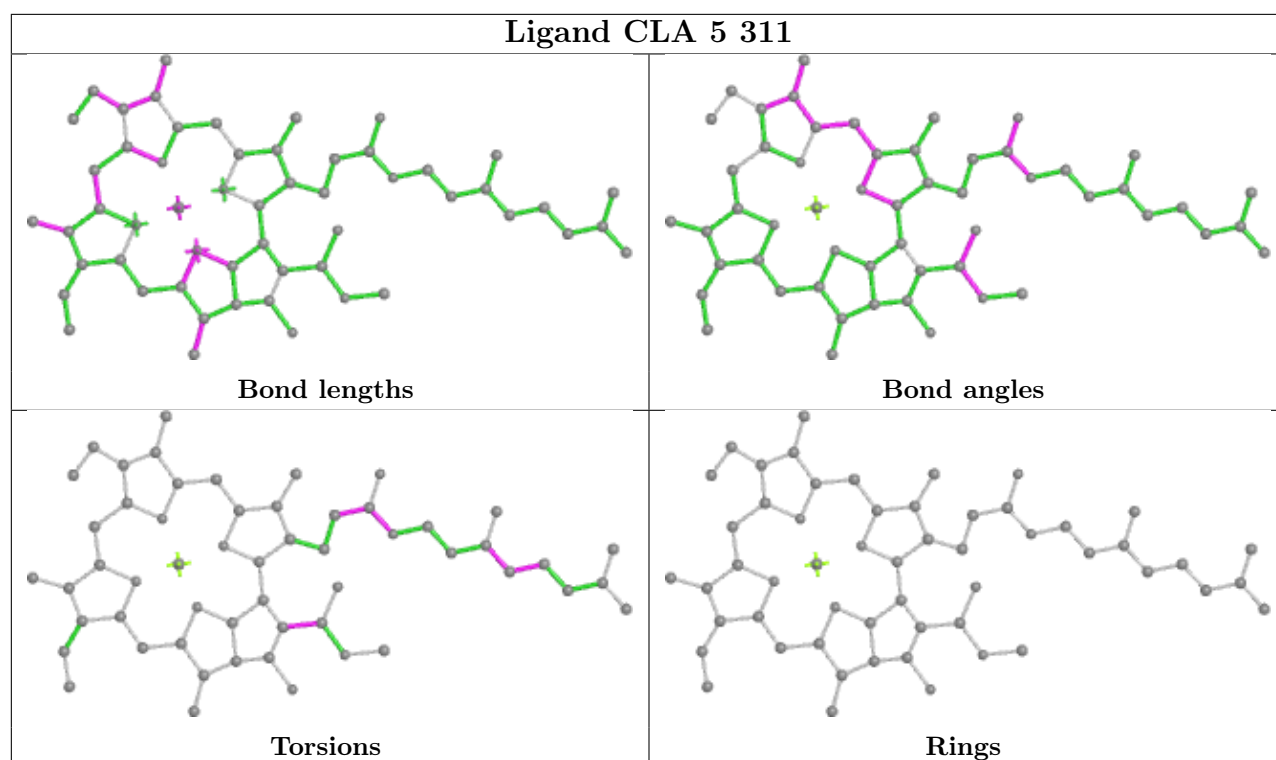


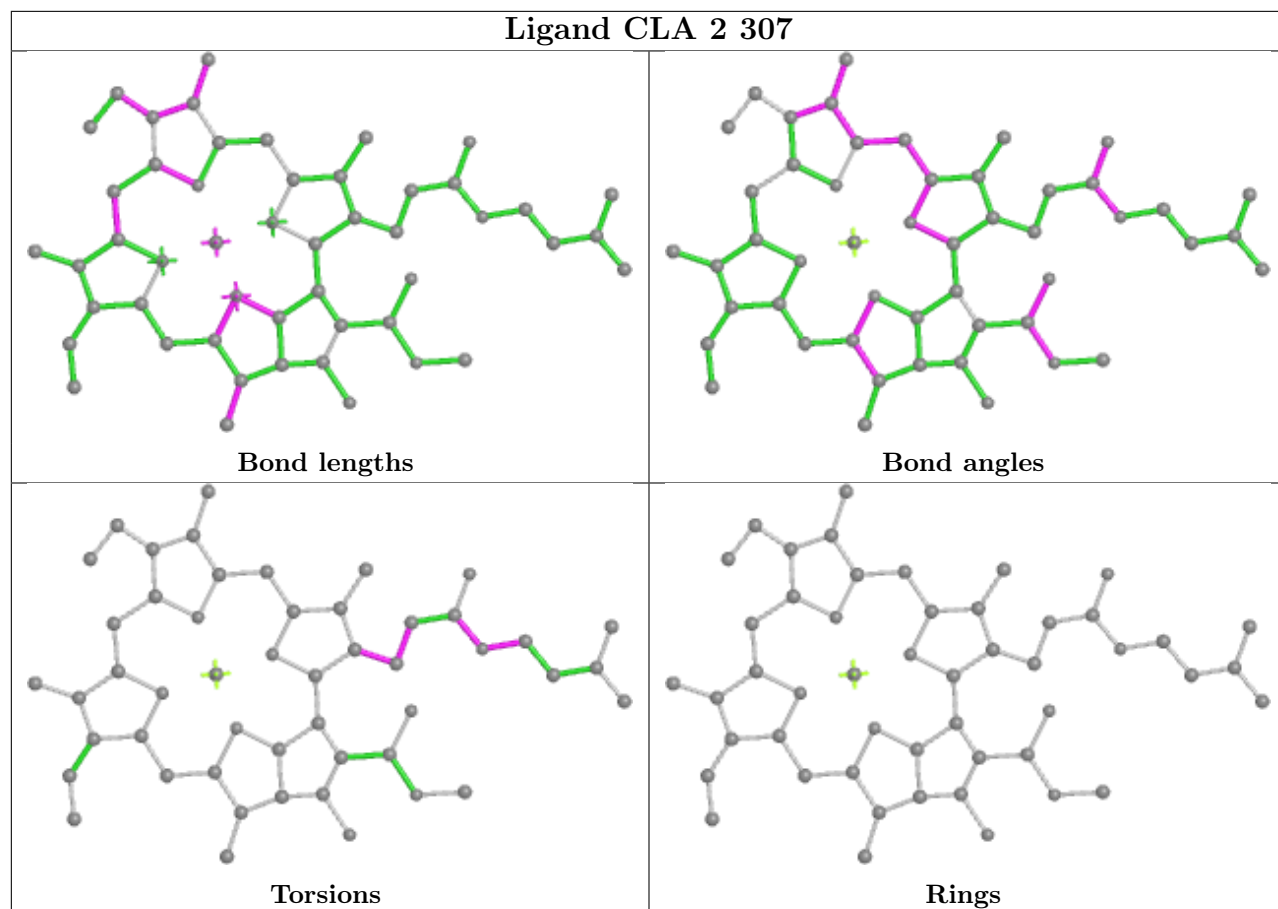


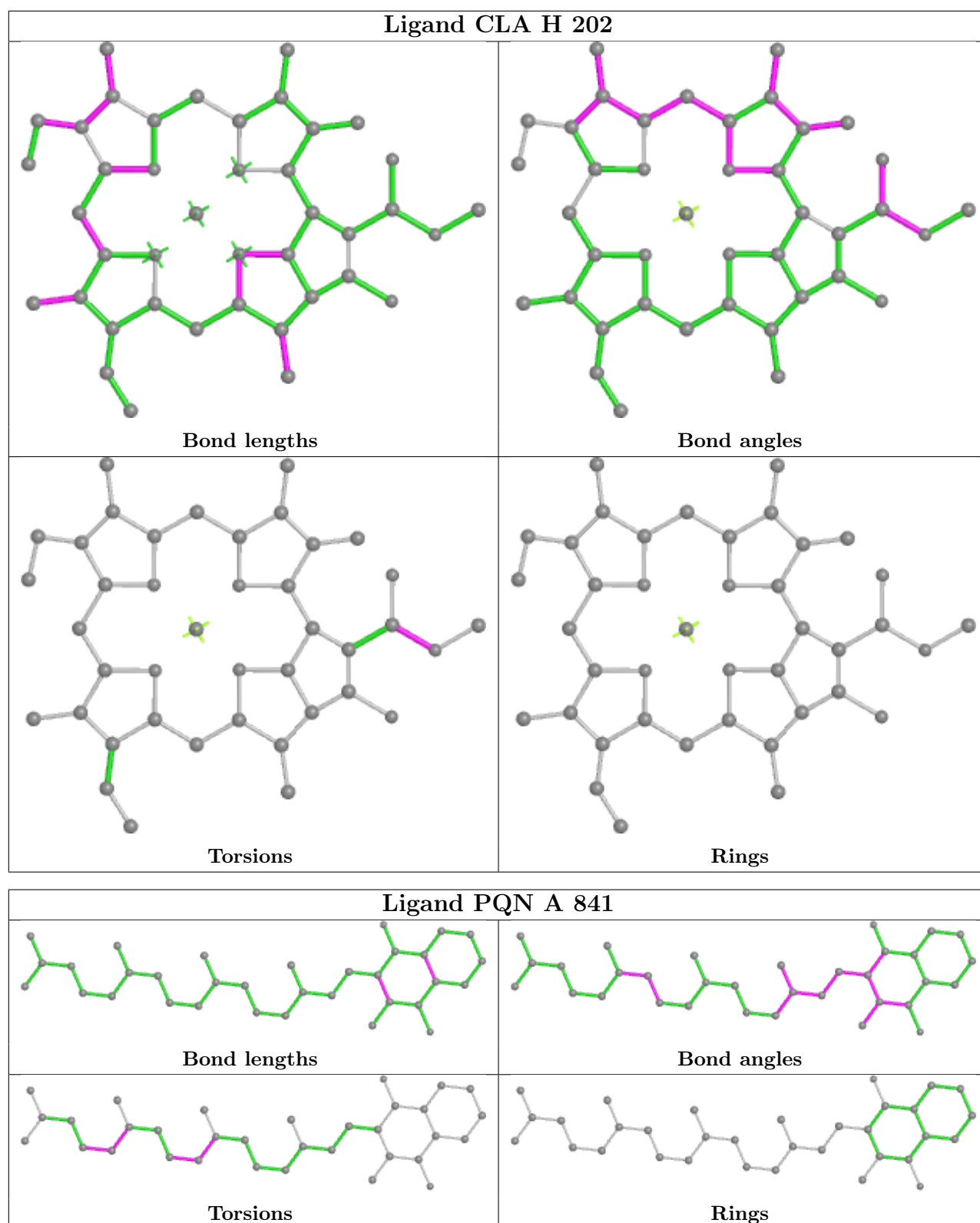


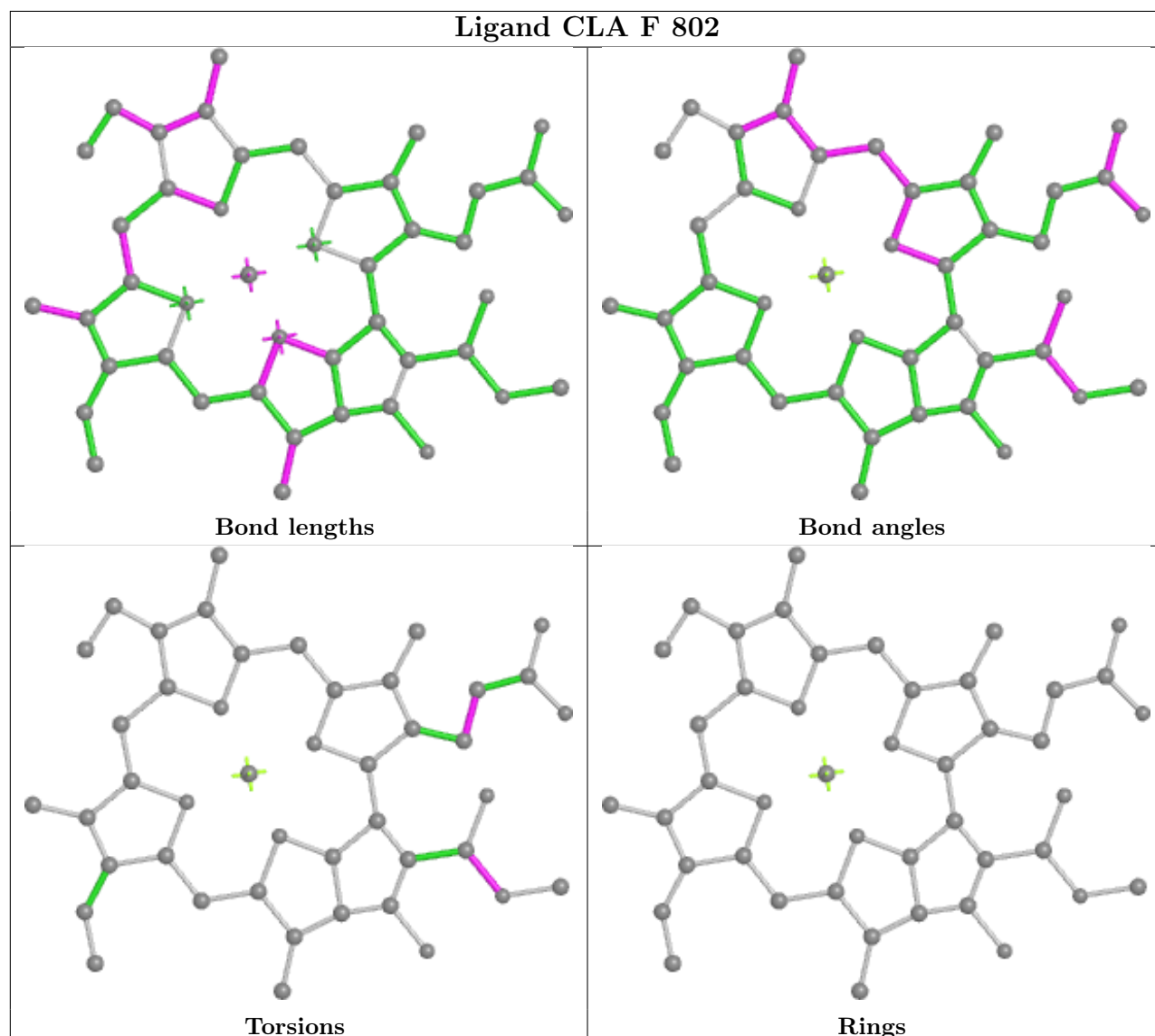
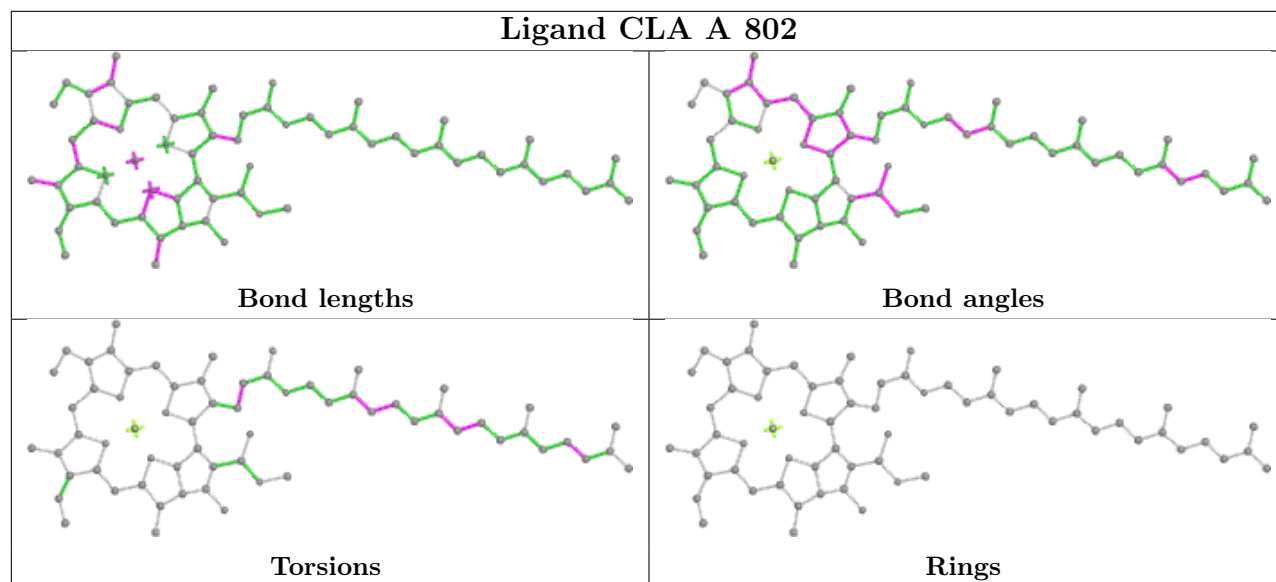


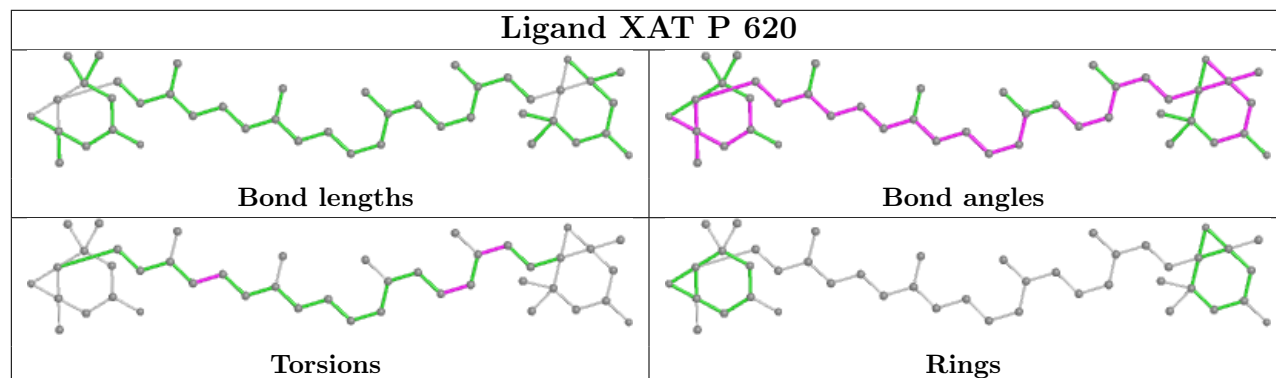
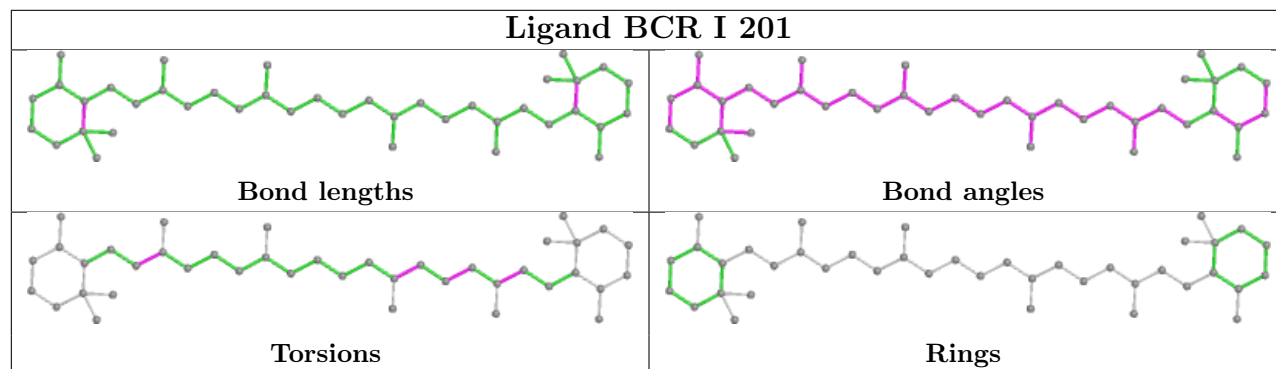
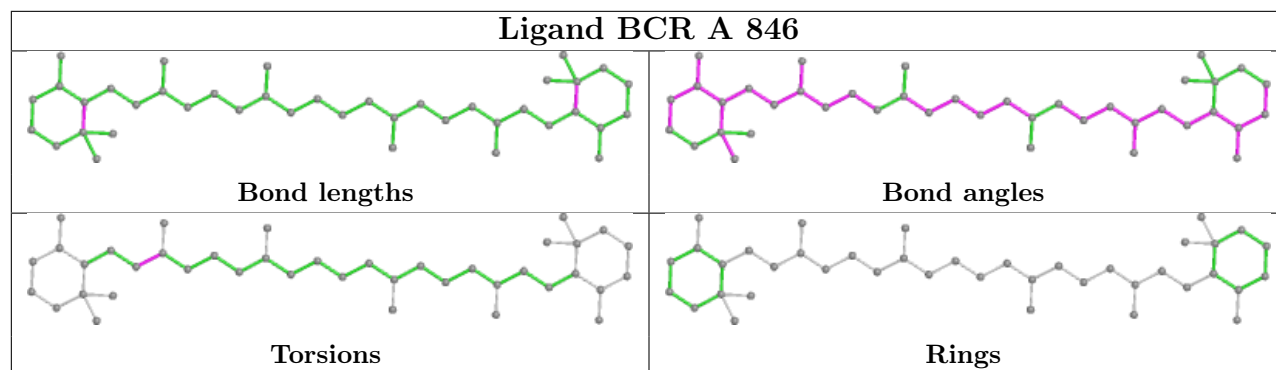
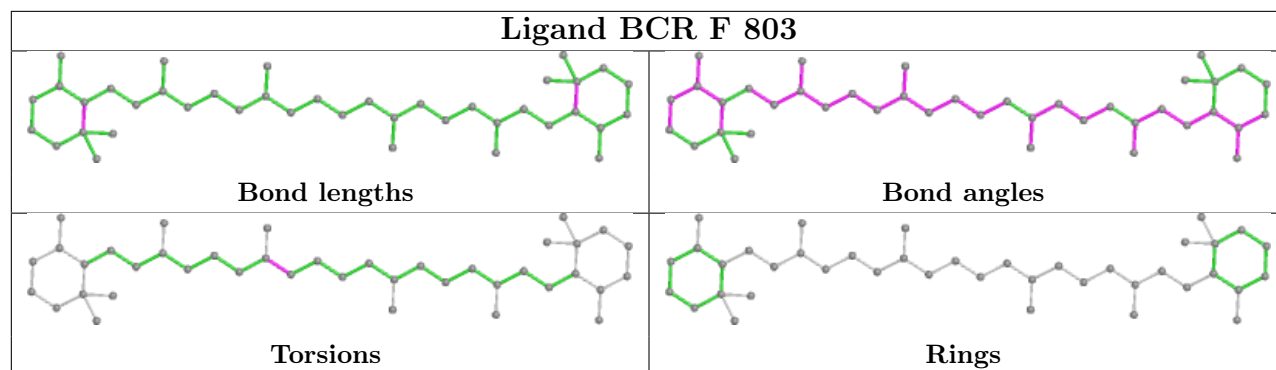


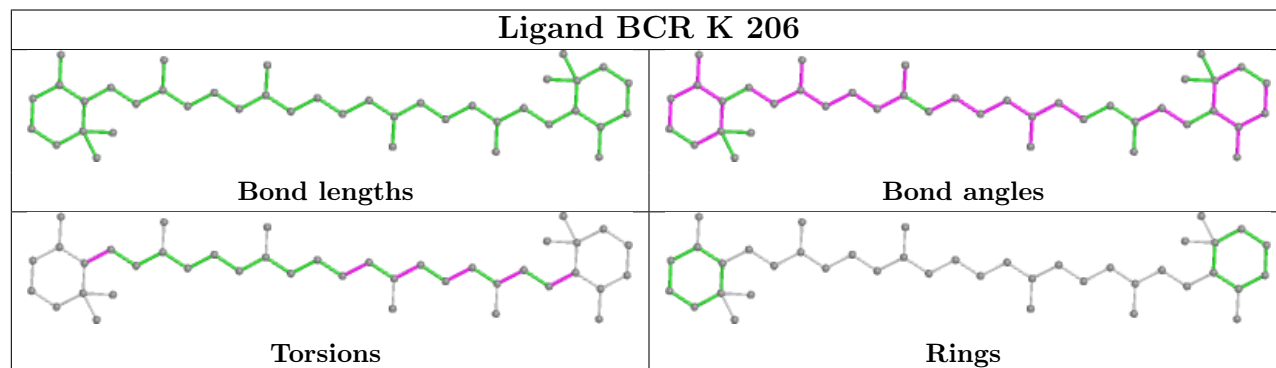
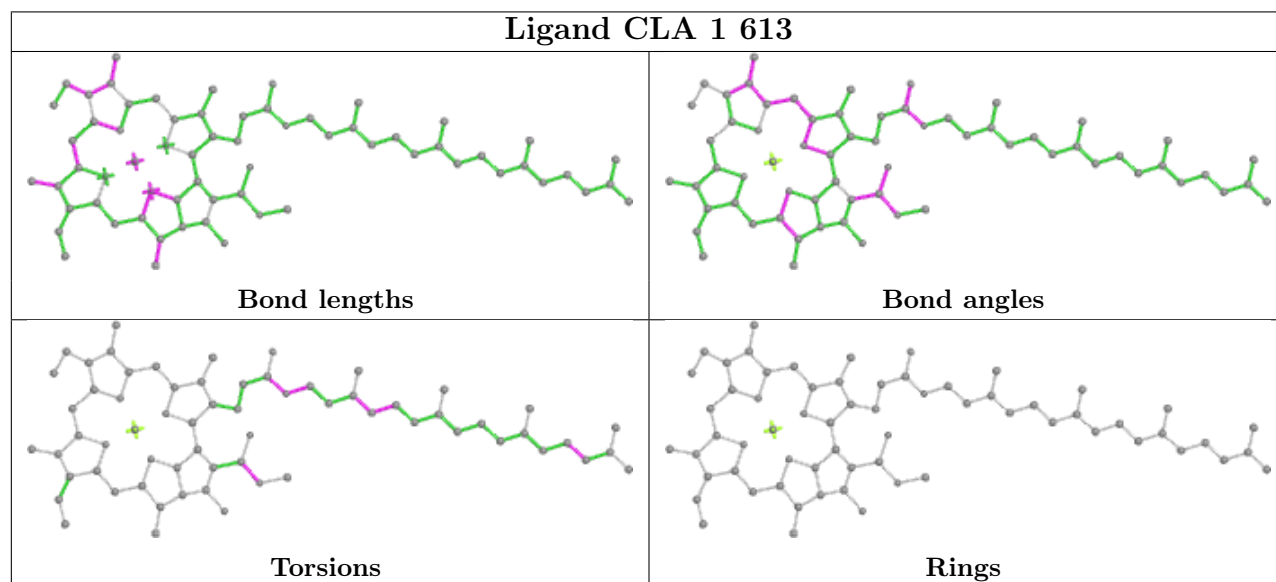
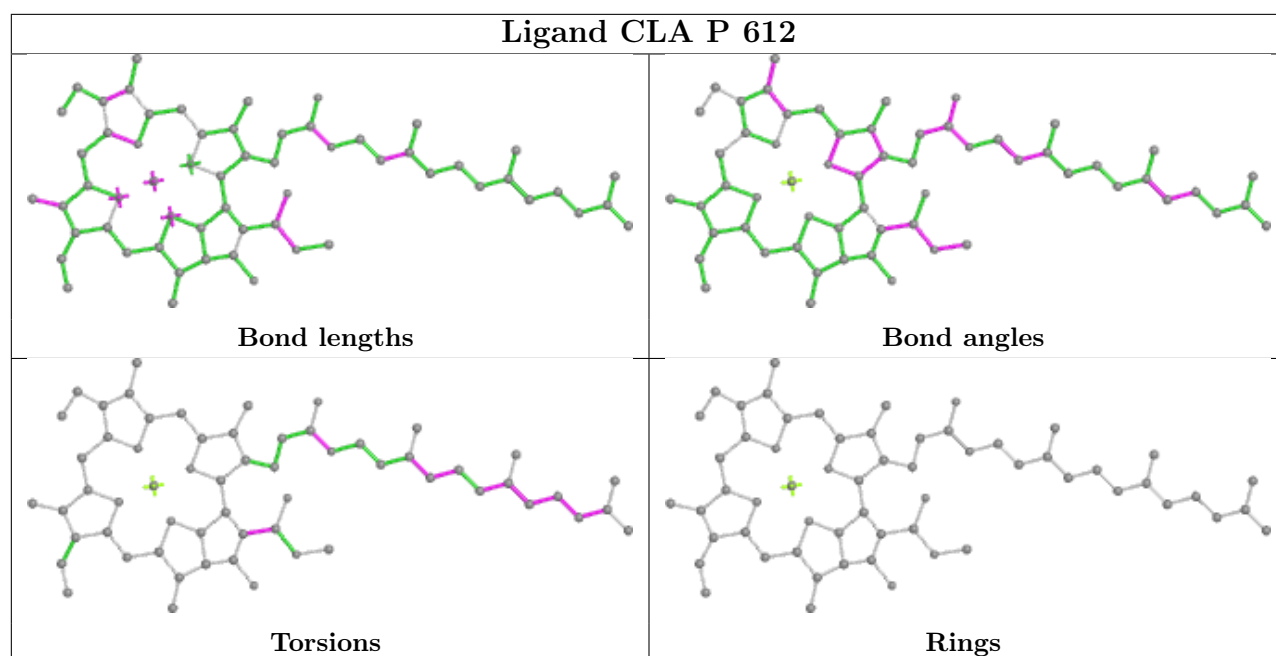


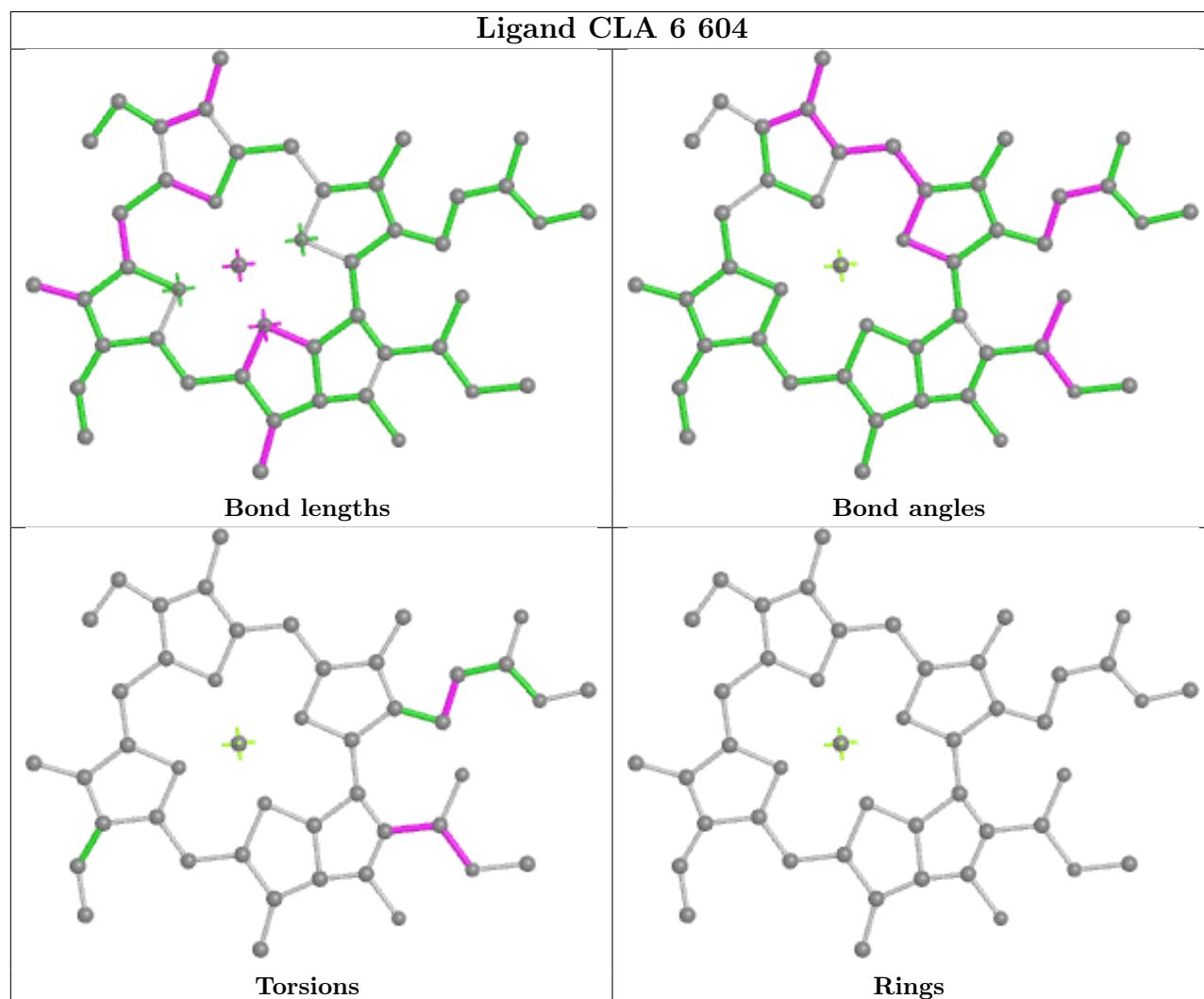
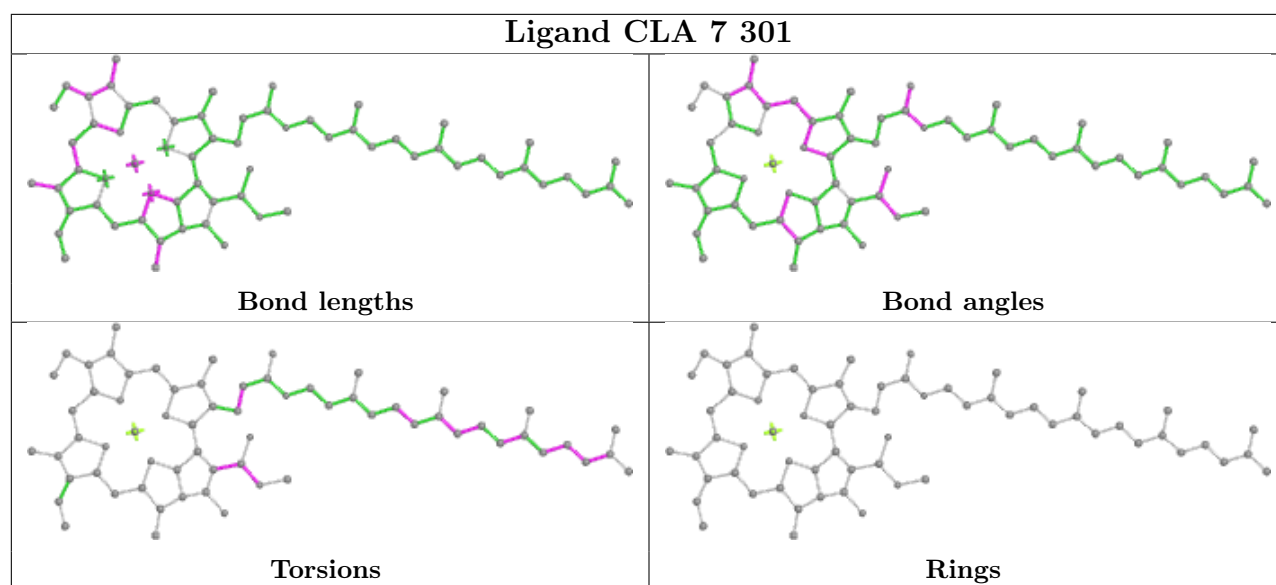


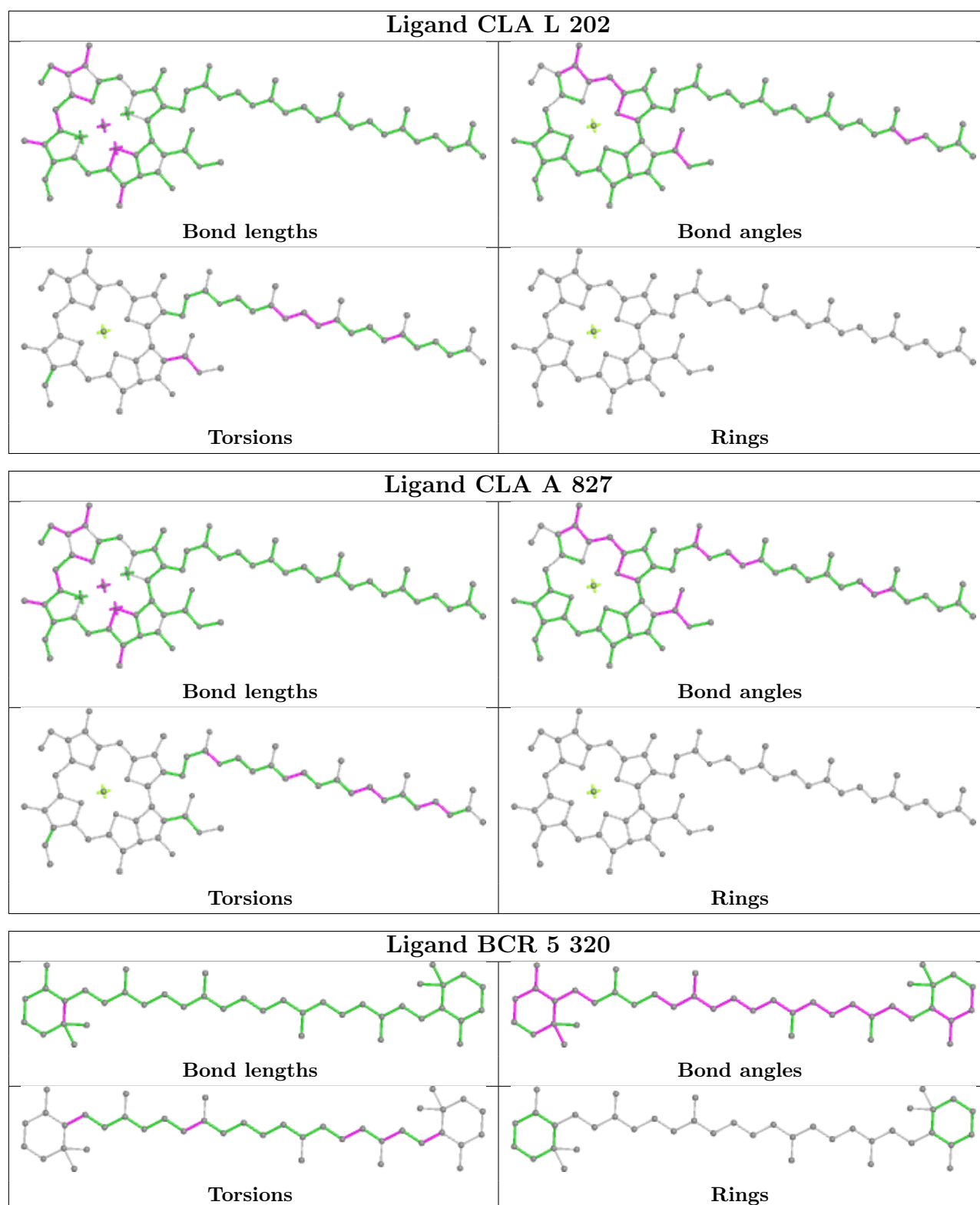


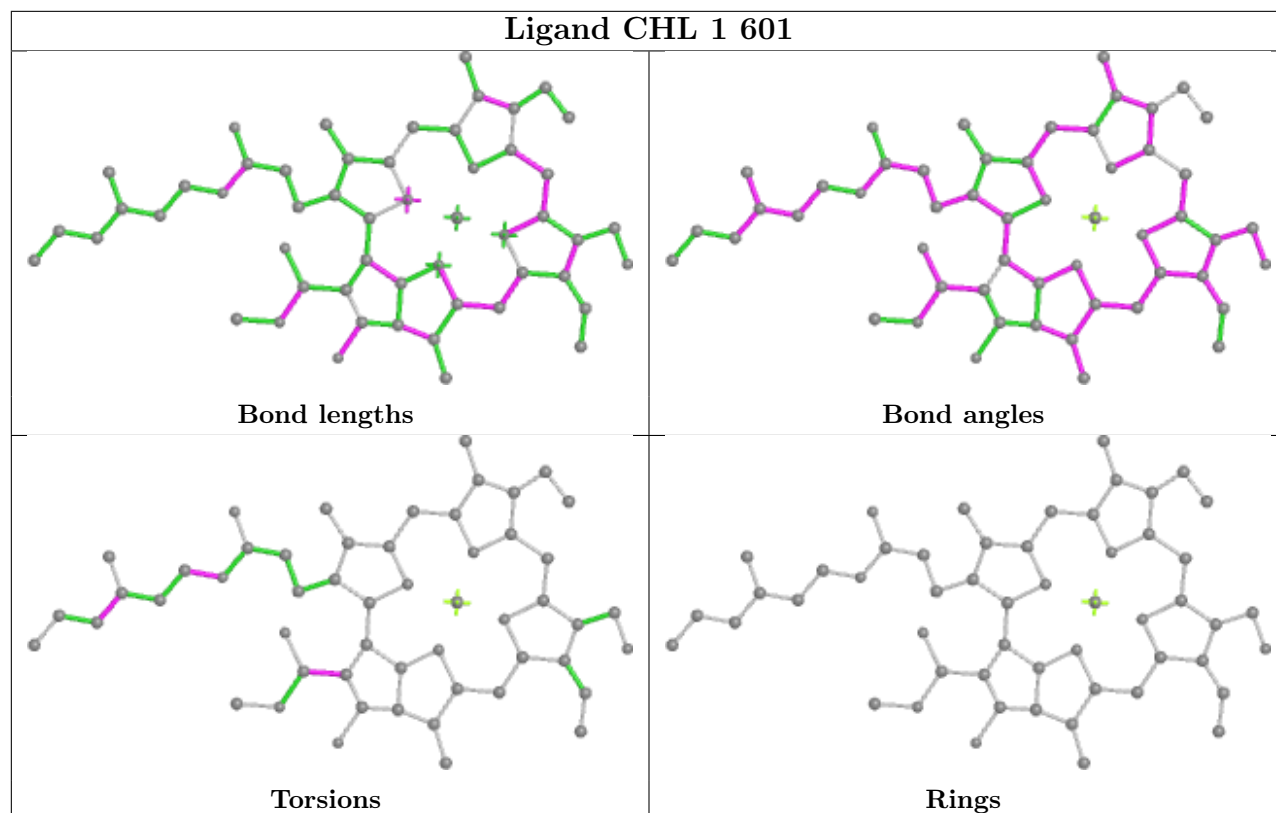
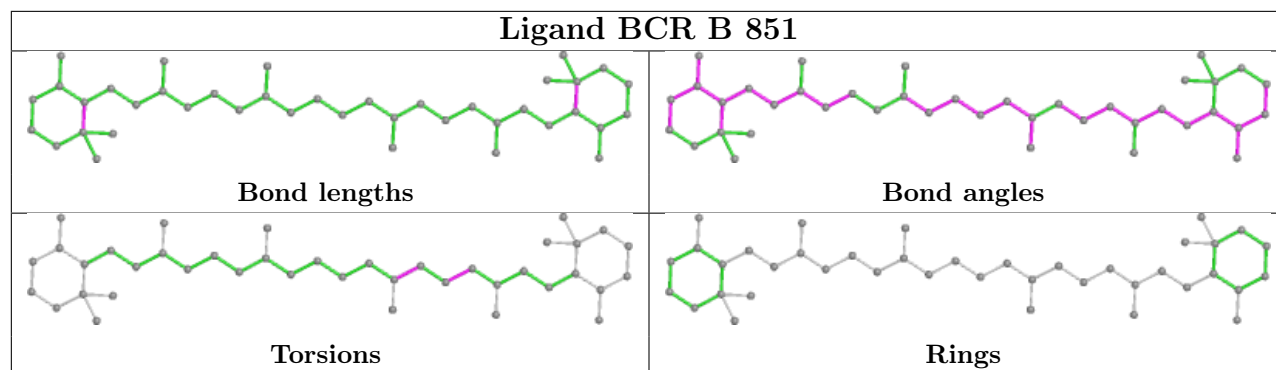


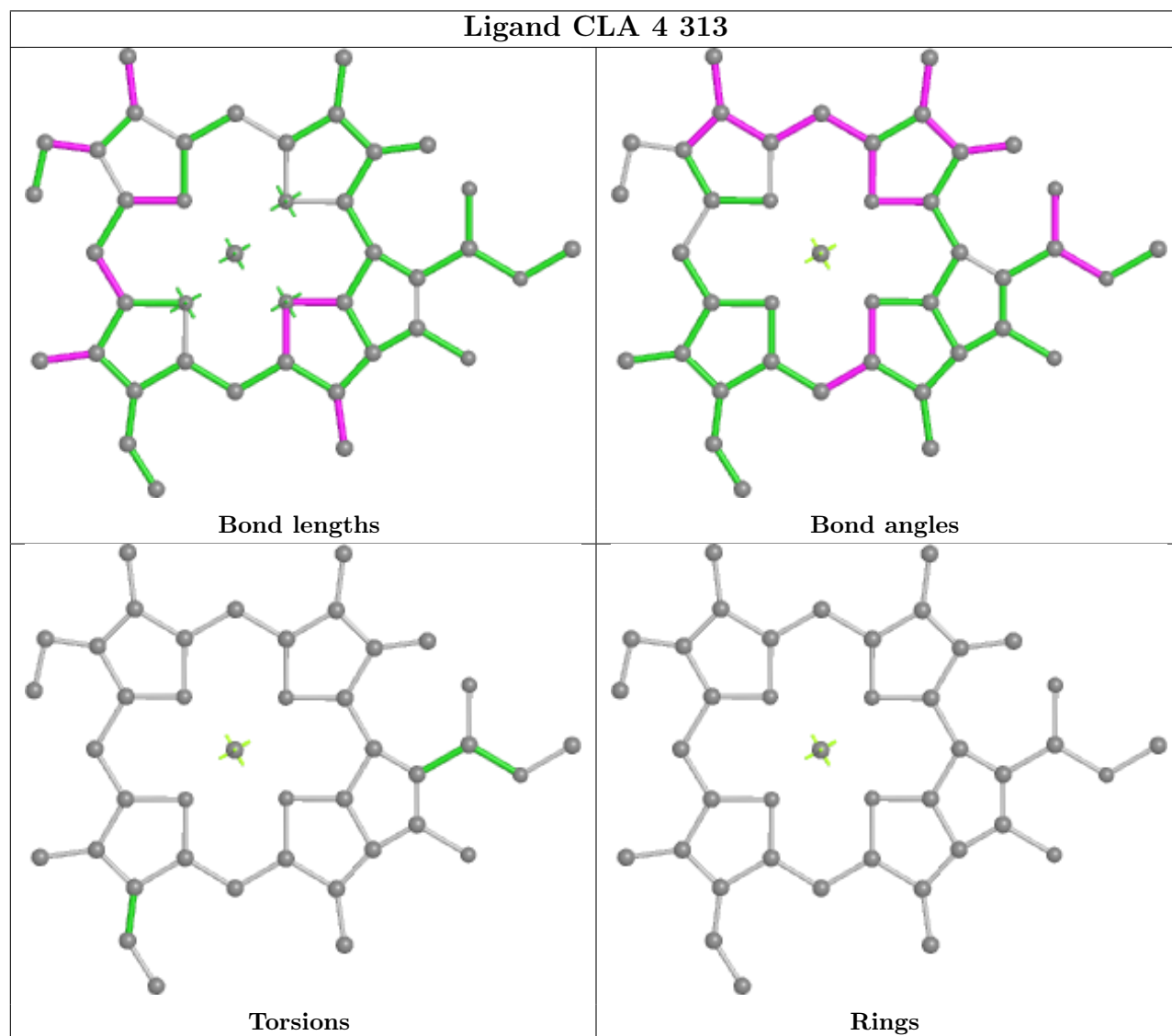
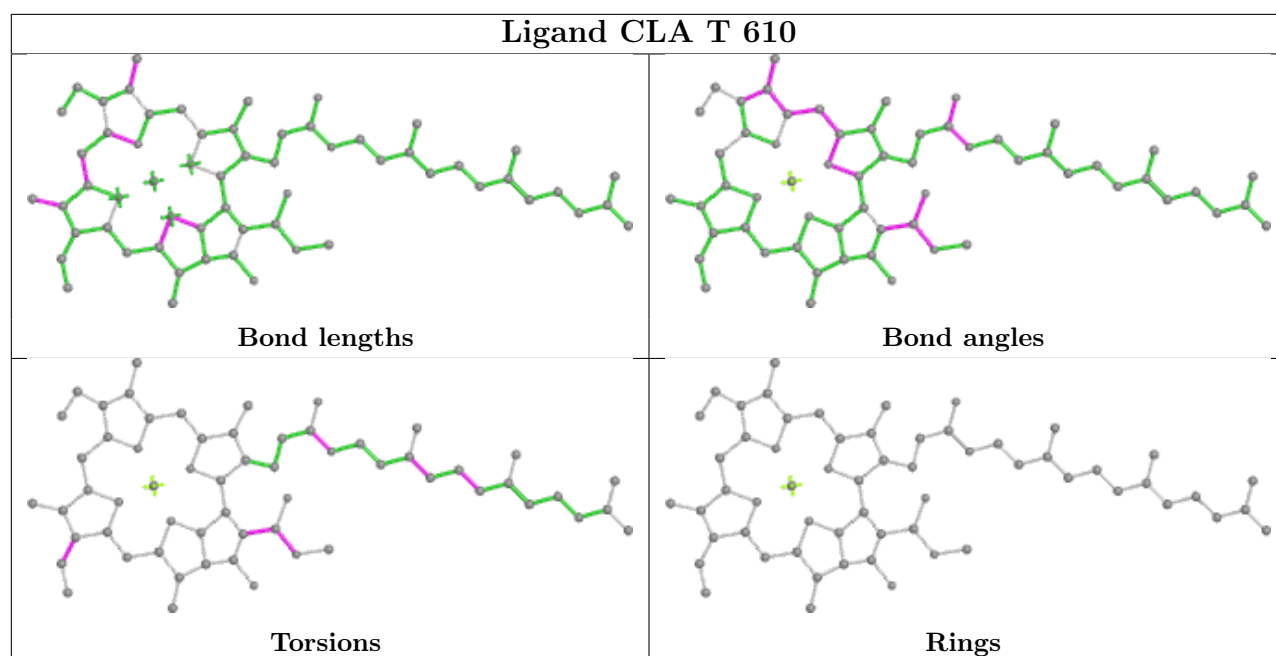


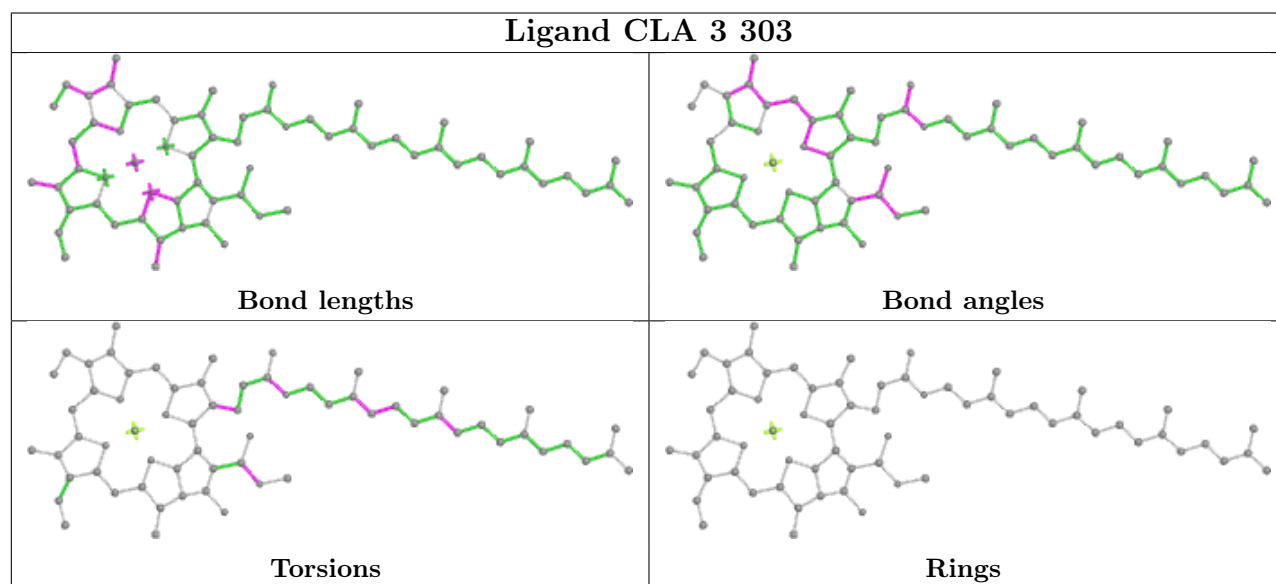
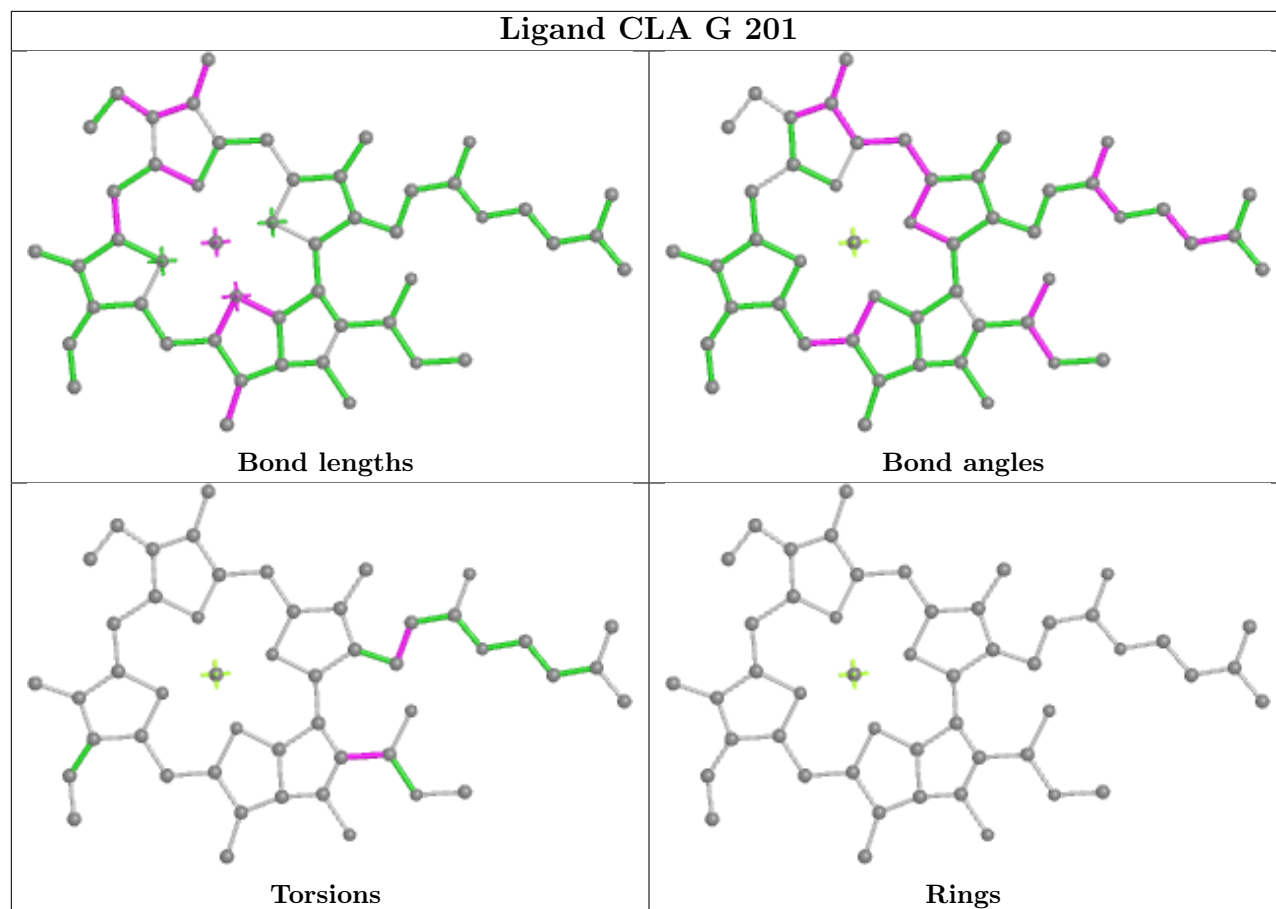


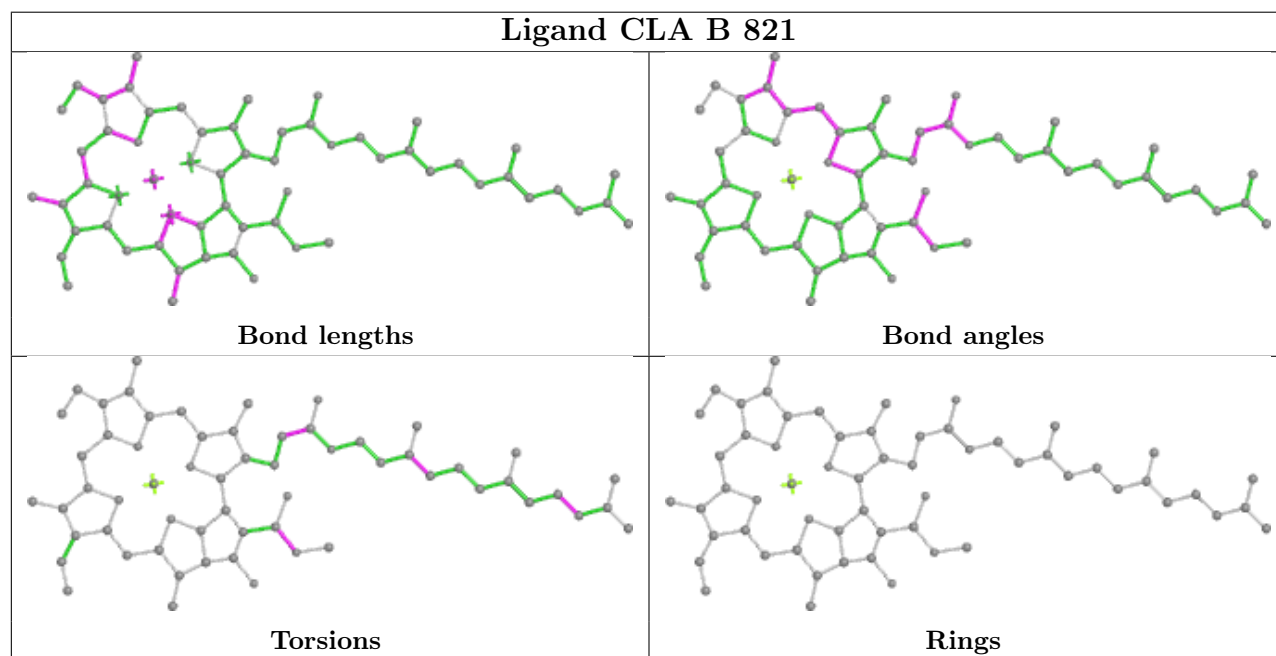
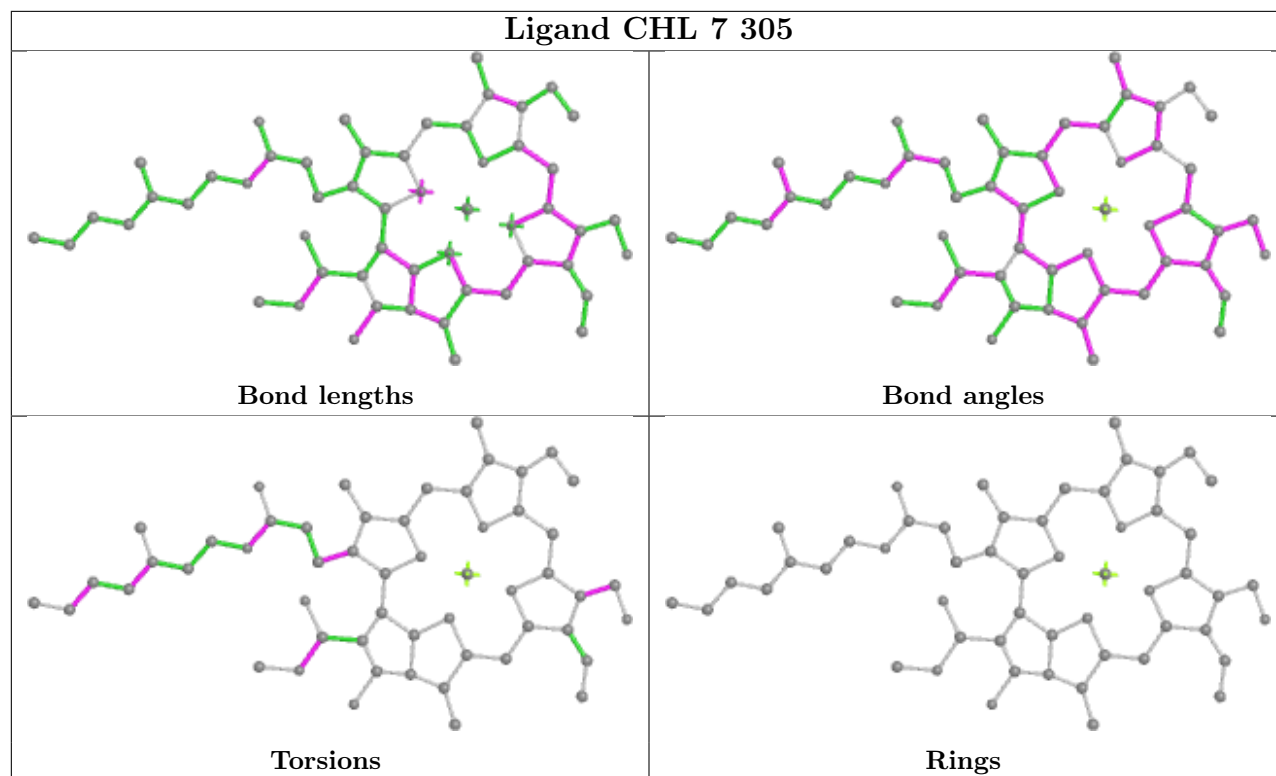


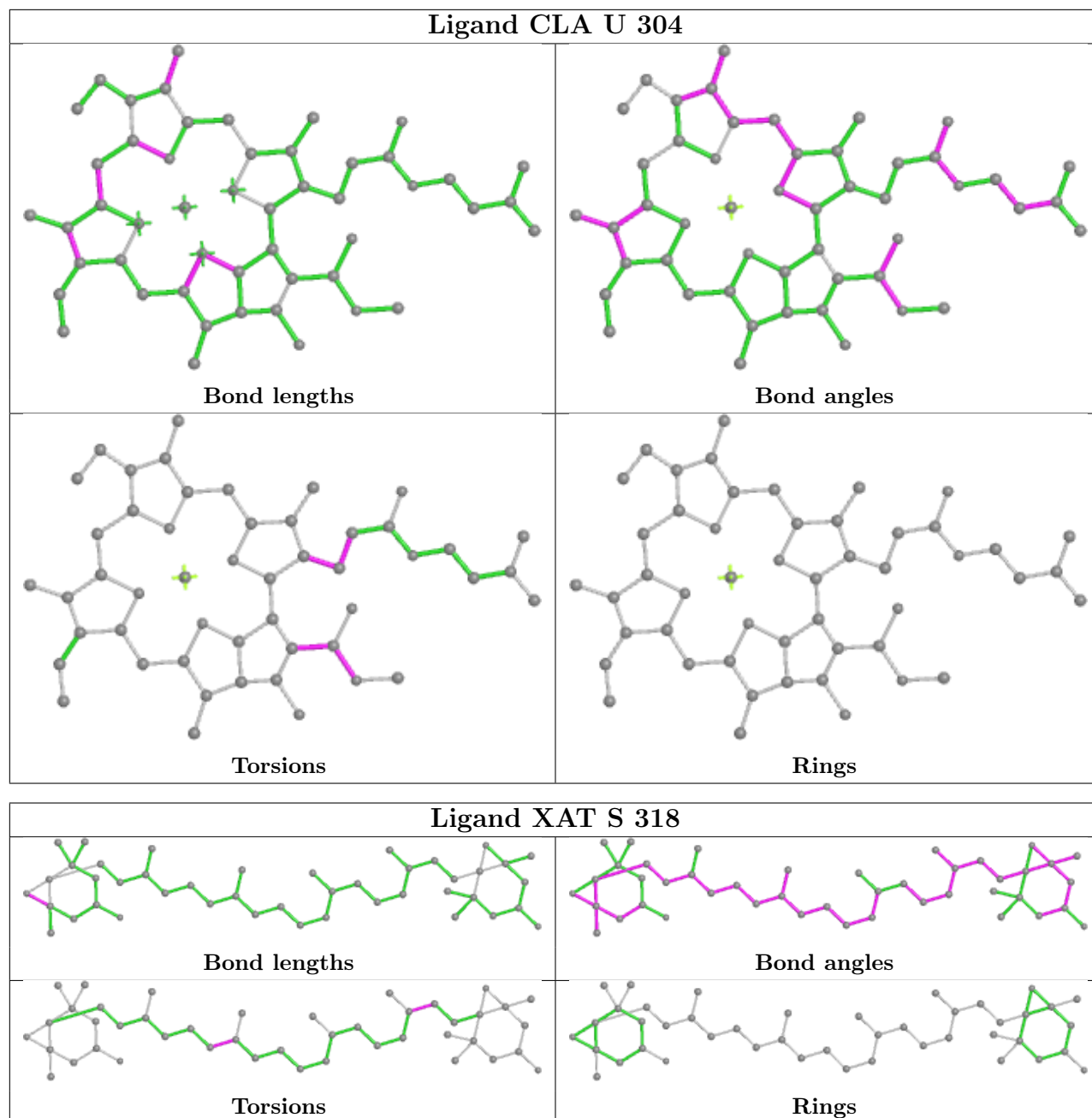


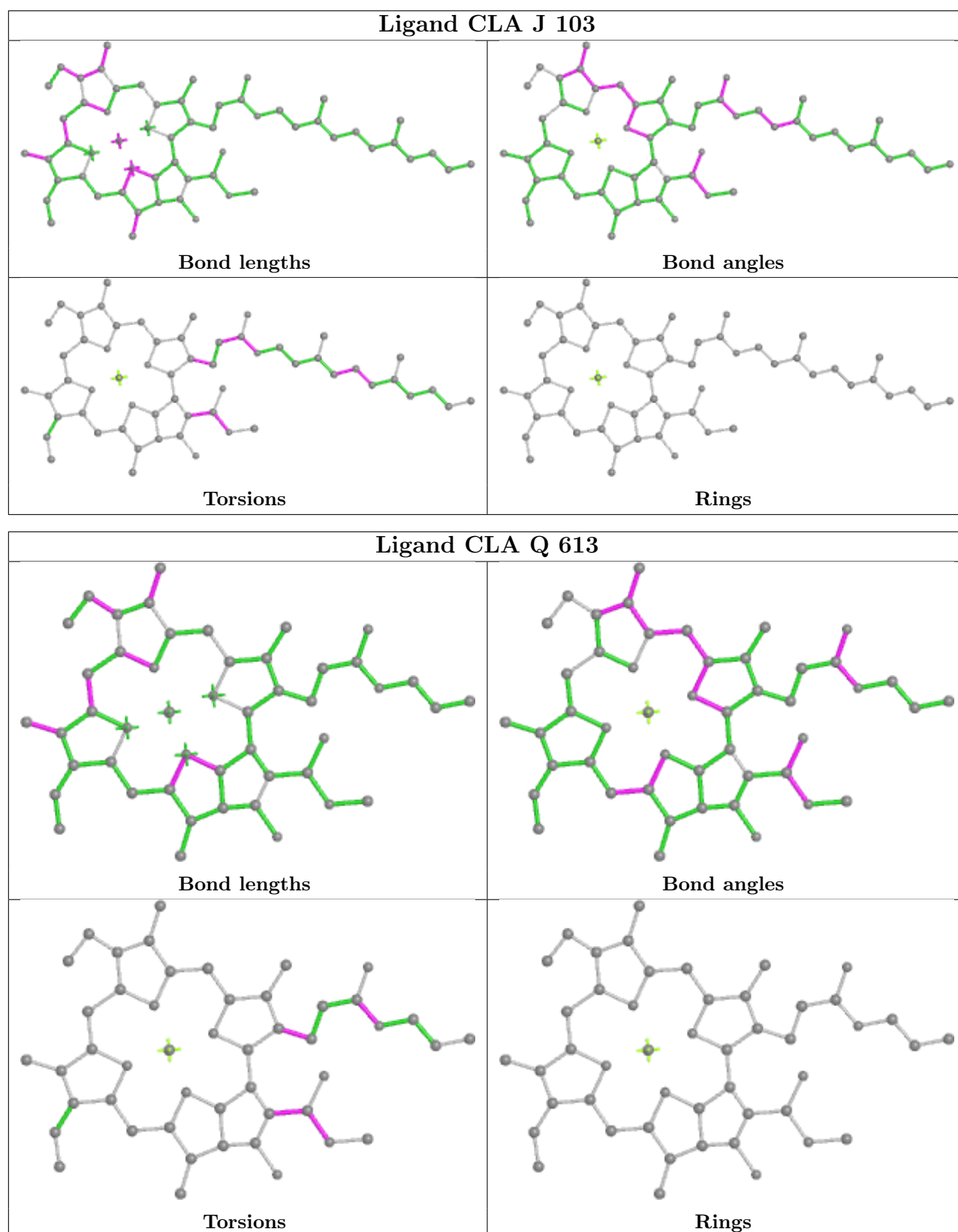


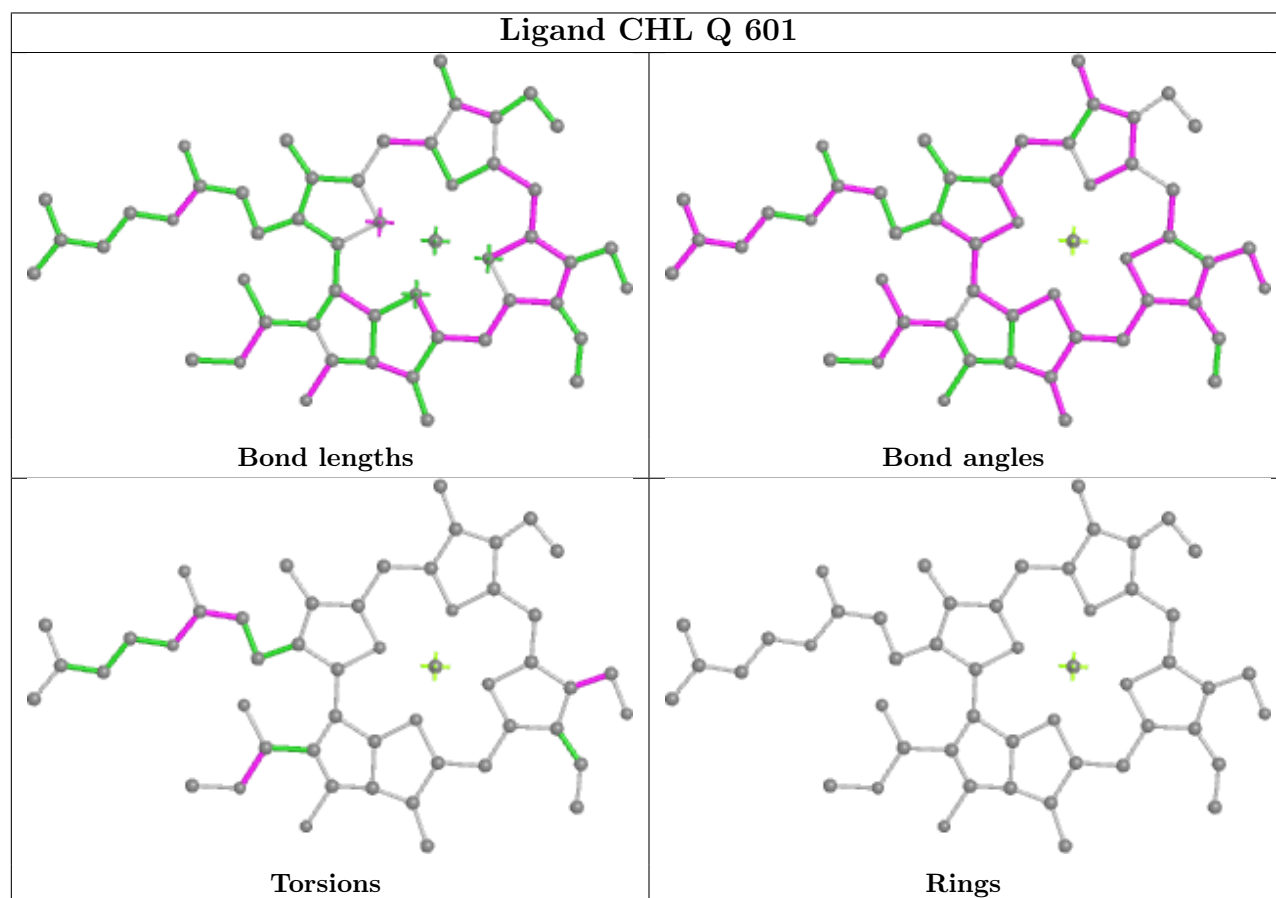
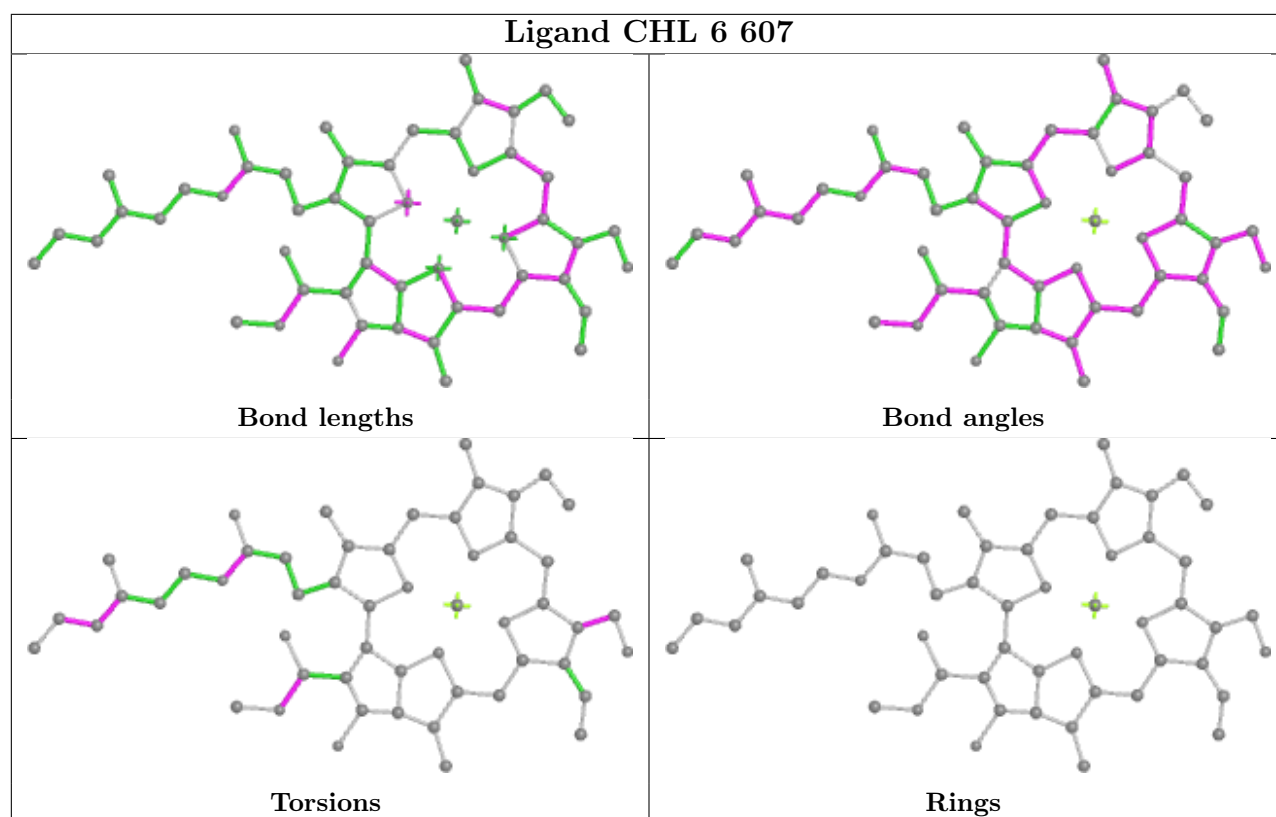


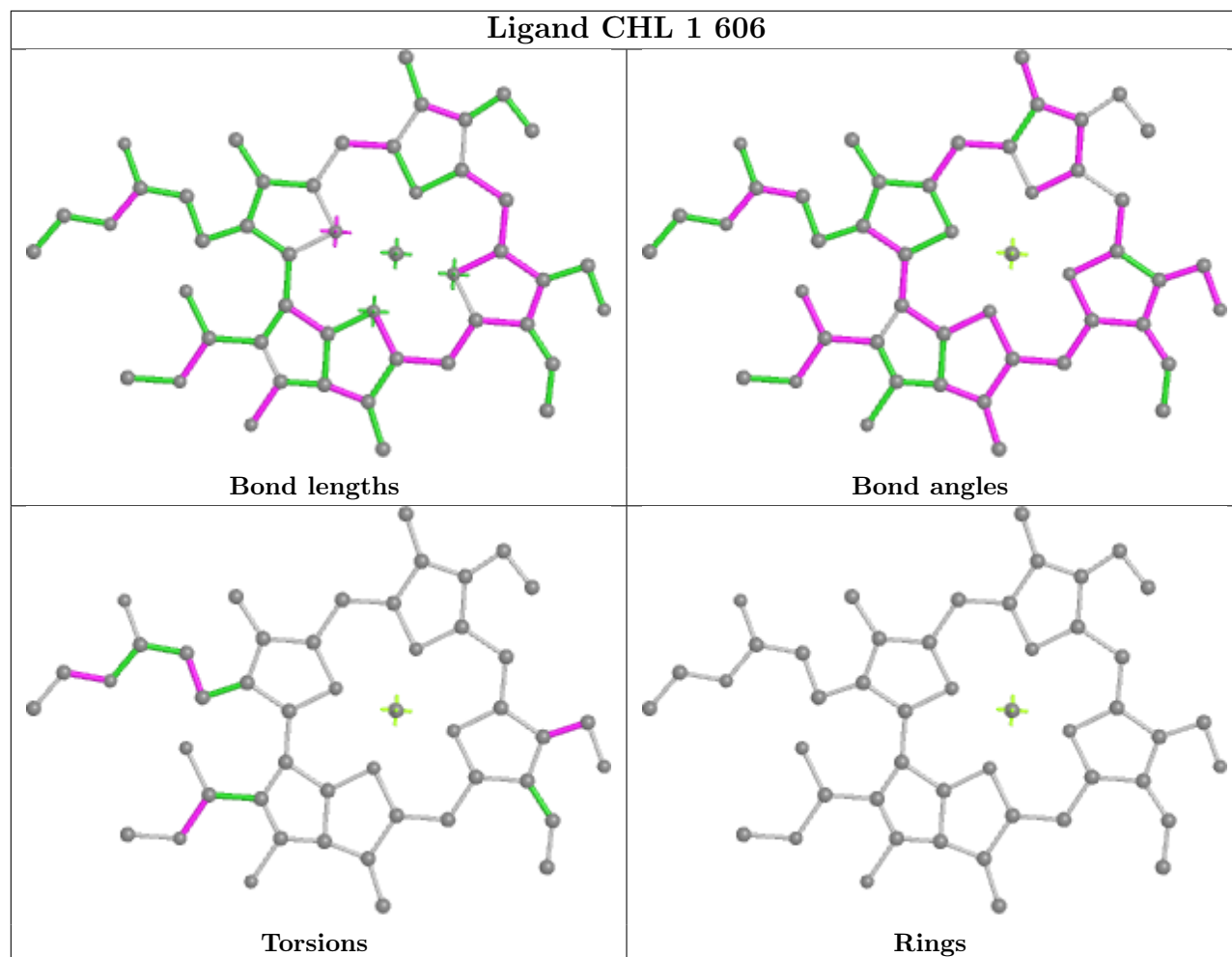


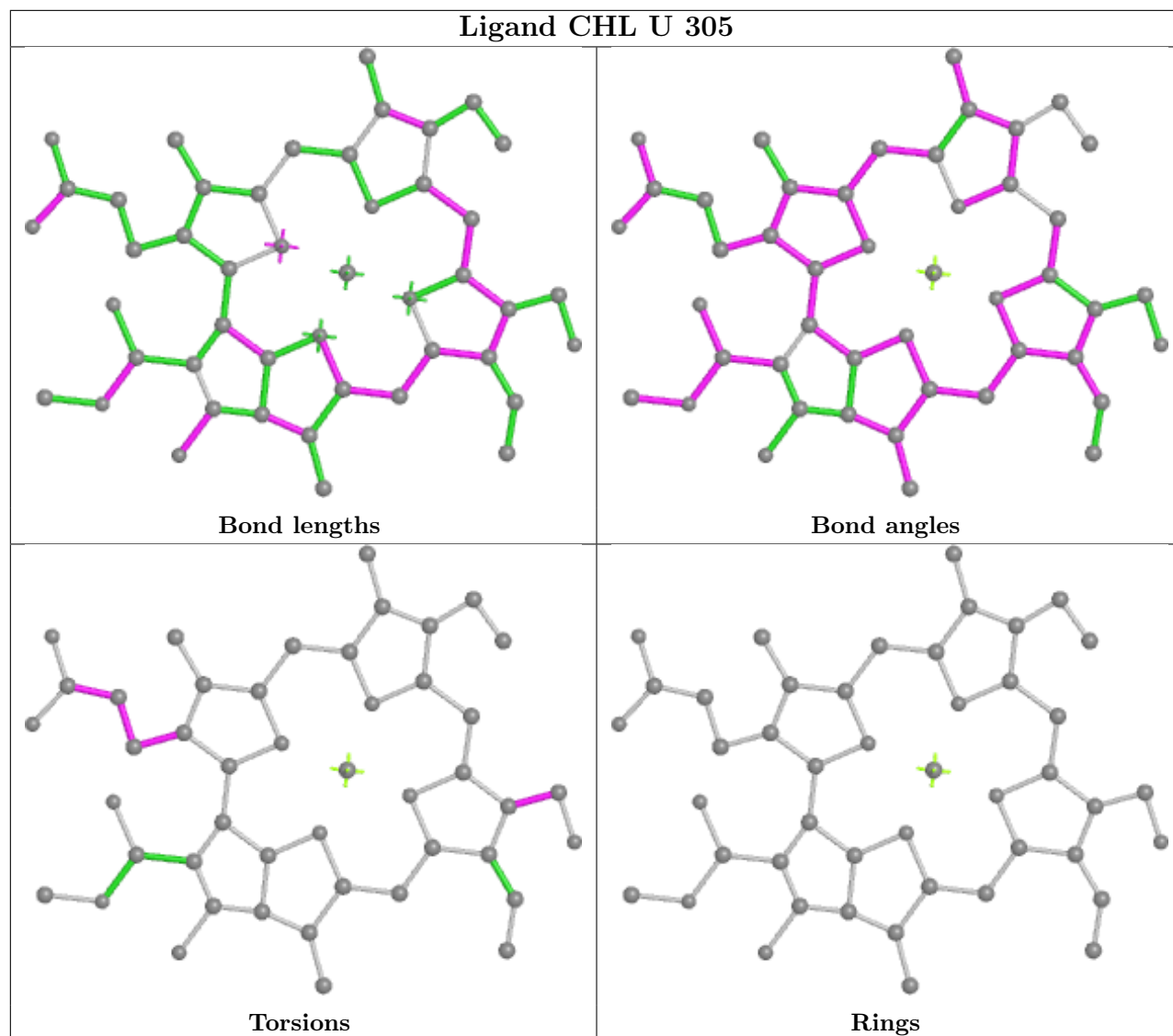


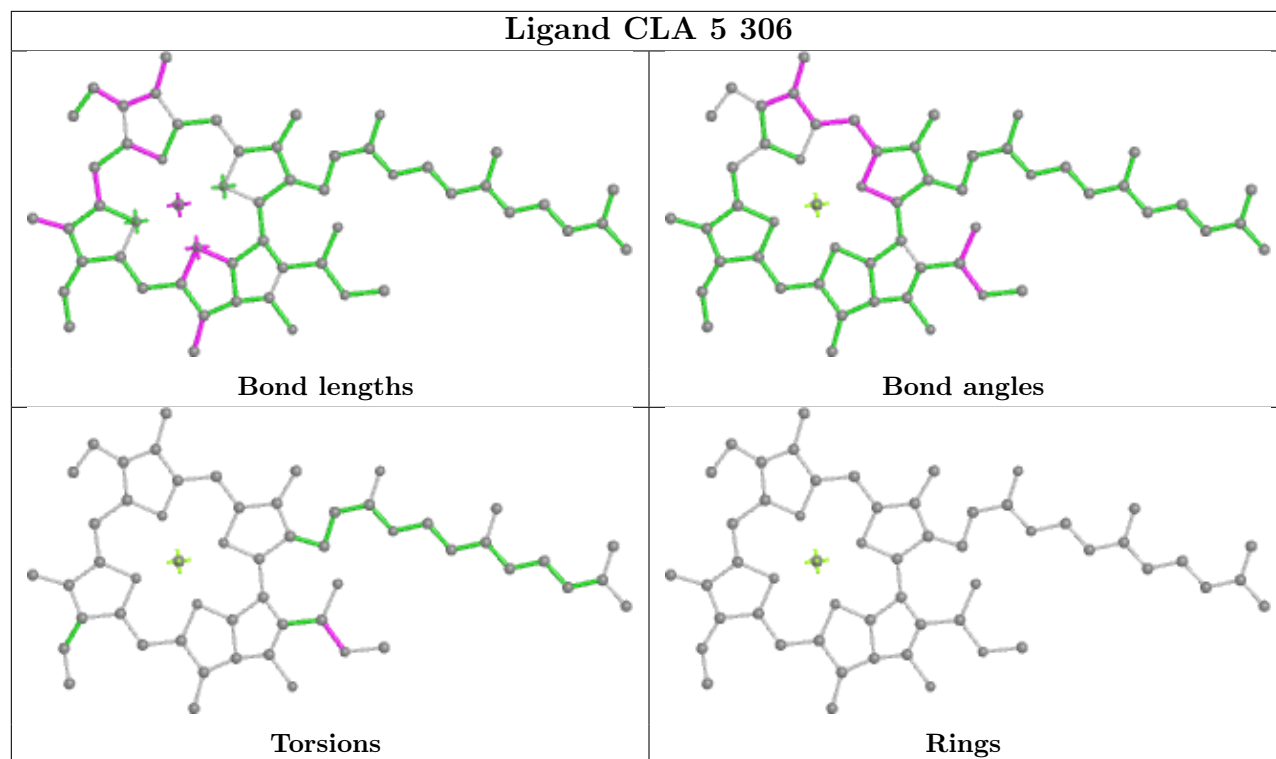


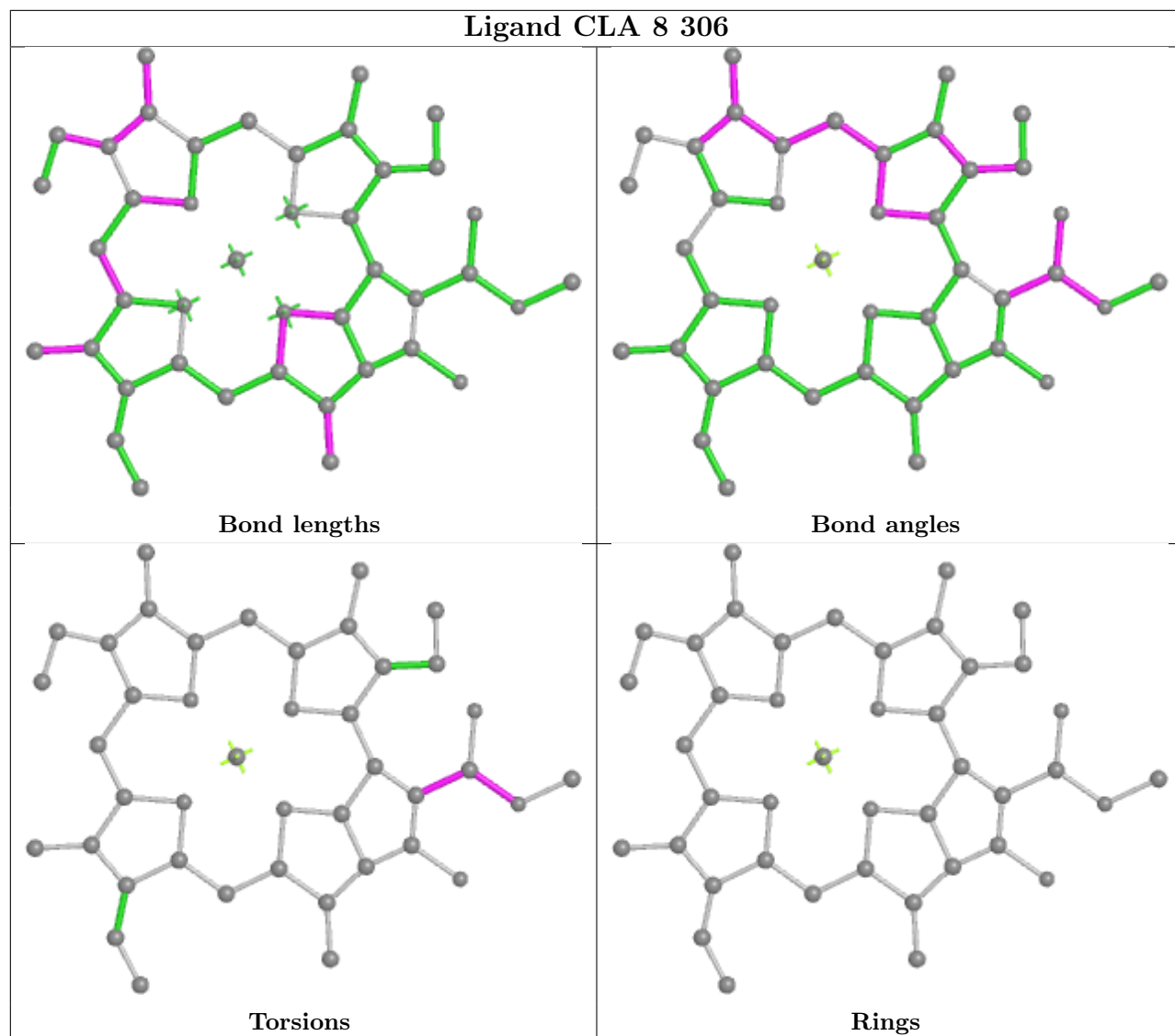


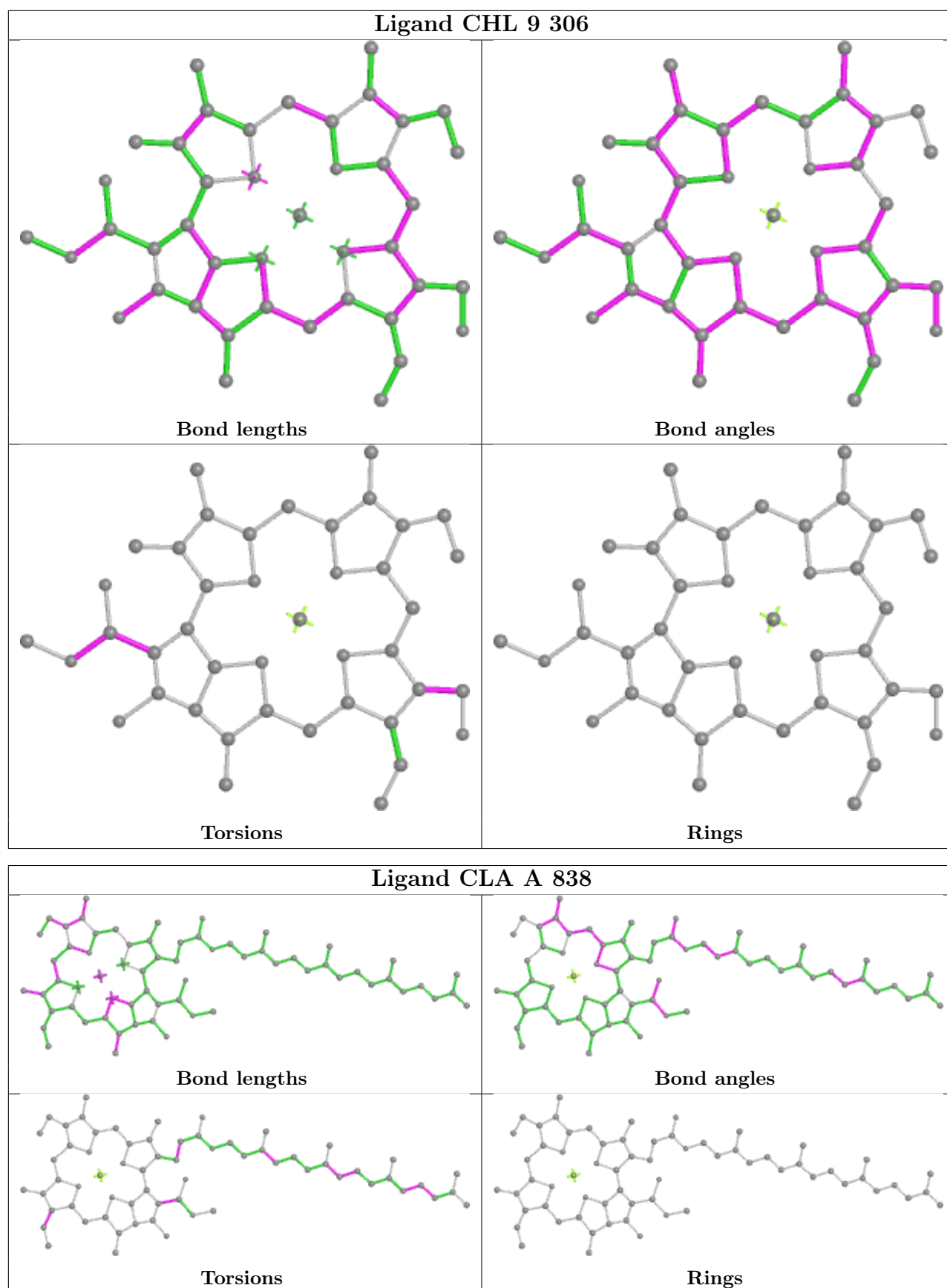


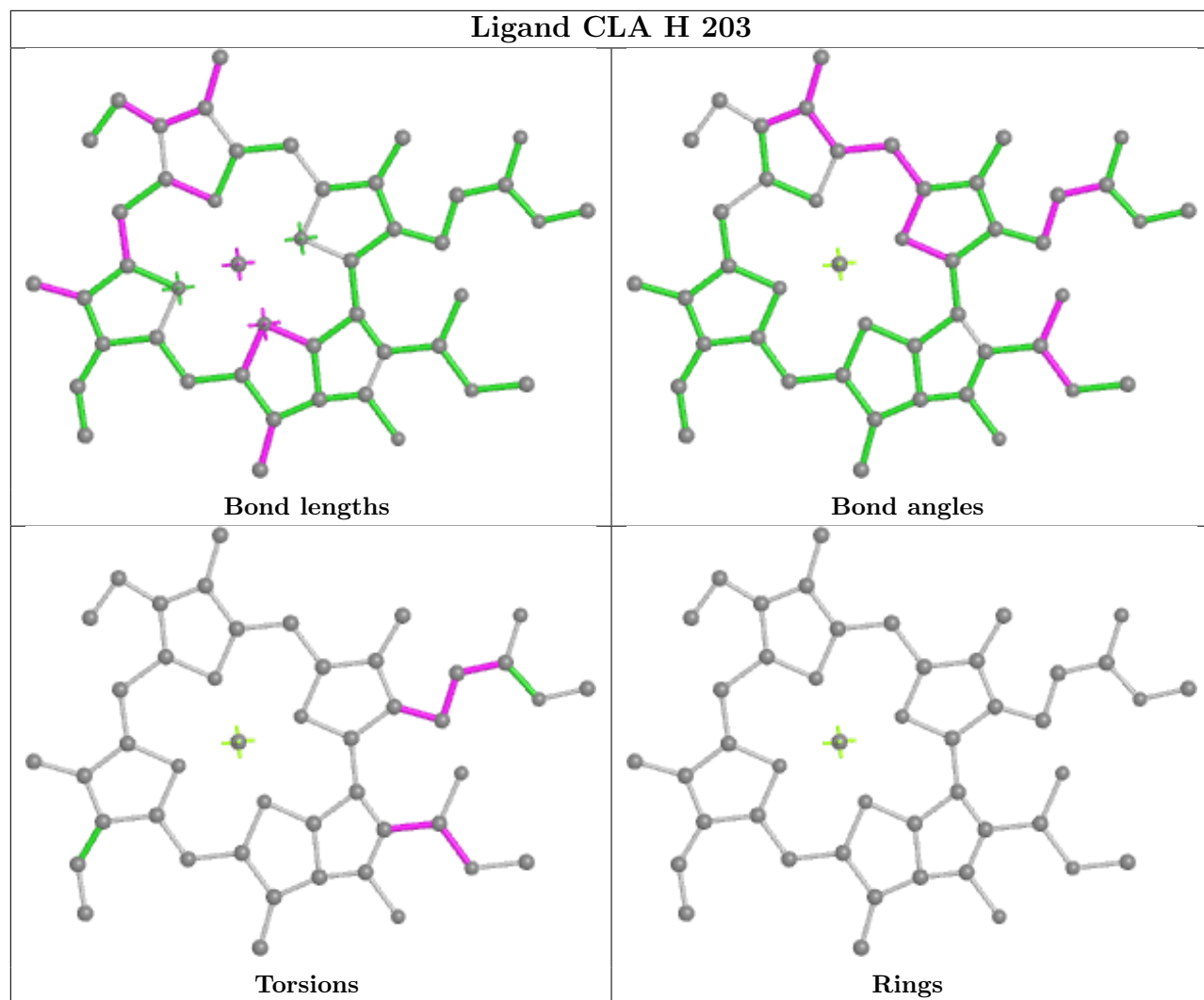


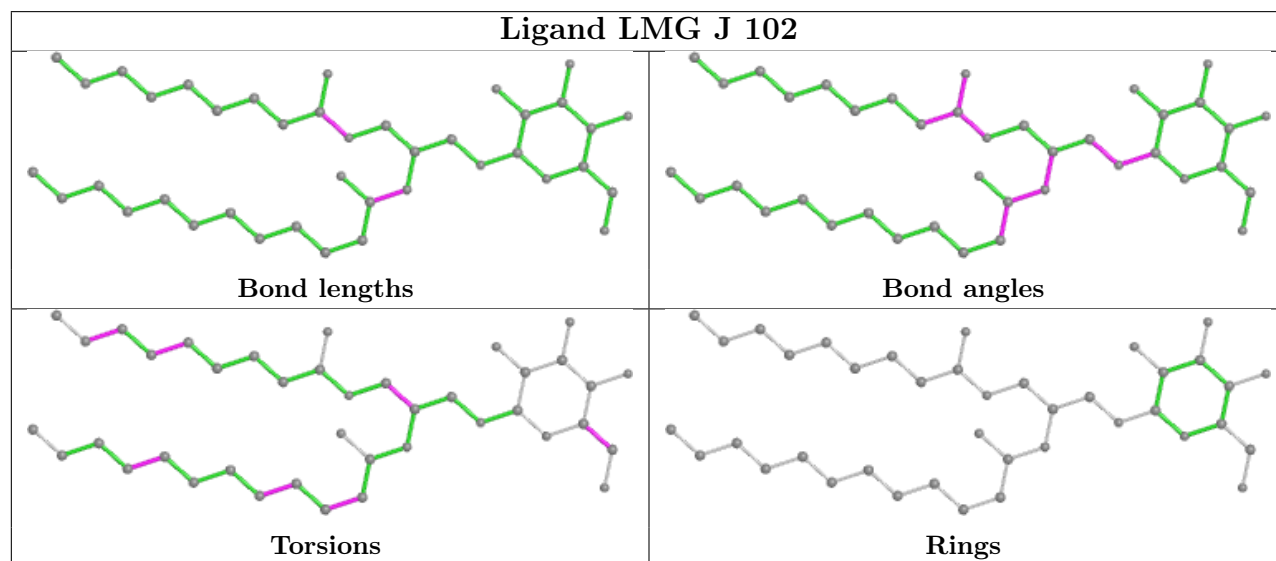
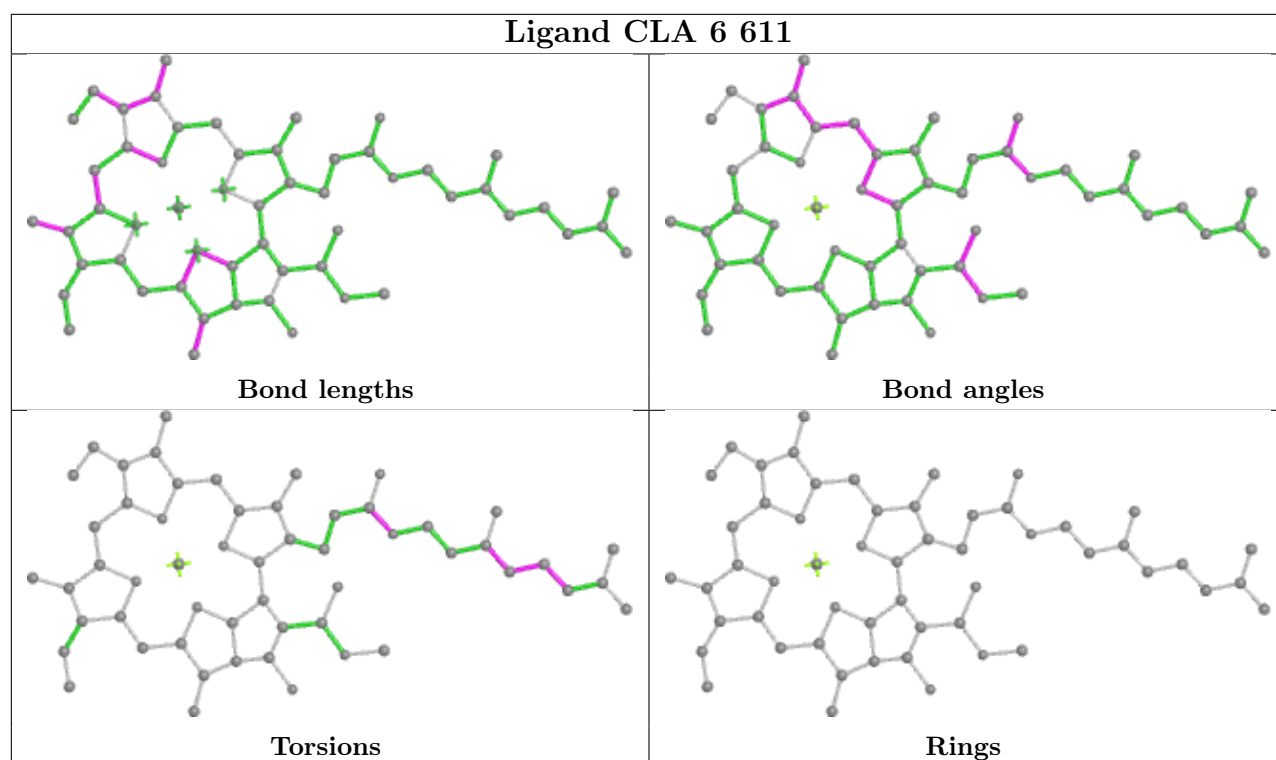


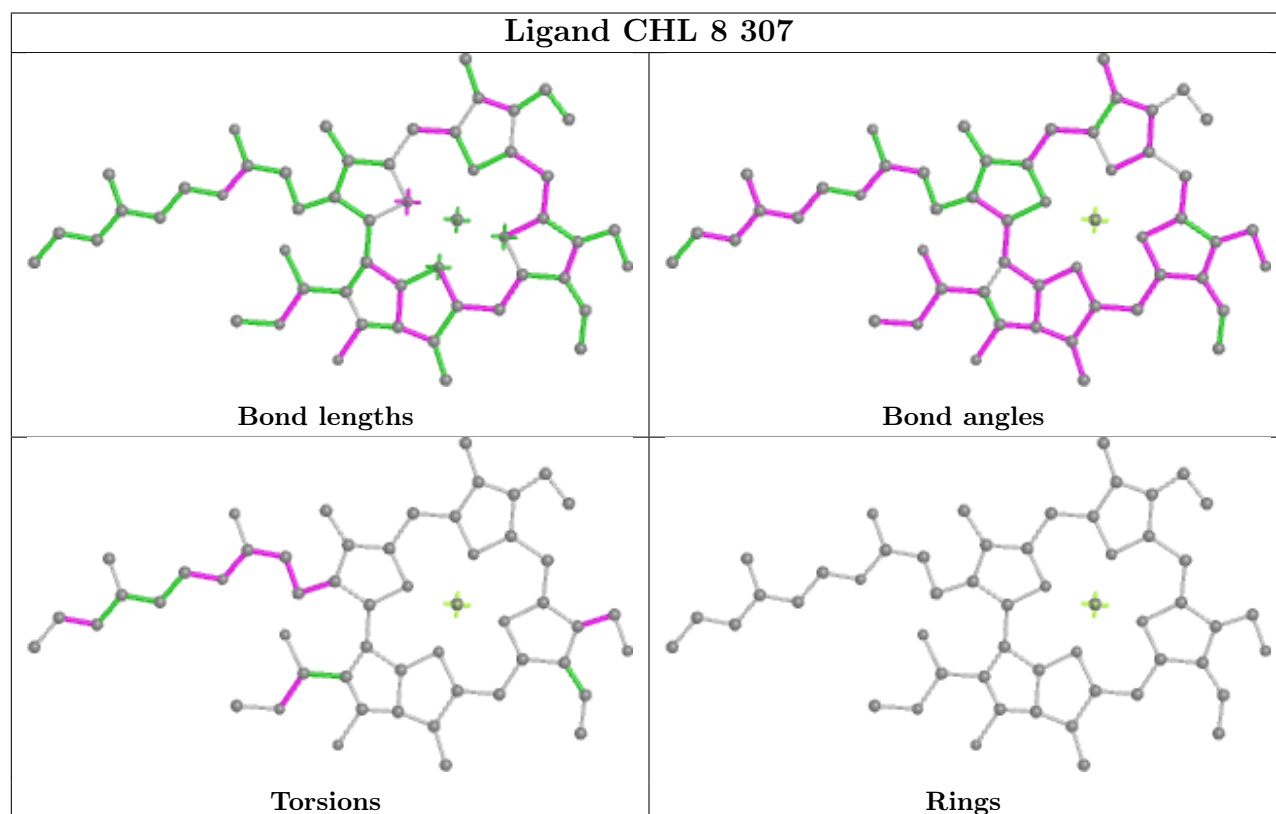
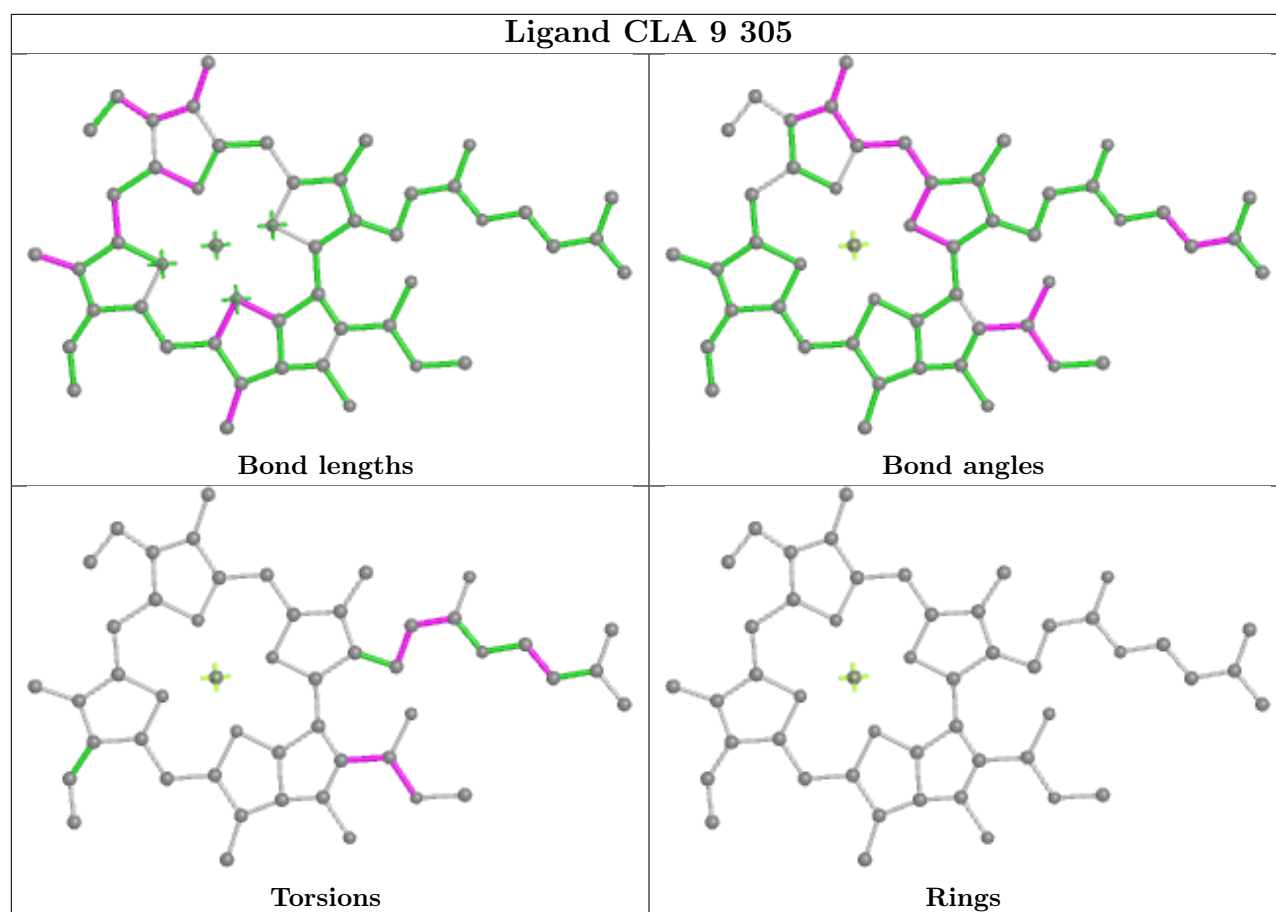


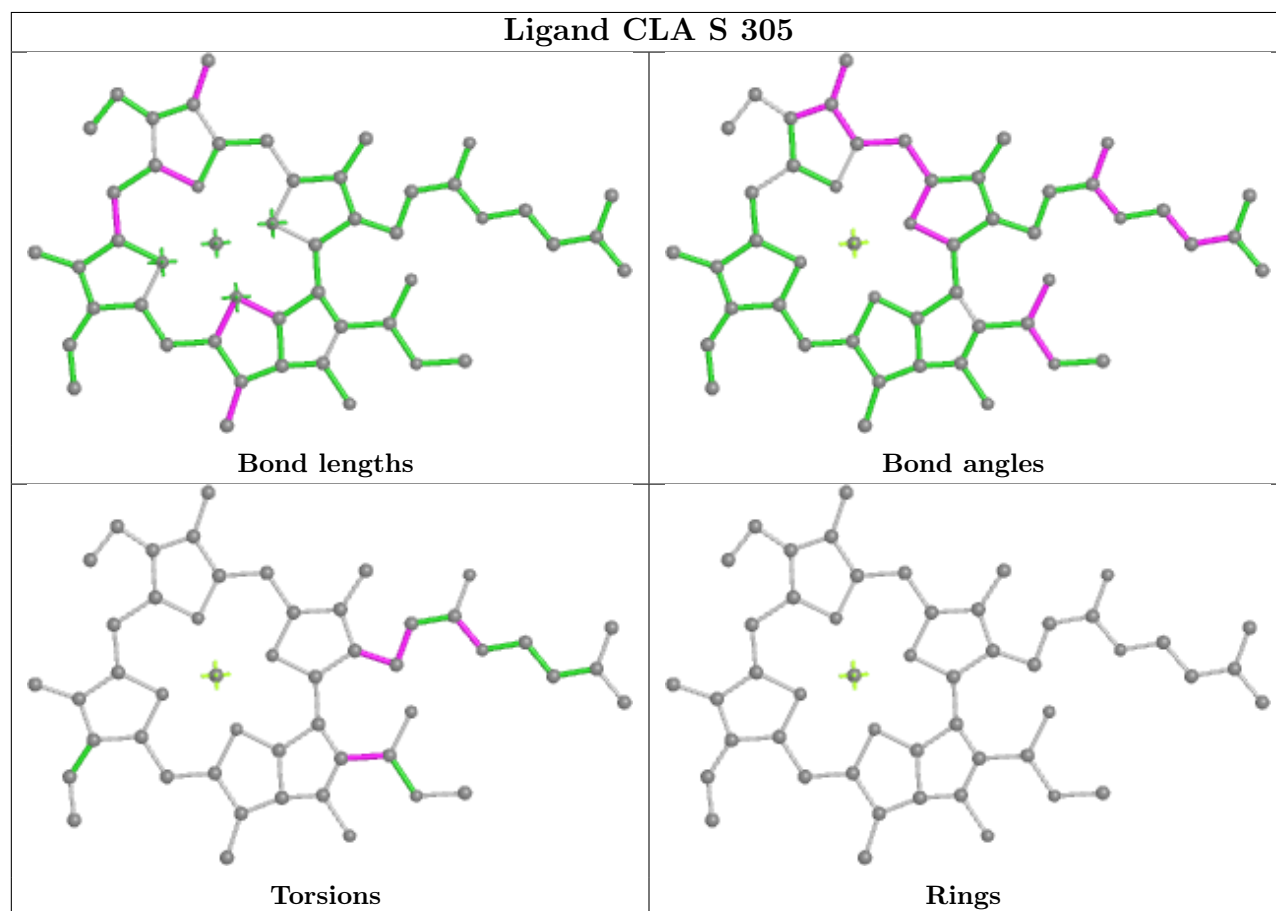
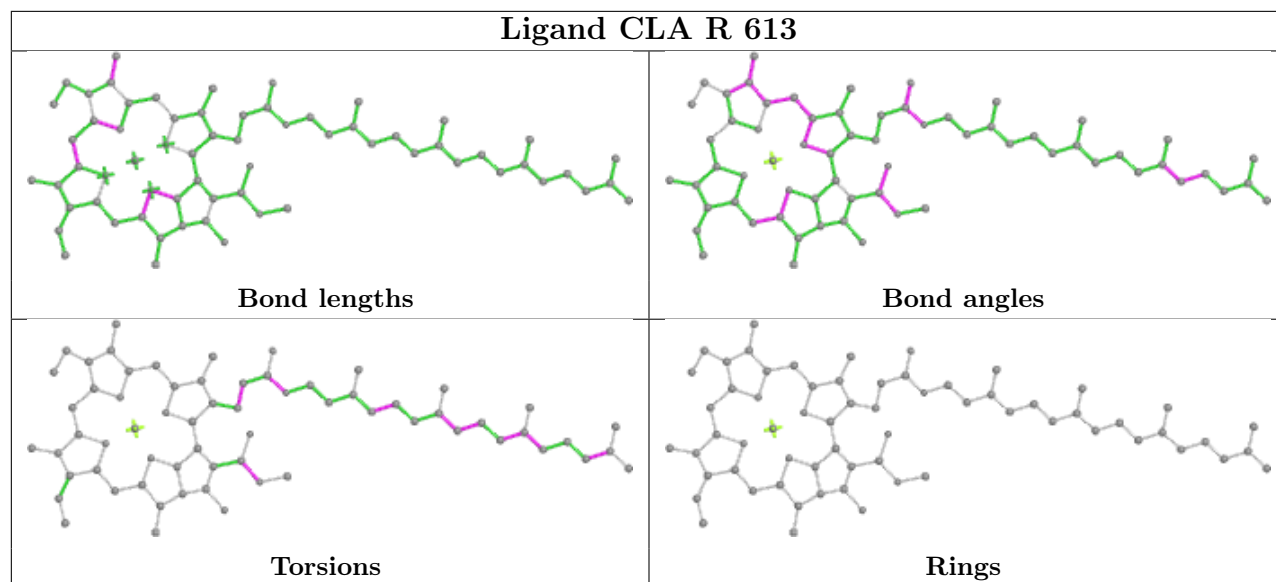


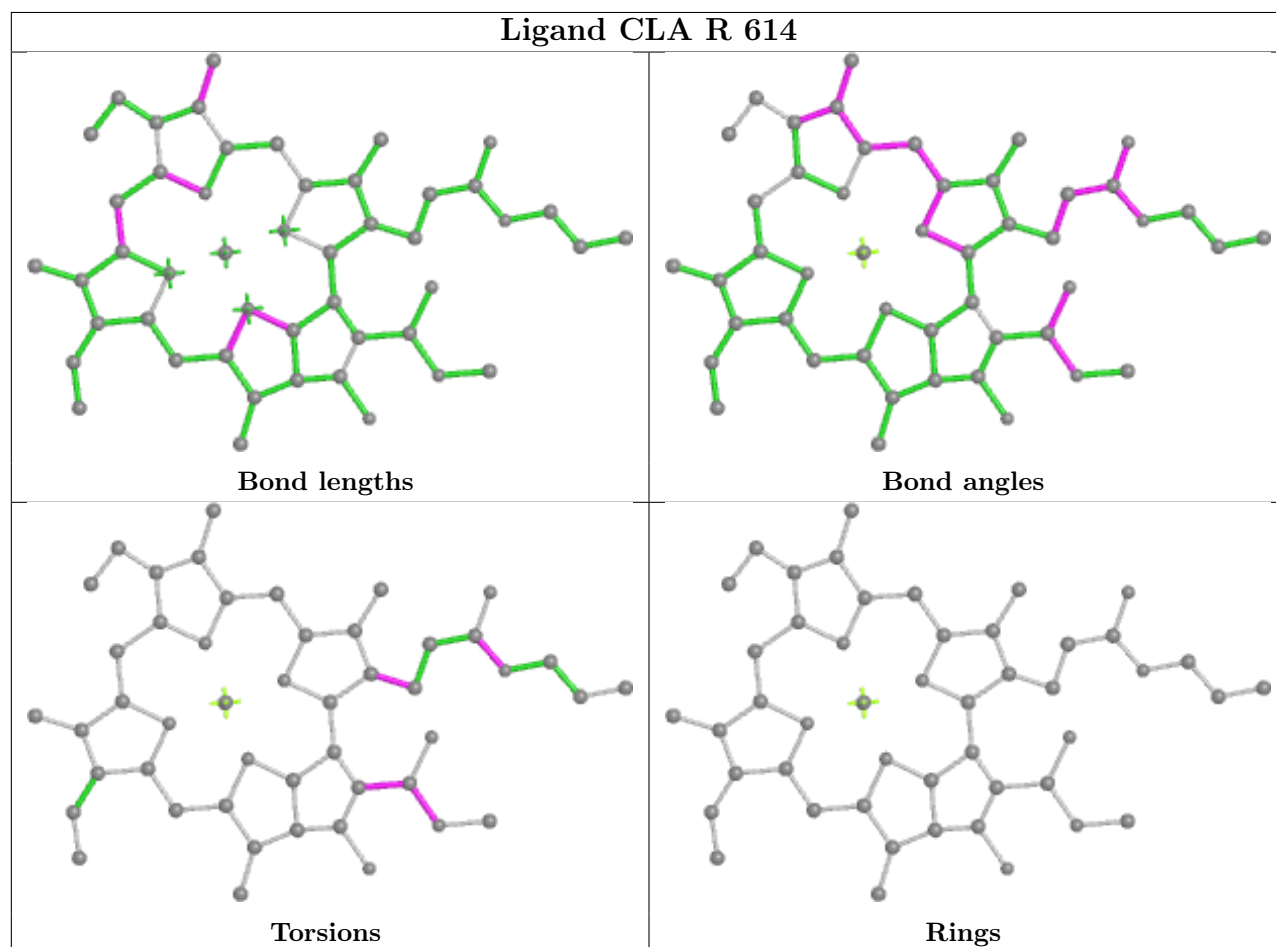
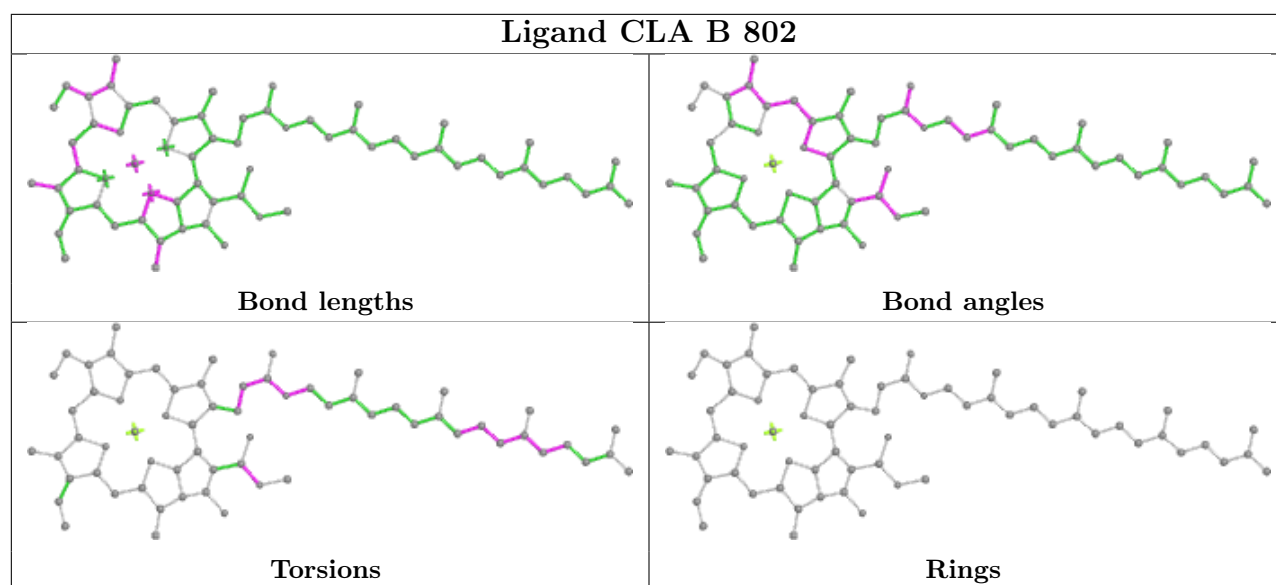


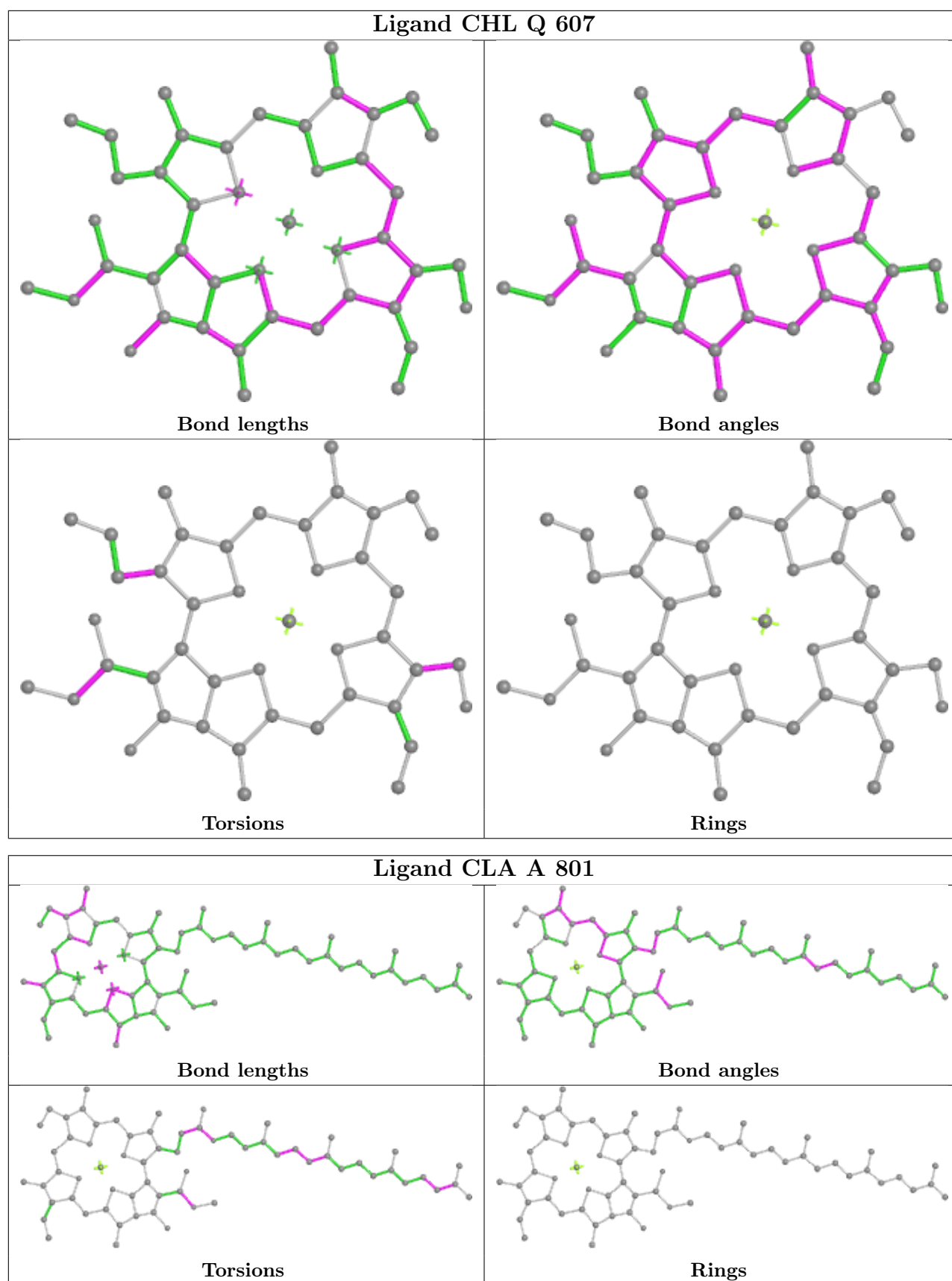


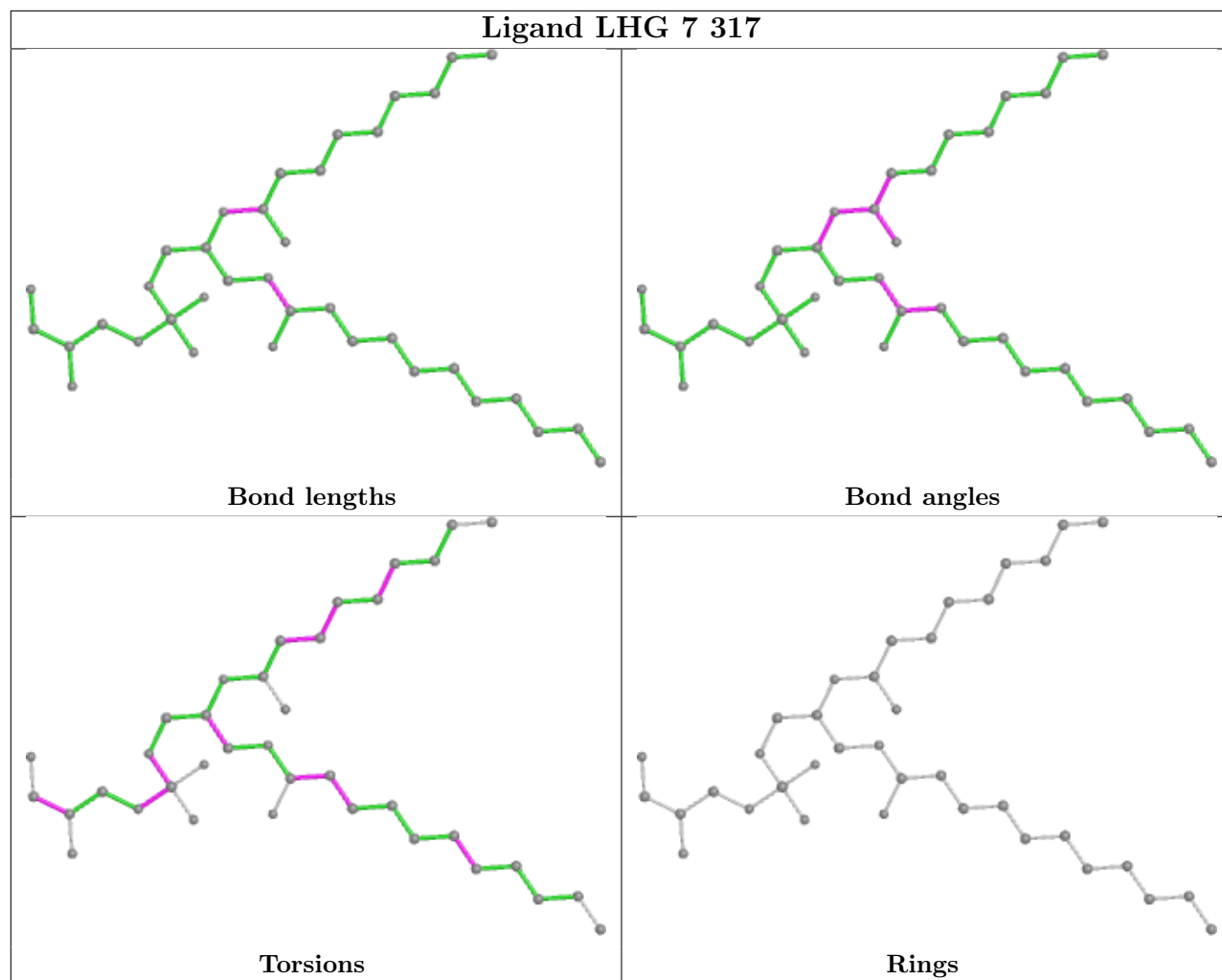


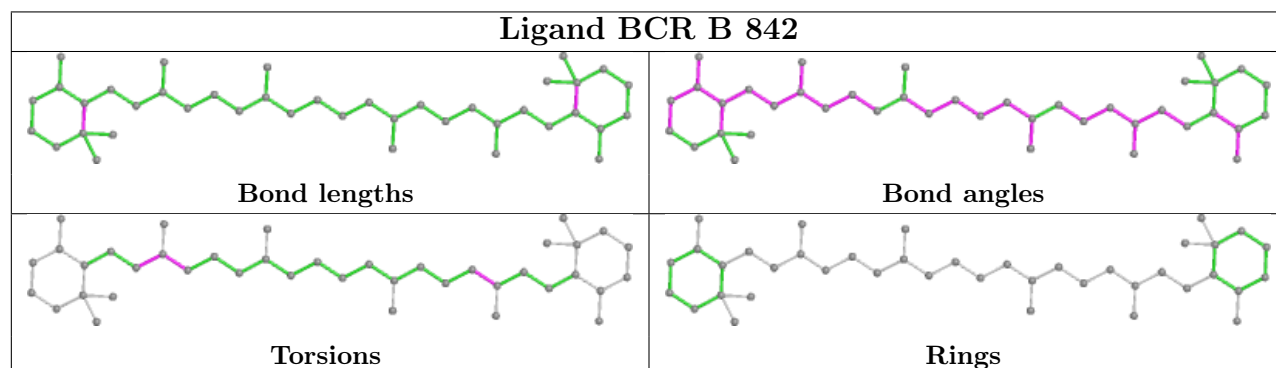
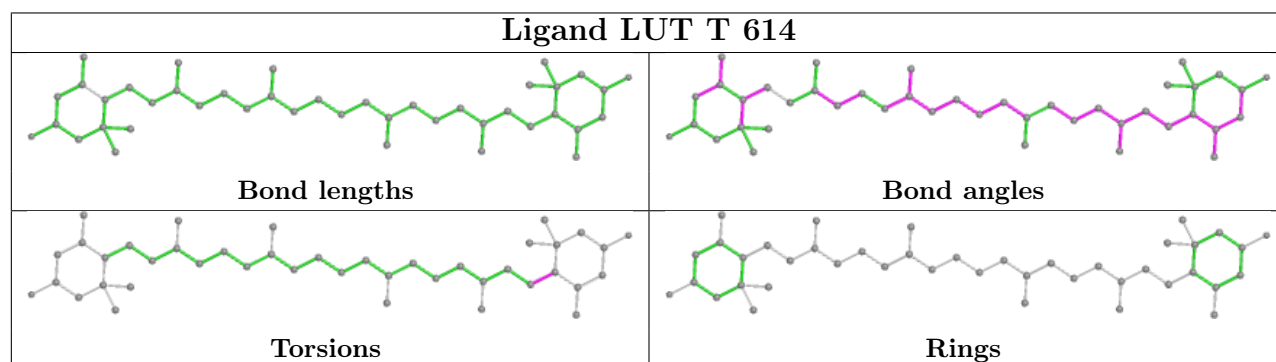
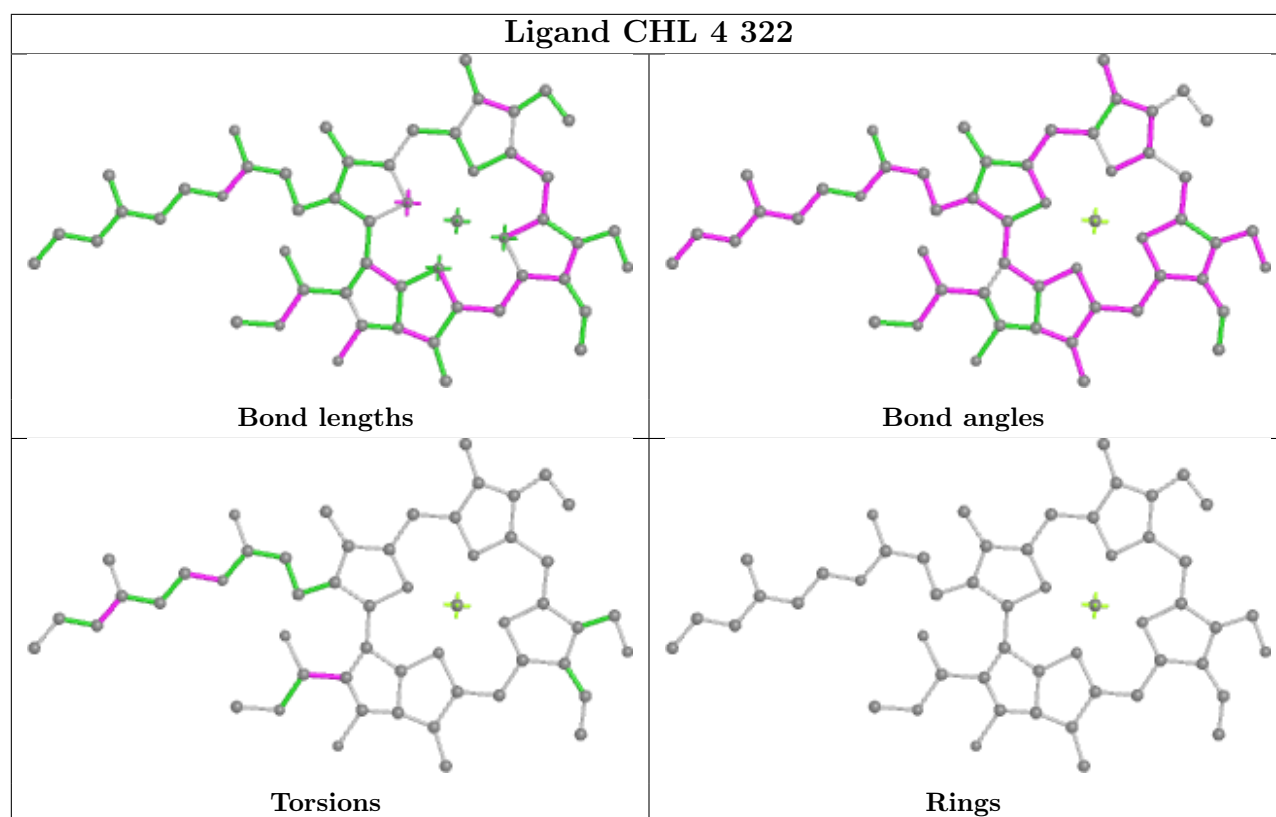


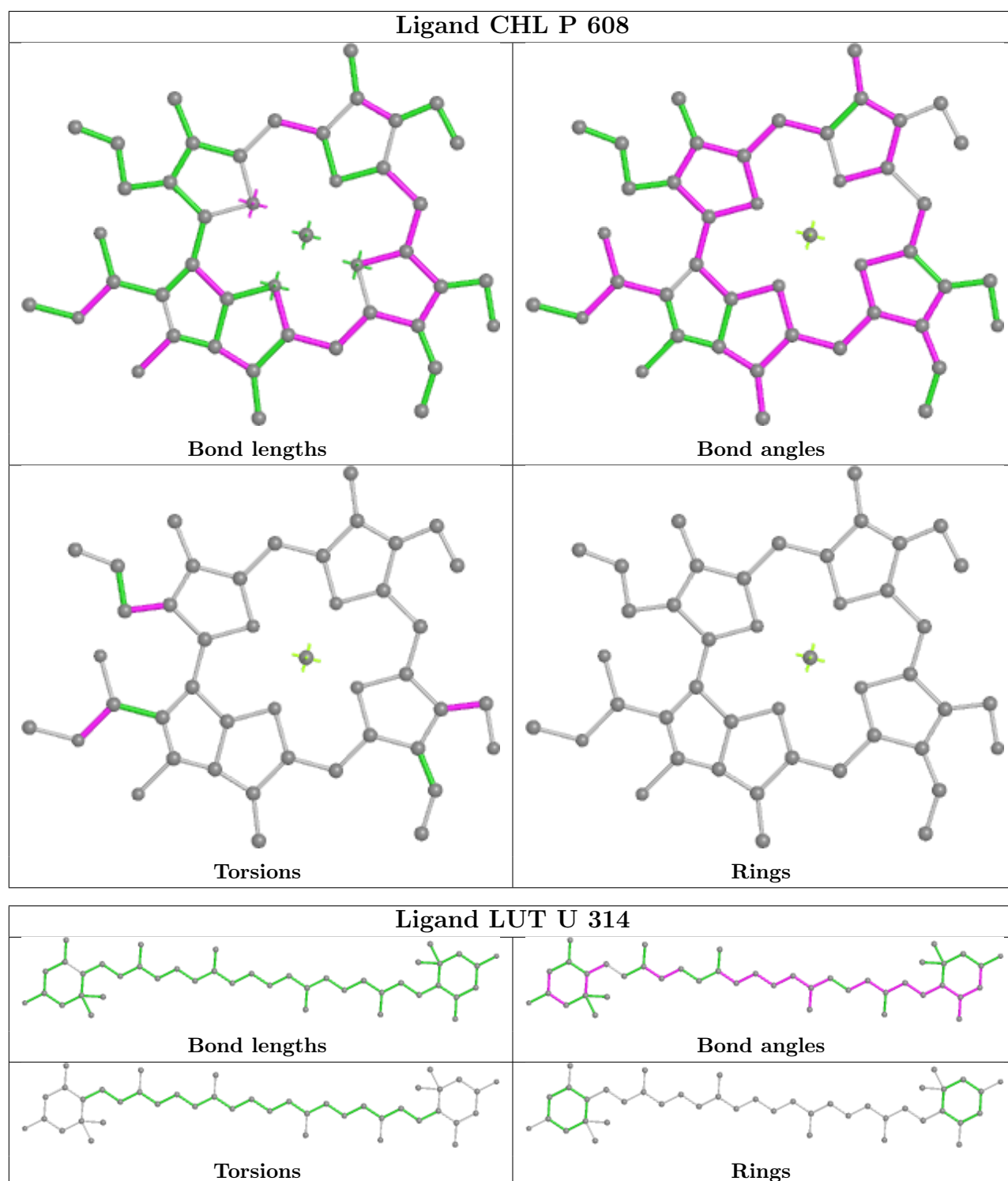


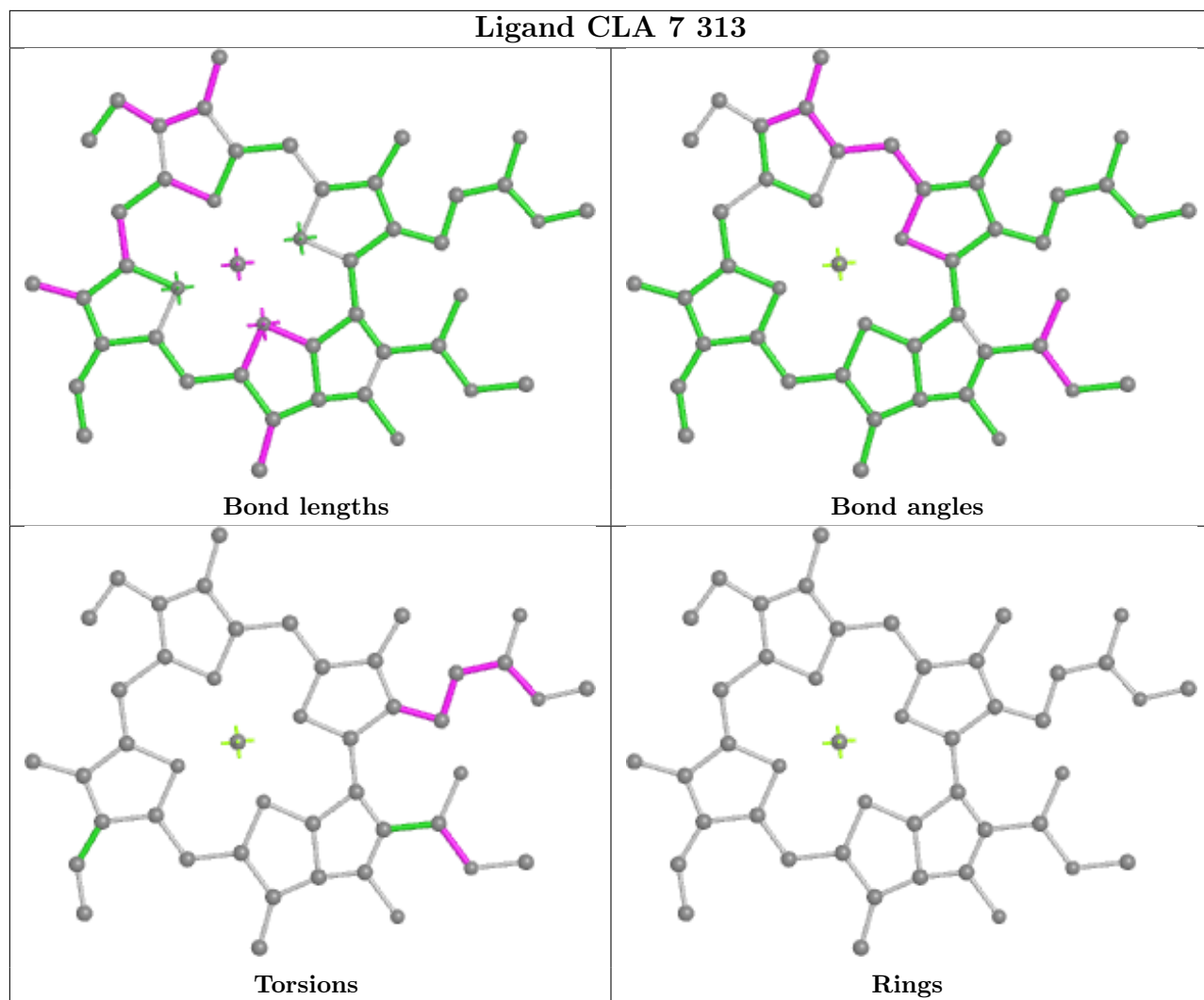


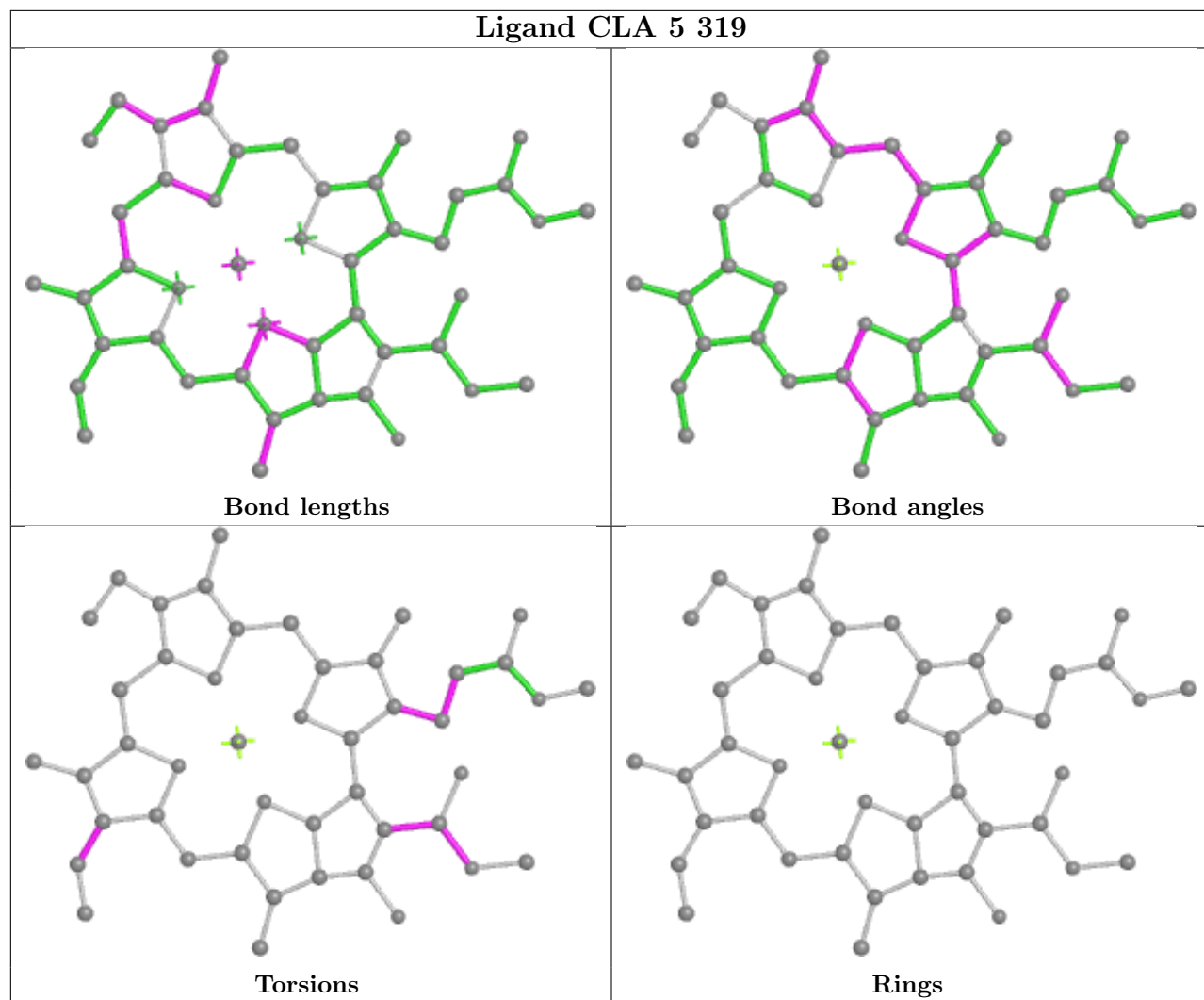


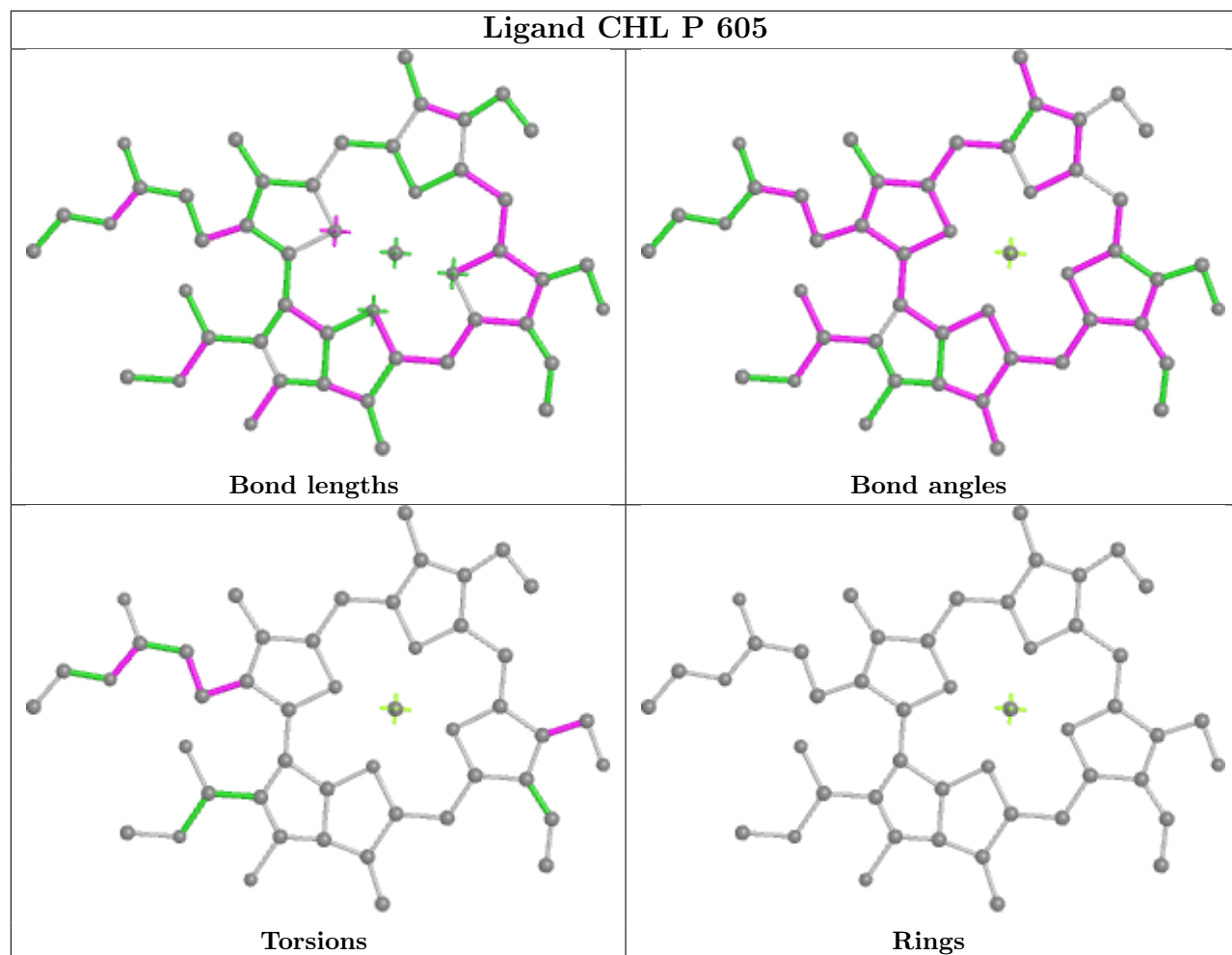


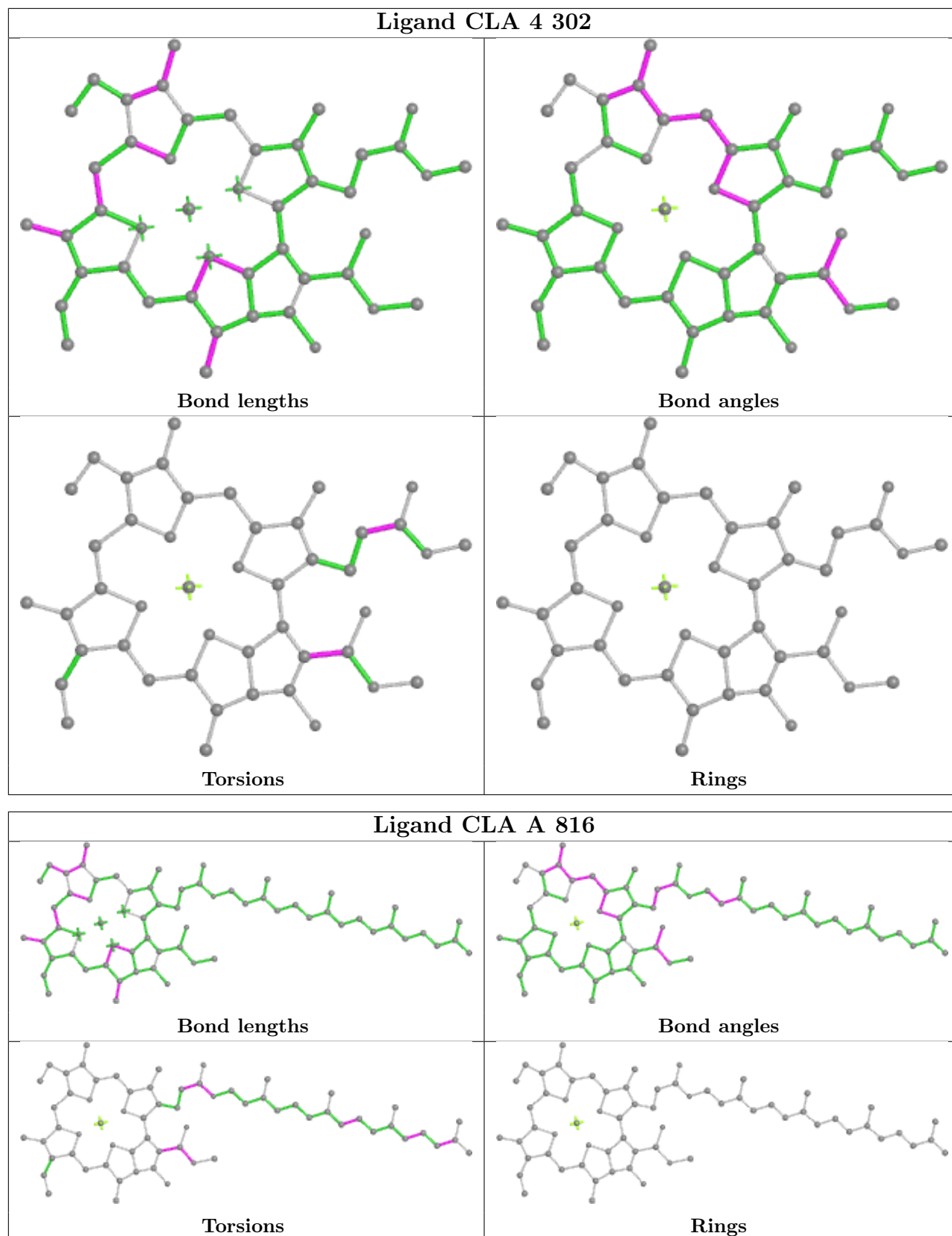


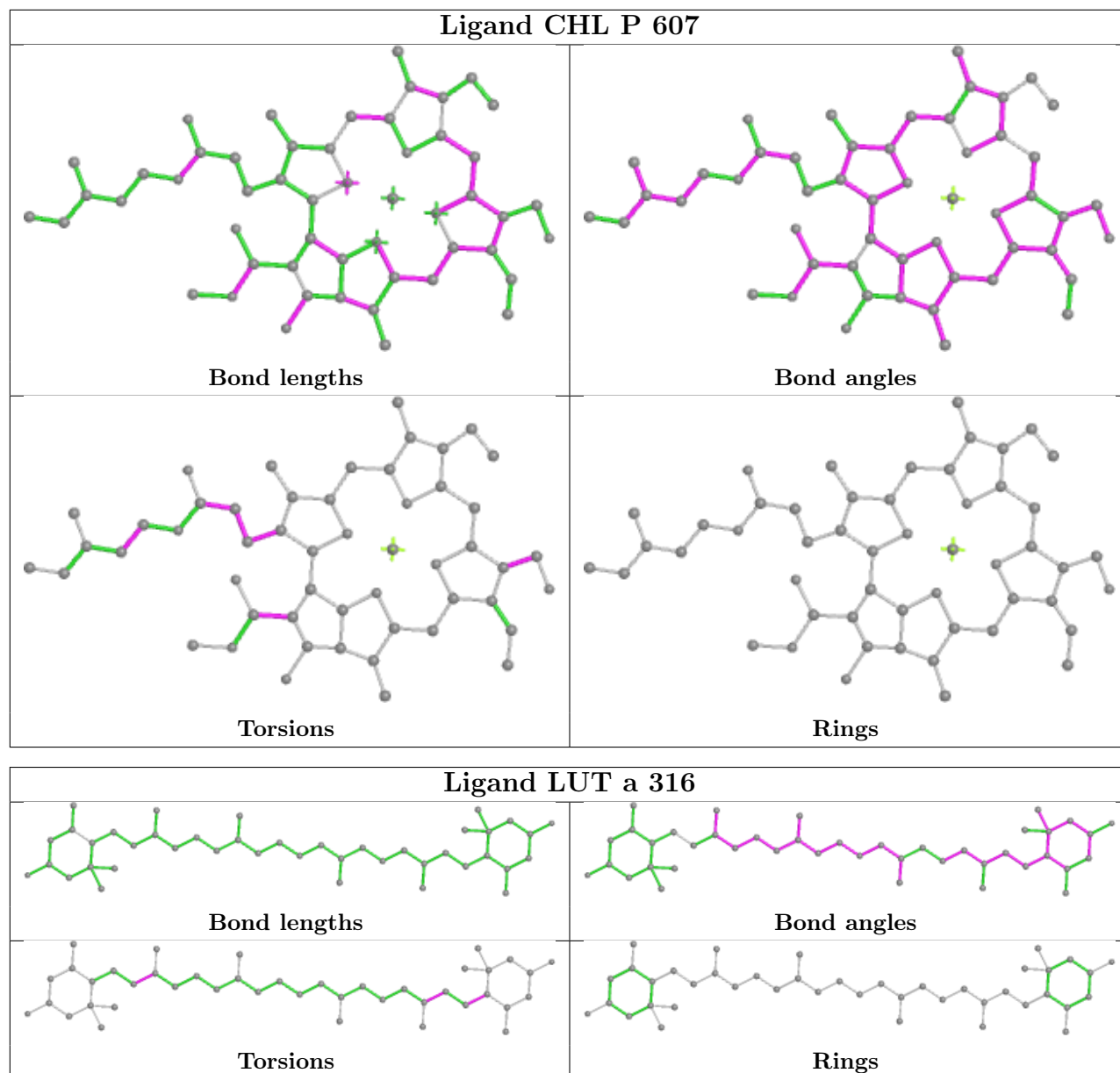


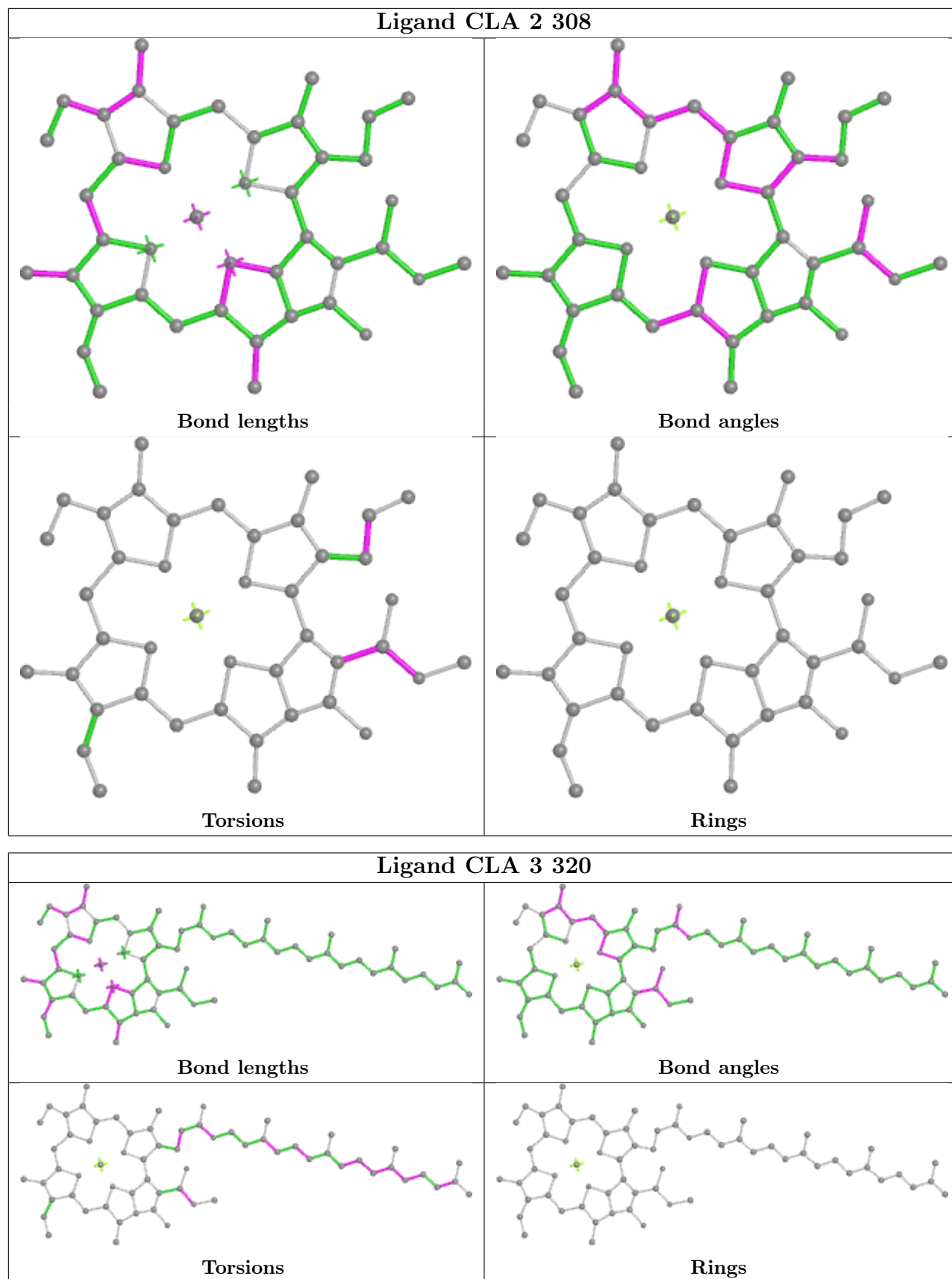


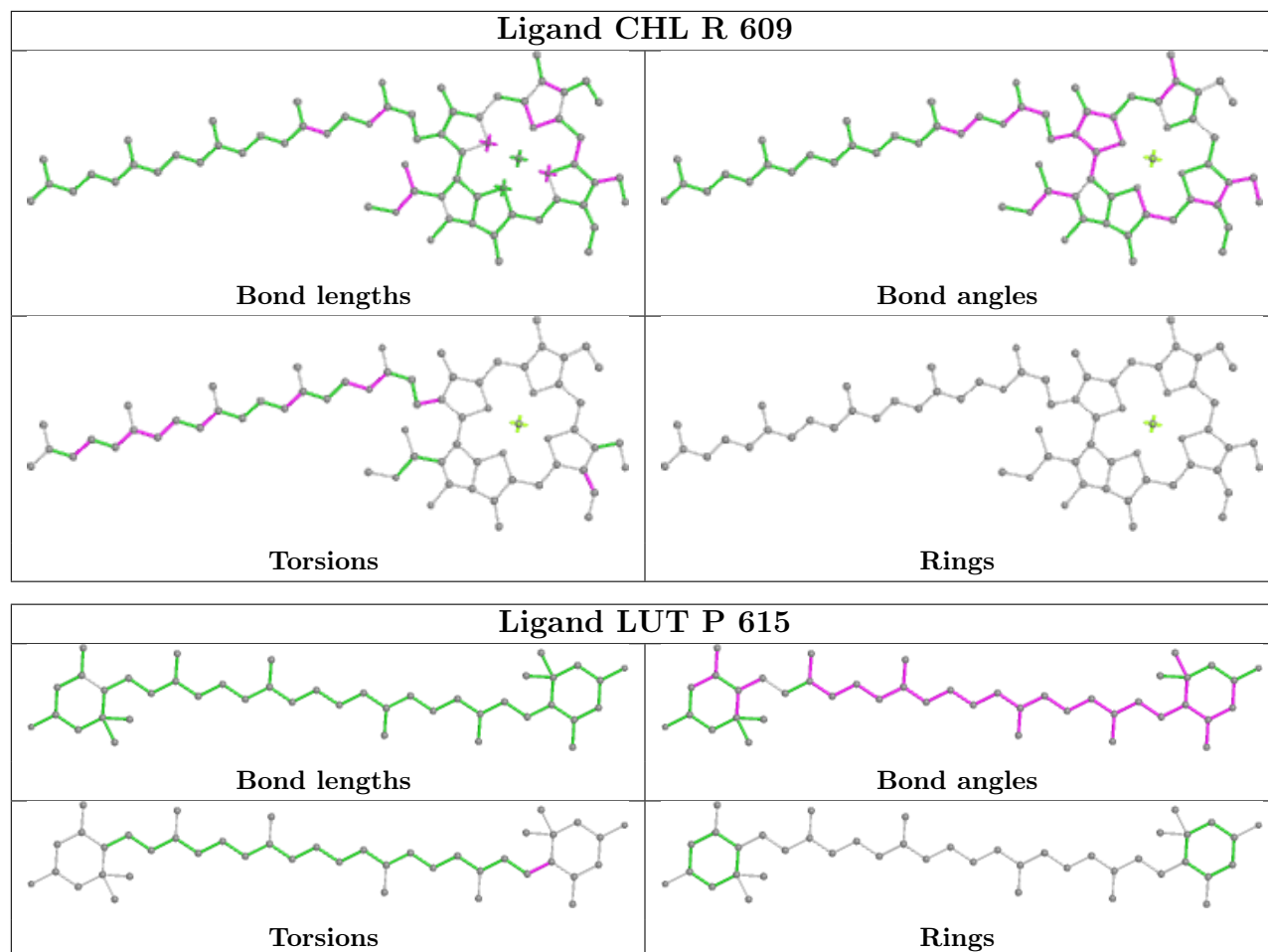


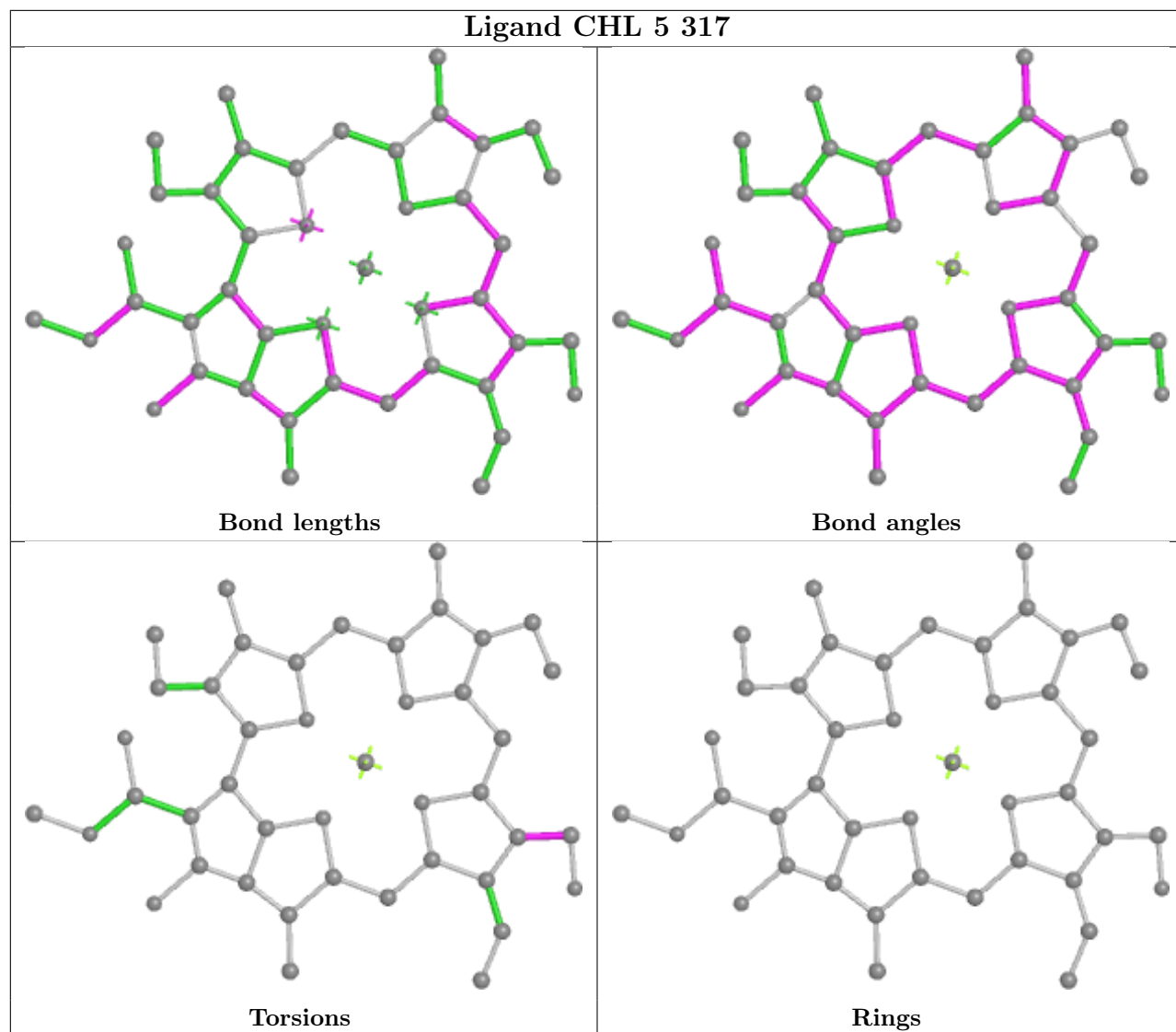


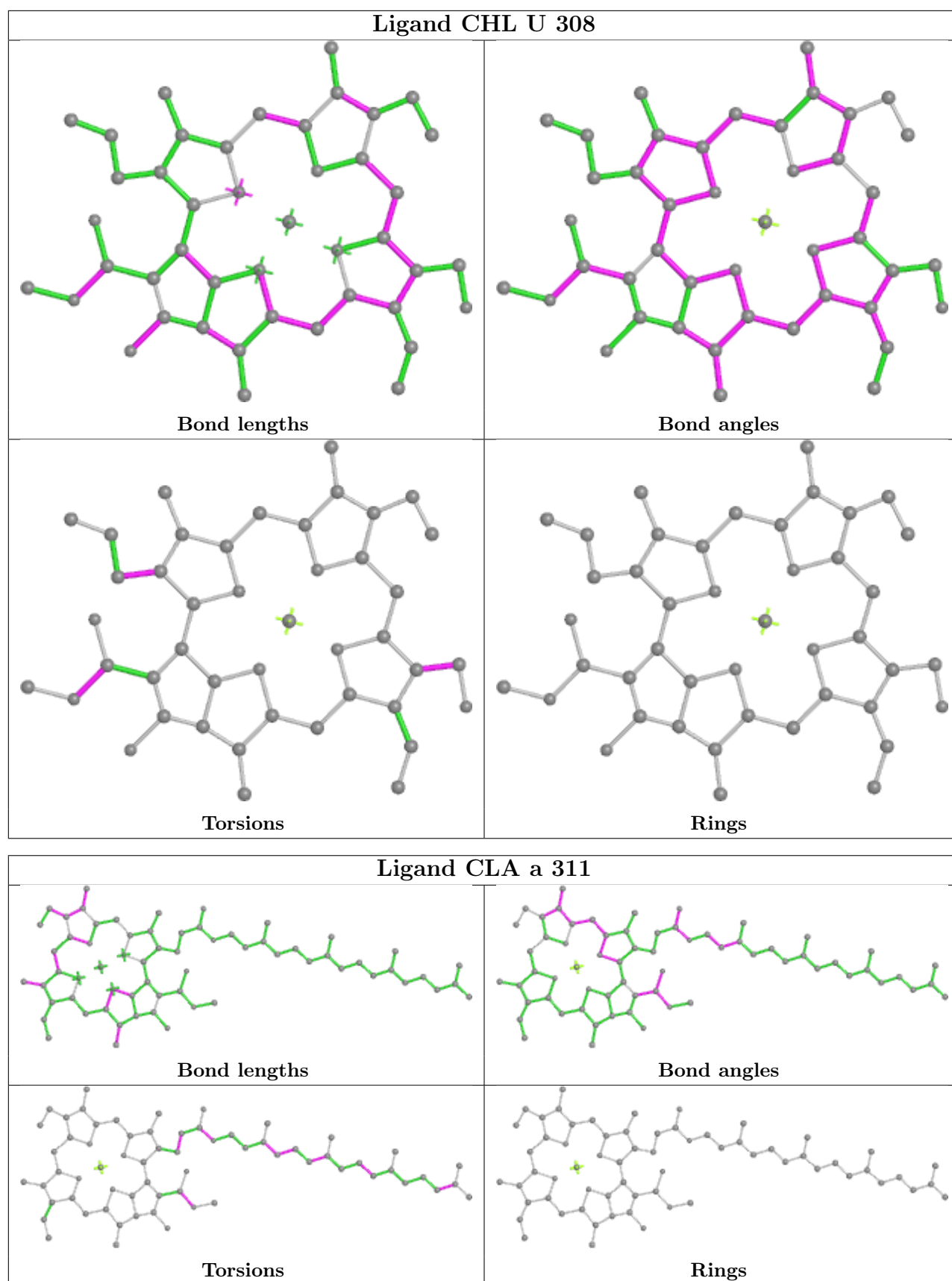


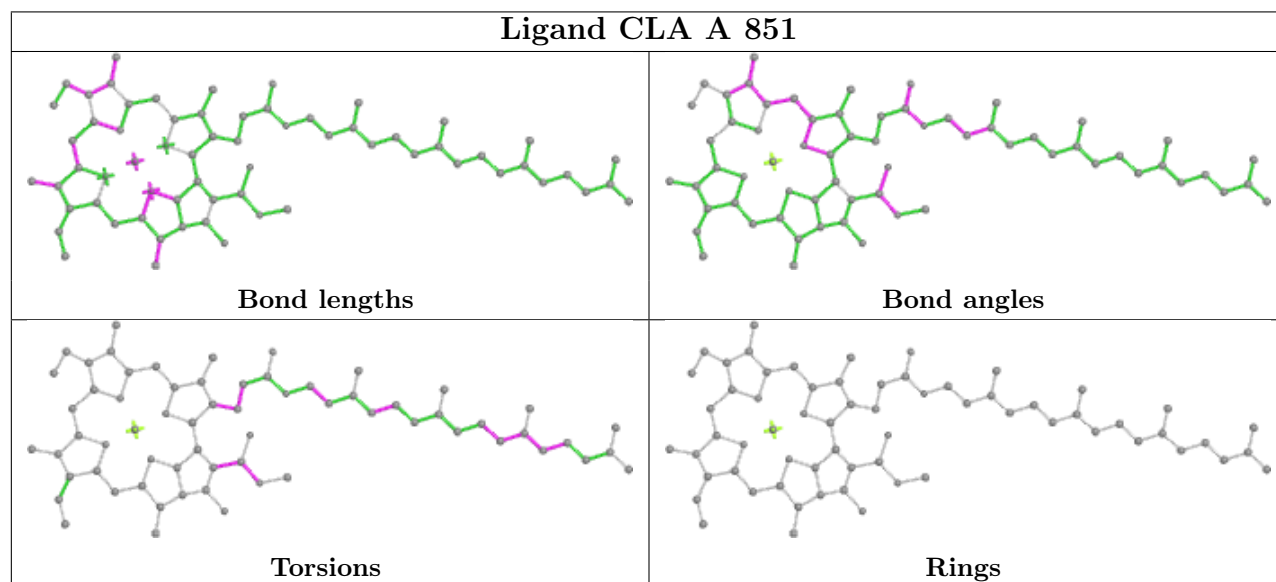
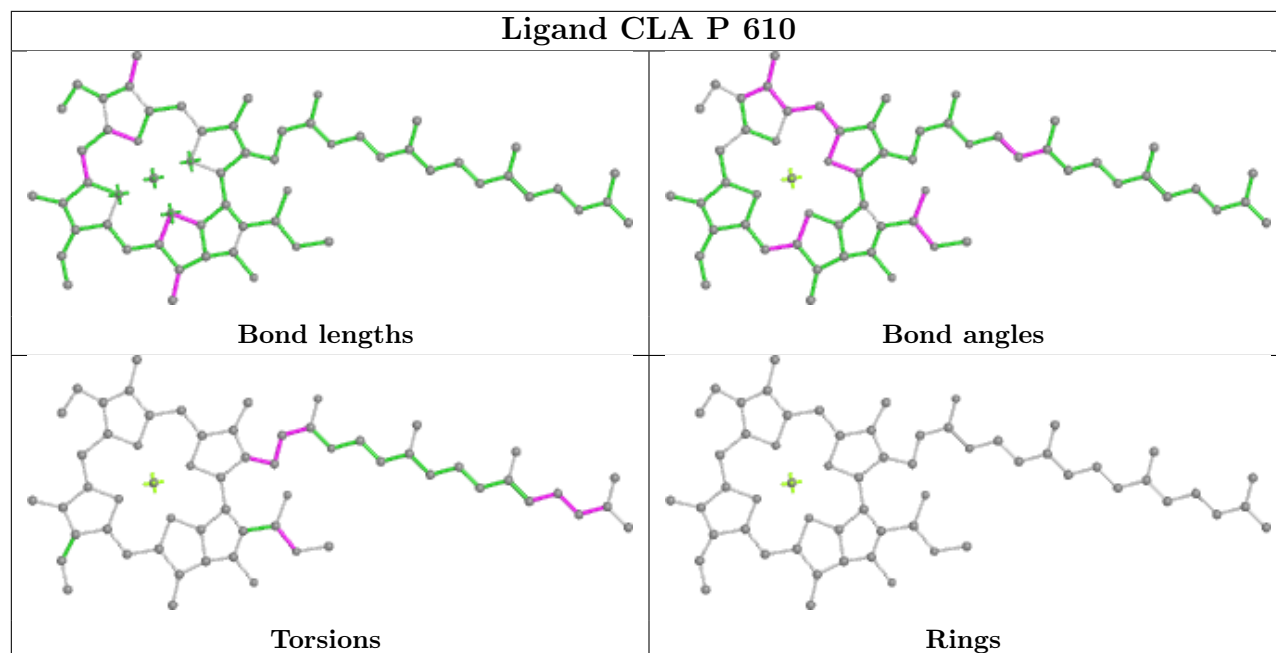




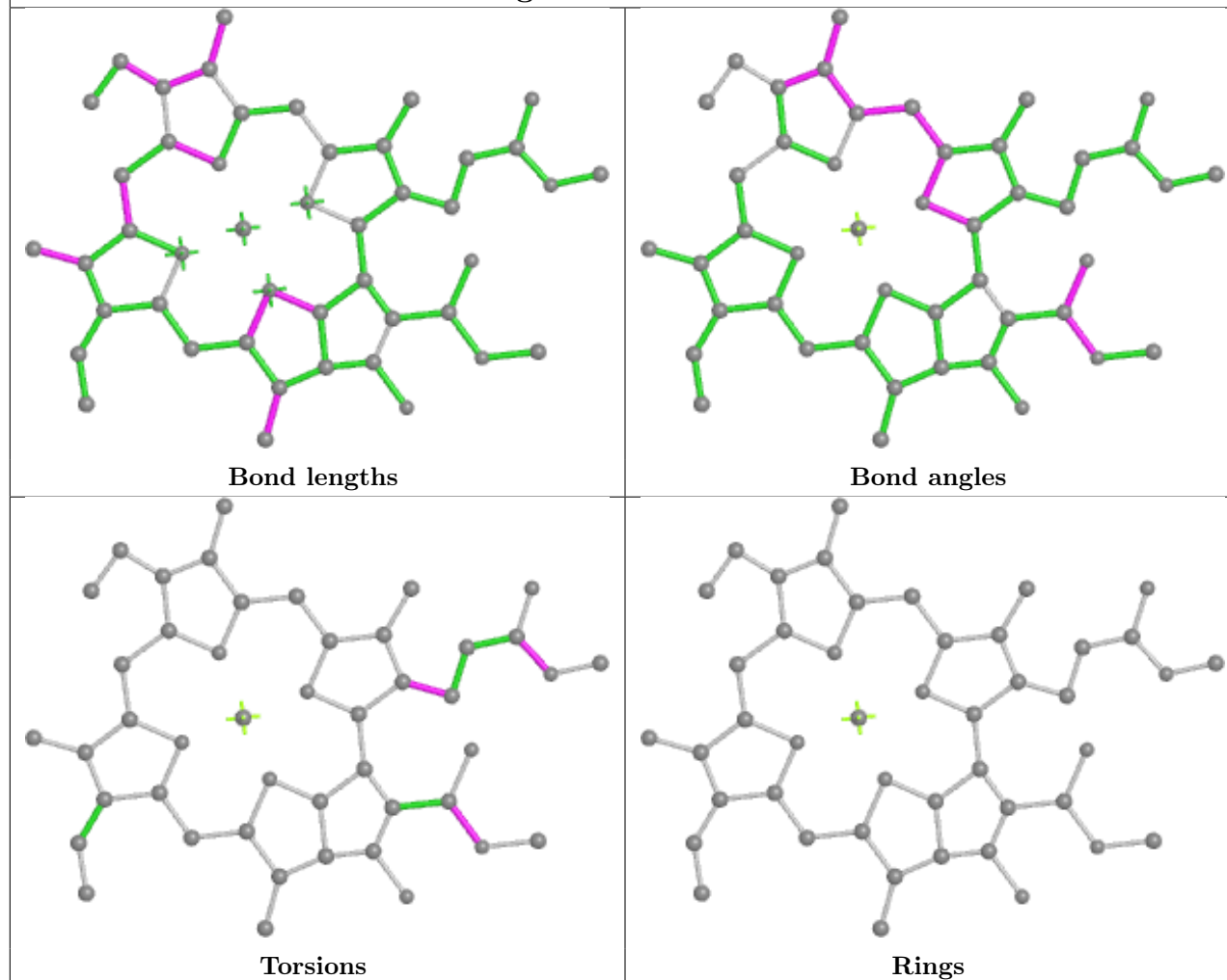




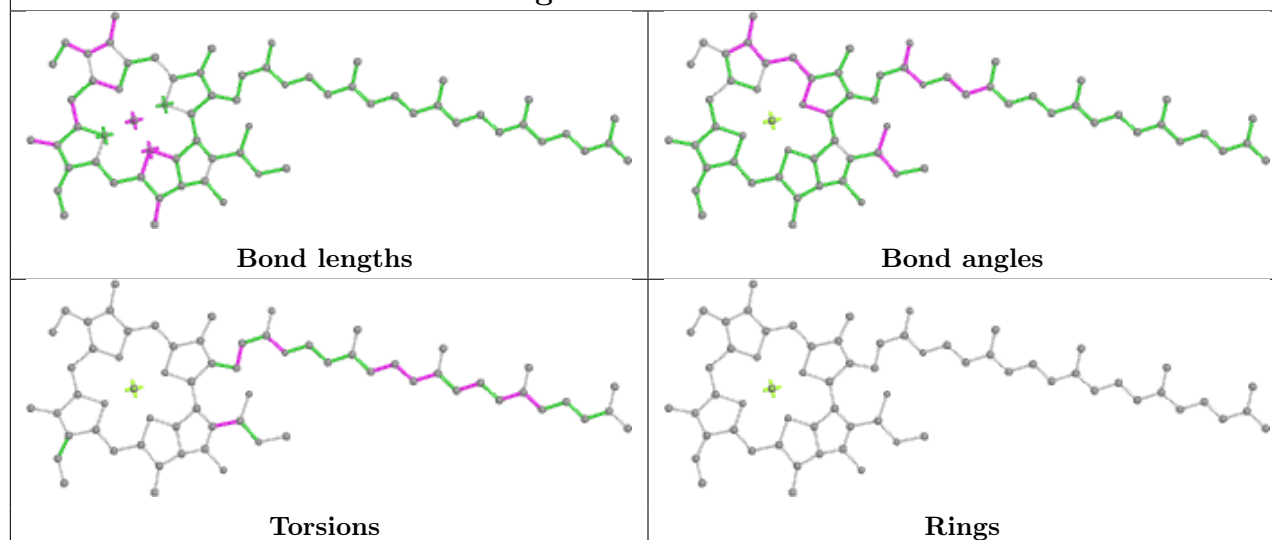


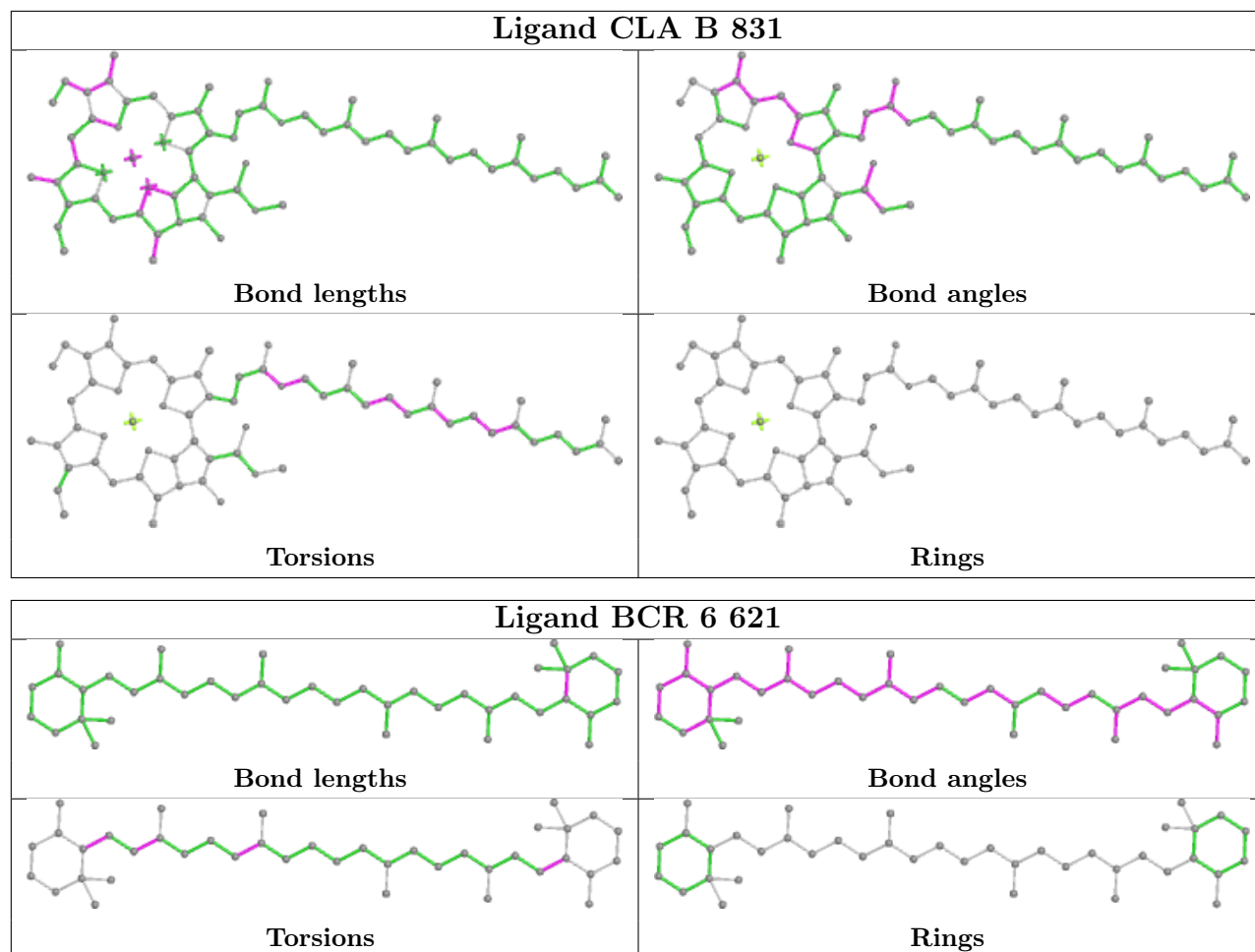


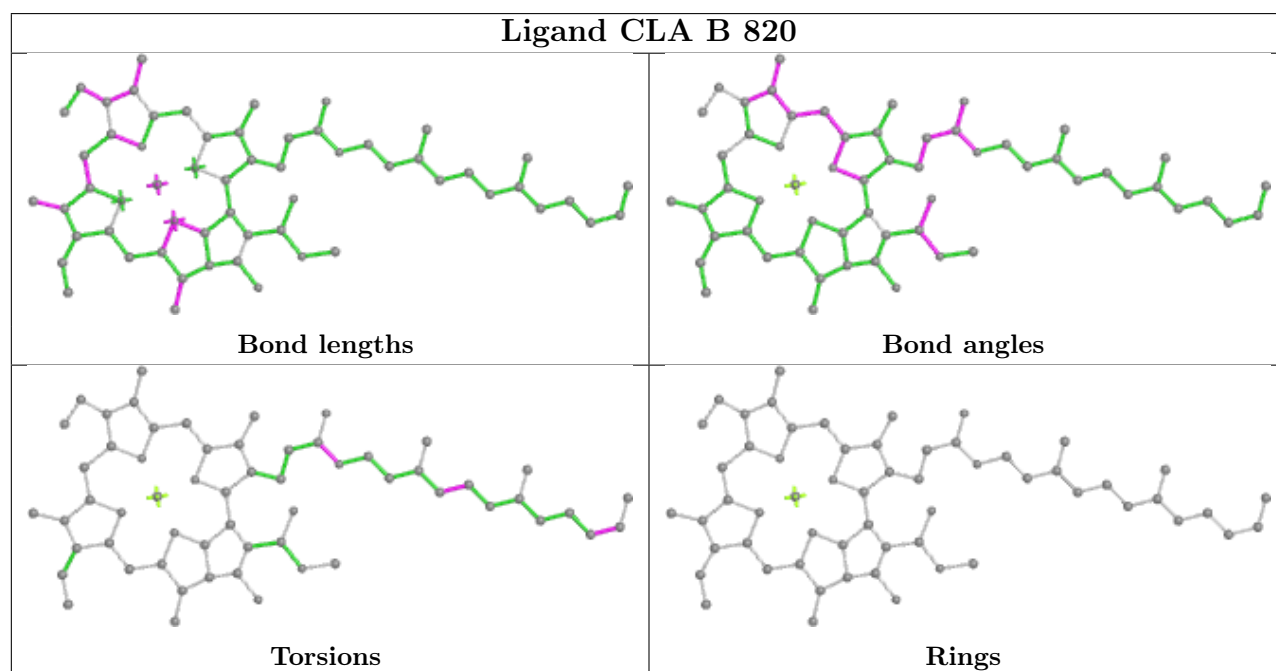
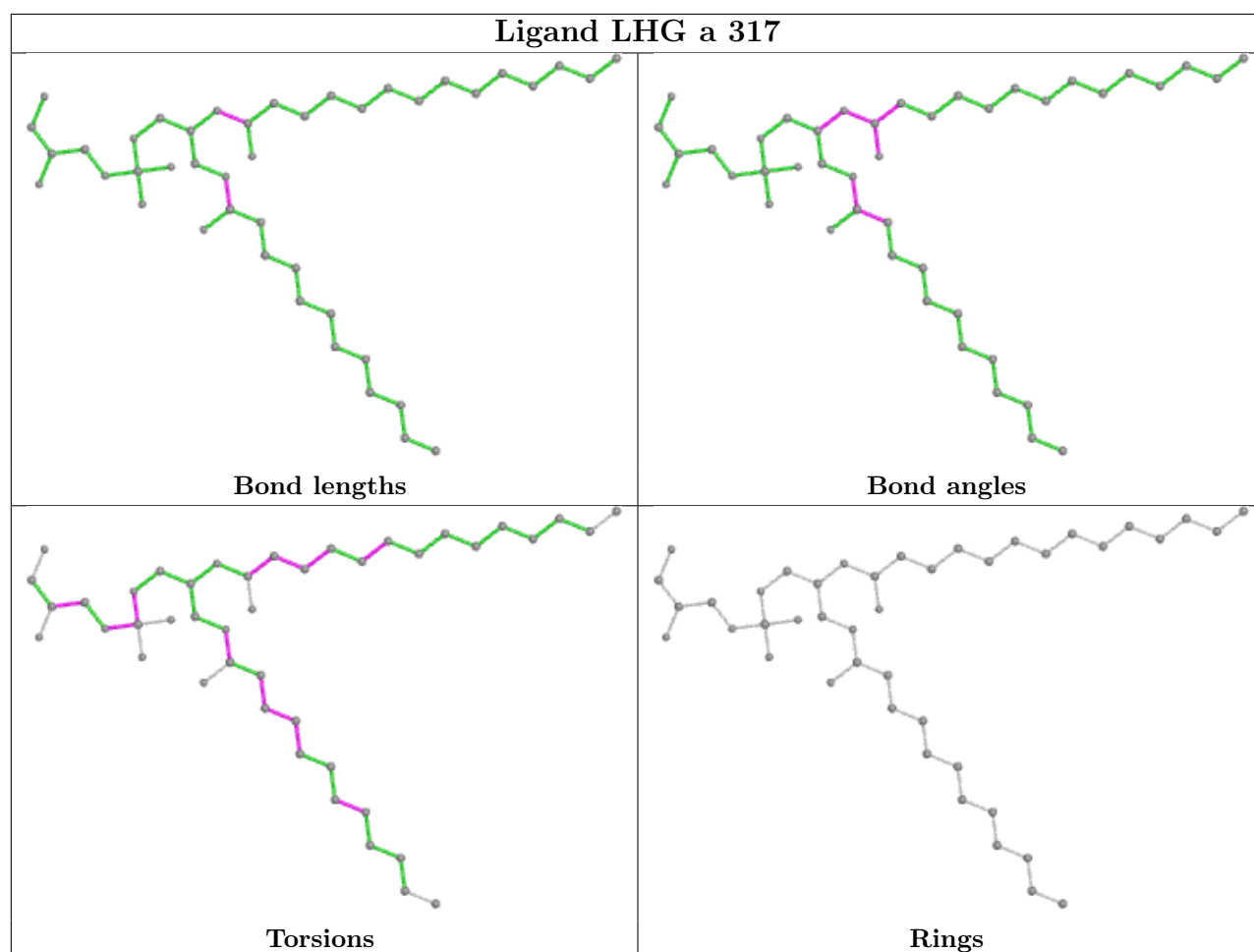
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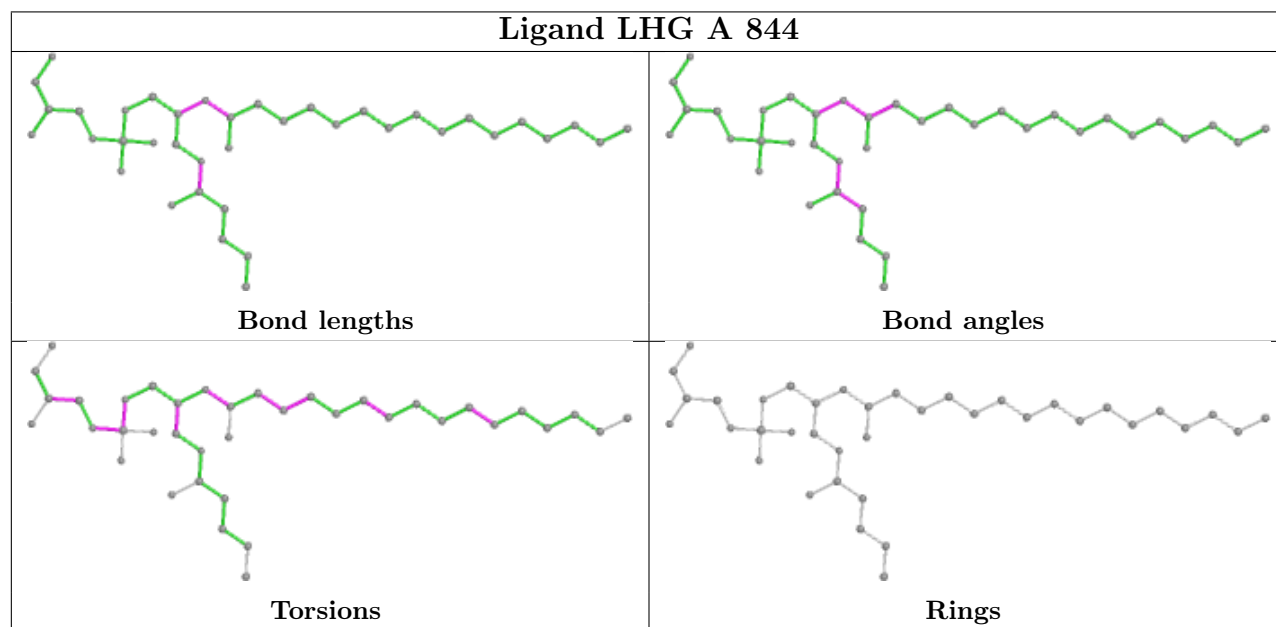
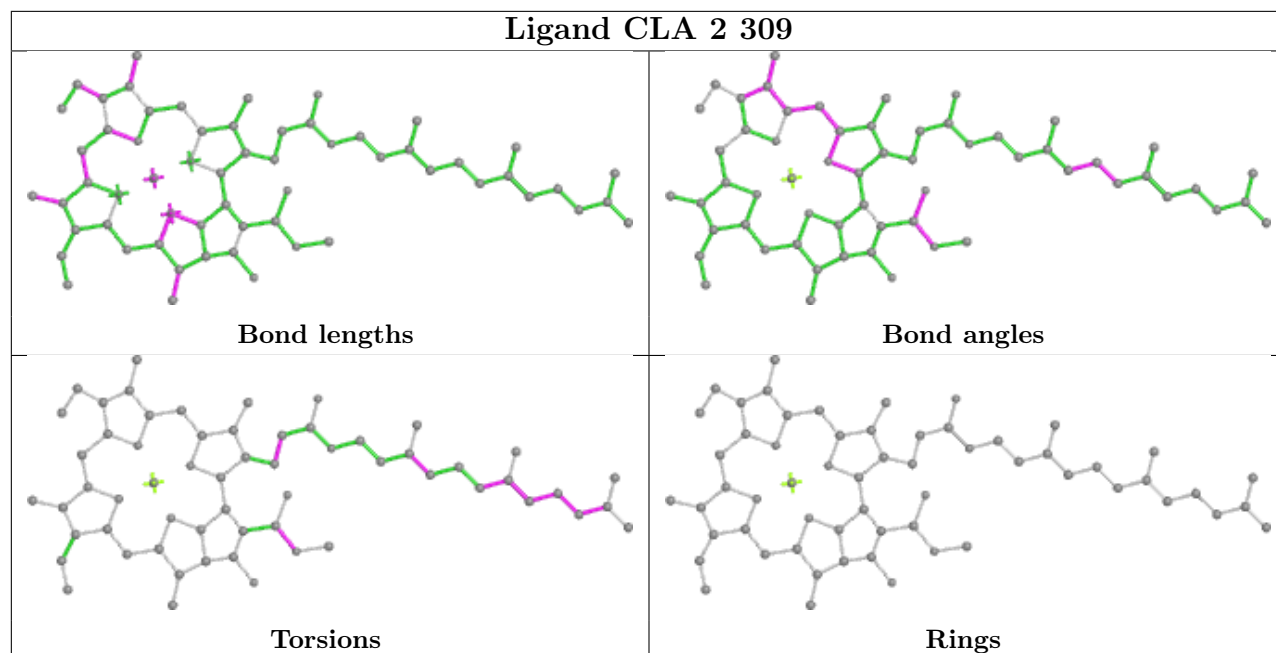


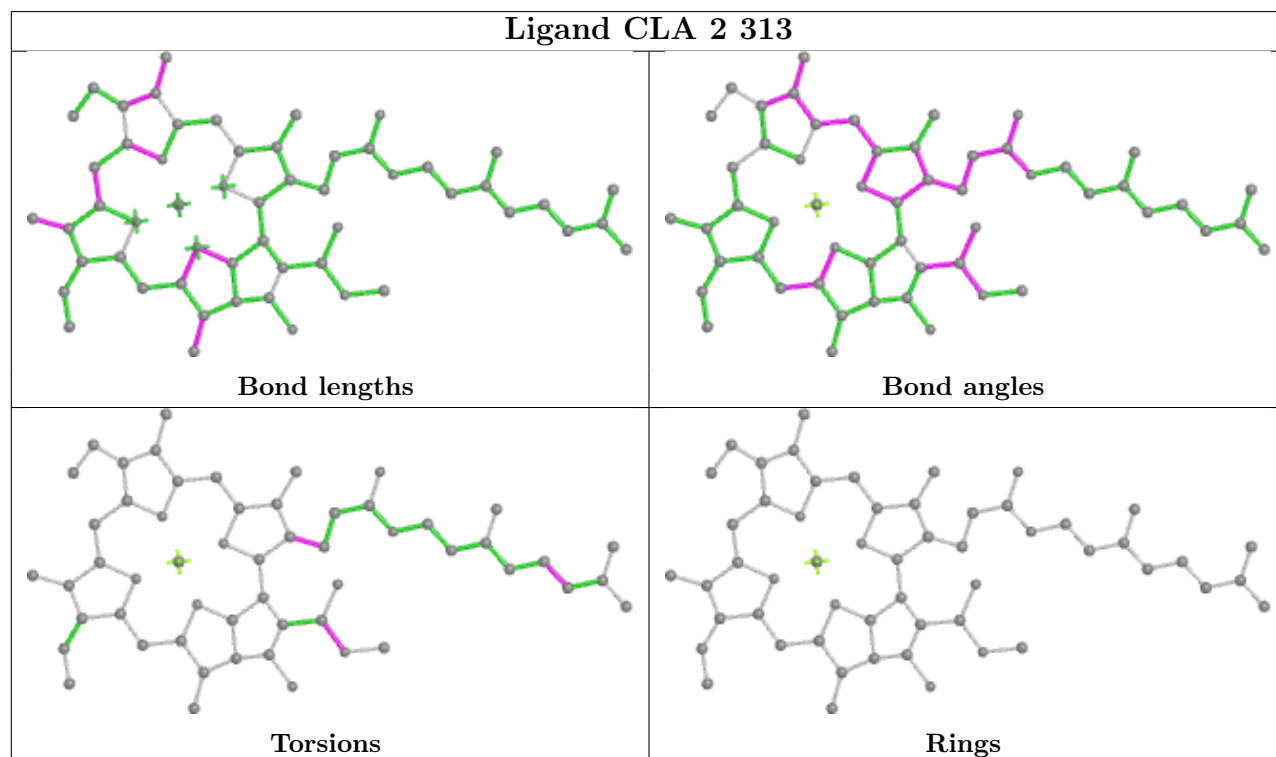
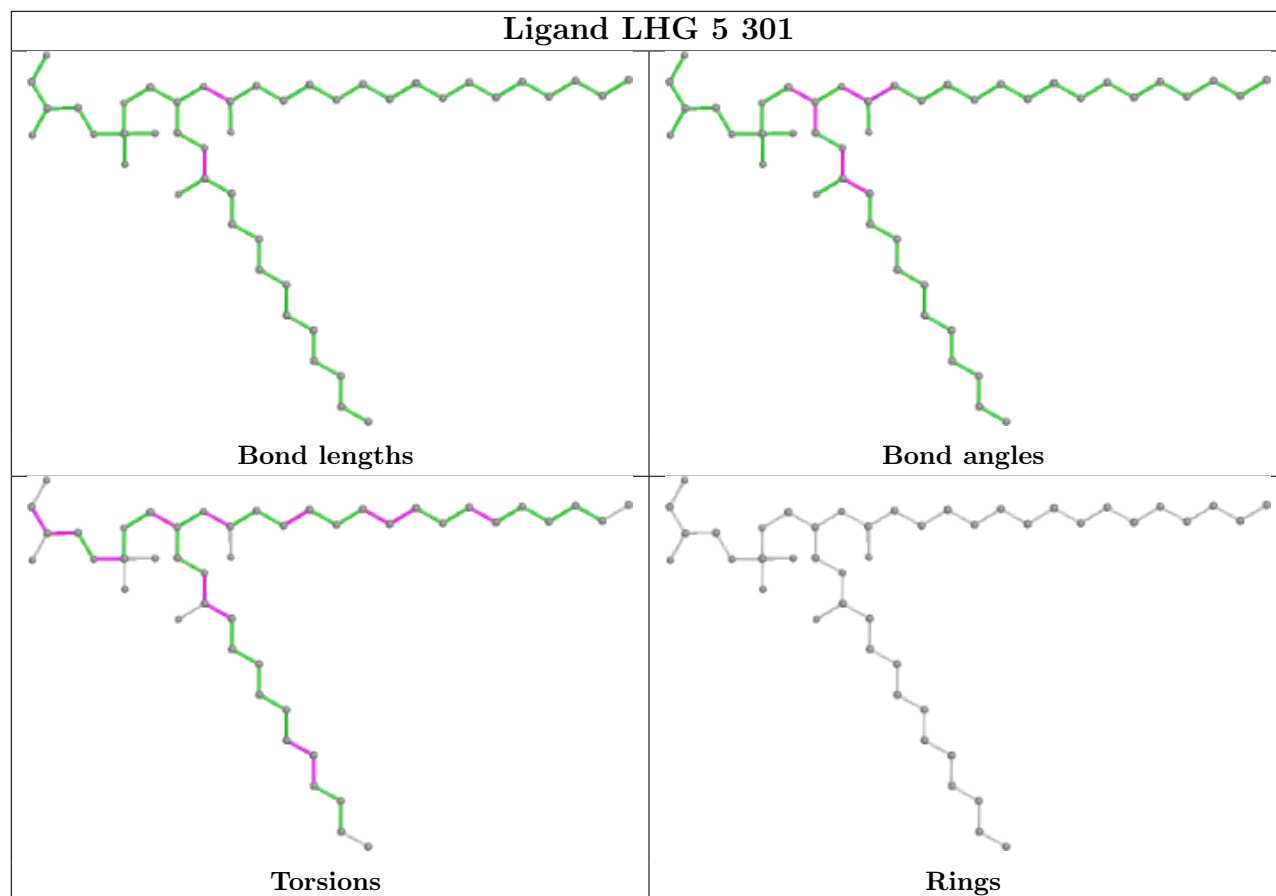
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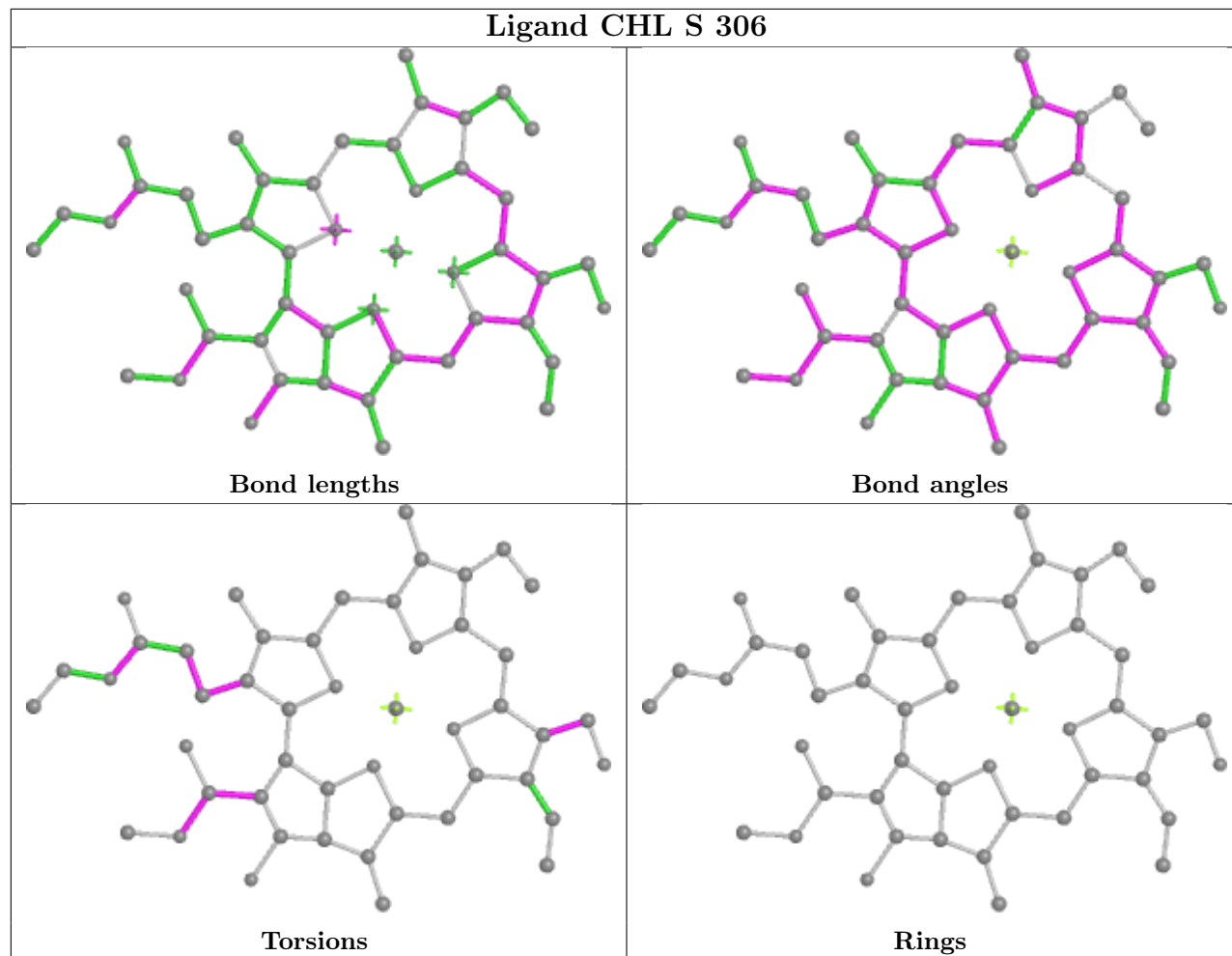
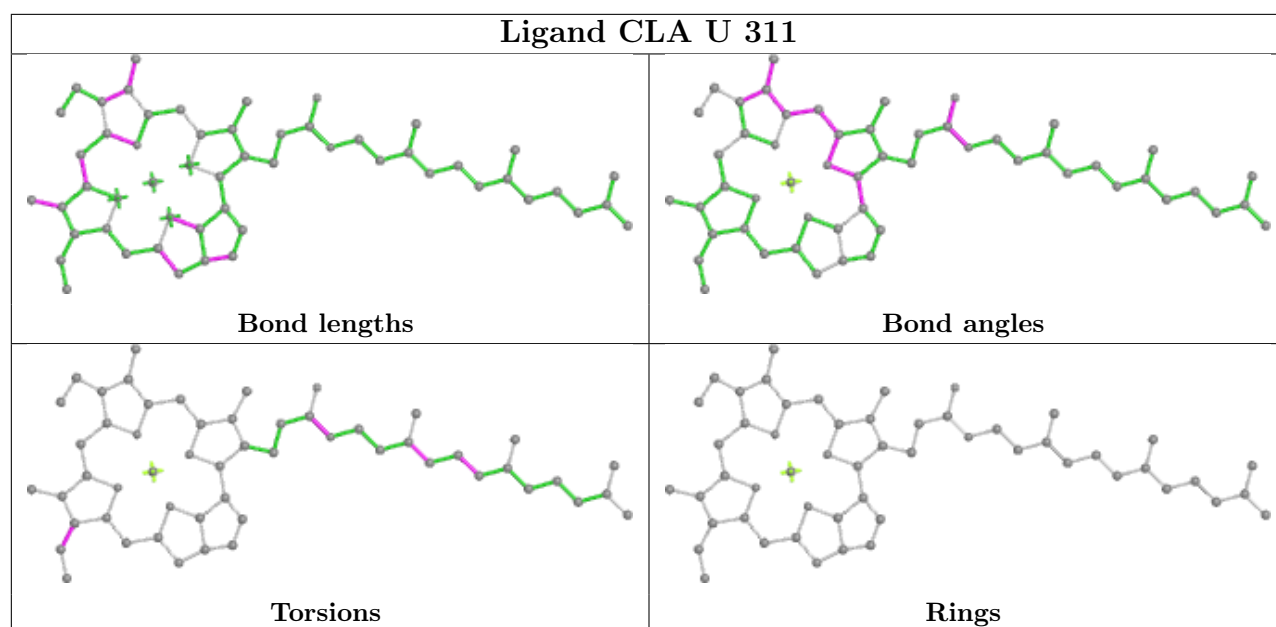


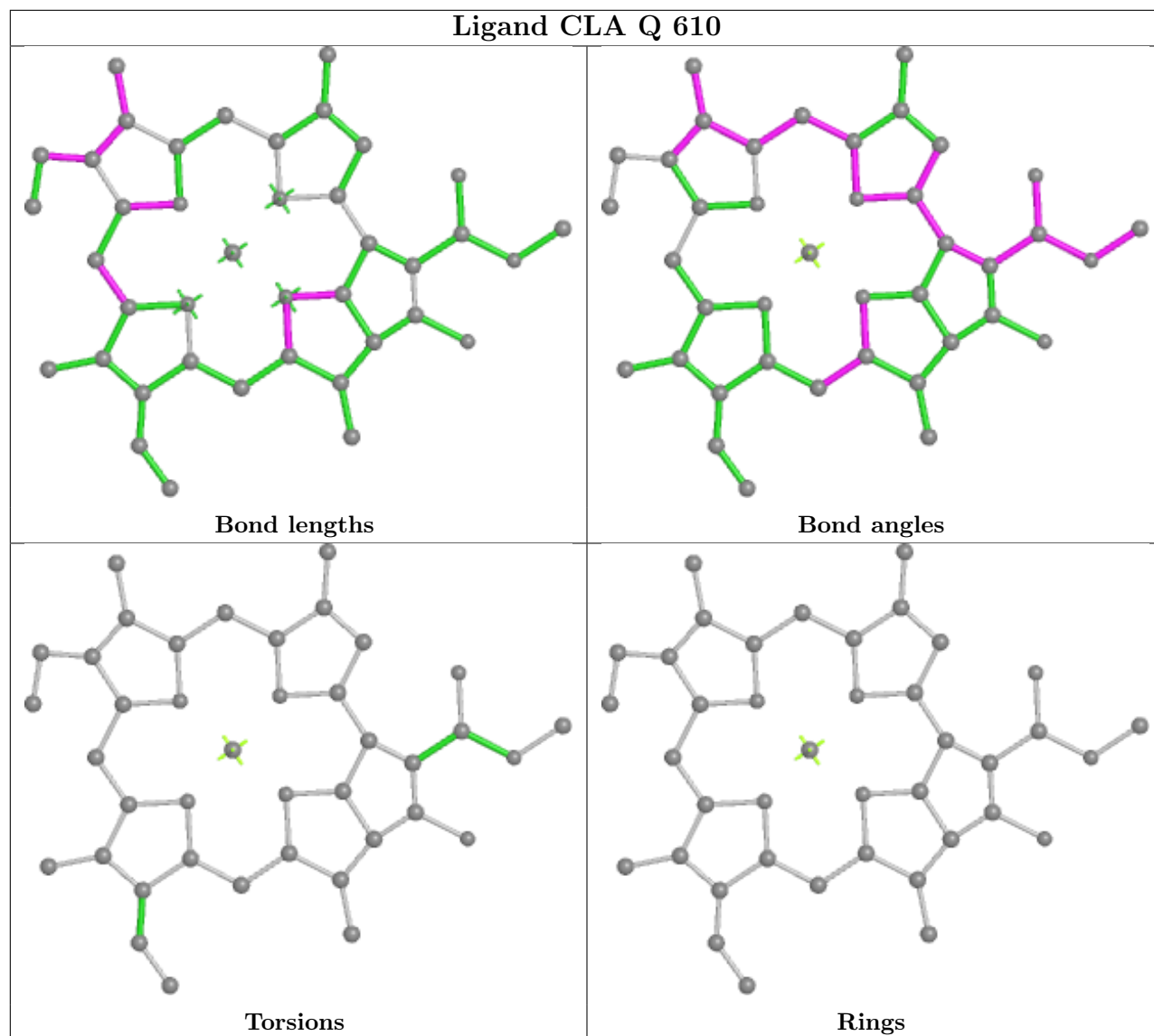


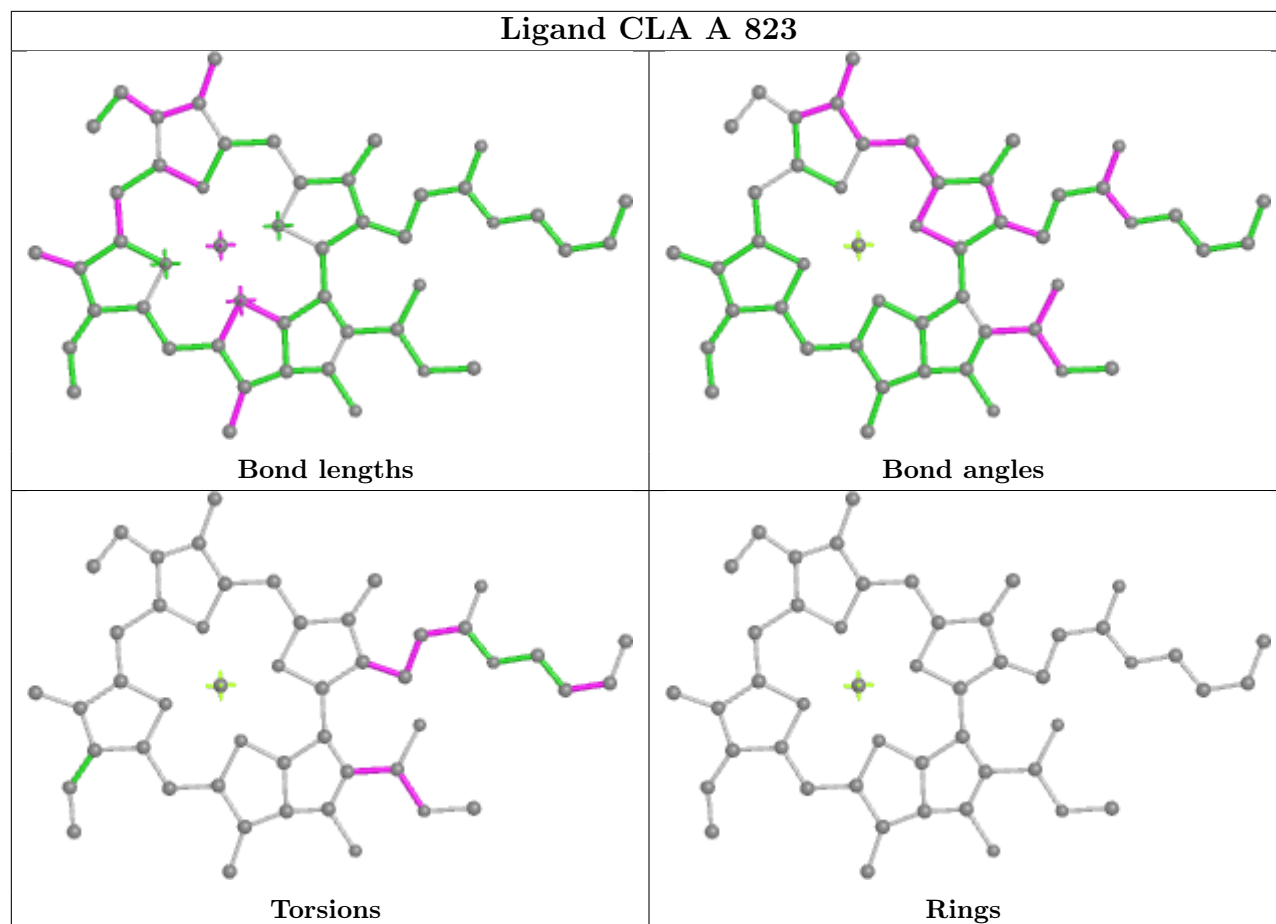


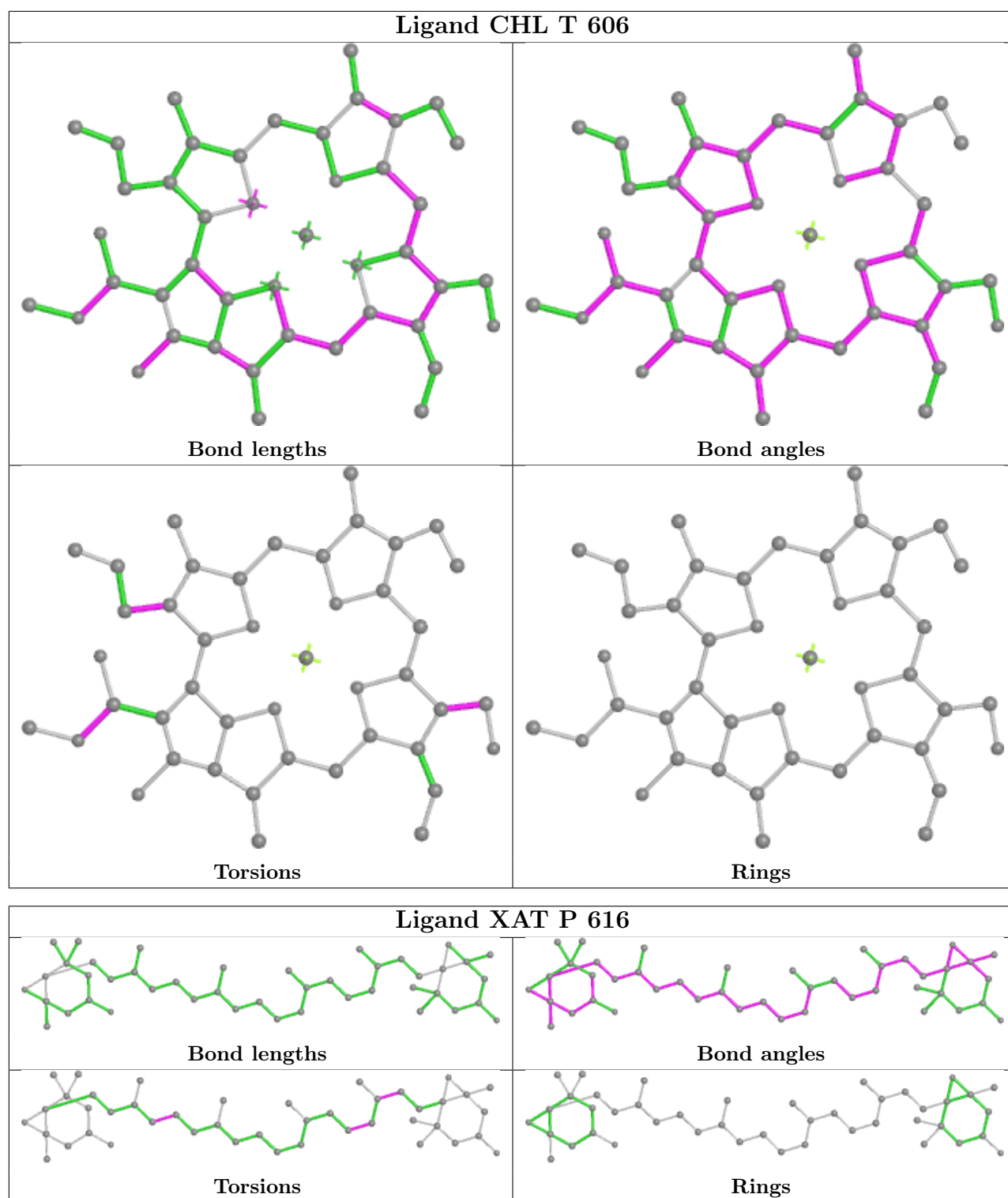


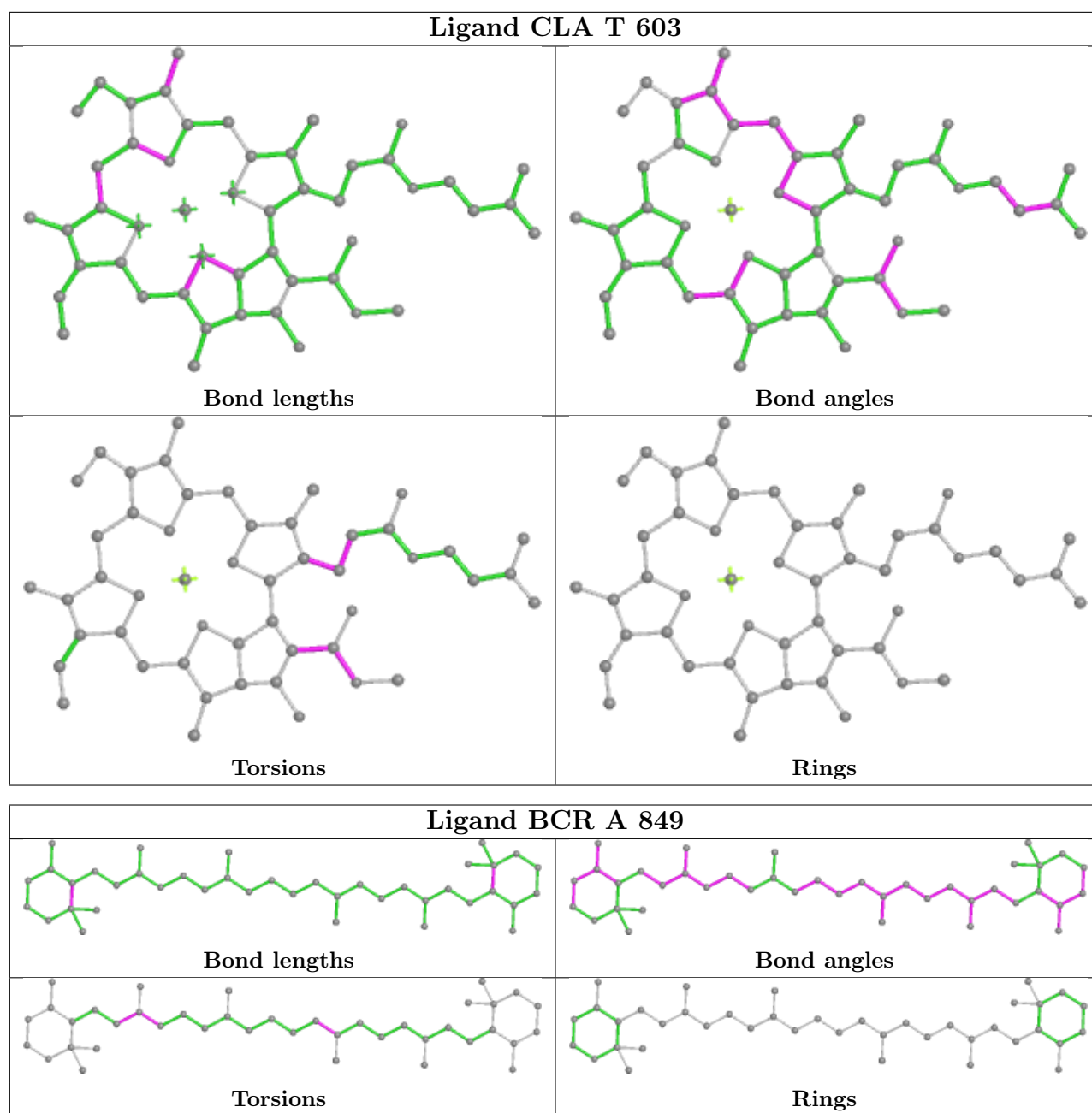


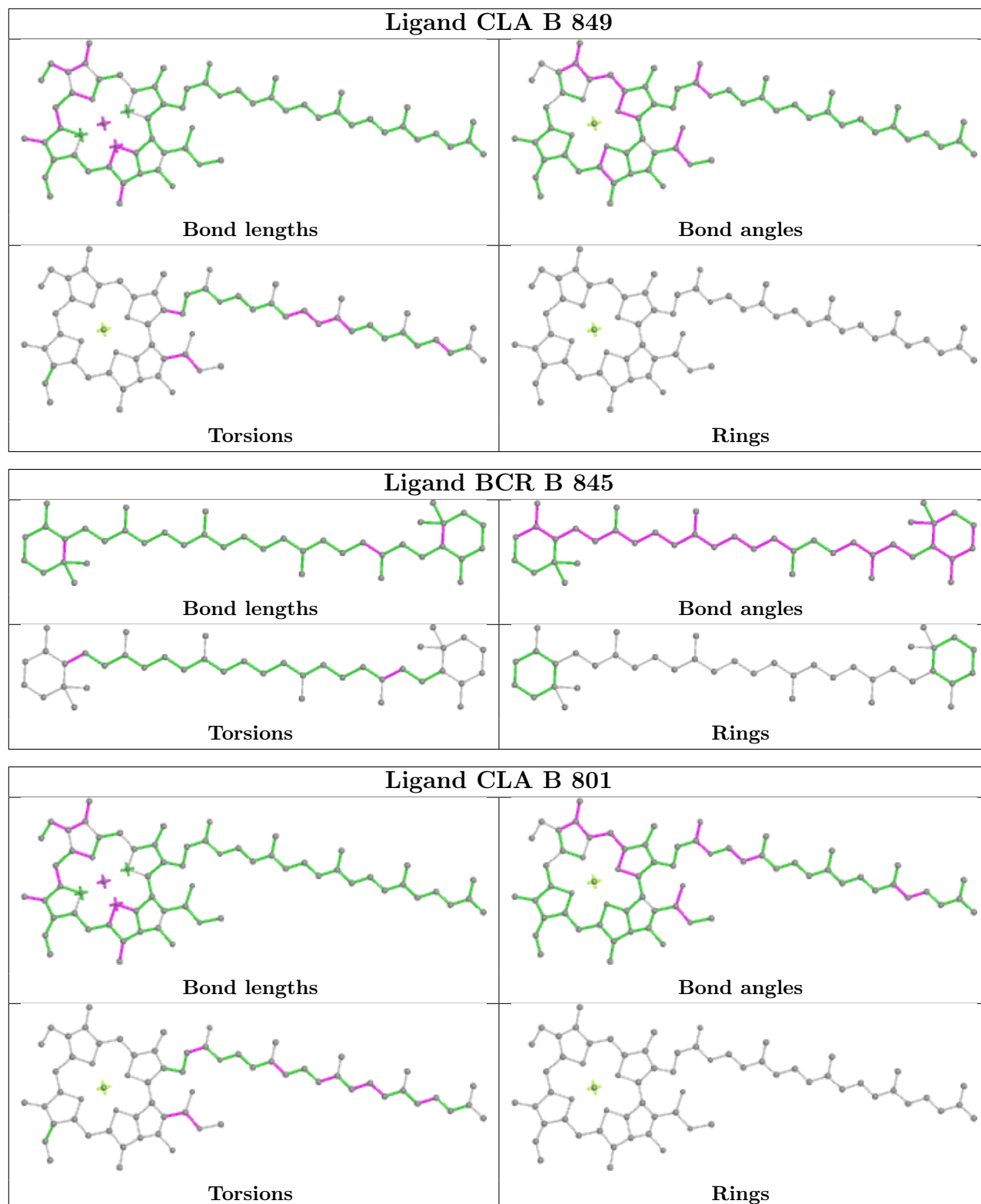


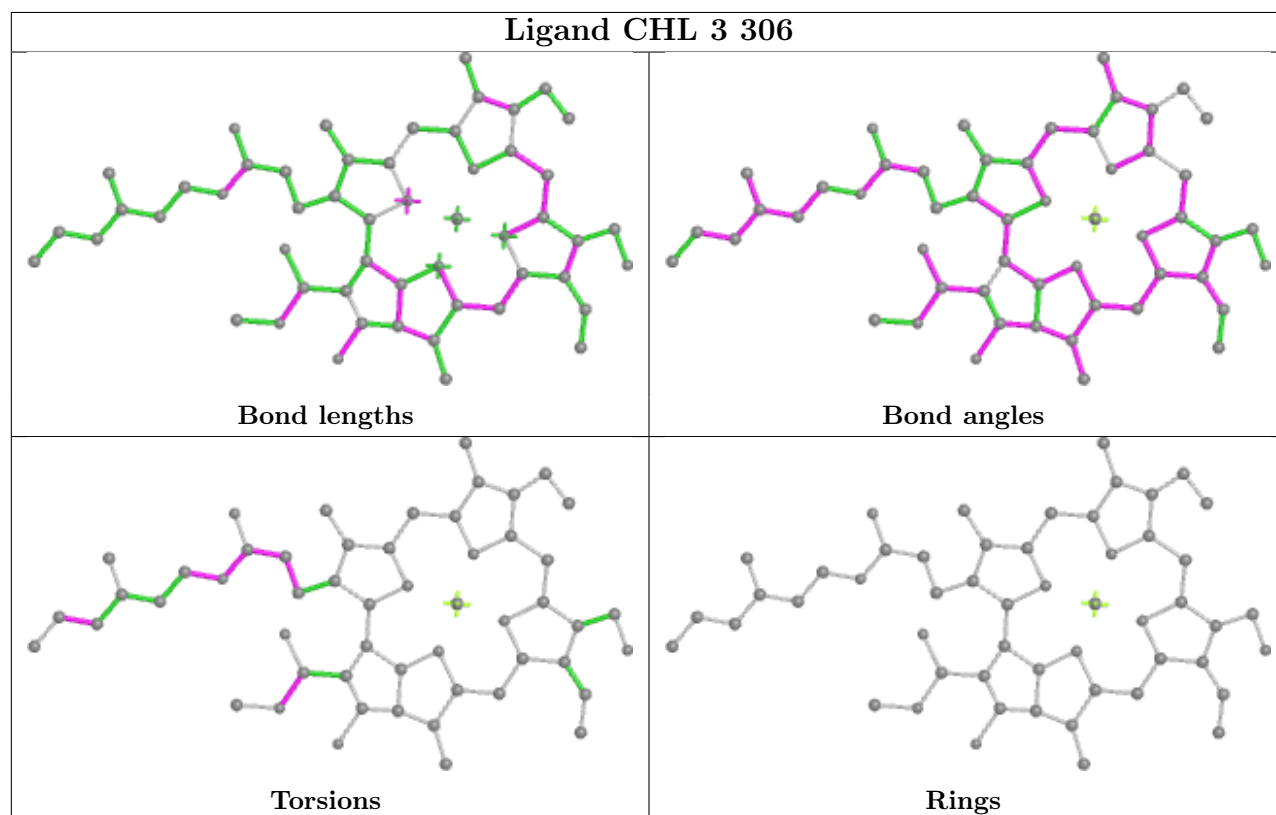
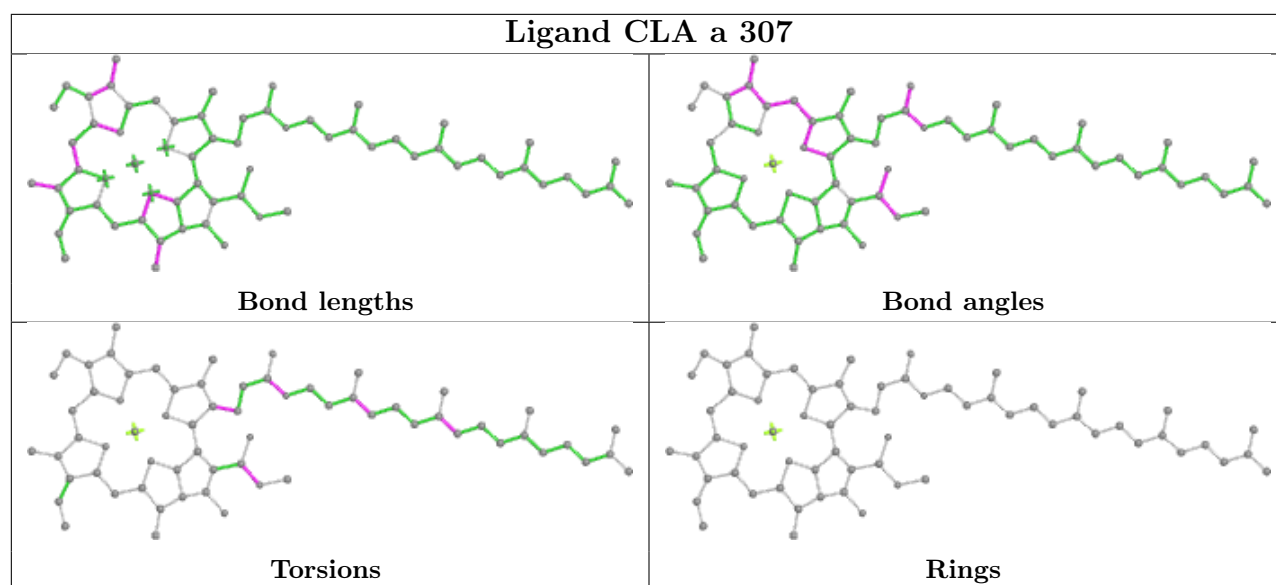


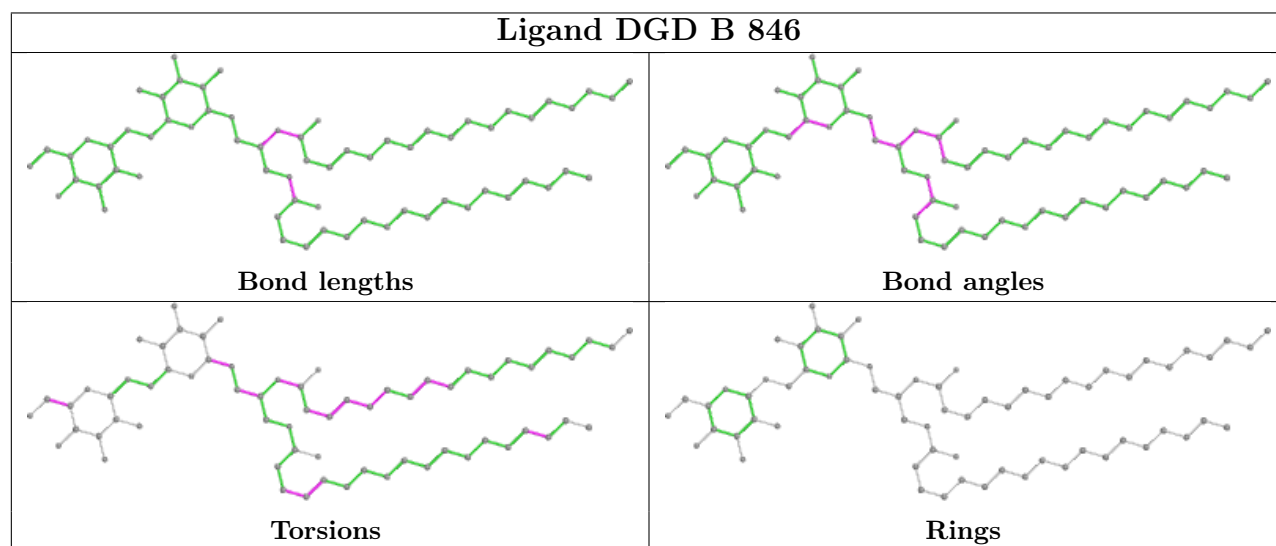
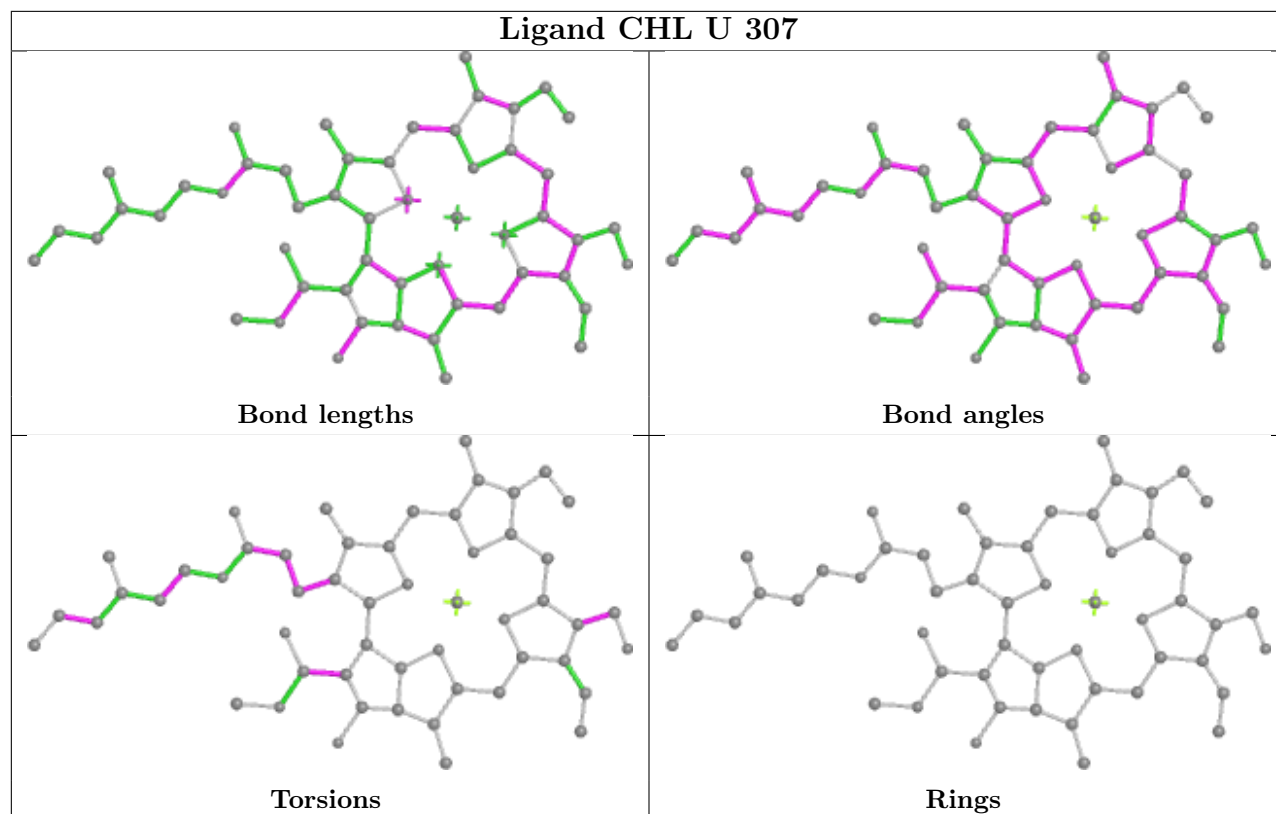


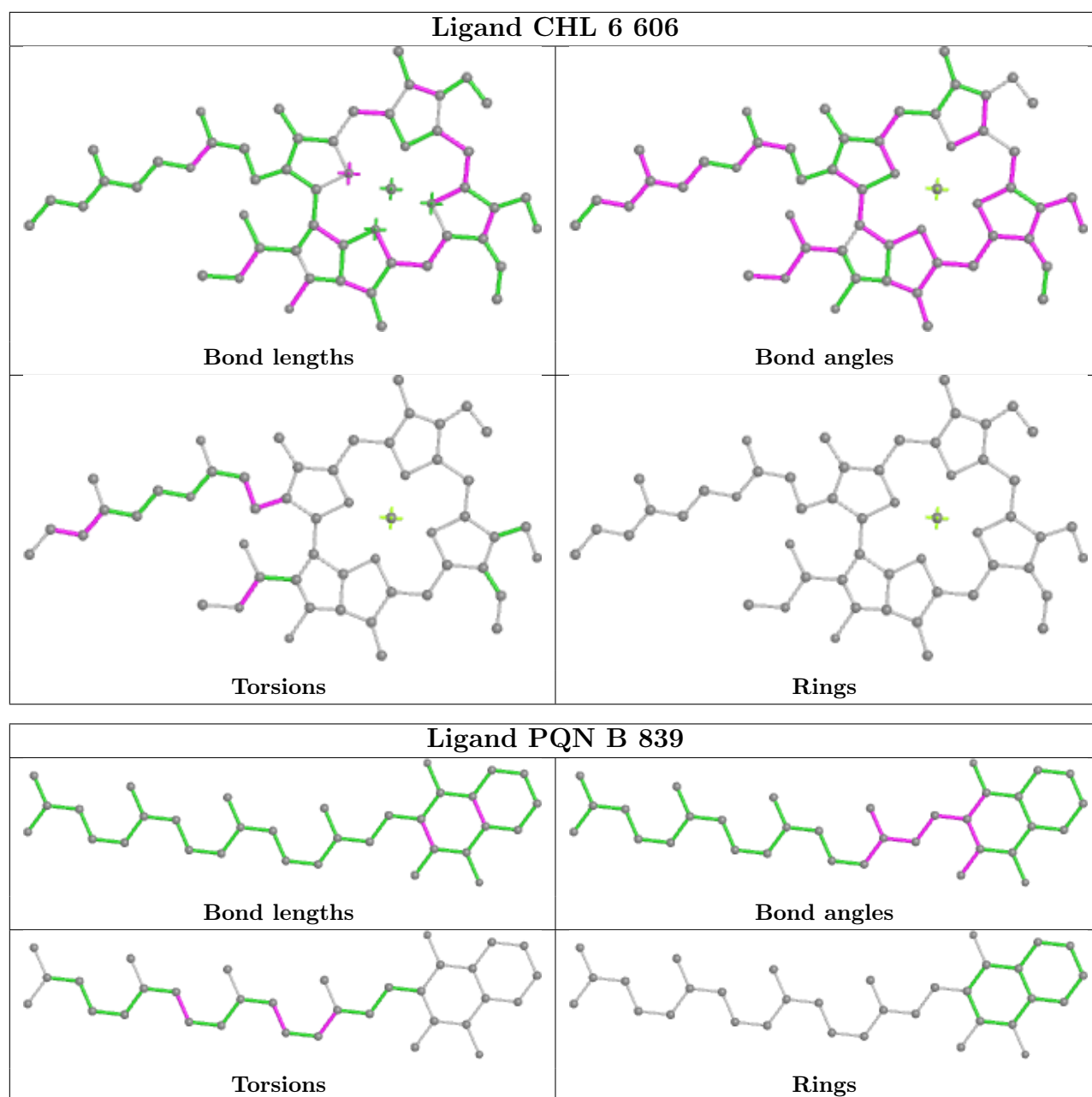


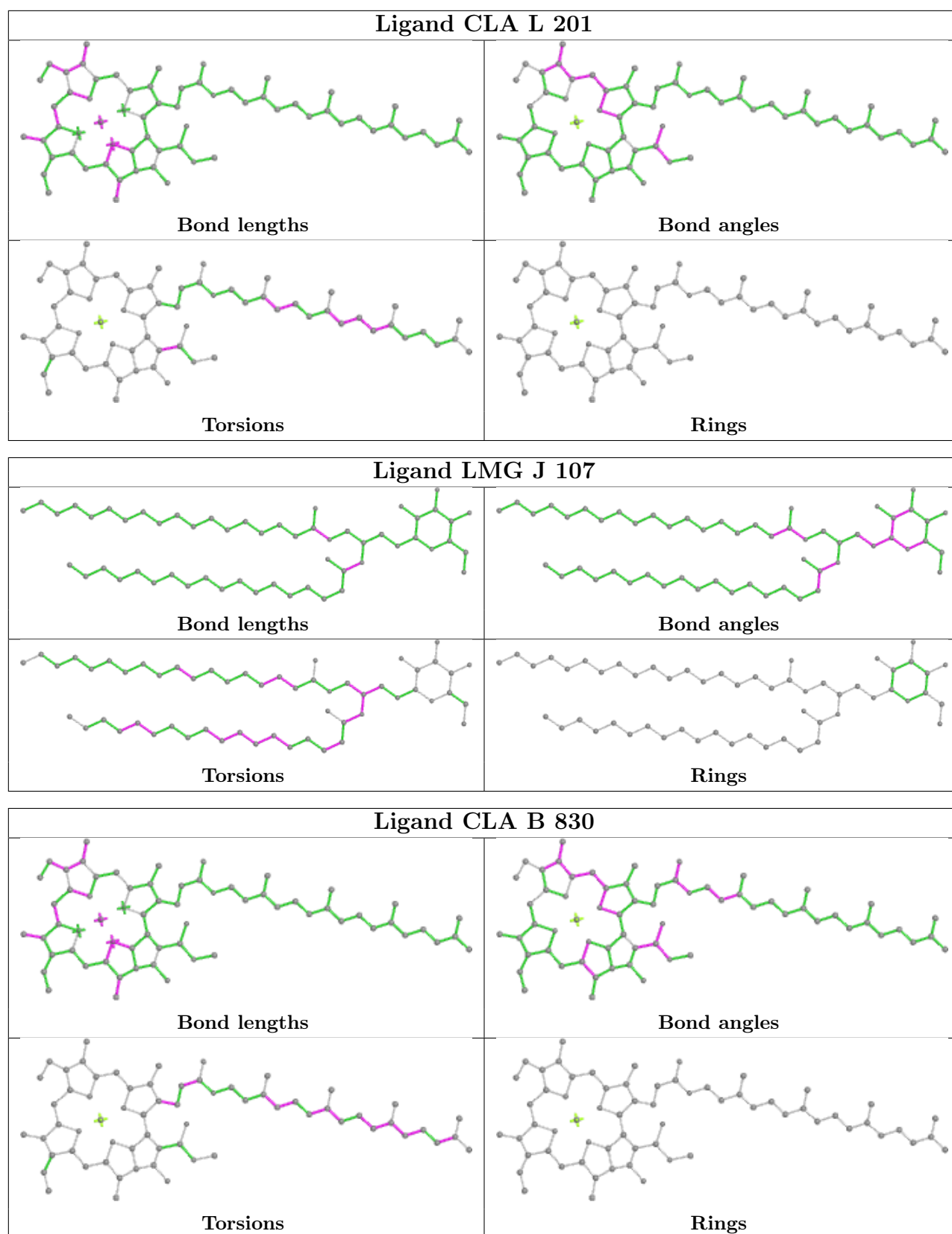


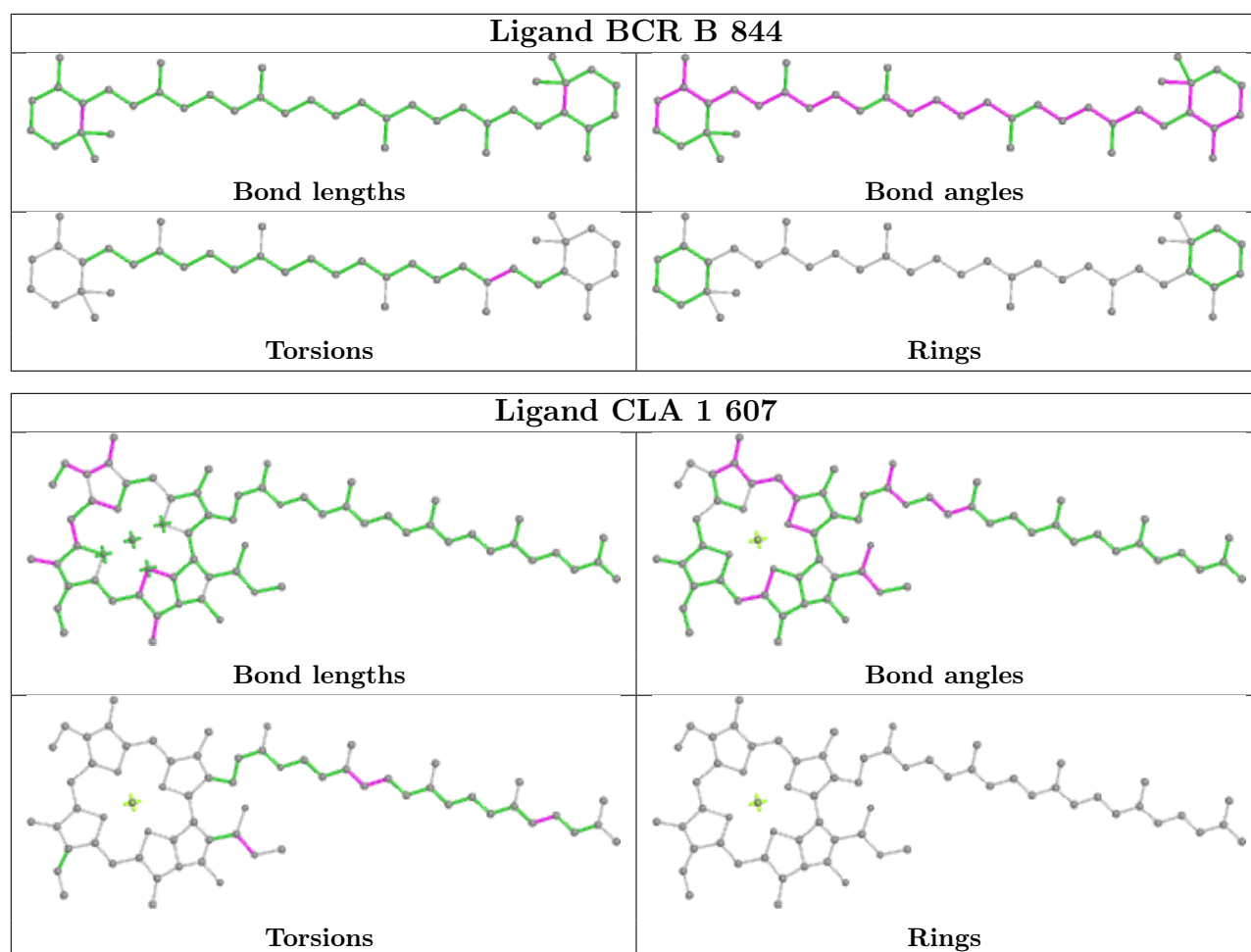


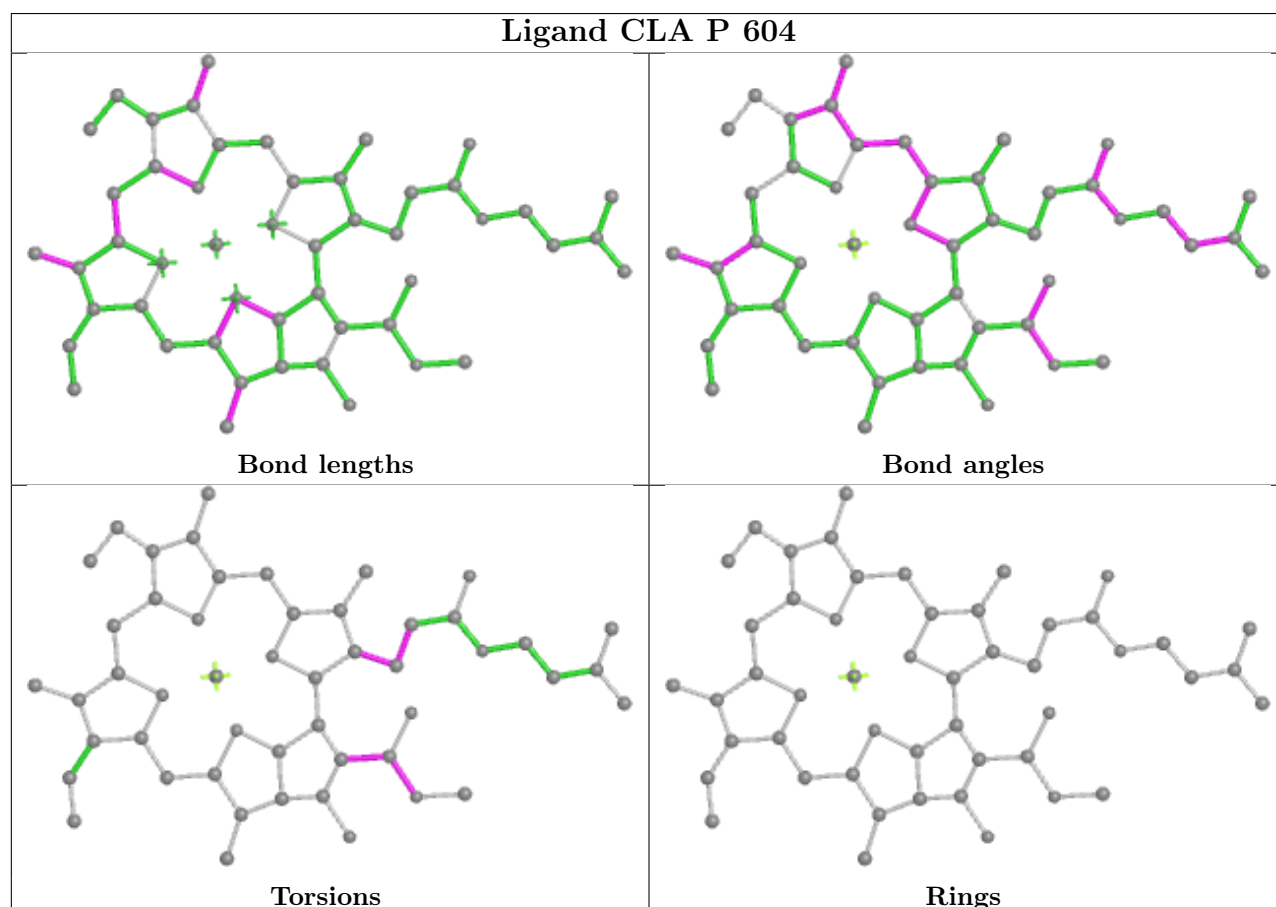
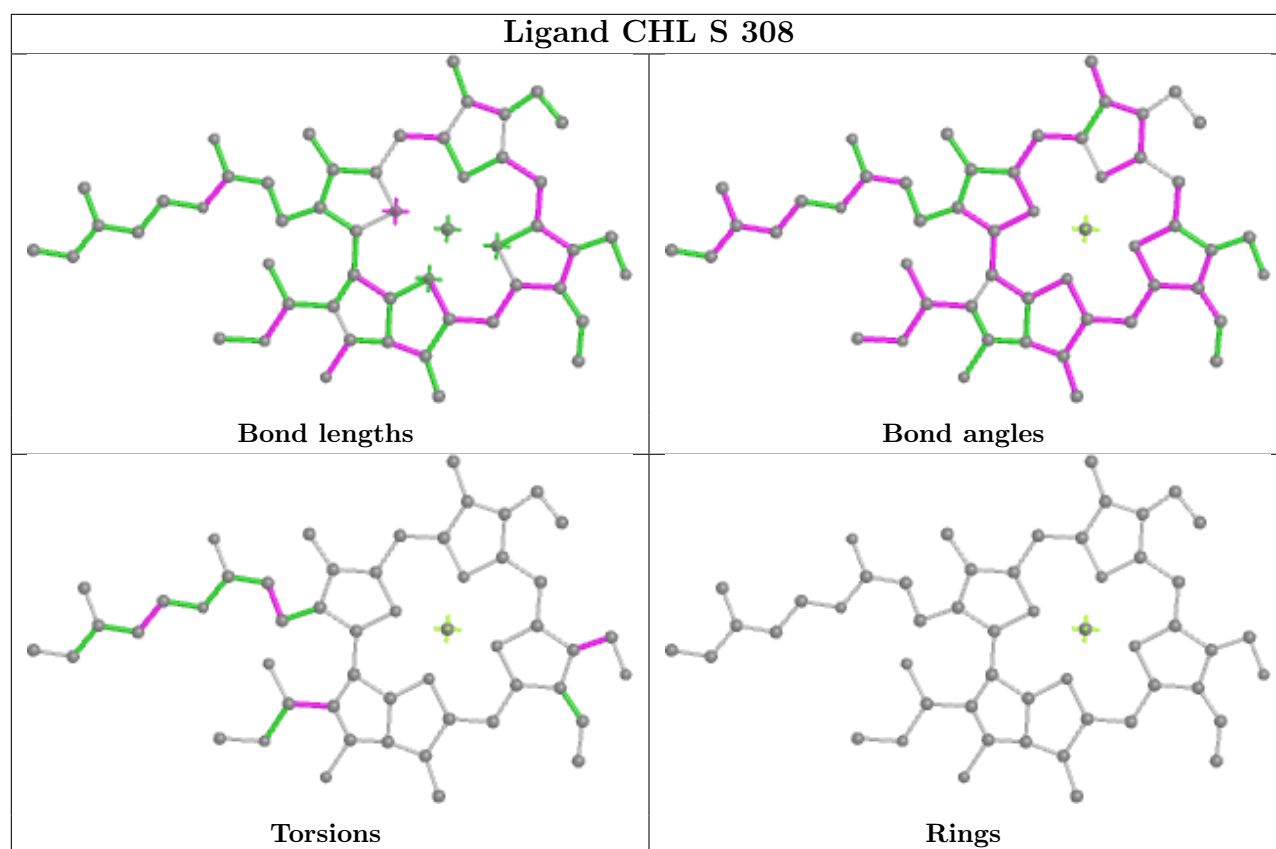


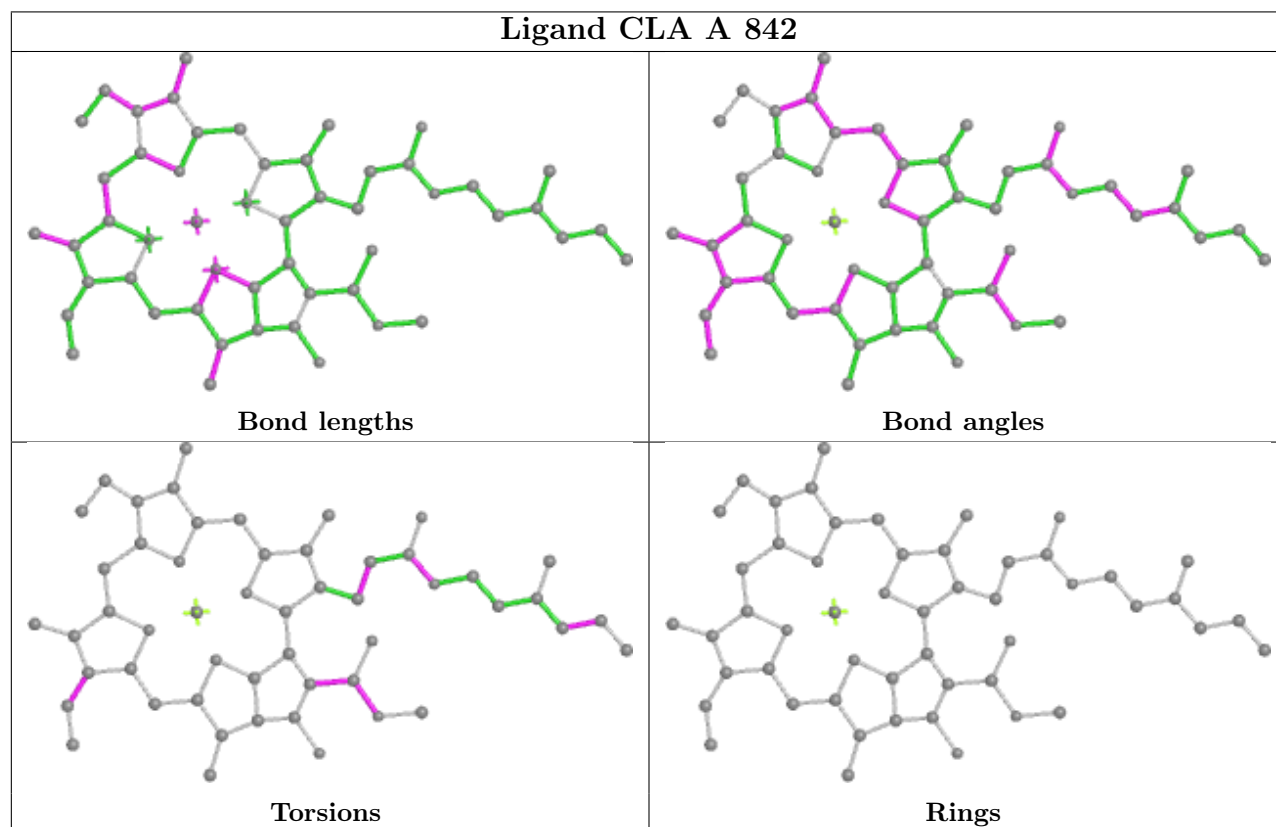
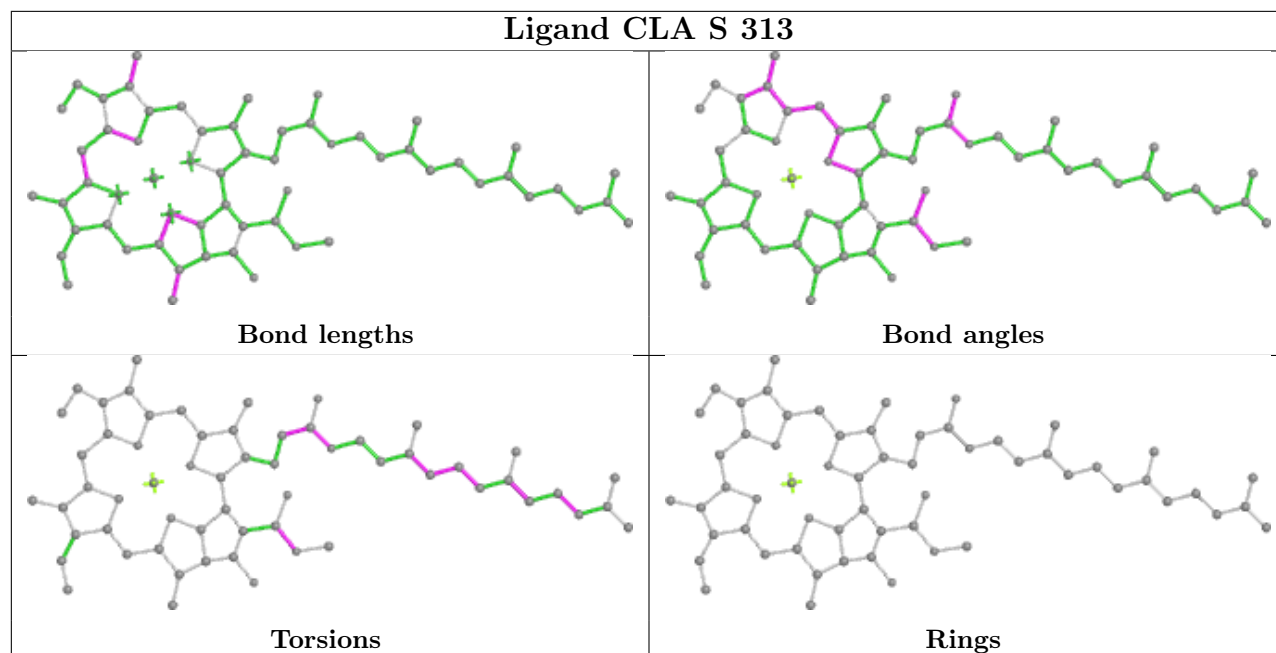


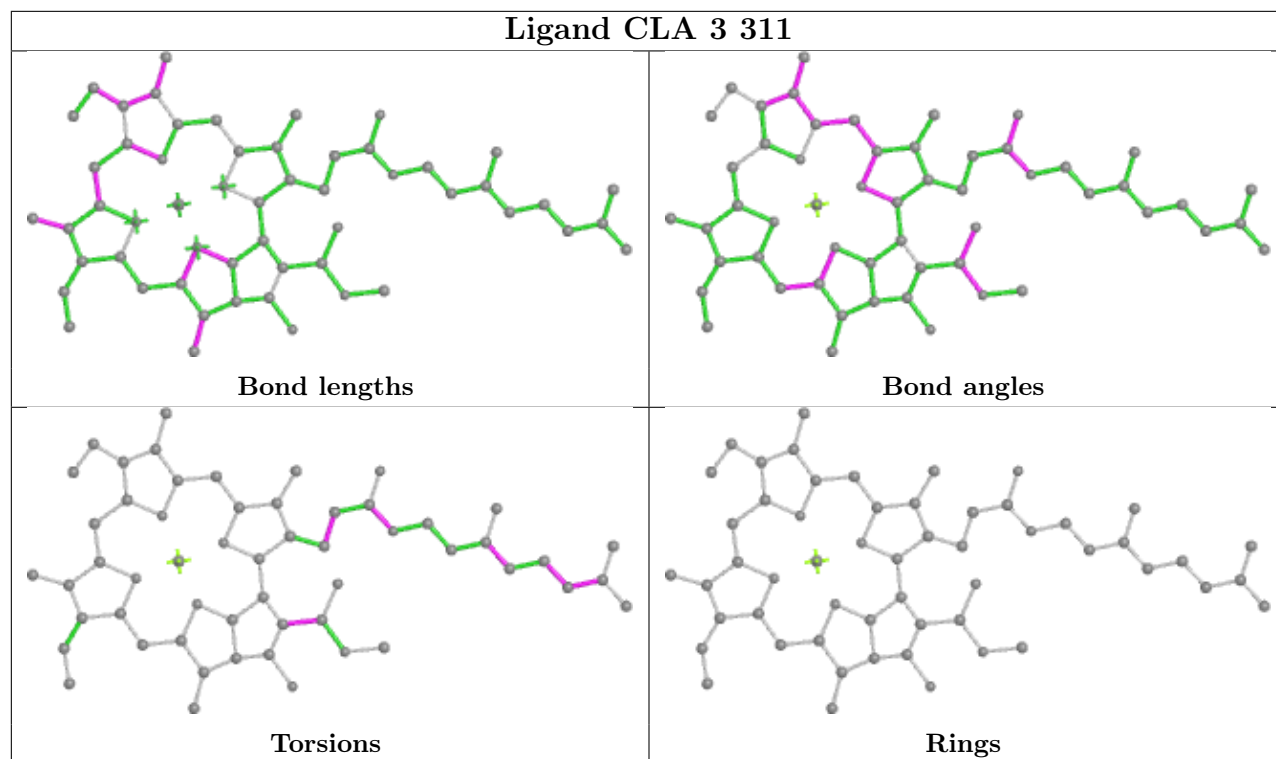
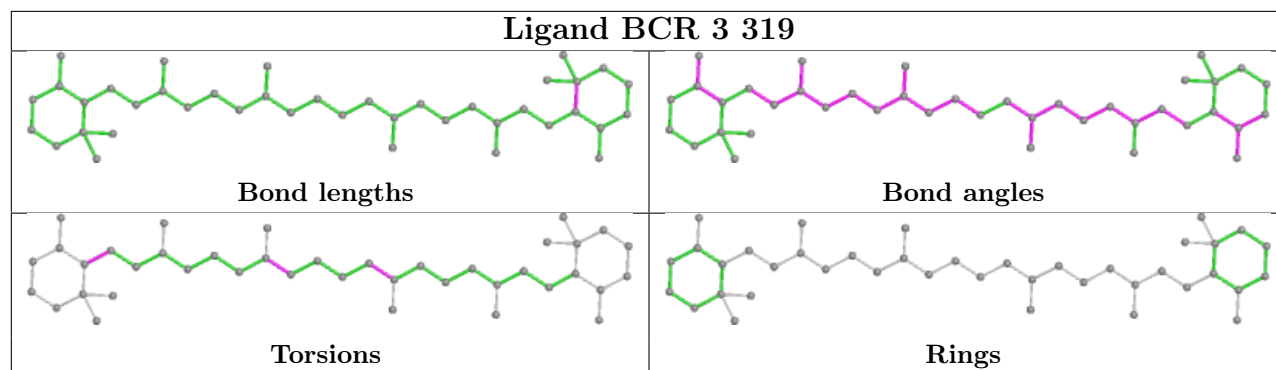


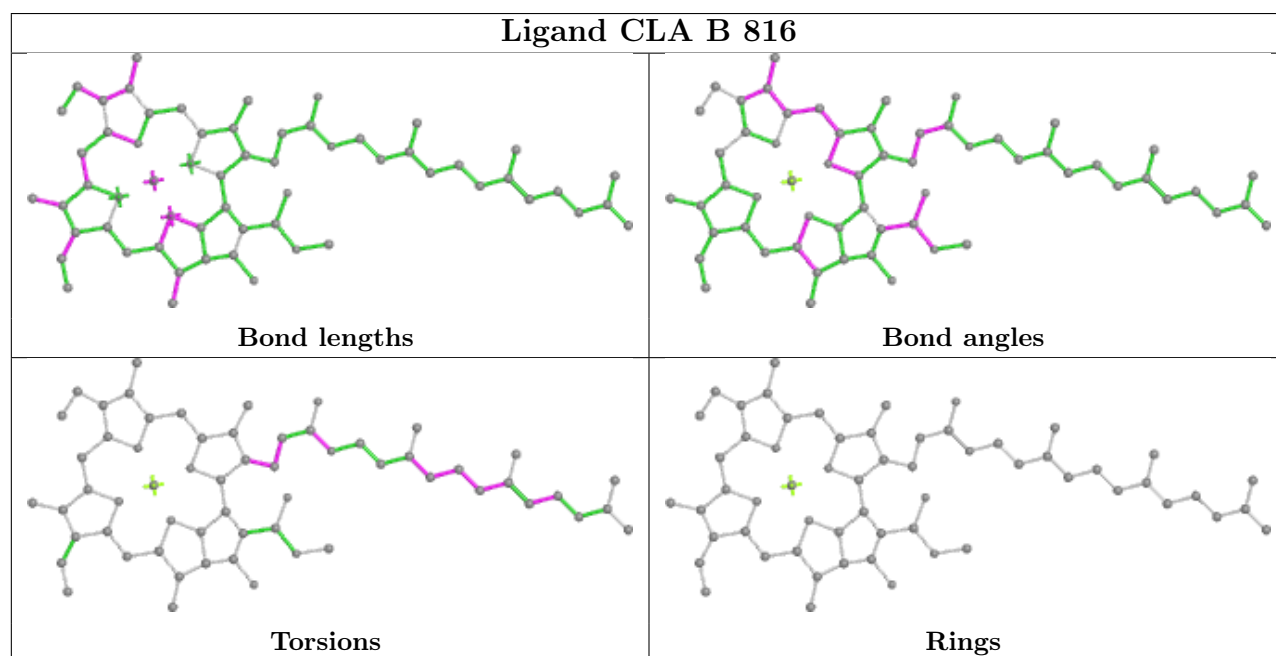
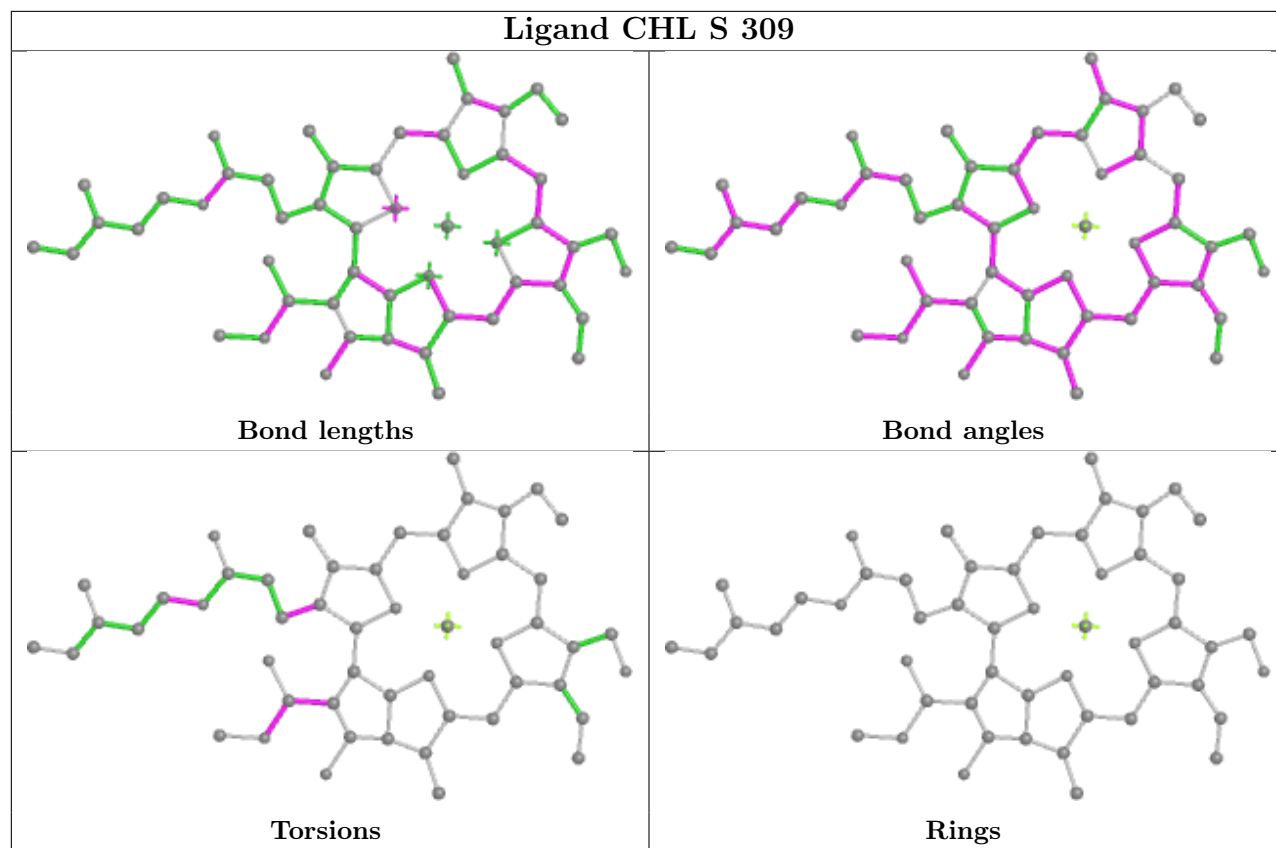


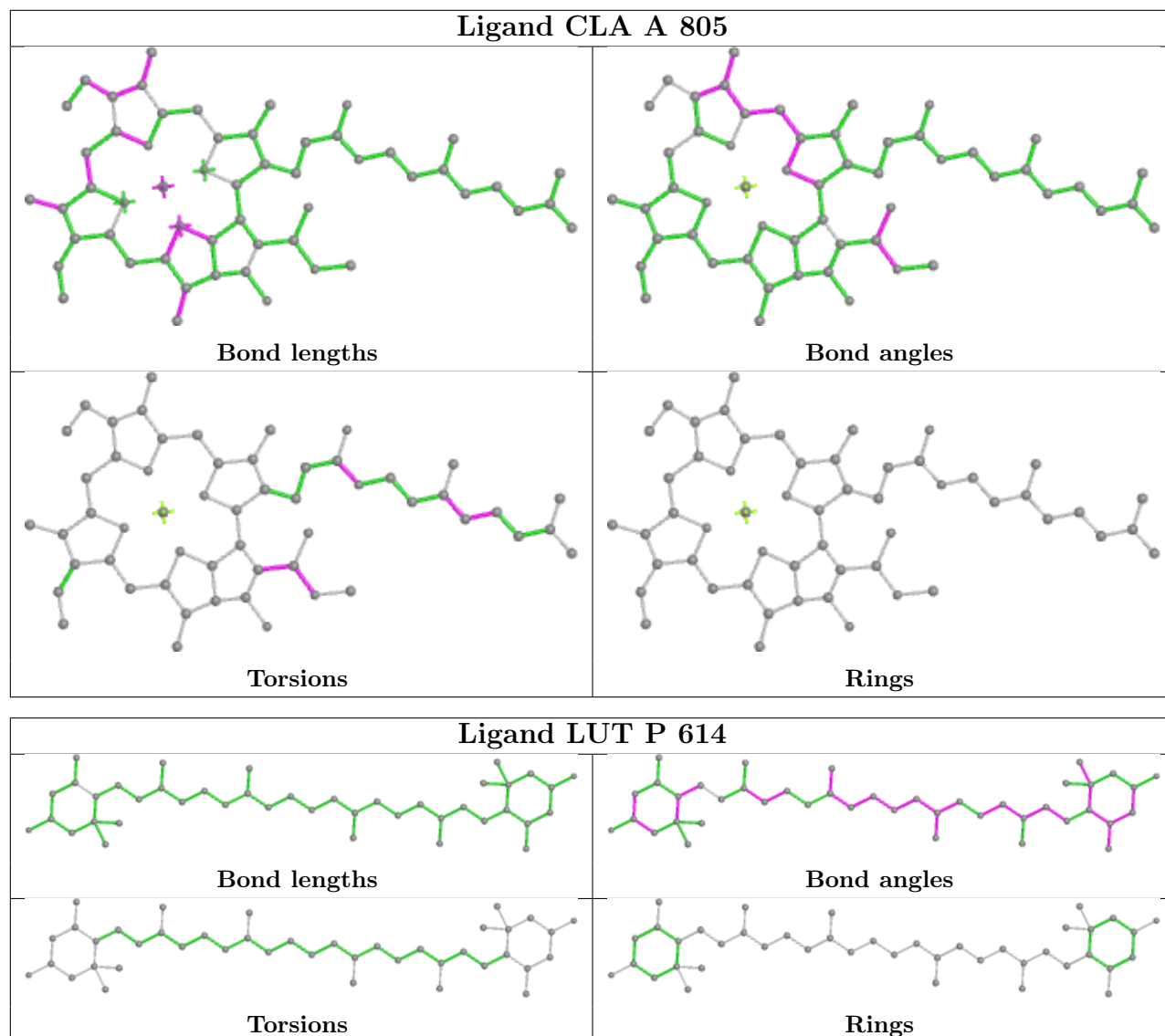


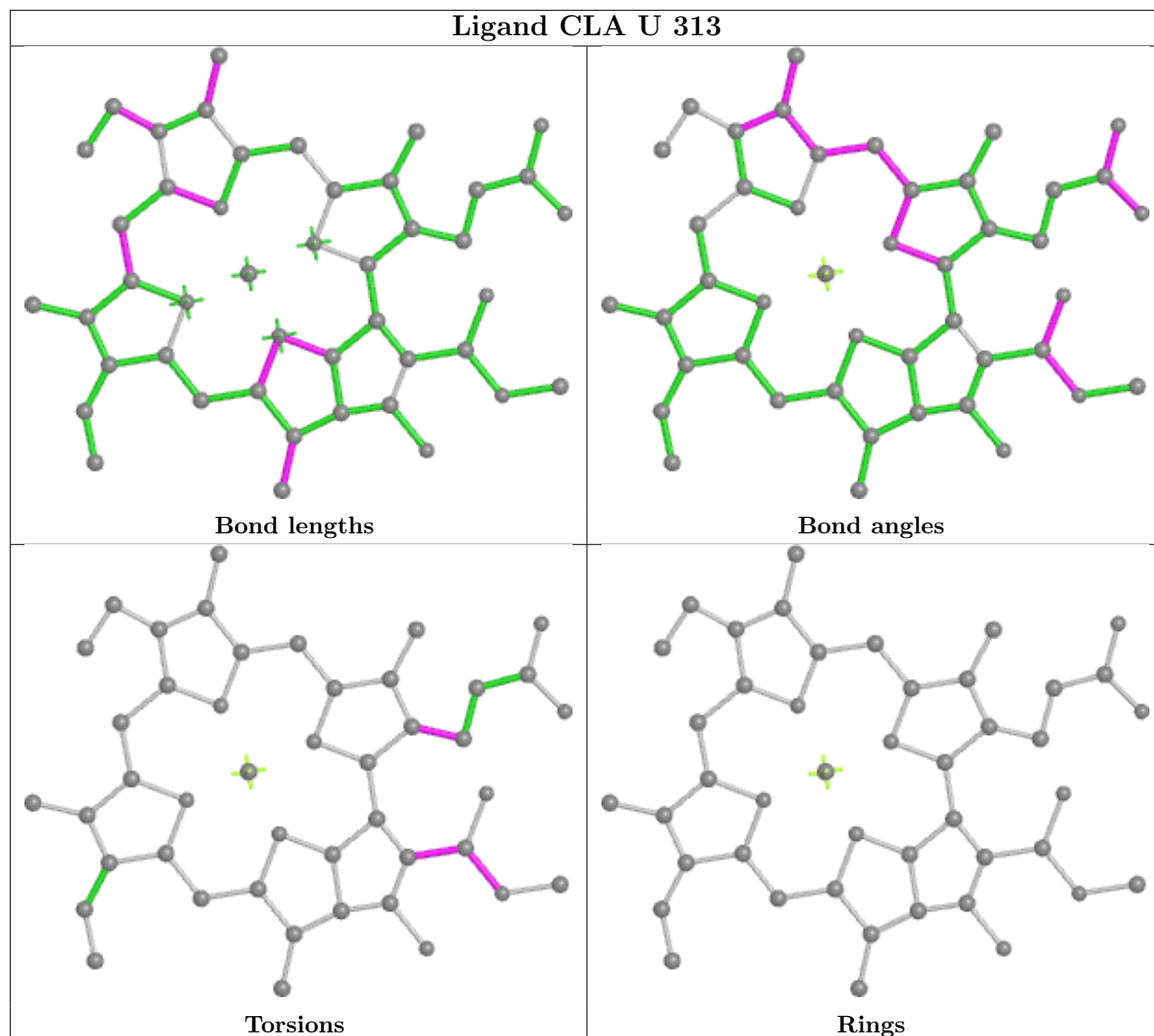


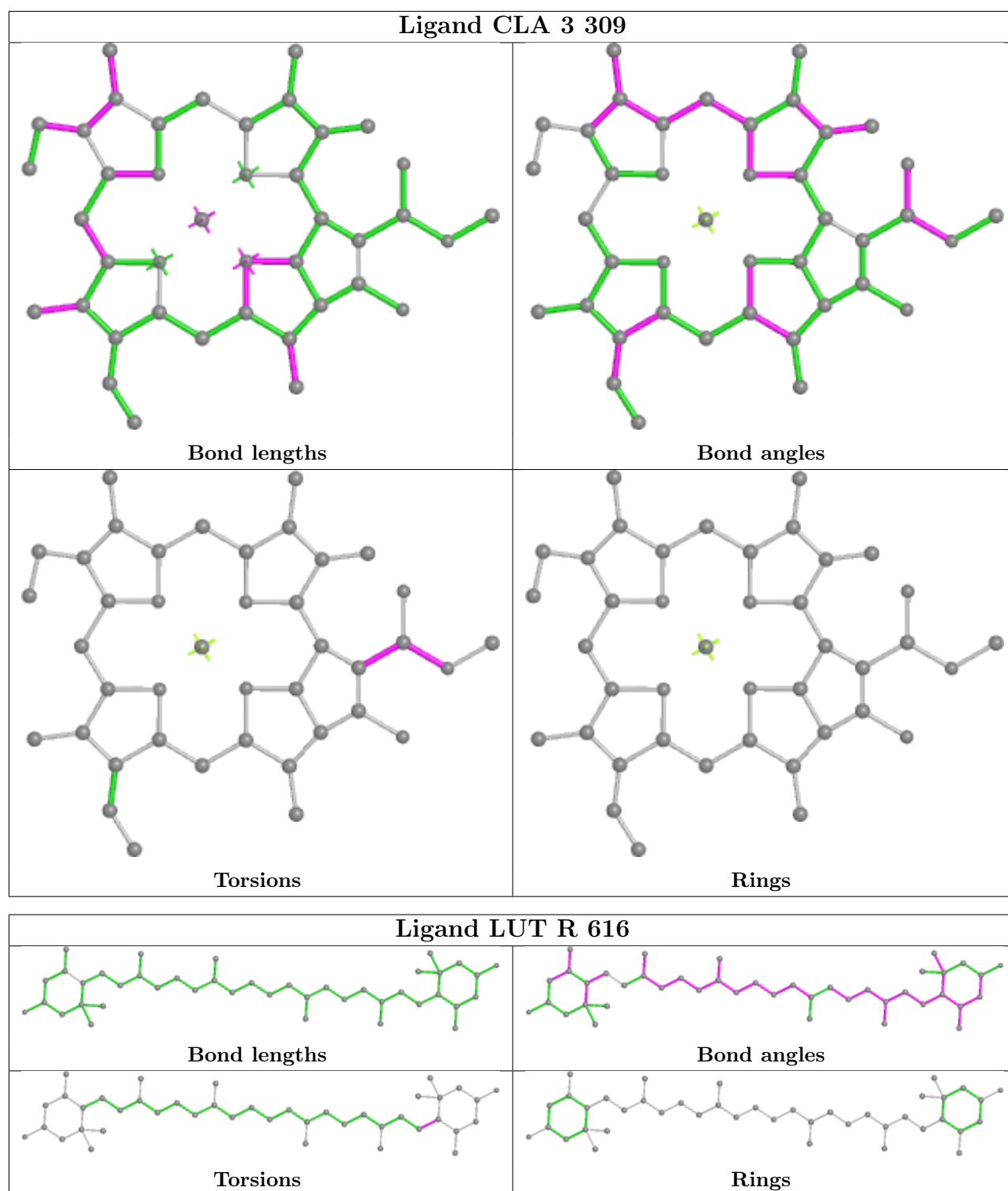


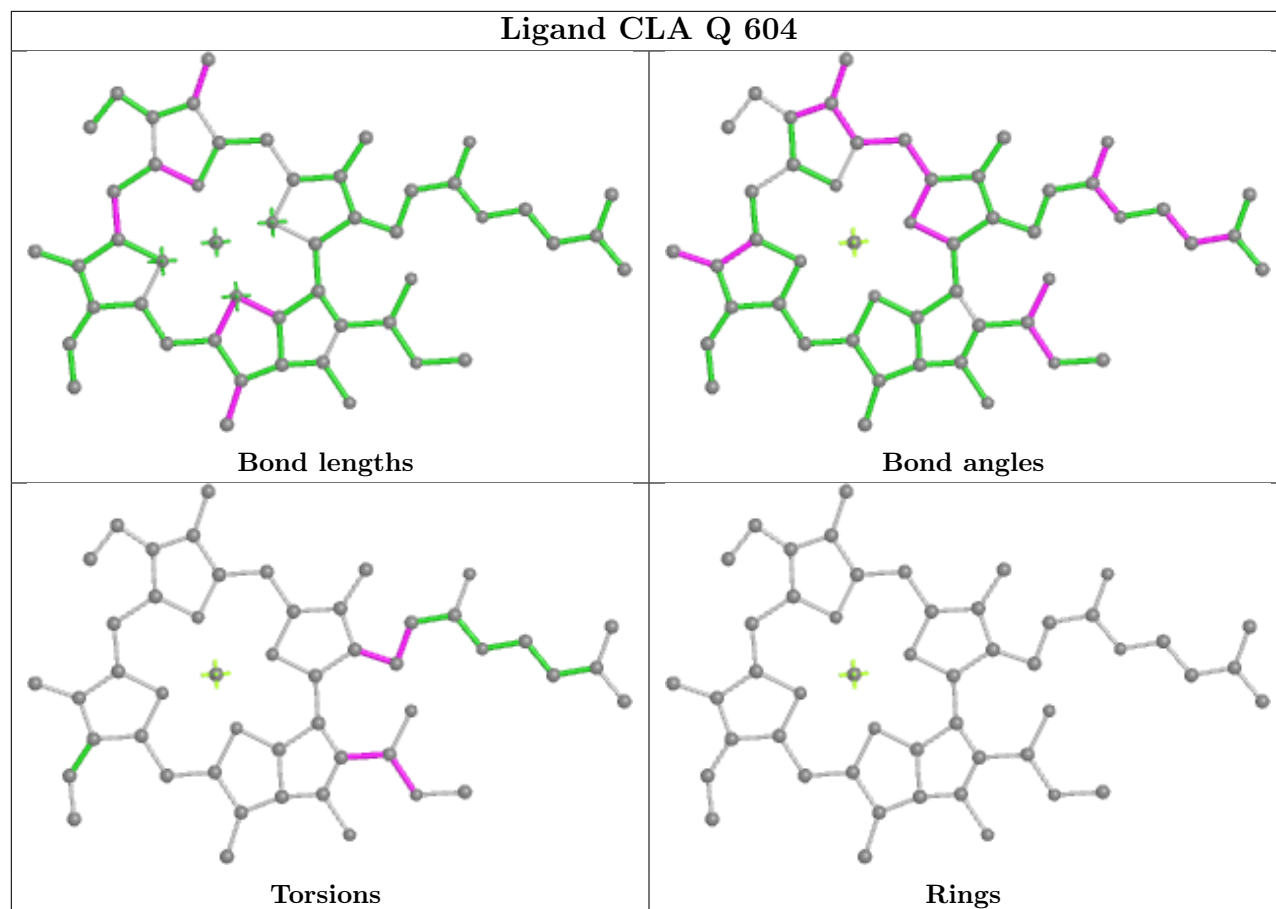


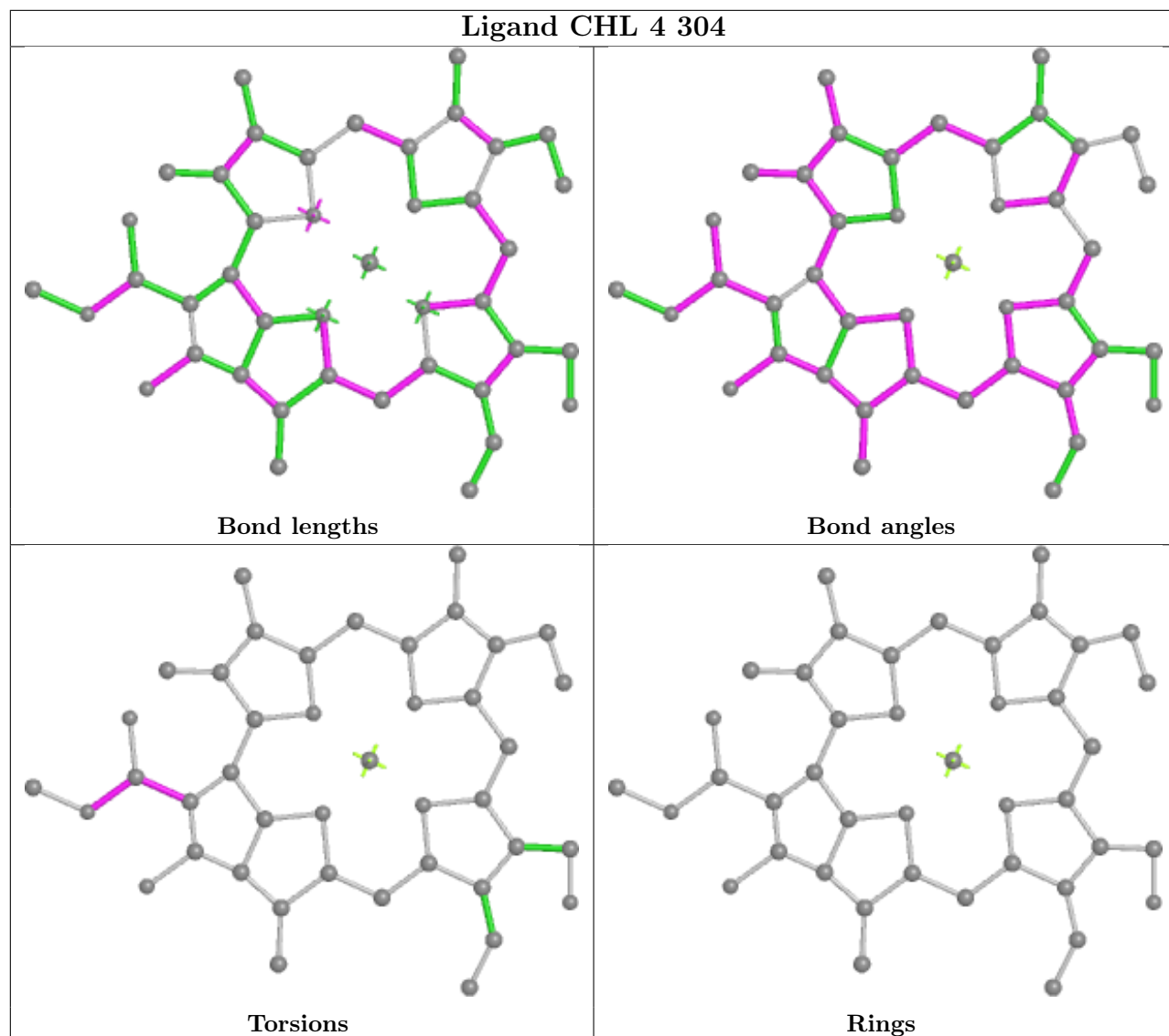


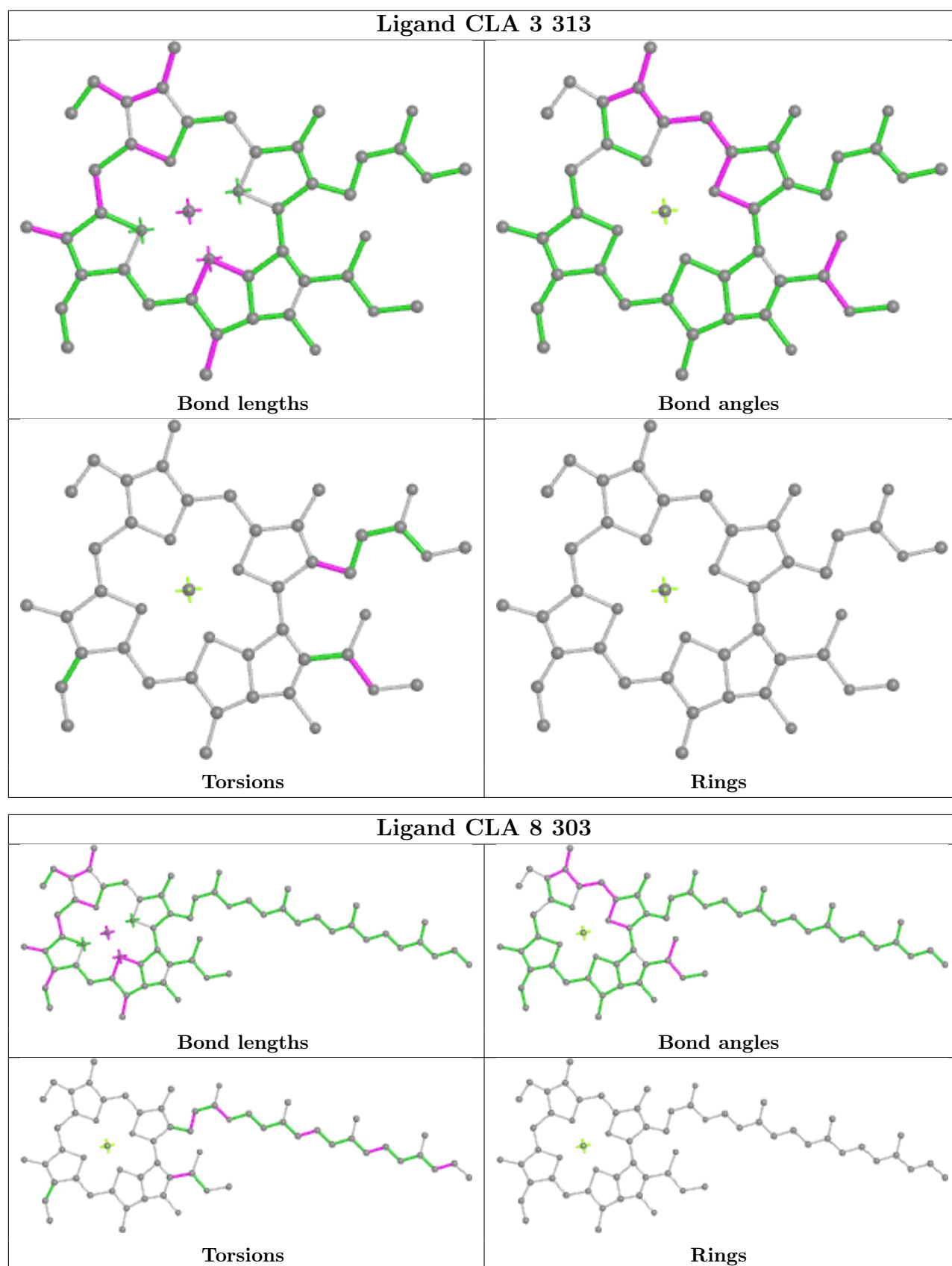


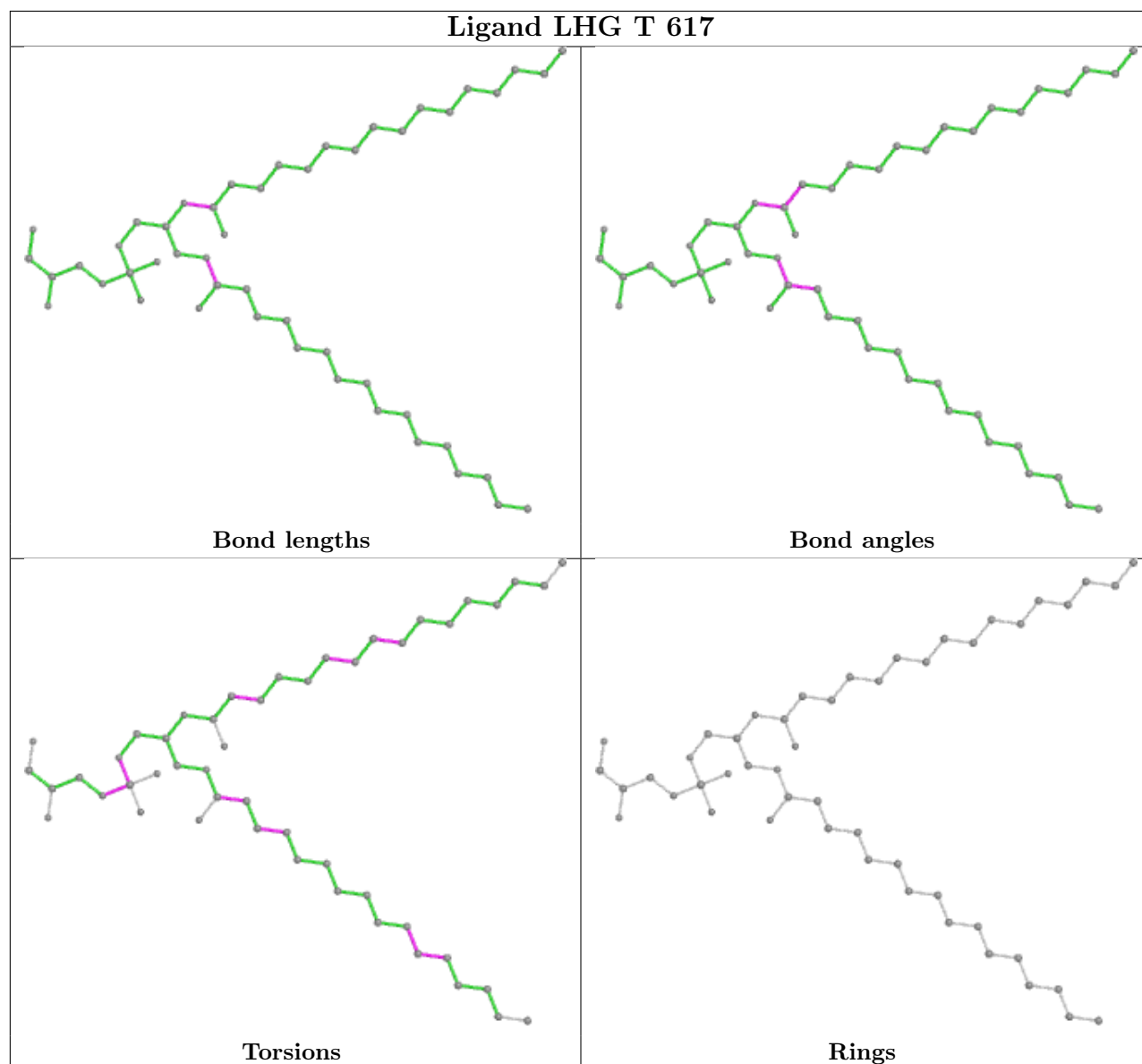
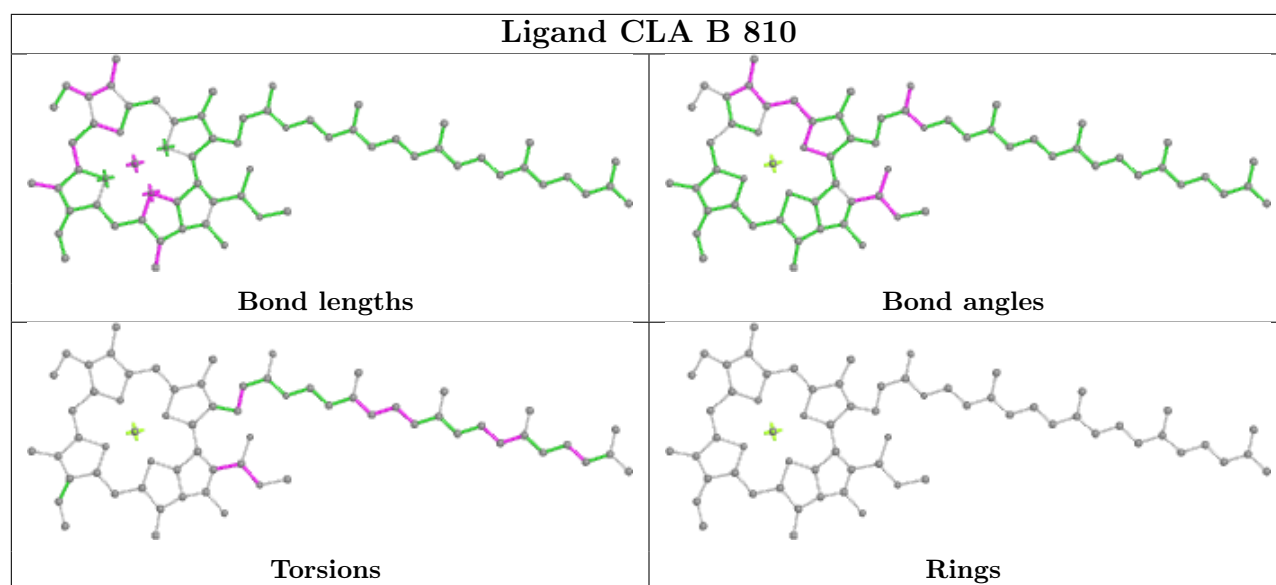


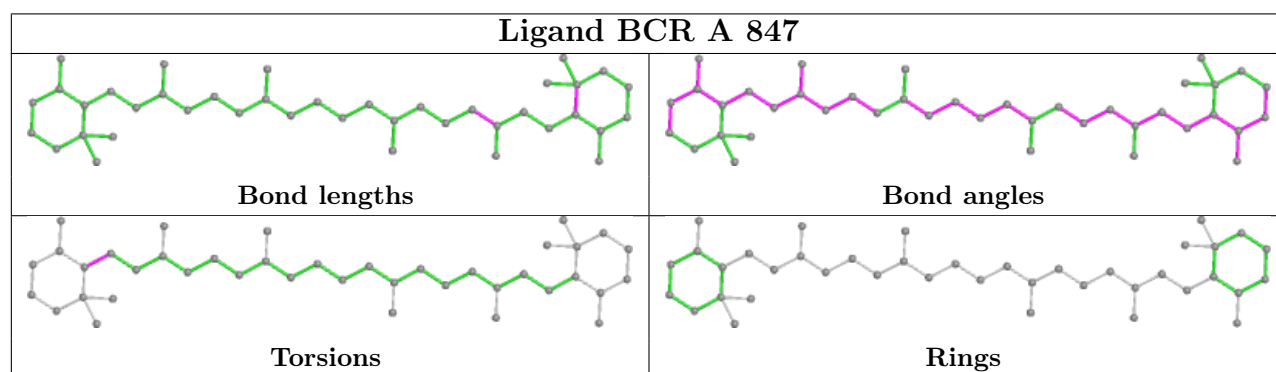
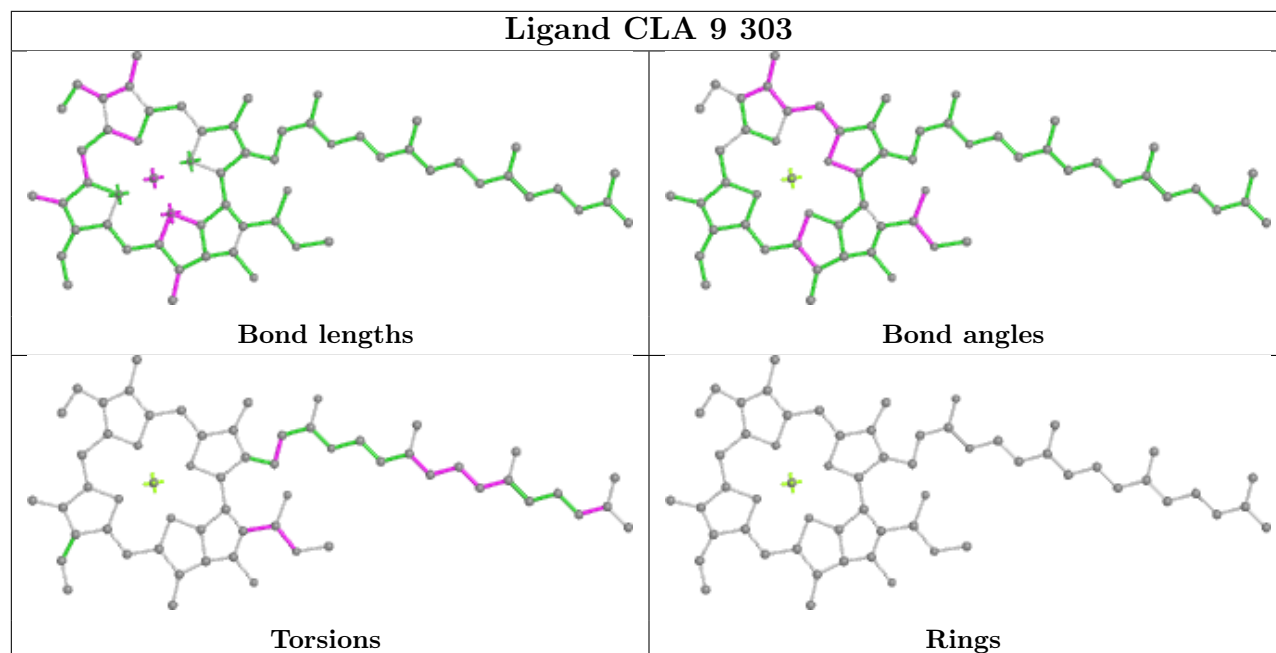
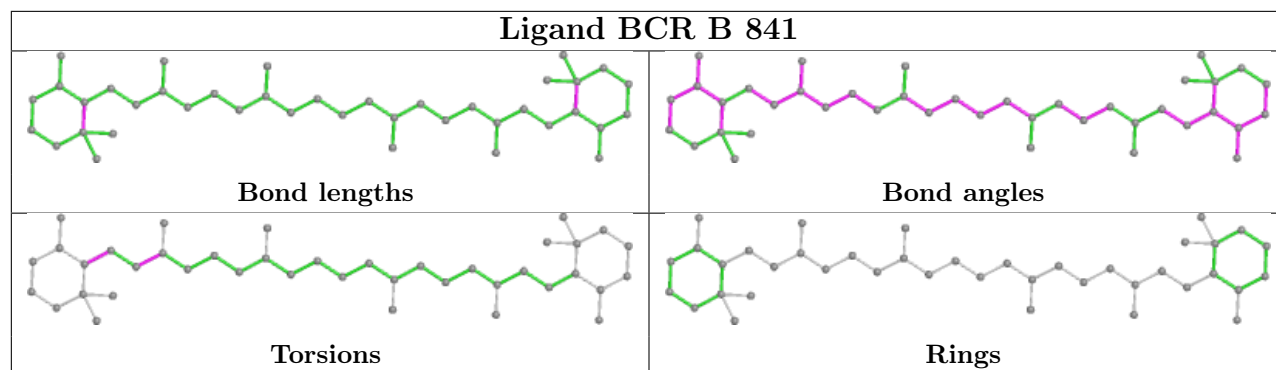


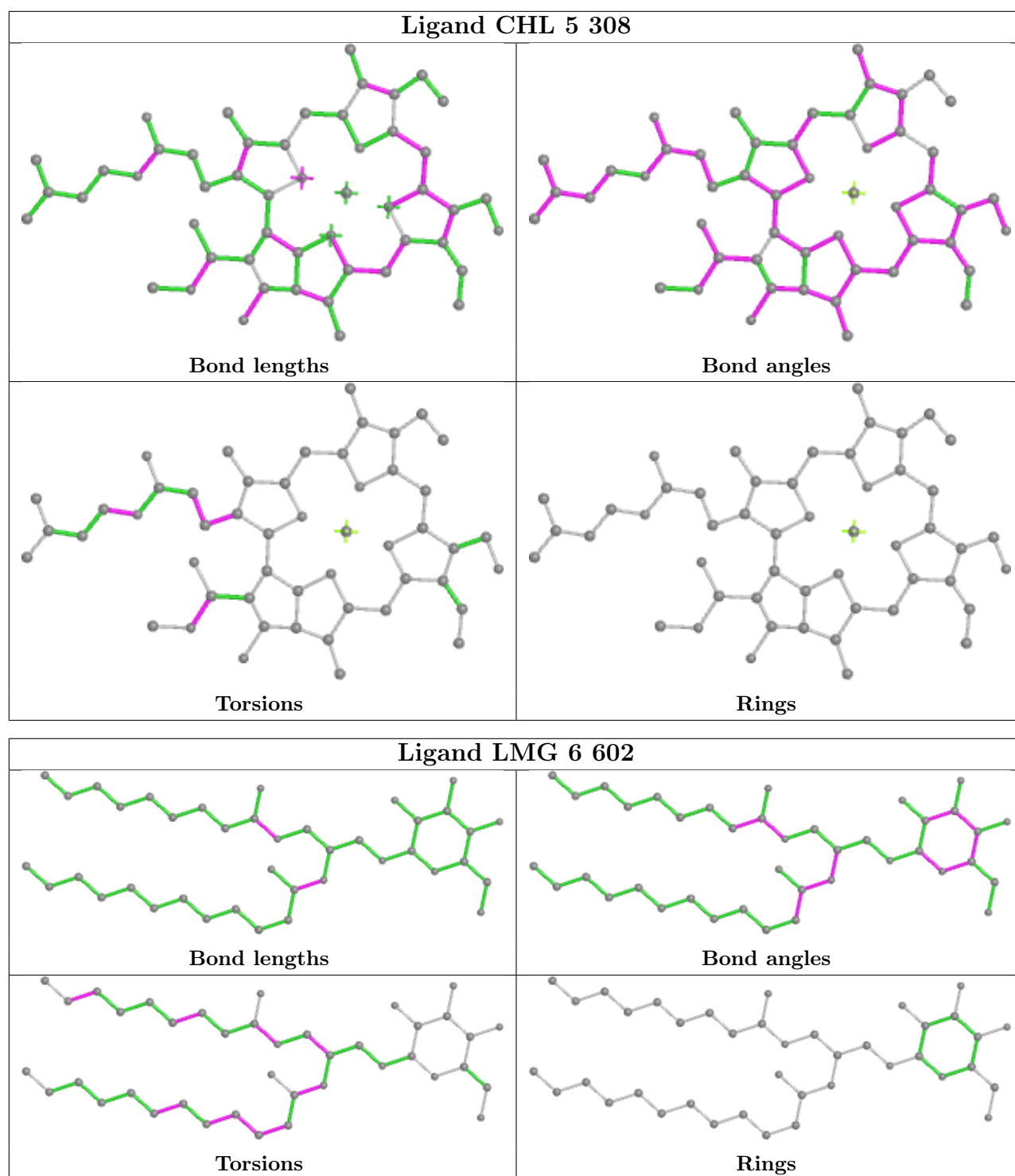


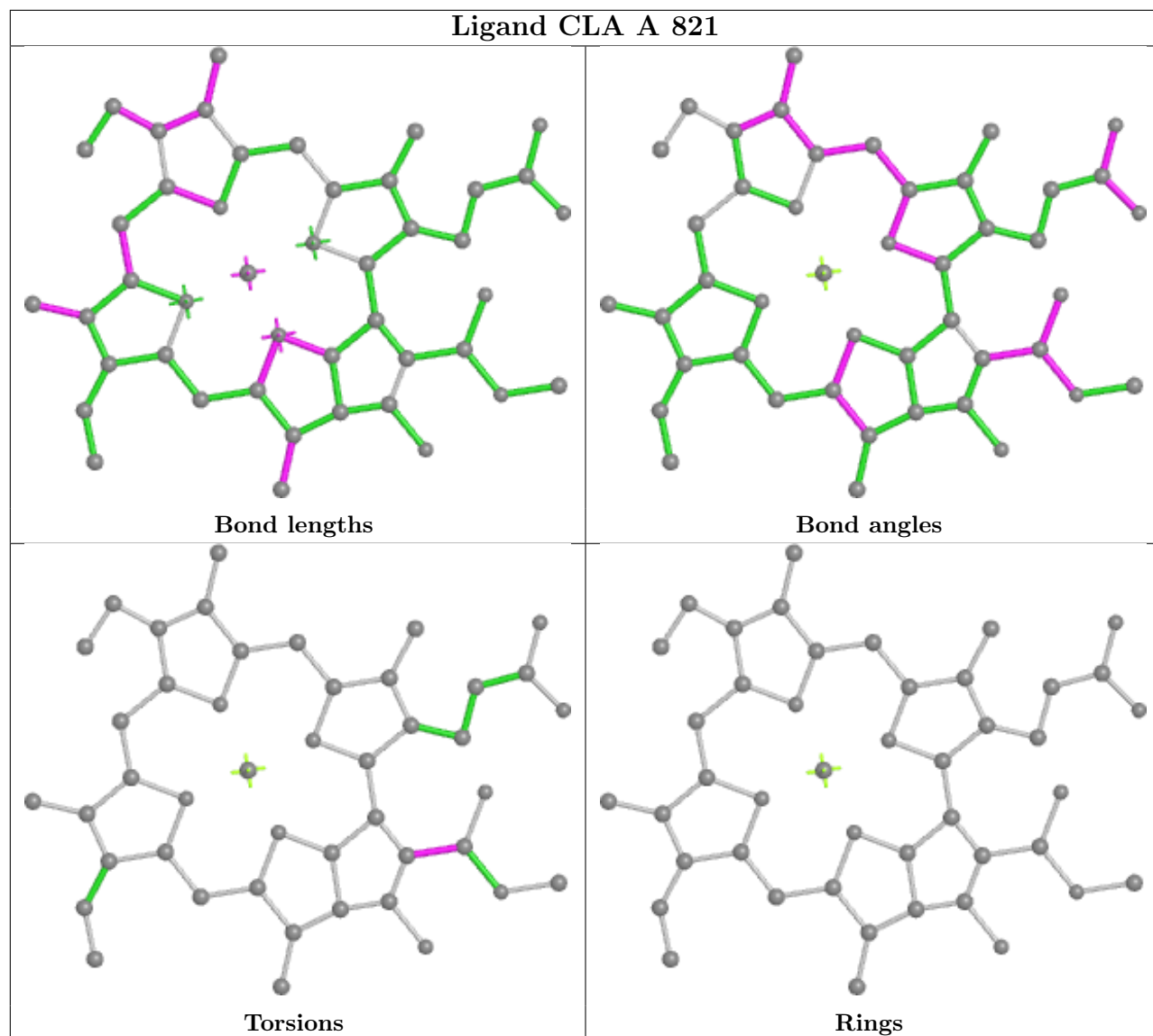


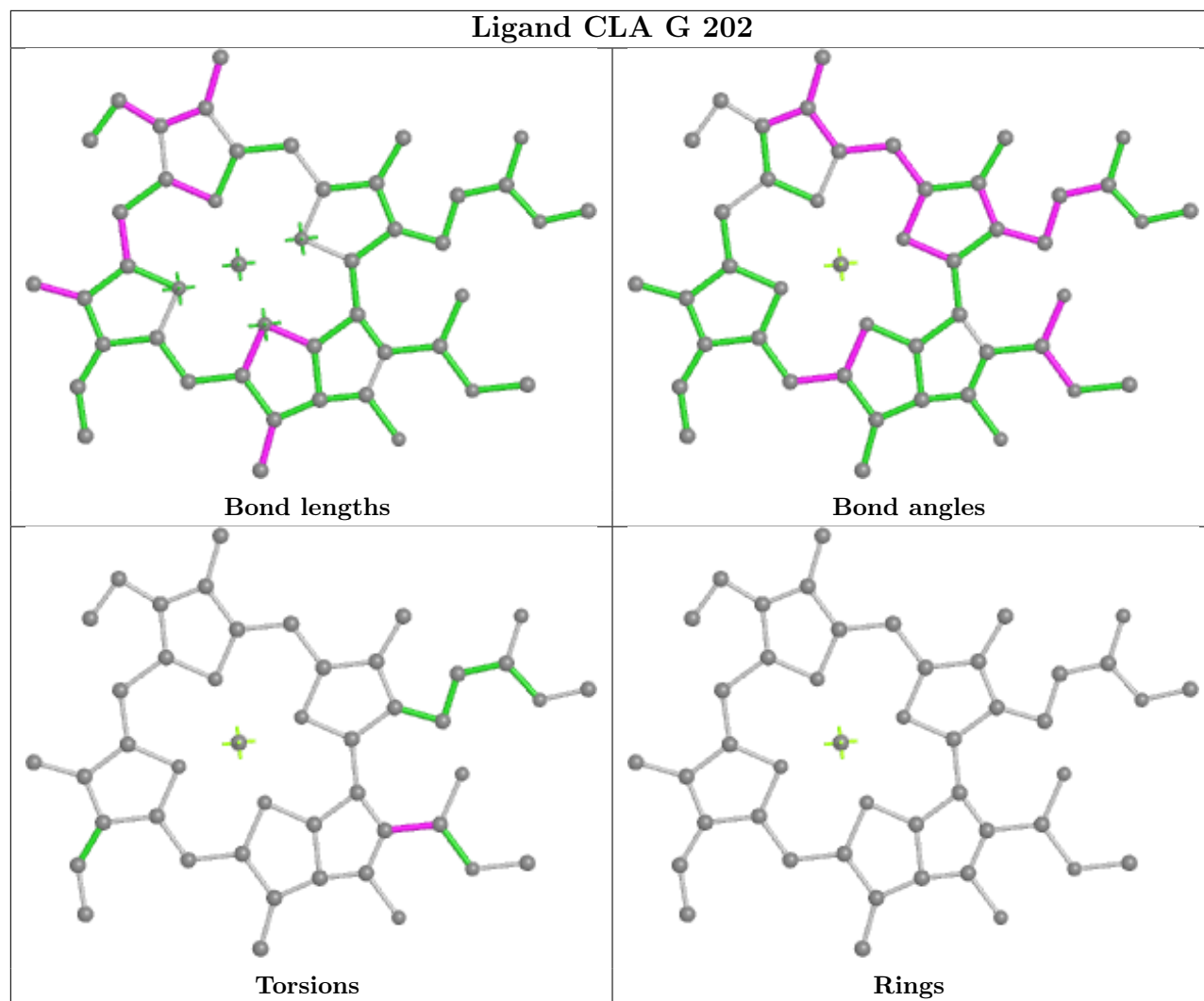


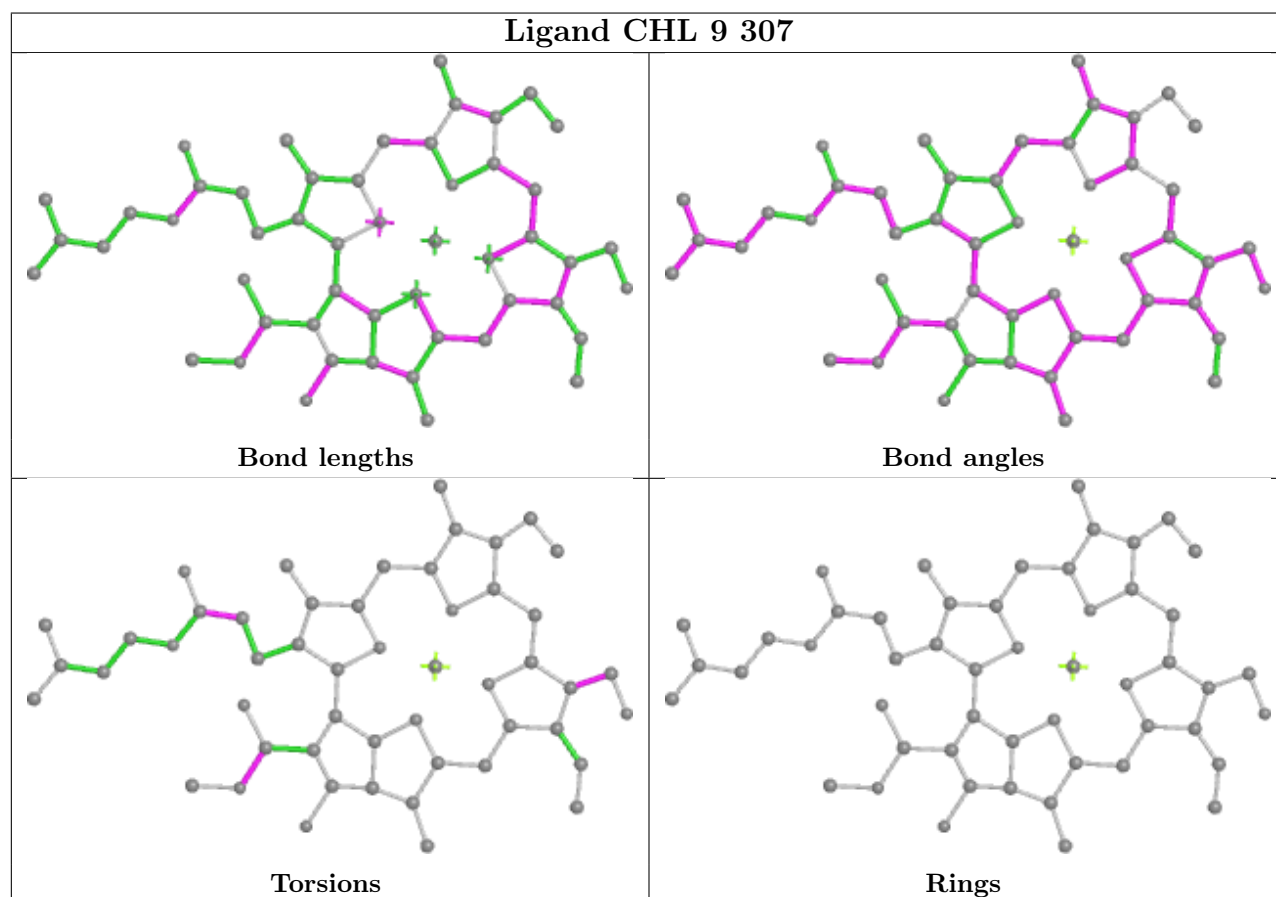
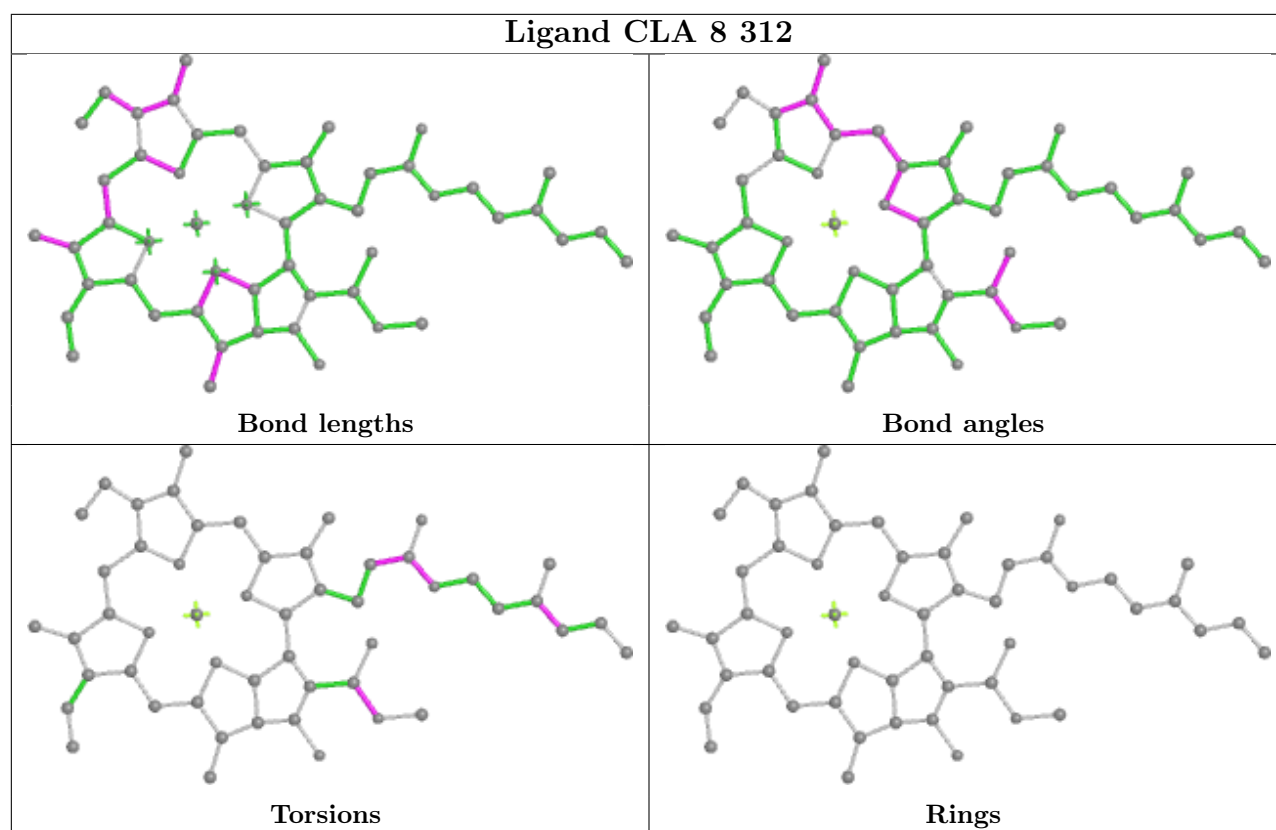


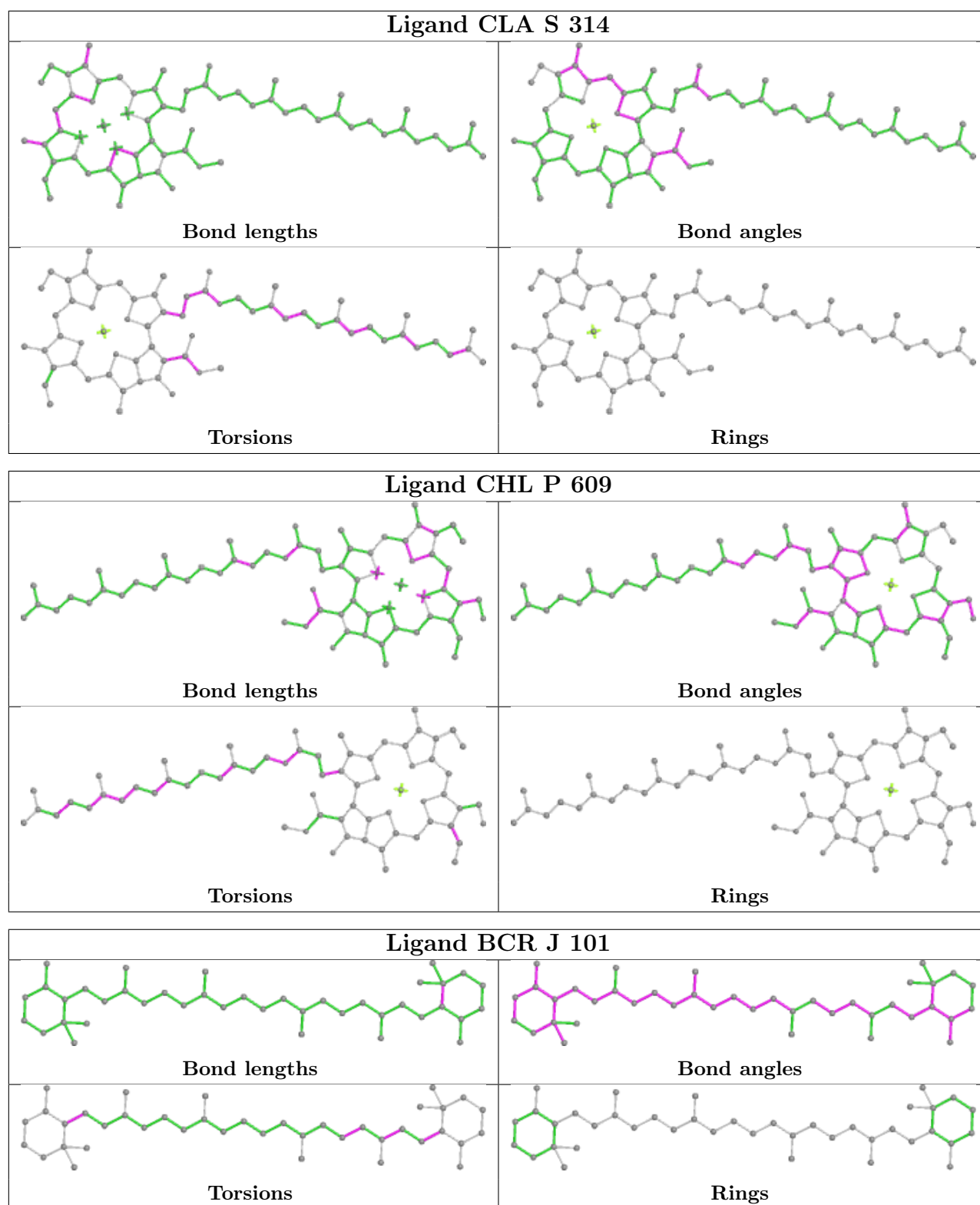


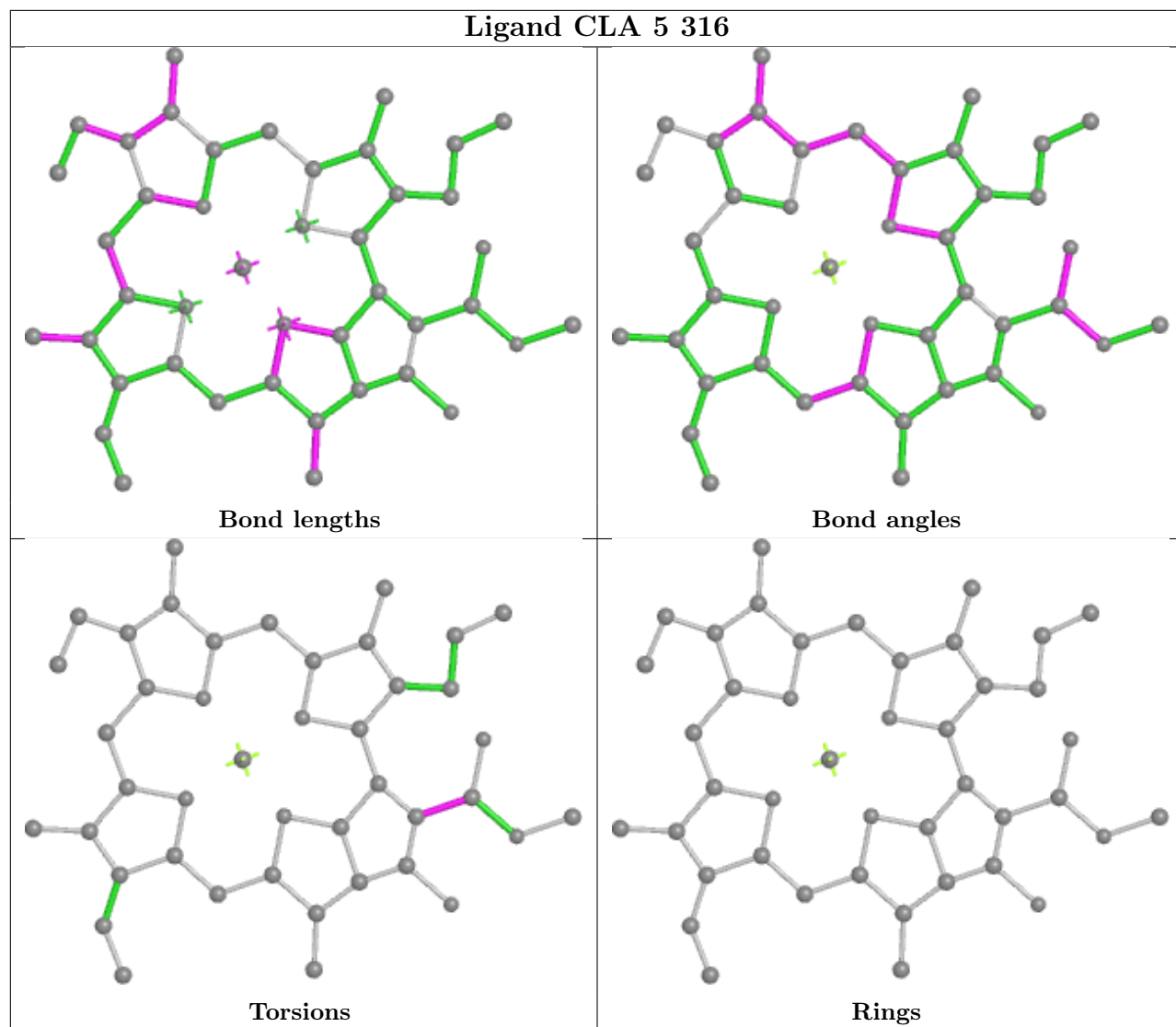


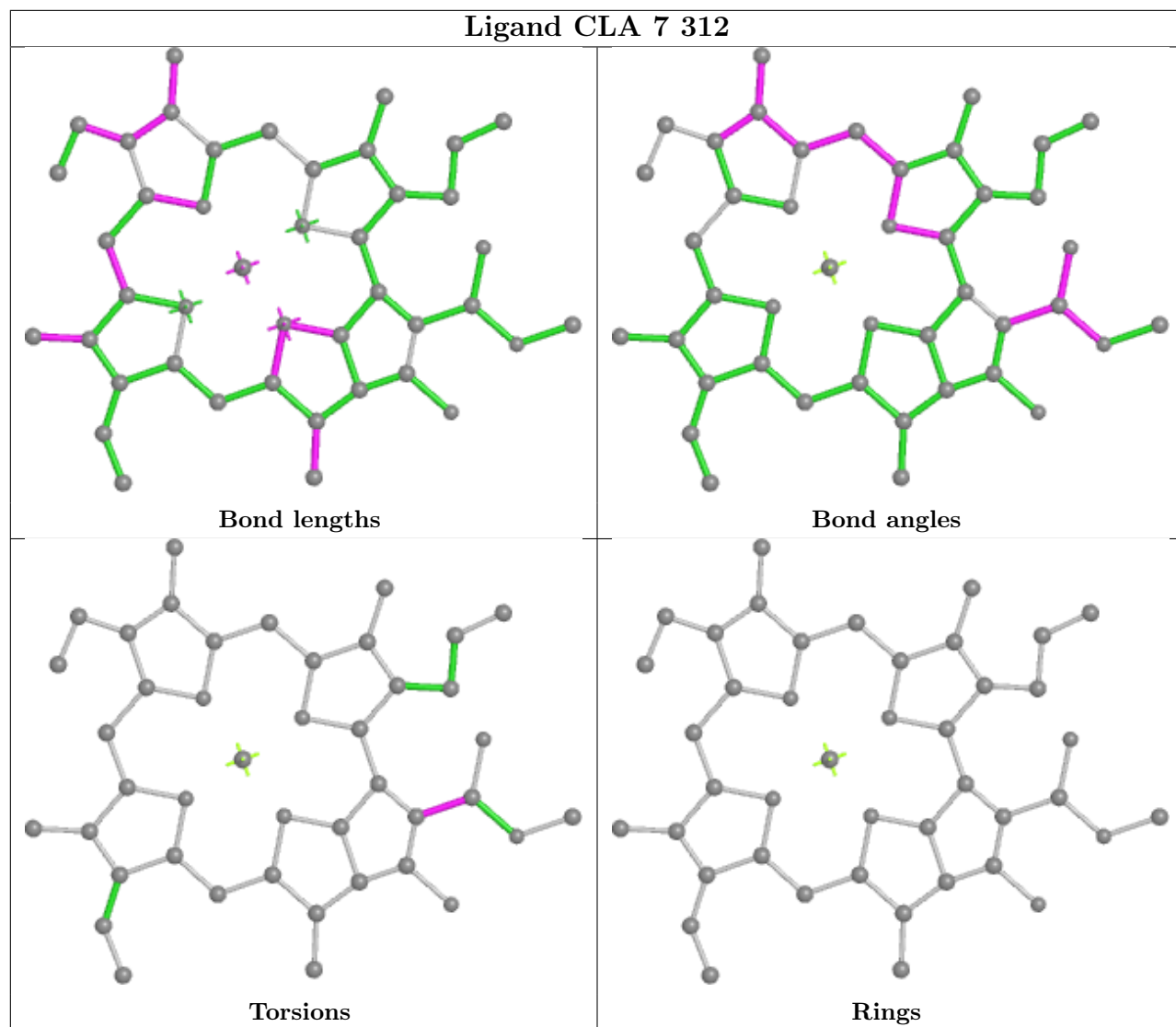


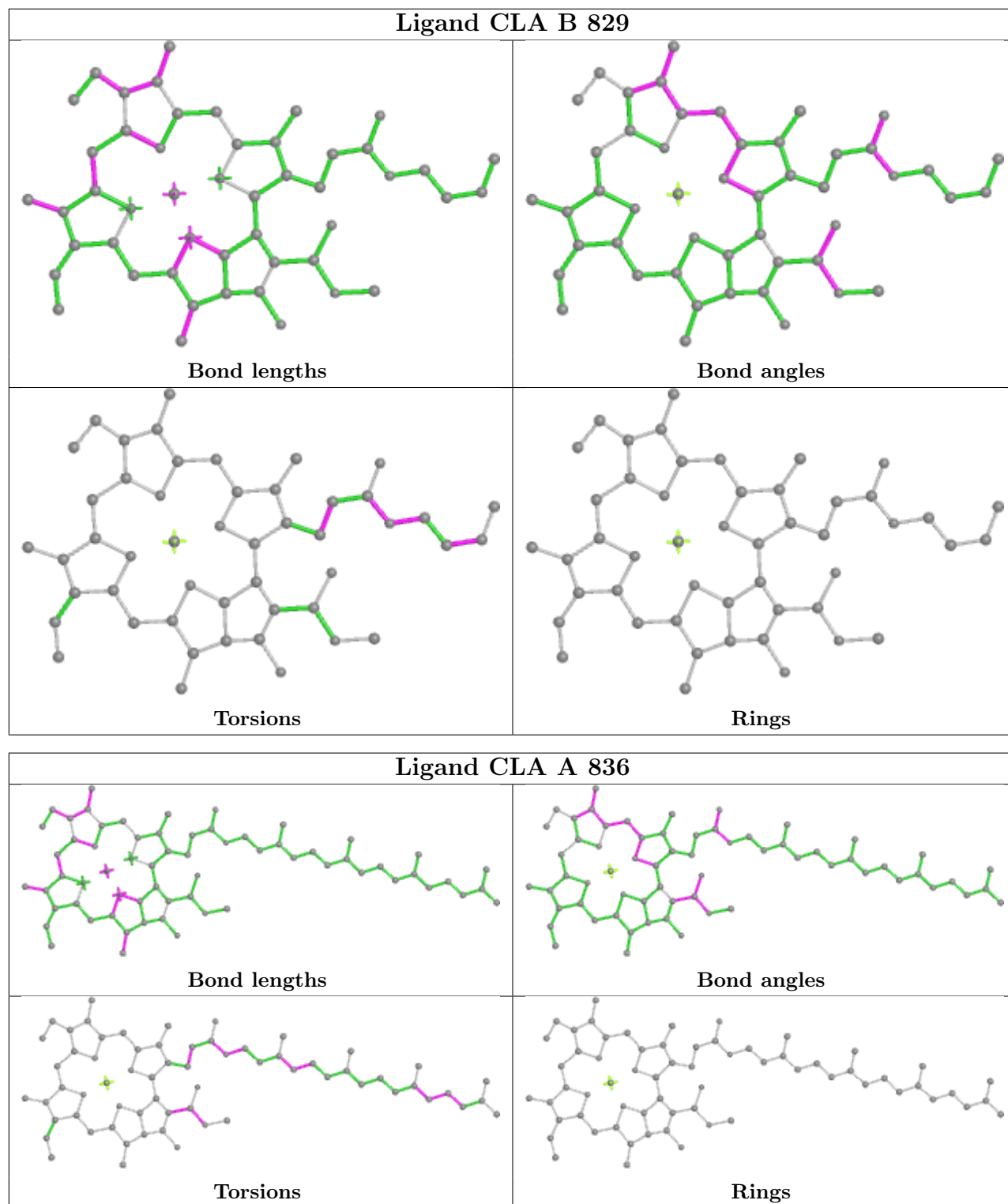


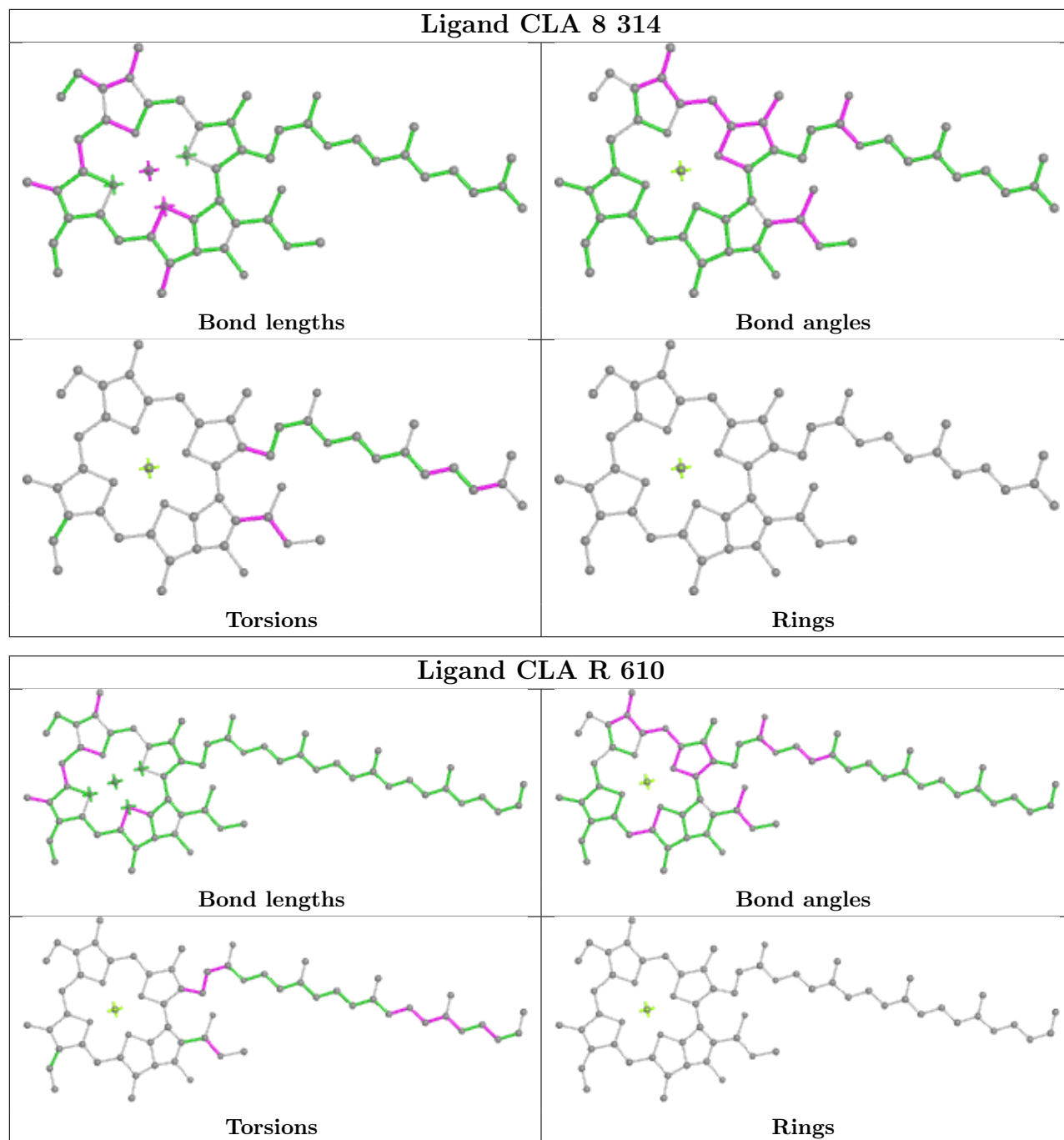


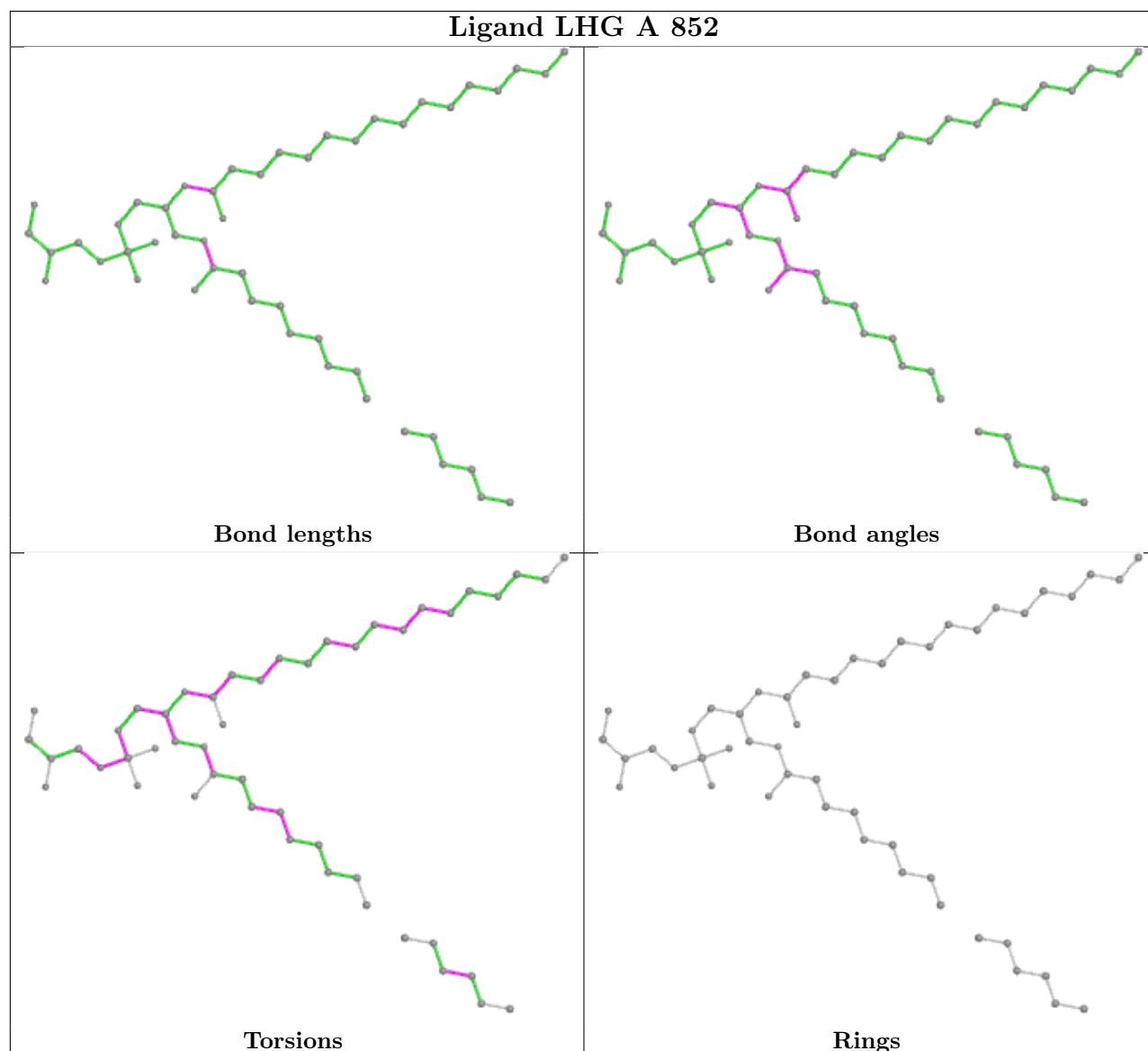
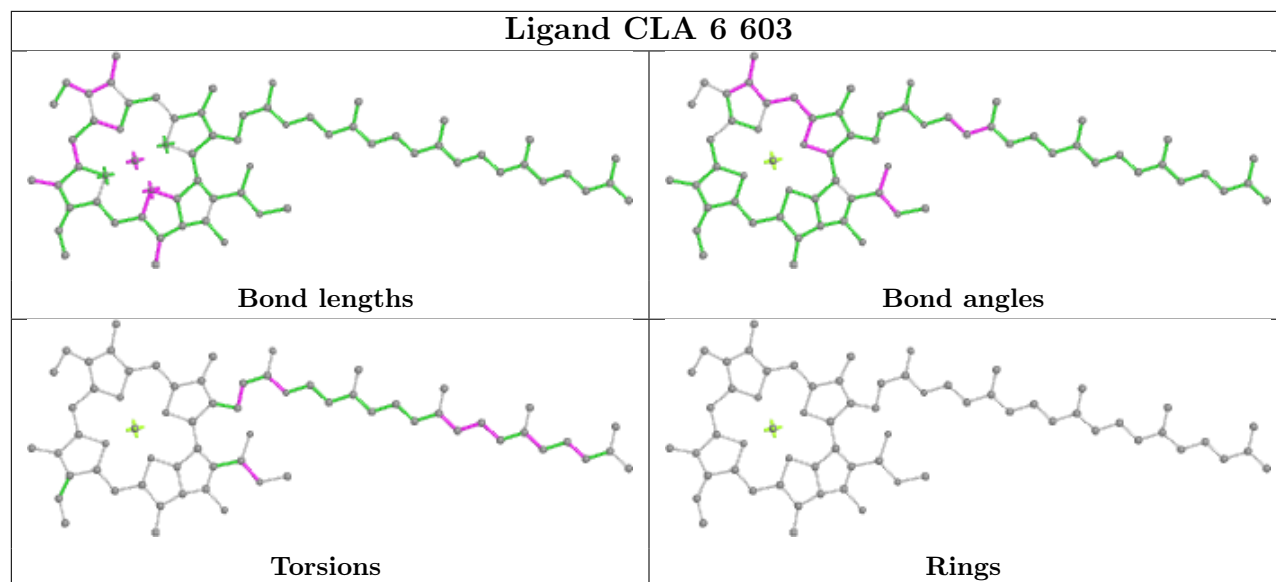


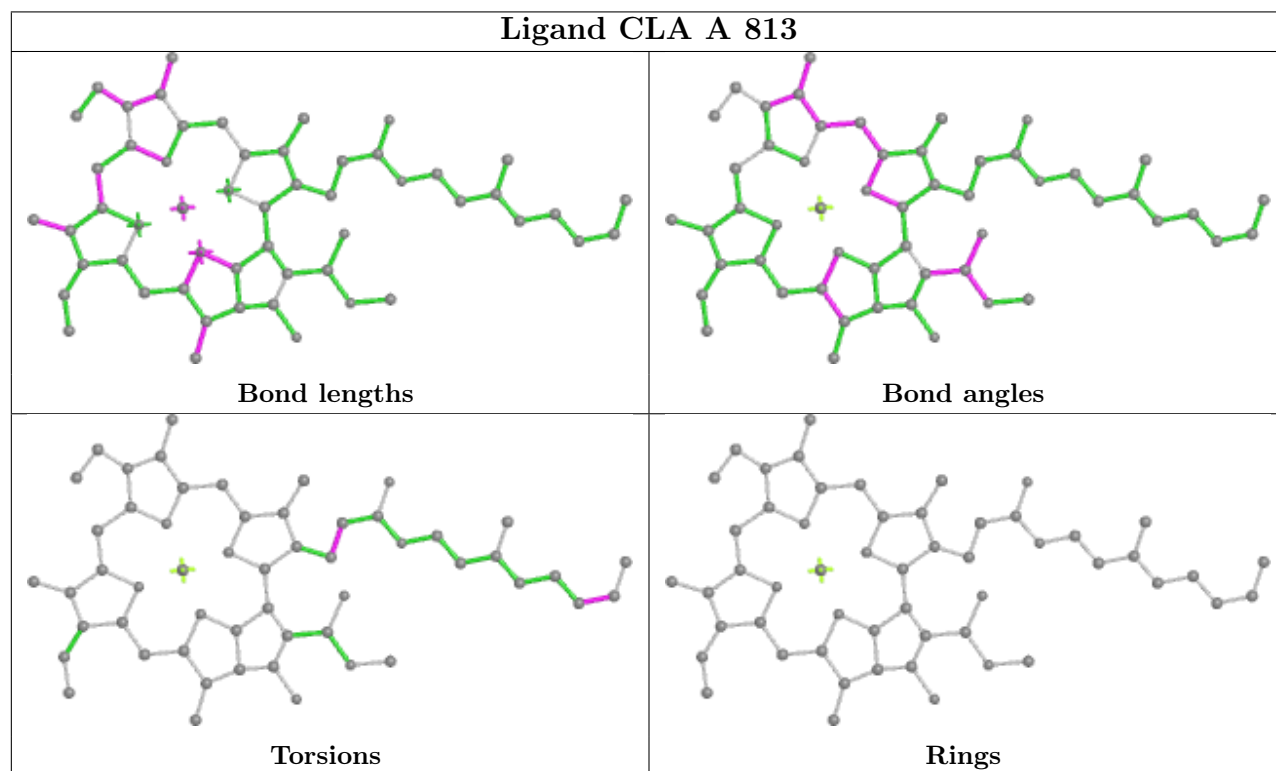
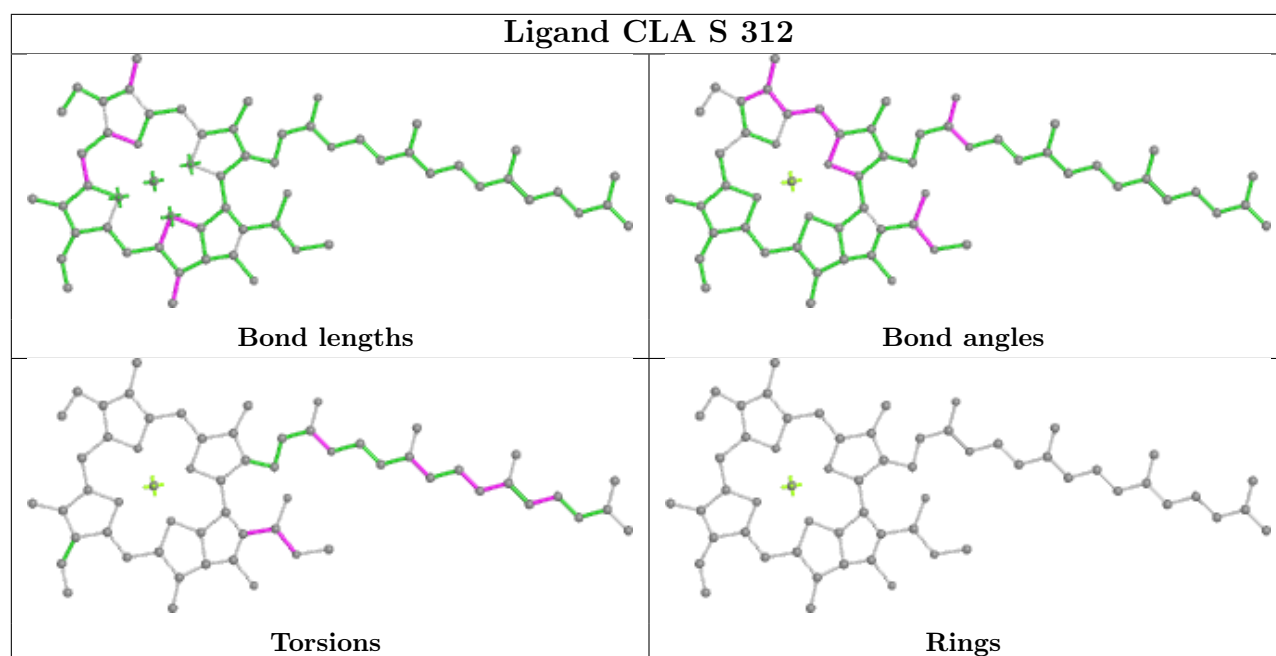


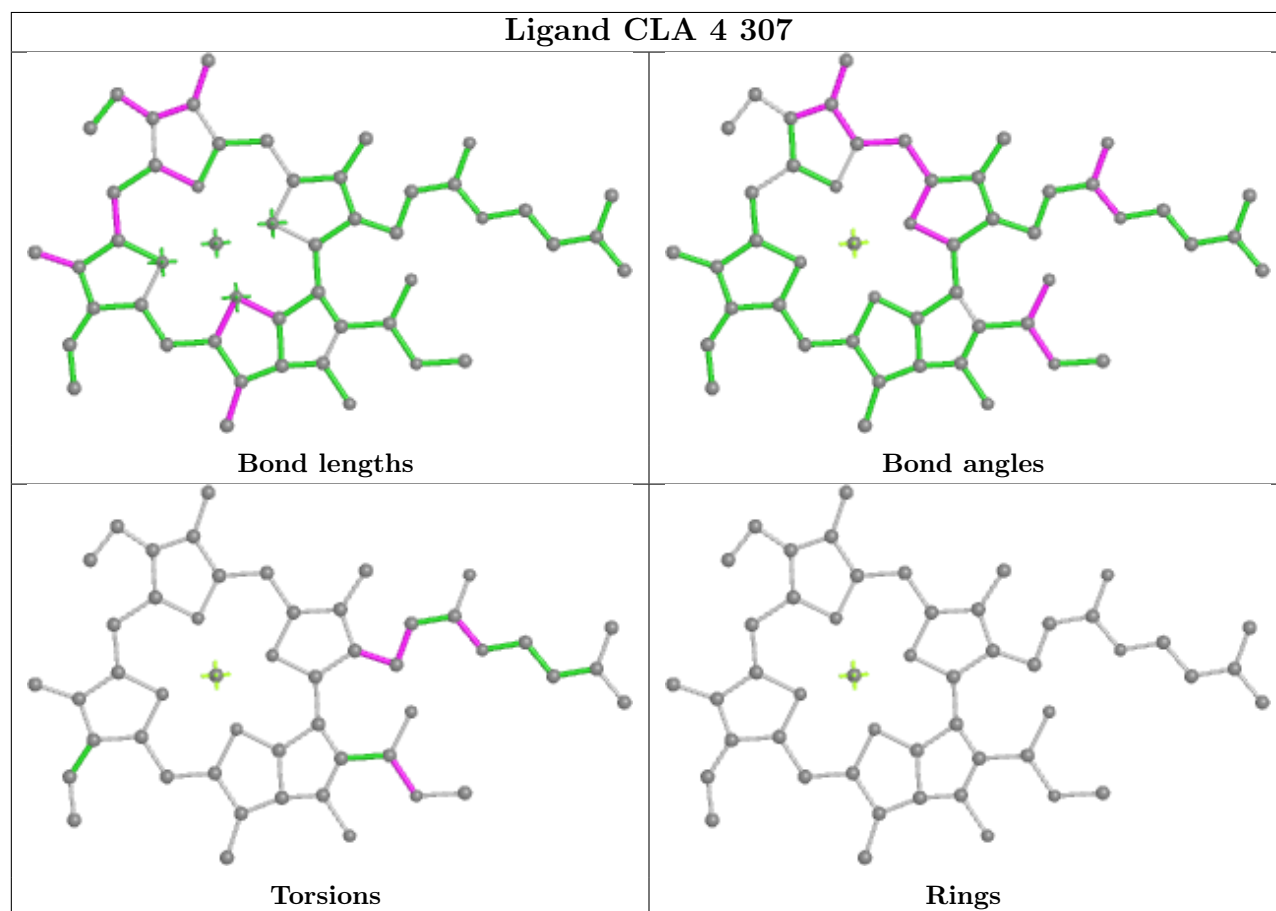
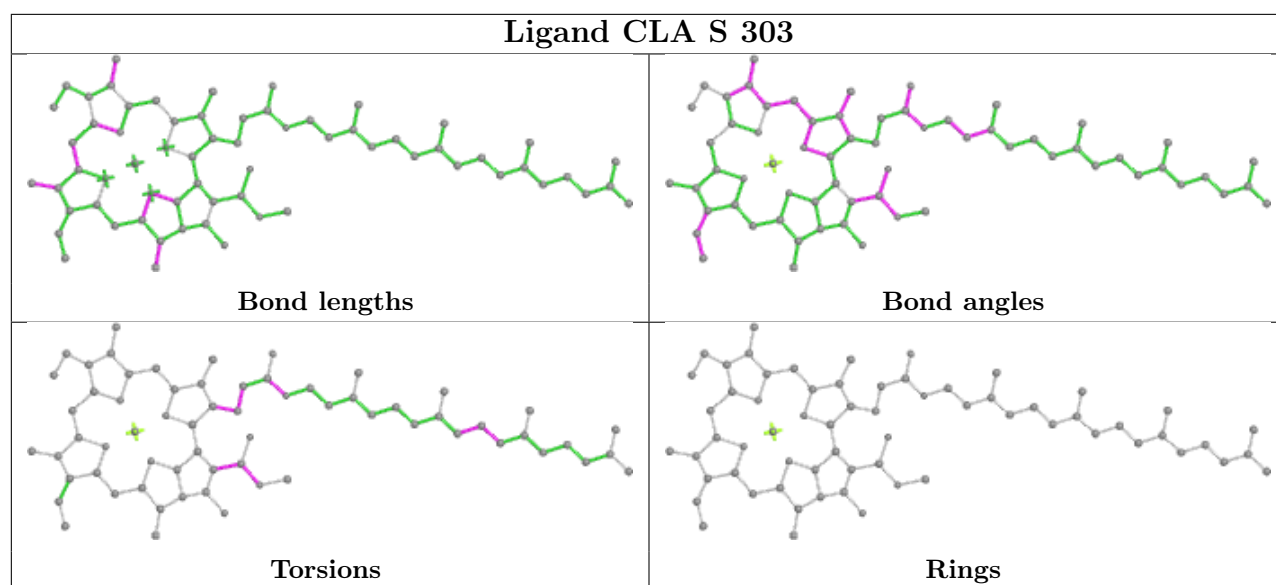


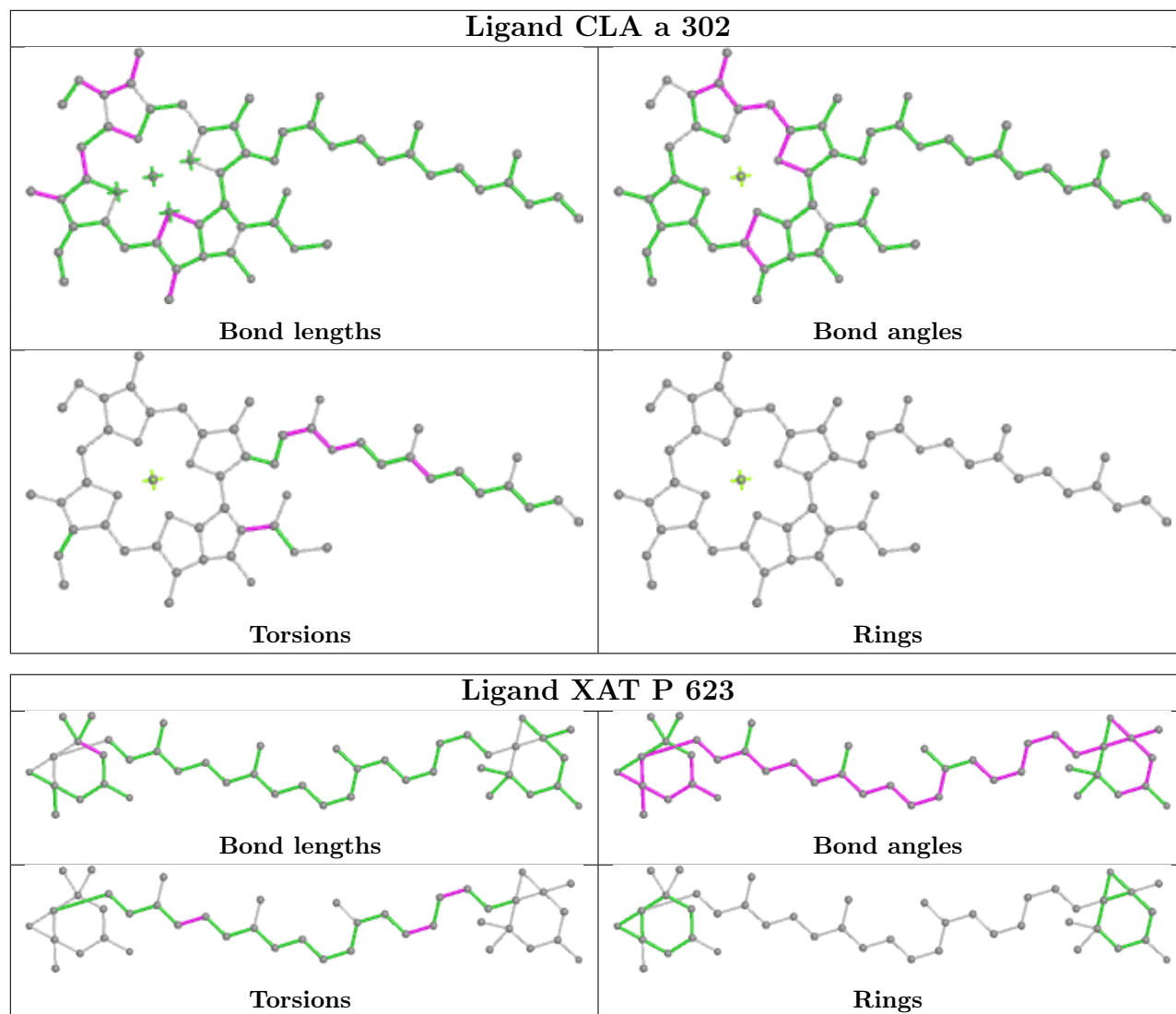


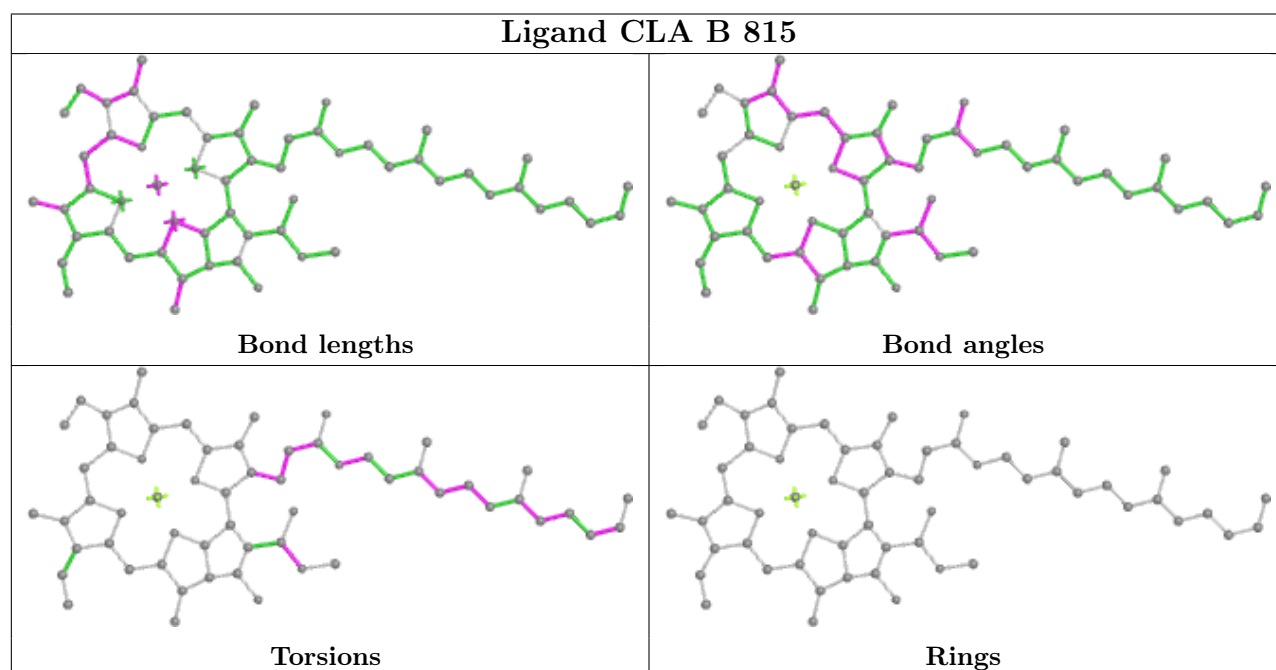
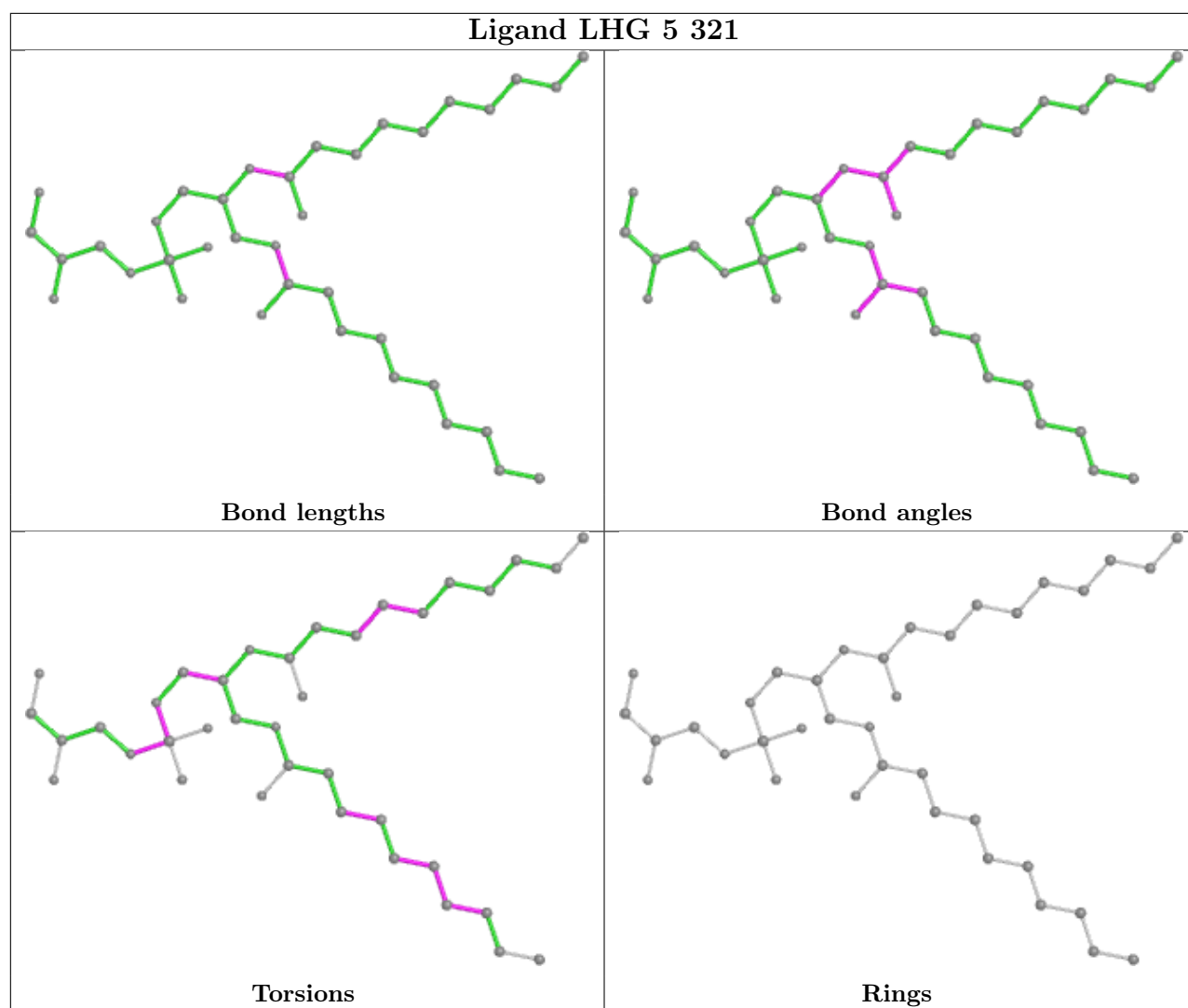


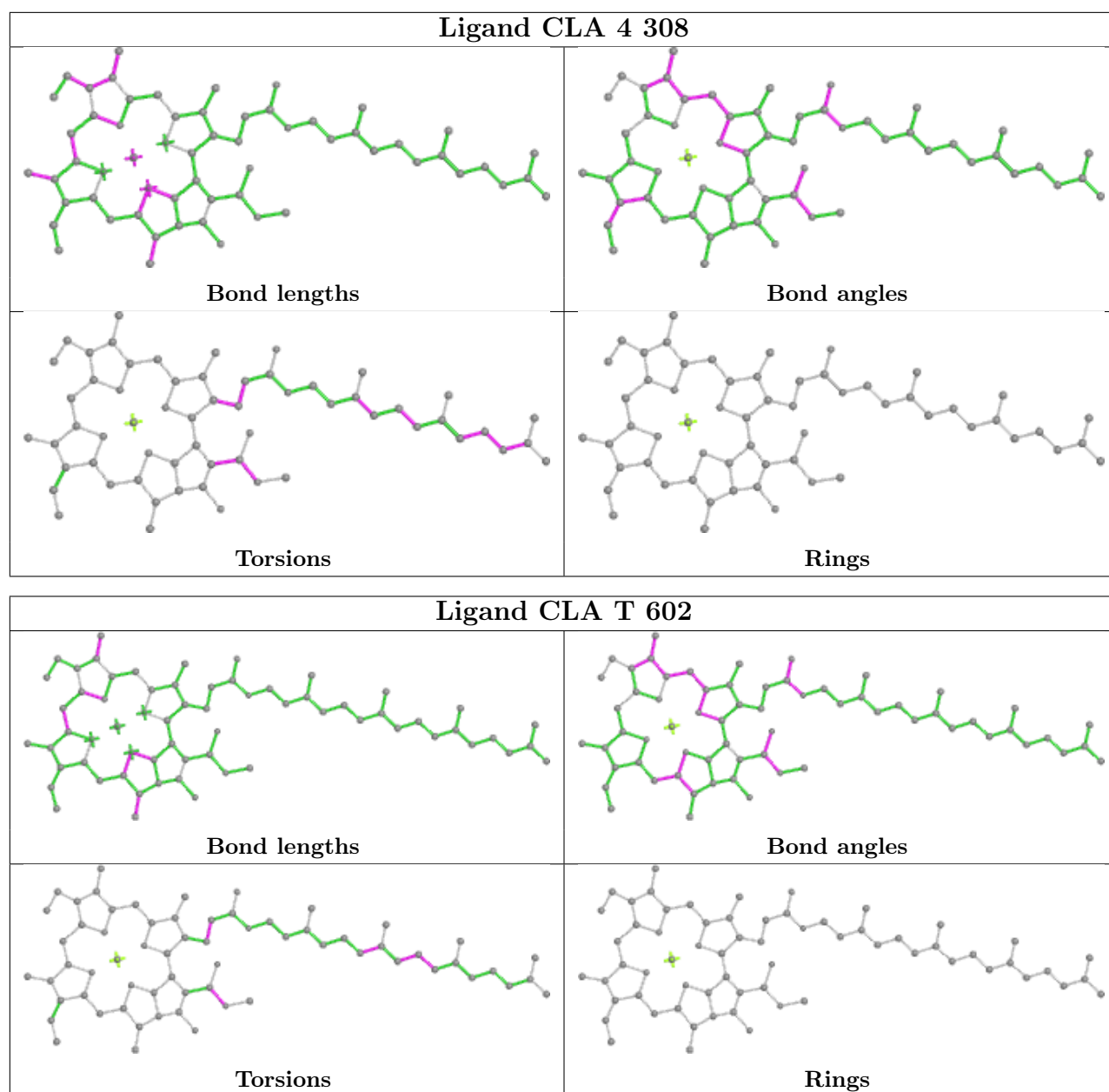


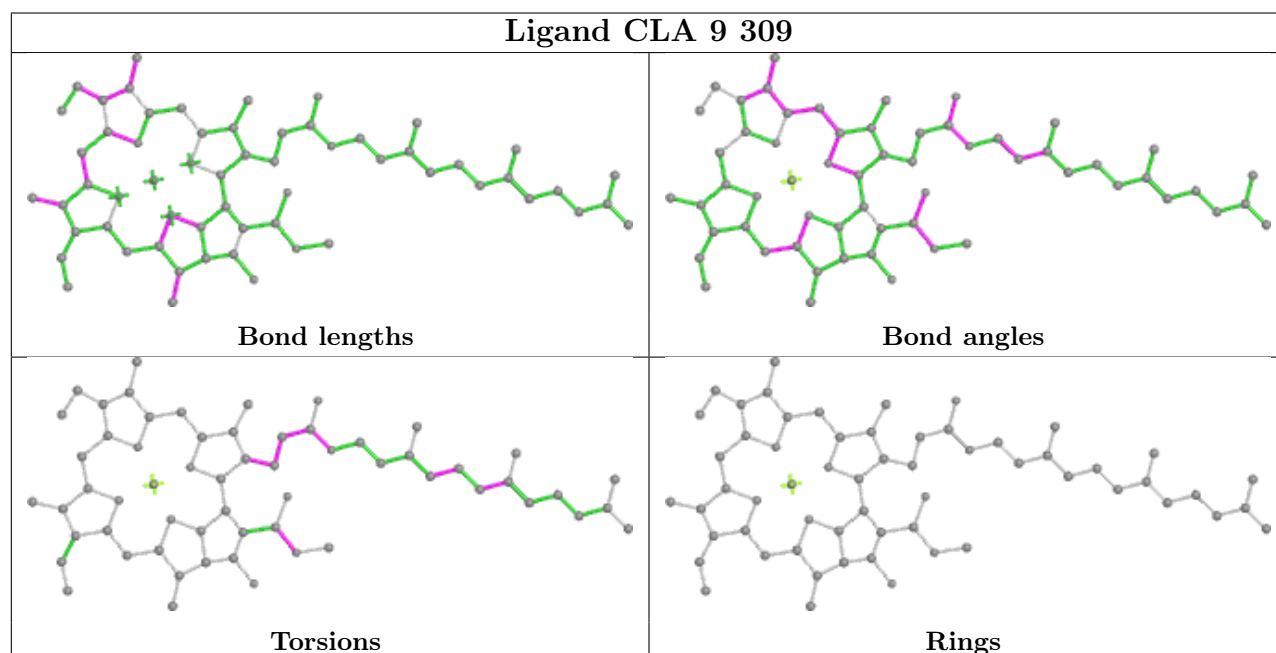
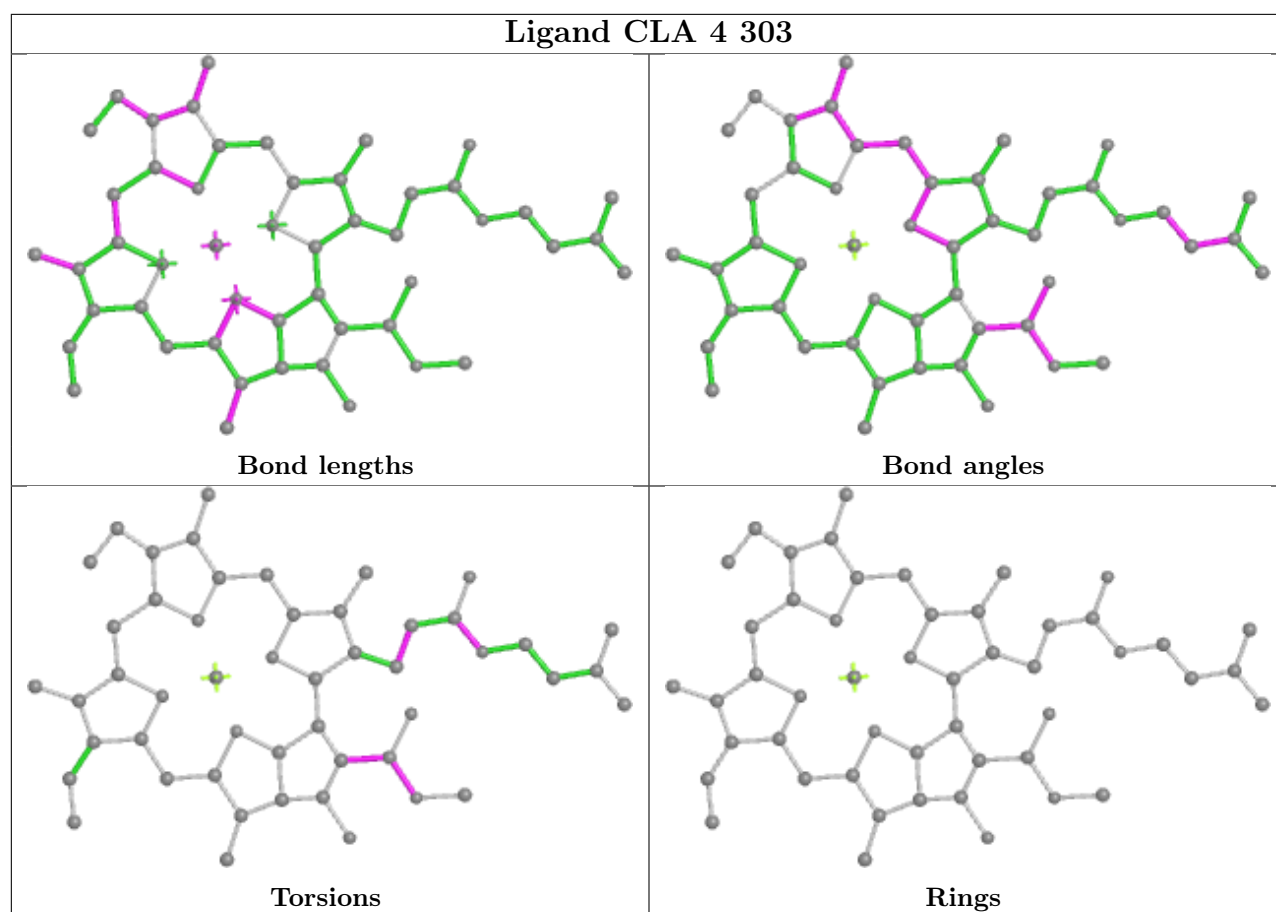


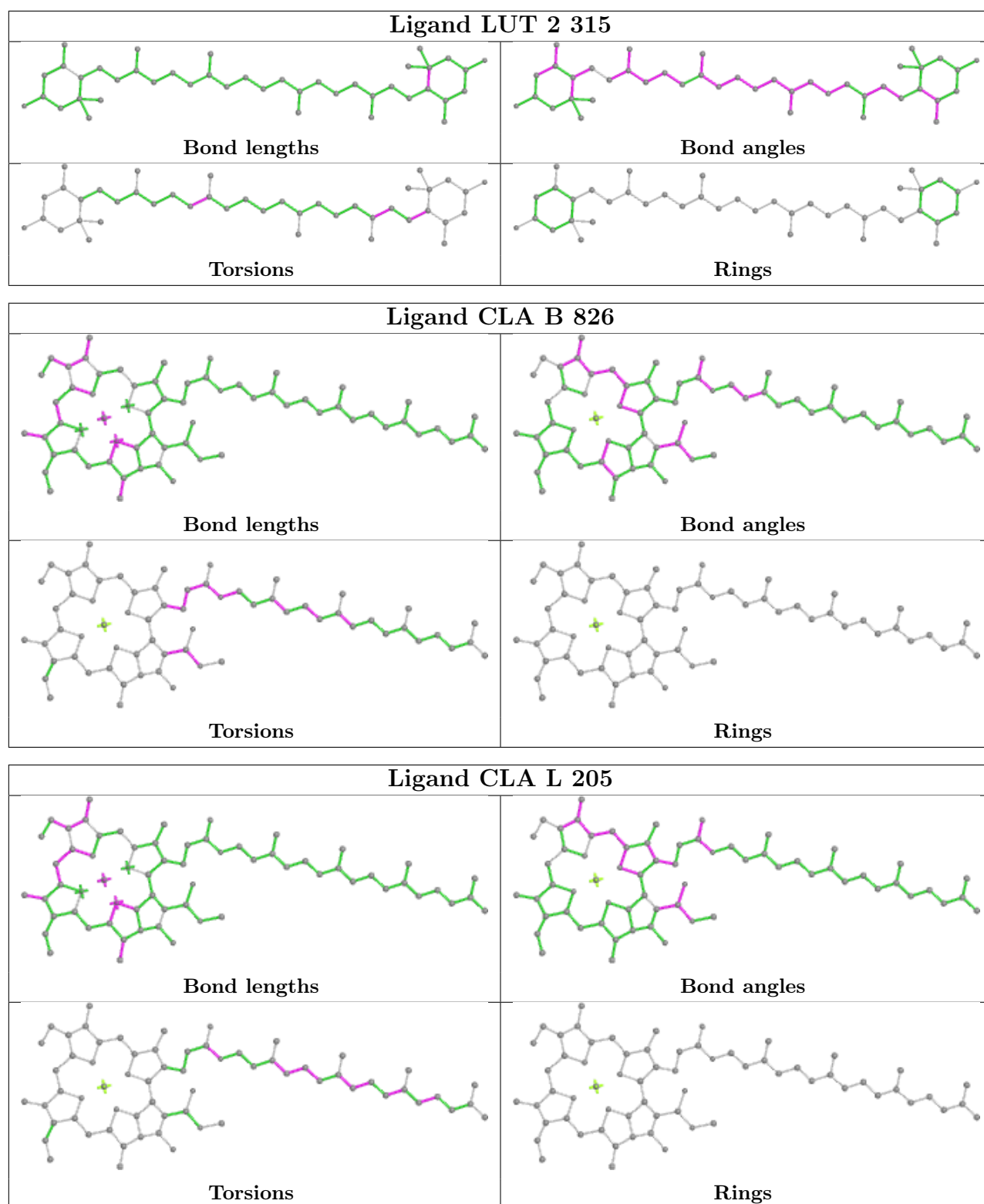


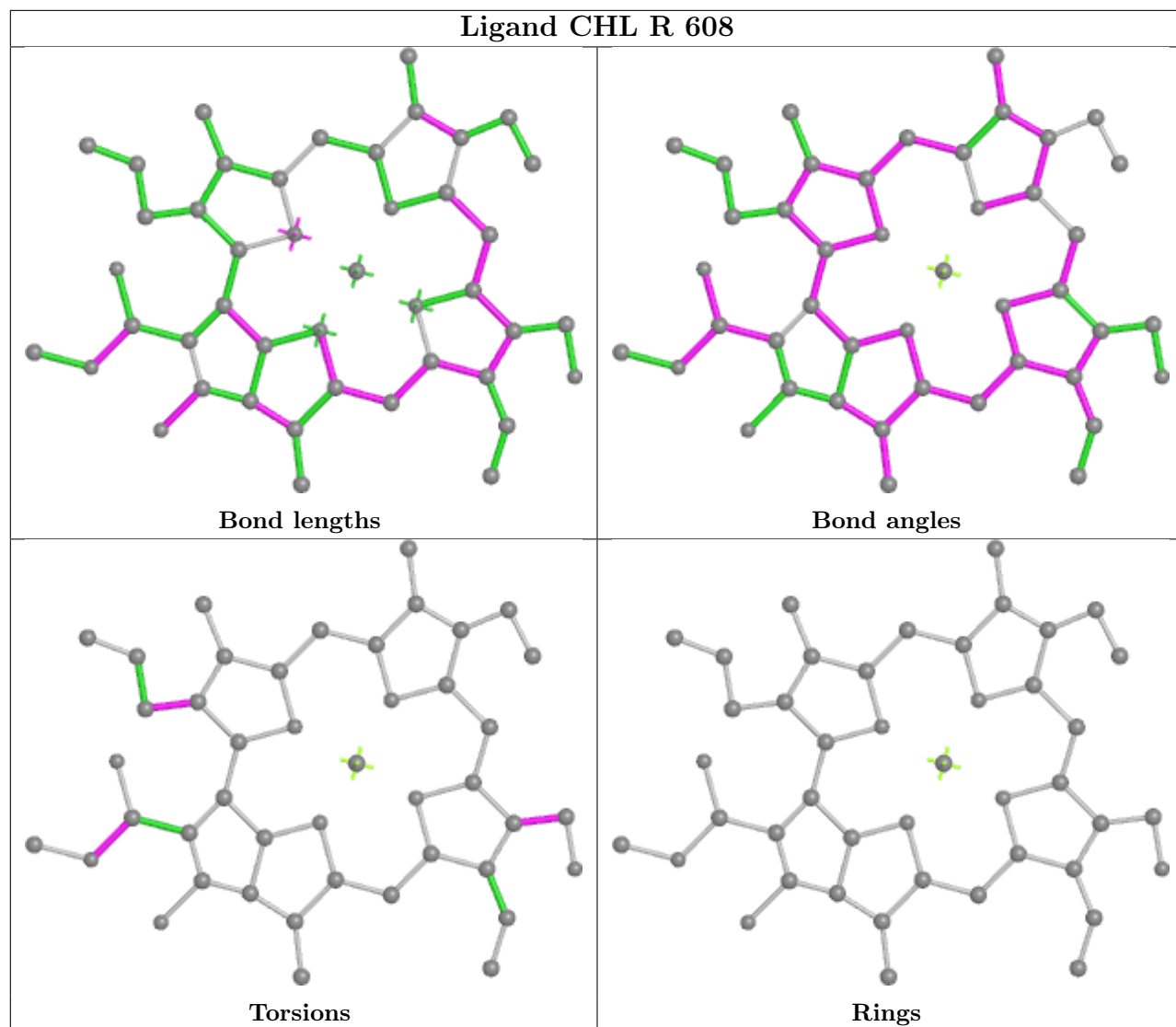


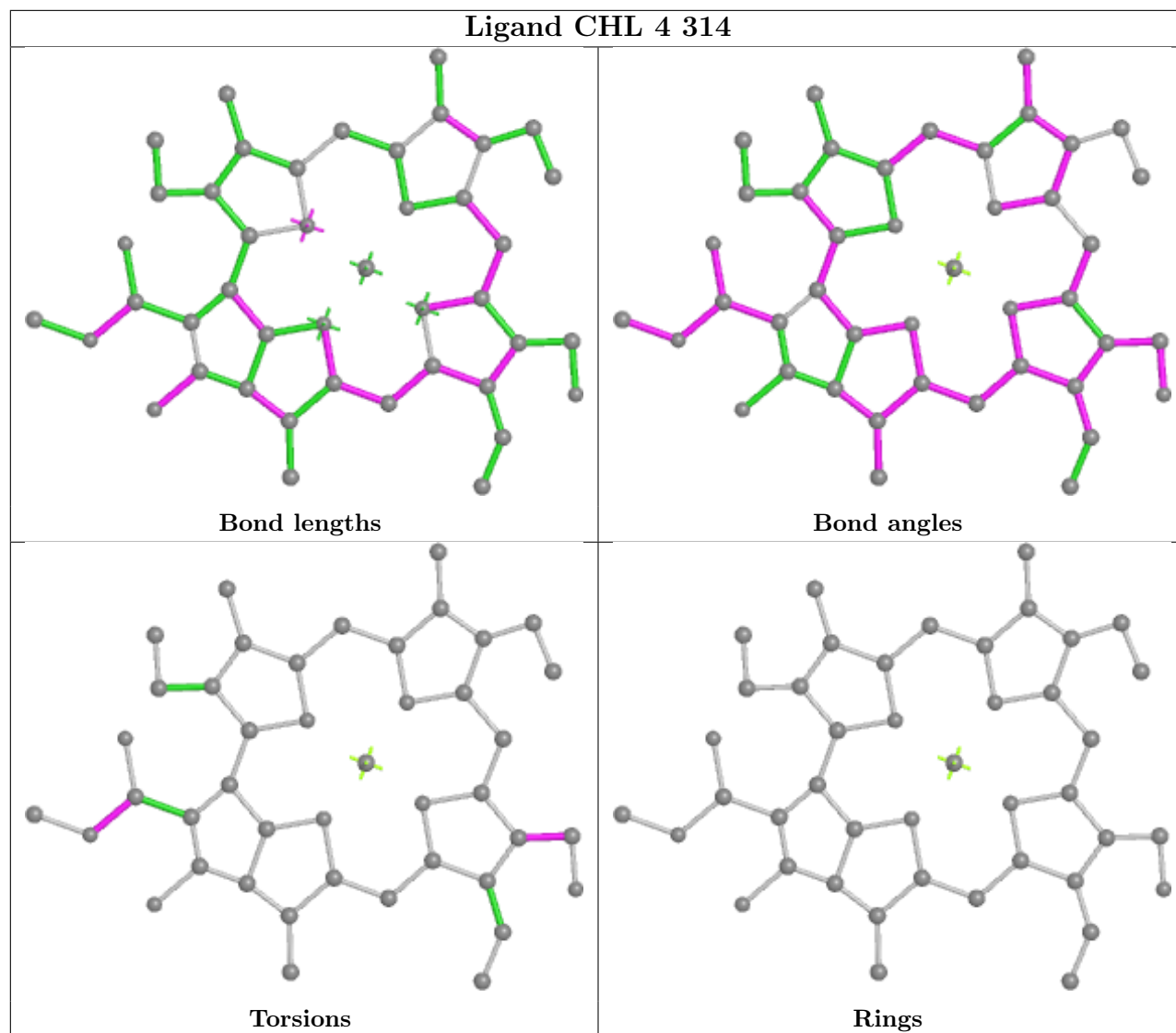


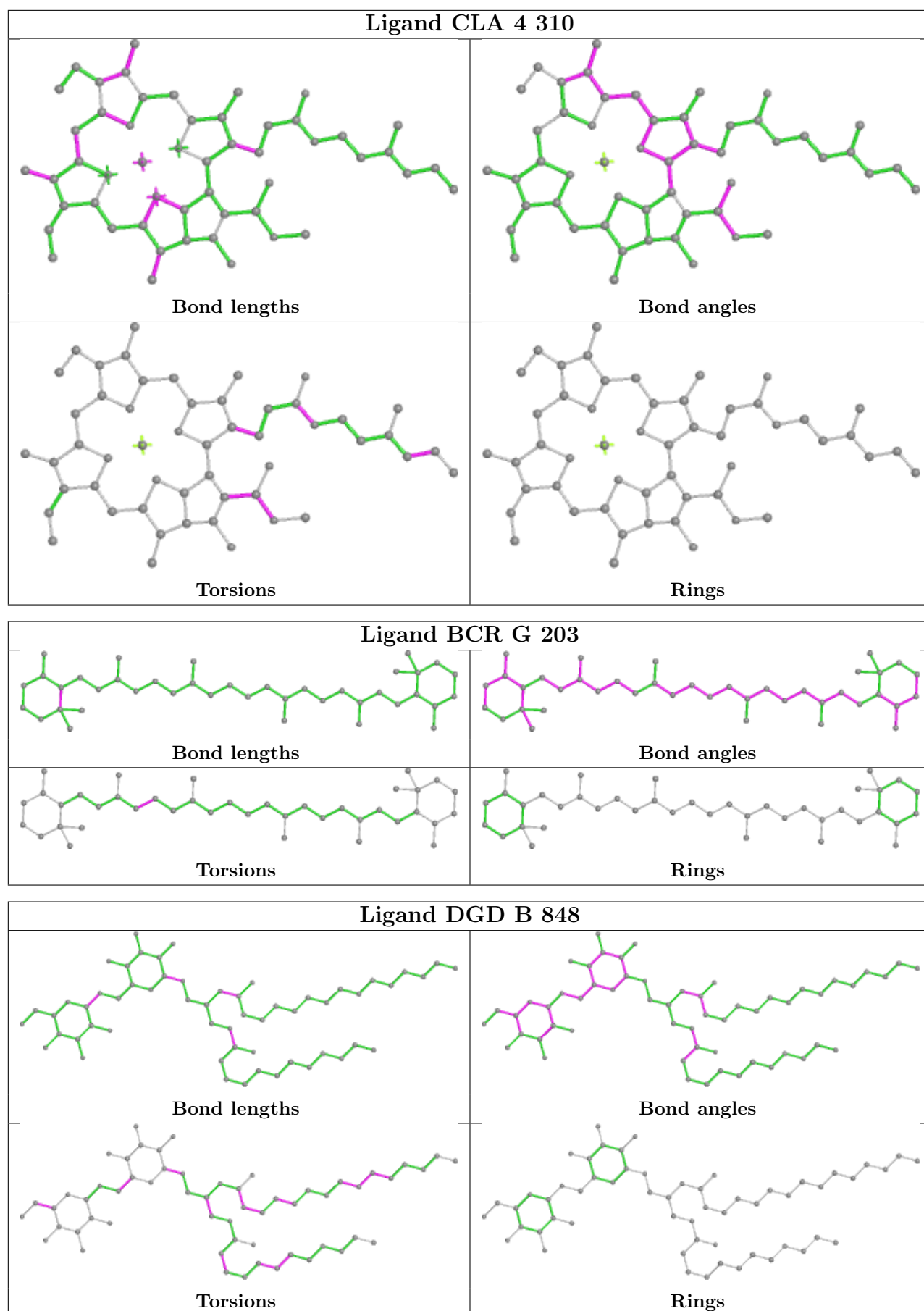


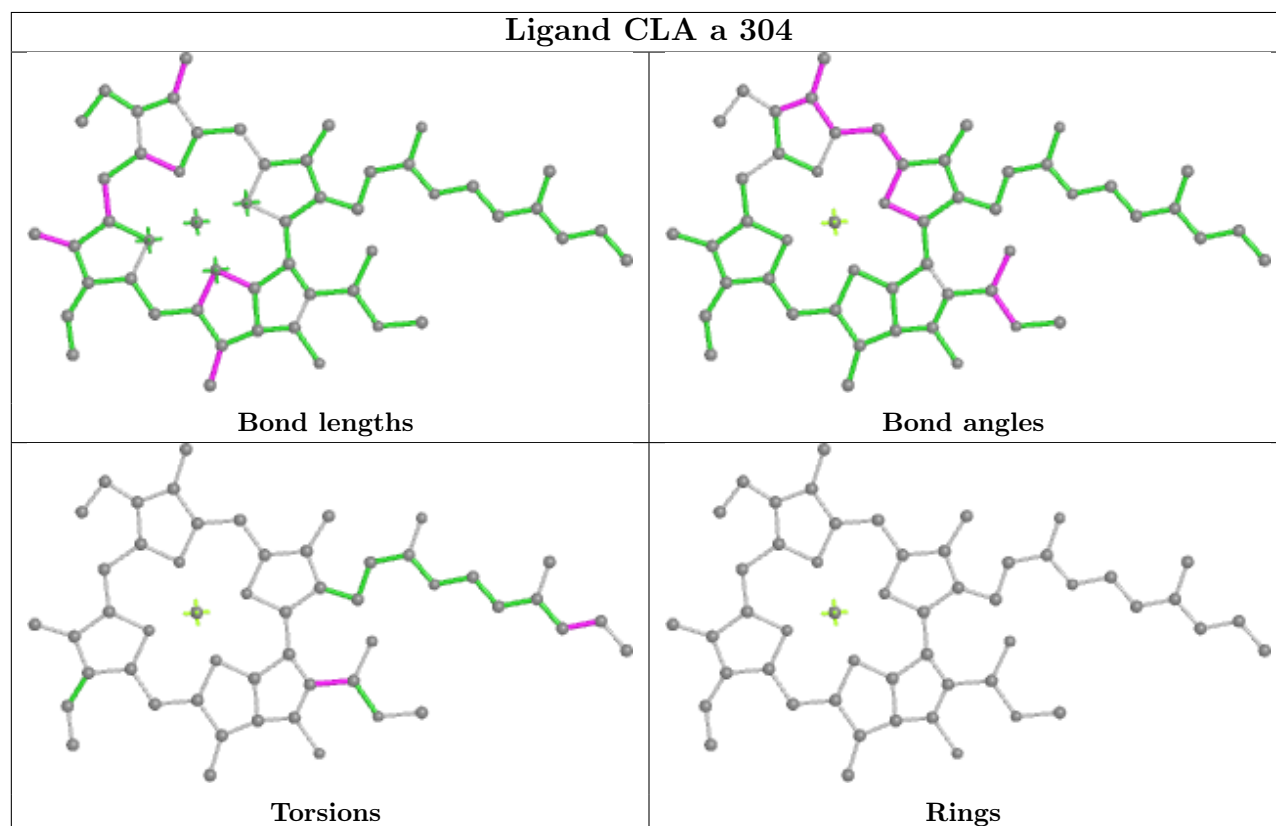
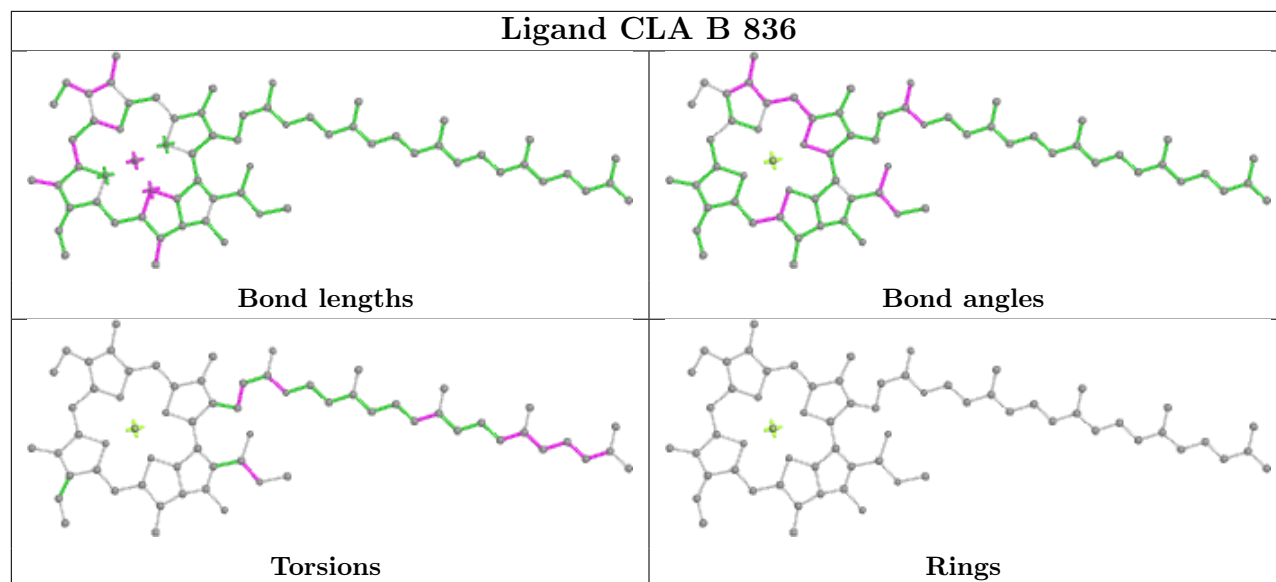


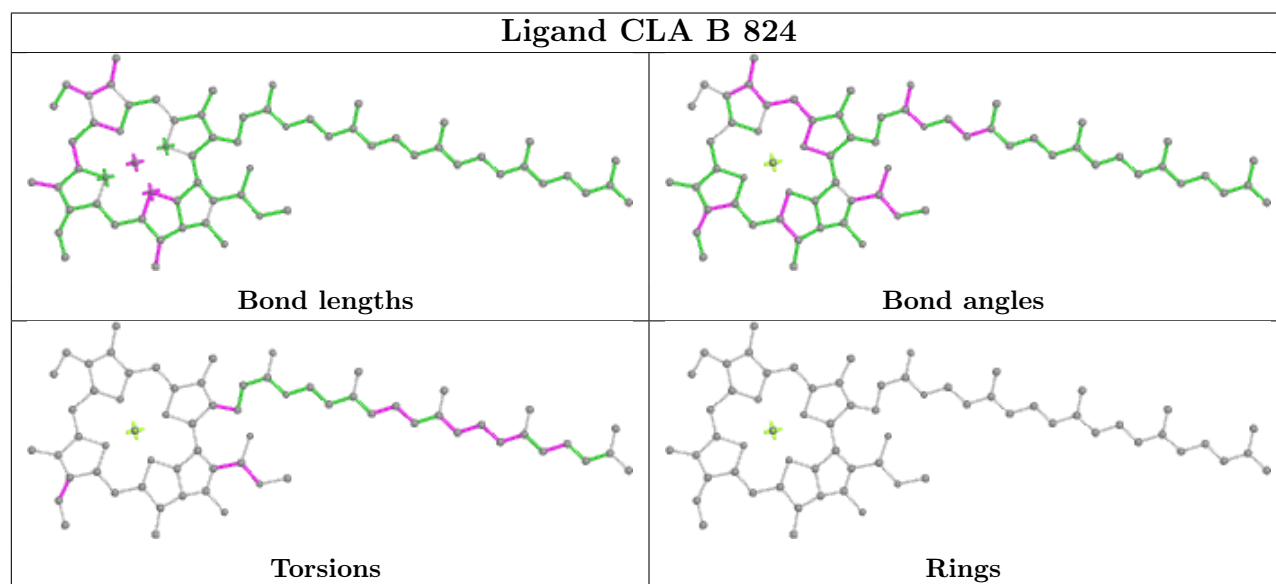
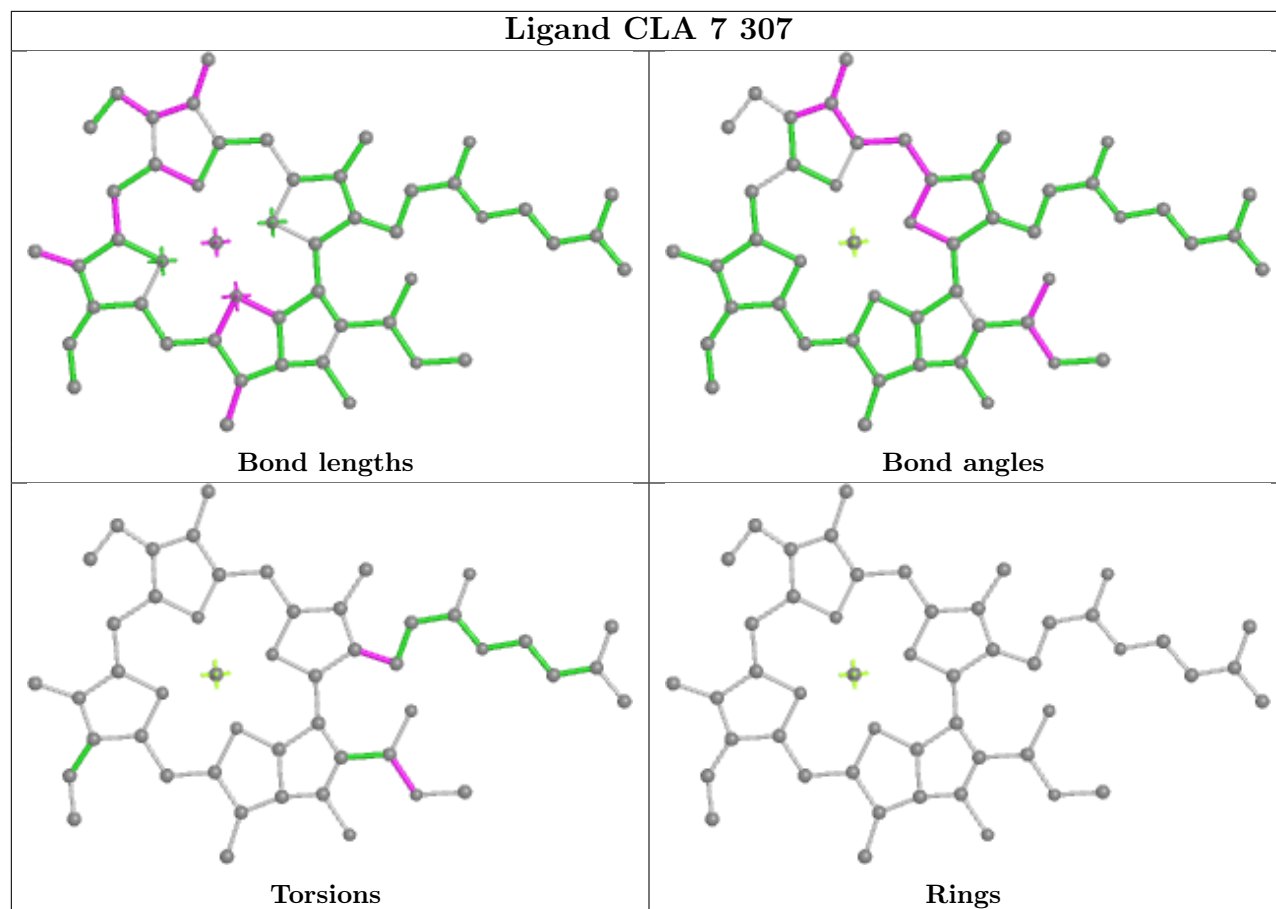


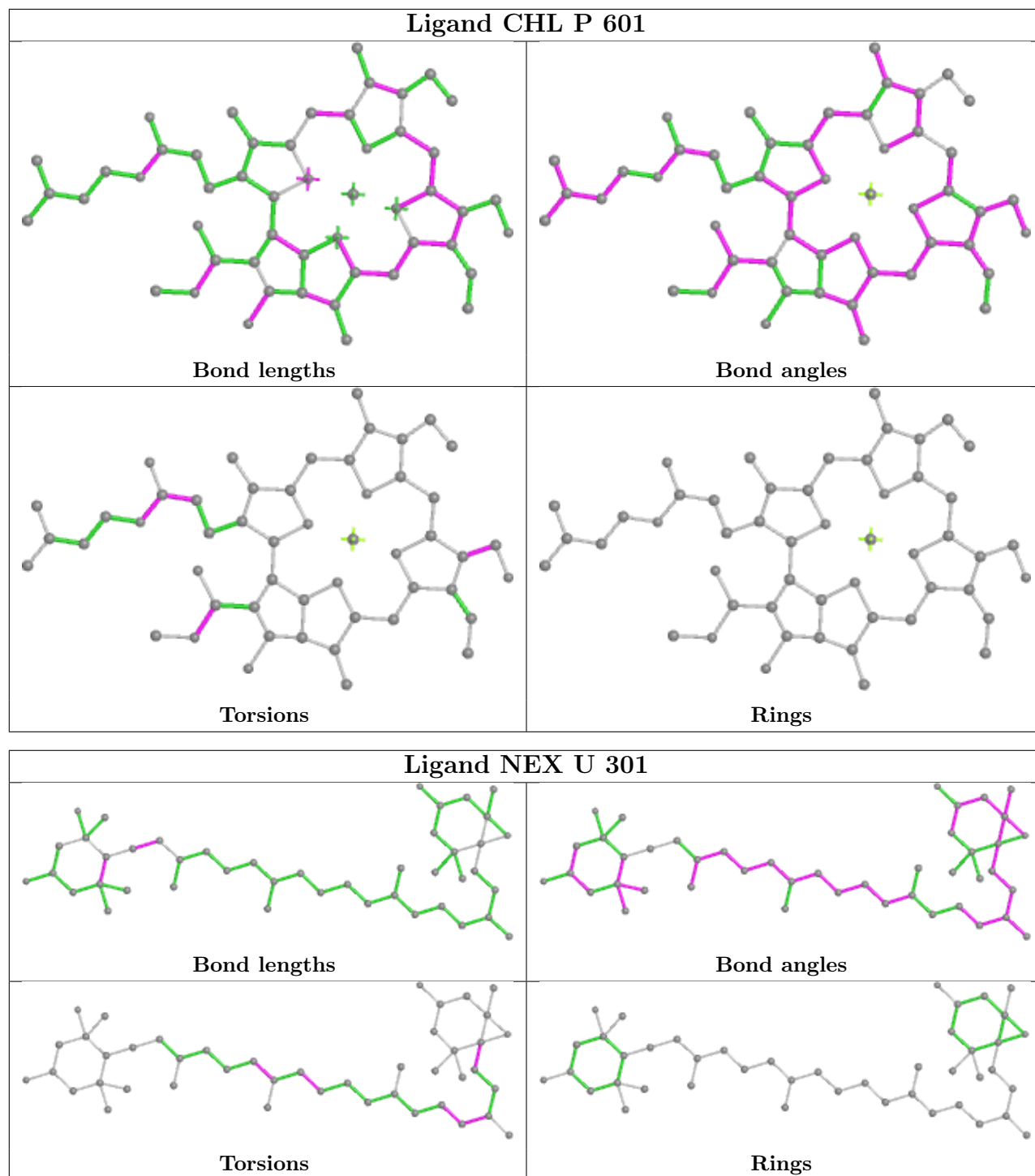


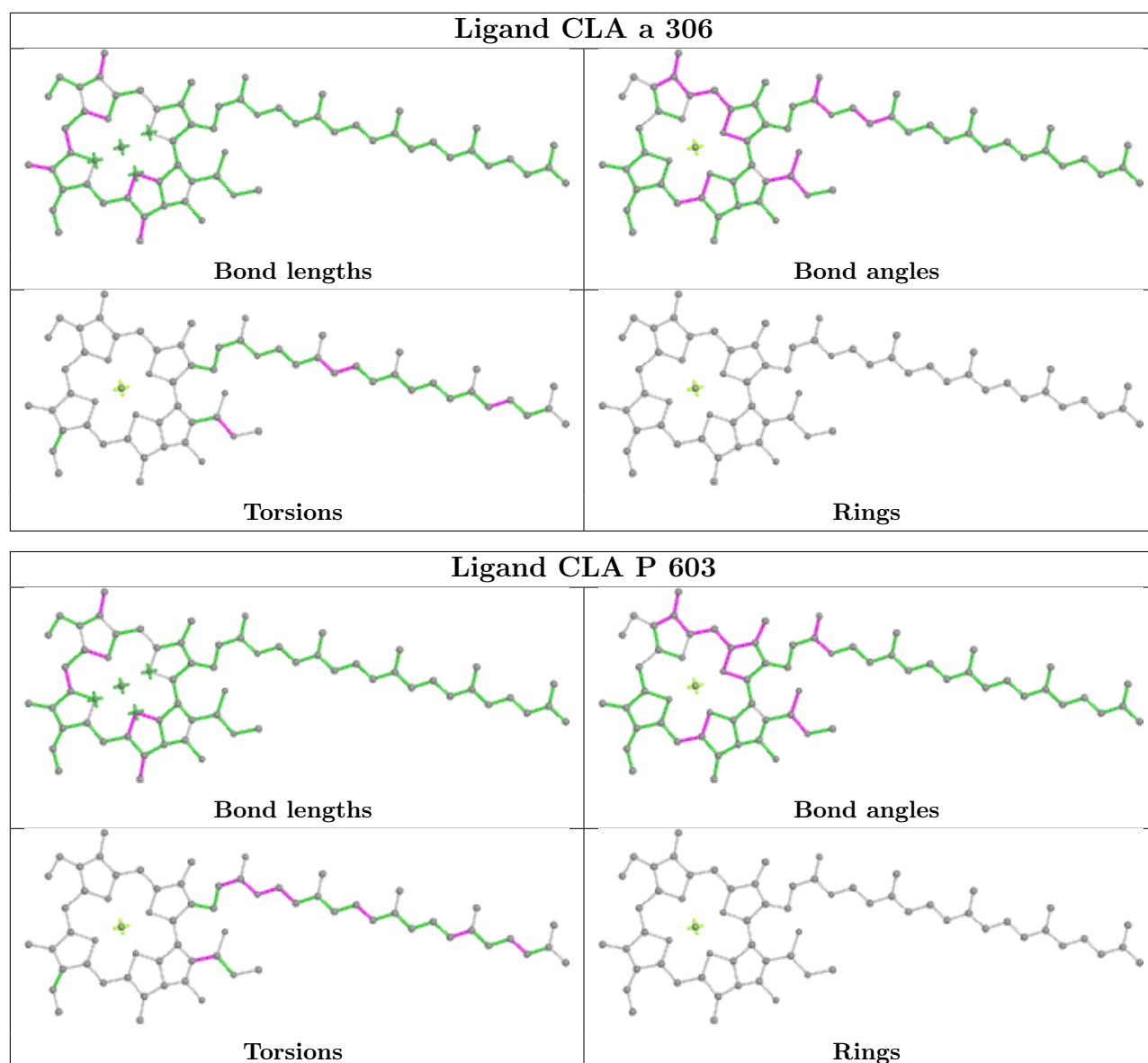


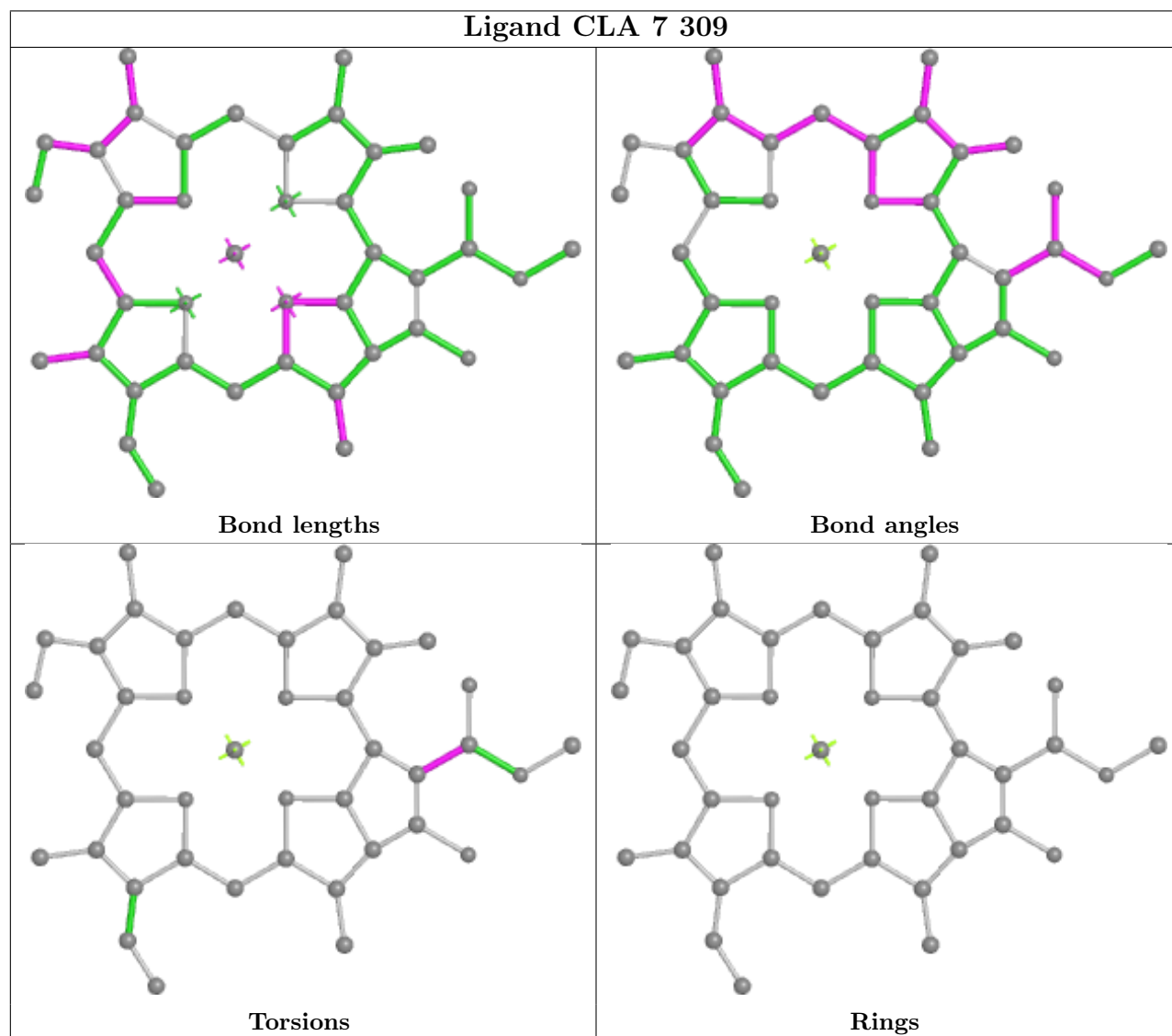
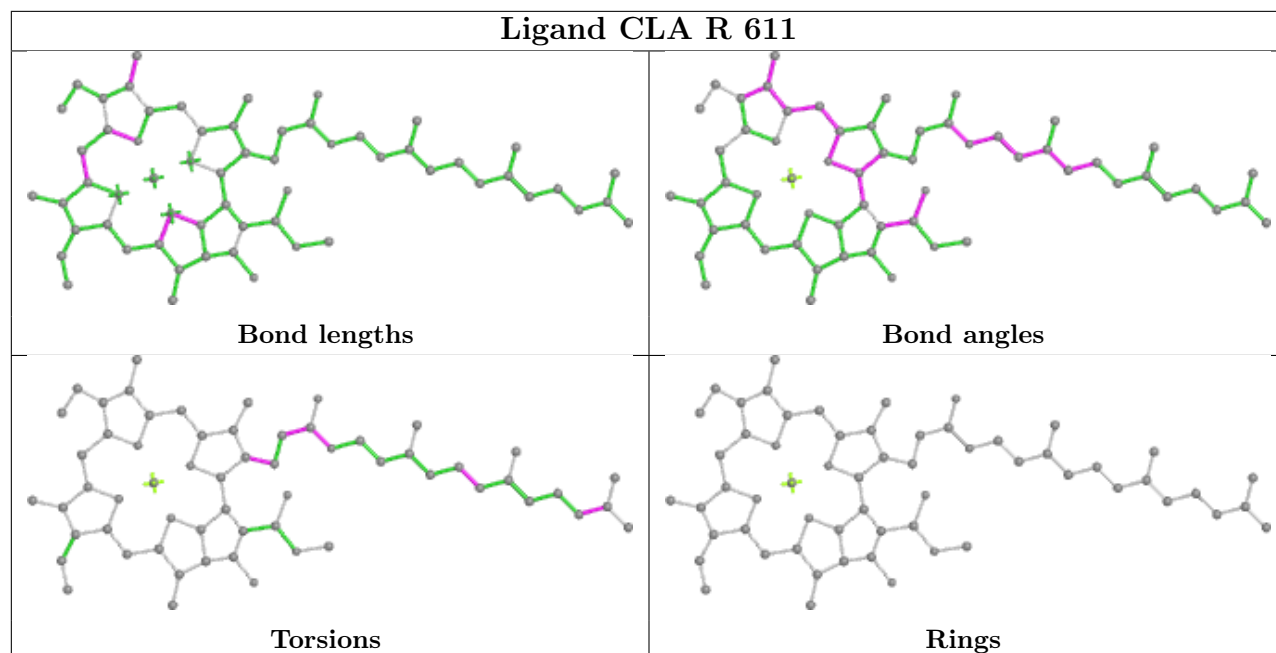


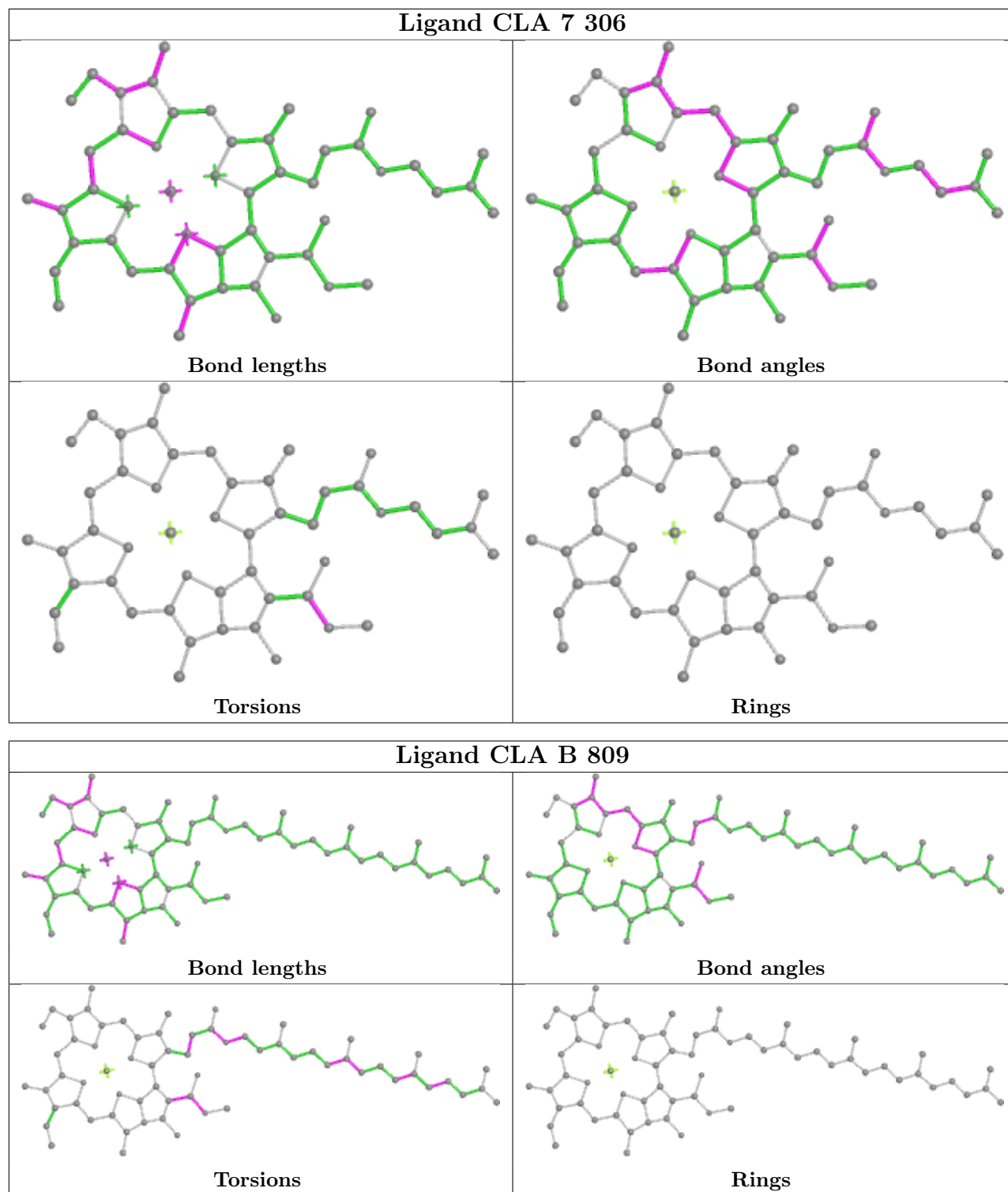


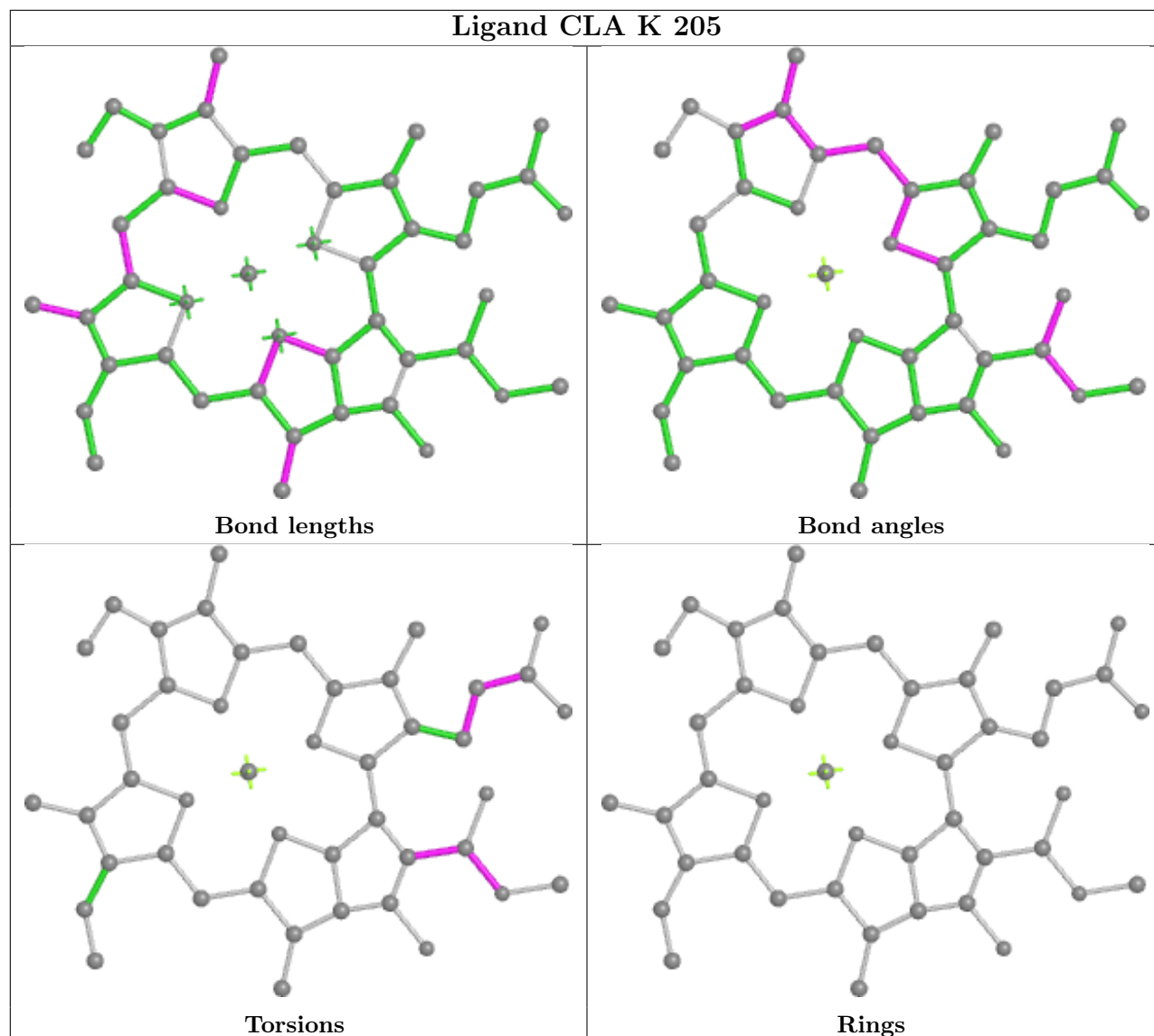


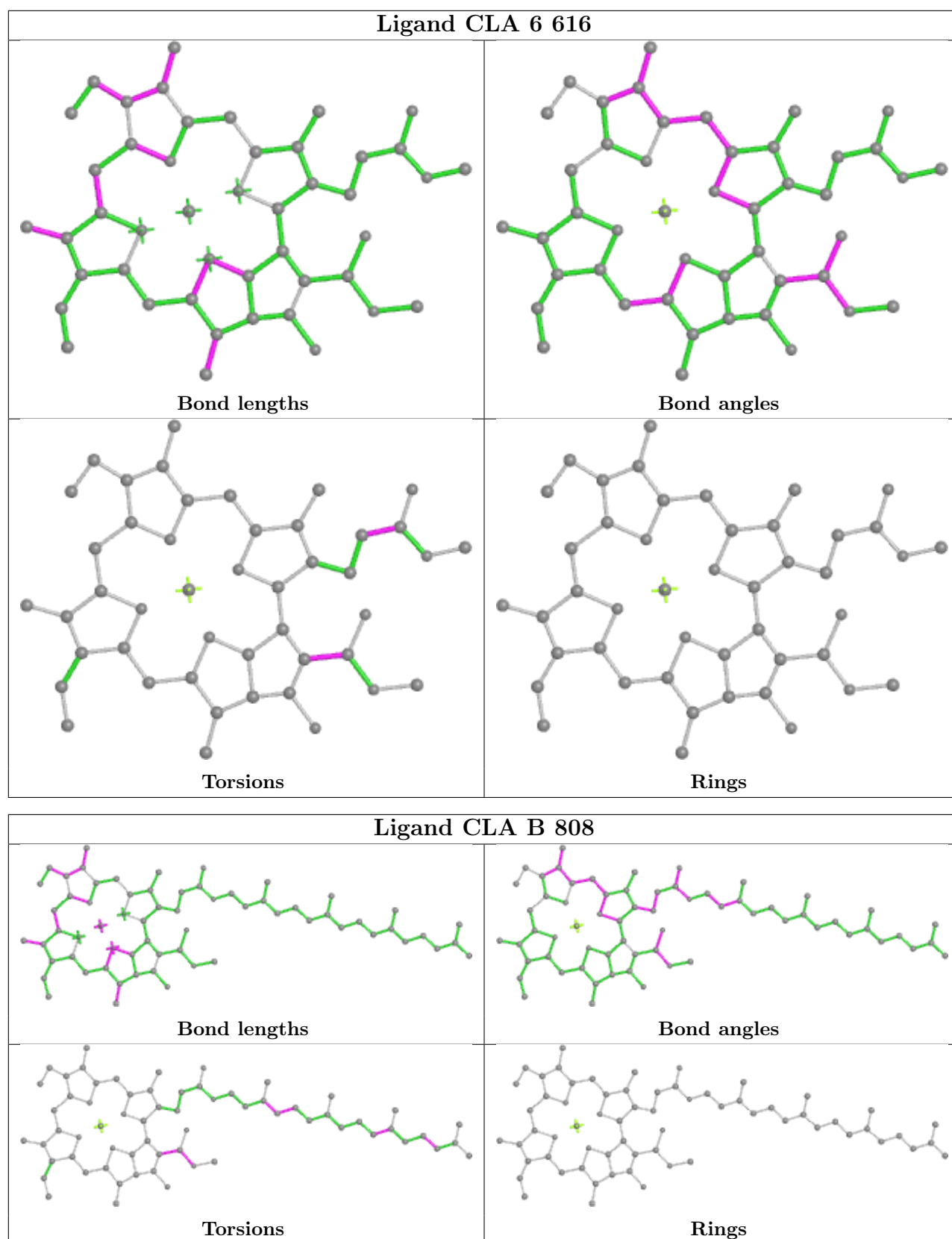


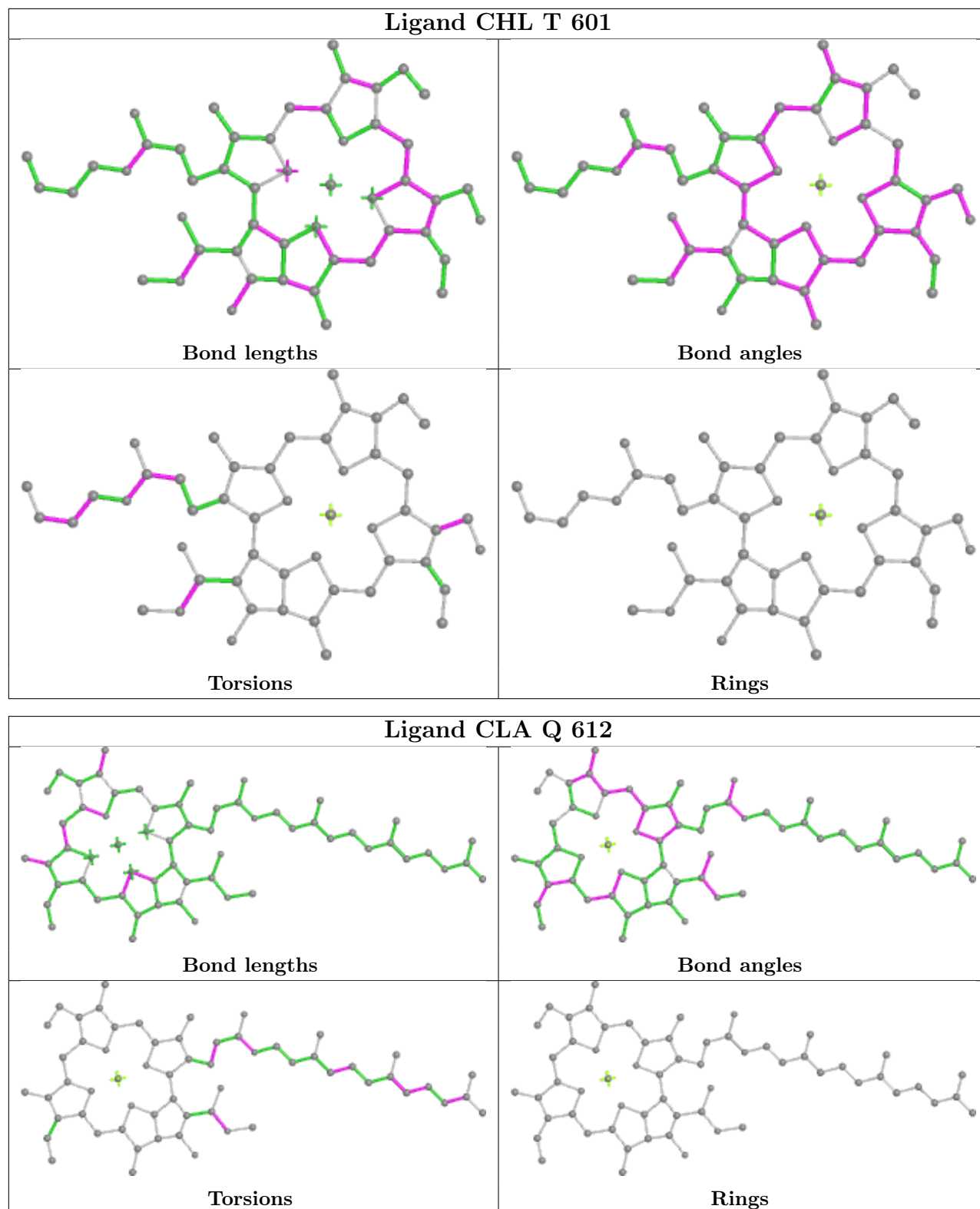


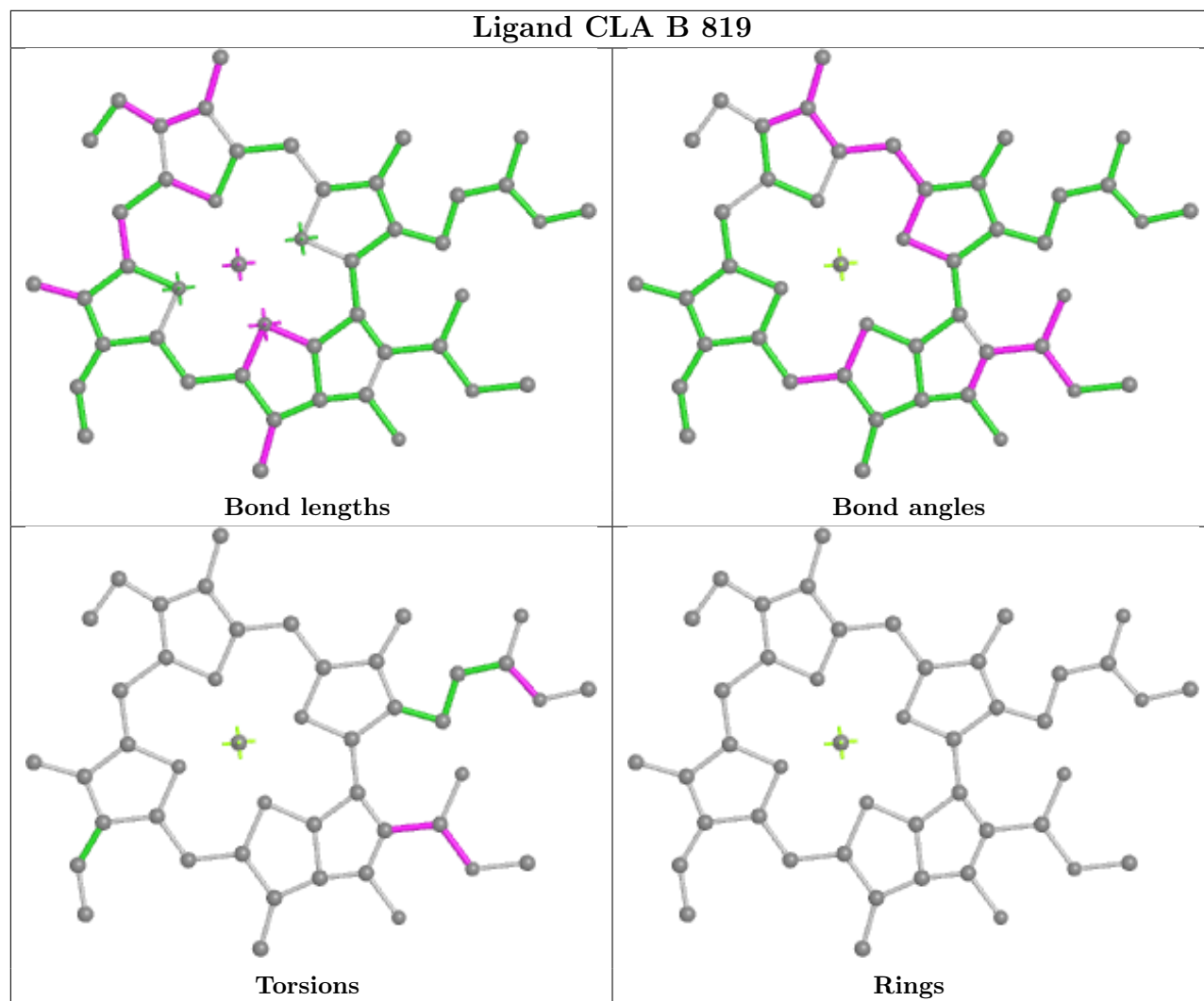
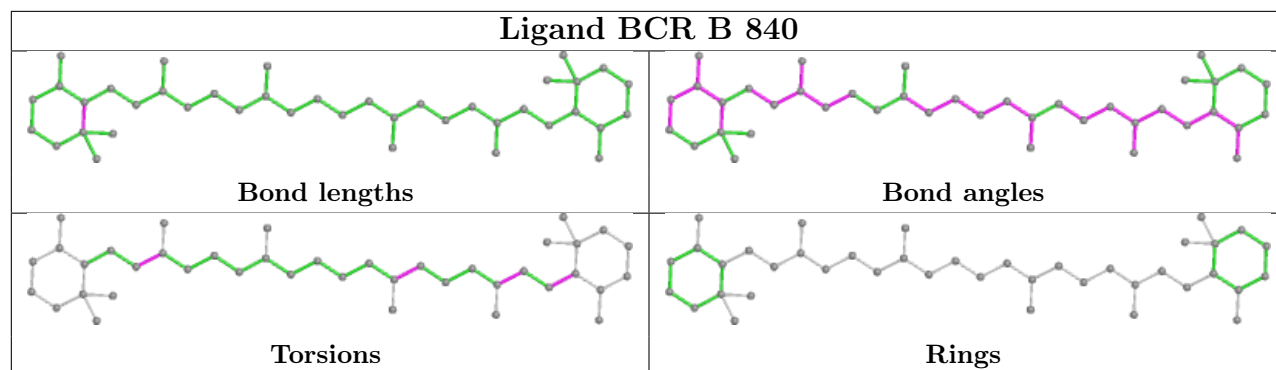


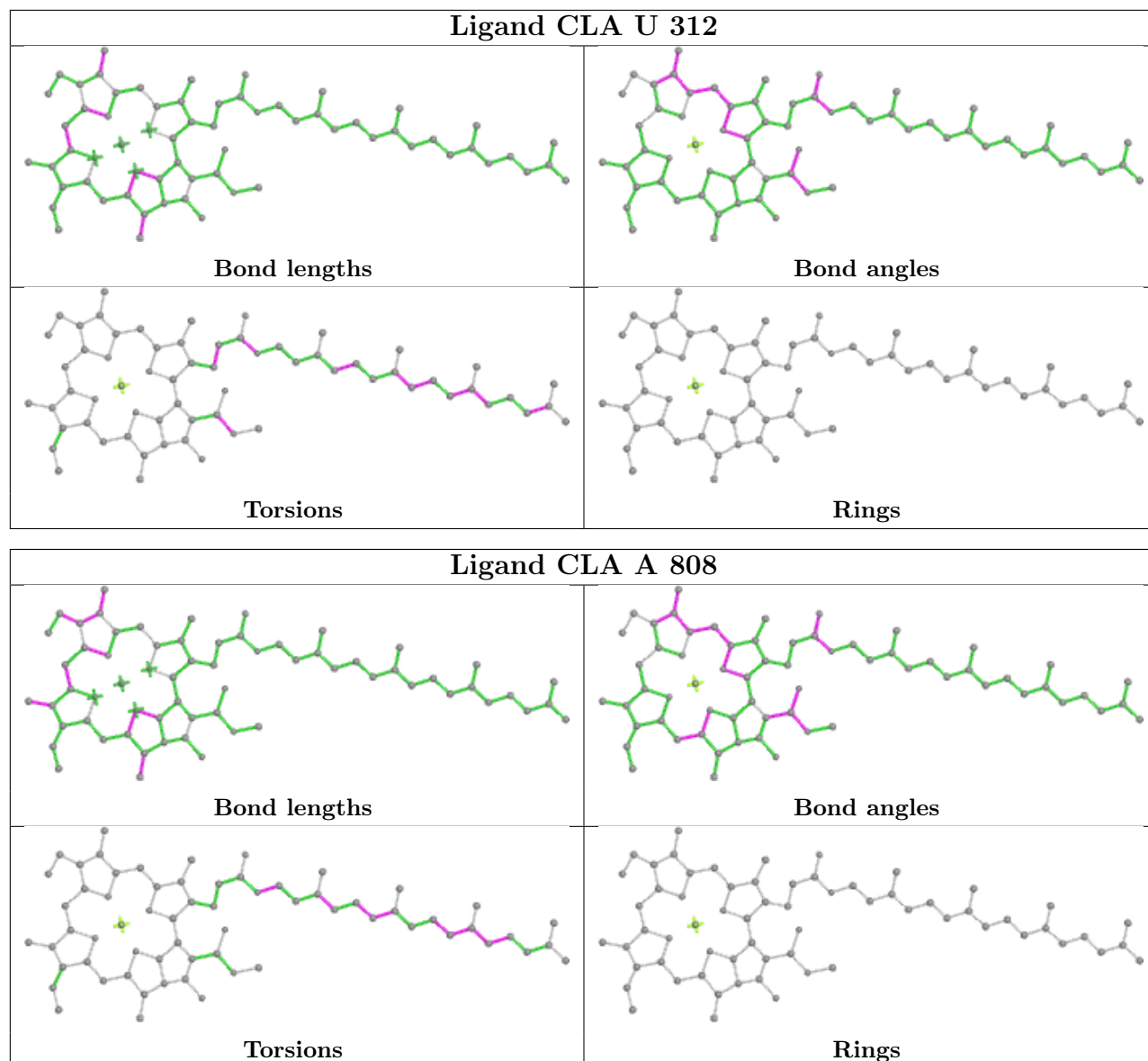


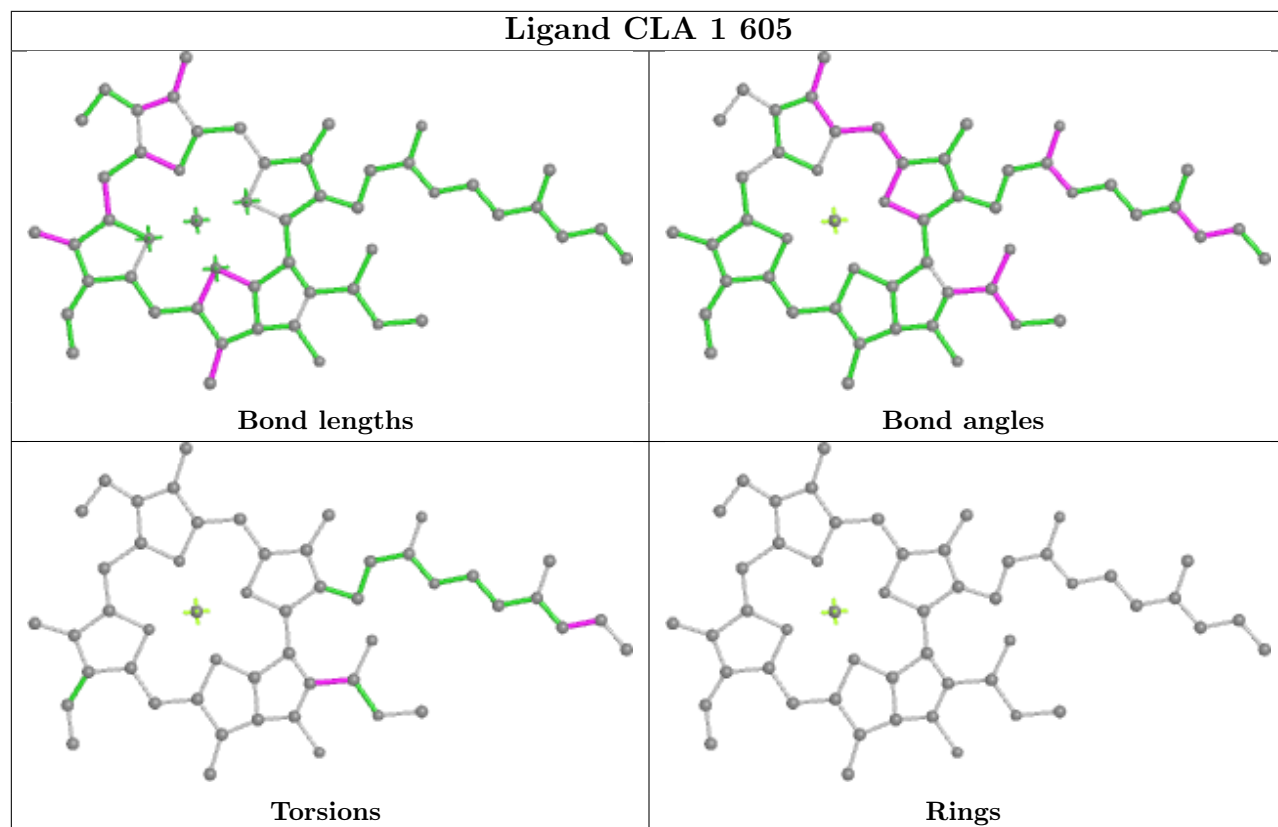


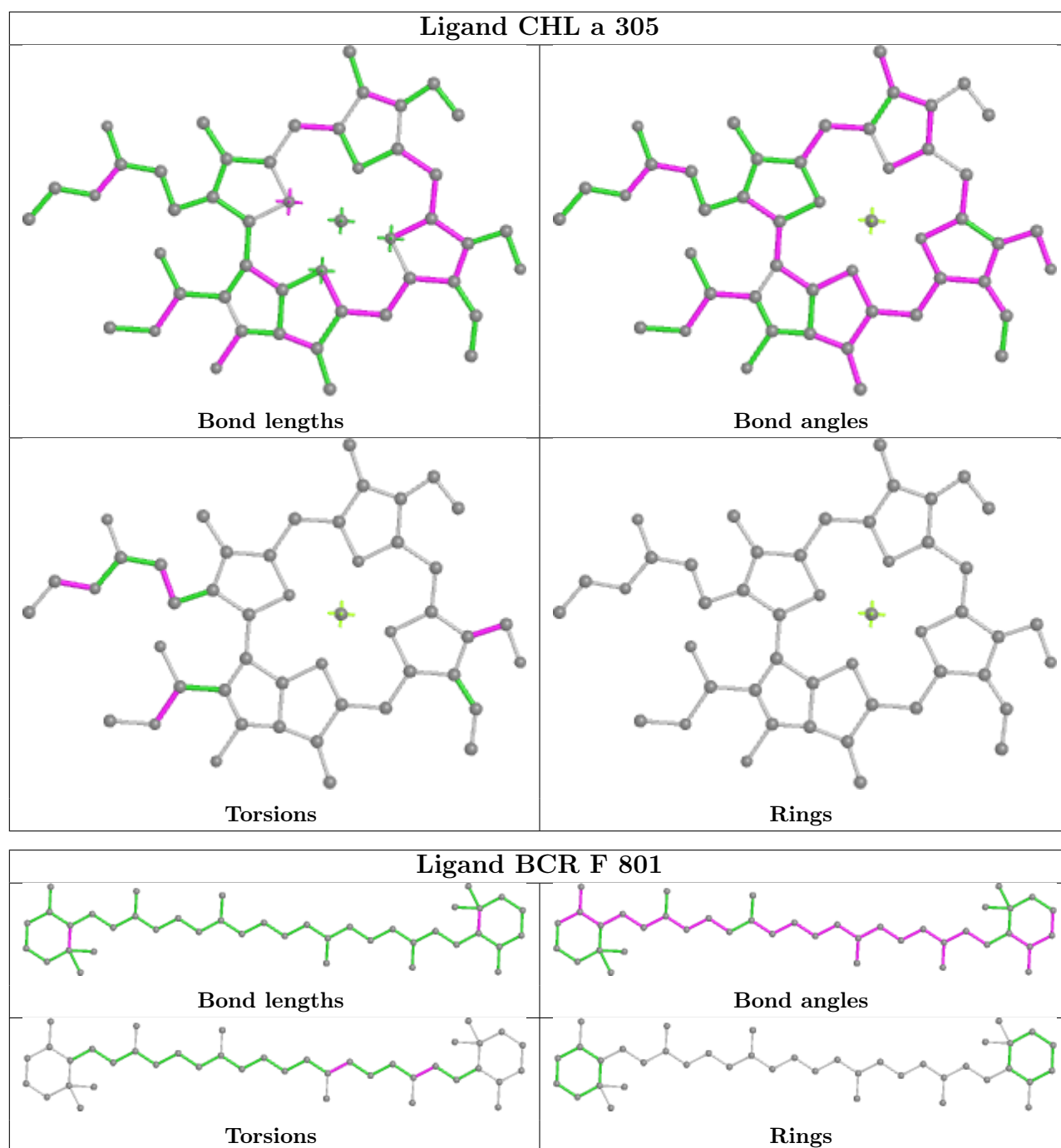


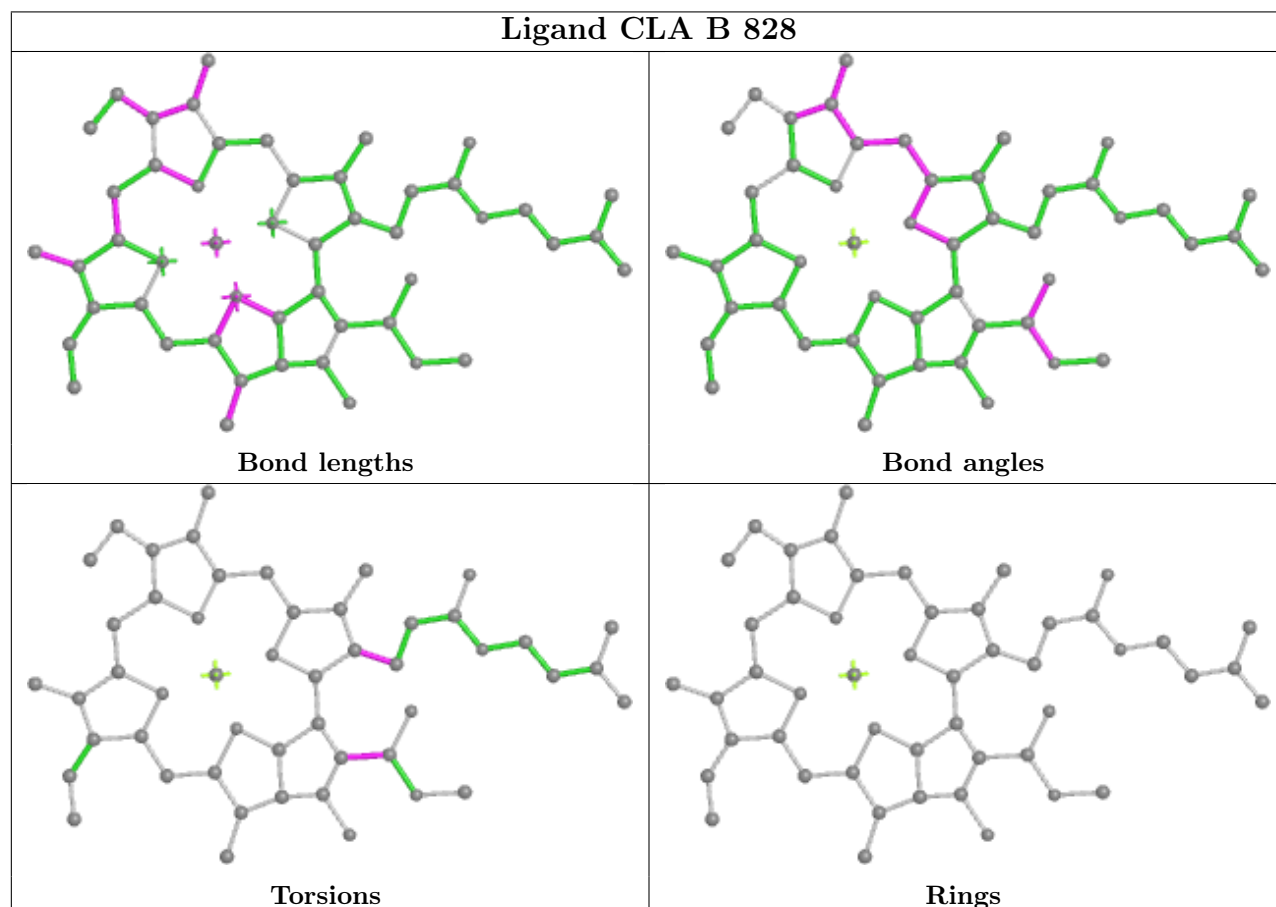
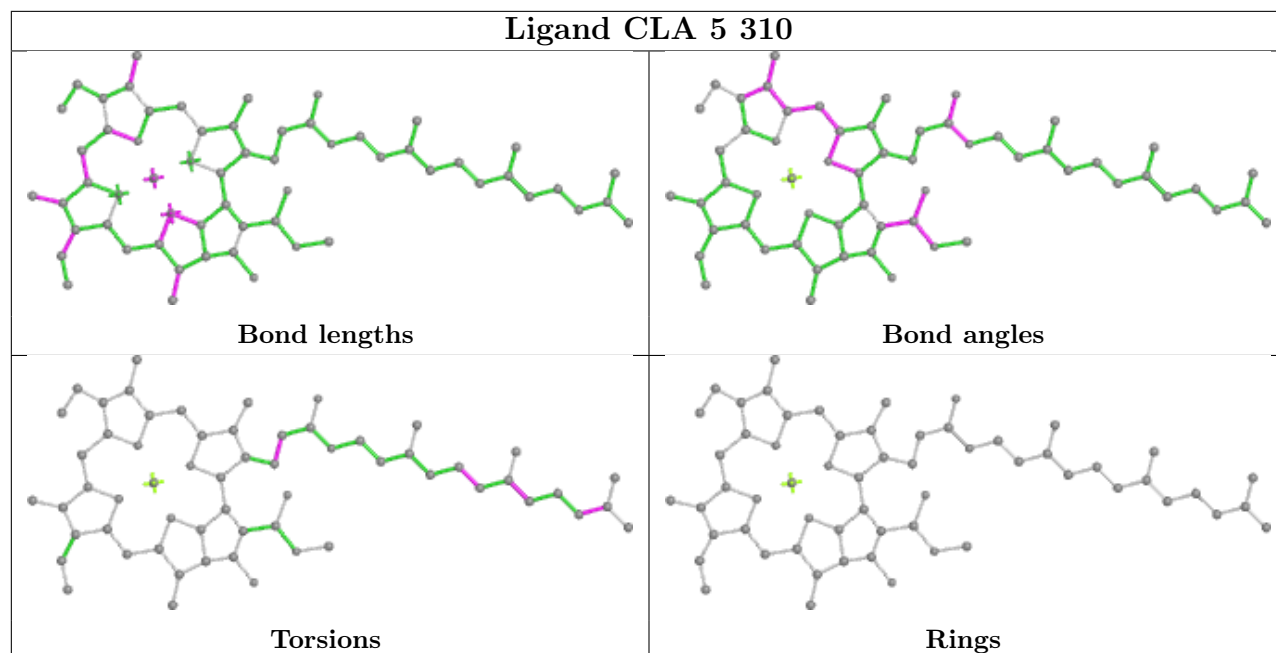


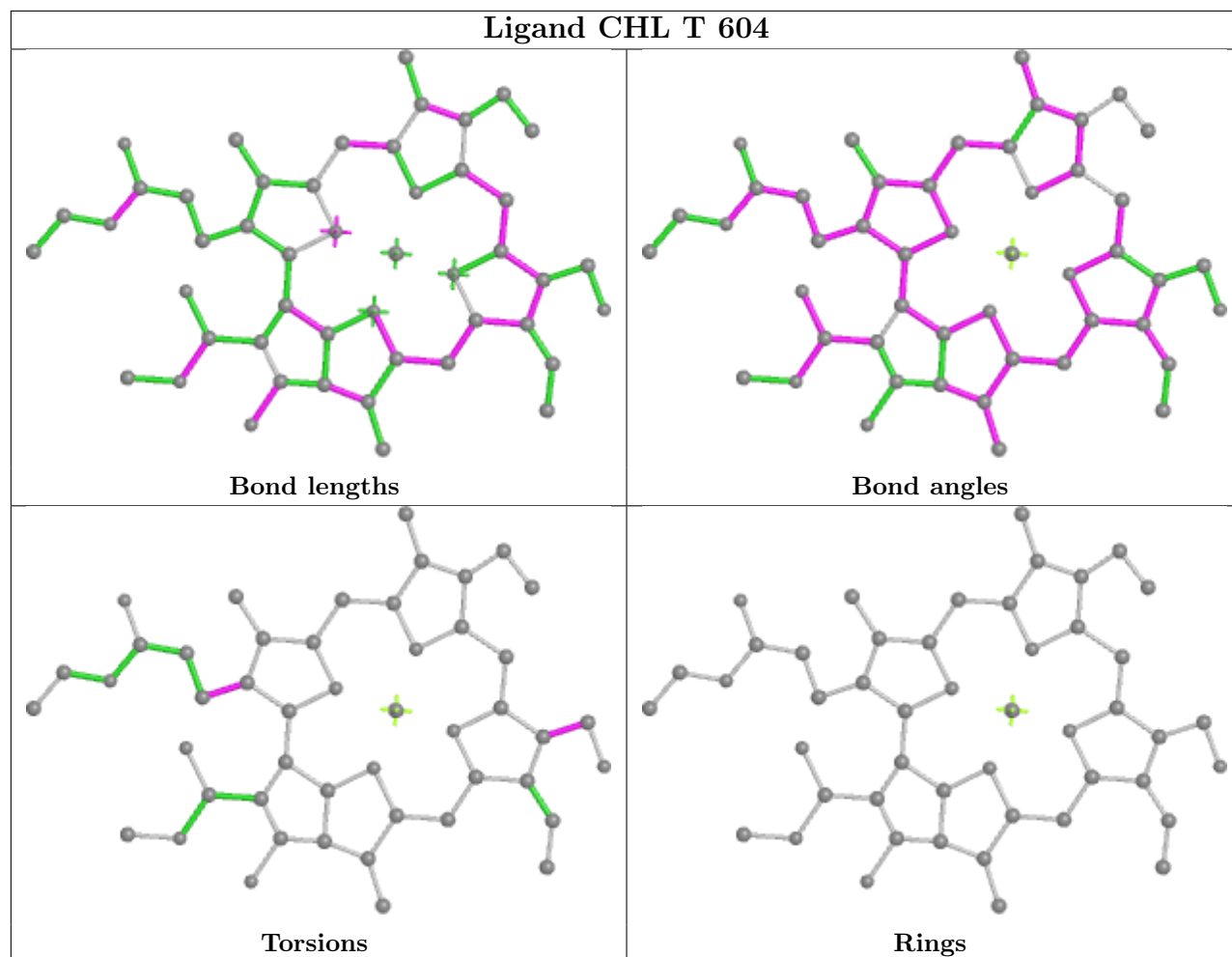


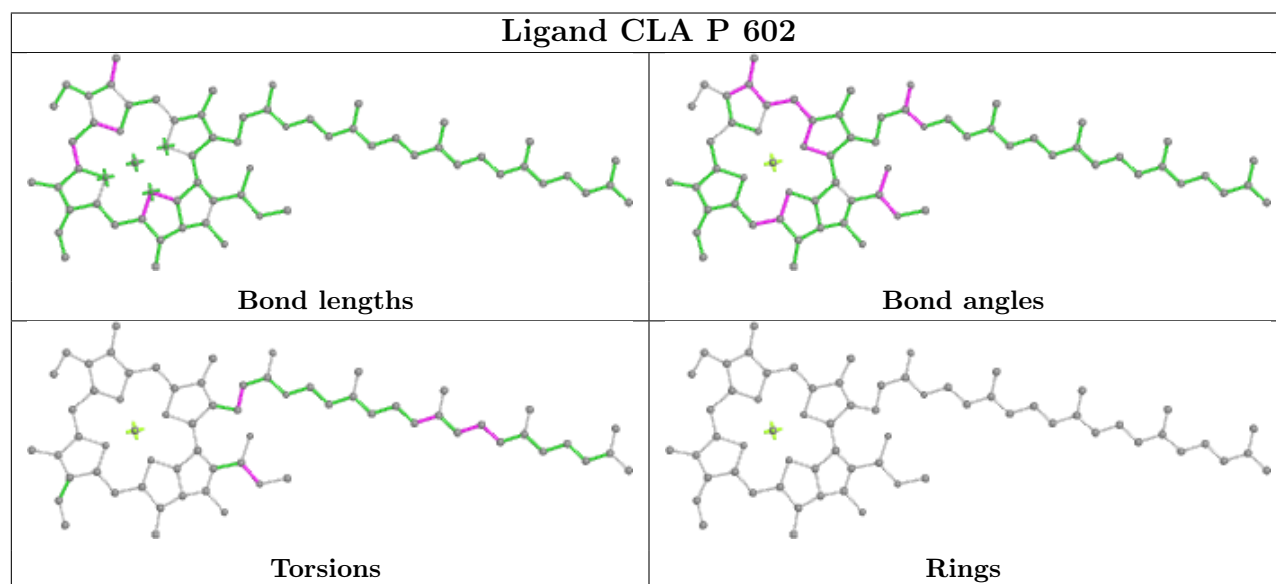
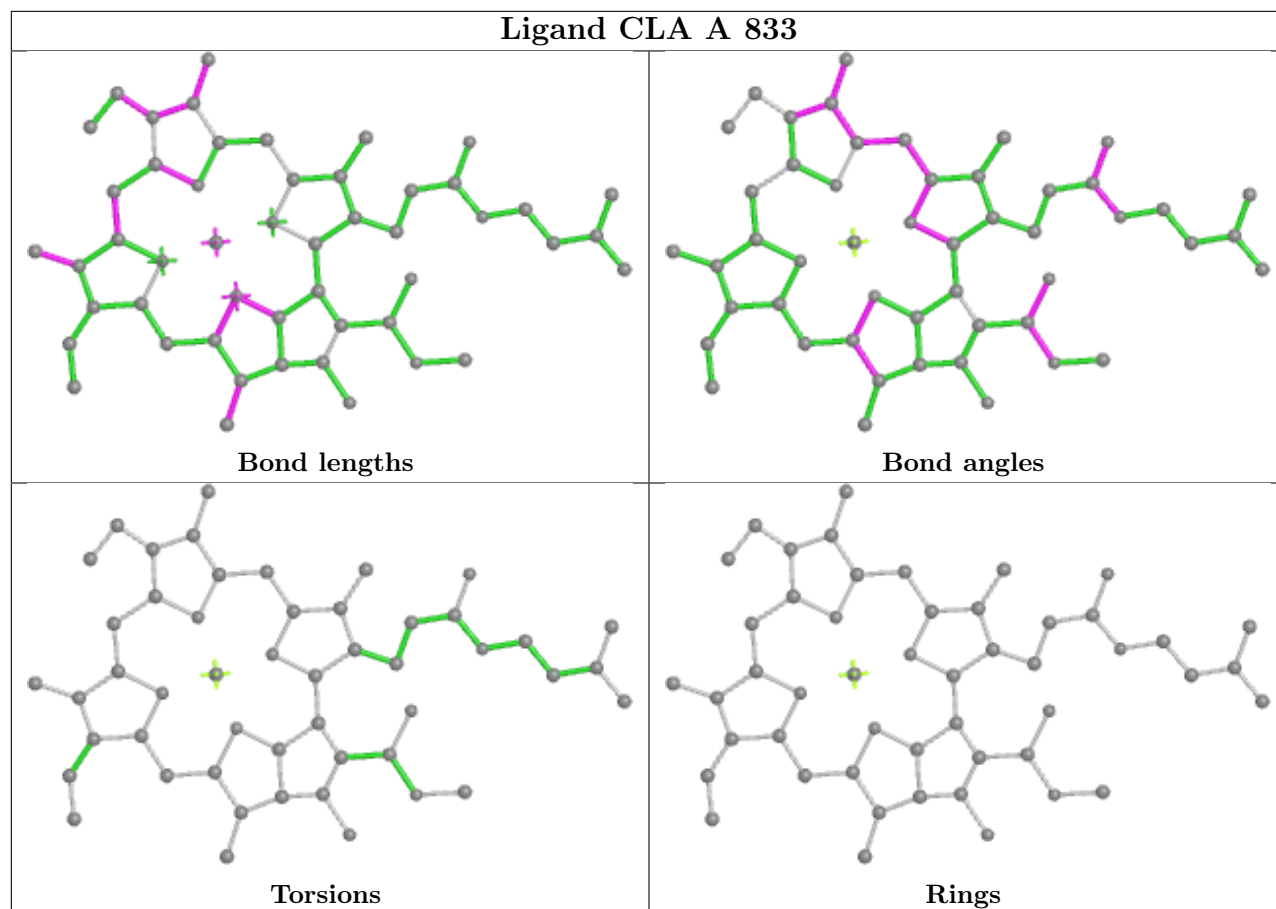


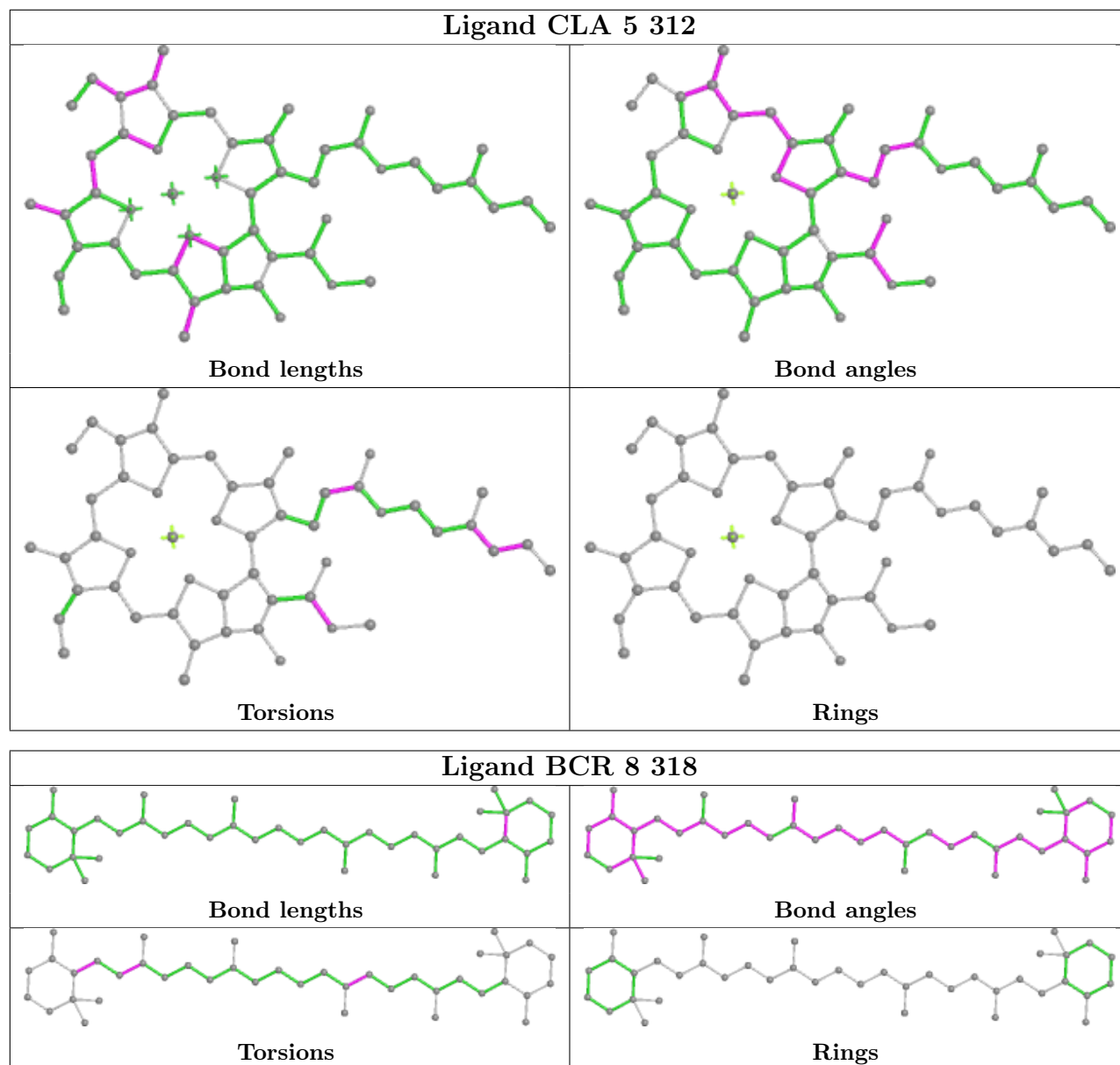


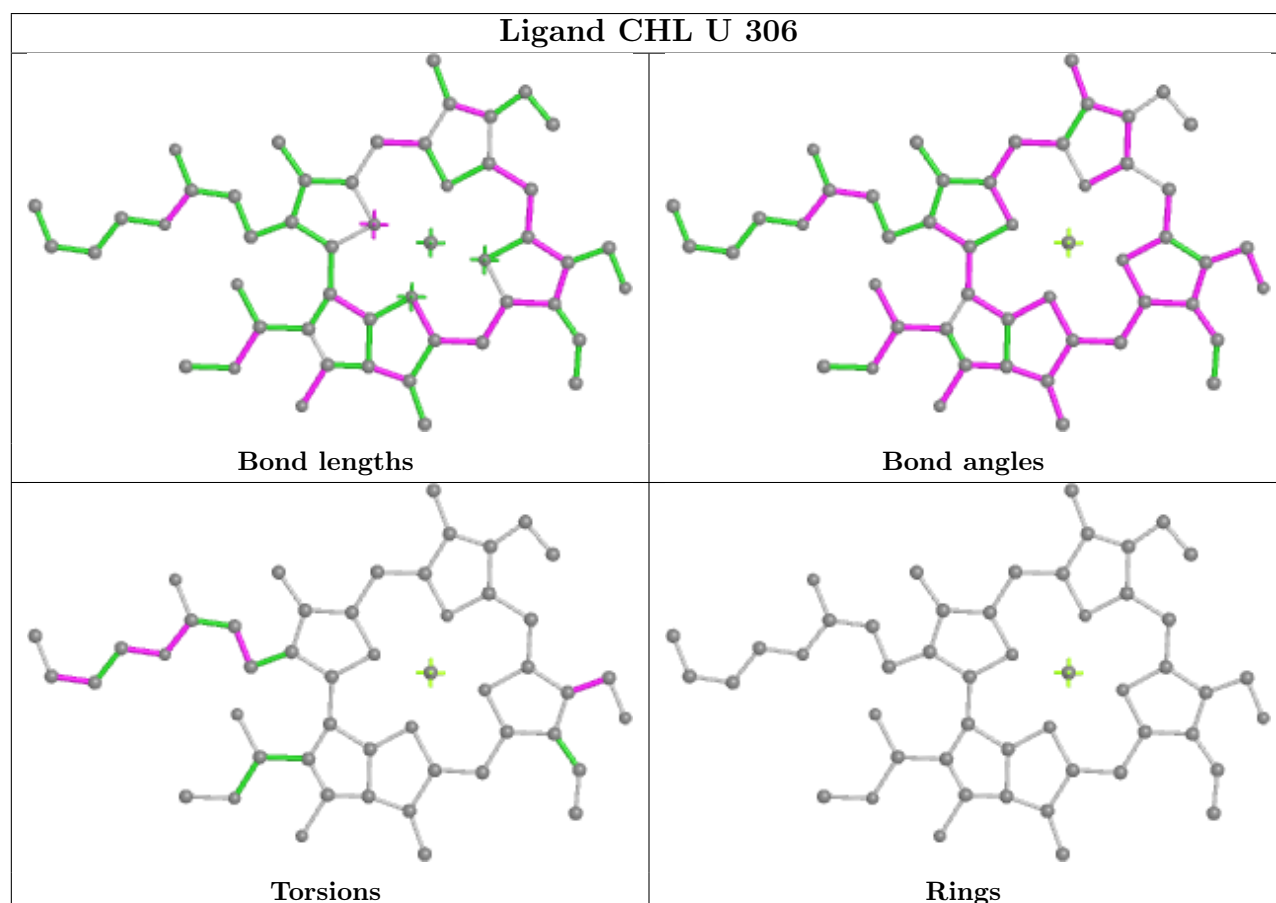
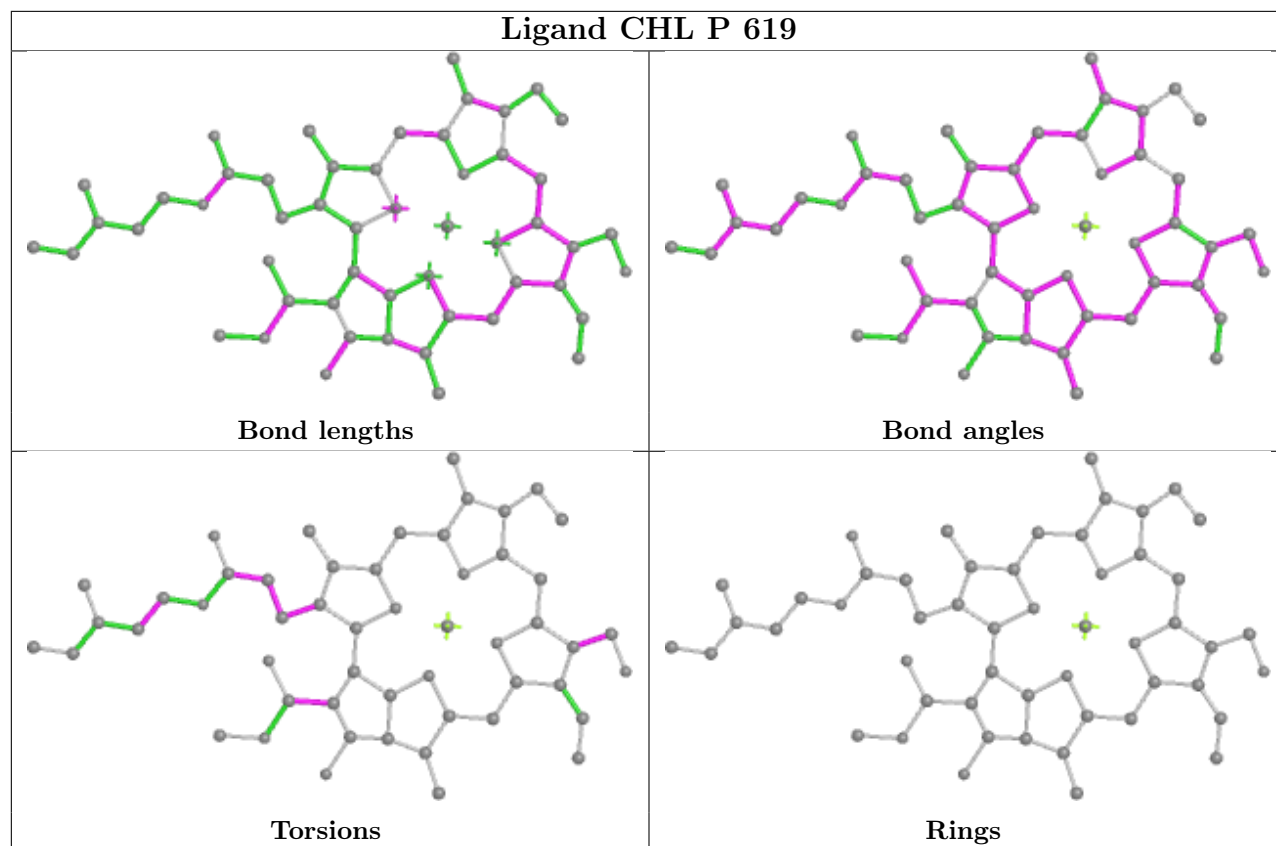


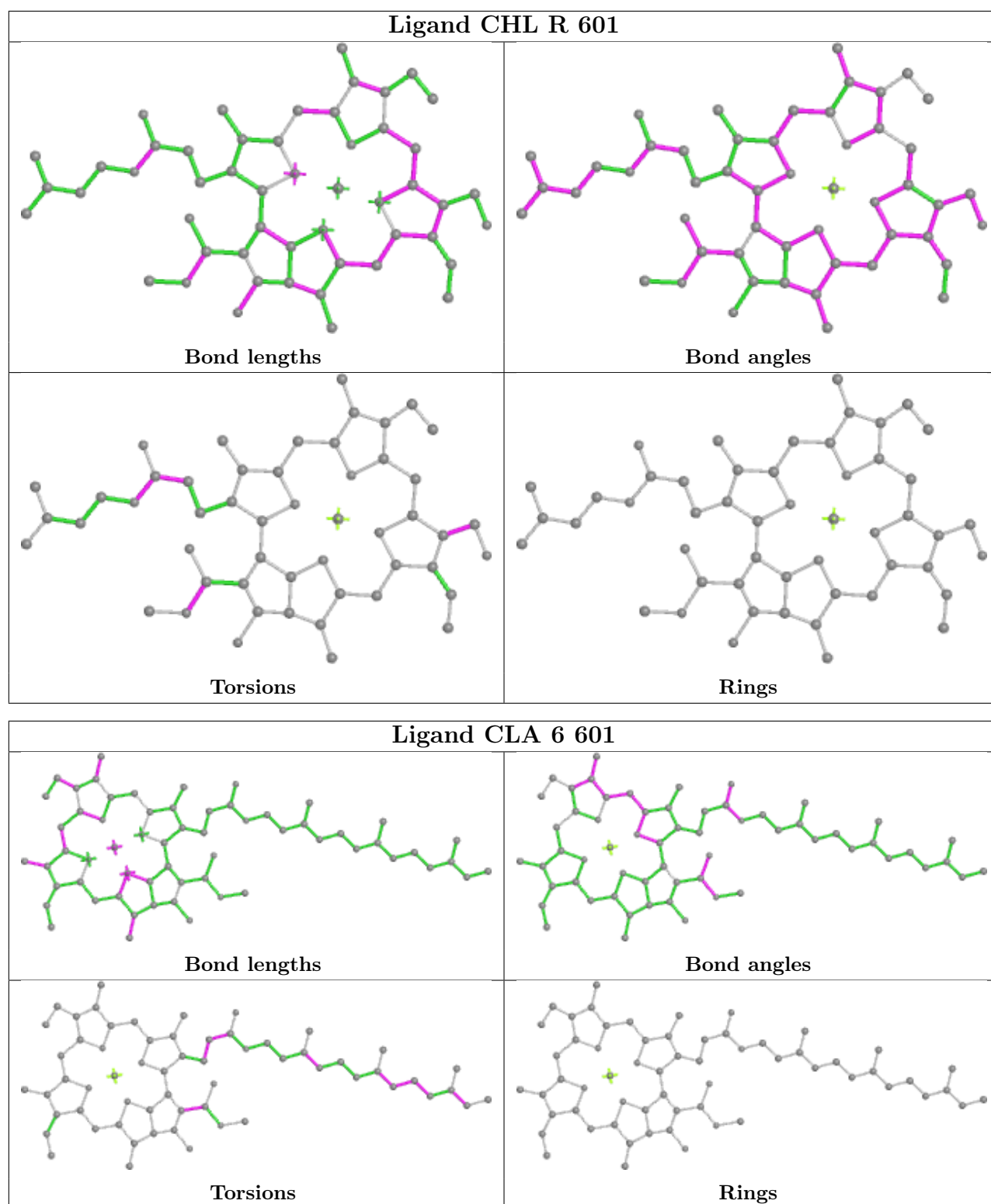


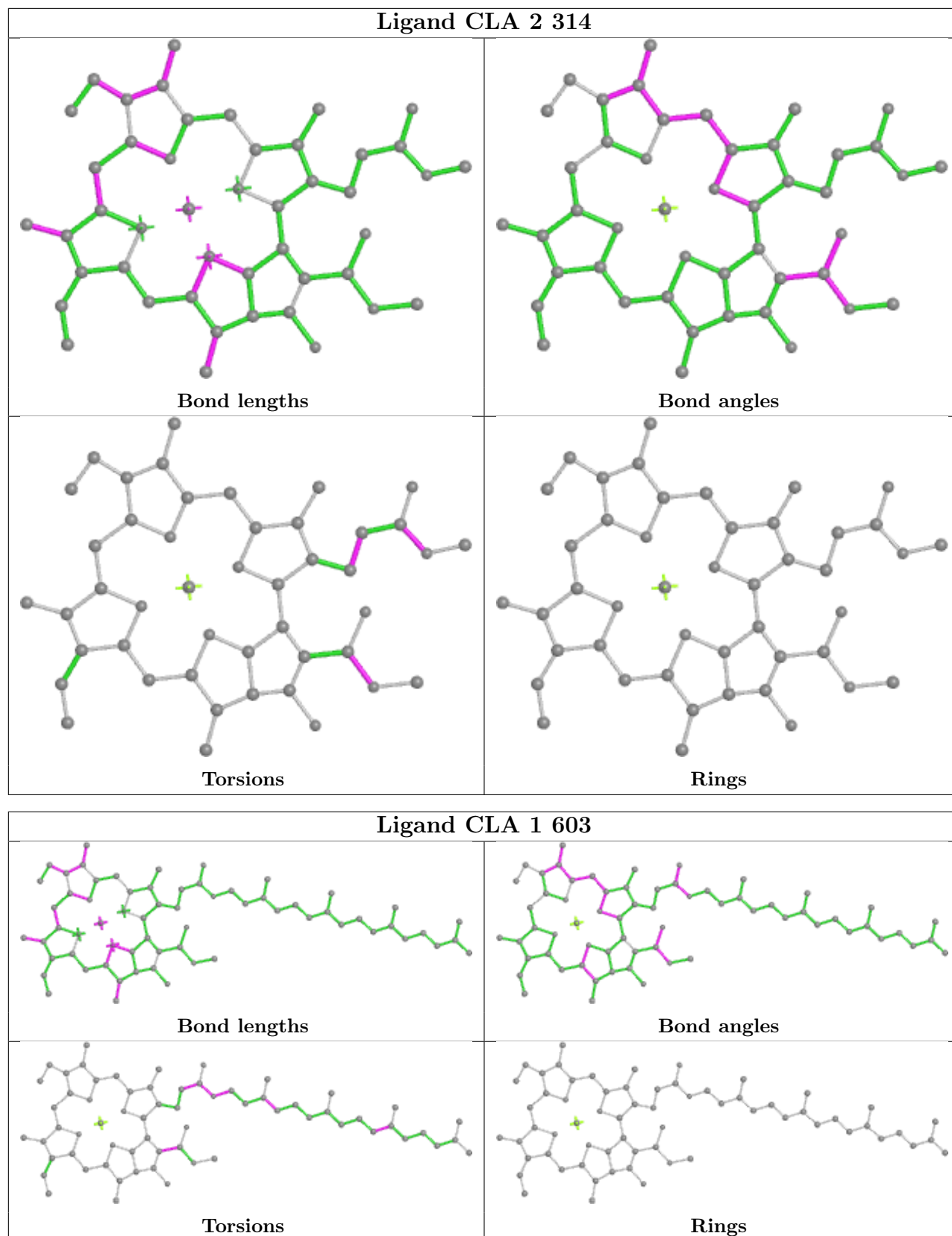


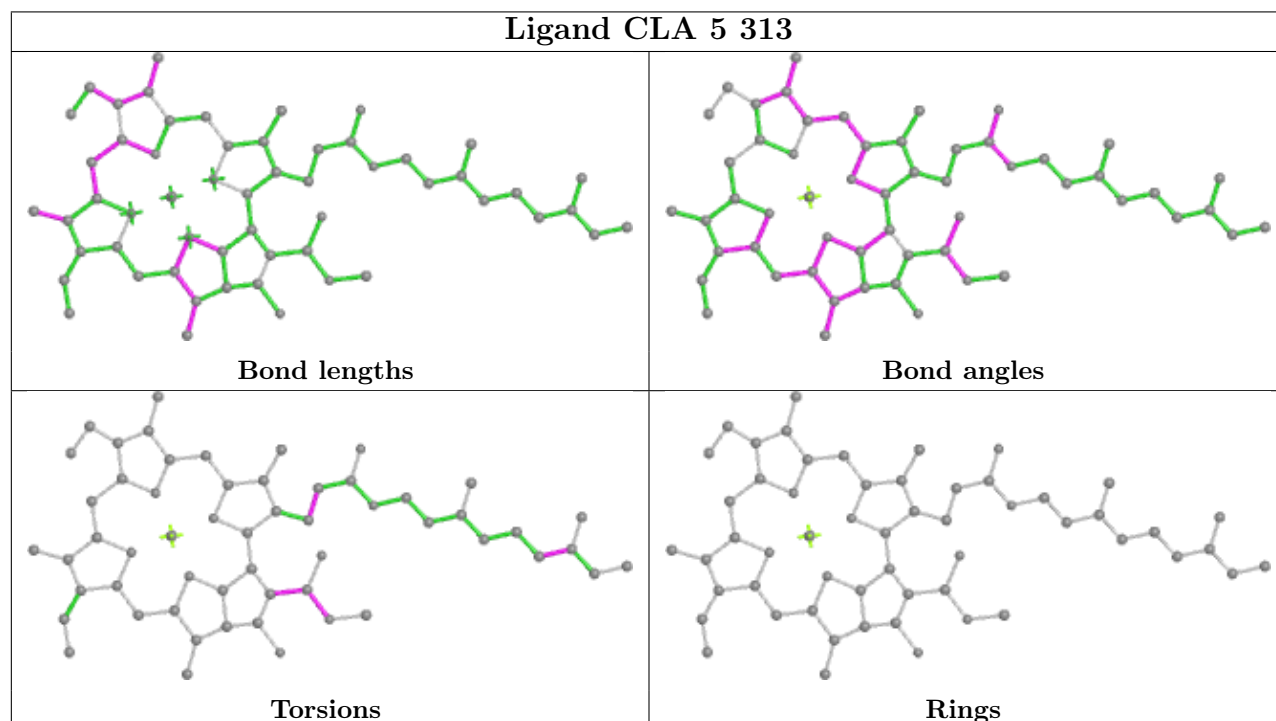
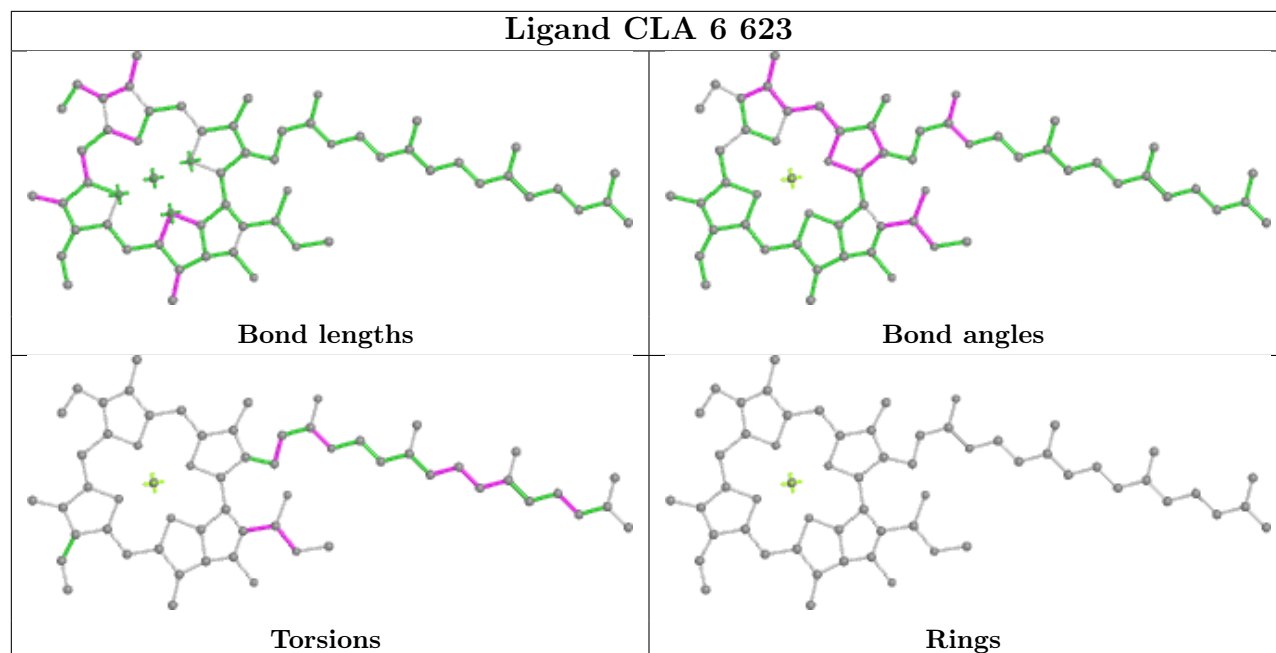


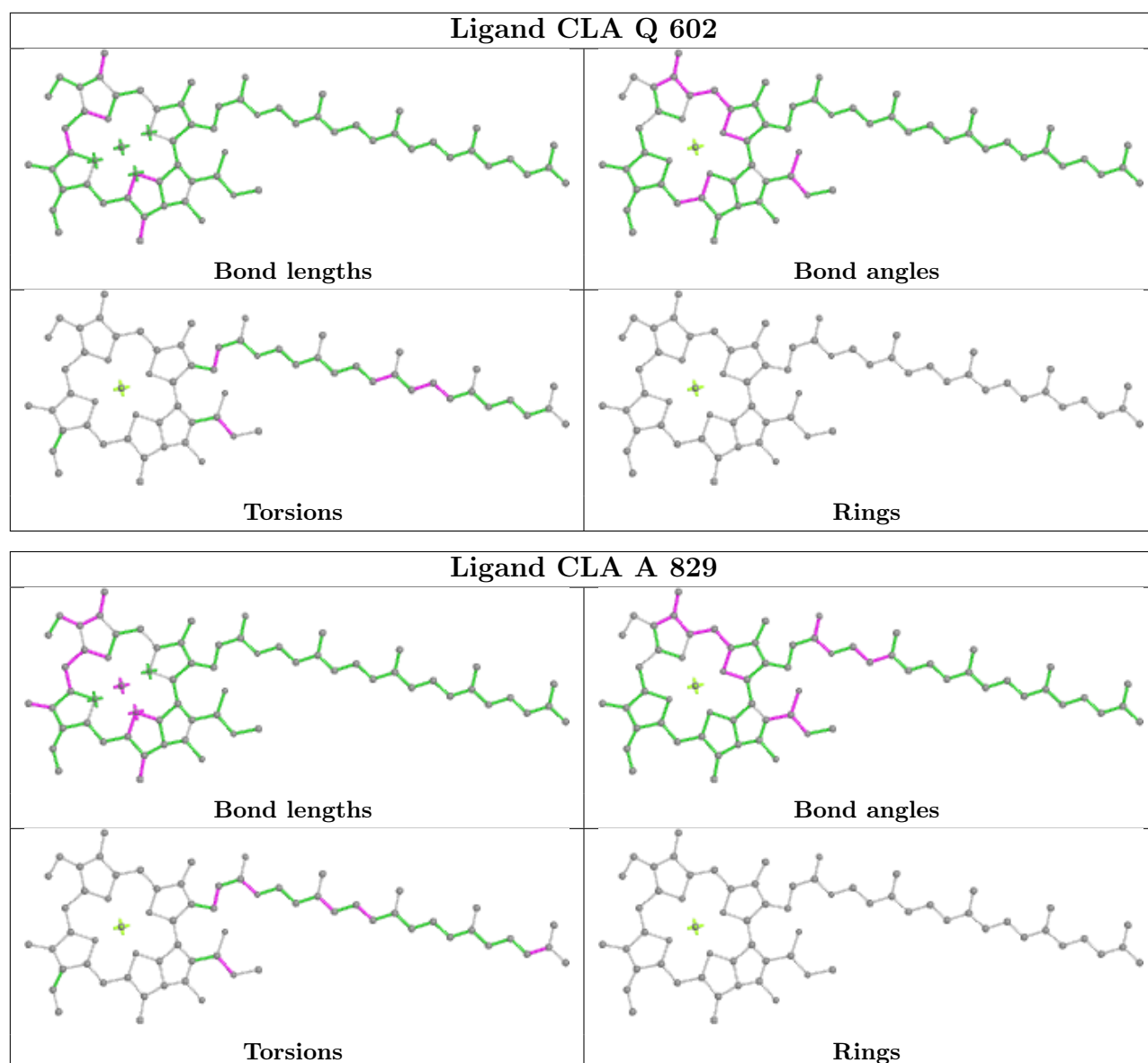


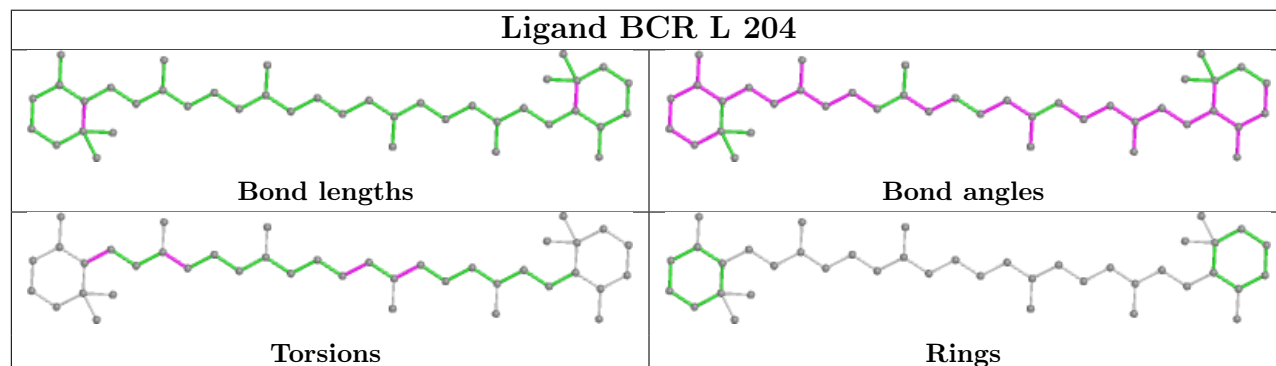
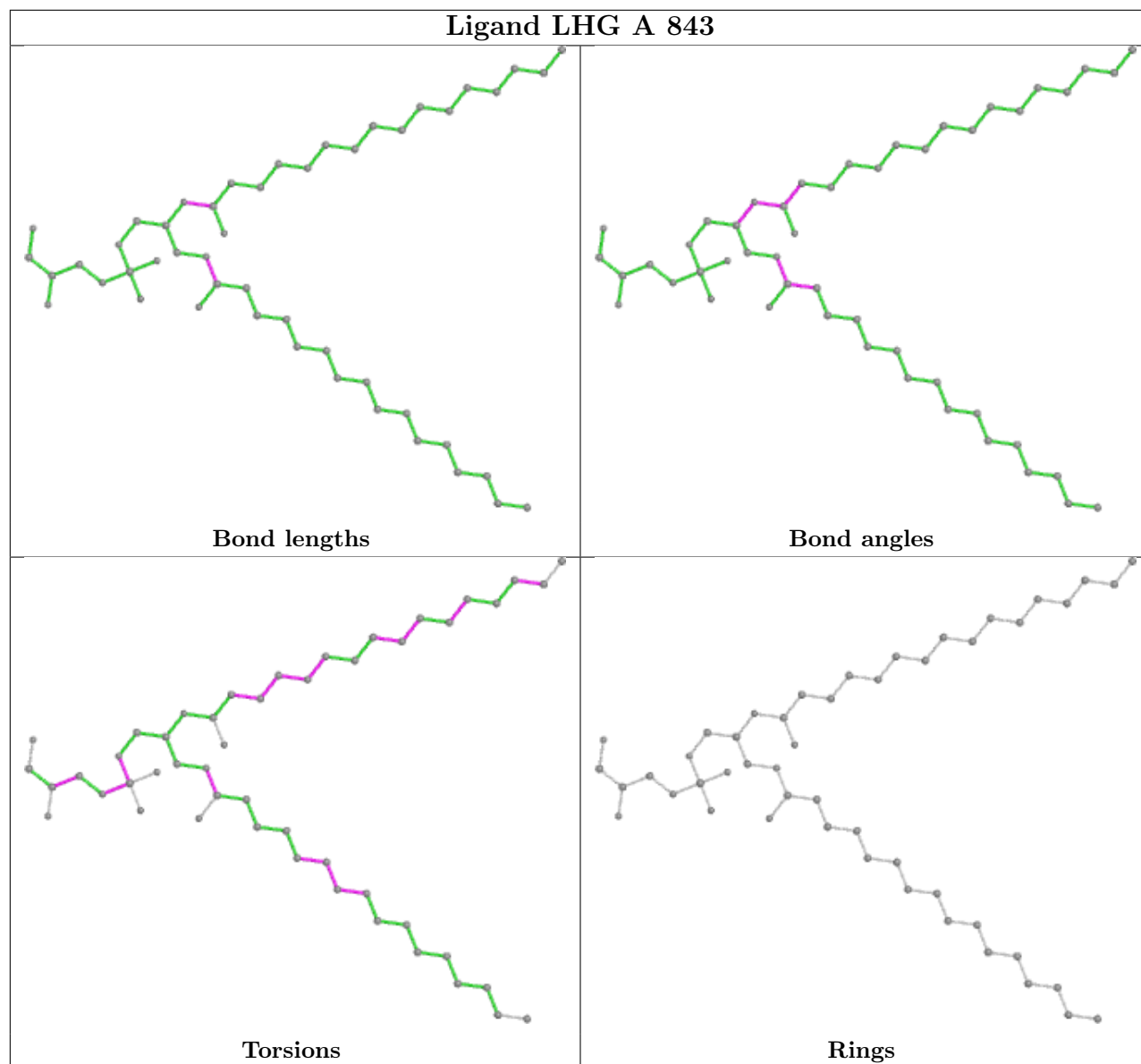


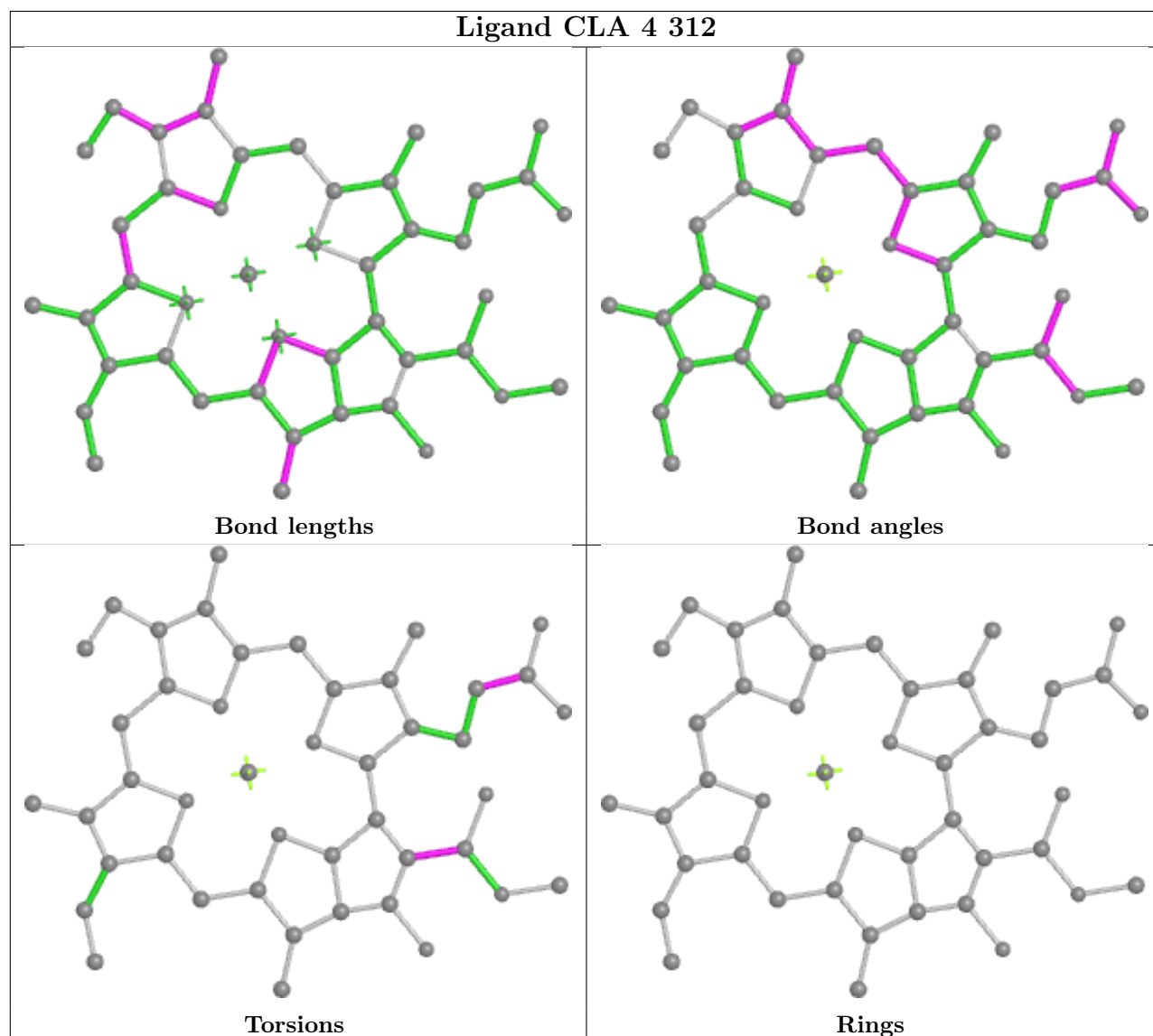
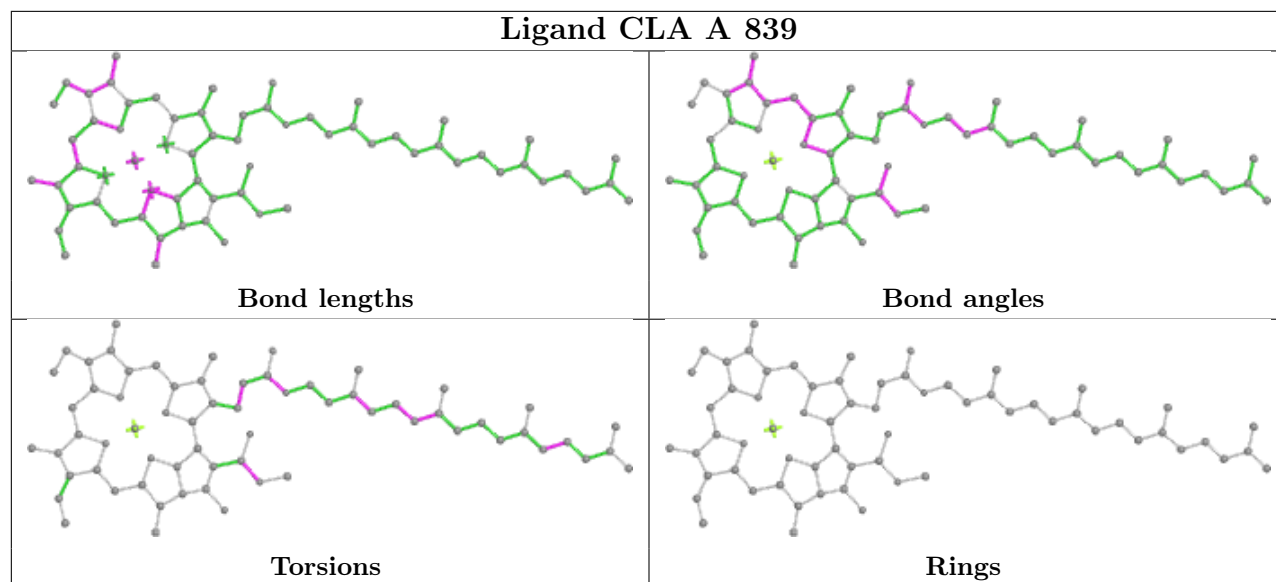


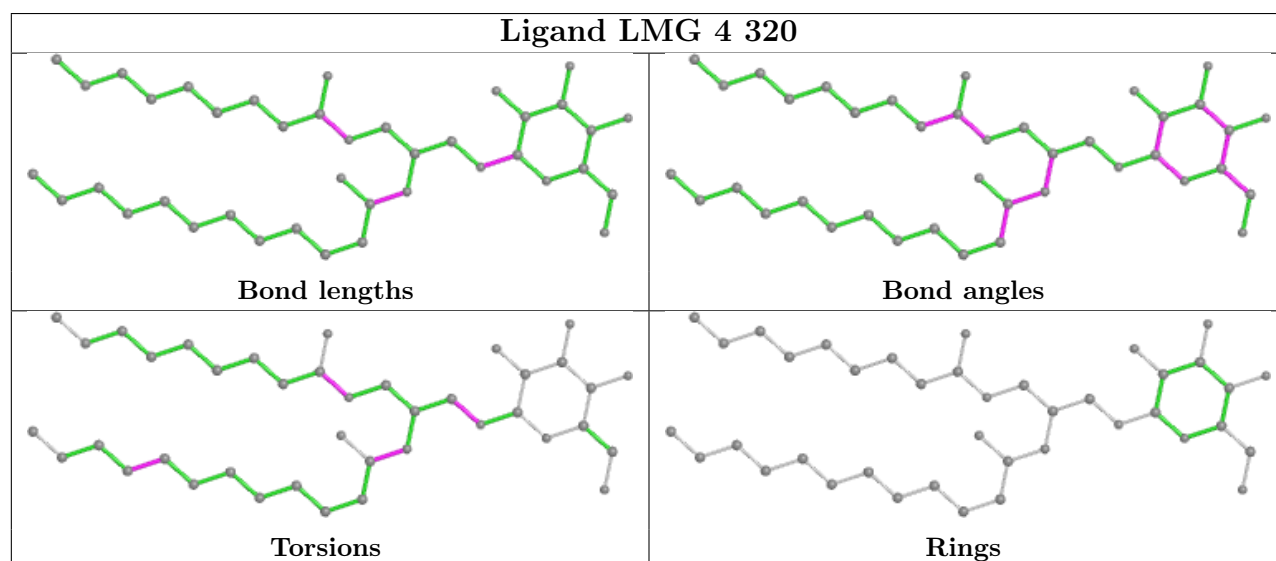
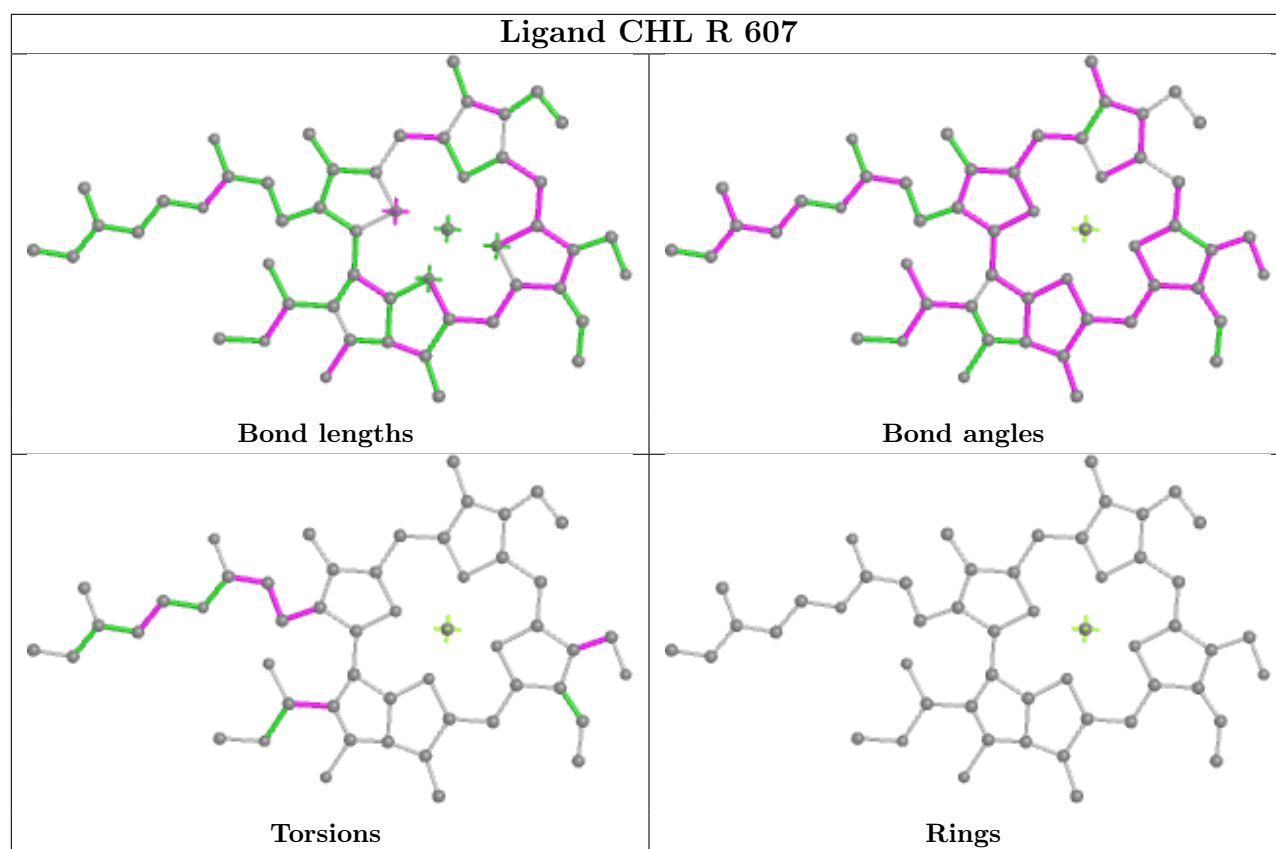


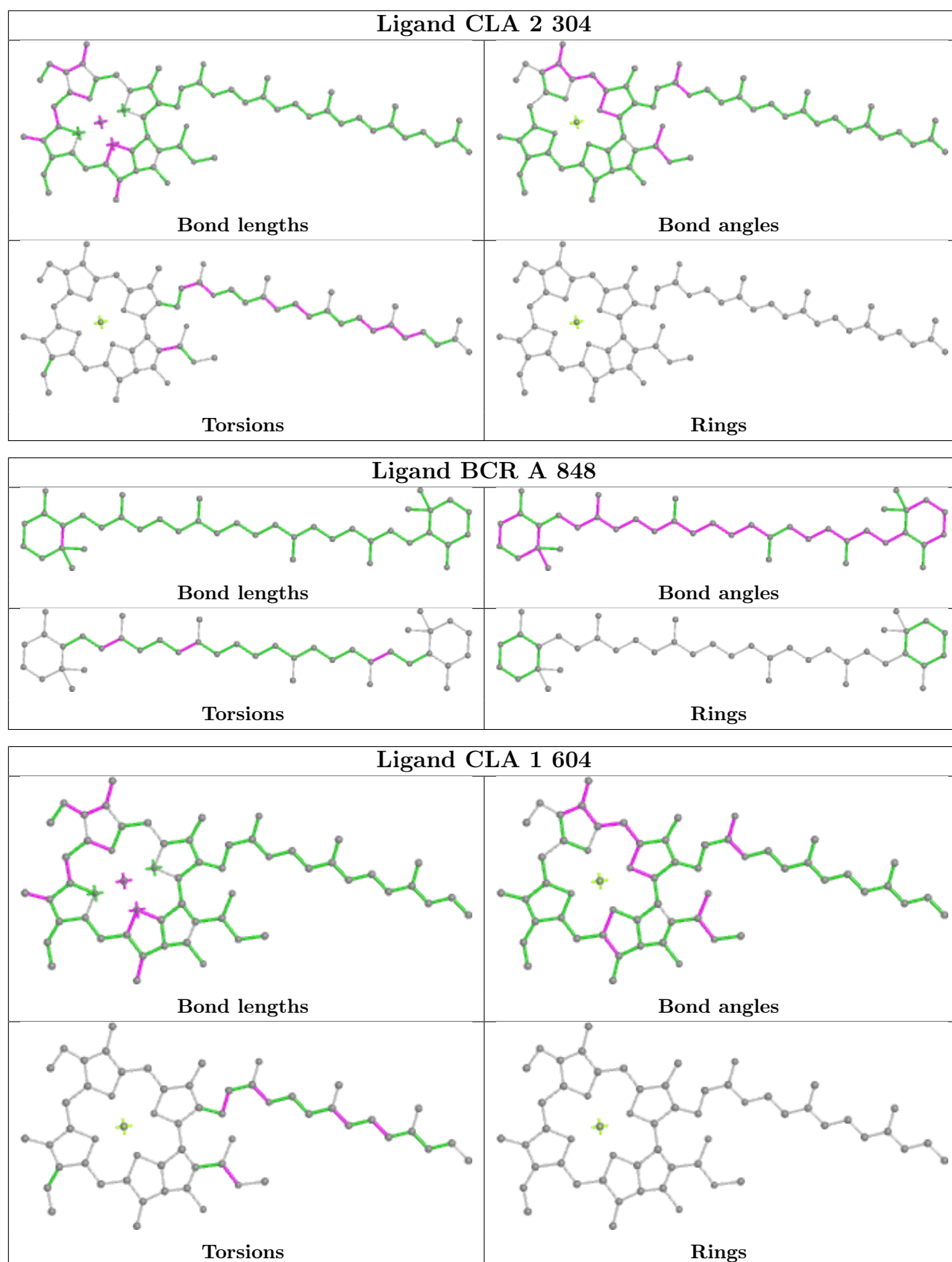


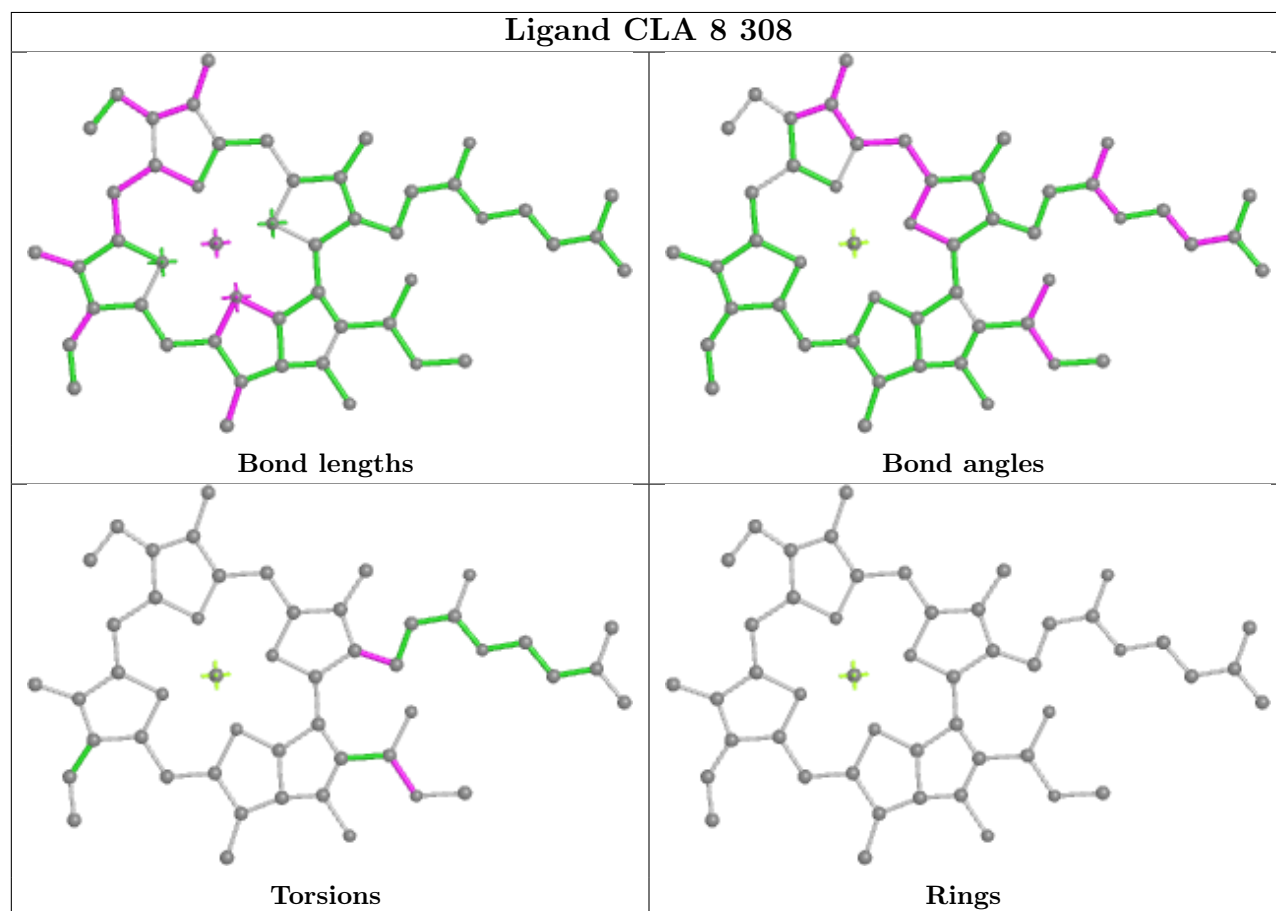
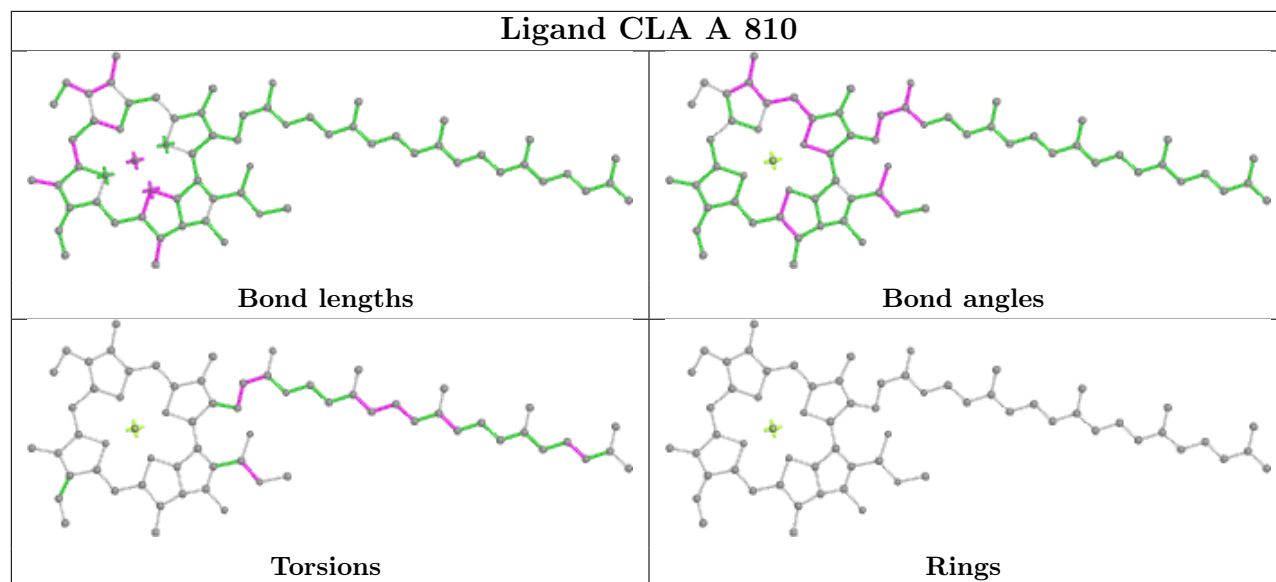


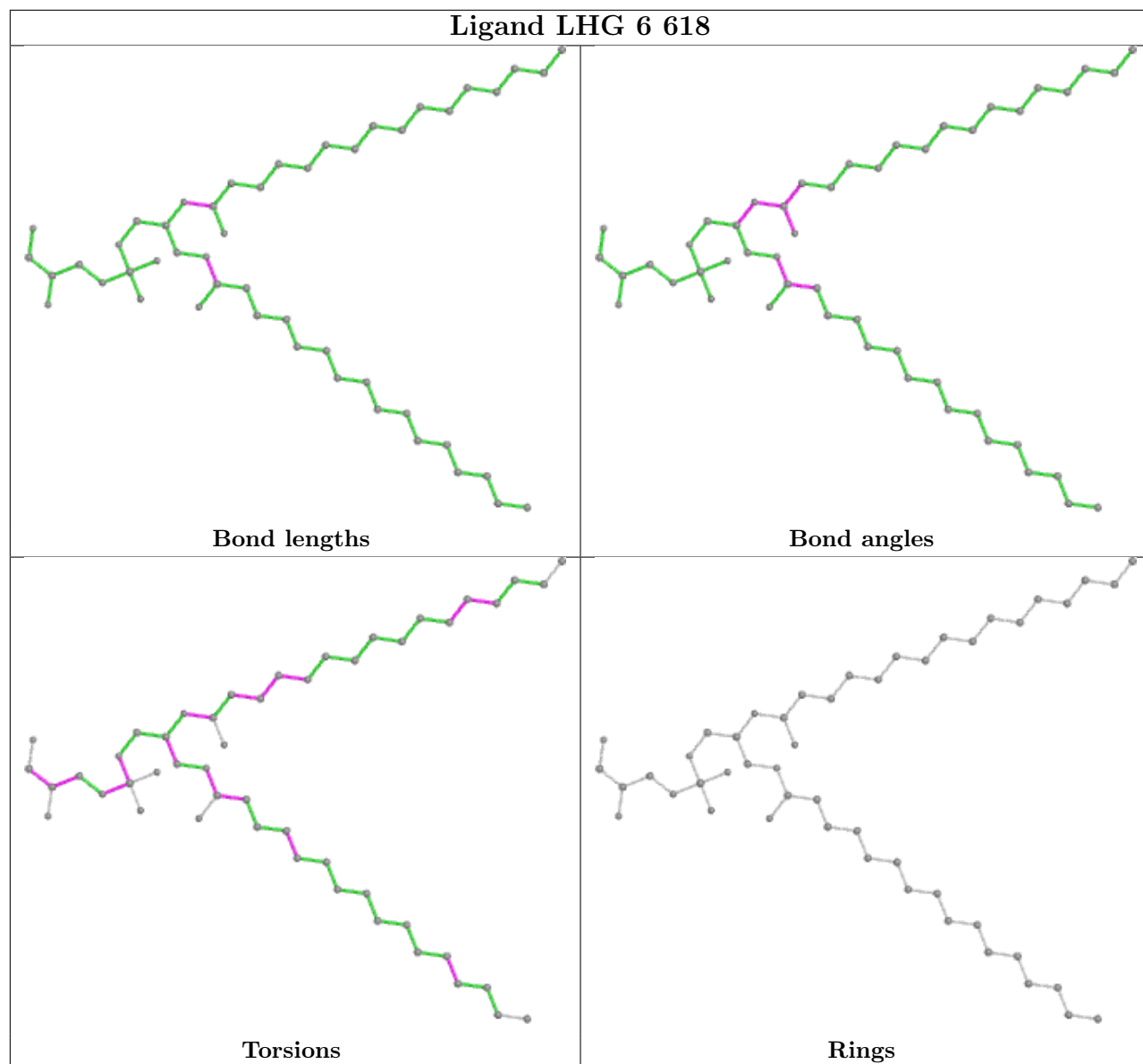


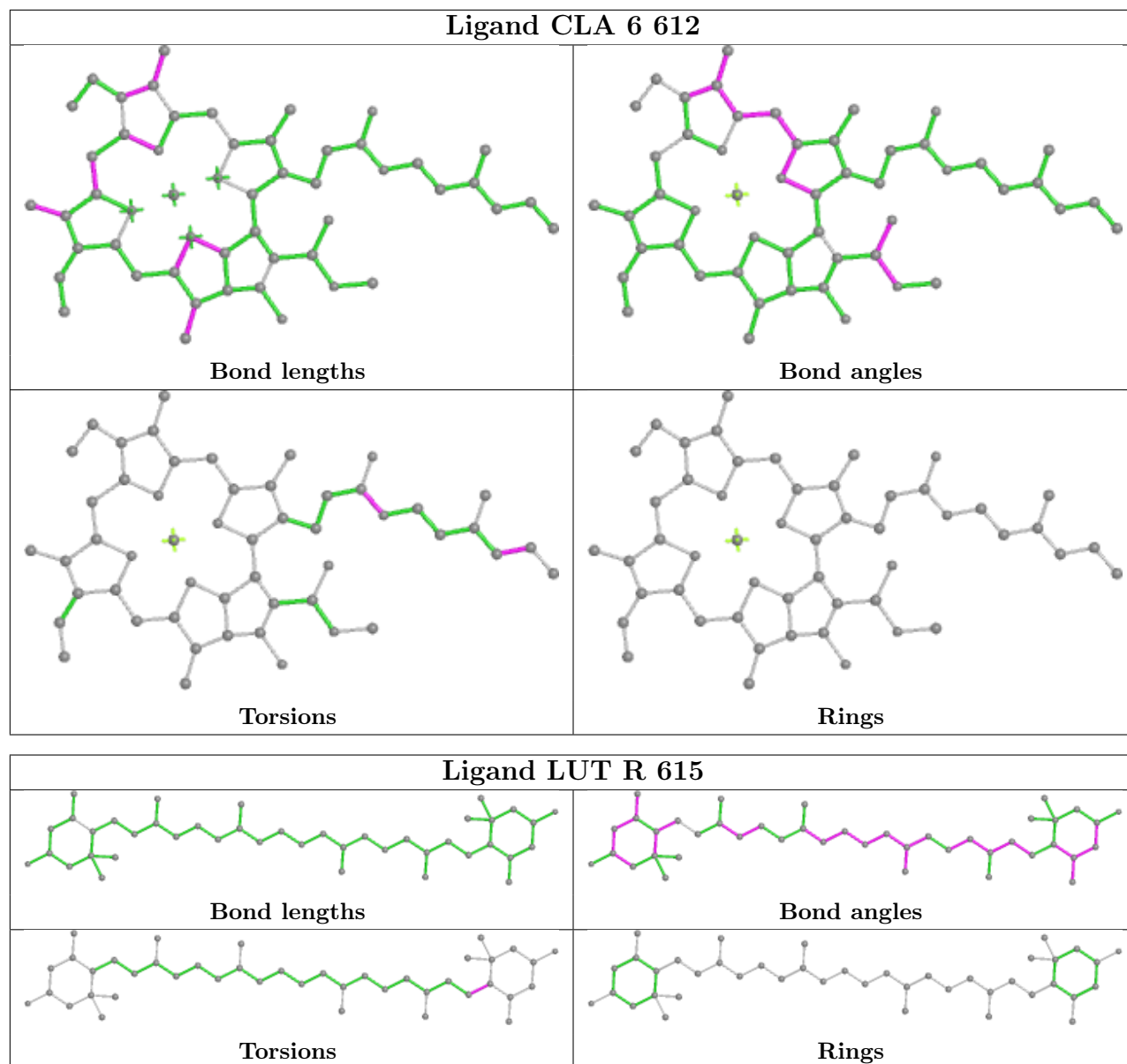


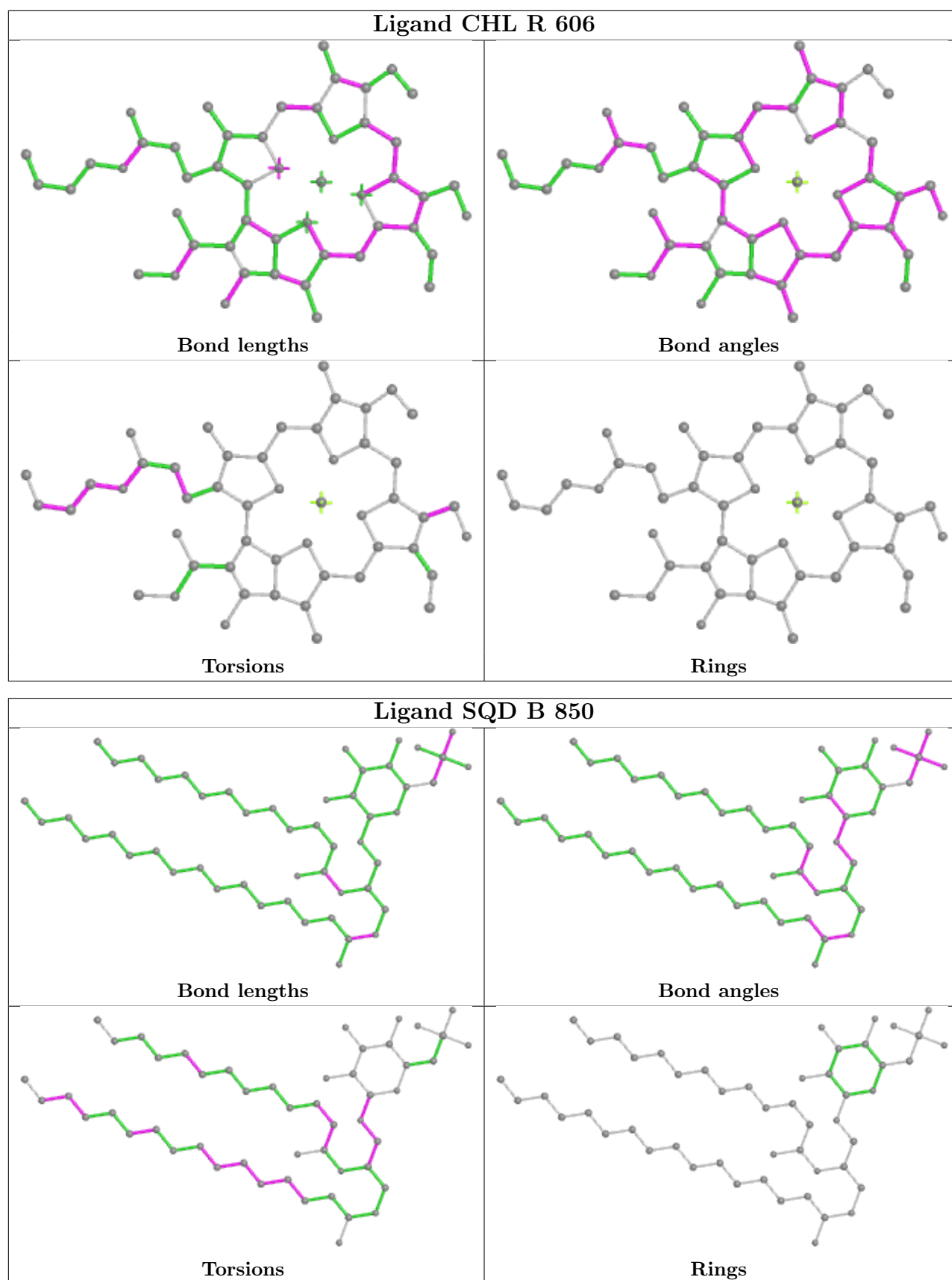


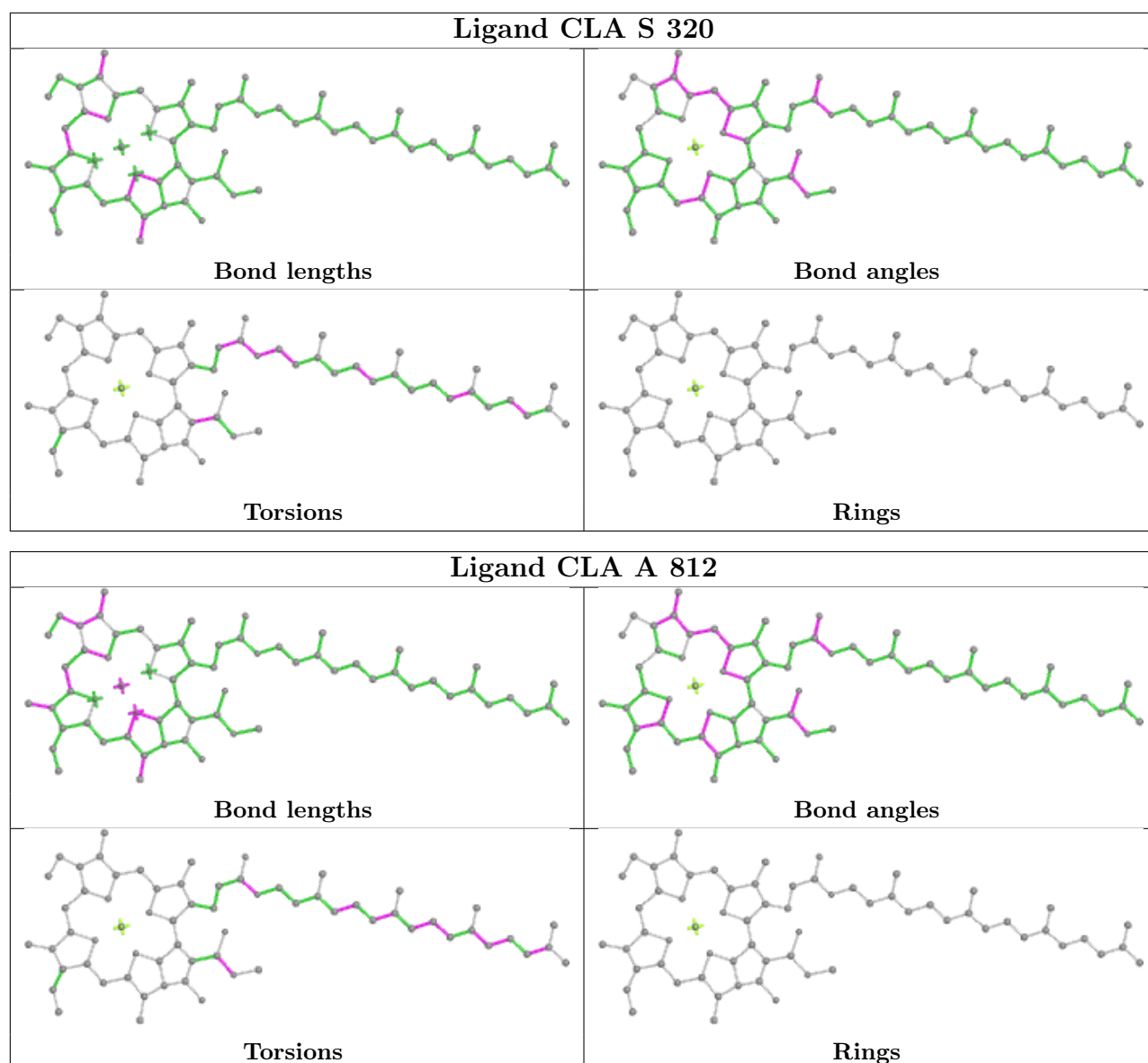


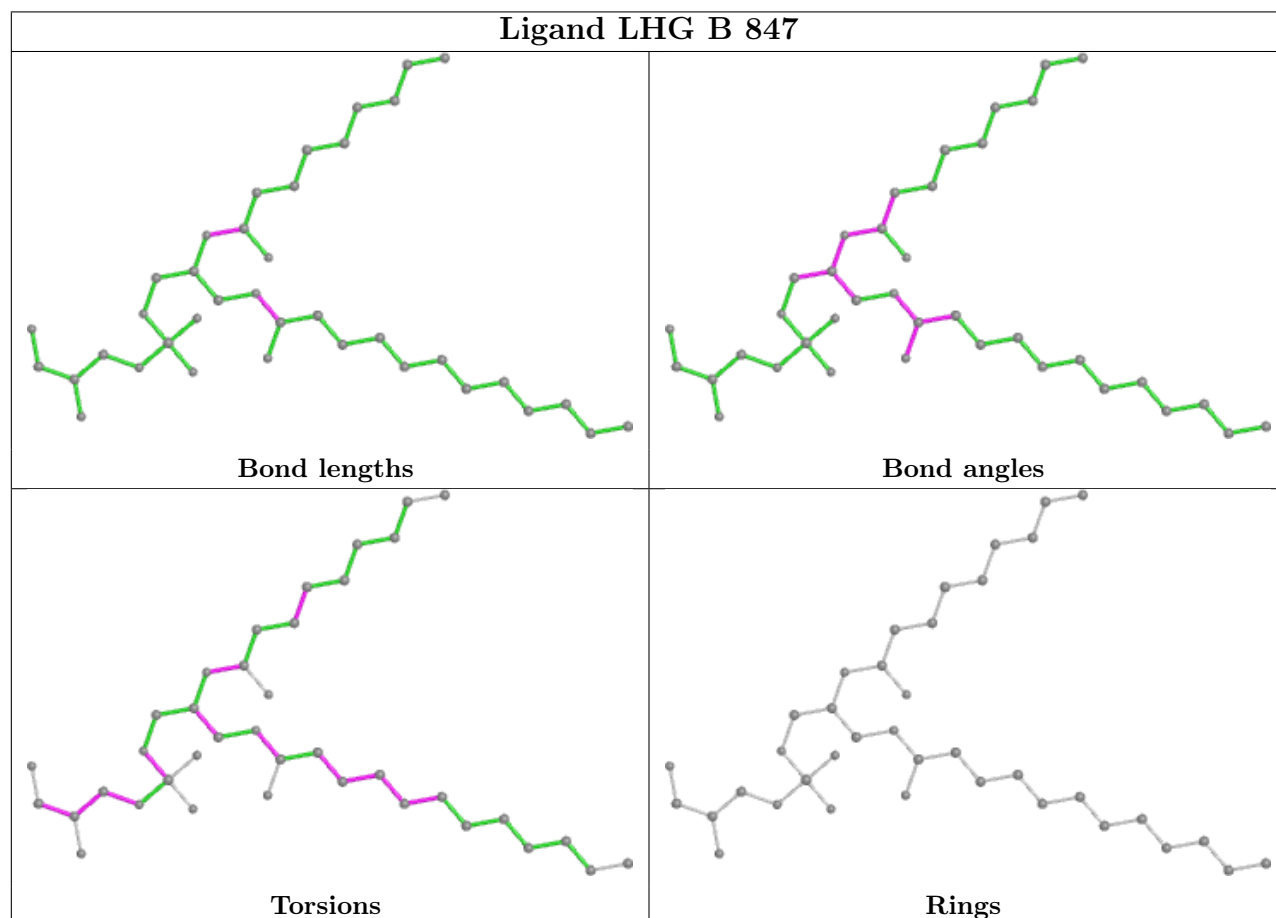
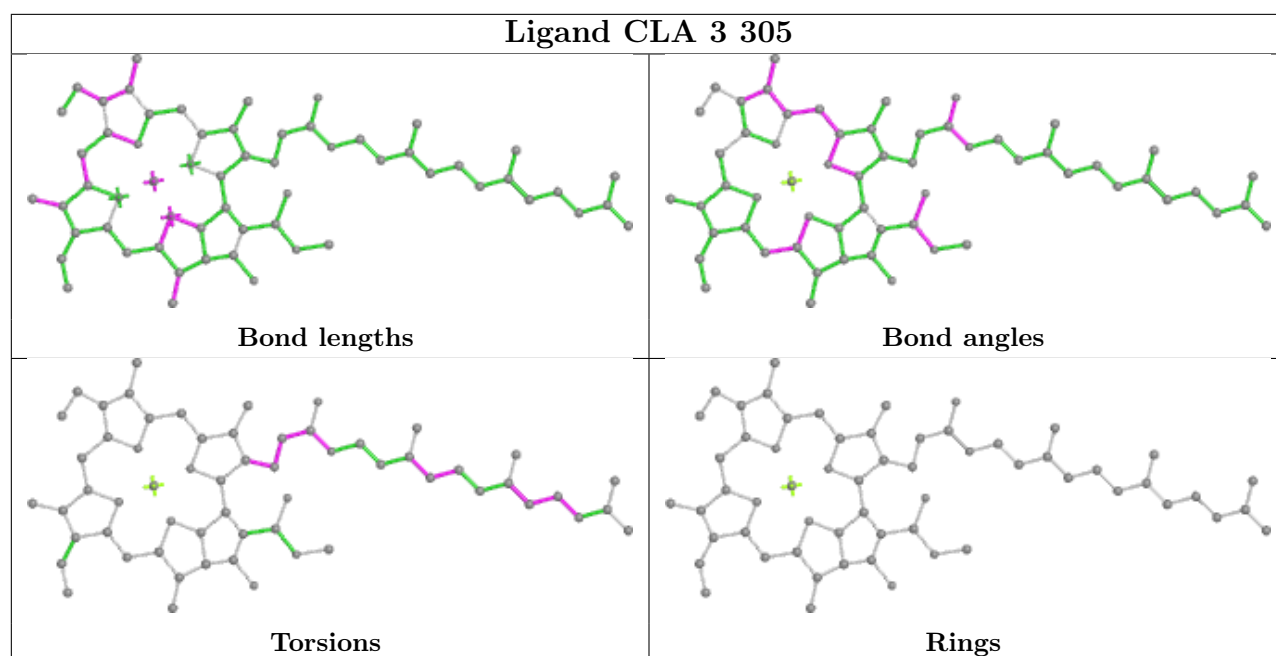


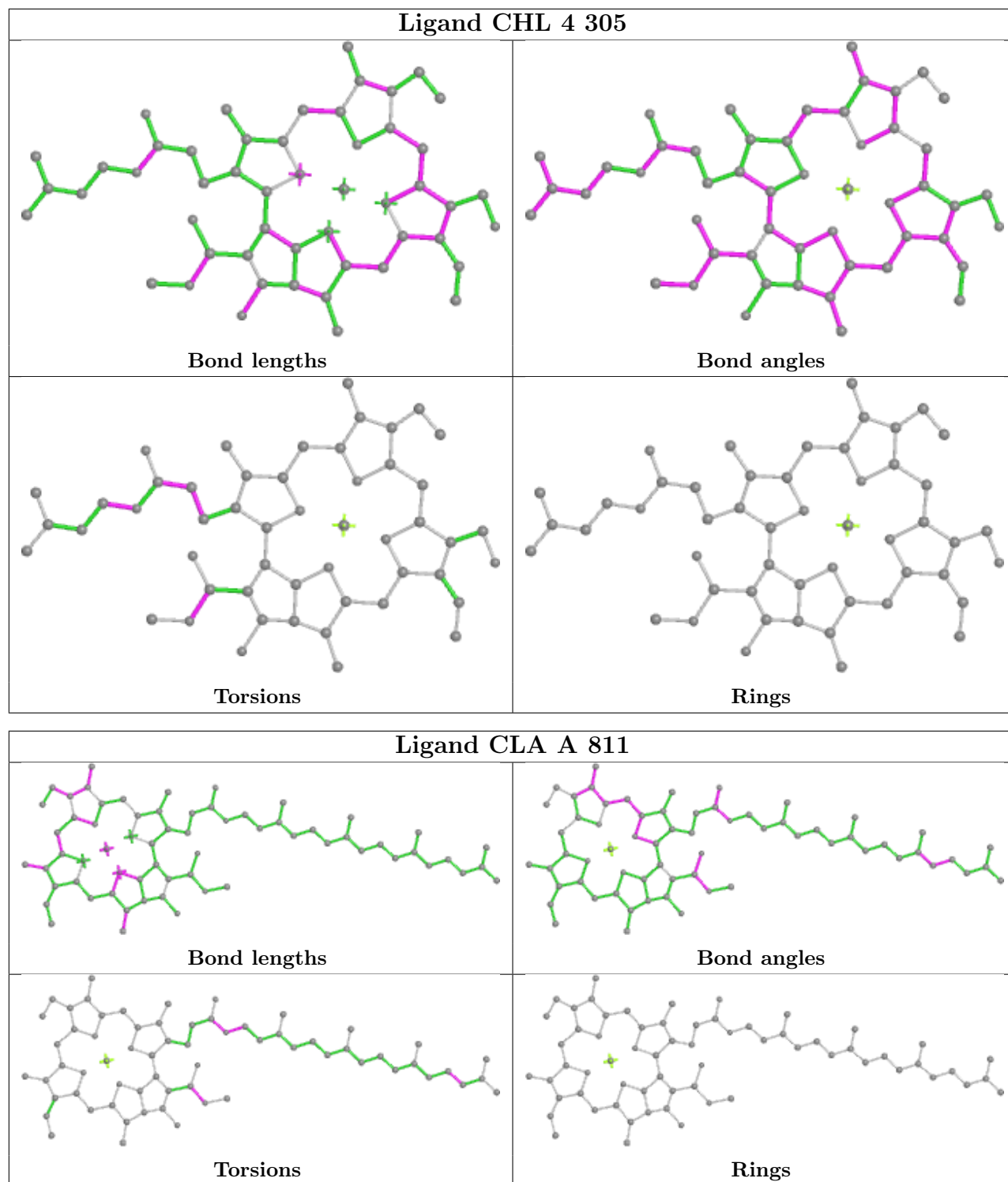


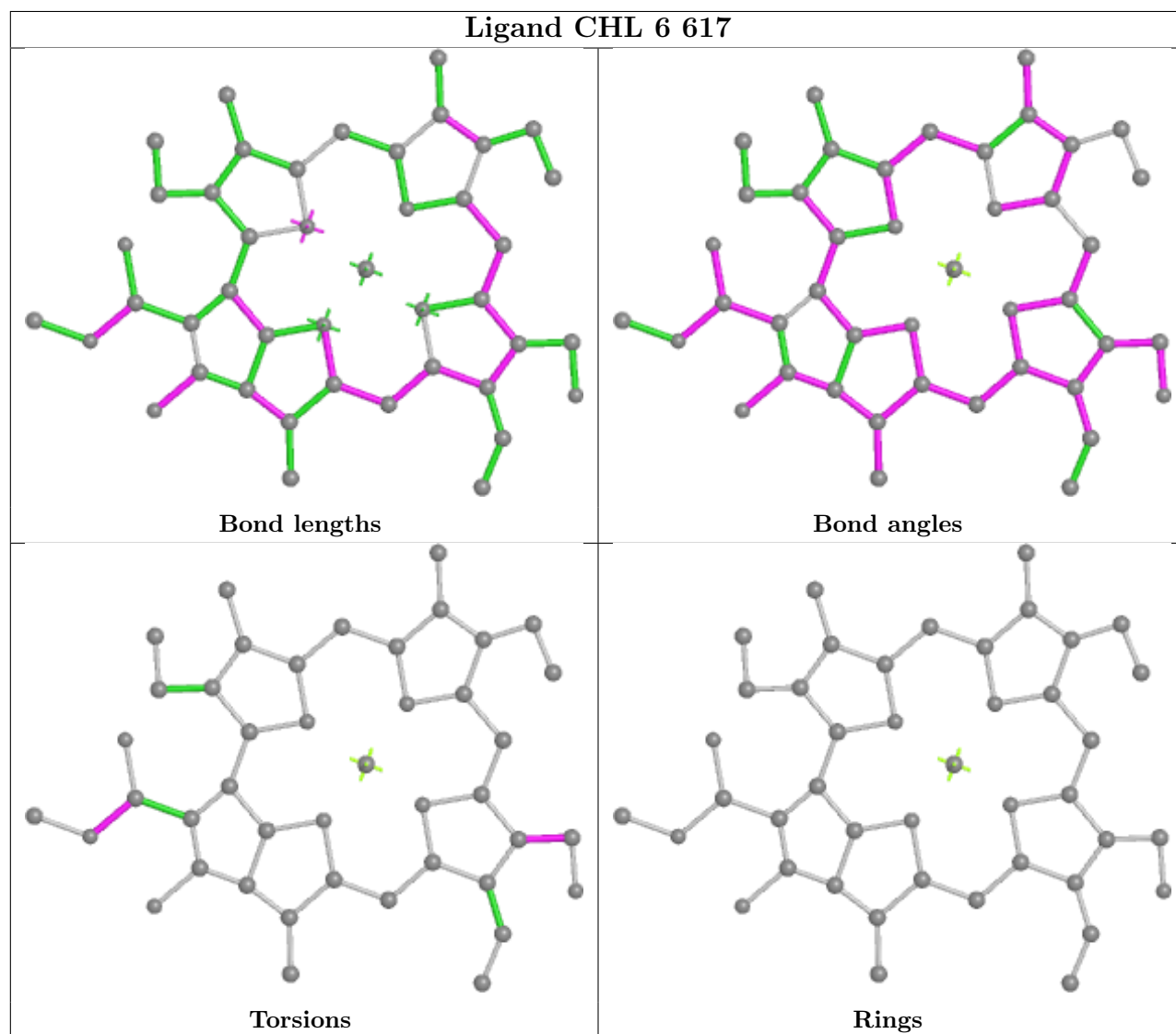
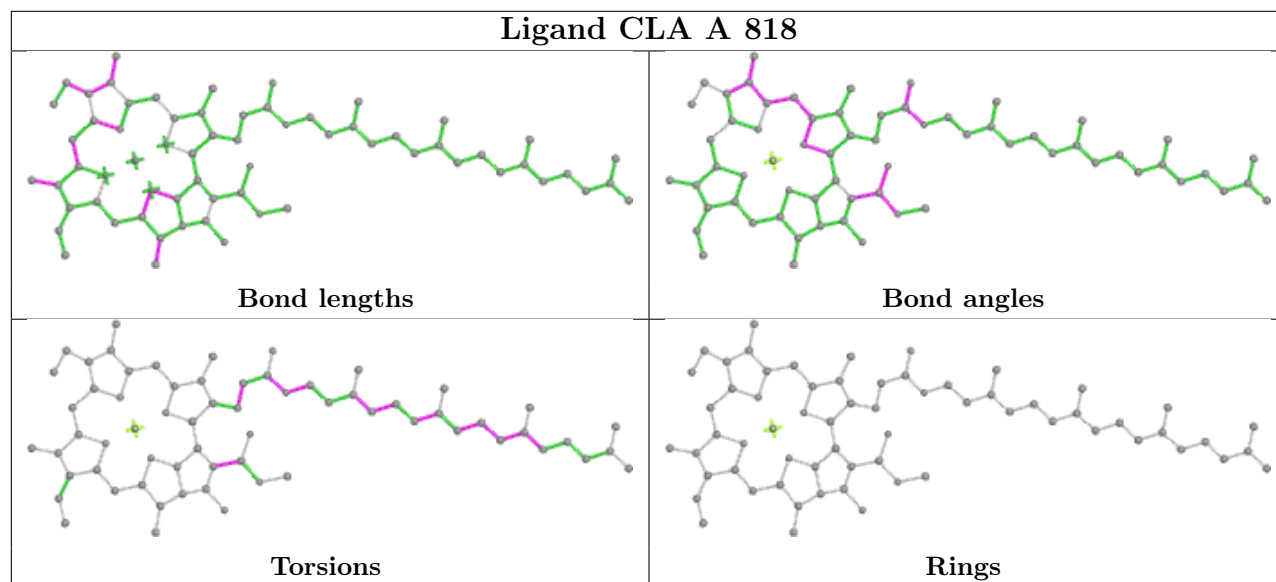


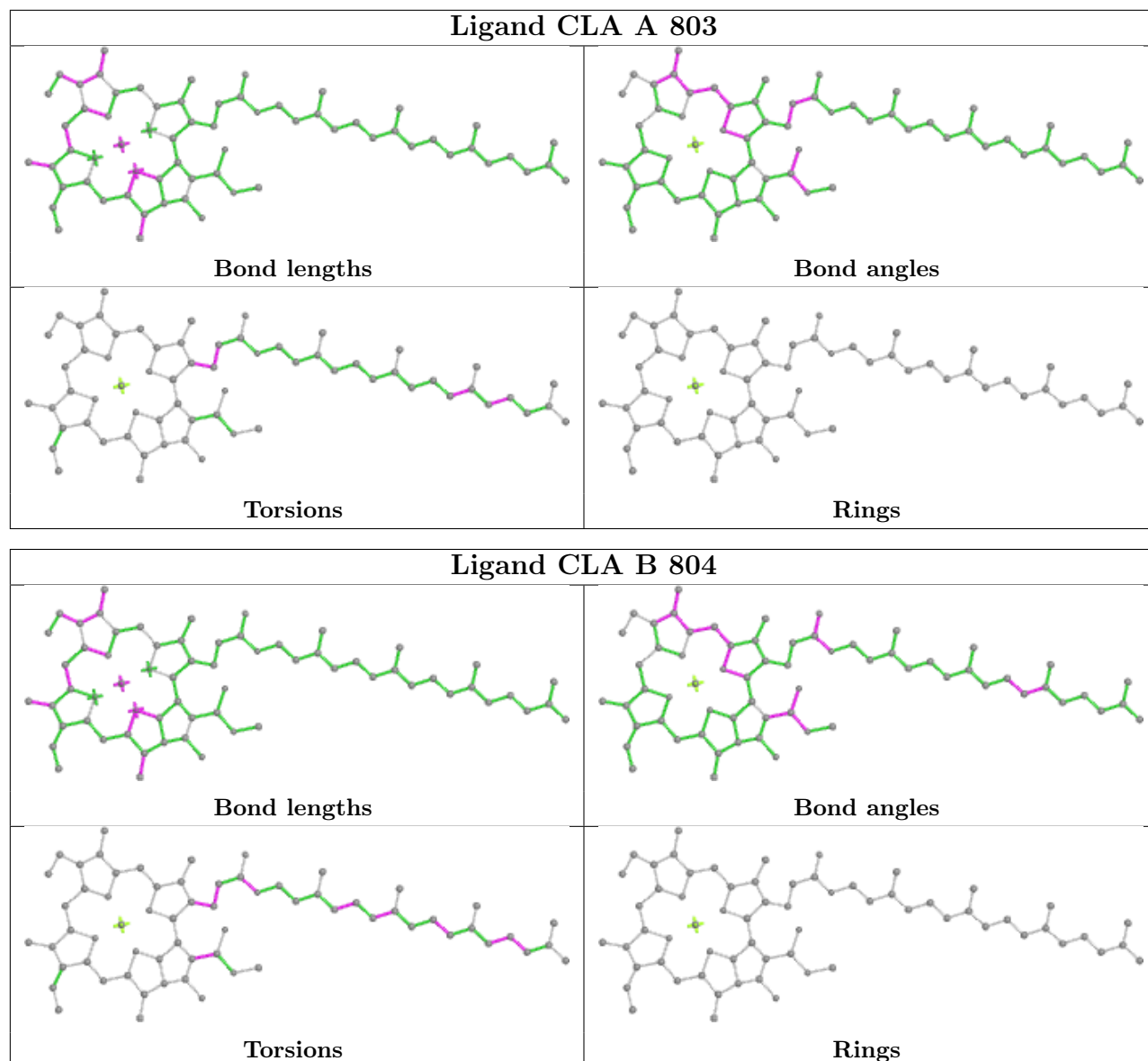


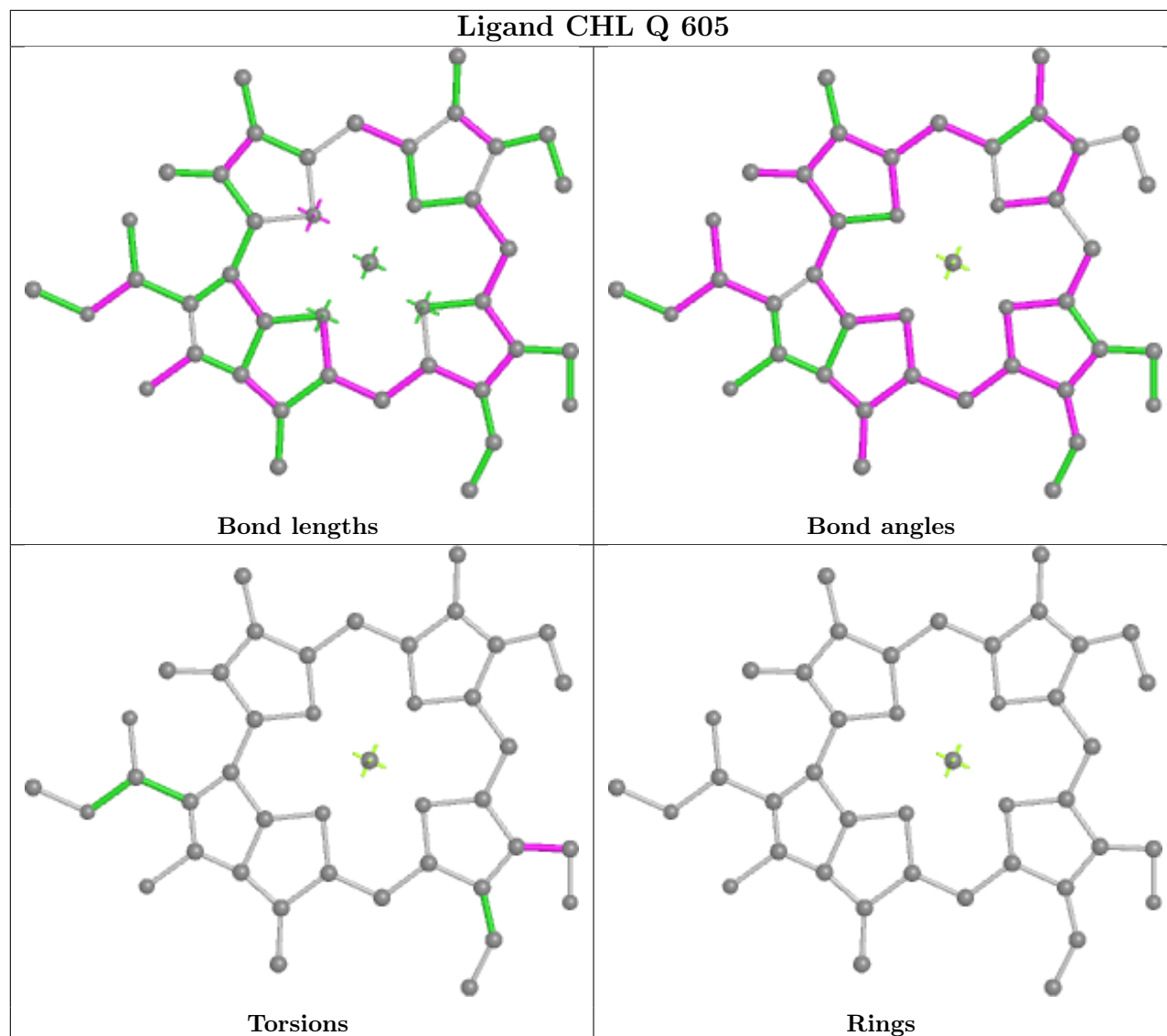


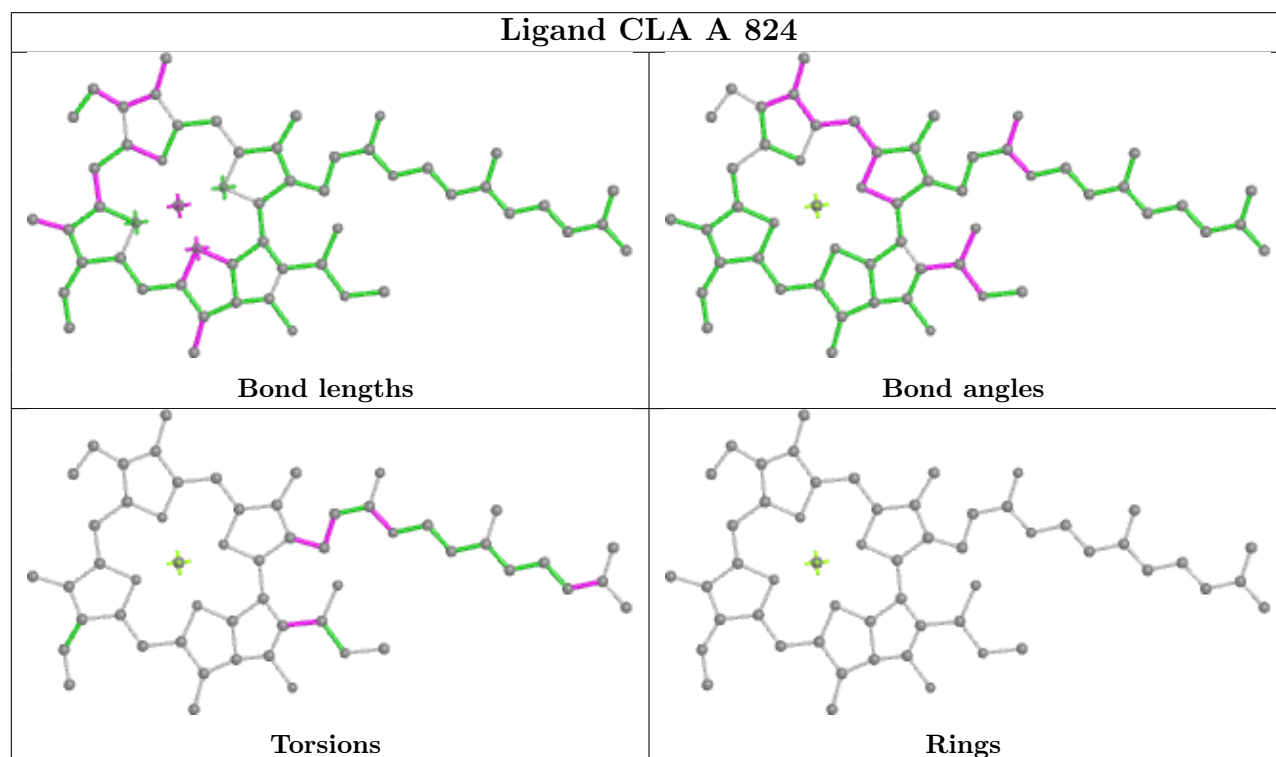
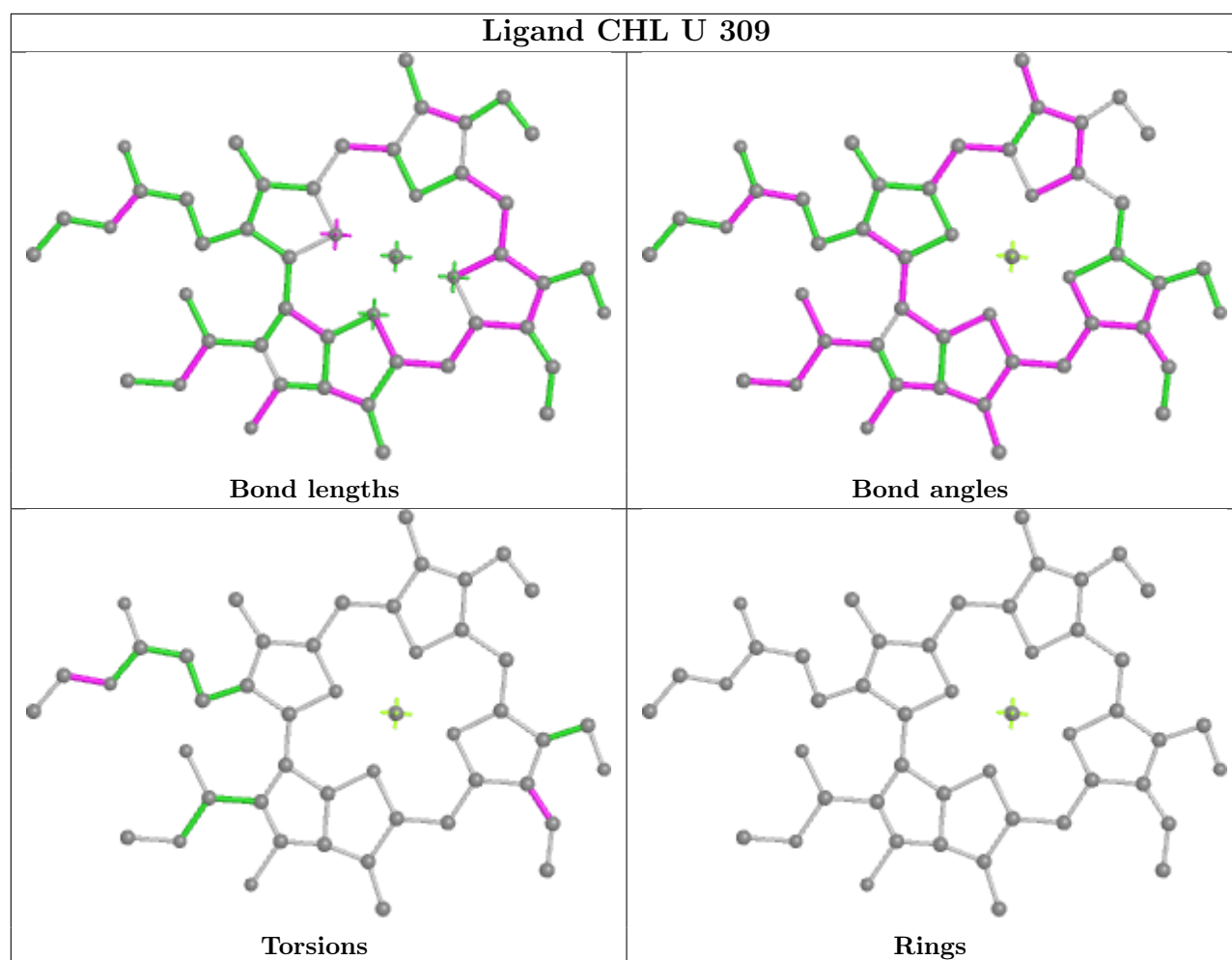


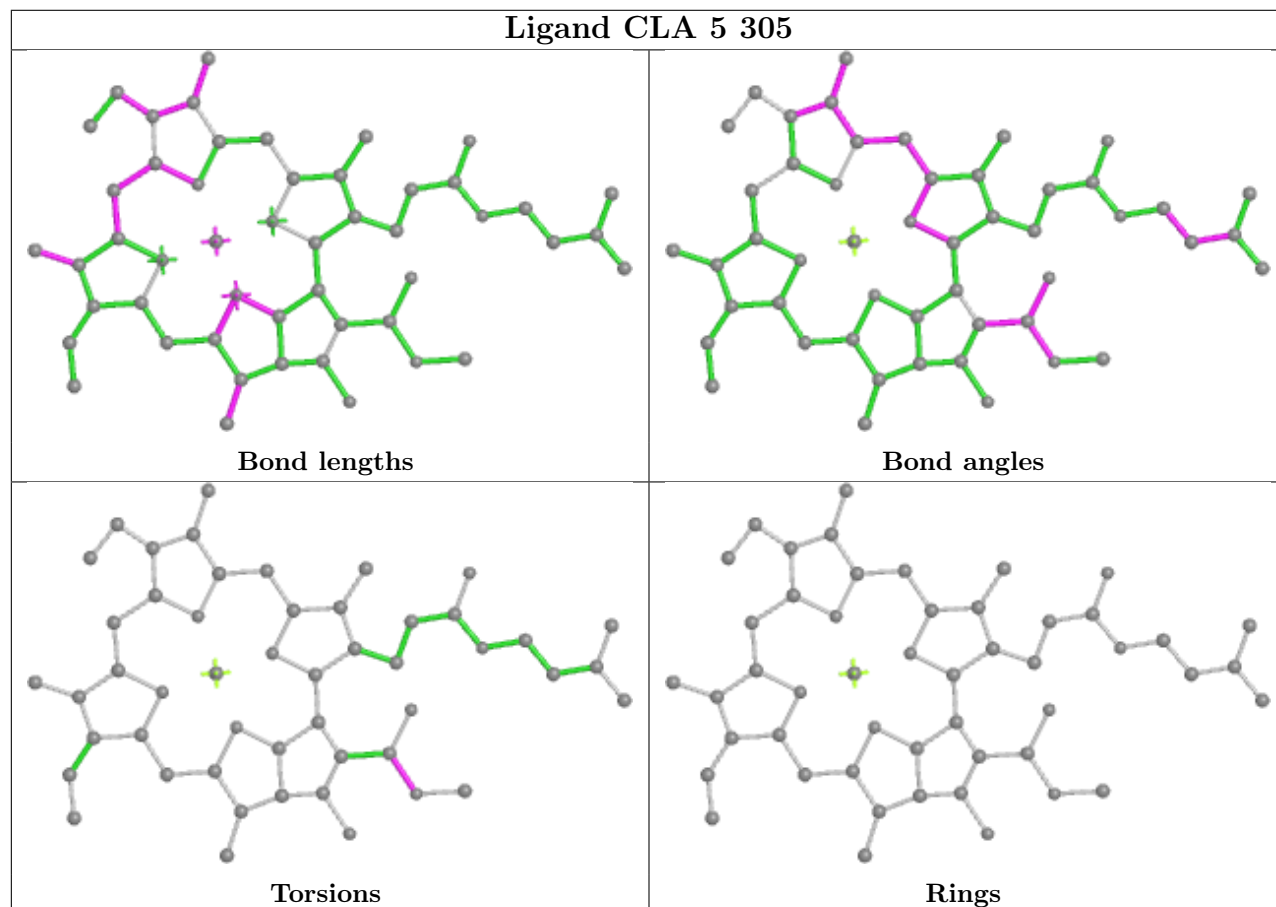
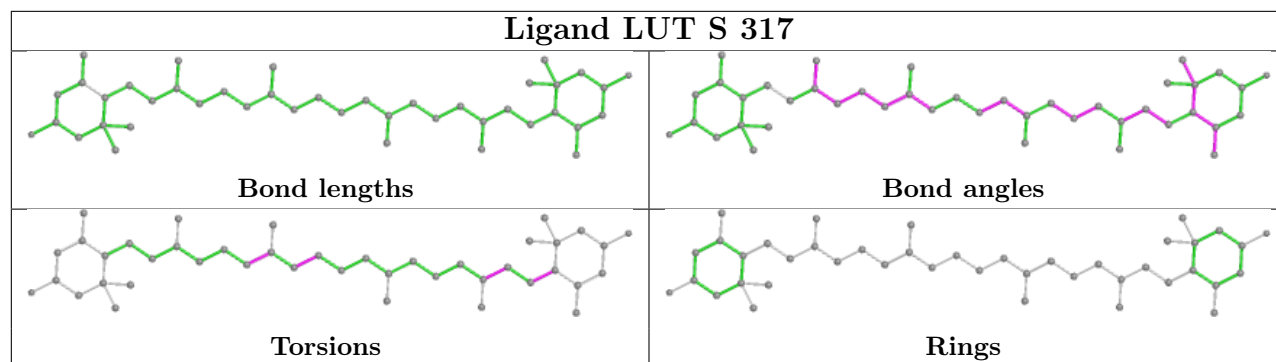
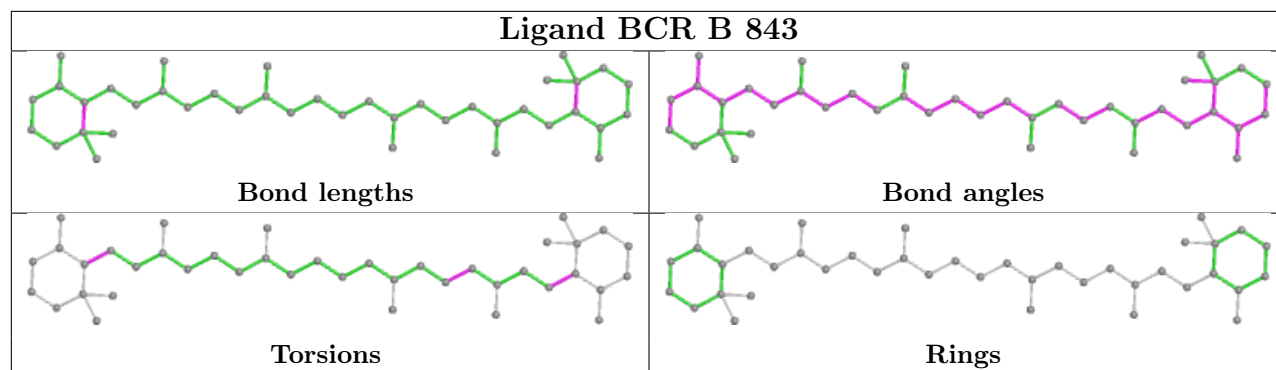












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

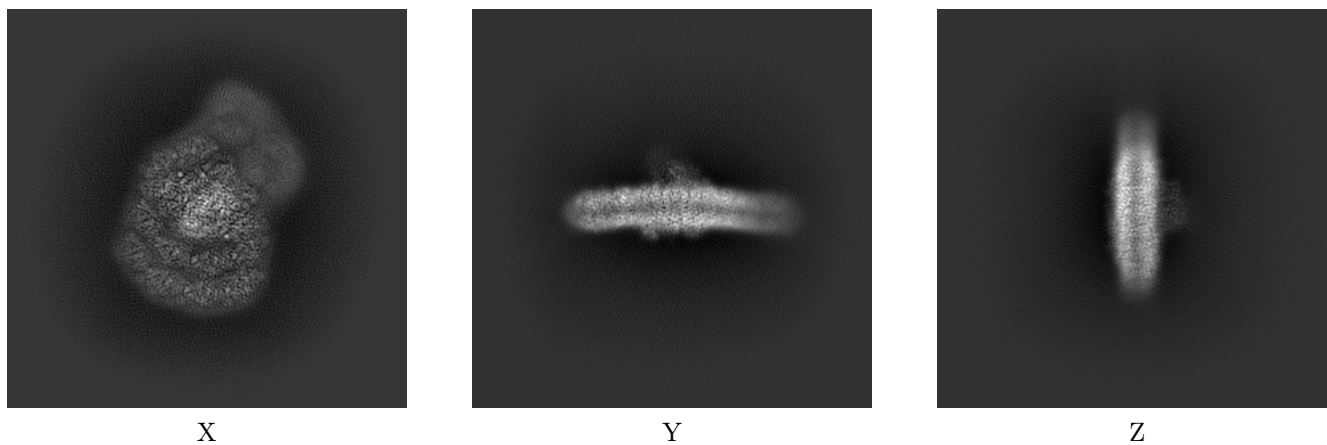
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-30536. These allow visual inspection of the internal detail of the map and identification of artifacts.

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

6.1 Orthogonal projections [i](#)

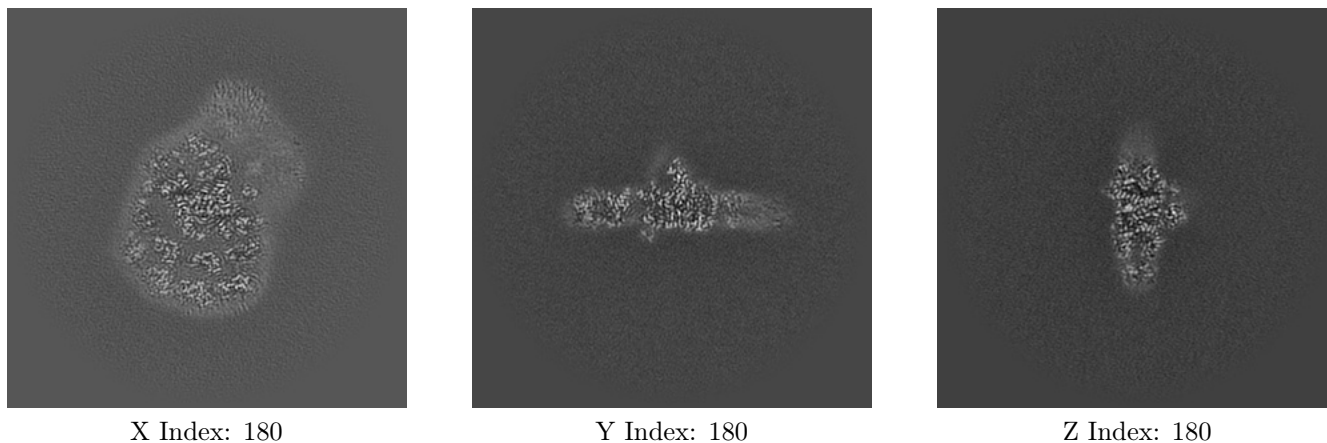
6.1.1 Primary map



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

6.2 Central slices [i](#)

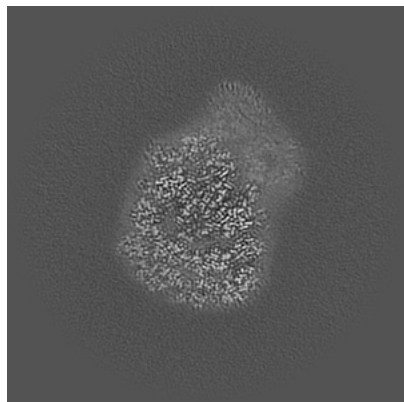
6.2.1 Primary map



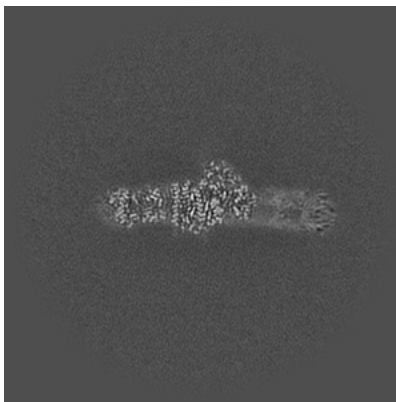
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

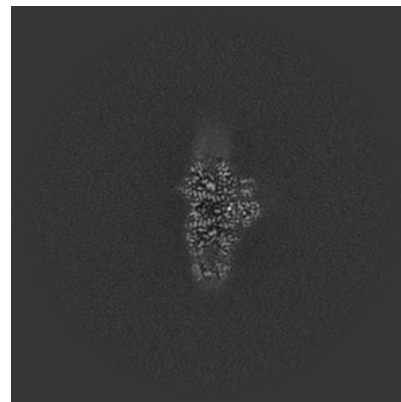
6.3.1 Primary map



X Index: 187



Y Index: 198



Z Index: 182

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

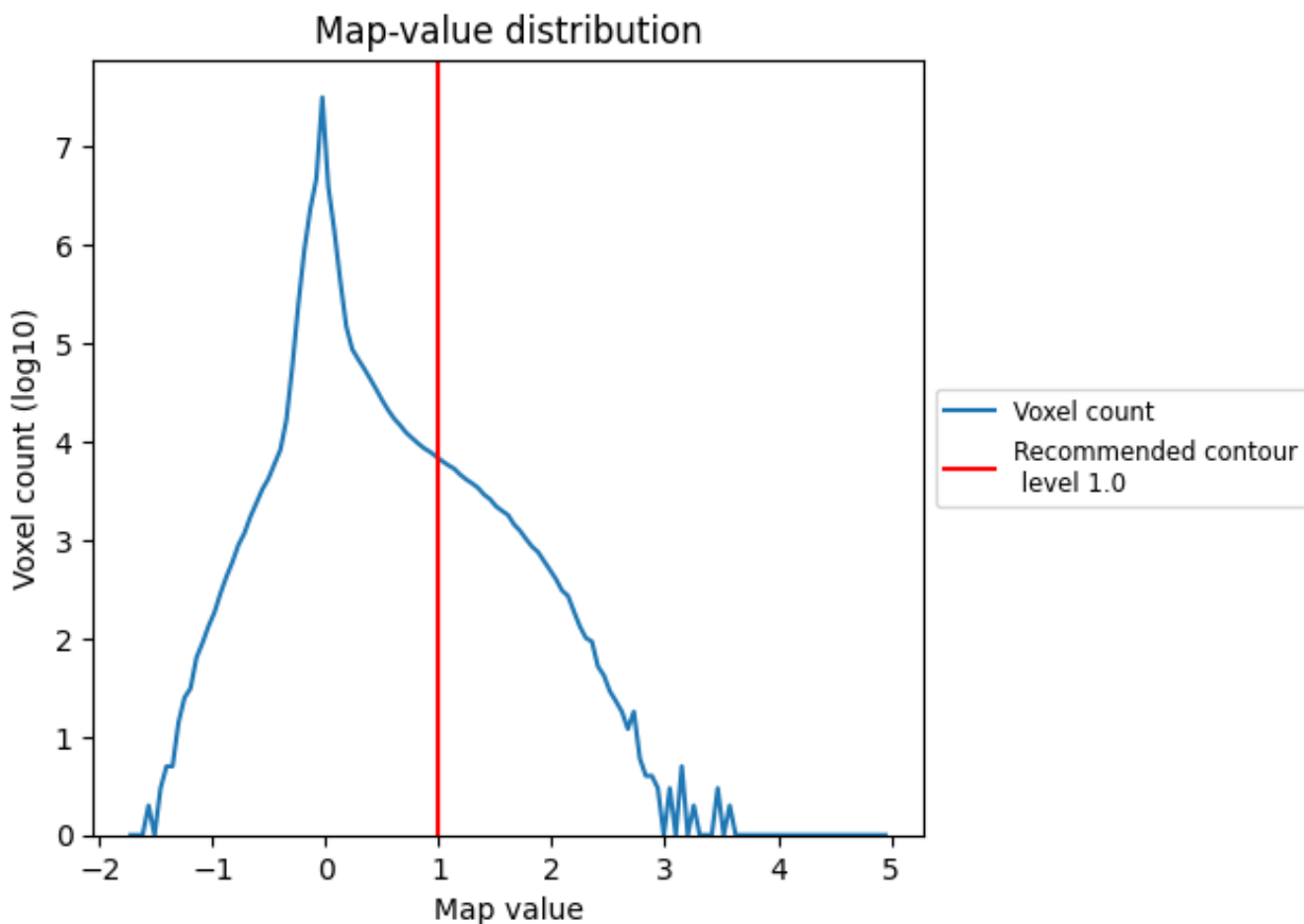
6.5 Mask visualisation

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

7 Map analysis [i](#)

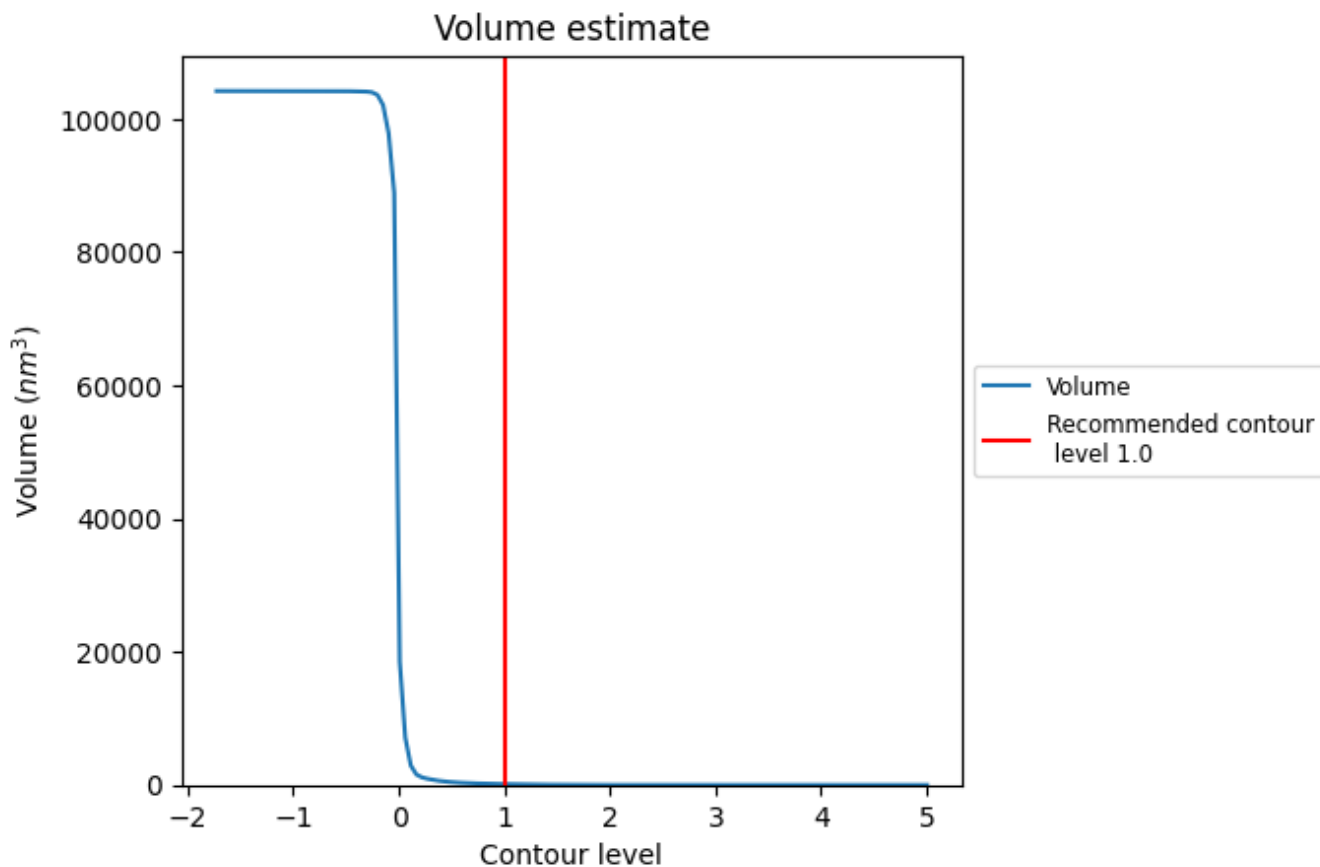
This section contains the results of statistical analysis of the map.

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.

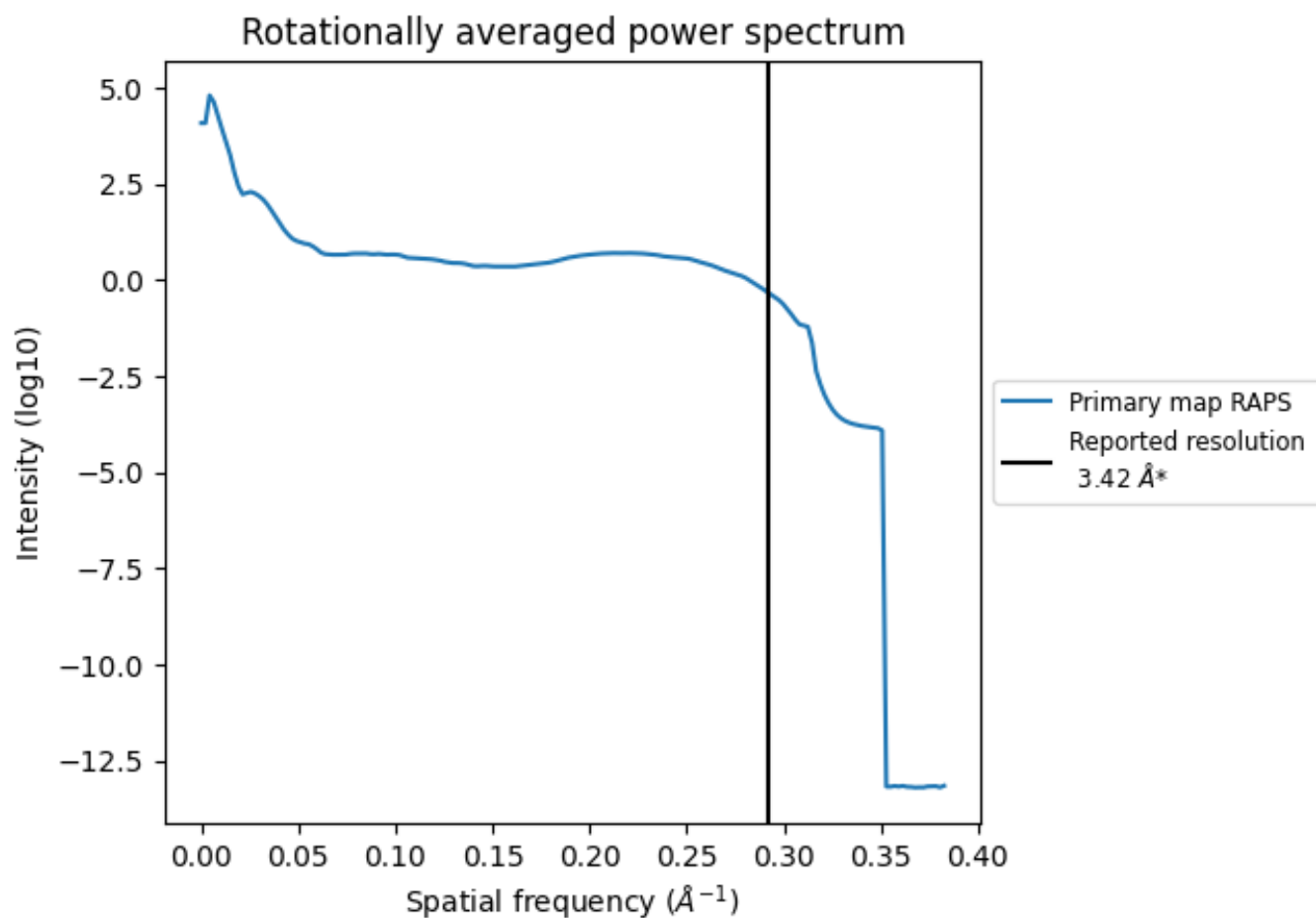
7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 128 nm³; this corresponds to an approximate mass of 115 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 0.292\AA^{-1}

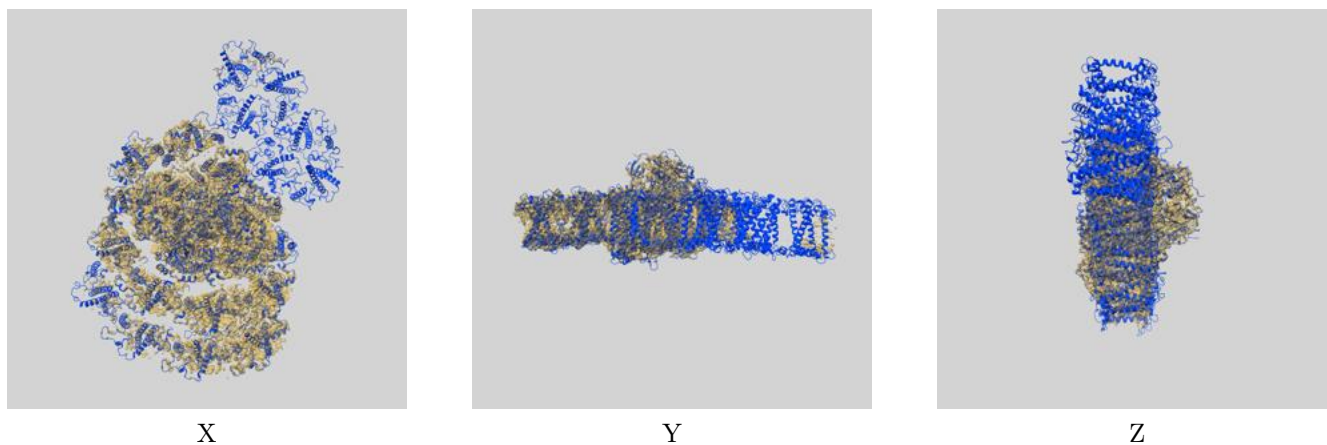
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

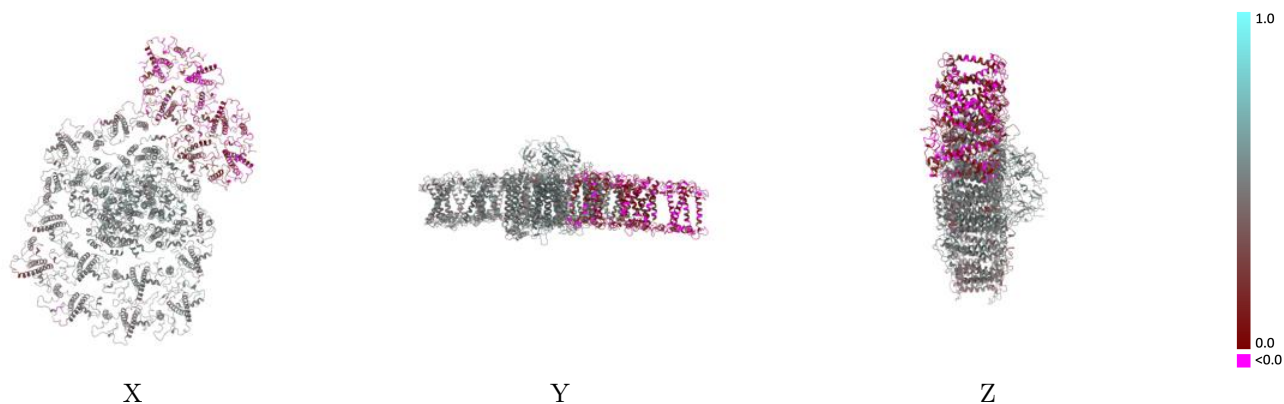
This section contains information regarding the fit between EMDB map EMD-30536 and PDB model 7D0J. Per-residue inclusion information can be found in section [3](#) on page [44](#).

9.1 Map-model overlay [i](#)



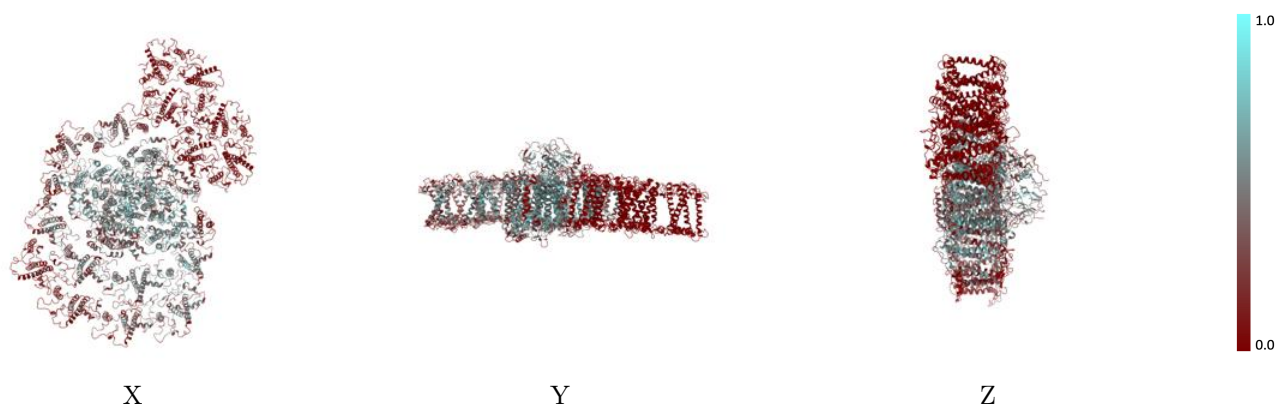
The images above show the 3D surface view of the map at the recommended contour level 1.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



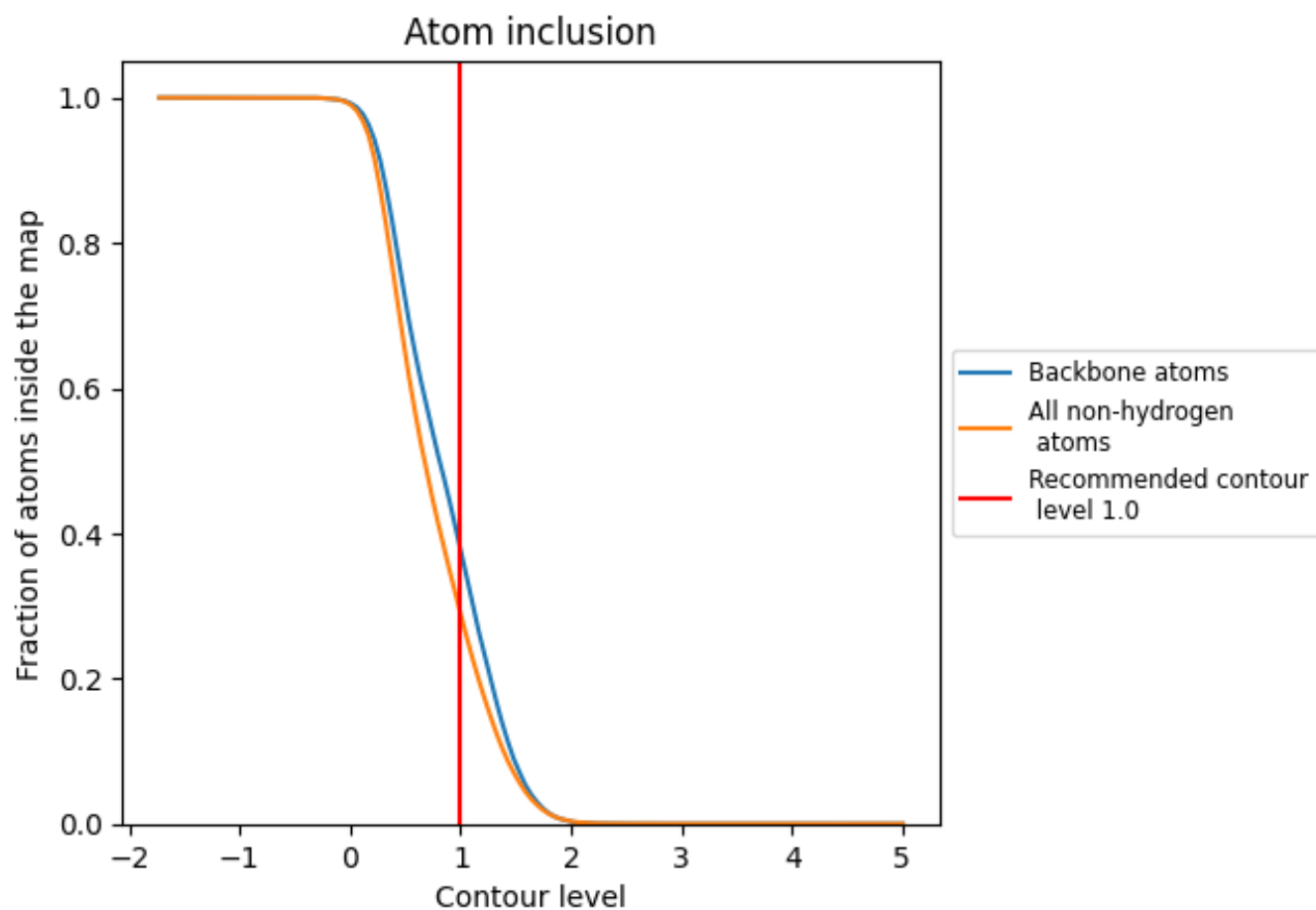
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (1.0).





























































9.4 Atom inclusion [i](#)



At the recommended contour level, 38% of all backbone atoms, 29% 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 (1.0) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.2895	 0.4070
1	 0.3153	 0.4760
2	 0.2701	 0.4450
3	 0.4267	 0.5110
4	 0.1245	 0.4380
5	 0.3906	 0.4980
6	 0.2671	 0.4690
7	 0.4372	 0.5110
8	 0.3667	 0.4930
9	 0.2294	 0.4440
A	 0.5312	 0.5300
B	 0.5205	 0.5290
C	 0.5714	 0.5210
D	 0.3739	 0.5140
E	 0.3706	 0.5020
F	 0.2698	 0.4750
G	 0.1380	 0.4410
H	 0.3034	 0.4750
I	 0.4734	 0.5110
J	 0.2902	 0.5190
K	 0.1582	 0.4560
L	 0.4356	 0.5030
O	 0.3058	 0.4670
P	 0.0000	 0.1620
Q	 0.0016	 0.0510
R	 0.0047	 0.0630
S	 0.0025	 0.2360
T	 0.0000	 0.1130
U	 0.0000	 0.1020
a	 0.0573	 0.3750

