



wwPDB EM Validation Summary Report ⓘ

Nov 16, 2022 – 01:20 PM JST

PDB ID : 6LY5
EMDB ID : EMD-30012
Title : Organization and energy transfer in a huge diatom PSI-FCPI supercomplex
Authors : Xiong, P.; Caizhe, X.
Deposited on : 2020-02-13
Resolution : 2.38 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:

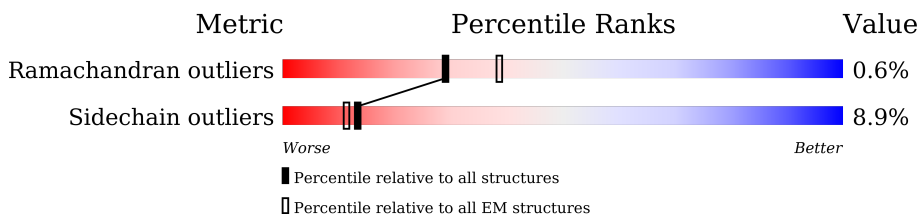
EMDB validation analysis : 0.0.1.dev43
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (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 2.38 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	168	95% 5%
2	B	223	54% 5% 41%
3	C	198	76% 7% 18%
4	D	207	74% 9% 17%
5	E	222	82% 15%
6	F	215	79% 5% 16%
7	G	245	76% 11% 13%
8	H	203	81% 16%
9	I	195	70% 13% 17%

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Mol	Chain	Length	Quality of chain
10	J	200	77% 6% 16%
11	K	207	80% 18%
12	L	229	6% 83% 14%
13	M	306	58% 39%
14	N	219	71% 90% 10%
15	O	205	13% 80% 16%
15	P	205	75% 9% 16%
15	Q	205	80% 16%
16	R	246	81% 14%
17	S	254	21% 78% 7% 13%
18	T	207	24% 81% 17%
19	W	198	32% 77% 19%
19	X	198	78% 77% 19%
20	a	743	91% 9%
21	b	733	89% 10%
22	c	80	90% 10%
23	d	132	85% 14%
24	e	63	97%
25	f	162	91% 9%
26	i	40	68% 15% 18%
27	j	42	79% 19%
28	l	172	72% 12% 16%
29	m	29	83% 14%
30	g	134	99%
31	h	139	53% 11% 36%

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Mol	Chain	Length	Quality of chain
32	U	160	
33	V	179	

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
36	CLA	A	305	X	-	-	-
36	CLA	A	306	X	-	-	-
36	CLA	A	307	X	-	-	-
36	CLA	A	308	X	-	-	-
36	CLA	A	309	X	-	-	-
36	CLA	A	310	X	-	-	-
36	CLA	A	311	X	-	-	-
36	CLA	A	313	X	-	-	-
36	CLA	A	314	X	-	-	-
36	CLA	B	305	X	-	-	-
36	CLA	B	306	X	-	-	-
36	CLA	B	307	X	-	-	-
36	CLA	B	308	X	-	-	-
36	CLA	B	309	X	-	-	-
36	CLA	B	311	X	-	-	-
36	CLA	C	205	X	-	-	-
36	CLA	C	206	X	-	-	-
36	CLA	C	207	X	-	-	-
36	CLA	C	208	X	-	-	-
36	CLA	C	209	X	-	-	-
36	CLA	C	210	X	-	-	-
36	CLA	C	211	X	-	-	-
36	CLA	C	212	X	-	-	-
36	CLA	C	214	X	-	-	-
36	CLA	D	306	X	-	-	-
36	CLA	D	307	X	-	-	-
36	CLA	D	308	X	-	-	-
36	CLA	D	309	X	-	-	-
36	CLA	D	310	X	-	-	-
36	CLA	D	312	X	-	-	-
36	CLA	D	313	X	-	-	-
36	CLA	D	315	X	-	-	-
36	CLA	D	316	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
36	CLA	D	317	X	-	-	-
36	CLA	E	308	X	-	-	-
36	CLA	E	311	X	-	-	-
36	CLA	E	312	X	-	-	-
36	CLA	E	313	X	-	-	-
36	CLA	E	314	X	-	-	-
36	CLA	E	315	X	-	-	-
36	CLA	E	316	X	-	-	-
36	CLA	E	317	X	-	-	-
36	CLA	F	309	X	-	-	-
36	CLA	F	310	X	-	-	-
36	CLA	F	311	X	-	-	-
36	CLA	F	312	X	-	-	-
36	CLA	F	313	X	-	-	-
36	CLA	F	314	X	-	-	-
36	CLA	F	316	X	-	-	-
36	CLA	F	317	X	-	-	-
36	CLA	G	309	X	-	-	-
36	CLA	G	310	X	-	-	-
36	CLA	G	311	X	-	-	-
36	CLA	G	312	X	-	-	-
36	CLA	G	313	X	-	-	-
36	CLA	G	314	X	-	-	-
36	CLA	G	315	X	-	-	-
36	CLA	G	316	X	-	-	-
36	CLA	G	319	X	-	-	-
36	CLA	H	305	X	-	-	-
36	CLA	H	306	X	-	-	-
36	CLA	H	307	X	-	-	-
36	CLA	H	308	X	-	-	-
36	CLA	H	309	X	-	-	-
36	CLA	H	310	X	-	-	-
36	CLA	H	311	X	-	-	-
36	CLA	H	312	X	-	-	-
36	CLA	H	314	X	-	-	-
36	CLA	H	315	X	-	-	-
36	CLA	H	316	X	-	-	-
36	CLA	H	317	X	-	-	-
36	CLA	H	318	X	-	-	-
36	CLA	I	305	X	-	-	-
36	CLA	I	306	X	-	-	-
36	CLA	I	307	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
36	CLA	I	308	X	-	-	-
36	CLA	I	309	X	-	-	-
36	CLA	I	310	X	-	-	-
36	CLA	I	311	X	-	-	-
36	CLA	I	312	X	-	-	-
36	CLA	I	313	X	-	-	-
36	CLA	I	314	X	-	-	-
36	CLA	J	307	X	-	-	-
36	CLA	J	309	X	-	-	-
36	CLA	J	310	X	-	-	-
36	CLA	J	311	X	-	-	-
36	CLA	J	312	X	-	-	-
36	CLA	J	313	X	-	-	-
36	CLA	J	315	X	-	-	-
36	CLA	J	316	X	-	-	-
36	CLA	J	317	X	-	-	-
36	CLA	K	307	X	-	-	-
36	CLA	K	308	X	-	-	-
36	CLA	K	309	X	-	-	-
36	CLA	K	310	X	-	-	-
36	CLA	K	311	X	-	-	-
36	CLA	K	312	X	-	-	-
36	CLA	K	313	X	-	-	-
36	CLA	K	315	X	-	-	-
36	CLA	K	316	X	-	-	-
36	CLA	L	308	X	-	-	-
36	CLA	L	309	X	-	-	-
36	CLA	L	310	X	-	-	-
36	CLA	L	311	X	-	-	-
36	CLA	L	313	X	-	-	-
36	CLA	L	314	X	-	-	-
36	CLA	L	316	X	-	-	-
36	CLA	L	320	X	-	-	-
36	CLA	M	306	X	-	-	-
36	CLA	M	307	X	-	-	-
36	CLA	M	308	X	-	-	-
36	CLA	M	309	X	-	-	-
36	CLA	M	310	X	-	-	-
36	CLA	M	311	X	-	-	-
36	CLA	M	312	X	-	-	-
36	CLA	M	314	X	-	-	-
36	CLA	M	316	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
36	CLA	N	307	X	-	-	-
36	CLA	N	308	X	-	-	-
36	CLA	N	309	X	-	-	-
36	CLA	N	310	X	-	-	-
36	CLA	N	311	X	-	-	-
36	CLA	N	312	X	-	-	-
36	CLA	N	313	X	-	-	-
36	CLA	N	316	X	-	-	-
36	CLA	N	317	X	-	-	-
36	CLA	N	318	X	-	-	-
36	CLA	N	319	X	-	-	-
36	CLA	O	306	X	-	-	-
36	CLA	O	307	X	-	-	-
36	CLA	O	308	X	-	-	-
36	CLA	O	309	X	-	-	-
36	CLA	O	310	X	-	-	-
36	CLA	O	311	X	-	-	-
36	CLA	O	314	X	-	-	-
36	CLA	O	316	X	-	-	-
36	CLA	P	301	X	-	-	-
36	CLA	P	308	X	-	-	-
36	CLA	P	309	X	-	-	-
36	CLA	P	310	X	-	-	-
36	CLA	P	311	X	-	-	-
36	CLA	P	312	X	-	-	-
36	CLA	P	313	X	-	-	-
36	CLA	P	316	X	-	-	-
36	CLA	P	318	X	-	-	-
36	CLA	P	319	X	-	-	-
36	CLA	Q	305	X	-	-	-
36	CLA	Q	306	X	-	-	-
36	CLA	Q	307	X	-	-	-
36	CLA	Q	308	X	-	-	-
36	CLA	Q	309	X	-	-	-
36	CLA	Q	312	X	-	-	-
36	CLA	Q	314	X	-	-	-
36	CLA	R	310	X	-	-	-
36	CLA	R	311	X	-	-	-
36	CLA	R	312	X	-	-	-
36	CLA	R	313	X	-	-	-
36	CLA	R	314	X	-	-	-
36	CLA	R	315	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
36	CLA	R	316	X	-	-	-
36	CLA	R	318	X	-	-	-
36	CLA	R	319	X	-	-	-
36	CLA	R	320	X	-	-	-
36	CLA	R	322	X	-	-	-
36	CLA	S	309	X	-	-	-
36	CLA	S	310	X	-	-	-
36	CLA	S	311	X	-	-	-
36	CLA	S	313	X	-	-	-
36	CLA	S	315	X	-	-	-
36	CLA	S	317	X	-	-	-
36	CLA	S	318	X	-	-	-
36	CLA	S	319	X	-	-	-
36	CLA	T	308	X	-	-	-
36	CLA	T	309	X	-	-	-
36	CLA	T	311	X	-	-	-
36	CLA	T	312	X	-	-	-
36	CLA	T	313	X	-	-	-
36	CLA	T	314	X	-	-	-
36	CLA	T	316	X	-	-	-
36	CLA	U	305	X	-	-	-
36	CLA	U	306	X	-	-	-
36	CLA	U	307	X	-	-	-
36	CLA	U	308	X	-	-	-
36	CLA	U	310	X	-	-	-
36	CLA	U	311	X	-	-	-
36	CLA	U	313	X	-	-	-
36	CLA	V	305	X	-	-	-
36	CLA	V	306	X	-	-	-
36	CLA	V	307	X	-	-	-
36	CLA	V	308	X	-	-	-
36	CLA	V	309	X	-	-	-
36	CLA	V	310	X	-	-	-
36	CLA	V	311	X	-	-	-
36	CLA	V	313	X	-	-	-
36	CLA	V	314	X	-	-	-
36	CLA	W	201	X	-	-	-
36	CLA	W	206	X	-	-	-
36	CLA	W	207	X	-	-	-
36	CLA	W	208	X	-	-	-
36	CLA	W	209	X	-	-	-
36	CLA	W	210	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
36	CLA	W	211	X	-	-	-
36	CLA	W	215	X	-	-	-
36	CLA	W	216	X	-	-	-
36	CLA	W	218	X	-	-	-
36	CLA	X	306	X	-	-	-
36	CLA	X	308	X	-	-	-
36	CLA	X	310	X	-	-	-
36	CLA	X	312	X	-	-	-
36	CLA	a	801	X	-	-	-
36	CLA	a	802	X	-	-	-
36	CLA	a	803	X	-	-	-
36	CLA	a	804	X	-	-	-
36	CLA	a	805	X	-	-	-
36	CLA	a	806	X	-	-	-
36	CLA	a	807	X	-	-	-
36	CLA	a	808	X	-	-	-
36	CLA	a	809	X	-	-	-
36	CLA	a	810	X	-	-	-
36	CLA	a	811	X	-	-	-
36	CLA	a	812	X	-	-	-
36	CLA	a	813	X	-	-	-
36	CLA	a	814	X	-	-	-
36	CLA	a	815	X	-	-	-
36	CLA	a	816	X	-	-	-
36	CLA	a	817	X	-	-	-
36	CLA	a	818	X	-	-	-
36	CLA	a	819	X	-	-	-
36	CLA	a	820	X	-	-	-
36	CLA	a	821	X	-	-	-
36	CLA	a	822	X	-	-	-
36	CLA	a	823	X	-	-	-
36	CLA	a	824	X	-	-	-
36	CLA	a	825	X	-	-	-
36	CLA	a	826	X	-	-	-
36	CLA	a	827	X	-	-	-
36	CLA	a	828	X	-	-	-
36	CLA	a	829	X	-	-	-
36	CLA	a	831	X	-	-	-
36	CLA	a	832	X	-	-	-
36	CLA	a	833	X	-	-	-
36	CLA	a	834	X	-	-	-
36	CLA	a	835	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
36	CLA	a	836	X	-	-	-
36	CLA	a	837	X	-	-	-
36	CLA	a	838	X	-	-	-
36	CLA	a	839	X	-	-	-
36	CLA	a	841	X	-	-	-
36	CLA	a	848	X	-	-	-
36	CLA	b	801	X	-	-	-
36	CLA	b	802	X	-	-	-
36	CLA	b	805	X	-	-	-
36	CLA	b	806	X	-	-	-
36	CLA	b	807	X	-	-	-
36	CLA	b	808	X	-	-	-
36	CLA	b	809	X	-	-	-
36	CLA	b	810	X	-	-	-
36	CLA	b	811	X	-	-	-
36	CLA	b	812	X	-	-	-
36	CLA	b	813	X	-	-	-
36	CLA	b	814	X	-	-	-
36	CLA	b	815	X	-	-	-
36	CLA	b	816	X	-	-	-
36	CLA	b	817	X	-	-	-
36	CLA	b	819	X	-	-	-
36	CLA	b	820	X	-	-	-
36	CLA	b	821	X	-	-	-
36	CLA	b	822	X	-	-	-
36	CLA	b	823	X	-	-	-
36	CLA	b	824	X	-	-	-
36	CLA	b	825	X	-	-	-
36	CLA	b	826	X	-	-	-
36	CLA	b	827	X	-	-	-
36	CLA	b	828	X	-	-	-
36	CLA	b	829	X	-	-	-
36	CLA	b	830	X	-	-	-
36	CLA	b	831	X	-	-	-
36	CLA	b	832	X	-	-	-
36	CLA	b	833	X	-	-	-
36	CLA	b	834	X	-	-	-
36	CLA	b	835	X	-	-	-
36	CLA	b	836	X	-	-	-
36	CLA	b	837	X	-	-	-
36	CLA	b	838	X	-	-	-
36	CLA	b	839	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
36	CLA	b	840	X	-	-	-
36	CLA	b	841	X	-	-	-
36	CLA	f	802	X	-	-	-
36	CLA	f	803	X	-	-	-
36	CLA	f	804	X	-	-	-
36	CLA	f	805	X	-	-	-
36	CLA	h	203	X	-	-	-
36	CLA	i	102	X	-	-	-
36	CLA	j	101	X	-	-	-
36	CLA	j	102	X	-	-	-
36	CLA	j	106	X	-	-	-
36	CLA	l	201	X	-	-	-
36	CLA	l	202	X	-	-	-
36	CLA	l	205	X	-	-	-
36	CLA	l	206	X	-	-	-

2 Entry composition [i](#)

There are 46 unique types of molecules in this entry. The entry contains 81344 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 FCPI-7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	168	1287	825	213	237	12	0	0

- Molecule 2 is a protein called FCPI-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	132	1013	662	166	176	9	0	0

- Molecule 3 is a protein called FCPI-11.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	163	1247	796	210	232	9	0	0

- Molecule 4 is a protein called FCPI-6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	D	172	1337	870	214	245	8	0	0

- Molecule 5 is a protein called FCPI-5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	E	188	1411	891	240	265	15	0	0

- Molecule 6 is a protein called FCPI-8.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	F	180	1375	880	230	253	12	0	0

- Molecule 7 is a protein called FCPI-4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	G	214	1668	1079	276	305	8	0	0

- Molecule 8 is a protein called FCPI-10.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	H	170	1291	832	213	236	10	0	0

- Molecule 9 is a protein called FCPI-3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	I	161	1250	807	208	228	7	0	0

- Molecule 10 is a protein called FCPI-9.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	J	167	1301	843	217	236	5	0	0

- Molecule 11 is a protein called FCPI-13.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	K	169	1304	850	214	232	8	0	0

- Molecule 12 is a protein called FCPI-14.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	L	196	1523	989	250	276	8	0	0

- Molecule 13 is a protein called FCPI-16.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	M	187	1423	914	248	255	6	0	0

- Molecule 14 is a protein called FCPI-21.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	219	Total	C	N	O	S	0	0
			1716	1119	282	309	6		

- Molecule 15 is a protein called FCPI.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	O	173	Total	C	N	O	S	0	0
			1302	837	216	241	8		
15	P	173	Total	C	N	O	S	0	0
			1296	834	213	241	8		
15	Q	173	Total	C	N	O	S	0	0
			1302	837	216	241	8		

- Molecule 16 is a protein called FCPI-24.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	R	211	Total	C	N	O	S	0	0
			1628	1061	266	294	7		

- Molecule 17 is a protein called FCPI-23.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	S	220	Total	C	N	O	S	0	0
			1722	1122	283	311	6		

- Molecule 18 is a protein called FCPI-12.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	T	172	Total	C	N	O	S	0	0
			1326	848	226	247	5		

- Molecule 19 is a protein called FCPI-17.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	W	160	Total	C	N	O	S	0	0
			1239	799	203	233	4		
19	X	161	Total	C	N	O	S	1	0
			1253	808	207	234	4		

- Molecule 20 is a protein called PsaA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
20	a	742	5858	3826	991	1013	28	0	0

- Molecule 21 is a protein called PsaB.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
21	b	732	5820	3828	980	994	18	1	0

- Molecule 22 is a protein called PsaC.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
22	c	80	597	368	104	114	11	0	0

- Molecule 23 is a protein called PsaD.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
23	d	132	1056	681	186	186	3	1	0

- Molecule 24 is a protein called PsaE.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
24	e	63	507	321	90	96	0	0

- Molecule 25 is a protein called PsaF.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
25	f	162	1223	789	211	220	3	0	0

- Molecule 26 is a protein called PsaI.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
26	i	33	256	176	40	38	2	0	0

- Molecule 27 is a protein called PsaJ.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	j	41	Total	C	N	O	S	0	0
			324	219	50	54	1		

- Molecule 28 is a protein called PsaL.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	l	144	Total	C	N	O	S	0	0
			1094	726	178	187	3		

- Molecule 29 is a protein called PsaM.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	m	28	Total	C	N	O	S	0	0
			198	130	32	34	2		

- Molecule 30 is a protein called PsaS.

Mol	Chain	Residues	Atoms				AltConf	Trace
30	g	134	Total	C	N	O	0	0
			670	402	134	134		

- Molecule 31 is a protein called PsaR.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	h	89	Total	C	N	O	S	0	0
			676	440	110	120	6		

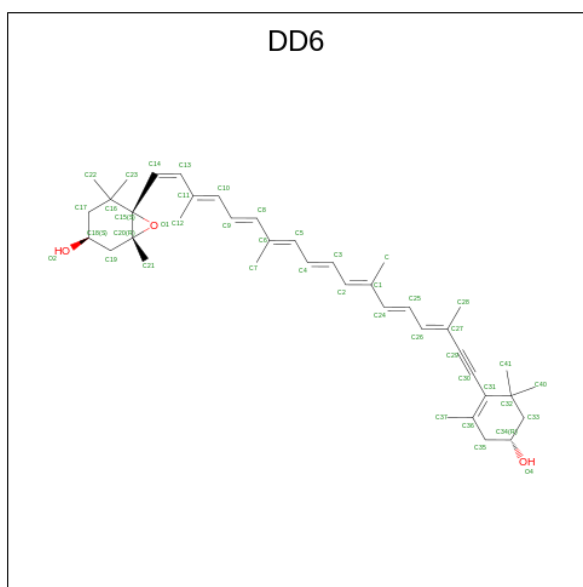
- Molecule 32 is a protein called FCPI-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	U	156	Total	C	N	O	S	0	0
			1194	766	199	221	8		

- Molecule 33 is a protein called FCPI-19.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	V	179	Total	C	N	O	S	0	0
			1361	871	234	252	4		

- Molecule 34 is (3S,3'R,5R,6S,7cis)-7',8'-didehydro-5,6-dihydro-5,6-epoxy-beta,beta-carotene -3,3'-diol (three-letter code: DD6) (formula: C₄₀H₅₄O₃).



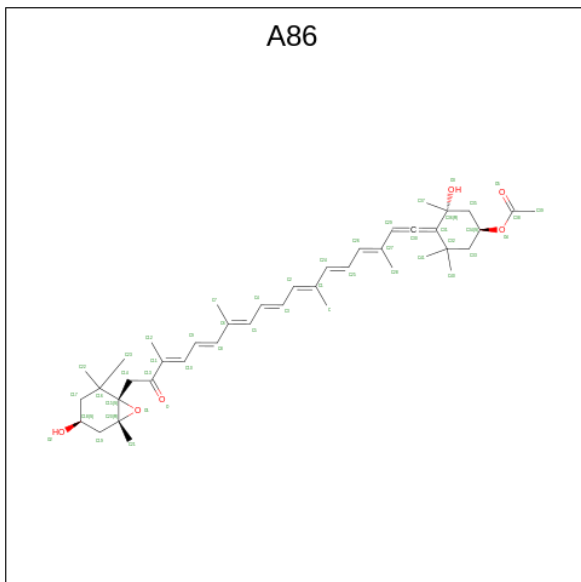
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
34	A	1	129	120	9	0
34	A	1	129	120	9	0
34	A	1	129	120	9	0
34	B	1	86	80	6	0
34	B	1	86	80	6	0
34	C	1	43	40	3	0
34	D	1	172	160	12	0
34	D	1	172	160	12	0
34	D	1	172	160	12	0
34	D	1	172	160	12	0
34	D	1	172	160	12	0
34	E	1	172	160	12	0
34	E	1	172	160	12	0
34	E	1	172	160	12	0
34	E	1	172	160	12	0

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Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
34	F	1	43	40	3	0
34	G	1	43	40	3	0
34	H	1	86	80	6	0
34	H	1	86	80	6	0
34	I	1	43	40	3	0
34	J	1	43	40	3	0
34	K	1	86	80	6	0
34	K	1	86	80	6	0
34	L	1	43	40	3	0
34	M	1	43	40	3	0
34	O	1	43	40	3	0
34	P	1	43	40	3	0
34	Q	1	43	40	3	0
34	R	1	86	80	6	0
34	R	1	86	80	6	0
34	S	1	86	80	6	0
34	S	1	86	80	6	0
34	W	1	86	80	6	0
34	W	1	86	80	6	0
34	a	1	43	40	3	0
34	j	1	43	40	3	0

- Molecule 35 is (3S,3'S,5R,5'R,6S,6'R,8'R)-3,5'-dihydroxy-8-oxo-6',7'-didehydro-5,5',6,6',7,8-hexahydro-5,6-epoxy-beta,beta-caroten-3'-yl acetate (three-letter code: A86) (formula: C₄₂H₅₈O₆).



Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
35	A	1	96	84	12	0
35	A	1	96	84	12	0
35	B	1	96	84	12	0
35	B	1	96	84	12	0
35	C	1	144	126	18	0
35	C	1	144	126	18	0
35	C	1	144	126	18	0
35	D	1	48	42	6	0
35	E	1	144	126	18	0
35	E	1	144	126	18	0
35	E	1	144	126	18	0
35	F	1	288	252	36	0

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Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
35	F	1	288	252	36	0
35	F	1	288	252	36	0
35	F	1	288	252	36	0
35	F	1	288	252	36	0
35	F	1	288	252	36	0
35	G	1	192	168	24	0
35	G	1	192	168	24	0
35	G	1	192	168	24	0
35	G	1	192	168	24	0
35	H	1	96	84	12	0
35	H	1	96	84	12	0
35	I	1	144	126	18	0
35	I	1	144	126	18	0
35	I	1	144	126	18	0
35	J	1	240	210	30	0
35	J	1	240	210	30	0
35	J	1	240	210	30	0
35	J	1	240	210	30	0
35	J	1	240	210	30	0
35	K	1	192	168	24	0
35	K	1	192	168	24	0

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Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
35	K	1	192	168	24	0
35	K	1	192	168	24	0
35	L	1	240	210	30	0
35	L	1	240	210	30	0
35	L	1	240	210	30	0
35	L	1	240	210	30	0
35	L	1	240	210	30	0
35	M	1	192	168	24	0
35	M	1	192	168	24	0
35	M	1	192	168	24	0
35	M	1	192	168	24	0
35	N	1	336	294	42	0
35	N	1	336	294	42	0
35	N	1	336	294	42	0
35	N	1	336	294	42	0
35	N	1	336	294	42	0
35	N	1	336	294	42	0
35	N	1	336	294	42	0
35	O	1	240	210	30	0
35	O	1	240	210	30	0
35	O	1	240	210	30	0

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Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
35	O	1	240	210	30	0
35	O	1	240	210	30	0
35	P	1	192	168	24	0
35	P	1	192	168	24	0
35	P	1	192	168	24	0
35	P	1	192	168	24	0
35	Q	1	192	168	24	0
35	Q	1	192	168	24	0
35	Q	1	192	168	24	0
35	Q	1	192	168	24	0
35	R	1	336	294	42	0
35	R	1	336	294	42	0
35	R	1	336	294	42	0
35	R	1	336	294	42	0
35	R	1	336	294	42	0
35	R	1	336	294	42	0
35	R	1	336	294	42	0
35	S	1	288	252	36	0
35	S	1	288	252	36	0
35	S	1	288	252	36	0
35	S	1	288	252	36	0

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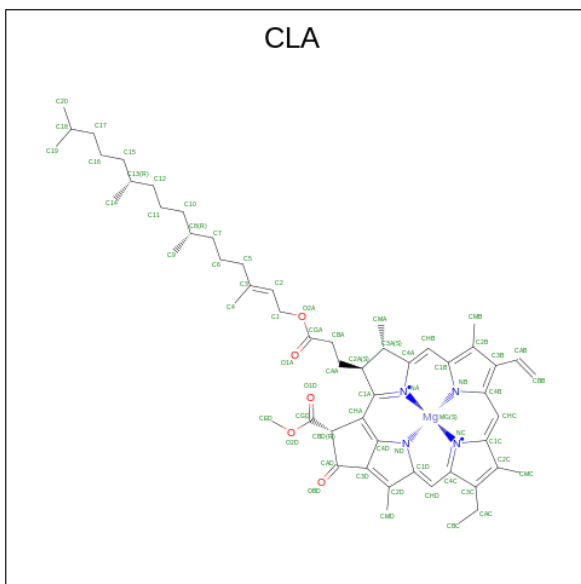
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
35	S	1	288	252	36	0
35	S	1	288	252	36	0
35	T	1	336	294	42	0
35	T	1	336	294	42	0
35	T	1	336	294	42	0
35	T	1	336	294	42	0
35	T	1	336	294	42	0
35	T	1	336	294	42	0
35	T	1	336	294	42	0
35	T	1	336	294	42	0
35	W	1	96	84	12	0
35	W	1	96	84	12	0
35	X	1	288	252	36	0
35	X	1	288	252	36	0
35	X	1	288	252	36	0
35	X	1	288	252	36	0
35	X	1	288	252	36	0
35	X	1	288	252	36	0
35	h	1	96	84	12	0
35	h	1	96	84	12	0
35	U	1	192	168	24	0
35	U	1	192	168	24	0

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Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
35	U	1	192	168	24	0
35	U	1	192	168	24	0
35	V	1	192	168	24	0
35	V	1	192	168	24	0
35	V	1	192	168	24	0
35	V	1	192	168	24	0

- Molecule 36 is CHLOROPHYLL A (three-letter code: CLA) (formula: $C_{55}H_{72}MgN_4O_5$).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
36	A	1	517	429	9	36	43	0
36	A	1	517	429	9	36	43	0
36	A	1	517	429	9	36	43	0
36	A	1	517	429	9	36	43	0
36	A	1	517	429	9	36	43	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
36	A	1	517	429	9	36	43	0
36	A	1	517	429	9	36	43	0
36	A	1	517	429	9	36	43	0
36	A	1	517	429	9	36	43	0
36	B	1	329	269	6	24	30	0
36	B	1	329	269	6	24	30	0
36	B	1	329	269	6	24	30	0
36	B	1	329	269	6	24	30	0
36	B	1	329	269	6	24	30	0
36	B	1	329	269	6	24	30	0
36	B	1	329	269	6	24	30	0
36	C	1	516	430	9	36	41	0
36	C	1	516	430	9	36	41	0
36	C	1	516	430	9	36	41	0
36	C	1	516	430	9	36	41	0
36	C	1	516	430	9	36	41	0
36	C	1	516	430	9	36	41	0
36	C	1	516	430	9	36	41	0
36	C	1	516	430	9	36	41	0
36	C	1	516	430	9	36	41	0
36	D	1	618	510	11	44	53	0
36	D	1	618	510	11	44	53	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
36	D	1	618	510	11	44	53	0
36	D	1	618	510	11	44	53	0
36	D	1	618	510	11	44	53	0
36	D	1	618	510	11	44	53	0
36	D	1	618	510	11	44	53	0
36	D	1	618	510	11	44	53	0
36	D	1	618	510	11	44	53	0
36	D	1	618	510	11	44	53	0
36	D	1	618	510	11	44	53	0
36	E	1	550	460	9	36	45	0
36	E	1	550	460	9	36	45	0
36	E	1	550	460	9	36	45	0
36	E	1	550	460	9	36	45	0
36	E	1	550	460	9	36	45	0
36	E	1	550	460	9	36	45	0
36	E	1	550	460	9	36	45	0
36	E	1	550	460	9	36	45	0
36	E	1	550	460	9	36	45	0
36	F	1	452	374	8	32	38	0
36	F	1	452	374	8	32	38	0
36	F	1	452	374	8	32	38	0

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Mol	Chain	Residues	Atoms					AltConf
36	F	1	Total	C	Mg	N	O	0
			452	374	8	32	38	
36	F	1	Total	C	Mg	N	O	0
			452	374	8	32	38	
36	F	1	Total	C	Mg	N	O	0
			452	374	8	32	38	
36	F	1	Total	C	Mg	N	O	0
			452	374	8	32	38	
36	F	1	Total	C	Mg	N	O	0
			452	374	8	32	38	
36	G	1	Total	C	Mg	N	O	0
			556	460	10	40	46	
36	G	1	Total	C	Mg	N	O	0
			556	460	10	40	46	
36	G	1	Total	C	Mg	N	O	0
			556	460	10	40	46	
36	G	1	Total	C	Mg	N	O	0
			556	460	10	40	46	
36	G	1	Total	C	Mg	N	O	0
			556	460	10	40	46	
36	G	1	Total	C	Mg	N	O	0
			556	460	10	40	46	
36	G	1	Total	C	Mg	N	O	0
			556	460	10	40	46	
36	G	1	Total	C	Mg	N	O	0
			556	460	10	40	46	
36	G	1	Total	C	Mg	N	O	0
			556	460	10	40	46	
36	H	1	Total	C	Mg	N	O	0
			760	632	13	52	63	
36	H	1	Total	C	Mg	N	O	0
			760	632	13	52	63	
36	H	1	Total	C	Mg	N	O	0
			760	632	13	52	63	
36	H	1	Total	C	Mg	N	O	0
			760	632	13	52	63	
36	H	1	Total	C	Mg	N	O	0
			760	632	13	52	63	
36	H	1	Total	C	Mg	N	O	0
			760	632	13	52	63	

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
36	H	1	760	632	13	52	63	0
36	H	1	760	632	13	52	63	0
36	H	1	760	632	13	52	63	0
36	H	1	760	632	13	52	63	0
36	H	1	760	632	13	52	63	0
36	H	1	760	632	13	52	63	0
36	H	1	760	632	13	52	63	0
36	I	1	555	459	10	40	46	0
36	I	1	555	459	10	40	46	0
36	I	1	555	459	10	40	46	0
36	I	1	555	459	10	40	46	0
36	I	1	555	459	10	40	46	0
36	I	1	555	459	10	40	46	0
36	I	1	555	459	10	40	46	0
36	I	1	555	459	10	40	46	0
36	I	1	555	459	10	40	46	0
36	I	1	555	459	10	40	46	0
36	J	1	562	464	10	40	48	0
36	J	1	562	464	10	40	48	0
36	J	1	562	464	10	40	48	0
36	J	1	562	464	10	40	48	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
36	J	1	562	464	10	40	48	0
36	J	1	562	464	10	40	48	0
36	J	1	562	464	10	40	48	0
36	J	1	562	464	10	40	48	0
36	J	1	562	464	10	40	48	0
36	J	1	562	464	10	40	48	0
36	K	1	529	441	9	36	43	0
36	K	1	529	441	9	36	43	0
36	K	1	529	441	9	36	43	0
36	K	1	529	441	9	36	43	0
36	K	1	529	441	9	36	43	0
36	K	1	529	441	9	36	43	0
36	K	1	529	441	9	36	43	0
36	K	1	529	441	9	36	43	0
36	K	1	529	441	9	36	43	0
36	K	1	529	441	9	36	43	0
36	L	1	527	439	9	36	43	0
36	L	1	527	439	9	36	43	0
36	L	1	527	439	9	36	43	0
36	L	1	527	439	9	36	43	0
36	L	1	527	439	9	36	43	0
36	L	1	527	439	9	36	43	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
36	L	1	527	439	9	36	43	0
36	L	1	527	439	9	36	43	0
36	L	1	527	439	9	36	43	0
36	M	1	525	429	10	40	46	0
36	M	1	525	429	10	40	46	0
36	M	1	525	429	10	40	46	0
36	M	1	525	429	10	40	46	0
36	M	1	525	429	10	40	46	0
36	M	1	525	429	10	40	46	0
36	M	1	525	429	10	40	46	0
36	M	1	525	429	10	40	46	0
36	M	1	525	429	10	40	46	0
36	M	1	525	429	10	40	46	0
36	M	1	525	429	10	40	46	0
36	N	1	601	489	12	48	52	0
36	N	1	601	489	12	48	52	0
36	N	1	601	489	12	48	52	0
36	N	1	601	489	12	48	52	0
36	N	1	601	489	12	48	52	0
36	N	1	601	489	12	48	52	0
36	N	1	601	489	12	48	52	0
36	N	1	601	489	12	48	52	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
36	N	1	601	489	12	48	52	0
36	N	1	601	489	12	48	52	0
36	N	1	601	489	12	48	52	0
36	N	1	601	489	12	48	52	0
36	O	1	506	420	9	36	41	0
36	O	1	506	420	9	36	41	0
36	O	1	506	420	9	36	41	0
36	O	1	506	420	9	36	41	0
36	O	1	506	420	9	36	41	0
36	O	1	506	420	9	36	41	0
36	O	1	506	420	9	36	41	0
36	O	1	506	420	9	36	41	0
36	O	1	506	420	9	36	41	0
36	O	1	506	420	9	36	41	0
36	P	1	686	570	12	48	56	0
36	P	1	686	570	12	48	56	0
36	P	1	686	570	12	48	56	0
36	P	1	686	570	12	48	56	0
36	P	1	686	570	12	48	56	0
36	P	1	686	570	12	48	56	0
36	P	1	686	570	12	48	56	0
36	P	1	686	570	12	48	56	0
36	P	1	686	570	12	48	56	0

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Mol	Chain	Residues	Atoms					AltConf
36	P	1	Total	C	Mg	N	O	0
			686	570	12	48	56	
36	P	1	Total	C	Mg	N	O	0
			686	570	12	48	56	
36	P	1	Total	C	Mg	N	O	0
			686	570	12	48	56	
36	P	1	Total	C	Mg	N	O	0
			686	570	12	48	56	
36	Q	1	Total	C	Mg	N	O	0
			458	380	8	32	38	
36	Q	1	Total	C	Mg	N	O	0
			458	380	8	32	38	
36	Q	1	Total	C	Mg	N	O	0
			458	380	8	32	38	
36	Q	1	Total	C	Mg	N	O	0
			458	380	8	32	38	
36	Q	1	Total	C	Mg	N	O	0
			458	380	8	32	38	
36	Q	1	Total	C	Mg	N	O	0
			458	380	8	32	38	
36	Q	1	Total	C	Mg	N	O	0
			458	380	8	32	38	
36	Q	1	Total	C	Mg	N	O	0
			458	380	8	32	38	
36	Q	1	Total	C	Mg	N	O	0
			458	380	8	32	38	
36	R	1	Total	C	Mg	N	O	0
			661	543	12	48	58	
36	R	1	Total	C	Mg	N	O	0
			661	543	12	48	58	
36	R	1	Total	C	Mg	N	O	0
			661	543	12	48	58	
36	R	1	Total	C	Mg	N	O	0
			661	543	12	48	58	
36	R	1	Total	C	Mg	N	O	0
			661	543	12	48	58	
36	R	1	Total	C	Mg	N	O	0
			661	543	12	48	58	
36	R	1	Total	C	Mg	N	O	0
			661	543	12	48	58	
36	R	1	Total	C	Mg	N	O	0
			661	543	12	48	58	
36	R	1	Total	C	Mg	N	O	0
			661	543	12	48	58	

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Mol	Chain	Residues	Atoms					AltConf
36	R	1	Total	C	Mg	N	O	0
			661	543	12	48	58	
36	R	1	Total	C	Mg	N	O	0
			661	543	12	48	58	
36	R	1	Total	C	Mg	N	O	0
			661	543	12	48	58	
36	S	1	Total	C	Mg	N	O	0
			658	544	12	48	54	
36	S	1	Total	C	Mg	N	O	0
			658	544	12	48	54	
36	S	1	Total	C	Mg	N	O	0
			658	544	12	48	54	
36	S	1	Total	C	Mg	N	O	0
			658	544	12	48	54	
36	S	1	Total	C	Mg	N	O	0
			658	544	12	48	54	
36	S	1	Total	C	Mg	N	O	0
			658	544	12	48	54	
36	S	1	Total	C	Mg	N	O	0
			658	544	12	48	54	
36	S	1	Total	C	Mg	N	O	0
			658	544	12	48	54	
36	S	1	Total	C	Mg	N	O	0
			658	544	12	48	54	
36	S	1	Total	C	Mg	N	O	0
			658	544	12	48	54	
36	T	1	Total	C	Mg	N	O	0
			408	340	7	28	33	
36	T	1	Total	C	Mg	N	O	0
			408	340	7	28	33	
36	T	1	Total	C	Mg	N	O	0
			408	340	7	28	33	
36	T	1	Total	C	Mg	N	O	0
			408	340	7	28	33	
36	T	1	Total	C	Mg	N	O	0
			408	340	7	28	33	
36	T	1	Total	C	Mg	N	O	0
			408	340	7	28	33	

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
36	T	1	408	340	7	28	33	0
36	W	1	629	513	12	48	56	0
36	W	1	629	513	12	48	56	0
36	W	1	629	513	12	48	56	0
36	W	1	629	513	12	48	56	0
36	W	1	629	513	12	48	56	0
36	W	1	629	513	12	48	56	0
36	W	1	629	513	12	48	56	0
36	W	1	629	513	12	48	56	0
36	W	1	629	513	12	48	56	0
36	W	1	629	513	12	48	56	0
36	W	1	629	513	12	48	56	0
36	W	1	629	513	12	48	56	0
36	W	1	629	513	12	48	56	0
36	W	1	629	513	12	48	56	0
36	X	1	368	296	8	32	32	0
36	X	1	368	296	8	32	32	0
36	X	1	368	296	8	32	32	0
36	X	1	368	296	8	32	32	0
36	X	1	368	296	8	32	32	0
36	X	1	368	296	8	32	32	0
36	X	1	368	296	8	32	32	0
36	X	1	368	296	8	32	32	0
36	X	1	368	296	8	32	32	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
36	a	1	Total 2437	C 2027	Mg 41	N 164	O 205	0
36	a	1	Total 2437	C 2027	Mg 41	N 164	O 205	0
36	a	1	Total 2437	C 2027	Mg 41	N 164	O 205	0
36	a	1	Total 2437	C 2027	Mg 41	N 164	O 205	0
36	a	1	Total 2437	C 2027	Mg 41	N 164	O 205	0
36	a	1	Total 2437	C 2027	Mg 41	N 164	O 205	0
36	a	1	Total 2437	C 2027	Mg 41	N 164	O 205	0
36	a	1	Total 2437	C 2027	Mg 41	N 164	O 205	0
36	a	1	Total 2437	C 2027	Mg 41	N 164	O 205	0
36	a	1	Total 2437	C 2027	Mg 41	N 164	O 205	0
36	a	1	Total 2437	C 2027	Mg 41	N 164	O 205	0
36	a	1	Total 2437	C 2027	Mg 41	N 164	O 205	0
36	a	1	Total 2437	C 2027	Mg 41	N 164	O 205	0
36	a	1	Total 2437	C 2027	Mg 41	N 164	O 205	0
36	a	1	Total 2437	C 2027	Mg 41	N 164	O 205	0
36	a	1	Total 2437	C 2027	Mg 41	N 164	O 205	0
36	a	1	Total 2437	C 2027	Mg 41	N 164	O 205	0
36	a	1	Total 2437	C 2027	Mg 41	N 164	O 205	0
36	b	1	Total 2337	C 1947	Mg 39	N 156	O 195	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
36	b	1	Total 2337	C 1947	Mg 39	N 156	O 195	0
36	b	1	Total 2337	C 1947	Mg 39	N 156	O 195	0
36	b	1	Total 2337	C 1947	Mg 39	N 156	O 195	0
36	b	1	Total 2337	C 1947	Mg 39	N 156	O 195	0
36	b	1	Total 2337	C 1947	Mg 39	N 156	O 195	0
36	b	1	Total 2337	C 1947	Mg 39	N 156	O 195	0
36	b	1	Total 2337	C 1947	Mg 39	N 156	O 195	0
36	b	1	Total 2337	C 1947	Mg 39	N 156	O 195	0
36	b	1	Total 2337	C 1947	Mg 39	N 156	O 195	0
36	b	1	Total 2337	C 1947	Mg 39	N 156	O 195	0
36	b	1	Total 2337	C 1947	Mg 39	N 156	O 195	0
36	b	1	Total 2337	C 1947	Mg 39	N 156	O 195	0
36	b	1	Total 2337	C 1947	Mg 39	N 156	O 195	0
36	b	1	Total 2337	C 1947	Mg 39	N 156	O 195	0
36	b	1	Total 2337	C 1947	Mg 39	N 156	O 195	0
36	b	1	Total 2337	C 1947	Mg 39	N 156	O 195	0
36	b	1	Total 2337	C 1947	Mg 39	N 156	O 195	0
36	f	1	Total 247	C 207	Mg 4	N 16	O 20	0
36	f	1	Total 247	C 207	Mg 4	N 16	O 20	0
36	f	1	Total 247	C 207	Mg 4	N 16	O 20	0
36	f	1	Total 247	C 207	Mg 4	N 16	O 20	0

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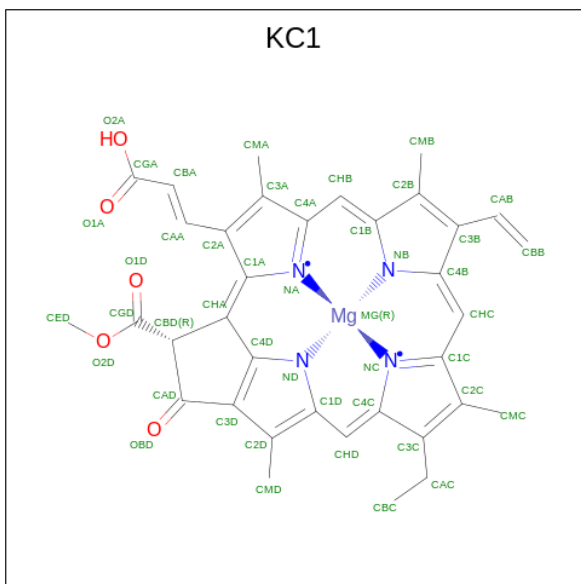
Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
36	i	1	65	55	1	4	5	0
36	j	1	172	144	3	12	13	0
36	j	1	172	144	3	12	13	0
36	j	1	172	144	3	12	13	0
36	l	1	294	244	5	20	25	0
36	l	1	294	244	5	20	25	0
36	l	1	294	244	5	20	25	0
36	l	1	294	244	5	20	25	0
36	l	1	294	244	5	20	25	0
36	h	1	65	55	1	4	5	0
36	U	1	449	371	8	32	38	0
36	U	1	449	371	8	32	38	0
36	U	1	449	371	8	32	38	0
36	U	1	449	371	8	32	38	0
36	U	1	449	371	8	32	38	0
36	U	1	449	371	8	32	38	0
36	U	1	449	371	8	32	38	0
36	U	1	449	371	8	32	38	0
36	V	1	545	457	9	36	43	0
36	V	1	545	457	9	36	43	0
36	V	1	545	457	9	36	43	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
36	V	1	Total 545	C 457	Mg 9	N 36	O 43	0
36	V	1	Total 545	C 457	Mg 9	N 36	O 43	0
36	V	1	Total 545	C 457	Mg 9	N 36	O 43	0
36	V	1	Total 545	C 457	Mg 9	N 36	O 43	0
36	V	1	Total 545	C 457	Mg 9	N 36	O 43	0
36	V	1	Total 545	C 457	Mg 9	N 36	O 43	0

- Molecule 37 is Chlorophyll c1 (three-letter code: KC1) (formula: $C_{35}H_{30}MgN_4O_5$).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
37	A	1	Total 45	C 35	Mg 1	N 4	O 5	0
37	B	1	Total 45	C 35	Mg 1	N 4	O 5	0
37	C	1	Total 45	C 35	Mg 1	N 4	O 5	0
37	D	1	Total 45	C 35	Mg 1	N 4	O 5	0
37	E	1	Total 45	C 35	Mg 1	N 4	O 5	0

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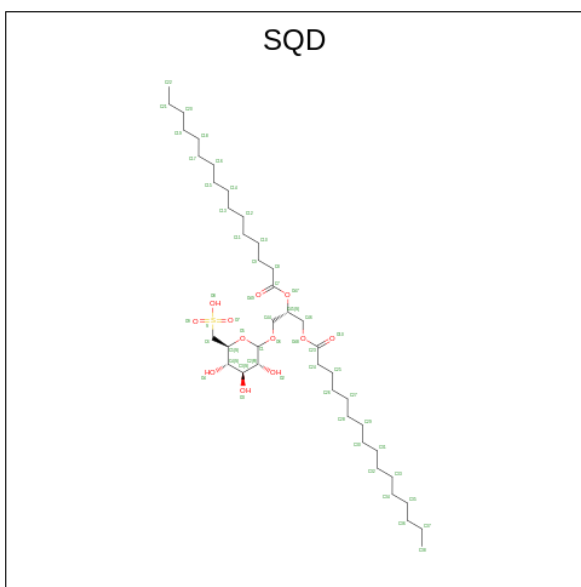
Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
37	F	1	Total 90	C 70	Mg 2	N 8	O 10	0
37	F	1	Total 90	C 70	Mg 2	N 8	O 10	0
37	G	1	Total 135	C 105	Mg 3	N 12	O 15	0
37	G	1	Total 135	C 105	Mg 3	N 12	O 15	0
37	G	1	Total 135	C 105	Mg 3	N 12	O 15	0
37	H	1	Total 45	C 35	Mg 1	N 4	O 5	0
37	J	1	Total 45	C 35	Mg 1	N 4	O 5	0
37	K	1	Total 45	C 35	Mg 1	N 4	O 5	0
37	L	1	Total 90	C 70	Mg 2	N 8	O 10	0
37	L	1	Total 90	C 70	Mg 2	N 8	O 10	0
37	M	1	Total 135	C 105	Mg 3	N 12	O 15	0
37	M	1	Total 135	C 105	Mg 3	N 12	O 15	0
37	M	1	Total 135	C 105	Mg 3	N 12	O 15	0
37	N	1	Total 45	C 35	Mg 1	N 4	O 5	0
37	O	1	Total 90	C 70	Mg 2	N 8	O 10	0
37	O	1	Total 90	C 70	Mg 2	N 8	O 10	0
37	P	1	Total 90	C 70	Mg 2	N 8	O 10	0
37	P	1	Total 90	C 70	Mg 2	N 8	O 10	0
37	Q	1	Total 90	C 70	Mg 2	N 8	O 10	0
37	Q	1	Total 90	C 70	Mg 2	N 8	O 10	0
37	R	1	Total 45	C 35	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
37	S	1	Total 45	C 35	Mg 1	N 4	O 5	0
37	T	1	Total 90	C 70	Mg 2	N 8	O 10	0
37	T	1	Total 90	C 70	Mg 2	N 8	O 10	0
37	W	1	Total 90	C 70	Mg 2	N 8	O 10	0
37	W	1	Total 90	C 70	Mg 2	N 8	O 10	0
37	X	1	Total 45	C 35	Mg 1	N 4	O 5	0
37	U	1	Total 45	C 35	Mg 1	N 4	O 5	0
37	V	1	Total 45	C 35	Mg 1	N 4	O 5	0

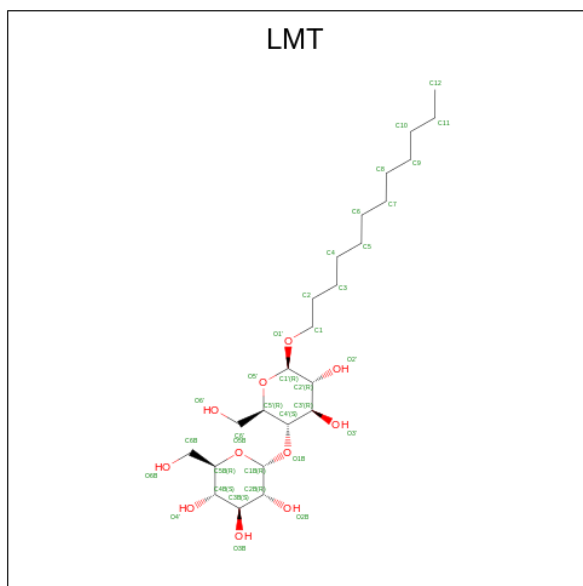
- Molecule 38 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (three-letter code: SQD) (formula: $C_{41}H_{78}O_{12}S$).



Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	S	
38	A	1	Total 28	C 15	O 12	S 1	0
38	b	1	Total 46	C 33	O 12	S 1	0

- Molecule 39 is DODECYL-BETA-D-MALTOSE (three-letter code: LMT) (formula:

C₂₄H₄₆O₁₁).



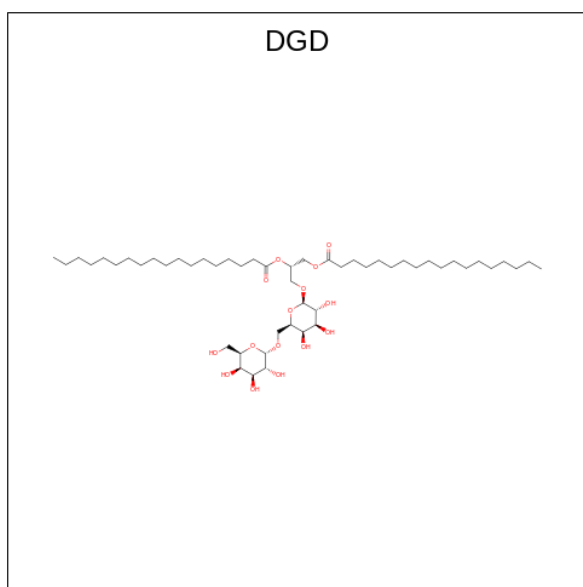
Mol	Chain	Residues	Atoms			AltConf
39	B	1	Total	C	O	0
			70	48	22	
39	B	1	Total	C	O	0
			70	48	22	
39	E	1	Total	C	O	0
			93	65	28	
39	E	1	Total	C	O	0
			93	65	28	
39	E	1	Total	C	O	0
			93	65	28	
39	F	1	Total	C	O	0
			68	46	22	
39	F	1	Total	C	O	0
			68	46	22	
39	G	1	Total	C	O	0
			70	48	22	
39	G	1	Total	C	O	0
			70	48	22	
39	I	1	Total	C	O	0
			70	48	22	
39	I	1	Total	C	O	0
			70	48	22	
39	K	1	Total	C	O	0
			66	44	22	
39	K	1	Total	C	O	0
			66	44	22	

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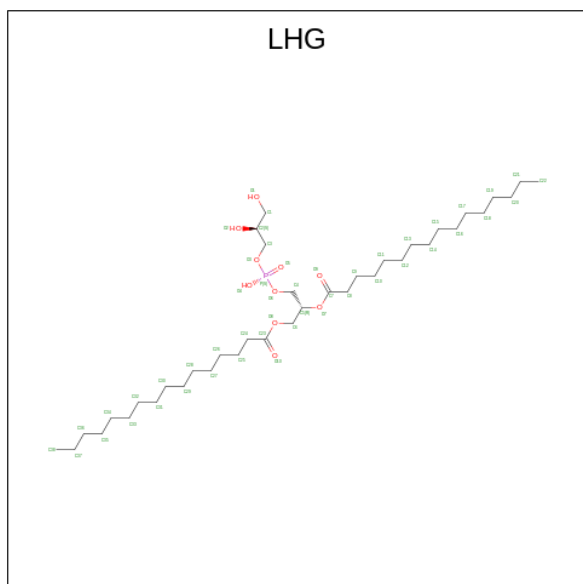
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
39	L	1	66	44	22	0
39	L	1	66	44	22	0
39	P	1	46	34	12	0
39	P	1	46	34	12	0
39	a	1	102	69	33	0
39	a	1	102	69	33	0
39	a	1	102	69	33	0
39	b	1	59	43	16	0
39	b	1	59	43	16	0
39	f	1	24	18	6	0
39	h	1	35	24	11	0
39	U	1	70	48	22	0
39	U	1	70	48	22	0

- Molecule 40 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (three-letter code: DGD) (formula: C₅₁H₉₆O₁₅).



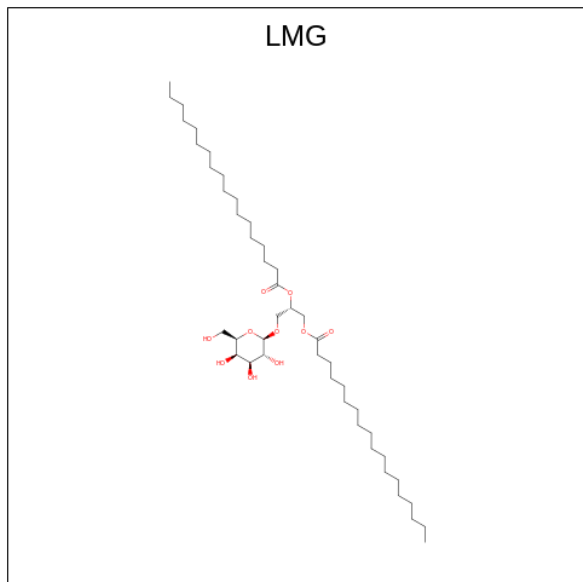
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
40	C	1	57	42	15	0
40	L	1	47	32	15	0
40	b	1	60	45	15	0

- Molecule 41 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula: $C_{38}H_{75}O_{10}P$).



Mol	Chain	Residues	Atoms				AltConf
41	D	1	Total	C	O	P	0
			95	73	20	2	
41	D	1	Total	C	O	P	0
			95	73	20	2	
41	E	1	Total	C	O	P	0
			49	38	10	1	
41	F	1	Total	C	O	P	0
			74	54	18	2	
41	F	1	Total	C	O	P	0
			74	54	18	2	
41	G	1	Total	C	O	P	0
			136	103	30	3	
41	G	1	Total	C	O	P	0
			136	103	30	3	
41	G	1	Total	C	O	P	0
			136	103	30	3	
41	I	1	Total	C	O	P	0
			49	38	10	1	
41	O	1	Total	C	O	P	0
			91	69	20	2	
41	O	1	Total	C	O	P	0
			91	69	20	2	
41	Q	1	Total	C	O	P	0
			49	38	10	1	
41	R	1	Total	C	O	P	0
			49	38	10	1	
41	a	1	Total	C	O	P	0
			122	89	30	3	
41	a	1	Total	C	O	P	0
			122	89	30	3	
41	a	1	Total	C	O	P	0
			122	89	30	3	
41	b	1	Total	C	O	P	0
			49	38	10	1	
41	f	1	Total	C	O	P	0
			91	69	20	2	
41	f	1	Total	C	O	P	0
			91	69	20	2	
41	i	1	Total	C	O	P	0
			46	35	10	1	
41	j	1	Total	C	O	P	0
			49	38	10	1	
41	l	1	Total	C	O	P	0
			48	37	10	1	

- Molecule 42 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: LMG) (formula: C₄₅H₈₆O₁₀).



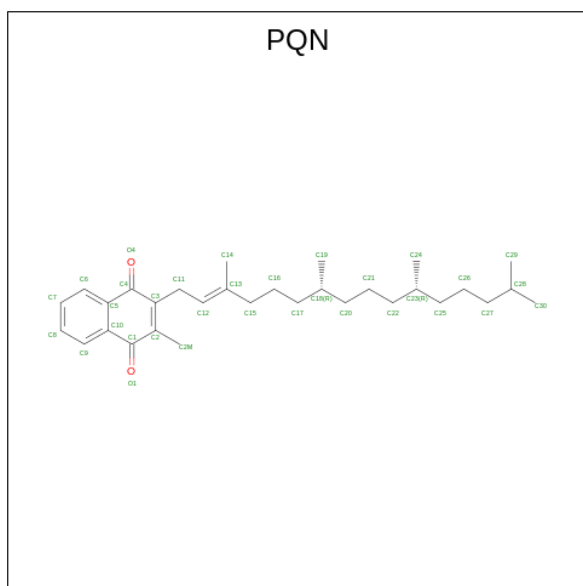
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
42	D	1	83	63	20	0
42	D	1	83	63	20	0
42	E	1	86	66	20	0
42	E	1	86	66	20	0
42	G	1	110	90	20	0
42	G	1	110	90	20	0
42	I	1	55	45	10	0
42	J	1	99	79	20	0
42	J	1	99	79	20	0
42	L	1	33	23	10	0
42	a	1	54	44	10	0
42	j	1	52	42	10	0

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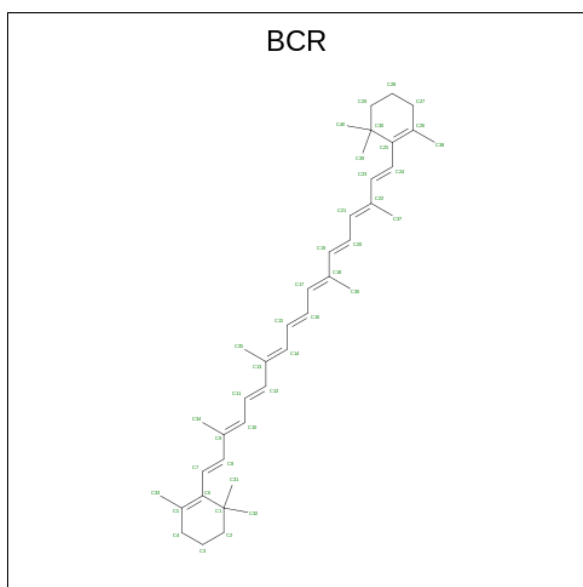
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
42	m	1	37	27	10	0
42	h	1	45	35	10	0
42	V	1	92	72	20	0
42	V	1	92	72	20	0

- Molecule 43 is PHYLLOQUINONE (three-letter code: PQN) (formula: $C_{31}H_{46}O_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
43	a	1	33	31	2	0
43	b	1	33	31	2	0

- Molecule 44 is BETA-CAROTENE (three-letter code: BCR) (formula: $C_{40}H_{56}$).



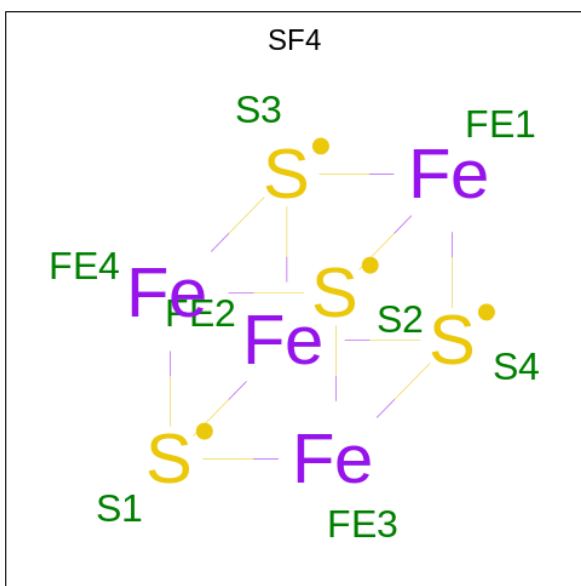
Mol	Chain	Residues	Atoms	AltConf
44	a	1	Total C 160 160	0
44	a	1	Total C 160 160	0
44	a	1	Total C 160 160	0
44	a	1	Total C 160 160	0
44	b	1	Total C 200 200	0
44	b	1	Total C 200 200	0
44	b	1	Total C 200 200	0
44	b	1	Total C 200 200	0
44	b	1	Total C 200 200	0
44	f	1	Total C 80 80	0
44	f	1	Total C 80 80	0
44	i	1	Total C 80 80	0
44	i	1	Total C 80 80	0
44	j	1	Total C 40 40	0

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Mol	Chain	Residues	Atoms	AltConf
44	l	1	Total C 80 80	0
44	l	1	Total C 80 80	0
44	m	1	Total C 40 40	0
44	h	1	Total C 40 40	0

- Molecule 45 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe₄S₄) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	AltConf
45	b	1	Total Fe S 8 4 4	0
45	c	1	Total Fe S 16 8 8	0
45	c	1	Total Fe S 16 8 8	0

- Molecule 46 is water.

Mol	Chain	Residues	Atoms	AltConf
46	a	64	Total O 64 64	0
46	b	72	Total O 72 72	0

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Mol	Chain	Residues	Atoms	AltConf
46	c	7	Total O 7 7	0
46	d	4	Total O 4 4	0
46	f	2	Total O 2 2	0
46	j	1	Total O 1 1	0
46	l	3	Total O 3 3	0

3 Residue-property plots [i](#)

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

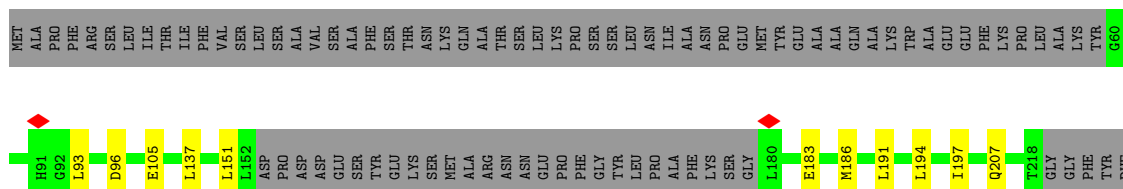
- Molecule 1: FCPI-7

Chain A: 95% 5%



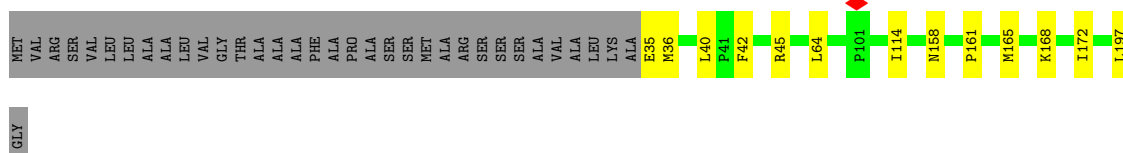
- Molecule 2: FCPI-1

Chain B: 54% 5% 41%



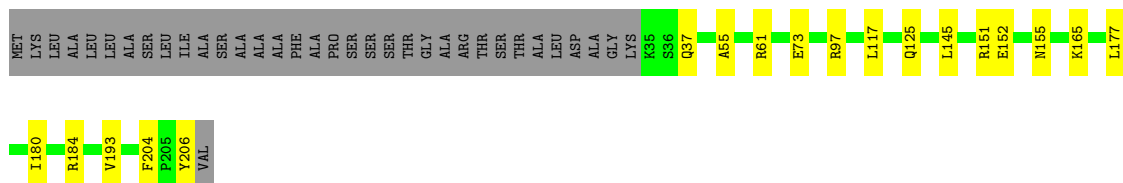
- Molecule 3: FCPI-11

Chain C: 76% 7% 18%

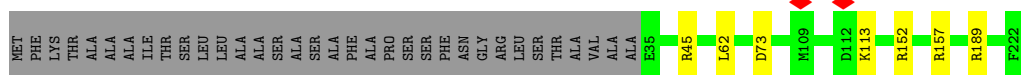
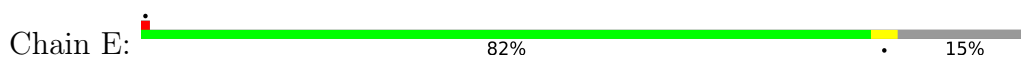


- Molecule 4: FCPI-6

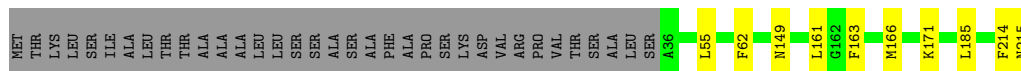
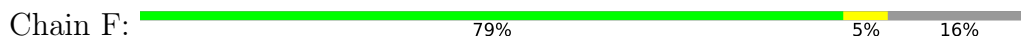
Chain D: 74% 9% 17%



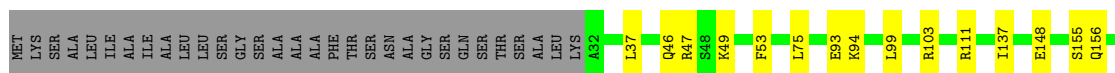
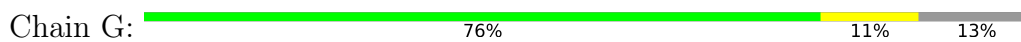
- Molecule 5: FCPI-5



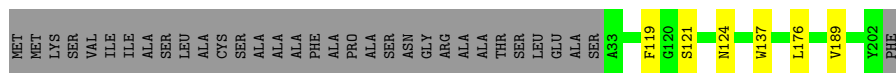
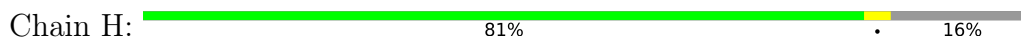
• Molecule 6: FCPI-8



• Molecule 7: FCPI-4



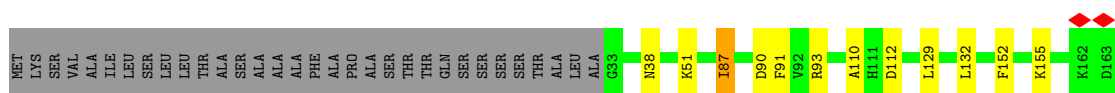
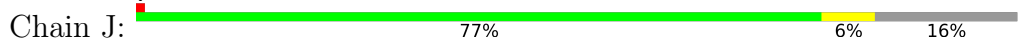
• Molecule 8: FCPI-10

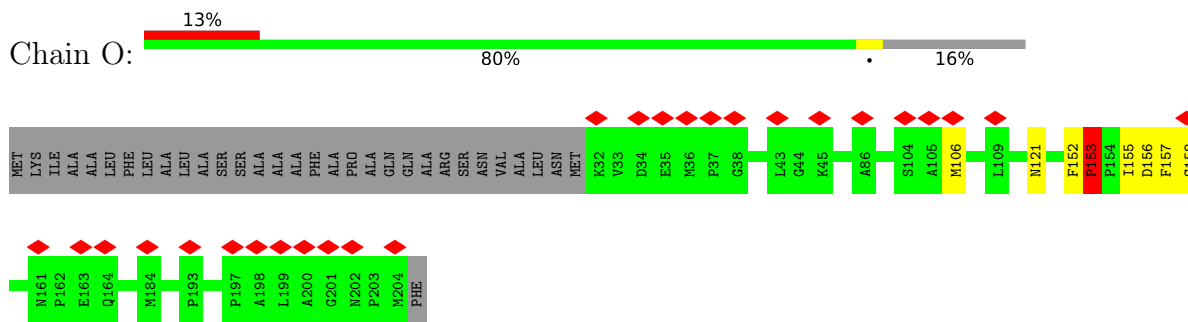


• Molecule 9: FCPI-3

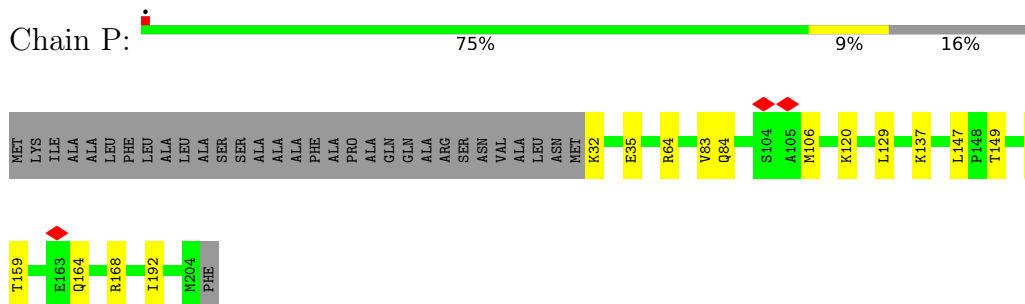


• Molecule 10: FCPI-9

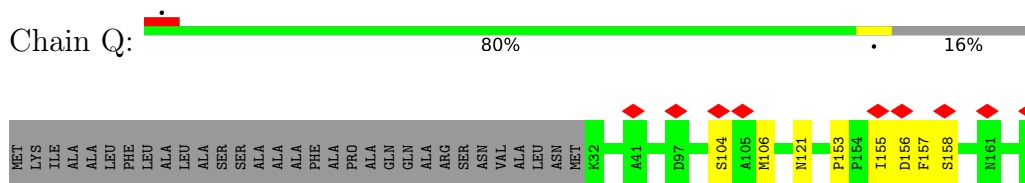




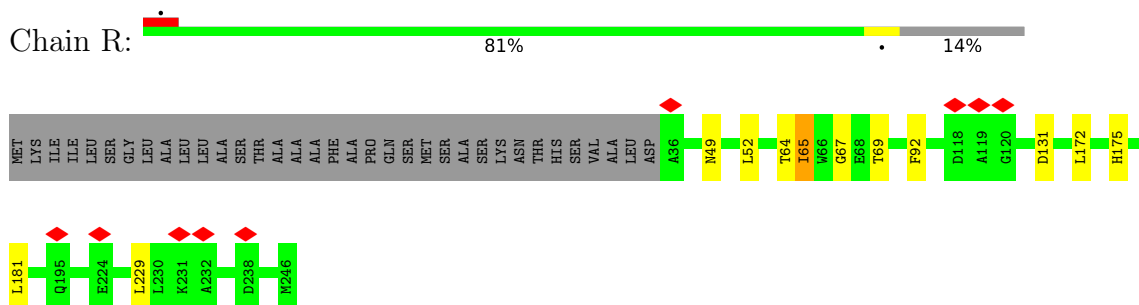
• Molecule 15: FCPI



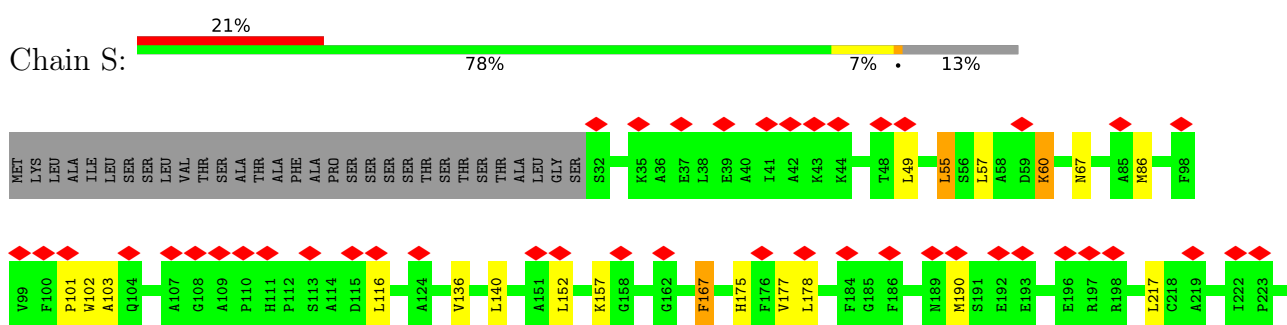
• Molecule 15: FCPI

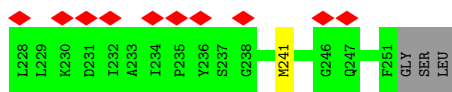


• Molecule 16: FCPI-24

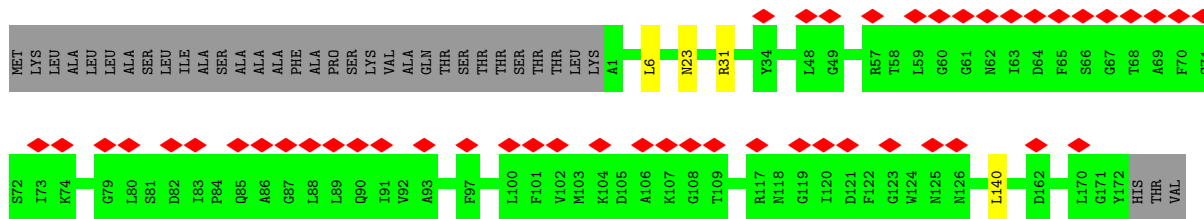
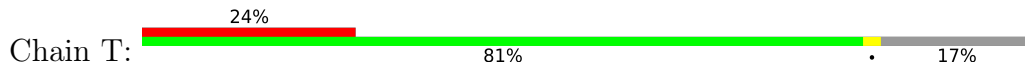


• Molecule 17: FCPI-23

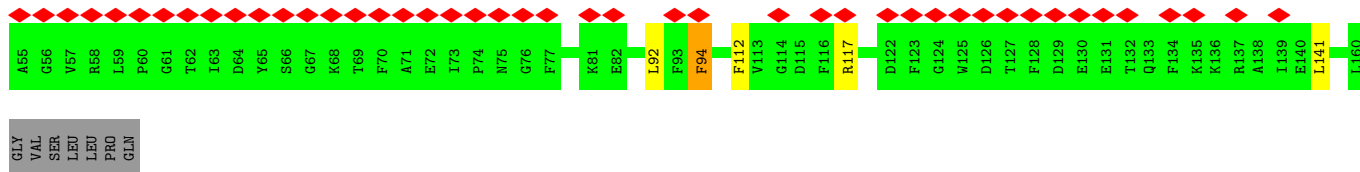
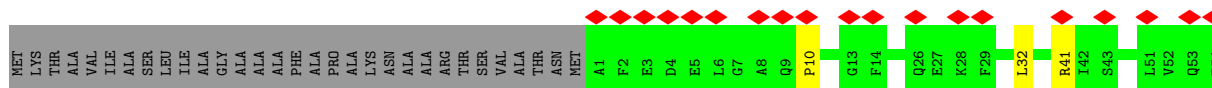
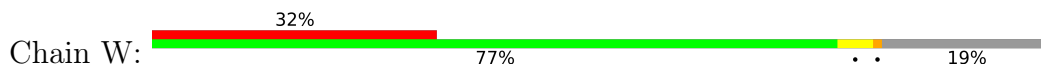




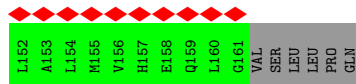
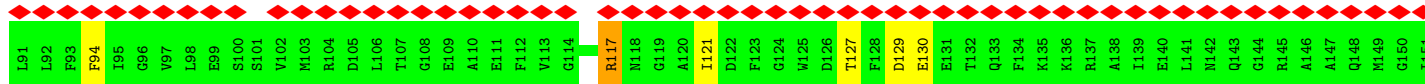
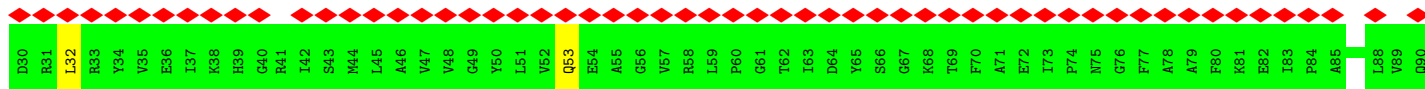
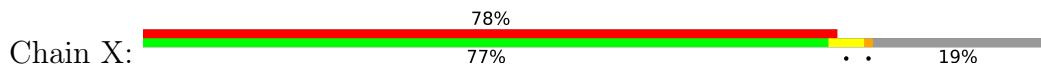
• Molecule 18: FCPI-12



• Molecule 19: FCPI-17



• Molecule 19: FCPI-17

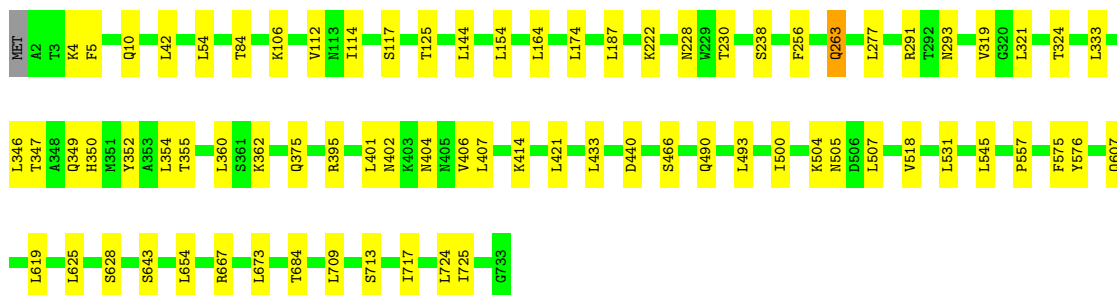
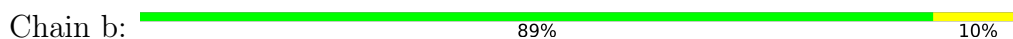


• Molecule 20: PsaA

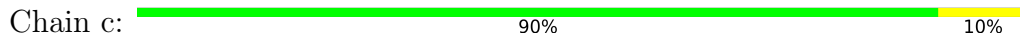




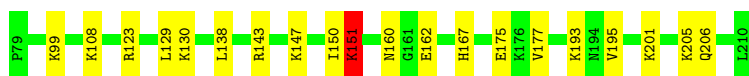
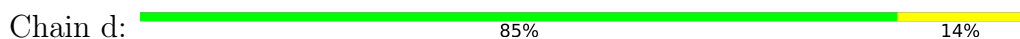
• Molecule 21: PsaB



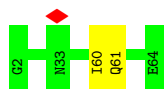
• Molecule 22: PsaC



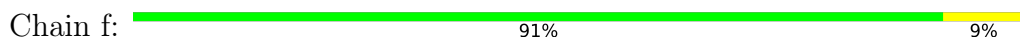
• Molecule 23: PsaD



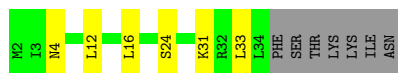
• Molecule 24: PsaE



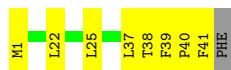
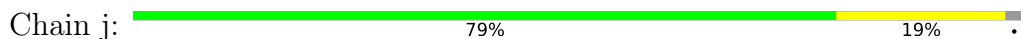
• Molecule 25: PsaF



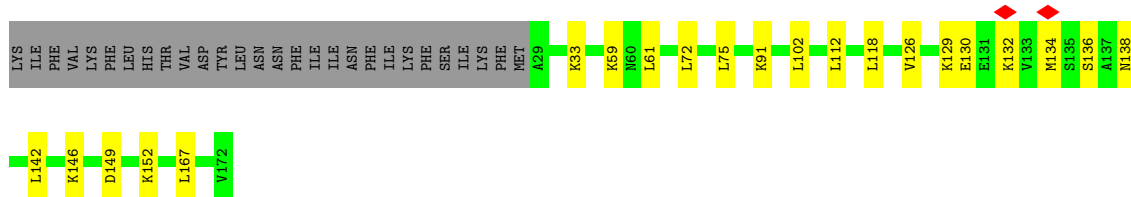
• Molecule 26: PsaI



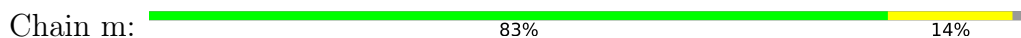
• Molecule 27: PsaJ



• Molecule 28: PsaL



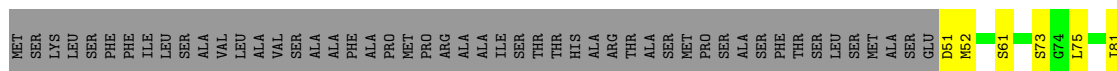
• Molecule 29: PsaM



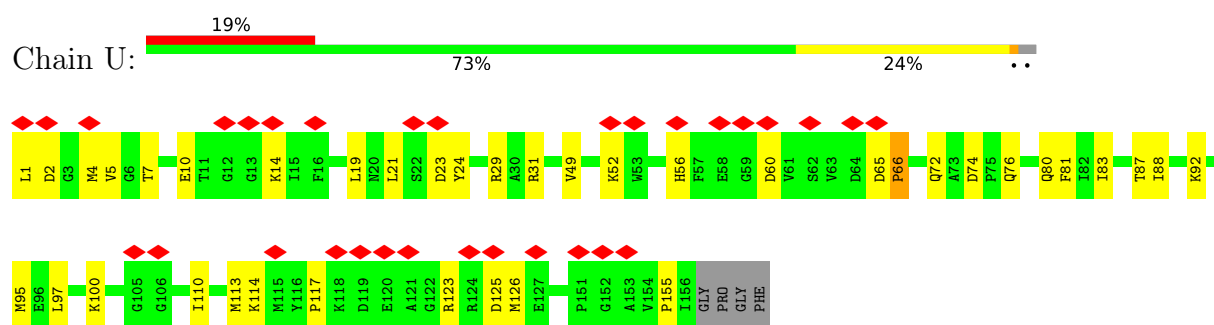
• Molecule 30: PsaS



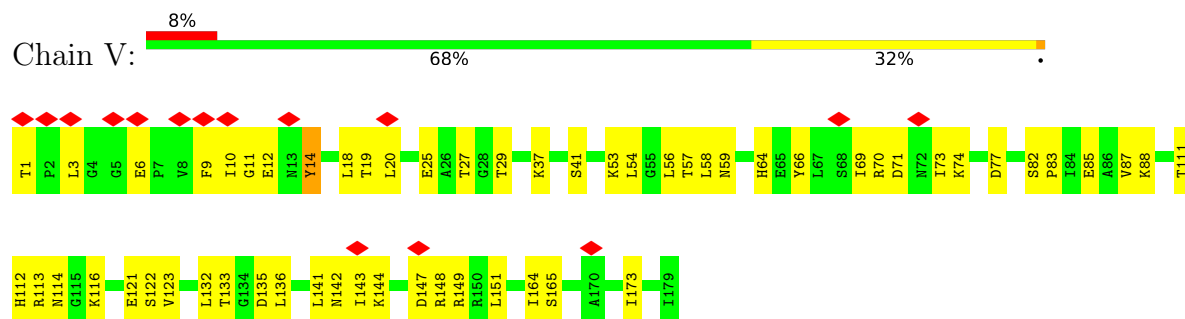
• Molecule 31: PsaR



• Molecule 32: FCPI-2



- Molecule 33: FCPI-19



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	164480	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	0.163	Depositor
Minimum map value	-0.055	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.016	Depositor
Map size (Å)	567.32, 567.32, 567.32	wwPDB
Map dimensions	520, 520, 520	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.091, 1.091, 1.091	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: KC1, BCR, A86, LMT, LHG, SQD, CLA, DGD, DD6, PQN, LMG, SF4

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	0.47	0/1319	0.67	1/1786 (0.1%)
2	B	0.51	2/1039 (0.2%)	0.98	7/1412 (0.5%)
3	C	0.37	0/1275	0.63	1/1726 (0.1%)
4	D	0.54	3/1373 (0.2%)	0.70	1/1860 (0.1%)
5	E	0.49	0/1439	0.70	2/1944 (0.1%)
6	F	0.47	0/1411	0.68	2/1908 (0.1%)
7	G	0.43	1/1714 (0.1%)	0.59	0/2321
8	H	0.55	1/1326 (0.1%)	0.79	3/1798 (0.2%)
9	I	0.40	0/1285	0.67	5/1746 (0.3%)
10	J	0.46	0/1339	0.73	3/1811 (0.2%)
11	K	0.51	0/1346	0.72	1/1826 (0.1%)
12	L	0.53	1/1571 (0.1%)	0.73	3/2141 (0.1%)
13	M	0.46	1/1464 (0.1%)	0.72	1/1982 (0.1%)
14	N	0.53	0/1770	0.90	6/2405 (0.2%)
15	O	0.55	3/1335 (0.2%)	0.81	4/1817 (0.2%)
15	P	0.40	1/1329 (0.1%)	0.93	4/1810 (0.2%)
15	Q	0.56	3/1335 (0.2%)	0.80	2/1817 (0.1%)
16	R	0.40	0/1680	0.71	5/2282 (0.2%)
17	S	0.44	0/1776	0.84	8/2413 (0.3%)
18	T	0.40	0/1353	0.64	2/1823 (0.1%)
19	W	0.55	1/1265 (0.1%)	0.88	8/1707 (0.5%)
19	X	0.59	3/1282 (0.2%)	0.98	11/1729 (0.6%)
20	a	0.44	3/6053 (0.0%)	0.59	5/8238 (0.1%)
21	b	0.39	0/6031	0.57	8/8231 (0.1%)
22	c	0.46	0/607	0.61	0/822
23	d	1.90	2/1086 (0.2%)	1.23	8/1461 (0.5%)
24	e	0.57	0/517	0.56	0/701
25	f	0.47	1/1248 (0.1%)	0.58	2/1687 (0.1%)
26	i	0.49	0/262	0.75	0/356
27	j	0.46	0/333	0.79	2/455 (0.4%)
28	l	0.47	1/1121 (0.1%)	0.69	6/1520 (0.4%)
29	m	0.44	0/198	0.58	1/269 (0.4%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
31	h	0.33	0/698	0.54	0/951
32	U	0.42	0/1225	0.83	4/1657 (0.2%)
33	V	0.26	0/1393	0.48	0/1894
All	All	0.53	27/51798 (0.1%)	0.72	116/70306 (0.2%)

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
10	J	0	1
12	L	0	2
14	N	0	7
15	O	0	1
15	P	0	1
15	Q	0	1
17	S	0	2
19	W	0	3
23	d	0	5
30	g	0	1
33	V	0	1
All	All	0	25

The worst 5 of 27 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	d	151[A]	LYS	CA-C	43.55	2.66	1.52
23	d	151[B]	LYS	CA-C	43.55	2.66	1.52
19	X	94	PHE	CE2-CZ	9.29	1.55	1.37
2	B	186	MET	C-N	8.97	1.54	1.34
4	D	73	GLU	CB-CG	-7.17	1.38	1.52

The worst 5 of 116 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	d	151[A]	LYS	CB-CA-C	-22.80	64.81	110.40
23	d	151[B]	LYS	CB-CA-C	-22.80	64.81	110.40
15	P	156	ASP	O-C-N	-20.21	90.36	122.70
32	U	65	ASP	C-N-CD	-19.93	76.74	120.60
23	d	151[A]	LYS	CA-C-N	-15.35	83.44	117.20

There are no chirality outliers.

5 of 25 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
10	J	91	PHE	Mainchain
12	L	228	HIS	Peptide
12	L	47	ASN	Peptide
14	N	112	PRO	Peptide
14	N	172	ASP	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	166/168 (99%)	150 (90%)	14 (8%)	2 (1%)	13	17
2	B	128/223 (57%)	121 (94%)	7 (6%)	0	100	100
3	C	161/198 (81%)	150 (93%)	9 (6%)	2 (1%)	13	17
4	D	170/207 (82%)	160 (94%)	9 (5%)	1 (1%)	25	34
5	E	186/222 (84%)	178 (96%)	8 (4%)	0	100	100
6	F	178/215 (83%)	165 (93%)	13 (7%)	0	100	100
7	G	212/245 (86%)	197 (93%)	14 (7%)	1 (0%)	29	39
8	H	168/203 (83%)	151 (90%)	17 (10%)	0	100	100
9	I	159/195 (82%)	146 (92%)	13 (8%)	0	100	100
10	J	165/200 (82%)	145 (88%)	17 (10%)	3 (2%)	8	9
11	K	167/207 (81%)	152 (91%)	15 (9%)	0	100	100
12	L	194/229 (85%)	176 (91%)	18 (9%)	0	100	100
13	M	185/306 (60%)	169 (91%)	15 (8%)	1 (0%)	29	39

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
14	N	217/219 (99%)	174 (80%)	40 (18%)	3 (1%)	11	14
15	O	171/205 (83%)	147 (86%)	21 (12%)	3 (2%)	8	9
15	P	171/205 (83%)	153 (90%)	16 (9%)	2 (1%)	13	17
15	Q	171/205 (83%)	150 (88%)	19 (11%)	2 (1%)	13	17
16	R	209/246 (85%)	182 (87%)	25 (12%)	2 (1%)	15	21
17	S	218/254 (86%)	184 (84%)	29 (13%)	5 (2%)	6	6
18	T	170/207 (82%)	164 (96%)	6 (4%)	0	100	100
19	W	158/198 (80%)	133 (84%)	25 (16%)	0	100	100
19	X	160/198 (81%)	146 (91%)	13 (8%)	1 (1%)	25	34
20	a	740/743 (100%)	713 (96%)	26 (4%)	1 (0%)	51	67
21	b	731/733 (100%)	699 (96%)	31 (4%)	1 (0%)	51	67
22	c	78/80 (98%)	74 (95%)	4 (5%)	0	100	100
23	d	131/132 (99%)	125 (95%)	6 (5%)	0	100	100
24	e	61/63 (97%)	60 (98%)	1 (2%)	0	100	100
25	f	160/162 (99%)	152 (95%)	8 (5%)	0	100	100
26	i	31/40 (78%)	31 (100%)	0	0	100	100
27	j	39/42 (93%)	37 (95%)	1 (3%)	1 (3%)	5	4
28	l	142/172 (83%)	131 (92%)	11 (8%)	0	100	100
29	m	26/29 (90%)	26 (100%)	0	0	100	100
31	h	87/139 (63%)	87 (100%)	0	0	100	100
32	U	154/160 (96%)	123 (80%)	26 (17%)	5 (3%)	4	3
33	V	177/179 (99%)	152 (86%)	20 (11%)	5 (3%)	5	4
All	All	6441/7429 (87%)	5903 (92%)	497 (8%)	41 (1%)	29	34

5 of 41 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
10	J	87	ILE
15	O	153	PRO
15	O	155	ILE
15	Q	153	PRO
17	S	103	ALA

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	137/137 (100%)	131 (96%)	6 (4%)	28	42
2	B	105/180 (58%)	99 (94%)	6 (6%)	20	30
3	C	131/153 (86%)	121 (92%)	10 (8%)	13	18
4	D	140/163 (86%)	126 (90%)	14 (10%)	7	10
5	E	142/164 (87%)	137 (96%)	5 (4%)	36	52
6	F	142/169 (84%)	134 (94%)	8 (6%)	21	31
7	G	172/193 (89%)	145 (84%)	27 (16%)	2	2
8	H	131/154 (85%)	128 (98%)	3 (2%)	50	68
9	I	124/152 (82%)	104 (84%)	20 (16%)	2	2
10	J	130/154 (84%)	123 (95%)	7 (5%)	22	33
11	K	133/160 (83%)	130 (98%)	3 (2%)	50	68
12	L	159/180 (88%)	158 (99%)	1 (1%)	86	93
13	M	142/247 (58%)	137 (96%)	5 (4%)	36	52
14	N	176/176 (100%)	169 (96%)	7 (4%)	31	47
15	O	138/159 (87%)	135 (98%)	3 (2%)	52	69
15	P	137/159 (86%)	120 (88%)	17 (12%)	4	5
15	Q	138/159 (87%)	135 (98%)	3 (2%)	52	69
16	R	167/193 (86%)	161 (96%)	6 (4%)	35	51
17	S	177/204 (87%)	167 (94%)	10 (6%)	21	31
18	T	136/163 (83%)	134 (98%)	2 (2%)	65	79
19	W	125/151 (83%)	125 (100%)	0	100	100
19	X	127/151 (84%)	124 (98%)	3 (2%)	49	66
20	a	606/606 (100%)	548 (90%)	58 (10%)	8	11
21	b	593/593 (100%)	523 (88%)	70 (12%)	5	6
22	c	67/69 (97%)	59 (88%)	8 (12%)	5	6
23	d	111/111 (100%)	91 (82%)	20 (18%)	1	2

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
24	e	55/55 (100%)	53 (96%)	2 (4%)	35	51
25	f	119/125 (95%)	108 (91%)	11 (9%)	9	12
26	i	29/36 (81%)	23 (79%)	6 (21%)	1	1
27	j	34/35 (97%)	29 (85%)	5 (15%)	3	3
28	l	114/143 (80%)	100 (88%)	14 (12%)	4	5
29	m	20/23 (87%)	17 (85%)	3 (15%)	3	3
31	h	70/109 (64%)	55 (79%)	15 (21%)	1	1
32	U	119/121 (98%)	87 (73%)	32 (27%)	0	0
33	V	137/137 (100%)	84 (61%)	53 (39%)	0	0
All	All	5183/5884 (88%)	4720 (91%)	463 (9%)	13	13

5 of 463 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
21	b	112	VAL
33	V	114	ASN
21	b	643	SER
33	V	85	GLU
32	U	87	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 117 such sidechains are listed below:

Mol	Chain	Res	Type
18	T	23	ASN
32	U	148	HIS
20	a	447	ASN
32	U	80	GLN
21	b	671	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](#)

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

589 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
35	A86	O	305	-	44,50,50	1.42	4 (9%)	51,76,76	1.95	16 (31%)
45	SF4	c	102	-	0,12,12	-	-	-	-	-
36	CLA	I	306	9	65,73,73	1.65	13 (20%)	76,113,113	2.44	22 (28%)
34	DD6	J	304	-	39,45,45	2.00	3 (7%)	52,67,67	1.87	12 (23%)
39	LMT	F	320	-	36,36,36	0.38	0	47,47,47	0.67	1 (2%)
34	DD6	I	303	-	39,45,45	2.03	3 (7%)	52,67,67	1.95	15 (28%)
35	A86	I	302	-	44,50,50	1.30	4 (9%)	51,76,76	2.66	17 (33%)
36	CLA	M	307	-	65,73,73	1.46	9 (13%)	76,113,113	1.56	9 (11%)
35	A86	N	303	-	44,50,50	1.31	5 (11%)	51,76,76	3.31	22 (43%)
36	CLA	B	309	2	52,60,73	2.05	10 (19%)	60,97,113	2.20	19 (31%)
36	CLA	E	311	-	65,73,73	1.40	7 (10%)	76,113,113	1.47	6 (7%)
36	CLA	b	839	-	65,73,73	1.42	8 (12%)	76,113,113	1.52	9 (11%)
35	A86	K	302	-	44,50,50	1.38	4 (9%)	51,76,76	3.29	20 (39%)
34	DD6	S	306	-	39,45,45	1.96	3 (7%)	52,67,67	2.00	13 (25%)
36	CLA	S	311	35	46,54,73	1.81	9 (19%)	53,90,113	1.64	10 (18%)
34	DD6	j	103	-	39,45,45	1.99	3 (7%)	52,67,67	1.83	12 (23%)
35	A86	M	304	-	44,50,50	1.23	3 (6%)	51,76,76	2.06	14 (27%)
35	A86	B	303	-	44,50,50	1.30	3 (6%)	51,76,76	4.01	27 (52%)
36	CLA	E	308	5	49,57,73	1.63	10 (20%)	55,93,113	1.62	9 (16%)
36	CLA	Q	312	-	41,49,73	1.85	8 (19%)	47,84,113	1.81	7 (14%)
36	CLA	S	312	17	65,73,73	1.46	7 (10%)	76,113,113	1.50	9 (11%)
41	LHG	l	208	-	47,47,48	0.95	2 (4%)	50,53,54	1.02	3 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
34	DD6	R	308	-	39,45,45	2.02	3 (7%)	52,67,67	2.12	13 (25%)
44	BCR	h	201	-	41,41,41	1.26	5 (12%)	56,56,56	1.42	10 (17%)
35	A86	U	304	32,37	44,50,50	1.21	3 (6%)	51,76,76	2.34	19 (37%)
34	DD6	A	301	-	39,45,45	2.04	3 (7%)	52,67,67	2.08	15 (28%)
34	DD6	E	301	-	39,45,45	1.98	3 (7%)	52,67,67	1.93	10 (19%)
37	KC1	M	318	-	48,53,53	5.42	28 (58%)	55,89,89	6.65	32 (58%)
36	CLA	O	307	-	65,73,73	1.43	8 (12%)	76,113,113	1.48	6 (7%)
36	CLA	W	218	19	43,51,73	1.75	8 (18%)	49,86,113	1.90	9 (18%)
36	CLA	J	307	10	61,69,73	1.46	7 (11%)	71,108,113	1.58	11 (15%)
35	A86	X	314	19	44,50,50	1.26	4 (9%)	51,76,76	2.07	13 (25%)
36	CLA	Q	309	15	46,54,73	1.73	7 (15%)	53,90,113	1.73	10 (18%)
42	LMG	D	320	41	46,46,55	0.98	2 (4%)	54,54,63	1.03	3 (5%)
36	CLA	Q	308	-	65,73,73	1.45	7 (10%)	76,113,113	1.54	10 (13%)
36	CLA	P	310	41,15	65,73,73	1.45	7 (10%)	76,113,113	1.44	8 (10%)
36	CLA	M	311	35,13	65,73,73	1.47	7 (10%)	76,113,113	1.41	6 (7%)
36	CLA	a	833	-	50,58,73	1.65	11 (22%)	58,95,113	1.69	7 (12%)
44	BCR	f	806	-	41,41,41	1.18	3 (7%)	56,56,56	1.23	7 (12%)
35	A86	Q	303	-	44,50,50	1.33	5 (11%)	51,76,76	2.05	15 (29%)
37	KC1	Q	311	15	48,53,53	3.07	20 (41%)	55,89,89	6.90	36 (65%)
36	CLA	V	307	-	51,59,73	1.67	6 (11%)	59,96,113	1.49	6 (10%)
39	LMT	a	854	-	36,36,36	0.40	0	47,47,47	0.75	0
35	A86	X	304	19	44,50,50	1.34	4 (9%)	51,76,76	3.26	20 (39%)
34	DD6	C	201	-	39,45,45	2.03	3 (7%)	52,67,67	1.92	13 (25%)
36	CLA	I	305	-	61,69,73	2.03	11 (18%)	71,108,113	1.76	12 (16%)
36	CLA	a	804	-	65,73,73	1.44	10 (15%)	76,113,113	1.42	11 (14%)
36	CLA	b	836	-	58,66,73	2.01	13 (22%)	67,104,113	3.05	24 (35%)
36	CLA	A	313	-	41,49,73	1.84	9 (21%)	47,84,113	1.83	7 (14%)
35	A86	E	305	5	44,50,50	1.23	4 (9%)	51,76,76	2.04	14 (27%)
36	CLA	M	316	36	42,50,73	1.78	8 (19%)	48,85,113	1.61	6 (12%)
36	CLA	a	821	-	49,57,73	1.57	8 (16%)	55,93,113	1.70	6 (10%)
36	CLA	l	201	-	65,73,73	1.40	8 (12%)	76,113,113	1.55	10 (13%)
44	BCR	b	843	-	41,41,41	1.18	3 (7%)	56,56,56	1.18	5 (8%)
36	CLA	I	314	-	41,49,73	1.84	7 (17%)	47,84,113	1.68	6 (12%)
35	A86	L	307	-	44,50,50	1.24	4 (9%)	51,76,76	1.93	11 (21%)
36	CLA	W	206	19	61,69,73	1.51	5 (8%)	71,108,113	1.63	7 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
36	CLA	a	828	-	65,73,73	1.36	7 (10%)	76,113,113	1.57	8 (10%)
35	A86	F	301	-	44,50,50	1.24	4 (9%)	51,76,76	2.32	16 (31%)
36	CLA	f	804	46	65,73,73	2.02	17 (26%)	76,113,113	2.93	29 (38%)
41	LHG	I	316	-	48,48,48	0.95	2 (4%)	51,54,54	1.00	2 (3%)
37	KC1	L	315	12,35	48,53,53	3.06	19 (39%)	55,89,89	6.27	36 (65%)
36	CLA	U	310	-	65,73,73	1.48	7 (10%)	76,113,113	1.62	13 (17%)
39	LMT	f	807	-	24,24,36	0.43	0	29,29,47	0.58	0
37	KC1	D	314	4	48,53,53	2.90	19 (39%)	55,89,89	5.52	34 (61%)
36	CLA	U	309	32	46,54,73	1.84	7 (15%)	53,90,113	1.84	11 (20%)
36	CLA	O	308	15	65,73,73	1.45	8 (12%)	76,113,113	1.53	9 (11%)
36	CLA	M	308	-	52,60,73	1.65	10 (19%)	60,97,113	1.71	9 (15%)
39	LMT	U	314	-	36,36,36	0.40	0	47,47,47	0.69	1 (2%)
35	A86	L	306	37	44,50,50	1.24	3 (6%)	51,76,76	2.98	19 (37%)
36	CLA	Q	314	-	65,73,73	1.45	6 (9%)	76,113,113	4.16	13 (17%)
36	CLA	C	206	-	61,69,73	1.48	7 (11%)	71,108,113	1.48	7 (9%)
35	A86	W	202	19,36	44,50,50	1.50	6 (13%)	51,76,76	3.63	29 (56%)
44	BCR	a	844	-	41,41,41	1.07	2 (4%)	56,56,56	1.29	5 (8%)
35	A86	P	304	-	44,50,50	1.33	5 (11%)	51,76,76	2.74	17 (33%)
36	CLA	a	802	-	65,73,73	1.45	7 (10%)	76,113,113	1.83	12 (15%)
35	A86	H	301	-	44,50,50	1.29	3 (6%)	51,76,76	4.88	20 (39%)
36	CLA	Q	310	15	65,73,73	2.92	15 (23%)	76,113,113	2.92	21 (27%)
41	LHG	D	318	36	45,45,48	0.30	0	48,51,54	0.39	0
35	A86	R	301	-	44,50,50	1.47	4 (9%)	51,76,76	3.48	24 (47%)
36	CLA	b	829	-	65,73,73	1.44	9 (13%)	76,113,113	1.37	7 (9%)
36	CLA	V	311	33	65,73,73	1.40	8 (12%)	76,113,113	1.76	13 (17%)
36	CLA	O	306	-	61,69,73	1.49	9 (14%)	71,108,113	1.46	6 (8%)
43	PQN	b	842	-	34,34,34	1.56	2 (5%)	42,45,45	1.19	4 (9%)
36	CLA	N	311	14	46,54,73	1.72	7 (15%)	53,90,113	1.86	10 (18%)
35	A86	T	307	-	44,50,50	1.24	3 (6%)	51,76,76	3.14	21 (41%)
35	A86	W	203	36	44,50,50	1.37	4 (9%)	51,76,76	2.83	20 (39%)
41	LHG	O	317	-	41,41,48	1.00	2 (4%)	44,47,54	1.08	3 (6%)
36	CLA	b	817	-	59,67,73	1.91	11 (18%)	68,105,113	2.25	18 (26%)
36	CLA	V	308	-	65,73,73	1.43	7 (10%)	76,113,113	1.50	9 (11%)
36	CLA	Q	307	15	50,58,73	1.63	8 (16%)	56,94,113	1.59	7 (12%)
36	CLA	a	829	-	65,73,73	1.45	9 (13%)	76,113,113	1.74	12 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
35	A86	L	304	-	44,50,50	1.39	4 (9%)	51,76,76	2.99	15 (29%)
36	CLA	a	823	-	55,63,73	1.95	11 (20%)	64,101,113	2.18	18 (28%)
36	CLA	a	831	-	65,73,73	1.42	10 (15%)	76,113,113	1.38	9 (11%)
36	CLA	C	207	-	65,73,73	2.00	14 (21%)	76,113,113	2.81	23 (30%)
37	KC1	M	317	-	48,53,53	2.95	21 (43%)	55,89,89	5.39	34 (61%)
36	CLA	O	316	-	65,73,73	1.83	11 (16%)	76,113,113	2.59	25 (32%)
36	CLA	V	313	-	65,73,73	1.46	8 (12%)	76,113,113	1.34	8 (10%)
36	CLA	C	211	-	65,73,73	1.44	10 (15%)	76,113,113	1.46	8 (10%)
44	BCR	a	847	-	41,41,41	1.23	4 (9%)	56,56,56	1.25	5 (8%)
35	A86	K	301	-	44,50,50	1.25	4 (9%)	51,76,76	2.26	13 (25%)
36	CLA	a	822	-	51,59,73	1.89	8 (15%)	59,96,113	2.05	14 (23%)
36	CLA	F	312	-	65,73,73	1.43	7 (10%)	76,113,113	1.44	8 (10%)
36	CLA	G	316	-	49,57,73	1.66	9 (18%)	55,93,113	1.61	7 (12%)
36	CLA	B	306	-	46,54,73	1.71	8 (17%)	53,90,113	1.76	8 (15%)
34	DD6	K	304	-	39,45,45	2.02	3 (7%)	52,67,67	1.87	13 (25%)
45	SF4	c	101	22	0,12,12	-	-	-	-	-
35	A86	G	302	-	44,50,50	1.18	3 (6%)	51,76,76	1.92	13 (25%)
37	KC1	V	312	33	48,53,53	3.13	21 (43%)	55,89,89	5.51	34 (61%)
36	CLA	a	809	-	56,64,73	1.49	9 (16%)	65,102,113	1.51	9 (13%)
37	KC1	N	314	14	48,53,53	3.16	22 (45%)	55,89,89	4.92	33 (60%)
36	CLA	R	316	-	46,54,73	1.73	9 (19%)	53,90,113	2.13	16 (30%)
36	CLA	P	309	41	65,73,73	1.44	8 (12%)	76,113,113	1.48	6 (7%)
35	A86	V	302	-	44,50,50	1.32	4 (9%)	51,76,76	2.92	21 (41%)
36	CLA	O	314	-	41,49,73	1.83	8 (19%)	47,84,113	1.80	7 (14%)
36	CLA	L	313	-	65,73,73	1.39	7 (10%)	76,113,113	1.59	7 (9%)
36	CLA	X	315	-	41,49,73	1.83	5 (12%)	47,84,113	1.78	8 (17%)
39	LMT	E	323	-	36,36,36	0.35	0	47,47,47	0.82	1 (2%)
36	CLA	a	824	-	65,73,73	1.45	8 (12%)	76,113,113	1.94	18 (23%)
35	A86	P	303	-	44,50,50	1.44	6 (13%)	51,76,76	3.47	23 (45%)
36	CLA	A	314	-	65,73,73	1.56	9 (13%)	76,113,113	1.92	12 (15%)
36	CLA	H	316	-	65,73,73	1.45	9 (13%)	76,113,113	1.45	7 (9%)
36	CLA	L	316	-	41,49,73	1.81	6 (14%)	47,84,113	1.75	8 (17%)
36	CLA	P	313	-	65,73,73	1.42	7 (10%)	76,113,113	1.44	6 (7%)
36	CLA	O	310	15	46,54,73	1.72	8 (17%)	53,90,113	1.73	10 (18%)
37	KC1	O	315	15	48,53,53	3.07	20 (41%)	55,89,89	6.90	36 (65%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
36	CLA	L	309	12	65,73,73	1.43	8 (12%)	76,113,113	1.45	8 (10%)
34	DD6	L	305	-	39,45,45	2.04	3 (7%)	52,67,67	2.00	15 (28%)
36	CLA	F	310	-	56,64,73	1.50	7 (12%)	65,102,113	1.64	12 (18%)
39	LMT	h	205	-	36,36,36	0.41	0	47,47,47	0.70	1 (2%)
35	A86	T	301	36	44,50,50	1.25	4 (9%)	51,76,76	2.07	16 (31%)
35	A86	U	301	-	44,50,50	1.37	3 (6%)	51,76,76	3.80	25 (49%)
34	DD6	P	305	-	39,45,45	2.02	3 (7%)	52,67,67	2.06	16 (30%)
36	CLA	E	313	-	65,73,73	1.95	13 (20%)	76,113,113	2.19	20 (26%)
36	CLA	P	318	-	51,59,73	1.66	7 (13%)	59,96,113	1.56	7 (11%)
37	KC1	S	316	-	48,53,53	3.10	20 (41%)	55,89,89	6.04	36 (65%)
36	CLA	W	209	19	57,65,73	1.59	7 (12%)	66,103,113	1.55	10 (15%)
36	CLA	a	836	-	65,73,73	1.34	8 (12%)	76,113,113	1.71	10 (13%)
36	CLA	P	314	-	60,68,73	1.66	9 (15%)	70,107,113	1.70	14 (20%)
35	A86	R	309	-	44,50,50	1.23	4 (9%)	51,76,76	2.84	16 (31%)
36	CLA	b	822	-	46,54,73	1.66	8 (17%)	53,90,113	1.62	9 (16%)
35	A86	N	320	-	44,50,50	1.38	6 (13%)	51,76,76	3.30	24 (47%)
36	CLA	E	316	-	65,73,73	1.45	6 (9%)	76,113,113	1.63	11 (14%)
42	LMG	E	318	-	46,46,55	0.98	2 (4%)	54,54,63	1.06	2 (3%)
35	A86	R	303	-	44,50,50	1.36	5 (11%)	51,76,76	3.63	21 (41%)
36	CLA	D	308	-	65,73,73	1.43	8 (12%)	76,113,113	1.65	12 (15%)
36	CLA	B	308	-	65,73,73	1.41	7 (10%)	76,113,113	1.64	12 (15%)
36	CLA	F	316	6	41,49,73	1.78	9 (21%)	47,84,113	1.66	9 (19%)
36	CLA	S	320	-	65,73,73	1.49	6 (9%)	76,113,113	1.38	8 (10%)
36	CLA	R	319	16	45,53,73	1.75	9 (20%)	52,89,113	2.00	14 (26%)
35	A86	F	302	-	44,50,50	1.24	4 (9%)	51,76,76	1.92	11 (21%)
36	CLA	b	841	41	65,73,73	1.42	12 (18%)	76,113,113	1.99	17 (22%)
39	LMT	U	315	-	36,36,36	0.40	0	47,47,47	0.74	1 (2%)
36	CLA	U	307	-	50,58,73	1.68	8 (16%)	58,95,113	1.51	6 (10%)
36	CLA	C	209	-	65,73,73	1.48	9 (13%)	76,113,113	1.44	9 (11%)
36	CLA	E	314	-	65,73,73	1.36	8 (12%)	76,113,113	1.66	13 (17%)
37	KC1	P	315	35	48,53,53	3.07	21 (43%)	55,89,89	6.91	36 (65%)
36	CLA	W	212	19	65,73,73	1.48	6 (9%)	76,113,113	1.75	10 (13%)
36	CLA	U	306	32	65,73,73	2.14	16 (24%)	76,113,113	2.65	23 (30%)
37	KC1	Q	313	-	48,53,53	3.07	20 (41%)	55,89,89	6.90	36 (65%)
36	CLA	b	820	21	60,68,73	1.50	9 (15%)	70,107,113	1.47	8 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
42	LMG	V	315	-	46,46,55	0.98	2 (4%)	54,54,63	4.29	4 (7%)
35	A86	D	302	-	44,50,50	1.23	4 (9%)	51,76,76	2.08	11 (21%)
35	A86	T	304	-	44,50,50	1.11	3 (6%)	51,76,76	1.69	11 (21%)
44	BCR	a	845	-	41,41,41	1.18	2 (4%)	56,56,56	1.19	5 (8%)
36	CLA	a	826	-	65,73,73	1.40	7 (10%)	76,113,113	1.65	9 (11%)
35	A86	S	303	17	44,50,50	1.32	5 (11%)	51,76,76	3.30	22 (43%)
36	CLA	G	319	7	50,58,73	2.05	14 (28%)	58,95,113	3.97	26 (44%)
36	CLA	X	312	-	41,49,73	1.81	7 (17%)	47,84,113	1.95	8 (17%)
37	KC1	K	314	11	48,53,53	2.91	19 (39%)	55,89,89	5.96	36 (65%)
36	CLA	M	314	-	41,49,73	1.81	7 (17%)	47,84,113	1.71	7 (14%)
36	CLA	b	831	-	50,58,73	1.66	10 (20%)	58,95,113	1.65	8 (13%)
42	LMG	a	852	-	54,54,55	0.90	2 (3%)	62,62,63	1.03	3 (4%)
36	CLA	Q	306	-	65,73,73	1.43	8 (12%)	76,113,113	1.48	6 (7%)
35	A86	K	306	11	44,50,50	1.22	3 (6%)	51,76,76	3.50	21 (41%)
36	CLA	R	315	-	65,73,73	1.44	7 (10%)	76,113,113	1.47	7 (9%)
35	A86	F	306	-	44,50,50	1.26	4 (9%)	51,76,76	2.04	13 (25%)
36	CLA	j	106	27	42,50,73	1.75	9 (21%)	48,85,113	1.74	8 (16%)
35	A86	S	305	-	44,50,50	1.27	3 (6%)	51,76,76	2.95	20 (39%)
37	KC1	A	312	1	48,53,53	2.88	19 (39%)	55,89,89	6.87	40 (72%)
37	KC1	T	310	-	48,53,53	4.86	28 (58%)	55,89,89	7.31	33 (60%)
36	CLA	a	810	36	62,70,73	1.44	8 (12%)	72,109,113	1.51	8 (11%)
36	CLA	W	214	19	41,49,73	2.04	7 (17%)	47,84,113	2.00	14 (29%)
36	CLA	f	802	-	65,73,73	1.51	8 (12%)	76,113,113	1.43	10 (13%)
36	CLA	R	321	16	65,73,73	1.47	7 (10%)	76,113,113	1.58	9 (11%)
36	CLA	N	308	14	65,73,73	1.67	7 (10%)	76,113,113	1.84	20 (26%)
42	LMG	j	105	-	52,52,55	0.91	2 (3%)	60,60,63	1.00	3 (5%)
36	CLA	a	813	-	45,53,73	1.62	10 (22%)	52,89,113	1.89	9 (17%)
35	A86	U	303	36	44,50,50	1.23	4 (9%)	51,76,76	2.00	14 (27%)
37	KC1	M	313	36,13	48,53,53	2.95	20 (41%)	55,89,89	6.15	36 (65%)
36	CLA	O	312	-	39,48,73	2.10	10 (25%)	45,82,113	1.56	8 (17%)
36	CLA	L	320	12	65,73,73	1.43	7 (10%)	76,113,113	1.44	6 (7%)
36	CLA	J	312	10	65,73,73	1.43	7 (10%)	76,113,113	1.57	8 (10%)
35	A86	J	302	-	44,50,50	1.26	4 (9%)	51,76,76	2.08	12 (23%)
35	A86	N	305	-	44,50,50	1.65	8 (18%)	51,76,76	2.29	17 (33%)
36	CLA	T	309	18	65,73,73	1.45	7 (10%)	76,113,113	1.51	9 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
42	LMG	G	324	-	55,55,55	0.90	2 (3%)	63,63,63	1.00	3 (4%)
36	CLA	C	214	-	41,49,73	1.77	9 (21%)	47,84,113	1.72	9 (19%)
36	CLA	T	308	18	61,69,73	1.50	5 (8%)	71,108,113	1.53	9 (12%)
39	LMT	I	318	-	36,36,36	0.39	0	47,47,47	0.75	1 (2%)
36	CLA	I	310	35	65,73,73	1.39	7 (10%)	76,113,113	1.55	7 (9%)
36	CLA	b	807	-	45,53,73	1.66	7 (15%)	52,89,113	1.76	8 (15%)
36	CLA	a	811	-	54,62,73	1.60	8 (14%)	62,99,113	1.51	7 (11%)
36	CLA	T	313	18	65,73,73	1.46	6 (9%)	76,113,113	1.42	9 (11%)
39	LMT	b	851	-	24,24,36	0.42	0	29,29,47	0.81	0
36	CLA	H	309	8	65,73,73	1.44	8 (12%)	76,113,113	1.44	7 (9%)
35	A86	X	302	35	44,50,50	1.22	4 (9%)	51,76,76	2.97	18 (35%)
36	CLA	a	837	-	65,73,73	1.38	7 (10%)	76,113,113	1.53	8 (10%)
36	CLA	S	319	17	65,73,73	1.49	8 (12%)	76,113,113	1.57	11 (14%)
36	CLA	a	830	-	50,58,73	2.05	12 (24%)	58,95,113	3.35	18 (31%)
36	CLA	H	310	8	46,54,73	2.01	10 (21%)	53,90,113	2.83	19 (35%)
36	CLA	A	305	1	49,57,73	1.65	8 (16%)	55,93,113	1.54	7 (12%)
39	LMT	E	321	-	23,23,36	0.45	0	28,28,47	0.59	0
41	LHG	O	318	15	48,48,48	0.88	3 (6%)	51,54,54	1.22	4 (7%)
37	KC1	R	317	-	48,53,53	2.91	20 (41%)	55,89,89	6.06	36 (65%)
35	A86	S	302	-	44,50,50	1.20	3 (6%)	51,76,76	2.68	15 (29%)
36	CLA	a	818	-	65,73,73	1.40	10 (15%)	76,113,113	1.71	10 (13%)
34	DD6	S	307	-	39,45,45	2.03	3 (7%)	52,67,67	2.07	15 (28%)
41	LHG	b	850	36	48,48,48	0.92	2 (4%)	51,54,54	1.04	3 (5%)
34	DD6	E	303	-	39,45,45	2.00	3 (7%)	52,67,67	2.00	10 (19%)
41	LHG	Q	315	36	48,48,48	0.93	2 (4%)	51,54,54	1.04	3 (5%)
36	CLA	F	309	-	65,73,73	1.42	6 (9%)	76,113,113	1.57	11 (14%)
36	CLA	M	310	35,13	46,54,73	2.28	10 (21%)	53,90,113	1.84	13 (24%)
41	LHG	G	320	-	39,39,48	1.04	2 (5%)	42,45,54	1.11	3 (7%)
36	CLA	V	305	35	61,69,73	1.66	7 (11%)	71,108,113	1.57	9 (12%)
36	CLA	A	311	-	65,73,73	1.42	9 (13%)	76,113,113	1.43	7 (9%)
41	LHG	F	319	-	40,40,48	1.03	2 (5%)	43,46,54	1.10	3 (6%)
36	CLA	N	313	14	41,49,73	1.89	8 (19%)	47,84,113	1.90	12 (25%)
36	CLA	a	827	-	62,70,73	1.46	8 (12%)	72,109,113	1.70	10 (13%)
35	A86	P	307	-	44,50,50	1.22	3 (6%)	51,76,76	2.05	13 (25%)
36	CLA	a	820	-	65,73,73	1.39	8 (12%)	76,113,113	1.54	10 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
35	A86	V	304	-	44,50,50	1.48	6 (13%)	51,76,76	3.49	18 (35%)
36	CLA	A	308	-	65,73,73	1.41	7 (10%)	76,113,113	1.59	9 (11%)
36	CLA	I	311	9	65,73,73	1.36	7 (10%)	76,113,113	1.64	9 (11%)
35	A86	X	301	-	44,50,50	1.55	5 (11%)	51,76,76	3.61	28 (54%)
36	CLA	S	314	17	65,73,73	1.57	9 (13%)	76,113,113	1.56	13 (17%)
36	CLA	b	815	-	65,73,73	1.43	8 (12%)	76,113,113	1.48	7 (9%)
36	CLA	b	824	-	53,61,73	2.22	14 (26%)	61,98,113	2.40	22 (36%)
37	KC1	G	317	-	48,53,53	2.92	22 (45%)	55,89,89	5.07	35 (63%)
36	CLA	b	837	-	65,73,73	1.40	8 (12%)	76,113,113	1.59	11 (14%)
35	A86	N	302	-	44,50,50	1.19	3 (6%)	51,76,76	2.68	15 (29%)
35	A86	P	306	-	44,50,50	1.22	3 (6%)	51,76,76	1.89	13 (25%)
36	CLA	K	310	-	62,70,73	1.98	16 (25%)	72,109,113	2.51	26 (36%)
37	KC1	E	309	-	48,53,53	2.94	20 (41%)	55,89,89	5.56	37 (67%)
35	A86	E	307	36	44,50,50	1.24	4 (9%)	51,76,76	2.07	12 (23%)
36	CLA	a	816	-	65,73,73	1.69	9 (13%)	76,113,113	2.11	16 (21%)
36	CLA	H	307	8	60,68,73	1.48	8 (13%)	70,107,113	1.99	18 (25%)
36	CLA	a	803	36	55,63,73	1.53	8 (14%)	64,101,113	1.72	12 (18%)
42	LMG	h	206	-	45,45,55	0.99	2 (4%)	53,53,63	1.03	3 (5%)
37	KC1	W	217	-	48,53,53	3.14	19 (39%)	55,89,89	4.85	35 (63%)
36	CLA	X	307	19,35	50,58,73	1.76	7 (14%)	58,95,113	1.94	13 (22%)
36	CLA	b	810	-	65,73,73	1.36	9 (13%)	76,113,113	1.42	8 (10%)
42	LMG	V	316	-	46,46,55	0.98	2 (4%)	54,54,63	1.04	3 (5%)
36	CLA	R	310	-	61,69,73	1.51	8 (13%)	71,108,113	1.51	6 (8%)
36	CLA	W	207	34	65,73,73	1.47	6 (9%)	76,113,113	1.52	9 (11%)
35	A86	C	204	-	44,50,50	1.84	14 (31%)	51,76,76	2.68	16 (31%)
36	CLA	b	813	-	54,62,73	1.58	9 (16%)	67,100,113	1.47	11 (16%)
44	BCR	b	846	-	41,41,41	1.15	4 (9%)	56,56,56	1.44	10 (17%)
36	CLA	b	827	-	65,73,73	1.57	8 (12%)	76,113,113	1.44	10 (13%)
35	A86	R	306	-	44,50,50	1.34	4 (9%)	51,76,76	2.91	16 (31%)
44	BCR	b	845	-	41,41,41	1.20	3 (7%)	56,56,56	1.37	8 (14%)
36	CLA	J	311	-	46,54,73	1.74	10 (21%)	53,90,113	1.59	9 (16%)
36	CLA	T	312	18	46,54,73	1.74	6 (13%)	53,90,113	1.79	11 (20%)
35	A86	R	305	-	44,50,50	1.22	4 (9%)	51,76,76	1.81	11 (21%)
36	CLA	a	801	-	65,73,73	1.44	10 (15%)	76,113,113	1.61	14 (18%)
36	CLA	B	307	-	46,54,73	1.74	8 (17%)	53,90,113	1.65	9 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
36	CLA	W	208	-	45,53,73	1.75	7 (15%)	52,89,113	1.60	6 (11%)
34	DD6	M	303	-	39,45,45	2.03	3 (7%)	52,67,67	1.96	11 (21%)
36	CLA	H	318	-	50,58,73	1.63	10 (20%)	58,95,113	1.63	10 (17%)
34	DD6	H	303	-	39,45,45	1.99	3 (7%)	52,67,67	1.97	12 (23%)
36	CLA	G	310	-	65,73,73	1.41	9 (13%)	76,113,113	1.36	6 (7%)
36	CLA	b	802	-	65,73,73	1.45	8 (12%)	76,113,113	1.42	9 (11%)
41	LHG	f	809	-	41,41,48	1.01	2 (4%)	44,47,54	1.09	3 (6%)
36	CLA	b	806	-	65,73,73	1.42	9 (13%)	76,113,113	1.76	12 (15%)
37	KC1	J	314	-	48,53,53	2.92	19 (39%)	55,89,89	6.21	35 (63%)
35	A86	G	304	-	44,50,50	1.43	5 (11%)	51,76,76	3.69	25 (49%)
36	CLA	a	834	20	45,53,73	1.75	7 (15%)	52,89,113	1.70	8 (15%)
42	LMG	m	102	-	37,37,55	1.08	2 (5%)	45,45,63	1.08	3 (6%)
34	DD6	D	301	-	39,45,45	2.01	3 (7%)	52,67,67	1.99	13 (25%)
36	CLA	b	832	-	49,57,73	1.52	8 (16%)	55,93,113	1.75	8 (14%)
36	CLA	U	311	32	65,73,73	1.46	8 (12%)	76,113,113	1.65	12 (15%)
35	A86	R	304	16,36	44,50,50	1.30	3 (6%)	51,76,76	2.95	17 (33%)
36	CLA	C	208	-	65,73,73	1.45	9 (13%)	76,113,113	1.43	9 (11%)
36	CLA	L	308	-	61,69,73	1.83	12 (19%)	71,108,113	2.35	17 (23%)
37	KC1	T	315	-	48,53,53	3.05	19 (39%)	55,89,89	5.84	34 (61%)
36	CLA	W	211	19	65,73,73	1.45	7 (10%)	76,113,113	1.60	11 (14%)
35	A86	Q	301	-	44,50,50	1.33	5 (11%)	51,76,76	2.73	17 (33%)
39	LMT	a	851	-	36,36,36	0.43	0	47,47,47	0.74	1 (2%)
36	CLA	V	310	33	65,73,73	1.44	7 (10%)	76,113,113	1.43	7 (9%)
37	KC1	W	213	-	48,53,53	3.12	20 (41%)	55,89,89	5.79	34 (61%)
36	CLA	b	819	-	59,67,73	1.63	9 (15%)	68,105,113	2.04	15 (22%)
41	LHG	i	104	-	45,45,48	0.98	2 (4%)	48,51,54	1.03	2 (4%)
36	CLA	N	307	-	61,69,73	1.53	6 (9%)	71,108,113	1.45	6 (8%)
35	A86	H	304	-	44,50,50	1.24	4 (9%)	51,76,76	2.31	17 (33%)
34	DD6	F	303	-	39,45,45	2.00	3 (7%)	52,67,67	1.91	14 (26%)
36	CLA	P	312	15	46,54,73	1.72	7 (15%)	53,90,113	1.71	10 (18%)
38	SQD	A	315	-	27,28,54	1.50	4 (14%)	36,39,65	1.29	5 (13%)
36	CLA	b	830	-	65,73,73	1.49	10 (15%)	76,113,113	1.82	13 (17%)
36	CLA	H	306	-	61,69,73	1.48	9 (14%)	71,108,113	1.42	6 (8%)
36	CLA	X	306	-	61,69,73	1.54	5 (8%)	71,108,113	1.46	8 (11%)
35	A86	h	202	-	44,50,50	1.24	4 (9%)	51,76,76	1.74	10 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
44	BCR	m	101	-	41,41,41	1.15	4 (9%)	56,56,56	1.34	7 (12%)
41	LHG	a	843	36	26,26,48	1.24	2 (7%)	29,32,54	1.31	2 (6%)
37	KC1	C	213	-	48,53,53	2.99	19 (39%)	55,89,89	4.91	31 (56%)
36	CLA	H	305	8	48,56,73	1.71	7 (14%)	55,92,113	1.59	8 (14%)
36	CLA	b	823	-	55,63,73	1.49	7 (12%)	64,101,113	1.61	7 (10%)
36	CLA	L	314	12	65,73,73	1.41	8 (12%)	76,113,113	1.58	10 (13%)
36	CLA	l	204	28	49,57,73	2.30	14 (28%)	55,93,113	2.26	17 (30%)
36	CLA	P	319	-	60,68,73	2.34	11 (18%)	70,107,113	2.21	15 (21%)
39	LMT	B	313	-	36,36,36	0.43	0	47,47,47	0.73	1 (2%)
36	CLA	B	311	2	55,63,73	1.63	6 (10%)	64,101,113	1.79	13 (20%)
36	CLA	a	835	-	51,59,73	1.65	10 (19%)	59,96,113	1.49	9 (15%)
44	BCR	f	801	-	41,41,41	1.12	2 (4%)	56,56,56	1.19	5 (8%)
34	DD6	Q	302	-	39,45,45	2.04	3 (7%)	52,67,67	2.04	16 (30%)
35	A86	F	304	36	44,50,50	1.25	4 (9%)	51,76,76	2.03	13 (25%)
36	CLA	R	312	-	65,73,73	1.49	9 (13%)	76,113,113	1.59	11 (14%)
36	CLA	b	811	-	65,73,73	1.43	8 (12%)	76,113,113	1.63	10 (13%)
36	CLA	H	315	8	65,73,73	1.48	9 (13%)	76,113,113	1.60	14 (18%)
36	CLA	b	833	-	58,66,73	1.50	8 (13%)	67,104,113	1.63	11 (16%)
36	CLA	a	814	-	50,58,73	1.62	9 (18%)	58,95,113	1.87	10 (17%)
36	CLA	a	812	-	65,73,73	1.41	7 (10%)	76,113,113	1.54	8 (10%)
36	CLA	b	825	-	65,73,73	1.40	9 (13%)	76,113,113	1.54	10 (13%)
42	LMG	J	319	-	44,44,55	0.99	2 (4%)	52,52,63	1.11	3 (5%)
36	CLA	H	308	8	63,72,73	1.45	8 (12%)	73,112,113	1.44	10 (13%)
41	LHG	G	301	-	48,48,48	0.77	2 (4%)	51,54,54	1.28	6 (11%)
41	LHG	F	318	-	32,32,48	0.88	1 (3%)	36,37,54	1.72	6 (16%)
36	CLA	a	839	46	65,73,73	1.38	8 (12%)	76,113,113	1.49	9 (11%)
35	A86	L	319	-	44,50,50	1.43	6 (13%)	51,76,76	3.47	24 (47%)
41	LHG	a	842	-	47,47,48	0.76	1 (2%)	50,53,54	1.27	4 (8%)
36	CLA	D	309	-	55,63,73	2.08	13 (23%)	64,101,113	2.97	25 (39%)
36	CLA	h	203	-	65,73,73	1.40	8 (12%)	76,113,113	1.59	10 (13%)
37	KC1	O	313	15	48,53,53	3.07	21 (43%)	55,89,89	6.91	36 (65%)
36	CLA	T	311	18	65,73,73	1.52	9 (13%)	76,113,113	2.03	16 (21%)
36	CLA	J	316	-	46,54,73	1.72	10 (21%)	53,90,113	1.84	10 (18%)
36	CLA	a	808	20	65,73,73	1.44	10 (15%)	76,113,113	1.50	10 (13%)
44	BCR	a	846	-	41,41,41	1.15	3 (7%)	56,56,56	1.19	3 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
36	CLA	R	314	16	46,54,73	1.74	8 (17%)	53,90,113	1.91	11 (20%)
36	CLA	K	315	-	41,49,73	1.76	7 (17%)	47,84,113	1.86	7 (14%)
36	CLA	G	312	7	58,66,73	1.48	10 (17%)	67,104,113	1.57	8 (11%)
35	A86	N	306	-	44,50,50	1.22	3 (6%)	51,76,76	2.83	16 (31%)
36	CLA	B	305	2	65,73,73	1.44	7 (10%)	76,113,113	1.50	9 (11%)
36	CLA	F	311	-	52,60,73	1.62	9 (17%)	60,97,113	1.62	8 (13%)
35	A86	F	307	-	44,50,50	1.31	3 (6%)	51,76,76	3.94	22 (43%)
36	CLA	W	201	19	48,56,73	1.72	7 (14%)	55,92,113	1.57	7 (12%)
40	DGD	b	849	-	61,61,67	1.05	7 (11%)	75,75,81	1.49	11 (14%)
36	CLA	J	317	10	47,55,73	1.70	9 (19%)	54,91,113	1.50	6 (11%)
35	A86	X	305	-	44,50,50	1.29	4 (9%)	51,76,76	3.04	18 (35%)
36	CLA	D	316	-	52,60,73	1.61	10 (19%)	60,97,113	1.82	13 (21%)
36	CLA	V	309	33	43,51,73	1.76	8 (18%)	49,86,113	2.05	12 (24%)
44	BCR	b	844	-	41,41,41	1.11	3 (7%)	56,56,56	1.31	5 (8%)
36	CLA	X	309	19	44,53,73	1.82	6 (13%)	50,89,113	1.83	12 (24%)
36	CLA	D	317	-	58,66,73	1.52	8 (13%)	67,104,113	1.50	8 (11%)
36	CLA	F	313	-	52,60,73	1.60	9 (17%)	60,97,113	1.55	8 (13%)
36	CLA	b	814	-	55,63,73	1.52	9 (16%)	64,101,113	1.50	7 (10%)
37	KC1	U	312	32,35	48,53,53	3.16	21 (43%)	55,89,89	4.86	31 (56%)
34	DD6	E	304	-	39,45,45	1.99	3 (7%)	52,67,67	1.78	10 (19%)
39	LMT	a	853	-	33,33,36	0.42	0	44,44,47	0.74	1 (2%)
45	SF4	b	803	20,21	0,12,12	-	-	-	-	-
36	CLA	b	821	46	65,73,73	1.43	10 (15%)	76,113,113	1.49	9 (11%)
36	CLA	M	315	13	47,55,73	1.81	10 (21%)	54,91,113	1.68	8 (14%)
44	BCR	l	203	-	41,41,41	1.23	4 (9%)	56,56,56	1.21	5 (8%)
35	A86	I	301	-	44,50,50	1.23	3 (6%)	51,76,76	2.39	18 (35%)
36	CLA	b	828	-	65,73,73	1.45	8 (12%)	76,113,113	1.58	14 (18%)
36	CLA	a	819	-	45,53,73	1.74	10 (22%)	52,89,113	2.32	10 (19%)
36	CLA	D	310	-	65,73,73	1.35	8 (12%)	76,113,113	1.57	8 (10%)
36	CLA	a	838	-	65,73,73	1.41	10 (15%)	76,113,113	1.44	9 (11%)
39	LMT	B	312	-	36,36,36	0.42	0	47,47,47	0.66	1 (2%)
39	LMT	E	320	-	36,36,36	0.37	0	47,47,47	0.67	0
35	A86	F	305	-	44,50,50	1.35	6 (13%)	51,76,76	2.84	20 (39%)
36	CLA	F	314	35,6	65,73,73	1.42	7 (10%)	76,113,113	1.56	10 (13%)
34	DD6	A	303	-	39,45,45	2.00	3 (7%)	52,67,67	1.86	9 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
36	CLA	b	809	-	65,73,73	1.40	8 (12%)	76,113,113	1.39	7 (9%)
36	CLA	S	309	-	61,69,73	1.53	8 (13%)	71,108,113	1.41	8 (11%)
36	CLA	N	319	14	42,50,73	3.74	14 (33%)	48,85,113	6.10	30 (62%)
36	CLA	C	205	-	43,51,73	1.69	7 (16%)	49,86,113	1.74	9 (18%)
41	LHG	R	323	-	48,48,48	0.94	2 (4%)	51,54,54	1.04	3 (5%)
34	DD6	W	204	36	39,45,45	2.04	3 (7%)	52,67,67	2.01	13 (25%)
36	CLA	S	321	-	52,60,73	1.66	8 (15%)	60,97,113	1.76	10 (16%)
36	CLA	b	840	-	65,73,73	1.40	9 (13%)	76,113,113	1.56	13 (17%)
34	DD6	D	304	-	39,45,45	1.97	3 (7%)	52,67,67	1.91	12 (23%)
36	CLA	b	834	-	65,73,73	1.47	8 (12%)	76,113,113	1.41	8 (10%)
36	CLA	C	212	35	65,73,73	1.38	8 (12%)	76,113,113	1.68	12 (15%)
36	CLA	N	316	14	65,73,73	1.47	7 (10%)	76,113,113	1.40	7 (9%)
36	CLA	R	318	35	41,49,73	1.83	7 (17%)	47,84,113	1.76	9 (19%)
36	CLA	l	206	46	50,58,73	1.59	7 (14%)	58,95,113	1.63	8 (13%)
36	CLA	U	305	-	61,69,73	1.52	6 (9%)	71,108,113	1.43	7 (9%)
36	CLA	N	318	-	47,55,73	1.74	6 (12%)	54,91,113	1.84	10 (18%)
37	KC1	H	313	-	48,53,53	2.88	21 (43%)	55,89,89	5.03	32 (58%)
39	LMT	P	321	-	23,23,36	0.43	0	28,28,47	0.61	0
34	DD6	A	304	-	39,45,45	2.00	3 (7%)	52,67,67	1.90	12 (23%)
36	CLA	N	317	14	54,62,73	1.64	6 (11%)	62,99,113	1.66	9 (14%)
35	A86	T	305	18	44,50,50	1.48	5 (11%)	51,76,76	3.68	22 (43%)
34	DD6	H	302	-	39,45,45	1.98	3 (7%)	52,67,67	1.92	15 (28%)
36	CLA	L	310	-	54,62,73	1.61	7 (12%)	62,99,113	1.41	6 (9%)
36	CLA	R	311	16	65,73,73	1.44	6 (9%)	76,113,113	1.48	8 (10%)
40	DGD	L	302	42	48,48,67	0.98	2 (4%)	62,62,81	1.05	4 (6%)
42	LMG	D	321	-	37,37,55	1.08	2 (5%)	45,45,63	1.02	2 (4%)
36	CLA	W	215	-	48,56,73	1.88	8 (16%)	55,92,113	1.50	8 (14%)
44	BCR	b	847	-	41,41,41	1.18	3 (7%)	56,56,56	1.26	7 (12%)
36	CLA	K	311	-	46,54,73	1.75	7 (15%)	53,90,113	1.63	10 (18%)
36	CLA	D	307	41	61,69,73	1.45	8 (13%)	71,108,113	1.73	16 (22%)
37	KC1	F	308	6	48,53,53	2.95	21 (43%)	55,89,89	6.07	33 (60%)
35	A86	T	306	-	44,50,50	1.23	4 (9%)	51,76,76	2.88	18 (35%)
36	CLA	j	101	27	65,73,73	1.40	8 (12%)	76,113,113	1.37	7 (9%)
39	LMT	P	320	-	23,23,36	0.43	0	28,28,47	0.62	0
36	CLA	a	841	41	52,60,73	1.65	8 (15%)	60,97,113	1.64	9 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
37	KC1	P	317	15	48,53,53	2.81	20 (41%)	55,89,89	5.84	35 (63%)
36	CLA	a	825	-	65,73,73	1.53	7 (10%)	76,113,113	1.77	11 (14%)
36	CLA	P	308	-	61,69,73	1.50	9 (14%)	71,108,113	1.46	6 (8%)
36	CLA	G	315	-	56,64,73	1.92	12 (21%)	65,102,113	2.50	19 (29%)
36	CLA	I	312	9	52,60,73	1.67	8 (15%)	60,97,113	1.50	7 (11%)
36	CLA	S	310	17	65,73,73	1.45	7 (10%)	76,113,113	1.70	12 (15%)
36	CLA	b	835	-	45,53,73	1.74	9 (20%)	52,89,113	1.74	10 (19%)
35	A86	N	301	-	44,50,50	1.46	4 (9%)	51,76,76	3.73	26 (50%)
34	DD6	K	305	-	39,45,45	2.00	3 (7%)	52,67,67	2.00	14 (26%)
36	CLA	H	314	-	41,49,73	1.74	8 (19%)	47,84,113	1.95	7 (14%)
36	CLA	R	313	-	65,73,73	1.41	8 (12%)	76,113,113	1.37	7 (9%)
36	CLA	a	848	36	65,73,73	1.72	11 (16%)	76,113,113	1.97	19 (25%)
36	CLA	E	310	-	65,73,73	1.47	6 (9%)	76,113,113	1.59	9 (11%)
36	CLA	R	320	16	45,53,73	1.80	8 (17%)	52,89,113	1.86	14 (26%)
36	CLA	I	309	9	46,54,73	1.74	7 (15%)	53,90,113	2.08	10 (18%)
36	CLA	G	307	-	41,50,73	2.21	12 (29%)	46,85,113	3.26	17 (36%)
36	CLA	I	308	9	65,73,73	2.07	15 (23%)	76,113,113	2.55	21 (27%)
44	BCR	i	101	-	41,41,41	1.09	2 (4%)	56,56,56	1.25	7 (12%)
36	CLA	b	838	-	47,55,73	1.59	7 (14%)	54,91,113	1.66	8 (14%)
36	CLA	I	313	-	41,49,73	1.79	7 (17%)	47,84,113	1.73	7 (14%)
36	CLA	O	311	-	58,66,73	1.51	7 (12%)	67,104,113	1.51	6 (8%)
35	A86	J	301	-	44,50,50	1.26	4 (9%)	51,76,76	2.23	18 (35%)
36	CLA	b	808	-	65,73,73	1.42	8 (12%)	76,113,113	1.49	10 (13%)
36	CLA	K	313	-	65,73,73	1.44	9 (13%)	76,113,113	1.62	10 (13%)
34	DD6	a	849	-	39,45,45	2.01	3 (7%)	52,67,67	1.84	13 (25%)
36	CLA	b	812	21	65,73,73	1.41	9 (13%)	76,113,113	1.61	13 (17%)
36	CLA	V	306	33	65,73,73	1.50	6 (9%)	76,113,113	1.62	11 (14%)
36	CLA	P	311	-	65,73,73	1.45	7 (10%)	76,113,113	1.54	10 (13%)
36	CLA	K	316	-	65,73,73	1.45	9 (13%)	76,113,113	1.32	5 (6%)
35	A86	U	302	-	44,50,50	1.33	4 (9%)	51,76,76	3.12	22 (43%)
34	DD6	B	302	-	39,45,45	2.01	3 (7%)	52,67,67	2.07	16 (30%)
36	CLA	G	311	-	65,73,73	1.40	9 (13%)	76,113,113	1.40	8 (10%)
41	LHG	E	322	-	48,48,48	0.93	2 (4%)	51,54,54	0.99	2 (3%)
39	LMT	L	303	-	36,36,36	1.33	6 (16%)	47,47,47	0.96	1 (2%)
35	A86	h	204	-	44,50,50	1.23	4 (9%)	51,76,76	2.14	11 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
36	CLA	f	803	-	65,73,73	1.81	14 (21%)	76,113,113	2.45	24 (31%)
39	LMT	G	322	-	36,36,36	0.39	0	47,47,47	0.69	0
36	CLA	M	309	-	65,73,73	1.46	7 (10%)	76,113,113	1.40	7 (9%)
35	A86	Q	316	15,36	44,50,50	1.65	8 (18%)	51,76,76	2.29	17 (33%)
36	CLA	D	306	4	45,53,73	1.81	9 (20%)	52,89,113	1.80	10 (19%)
39	LMT	G	323	-	36,36,36	0.39	0	47,47,47	0.82	0
36	CLA	A	309	1	46,54,73	1.73	9 (19%)	53,90,113	1.61	6 (11%)
39	LMT	K	317	-	32,32,36	0.43	0	43,43,47	0.70	0
36	CLA	U	308	32,35	56,64,73	1.59	8 (14%)	65,102,113	1.75	10 (15%)
34	DD6	D	303	-	39,45,45	2.97	8 (20%)	52,67,67	2.65	18 (34%)
34	DD6	G	303	-	39,45,45	1.99	3 (7%)	52,67,67	1.83	10 (19%)
35	A86	T	303	-	44,50,50	1.22	4 (9%)	51,76,76	3.14	21 (41%)
34	DD6	W	205	-	39,45,45	1.99	3 (7%)	52,67,67	2.03	15 (28%)
41	LHG	G	321	36	46,46,48	0.96	2 (4%)	49,52,54	1.06	2 (4%)
36	CLA	U	313	-	41,49,73	1.87	7 (17%)	47,84,113	1.92	11 (23%)
36	CLA	D	315	-	41,49,73	1.70	7 (17%)	47,84,113	2.05	9 (19%)
44	BCR	j	107	-	41,41,41	1.11	2 (4%)	56,56,56	1.22	7 (12%)
35	A86	X	303	36	44,50,50	1.47	5 (11%)	51,76,76	3.76	24 (47%)
37	KC1	X	311	-	48,53,53	3.14	19 (39%)	55,89,89	4.85	34 (61%)
36	CLA	I	307	-	54,62,73	1.51	8 (14%)	62,99,113	1.66	8 (12%)
39	LMT	L	318	-	32,32,36	0.45	0	43,43,47	0.79	1 (2%)
36	CLA	P	302	-	42,50,73	1.72	7 (16%)	48,85,113	1.92	9 (18%)
35	A86	C	202	3,36	44,50,50	1.40	5 (11%)	51,76,76	3.09	17 (33%)
36	CLA	b	826	21,46	64,72,73	1.48	10 (15%)	74,111,113	2.11	17 (22%)
36	CLA	E	317	-	46,54,73	1.76	7 (15%)	53,90,113	1.54	7 (13%)
37	KC1	F	315	-	48,53,53	2.84	18 (37%)	55,89,89	6.66	33 (60%)
39	LMT	F	321	-	34,34,36	0.65	0	45,45,47	1.61	6 (13%)
36	CLA	b	805	36	65,73,73	1.42	10 (15%)	76,113,113	1.40	14 (18%)
36	CLA	X	308	19	47,55,73	3.10	10 (21%)	54,91,113	2.43	19 (35%)
37	KC1	G	318	-	48,53,53	2.98	21 (43%)	55,89,89	4.77	36 (65%)
36	CLA	S	318	-	42,50,73	1.83	6 (14%)	48,85,113	1.77	9 (18%)
35	A86	S	301	-	44,50,50	1.46	4 (9%)	51,76,76	3.73	26 (50%)
36	CLA	J	310	-	65,73,73	1.39	7 (10%)	76,113,113	1.50	7 (9%)
36	CLA	l	205	-	65,73,73	1.53	10 (15%)	76,113,113	2.19	18 (23%)
35	A86	O	302	-	44,50,50	1.44	6 (13%)	51,76,76	3.47	23 (45%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
35	A86	M	302	-	44,50,50	1.29	4 (9%)	51,76,76	2.78	16 (31%)
36	CLA	T	314	-	65,73,73	1.44	7 (10%)	76,113,113	1.68	12 (15%)
36	CLA	X	313	19	42,50,73	2.62	8 (19%)	48,85,113	4.07	18 (37%)
36	CLA	G	314	7	41,49,73	1.79	9 (21%)	47,84,113	1.82	9 (19%)
34	DD6	E	306	-	39,45,45	2.03	3 (7%)	52,67,67	2.04	10 (19%)
39	LMT	I	317	-	36,36,36	0.41	0	47,47,47	0.75	1 (2%)
36	CLA	K	312	-	65,73,73	1.42	7 (10%)	76,113,113	1.45	7 (9%)
39	LMT	K	318	-	36,36,36	0.41	0	47,47,47	0.72	1 (2%)
35	A86	A	302	-	44,50,50	1.61	6 (13%)	51,76,76	4.76	25 (49%)
41	LHG	a	850	-	46,46,48	0.96	2 (4%)	49,52,54	1.04	3 (6%)
36	CLA	E	312	-	65,73,73	1.42	7 (10%)	76,113,113	1.57	9 (11%)
36	CLA	N	310	14	41,49,73	1.96	10 (24%)	47,84,113	2.42	15 (31%)
36	CLA	a	815	46	45,53,73	1.73	8 (17%)	52,89,113	1.63	6 (11%)
36	CLA	a	807	20	65,73,73	1.37	7 (10%)	76,113,113	1.63	12 (15%)
36	CLA	K	309	-	59,67,73	1.53	9 (15%)	68,105,113	1.41	8 (11%)
36	CLA	H	312	8	65,73,73	1.41	10 (15%)	76,113,113	1.57	13 (17%)
36	CLA	a	805	20	65,73,73	1.40	10 (15%)	76,113,113	1.43	9 (11%)
44	BCR	i	103	-	41,41,41	1.19	3 (7%)	56,56,56	1.32	7 (12%)
42	LMG	E	319	-	40,40,55	1.04	2 (5%)	48,48,63	1.11	3 (6%)
35	A86	S	304	-	44,50,50	1.24	4 (9%)	51,76,76	2.13	16 (31%)
35	A86	R	302	16	44,50,50	1.38	5 (11%)	51,76,76	2.80	15 (29%)
39	LMT	b	848	-	36,36,36	0.38	0	47,47,47	0.67	1 (2%)
34	DD6	R	307	-	39,45,45	2.00	2 (5%)	52,67,67	2.11	15 (28%)
36	CLA	L	312	12	46,54,73	1.77	8 (17%)	53,90,113	1.91	10 (18%)
36	CLA	P	301	15	65,73,73	1.44	8 (12%)	76,113,113	1.56	10 (13%)
34	DD6	O	304	-	39,45,45	1.90	3 (7%)	52,67,67	2.00	14 (26%)
36	CLA	A	307	-	60,68,73	1.46	7 (11%)	70,107,113	1.50	10 (14%)
36	CLA	G	309	7	65,73,73	1.38	8 (12%)	76,113,113	1.95	14 (18%)
36	CLA	W	210	-	46,54,73	1.69	6 (13%)	53,90,113	2.10	14 (26%)
35	A86	J	305	-	44,50,50	1.24	3 (6%)	51,76,76	2.08	15 (29%)
36	CLA	M	312	36,13	47,55,73	1.71	9 (19%)	54,91,113	1.71	9 (16%)
43	PQN	a	840	-	34,34,34	1.58	2 (5%)	42,45,45	1.15	4 (9%)
36	CLA	Q	305	-	61,69,73	1.50	8 (13%)	71,108,113	1.46	6 (8%)
35	A86	M	301	-	44,50,50	1.36	4 (9%)	51,76,76	3.39	22 (43%)
36	CLA	P	316	-	41,49,73	1.84	8 (19%)	47,84,113	1.81	7 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
35	A86	G	305	-	44,50,50	1.23	3 (6%)	51,76,76	2.23	15 (29%)
36	CLA	G	313	7	65,73,73	1.49	6 (9%)	76,113,113	1.96	14 (18%)
44	BCR	l	207	-	41,41,41	1.08	2 (4%)	56,56,56	1.35	8 (14%)
42	LMG	J	318	-	55,55,55	0.89	2 (3%)	63,63,63	1.02	3 (4%)
36	CLA	D	312	-	65,73,73	1.46	9 (13%)	76,113,113	1.40	9 (11%)
36	CLA	b	818	-	55,63,73	1.53	7 (12%)	64,101,113	1.79	11 (17%)
36	CLA	C	210	3	46,54,73	1.79	6 (13%)	53,90,113	1.68	9 (16%)
35	A86	J	306	-	44,50,50	1.25	3 (6%)	51,76,76	1.96	11 (21%)
35	A86	O	301	-	44,50,50	1.25	4 (9%)	51,76,76	2.07	14 (27%)
35	A86	N	304	-	44,50,50	2.90	7 (15%)	51,76,76	7.45	18 (35%)
36	CLA	E	315	-	65,73,73	1.96	15 (23%)	76,113,113	2.57	24 (31%)
36	CLA	S	315	17	43,51,73	1.91	9 (20%)	49,86,113	2.11	10 (20%)
35	A86	G	306	-	44,50,50	1.21	4 (9%)	51,76,76	2.34	18 (35%)
36	CLA	O	309	-	65,73,73	1.46	8 (12%)	76,113,113	1.53	10 (13%)
35	A86	E	302	-	44,50,50	1.23	4 (9%)	51,76,76	2.19	13 (25%)
35	A86	A	316	-	44,50,50	1.23	4 (9%)	51,76,76	2.16	16 (31%)
35	A86	V	301	35	44,50,50	1.23	4 (9%)	51,76,76	2.22	16 (31%)
42	LMG	I	315	-	55,55,55	0.89	2 (3%)	63,63,63	1.00	3 (4%)
34	DD6	B	304	-	39,45,45	2.01	3 (7%)	52,67,67	2.14	16 (30%)
35	A86	K	303	-	44,50,50	1.31	4 (9%)	51,76,76	2.80	17 (33%)
35	A86	S	308	37	44,50,50	1.23	4 (9%)	51,76,76	2.12	16 (31%)
36	CLA	l	202	28	65,73,73	1.44	9 (13%)	76,113,113	1.40	10 (13%)
36	CLA	D	313	-	65,73,73	1.36	7 (10%)	76,113,113	1.66	11 (14%)
41	LHG	f	808	25	48,48,48	0.95	2 (4%)	51,54,54	1.02	3 (5%)
36	CLA	J	309	-	65,73,73	1.45	6 (9%)	76,113,113	1.34	7 (9%)
36	CLA	b	801	46	65,73,73	1.46	8 (12%)	76,113,113	1.57	11 (14%)
36	CLA	J	308	-	61,69,73	1.47	6 (9%)	71,108,113	1.76	11 (15%)
36	CLA	i	102	26	65,73,73	1.44	7 (10%)	76,113,113	1.59	8 (10%)
36	CLA	X	310	19	41,49,73	1.88	7 (17%)	47,84,113	2.18	11 (23%)
36	CLA	D	311	-	46,54,73	1.71	9 (19%)	53,90,113	1.63	7 (13%)
36	CLA	b	816	-	60,68,73	1.92	12 (20%)	70,107,113	2.01	18 (25%)
35	A86	C	203	-	44,50,50	1.24	4 (9%)	51,76,76	2.07	16 (31%)
36	CLA	N	315	-	41,49,73	1.82	6 (14%)	47,84,113	1.98	10 (21%)
37	KC1	L	317	-	48,53,53	2.96	20 (41%)	55,89,89	5.42	36 (65%)
36	CLA	S	313	-	46,54,73	1.74	6 (13%)	53,90,113	1.99	12 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
36	CLA	J	313	-	65,73,73	1.44	9 (13%)	76,113,113	1.44	8 (10%)
36	CLA	a	832	-	65,73,73	1.40	9 (13%)	76,113,113	1.59	13 (17%)
36	CLA	N	309	14	51,59,73	1.67	9 (17%)	59,96,113	1.81	8 (13%)
35	A86	B	301	-	44,50,50	1.23	4 (9%)	51,76,76	1.98	13 (25%)
36	CLA	S	317	-	41,49,73	1.84	6 (14%)	47,84,113	1.70	8 (17%)
42	LMG	G	325	-	55,55,55	0.89	2 (3%)	63,63,63	1.01	3 (4%)
36	CLA	T	316	-	41,49,73	1.82	7 (17%)	47,84,113	1.71	7 (14%)
42	LMG	L	321	40	33,33,55	1.13	2 (6%)	41,41,63	1.15	3 (7%)
36	CLA	a	817	-	65,73,73	1.38	8 (12%)	76,113,113	1.84	13 (17%)
41	LHG	j	104	-	48,48,48	0.93	2 (4%)	51,54,54	1.04	3 (5%)
35	A86	T	302	18	44,50,50	1.24	3 (6%)	51,76,76	2.85	21 (41%)
36	CLA	f	805	25	52,60,73	1.55	7 (13%)	60,97,113	1.65	9 (15%)
35	A86	V	303	35	44,50,50	1.28	4 (9%)	51,76,76	3.25	22 (43%)
36	CLA	H	317	8	65,73,73	1.46	8 (12%)	76,113,113	1.37	7 (9%)
37	KC1	G	308	-	48,53,53	2.94	21 (43%)	55,89,89	5.62	35 (63%)
35	A86	L	301	-	44,50,50	1.25	4 (9%)	51,76,76	2.01	14 (27%)
36	CLA	K	307	-	61,69,73	1.91	13 (21%)	71,108,113	2.94	22 (30%)
36	CLA	j	102	-	65,73,73	1.77	10 (15%)	76,113,113	2.26	18 (23%)
36	CLA	a	806	-	65,73,73	1.72	9 (13%)	76,113,113	1.90	17 (22%)
41	LHG	D	319	42	48,48,48	0.93	2 (4%)	51,54,54	1.06	3 (5%)
36	CLA	H	311	-	65,73,73	1.36	7 (10%)	76,113,113	1.59	9 (11%)
35	A86	O	303	-	44,50,50	1.34	5 (11%)	51,76,76	2.73	17 (33%)
35	A86	I	304	-	44,50,50	1.47	4 (9%)	51,76,76	3.38	21 (41%)
36	CLA	N	312	-	47,55,73	1.62	6 (12%)	54,91,113	1.65	6 (11%)
36	CLA	V	314	-	65,73,73	1.98	14 (21%)	76,113,113	2.97	22 (28%)
35	A86	J	303	-	44,50,50	1.41	4 (9%)	51,76,76	2.80	20 (39%)
38	SQD	b	804	-	45,46,54	1.27	4 (8%)	54,57,65	1.21	4 (7%)
36	CLA	A	310	-	65,73,73	1.40	8 (12%)	76,113,113	1.49	7 (9%)
36	CLA	J	315	-	41,49,73	1.77	7 (17%)	47,84,113	1.81	8 (17%)
36	CLA	M	306	37,13	55,63,73	1.52	10 (18%)	64,101,113	1.57	11 (17%)
36	CLA	L	311	-	65,73,73	1.42	8 (12%)	76,113,113	1.48	9 (11%)
36	CLA	K	308	-	65,73,73	1.45	6 (9%)	76,113,113	1.50	8 (10%)
35	A86	O	319	35,36	44,50,50	1.28	5 (11%)	51,76,76	2.93	18 (35%)
35	A86	M	305	-	44,50,50	1.34	4 (9%)	51,76,76	2.88	15 (29%)
36	CLA	R	322	16	52,60,73	1.66	7 (13%)	60,97,113	1.77	11 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
36	CLA	A	306	-	61,69,73	1.93	13 (21%)	71,108,113	2.41	25 (35%)
37	KC1	B	310	2	48,53,53	3.13	20 (41%)	55,89,89	5.04	34 (61%)
35	A86	Q	304	-	44,50,50	1.39	6 (13%)	51,76,76	3.30	24 (47%)
36	CLA	W	216	19,35	45,53,73	2.27	10 (22%)	52,89,113	2.80	14 (26%)
36	CLA	F	317	6	56,64,73	1.95	13 (23%)	65,102,113	2.70	23 (35%)
40	DGD	C	215	-	58,58,67	0.90	2 (3%)	72,72,81	0.96	3 (4%)
34	DD6	D	305	-	39,45,45	2.00	3 (7%)	52,67,67	1.63	9 (17%)

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
35	A86	O	305	-	-	14/34/90/90	0/3/3/3
45	SF4	c	102	-	-	-	0/6/5/5
36	CLA	I	306	9	2/2/15/20	15/37/115/115	-
34	DD6	J	304	-	-	5/26/80/80	0/3/3/3
39	LMT	F	320	-	-	12/21/61/61	0/2/2/2
34	DD6	I	303	-	-	4/26/80/80	0/3/3/3
36	CLA	M	307	-	1/1/15/20	12/37/115/115	-
35	A86	I	302	-	-	7/34/90/90	0/3/3/3
35	A86	N	303	-	-	4/34/90/90	0/3/3/3
36	CLA	B	309	2	1/1/12/20	6/22/100/115	-
36	CLA	E	311	-	1/1/15/20	16/37/115/115	-
36	CLA	b	839	-	1/1/15/20	4/37/115/115	-
35	A86	K	302	-	-	8/34/90/90	0/3/3/3
34	DD6	S	306	-	-	5/26/80/80	0/3/3/3
36	CLA	S	311	35	1/1/11/20	2/15/93/115	-
34	DD6	j	103	-	-	9/26/80/80	0/3/3/3
36	CLA	E	308	5	1/1/11/20	8/18/96/115	-
36	CLA	Q	312	-	1/1/10/20	3/8/86/115	-
35	A86	B	303	-	-	13/34/90/90	0/3/3/3
35	A86	M	304	-	-	14/34/90/90	0/3/3/3
36	CLA	S	312	17	-	17/37/115/115	-
41	LHG	l	208	-	-	34/52/52/53	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
34	DD6	R	308	-	-	10/26/80/80	0/3/3/3
44	BCR	h	201	-	-	9/29/63/63	0/2/2/2
35	A86	U	304	32,37	-	11/34/90/90	0/3/3/3
34	DD6	A	301	-	-	7/26/80/80	0/3/3/3
34	DD6	E	301	-	-	4/26/80/80	0/3/3/3
37	KC1	M	318	-	-	10/15/71/71	-
36	CLA	O	307	-	1/1/15/20	14/37/115/115	-
36	CLA	W	218	19	1/1/10/20	9/11/89/115	-
36	CLA	J	307	10	1/1/14/20	9/33/111/115	-
35	A86	X	314	19	-	3/34/90/90	1/3/3/3
36	CLA	Q	309	15	1/1/11/20	7/15/93/115	-
42	LMG	D	320	41	-	24/41/61/70	0/1/1/1
36	CLA	Q	308	-	1/1/15/20	18/37/115/115	-
36	CLA	P	310	41,15	1/1/15/20	11/37/115/115	-
36	CLA	M	311	35,13	1/1/15/20	10/37/115/115	-
36	CLA	a	833	-	1/1/12/20	2/19/97/115	-
44	BCR	f	806	-	-	9/29/63/63	0/2/2/2
35	A86	Q	303	-	-	8/34/90/90	0/3/3/3
37	KC1	Q	311	15	-	2/15/71/71	-
36	CLA	V	307	-	1/1/12/20	5/21/99/115	-
39	LMT	a	854	-	-	16/21/61/61	0/2/2/2
35	A86	X	304	19	-	7/34/90/90	0/3/3/3
34	DD6	C	201	-	-	7/26/80/80	0/3/3/3
36	CLA	I	305	-	2/2/14/20	10/33/111/115	-
36	CLA	a	804	-	1/1/15/20	16/37/115/115	-
36	CLA	b	836	-	1/1/13/20	8/29/107/115	-
36	CLA	A	313	-	1/1/10/20	2/8/86/115	-
36	CLA	M	316	36	1/1/10/20	4/10/88/115	-
35	A86	E	305	5	-	5/34/90/90	0/3/3/3
36	CLA	a	821	-	1/1/11/20	4/18/96/115	-
36	CLA	l	201	-	1/1/15/20	16/37/115/115	-
44	BCR	b	843	-	-	9/29/63/63	0/2/2/2
36	CLA	I	314	-	1/1/10/20	0/8/86/115	-
35	A86	L	307	-	-	8/34/90/90	1/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
36	CLA	W	206	19	1/1/14/20	10/33/111/115	-
36	CLA	a	828	-	1/1/15/20	20/37/115/115	-
35	A86	F	301	-	-	4/34/90/90	0/3/3/3
36	CLA	f	804	46	2/2/15/20	10/37/115/115	-
41	LHG	I	316	-	-	30/53/53/53	-
37	KC1	L	315	12,35	-	6/15/71/71	-
36	CLA	U	310	-	1/1/15/20	17/37/115/115	-
39	LMT	f	807	-	-	7/15/35/61	0/1/1/2
37	KC1	D	314	4	-	5/15/71/71	-
36	CLA	U	309	32	-	4/15/93/115	-
36	CLA	O	308	15	1/1/15/20	13/37/115/115	-
36	CLA	M	308	-	1/1/12/20	5/22/100/115	-
39	LMT	U	314	-	-	14/21/61/61	0/2/2/2
36	CLA	Q	314	-	1/1/15/20	22/37/115/115	-
35	A86	L	306	37	-	10/34/90/90	0/3/3/3
36	CLA	C	206	-	1/1/14/20	15/33/111/115	-
35	A86	W	202	19,36	-	8/34/90/90	0/3/3/3
44	BCR	a	844	-	-	6/29/63/63	0/2/2/2
35	A86	P	304	-	-	6/34/90/90	0/3/3/3
36	CLA	a	802	-	2/2/15/20	11/37/115/115	-
35	A86	H	301	-	-	5/34/90/90	0/3/3/3
36	CLA	Q	310	15	-	20/37/115/115	-
41	LHG	D	318	36	-	30/50/50/53	-
35	A86	R	301	-	-	9/34/90/90	0/3/3/3
36	CLA	b	829	-	1/1/15/20	9/37/115/115	-
36	CLA	V	311	33	1/1/15/20	13/37/115/115	-
36	CLA	O	306	-	1/1/14/20	9/33/111/115	-
43	PQN	b	842	-	-	11/23/43/43	0/2/2/2
36	CLA	N	311	14	1/1/11/20	4/15/93/115	-
35	A86	T	307	-	-	9/34/90/90	0/3/3/3
35	A86	W	203	36	-	6/34/90/90	0/3/3/3
41	LHG	O	317	-	-	33/46/46/53	-
36	CLA	b	817	-	2/2/13/20	9/30/108/115	-
36	CLA	V	308	-	1/1/15/20	18/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
36	CLA	Q	307	15	1/1/11/20	4/19/97/115	-
36	CLA	a	829	-	1/1/15/20	13/37/115/115	-
35	A86	L	304	-	-	6/34/90/90	0/3/3/3
36	CLA	a	823	-	2/2/13/20	10/25/103/115	-
36	CLA	a	831	-	1/1/15/20	14/37/115/115	-
36	CLA	C	207	-	1/1/15/20	16/37/115/115	-
37	KC1	M	317	-	-	3/15/71/71	-
36	CLA	O	316	-	1/1/15/20	26/37/115/115	-
36	CLA	V	313	-	1/1/15/20	13/37/115/115	-
36	CLA	C	211	-	1/1/15/20	11/37/115/115	-
44	BCR	a	847	-	-	6/29/63/63	0/2/2/2
35	A86	K	301	-	-	6/34/90/90	1/3/3/3
36	CLA	a	822	-	1/1/12/20	4/21/99/115	-
36	CLA	F	312	-	1/1/15/20	20/37/115/115	-
36	CLA	G	316	-	1/1/11/20	8/18/96/115	-
36	CLA	B	306	-	1/1/11/20	4/15/93/115	-
34	DD6	K	304	-	-	2/26/80/80	0/3/3/3
45	SF4	c	101	22	-	-	0/6/5/5
35	A86	G	302	-	-	7/34/90/90	0/3/3/3
37	KC1	V	312	33	-	7/15/71/71	-
36	CLA	a	809	-	1/1/13/20	9/27/105/115	-
37	KC1	N	314	14	-	7/15/71/71	-
36	CLA	R	316	-	1/1/11/20	8/15/93/115	-
36	CLA	P	309	41	1/1/15/20	14/37/115/115	-
36	CLA	O	314	-	1/1/10/20	3/8/86/115	-
35	A86	V	302	-	-	5/34/90/90	0/3/3/3
36	CLA	L	313	-	1/1/15/20	8/37/115/115	-
36	CLA	X	315	-	-	3/8/86/115	-
39	LMT	E	323	-	-	11/21/61/61	0/2/2/2
36	CLA	a	824	-	1/1/15/20	11/37/115/115	-
35	A86	P	303	-	-	9/34/90/90	0/3/3/3
36	CLA	A	314	-	1/1/15/20	20/37/115/115	-
36	CLA	H	316	-	1/1/15/20	16/37/115/115	-
36	CLA	L	316	-	1/1/10/20	1/8/86/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
36	CLA	P	313	-	1/1/15/20	12/37/115/115	-
36	CLA	O	310	15	1/1/11/20	7/15/93/115	-
37	KC1	O	315	15	-	2/15/71/71	-
36	CLA	L	309	12	1/1/15/20	12/37/115/115	-
34	DD6	L	305	-	-	7/26/80/80	0/3/3/3
36	CLA	F	310	-	1/1/13/20	10/27/105/115	-
39	LMT	h	205	-	-	10/21/61/61	0/2/2/2
35	A86	T	301	36	-	4/34/90/90	1/3/3/3
35	A86	U	301	-	-	8/34/90/90	0/3/3/3
34	DD6	P	305	-	-	2/26/80/80	0/3/3/3
36	CLA	E	313	-	2/2/15/20	8/37/115/115	-
36	CLA	P	318	-	1/1/12/20	7/21/99/115	-
37	KC1	S	316	-	-	6/15/71/71	-
36	CLA	W	209	19	1/1/13/20	13/28/106/115	-
36	CLA	a	836	-	1/1/15/20	11/37/115/115	-
36	CLA	P	314	-	-	21/31/109/115	-
36	CLA	b	822	-	1/1/11/20	5/15/93/115	-
35	A86	R	309	-	-	8/34/90/90	0/3/3/3
36	CLA	E	316	-	1/1/15/20	17/37/115/115	-
35	A86	N	320	-	-	10/34/90/90	0/3/3/3
42	LMG	E	318	-	-	24/41/61/70	0/1/1/1
35	A86	R	303	-	-	7/34/90/90	0/3/3/3
36	CLA	D	308	-	1/1/15/20	16/37/115/115	-
36	CLA	B	308	-	1/1/15/20	14/37/115/115	-
36	CLA	F	316	6	1/1/10/20	1/8/86/115	-
36	CLA	S	320	-	-	16/37/115/115	-
36	CLA	R	319	16	1/1/11/20	5/13/91/115	-
35	A86	F	302	-	-	8/34/90/90	0/3/3/3
36	CLA	b	841	41	1/1/15/20	9/37/115/115	-
39	LMT	U	315	-	-	17/21/61/61	0/2/2/2
36	CLA	U	307	-	1/1/12/20	1/19/97/115	-
36	CLA	C	209	-	1/1/15/20	10/37/115/115	-
36	CLA	E	314	-	1/1/15/20	8/37/115/115	-
37	KC1	P	315	35	-	2/15/71/71	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
36	CLA	W	212	19	-	15/37/115/115	-
36	CLA	U	306	32	1/1/15/20	20/37/115/115	-
37	KC1	Q	313	-	-	2/15/71/71	-
36	CLA	b	820	21	1/1/14/20	15/31/109/115	-
42	LMG	V	315	-	-	24/41/61/70	0/1/1/1
35	A86	D	302	-	-	7/34/90/90	0/3/3/3
35	A86	T	304	-	-	0/34/90/90	0/3/3/3
44	BCR	a	845	-	-	9/29/63/63	0/2/2/2
36	CLA	a	826	-	1/1/15/20	12/37/115/115	-
35	A86	S	303	17	-	4/34/90/90	0/3/3/3
36	CLA	X	312	-	1/1/10/20	3/8/86/115	-
36	CLA	G	319	7	1/1/12/20	8/19/97/115	-
37	KC1	K	314	11	-	5/15/71/71	-
36	CLA	M	314	-	1/1/10/20	2/8/86/115	-
36	CLA	b	831	-	1/1/12/20	7/19/97/115	-
42	LMG	a	852	-	-	26/49/69/70	0/1/1/1
36	CLA	Q	306	-	1/1/15/20	14/37/115/115	-
36	CLA	R	315	-	1/1/15/20	11/37/115/115	-
35	A86	K	306	11	-	8/34/90/90	0/3/3/3
36	CLA	j	106	27	1/1/10/20	6/10/88/115	-
35	A86	F	306	-	-	0/34/90/90	1/3/3/3
35	A86	S	305	-	-	9/34/90/90	0/3/3/3
37	KC1	A	312	1	-	2/15/71/71	-
37	KC1	T	310	-	-	11/15/71/71	-
36	CLA	a	810	36	1/1/14/20	15/34/112/115	-
36	CLA	W	214	19	-	3/8/86/115	-
36	CLA	f	802	-	1/1/15/20	16/37/115/115	-
36	CLA	R	321	16	-	9/37/115/115	-
36	CLA	N	308	14	1/1/15/20	15/37/115/115	-
42	LMG	j	105	-	-	31/47/67/70	0/1/1/1
36	CLA	a	813	-	1/1/11/20	2/13/91/115	-
35	A86	U	303	36	-	17/34/90/90	0/3/3/3
37	KC1	M	313	36,13	-	5/15/71/71	-
36	CLA	O	312	-	-	4/8/82/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
36	CLA	L	320	12	1/1/15/20	11/37/115/115	-
36	CLA	J	312	10	1/1/15/20	10/37/115/115	-
35	A86	J	302	-	-	5/34/90/90	1/3/3/3
35	A86	N	305	-	-	2/34/90/90	0/3/3/3
36	CLA	T	309	18	1/1/15/20	18/37/115/115	-
42	LMG	G	324	-	-	31/50/70/70	0/1/1/1
36	CLA	C	214	-	1/1/10/20	2/8/86/115	-
36	CLA	T	308	18	1/1/14/20	8/33/111/115	-
39	LMT	I	318	-	-	17/21/61/61	0/2/2/2
36	CLA	I	310	35	1/1/15/20	10/37/115/115	-
36	CLA	b	807	-	1/1/11/20	3/13/91/115	-
36	CLA	a	811	-	1/1/12/20	6/24/102/115	-
36	CLA	T	313	18	1/1/15/20	8/37/115/115	-
39	LMT	b	851	-	-	7/15/35/61	0/1/1/2
36	CLA	H	309	8	1/1/15/20	15/37/115/115	-
35	A86	X	302	35	-	6/34/90/90	0/3/3/3
36	CLA	a	837	-	1/1/15/20	10/37/115/115	-
36	CLA	S	319	17	1/1/15/20	6/37/115/115	-
36	CLA	a	830	-	-	10/19/97/115	-
36	CLA	H	310	8	1/1/11/20	5/15/93/115	-
36	CLA	A	305	1	1/1/11/20	4/18/96/115	-
39	LMT	E	321	-	-	9/15/35/61	0/1/1/2
41	LHG	O	318	15	-	30/53/53/53	-
37	KC1	R	317	-	-	3/15/71/71	-
35	A86	S	302	-	-	6/34/90/90	0/3/3/3
36	CLA	a	818	-	1/1/15/20	14/37/115/115	-
34	DD6	S	307	-	-	6/26/80/80	0/3/3/3
41	LHG	b	850	36	-	27/53/53/53	-
34	DD6	E	303	-	-	7/26/80/80	0/3/3/3
41	LHG	Q	315	36	-	33/53/53/53	-
36	CLA	F	309	-	1/1/15/20	13/37/115/115	-
36	CLA	M	310	35,13	1/1/11/20	5/15/93/115	-
41	LHG	G	320	-	-	18/44/44/53	-
36	CLA	V	305	35	1/1/14/20	11/33/111/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
36	CLA	A	311	-	1/1/15/20	18/37/115/115	-
41	LHG	F	319	-	-	33/45/45/53	-
36	CLA	N	313	14	1/1/10/20	2/8/86/115	-
36	CLA	a	827	-	1/1/14/20	14/34/112/115	-
35	A86	P	307	-	-	2/34/90/90	0/3/3/3
36	CLA	a	820	-	1/1/15/20	11/37/115/115	-
35	A86	V	304	-	-	9/34/90/90	0/3/3/3
36	CLA	A	308	-	1/1/15/20	13/37/115/115	-
36	CLA	I	311	9	1/1/15/20	17/37/115/115	-
35	A86	X	301	-	-	8/34/90/90	0/3/3/3
36	CLA	S	314	17	-	9/37/115/115	-
36	CLA	b	815	-	1/1/15/20	19/37/115/115	-
36	CLA	b	824	-	1/1/12/20	12/23/101/115	-
37	KC1	G	317	-	-	6/15/71/71	-
36	CLA	b	837	-	1/1/15/20	8/37/115/115	-
35	A86	N	302	-	-	6/34/90/90	0/3/3/3
35	A86	P	306	-	-	3/34/90/90	0/3/3/3
36	CLA	K	310	-	2/2/14/20	14/34/112/115	-
37	KC1	E	309	-	-	5/15/71/71	-
35	A86	E	307	36	-	3/34/90/90	0/3/3/3
36	CLA	a	816	-	1/1/15/20	20/37/115/115	-
36	CLA	H	307	8	1/1/14/20	5/31/109/115	-
36	CLA	a	803	36	1/1/13/20	5/25/103/115	-
42	LMG	h	206	-	-	24/40/60/70	0/1/1/1
37	KC1	W	217	-	-	4/15/71/71	-
36	CLA	X	307	19,35	-	6/19/97/115	-
36	CLA	b	810	-	1/1/15/20	8/37/115/115	-
42	LMG	V	316	-	-	24/41/61/70	0/1/1/1
36	CLA	R	310	-	1/1/14/20	16/33/111/115	-
36	CLA	W	207	34	1/1/15/20	15/37/115/115	-
35	A86	C	204	-	-	12/34/90/90	0/3/3/3
36	CLA	b	813	-	1/1/13/20	3/25/101/115	-
44	BCR	b	846	-	-	8/29/63/63	0/2/2/2
36	CLA	b	827	-	1/1/15/20	10/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
35	A86	R	306	-	-	8/34/90/90	0/3/3/3
44	BCR	b	845	-	-	7/29/63/63	0/2/2/2
36	CLA	J	311	-	1/1/11/20	3/15/93/115	-
36	CLA	T	312	18	1/1/11/20	5/15/93/115	-
35	A86	R	305	-	-	5/34/90/90	0/3/3/3
36	CLA	a	801	-	1/1/15/20	10/37/115/115	-
36	CLA	B	307	-	1/1/11/20	5/15/93/115	-
36	CLA	W	208	-	1/1/11/20	5/13/91/115	-
34	DD6	M	303	-	-	3/26/80/80	0/3/3/3
36	CLA	H	318	-	1/1/12/20	8/19/97/115	-
34	DD6	H	303	-	-	6/26/80/80	0/3/3/3
36	CLA	G	310	-	1/1/15/20	5/37/115/115	-
36	CLA	b	802	-	1/1/15/20	10/37/115/115	-
41	LHG	f	809	-	-	28/46/46/53	-
36	CLA	b	806	-	1/1/15/20	14/37/115/115	-
37	KC1	J	314	-	-	4/15/71/71	-
35	A86	G	304	-	-	8/34/90/90	0/3/3/3
36	CLA	a	834	20	1/1/11/20	5/13/91/115	-
42	LMG	m	102	-	-	14/32/52/70	0/1/1/1
34	DD6	D	301	-	-	11/26/80/80	0/3/3/3
36	CLA	b	832	-	1/1/11/20	4/18/96/115	-
36	CLA	U	311	32	1/1/15/20	21/37/115/115	-
36	CLA	C	208	-	1/1/15/20	17/37/115/115	-
35	A86	R	304	16,36	-	8/34/90/90	0/3/3/3
36	CLA	L	308	-	2/2/14/20	20/33/111/115	-
37	KC1	T	315	-	-	7/15/71/71	-
36	CLA	W	211	19	1/1/15/20	8/37/115/115	-
35	A86	Q	301	-	-	6/34/90/90	0/3/3/3
39	LMT	a	851	-	-	15/21/61/61	0/2/2/2
36	CLA	V	310	33	1/1/15/20	8/37/115/115	-
37	KC1	W	213	-	-	5/15/71/71	-
36	CLA	b	819	-	1/1/13/20	5/30/108/115	-
41	LHG	i	104	-	-	29/50/50/53	-
36	CLA	N	307	-	1/1/14/20	7/33/111/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
35	A86	H	304	-	-	8/34/90/90	0/3/3/3
34	DD6	F	303	-	-	8/26/80/80	0/3/3/3
36	CLA	P	312	15	1/1/11/20	7/15/93/115	-
38	SQD	A	315	-	-	11/22/42/69	0/1/1/1
36	CLA	b	830	-	1/1/15/20	5/37/115/115	-
36	CLA	H	306	-	1/1/14/20	6/33/111/115	-
36	CLA	X	306	-	1/1/14/20	9/33/111/115	-
35	A86	h	202	-	-	3/34/90/90	1/3/3/3
44	BCR	m	101	-	-	9/29/63/63	0/2/2/2
41	LHG	a	843	36	-	10/31/31/53	-
37	KC1	C	213	-	-	6/15/71/71	-
36	CLA	H	305	8	1/1/11/20	8/17/95/115	-
36	CLA	b	823	-	1/1/13/20	4/25/103/115	-
36	CLA	L	314	12	1/1/15/20	19/37/115/115	-
36	CLA	l	204	28	-	8/18/96/115	-
36	CLA	P	319	-	1/1/14/20	14/31/109/115	-
39	LMT	B	313	-	-	16/21/61/61	0/2/2/2
36	CLA	B	311	2	1/1/13/20	13/25/103/115	-
36	CLA	a	835	-	1/1/12/20	1/21/99/115	-
44	BCR	f	801	-	-	9/29/63/63	0/2/2/2
34	DD6	Q	302	-	-	8/26/80/80	0/3/3/3
35	A86	F	304	36	-	4/34/90/90	0/3/3/3
36	CLA	R	312	-	1/1/15/20	12/37/115/115	-
36	CLA	b	811	-	1/1/15/20	10/37/115/115	-
36	CLA	H	315	8	1/1/15/20	14/37/115/115	-
36	CLA	b	833	-	1/1/13/20	9/29/107/115	-
36	CLA	a	814	-	1/1/12/20	2/19/97/115	-
36	CLA	a	812	-	1/1/15/20	14/37/115/115	-
36	CLA	b	825	-	1/1/15/20	13/37/115/115	-
42	LMG	J	319	-	-	23/39/59/70	0/1/1/1
36	CLA	H	308	8	1/1/15/20	15/35/113/115	-
41	LHG	G	301	-	-	24/53/53/53	-
41	LHG	F	318	-	-	15/34/34/53	-
36	CLA	a	839	46	1/1/15/20	15/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
35	A86	L	319	-	-	9/34/90/90	0/3/3/3
41	LHG	a	842	-	-	24/52/52/53	-
36	CLA	D	309	-	2/2/13/20	6/25/103/115	-
36	CLA	h	203	-	1/1/15/20	20/37/115/115	-
37	KC1	O	313	15	-	2/15/71/71	-
36	CLA	T	311	18	1/1/15/20	11/37/115/115	-
36	CLA	J	316	-	1/1/11/20	6/15/93/115	-
36	CLA	a	808	20	1/1/15/20	9/37/115/115	-
44	BCR	a	846	-	-	7/29/63/63	0/2/2/2
36	CLA	R	314	16	1/1/11/20	9/15/93/115	-
36	CLA	K	315	-	1/1/10/20	3/8/86/115	-
36	CLA	G	312	7	1/1/13/20	4/29/107/115	-
36	CLA	B	305	2	1/1/15/20	24/37/115/115	-
36	CLA	W	201	19	1/1/11/20	2/17/95/115	-
36	CLA	F	311	-	1/1/12/20	8/22/100/115	-
35	A86	F	307	-	-	6/34/90/90	0/3/3/3
35	A86	N	306	-	-	8/34/90/90	0/3/3/3
40	DGD	b	849	-	-	21/49/89/95	0/2/2/2
36	CLA	J	317	10	1/1/11/20	3/16/94/115	-
35	A86	X	305	-	-	8/34/90/90	0/3/3/3
36	CLA	D	316	-	1/1/12/20	9/22/100/115	-
36	CLA	V	309	33	1/1/10/20	2/11/89/115	-
44	BCR	b	844	-	-	6/29/63/63	0/2/2/2
36	CLA	X	309	19	-	6/13/91/115	-
36	CLA	D	317	-	1/1/13/20	10/29/107/115	-
36	CLA	F	313	-	1/1/12/20	6/22/100/115	-
36	CLA	b	814	-	1/1/13/20	3/25/103/115	-
37	KC1	U	312	32,35	-	4/15/71/71	-
34	DD6	E	304	-	-	4/26/80/80	0/3/3/3
39	LMT	a	853	-	-	10/18/58/61	0/2/2/2
45	SF4	b	803	20,21	-	-	0/6/5/5
36	CLA	b	821	46	1/1/15/20	11/37/115/115	-
36	CLA	M	315	13	-	6/16/94/115	-
44	BCR	l	203	-	-	10/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
35	A86	I	301	-	-	10/34/90/90	0/3/3/3
36	CLA	b	828	-	1/1/15/20	14/37/115/115	-
36	CLA	a	819	-	1/1/11/20	3/13/91/115	-
36	CLA	D	310	-	1/1/15/20	9/37/115/115	-
36	CLA	a	838	-	1/1/15/20	6/37/115/115	-
39	LMT	B	312	-	-	14/21/61/61	0/2/2/2
39	LMT	E	320	-	-	13/21/61/61	0/2/2/2
36	CLA	F	314	35,6	1/1/15/20	14/37/115/115	-
35	A86	F	305	-	-	8/34/90/90	0/3/3/3
34	DD6	A	303	-	-	5/26/80/80	0/3/3/3
36	CLA	b	809	-	1/1/15/20	16/37/115/115	-
36	CLA	S	309	-	1/1/14/20	8/33/111/115	-
36	CLA	N	319	14	1/1/10/20	3/10/88/115	-
36	CLA	C	205	-	1/1/10/20	2/11/89/115	-
41	LHG	R	323	-	-	29/53/53/53	-
34	DD6	W	204	36	-	7/26/80/80	0/3/3/3
36	CLA	S	321	-	-	10/22/100/115	-
36	CLA	b	840	-	1/1/15/20	12/37/115/115	-
34	DD6	D	304	-	-	8/26/80/80	0/3/3/3
36	CLA	b	834	-	1/1/15/20	10/37/115/115	-
36	CLA	C	212	35	1/1/15/20	23/37/115/115	-
36	CLA	N	316	14	1/1/15/20	11/37/115/115	-
36	CLA	R	318	35	1/1/10/20	2/8/86/115	-
36	CLA	I	206	46	1/1/12/20	6/19/97/115	-
36	CLA	U	305	-	1/1/14/20	11/33/111/115	-
36	CLA	N	318	-	1/1/11/20	5/16/94/115	-
37	KC1	H	313	-	-	6/15/71/71	-
39	LMT	P	321	-	-	10/14/34/61	0/1/1/2
34	DD6	A	304	-	-	4/26/80/80	0/3/3/3
36	CLA	N	317	14	1/1/12/20	8/24/102/115	-
36	CLA	L	310	-	1/1/12/20	2/24/102/115	-
34	DD6	H	302	-	-	2/26/80/80	0/3/3/3
35	A86	T	305	18	-	7/34/90/90	0/3/3/3
36	CLA	R	311	16	1/1/15/20	13/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
40	DGD	L	302	42	-	21/36/76/95	0/2/2/2
42	LMG	D	321	-	-	21/32/52/70	0/1/1/1
36	CLA	W	215	-	1/1/11/20	4/17/95/115	-
44	BCR	b	847	-	-	8/29/63/63	0/2/2/2
36	CLA	K	311	-	1/1/11/20	6/15/93/115	-
36	CLA	D	307	41	1/1/14/20	17/33/111/115	-
37	KC1	F	308	6	-	7/15/71/71	-
35	A86	T	306	-	-	6/34/90/90	0/3/3/3
36	CLA	j	101	27	1/1/15/20	17/37/115/115	-
39	LMT	P	320	-	-	8/14/34/61	0/1/1/2
36	CLA	a	841	41	1/1/12/20	7/22/100/115	-
37	KC1	P	317	15	-	4/15/71/71	-
36	CLA	a	825	-	2/2/15/20	15/37/115/115	-
36	CLA	P	308	-	1/1/14/20	9/33/111/115	-
36	CLA	G	315	-	2/2/13/20	11/27/105/115	-
36	CLA	I	312	9	1/1/12/20	4/22/100/115	-
36	CLA	S	310	17	1/1/15/20	14/37/115/115	-
36	CLA	b	835	-	1/1/11/20	3/13/91/115	-
35	A86	N	301	-	-	8/34/90/90	0/3/3/3
36	CLA	H	314	-	1/1/10/20	3/8/86/115	-
34	DD6	K	305	-	-	0/26/80/80	0/3/3/3
36	CLA	R	313	-	1/1/15/20	13/37/115/115	-
36	CLA	a	848	36	2/2/15/20	12/37/115/115	-
36	CLA	E	310	-	-	7/37/115/115	-
36	CLA	R	320	16	1/1/11/20	3/13/91/115	-
36	CLA	I	309	9	1/1/11/20	6/15/93/115	-
36	CLA	G	307	-	-	2/9/87/115	-
36	CLA	I	308	9	1/1/15/20	19/37/115/115	-
44	BCR	i	101	-	-	2/29/63/63	0/2/2/2
36	CLA	b	838	-	1/1/11/20	3/16/94/115	-
36	CLA	I	313	-	1/1/10/20	3/8/86/115	-
36	CLA	O	311	-	1/1/13/20	9/29/107/115	-
35	A86	J	301	-	-	11/34/90/90	0/3/3/3
36	CLA	b	808	-	1/1/15/20	12/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
36	CLA	K	313	-	1/1/15/20	13/37/115/115	-
34	DD6	a	849	-	-	6/26/80/80	0/3/3/3
36	CLA	b	812	21	1/1/15/20	6/37/115/115	-
36	CLA	V	306	33	1/1/15/20	19/37/115/115	-
36	CLA	P	311	-	1/1/15/20	17/37/115/115	-
36	CLA	K	316	-	1/1/15/20	10/37/115/115	-
34	DD6	B	302	-	-	4/26/80/80	0/3/3/3
35	A86	U	302	-	-	9/34/90/90	0/3/3/3
36	CLA	G	311	-	1/1/15/20	17/37/115/115	-
41	LHG	E	322	-	-	28/53/53/53	-
39	LMT	L	303	-	-	10/21/61/61	0/2/2/2
35	A86	h	204	-	-	1/34/90/90	0/3/3/3
36	CLA	f	803	-	2/2/15/20	13/37/115/115	-
39	LMT	G	322	-	-	17/21/61/61	0/2/2/2
36	CLA	M	309	-	1/1/15/20	13/37/115/115	-
35	A86	Q	316	15,36	-	2/34/90/90	0/3/3/3
36	CLA	D	306	4	1/1/11/20	4/13/91/115	-
39	LMT	G	323	-	-	16/21/61/61	0/2/2/2
36	CLA	A	309	1	1/1/11/20	7/15/93/115	-
39	LMT	K	317	-	-	14/17/57/61	0/2/2/2
36	CLA	U	308	32,35	1/1/13/20	10/27/105/115	-
34	DD6	D	303	-	-	9/26/80/80	0/3/3/3
34	DD6	G	303	-	-	4/26/80/80	0/3/3/3
35	A86	T	303	-	-	6/34/90/90	0/3/3/3
34	DD6	W	205	-	-	8/26/80/80	0/3/3/3
41	LHG	G	321	36	-	27/51/51/53	-
36	CLA	U	313	-	1/1/10/20	2/8/86/115	-
36	CLA	D	315	-	1/1/10/20	2/8/86/115	-
44	BCR	j	107	-	-	5/29/63/63	0/2/2/2
35	A86	X	303	36	-	9/34/90/90	0/3/3/3
37	KC1	X	311	-	-	3/15/71/71	-
36	CLA	I	307	-	1/1/12/20	4/24/102/115	-
39	LMT	L	318	-	-	13/17/57/61	0/2/2/2
36	CLA	P	302	-	-	5/10/88/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
36	CLA	b	826	21,46	1/1/14/20	10/36/114/115	-
35	A86	C	202	3,36	-	8/34/90/90	0/3/3/3
36	CLA	E	317	-	1/1/11/20	5/15/93/115	-
37	KC1	F	315	-	-	3/15/71/71	-
39	LMT	F	321	-	-	11/19/59/61	0/2/2/2
36	CLA	b	805	36	1/1/15/20	16/37/115/115	-
36	CLA	X	308	19	1/1/11/20	10/16/94/115	-
37	KC1	G	318	-	-	5/15/71/71	-
36	CLA	S	318	-	1/1/10/20	7/10/88/115	-
35	A86	S	301	-	-	8/34/90/90	0/3/3/3
36	CLA	J	310	-	1/1/15/20	11/37/115/115	-
36	CLA	l	205	-	2/2/15/20	14/37/115/115	-
35	A86	O	302	-	-	9/34/90/90	0/3/3/3
35	A86	M	302	-	-	7/34/90/90	0/3/3/3
36	CLA	T	314	-	1/1/15/20	15/37/115/115	-
36	CLA	X	313	19	-	5/10/88/115	-
36	CLA	G	314	7	1/1/10/20	2/8/86/115	-
34	DD6	E	306	-	-	4/26/80/80	0/3/3/3
39	LMT	I	317	-	-	13/21/61/61	0/2/2/2
36	CLA	K	312	-	1/1/15/20	6/37/115/115	-
39	LMT	K	318	-	-	12/21/61/61	0/2/2/2
35	A86	A	302	-	-	9/34/90/90	0/3/3/3
41	LHG	a	850	-	-	36/51/51/53	-
36	CLA	E	312	-	1/1/15/20	15/37/115/115	-
36	CLA	N	310	14	1/1/10/20	1/8/86/115	-
36	CLA	a	815	46	1/1/11/20	5/13/91/115	-
36	CLA	a	807	20	1/1/15/20	13/37/115/115	-
36	CLA	K	309	-	1/1/13/20	12/30/108/115	-
36	CLA	H	312	8	1/1/15/20	17/37/115/115	-
36	CLA	a	805	20	1/1/15/20	16/37/115/115	-
44	BCR	i	103	-	-	11/29/63/63	0/2/2/2
42	LMG	E	319	-	-	23/35/55/70	0/1/1/1
35	A86	S	304	-	-	9/34/90/90	0/3/3/3
35	A86	R	302	16	-	6/34/90/90	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
39	LMT	b	848	-	-	12/21/61/61	0/2/2/2
34	DD6	R	307	-	-	11/26/80/80	0/3/3/3
36	CLA	L	312	12	-	6/15/93/115	-
36	CLA	P	301	15	1/1/15/20	16/37/115/115	-
36	CLA	A	307	-	1/1/14/20	10/31/109/115	-
34	DD6	O	304	-	-	5/26/80/80	0/3/3/3
36	CLA	G	309	7	1/1/15/20	13/37/115/115	-
36	CLA	W	210	-	1/1/11/20	7/15/93/115	-
35	A86	J	305	-	-	6/34/90/90	0/3/3/3
36	CLA	M	312	36,13	1/1/11/20	10/16/94/115	-
43	PQN	a	840	-	-	7/23/43/43	0/2/2/2
36	CLA	Q	305	-	1/1/14/20	9/33/111/115	-
35	A86	M	301	-	-	8/34/90/90	0/3/3/3
36	CLA	P	316	-	1/1/10/20	3/8/86/115	-
36	CLA	G	313	7	1/1/15/20	16/37/115/115	-
35	A86	G	305	-	-	4/34/90/90	0/3/3/3
44	BCR	l	207	-	-	7/29/63/63	0/2/2/2
42	LMG	J	318	-	-	28/50/70/70	0/1/1/1
36	CLA	D	312	-	1/1/15/20	11/37/115/115	-
36	CLA	b	818	-	-	4/25/103/115	-
36	CLA	C	210	3	1/1/11/20	4/15/93/115	-
35	A86	J	306	-	-	10/34/90/90	0/3/3/3
35	A86	O	301	-	-	4/34/90/90	0/3/3/3
35	A86	N	304	-	-	8/34/90/90	0/3/3/3
36	CLA	E	315	-	2/2/15/20	16/37/115/115	-
36	CLA	S	315	17	1/1/10/20	3/11/89/115	-
35	A86	G	306	-	-	6/34/90/90	1/3/3/3
36	CLA	O	309	-	1/1/15/20	17/37/115/115	-
35	A86	E	302	-	-	4/34/90/90	0/3/3/3
35	A86	A	316	-	-	9/34/90/90	0/3/3/3
35	A86	V	301	35	-	10/34/90/90	1/3/3/3
42	LMG	I	315	-	-	32/50/70/70	0/1/1/1
34	DD6	B	304	-	-	2/26/80/80	0/3/3/3
35	A86	K	303	-	-	5/34/90/90	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
35	A86	S	308	37	-	12/34/90/90	0/3/3/3
36	CLA	l	202	28	1/1/15/20	11/37/115/115	-
36	CLA	D	313	-	1/1/15/20	8/37/115/115	-
41	LHG	f	808	25	-	29/53/53/53	-
36	CLA	J	309	-	1/1/15/20	8/37/115/115	-
36	CLA	b	801	46	1/1/15/20	8/37/115/115	-
36	CLA	J	308	-	-	12/33/111/115	-
36	CLA	i	102	26	1/1/15/20	20/37/115/115	-
36	CLA	X	310	19	1/1/10/20	2/8/86/115	-
36	CLA	D	311	-	-	5/15/93/115	-
36	CLA	b	816	-	2/2/14/20	17/31/109/115	-
35	A86	C	203	-	-	8/34/90/90	1/3/3/3
36	CLA	N	315	-	-	0/8/86/115	-
37	KC1	L	317	-	-	3/15/71/71	-
36	CLA	S	313	-	1/1/11/20	6/15/93/115	-
36	CLA	J	313	-	1/1/15/20	13/37/115/115	-
36	CLA	a	832	-	1/1/15/20	14/37/115/115	-
36	CLA	N	309	14	1/1/12/20	7/21/99/115	-
36	CLA	S	317	-	1/1/10/20	3/8/86/115	-
35	A86	B	301	-	-	10/34/90/90	0/3/3/3
42	LMG	G	325	-	-	27/50/70/70	0/1/1/1
36	CLA	T	316	-	1/1/10/20	0/8/86/115	-
42	LMG	L	321	40	-	15/28/48/70	0/1/1/1
36	CLA	a	817	-	1/1/15/20	15/37/115/115	-
41	LHG	j	104	-	-	32/53/53/53	-
36	CLA	f	805	25	1/1/12/20	9/22/100/115	-
35	A86	T	302	18	-	7/34/90/90	0/3/3/3
35	A86	V	303	35	-	8/34/90/90	0/3/3/3
36	CLA	H	317	8	1/1/15/20	8/37/115/115	-
37	KC1	G	308	-	-	5/15/71/71	-
36	CLA	K	307	-	2/2/14/20	21/33/111/115	-
35	A86	L	301	-	-	5/34/90/90	1/3/3/3
36	CLA	j	102	-	1/1/15/20	13/37/115/115	-
36	CLA	a	806	-	2/2/15/20	10/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
41	LHG	D	319	42	-	30/53/53/53	-
36	CLA	H	311	-	1/1/15/20	9/37/115/115	-
36	CLA	V	314	-	1/1/15/20	17/37/115/115	-
35	A86	I	304	-	-	9/34/90/90	0/3/3/3
36	CLA	N	312	-	1/1/11/20	7/16/94/115	-
35	A86	O	303	-	-	6/34/90/90	0/3/3/3
35	A86	J	303	-	-	7/34/90/90	0/3/3/3
38	SQD	b	804	-	-	23/41/61/69	0/1/1/1
36	CLA	A	310	-	1/1/15/20	11/37/115/115	-
36	CLA	J	315	-	1/1/10/20	2/8/86/115	-
36	CLA	M	306	37,13	1/1/13/20	8/25/103/115	-
36	CLA	L	311	-	1/1/15/20	14/37/115/115	-
36	CLA	K	308	-	1/1/15/20	11/37/115/115	-
35	A86	O	319	35,36	-	8/34/90/90	0/3/3/3
35	A86	M	305	-	-	8/34/90/90	0/3/3/3
36	CLA	R	322	16	1/1/12/20	11/22/100/115	-
36	CLA	A	306	-	2/2/14/20	19/33/111/115	-
37	KC1	B	310	2	-	3/15/71/71	-
36	CLA	W	216	19,35	1/1/11/20	3/13/91/115	-
35	A86	Q	304	-	-	10/34/90/90	0/3/3/3
36	CLA	F	317	6	2/2/13/20	10/27/105/115	-
40	DGD	C	215	-	-	31/46/86/95	0/2/2/2
34	DD6	D	305	-	-	3/26/80/80	0/3/3/3

The worst 5 of 4148 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	M	318	KC1	C4C-NC	17.10	1.63	1.37
36	Q	310	CLA	CAA-C2A	15.78	1.83	1.54
37	M	318	KC1	C1A-NA	15.77	1.68	1.38
37	T	310	KC1	C1A-NA	14.39	1.66	1.38
36	X	308	CLA	C4B-NB	13.90	1.47	1.35

The worst 5 of 7259 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	N	304	A86	O1-C20-C21	-47.08	58.64	115.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	Q	314	CLA	C4-C3-C5	-24.40	74.22	115.27
42	V	315	LMG	O7-C10-C11	22.29	159.53	111.50
35	A	302	A86	C33-C32-C31	-21.39	88.43	109.21
36	N	319	CLA	CHD-C1D-ND	-21.33	104.86	124.45

5 of 321 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
36	A	305	CLA	ND
36	A	306	CLA	ND
36	A	306	CLA	C8
36	A	307	CLA	ND
36	A	308	CLA	ND

5 of 5822 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
34	A	301	DD6	C10-C11-C13-C14
34	A	301	DD6	C12-C11-C13-C14
34	A	301	DD6	C13-C14-C15-C20
34	A	301	DD6	C13-C14-C15-O1
34	A	303	DD6	C10-C11-C13-C14

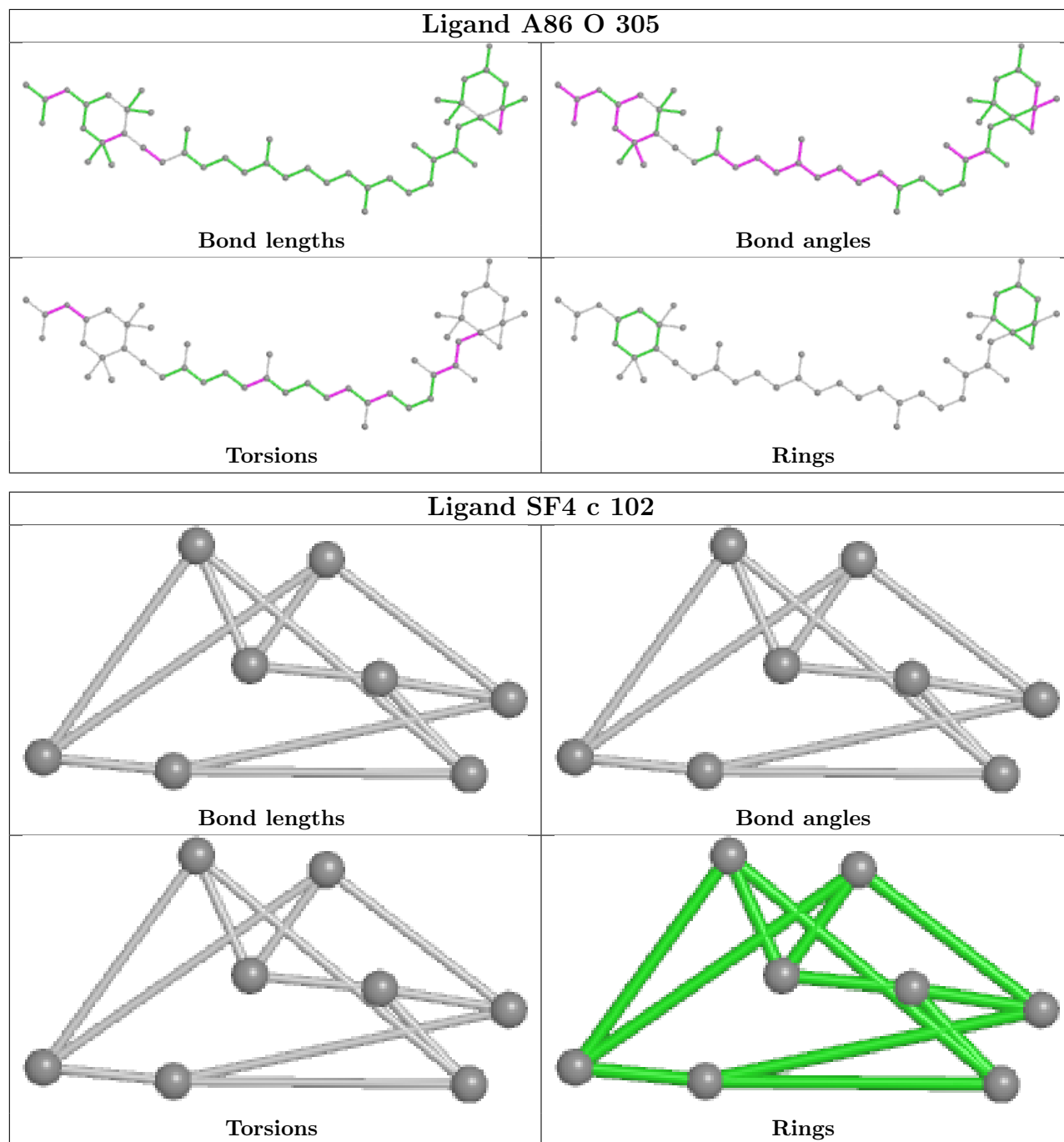
5 of 11 ring outliers are listed below:

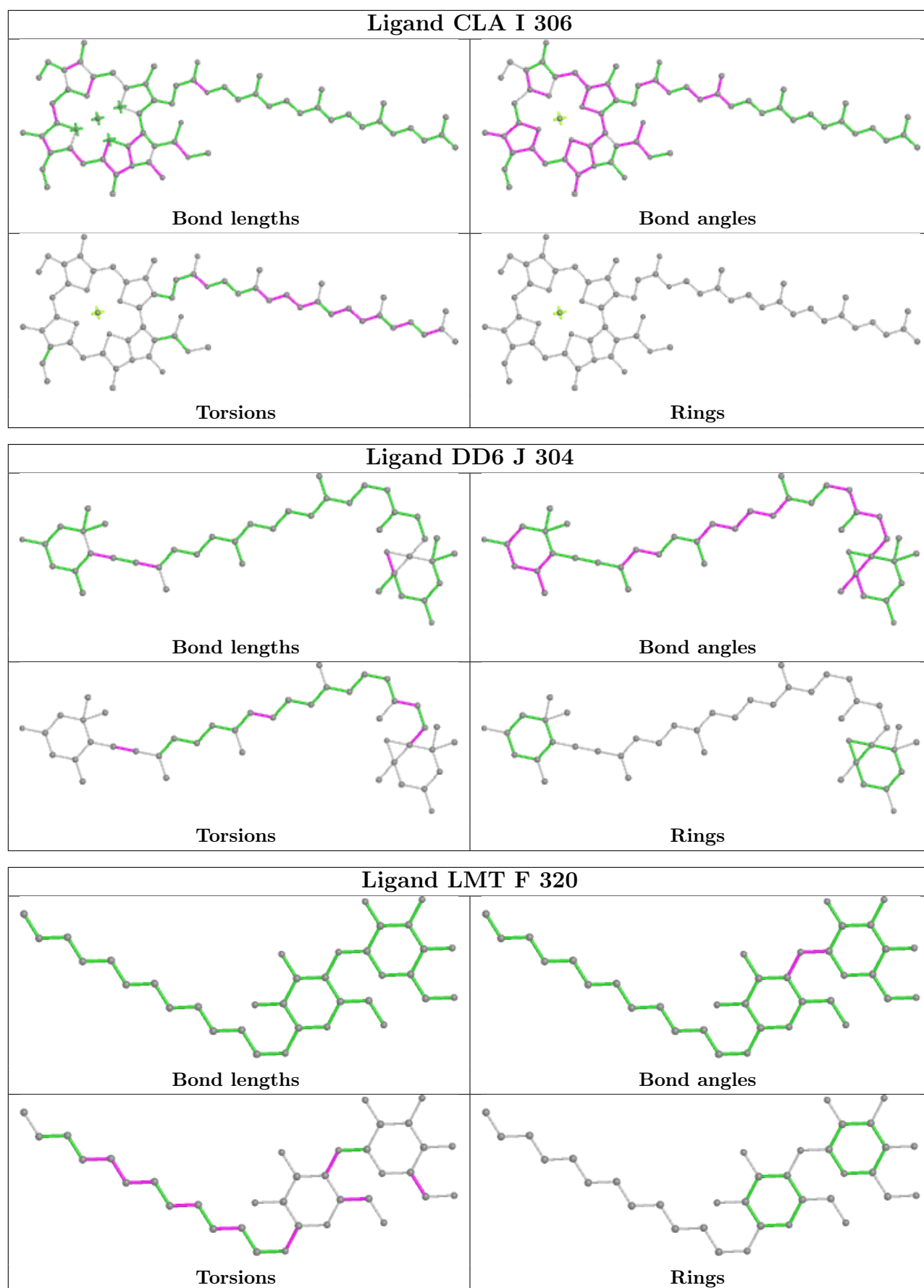
Mol	Chain	Res	Type	Atoms
35	V	301	A86	C31-C32-C33-C34-C35-C36
35	J	302	A86	C31-C32-C33-C34-C35-C36
35	K	301	A86	C31-C32-C33-C34-C35-C36
35	G	306	A86	C31-C32-C33-C34-C35-C36
35	T	301	A86	C31-C32-C33-C34-C35-C36

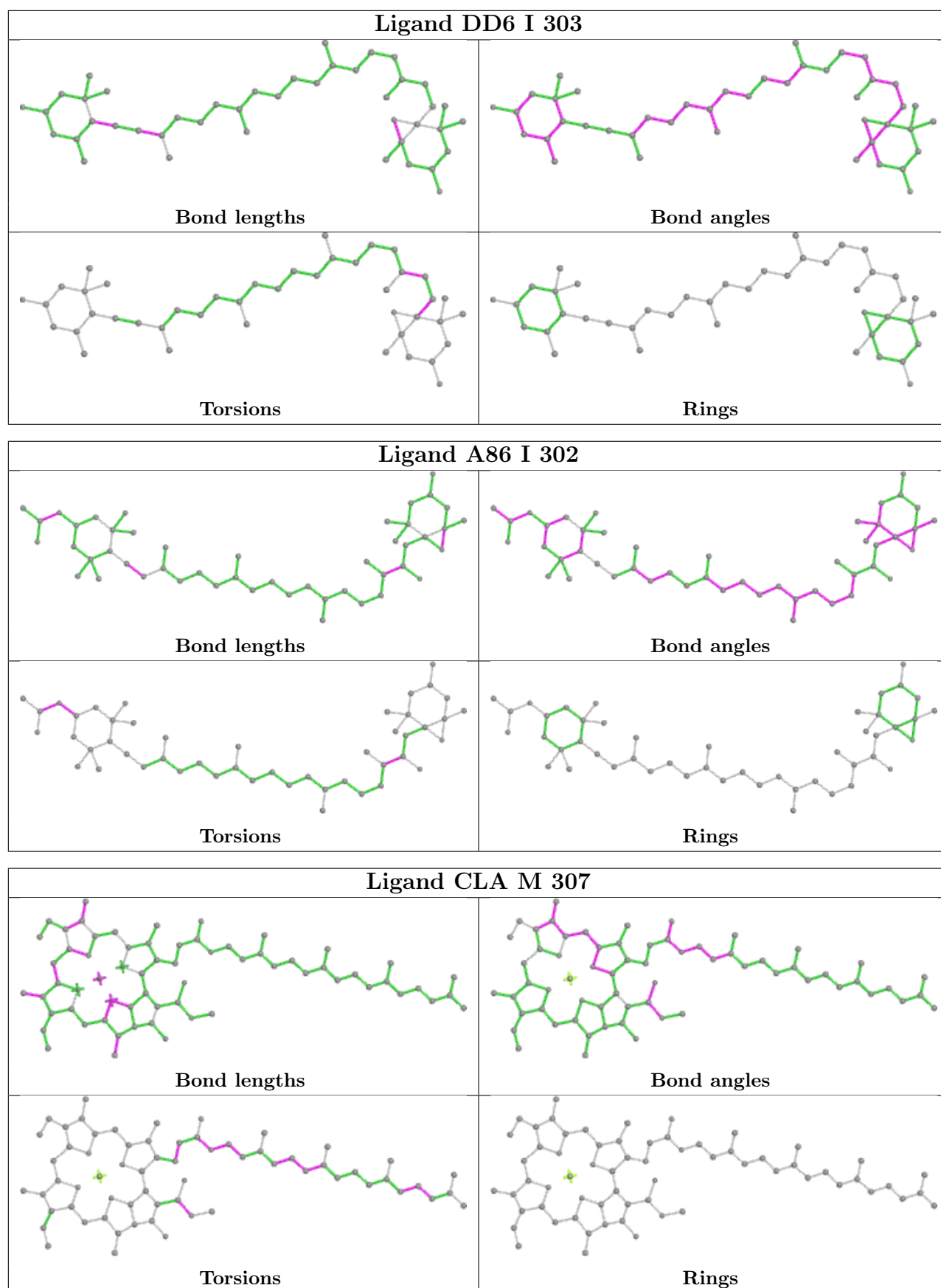
No monomer is involved in short contacts.

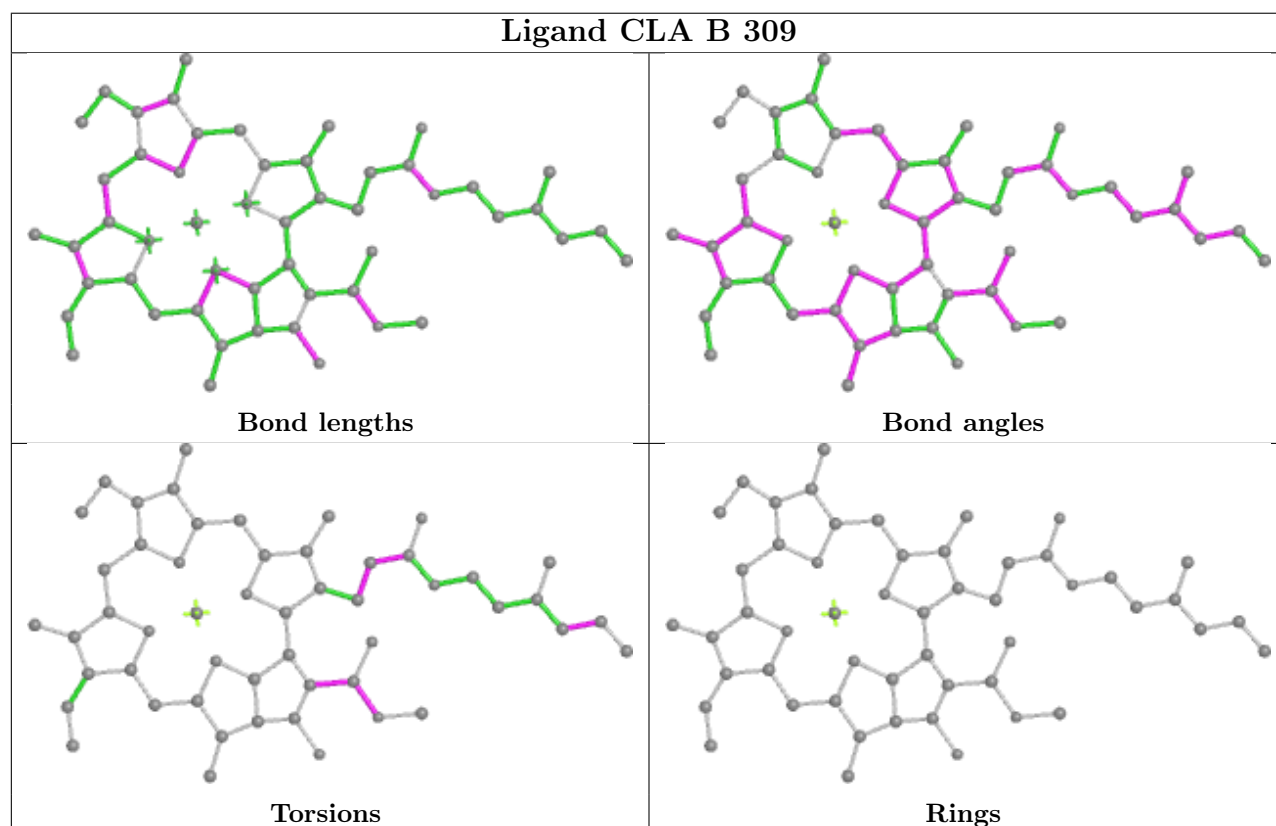
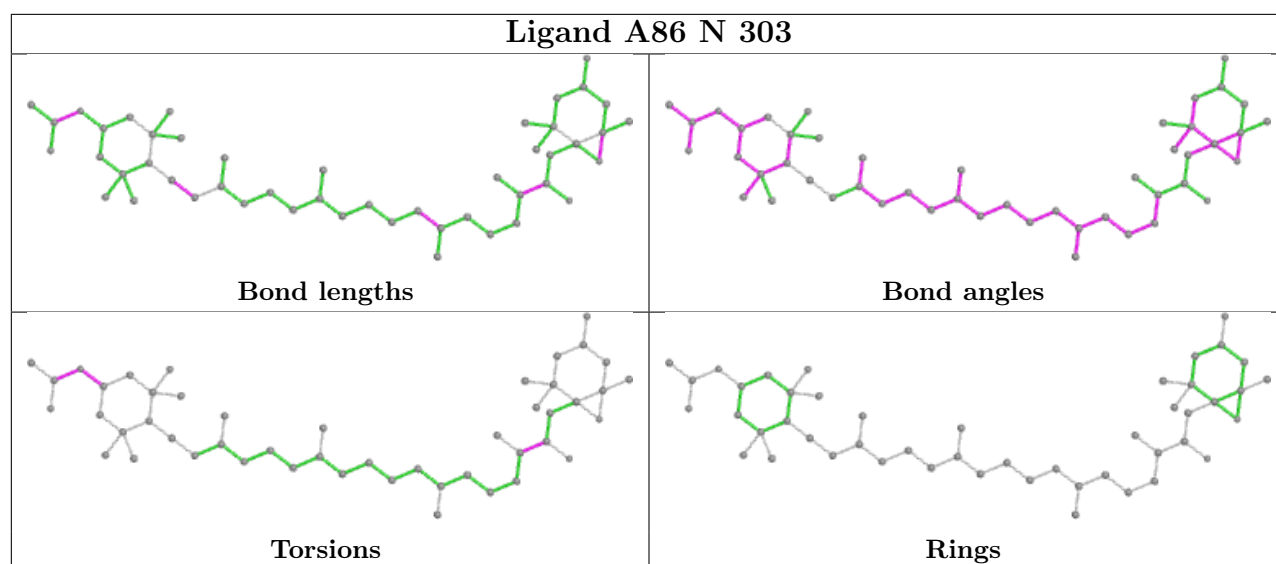
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

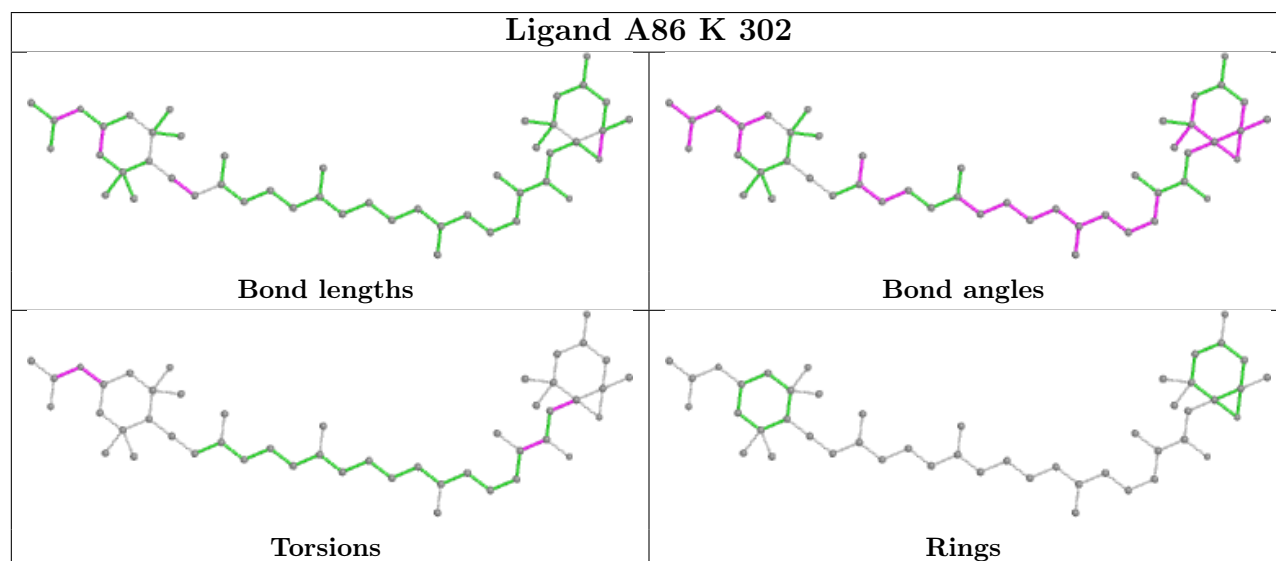
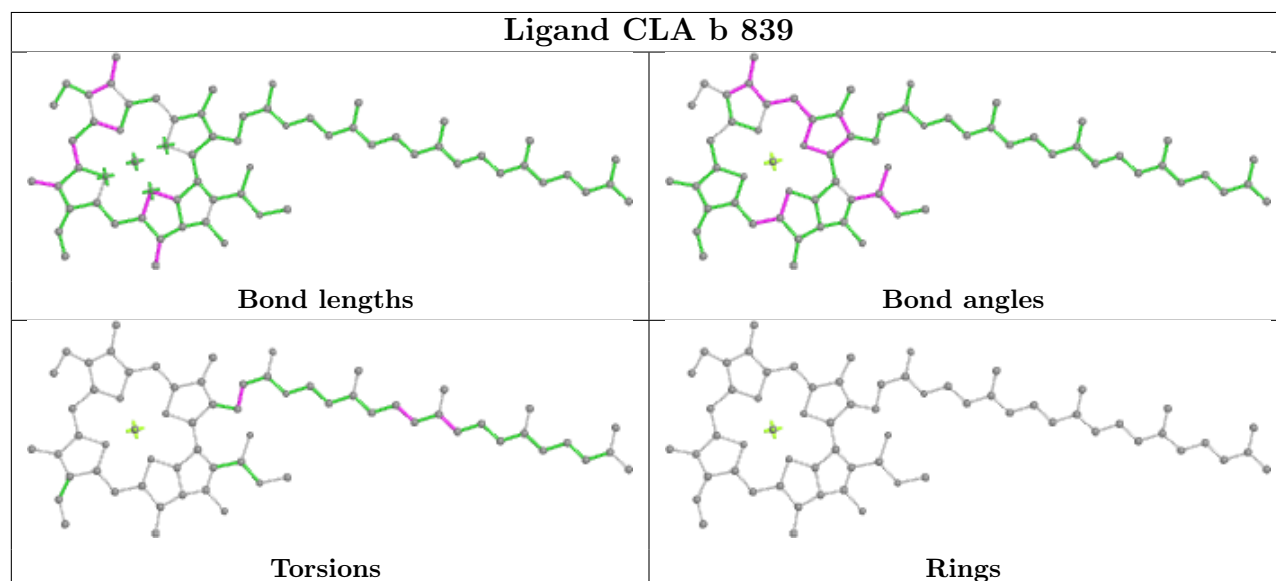
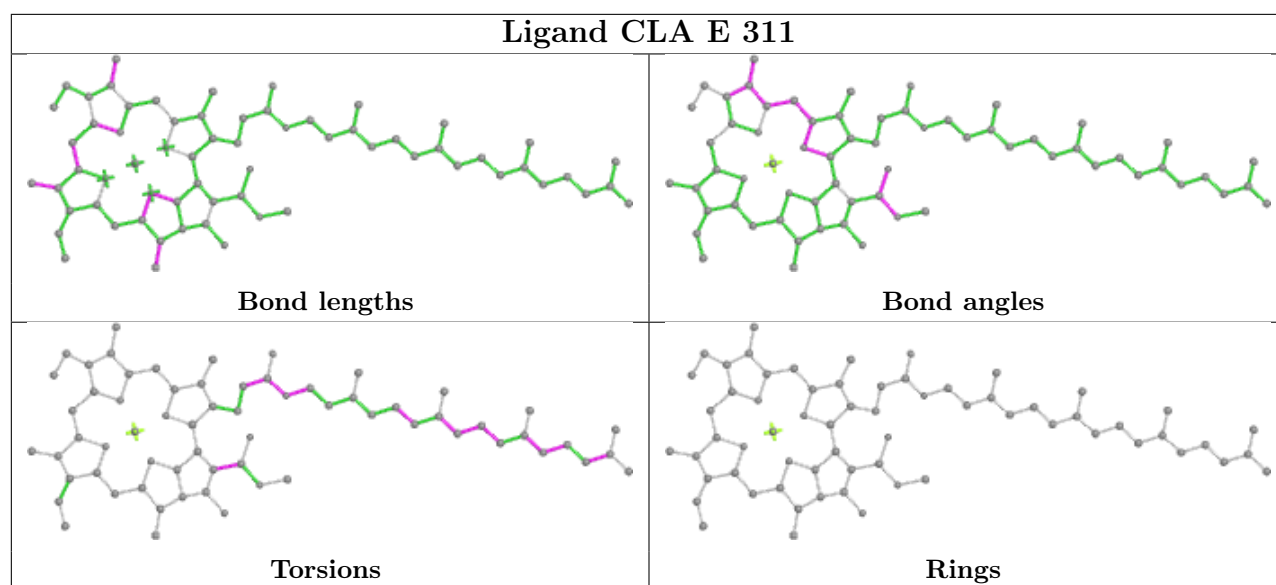
any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

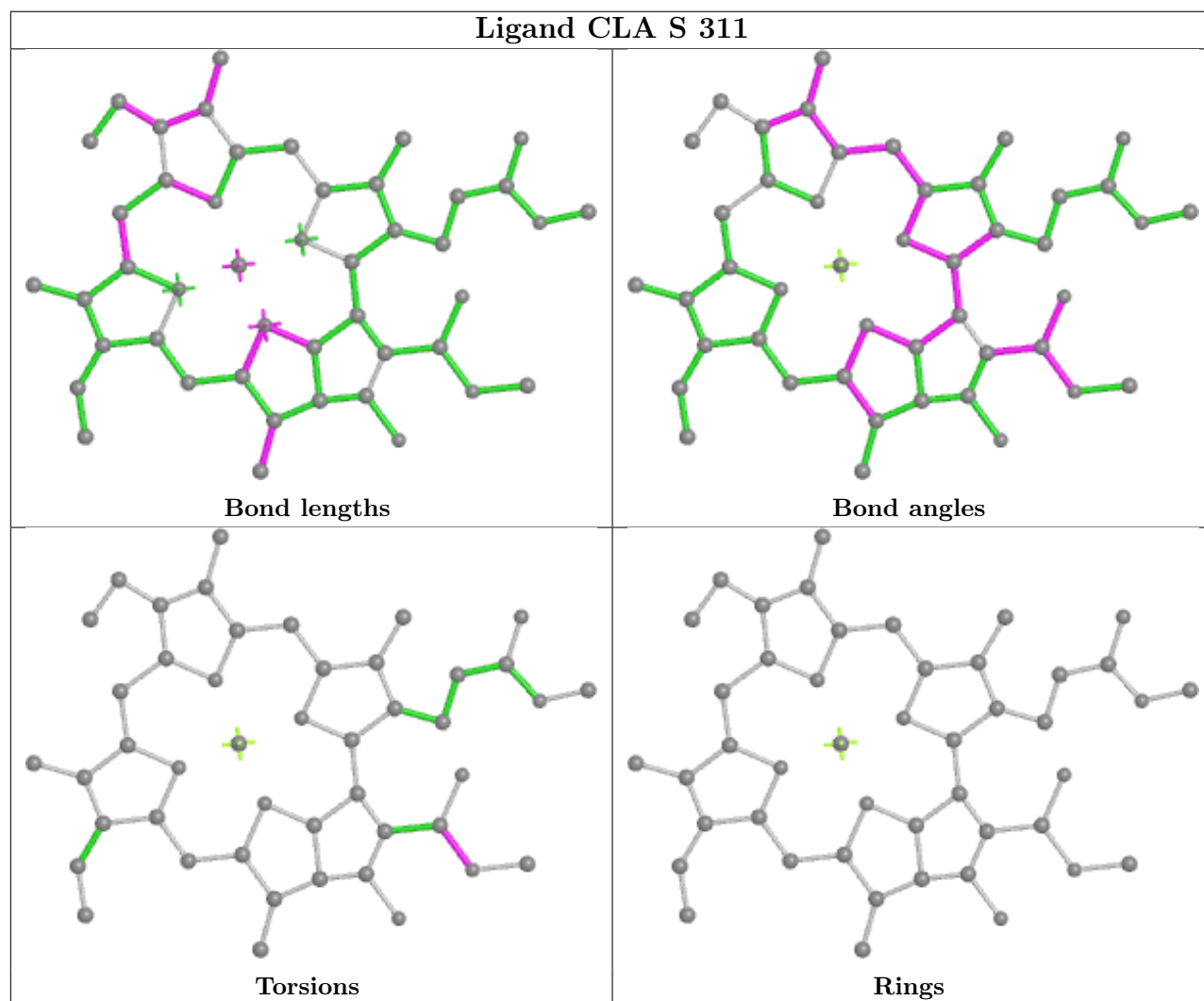
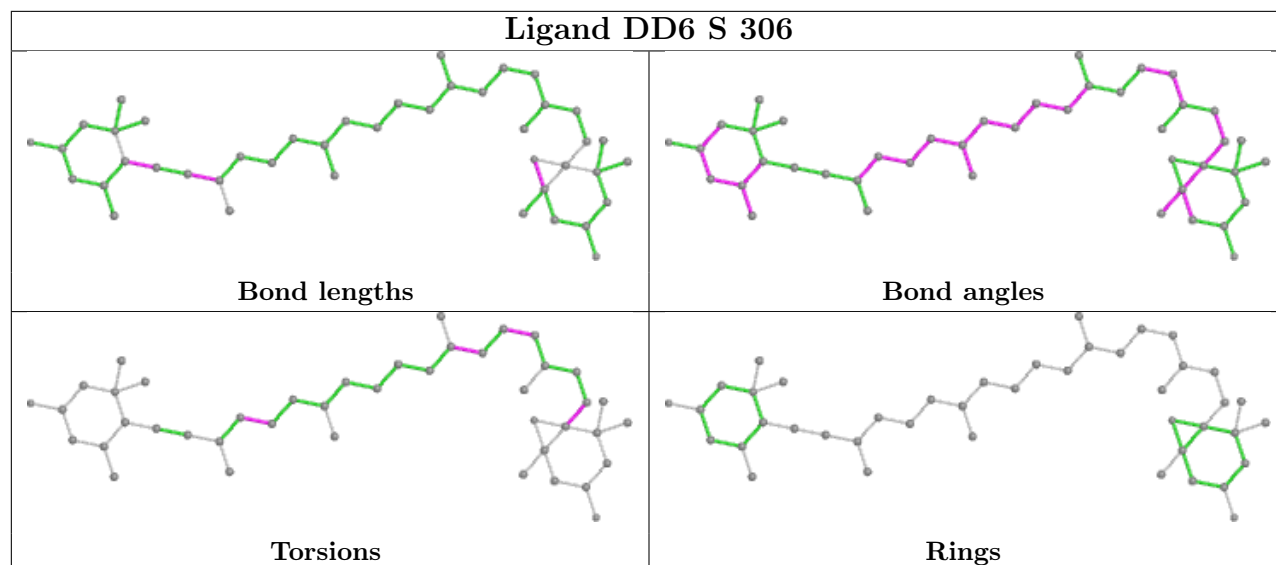


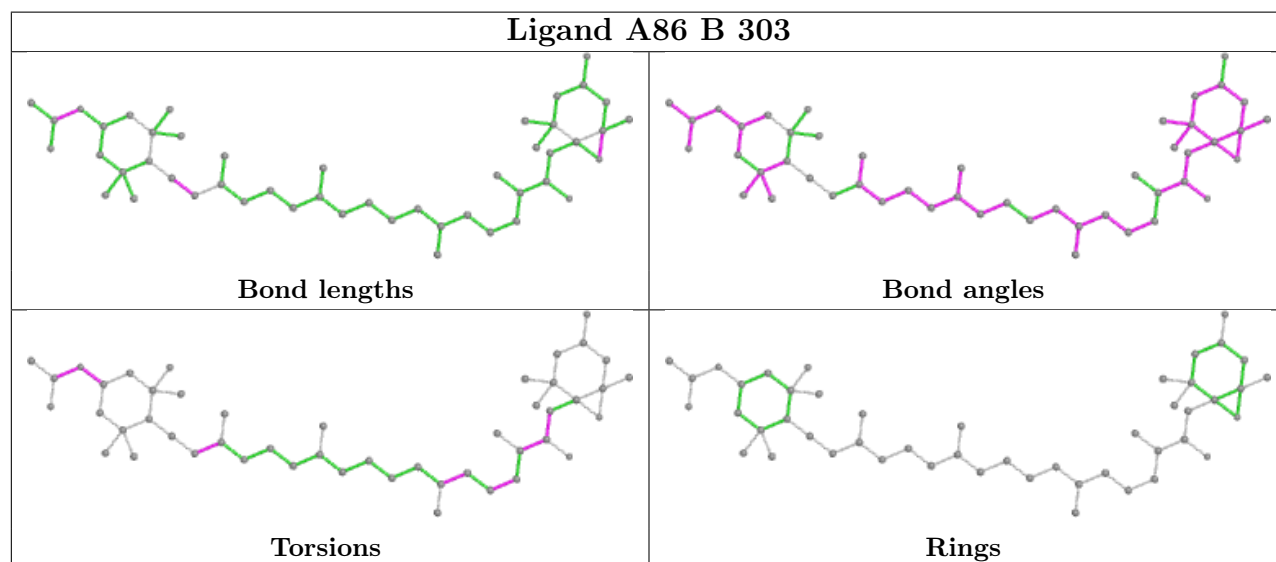
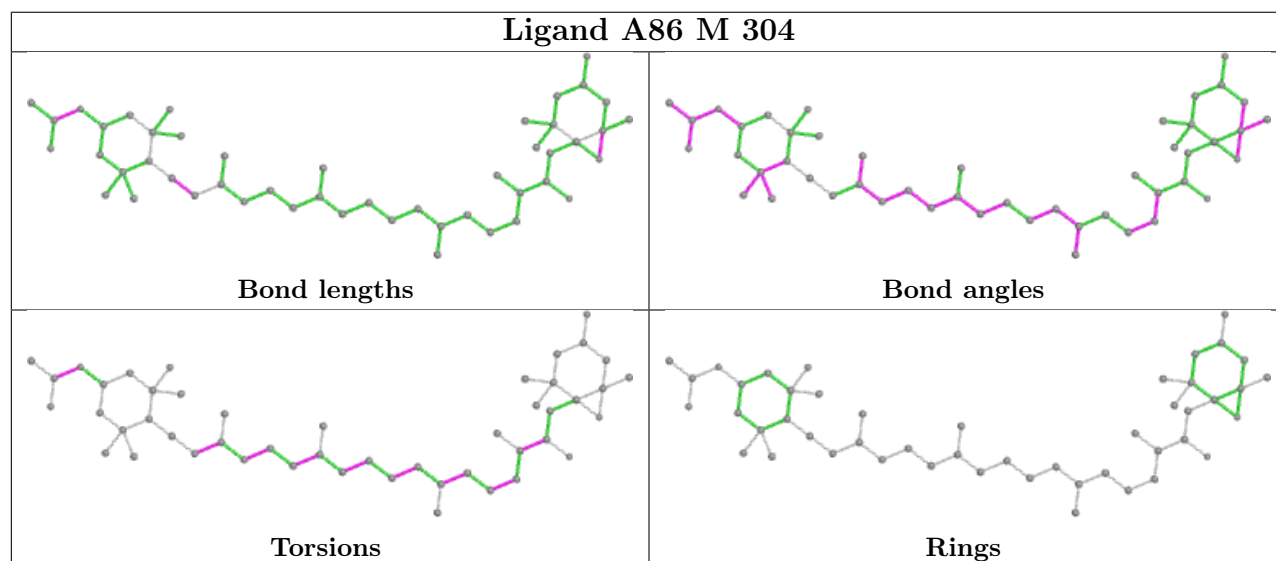
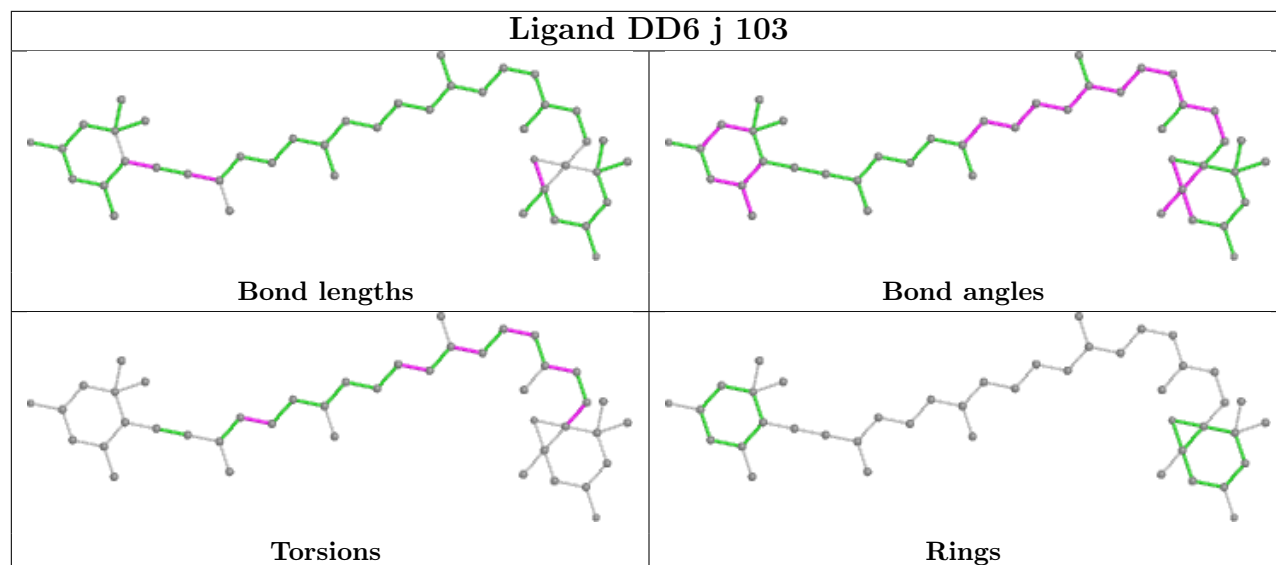


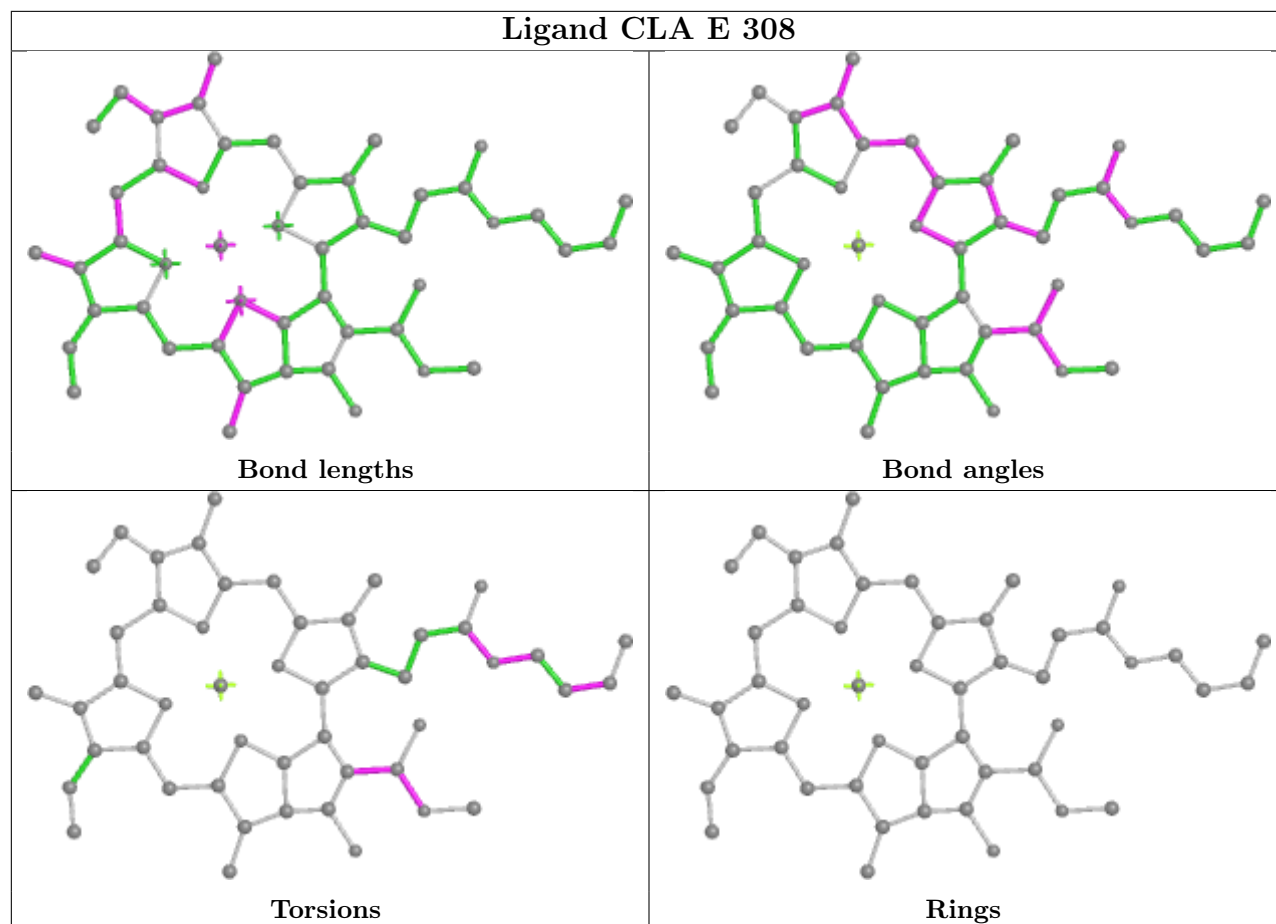


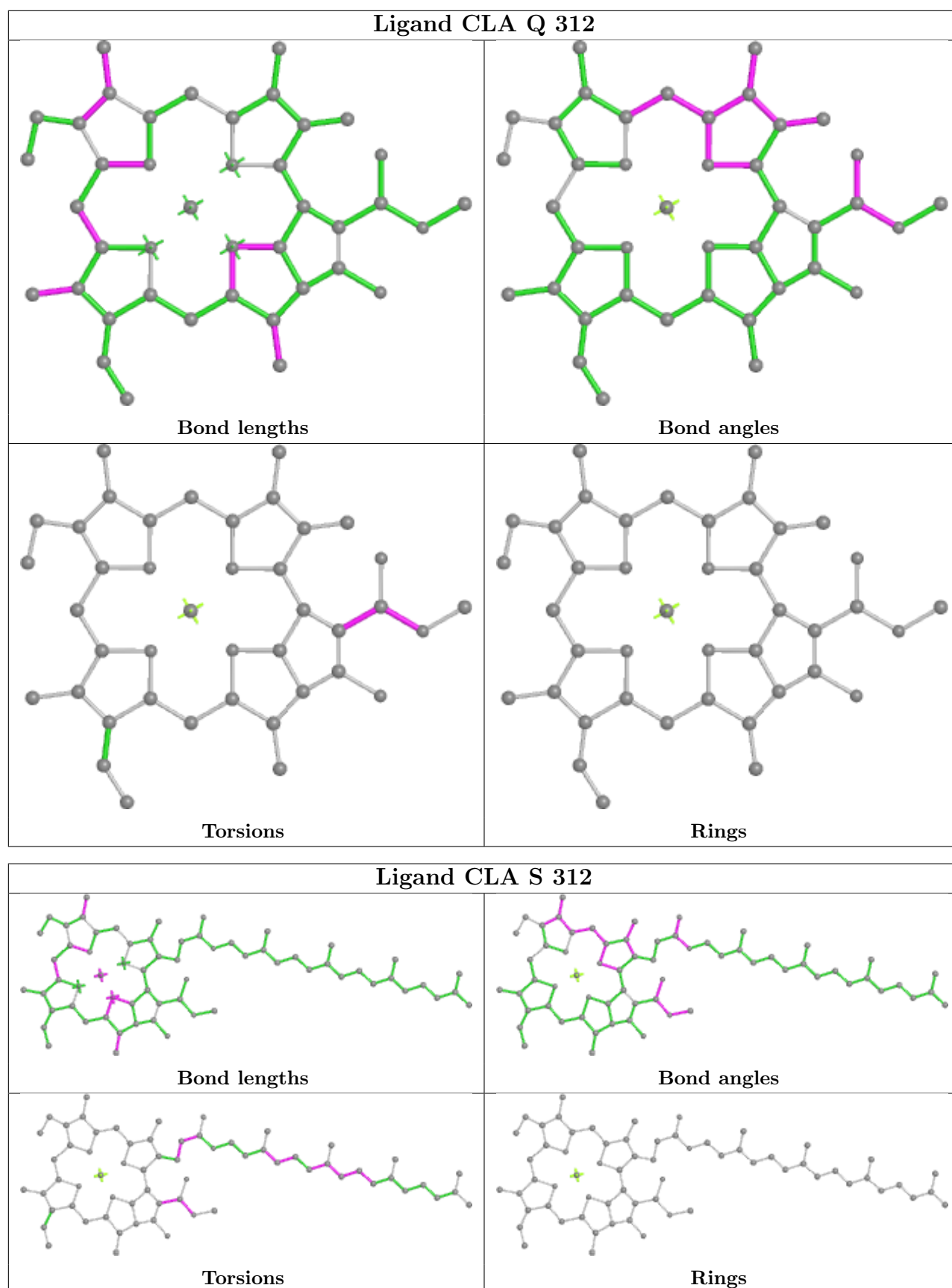


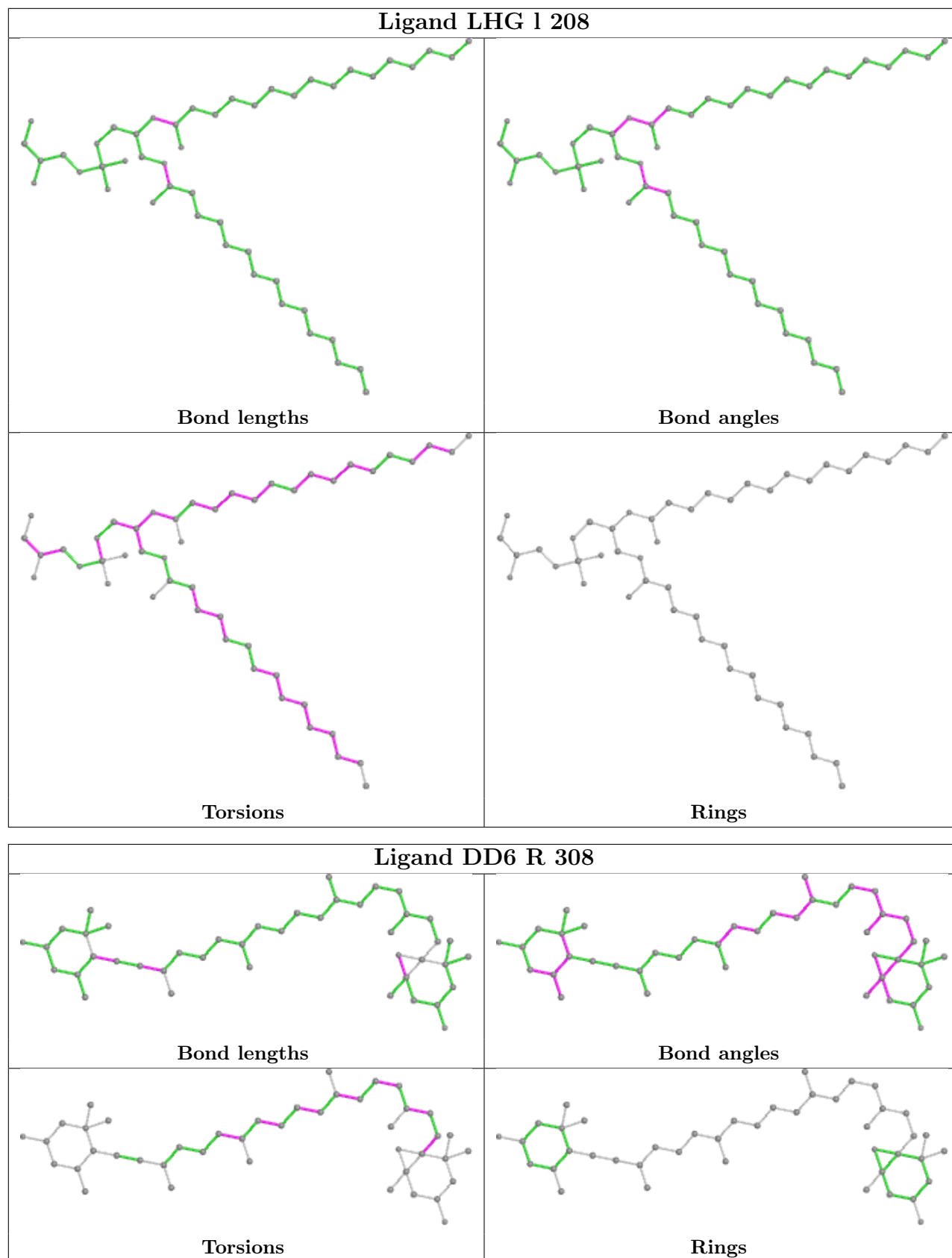


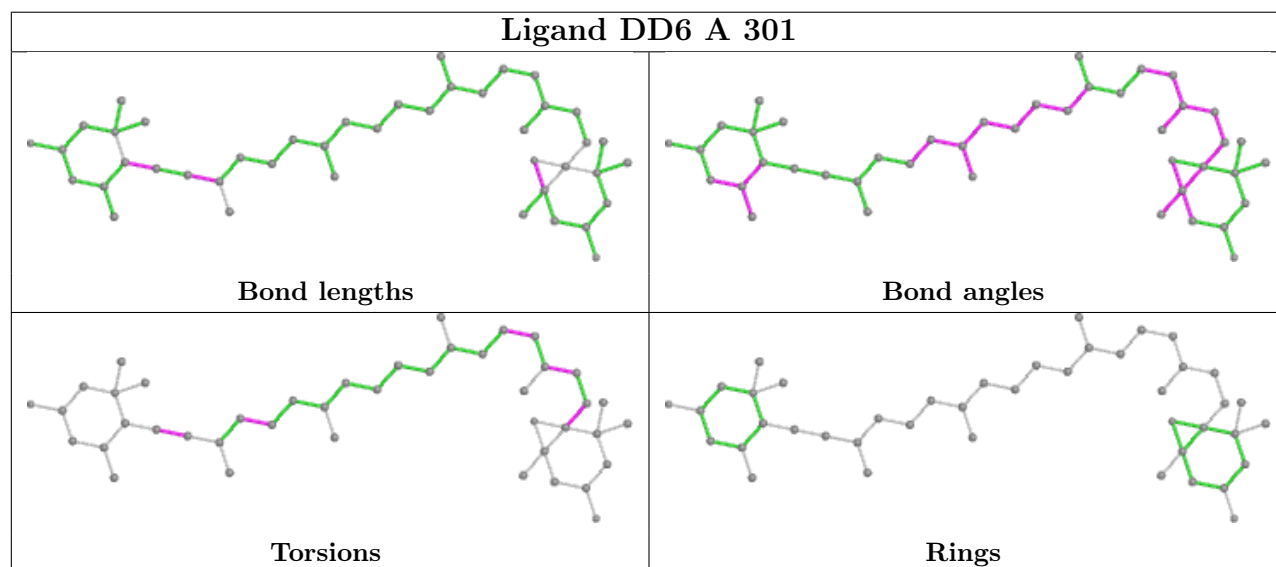
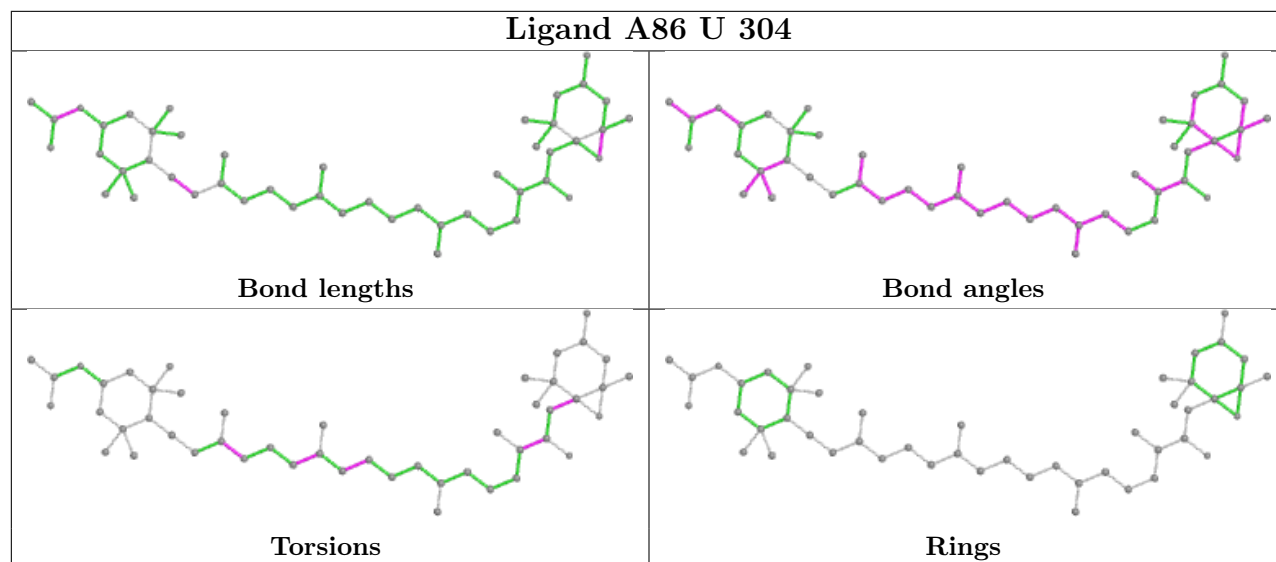
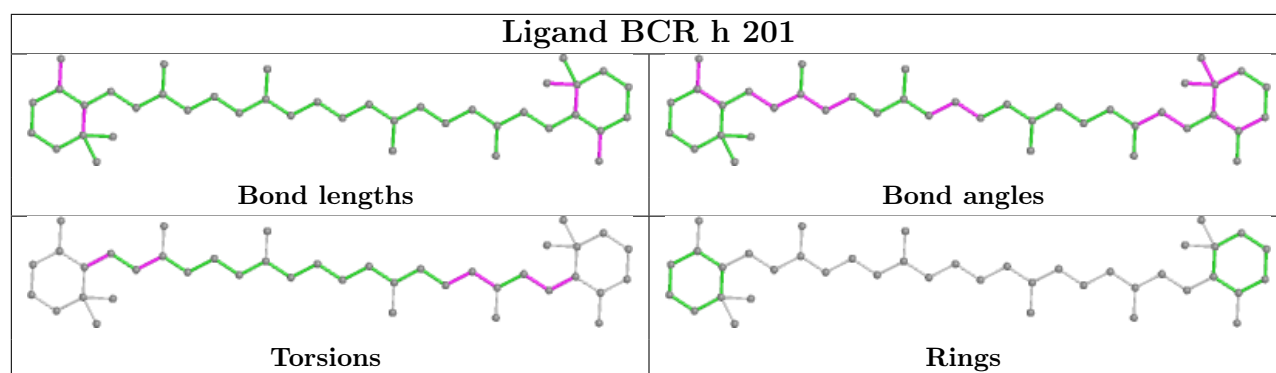


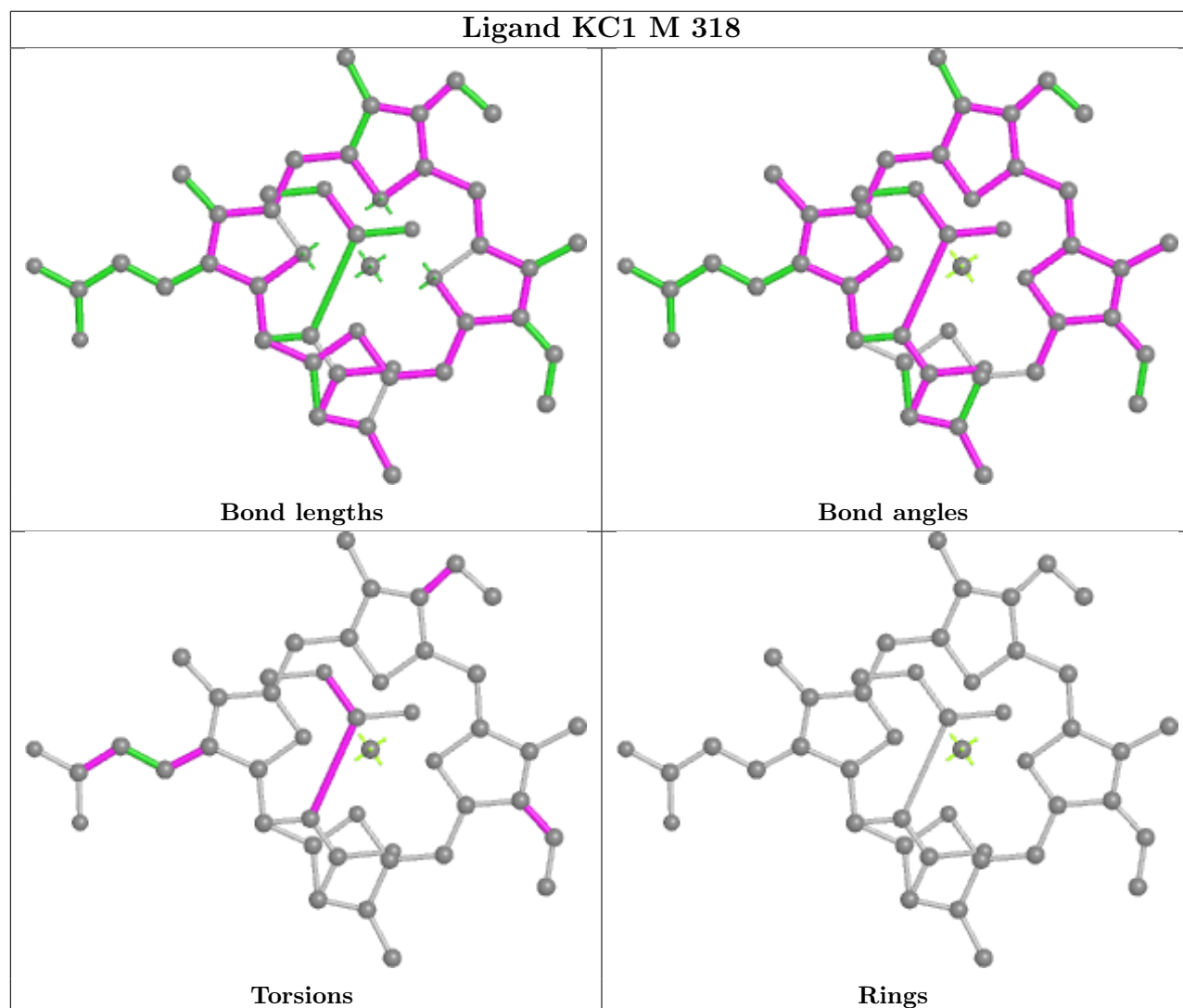
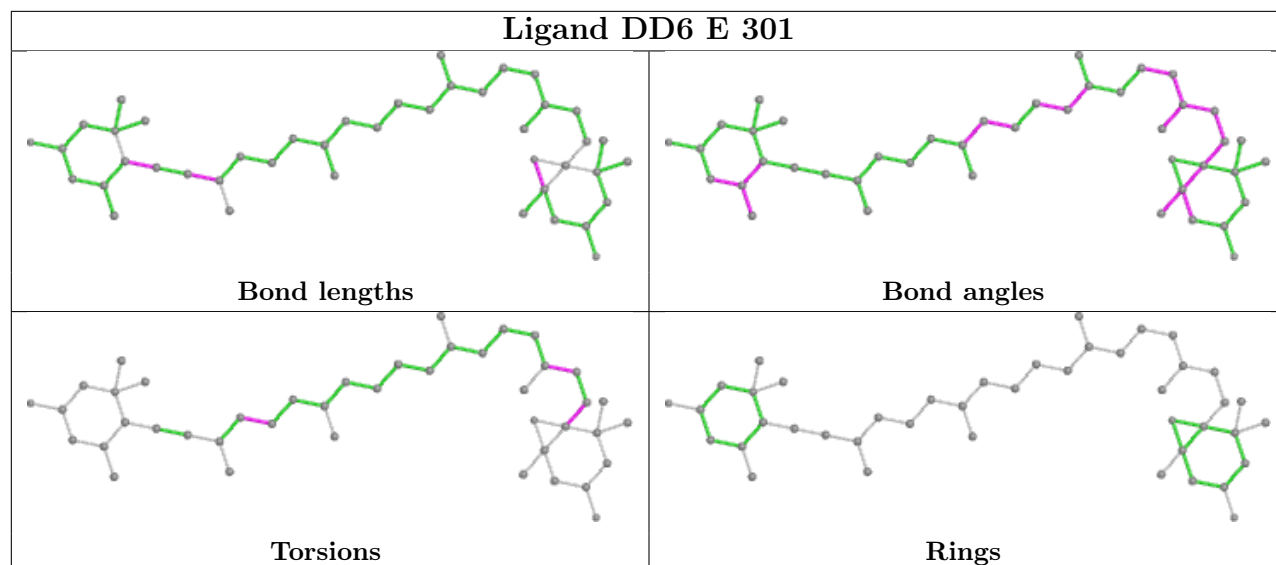


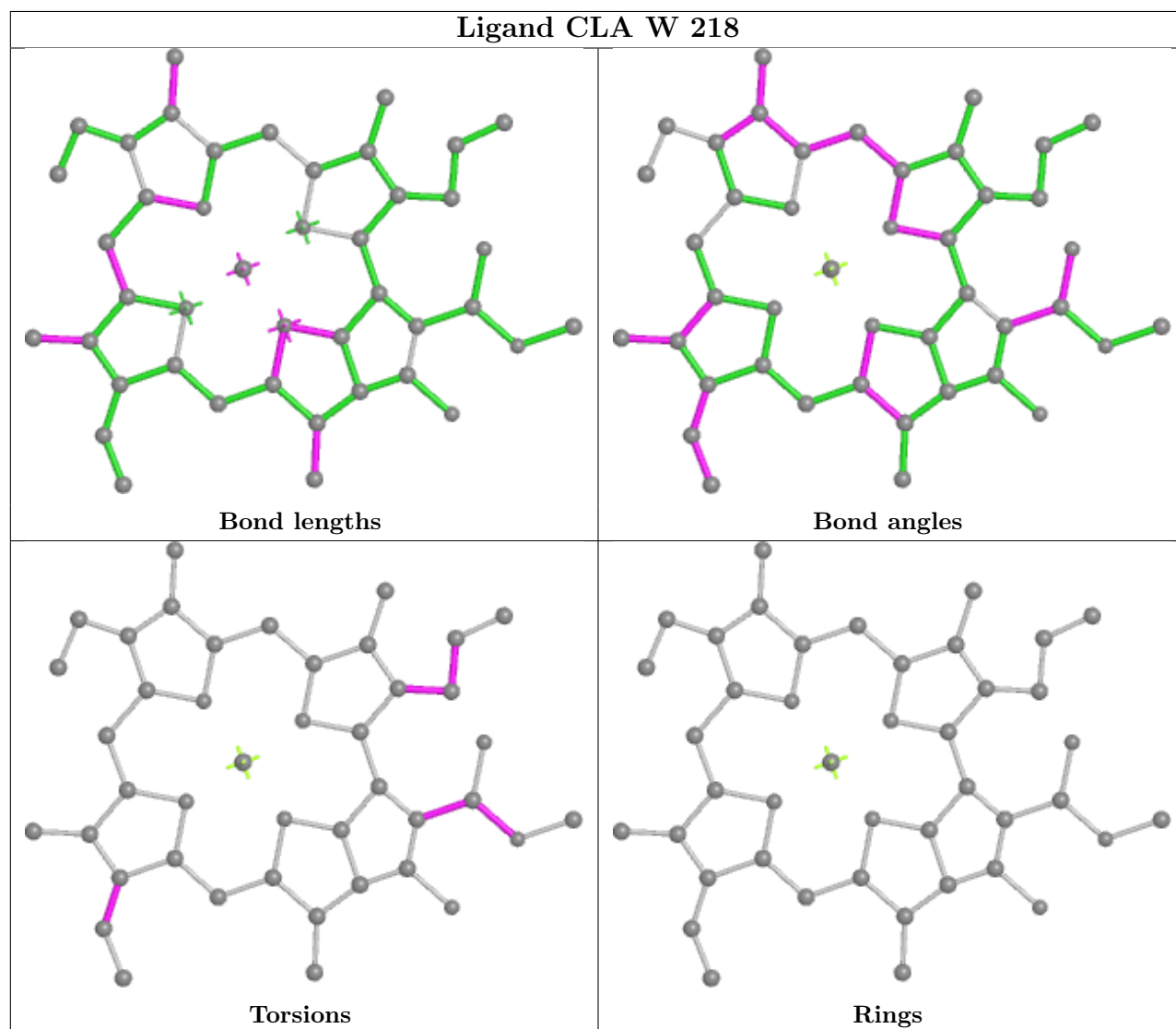
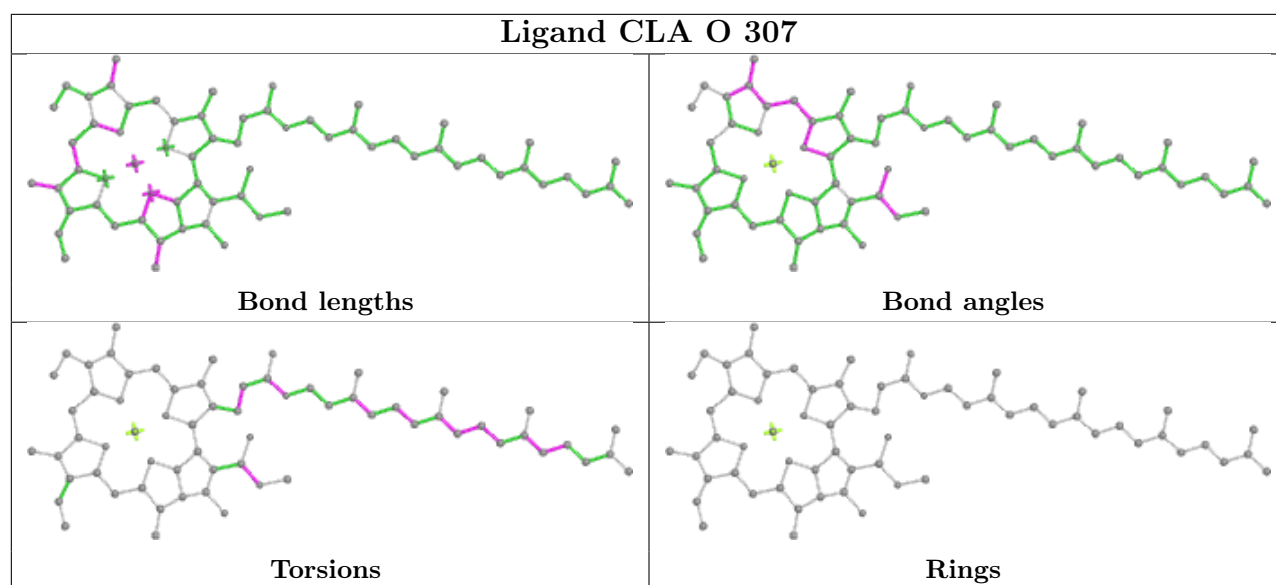


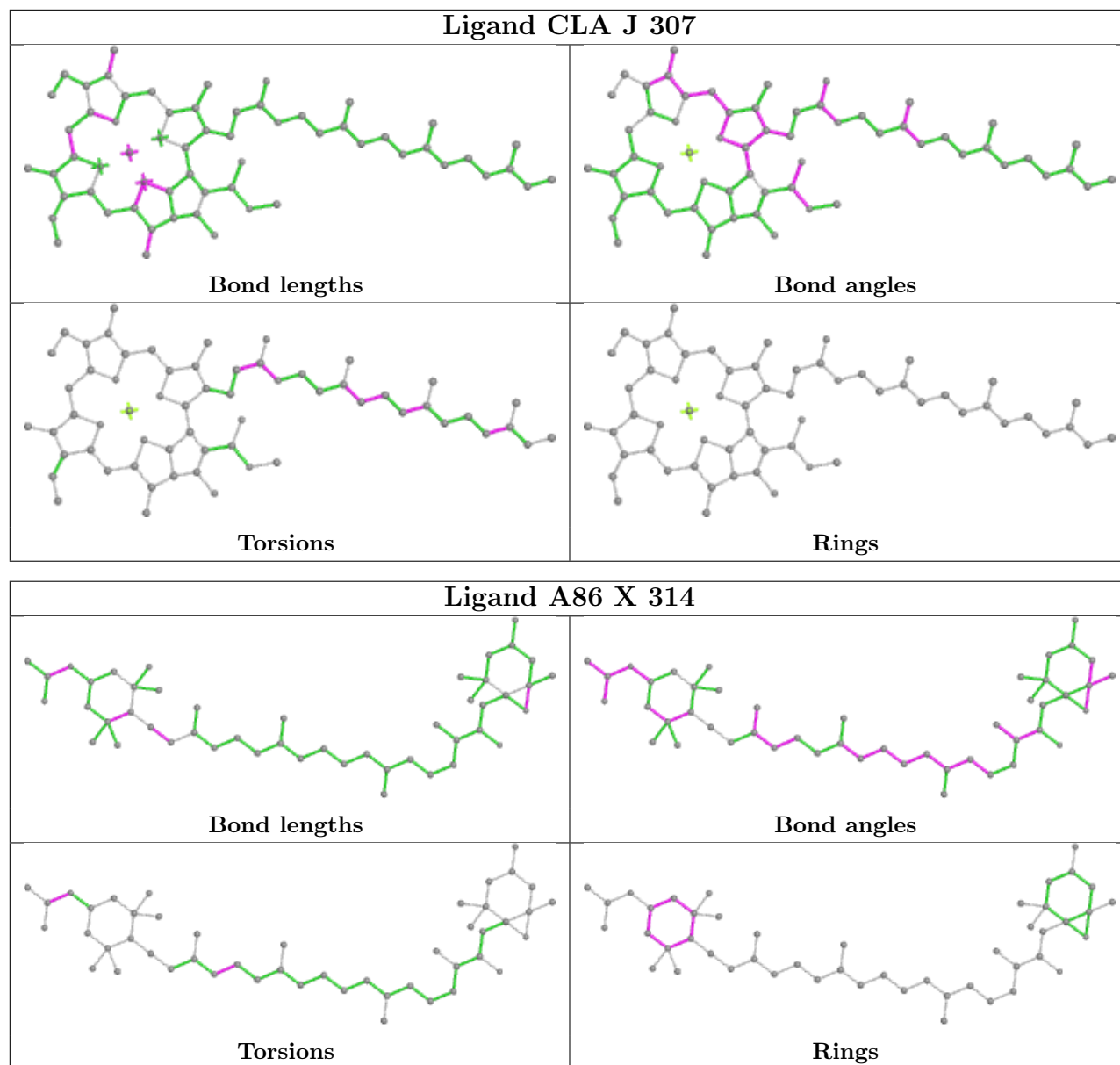


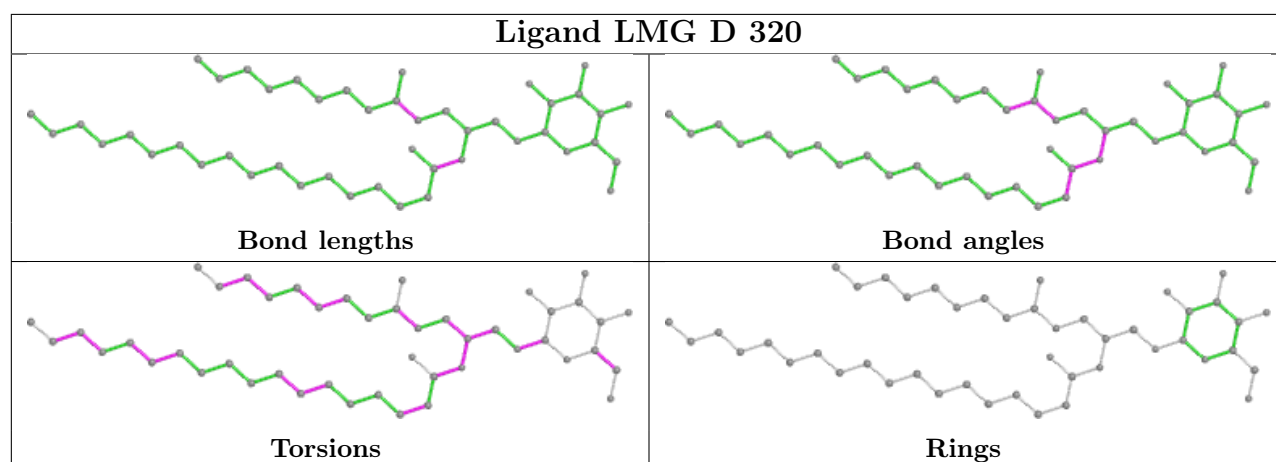
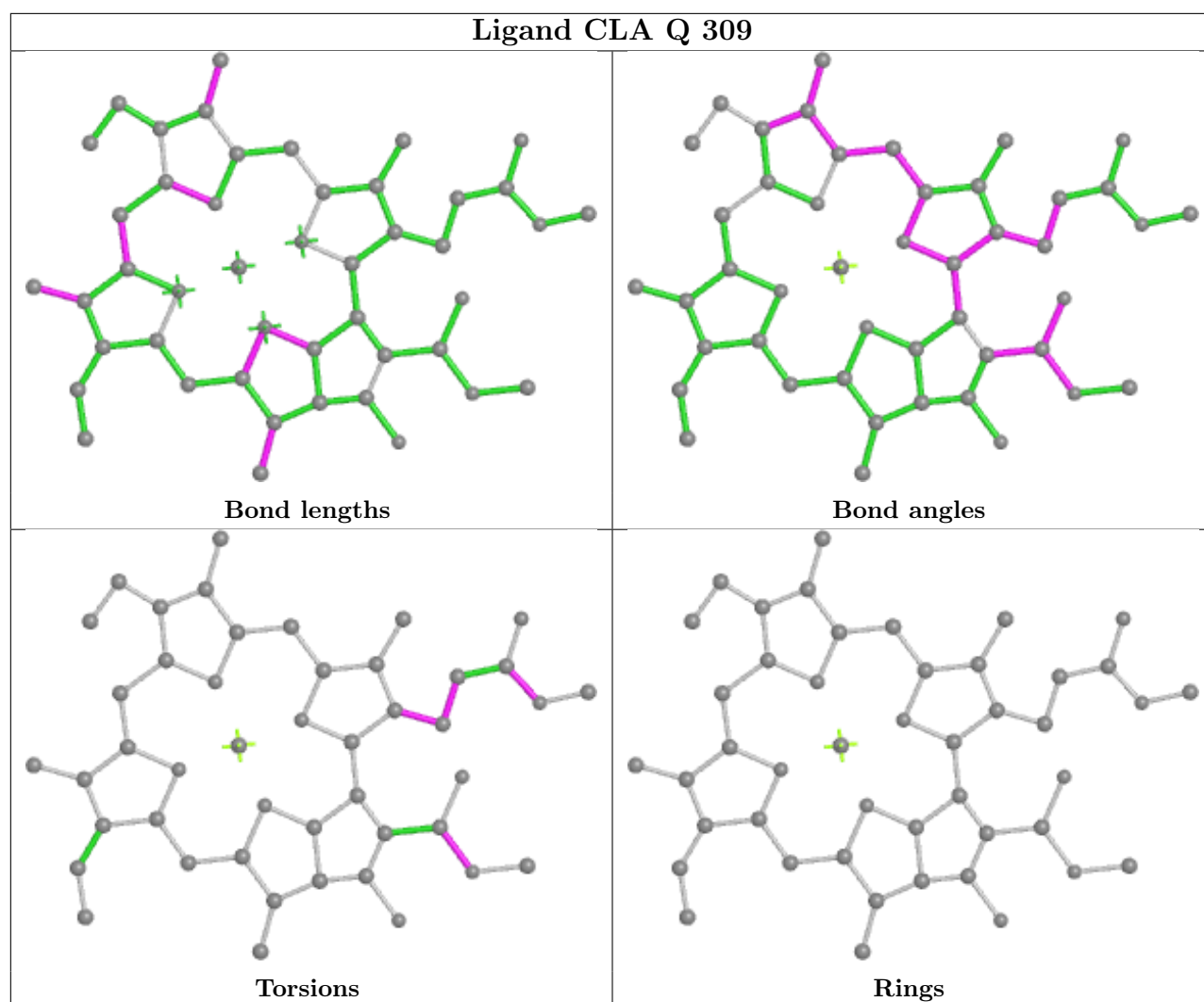


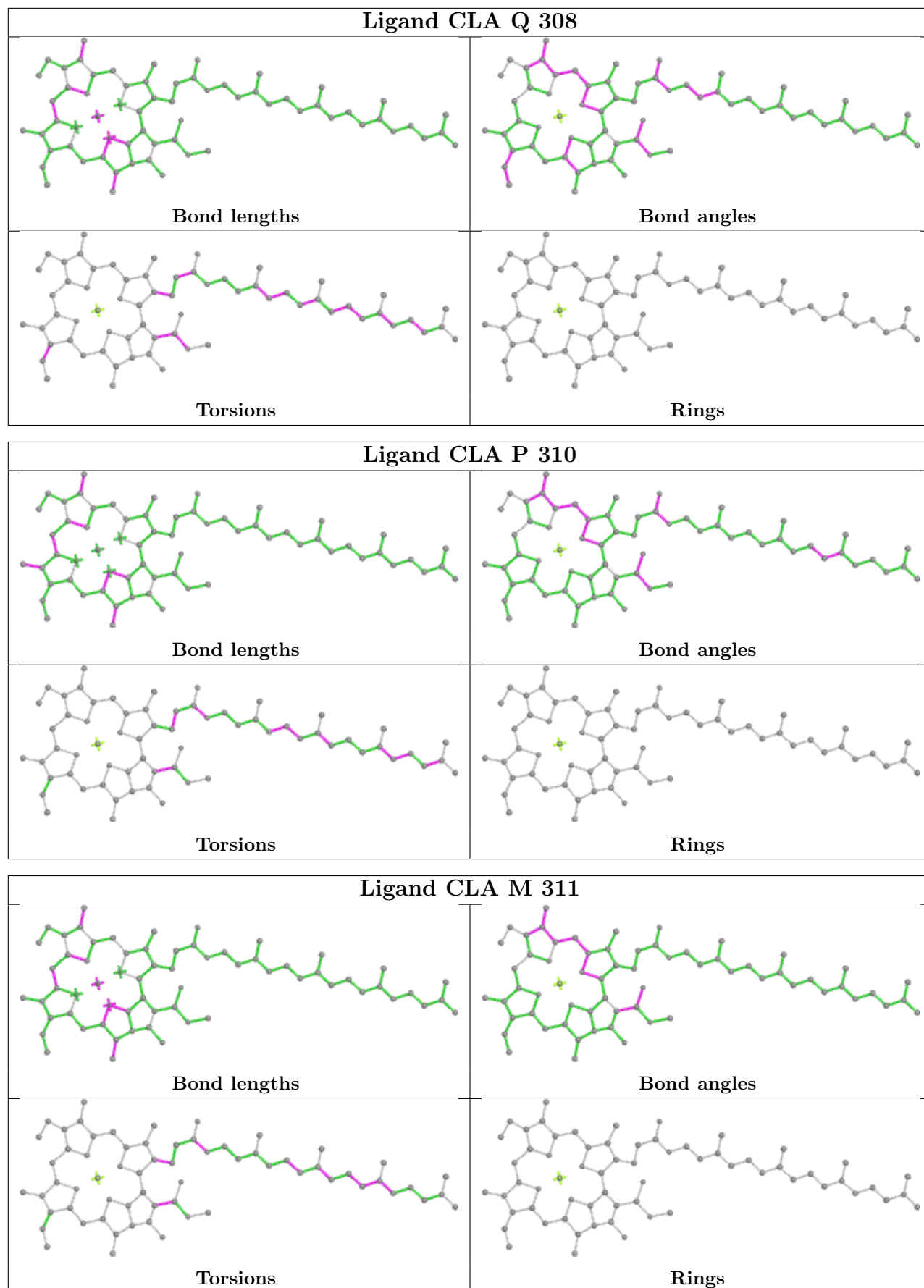


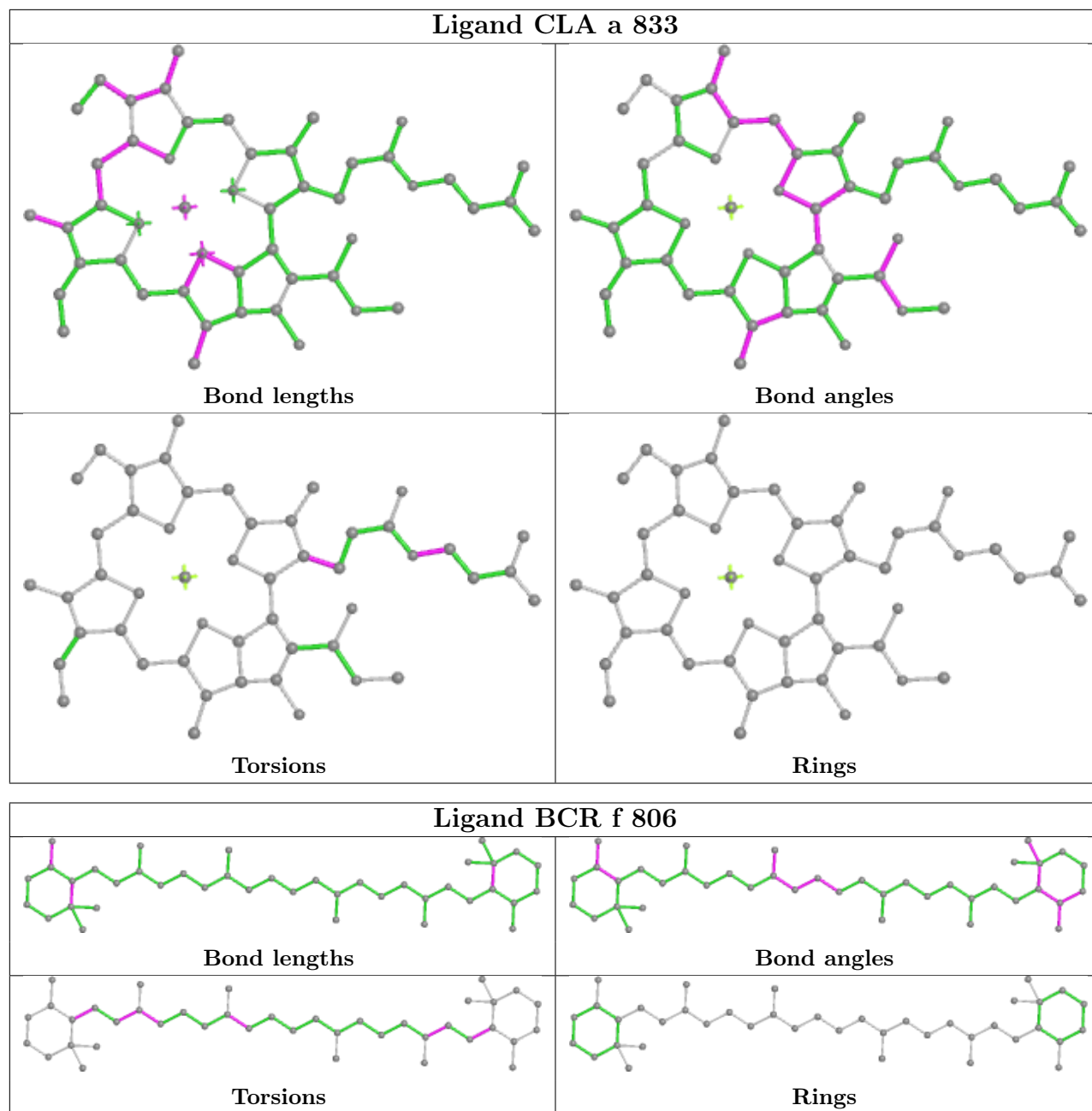


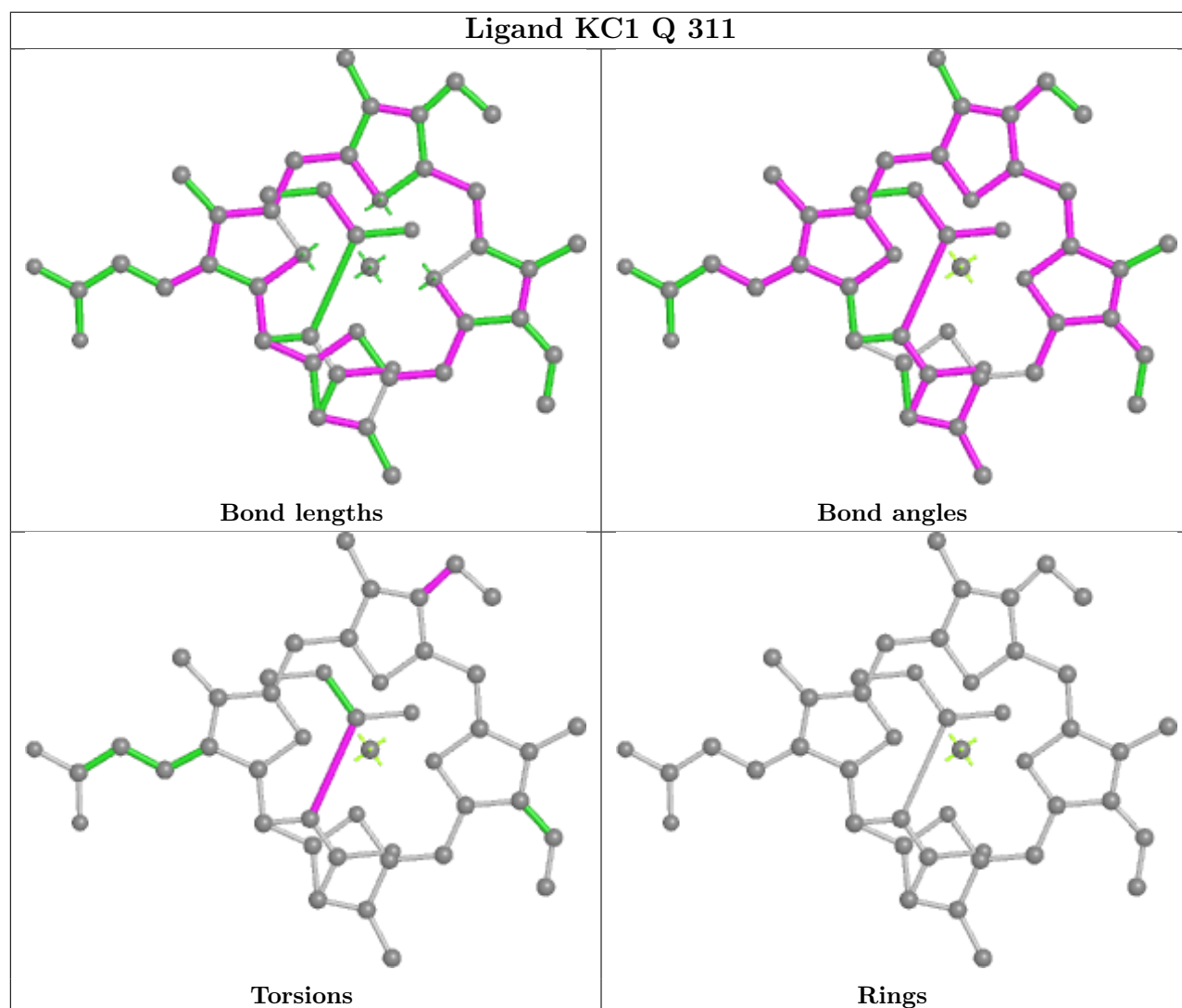
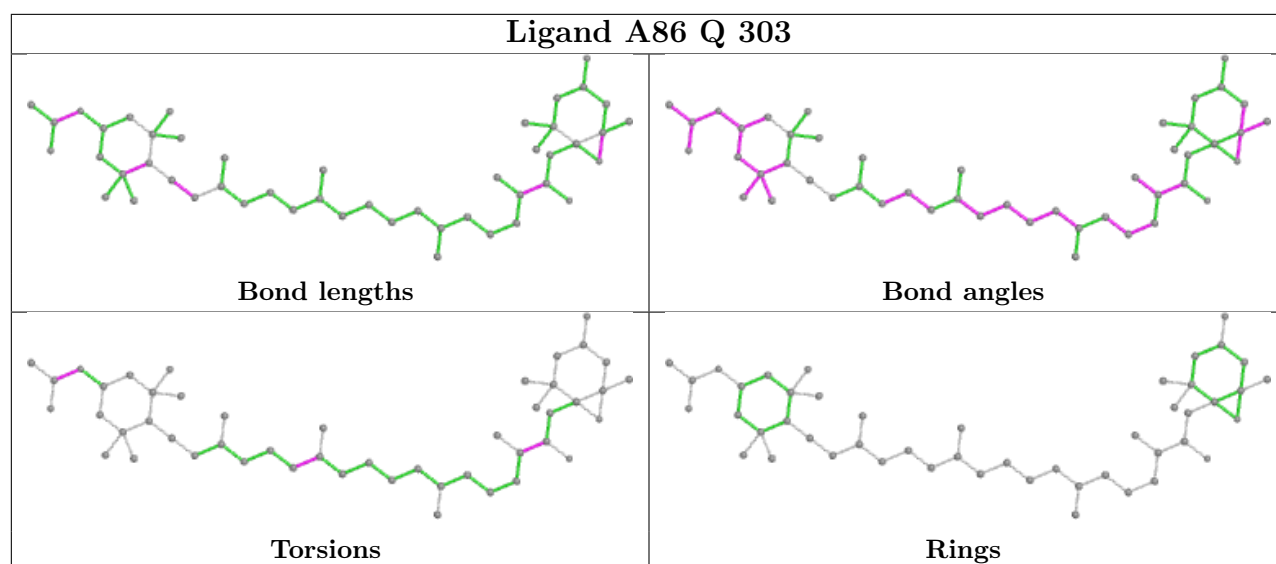


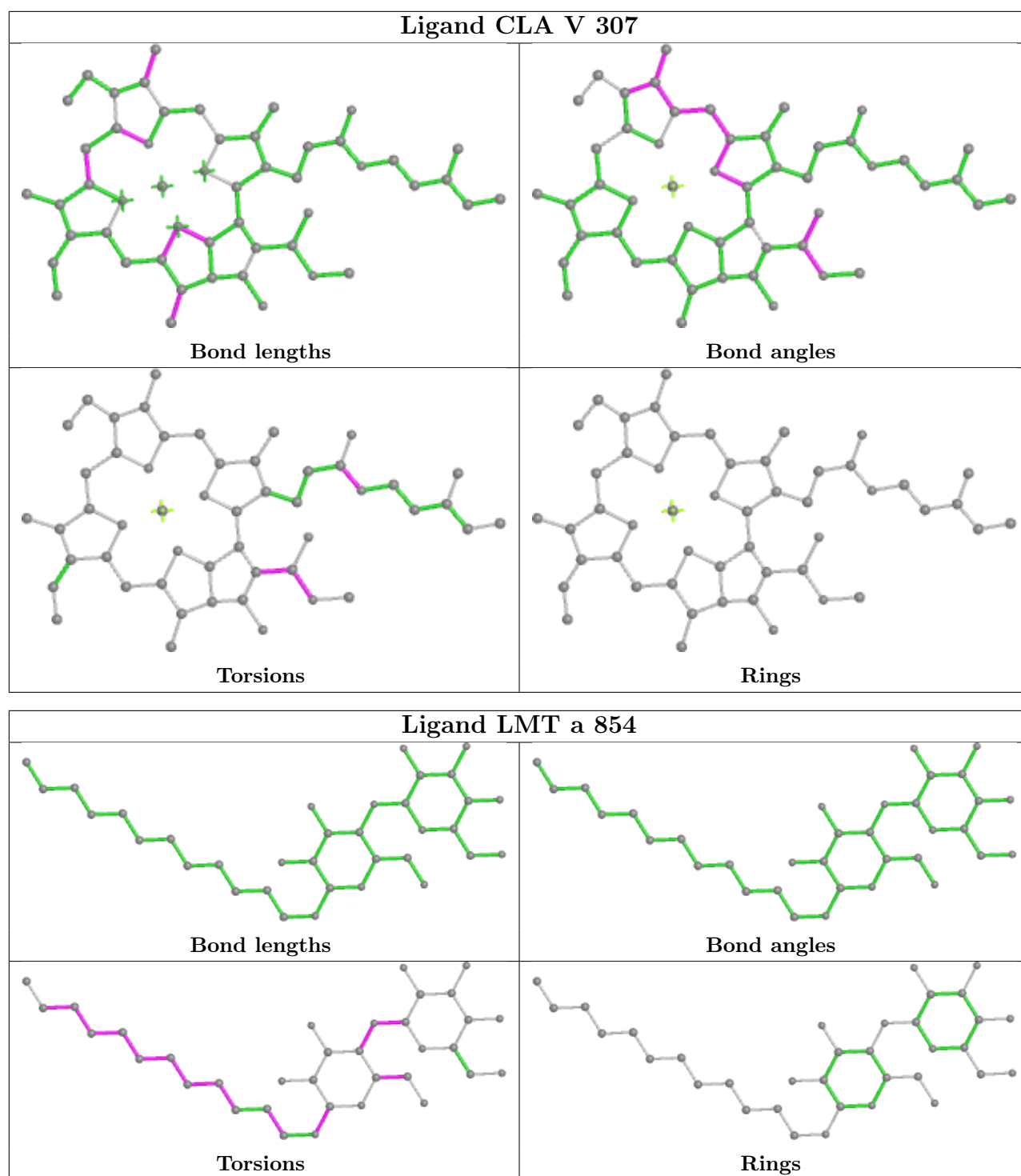


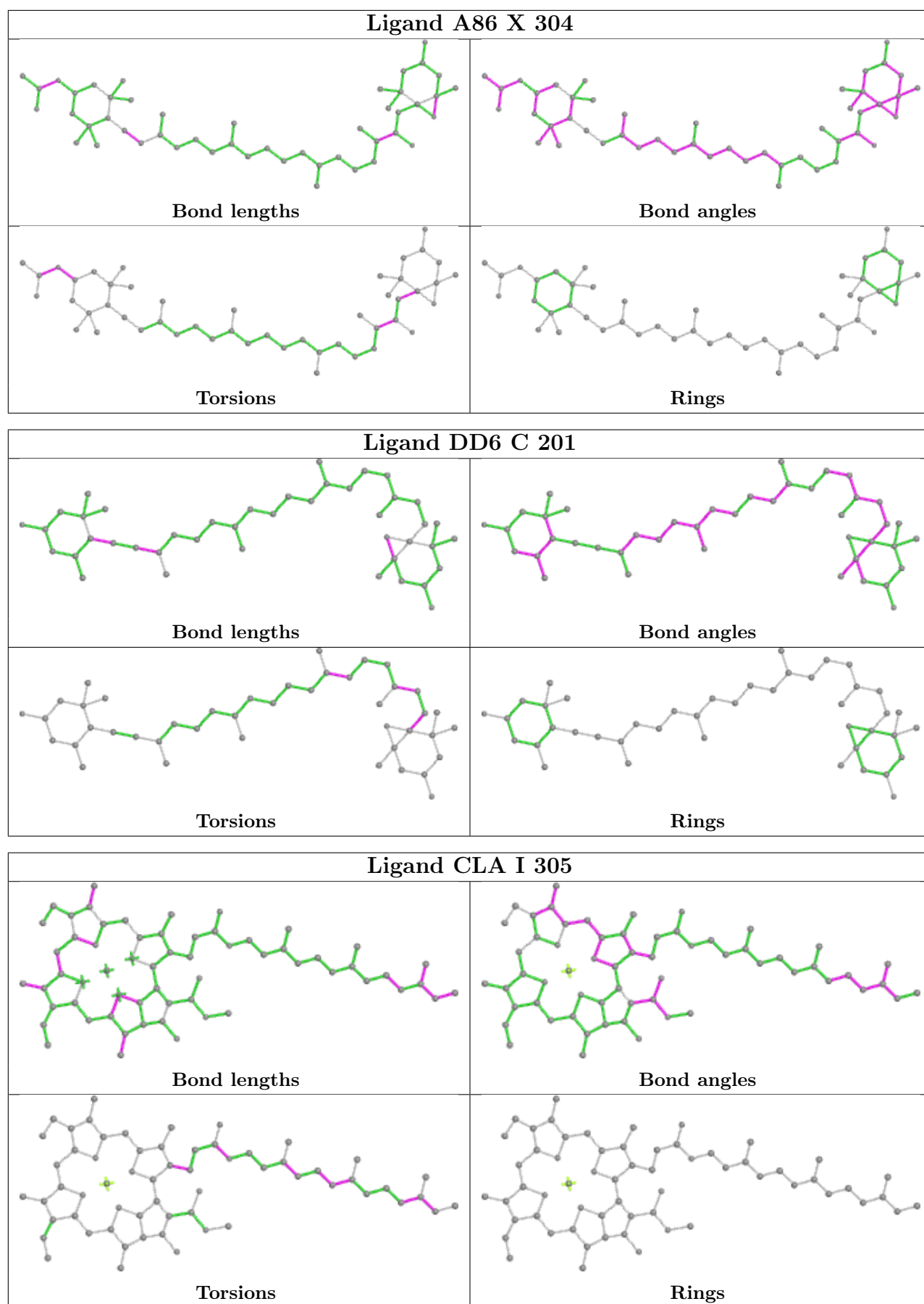


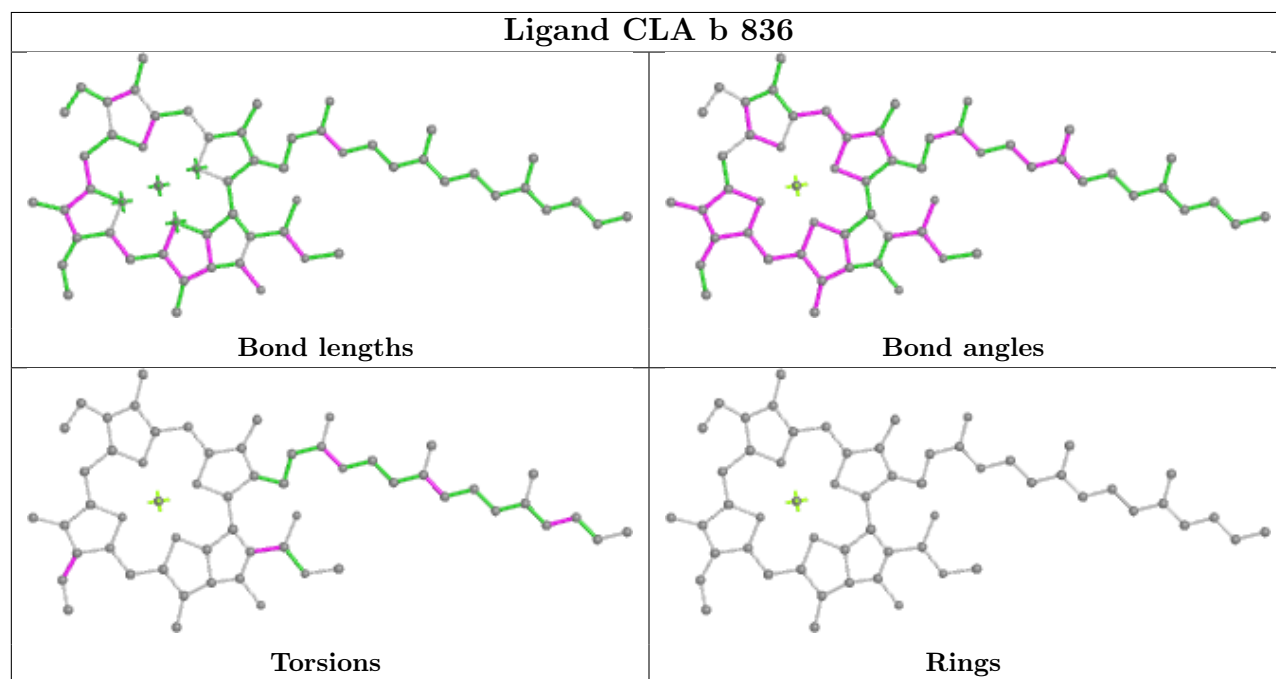
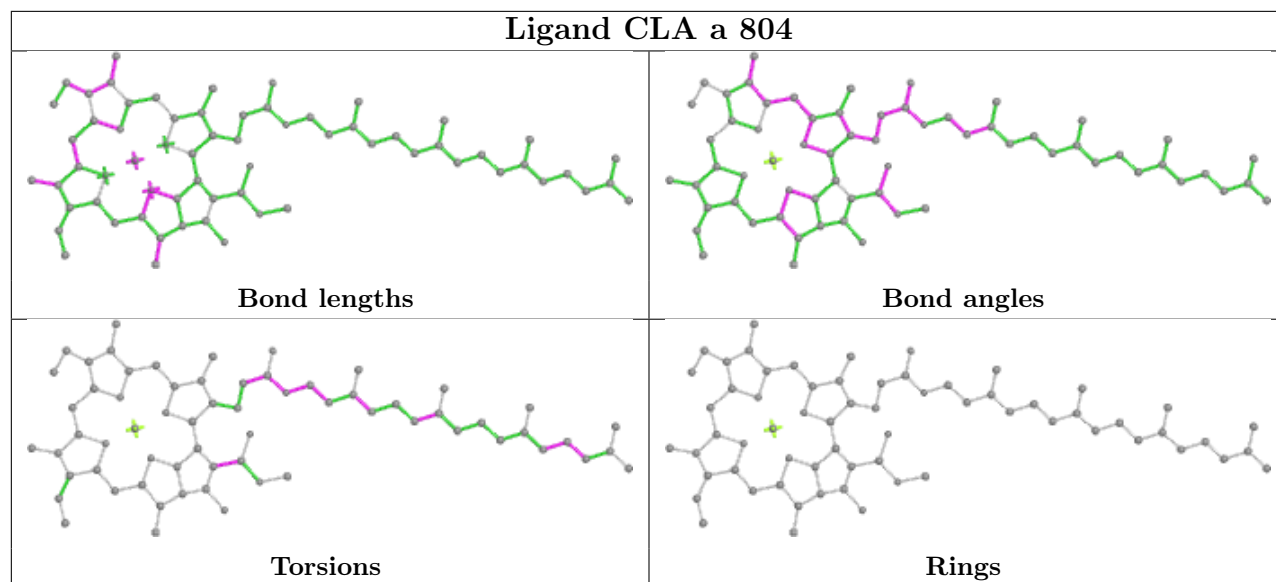


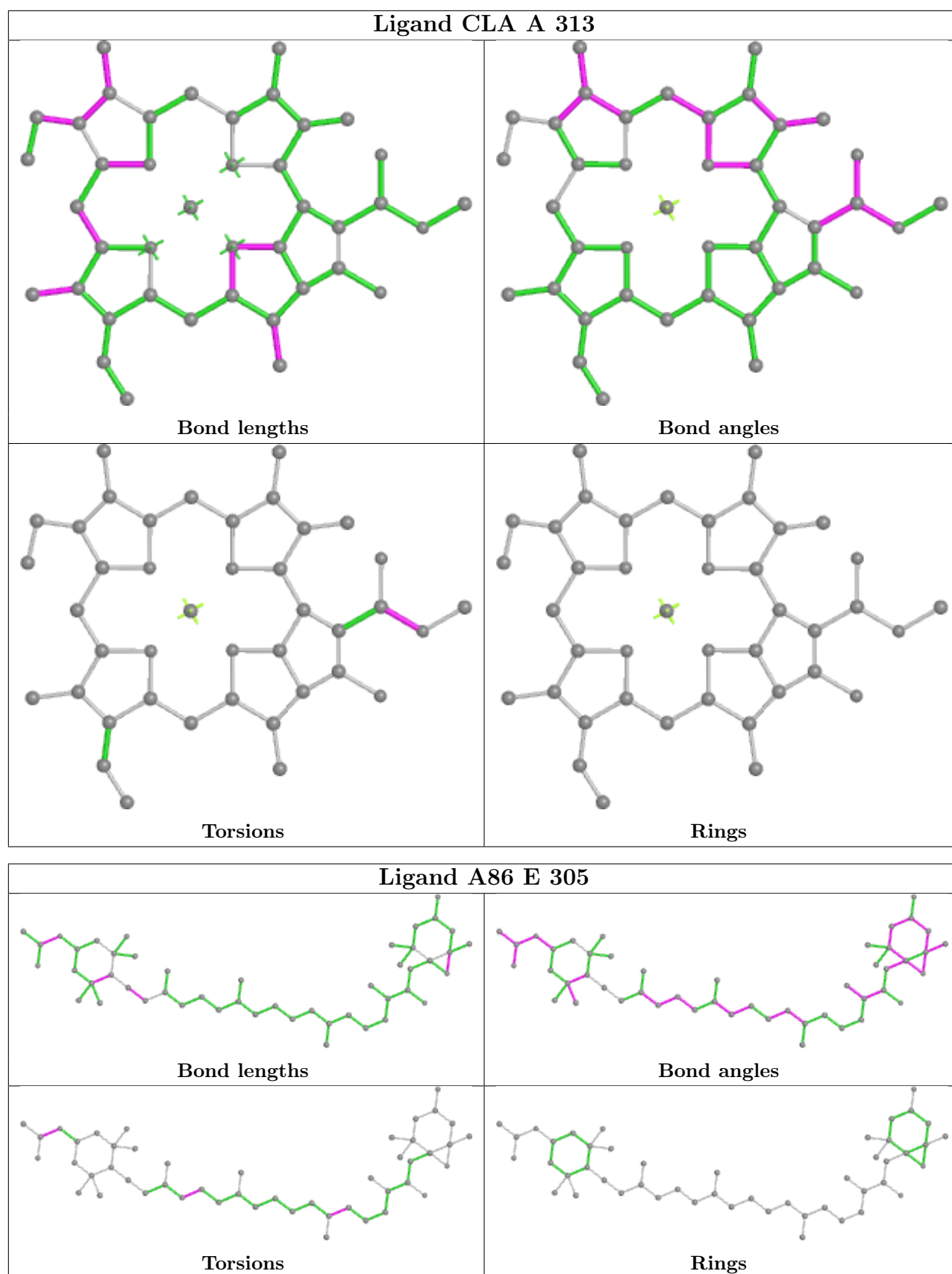


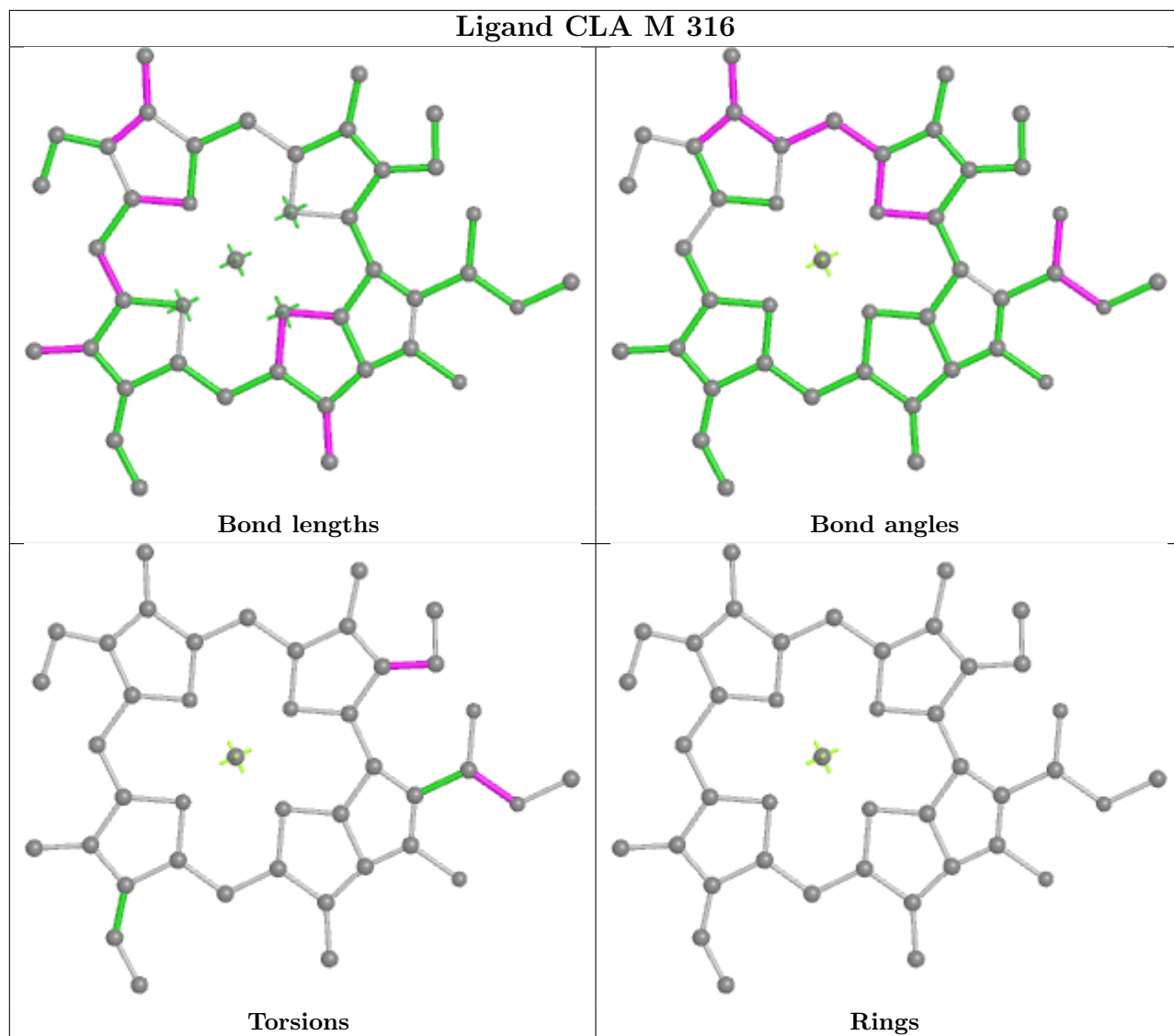


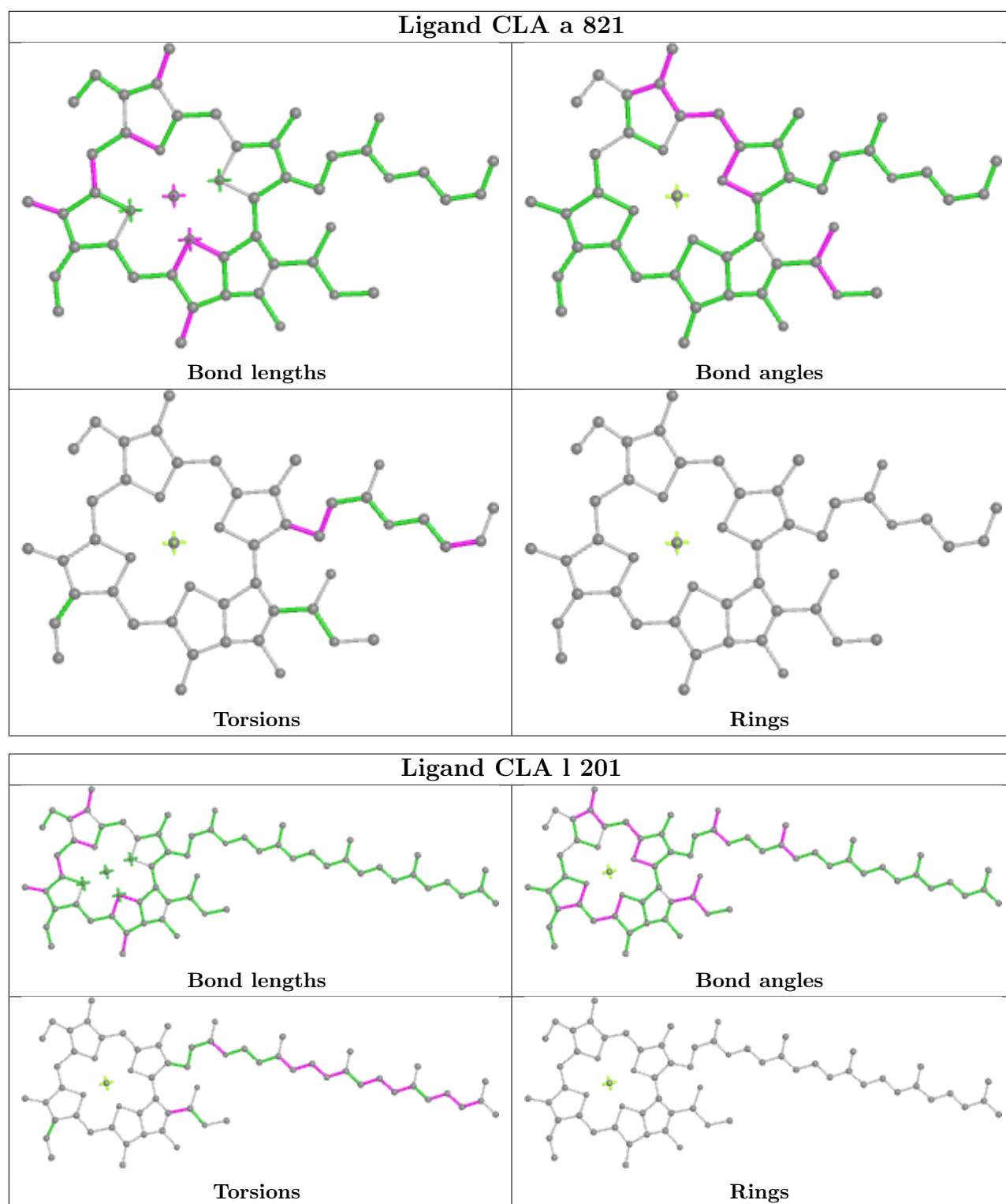


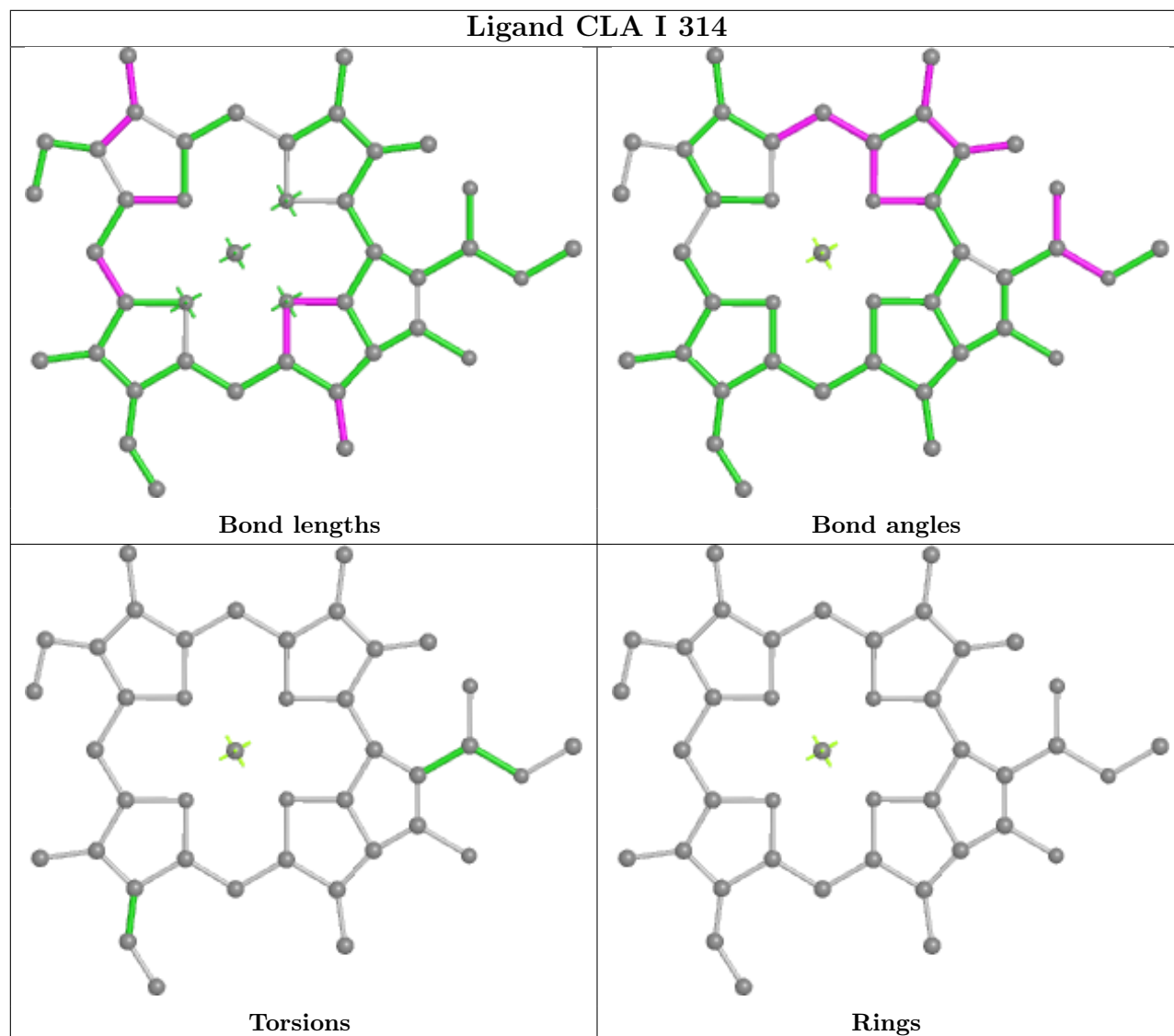
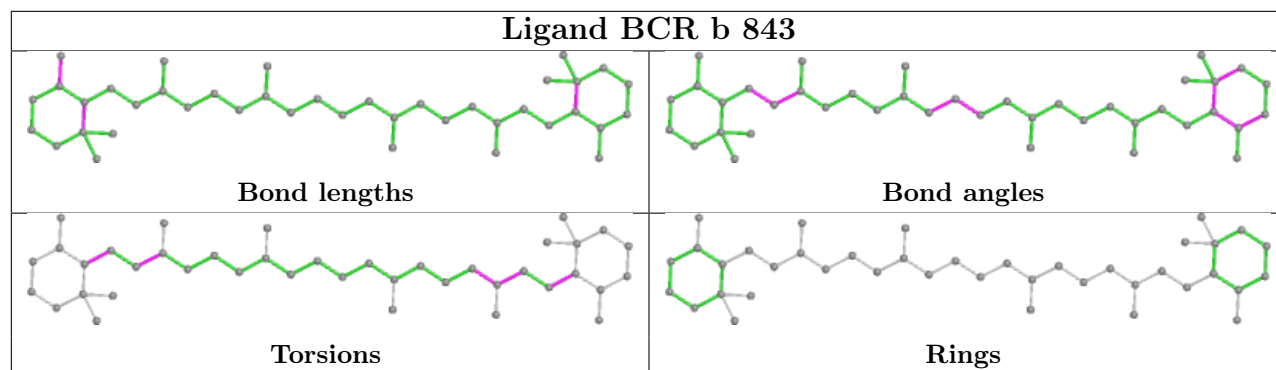


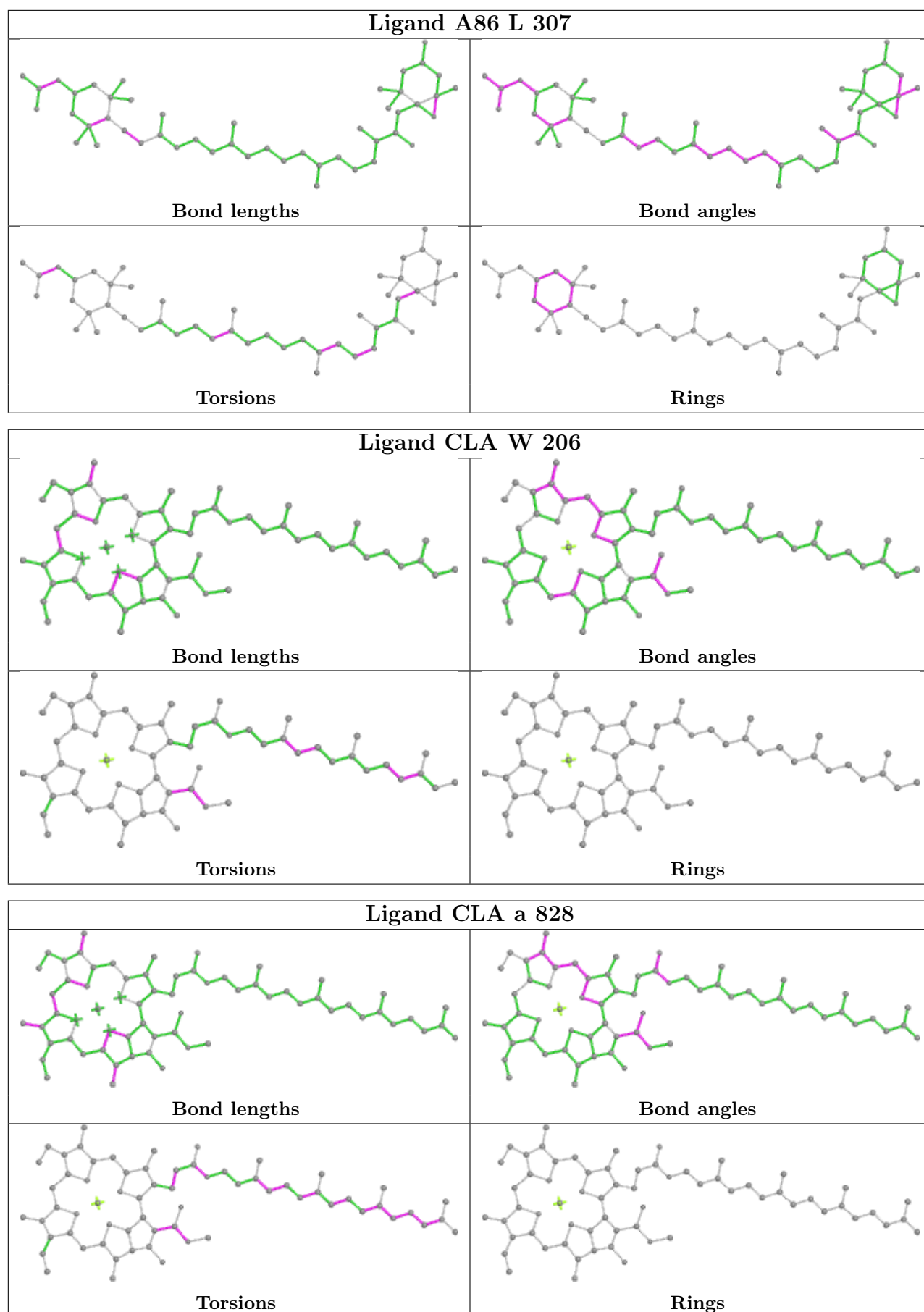


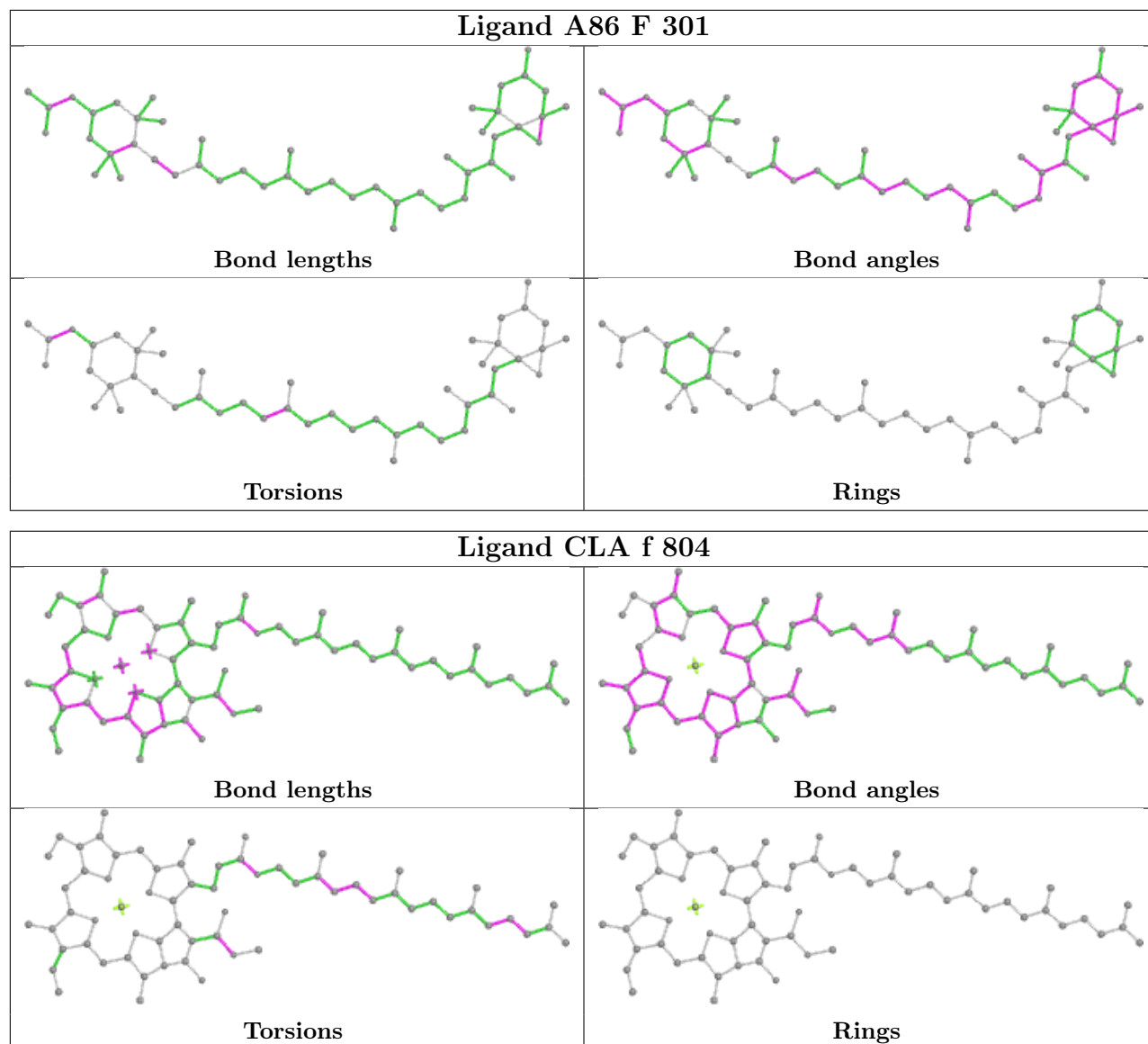


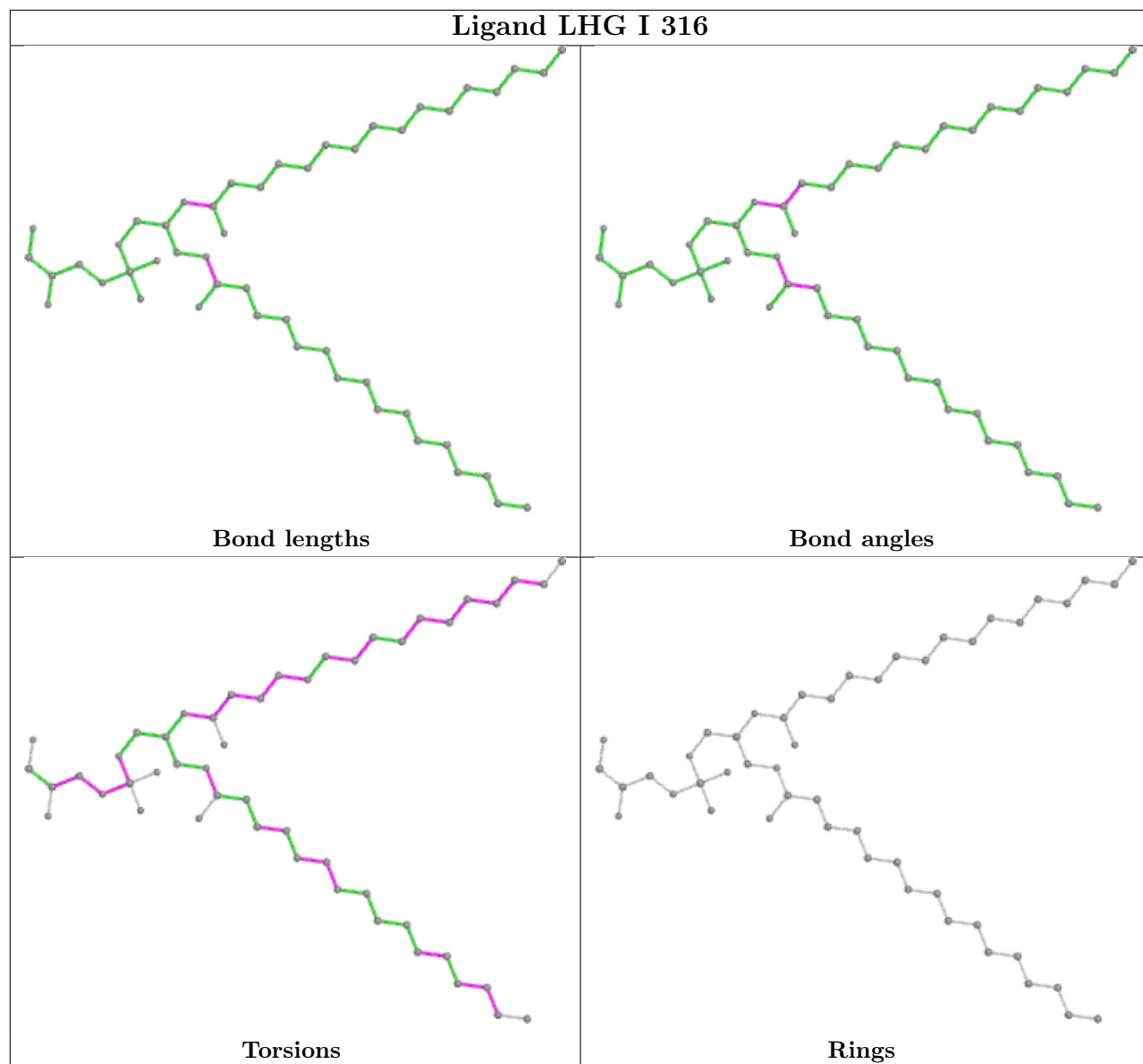


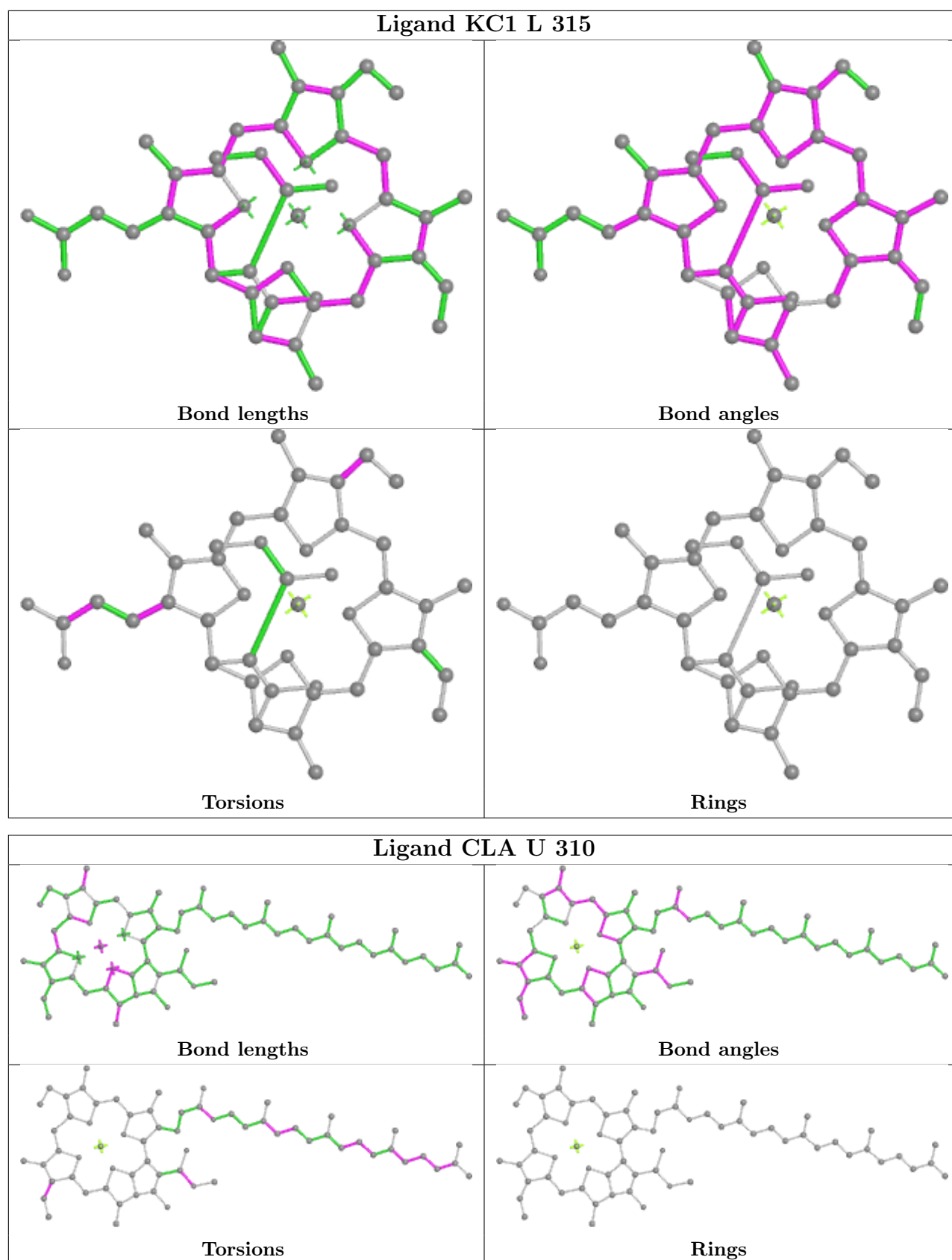


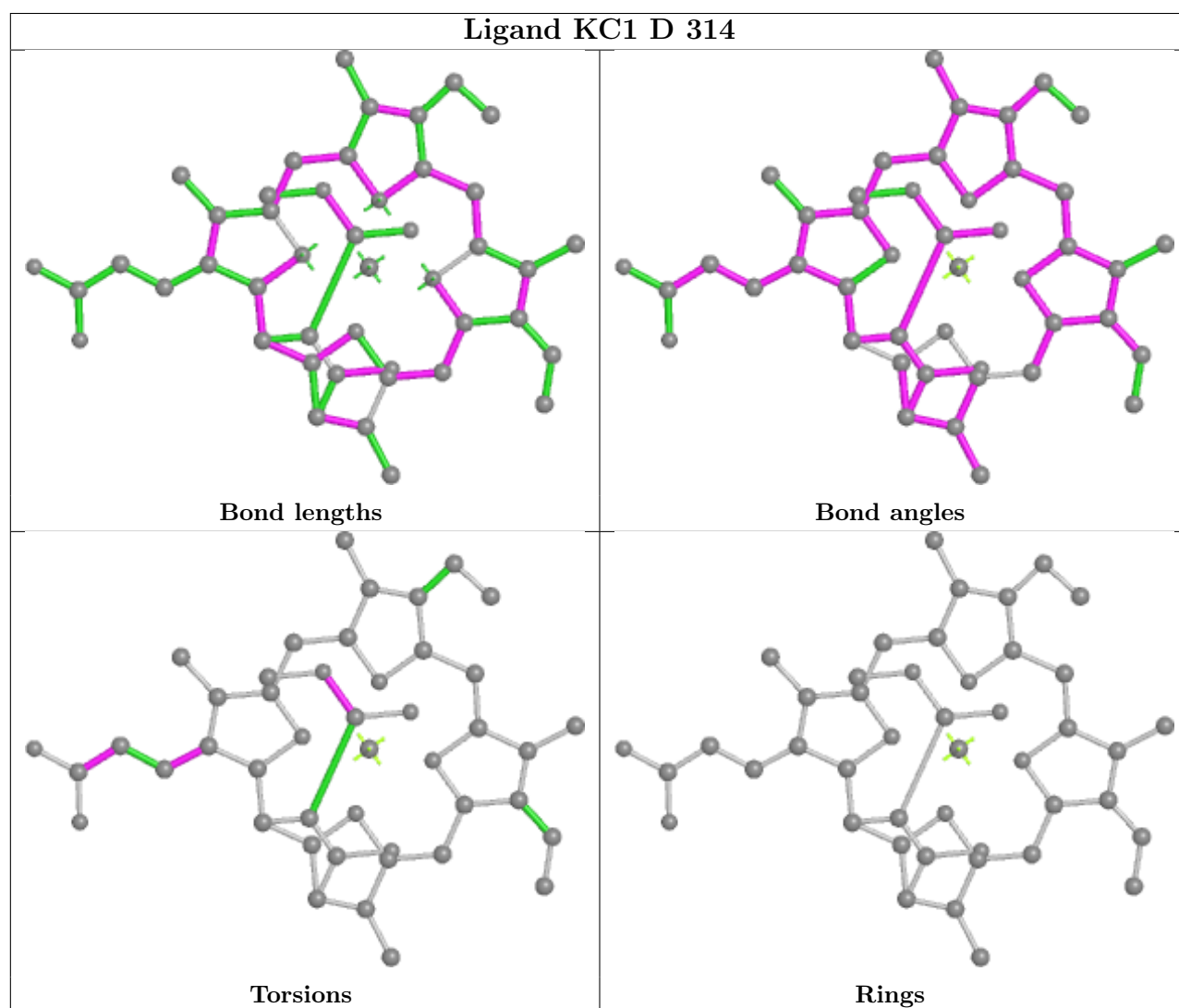
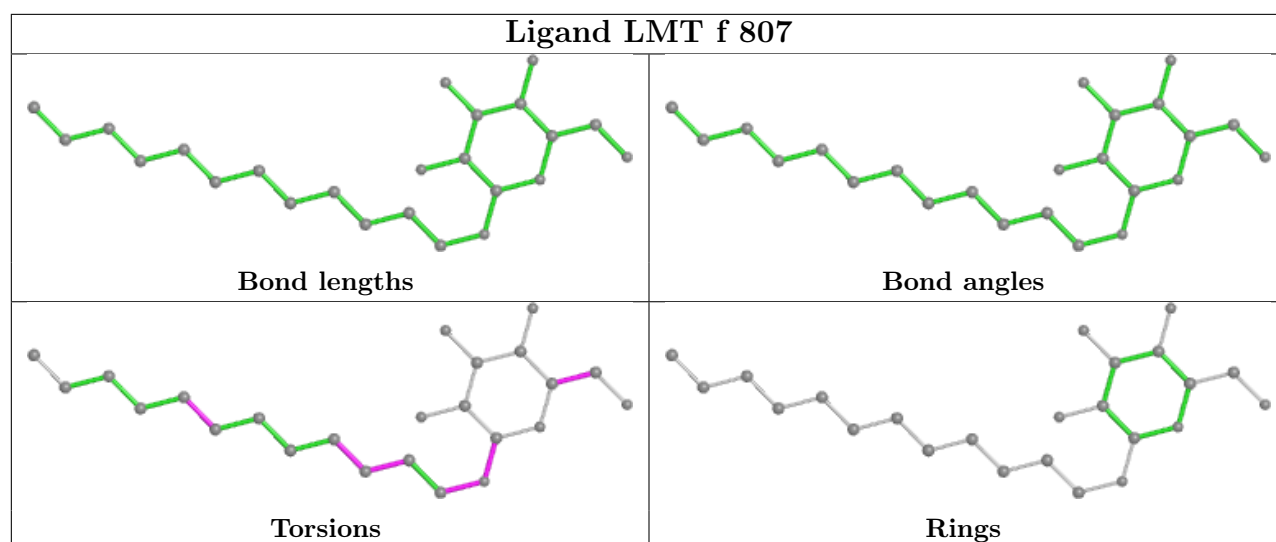


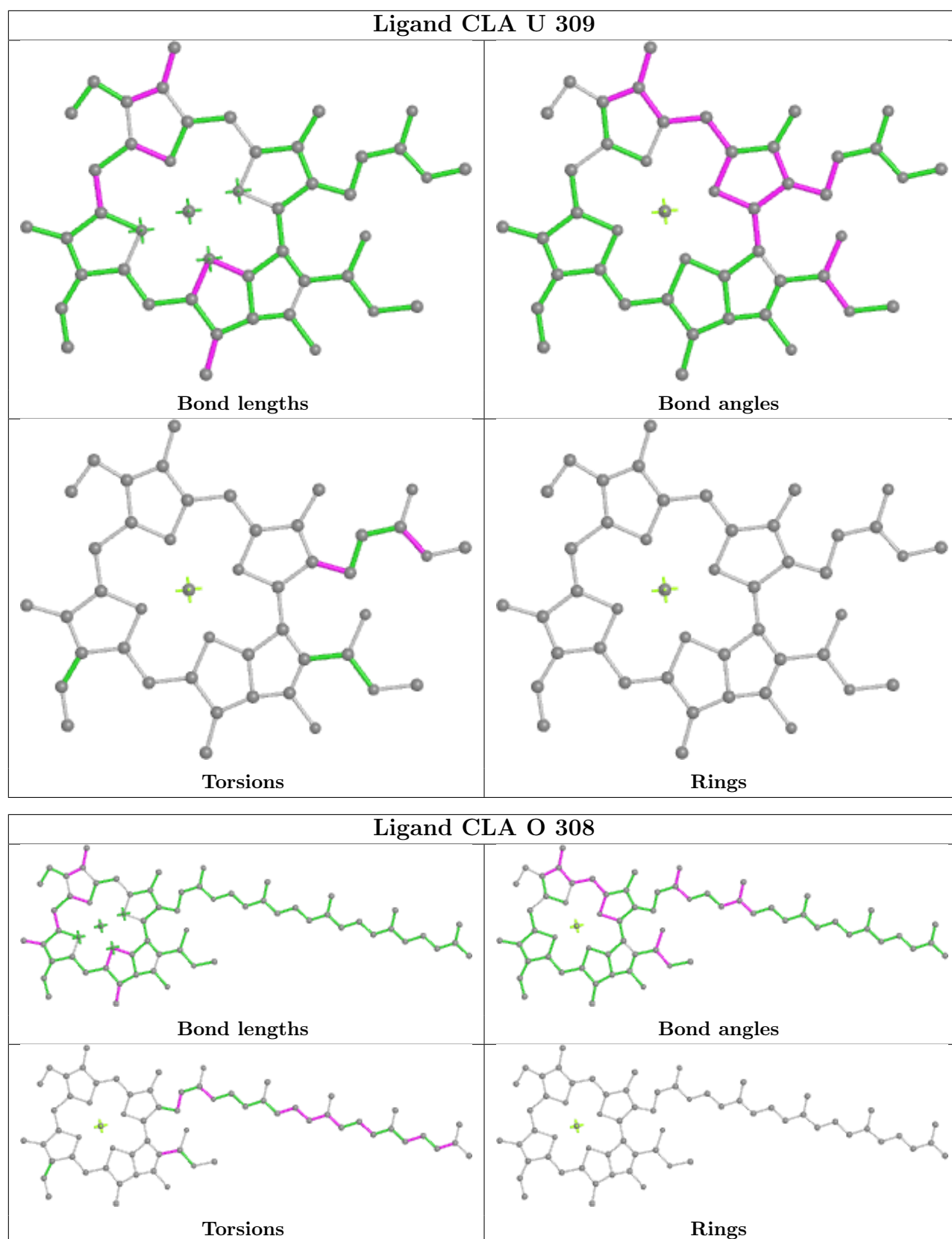


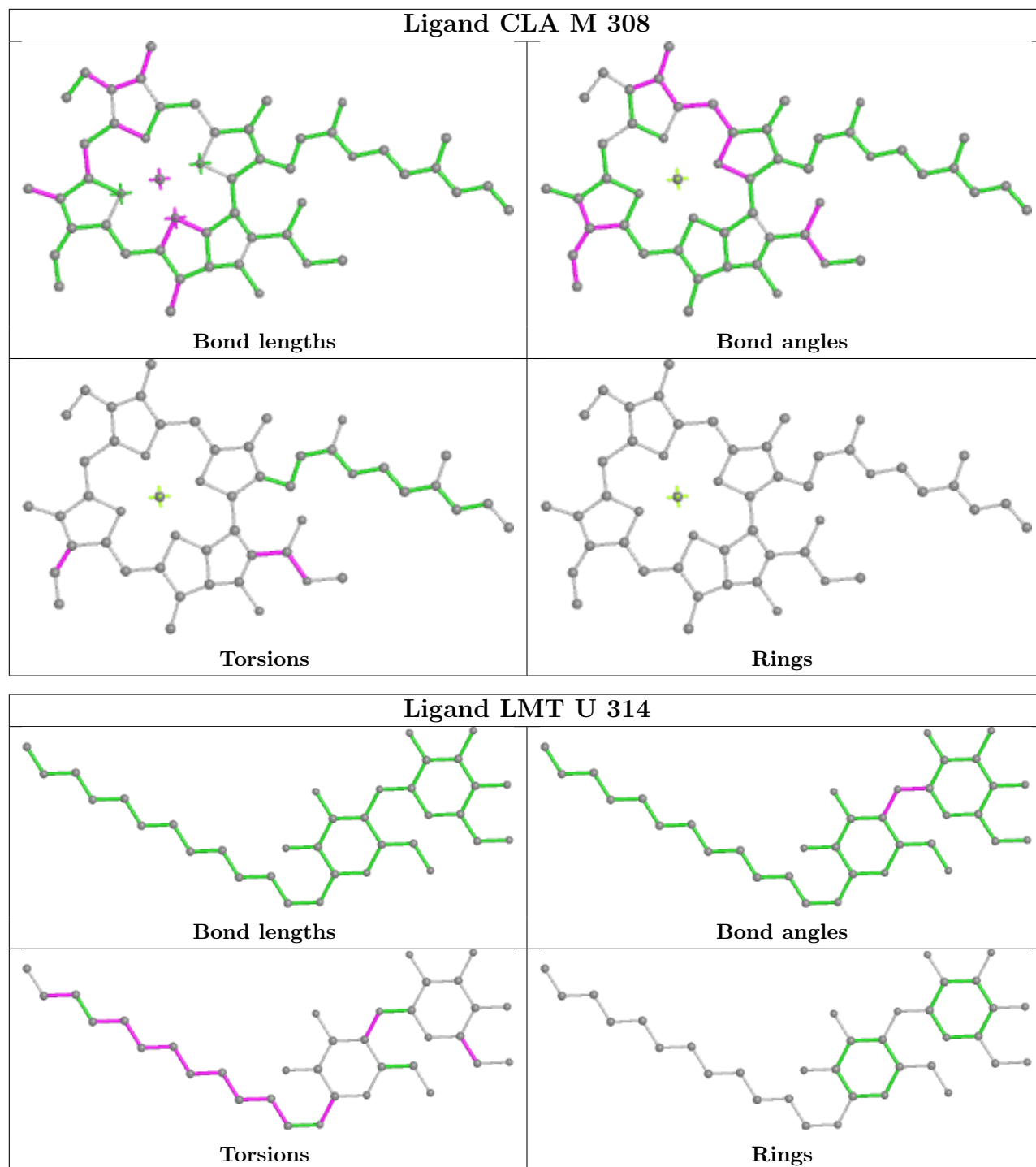


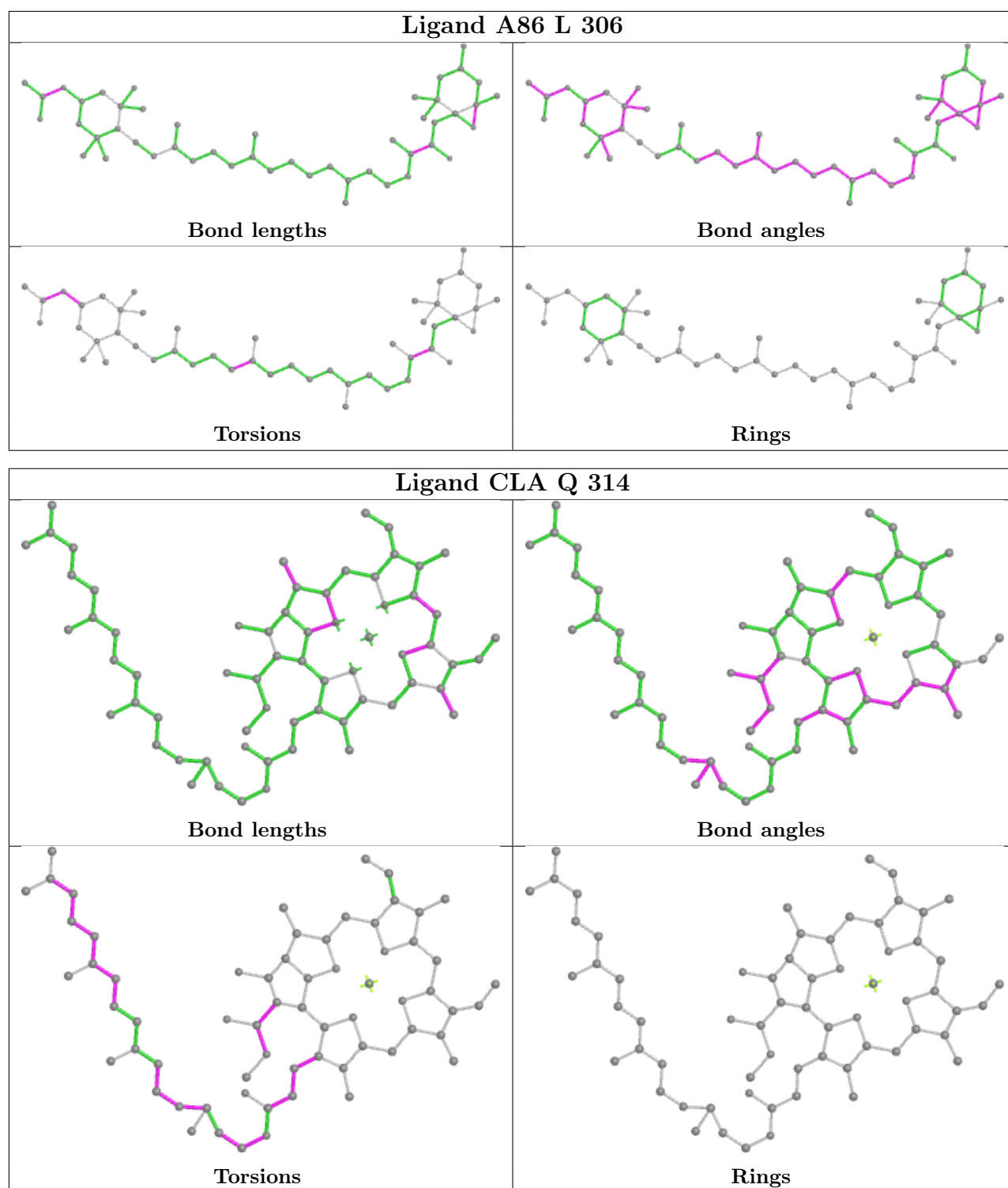


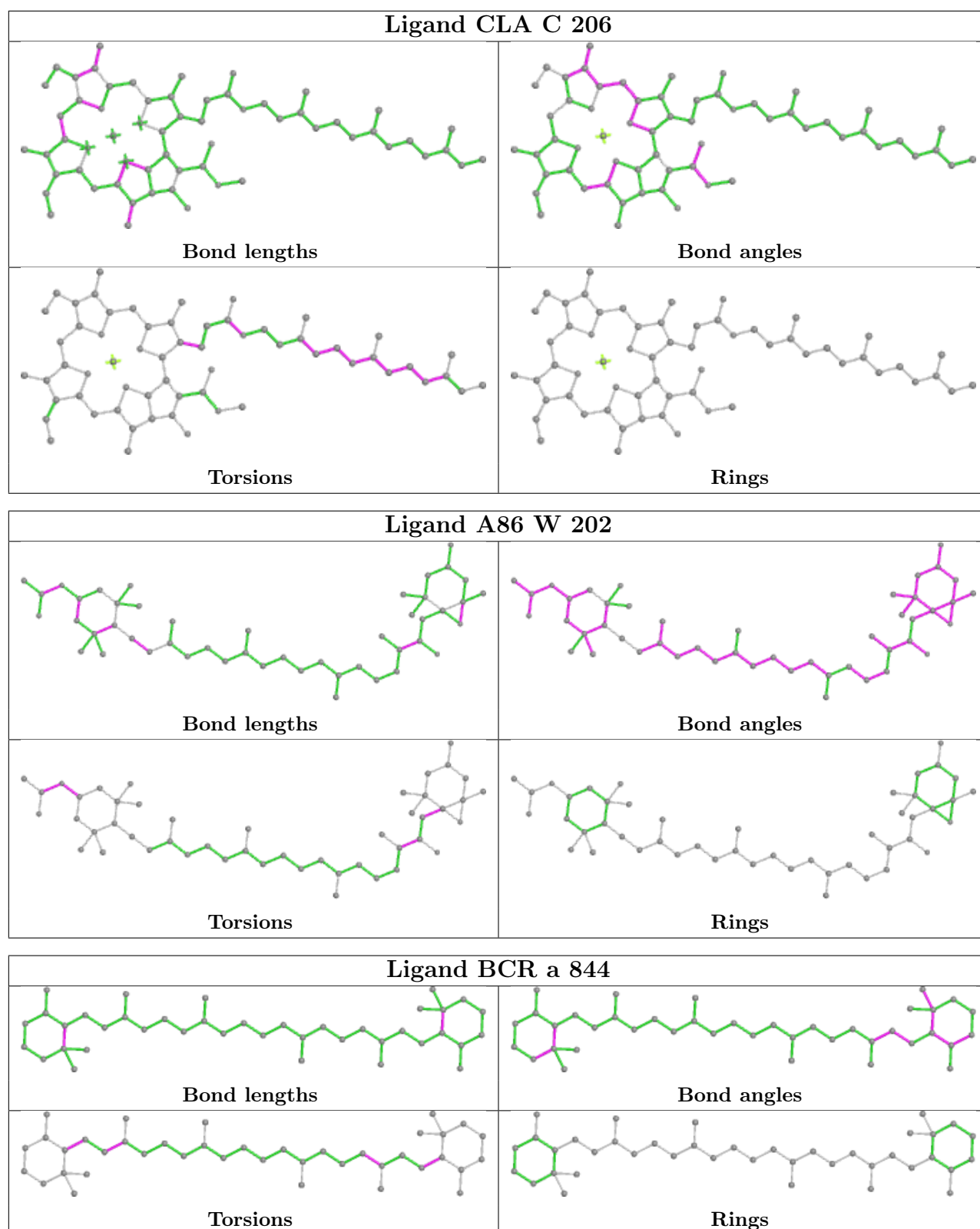


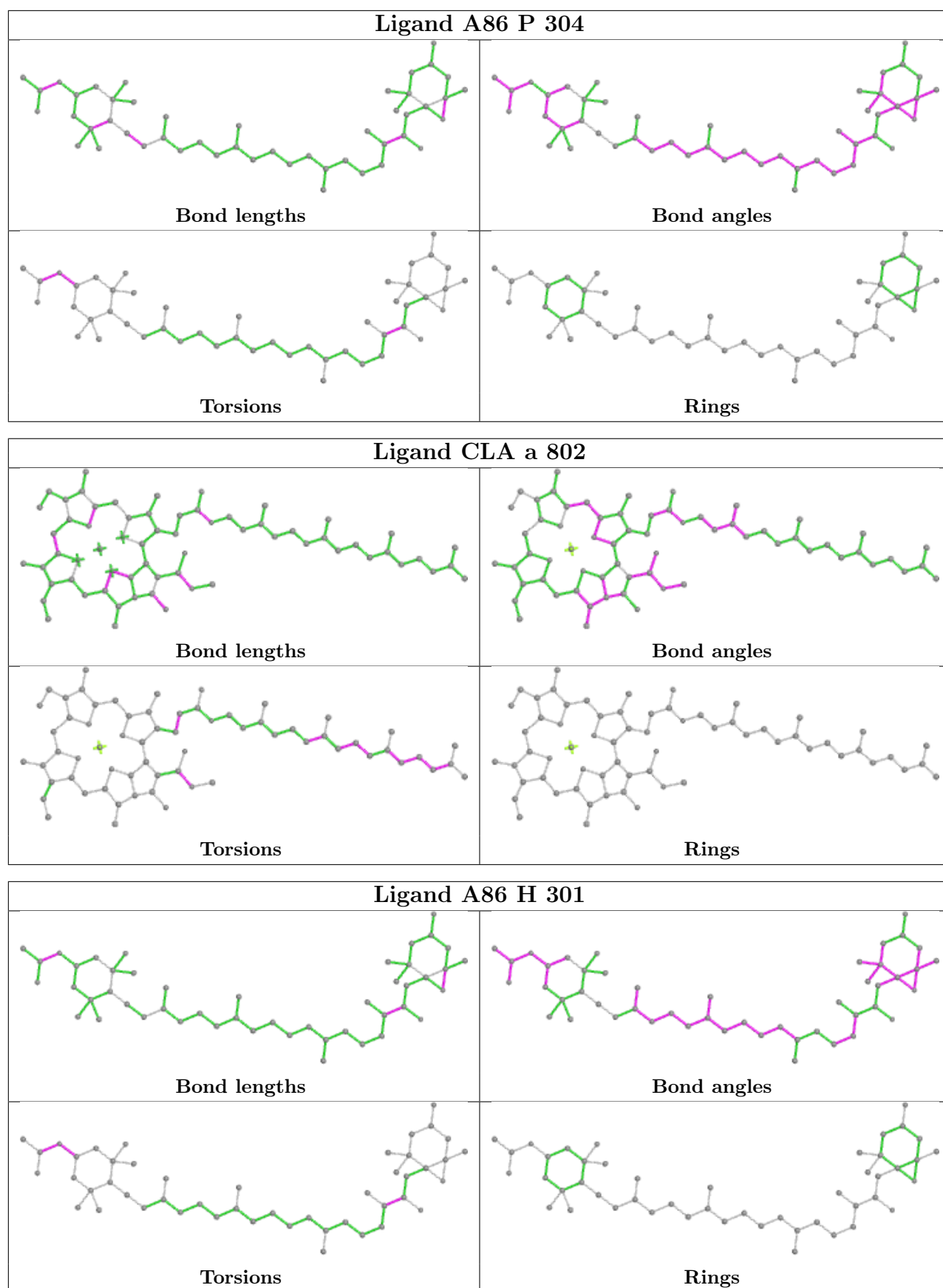


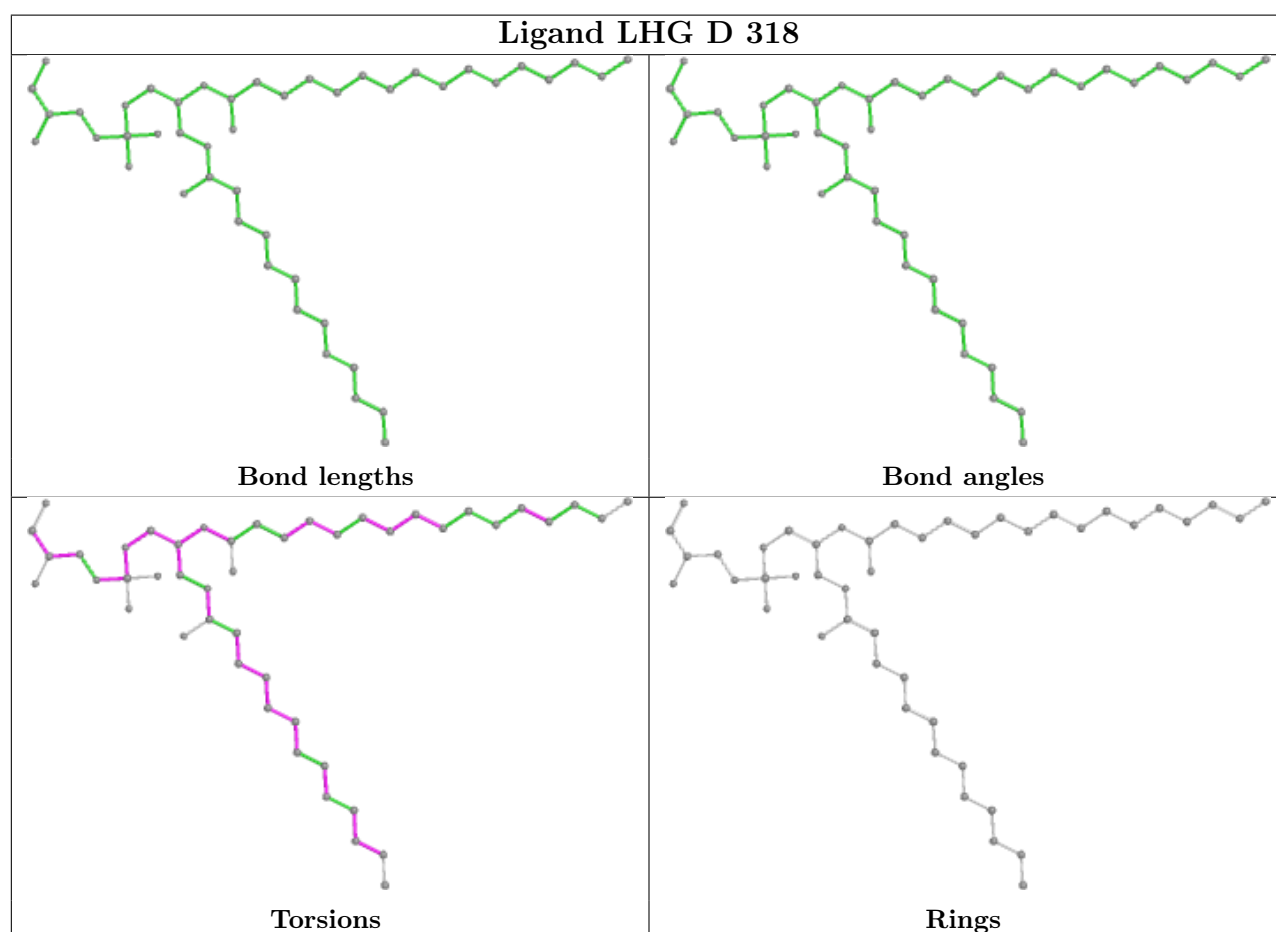
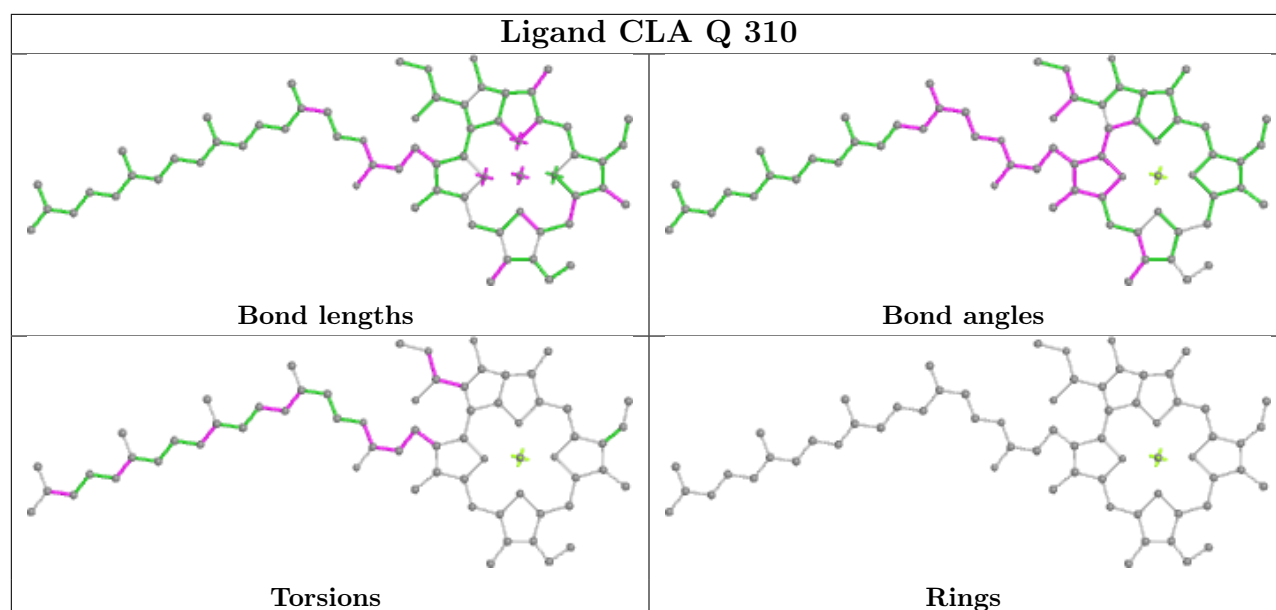


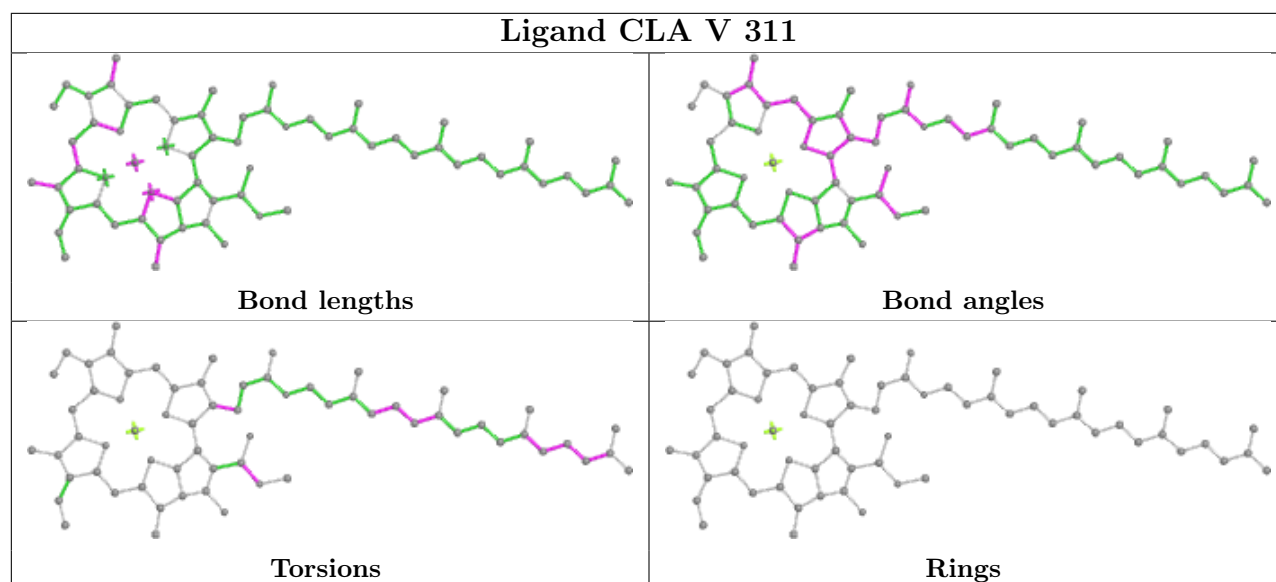
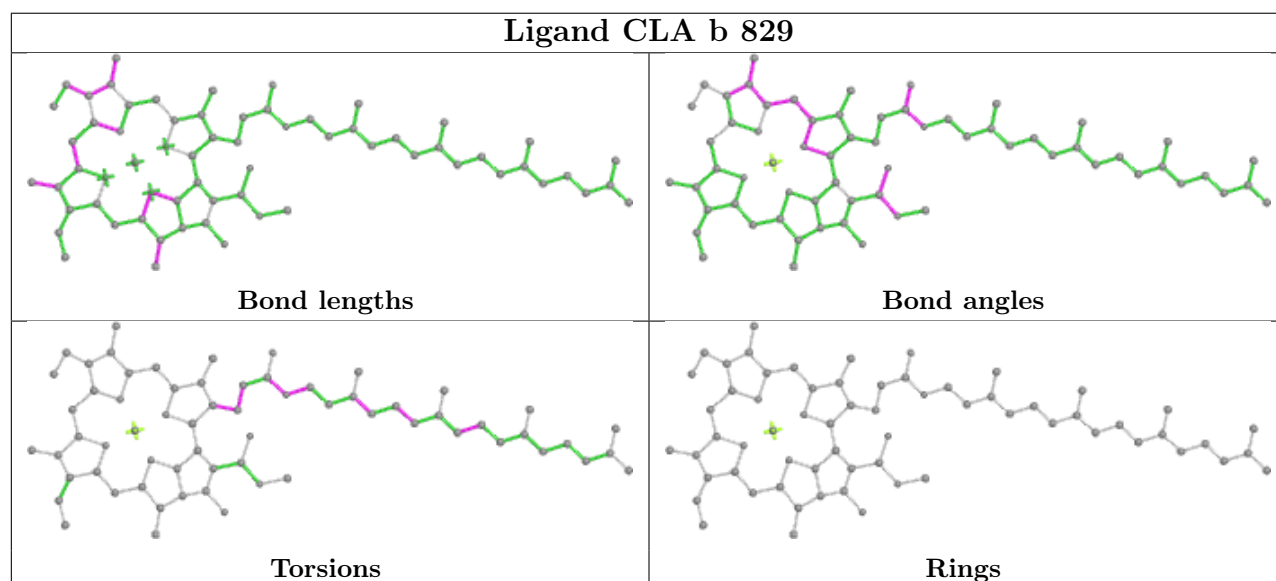
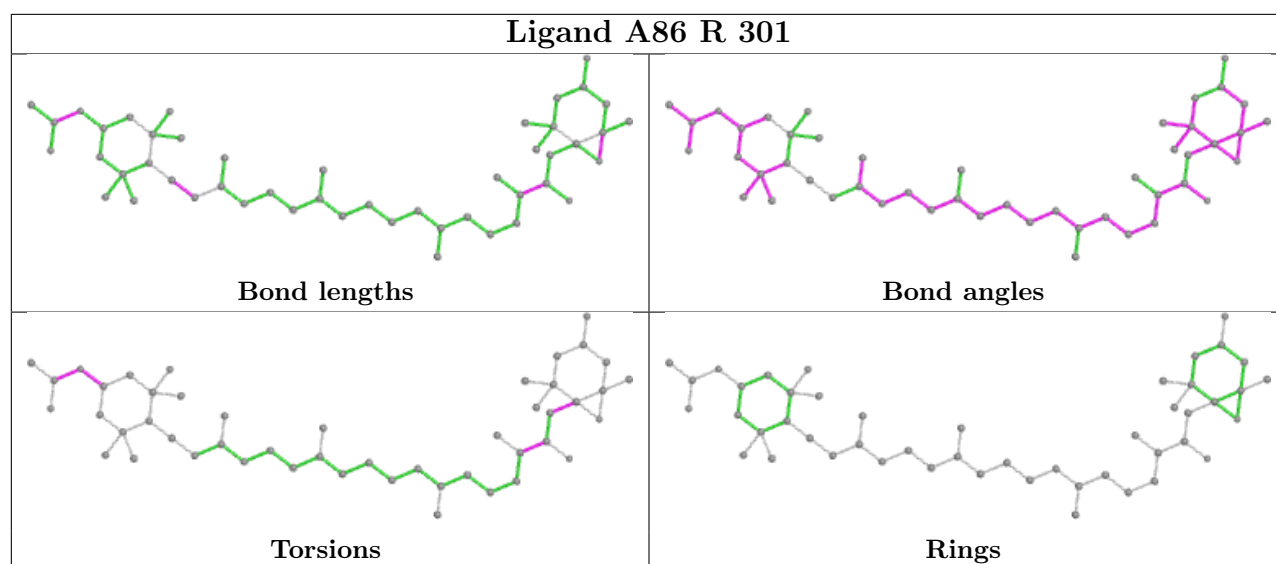


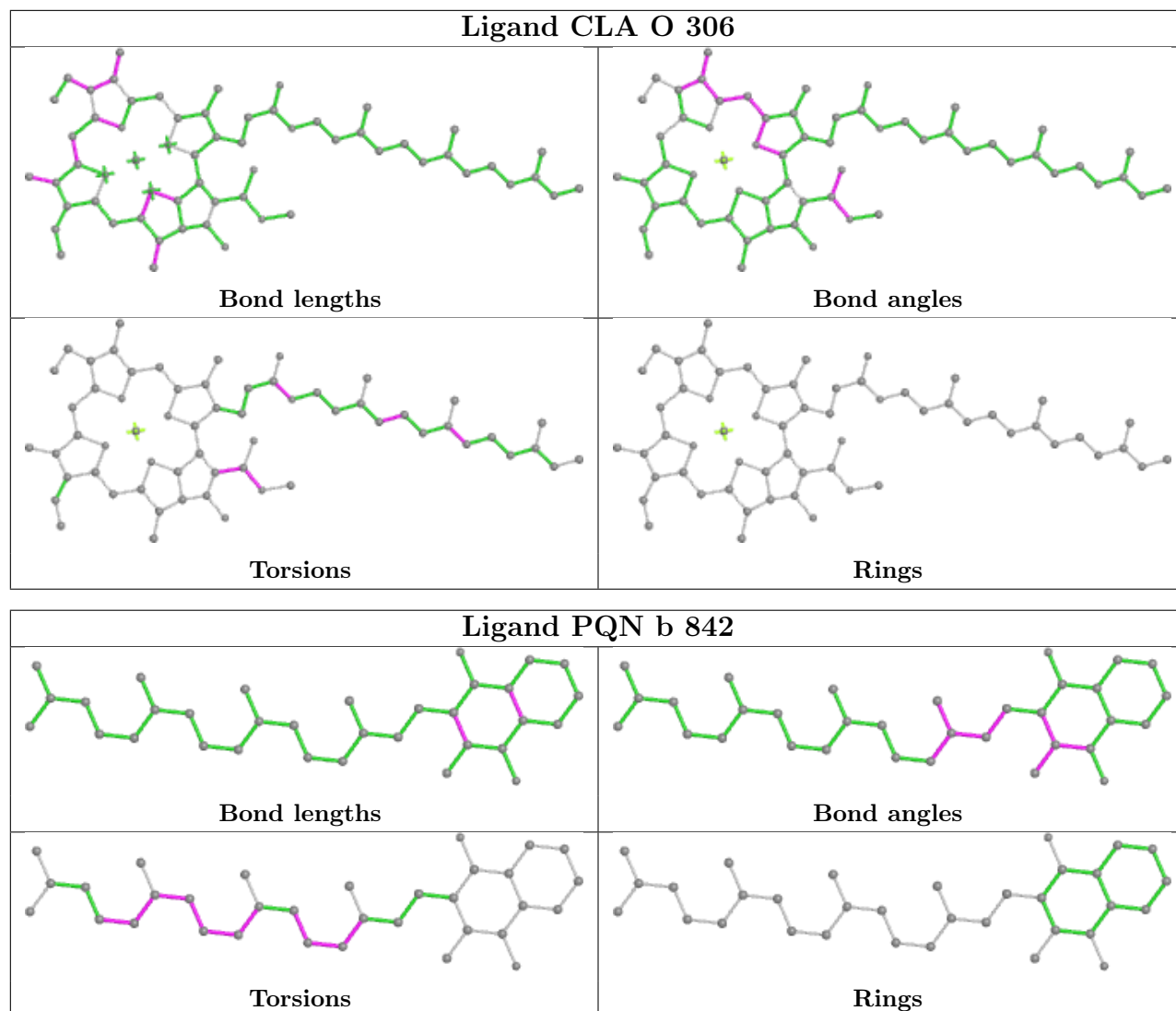


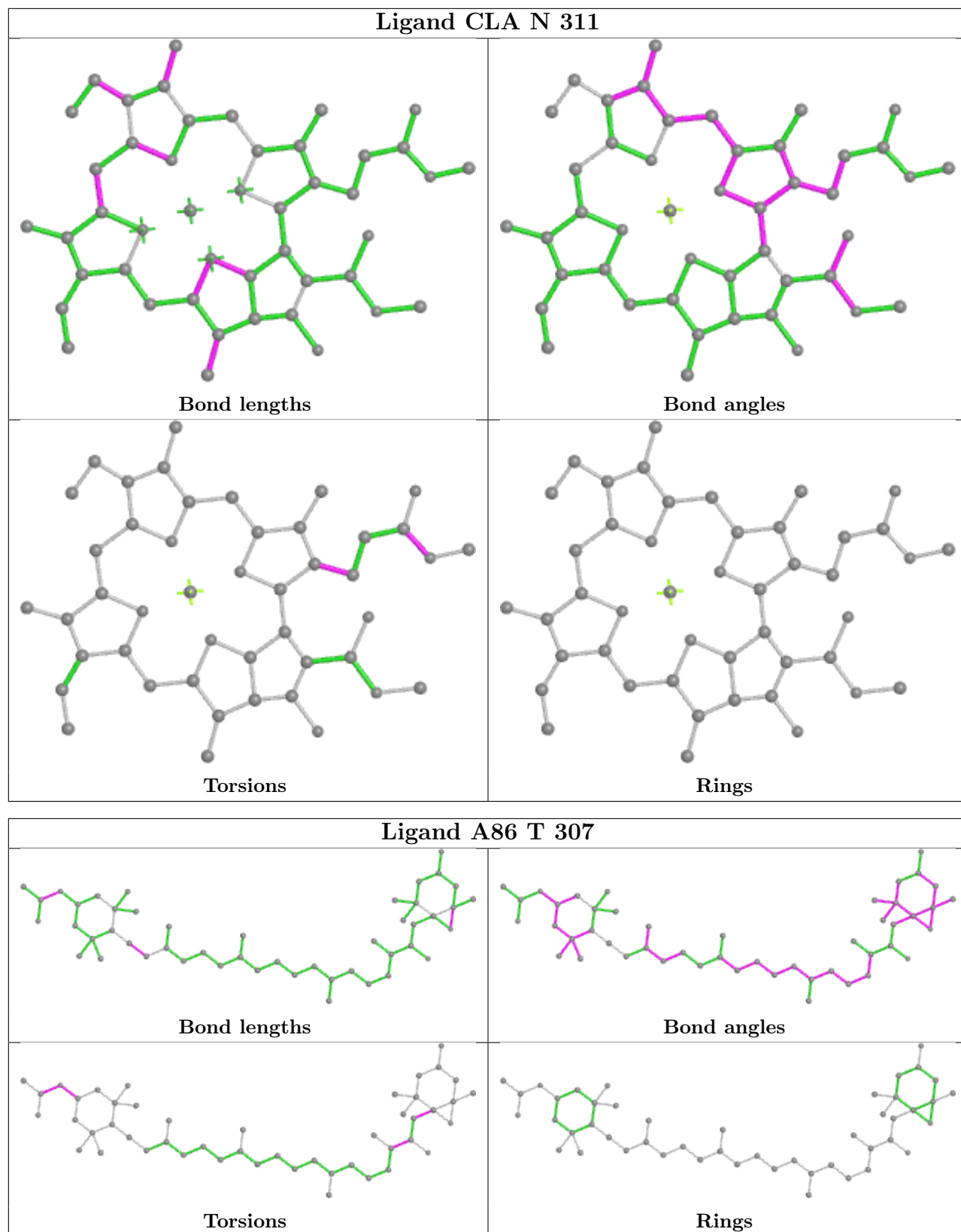


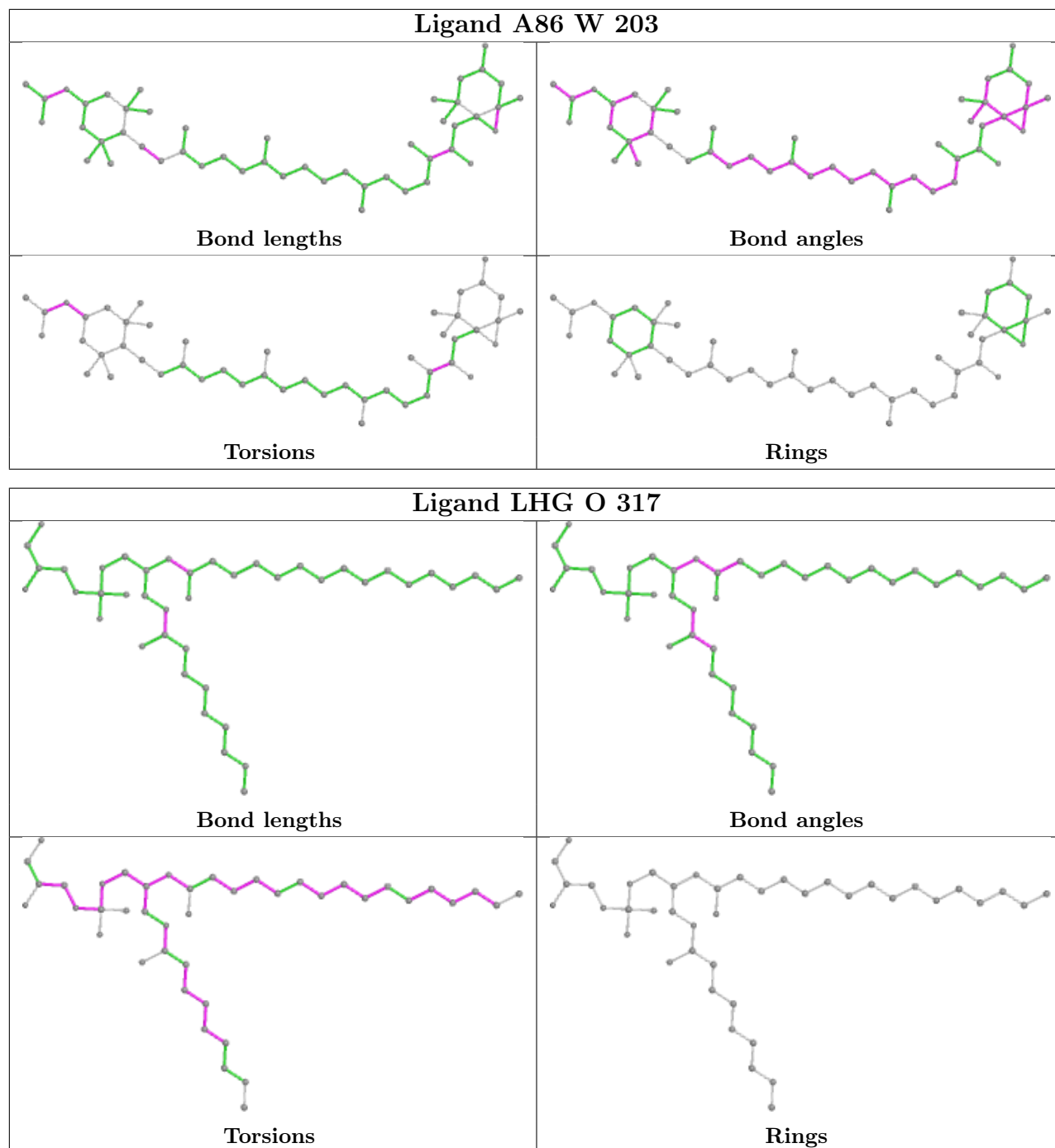


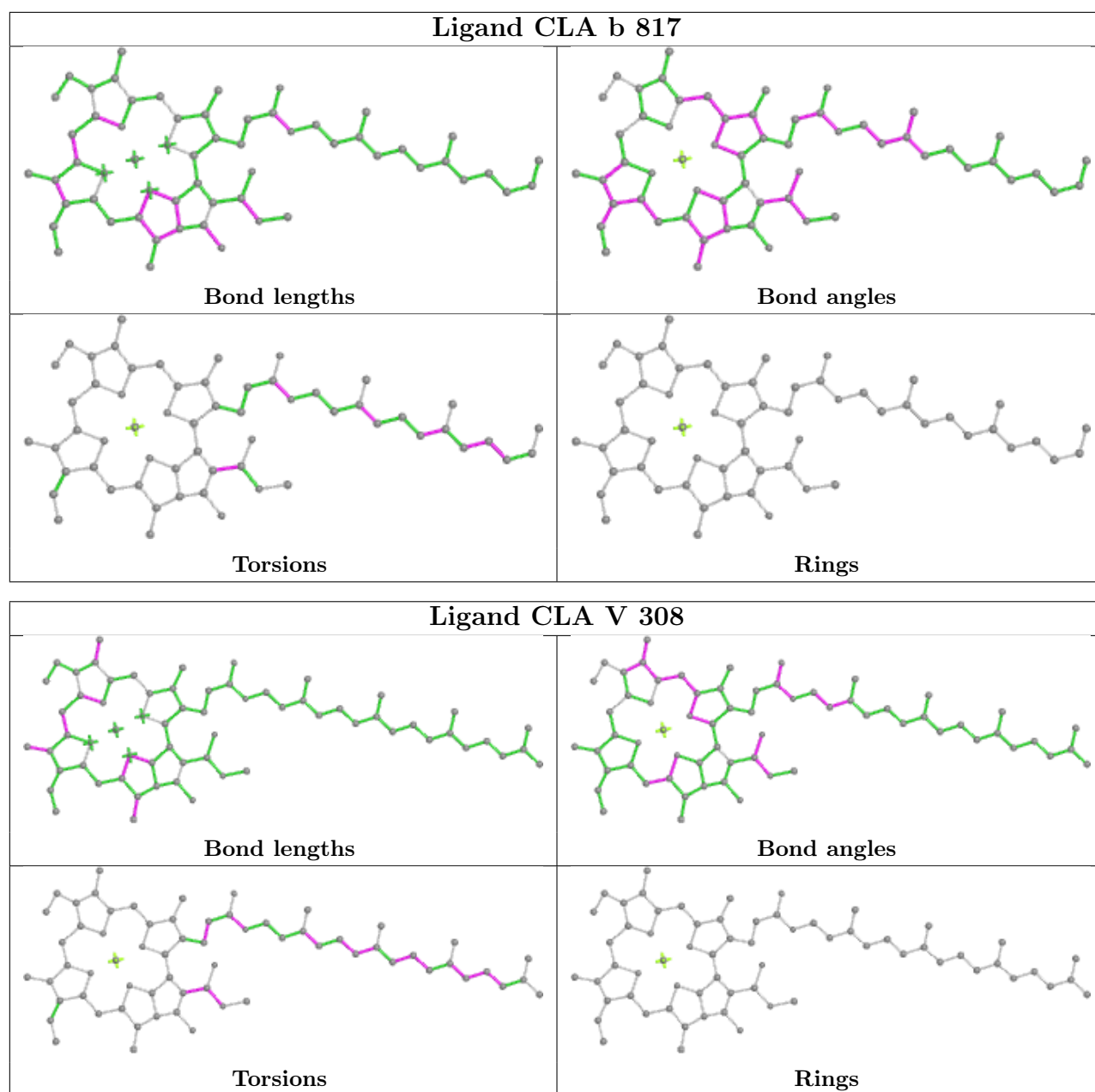


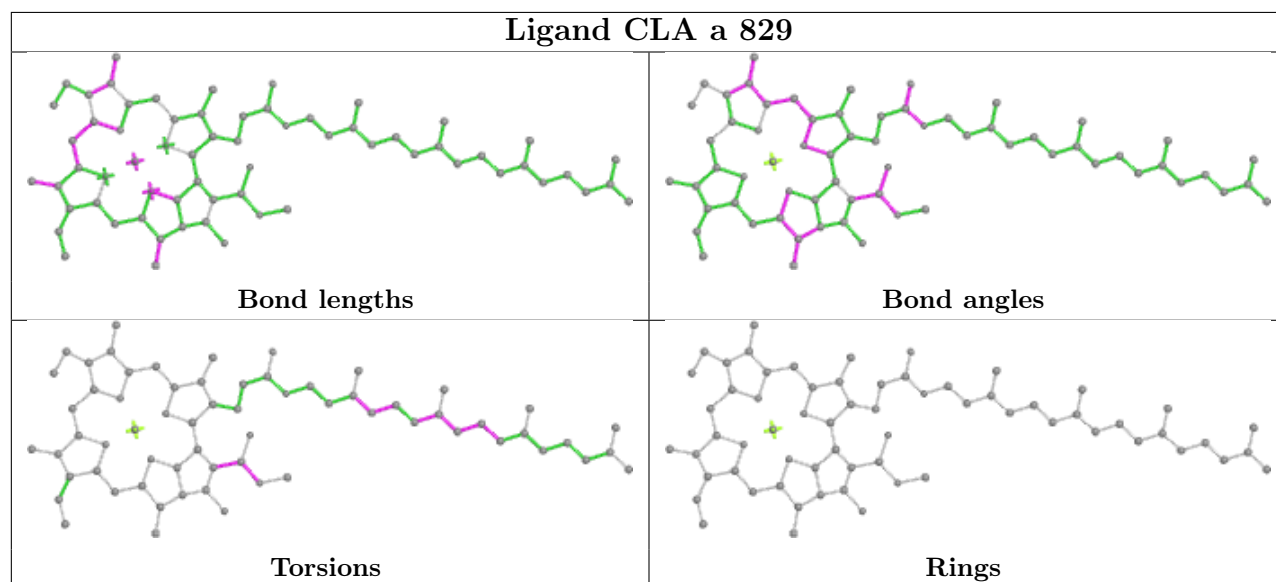
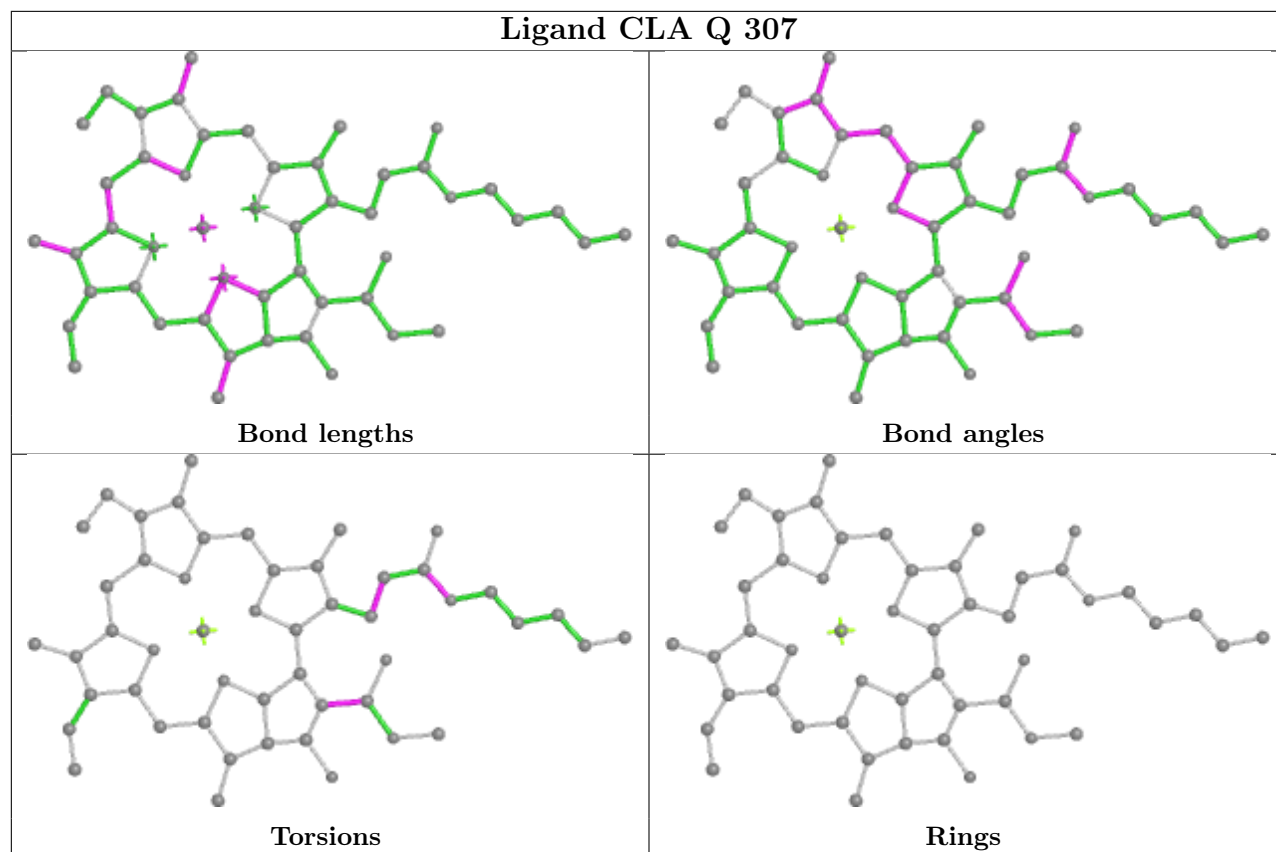


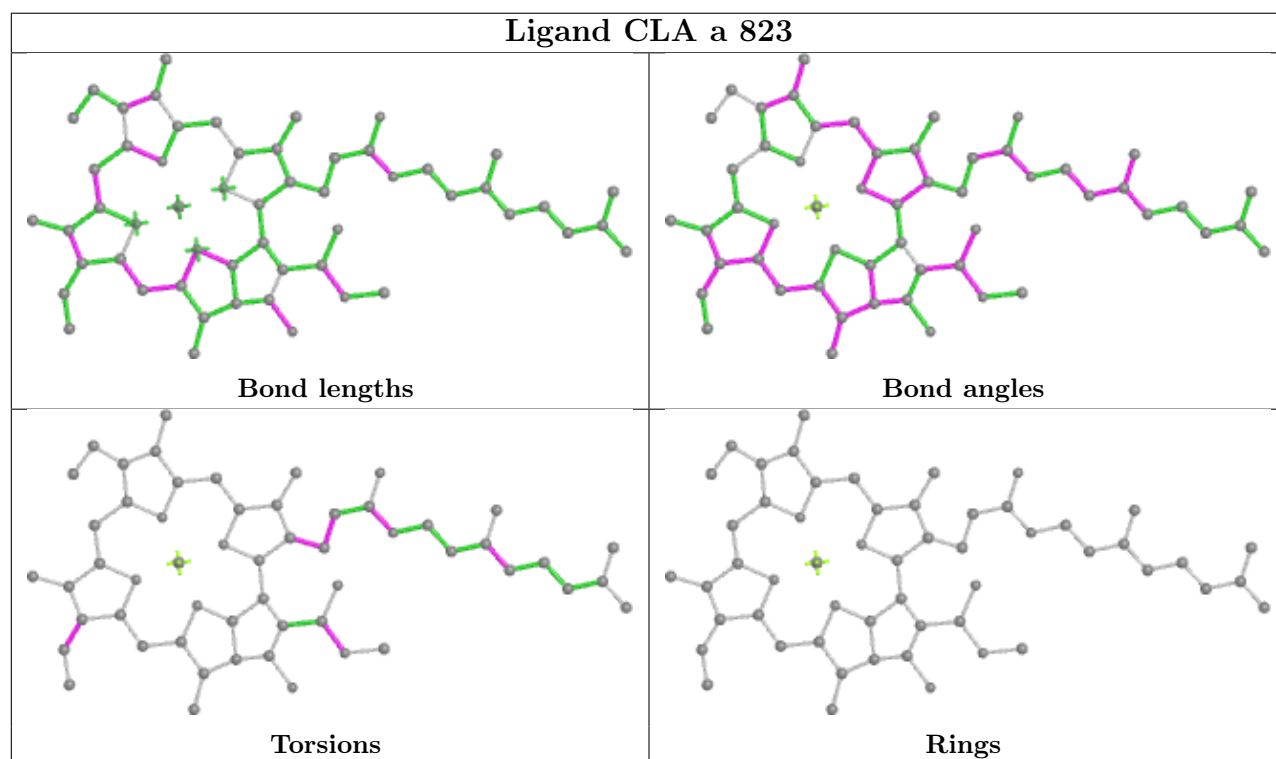
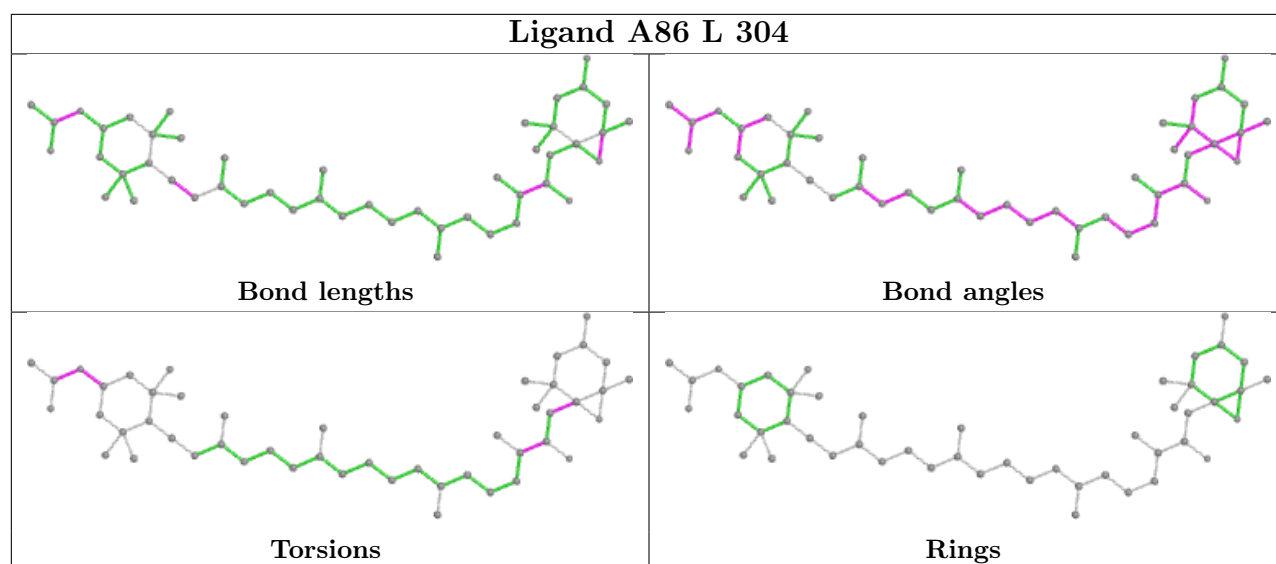


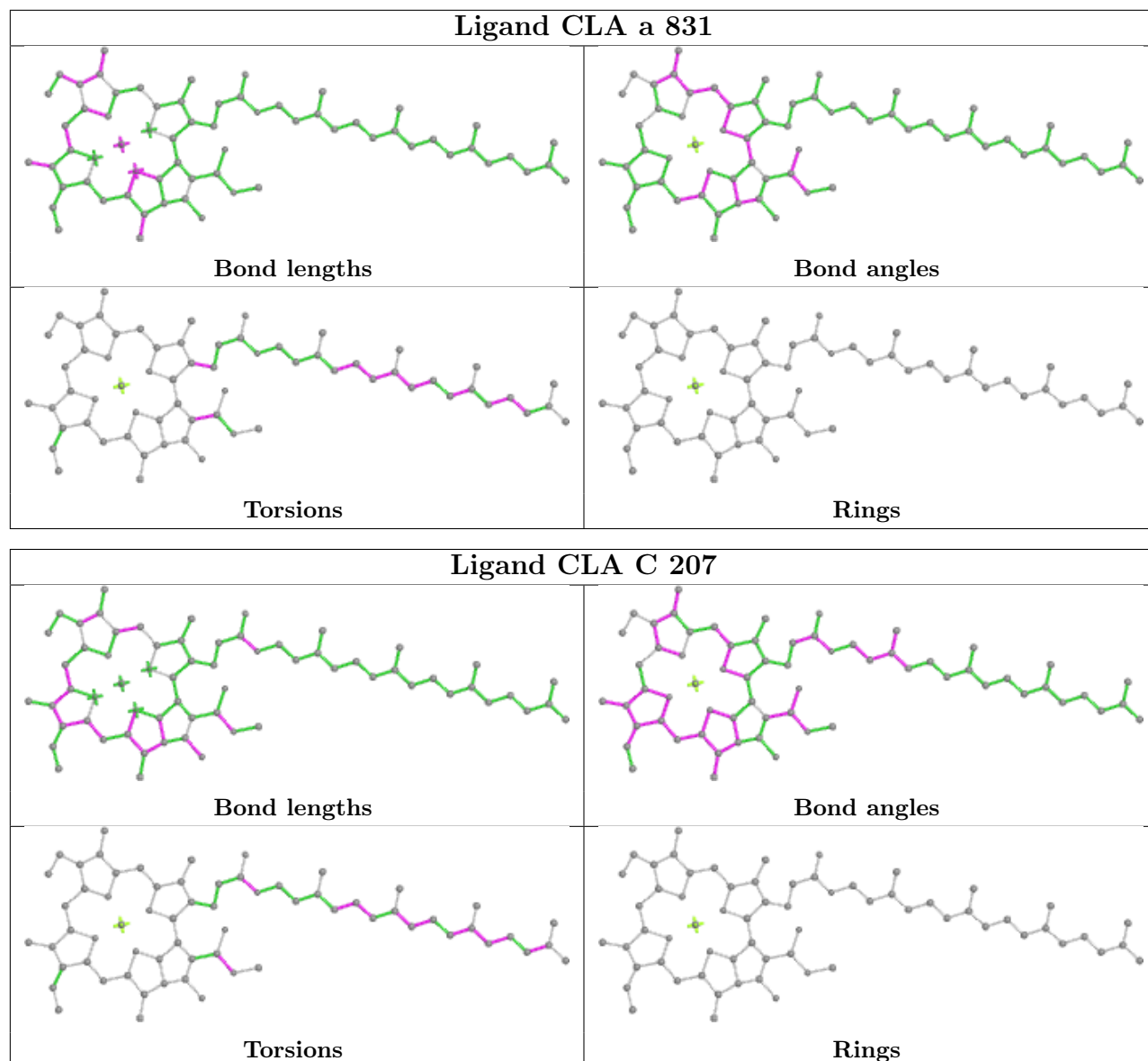


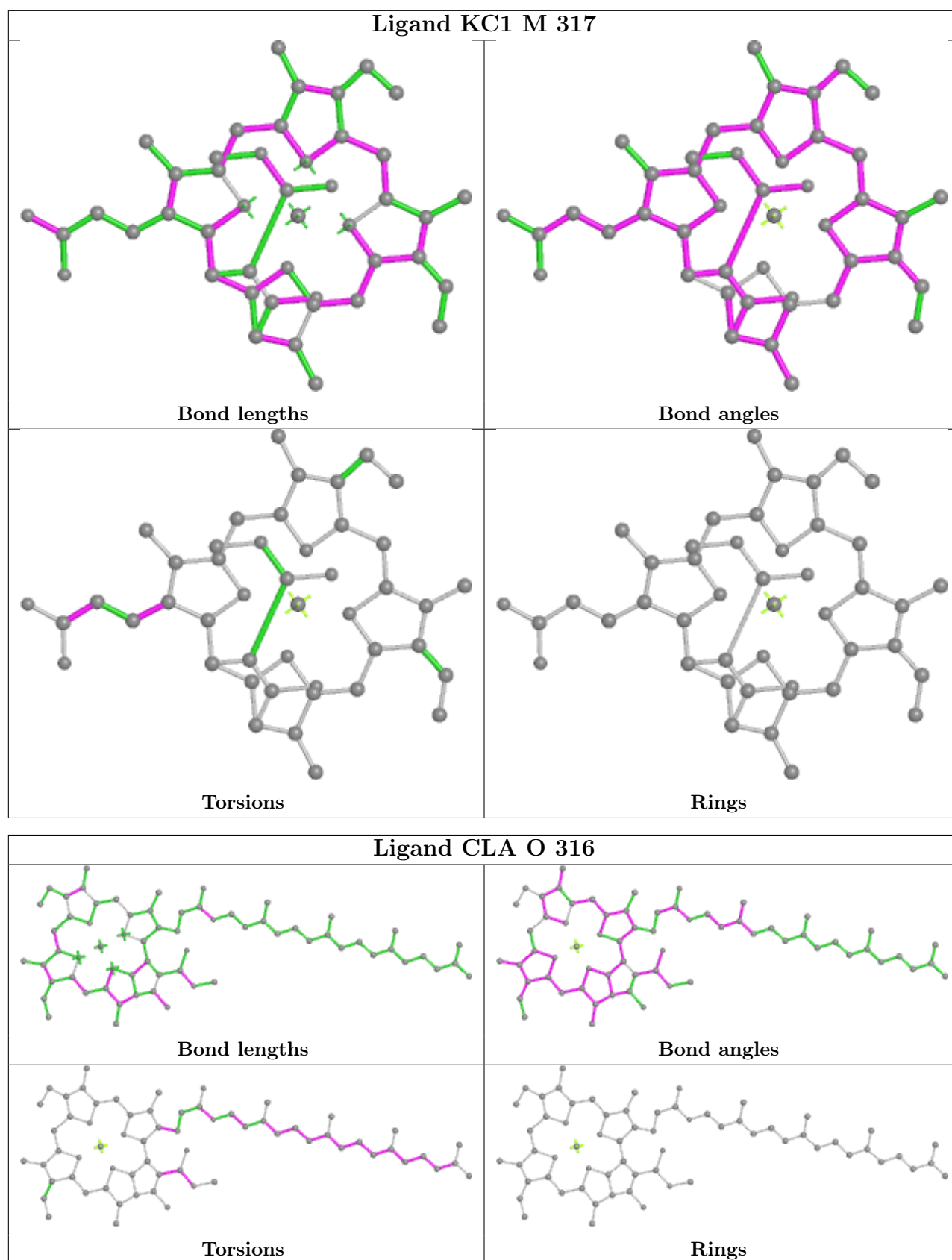


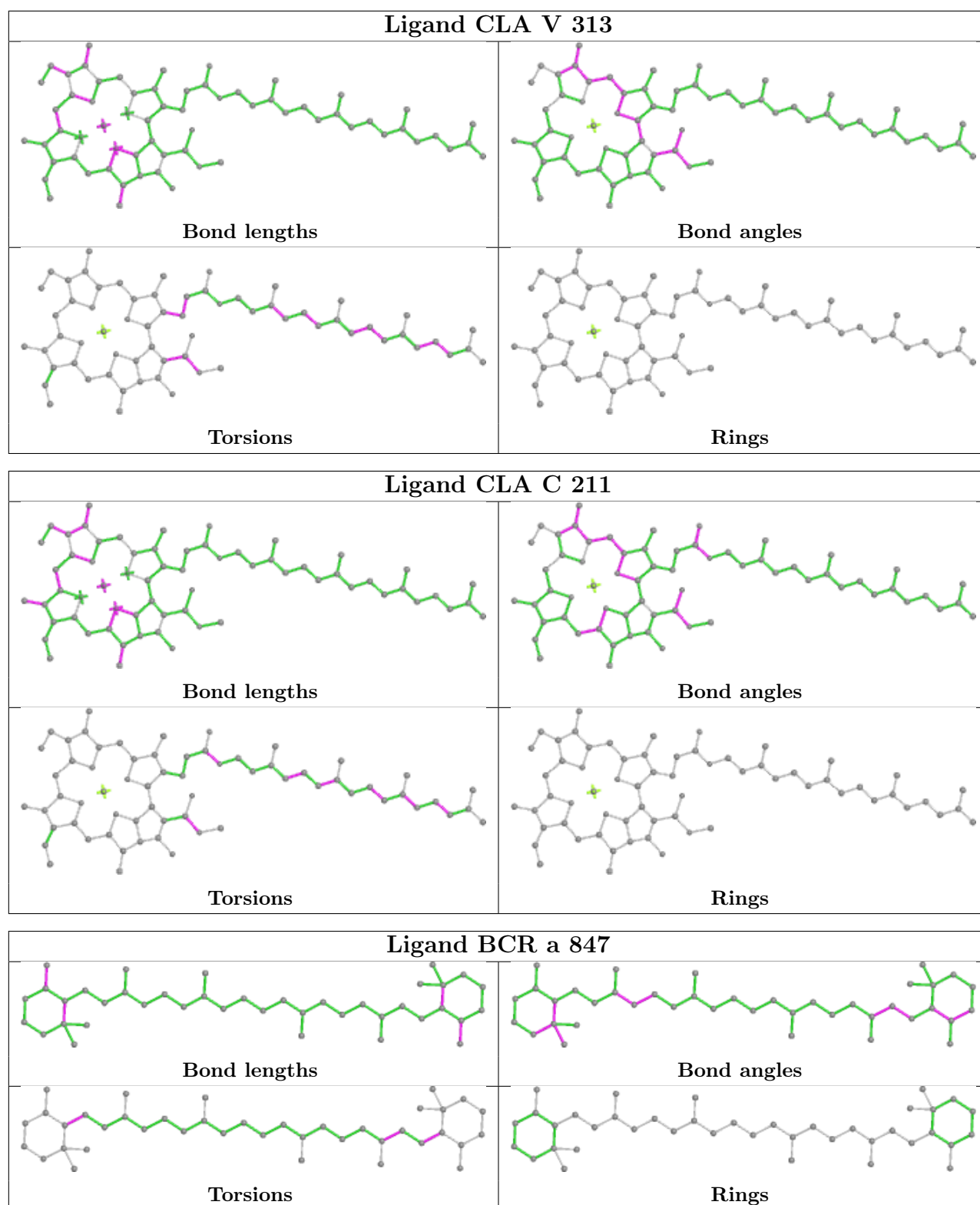


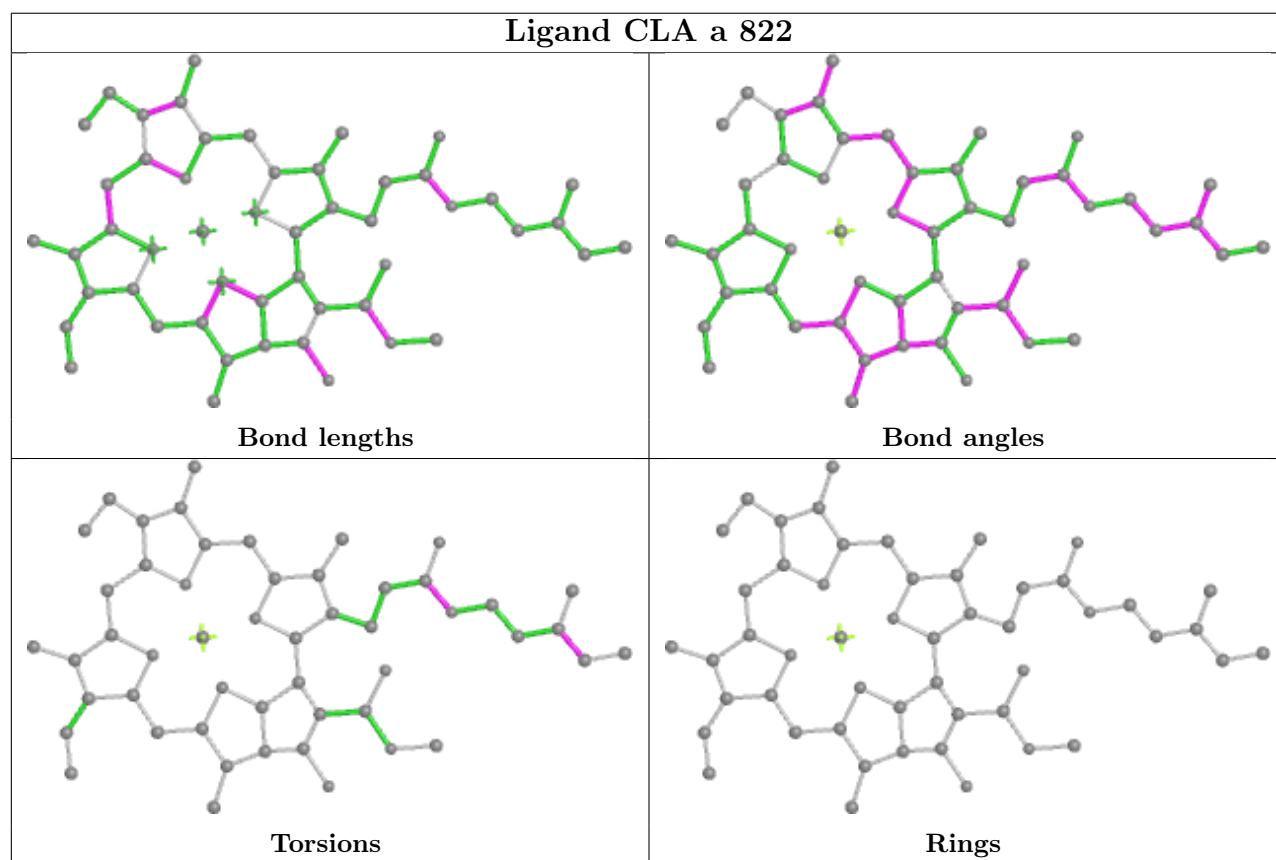
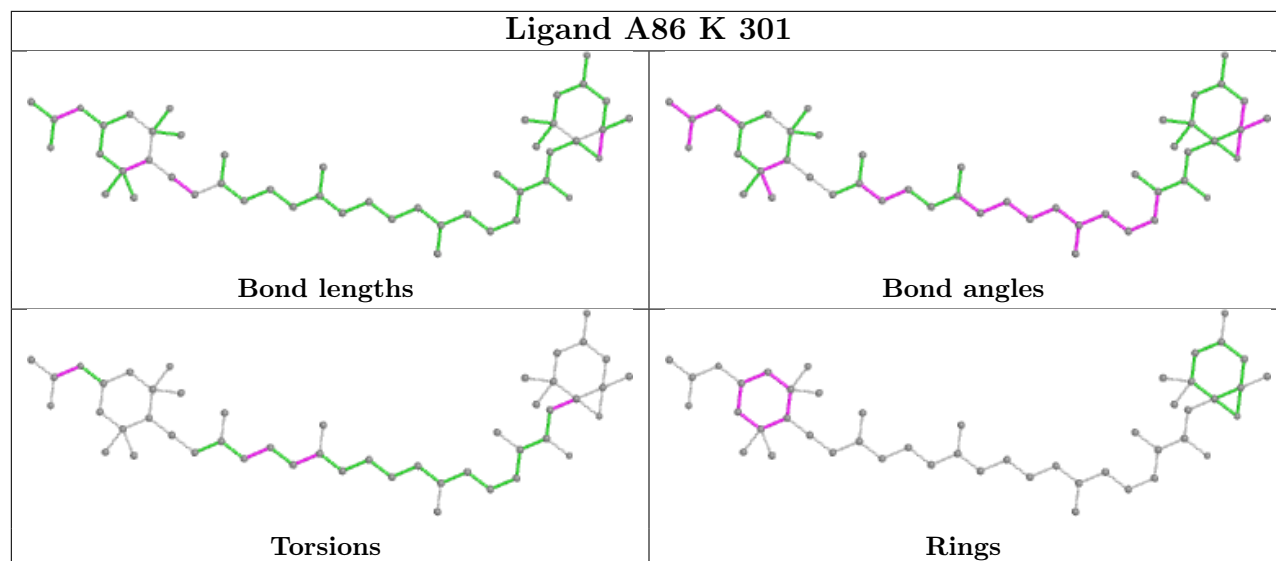


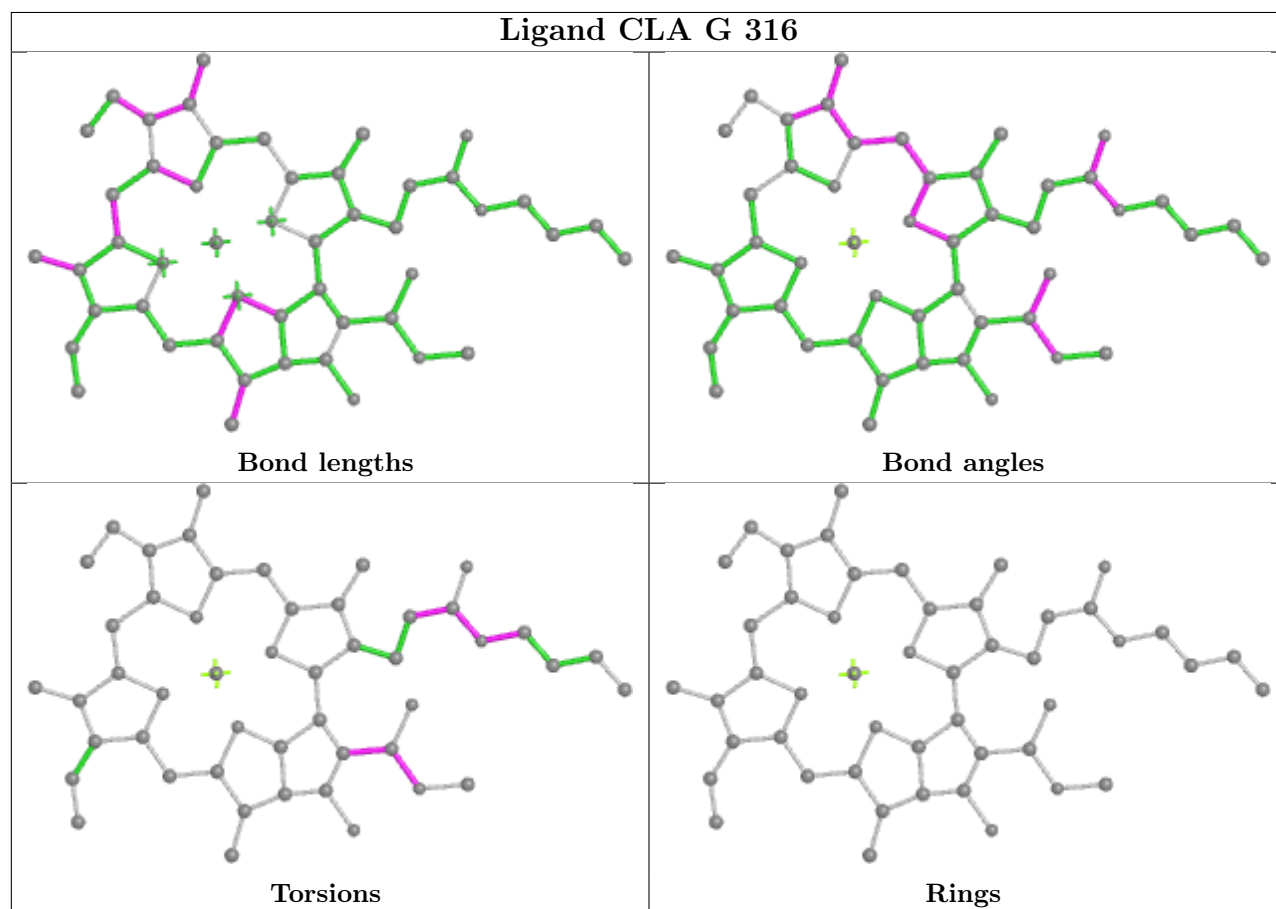
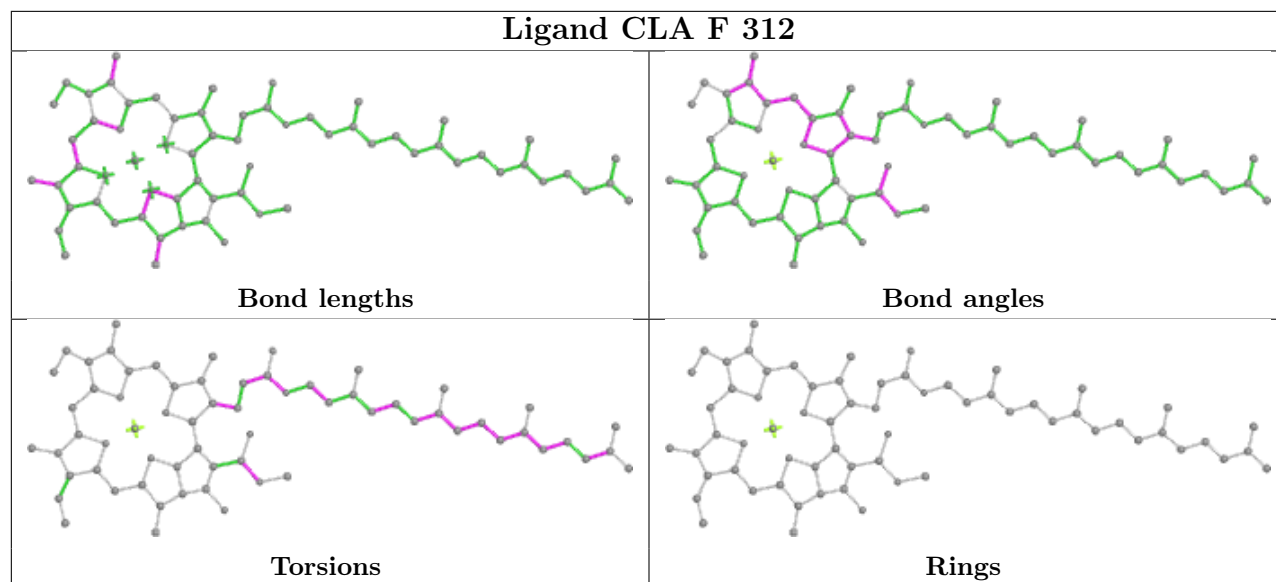


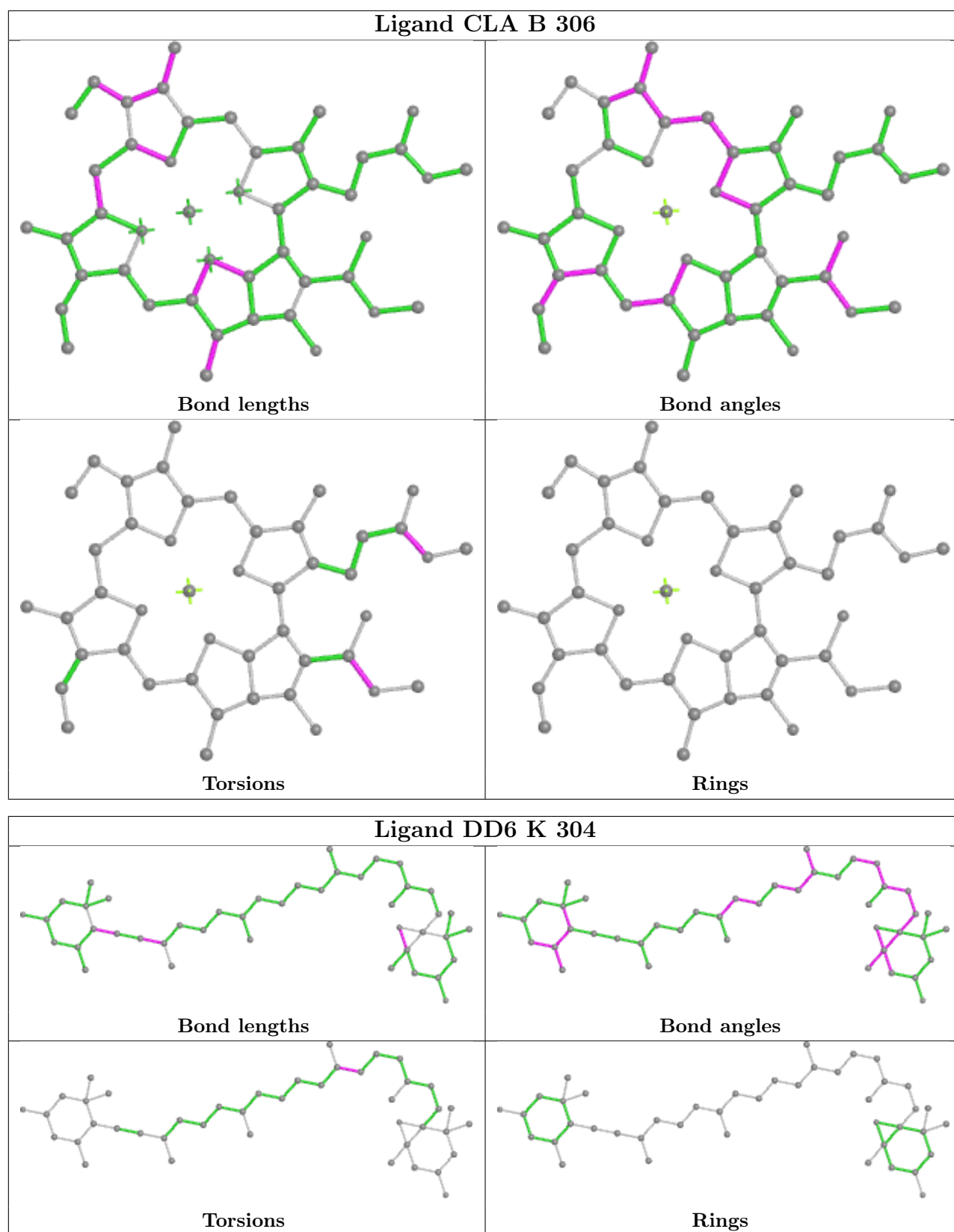


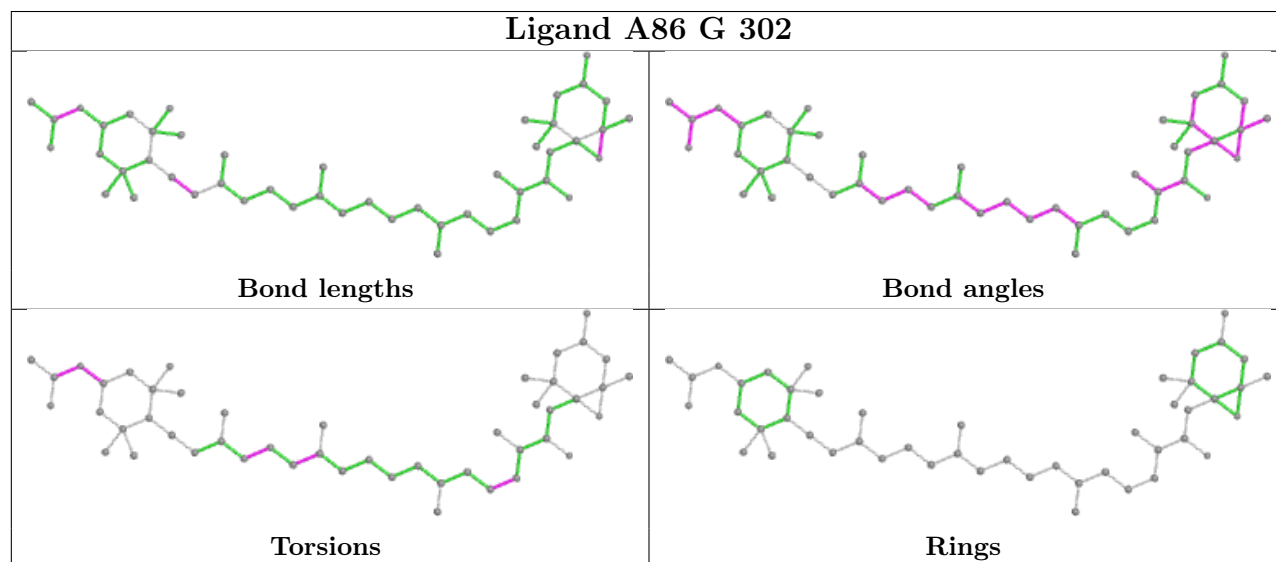
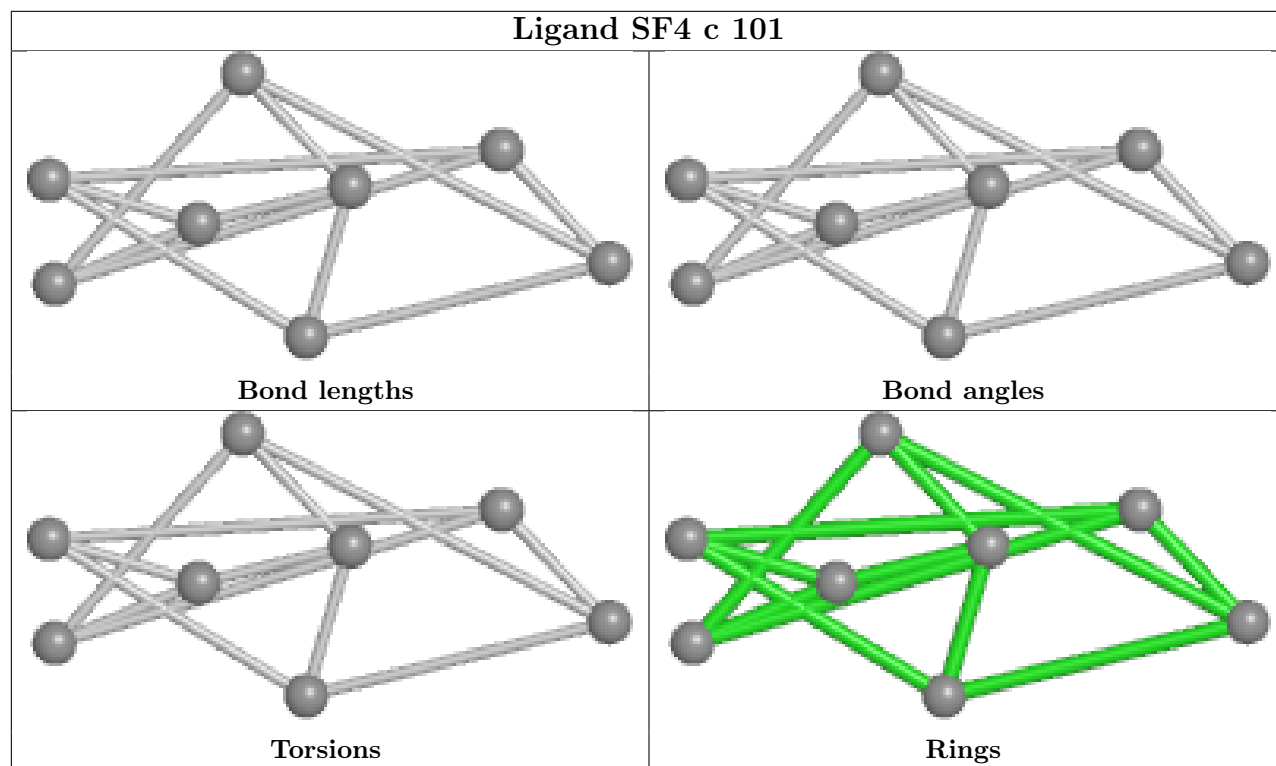


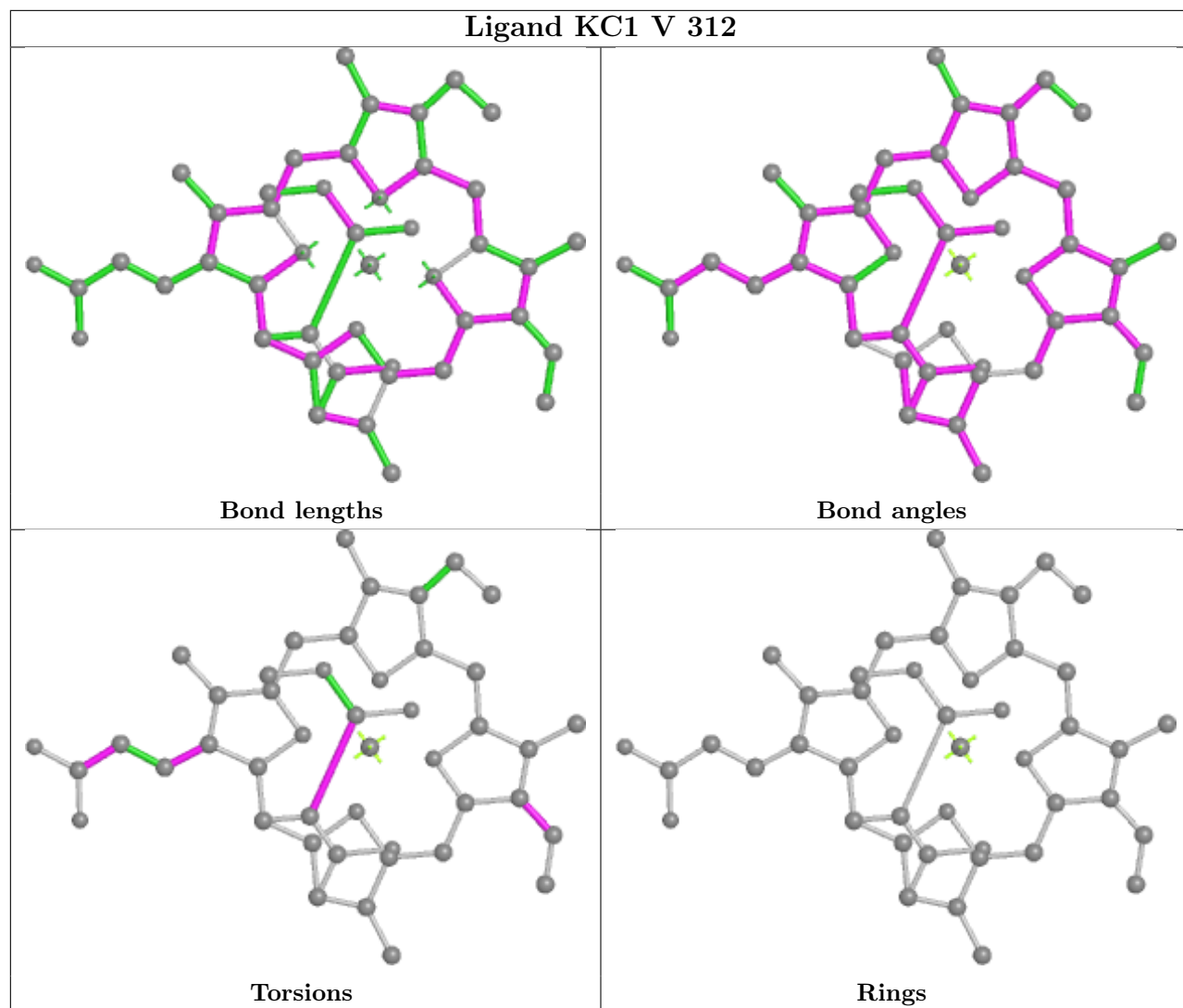


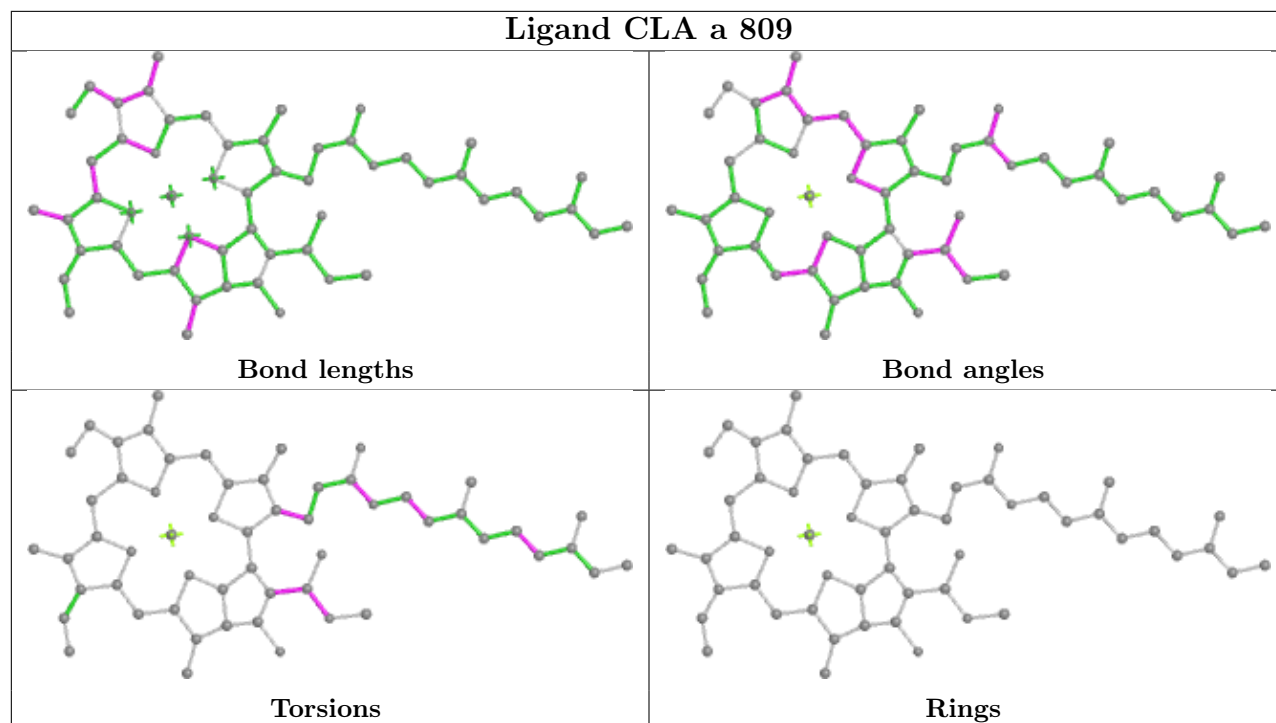


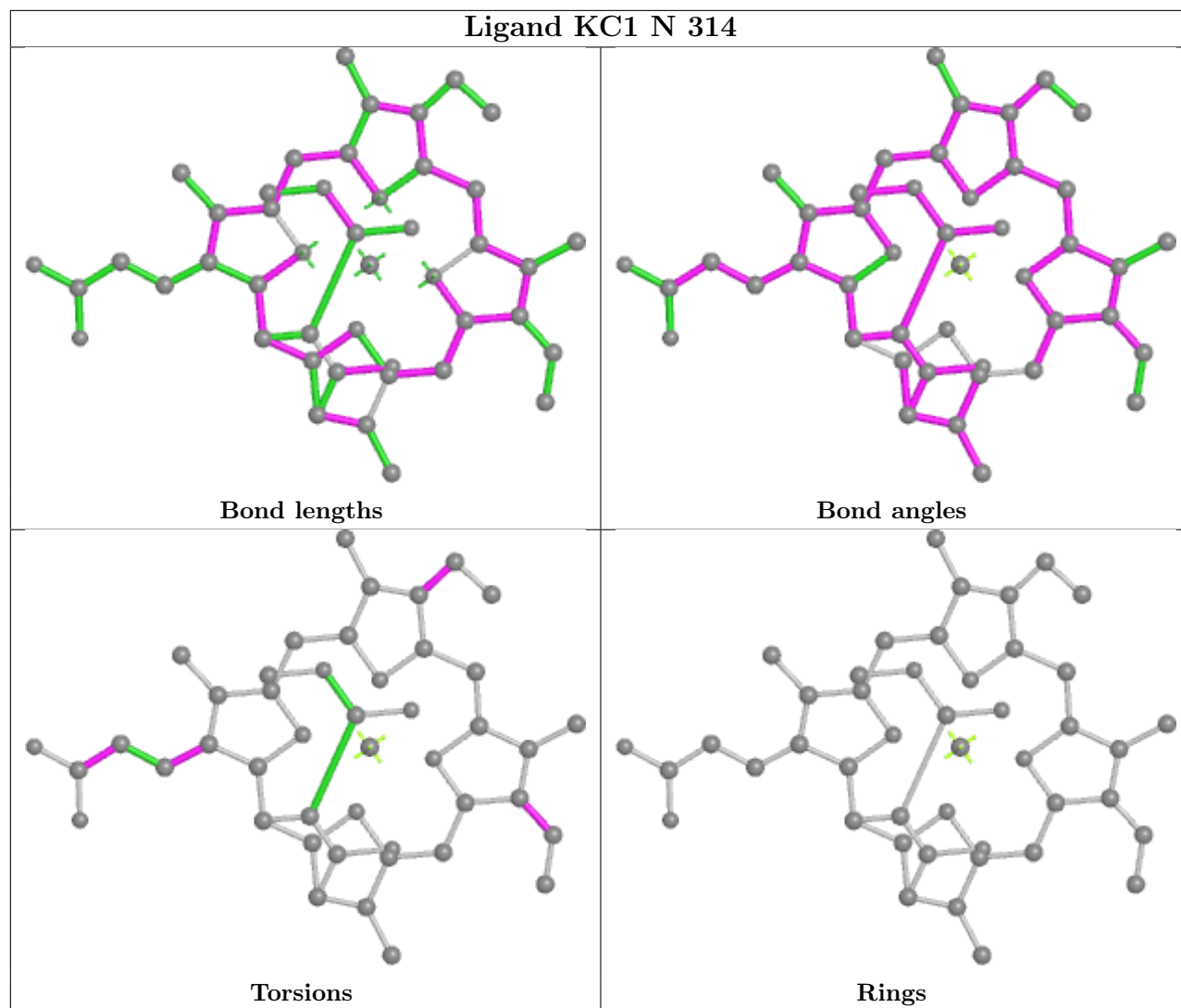


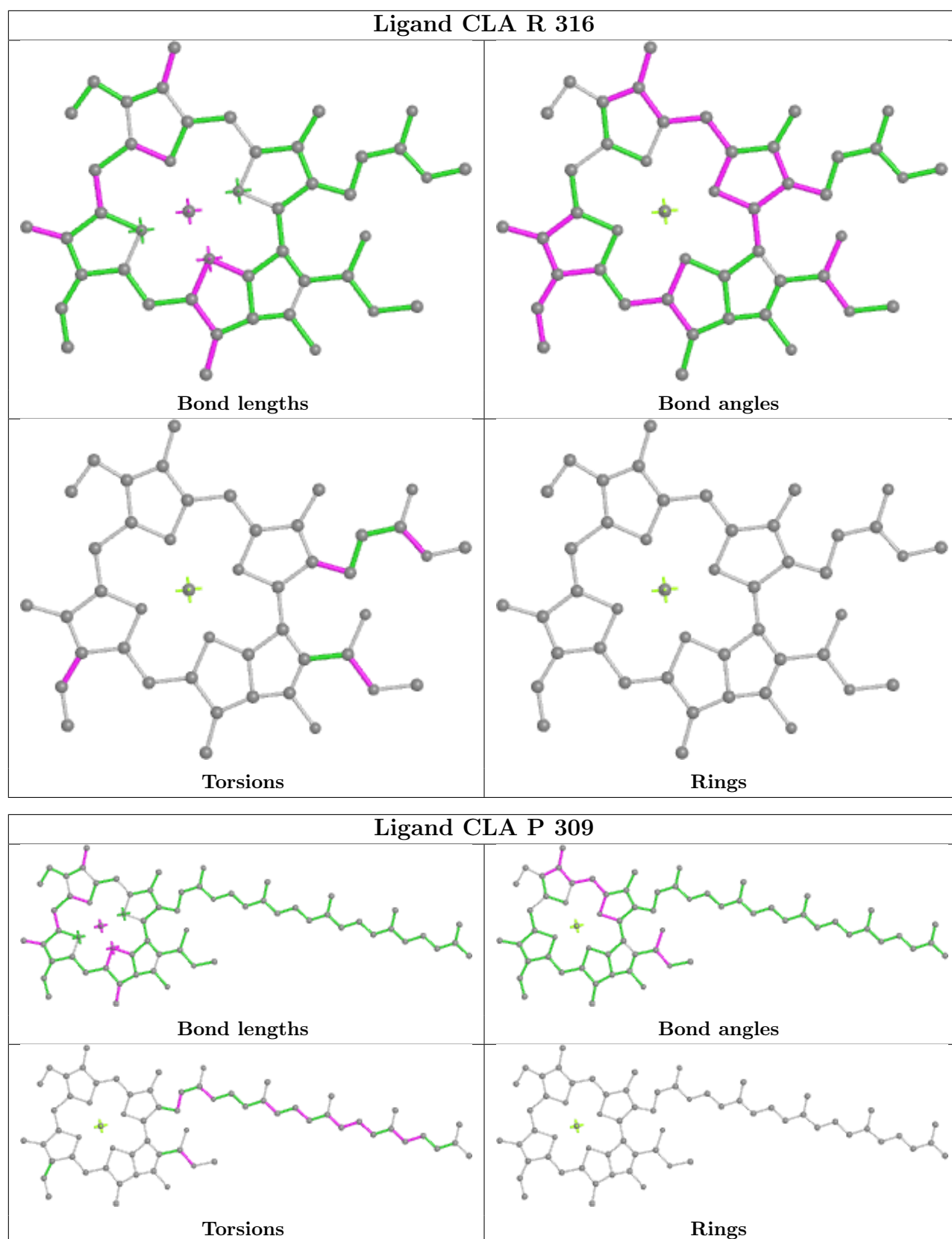


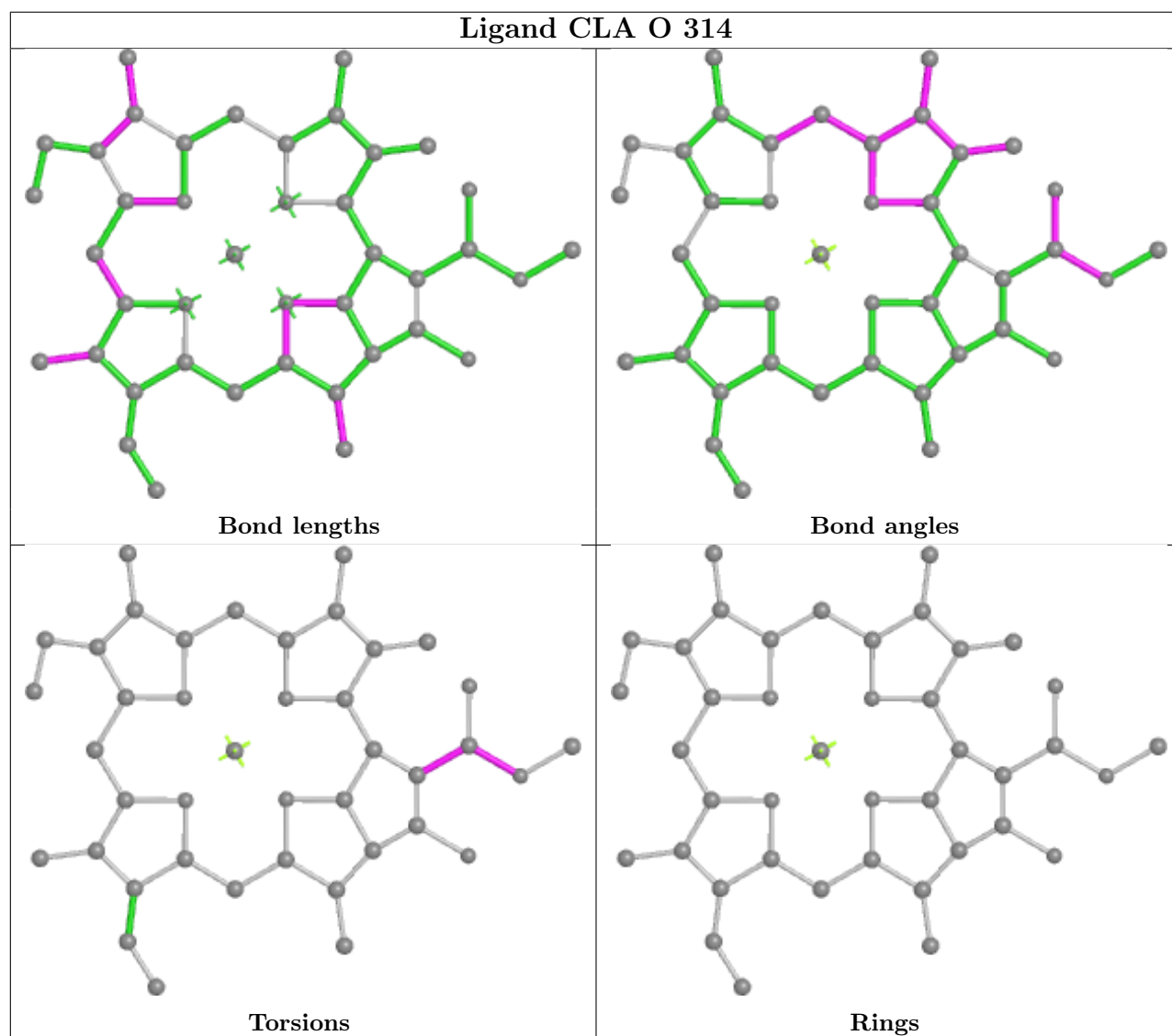
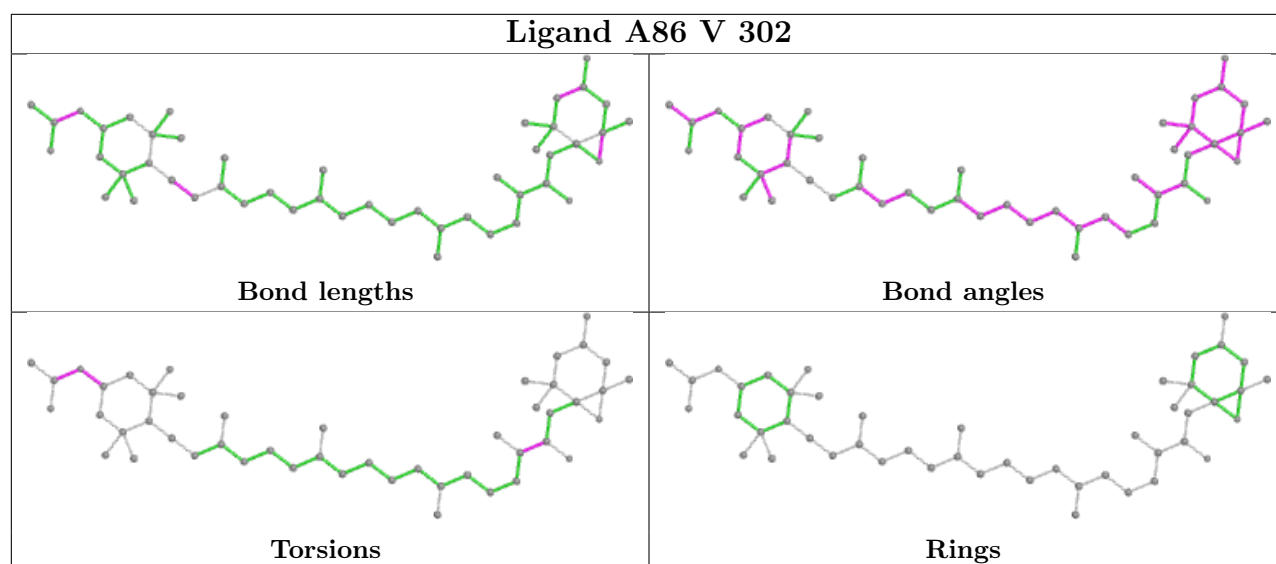


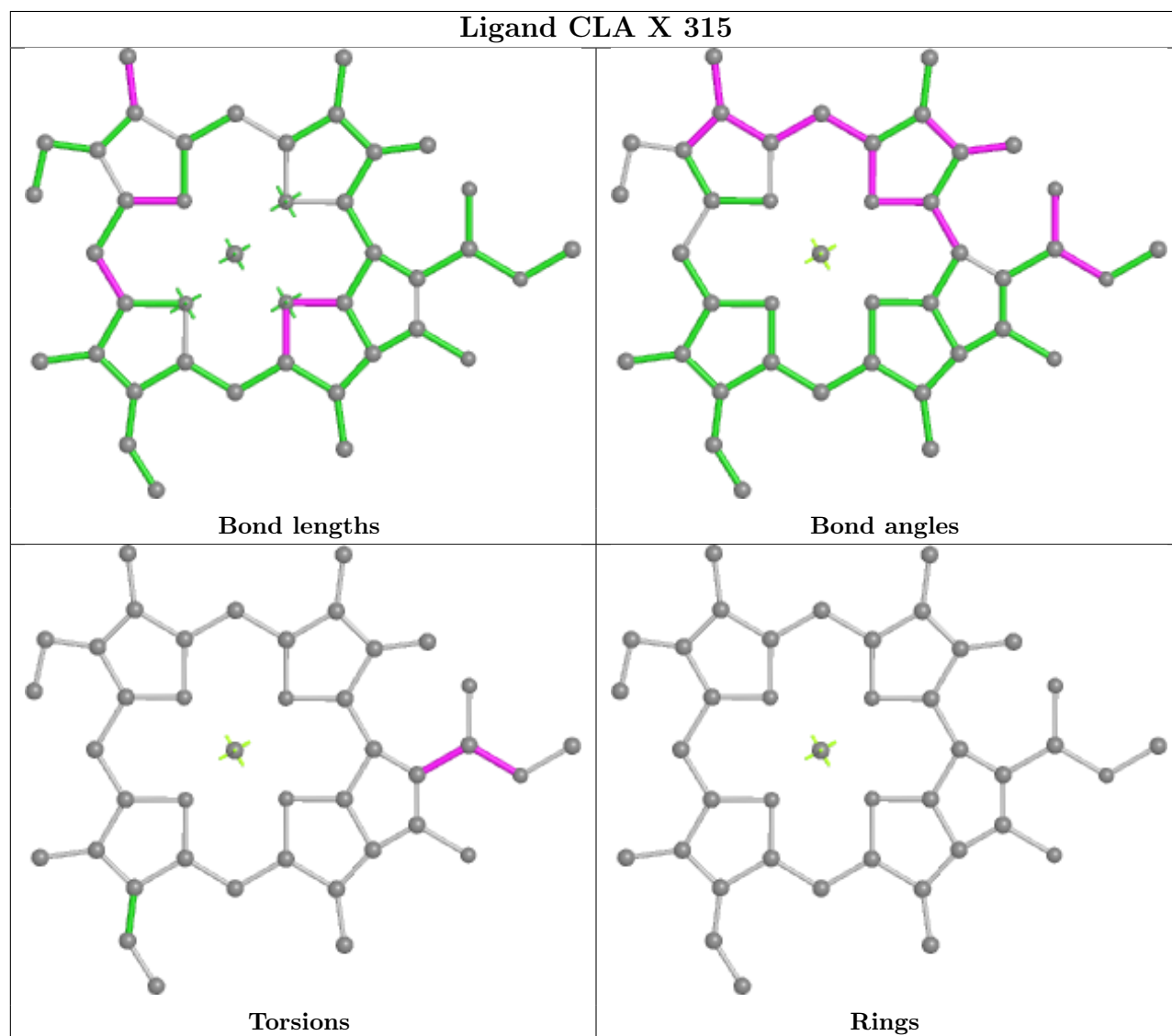
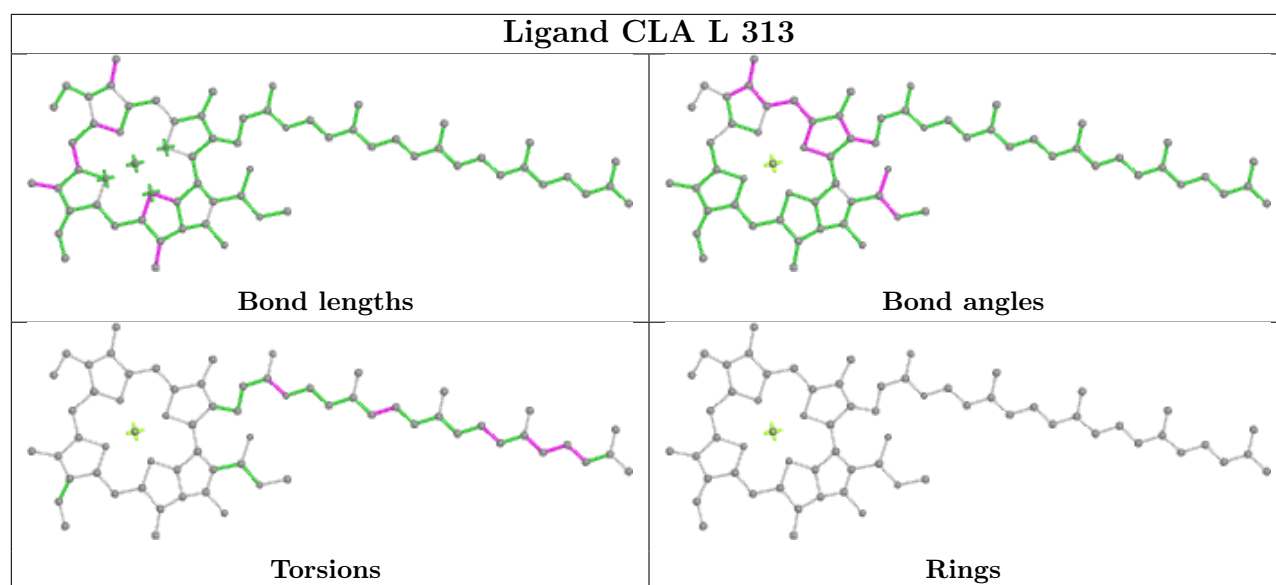


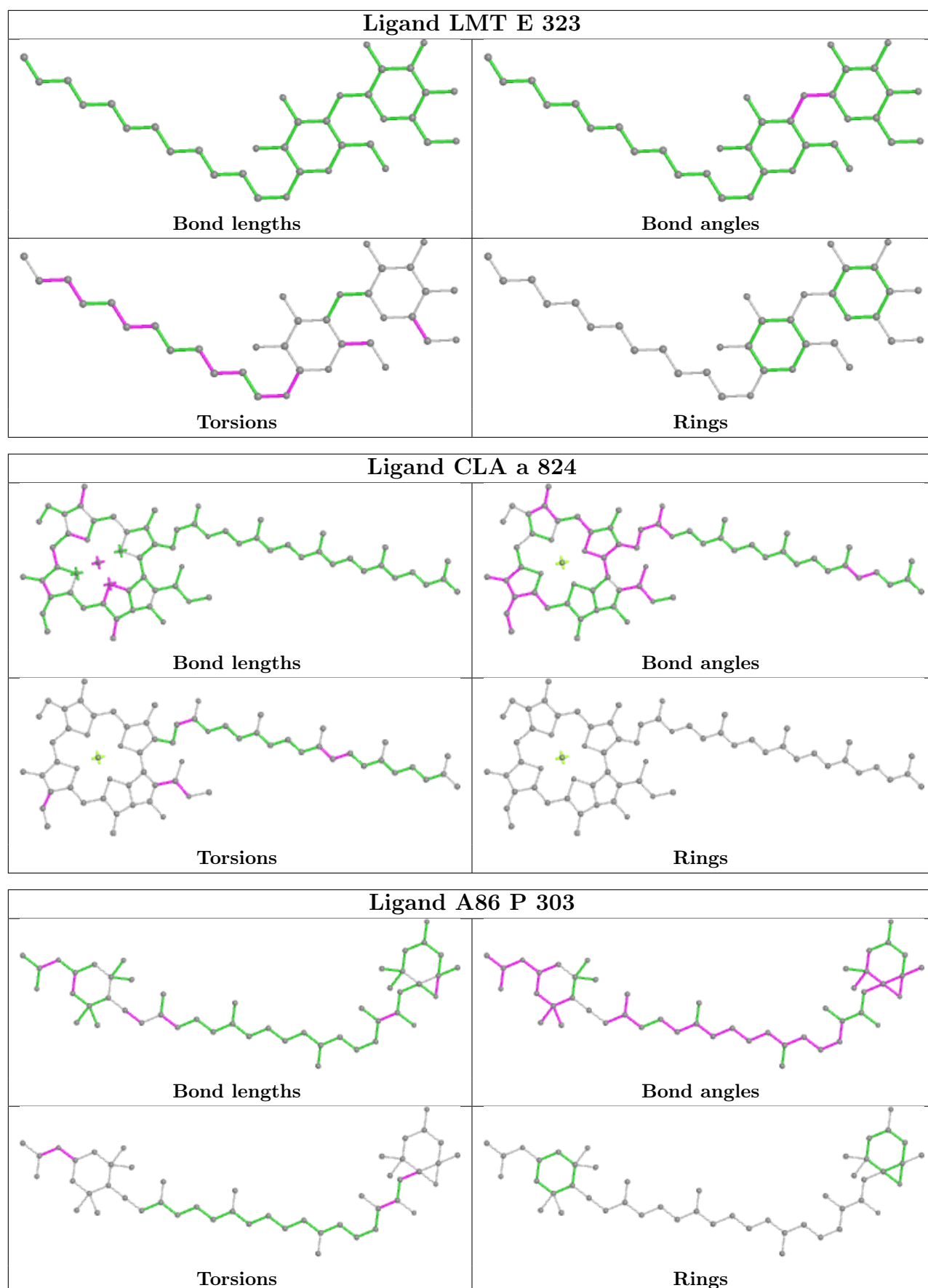


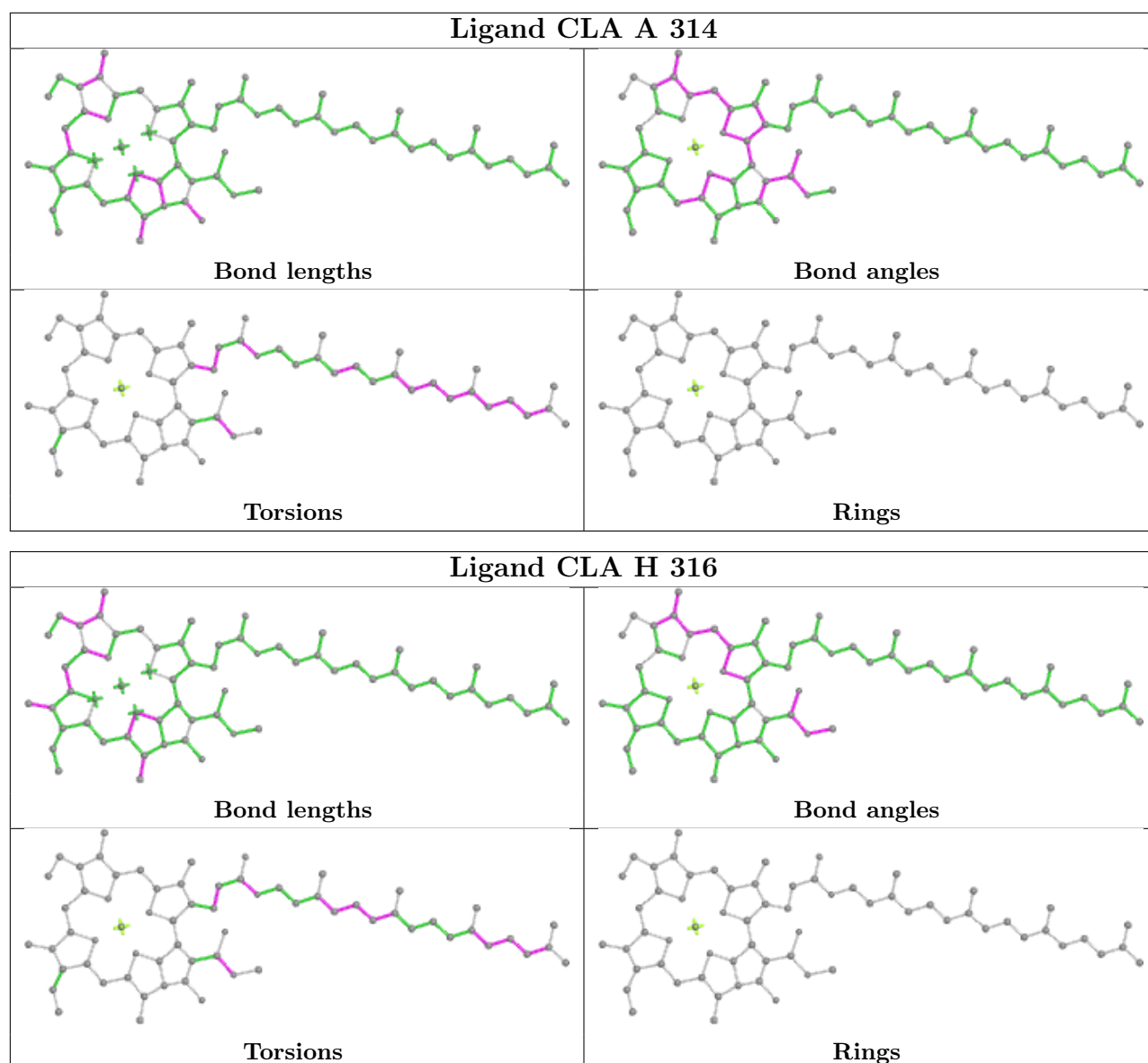


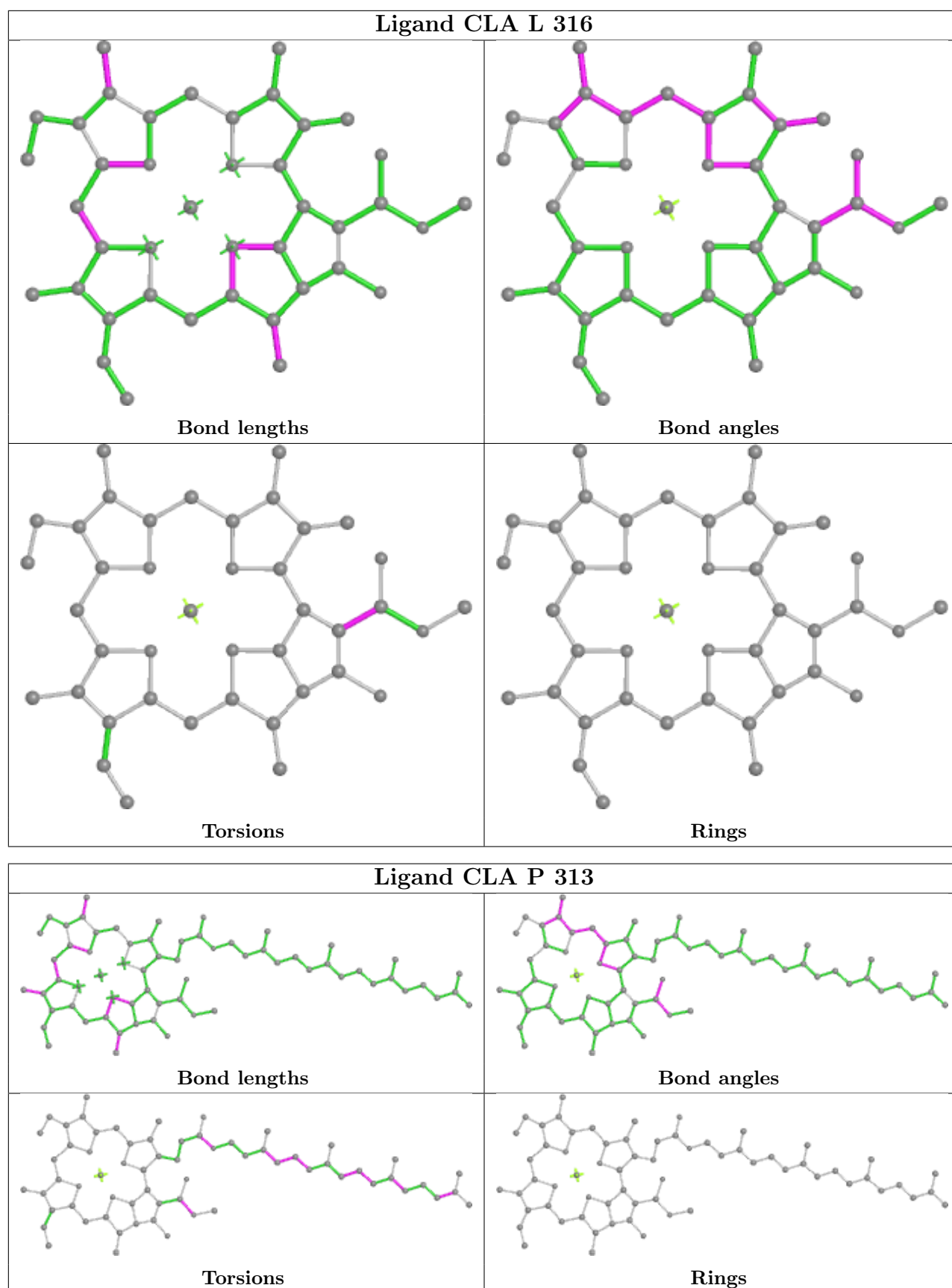


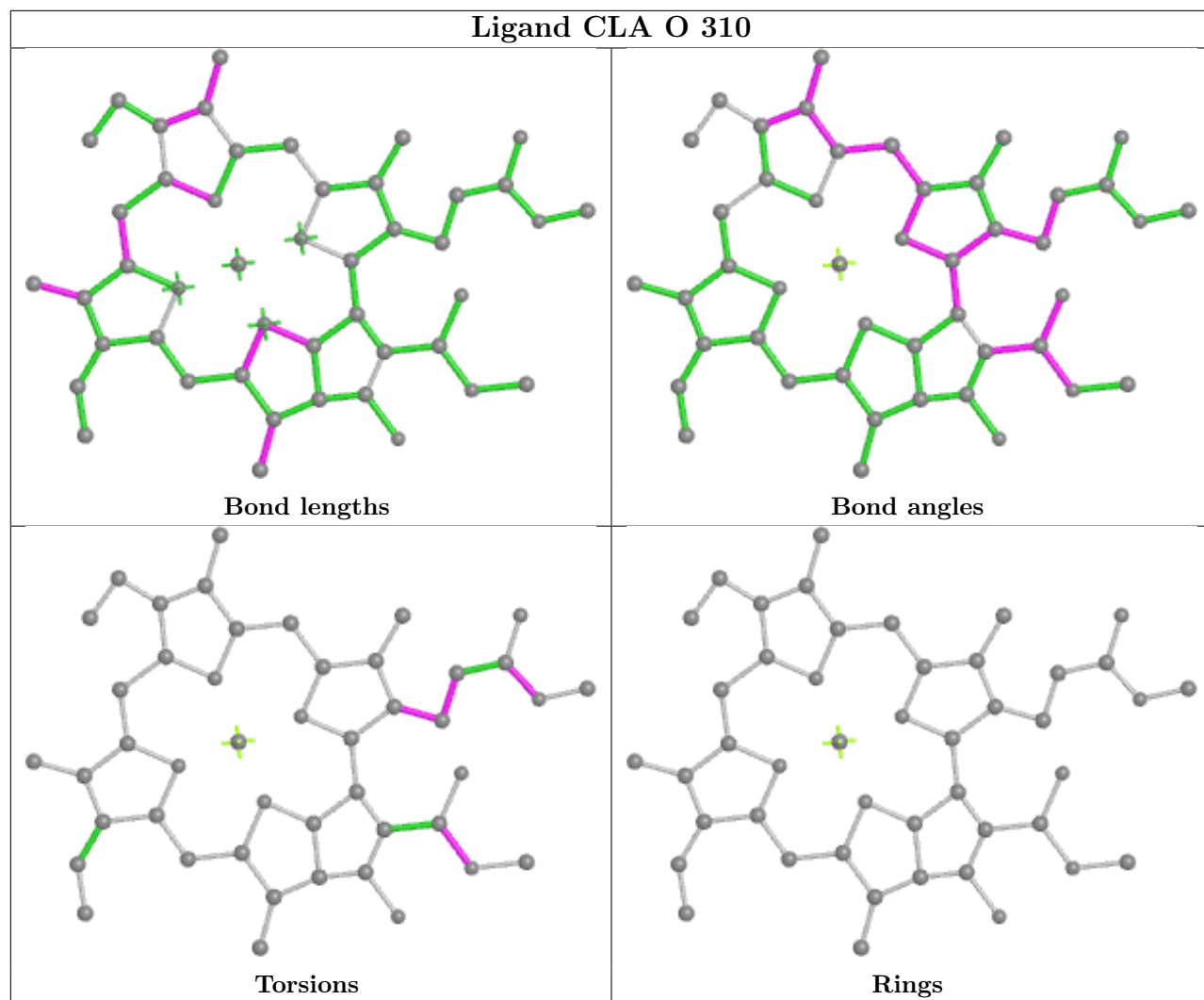


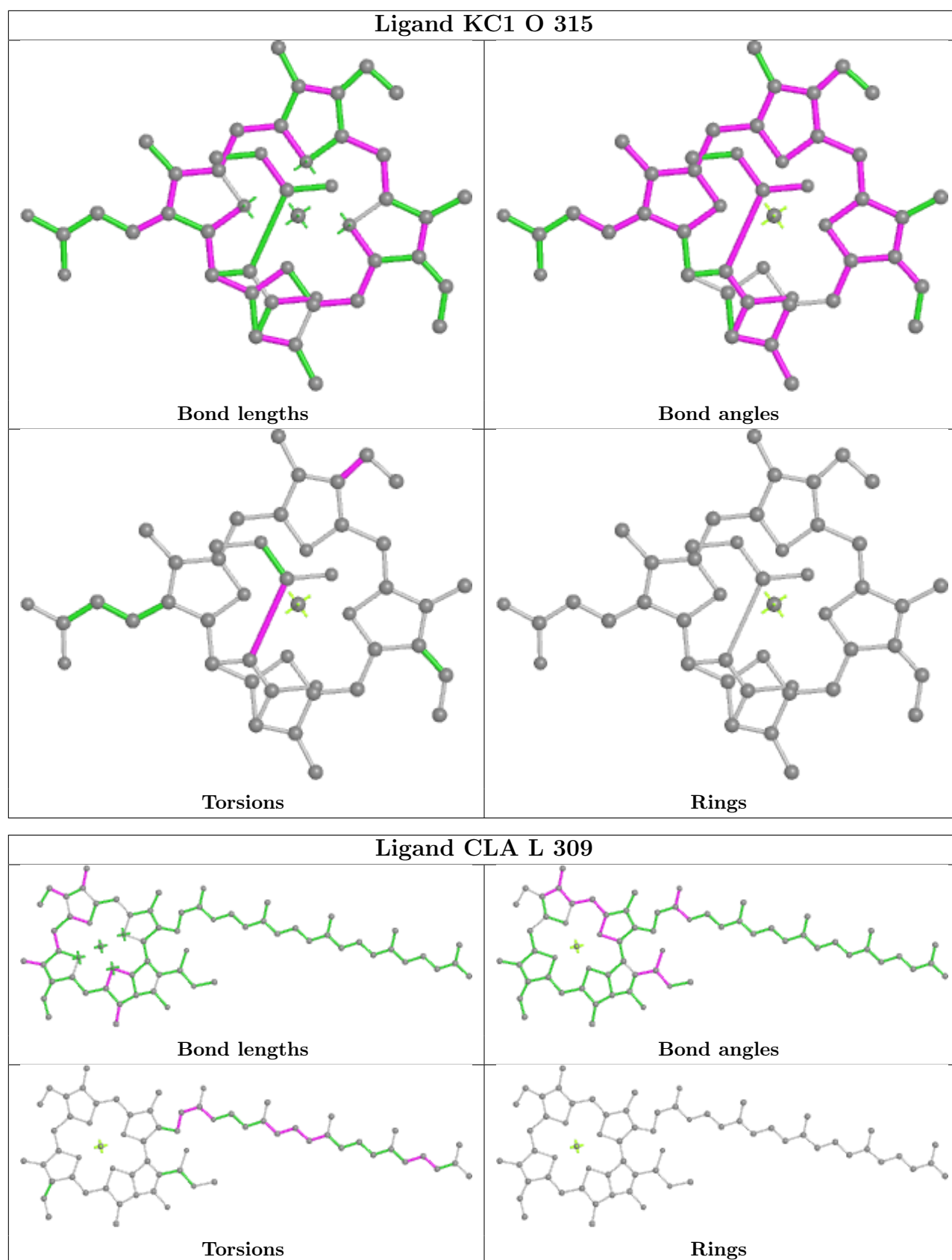


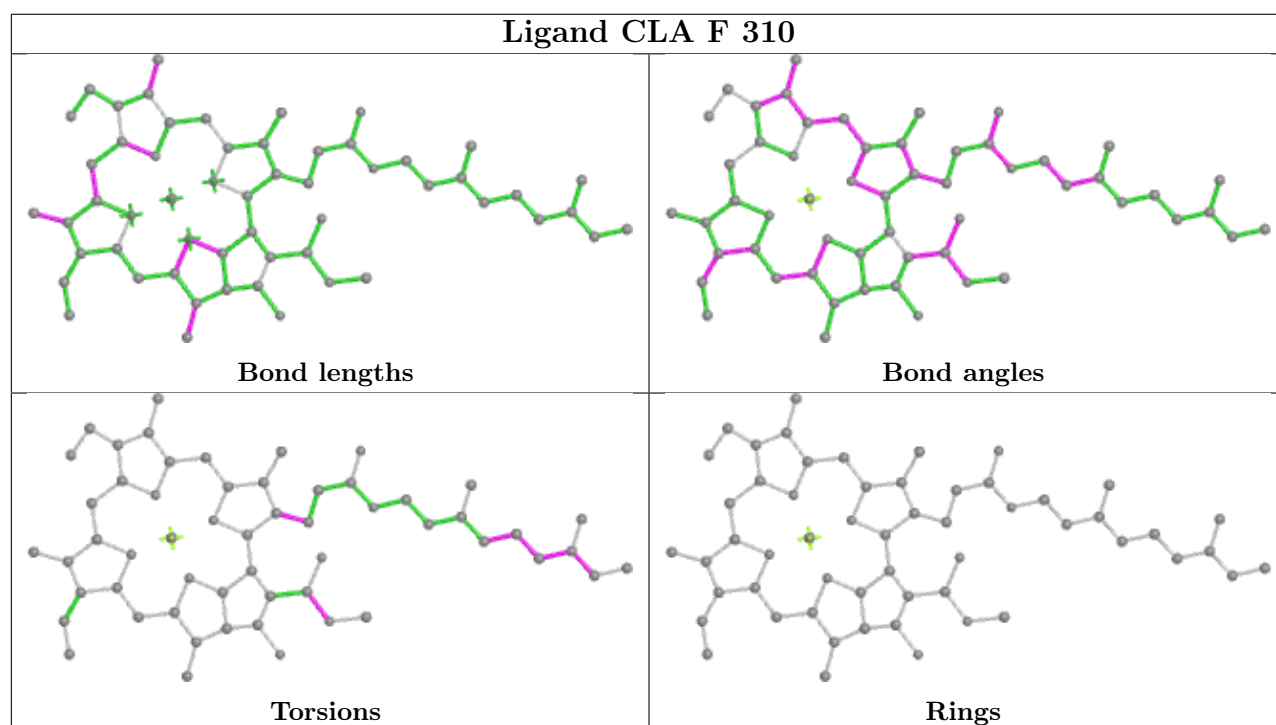
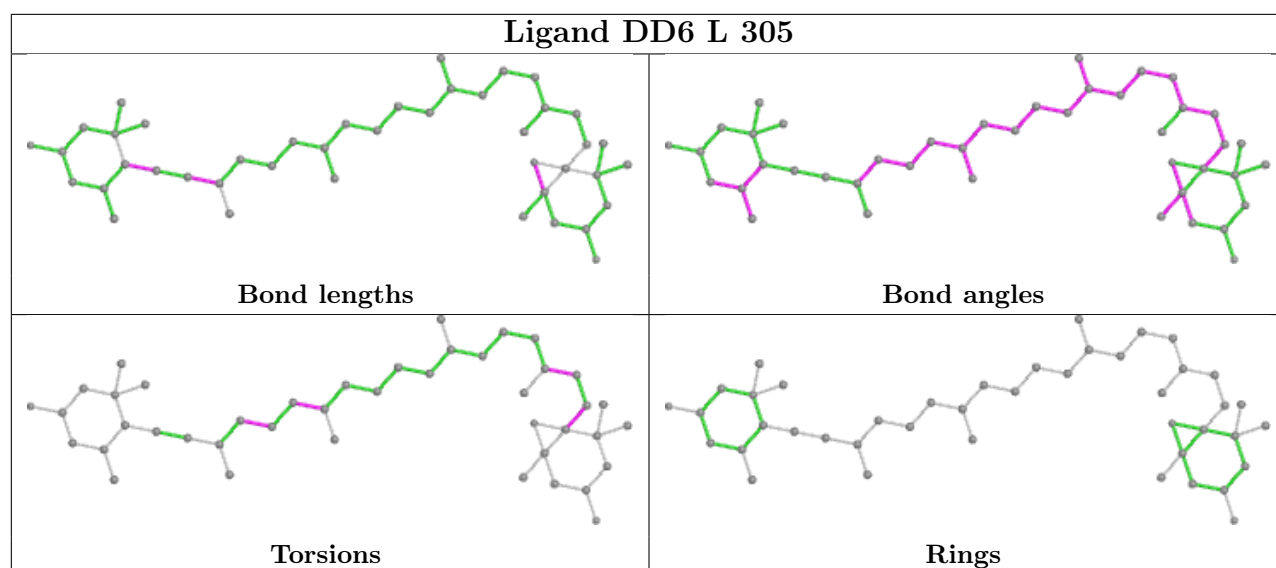


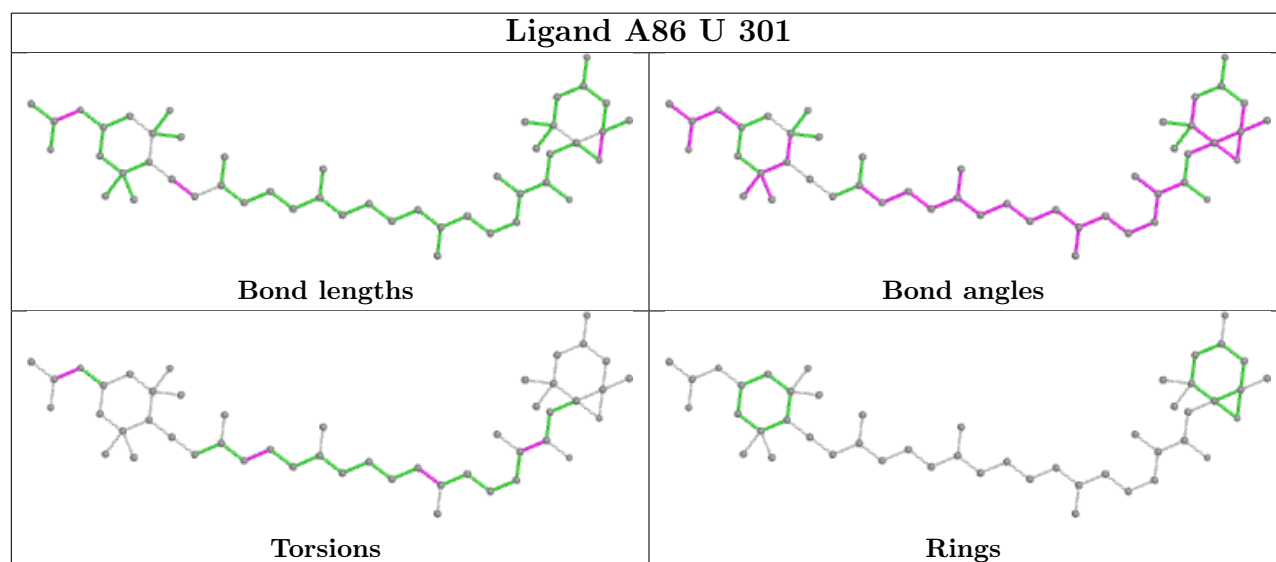
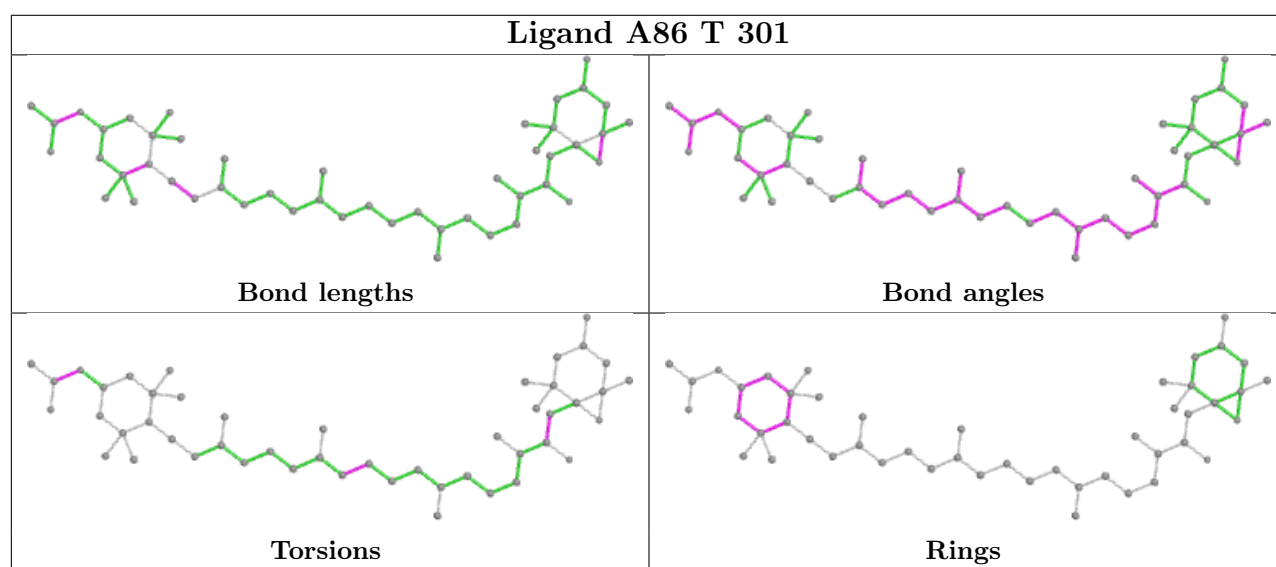
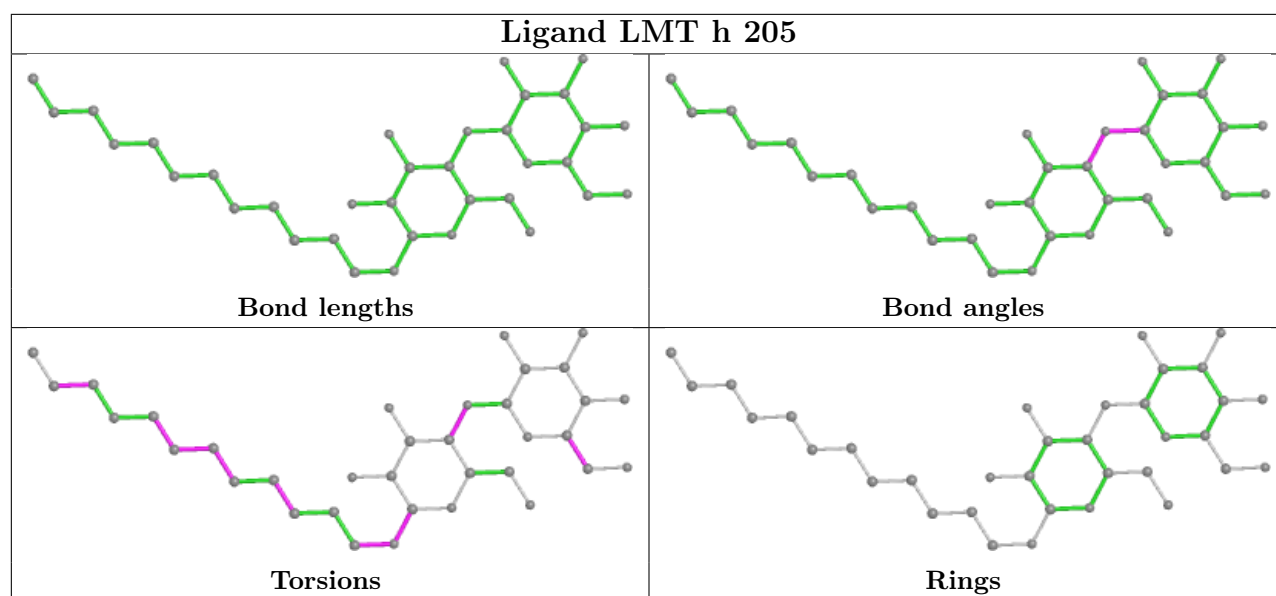


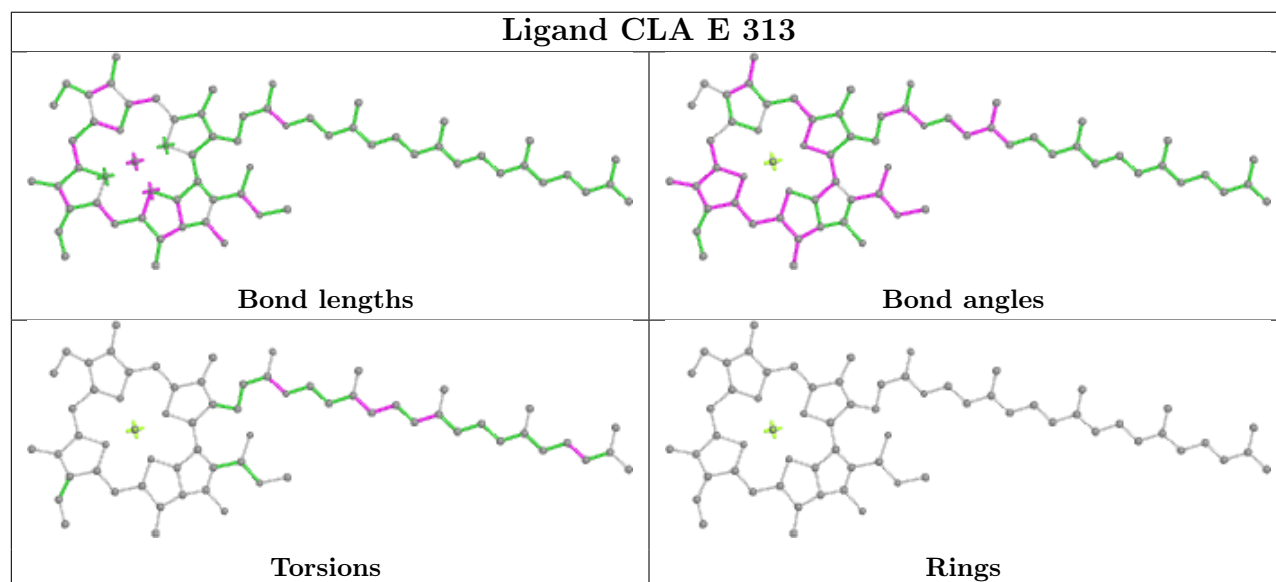
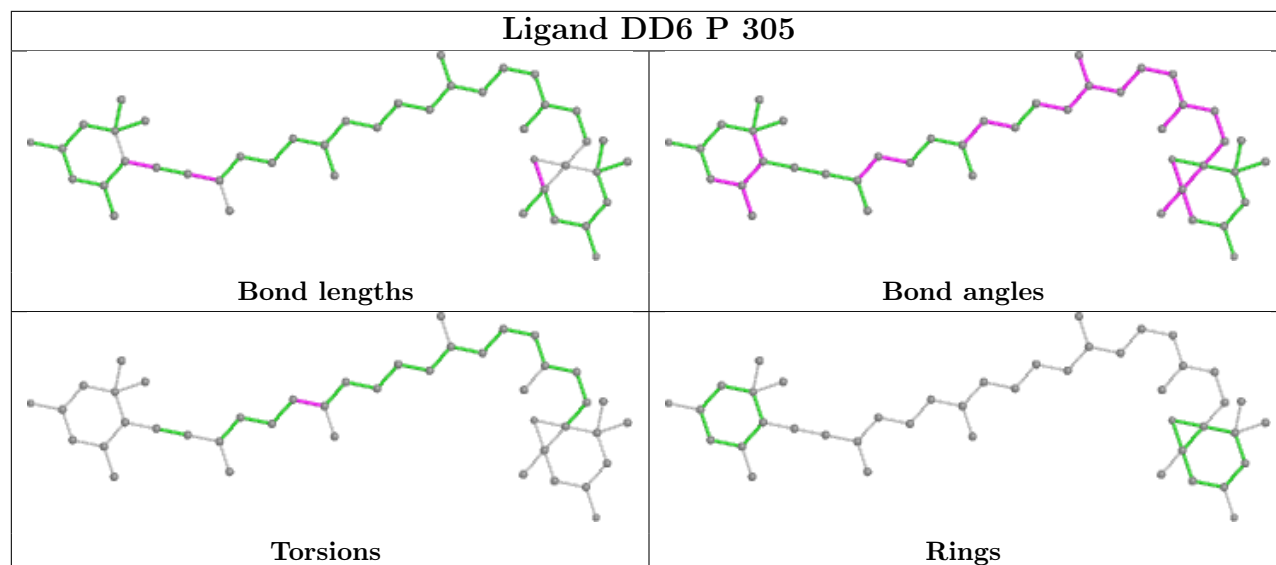


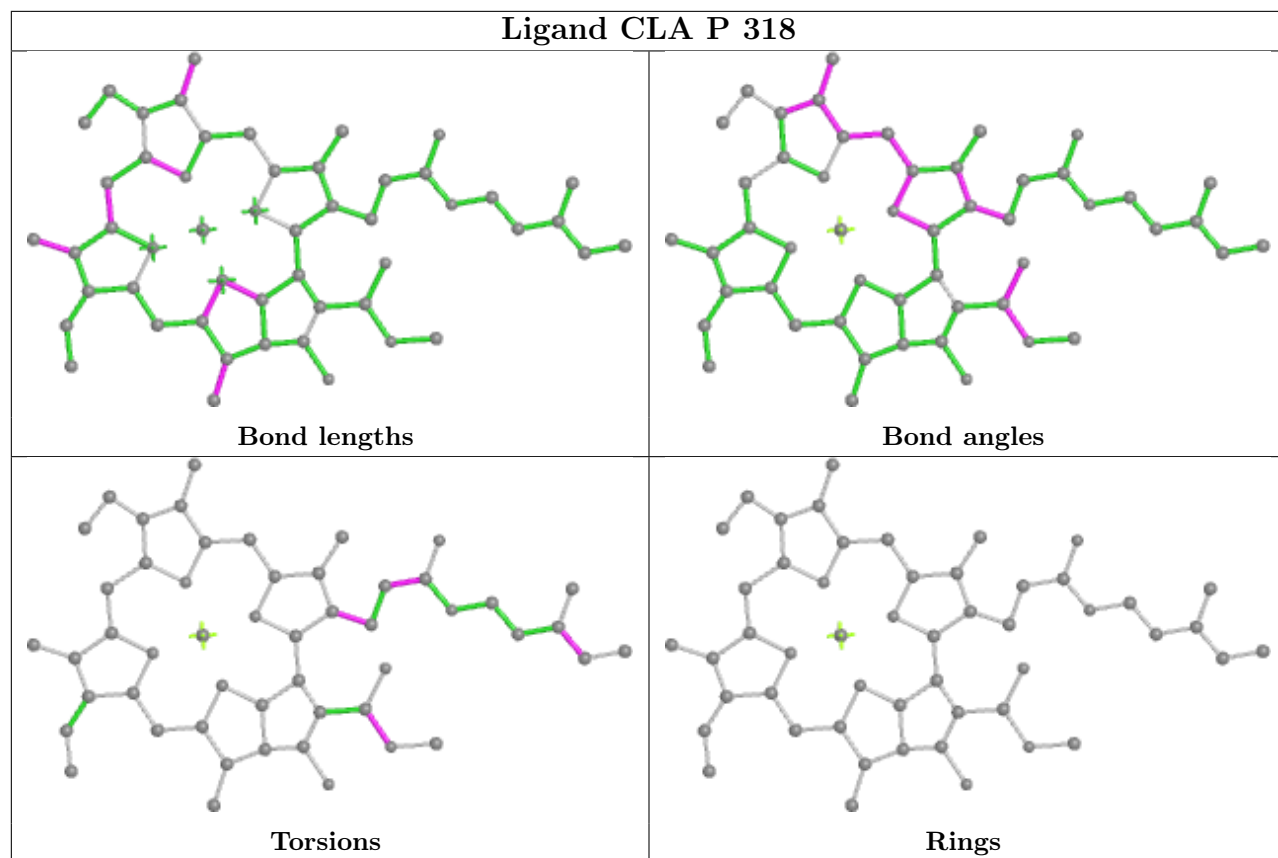


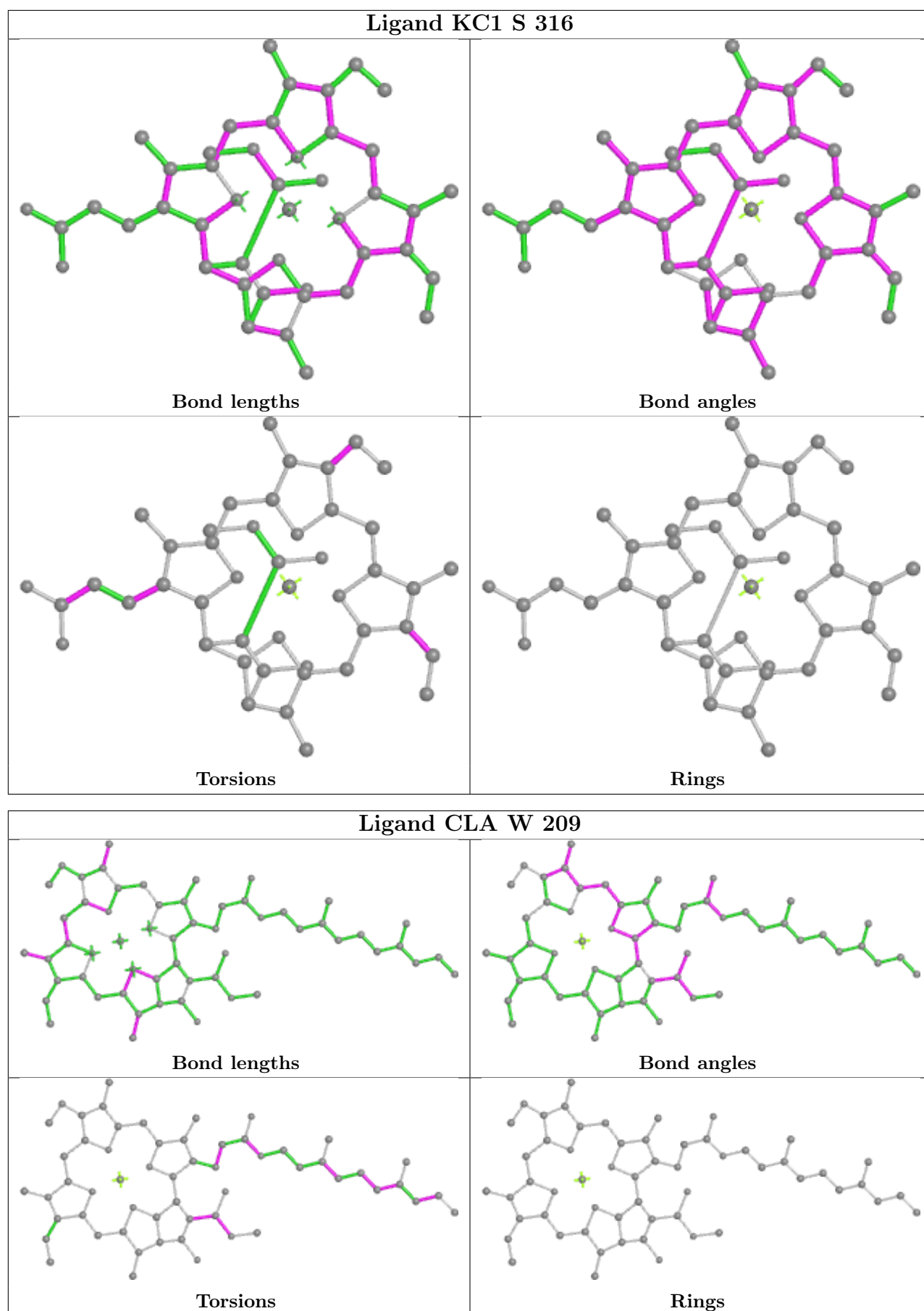


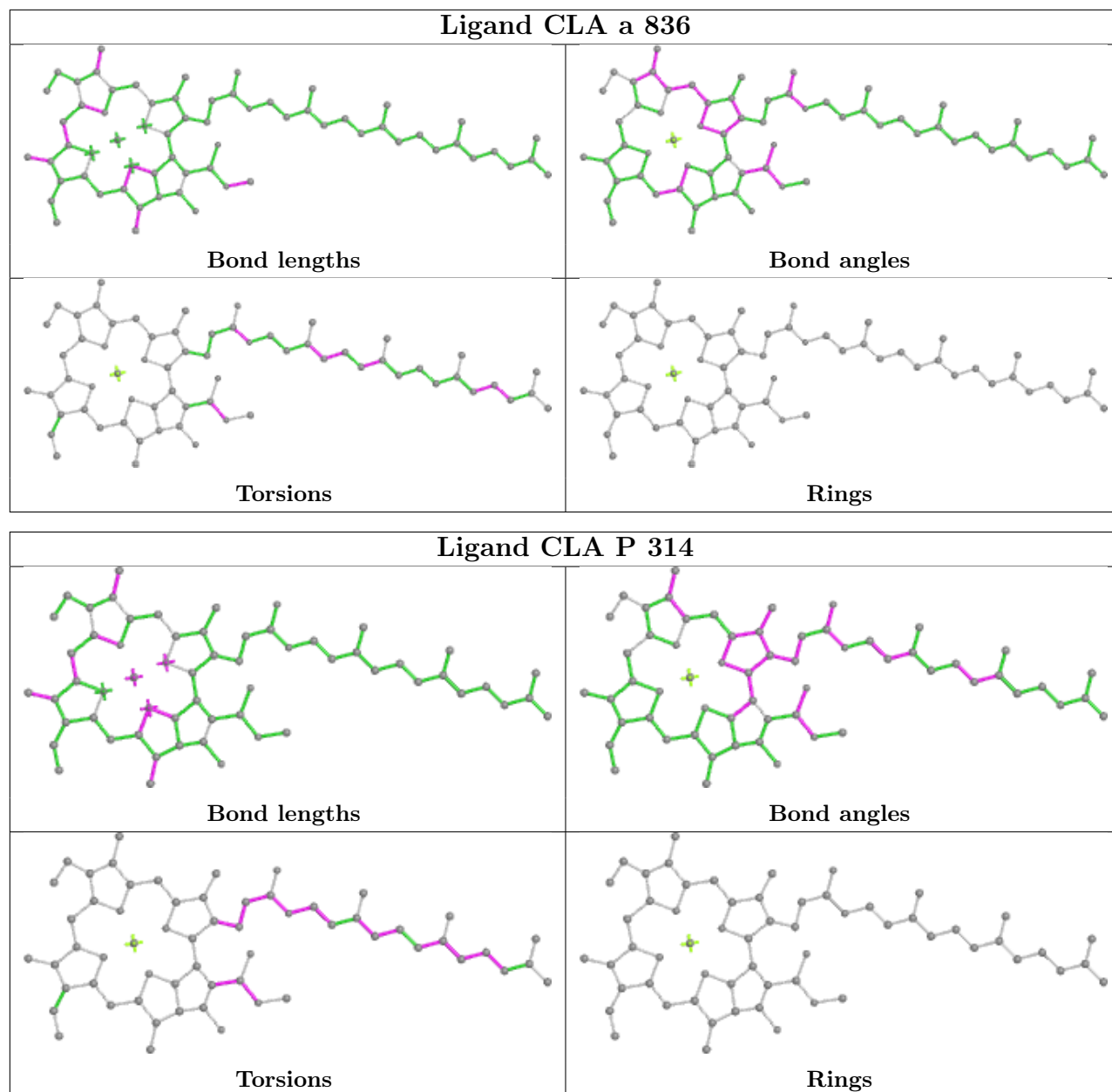


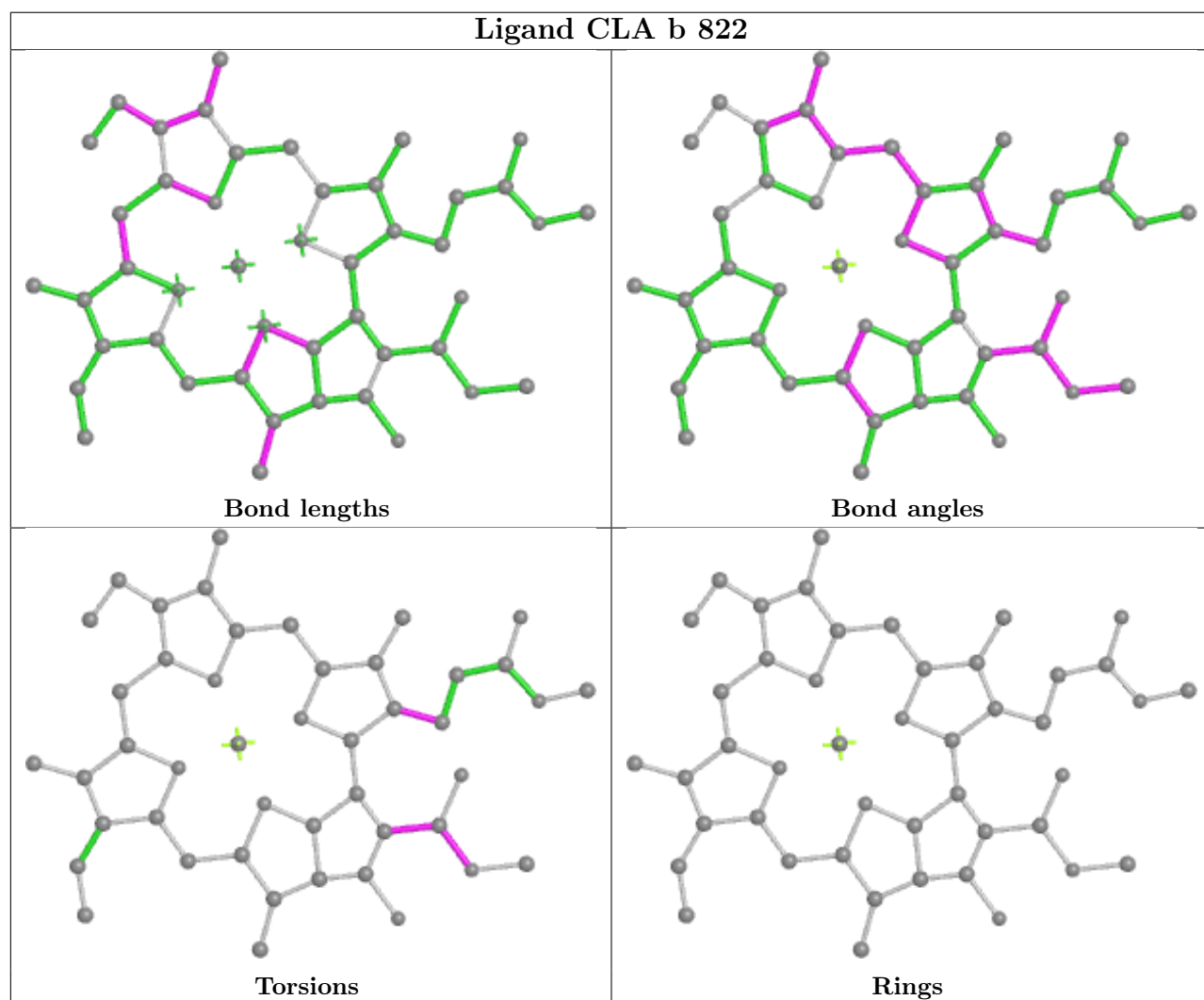
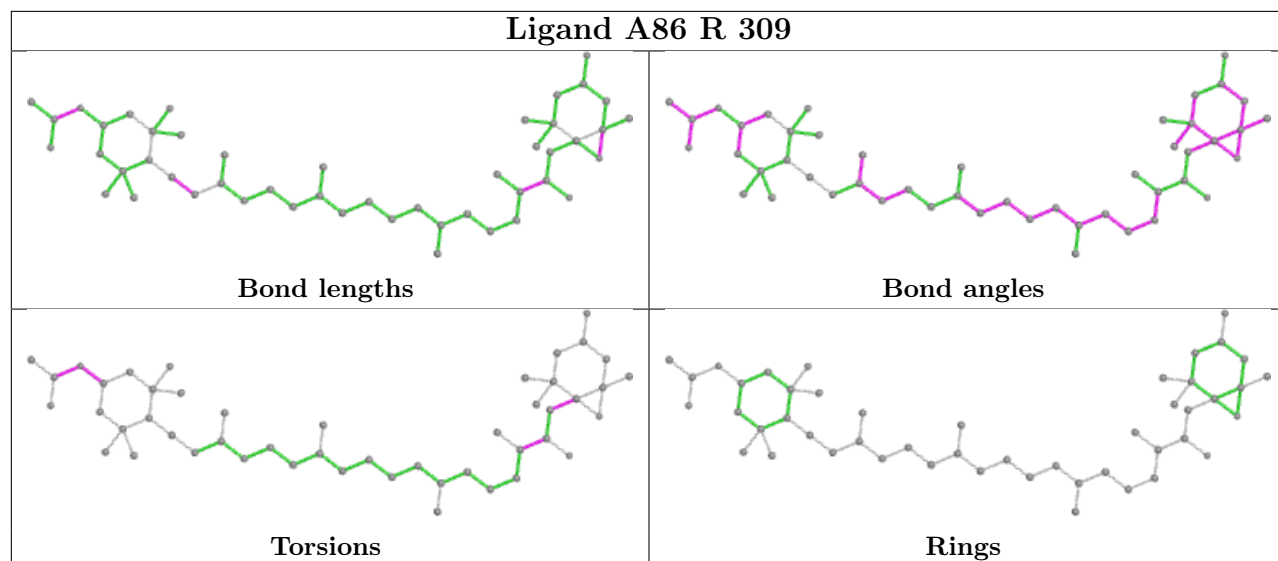


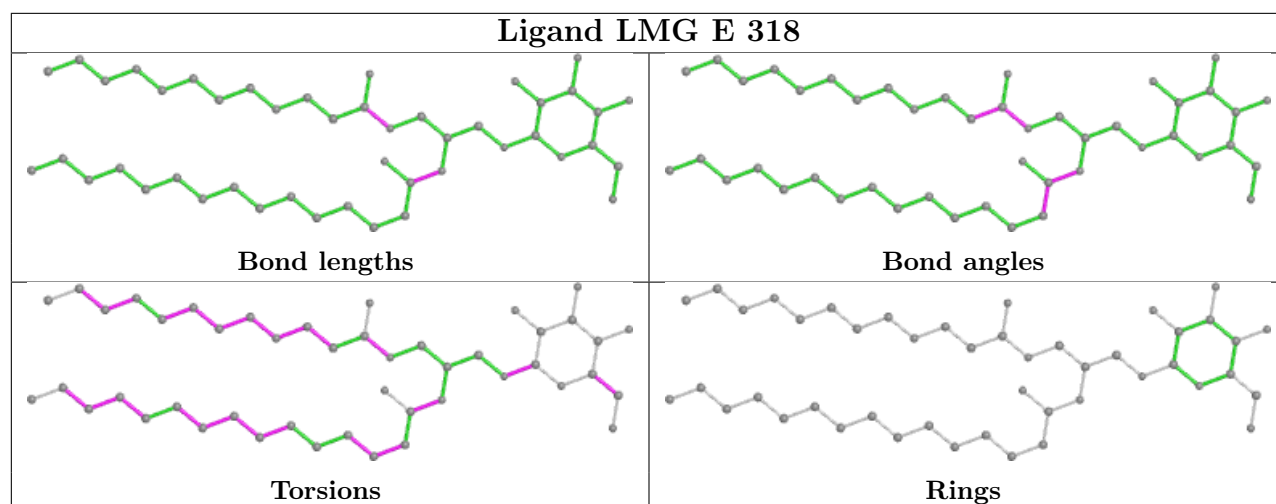
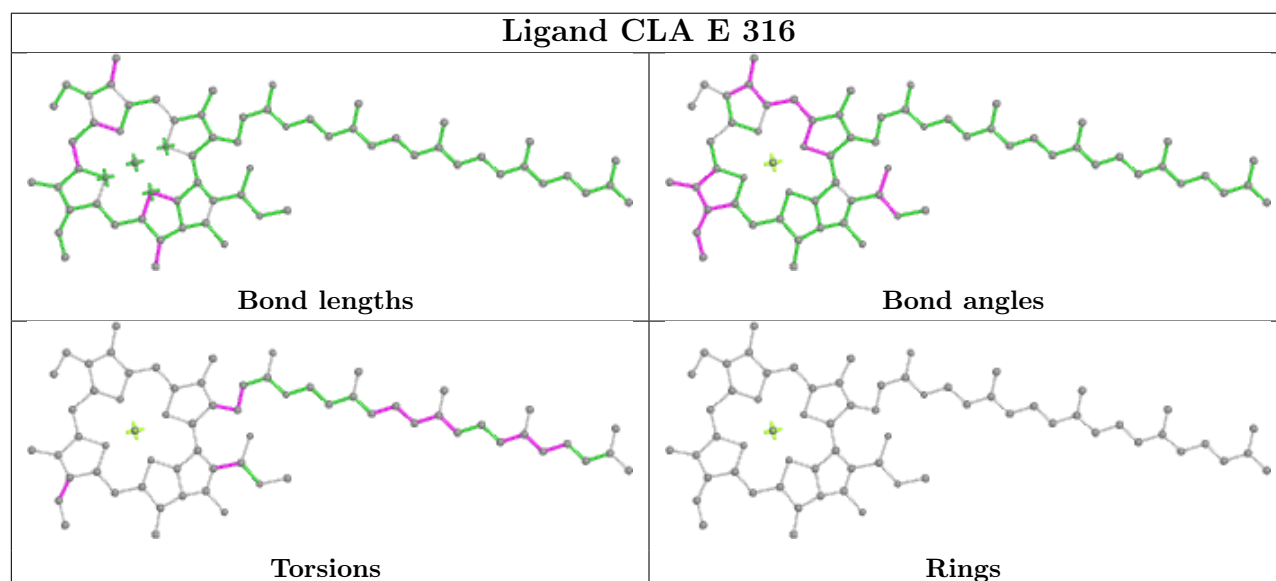
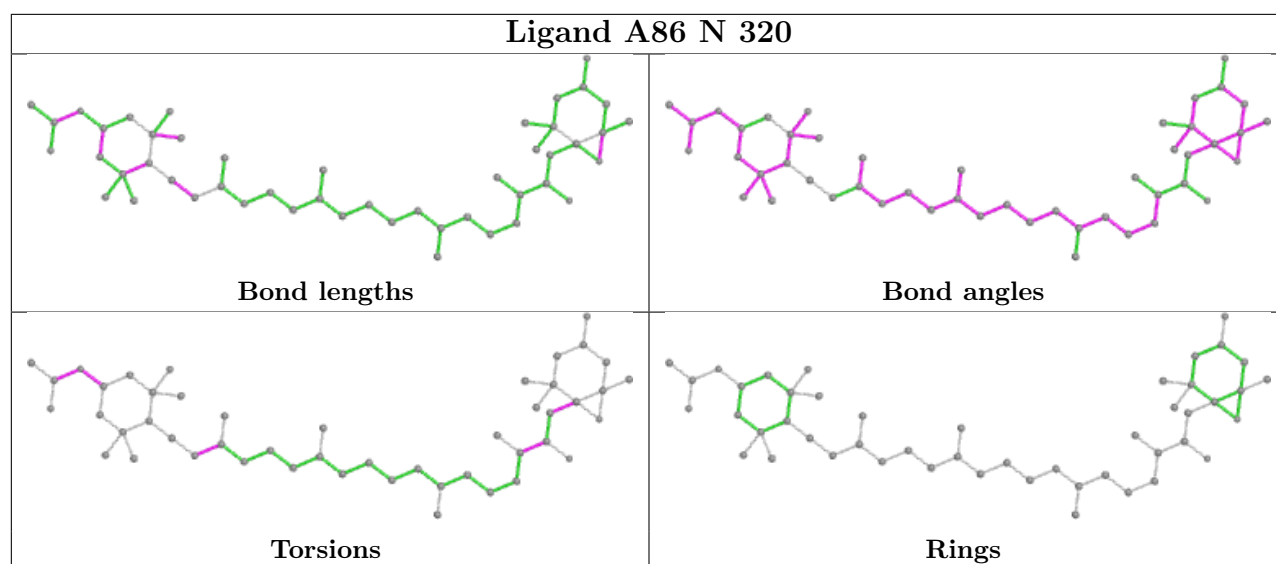


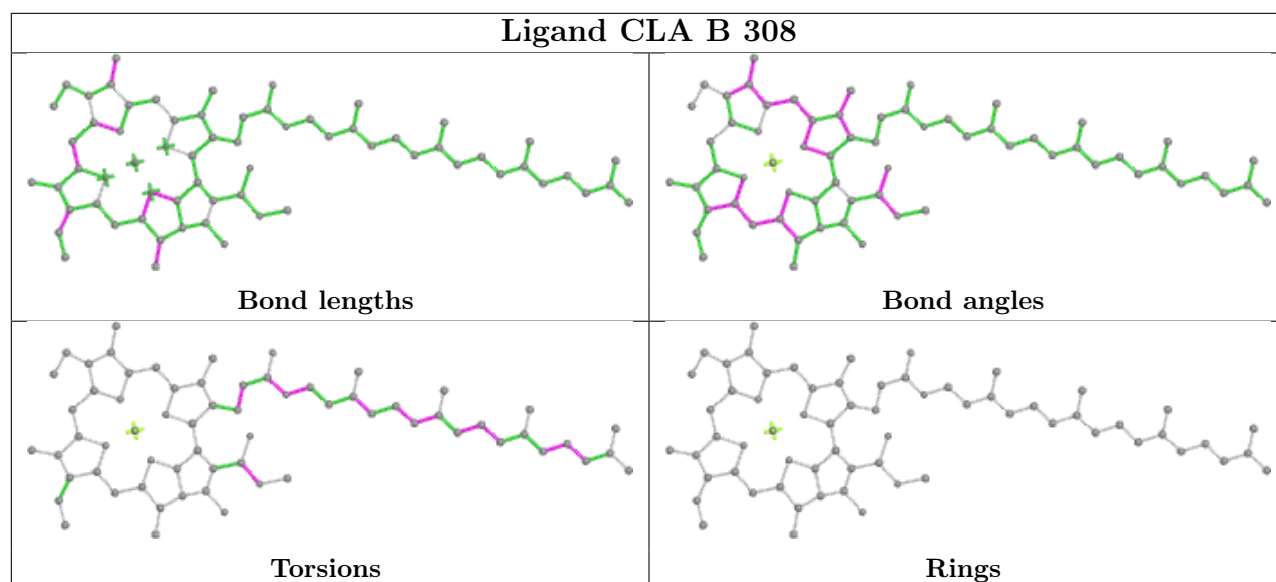
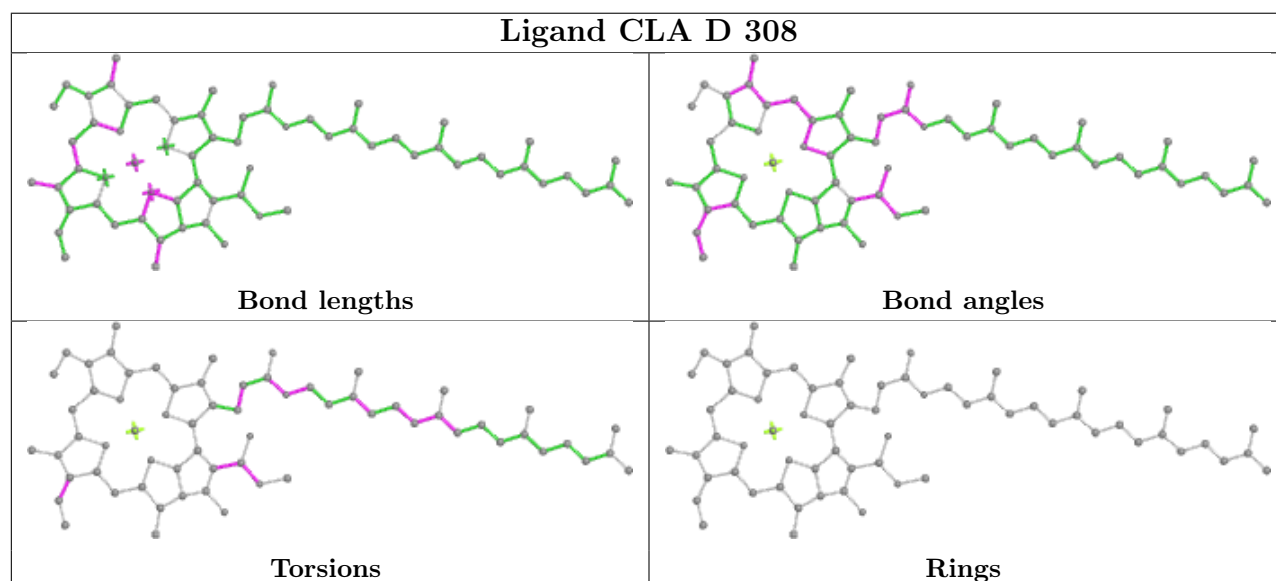
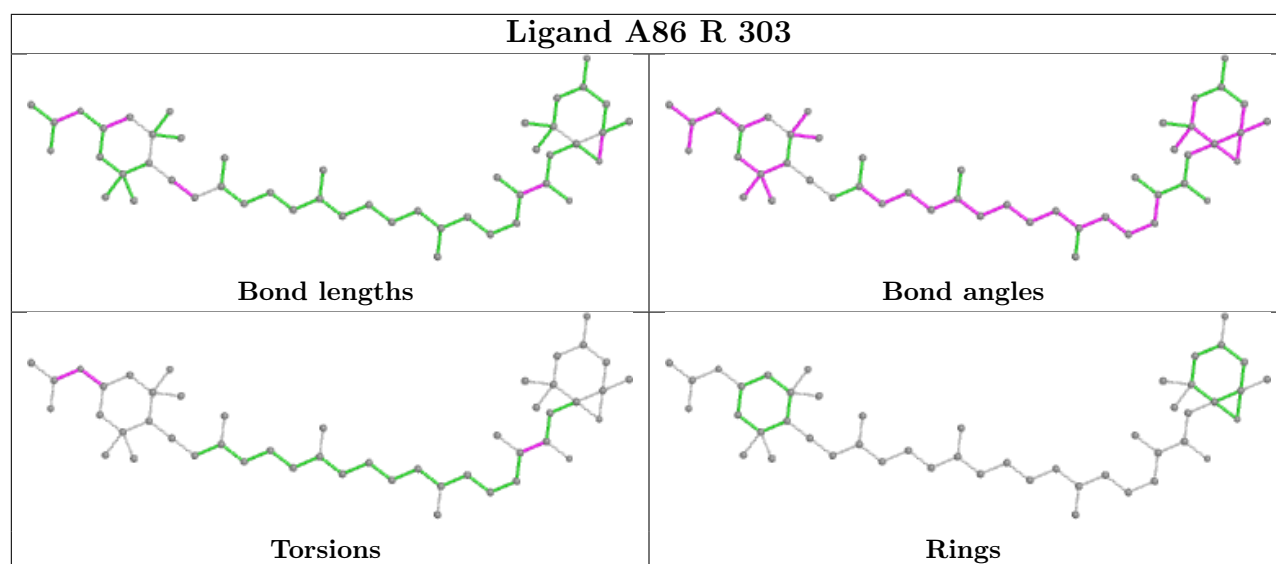


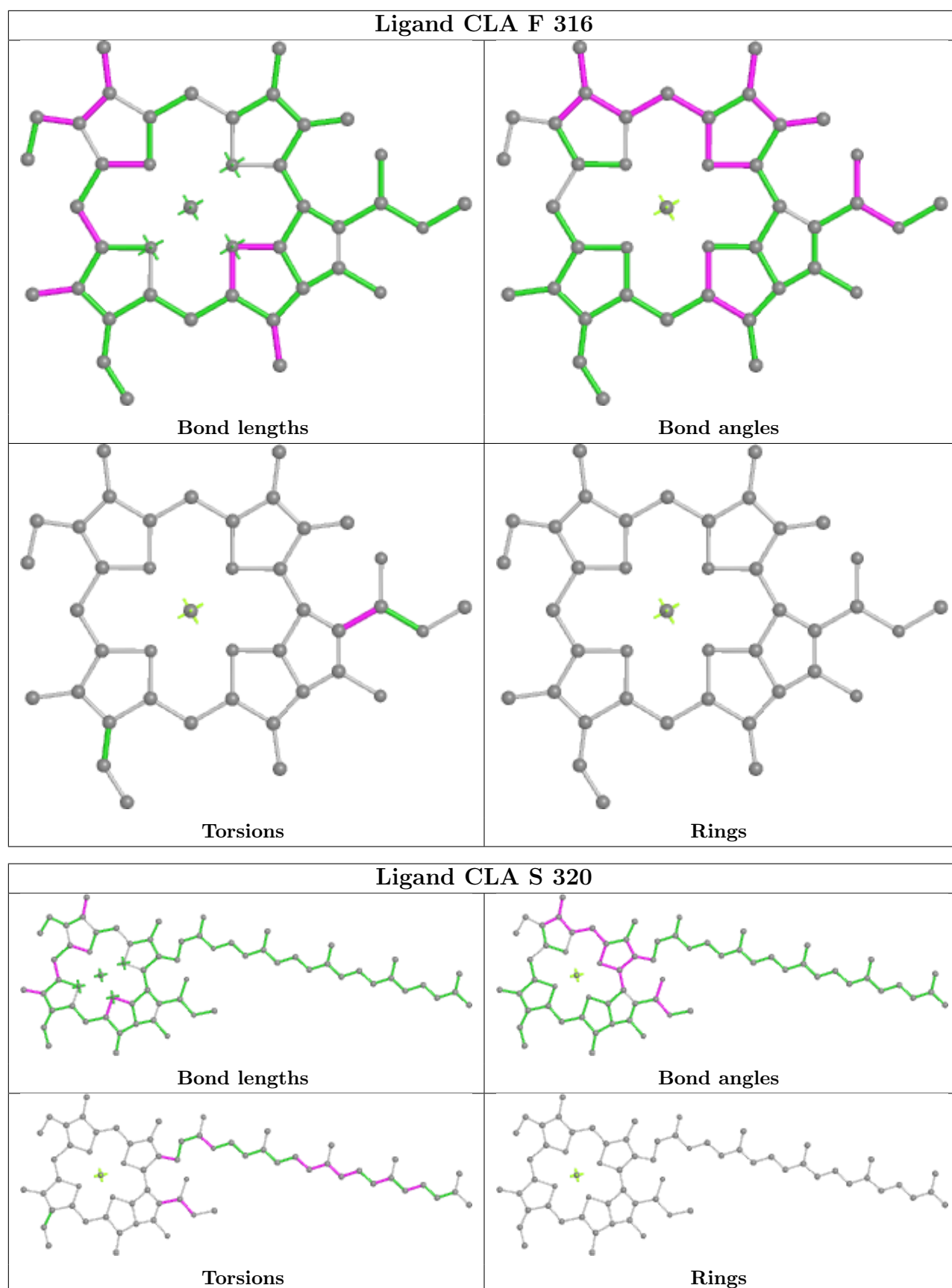


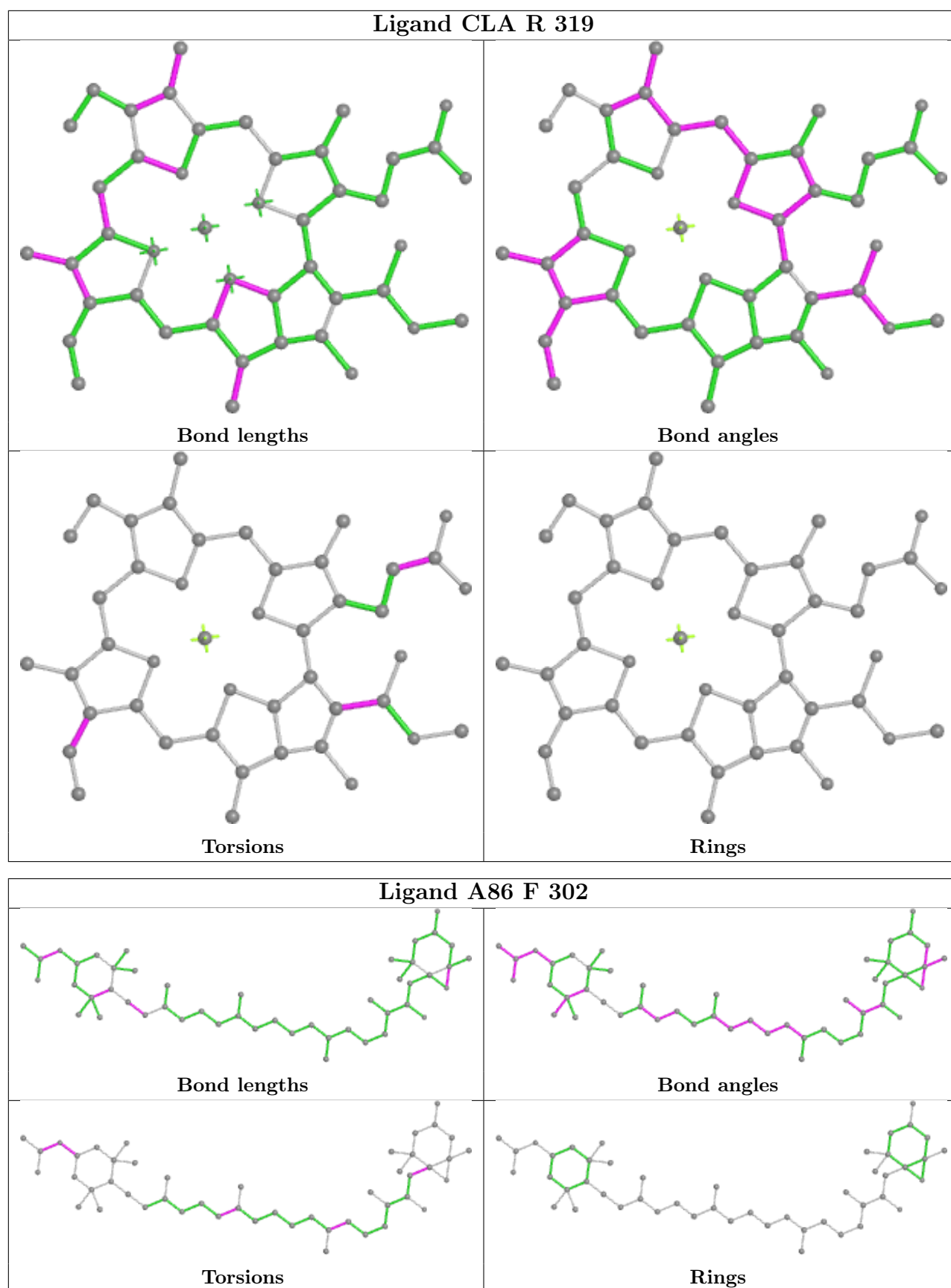


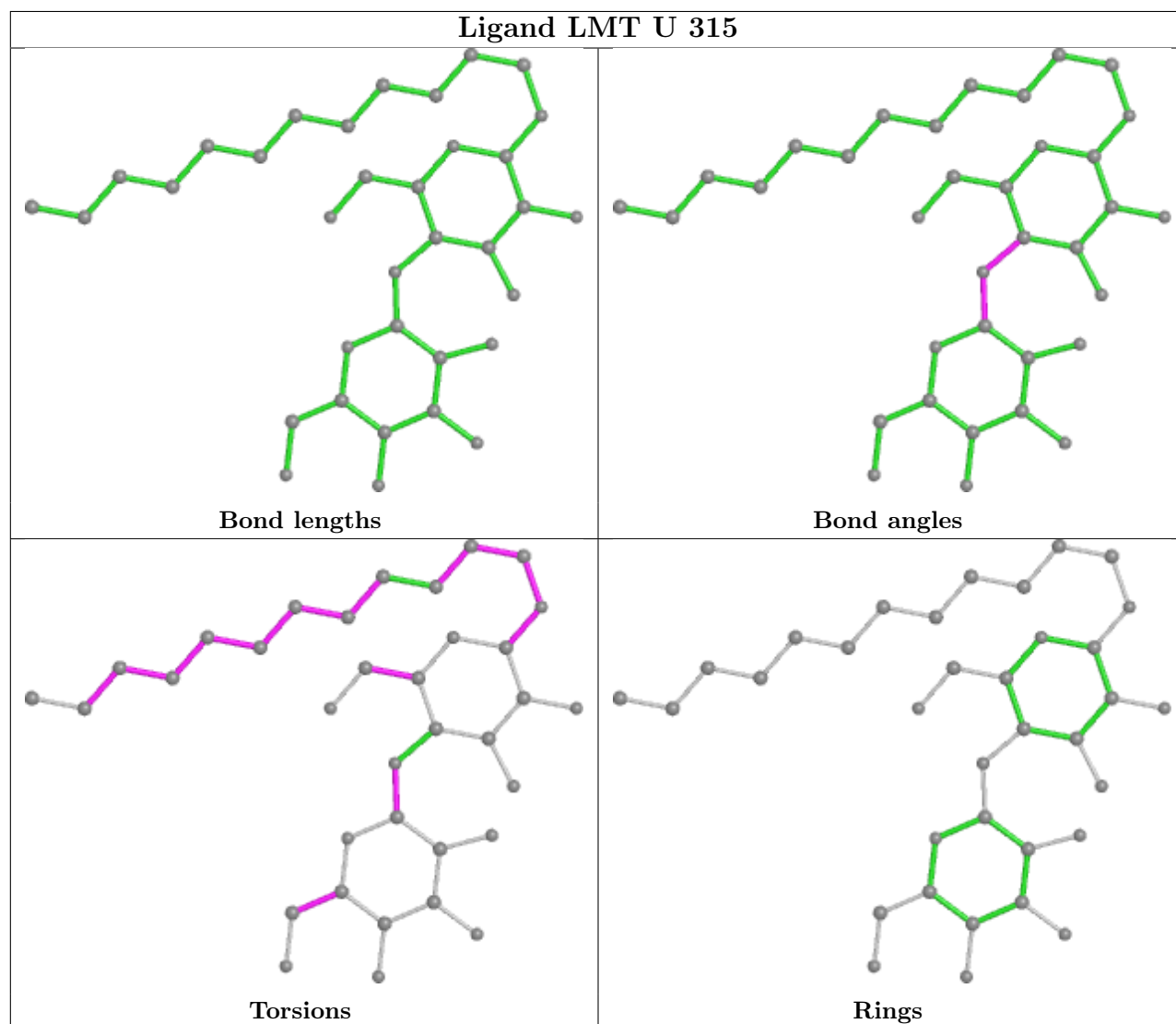
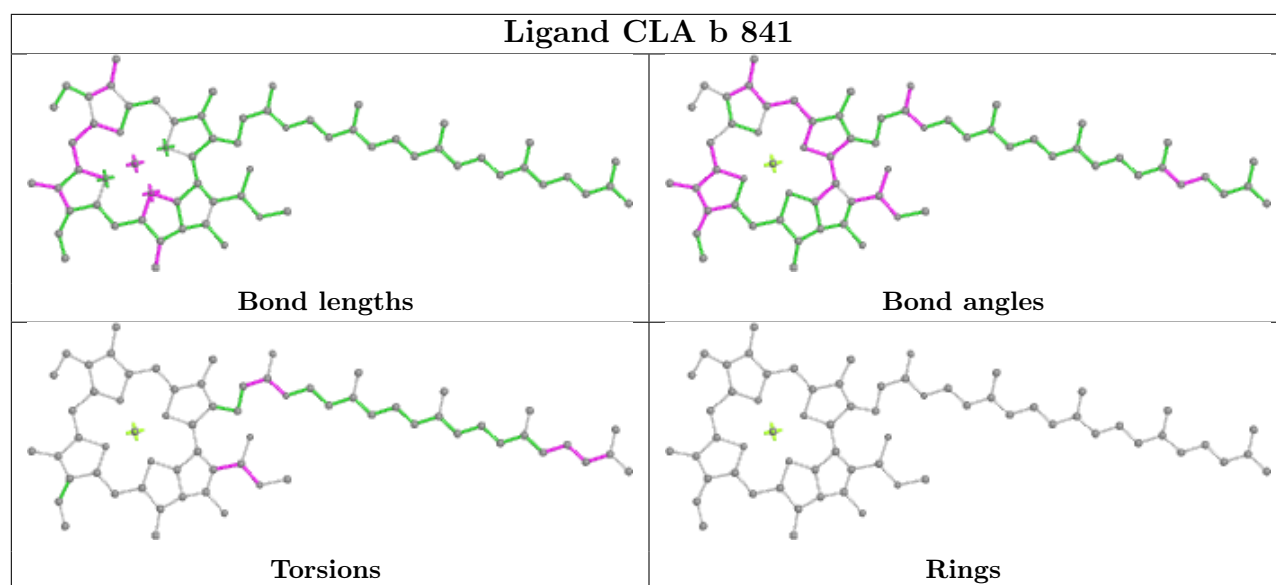


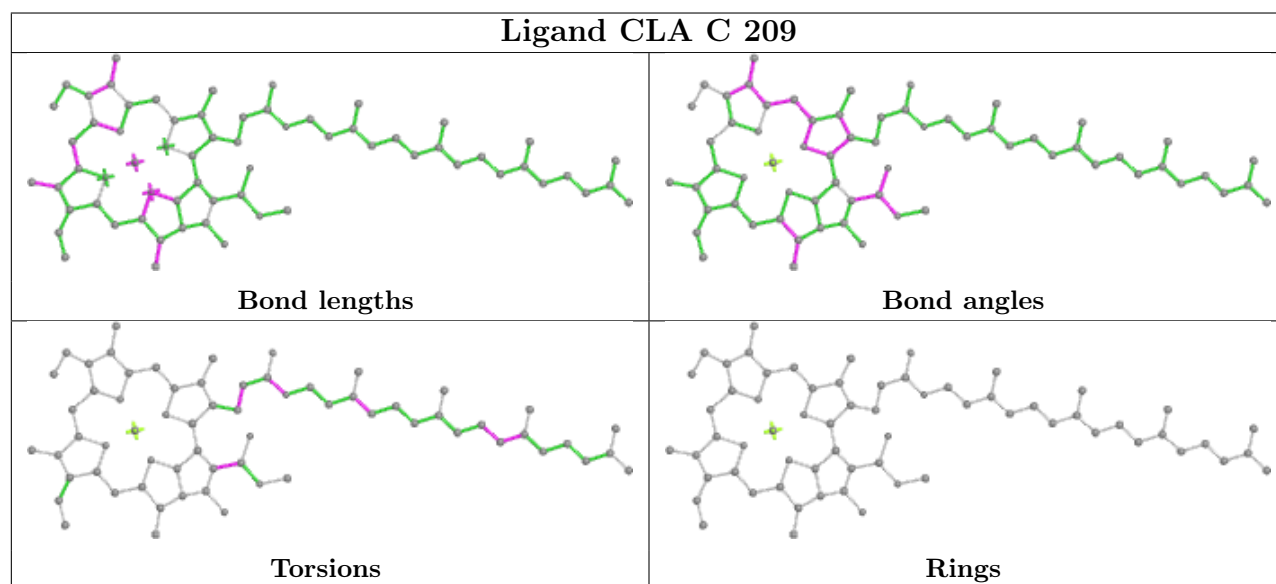
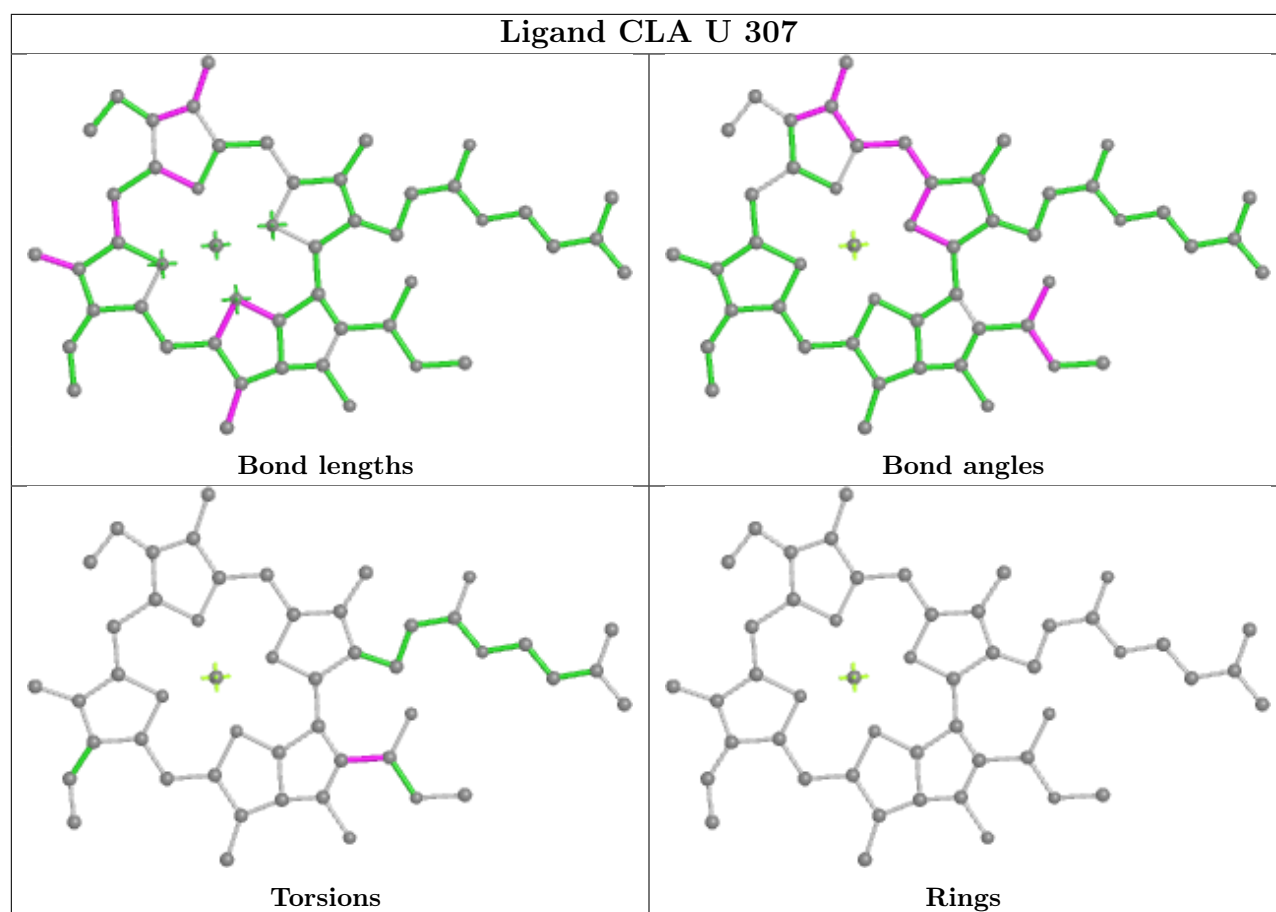


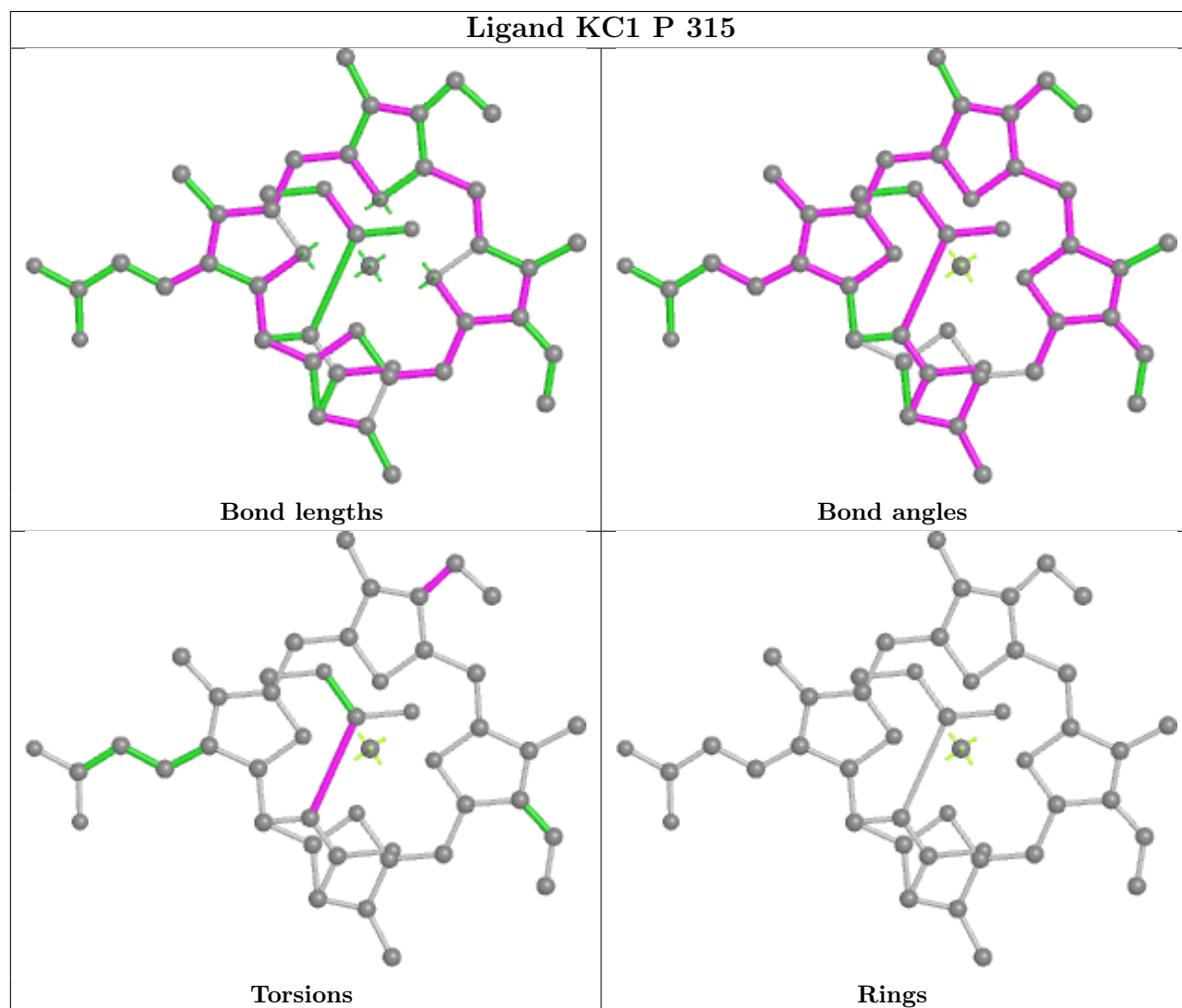
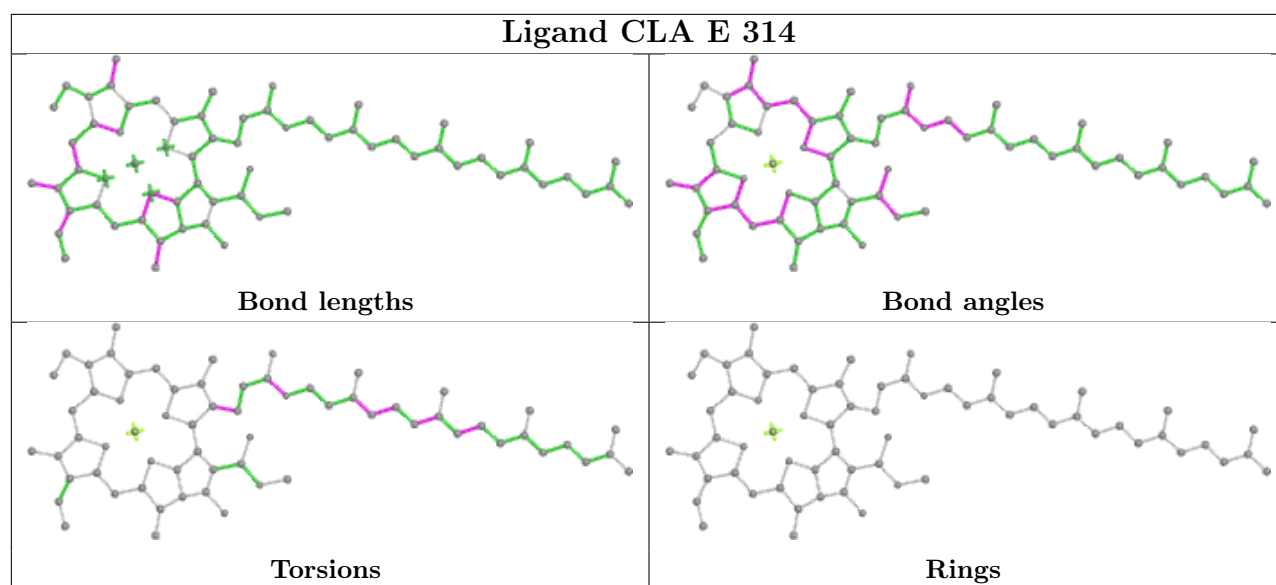


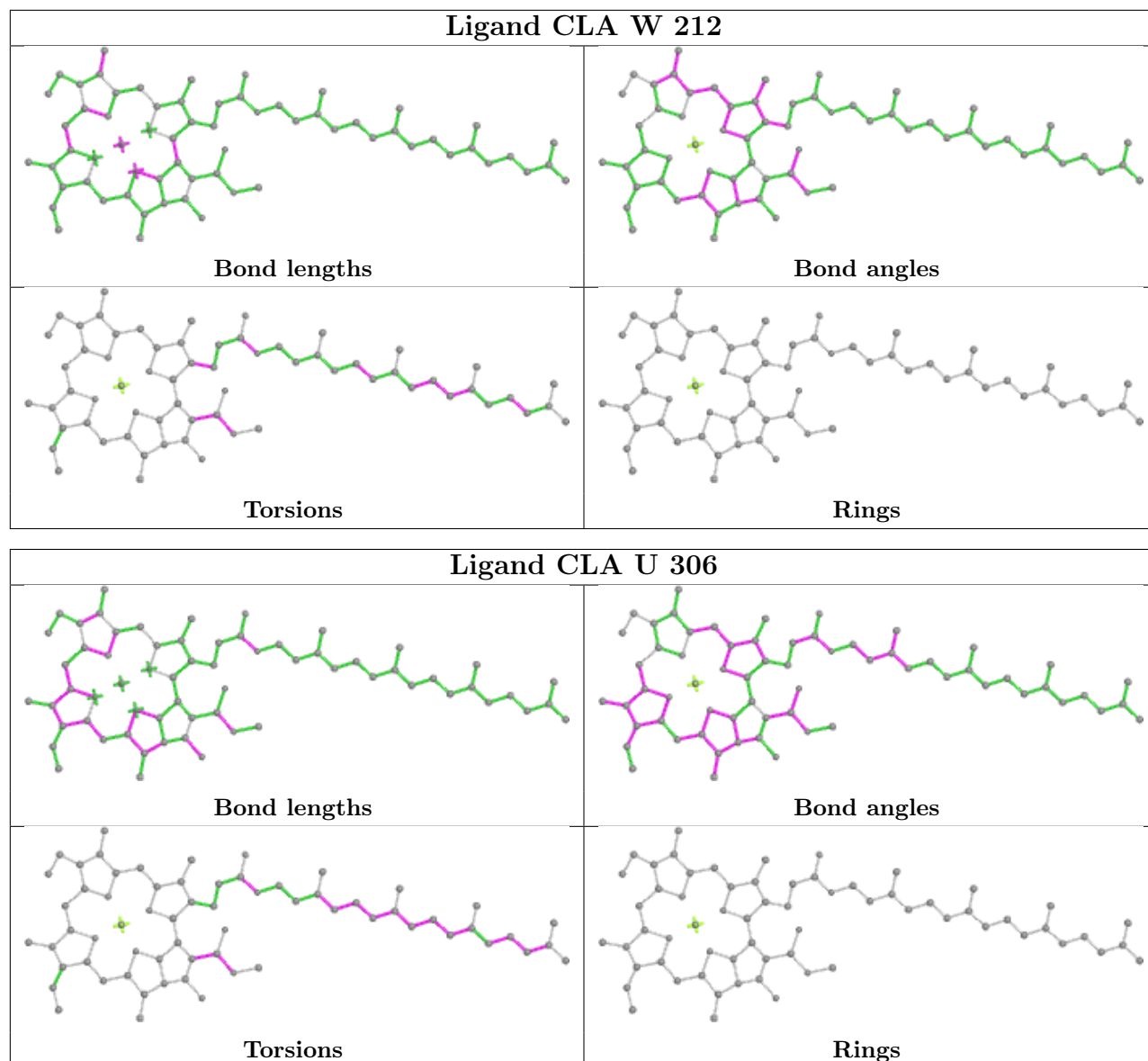


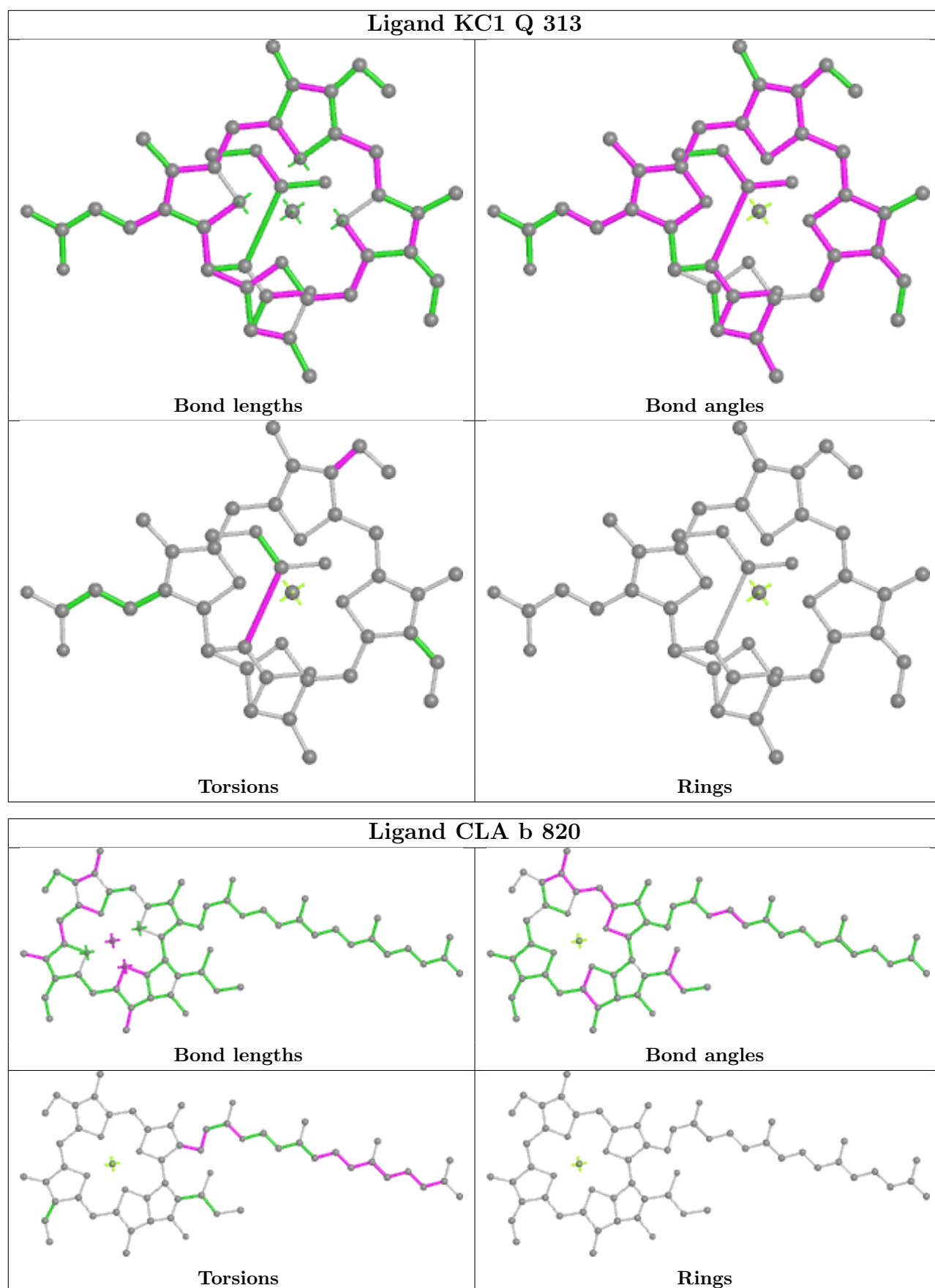


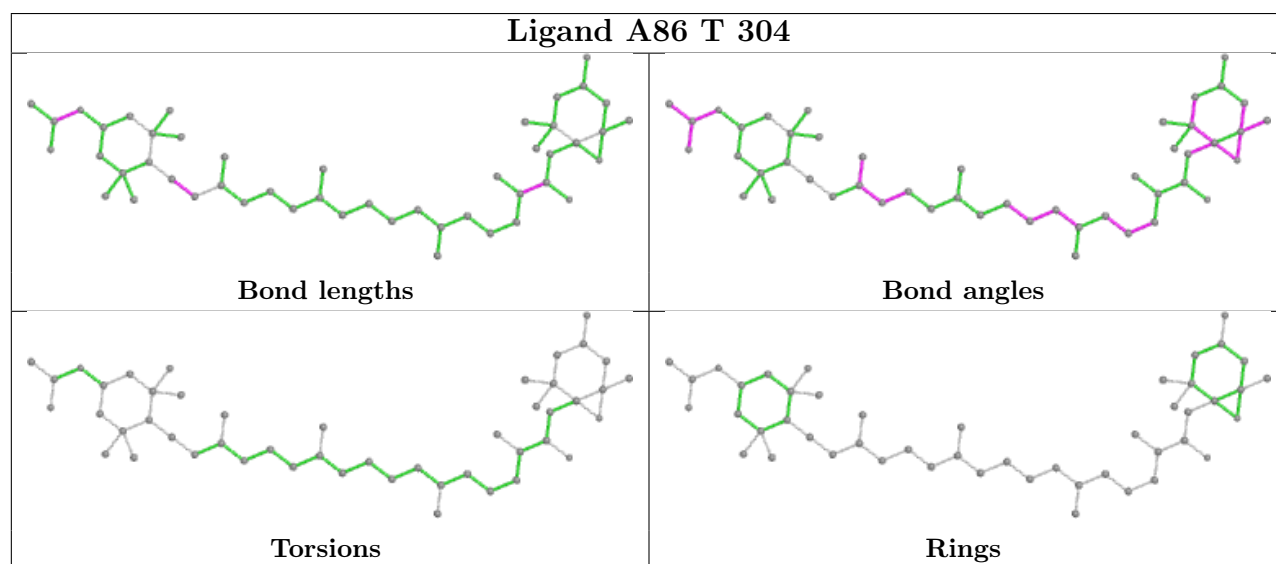
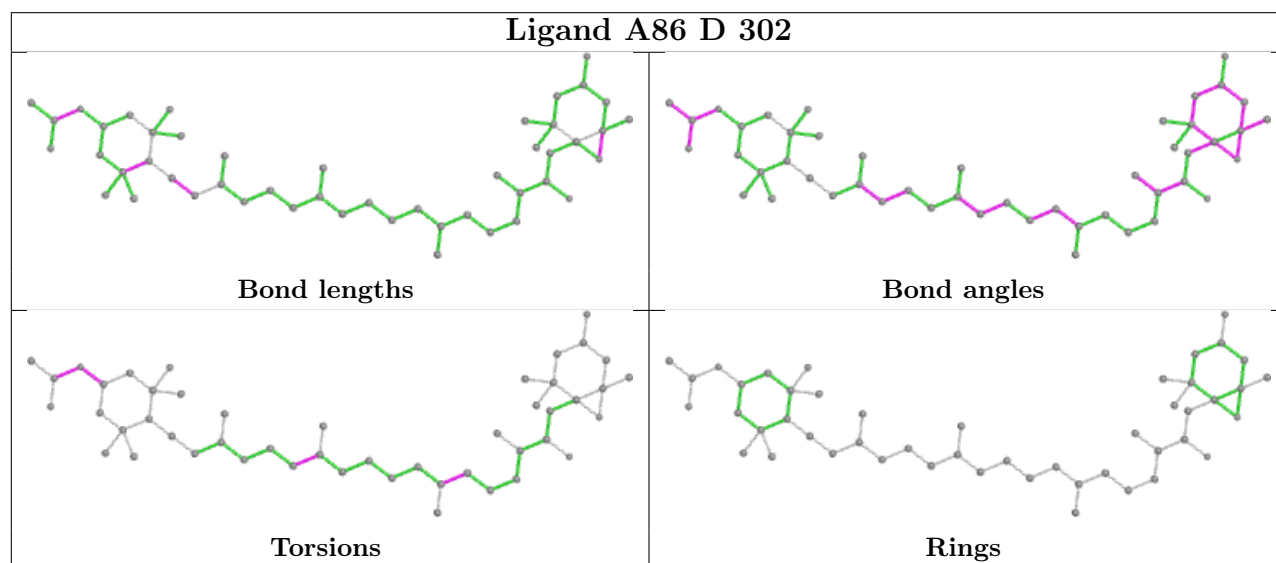
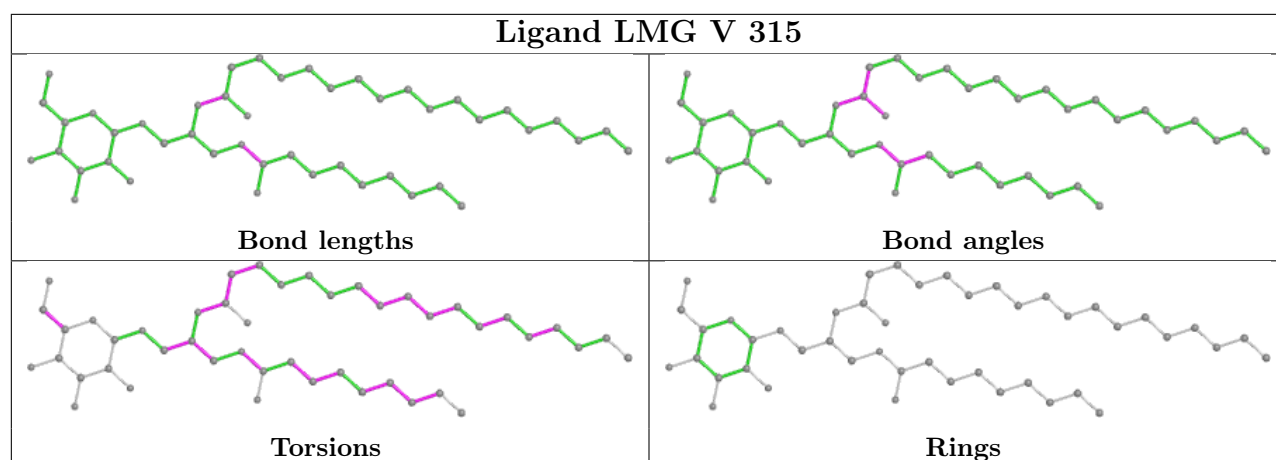


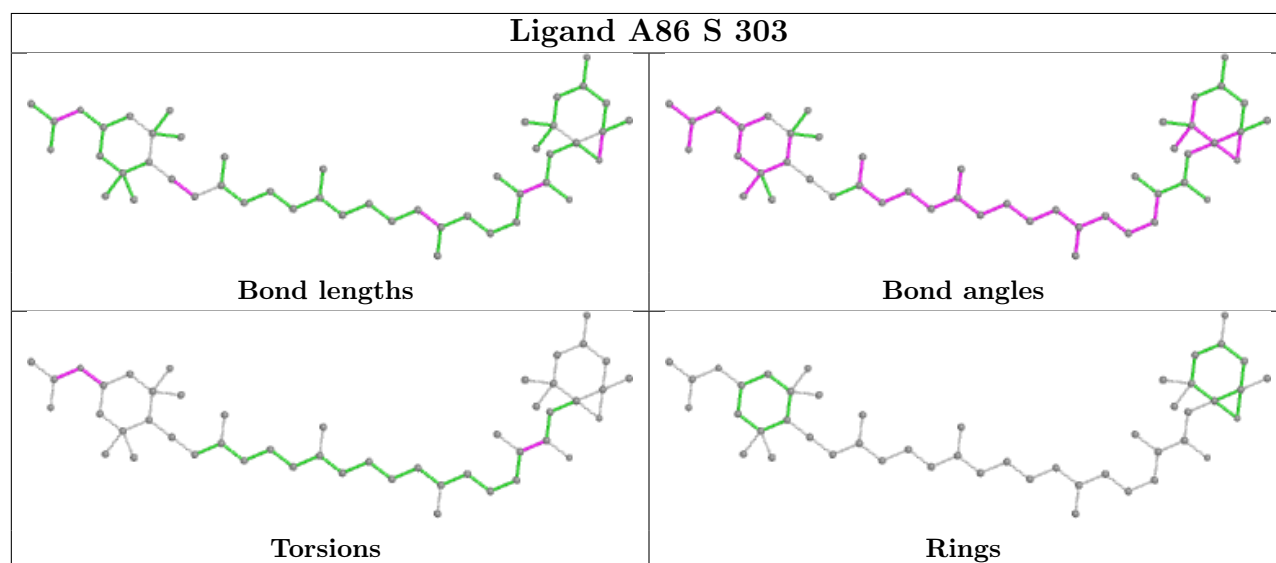
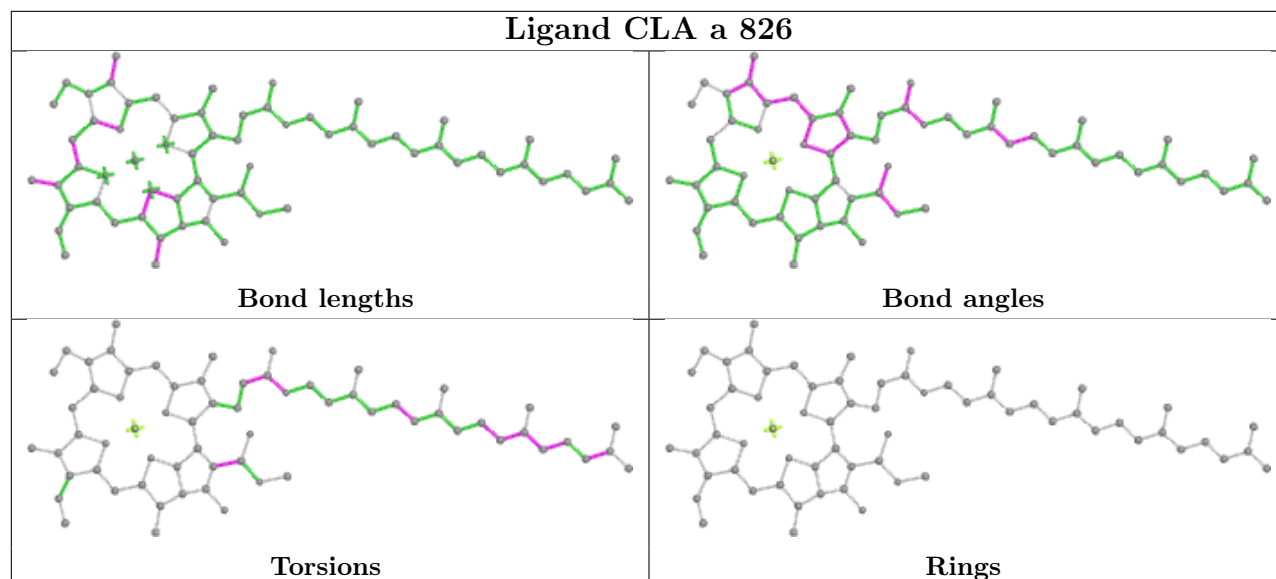
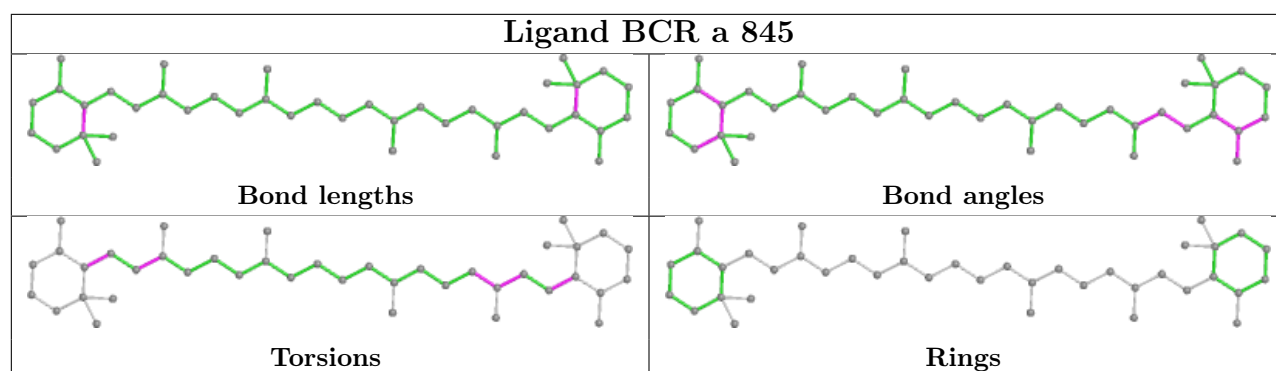


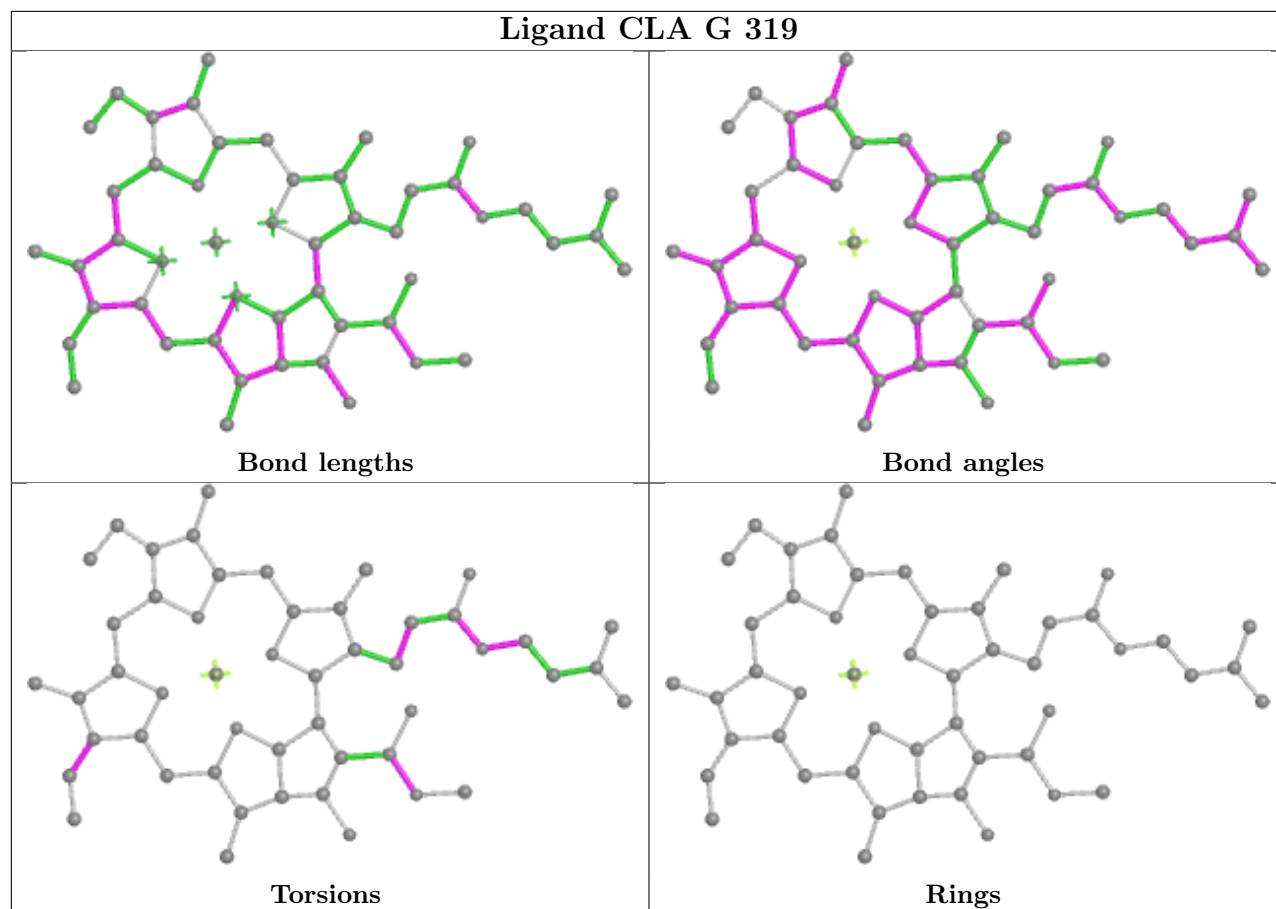


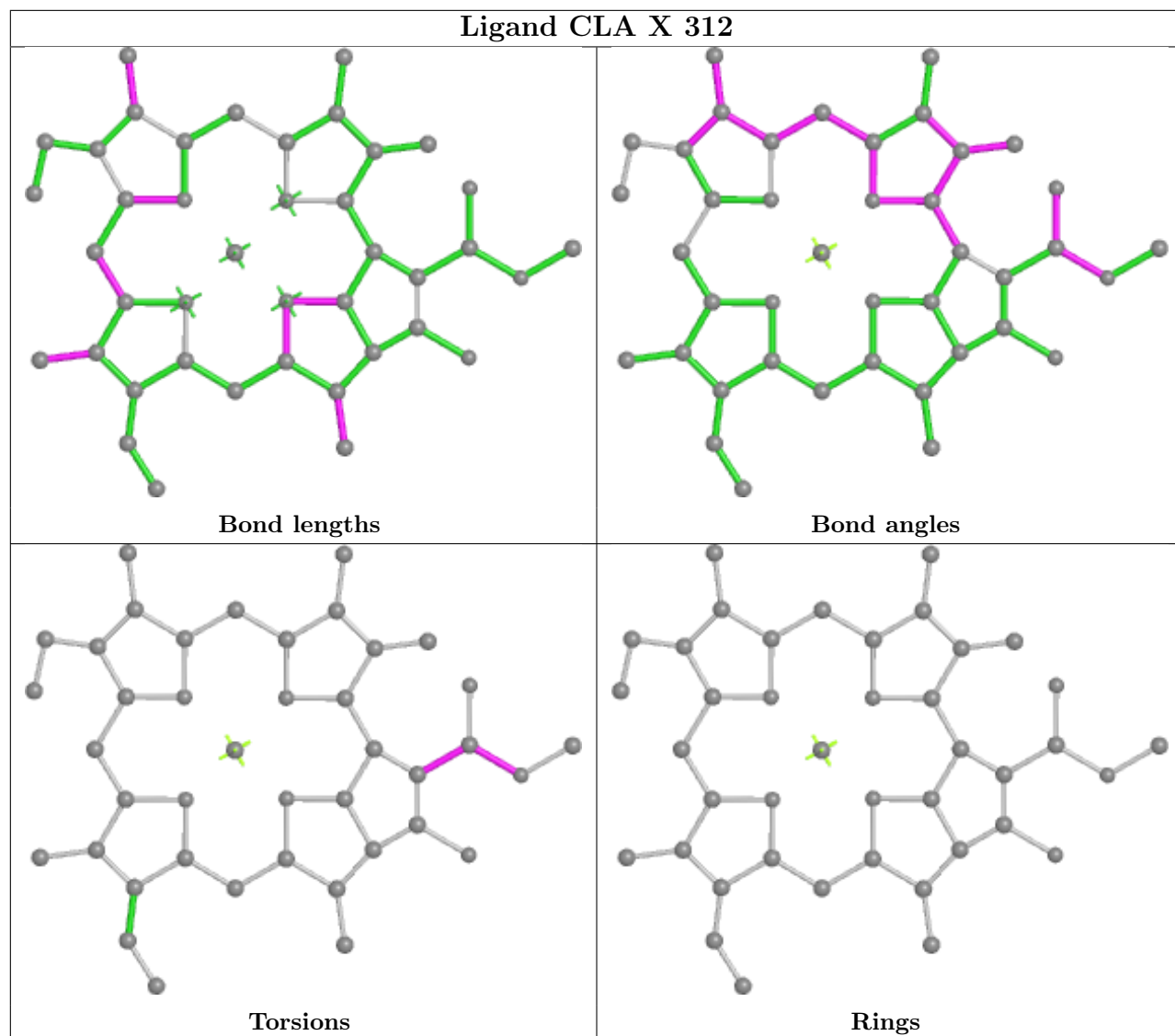


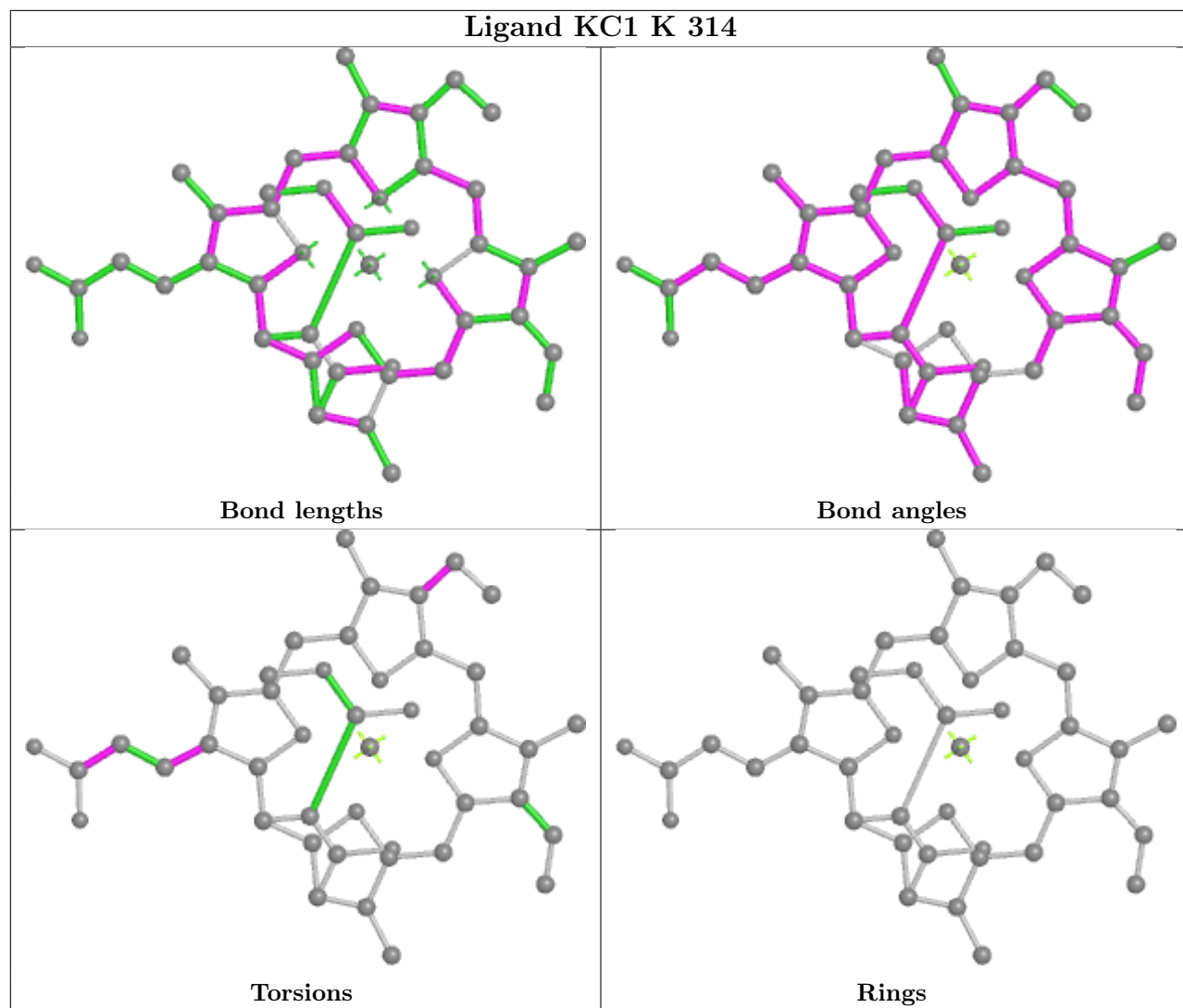


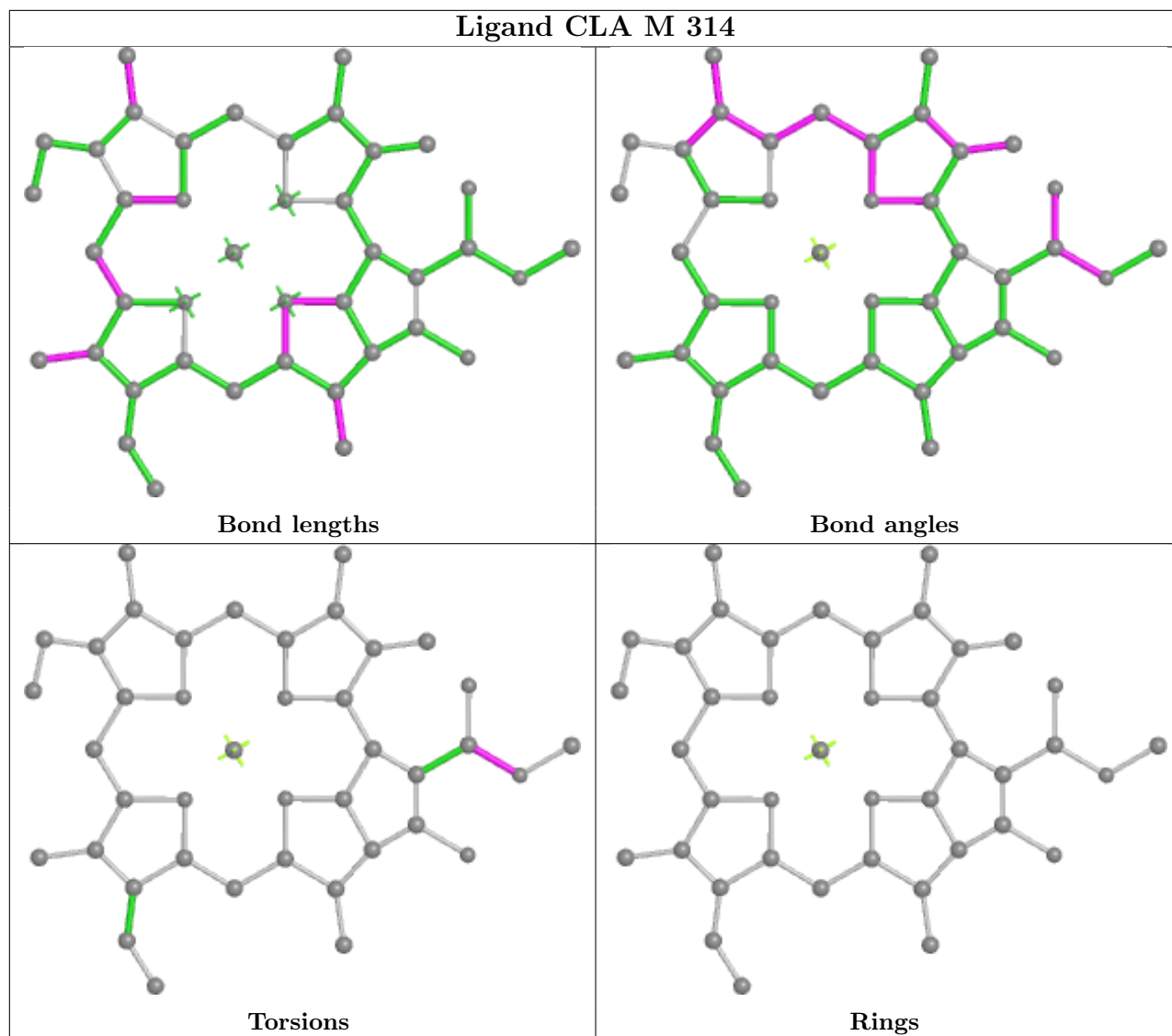


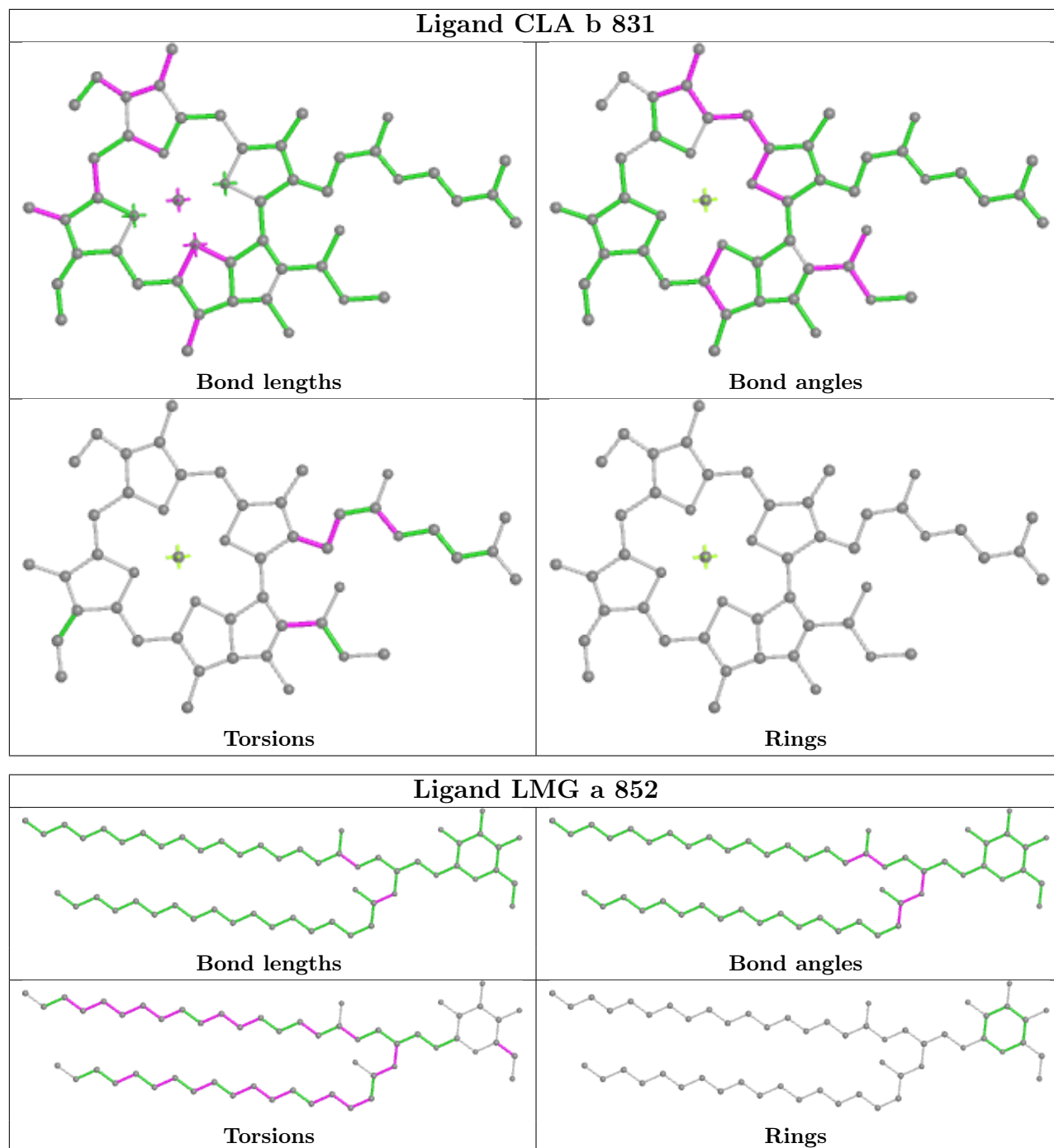


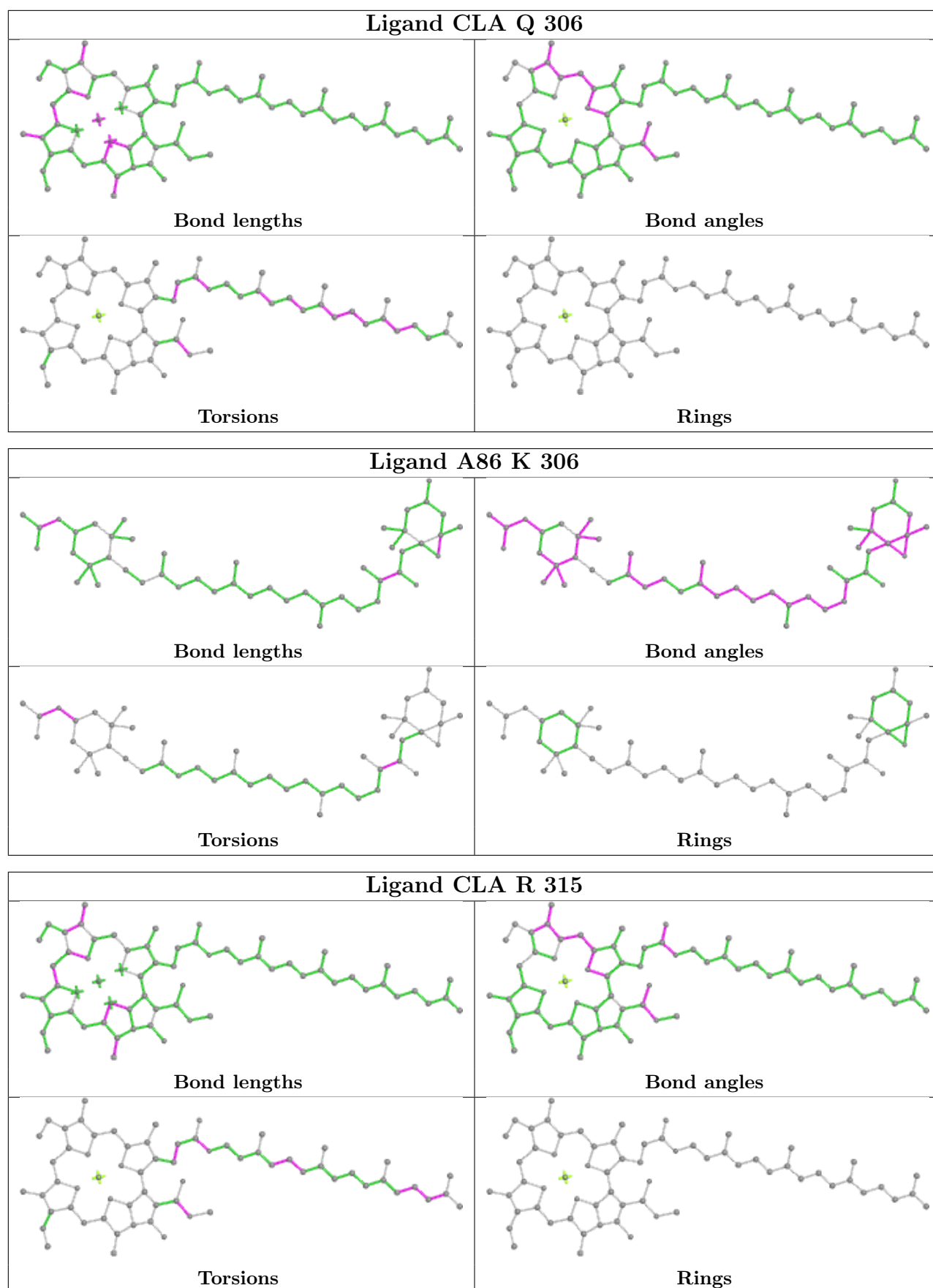


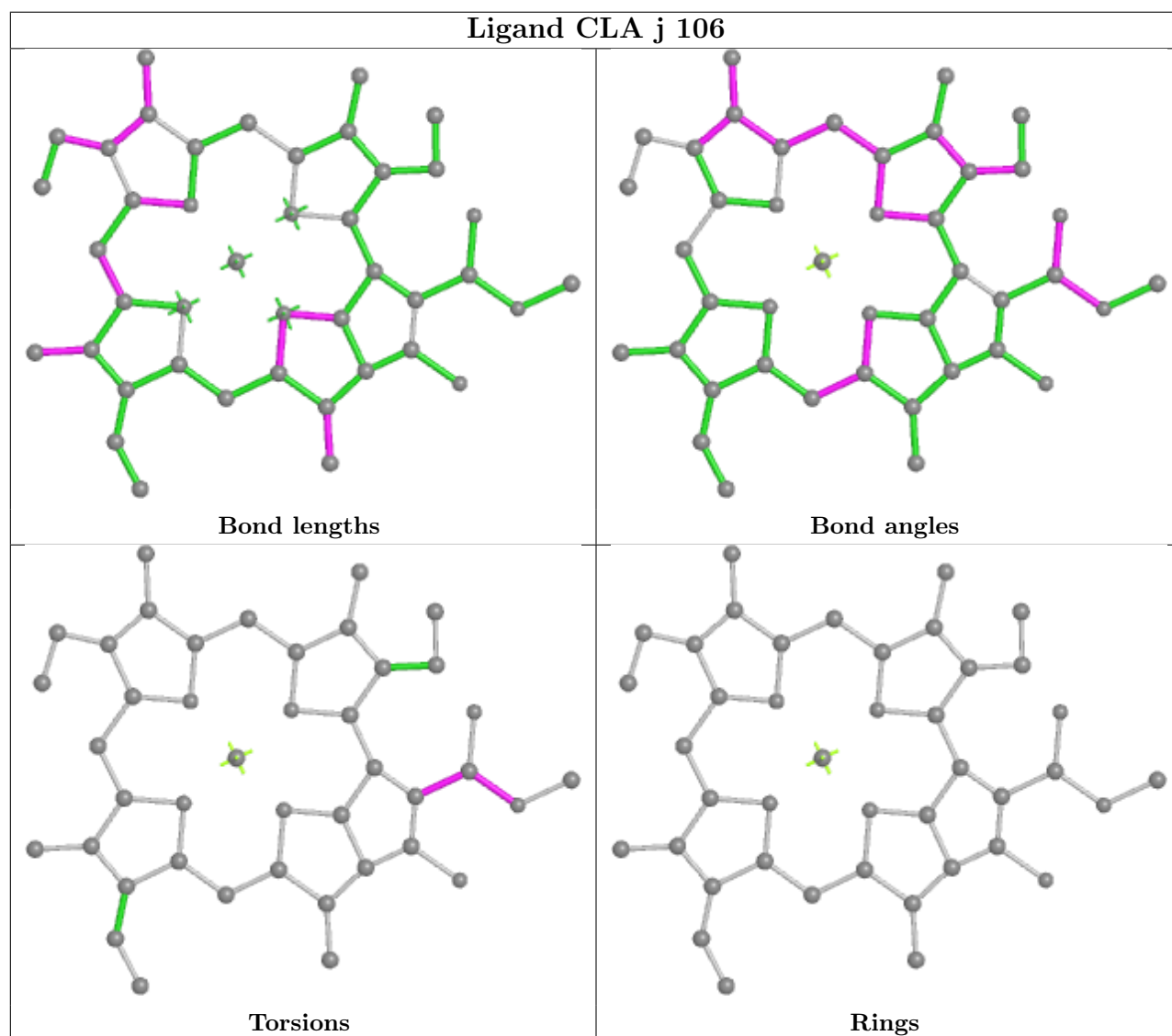
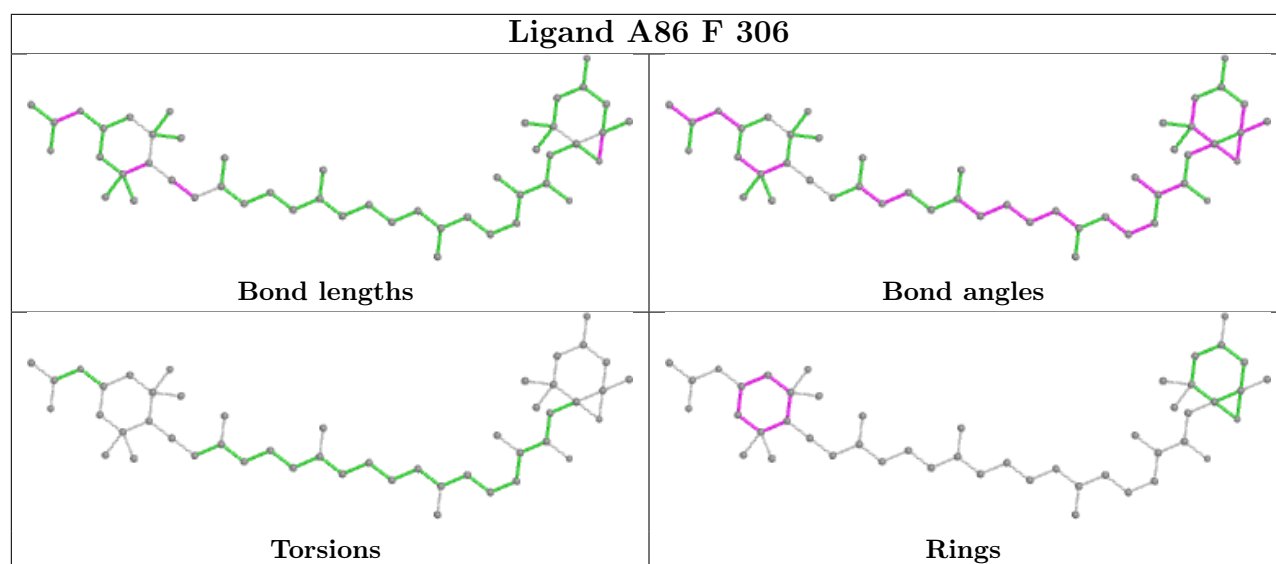


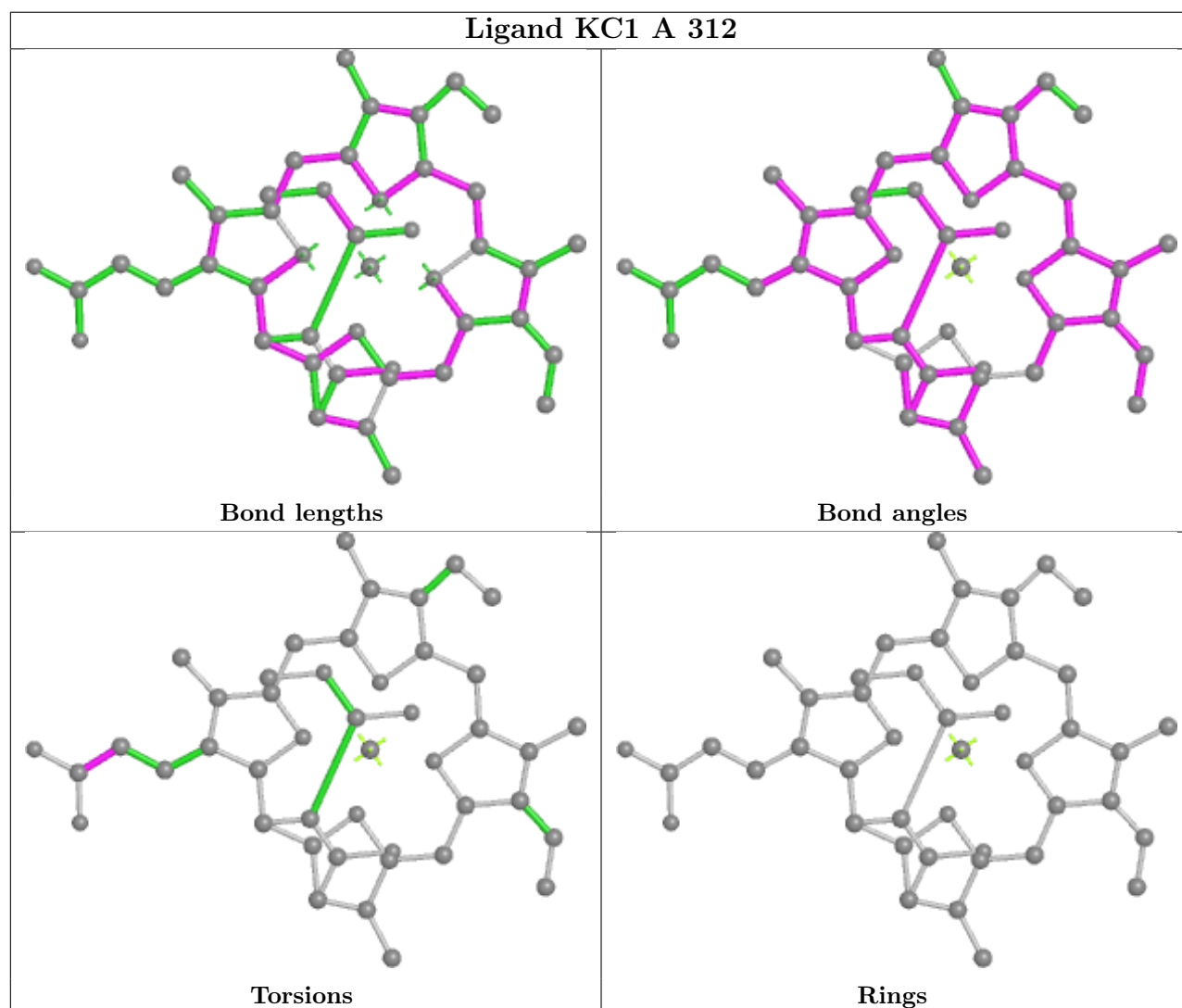
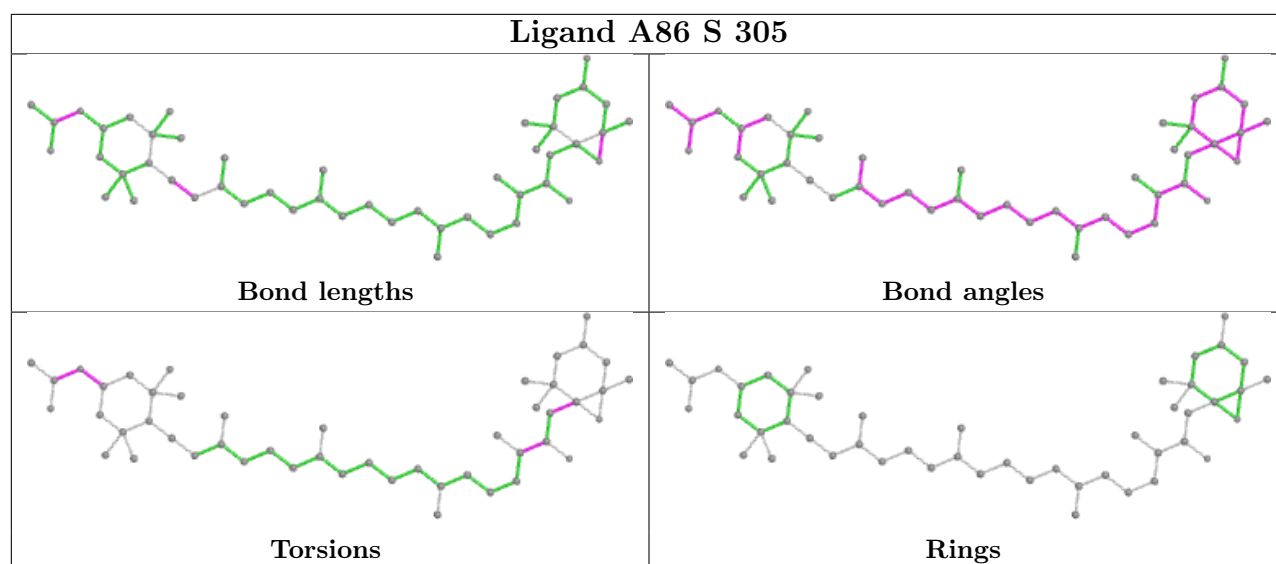


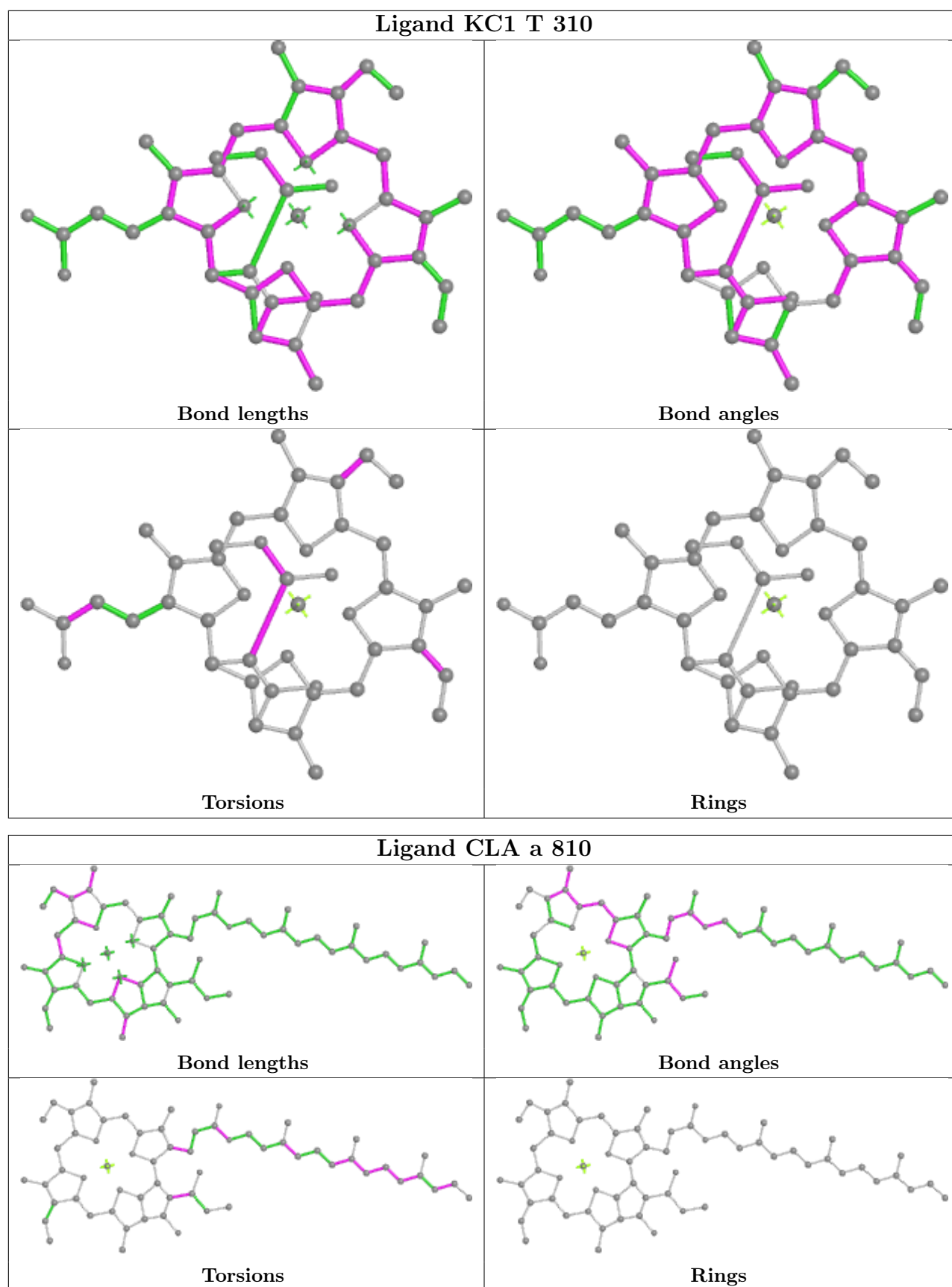


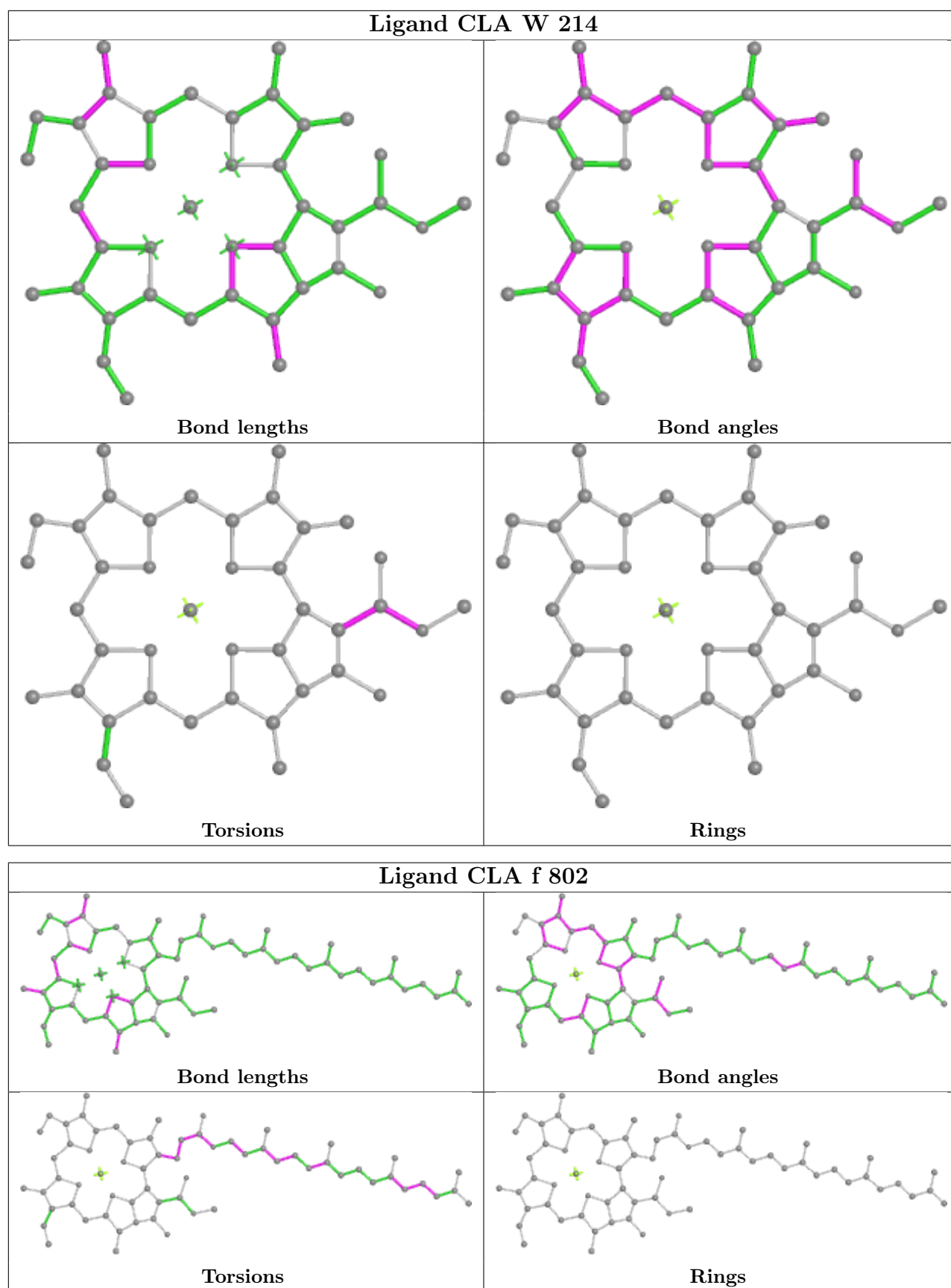


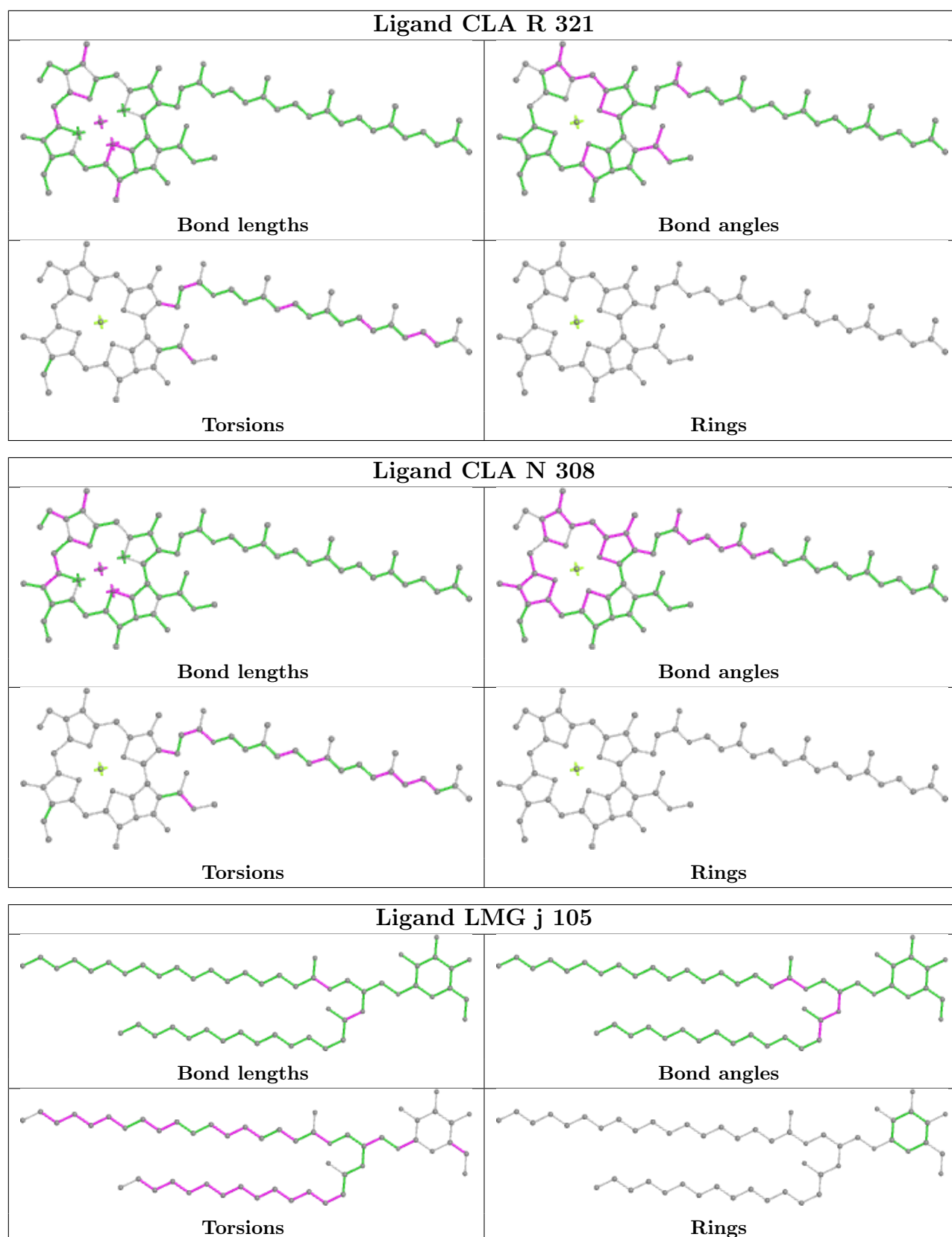


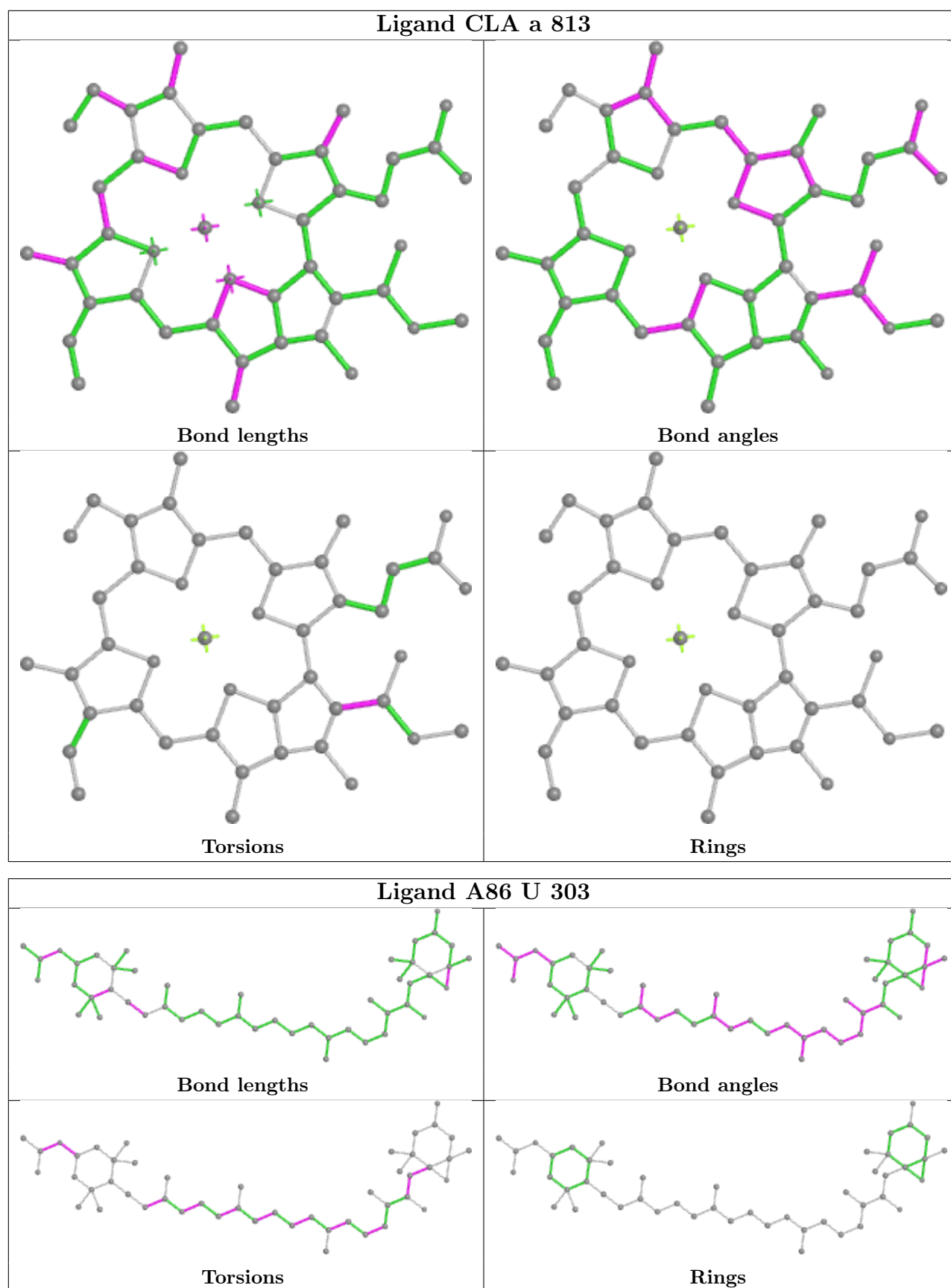


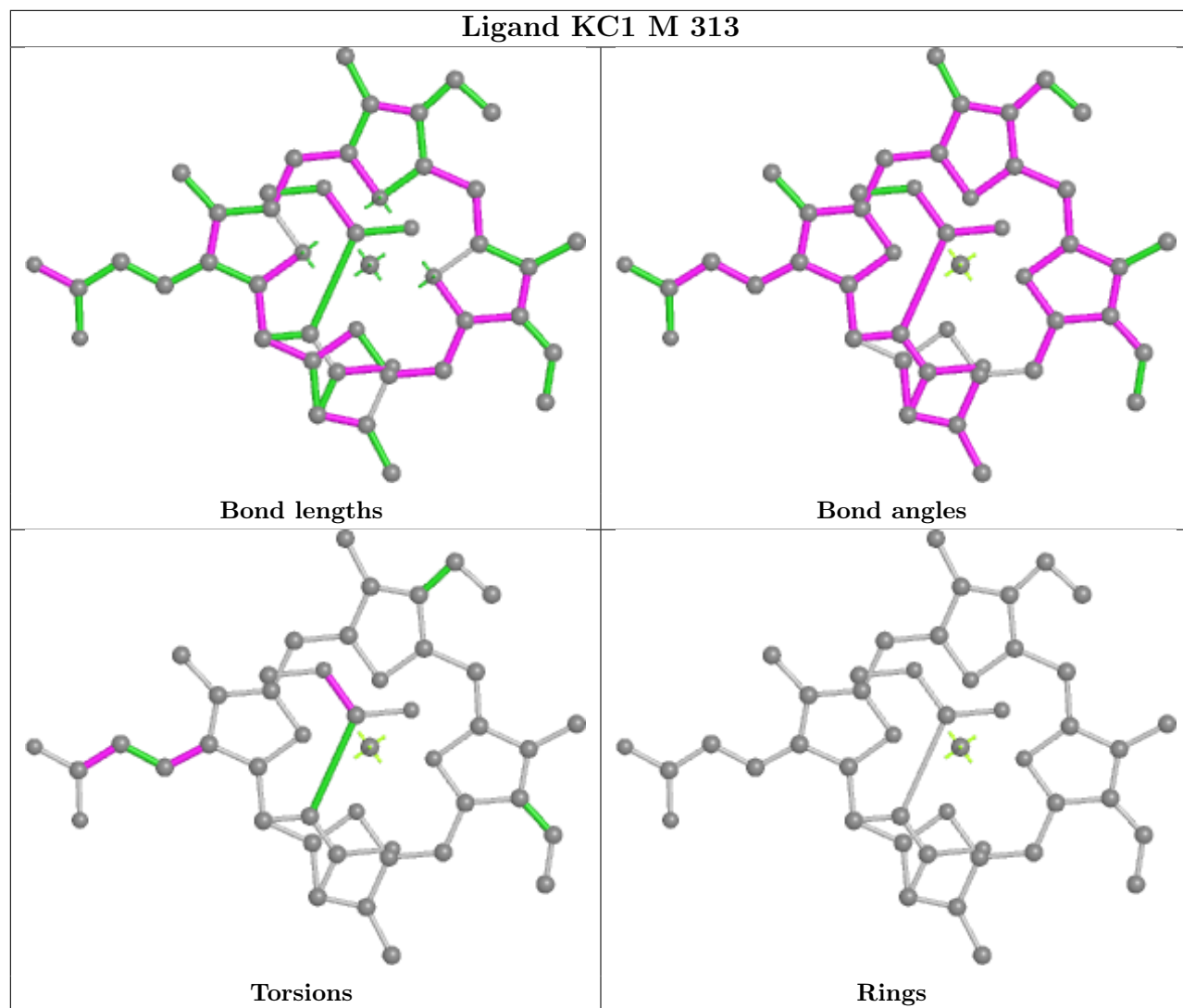


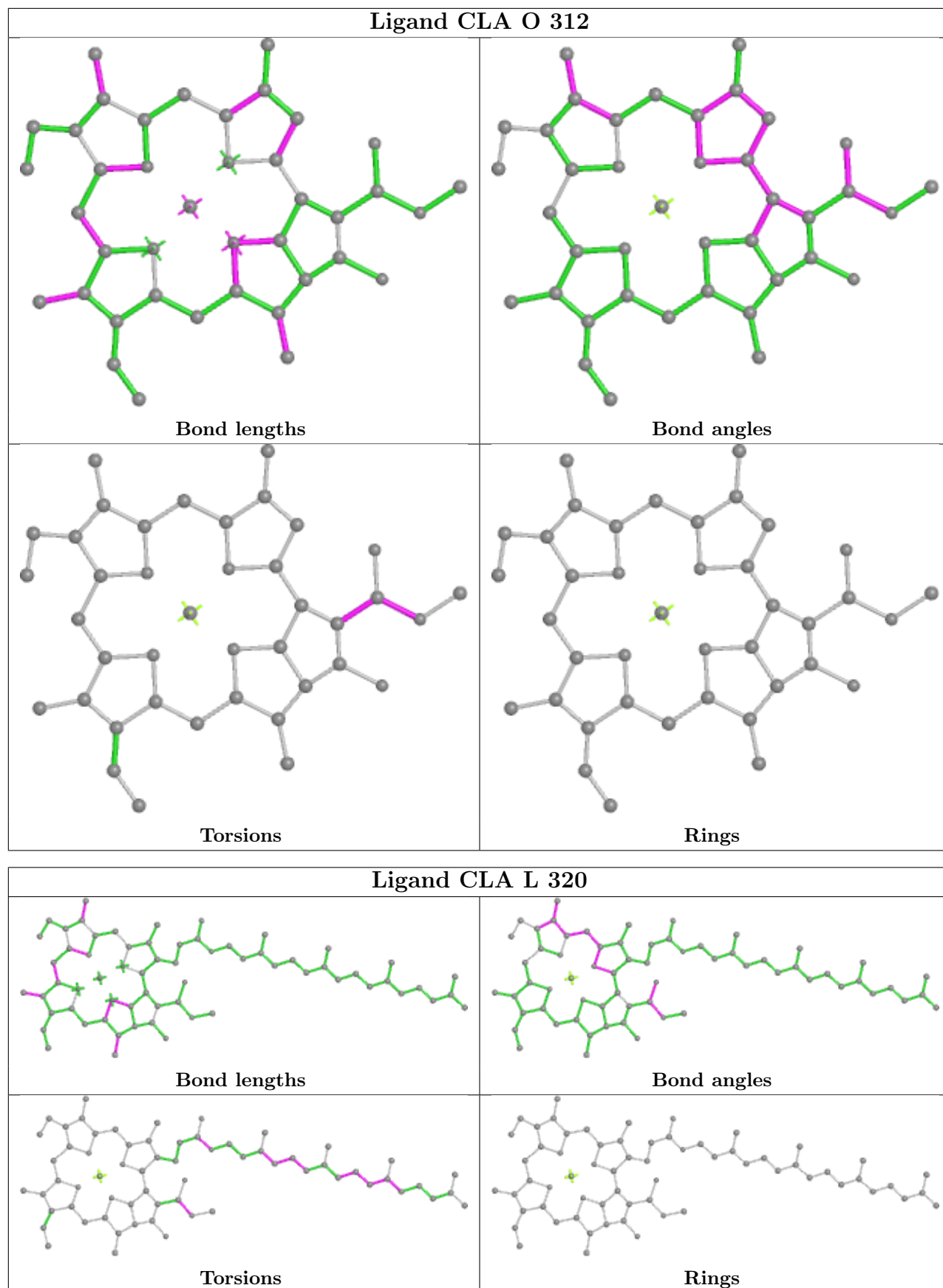


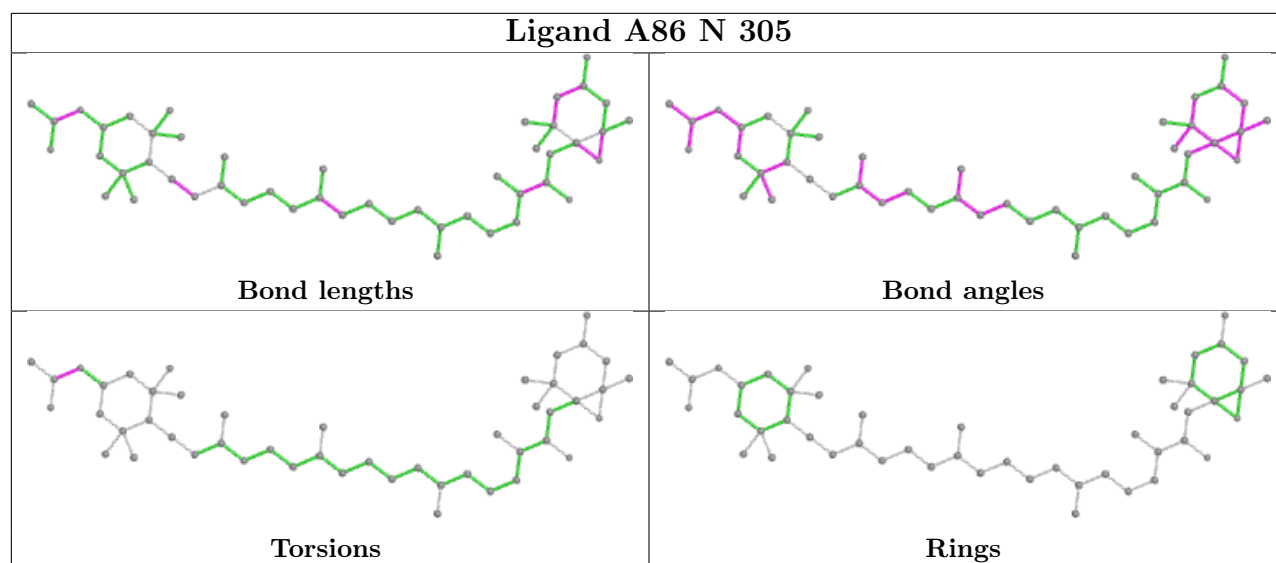
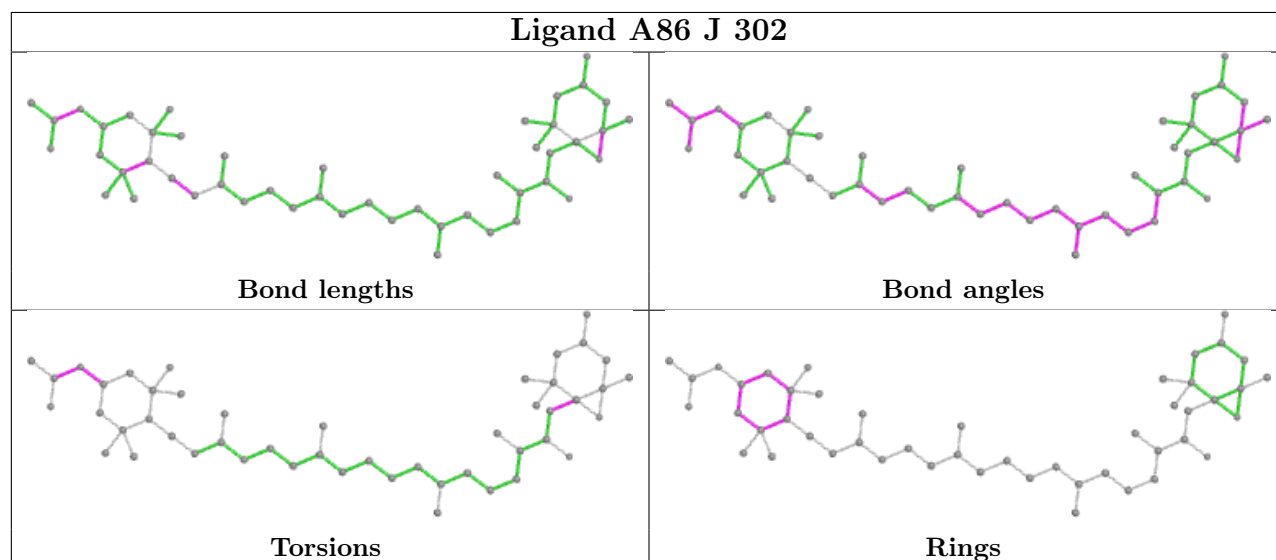
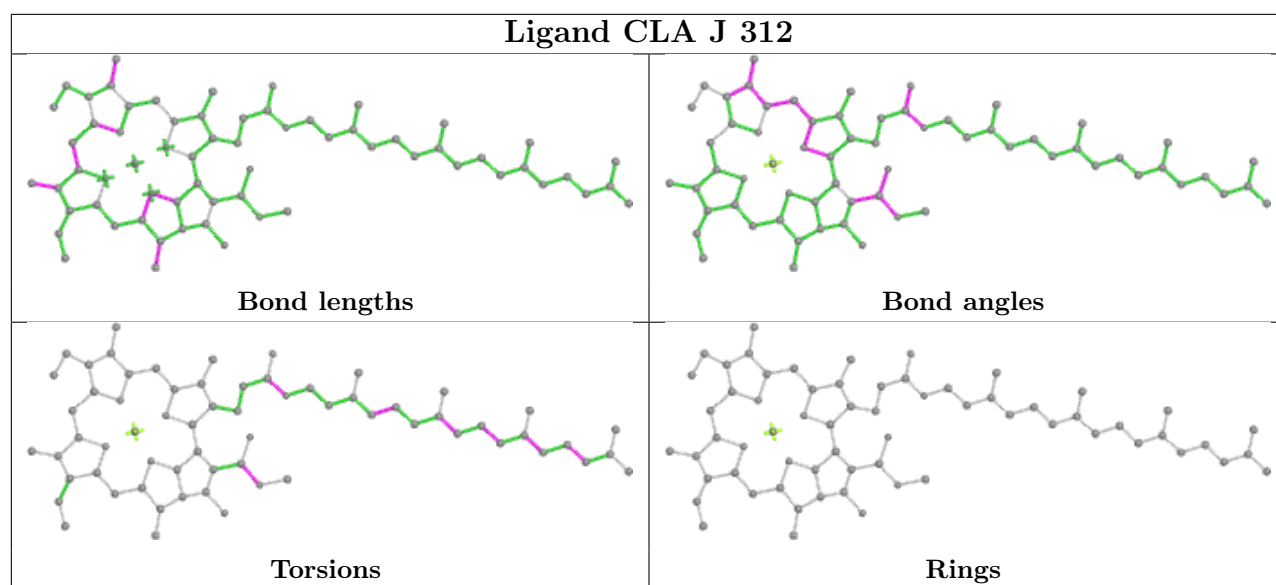


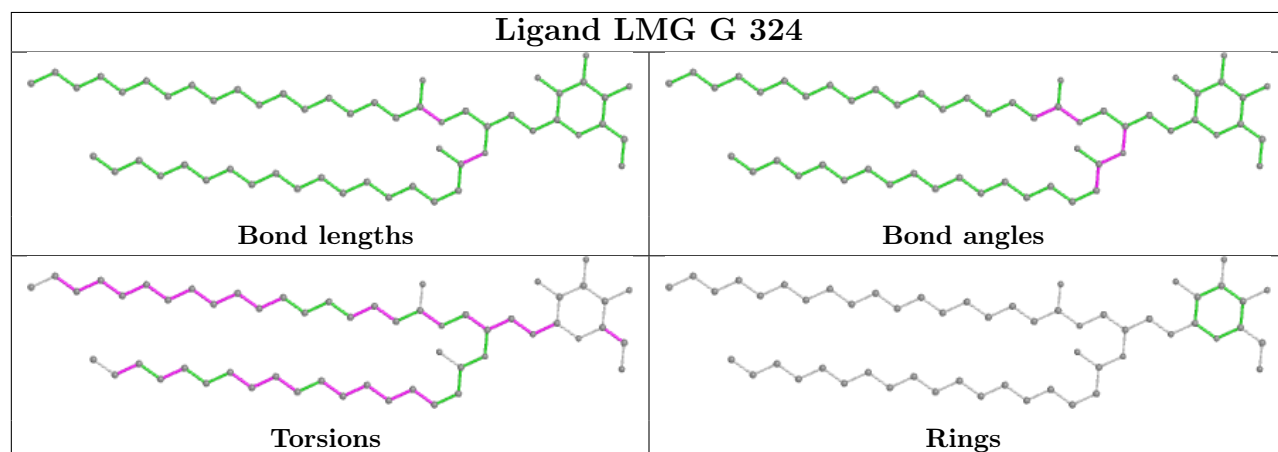
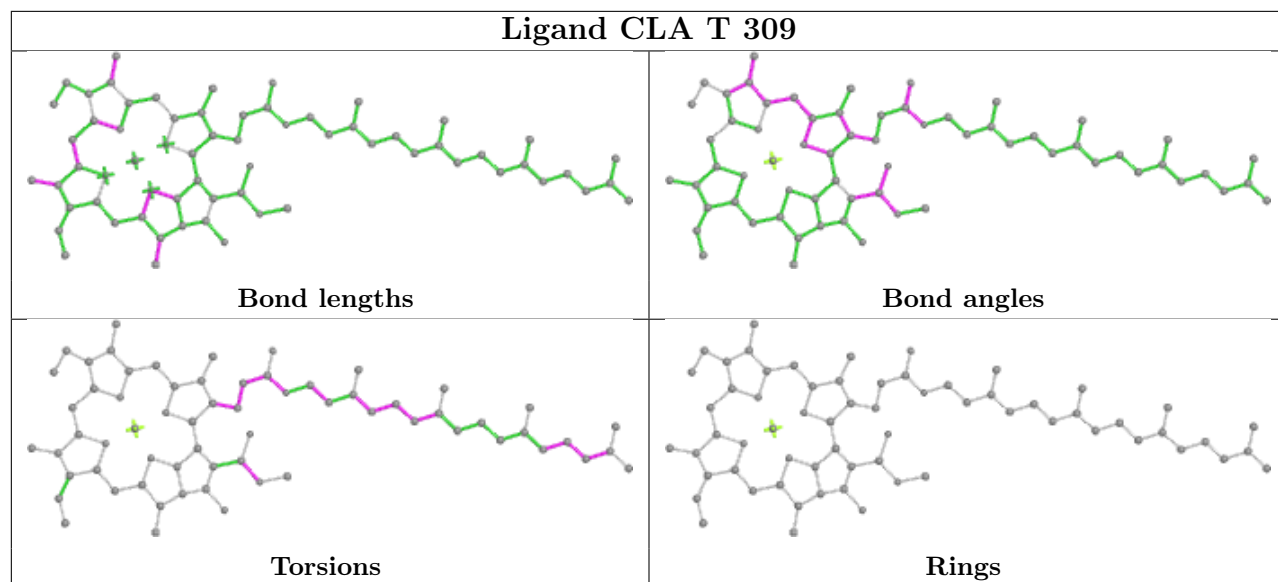


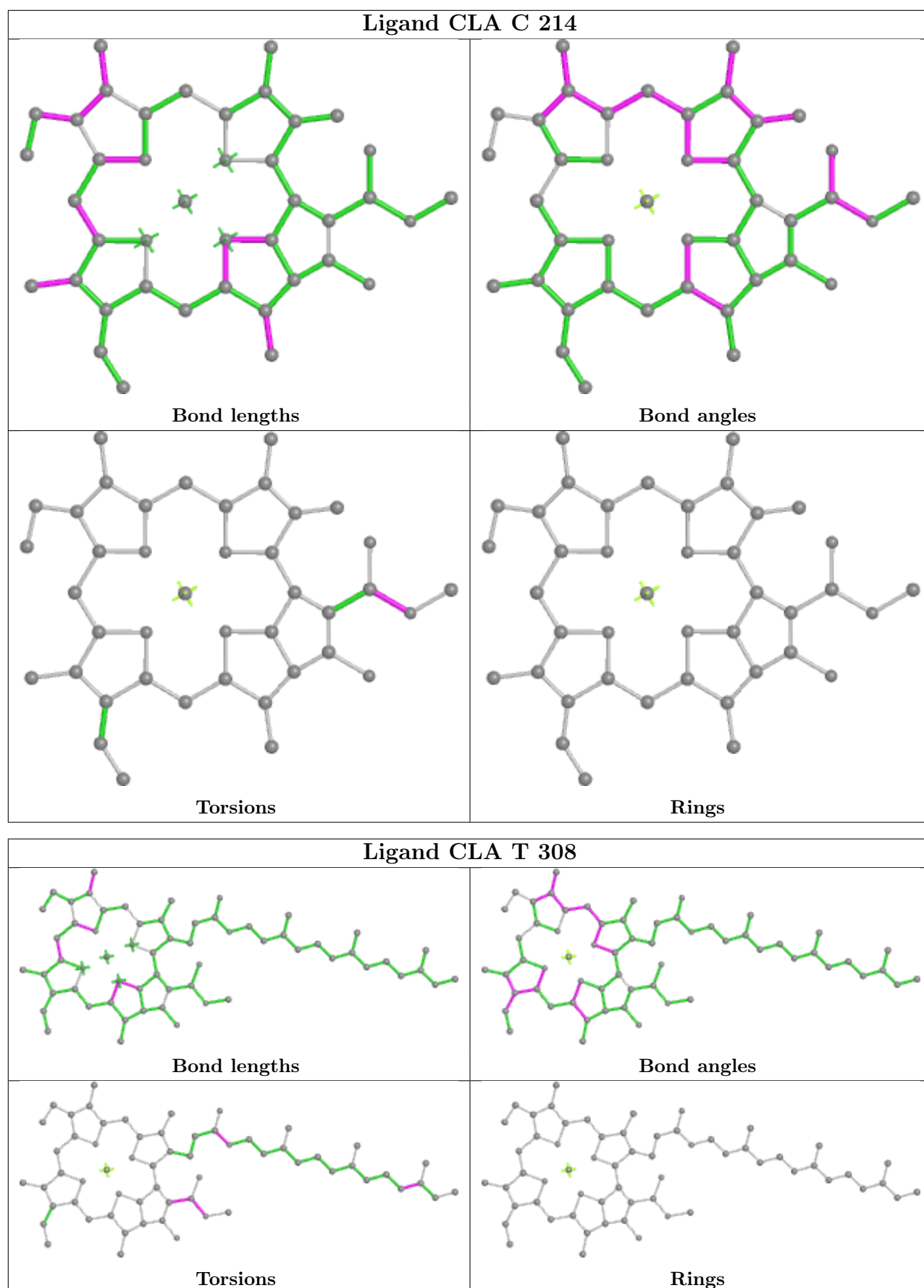


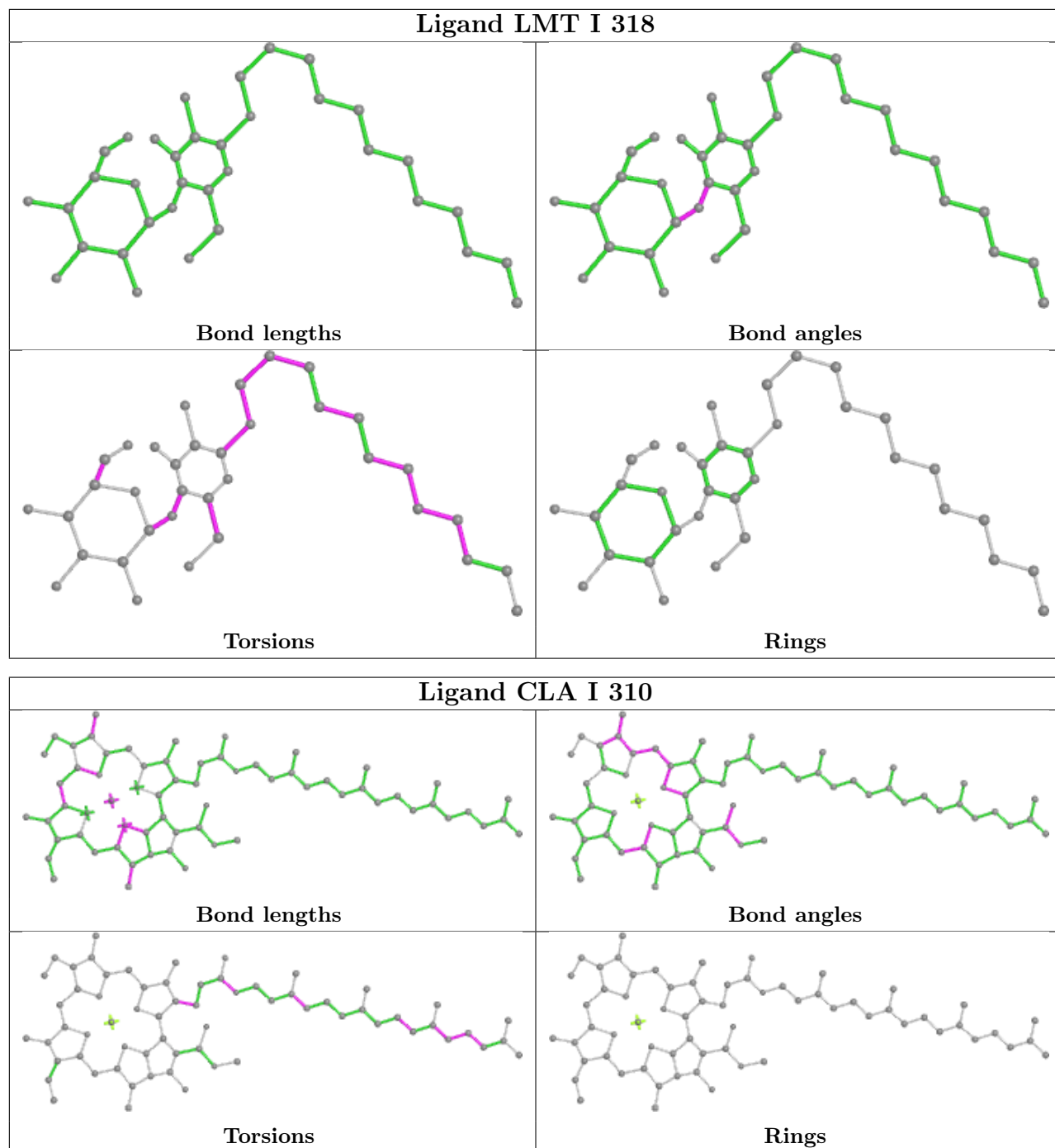


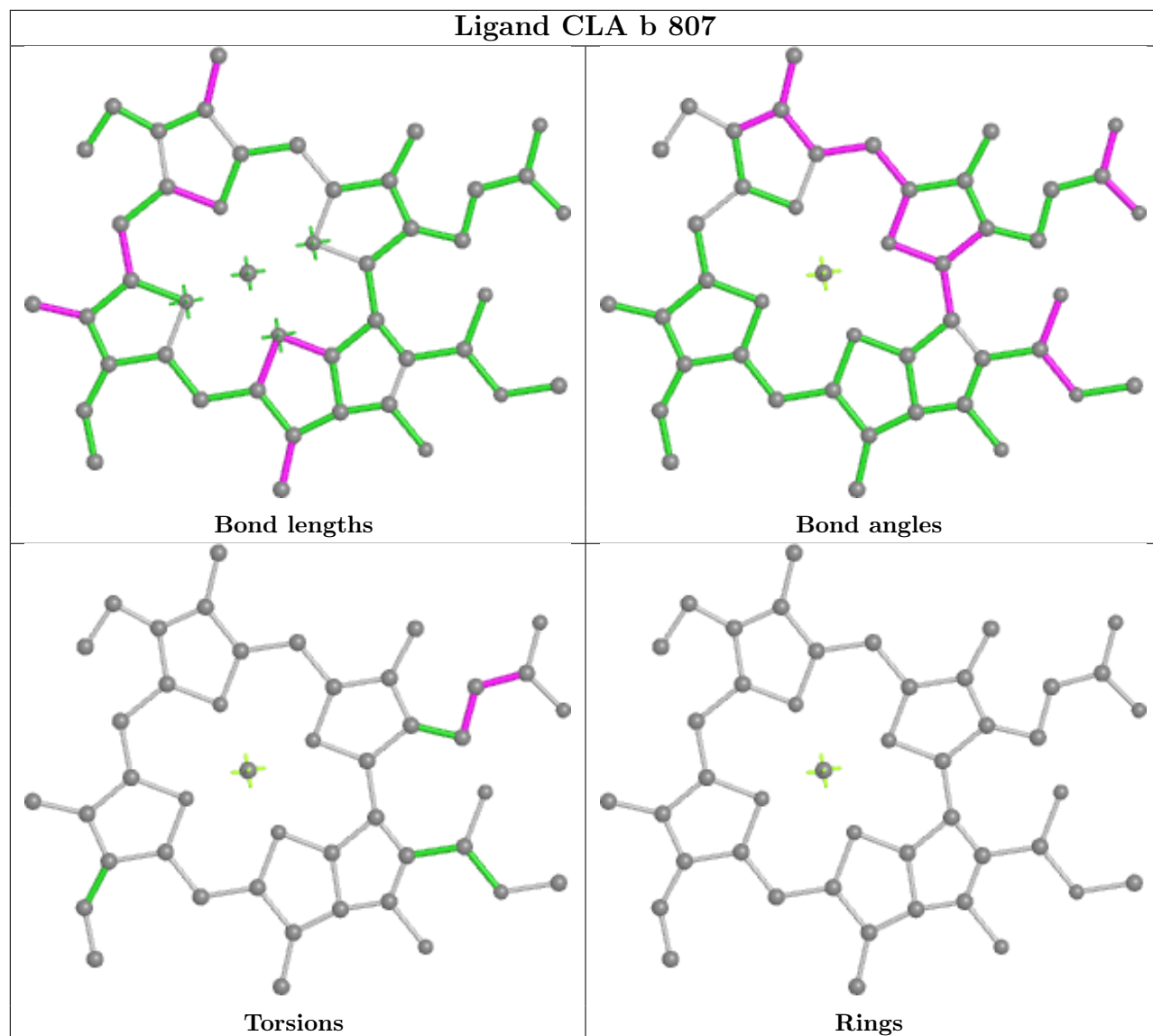


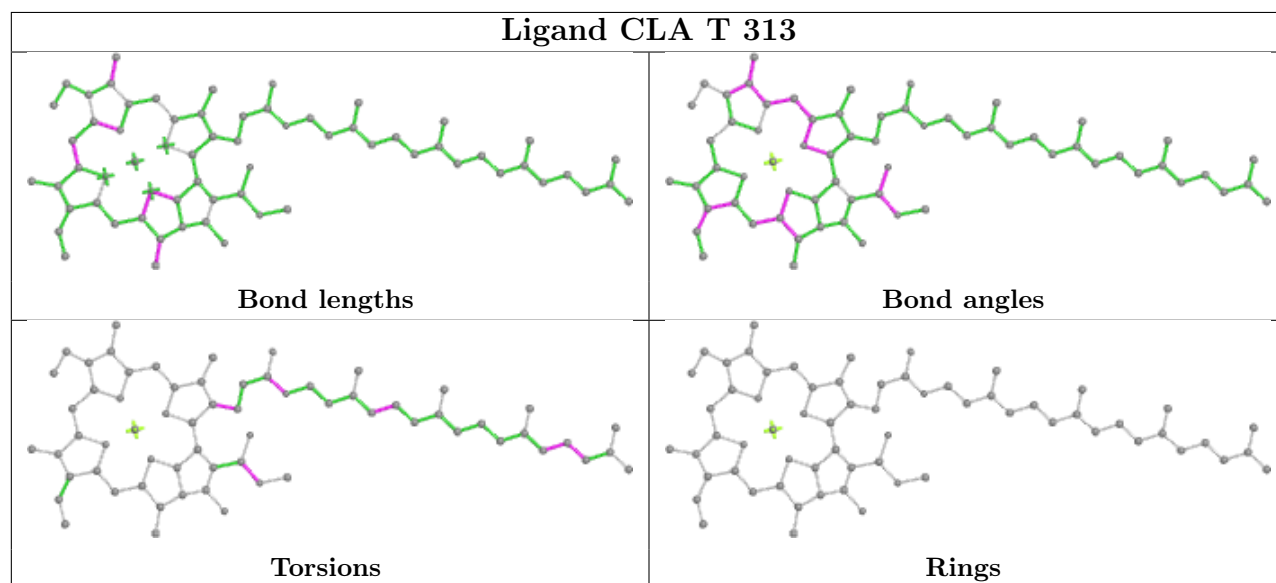
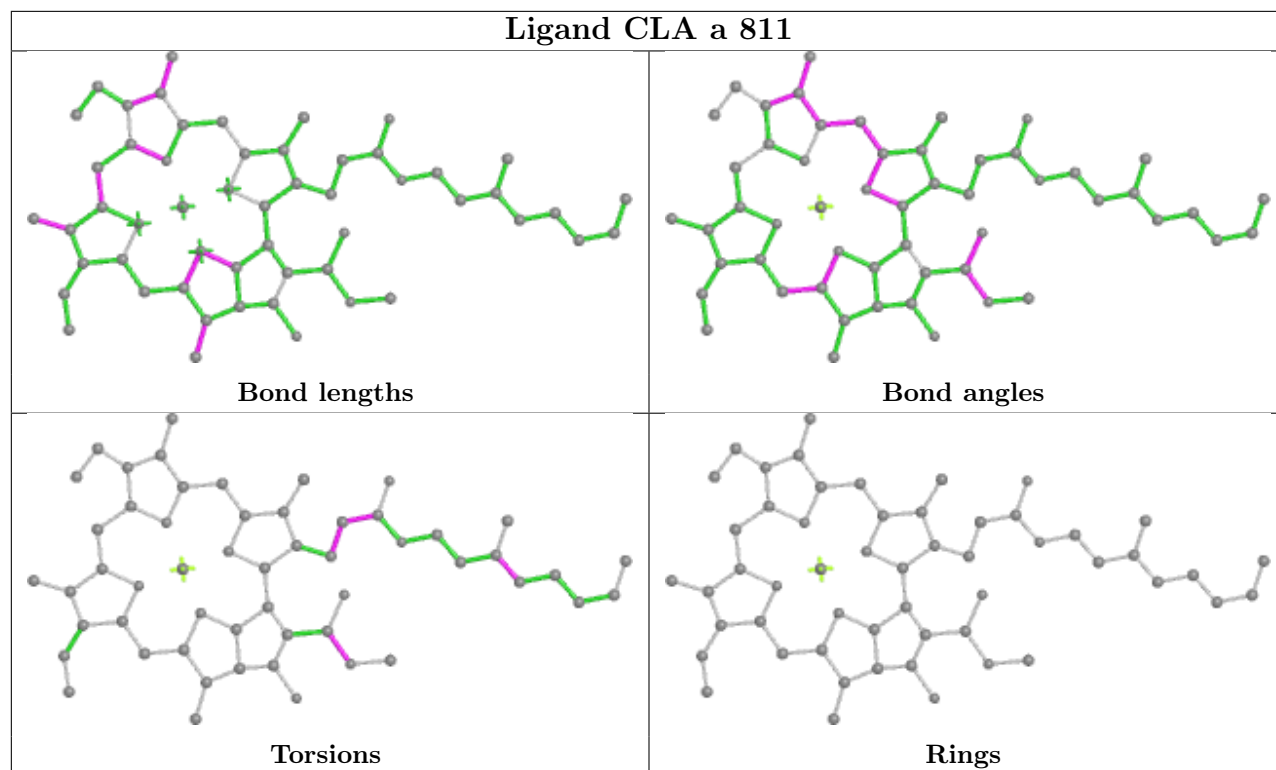


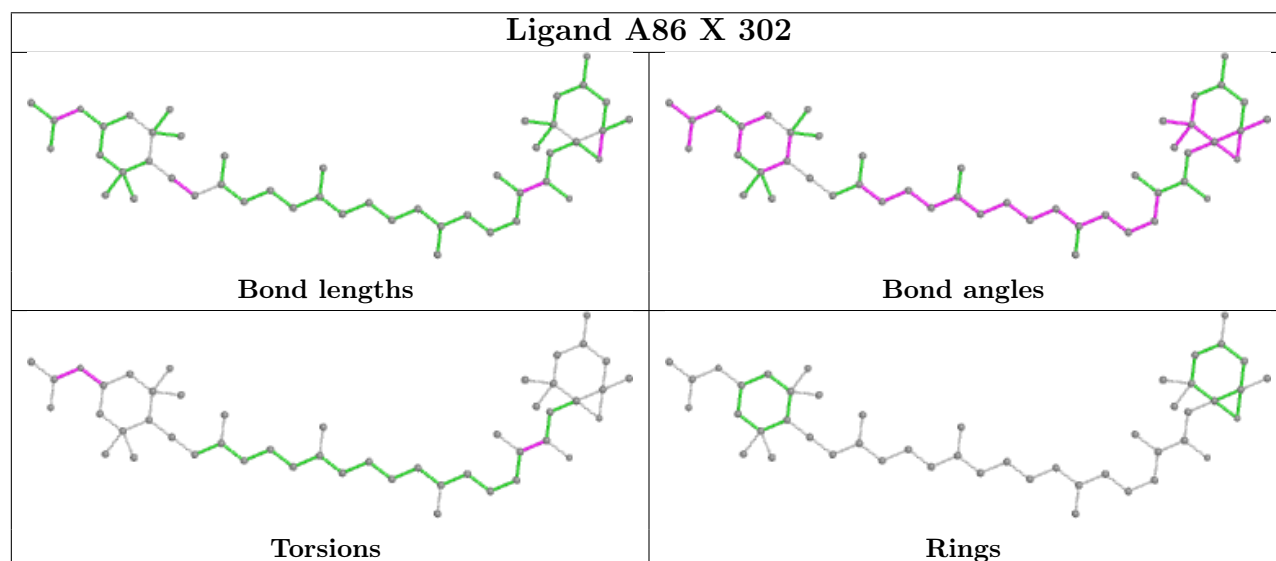
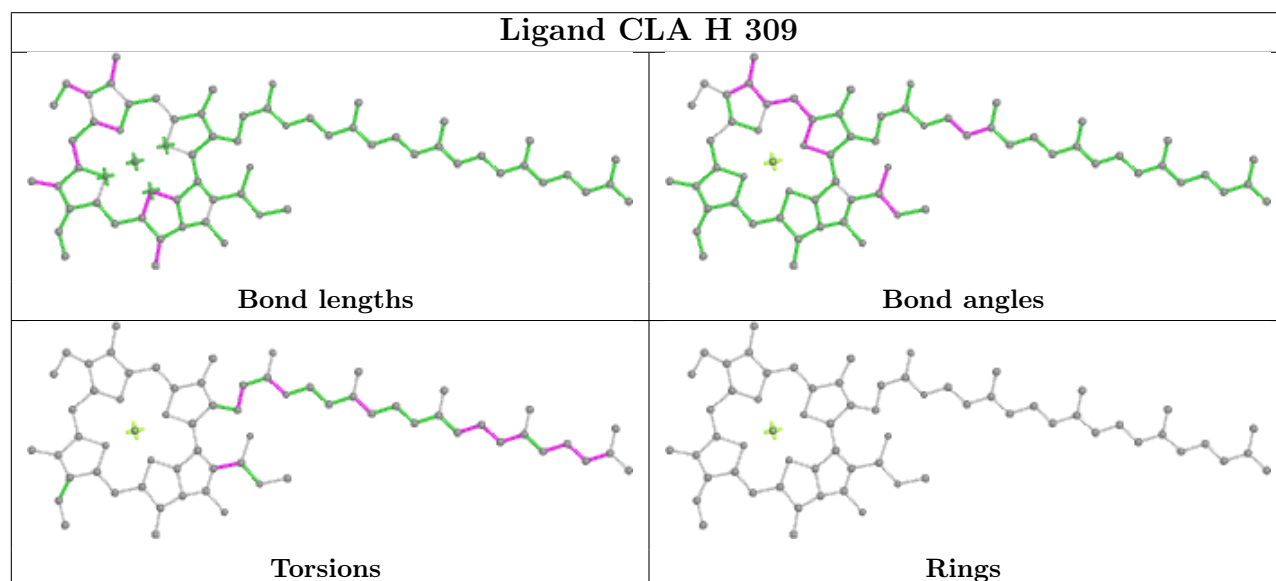
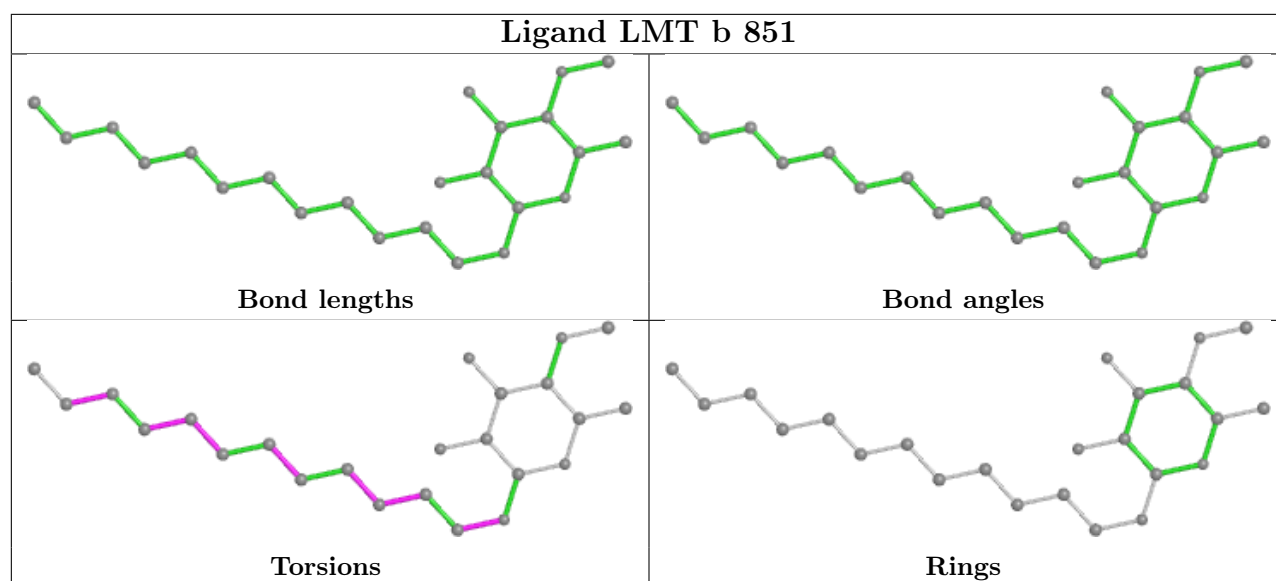


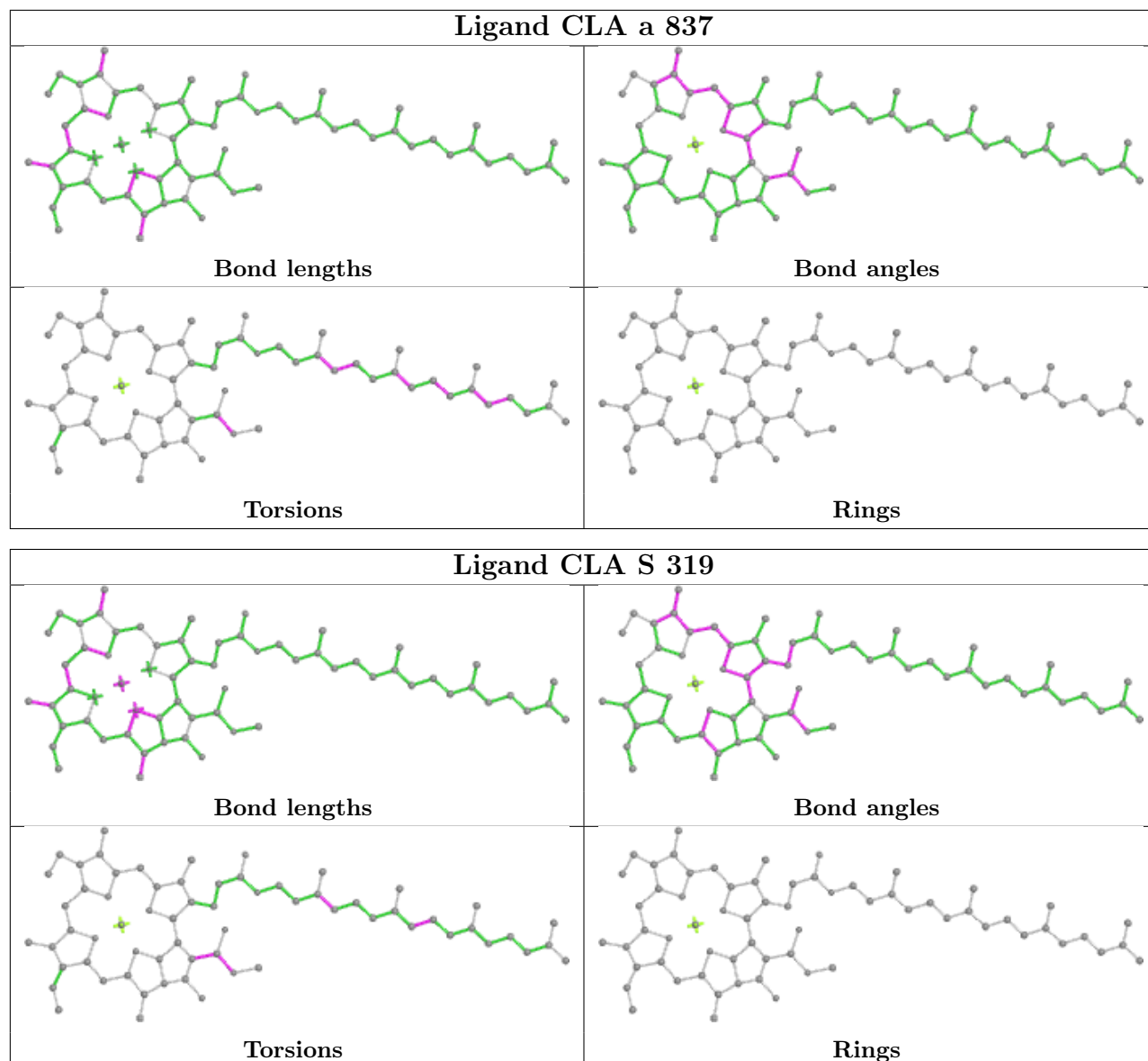


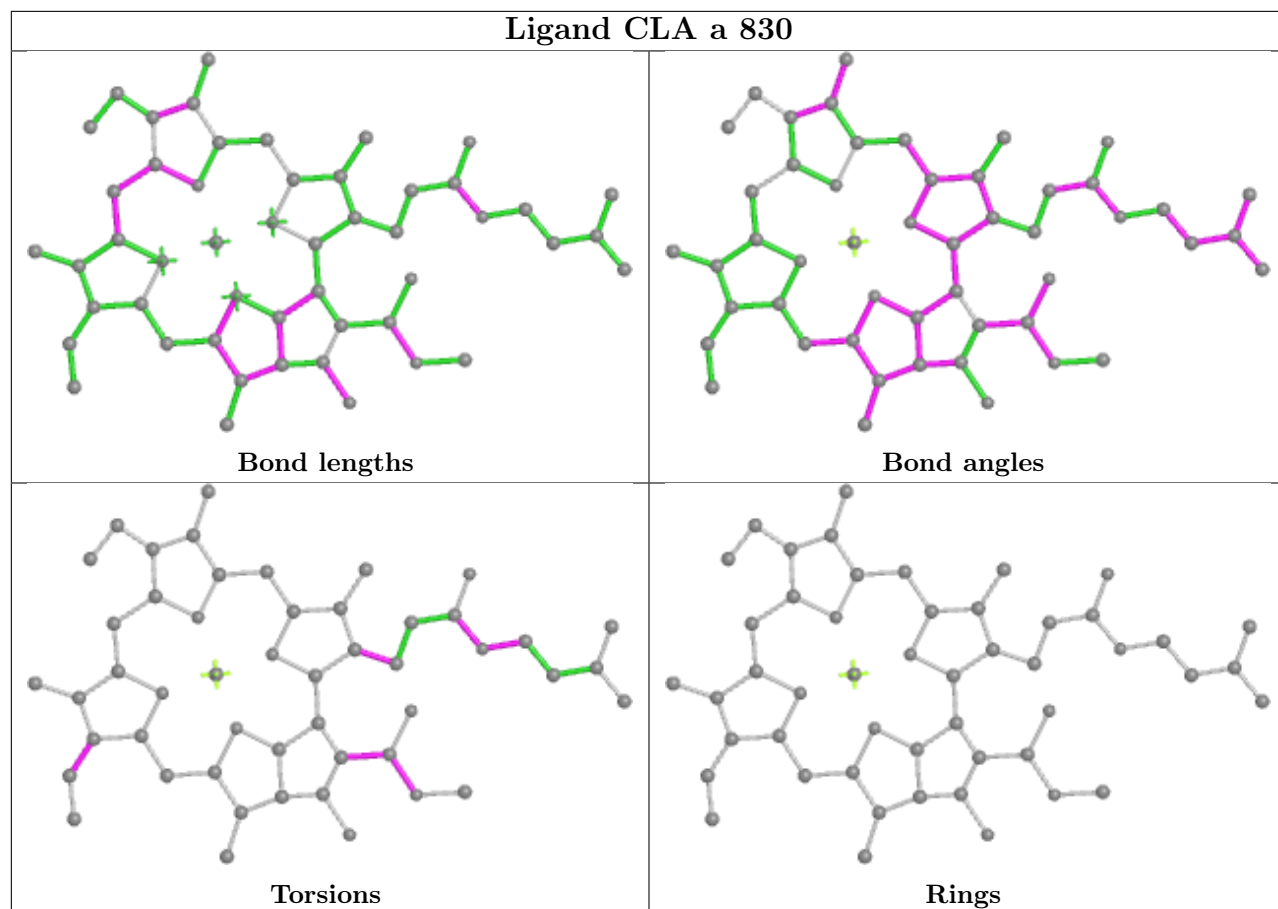


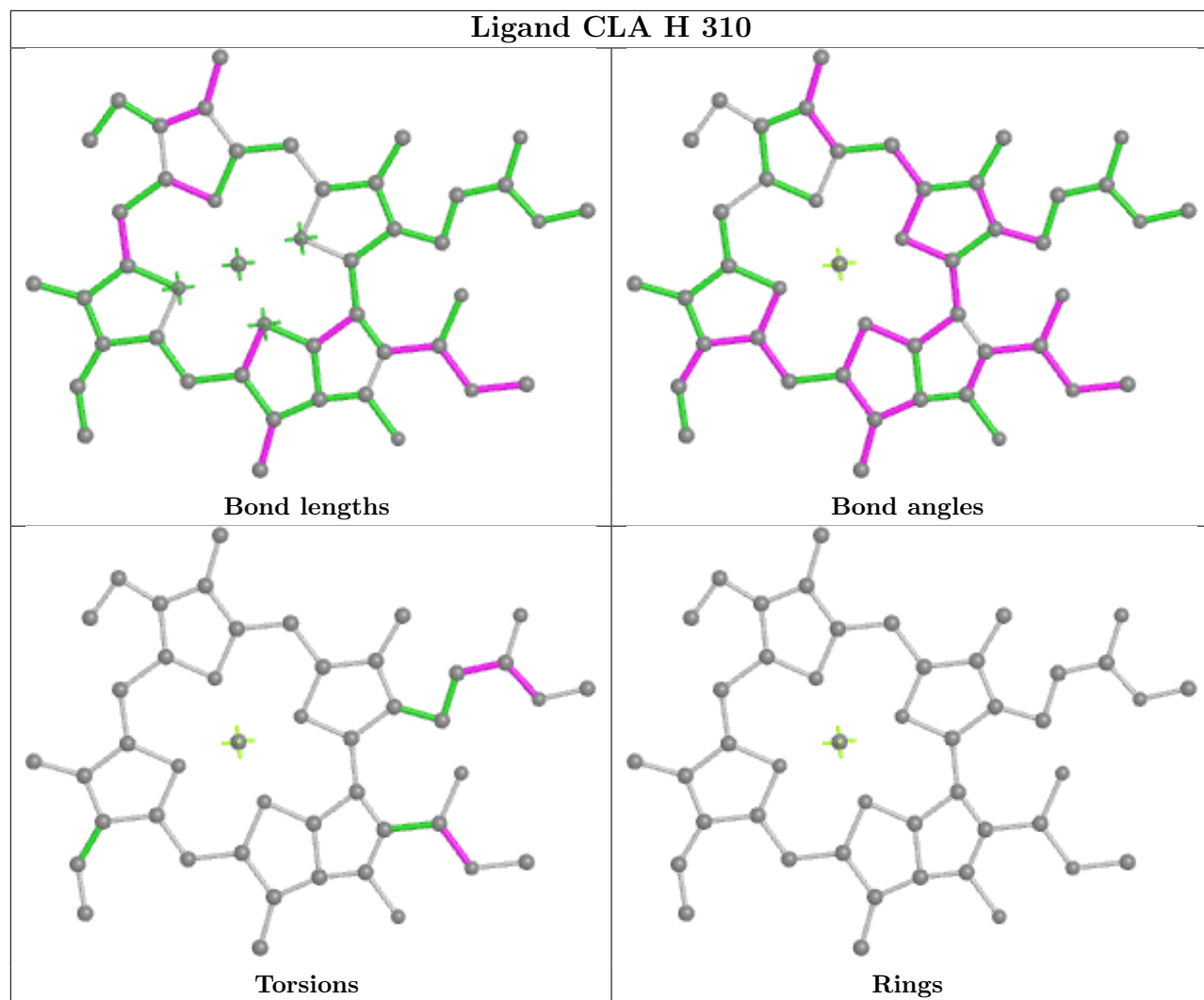


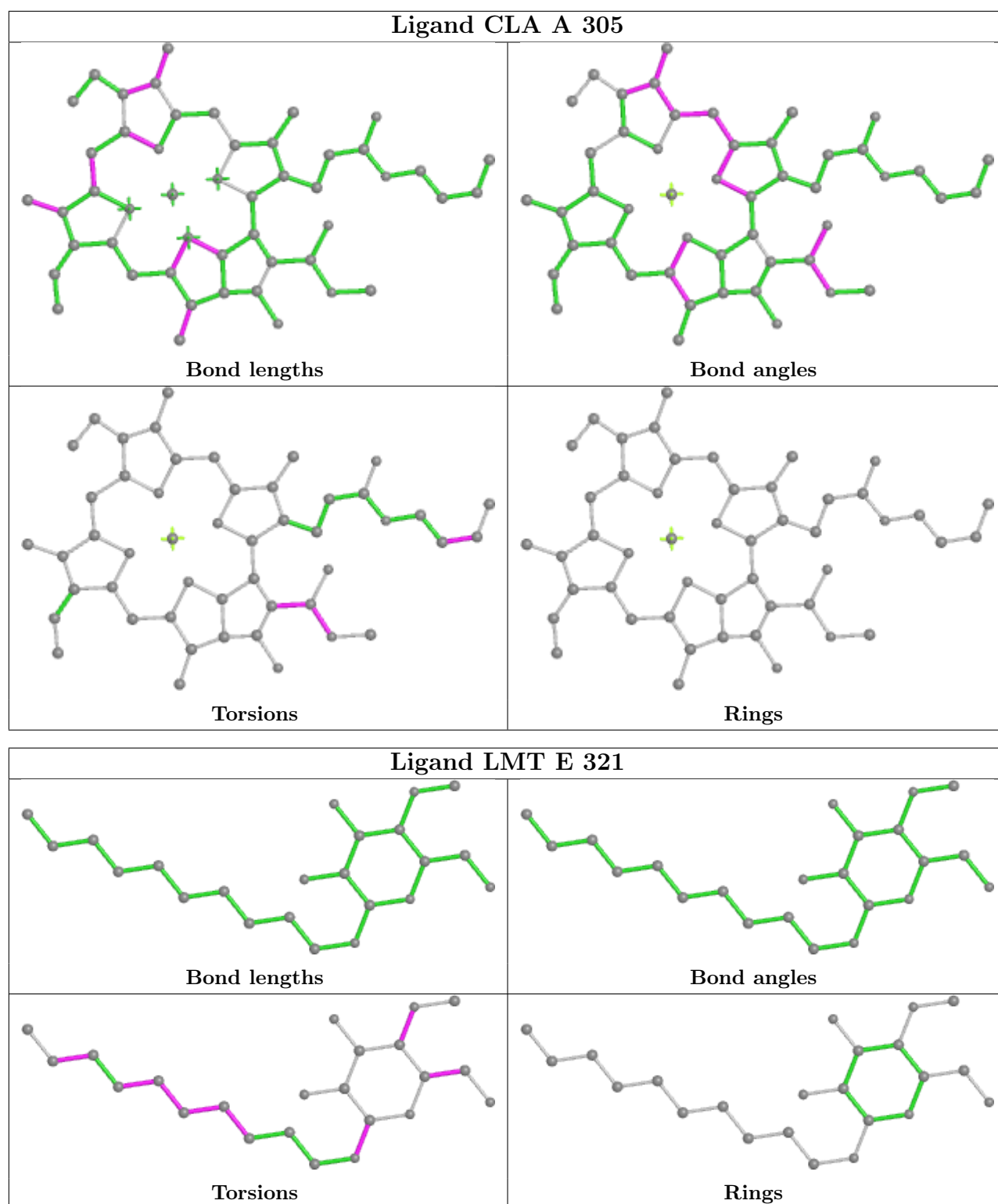


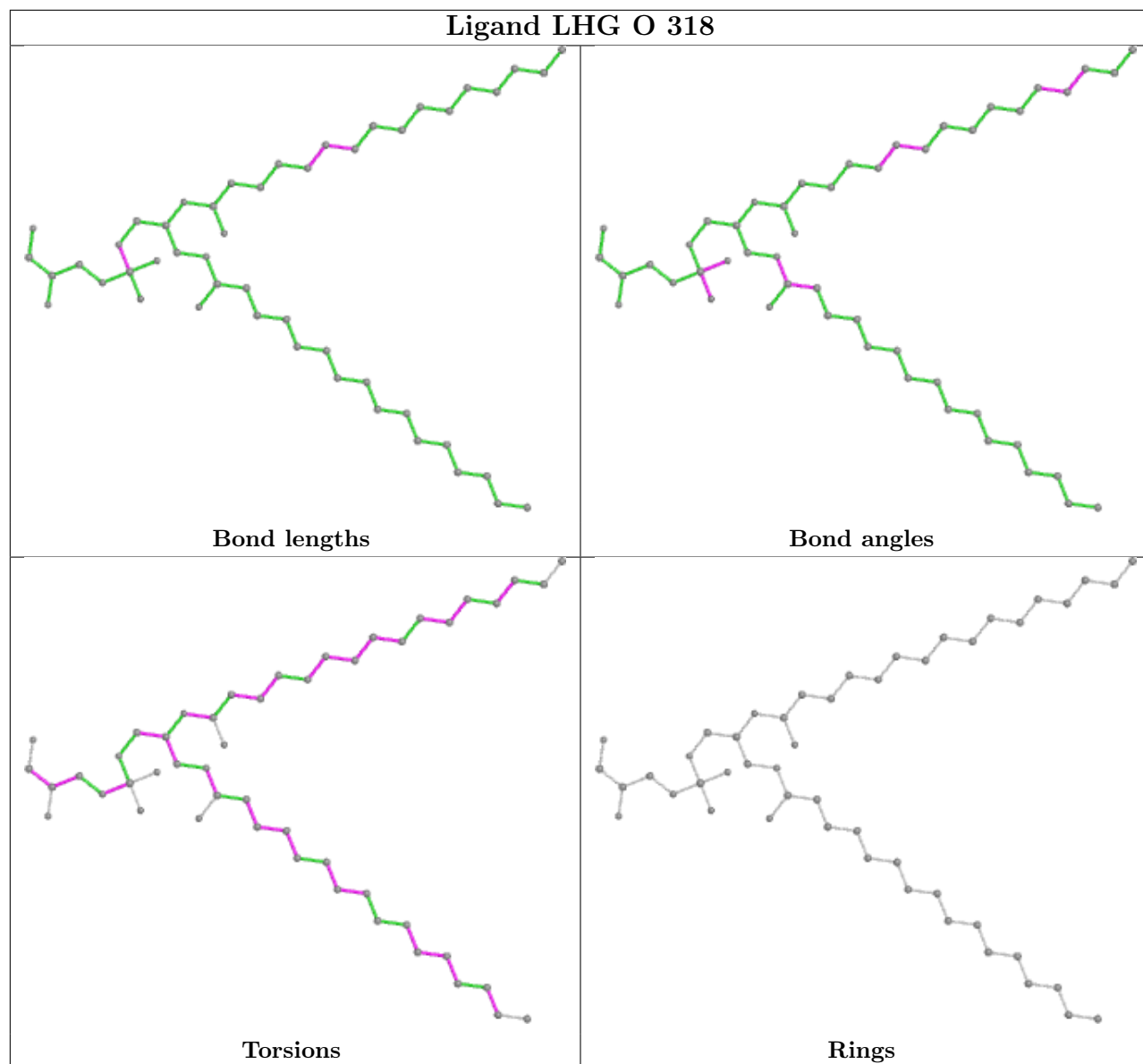


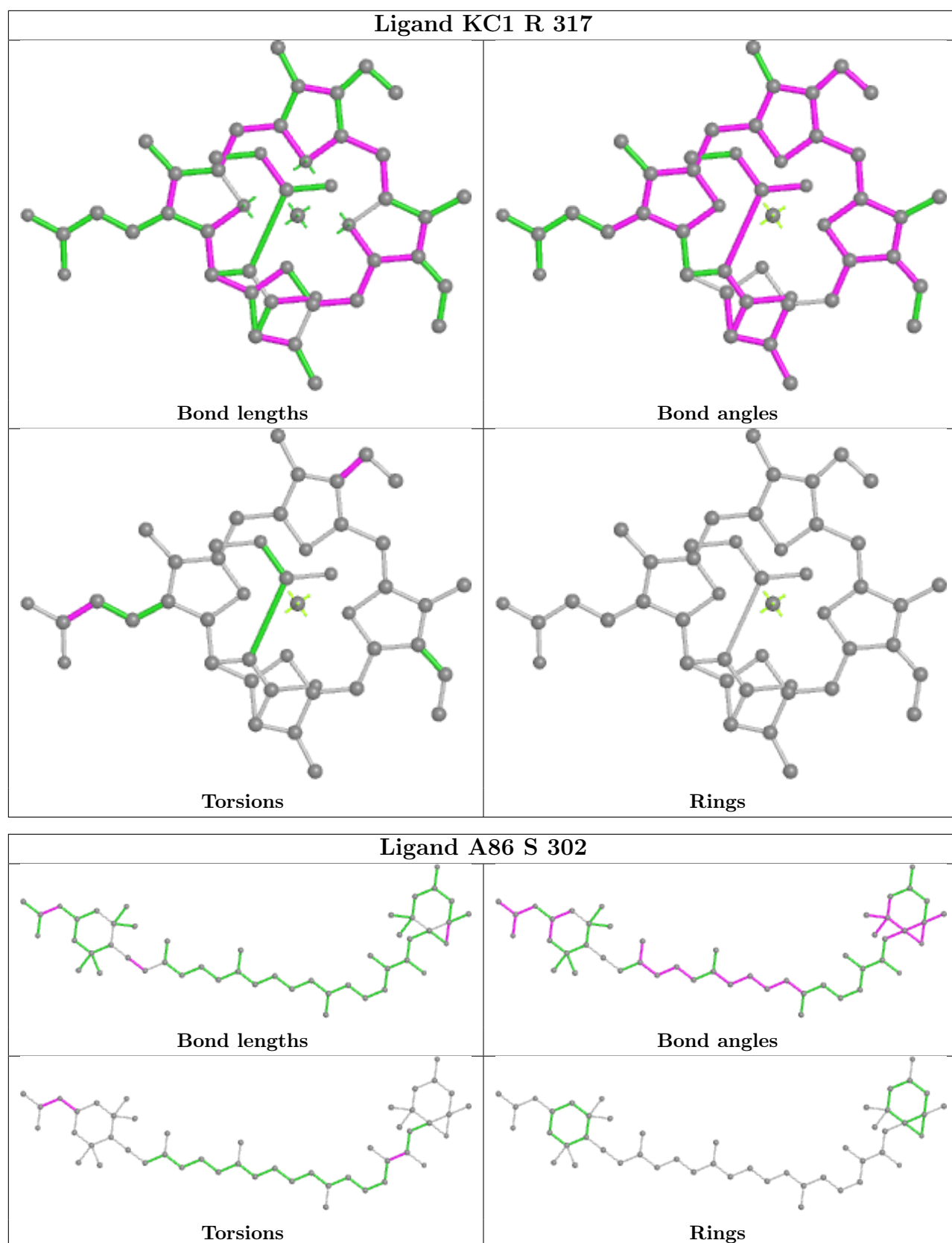


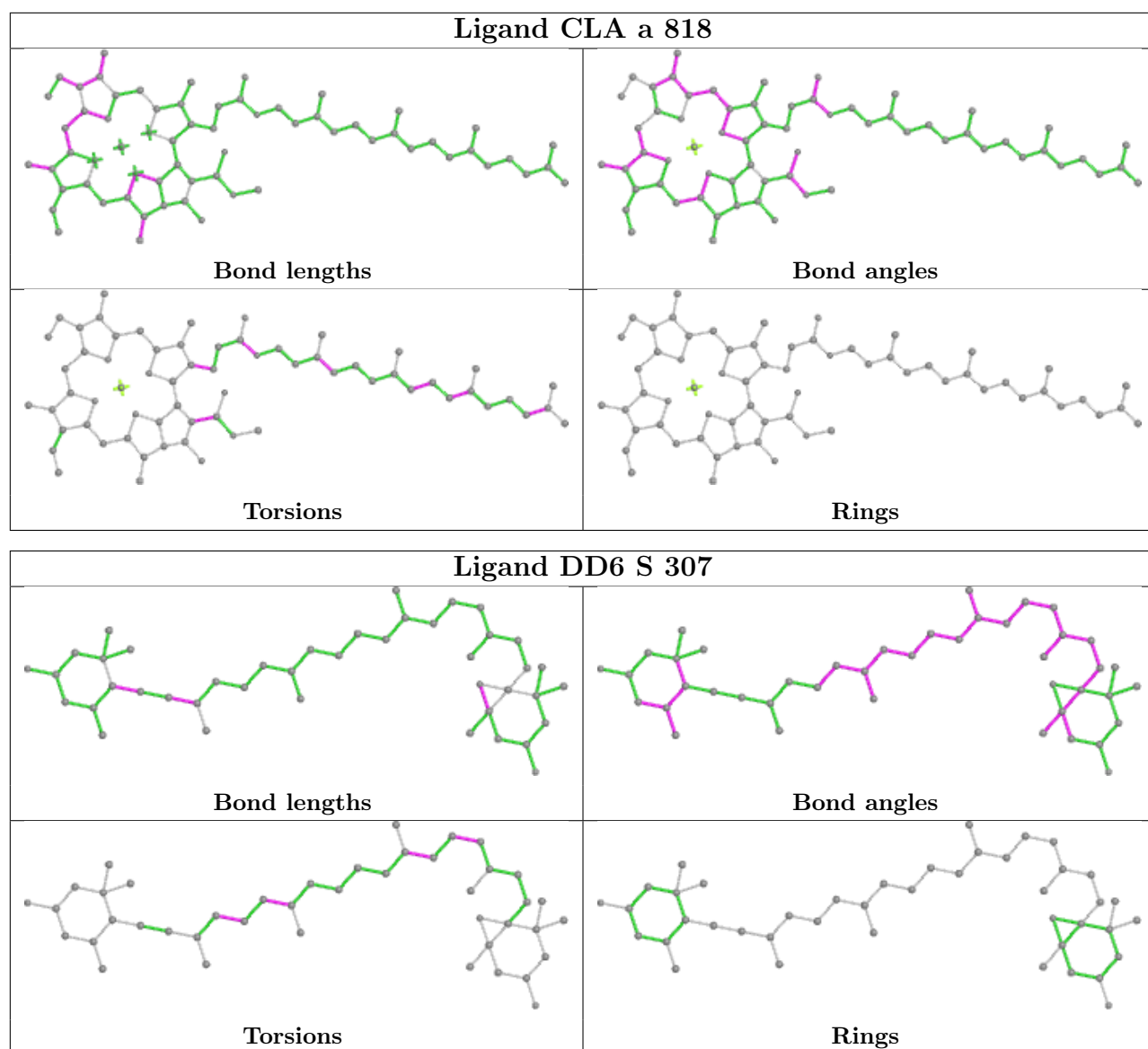


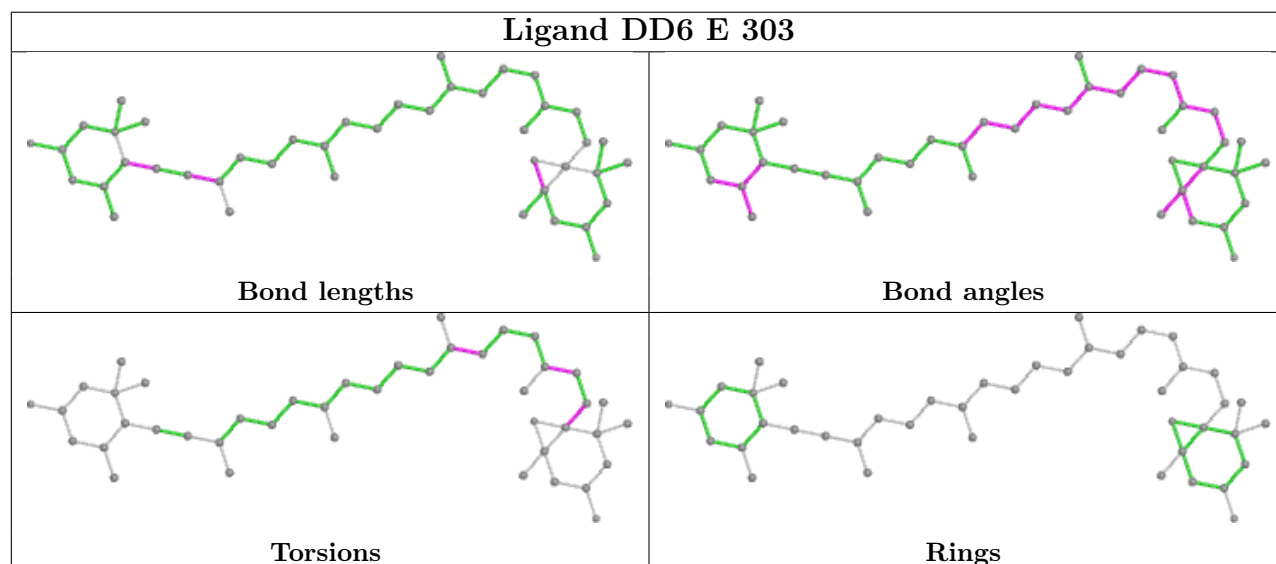
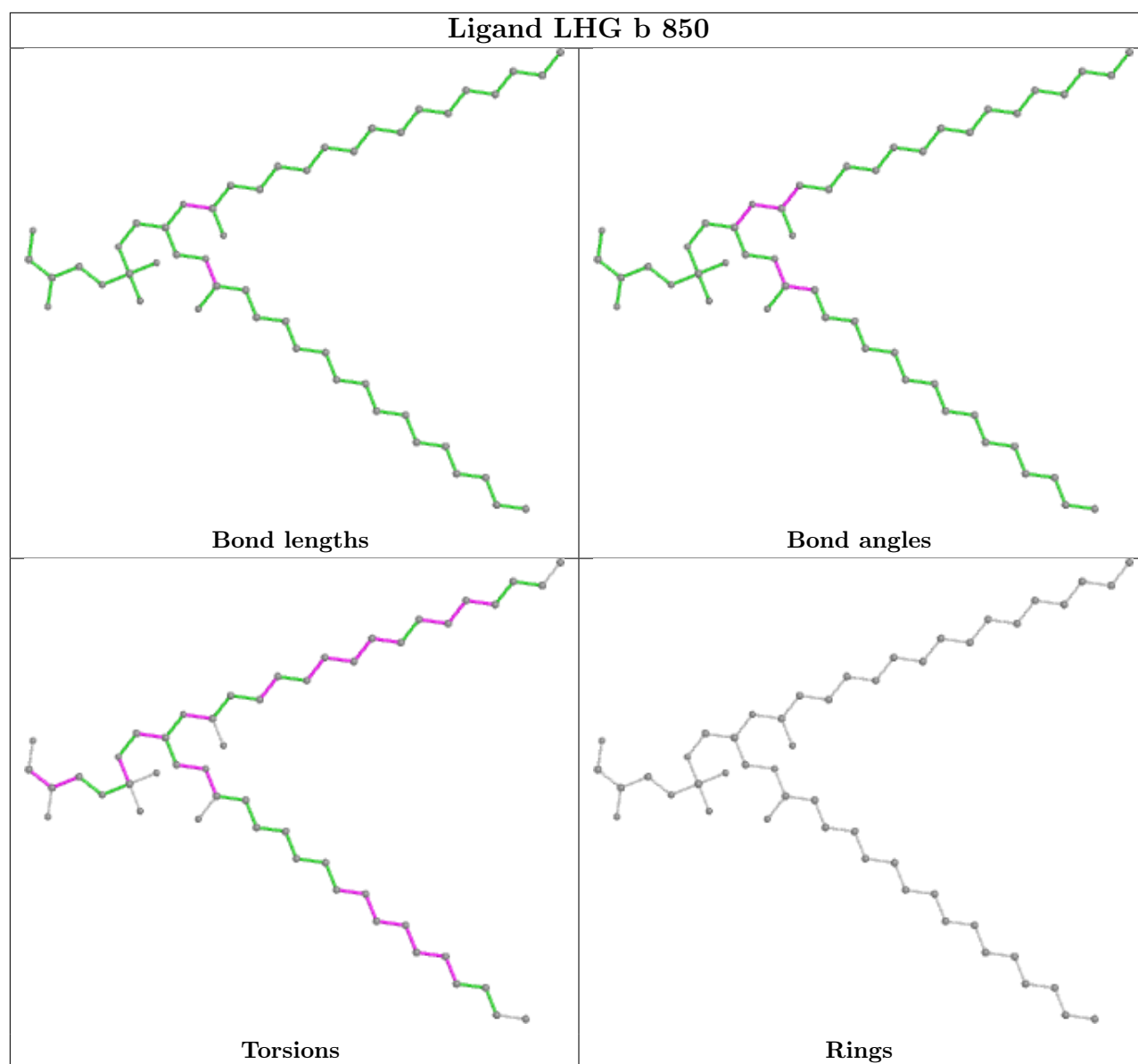


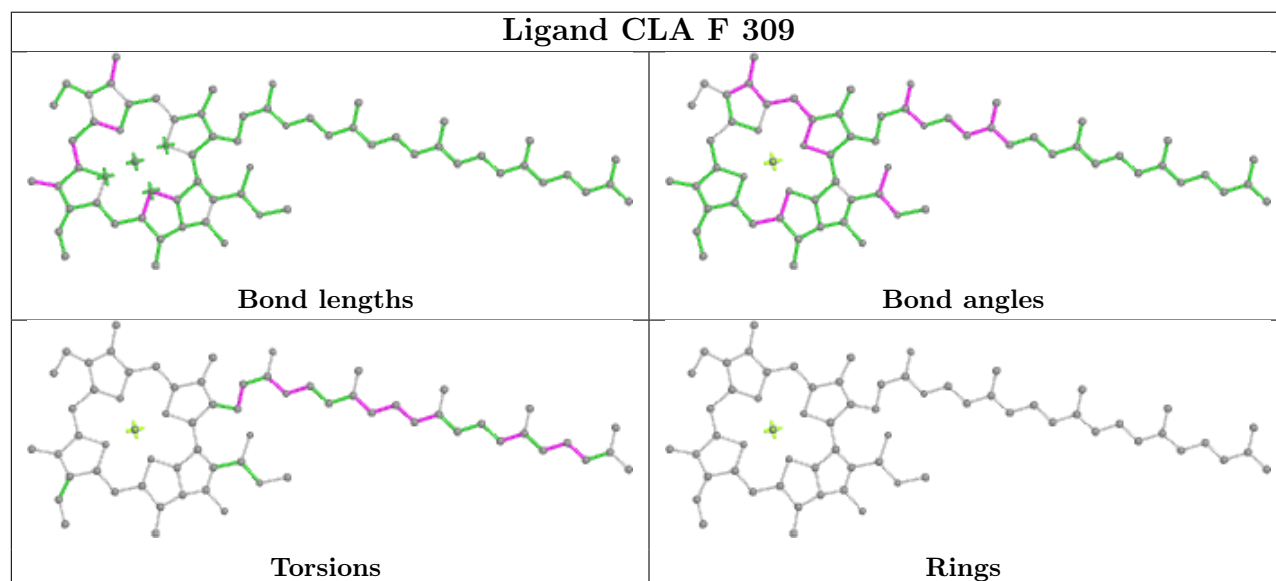
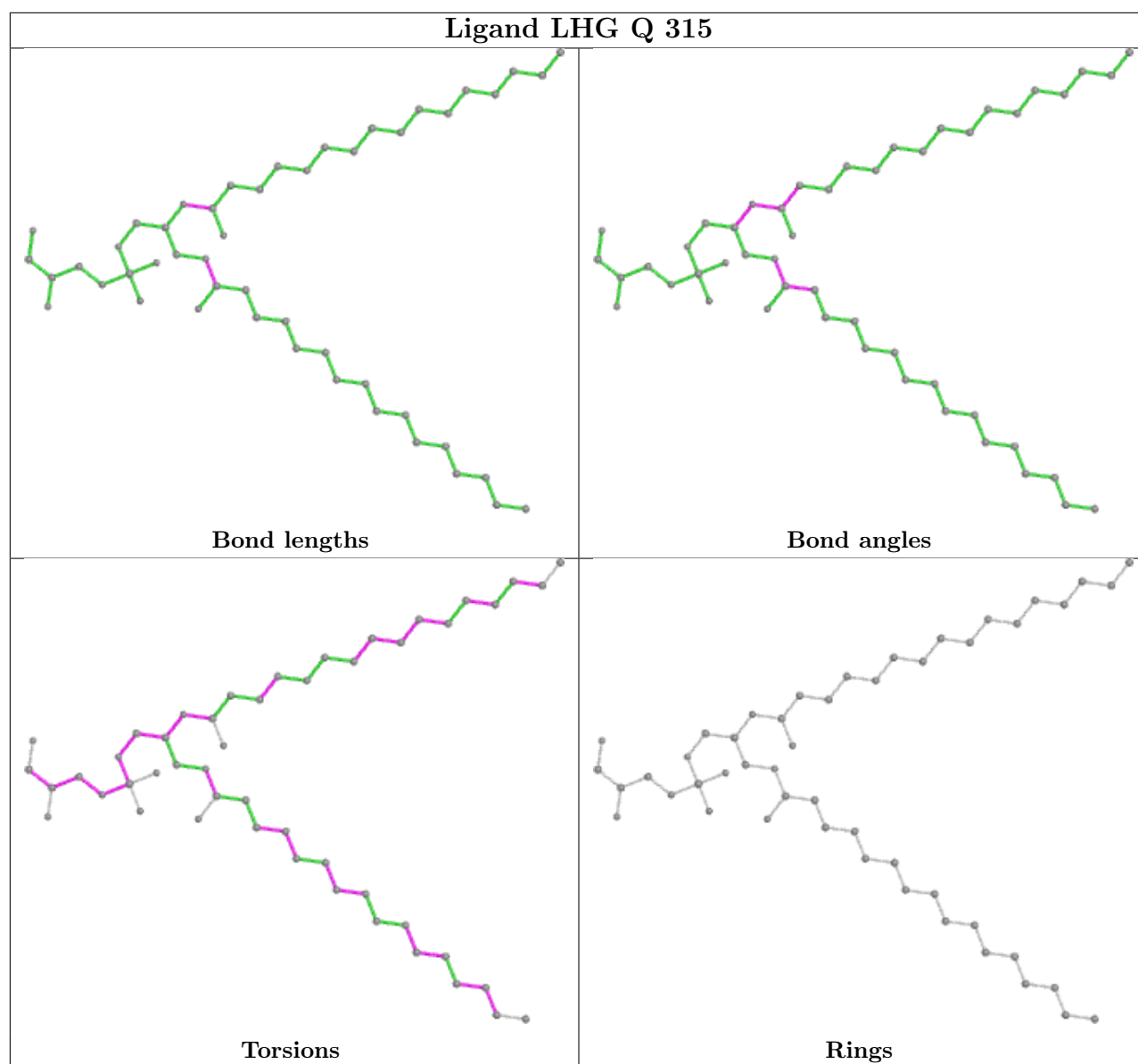


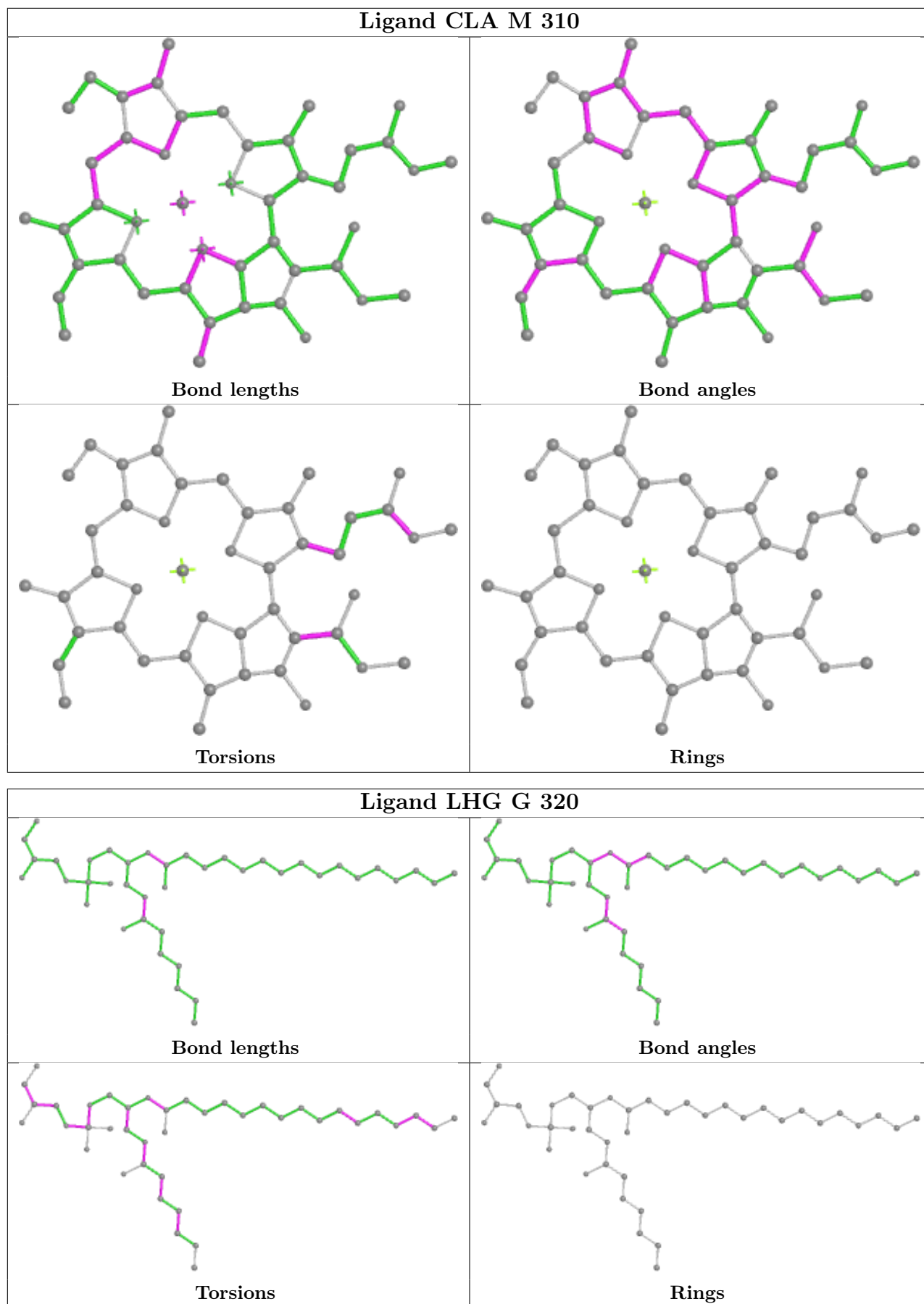


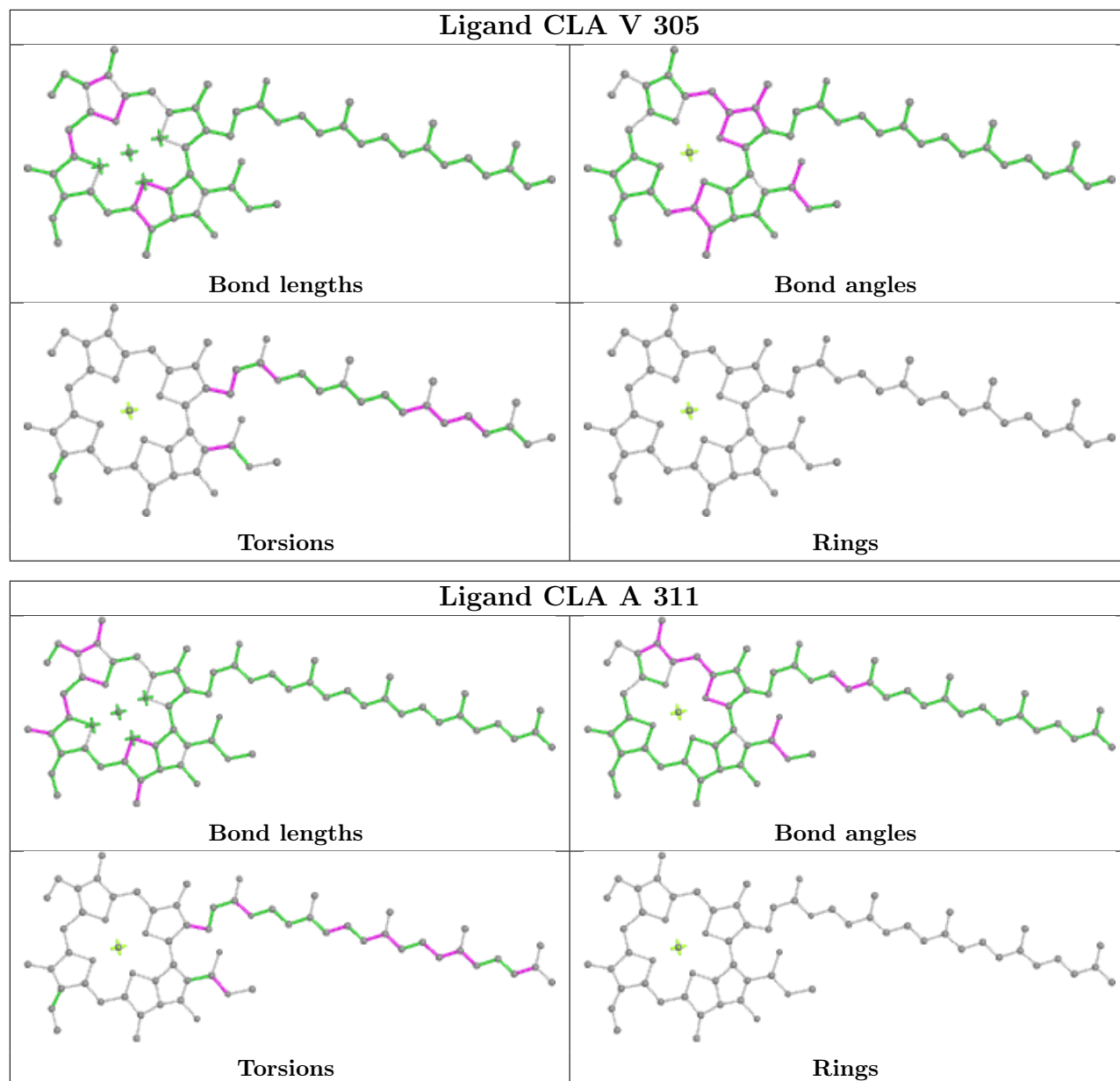


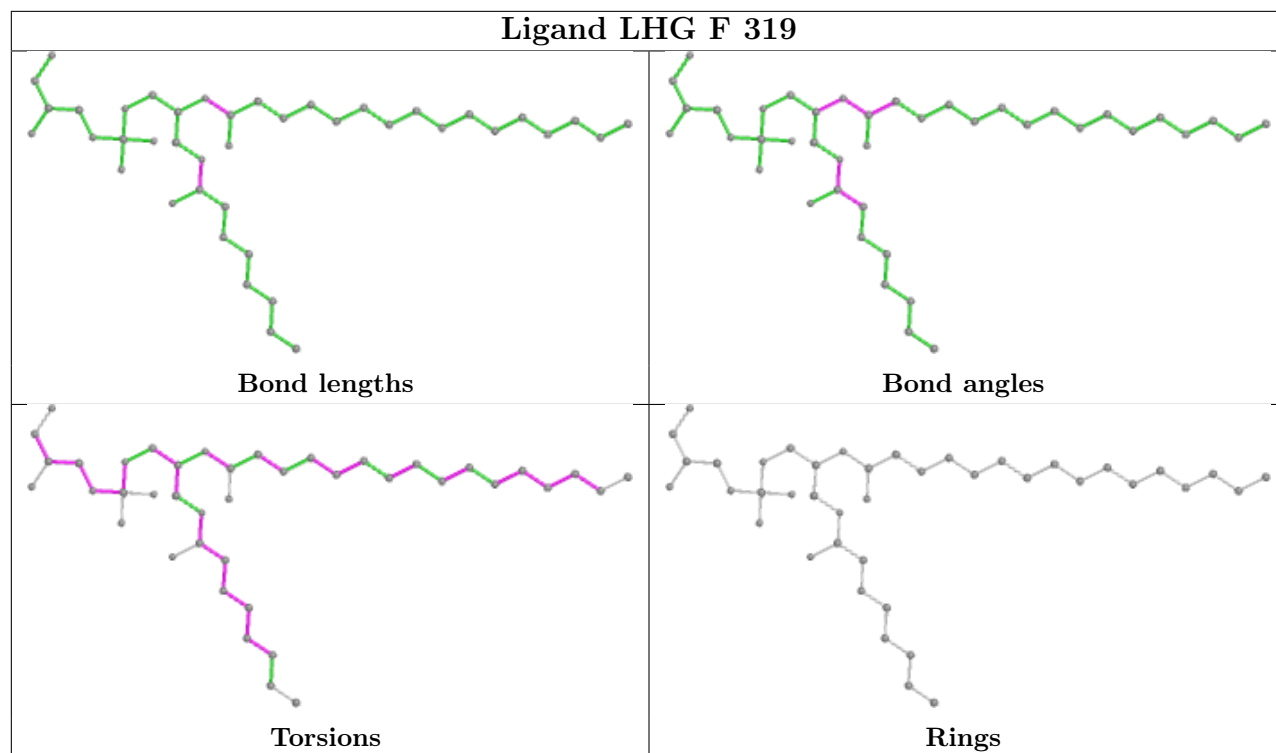


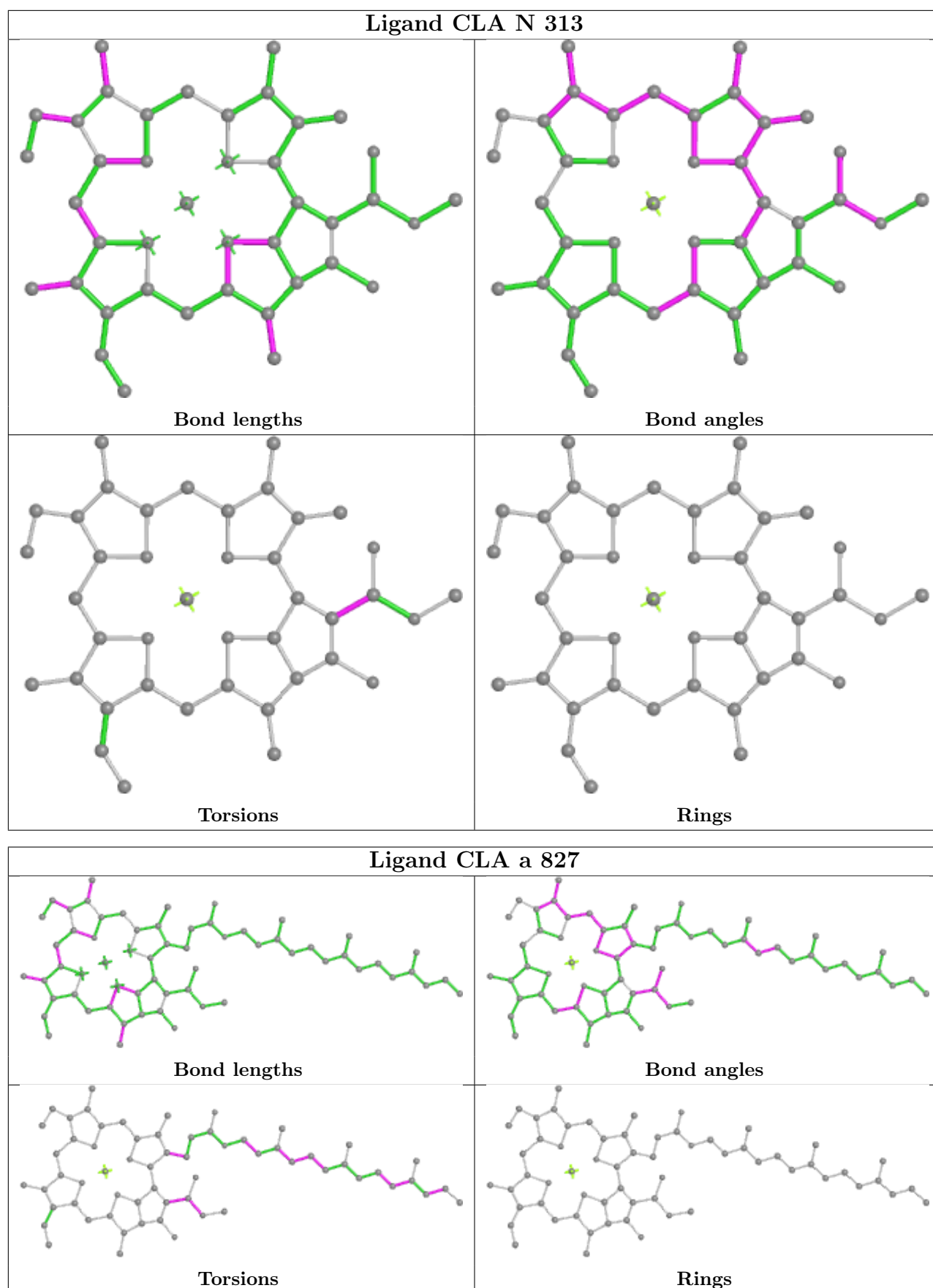


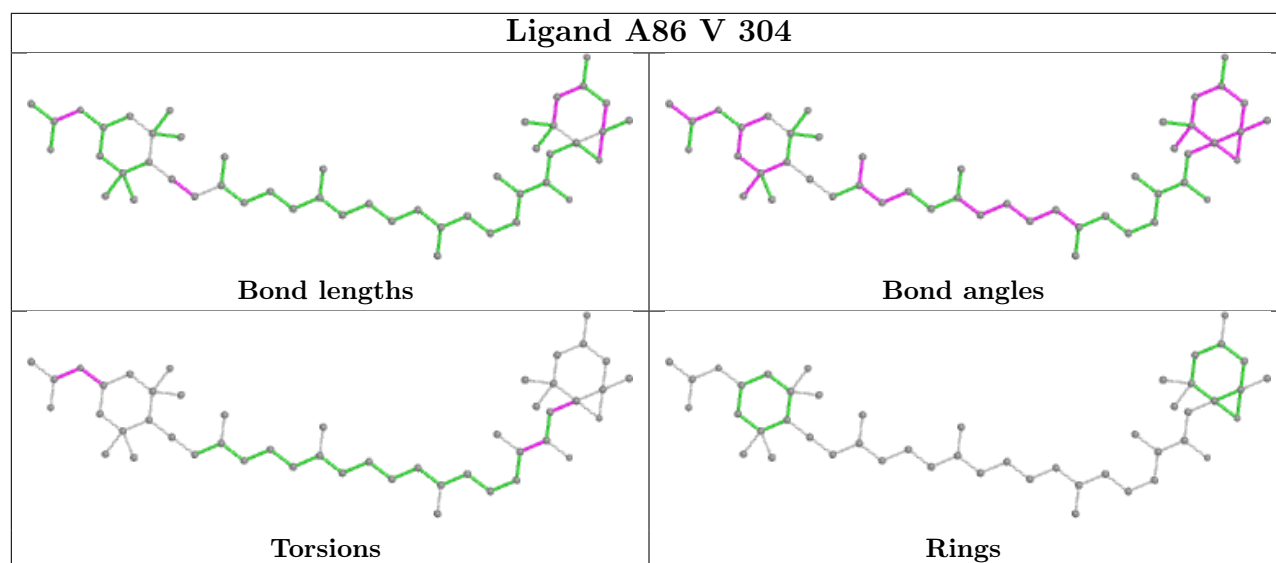
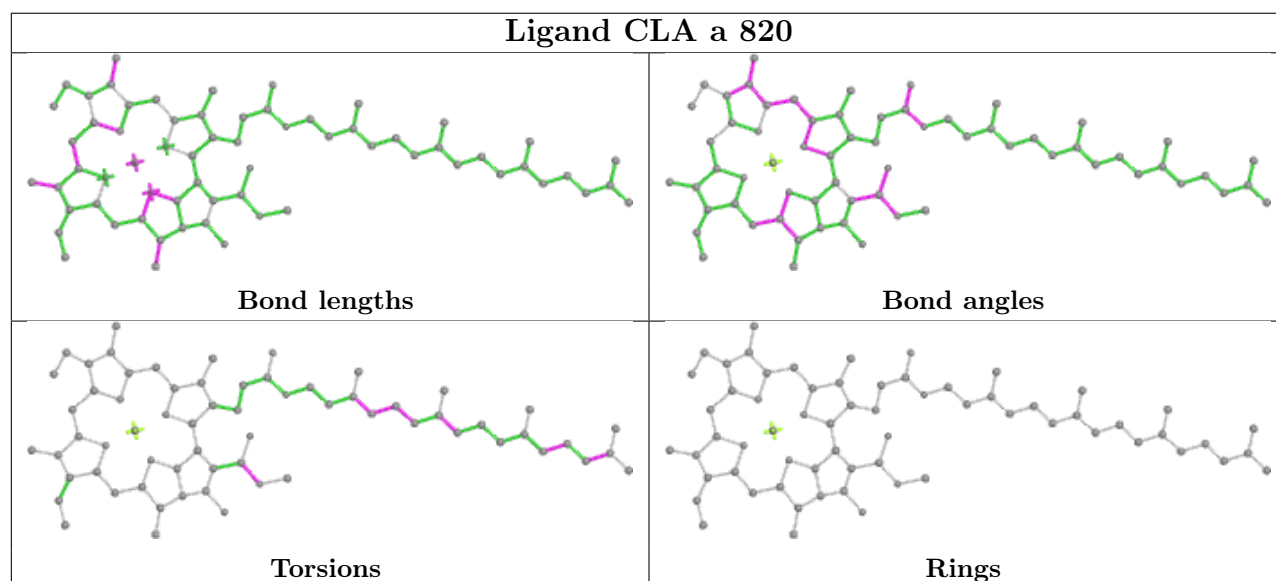
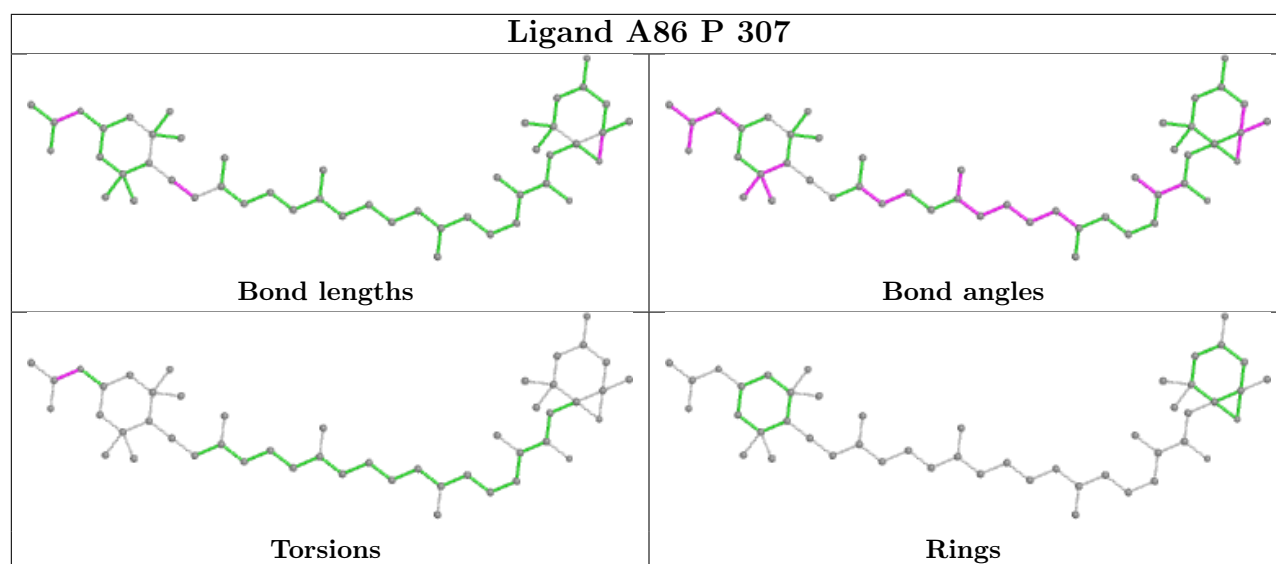


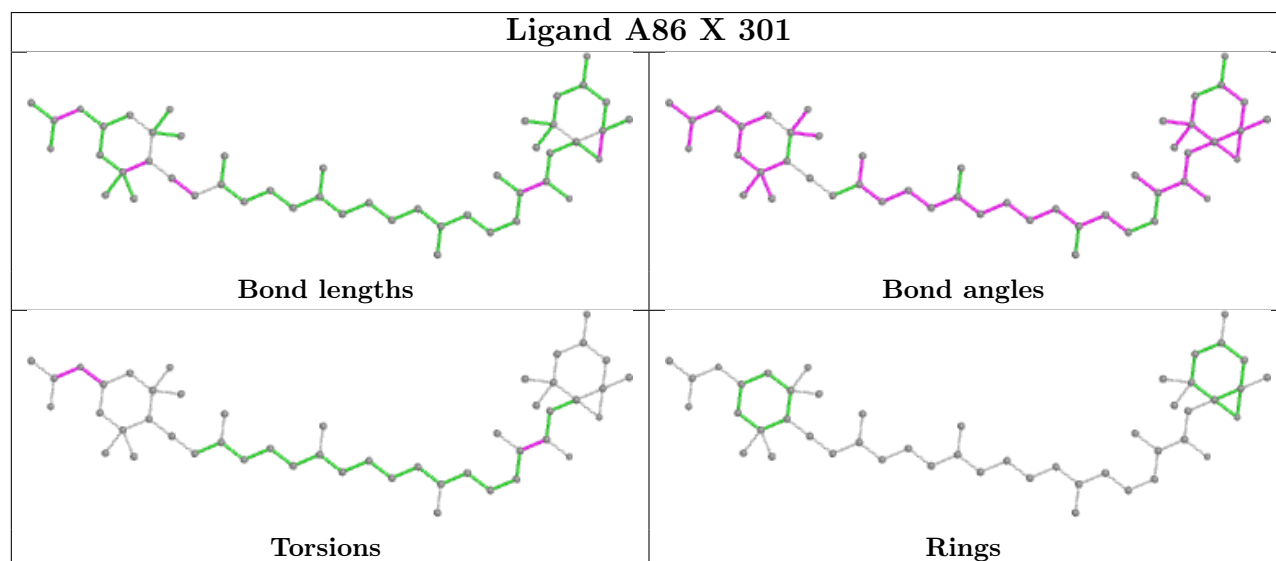
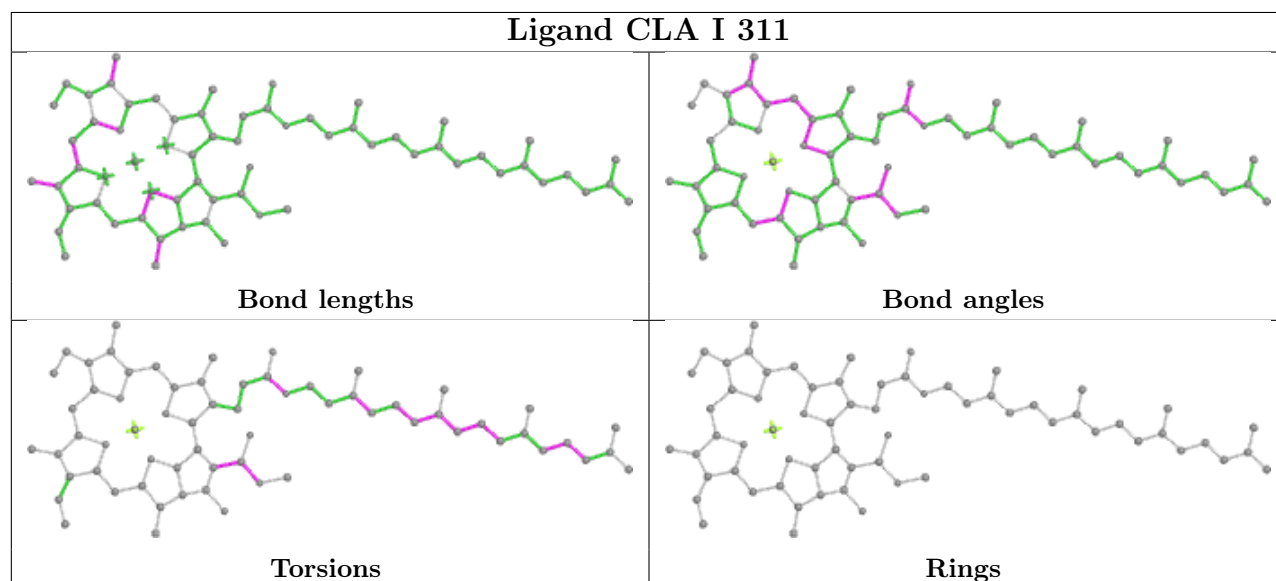
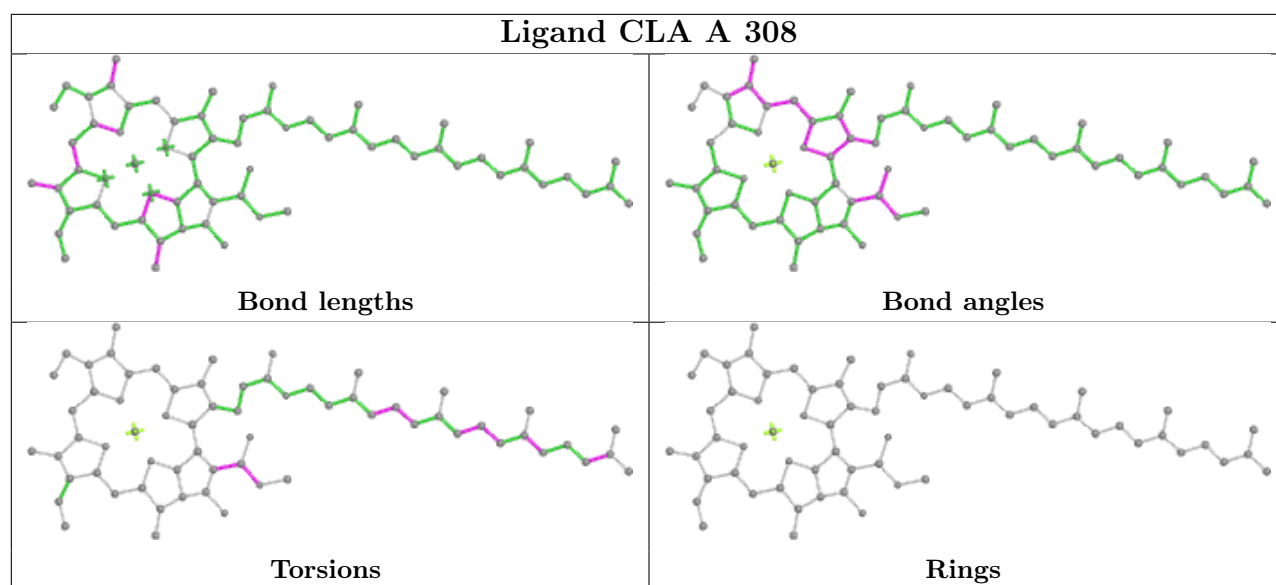


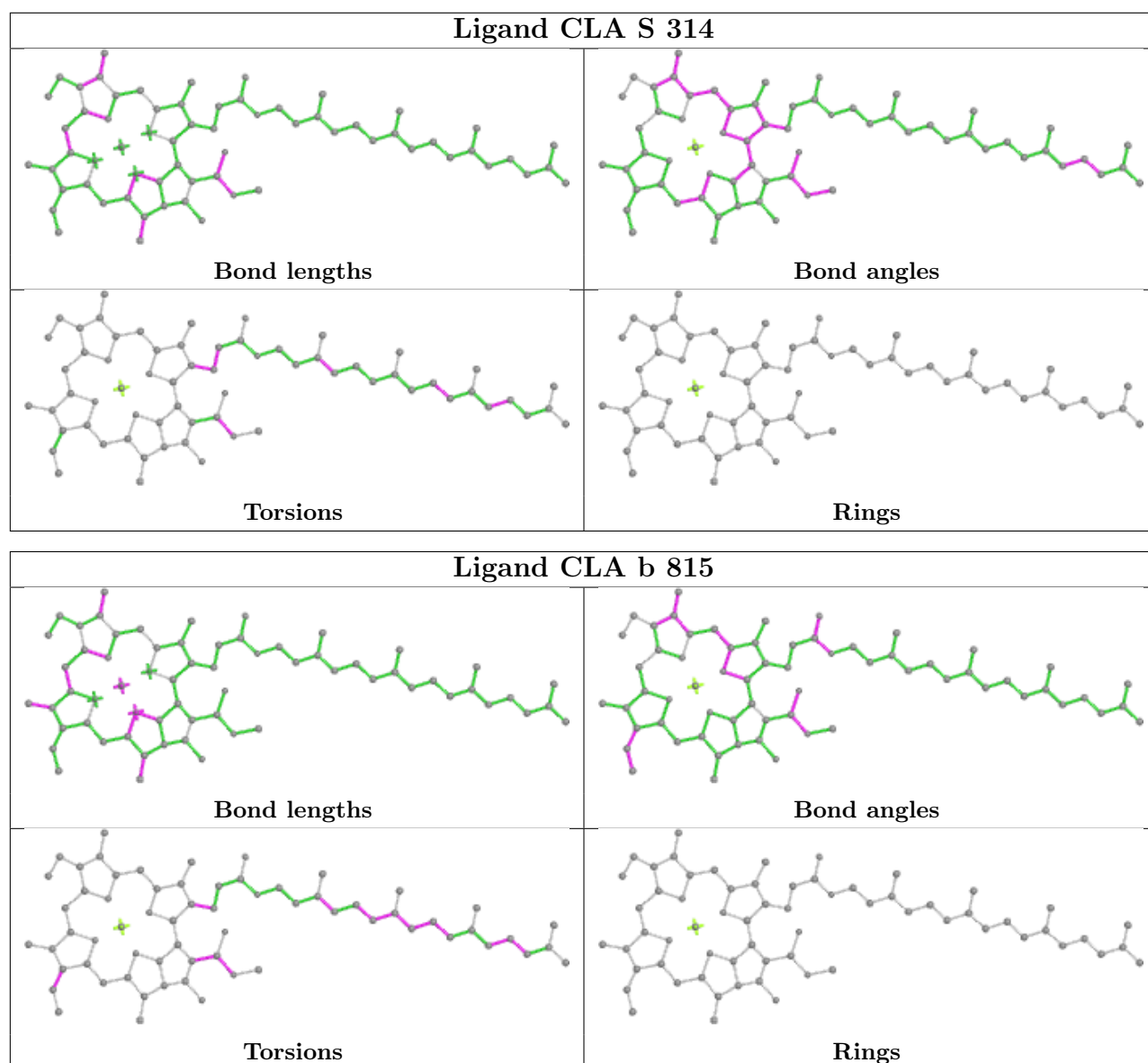


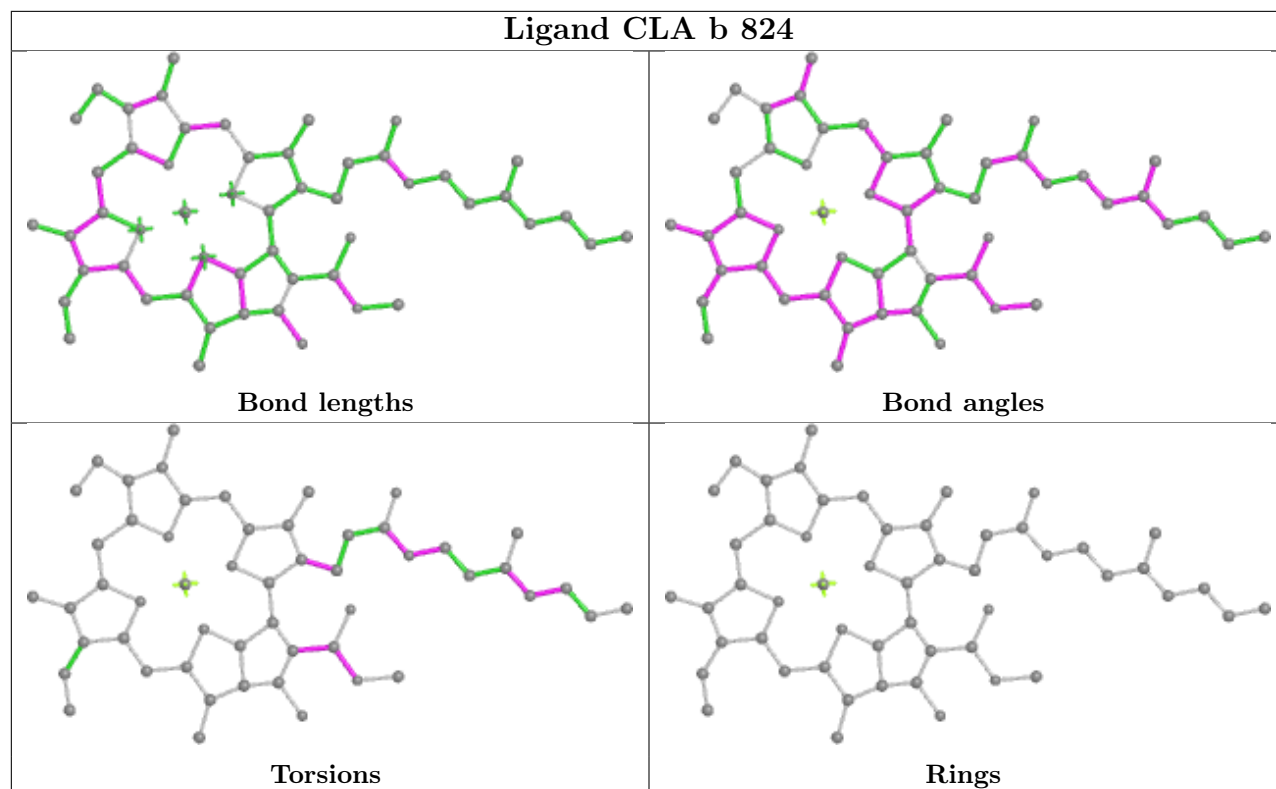


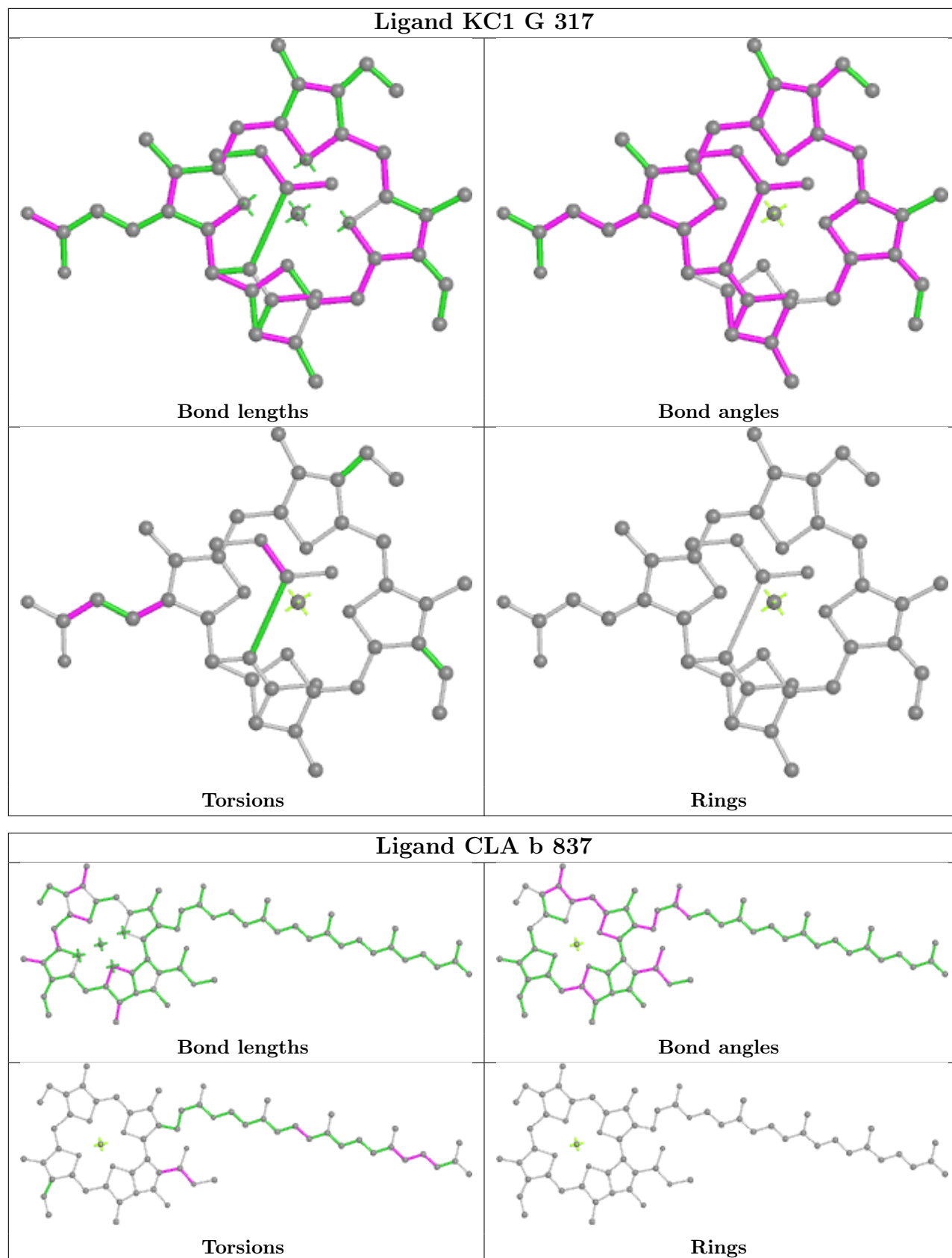


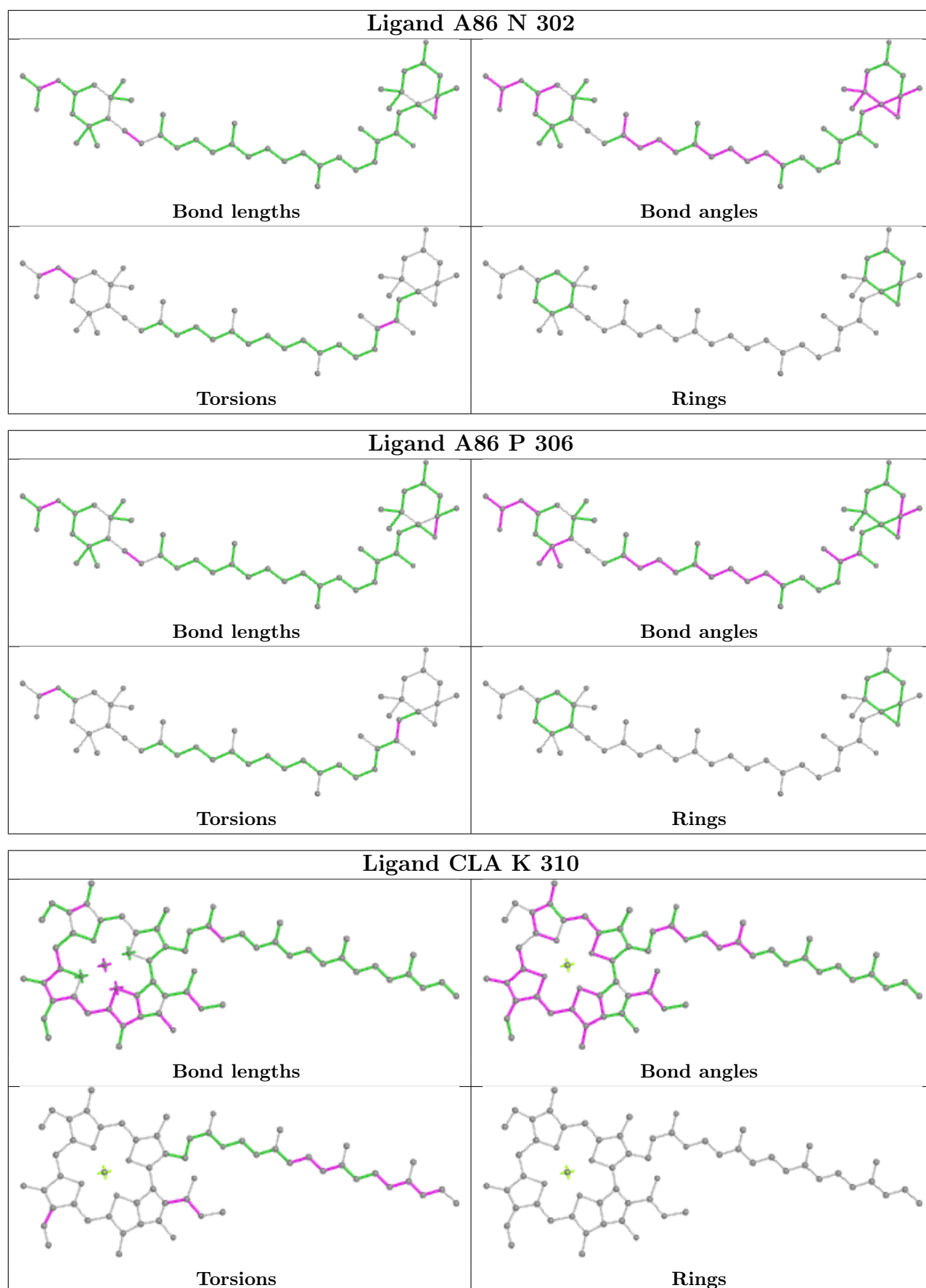


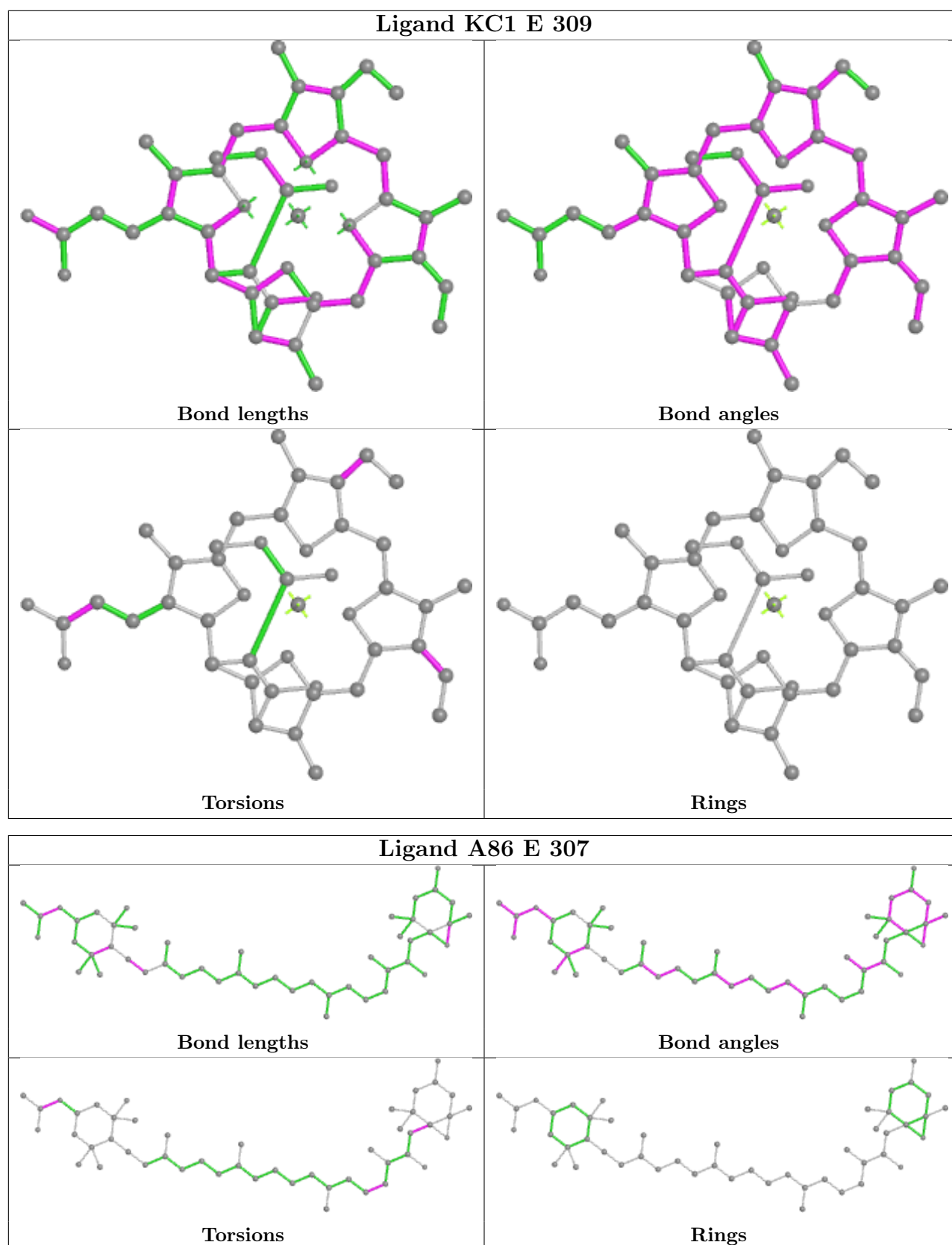


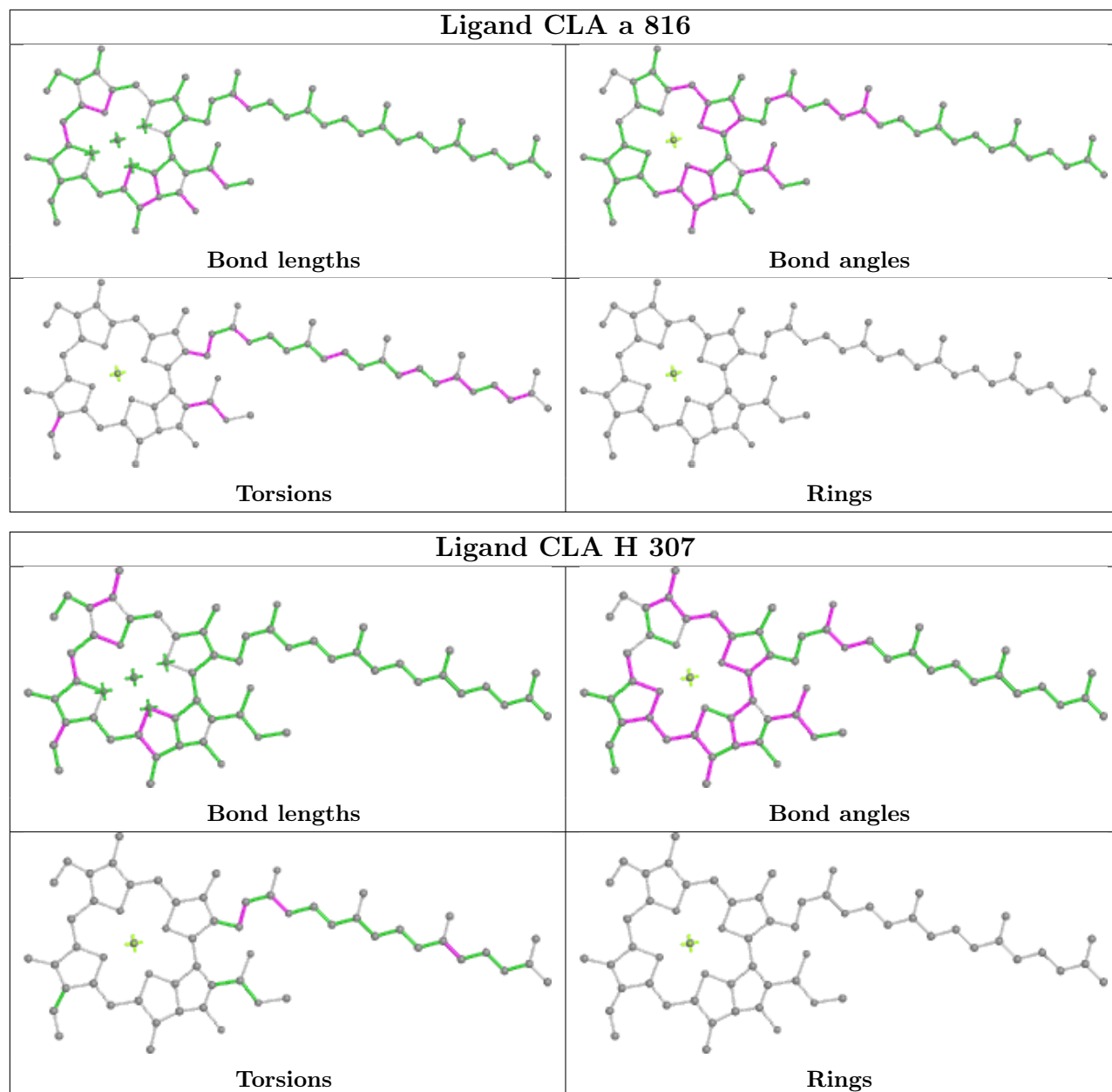


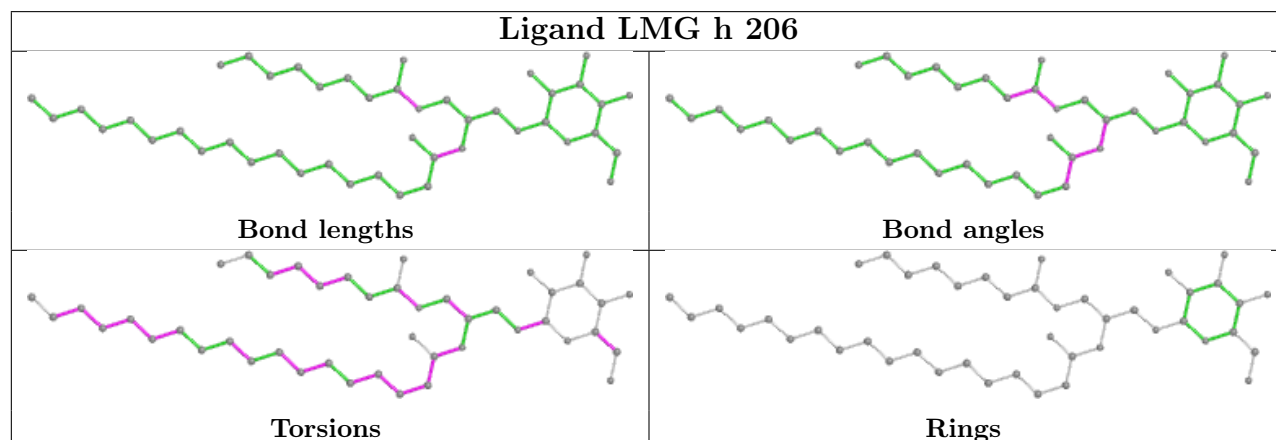
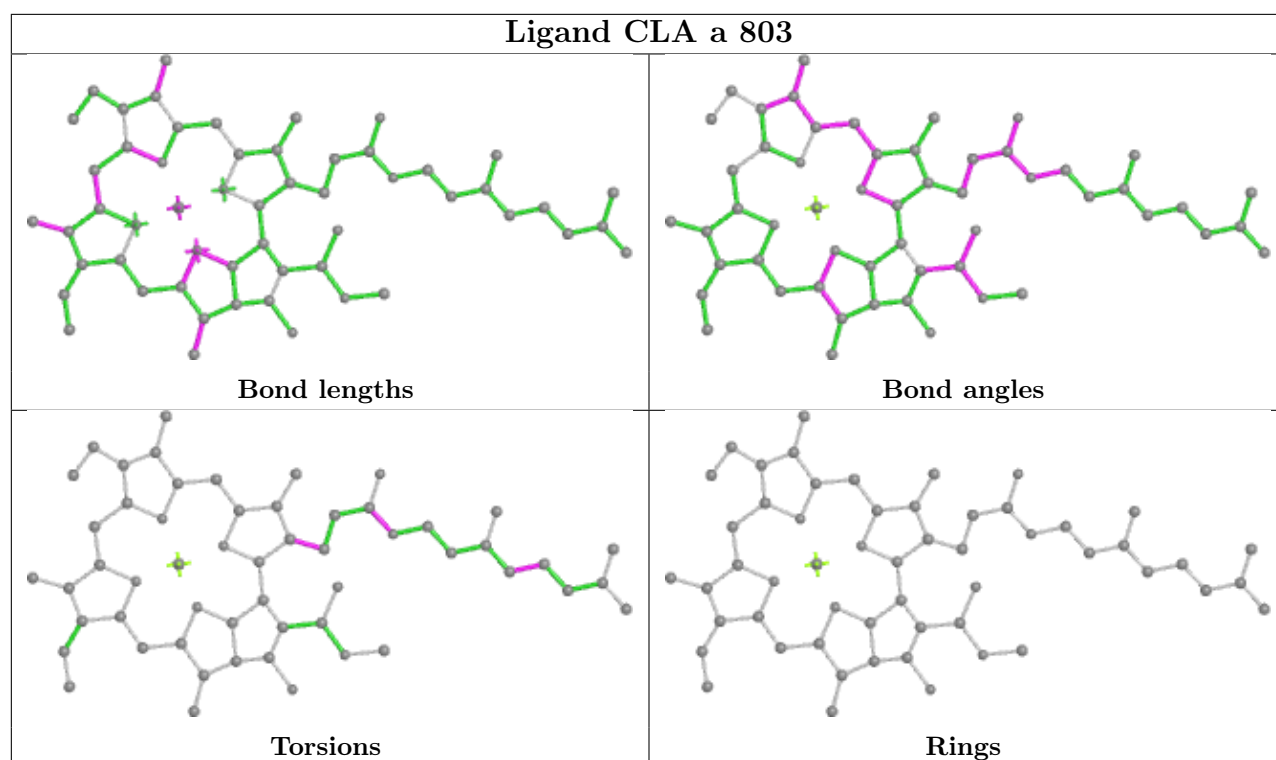


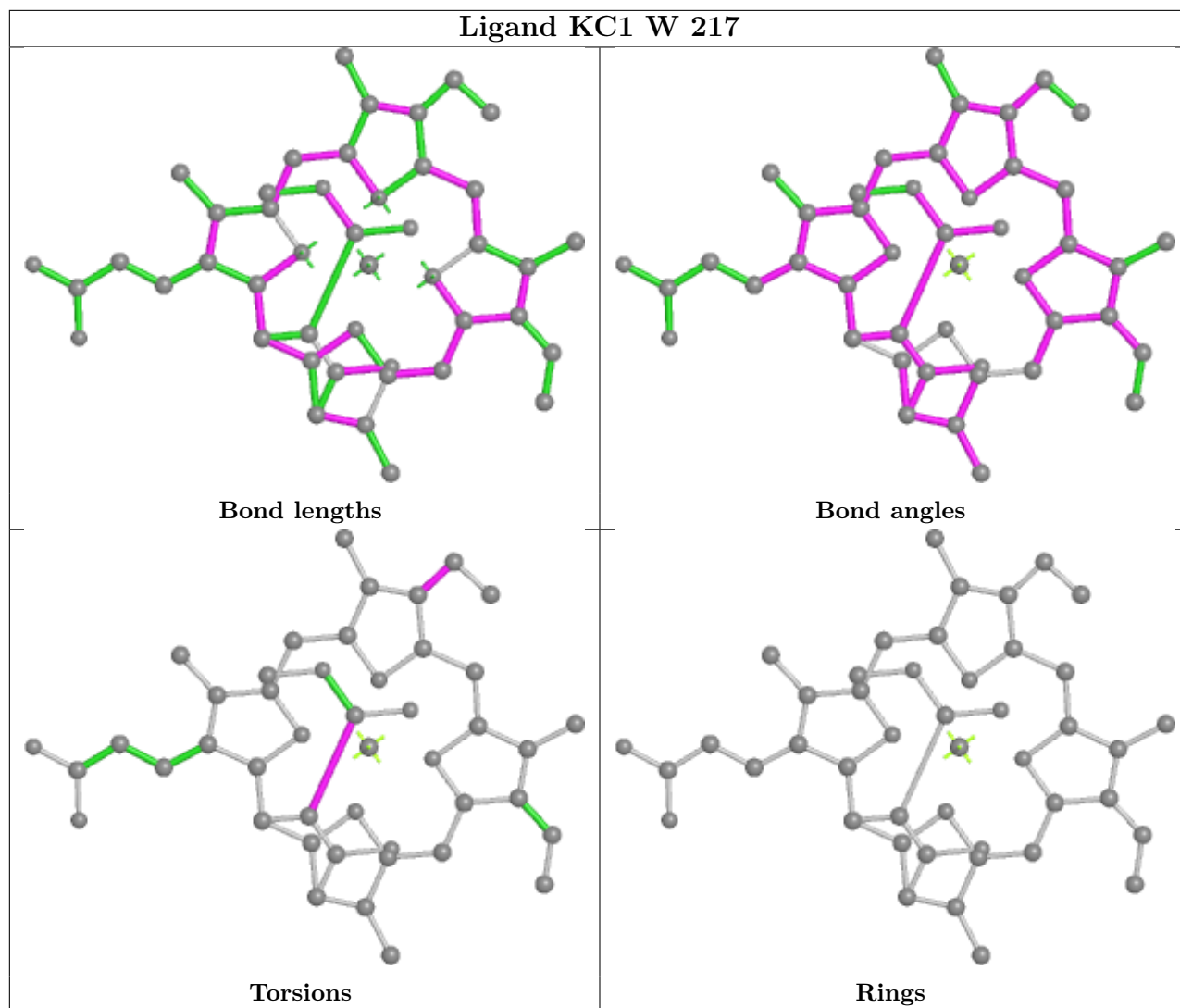


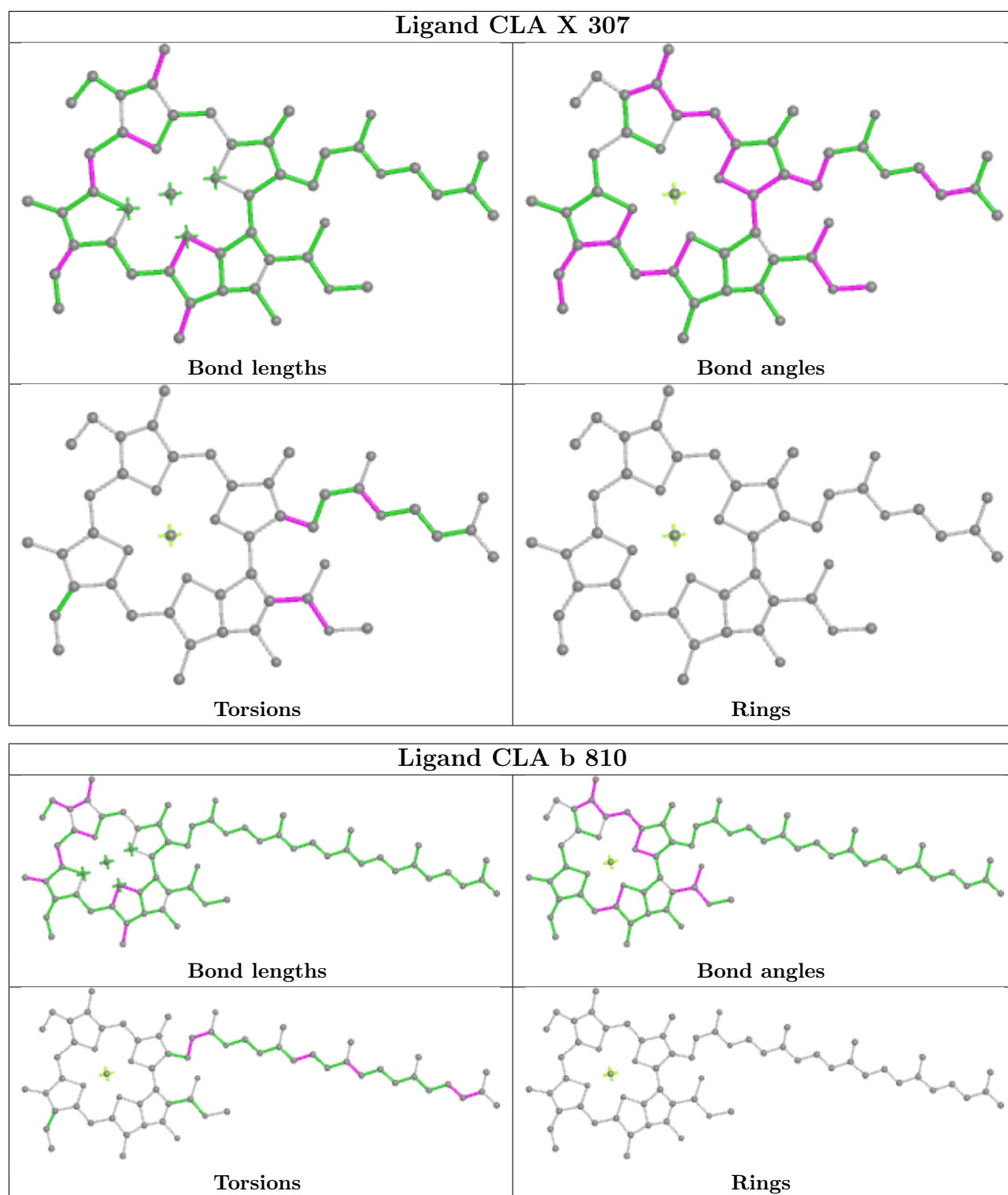


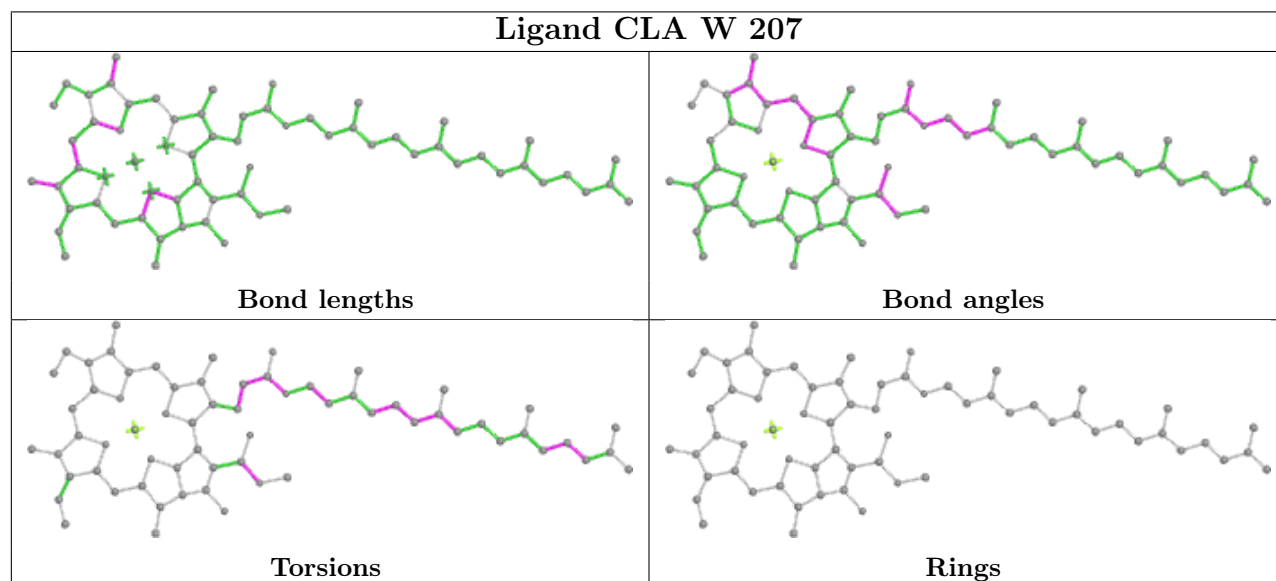
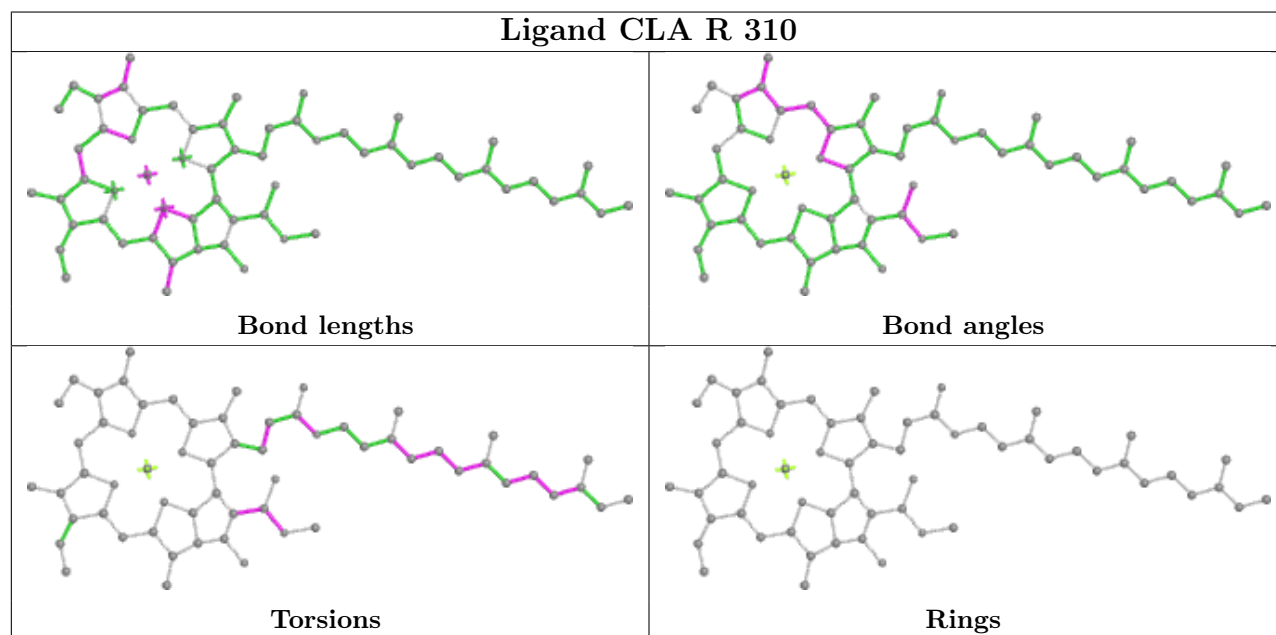
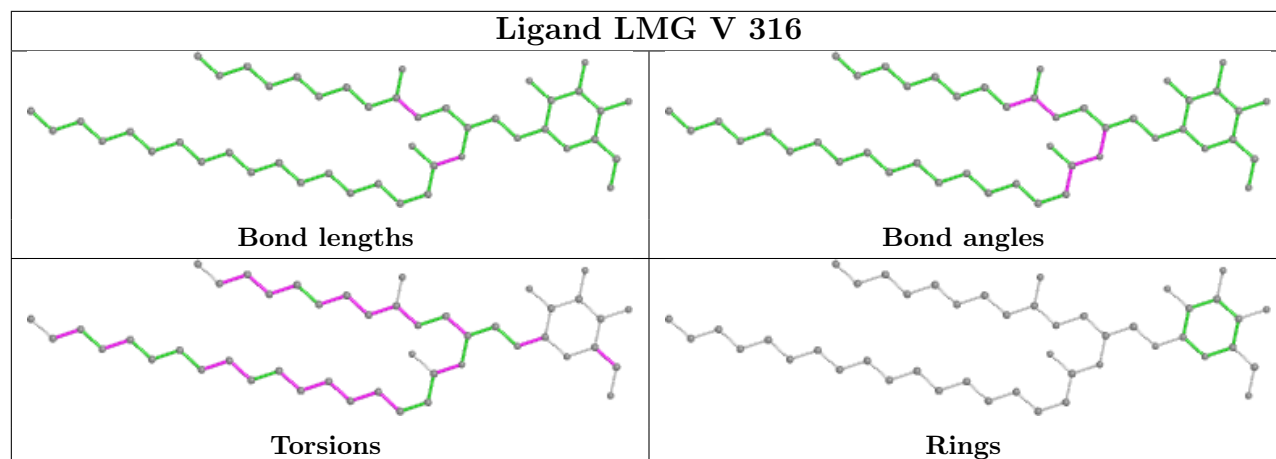


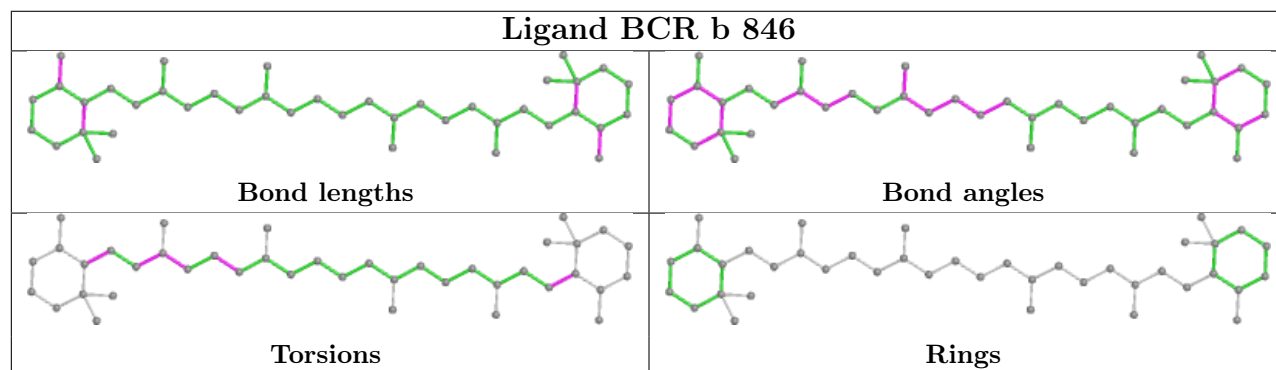
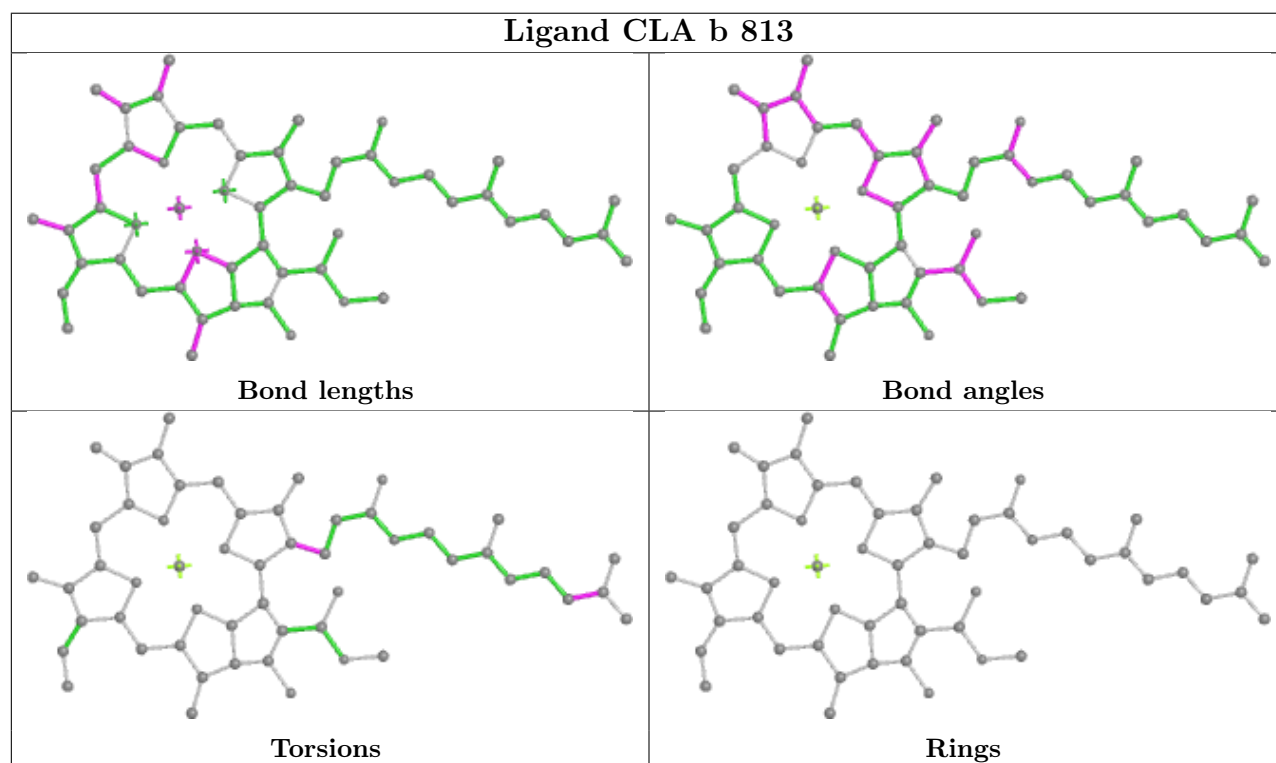
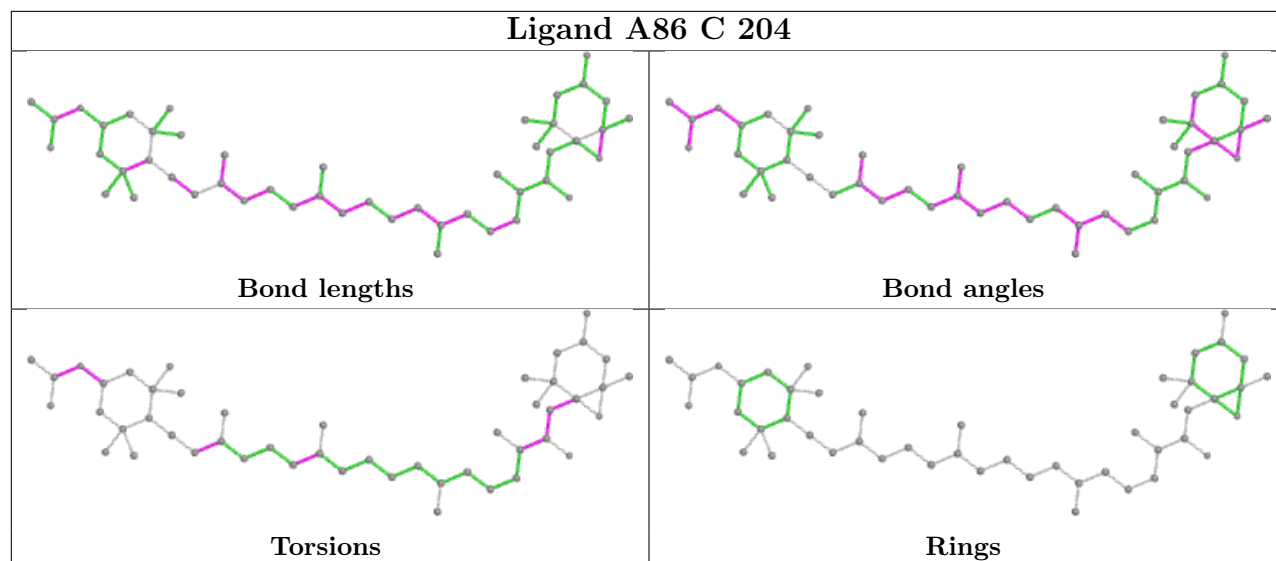


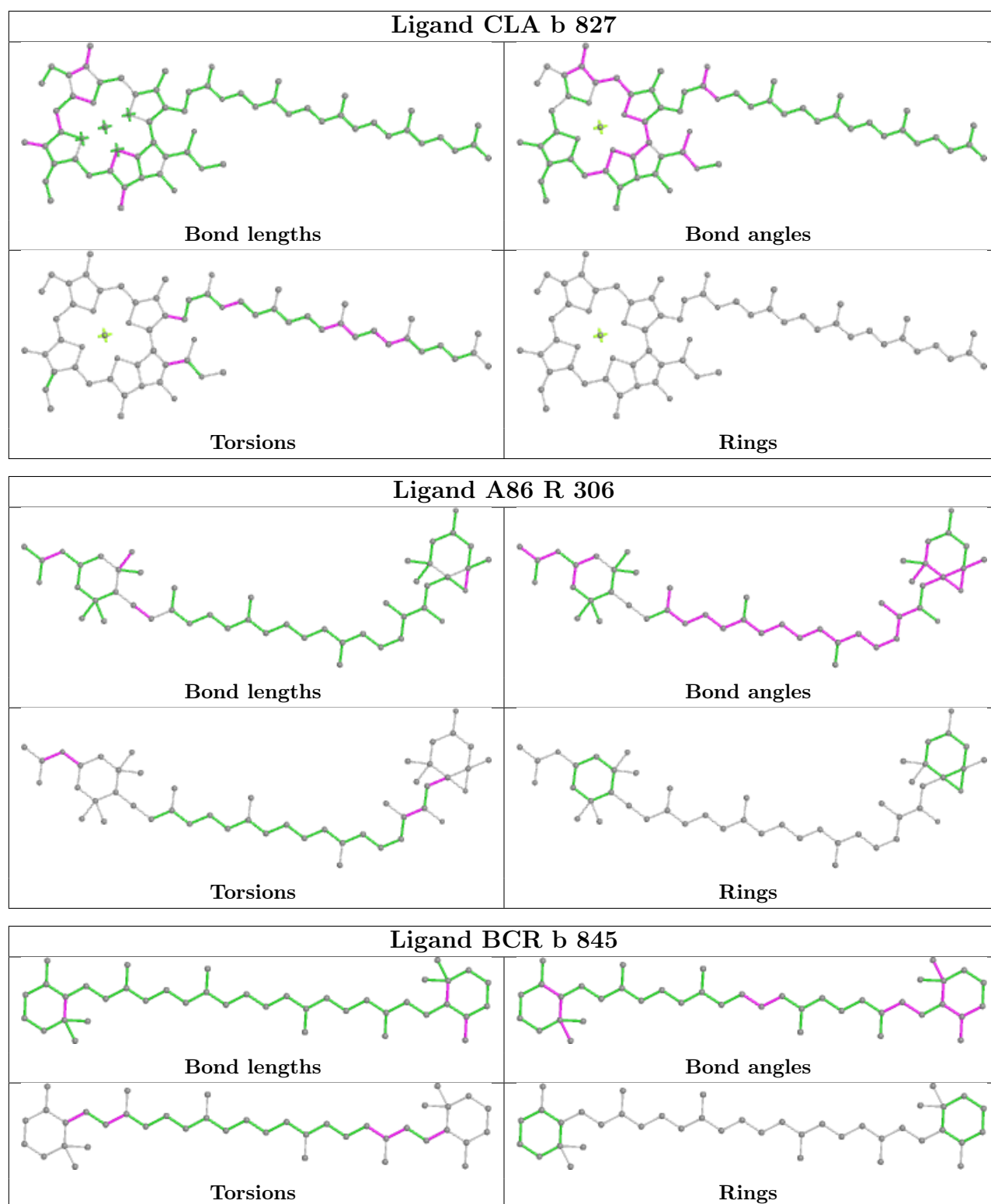


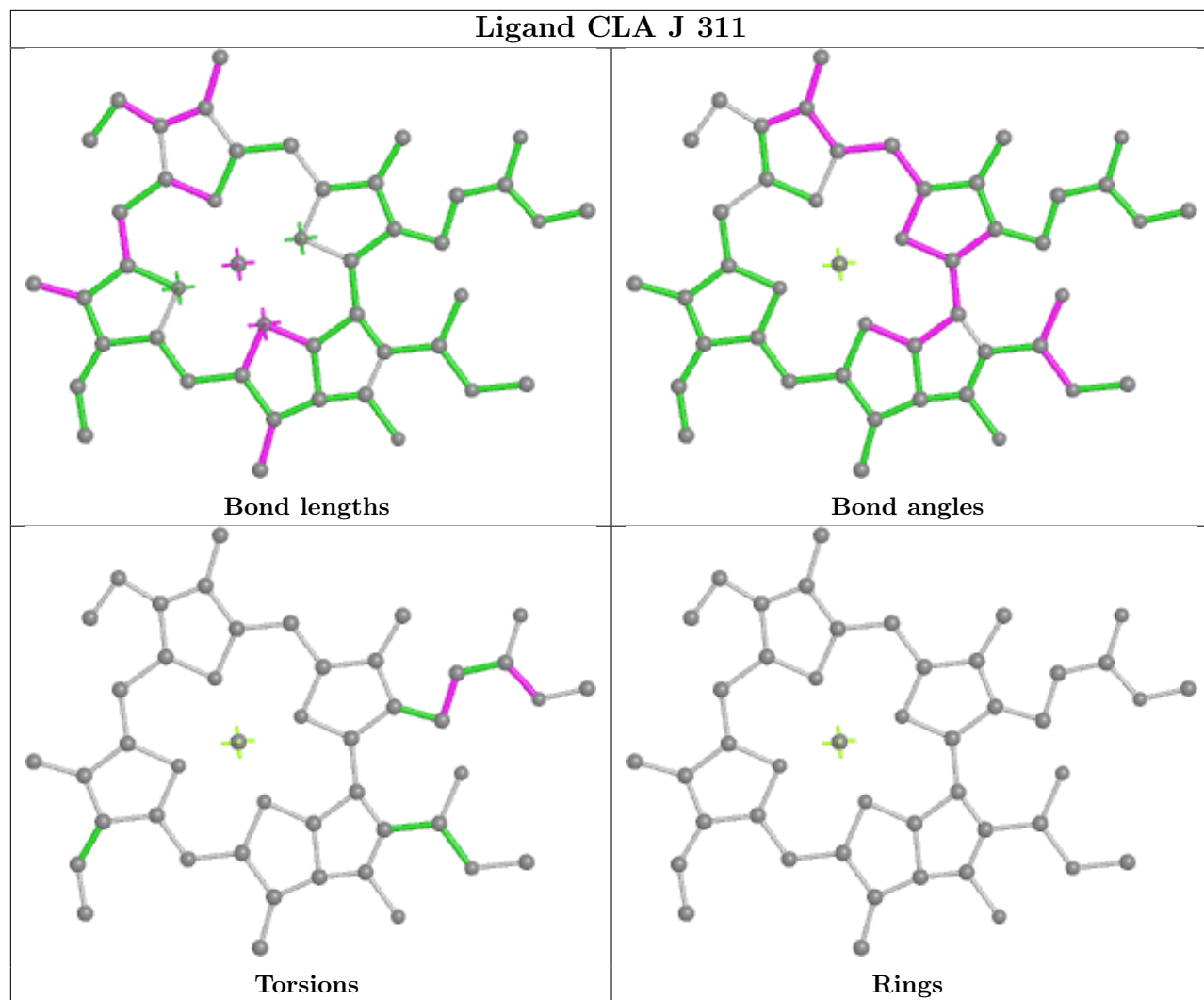


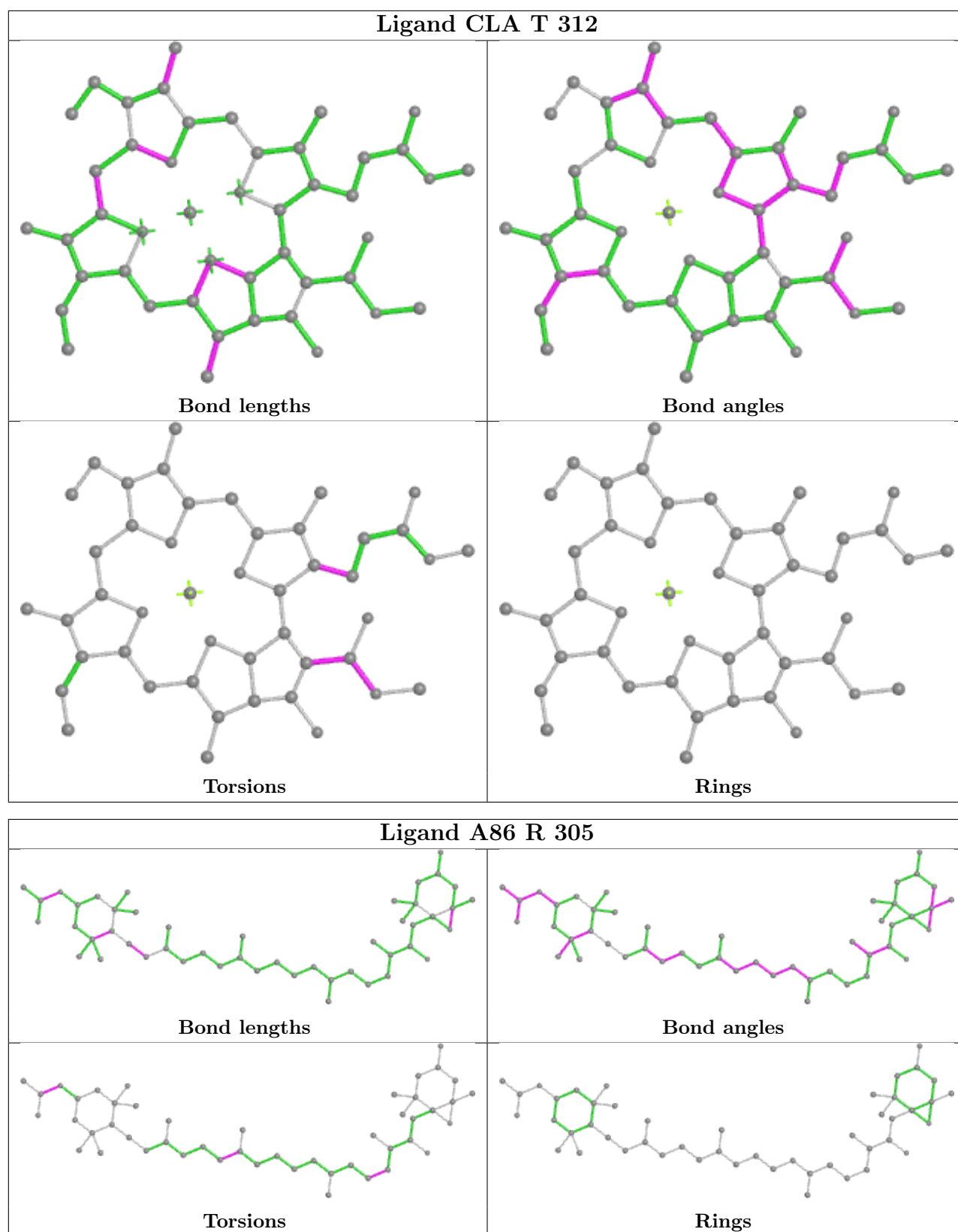


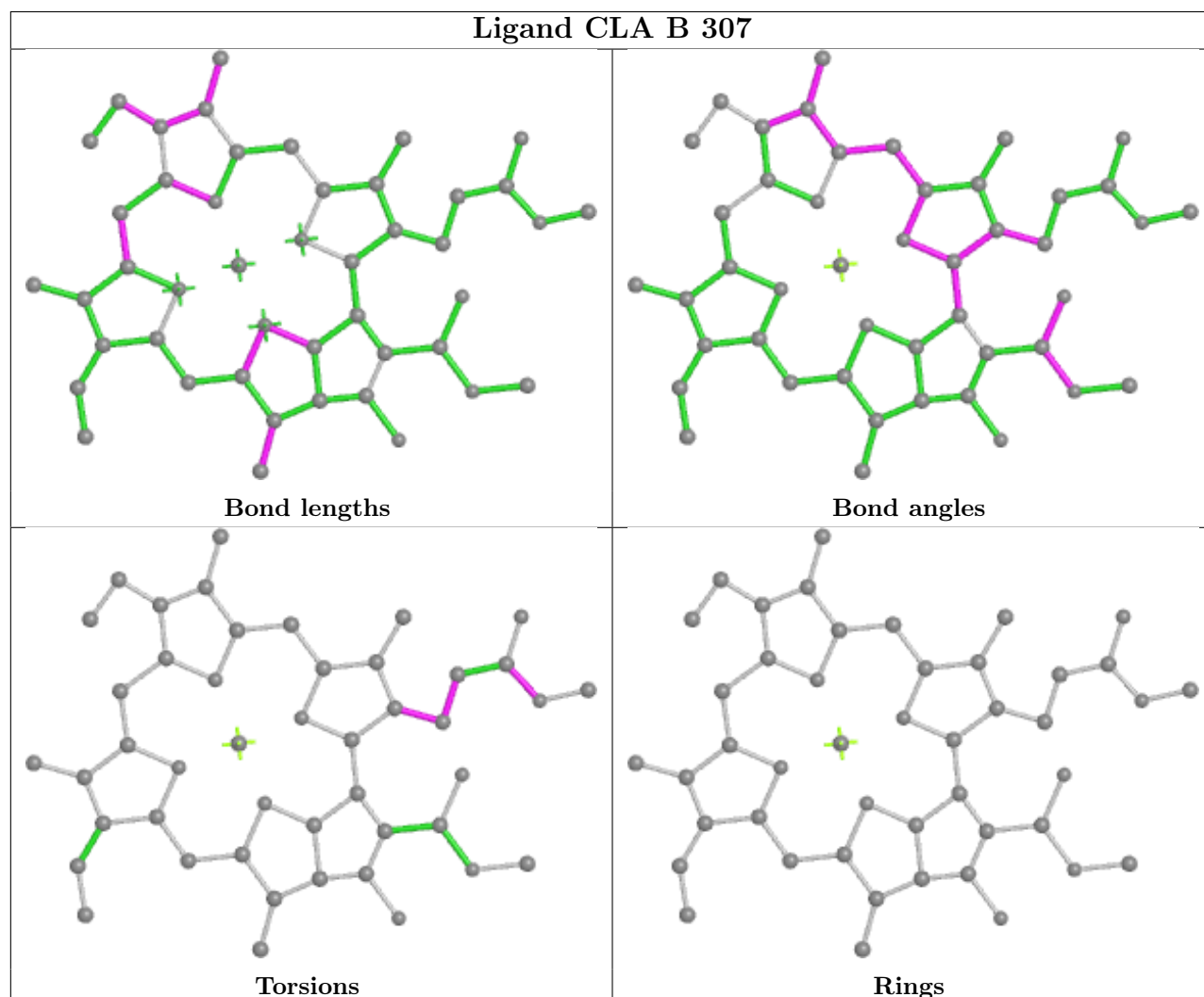
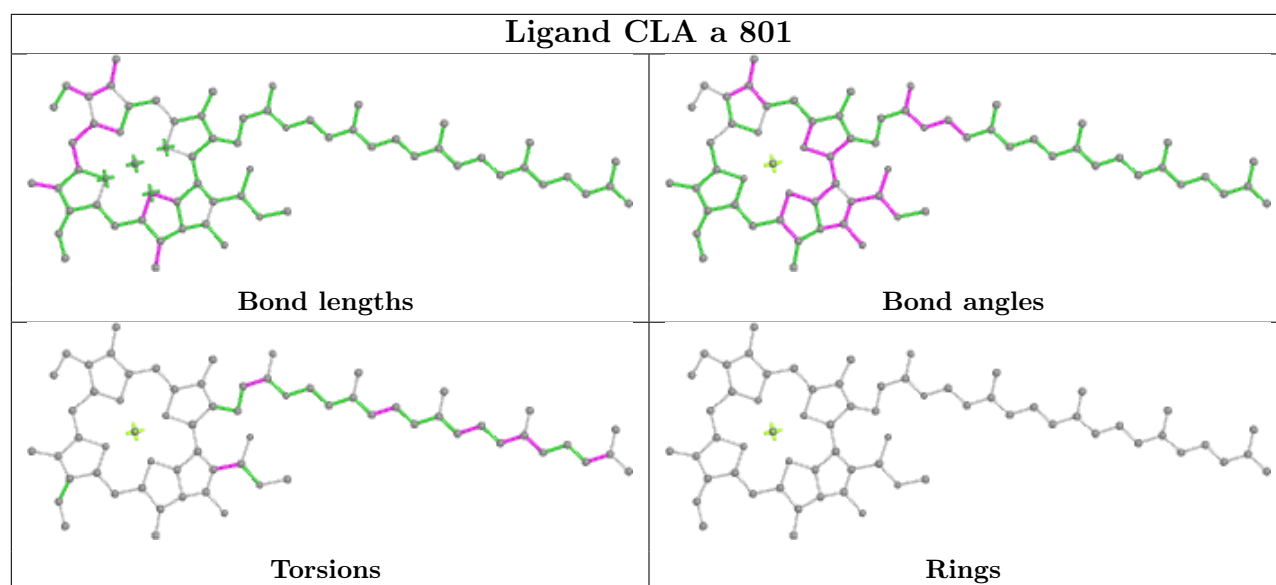


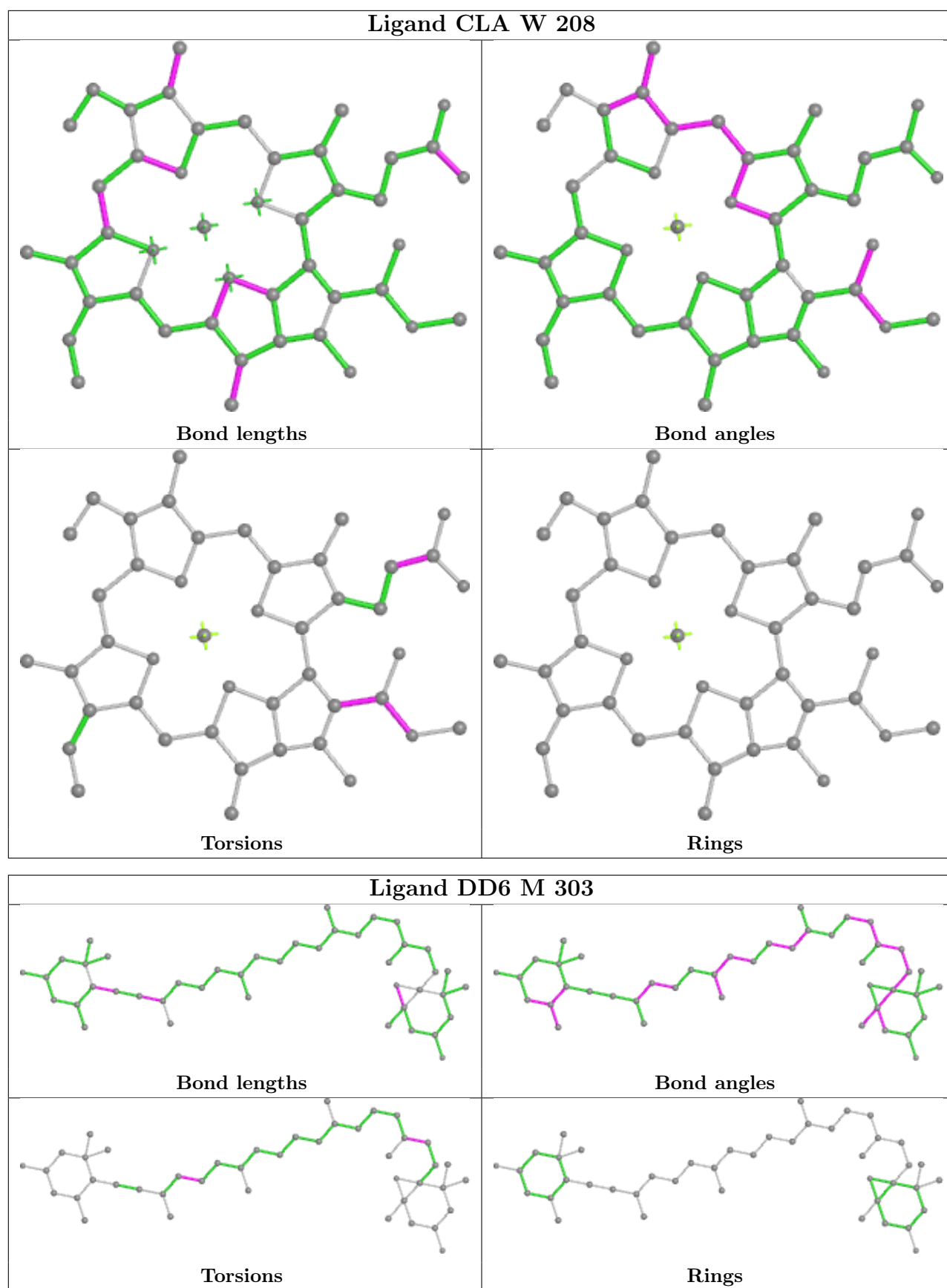


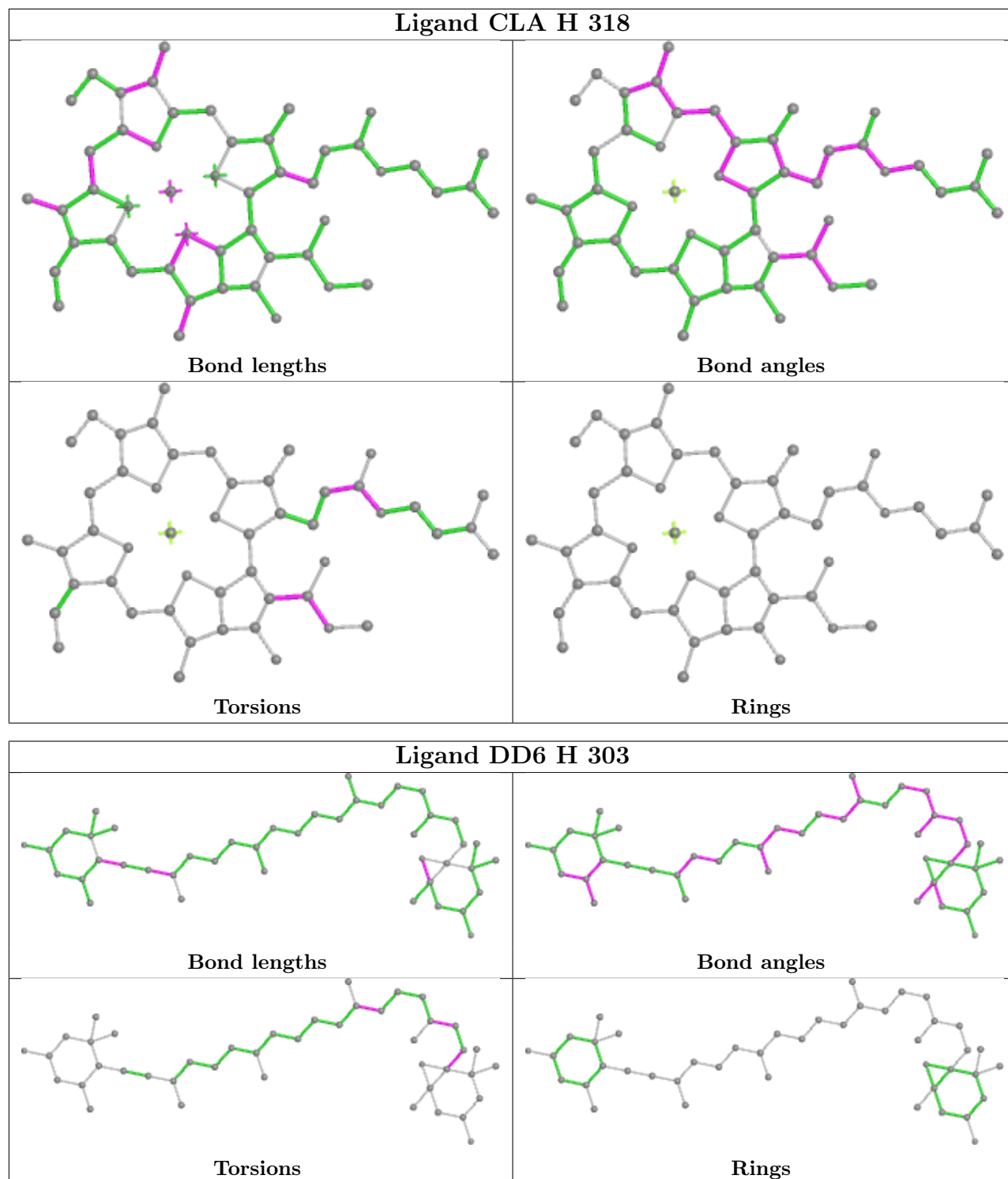


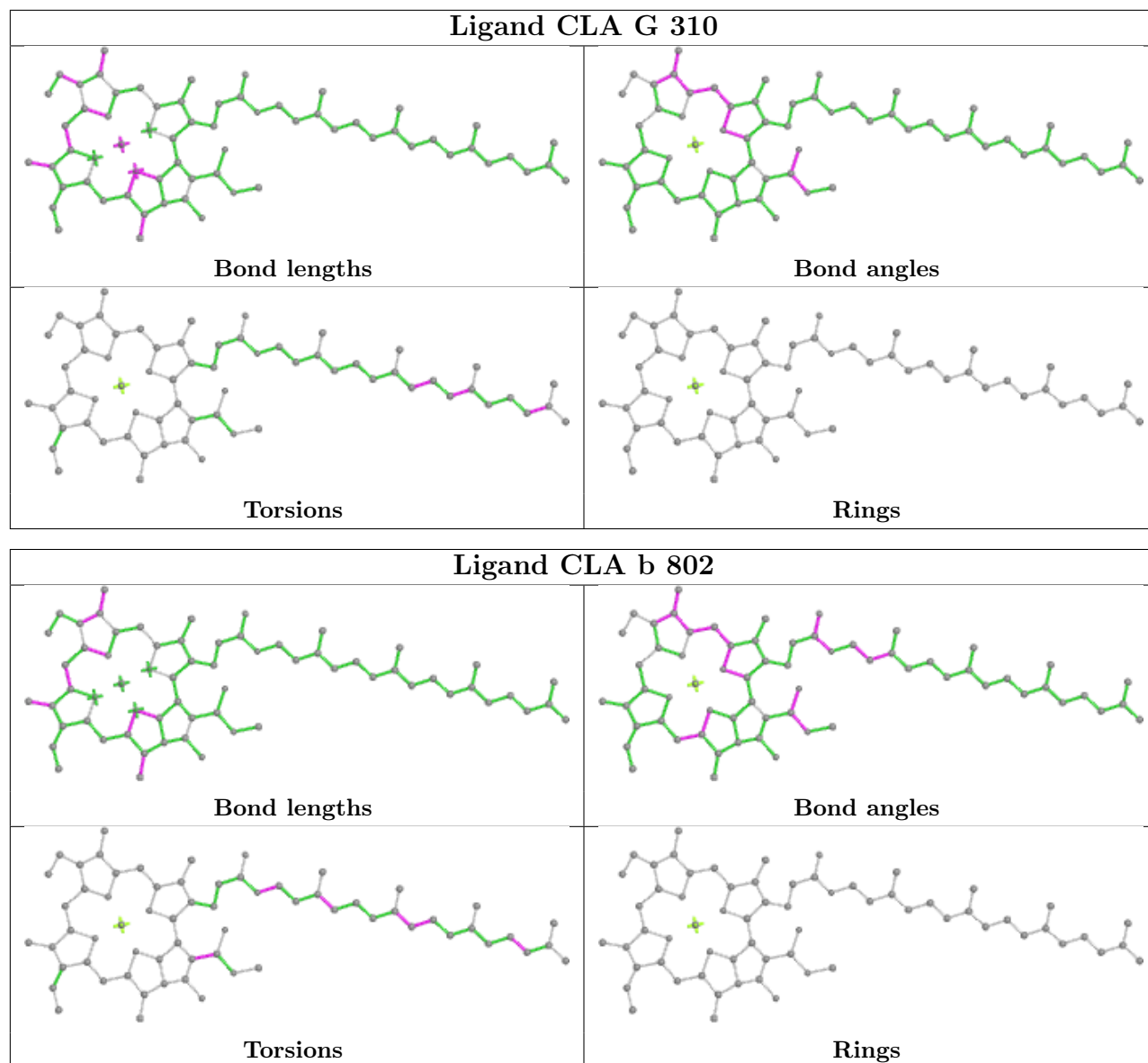


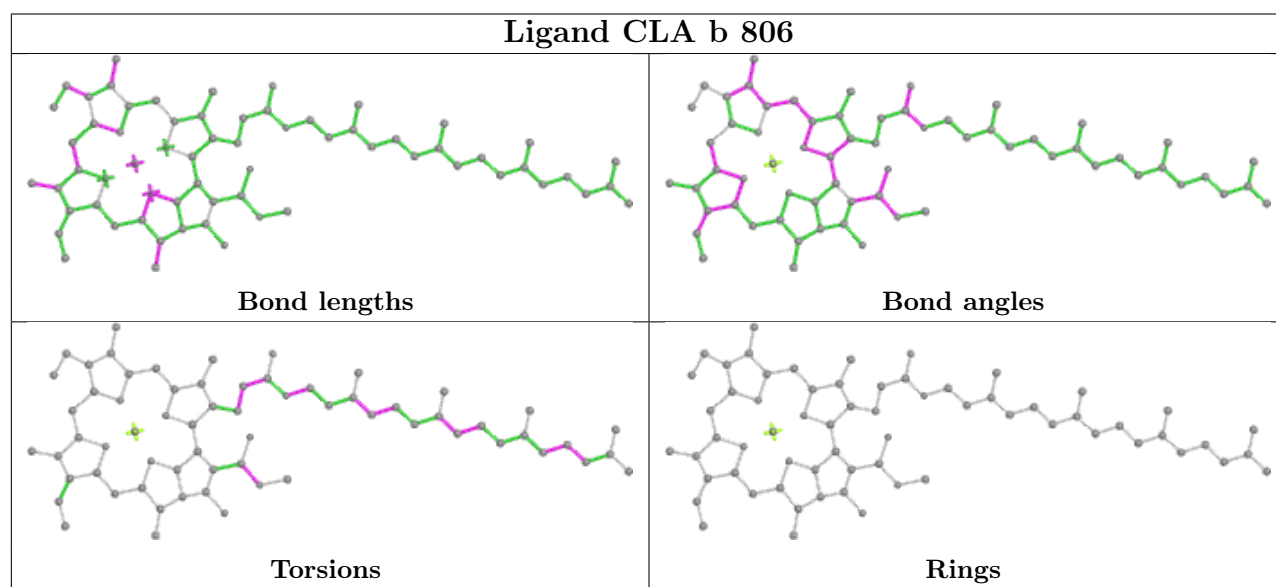
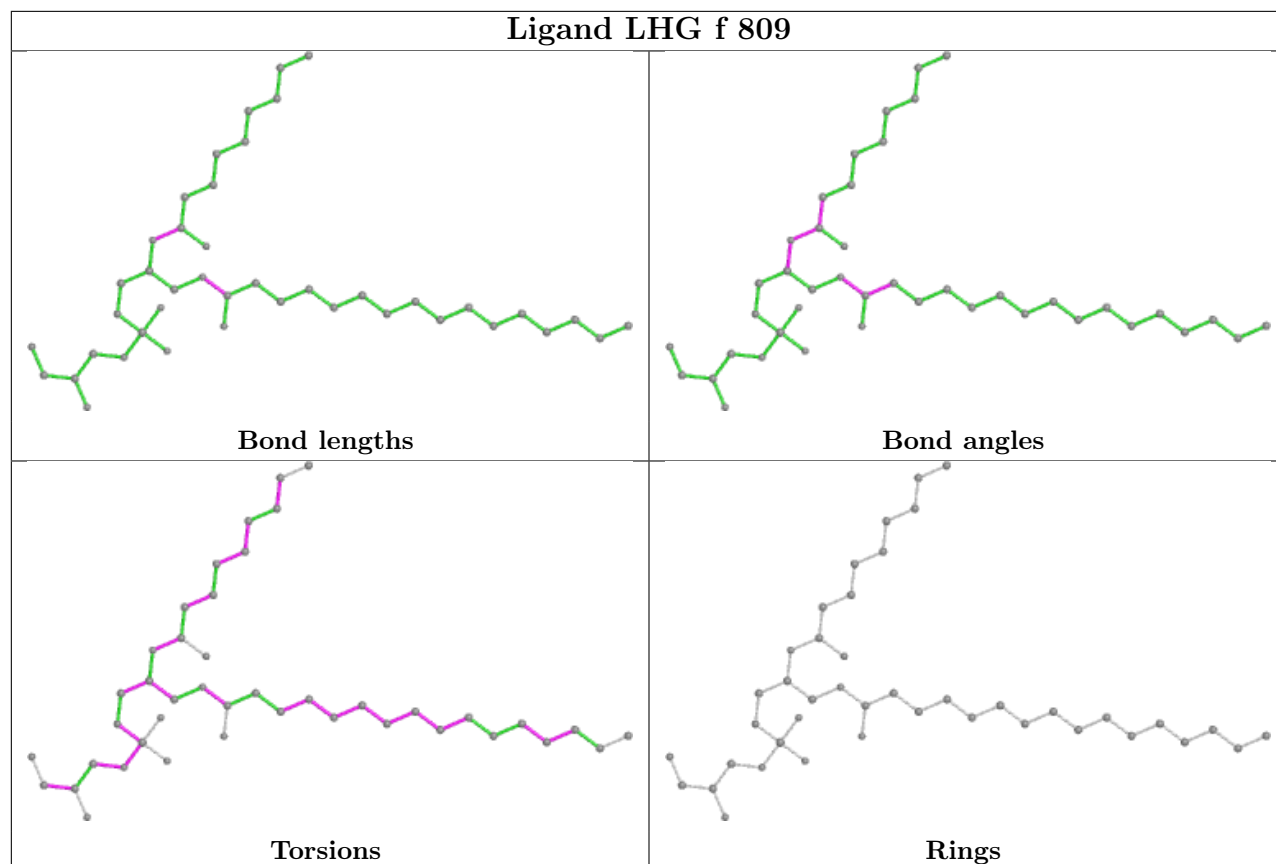


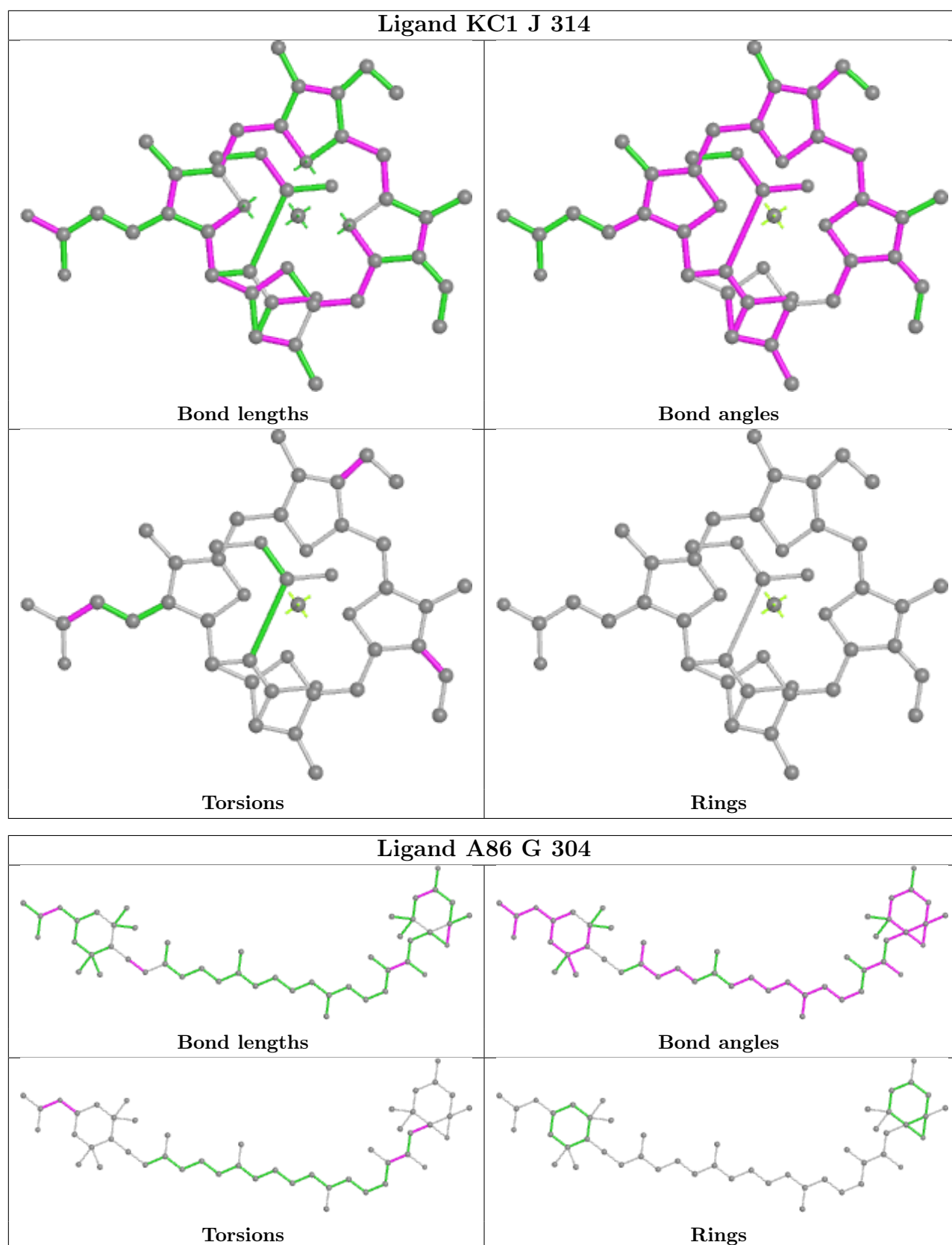


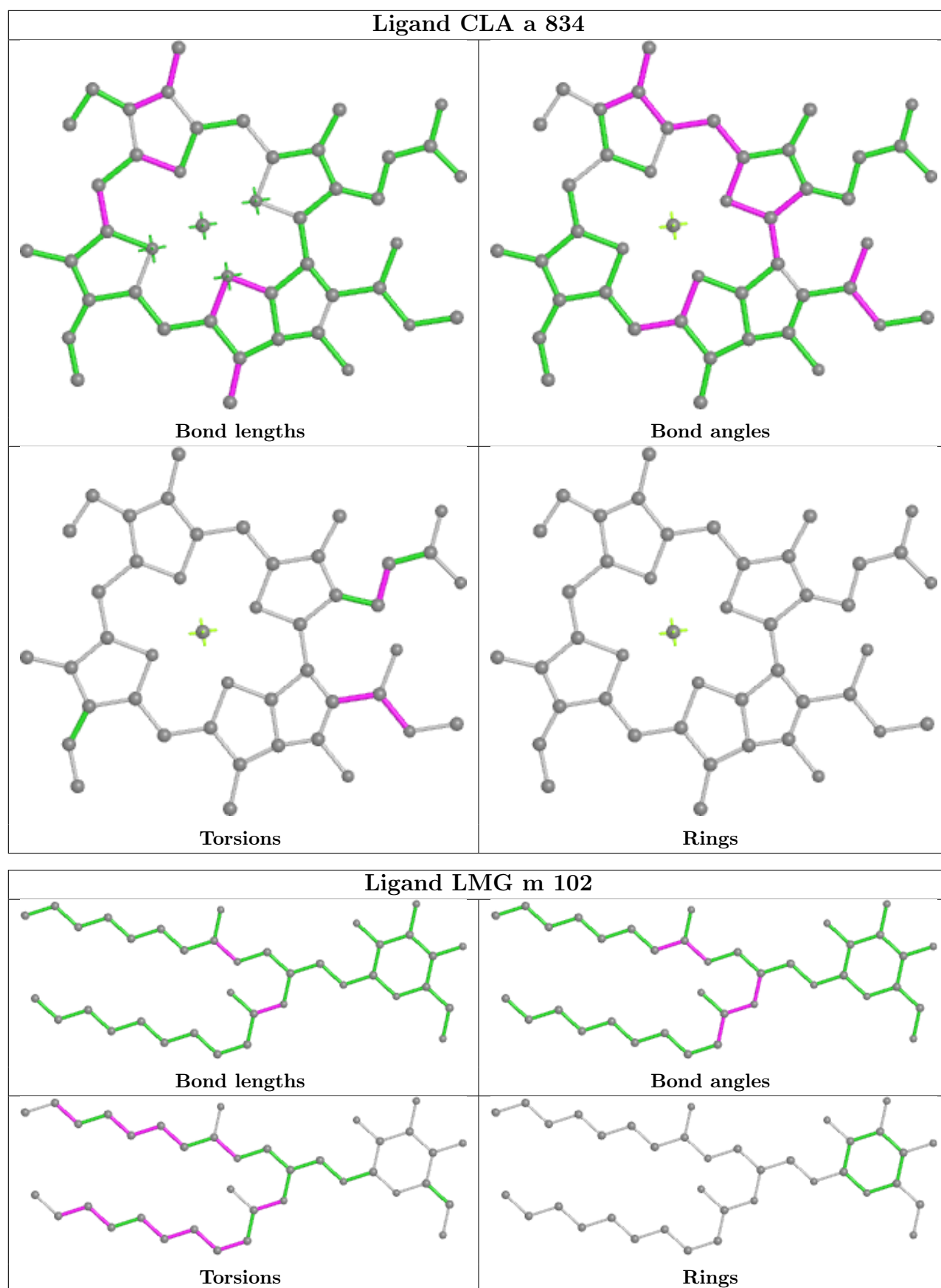


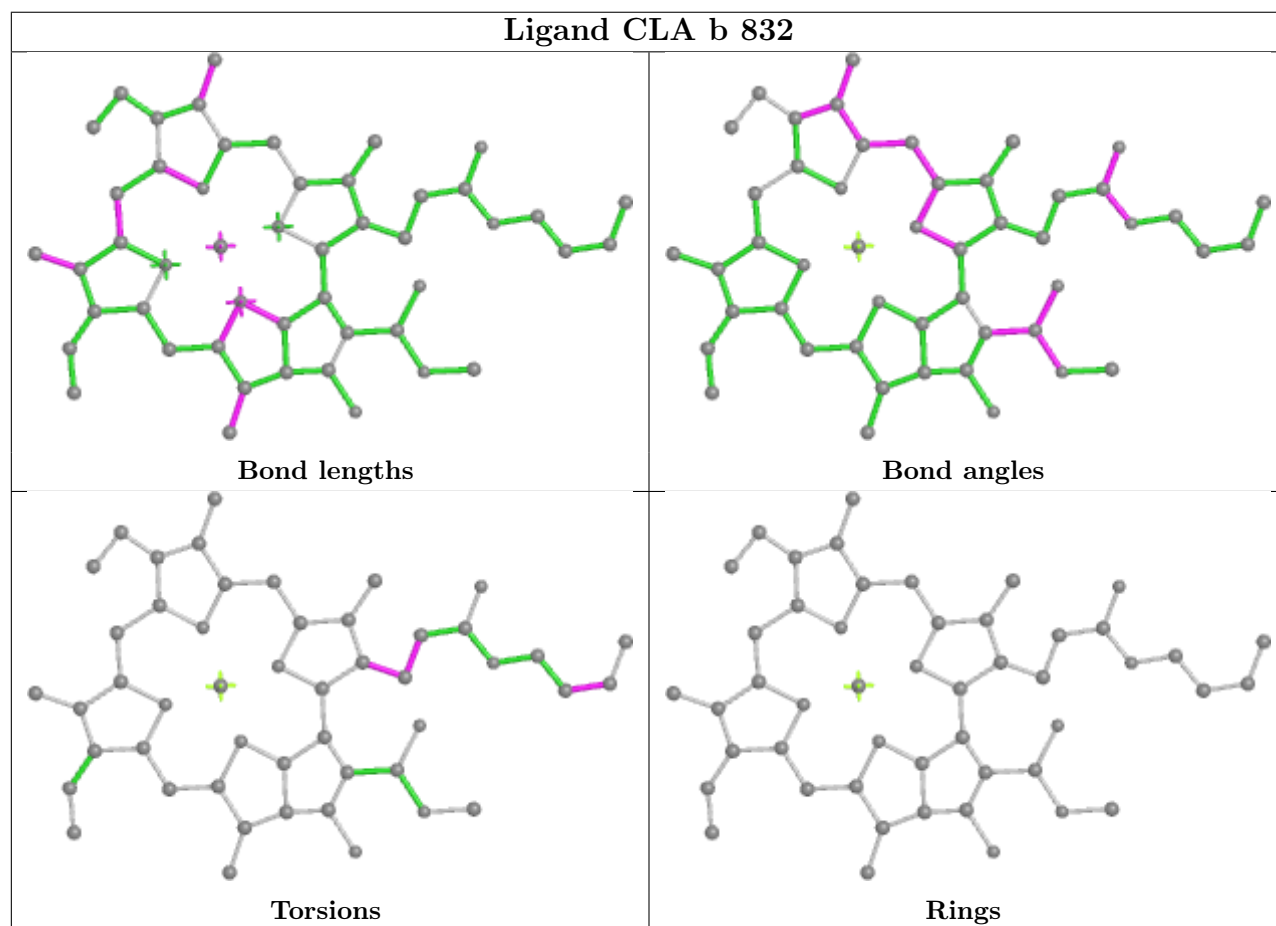
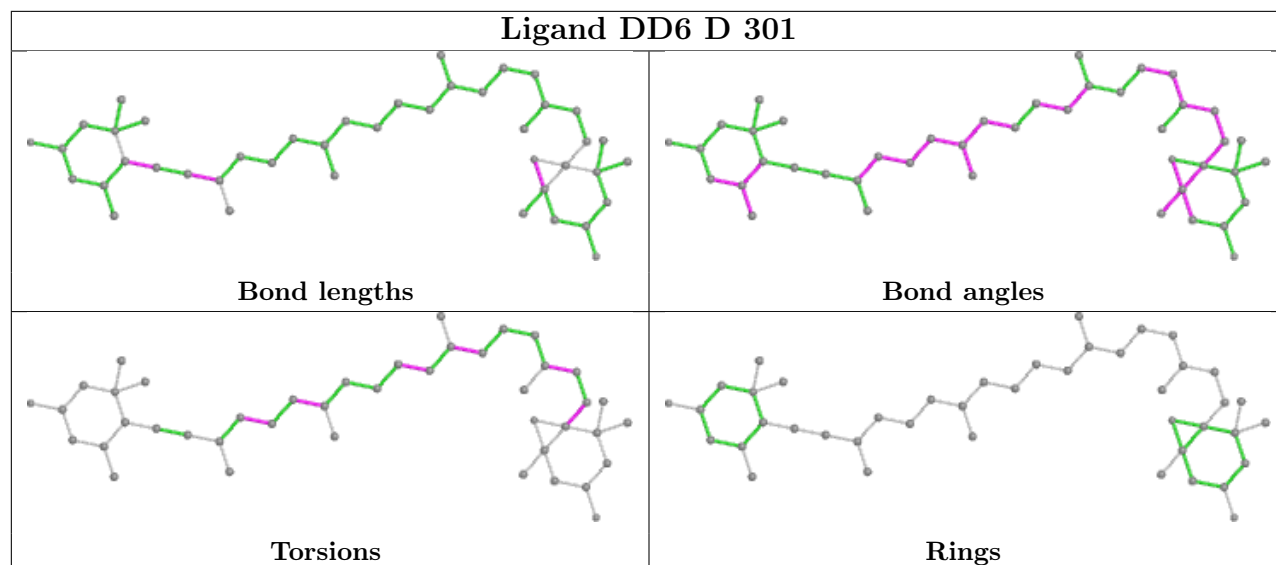


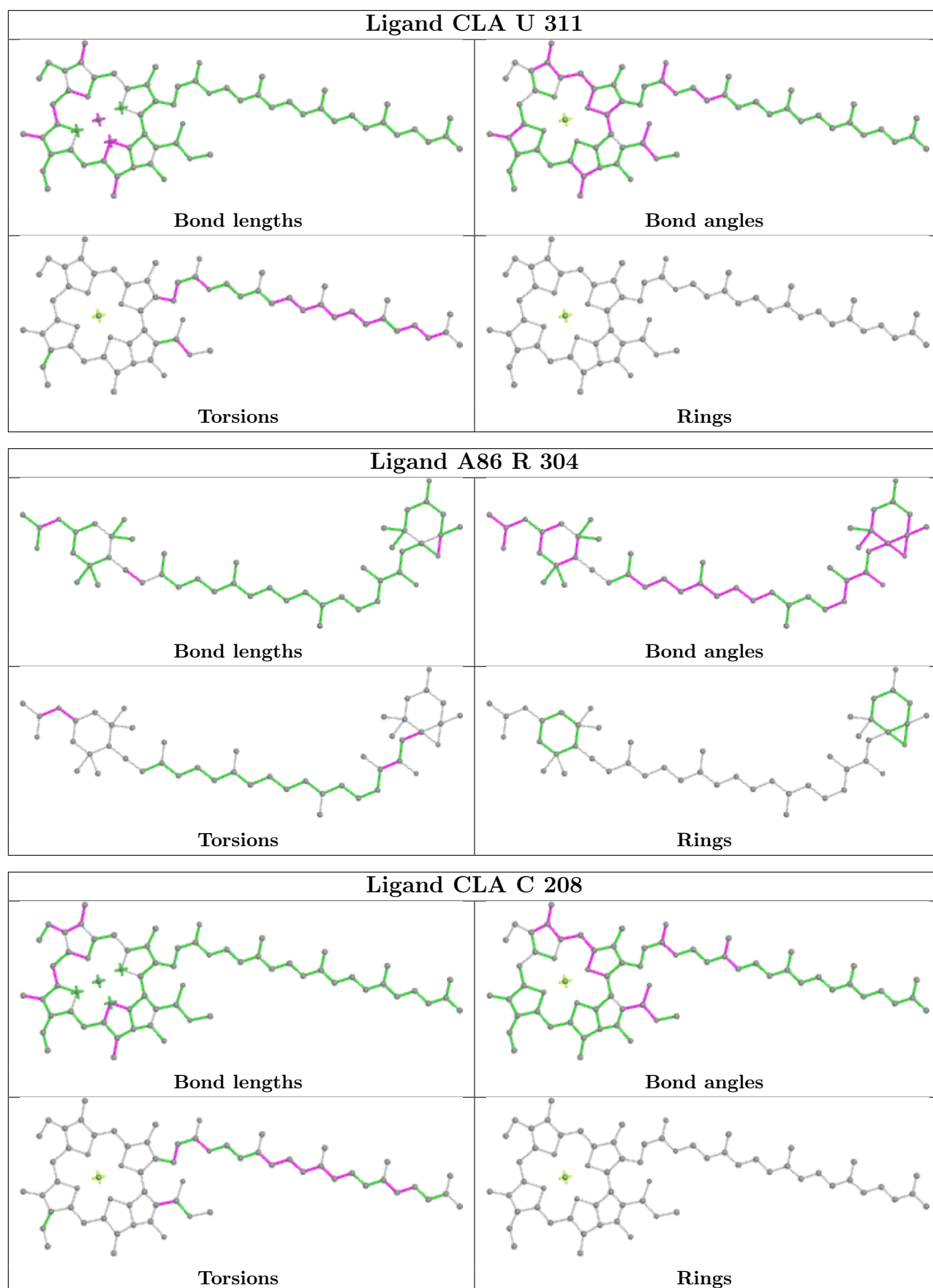


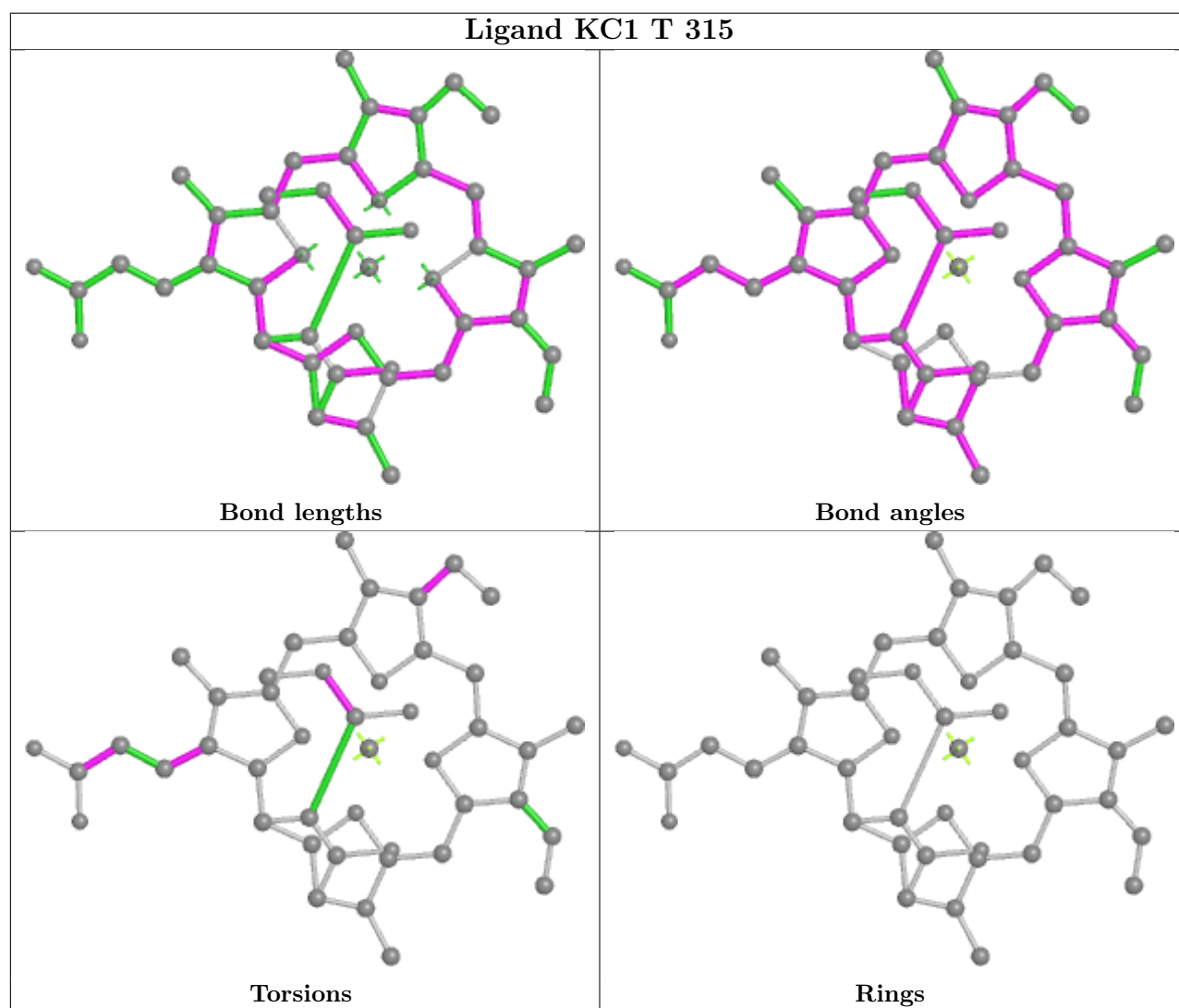
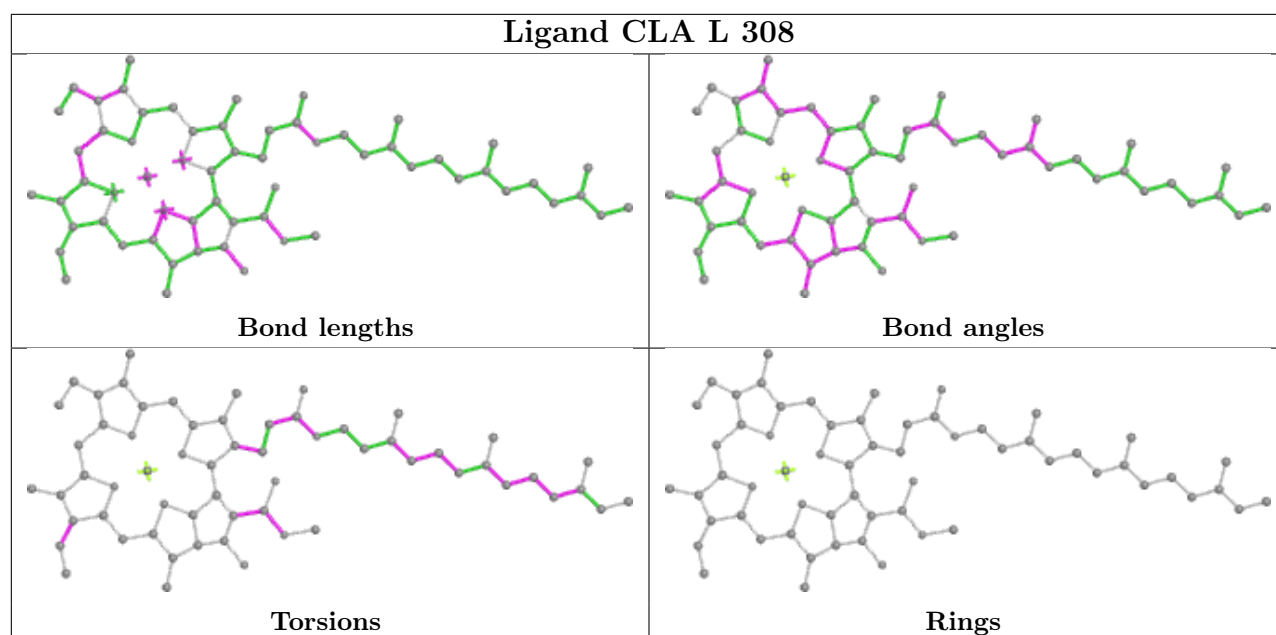


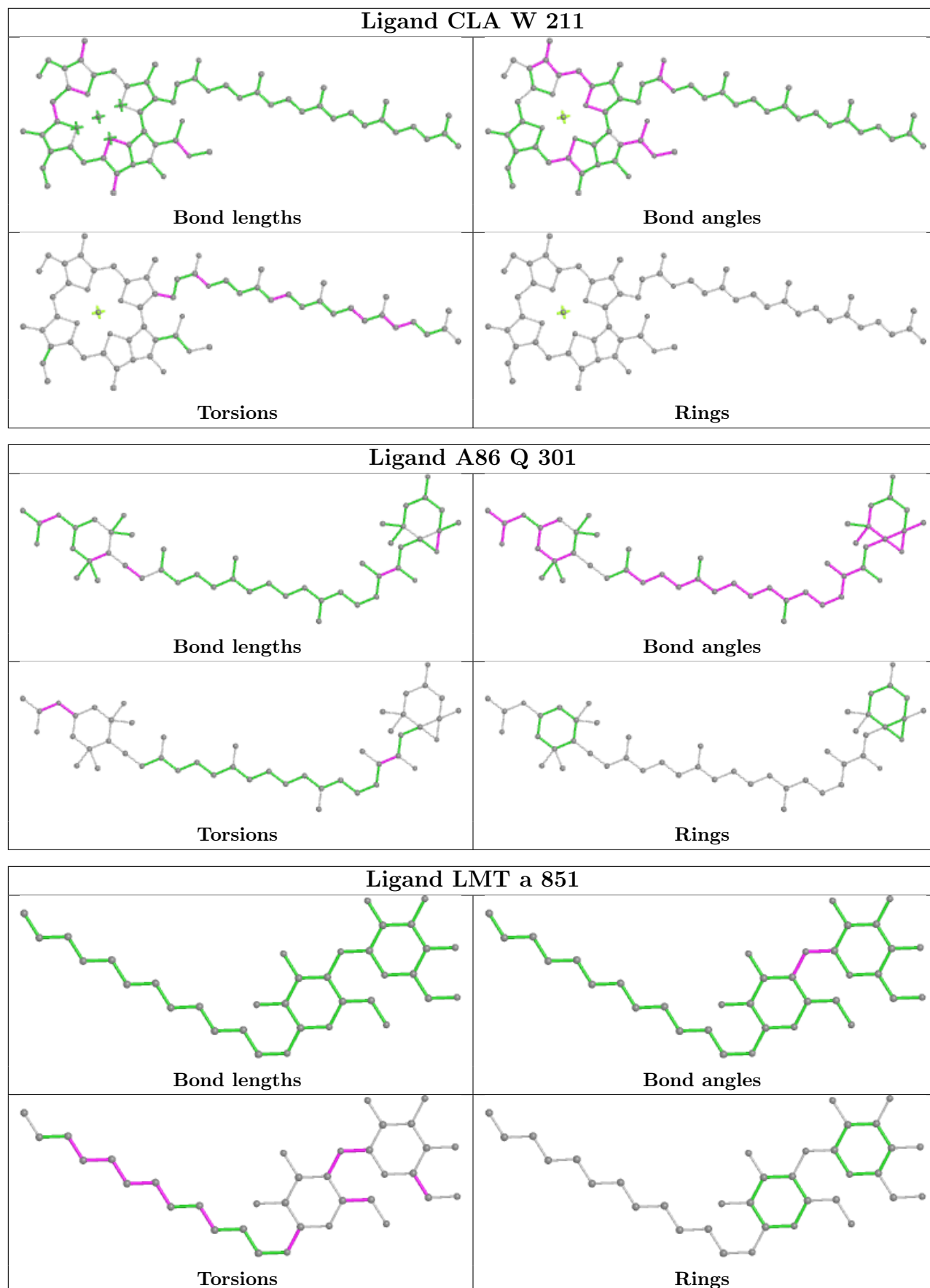


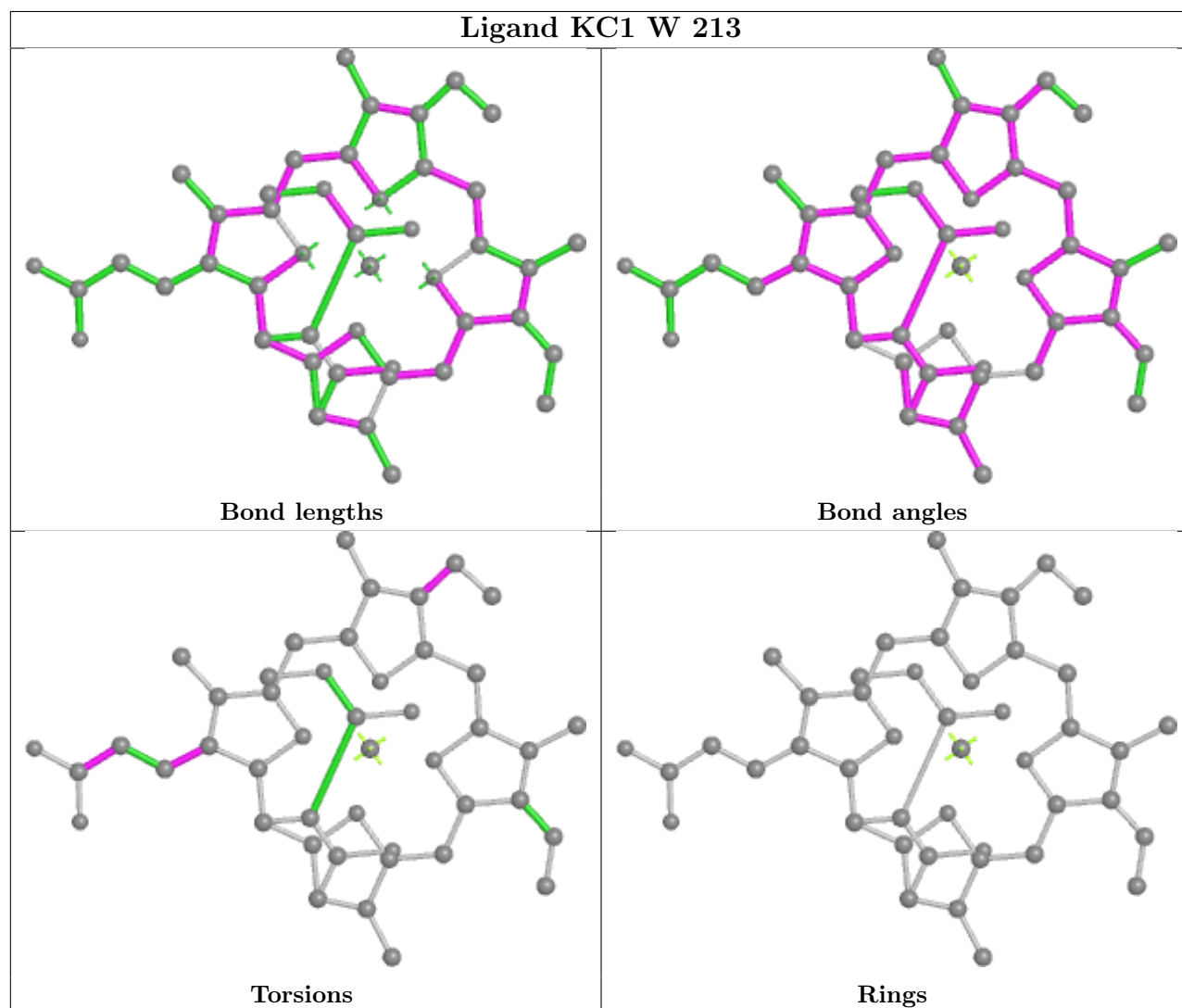
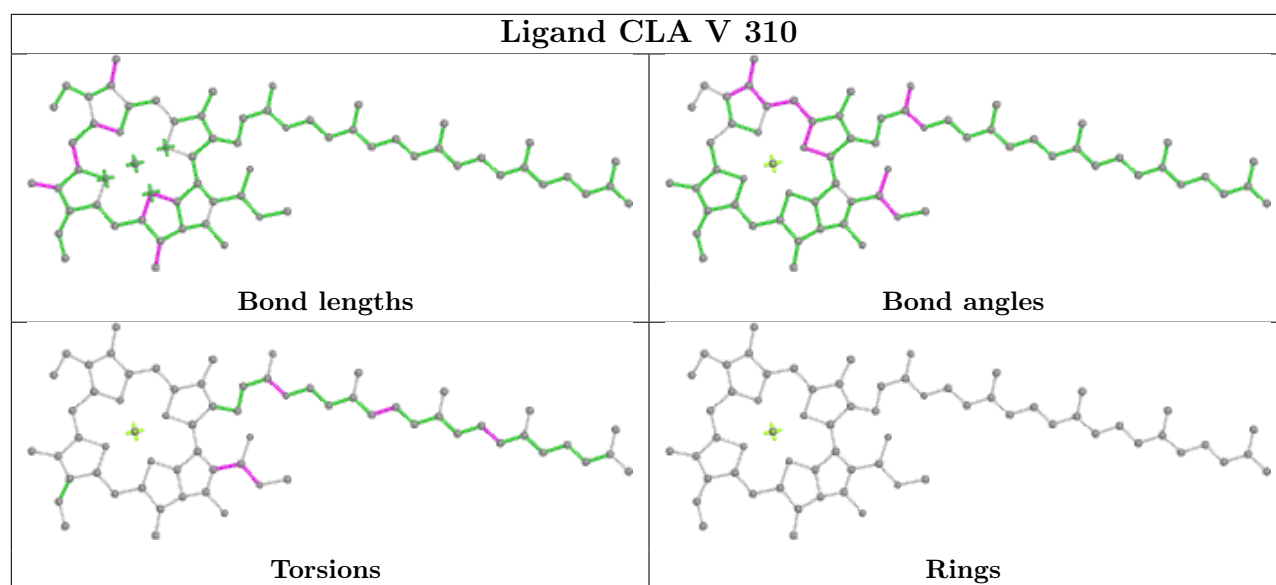


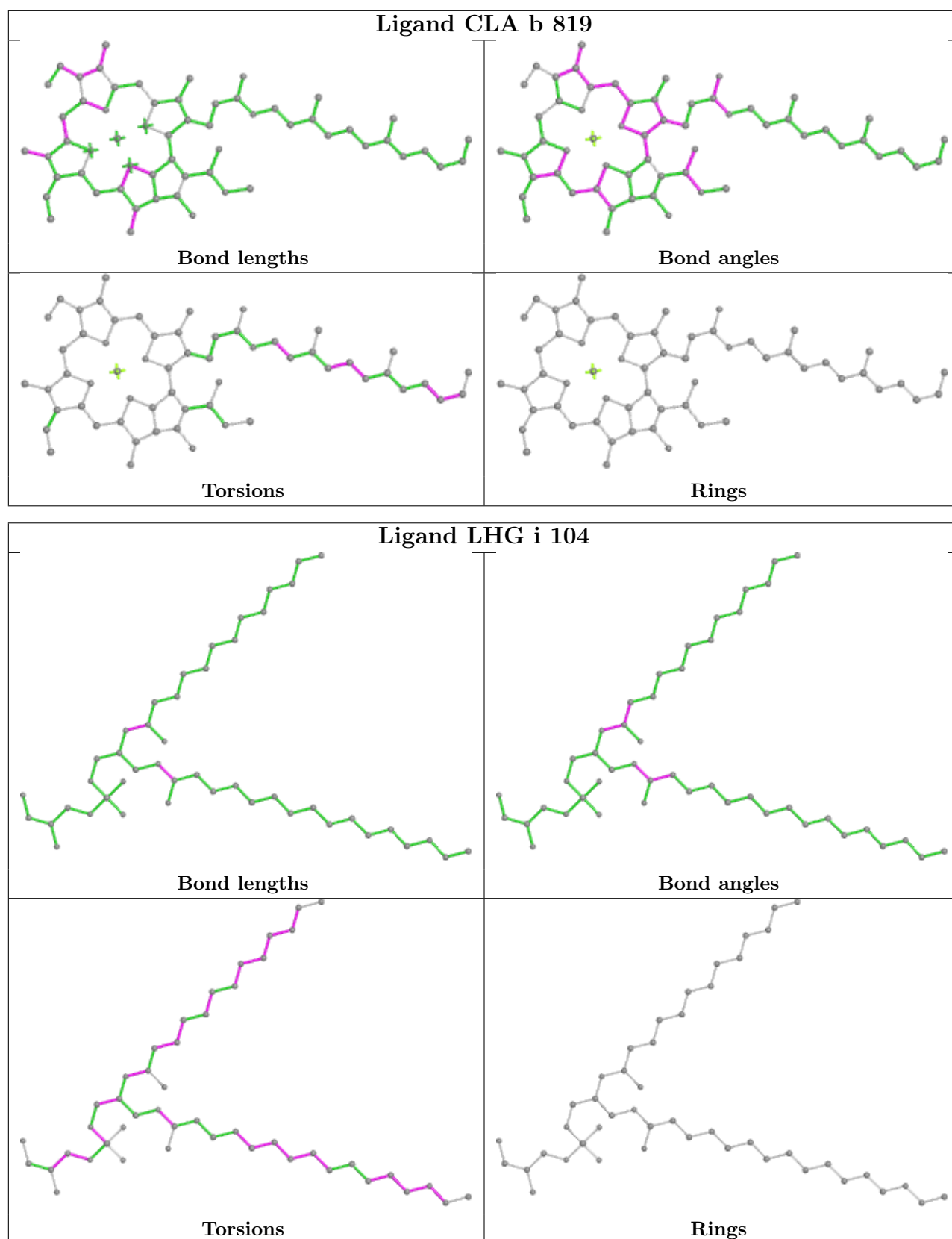


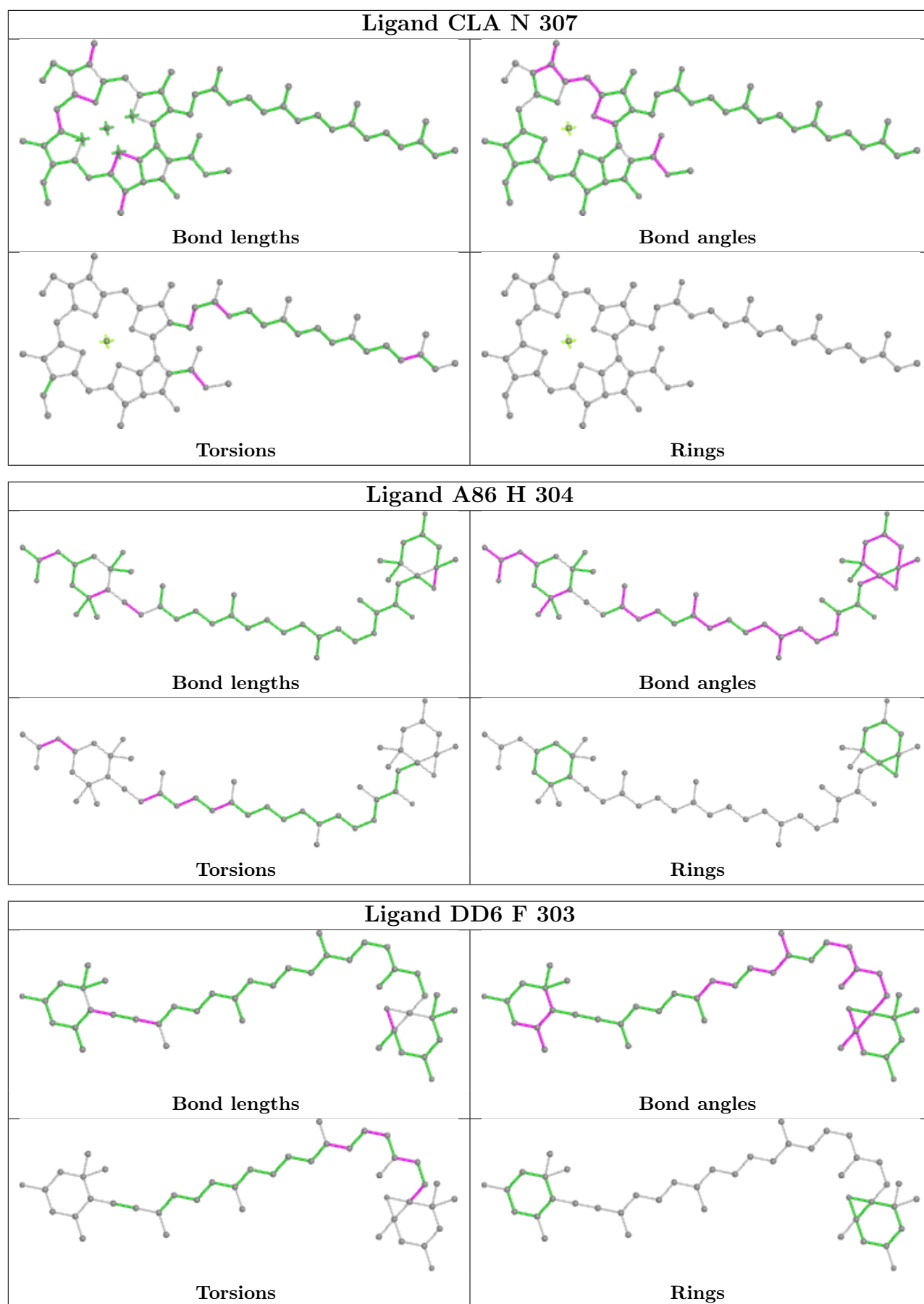


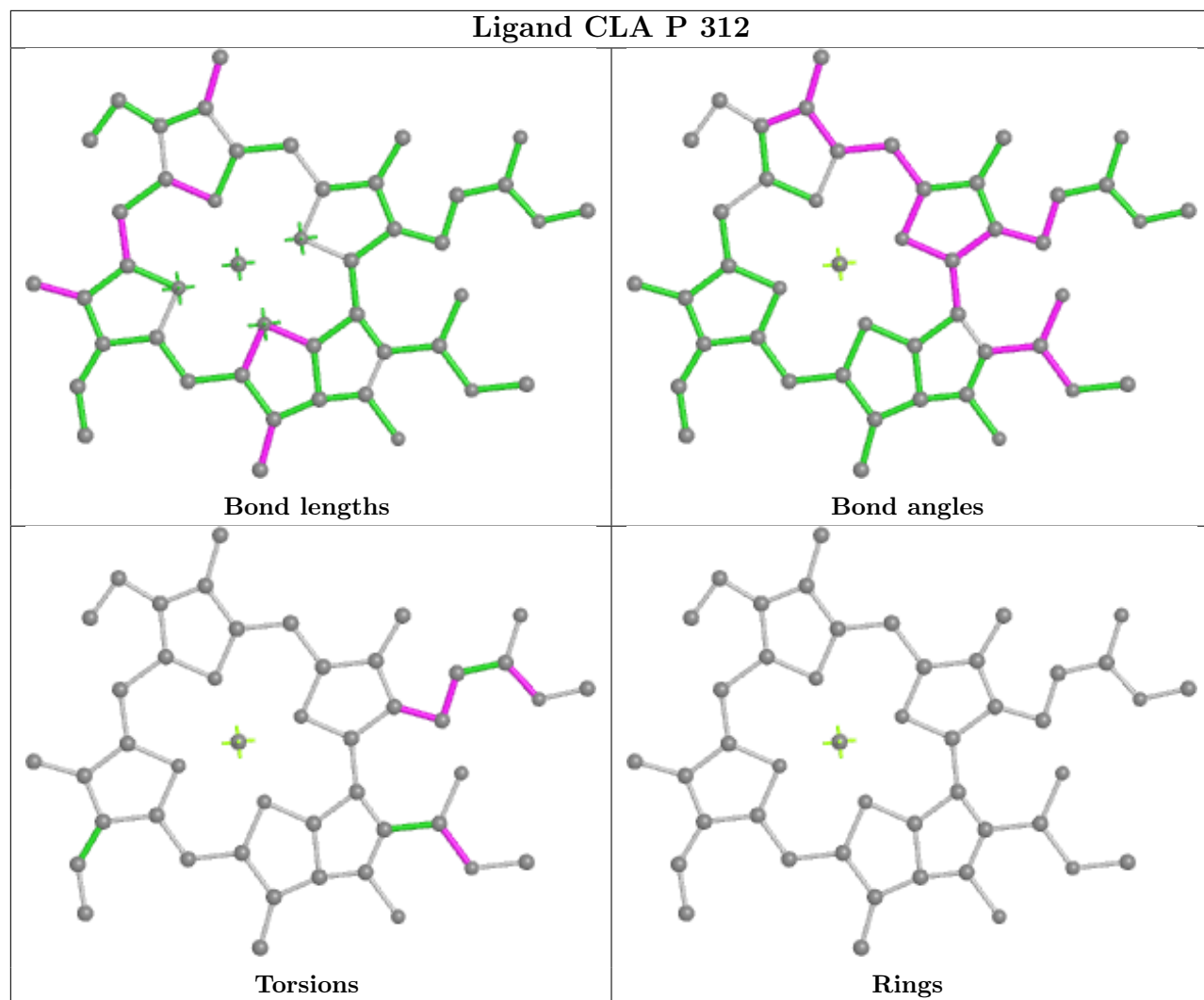


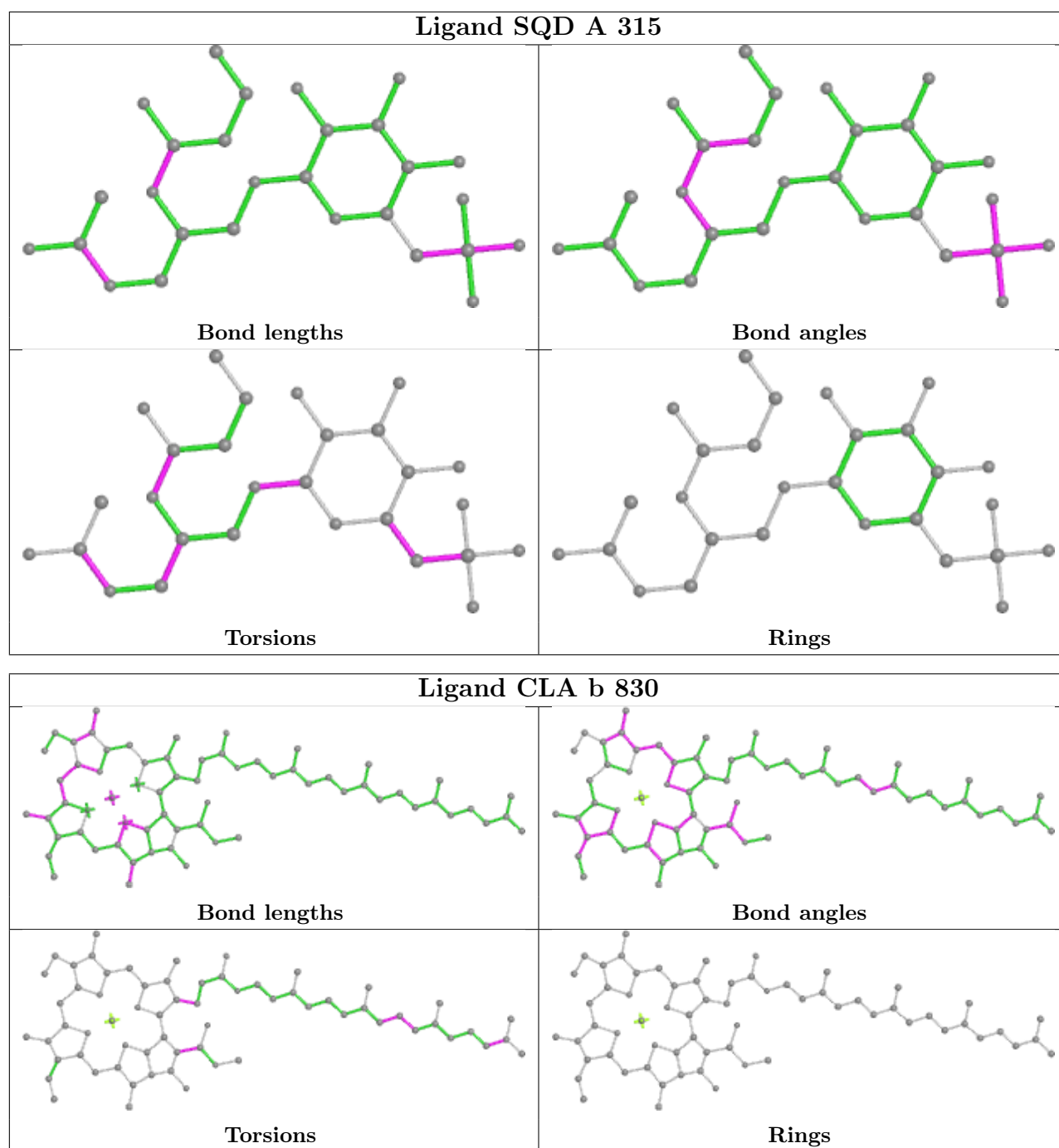


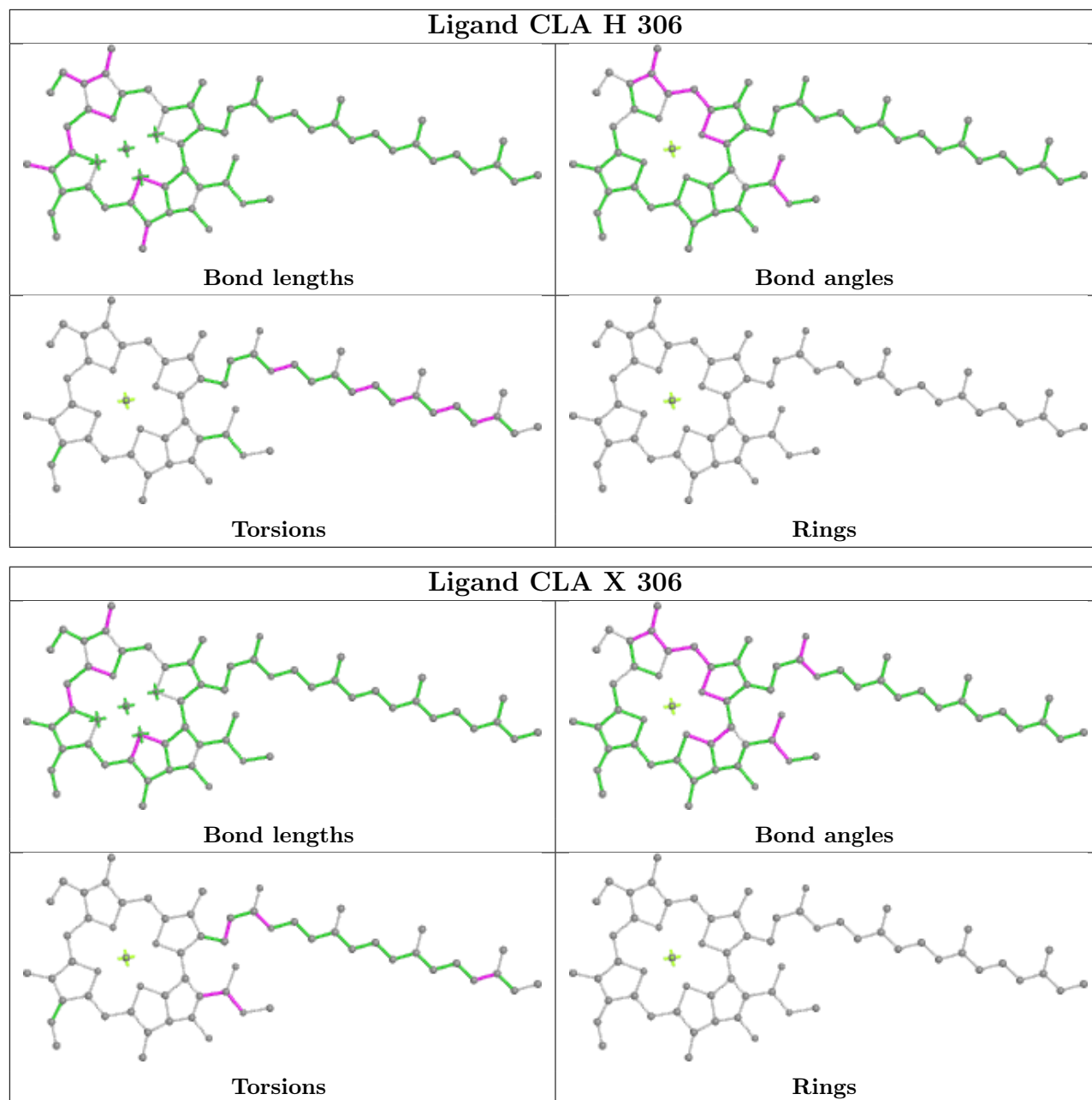


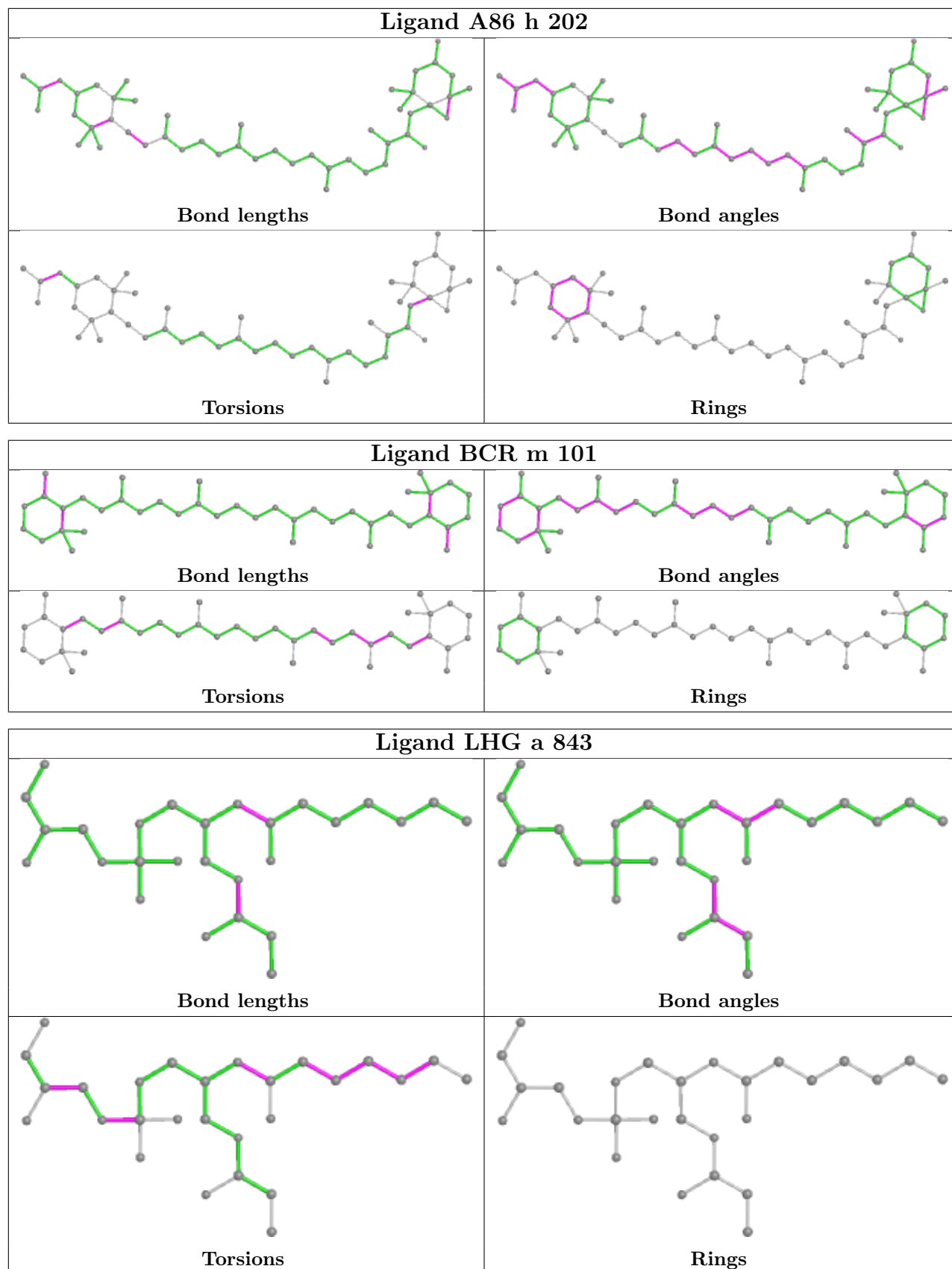


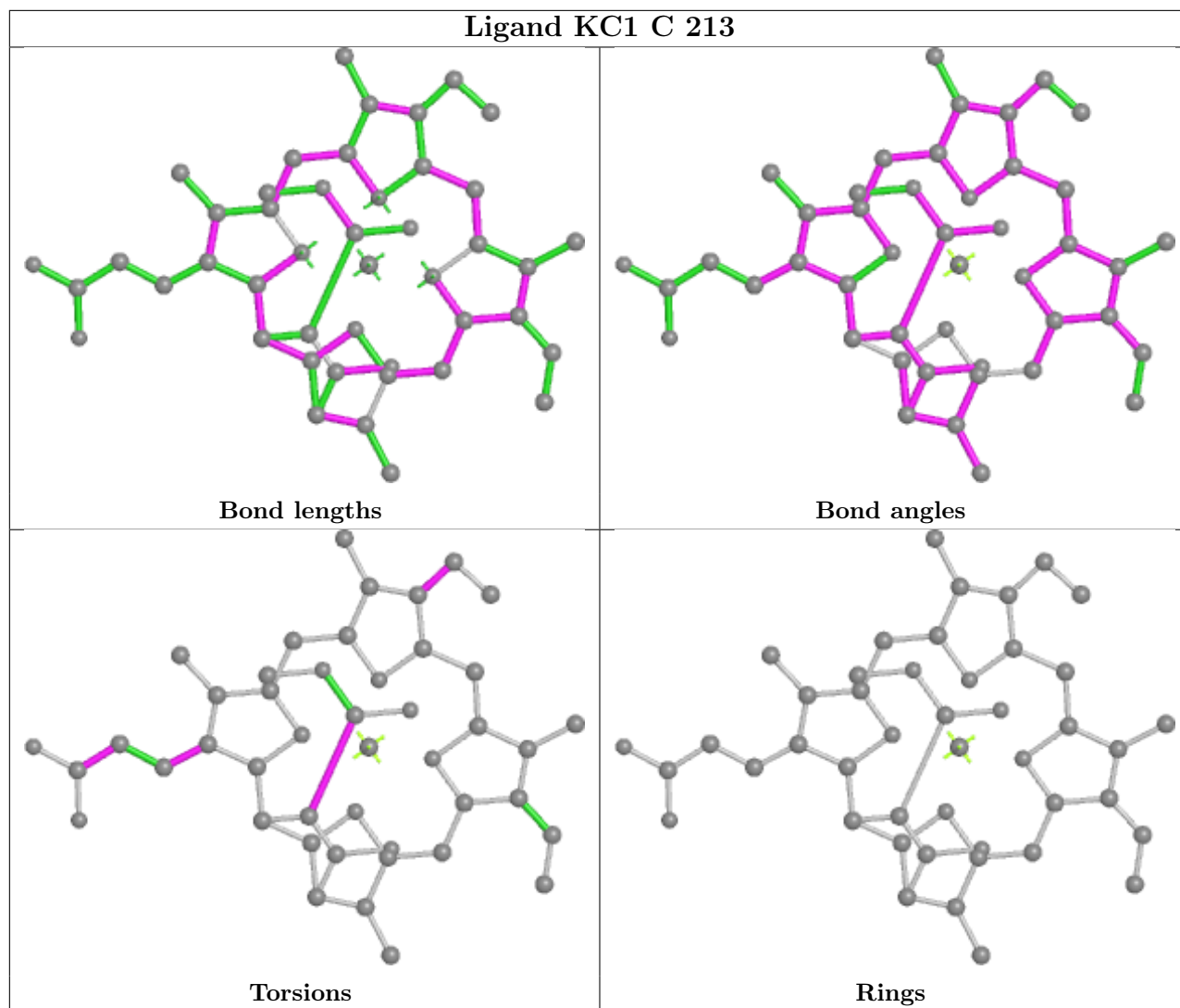


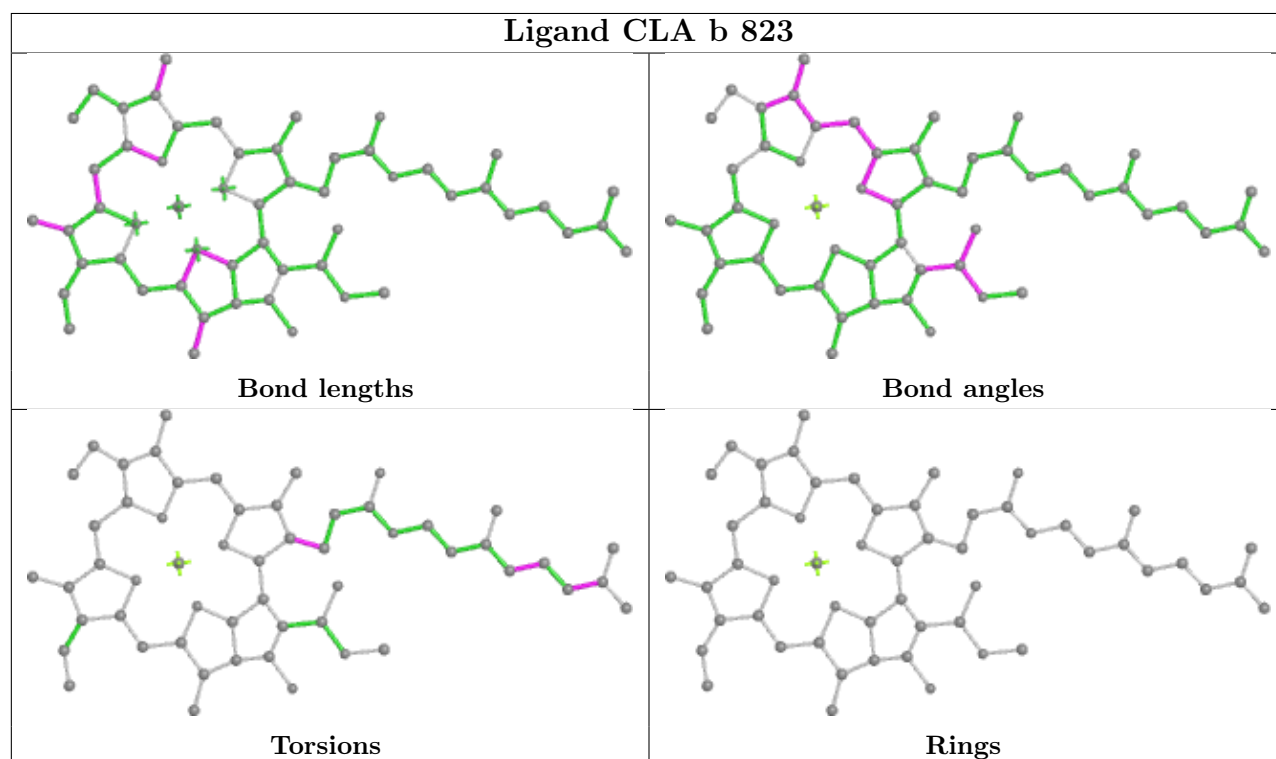
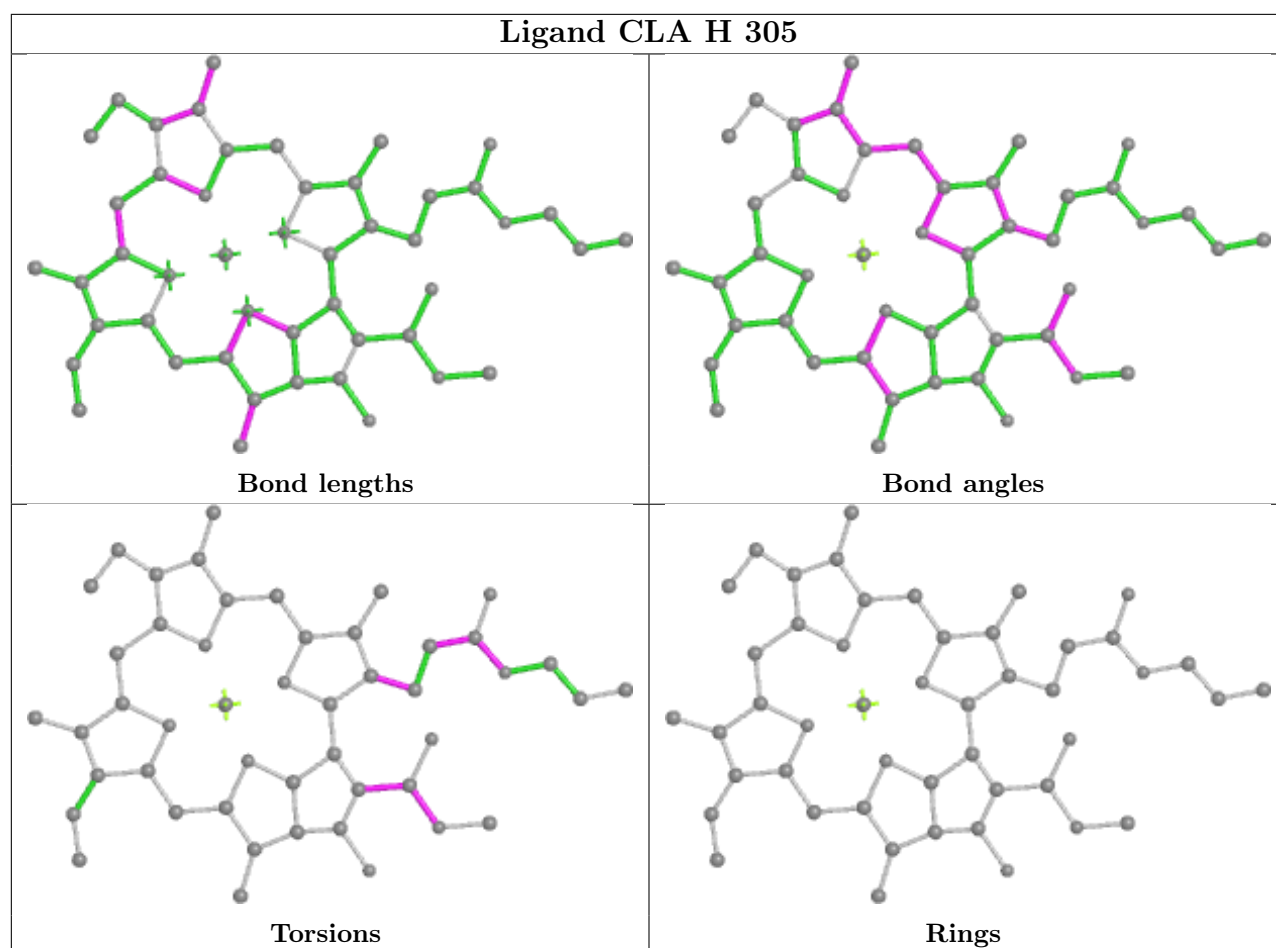


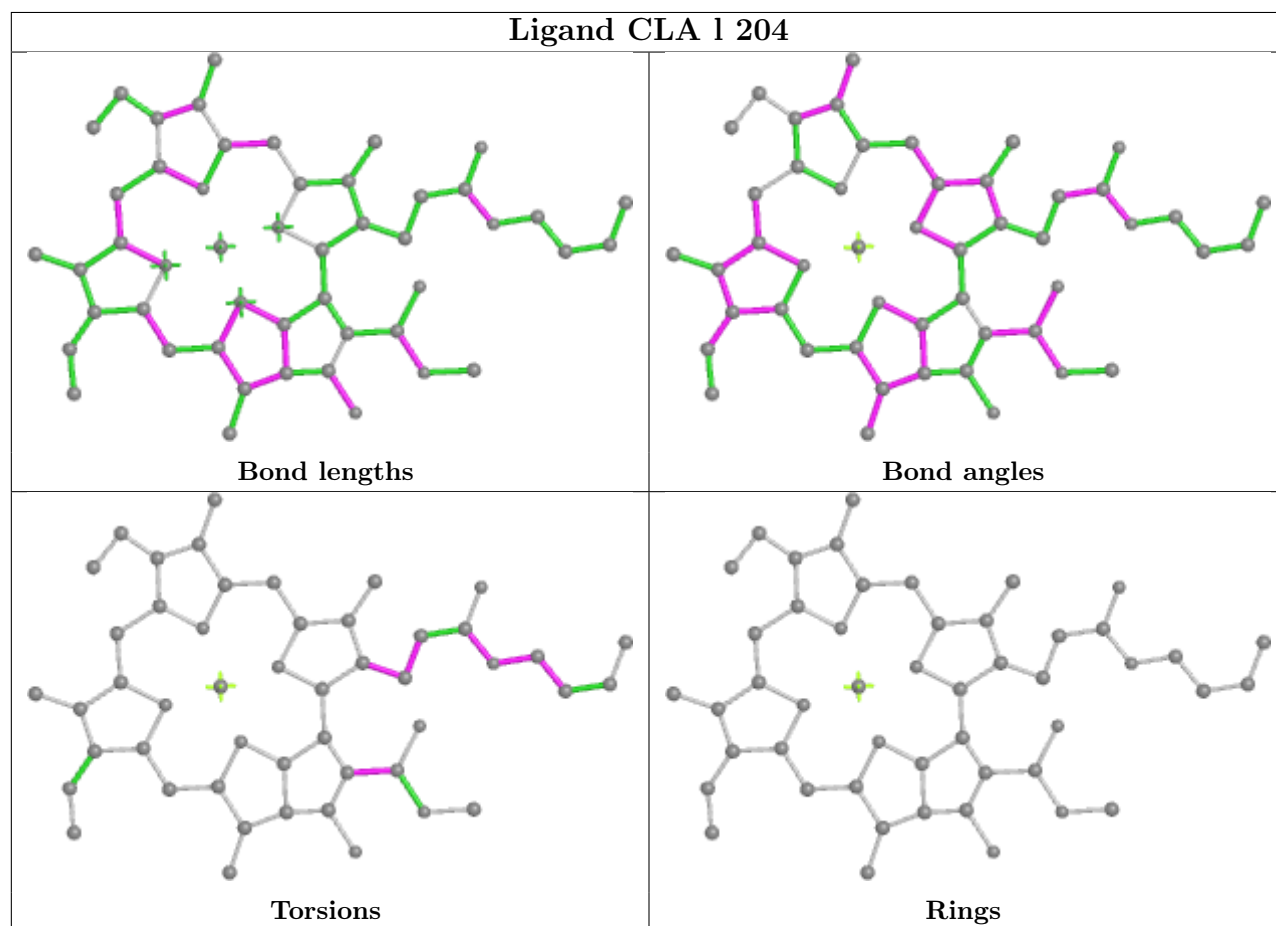
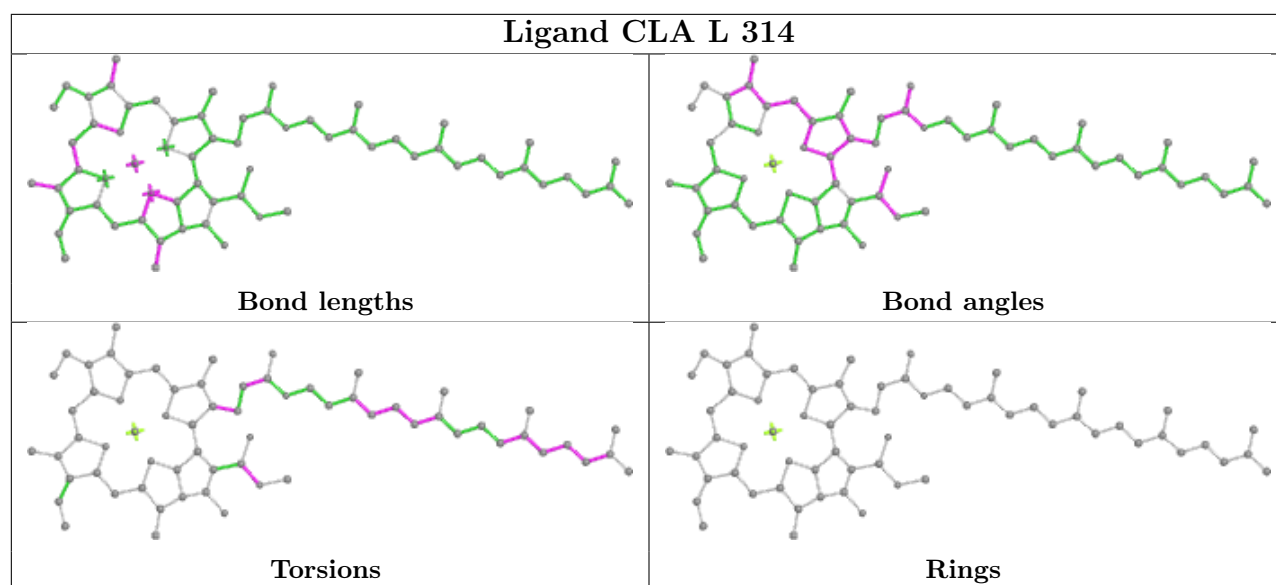


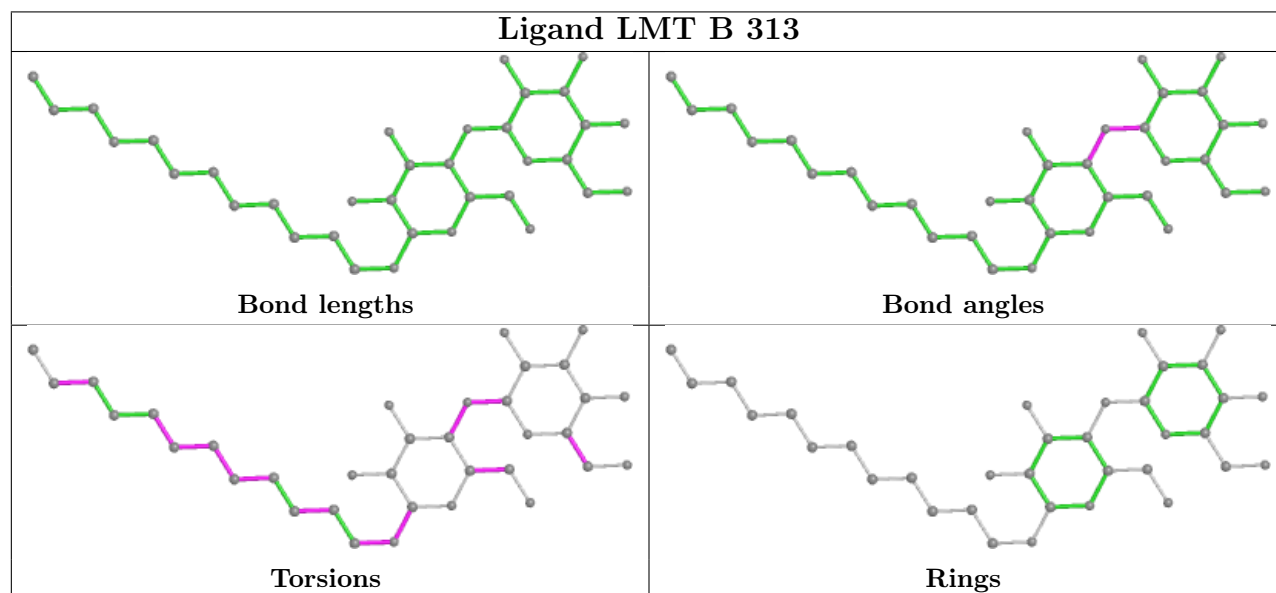
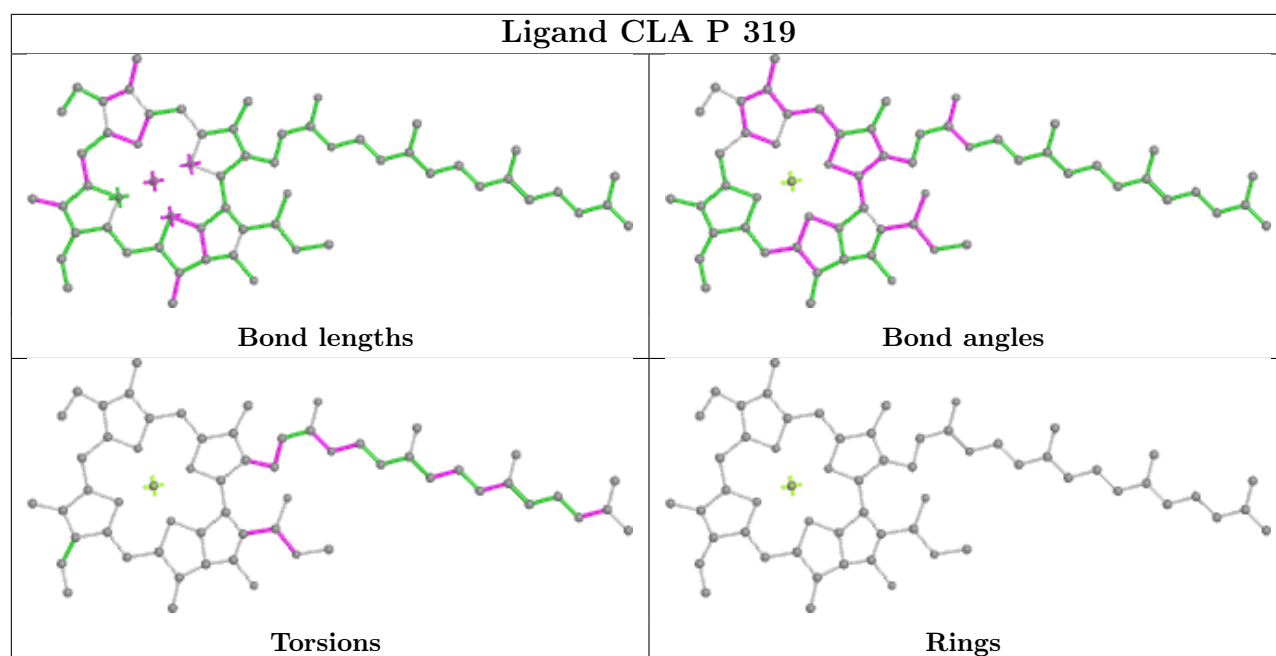


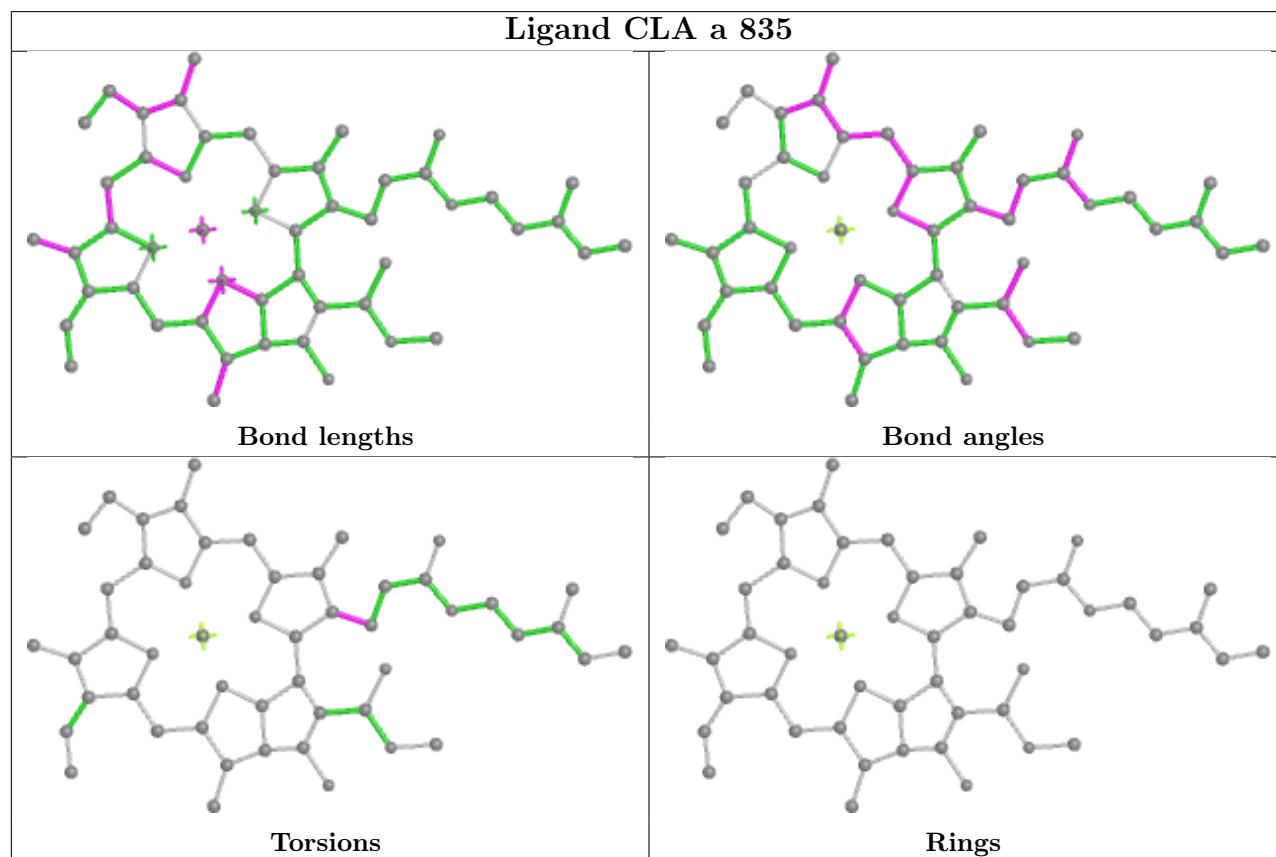
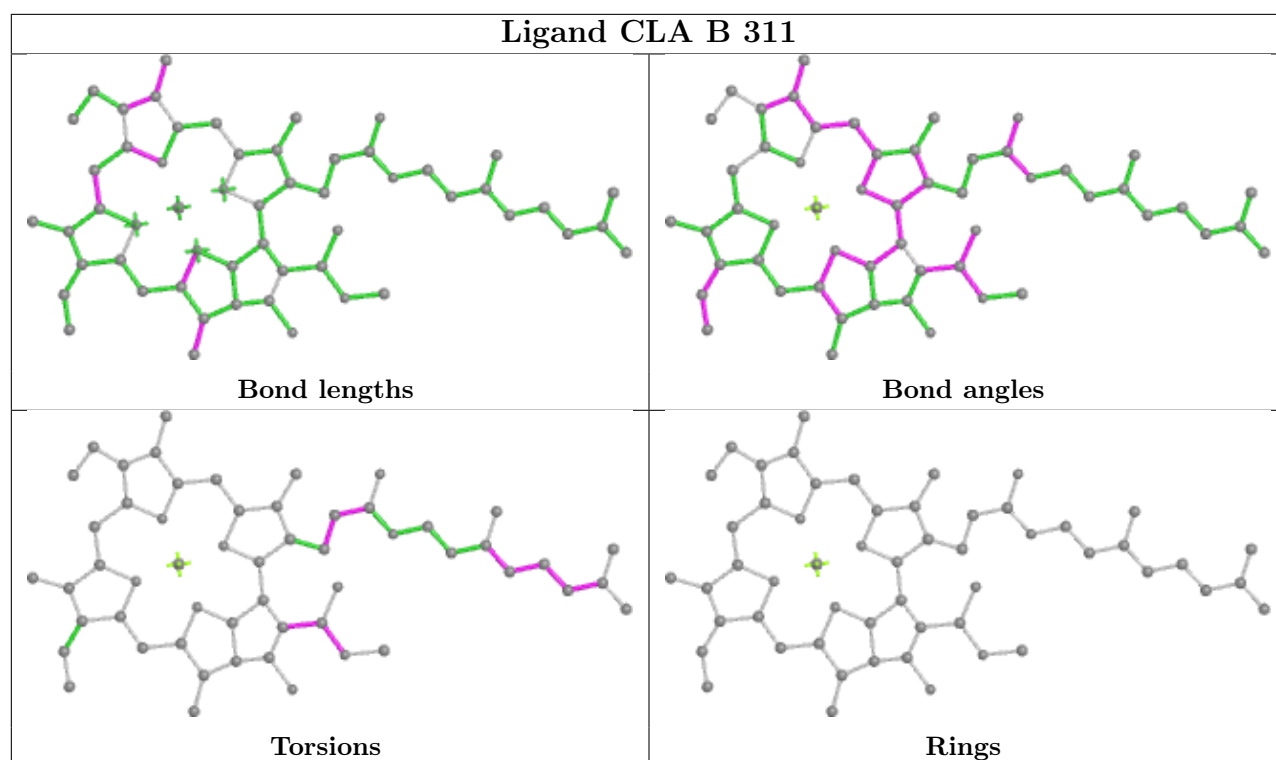


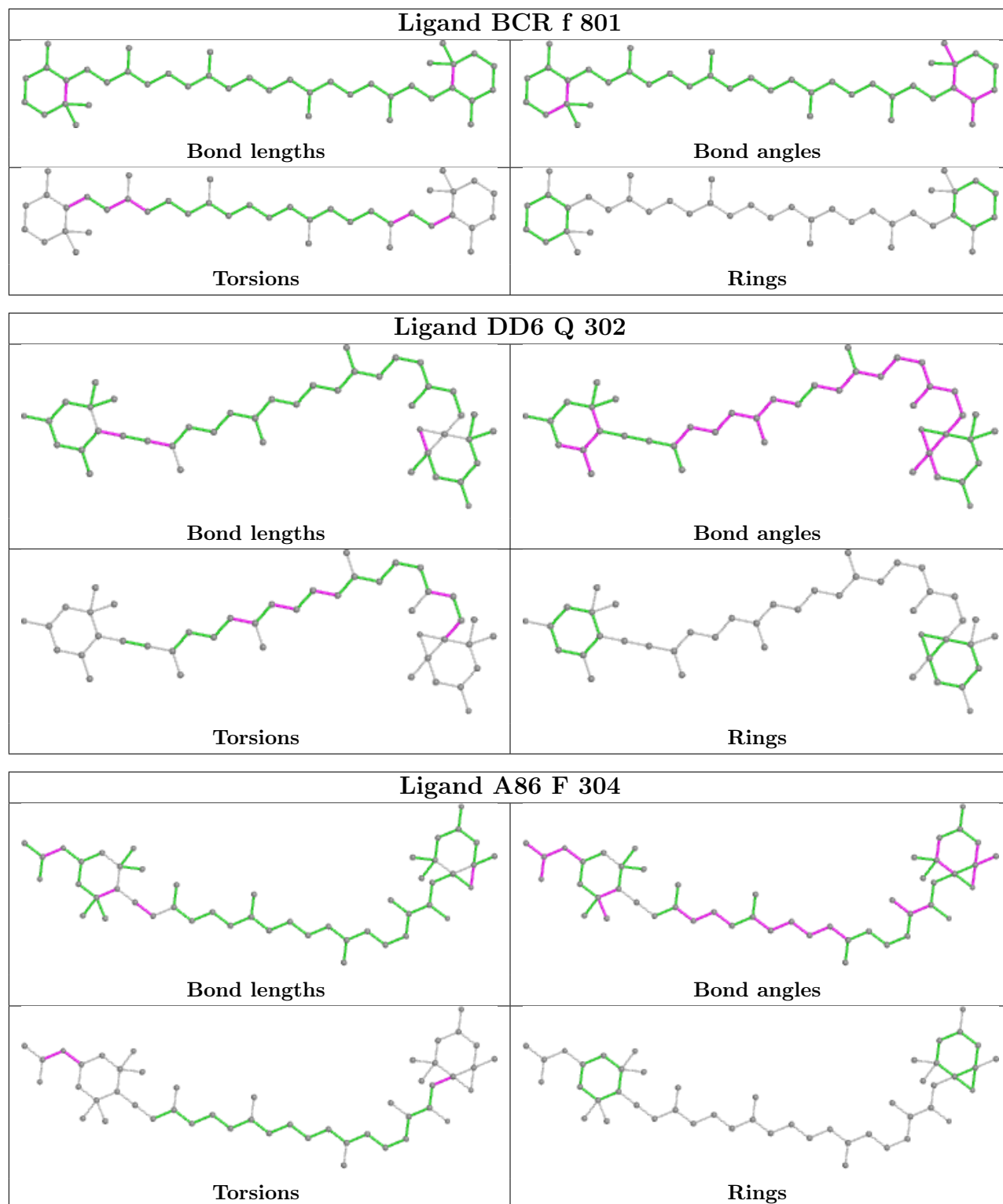


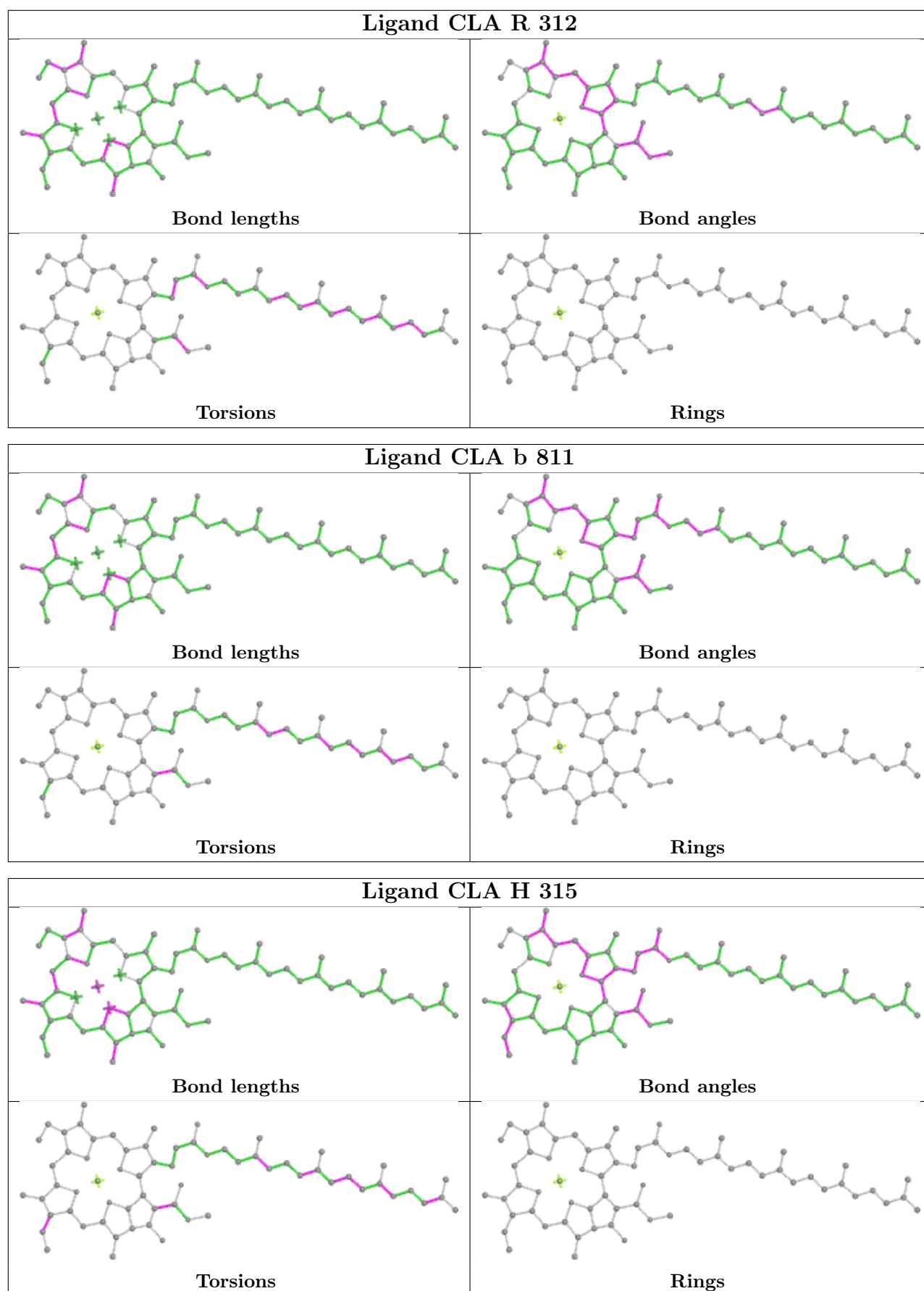


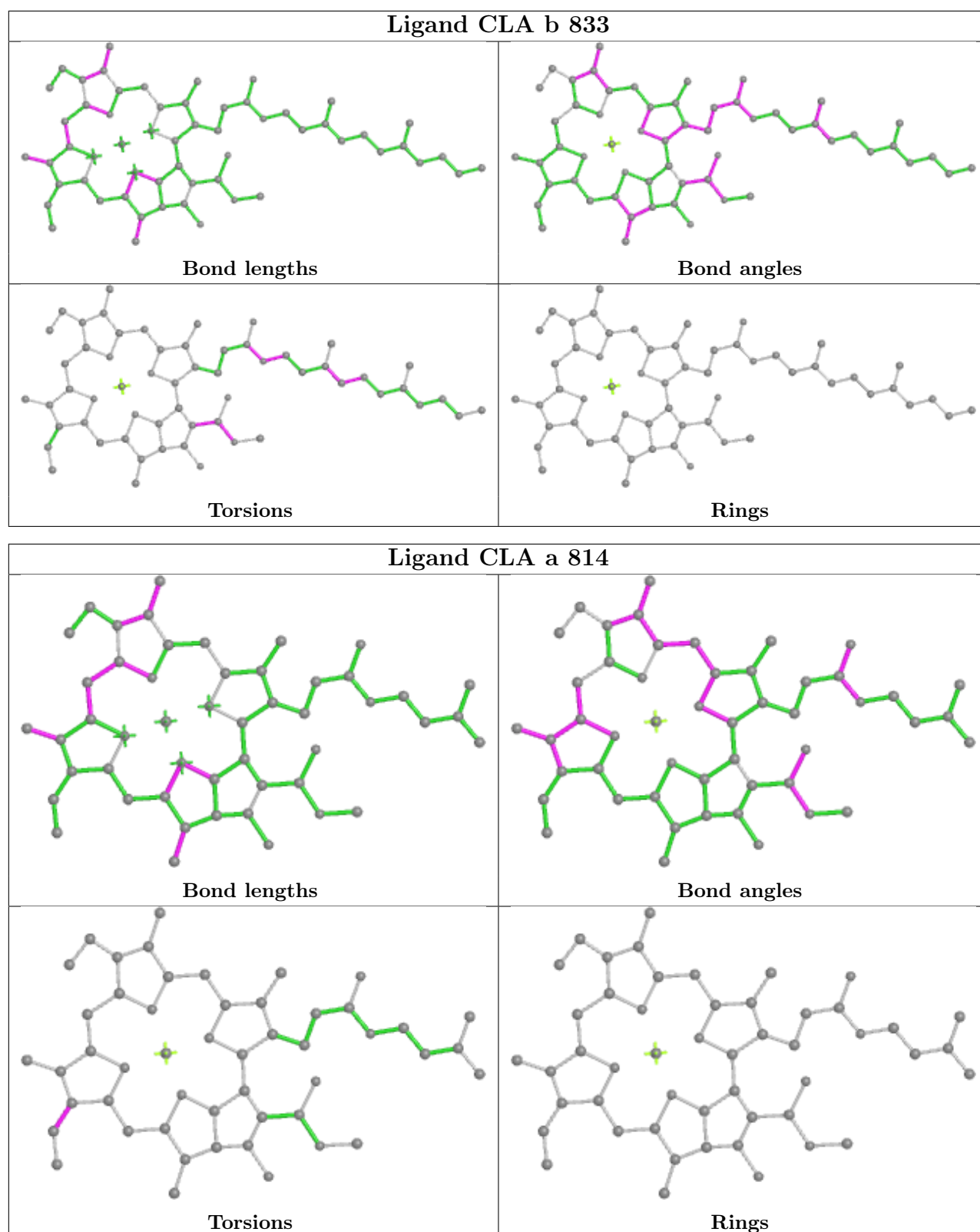


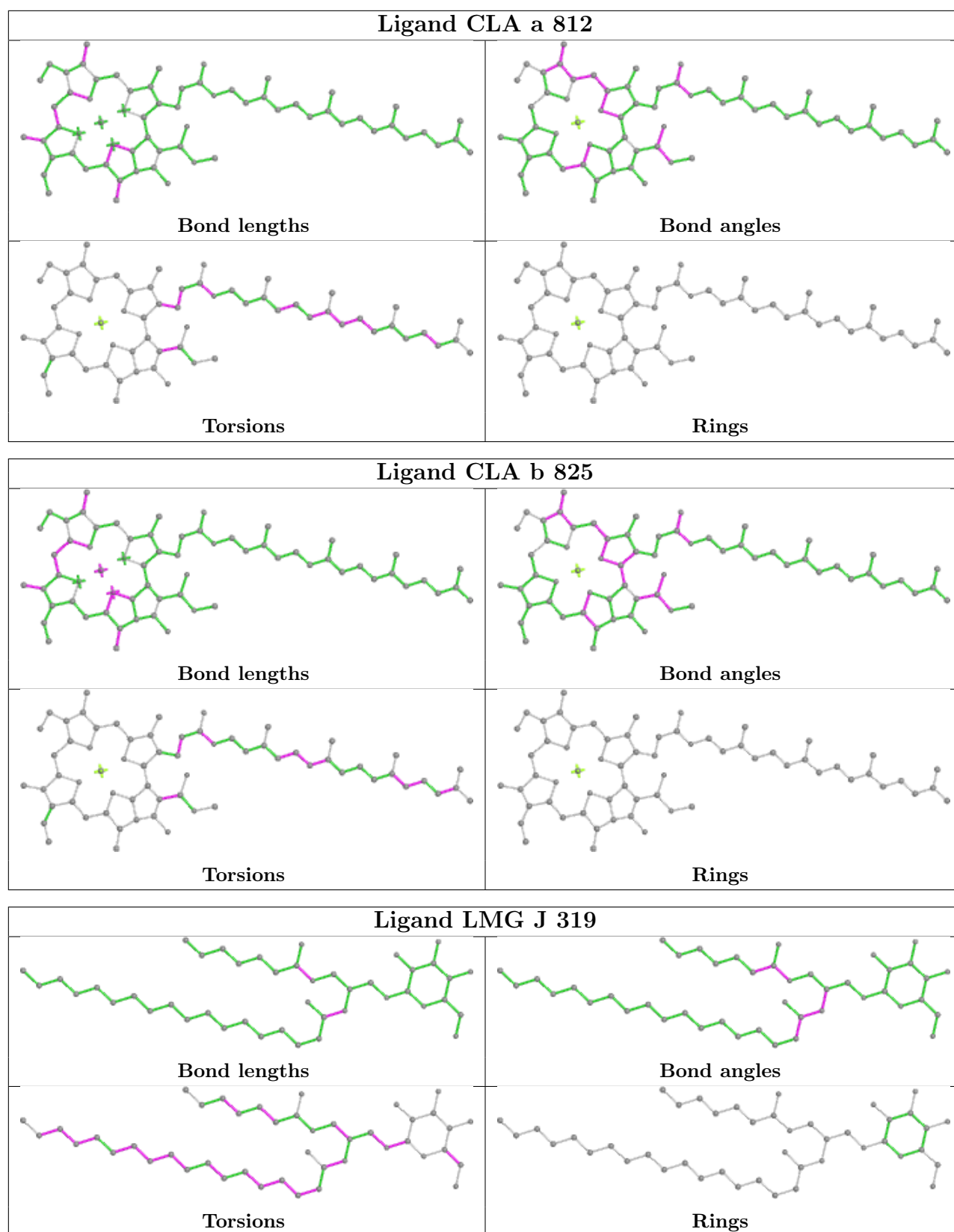


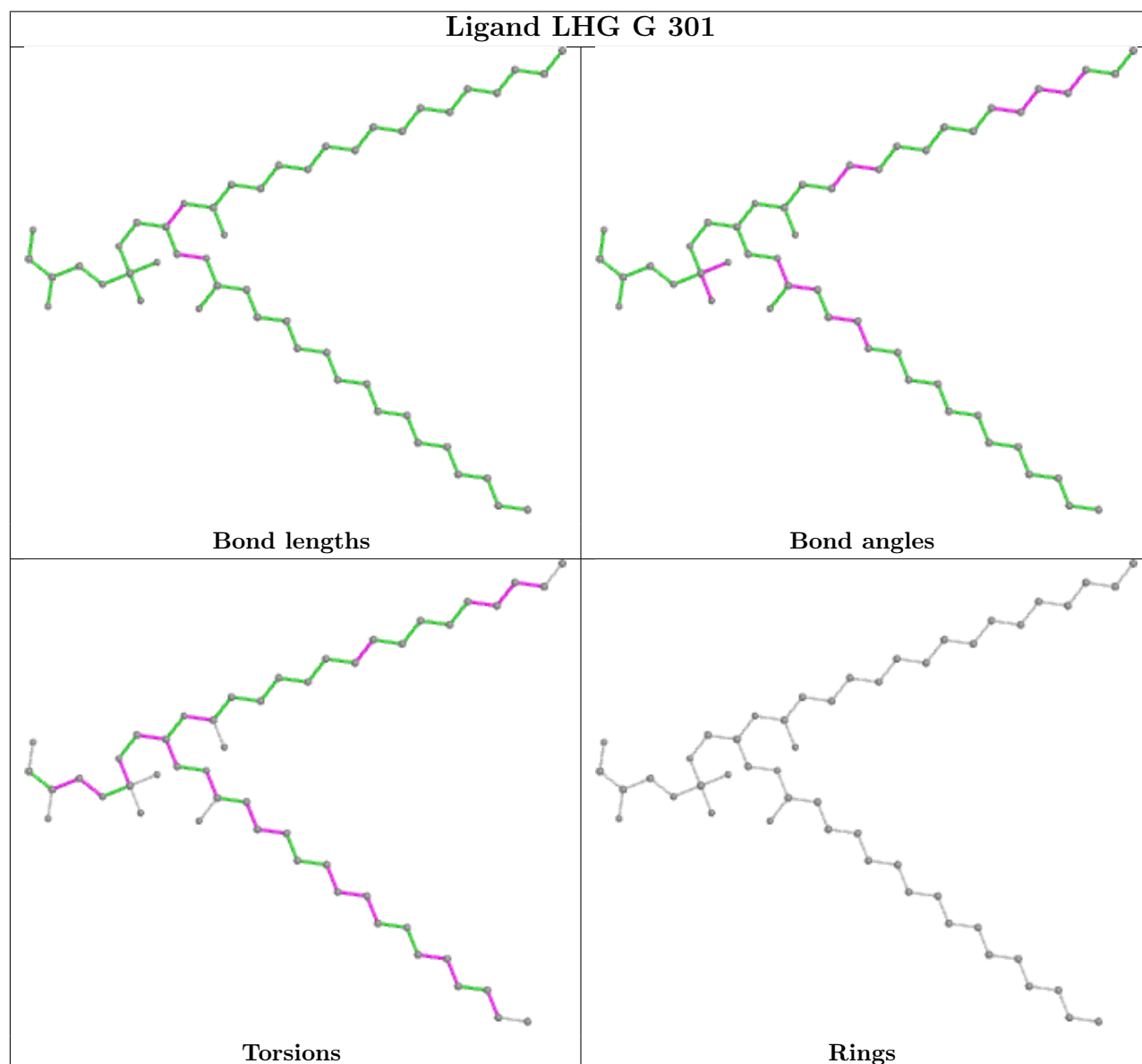
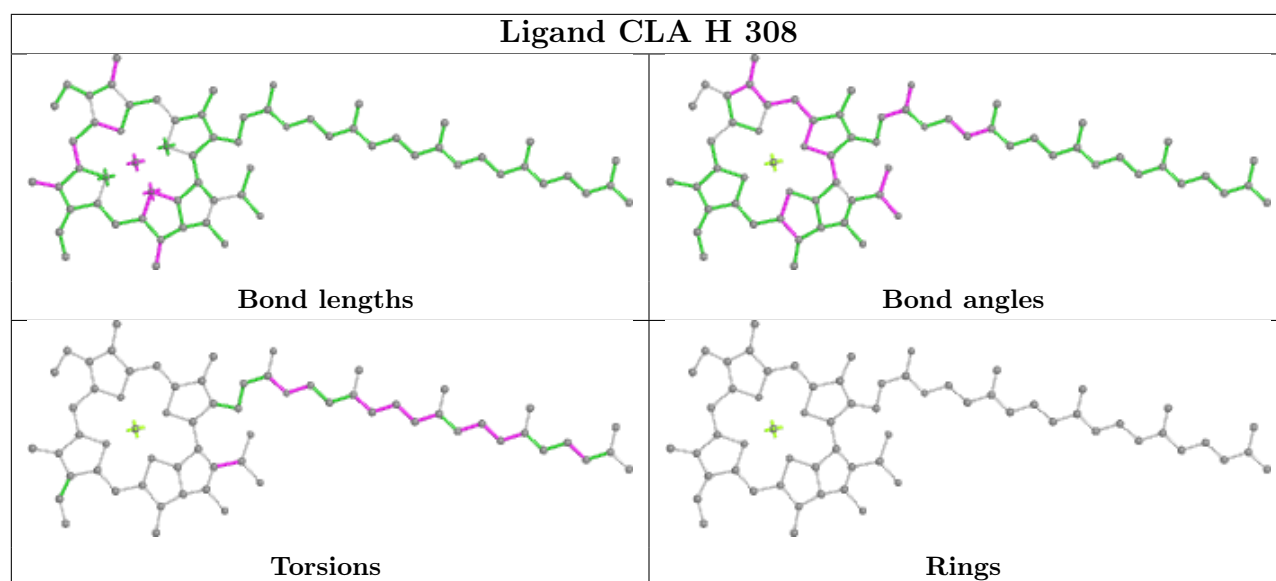


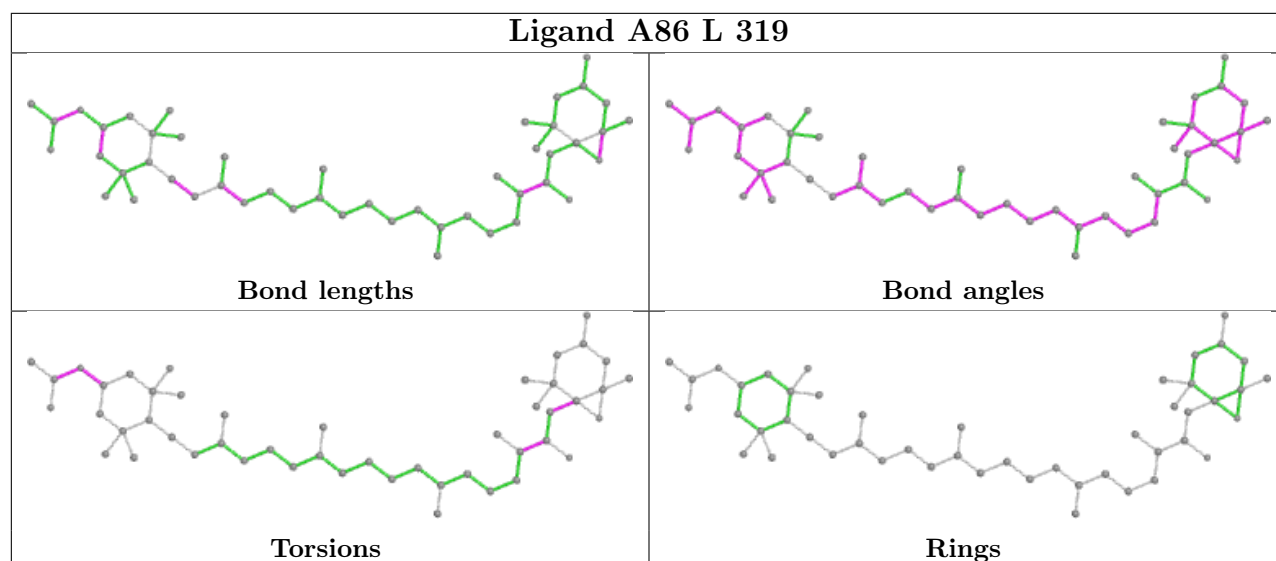
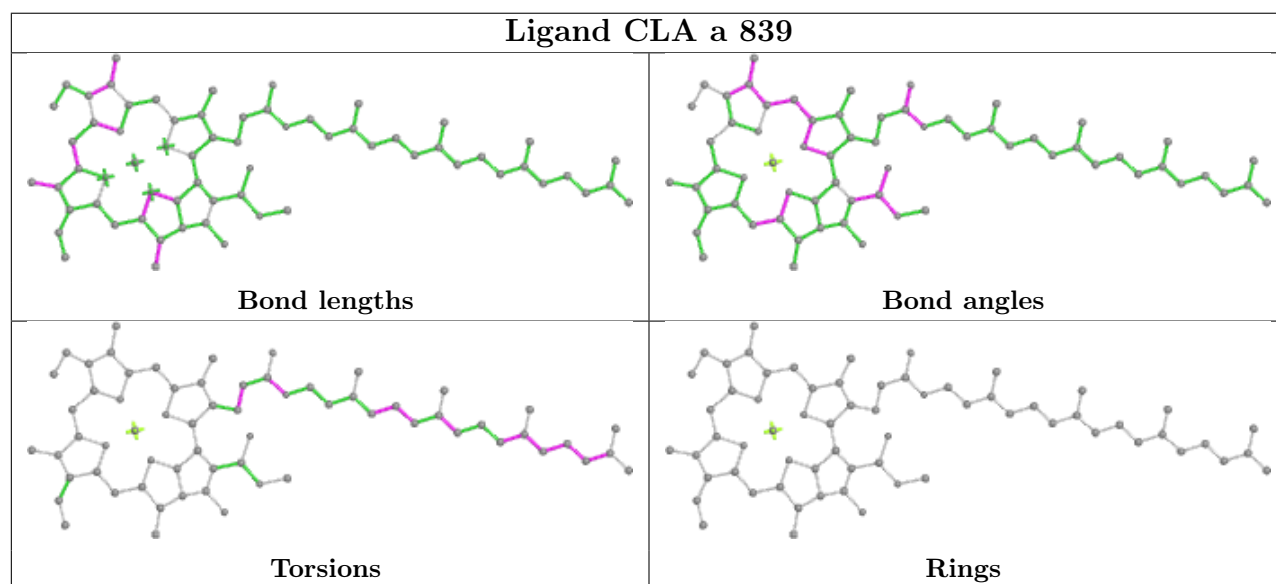
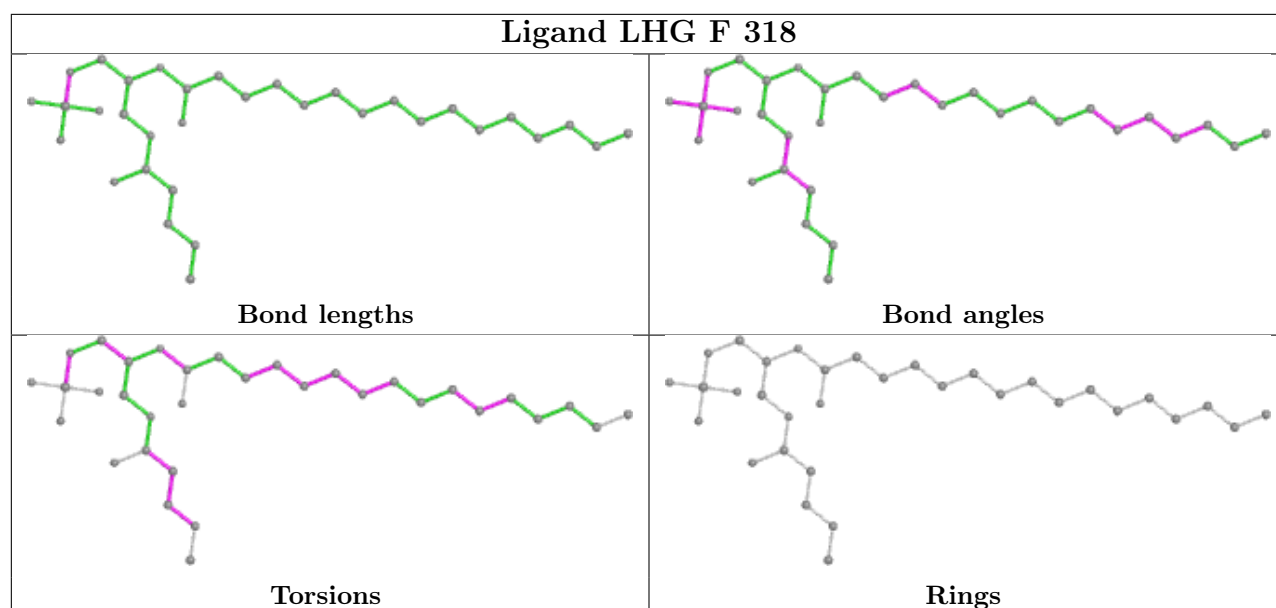


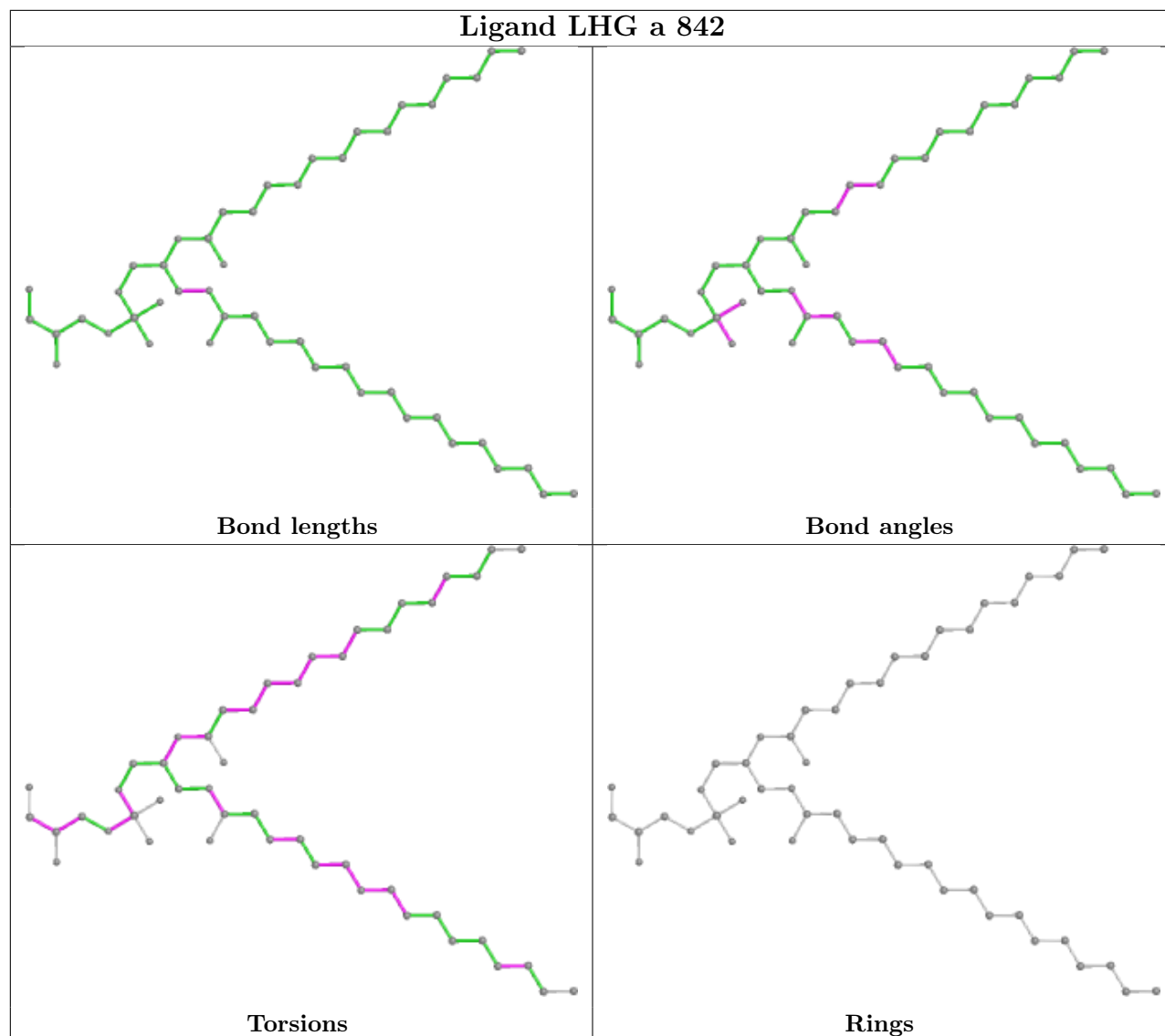


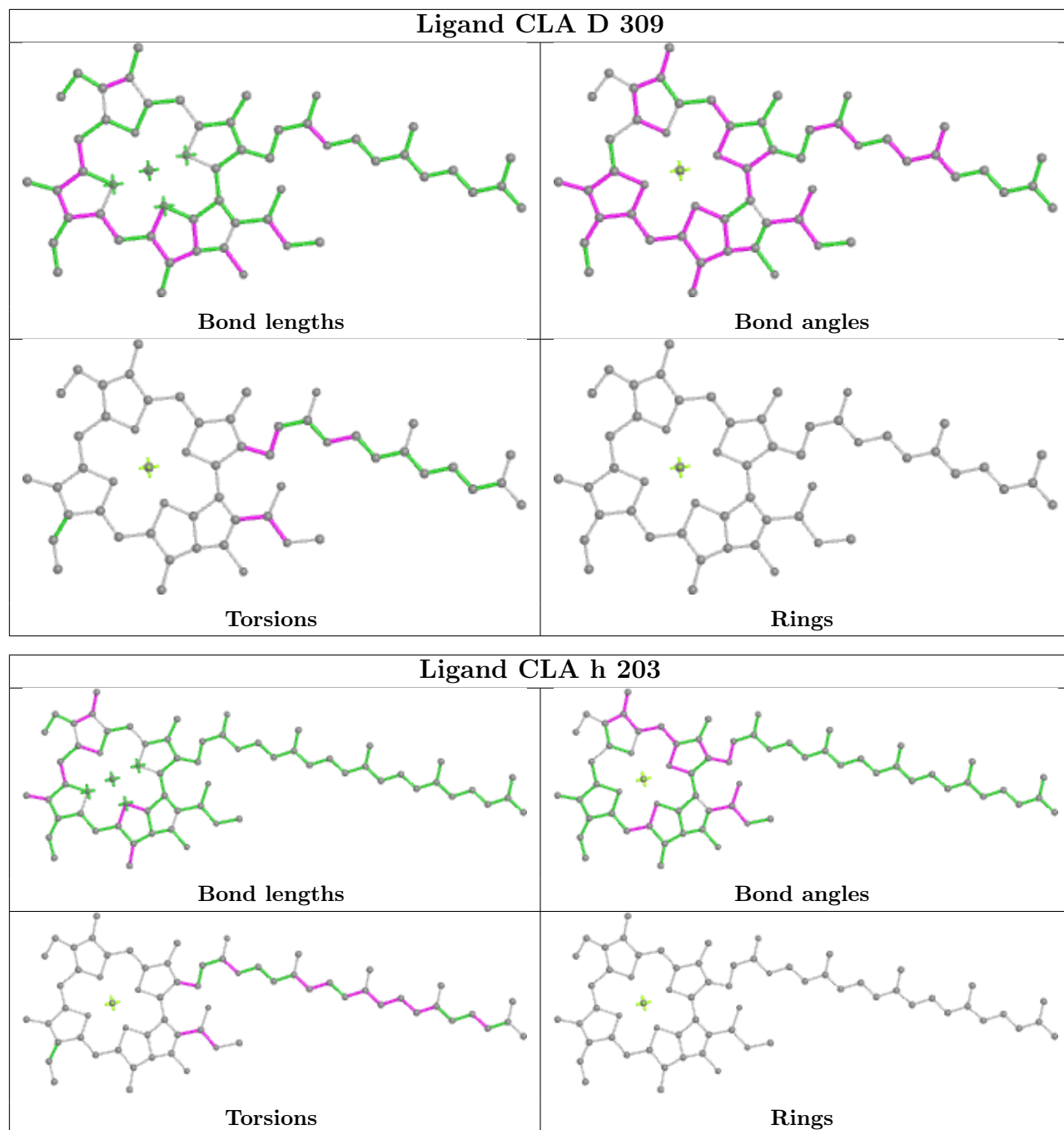


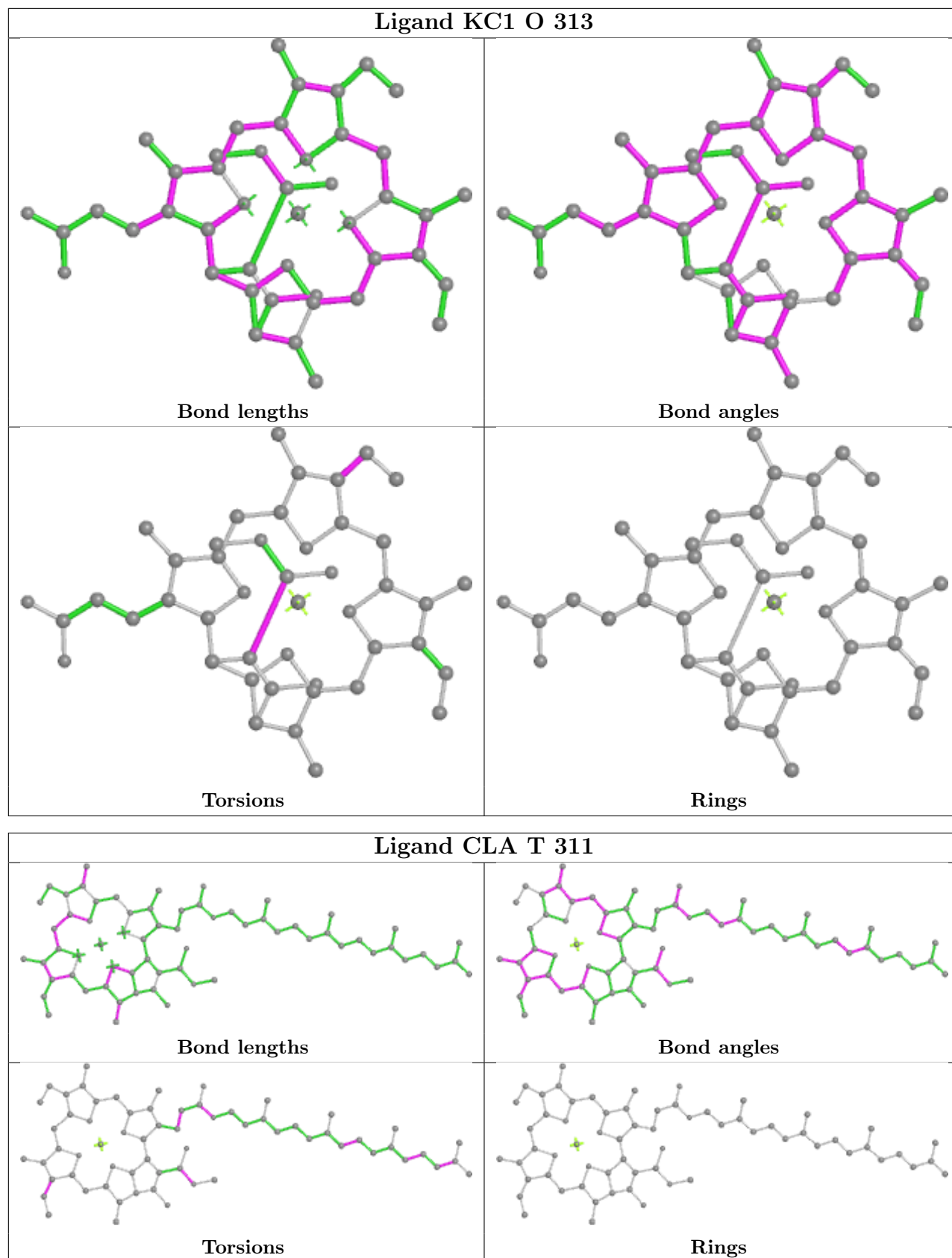


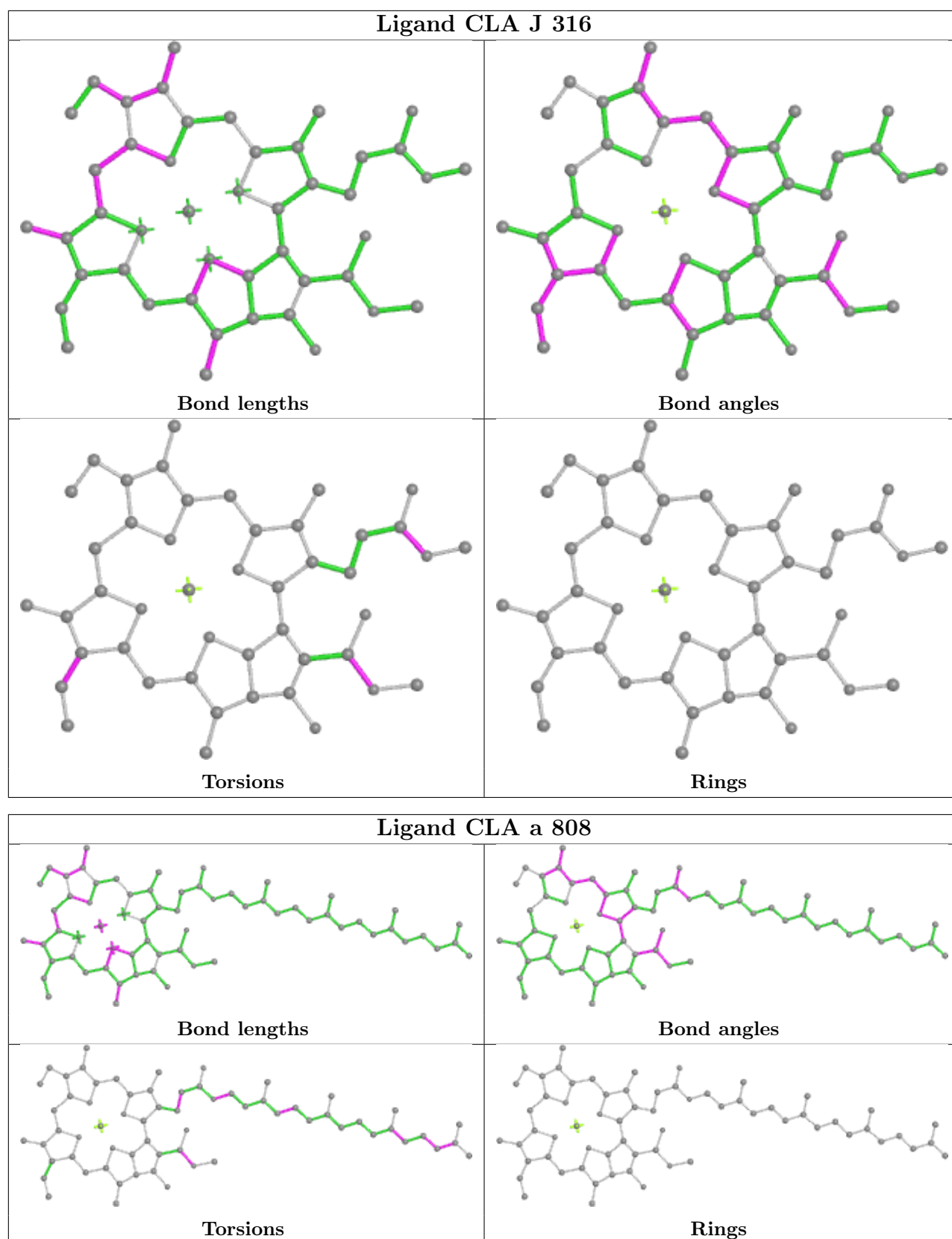


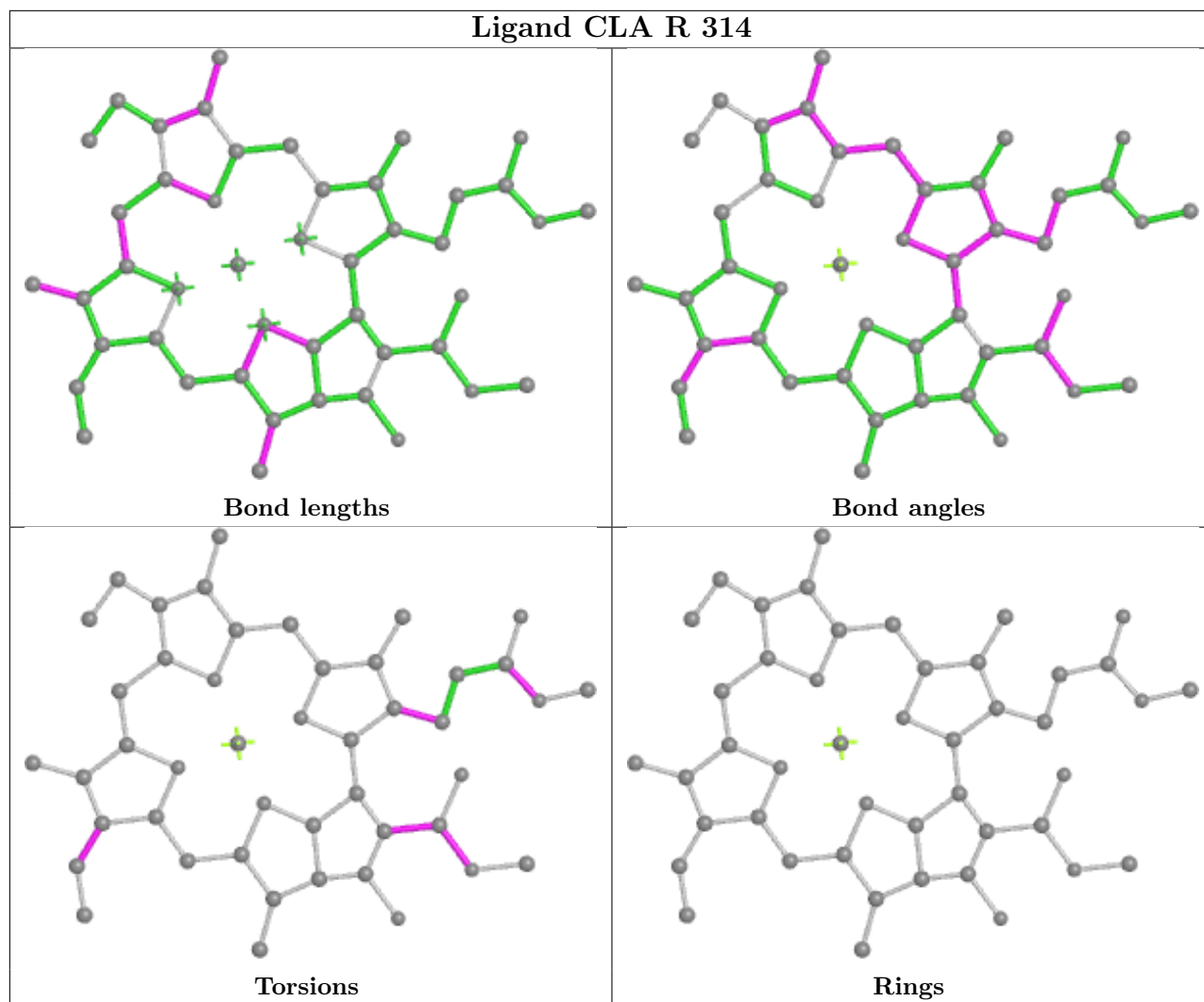
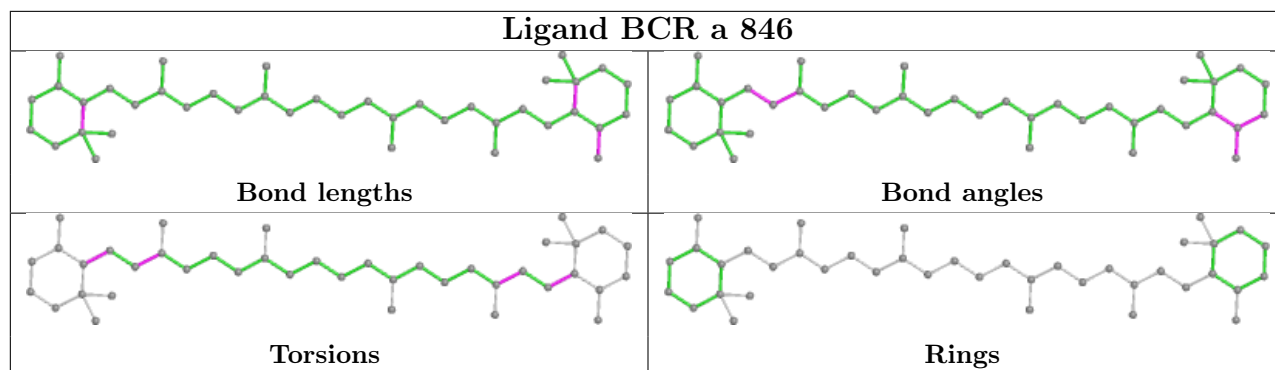


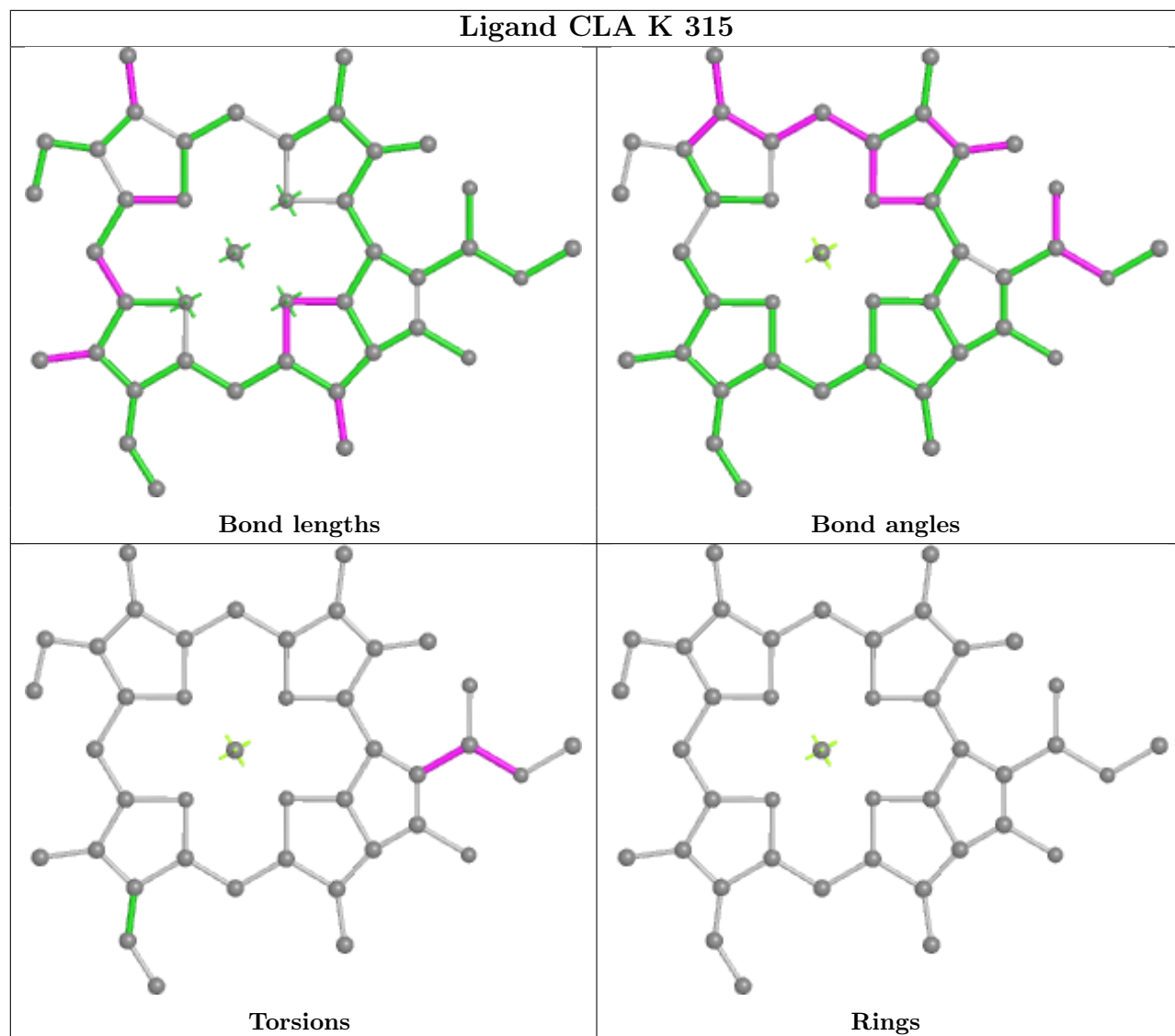


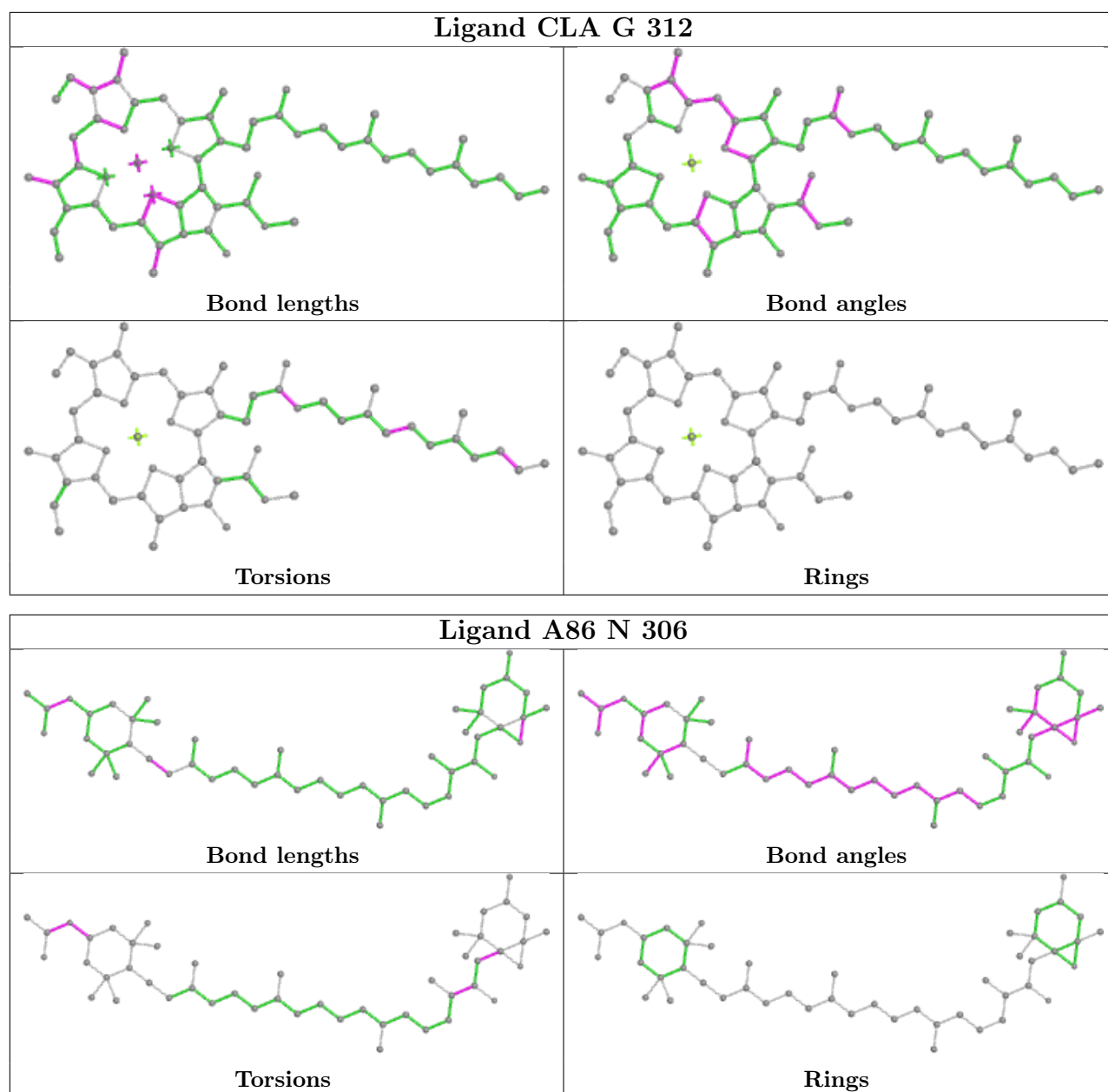


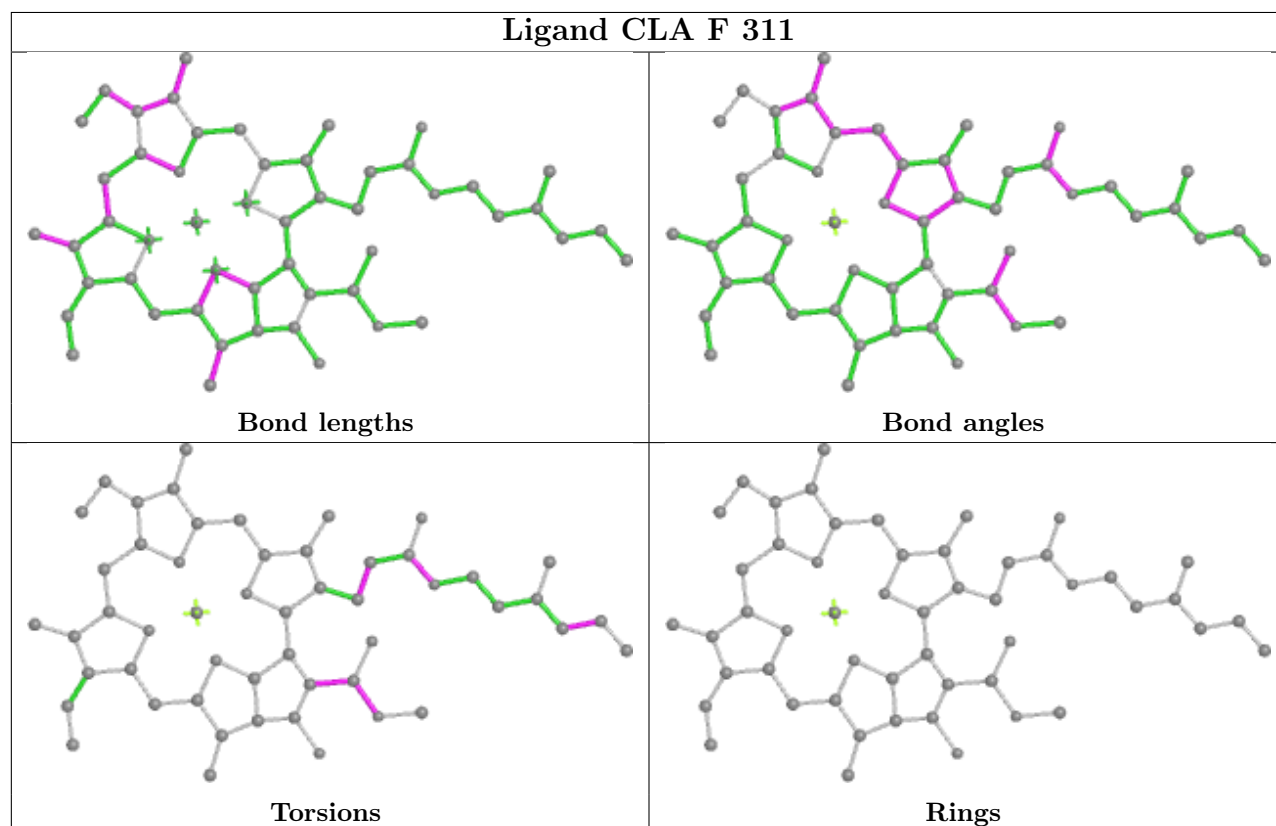
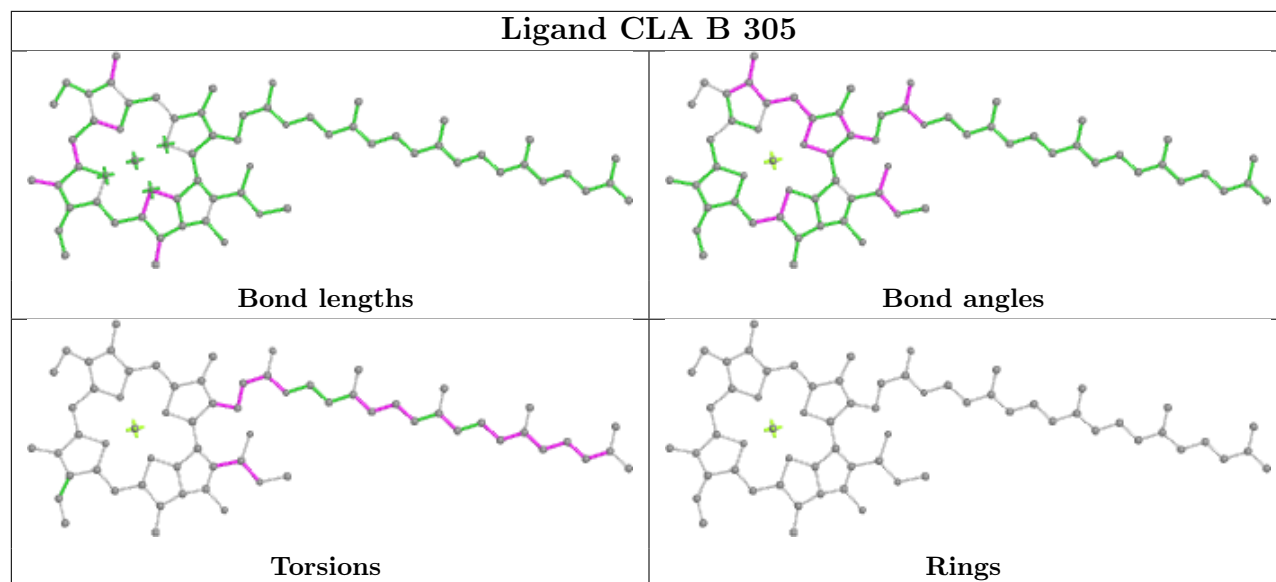


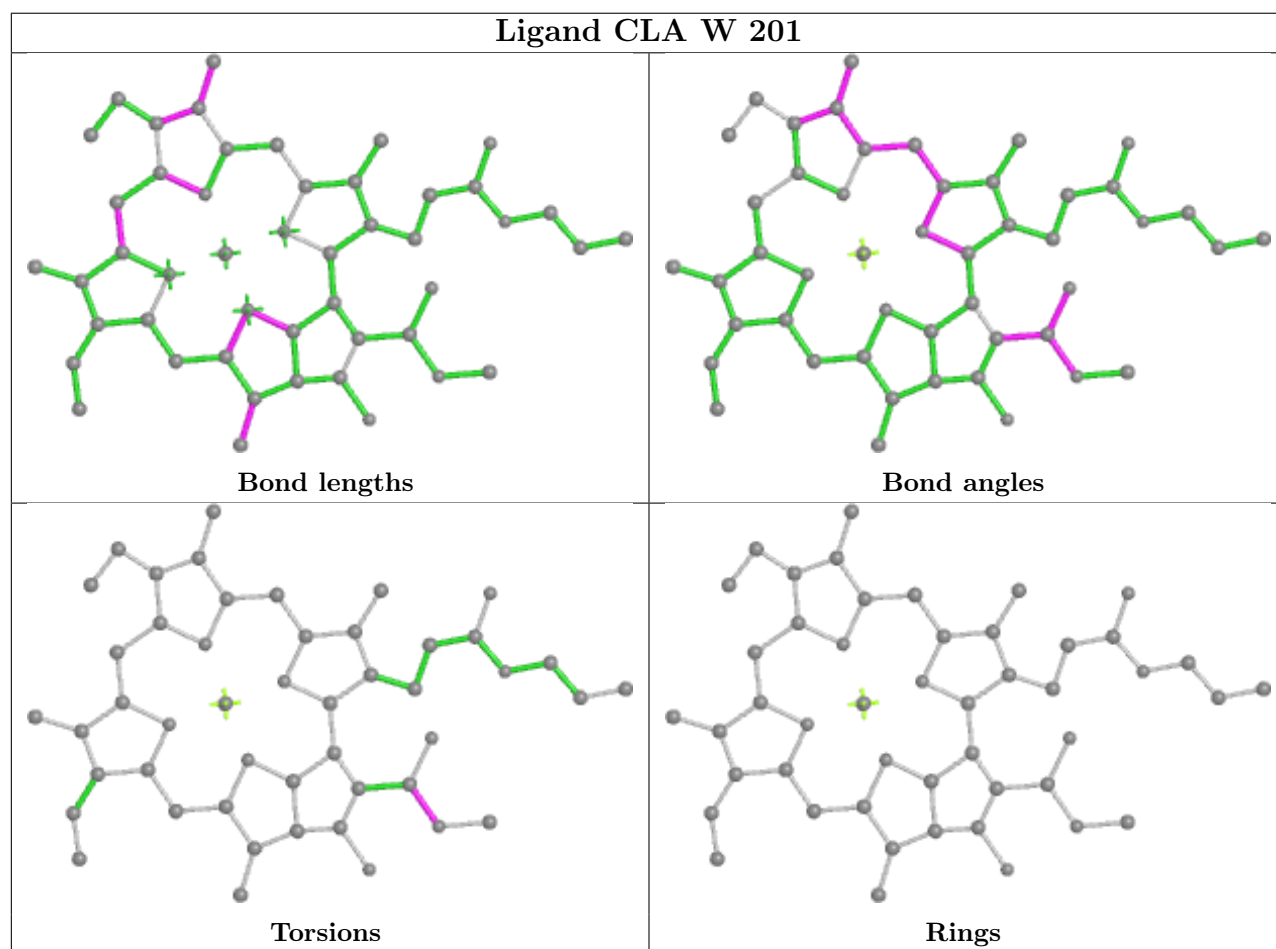
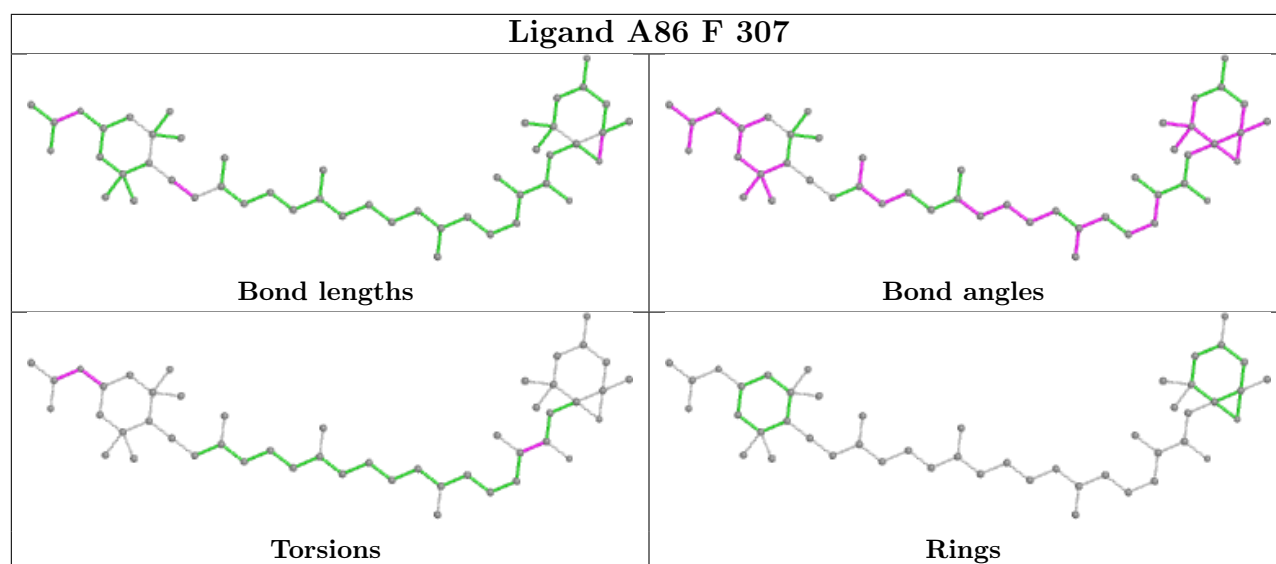


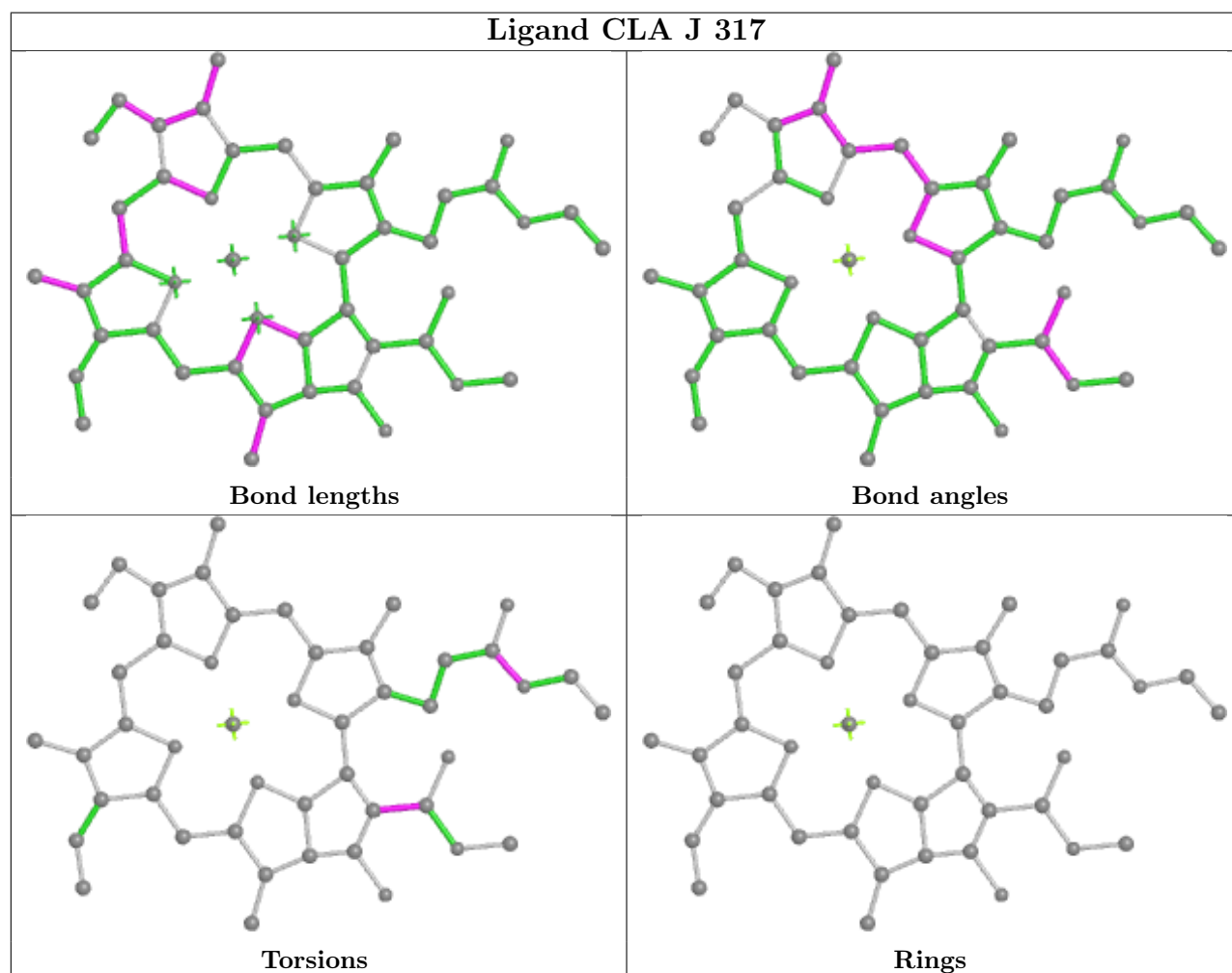
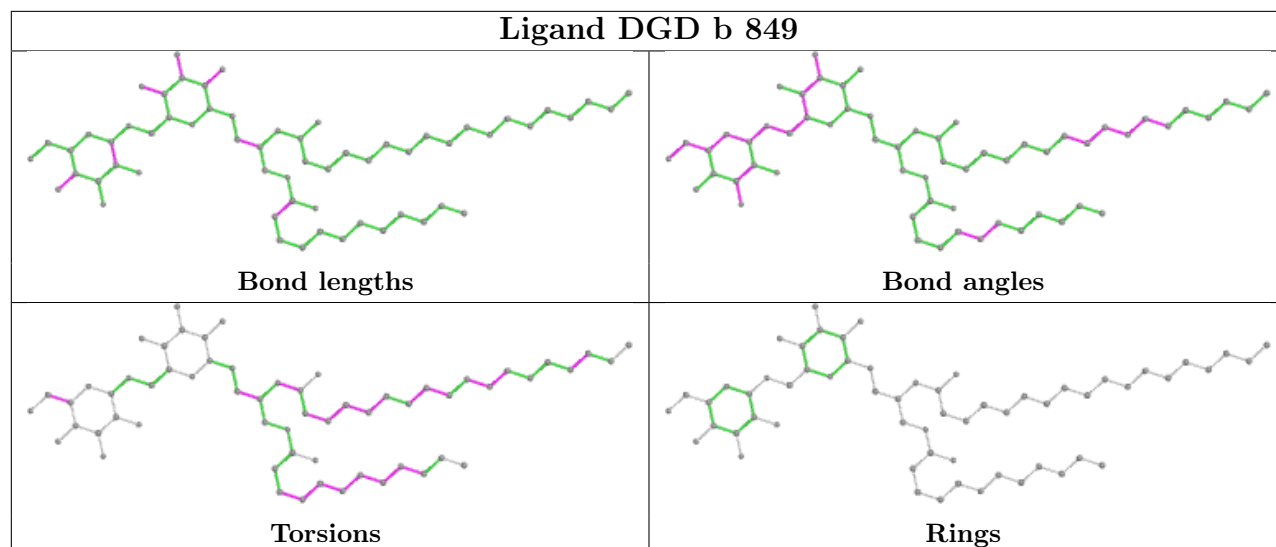


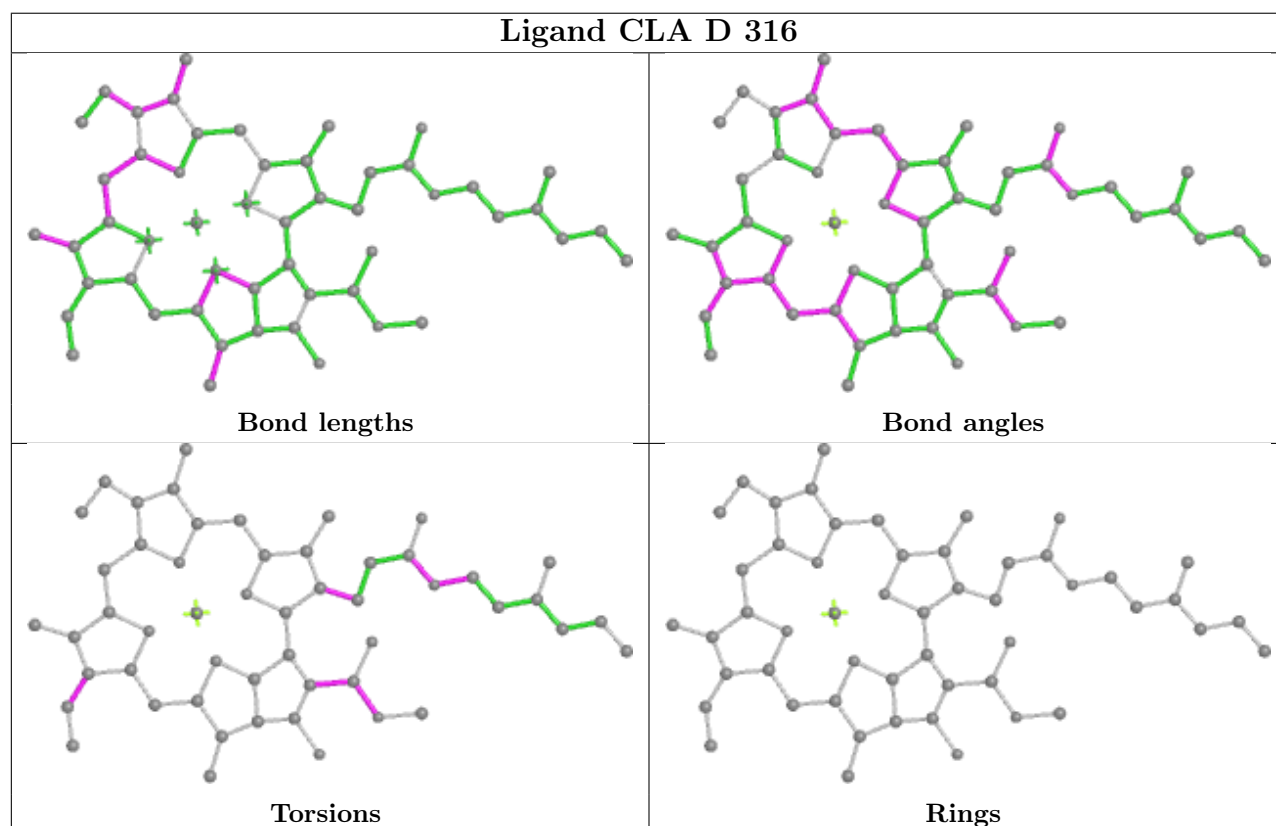
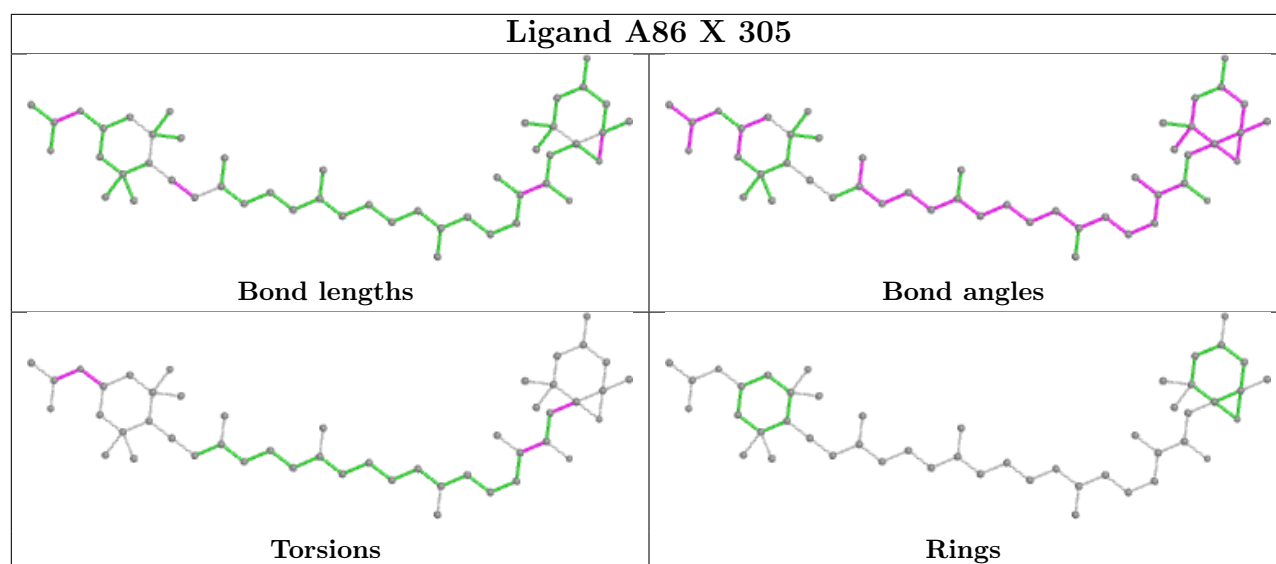


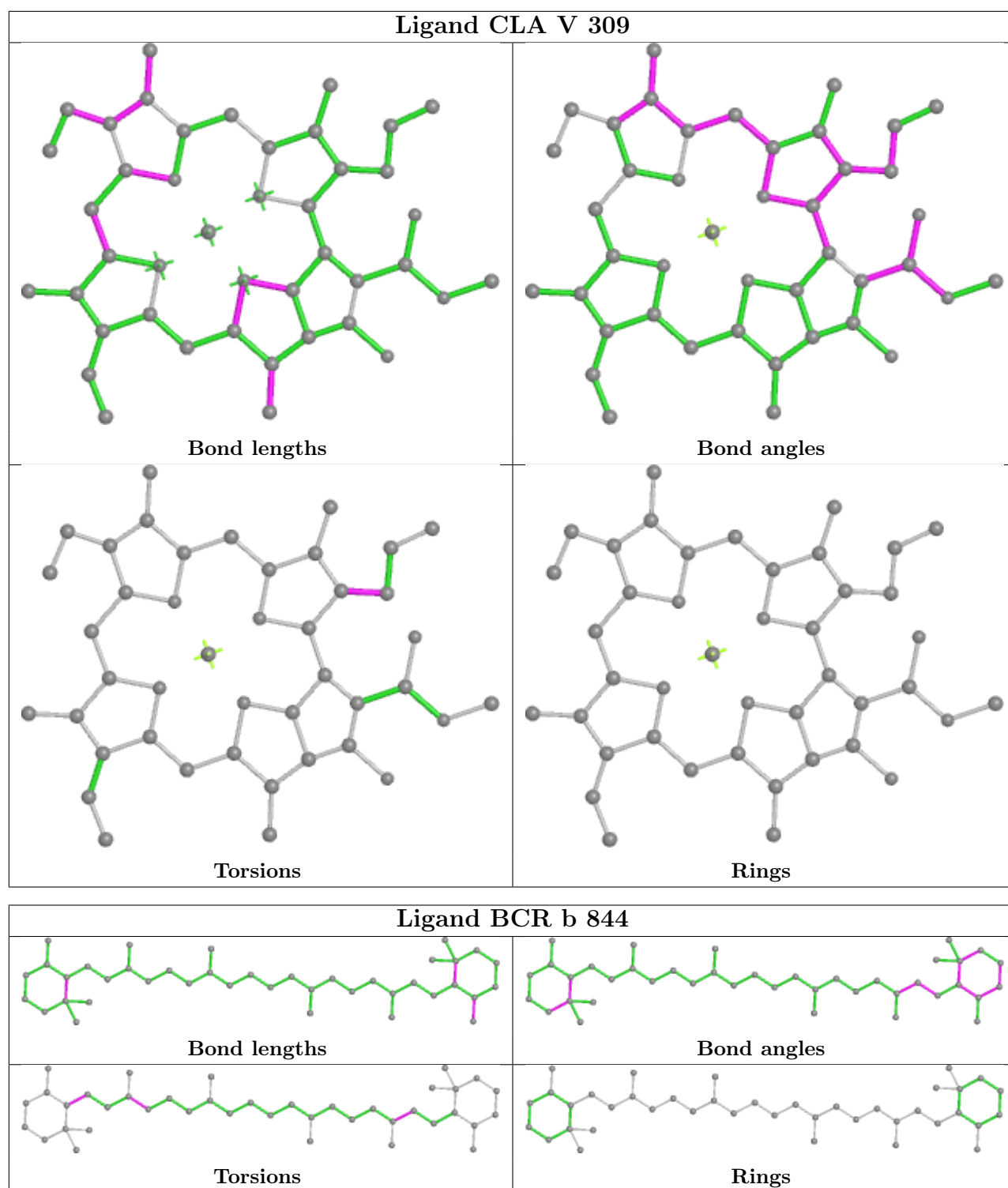


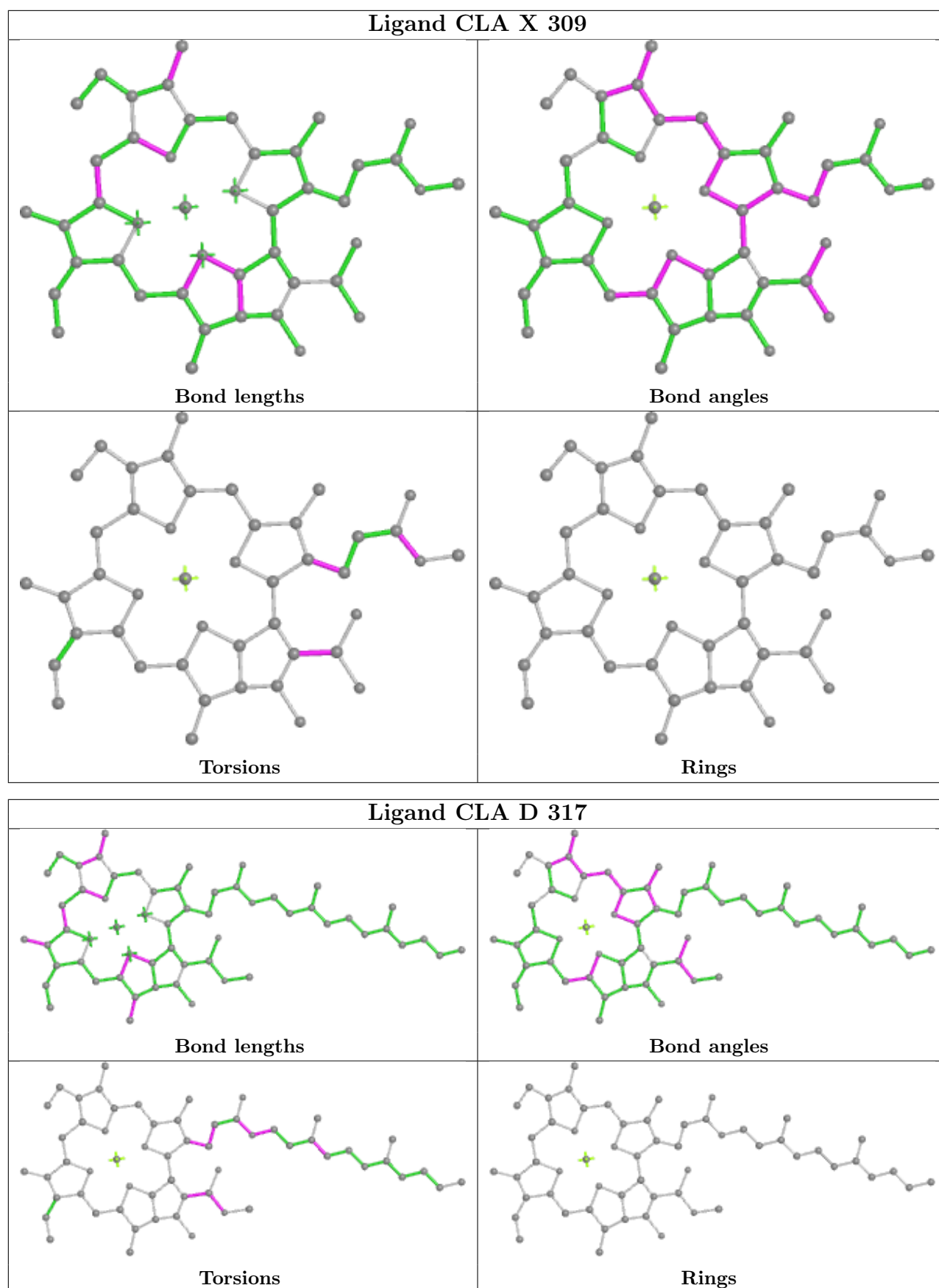


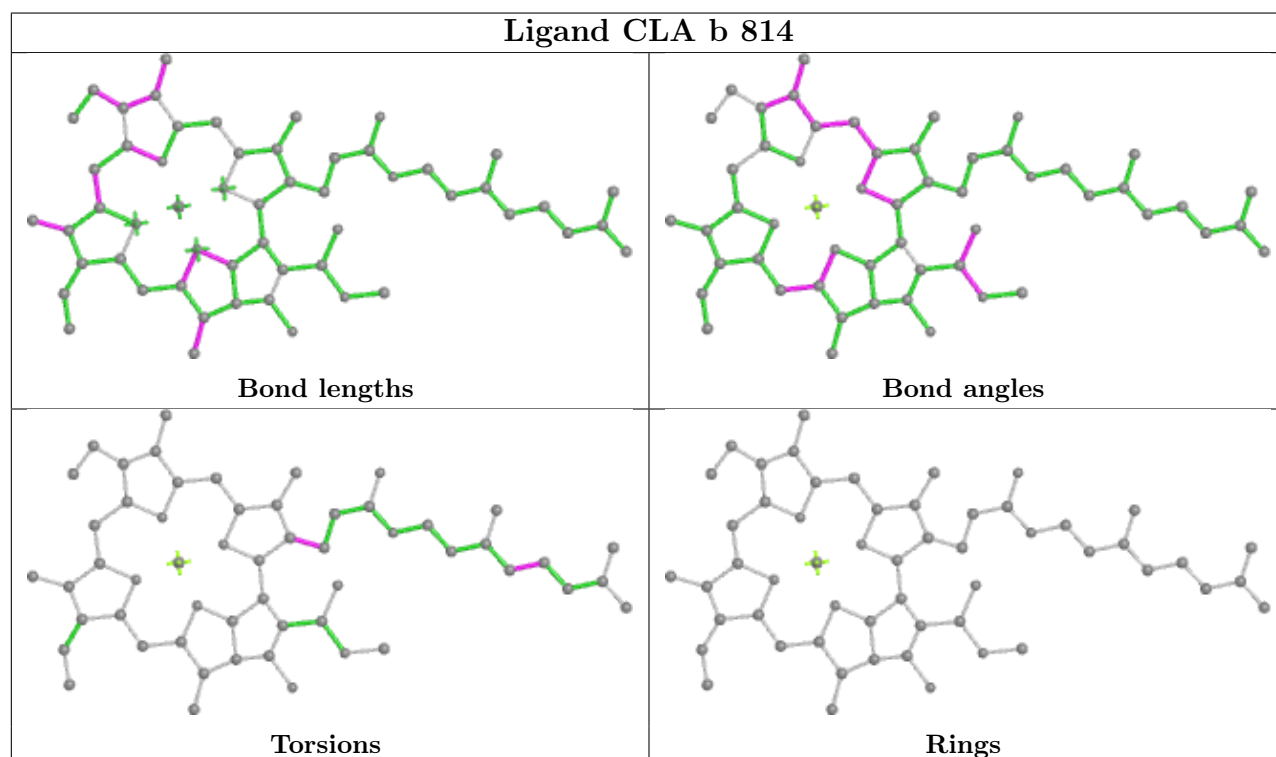
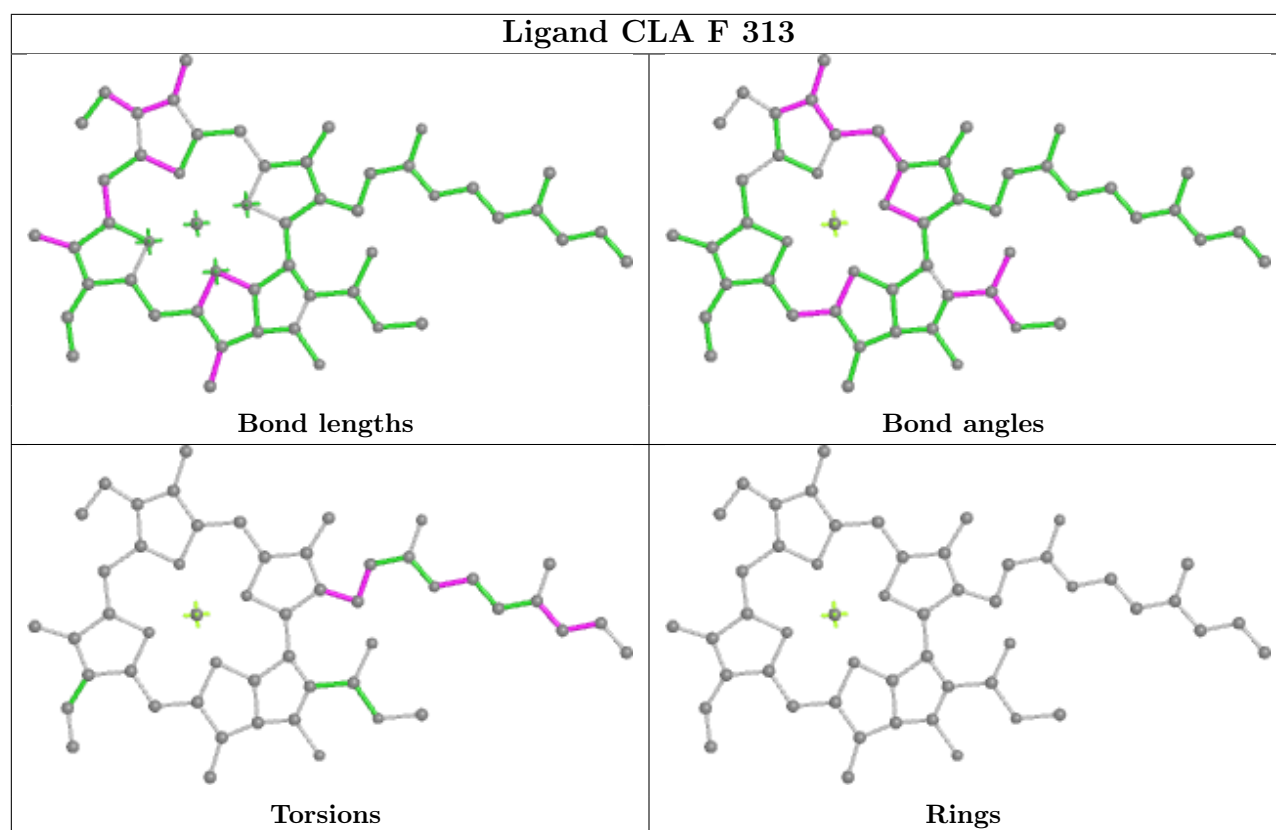


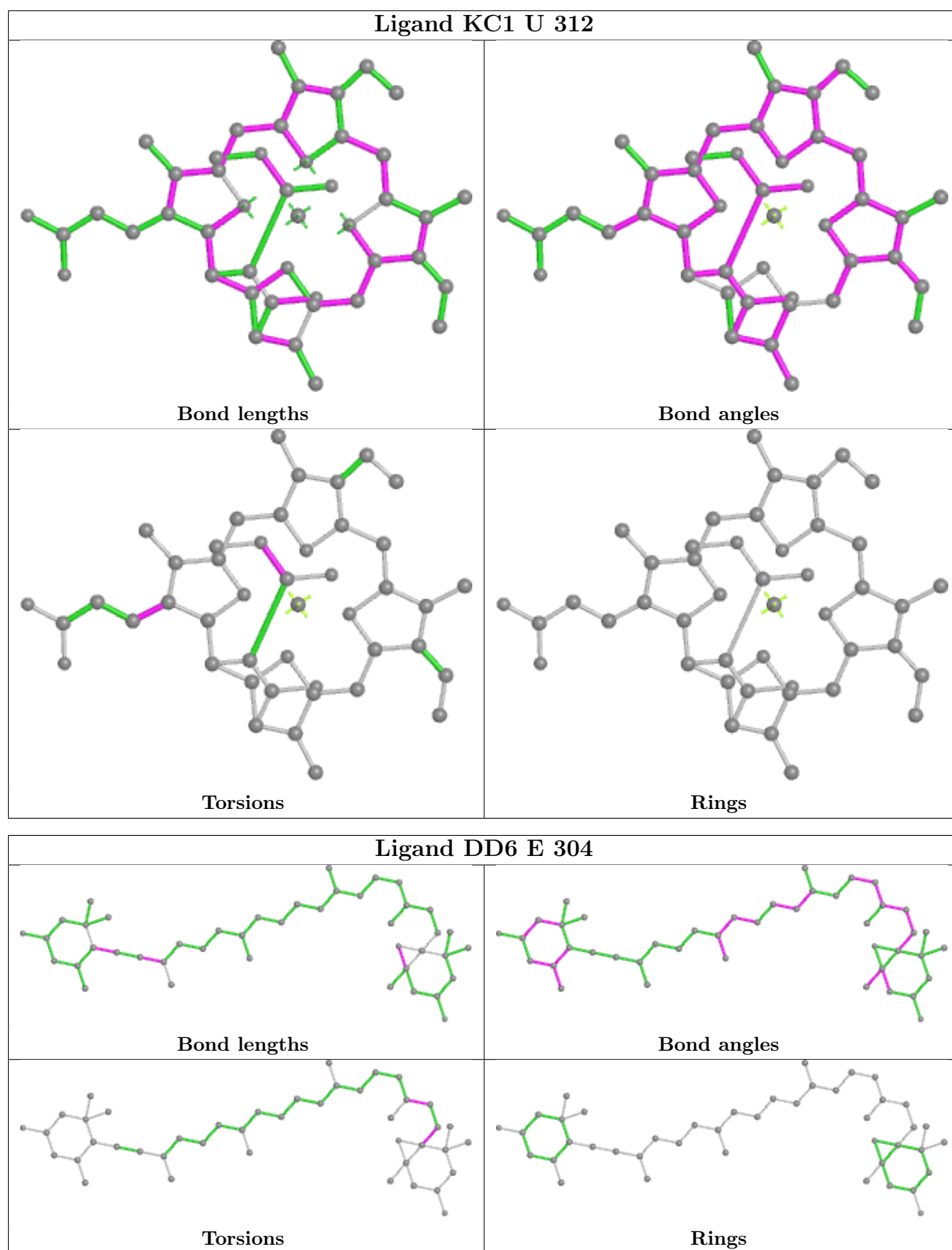


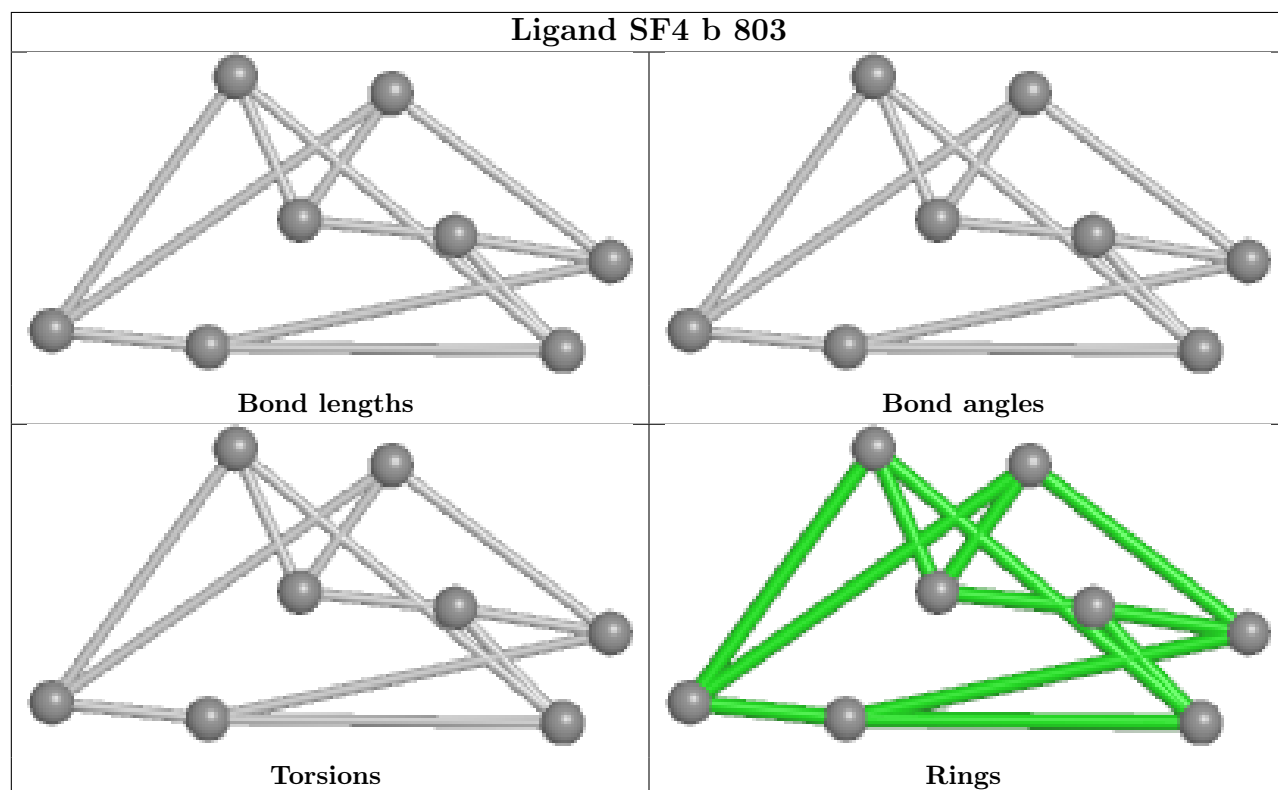
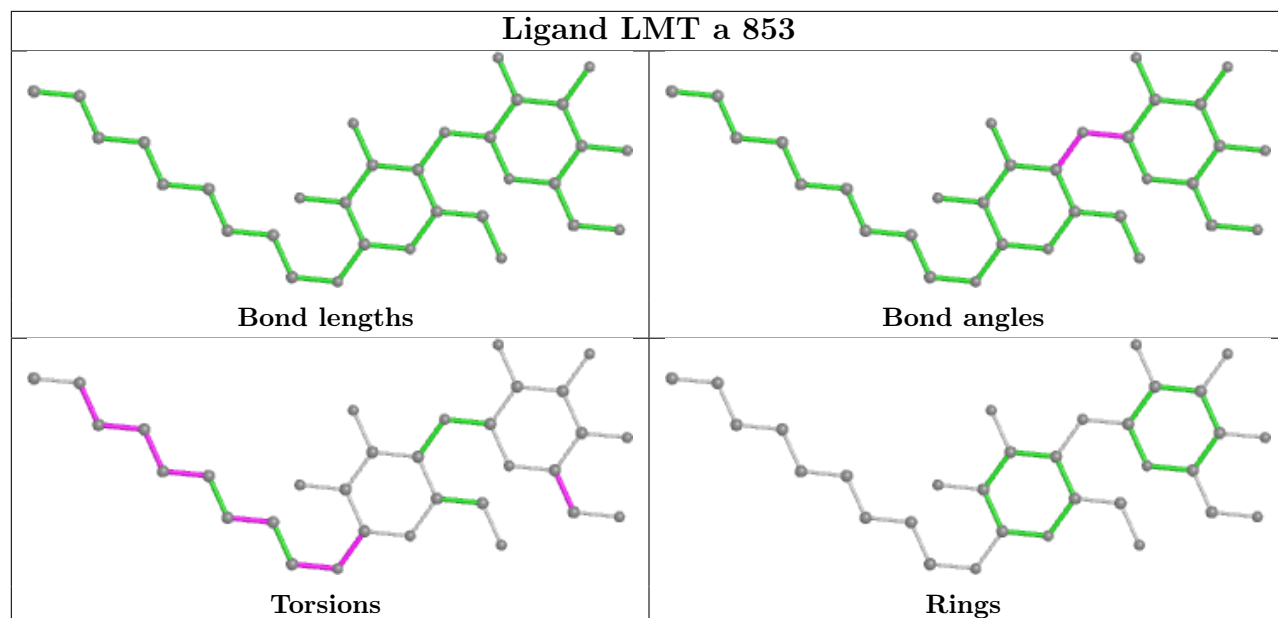


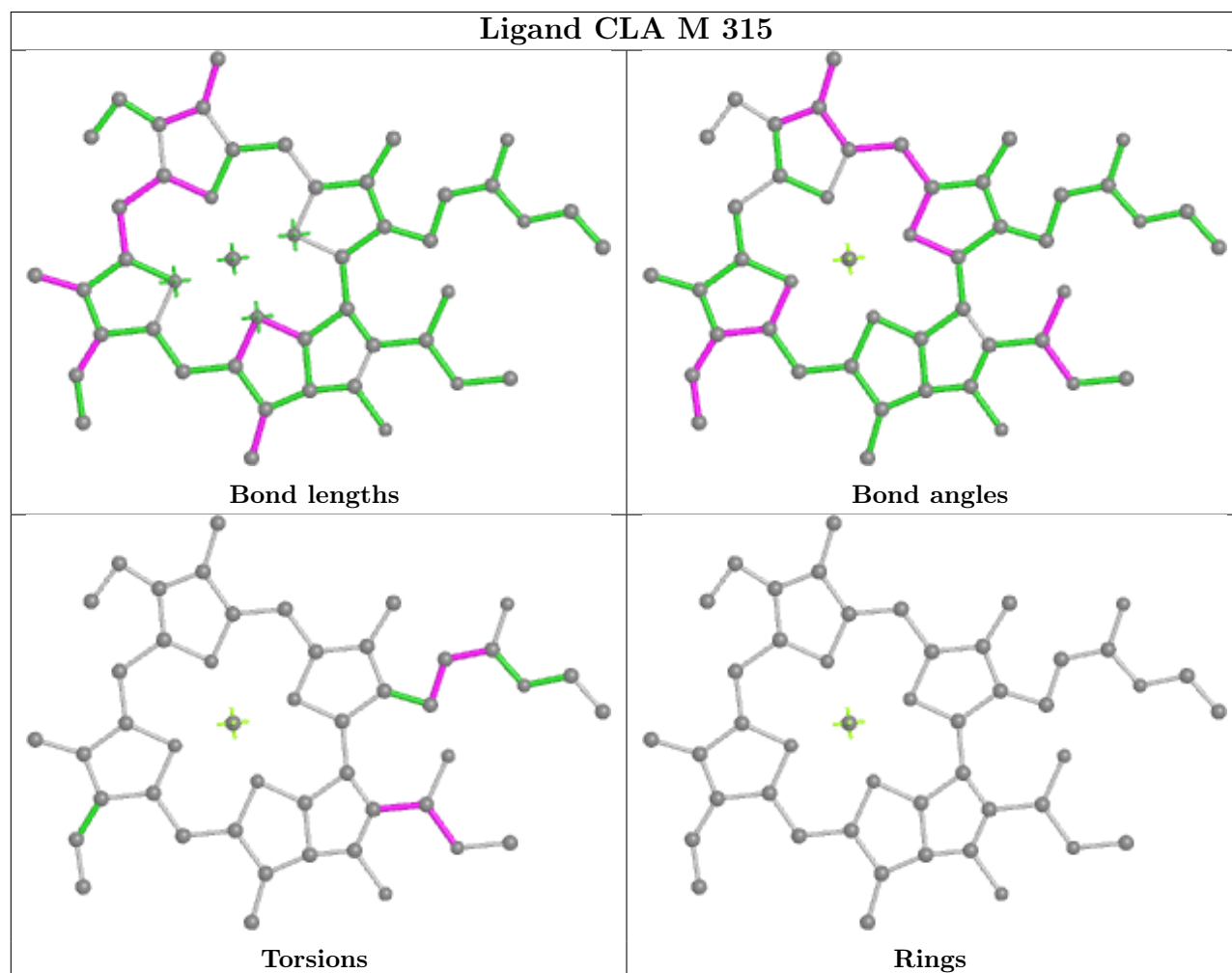
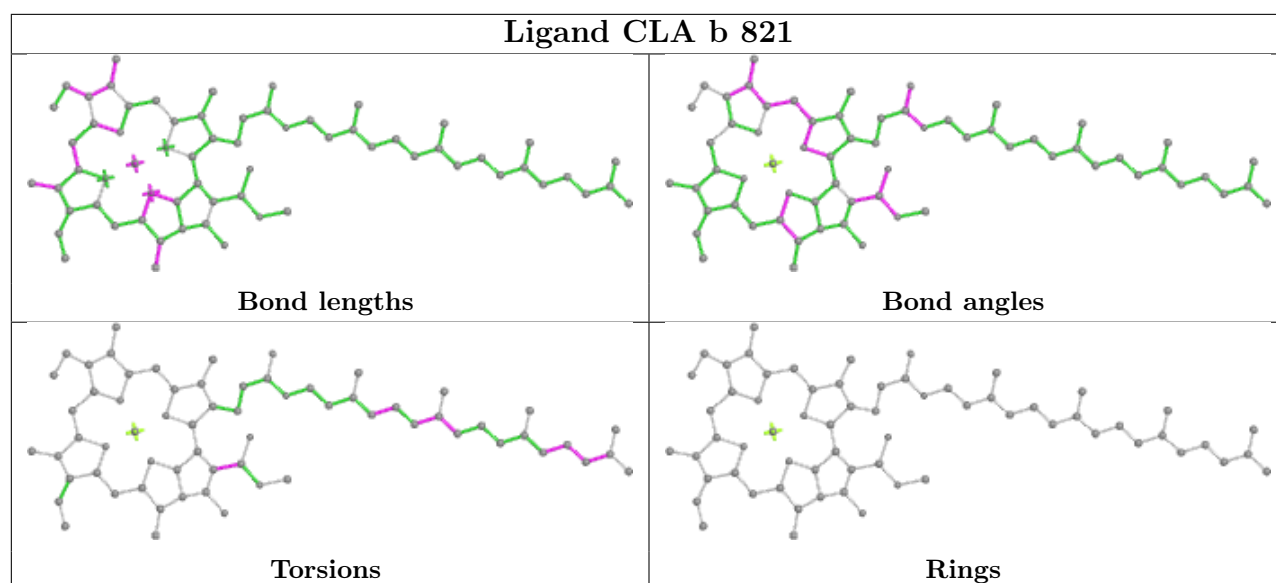


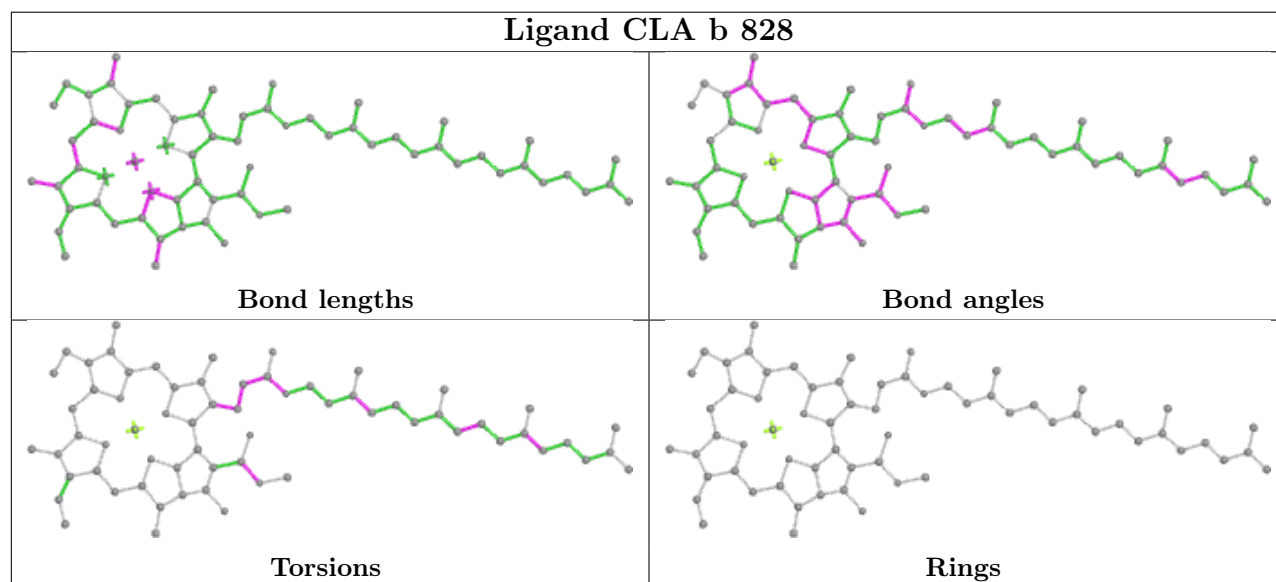
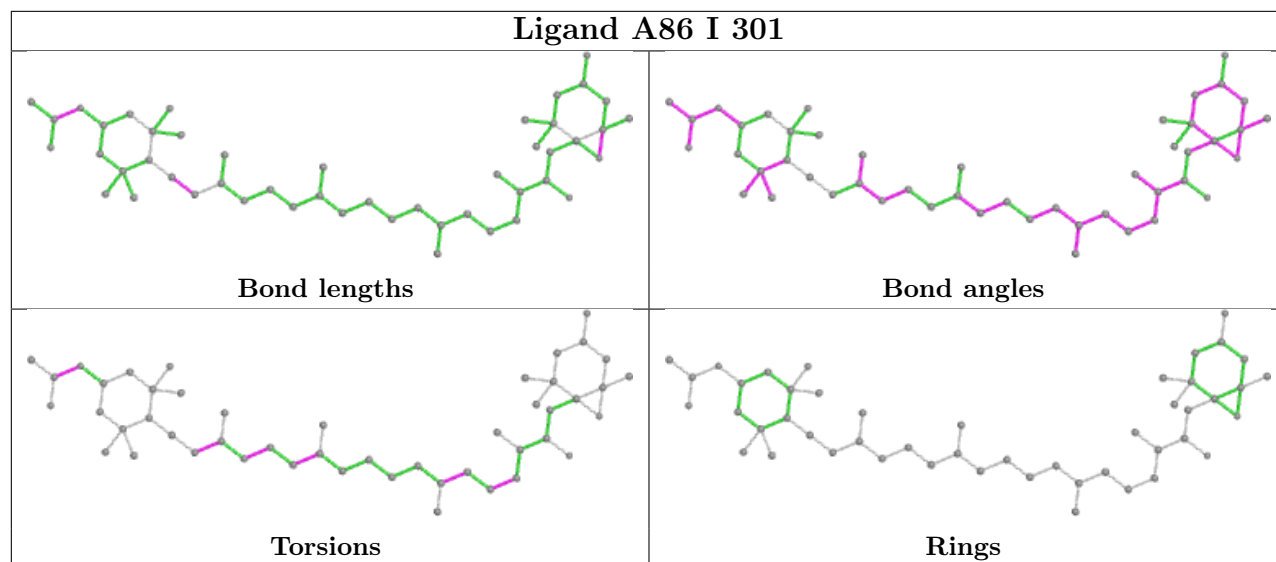
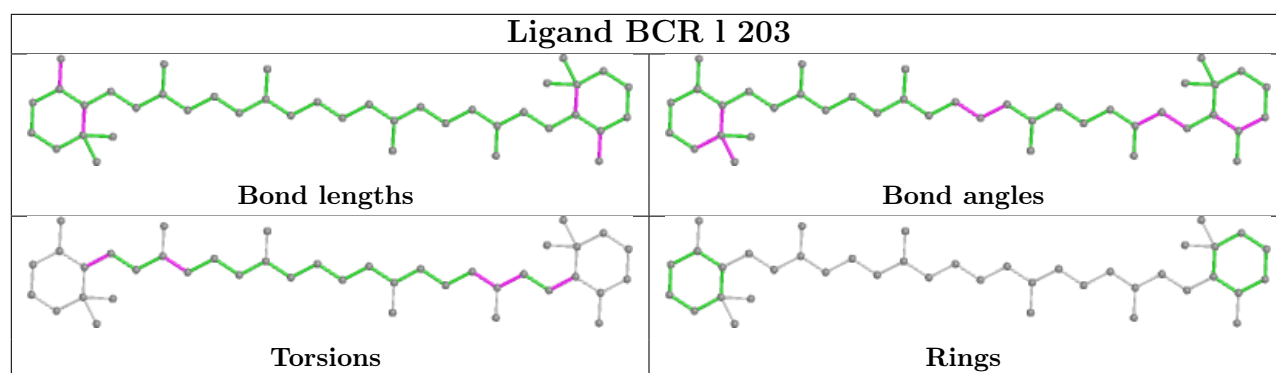


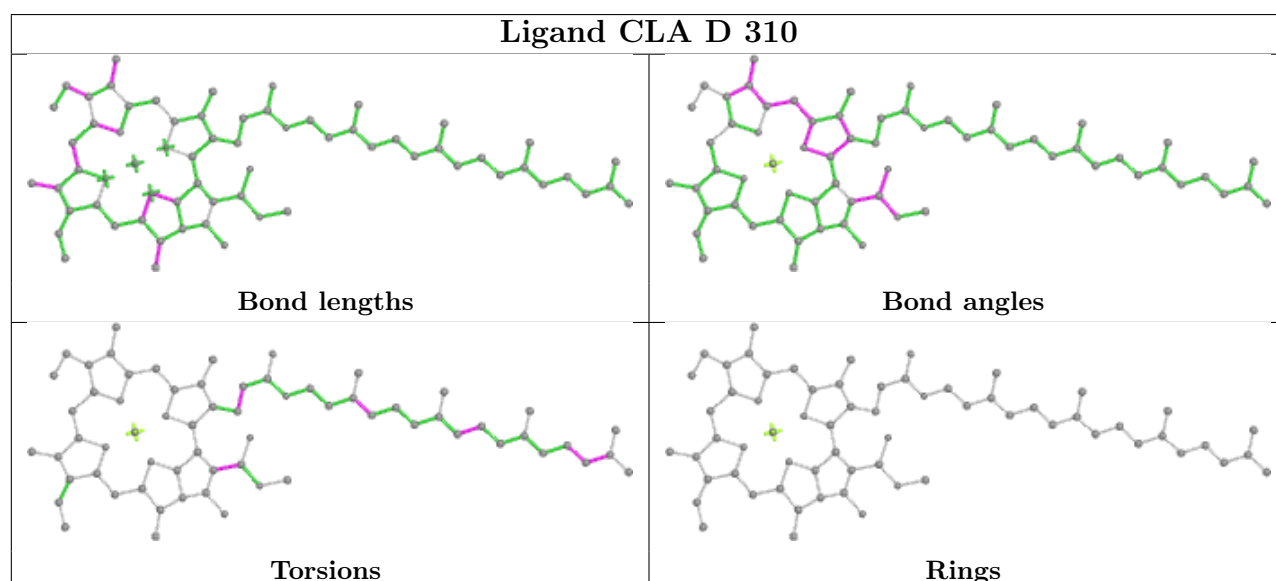
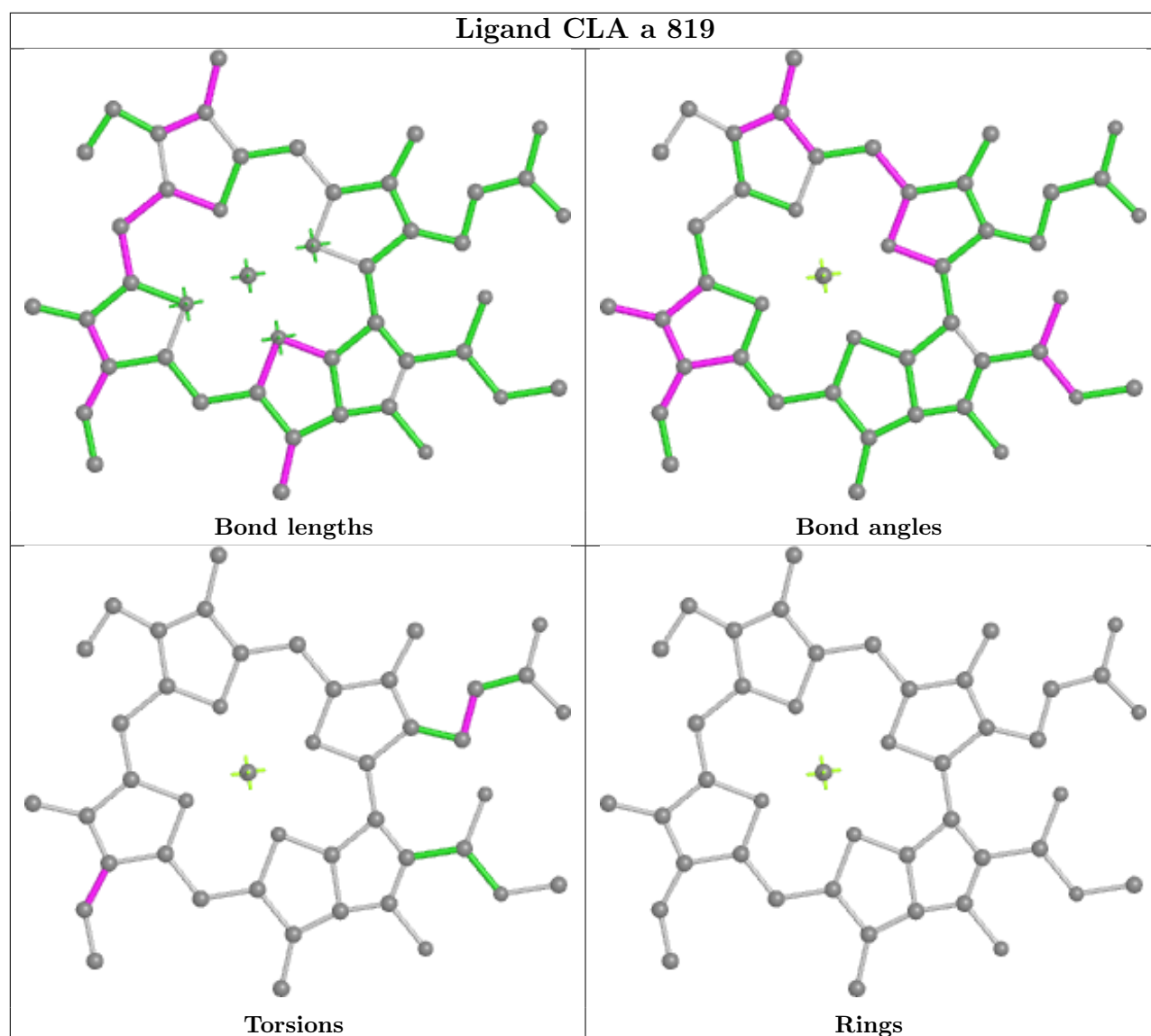


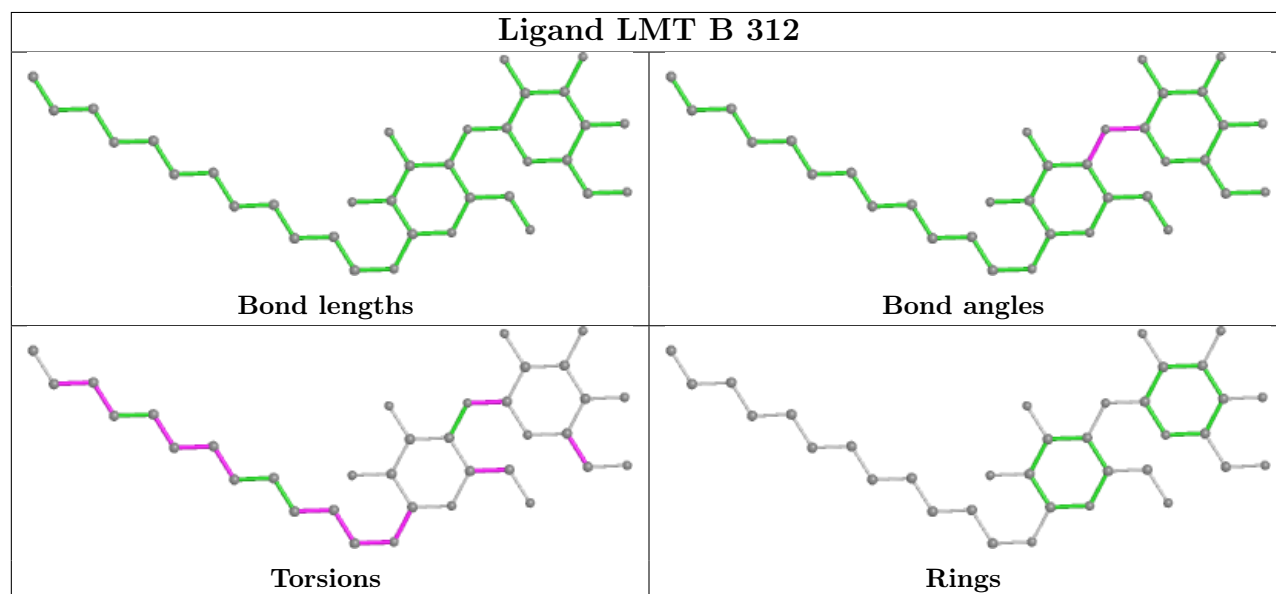
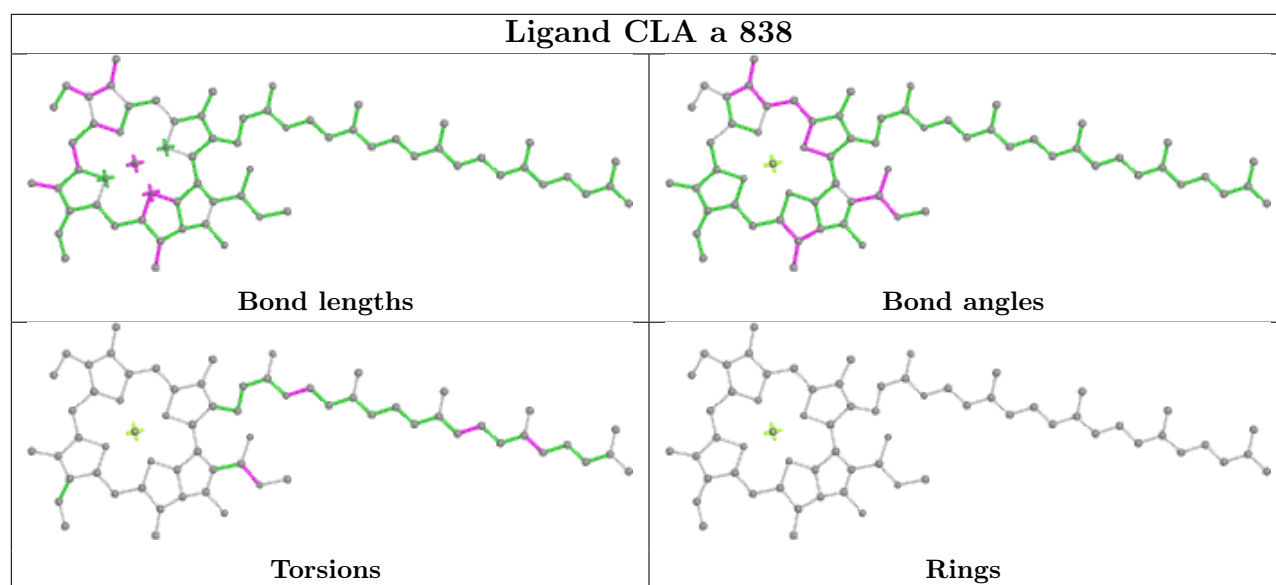


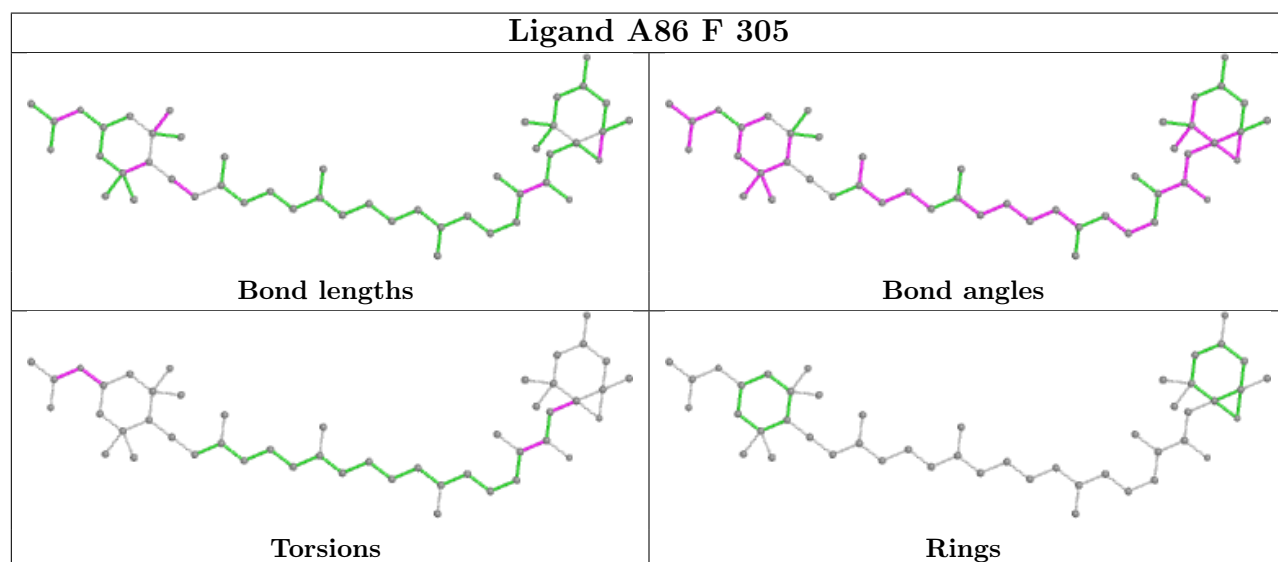
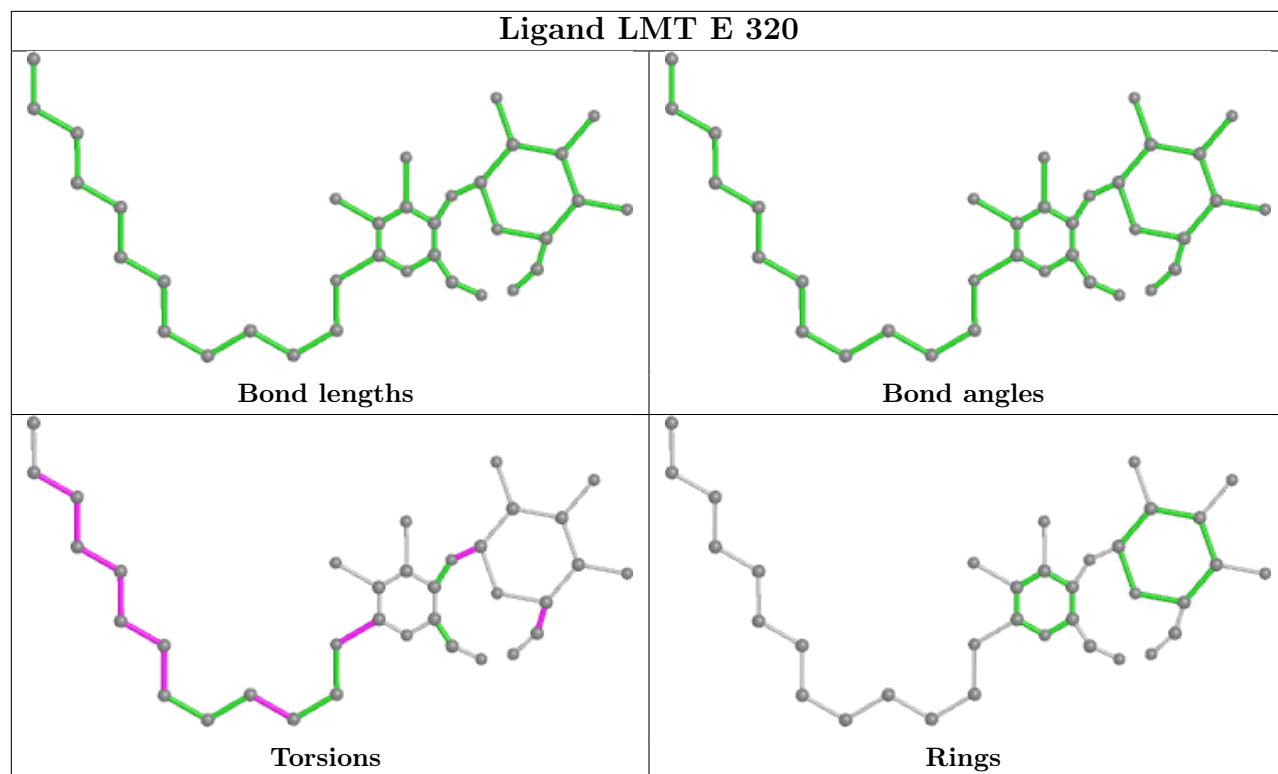


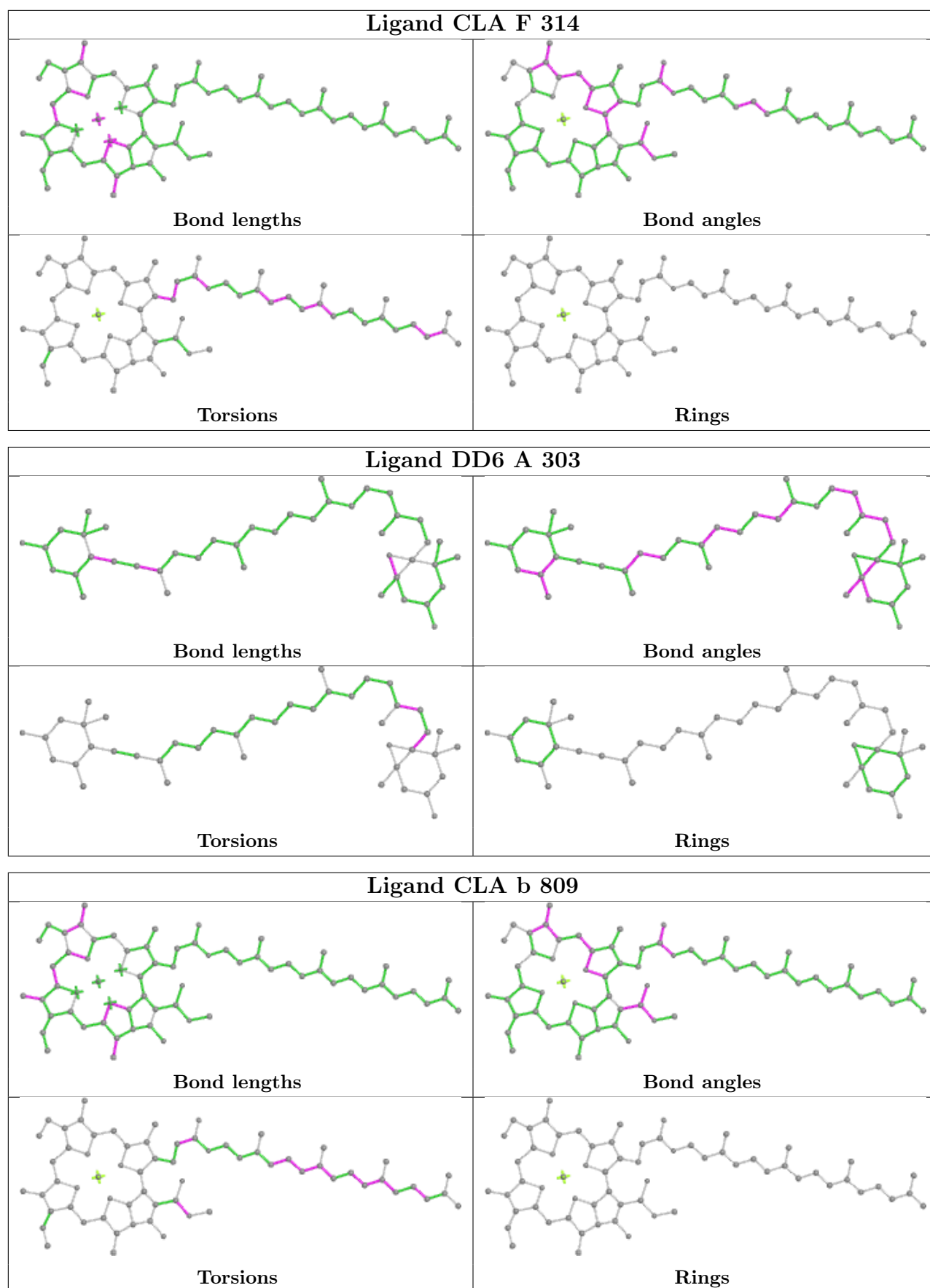


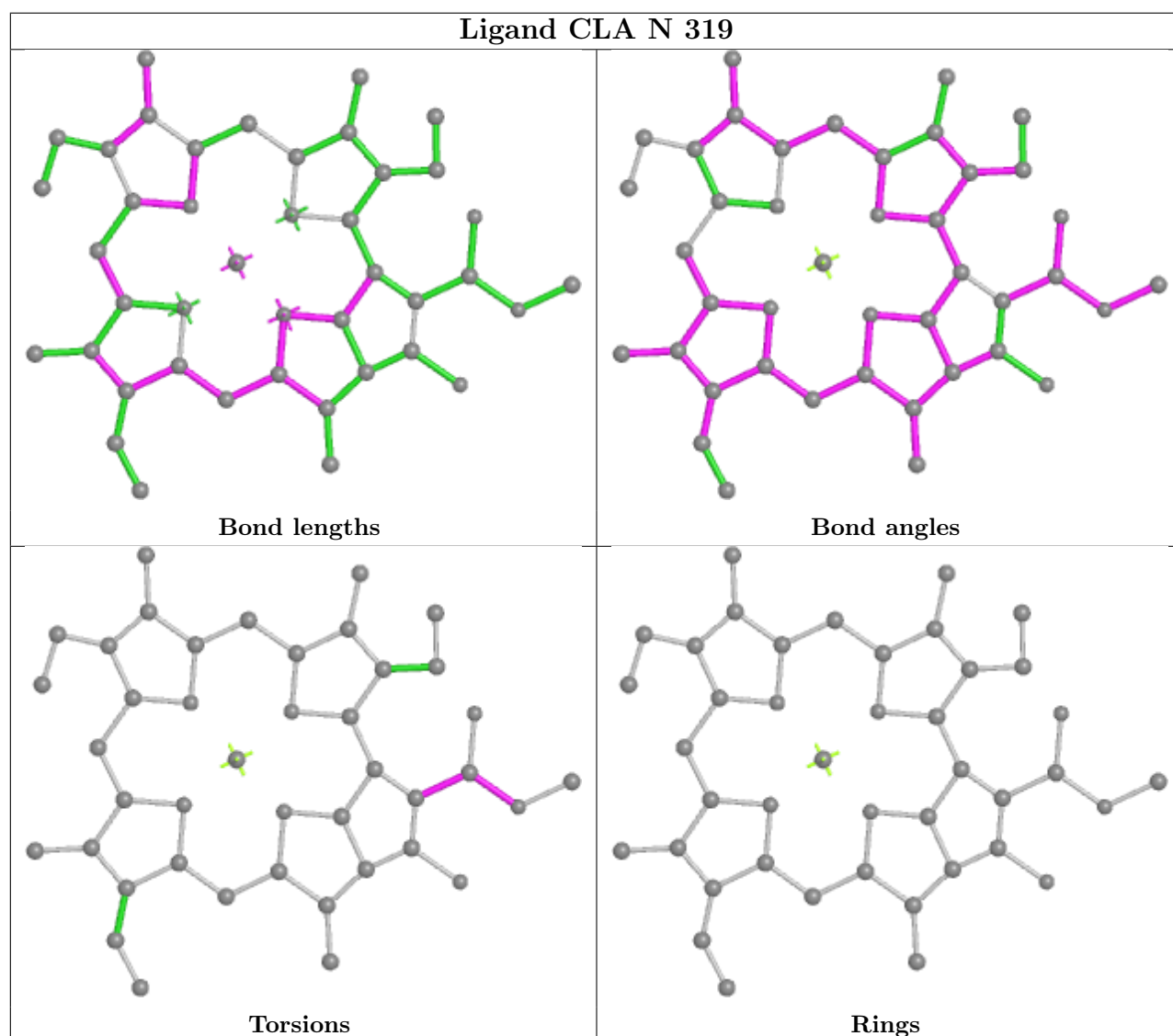
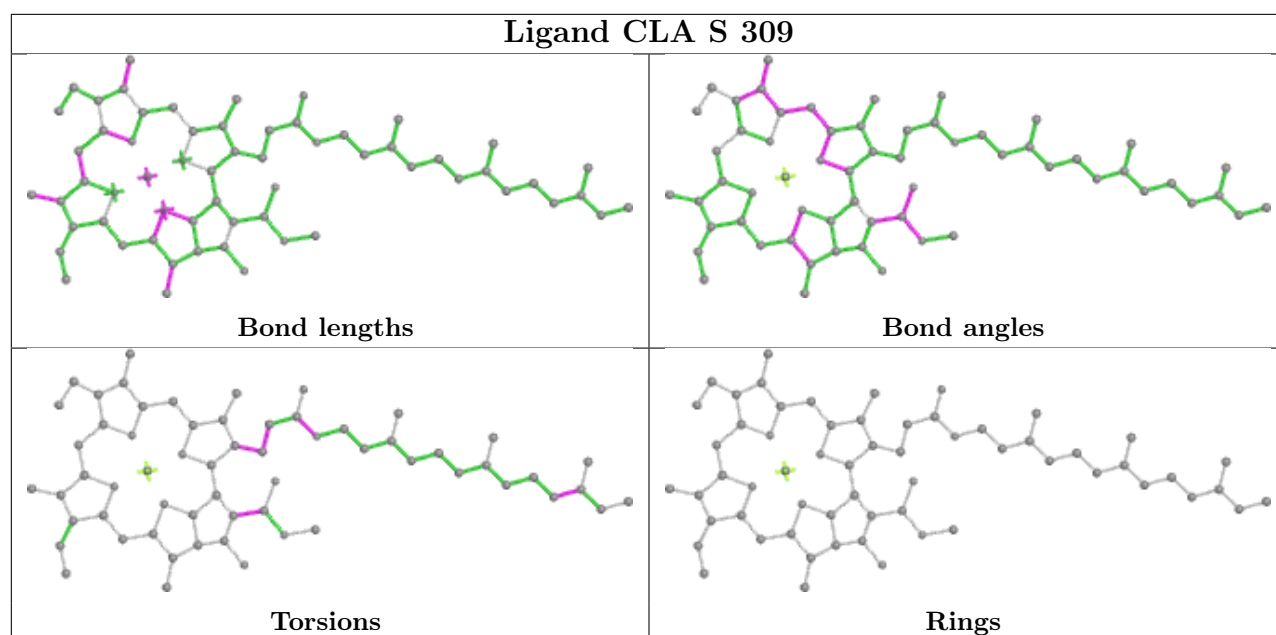


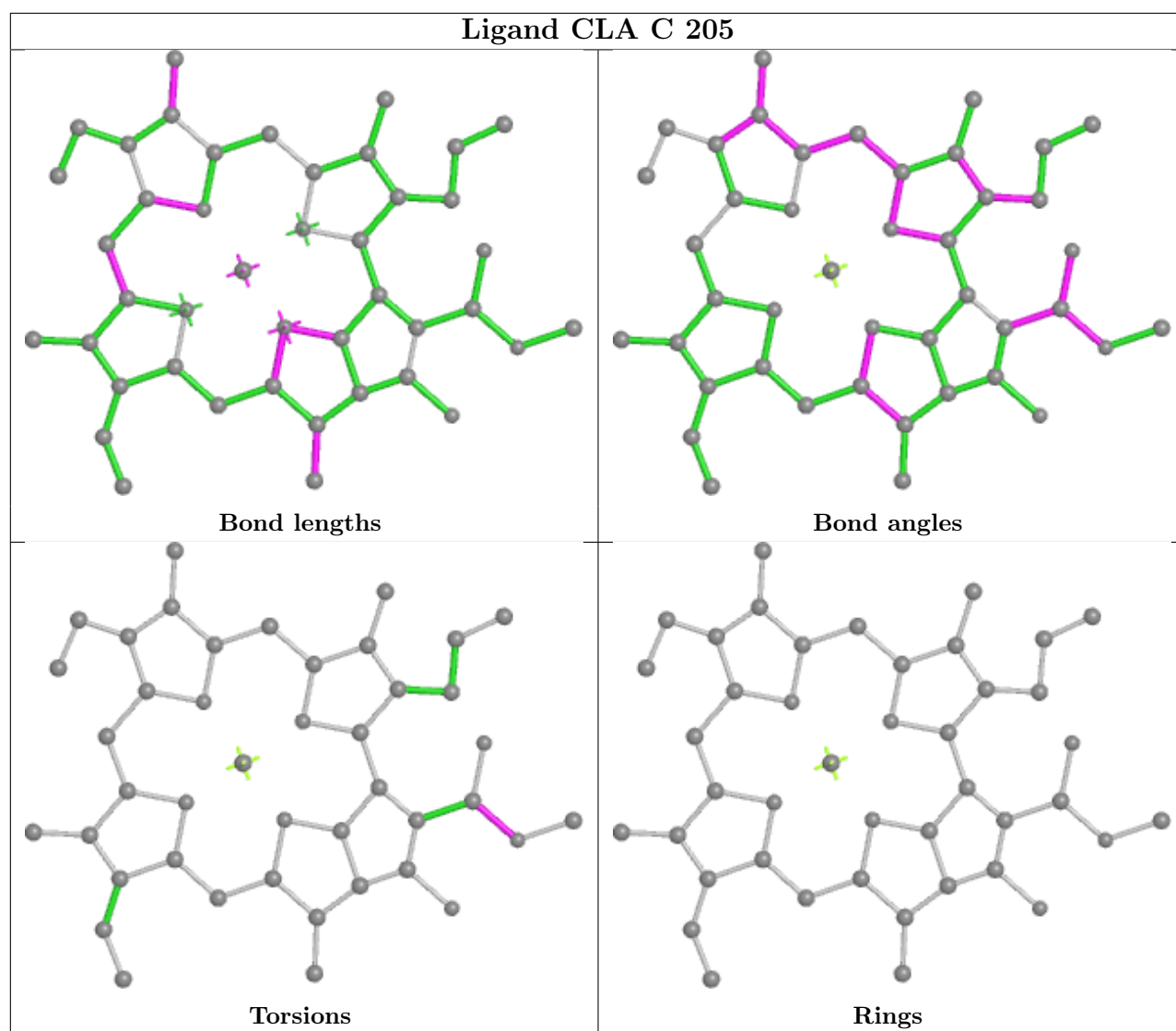


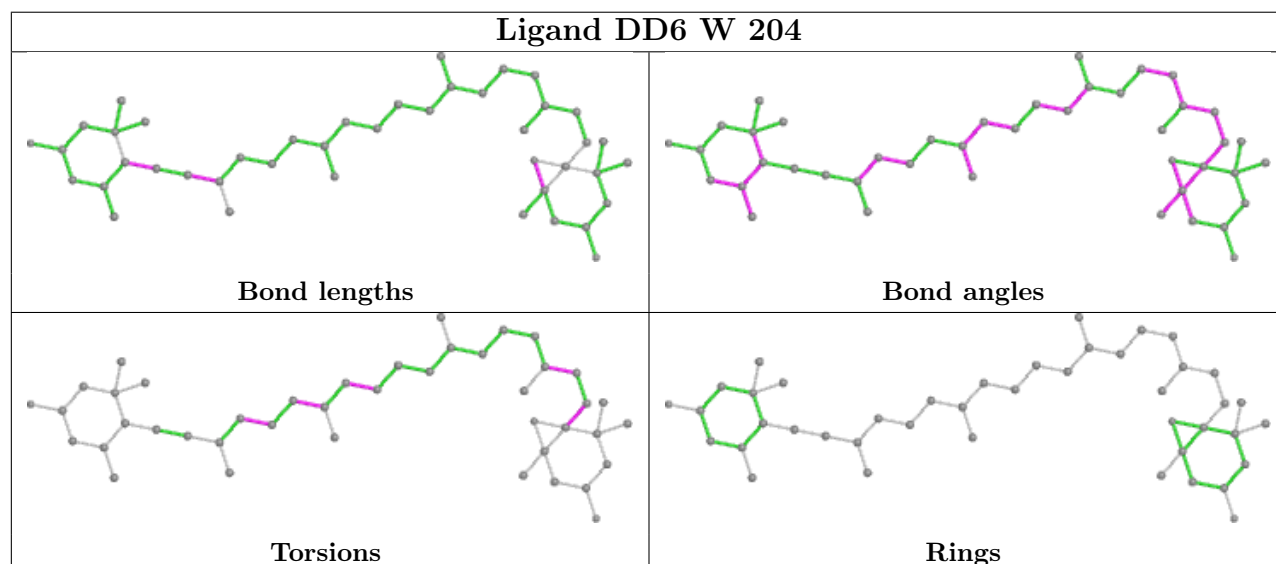
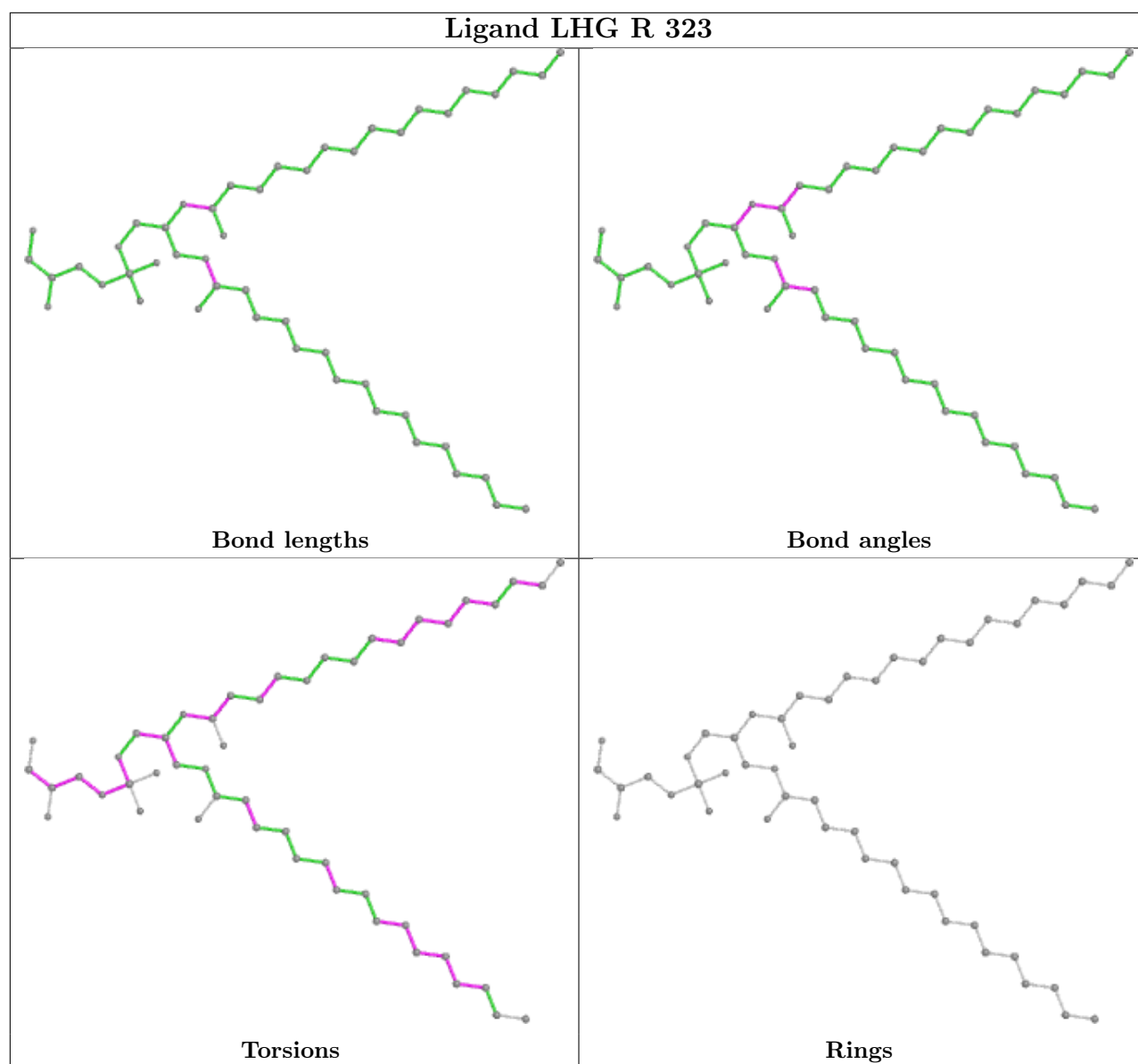


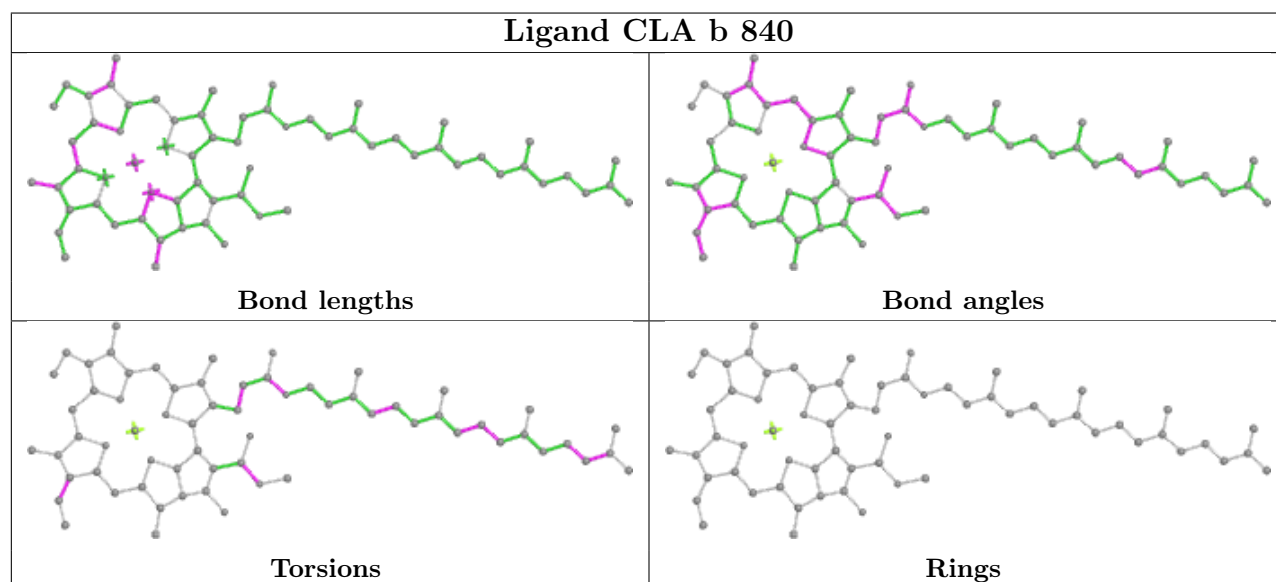
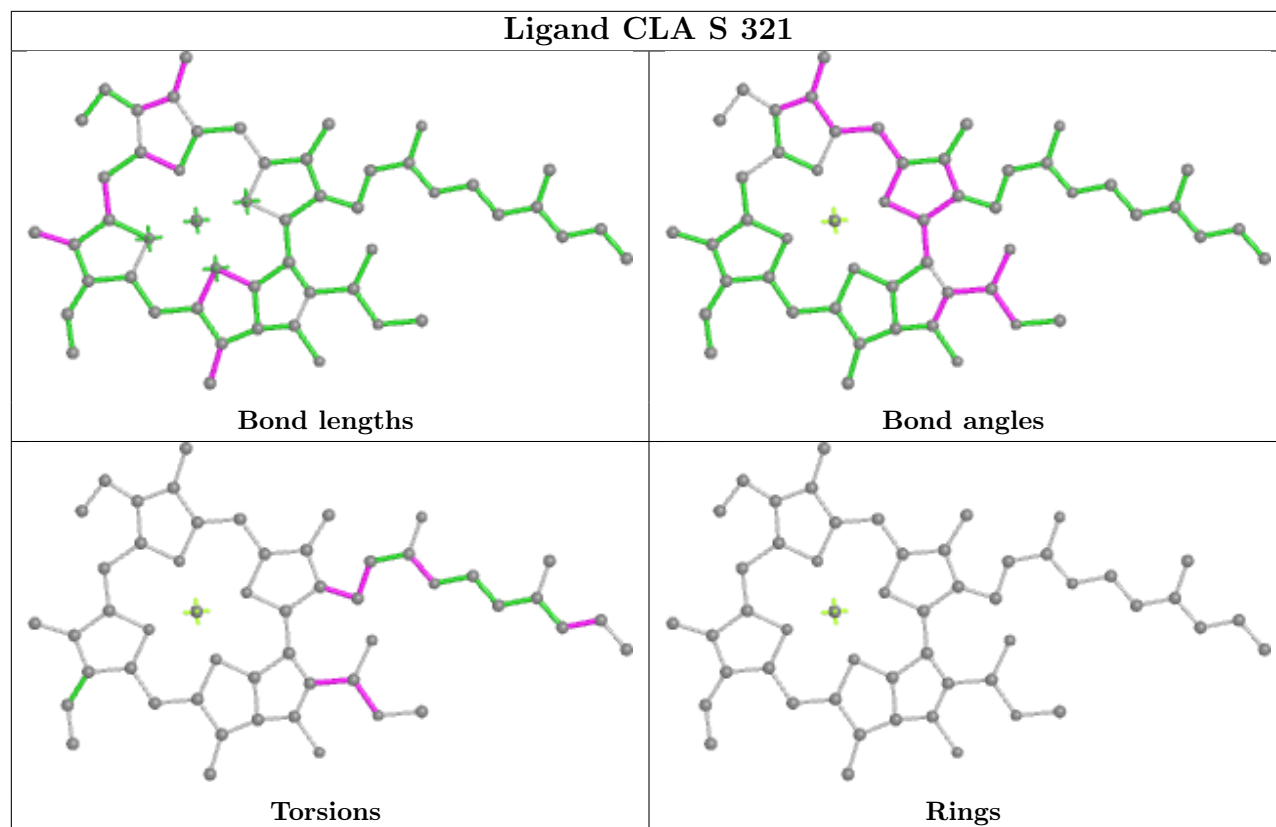


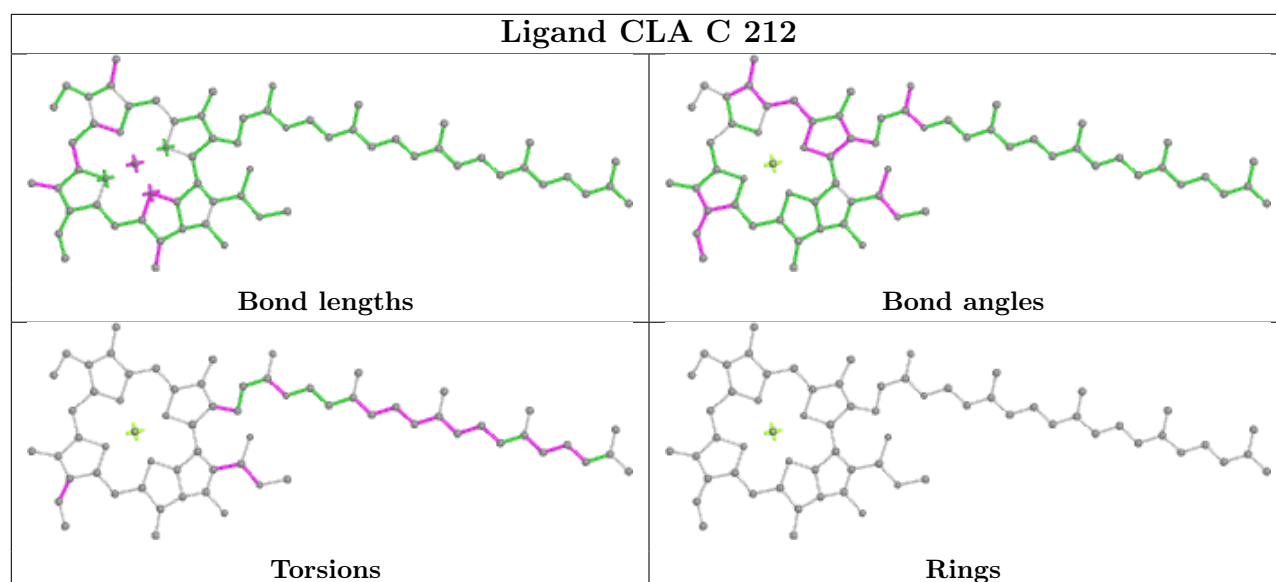
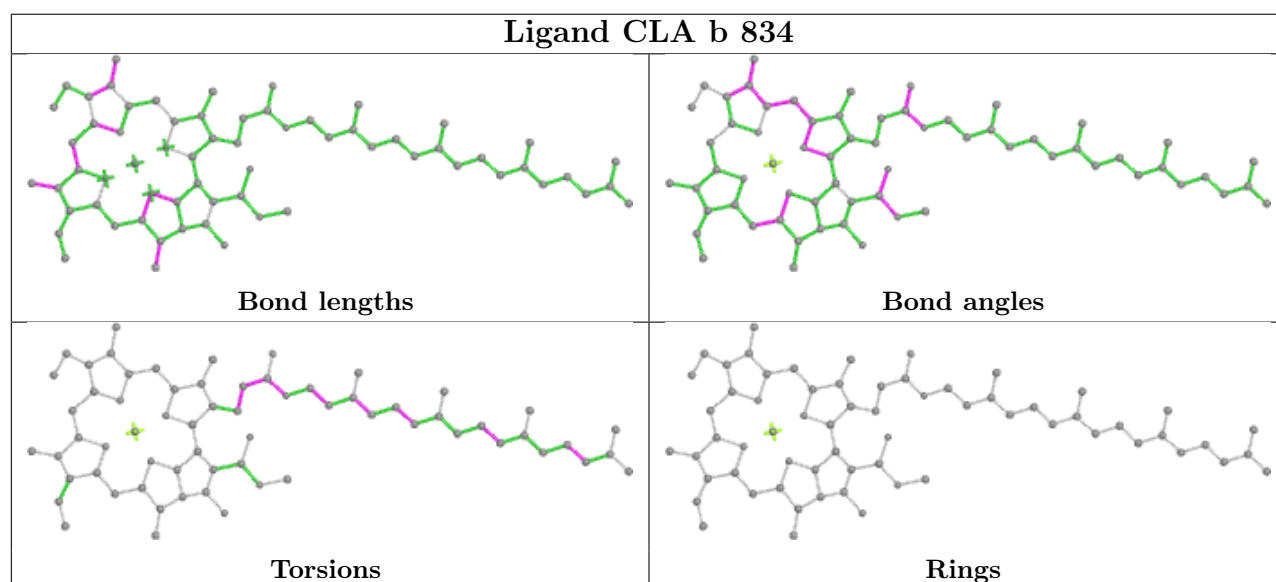
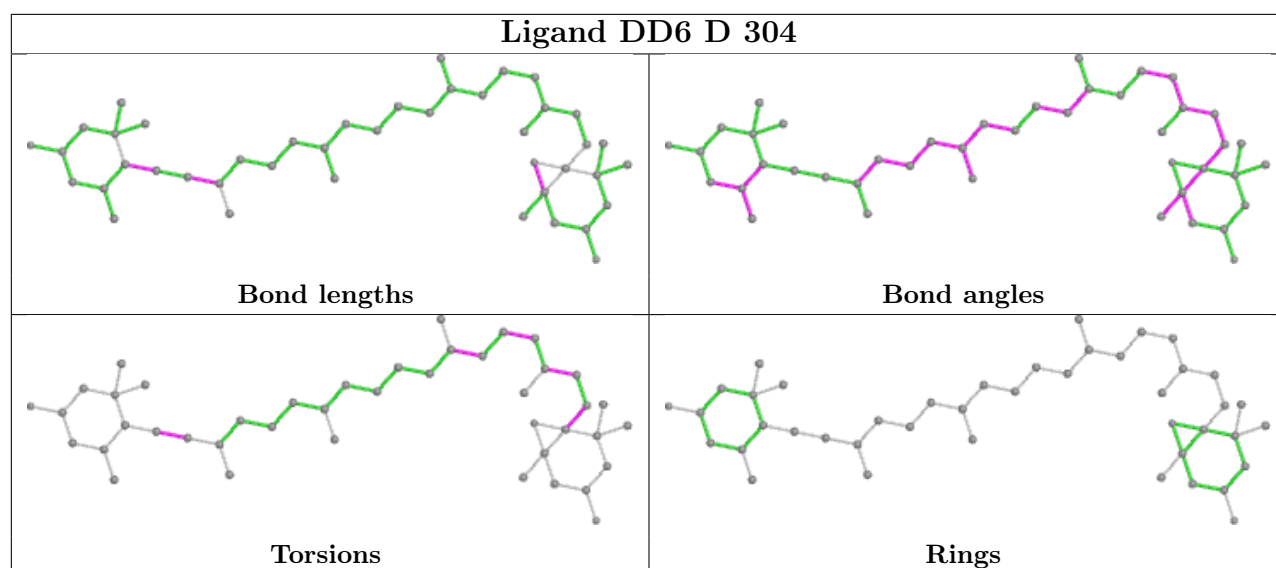


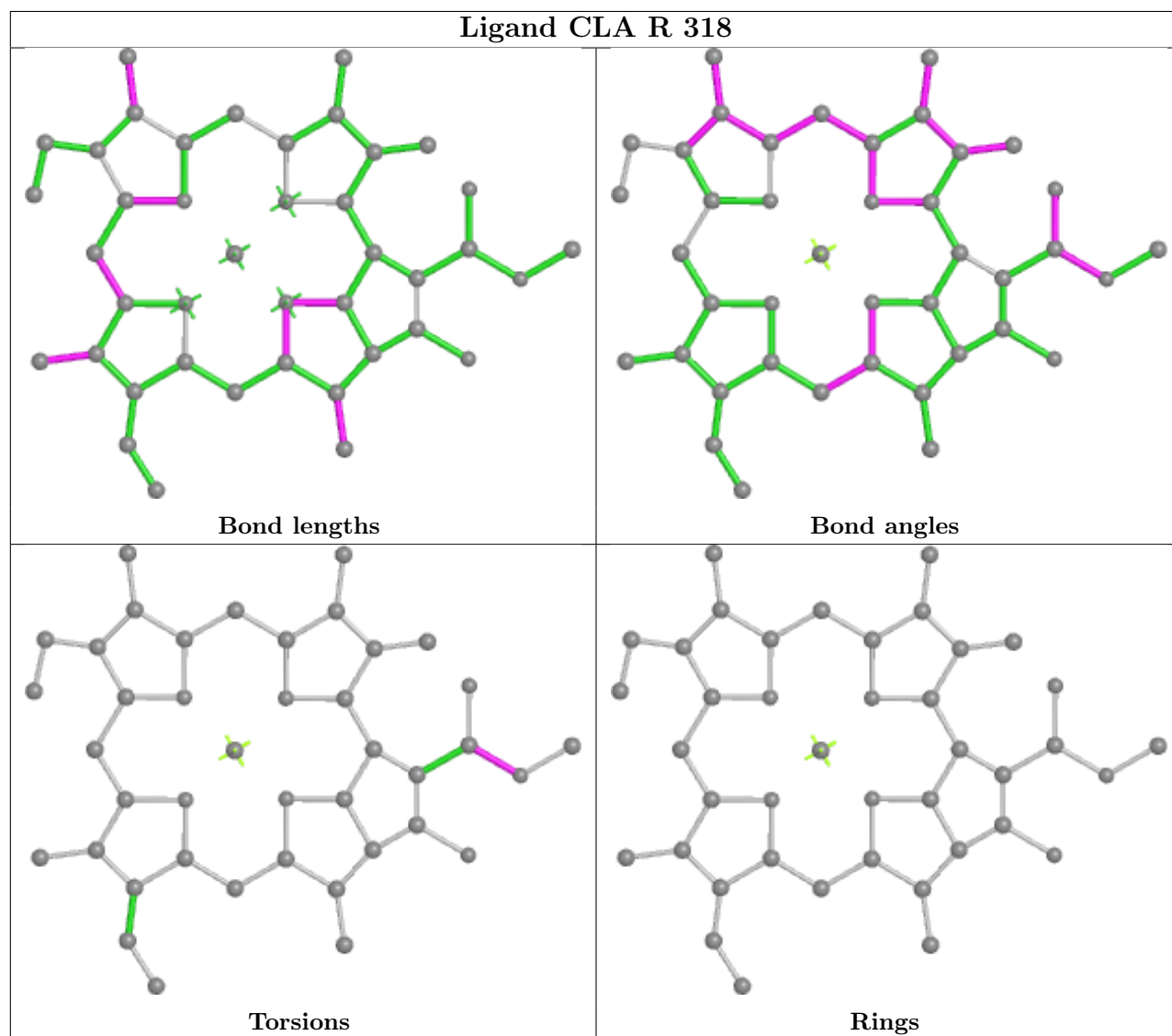
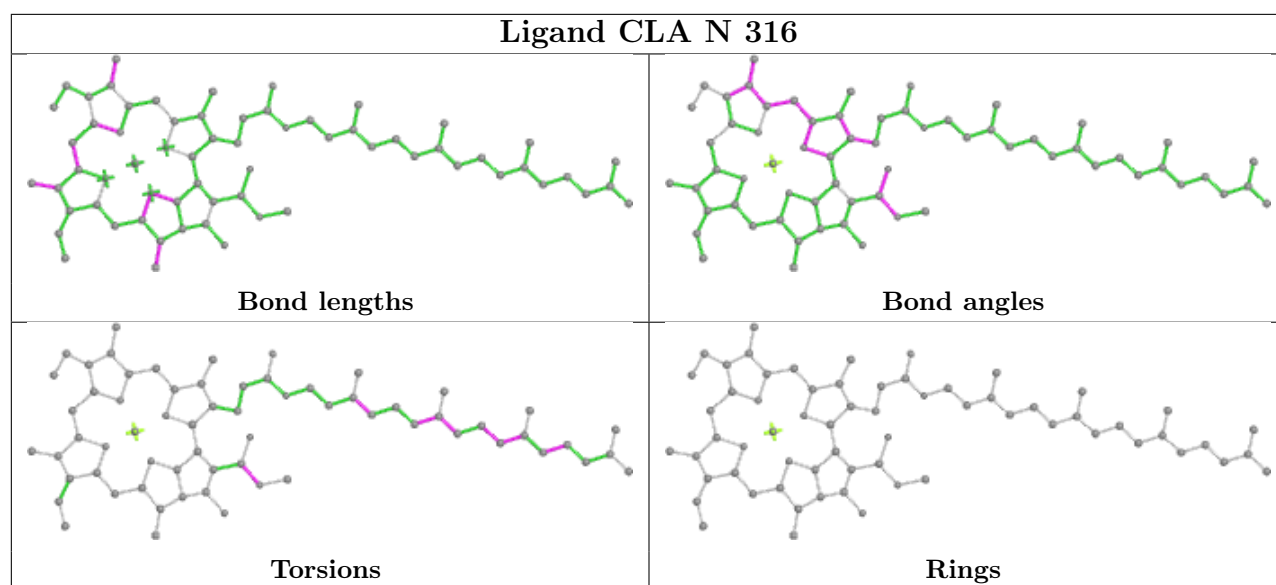


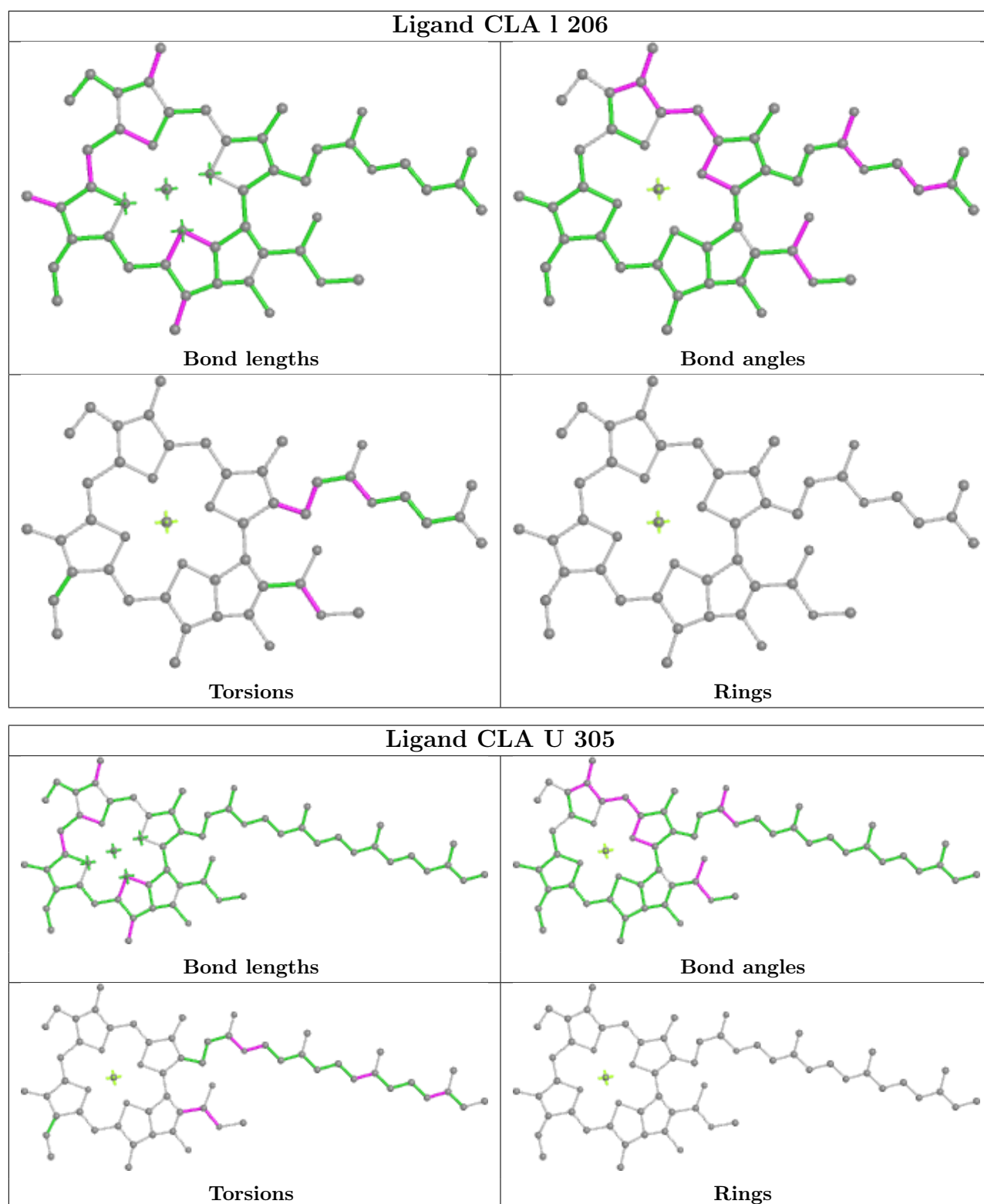


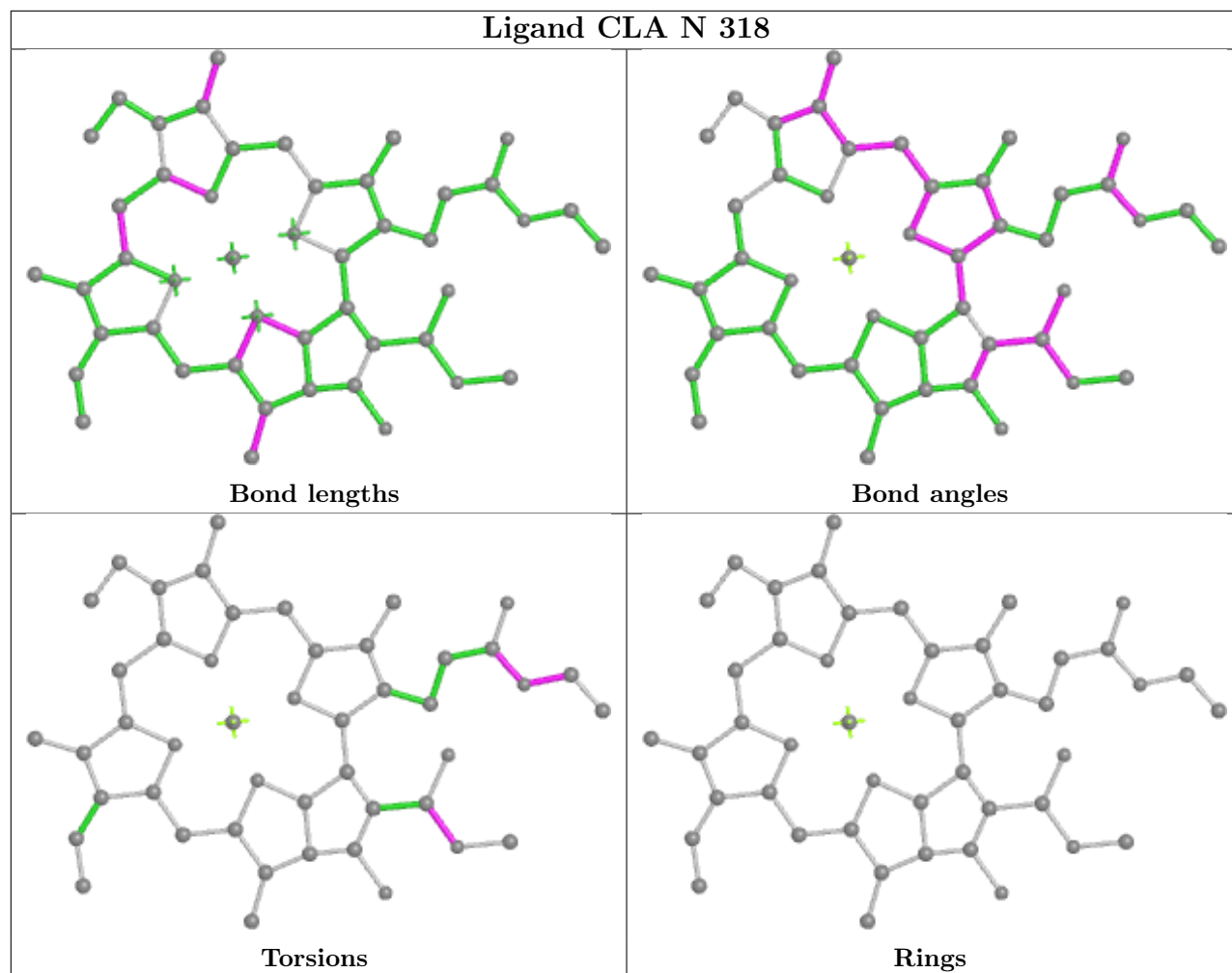


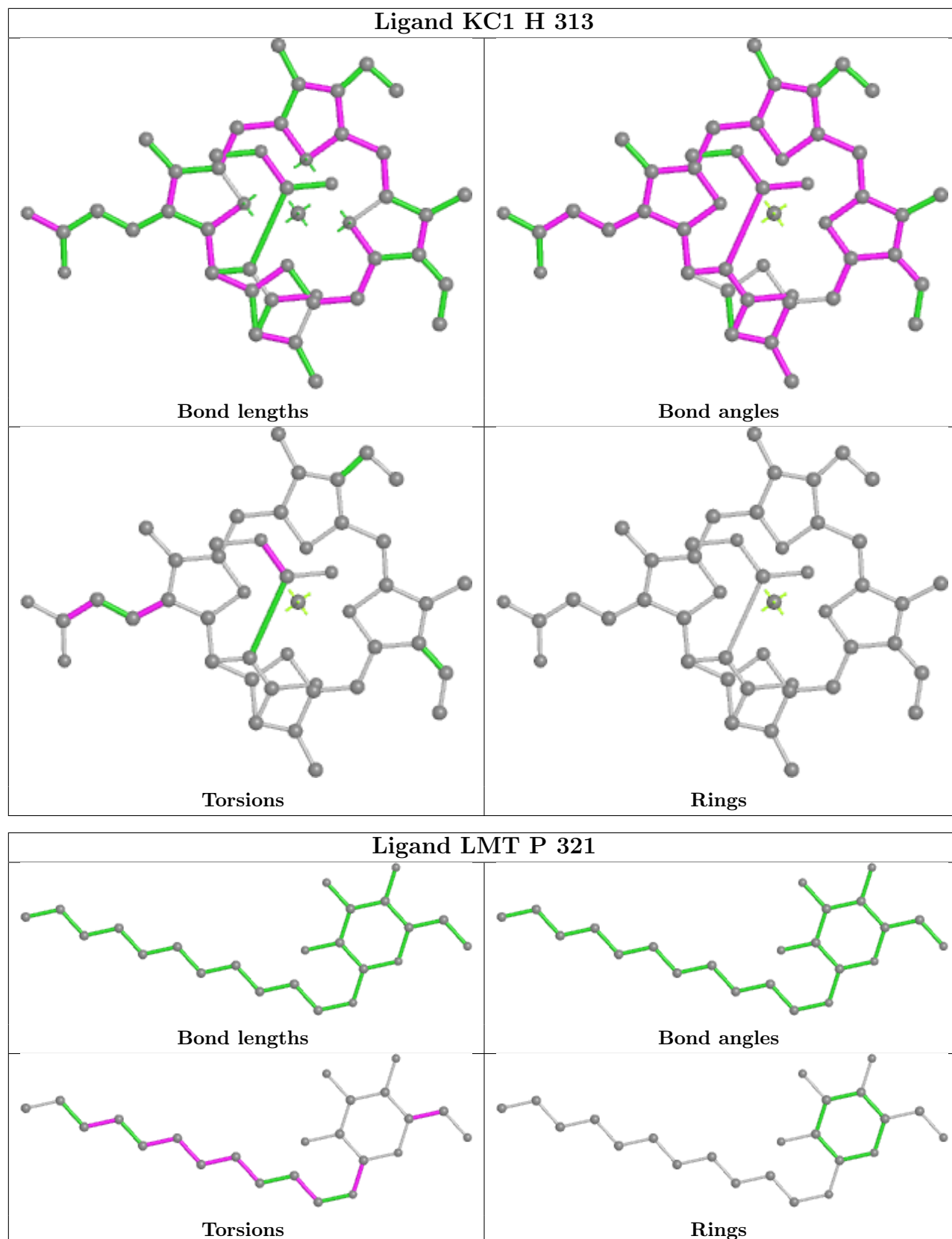


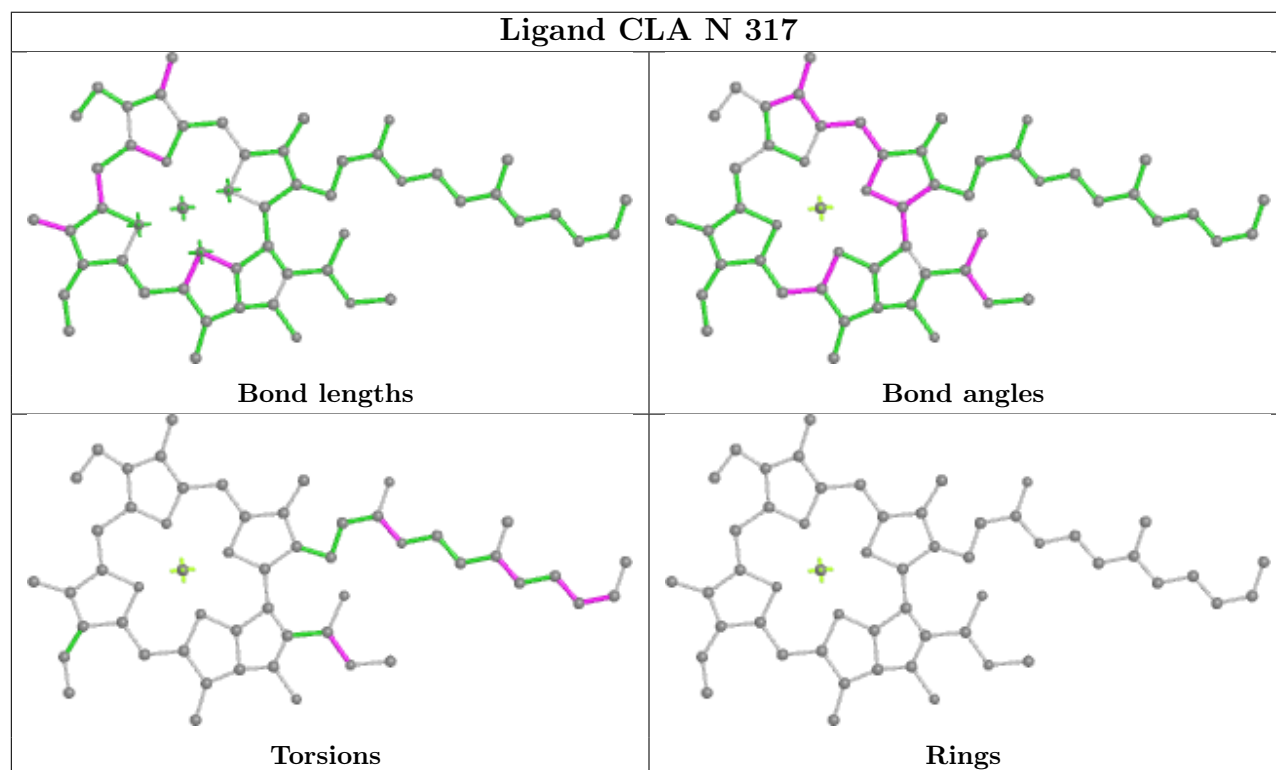
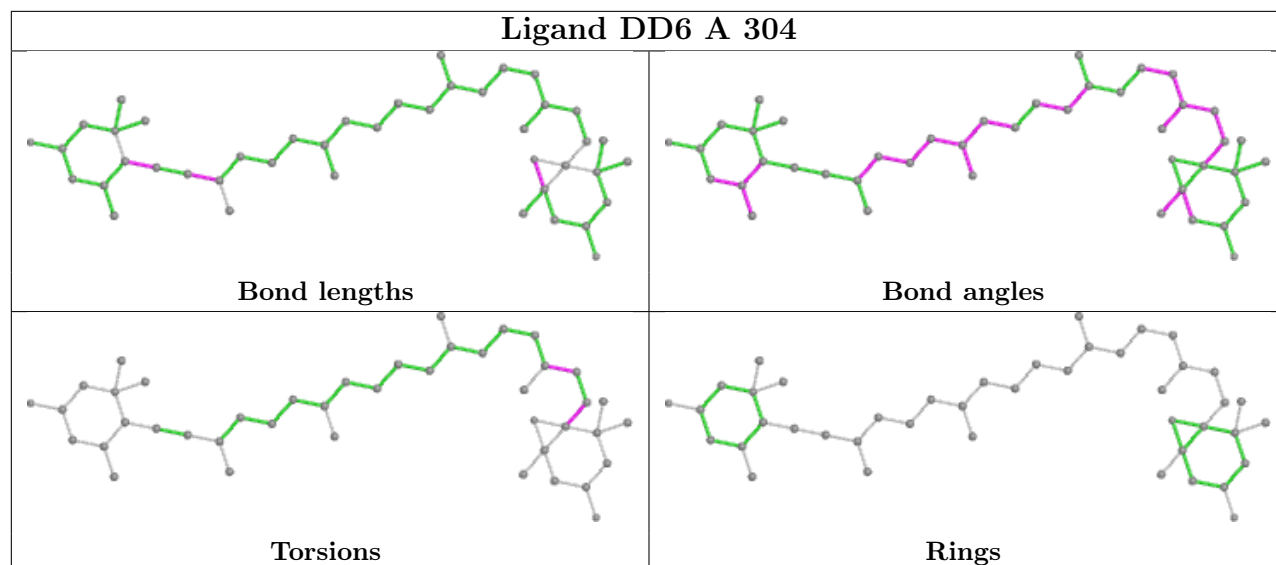


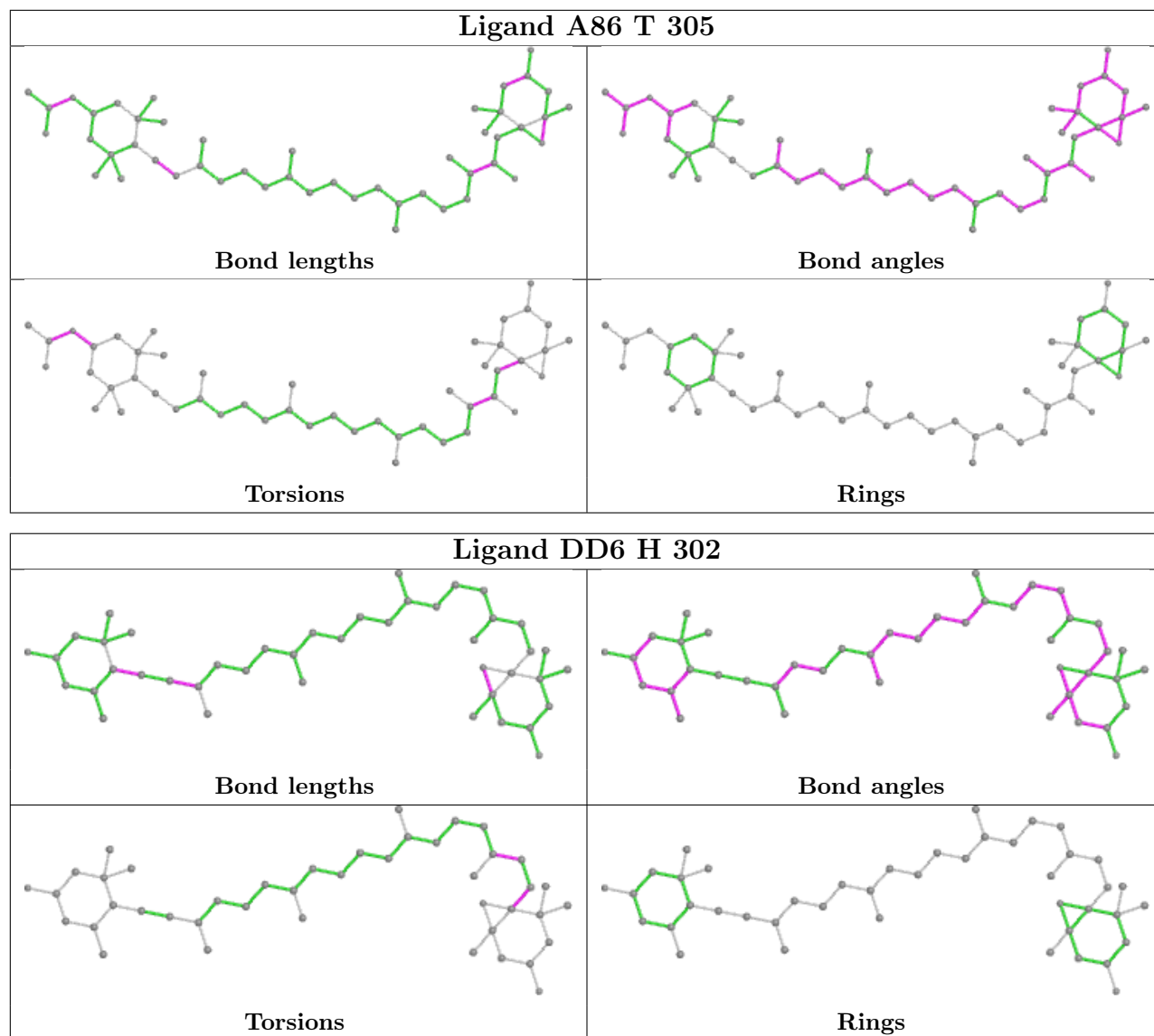


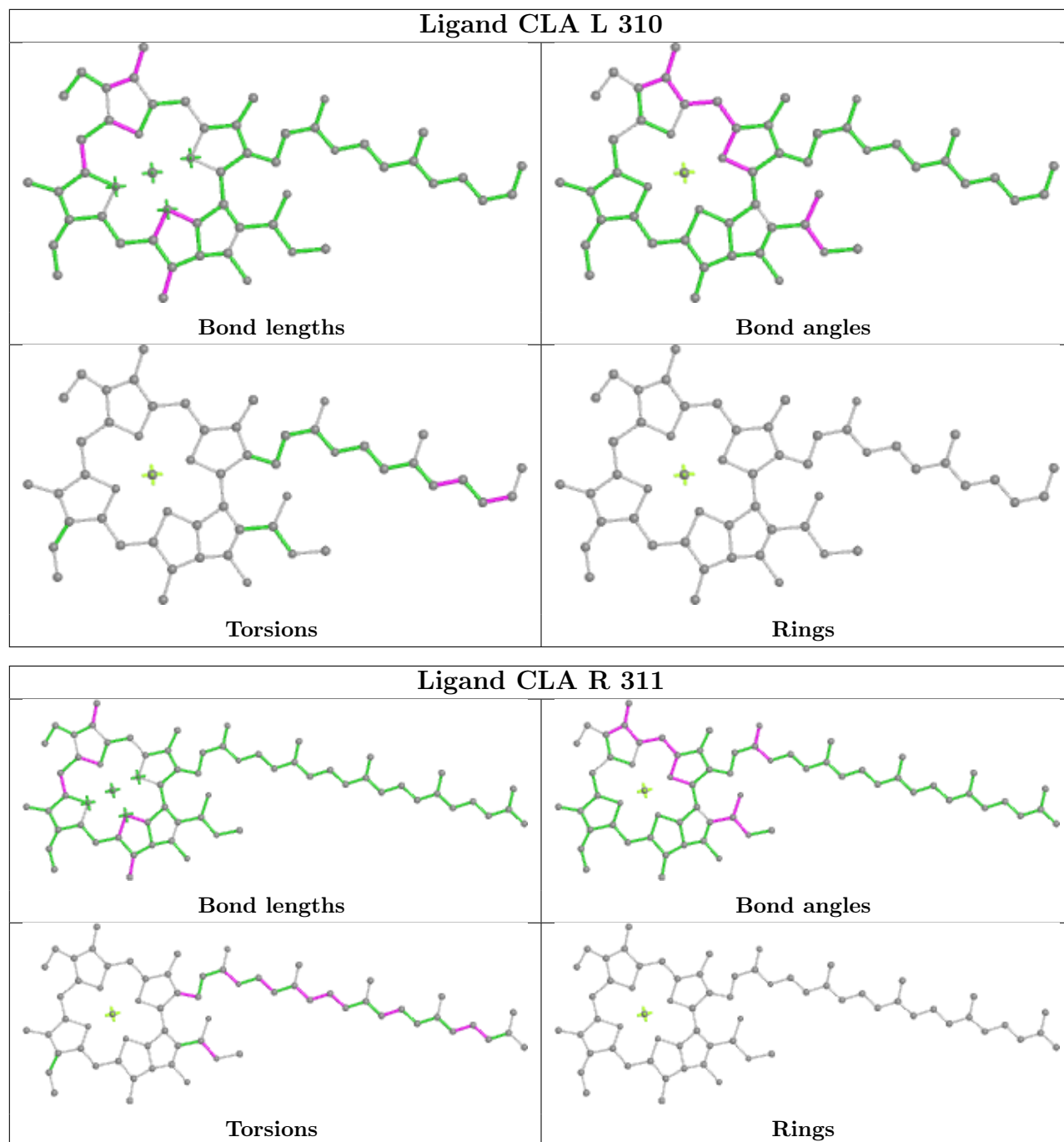


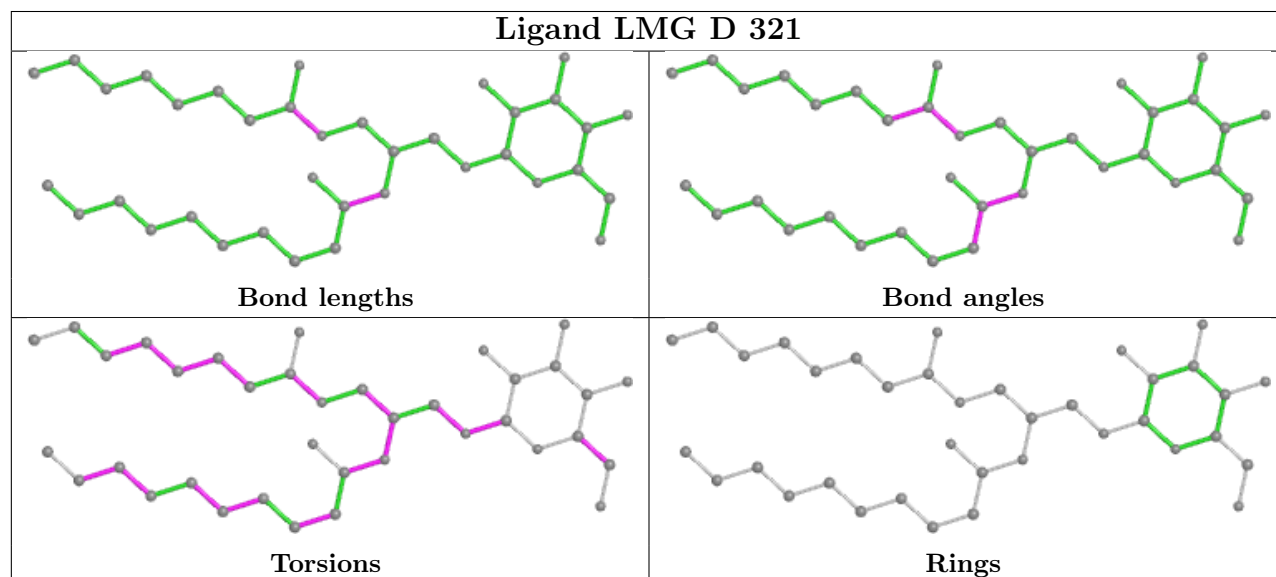
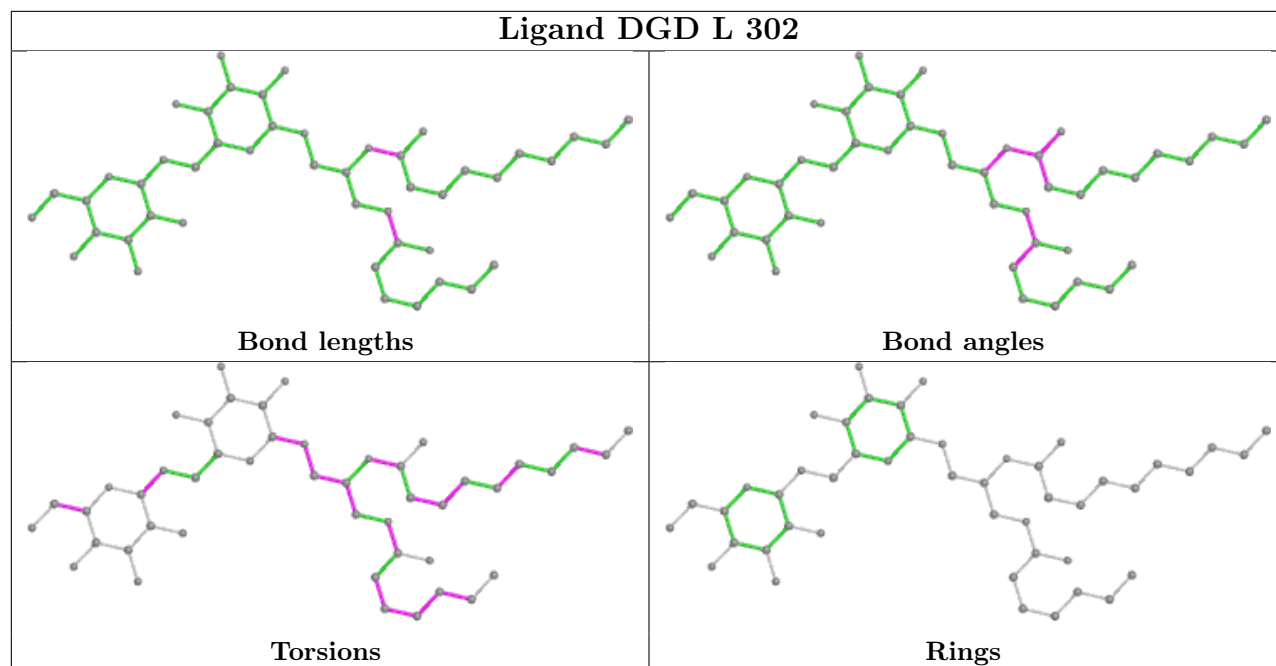


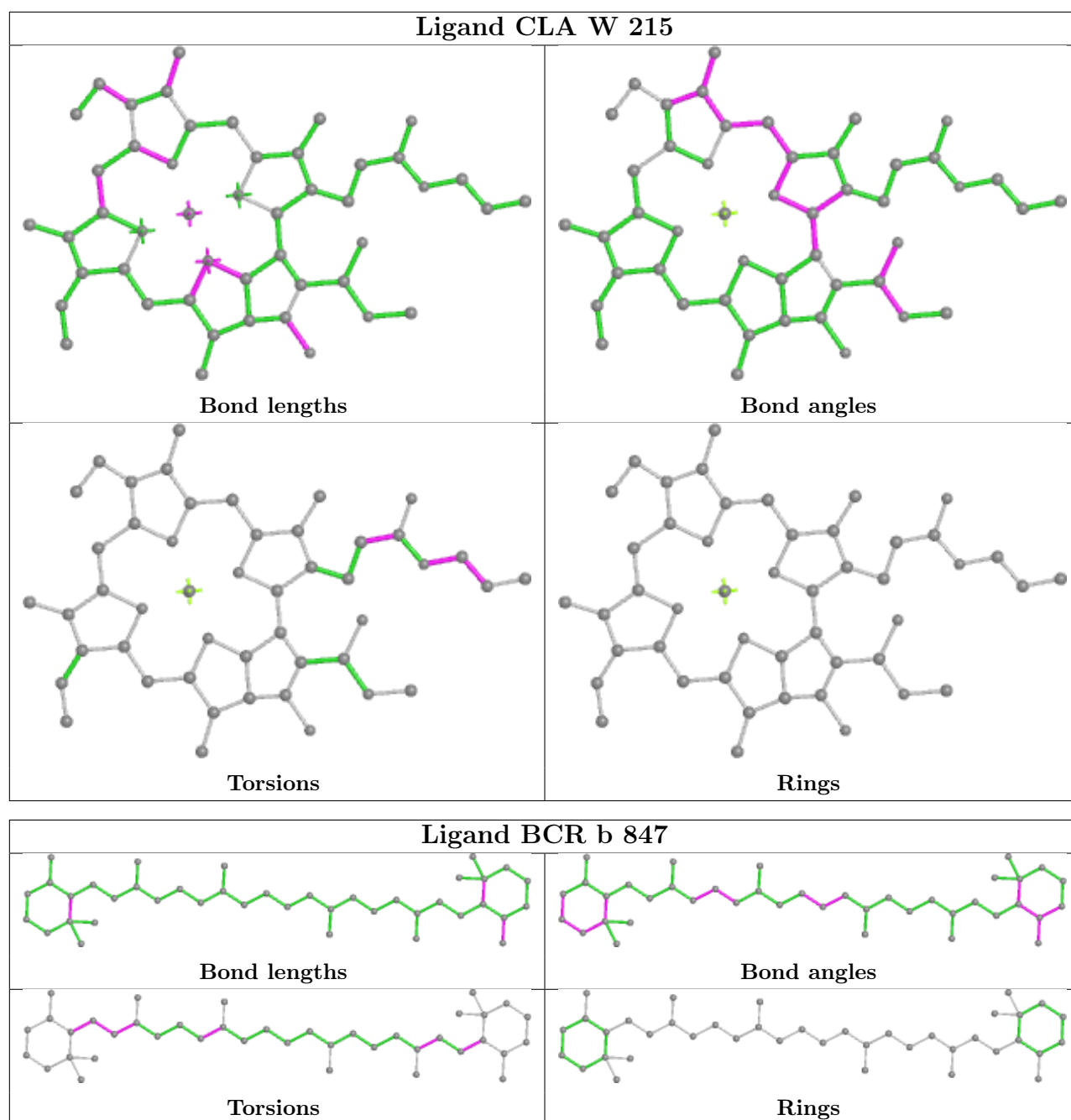


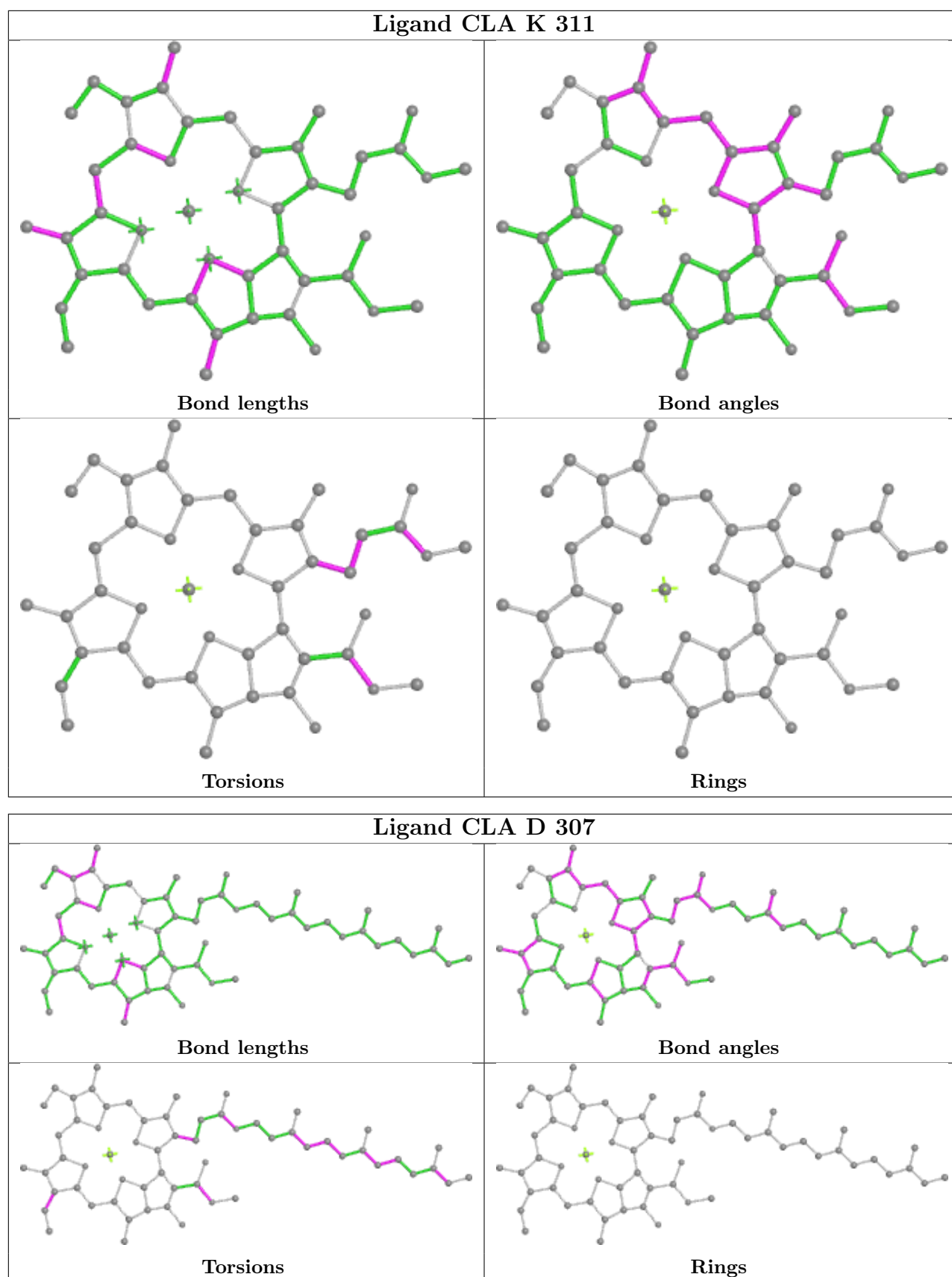


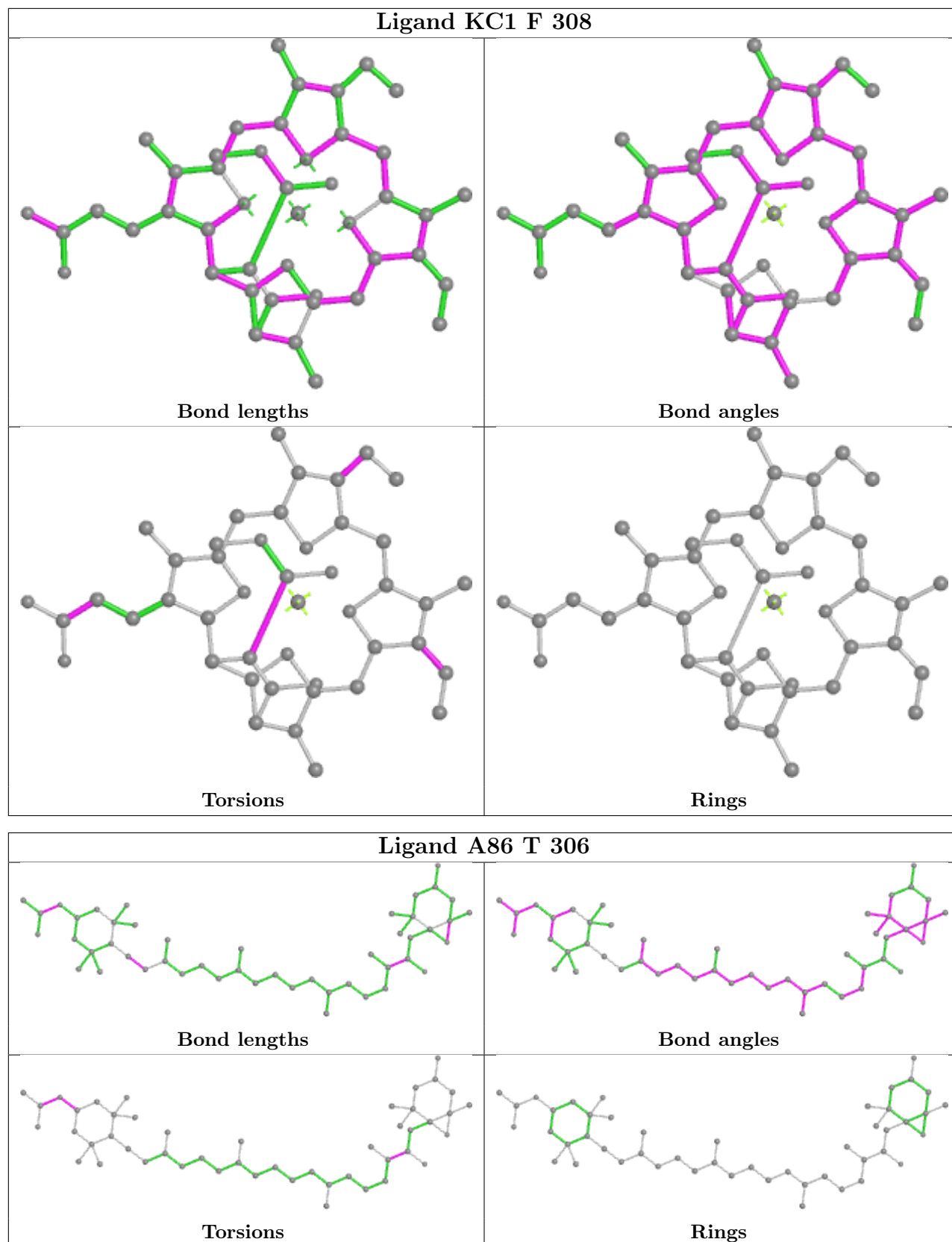


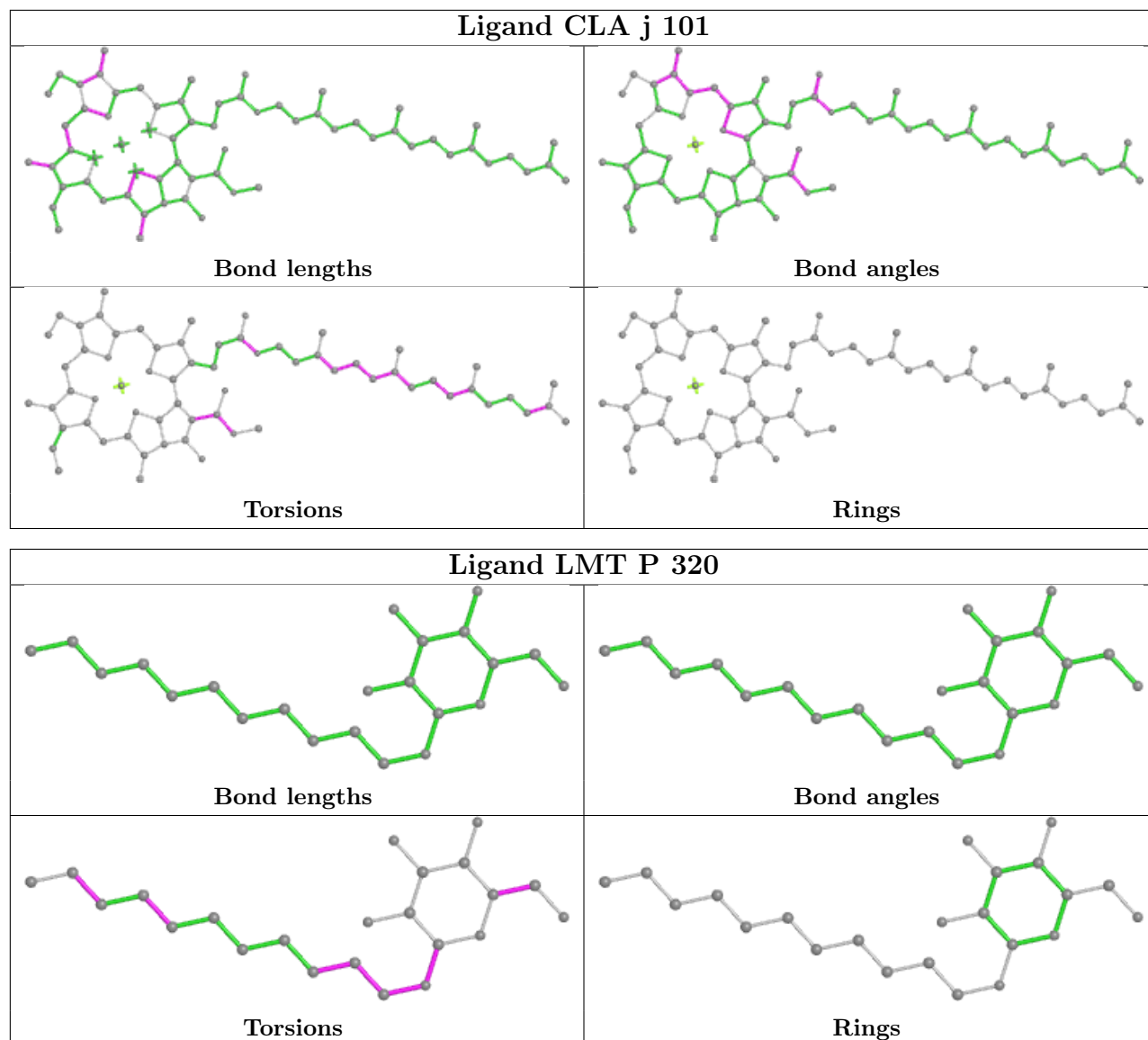


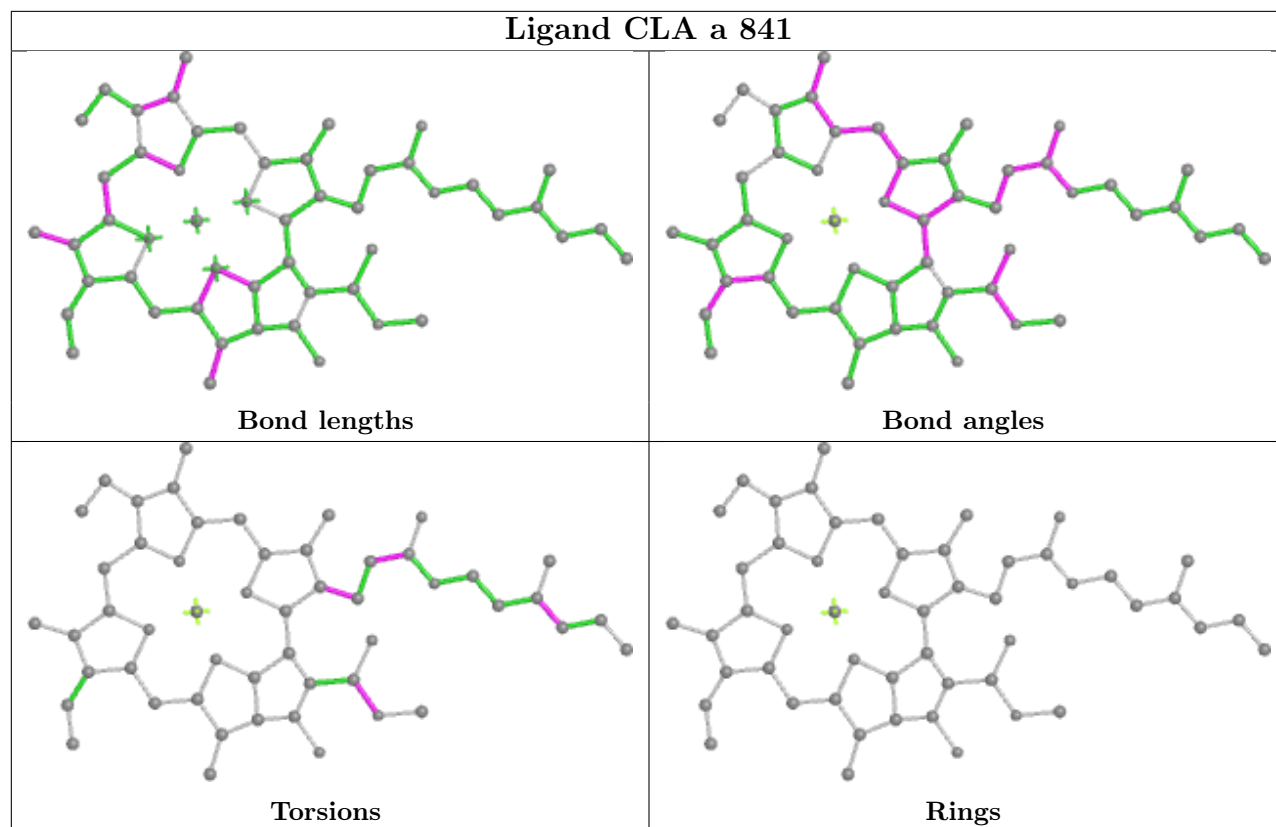


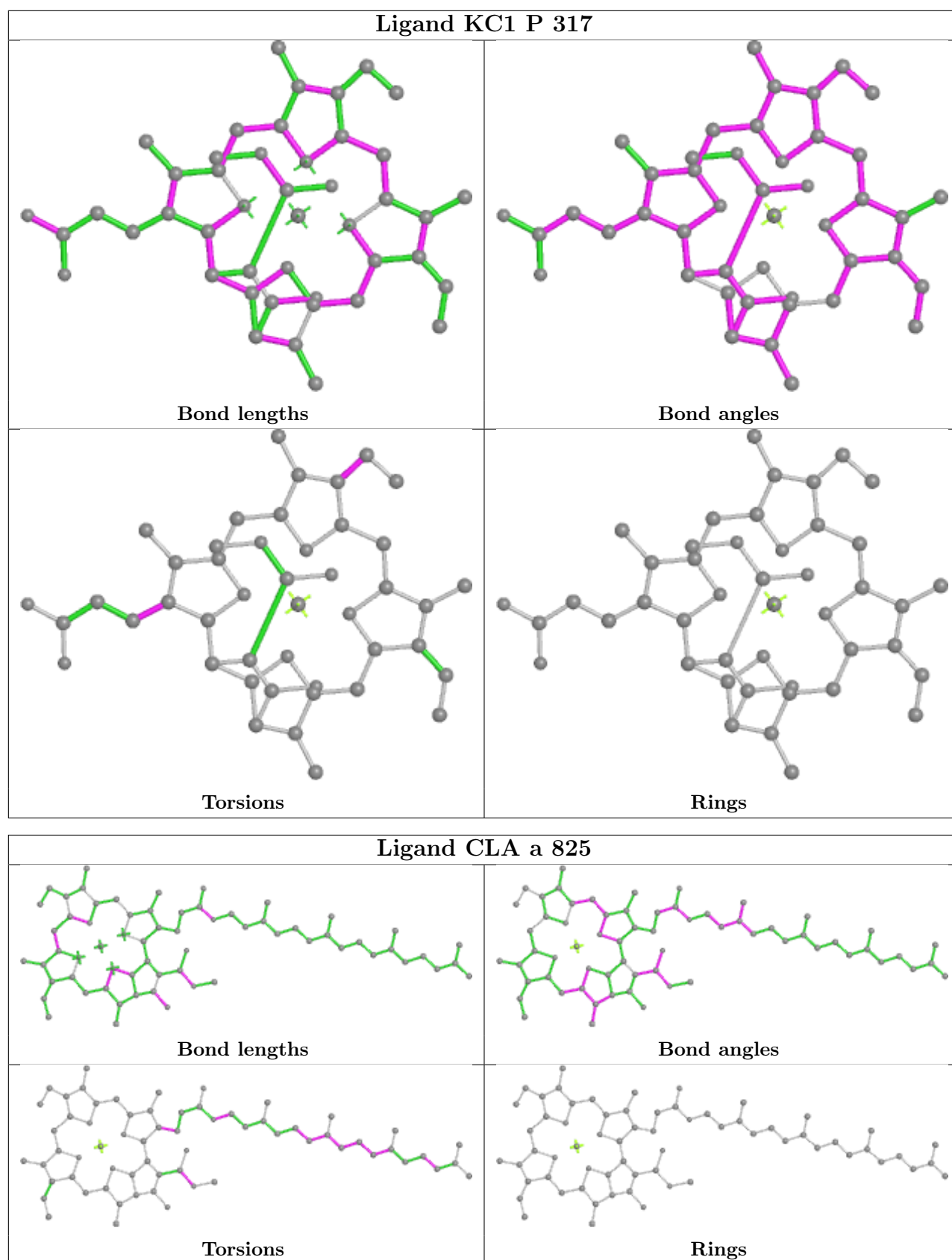


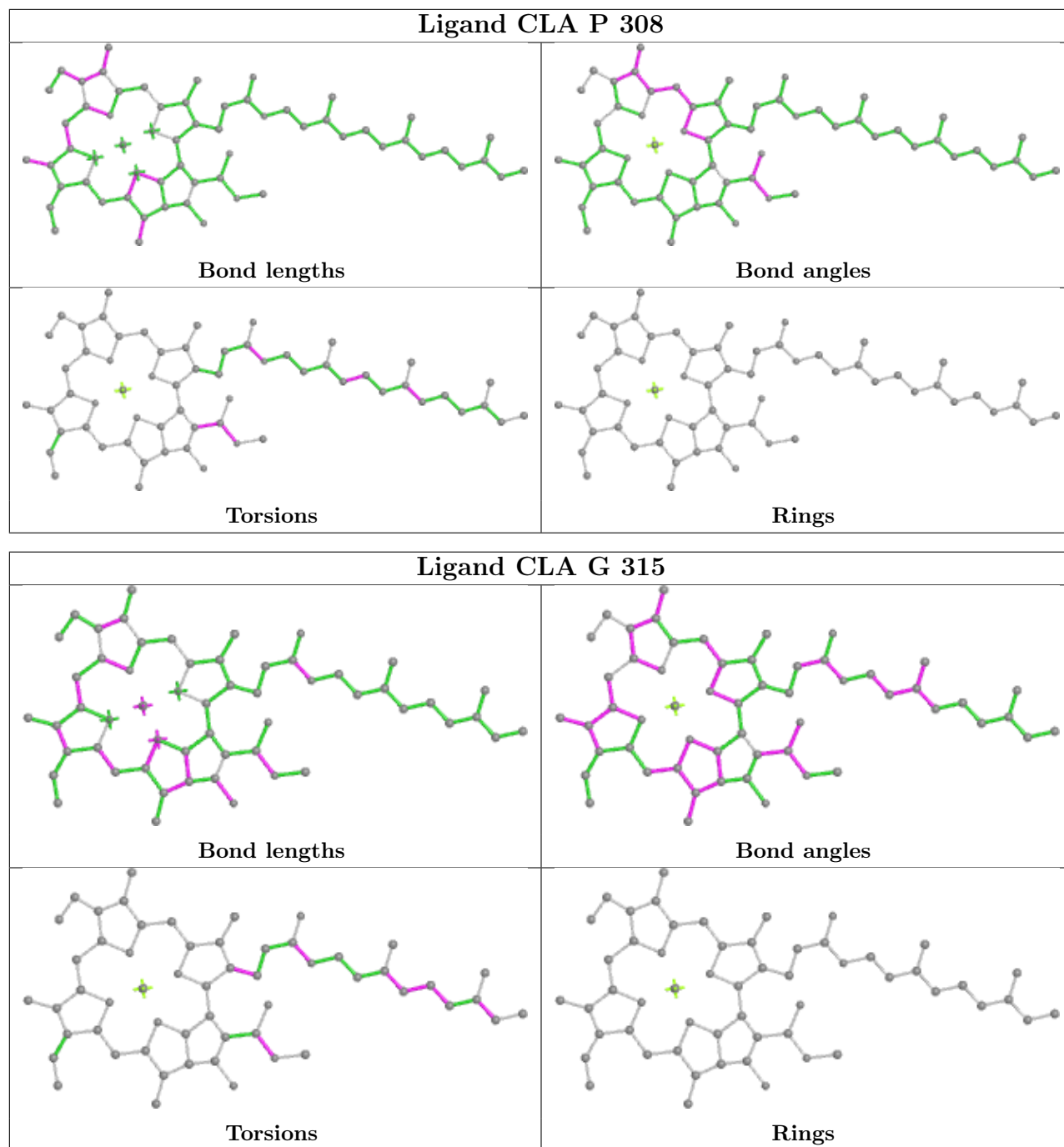


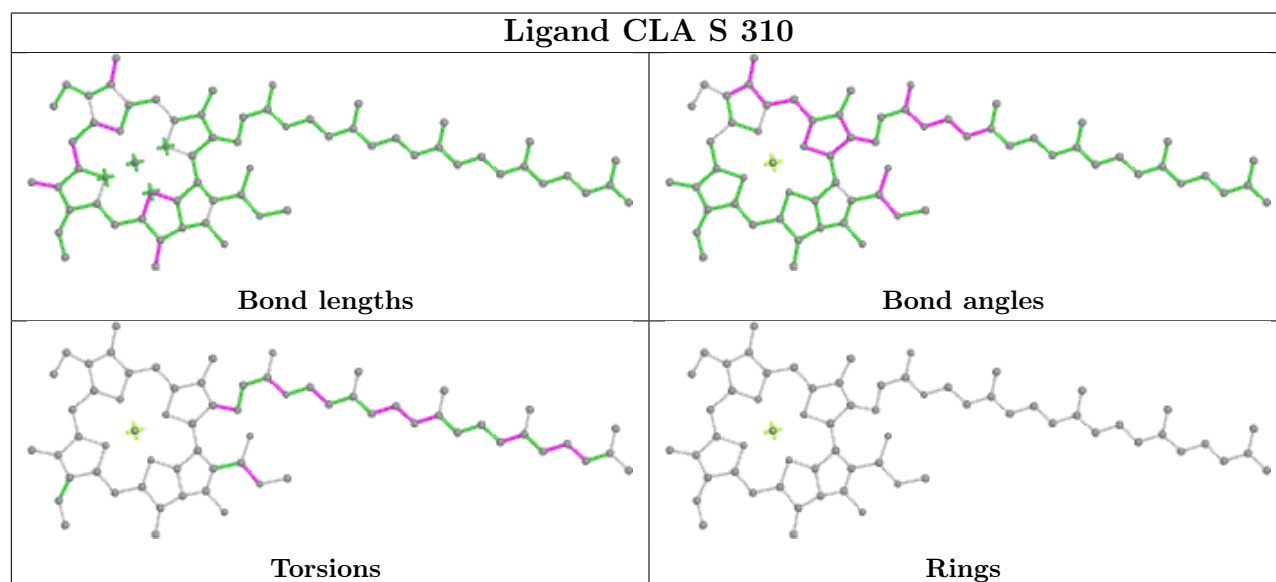
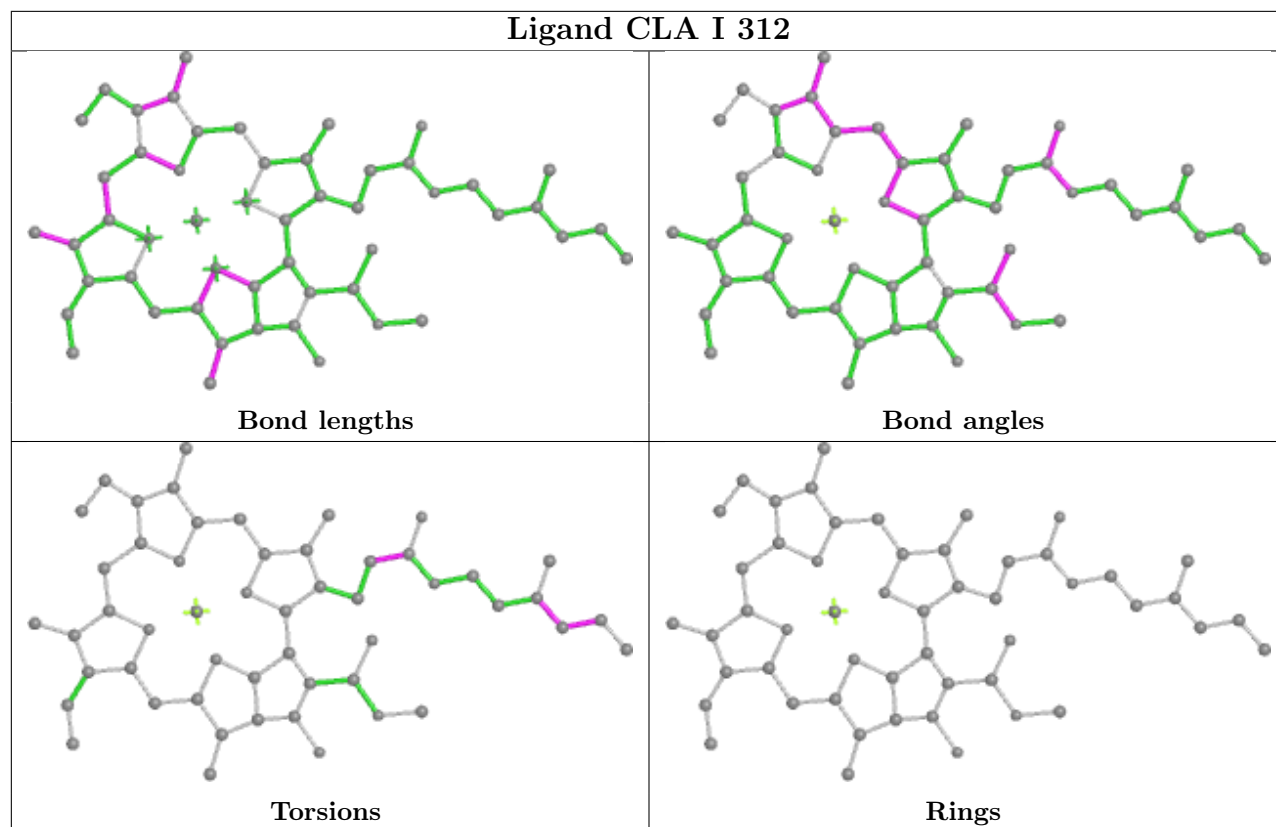


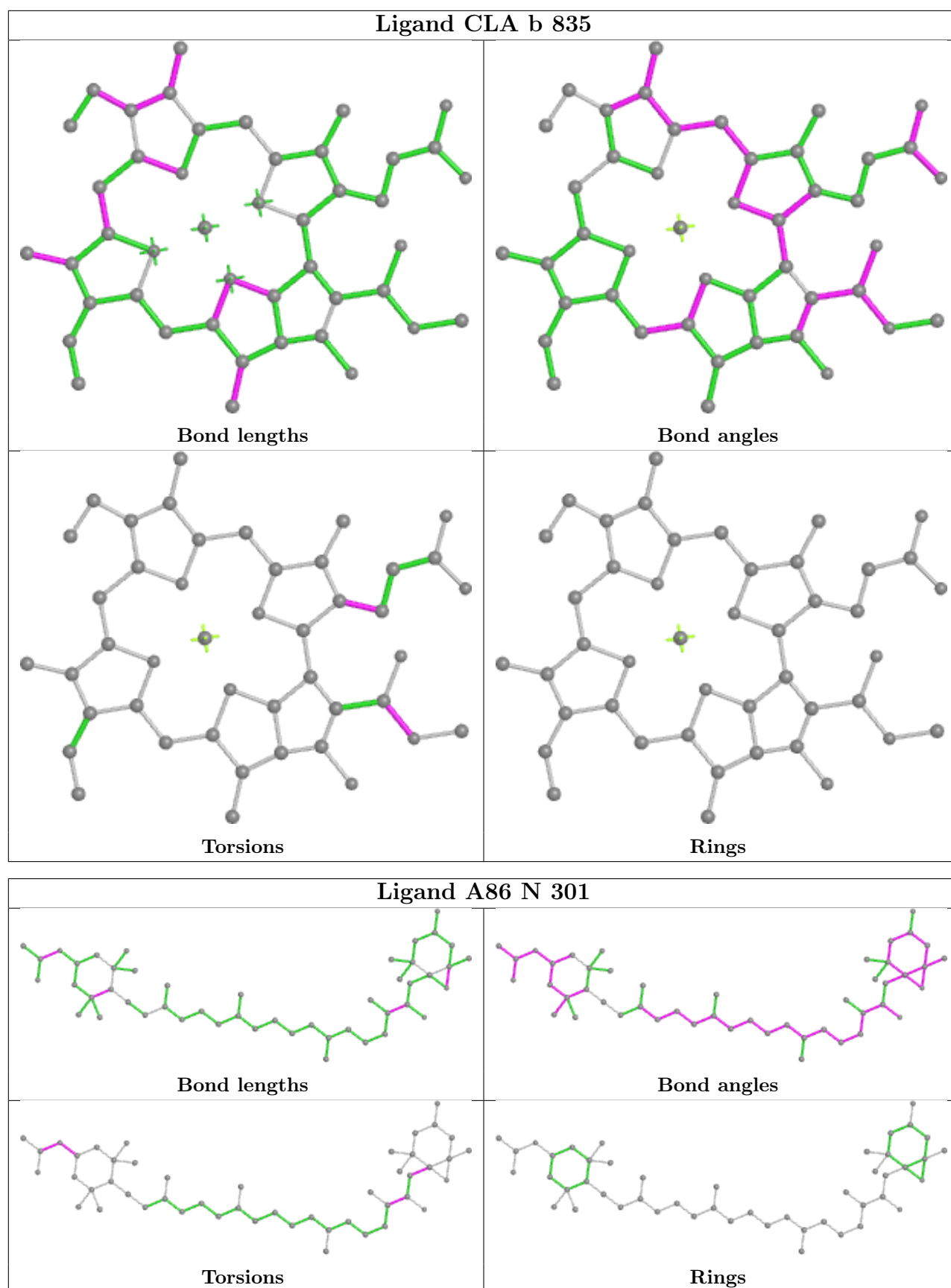


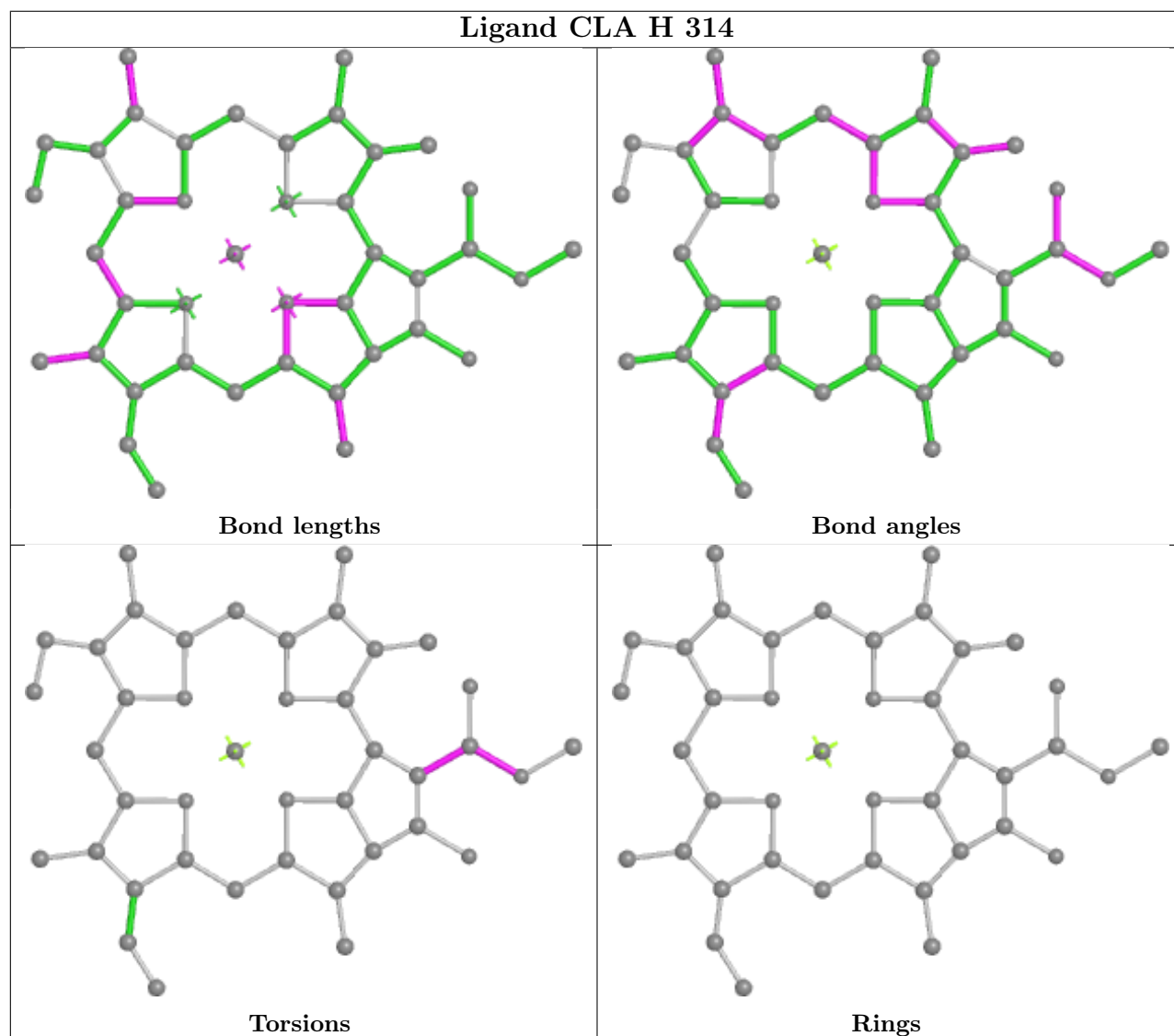
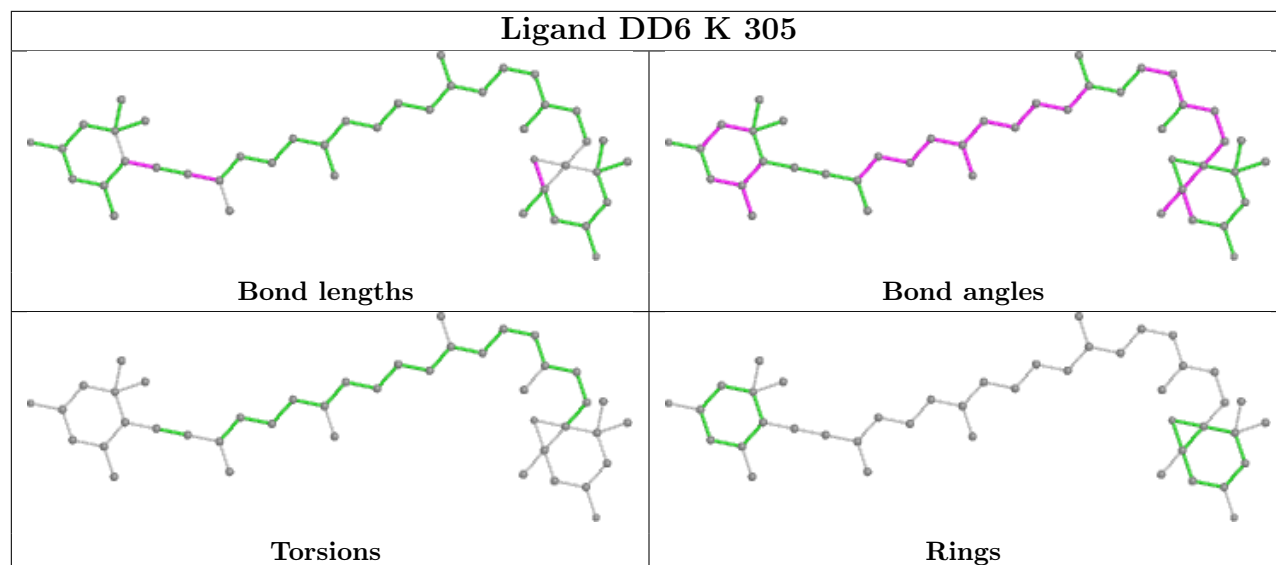


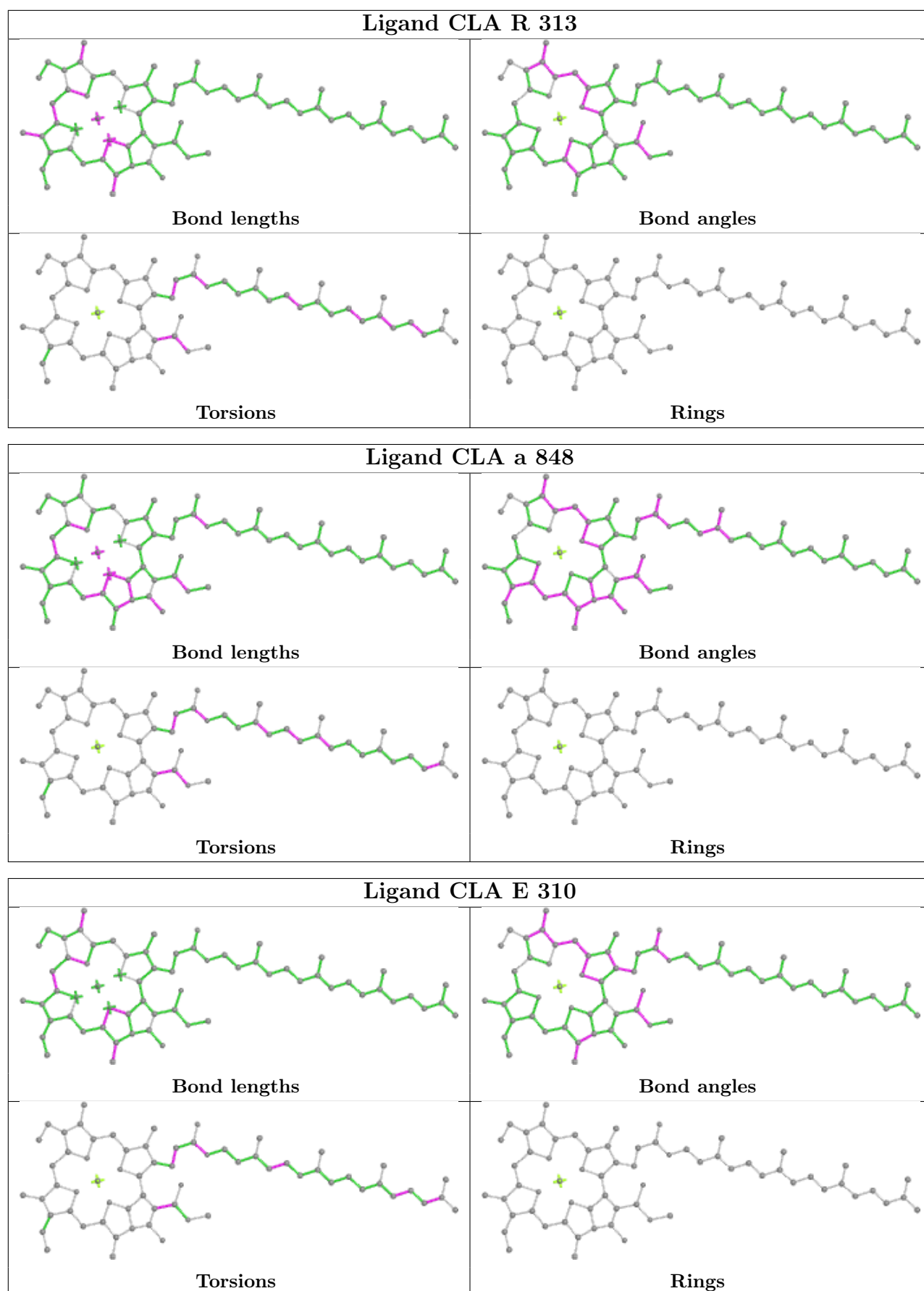


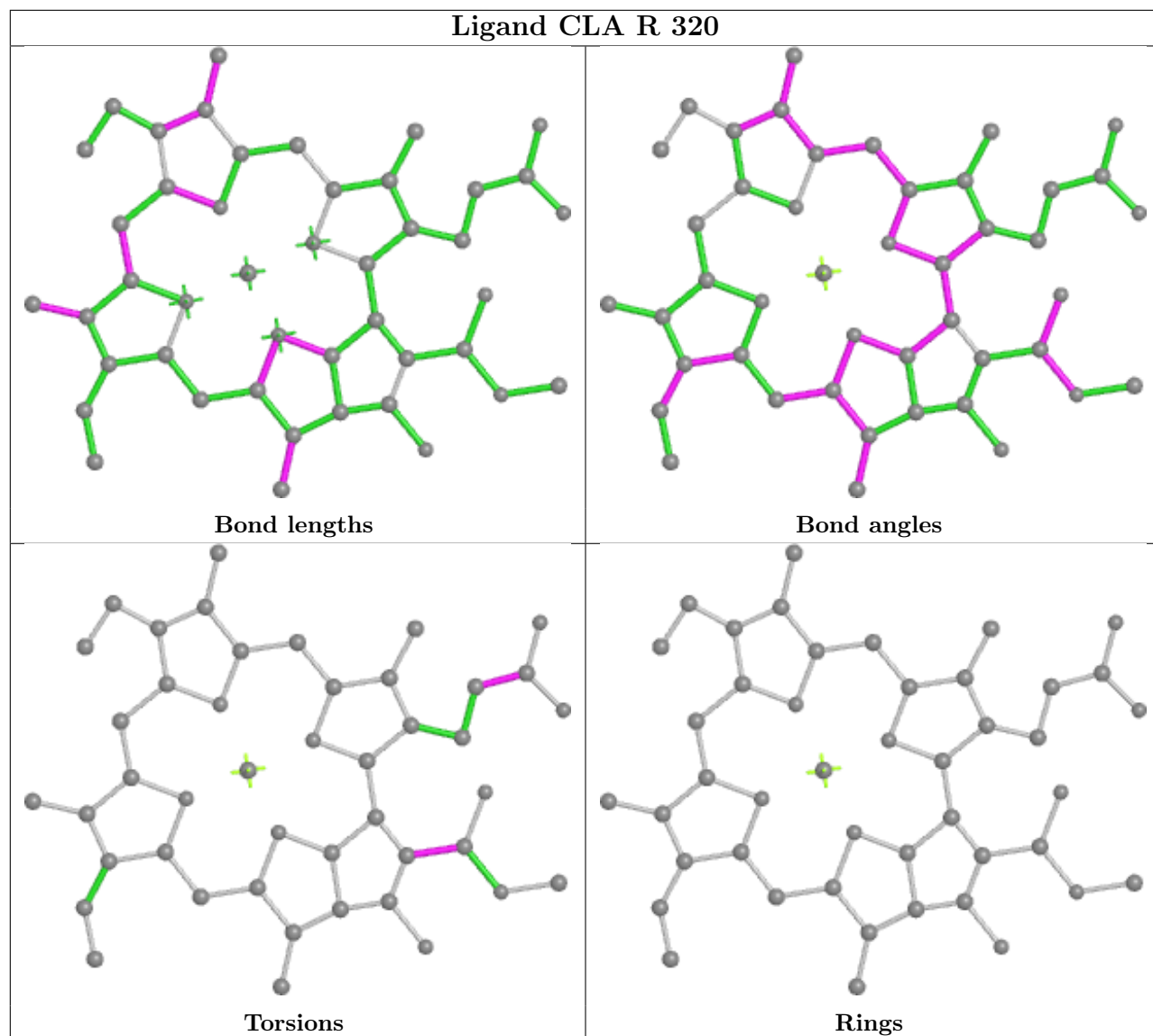


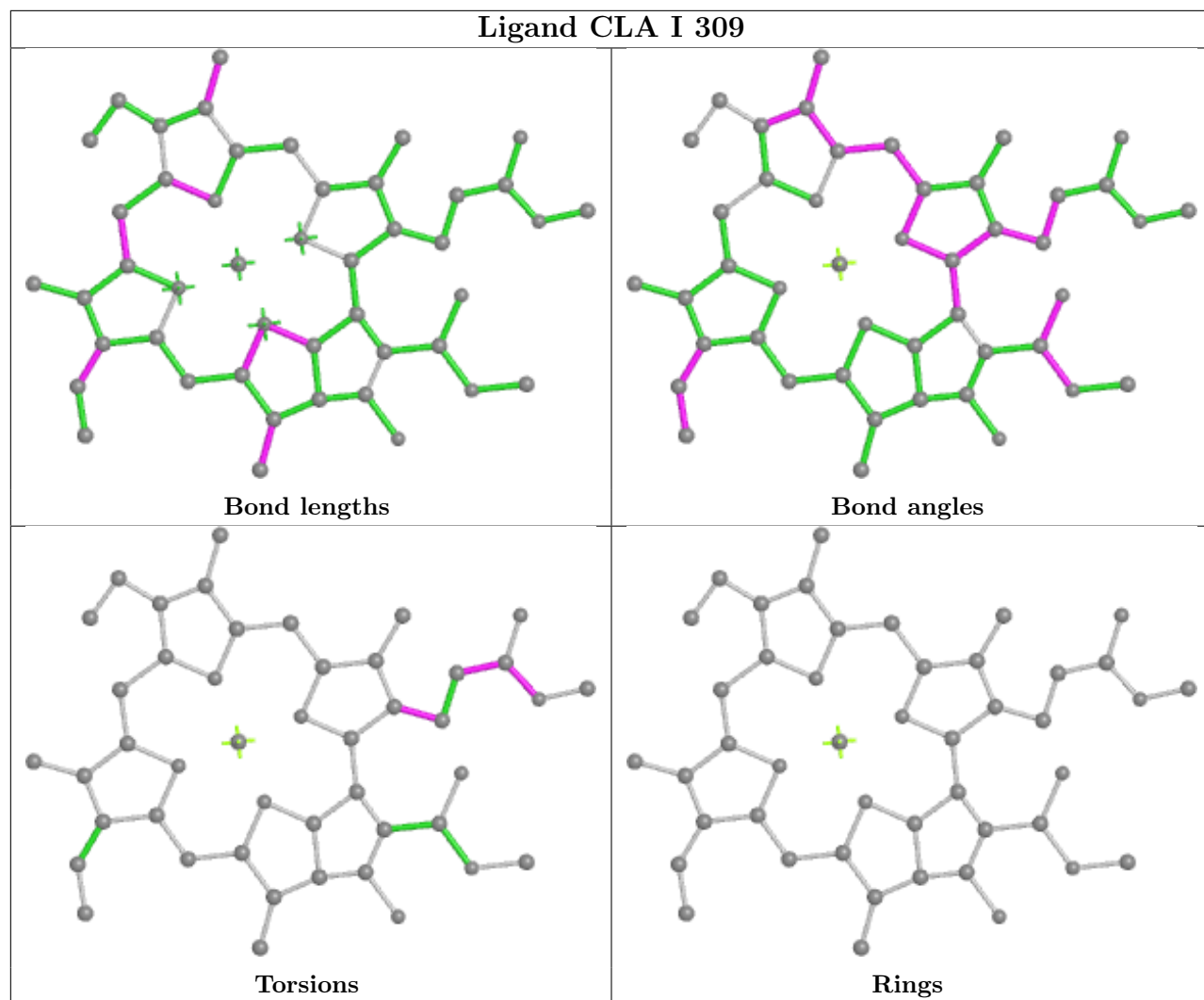


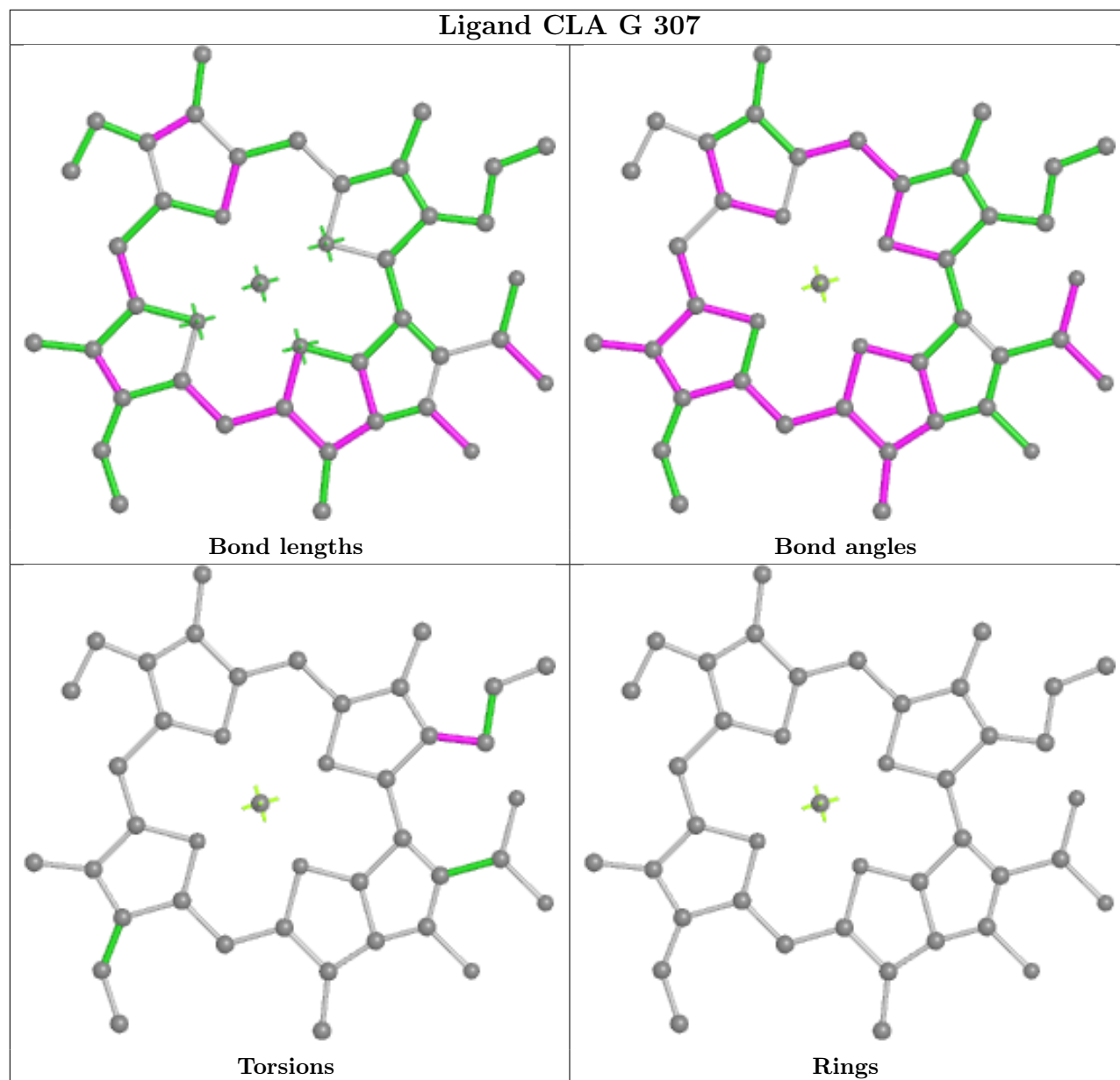


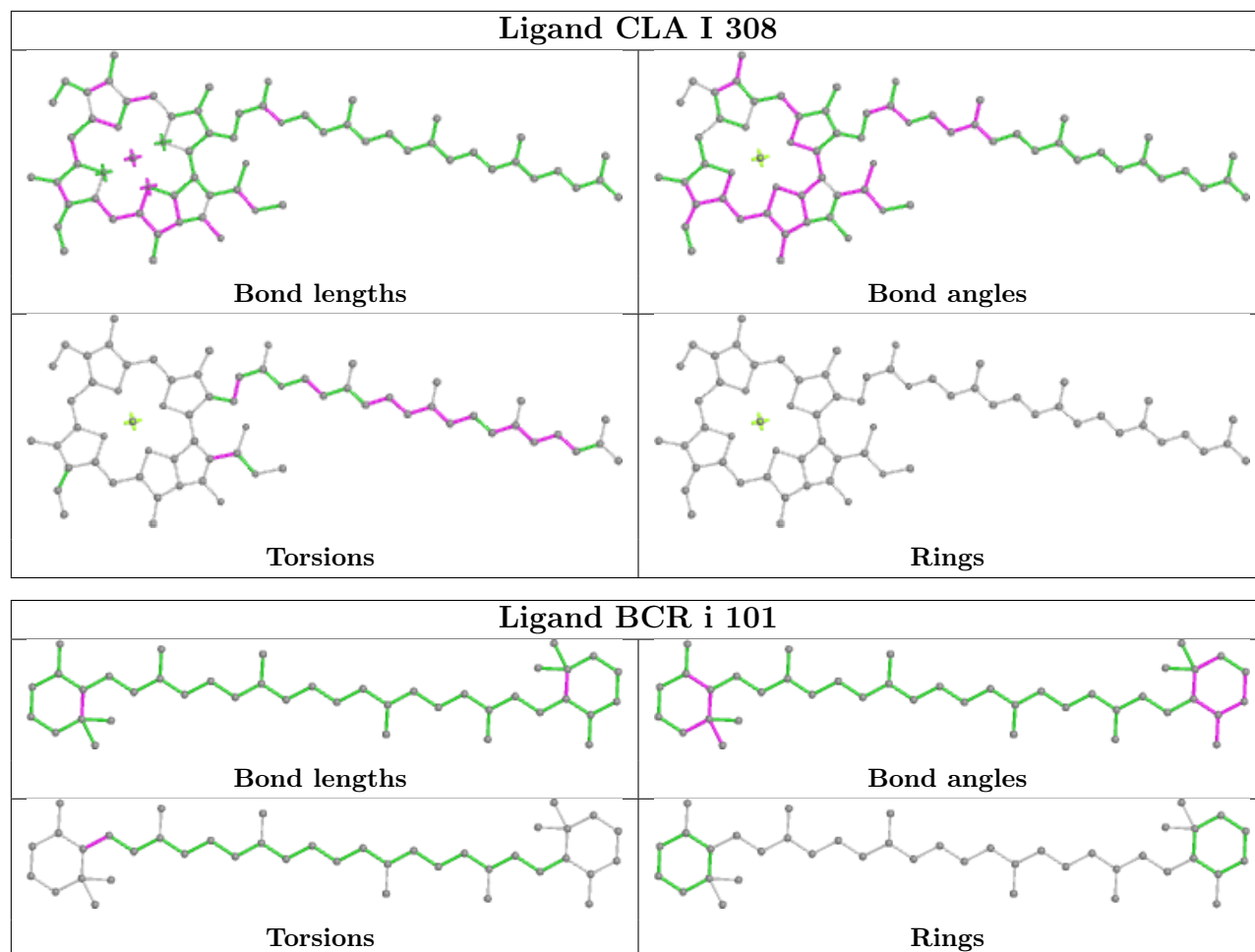


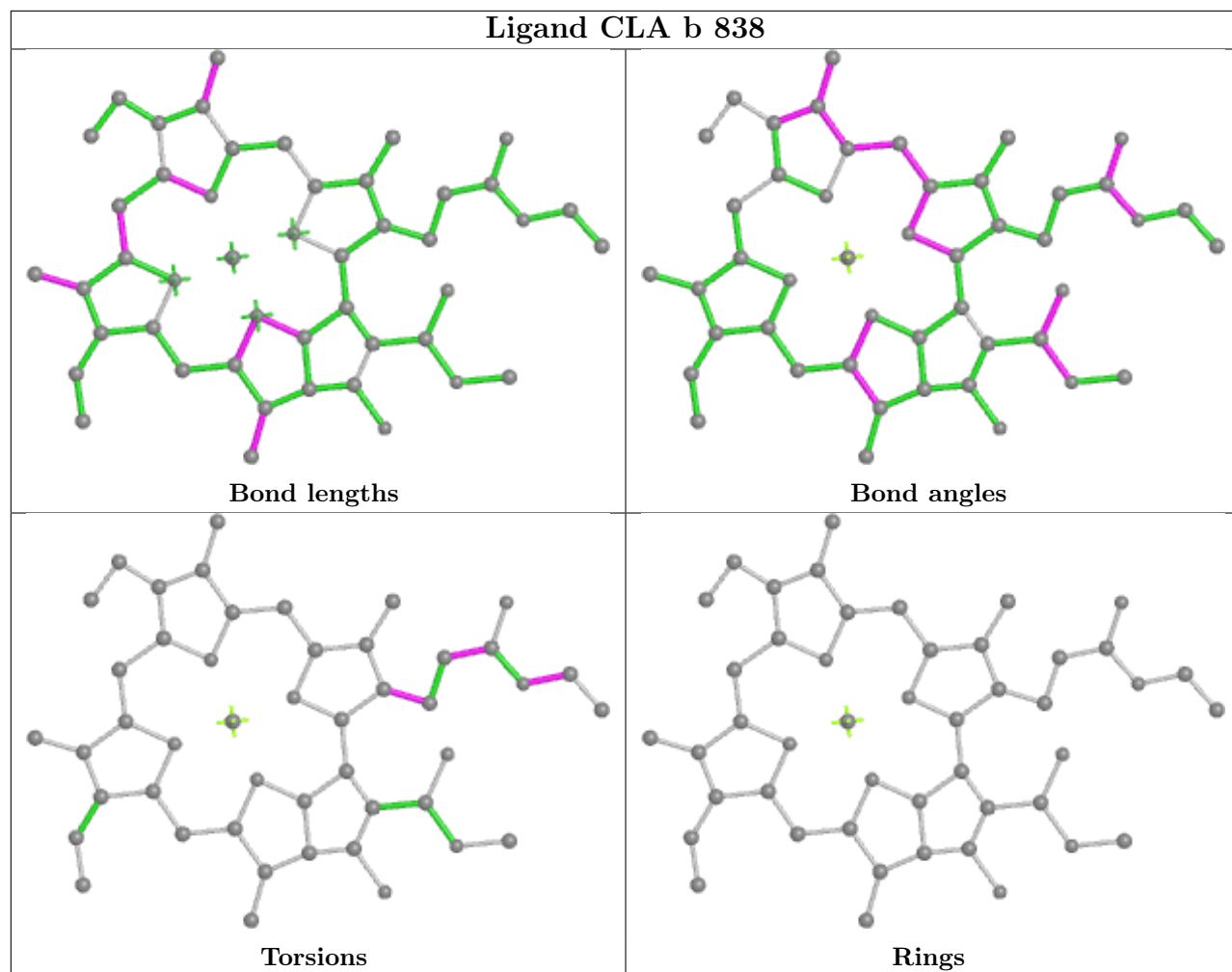


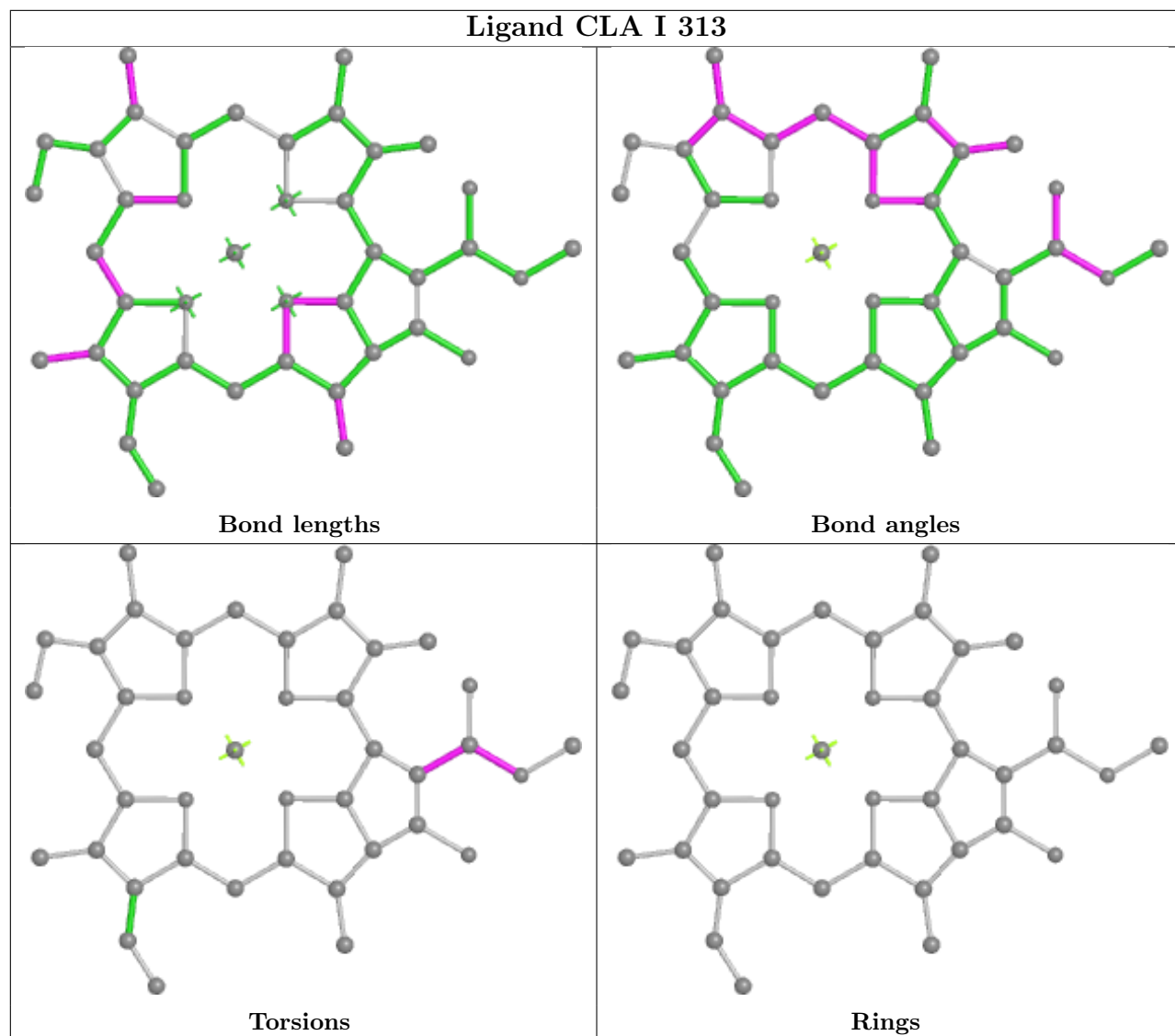


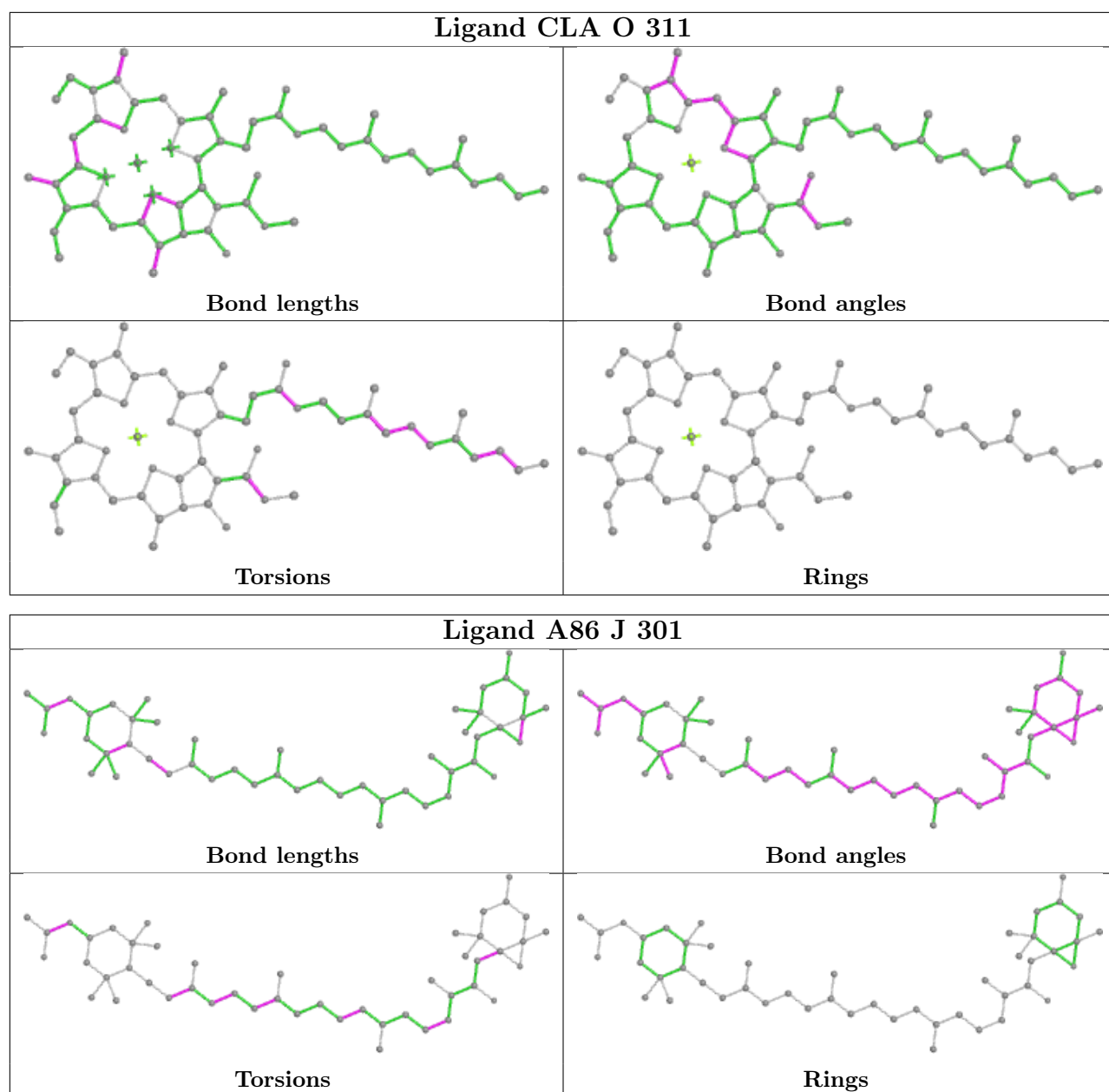


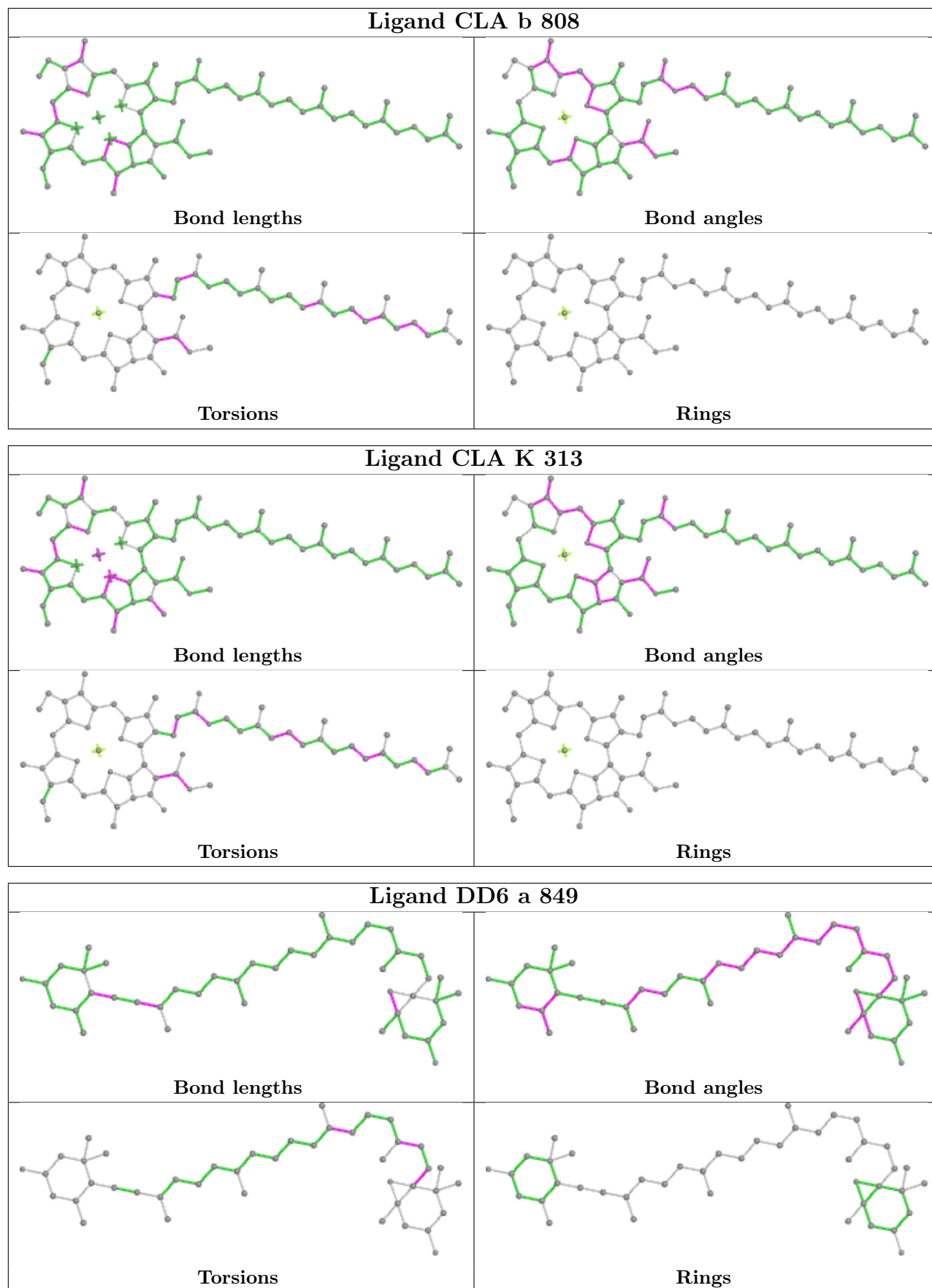


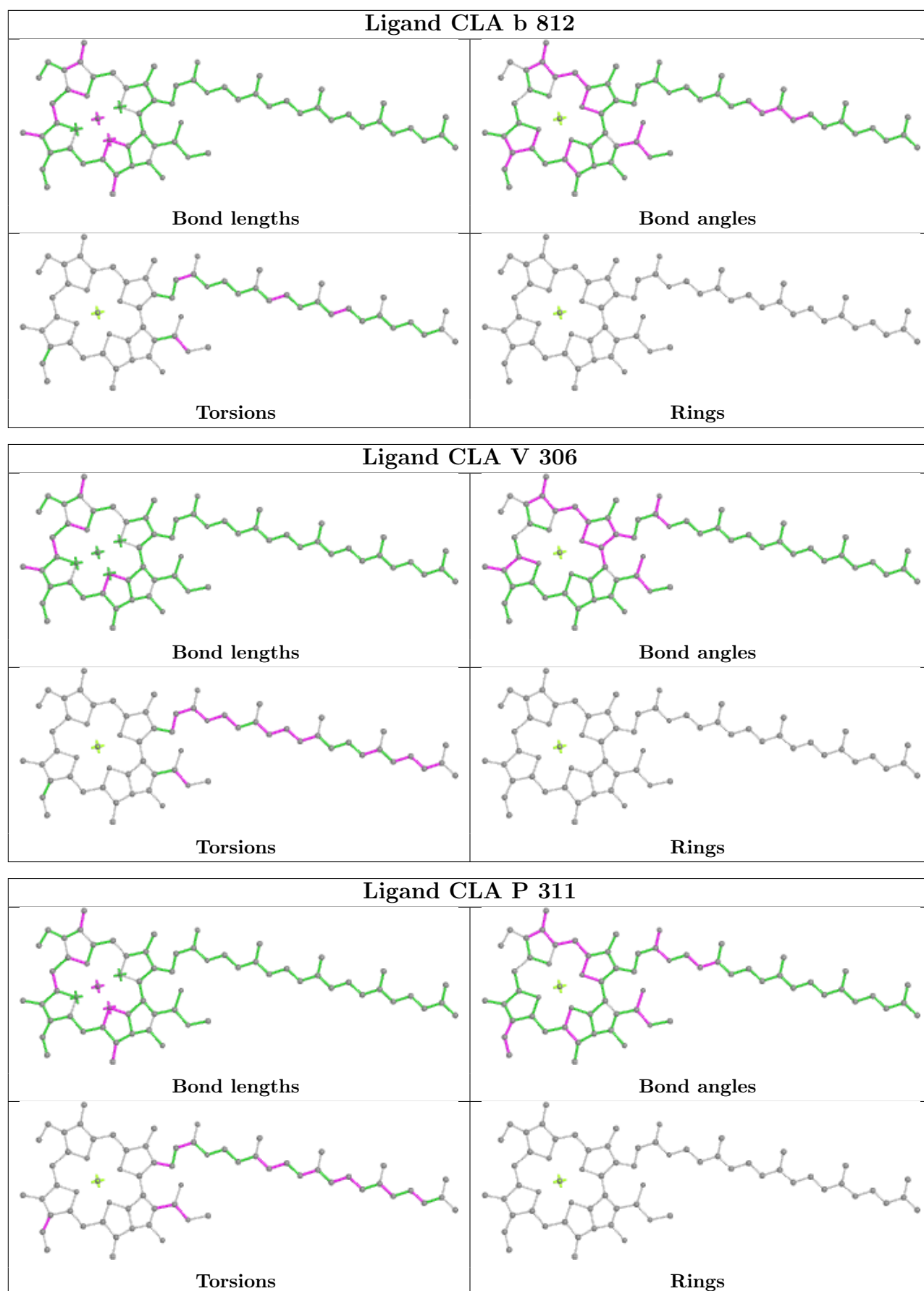


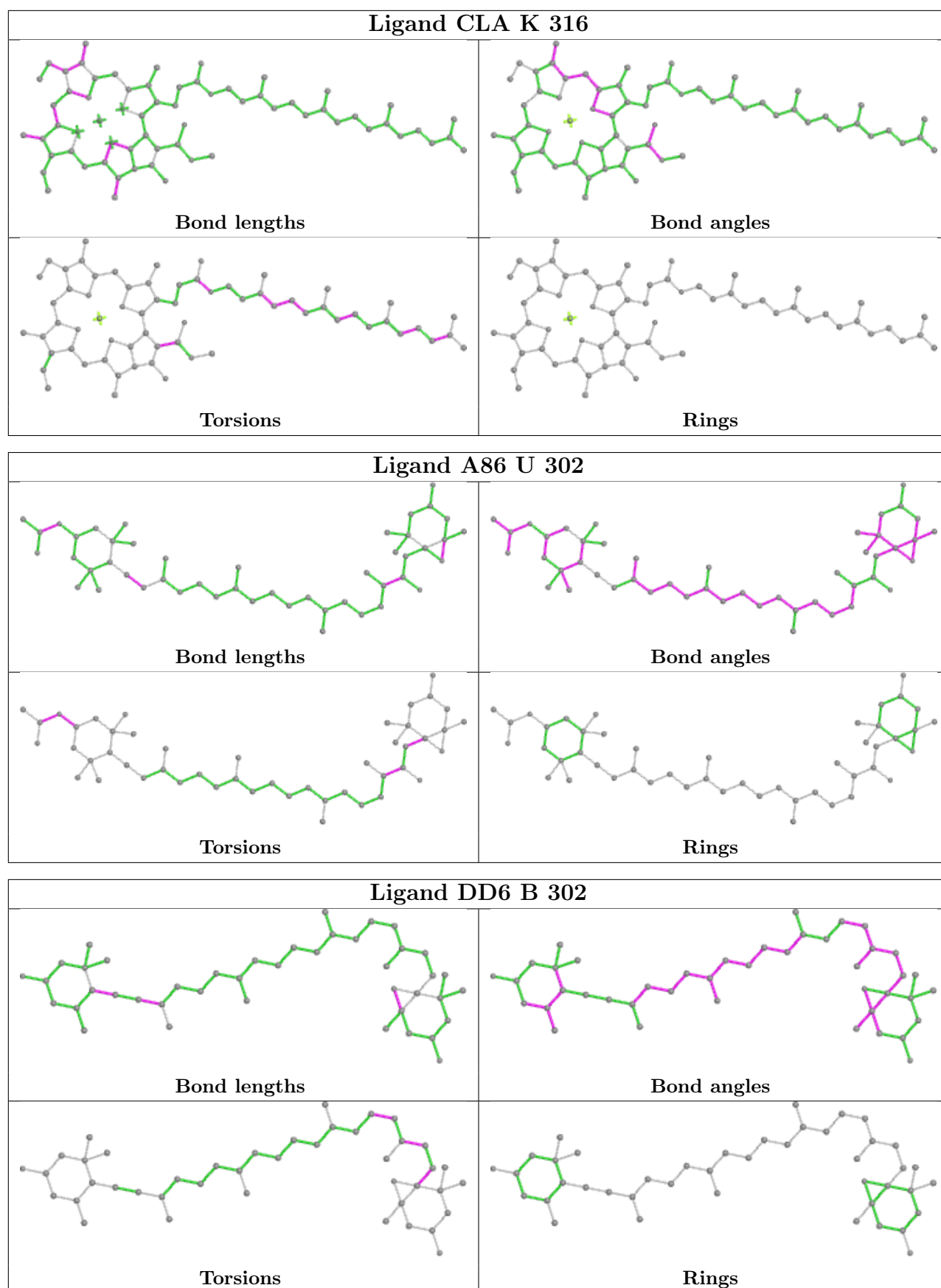


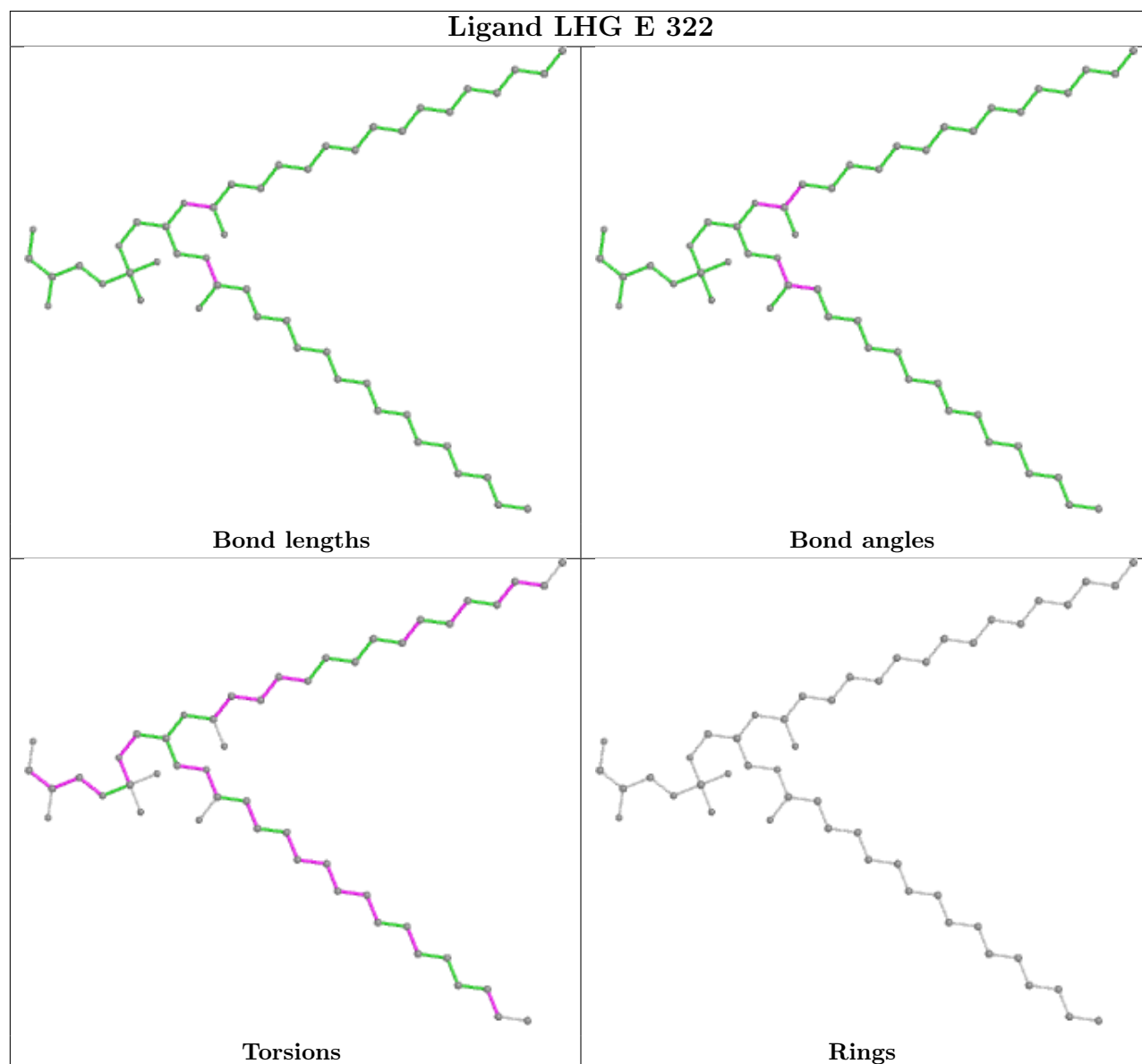
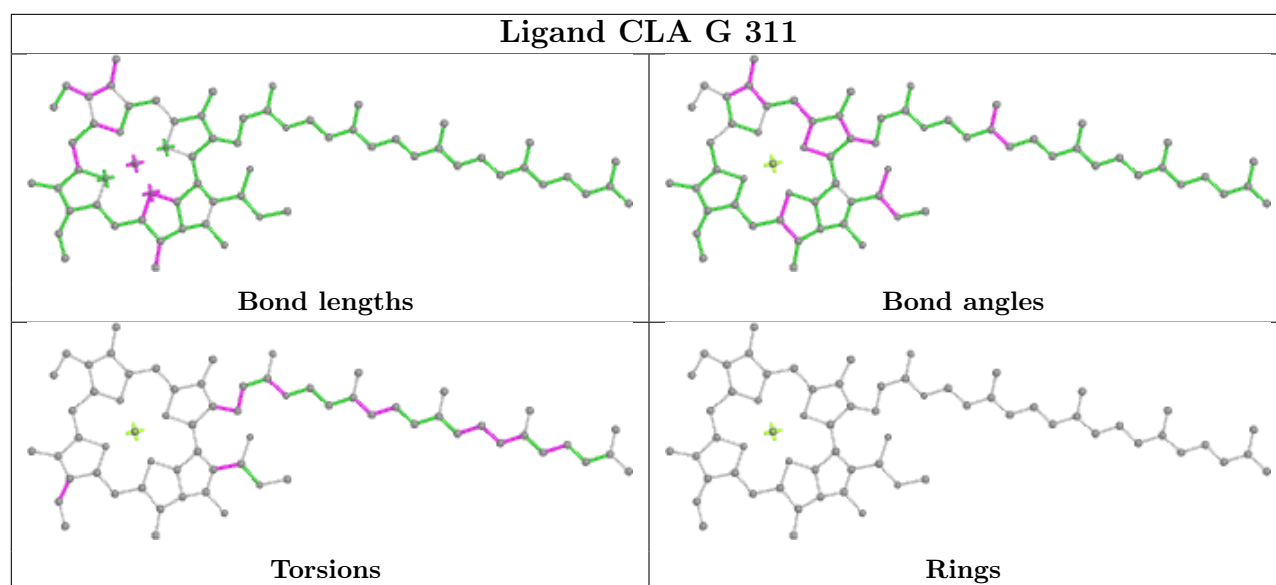


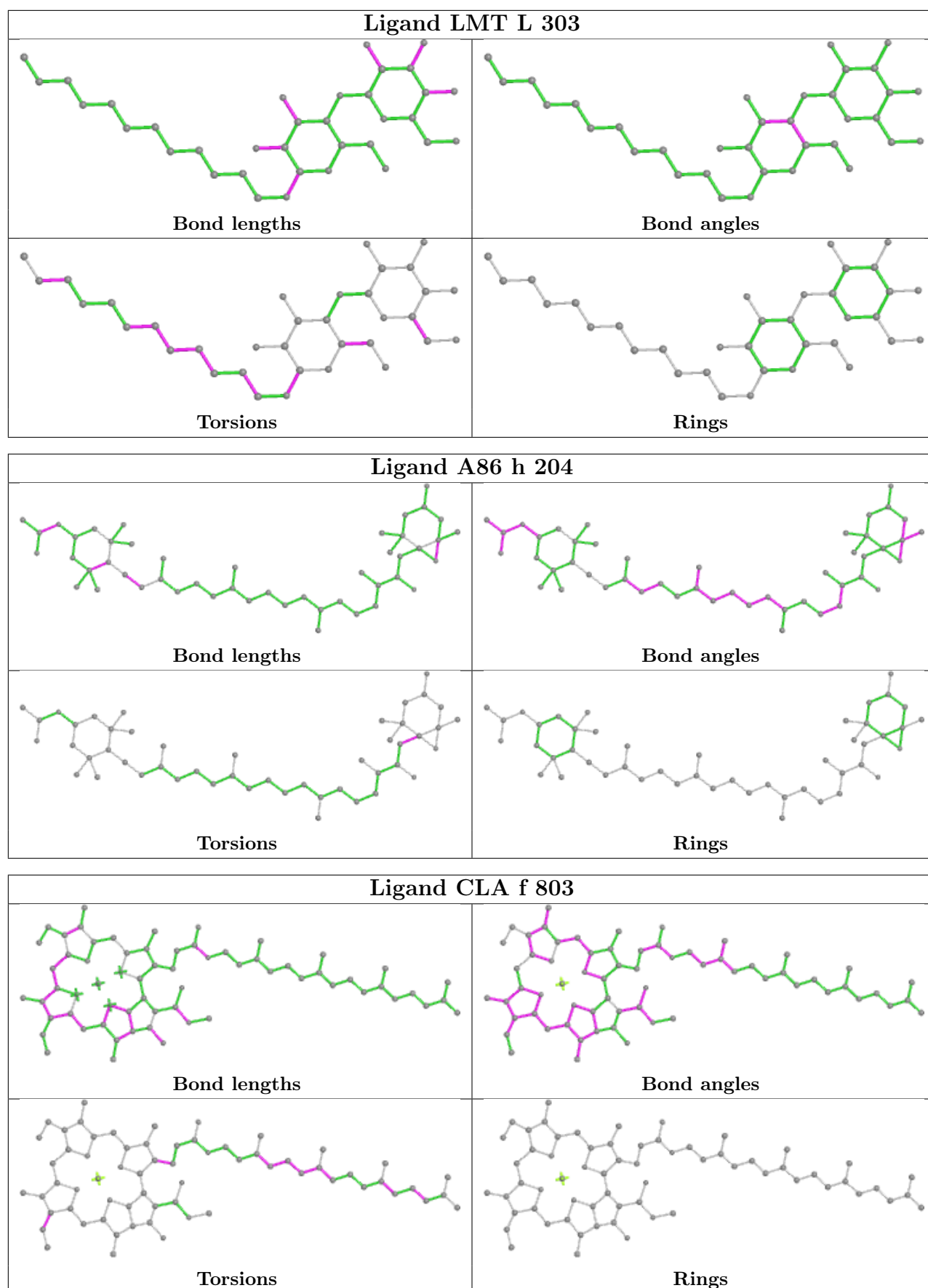


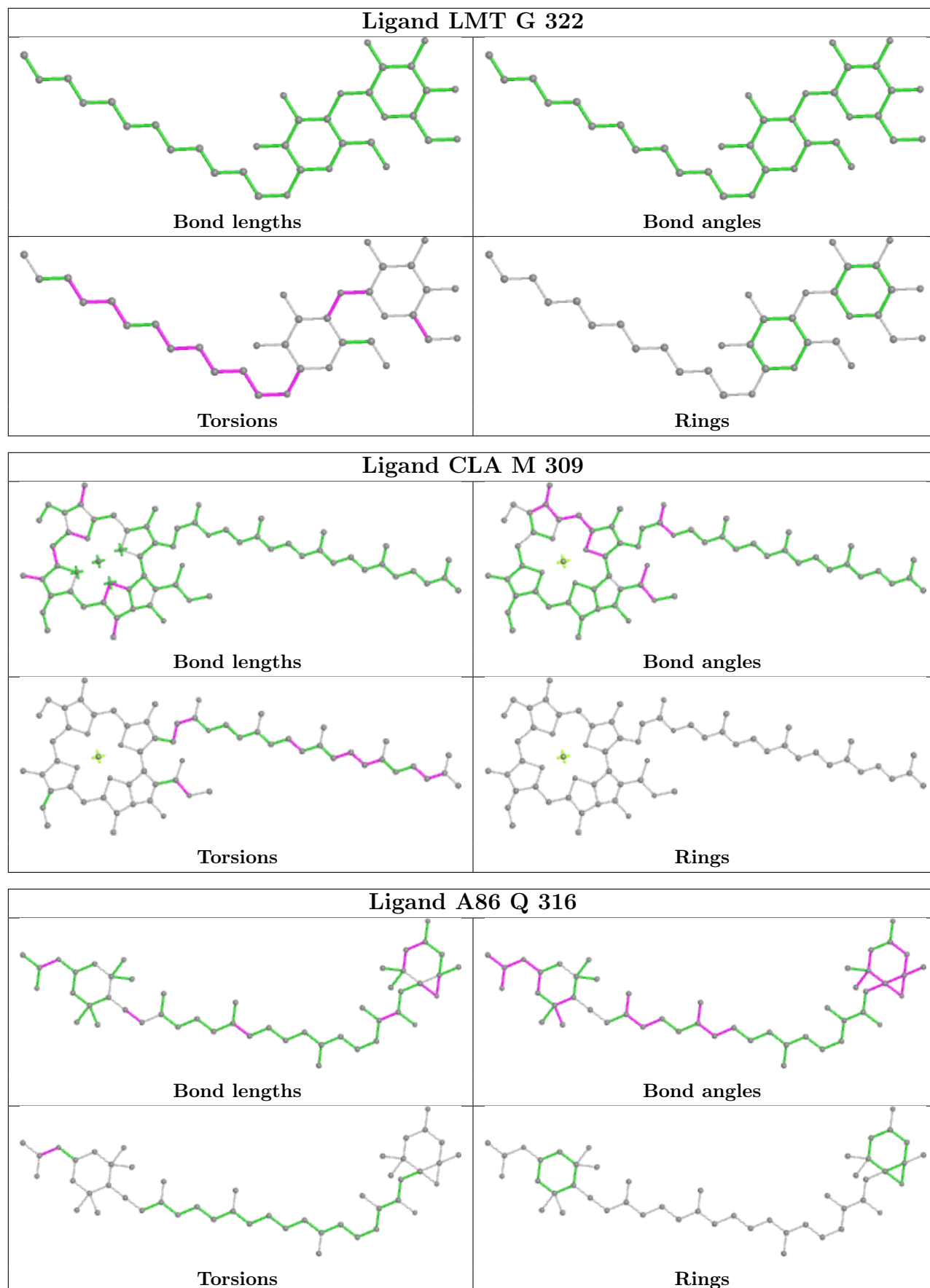


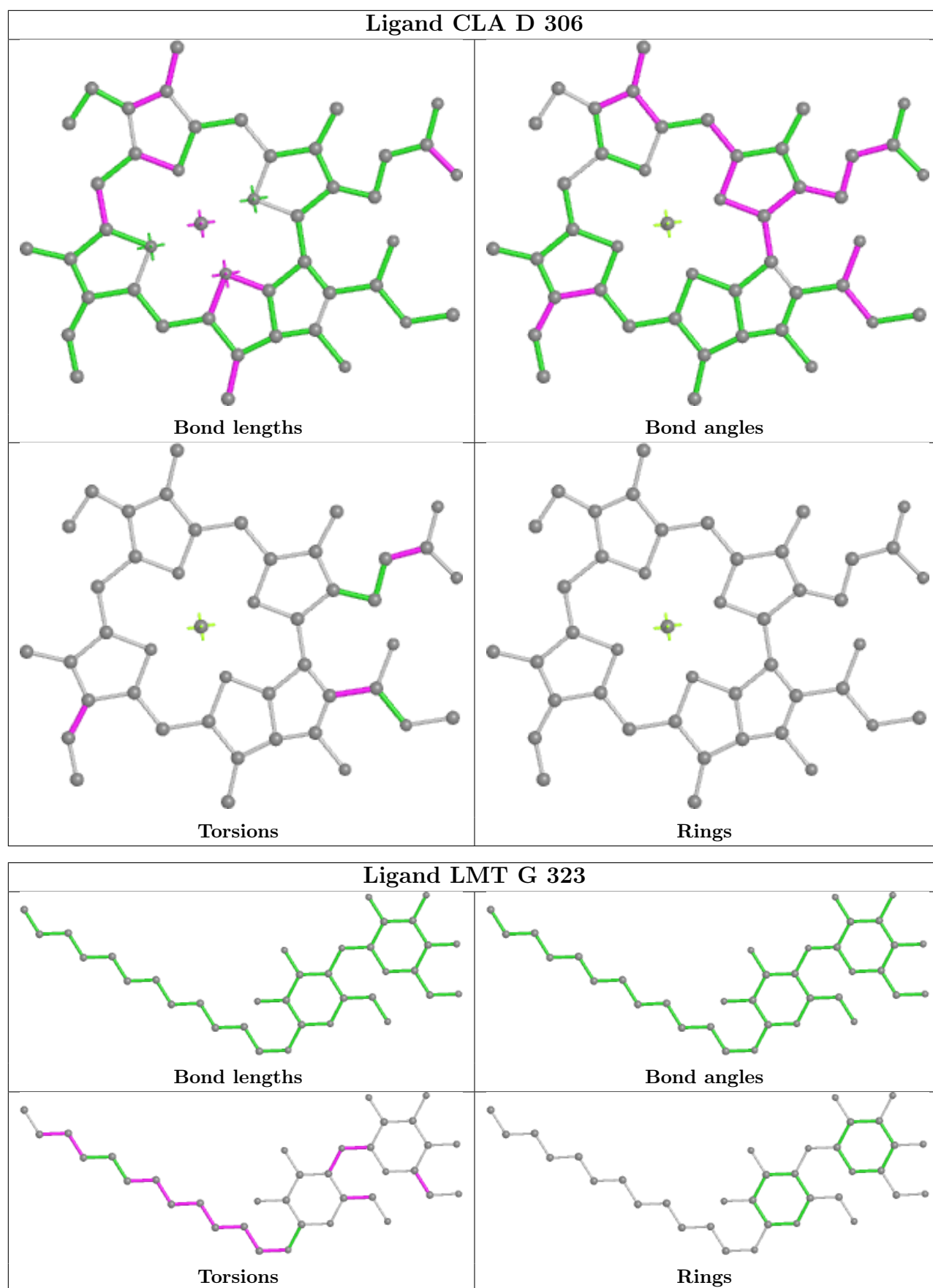


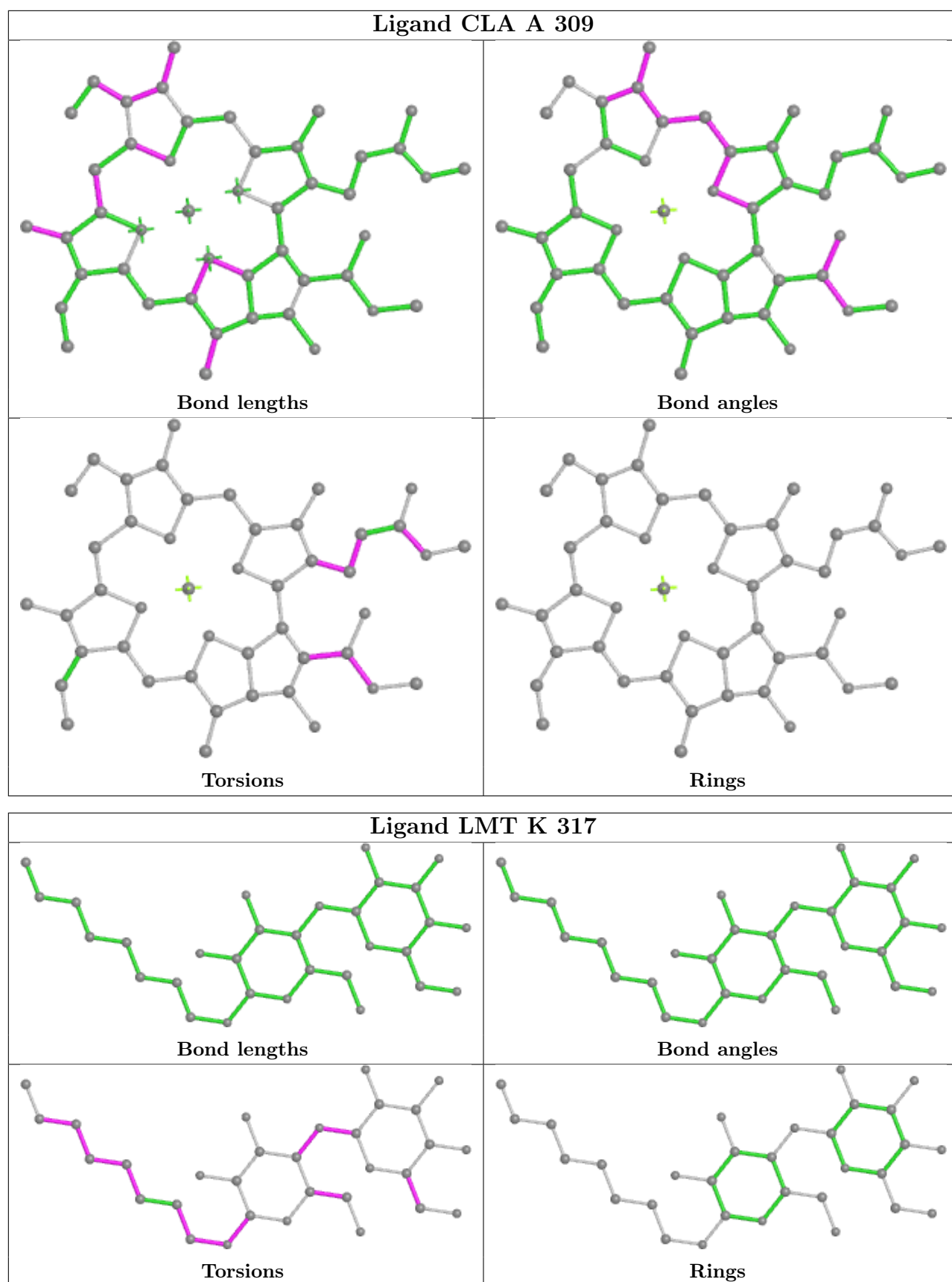


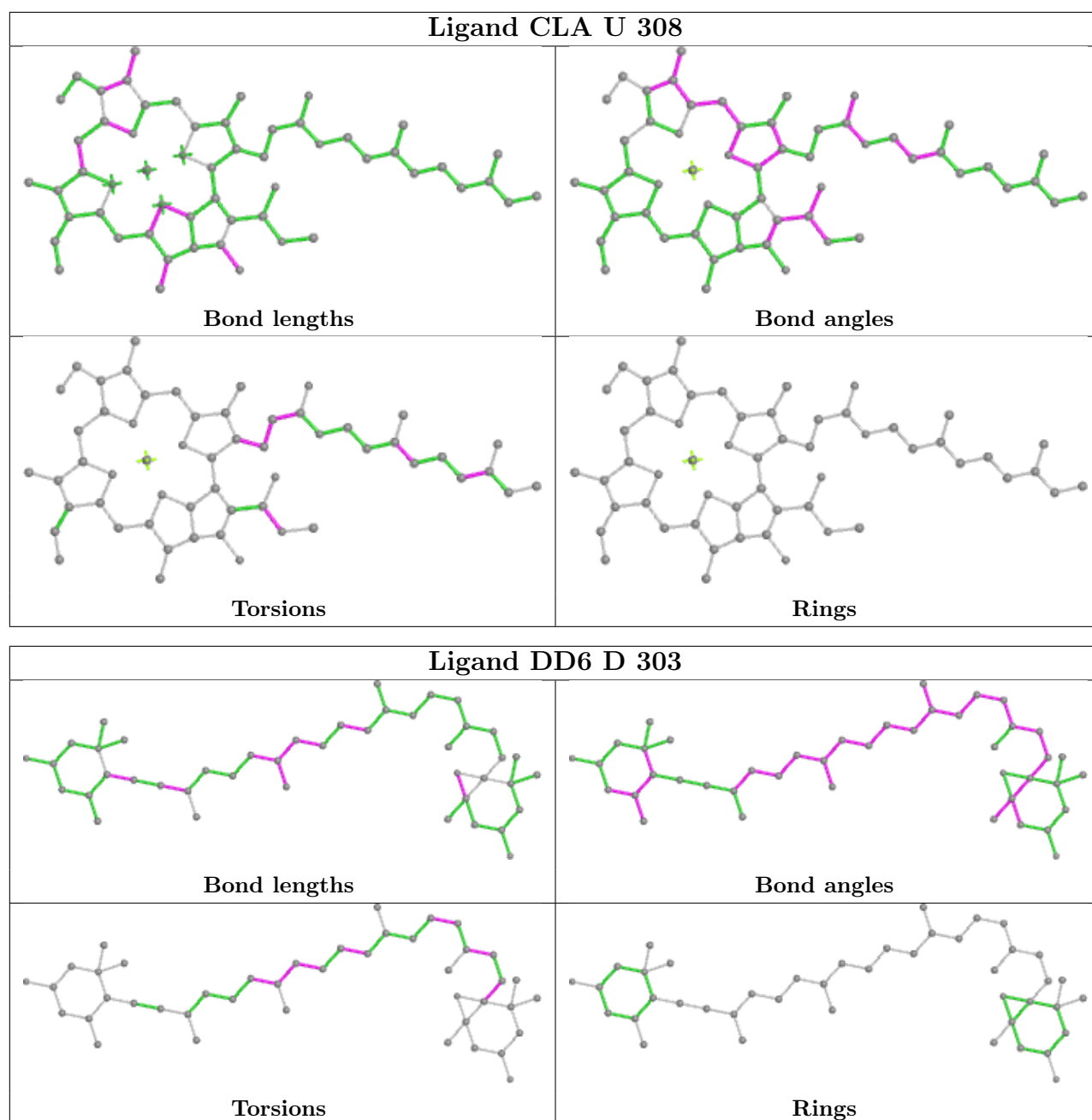


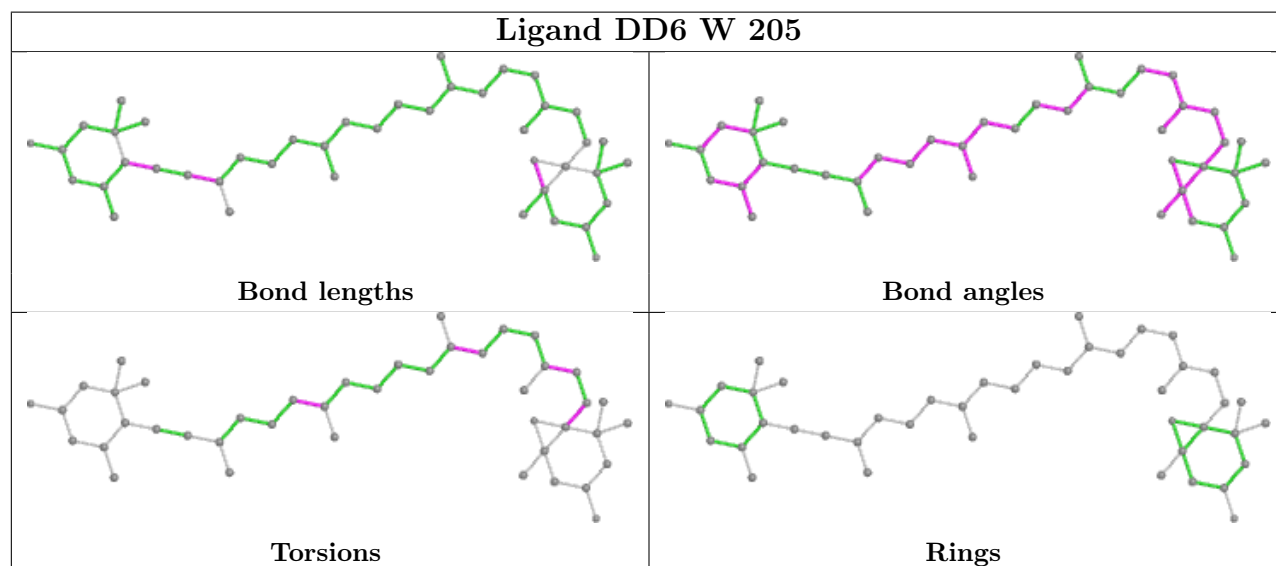
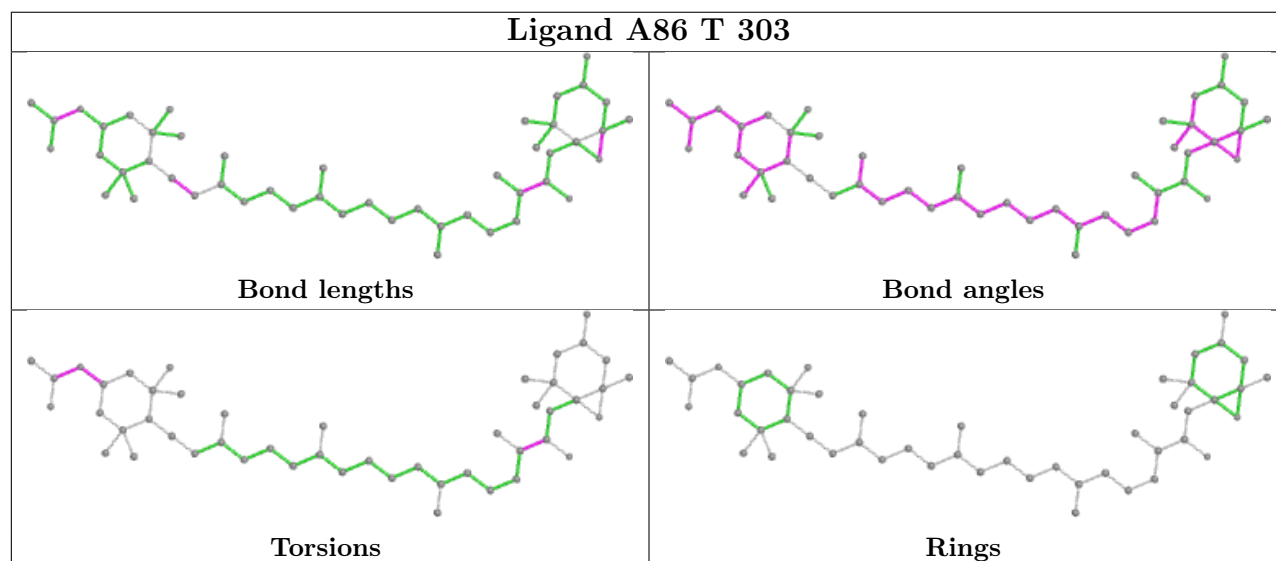
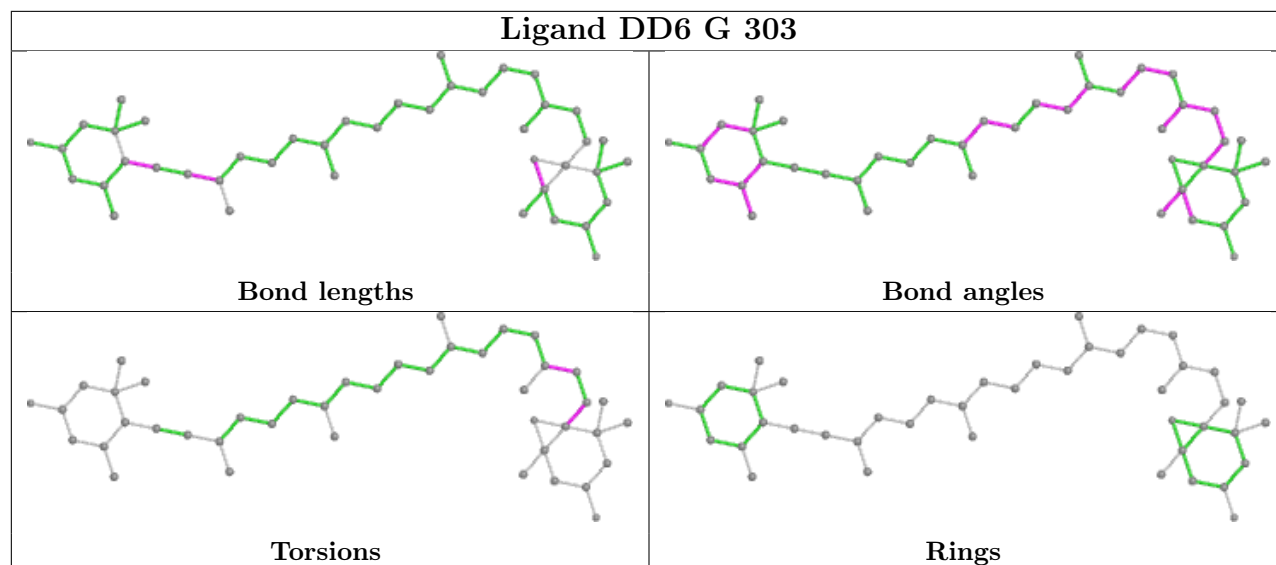


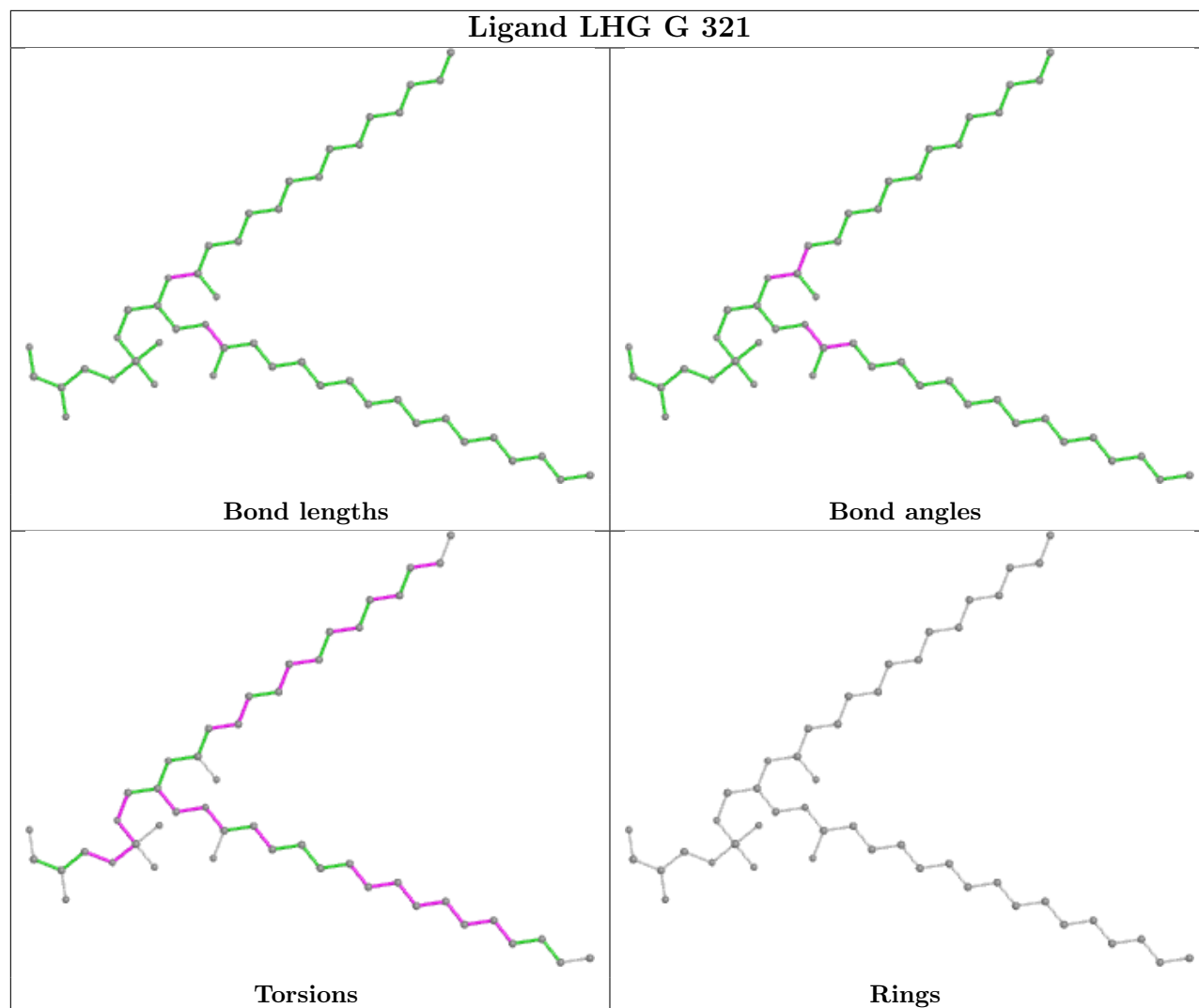


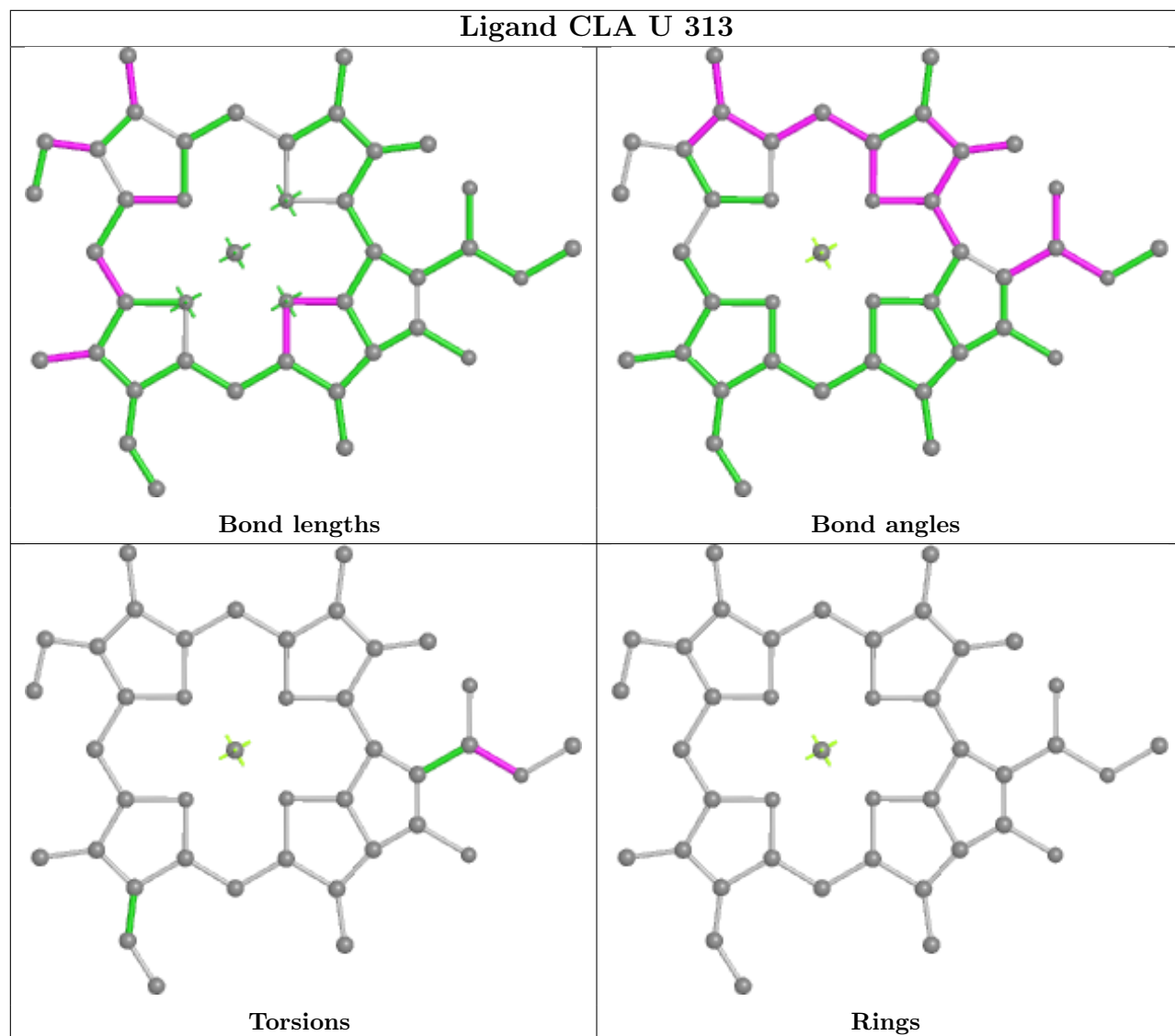


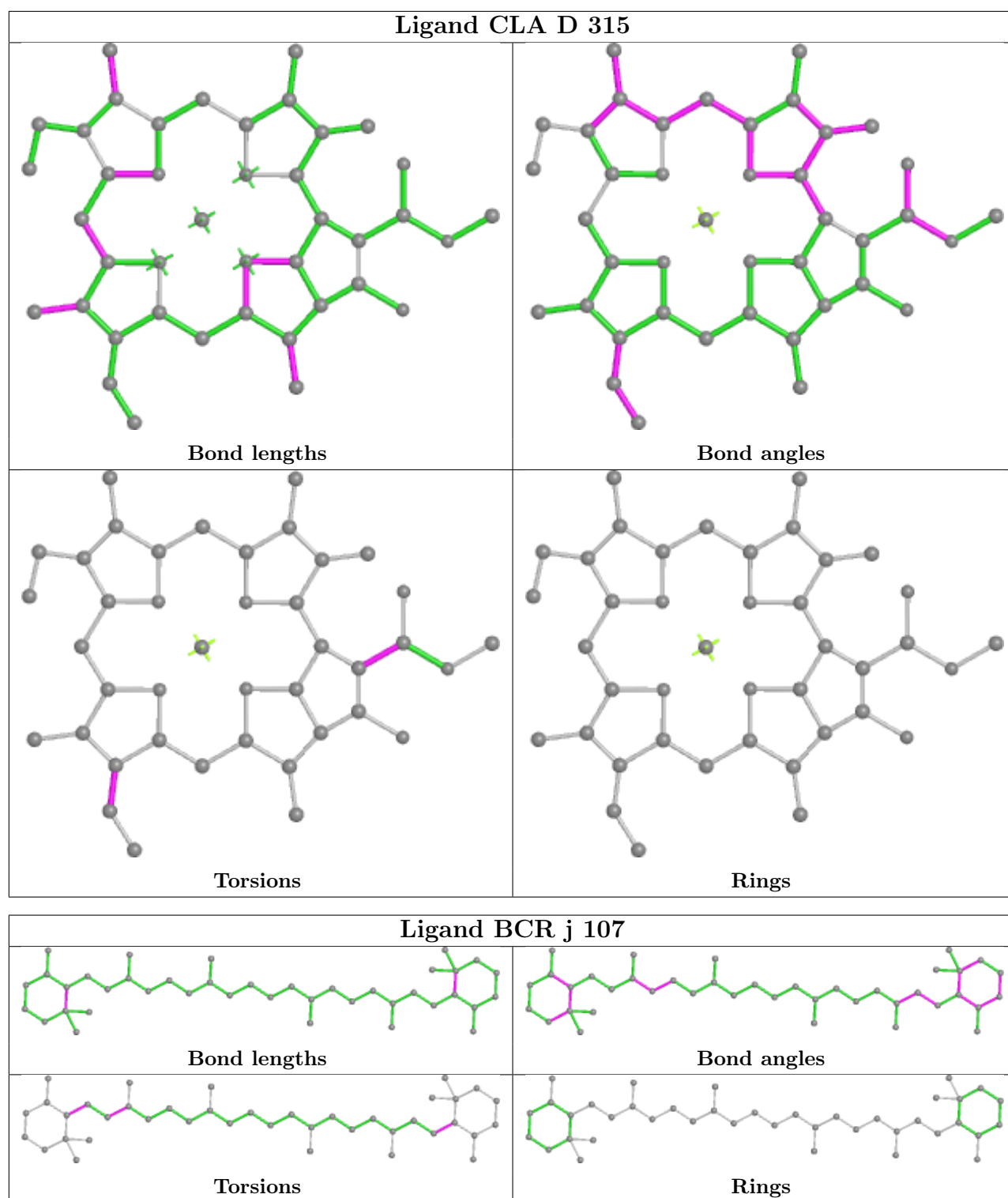


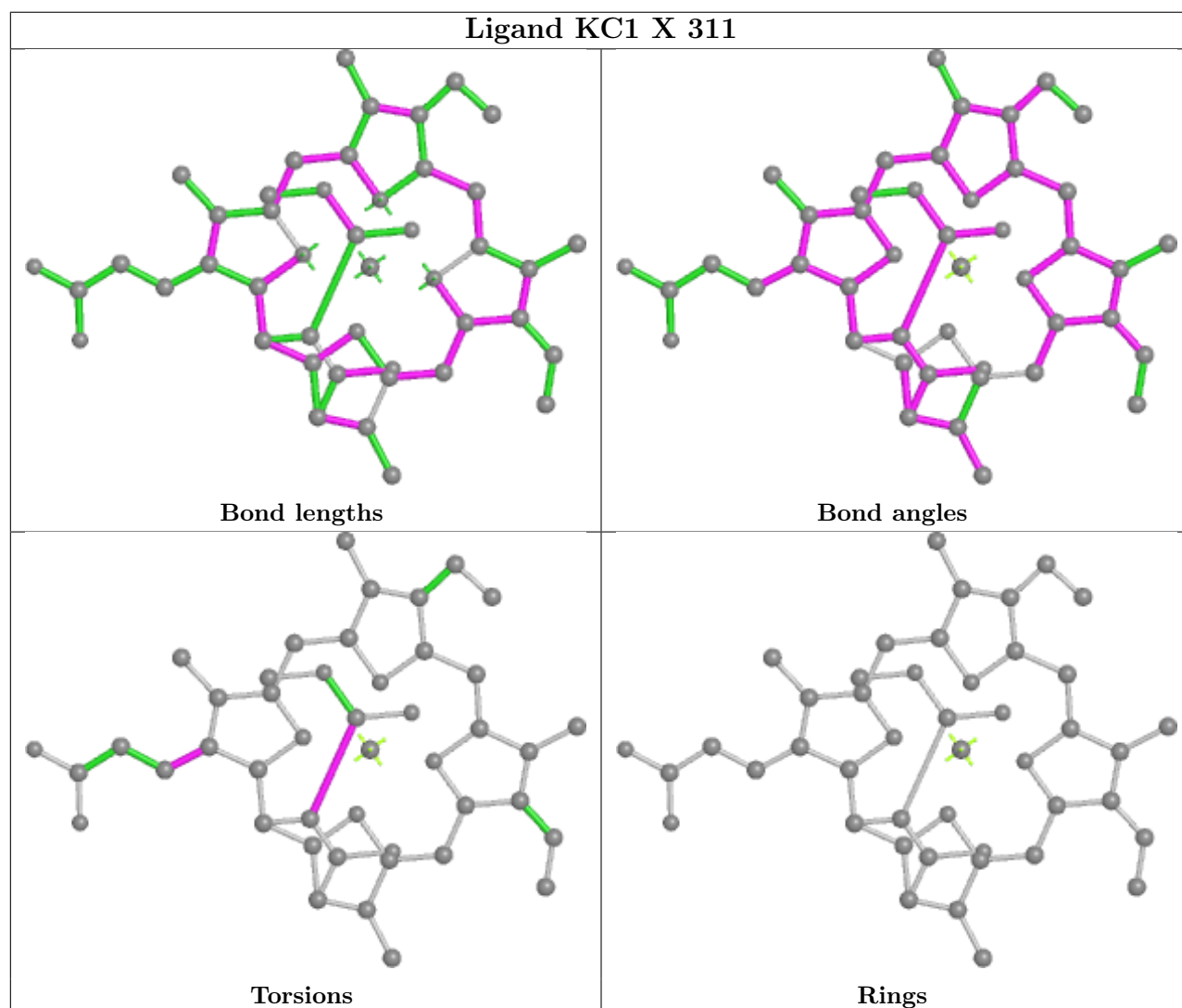
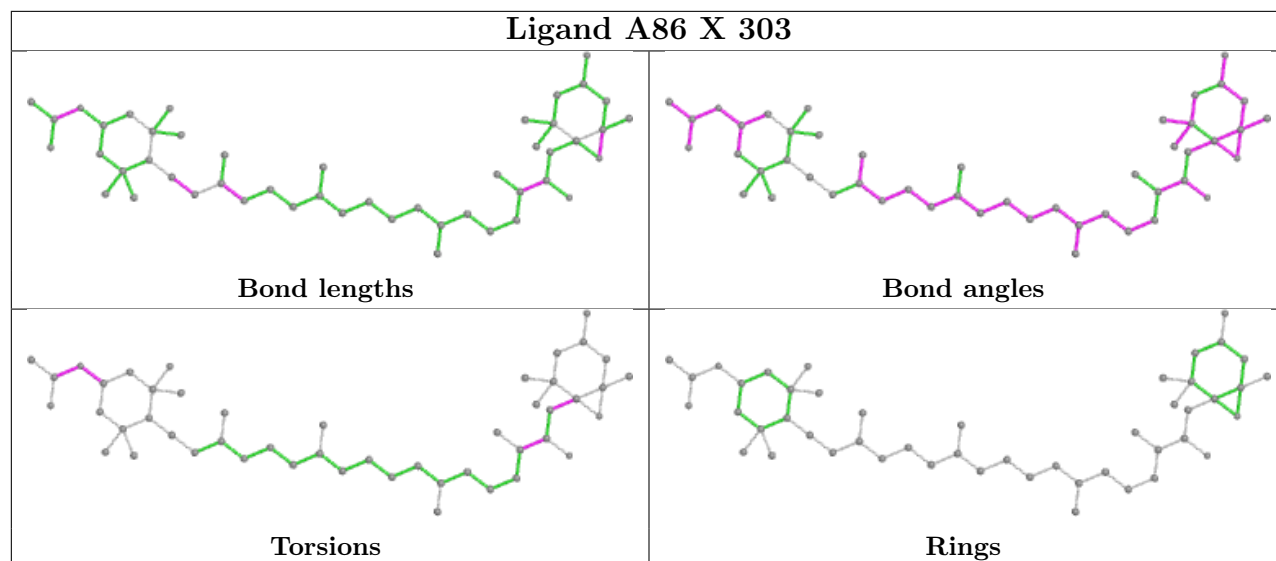


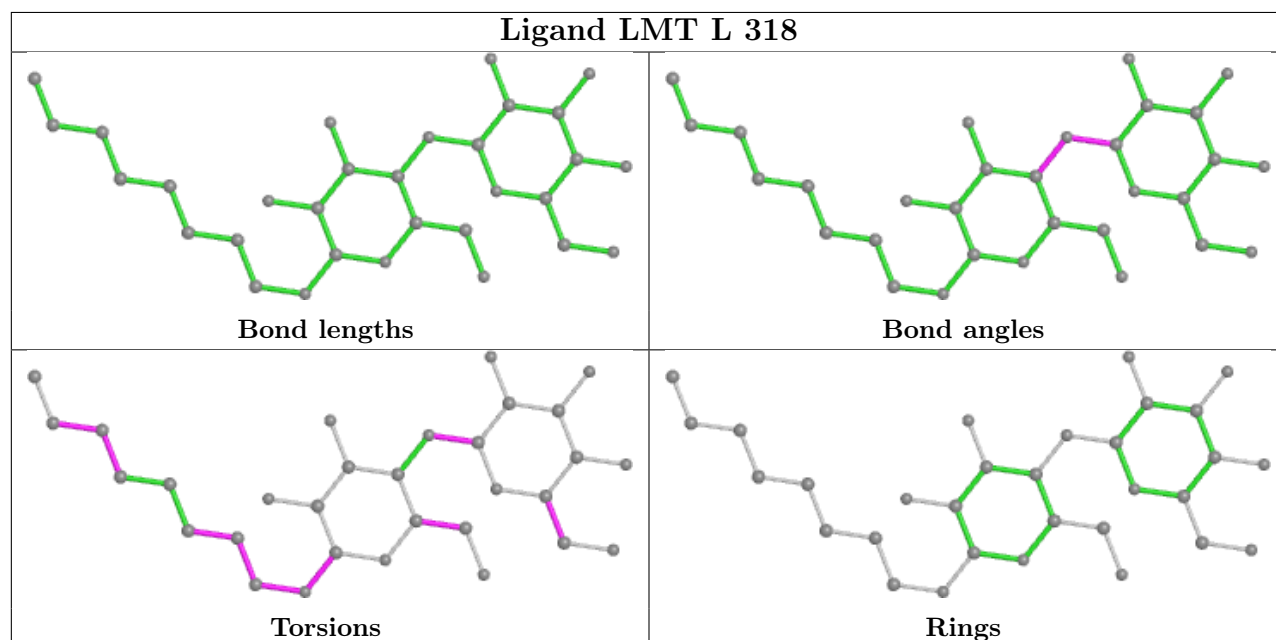
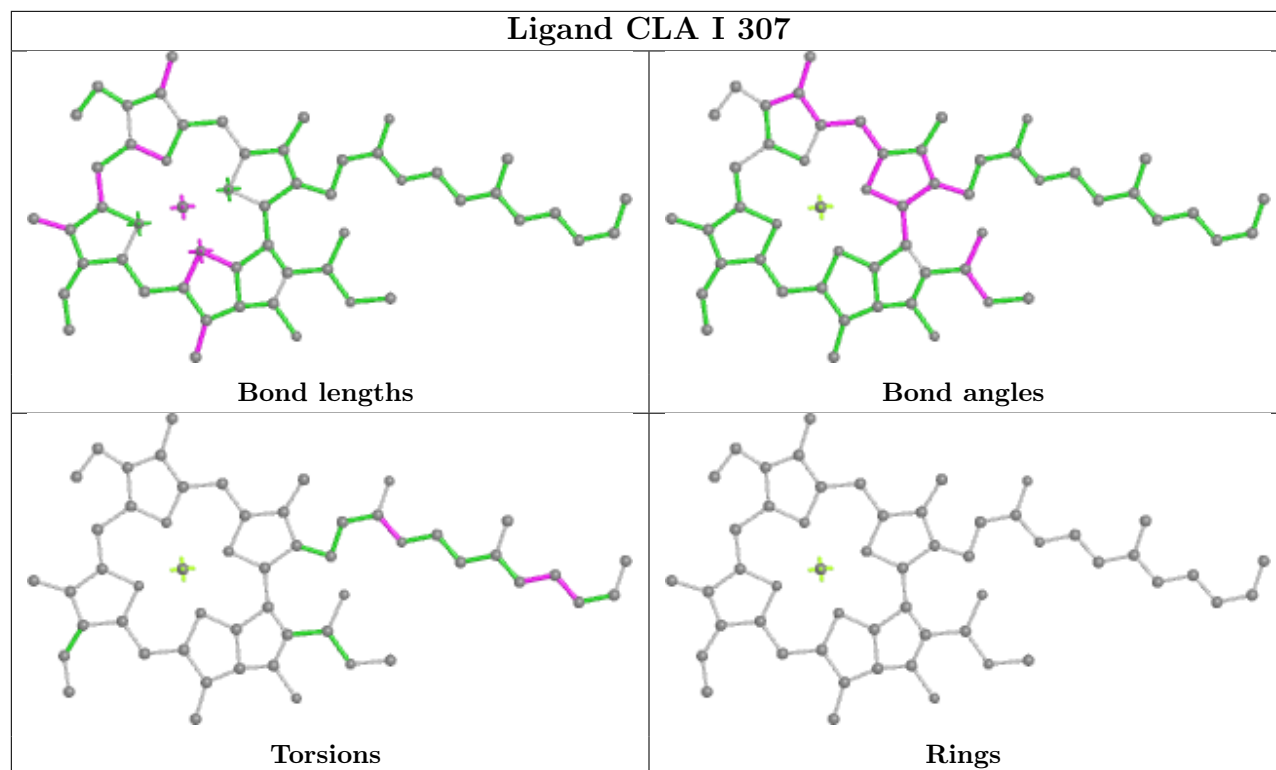


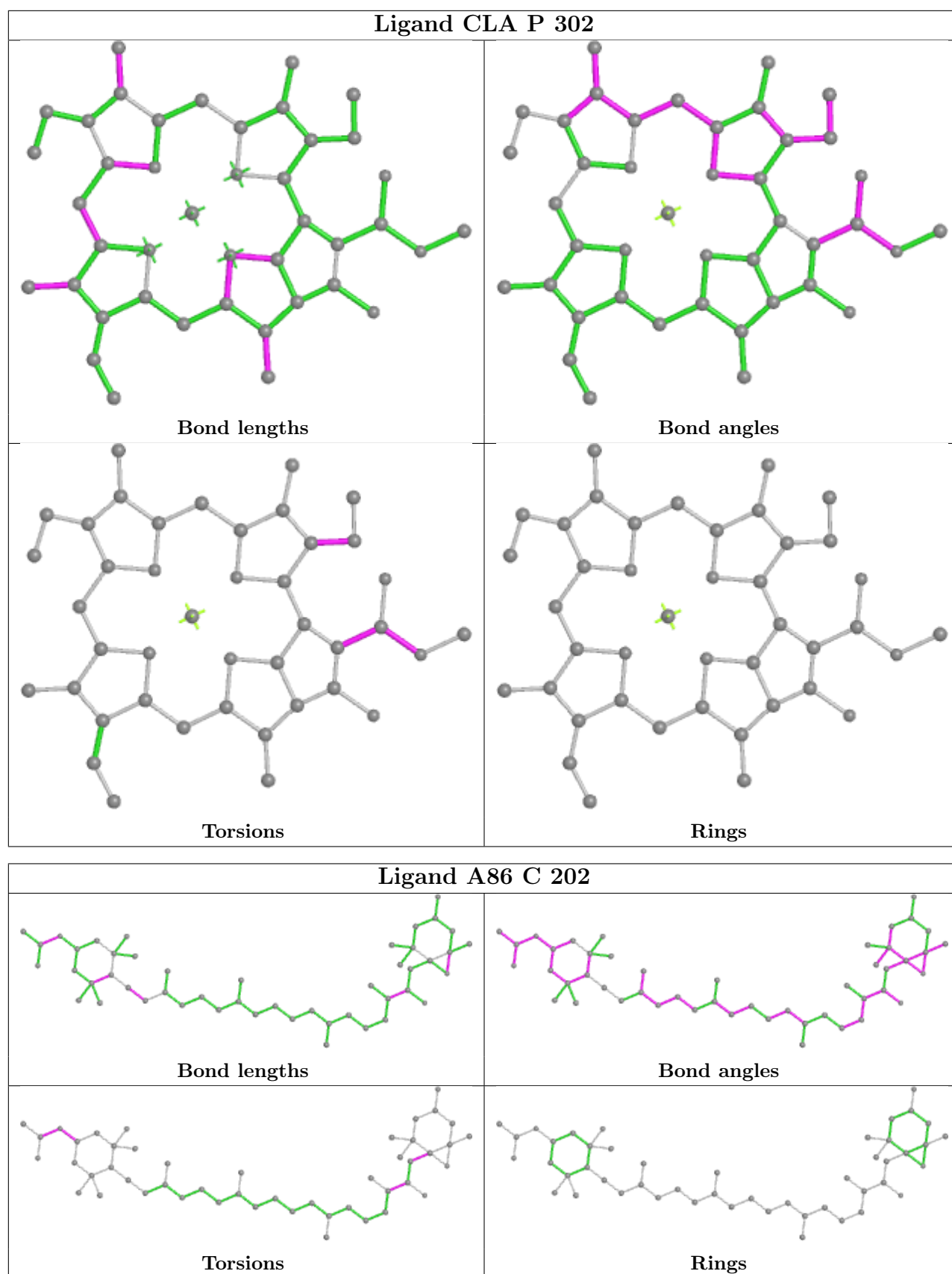


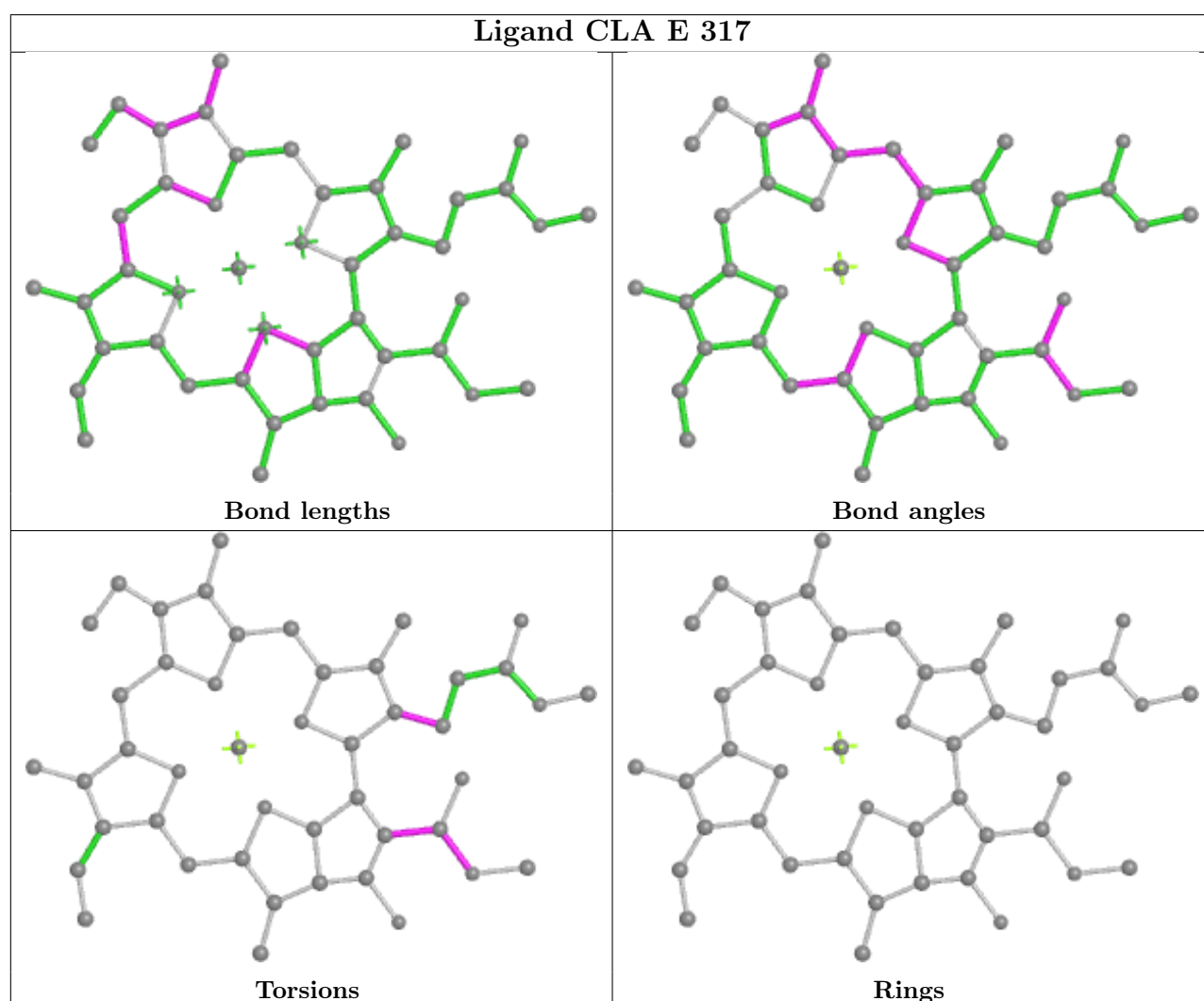
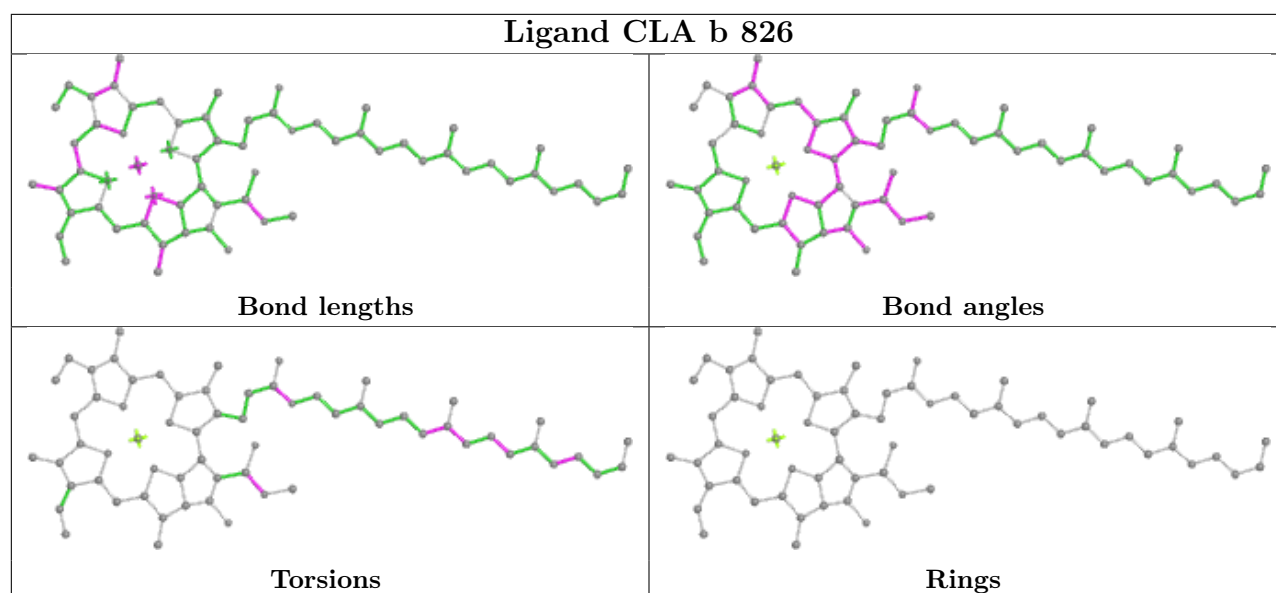


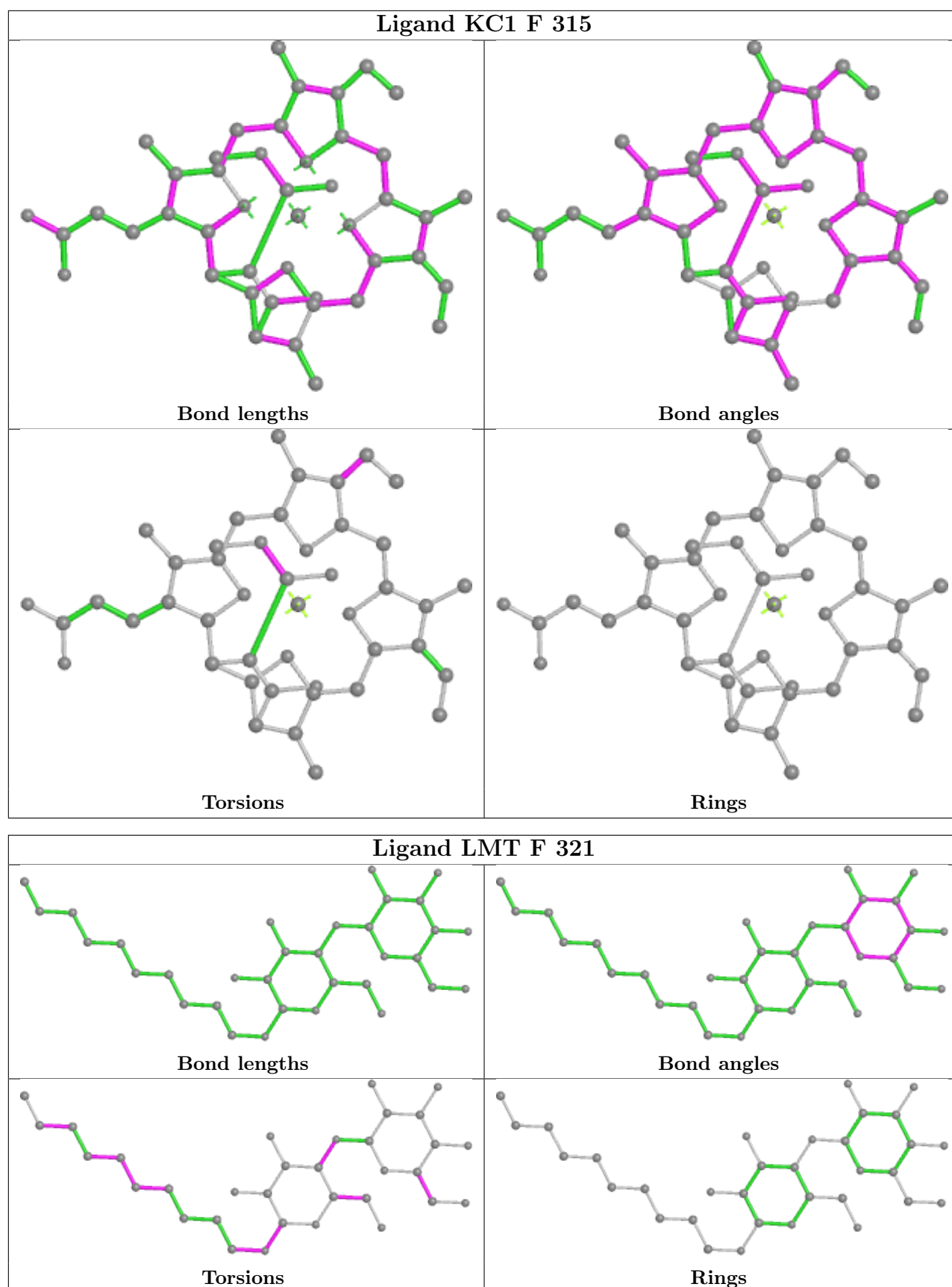


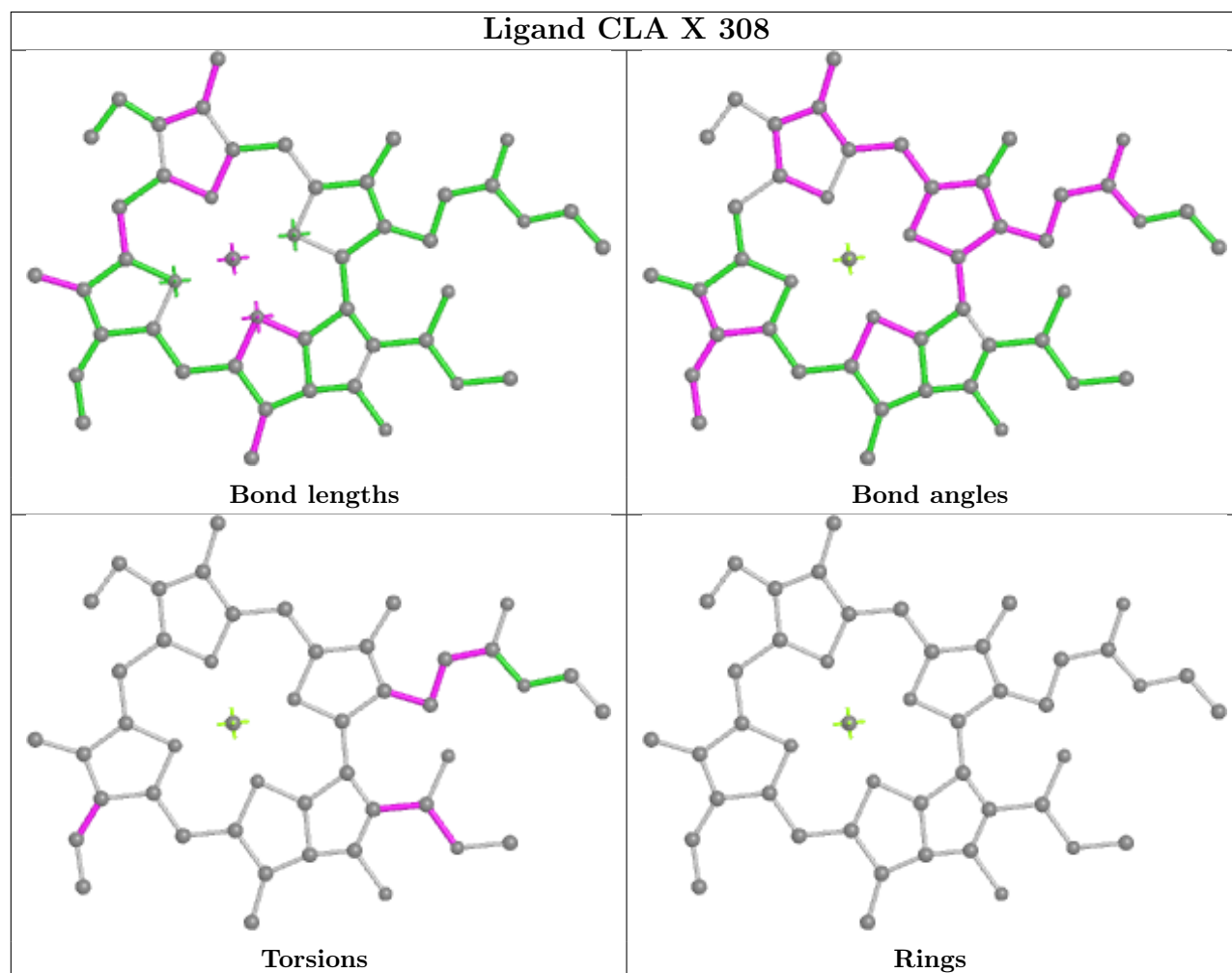
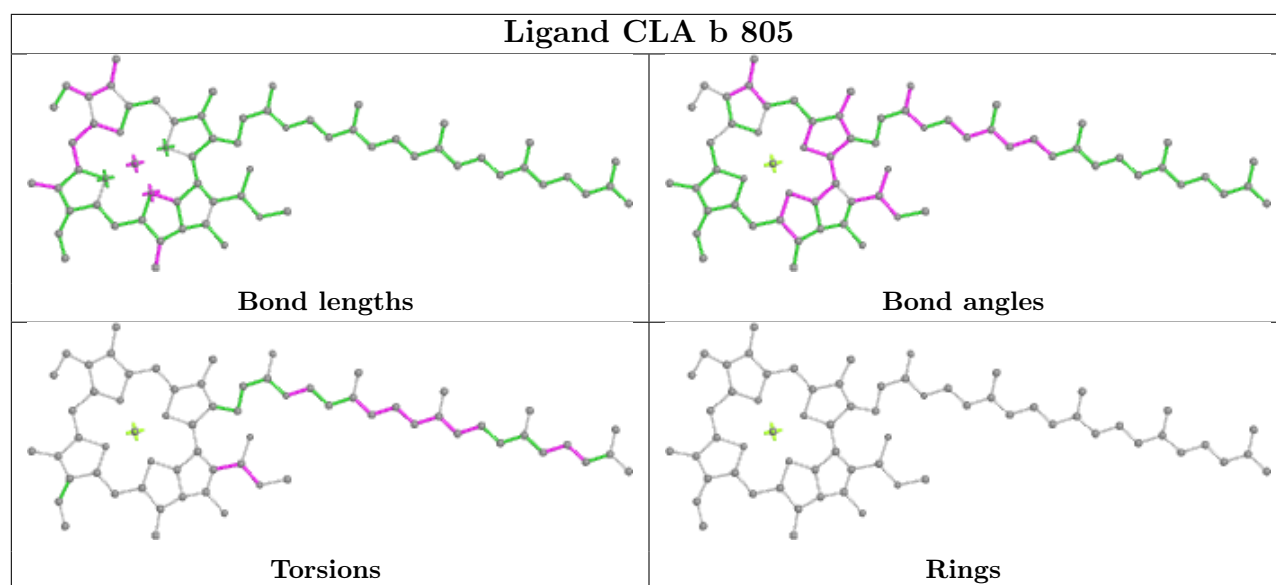


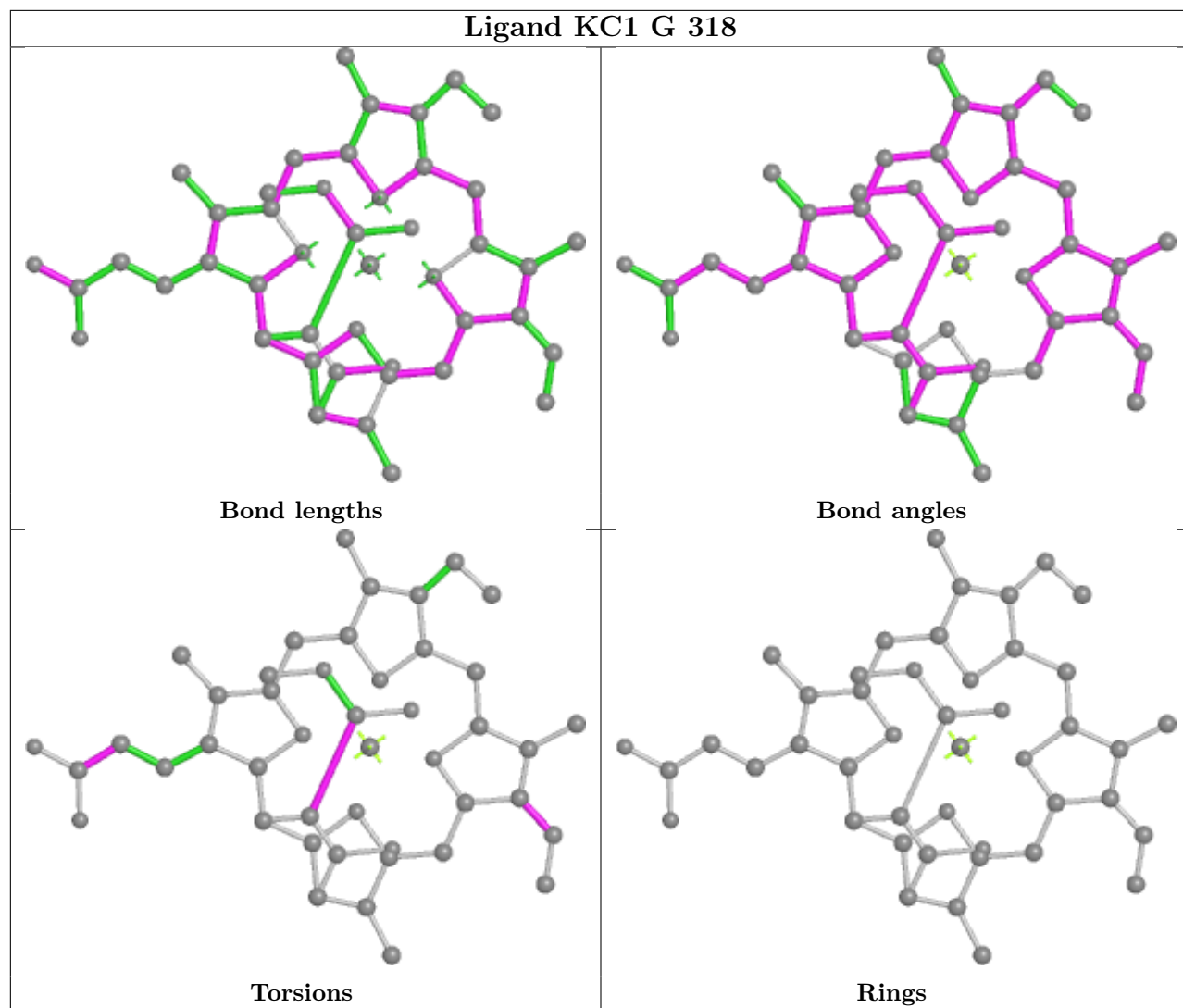


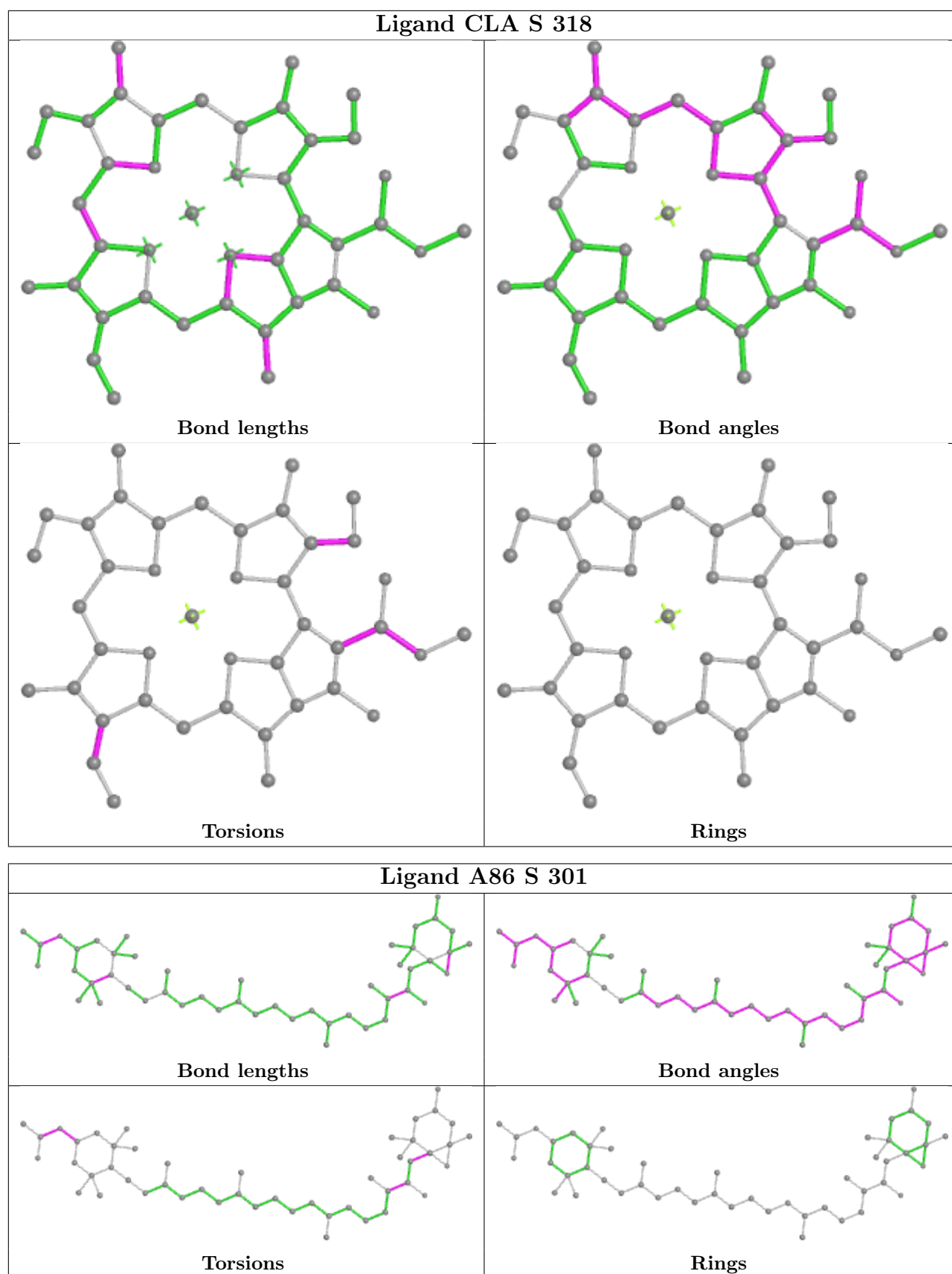


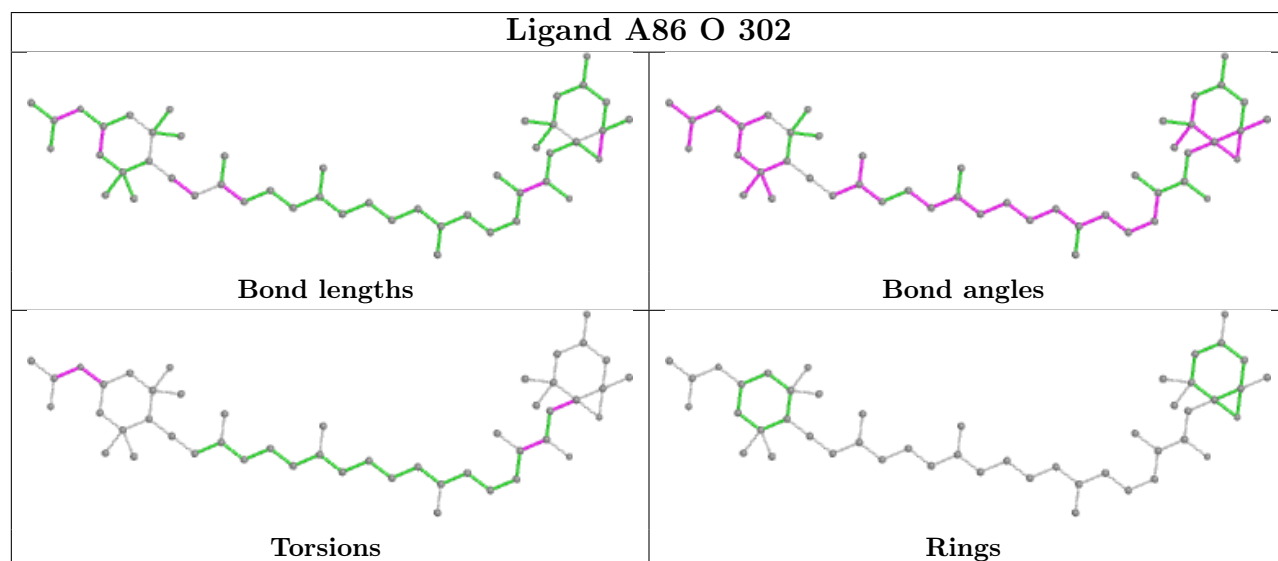
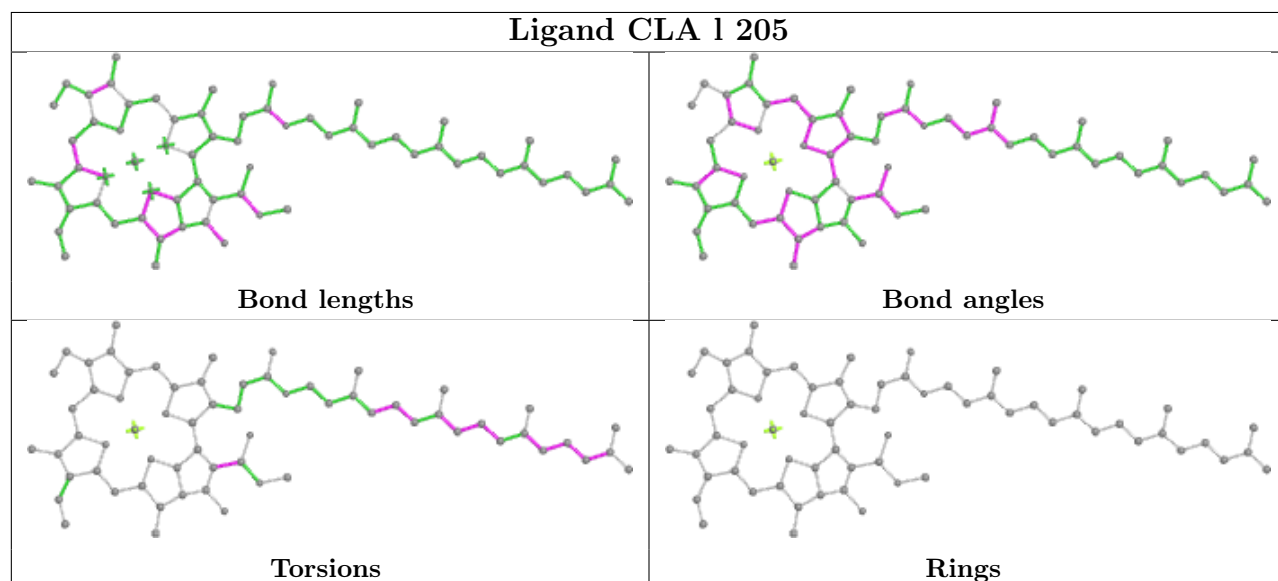
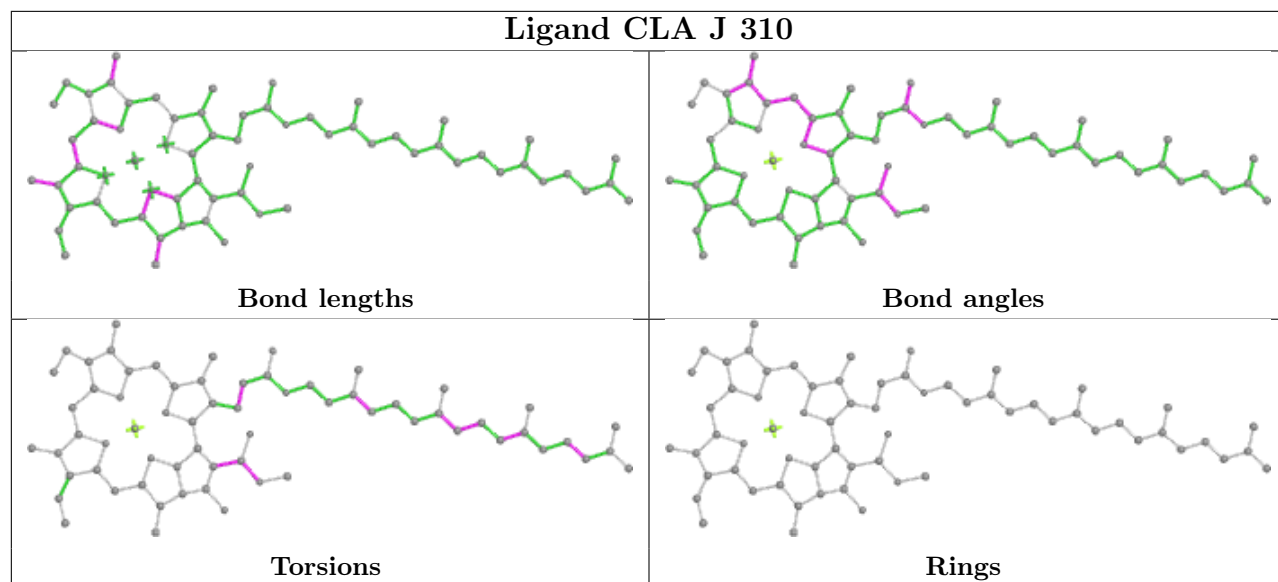


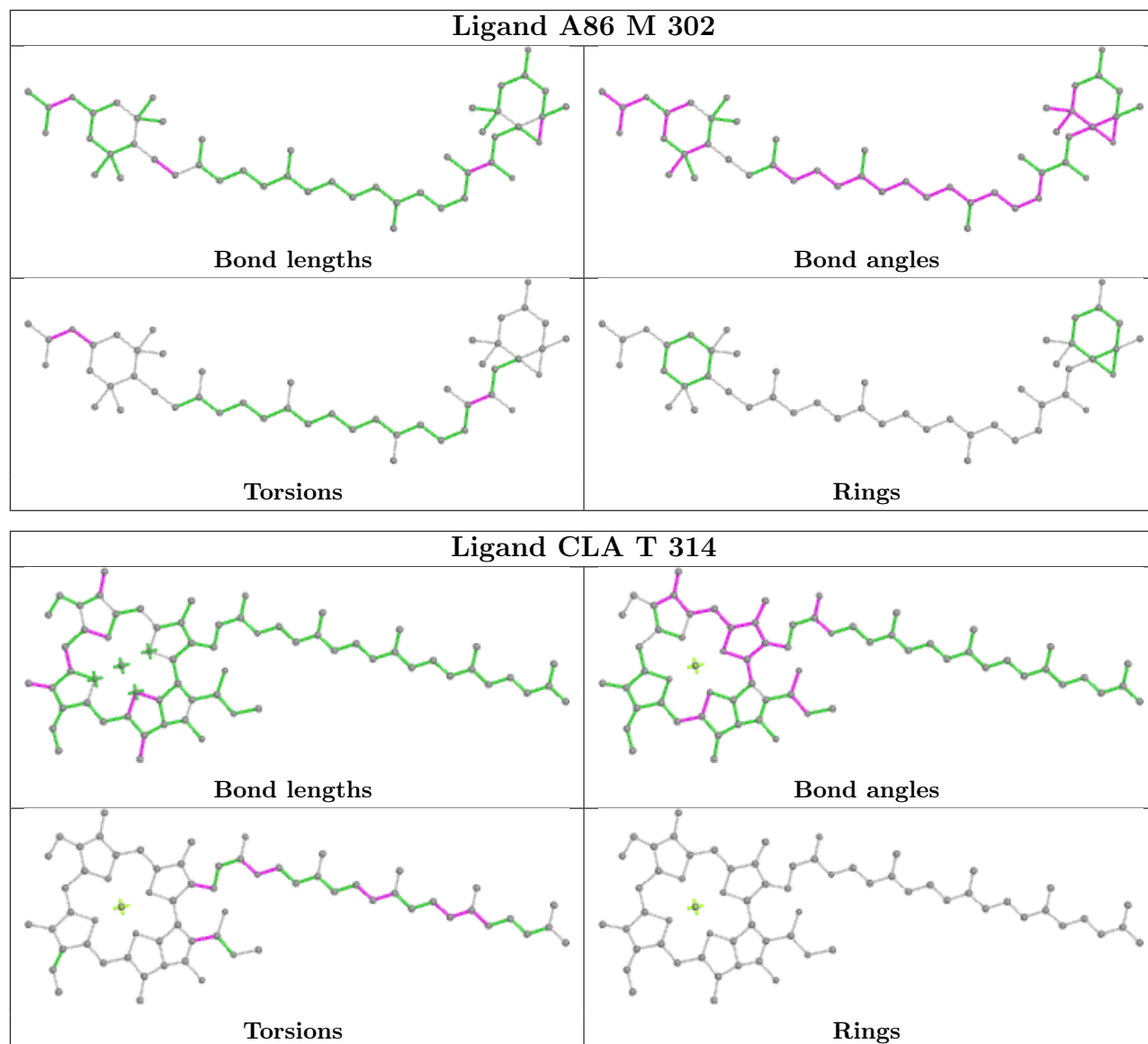


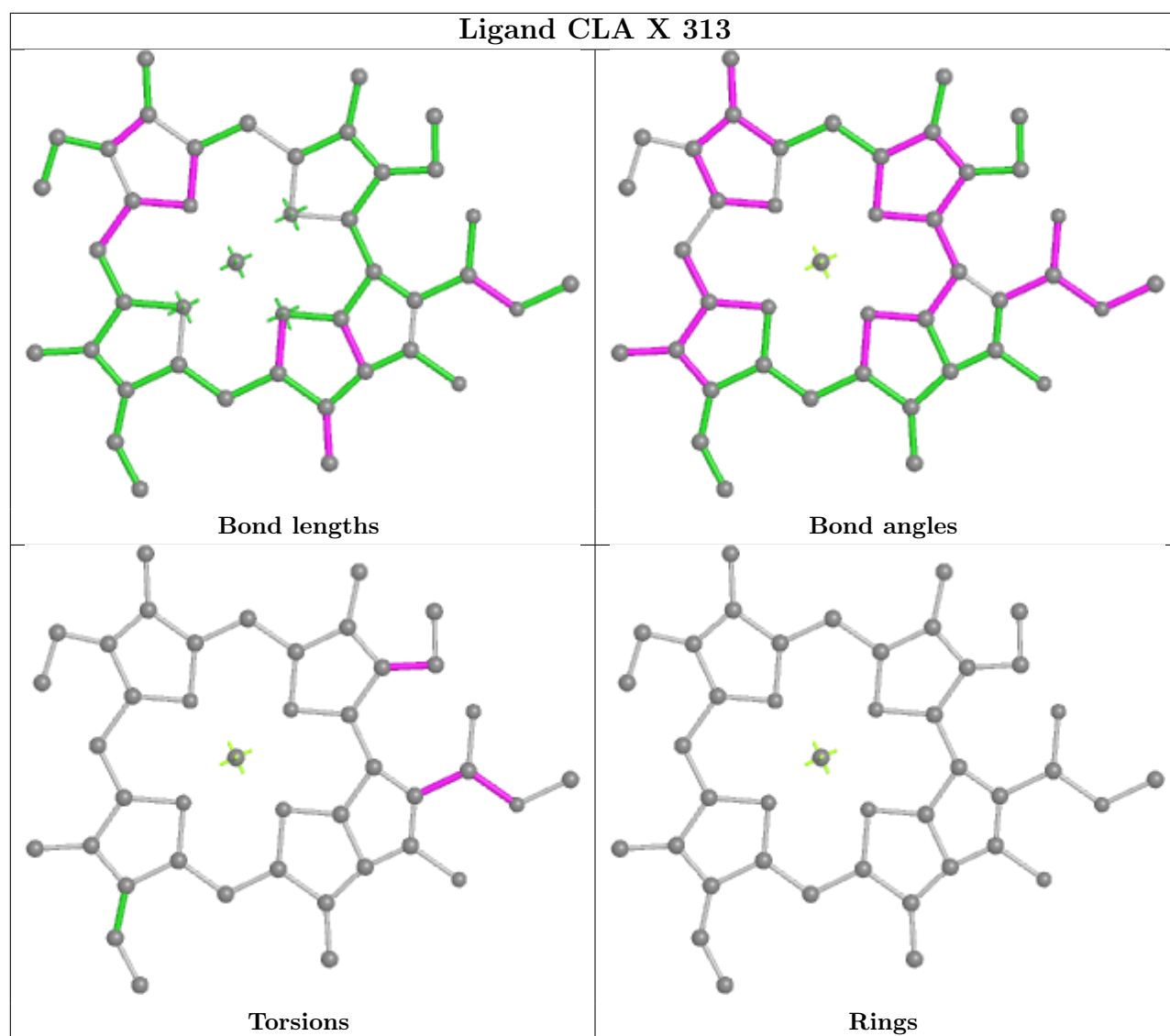


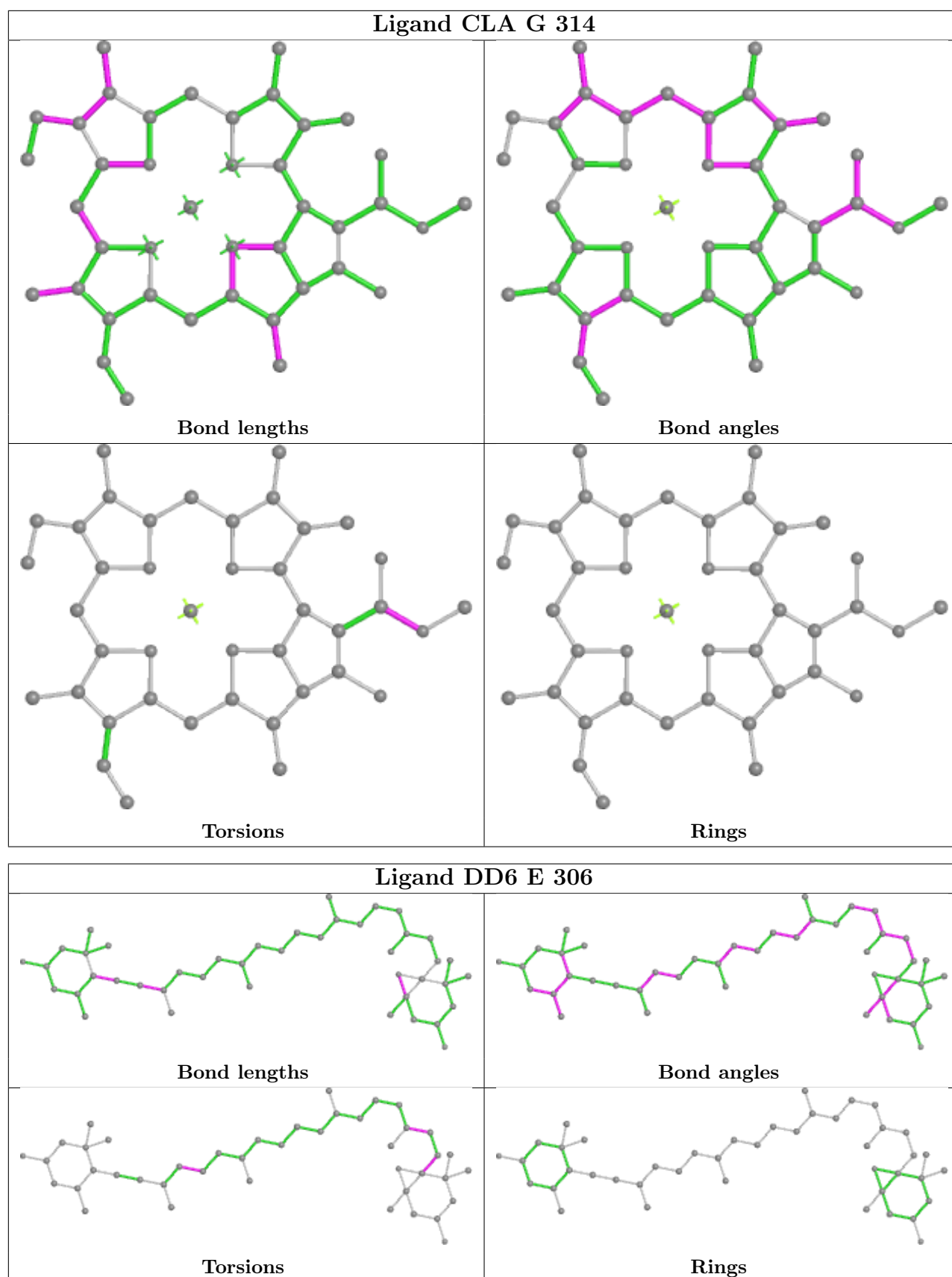


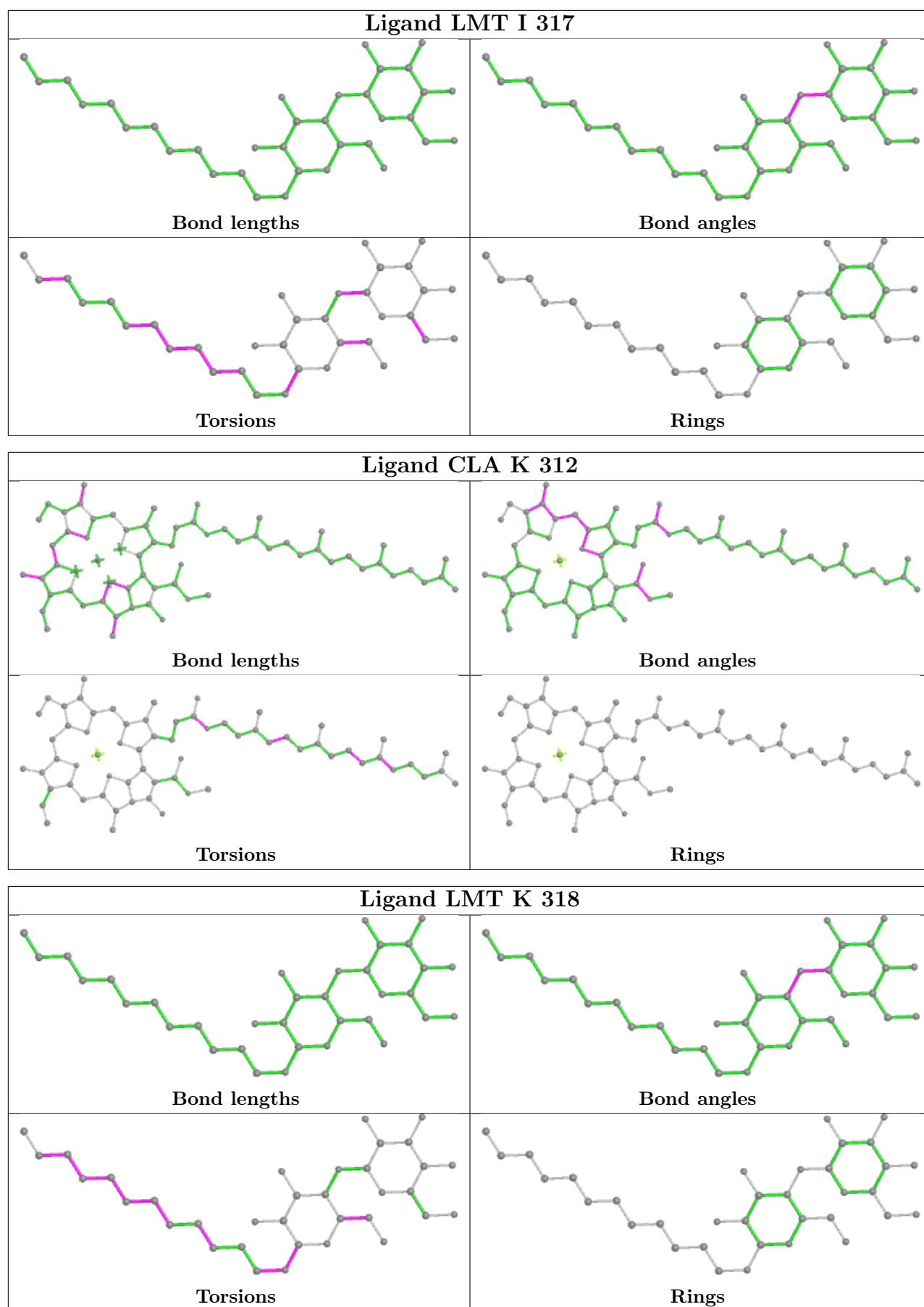


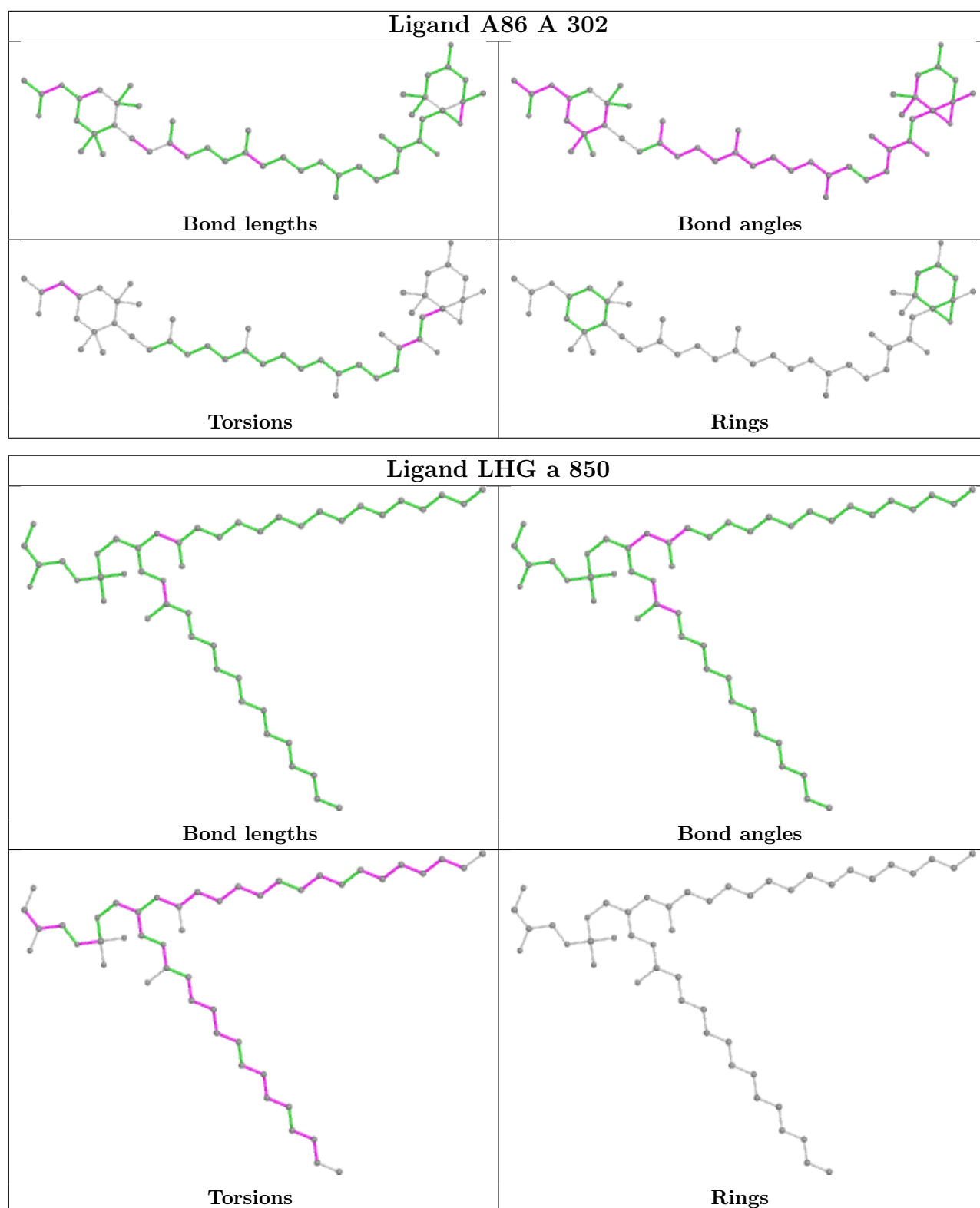


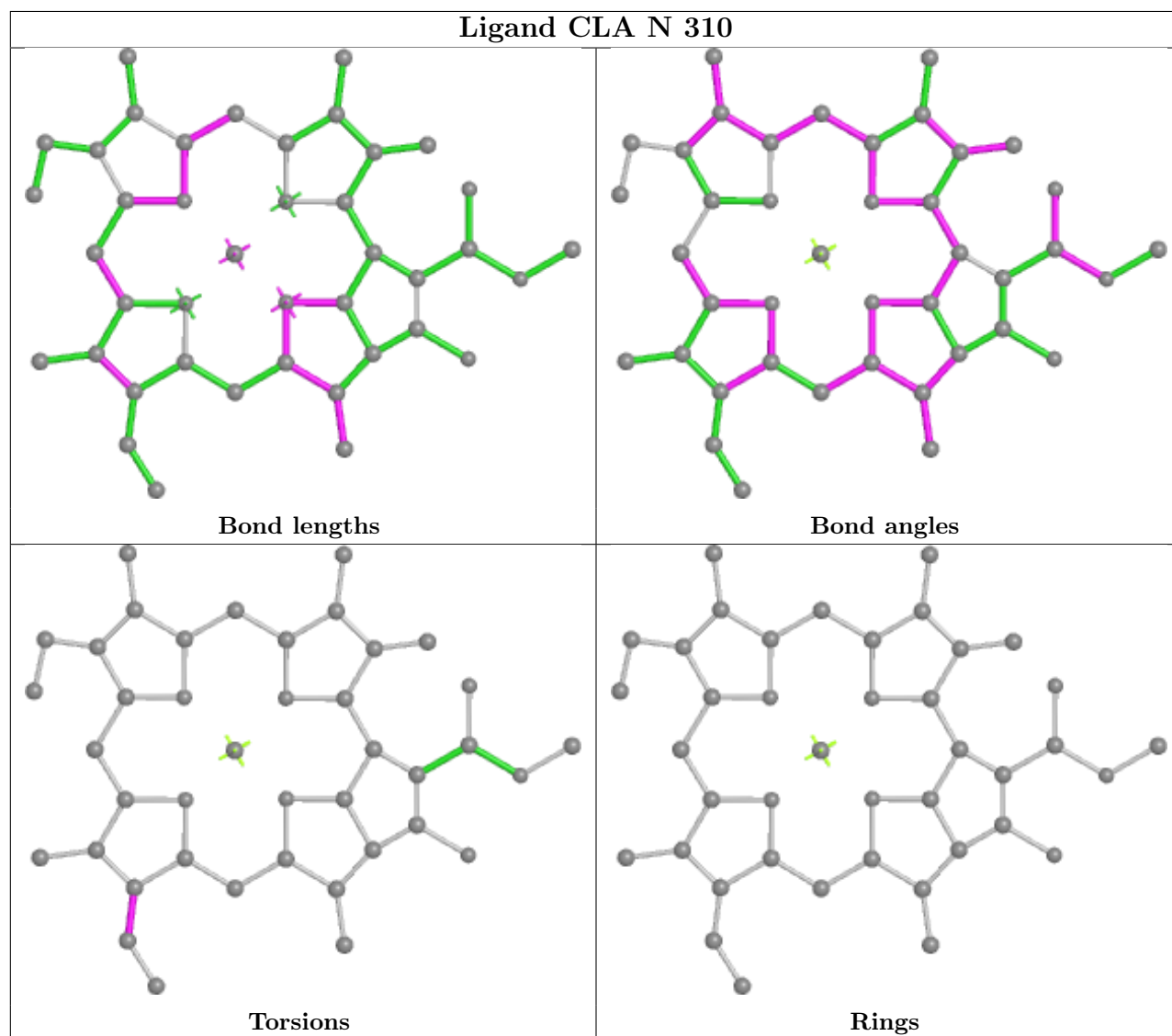
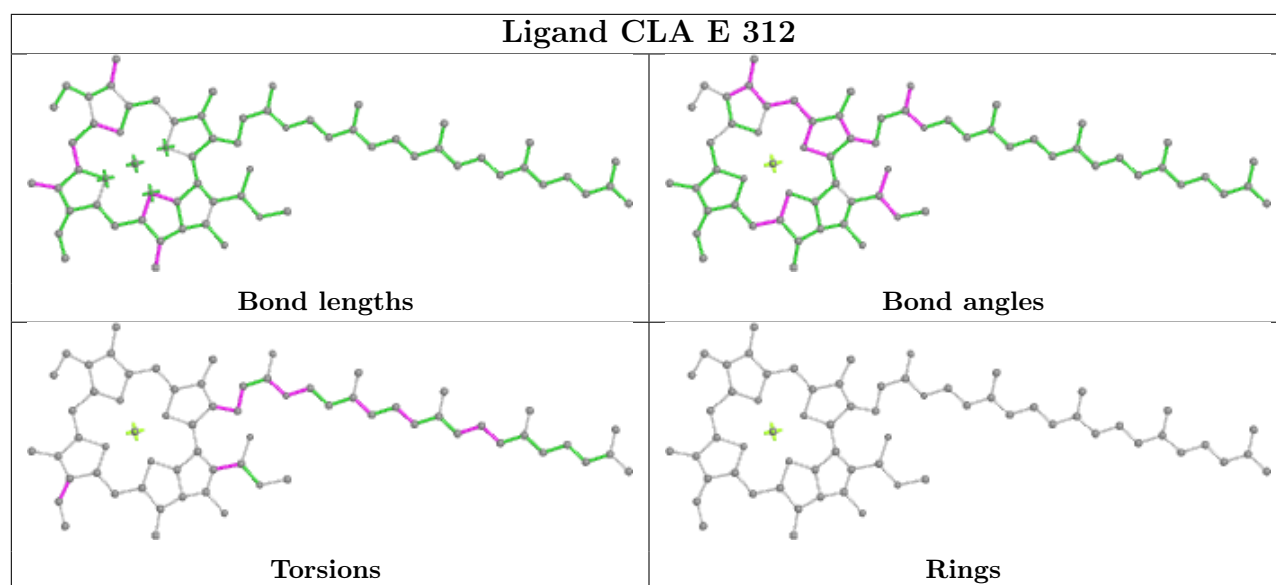


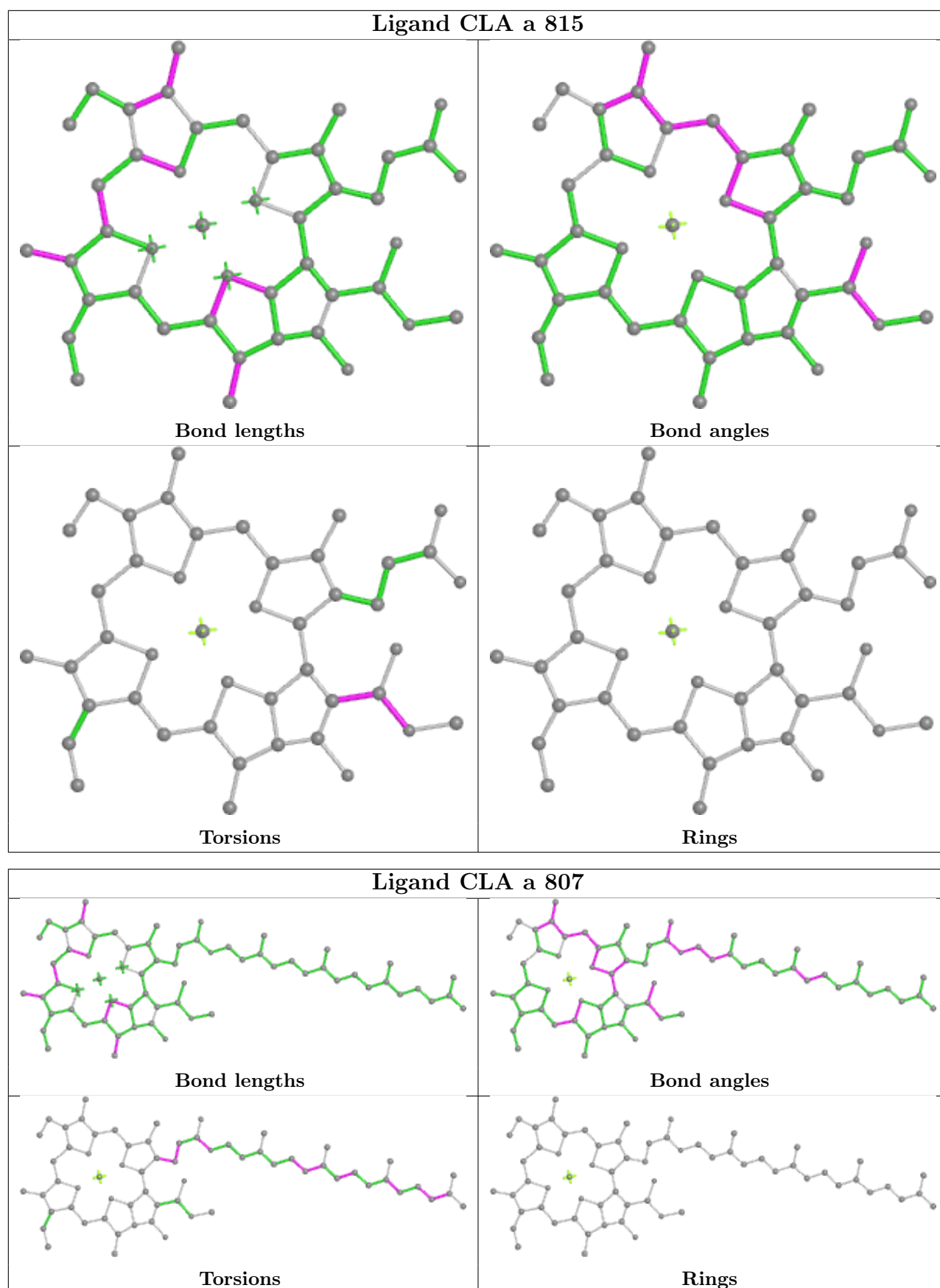


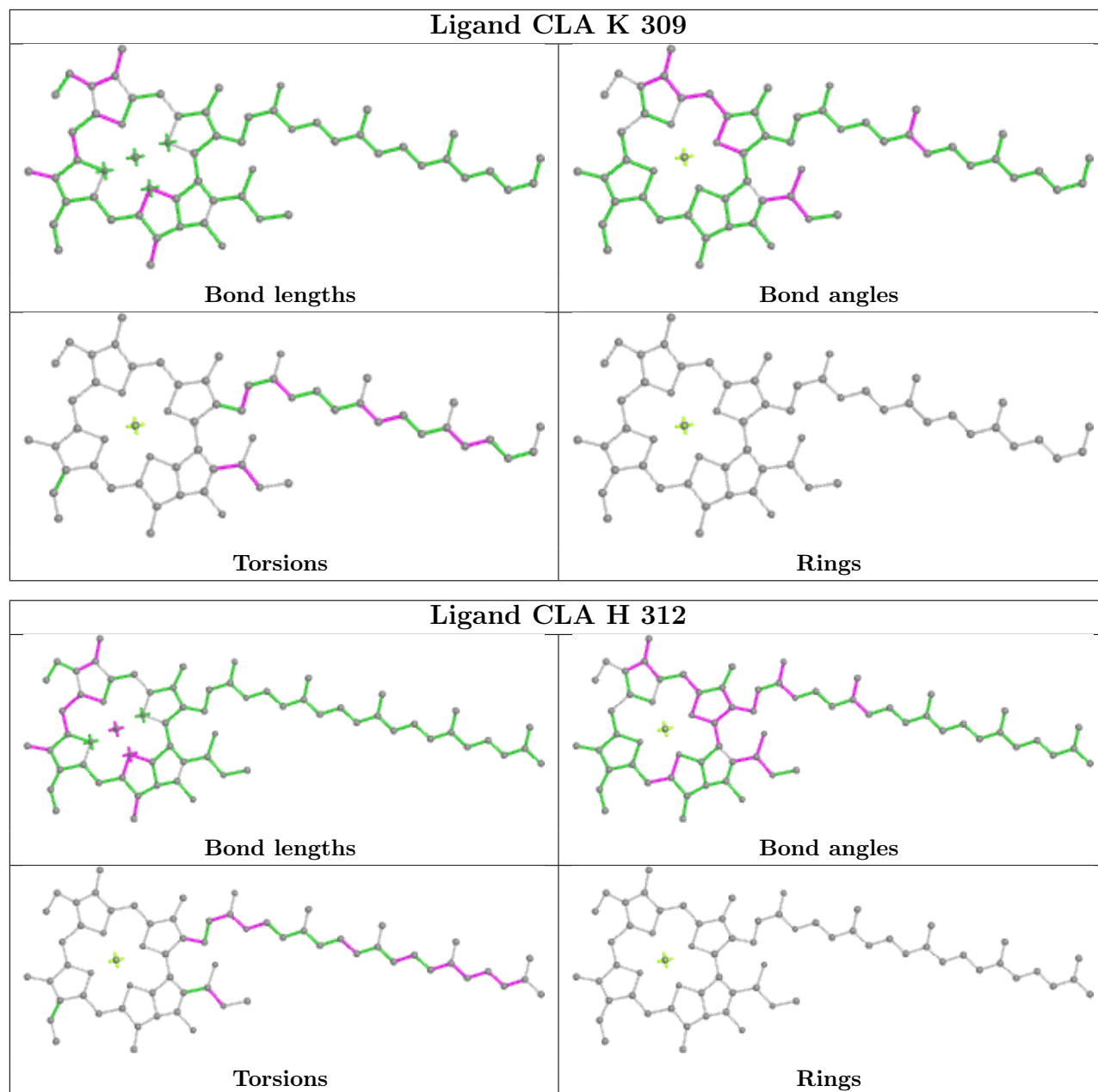


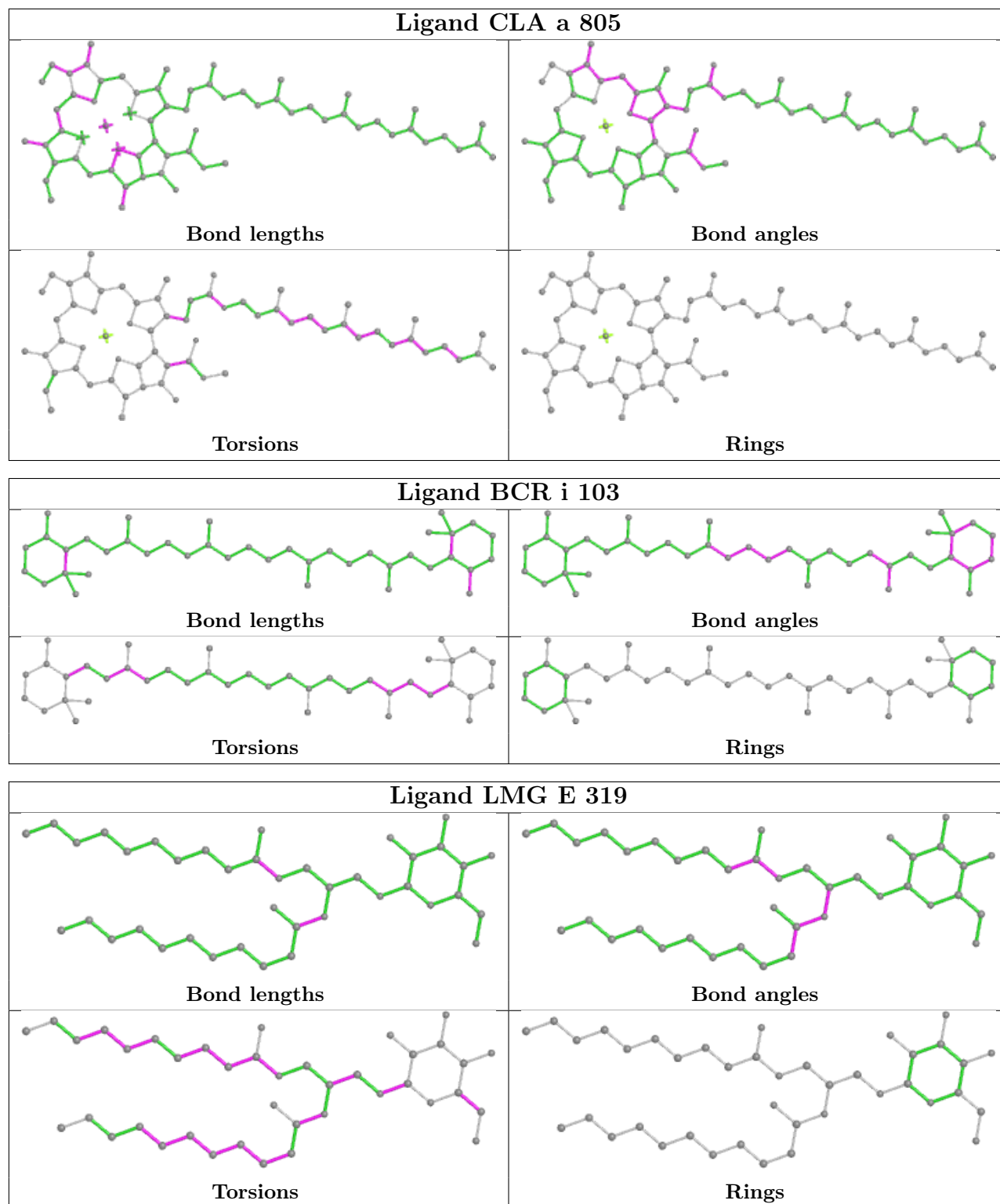


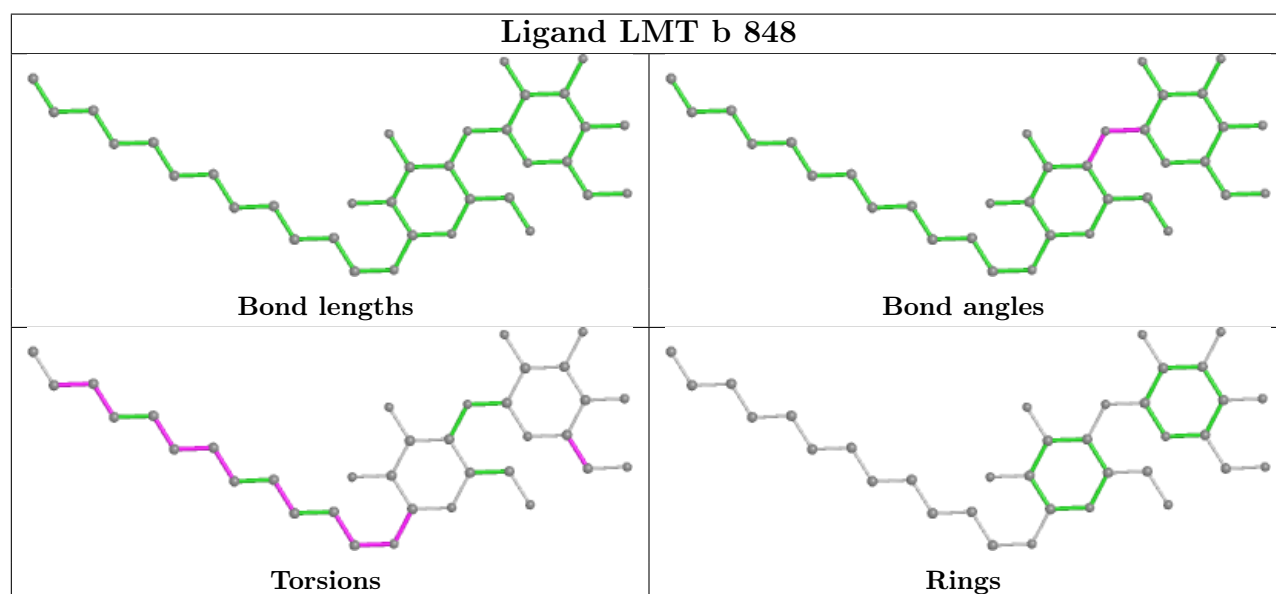
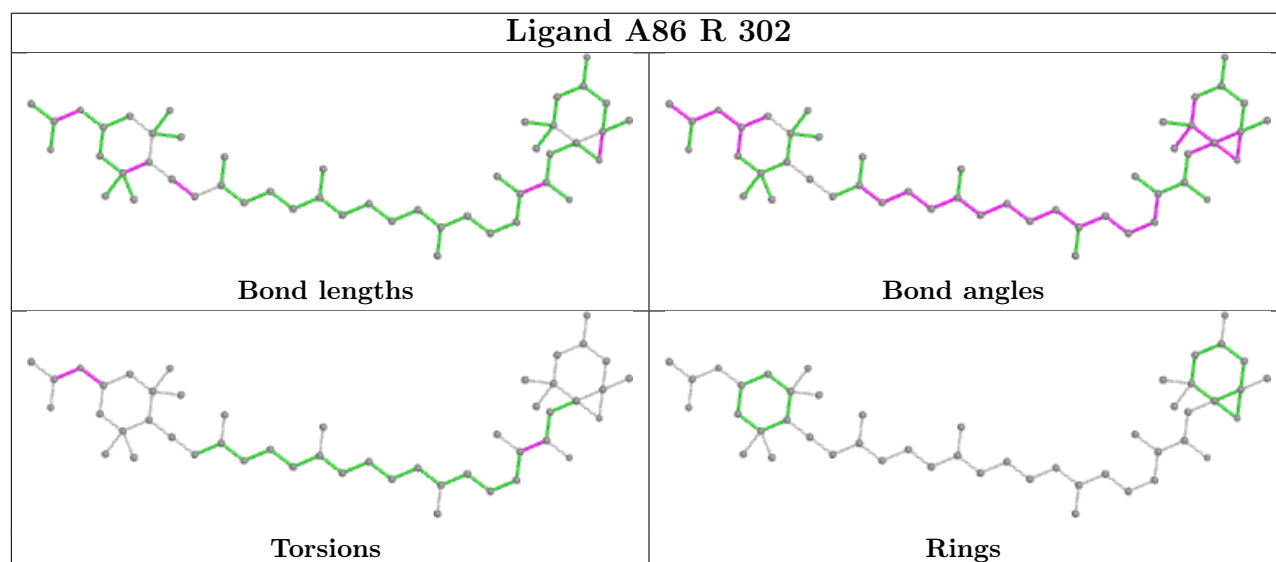
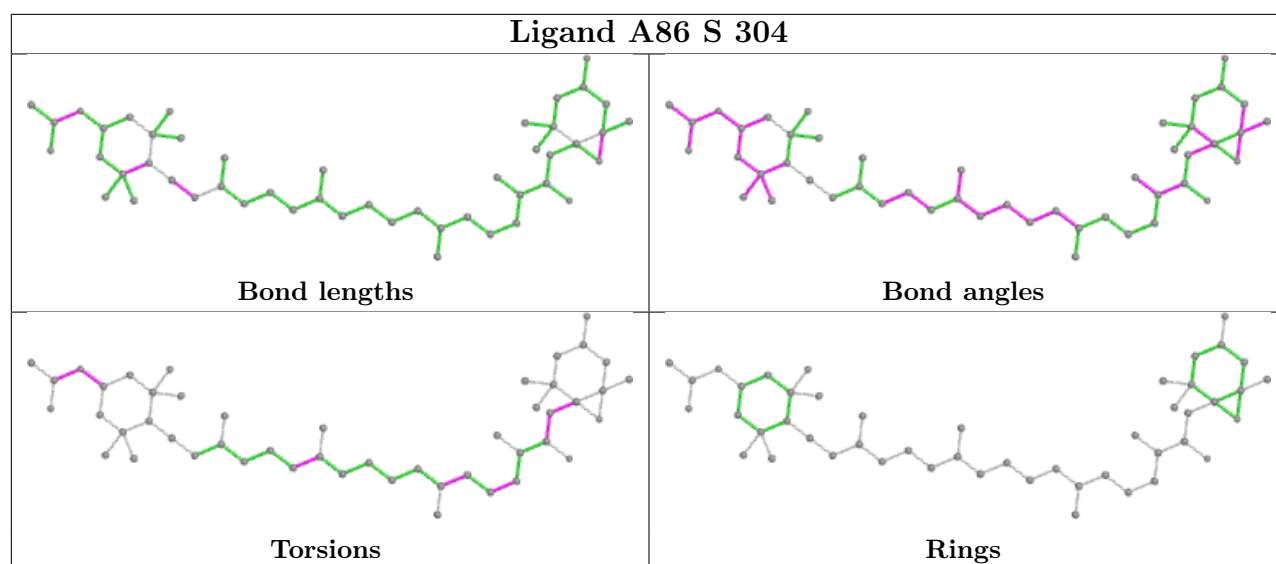


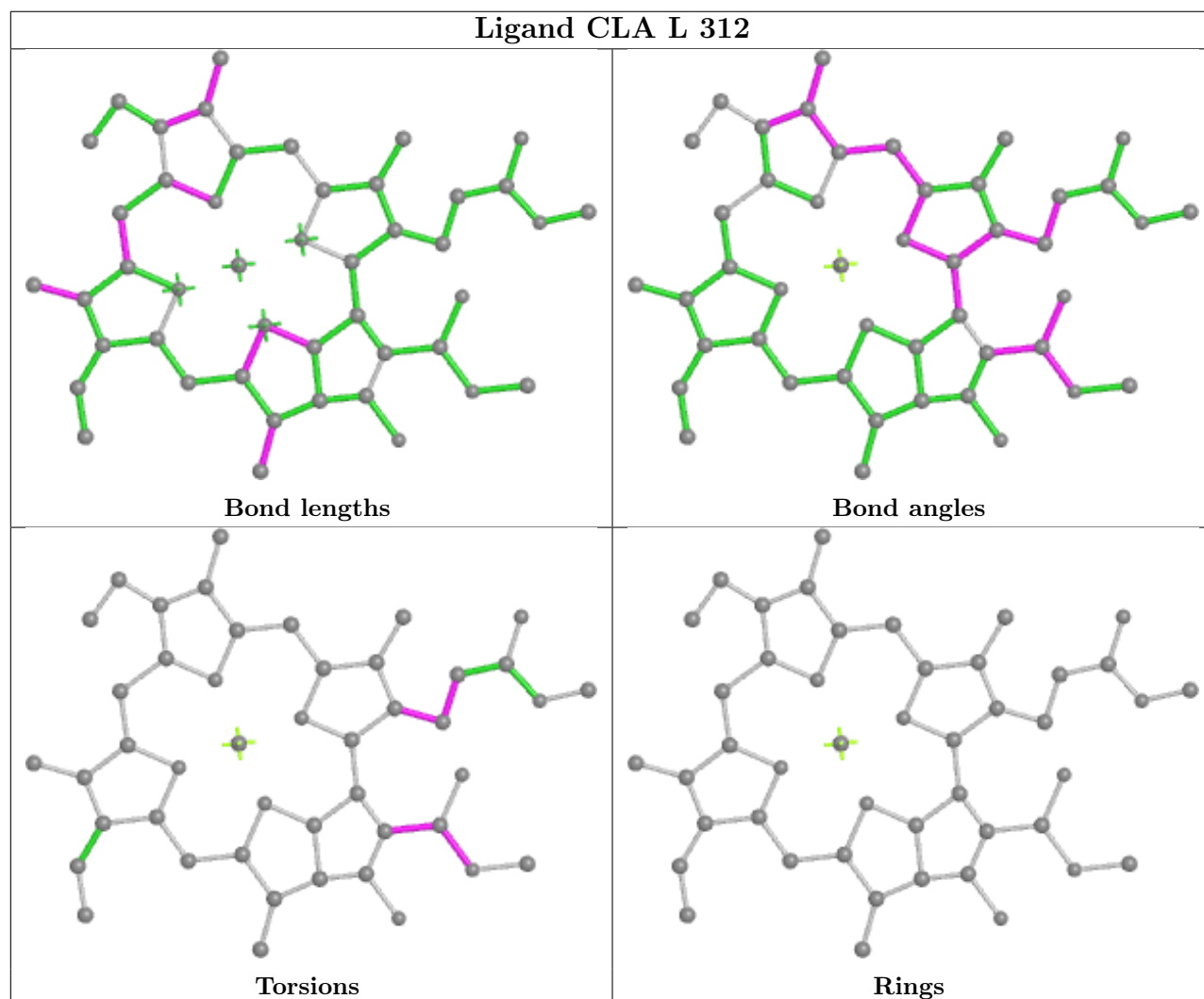
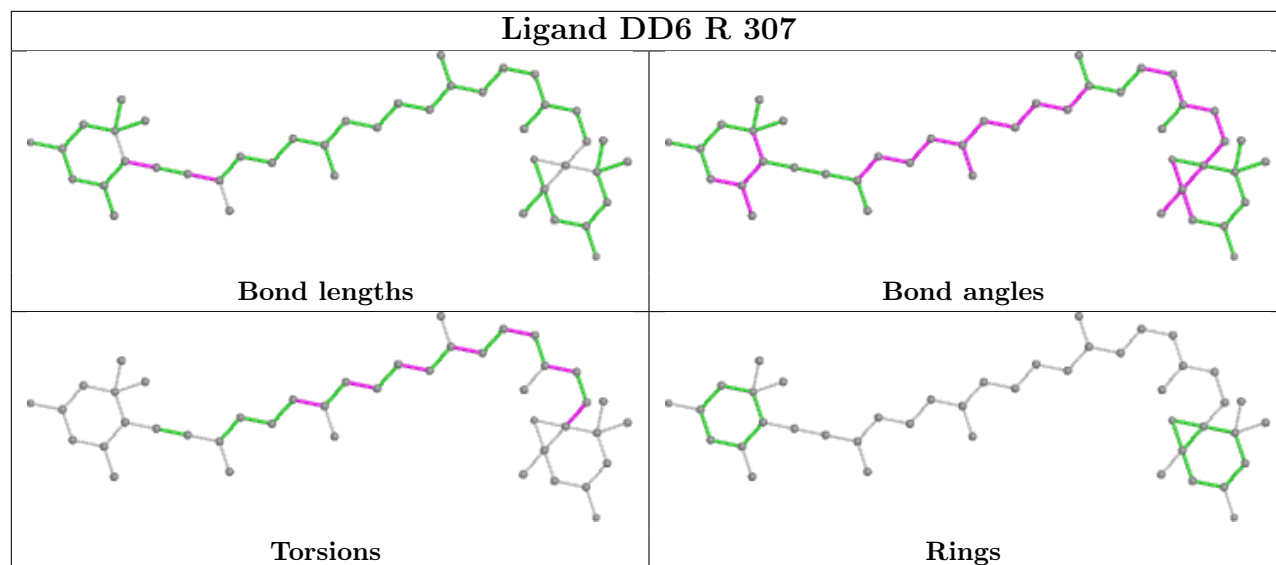


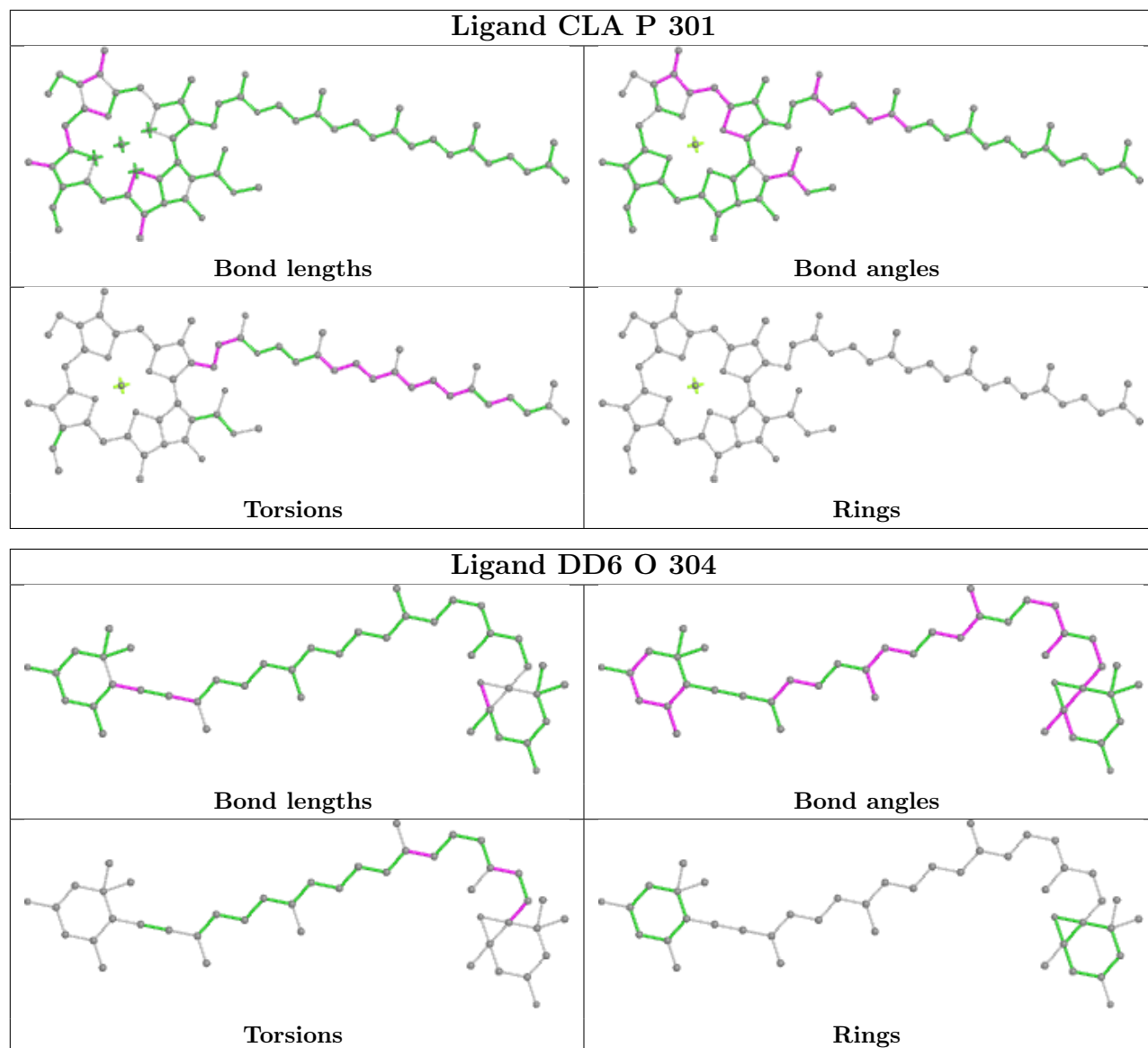


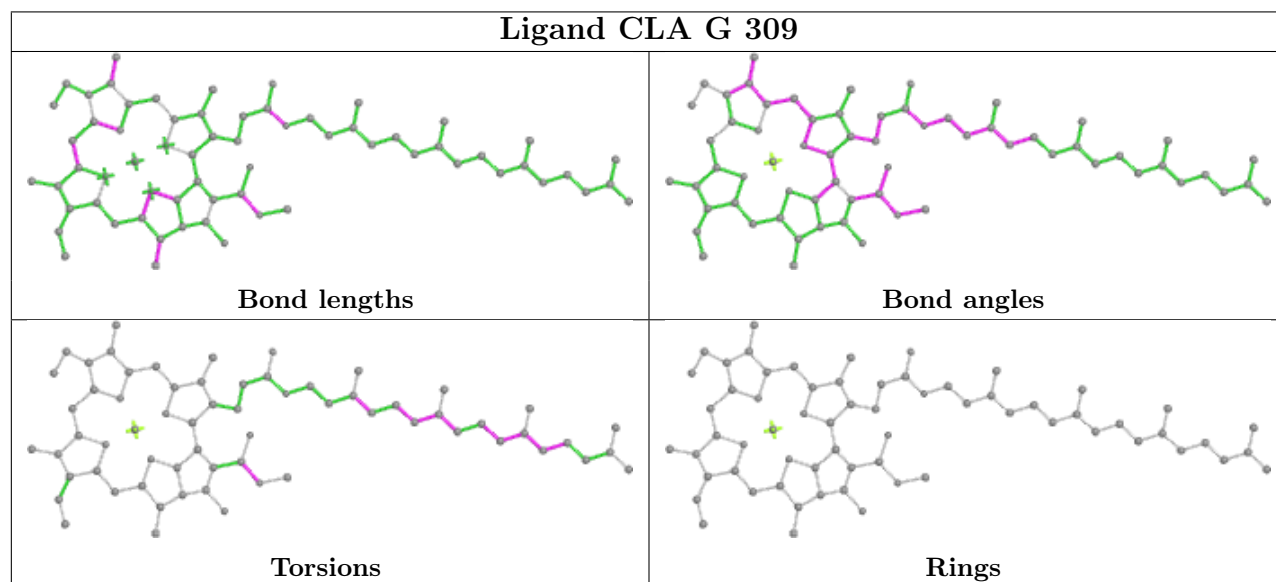
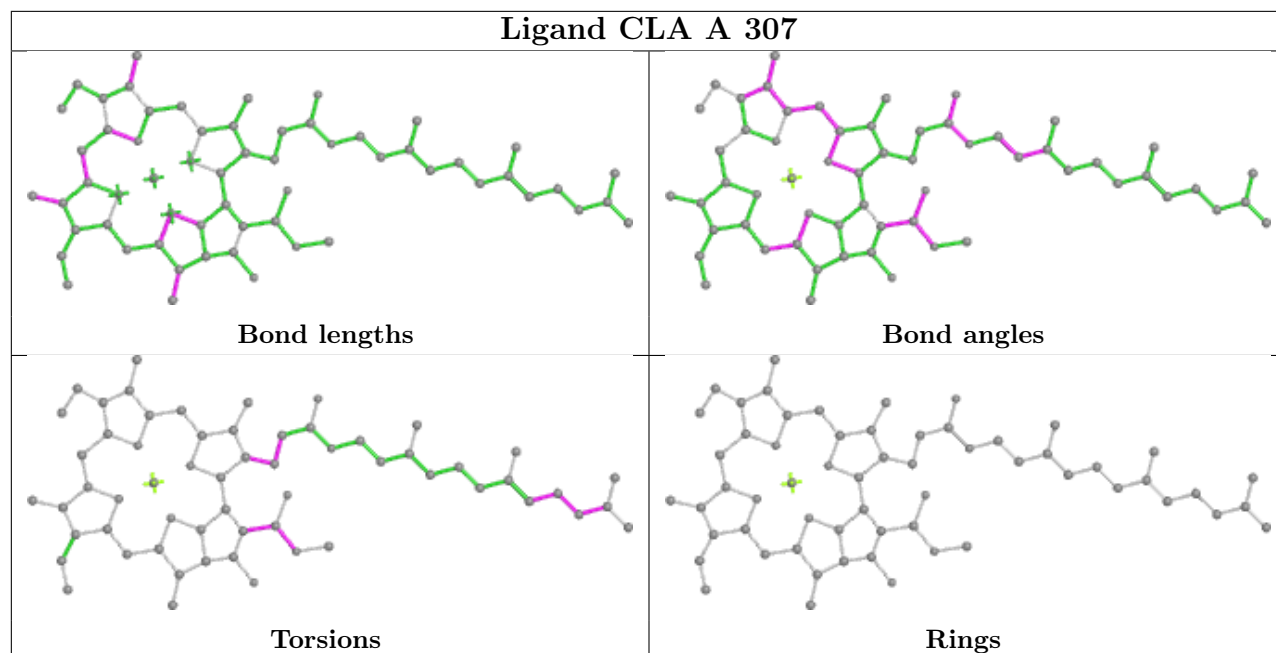


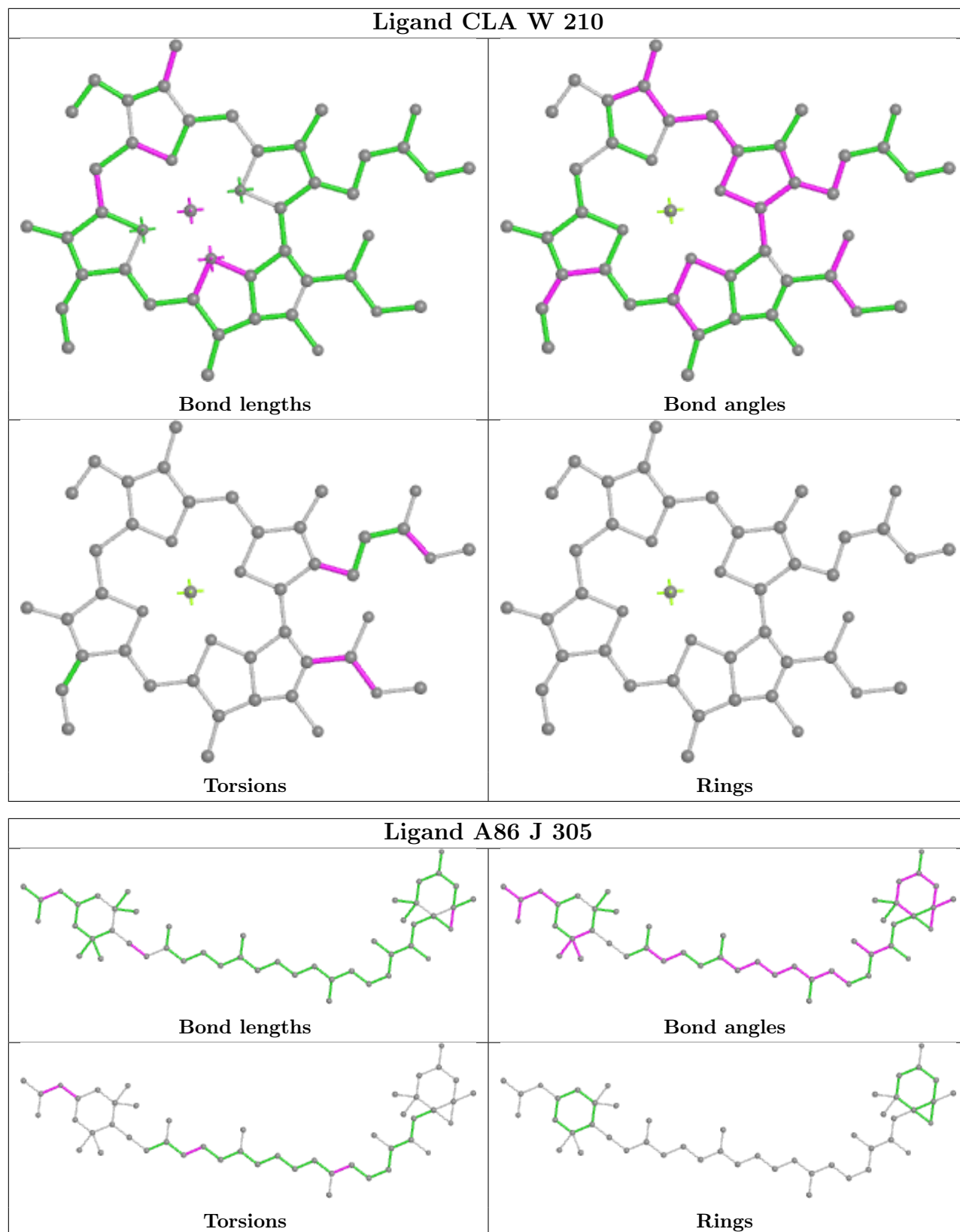


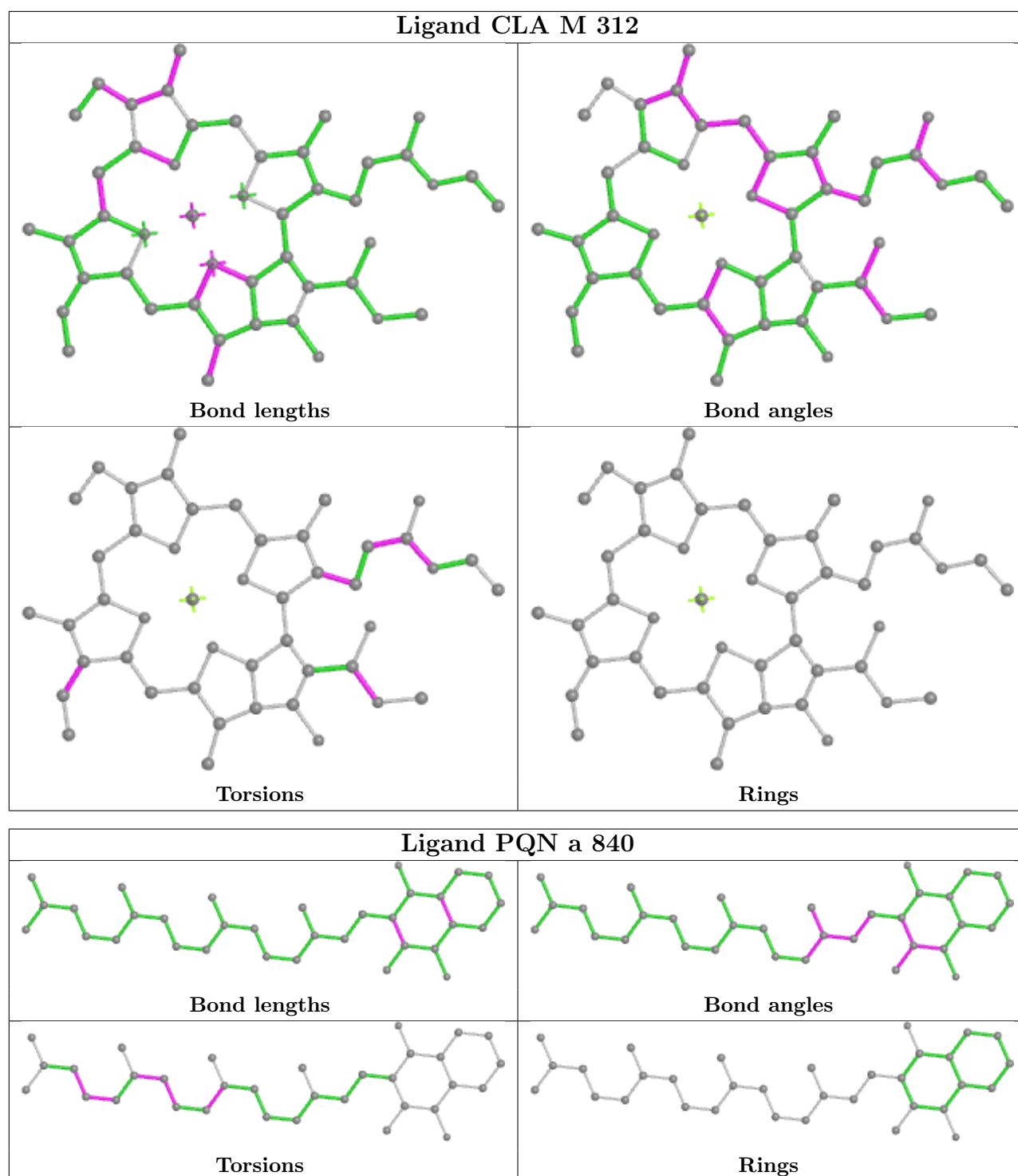


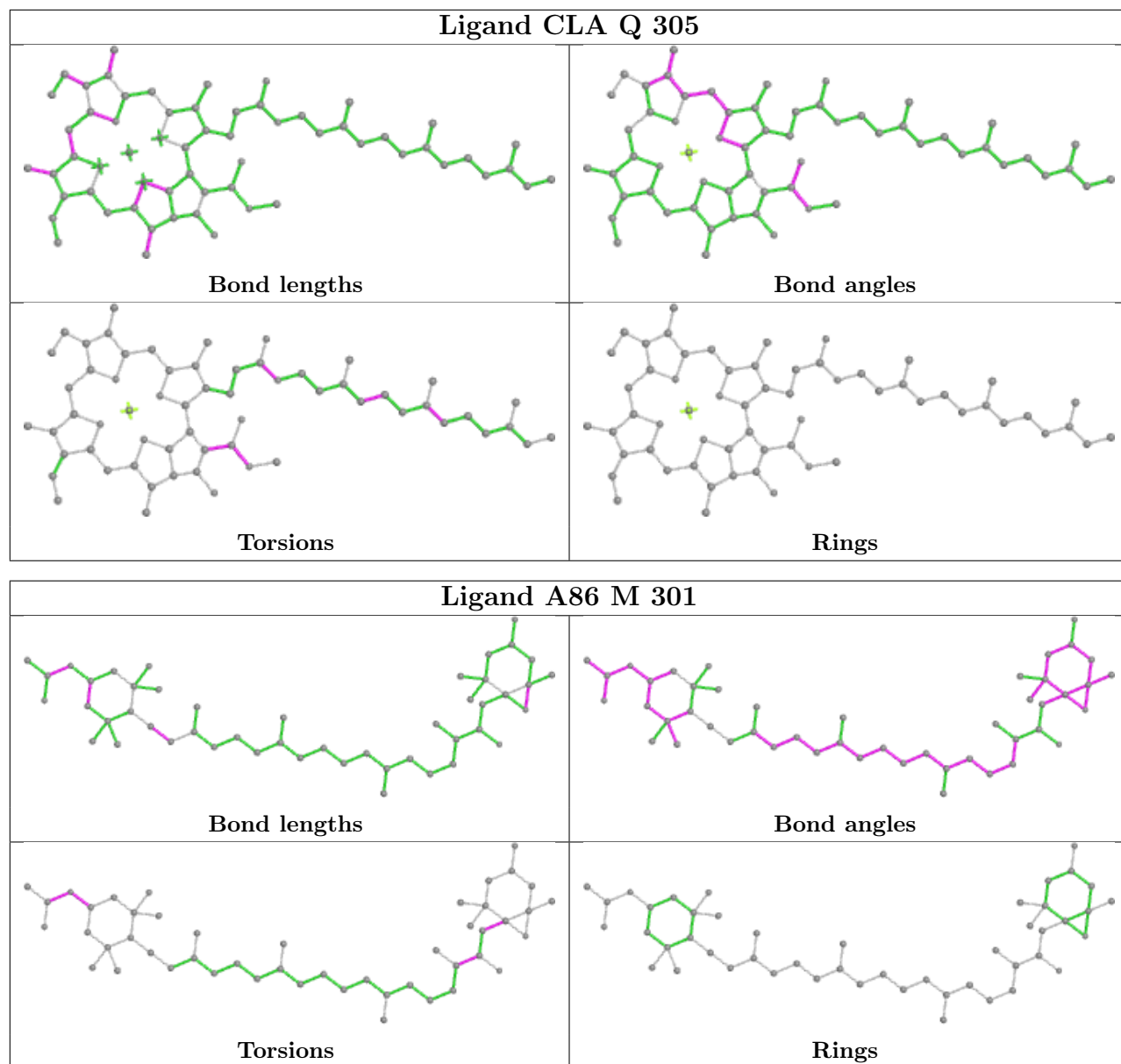


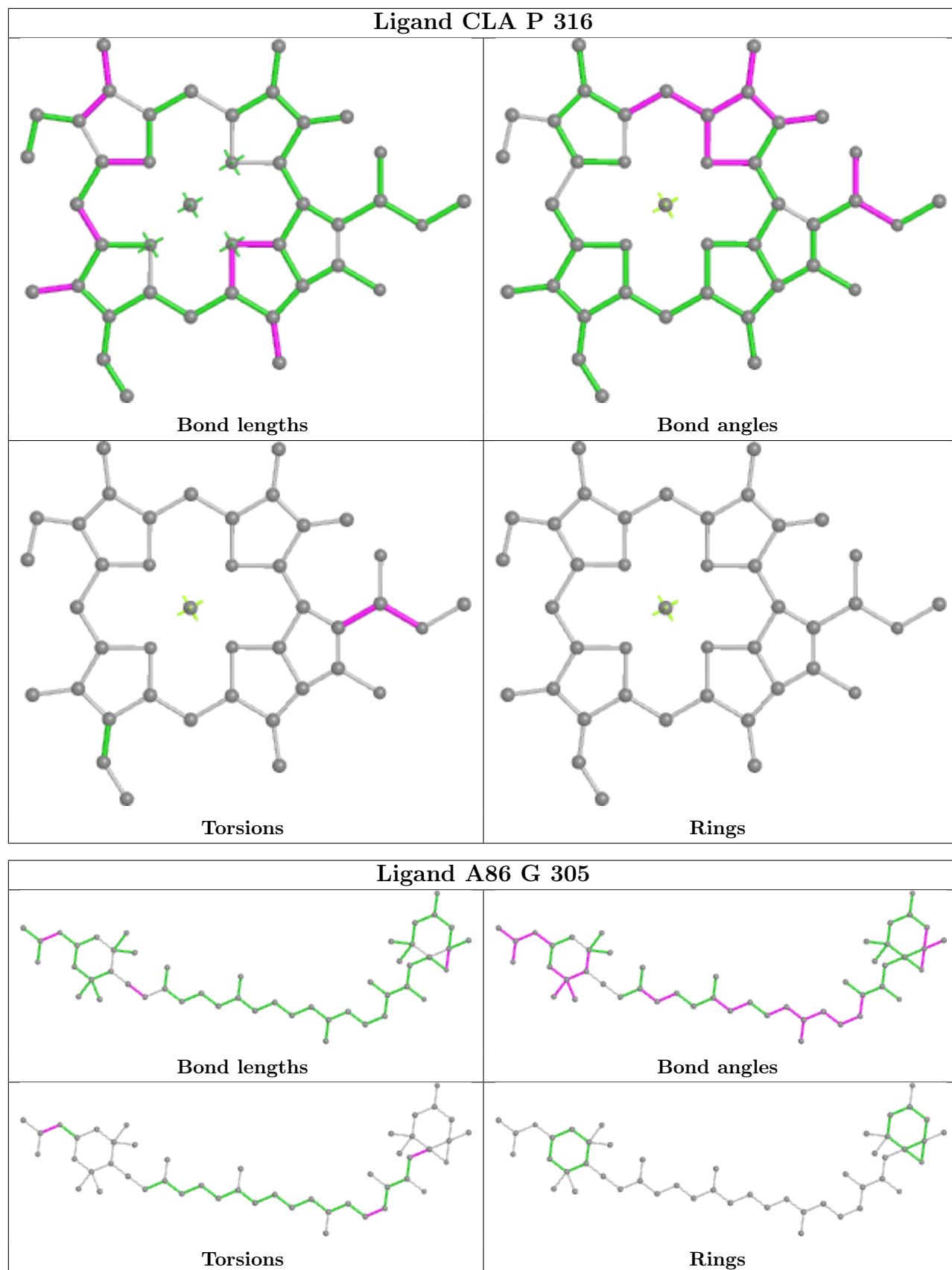


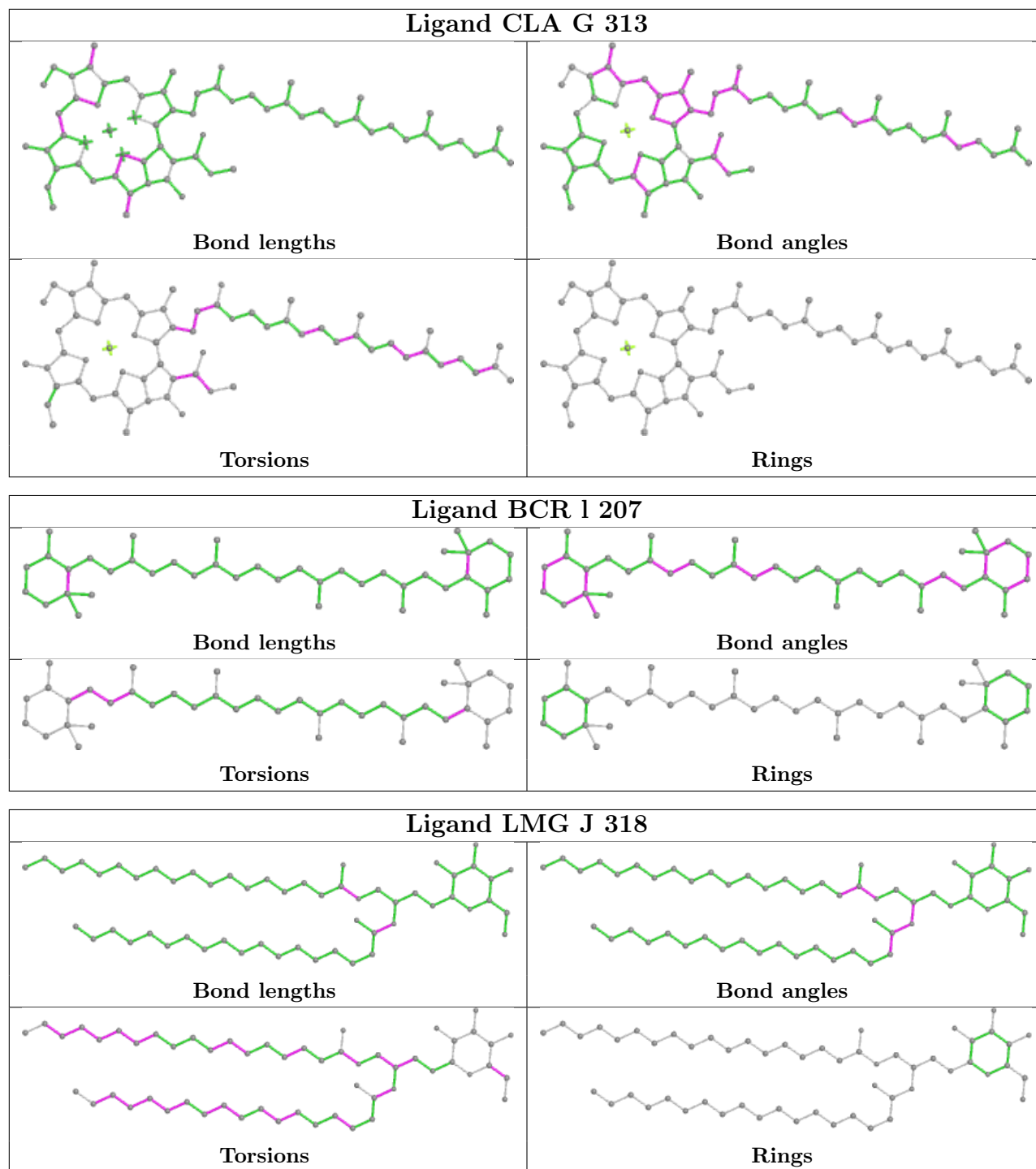


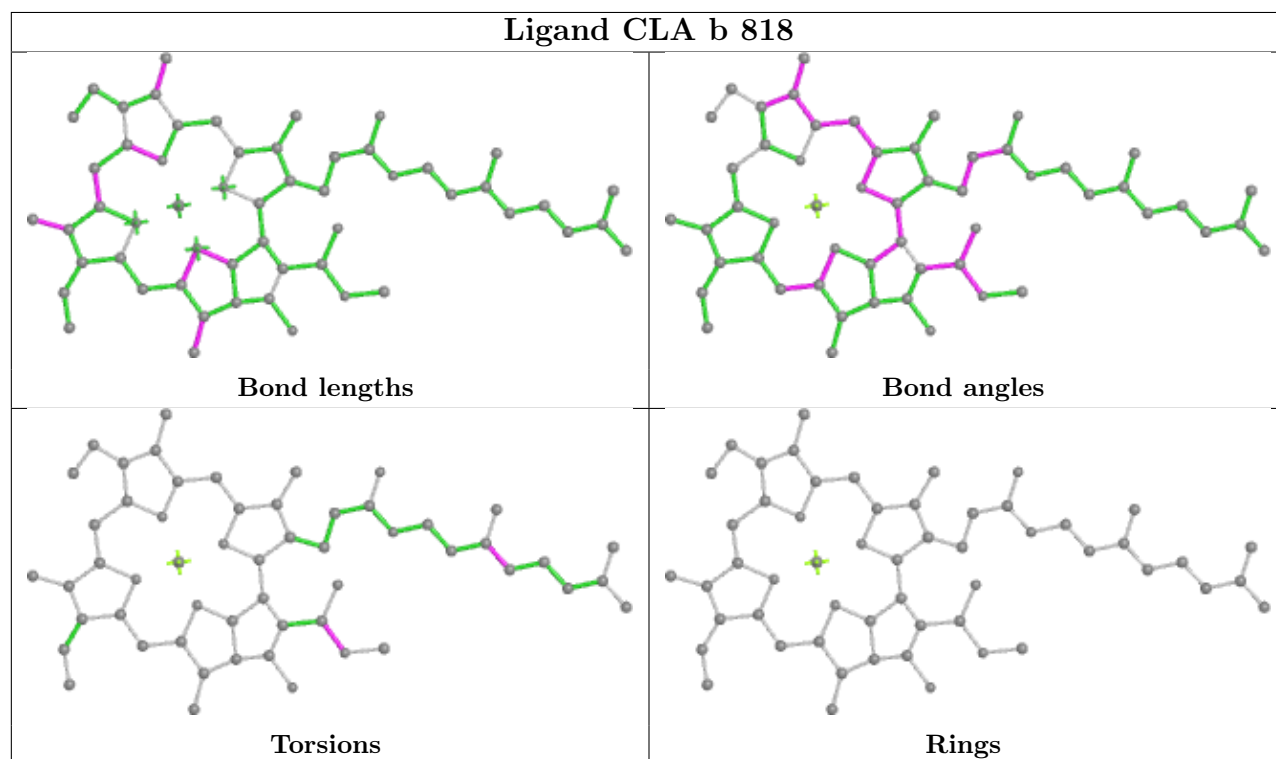
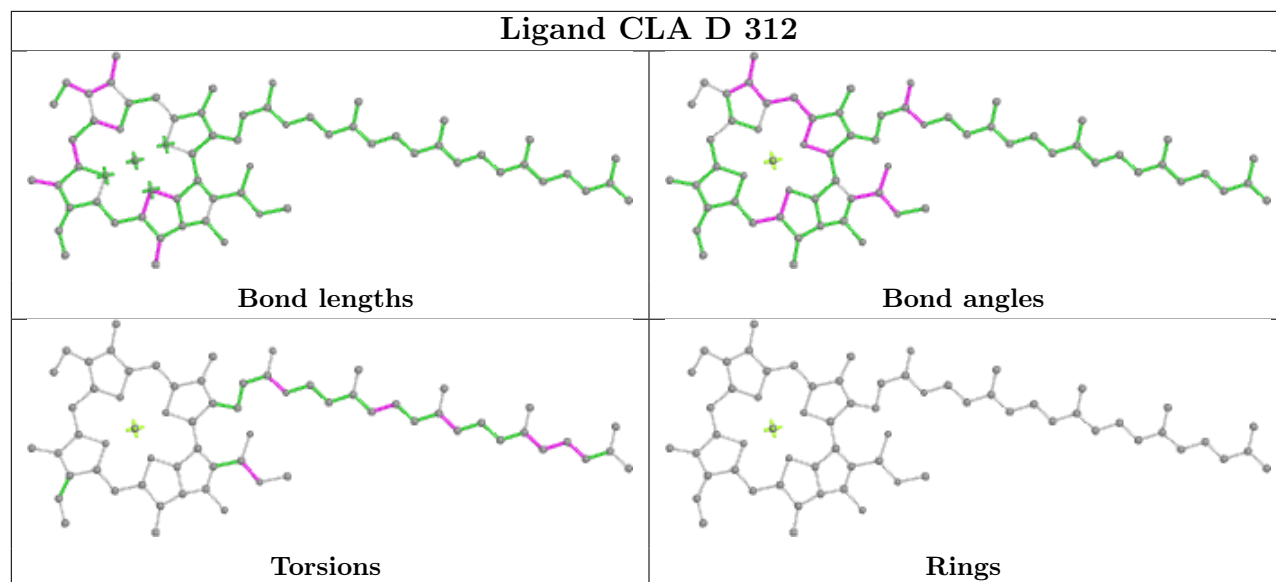


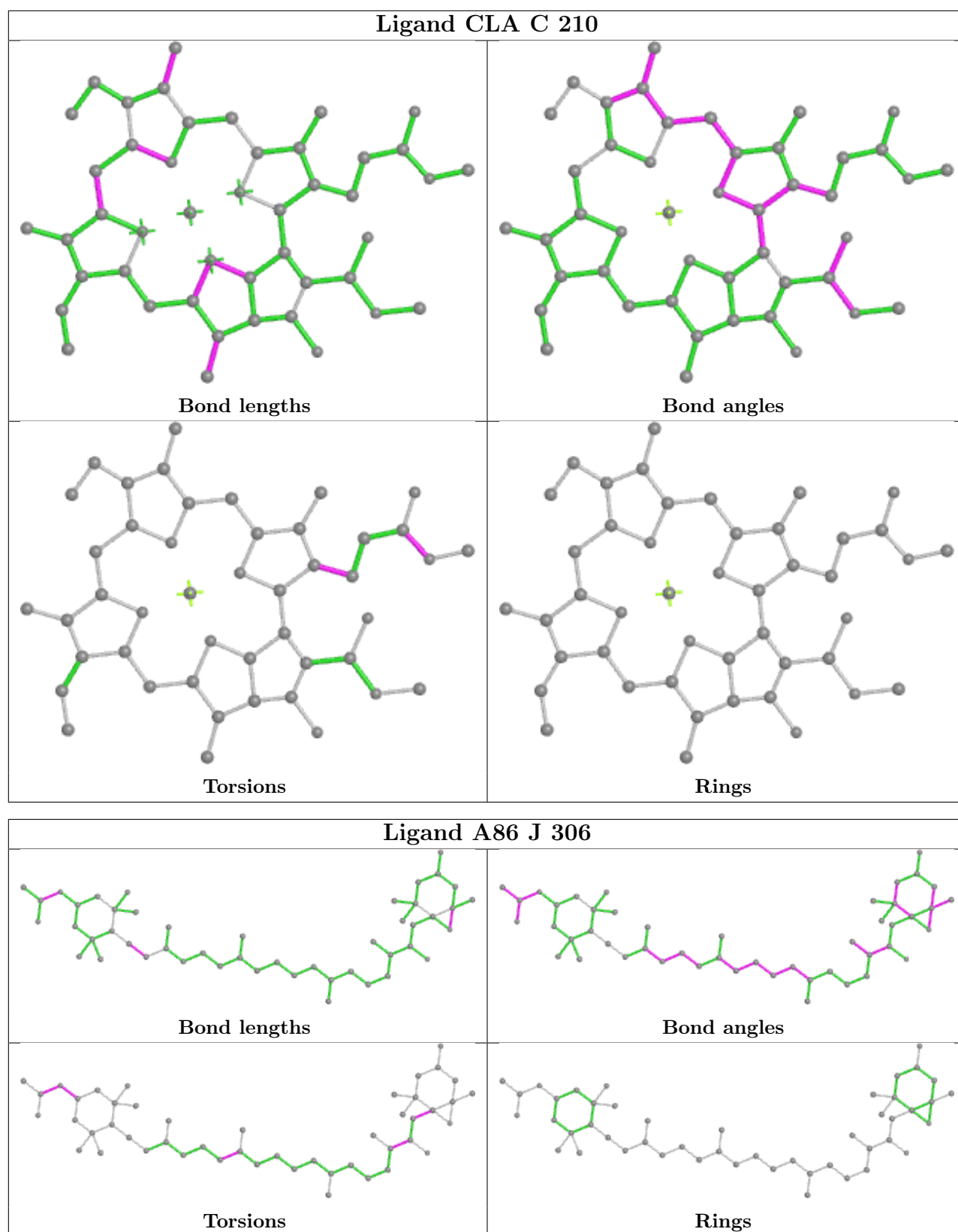


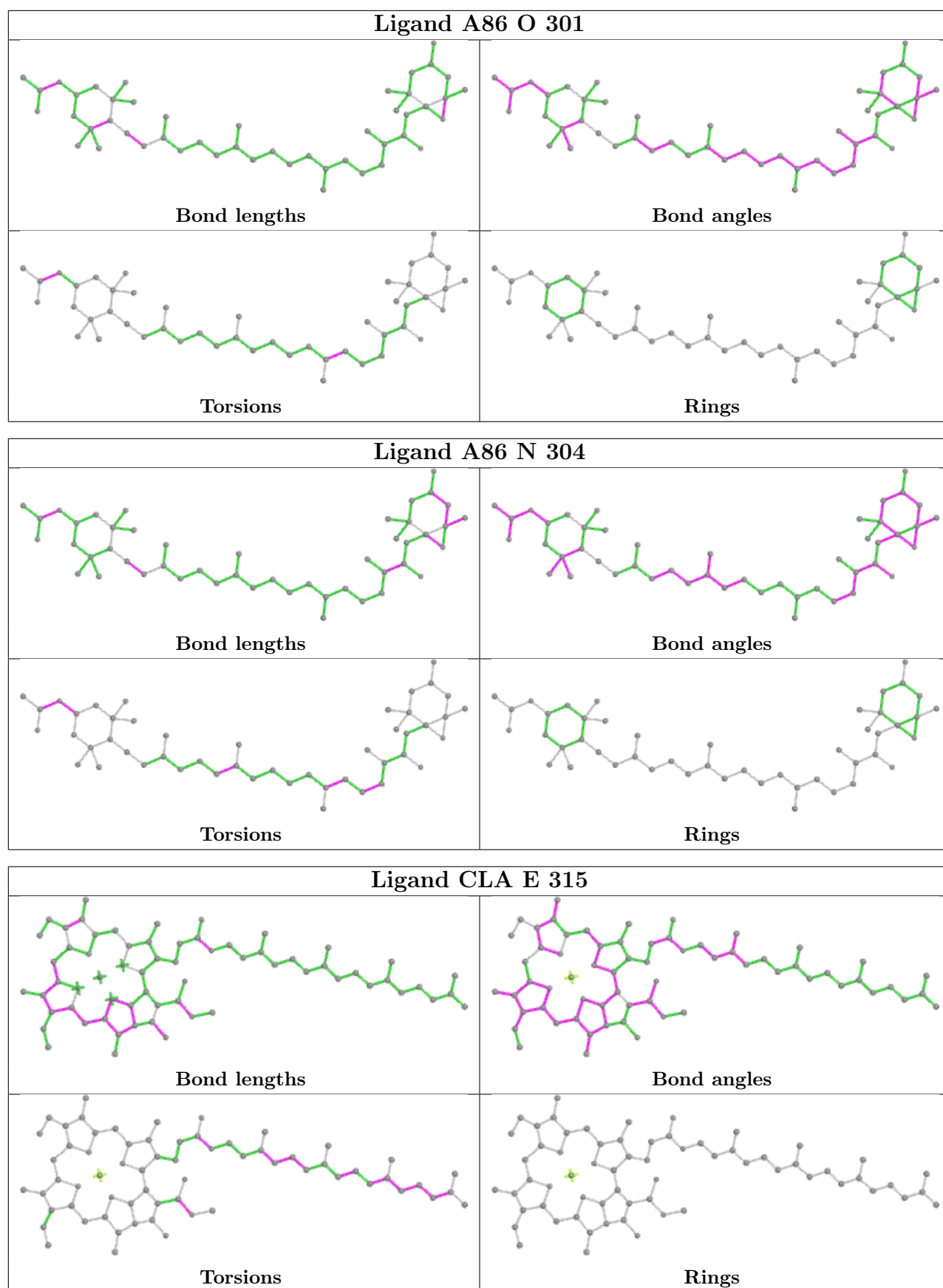


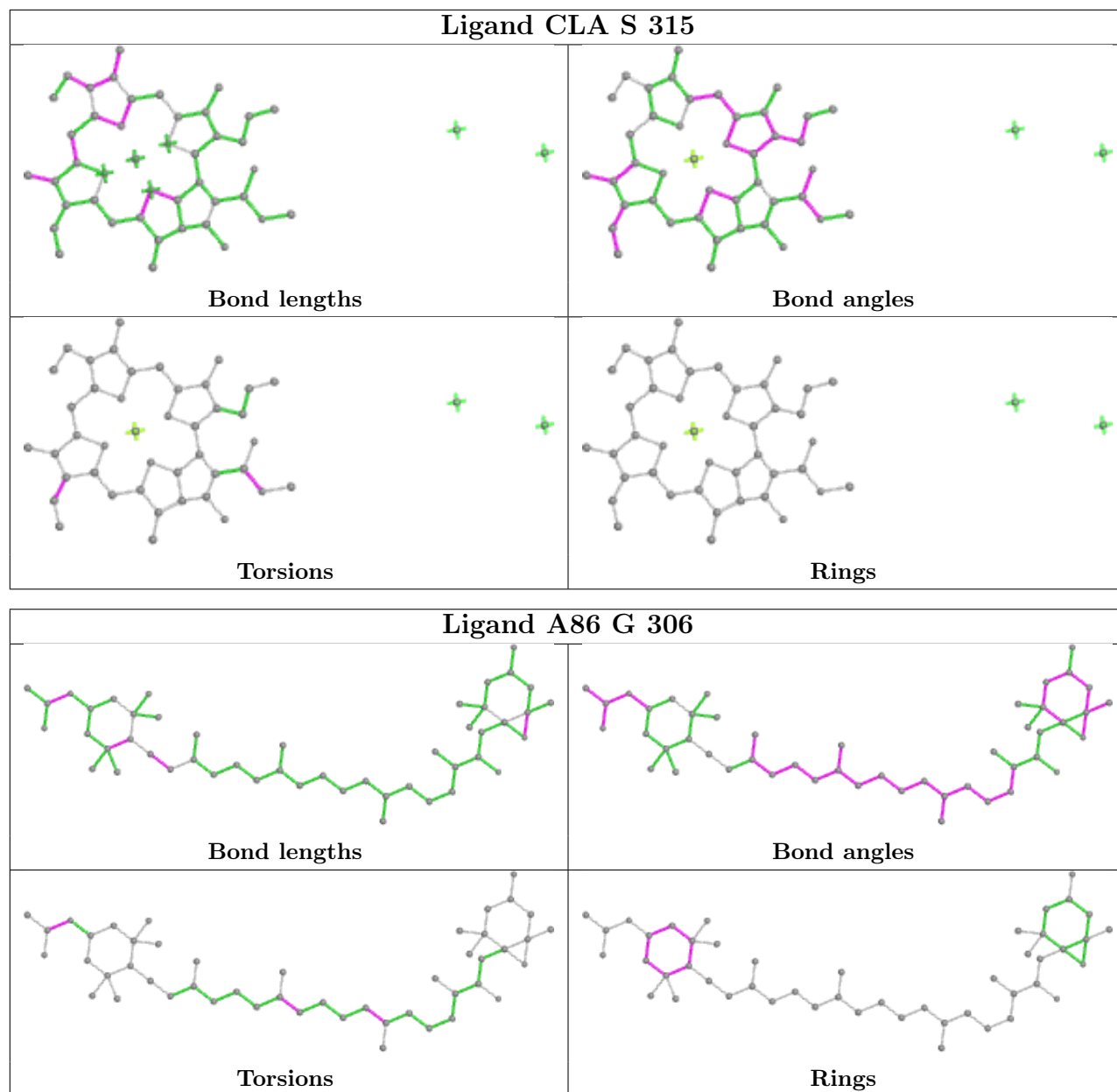


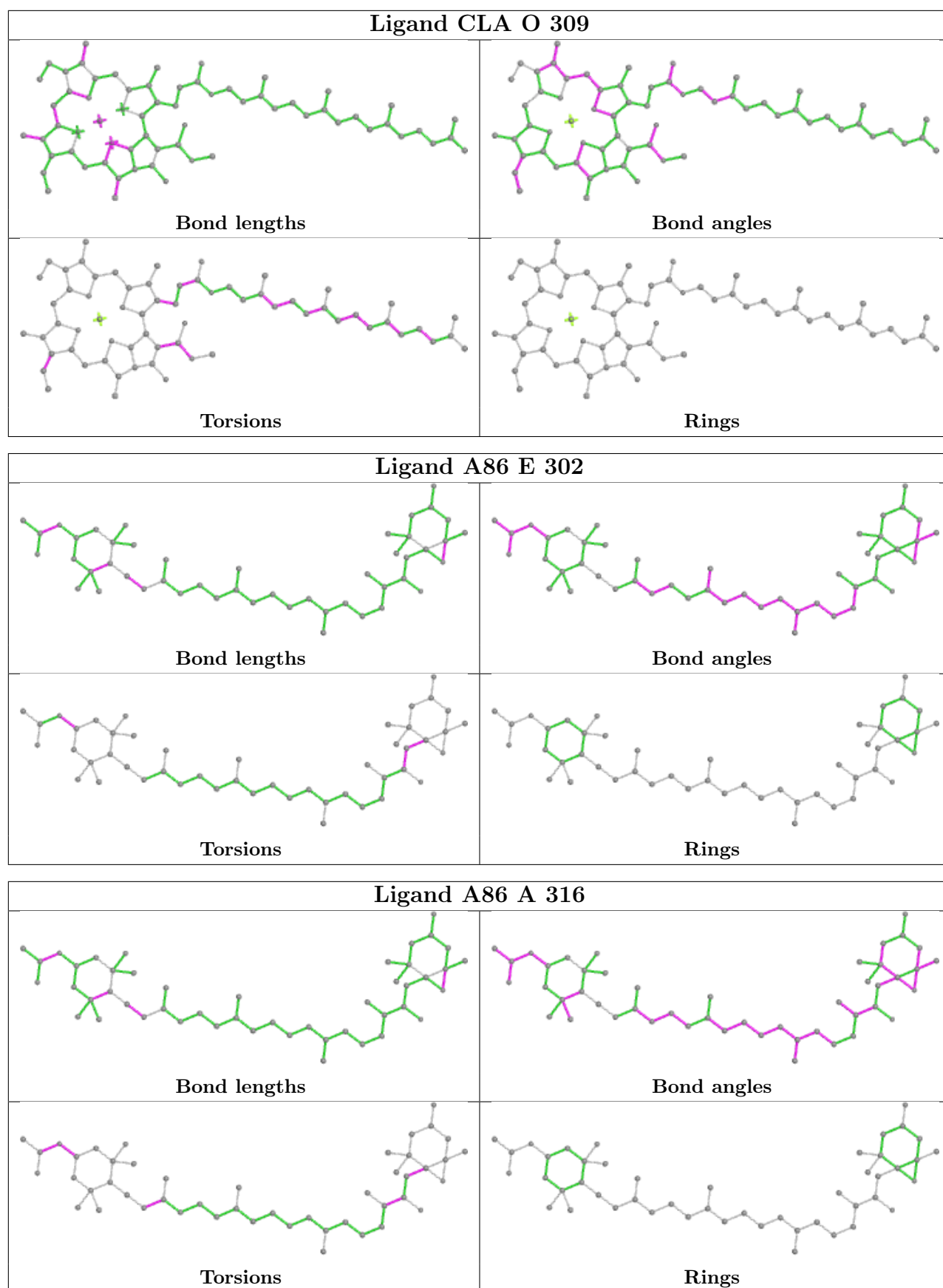


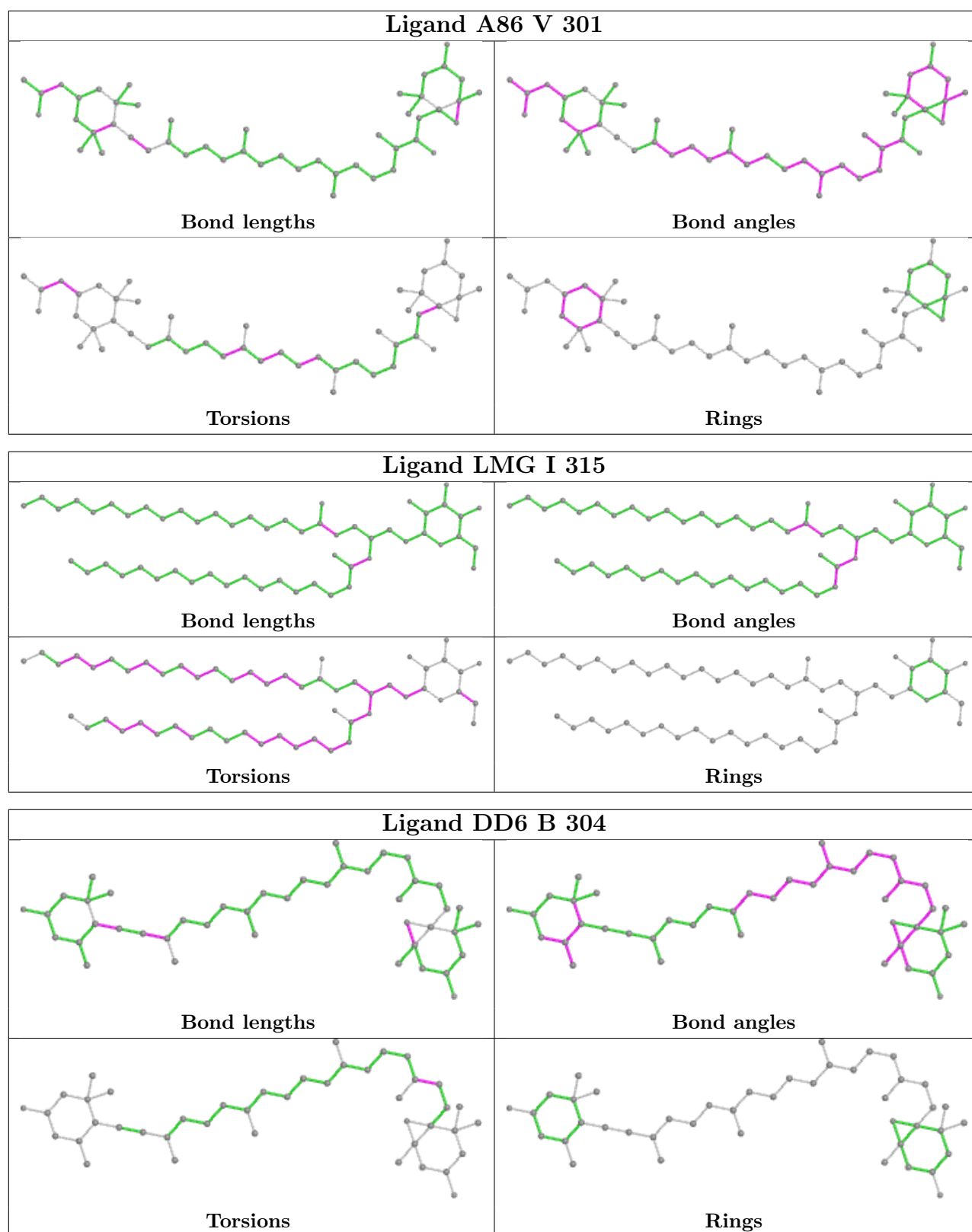


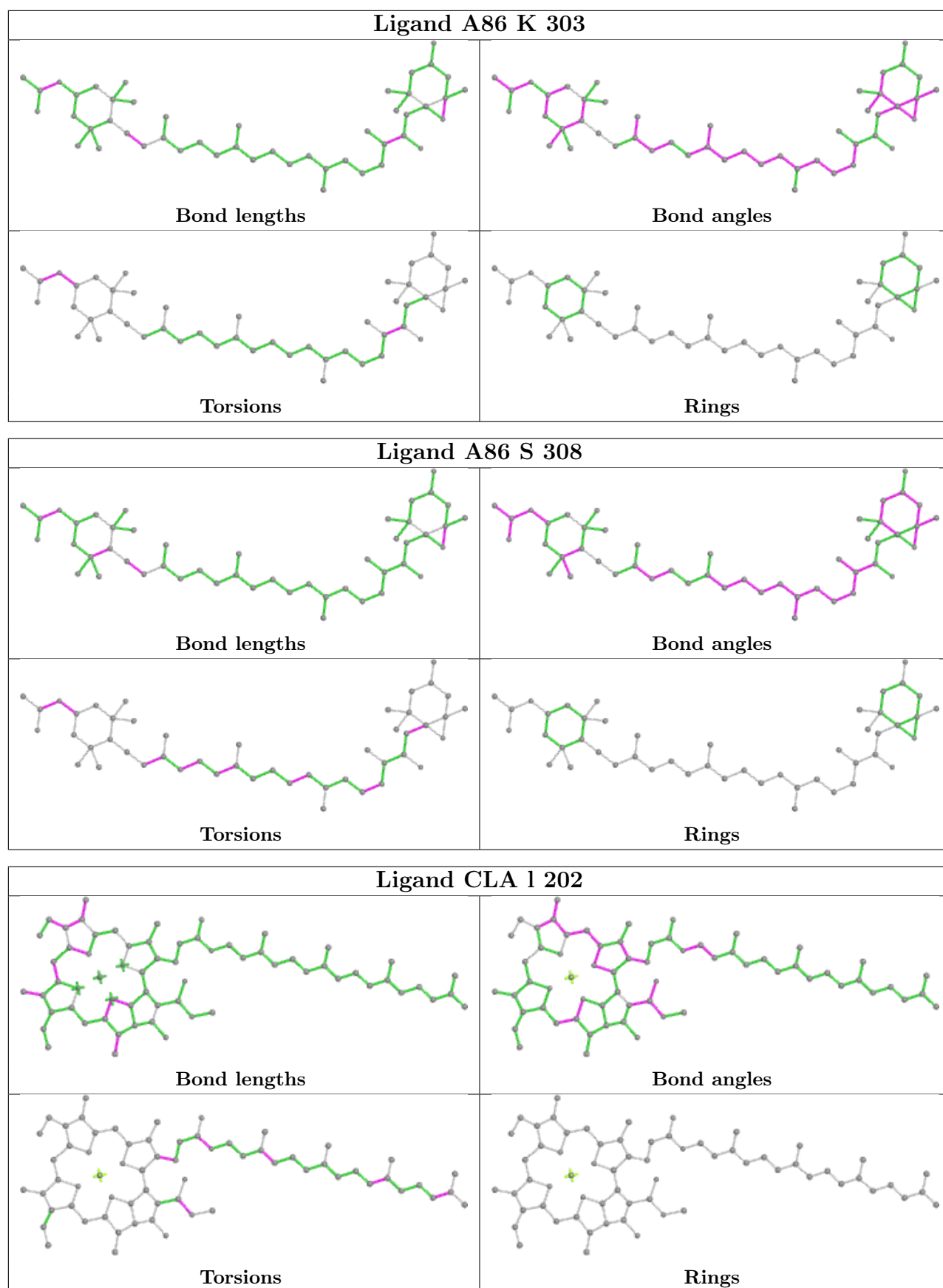


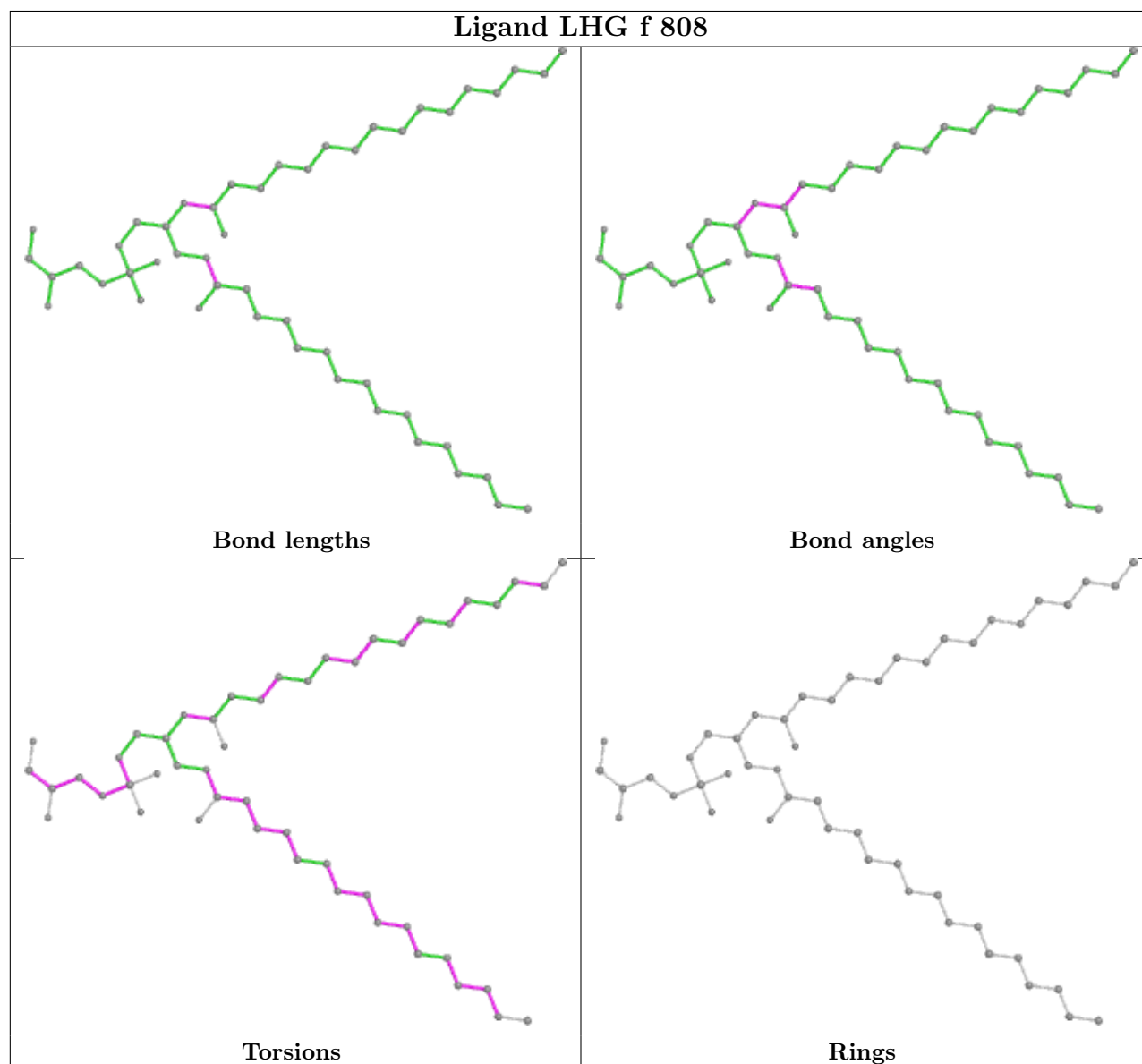
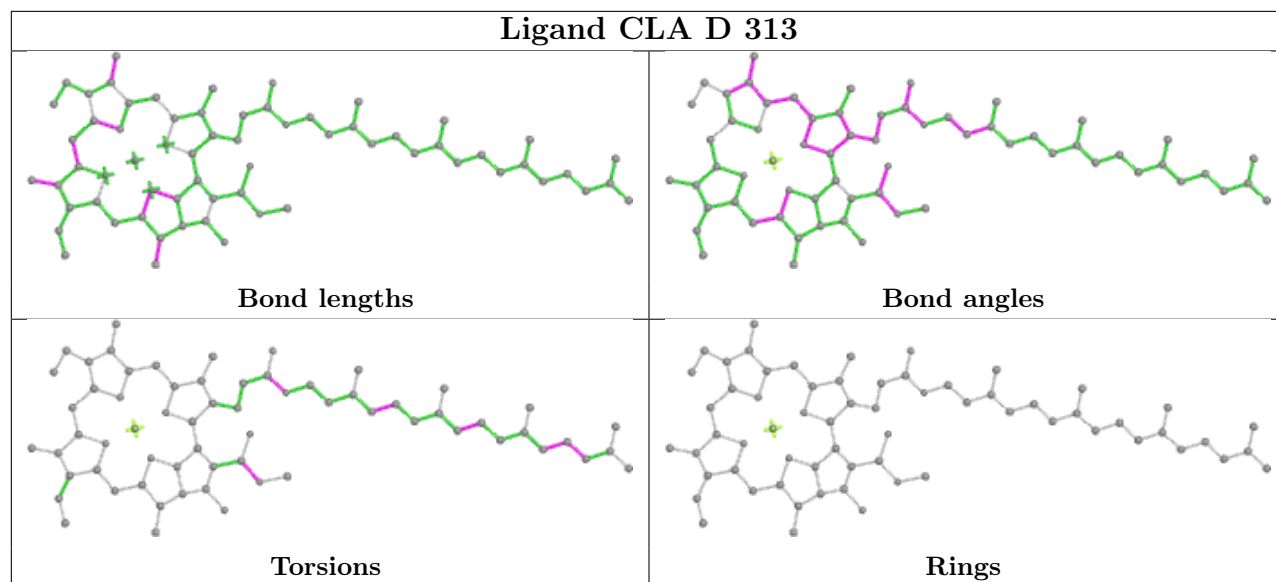


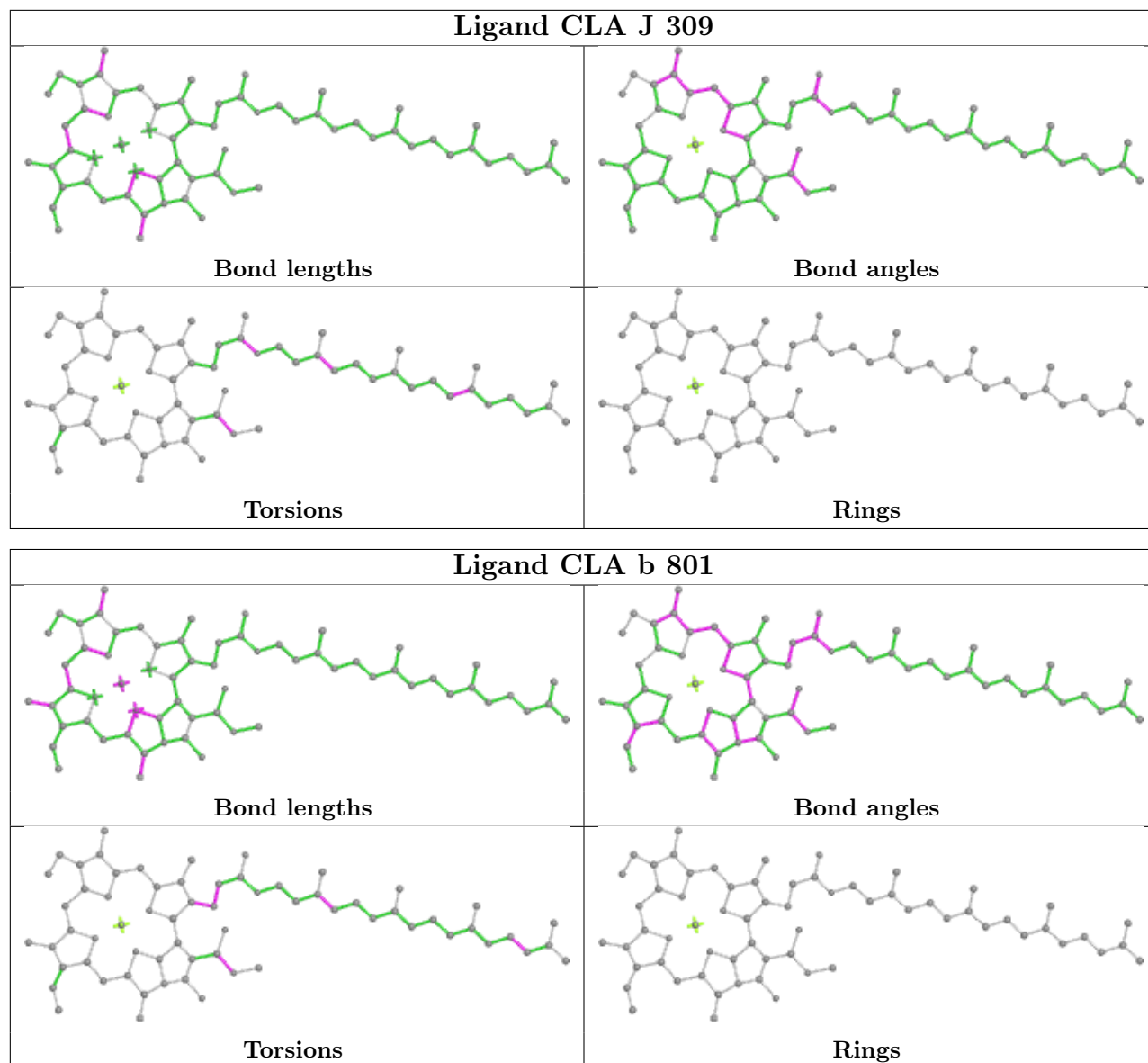


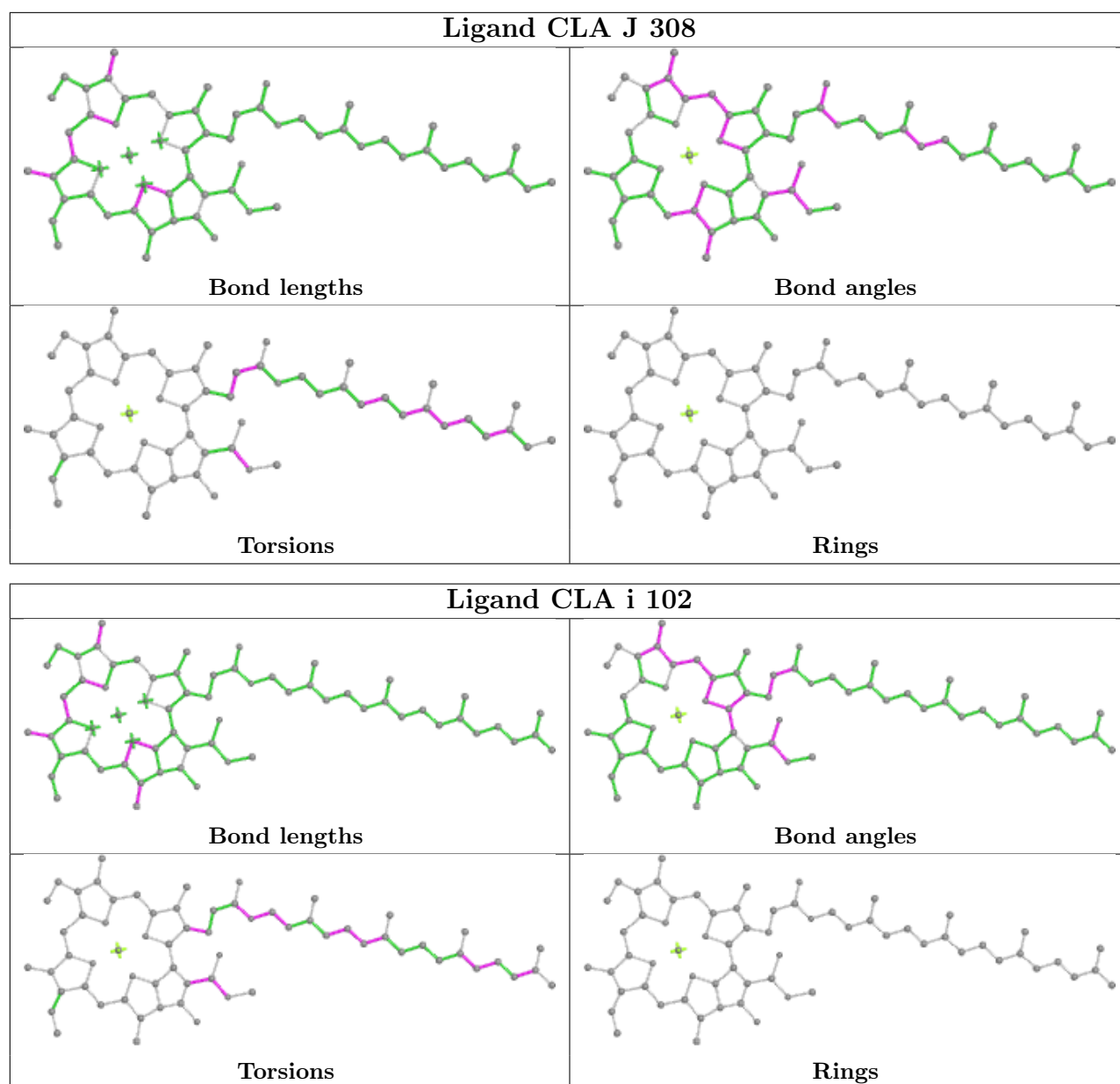


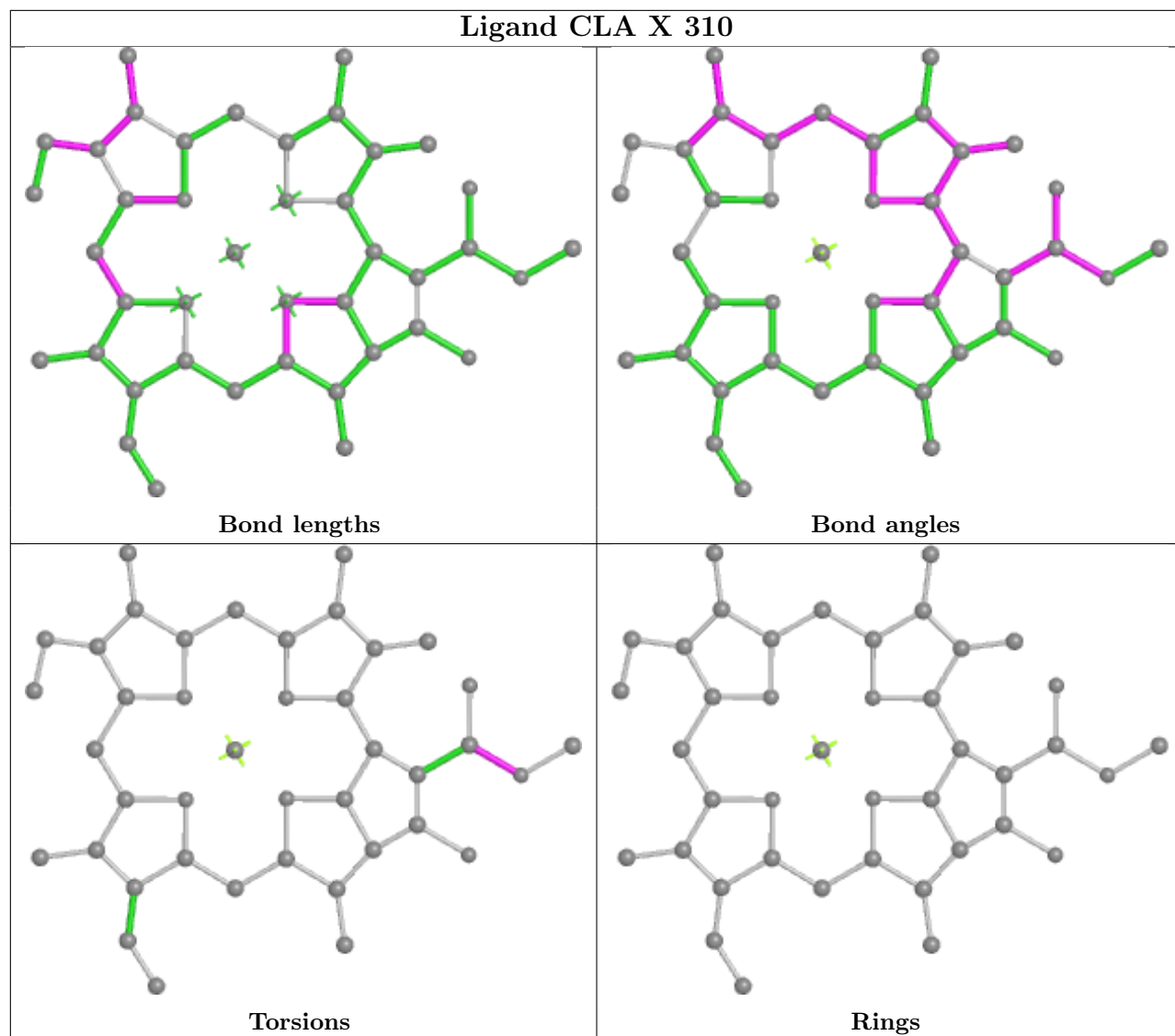


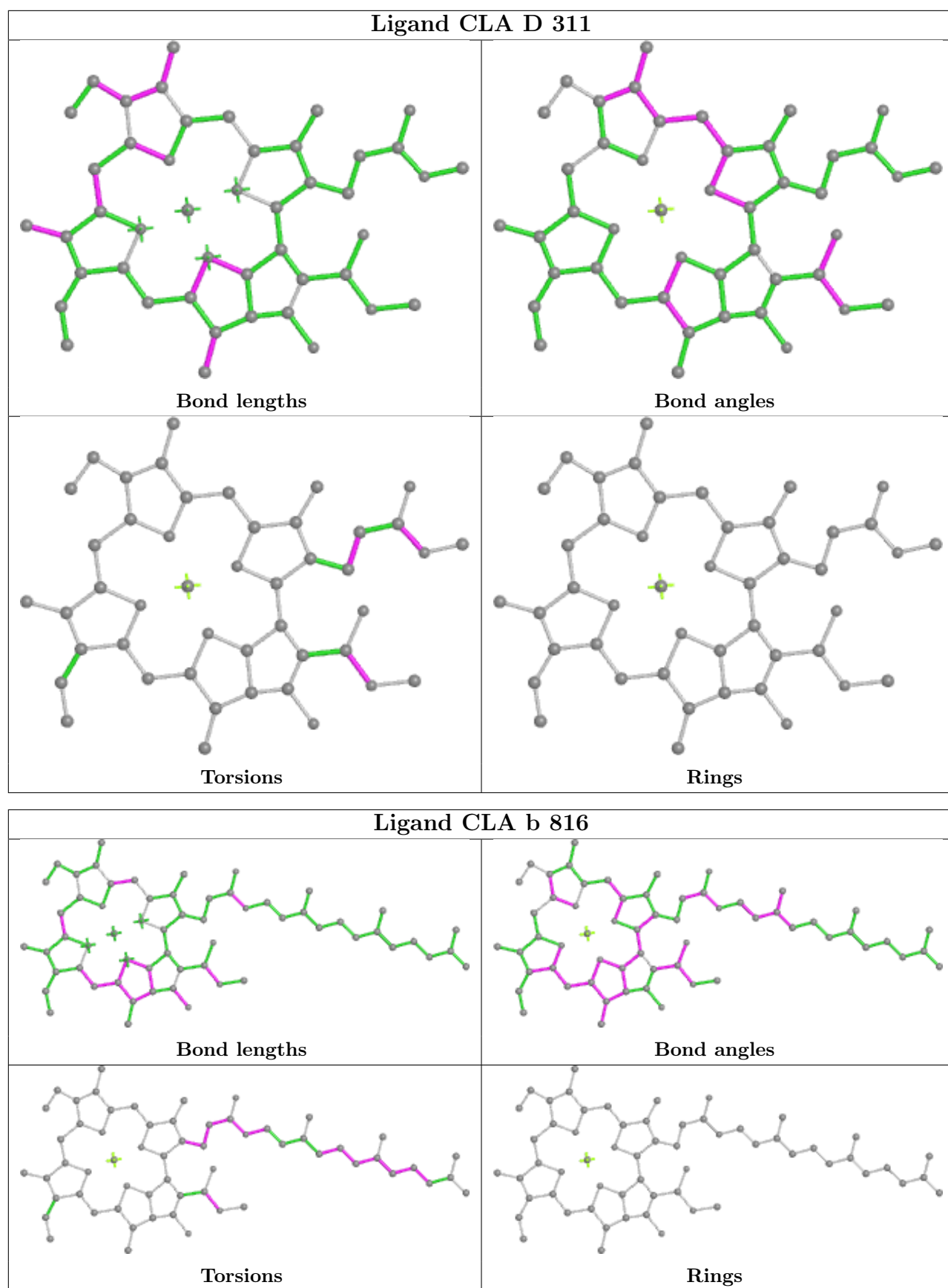


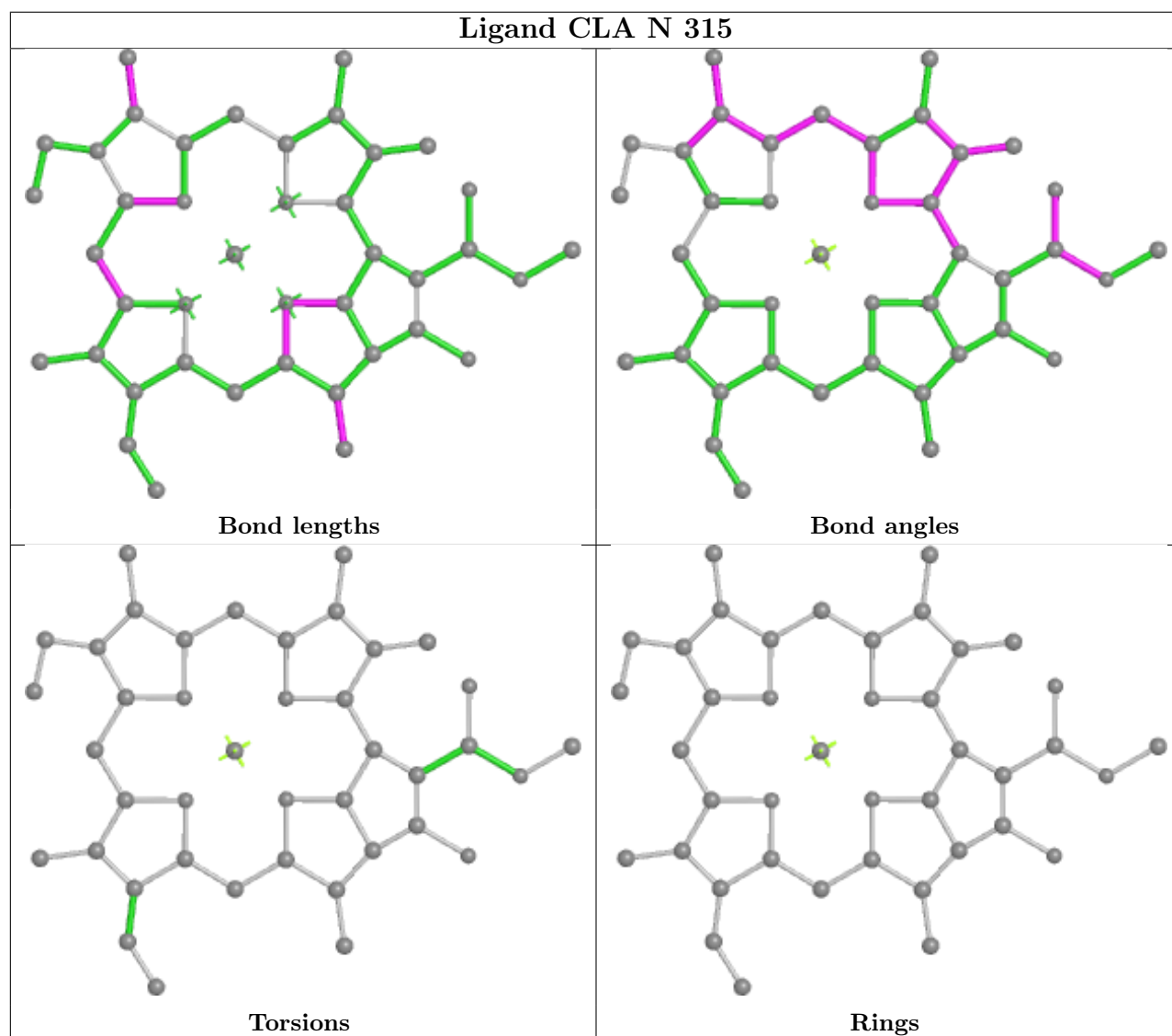
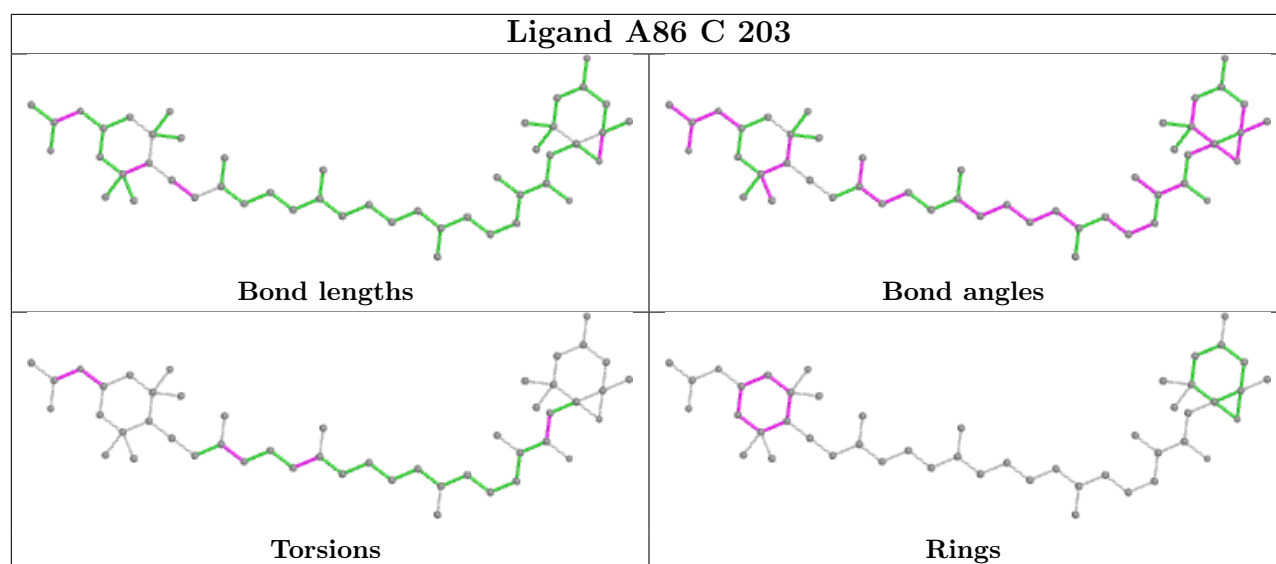


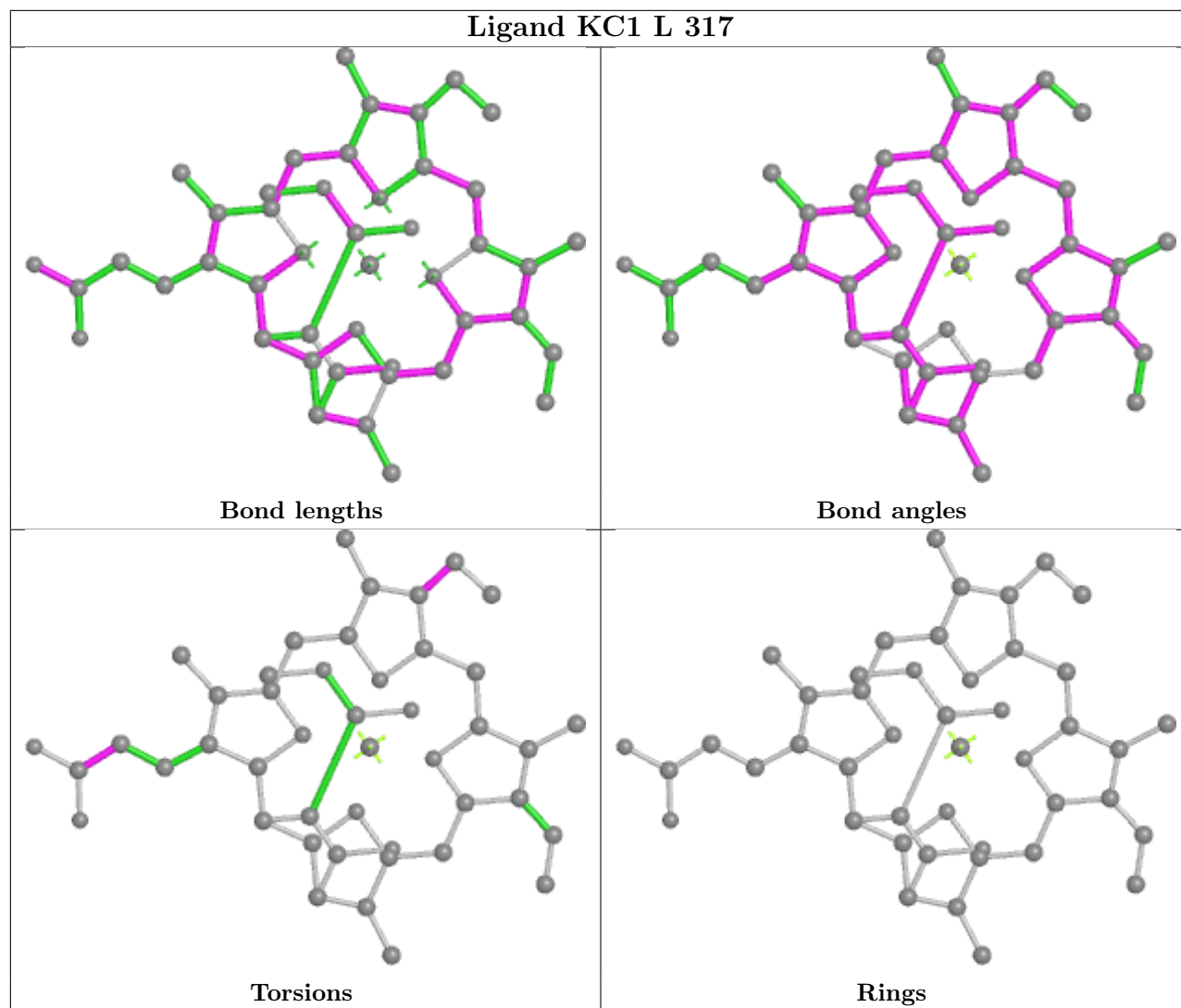


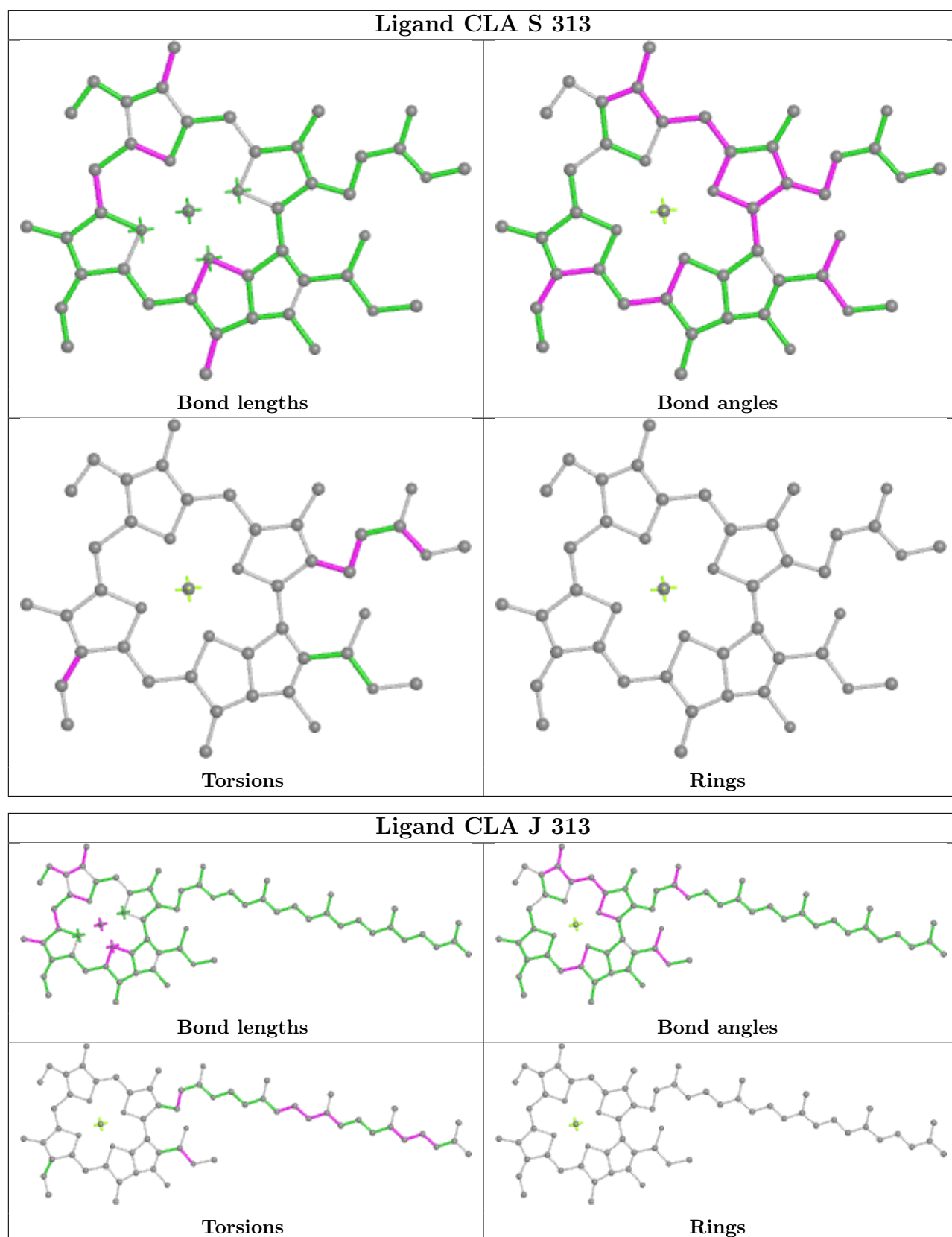


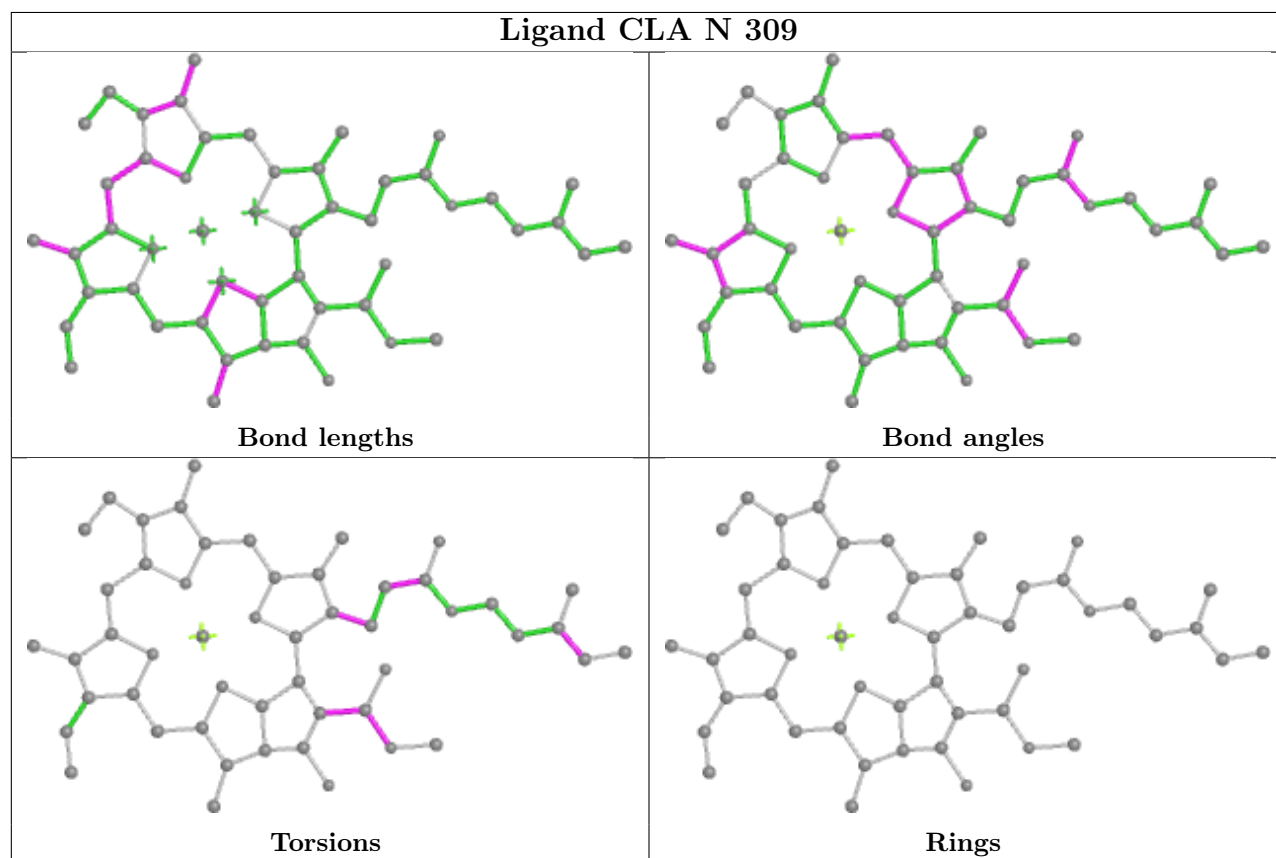
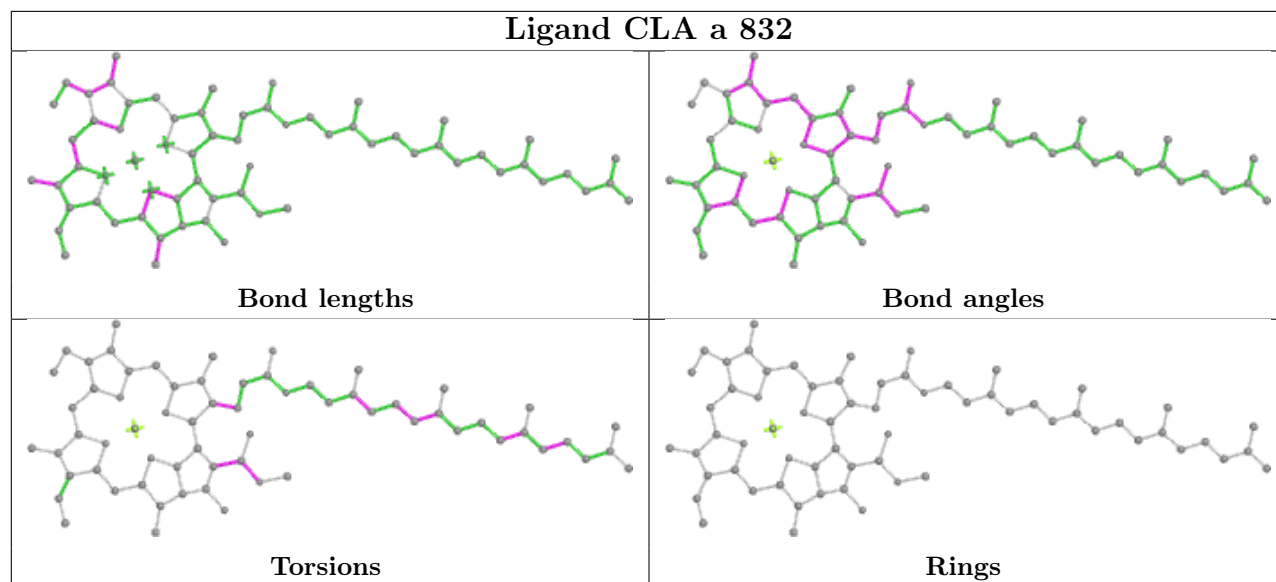


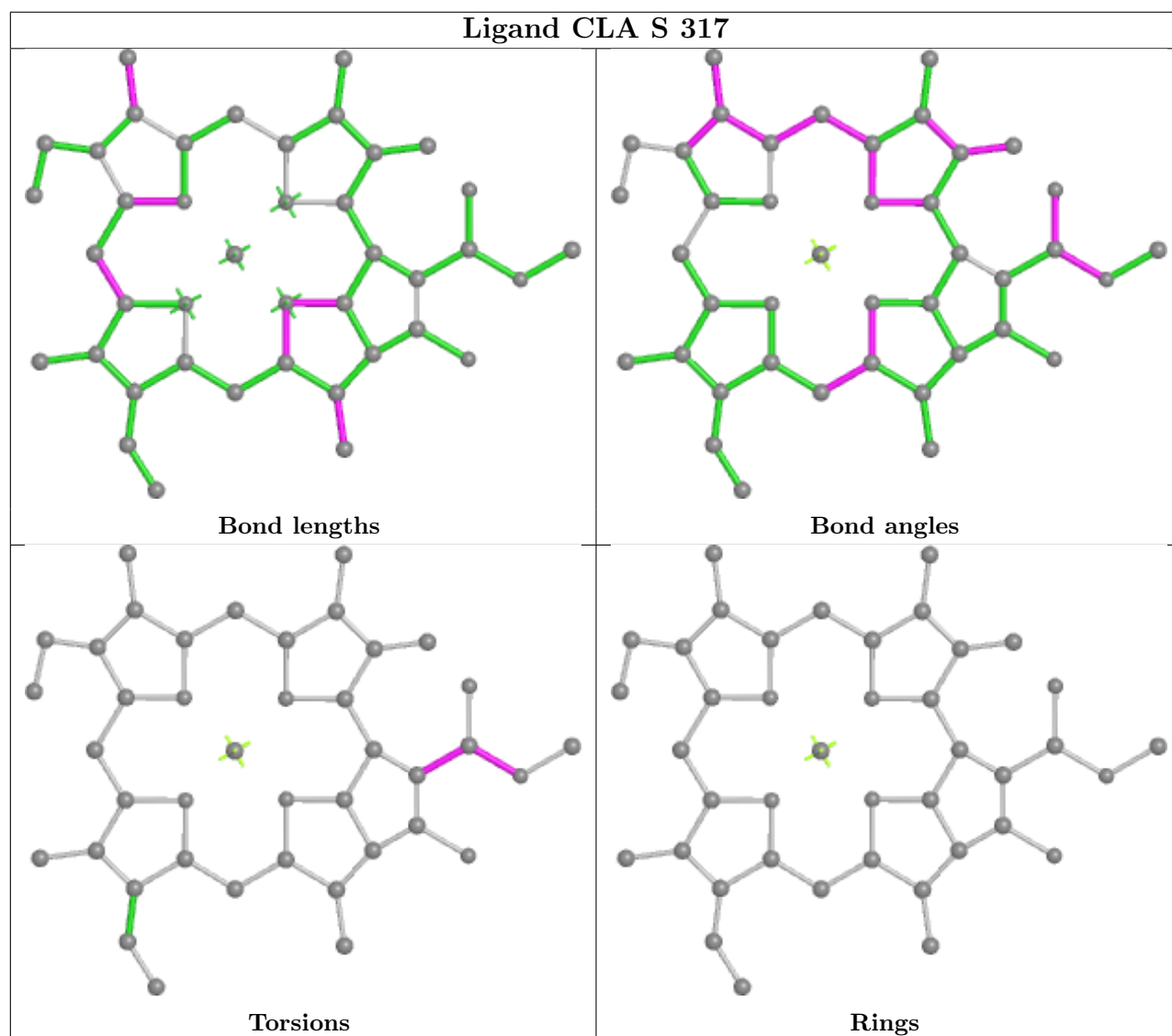
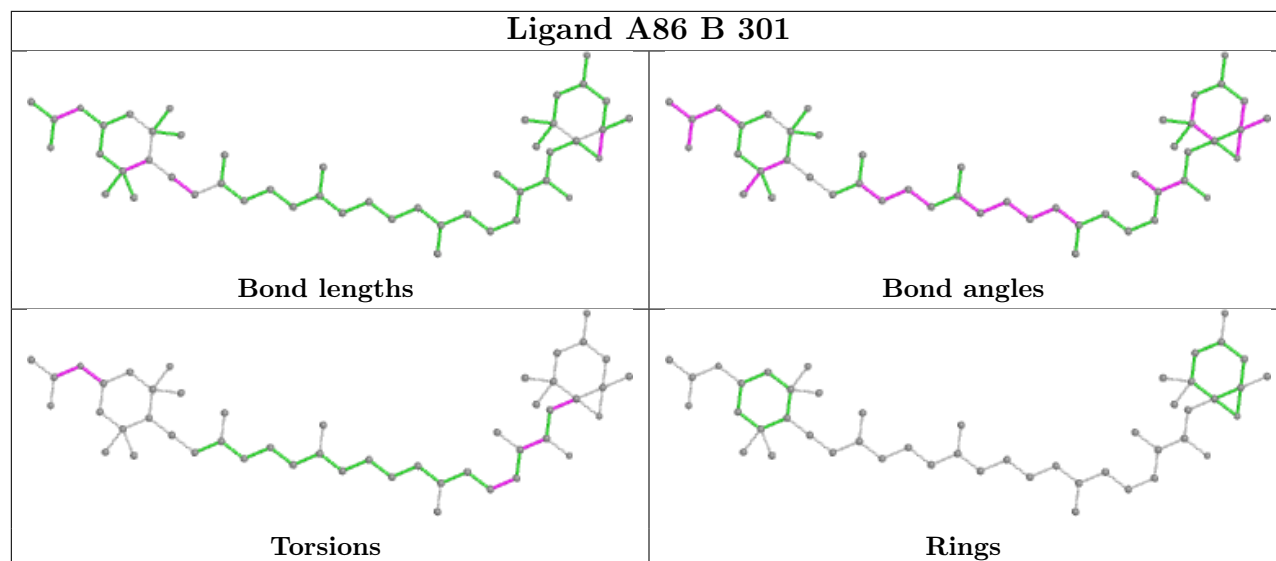


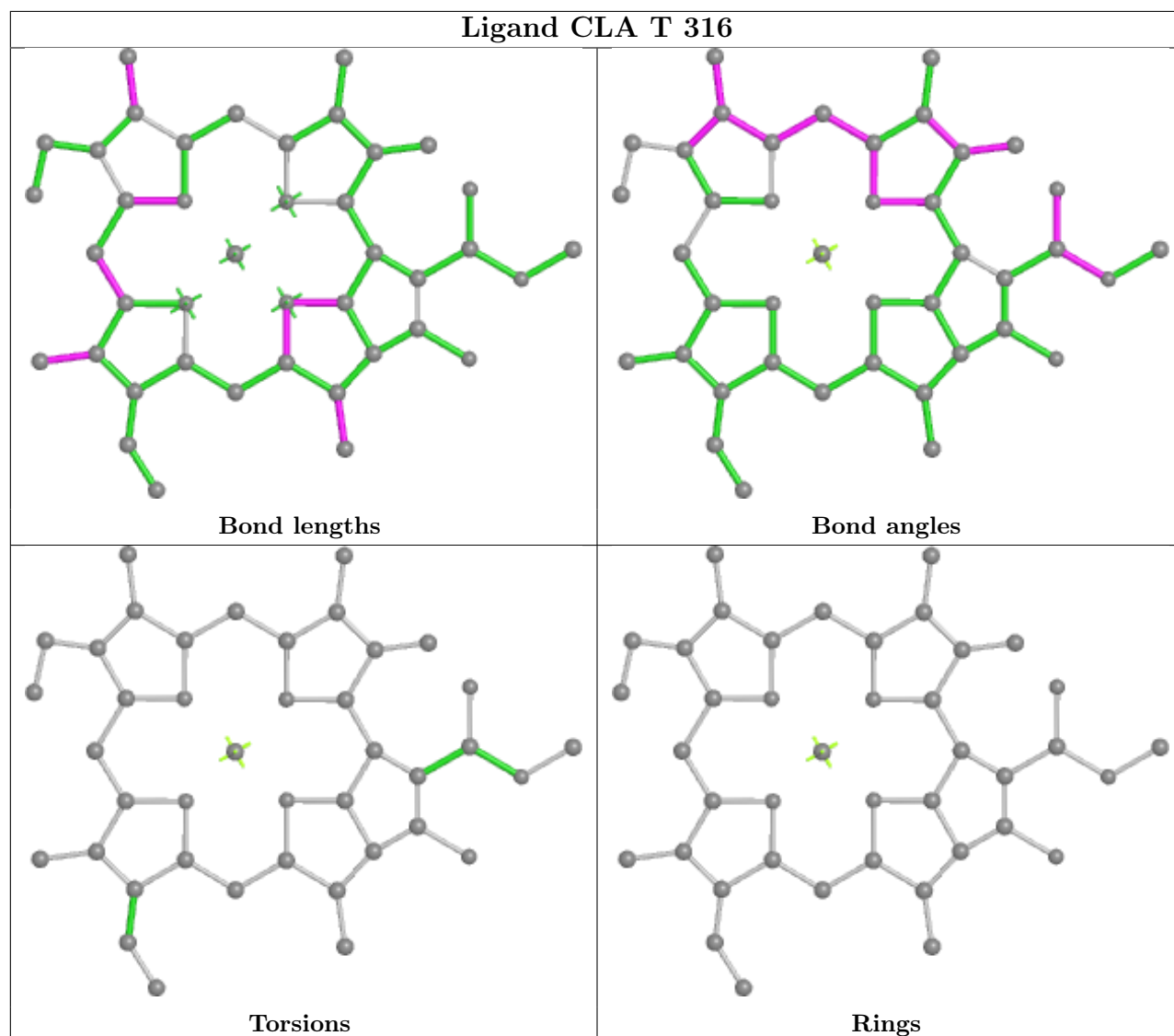
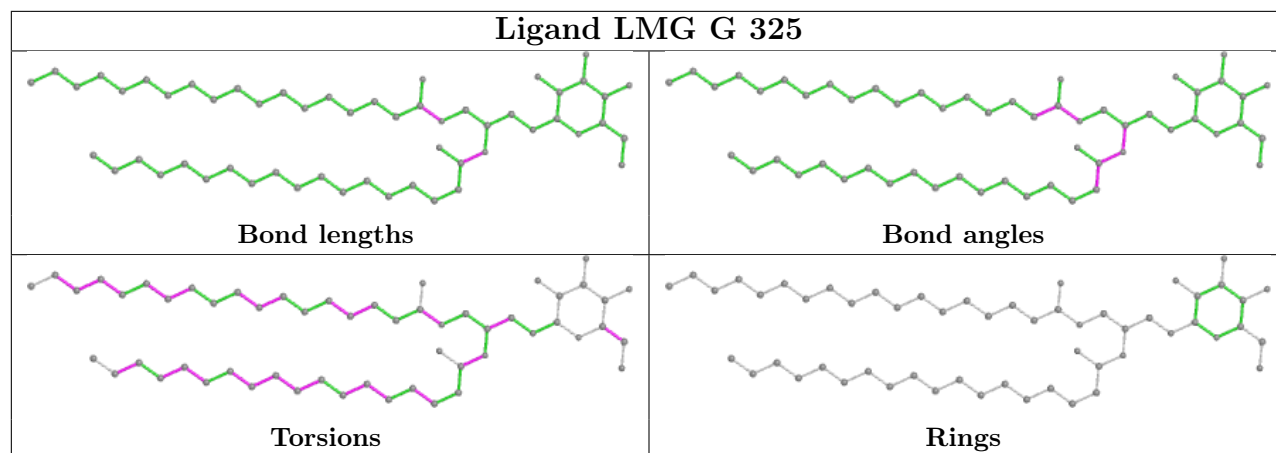


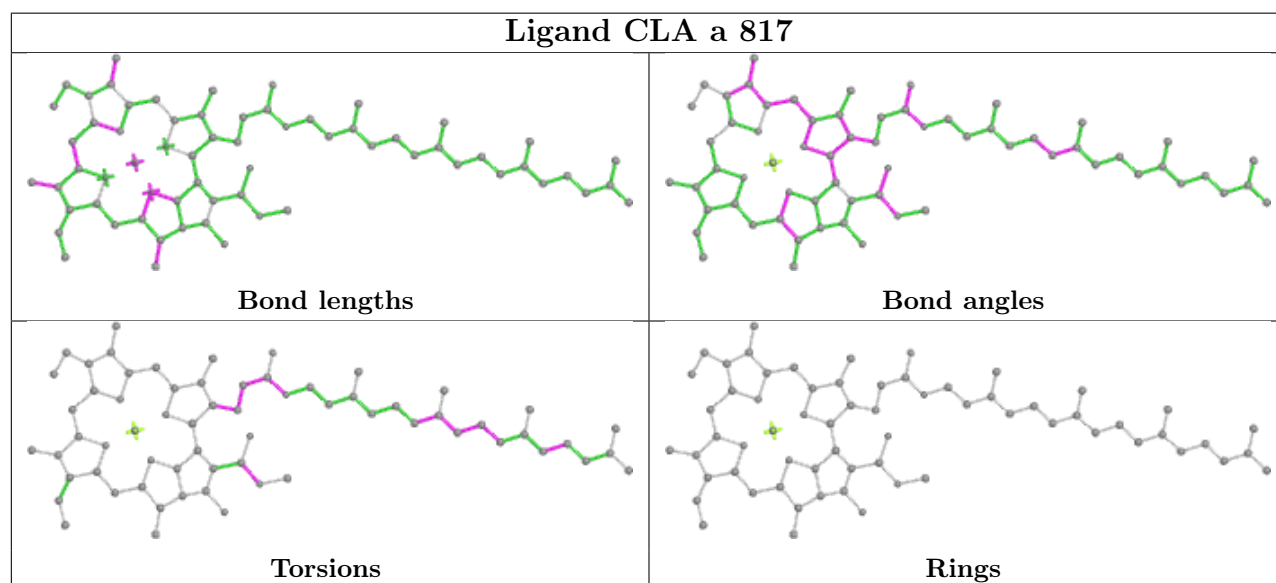
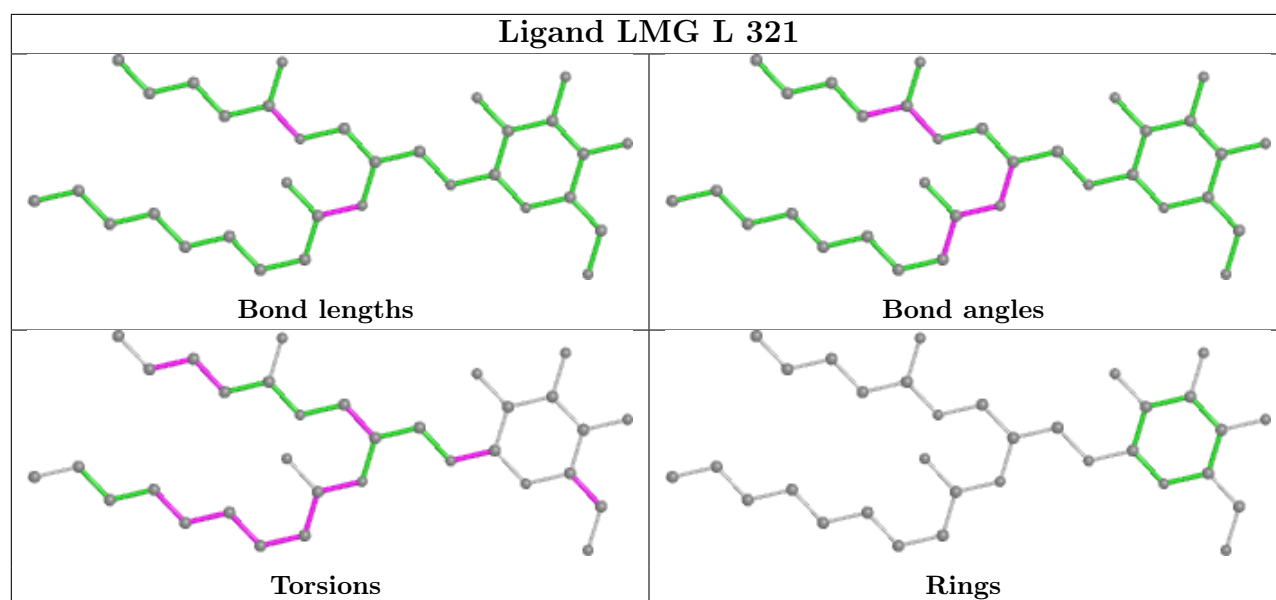


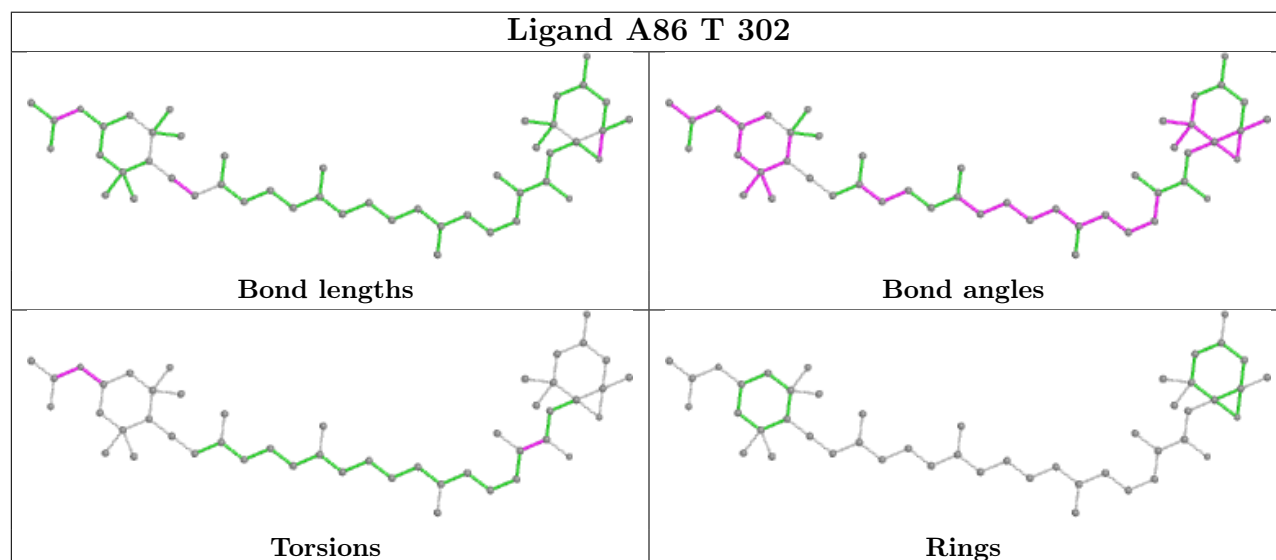
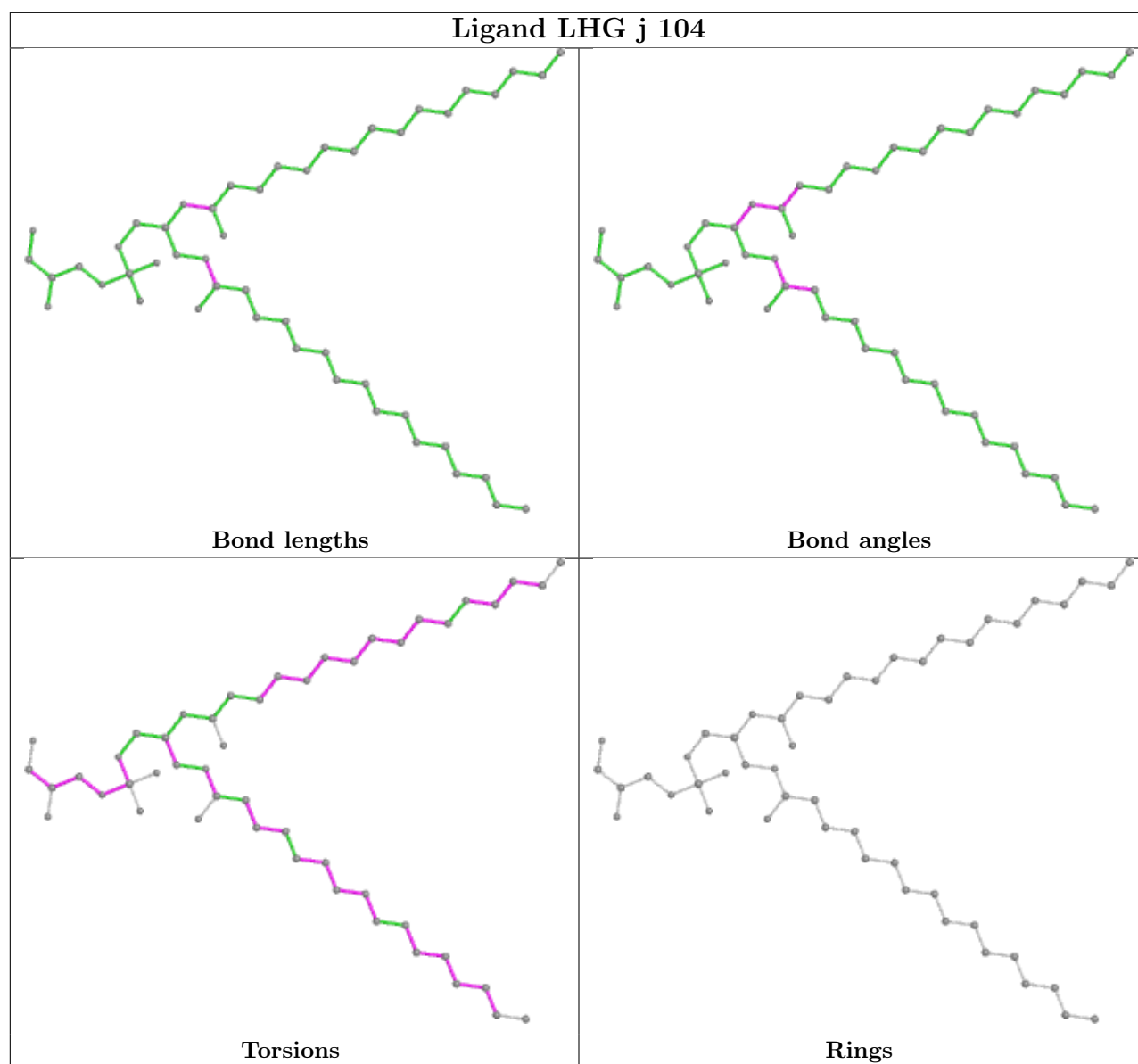


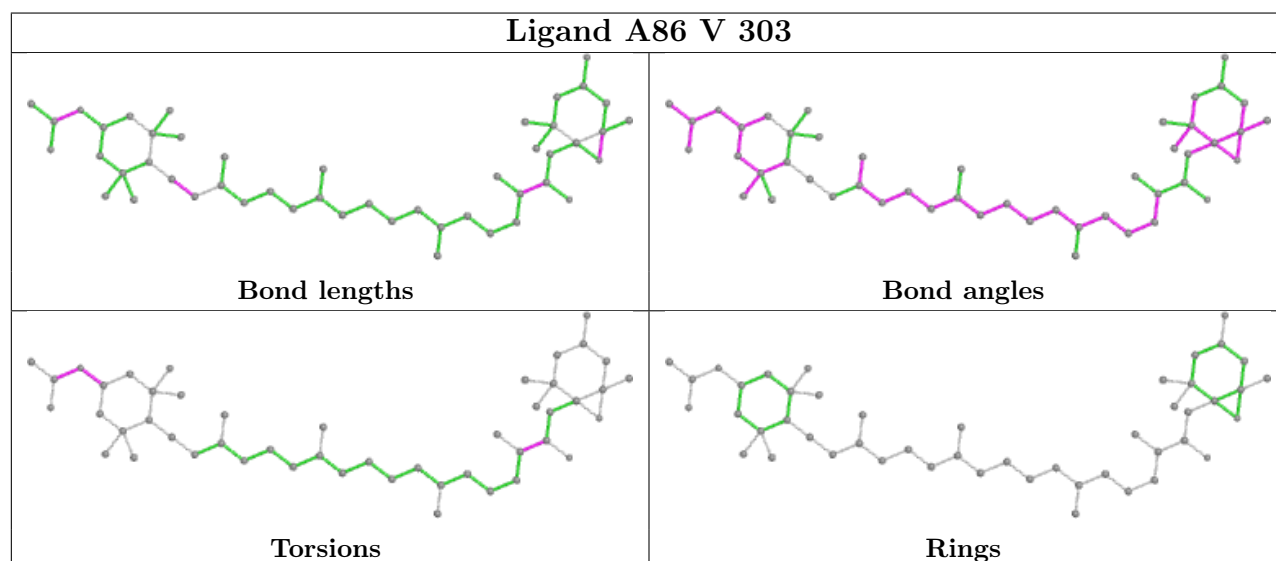
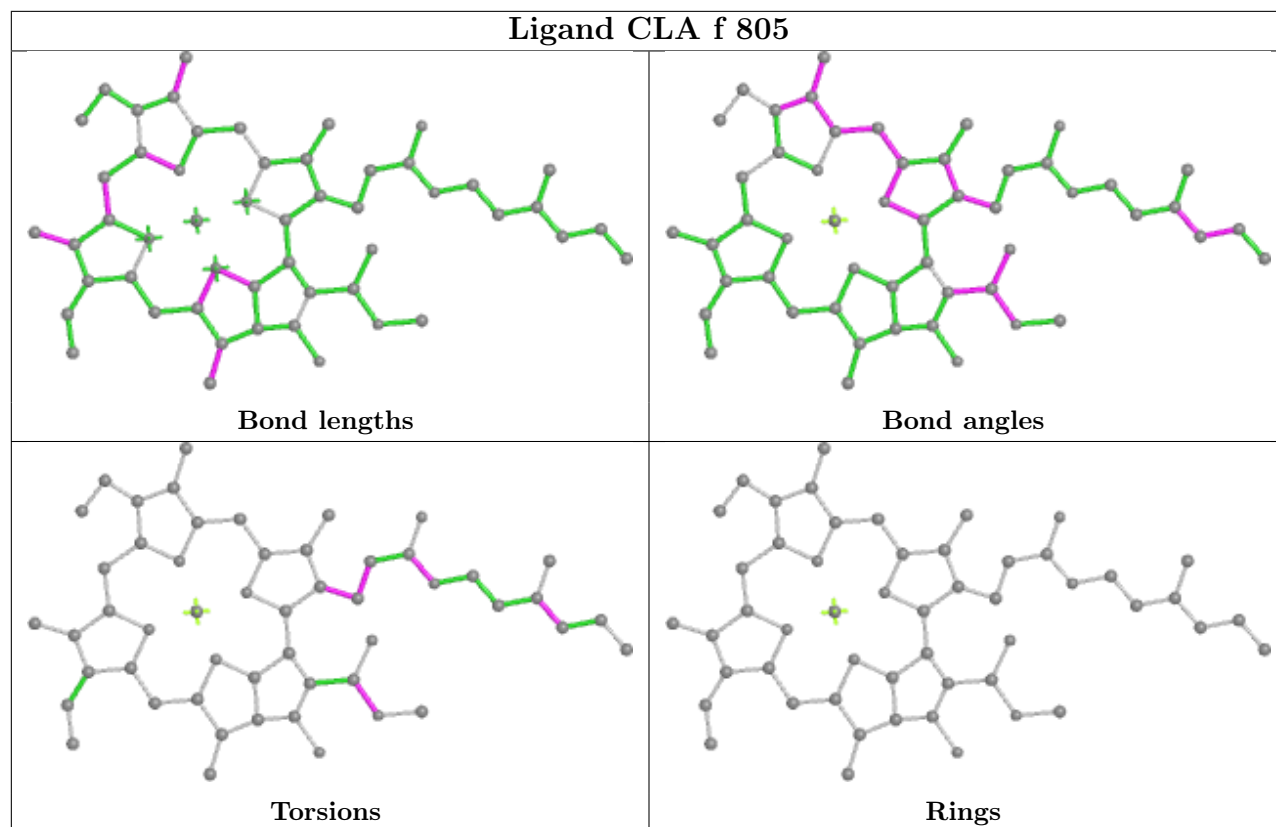


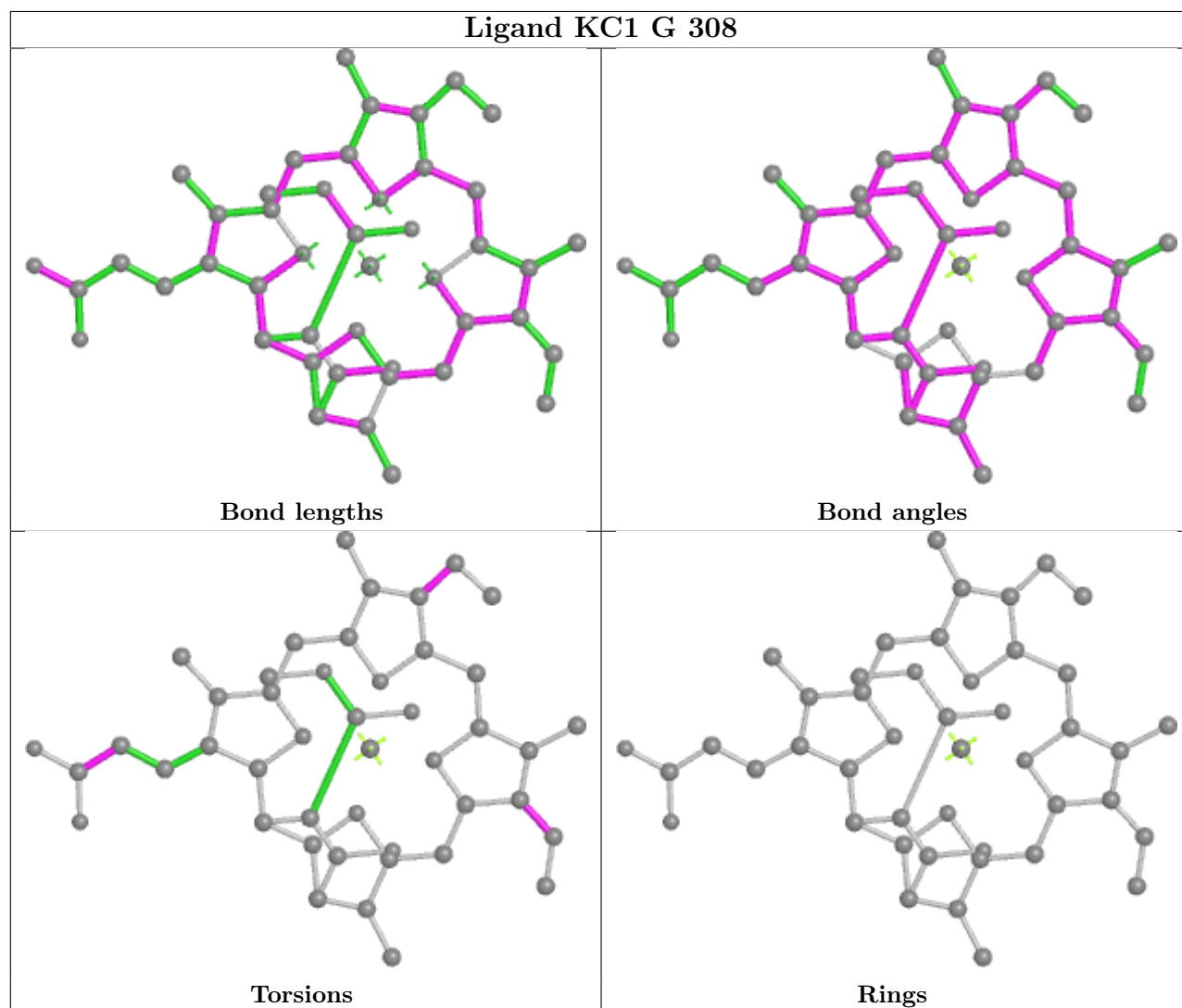
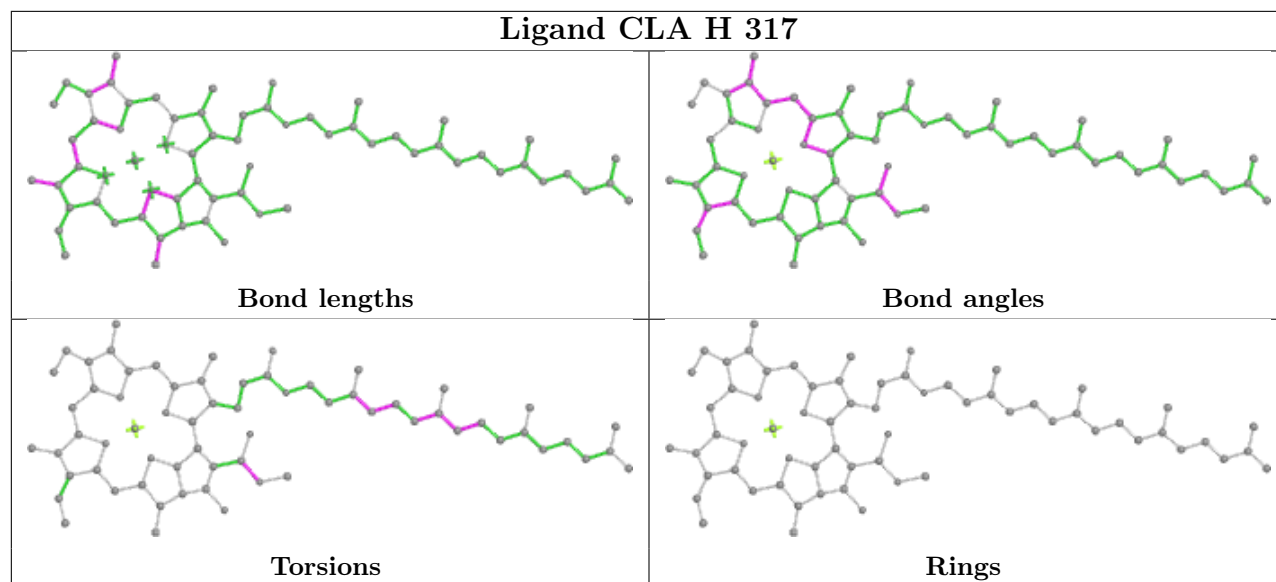


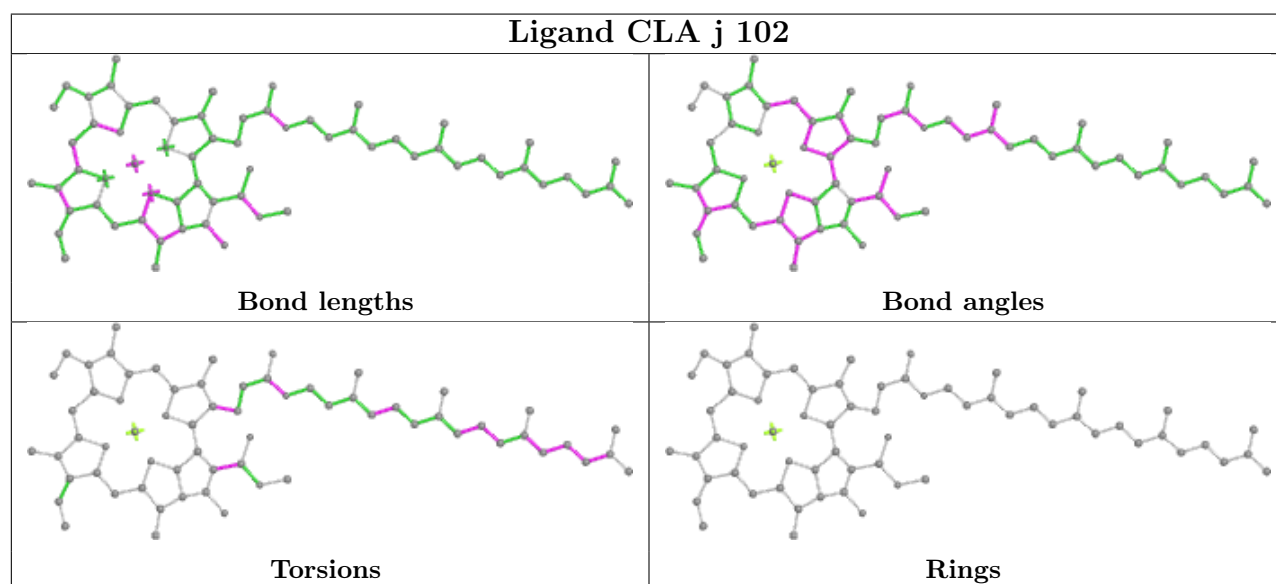
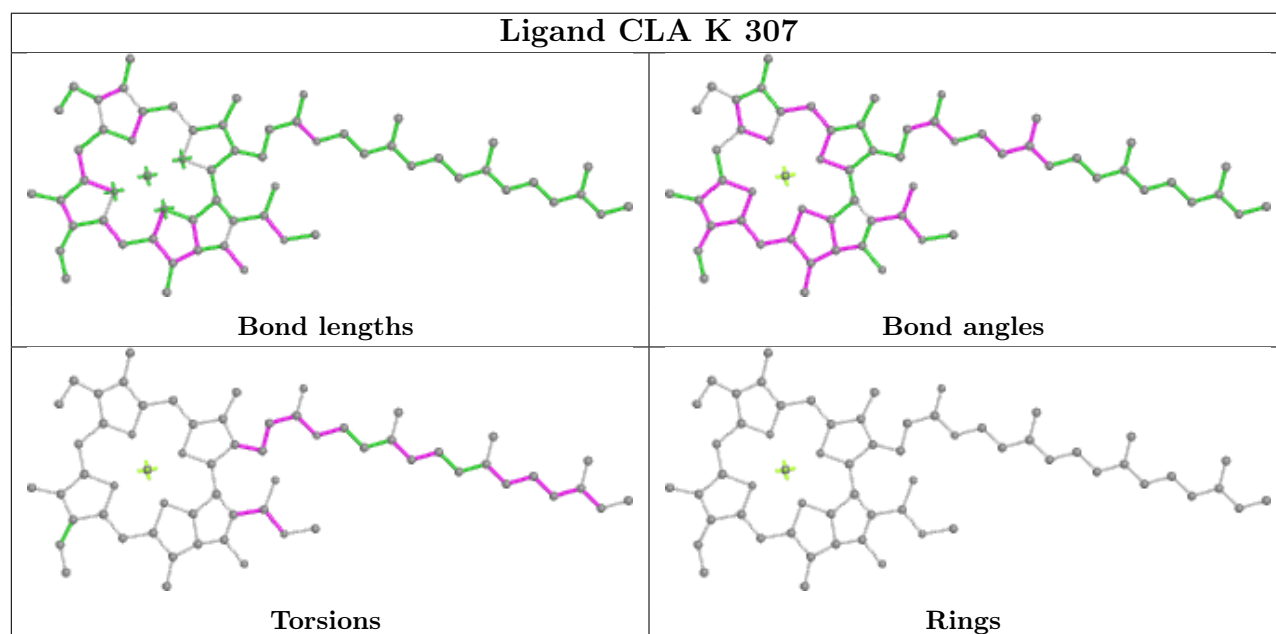
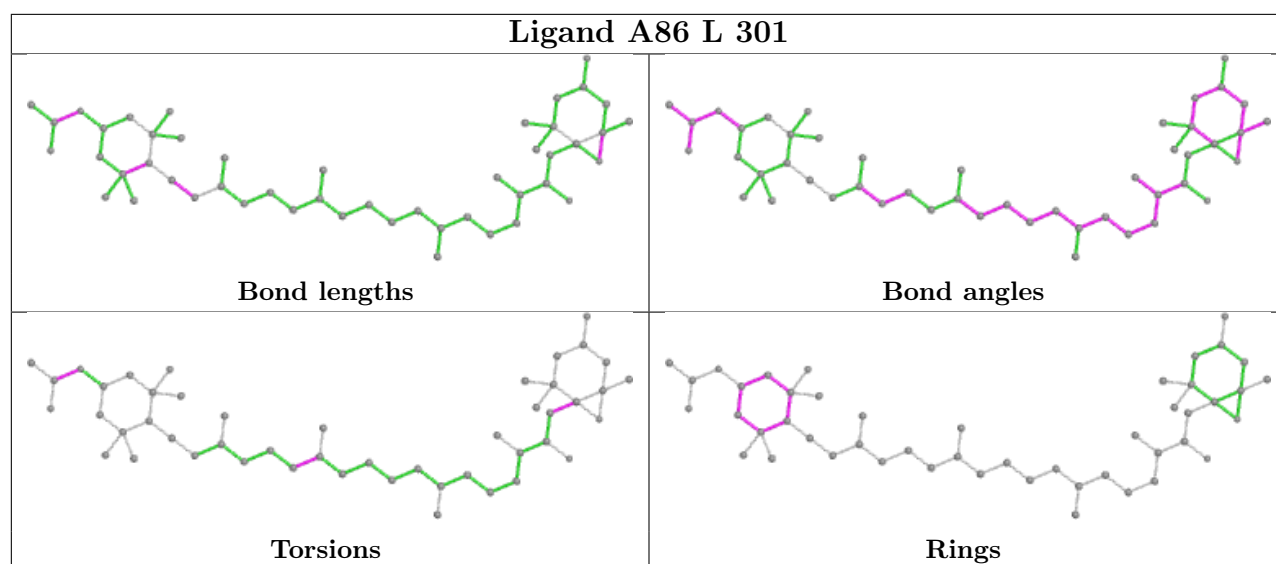


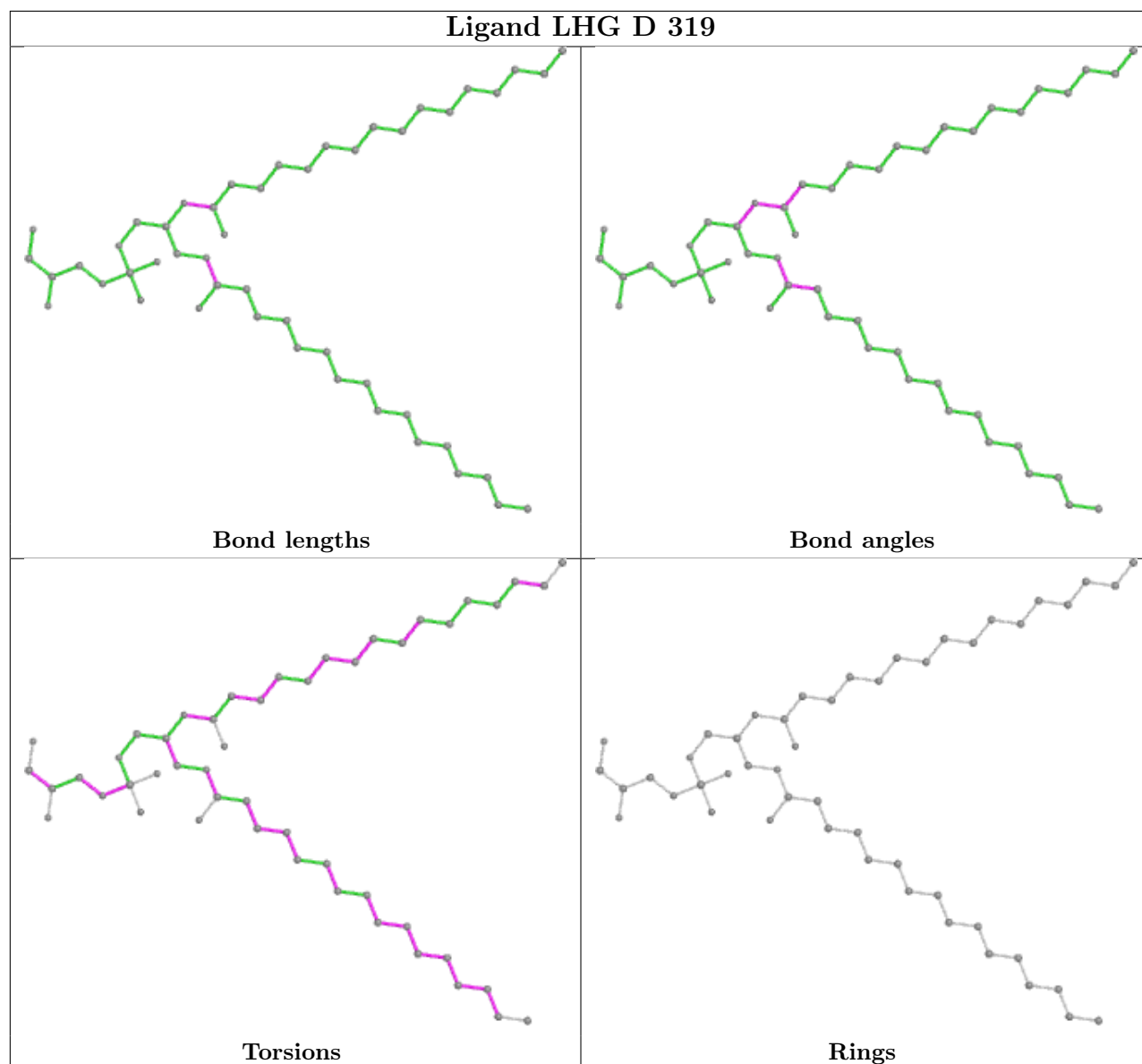
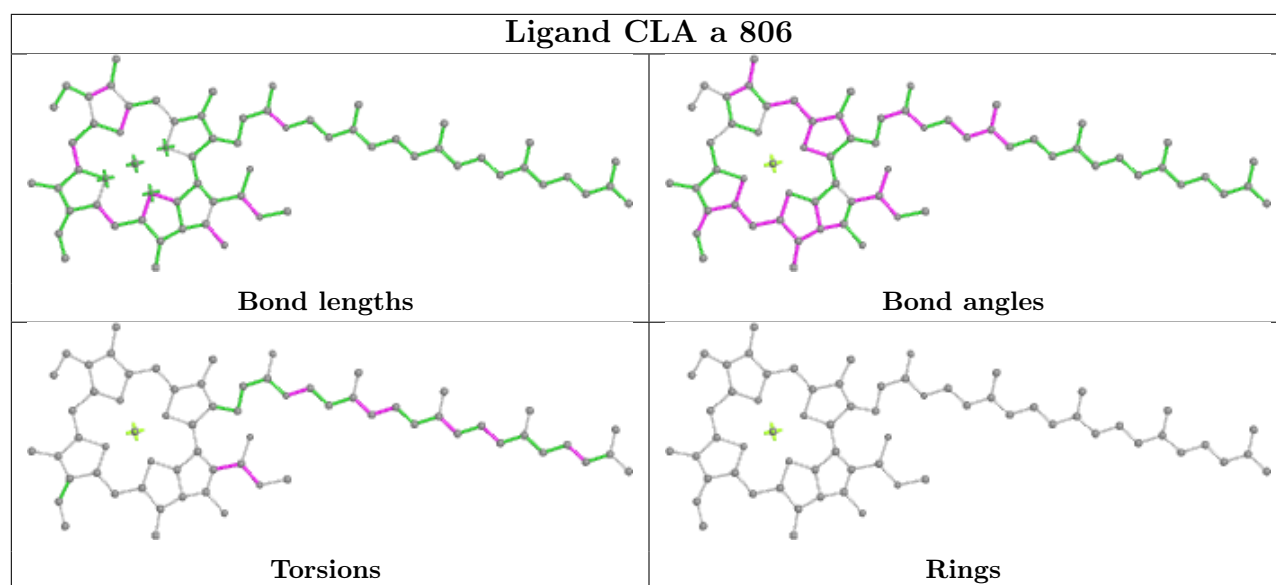


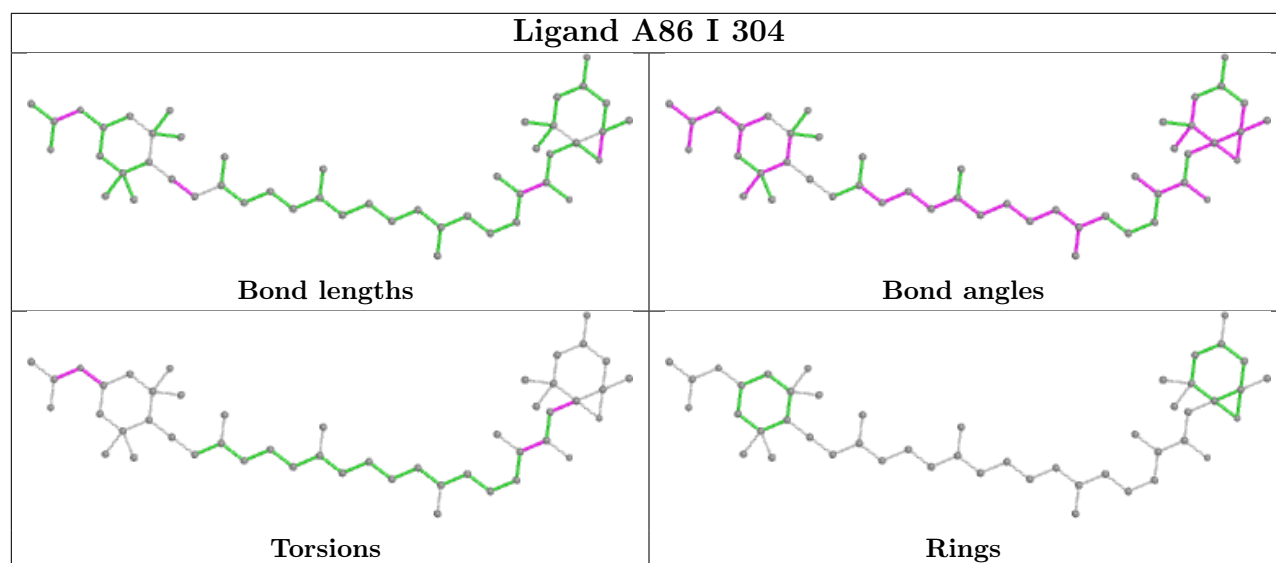
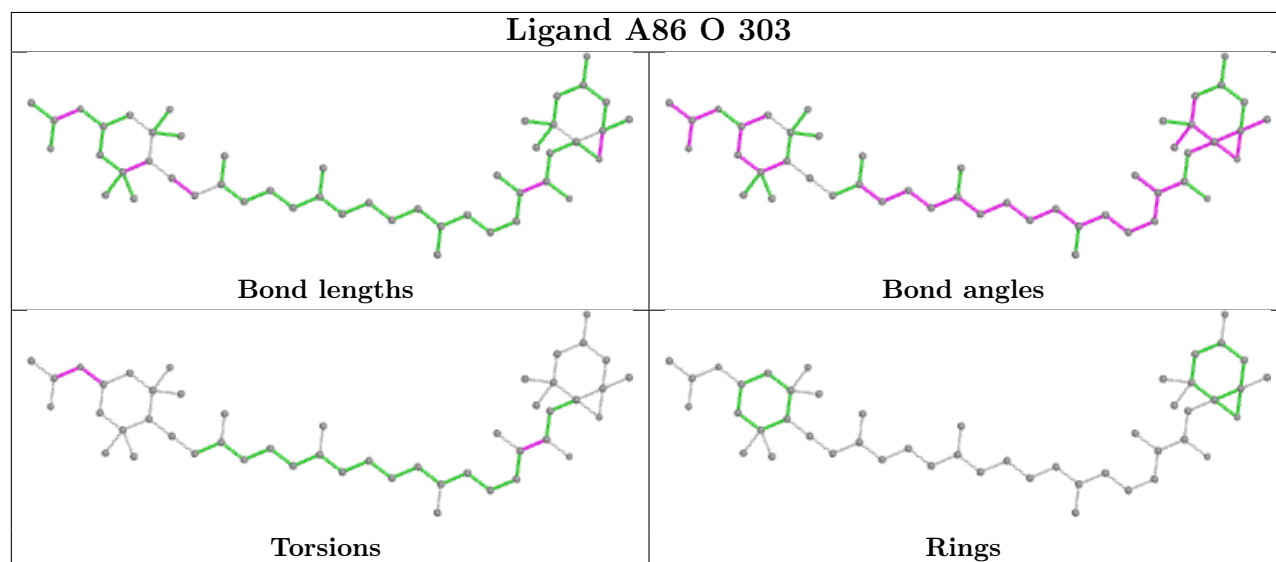
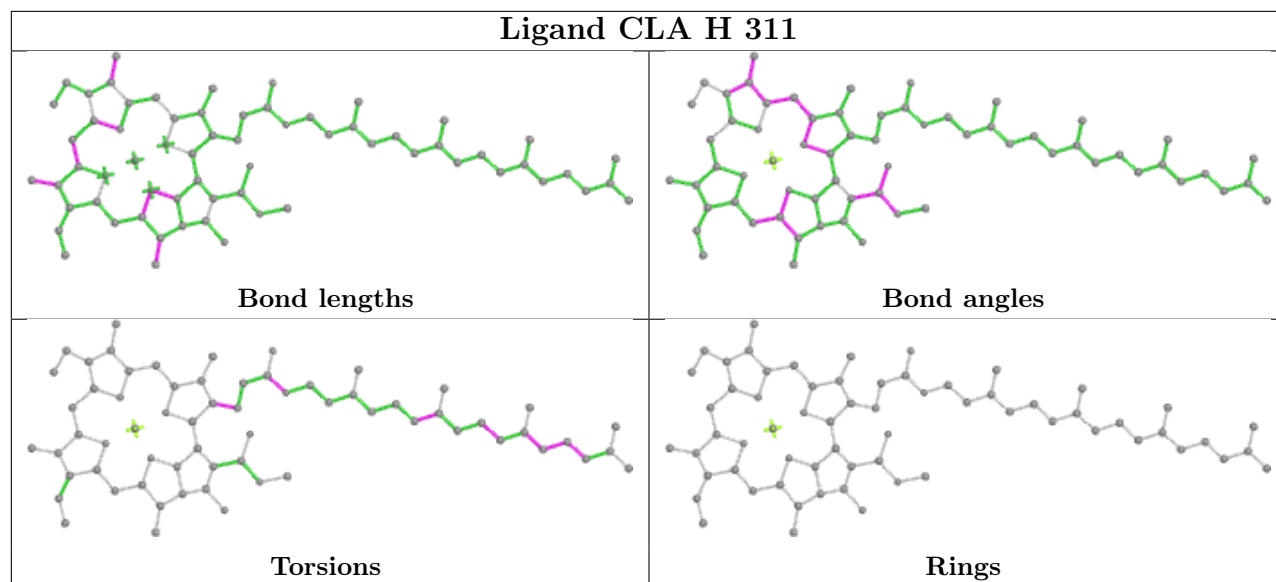


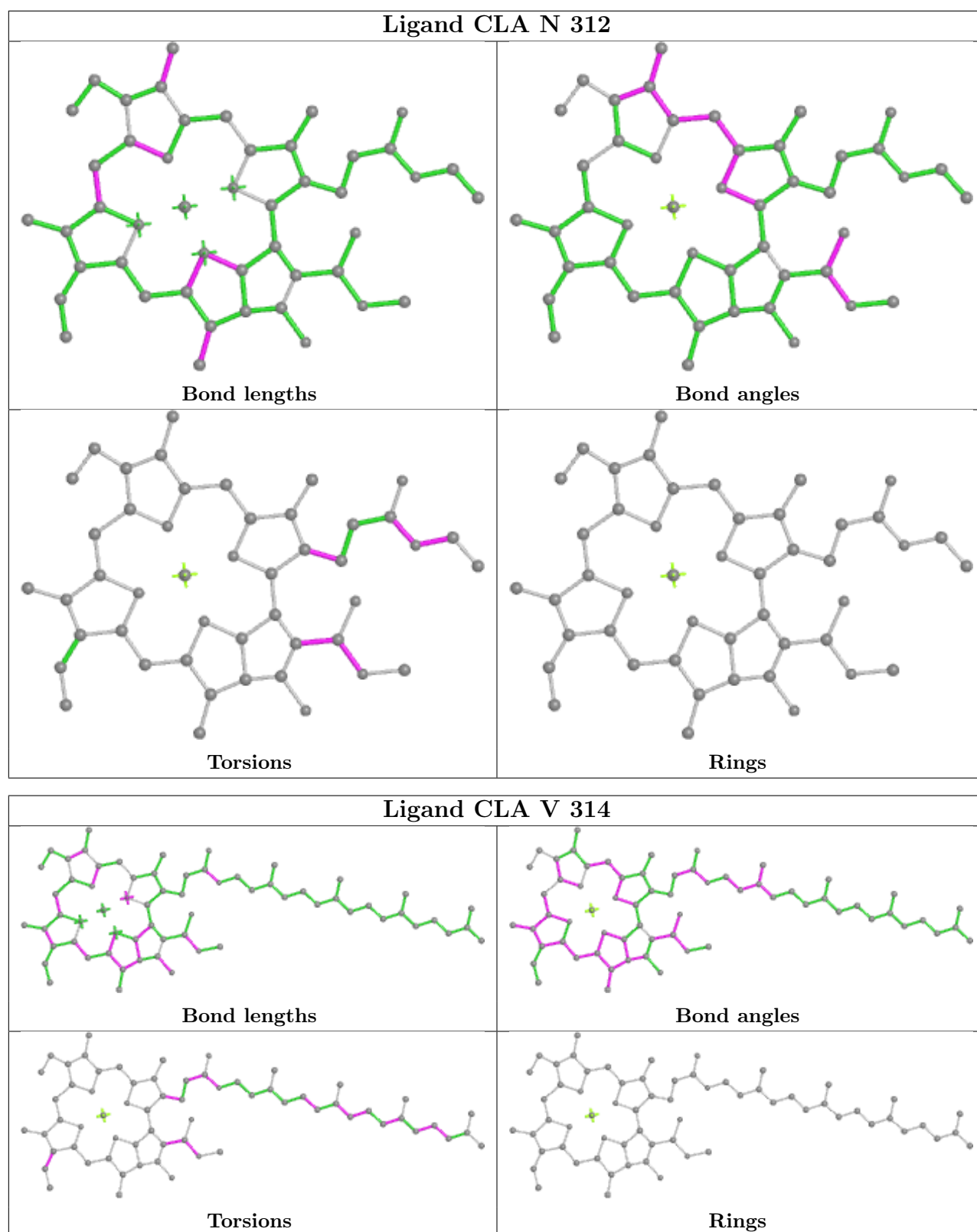


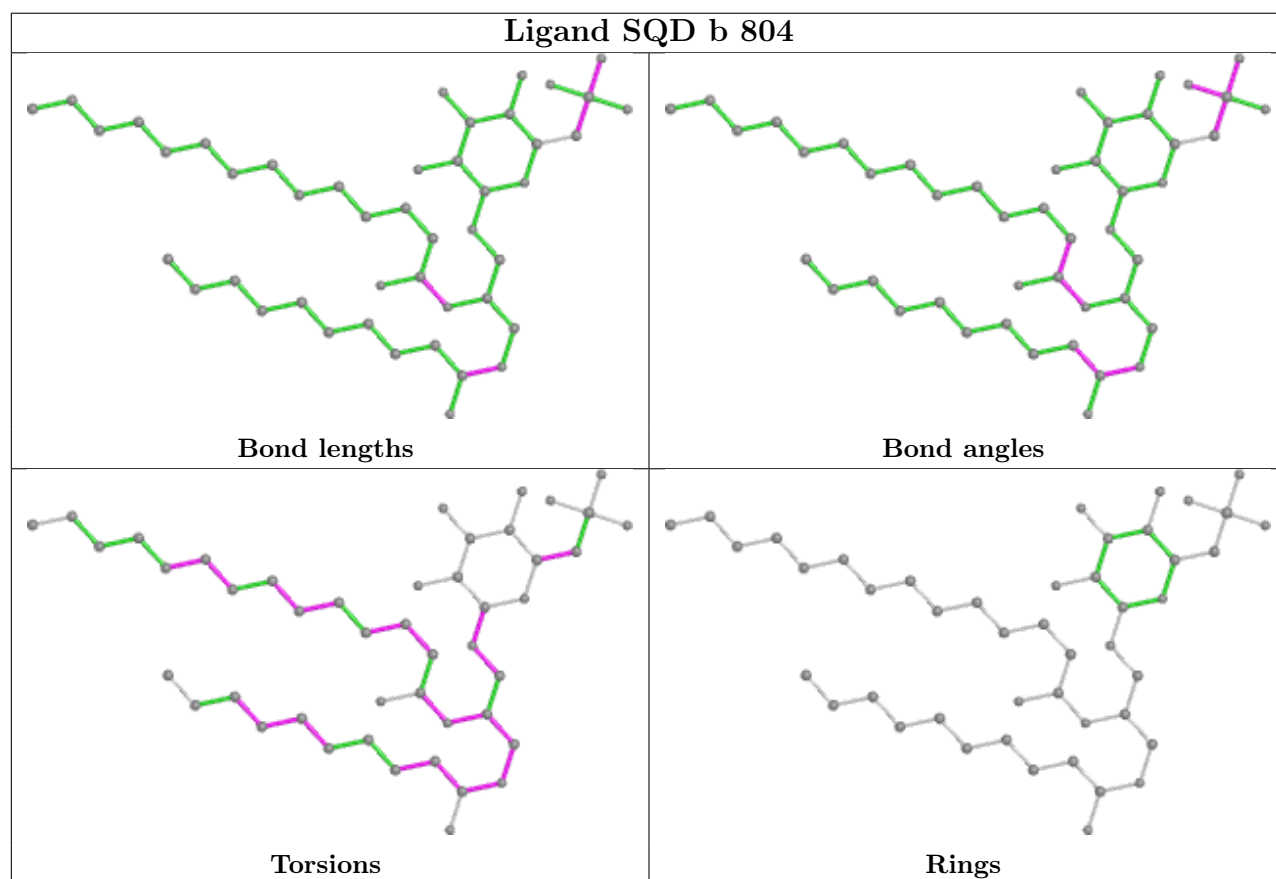
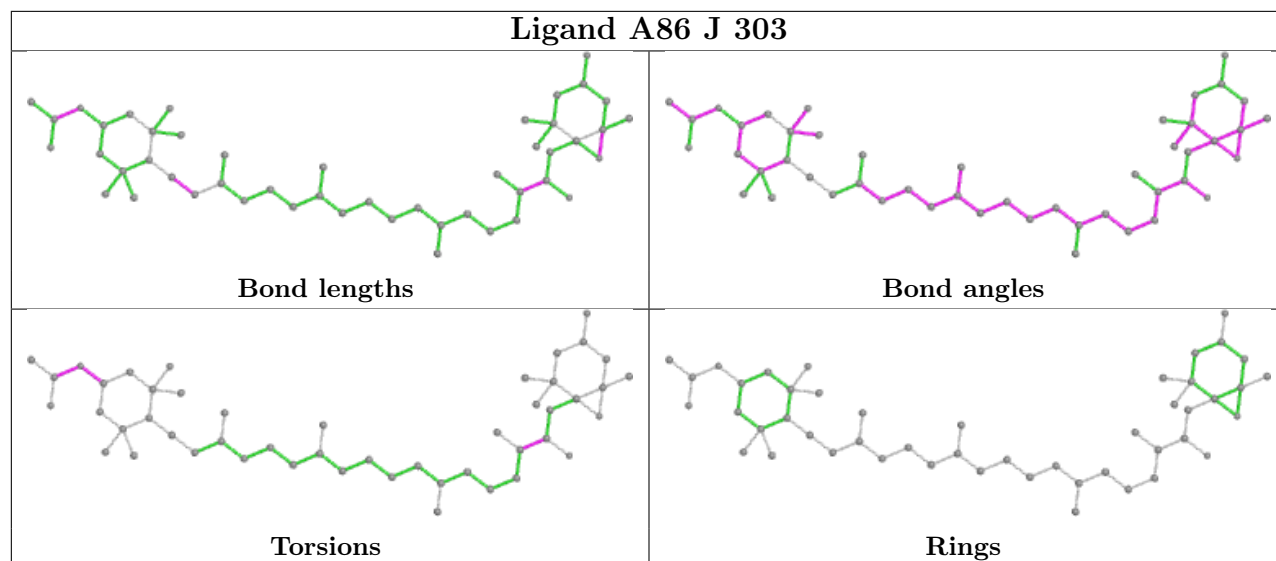


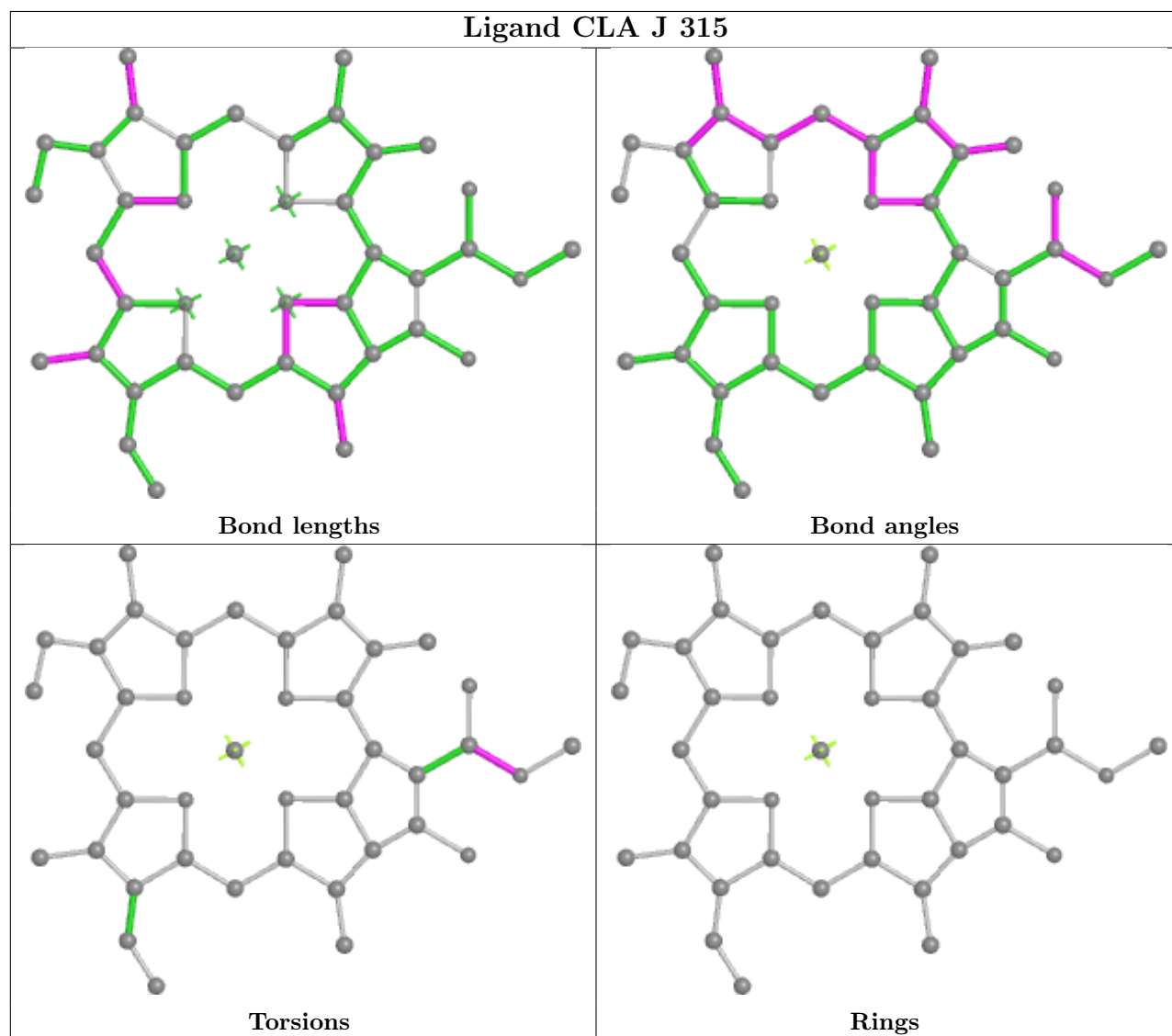
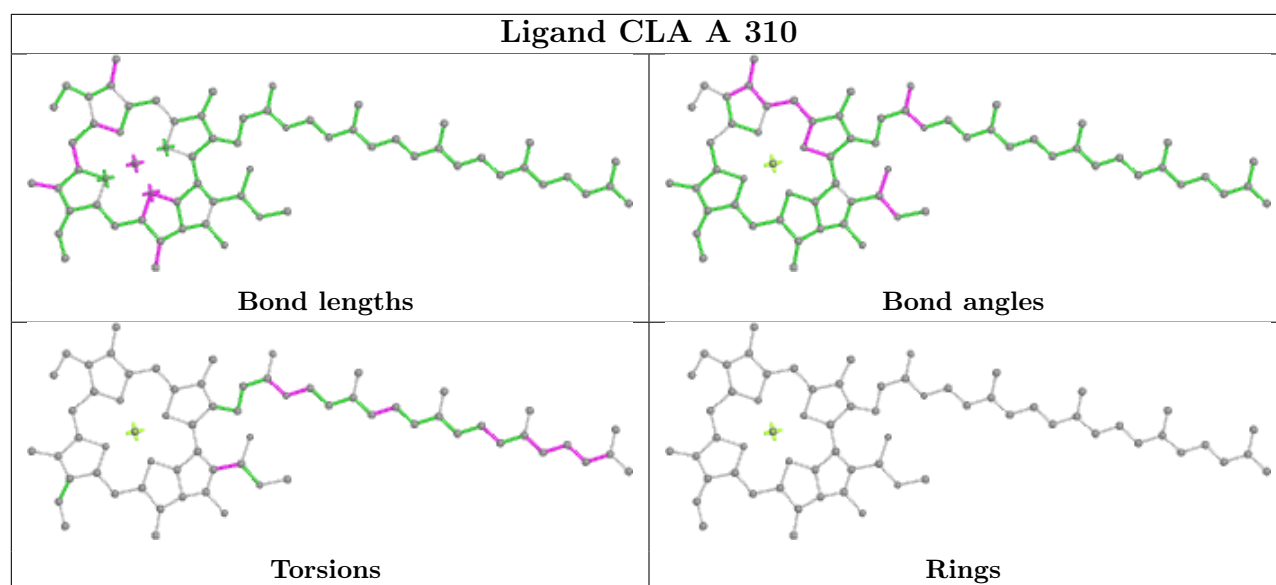


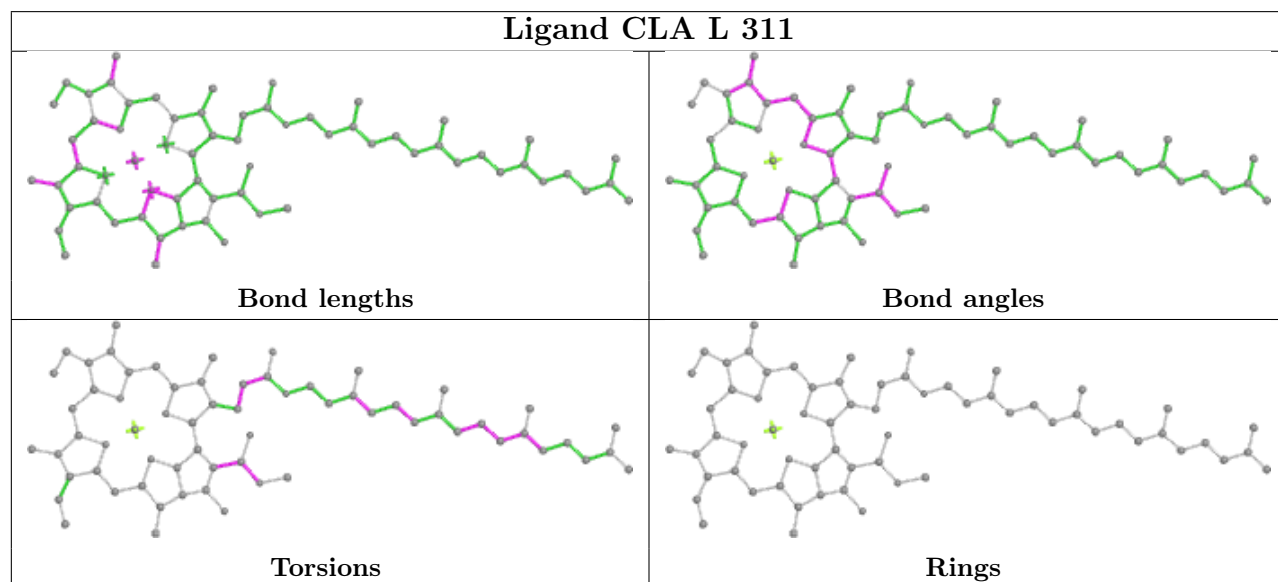
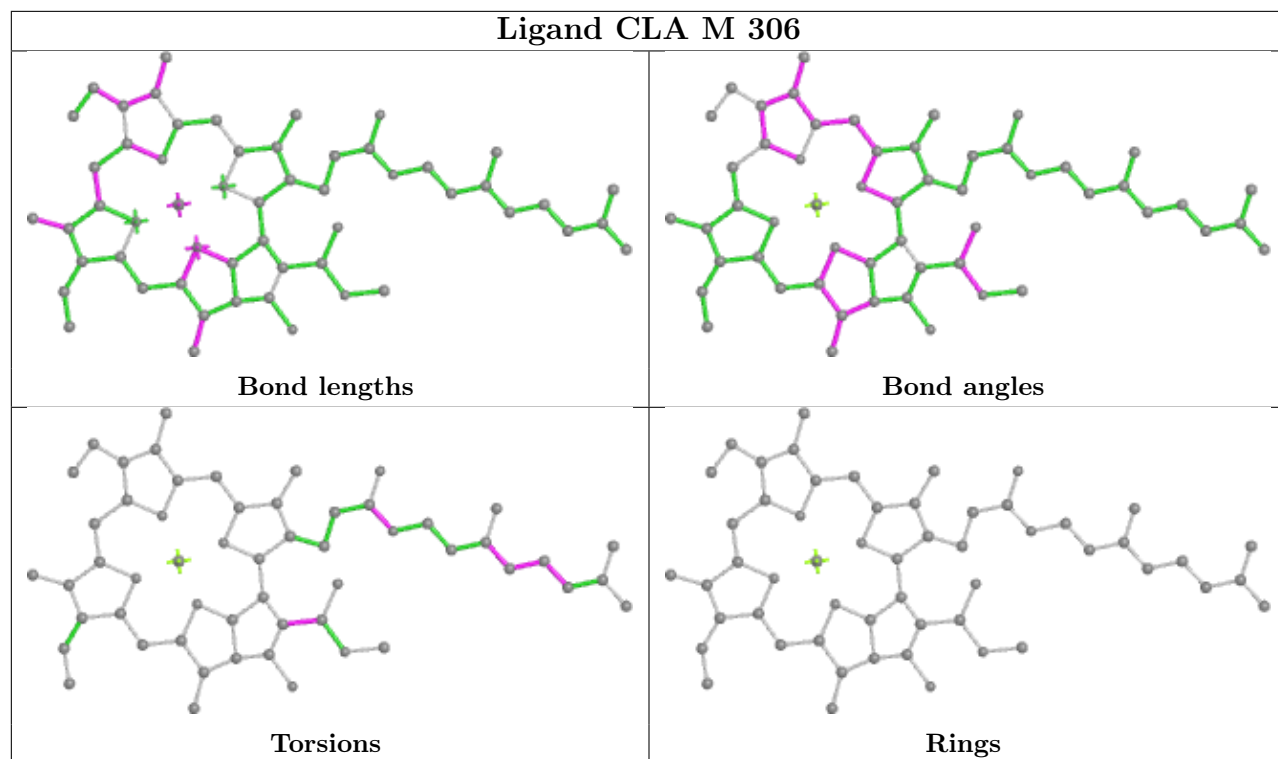


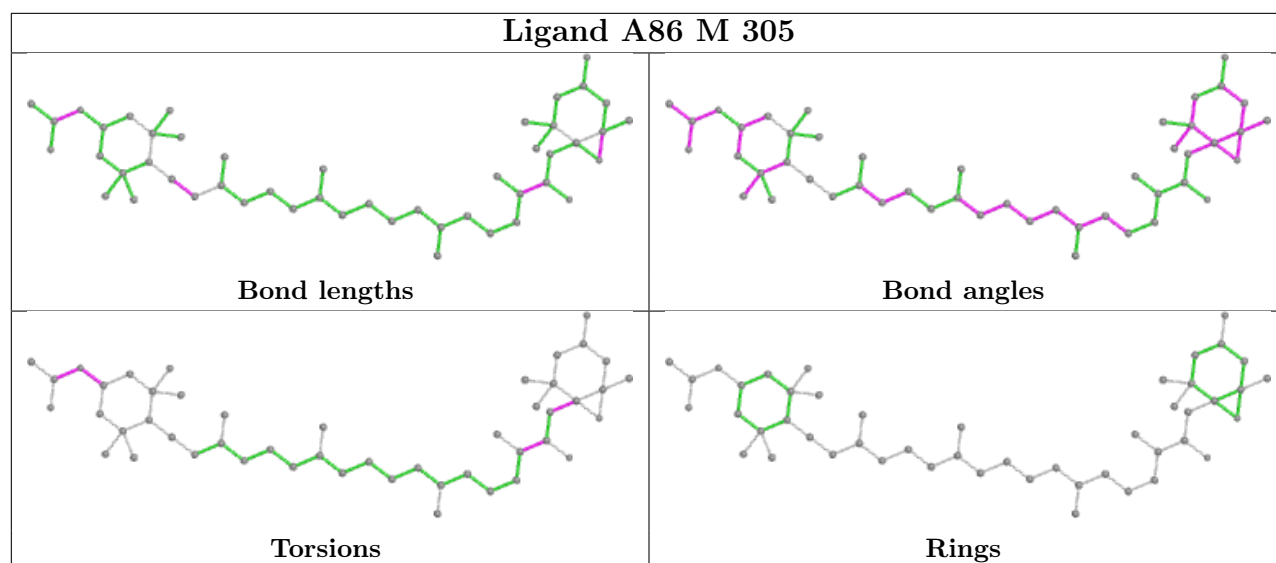
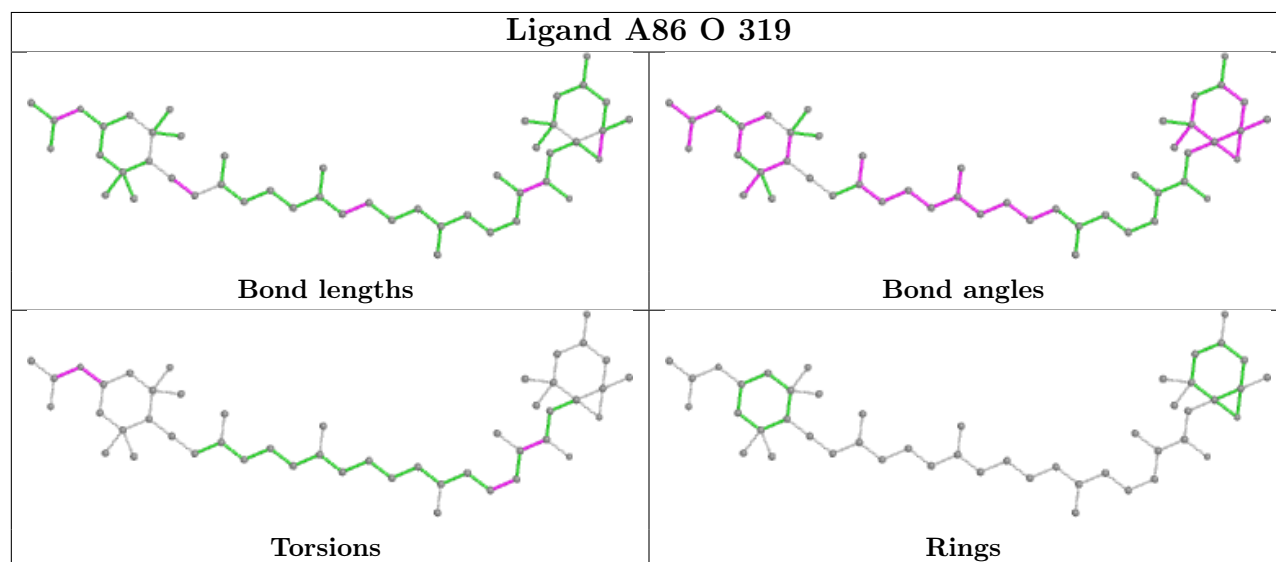
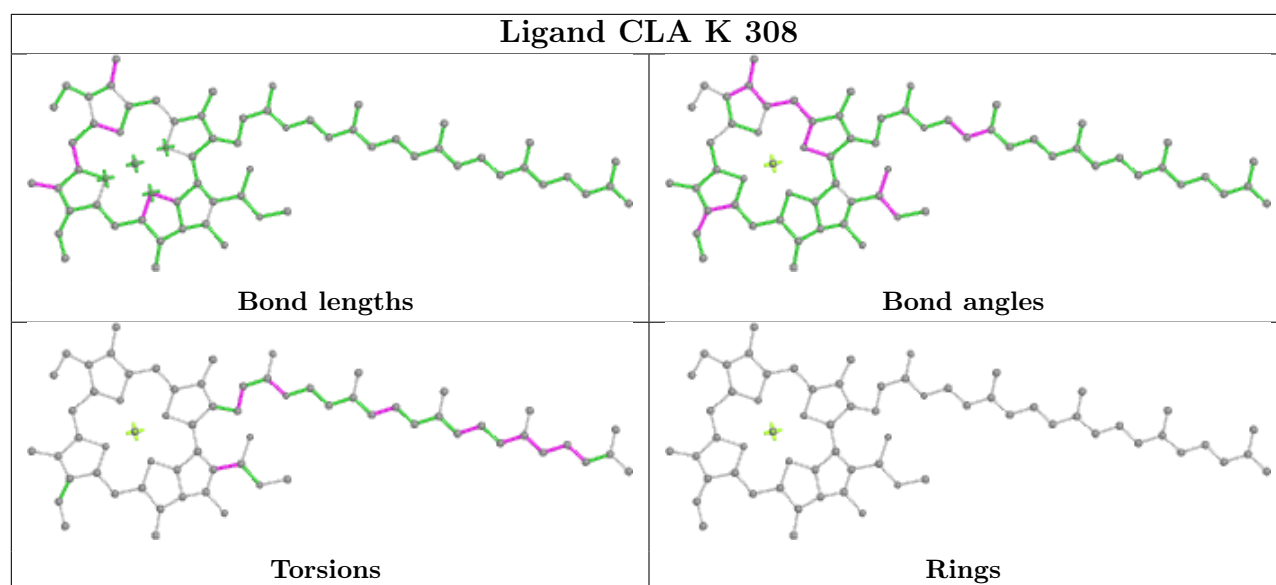


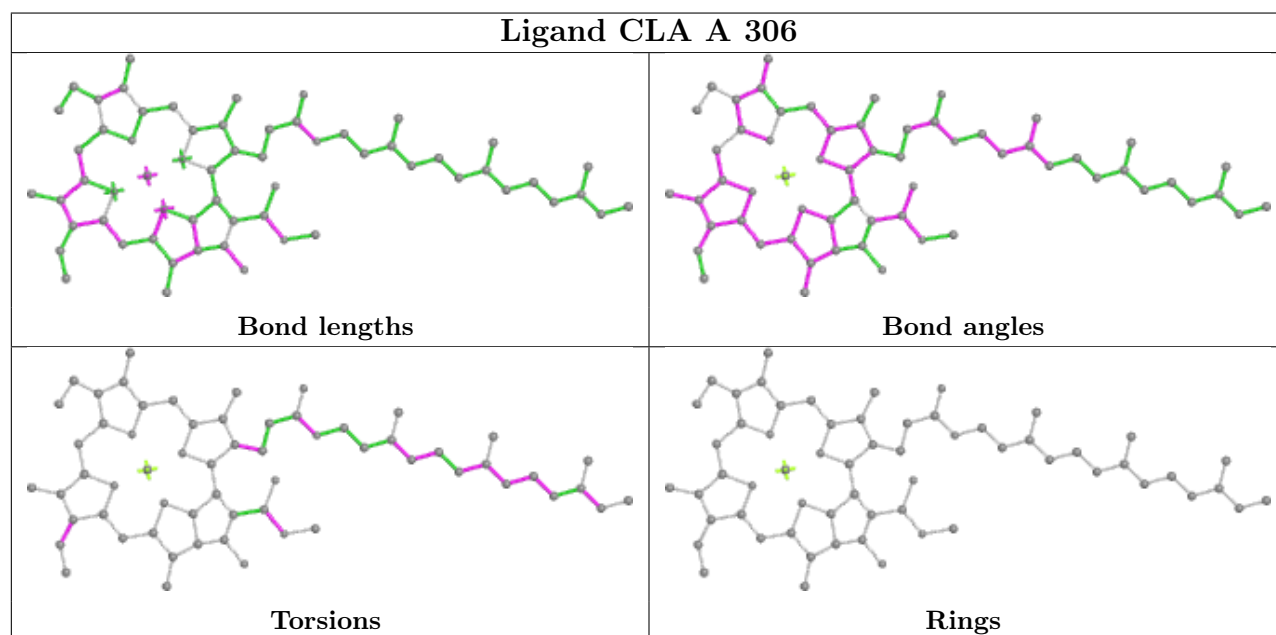
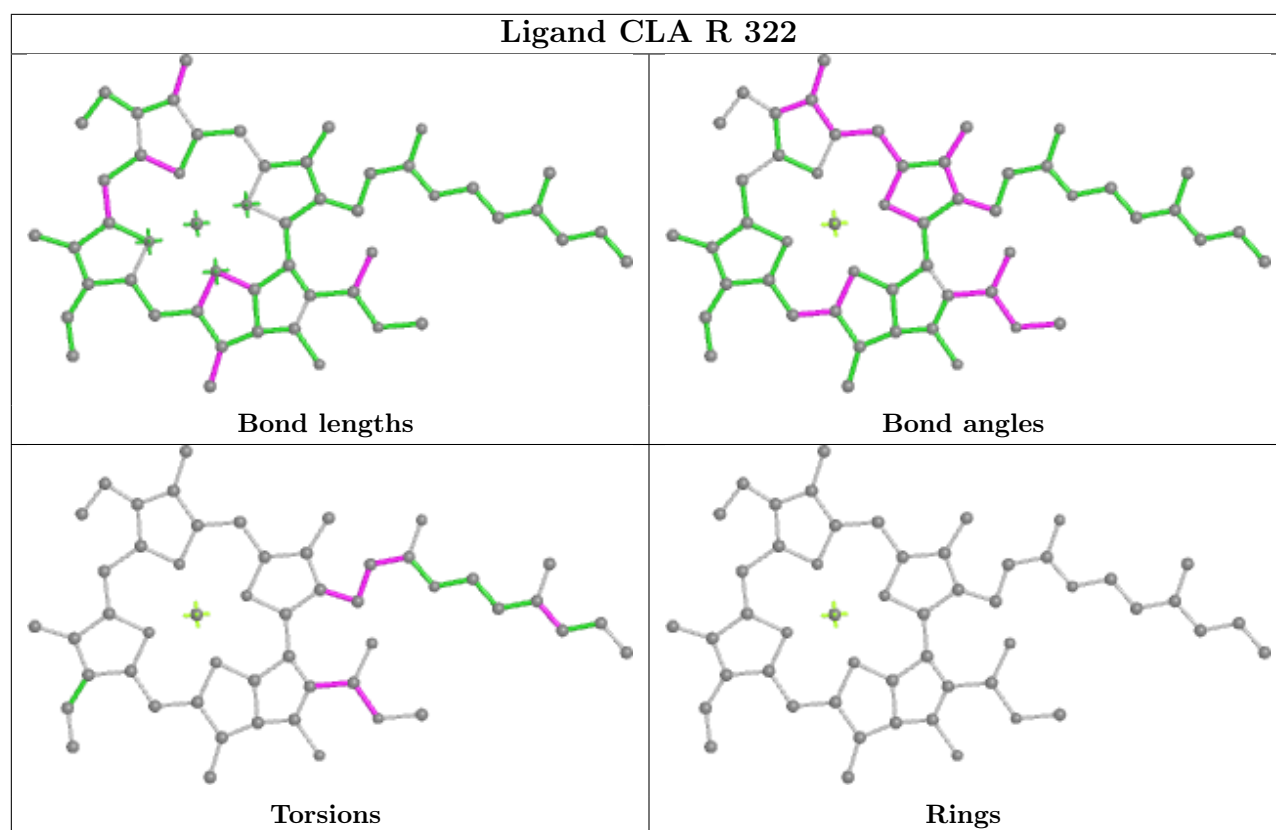


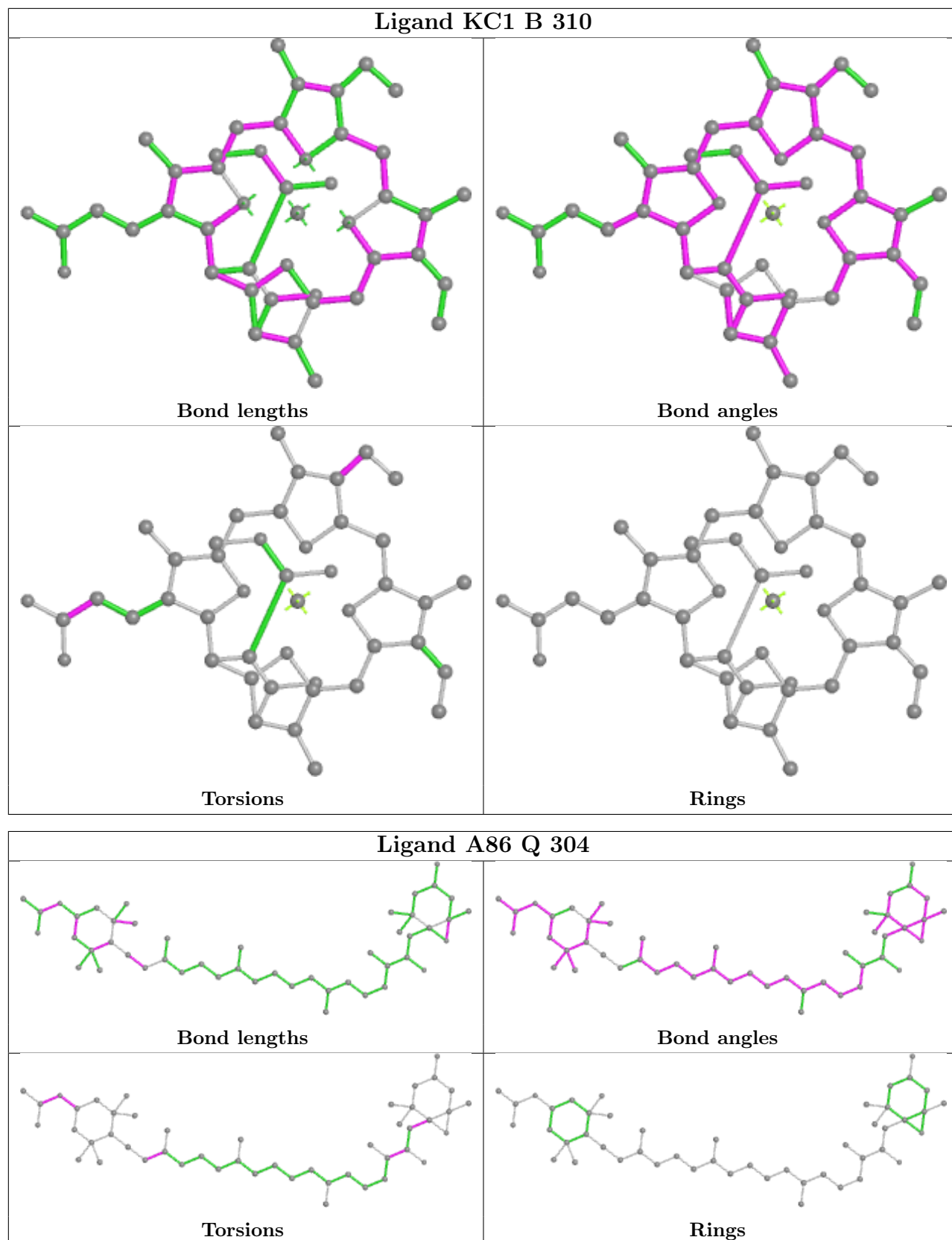


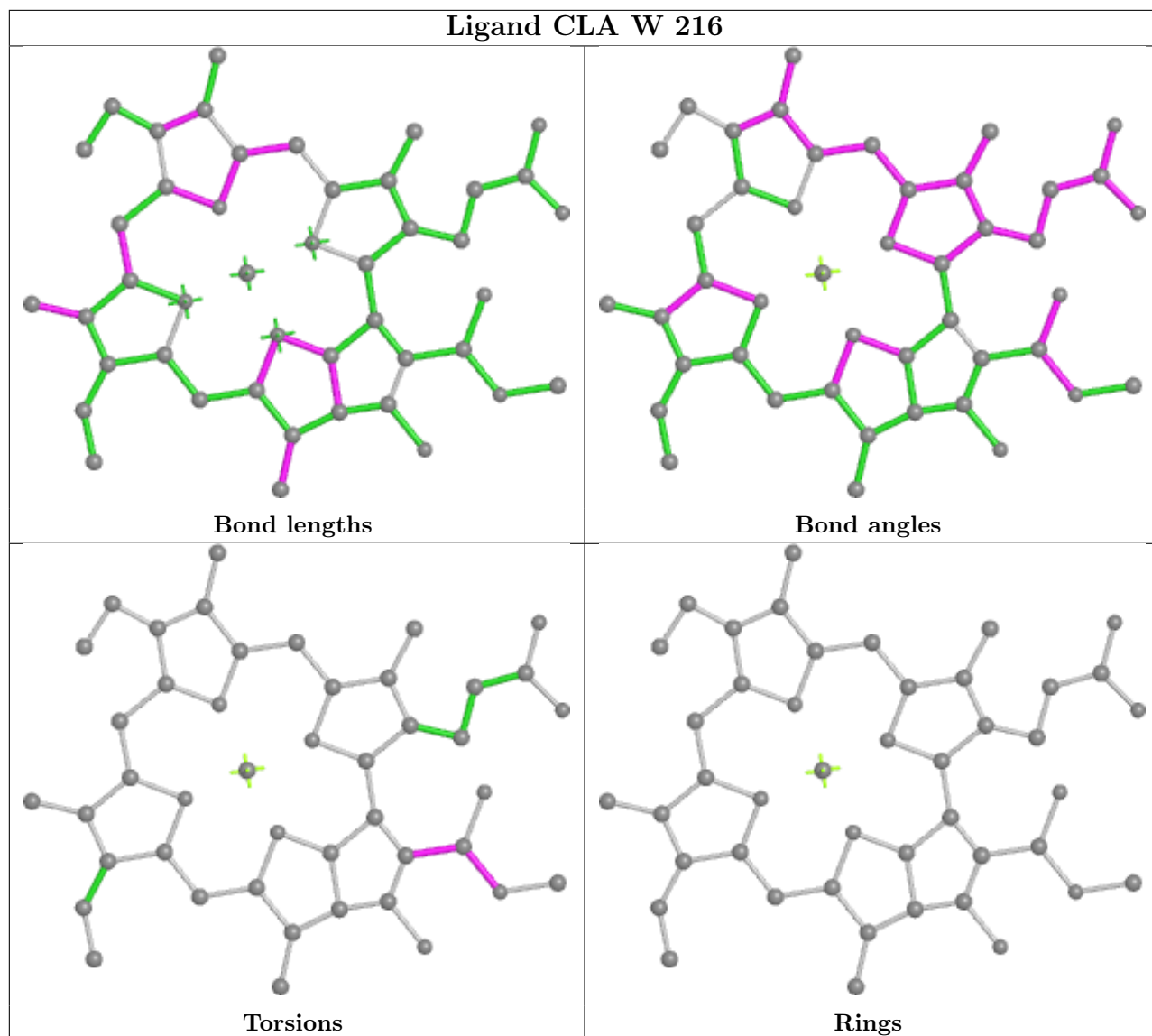


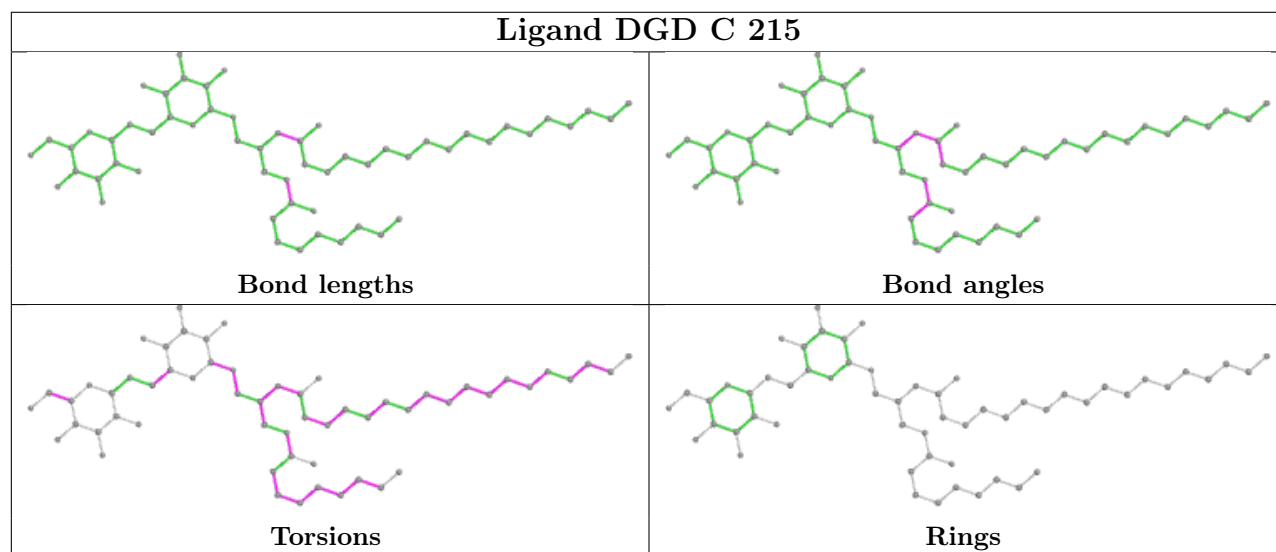
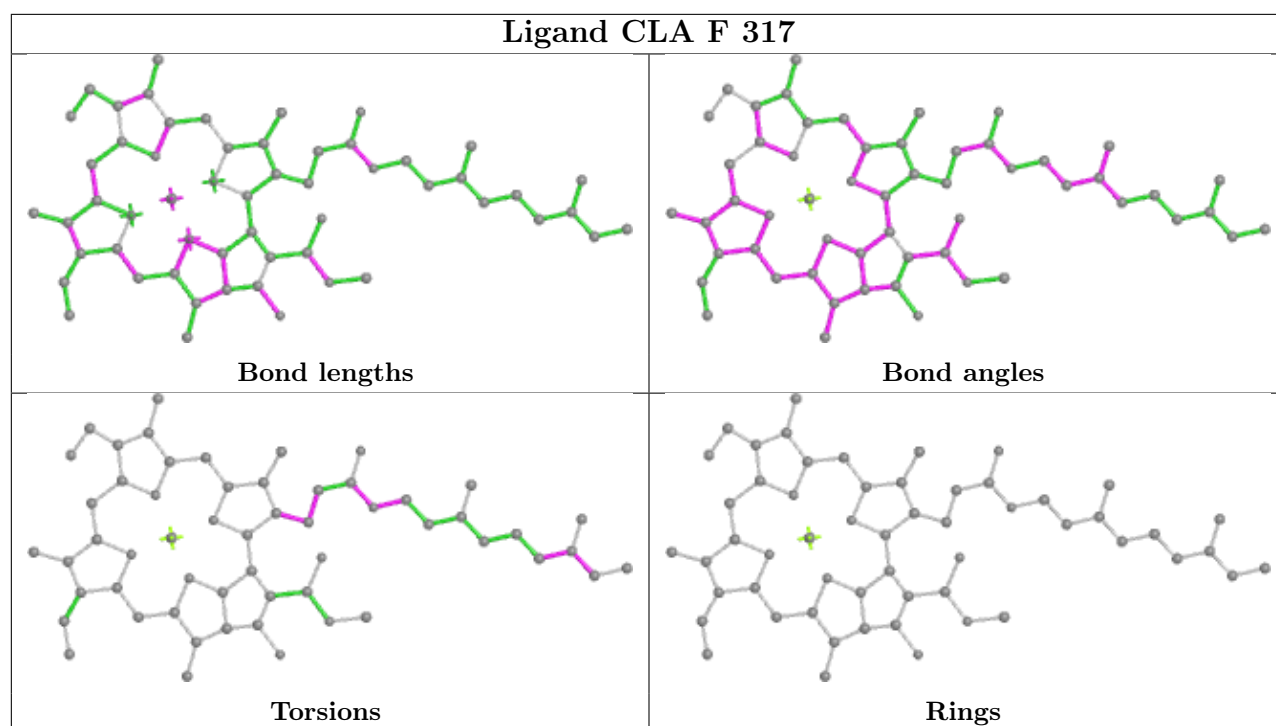


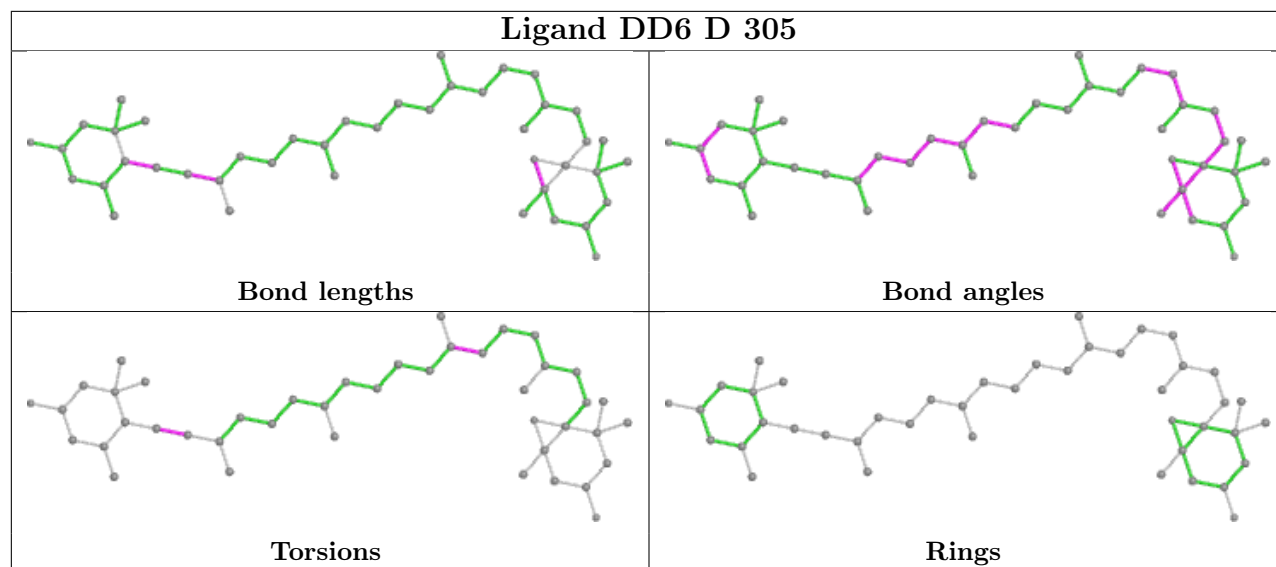












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

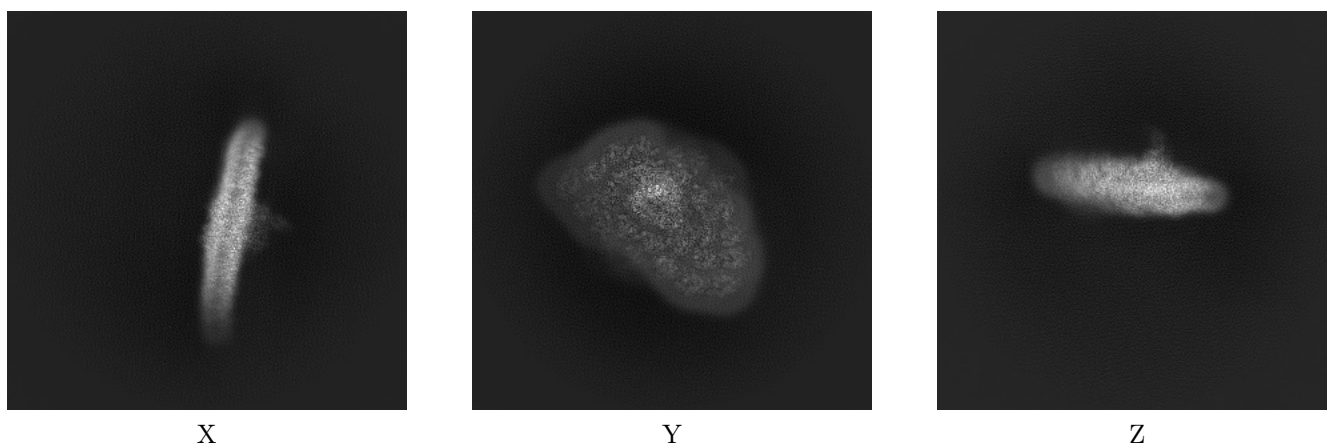
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-30012. 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](#)

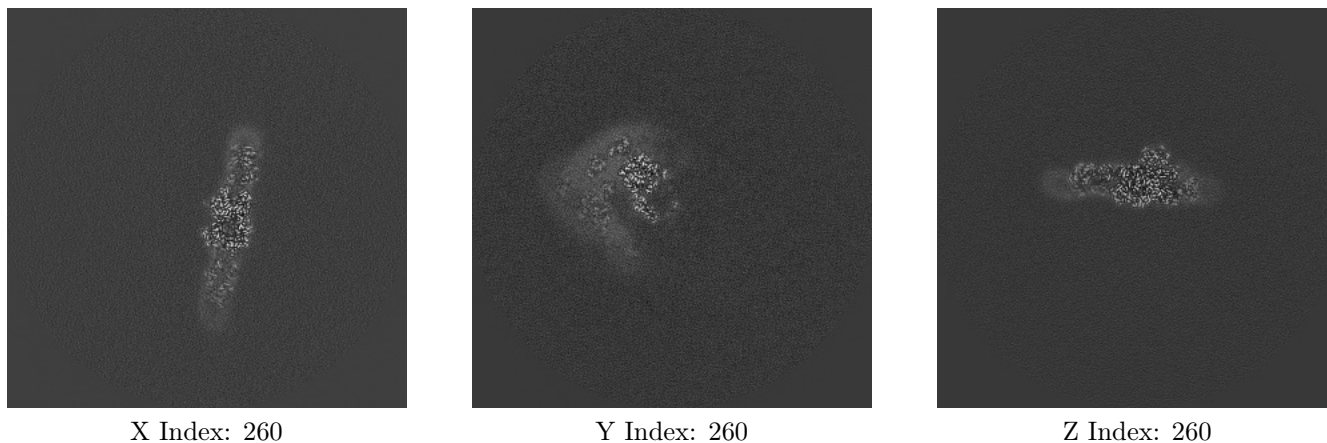
6.1.1 Primary map



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

6.2 Central slices [i](#)

6.2.1 Primary map



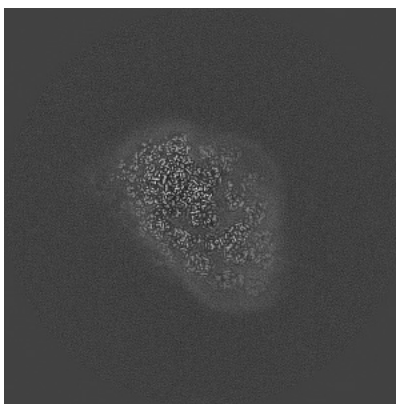
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

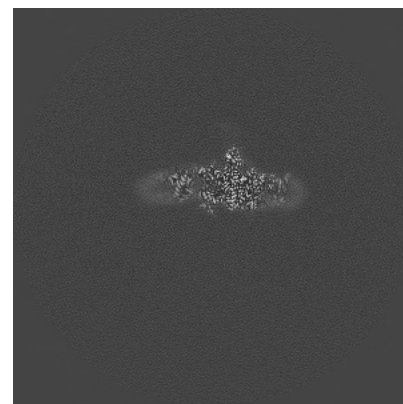
6.3.1 Primary map



X Index: 278



Y Index: 294



Z Index: 231

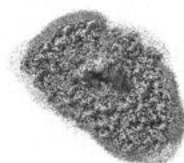
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views [i](#)

6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.016. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

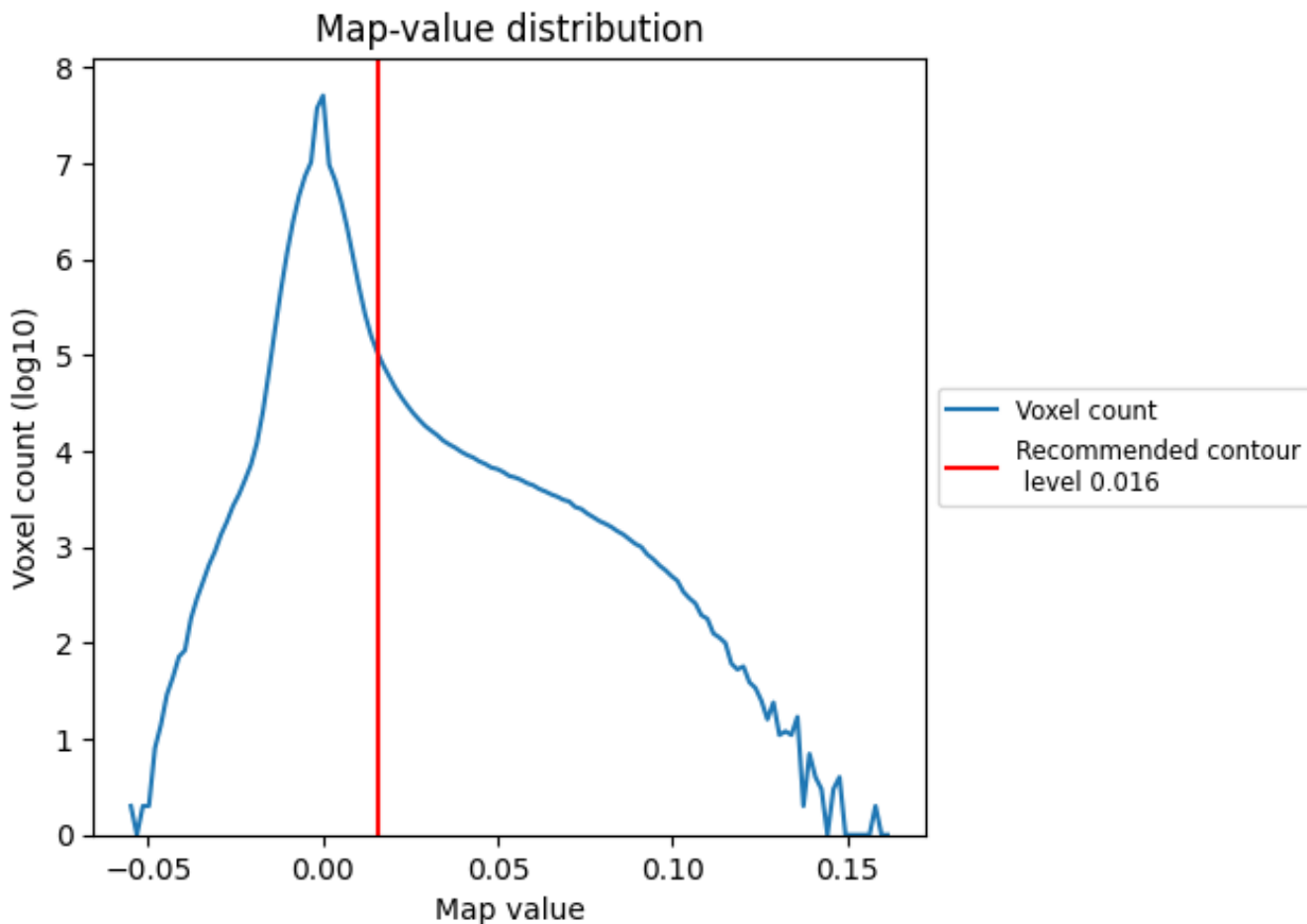
6.5 Mask visualisation

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

7 Map analysis [i](#)

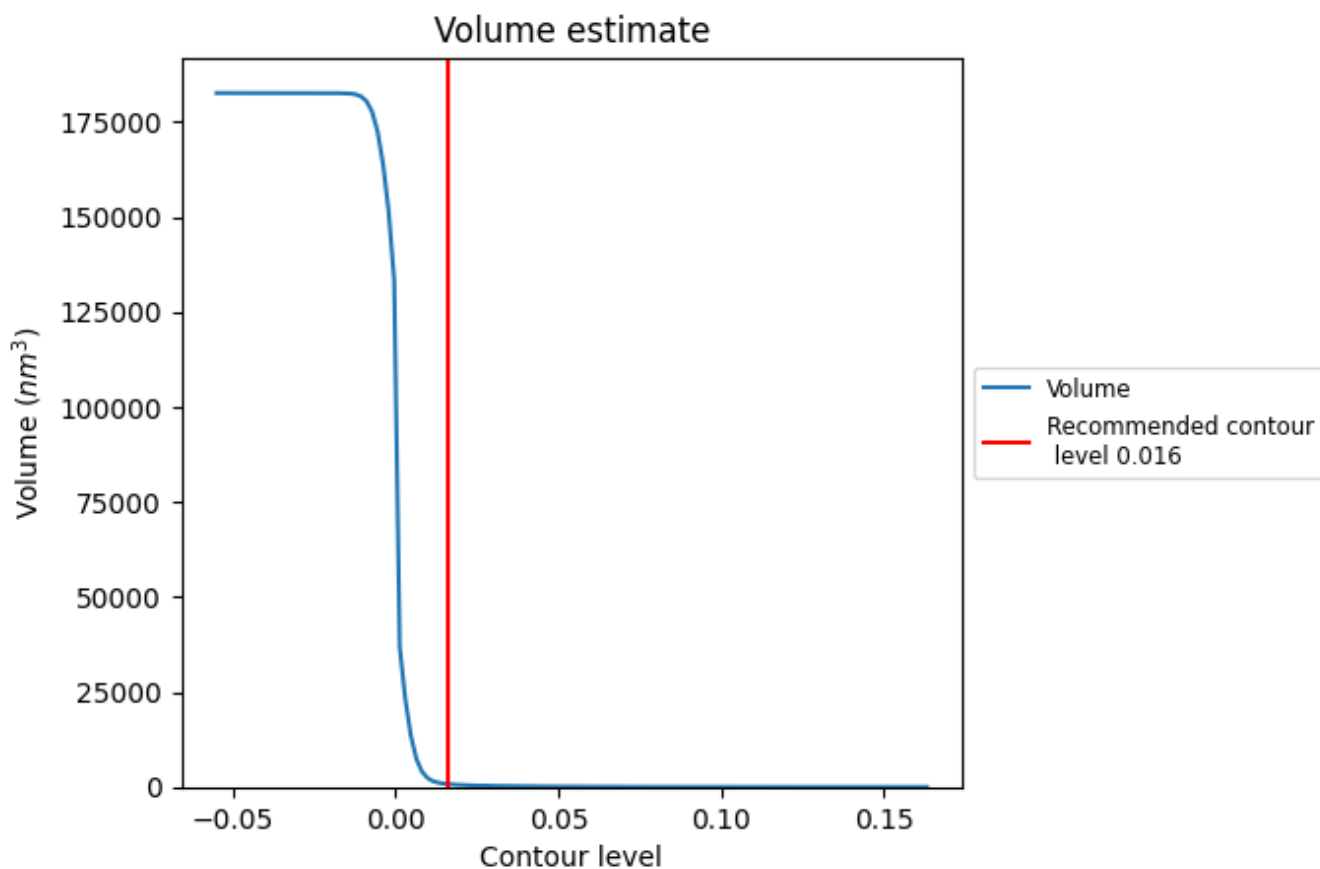
This section contains the results of statistical analysis of the map.

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.

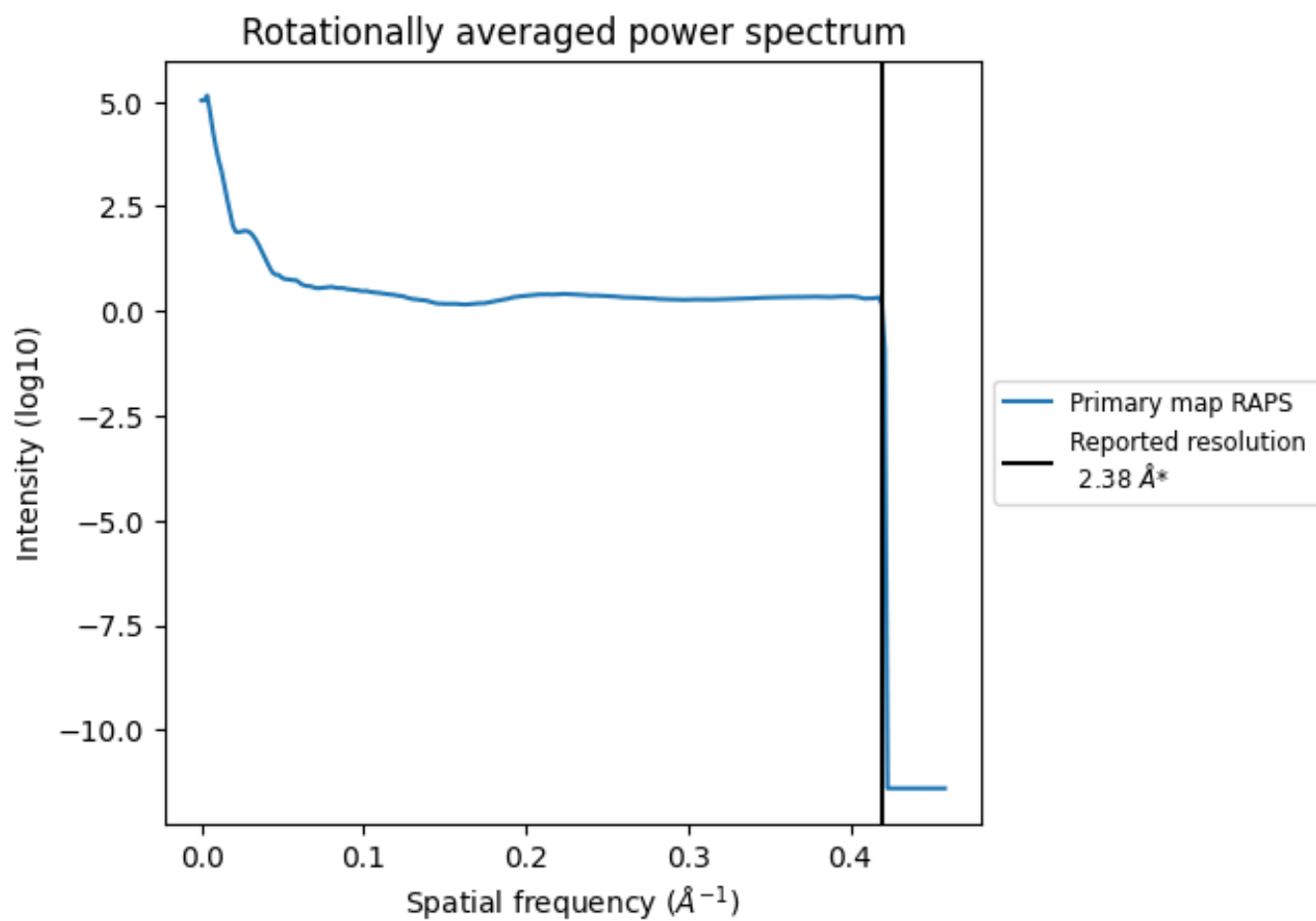
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 778 nm³; this corresponds to an approximate mass of 703 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 0.420 Å⁻¹

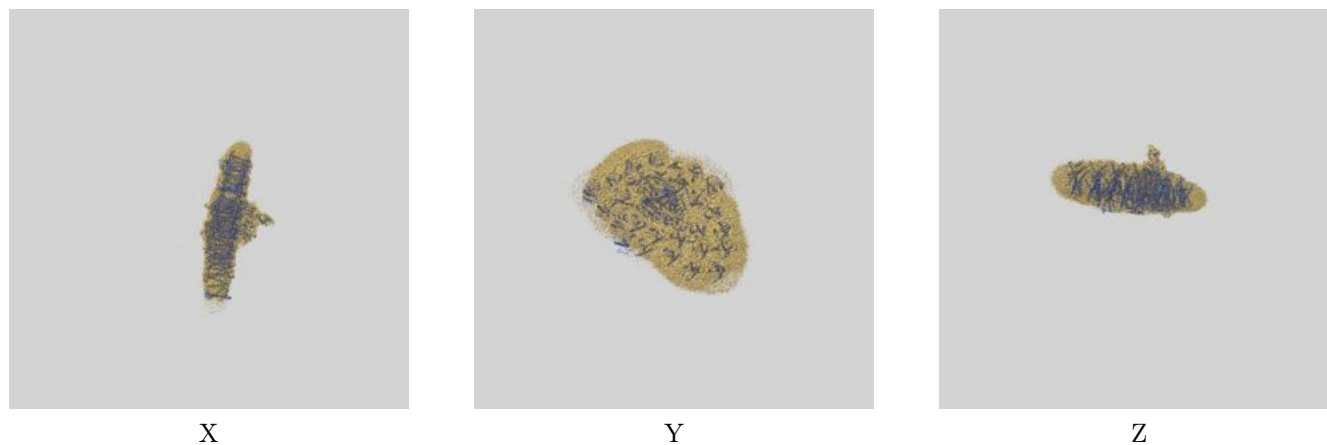
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

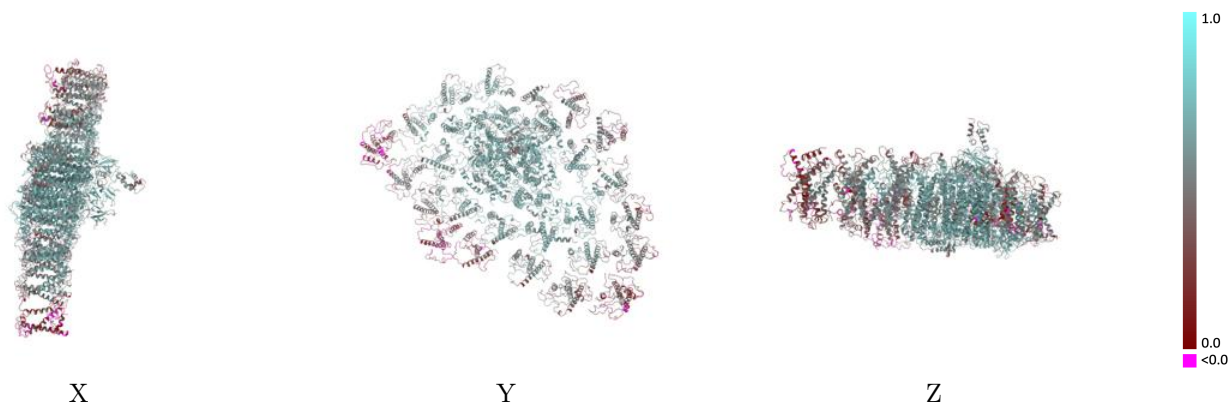
This section contains information regarding the fit between EMDB map EMD-30012 and PDB model 6LY5. Per-residue inclusion information can be found in section [3](#) on page [52](#).

9.1 Map-model overlay [i](#)



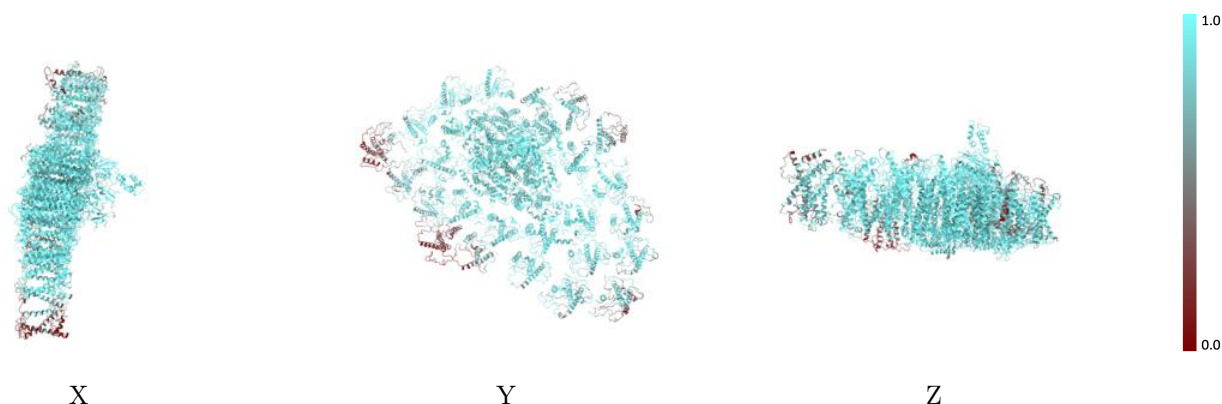
The images above show the 3D surface view of the map at the recommended contour level 0.016 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



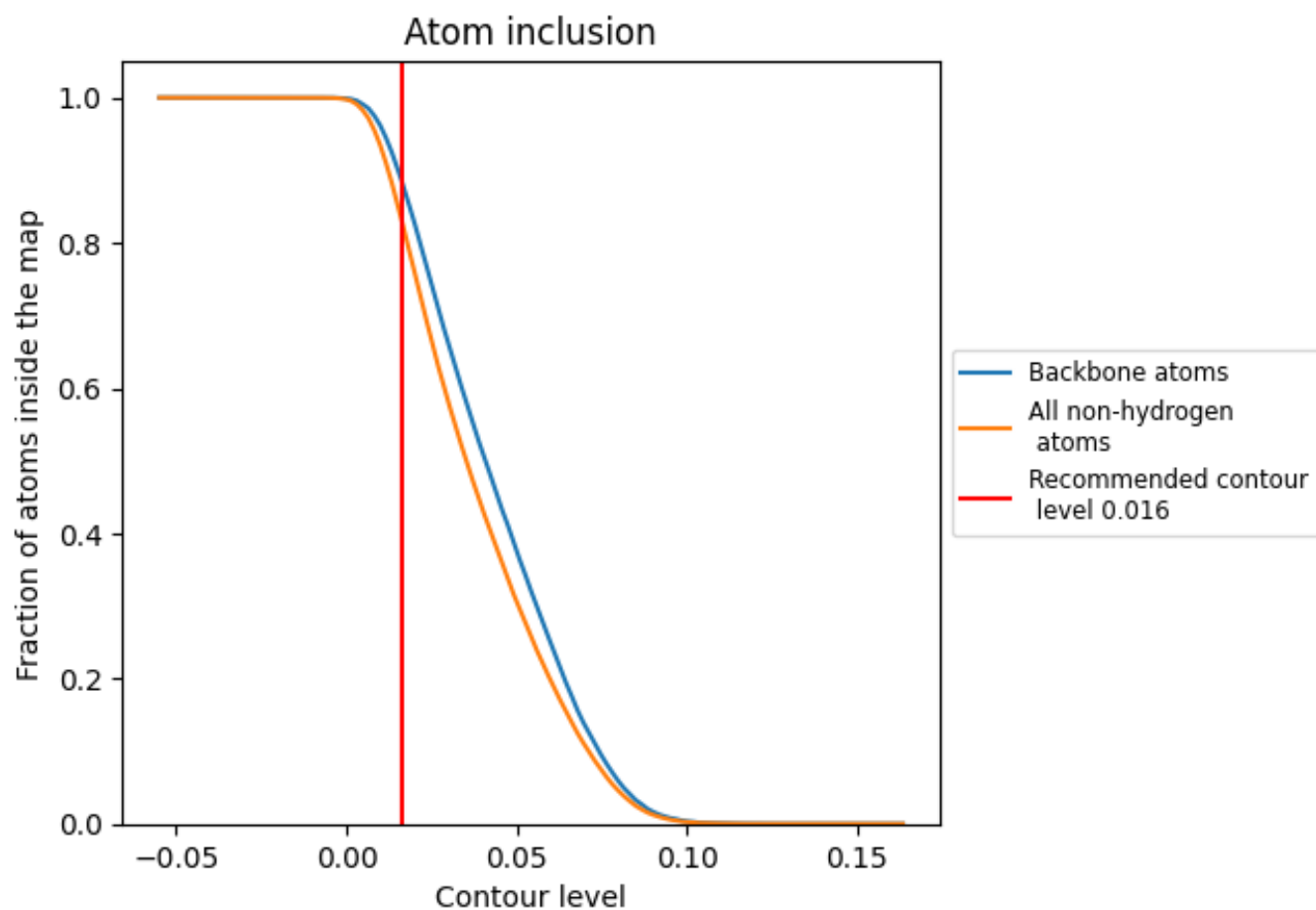
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.016).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 89% of all backbone atoms, 84% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary





The table lists the average atom inclusion at the recommended contour level (0.016) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8350	 0.5170
A	 0.9409	 0.5810
B	 0.8368	 0.4930
C	 0.8977	 0.5340
D	 0.9343	 0.5870
E	 0.9534	 0.6050
F	 0.9430	 0.5960
G	 0.9572	 0.6150
H	 0.8905	 0.5450
I	 0.9244	 0.5640
J	 0.9059	 0.5400
K	 0.8889	 0.5170
L	 0.8047	 0.4220
M	 0.8703	 0.4820
N	 0.3043	 0.1740
O	 0.6670	 0.4100
P	 0.8984	 0.5260
Q	 0.7763	 0.3880
R	 0.7926	 0.4220
S	 0.5669	 0.2610
T	 0.6282	 0.3920
U	 0.6600	 0.3880
V	 0.7548	 0.4470
W	 0.4971	 0.2640
X	 0.1526	 0.1400
a	 0.9829	 0.6690
b	 0.9909	 0.6730
c	 0.9766	 0.6620
d	 0.9463	 0.6200
e	 0.9209	 0.5940
f	 0.9318	 0.6150
g	 0.8866	 0.4480
h	 0.9692	 0.6040
i	 0.9433	 0.6250
j	 0.9381	 0.6250



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Chain	Atom inclusion	Q-score
l	 0.9575	 0.6310
m	 0.9418	 0.6140